New Journal of Chemistry

A new fluorescent sensor containing glutamic acid for Fe^{3+} and its resulting complex as a secondary sensor for PPi in purely aqueous solution

Ping Li* and Ying Wang*

School of chemistry and chemical engineering, University of Jinan, Jinan 250022, China.

*Corresponding author:

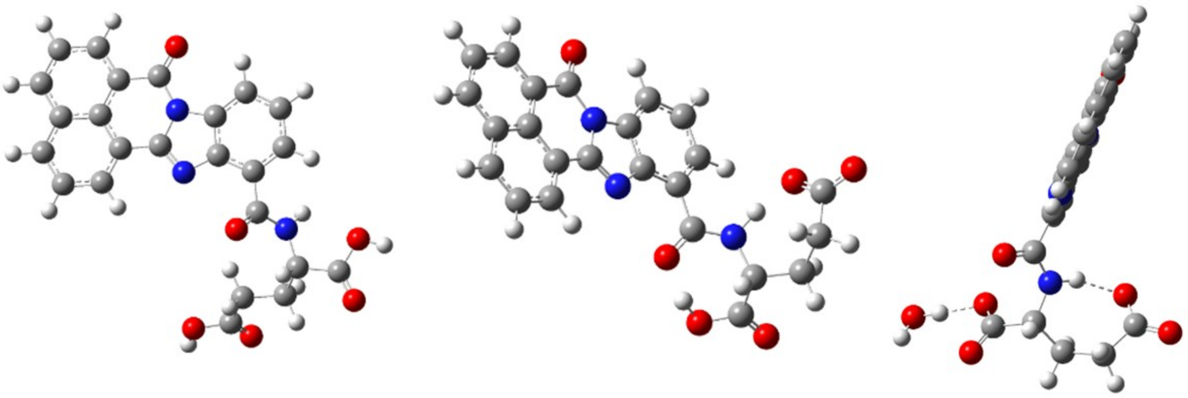
Ping Li

Ying Wang

School of chemistry and chemical engineering, University of Jinan, Jinan 250022, China.

E-mail address: chm_lip@ujn.edu.cn (P. Li),

15165089871@163.com (Y. Wang)



L L^- $L^{2-}\bullet H_2O$

Fig. S1. The optimization of L, L^- and $L^{2-}\bullet H_2O$ using TD-DFT calculating methods.

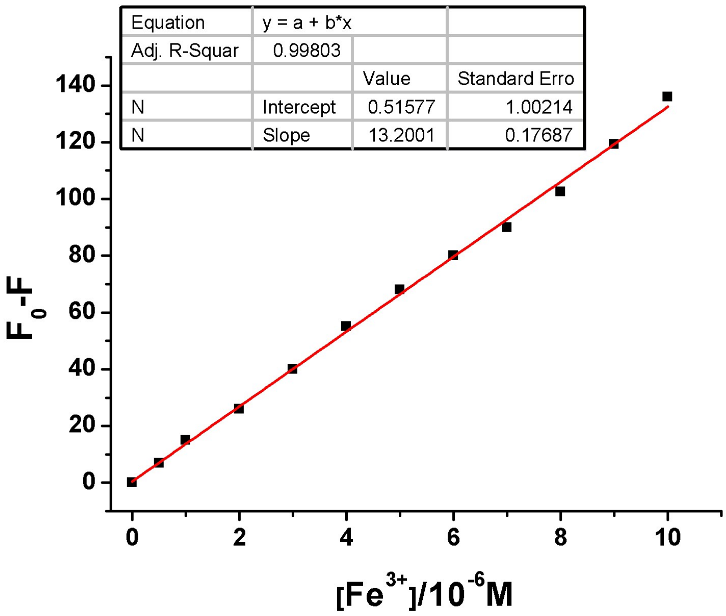
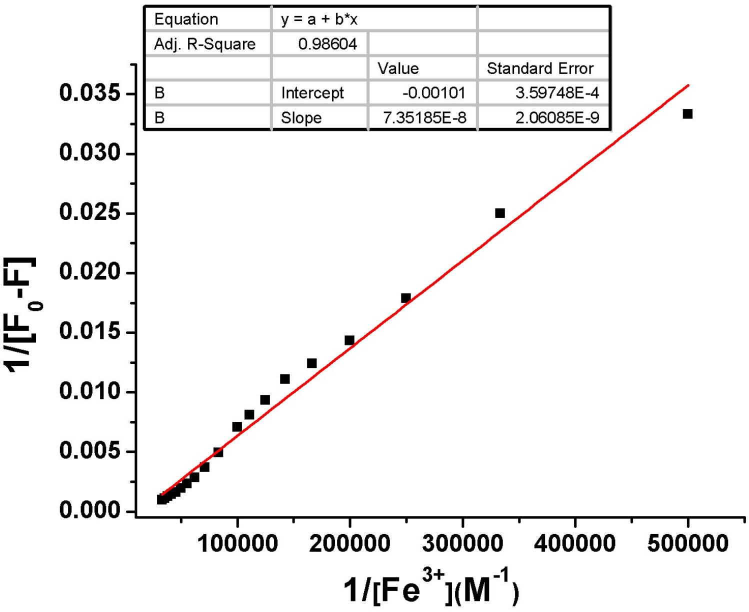


Fig. S2. The linear change ratio between fluorescence intensity (at 524 nm) and different concentration of Fe^{3+} in purely aqueous buffer (tris 10 mM, pH = 7.4) solution.



