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A smart copper (II) responsive binuclear gadolinium (III) complex based magnetic resonance imaging contrast agent

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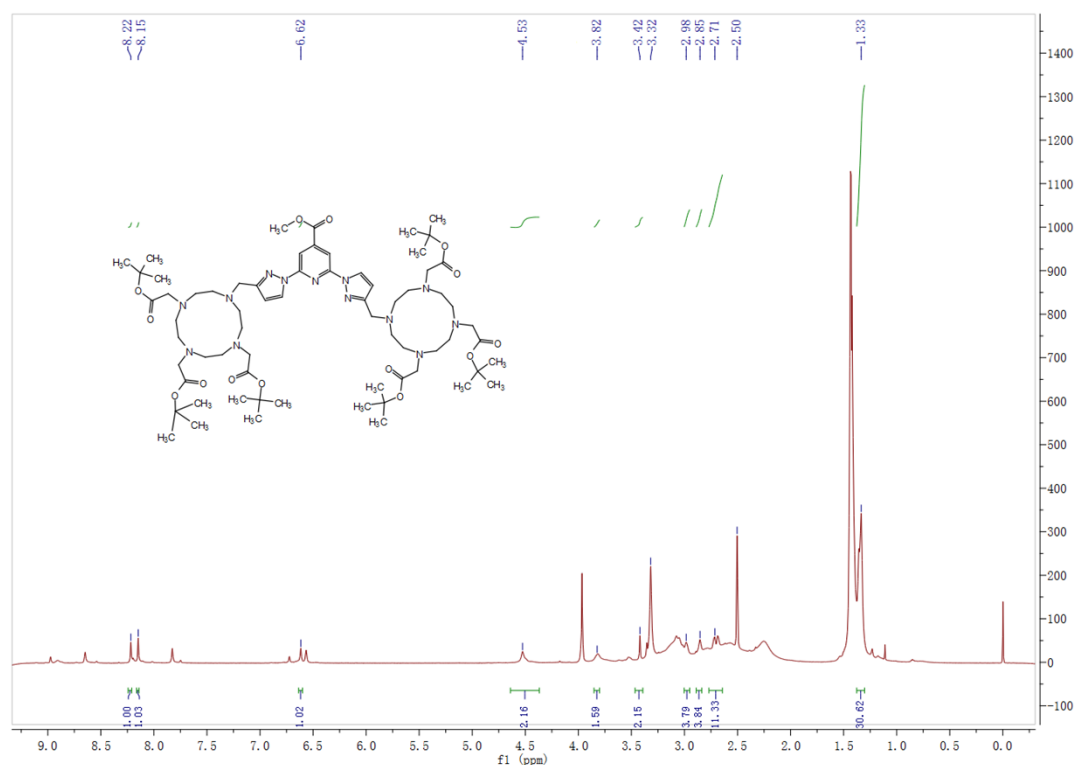


Fig. S1 ¹H NMR spectrum of Compound 3 in DMSO (600 MHz).

