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Rhodamine based Turn-On Chemosensor for Fe^{3+} in Aqueous Medium and Interactions of Its Fe^{3+} Complex with HSA.

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Figure S1. ^{1}H NMR spectrum of **1** in $CDCl_3$, in Bruker 300 MHz instrument.

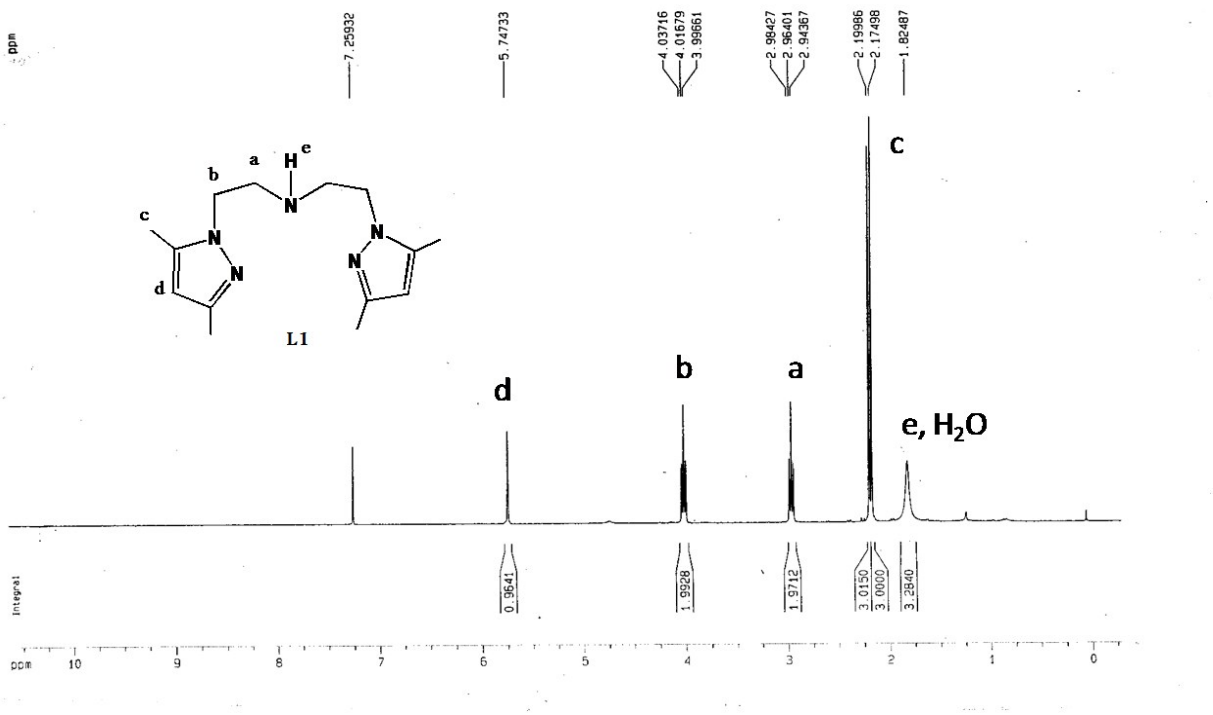


Figure S2. ^{1}H NMR spectrum of **2** in $CDCl_3$, in Bruker 300 MHz instrument.

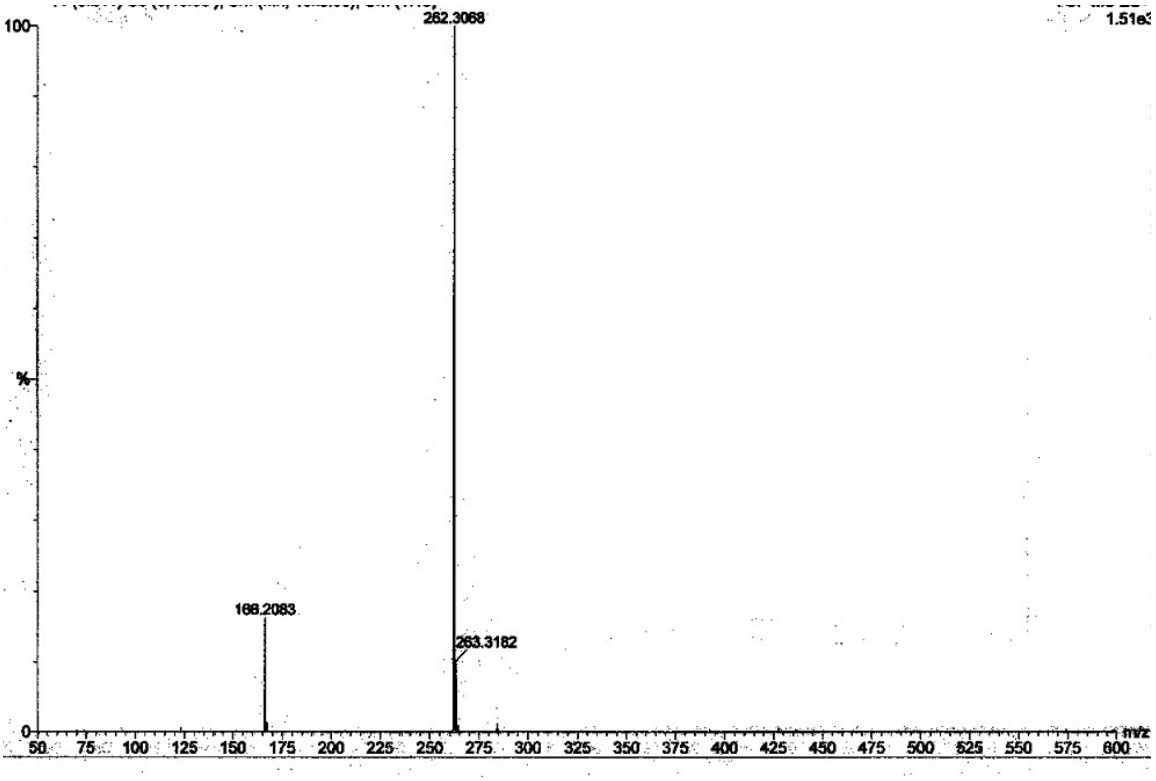


Figure S3. HRMS spectrum of **2** in MeCN**.**

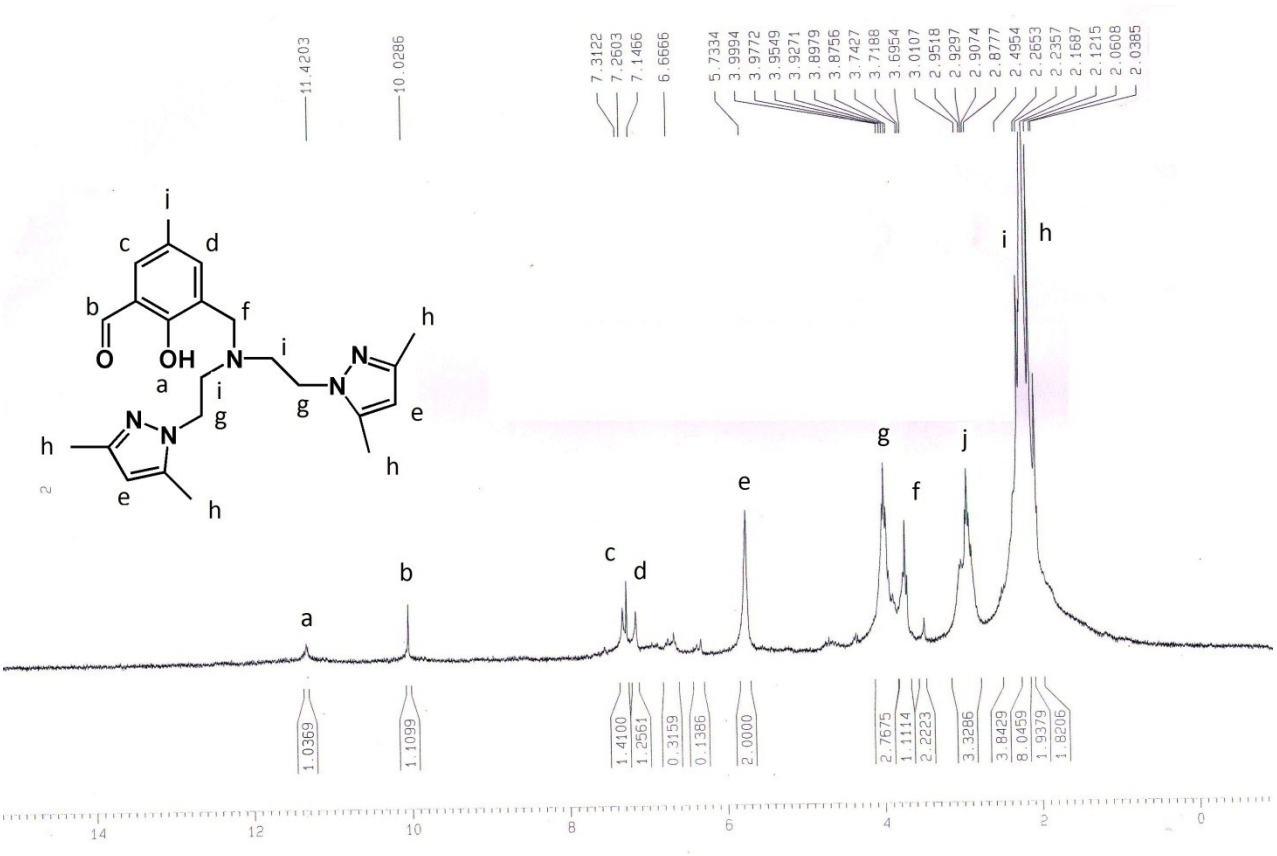


Figure S4. ^{1}H NMR spectrum of **3** in $CDCl_3$, in Bruker 300 MHz instrument.

