Supporting Information

Dual mode selective chemosensor for copper and fluoride ions: A fluorimetric, colorimetric and theoretical investigation

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nguchhait@yahoo.com (N.G.)

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1. Characterization:

1.1 ^{1}H NMR Spectra

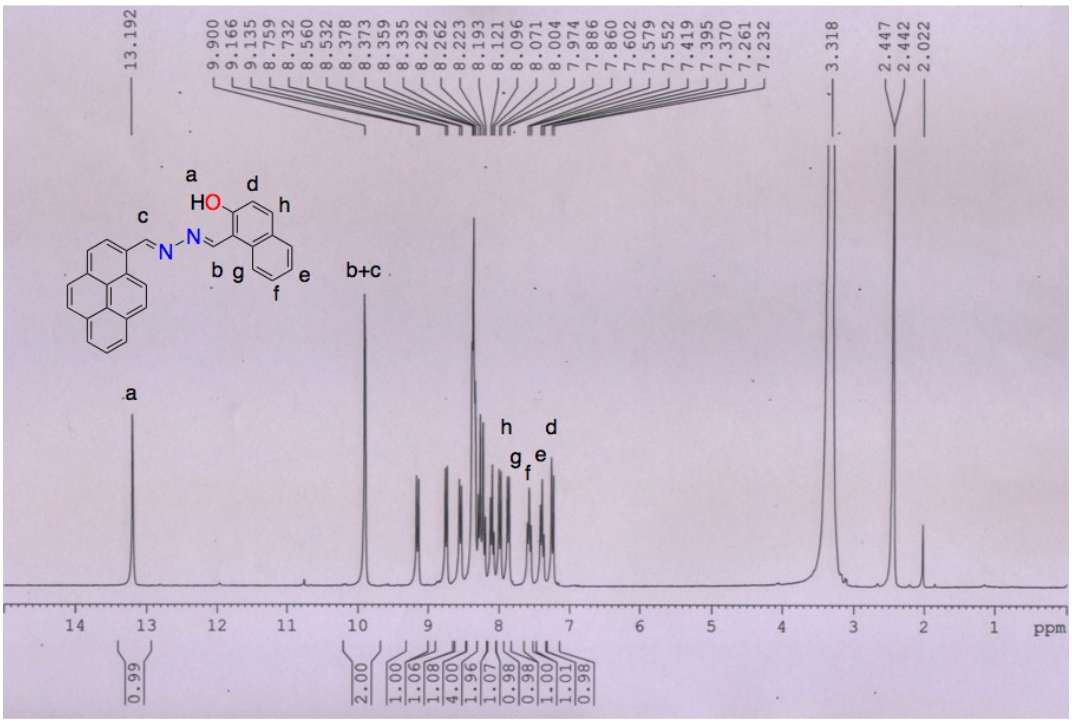


Fig. S1. ^{1}H NMR (300 MHz) spectrum of **1** in d_6-DMSO at 20 ºC

1.2 Mass (TOF-MS ES+) Spectra

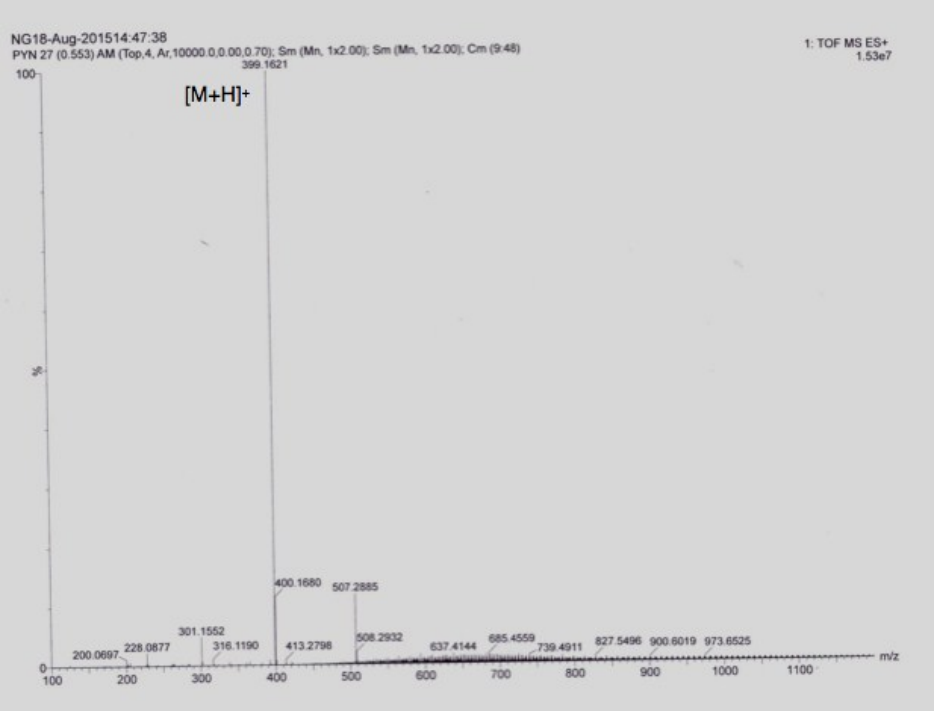


Fig. S2. Mass spectra (TOF-MS ES+) of **1**

2. X–ray Crystallographic Structures

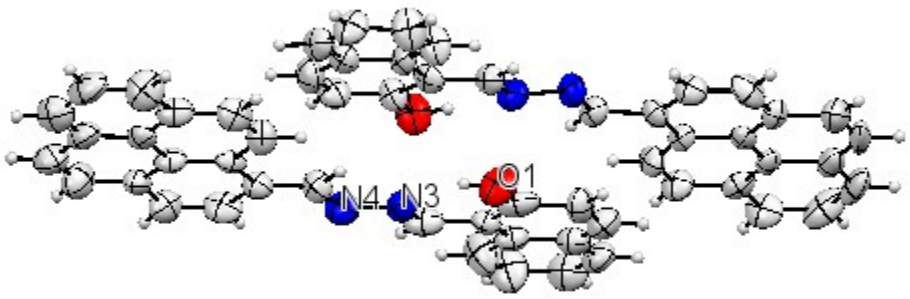


Fig. S3 ORTEP diagram of **1** (thermal ellipsoids set to 30% probability).

