

# Supporting Information

## **Fluorescence turn-on detection of Fe<sup>3+</sup> in pure water based on a cationic poly(perylene diimide) derivative**

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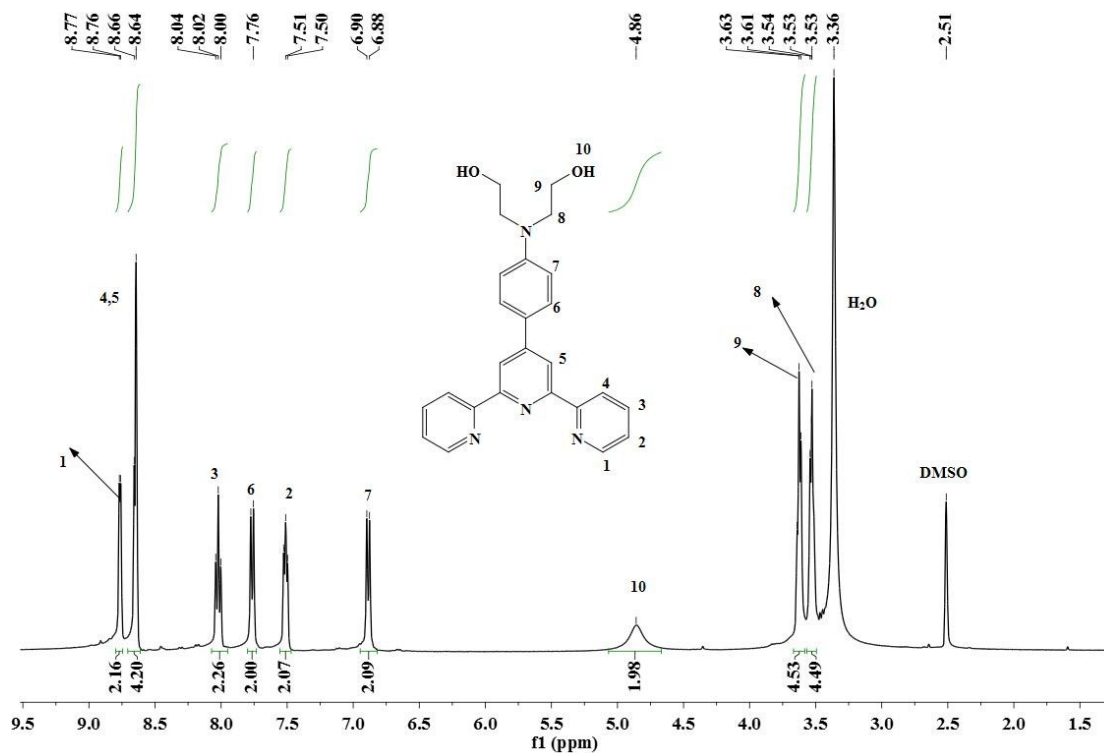


Fig. S1:  $^1\text{H}$  NMR of compound 1.

