Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Cationic Red-Emitting Probes for the Rapid and Selective Detection of SO_2 Derivatives in Aqueous and Cellular Environment

Palash Jana[#], Nishaben Patel[§], Virupakshi Soppina[§] and Sriram Kanvah[#]*

[#]Department of Chemistry and [§]Department of Biological Engineering, Indian Institute of Technology Gandhinagar, Gandhinagar Palaj-382355

*sriram@iitgn.ac.in; [§]vsoppina@iitgn.ac.in

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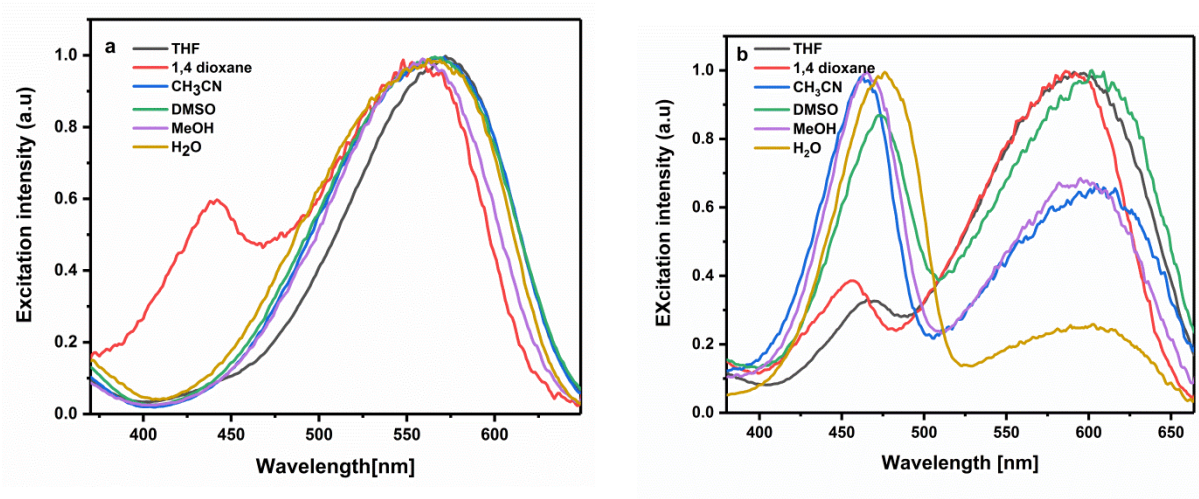

Fig. S1: a) Excitation spectra of compound (**1**) **b**) excitation spectra of compound (**2**)

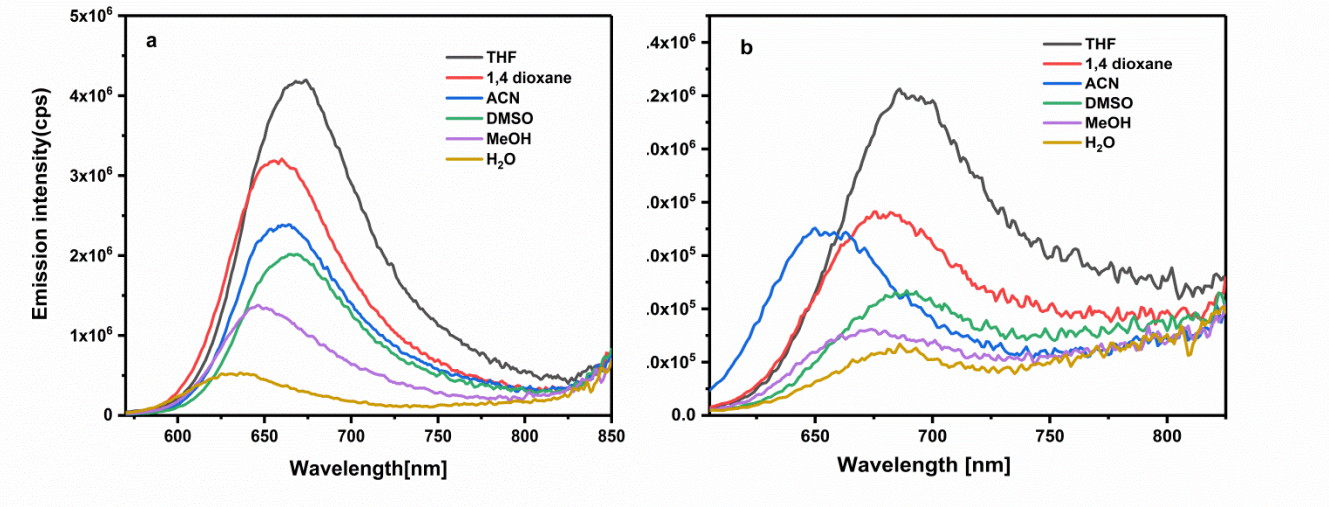

Fig. S2: **a)** Real emission spectra of dye (**1**) **b**) Real emission spectra of dye (**2**)

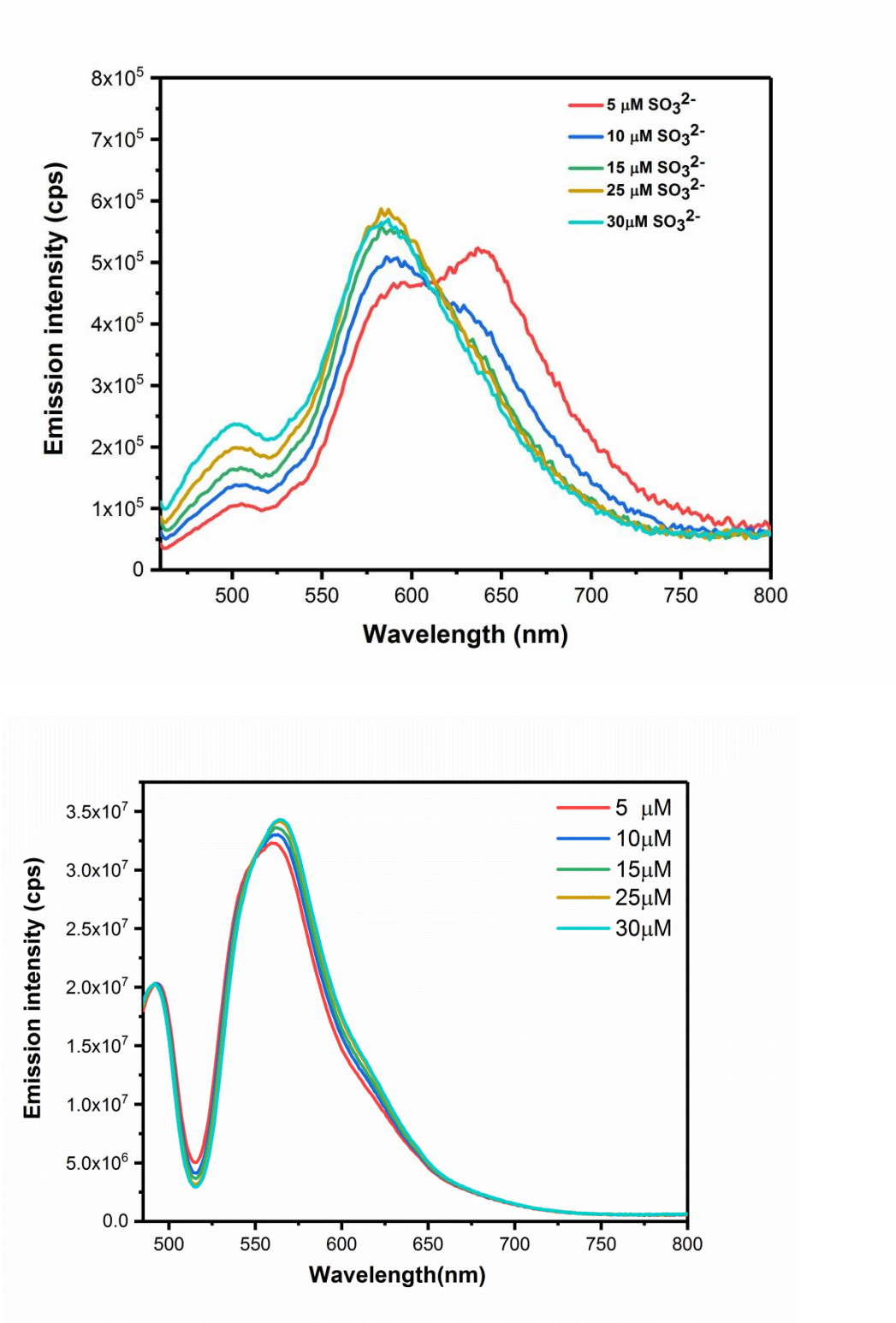

Fig S3: The emission spectra obtained for **1** and **2** upon excitation at isosbestic point (450 nm for **1** and 475 nm for **2**) in the presence of sulfite anion.

