

**Electronic Supplementary Information**  
**For the**  
**Manuscript Entitled**

**Arene-based Fluorescent Probes for the Selective**  
**Detection of Iron**

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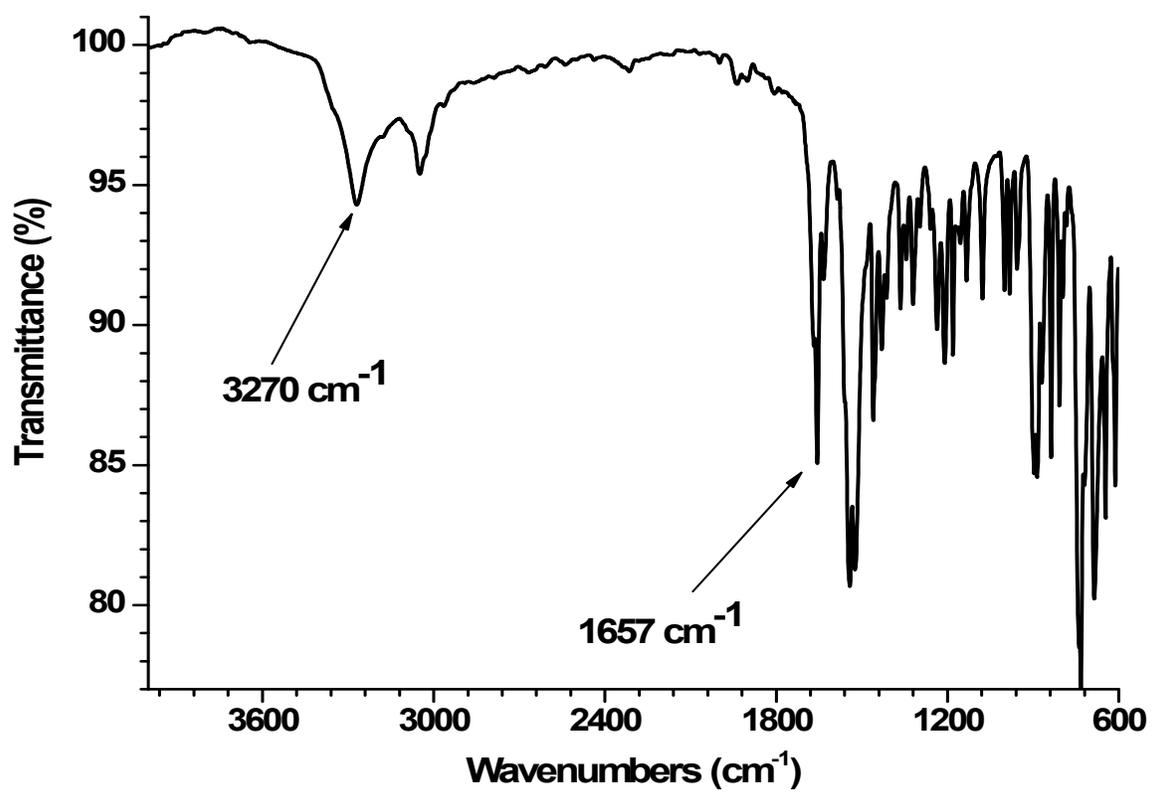


Figure S1. FTIR spectrum of probe L3.

