

## Supporting Information

### 1. Figure captions:

Fig. S1 PXRD patterns of complex **2** immersed in different solutions including  $\text{Cr}_2\text{O}_7^{2-}/\text{CrO}_4^{2-}/\text{Fe}^{3+}/\text{MDZ}/\text{benzaldehyde}/\text{aqueous}/\text{acidic}$  solution (pH = 3) and basic solution (pH = 13) for 2 days.

Fig. S2 The solid state emission spectra of the free ligands, complexes **1** and **3**.

Fig. S3 The solid state emission spectra of complex **2** at different excitation wavelength.

Fig. S4 Fluorescence lifetime decay curves of **2** and **4**.

Fig. S5 Emission spectra of **2** dispersed in different  $\text{M}(\text{NO}_3)_n$  solutions.

Fig. S6 The competing experiments of **2** for  $\text{Fe}^{3+}$  (a),  $\text{Cr}_2\text{O}_7^{2-}$  (b),  $\text{CrO}_4^{2-}$  (c), and MDZ (d).

Fig. S7 Emission spectra of **2** dispersed in different  $\text{Na}_n\text{X}$  solutions.

Fig. S8 Emission spectra of **2** dispersed in different antibiotic solutions.

Fig. S9 Emission spectra of **2** dispersed in different pH values. Insert: the  ${}^5\text{D}_0 \rightarrow {}^7\text{F}_2$  (616nm) transition intensities. ( $\lambda_{\text{ex}} = 352$  nm).

Fig. S10 Emission spectra of **2** dispersed in pH = 3 acidic solutions upon incremental addition of  $\text{Fe}^{3+}$ (a),  $\text{Cr}_2\text{O}_7^{2-}$  (b), and MDZ(c) (1 mM, 30 uL addition each time), and Stern-Volmer plot of **2** for  $\text{Fe}^{3+}$ (d),  $\text{Cr}_2\text{O}_7^{2-}$  (e),  $\text{CrO}_4^{2-}$ (f). ( $\lambda_{\text{ex}} = 352$  nm)

Fig. S11 The luminescence intensity ( ${}^5\text{D}_0 \rightarrow {}^7\text{F}_2$ ) of three recyclable experiments of **2** for  $\text{Fe}^{3+}$ (a),  $\text{Cr}_2\text{O}_7^{2-}$ (b),  $\text{CrO}_4^{2-}$ (c), MDZ(d).

Fig. S12 UV-vis spectra of Phen ligand, 2,3'-oba (a), various cations (b), various anions (c), and MDZ(d).

Fig. S13 FT-IR of **2** and **2** immersed in MDZ.

Fig. S14 PXRD patterns of **2**@ $\text{Fe}^{3+}$ ,  $\text{Cr}_2\text{O}_7^{2-}$ ,  $\text{CrO}_4^{2-}$  and MDZ after water washing.

Fig. S15 EDS of **2** after immersing in  $\text{Fe}^{3+}$  aqueous solution.

Fig. S16 HOMO and LUMO energies for antibiotics arranged in ascending order of HUMO energies.

Table S1 Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] of **1-4** selected.

Table S2 **HOMO** and **LUMO** energies value of antibiotics.

2. The solvent sensing experiment was performed as follows: Complex **2** (2.5 mg) was immersed in different organic solvents (3 mL), treated by ultrasonication for 30 minutes, including formaldehyde, ethyl acetate, isopropanol, dimethylformamide (DMF), water, acetonitrile, benzene, acetone, dimethyl sulfoxide (DMSO), xylene, ethanol, methanol and benzaldehyde.

The metal ions sensing experiment was performed as follows: Complex **2** (2.5 mg) was immersed in aqueous solution ( $10^{-2}$  mol/L, 10mL) of  $M(NO_3)_n$  ( $M^{n+} = Fe^{2+}, Ca^{2+}, K^+, Cr^{3+}, Ba^{2+}, Al^{3+}, Mg^{2+}, Ni^{2+}, Na^+, Li^+, Co^{2+}, Cd^{2+}, Ag^+, Zn^{2+}, Cu^{2+}$  and  $Fe^{3+}$ ), treated by ultrasonication for 30 min.

The anions sensing experiment was performed as follows: Complex **2** (2.5 mg) was immersed in aqueous solution ( $10^{-2}$  mol/L, 3mL) of  $Na_nX$  ( $Na_nX = NO_3^-, SO_4^{2-}, ClO_4^-, SCN^-, Br^-, I^-, Cl^-, HSO_3^-, NO_2^-, SO_3^{2-}, Cr_2O_7^{2-}$  and  $CrO_4^{2-}$ ), treated by ultrasonication for 30 min.

The antibiotics sensing experiment was performed as follows: Complex **2** (2.5 mg) was immersed in aqueous solution ( $10^{-2}$  mol/L, 3mL) of antibiotics, including sulfamethazine (SMZ), sulfadiazine (SDZ), thiamphenicol (THI), metronidazole (MDZ), dithiazoline (DTZ), chloramphenicol (CAP), nitrofurantoin (NFT) and nitrofurazone (NFZ).

