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Electronic Supplementary Information

A highly luminescent terbium-organic framework for reversible detection of mercury ions in aqueous solution

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Luminescent Sensing Measurements

A well-ground powder of $[TbL_{1.5}(H_2O)_2]\cdot H_2O$ (2 mg) was immersed in an aqueous solution (4 mL) containing different nitrate salts of metal cations and the mixture was well stirred for one hour at room temperature. The steady state luminescent emission of each sample was measured after two days of aging and stirred vigorously before testing.

Table S1 Crystal data and structure refinement parameters for complex **1**

Complex	**1**
Empirical formula	$C_{19.50}H_{16.50}N_{1.50}O_9Tb$
Formula weight	574.76
Crystal system	Triclinic
Space group	P-1
a / Å	9.9199(4)
b / Å	10.4905(4)
c / Å	13.4316(8)
α (°)	105.687(4)
β (°)	101.880(5)
γ (°)	94.436(3)
V /Å^3	1303.68(11)
Z	2
Calculated density / mg·m^{-3}	1.464
Absorption coefficient/ mm^{-1}	2.755
Crystal size / mm	0.35 x 0.15 x 0.05
Reflections collected / unique	14207 / 9460
GOF	1.065
R_1[a] / wR_2[b][$I > 2\sigma(I)$]	0.0521/0.1490
R_1, wR_2 (all data)	0.0738/0.1734

[a] $R_1 = \Sigma||F_o| - |F_c||/|F_o|$. [b] $wR_2 = [\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$.

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Table S2 Selected bond lengths (Å) and angles (°) for **1**

Tb(1)-O(2)#1	2.300(5)	Tb(1)-O(5)	2.439(5)
Tb(1)-O(3)#2	2.309(5)	Tb(1)-O(6)	2.495(6)
Tb(1)-O(1)	2.328(4)	O(2)-Tb(1)#1	2.300(5)
Tb(1)-O(4)#3	2.333(4)	O(3)-Tb(1)#2	2.309(5)
Tb(1)-O(2W)	2.435(5)	O(4)-Tb(1)#4	2.333(4)
Tb(1)-O(1W)	2.436(5)		
O(2)#1-Tb(1)-O(3)#2	146.90(18)	O(2W)-Tb(1)-O(1W)	73.04(15)
O(2)#1-Tb(1)-O(1)	100.87(17)	O(2)#1-Tb(1)-O(5)	77.35(17)
O(3)#2-Tb(1)-O(1)	86.91(17)	O(3)#2-Tb(1)-O(5)	72.99(17)
O(2)#1-Tb(1)-O(4)#3	85.09(19)	O(1)-Tb(1)-O(5)	129.05(18)
O(3)#2-Tb(1)-O(4)#3	102.07(18)	O(4)#3-Tb(1)-O(5)	77.16(18)
O(1)-Tb(1)-O(4)#3	153.75(18)	O(2W)-Tb(1)-O(5)	129.11(15)
O(2)#1-Tb(1)-O(2W)	142.07(19)	O(1W)-Tb(1)-O(5)	144.10(17)
O(3)#2-Tb(1)-O(2W)	70.47(18)	O(2)#1-Tb(1)-O(6)	71.79(19)
O(1)-Tb(1)-O(2W)	82.86(17)	O(3)#2-Tb(1)-O(6)	78.74(18)
O(4)#3-Tb(1)-O(2W)	77.22(18)	O(1)-Tb(1)-O(6)	77.63(18)
O(2)#1-Tb(1)-O(1W)	71.58(18)	O(4)#3-Tb(1)-O(6)	128.08(18)
O(3)#2-Tb(1)-O(1W)	141.00(18)	O(2W)-Tb(1)-O(6)	144.22(18)
O(1)-Tb(1)-O(1W)	75.28(18)	O(1W)-Tb(1)-O(6)	128.61(17)
O(4)#3-Tb(1)-O(1W)	82.62(18)	O(5)-Tb(1)-O(6)	53.06(13)

[a] Symmetry codes for 1: #1 -x+1,-y+1,-z+1; #2 -x+1,-y+2,-z+1; #3 x+1,y-1,z; #4 x-1,y+1,z; #5 -x+2,-y+1,-z+2.