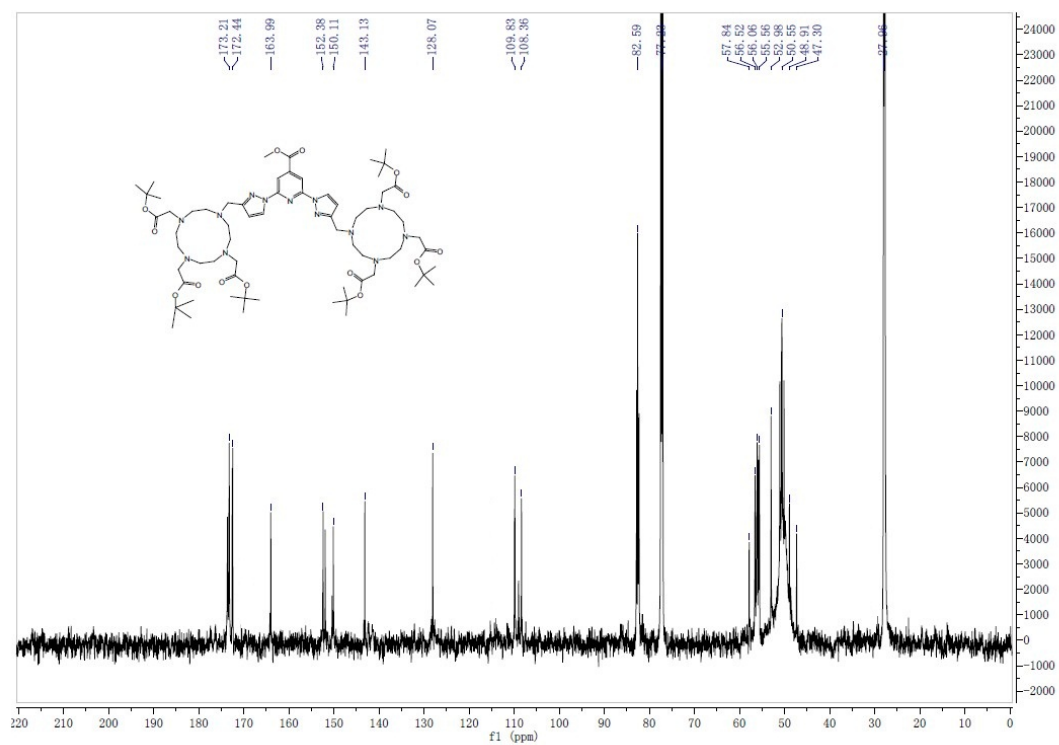
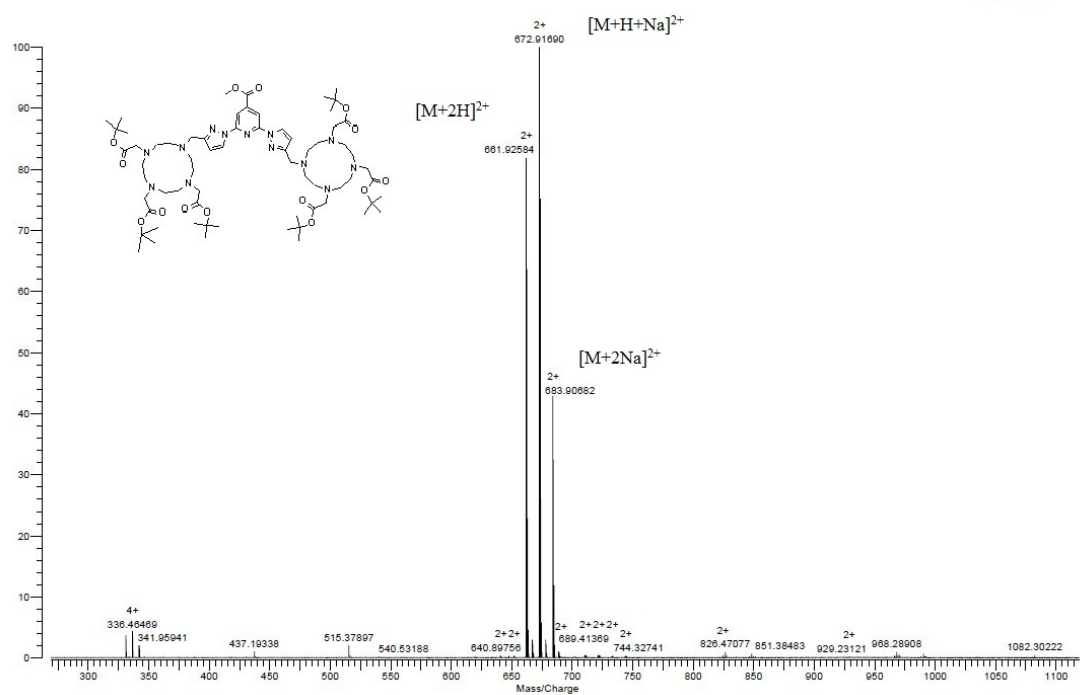


Fig. S2 ^{13}C NMR spectrum of Compound 3 in CDCl_3 (151 MHz).



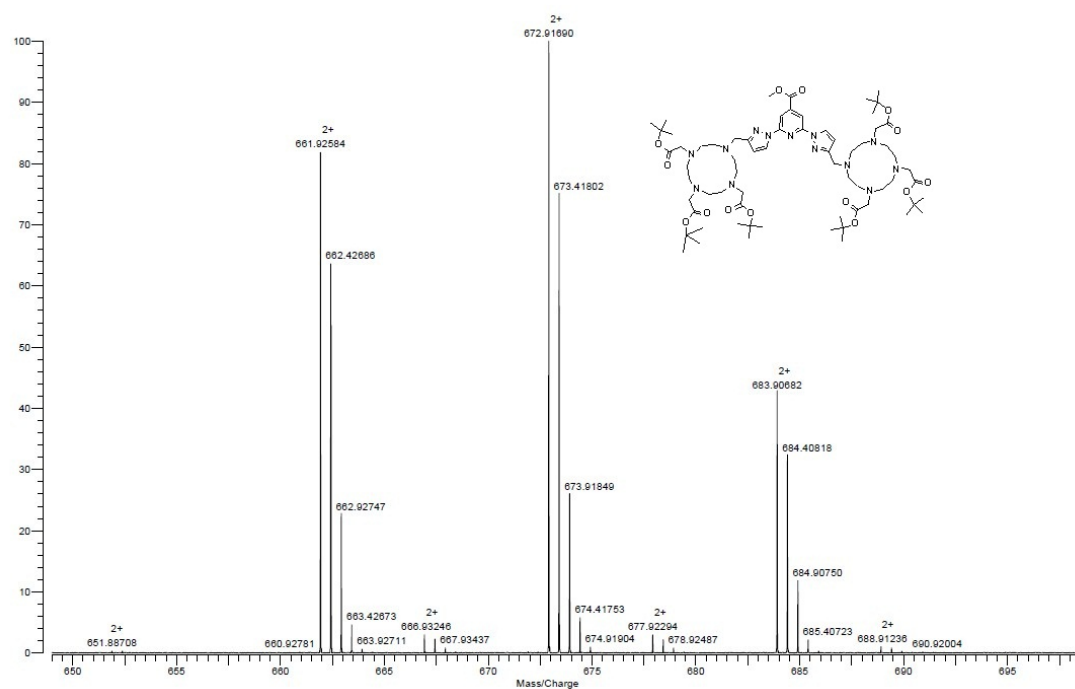


Fig. S3 HRMS (ESI) spectrum and expanded view of **Compound 3**. The peaks at $m/z = 661.92584$, 672.91690 , and 683.90682 correspond to $[M + 2H]^{2+}$ (calc. 661.92650), $[M + H + Na]^{2+}$ (calc. 672.91747), and $[M + 2Na]^{2+}$ (calc. 683.90844) respectively.

