Supporting information

A Series of Cadmium(II) Coordination Polymers Based on a Versatile Multi N-Donor Tecton or Mixed Carboxylate Ligands: Synthesis, Structure and Selectively Sensing Property

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Table S1 Selected bond lengths [Å] and bond angles [º] for complexes **1 - 5**

1			
Cd(1)-N(7)	2.196(5)	Cd(1)-N(5)#1	2.215(4)
Cd(1)-N(11)#2	2.223(4)	Cd(1)-N(1)	2.370(3)
N(7)-Cd(1)-N(5)#1	141.31(15)	N(7)-Cd(1)-N(11)#2	98.07(15)
N(5)#1-Cd(1)-N(11)#2	116.17(15)	N(7)-Cd(1)-N(1)	99.88(16)
N(5)#1-Cd(1)-N(1)	83.28(12)	N(11)#2-Cd(1)-N(1)	113.39(16)
2			
Cd(1)-O(1W)	2.323(4)	Cd(1)-N(2)	2.330(4)
O(1W)-Cd(1)-O(1W)#3	179.999(1)	O(1W)-Cd(1)-N(2)	85.99(12)
O(1W)-Cd(1)-N(2)#3	94.01(12)	N(2)-Cd(1)-N(2)#4	90.9(2)
N(2)-Cd(1)-N(2)#3	179.999(1)	O(1W)-Cd(1)-N(2)#5	94.01(12)
N(2)-Cd(1)-N(2)#5	89.1(2)	N(2)#4-Cd(1)-N(2)#5	180.00(14)
3			
Cd(1)-O(2)#6	2.292(2)	Cd(1)-N(1)	2.301(3)
Cd(1)-O(4)#9	2.346(2)	Cd(2)-N(2)#11	2.208(3)

Cd(2)-N(5)	2.225(3)	Cd(2)-O(3)	2.328(3)
Cd(2)-O(1)	2.358(2)	Cd(2)-O(1)#12	2.382(2)
Cd(2)-O(4)#13	2.560(2)	Cd(2)-O(3)#13	2.583(3)
O(2)#6-Cd(1)-O(2)#7	180.00(12)	O(2)#6-Cd(1)-N(1)	93.77(10)
O(2)#7-Cd(1)-N(1)	86.23(10)	O(2)#6-Cd(1)-N(1)#8	86.23(10)
O(2)#7-Cd(1)-N(1)#8	93.77(10)	N(1)-Cd(1)-N(1)#8	180.00(10)
O(2)#6-Cd(1)-O(4)#9	85.71(8)	O(2)#7-Cd(1)-O(4)#9	94.29(8)
N(1)-Cd(1)-O(4)#9	93.41(9)	N(1)#8-Cd(1)-O(4)#9	86.59(9)
O(2)#6-Cd(1)-O(4)#10	94.29(8)	N(1)-Cd(1)-O(4)#10	86.59(9)
O(4)#9-Cd(1)-O(4)#10	180.0	N(2)#11-Cd(2)-N(5)	176.09(11)
N(2)#11-Cd(2)-O(3)	98.17(10)	N(5)-Cd(2)-O(3)	83.11(11)
N(2)#11-Cd(2)-O(1)	93.08(10)	N(5)-Cd(2)-O(1)	90.79(10)
O(3)-Cd(2)-O(1)	79.19(9)	N(2)#11-Cd(2)-O(1)#12	94.00(10)
N(5)-Cd(2)-O(1)#12	86.06(11)	O(3)-Cd(2)-O(1)#12	156.82(10)
O(1)-Cd(2)-O(1)#12	80.54(9)	N(2)#11-Cd(2)-O(4)#13	90.42(9)
N(5)-Cd(2)-O(4)#13	85.79(9)	O(3)-Cd(2)-O(4)#13	122.31(8)
O(1)-Cd(2)-O(4)#13	157.47(8)	O(1)#12-Cd(2)-O(4)#13	77.02(8)
N(2)#11-Cd(2)-O(3)#13	86.39(10)	N(5)-Cd(2)-O(3)#13	90.47(10)
O(3)-Cd(2)-O(3)#13	73.09(10)	O(1)-Cd(2)-O(3)#13	151.89(8)
O(1)#12-Cd(2)-O(3)#13	127.56(8)	O(4)#13-Cd(2)-O(3)#13	50.55(7)
4			
Cd(1)-O(1)	2.199(3)	Cd(1)-N(7)	2.334(4)
Cd(1)-N(9)#14	2.385(4)	Cd(1)-N(6)#15	2.396(3)
Cd(1)-N(12)#16	2.408(4)	Cd(1)-O(6)	2.475(3)
Cd(2)-O(3)#17	2.250(3)	Cd(2)-N(3)#18	2.293(3)
Cd(2)-N(1)	2.296(4)	Cd(2)-N(5)#15	2.310(3)
Cd(2)-O(6)	2.420(3)	Cd(2)-N(10)#14	2.427(3)
O(1)-Cd(1)-N(7)	89.53(13)	O(1)-Cd(1)-N(9)#14	97.28(13)
N(7)-Cd(1)-N(9)#14	94.89(13)	O(1)-Cd(1)-N(6)#15	102.93(11)
N(7)-Cd(1)-N(6)#15	166.40(13)	N(9)#14-Cd(1)-N(6)#15	88.99(11)
O(1)-Cd(1)-N(12)#16	100.85(13)	N(7)-Cd(1)-N(12)#16	88.57(13)
N(9)#14-Cd(1)-N(12)#16	161.57(12)	N(6)#15-Cd(1)-N(12)#16	83.79(12)
O(1)-Cd(1)-O(6)	171.49(12)	N(7)-Cd(1)-O(6)	82.14(12)