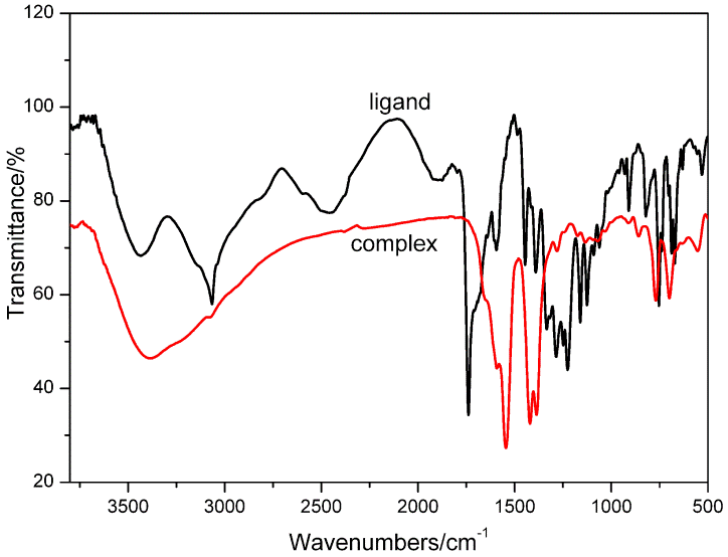

Fig. S1. FT-IR spectra.

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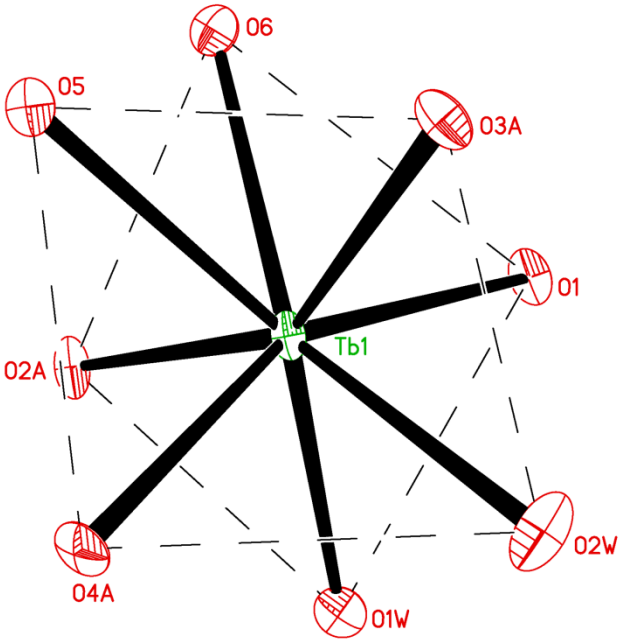

Fig. S2 The distorted square antiprism coordination polyhedron of the Tb^{3+} in **1**.

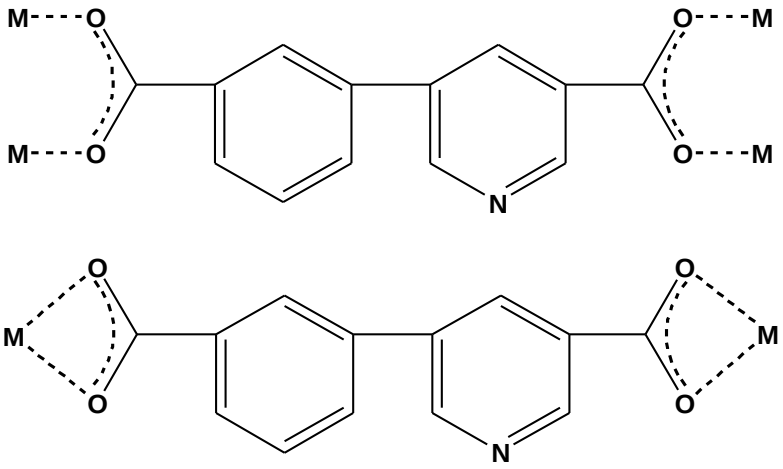

Fig. S3 Coordination modes of ligand in **1**.

