Supporting Information for

A benzimidazole-based 'turn-on' fluorescent probe for highly sensitive detection of $Fe^{3+/2+}$: synthesis, performance, DFT calculations and applications

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TABLE OF CONTENTS **PAGE**

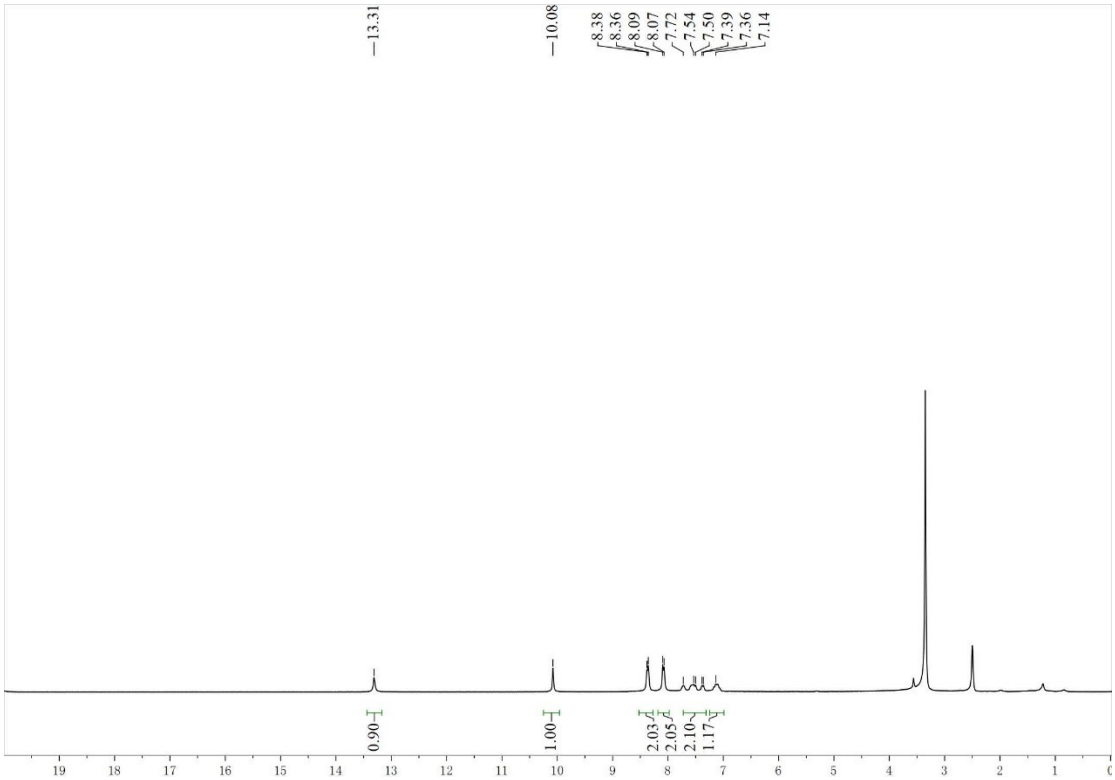


Fig. S1. ^{1}H NMR spectra of compound 3

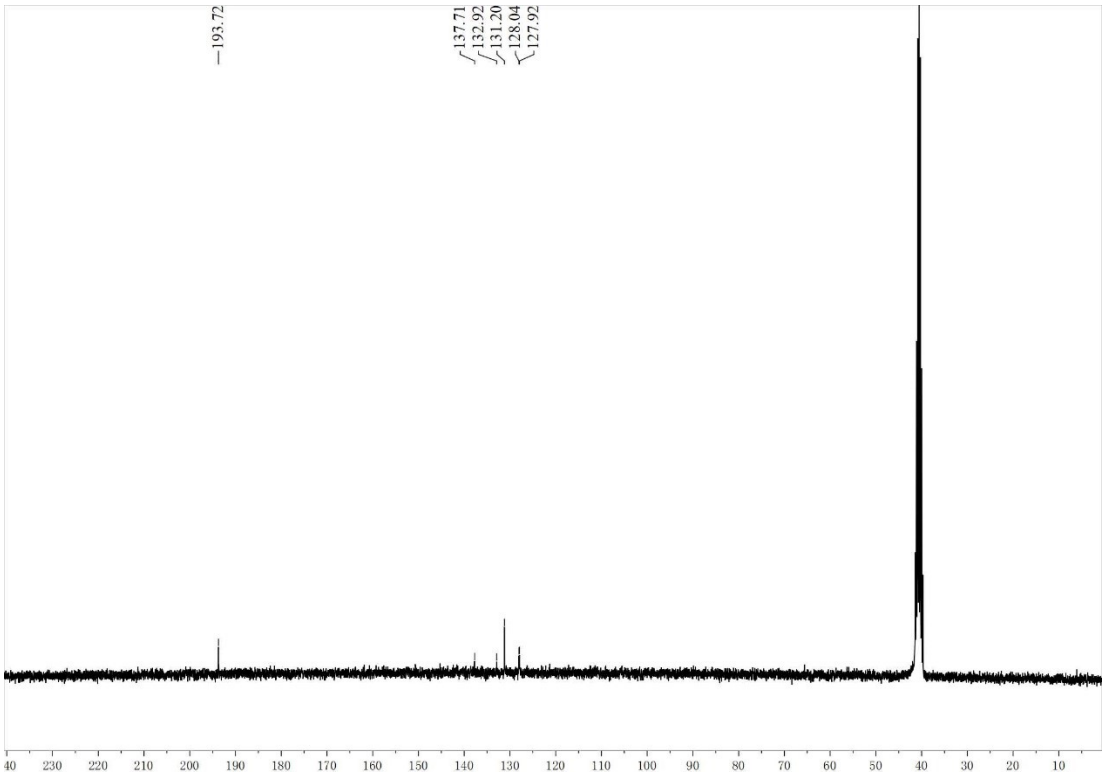


