Supporting information

Different Effect in the Selective Detection of Aniline and Fe3+ by Lanthanide-Based Coordination Polymers Containing Multiple Reactive Sites

Xinfang Liu,[a,*] Liyong Du,[b] Rongfang Li,[a] Ningning Ma,[a] Mengdi You[a] and Xun Feng[a,*]

[a] College of Chemistry and Chemical Engineering, Henan Key Laboratory of Function Oriented Porous Materials, Luoyang Normal University, Luoyang, 471934, China.
[b] School of Chemical and Material Engineering, Jiangnan University, Wuxi, 214122, PR China.

Table S1. Crystal data and refinement parameters of **1-Eu** and **2-Tb**.

	1-Eu	**2-Tb**
Empirical formula	$C_{14}H_{16}NO_{11}Eu$	$C_{14}H_{16}NO_{11}Tb$
Formula weight	526.24	533.20
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
a/Å	12.4793(8)	12.4886(7)
b/Å	13.8564(6)	14.0071(6)
c/Å	10.7865(6)	10.8593(6)
β/°	113.602(7)	114.000(6)
Volume/Å^3	1709.16(18)	1735.38(17)
Z	4	4
ρ_{calc}g/cm^3	2.045	2.041
μ/mm^{-1} /F(000)	3.732 / 1032.0	4.137/1040.0
Crystal size/mm^{3}F(000)	0.21 × 0.19 × 0.18	0.21 × 0.20 × 0.18
2Θ range for data	6.876 to 54.932	6.826 to 58.568
Index ranges Radiation	$-16 \le h \le 15$, $-17 \le k \le 17$, $-12 \le l \le 13$	$-13 \le h \le 16$, $-18 \le k \le 16$, $-14 \le l \le 9$
Data/restraints/parameters	3391/0/251	4082/0/250
Final R indexes [I>=2σ]	$R_1 = 0.0409$, $wR_2 = 0.0989$	$R_1 = 0.0349$, $wR_2 =$
Final R indexes [all	$R_1 = 0.0445$, $wR_2 = 0.1024$	R1= 0.0407, wR2 =
Largest diff. peak/hole / e Å^{-3}	2.73/-2.58	1.41/-1.52

Table S2. Selected bond lengths and bond angles in **1-Eu**

Bond	Length/Å	Bond	Length/Å
Eu1-O1#1	2.522(3)	Eu1-O9	2.489(3)
Eu1-O4	2.454(3)	Eu1-O10	2.475(3)
Eu1-O6	2.378(4)	Eu1-O2#1	2.510(3)
Eu1-O7	2.400(4)	Eu1-N1	2.543(4)
Eu1-O8	2.445(3)		
Bond	Angle/°	Bond	Angle/°
O2#1-Eu1-N1	133.84(12)	O6-Eu1-N1	63.43(12)
O2#1-Eu1- O1#1	51.98(12)	O9-Eu1-O6	73.43(12)
O4-Eu1-O6	126.91(12)	O9-Eu1-O7	134.59(12)
O4-Eu1-O7	77.32(12)	O9-Eu1-O8	68.05(12)
O4-Eu1-O8	135.97(12)	O9-Eu1-O1#1	98.75(11)
O4-Eu1-O9	145.89(13)	O9-Eu1-O2#1	72.11(11)
O4-Eu1-O10	81.46(12)	O9-Eu1-N1	129.20(12)
O4-Eu1-O2#1	78.61(11)	O8-Eu1-O1#1	70.32(11)
O4-Eu1-O1#1	75.68(11)	O8-Eu1-O2#1	100.59(11)
O4-Eu1-N1	63.57(12)	O8-Eu1-N1	124.78(12)
O7-Eu1-O8	67.59(12)	O10-Eu1-O6	77.37(14)
O7-Eu1-O1#1	75.02(12)	O10-Eu1-O7	144.80(12)
O7-Eu1-O2#1	125.61(12)	O10-Eu1-O8	141.76(11)
O7-Eu1-N1	72.34(13)	O10-Eu1-O9	74.91(11)
O6-Eu1-O7	89.65(12)	O10-Eu1-O1#1	126.07(12)
O6-Eu1-O8	79.73(11)	O10-Eu1-O2#1	76.07(12)
O6-Eu1-O1#1	149.70(11)	O10-Eu1-N1	73.14(12)
O6-Eu1-O2#1	142.44(11)	O1#1-Eu1-N1	132.00(11)

#1, -1+x, y, -1+z.