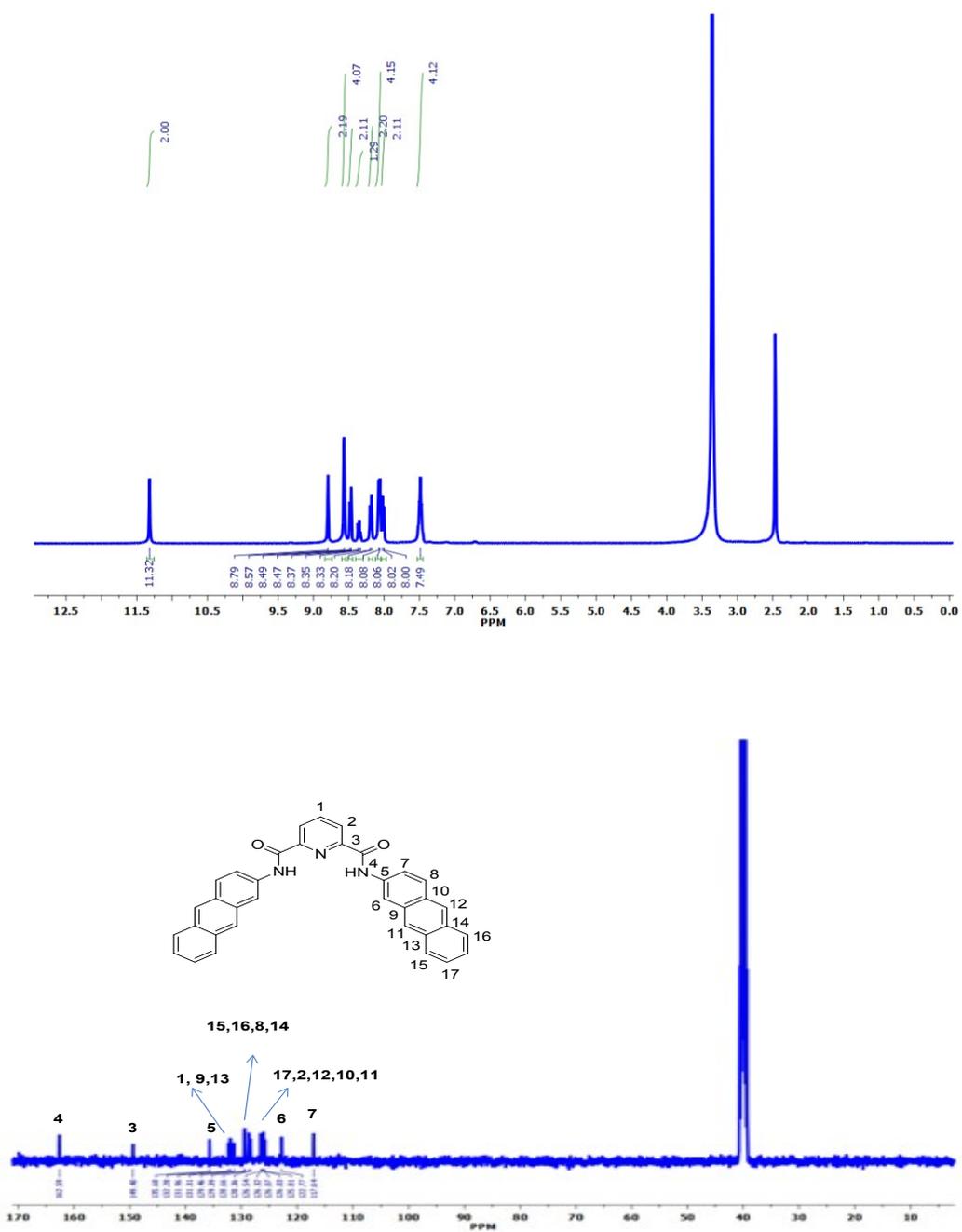


Figure S2.  $^1\text{H}$  (top) and  $^{13}\text{C}$  (bottom) NMR spectra of probe L3 in  $\text{CDCl}_3$ .

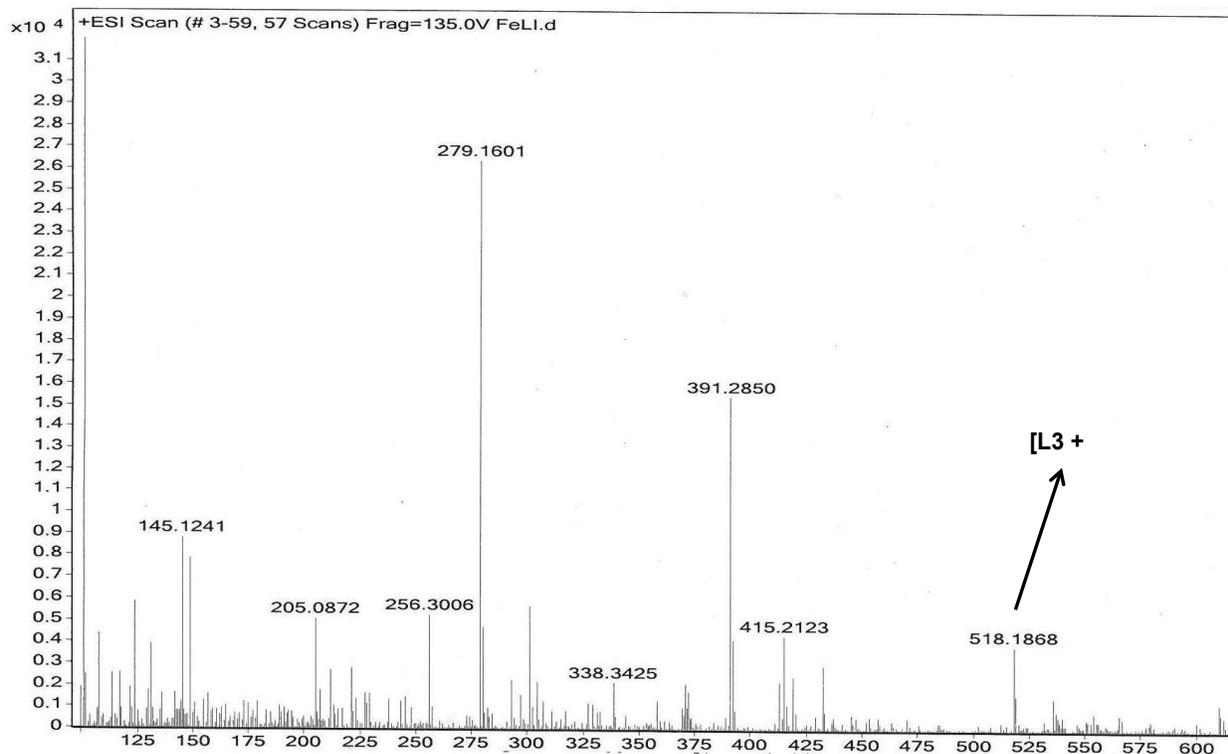


Figure S3. ESI<sup>+</sup>-MS spectrum of probe L3 in THF.