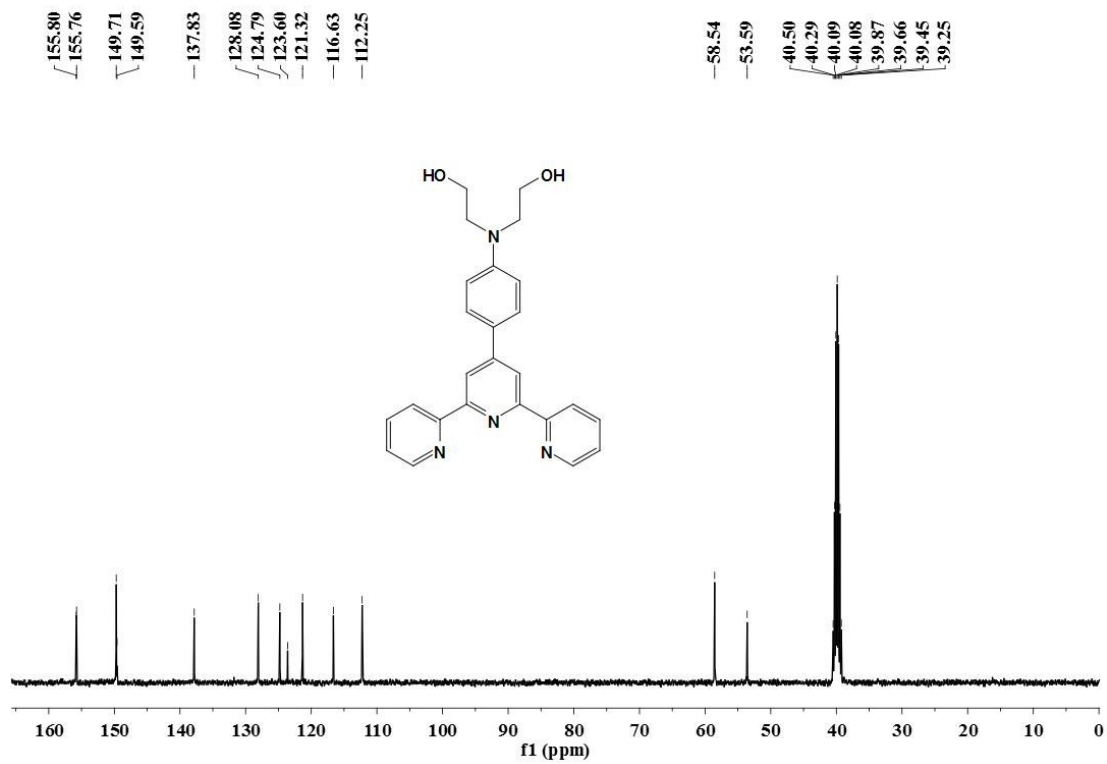
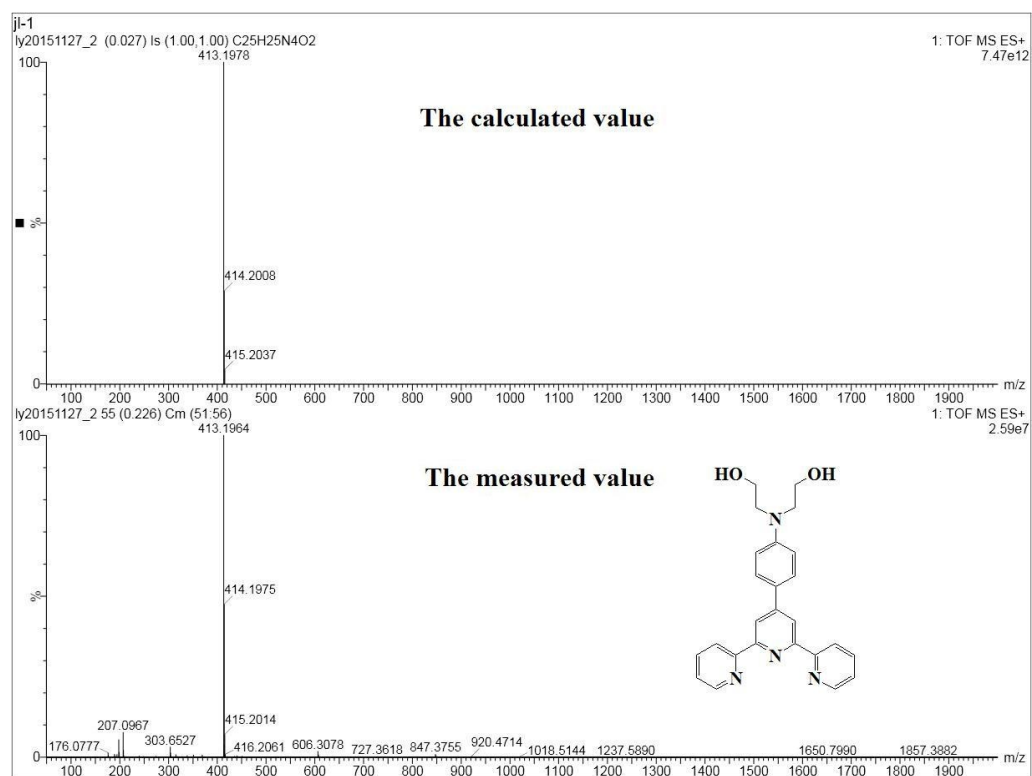
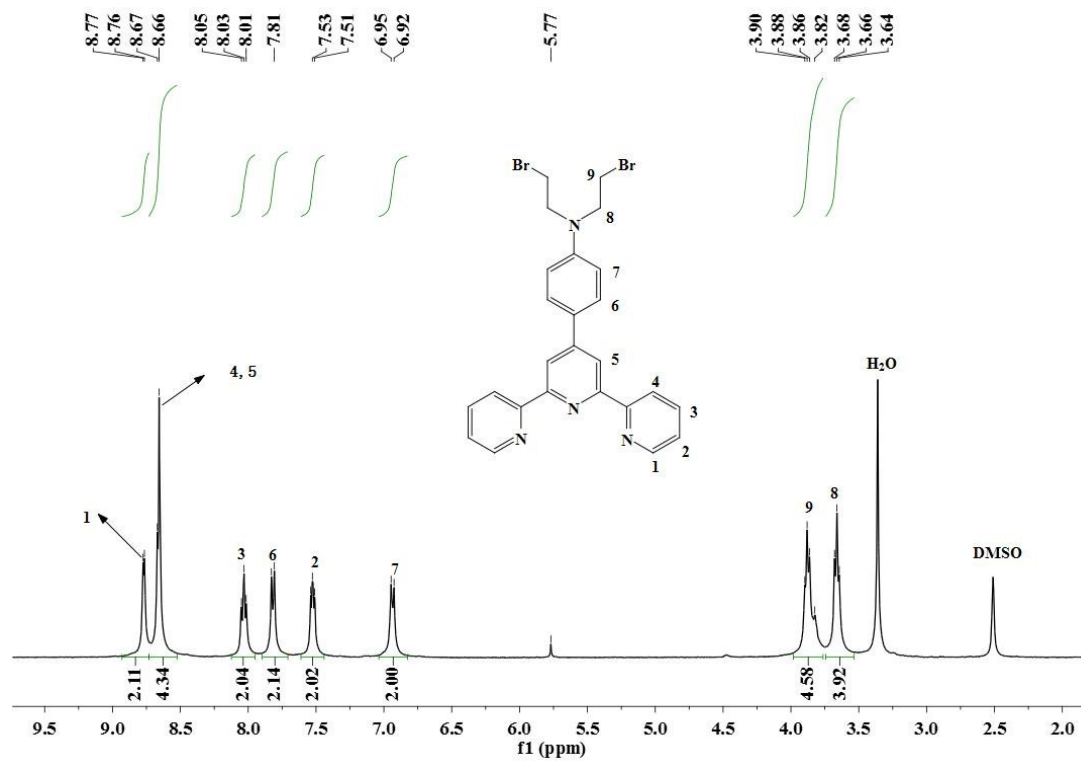