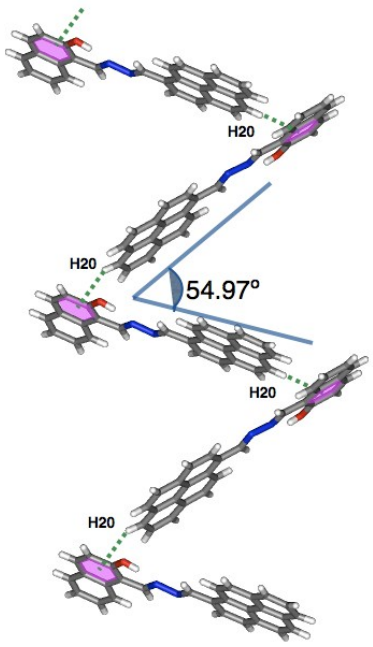


Fig. S4 1D polymer through CH…π interaction

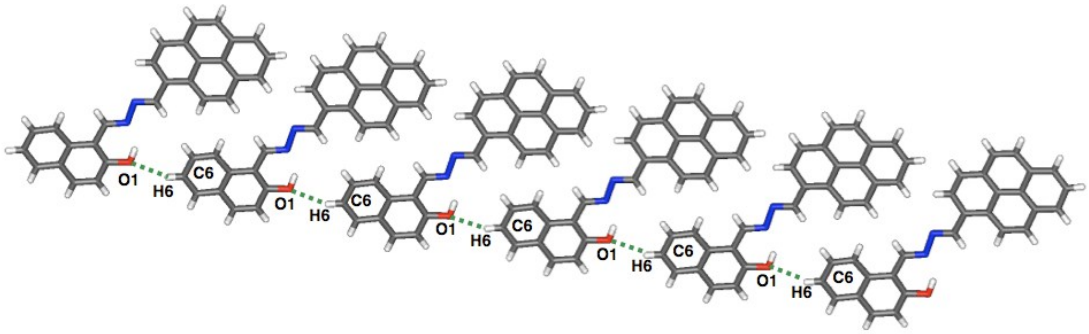


Fig. S5 1D polymer through intermolecular H-bonding interaction

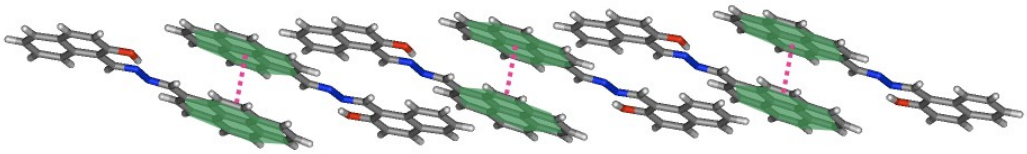


Fig. S6 Different type of π…π interaction

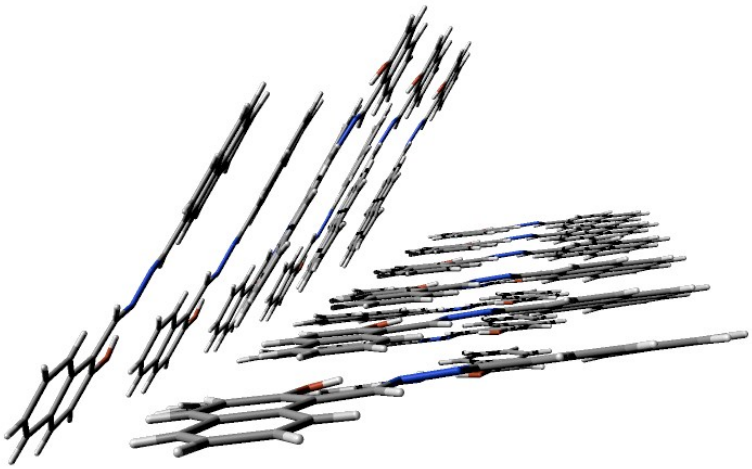


Fig. S7 2D polymeric structure of **1**

3. UV–Vis Spectra

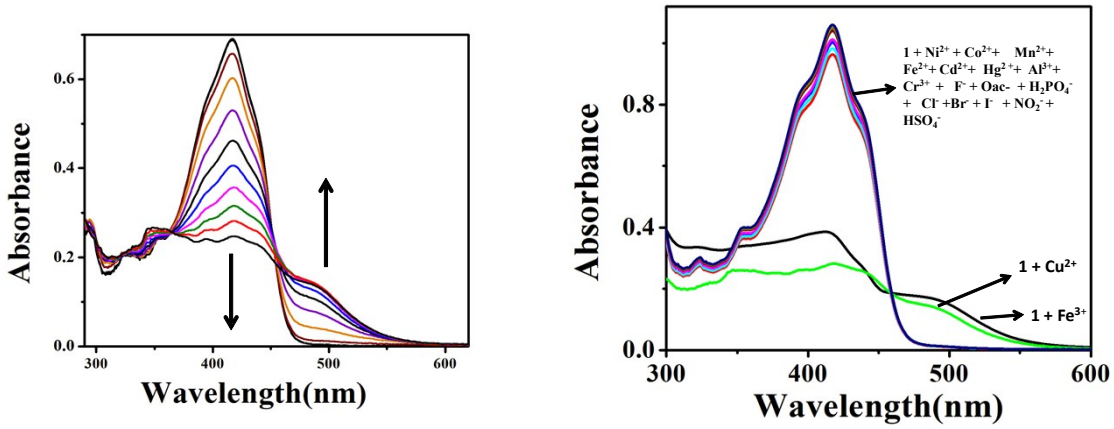


