

Supporting Information

A fluorescent probe for the selective detection of sulfate ions in water

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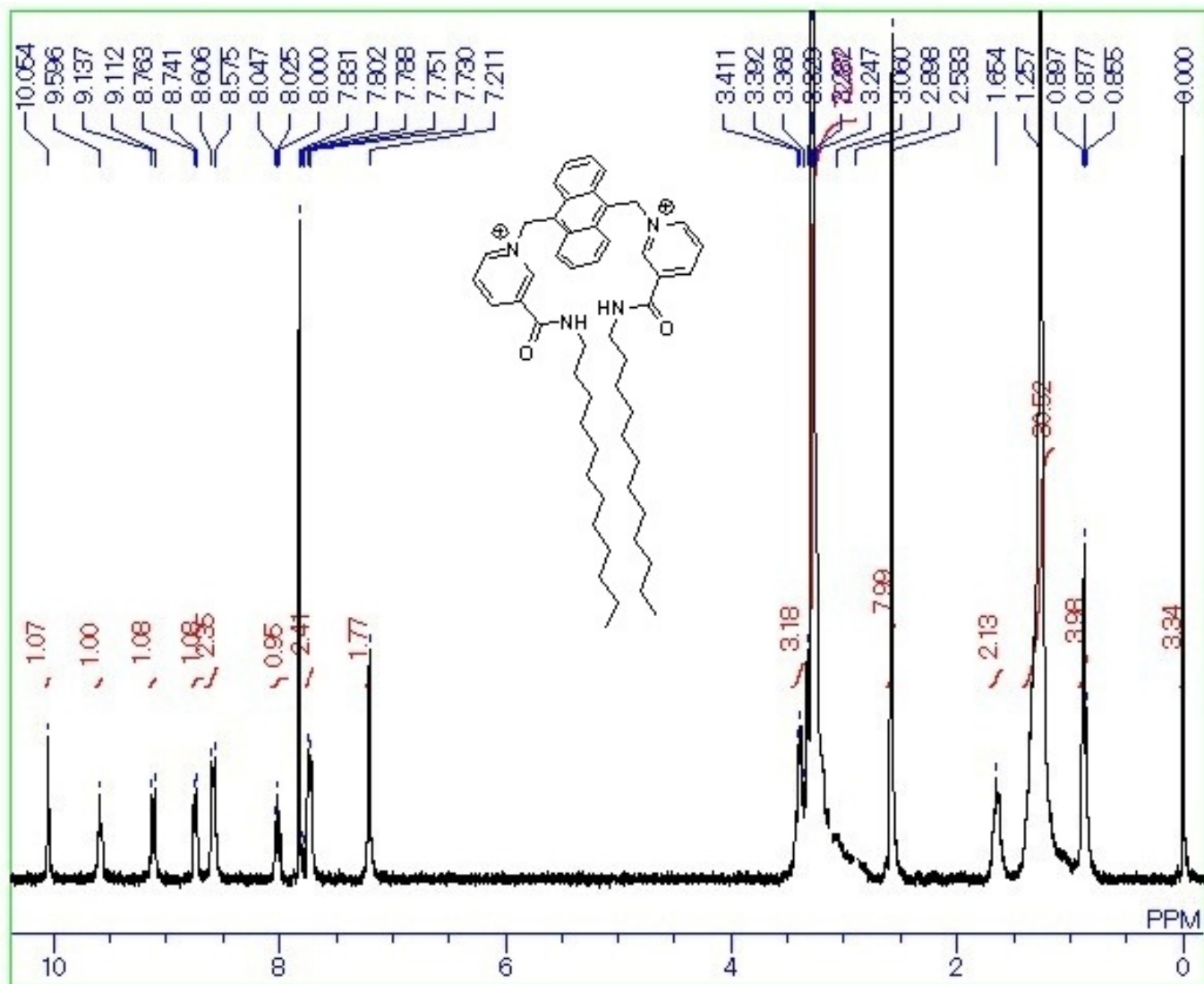


Figure S1. ^1H NMR spectrum of probe 1.

