Electronic Supplementary Material (ESI) for RSC Advances.

Design and Synthesis of a Rhodol Isomer and Its Derivatives with High Selectivity and Sensitivity for Sensing Hg^{2+} and F^- in Aqueous Media

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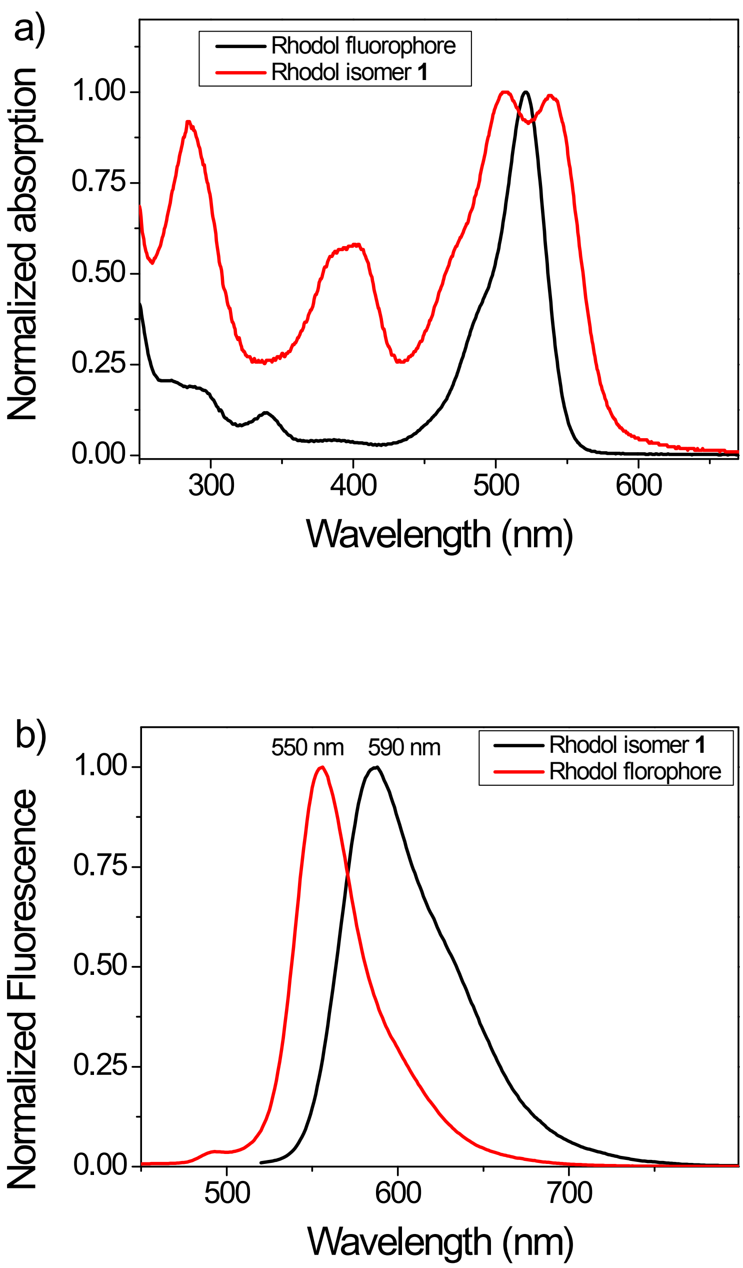

Figure S1. Absorption and fluorescence emission spectra of the rhodol fluorophore and the rhodol isomer 1 in water at pH 7. a) Absorption spectra of the rhodol fluorophore and the rhodol isomer **1**,

b) Fluorescence emission spectra of the rhodol fluorophore and the rhodol isomer **1**.

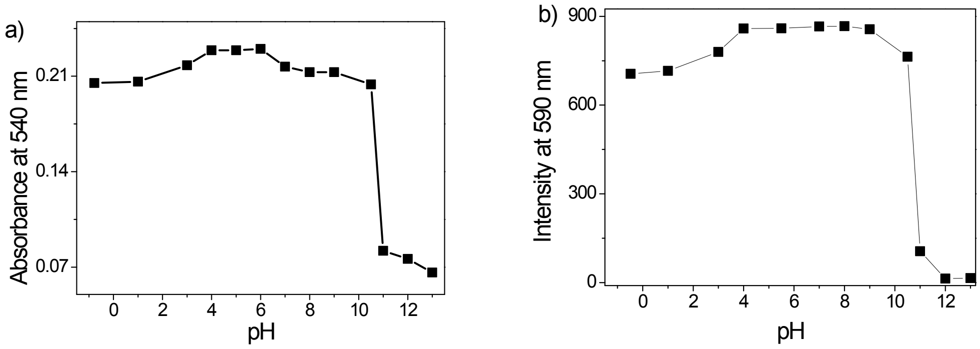

Figure S2. Absorption a) and fluorescence emission b) spectra of the rhodol isomer **1** under different pH conditions in water.

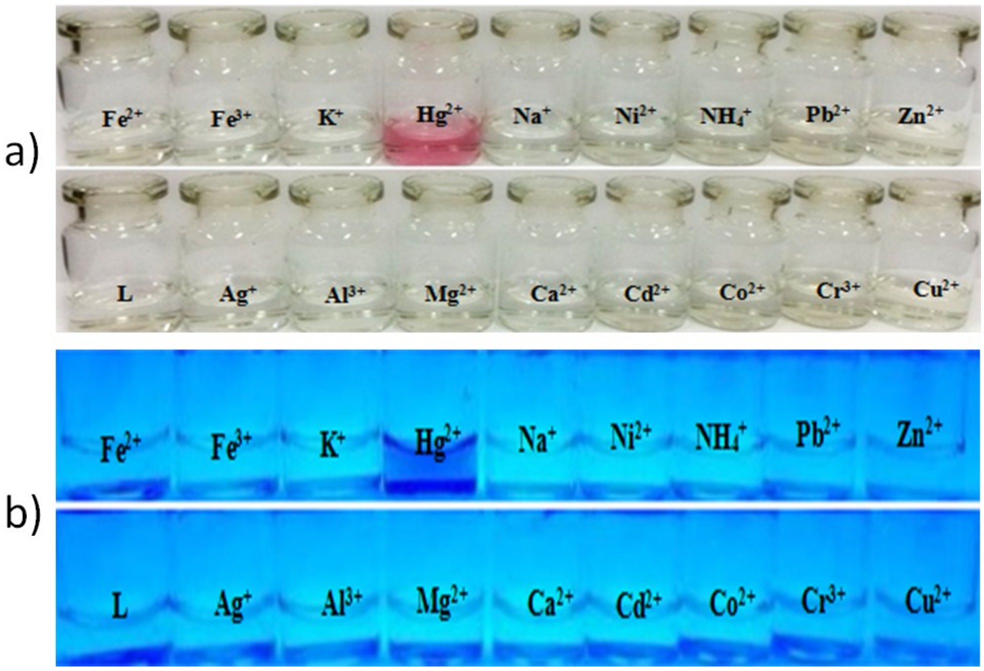

Figure S3. (a) Photograph of 2 in the presence of various metal ions. (b) fluorescence changes of 2 under UV 365 nm excitation in the presence of different metal ions.

