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Structural alteration of myoglobin with two homologous cationic surfactants and effect of β-cyclodextrin: multifaceted insight and molecular docking study

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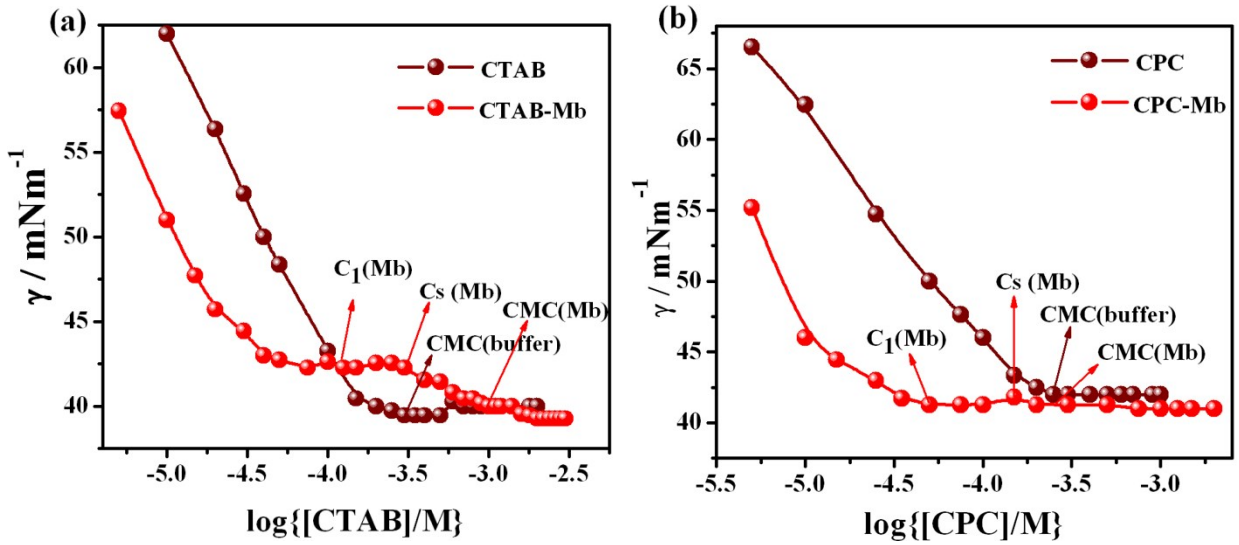


Fig. S1 Tensiometric profile for the interactions of Mb with (a) CTAB and (b) CPC in a 10 mM phosphate buffer media of pH 7.4 at 298 K. [Mb] = 5 μM.

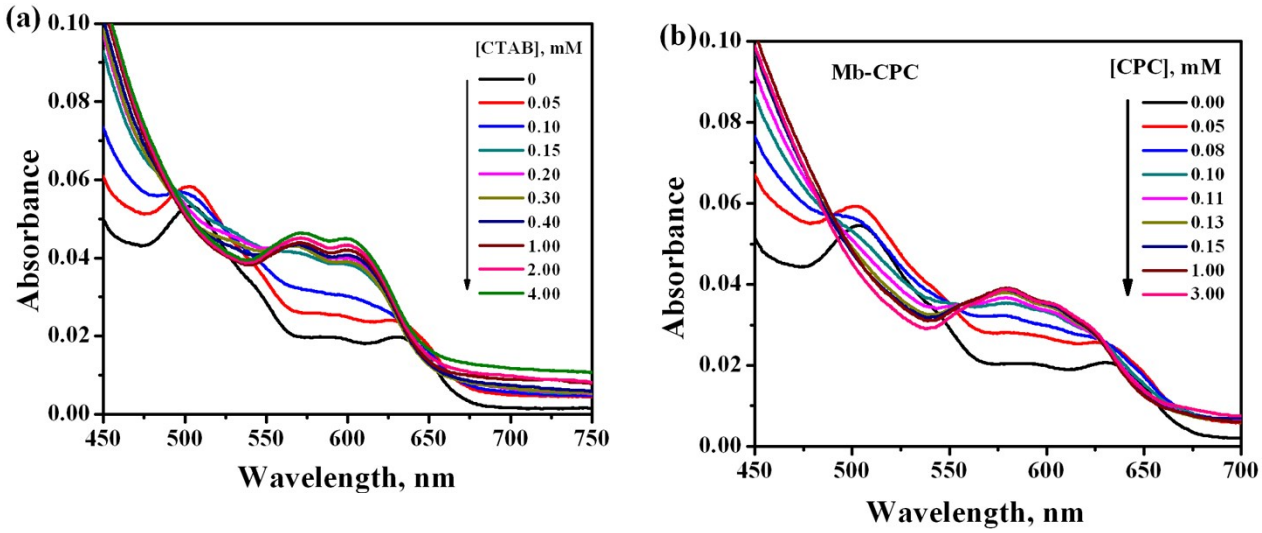


Fig. S2 Absorption spectra of visible region of Mb in the absence and presence of (a) CTAB and (b) CPC at pH 7.4 and 298 K, [Mb] = 5 μM.