Fig. S1

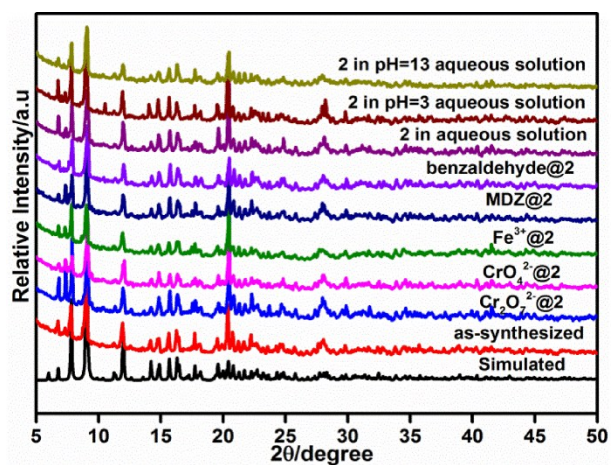


Fig. S2

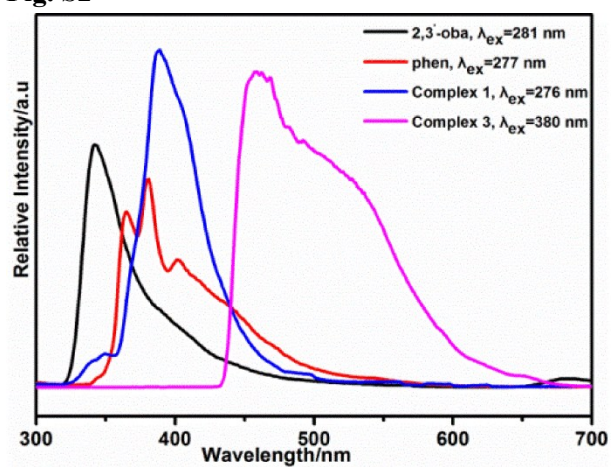


Fig. S3

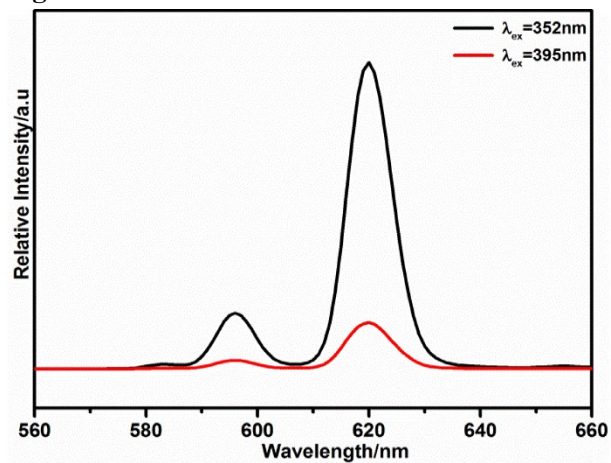


Fig. S4

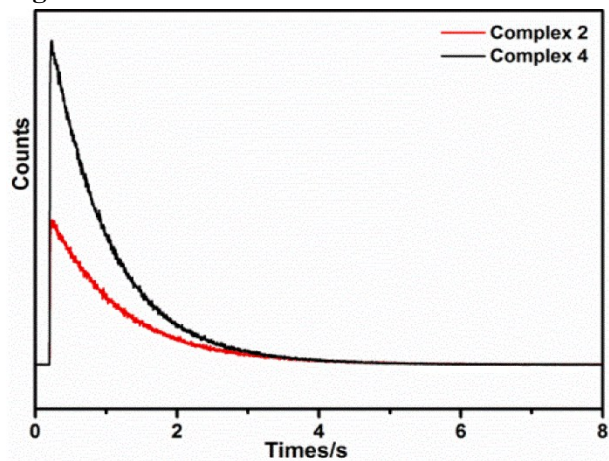


Fig. S5

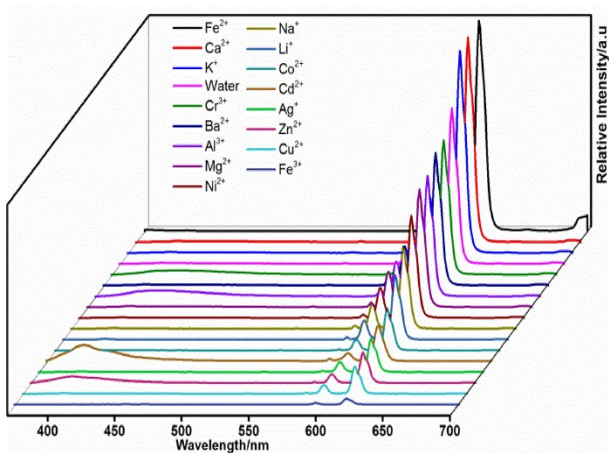


Fig. S6

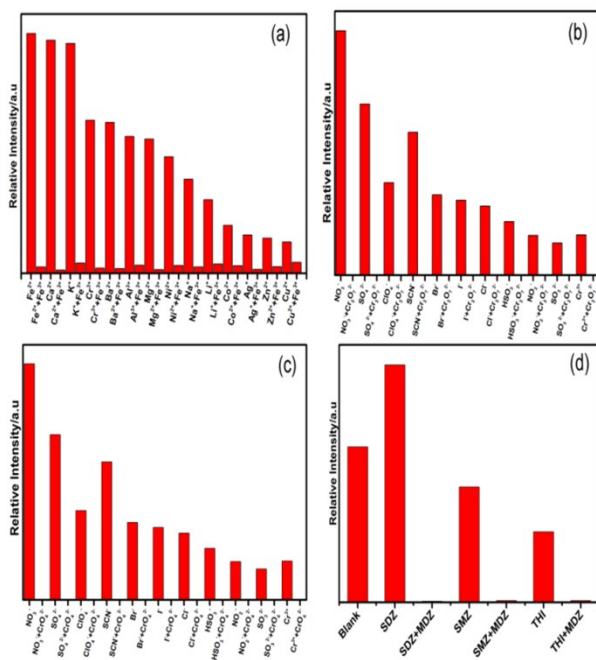


Fig. S7

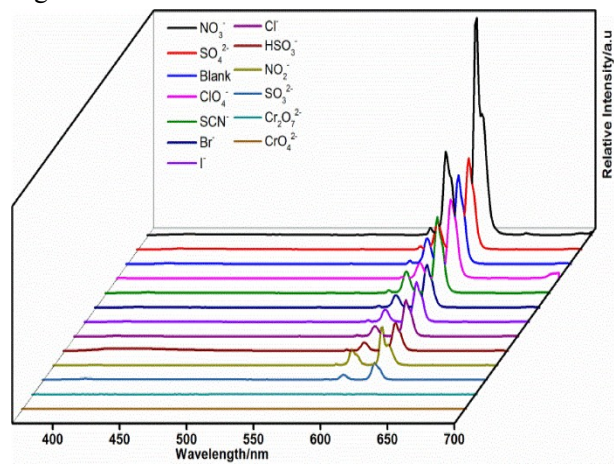


Fig. S8

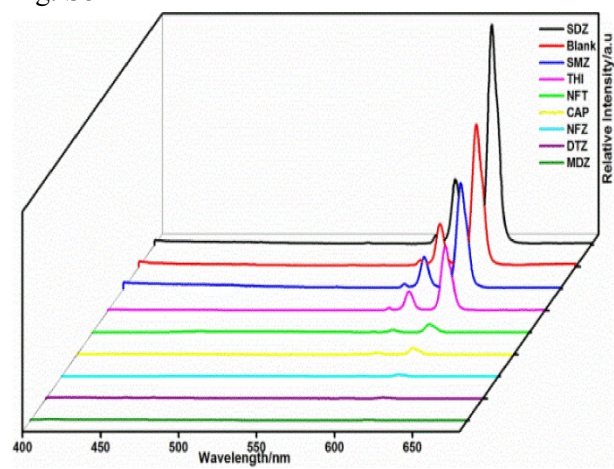


Fig. S9

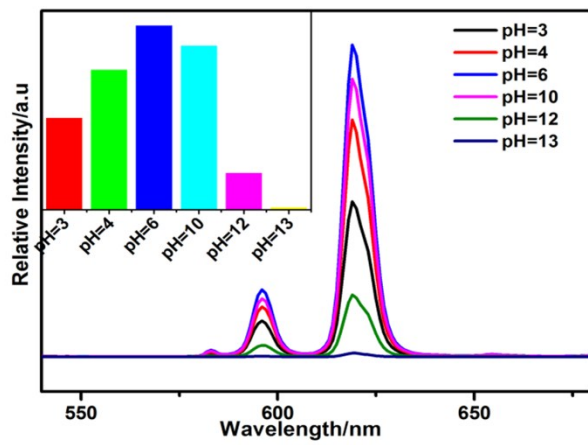


Fig. S10

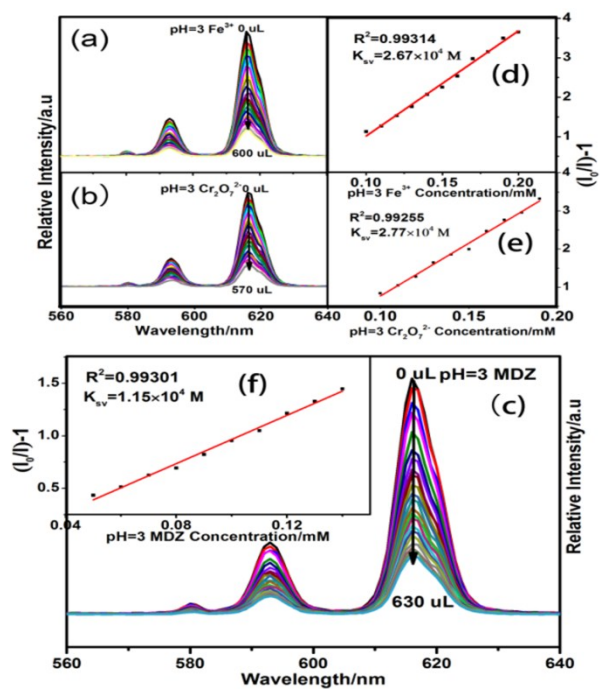


Fig. S11

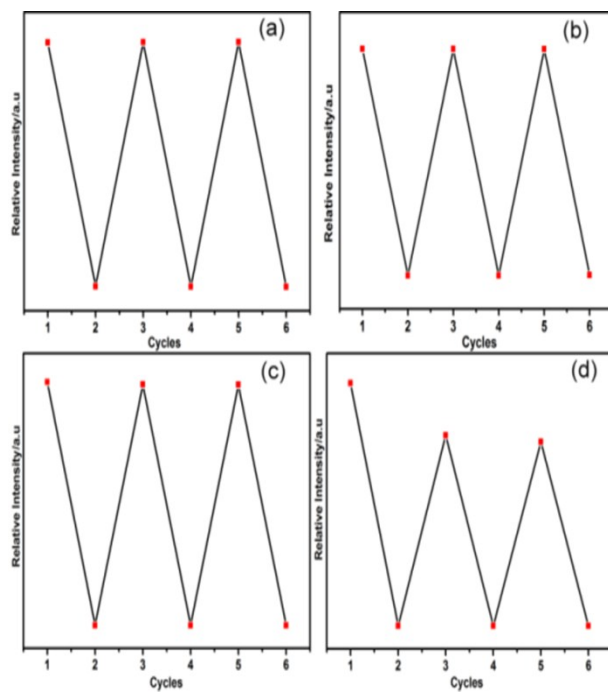


Fig. S12

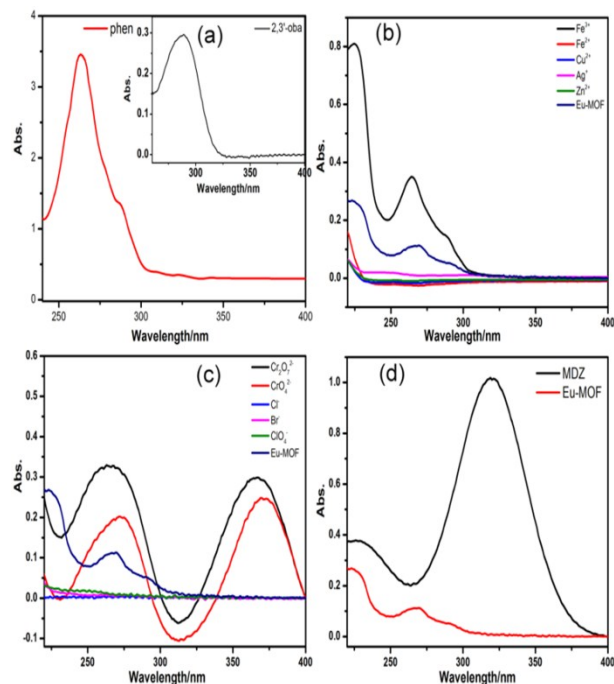


Fig. S13

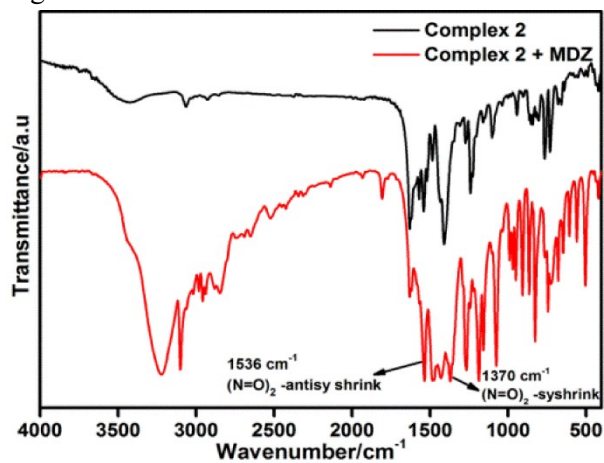


Fig. S14

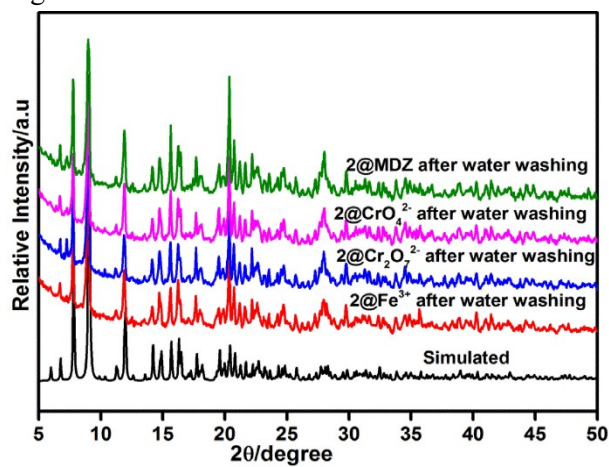


Fig. S15

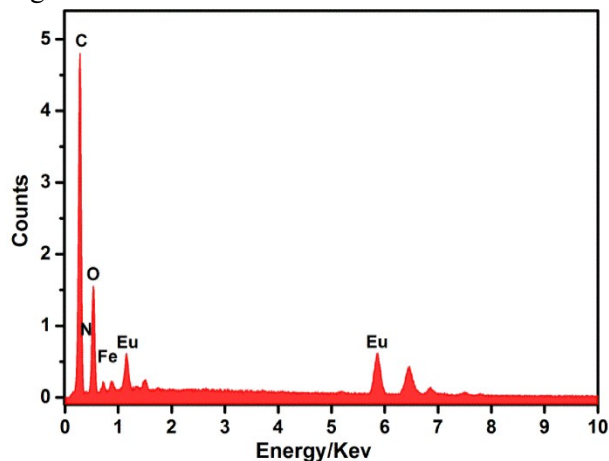


Fig. S16

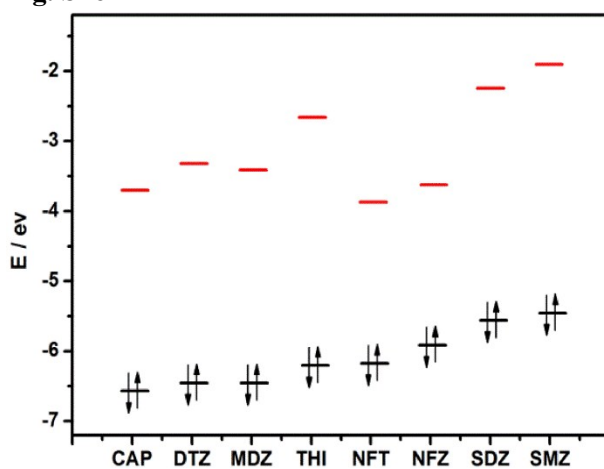