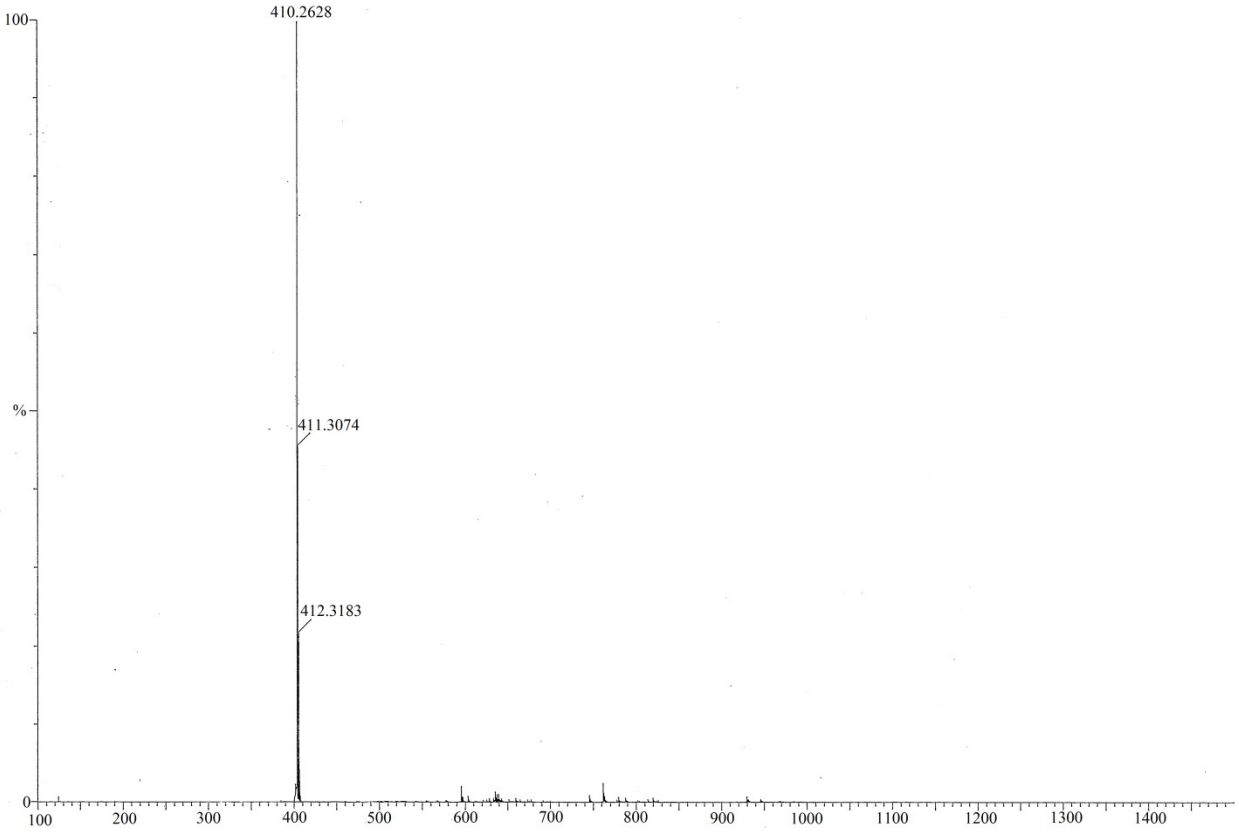


Figure S5. HRMS spectrum of **3** in MeCN

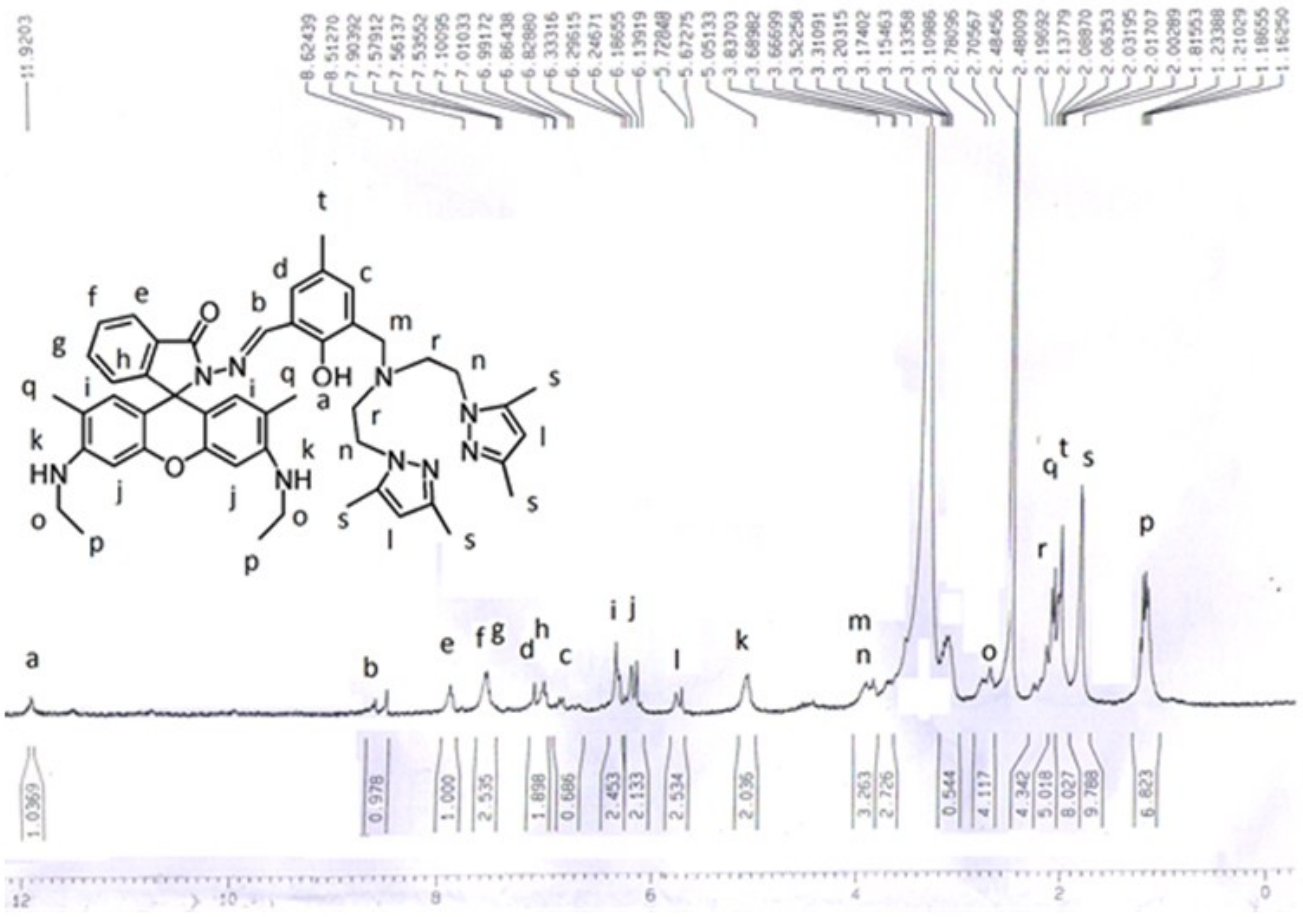


Figure S6. ^{1}H NMR spectrum of H**L**^{6} in $CDCl_3$, in Bruker 300 MHz instrument.

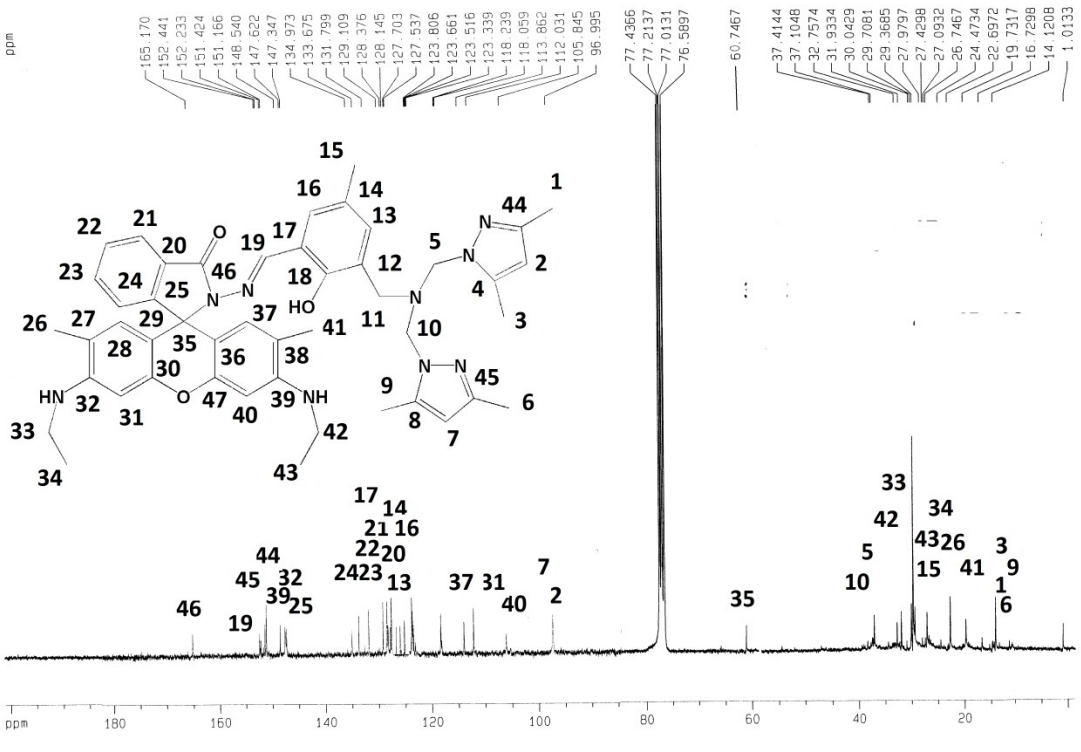


Figure S7. ^{13}C NMR spectrum of H**L**^{6} in $CDCl_3$, in Bruker 300 MHz instrument.

