Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Different Mechanisms of Ultrafast Excited State Deactivation of Coumarin 500 in Dioxane and Methanol Solvents: Experimental and Theoretical Study

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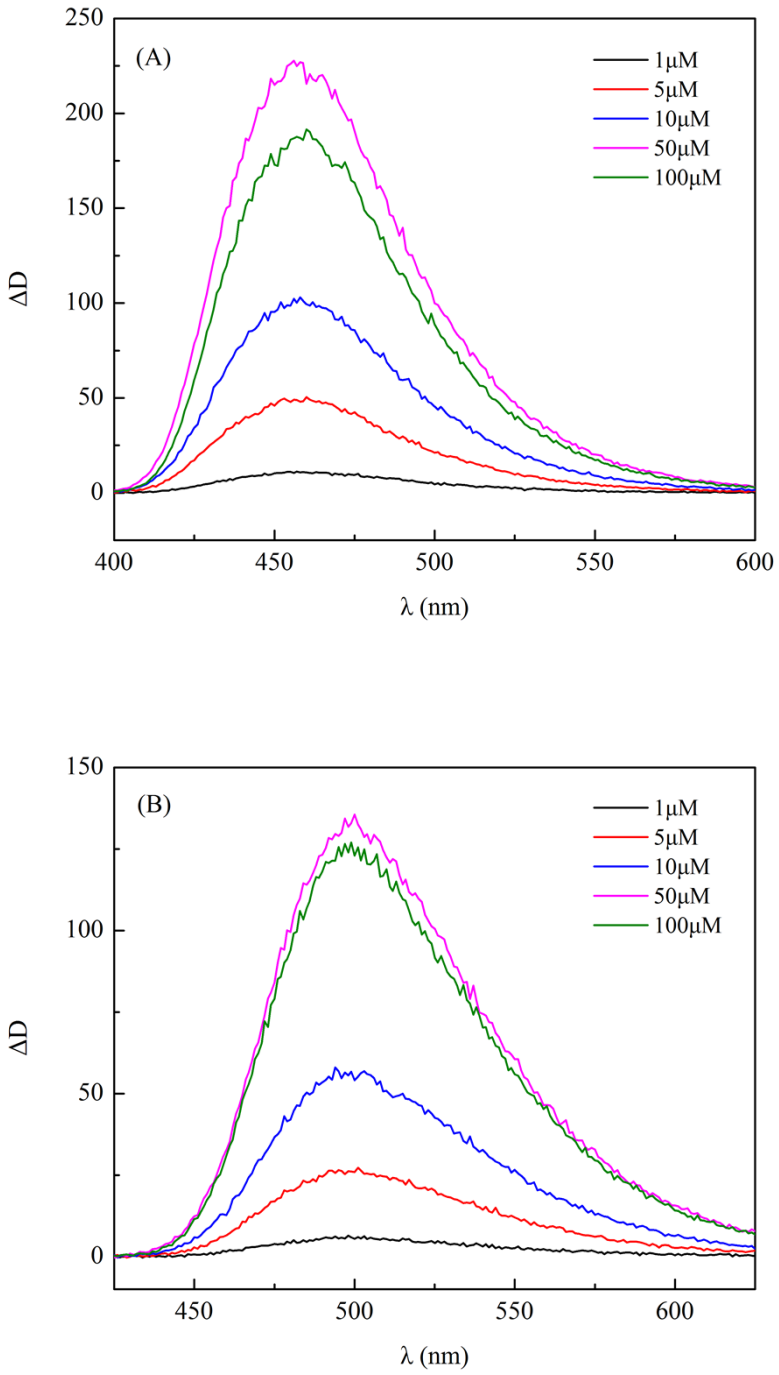

Figure S1. Fluorescence spectra of C500 in (A) Diox and (B) MeOH solvents at different concentrations.