Table S3. Selected bond lengths and bond angles in **2-Tb**

Bond	Length/Å	Bond	Length/Å
Tb-O4	2.408(3)	Tb-O8	2.480(4)
Tb-O9	2.426(3)	Tb-O2#1	2.487(3)
Tb-O6	2.333(3)	Tb-N1	2.502(4)
Tb-O7	2.460(3)	Tb-O1#1	2.493(3)
Tb-O10	2.395(3)		
Bond	Angle/°	Bond	Angle/°
O4-Tb-O9	136.50(12)	O6-Tb-O1#1	140.96(12)
O4-Tb-O7	81.87(12)	O7-Tb-O8	74.75(12)
O4-Tb-O8	145.31(13)	O7-Tb-O2#1	74.81(12)
O4-Tb-O2#1	76.24(11)	O7-Tb – N1	72.43(12)
O4-Tb-N1	64.24(11)	O7-Tb – O2#1	125.50(11)
O4 -Tb-O1#1	78.07(12)	O10-Tb-O4	78.49(12)
O9 -Tb-O7	141.03(12)	O10-Tb-O7	144.46(13)
O9 -Tb-O8	67.97(12)	O10-Tb-O8	134.01(12)
O9-Tb-O2#1	71.26(11)	O10-Tb-O2#1	77.79(13)
O9-Tb-N1	124.27(12)	O10-Tb-N1	72.41(13)
O9-Tb – O1#1	102.73(13)	O10-Tb-O1#1	128.39(12)
O6-Tb-O4	128.19(12)	O10-Tb-O9	67.11(13)
O6-Tb-O9	78.02(11)	O8-Tb-O2#1	96.81(12)
O6-Tb-O7	80.80(12)	O8-Tb-N1	129.01(12)
O6-Tb-O10	88.46(12)	O8-Tb-O1#1	71.34(13)
O6-Tb-O8	73.12(12)	O2#1 -Tb-N1	134.06(11)
O6-Tb-O2#1	149.20(11)	O2#1 -Tb-O1#1	52.20(12)
O6-Tb-N1	64.01(11)	O1#1-Tb-N1	132.58(13)

#1, 1+x, y, 1+z; #2, -1+x, y, -1+z.

Table S4. Hydrogen bonds for 1-Eu and 2-Tb.

1-Eu				
D-H-A	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
O7-H7A···O3#1	0.86	1.95	2.806(5)	170.7
O8-H8B···O4#1	0.88	1.88	2.706(5)	155.8
O9-H9B···O2#2	0.87	2.06	2.745(5)	135.8
O10-H10B···O11	0.88	1.99	2.831(5)	159.7
2-Tb				
D-H-A (2-Eu)	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
O(7)-H(7A)-O(4)#1	0.85	2.09	2.896(4)	157.2
O(7)-H(7B)-O(5)#2	0.87	1.96	2.791(4)	159.4
O(9)-H(9B)-O(2)#3	0.88	1.86	2.735(5)	174.6
O(11)-H(11A)-O(10)	0.85	2.10	2.857(5)	148.0

For **1-Eu**: #1, +x, 0.5-y, 0.5+z; 2, +x, 0.5-y, -0.5+z.

For **2-Tb**: #1, x, 1.5-y, 0.5+z; #2, x, 1.5-y, 0.5+z; #3, 1-x, 1-y, 1-z.