Table S1

1			
La(1)-La(1)#1	4.0991(5)	La(2)-La(2)#2	4.2291(5)
La(1)-O(10)	2.601(3)	La(2)-O(7)#2	2.528(3)
La(1)-O(14)	2.480(3)	La(2)-O(7)	2.676(3)
La(1)-O(11)	2.494(3)	La(2)-O(2)	2.431(3)
La(1)-N(1)	2.689(4)	La(2)-N(4)	2.712(4)
La(1)-O(9)	2.512(3)	La(2)-O(5)	2.638(3)
La(1)-O(12)	2.438(3)	La(2)-O(3)	2.559(3)
La(1)-O(13)	2.945(3)	La(2)-O(6)	2.575(3)
La(1)-O(13)#1	2.471(3)	La(2)-N(3)	2.716(4)
La(1)-N(2)	2.736(4)	La(2)-O(4)	2.534(3)
O(10)-La(1)-N(1)	92.13(11)	O(7)#2-La(2)-O(7)	71.31(11)
O(10)-La(1)-O(13)	124.87(10)	O(7)#2-La(2)-N(4)	81.83(11)
O(10)-La(1)-N(2)	74.25(10)	O(7)-La(2)-N(4)	142.52(11)
O(14)-La(1)-O(10)	87.77(11)	O(7)#2-La(2)-O(5)	150.66(11)
O(14)-La(1)-O(11)	81.71(12)	O(7)#2-La(2)-O(3)	67.69(10)
O(14)-La(1)-N(1)	131.57(12)	O(7)#2-La(2)-O(6)	118.10(10)
O(14)-La(1)-O(9)	135.38(11)	O(7)#2-La(2)-N(3)	93.13(11)



