Supplementary Information

Aggregation induced emissive pyrimido fused tetraphenylethene benzothiazole probe for sensitive and selective detection of Fe^{3+} ions

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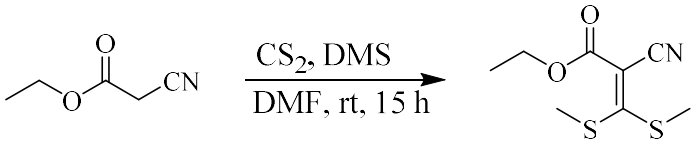
Experimental Section

Synthesis of ethyl 2-cyano-3,3-bis(methylthio)acrylate (2):



2

Scheme S1. Synthesis of ethyl 2-cyano-3,3-bis(methylthio)acrylate (**2**):

To a mixture of potassium hydroxide (0.424 g, 10.60 mmol) in 15 ml of dry DMF the reaction mixture was stirred at r.t. for 20 min. Then ethyl cyanoacetate (1 g, 8.84 mmol) was added dropwise at r.t. The resulting mixture was stirred at r.t for 1 h and carbon disulfide (0.8077 g, 10.60 mmol) was added at 0 ℃. The mixture stirred at 0℃ for 1.5 h and dimethyl sulfate (2.23 g, 17.68 mmol) was added slowly at 0℃. Then the resulting reaction mixture was stirred at r.t for 12 h and after completion of the reaction was monitored by TLC plate. The above reaction mixture was poured in to ice water with constant stirring and compound 2 was precipitated out. Further washed with water and dried to afford a yellow solid (**2,** 60%). Then it was used without further purification. FT-IR (cm^{-1} KBr) 2210, 1661, 1445, 1316, 1210, 935; ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm: 4.3 (q, 2H, J = 7.2 Hz), 2.75 (s, 3H), 2.6 (s, 3H), 1.37 (t, 3H, J = 7.09 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.8, 162.4, 116.1, 98.8, 61.8, 20.9, 18.9, 14.2; ESI-mass m/z: calcd 217.30 $[M]^+$, found 218.00 $[M+H]^+$; HRMS m/z: $[M+H]^+$ calcd. for $C_8H_{12}NO_2S_2$ 218.03040; found 218.03134 $[M+H]^+$.

