

Figure S3. FT-MS of NL .

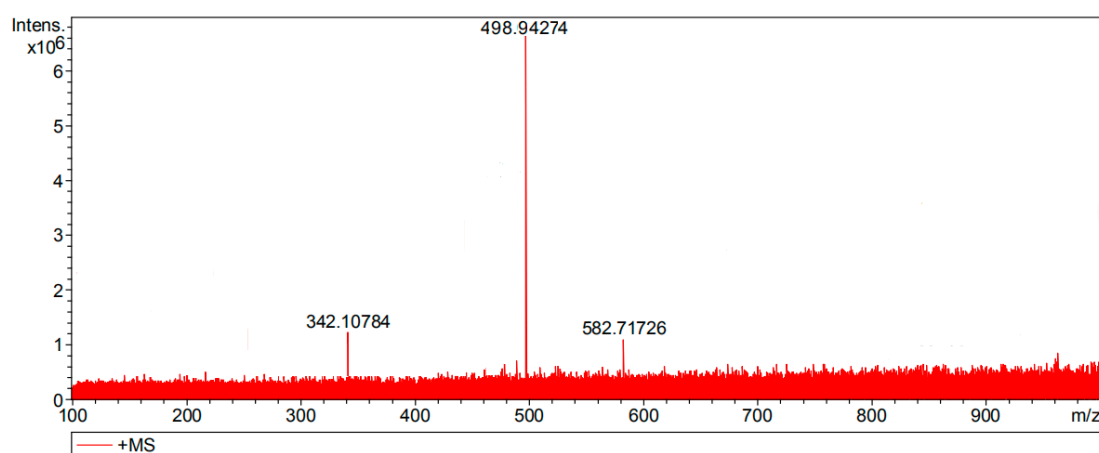


Figure S4. FT-MS of NL-Fe<sup>3+</sup> complex.

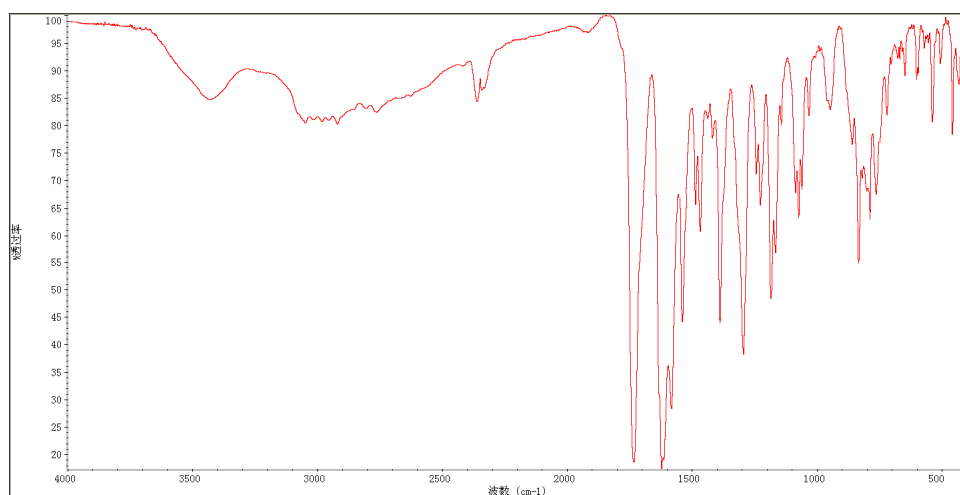


Figure S5. IR of NL-Fe<sup>3+</sup> complex .

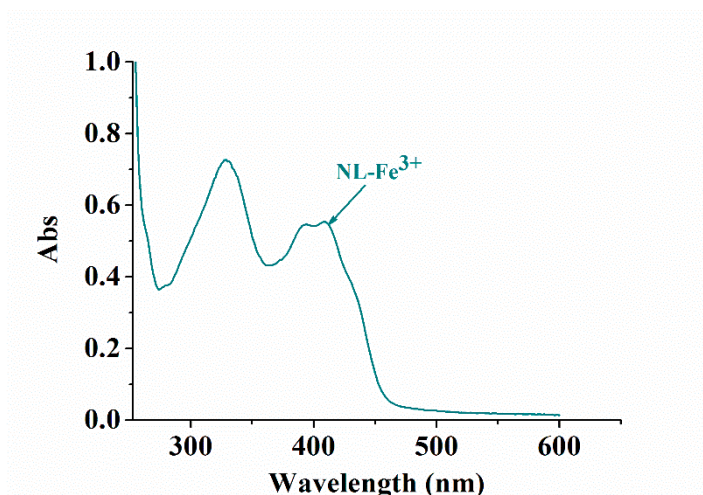


Figure S6. UV-Vis of NL-Fe<sup>3+</sup> complex .