O(14)-La(1)-O(13)	46.71(10)	O(7)-La(2)-N(3)	143.92(11)
O(14)-La(1)-N(2)	73.10(11)	O(7)#2-La(2)-O(4)	152.26(11)
O(11)-La(1)-O(10)	74.52(10)	O(2)-La(2)-O(7)	72.68(10)
O(11)-La(1)-N(1)	144.35(12)	O(2)-La(2)-O(7)#2	73.70(11)
O(11)-La(1)-O(9)	72.02(11)	O(2)-La(2)-N(4)	124.55(12)
O(11)-La(1)-O(13)	70.30(10)	O(2)-La(2)-O(5)	77.57(11)
O(11)-La(1)-N(2)	140.24(11)	O(2)-La(2)-O(3)	132.86(10)
N(1)-La(1)-O(13)	139.26(10)	O(2)-La(2)-O(6)	100.22(12)
N(1)-La(1)-N(2)	60.47(12)	O(2)-La(2)-N(3)	71.73(12)
O(9)-La(1)-O(10)	51.11(10)	O(2)-La(2)-O(4)	124.85(11)
O(9)-La(1)-N(1)	73.93(12)	N(4)-La(2)-N(3)	60.68(13)
O(9)-La(1)-O(13)	140.98(10)	O(5)-La(2)-O(7)	105.67(11)
O(9)-La(1)-N(2)	105.52(11)	O(5)-La(2)-N(4)	110.42(12)
O(12)-La(1)-O(10)	148.54(10)	O(5)-La(2)-N(3)	72.07(12)
O(12)-La(1)-O(14)	83.80(12)	O(3)-La(2)-O(7)	70.13(10)
O(12)-La(1)-O(11)	133.49(11)	O(3)-La(2)-N(4)	75.78(12)