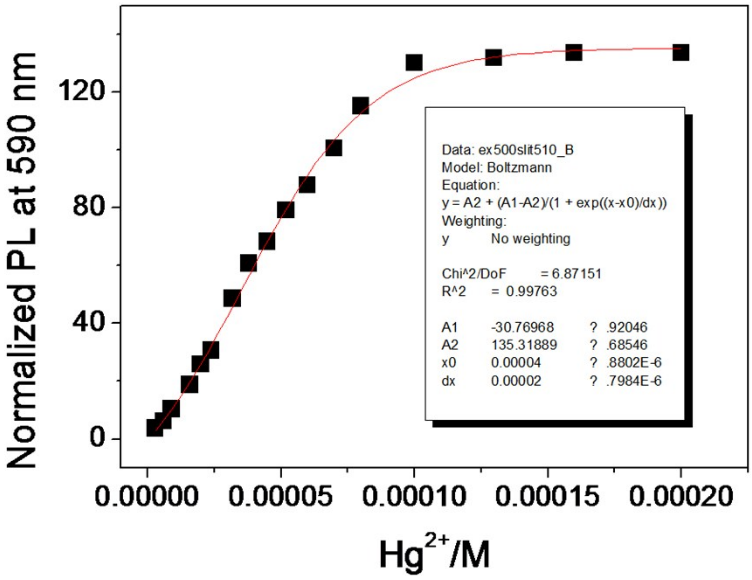

Figure S4. Measurement of the fluorescence turn-on constant ($K_{turn-on}$) of **2**.[S1]

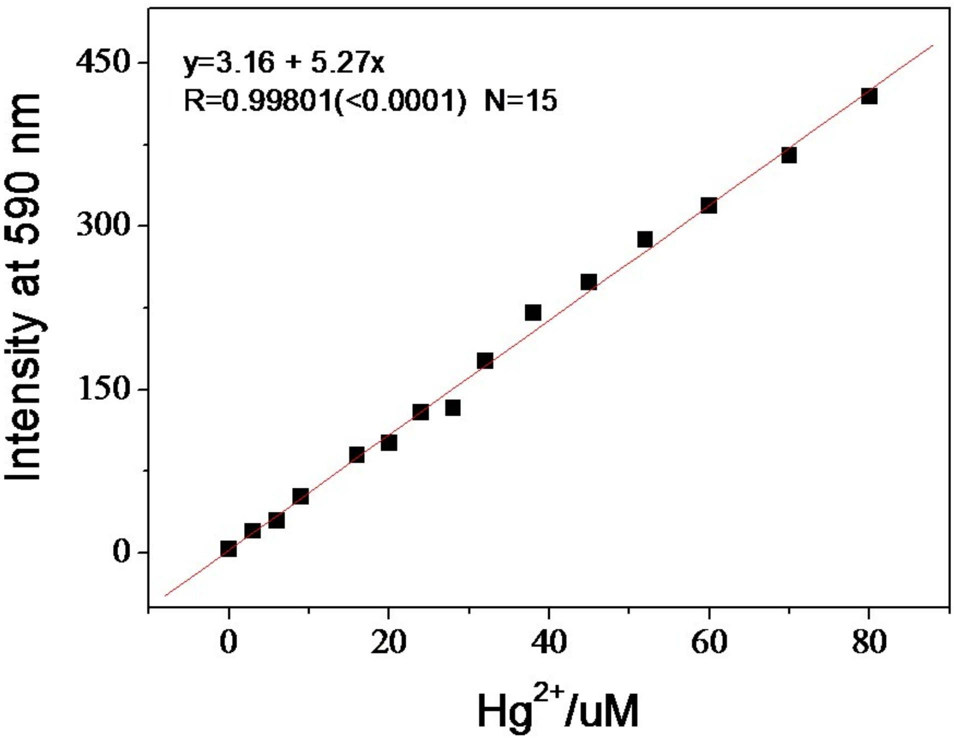

Figure S5 Emission (at 590 nm) of **2** (10 µM) at different concentrations of Hg^{2+} added. A linear relationship between the fluorescence intensity and the Hg^{2+} concentration could be obtained in the 0 - 80 µM concentration range (R = 0.9980). The detection limit was then calculated with the equation: detection limit = 3σbi/m, where σbi is the standard deviation of blank measurements (σbi = 5.8197 $\times 10^{-8}$, derived from 20 measurements), m is the slope between intensity *versus* sample concentration. The detection limit was measured to be 3.31×10^{-9} M.

[S1] P. Du and S. J. Lippard, *Inorg. Chem.*, 2010, **49**, 10753.