Fig. S2:  $^{13}\text{C}$  NMR of compound 1.



**Fig. S3:** HRMS spectra of compound 1.



**Fig. S4:** <sup>1</sup>H NMR of compound 2.

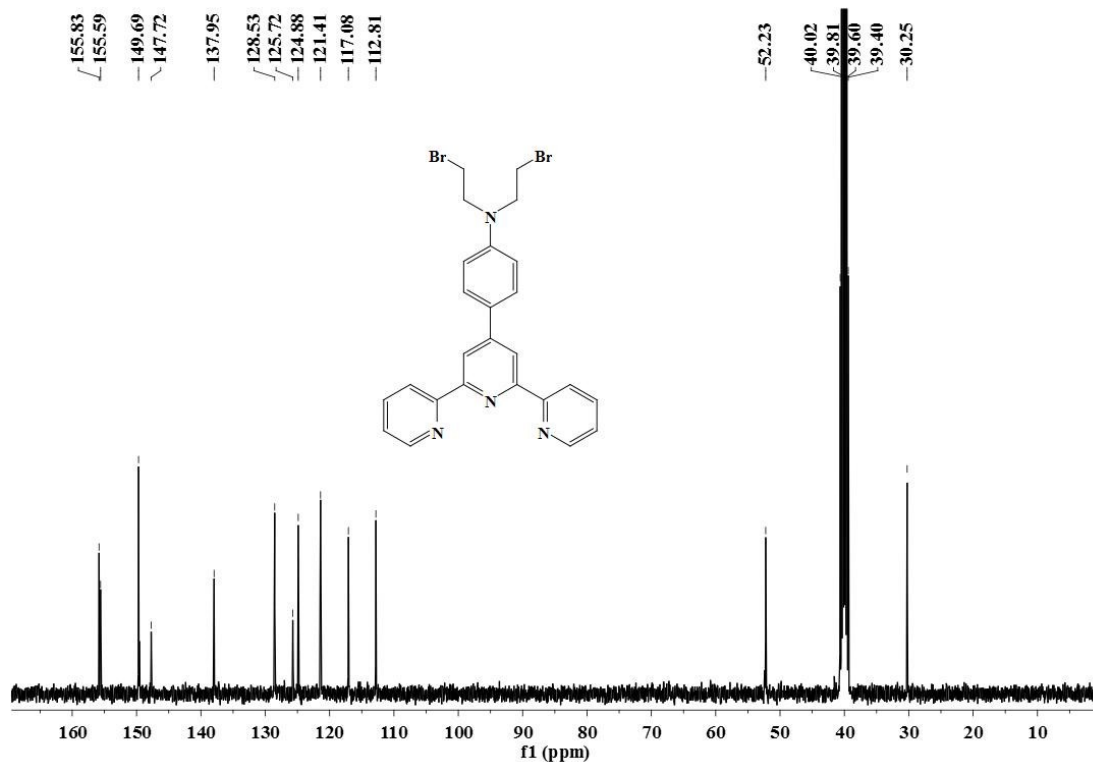


Fig. S5:  $^{13}\text{C}$  NMR of compound 2.