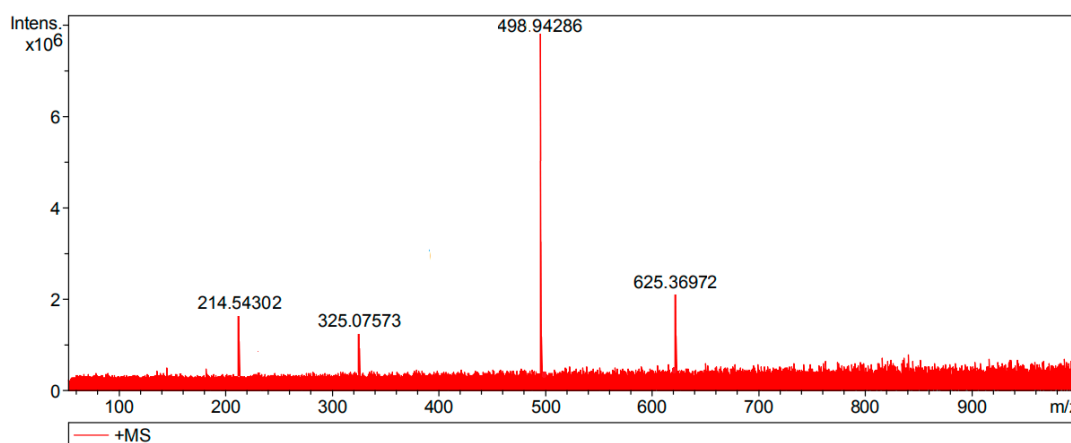


Figure S7. FT-MS by adding Fe<sup>3+</sup> into NL .

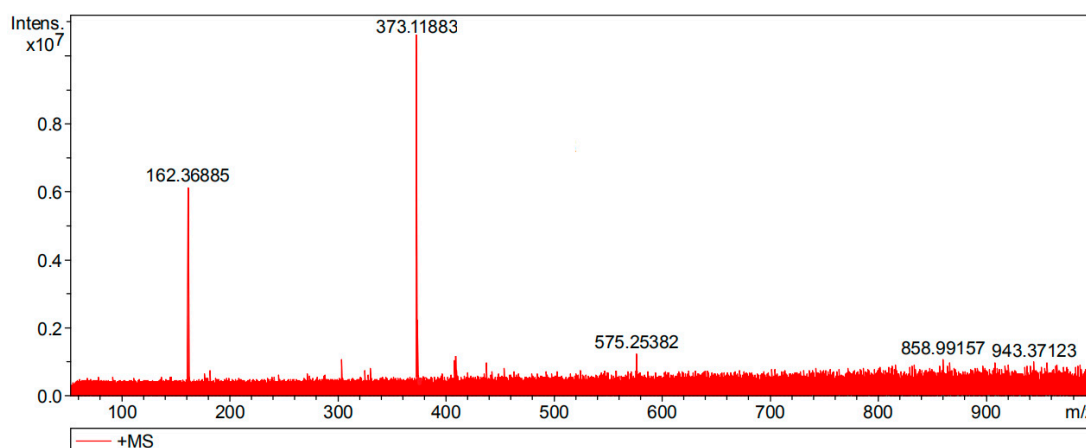
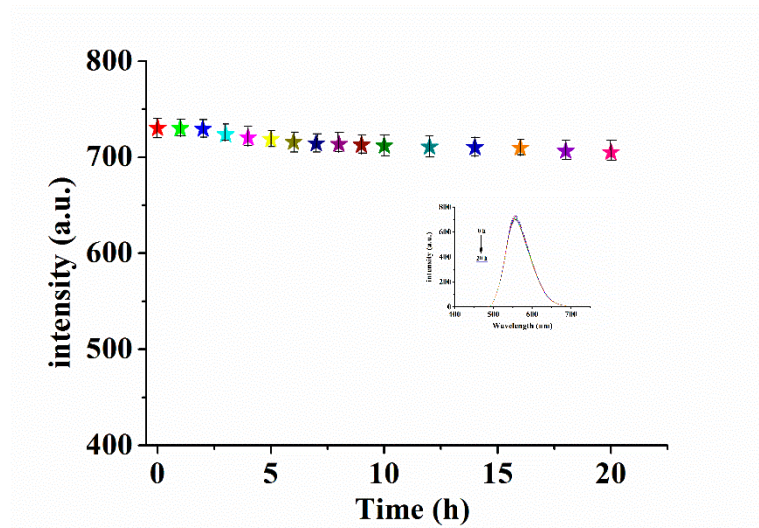
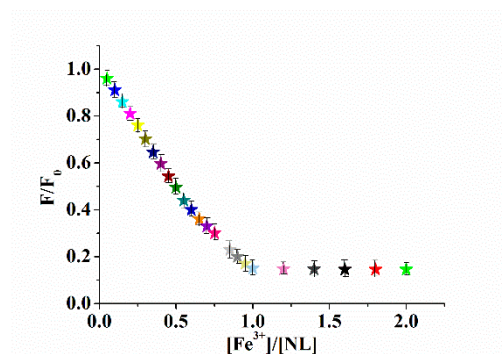