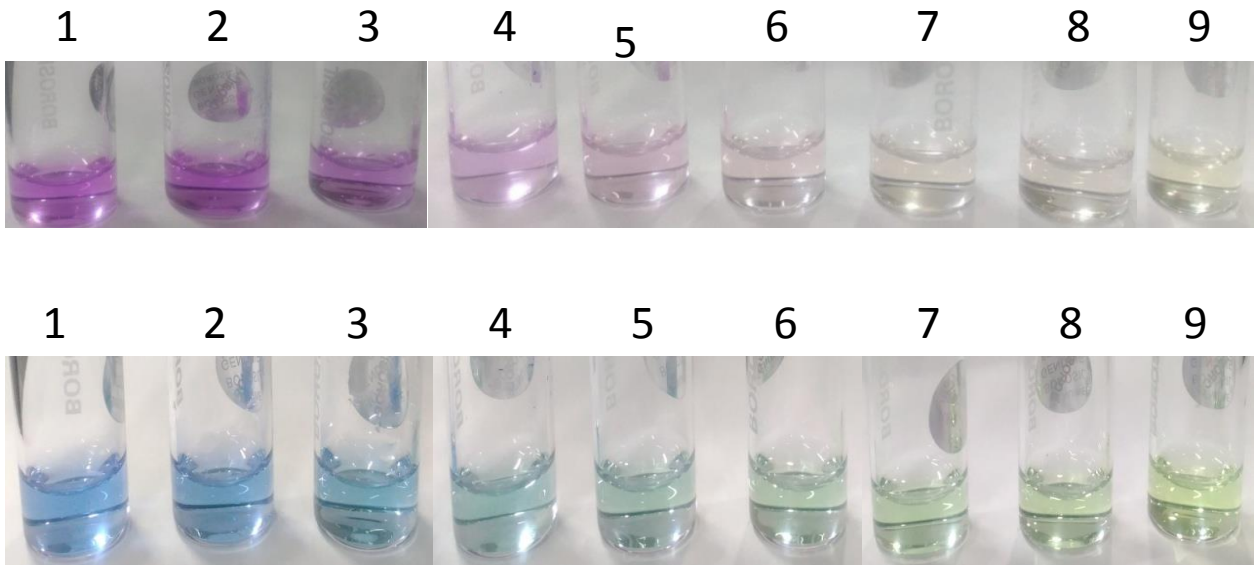

Fig. S4: Visual detection of probes **1** (above panel) and probe (**2**) below panel with the different concentration of SO_3^{2-} anion 1) Blank 2) 5μM; 3) 10 μM ; 4) 15 μM; 5) 20 μM; 6) 25 μM; 7) 30 μM; 8) 35 μM; 9) 40μM

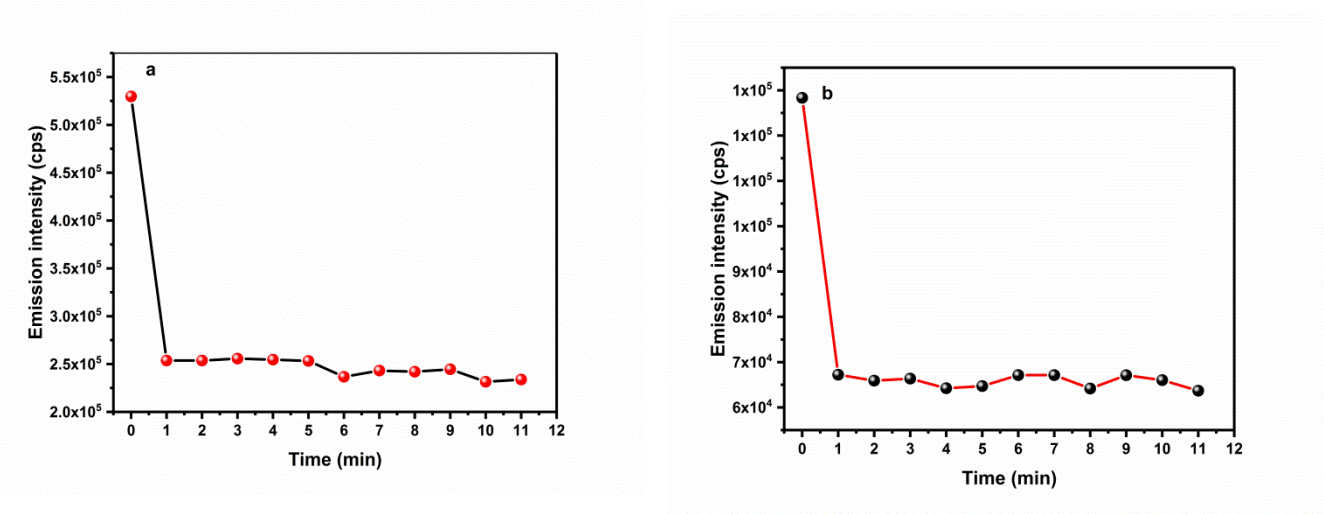

Fig. S5: Kinetic response of **a**) compound **1 & b**) compound **2** in PBS buffer solution (pH = 7.4, 10mM) : Sulfite Concentration: 30µM

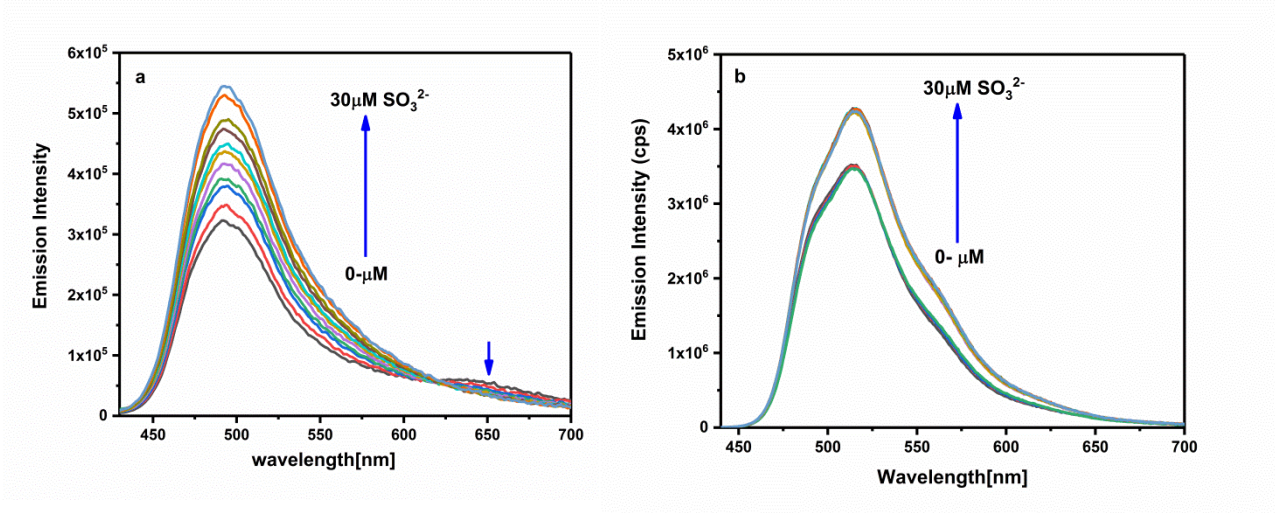

Fig. S6: Fluorescence spectra of **a**) compound **1 b**) compound **2** (10µM) in PBS buffer solution (10mM, pH = 7.4, containing 1% DMSO) with the addition of different concentration of $[SO_3^{2-}]$/µM: 0 (1); 2.85 (2); 5.7 (3); 8.5 (4); 11.4 (5); 14.2 (6); 17.2 (7); 20 (8); 22.8 (9); 25.6 (10); 30 (11). λ_{ex} = 410nm, for compound **1** & λ_{ex} = 430 nm for compound **2**. Each spectrum was recorded after 1 min.