Equation	y = a + b*x		
Adj. R-Square	0.98604		
		Value	Standard Error
B	Intercept	-0.00101	3.59748E-4
B	Slope	7.35185E-8	2.06085E-9

Fig. S3. Benesi–Hildebrand plot based on a 1:1 binding stoichiometry between L and Fe^{3+}.

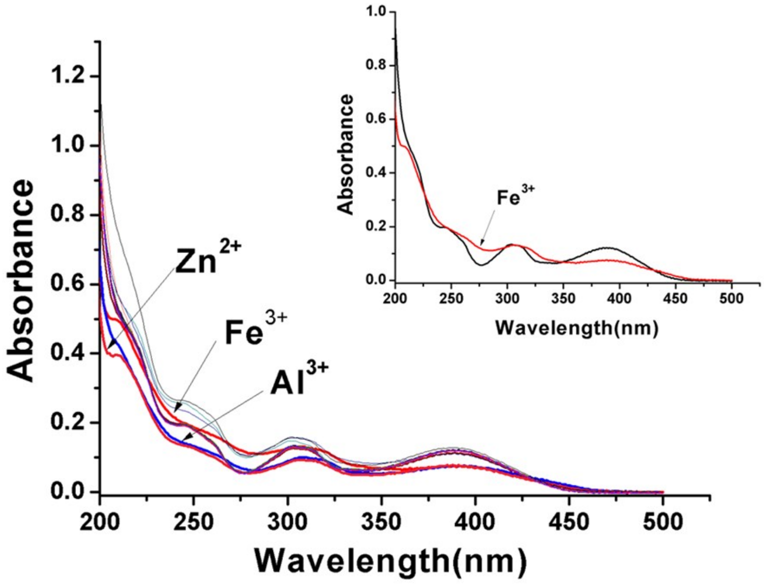


Fig. S4. Absorption spectrum of L (1 × 10^{-5} M) towards 5 equiv. of various metal ions including Na^+, Li^+, K^+, Mg^{2+}, Ca^{2+}, Zn^{2+}, Cd^{2+}, Fe^{2+}, Ag^+, Cu^{2+}, Co^{2+}, Ni^{2+}, Mn^{2+}, Cr^{3+}, Sr^{3+}, Al^+ and Fe^{3+}, only Fe^{3+} in purely aqueous buffer (tris 10 mM, pH = 7.4) solution. Insert: Absorption spectrum of free L and L-Fe^{3+}complex in the presence of 5 equiv. of Fe^{3+}.

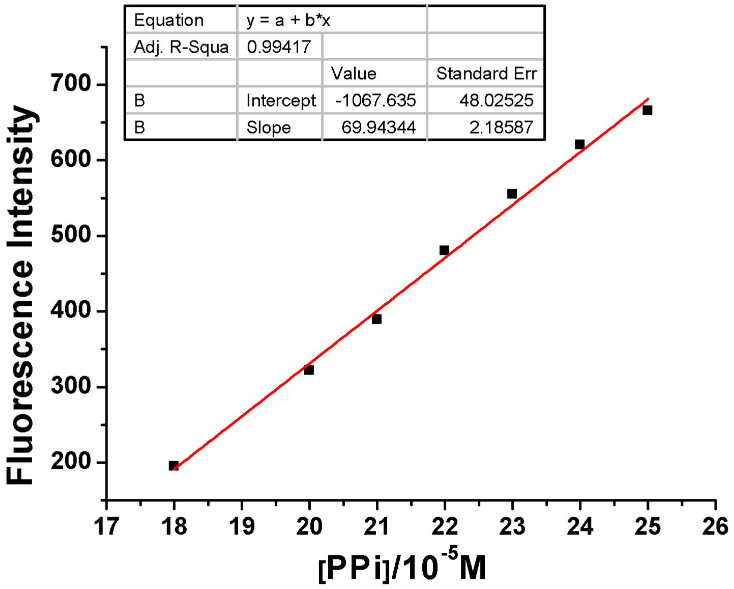


Fig. S5. The linear change ratio between fluorescence intensity of L-Fe^{3+} complex (at 524 nm) and different concentration of PPi in purely aqueous buffer (tris 10 mM, pH = 7.4) solution.

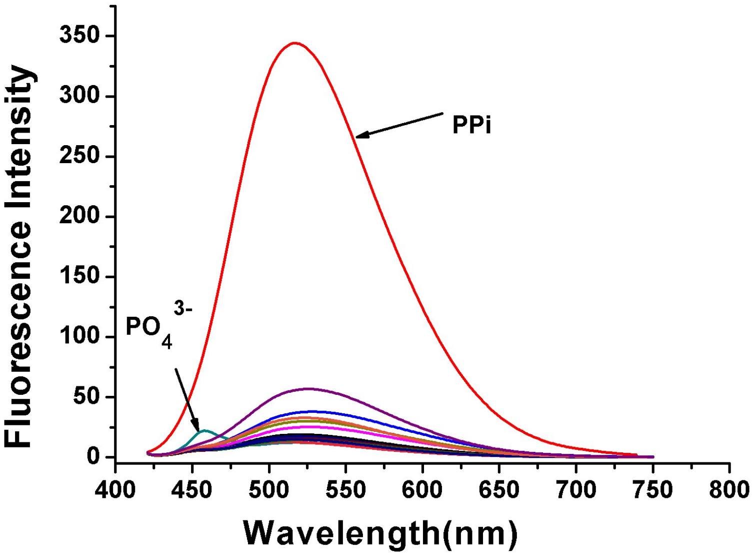


Fig. S6. Fluorescence selectivity of L-Fe^{3+} complex towards various anions including PPi, EDTA, PO_4^{3-}, $H_2PO_4^-$, $S_2O_3^{2-}$, HSO_3^-, CrO_4^{2-}, NO_2^-, NO_3^-, S^{2-}, F^-, Cl^-, Br^- in purely aqueous buffer (tris 10 mM, pH = 7.4) solution.