N(9)#14-Cd(1)-O(6)	81.76(12)	N(6)#15-Cd(1)-O(6)	85.54(11)
N(12)#16-Cd(1)-O(6)	80.79(12)	O(3)#17-Cd(2)-N(3)#18	100.04(13)
O(3)#17-Cd(2)-N(1)	91.71(14)	N(3)#18-Cd(2)-N(1)	93.04(13)
O(3)#17-Cd(2)-N(5)#15	163.24(13)	N(3)#18-Cd(2)-N(5)#15	96.51(12)
N(1)-Cd(2)-N(5)#15	90.00(13)	O(3)#17-Cd(2)-O(6)	84.66(12)
N(3)#18-Cd(2)-O(6)	173.89(11)	N(1)-Cd(2)-O(6)	90.71(13)
N(5)#15-Cd(2)-O(6)	78.64(12)	O(3)#17-Cd(2)-N(10)#14	91.82(13)
N(3)#18-Cd(2)-N(10)#14	92.14(12)	N(1)-Cd(2)-N(10)#14	173.13(13)
N(5)#15-Cd(2)-N(10)#14	84.93(12)	O(6)-Cd(2)-N(10)#14	83.76(12)
5			
Cd(1)-O(4)#19	2.255(2)	Cd(1)-N(2)#20	2.292(3)
Cd(1)-O(1)	2.331(3)	Cd(1)-O(8)	2.338(4)
Cd(1)-O(2)	2.359(3)	Cd(1)-O(6)#21	2.375(3)
Cd(2)-N(5)	2.192(3)	Cd(2)-O(5)#22	2.243(3)
Cd(2)-N(1)#23	2.256(3)	Cd(2)-O(7)	2.323(4)
Cd(2)-O(3)	2.395(3)		
O(4)#19-Cd(1)-N(2)#20	121.77(10)	O(4)#19-Cd(1)-O(1)	93.44(10)
N(2)#20-Cd(1)-O(1)	142.41(11)	O(4)#19-Cd(1)-O(8)	84.35(11)
N(2)#20-Cd(1)-O(8)	103.76(13)	O(1)-Cd(1)-O(8)	91.49(14)
O(4)#19-Cd(1)-O(2)	147.25(11)	N(2)#20-Cd(1)-O(2)	90.87(11)
O(1)-Cd(1)-O(2)	55.88(10)	O(8)-Cd(1)-O(2)	85.27(15)
O(4)#19-Cd(1)-O(6)#21	80.93(10)	N(2)#20-Cd(1)-O(6)#21	82.78(10)
O(1)-Cd(1)-O(6)#21	91.07(10)	O(8)-Cd(1)-O(6)#21	165.18(11)
O(2)-Cd(1)-O(6)#21	108.16(12)	N(5)-Cd(2)-O(5)#22	92.32(11)
N(5)-Cd(2)-N(1)#23	130.23(11)	O(5)#22-Cd(2)-N(1)#23	136.83(10)
N(5)-Cd(2)-O(7)	91.81(15)	O(5)#22-Cd(2)-O(7)	91.56(15)
N(1)#23-Cd(2)-O(7)	93.66(13)	N(5)-Cd(2)-O(3)	103.20(12)
O(5)#22-Cd(2)-O(3)	83.09(10)	N(1)#23-Cd(2)-O(3)	80.45(10)
O(7)-Cd(2)-O(3)	164.21(15)		