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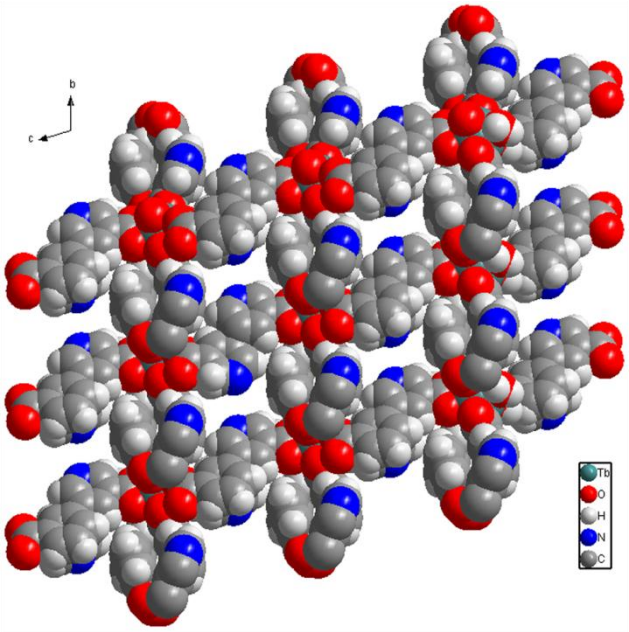

Fig. S4 Space-filled model of **1** showing the 1D channels viewed along the *a*-axis; the guest water are omitted for clarity.

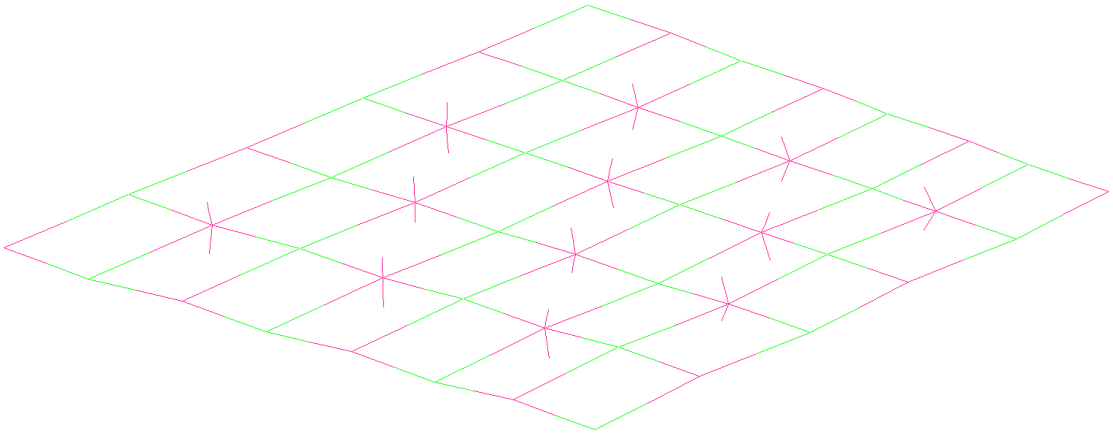

Fig. S5 The (4, 4)-connected topological network. Hydrogen atoms and lattice solvent molecules have been omitted for clarity.