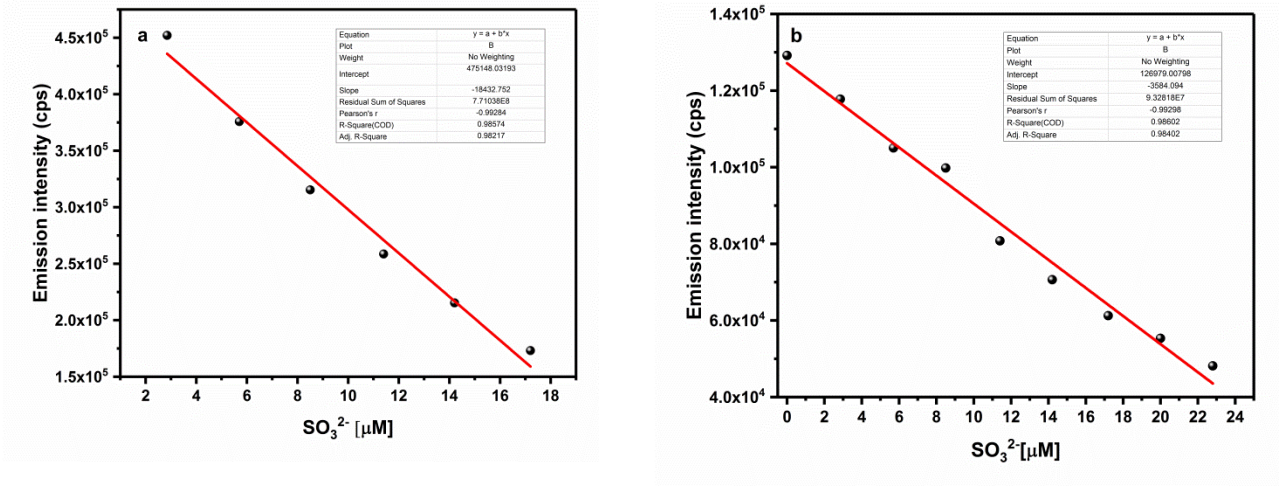

Fig. S7: The relationship between fluorescence intensity of **a**) compound (**1**) [at 647nm] **b**) compound **2** [670nm] and concentration of sulfite from 0-30μM SO_3^{2-} in PBS buffer solution (at pH = 7.4, 10mM). The detection limit for dye **1:** 1.47μM & for dye **2:** 2.8μM

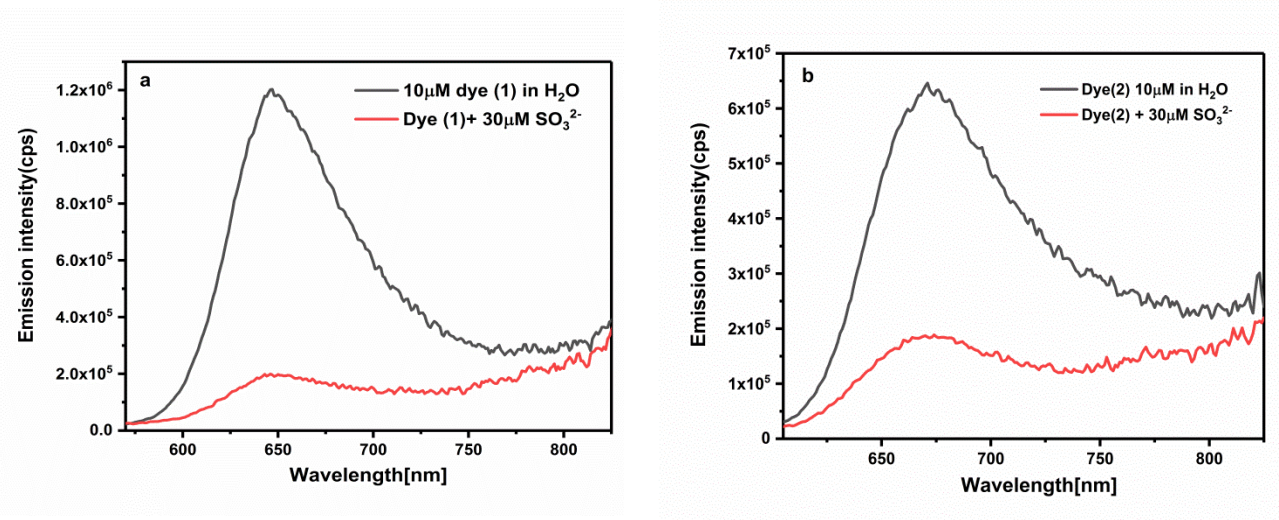

Fig. S8: a) Sulfite detection in H_2O for dye (**1**) b) Sulfite detection in H_2O for dye (**2**)

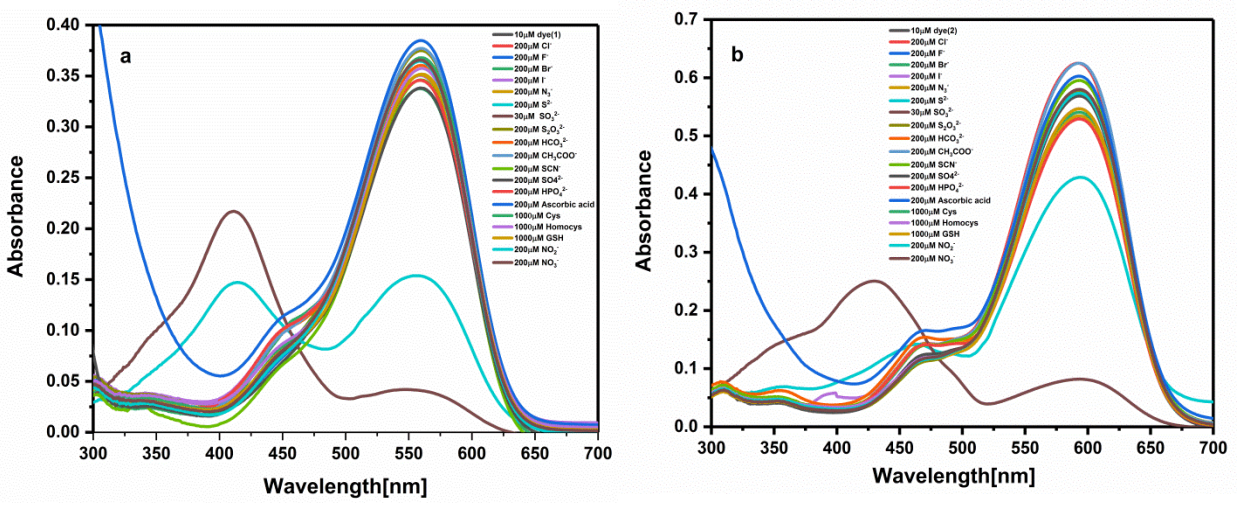

Fig. S9: Absorbance spectra of **a**) compound (**1**) & **b**) compound (**2**) with various analytes in PBS buffer solution (pH = 7.4)