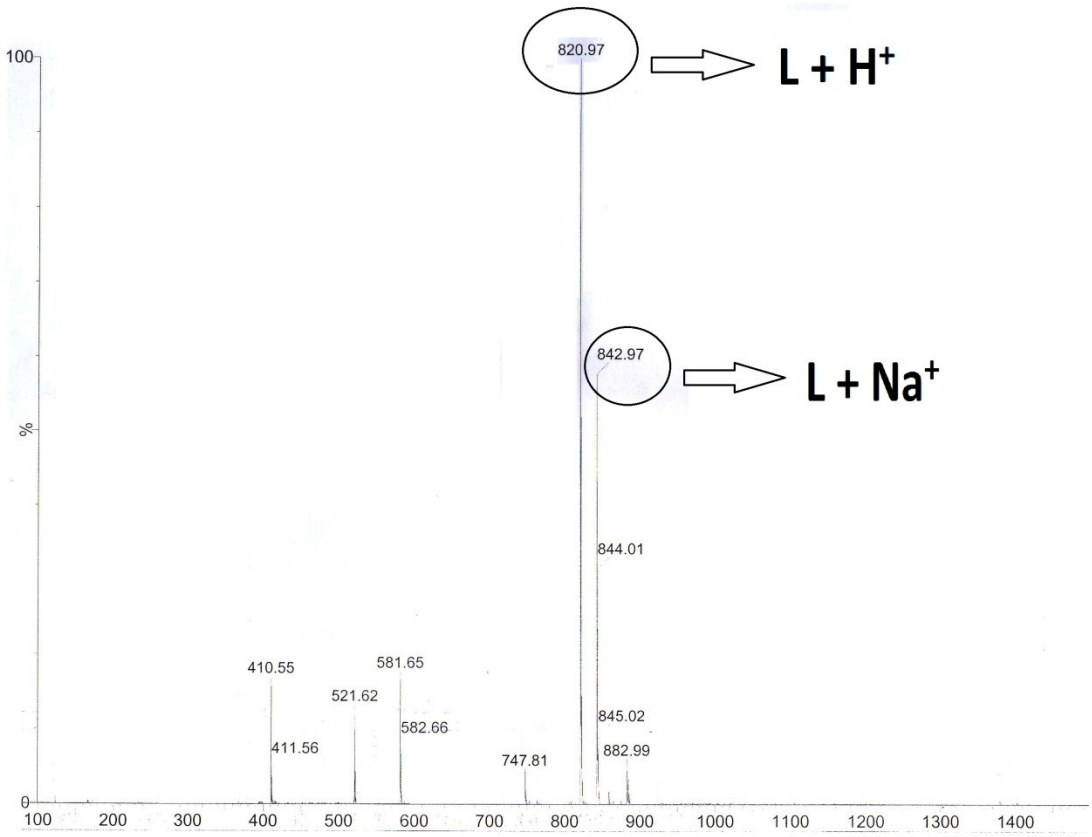


Figure S8. Mass spectra of HL^6

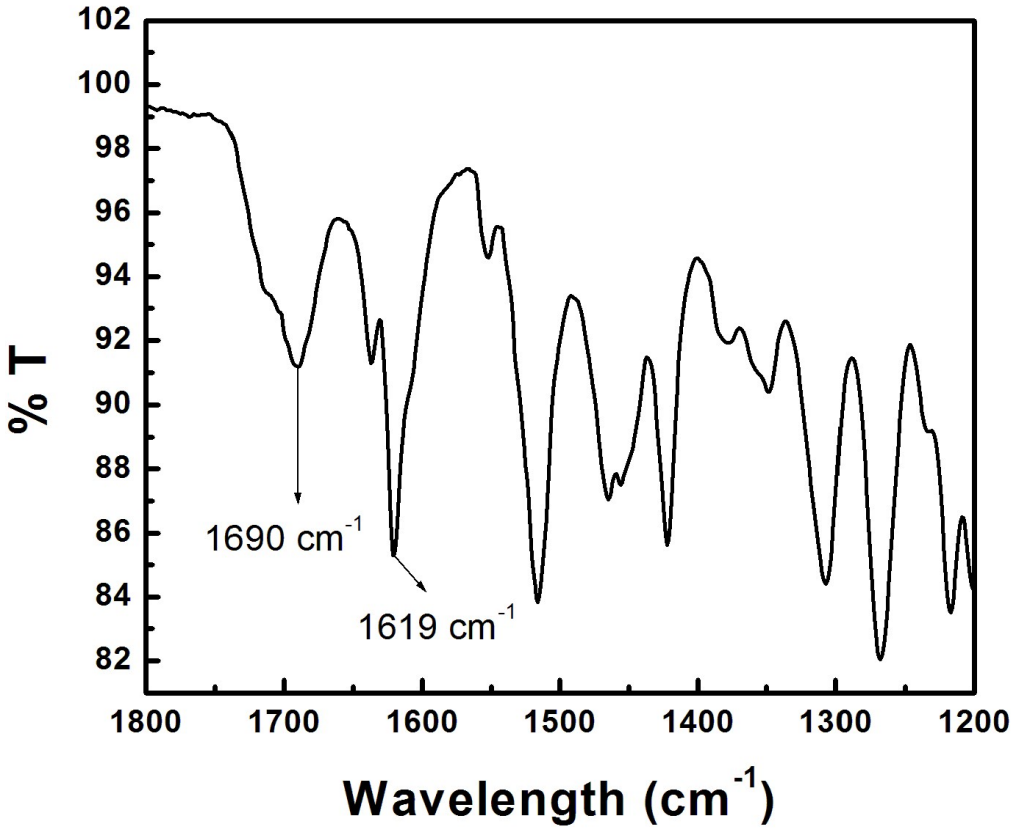


Figure S9. IR spectra of H**L**[6].