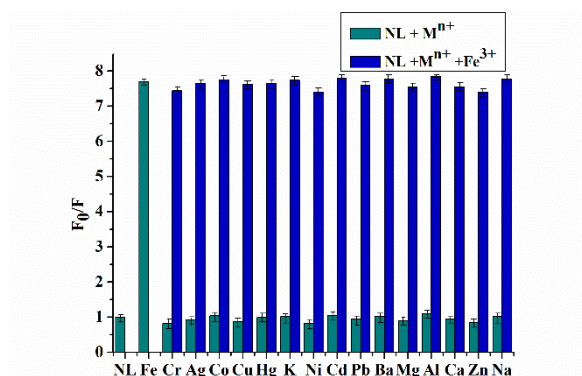
Figure S8. FT-MS of NL-Fe<sup>3+</sup>+PPI .



**Figure S9.** Fluorescence spectra of NL (10  $\mu\text{M}$ ) at different times in DMSO/H<sub>2</sub>O (2:8/v:v, 20 mM HEPES, pH=7.2) solutions ( $\lambda_{\text{ex}}$ =410nm).



**Figure S10.** Fluorescence intensities of NL (10  $\mu\text{M}$ ) at 557nm as a function of Fe<sup>3+</sup> concentration (0-20  $\mu\text{M}$ ) in DMSO/H<sub>2</sub>O (2:8/v:v, 20 mM HEPES, pH=7.2) solutions ( $\lambda_{\text{ex}}$ =410 nm).



**Figure S11.** Fluorescence response of NL (10  $\mu\text{M}$ ) to Fe<sup>3+</sup> (20  $\mu\text{M}$ ) in the presence of other common metal ions (20  $\mu\text{M}$ ). The green bars represent the enhancement degree of NL in the presence of cations of interest (all are 20  $\mu\text{M}$ ). The blue bars represent the changes of the emission that occurs upon the subsequent addition of Fe<sup>3+</sup> (20  $\mu\text{M}$ ) to the above solution ( $\lambda_{\text{ex}}$ =410 nm).

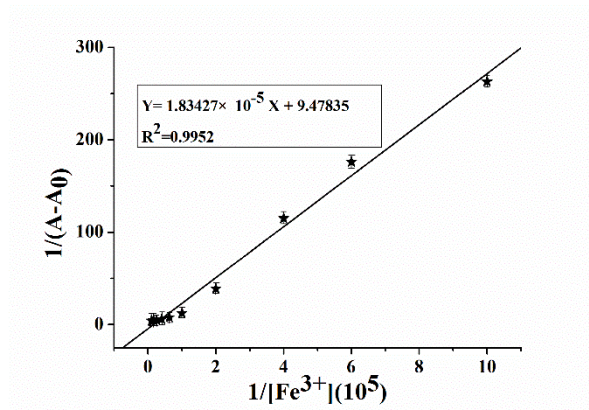


Figure S12. The Benesi-Hildebrand plot of NL(10  $\mu$ M) with  $Fe^{3+}$ (20  $\mu$ M) by UV-Vis spectroscopy.