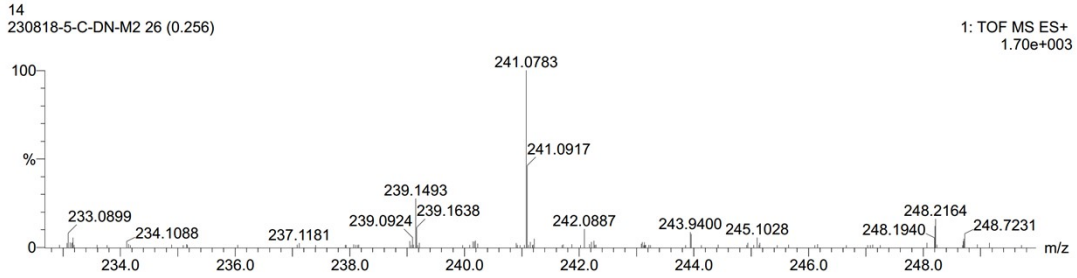
Fig. S2. ^{13}C NMR spectra of compound 3

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
211 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 14-14 H: 10-10 N: 0-100 O: 0-100 Na: 0-1 F: 1-1

14
230818-5-C-DN-M2 26 (0.256)



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
241.0783	241.0777	0.6	2.5	10.5	172.4	n/a	n/a	C14 H10 N2 O F