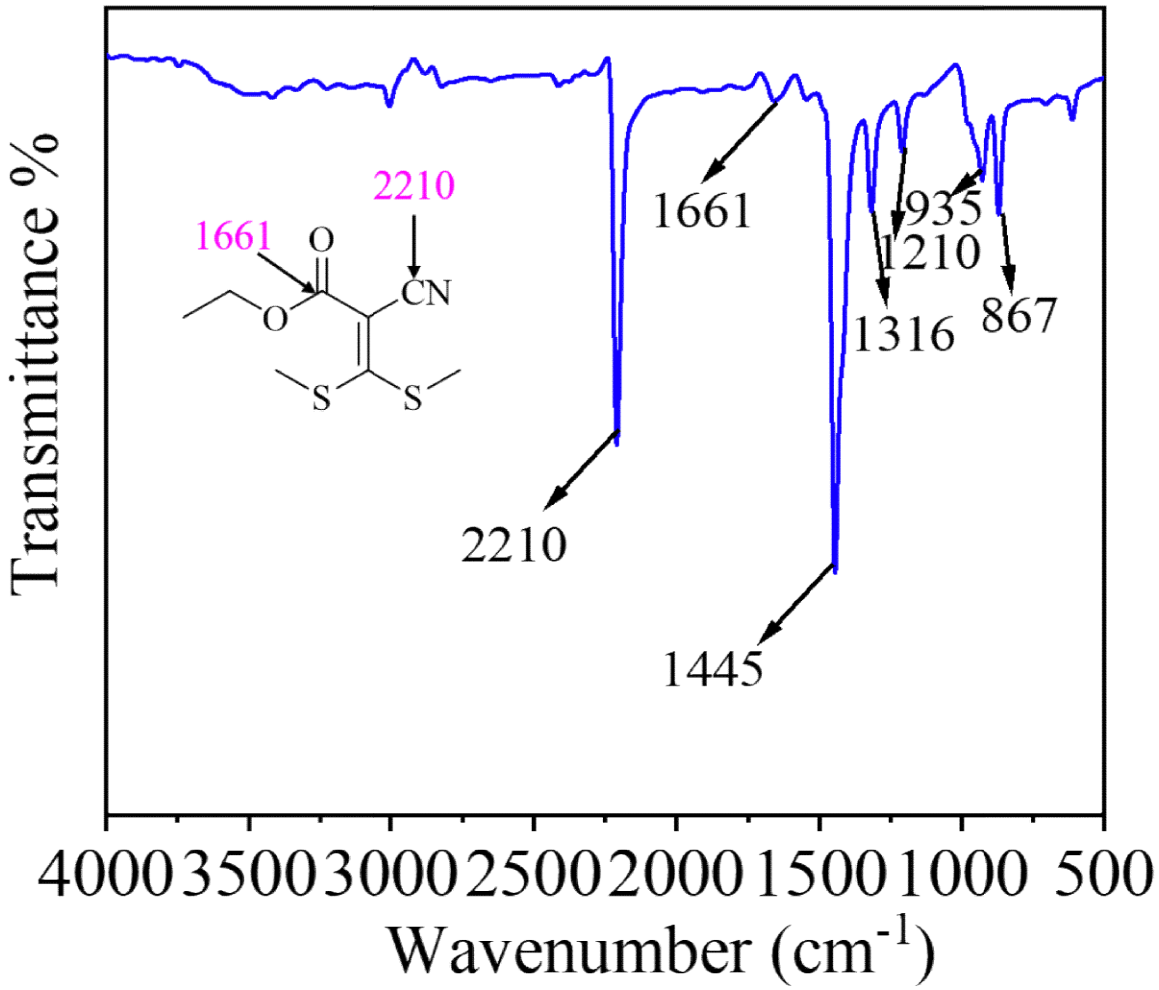


Figure S1**.** FT-IR spectra of compound 2

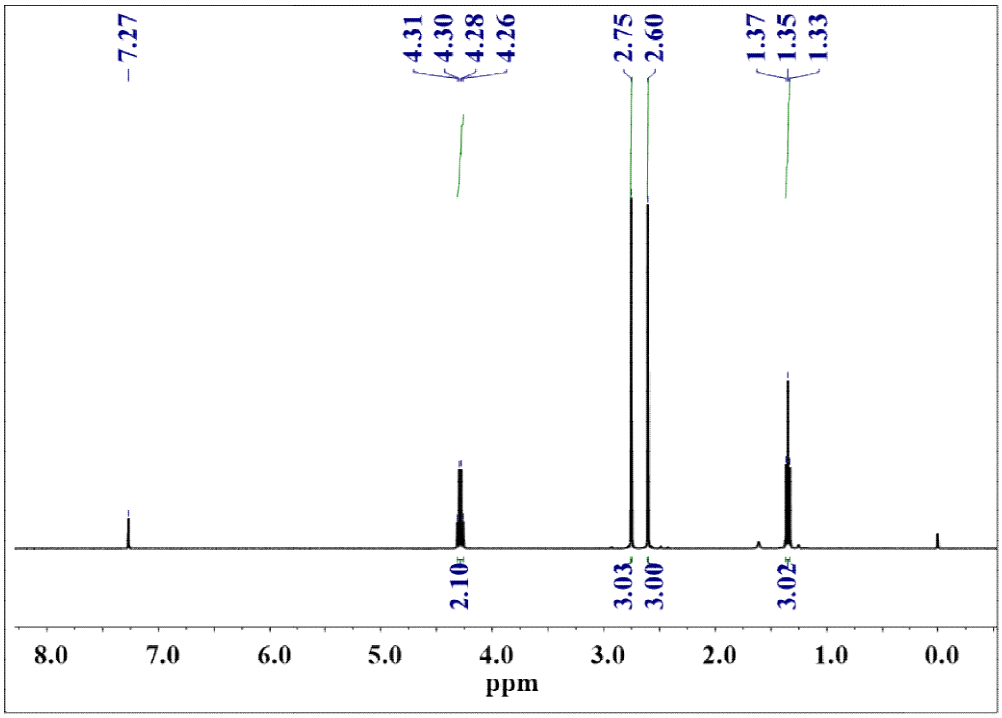


Figure S2. ^{1}H NMR spectra of compound 2.

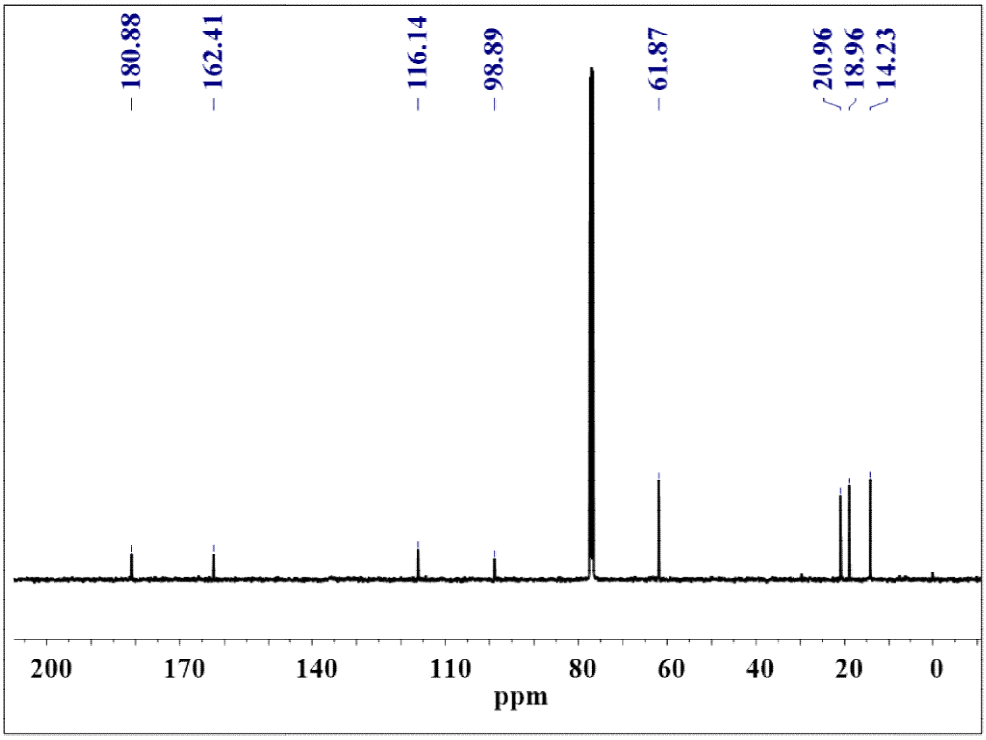


Figure S3. ^{13}C NMR spectra of compound 2.

