

## Electronic Supplementary Information (ESI)

### A novel boronic acid-based fluorescent sensor for selectively recognizing Fe<sup>3+</sup> ion in real time

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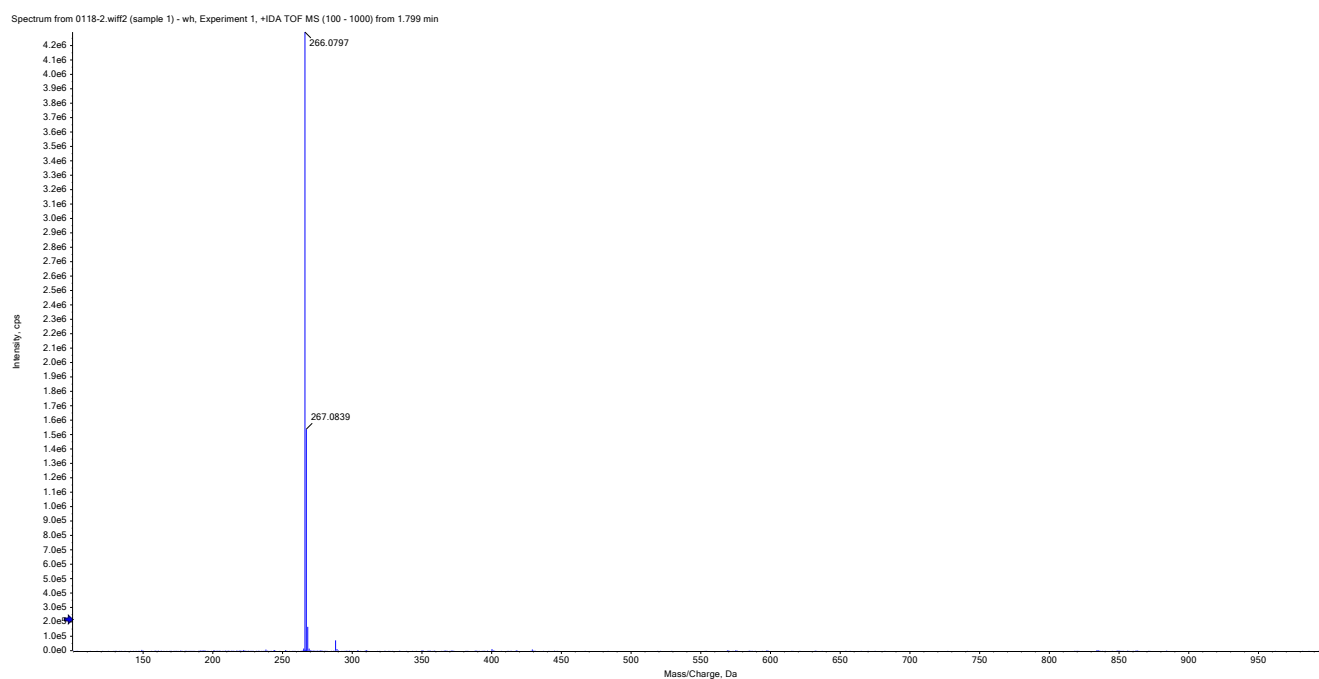