Fig. S3. HRMS spectra of compound 3

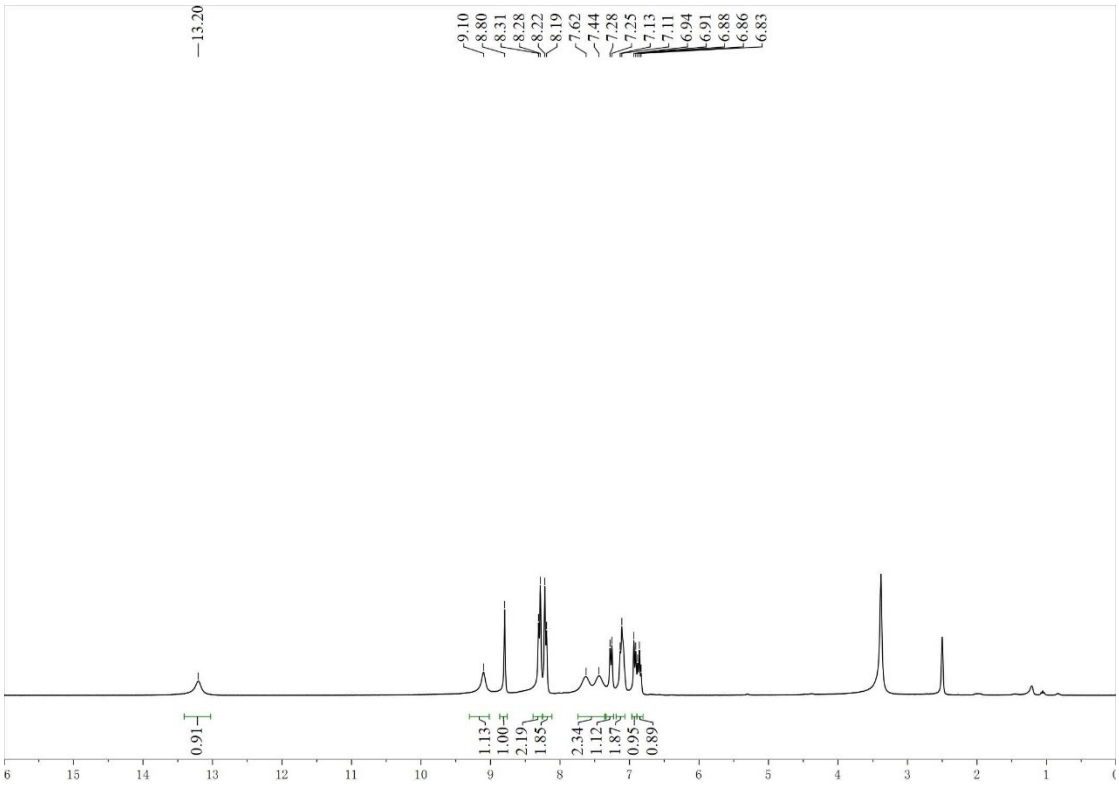


Fig. S4. ^{1}H NMR spectra of probe FBBAP

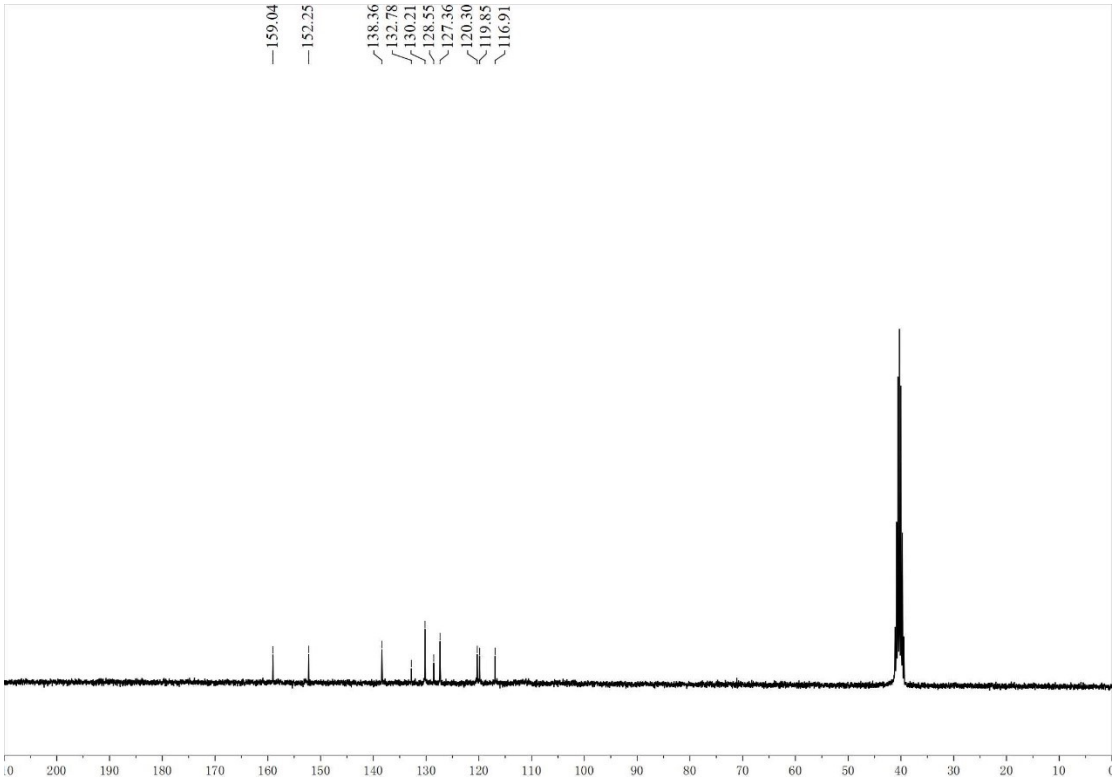


Fig. S5. ^{13}C NMR spectra of probe FBBAP

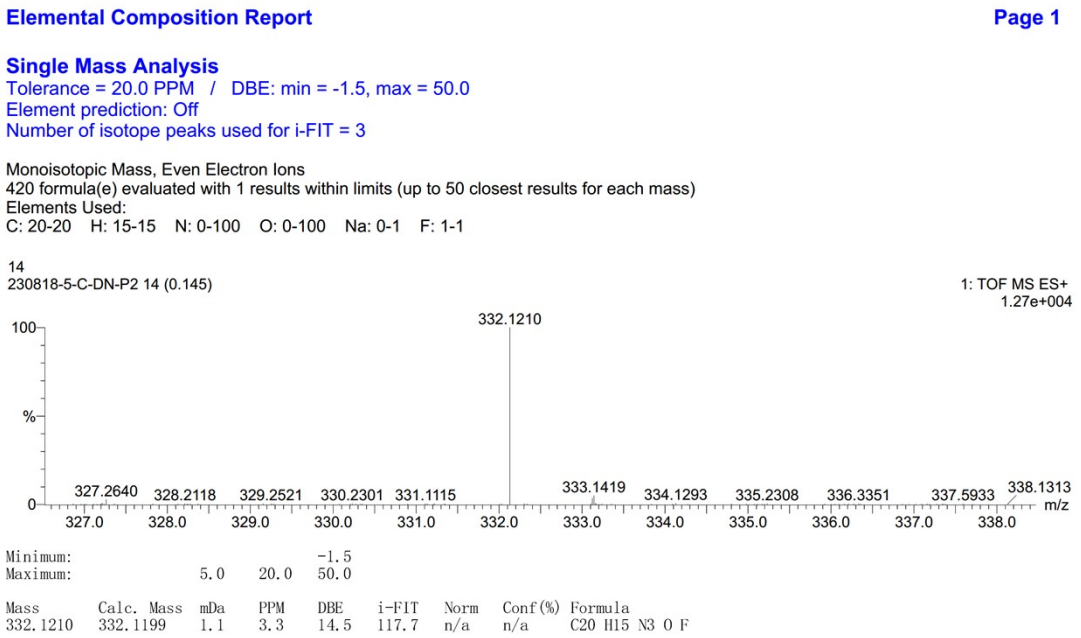


Fig. S6. HRMS spectra of probe FBBAP

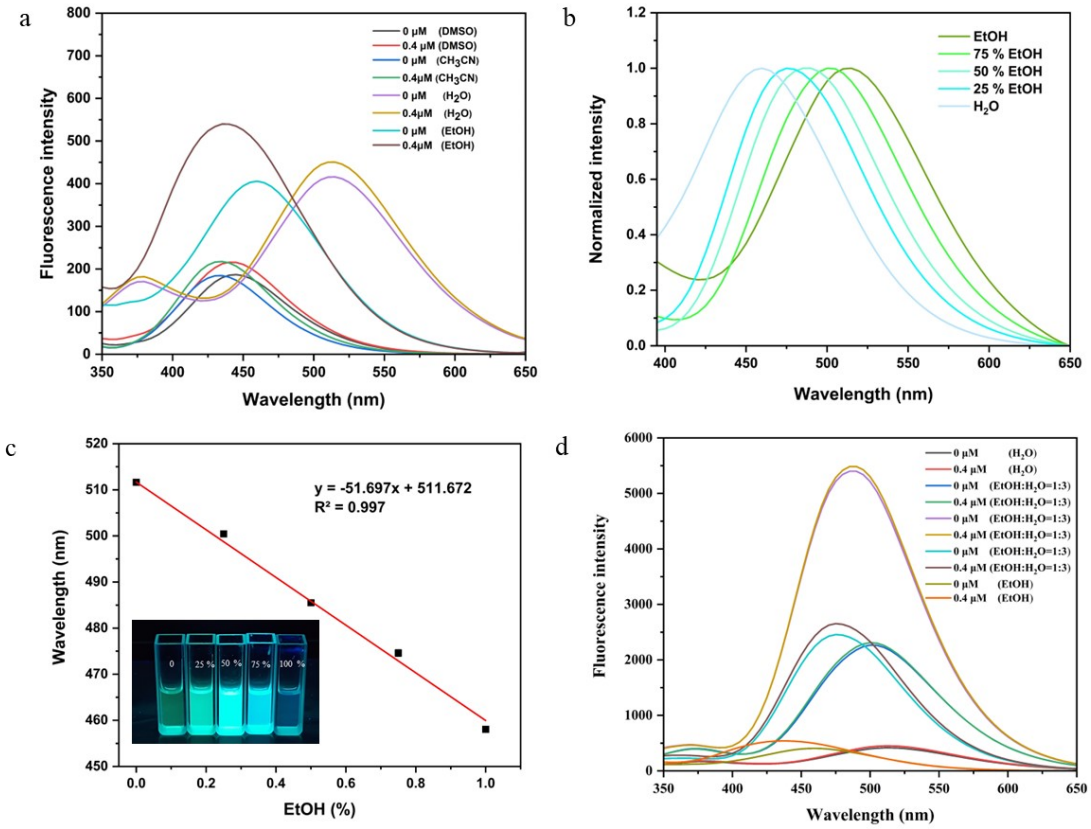