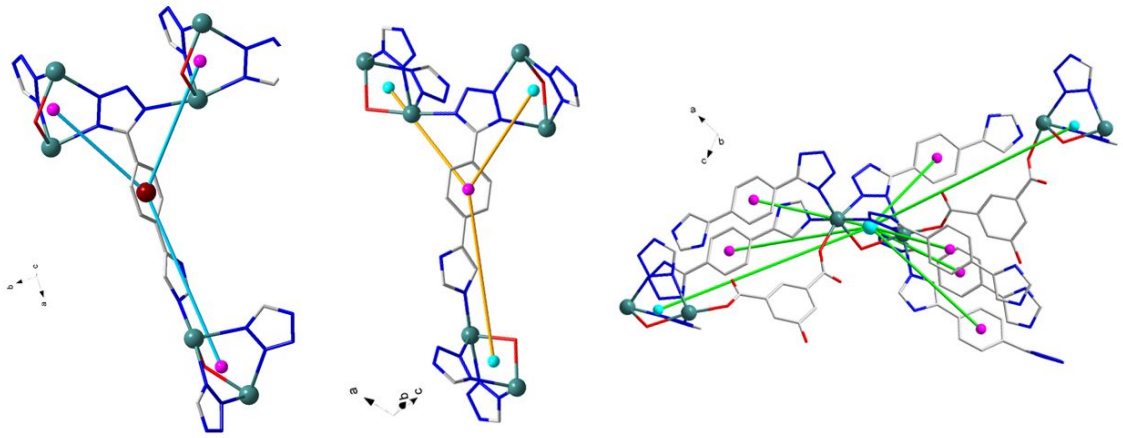
Symmetry transformations used to generate equivalent atoms: #1 -*x*, *y*+1/2, -*z*, #2 *x*, *y*-1, *z*, #3 -*x*, -*y*+2, -*z*+1, #4 *x*, *y*, -*z*+1, #5 -*x*, -*y*+2, *z*, #6 -*x*+1, -*y*+1, -*z*+1, #7 *x*, *y*+1, *z*-1, #8 -*x*+1, -*y*+2, -*z*, #9 -*x*+2, -*y*+1, -*z*+1, #10 *x*-1, *y*+1, *z*-1, #11 *x*, *y*, *z*+1, #12 -*x*+1, -*y*+1, -*z*+2, #13 -*x*+2, -*y*+1, -*z*+2, #14 -*x*+3/2, *y*-1/2, -*z*+1/2, #15 *x*-1/2, -*y*+3/2, *z*-1/2, #16 -*x*+3/2, *y*+1/2, -*z*+1/2, #17 *x*+1/2,

-*y*+1/2, *z*+1/2, #18 -*x*+3, -*y*+1, -*z*+1, #19 *x*-1, *y*+1, *z*, #20 -*x*, -*y*+1, -*z*+2, #21 -*x*+1, -*y*+1, -*z*+1, #22 -*x*+2, -*y*, -*z*+1, #23 -*x*+1, -*y*, -*z*+2.

Table S2. Hydrogen bonding interactions for complexes **1** and **3** - **5** (Å, °)