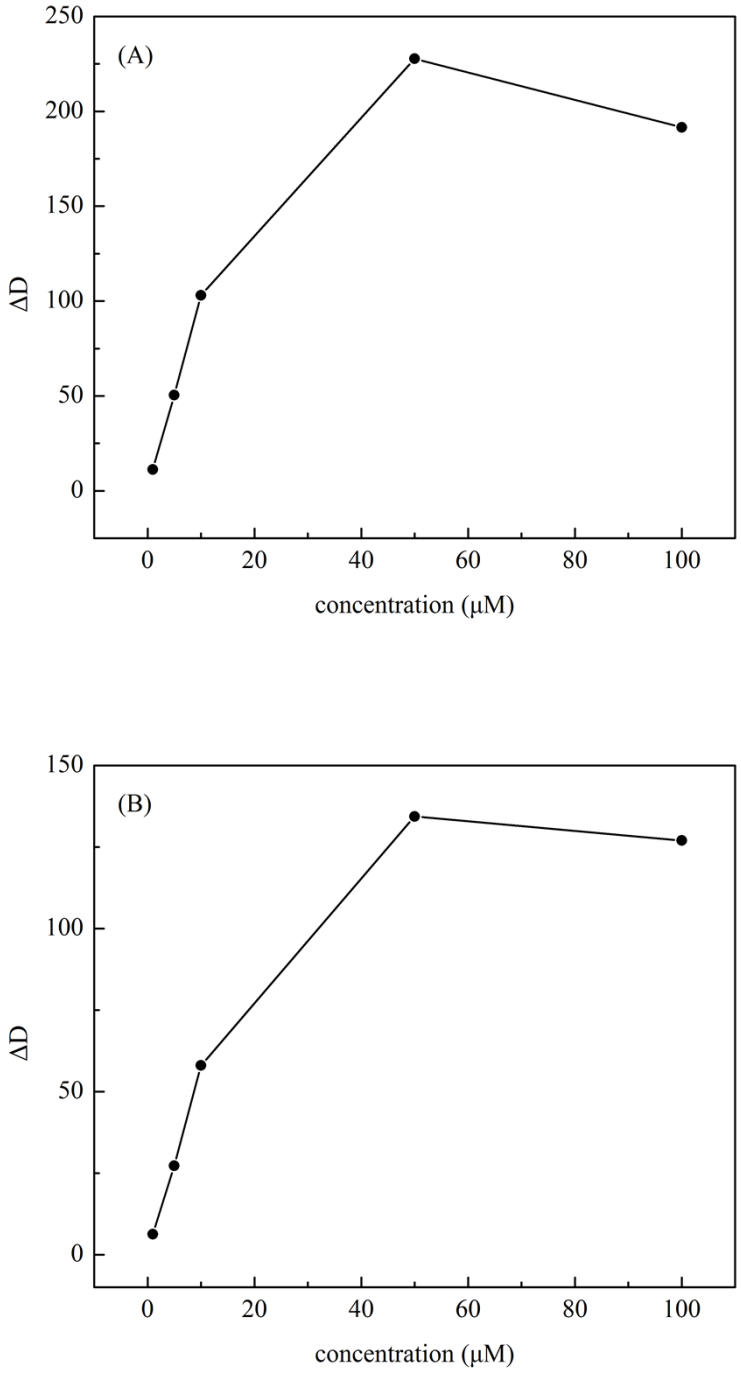

Figure S2. Intensity of the fluoerscence as function of concentration in (A) Diox and (B) MeOH solvents.

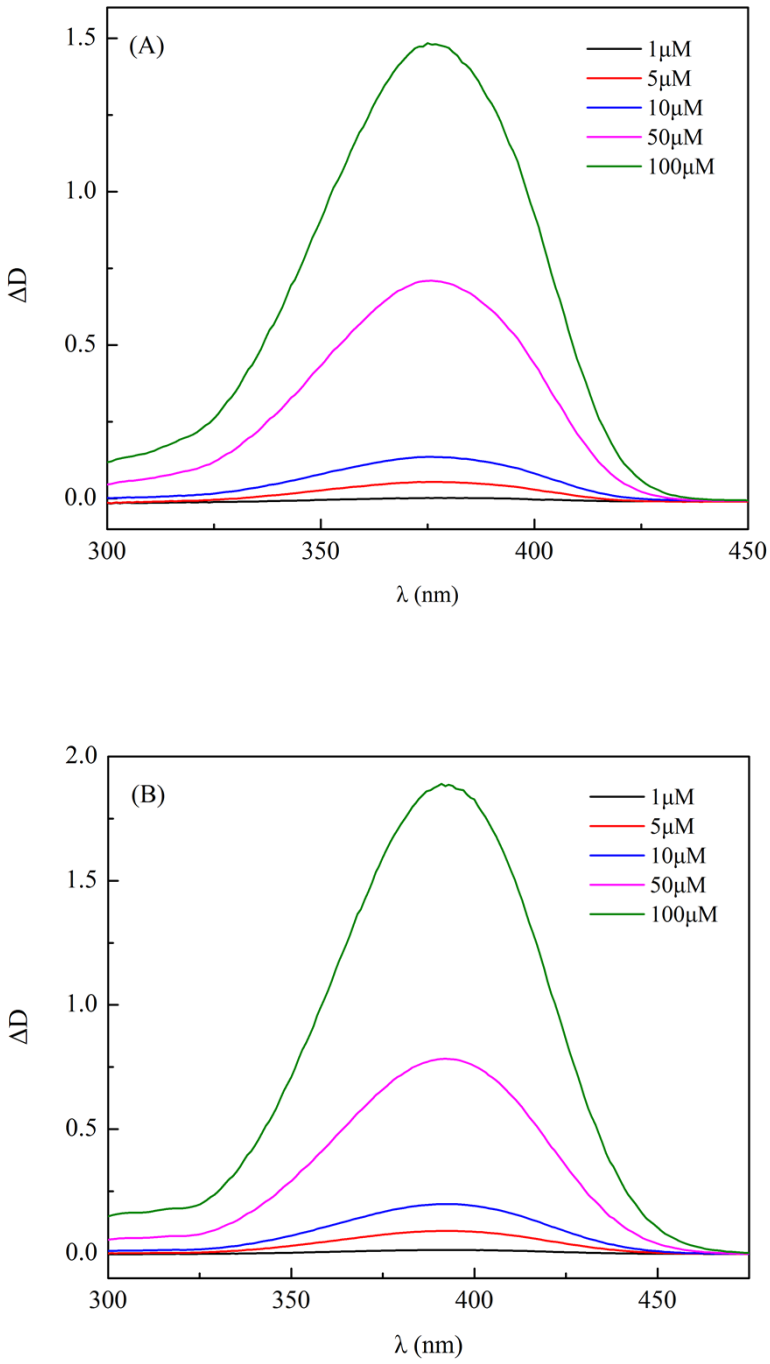

Figure S3. Absorption spectra of C500 in (A) Diox and (B) MeOH solvents at different concentrations.