Table S5. K_{SV} values and LODs for the recently reported MOF-based luminescence probes for Fe^{3+}

MOF-based sensor	Linear Range [μM]	LOD [μM]	$K_{SV\times}10^4$ [M^{-1}]	Ref.
$[Eu_2(2,3'\text{-oba})_3(phen)_2]_n$	0-180	7.93	1.37	[1]
$\{[Eu(L)(HCOO)]\cdot H_2O\}_n$	0-100	1.0	0.7461	[2]
$[Tb(TBOT)(H_2O)](H_2O)_4(DMF)(NMP)_{0.5}$	0-100	10	0.551	[3]
$\{Zn_2(NO_3)_2(4,4'\text{-bpy})_2(TBA)\}$	100-300	7.18	0.748	[4]
Zn-DTA	50-200	0.82	0.84	[5]
Cd-DTA	50-200	1.07	0.64	[5]
$[Cd_2(btc)(bib)(HCOO)(H_2O)\cdot H_2O]_n$	0-130	1.56	0.605	[6]
1-Eu	0-1600	0.1565	1.629	This work
2-Tb	0-1600	0.1567	1.626	This work

Table S6. K_{SV} values and LODs for the recently reported MOF-based luminescence probes for aniline

MOF-based sensor	Medium	Linear Range [mM]	LOD [μM]	K_{SV} [M^{-1}]	Ref.
$[Ln(BTB)(H_2O)]_n$	ethanol	0.005-5	5	1750	[7]
Zn-Eu	methanol	0.05-0.5	7.5	1200.2	[8]
Zn-Tb	methanol	0.05-0.5	5.2	987.6	[8]
$[EMI]_2[Eu_2(BDC)_3(H_2BDC)Cl]$	DMF water	0.1-5 0.1-5	10 6.8	- -	[9]
$Eu(BDC)Cl(H_2O)]$	DMF water	0.01-5 0.5-10	7 9	- -	[9]
1-Eu	DMF	0-3.3	0.92	1696	This work

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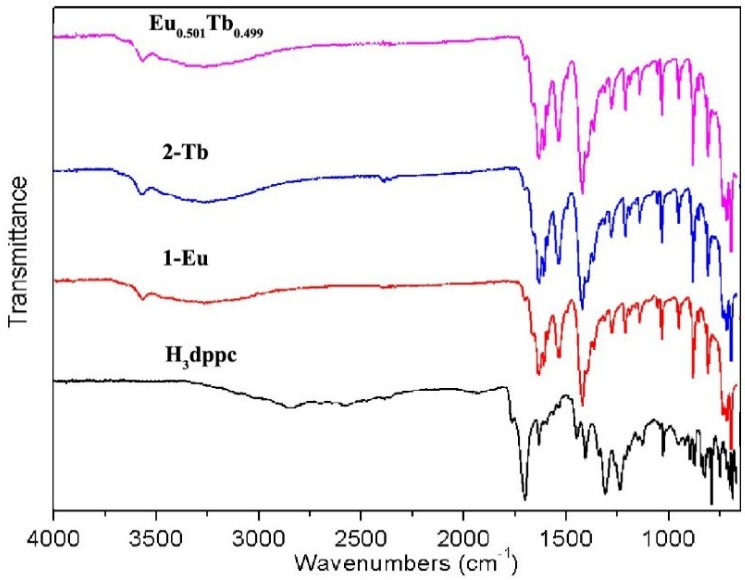

Fig. S1 IR spectra of H_3dppc ligand and complexes **1-Eu**, **2-Tb** and **$Eu_{0.501}Tb_{0.499}$**.

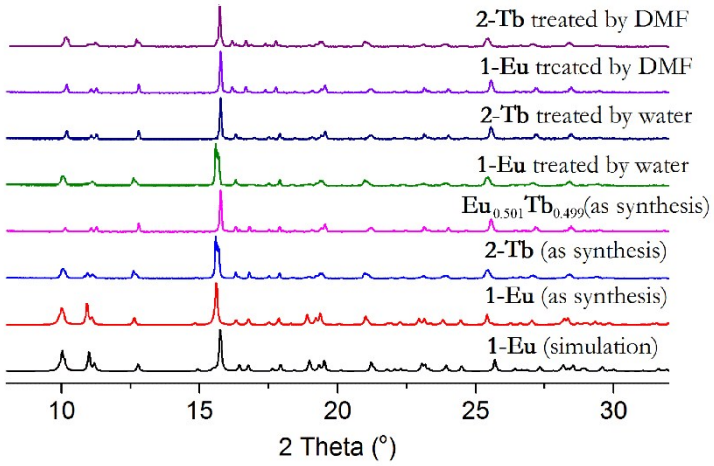

Fig. S2 PXRD patterns of complexes **1-Eu**, **2-Tb** and $\mathbf{Eu_{0.501}Tb_{0.499}}$ before and after being treated by water and DMF (for the first two Ln-CPs). The treatment process is as follows: 5mg of **1-Eu** or **2-Tb** was immersed in 5mL of H_2O or DMF for 24 h, filtered and dried in air.