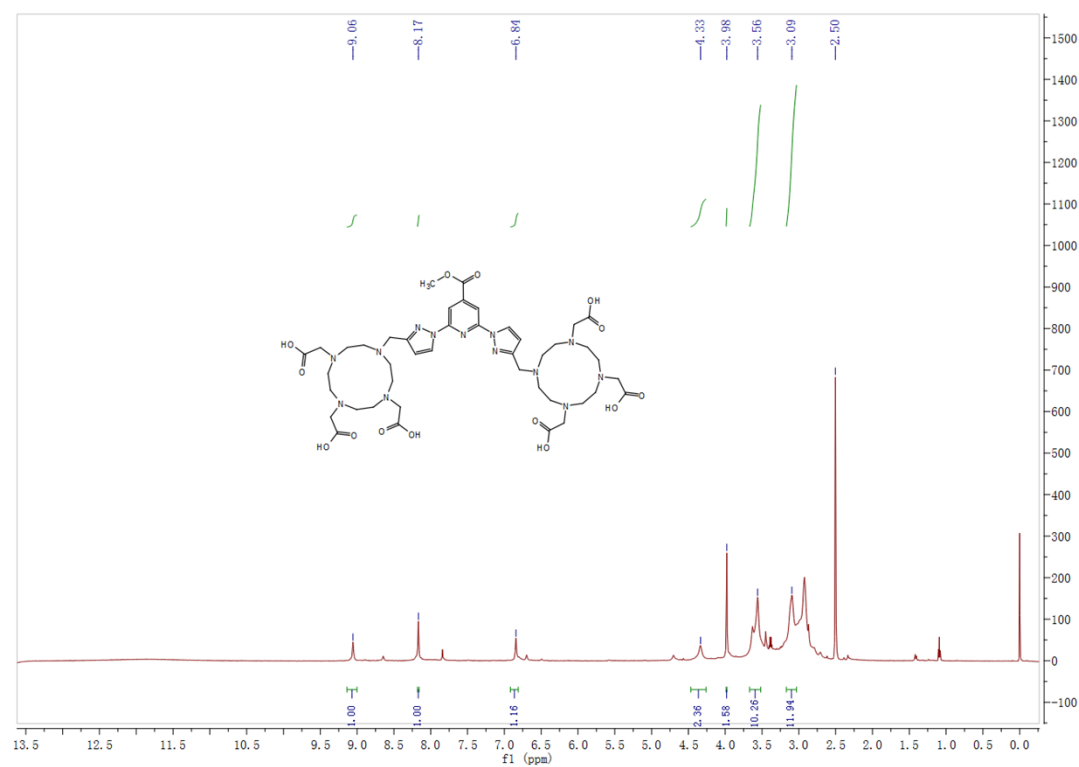


Fig. S4 1H NMR spectrum of Compound 4 in DMSO (600 MHz).

