Electronic Supplementary Information

Supramolecular interaction of sanguinarine dye with sulfobutylether-β-cyclodextrin: Modulation in the photophysical properties and antibacterial activity

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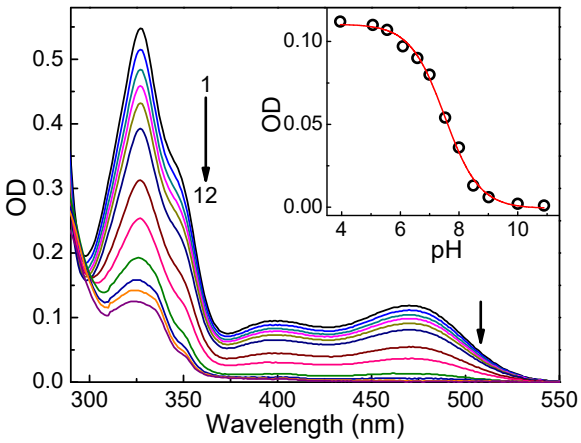

Fig. S1 Absorption spectra of sanguinarine at different pH values. pH: 4.0 (1), 5.1 (2), 5.6 (3), 6.1 (4), 6.6 (5), 7.1 (6), 7.6 (7), 8.1 (8), 8.6 (9), 9.1 (10), 10.1 (11) and 11.0 (12). **Inset** shows the pK_a curve (variation in absorbance with pH at 470 nm).

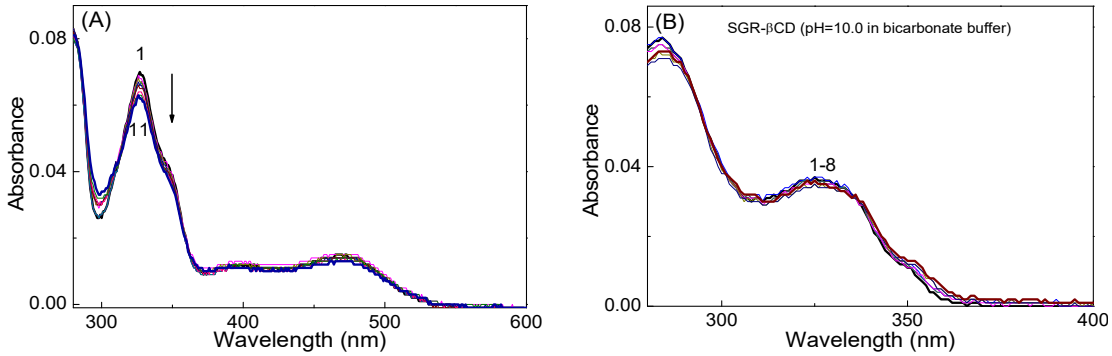

Fig. S2 (A) Absorption spectra of sanguinarine at different concentrations of βCD at pH 6.0. [βCD]/ μM: (1) 0, (2) 2, (3) 7, (4) 22, (5) 44, (6) 144, (7) 226, (8) 376, (9) 553, (10) 724 and (11) 889. (B) Absorption spectra of sanguinarine at different concentrations of βCD at pH 10. [βCD]/ μM: (1) 0, (2) 12, (3) 25, (4) 50, (5) 98, (6) 249, (7) 455 and (8) 677.

Method M1

In the present systems, the binding constant (*K*) for the different forms of the sanguinarine (SGR) dye with both the $SBE_7\beta CD$ and βCD macrocyclic hosts (H) were estimated at suitable pH conditions by the fluorescence titration method assuming 1:1 complexation stoichiometry. At any stage, the observed fluorescence intensity I_f corresponds to the sum of the fluorescence intensities arising from the free SGR and H:SGR and are directly proportional to their respective concentrations present in the solution. Therefore, one can write

$$I_f = I_f^0 \frac{[SGR]_{eq}}{[SGR]_0} + I_{H:SGR} \frac{[H:SGR]_{eq}}{[SGR]_0} \quad (S1)$$

where I_f^0 is the fluorescence intensity in the absence of host and $I_{H:SGR}$ is the fluorescence intensity when all SGR molecules are complexed with the host in a 1:1 complex. $[SGR]_0$ and $[H]_0$ are the total concentrations of SGR and H used. Equation S1 can be rearranged into a modified Benesi-Hildebrand equation as in equation S2,[1]