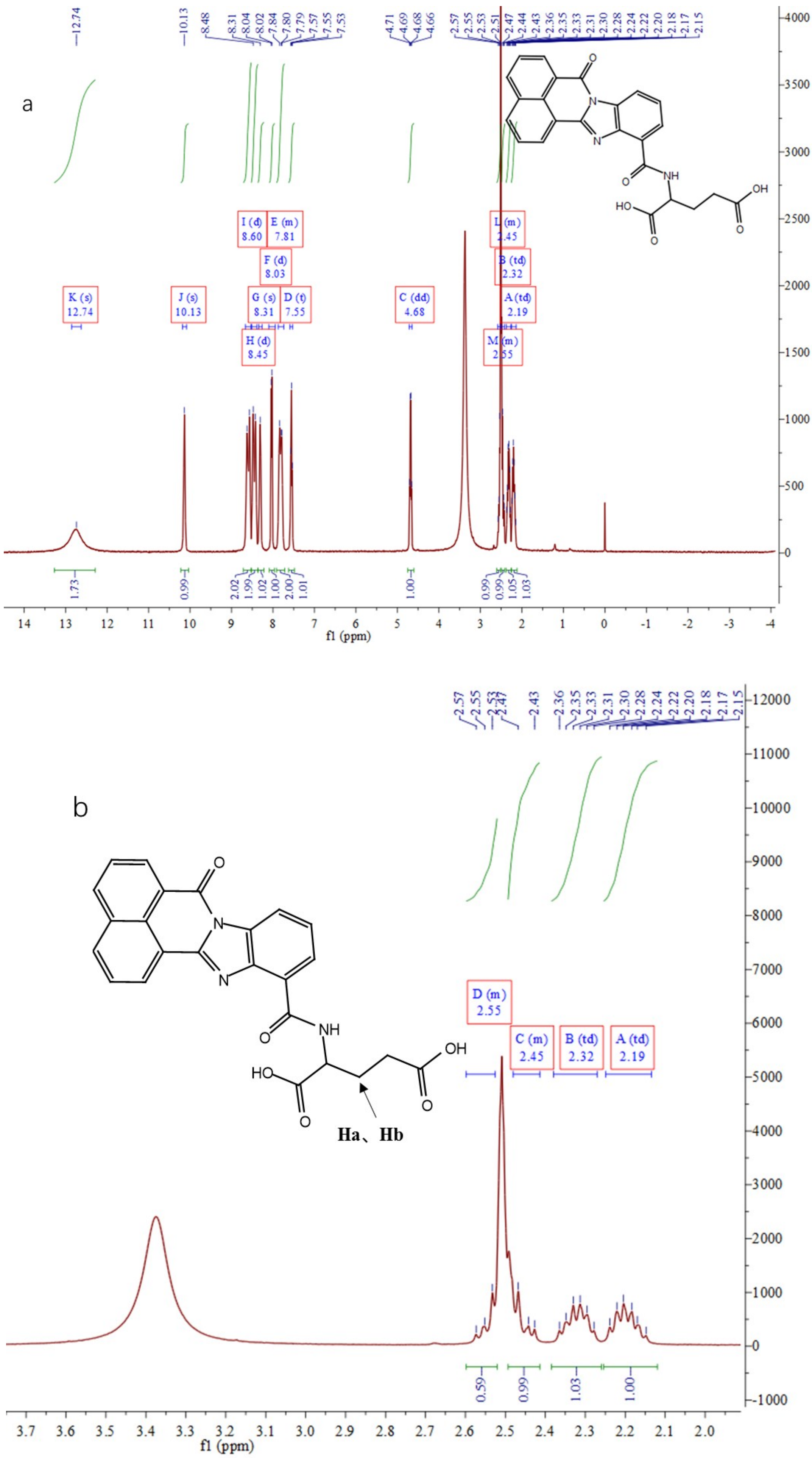


Fig. S7. (a) whole ^{1}H NMR spectrum and (b) partial ^{1}H NMR spectrum in detail of probe L in DMSO-d_6.