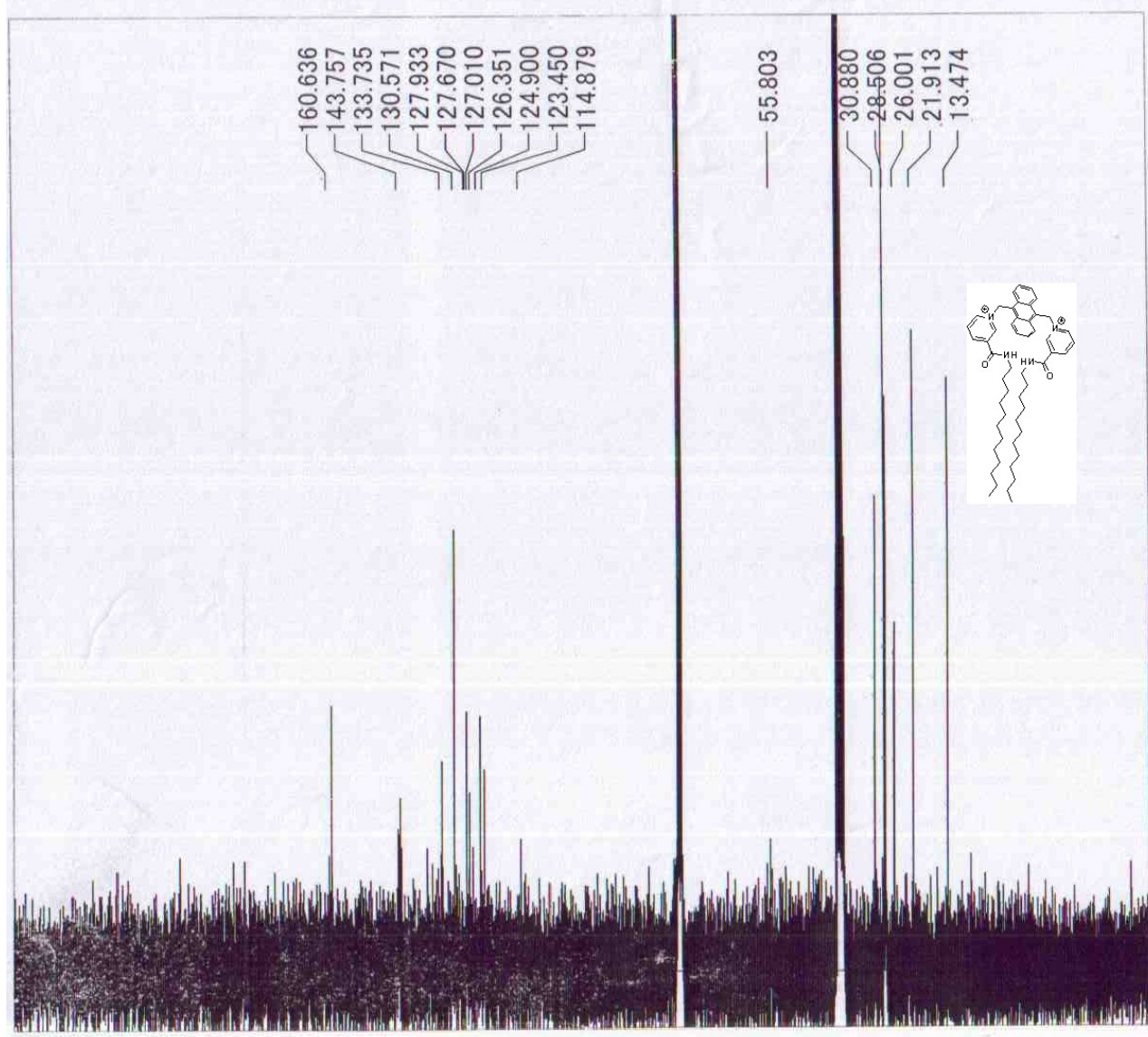


Figure S2. ^{13}C NMR spectrum of probe 1.