Fig. S7. (a) Fluorescence spectra of probe FBBAP (10 μM) with $Fe^{3+/2+}$ (0.4 μM) in different solvents; (b) The emission wavelength changes of the probe under different ratios of ethanol. (c) The linear relationship between the emission wavelength of probe FBBAP and different proportions of ethanol. Insert: The luminescence of probe FBBAP under different ratios of ethanol. (d) Fluorescence spectra of probe FBBAP (10 μM) with $Fe^{3+/2+}$ (0.4 μM) in different ratios of ethanol.

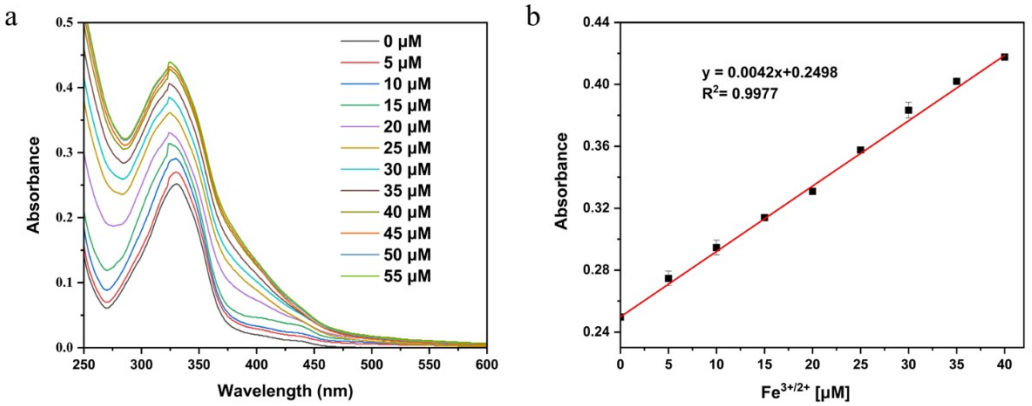


Fig. S8. (a) Absorption spectrum of probe FBBAP (10 μM) with $Fe^{3+/2+}$ (0-55 μM) in EtOH at 25°C. (b) Plot of fluorescence intensity with 0-40 μM $Fe^{3+/2+}$. Tests were performed in triplicate.