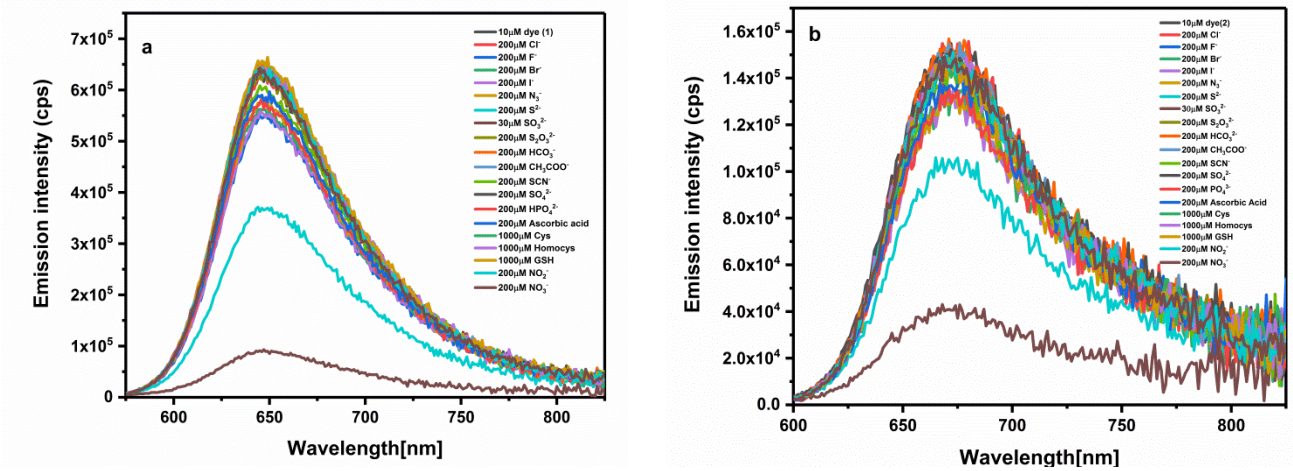

Fig. S10: Fluorescence spectra of **a**) compound **1** & **b**) compound **2** with various analytes in PBS buffer solution (pH = 7.4, 10mM)

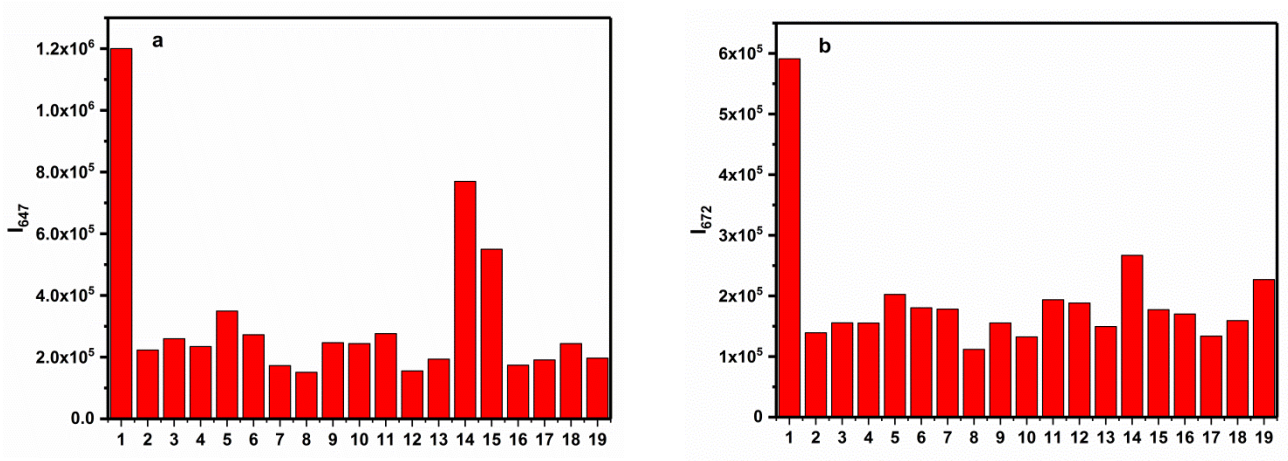

Fig. S11: **Competitive Experiment:** Fluorescence intensity of a) dye **1** measured at 647nm and b) dye **2** measured at 672nm in phosphate buffer solution (10mM, pH = 7.4, containing 1% DMSO) with various analytes. The concentration of secondary analytes used are 200μM (20 equiv unless specified.) and concentration of sulfite used is 30μM SO_3^{2-} (3equiv.): The secondary analytes used are 2) Cl^- 3) F^- 4) Br^- 5) I^- 6) N_3^- 7) S^{2-} 8) $S_2O_3^{2-}$ 9) HCO_3^-10) CH_3COO^- 11) SCN^- 12) SO_4^{2-} 13) HPO_4^{2-} 14) Ascorbic acid 15) Cys (100 equiv.) 16) Homocys (100 equiv.) 17) GSH (100 equiv.) 18) NO_2^- 19) NO_3^- The column (**1**) in each plot corresponds to the free dye **1** and dye **2** [10μM (1equiv.)]

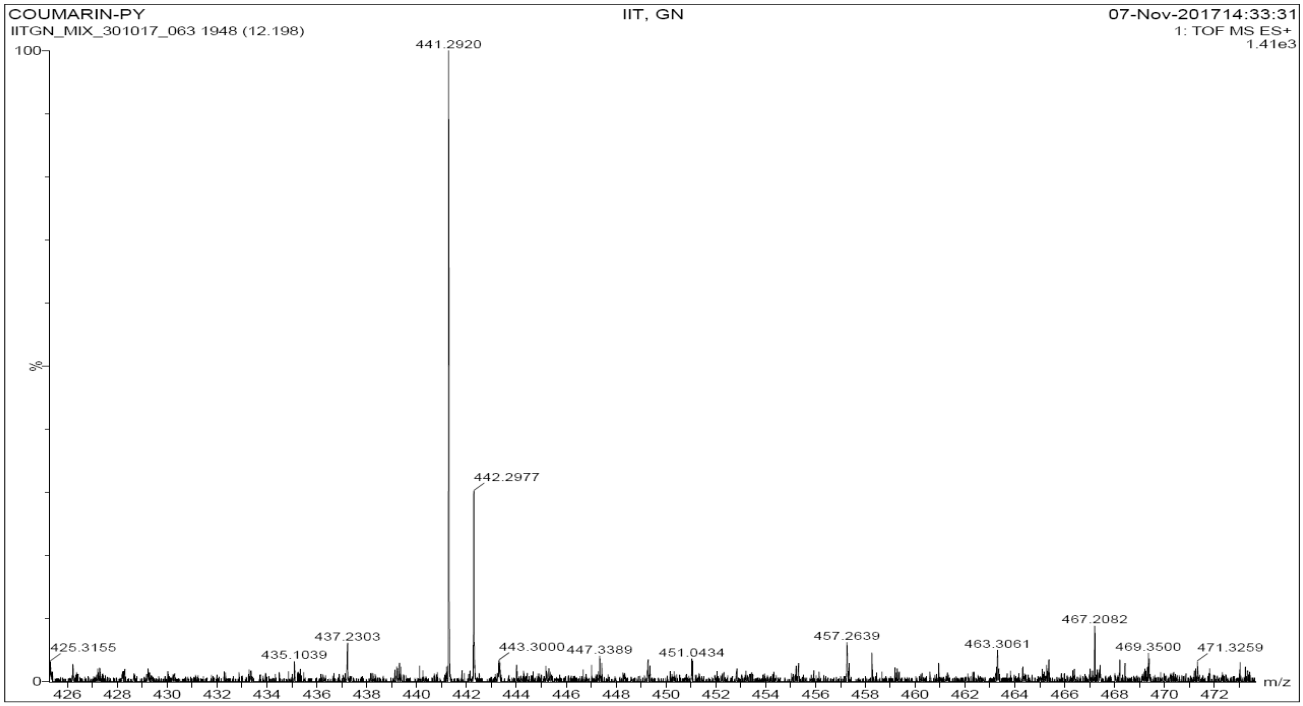

Fig. S12: Mass spectra of compound [**1**-SO_3^-+ H^+]