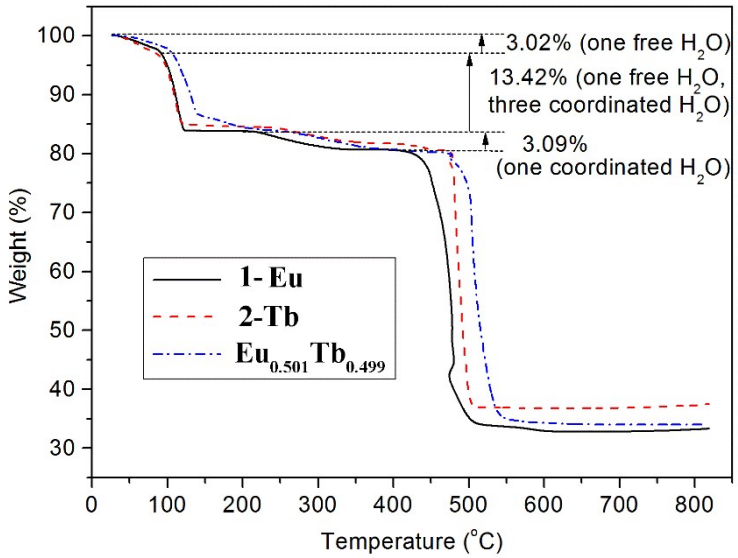

Fig. S3 TG curves of complexes **1-Eu** and **2-Tb**.

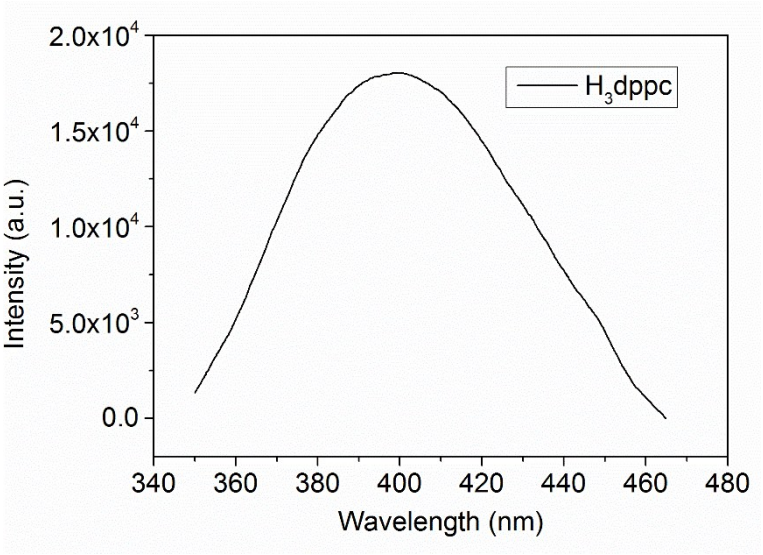

Fig. S4 Emission spectrum of the free ligand H_3dppc.