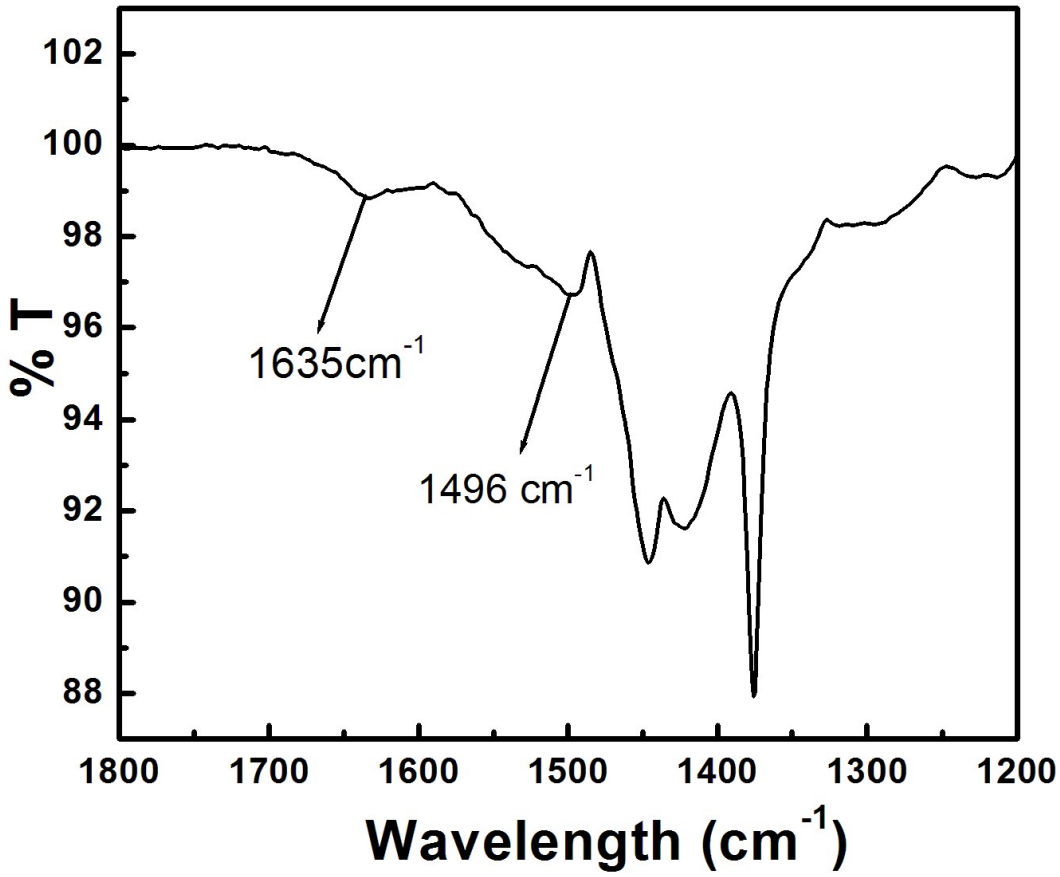


Figure S10. IR Spectrum of $[\mathbf{L^6}\text{-Fe}]^{2+}$ complex

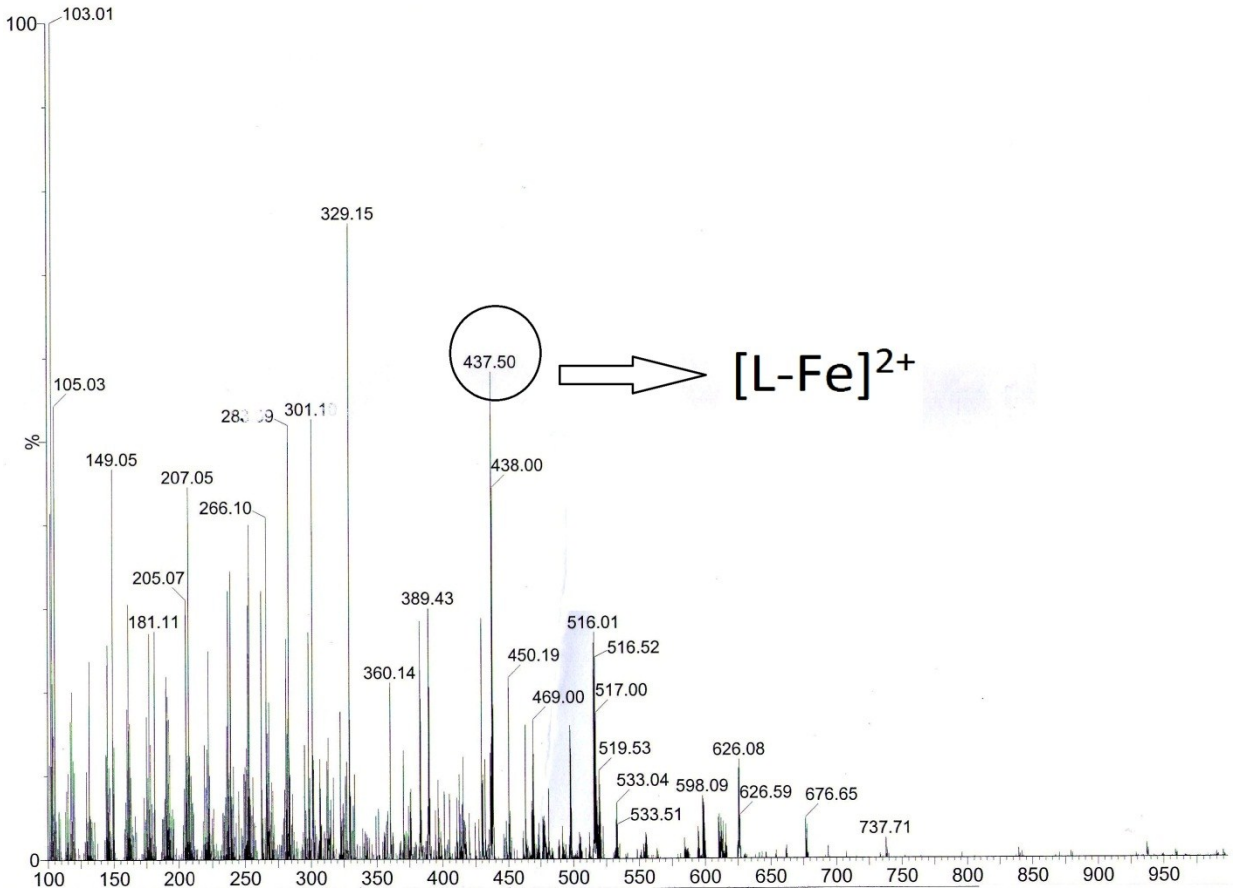


Figure S11a. Mass spectra of **[L^{6}**-Fe]$^{2+}$ complex

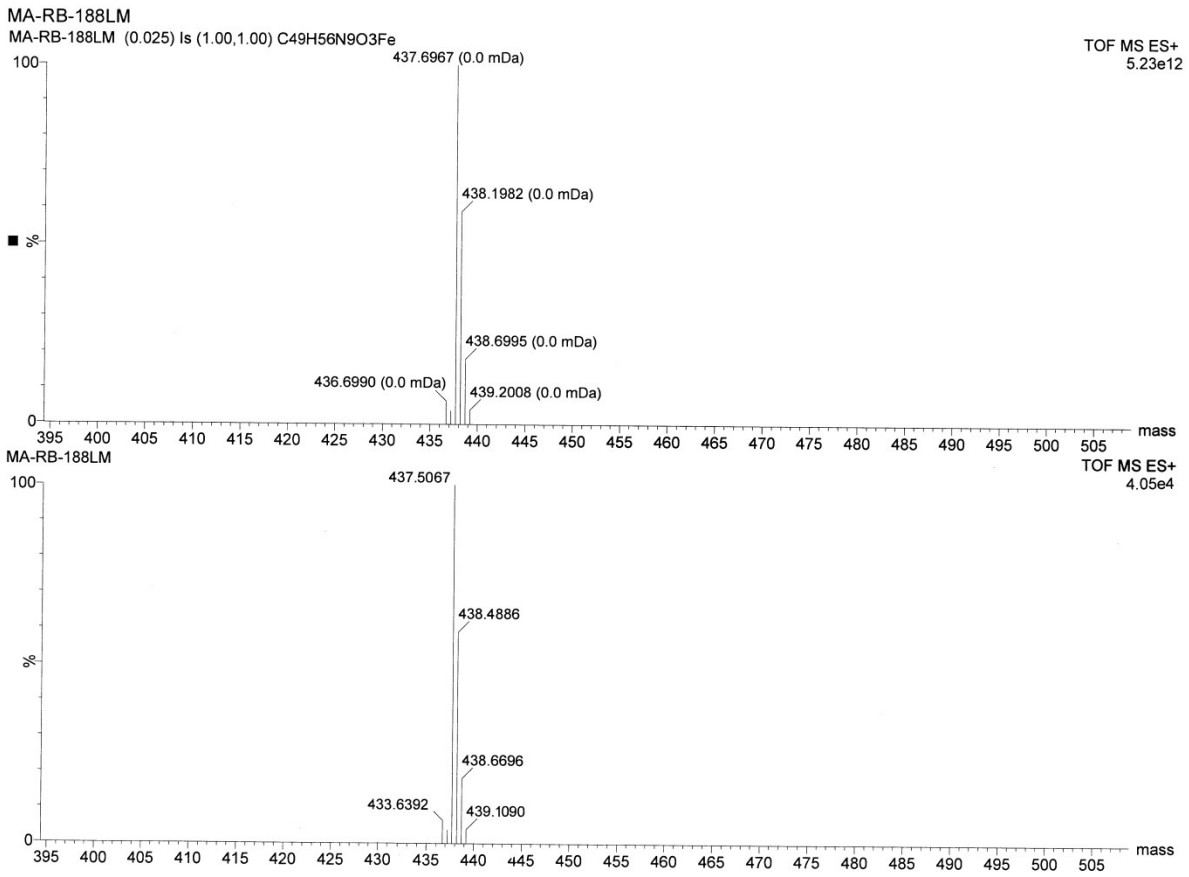


Figure S11b. Simulated Mass spectra of $[\mathbf{L}^{6}\text{-Fe}]^{2+}$ complex

Solution preparation for UV-Vis and fluorescence studies.

10 ml 1.0 x 10^{-3} M solutions of the probe **HL^6** and $Fe(NO_3)_3.9H_2O$ were prepared separately by dissolving appropriate amount of the materials in MeCN and used as stocks for all the UV-Vis and fluorescence studies. Similarly, 1.0 x 10^{-3} M 250 μL HSA solution was prepared freshly in 10 mM Tris buffer prepared by dissolving appropriate amount of HEPES in 100 ml water and pH was adjusted at 7.24 using HCl and NaOH as required. For UV-Vis spectral studies a 2.5 ml aliquot of the buffer solution was pipetted out into a cuvette to which 50 μM of the probe was added. Now, to this buffer solution Fe^{3+} was added starting from 0 to 58 μM at a regular interval of volume. UV-Vis spectra were recorded for each of these solutions. For fluorescence studies, to 20 μM **HL^6** was used instead of 50 μM as in UV-Vis studies keeping other conditions the same and Fe^{3+} was added starting from 0 to 41 μM at a regular incremental volume and fluorescence studies were performed for each solution. Again, for protein binding studies, to 10 μM [**L^6**-Fe]$^{2+}$ complex solution (prepared by mixing equimolar concentration of HL^6 and Fe^{3+}) HSA solution was varied between 0 and 10 μM. For both emission and absorption studies 1 cm path length of the cuvette was used. 2 nm x 2 nm slit widths were used for all fluorescence studies.