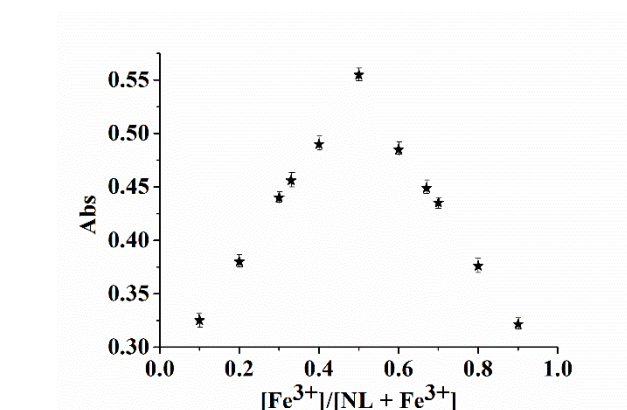


Figure S13. The Job's plot of the reaction between NL and  $Fe^{3+}$  by UV-Vis spectroscopy.

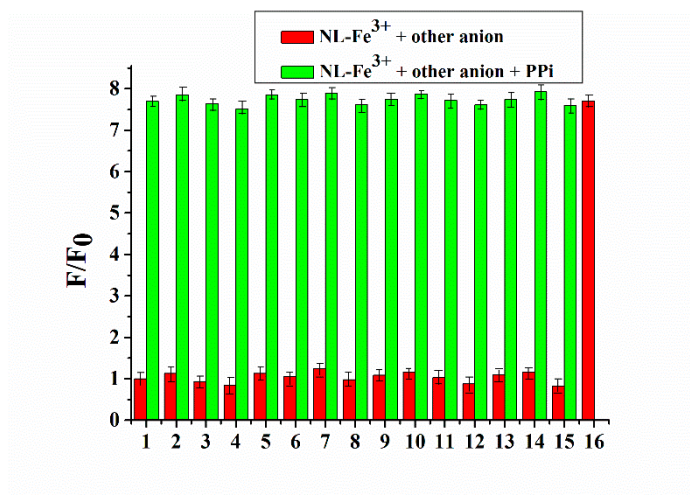
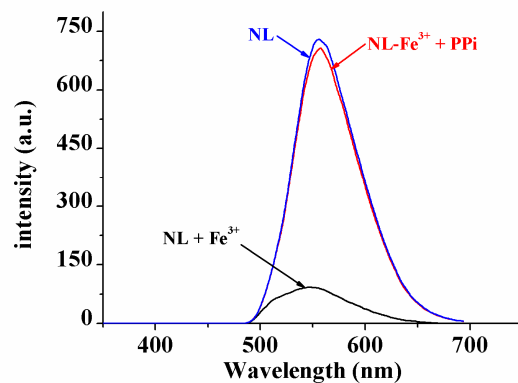
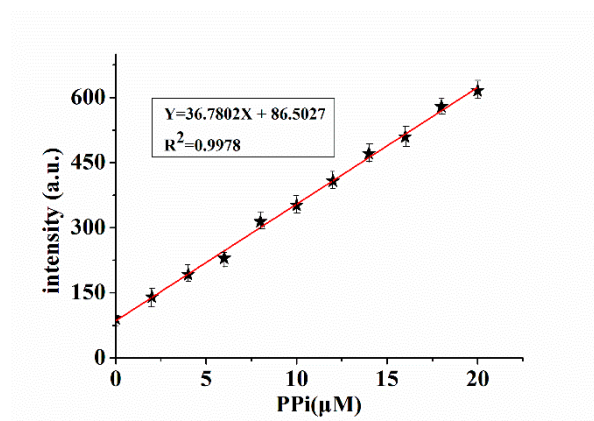