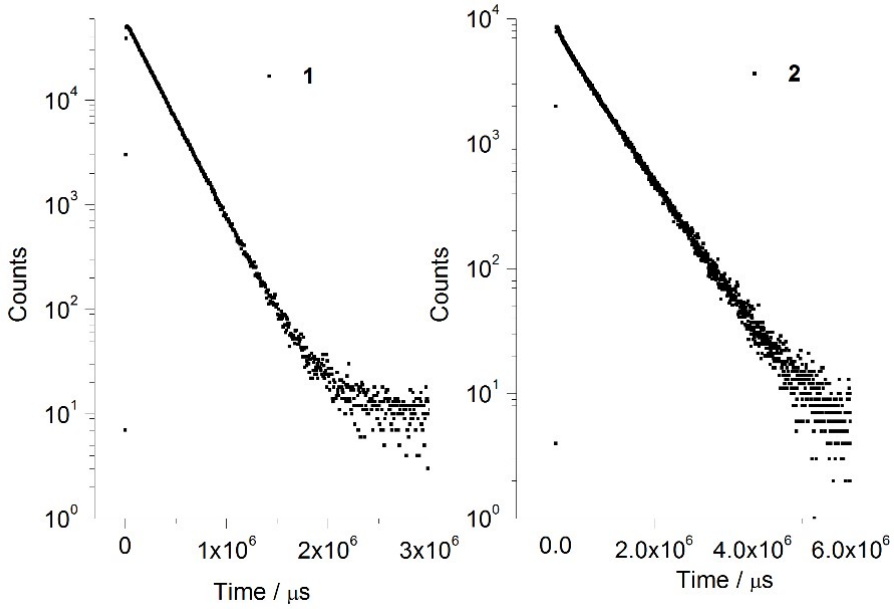

Fig. S5 Luminescence decay lifetimes of **1-Eu** and **2-Tb** upon excited at 300 nm and 330 nm, respectively

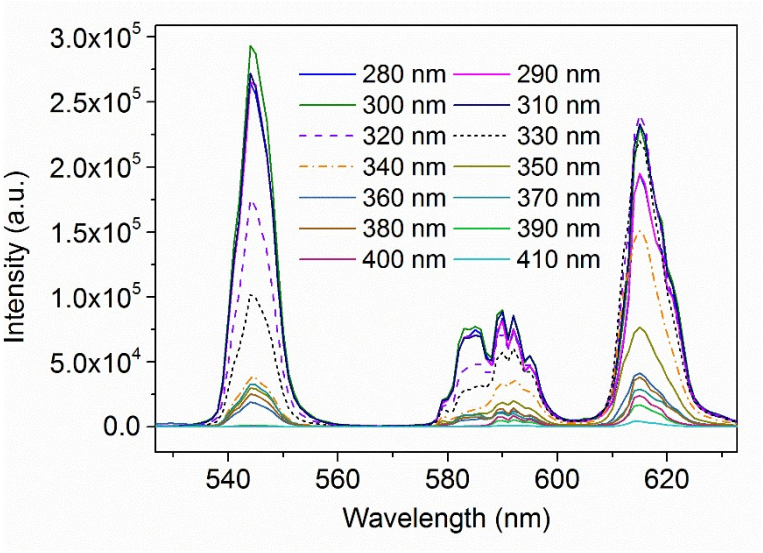

Fig. S6 Solid emission spectra of $\mathbf{Eu_{0.501}Tb_{0.499}}$ when excited under a series of excitation wavelength