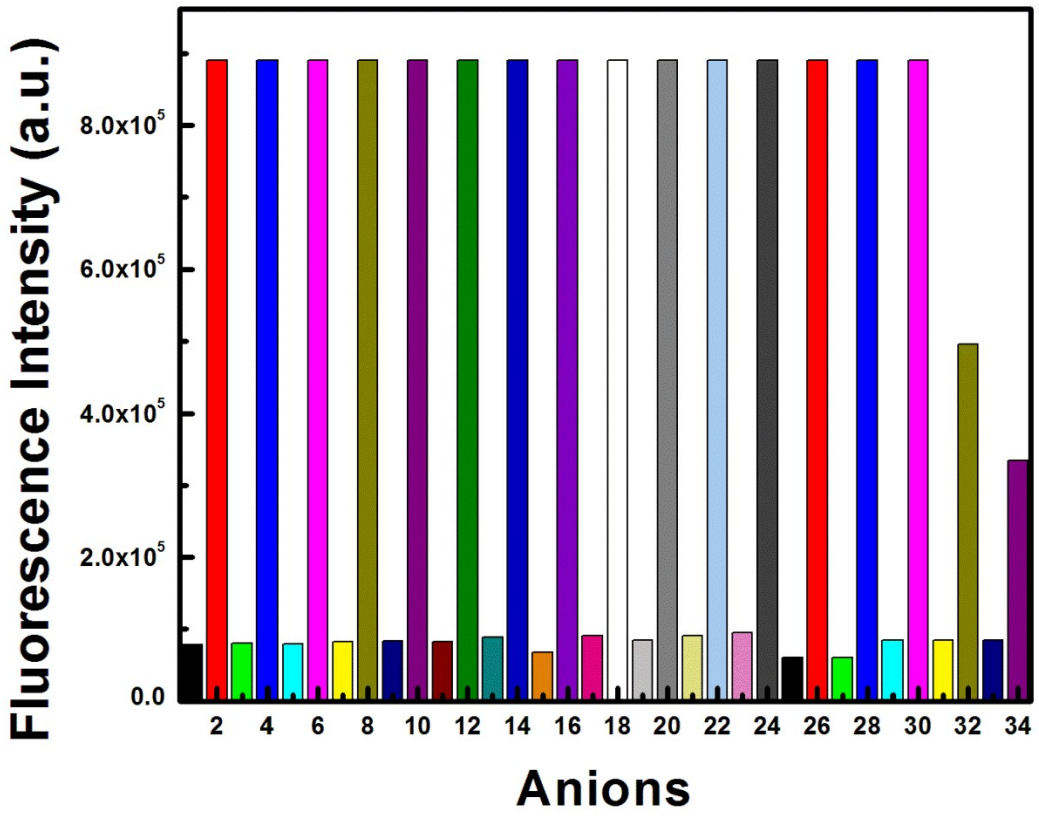


Figure S12a. Fluorescence emission of HL^6 (50 μM) induced by different anions (250 μM). (1-34 are HL^6, HL^6+Fe^{3+}, $HL^6+ CN^-$, $HL^6+ CN^-+Fe^{3+}$, $HL^6+ SO_4^{2-}$, $HL^6+ SO_4^{2-}+Fe^{3+}$, $HL^6+ NO_3^-$, $HL^6+ NO_3^-+Fe^{3+}$, $HL^6+ PO_4^{3-}$, $HL^6+ PO_4^{3-}+Fe^{3+}$, $HL^6+ S^{2-}$, $HL^6+ S^{2-}+Fe^{3+}$, $HL^6+ Cl^-$, $HL^6+ Cl^-+Fe^{3+}$, $HL^6+ Br^-$, $HL^6+ Br^-+Fe^{3+}$, $HL^6+ OAc^-$, $HL^6+ OAc^-+Fe^{3+}$, $HL^6+ H_2AsO_4^-$, $HL^6+ H_2AsO_4^-+Fe^{3+}$, $HL^6+ ClO_4^-$, $HL^6+ ClO_4^-+Fe^{3+}$, $HL^6+ S_2O_4^{2-}$, $HL^6+ S_2O_4^{2-}+Fe^{3+}$, $HL^6+ HCO_3^-$, $HL^6+ HCO_3^-+Fe^{3+}$, $HL^6+ SCN^-$, $HL^6+ SCN^-+Fe^{3+}$, $HL^6+ P_2O_7^{4-}$, $HL^6+ P_2O_7^{4-}+Fe^{3+}$, $HL^6+ F^{-+}$,$HL^6+ F^-+Fe^{3+}$, $HL^6+ I^-$, $HL^6+ I^-+Fe^{3}$). Here ferric nitrate used.

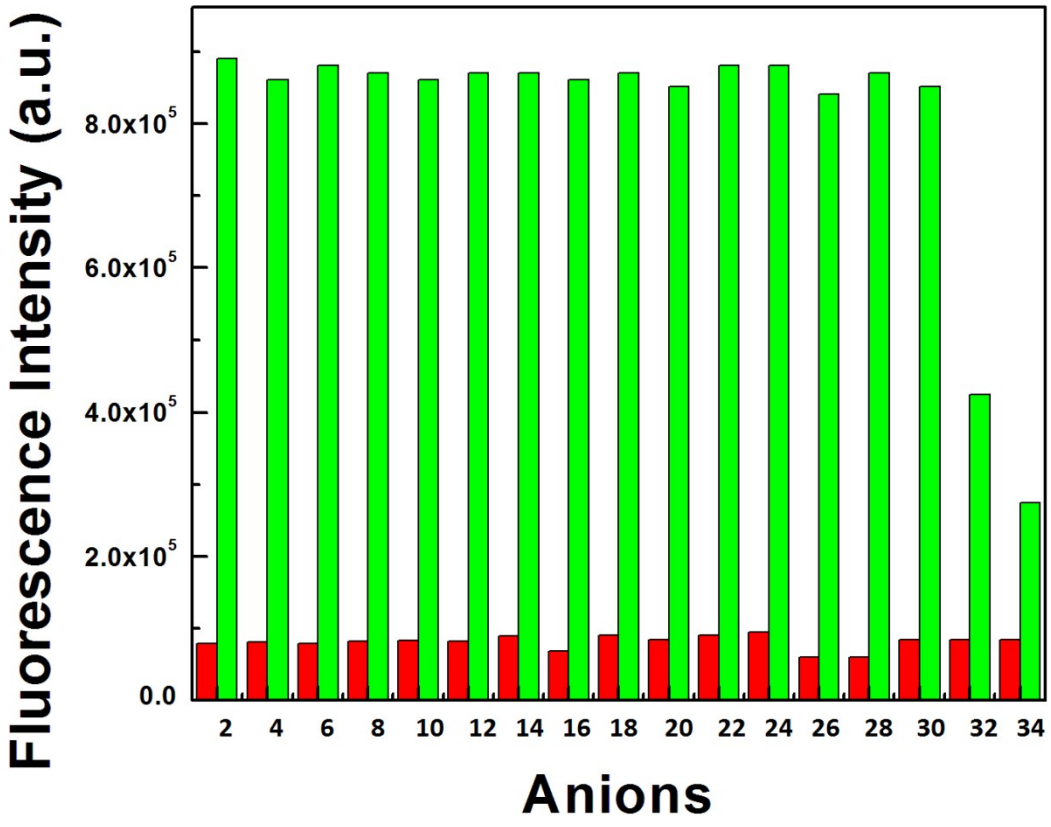


Figure S12b. Fluorescence emission of HL^6 (50 μM) induced by different anions (250 μM). (1-34 are HL^6, HL^6+Fe^{3+}, $HL^6+ CN^-$, $HL^6+ CN^-+Fe^{3+}$, $HL^6+ SO_4^{2-}$, $HL^6+ SO_4^{2-}+Fe^{3+}$, $HL^6+ NO_3^-$, $HL^6+ NO_3^-+Fe^{3+}$, $HL^6+ PO_4^{3-}$, $HL^6+ PO_4^{3-}+Fe^{3+}$, $HL^6+ S^{2-}$, $HL^6+ S^{2-}+Fe^{3+}$, $HL^6+ Cl^-$, $HL^6+ Cl^-+Fe^{3+}$, $HL^6+ Br^-$, $HL^6+ Br^-+Fe^{3+}$, $HL^6+ OAc^-$, $HL^6+ OAc^-+Fe^{3+}$, $HL^6+ H_2AsO_4^-$, $HL^6+ H_2AsO_4^-+Fe^{3+}$, $HL^6+ ClO_4^-$, $HL^6+ ClO_4^-+Fe^{3+}$, $HL^6+ S_2O_4^{2-}$, $HL^6+ S_2O_4^{2-}+Fe^{3+}$, $HL^6+ HCO_3^-$, $HL^6+ HCO_3^-+Fe^{3+}$, $HL^6+ SCN^-$, $HL^6+ SCN^-+Fe^{3+}$, $HL^6+ P_2O_7^{4-}$, $HL^6+ P_2O_7^{4-}+Fe^{3+}$, $HL^6+ F^{-+}$,$HL^6+ F^-+Fe^{3+}$, $HL^6+ I^-$, $HL^6+ I^-+Fe^{3}$). Here ferric perchlorate used.