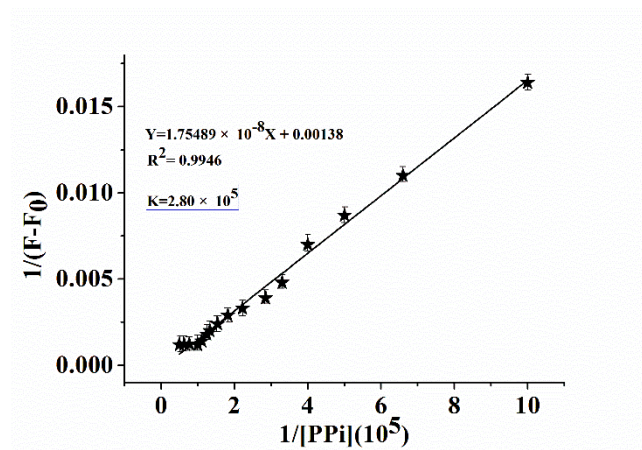
Figure S14. Fluorescence response of NL- $Fe^{3+}$  (10  $\mu$ M) in the presence of various analytes (40  $\mu$ M): (1)  $NO_2^-$ , (2)  $S^{2-}$ , (3)  $F^-$ , (4)  $SCN^-$ , (5)  $Ac^-$ , (6)  $HCO_3^-$ , (7)  $HSO_4^-$ , (8)  $CO_3^{2-}$ , (9)  $Cl^-$ , (10)  $Br^-$ , (11)  $SO_4^{2-}$ , (12) AMP, (13) ADP, (14) ATP, (15) Pi, (16) PPI ( $\lambda_{ex}=410$  nm).



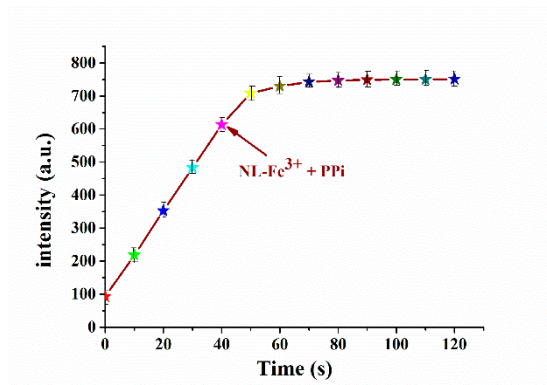
**Figure S15.** Fluorescence spectra of NL (10  $\mu\text{M}$ ), sequential upon addition of  $\text{Fe}^{3+}$  (20  $\mu\text{M}$ ) and PPI (40  $\mu\text{M}$ ) in DMSO/ $\text{H}_2\text{O}$  (2:8/v:v, 20 mM HEPES, pH=7.2) solutions ( $\lambda_{\text{ex}}$ =410 nm).



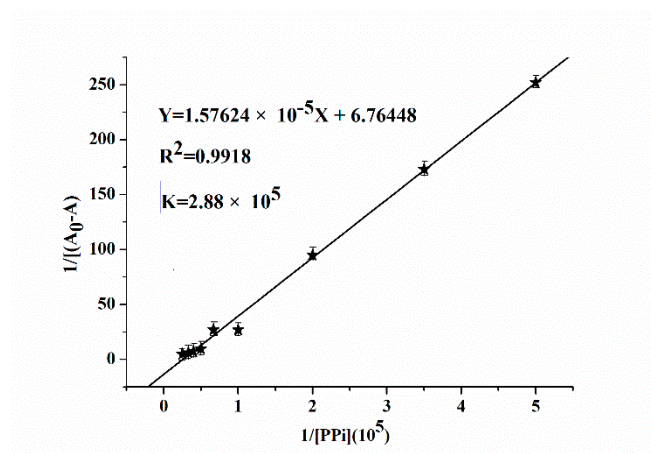
**Figure S16.** The linear responses of NL- $\text{Fe}^{3+}$  (10  $\mu\text{M}$ ) versus the concentration of PPI (0-20  $\mu\text{M}$ ) in DMSO/ $\text{H}_2\text{O}$  (2:8/v:v, 20 mM HEPES, pH=7.2) solutions.



