**Supporting Information for**

**Anion-Induced Deprotonation as a Simple Strategy to Improve Analytical Performance of an Amphiphilic Probe at Mesoscopic Interface**

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**Experimental Section**

**Materials and methods:** All reagents including reagents, solvents and silica gel were obtained from the best-known local supplier and were used directly without further purification. Solvents were distilled and dried prior to use. FTIR spectra were recorded on a Perkin-Elmer FT-IR Spectrum BX system. 1H- and 13C-NMR spectra were recorded with a Bruker Advance DRX 400 spectrometer operating at 400 and 100 MHz respectively. Chemical shifts were reported in ppm downfield from the internal standard, tetramethylsilane (TMS). Mass spectra were recorded on Micro mass Q-TOF Micro TM spectrometer.

**UV-visible and fluorescence experiment:** The UV−vis and fluorescence spectra were recorded on a Shimadzu model 2100 UV-vis spectrometer and Cary Eclipse spectrofluorimeter respectively. In the fluorescence experiment, the slit widths (for both the excitation and emission channel) were fixed at 5 nm and the excitation wavelength was chosen 350 nm.

**Sample preparation for studies:** All the sensing studies have been performed in aqueous medium. The 10 μL DMSO solution of **1** from a stock (1 × 10−3 M) was added in PBS buffer (pH 7.0) make the final volume of **1** mL ([**1**] = 1 × 10−5 M). For sensing studies, the aqueous solutions of the metal ions were added directly to the aqueous solution of **1** (1.2 – 1.5 equiv.). Similarly, to check the influence of pH of the medium, buffered solutions of different pH (HCO2Na/ HCl buffer for pH 2-4.5, CH3CO2Na/ HCl buffer for pH 5-6.5, PBS for pH 7-9 and Na2B4O7·10H2O/NaOH for pH 9.5-10.5) have been used. The final concentration of DMSO in the solution did not exceed 1%.For studying in micelle medium, the aqueous solutions of Brij-58, SDS and CTAB wereat concentrations 1, 1.5 and 8 mM respectively used for the sensing studies.

**1H NMR titration studies.** 1H NMR titration with compound **1** was performed upon dissolving **1** (5 mM) in DMSO-d6 medium. To that Hg2+ was added (0 to 1.25 equiv.) and the spectra were recorded using identical parameters. Then 1H-NMR spectra of **1** was recorded with Hg2+ ion (1 equiv.) both in presence and absence of tertbutyl ammonium acetate (1 equiv.).

**Determination of fluorescence quantum yield:** The fluorescence quantum yield was calculated by using rhodamine 6G (φ = 0.94 in EtOH) as a reference. And the quantum yield is calculated using the equation

φunk = φstd[(Iunk/Aunk)/(Istd/Astd)](ηunk/ηstd)2

where, φunk and φstd are the radiative quantum yields of the sample and standard, Iunk and Istd are the integrated emission intensities of the corrected spectra for the sample and standard, Aunk and Astd are the absorbances of the sample and standard at the excitation wavelength, and ηunk and ηstd are the indices of refraction of the sample and standard solutions, respectively.

**Synthesis and Characterization of Compound 1**

**Synthesis:**1-Pyrenecarboxaldehyde (100 mg, 0.44 mmol) and indole (103 mg, 0.88 mmol) were dissolved in methanol (4 mL). To that mixture, I2 (5 mol%) was added and stirred for 30 min at room temperature. Then a solution of 2,3-dichloro- 5,6-dicyano-1,4-benzoquinone (DDQ; 1 mmol) in methanol (4 mL) was added dropwise to that reaction mixture and stirred overnight at RT. The resulting reaction mixture was filtered, washed thoroughly with CH3CN and then dried. The final compound was obtained as red powder solid. Yield: 120 mg (62%), m.p. 262–265 °C.

**Characterization Data:** 1H NMR (400 MHz, [D6]DMSO): d = 6.1 (d, J=7.2 Hz, 2H), 6.72 (t, J = 16 Hz, 2 H), 7.20 (t, J = 16 Hz, 2H), 7.60 (d, J = 8 Hz, 2H), 8.00 (dd, J = 9.2 Hz, 2H), 8.14–8.16 (m, 2 H), 8.28 (d, J = 7.6 Hz, 1H), 8.40 – 8.52 (m, 4H), 8.72 ppm (s, 1H); 13C NMR (400 MHz, [D6]DMSO): d = 99.0, 116.2, 120.4, 124.0, 124.2, 124.4, 124.6, 125.4, 126.1, 126.5, 127.6, 127.5, 127.8, 128.0, 129.4, 130.7, 131.6, 133.4, 133.8, 142.0, 147.2, 152. 8, 164.2 ppm; IR (KBr): υ = 2204, 1520, 1475, 1410, 1342, 1232, 1192, 1170, 1125, 765 cm-1; HRMS (ESI): m/z calcd for C33H20N2: 445.1707 [M+H]+; found: 445.1701.

**Additional Spectral Data**



**Figure S1.** pH-dependent change in absorbance of compound **1** (10 mM) in different buffered medium.



**Figure S2.** UV-visible spectra of compound **1** (10 mM) in different medium (water and ethanol).



**Figure S3.** Fluorescence spectra of compound **1** (10 mM, λex = 390 nm) in water and Brij-58 (1 mM) micelle.



**Figure S4.** (a) Job’s plot analysis of compound **1** with Hg2+ ion in Brij-58 (1 mM) micelle. (b) Determination of binding constant of compound **1** withHg2+using non-linear one-site total binding model.



**Figure S5.** (a) UV-visible spectra compound **1** (10 mM) in SDS (8 mM) micelle and water. (b) UV-visible spectra compound **1** (10 mM) in CTAB (1.5 mM) micelle and water.



**Figure S6.** Change in absorbance of compound **1** (10 mM) with different metal ions (1.2 equiv.) in SDS micelle (8 mM).



**Figure S7.** Job’s plot analysis of compound **1** with AcO- ion in Brij-58 (1 mM) micelle.



**Figure S8.** Determination of binding constant of Hg2+ with compound **1** + NaOAc (1:1) mixturein Brij-58 micelle(1 mM) using non-linear one-site total binding model.



**Figure S9.** (a) UV-visible spectra of compound **1** (10 mM) with H2PO4- (1.0 equiv.) in Brij-58 micelle (1 mM). (b) UV-visible titration of compound **1** + H2PO4- (10 mM, 1:1) with Hg2+ ions in Brij-58 micelle (1 mM).



**Figure S10.** Change in absorbance of compound **1** with Hg2+ ions in presence of NaOAc (1:1) and NaH2PO4 (1:1) in Brij-58 micelle.



**Figure S11.** 1H-NMR titration of **1** (5 mM) with Hg2+ (0 – 1.5 equiv.) in DMSO-d6 medium (inset shows structure of compound **1** with assigned protons).