Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Comparison of two 5-(thiophene-2-yl)oxazole derived "turn on" fluorescence chemosensors for detection of Ga^{3+} and practical applications

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Calculation of quantum yield, detection limit, association constant

The quantum yield was calculated according to the following formula (1):

$$\Phi_u = \Phi_s \frac{F_u A_s n_u^2}{F_s A_u n_s^2}$$

Φ, F, A, and n represent the quantum yield, the integrated area under the corrected emission spectra, the absorbance intensity at the excitation wavelength and the refractive index of solvent, respectively. In addition, s refers to rhodamine B as the standard, and u refers to the target. The quantum yield (Φ) of rhodamine B dissolved in anhydrous ethanol is 0.97.

The detection limit of **L1** and **L2** for Ga^{3+} were calculated by the following formula (2):

$$LOD = 3\sigma/s$$

where σ is the standard deviation of 10 times the intensity of free **L1** and **L2** (**L1**-Ga^{3+} and **L2**-Ga^{3+}), and s is the slope of the emission intensity of **L1** and **L2** (**L1**-Ga^{3+} and **L2**-Ga^{3+}) as a function of the Ga^{3+} concentration.

The association constant between **L1** and **L2** for Ga^{3+} were calculated by the following formula (3):

$$\frac{1}{\Delta F} = \frac{1}{\Delta F_{max}} + \frac{1}{K\Delta F_{max}} \cdot \frac{1}{[Ga^{3+}]^2}$$

where $\Delta F = F - F_0$ and $\Delta F_{max} = F_{max} - F_0$, with F_0, F and F_{max} being the fluorescence intensities of the free sensor, at various concentration of Ga^{3+} and at the maximum concentration of Ga^{3+} respectively.

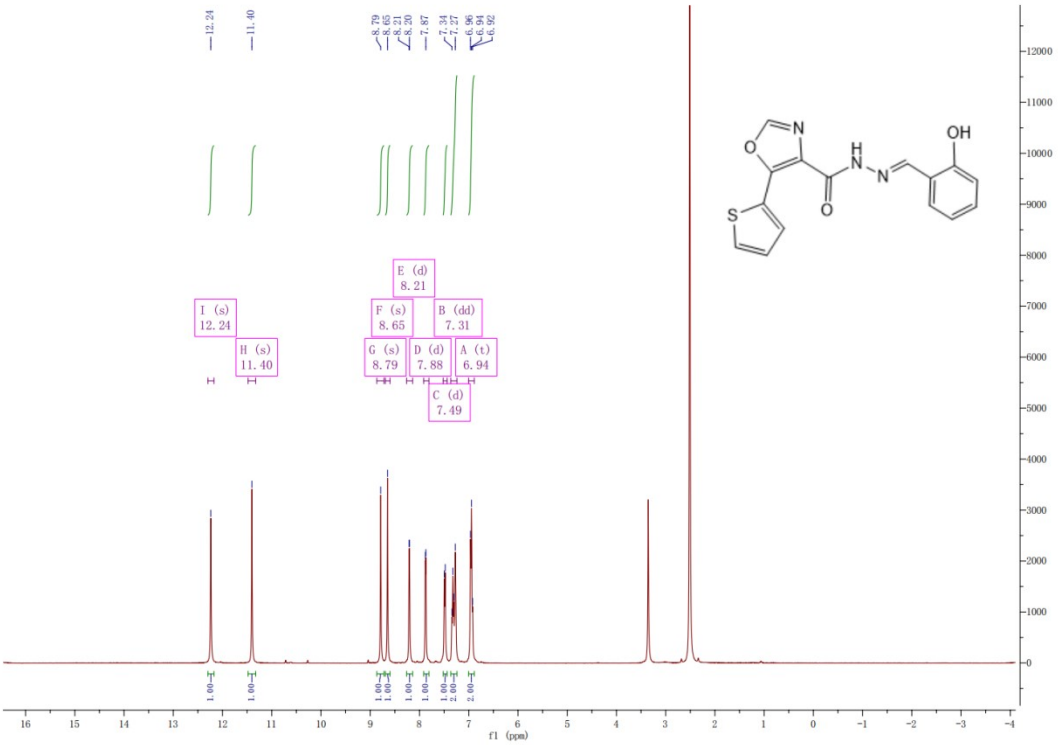

Fig. S1. [1]H NMR in DMSO-d_6 spectrum of **L1**.