O(12)-La(1)-N(1)	71.70(11)	O(3)-La(2)-O(5)	140.14(11)
O(12)-La(1)-O(9)	139.98(11)	O(3)-La(2)-O(6)	76.25(11)
O(12)-La(1)-O(13)#1	76.20(11)	O(3)-La(2)-N(3)	134.74(12)
O(12)-La(1)-O(13)	67.67(10)	O(6)-La(2)-O(7)	49.37(10)
O(12)-La(1)-N(2)	74.30(11)	O(6)-La(2)-N(4)	135.07(13)
O(13)#1-La(1)-O(10)	130.69(10)	O(6)-La(2)-O(5)	72.67(12)
O(13)#1-La(1)-O(14)	128.68(11)	O(6)-La(2)-N(3)	144.74(12)
O(13)#1-La(1)-O(11)	79.16(11)	O(4)-La(2)-O(7)	130.78(10)
O(13)#1-La(1)-N(1)	85.69(11)	O(4)-La(2)-N(4)	70.61(11)
O(13)#1-La(1)-O(9)	81.42(11)	O(4)-La(2)-O(5)	49.97(11)
O(13)#1-La(1)-O(13)	81.99(11)	O(4)-La(2)-O(3)	101.43(11)
O(13)#1-La(1)-N(2)	140.53(11)	O(4)-La(2)-O(6)	81.41(11)
N(2)-La(1)-O(13)	109.73(10)	O(4)-La(2)-N(3)	76.42(12)

Symmetry transformations used to generate equivalent atoms: 1, #1 -x,-y+1,-z;  
#2 -x+1,-y+1,-z+1.