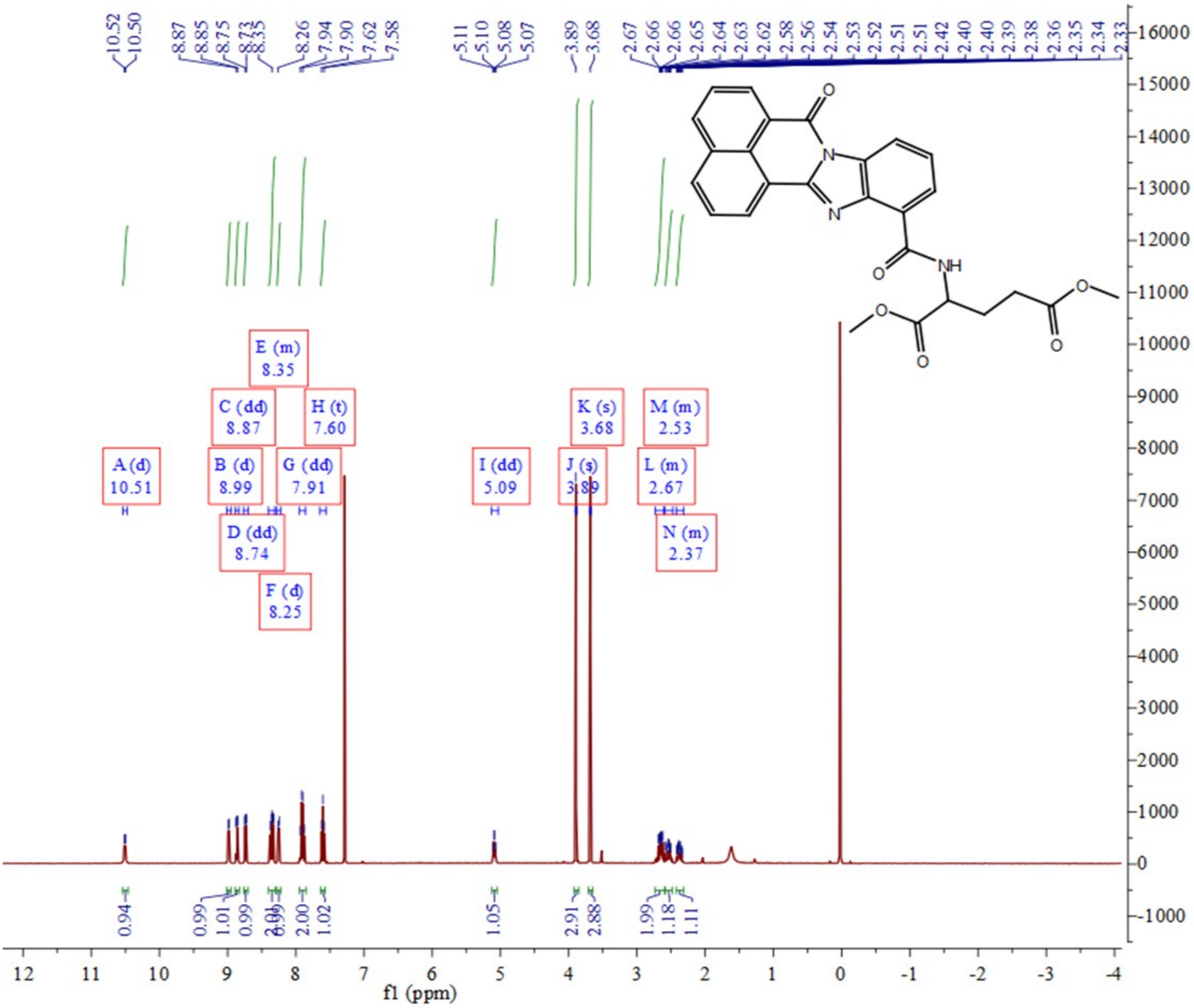


Fig. S8. ^{1}H NMR spectrum of compound 3 in CDCl$_3$.