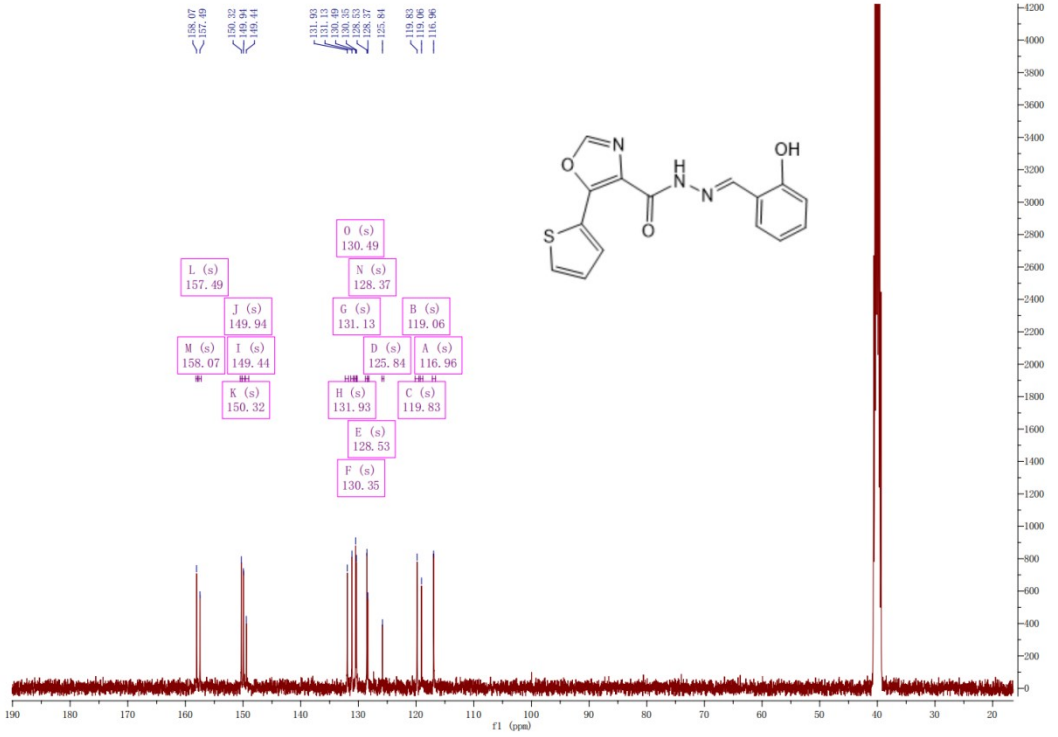

Fig. S2. 13C-NMR in DMSO-d_6 spectrum of **L1**.

