Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2023

Electronic Supplementary Information

Bis-chalcone based colorimetric probe for the selective detection of bisulfite/sulfite anions: exploring surfactant promoted Michael addition of anions to α, β-unsaturated ketone.

Sowmya P, Sivakrishna Prakash, and Abraham Joseph*

Department of Chemistry, University of Calicut, Calicut University P O, 673 635, Kerala, India. abrahamjoseph@uoc.ac.in

Synthesis of the probe (1E,4E)-1,5-di(thiophen-2-yl) penta-1,4-dien-3-one

To a mixture of 1.87 ml (0.02 mol) of thiophene-2-carboxaldehyde, 2g (0.05 mol) NaOH in water (0.1g/ml ratio), 40 mL of EtOH and 60 mL of water, 0.74 ml (0.01 mol) of acetone was added dropwise. The reaction was carried out at room temperature for 1 h and the reaction mixture was poured into crushed ice. The yellow crystalline solid was collected by filtration and dried to give 2.19 g (89%) of product, mp 114-116.5 °C: ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.83 (d, 2 H, J = 15 Hz),7.40 (d, 2 H, J = 5.0 Hz), 7.33 (d, 2 H, J = 3.6 Hz), 7.08 (dd, 2H, J = 3.6, 5.0 Hz), 6.82 (d, 2 H, J = 15 Hz); ^{13}C NMR (400 MHz, $CDCl_3$): δ 187.8, 140.3,135.6, 131.9, 128.8, 128.3, 124.4; MS (EI, 70 eV): *m/z* (%) 246 ; Ir (KBr) 3087, 1661, 1604,1565, 1105, 749, 729 cm-1.

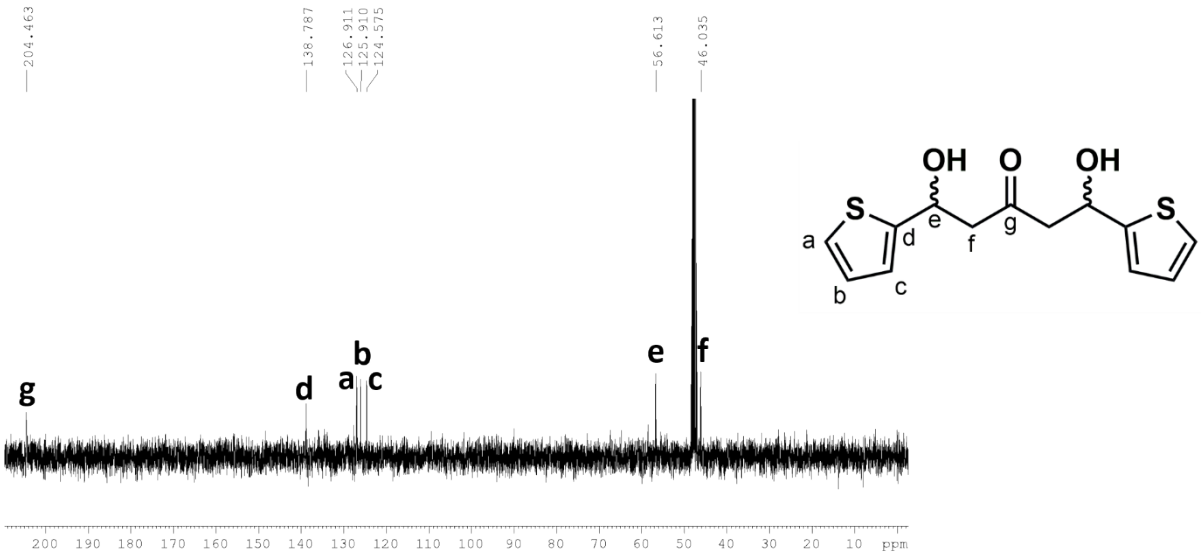

Fig. S1. ^{13}C NMR spectra of the probe-OH adduct in CD_3OD.