Fig. S8 UV-vis spectral changes of **1** (1.0 x 10^{-6} M) upon addition of (0–2 equiv.) Cu $(ClO_4)_2$ in methanol water mixture (7:3, v/v) (left) and UV-vis spectral changes of sensor **1** (1x10^{-6} M) in presence of various metal ions and anions (2 equiv.) in methanol water mixture (7:3, v/v) (right).

4. Emission Spectra

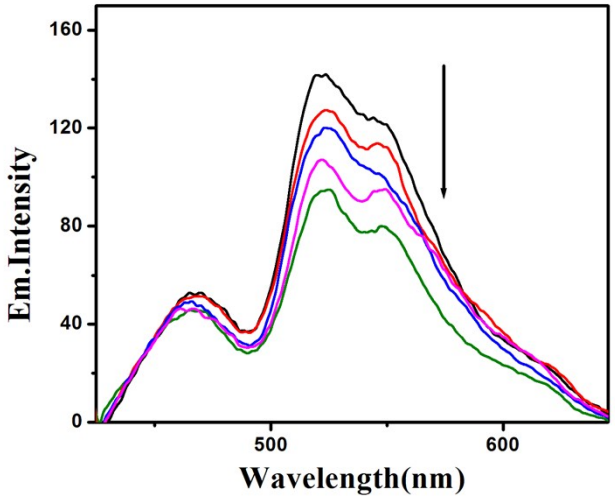


Fig. S9 Emission spectral changes of Sensor **1** ($1x10^{-7}$ M) with dilution in methanol water mixture (7:3, v/v).