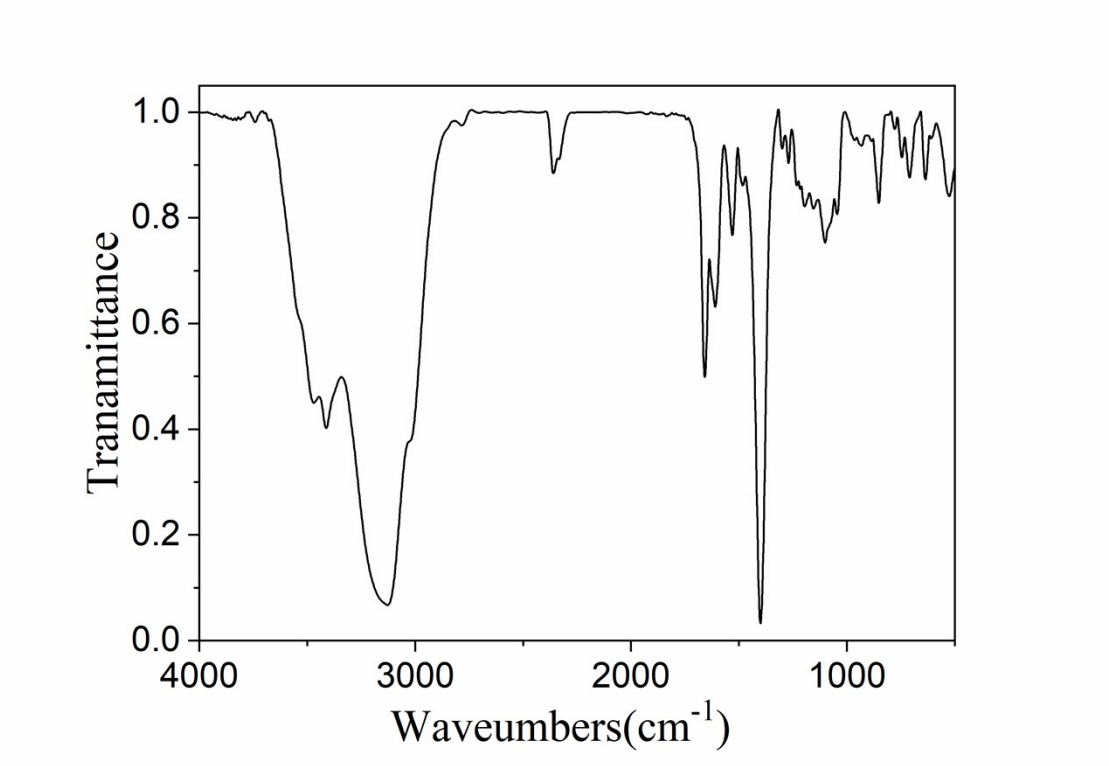

Figure S3. The FTIR spectrum of **L1**.

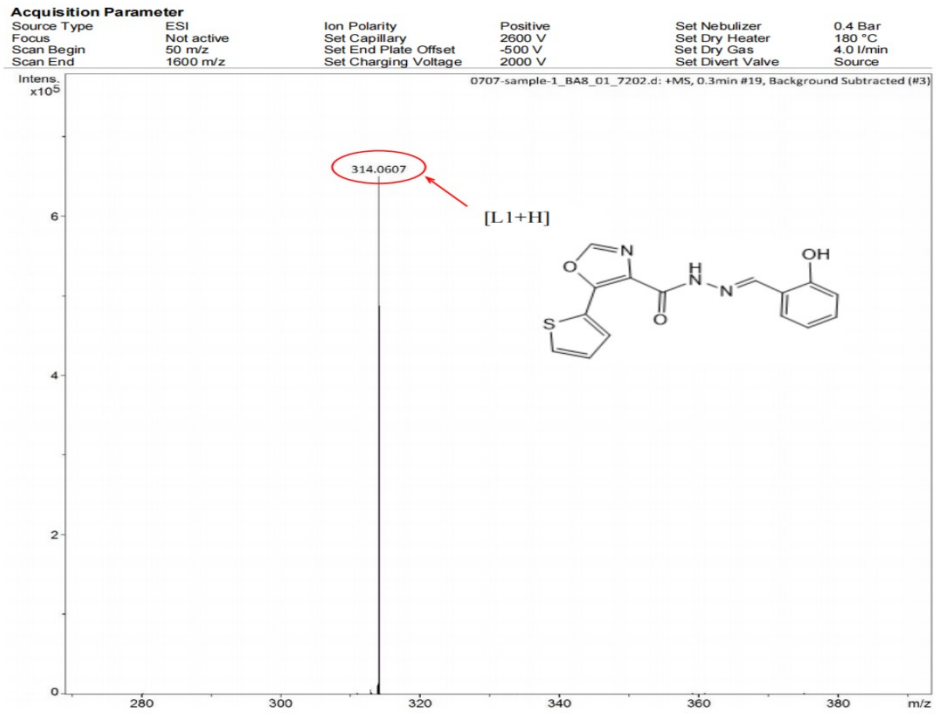

Figure S4. ESI-MS spectrum of **L1**.