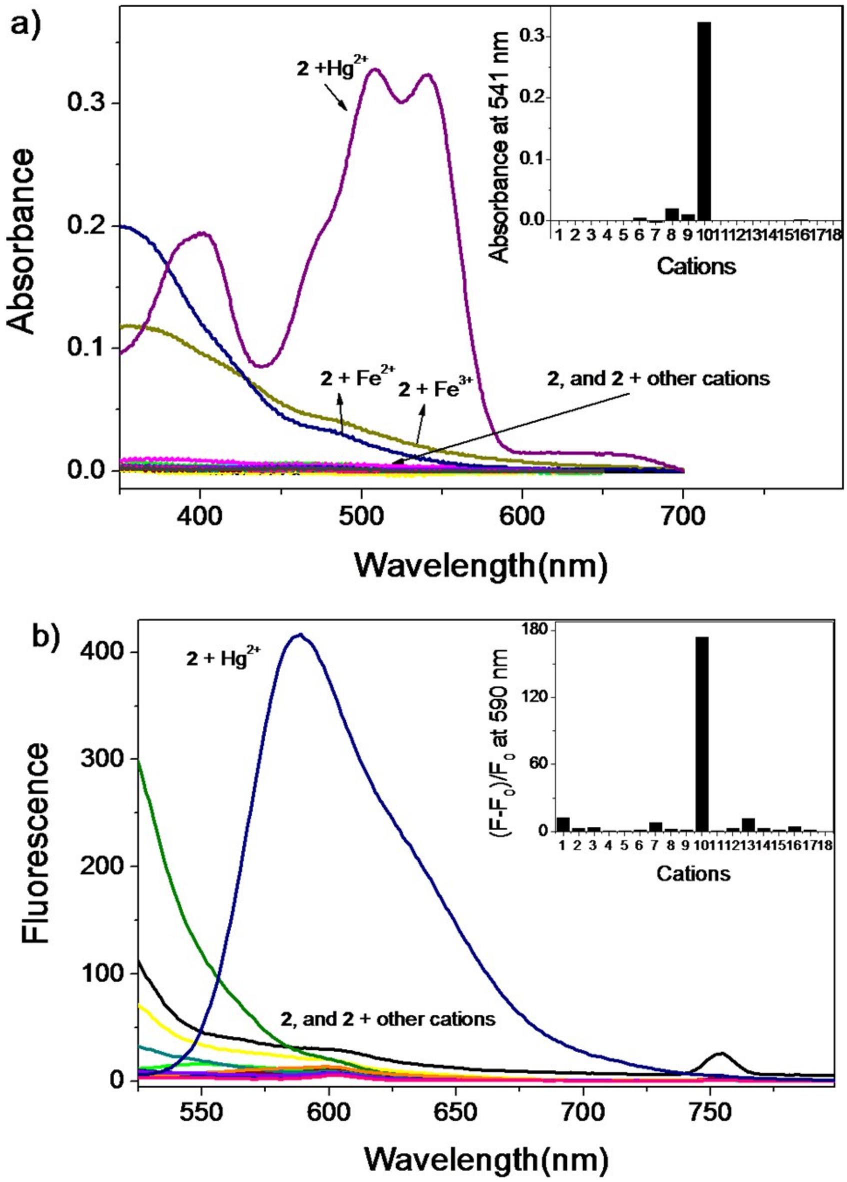

Figure S6. Absorption a) and Fluorescence b) spectra of **2** (10 μM) and those in the presence of different nitrate salts (10 equiv.). Insets of a) and b): (1) **2** + Ag^{+};(2) **2** + Al^{3+}; (3) **2** + Ca^{2+}; (4) **2** + Cd^{2+}; (5) **2** + Co^{2+}; (6) **2** + Cr^{3+}; (7) **2** + Cu^{2+}; (8) **2** + Fe^{2+}; (9) **2** + Fe^{3+}; (10) **2** + Hg^{2+}; (11) **2** + K^{+}; (12) **2** + Mg^{2+}; (13) **2** + Na^{+}; (14) **2** + NH_4^{+}; (15) **2** + Ni^{2+}; (16) **2** + Pb^{2+};(17) **2** + Zn^{2+} and (18) **2** alone. λ_{ex} = 500 nm.

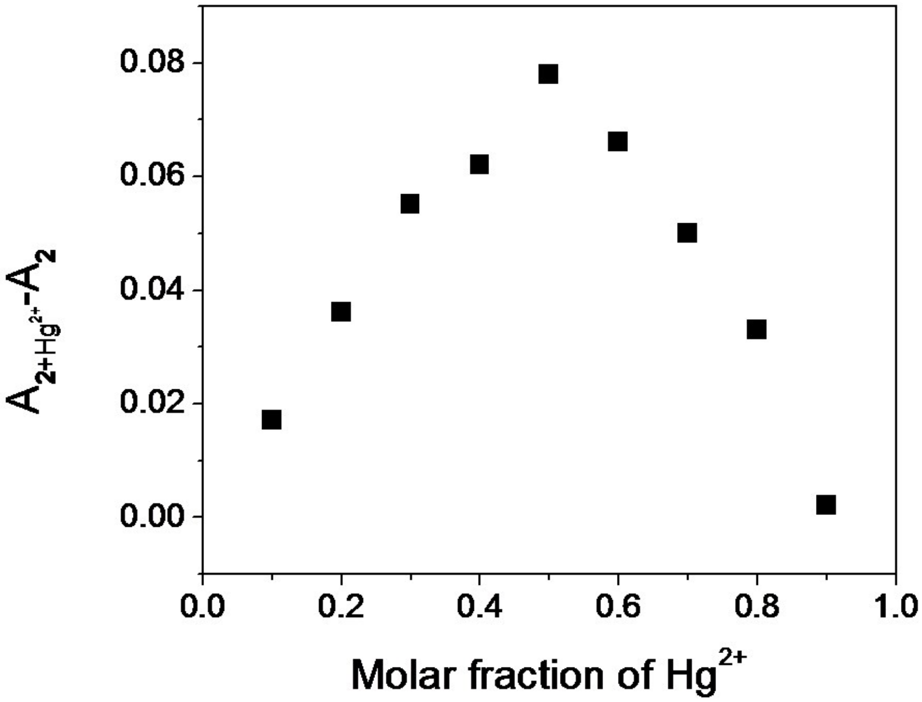

Figure S7. Job's plot of **2** showing the 1:1 stoichiometry of the complex between Hg^{2+} ion and **2**. The total of **2** and Hg^{2+} is 10 *u*M.

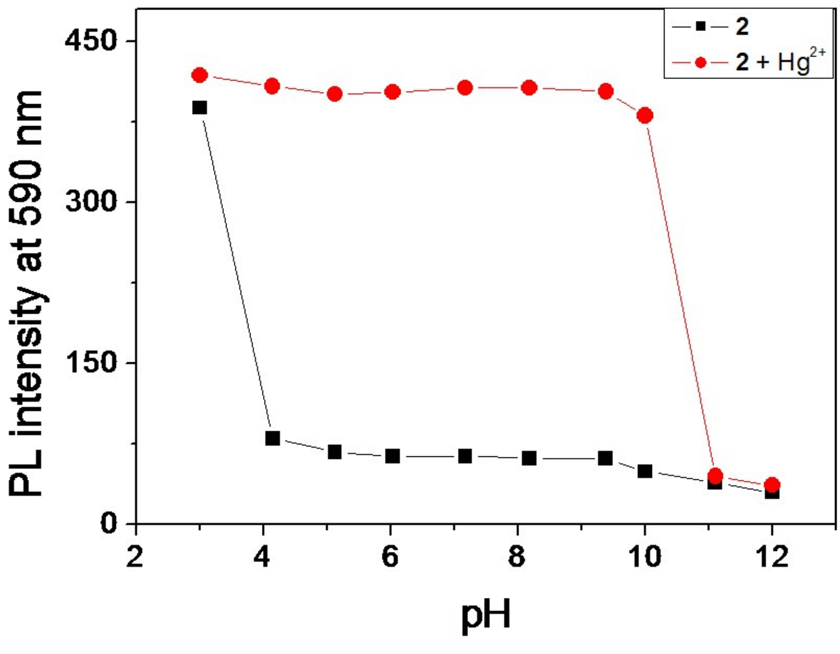

Figure S8 Fluorescence response of **2** (10 uM) and **2** + Hg^{2+} (5.0 equiv) as a function of different pH values.