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**2**

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Eu(1)-Eu(1)#1	4.1475(6)	Eu(2)-Eu(2)#2	3.9251(6)
Eu(1)-N(1)	2.650(5)	Eu(2)-N(3)	2.555(5)
Eu(1)-N(2)	2.547(5)	Eu(2)-N(4)	2.647(4)
Eu(1)-O(1)	2.362(4)	Eu(2)-O(3)	2.446(3)
Eu(1)-O(2)#1	2.335(4)	Eu(2)-O(4)	2.452(4)
Eu(1)-O(6)	2.488(4)	Eu(2)-O(8)#2	2.385(4)
Eu(1)-O(7)	2.400(3)	Eu(2)-O(8)	2.642(4)
Eu(1)-O(11)	2.360(4)	Eu(2)-O(9)	2.476(4)
Eu(1)-O(12)#1	2.330(4)	Eu(2)-O(13)	2.398(3)
		Eu(2)-O(14)#2	2.350(4)
N(2)-Eu(1)-N(1)	63.02(15)	O(3)-Eu(2)-O(4)	53.17(12)

O(1)-Eu(1)-N(1)	66.78(14)	O(3)-Eu(2)-O(8)	156.51(12)
O(1)-Eu(1)-N(2)	78.34(16)	O(3)-Eu(2)-O(9)	144.07(13)
O(1)-Eu(1)-O(6)	143.60(14)	O(4)-Eu(2)-N(3)	72.27(14)
O(1)-Eu(1)-O(7)	139.85(15)	O(4)-Eu(2)-N(4)	120.09(14)
O(2)#1-Eu(1)-N(1)	145.99(16)	O(4)-Eu(2)-O(8)	137.44(11)
O(2)#1-Eu(1)-N(2)	141.82(16)	O(4)-Eu(2)-O(9)	134.66(13)
O(2)#1-Eu(1)-O(1)	129.13(16)	O(8)#2-Eu(2)-N(3)	148.29(14)
O(2)#1-Eu(1)-O(6)	73.39(13)	O(8)#2-Eu(2)-N(4)	141.75(13)
O(2)#1-Eu(1)-O(7)	86.45(16)	O(8)-Eu(2)-N(4)	101.16(13)
O(2)#1-Eu(1)-O(11)	74.97(14)	O(8)#2-Eu(2)-O(3)	88.11(12)
O(6)-Eu(1)-N(1)	112.39(13)	O(8)#2-Eu(2)-O(4)	76.34(13)
O(6)-Eu(1)-N(2)	70.48(14)	O(8)#2-Eu(2)-O(8)	77.43(13)
O(7)-Eu(1)-N(1)	73.10(13)	O(8)#2-Eu(2)-O(9)	126.92(12)
O(7)-Eu(1)-N(2)	82.23(14)	O(8)#2-Eu(2)-O(13)	80.14(12)
O(7)-Eu(1)-O(6)	53.93(12)	O(9)-Eu(2)-N(3)	75.39(14)
O(11)-Eu(1)-N(1)	77.19(13)	O(9)-Eu(2)-N(4)	68.42(13)
O(11)-Eu(1)-N(2)	140.20(15)	O(9)-Eu(2)-O(8)	50.36(11)
O(11)-Eu(1)-O(1)	85.55(15)	O(13)-Eu(2)-N(3)	86.87(14)
O(11)-Eu(1)-O(6)	130.66(12)	O(13)-Eu(2)-N(4)	135.84(14)
O(11)-Eu(1)-O(7)	87.45(13)	O(13)-Eu(2)-O(3)	126.85(13)
O(12)#1-Eu(1)-N(1)	133.75(15)	O(13)-Eu(2)-O(4)	73.70(12)
O(12)#1-Eu(1)-N(2)	81.48(15)	O(13)-Eu(2)-O(8)	69.21(11)
O(12)#1-Eu(1)-O(1)	78.29(15)	O(13)-Eu(2)-O(9)	73.63(12)
O(12)#1-Eu(1)-O(2)#1	79.94(17)	O(14)#2-Eu(2)-N(3)	132.35(14)
O(12)#1-Eu(1)-O(6)	78.94(13)	O(14)#2-Eu(2)-N(4)	71.62(14)
O(12)#1-Eu(1)-O(7)	132.87(14)	O(14)#2-Eu(2)-O(3)	82.24(13)
O(12)#1-Eu(1)-O(11)	130.56(13)	O(14)#2-Eu(2)-O(4)	124.91(13)
N(3)-Eu(2)-N(4)	62.65(15)	O(14)#2-Eu(2)-O(8)	75.63(12)
N(3)-Eu(2)-O(8)	124.48(13)	O(14)#2-Eu(2)-O(8)#2	71.07(12)
O(3)-Eu(2)-N(3)	76.75(14)	O(14)#2-Eu(2)-O(9)	100.36(13)
O(3)-Eu(2)-N(4)	78.82(13)	O(14)#2-Eu(2)-O(13)	138.46(12)

Symmetry transformations used to generate equivalent atoms:**2**, #1 -x+1,-y+1,-z+1;  
#2 -x,-y+2,-z+1.