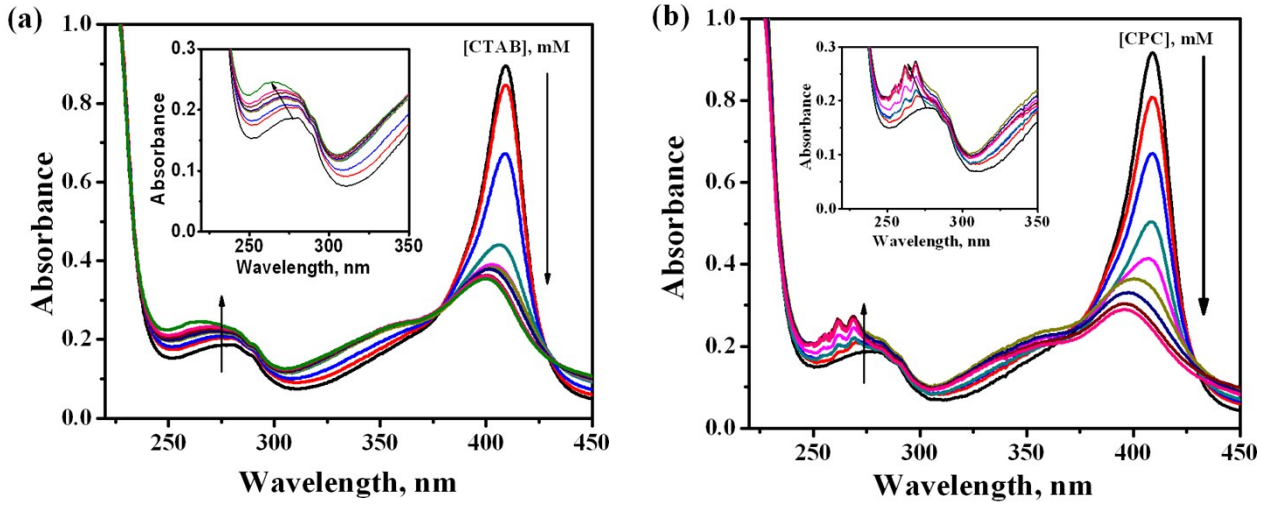


Fig. S3 Absorption spectra of Mb in the absence and presence of (a) CTAB and (b) CPC at pH 7.4 and 298 K, [Mb] = 5 μM.

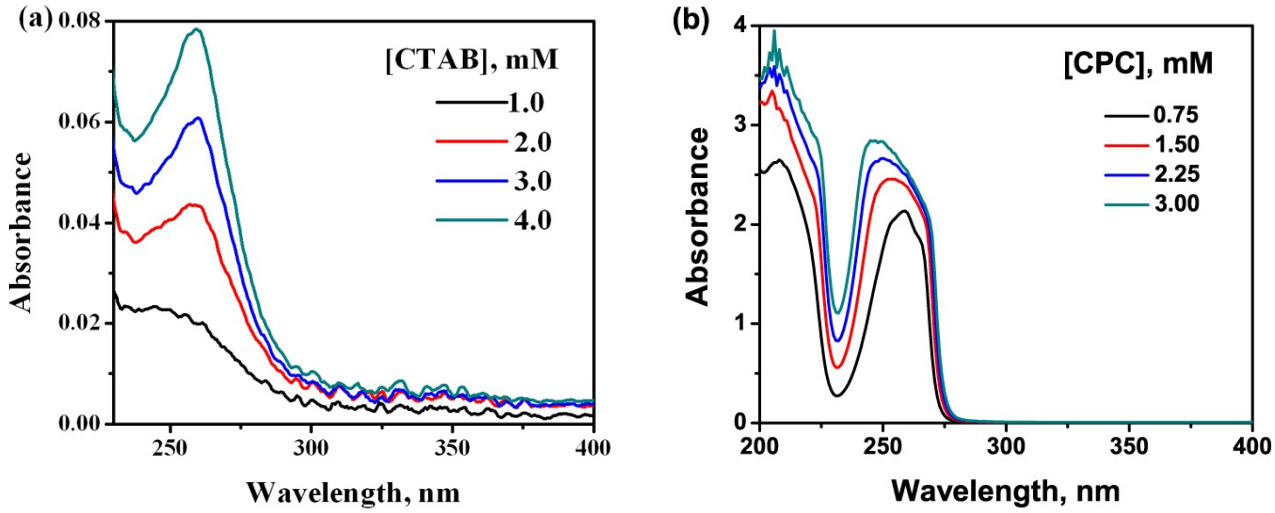
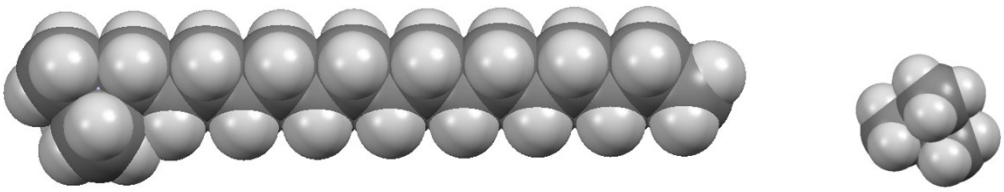
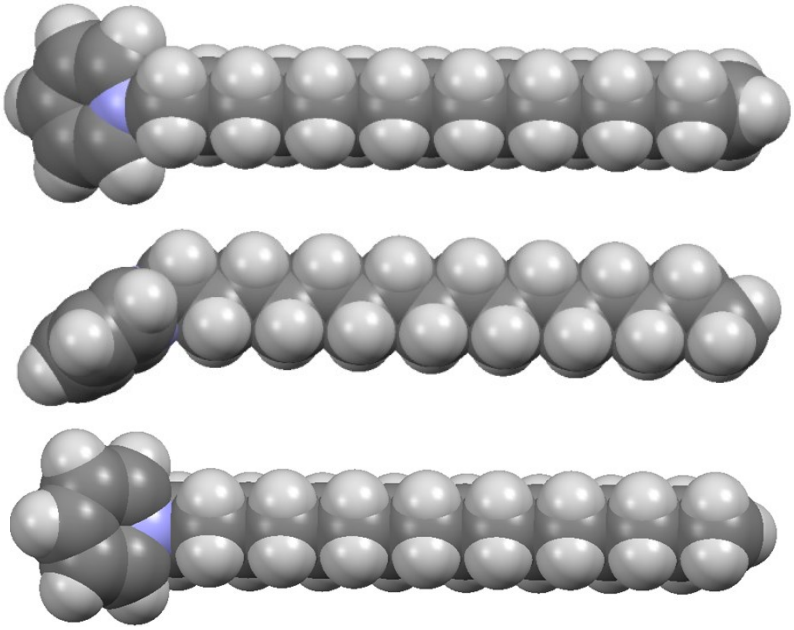


Fig. S4 Absorption spectra of (a) CTAB and (b) CPC.



(a)



(b)

Fig. S5 Space filling structures of (a) CTAB and (b) CPC.