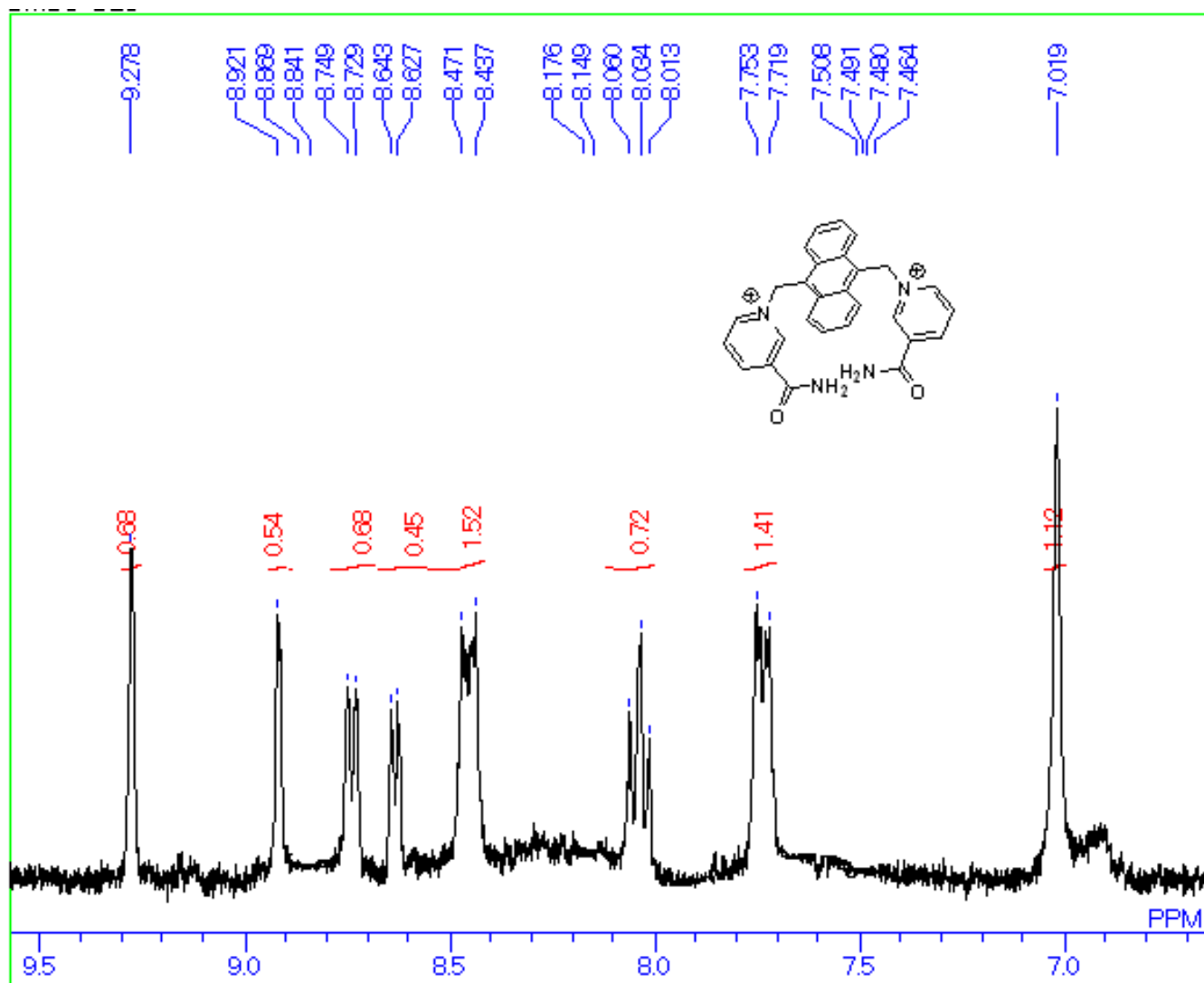


Figure S3. ¹H NMR spectrum of probe 2.

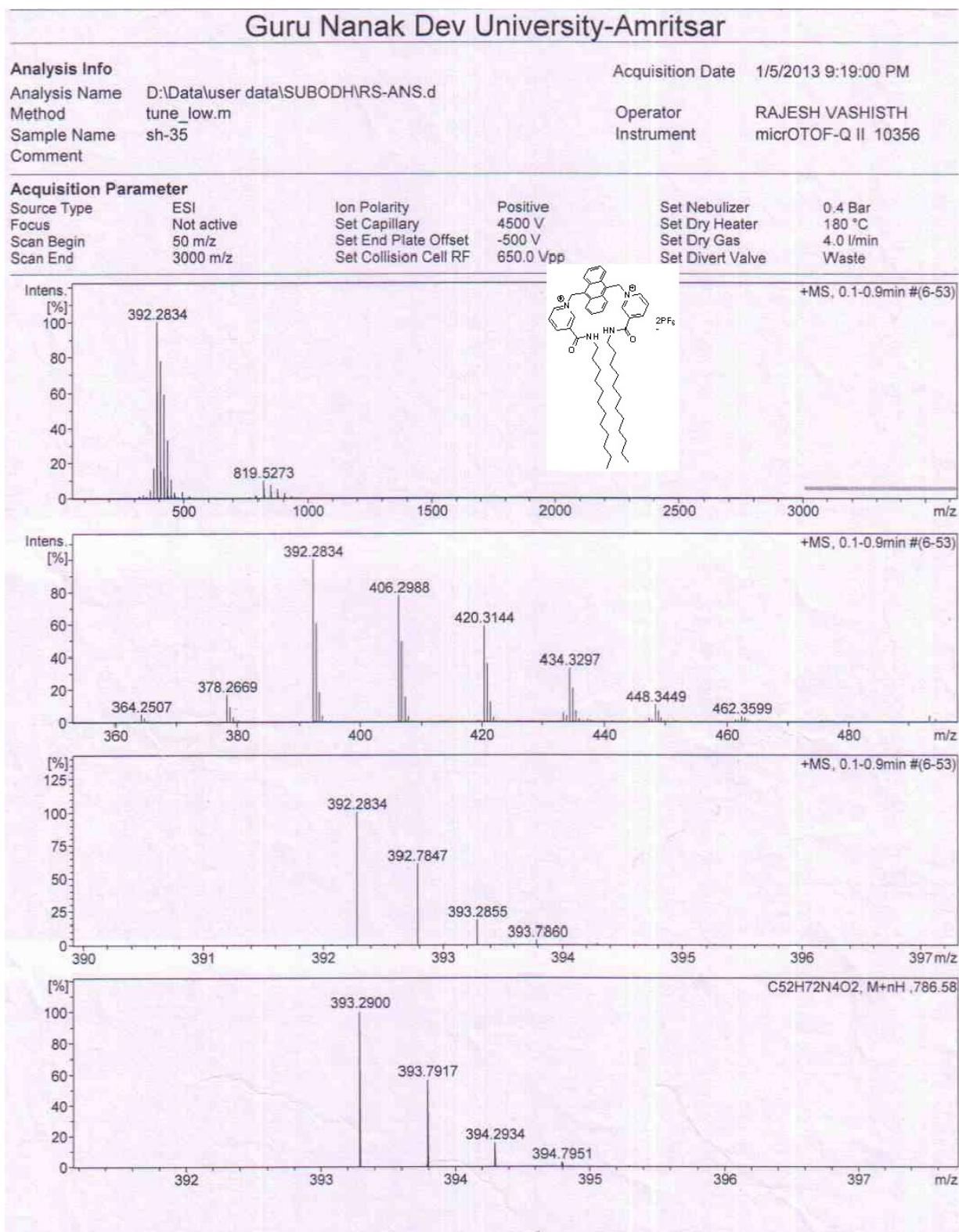


Figure S4. HRMS of probe 1.

