

A convenient tool for real-time detection of iron content in human food

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Fig. S1. ^1H NMR spectra of compound 1

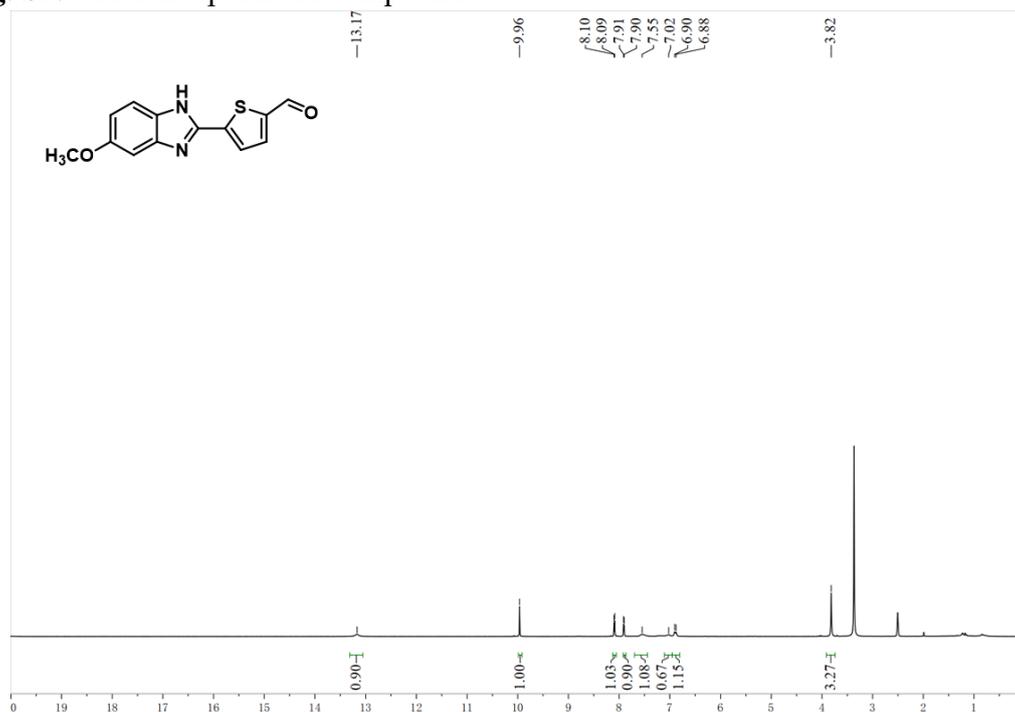


Fig. S2. ^{13}C NMR spectra of compound 1

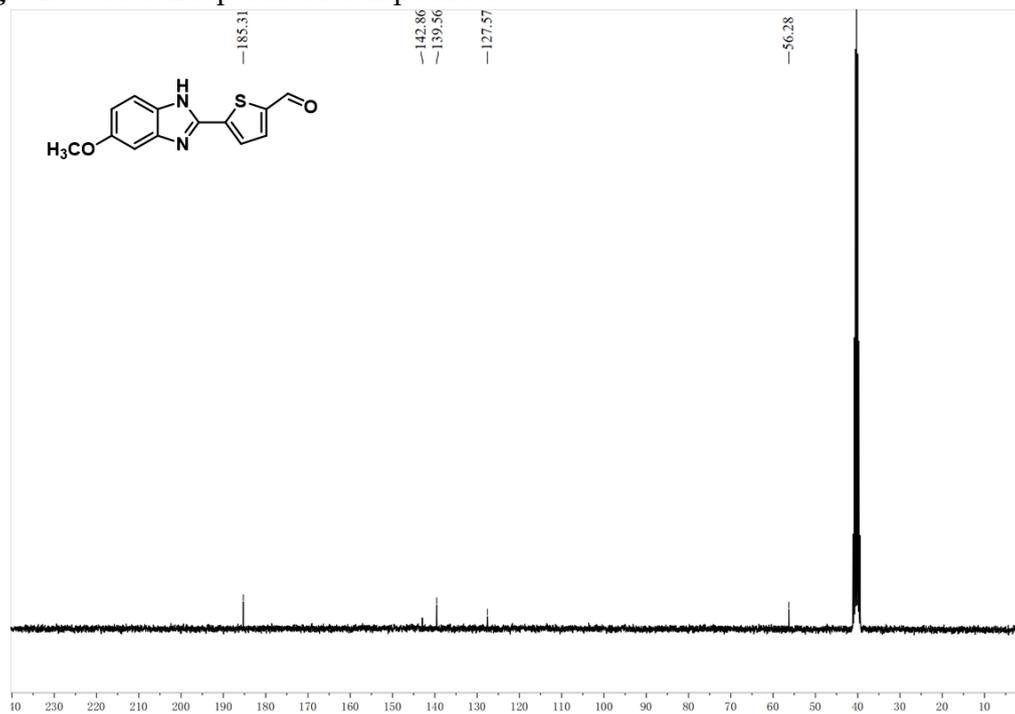


Fig. S3. HRMS spectra of compound 1

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

382 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

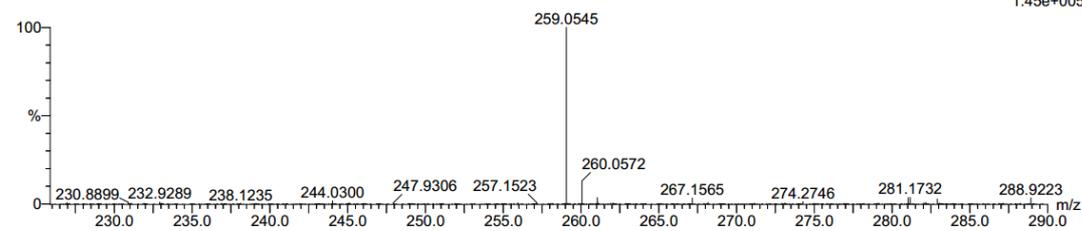
Elements Used:

C: 13-13 H: 11-11 N: 0-100 O: 0-100 Na: 0-1 S: 1-2

28

240621-10-M11 27 (0.178)

1: TOF MS ES+
1.45e+005



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
259.0545	259.0541	0.4	1.5	9.5	447.1	n/a	n/a	C13 H11 N2 O2 S

Fig. S4. ¹H NMR spectra of probe OMTP

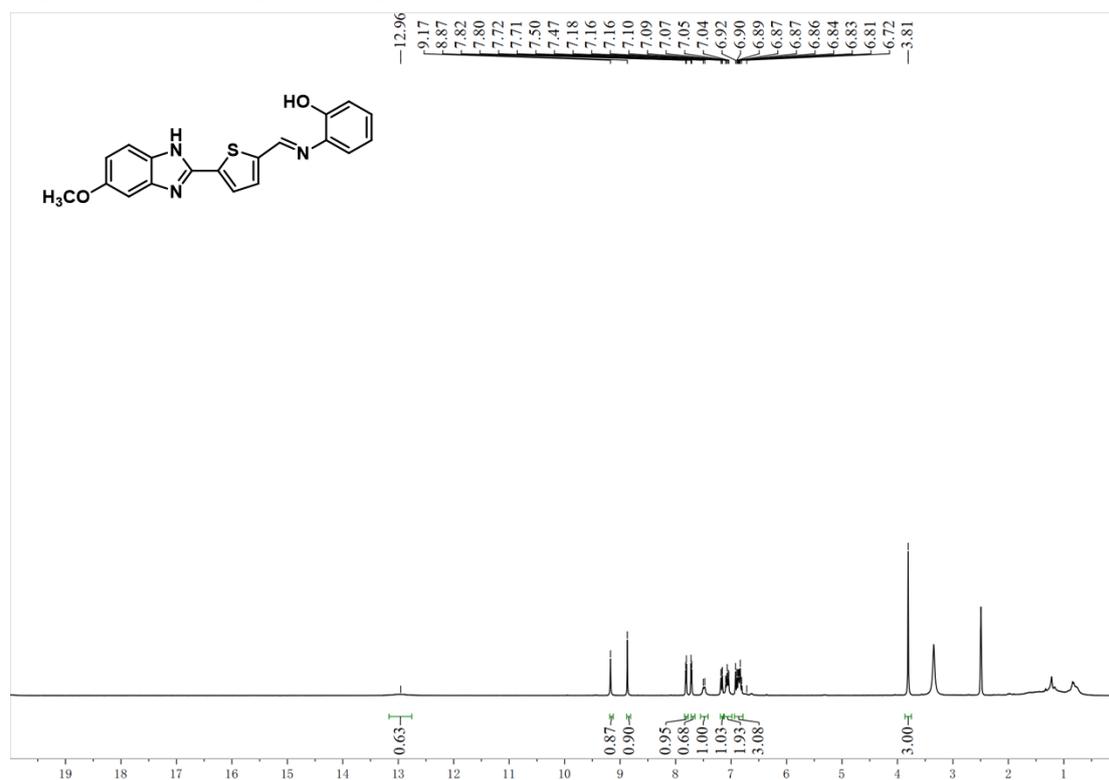


Fig. S5. ^{13}C NMR spectra of probe OMTP

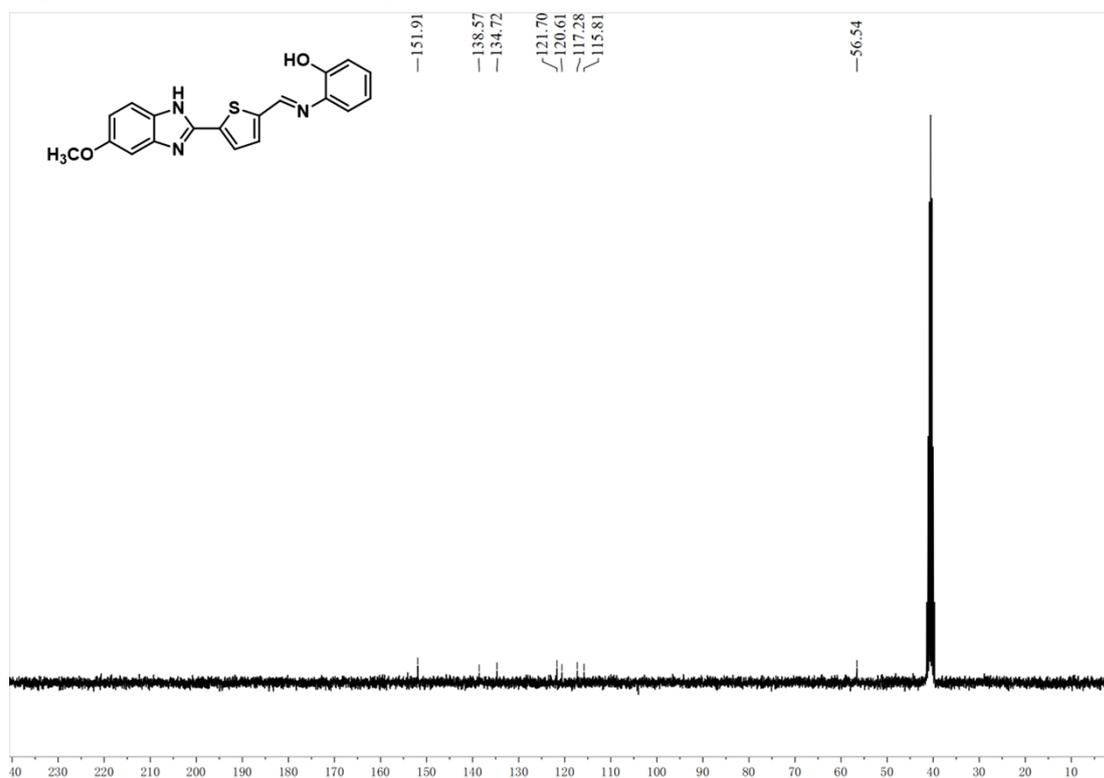


Fig. S6. HRMS spectra of probe OMTP

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

780 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