3

Gd(1)-O(12)	2.480(3)	Gd(2)-Gd(2)#1	3.9165(5)
Gd(1)-O(14)	2.353(3)	Gd(2)-O(6)	2.399(3)
Gd(1)-O(11)	2.385(3)	Gd(2)-O(4)	2.484(4)
Gd(1)-O(9)	2.354(4)	Gd(2)-O(3)	2.638(3)
Gd(1)-C(54)	2.786(5)	Gd(2)-O(3)#1	2.377(3)
Gd(1)-O(10)	2.329(3)	Gd(2)-O(7)	2.345(3)
Gd(1)-O(13)	2.326(4)	Gd(2)-O(2)	2.451(3)
Gd(1)-N(1)	2.634(4)	Gd(2)-O(1)	2.438(3)
Gd(1)-N(2)	2.553(4)	Gd(2)-N(3)	2.635(4)
		Gd(2)-N(4)	2.552(4)

O(12)-Gd(1)-N(1)	113.03(11)	O(6)-Gd(2)-O(1)	127.53(11)
O(12)-Gd(1)-N(2)	70.89(13)	O(6)-Gd(2)-C(13)	66.43(12)
O(14)-Gd(1)-N(1)	76.62(12)	O(6)-Gd(2)-N(3)	135.67(12)
O(14)-Gd(1)-O(12)	130.70(12)	O(4)-Gd(2)-O(3)	50.27(11)
O(14)-Gd(1)-O(11)	87.67(12)	O(4)-Gd(2)-N(4)	75.76(12)
O(14)-Gd(1)-N(2)	140.07(13)	O(4)-Gd(2)-N(3)	68.56(12)
O(11)-Gd(1)-N(1)	73.79(12)	O(3)#1-Gd(2)-O(6)	80.11(11)
O(11)-Gd(1)-O(12)	53.62(11)	O(3)#1-Gd(2)-O(4)	126.74(11)
O(11)-Gd(1)-N(2)	82.66(13)	O(3)#1-Gd(2)-O(3)	77.42(12)
N(2)-Gd(1)-N(1)	63.47(13)	O(3)#1-Gd(2)-N(4)	147.47(13)
O(9)-Gd(1)-N(1)	67.23(13)	O(3)#1-Gd(2)-O(2)	75.90(12)
O(9)-Gd(1)-O(12)	144.65(13)	O(3)#1-Gd(2)-O(1)	88.37(11)
O(9)-Gd(1)-O(14)	84.55(14)	O(3)#1-Gd(2)-N(3)	141.85(12)
O(9)-Gd(1)-O(11)	141.01(13)	N(4)-Gd(2)-O(3)	124.65(11)
O(9)-Gd(1)-N(2)	79.27(14)	N(4)-Gd(2)-N(3)	63.54(14)
O(10)-Gd(1)-N(1)	134.17(14)	O(7)-Gd(2)-O(6)	137.90(11)
O(10)-Gd(1)-O(12)	79.19(12)	O(7)-Gd(2)-O(4)	100.36(13)
O(10)-Gd(1)-O(14)	130.09(13)	O(7)-Gd(2)-O(3)	75.21(11)
O(10)-Gd(1)-O(11)	132.80(13)	O(7)-Gd(2)-O(3)#1	70.92(11)
O(10)-Gd(1)-N(2)	81.79(14)	O(7)-Gd(2)-N(4)	133.50(13)
O(10)-Gd(1)-O(9)	78.16(14)	O(7)-Gd(2)-O(2)	124.70(12)
O(13)-Gd(1)-N(1)	145.38(14)	O(7)-Gd(2)-O(1)	82.30(11)
O(13)-Gd(1)-O(12)	73.05(13)	O(7)-Gd(2)-N(3)	71.89(12)
O(13)-Gd(1)-O(14)	74.96(13)	O(2)-Gd(2)-O(4)	134.90(12)
O(13)-Gd(1)-O(11)	85.66(15)	O(2)-Gd(2)-O(3)	137.37(11)
O(13)-Gd(1)-N(2)	141.98(14)	O(2)-Gd(2)-N(4)	71.99(13)
O(13)-Gd(1)-O(9)	128.32(14)	O(2)-Gd(2)-N(3)	120.40(12)
O(13)-Gd(1)-O(10)	80.04(16)	O(1)-Gd(2)-O(4)	143.96(12)
O(6)-Gd(2)-O(4)	73.17(12)	O(1)-Gd(2)-O(3)	156.30(11)
O(6)-Gd(2)-O(3)	69.02(10)	O(1)-Gd(2)-N(4)	76.76(12)
O(6)-Gd(2)-N(4)	86.27(12)	O(1)-Gd(2)-O(2)	53.49(11)
O(6)-Gd(2)-O(2)	74.08(11)	O(1)-Gd(2)-N(3)	78.51(12)
O(6)-Gd(2)-C(14)	100.70(14)	N(3)-Gd(2)-O(3)	101.03(12)

Symmetry transformations used to generate equivalent atoms:**3**, #1 -x,-y+1,-z+2.