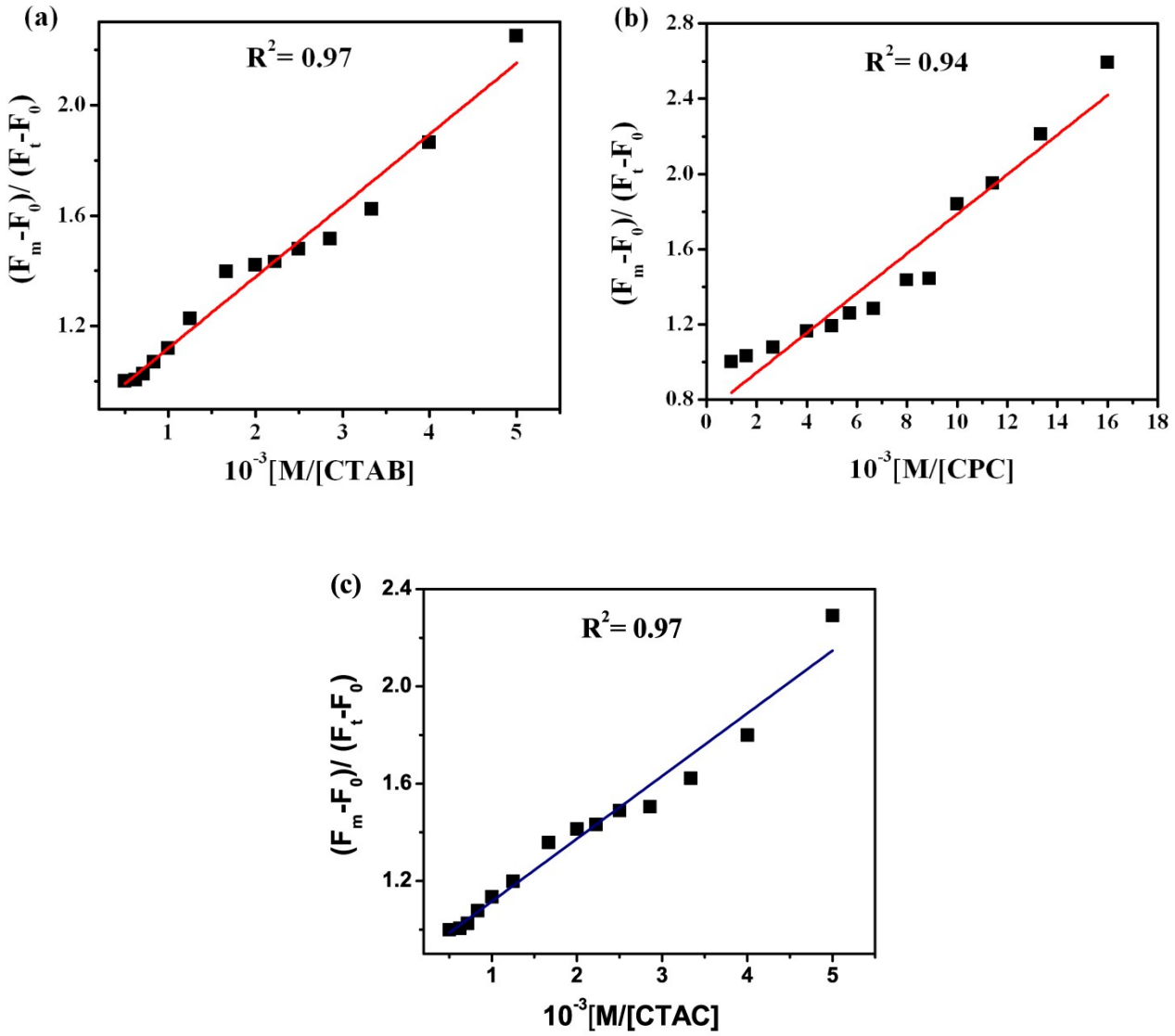


Fig. S6 Plot of (a) $(F_m-F_0)/(F_t-F_0)$ *versus* [M]/[CTAB], (b) $(F_m-F_0)/(F_t-F_0)$ *versus* [M]/[CPC] and (c) $(F_m-F_0)/(F_t-F_0)$ *versus* [M]/[CTAC] based on Almgreen equation.

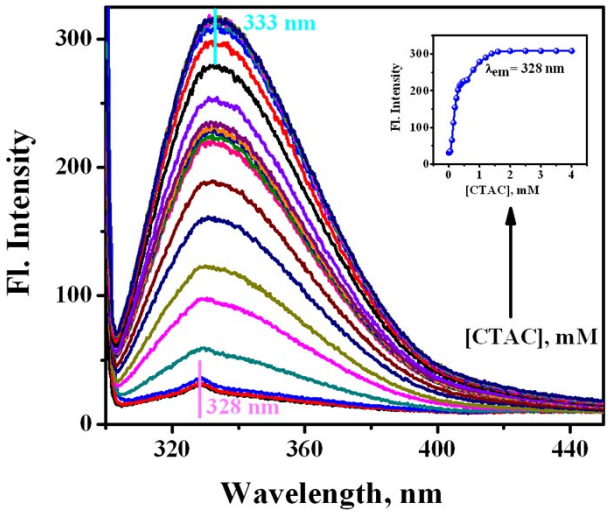


Fig. S7 Representative fluorescence emission spectra of Mb with increasing concentrations of CTAC. Inset: Trend in emission intensity with increasing concentrations of CTAC.

