Supporting Information

A stable LnMOF as a highly efficient and selective luminescent sensor for detecting malachite green in water and real samples

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1. Figure captions:

Table S4 HOMO and LUMO energy levels of selected antibiotics.

2. The antibiotics sensing experiment was performed as follows: Compound **3** (5 mg) was immersed in aqueous solution (0.01 mol/L, 3 mL) of antibiotics, including Ciprofloxacin (CPFX), Lincomycin hydrochloride (LIN), Penicillin (PCL), Azithromycin (AZM), Roxithromycin (ROX), Potassium antimony tartrate (PAT), Malachite green (MG), and treated by ultrasonication for 30 min.

Fig. S1

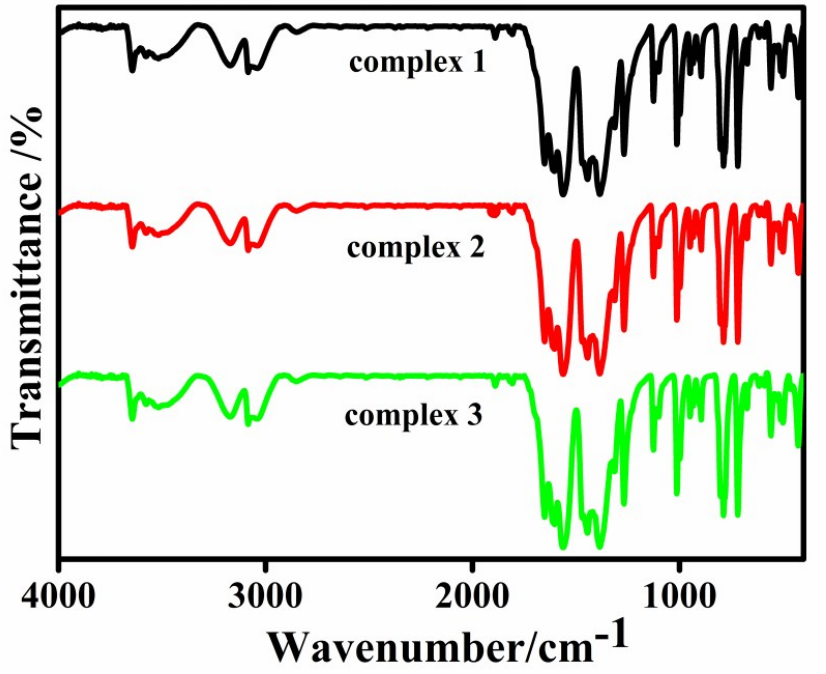


Fig. S2

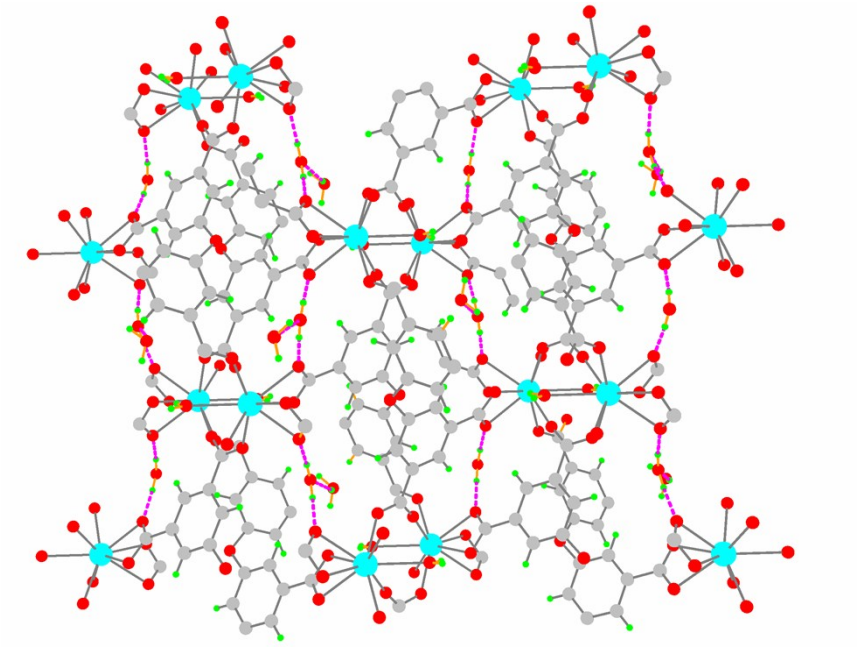
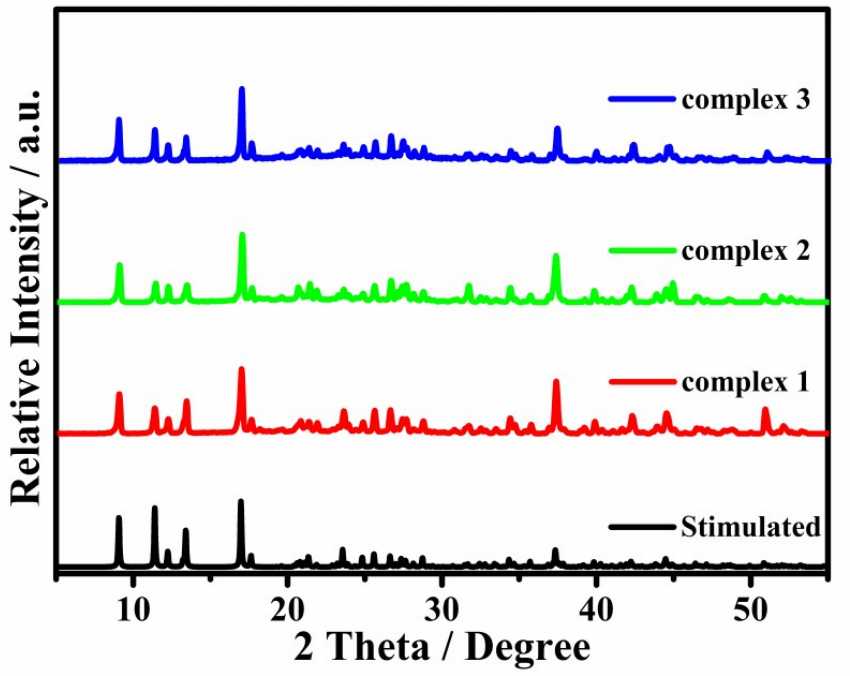


Fig. S3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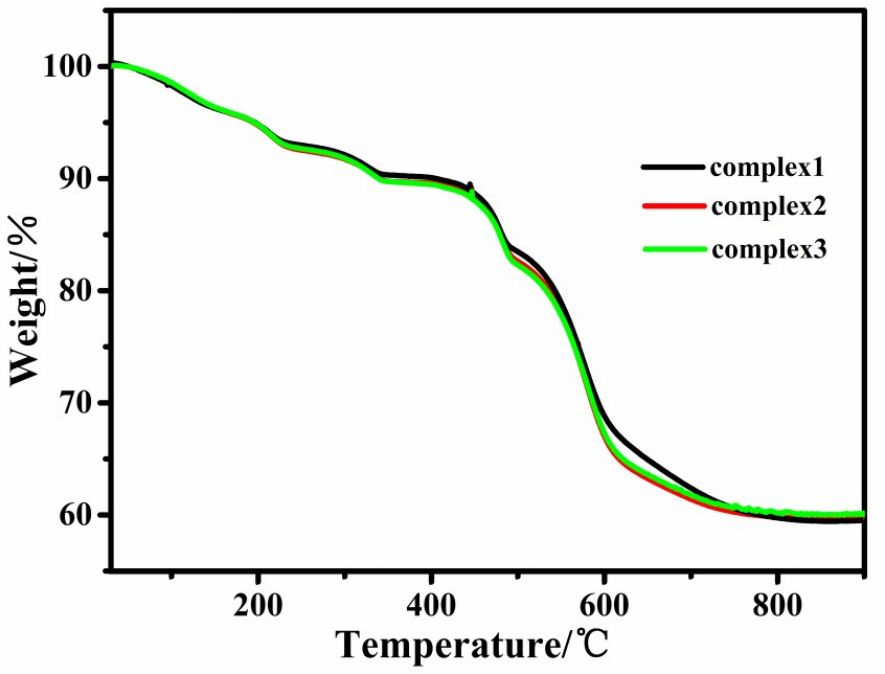
complex 2
complex 1
Stimulated
Relative Intensity / a.u.
10
20
30
40
50
2 Theta / Degree