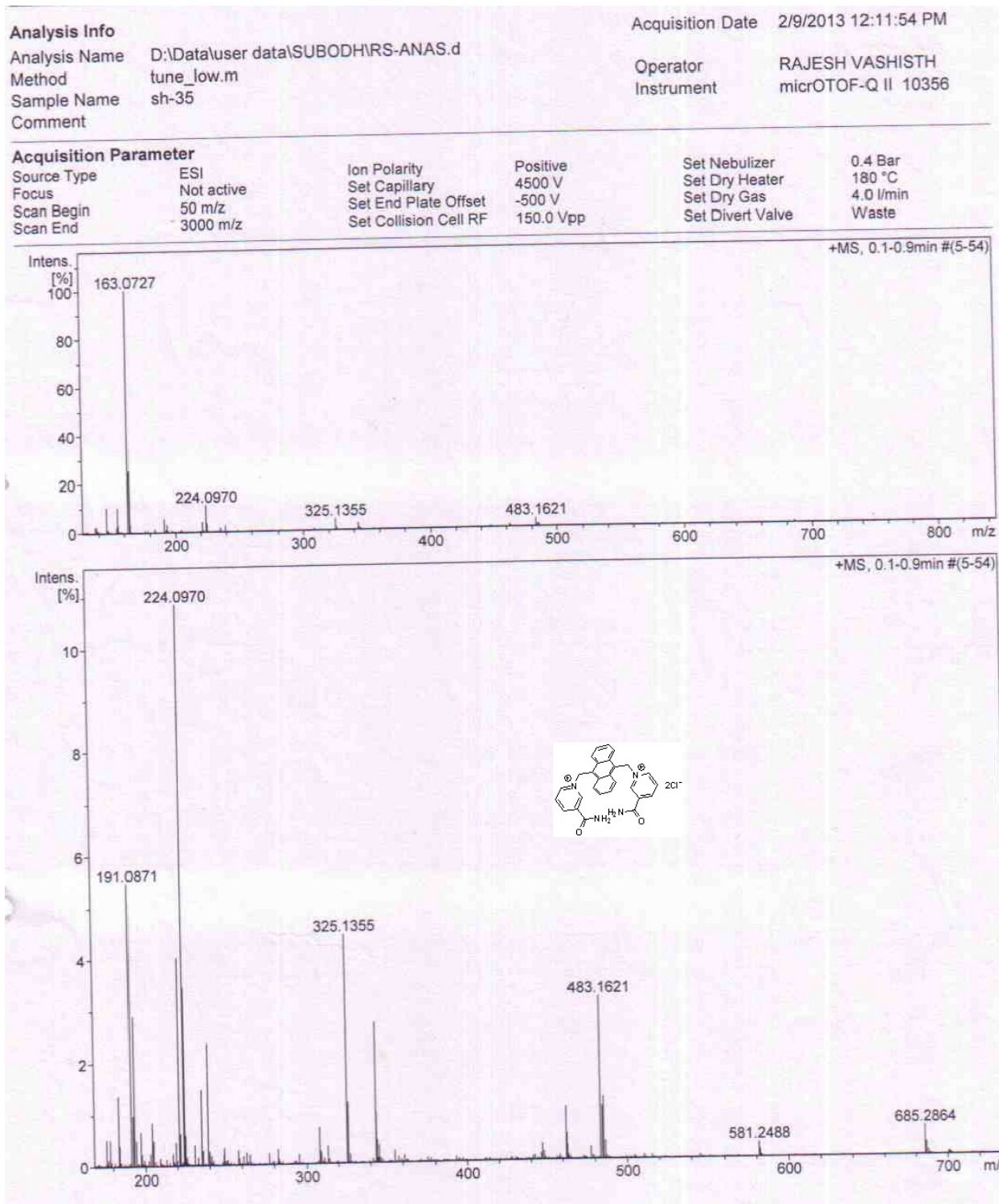


Figure S5. HRMS of probe 2

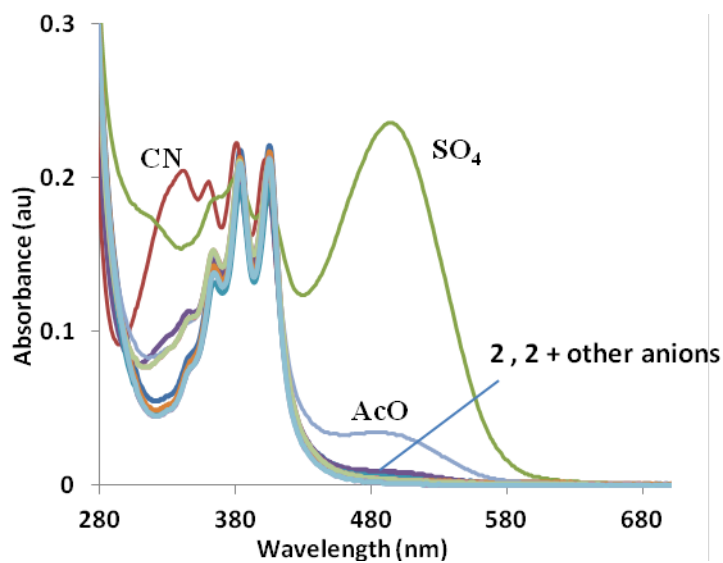


Figure S6: The effect of addition of anions on the UV-Vis spectrum of probe **2** (10 μM, DMSO) (SO₄²⁻ 50 μM, other anions 200 μM)

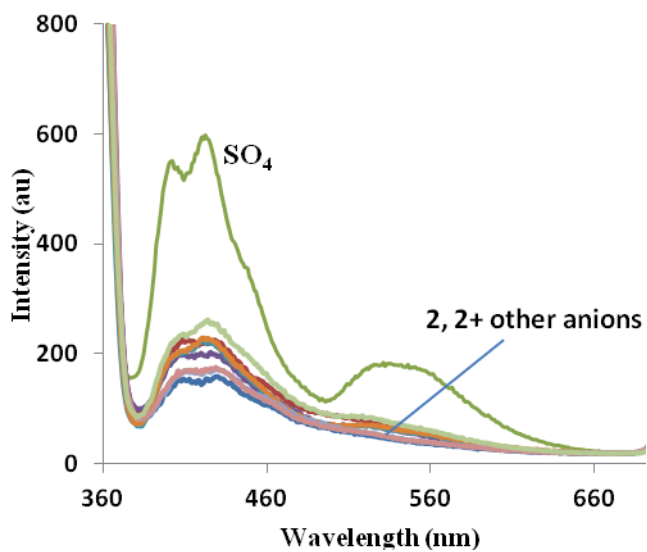


Figure S7:- The effect of addition of anions on the fluorescence spectrum of probe **2** (10 μM, DMSO), λ_{ex} 360 nm. (SO₄²⁻ 50 μM, other anions 200 μM).

