

Supporting Information

Construction of a high-nuclearity Nd(III) nanoring for the NIR Luminescent detection of antibiotics

Wenxin Hao, Xiaoping Yang, Yanan Ma, Mengyu Niu, Dongliang Shi, and Desmond Schipper

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1. IR spectra of the free ligand H₂L and 1

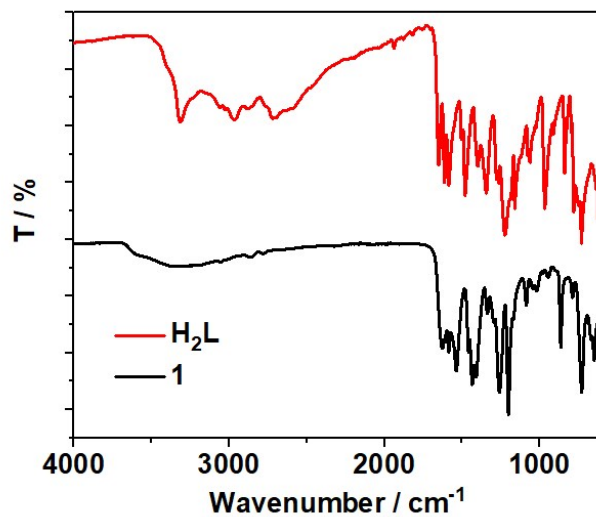


Figure S1. IR spectra of free ligand H₂L and 1.

2. The thermogravimetric analysis of 1

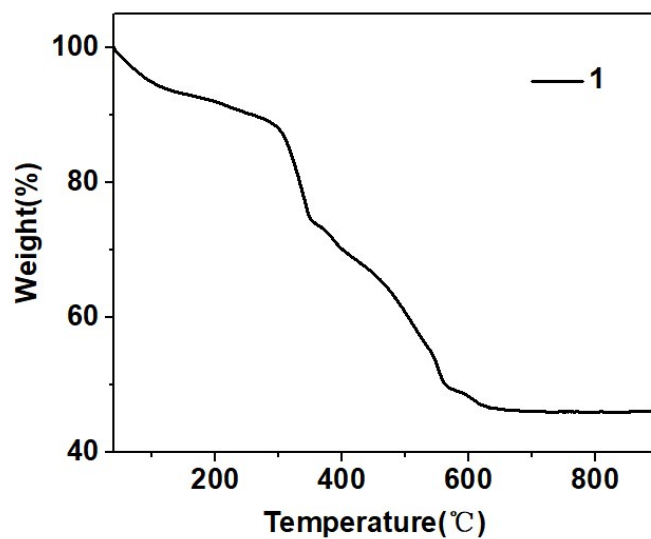


Figure S2. The thermogravimetric analysis of 1.

3. Powder XRD patterns of **1**

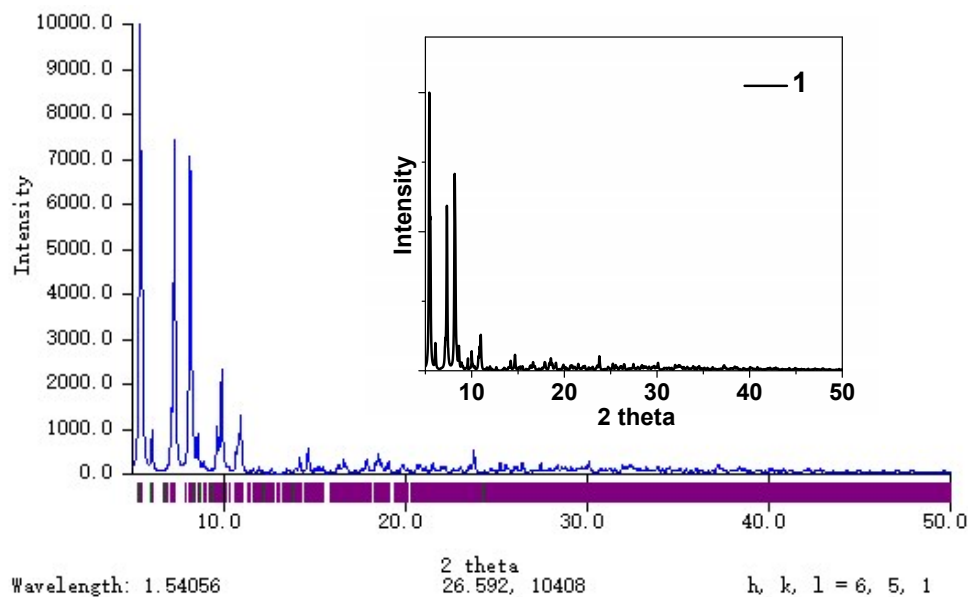


Figure S3. Powder XRD pattern of **1**.

4. UV-vis absorption spectra of the free ligand H_2L and **1**

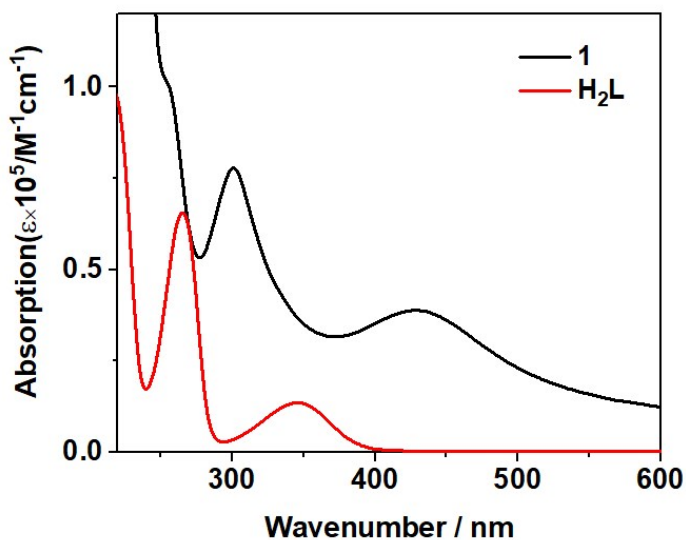


Figure S4. UV-vis absorption spectra of the free ligand H_2L and **1** in CH_3CN ($c = 5 \mu M$).

5. The NIR emission lifetime of 1

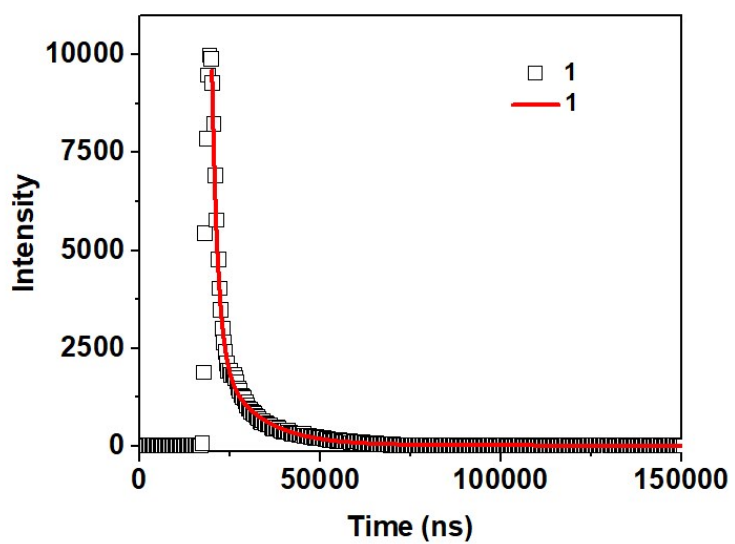
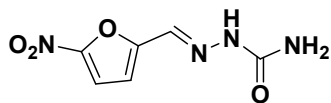
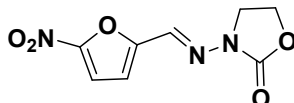


Figure S5. The NIR emission lifetime of **1** in CH₃CN (10 μM).