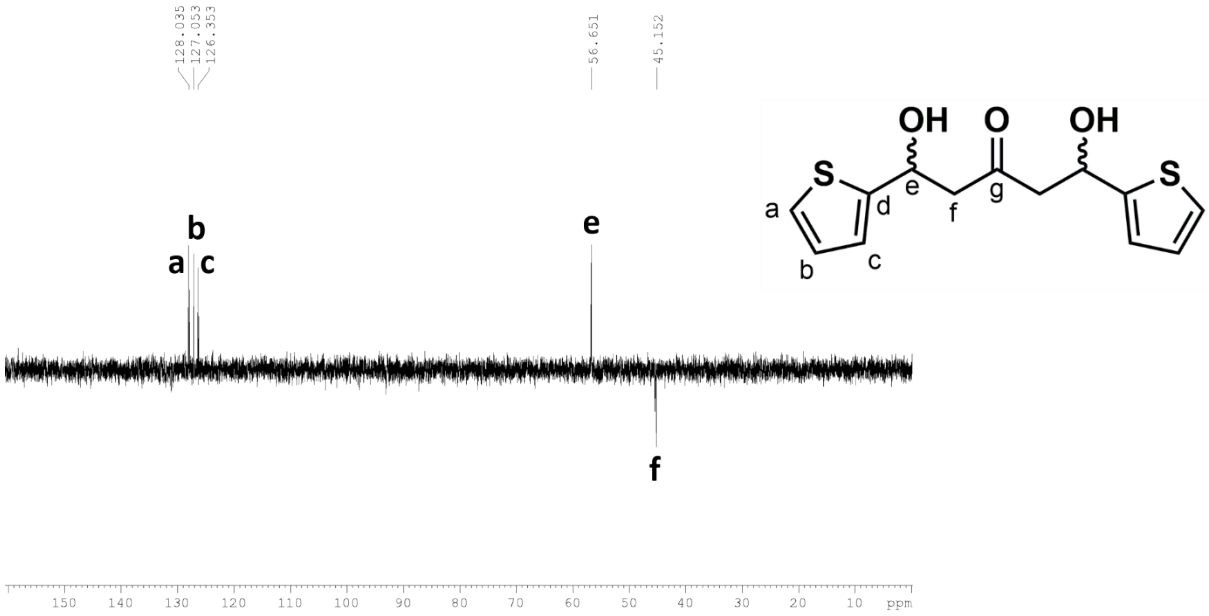

Fig. S2. DEPT analysis spectra of the probe-OH adduct in CD_3OD.

