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Deciphering the role of head group of cationic surfactants on the binding interaction with heme protein and releasing by β-cyclodextrin

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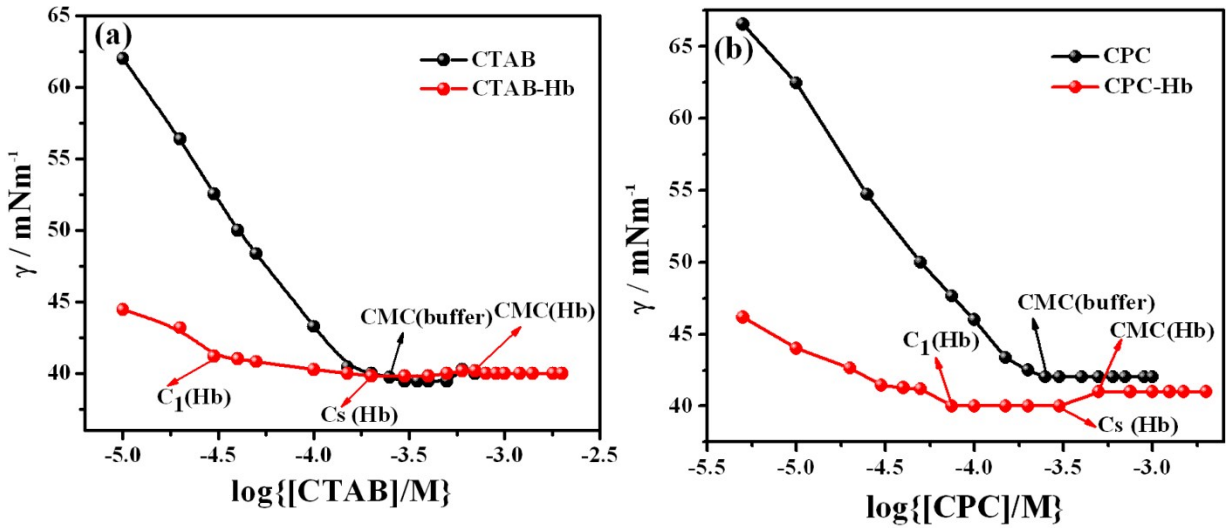


Fig. S1 Tensiometric profile for the interaction of Hb with (a) CTAB and (b) CPC in 10 mM phosphate buffer media of pH 7.4 at 298 K. [Hb] = 5 μM.