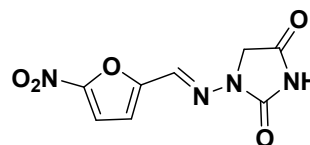
6. Chemical structures of antibiotics



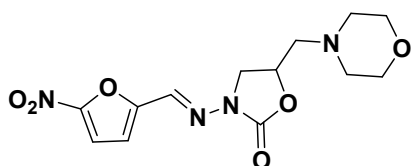
Nitrofurazone (NFZ)



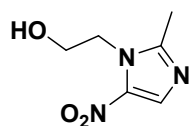
Furazolidone (FZD)



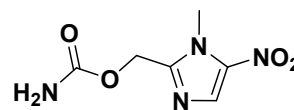
Nitrofurantion (NFT)



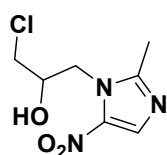
Furaltadone (FTD)



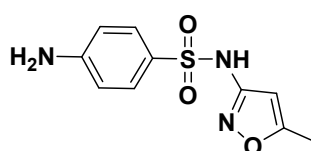
Metronidazole (MDZ)



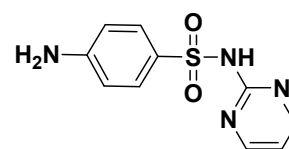
Ronidazole (RDZ)



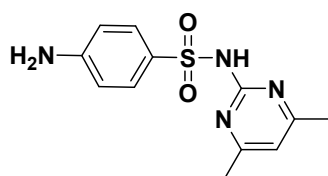
Omidazole (ODZ)



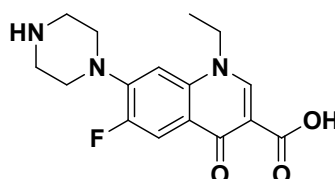
Sulfamethoxazole (SMX)



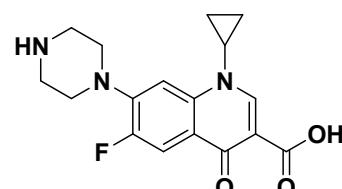
Sulfadiazine (SDZ)



Sulfamethazine (SMZ)



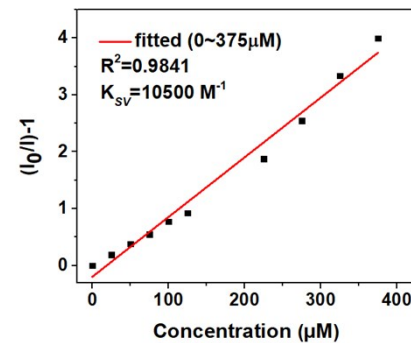
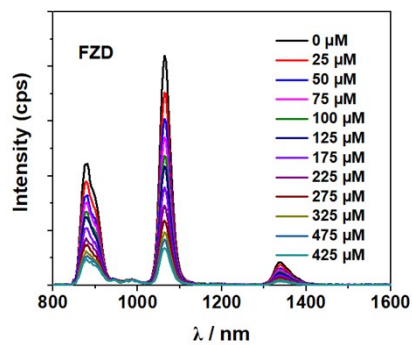
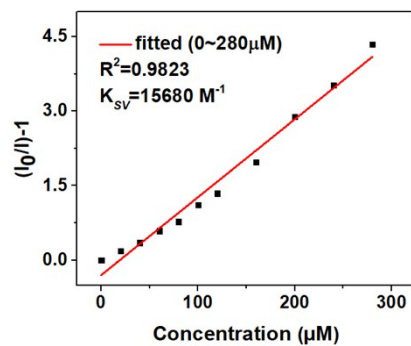
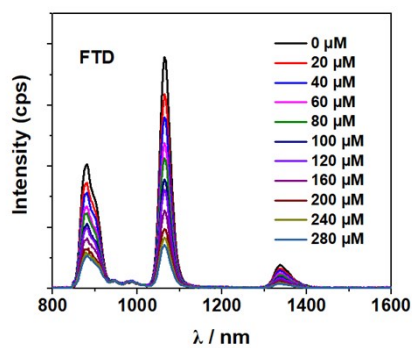
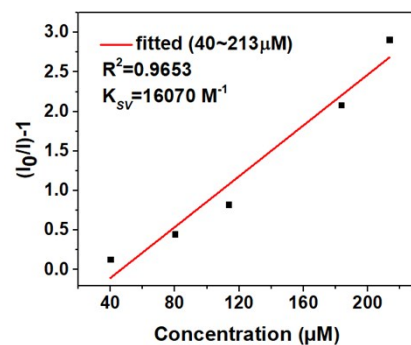
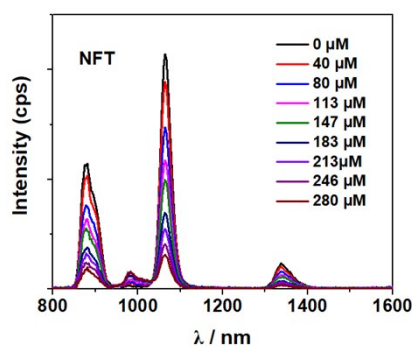
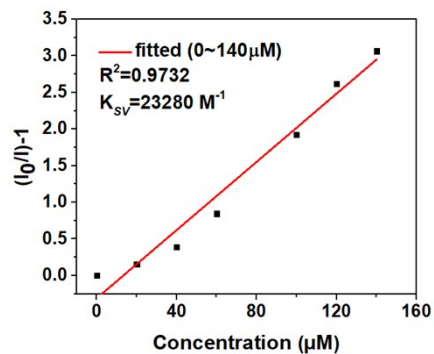
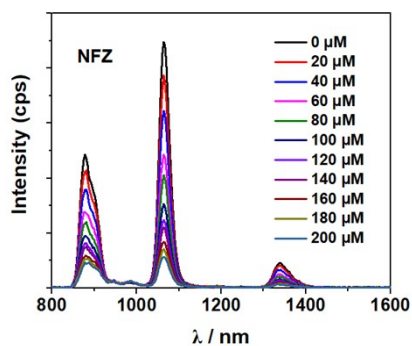
Norfloxacin (NFX)

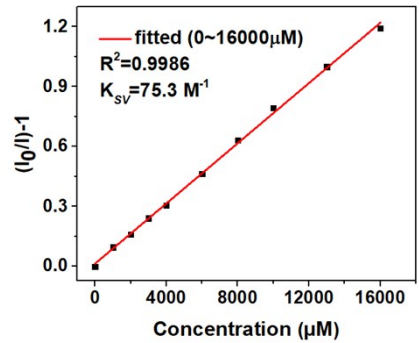
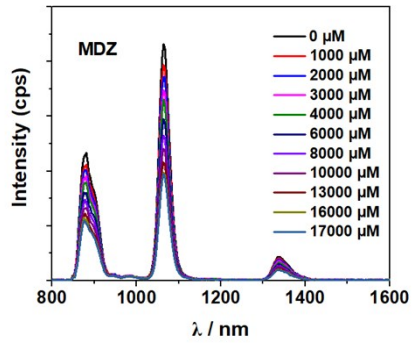
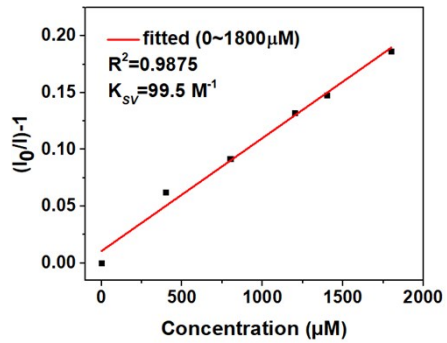
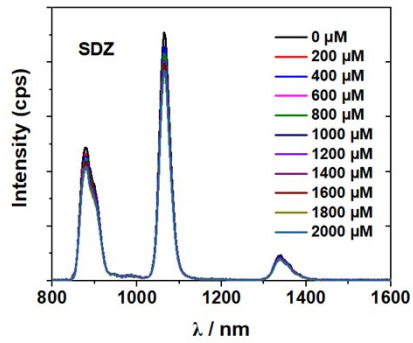
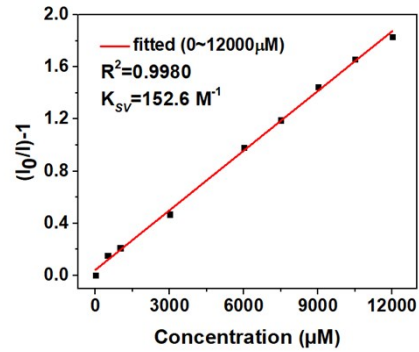
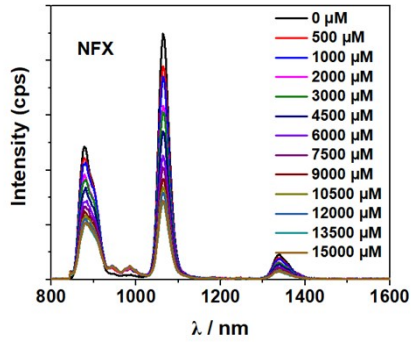
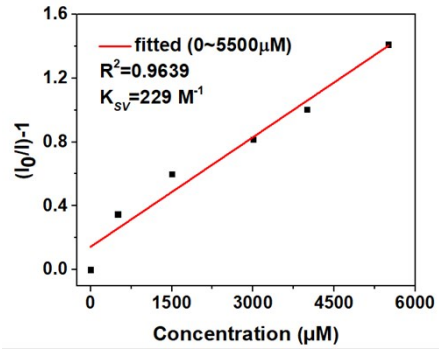
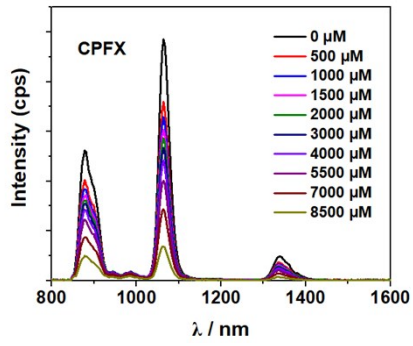