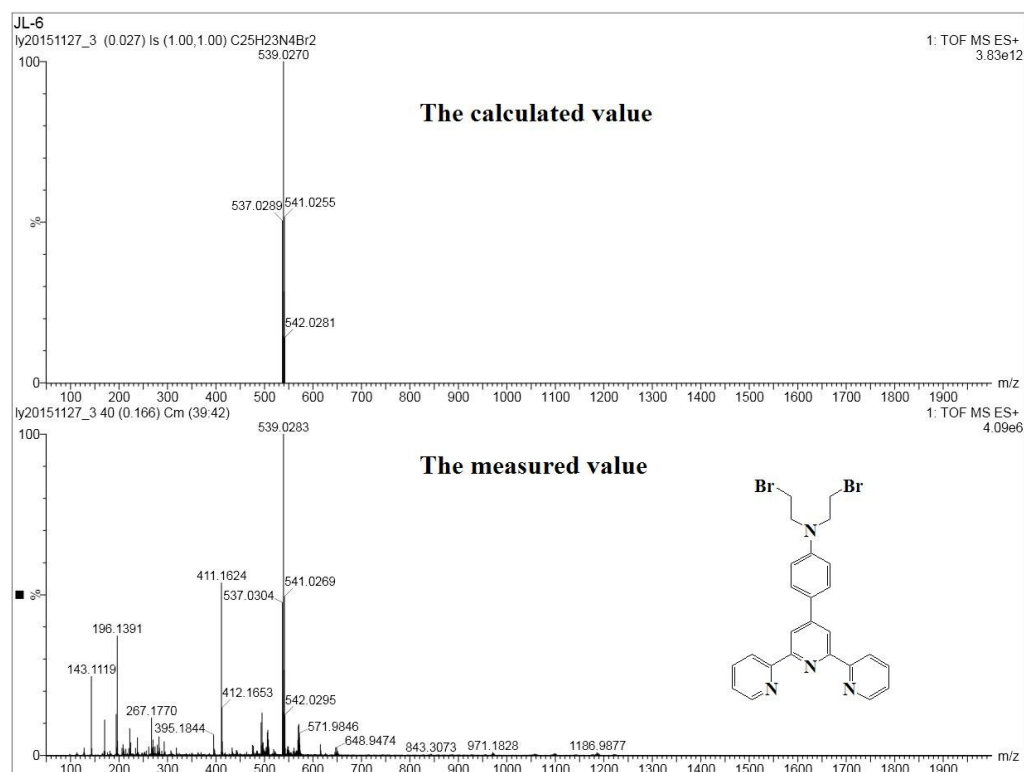
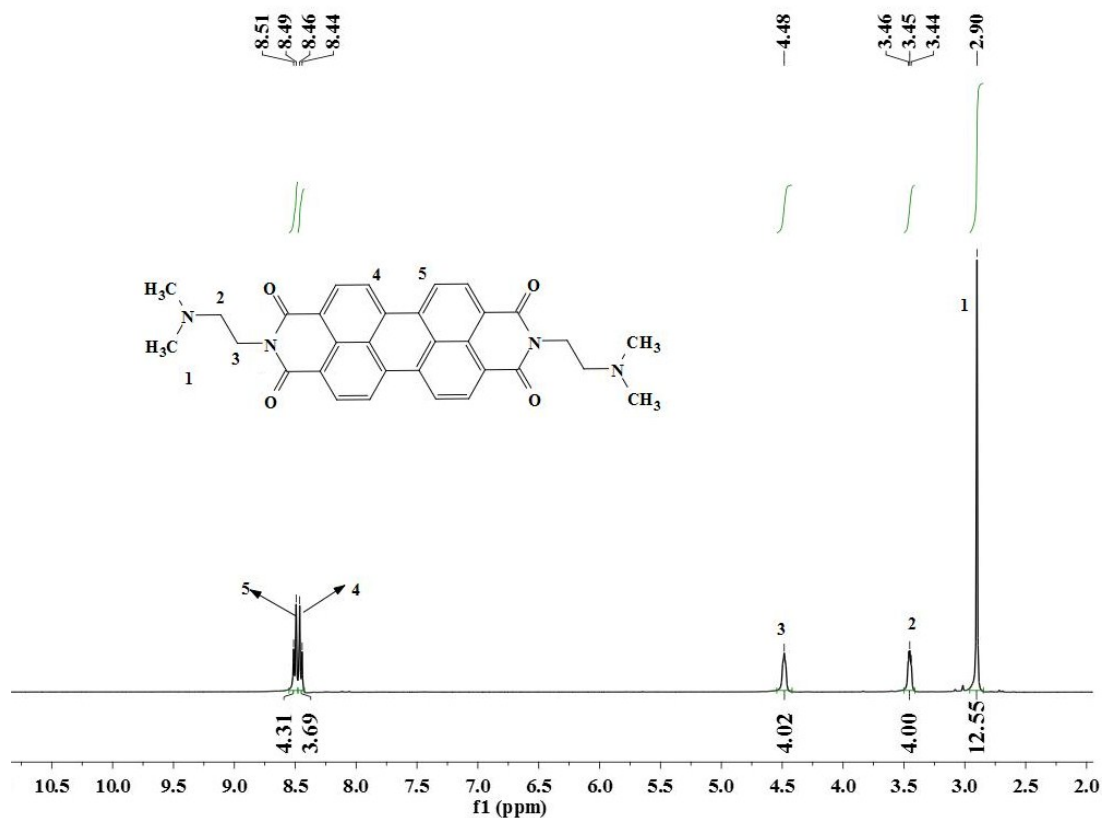