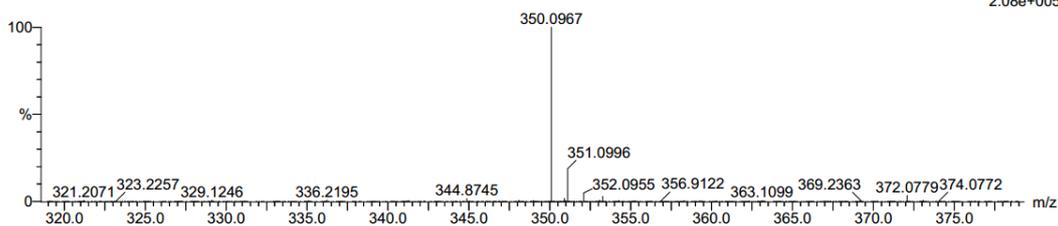
Elements Used:

C: 19-19 H: 16-16 N: 0-100 O: 0-100 Na: 0-1 S: 1-2

28

240621-10-P11 22 (0.152)

1: TOF MS ES+
2.08e+005



Minimum:

Maximum: 5.0 10.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
350.0967	350.0963	0.4	1.1	13.5	476.7	n/a	n/a	C19 H16 N3 O2 S

Fig. S7 Reaction mechanism for the hydrolysis of probe OMTP.

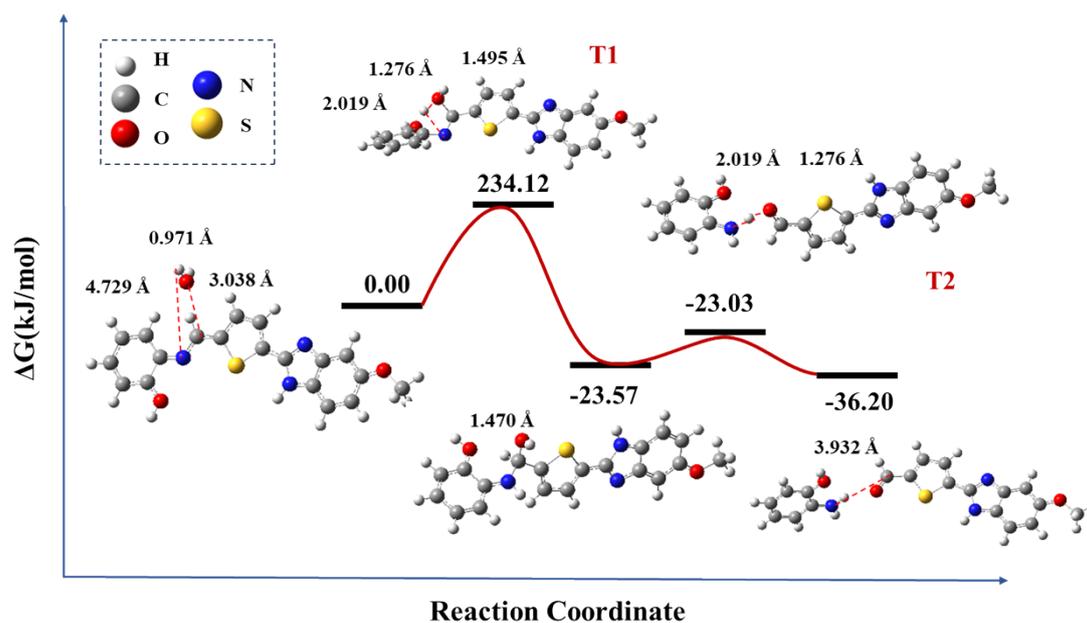


Fig. S8 Initial and final structures of Fe^{3+} , Cu^{2+} , and Al^{3+} catalyzed hydrolysis probe OMTP