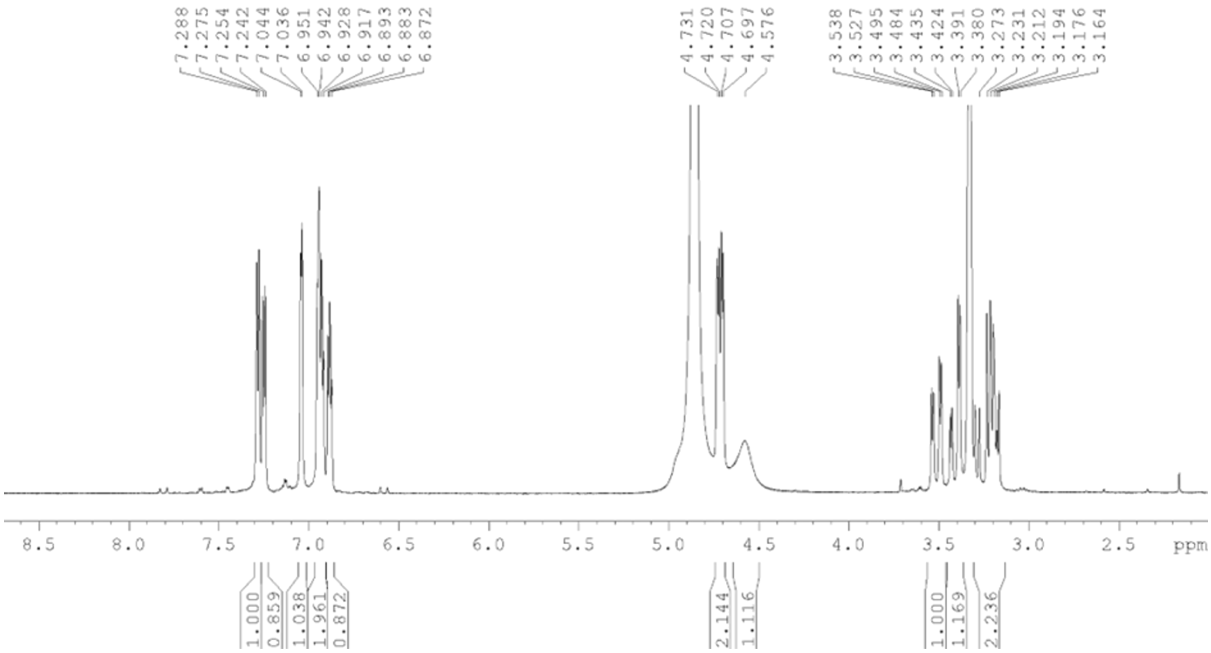

Fig. S3. ^{1}H NMR spectra of the probe-OH adduct in CD_3OD.

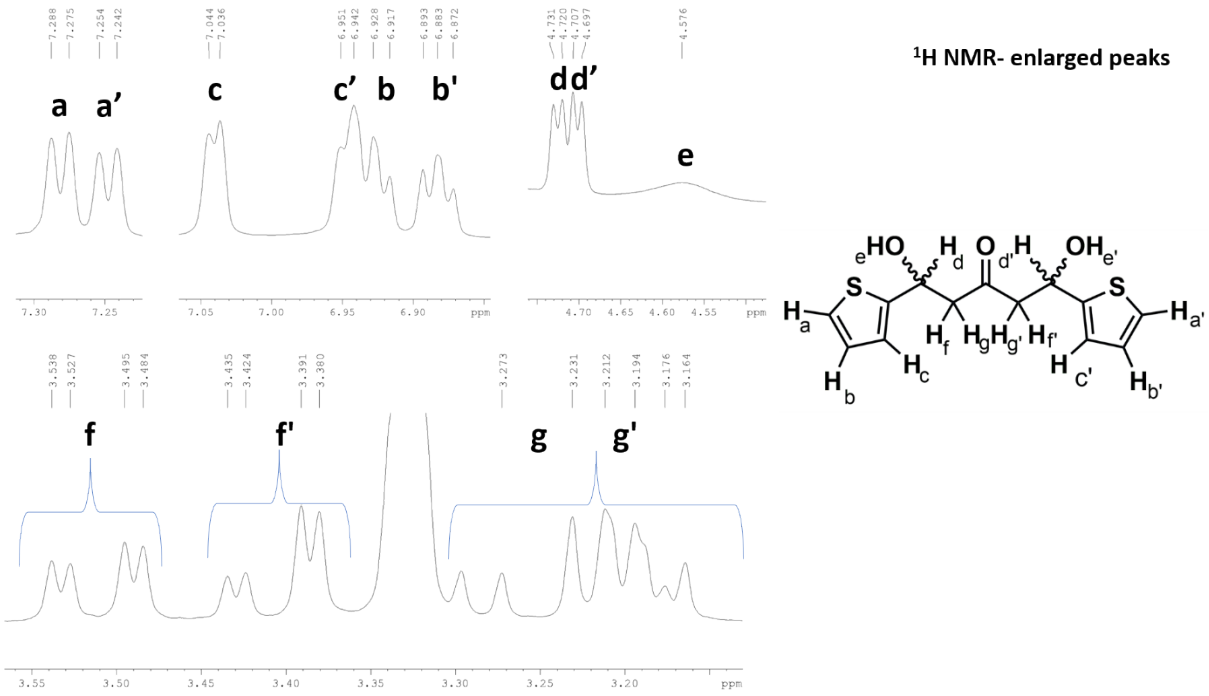

Fig. S4. Enlarged ^{1}H NMR spectra of the probe-OH adduct in CD_3OD.