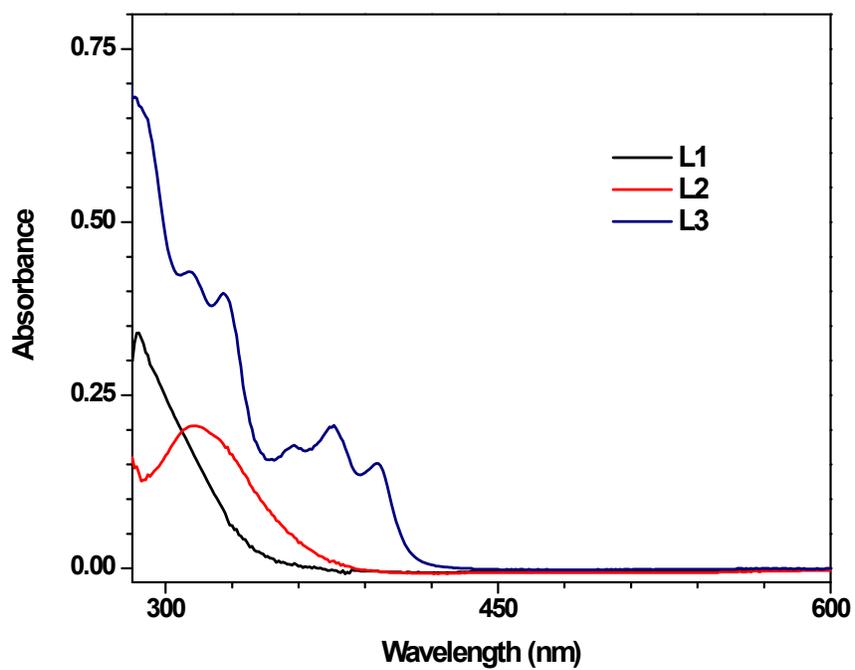
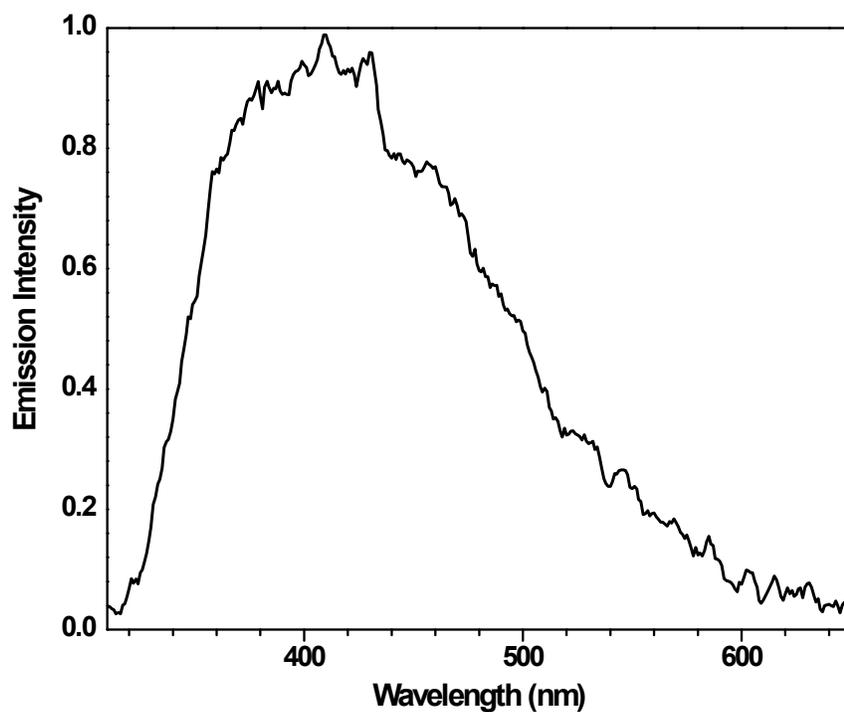
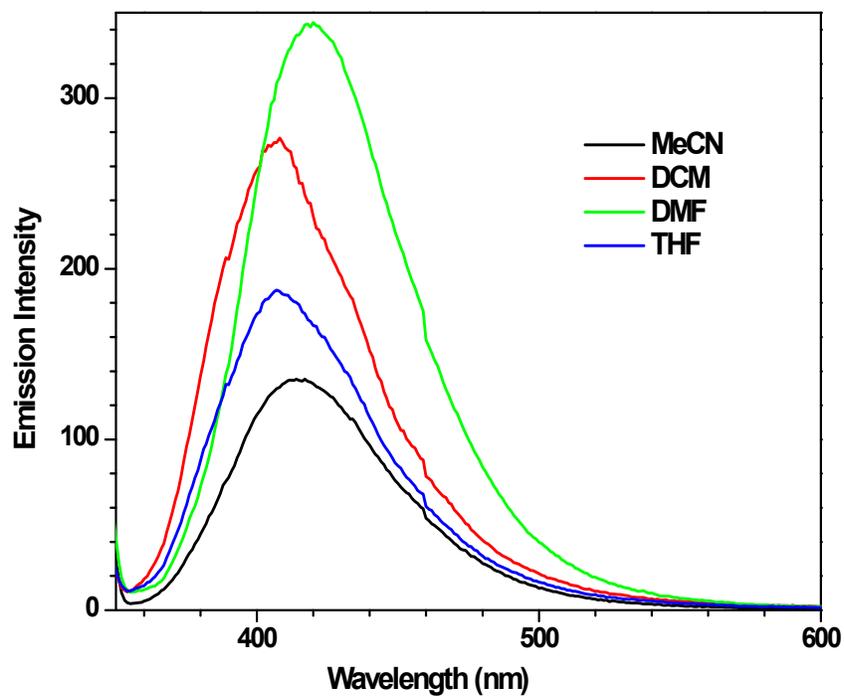


Figure S4. UV-Vis spectra of probes L1, L2 and L3 (20  $\mu$ M) in THF.