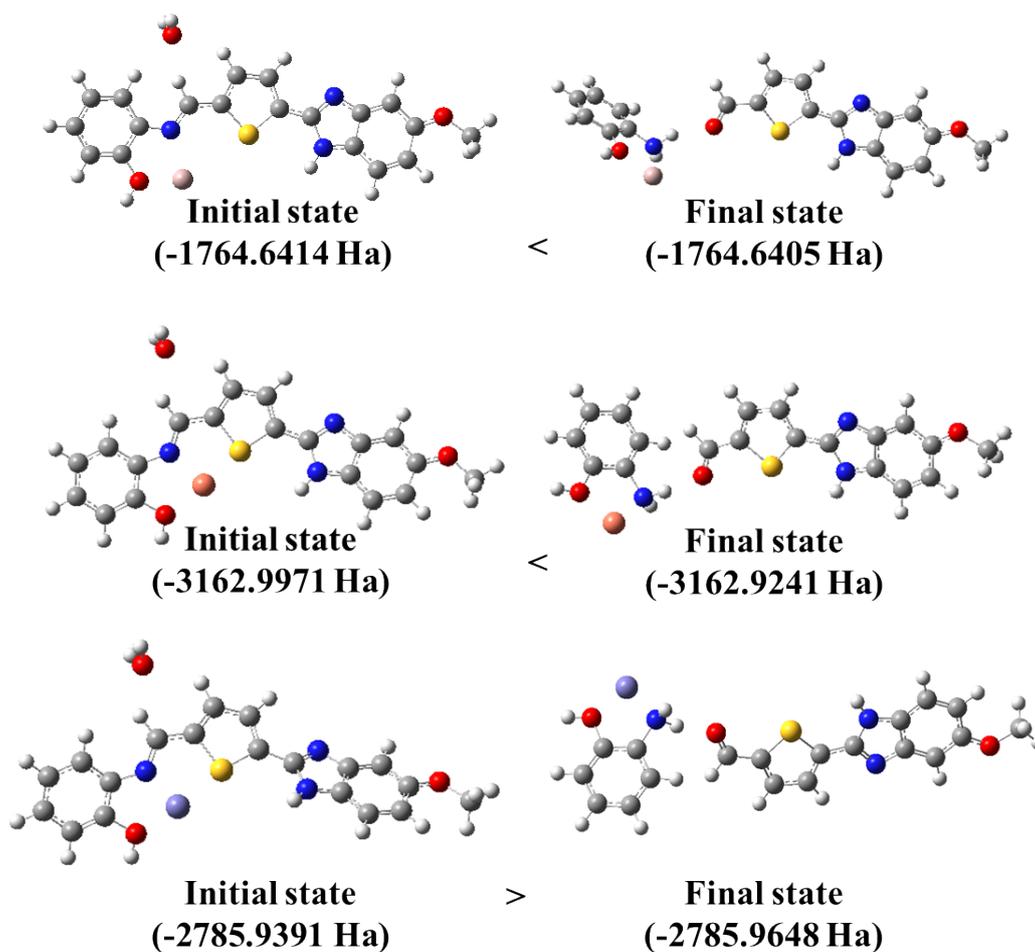


Fig. S9 (a) Changes in fluorescence intensity of probe OMTP (10 μM) with $\text{Fe}^{3+/2+}$ (1.0 μM) in EtOH with different proportions of H_2O ; (b) Changes in fluorescence intensity of probe OMTP (10 μM) with $\text{Fe}^{3+/2+}$ (1.0 μM) in different pH solution.

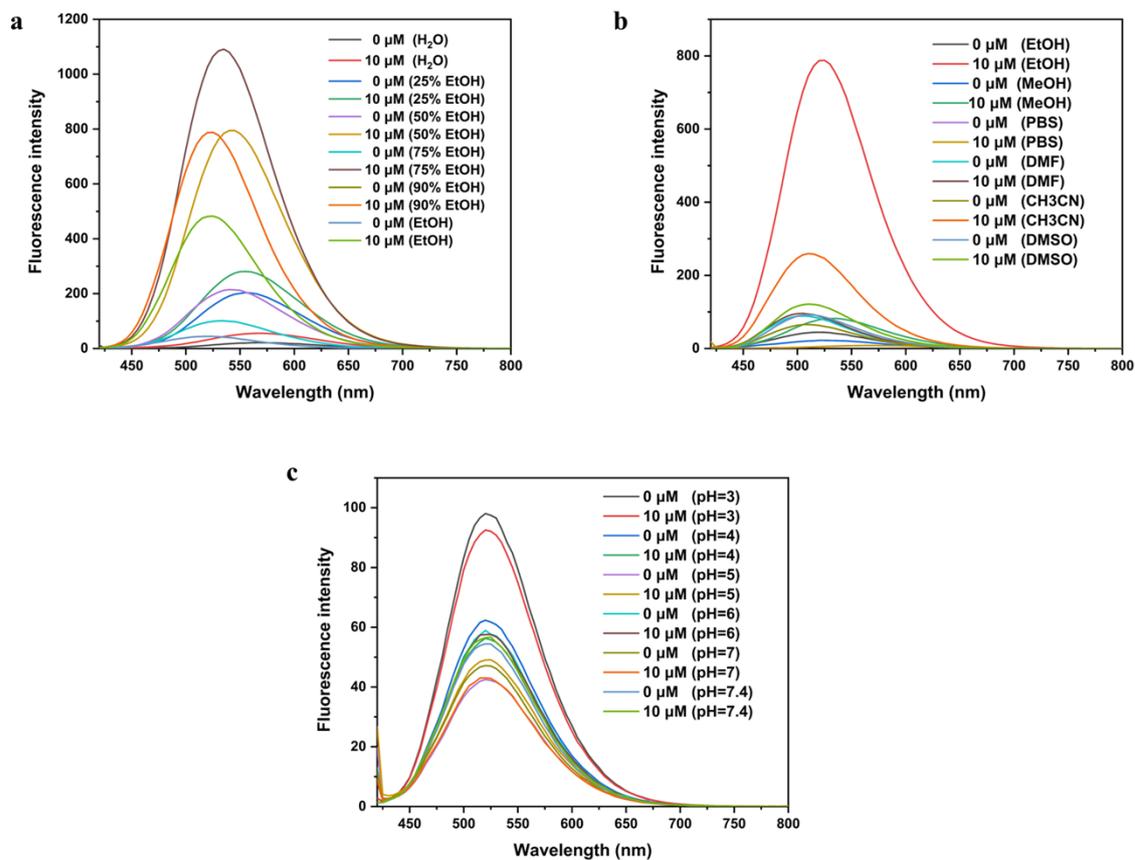


Fig. S10 Absorption spectrum (a) and linear curve (b) of probe MBBP with $\text{Fe}^{3+}/2+$.