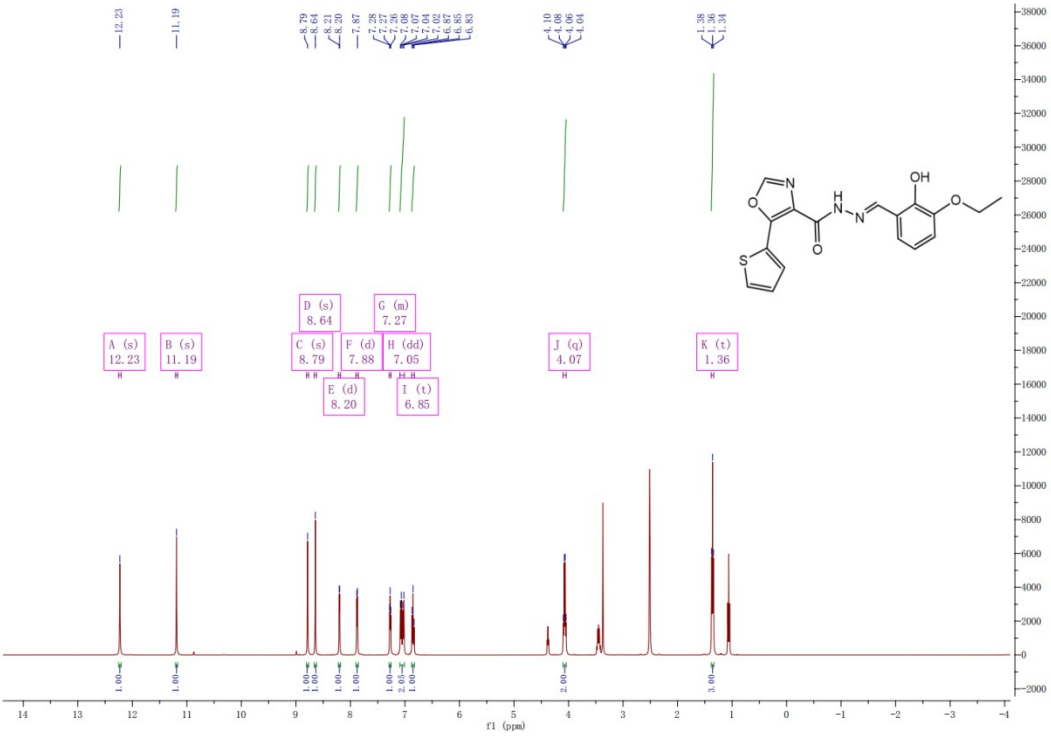

Fig. S5. ^{1}H NMR in DMSO-d_6 spectrum of **L2**.

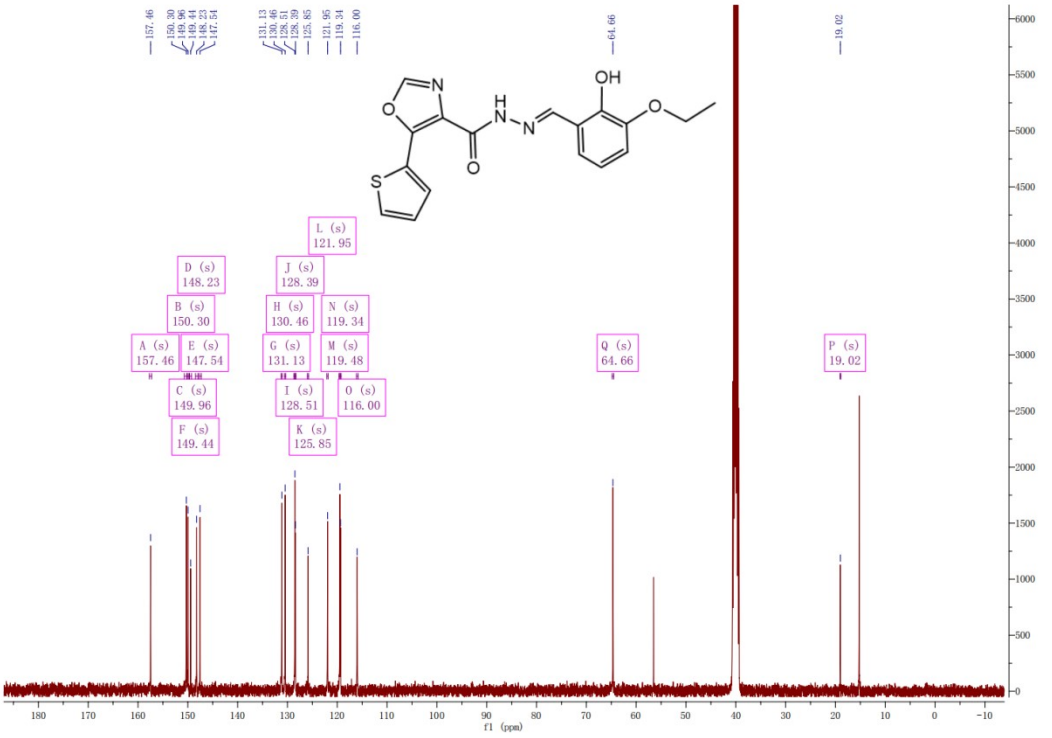

Fig. S6. ^{13}C NMR in DMSO-d_6 spectrum of **L2**.