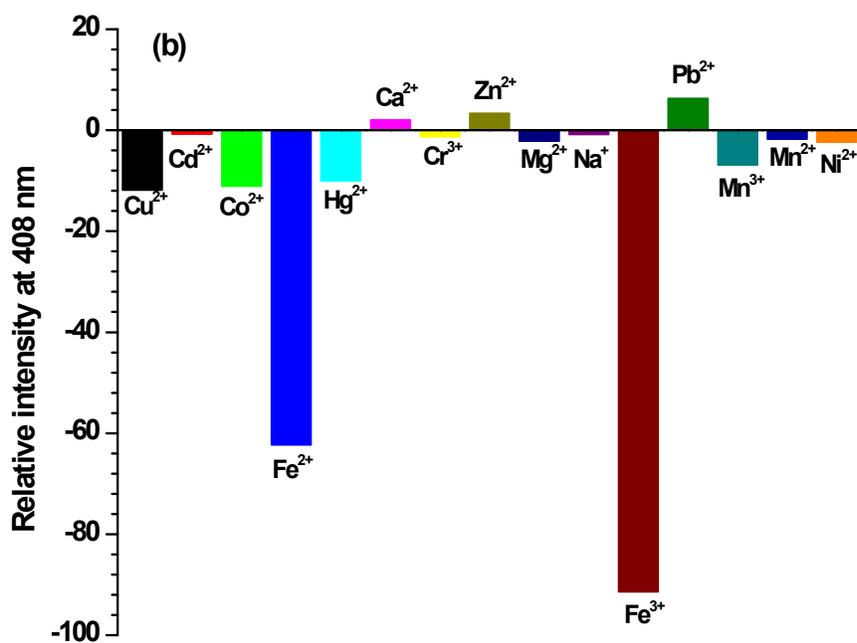
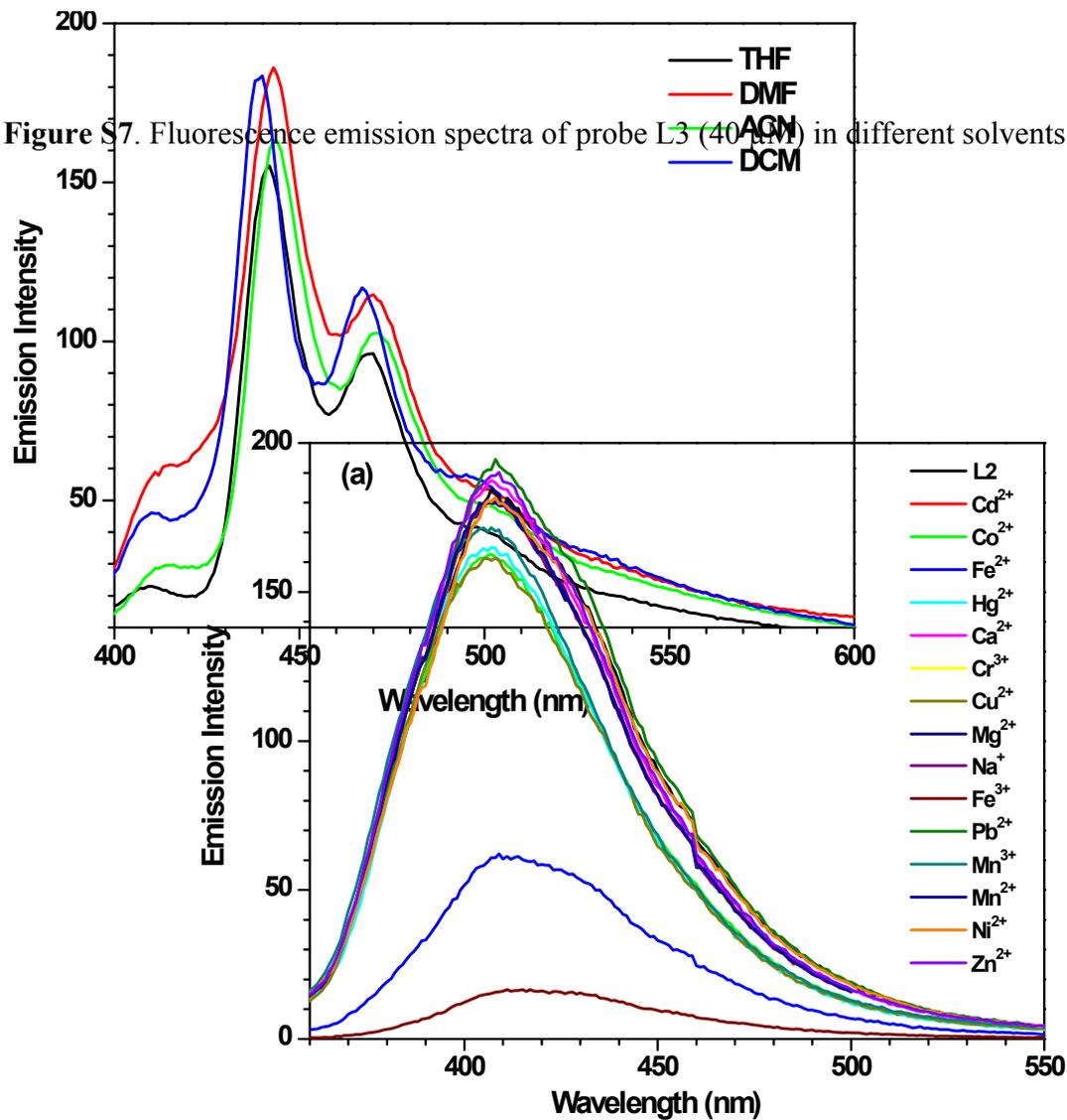