$$I_f = \frac{I_f^0 + I_{H:SGR} K[H]_0}{1 + K[H]_0} \quad (S2)$$

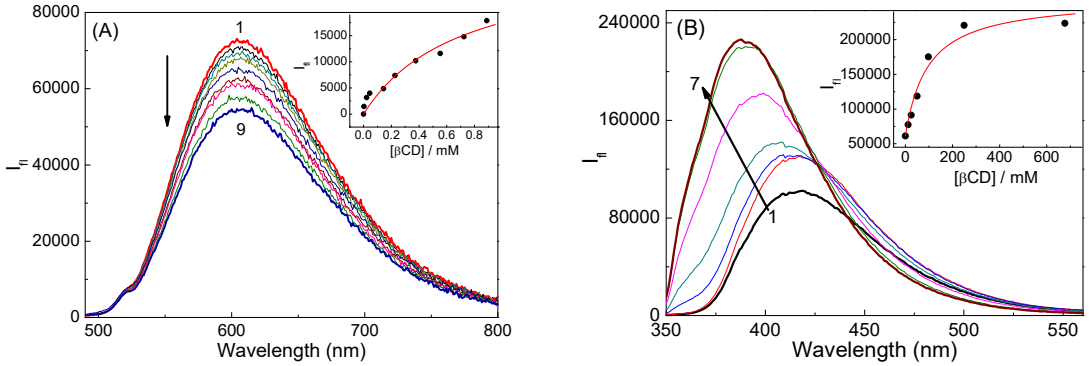

Fig. S3 (A) Fluorescence spectra of SG^+ at different concentrations of βCD at pH 6.0. [βCD] / μM: (1) 0.0, (2) 2.4, (3) 21.5, (4) 144.2, (5) 226.2, (6) 375.6, (7) 553.0, (8) 724.0 and (9) 889.0. (B) Fluorescence spectra of SGOH at different concentrations of βCD at pH 10.0. [βCD] / μM: (1) 0.0, (2) 12.0, (3) 25.0, (4) 49.5, (5) 98.0, (6) 249.0 and (7) 676.5.

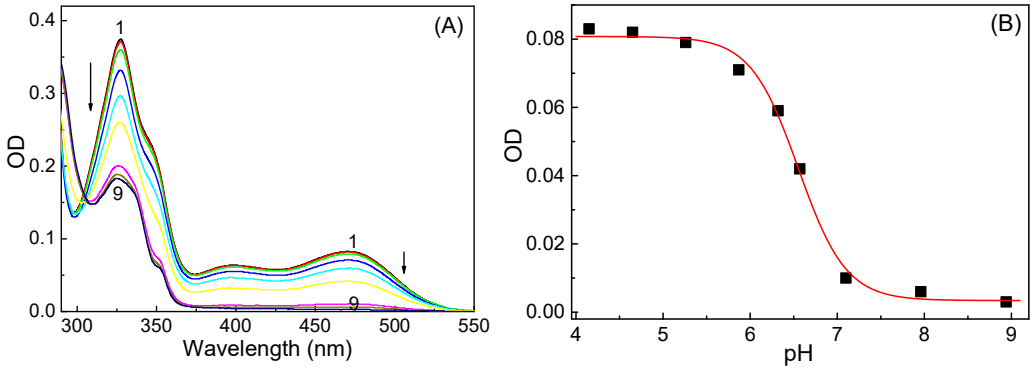

Fig. S4 (A) Absorption spectra of sanguinarine in the presence of 2 mM βCD at different pH values. pH: 1) 4.15, 2) 4.65, 3) 5.26, 4) 5.87, 5) 6.32, 6) 6.57, 7) 7.10, 8) 7.96 and 9) 8.94. (B) pK_a curve of SGR in the presence of βCD (variation in absorbance with pH at 470 nm).

Table S1. Changes in the pK_a value obtained from absorption studies of SGR in the presence of SBE_7βCD and βCD hosts.

Systems	**pK_a (abs)**	**ΔpK_a (abs)**
SGR	7.5	---
SGR-SBE_7βCD (2mM)	8.1	+0.6
SGR-βCD (2mM)	6.55	-0.95