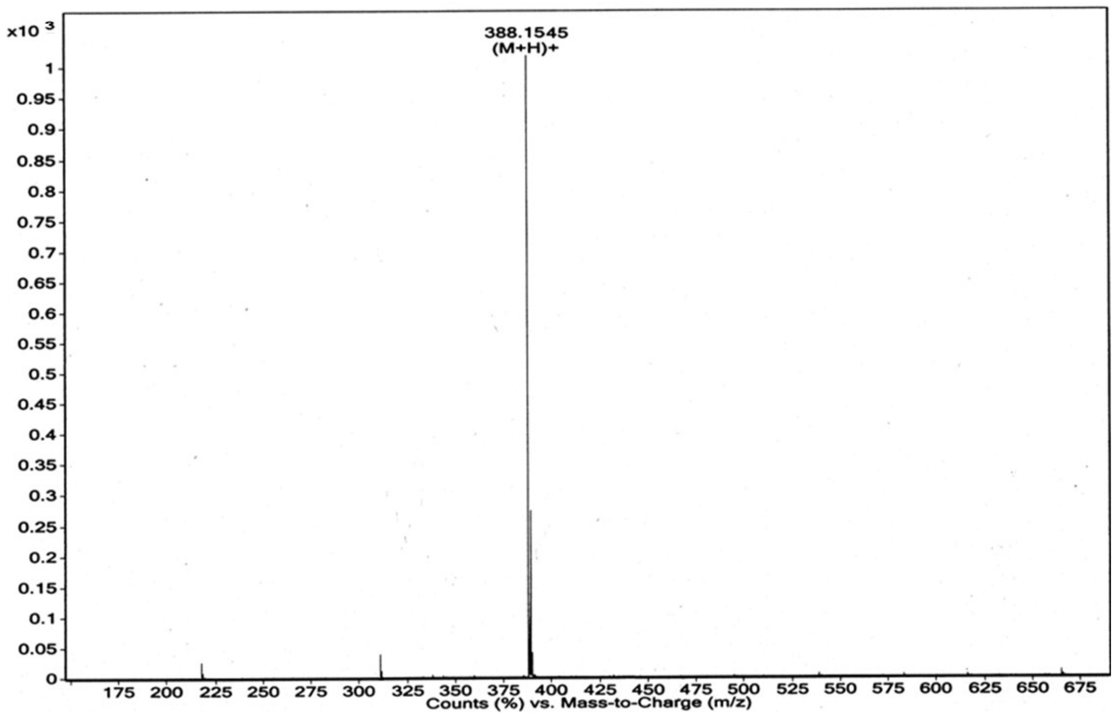

Figure S9 HRMS spectra of **2** upon addition of Hg^{2+} (2.0 equiv.). The peak (m/z) at 388.1545 corresponds to rhodol isomer **1** + H^+ (Calcd: 388.1543).

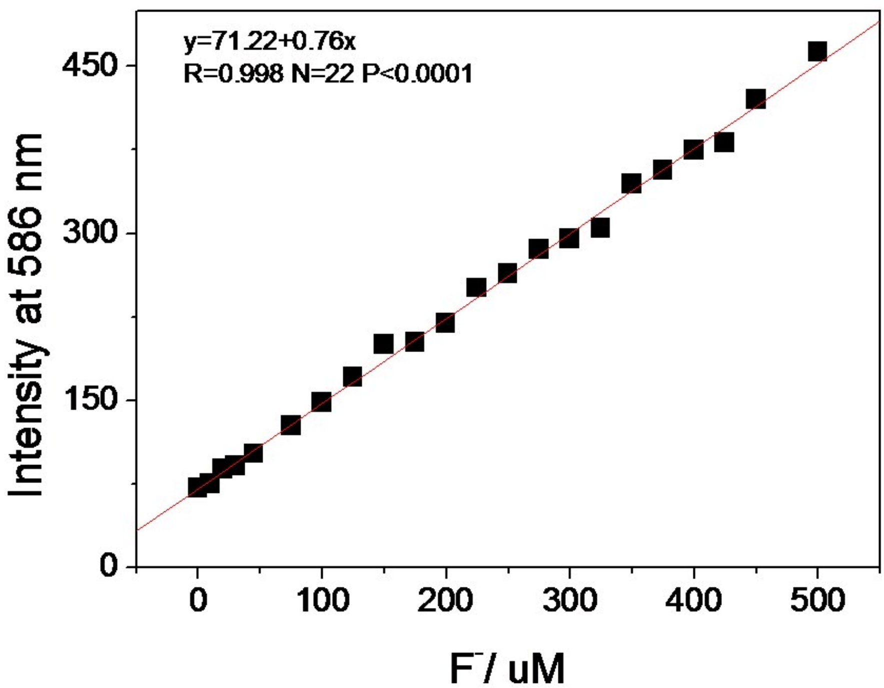

Figure S10. Emission at 586 nm of **3** (5 μM) at different concentrations of F^- added. A linear relationship between the fluorescence intensity and the F^- concentration could be obtained in the 0 - 500 μM concentration range (R = 0.9980). The detection limit was then calculated with the equation: detection limit = 3σbi/m, where σbi is the standard deviation of blank measurements (σbi = 1.4225, derived from 10 measurements), m is the slope between intensity *versus* sample concentration. The detection limit was measured to be 5.61 ×10^{-6} M.