Fig.S4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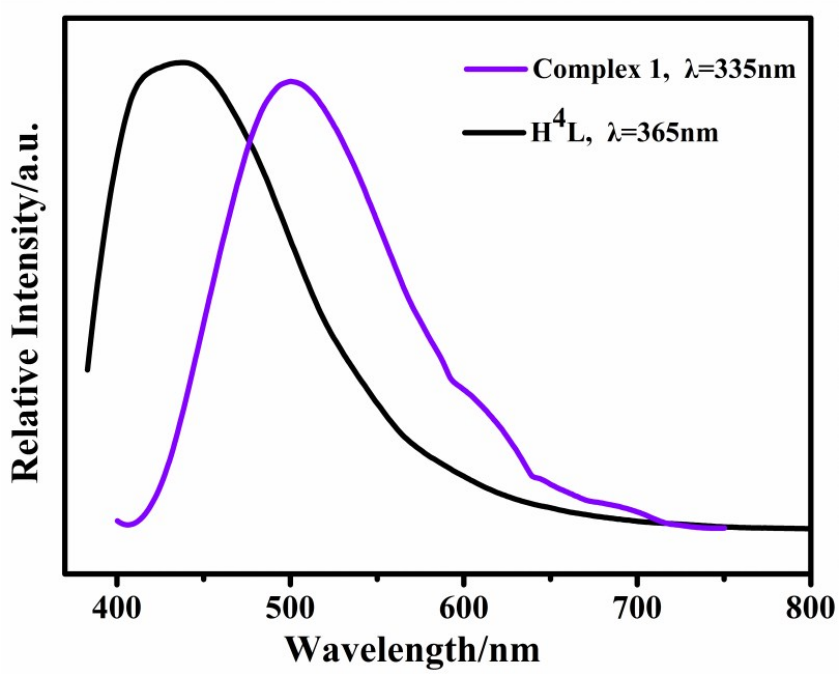
complex2
complex3
Weight/%
100
90
80
70
60
200
400
600
800
Temperature/℃

Fig. S5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H4L, λ=365nm
Relative Intensity/a.u.
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500
600
700
800
Wavelength/nm

Fig.S6

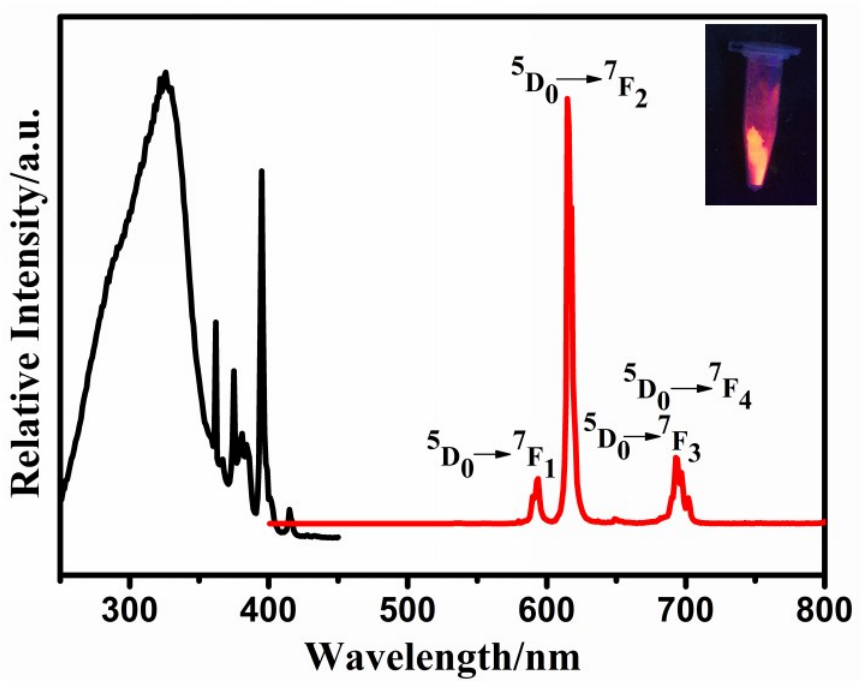

5D0→7F2
5D0→7F4
5D0→7F3
5D0→7F1
Relative Intensity/a.u.
300
400
500
600
700
800
Wavelength/nm