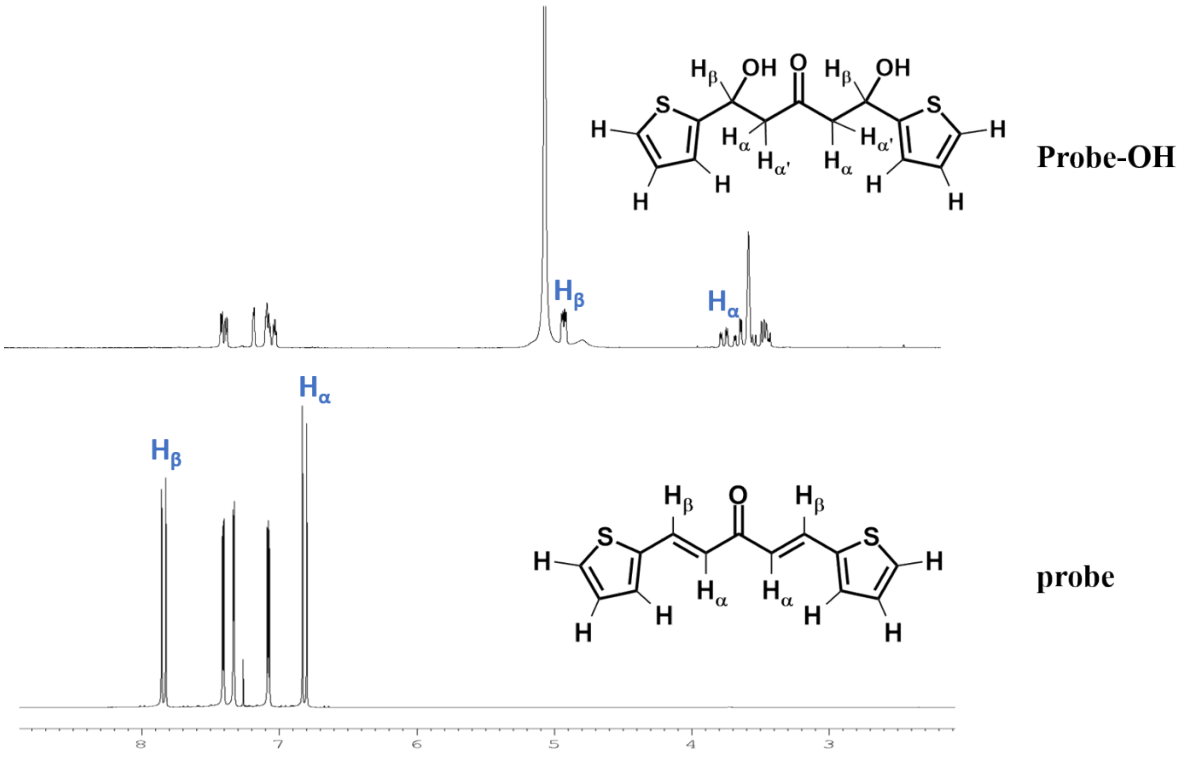

Fig. S5. ^{1}H NMR spectra of the probe and probe-OH in $CDCl_3$ and CD_3OD respectively.