Ciprofloxacin (CPFX)

Figure S6. Chemical structures of antibiotics.

7. NIR luminescent sensing of 1 to antibiotics





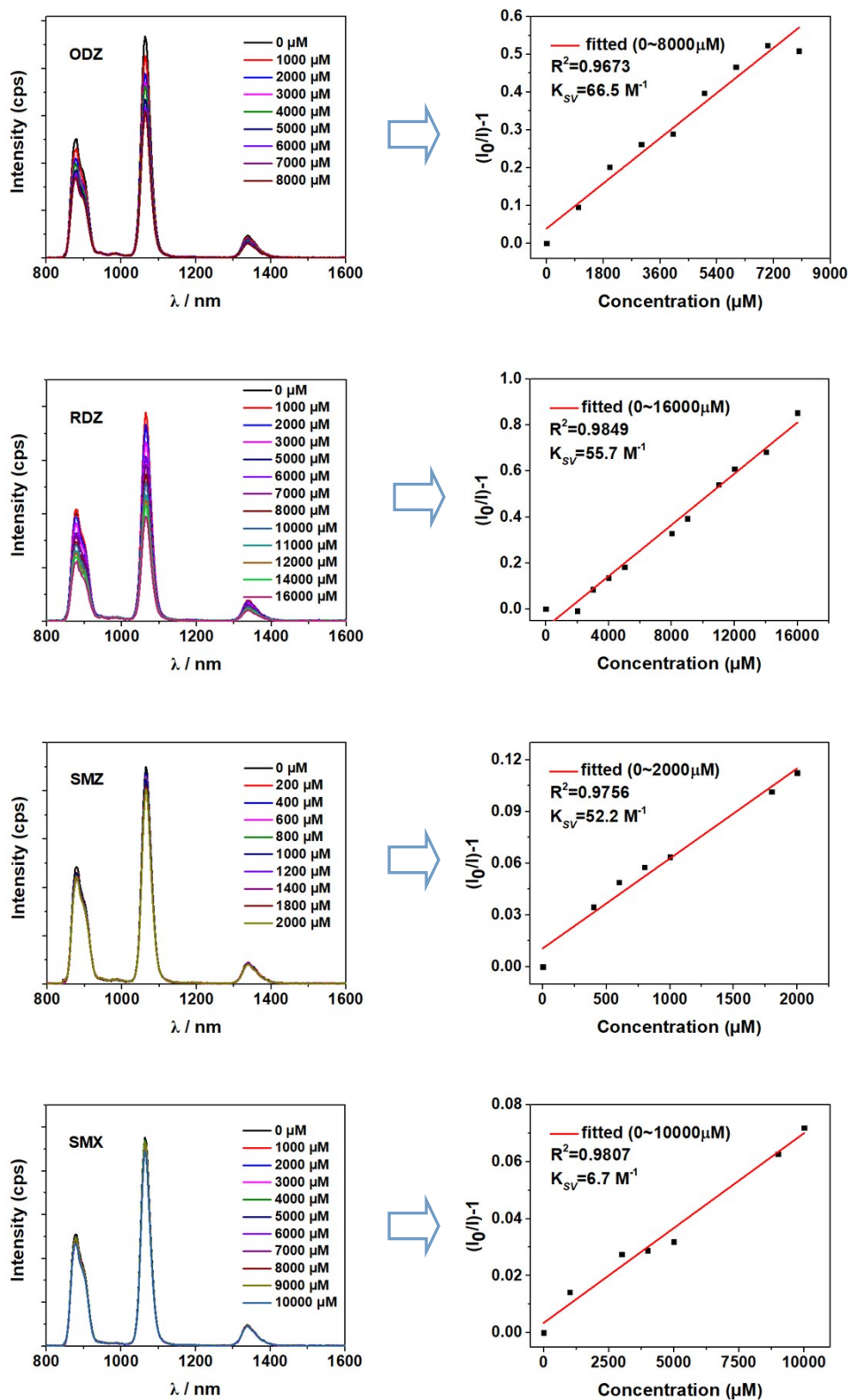


Figure S7. NIR luminescent sensing of **1** (10 μM) to antibiotics in CH_3CN ($\lambda_{\text{ex}} = 404 \text{ nm}$).

8. The NIR luminescent quenching of 1 caused by antibiotics

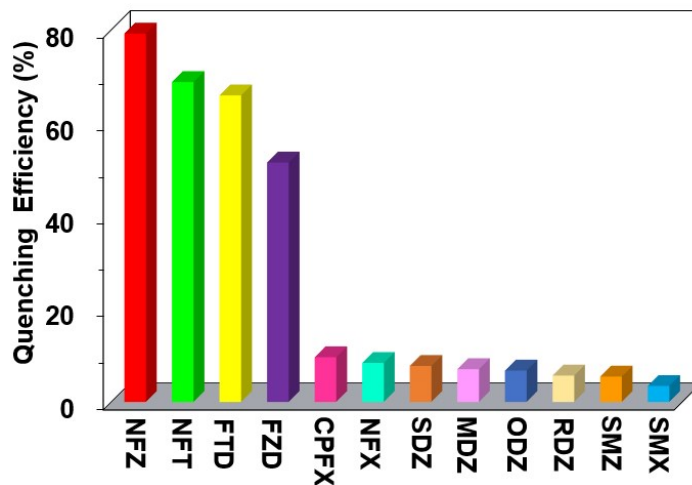


Figure S8. Percentages of NIR emission quenching of 1 (10 μ M) caused by antibiotics (190 μ M).