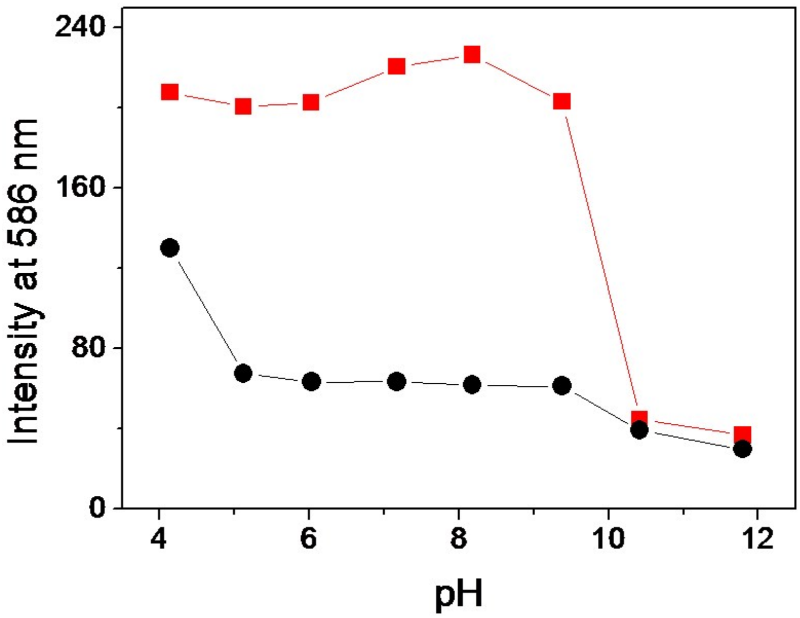

Figure S11 Fluorescence response of **3** (5 uM) (black dot) and after addition of F^- (40 eq.) (red dot) in DMSO–water (v/v = 1 : 1) as a function of different pH values. λ_{ex} = 514 nm.

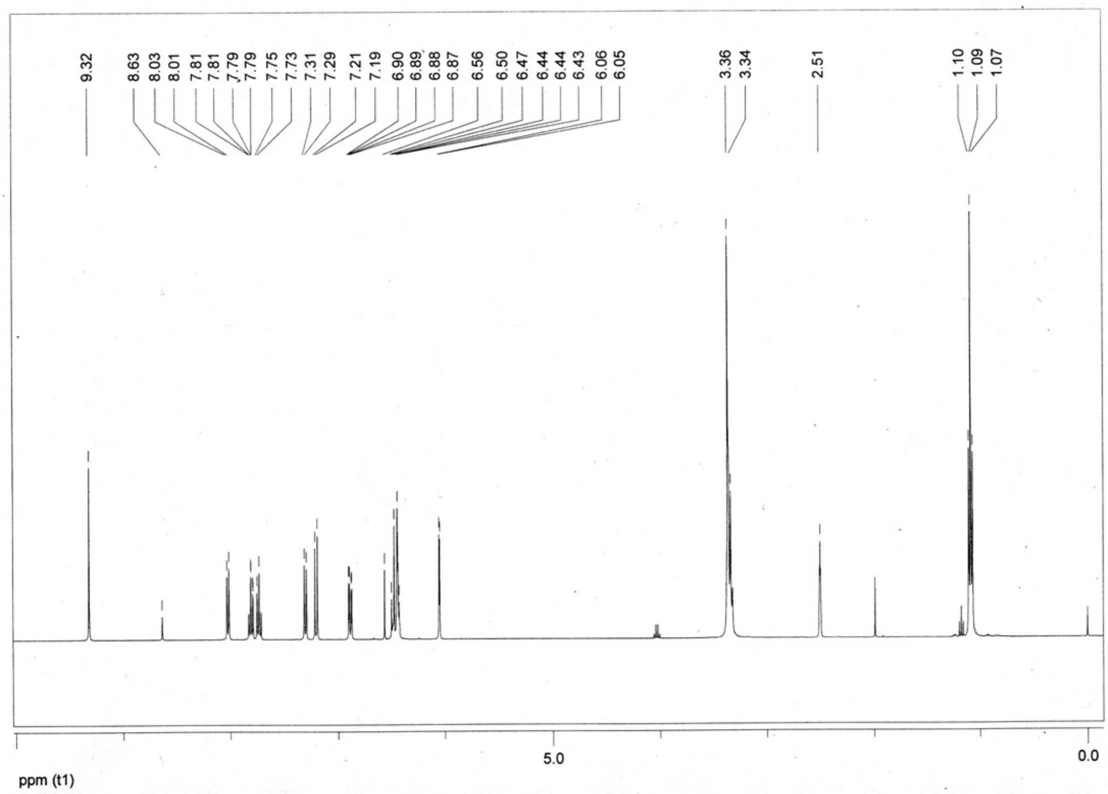

Fig. S12.[1]H NMR of **1** (400 MHz, DMSO-d_6)

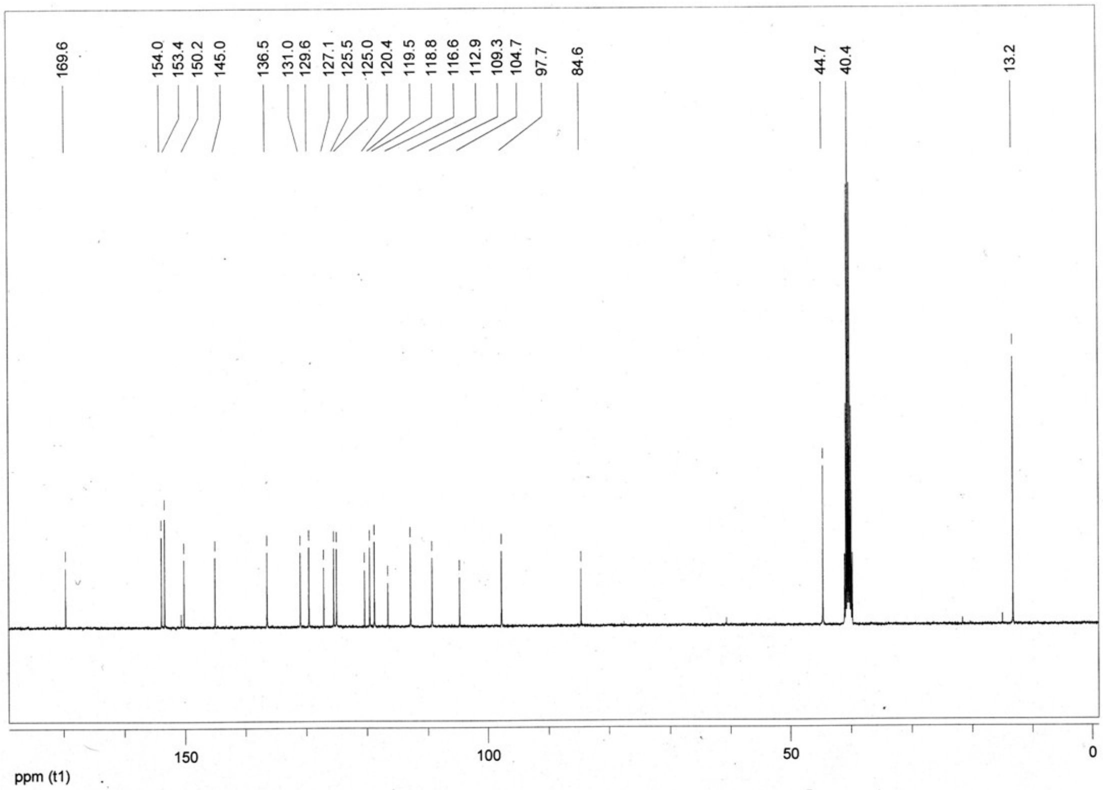

Fig. S13. ^{13}C NMR of **1** (100 MHz, DMSO-d_6).