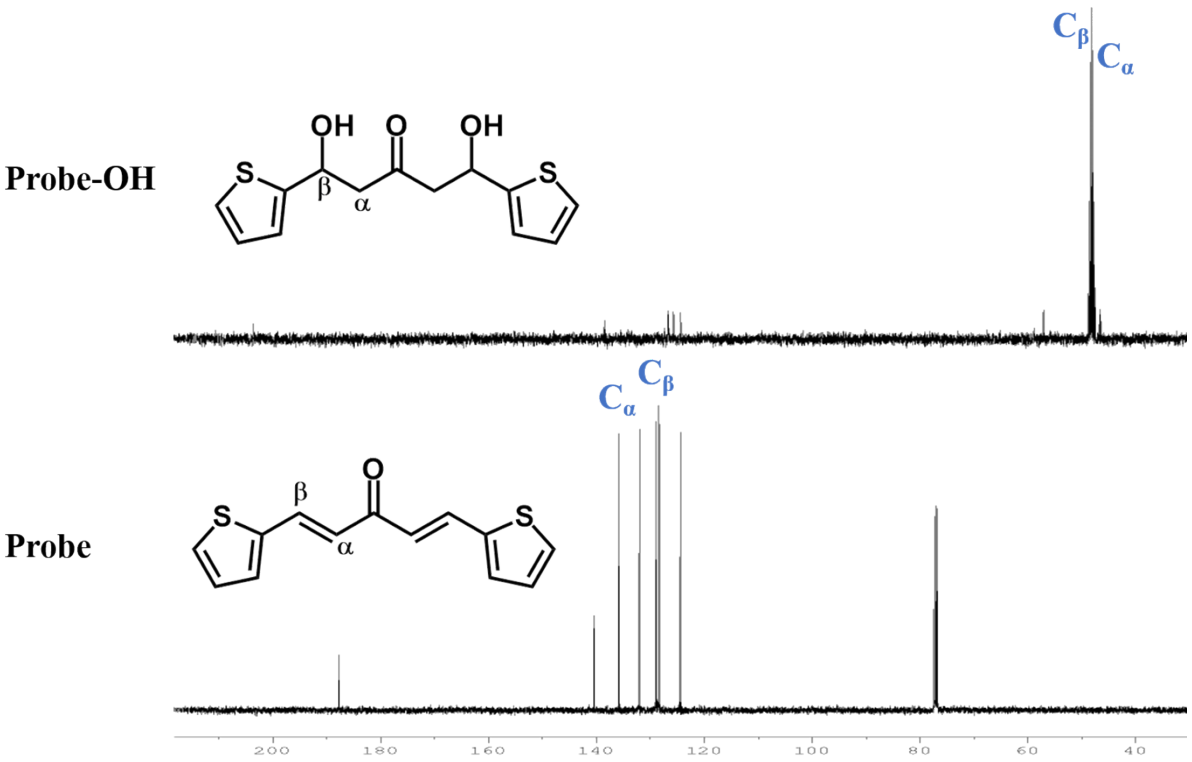

Fig. S6. ^{13}C NMR spectra of the probe and probe-OH in $CDCl_3$ and CD_3OD respectively.