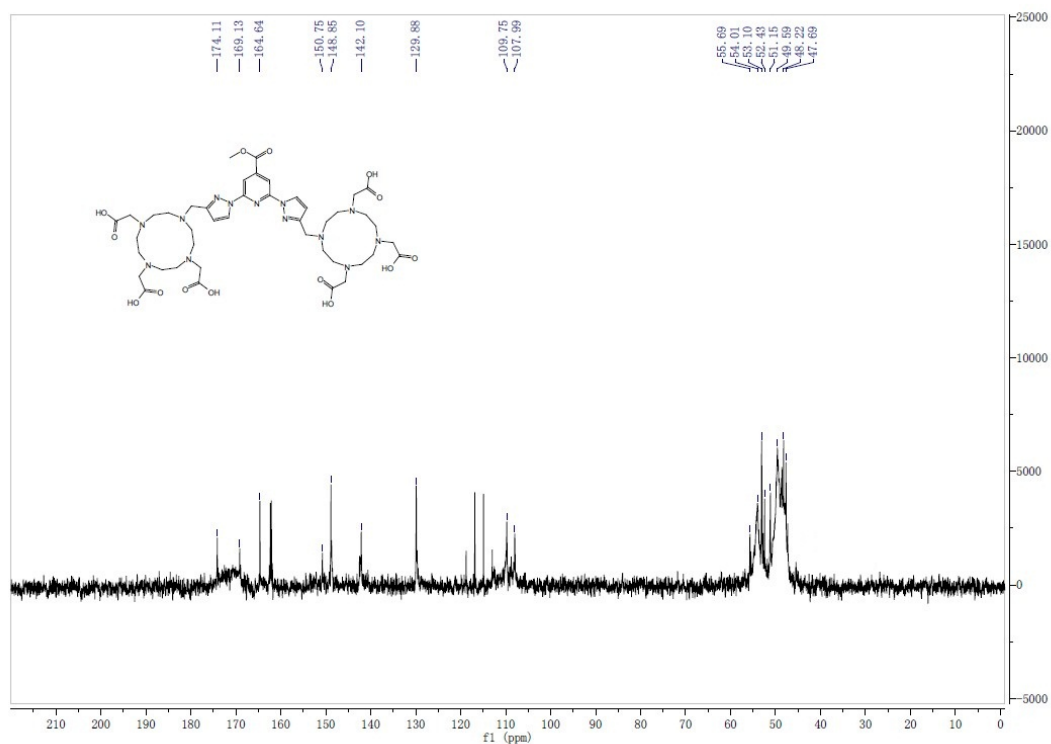


Fig. S5 ¹³C NMR spectrum of Compound 4 in D₂O (151 MHz).

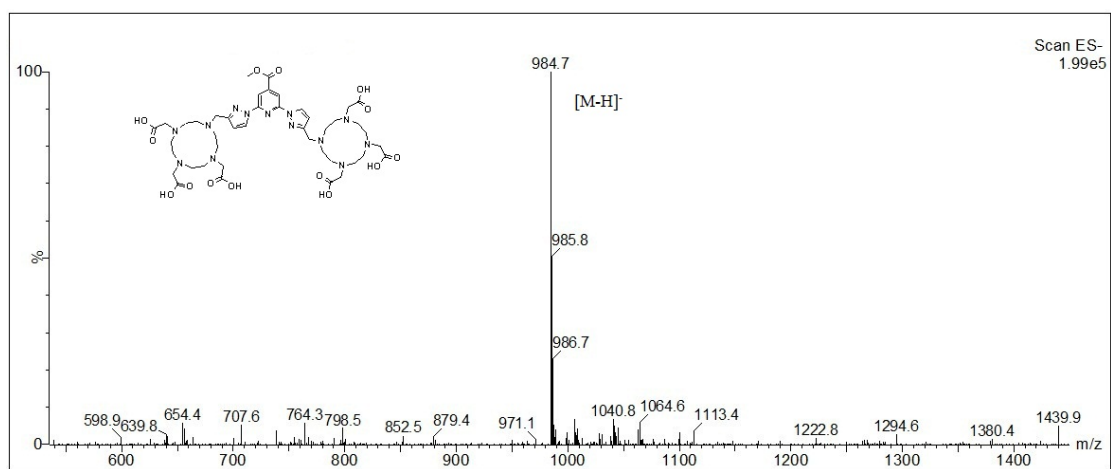


Fig. S6 MALDI-TOF-MS spectrum of **Compound 4**. The peak at $m/z = 984.7$ correspond to $[M - H]^+$ (calc. 984.46).

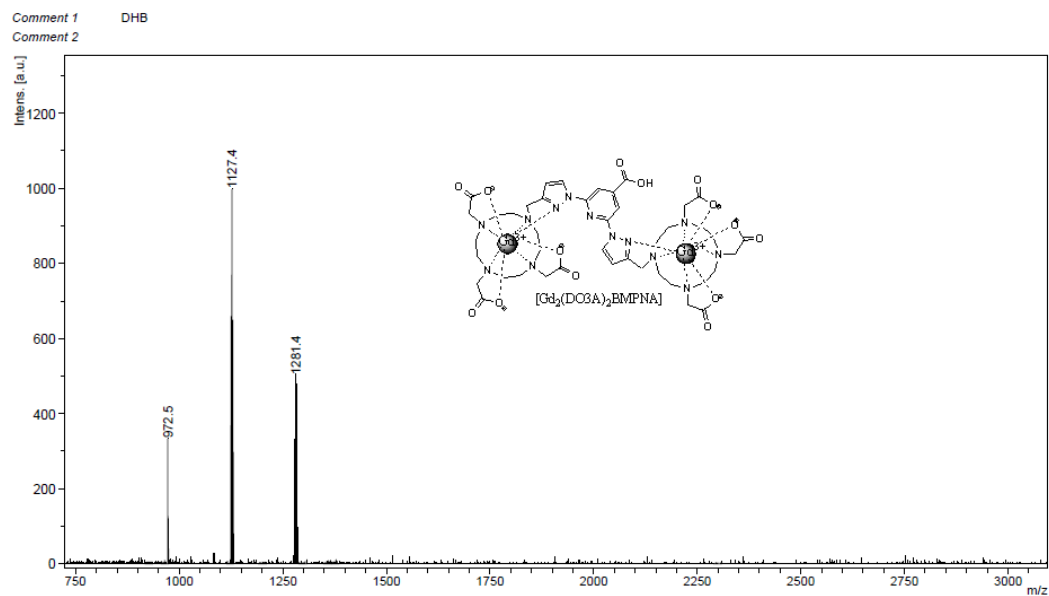


Fig. S7 MALDI-TOF-MS spectrum of $[\text{Gd}_2(\text{DO3A})_2\text{BMPNA}]$. The peak at $m/z = 1281.4$ correspond to $[\text{M} + \text{H}]^+$ (calc. 1281.46).