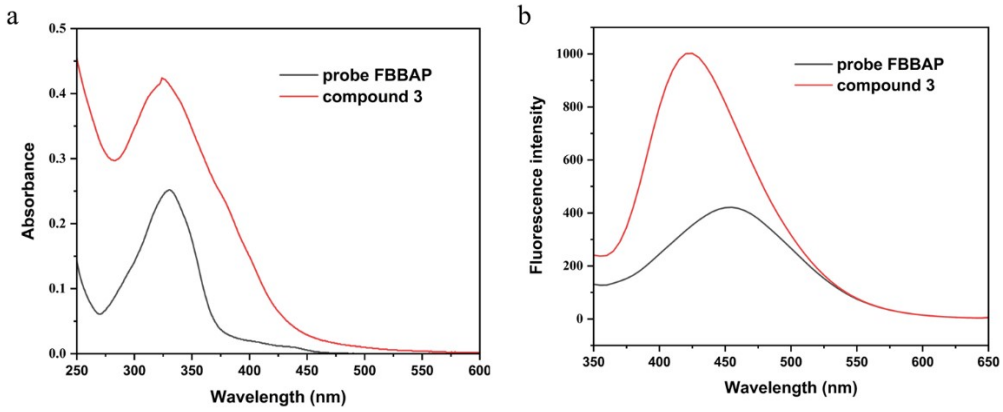


Fig. S9. The UV (a) and fluorescence spectra (b) of probe FBBAP and compound 3.

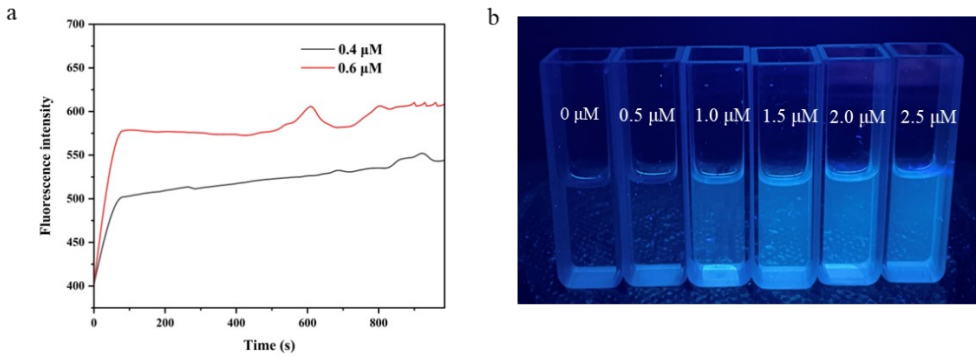


Fig. S10. (a) The variation of fluorescence intensity of probe FBBAP with time after adding $Fe^{3+/2+}$. (b) Changes in probe FBBAP at 365nm after adding different concentrations of $Fe^{3+/2+}$.