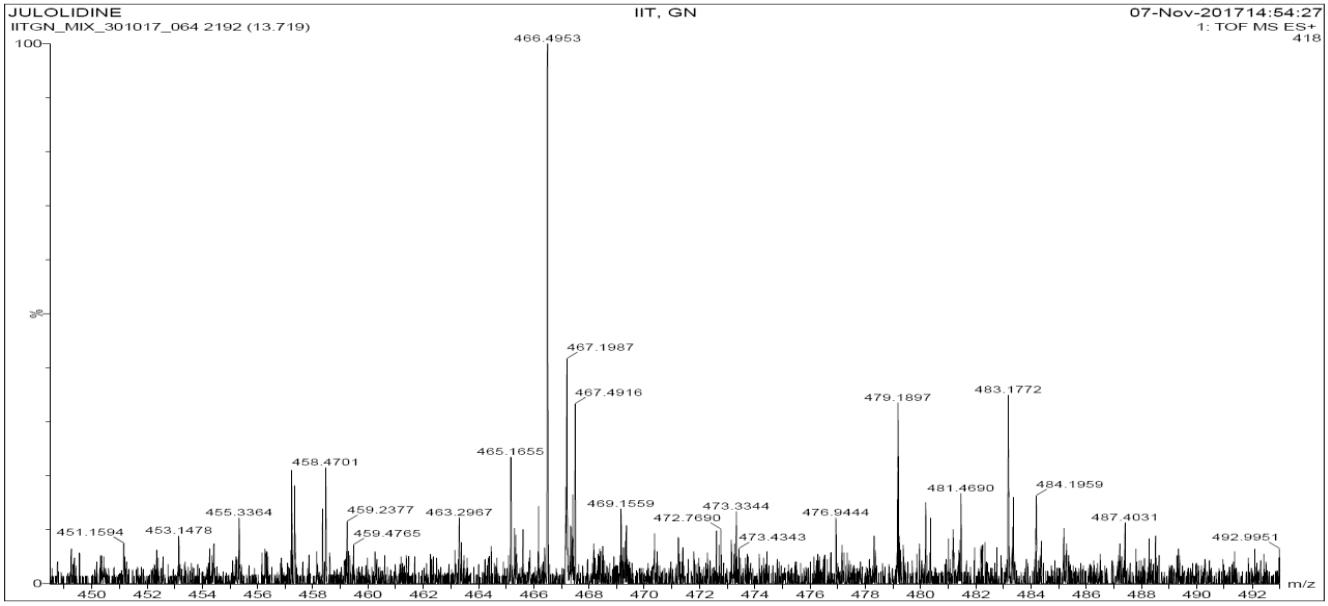

Fig. S13: Mass spectra of compound [**2**-SO_3H + H^+]

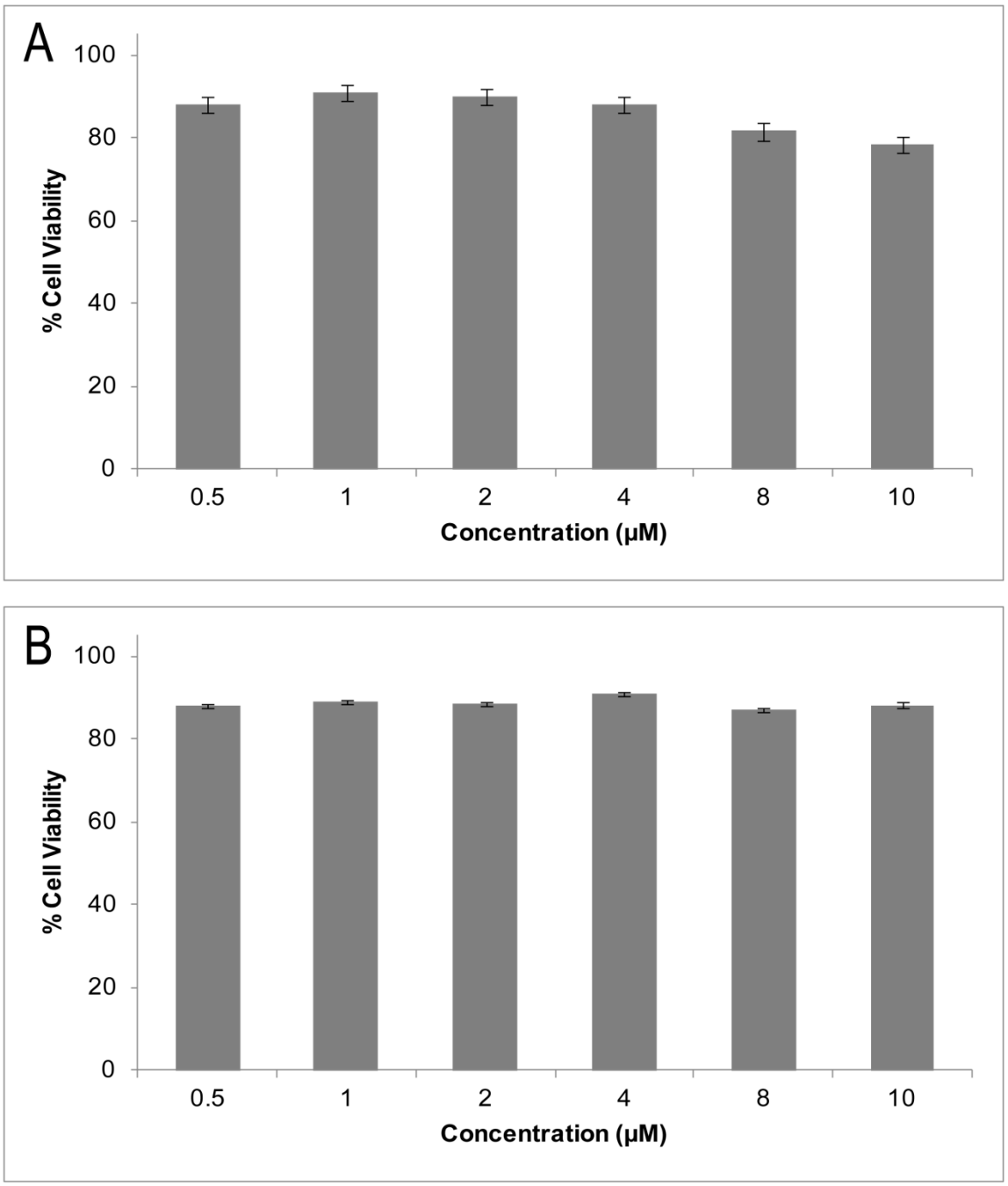

Fig. S14: Standard MTT assays were performed to test cytotoxicity of a) dye **1** and b) dye **2** in HeLa cells. Incubation was for 24 h after treatment. Experiment was performed three times in triplicates.