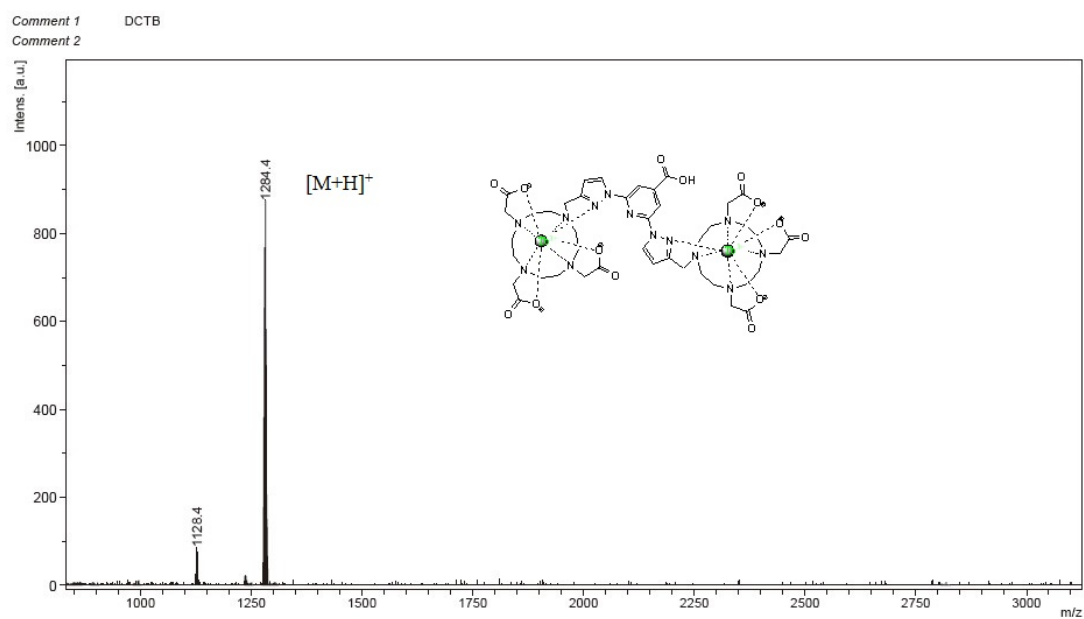


Fig. S8 MALDI-TOF-MS spectrum of $[\text{Tb}_2(\text{DO3A})_2\text{BMPNA}]$. The peak at $m/z = 1284.4$ correspond to $[\text{M} + \text{H}]^+$ (calc. 1284.3).