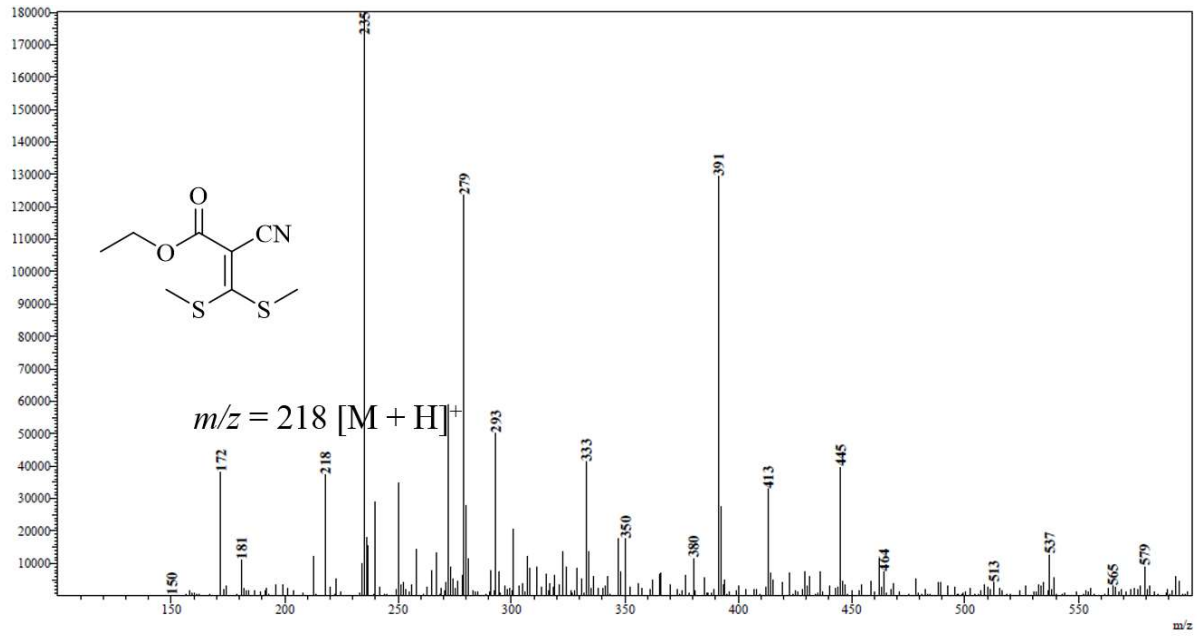


Figure S4. Mass spectrum of compound 2.