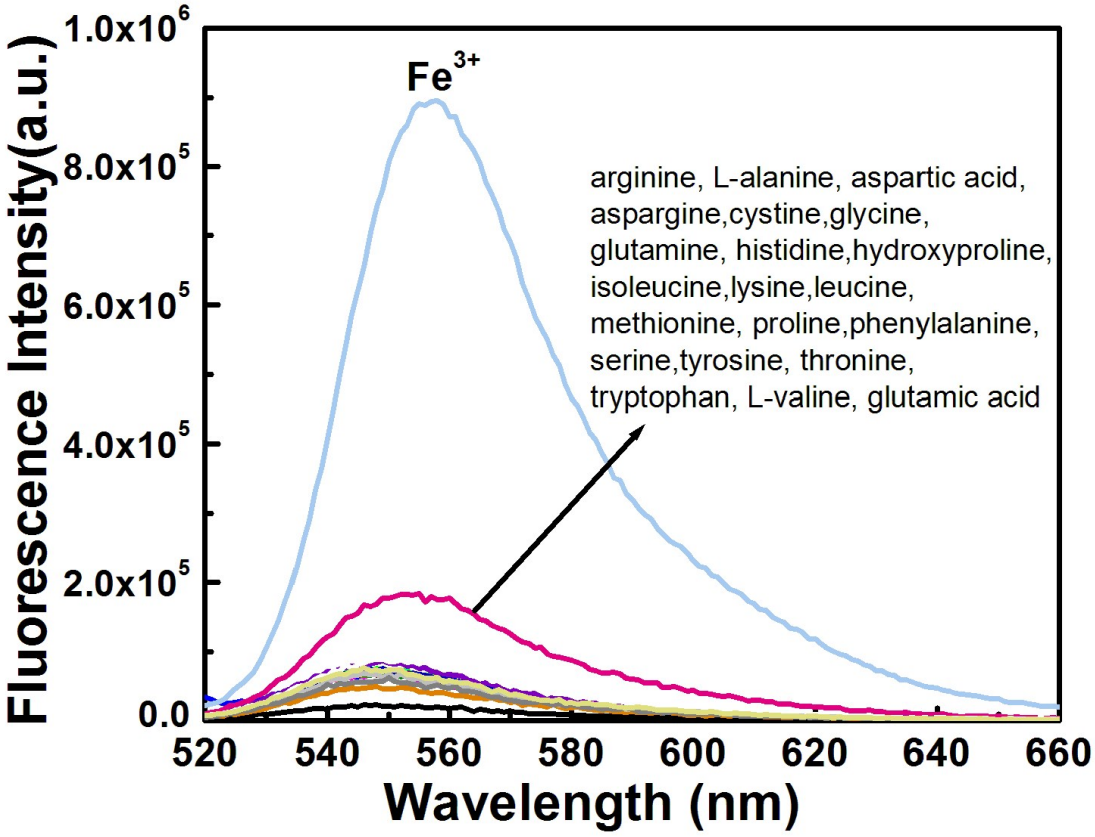


Figure S13. Fluorescence emission induced by different amino acids.

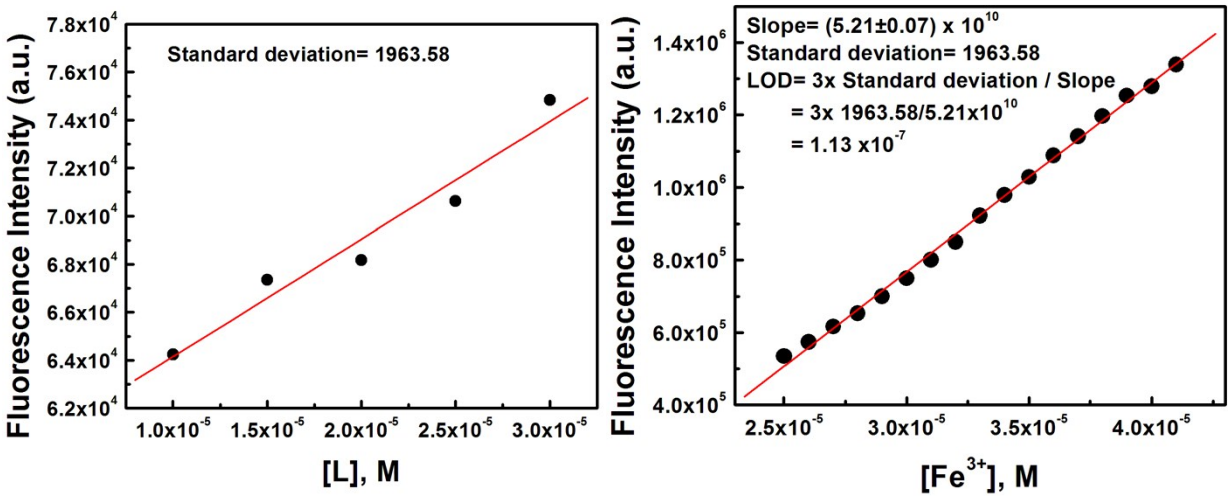


Figure S14. Determination of Limit of detection (LOD) of Fe^{3+} by L from the slope of the plot of FI vs. [Fe^{3+}] and the standard deviation of the blank (intercept) determined from the plot of FI vs. [L] utilizing 3σ method.

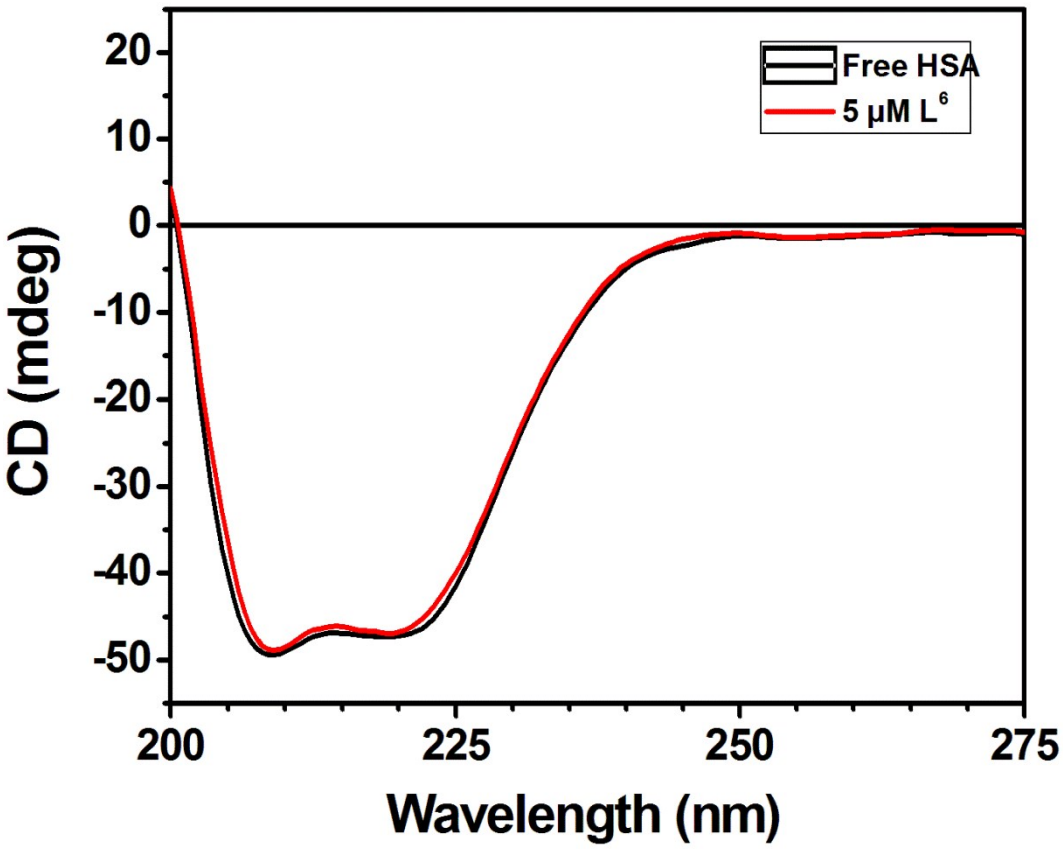


Figure S15. Effect of **L**^{6} on intrinsic circular dichroic (CD) spectrum of HAS; CD spectrum of 1.0 μM HSA treated with 5.0 μM **L**^{6}, at 25 °C.

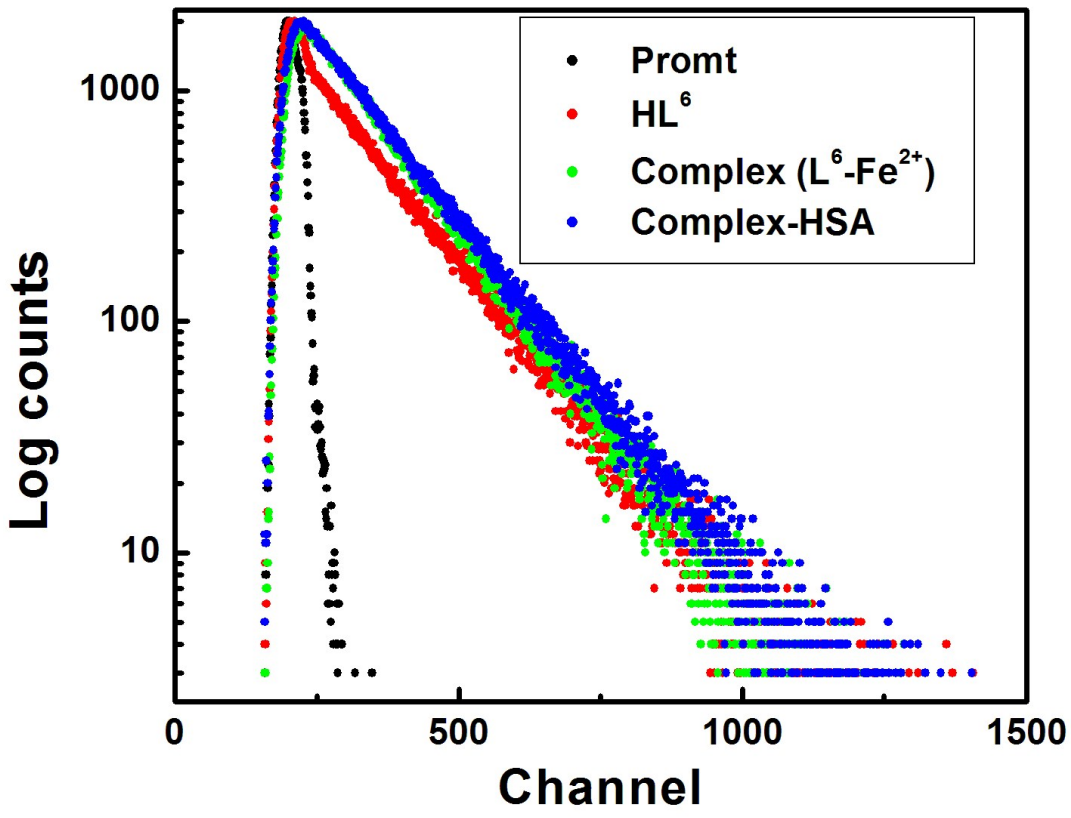


Figure S16. Fluorescence decay curves of HL^6, $[L^6\text{-}Fe]^{2+}$ and $[L^6\text{-}Fe]^{2+}$ in presence of HSA.