Fig. S1 HRMS spectrum of compound 2

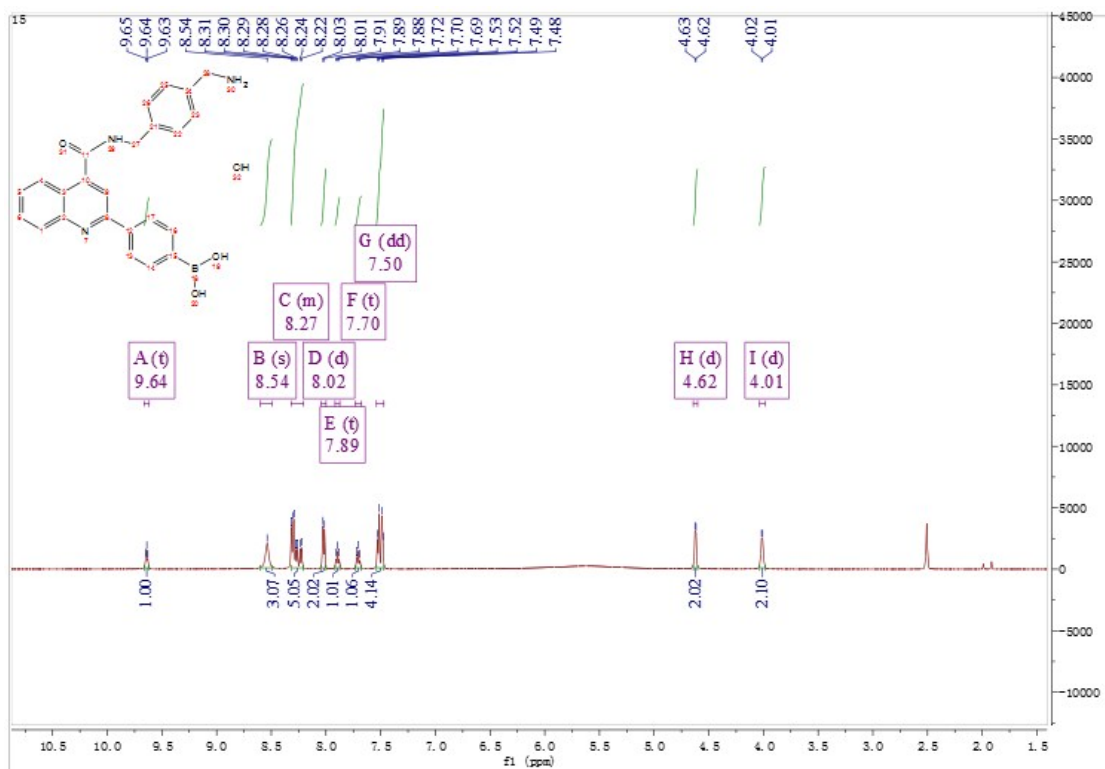


Fig. S2 <sup>1</sup>H