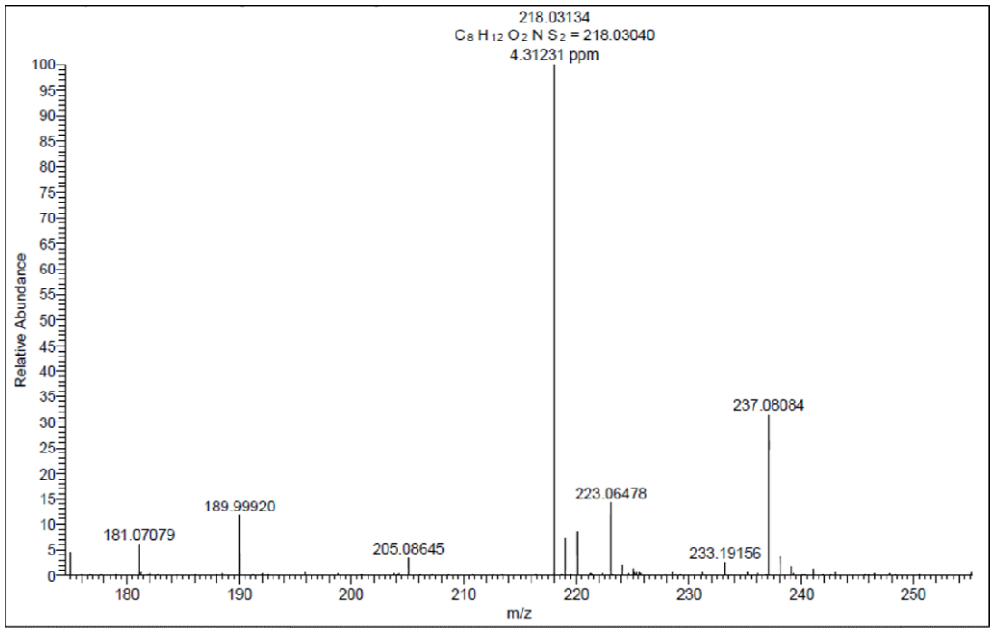
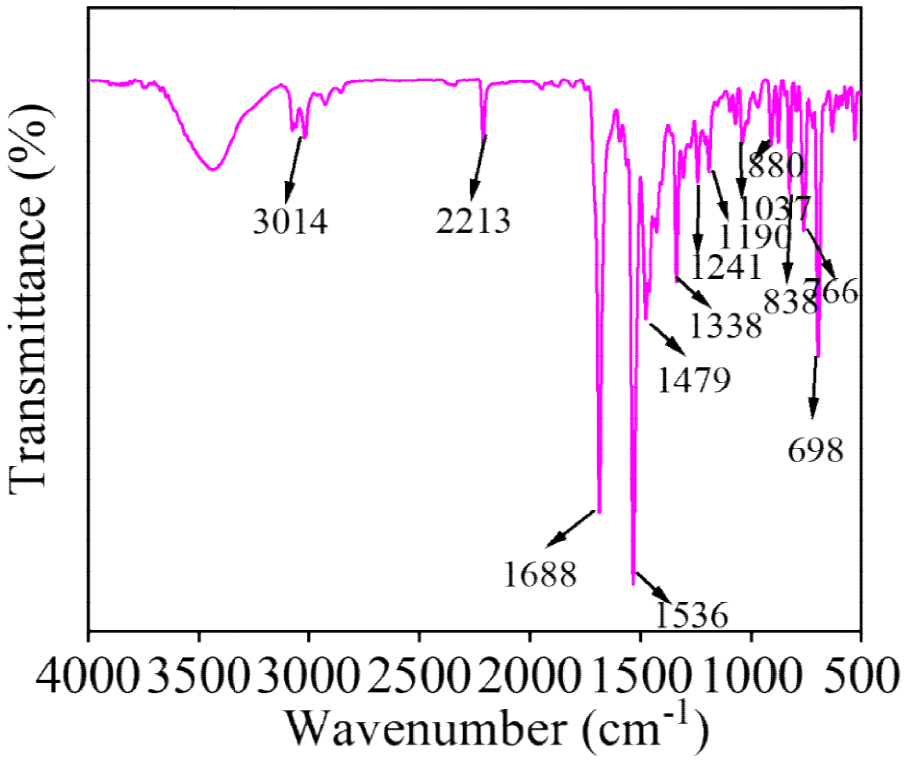


Figure S5. HRMS spectrum of compound 2.