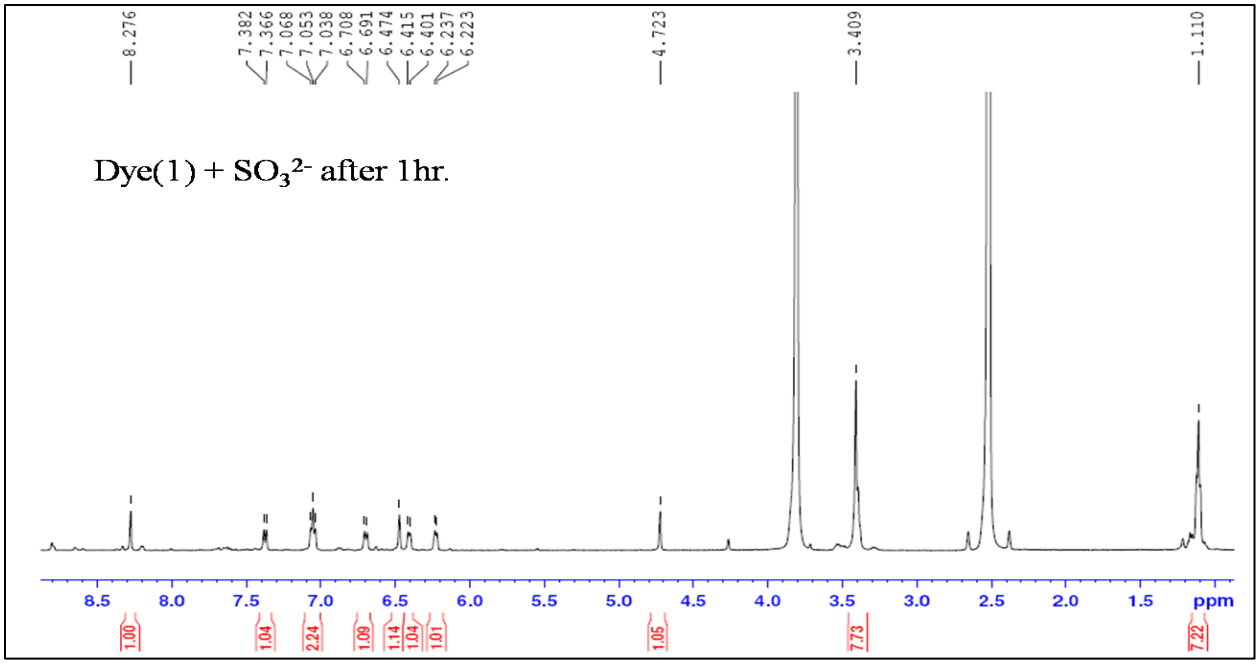

Fig. S15: Time-dependent ^{1}H-NMR spectra of dye) in presence of SO_3^{2-} (DMSO-d_6:D_2O:8:2) [Dye: Na_2SO_3: 1equiv. (1mM) : 3equiv. (3mM)]

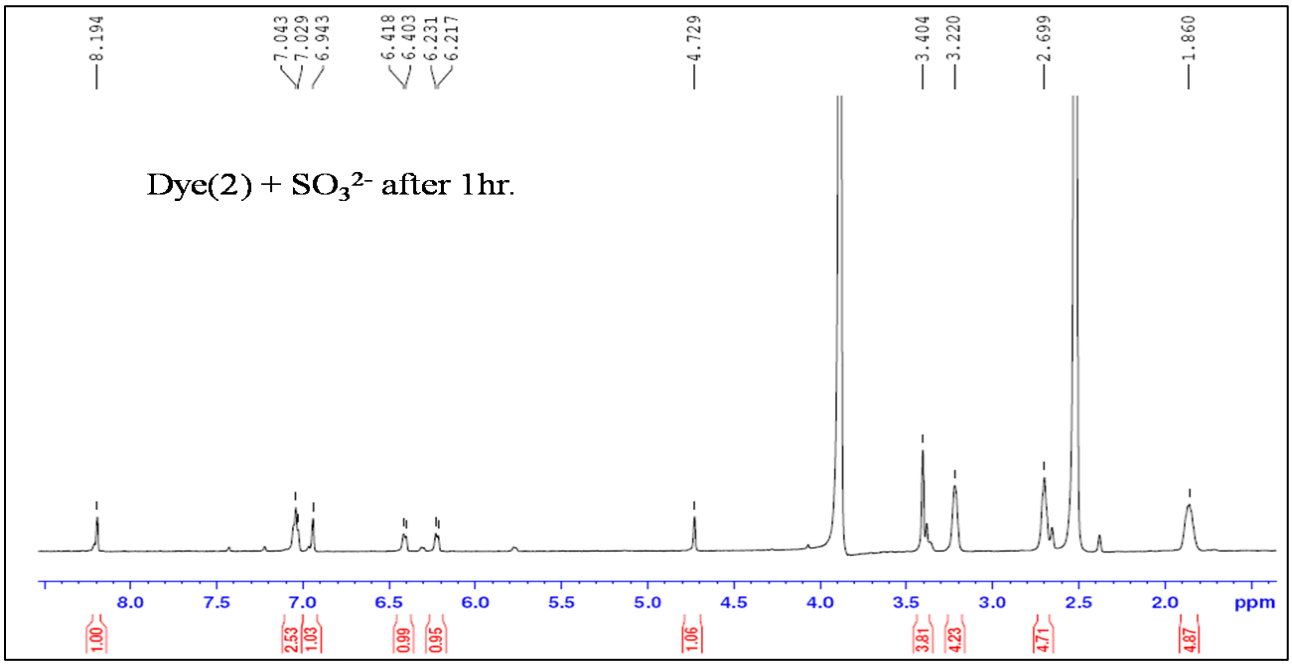

Fig. S16: Time-dependent ^{1}H-NMR spectra of dye **2** in presence of SO_3^{2-} (DMSO-d_6:D_2O:8:2) [Dye: Na_2SO_3: 1equiv. (1mM) : 3equiv (3mM)]