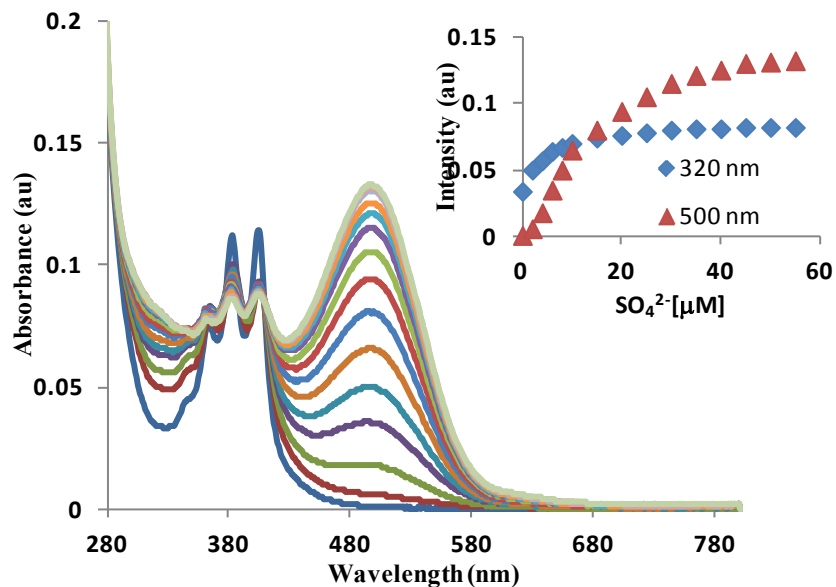


Figure S8:- Change in the UV-Vis spectrum of probe 2 (10 μM , DMSO) upon gradual addition of sulfate ions. Inset shows the change in absorbance intensity at 320 nm and 500 nm with concentration of sulfate ions.

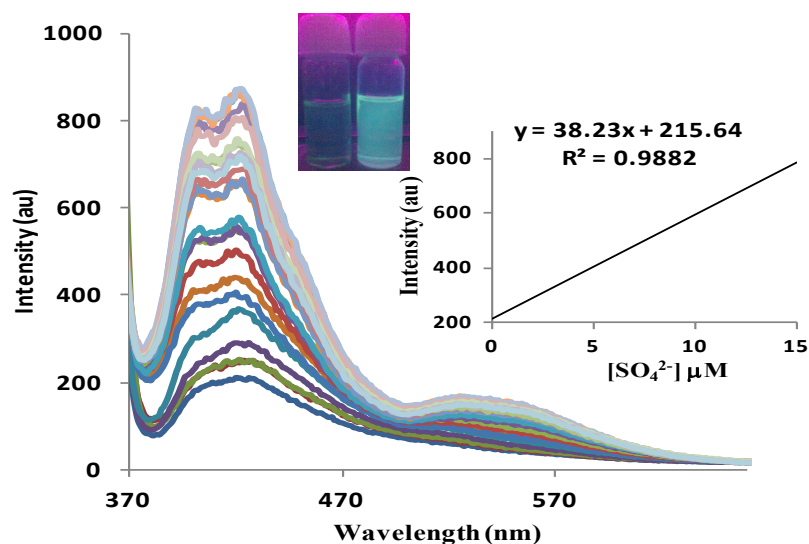


Figure S9:- The change in fluorescence spectrum of probe 1 (10 μM , DMSO) upon gradual addition of sulfate ions. Inset shows the linear increase in fluorescence at 421 nm between 0-15 μM of sulfate ions and the fluorescence color change under illumination at 365 nm.

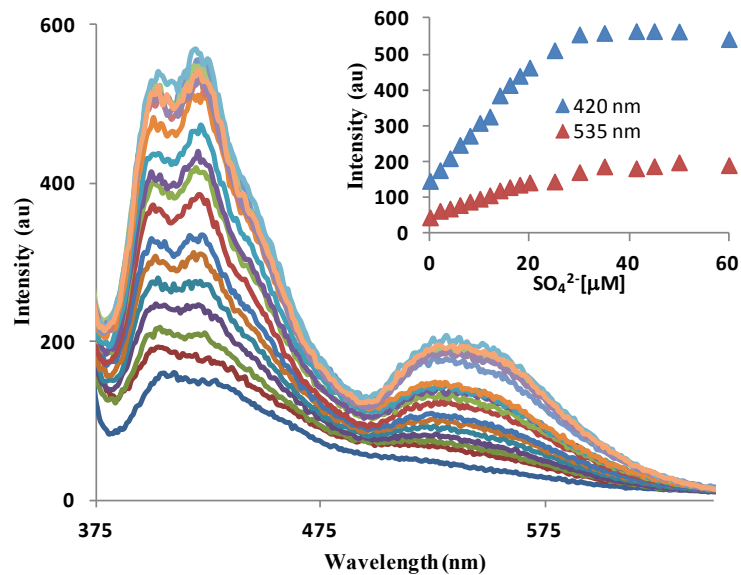


Figure S10:- Change in the fluorescence spectrum of probe **2** (10 μM, DMSO) upon gradual addition of sulfate ions, $\lambda_{\text{ex}} = 360$ nm. Inset shows the change in fluorescence intensity at 420 nm and 535 nm with concentration of sulfate ions.