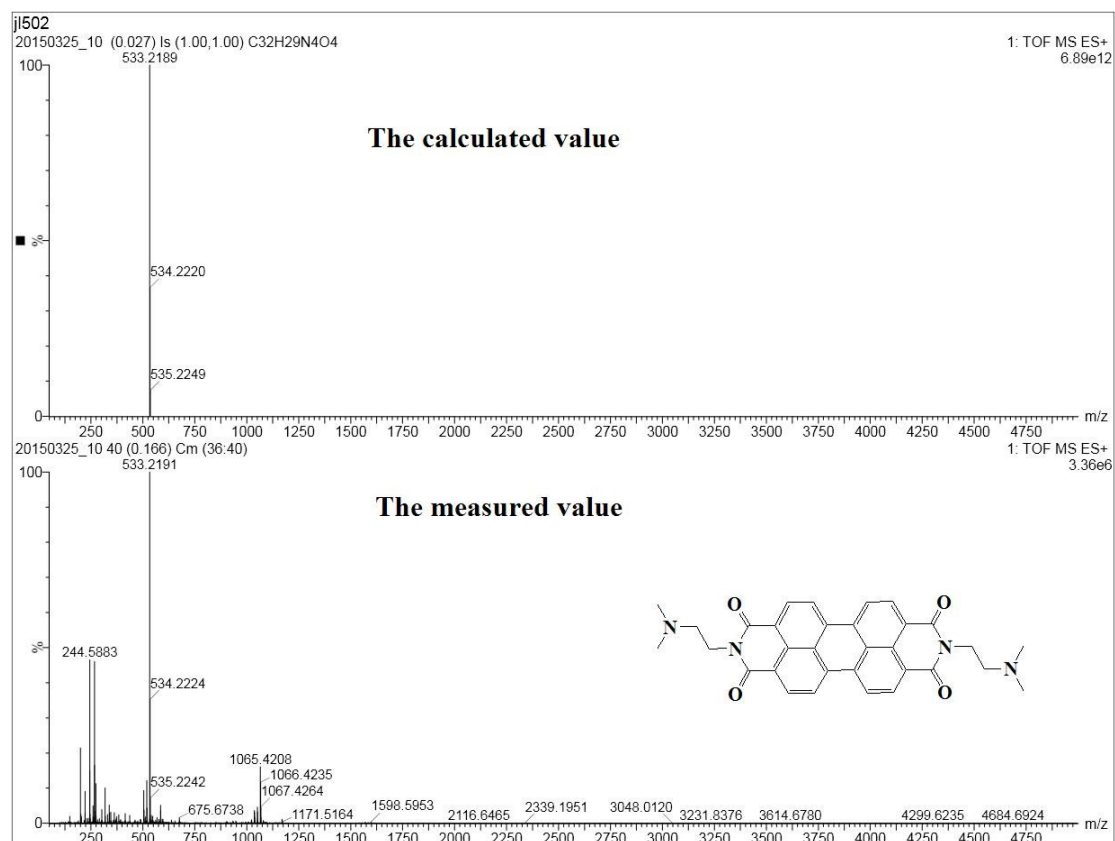