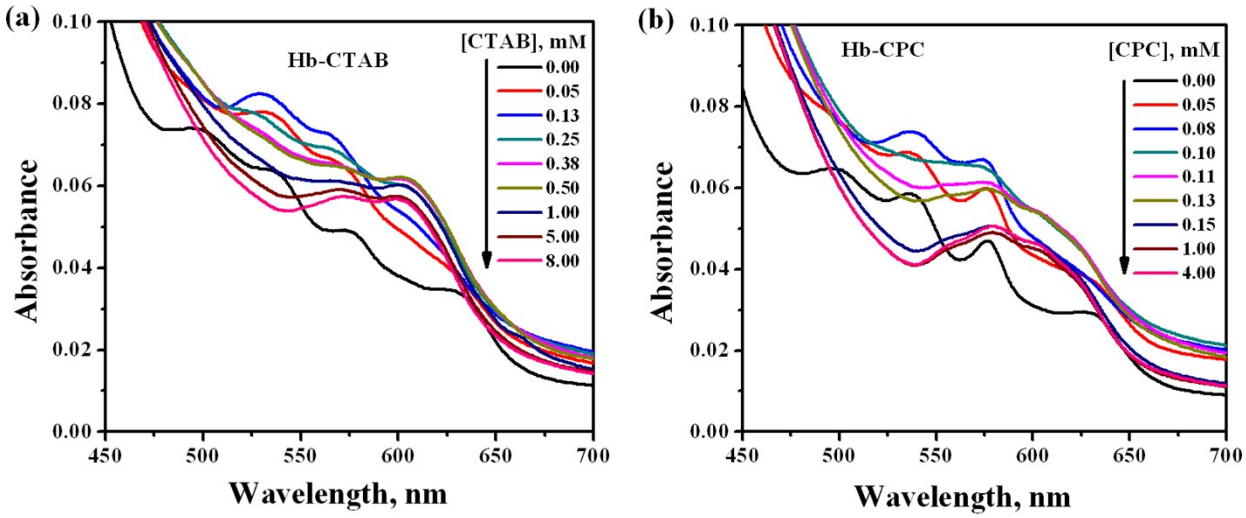


Fig. S2 Absorption spectra of visible region of hemoglobin in absence and presence of (a) CTAB and (b) CPC at pH 7.4 and 298 K, [Hb] = 5 μM.

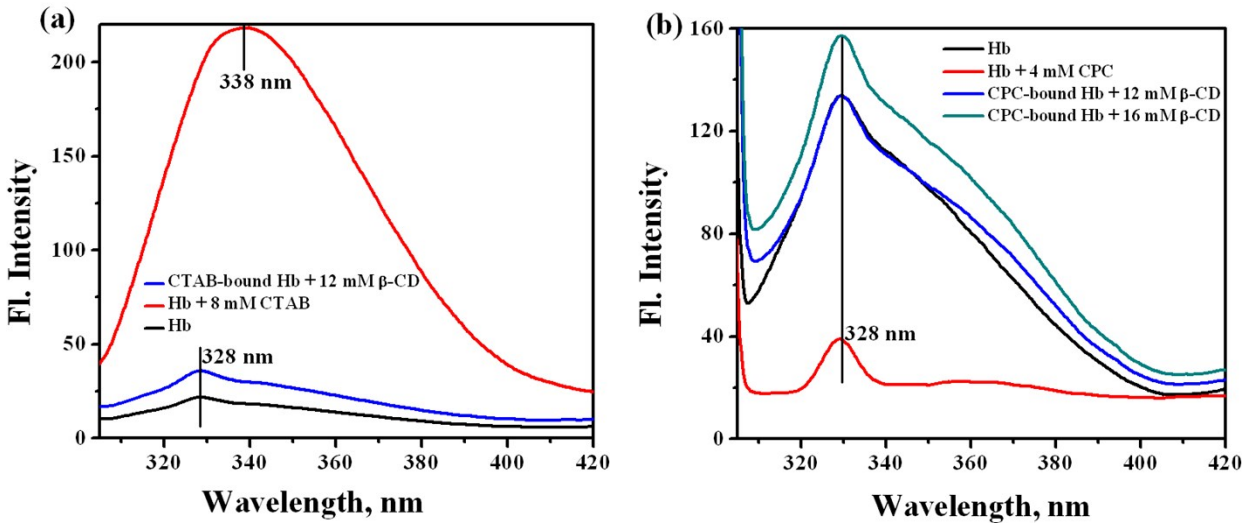


Fig. S3 (a) Fluorescence emission spectrum of Hb, CTAB-bond Hb and CTAB-bond Hb with 12 mM β-CD and (b) fluorescence emission spectrum of Hb, CPC-bond Hb and CPC-bond Hb with 12, 16 mM β-CD at 298 K and 10 mM phosphate buffer (pH 7.4).

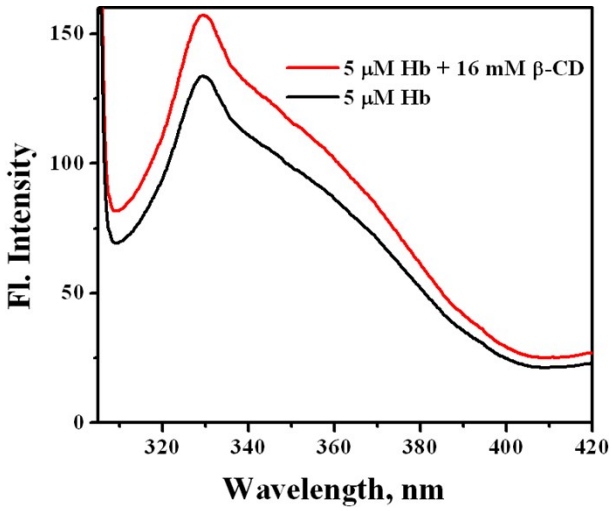


Fig. S4 Fluorescence emission spectrum of 5 μM Hb and in presence of 16 mm β-CD.