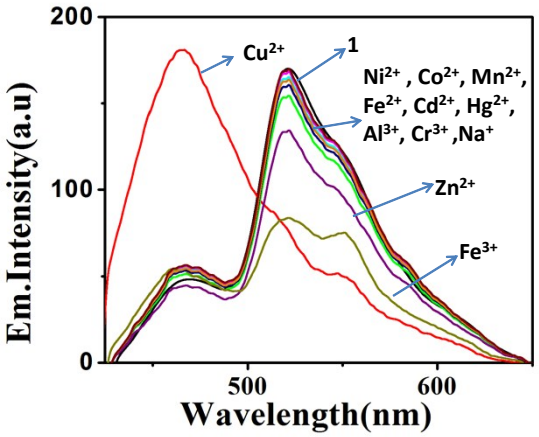


Fig. S10 Emission spectral changes of sensor **1**($1x10^{-7}$ M) in presence of various metal ions (2 equiv.) in methanol water mixture (7:3, v/v)

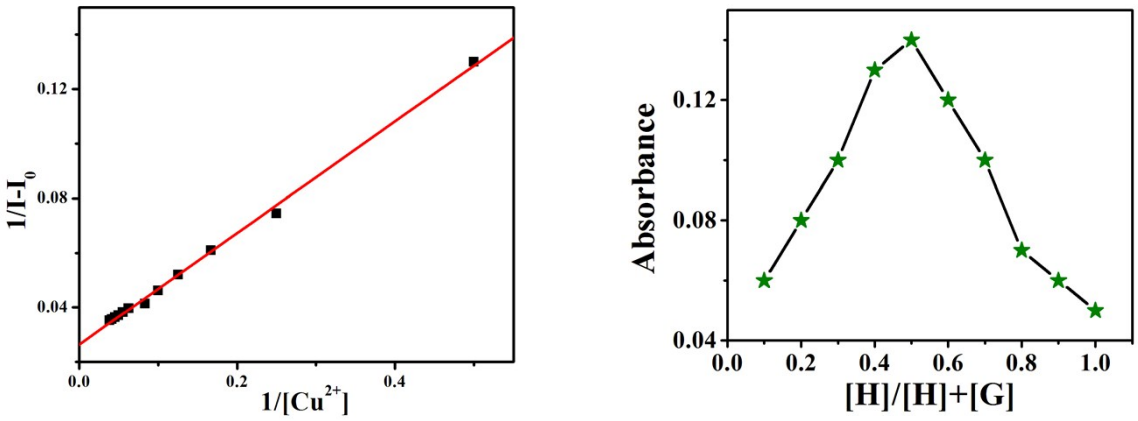


Fig. S11 B-H plot from fluorescence titration spectra at 466 nm (left) and Job's plot from Uv-vis titration at 490 nm (right) of receptor **1** with Cu^{2+} showing 1:1 binding stoichiometry.