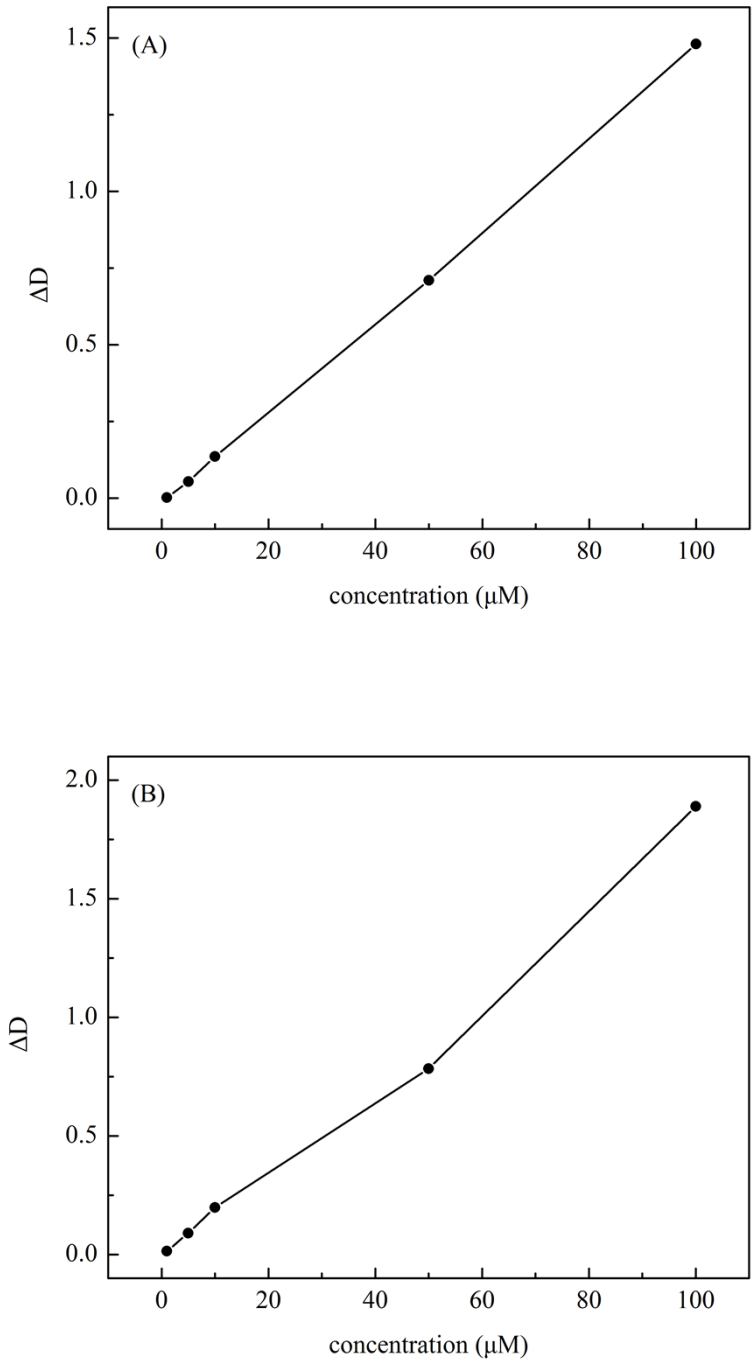

Figure S4. Absorption intensity variation with concentration in (A) Diox and (B) MeOH solvents.

solvent	π^*	*a*	*b*
Diox	0.55	0	0.37
MeOH	0.6	0.93	0.62

Table S1. KT Parameters in Diox and MeOH solvents.

	C500		C500-$(MeOH)_3$	
	BP86(RI)	CAM-B3LYP	BP86(RI)	CAM-B3LYP
S_1	413 (0.226) H→L 86.4%	311 (0.485) H→L 68.8%	511 (0.000) H-1→L 96.1%	309 (0.501) H→L 68.7%
S_2	345 (0.072) H-1→L 87.0%	264 (0.004) H-1→L 52.5%	420 (0.227) H→L 84.2%	264 (0.001) H-1→L 56%

Table S2. Calculated electronic excitation energies (nm), the corresponding oscillation strengths and FMOs for hydrogen-bonded complexes C500 and C500-$(MeOH)_3$ in low-lying electronically excited states by BP86(RI) and CAM-B3LYP.