Characterization Data

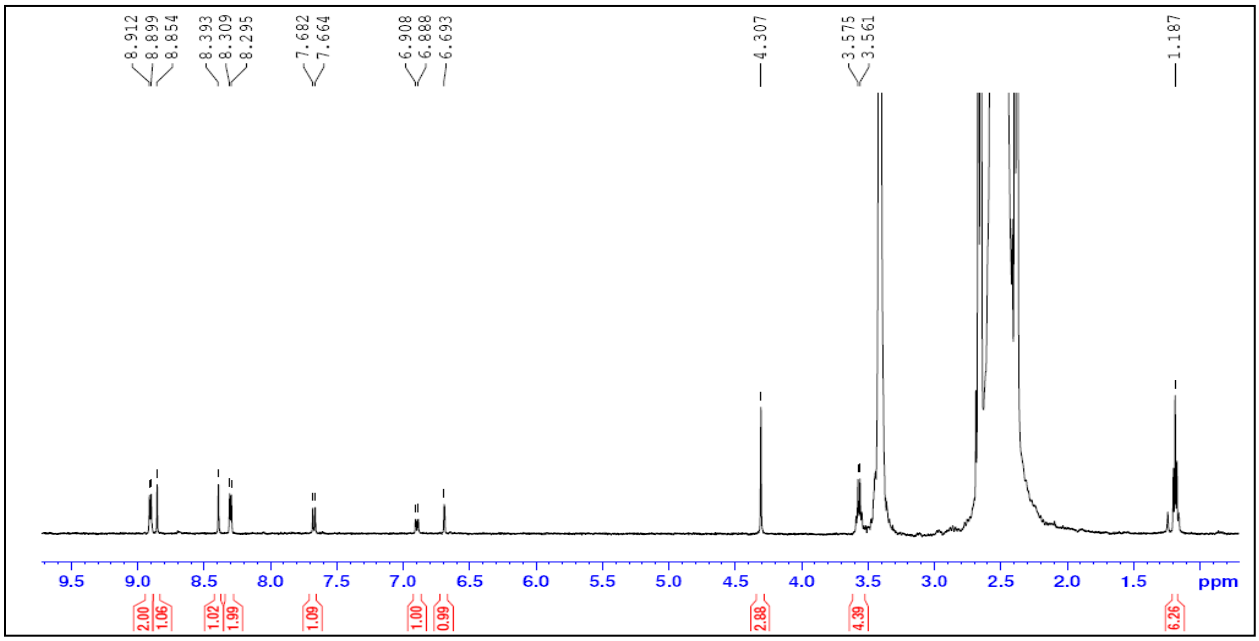

Fig. S17: ^{1}H-NMR spectra of compound **1**

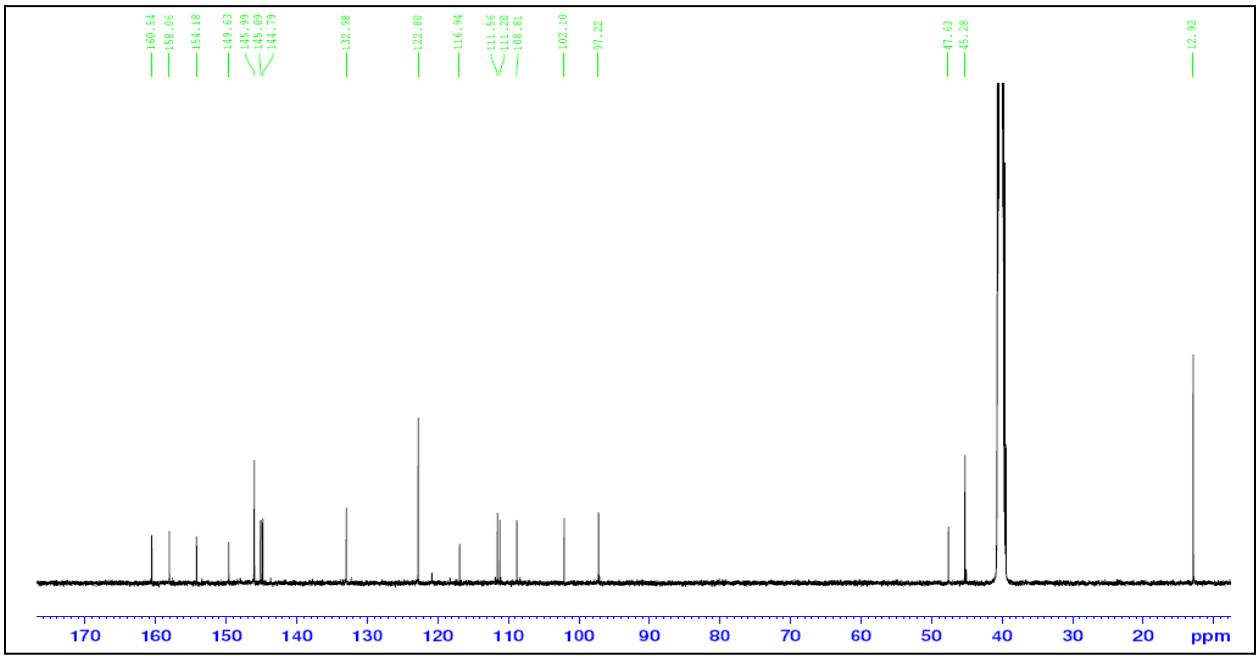

Fig. S18: ^{13}C-NMR spectra of compound **1**

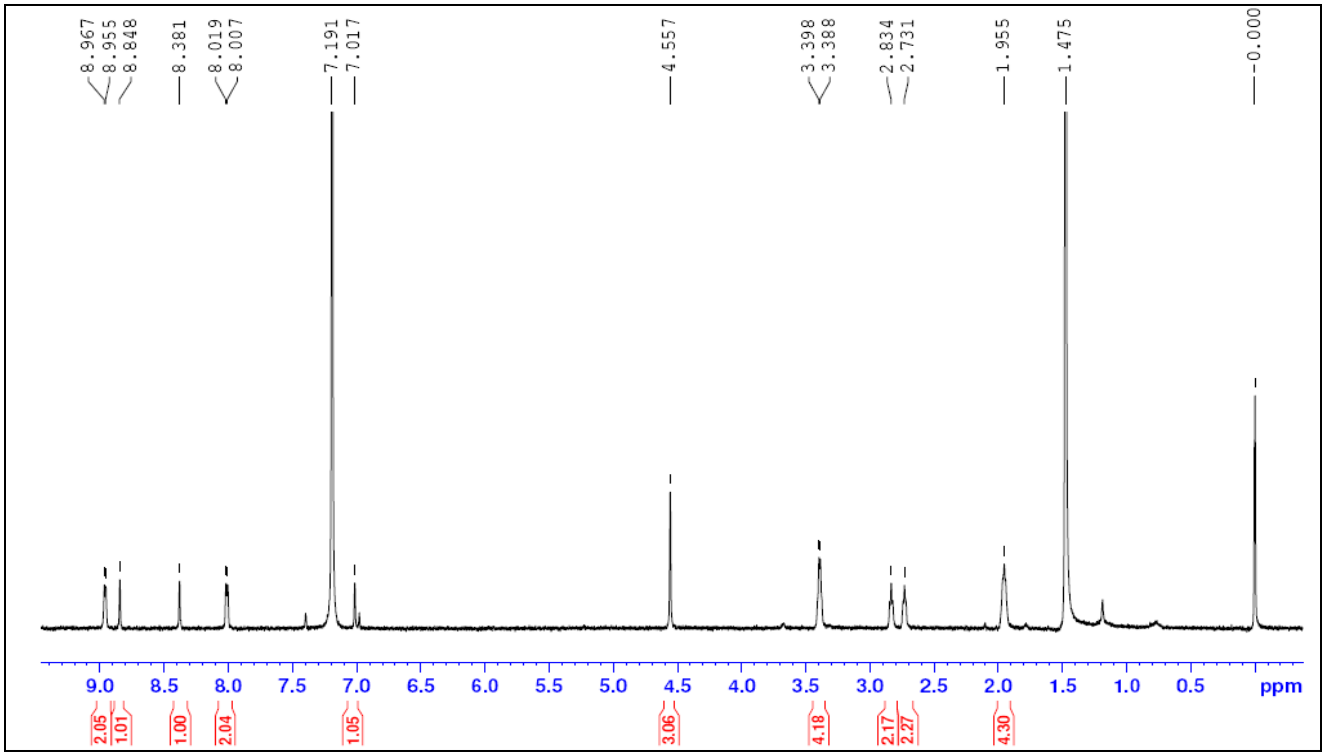

Fig. S19: ^{1}H-NMR spectra of compound **2**