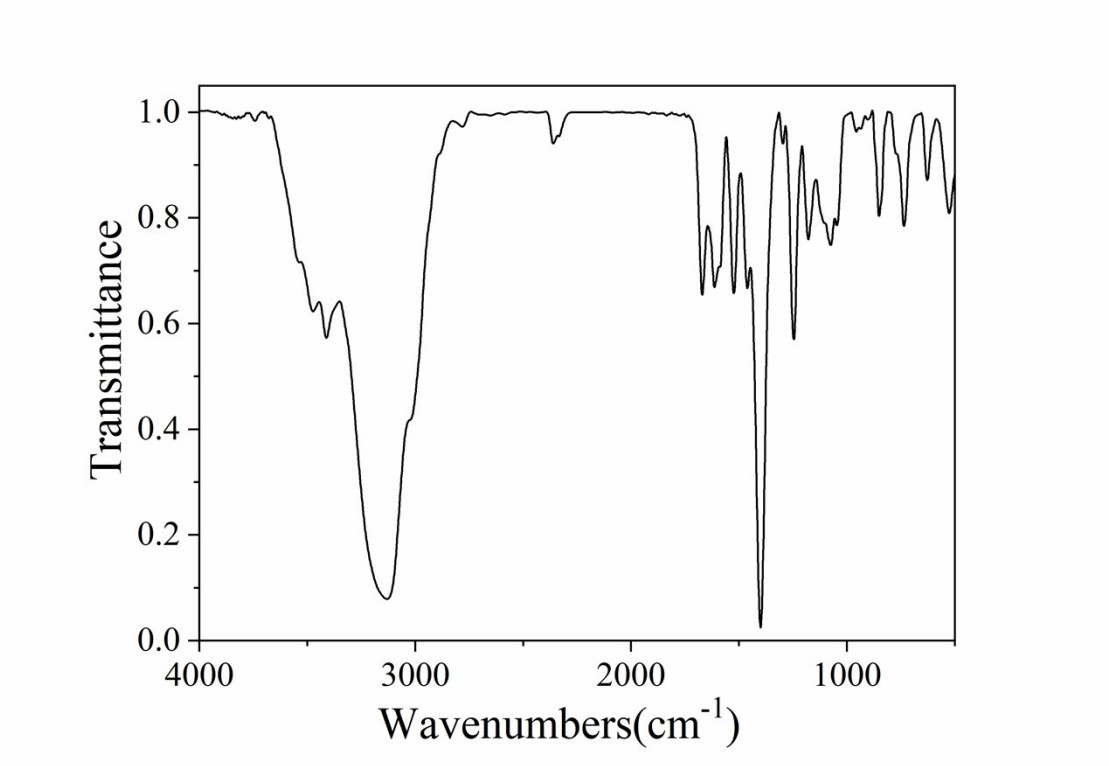

Figure S7. The FTIR spectrum of **L2**.

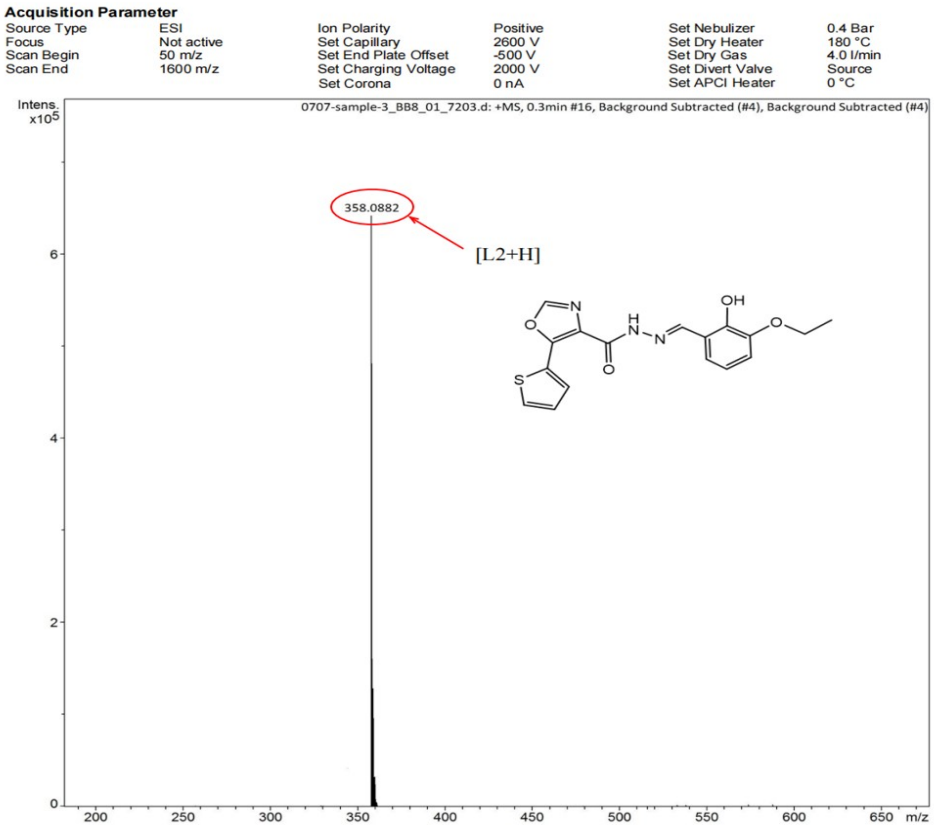

Fig. S8. ESI-MS spectrum of the probe **L2**.