**Figure S5.** Fluorescence emission spectrum of L1 (100 μM) in MeOH (Ex- 300 nm).

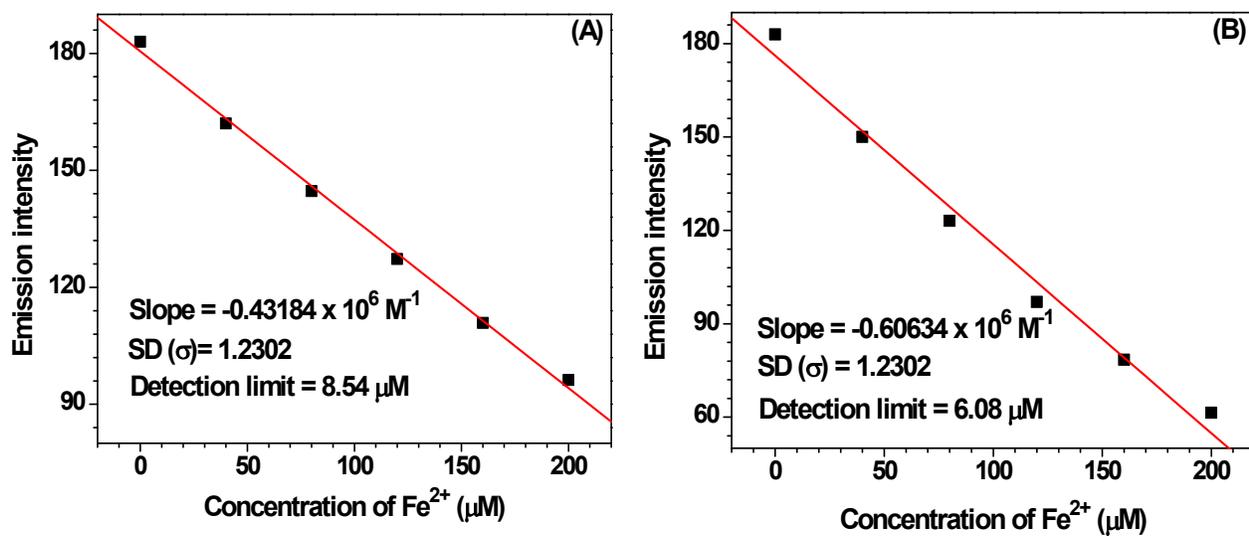


**Figure S6.** Fluorescence emission spectra of probe L2 (40 μM) in different solvents.

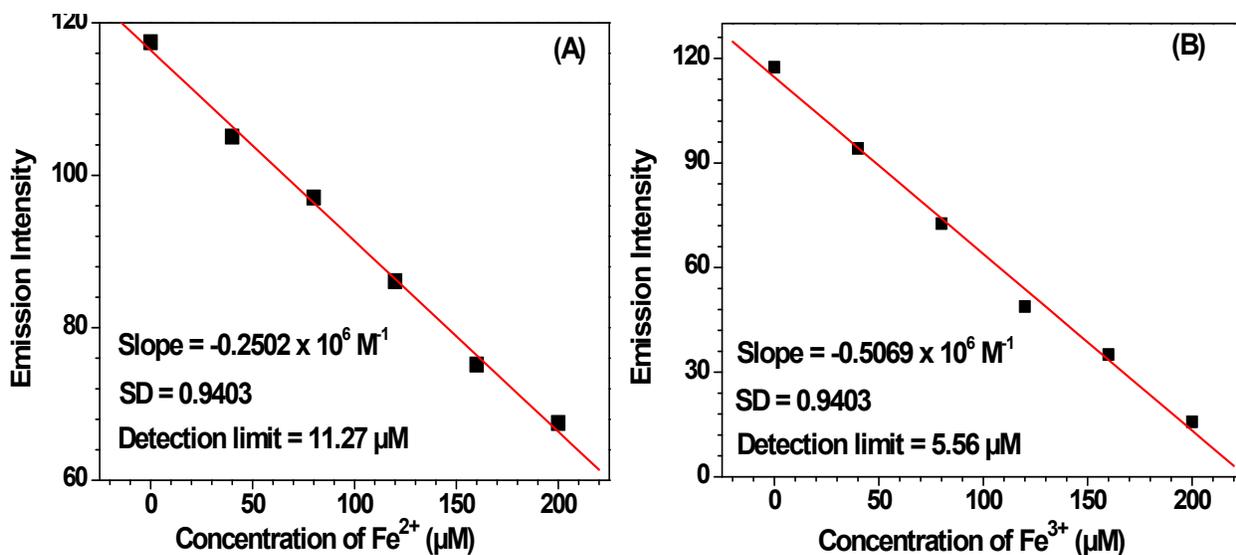
Figure S7. Fluorescence emission spectra of probe L3 (40  $\mu$ M) in different solvents.