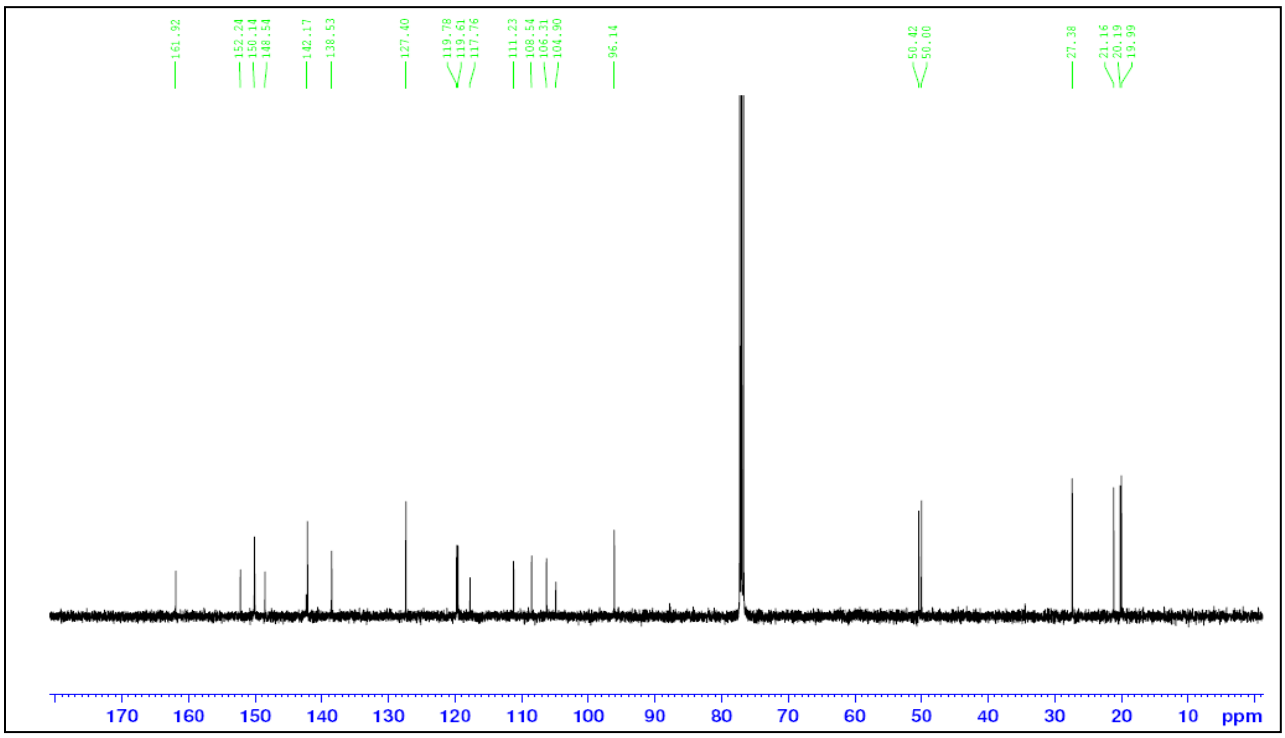

Fig. S20: ^{13}C-NMR spectra of compound **2**

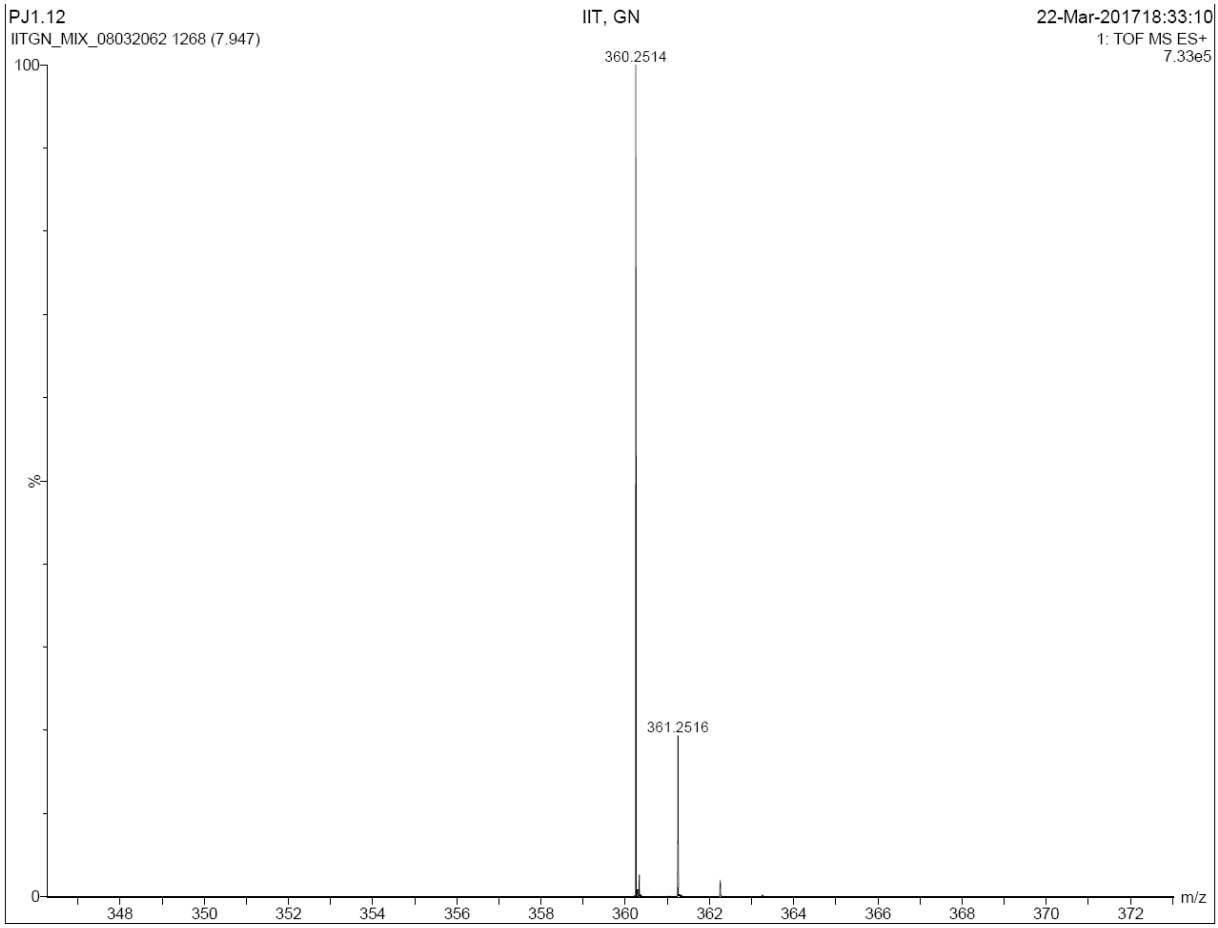

Fig. S21: HRMS spectra of compound **1**

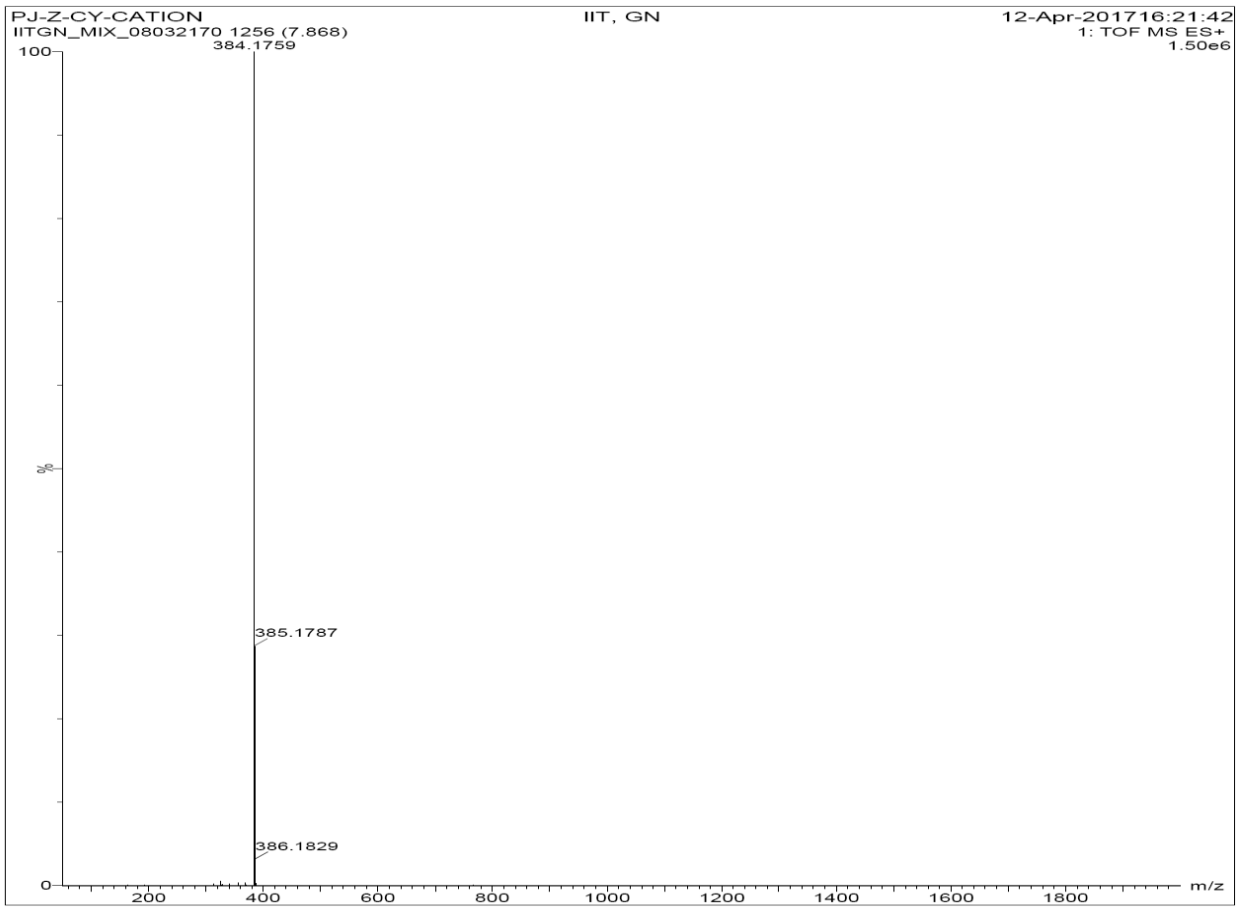

Fig. S22: HRMS spectra of compound (**2**)