Fig.S7

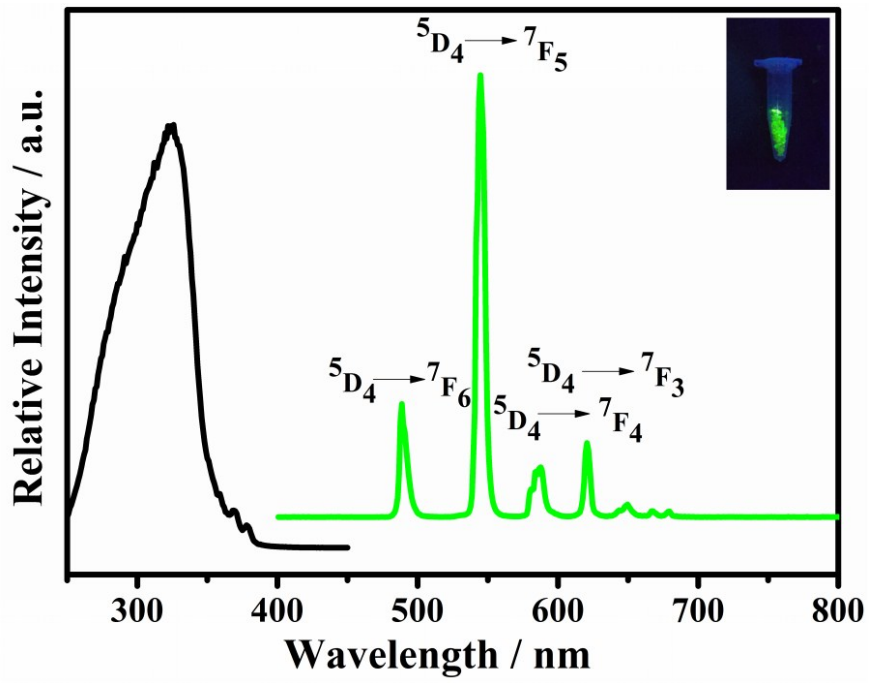
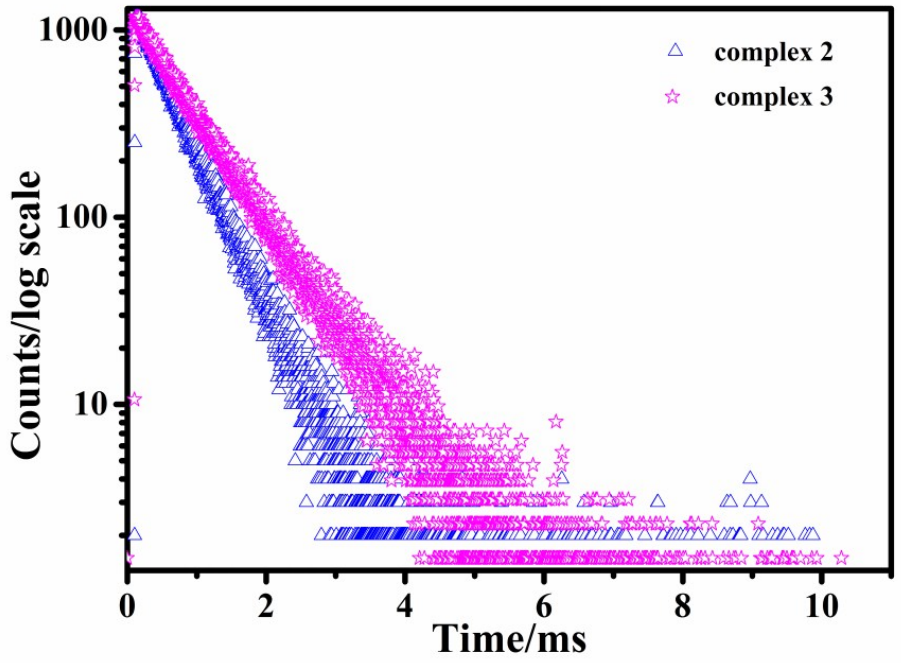