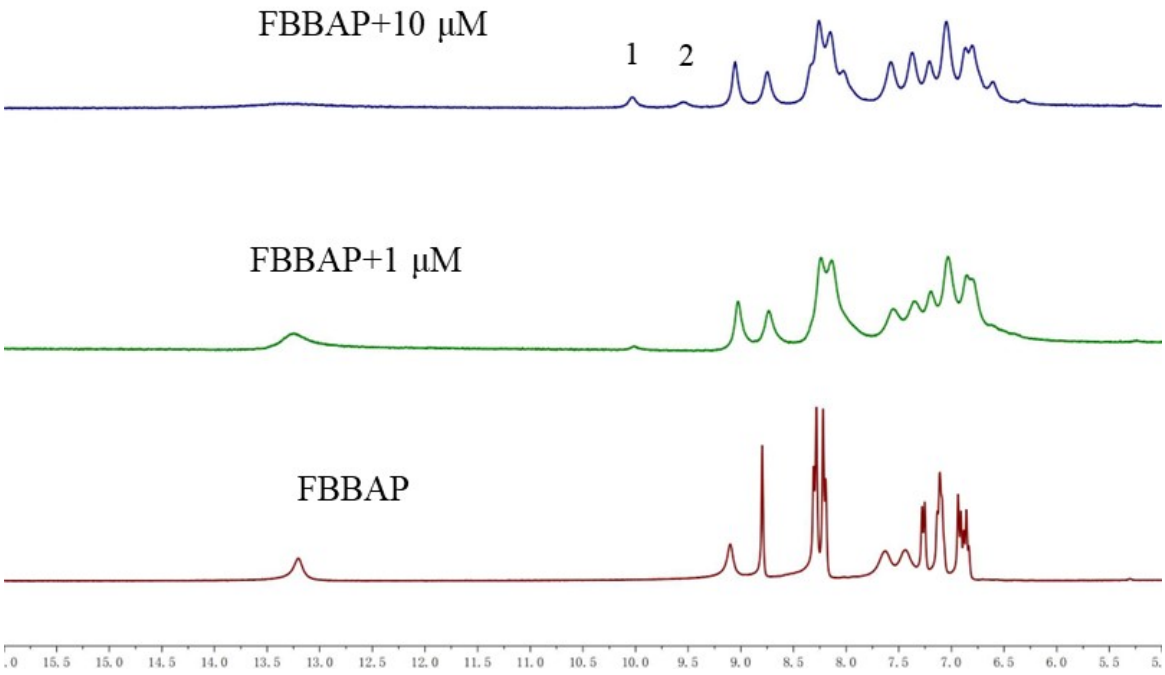


Fig. S11. The NMR mechanism diagram of the probe FBBAP after adding different concentrations of $Fe^{3+/2+}$.

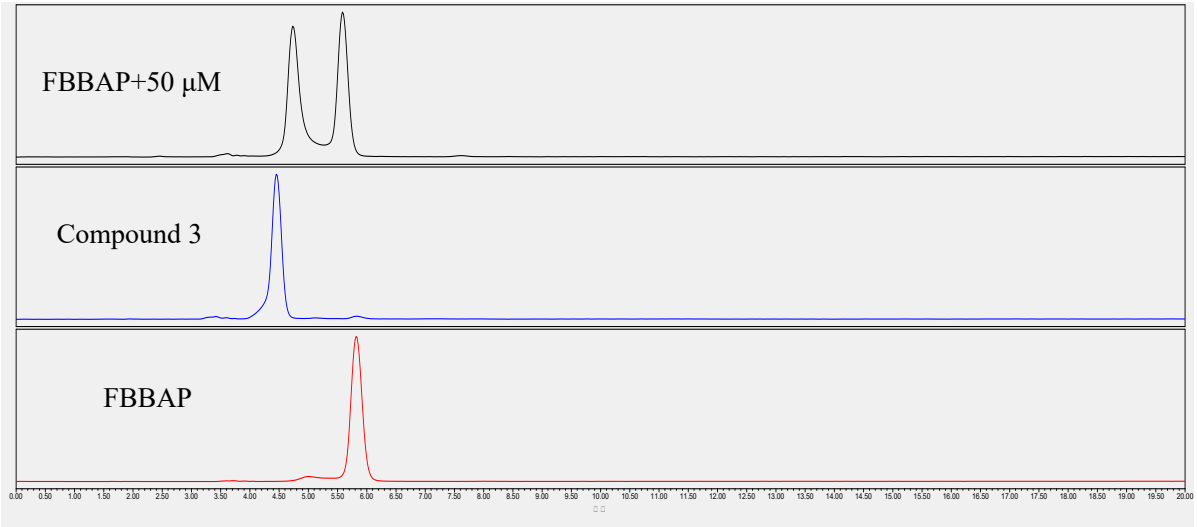


Fig. S12. High performance liquid chromatography of probe FBBAP, compound 3, and FBBAP+$Fe^{3+/2+}$ (50 μM).