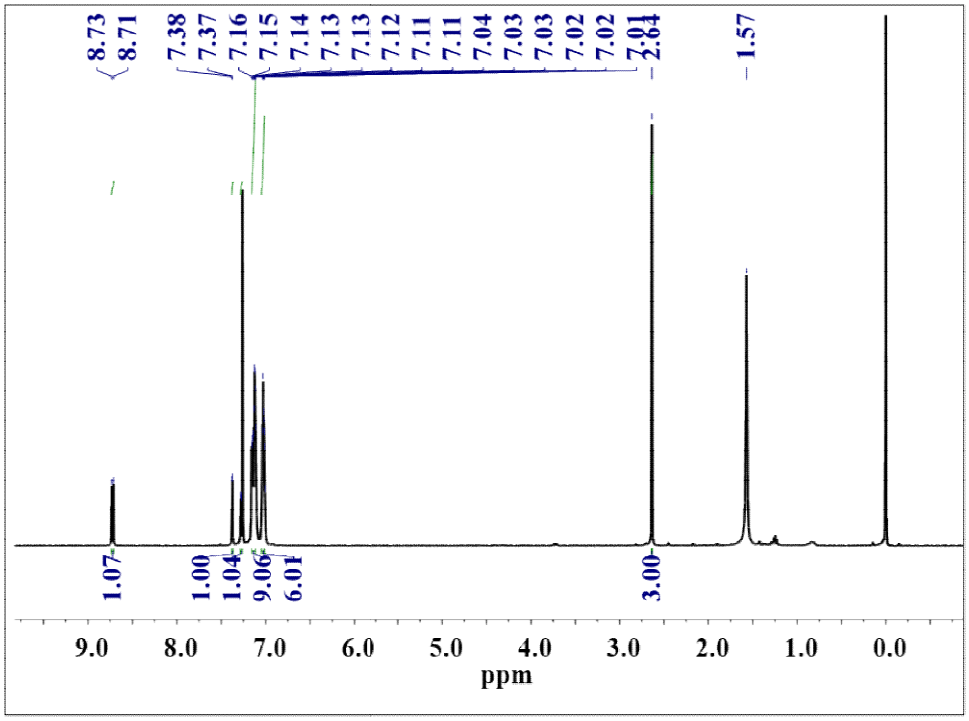


Figure S6. FT-IR spectra of compound TPE-1

Figure S7. ^{1}H NMR spectra of compound TPE-1

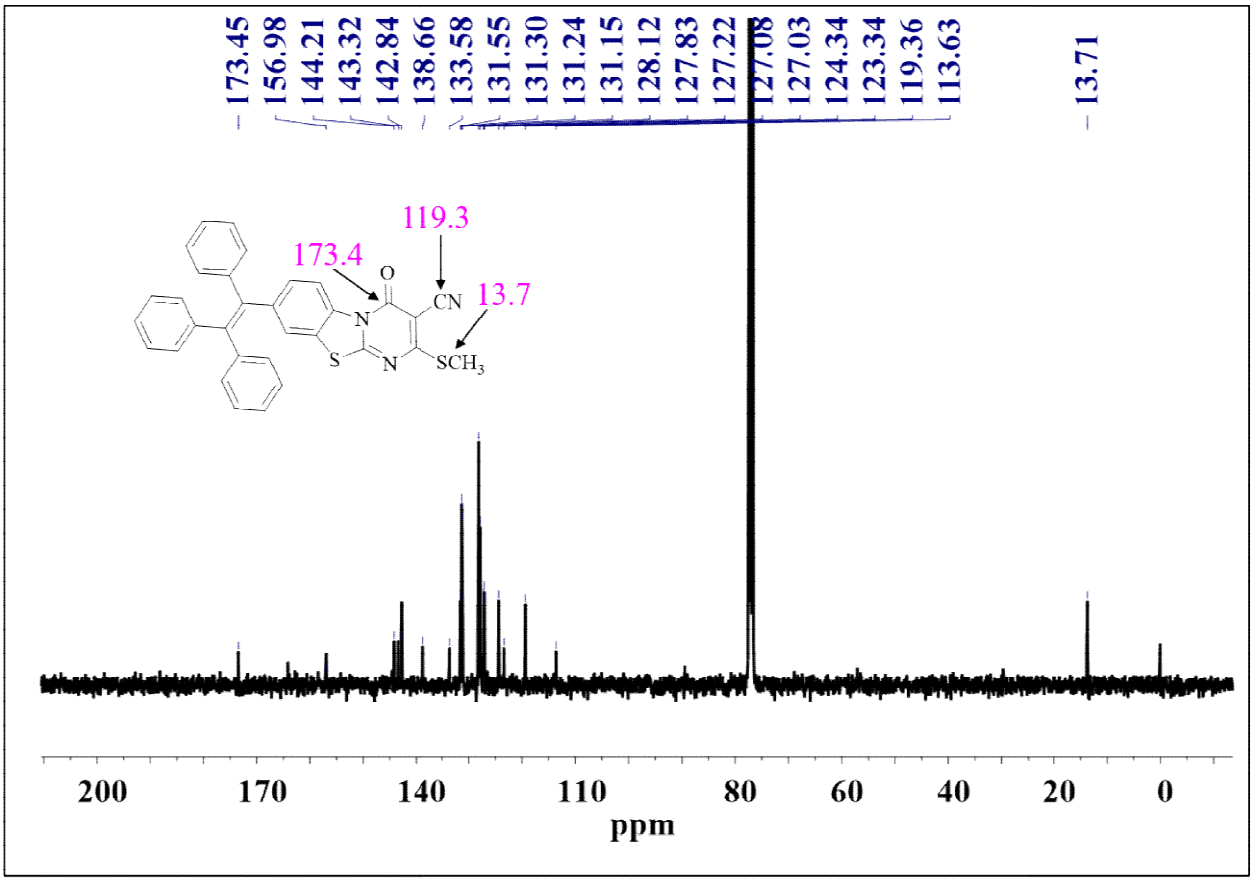