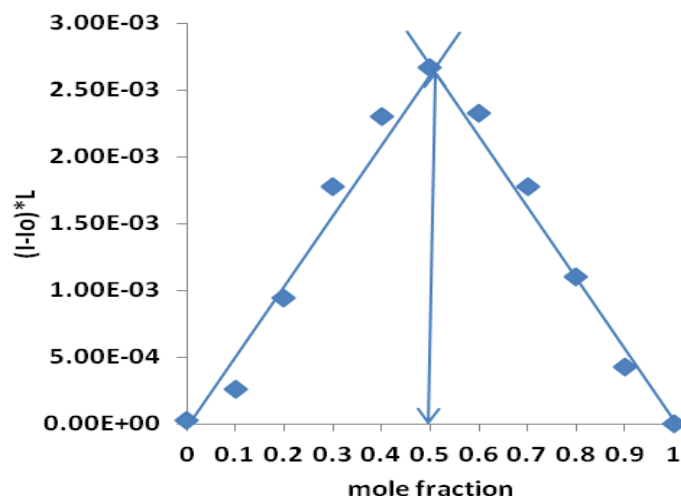


Figure S11: Job's plot points towards 1:1 stoichiometry between probe **1** and sulfate ions in DMSO as determined by fluorescence studies

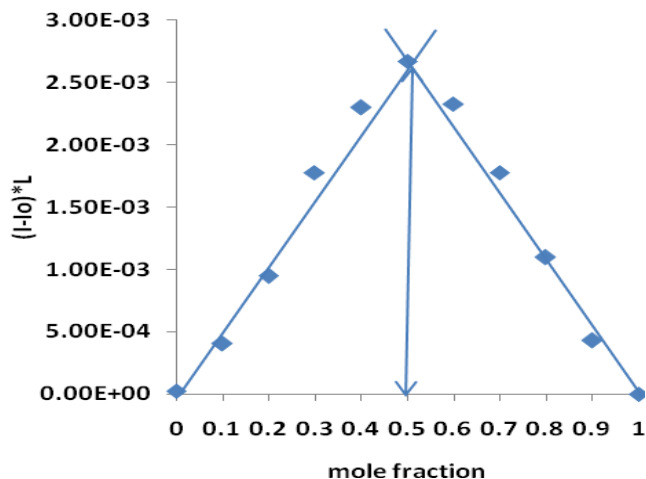


Figure S12. Job's plot pointing towards 1:1 stoichiometry between probe **2** and sulfate ions in DMSO as determined by fluorescence studies

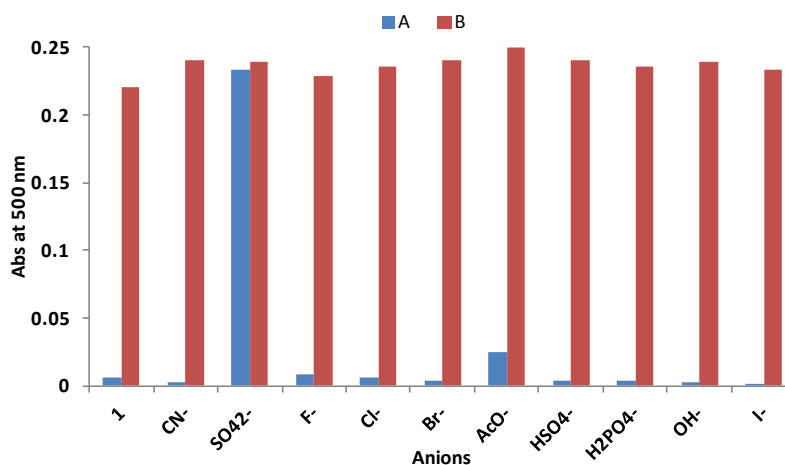


Figure S13. Absorbance response of **1** (10 μ M, DMSO) towards various anions (50 μ M each). Red bars represent selectivity (Abs at 500 nm) of **1** upon addition of different anions; blue bars represent competitive selectivity of **1** towards sulfate ions (50 μ M) in the presence of other anions (200 μ M).

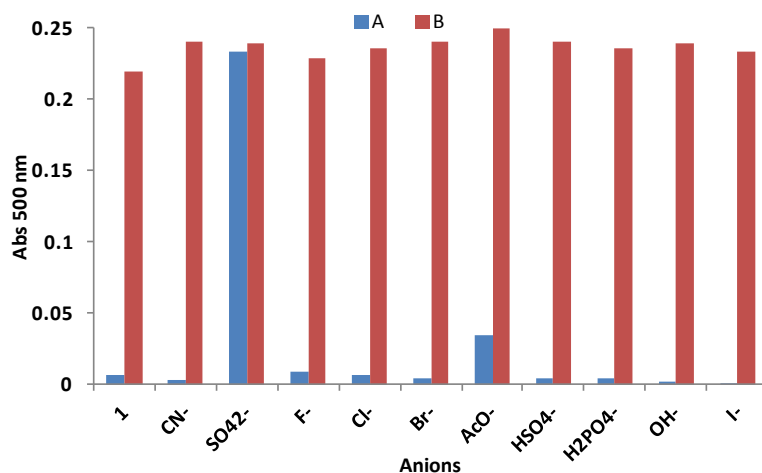


Figure S14. Absorbance response of **2** (10 μ M, DMSO) towards various anions (50 μ M each). Red bars represent selectivity (Abs at 500 nm) of **2** upon addition of different anions; blue bars represent competitive selectivity of **2** toward sulfate ions (50 μ M) in the presence of other anions (50 μ M).