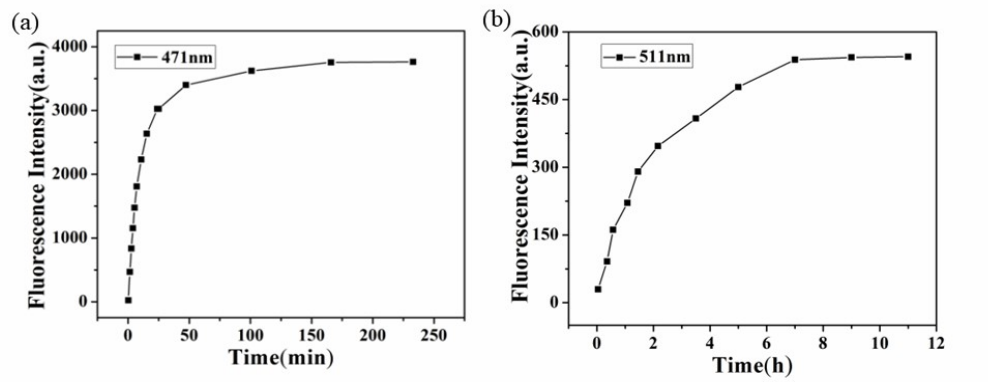

Fig. S9. Fluorescence emission intensity of **L1** (a) at 471 nm towards Ga^{3+} (5 equiv.) and **L2** (b) at 511 nm towards Ga^{3+} (10 equiv.) as a function of time.

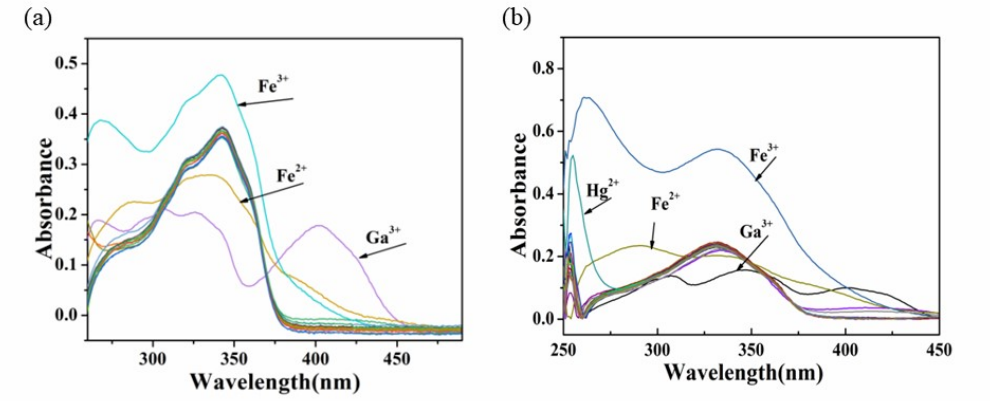

Fig. S10. UV-vis spectra of **L1** (a) and **L2** (b) in the presence of different metal ions (Ga^{3+}, Al^{3+}, In^{3+}, Zn^{2+}, Cd^{2+}, Hg^{2+}, Cu^{2+}, Ag^{+}, Ni^{2+}, Co^{2+}, Fe^{3+}, Mn^{2+}, Cr^{3+}, Ca^{2+}, Ba^{2+}, Li^{+}, Na^{+}, and K^{+}.) (5 equiv. for **L1** and 10 equiv. for **L2**) in DMSO/H_2O buffer solution (V/V = 9:1, Tris = 10 mM, pH = 7.4).

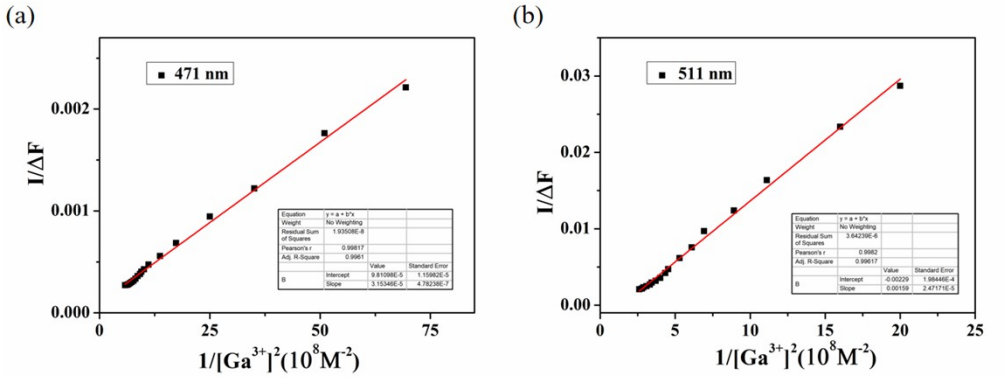

Fig. S11. Benesi-Hildebrand plot of **L1** (a) and **L2** (b), assuming 1:2 stoichiometry for association between sensors and Ga^{3+}.