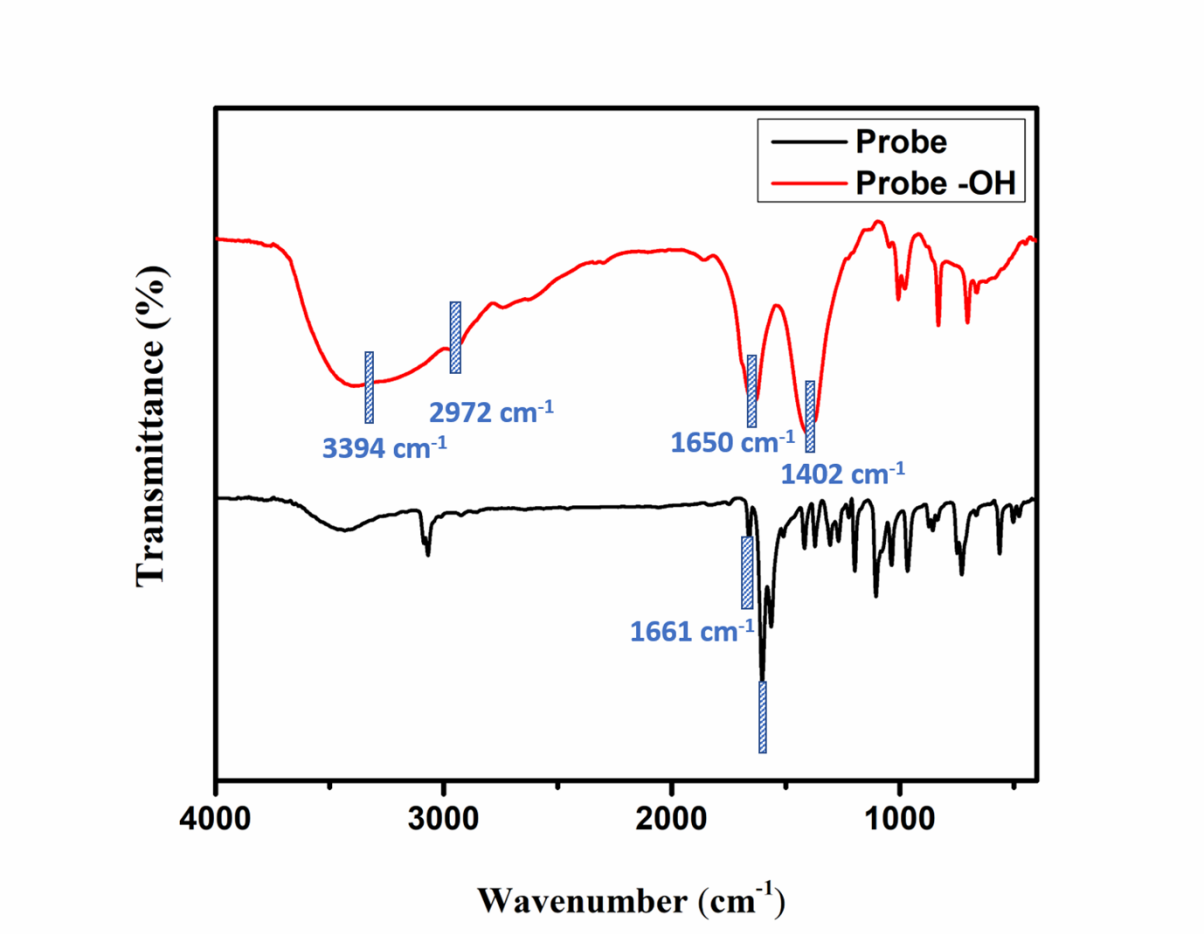

Fig. S7. FT-IR spectrum of the probe and probe-OH.