NMR spectrum of 3

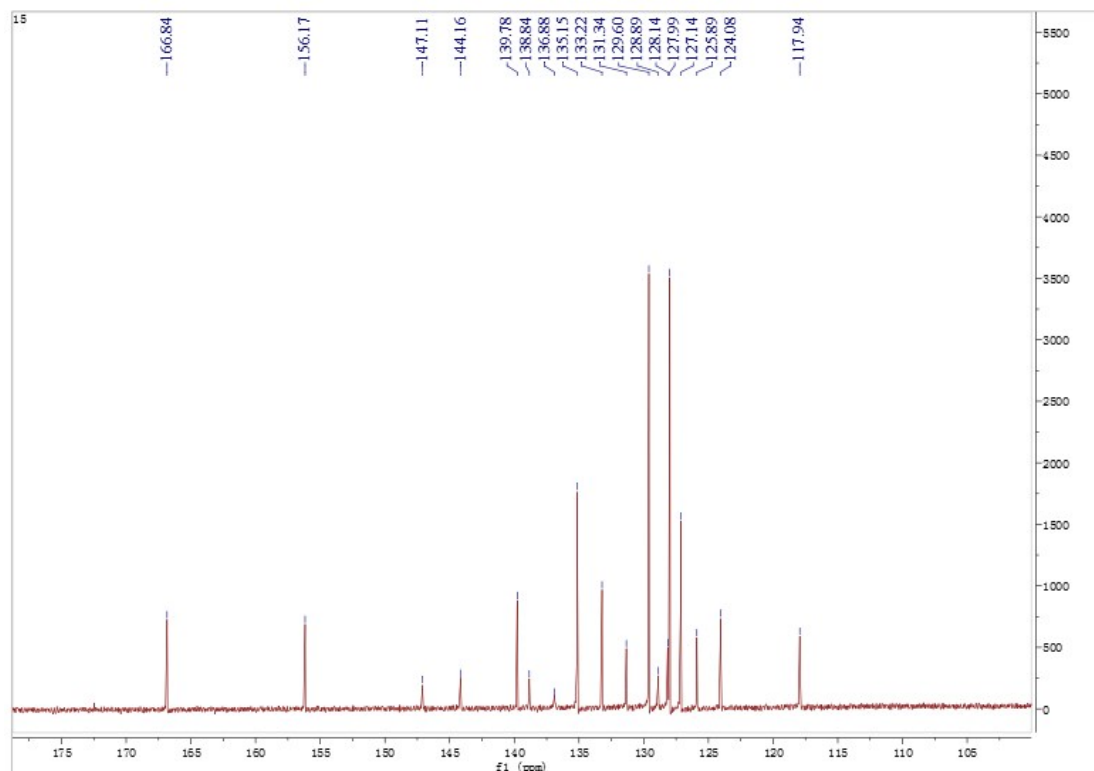


Fig. S3 <sup>13</sup>C NMR spectrum of 3