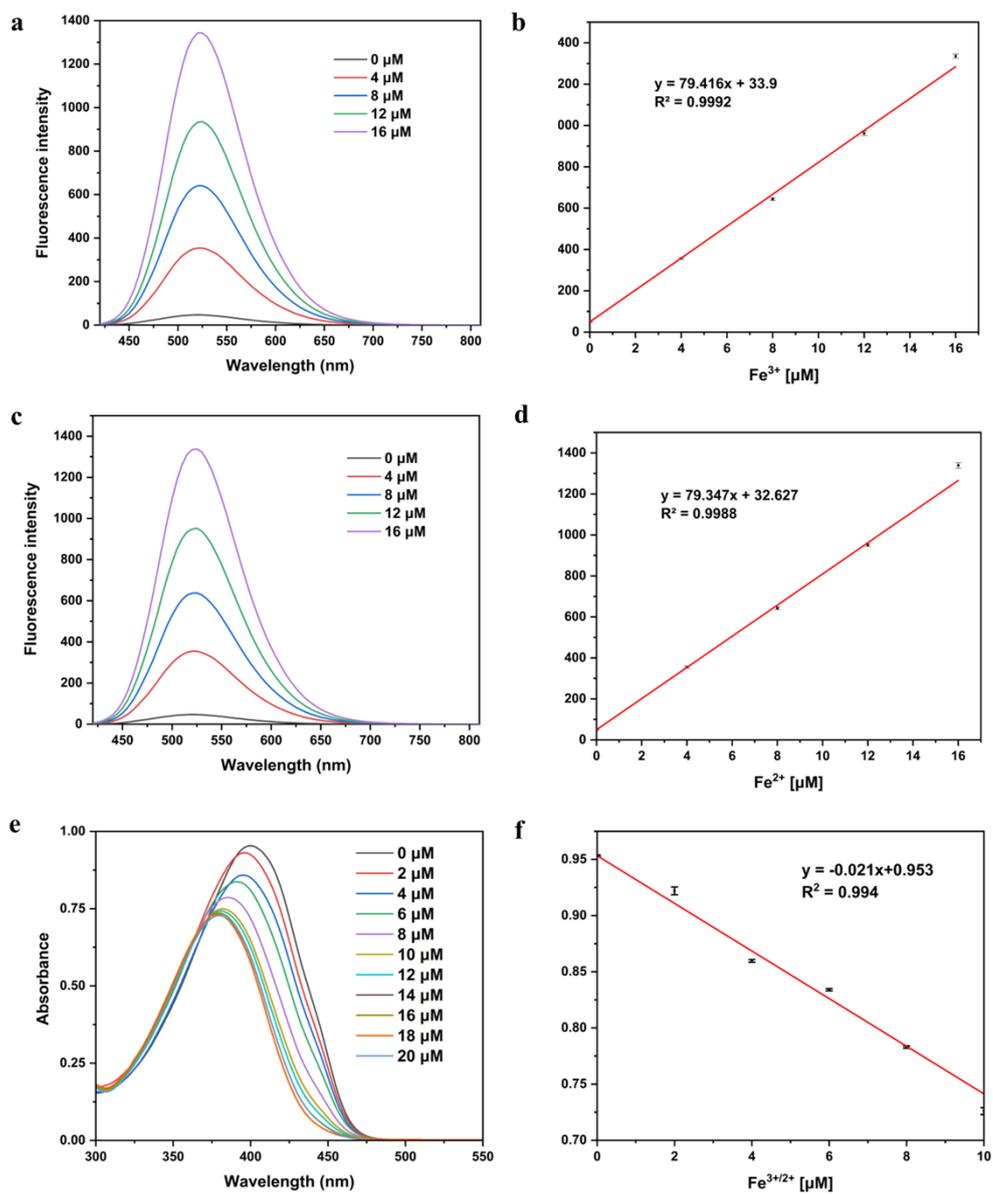


Fig. S11 High-performance liquid chromatography of compound 1, OMTP+Fe^{3+/2+} (50 μM) and probe OMTP.

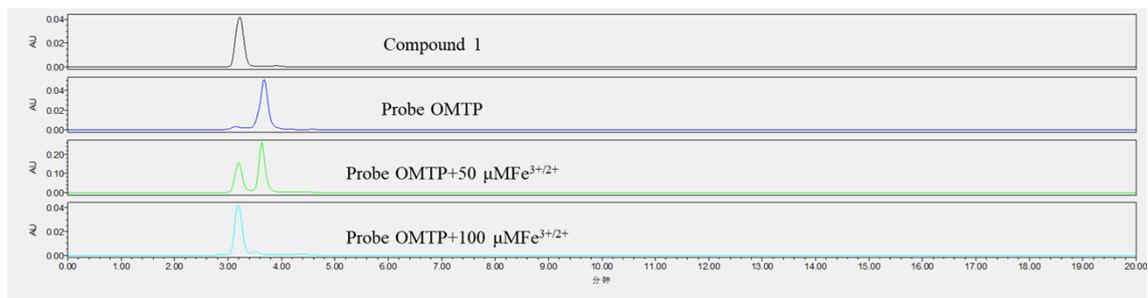


Fig. S12 HPLC-MS results for probe OMTP+Fe^{3+/2+} (50 μmol/L).