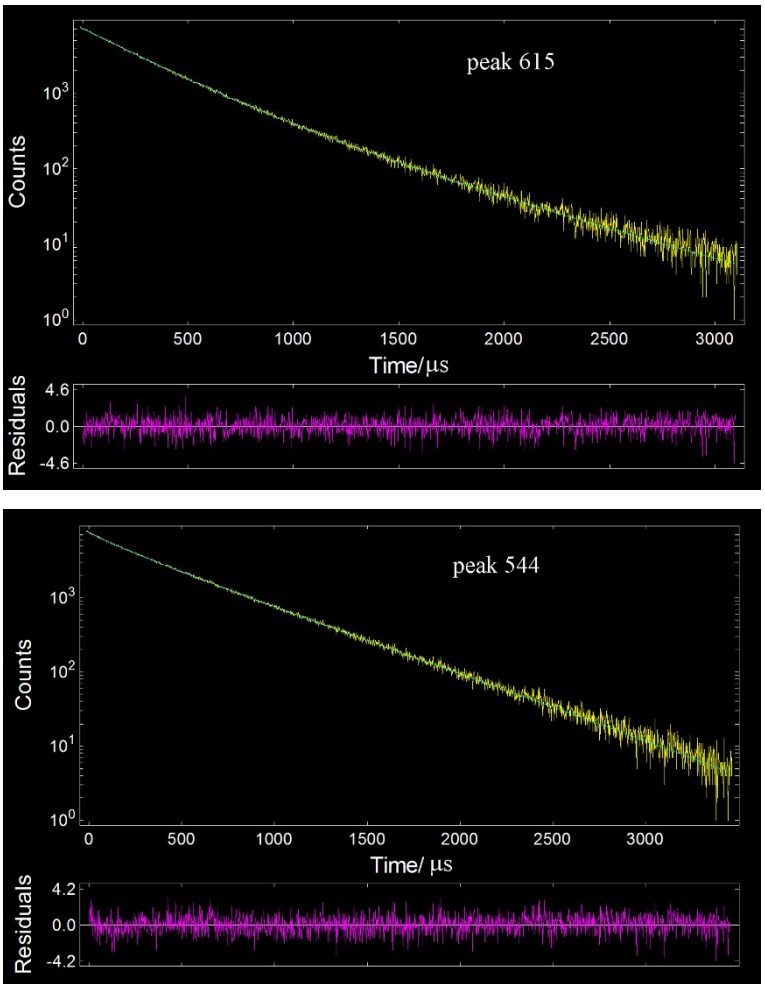

Fig. S7 Luminescence decay lifetimes of peaks 615 and 544 in $\mathbf{Eu_{0.501}Tb_{0.499}}$-MOF upon excited at 310 nm

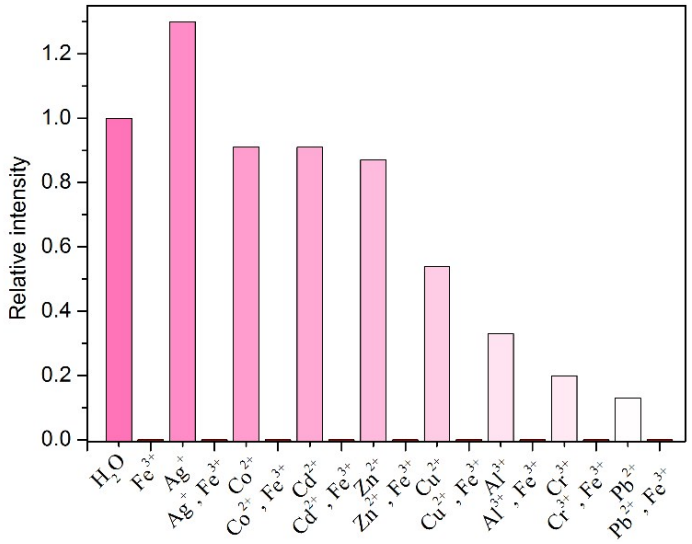

Fig. S8 Luminescent detection of different metal ions without or with Fe^{3+} by **1-Eu**

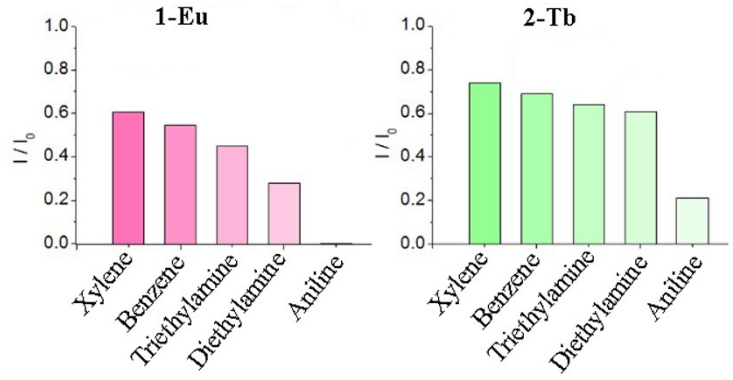

Fig. S9 Relative fluorescence intensities of **1-Eu** and **2-Tb** dispersed in DMF solution of aromatic series and amine series (0.1 mol/L) (the concentration of aniline used to quench the fluorescence of **1-Eu** is 0.01 mol/L).