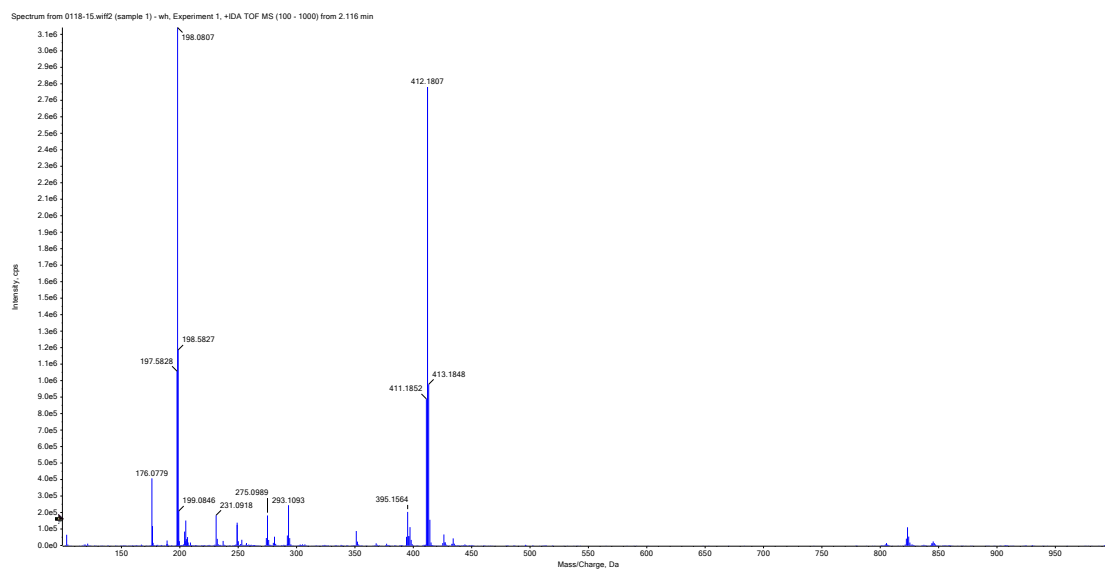


Fig. S4 HRMS spectrum of compound 3

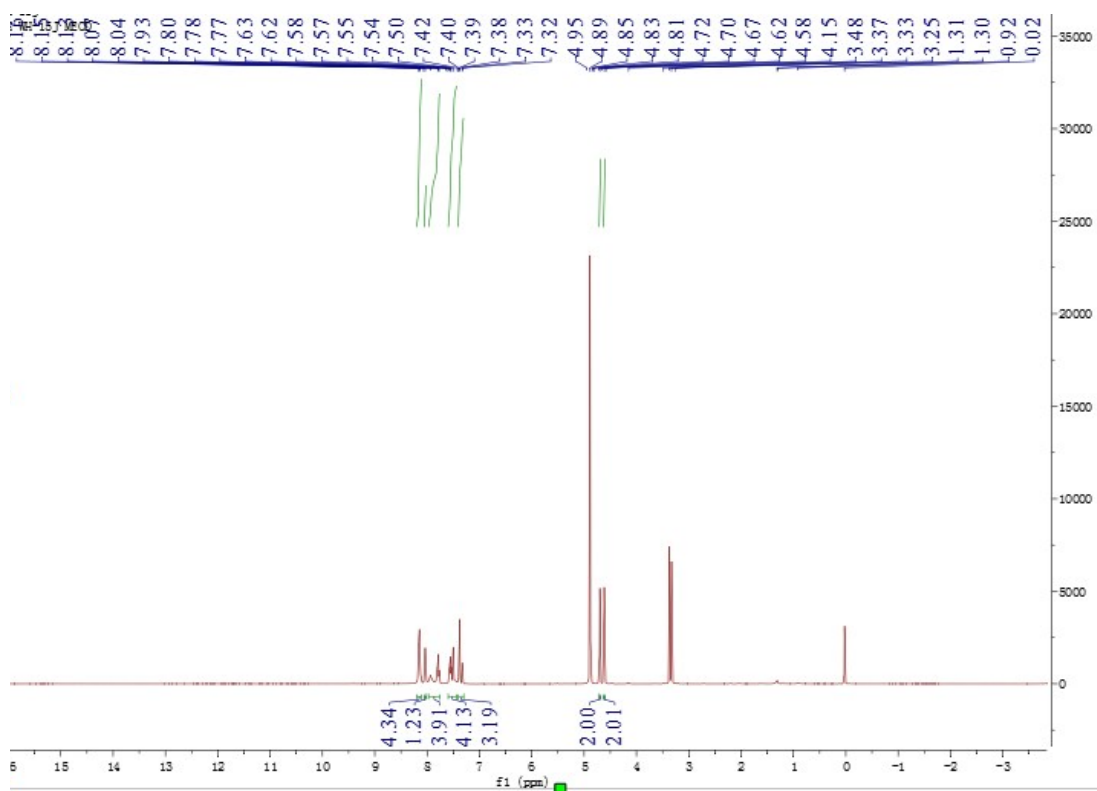