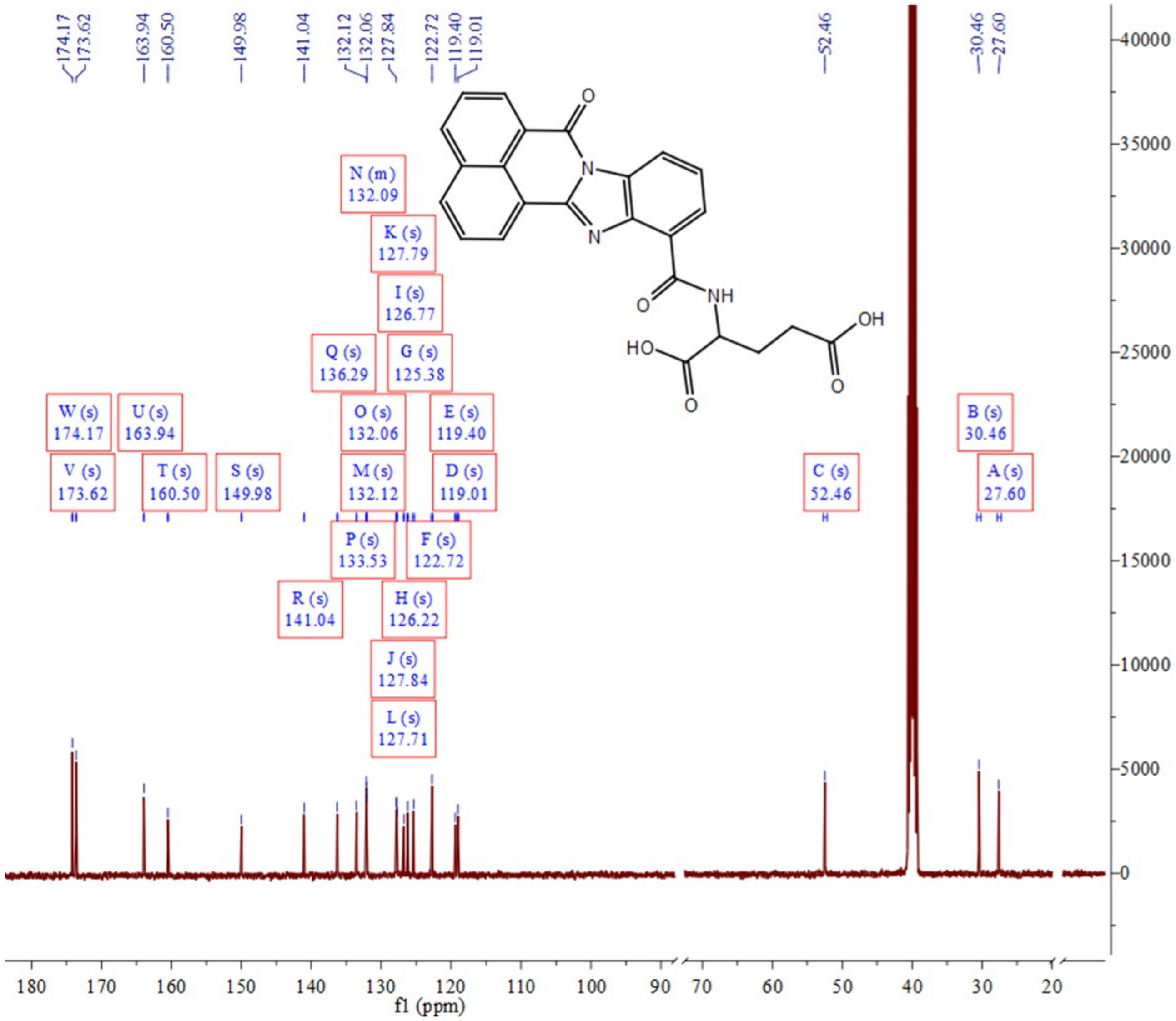


Fig. S9. ^{13}C NMR spectrum of probe L in DMSO-d_6.

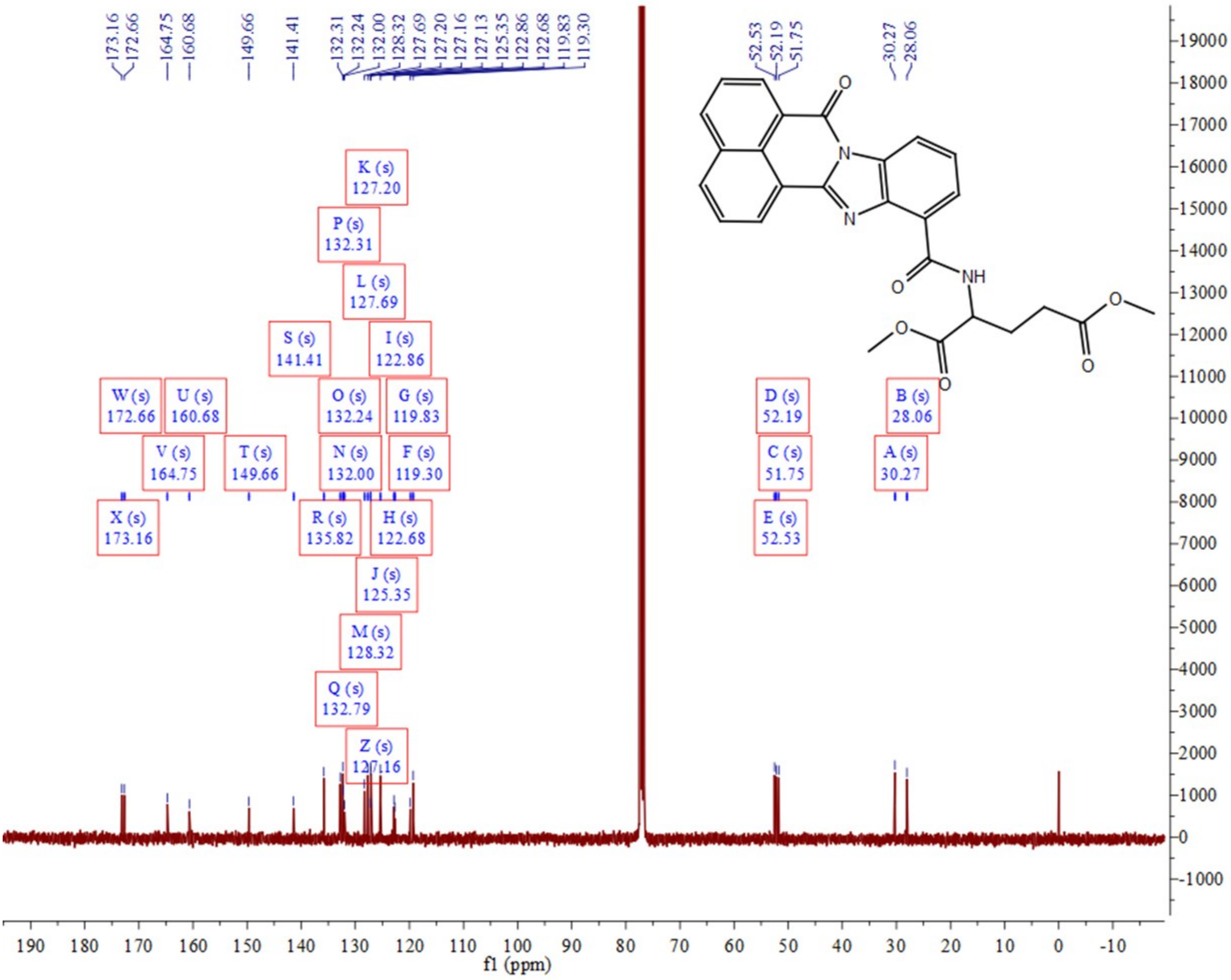


Fig. S10. ^{13}C NMR spectrum of compound 3 in $CDCl_3$.