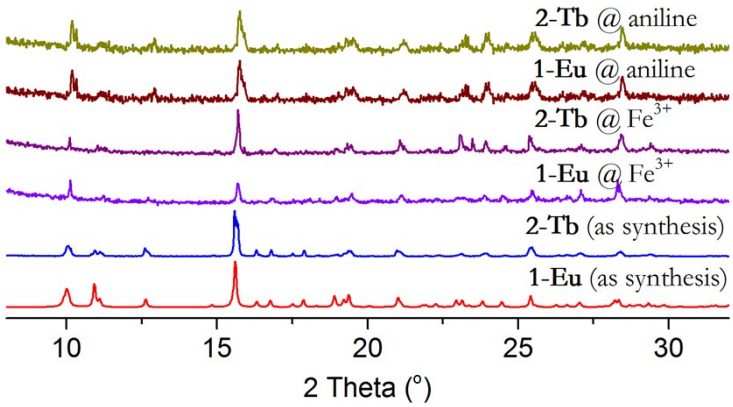

Fig. S10 PXRD patterns of complexes **1-Eu** and **2-Tb** before and after treatment by Fe^{3+} aqueous solution or aniline. The treatment process is as follows: 5mg of 1-Eu or 2-Tb was immersed in 5mL of $Fe(NO_3)_3$ aqueous solution (10^{-2} mol/L) or DMF for 24 h, filtered and dried in air.

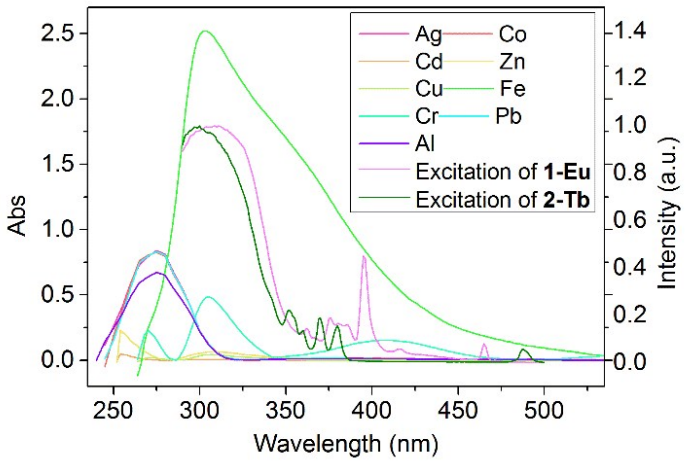

Figure S11. UV-Vis adsorption spectra of aqueous solutions of different metal ions (10^{-3} mol/L) and excitation of **1-Eu** and **2-Tb** (2 mg) dispersed in aqueous solution (2 mL).

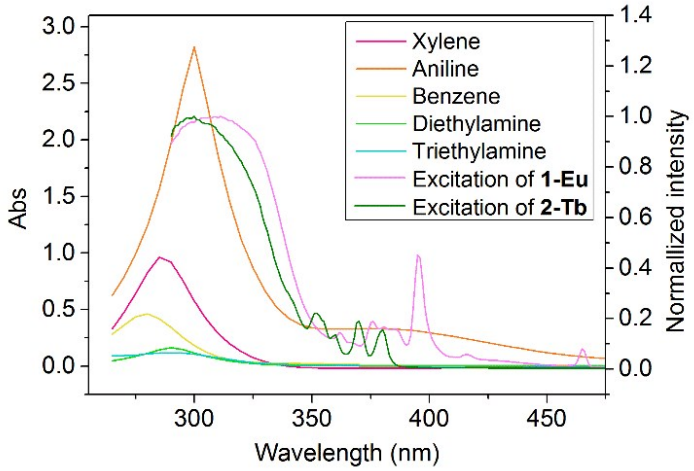

Figure S12. UV-Vis adsorption spectra of aqueous solutions of different organics (10^{-3} mol/L) in DMF solution and excitation of **1-Eu** and **2-Tb** (2 mg) dispersed in DMF solution (2 mL).