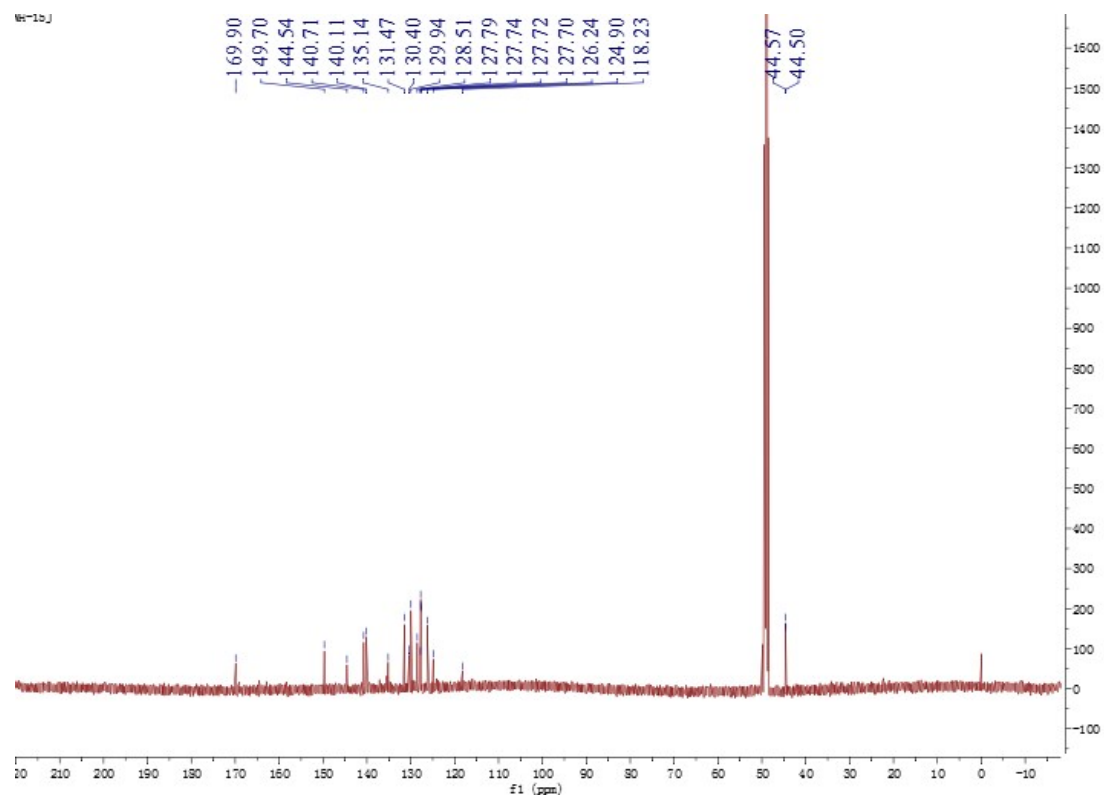
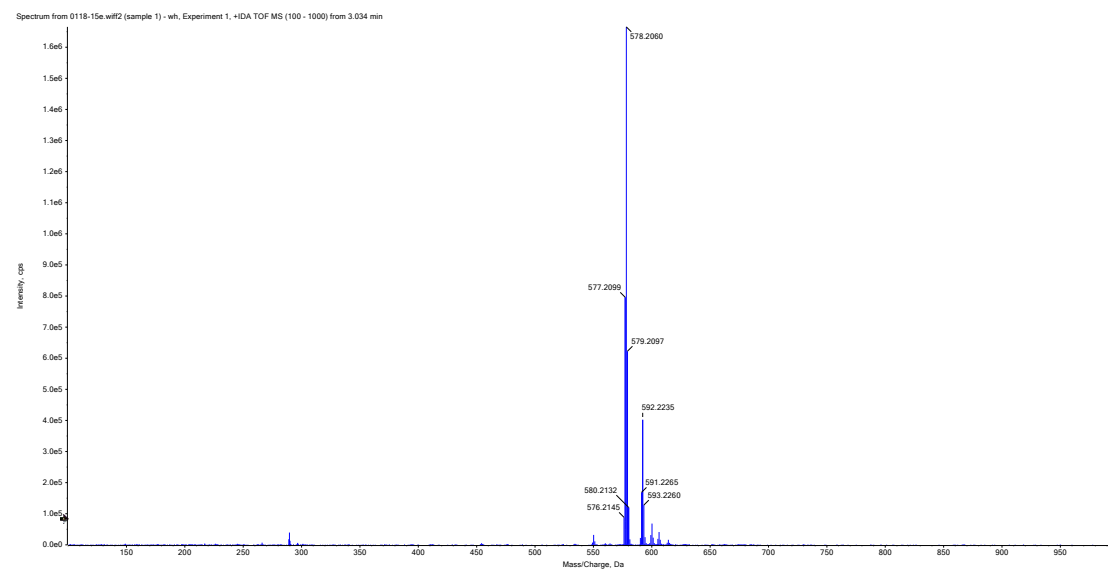