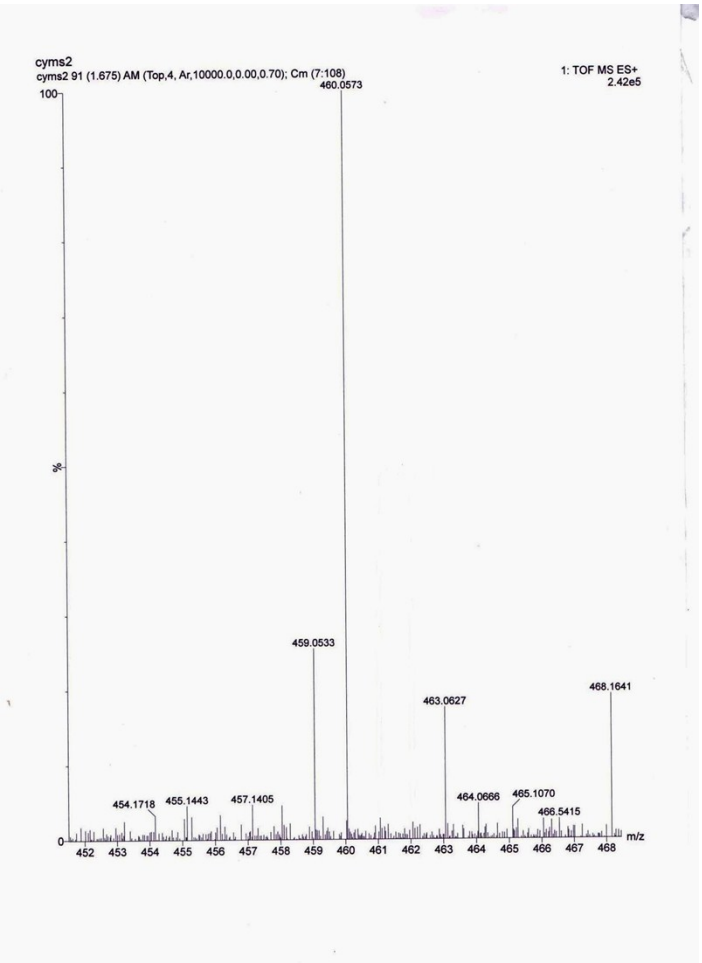


Fig. S12 Mass spectra (TOF-MS ES+) of **1**-Cu^{2+} complex

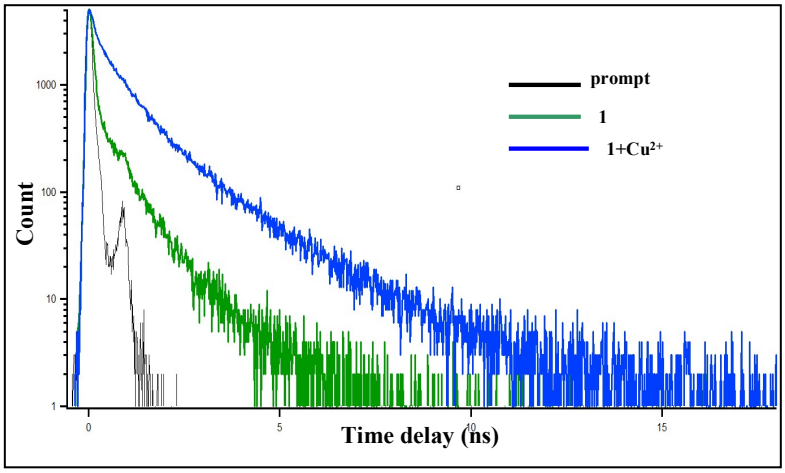


Fig. S13 Fluorescence decay profile of **1** and **1** in presence of 2 equivalents of Cu^{2+}, λ_{ex} = 375 nm, $\lambda_{em\ (max)}$ = 570 nm

5. Theoretically optimized structure

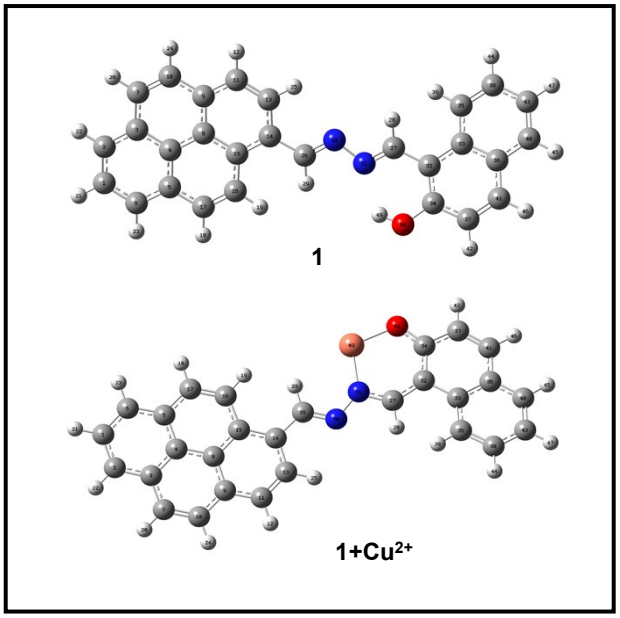


Fig. S14 Theoretically optimized structure of **1** and **1**-Cu^{2+}

6. UV–Vis Spectral data of 1 with F^-

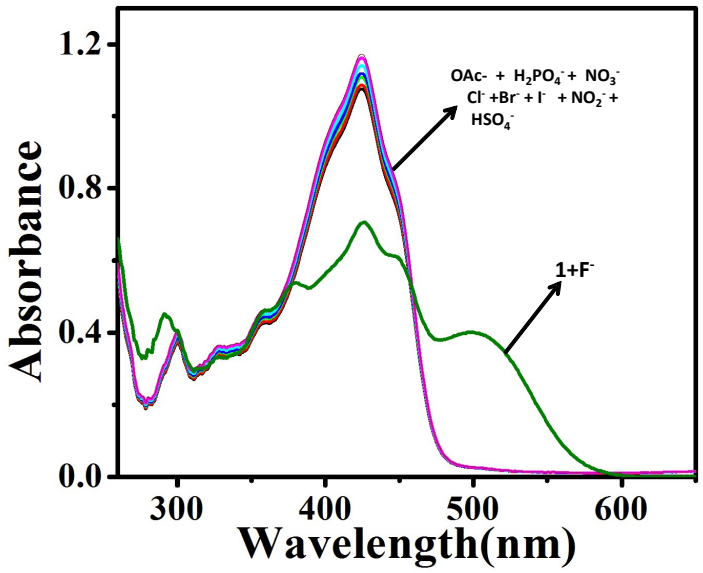


Fig. S15 UV-Vis spectral changes of sensor **1** ($1x10^{-6}$ M) in presence of various anions (2 equiv.) in DMSO-water mixture (7:3, v/v)