9. The visible emission quenching of free H₂L ligand to antibiotics

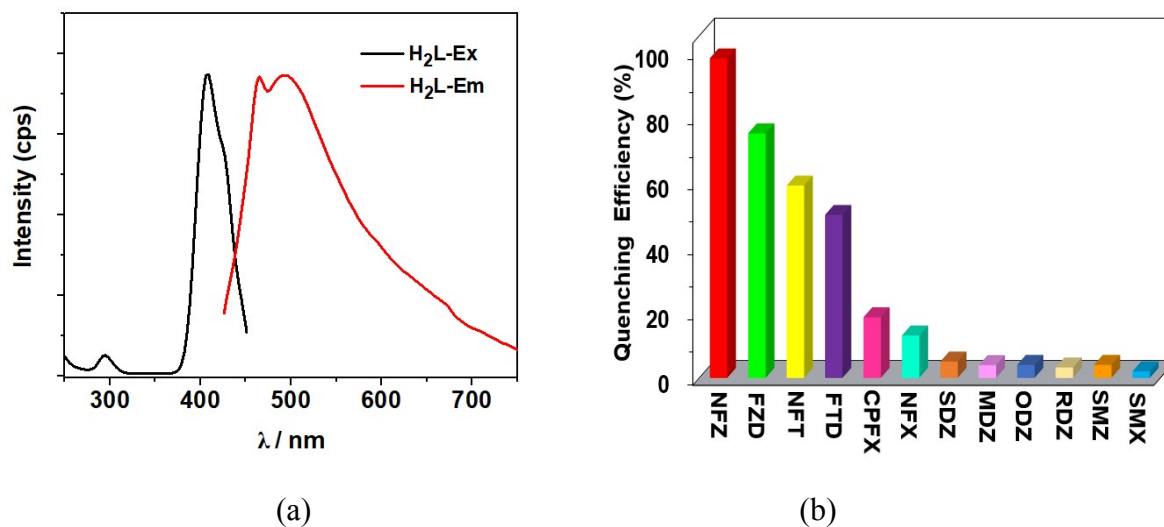
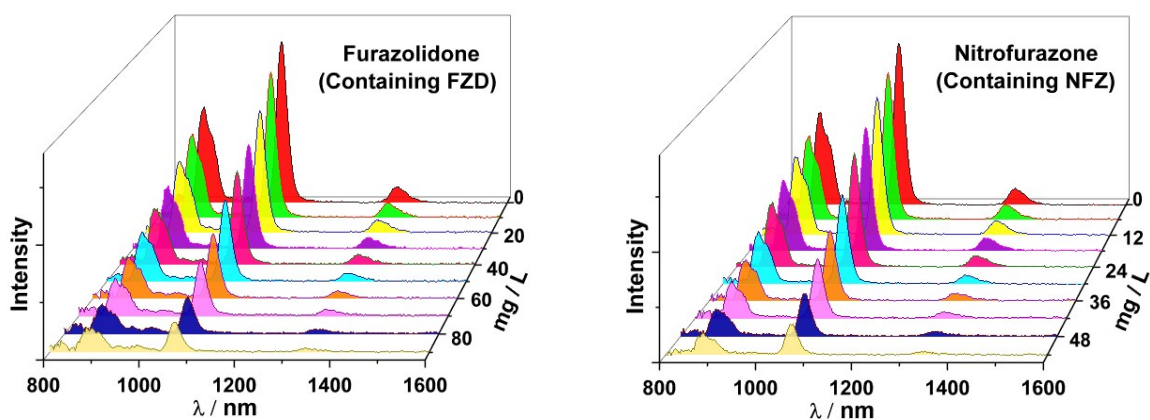


Figure S9. (a) The excitation (λ_{em} = 492 nm) and emission (λ_{ex} = 409 nm) spectra of the free H₂L ligand; (b) Percentages of visible emission quenching of the free H₂L ligand (10 μ M) caused by antibiotics (190 μ M). (λ_{ex} = 409 nm)

10. The luminescent response of **1** to antibiotic drugs sold in pharmacy



(a)



(b)

Figure S10. (a) The photos of antibiotic drugs furazolidone (containing FZD) and nitrofurazone (containing NFZ) sold in pharmacy; (b) The luminescent response of **1** ($10 \mu\text{M}$) to furazolidone and nitrofurazone in CH_3CN . ($\lambda_{\text{ex}} = 404 \text{ nm}$)

11. The luminescent response of recycled 1 to antibiotic drugs sold in pharmacy

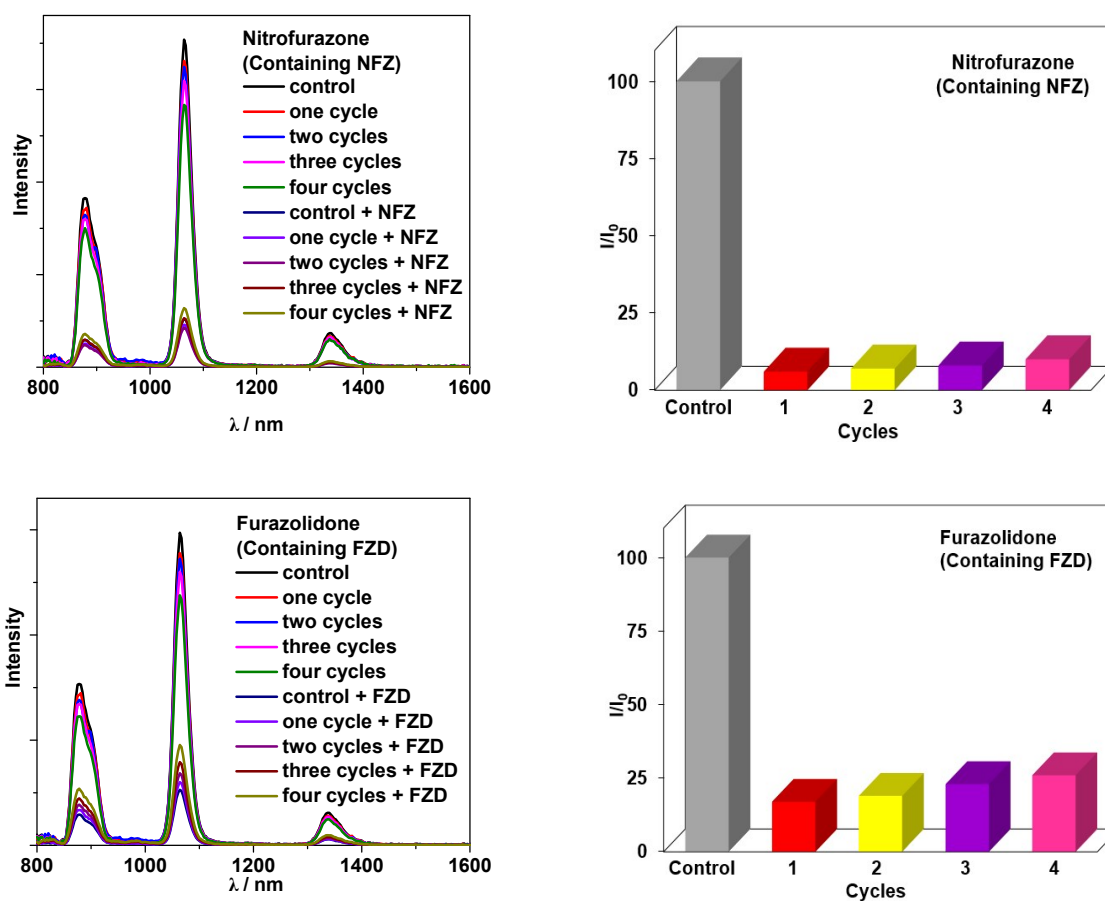


Figure S11. The luminescence quenching of **1** ($10 \mu\text{M}$) after 1-4 times recycled with the addition of 80 mg/L of nitrofurazone and furazolidone sold in pharmacy in CH_3CN . ($\lambda_{\text{ex}} = 404 \text{ nm}$)

12. X-Ray Crystallography

Table S1. Selected bond lengths (Å) and angles (°) for **1**.