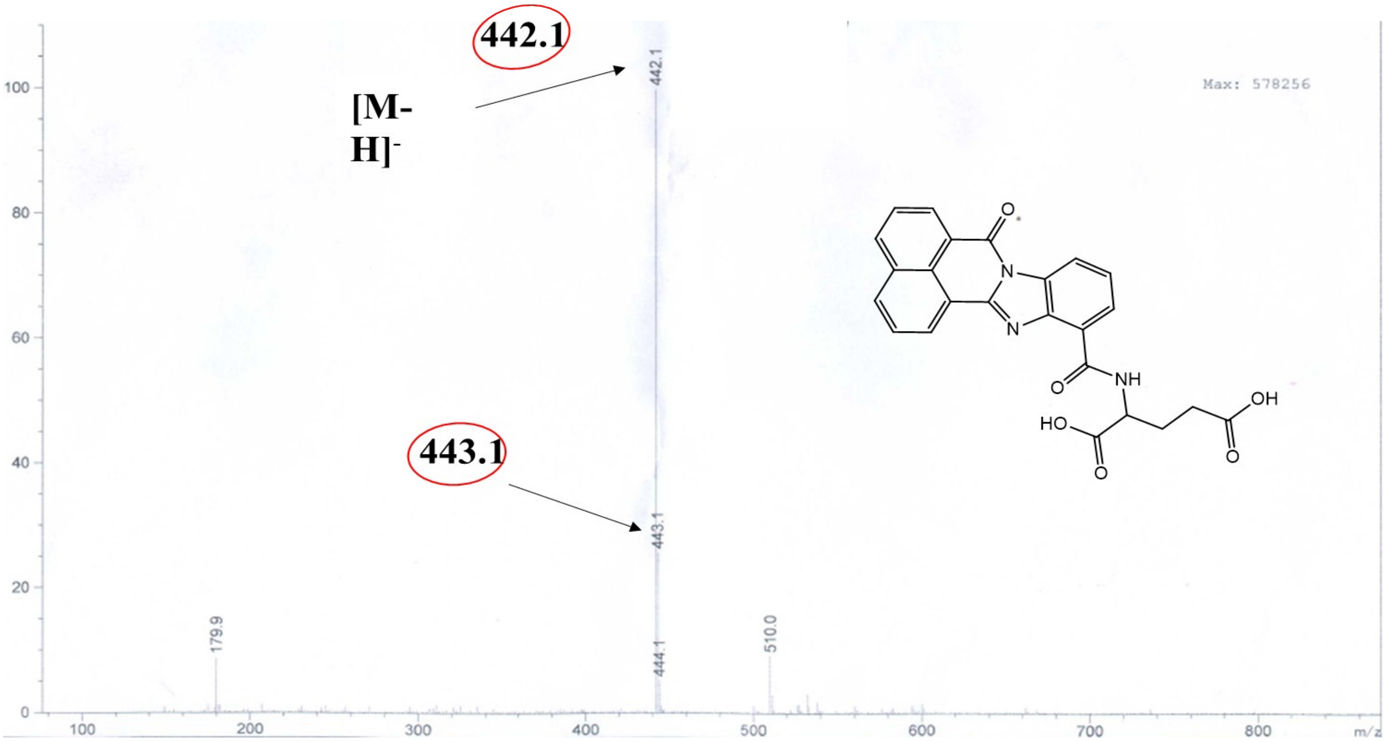


Fig. S11. ESI-MS of complex L.