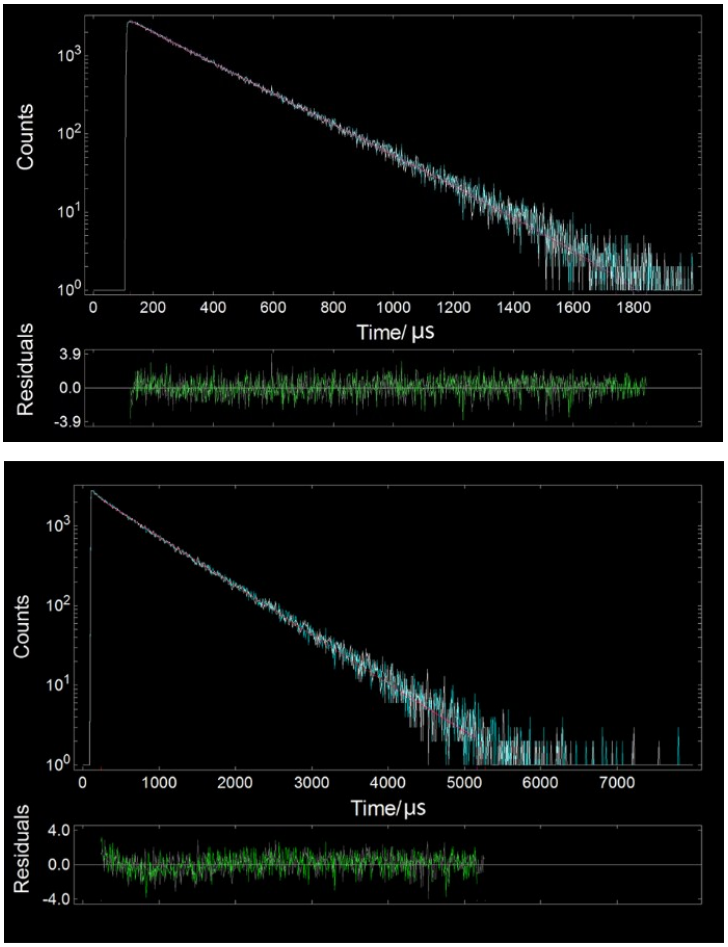

Fig. S13 Luminescence lifetimes of **1-Eu** or **2-Tb** in aqueous solution without (top) or with Fe^{3+} (bottom)

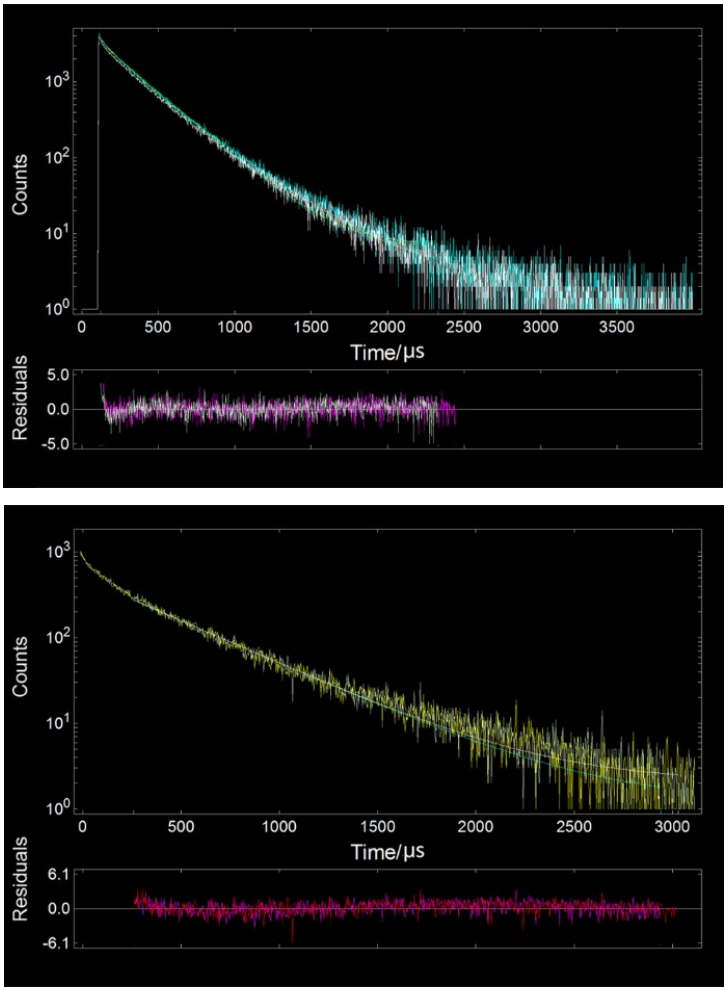

Fig. S14 Luminescence lifetimes of **1-Eu** or **2-Tb** in DMF solution without (top) or with aniline (bottom)