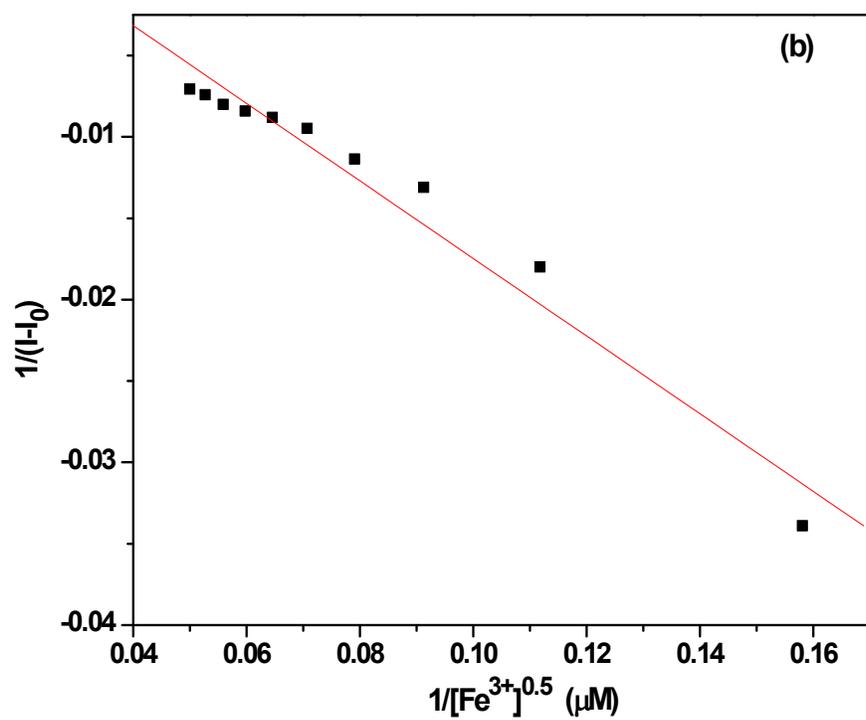
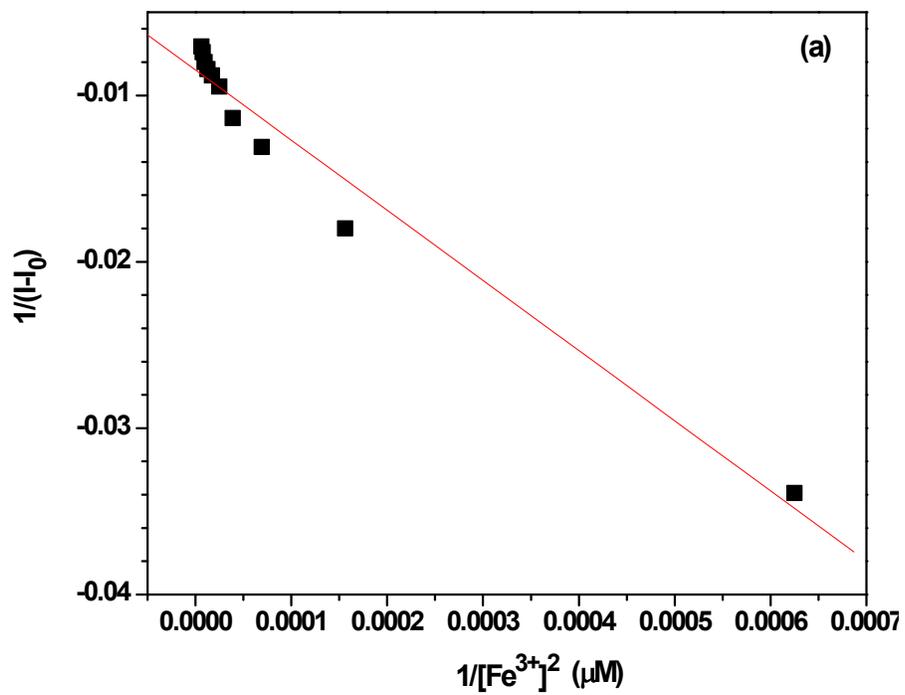
**Figure S8.** (a) Fluorescence emission spectra of L2 (40  $\mu\text{M}$ ) in THF and after its interaction with 10 equivalents of assorted metal ions. (b) Bar diagram exhibiting change in emission intensity of L2 (40  $\mu\text{M}$ ) in THF after addition of 10 equivalents of assorted metal ions.



**Figure S9.** Determination of detection limit of probe L2 towards (A)  $\text{Fe}^{2+}$  (B)  $\text{Fe}^{3+}$  ions (Concentration was linear from 0 - 200  $\mu\text{M}$ ).