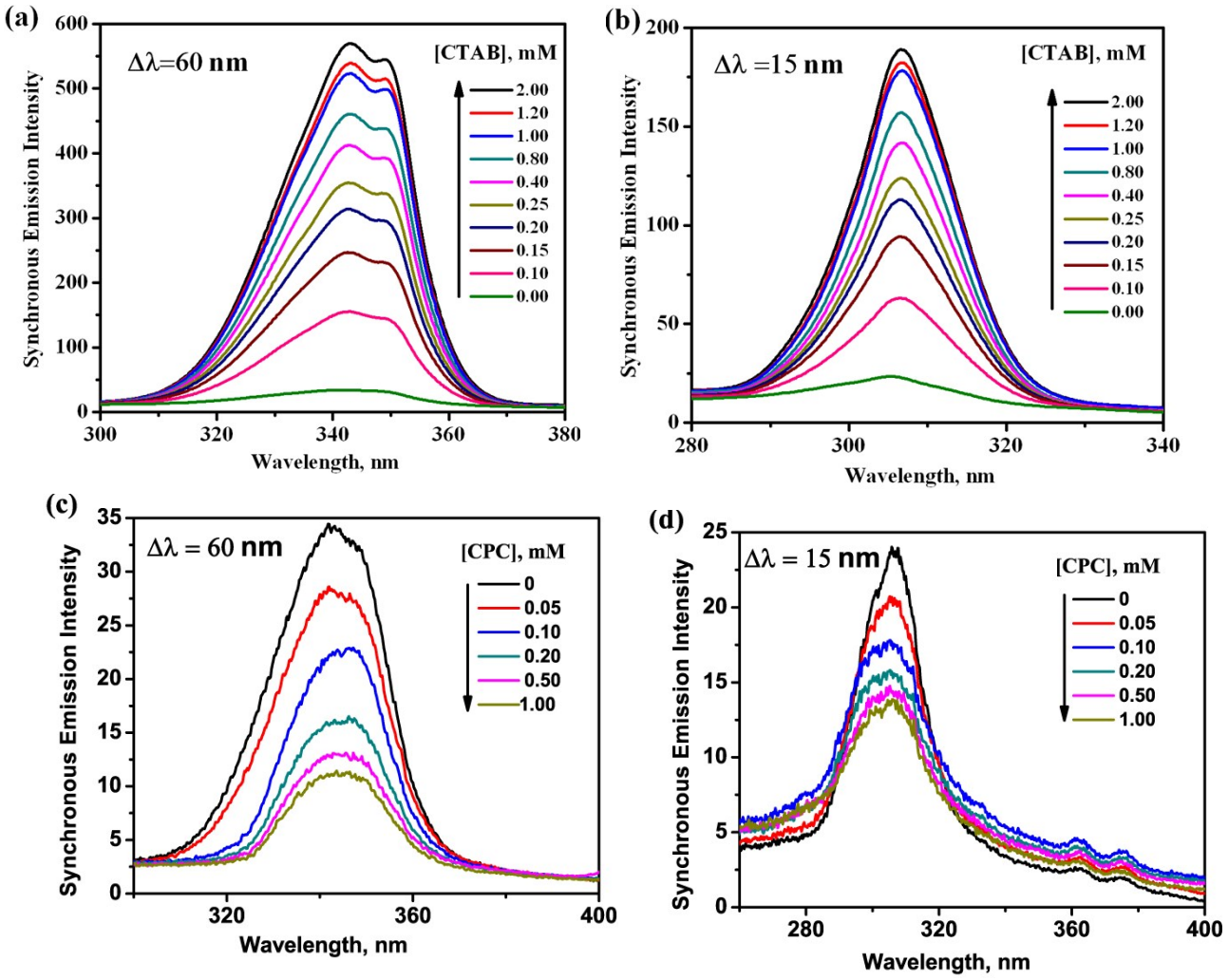


Fig. S8 Synchronous fluorescence spectra of Mb in the presence of increasing concentrations of surfactant at 298 K, pH 7.4, (a) & (b) in the presence of CTAB and (c) & (d) in the presence of CPC surfactant. (Δλ=60 and 15 nm for Trp & Tyr respectively), [Mb] = 5 μM.

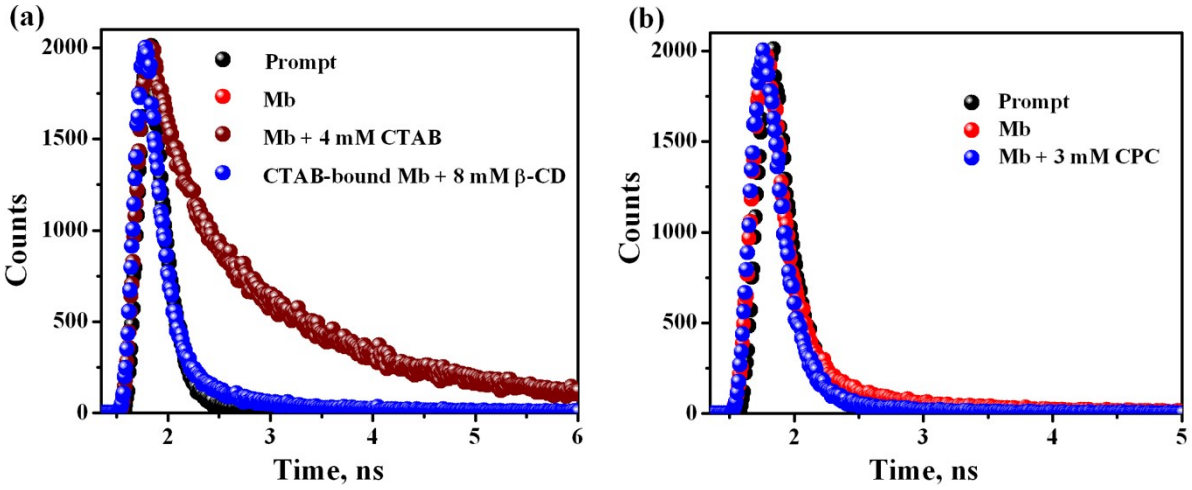


Fig. S9 (a) Fluorescence lifetime decays of native Mb, CTAB (4.0 mM) bound Mb and CTAB (4.0 mM) bound Mb in the presence of 10 mM β-CD (b) Fluorescence lifetime decays of native Mb and Mb in the presence of 3.0 mM CPC as marked in the figure. Prompt refers to the Instrument Response Function (IRF), *i.e.* the contribution from the laser diode which was deconvoluted during fitting.

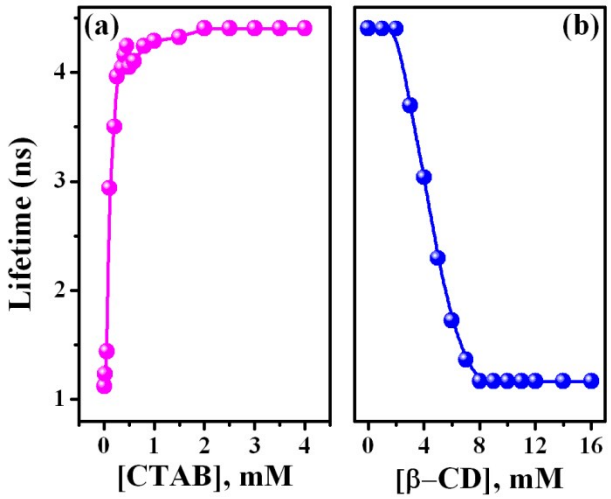


Fig. S10 Plots of the average fluorescence lifetimes of (a) native Mb *versus* [CTAB] for the surfactant binding process and (b) CTAB (4.0 mM) bound denatured Mb *versus* [β-CD] for the surfactant releasing process.