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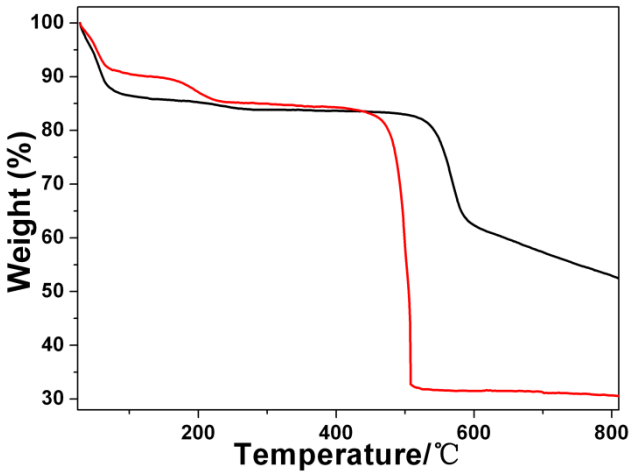

Fig. S6 TGA curves of **1**in nitrogen (black) and air (red) atmosphere.

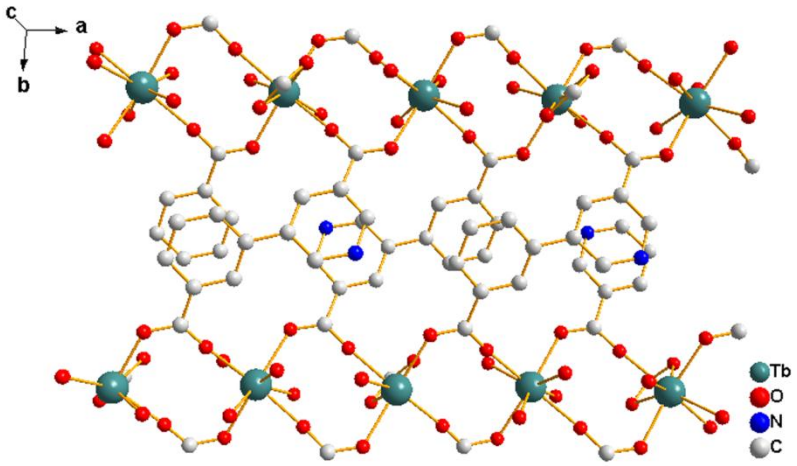

Fig. S7 The π-π stacking of adjacent aromatic rings

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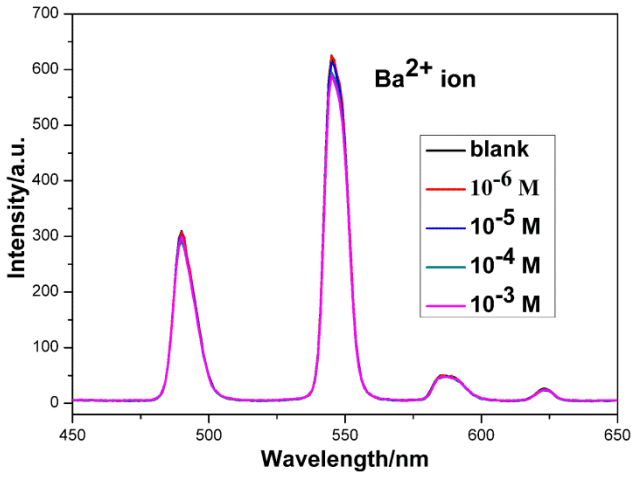