Relative Intensity / a.u.
Wavelength / nm
300
400
500
600
700
800
$^5D_4 \rightarrow {}^7F_5$
$^5D_4 \rightarrow {}^7F_6$
$^5D_4 \rightarrow {}^7F_4$
$^5D_4 \rightarrow {}^7F_3$

Fig. S8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0
2
4
6
8
10
complex 2
complex 3

Fig. S9

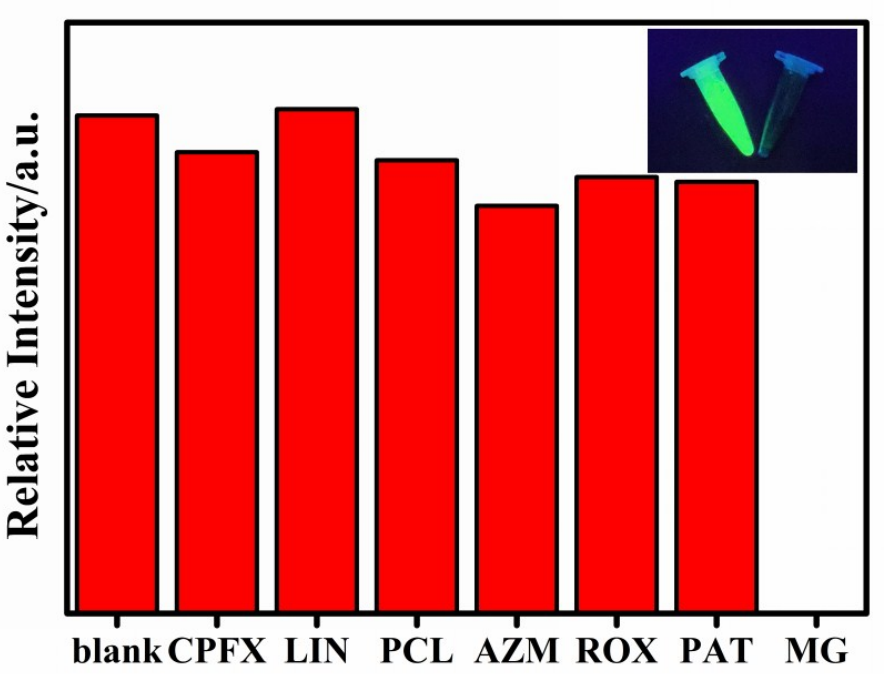


Fig. S10

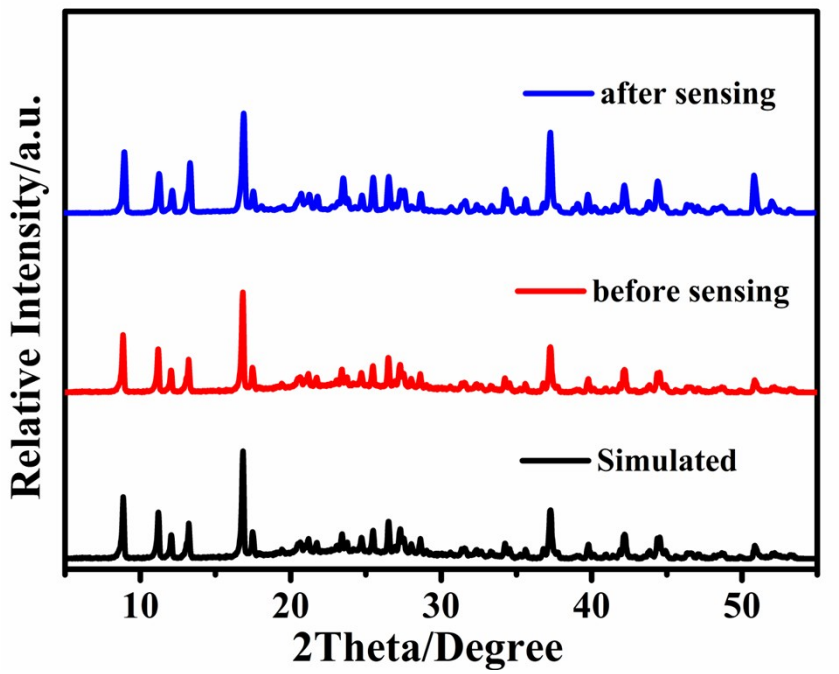


Fig. S11

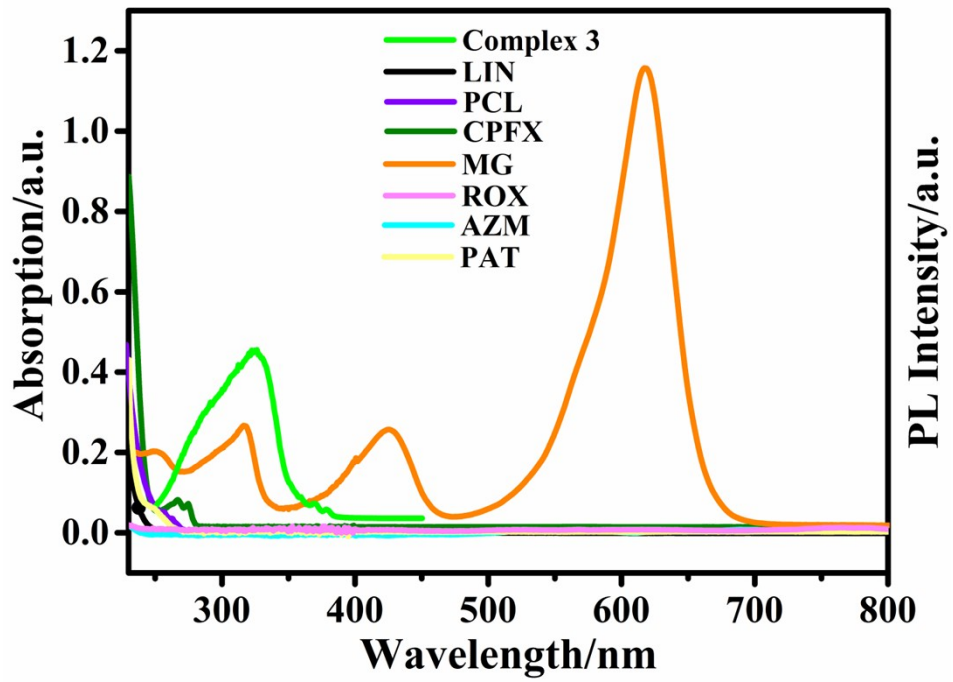
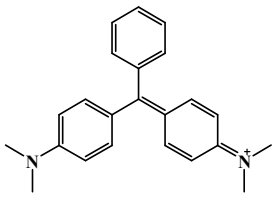
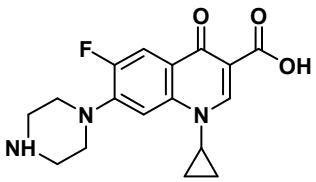