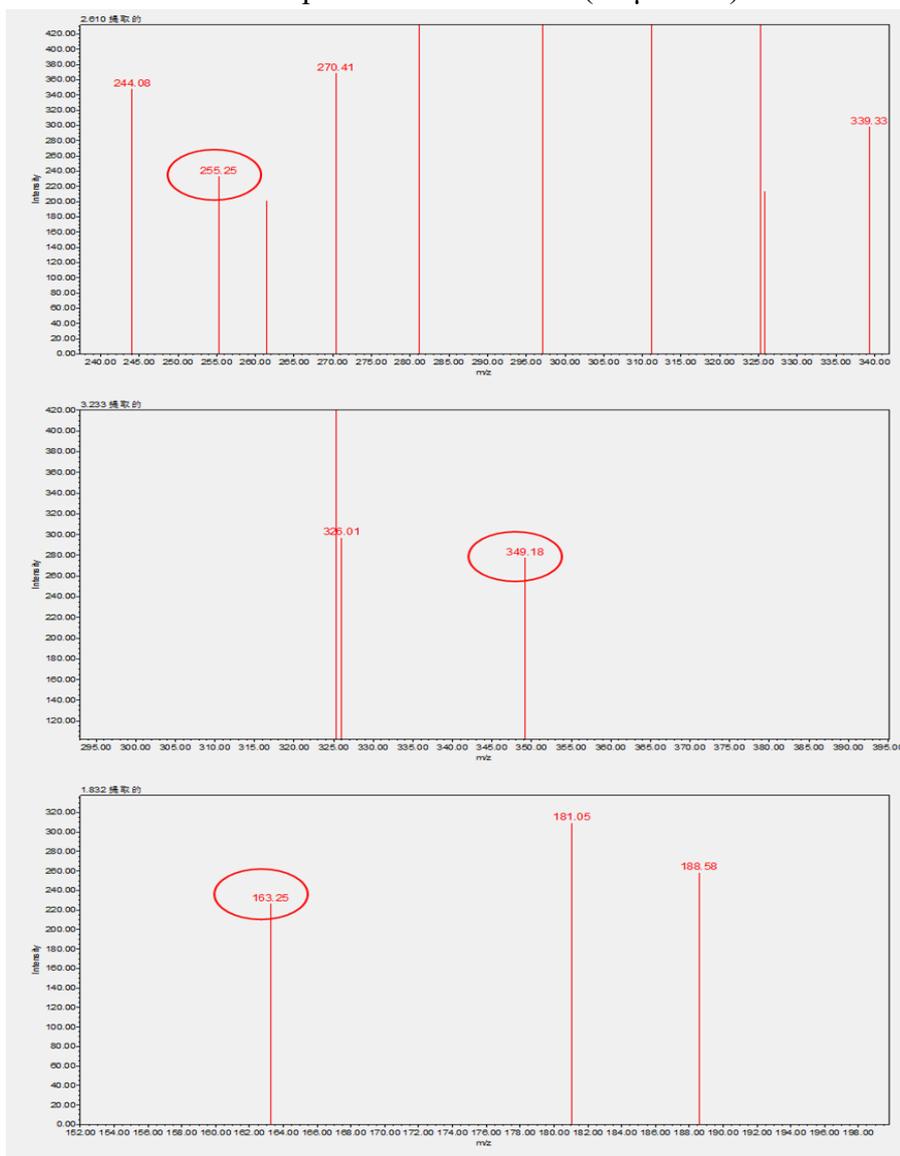


Fig. S13 (a) ^1H NMR mechanisms of probe OMTP, compound 1, and probe OMTP after addition of $\text{Fe}^{3+/2+}$; (b) Recognition mechanism of probe OMTP response to $\text{Fe}^{3+/2+}$.