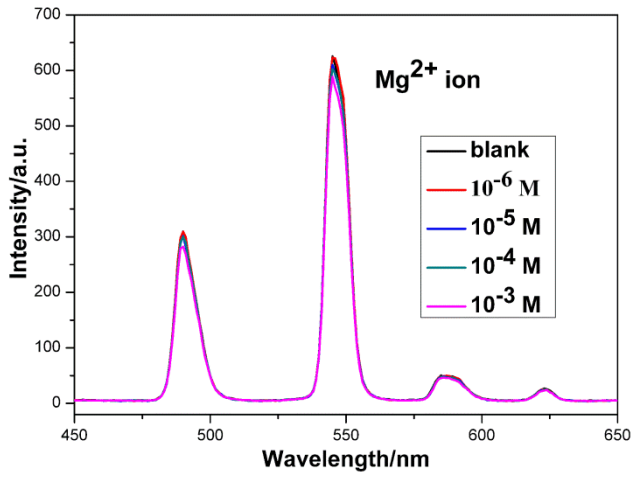

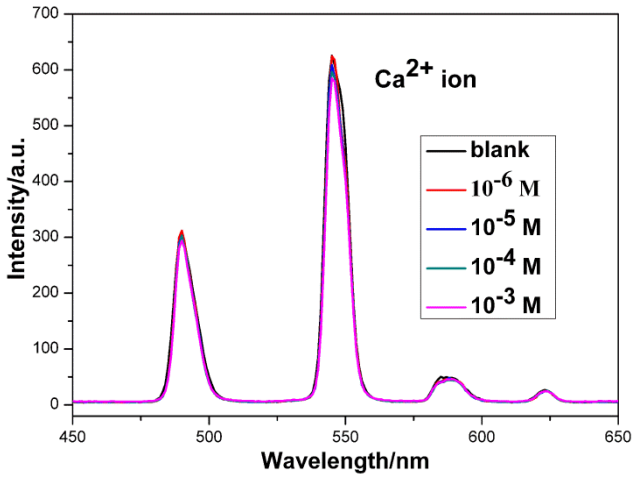

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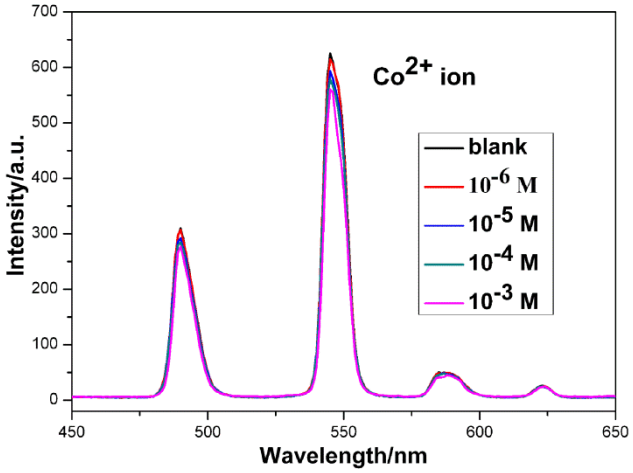