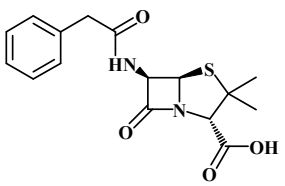


Table. S1

Kind	Name	Chemical Structure
Triphenylmethane	Malachite green (MG)	
Quinolones	Ciprofloxacin (CPFX)	
β-Lactams	Penicillin (PCL)	

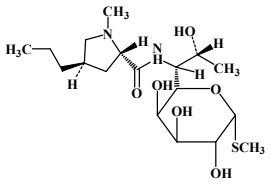
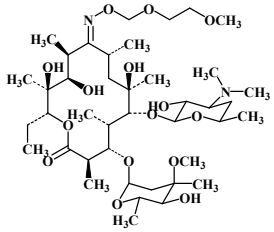
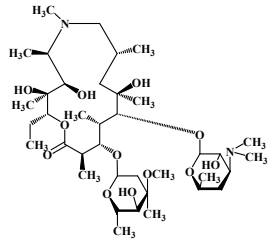
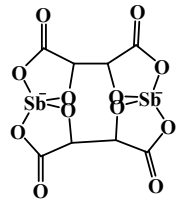
Lincosamides	Lincomycin hydrochloride (LIN)	
macrolides	Roxithromycin (ROX)	
	Azithromycin (AZM)	
Others	Potassium antimony tartrate (PAT)	