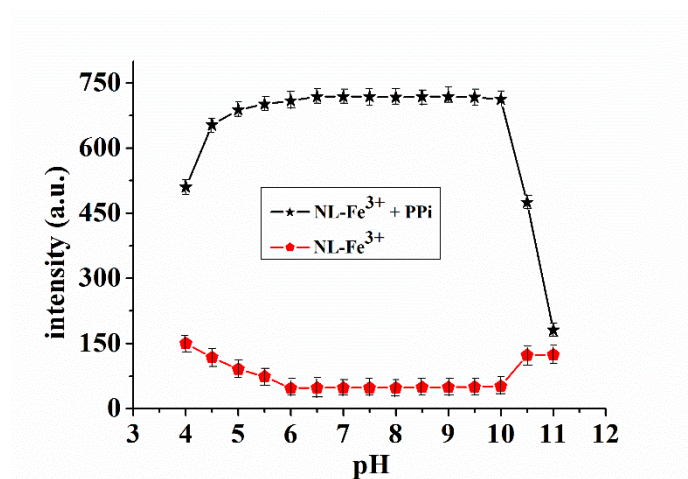
**Figure S17.** The decomplexation constant of NL- $\text{Fe}^{3+}$  toward PPI by fluorescence titration.



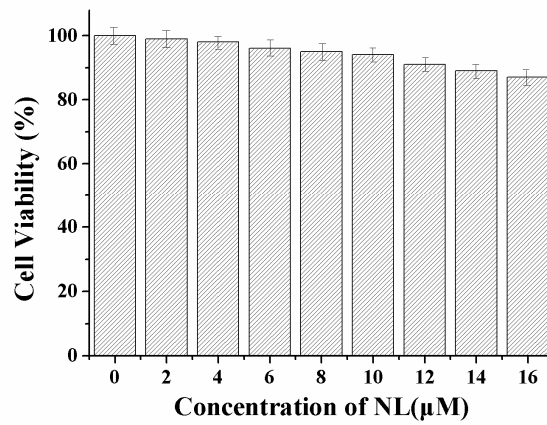
**Figure S18.** The fluorescence response time of NL-Fe<sup>3+</sup> (10 μM) in the presence of PPI (40 μM) in DMSO/H<sub>2</sub>O (2:8/v:v, 20 mM HEPES, pH=7.2) solutions.



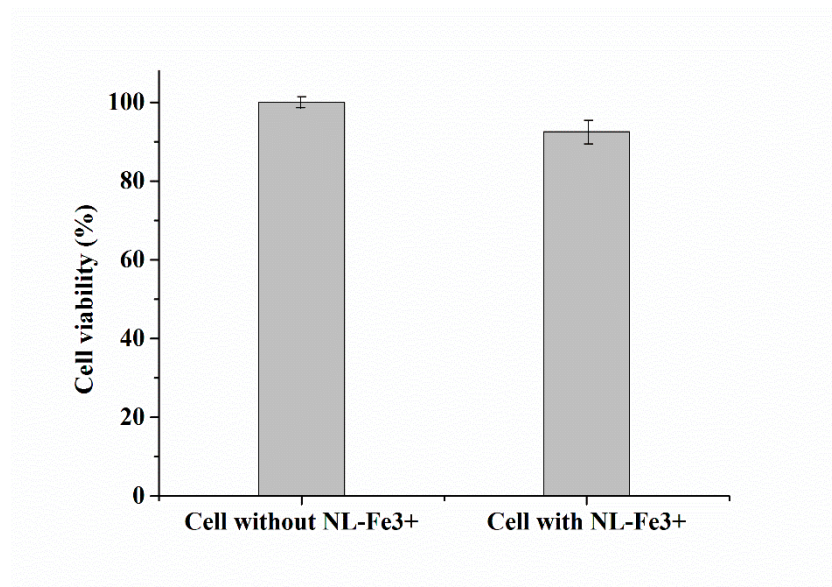
**Figure S19.** The decomplexation constant of NL-Fe<sup>3+</sup> toward PPI by UV-Vis spectroscopy.



**Figure S20.** Fluorescence intensity of NL-Fe<sup>3+</sup> (10 μM) in the absence and presence of PPI (40 μM) ion at various pH values in DMSO/H<sub>2</sub>O (2:8/v:v, 20 mM HEPES, pH=7.2) solutions.



**Figure S21.** Cell viability values (%) assessed using an MTT proliferation test versus incubation concentrations of NL. Hep G2 cells were cultured in the presence of NL (2-16 µM) at 25 °C for 24 h. Viability(%) = mean of absorbance value of treatment group/mean absorbance value of control × 100%.



**Figure S22.** MTT assay of Hep G2 cells treated with NL-Fe<sup>3+</sup> (10 µM) .