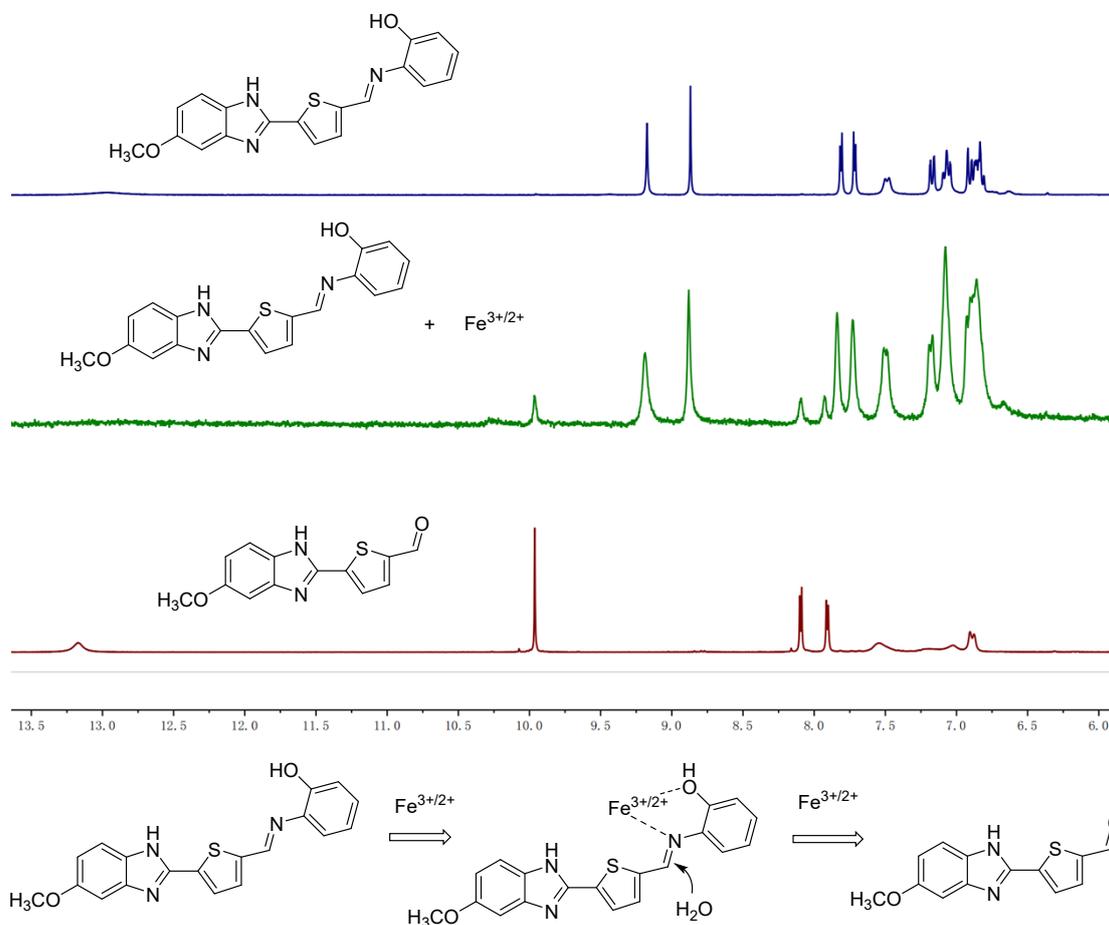


Fig. S14 The Job's plot examined between $\text{Fe}^{3+/2+}$ and OMTP.

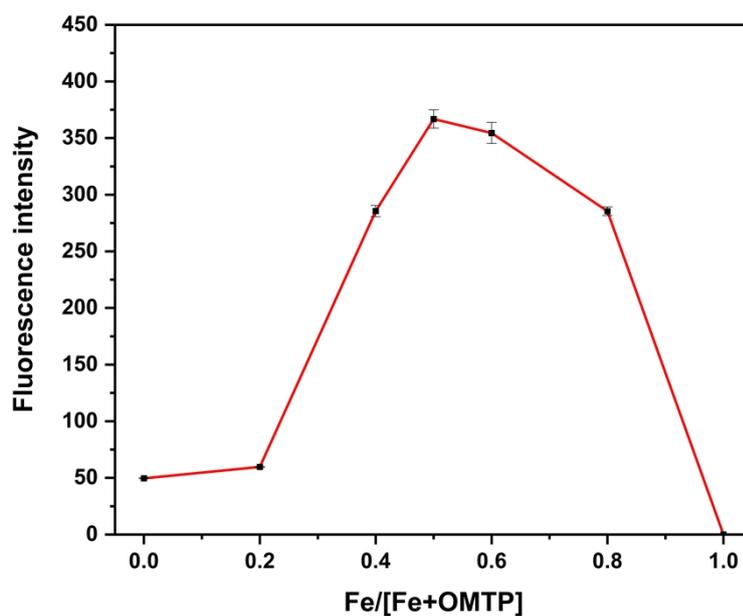


Fig. S15 The linear relationship between iron ion concentration and (R+G)/B in **Fig. 5a**, tests were performed in triplicate.

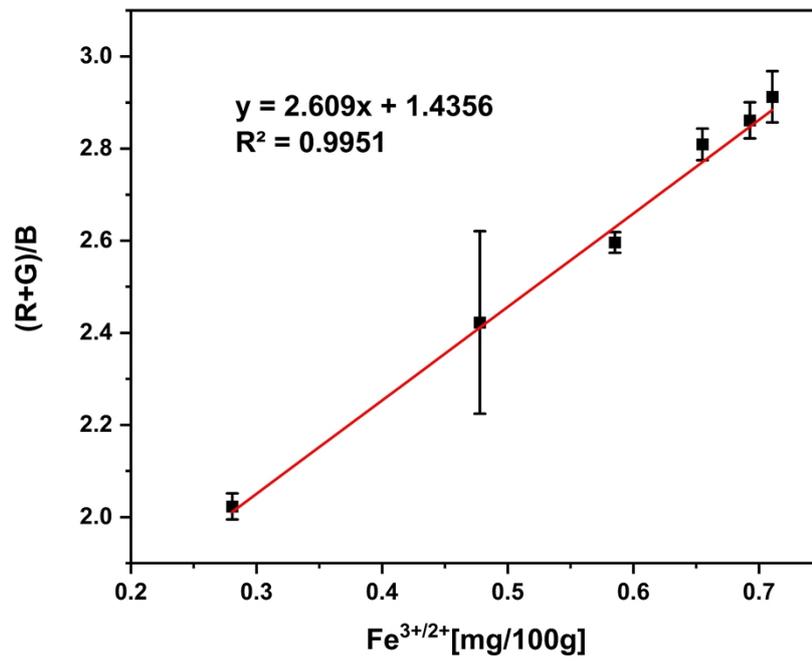


Fig. S16 (R+G)/B values of probe OMTP measured after application to various fruits and vegetables (H₂O and iron water), tests were performed in triplicate