Table S2

Compounds	**1**	**2**	**3**
Empirical formula	$C_{16}H_{13}GdO_{12}$	$C_{16}H_{13}EuO_{12}$	$C_{16}H_{13}TbO_{12}$
Formula weight	554.51	549.23	556.19
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	*P*nna	*P*nna	*P*nna
a (Å)	9.1964(18)	9.2104(18)	9.1988(18)
b (Å)	13.197(3)	13.203(3)	13.161(3)
c (Å)	14.447(3)	14.465(3)	14.406(3)
V (Å^3)	1753.4(6)	1759.0(6)	1744.1(6)

Z	4	4	4
D_{calcd} (g·cm^{-3})	2.101	2.074	2.118
μ (mm^{-1})	3.851	3.634	4.124
F(000)	1076.0	1072.0	1080.0
Temperature (K)	293	293	293
Refln. measured	18298	18527	17928
Independent refln.	3212	3197	3172
Observed refln.	3122	3137	3093
GOF	1.135	1.138	1.106
R_1[a] [$I > 2\sigma(I)$]	0.0233	0.0239	0.0293
wR_2[b]	0.0530	0.0529	0.0730
$\Delta\rho_{max}$/ $\Delta\rho_{min}$ (e.Å^3)	0.523/-1.328	0.527/–0.961	1.584/-1.443

Table S3

Compound **1**			
Gd(1)-O(1)^{i}	2.4705 (14)	Gd(1)-O(3)	2.3562 (15)
Gd(1)-O(1)^{ii}	2.4705 (14)	Gd(1)-O(3)^{iii}	2.3562 (15)
Gd(1)-O(2)^{i}	2.5904 (18)	Gd(1)-O(4)^{iv}	2.3525 (15)
Gd(1)-O(2)^{ii}	2.5904 (18)	Gd(1)-O(4)^{v}	2.3525 (15)
Gd(1)-O(6)	2.590 (3)	O(1)^{ii}-Gd(1)-O(1)^{i}	75.53 (7)
O(1)^{i}-Gd(1)-O(6)	142.24 (4)	O(1)^{i}-Gd(1)-O(2)^{i}	51.61 (5)
O(1)^{i}-Gd(1)-O(2)^{ii}	68.67 (6)	O(2)^{i}-Gd(1)-O(2)^{ii}	102.97 (9)
O(3)-Gd(1)-O(3)^{iii}	154.21 (8)	O(3)-Gd(1)-O(1)^{i}	122.18 (5)
O(3)-Gd(1)-O(1)^{ii}	79.65 (5)	O(3)-Gd(1)-O(6)	77.11 (4)
O(3)-Gd(1)-O(2)^{i}	70.82 (5)	O(3)-Gd(1)-O(2)^{ii}	127.34 (5)