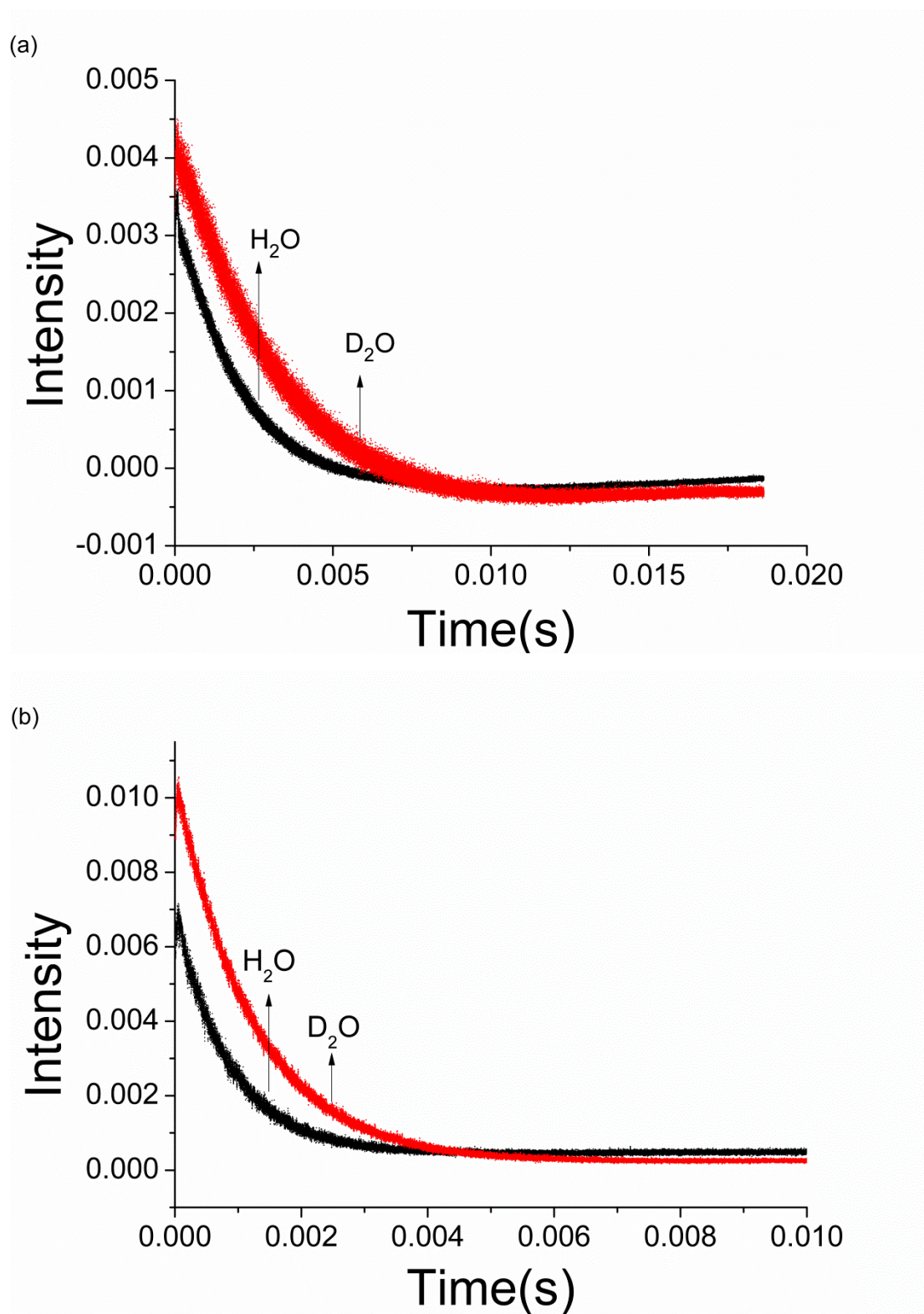


Fig. S9 (a) Luminescence decay of $[\text{Tb}_2(\text{DO3A})_2\text{BMPNA}]$ in H_2O and D_2O without addition of Cu^{2+} ;
(b) Luminescence decay of $[\text{Tb}_2(\text{DO3A})_2\text{BMPNA}]$ in H_2O and D_2O with addition of Cu^{2+} .

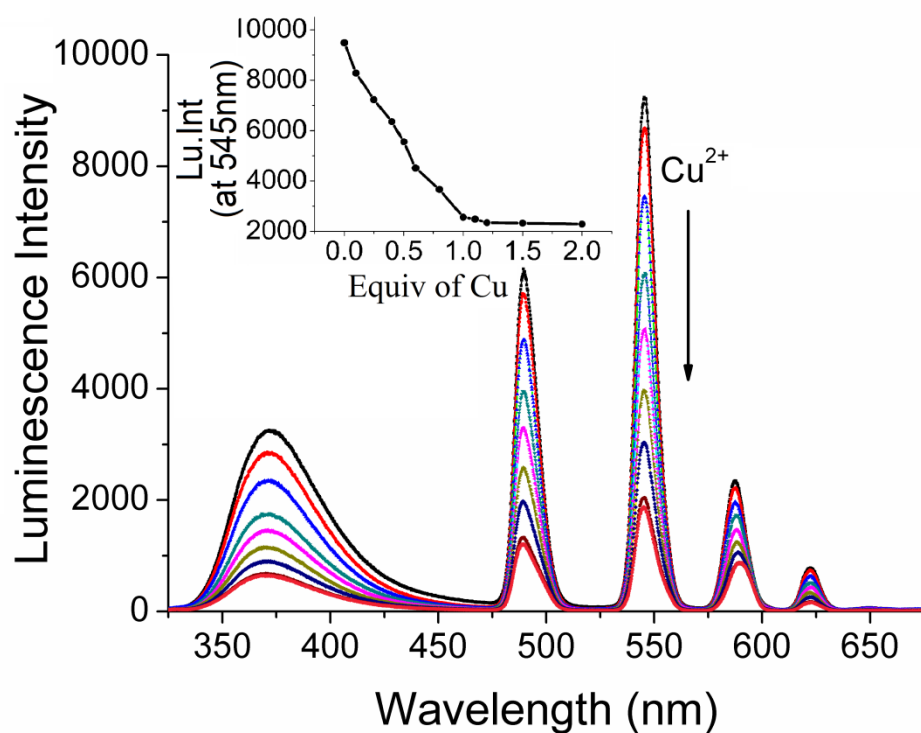


Fig. S10 Luminescence spectra of $[\text{Tb}_2(\text{DO3A})_2\text{BMPNA}]$ ($20\ \mu\text{M}$) upon addition of different concentrations of Cu^{2+} (0-2 equiv.) in HEPES-buffered (pH 7.4, 100 mM) aqueous solutions. Excitation wavelength: 295 nm. Inset shows the luminescence at 545 nm as a function of Cu^{2+} concentration suggesting a 1:1 binding ratio between $[\text{Tb}_2(\text{DO3A})_2\text{BMPNA}]$ and Cu^{2+} .