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

[CTAB], mM	τ_1, ns	τ_2, ns	a_1	a_2	$\langle\tau\rangle$, ns	χ^2
0	0.51	2.97	74.83	25.17	1.12	1.02
0.05	0.47	3.74	70.16	29.84	1.44	1.02
0.10	0.57	4.80	44.09	55.91	2.94	1.04
0.20	0.67	5.20	25.24	74.76	3.50	1.03
0.25	0.74	5.29	29.27	70.73	3.96	1.02
0.35	0.75	5.22	26.35	73.65	4.04	1.01
0.40	0.77	5.15	22.71	77.29	4.16	1.04
1.00	0.74	5.11	20.87	79.13	4.29	1.05
2.00	1.24	5.17	19.62	80.38	4.40	1.04
4.00	1.21	5.09	18.61	81.39	4.40	1.05

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

[β-CD], mM	τ_1, ns	τ_2, ns	a_1	a_2	$\langle\tau\rangle$, ns	χ^2
0	1.21	5.09	18.61	81.39	4.40	1.02
2.0	1.18	5.12	18.65	81.35	4.40	1.03
3.0	0.68	4.82	27.44	72.56	3.68	1.04
4.0	0.54	4.65	39.81	60.19	3.02	1.02
5.0	0.49	4.44	55.13	44.87	2.27	1.05
6.0	0.49	3.98	65.70	34.30	1.69	1.06
7.0	0.49	3.18	68.98	31.02	1.32	1.02
8.0	0.47	2.68	70.59	29.41	1.12	1.04
12.0	0.51	2.67	74.83	25.17	1.12	1.02
16.0	0.51	2.97	74.83	25.17	1.12	1.05

Table S3 Time-resolved fluorescence decay parameters of Mb with increasing the concentrations of CPC at pH 7.4 and 298 K

[CPC], mM	τ_1, ns	τ_2, ns	a_1	a_2	$\langle\tau\rangle$, ns	χ^2
0	0.51	2.97	74.83	25.17	1.12	1.02
1.00	0.44	2.08	90.43	9.57	0.60	1.02
3.00	0.44	2.08	90.43	9.57	0.60	1.02

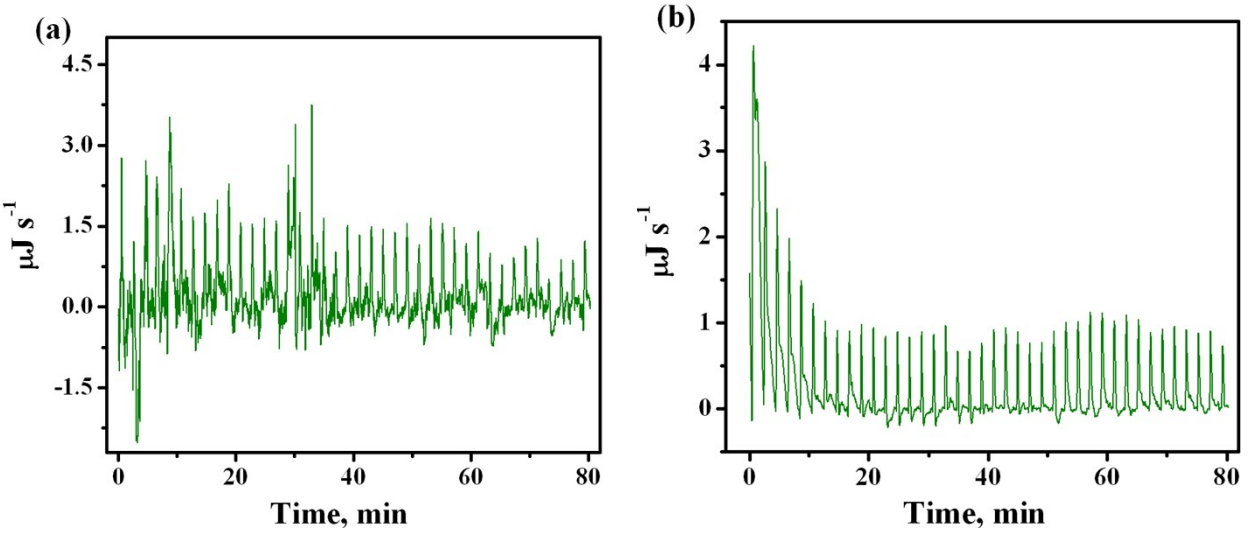


Fig. S11 Plot of the raw data for the integrated heat after correcting for the heat of dilution (a) CTAB and (b) CPC with Mb solution.