O(4)^{iv}-Gd(1)-O(4)^{v}	141.92 (9)	O(4)^{iv}-Gd(1)-O(3)	80.13 (6)
O(4)^{iv}-Gd(1)-O(3)^{iii}	91.47 (6)	O(4)^{iv}-Gd(1)-O(1)^{ii}	76.05 (6)
O(4)^{iv}-Gd(1)-O(2)^{i}	137.37 (6)	O(4)^{iv}-Gd(1)-O(2)^{ii}	70.77 (7)
O(4)^{iv}-Gd(1)-O(1)^{i}	139.18 (6)	O(4)^{v}-Gd(1)-O(3)	91.48 (6)
O(4)^{v}-Gd(1)-O(3)^{iii}	80.13 (6)	O(6)-Gd(1)-O(4)^{iv}	70.96 (5)
Compound **2**			
Eu(1)-O(1)^{i}	2.4821 (14)	Eu(1)-O(3)	2.3645 (16)
Eu(1)-O(1)^{ii}	2.4821 (14)	Eu(1)-O(3)^{iii}	2.3644 (16)
Eu(1)-O(2)^{i}	2.5945 (18)	Eu(1)-O(4)^{iv}	2.3639 (15)
Eu(1)-O(2)^{ii}	2.5945 (18)	Eu(1)-O(4)^{v}	2.3639 (15)
Eu(1)-O(6)	2.605 (3)	O(1)^{ii}-Eu(1)-O(1)^{i}	75.60 (7)
O(1)^{i}-Eu(1)-O(6)	142.20 (4)	O(1)^{i}-Eu(1)-O(2)^{i}	51.49 (5)
O(1)^{i}-Eu(1)-O(2)^{ii}	68.73 (6)	O(2)^{i}-Eu(1)-O(2)^{ii}	102.85 (9)
O(3)-Eu(1)-O(3)^{iii}	154.52 (8)	O(3)-Eu(1)-O(1)^{i}	121.96 (5)
O(3)-Eu(1)-O(1)^{ii}	79.58 (5)	O(3)-Eu(1)-O(6)	77.26 (4)
O(3)-Eu(1)-O(2)^{i}	70.72 (5)	O(3)-Eu(1)-O(2)^{ii}	127.24 (5)
O(4)^{iv}-Eu(1)-O(4)^{v}	141.87 (9)	O(4)^{iv}-Eu(1)-O(3)	80.24 (7)
O(4)^{iv}-Eu(1)-O(3)^{iii}	91.45 (6)	O(4)^{iv}-Eu(1)-O(1)^{ii}	76.02 (6)
O(4)^{iv}-Eu(1)-O(2)^{i}	137.41 (6)	O(4)^{iv}-Eu(1)-O(2)^{ii}	70.80 (7)
O(4)^{iv}-Eu(1)-O(1)^{i}	139.27 (6)	O(4)^{v}-Eu(1)-O(3)	91.45 (6)
O(4)^{v}-Eu(1)-O(3)^{iii}	80.24 (7)	O(6)-Eu(1)-O(4)^{iv}	70.93 (5)
Compound **3**			
Tb(1)-O(1)^{i}	2.4577 (17)	Tb(1)-O(3)	2.3366 (18)
Tb(1)-O(1)^{ii}	2.4577 (17)	Tb(1)-O(3)^{iii}	2.3366 (18)
Tb(1)-O(2)^{i}	2.582 (2)	Tb(1)-O(4)^{iv}	2.3384 (18)
Tb(1)-O(2)^{ii}	2.582 (2)	Tb(1)-O(4)^{v}	2.3384 (18)
Tb(1)-O(6)	2.583 (4)	O(1)^{ii}-Tb(1)-O(1)^{i}	75.68 (9)
O(1)^{i}-Tb(1)-O(6)	142.16 (4)	O(1)^{i}-Eu(1)-O(2)^{i}	51.86 (6)
O(1)^{i}-Tb(1)-O(2)^{ii}	68.64 (7)	O(2)^{i}-Eu(1)-O(2)^{ii}	103.13 (11)
O(3)-Tb(1)-O(3)^{iii}	153.84 (9)	O(3)-Eu(1)-O(1)^{i}	122.34 (6)

O(3)-Tb(1)-O(1)^{ii}	79.78 (6)	O(3)-Eu(1)-O(6)	76.92 (5)
O(3)-Tb(1)-O(2)^{i}	70.71 (6)	O(3)-Eu(1)-O(2)^{ii}	127.71 (6)
O(4)^{iv}-Tb(1)-O(4)^{v}	141.94 (11)	O(4)^{iv}-Eu(1)-O(3)	80.29 (8)
O(4)^{iv}-Tb(1)-O(3)^{iii}	91.21 (7)	O(4)^{iv}-Eu(1)-O(1)^{ii}	76.04 (7)
O(4)^{iv}-Tb(1)-O(2)^{i}	137.31 (7)	O(4)^{iv}-Eu(1)-O(2)^{ii}	70.76 (8)
O(4)^{iv}-Tb(1)-O(1)^{i}	139.14 (8)	O(4)^{v}-Eu(1)-O(3)	91.21 (7)
O(4)^{v}-Tb(1)-O(3)^{iii}	80.29 (8)	O(6)-Eu(1)-O(4)^{iv}	70.97 (6)

Table S4

Antibiotics	HOMO(eV)	LUMO(eV)	Band Gap(eV)
Complex 3	-7.21	-2.55	4.66
CPFX	-4.85	-1.90	2.95
PCL	-5.40	-1.66	3.74
LIN	-4.57	-0.40	4.17
ROX	-4.71	-0.85	3.86
MG	-7.04	-6.80	0.24
AZM	-4.08	-0.85	3.23
PAT	-0.30	5.39	5.69