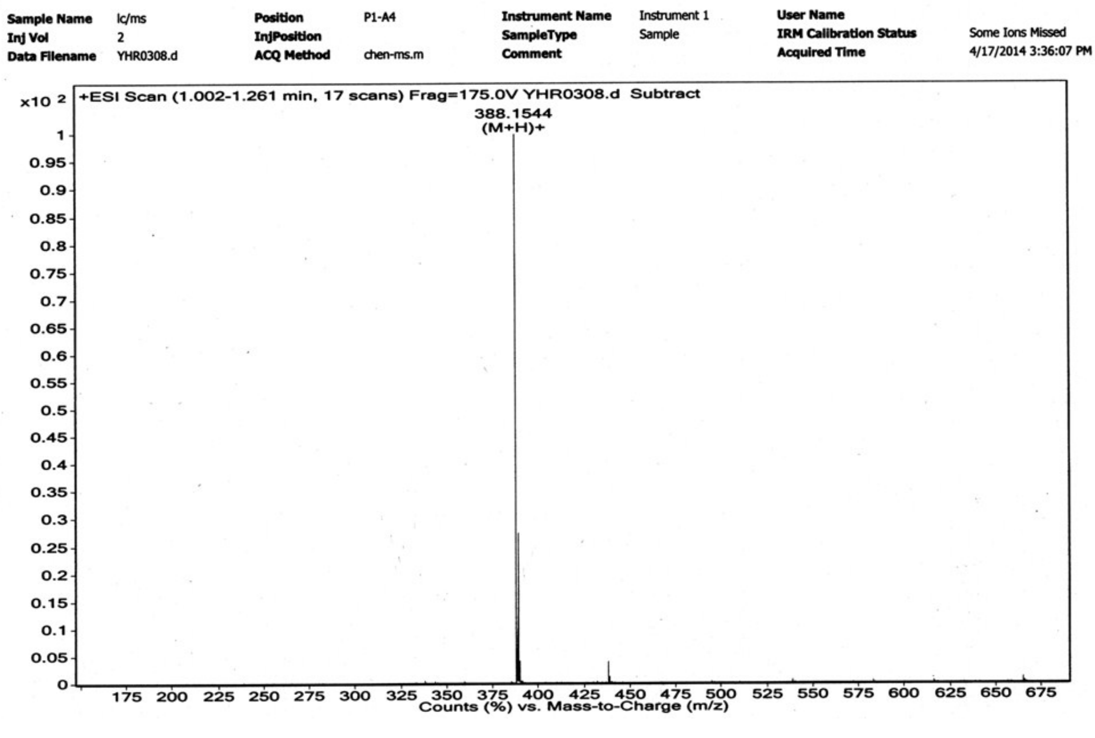

Fig. S14. HRMS (LC/MS) spectra of **1**. The peak at m/z = 388.1544 was assigned to the mass of **1**+H$^+$.

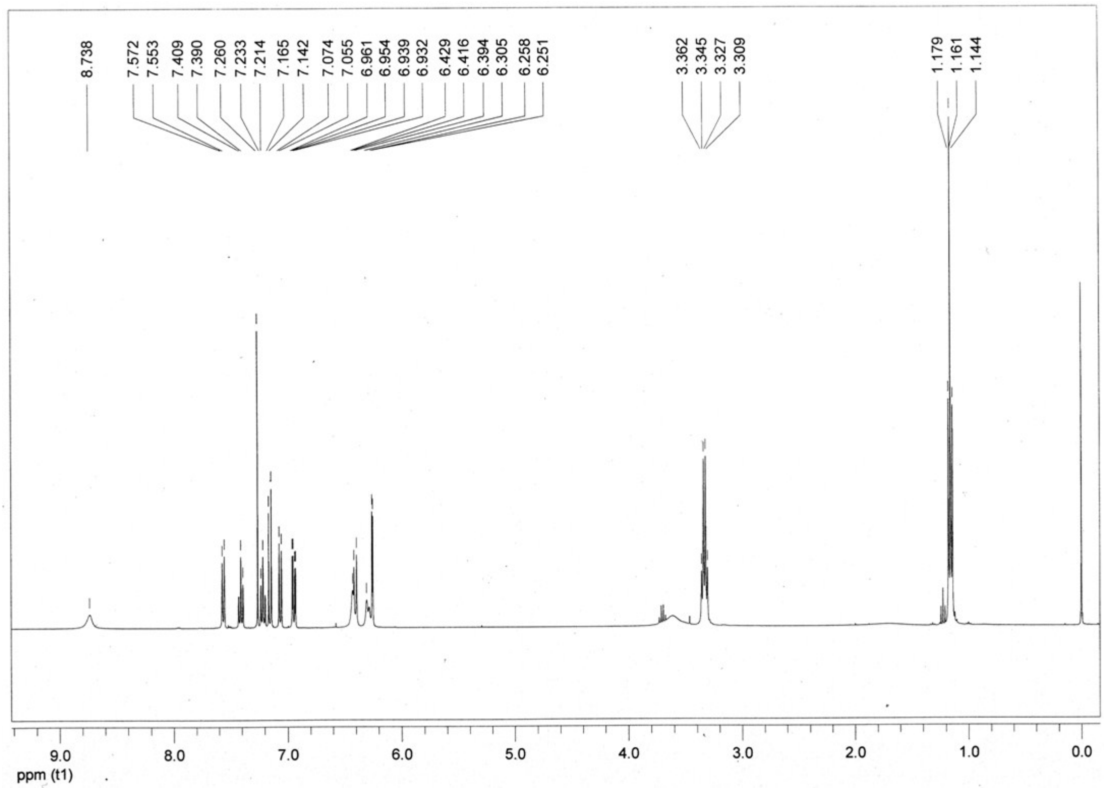

Fig. S15.^{1}H NMR of **2** (400 MHz, DMSO-d_6)