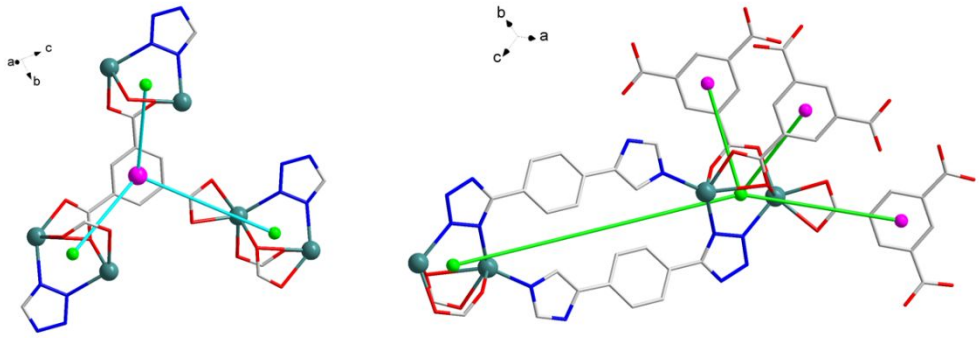
complex	D–H···A	D–H	H···A	D···A	∠DHA
1	N(6)-H(6A)···N(2)[a]	0.8600	2.5900	3.244(7)	134.00
	N(8)-H(8)···N(9)[b]	0.8600	2.1800	2.994(7)	158.00
	C(3)-H(3)···N(12)[a]	0.9300	2.4900	3.107(6)	124.00
3	C(19)-H(19)···N(10)[a]	0.9300	2.5500	3.304(7)	138.00
	C(5)-H(5)···N(3)	0.9300	2.5500	2.869(5)	101.00
4	N(2)-H(2A)···O(2)[a]	0.8600	2.0500	2.907(5)	175.00
	O(6)-H(6A)···N(11)[b]	0.9700	2.4000	3.051(5)	124.00
	O(6)-H(6B)···O(4)[c]	0.9700	1.7800	2.621(7)	143.00
	C(1)-H(1)···O(2)[a]	0.9300	2.5100	3.430(5)	168.00
	C(9)-H(9)···N(4)[d]	0.9300	2.5600	3.211(5)	128.00
	C(20)-H(20)···O(4)[c]	0.9300	2.5000	3.409(9)	166.00
	C(23)-H(23)···O(1)	0.9300	2.4300	2.741(7)	100.00
5	N(6)-H(6A)···O(9)[a]	0.8600	1.9400	2.792(5)	169.00
	C(15)-H(15)···O(1)[a]	0.9300	2.6000	3.226(4)	125.00
	C(17)-H(17)···O(4)	0.9300	2.4400	2.761(4)	100.00
	C(17)-H(17)···O(5)	0.9300	2.4000	2.723(4)	100.00

Symmetry codes: (a) *x*, -1+*y*, *z*; (b) -1-*x*, -1/2+*y*, 1-*z* for **1**. (a) -1+*x*, *y*, *z*; (b) 1-*x*, 1-*y*, 1-*z* for **3**. (a) 5/2-*x*, 1/2+*y*, 1/2-*z*; (b) 3/2-*x*, 1/2+*y*, 1/2-*z*; (c) 1/2+*x*, 1/2-*y*, 1/2+*z*; (d) -1/2+*x*, 3/2-*y*, -1/2+*z* for **4**. (a) 1-*x*, 1-*y*, 1-*z* for **5**.



(A) **(B)** **(C)**

Figure S1. Ball-and-stick representations of two kinds of 3-connected HL^- ligand (A and B) and 8-connected binuclear Cd(II) cluster of **4** (C).



(A) **(B)**

Figure S2. Ball-and-stick representations of the 3-connected btc^{3-} ligand (A) and 5-connected binuclear Cd(II) unit of **5** (B).