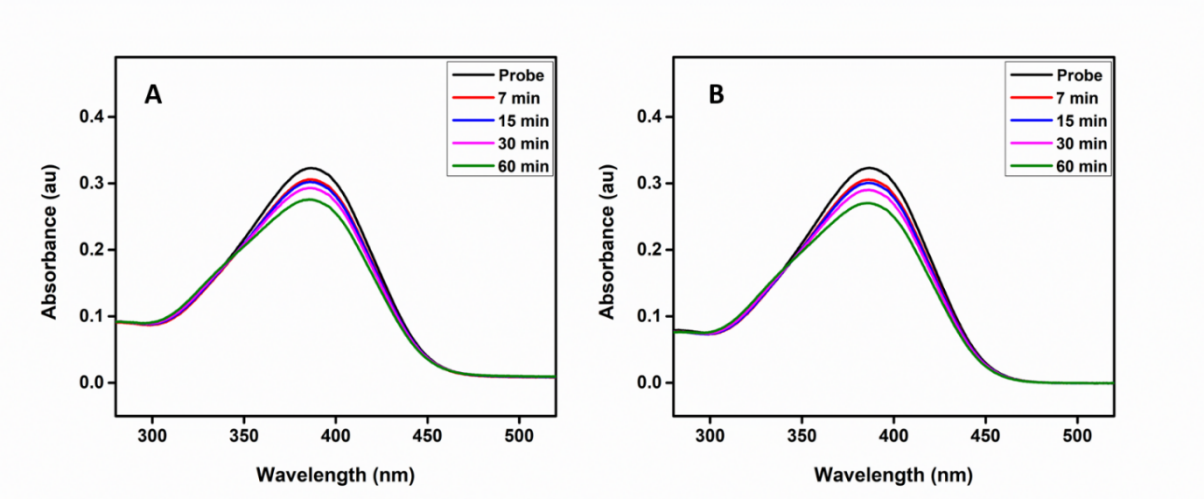

Fig. S8. (A) Absorption spectra of probe (10 μM) upon the addition of $NaHSO_3$ (200 μM) and (B) Na_2SO_3 (200 μM) respectively in HEPES buffer solution (20 mM, pH 7.4) in the absence of CTAB.

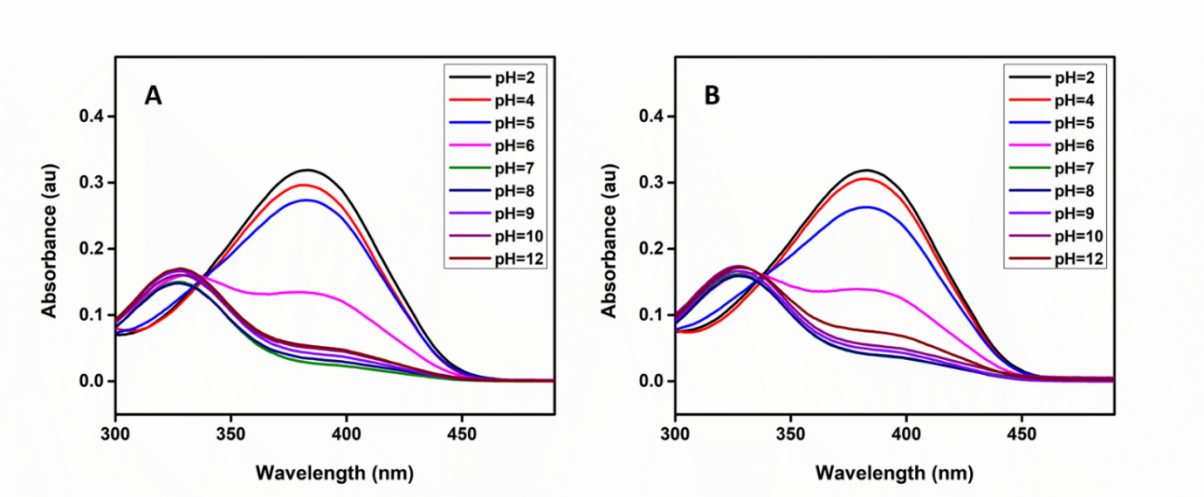

Fig. S9. (A) Spectra for the reaction between probe (10 μM) and $NaHSO_3$ (200 μM) and (B) Na_2SO_3 (200 μM) respectively at different pH values.