**Figure S10.** Determination of detection limit of probe L3 towards (A)  $\text{Fe}^{2+}$  (B)  $\text{Fe}^{3+}$  (Concentration was linear from 0 - 200  $\mu\text{M}$ ).



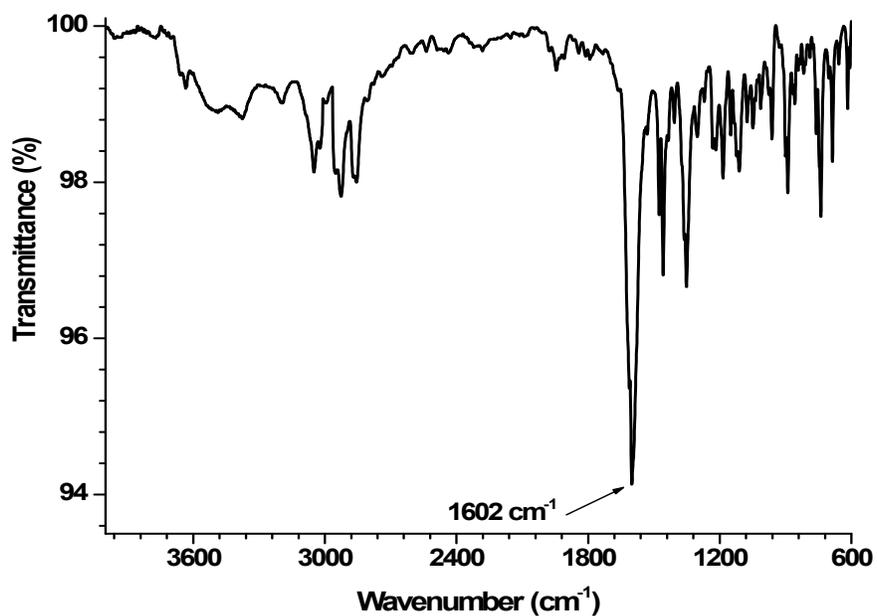


Figure S12. FTIR spectrum of complex 1.