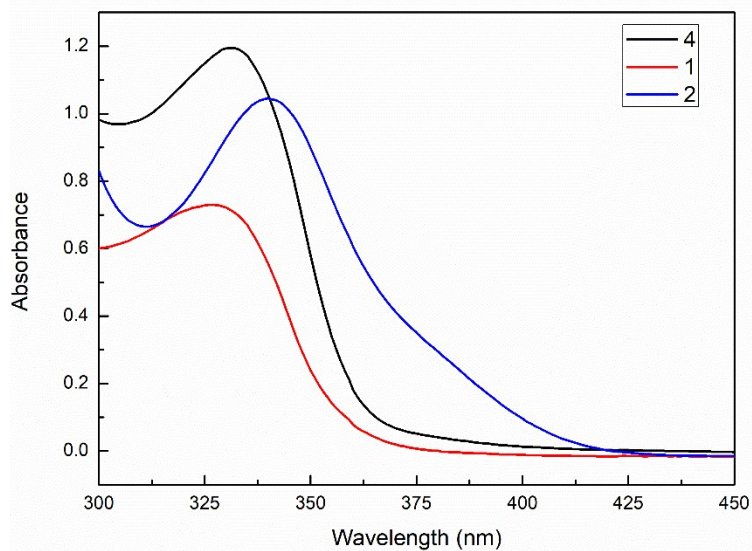
Fig. S5 <sup>1</sup>H NMR spectrum of 4



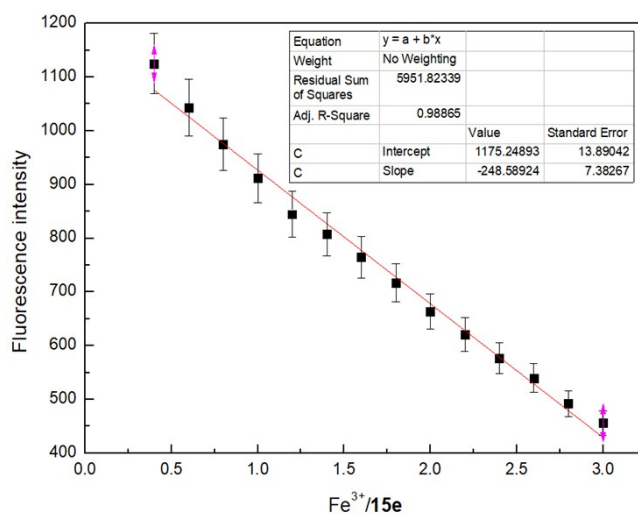
**Fig. S6**  $^{13}\text{C}$  NMR spectrum of **4**



**Fig. S7** HRMS spectrum of compound **4**



**Fig. S8** UV-vis absorption spectra of sensor **1**, **2** and **4** in DMSO/H<sub>2</sub>O (3:7, v/v).



**Fig. S9** Linear relationship between sensor **4** and Fe<sup>3+</sup> ion in DMSO/H<sub>2</sub>O (3:7, v/v).

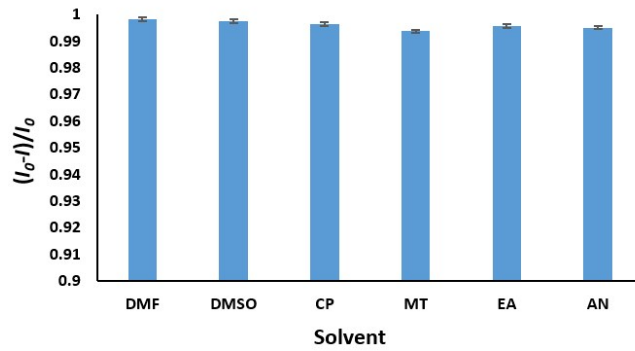
Linear Equation:  $Y = -248.58924X + 1175.24893$

$R^2 = 0.98865$

$S = 2.4858924 \times 10^6$

$$\delta = \sqrt{\frac{\sum (F_i - F_0)^2}{N - 1}} = 5.0 \quad (N=10) \quad K=3$$