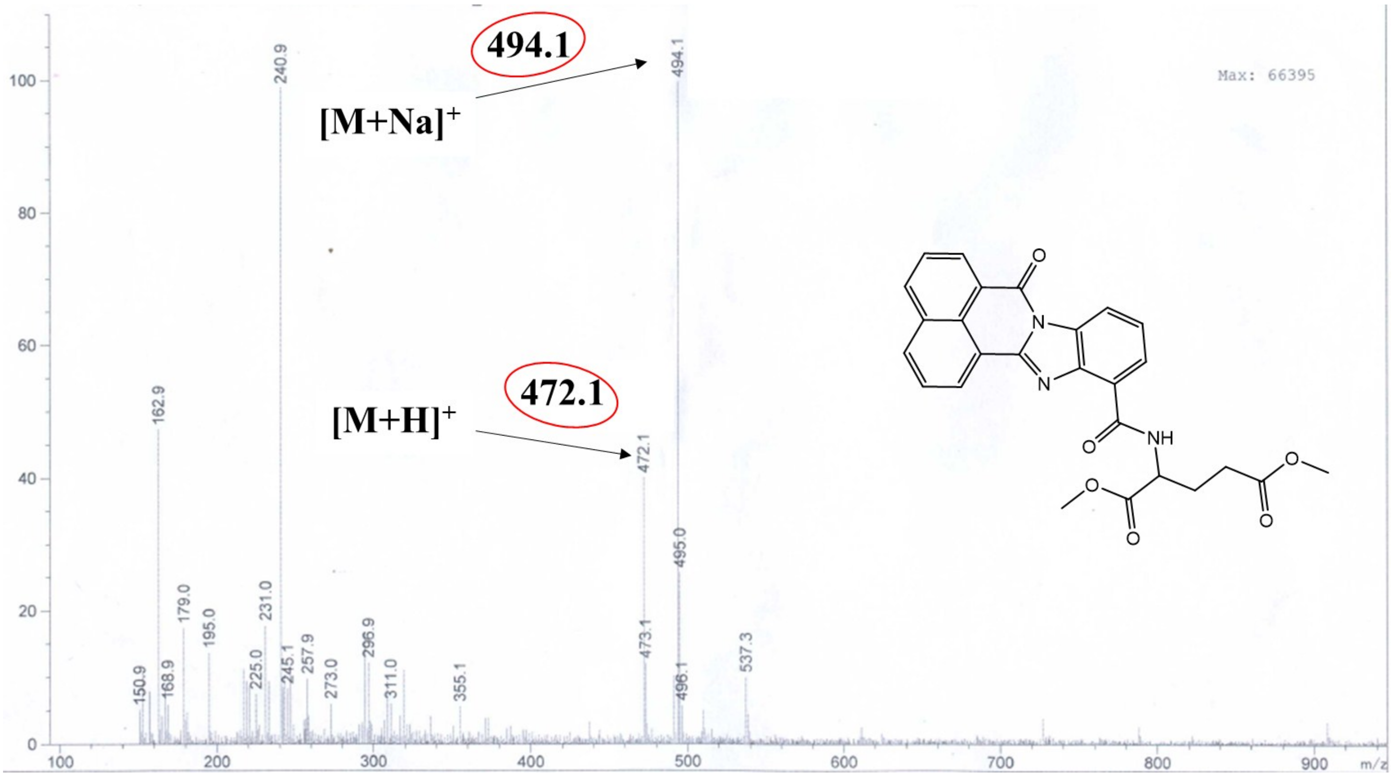


Fig. S12. ESI-MS of complex 3.

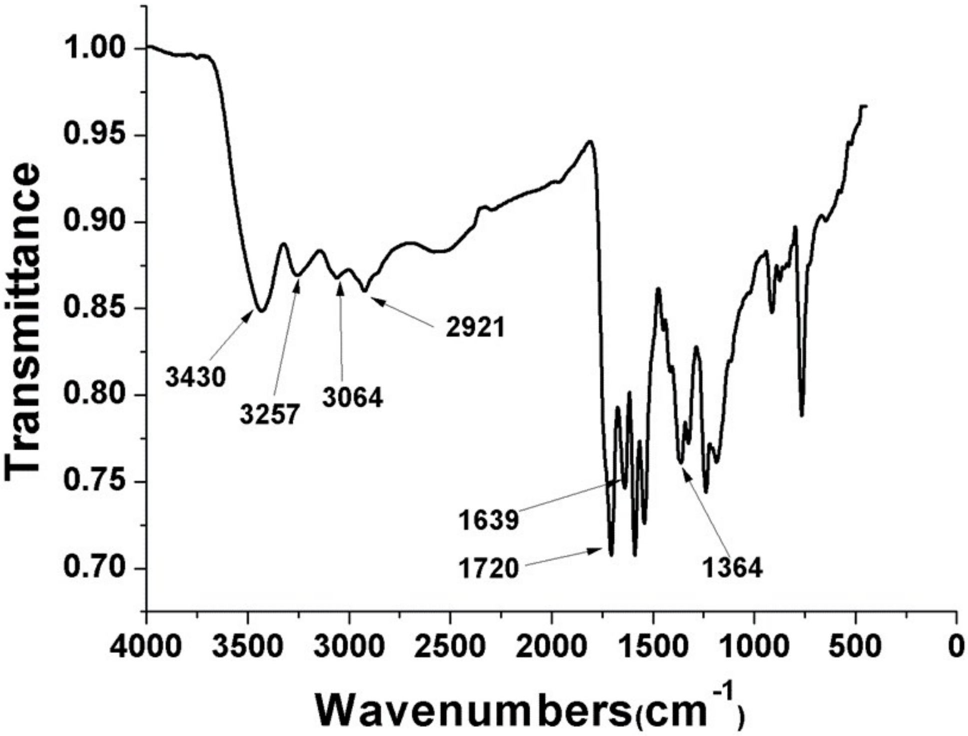


Fig. S13. The FTIR spectra of L.