Nd(1)-O(6)	2.354(15)	Nd(6)-O(19)	2.518(16)
Nd(1)-O(53)	2.374(17)	Nd(6)-O(18)	2.546(14)
Nd(1)-O(2)	2.385(16)	Nd(7)-O(79)	2.346(17)
Nd(1)-O(74)	2.39(3)	Nd(7)-O(18)	2.352(13)
Nd(1)-O(56)	2.422(16)	Nd(7)-O(23)	2.392(16)
Nd(1)-O(57)	2.429(17)	Nd(7)-O(27)	2.424(15)
Nd(1)-O(1)	2.48(2)	Nd(7)-O(26)	2.436(16)
Nd(1)-O(52)	2.493(19)	Nd(7)-O(22)	2.502(19)
Nd(2)-O(8)	2.364(16)	Nd(7)-O(78)	2.53(2)
Nd(2)-O(2)	2.405(17)	Nd(7)-O(76)	2.53(3)
Nd(2)-O(57)	2.417(17)	Nd(8)-O(36)	2.347(14)
Nd(2)-O(3)	2.446(16)	Nd(8)-O(29)	2.351(17)
Nd(2)-O(5)	2.466(14)	Nd(8)-O(26)	2.373(14)
Nd(2)-O(58)	2.502(16)	Nd(8)-O(23)	2.418(17)
Nd(2)-O(6)	2.508(14)	Nd(8)-O(24)	2.422(16)
Nd(2)-O(64)	2.56(2)	Nd(8)-O(25)	2.50(2)
Nd(2)-O(7)	2.568(18)	Nd(8)-O(28)	2.502(19)
Nd(3)-O(3)	2.406(16)	Nd(8)-O(77)	2.55(4)
Nd(3)-O(11)	2.407(17)	Nd(8)-O(76)	2.66(3)
Nd(3)-O(5)	2.418(14)	Nd(9)-O(32)	2.333(16)
Nd(3)-O(9)	2.420(15)	Nd(9)-O(29)	2.415(16)
Nd(3)-O(8)	2.446(15)	Nd(9)-O(24)	2.436(17)
Nd(3)-O(10)	2.520(18)	Nd(9)-O(35)	2.436(15)
Nd(3)-O(65)	2.54(2)	Nd(9)-O(61)	2.443(16)
Nd(3)-O(66)	2.60(2)	Nd(9)-O(30)	2.489(17)
Nd(3)-O(4)	2.620(15)	Nd(9)-O(69)	2.50(2)
Nd(4)-O(15)	2.313(18)	Nd(9)-O(36)	2.514(14)
Nd(4)-O(12)	2.321(18)	Nd(9)-O(31)	2.526(16)
Nd(4)-O(9)	2.337(15)	Nd(10)-O(30)	2.408(17)
Nd(4)-O(21)	2.371(14)	Nd(10)-O(63)	2.42(2)
Nd(4)-O(11)	2.413(16)	Nd(10)-O(33)	2.426(15)
Nd(4)-O(14)	2.435(17)	Nd(10)-O(35)	2.430(15)
Nd(4)-O(4)	2.585(16)	Nd(10)-O(38)	2.431(18)
Nd(4)-O(16)	2.606(16)	Nd(10)-O(32)	2.470(16)
Nd(5)-O(14)	2.388(16)	Nd(10)-O(70)	2.48(2)
Nd(5)-O(80)	2.389(16)	Nd(10)-O(37)	2.51(2)
Nd(5)-O(17)	2.422(15)	Nd(10)-O(34)	2.610(15)
Nd(5)-O(59)	2.434(18)	Nd(11)-O(42)	2.299(19)
Nd(5)-O(21)	2.438(14)	Nd(11)-O(39)	2.312(19)
Nd(5)-O(20)	2.445(14)	Nd(11)-O(48)	2.342(15)
Nd(5)-O(67)	2.50(2)	Nd(11)-O(33)	2.378(15)
Nd(5)-O(13)	2.50(2)	Nd(11)-O(38)	2.406(16)
Nd(5)-O(16)	2.629(17)	Nd(11)-O(41)	2.433(16)
Nd(6)-O(20)	2.358(14)	Nd(11)-O(43)	2.571(15)
Nd(6)-O(79)	2.429(16)	Nd(11)-O(34)	2.616(15)
Nd(6)-O(27)	2.441(15)	Nd(12)-O(41)	2.395(16)
Nd(6)-O(17)	2.445(14)	Nd(12)-O(48)	2.402(15)
Nd(6)-O(80)	2.478(16)	Nd(12)-O(51)	2.405(18)
Nd(6)-O(60)	2.482(15)	Nd(12)-O(47)	2.409(15)
Nd(6)-O(68)	2.49(2)	Nd(12)-O(44)	2.432(15)

Nd(12)-O(40)	2.510(18)	O(57)-Nd(2)-O(3)	133.0(6)
Nd(12)-O(71)	2.571(19)	O(8)-Nd(2)-O(5)	67.5(5)
Nd(12)-O(72)	2.58(2)	O(2)-Nd(2)-O(5)	95.3(5)
Nd(12)-O(43)	2.604(16)	O(57)-Nd(2)-O(5)	132.2(5)
Nd(13)-O(47)	2.368(14)	O(3)-Nd(2)-O(5)	67.6(5)
Nd(13)-O(54)	2.403(16)	O(8)-Nd(2)-O(58)	81.6(5)
Nd(13)-O(50)	2.405(17)	O(2)-Nd(2)-O(58)	137.9(5)
Nd(13)-O(51)	2.458(17)	O(57)-Nd(2)-O(58)	82.6(5)
Nd(13)-O(44)	2.459(15)	O(3)-Nd(2)-O(58)	142.9(5)
Nd(13)-O(62)	2.509(16)	O(5)-Nd(2)-O(58)	80.5(5)
Nd(13)-O(45)	2.551(14)	O(8)-Nd(2)-O(6)	128.0(5)
Nd(13)-O(46)	2.562(18)	O(2)-Nd(2)-O(6)	69.0(5)
Nd(13)-O(73)	2.58(2)	O(57)-Nd(2)-O(6)	67.6(5)
Nd(14)-O(50)	2.347(17)	O(3)-Nd(2)-O(6)	108.7(5)
Nd(14)-O(75)	2.36(3)	O(5)-Nd(2)-O(6)	64.7(5)
Nd(14)-O(45)	2.362(15)	O(58)-Nd(2)-O(6)	71.6(5)
Nd(14)-O(56)	2.377(16)	O(8)-Nd(2)-O(64)	96.8(6)
Nd(14)-O(54)	2.389(17)	O(2)-Nd(2)-O(64)	71.8(6)
Nd(14)-O(53)	2.450(17)	O(57)-Nd(2)-O(64)	77.1(6)
Nd(14)-O(49)	2.48(2)	O(3)-Nd(2)-O(64)	75.1(6)
Nd(14)-O(55)	2.510(19)	O(5)-Nd(2)-O(64)	142.6(6)
O(6)-Nd(1)-O(53)	104.8(5)	O(58)-Nd(2)-O(64)	132.5(6)
O(6)-Nd(1)-O(2)	71.9(5)	O(6)-Nd(2)-O(64)	134.1(6)
O(53)-Nd(1)-O(2)	151.5(6)	O(8)-Nd(2)-O(7)	67.4(6)
O(6)-Nd(1)-O(74)	151.3(9)	O(2)-Nd(2)-O(7)	135.8(6)
O(53)-Nd(1)-O(74)	90.6(9)	O(57)-Nd(2)-O(7)	84.9(6)
O(2)-Nd(1)-O(74)	105.4(9)	O(3)-Nd(2)-O(7)	117.4(5)
O(6)-Nd(1)-O(56)	87.3(5)	O(5)-Nd(2)-O(7)	127.8(6)
O(53)-Nd(1)-O(56)	69.6(5)	O(58)-Nd(2)-O(7)	68.2(5)
O(2)-Nd(1)-O(56)	136.7(6)	O(6)-Nd(2)-O(7)	133.5(5)
O(74)-Nd(1)-O(56)	75.4(9)	O(64)-Nd(2)-O(7)	67.7(6)
O(6)-Nd(1)-O(57)	69.9(5)	O(3)-Nd(3)-O(11)	150.4(5)
O(53)-Nd(1)-O(57)	137.2(6)	O(3)-Nd(3)-O(5)	69.0(5)
O(2)-Nd(1)-O(57)	69.5(6)	O(11)-Nd(3)-O(5)	133.7(5)
O(74)-Nd(1)-O(57)	82.2(9)	O(3)-Nd(3)-O(9)	135.9(5)
O(56)-Nd(1)-O(57)	67.8(5)	O(11)-Nd(3)-O(9)	69.2(5)
O(6)-Nd(1)-O(1)	130.8(6)	O(5)-Nd(3)-O(9)	93.9(5)
O(53)-Nd(1)-O(1)	94.0(7)	O(3)-Nd(3)-O(8)	68.6(6)
O(2)-Nd(1)-O(1)	70.4(7)	O(11)-Nd(3)-O(8)	132.9(5)
O(74)-Nd(1)-O(1)	70.4(10)	O(5)-Nd(3)-O(8)	67.0(5)
O(56)-Nd(1)-O(1)	141.8(7)	O(9)-Nd(3)-O(8)	67.3(5)
O(57)-Nd(1)-O(1)	122.3(6)	O(3)-Nd(3)-O(10)	81.6(6)
O(6)-Nd(1)-O(52)	73.2(5)	O(11)-Nd(3)-O(10)	69.0(6)
O(53)-Nd(1)-O(52)	71.6(6)	O(5)-Nd(3)-O(10)	139.3(6)
O(2)-Nd(1)-O(52)	80.6(6)	O(9)-Nd(3)-O(10)	126.6(6)
O(74)-Nd(1)-O(52)	135.4(9)	O(8)-Nd(3)-O(10)	127.5(6)
O(56)-Nd(1)-O(52)	129.8(6)	O(3)-Nd(3)-O(65)	92.1(6)
O(57)-Nd(1)-O(52)	138.0(6)	O(11)-Nd(3)-O(65)	79.0(6)
O(1)-Nd(1)-O(52)	70.5(7)	O(5)-Nd(3)-O(65)	139.7(6)
O(8)-Nd(2)-O(2)	135.5(5)	O(9)-Nd(3)-O(65)	74.8(6)
O(8)-Nd(2)-O(57)	151.7(6)	O(8)-Nd(3)-O(65)	73.0(6)
O(2)-Nd(2)-O(57)	69.4(6)	O(10)-Nd(3)-O(65)	65.8(7)
O(8)-Nd(2)-O(3)	69.3(5)	O(3)-Nd(3)-O(66)	82.8(6)
O(2)-Nd(2)-O(3)	66.2(6)	O(11)-Nd(3)-O(66)	86.0(6)