Fig. S6: HRMS spectra of compound 2.



**Fig. S7:** <sup>1</sup>H NMR of compound 3.



**Fig. S8:** HRMS spectra of compound 3.



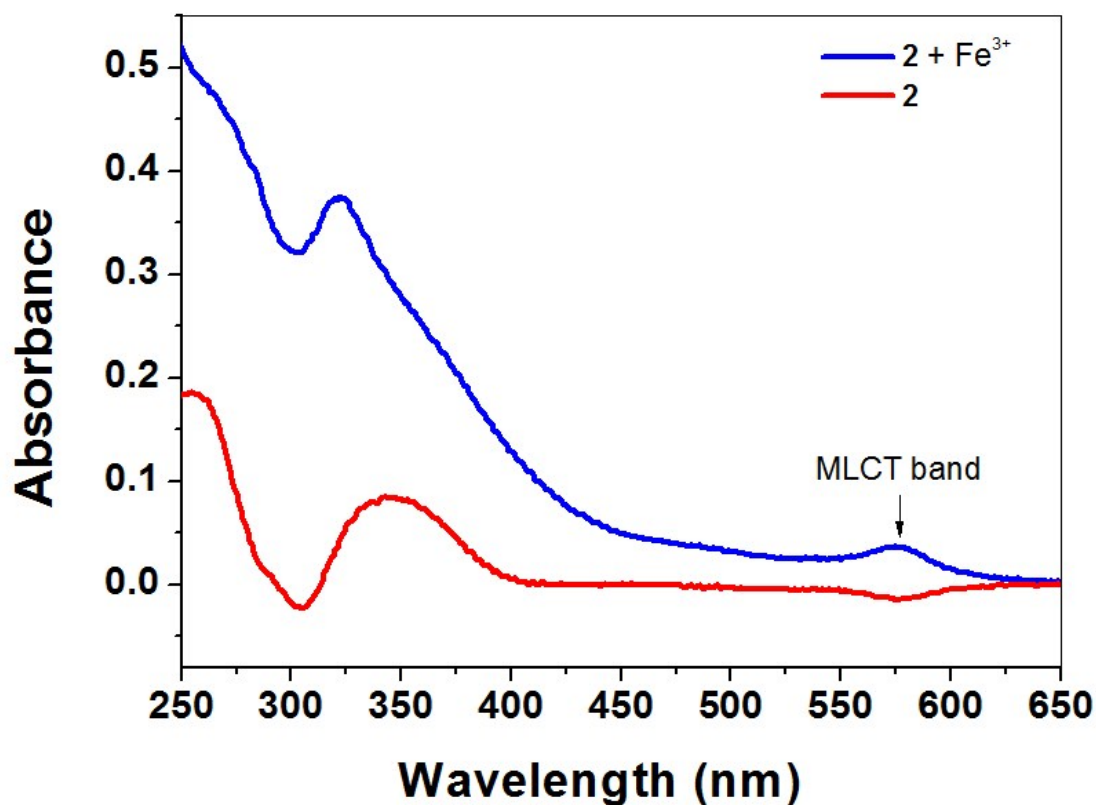


Fig. S11: UV-vis absorption spectra of compound **2** (20  $\mu\text{M}$ ) in the absence and presence of 4 equiv. of  $\text{Fe}^{3+}$  ions in water.

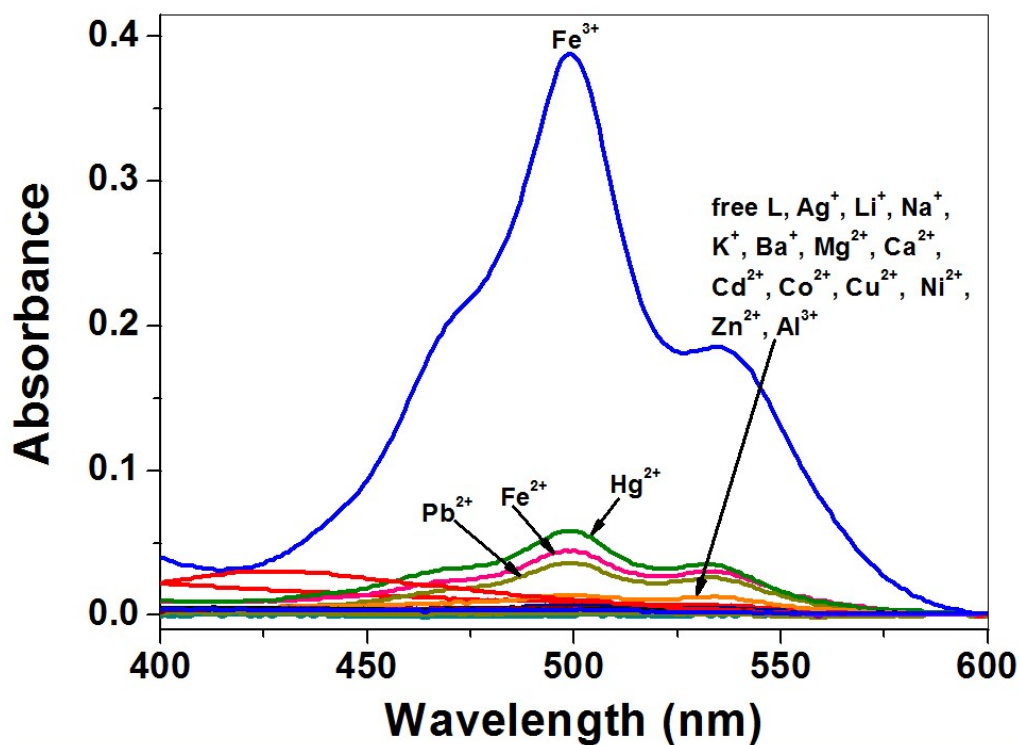


Fig. S12: UV-vis absorption spectra of **L** (10  $\mu\text{M}$ ) in water in the presence of various

relevant metal ions (5 equiv. for each metal ion).