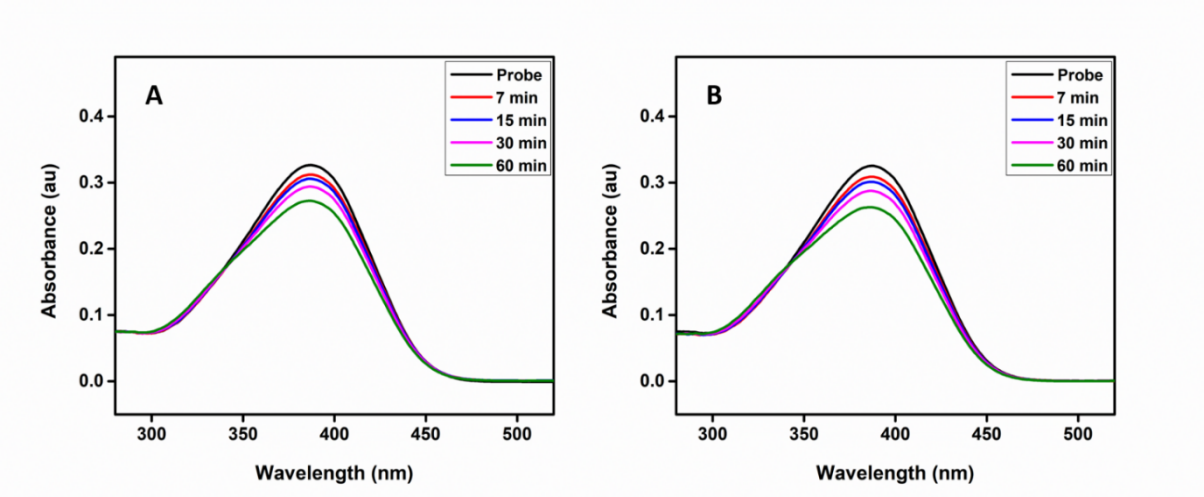

Fig. S10. (A) Absorption spectra of probe (10 μM) upon the addition of $NaHSO_3$ (200 μM) and (B) Na_2SO_3 (200 μM) respectively in HEPES buffer solution (20 mM, pH 7.4) in the presence of anionic surfactant SDBS.

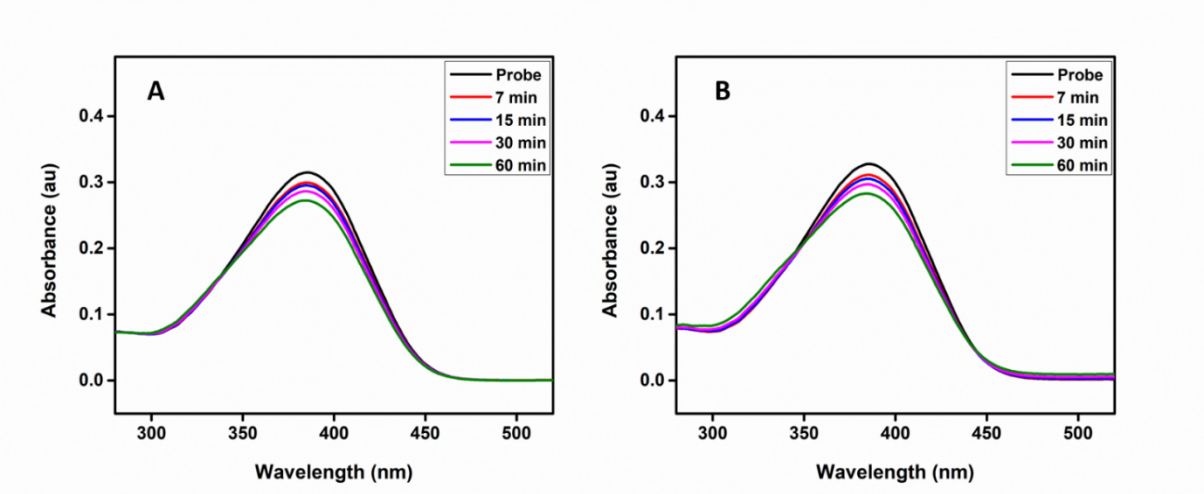

Fig. S11. (A) Absorption spectra of probe (10 μM) upon the addition of $NaHSO_3$ (200 μM) and (B) Na_2SO_3 (200 μM) respectively in HEPES buffer solution (20 mM, pH 7.4) in the presence of zwitter ionic surfactant CAPB.