O(5)-Nd(3)-O(66)	75.0(6)	O(59)-Nd(5)-O(20)	138.6(5)
O(9)-Nd(3)-O(66)	133.4(6)	O(21)-Nd(5)-O(20)	65.7(5)
O(8)-Nd(3)-O(66)	138.4(6)	O(14)-Nd(5)-O(67)	81.1(6)
O(10)-Nd(3)-O(66)	73.9(6)	O(80)-Nd(5)-O(67)	89.1(6)
O(65)-Nd(3)-O(66)	139.7(6)	O(17)-Nd(5)-O(67)	137.8(6)
O(3)-Nd(3)-O(4)	132.5(5)	O(59)-Nd(5)-O(67)	137.6(7)
O(11)-Nd(3)-O(4)	66.9(5)	O(21)-Nd(5)-O(67)	75.5(6)
O(5)-Nd(3)-O(4)	66.9(5)	O(20)-Nd(5)-O(67)	72.2(6)
O(9)-Nd(3)-O(4)	64.4(5)	O(14)-Nd(5)-O(13)	68.7(6)
O(8)-Nd(3)-O(4)	108.1(5)	O(80)-Nd(5)-O(13)	82.2(6)
O(10)-Nd(3)-O(4)	123.7(6)	O(17)-Nd(5)-O(13)	137.0(6)
O(65)-Nd(3)-O(4)	133.6(6)	O(59)-Nd(5)-O(13)	68.3(7)
O(66)-Nd(3)-O(4)	69.7(6)	O(21)-Nd(5)-O(13)	129.2(6)
O(15)-Nd(4)-O(12)	85.6(6)	O(20)-Nd(5)-O(13)	131.0(6)
O(15)-Nd(4)-O(9)	81.6(6)	O(67)-Nd(5)-O(13)	69.5(7)
O(12)-Nd(4)-O(9)	132.9(6)	O(14)-Nd(5)-O(16)	66.5(5)
O(15)-Nd(4)-O(21)	134.1(6)	O(80)-Nd(5)-O(16)	133.4(5)
O(12)-Nd(4)-O(21)	80.0(6)	O(17)-Nd(5)-O(16)	67.6(5)
O(9)-Nd(4)-O(21)	137.7(5)	O(59)-Nd(5)-O(16)	71.5(5)
O(15)-Nd(4)-O(11)	97.8(6)	O(21)-Nd(5)-O(16)	65.8(5)
O(12)-Nd(4)-O(11)	66.6(6)	O(20)-Nd(5)-O(16)	108.3(5)
O(9)-Nd(4)-O(11)	70.5(5)	O(67)-Nd(5)-O(16)	135.7(6)
O(21)-Nd(4)-O(11)	115.3(5)	O(13)-Nd(5)-O(16)	120.3(6)
O(15)-Nd(4)-O(14)	66.7(6)	O(20)-Nd(6)-O(79)	134.6(6)
O(12)-Nd(4)-O(14)	93.2(6)	O(20)-Nd(6)-O(27)	153.5(5)
O(9)-Nd(4)-O(14)	121.9(6)	O(79)-Nd(6)-O(27)	68.9(6)
O(21)-Nd(4)-O(14)	70.9(5)	O(20)-Nd(6)-O(17)	67.2(5)
O(11)-Nd(4)-O(14)	156.1(5)	O(79)-Nd(6)-O(17)	94.9(5)
O(15)-Nd(4)-O(4)	147.3(6)	O(27)-Nd(6)-O(17)	131.0(5)
O(12)-Nd(4)-O(4)	112.1(6)	O(20)-Nd(6)-O(80)	67.5(5)
O(9)-Nd(4)-O(4)	66.1(5)	O(79)-Nd(6)-O(80)	67.0(5)
O(21)-Nd(4)-O(4)	77.6(5)	O(27)-Nd(6)-O(80)	133.6(5)
O(11)-Nd(4)-O(4)	67.4(5)	O(17)-Nd(6)-O(80)	67.2(5)
O(14)-Nd(4)-O(4)	135.1(5)	O(20)-Nd(6)-O(60)	82.0(5)
O(15)-Nd(4)-O(16)	109.0(6)	O(79)-Nd(6)-O(60)	138.7(5)
O(12)-Nd(4)-O(16)	145.2(6)	O(27)-Nd(6)-O(60)	82.4(5)
O(9)-Nd(4)-O(16)	81.4(5)	O(17)-Nd(6)-O(60)	81.7(5)
O(21)-Nd(4)-O(16)	67.1(5)	O(80)-Nd(6)-O(60)	142.7(5)
O(11)-Nd(4)-O(16)	137.6(5)	O(20)-Nd(6)-O(68)	97.0(6)
O(14)-Nd(4)-O(16)	66.2(5)	O(79)-Nd(6)-O(68)	69.9(6)
O(4)-Nd(4)-O(16)	72.5(5)	O(27)-Nd(6)-O(68)	79.0(6)
O(14)-Nd(5)-O(80)	150.9(6)	O(17)-Nd(6)-O(68)	140.2(6)
O(14)-Nd(5)-O(17)	134.0(5)	O(80)-Nd(6)-O(68)	73.0(6)
O(80)-Nd(5)-O(17)	69.0(5)	O(60)-Nd(6)-O(68)	134.0(6)
O(14)-Nd(5)-O(59)	86.2(6)	O(20)-Nd(6)-O(19)	68.0(5)
O(80)-Nd(5)-O(59)	82.8(5)	O(79)-Nd(6)-O(19)	134.1(5)
O(17)-Nd(5)-O(59)	76.8(5)	O(27)-Nd(6)-O(19)	86.6(5)
O(14)-Nd(5)-O(21)	70.5(5)	O(17)-Nd(6)-O(19)	129.3(5)
O(80)-Nd(5)-O(21)	133.3(5)	O(80)-Nd(6)-O(19)	114.5(5)
O(17)-Nd(5)-O(21)	93.4(5)	O(60)-Nd(6)-O(19)	69.7(5)
O(59)-Nd(5)-O(21)	136.7(5)	O(68)-Nd(6)-O(19)	67.6(6)
O(14)-Nd(5)-O(20)	133.0(5)	O(20)-Nd(6)-O(18)	128.6(5)
O(80)-Nd(5)-O(20)	67.6(5)	O(79)-Nd(6)-O(18)	69.1(5)
O(17)-Nd(5)-O(20)	66.2(5)	O(27)-Nd(6)-O(18)	65.3(5)