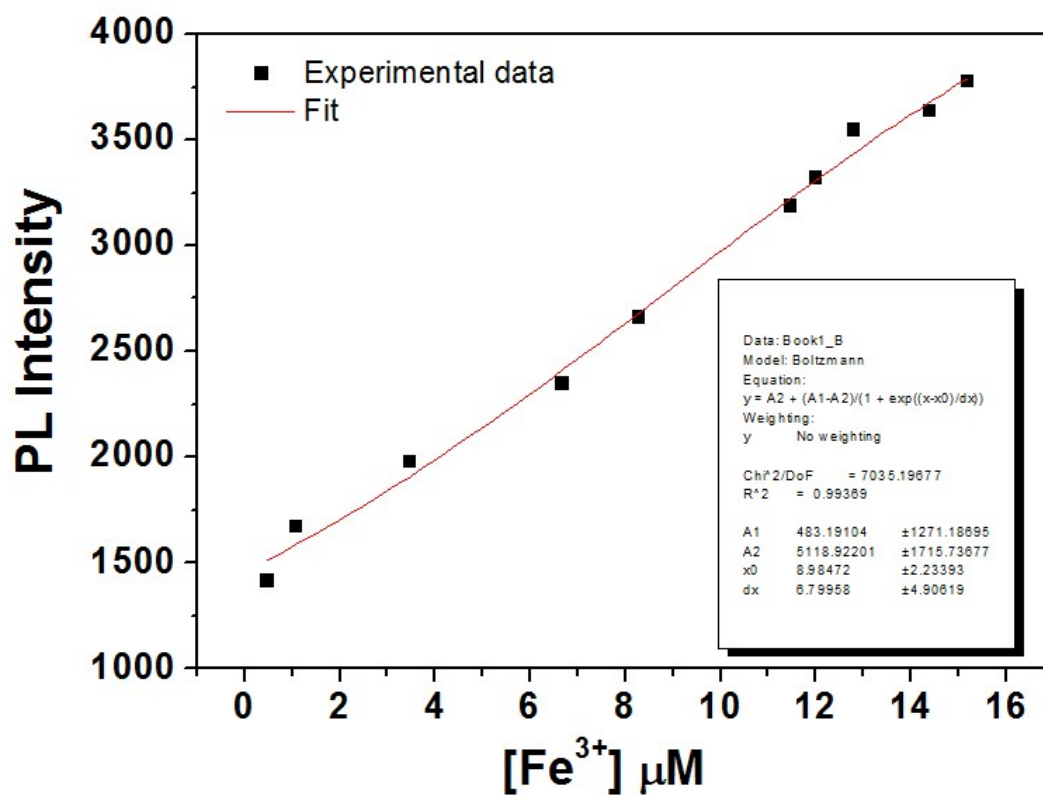


Fig. 13: Measurement of the fluorescence turn-on constant ( $K_{\text{turn-on}}$ ) of L.



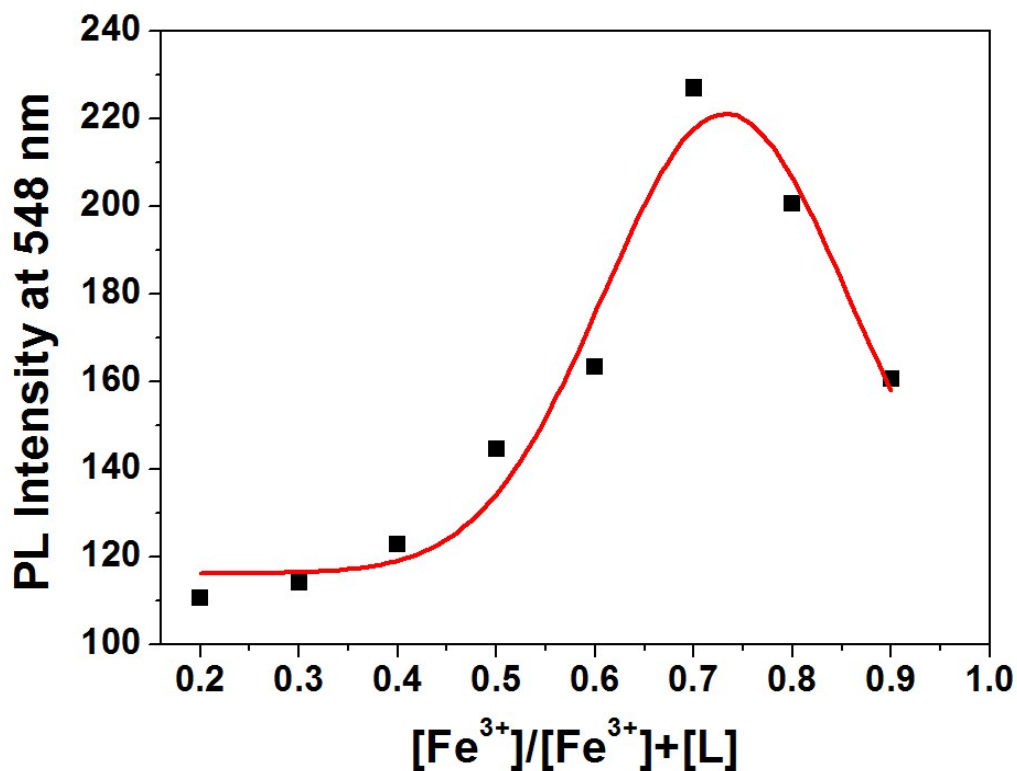


Fig. 14: Job's plot of **L** in water showing the 1:2 stoichiometry of the complex between **L** and  $\text{Fe}^{3+}$  ion. The total of the chemosensor and  $\text{Fe}^{3+}$  is  $50 \mu\text{M}$ .  $\lambda_{\text{ex}} = 495 \text{ nm}$ .