7. ^{1}H NMR titration

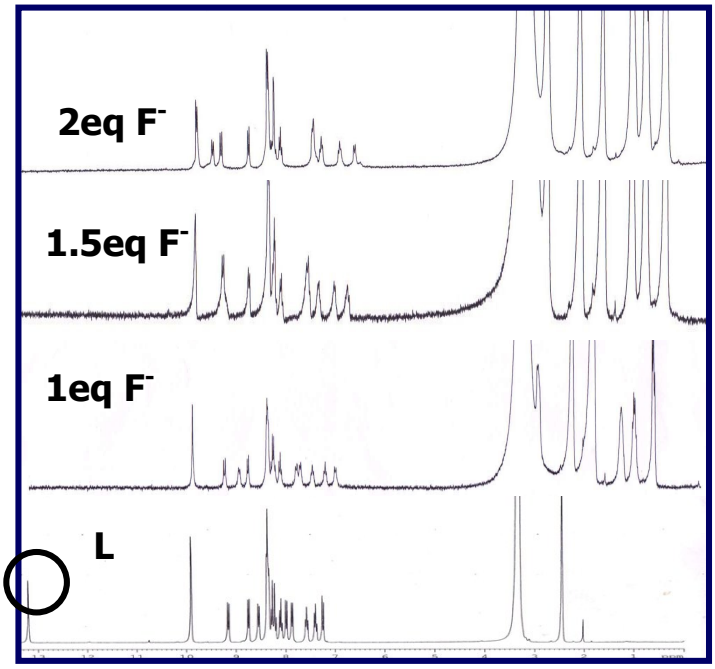


Fig. S16 ^{1}H NMR titration of **1**with tetrabutyl ammonium fluoride in DMSO-d_6

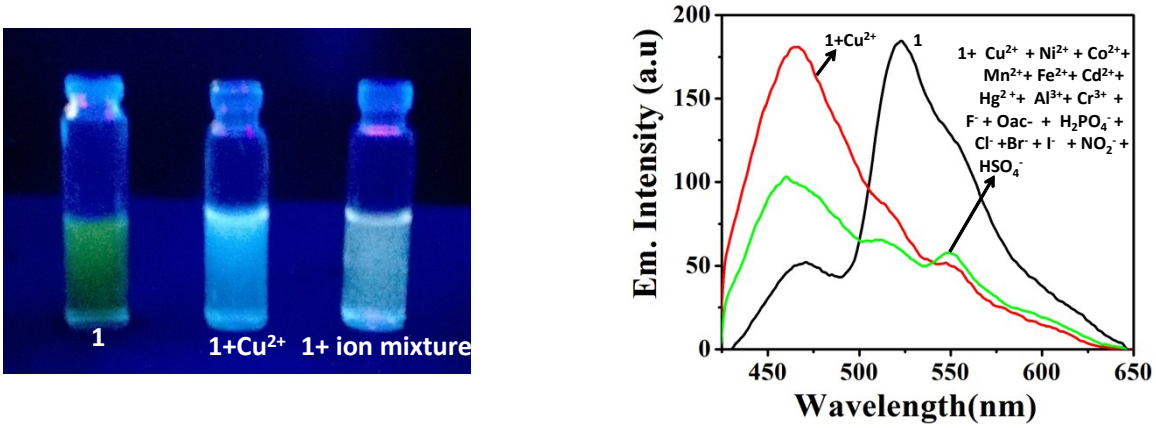


Fig. S17 Visual fluorescence change of **1**(1×10^{-5} M) (left) and fluorescence spectra of **1** (1×10^{-7} M) (right) in bare copper ion and in mixture of ions (Cu^{2+}, Ni^{2+}, Co^{2+}, Mn^{2+}, Fe^{2+}, Cd^{2+}, Hg^{2+}, Al^{3+}, Cr^{3+}, F^{-}, OAc^{-}, $H_2PO_4^{-}$, Cl^{-} ,Br^{-}, I^{-}, NO_2^{-} and HSO_4^{-}) in methanol water mixture (7:3, v/v)