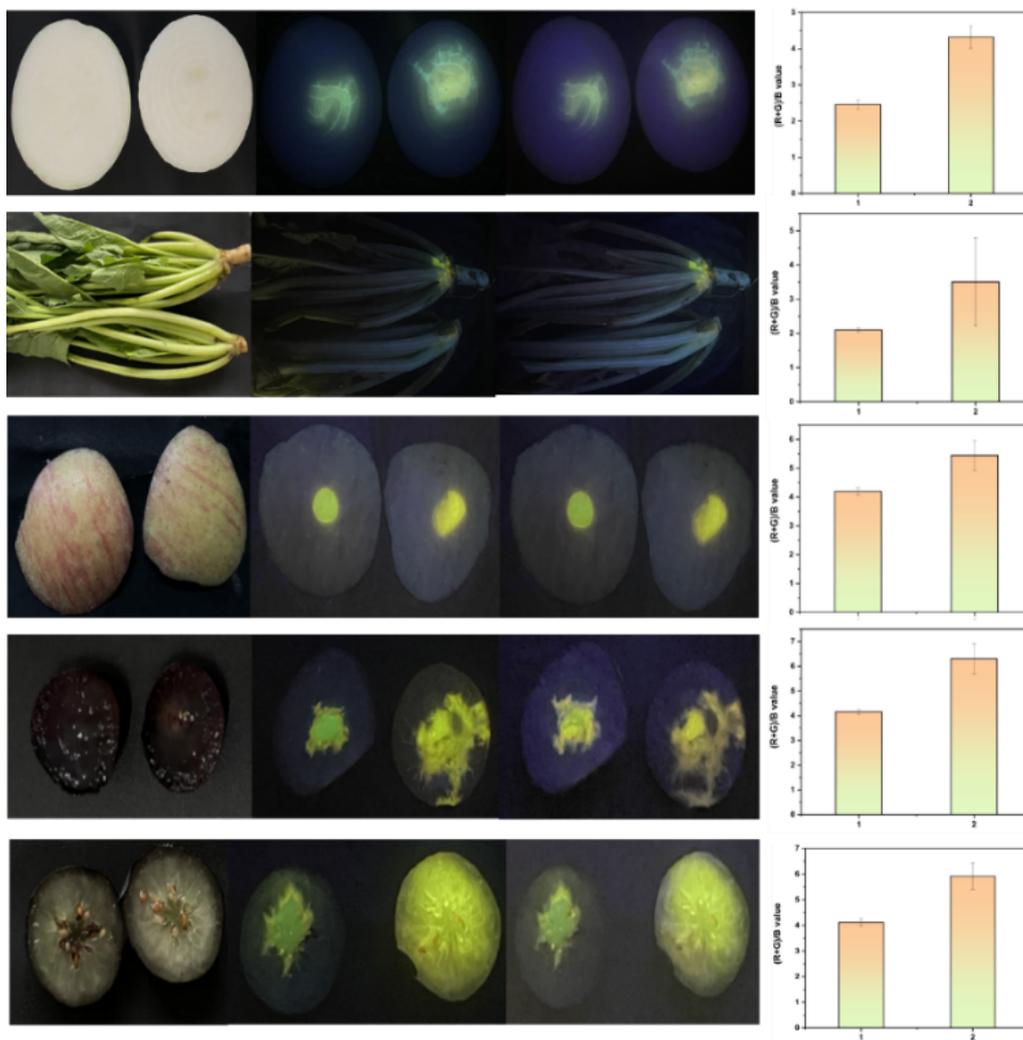


Table S1 Results for the probe and intermediate excited states calculated using three Functionals.

Functionals		CAM-B3LYP	B3LYP	PBE0	Actual value
Compound	λ_{abs} (nm)	344	386	364	380
	f	0.9105	0.5894	0.5265	/
	λ_{em} (nm)	639	542	518	527
	f	0.7859	1.0785	1.1808	/
Probe	λ_{abs} (nm)	398	436	416	410
	f	0.0025	0.3344	1.0942	/
OMTP	λ_{em} (nm)	495	545	515	530
	f	0.0026	0.0031	0.0069	/

Table S2 Determination of total iron content in actual samples.

Sample	Fe ³⁺ level found ($\mu\text{M/L}$)	Added ($\mu\text{M/L}$)	Found ($\mu\text{M/L}$)	Recovery/%	RSD/%(n=3)
Red wine 1	1.59	4.00	5.50	97.77	0.99
		8.00	9.74	101.88	0.90
Red wine 2	1.92	4.00	5.92	100.06	1.19
		8.00	9.92	100.04	1.04
Beer 1	0.00	4.00	3.90	97.62	0.37
		8.00	8.18	102.20	1.91
Beer 2	0.00	4.00	3.93	98.22	0.91
		8.00	8.18	98.58	1.54
Milk 1	0.00	4.00	3.86	96.52	0.57
		8.00	8.02	100.31	1.42
Milk 2	0.00	4.00	3.87	96.78	0.21
		8.00	7.95	99.42	1.88