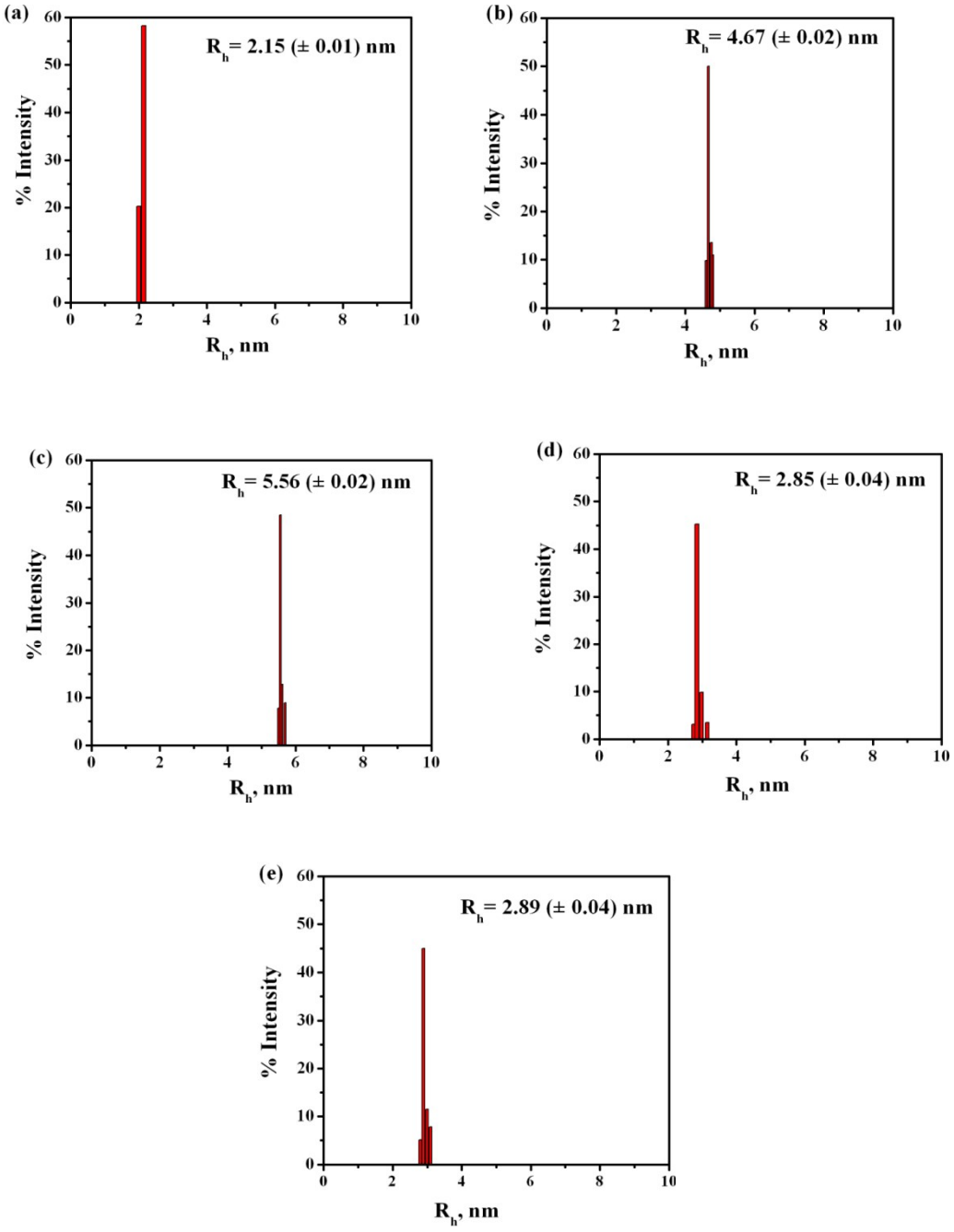


Fig. S12 Hydrodynamic radius (R_h) of Mb (a) in the native state (b) in the presence of 8 mM CTAB (c) in the presence of 4 mM CPC (d) CTAB-bound Mb in the presence 12 mM β-CD and (e) CPC-bound Mb in the presence 12 mM β-CD in a 10 mM sodium phosphate buffer at pH 7.4.

Table S4 Secondary structural content of Mb in the presence of different concentrations of surfactant in phosphate buffer medium at pH 7.4 and 298 K

[CTAB], mM	α-helix (%)	β-sheet (%)	Random coil (%)
0	81.70	10.50	7.80
0.04	78.10	11.40	10.50
0.13	69.30	18.20	12.50
0.20	55.70	26.20	18.10
0.32	52.60	27.12	20.28
0.52	50.80	28.10	21.20

[CPC], mM	α-helix (%)	β-sheet (%)	Random coil (%)
0	81.70	10.50	7.80
0.008	71.80	18.70	9.50
0.015	55.60	33.20	11.20
0.030	56.70	29.50	13.80
0.075	54.20	30.30	15.50
0.150	18.30	54.10	35.80

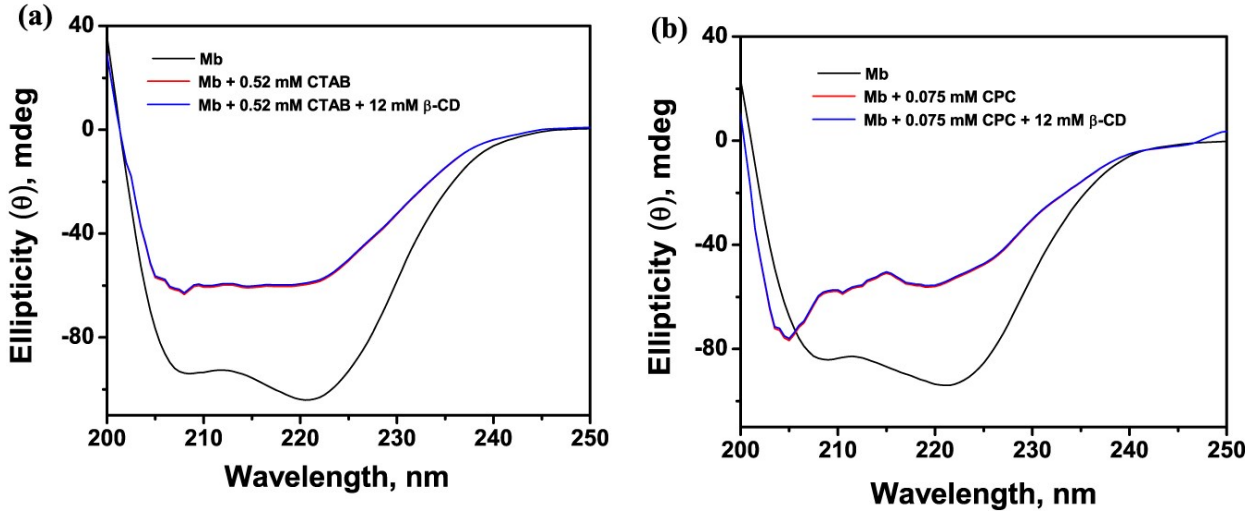


Fig. S13 Far-UV CD spectra of Mb, Mb in the presence of surfactant and surfactant bound Mb in the presence of 12 mM β-CD at pH 7.4 and 298 K.

Table S5 Secondary structural content of surfactant bound Mb in the presence of 12 mM β-CD at pH 7.4 and 298 K.

System	α-helix (%)	β-sheet (%)	Random coil (%)
Mb + 0.52 mM CTAB + 12 mM β-CD	50.85	28.15	21.20
Mb + 0.075 mM CPC + 12 mM β-CD	18.32	54.15	35.80