Figure S8. ^{13}C NMR spectra of compound TPE-1

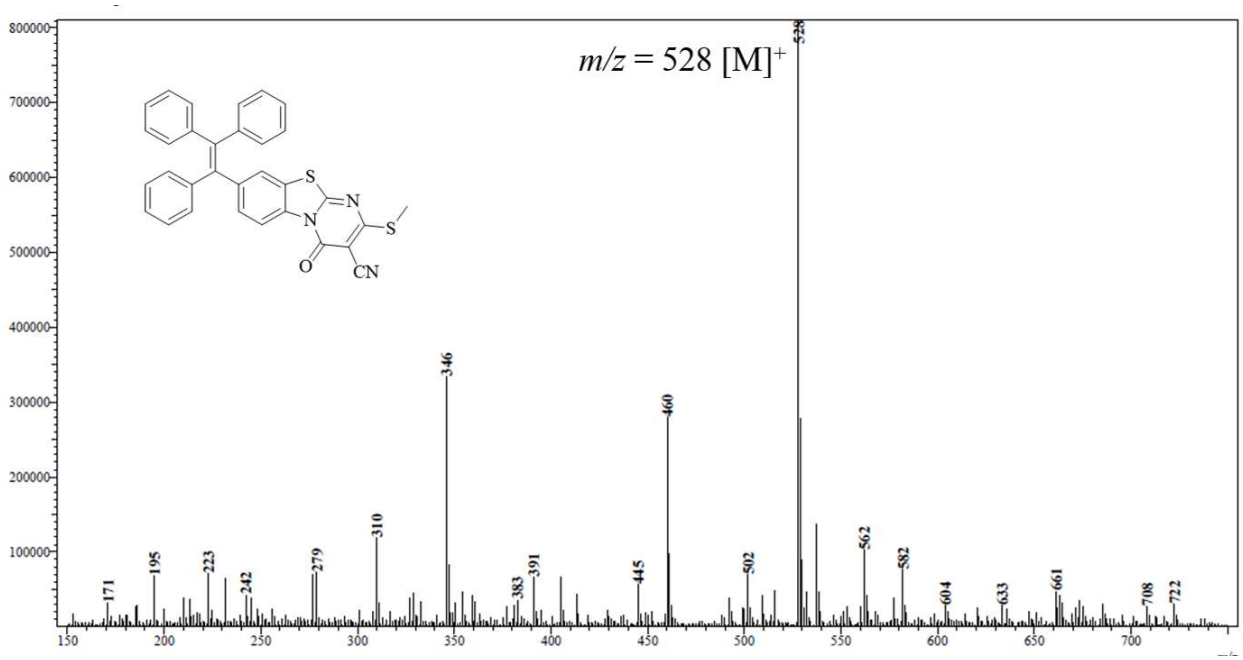


Figure S9. Mass spectrum of TPE-1.

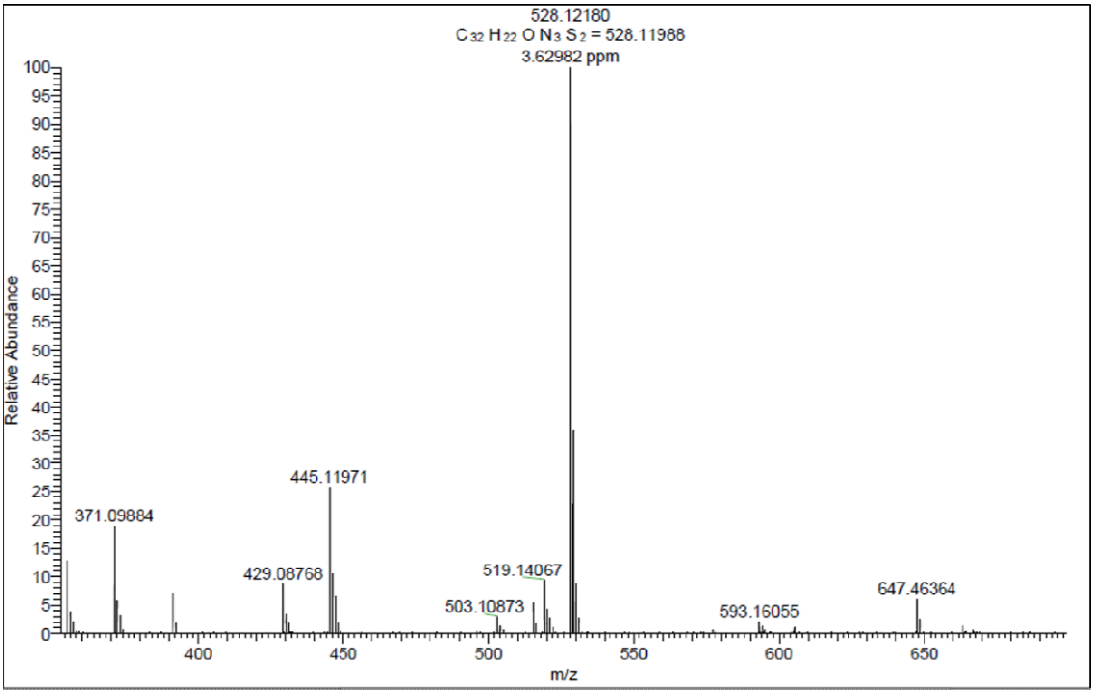


Figure S10. HRMS spectrum of compound TPE-1.