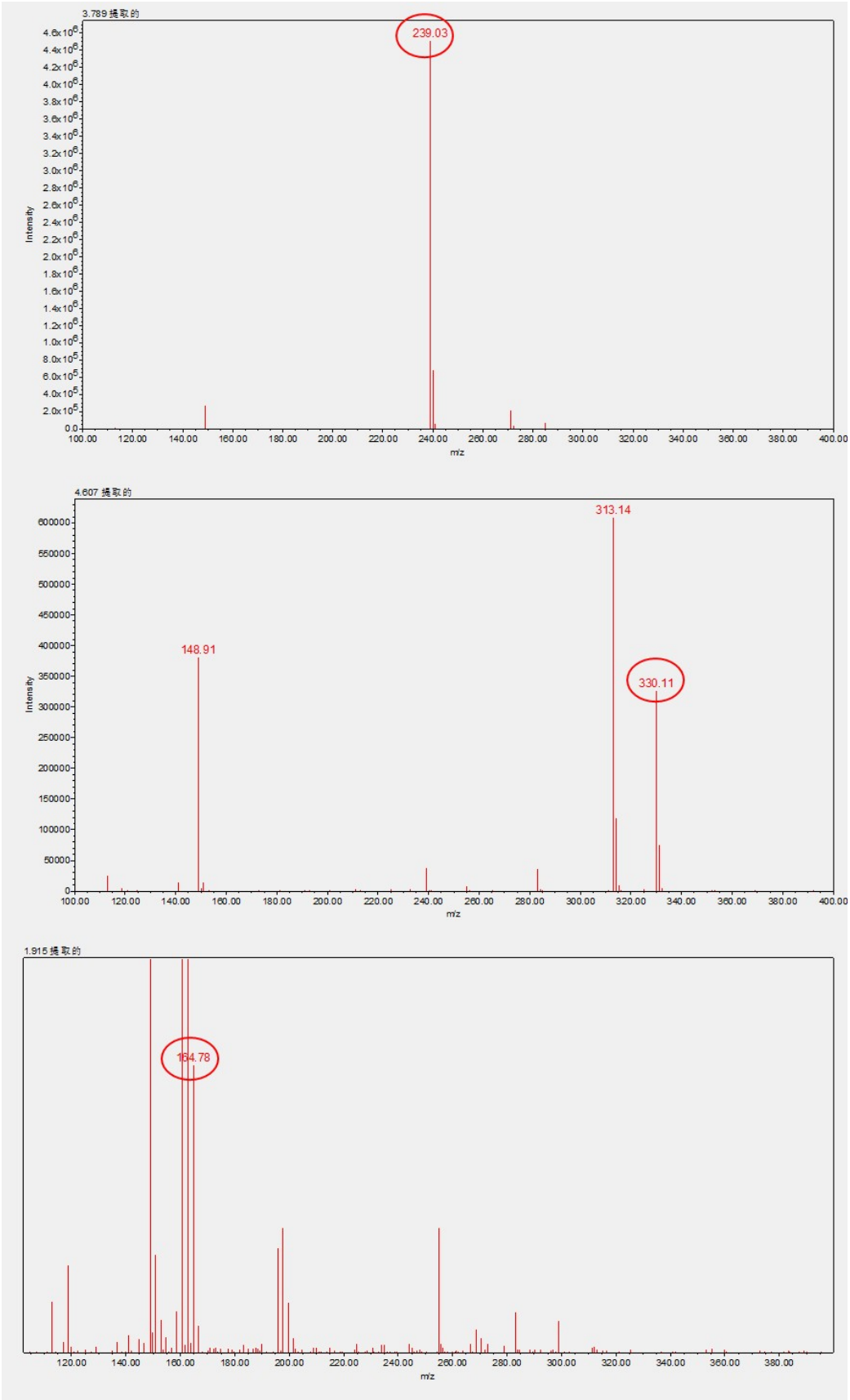


Fig. S13. The experimental results of HPLC-MS after probe FBBAP response to $Fe^{3+/2+}$.

Table S1 Calculation Results of Excited States of Probes and Intermediates by Three Functional Methods. EtOH was used as the solvent (PCM model).

Functionals		Cam-B3LYP	M06-2X	PBE0	Experimental value
Compound 3	λ_{abs} (nm)	321.28	336.50	345.57	330
	CI coefficient	0.61	0.57	0.70	/
	λ_{em} (nm)	425.59	367.99	434.16	420
	CI coefficient	0.71	0.70	0.70	/
	f	1.3126	1.2505	1.4414	/
Probe FBBAP	λ_{abs} (nm)	355.61	344.39	394.33	349
	CI coefficient	0.69	0.67	0.70	/
	λ_{em} (nm)	469.32	382.83	471.91	460
	CI coefficient	0.68	0.63	0.67	/
	f	0.0130	0.0767	0.0330	/

Table S2 Determination of total iron content in really samples

Sample	Fe^{3+} level found （μM）	Added (μM)	Found (μM)	Recovery/%	RSD/%(n=3)
Red wine 1	0.34	0.2	0.54	103.40	0.01
		0.4	0.72	95.33	0.02
Red wine 2	0.46	0.2	0.66	95.63	0.02
		0.4	0.86	99.23	0.09
Water	0.00	0.2	0.20	98.12	0.28
		0.4	0.39	98.04	0.29
Milk 1	0.00	0.2	0.19	96.83	0.55
		0.4	0.42	106.02	0.12
Milk 2	0.00	0.2	0.19	96.53	0.62
		0.4	0.40	101.11	0.48