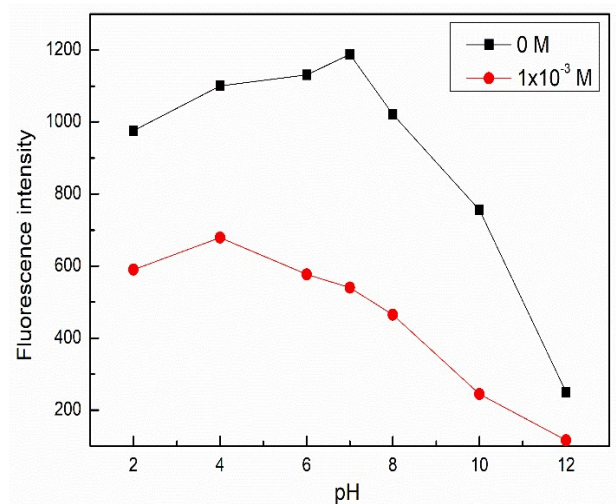
$LOD = K \times \delta / S = 6.0 \times 10^{-6} \text{ M}$



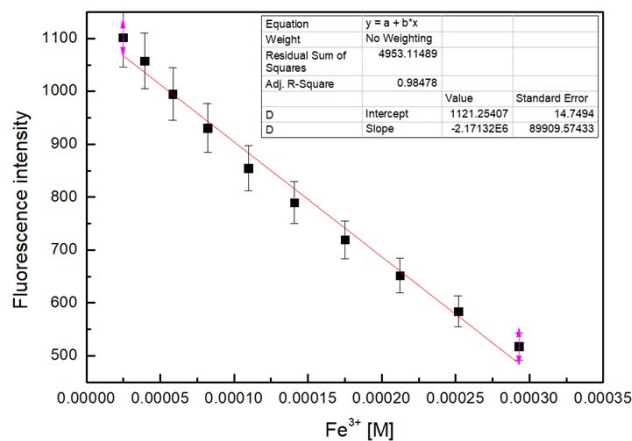
**Fig. S10** Relative fluorescence intensity of sensor **4** ( $1 \times 10^{-4}$  M) in the presence of 10 equiv. of  $\text{Fe}^{3+}$  ion in different polar solvents / DMSO (9:1, v/v) solution, at room temperature. From left to right: N, N-dimethylformamide (DMF), dimethylsulfoxide (DMSO), acetone (CP), methyl alcohol (MT), ethyl alcohol (EA), acetonitrile (AN).



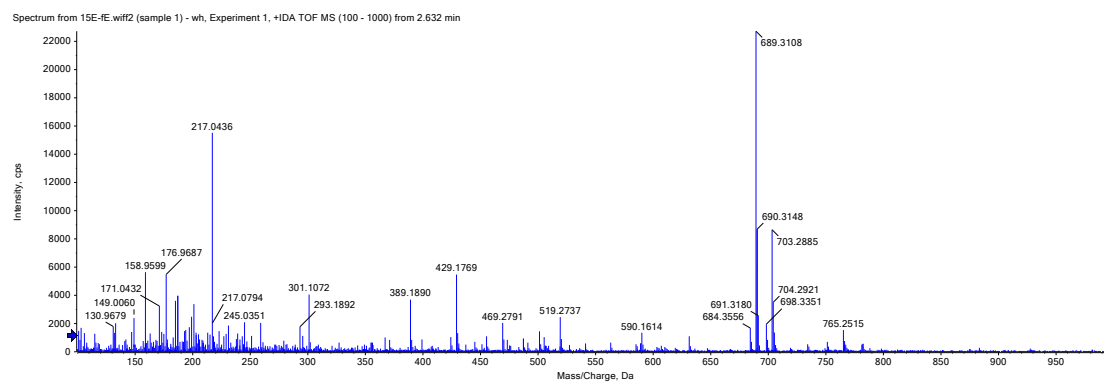
**Fig. S11** Photograph of **4** ( $10^{-4}$  M) upon adding 10 equiv. of various ions in DMSO/ $\text{H}_2\text{O}$  (1:9, v/v) which was observed under a UV-lamp (365 nm).