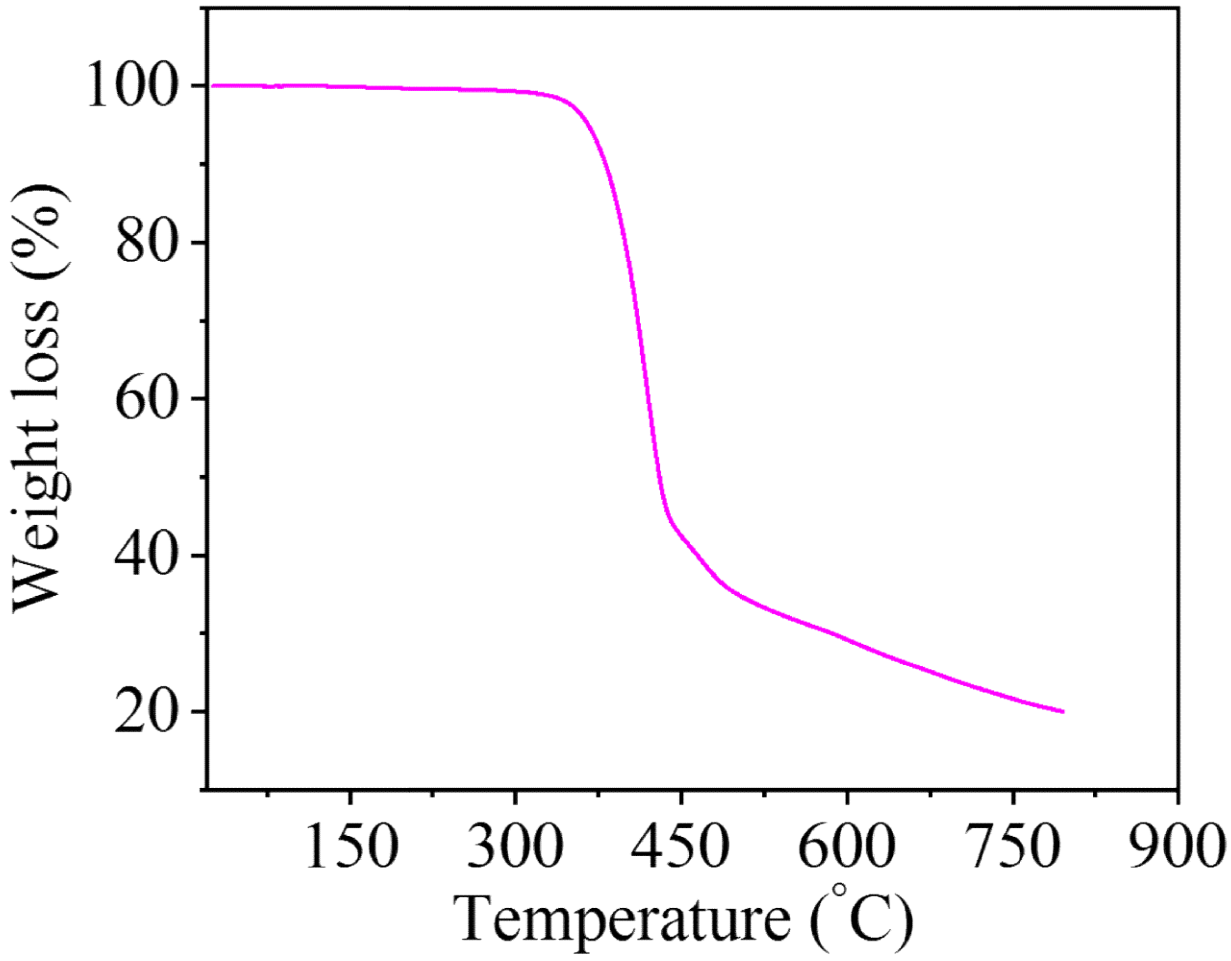


Figure S11. Thermogravimetric analysis (TGA) of TPE-1.