O(17)-Nd(6)-O(18)	65.7(5)	O(36)-Nd(8)-O(77)	141.5(10)
O(80)-Nd(6)-O(18)	110.3(5)	O(29)-Nd(8)-O(77)	94.5(9)
O(60)-Nd(6)-O(18)	72.1(5)	O(26)-Nd(8)-O(77)	106.8(9)
O(68)-Nd(6)-O(18)	132.8(6)	O(23)-Nd(8)-O(77)	78.4(10)
O(19)-Nd(6)-O(18)	134.9(5)	O(24)-Nd(8)-O(77)	73.5(10)
O(79)-Nd(7)-O(18)	73.9(5)	O(25)-Nd(8)-O(77)	139.2(10)
O(79)-Nd(7)-O(23)	150.7(6)	O(28)-Nd(8)-O(77)	68.1(10)
O(18)-Nd(7)-O(23)	99.5(5)	O(36)-Nd(8)-O(76)	154.6(7)
O(79)-Nd(7)-O(27)	70.6(6)	O(29)-Nd(8)-O(76)	129.3(6)
O(18)-Nd(7)-O(27)	68.5(5)	O(26)-Nd(8)-O(76)	66.4(6)
O(23)-Nd(7)-O(27)	134.5(6)	O(23)-Nd(8)-O(76)	68.6(7)
O(79)-Nd(7)-O(26)	137.6(5)	O(24)-Nd(8)-O(76)	105.3(7)
O(18)-Nd(7)-O(26)	86.8(5)	O(25)-Nd(8)-O(76)	118.0(7)
O(23)-Nd(7)-O(26)	68.5(5)	O(28)-Nd(8)-O(76)	70.8(7)
O(27)-Nd(7)-O(26)	67.2(5)	O(77)-Nd(8)-O(76)	40.6(9)
O(79)-Nd(7)-O(22)	77.6(6)	O(32)-Nd(9)-O(29)	135.0(6)
O(18)-Nd(7)-O(22)	74.9(5)	O(32)-Nd(9)-O(24)	153.0(6)
O(23)-Nd(7)-O(22)	73.2(6)	O(29)-Nd(9)-O(24)	68.8(6)
O(27)-Nd(7)-O(22)	136.6(5)	O(32)-Nd(9)-O(35)	67.8(5)
O(26)-Nd(7)-O(22)	133.8(6)	O(29)-Nd(9)-O(35)	94.8(5)
O(79)-Nd(7)-O(78)	69.1(6)	O(24)-Nd(9)-O(35)	131.1(5)
O(18)-Nd(7)-O(78)	134.1(6)	O(32)-Nd(9)-O(61)	81.5(5)
O(23)-Nd(7)-O(78)	99.7(6)	O(29)-Nd(9)-O(61)	139.2(5)
O(27)-Nd(7)-O(78)	120.4(6)	O(24)-Nd(9)-O(61)	82.6(5)
O(26)-Nd(7)-O(78)	139.0(6)	O(35)-Nd(9)-O(61)	82.3(5)
O(22)-Nd(7)-O(78)	71.5(6)	O(32)-Nd(9)-O(30)	68.2(5)
O(79)-Nd(7)-O(76)	125.7(7)	O(29)-Nd(9)-O(30)	66.8(6)
O(18)-Nd(7)-O(76)	154.4(7)	O(24)-Nd(9)-O(30)	132.9(5)
O(23)-Nd(7)-O(76)	71.2(7)	O(35)-Nd(9)-O(30)	68.0(5)
O(27)-Nd(7)-O(76)	100.5(7)	O(61)-Nd(9)-O(30)	143.6(5)
O(26)-Nd(7)-O(76)	67.6(7)	O(32)-Nd(9)-O(69)	97.3(6)
O(22)-Nd(7)-O(76)	122.1(7)	O(29)-Nd(9)-O(69)	69.4(6)
O(78)-Nd(7)-O(76)	71.4(7)	O(24)-Nd(9)-O(69)	78.3(6)
O(36)-Nd(8)-O(29)	73.0(5)	O(35)-Nd(9)-O(69)	140.4(6)
O(36)-Nd(8)-O(26)	100.3(5)	O(61)-Nd(9)-O(69)	133.5(6)
O(29)-Nd(8)-O(26)	150.4(6)	O(30)-Nd(9)-O(69)	72.4(6)
O(36)-Nd(8)-O(23)	86.6(5)	O(32)-Nd(9)-O(36)	129.1(5)
O(29)-Nd(8)-O(23)	137.1(5)	O(29)-Nd(9)-O(36)	69.0(5)
O(26)-Nd(8)-O(23)	69.1(5)	O(24)-Nd(9)-O(36)	65.3(5)
O(36)-Nd(8)-O(24)	68.1(5)	O(35)-Nd(9)-O(36)	65.8(5)
O(29)-Nd(8)-O(24)	70.1(6)	O(61)-Nd(9)-O(36)	72.9(5)
O(26)-Nd(8)-O(24)	135.3(6)	O(30)-Nd(9)-O(36)	110.8(5)
O(23)-Nd(8)-O(24)	67.3(5)	O(69)-Nd(9)-O(36)	132.1(6)
O(36)-Nd(8)-O(25)	74.8(6)	O(32)-Nd(9)-O(31)	68.3(5)
O(29)-Nd(8)-O(25)	77.8(6)	O(29)-Nd(9)-O(31)	133.6(5)
O(26)-Nd(8)-O(25)	72.6(6)	O(24)-Nd(9)-O(31)	85.6(5)
O(23)-Nd(8)-O(25)	133.2(6)	O(35)-Nd(9)-O(31)	130.0(5)
O(24)-Nd(8)-O(25)	136.3(6)	O(61)-Nd(9)-O(31)	68.7(5)
O(36)-Nd(8)-O(28)	134.2(6)	O(30)-Nd(9)-O(31)	114.9(5)
O(29)-Nd(8)-O(28)	70.1(6)	O(69)-Nd(9)-O(31)	67.9(6)
O(26)-Nd(8)-O(28)	98.5(6)	O(36)-Nd(9)-O(31)	134.2(5)
O(23)-Nd(8)-O(28)	139.2(6)	O(30)-Nd(10)-O(63)	83.4(6)
O(24)-Nd(8)-O(28)	120.9(6)	O(30)-Nd(10)-O(33)	133.4(5)
O(25)-Nd(8)-O(28)	71.7(6)	O(63)-Nd(10)-O(33)	136.6(6)