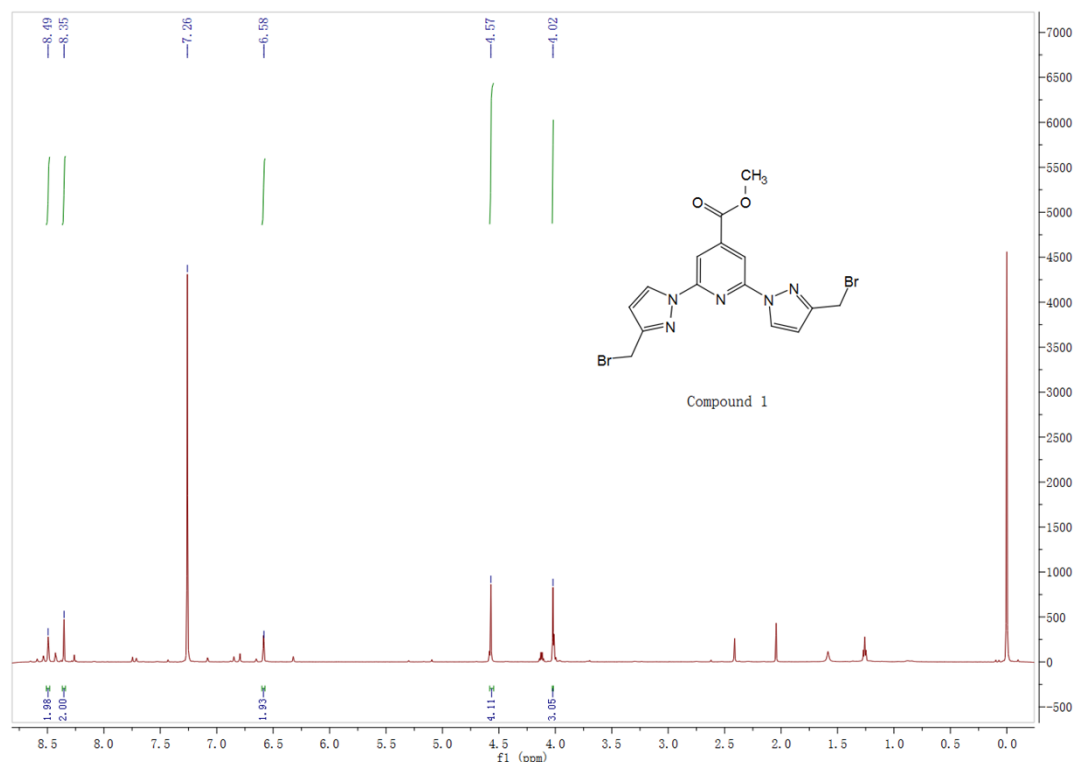


Fig. S11 ^1H NMR spectrum of Compound 1 in CDCl_3 (600 MHz).

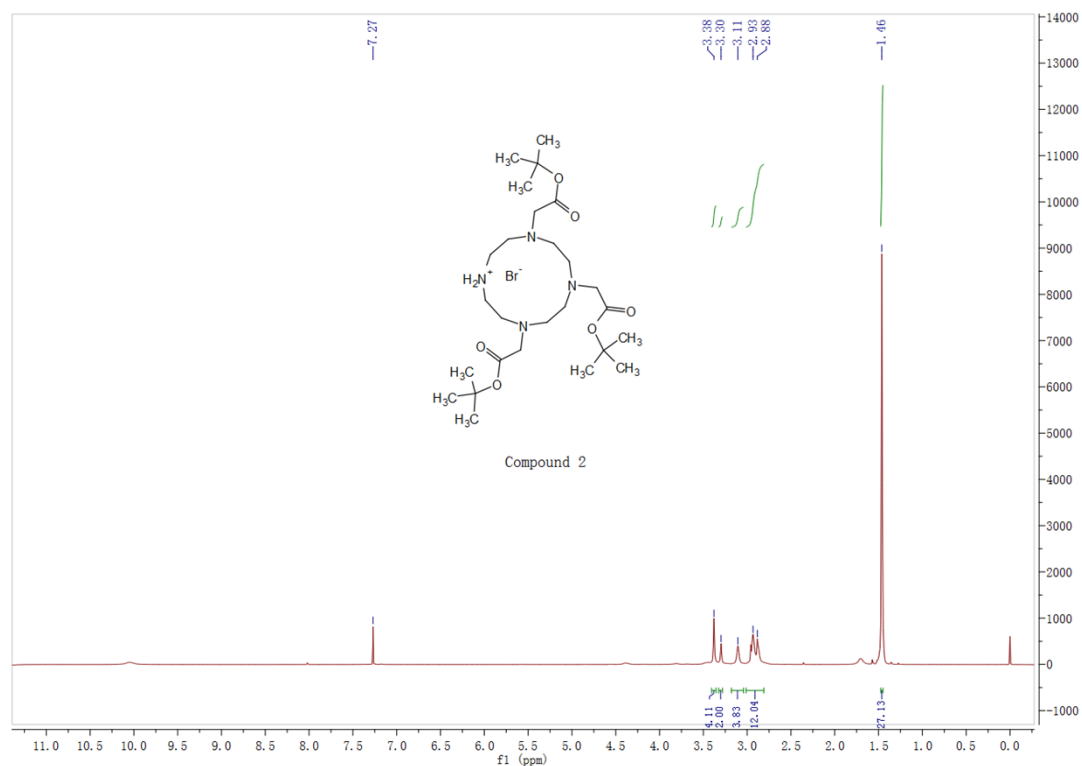


Fig. S12 ^1H NMR spectrum of Compound 2 in CDCl_3 (600 MHz).