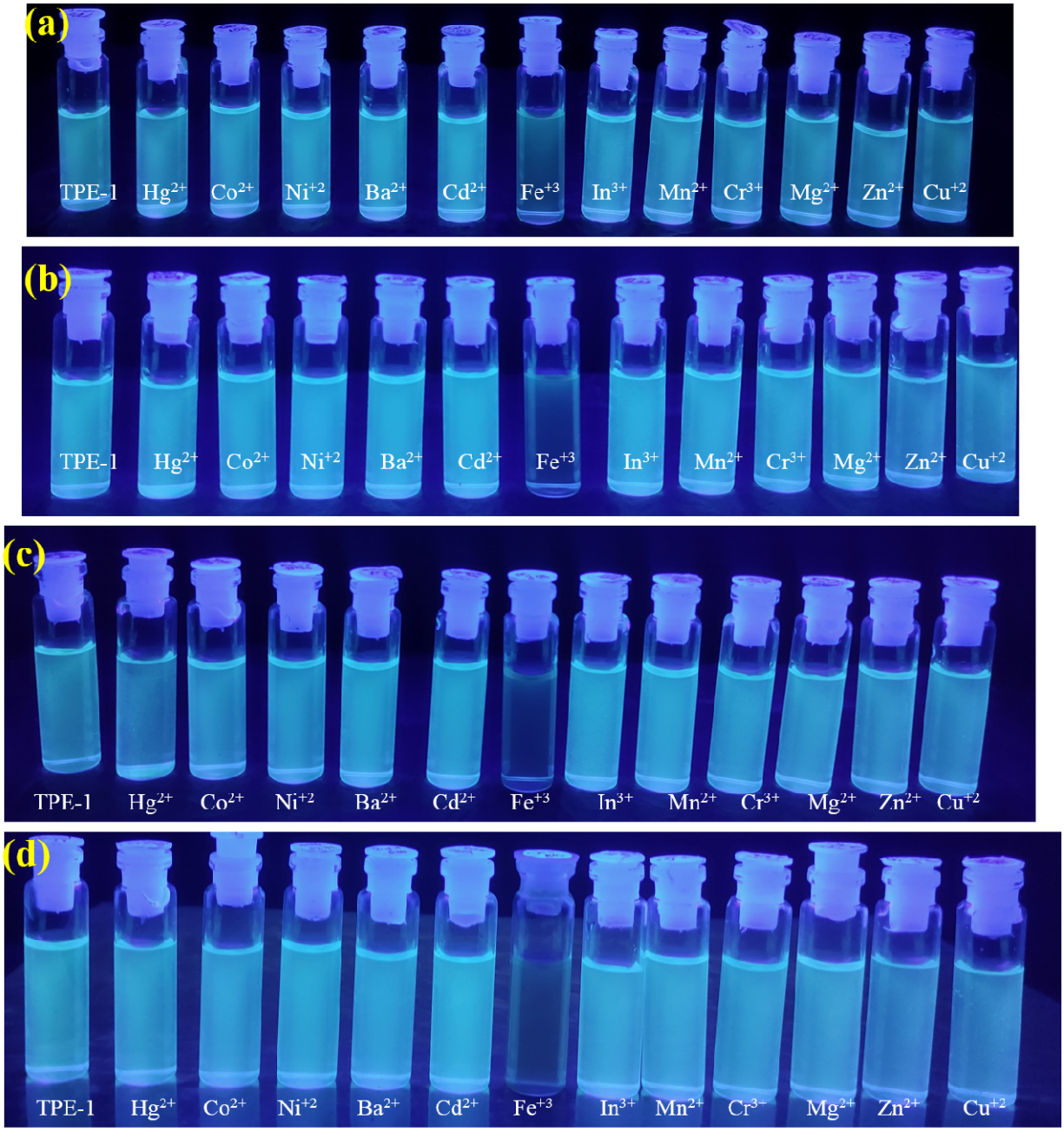


Figure S12. Photographic images of TPE-1 with (a) 100 equiv.; (b) 200 equiv., (c) 300 equiv. and (d) 500 equiv. of various metals ions in DMSO: H_2O (10:90).

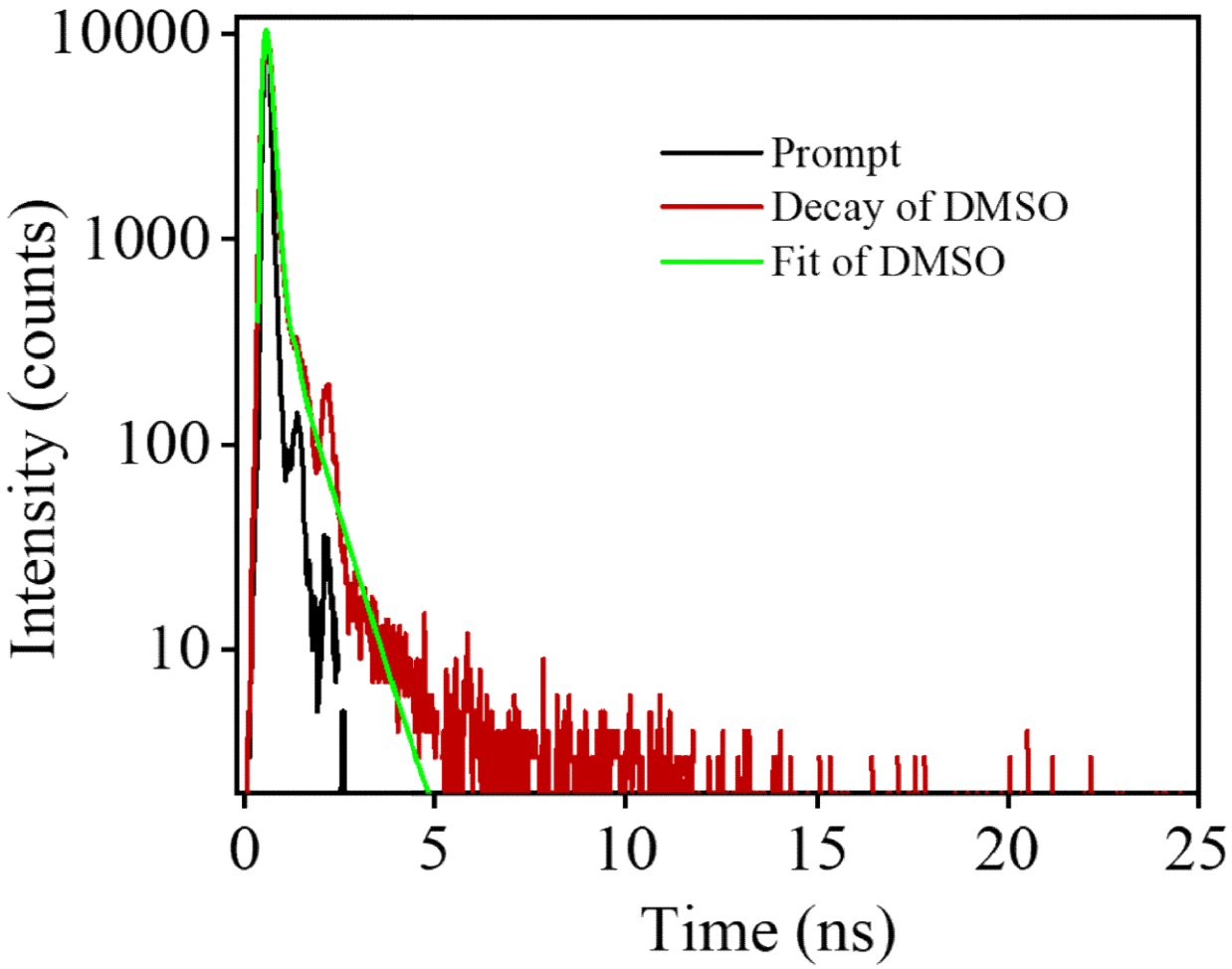


Figure S13. TCSPC measurements of TPE-1 (1×10^{-5} M) in DMSO.