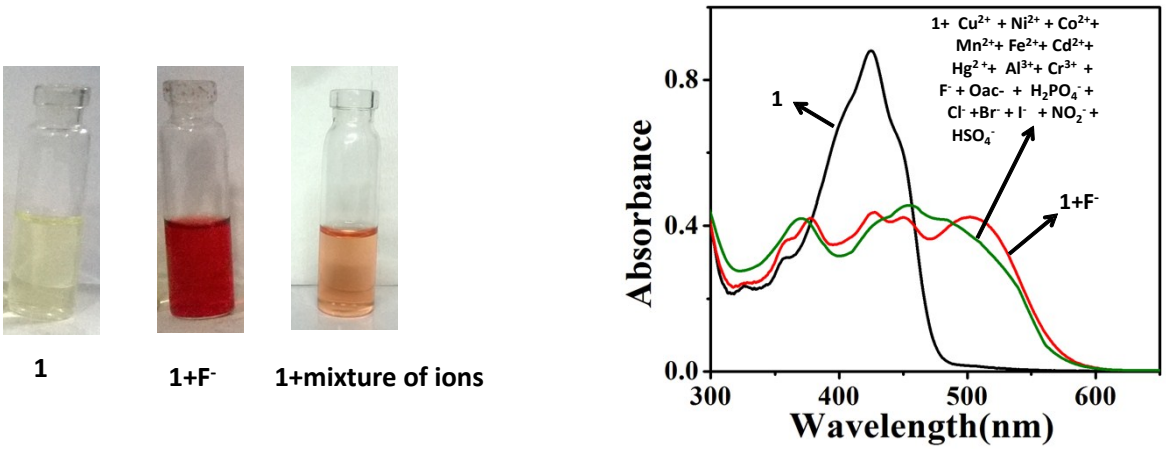


Fig. S18 Naked-eye color change of **1**(1×10^{-4} M) (left) and Uv-vis spectra of **1** (1×10^{-6} M) (right) in bare fluoride and in mixture of ions (Cu^{2+}, Ni^{2+}, Co^{2+}, Mn^{2+}, Fe^{2+}, Cd^{2+}, Hg^{2+}, Al^{3+}, Cr^{3+}, F^{-}, Oac^{-}, $H_2PO_4^{-}$, Cl^{-} ,Br^{-}, I^{-}, NO_2^{-} and HSO_4^{-}) in DMSO water mixture (7:3, v/v)

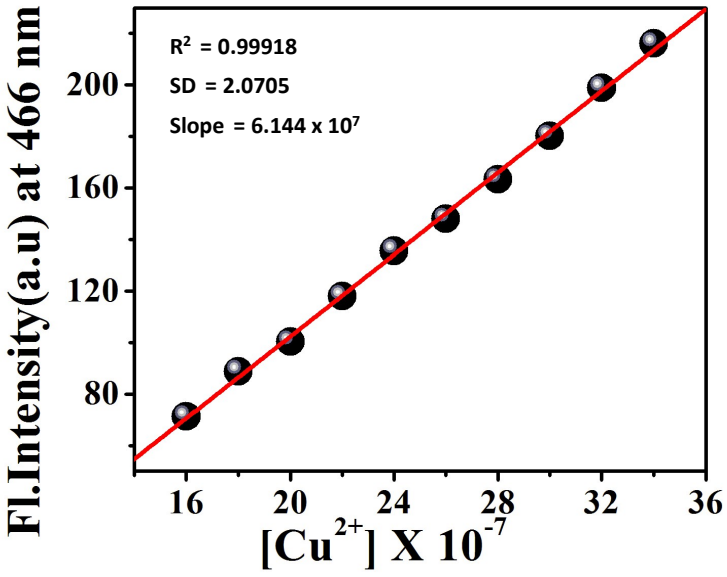


Fig.S19 Determination of detection limit of Cu^{2+} by **1**(1×10^{-7}) in methanol water mixture (7:3, v/v) at λ_{em} =466nm.