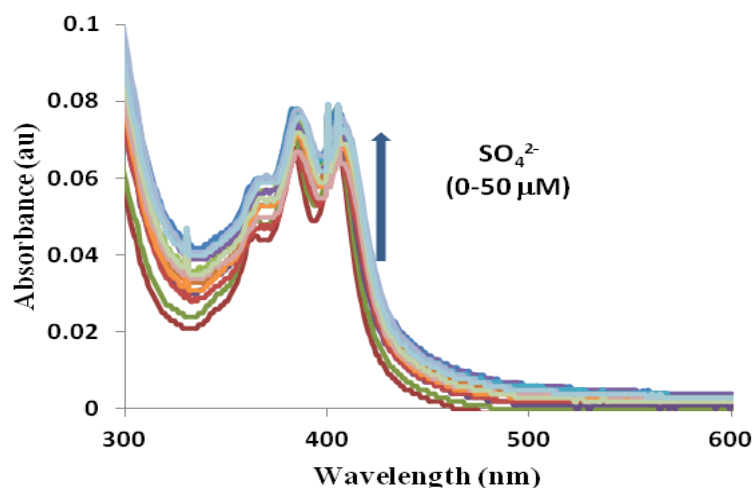


Figure S15: Effect of gradual addition of sodium sulfate on the UV-Vis spectrum of probe **1** (10 μ M, HEPES buffer-DMSO; 9:1, pH = 7.4).

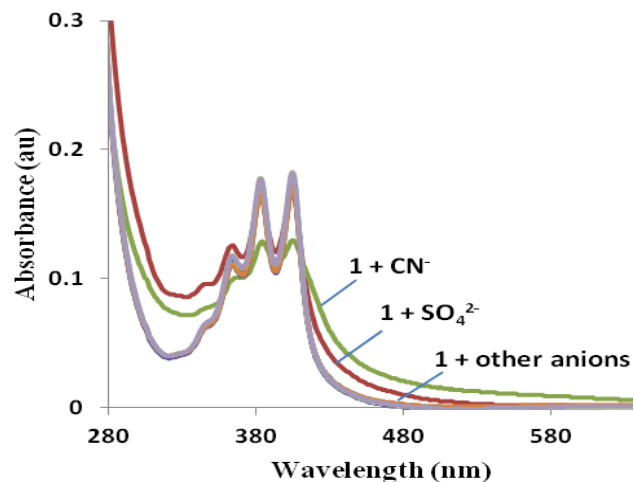


Figure S16. Effect of anions on the UV-Vis spectrum of probe **1** (10 μM, HEPES buffer – DMSO; 9:1, pH = 7.4).

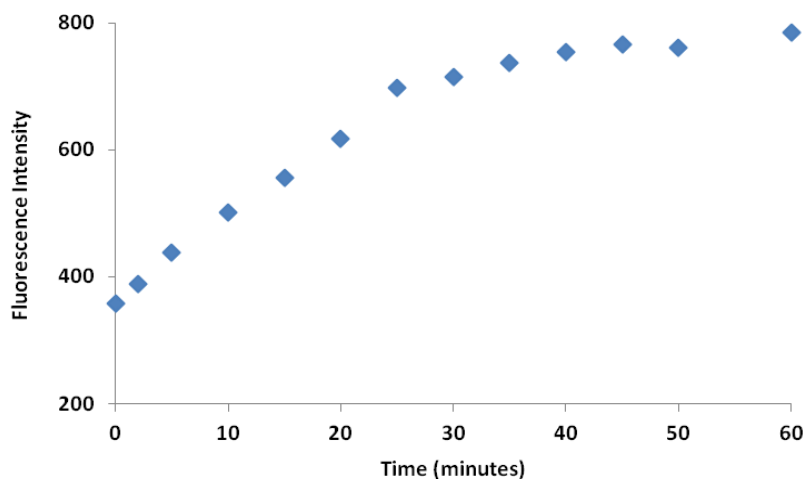


Figure S17:- Kinetic studies of the **1**-SO₄²⁻ (5 eq.) solution showed the completion of the fluorescence enhancement within 30 minutes.

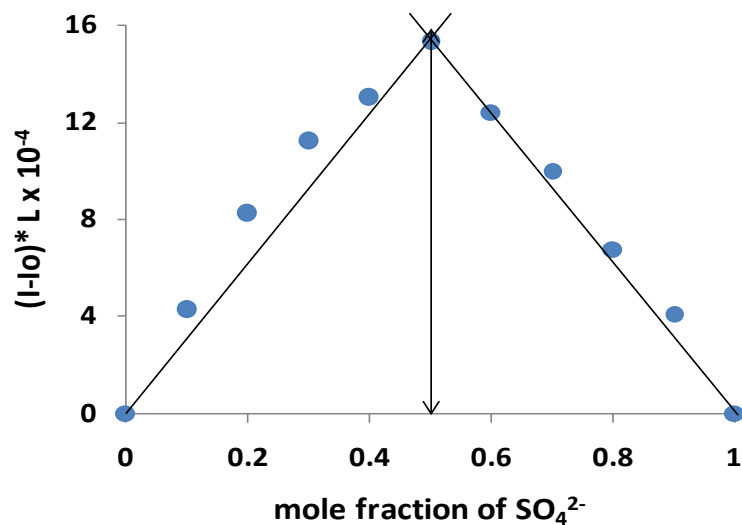


Figure S18: Job's plot pointing to 1:1 stoichiometry between probe **1** and sulfate ions.