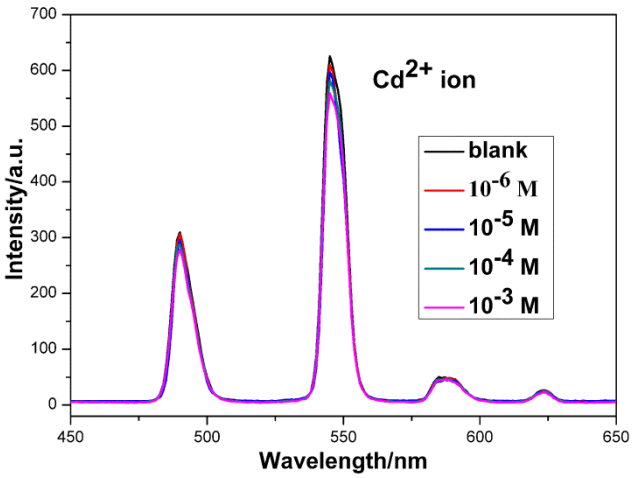

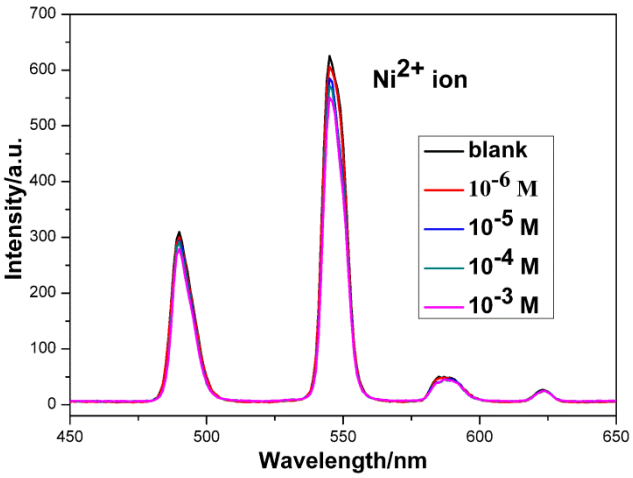

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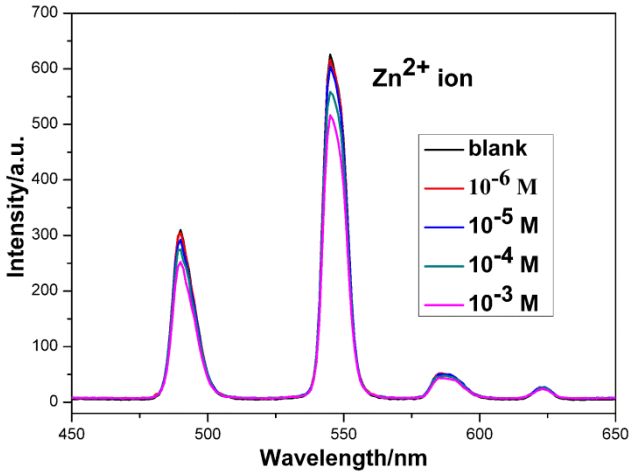