**4**

Tb(1)-O(1)#1	2.331(3)	Tb(2)-O(12)	2.440(4)
Tb(1)-O(9)#2	2.372(3)	Tb(2)-O(5)	2.326(3)
Tb(1)-O(10)#2	2.488(3)	Tb(2)-O(6)	2.364(4)
Tb(1)-O(15)#3	2.340(4)	Tb(2)-O(6)#5	2.635(3)
Tb(1)-O(14)#4	2.333(4)	Tb(2)-O(7)#5	2.468(4)
Tb(2)-O(4)#5	2.380(3)	Tb(2)-O(11)	2.423(3)
Tb(1)-N(1)	2.627(4)	Tb(2)-N(3)	2.617(4)
Tb(1)-N(2)	2.529(4)	Tb(2)-N(4)	2.544(4)

Tb(1)-O(2)	2.317(4)		
O(1)#1-Tb(1)-O(9)#2	87.93(13)	O(5)-Tb(2)-O(12)	124.57(12)
O(1)#1-Tb(1)-O(10)#2	131.51(13)	O(5)-Tb(2)-O(6)#5	75.21(11)
O(1)#1-Tb(1)-N(1)	76.55(12)	O(5)-Tb(2)-O(6)	71.48(12)
O(1)#1-Tb(1)-O(15)#3	74.43(13)	O(5)-Tb(2)-O(7)#5	100.27(13)
O(1)#1-Tb(1)-O(14)#4	83.82(14)	O(5)-Tb(2)-O(4)#5	138.37(11)
O(1)#1-Tb(1)-N(2)	140.33(13)	O(5)-Tb(2)-O(11)	82.42(12)
O(9)#2-Tb(1)-O(10)#2	53.86(12)	O(5)-Tb(2)-N(4)	133.34(14)
O(9)#2-Tb(1)-N(1)	74.00(13)	O(5)-Tb(2)-N(3)	71.56(13)
O(9)#2-Tb(1)-N(2)	82.86(14)	O(6)#5-Tb(2)-Tb(2)#5	36.20(8)
O(10)#2-Tb(1)-N(1)	113.00(12)	O(6)-Tb(2)-O(12)	75.42(12)
O(10)#2-Tb(1)-N(2)	70.25(14)	O(6)-Tb(2)-O(6)#5	77.37(13)
N(1)-Tb(1)-C(40)#2	94.15(14)	O(6)-Tb(2)-O(7)#5	126.89(12)
O(15)#3-Tb(1)-O(9)#2	85.65(15)	O(6)-Tb(2)-O(4)#5	79.79(12)
O(15)#3-Tb(1)-O(10)#2	74.06(13)	O(6)-Tb(2)-O(11)	88.49(12)
O(15)#3-Tb(1)-N(1)	144.93(14)	O(6)-Tb(2)-N(4)	147.03(14)
O(15)#3-Tb(1)-N(2)	142.40(14)	O(6)-Tb(2)-N(3)	142.07(13)
O(14)#4-Tb(1)-O(9)#2	141.23(14)	O(7)#5-Tb(2)-O(6)#5	50.52(11)
O(14)#4-Tb(1)-O(10)#2	144.57(13)	O(7)#5-Tb(2)-N(4)	75.84(13)
O(14)#4-Tb(1)-N(1)	67.23(14)	O(7)#5-Tb(2)-N(3)	68.47(13)
O(14)#4-Tb(1)-O(15)#3	127.62(14)	O(4)#5-Tb(2)-O(12)	73.71(13)
O(14)#4-Tb(1)-N(2)	79.83(15)	O(4)#5-Tb(2)-O(6)#5	69.48(11)
N(2)-Tb(1)-N(1)	63.82(13)	O(4)#5-Tb(2)-O(7)#5	73.60(13)
O(2)-Tb(1)-O(1)#1	129.27(14)	O(4)#5-Tb(2)-O(11)	126.97(12)
O(2)-Tb(1)-O(9)#2	133.26(13)	O(4)#5-Tb(2)-N(4)	86.09(13)
O(2)-Tb(1)-O(10)#2	79.40(13)	O(4)#5-Tb(2)-N(3)	135.89(13)
O(2)-Tb(1)-N(1)	134.31(14)	O(11)-Tb(2)-O(12)	53.31(12)
O(2)-Tb(1)-O(15)#3	80.17(16)	O(11)-Tb(2)-O(6)#5	156.37(11)
O(2)-Tb(1)-O(14)#4	78.06(14)	O(11)-Tb(2)-O(7)#5	143.77(13)
O(2)-Tb(1)-N(2)	82.04(14)	O(11)-Tb(2)-N(4)	76.47(12)
O(12)-Tb(2)-O(6)#5	137.26(12)	O(11)-Tb(2)-N(3)	78.53(13)
O(12)-Tb(2)-O(7)#5	135.12(13)	N(4)-Tb(2)-O(6)#5	124.94(12)
O(12)-Tb(2)-N(4)	72.05(14)	N(4)-Tb(2)-N(3)	63.75(14)
O(12)-Tb(2)-N(3)	120.58(13)	N(3)-Tb(2)-O(6)#5	101.06(12)

Symmetry transformations used to generate equivalent atoms: 4, #1 -x+2,-y,-z; #2 x,y,z-1; #3 -x+1,y-1/2,-z+1/2; #4 x+1,-y+1/2,z-1/2; #5 -x+1,-y,-z+1.

**Table S2**

Analytes	HUMO(ev)	LUMO(ev)
CAP	-6.579	-3.692
DTZ	-6.427	-3.336
MDZ	-6.42	-3.425
THI	-6.206	-2.661

NFT	-6.205	-3.864
NFZ	-5.905	-3.624
SDZ	-5.538	-2.26
SMZ	-5.457	-1.898

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