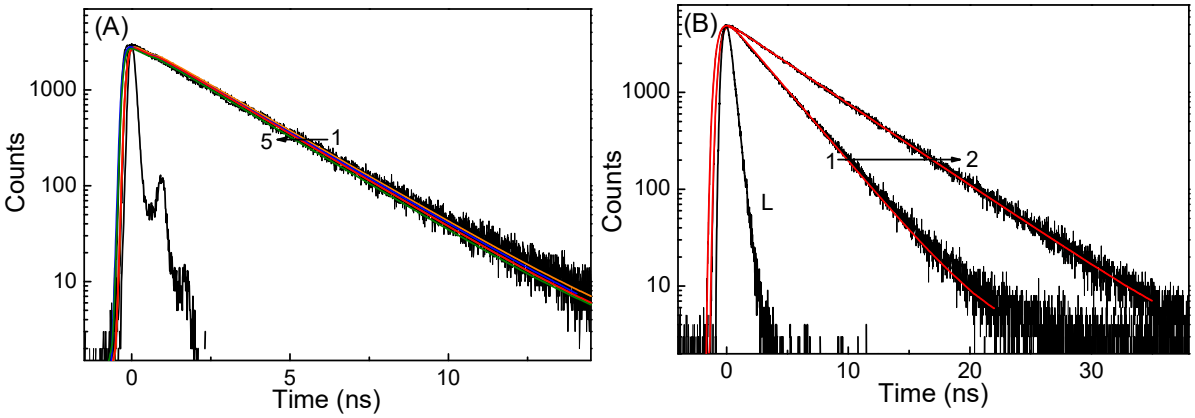

Fig. S5 (A) Lifetime decay traces of SG^+ form at different concentrations of βCD at pH 6.0 [βCD]/mM: (1) 0.0, (2) 0.24, (3) 0.87, (4) 1.7 and (5) 2.9. λ_{ex} = 445 nm, λ_{em} = 605 nm. (B) Lifetime decay traces of SGOH form in the absence (1) and presence (2) of 1 mM of βCD at pH 10. λ_{ex} = 339 nm, λ_{em} = 380 nm.

Table S2. Excited-state decay time constants for SG^+ form monitored at 605 nm and SGOH form monitored at 380 nm at the saturated concentration of $SBE_7\beta CD$ and βCD.

Systems	τ_1 (ns), a_1 (%)	τ_2 (ns), a_2 (%)	$\langle\tau\rangle$ (ns)	τ_r (ps)
SG^+	2.28 (100)	---	2.28	186 ± 50
SG^+:$SBE_7\beta CD$ (350 μM)	2.32 (79)	0.84 (21)	2.00	575 ± 50
SG^+:βCD (2.9 mM)	2.17 (100)	---	2.17	285 ± 50
SGOH	3.03 (100)	---	3.03	
SGOH:$SBE_7\beta CD$ (1.2 mM)	5.11 (97)	2.25 (3%)	5.02	
SGOH:βCD (1 mM)	5.07 (100)	---	5.07	

Table S3. Minimal inhibitory concentration of sanguinarine (SGR) at different solution conditions towards four pathogenic bacteria at physiological pH 7.4. All the experiments are done in duplicate and each repeated thrice.

Systems	Minimum inhibitory concentration in μM (μg/ml)			
	B. cereus	*S. aureus*	*E. coli*	*S. typhimurium*
SGR	14.7	29.4	14.7	14.7
SGR-$SBE_7\beta CD$ (2mM)	7.5	14.7	7.5	14.7
SGR-βCD (2mM)	14.7	29.4	14.7	14.7

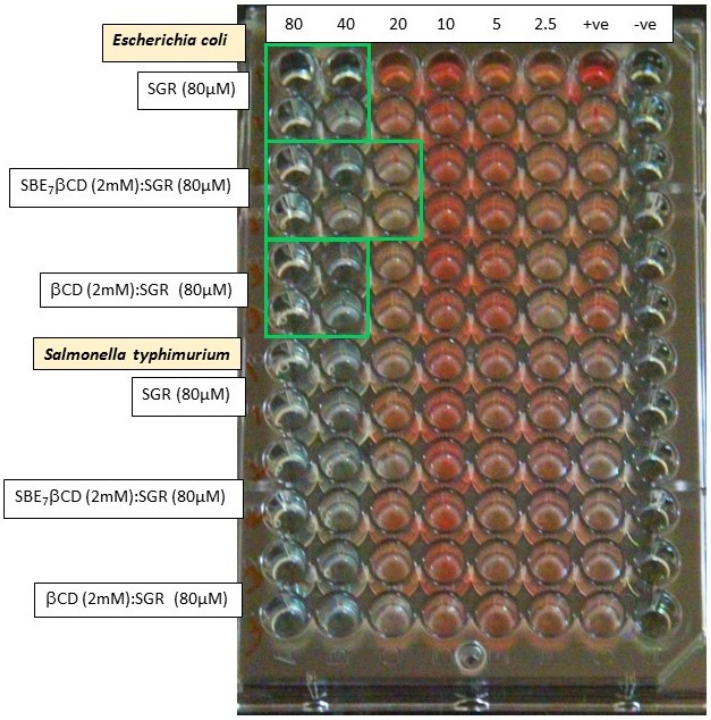

Fig. S6 Antibacterial study of SGR in the absence and presence of $SBE_7\beta CD$ (2 mM) and βCD (2mM) against *E. coli and S. typhimurium* at physiological pH 7.4.

Reference

1. M. K. Singh, H. Pal, A. S. R. Koti, A. V. Sapre, *J. Phys. Chem. A*, 2004, **108**, 1465-1474.