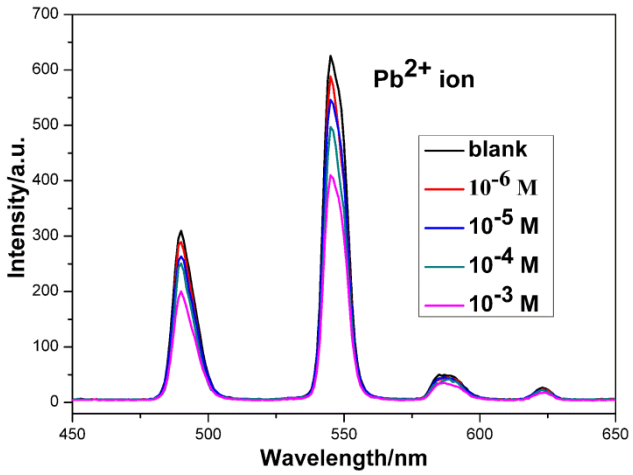

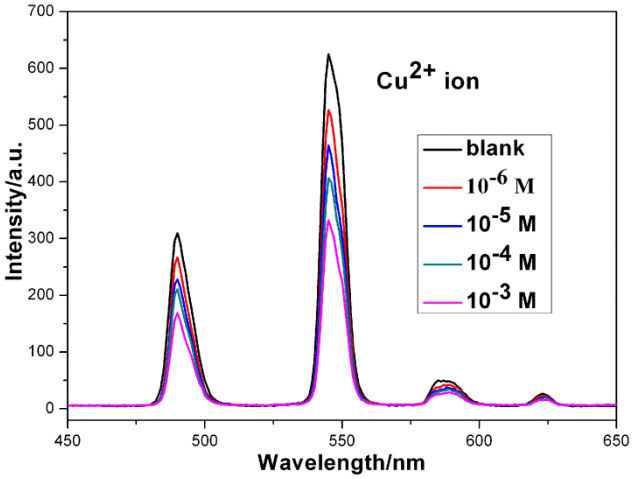

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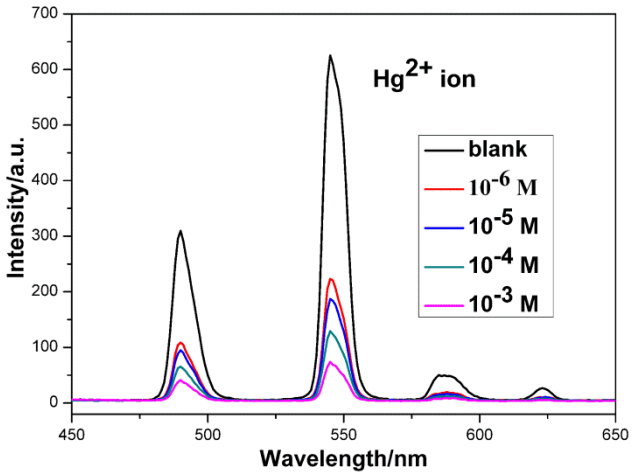

Fig. S8 Emission spectra of **1** in different metal ionic aqueous solutions at various concentrations (excited at 314 nm).

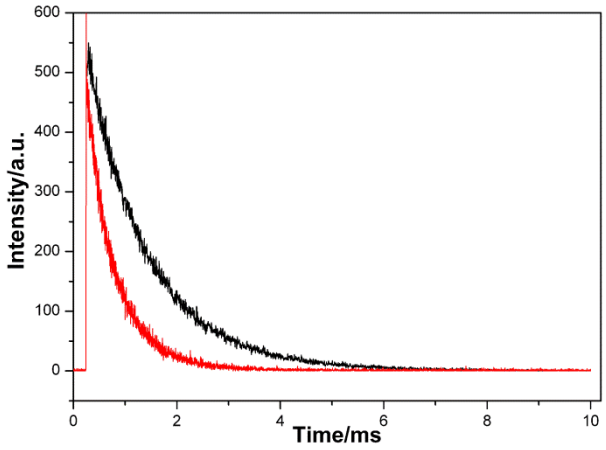

Fig. S9 Luminescence decay profiles of **1** (black) and Hg^{2+}-incorporated **1** (red).

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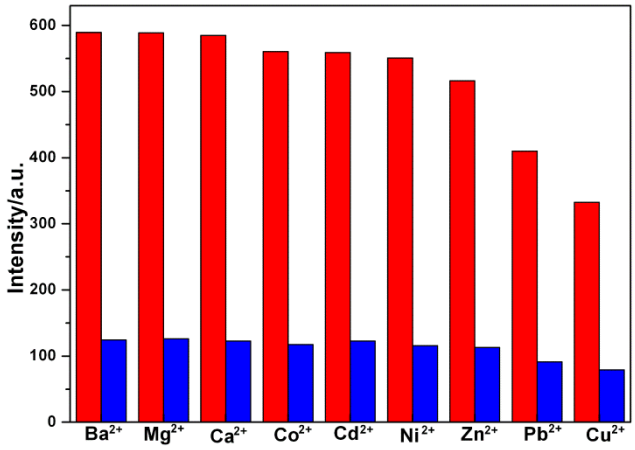

Fig. S10 The emission intensities of **1** at 545 nm in different 10^{-3} mol L^{-1} metal ions(red) or mixture of 10^{-3} mol L^{-1} metal ions and 10^{-4} mol L^{-1} Hg^{2+} ions (blue) aqueous solutions (excited at 314 nm).

Table S3 Quenching effect coefficients (Ksv) of different metal ions on the luminescence intensity of **1**.

Metal ion	Ba^{2+}	Mg^{2+}	Ca^{2+}	Co^{2+}	Cd^{2+}	Ni^{2+}	Zn^{2+}	Pb^{2+}	Cu^{2+}	Hg^{2+}
Ksv [M^{-1}]	61	62	69	116	118	135	211	525	880	7465