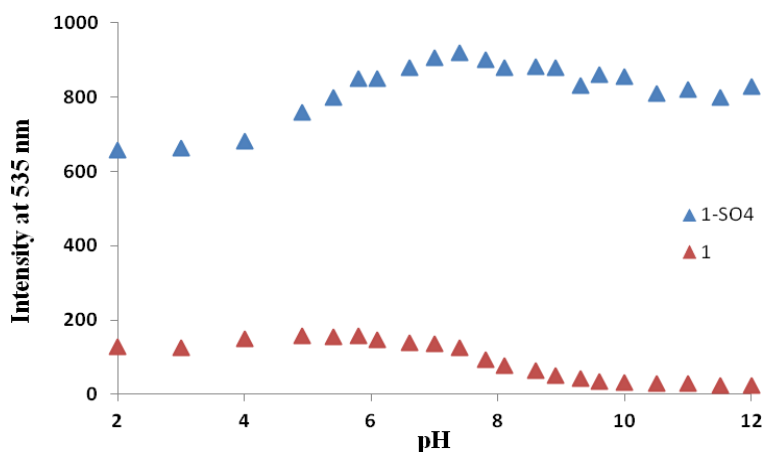


Figure S19- The effect of pH on the fluorescence intensity at 535 nm of both probe **1** and its complex with sulfate ions in 90 % aqueous-DMSO solution.

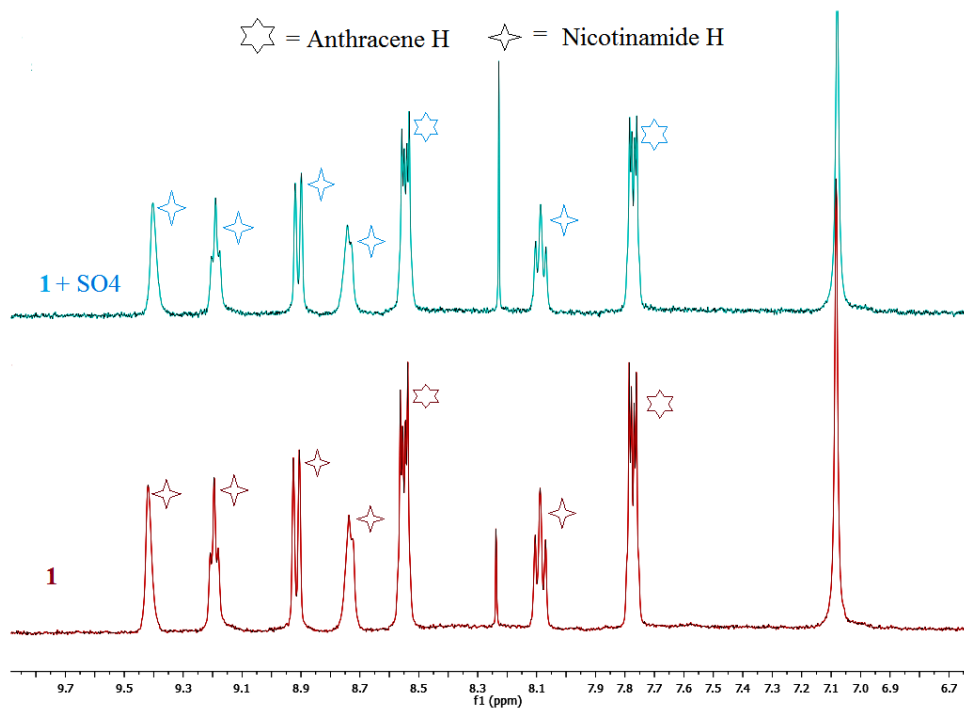


Figure S20. ^1H NMR spectrum of probe **1** before and after the addition of 1 eq. of Na_2SO_4 in DMSO- d_6 - H_2O (8:2).

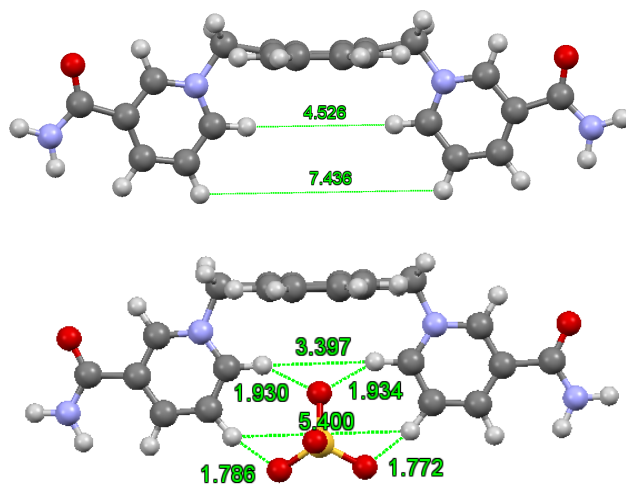


Figure S21. The optimized structures of probe **2** and its complex with sulfate ion at B3LYP-3-21G* level.