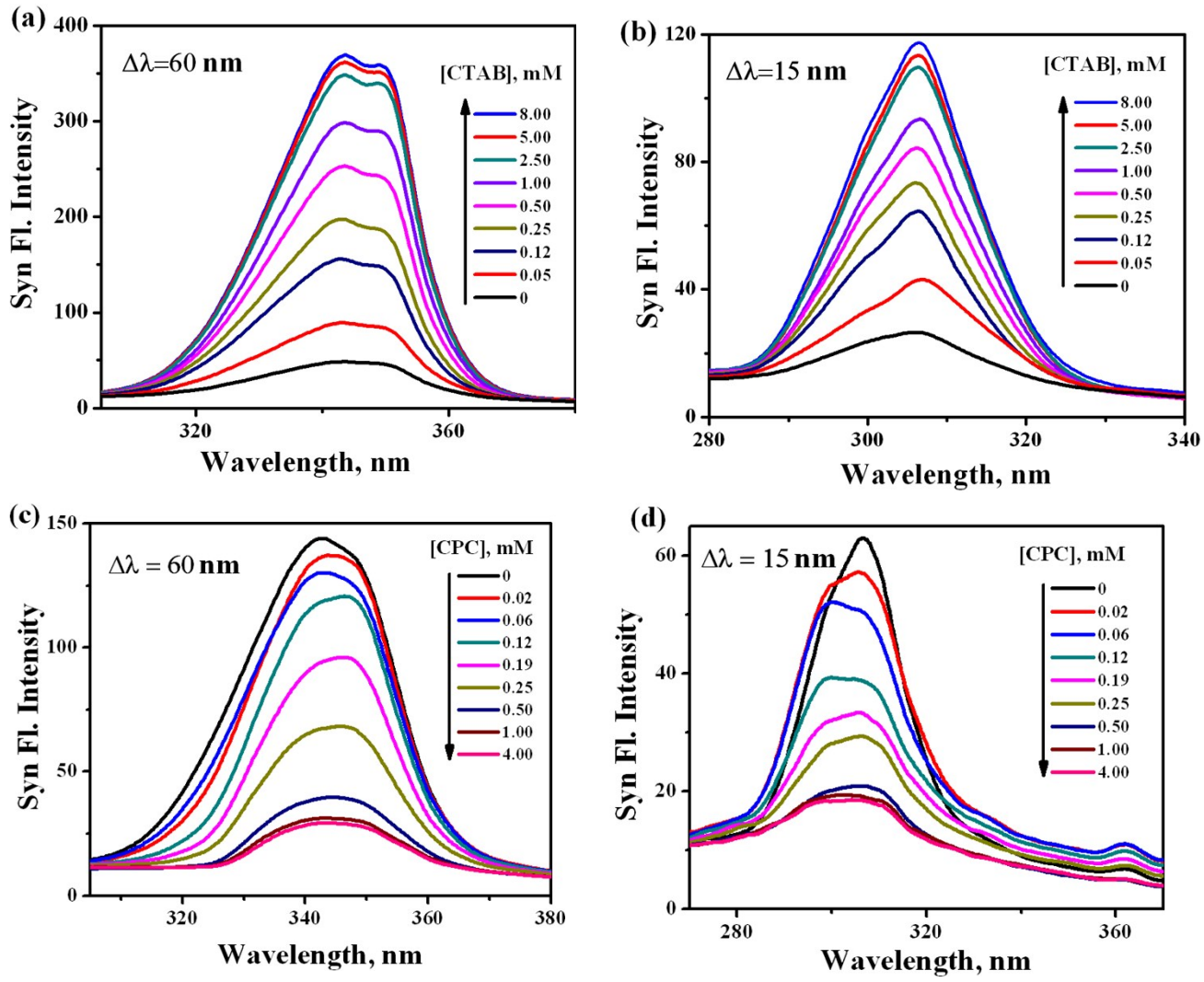


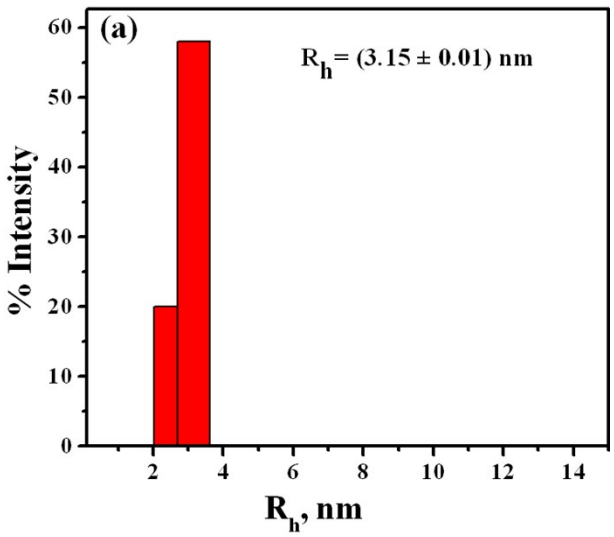
Fig. S5. Synchronous fluorescence spectra of Hb in presence of increasing concentrations of surfactant at 298 K, pH 7.4, (a) & (b) in presence of CTAB and (c) & (d) in presence of CPC surfactant. (Δλ=60 and 15 nm for Trp & Tyr respectively), [Hb] = 5 μM.

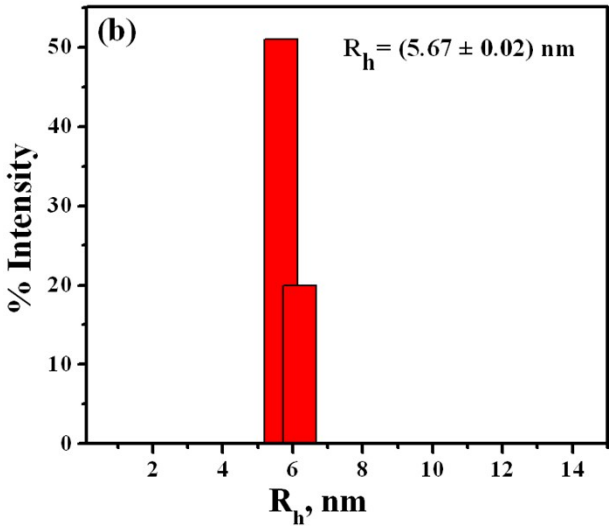
Table S1 Time-resolved fluorescence decay parameters of Hb with increasing concentrations of CTAB at pH 7.4 and 298 K

[CTAB] mM	τ_1 (ns)	τ_2 (ns)	τ_3 (ns)	α_1	α_2	α_3	$\langle\tau\rangle$ (ns)	χ^2
0	1.84	5.27	0.04	12.96	10.11	76.93	0.80	1.09
0.05	2.02	4.31	0.05	7.08	20.44	72.48	1.06	1.04
0.13	1.81	5.38	0.06	18.18	34.31	47.50	2.20	1.06
0.25	1.95	5.32	0.03	13.08	18.85	68.07	2.26	1.01
0.50	1.26	5.27	0.01	21.73	50.58	27.69	2.94	1.06
1.00	1.78	5.42	0.08	20.60	53.10	26.29	3.27	1.03
2.00	1.79	5.70	0.07	19.98	52.89	27.13	3.38	1.02
2.50	1.64	5.27	0.02	25.00	58.21	16.79	3.48	1.07
5.00	1.65	5.22	0.02	26.58	59.31	14.10	3.54	1.05
8.00	1.62	5.22	0.02	25.02	59.99	14.99	3.54	1.04