O(30)-Nd(10)-O(35)	69.4(5)	O(42)-Nd(11)-O(34)	144.6(6)
O(63)-Nd(10)-O(35)	76.8(6)	O(39)-Nd(11)-O(34)	109.2(6)
O(33)-Nd(10)-O(35)	94.1(5)	O(48)-Nd(11)-O(34)	81.9(5)
O(30)-Nd(10)-O(38)	150.8(5)	O(33)-Nd(11)-O(34)	67.2(5)
O(63)-Nd(10)-O(38)	87.1(6)	O(38)-Nd(11)-O(34)	67.2(5)
O(33)-Nd(10)-O(38)	69.4(5)	O(41)-Nd(11)-O(34)	137.9(5)
O(35)-Nd(10)-O(38)	134.7(5)	O(43)-Nd(11)-O(34)	73.4(5)
O(30)-Nd(10)-O(32)	67.4(5)	O(41)-Nd(12)-O(48)	69.7(5)
O(63)-Nd(10)-O(32)	138.4(6)	O(41)-Nd(12)-O(51)	149.7(6)
O(33)-Nd(10)-O(32)	66.1(5)	O(48)-Nd(12)-O(51)	135.8(6)
O(35)-Nd(10)-O(32)	65.8(5)	O(41)-Nd(12)-O(47)	133.2(5)
O(38)-Nd(10)-O(32)	132.2(6)	O(48)-Nd(12)-O(47)	67.2(5)
O(30)-Nd(10)-O(70)	88.2(6)	O(51)-Nd(12)-O(47)	68.6(6)
O(63)-Nd(10)-O(70)	137.0(7)	O(41)-Nd(12)-O(44)	134.2(5)
O(33)-Nd(10)-O(70)	75.9(6)	O(48)-Nd(12)-O(44)	94.5(5)
O(35)-Nd(10)-O(70)	138.2(6)	O(51)-Nd(12)-O(44)	69.0(5)
O(38)-Nd(10)-O(70)	80.1(7)	O(47)-Nd(12)-O(44)	67.2(5)
O(32)-Nd(10)-O(70)	73.2(6)	O(41)-Nd(12)-O(40)	67.6(6)
O(30)-Nd(10)-O(37)	81.5(6)	O(48)-Nd(12)-O(40)	125.6(6)
O(63)-Nd(10)-O(37)	67.9(7)	O(51)-Nd(12)-O(40)	82.3(6)
O(33)-Nd(10)-O(37)	129.2(6)	O(47)-Nd(12)-O(40)	128.0(6)
O(35)-Nd(10)-O(37)	136.3(6)	O(44)-Nd(12)-O(40)	139.7(6)
O(38)-Nd(10)-O(37)	69.4(6)	O(41)-Nd(12)-O(71)	78.5(6)
O(32)-Nd(10)-O(37)	131.3(6)	O(48)-Nd(12)-O(71)	74.1(6)
O(70)-Nd(10)-O(37)	69.2(7)	O(51)-Nd(12)-O(71)	92.4(6)
O(30)-Nd(10)-O(34)	133.7(5)	O(47)-Nd(12)-O(71)	73.0(6)
O(63)-Nd(10)-O(34)	70.7(6)	O(44)-Nd(12)-O(71)	139.9(6)
O(33)-Nd(10)-O(34)	66.6(5)	O(40)-Nd(12)-O(71)	65.9(6)
O(35)-Nd(10)-O(34)	67.8(5)	O(41)-Nd(12)-O(72)	86.1(6)
O(38)-Nd(10)-O(34)	66.9(5)	O(48)-Nd(12)-O(72)	133.3(6)
O(32)-Nd(10)-O(34)	108.6(5)	O(51)-Nd(12)-O(72)	82.9(6)
O(70)-Nd(10)-O(34)	136.5(6)	O(47)-Nd(12)-O(72)	137.9(6)
O(37)-Nd(10)-O(34)	119.9(6)	O(44)-Nd(12)-O(72)	74.0(6)
O(42)-Nd(11)-O(39)	85.0(7)	O(40)-Nd(12)-O(72)	74.9(6)
O(42)-Nd(11)-O(48)	133.1(6)	O(71)-Nd(12)-O(72)	140.7(6)
O(39)-Nd(11)-O(48)	81.7(6)	O(41)-Nd(12)-O(43)	66.7(5)
O(42)-Nd(11)-O(33)	79.5(6)	O(48)-Nd(12)-O(43)	64.3(5)
O(39)-Nd(11)-O(33)	134.0(6)	O(51)-Nd(12)-O(43)	133.4(5)
O(48)-Nd(11)-O(33)	138.1(5)	O(47)-Nd(12)-O(43)	108.3(5)
O(42)-Nd(11)-O(38)	91.1(6)	O(44)-Nd(12)-O(43)	67.7(5)
O(39)-Nd(11)-O(38)	66.7(6)	O(40)-Nd(12)-O(43)	122.7(6)
O(48)-Nd(11)-O(38)	123.3(6)	O(71)-Nd(12)-O(43)	132.5(5)
O(33)-Nd(11)-O(38)	70.6(5)	O(72)-Nd(12)-O(43)	69.6(5)
O(42)-Nd(11)-O(41)	67.4(6)	O(47)-Nd(13)-O(54)	153.6(6)
O(39)-Nd(11)-O(41)	97.4(6)	O(47)-Nd(13)-O(50)	135.5(6)
O(48)-Nd(11)-O(41)	70.0(5)	O(54)-Nd(13)-O(50)	68.1(6)
O(33)-Nd(11)-O(41)	115.4(5)	O(47)-Nd(13)-O(51)	68.4(6)
O(38)-Nd(11)-O(41)	154.9(6)	O(54)-Nd(13)-O(51)	132.5(6)
O(42)-Nd(11)-O(43)	112.5(6)	O(50)-Nd(13)-O(51)	67.1(6)
O(39)-Nd(11)-O(43)	146.7(6)	O(47)-Nd(13)-O(44)	67.4(5)
O(48)-Nd(11)-O(43)	65.6(5)	O(54)-Nd(13)-O(44)	131.0(5)
O(33)-Nd(11)-O(43)	78.5(5)	O(50)-Nd(13)-O(44)	94.3(6)
O(38)-Nd(11)-O(43)	136.8(5)	O(51)-Nd(13)-O(44)	67.7(5)
O(41)-Nd(11)-O(43)	66.7(5)	O(47)-Nd(13)-O(62)	82.5(5)

O(54)-Nd(13)-O(62)	82.6(5)	O(75)-Nd(14)-O(45)	151.8(9)
O(50)-Nd(13)-O(62)	136.3(6)	O(50)-Nd(14)-O(56)	151.9(6)
O(51)-Nd(13)-O(62)	143.2(6)	O(75)-Nd(14)-O(56)	91.3(10)
O(44)-Nd(13)-O(62)	80.8(5)	O(45)-Nd(14)-O(56)	103.2(5)
O(47)-Nd(13)-O(45)	127.2(5)	O(50)-Nd(14)-O(54)	69.3(6)
O(54)-Nd(13)-O(45)	67.0(5)	O(75)-Nd(14)-O(54)	82.5(9)
O(50)-Nd(13)-O(45)	68.2(5)	O(45)-Nd(14)-O(54)	70.3(5)
O(51)-Nd(13)-O(45)	109.1(5)	O(56)-Nd(14)-O(54)	136.5(6)
O(44)-Nd(13)-O(45)	64.0(5)	O(50)-Nd(14)-O(53)	136.5(6)
O(62)-Nd(13)-O(45)	70.8(5)	O(75)-Nd(14)-O(53)	75.2(9)
O(47)-Nd(13)-O(46)	68.0(5)	O(45)-Nd(14)-O(53)	87.4(5)
O(54)-Nd(13)-O(46)	86.2(6)	O(56)-Nd(14)-O(53)	69.1(6)
O(50)-Nd(13)-O(46)	137.0(6)	O(54)-Nd(14)-O(53)	67.7(6)
O(51)-Nd(13)-O(46)	117.3(6)	O(50)-Nd(14)-O(49)	71.0(6)
O(44)-Nd(13)-O(46)	127.9(5)	O(75)-Nd(14)-O(49)	70.3(10)
O(62)-Nd(13)-O(46)	68.0(5)	O(45)-Nd(14)-O(49)	131.1(6)
O(45)-Nd(13)-O(46)	133.0(5)	O(56)-Nd(14)-O(49)	94.5(6)
O(47)-Nd(13)-O(73)	97.4(6)	O(54)-Nd(14)-O(49)	122.8(6)
O(54)-Nd(13)-O(73)	77.4(6)	O(53)-Nd(14)-O(49)	141.4(6)
O(50)-Nd(13)-O(73)	72.3(6)	O(50)-Nd(14)-O(55)	80.4(6)
O(51)-Nd(13)-O(73)	74.7(6)	O(75)-Nd(14)-O(55)	135.3(10)
O(44)-Nd(13)-O(73)	142.3(6)	O(45)-Nd(14)-O(55)	72.8(6)
O(62)-Nd(13)-O(73)	133.2(6)	O(56)-Nd(14)-O(55)	72.0(6)
O(45)-Nd(13)-O(73)	134.1(6)	O(54)-Nd(14)-O(55)	137.7(6)
O(46)-Nd(13)-O(73)	68.8(6)	O(53)-Nd(14)-O(55)	130.4(6)
O(50)-Nd(14)-O(75)	105.3(10)	O(49)-Nd(14)-O(55)	70.1(7)
O(50)-Nd(14)-O(45)	72.4(5)		