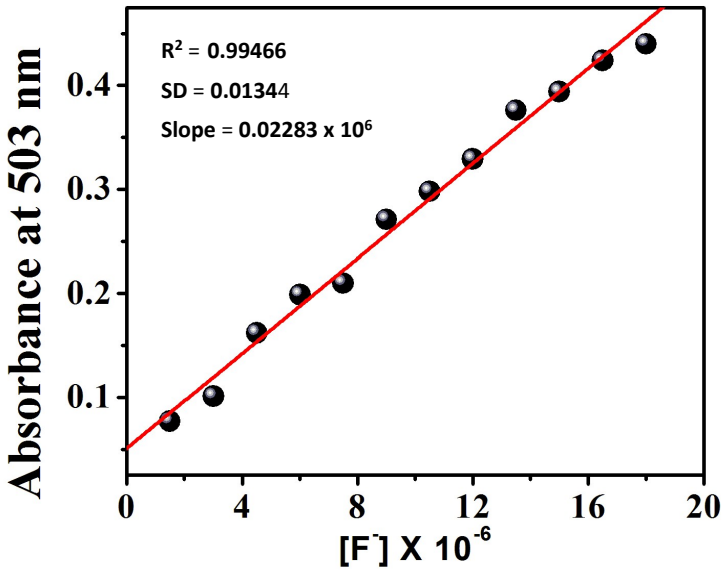


Fig. S20 Determination of detection limit of F^- by **1**(1×10^{-6}) in DMSO water mixture (7:3, v/v) at λ_{abs} =503nm.

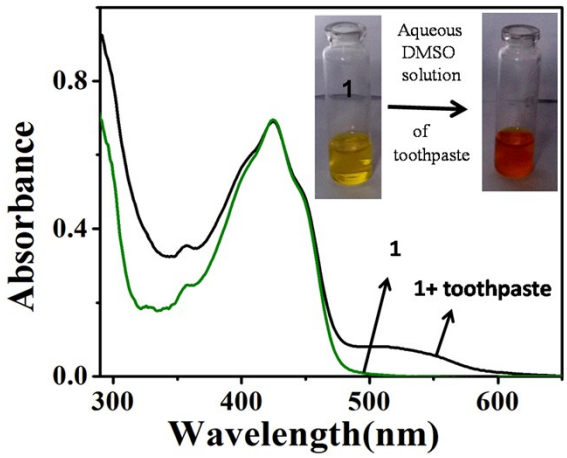
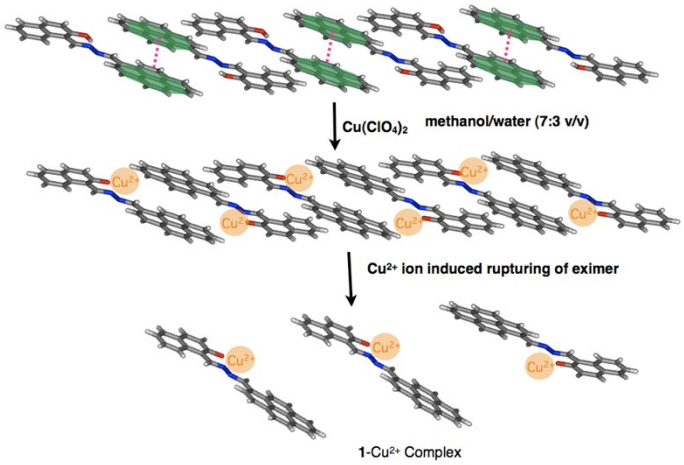
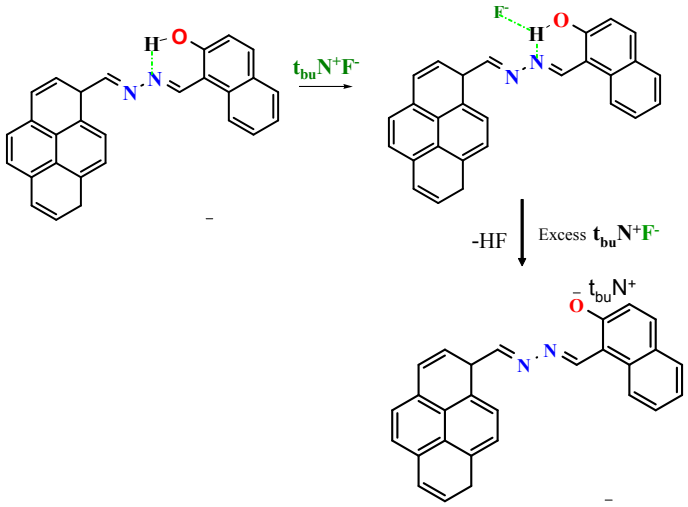


Fig. S21 Uv-vis spectra of **1** (1×10^{-5} M) and **1** in presence of toothpaste in aqueous DMSO solution and Naked-eye color change (inset).



Scheme S1. The plausible representation of the complexation of **1** with Cu^{2+}



Scheme S2. The plausible representation of the H-bonded form and the deprotonated form of receptor **1**.