Table S2 Time-resolved fluorescence decay parameters of CTAB-bound Hb with increasing concentrations of β-CD at pH 7.4 and 298 K

[β-CD] mM	τ_1 (ns)	τ_2 (ns)	τ_3 (ns)	α_1	α_2	α_3	$\langle\tau\rangle$ (ns)	χ^2
0	1.62	5.22	0.02	25.02	59.99	14.99	3.54	1.04
3.0	0.60	5.04		33.76	20.44		3.54	1.04
4.0	0.57	4.35		38.60	61.40		2.89	1.02
5.0	0.54	4.18		45.27	54.73		2.53	1.02
6.0	0.52	4.13		50.20	49.72		2.32	1.02
7.0	0.51	4.16		55.46	44.54		2.14	1.04
8.0	0.48	3.89		59.99	40.01		1.84	1.00
9.0	0.47	3.74		70.16	29.84		1.45	1.04
10.0	0.46	3.43		83.36	16.64		0.95	1.02
16.0	0.46	2.65		77.75	22.25		0.95	1.05





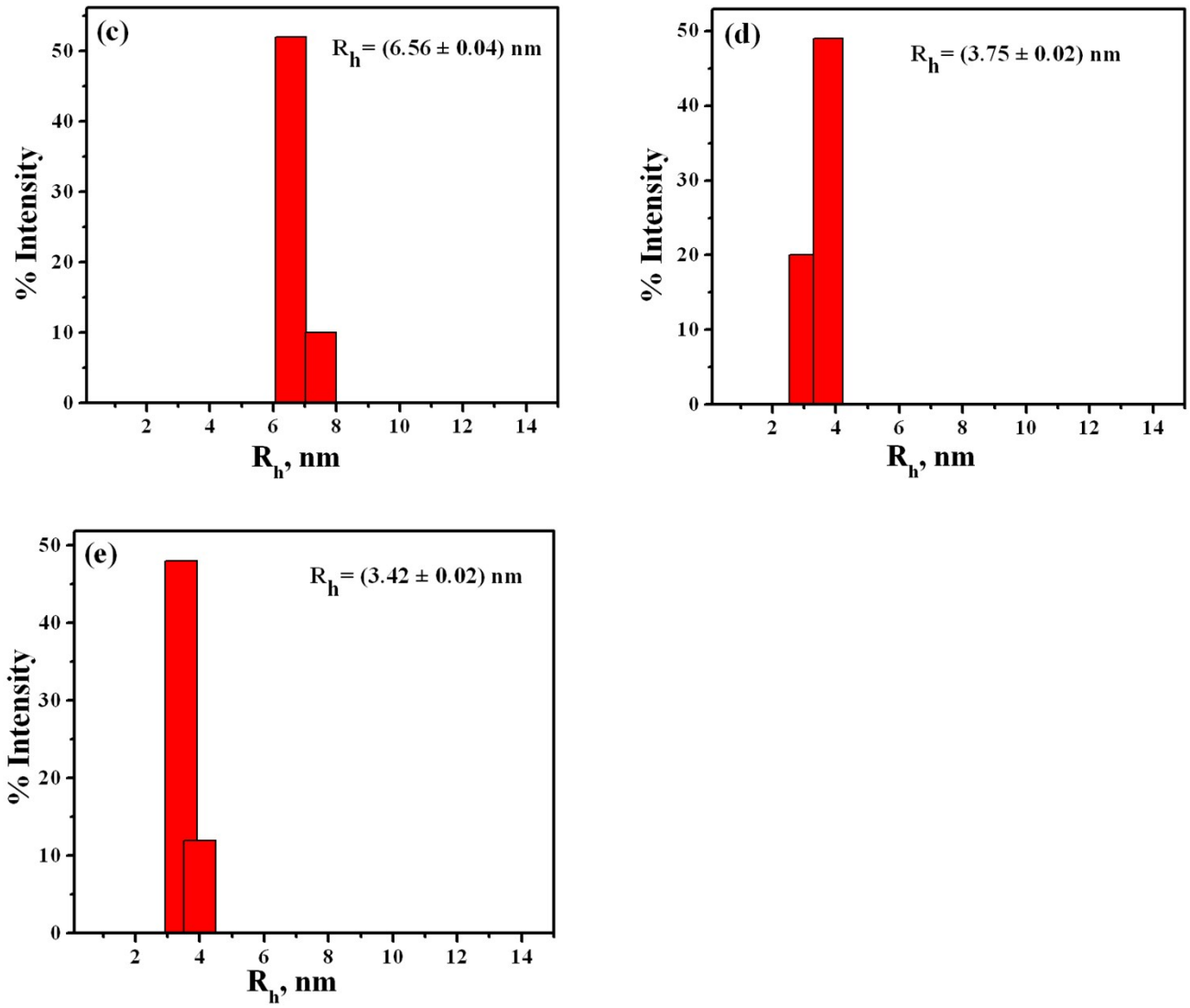


Fig. S6 Hydrodynamic radius (R_h) of Hb (a) in native state, (b) in presence of 8 mM CTAB, (c) in presence of 4 mM CPC, (d) CTAB-bound Hb in presence 12 mM β-CD and (e) CPC-bound Hb in presence 12 mM β-CD at pH 7.4 in 10 mM sodium phosphate buffer.

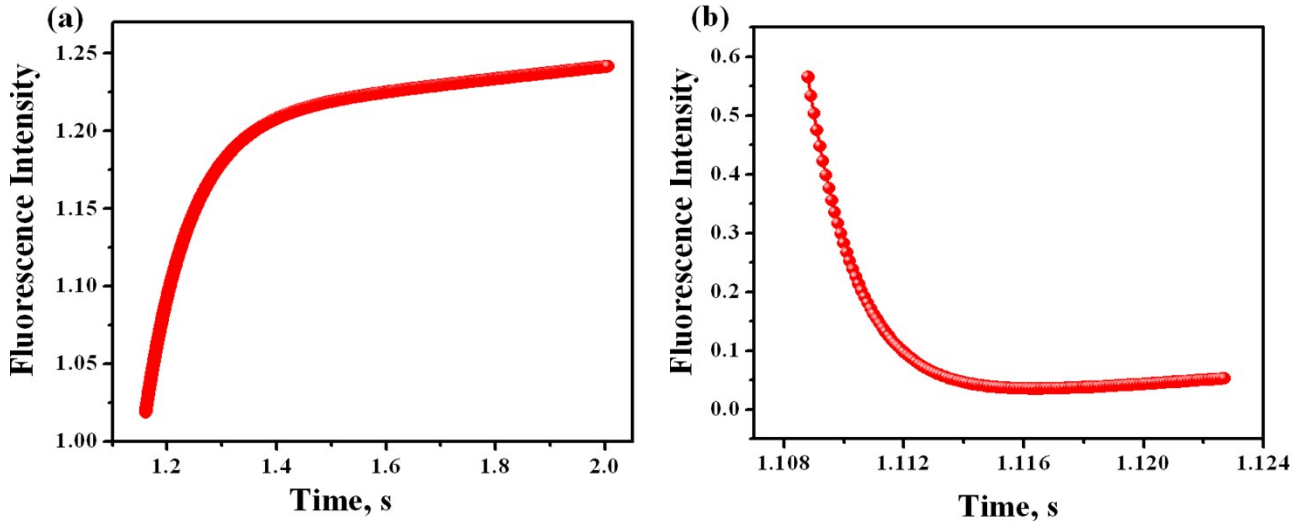


Fig. S7 Representative time course fluorescence kinetic profile for the binding interaction of (a) CTAB and (b) CPC with heme protein Hb in 10 mM phosphate buffer medium (pH = 7.4) at 298 K. λex = 295 nm, $\lambda_{monitored} = \lambda_{em}$ = 334 nm, [CTAB], [CPC] = 5 mM and [Hb] = 5 μM.