Table S1. Life time of $[L^6\text{-}Fe]^{2+}$ complex in different protein concentration monitored 450 nm plate.

[HSA], μM	Life time(ns)
0	3.26
2	3.50
4	3.51
6	3.52
8	3.53
10	3.59

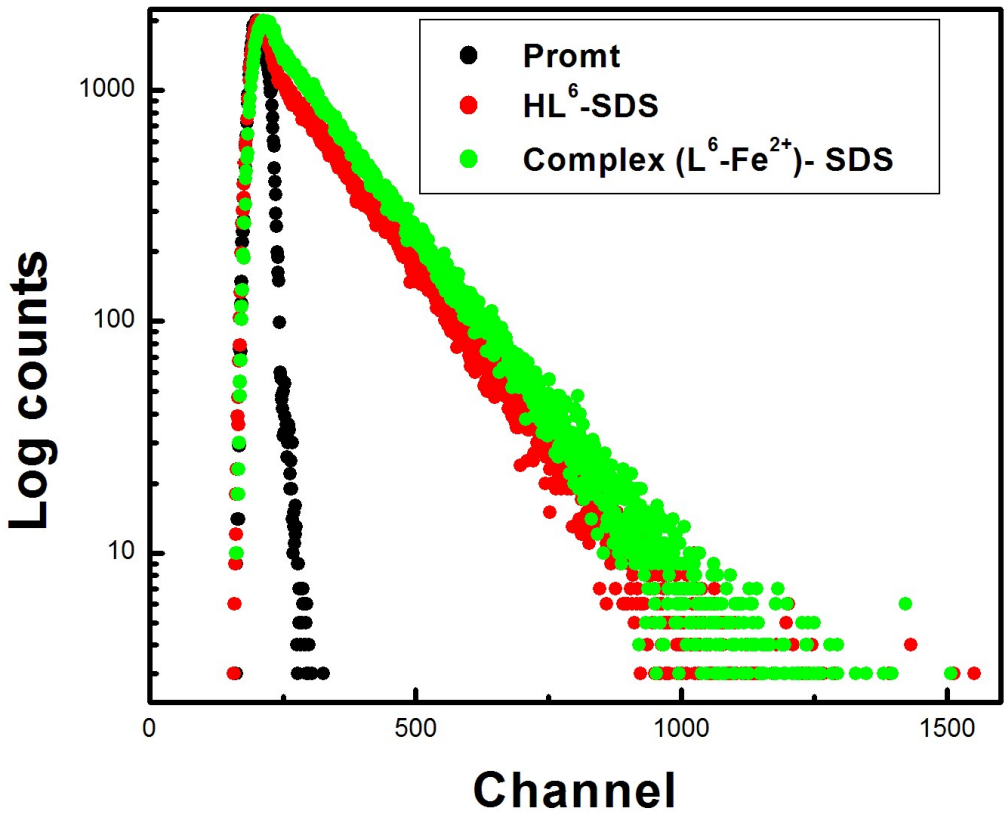


Figure S17. Fluorescence decay curves of $HL^6$and $[L^6\text{-}Fe]^{2+}$ in presence of SDS.

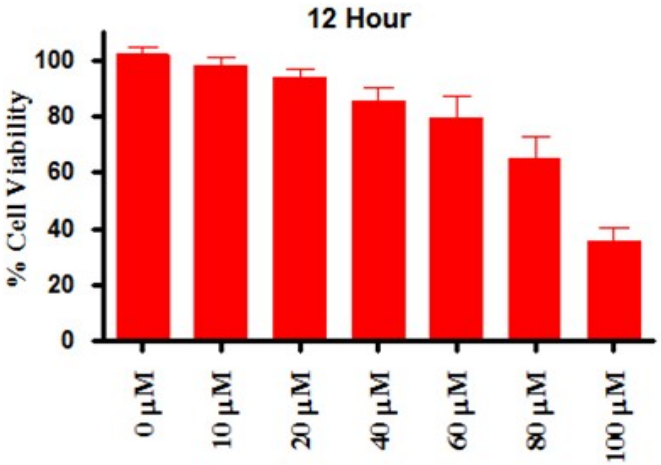
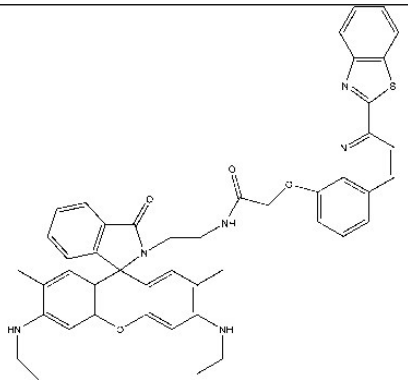
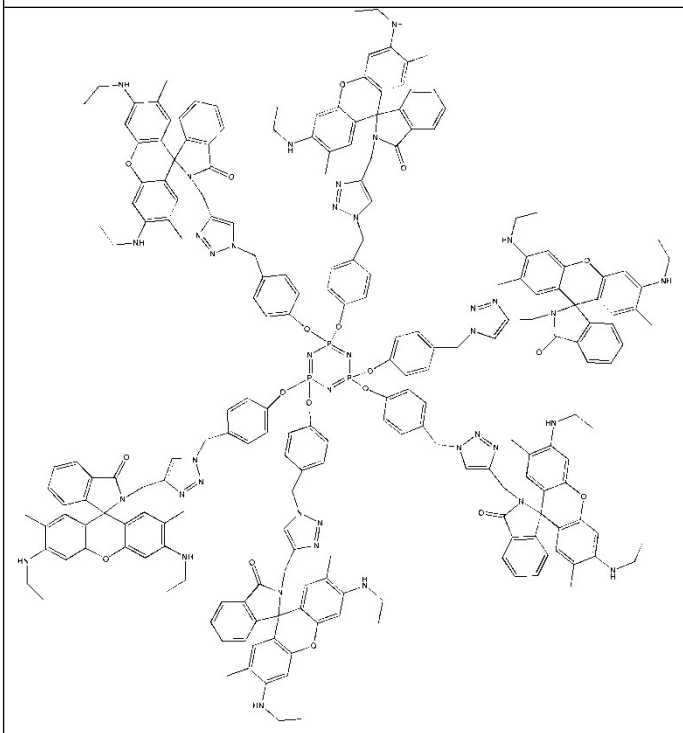
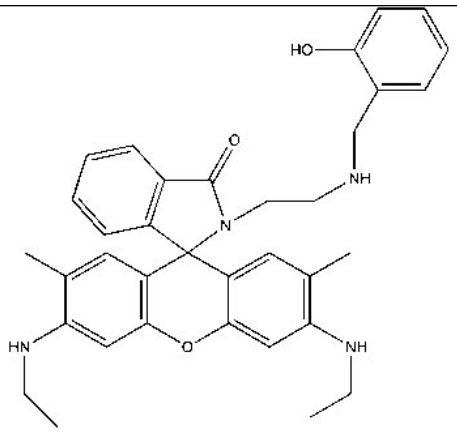
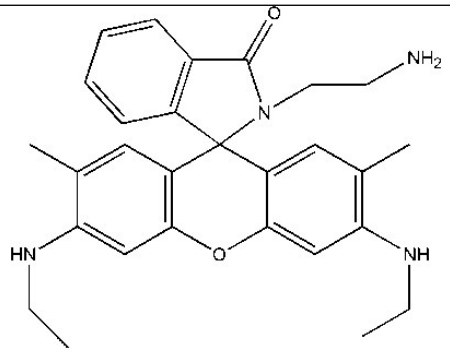
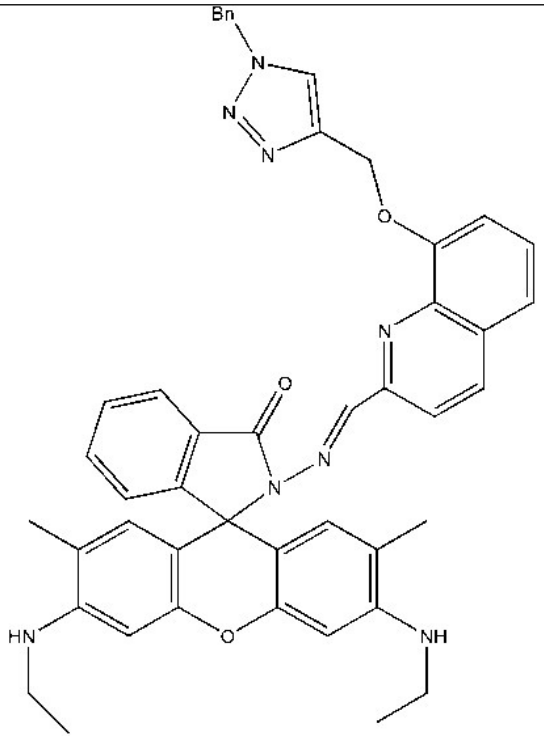
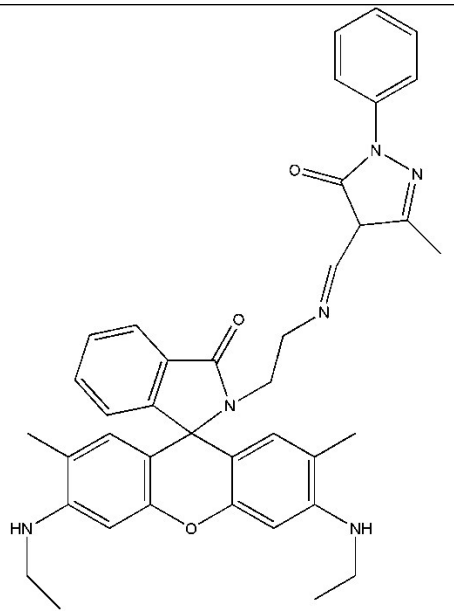
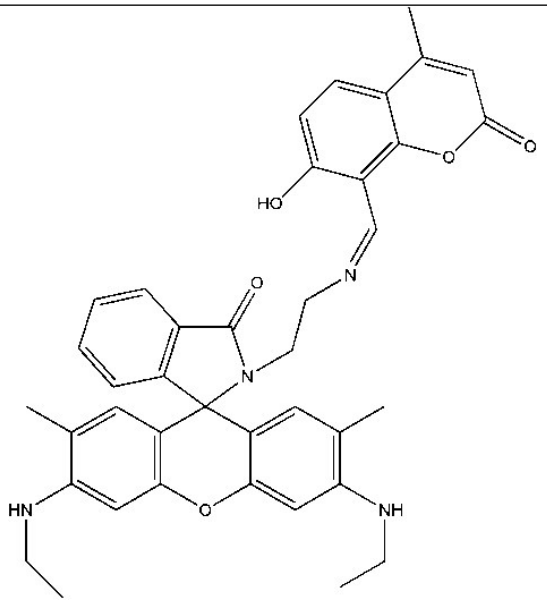