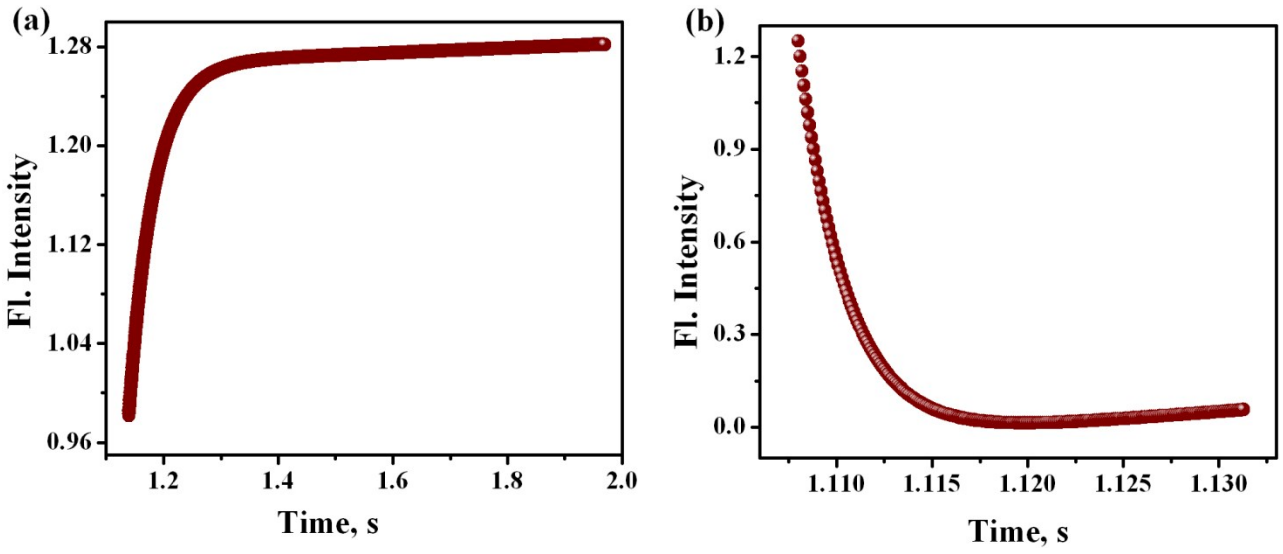


Fig. S14 Representative time course fluorescence kinetic profile for the binding interactions of (a) CTAB and (b) CPC with Mb in a 10 mM phosphate buffer medium (pH = 7.4) at 298 K. λ_{ex} = 295 nm, $\lambda_{monitored} = \lambda_{em}$ = 334 nm, [CTAB], [CPC] = 5 mM and [Mb] = 5 μM.

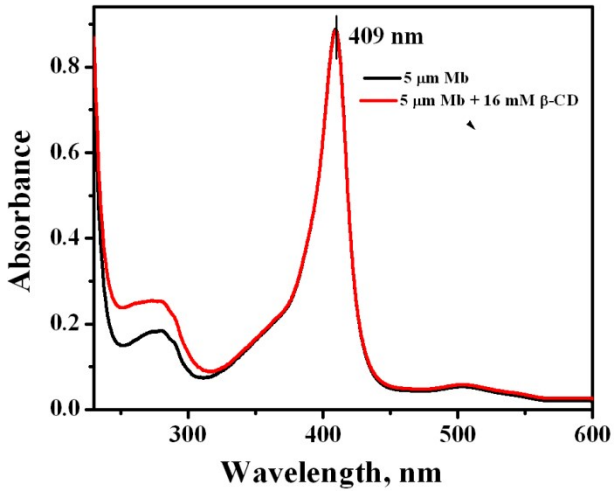


Fig. S15 Absorption spectra of Mb in the absence and presence of β-CD at pH 7.4 and 298 K, [Mb] = 5 μM.

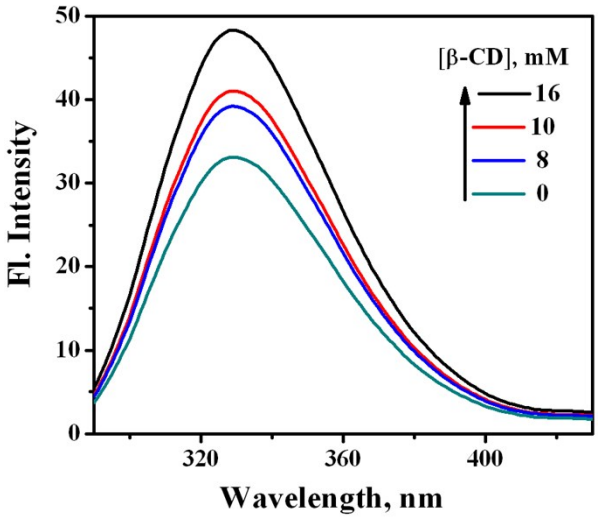


Fig. S16 Emission spectra of Mb in the absence and presence of β-CD at pH 7.4 and 298 K, [Mb] = 5 μM.

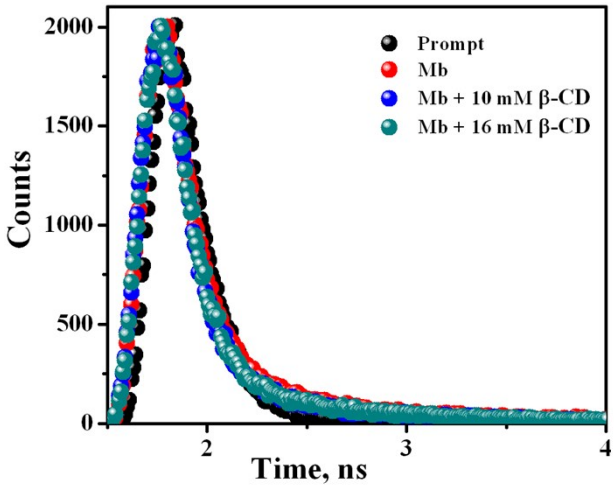


Fig. S17 Fluorescence lifetime decays of native Mb, and native Mb in the presence of β-CD as marked in the figure. Prompt refers to the Instrument Response Function (IRF), *i.e*. the contribution from the laser diode which was deconvoluted during fitting.

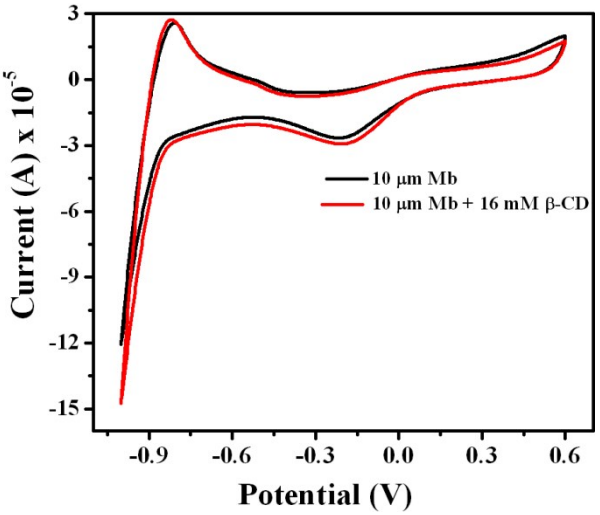


Fig. S18 Cyclic voltammograms profile of Mb and Mb in the presence of 16 mM β-CD at the scan rate of50 mV s^{-1} (at 298K, pH 7.4).