**Fig. S12** Fluorescence responses of sensor **4** ( $1 \times 10^{-4}$  M) to  $\text{Fe}^{3+}$  ion in DMSO/ $\text{H}_2\text{O}$  (3:7, v/v, phosphate buffer, 0.1 M) at different pH values. Concentrations of  $\text{Fe}^{3+}$  ion are given in the plot.

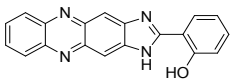
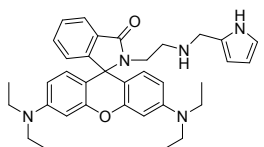


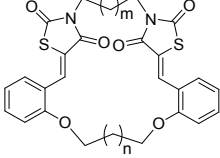
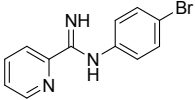
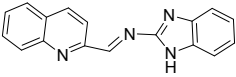
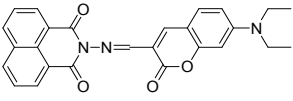
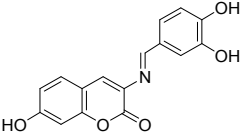
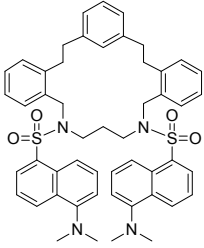
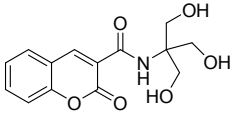
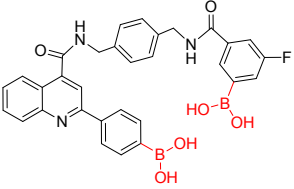
**Fig. S13** Linear relationship between sensor **4** and  $\text{Fe}^{3+}$  ion in rabbit plasma



**Fig. S14** HRMS spectrum of compound **4-2Fe<sup>3+</sup>** (calculated 689.0658, found 689.3108).

**Table1** Key information of some reported  $\text{Fe}^{3+}$  sensors

	Sensor	Buffer	Response time	LOD
Gao <i>et al.</i> reported <sup>1</sup>		$\text{CH}_3\text{CN}$ /HEPES(1:4)	60 min	$4.8 \times 10^{-6}$ M
Bao <i>et al.</i> reported <sup>2</sup>		$\text{MeOH}/\text{H}_2\text{O}$ (3:2)	10min	$0.031 \times 10^{-6}$ M

Sepay <i>et al.</i> reported <sup>3</sup>		Ethanol/H <sub>2</sub> O (3:1)	No data	9.8×10 <sup>-6</sup> M
Nandre <i>et al.</i> reported <sup>4</sup>		MeOH	No data	0.6×10 <sup>-6</sup> M
Kar <i>et al.</i> reported <sup>5</sup>		CH <sub>3</sub> CN/HEPES(1:4)	1 min	4.0×10 <sup>-6</sup> M
Li <i>et al.</i> reported <sup>6</sup>		THF/H <sub>2</sub> O (1:1)	No data	0.38 × 10 <sup>-6</sup> M
García-Beltrán <i>et al.</i> reported <sup>7</sup>		DMSO/HEPES(1:99)	6 min	51.7 × 10 <sup>-6</sup> M
Dai <i>et al.</i> reported <sup>8</sup>		DMSO/HEPES(3:1)	No data	91.1×10 <sup>-6</sup> M
Yao <i>et al.</i> reported <sup>9</sup>		H <sub>2</sub> O	No data	No data
Our sensor 4		DMSO/ H <sub>2</sub> O (3:7)	Within a record time (0.5min)	5.8×10 <sup>-6</sup> M

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