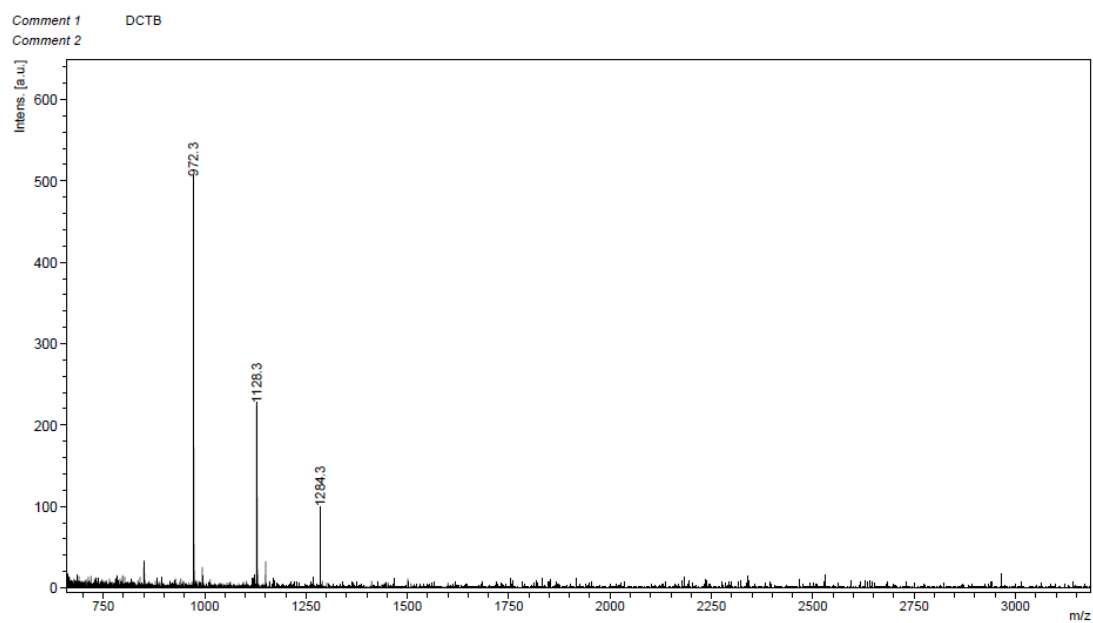


Fig. S13 MALDI-TOF-MS spectrum of $[\text{Gd}_2(\text{DO3A})_2\text{BMPNA}]$ in the presence of Zn^{2+} at room temperature after 7 days . No metal-ion exchange was observed.

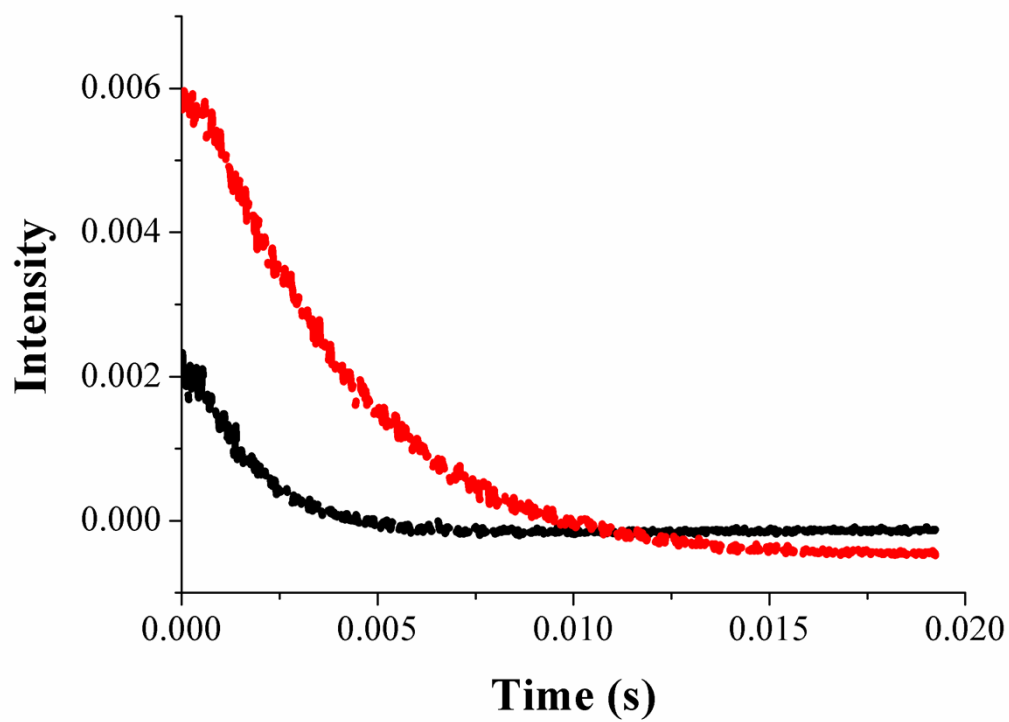


Fig. S14 Luminescence decay of [Tb₂(DO₃A)₂BMPNA] in H₂O (black) and D₂O (red) with addition of Cu²⁺ and phosphate.