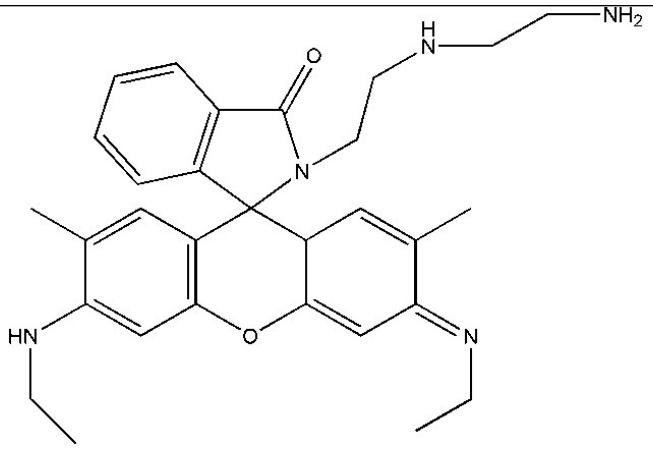
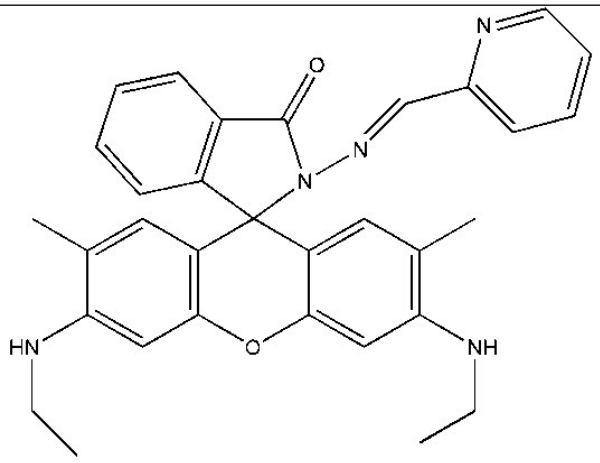
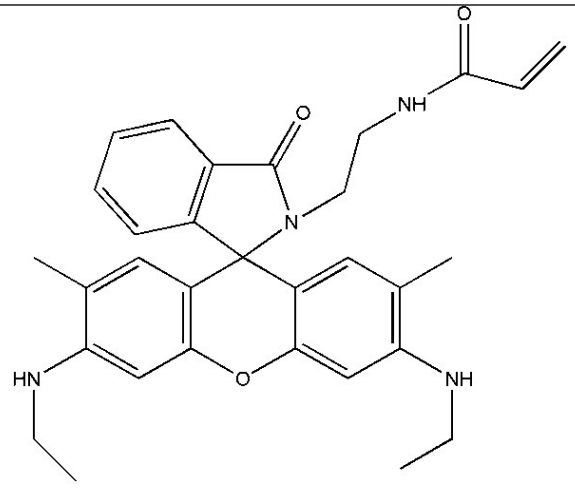
Figure S18. Cell viability assay performed by using ligand HL^6.

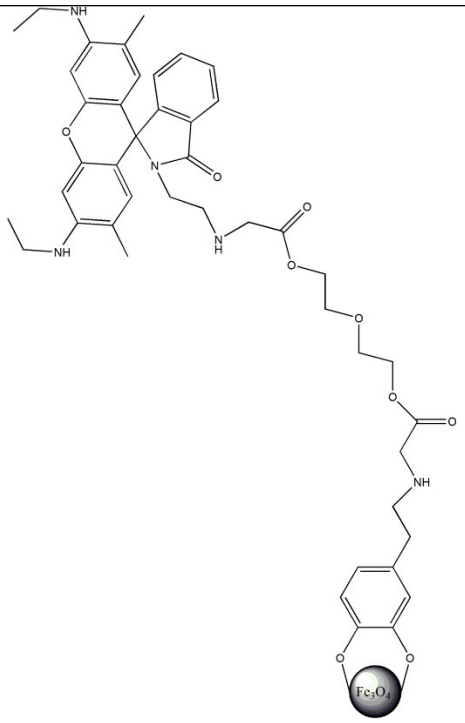
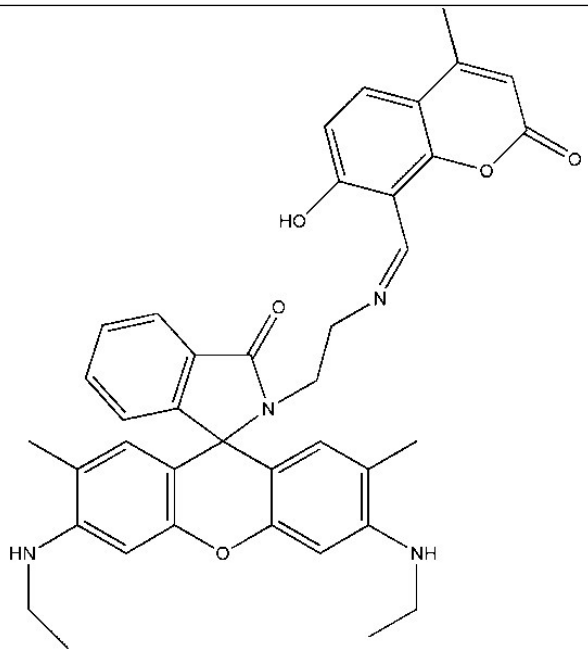
Table S2. Comparison of results of the probe HL^6 with other reported Fe^{3+} sensors.

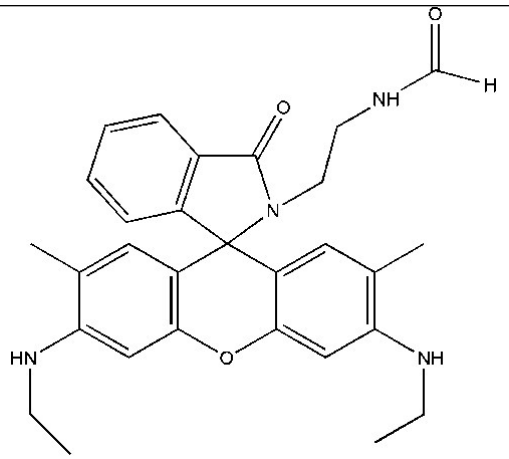
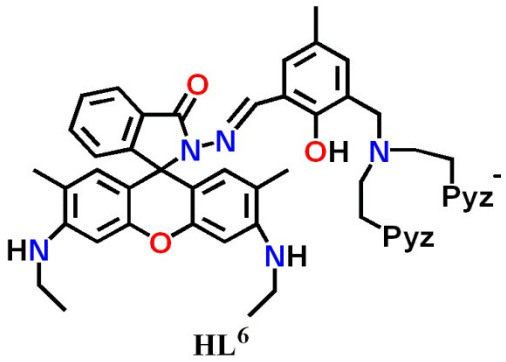
Ligand	Solvent(s)	Limit of Detection	Ref
	CH_3OH/H_2O (2/3)	0.01μM	38
	THF/H_2O (99:1)	4.8μM	39

	EtOH	-	40
	10% Aqueous ethanol	-	41
	Tris-HCl: CH_3CN(1:1)	0.05µM	42

	H_2O: CH_3CN(1:1)	6.1µM	43
	Ethanol	5.6ppb	44

	DMF/H_2O	-	45
	H_2O: CH_3CN(1:1)	0.09 µM	46
	Hydrogel formation insluble in H_2O	-	47

	Aqueous	2ppb	48
	Aqueous	0.72µM	49

	Aqueous	0.01μM	50
	Aqueous	0.11 μM	This work