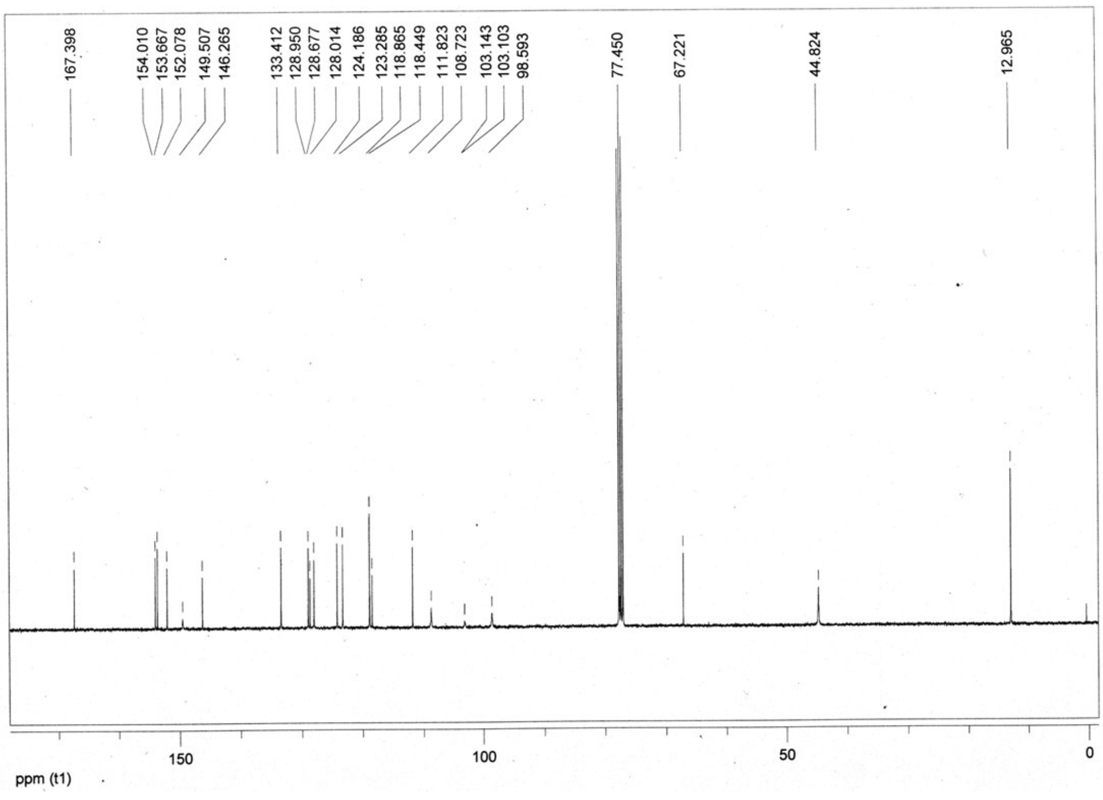

Fig. S16 ^{13}C NMR of **2** (100 MHz, DMSO-d_6).

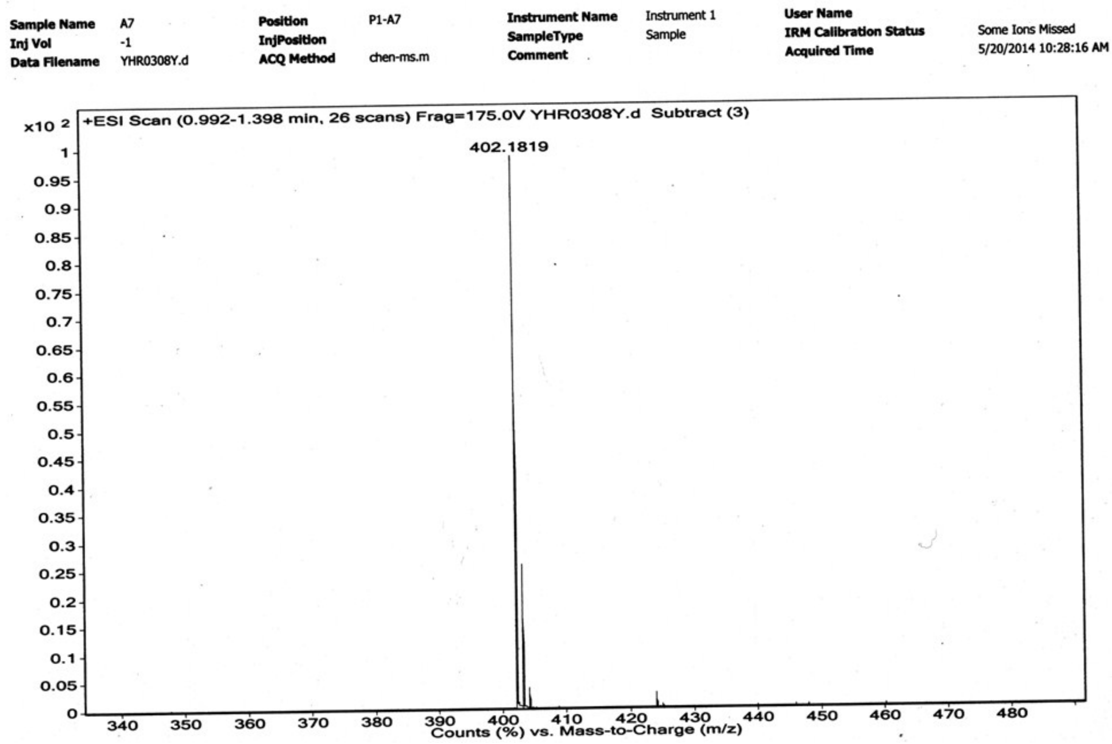

Fig. S17. HRMS (LC/MS) spectra of **2**. The peak at m/z = 402.1819 was assigned to the mass of **2**+H+.