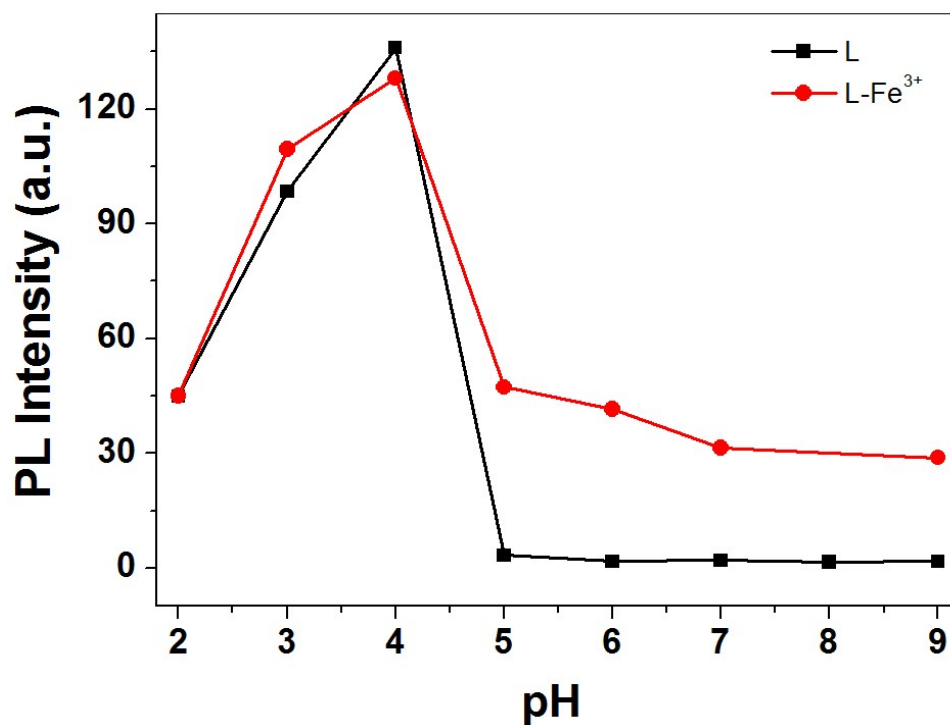
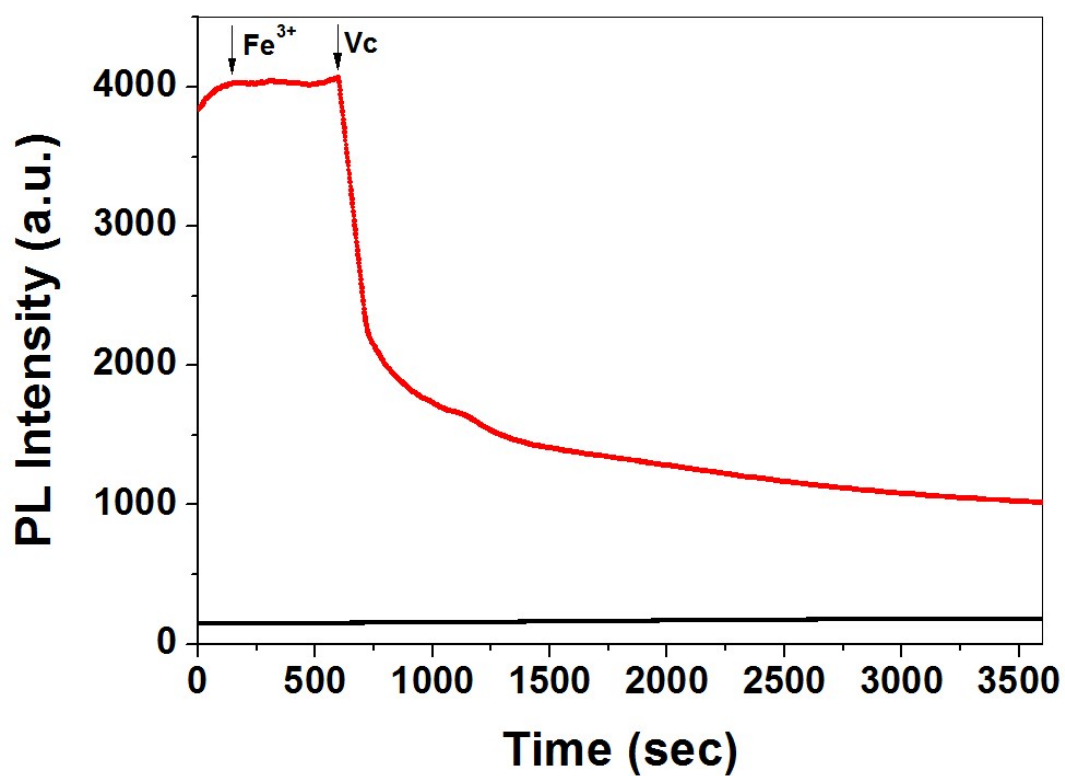


Fig. S15: Profile of pH dependence of the fluorescence intensity of **L** ( $2.5 \mu\text{M}$ ) at 548 nm in the absence and presence of  $\text{Fe}^{3+}$  (4 equiv.) in water.  $\lambda_{\text{ex}} = 495 \text{ nm}$ .



**Fig. S16:** The kinetic assay of redox conversion of iron from  $\text{Fe}^{3+}$  to  $\text{Fe}^{2+}$ . The emission spectra were recorded at 548 nm ( $\lambda_{\text{ex}} = 495$  nm) in water.  $[\text{L}] = 2.5 \mu\text{M}$ .  $[\text{Fe}^{3+}] = 10 \mu\text{M}$ .  $[\text{Vc}] = 0.83 \text{ mM}$