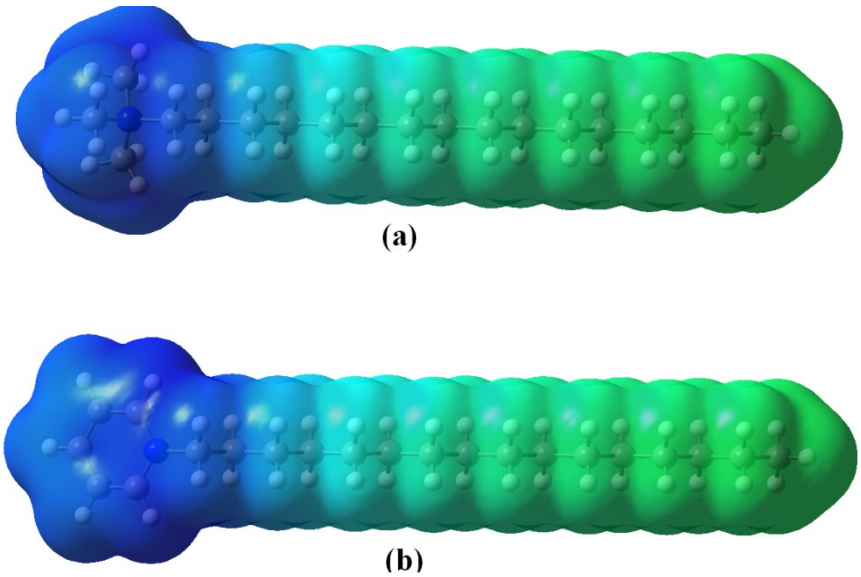
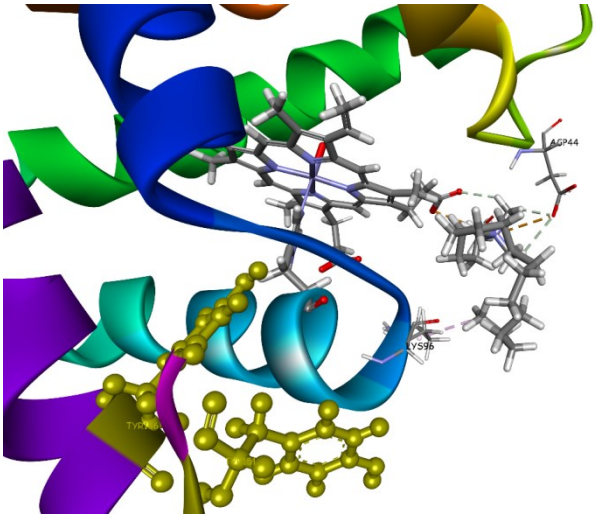
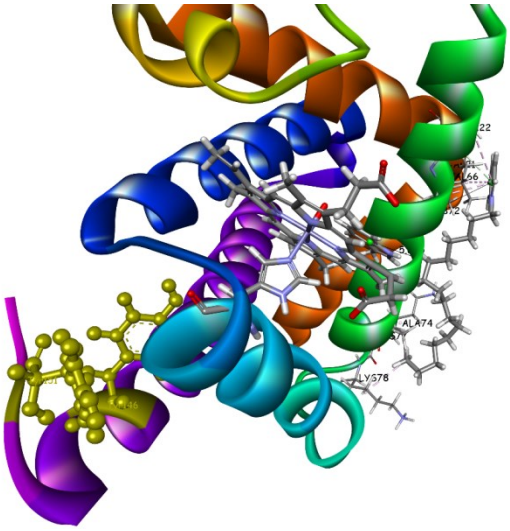


Fig. S19 MEP of (a) CTAB and (b) CPC



(a)



(b)

Fig. S20 Docking poses of various amino acid residues of Mb involved in the binding of (a) CTAB and (b) CPC.

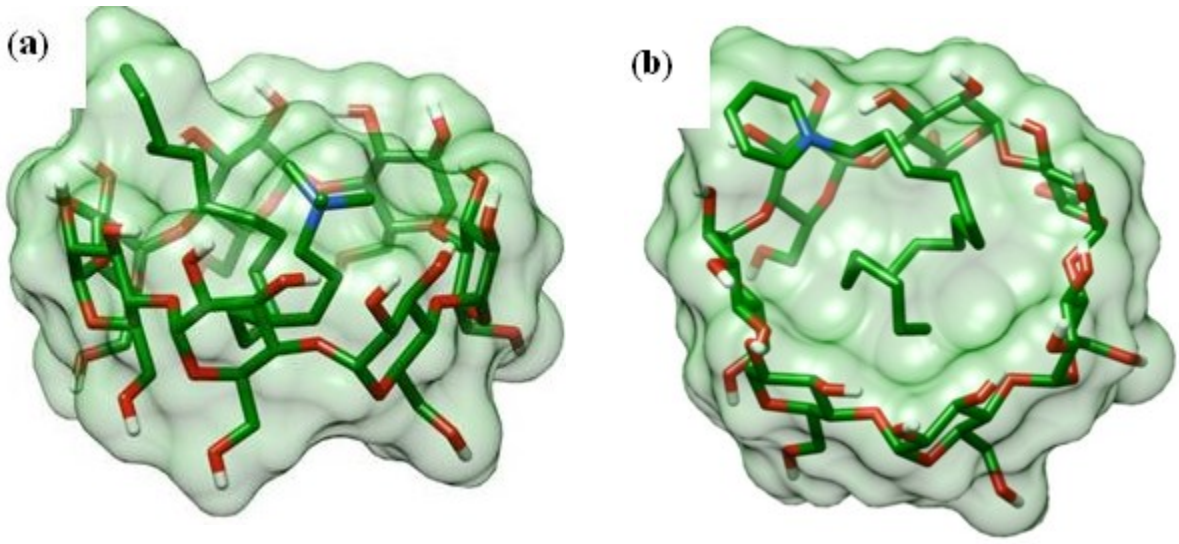


Fig. S21 Docking pose showing the interactions of the β-CD with (a) CTAB and (b) CPC.