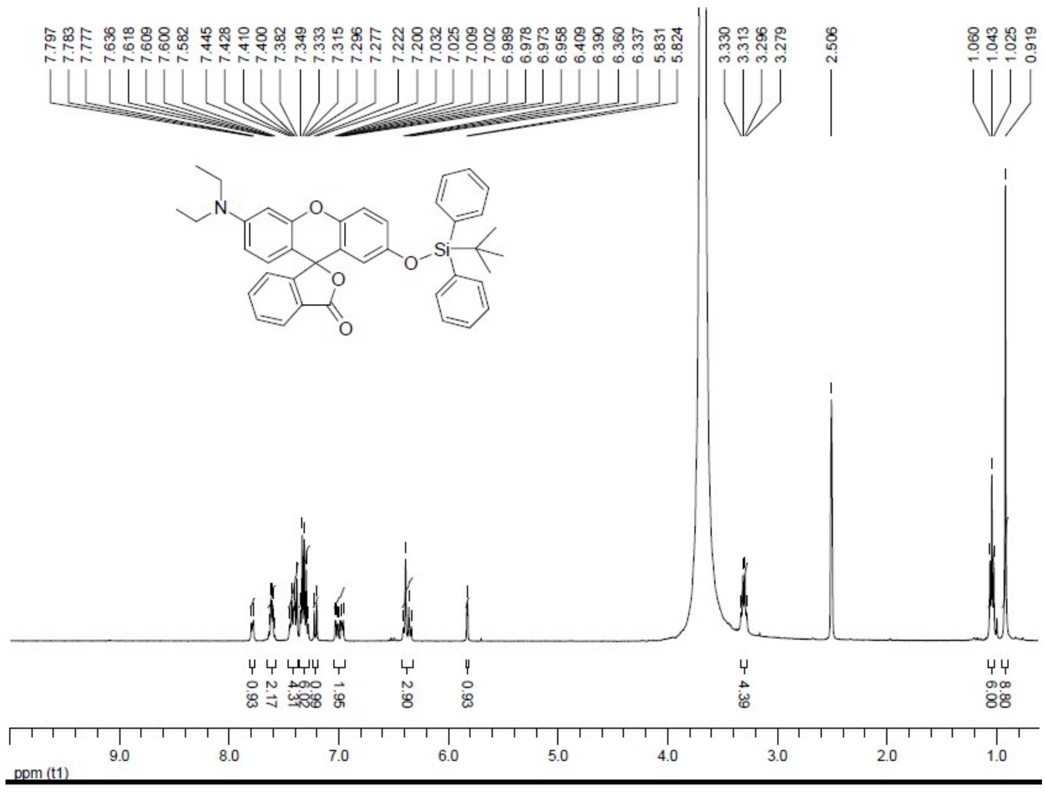

Fig. S18.[1]H NMR of **3** (400 MHz, DMSO-d_6)

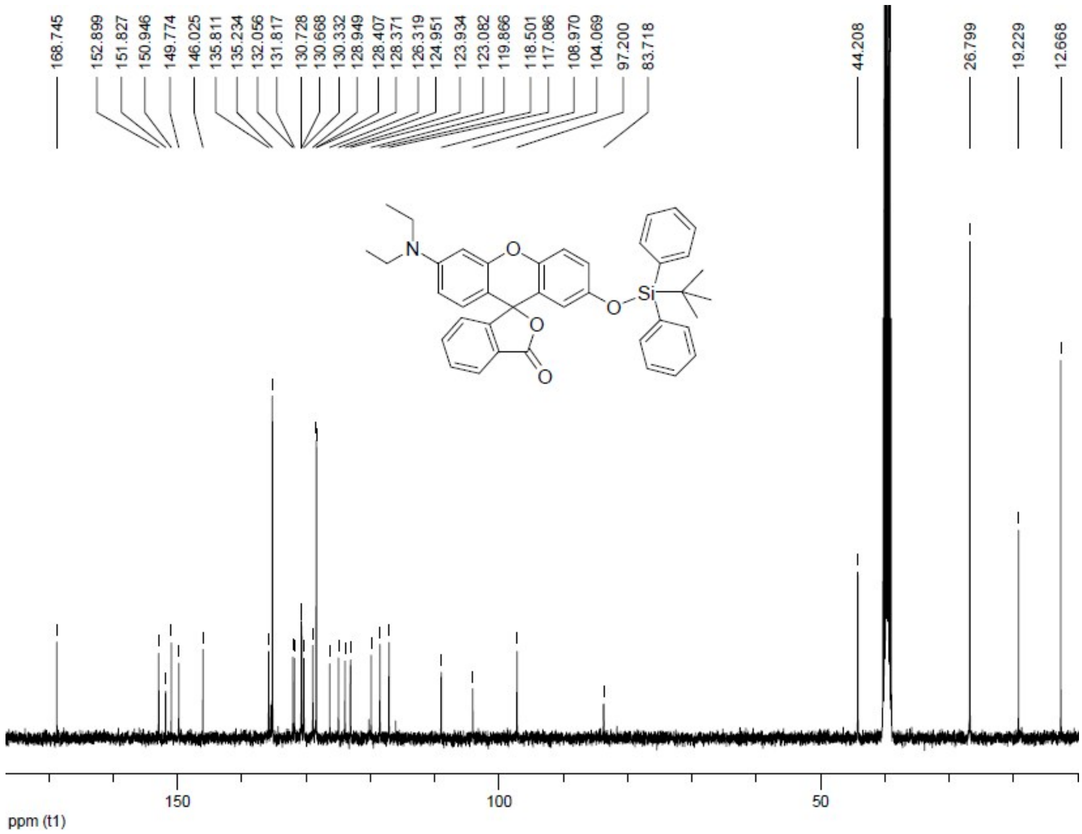

Fig. S19. ^{13}C NMR of **3** (100 MHz, DMSO-d_6).

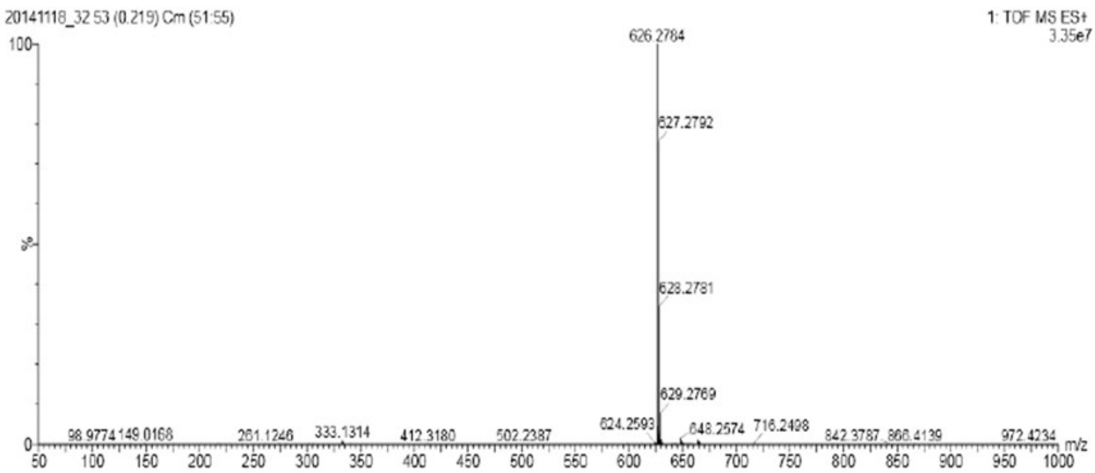

Fig. S20. HRMS (LC/MS) spectra of **3**. The peak at m/z = 626.28 was assigned to the mass of **3**+H^+.