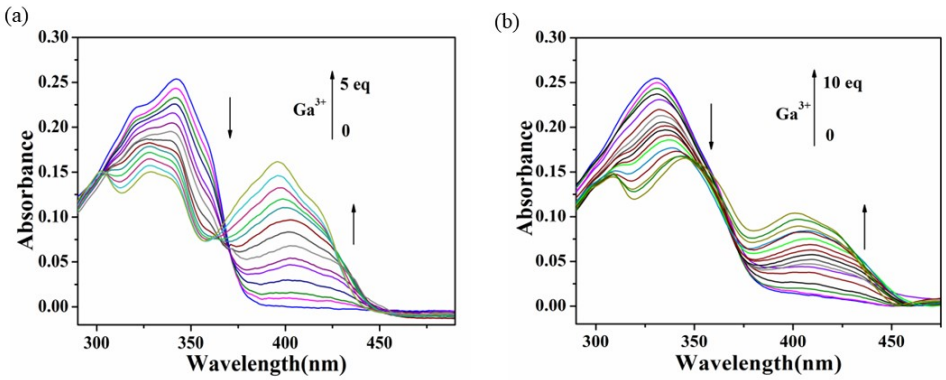

Fig. S12. Absorbance titration spectra of complex **L1** (a) and **L2** (b) with addition of Ga^{3+} (5 equiv. for **L1** and 10 equiv. for **L2**) in DMSO/H_2O tris buffer solution (V/V = 9:1, Tris = 10 mM, pH = 7.4)

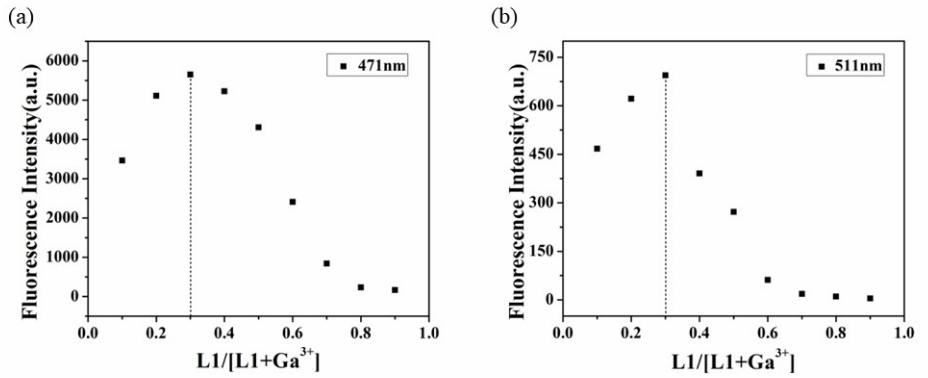

Fig. S13. Job's plot of the **L1** (a) and **L2** (b) in DMSO/H_2O buffer solution (V/V = 9:1, Tris = 10 mM, pH = 7.4).

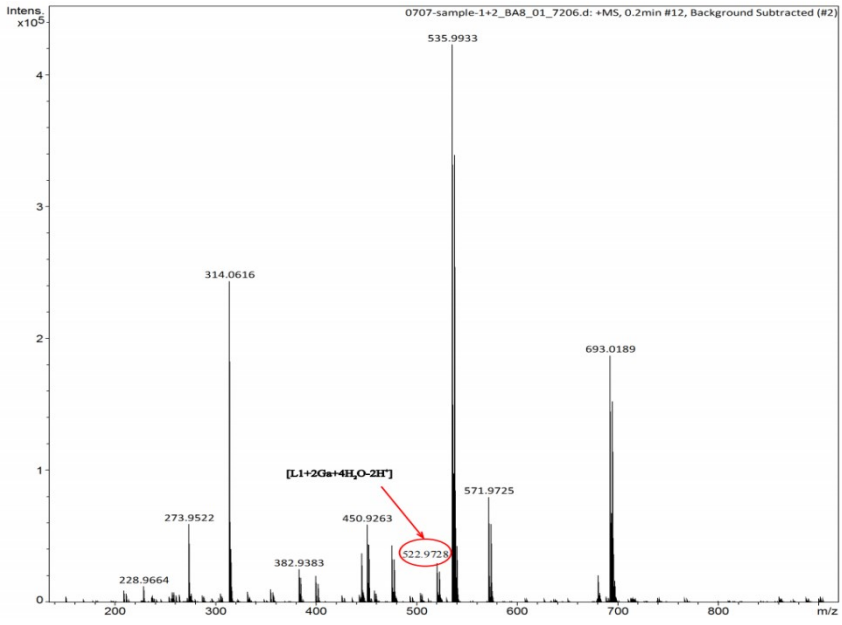

Figure S14. ESI-MS of **L1** with addition of Ga^{3+}.