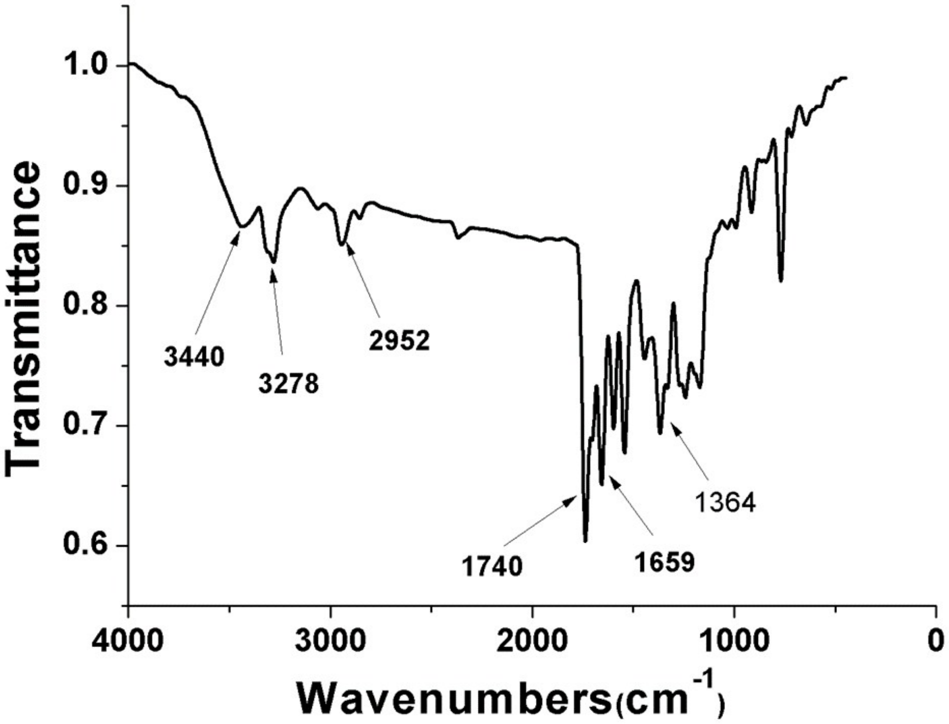


Fig. S14. The FTIR spectra of compound 3.

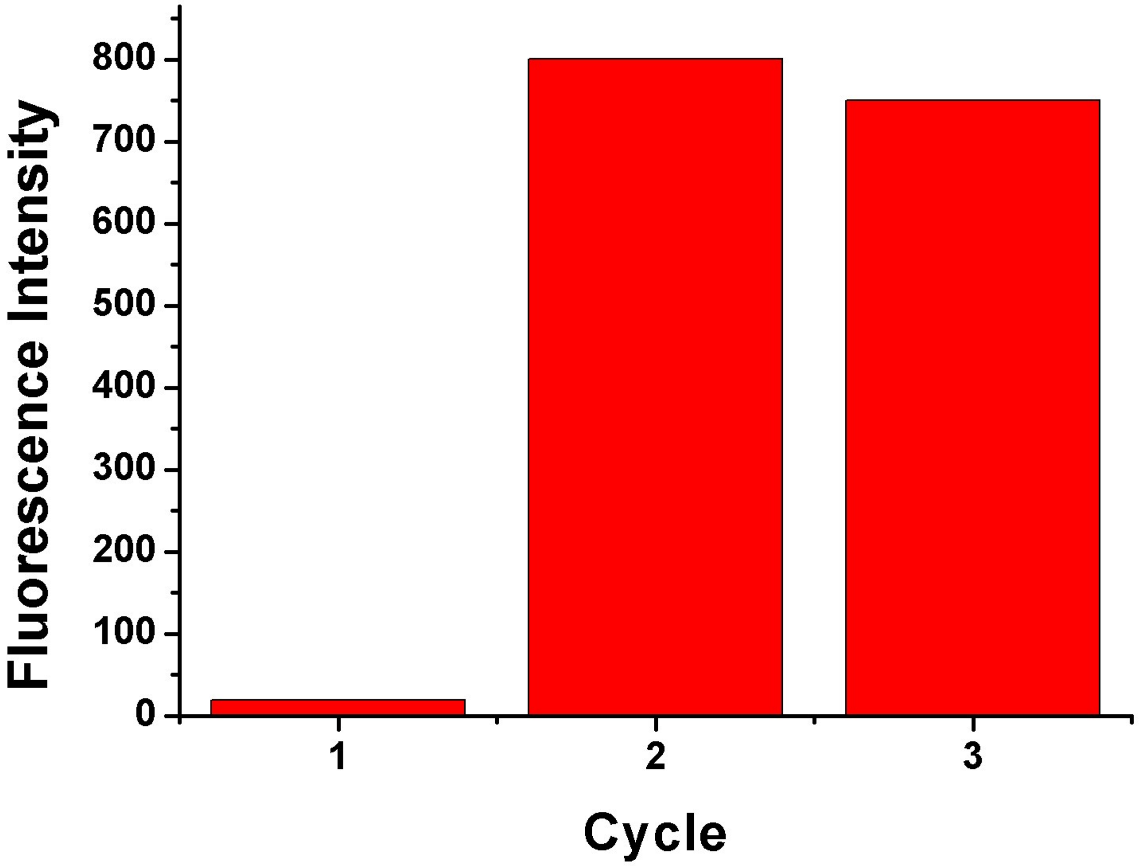


Fig. S15. Reversible switching of the emission of **L** by sequential addition of Fe^{3+} and PPi. (1: the fluorescence intensity of **L** in the presence of 3 equiv. of Fe^{3+}; 2: the fluorescence intensity of 1 in the presence of 40 equiv. of PPi; 3: the fluorescence intensity of 2 in the presence of 10 equiv. of Fe^{3+}.)