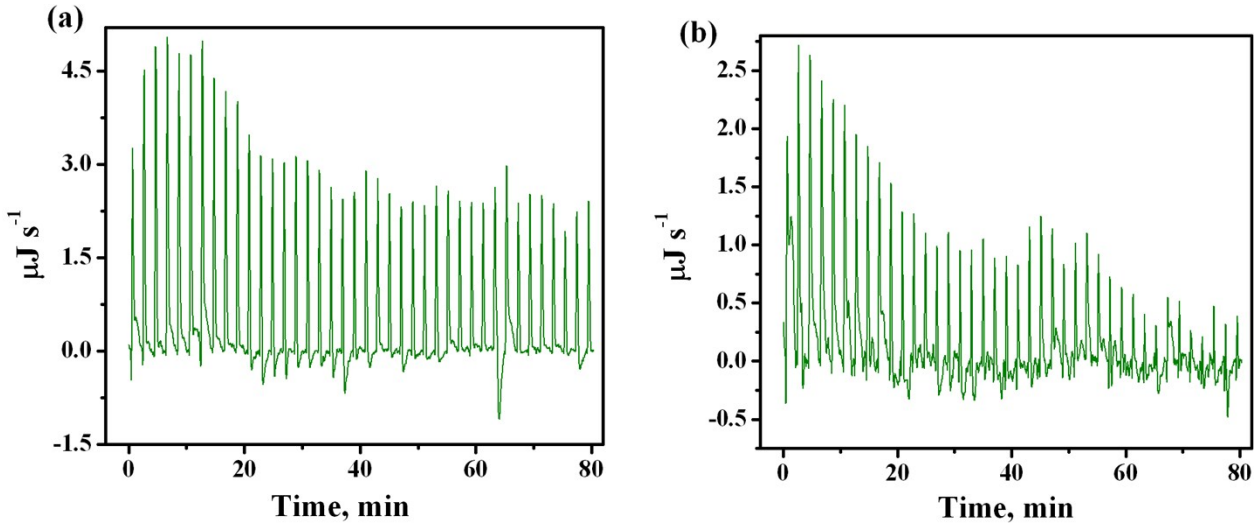


Fig. S8 Plot of raw data for the integrated heat after correction for heat of dilution, (a) CTAB and (b) CPC with Hb solution.

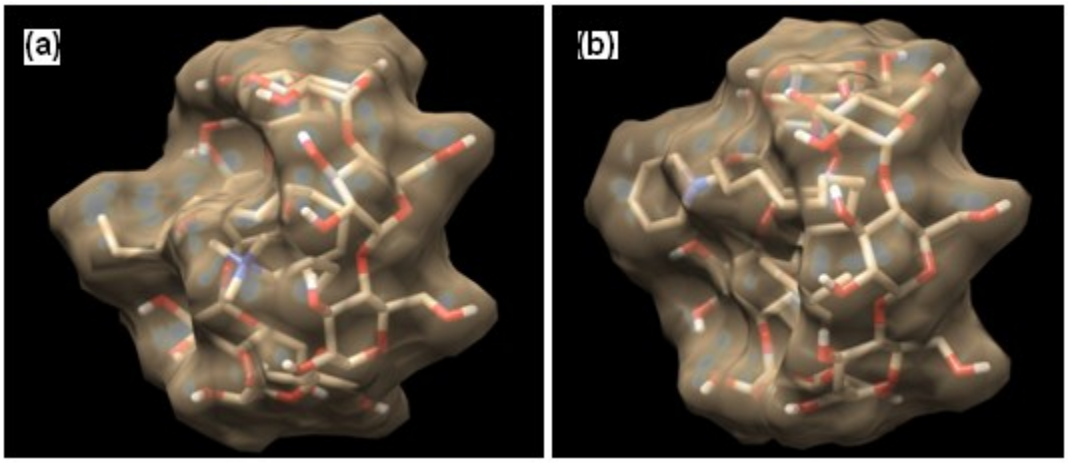


Fig. S9 Docking pose showing the interaction of the β-CD with (a) CTAB and (b) CPC