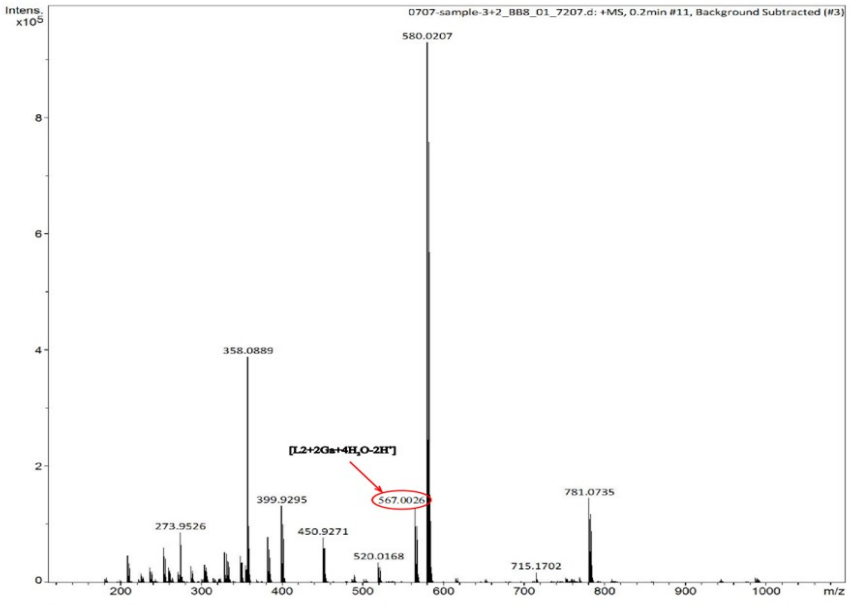

Figure S15. ESI-MS of **L2** with addition of Ga^{3+}.

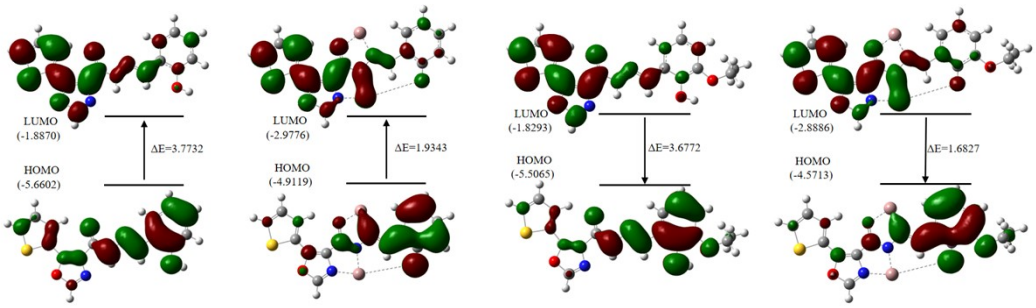

Fig. S16. The HOMO and LUMO orbital distributions and energy levels of **L1**, **L1**-Ga^{3+} and **L2**, **L2**-Ga^{3+}.

Table S1 Determination of the Ga^{3+} concentration in tap water samples with **L1**

Sample	Ga^{3+} added ($mol \cdot L^{-1}$)	Ga^{3+} recovered ($mol \cdot L^{-1}$)	Recovery (%)	RSD (%)
1	1.00×10^{-5}	0.93×10^{-5}	93.37	0.21
2	3.00×10^{-5}	2.97×10^{-5}	98.99	0.24
3	5.00×10^{-5}	4.88×10^{-5}	97.51	0.35

Table S2 Determination of the Ga^{3} concentration in tap water samples with **L2**

Sample	Ga^{3+} added ($mol \cdot L^{-1}$)	Ga^{3+} recovered ($mol \cdot L^{-1}$)	Recovery (%)	RSD (%)
1	4.00×10^{-5}	4.09×10^{-5}	102.20	0.34
2	6.00×10^{-5}	5.85×10^{-5}	97.43	0.16
3	7.00×10^{-5}	6.82×10^{-5}	97.48	0.14

R.S.D = SD/X. Where SD is the standard deviation of 3 recovered measurements, and X is the arithmetic average value of 3 recovered measurements.