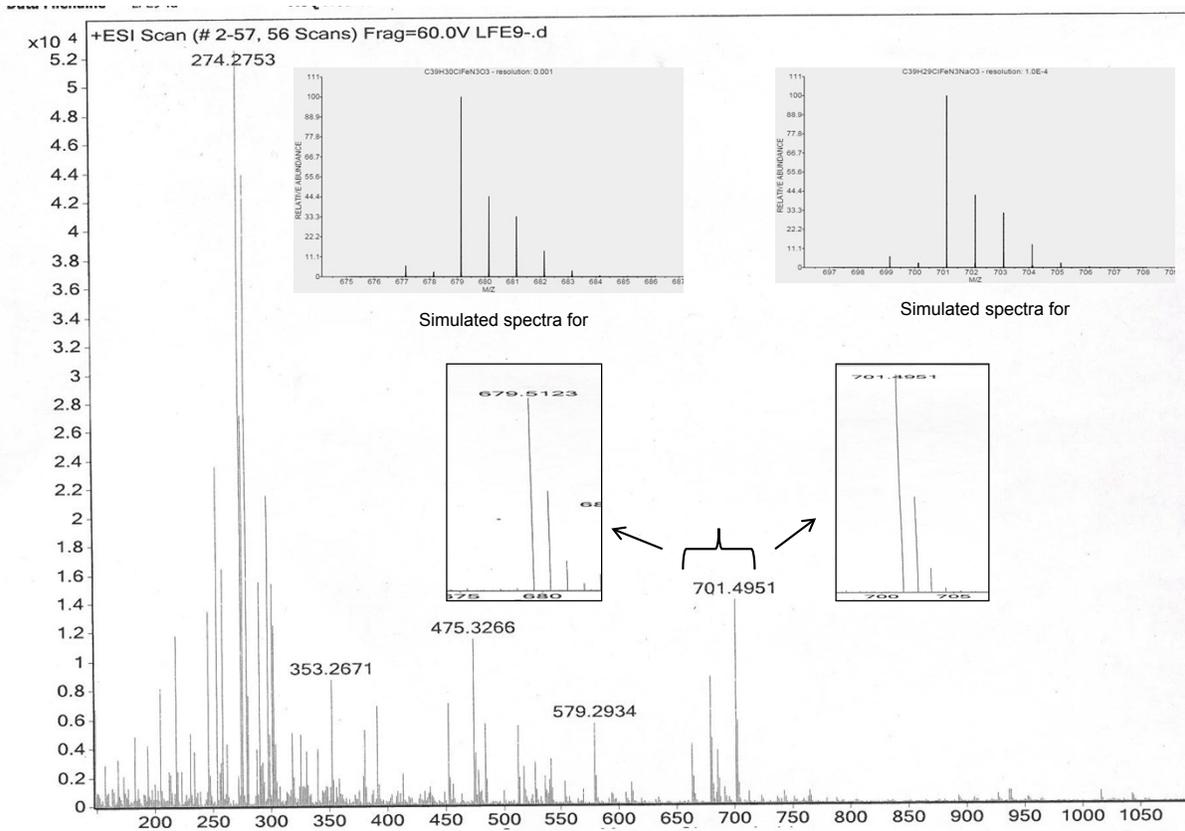
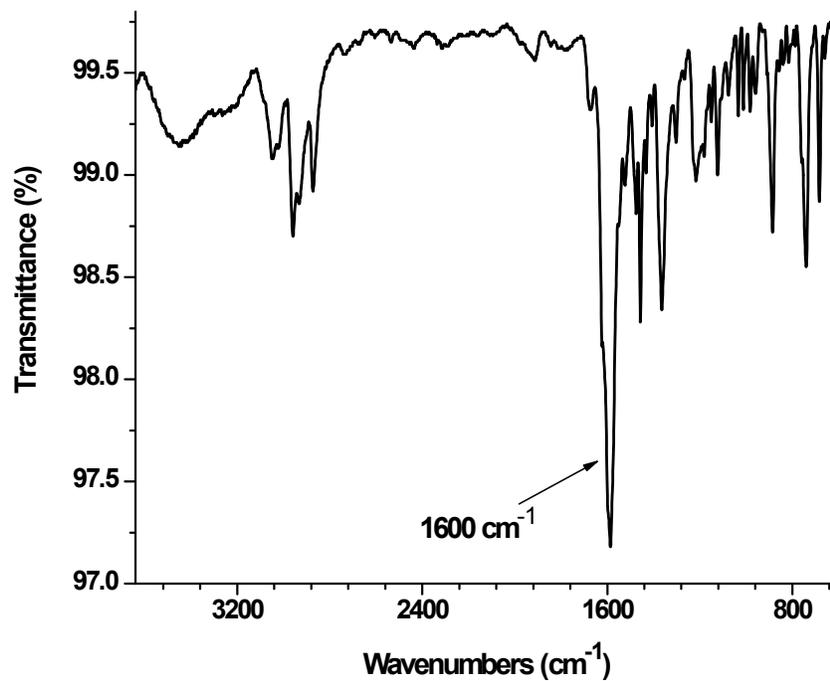
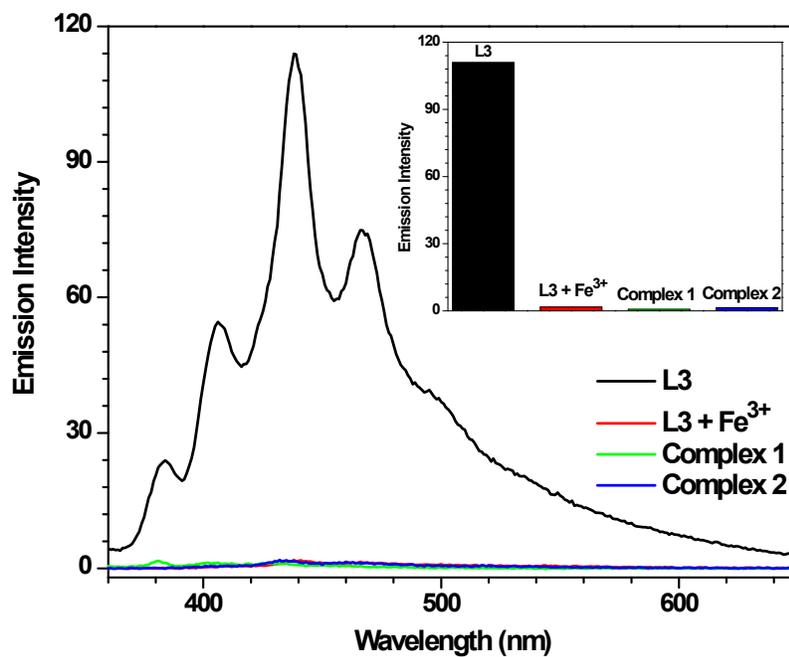


Figure S13. ESI<sup>+</sup>-MS spectrum of a mixture of L3 and FeCl<sub>3</sub> in THF along with the simulated spectrum.



**Figure S14.** FTIR spectrum of complex 2.



**Figure S15.** Emission spectra of probe L3 (40  $\mu\text{M}$ ); in presence of 10 equiv of Fe<sup>3+</sup> ion; complex 1; and complex 2 (40  $\mu\text{M}$ ) in THF.

**Table S1.** Crystallographic data collection and structure solution parameters for complex **2**.

	<b>2</b>
Formula	C <sub>84</sub> H <sub>74</sub> FeN <sub>7</sub> O <sub>4</sub>
Formula weight	1301.35
T (K)	298(2)
System	Monoclinic
Space group	I 2
<i>a</i> (Å)	13.412(3)
<i>b</i> (Å)	10.469(2)
<i>c</i> (Å)	29.031(7)
$\alpha$ (°)	90
$\beta$ (°)	100.999(19)
$\gamma$ (°)	90
<i>V</i> (Å <sup>3</sup> )	4001.4(15)
<i>Z</i>	2
$\rho_{\text{calc}}$ (mg/m <sup>3</sup> )	1.080
<i>F</i> (000)	1370
Goodness-of-fit (GOF) on <i>F</i> <sup>2</sup>	0.871
Final <i>R</i> indices [ <i>I</i> > 2σ( <i>I</i> )]	<i>R</i> <sub>1</sub> = 0.1190, <i>WR</i> <sub>2</sub> = 0.2699
<i>R</i> indices (all data)	<i>R</i> <sub>1</sub> = 0.2560, <i>WR</i> <sub>2</sub> = 0.3413