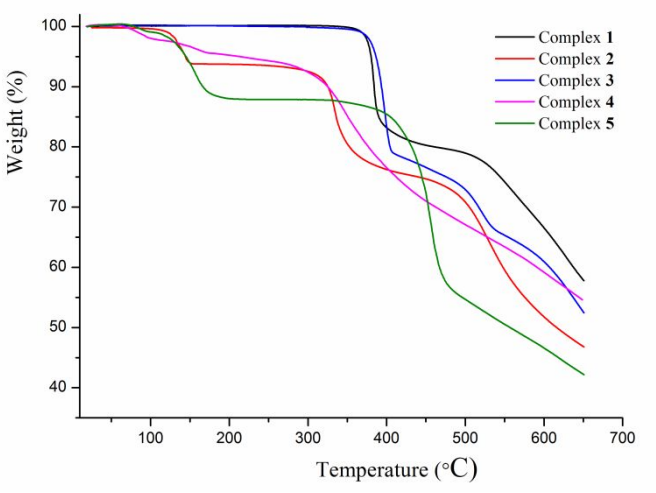
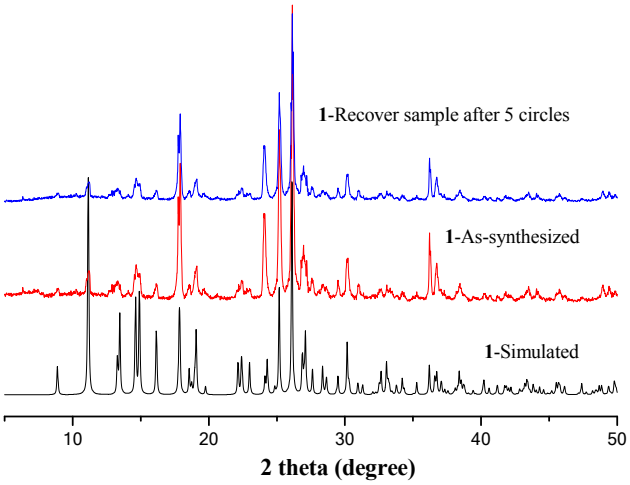
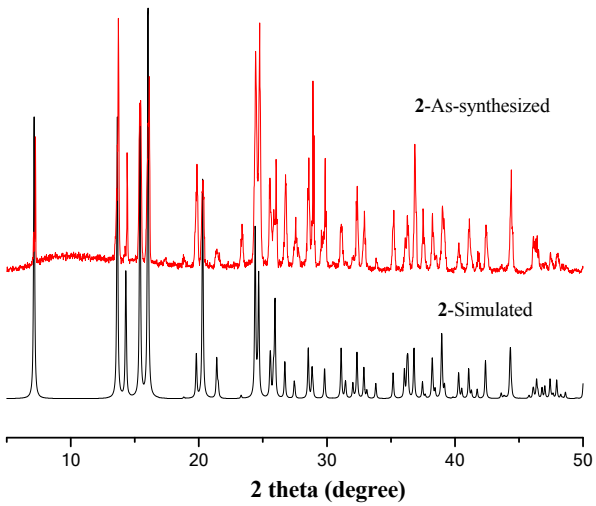
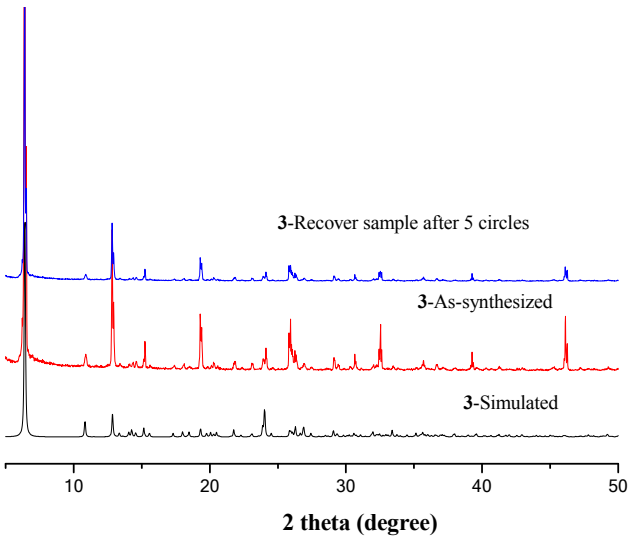
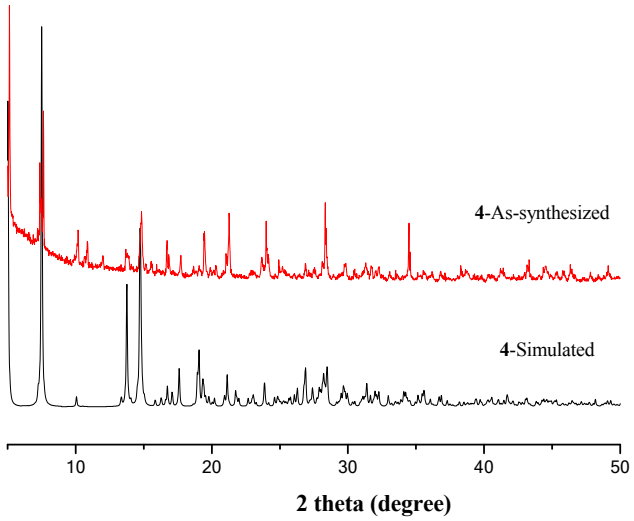


Figure S3. The TG curves of complexes **1 – 5.**




2-As-synthesized
2-Simulated
10
20
30
40
50
2 theta (degree)


3-Recover sample after 5 circles
3-As-synthesized
3-Simulated
10
20
30
40
50
2 theta (degree)



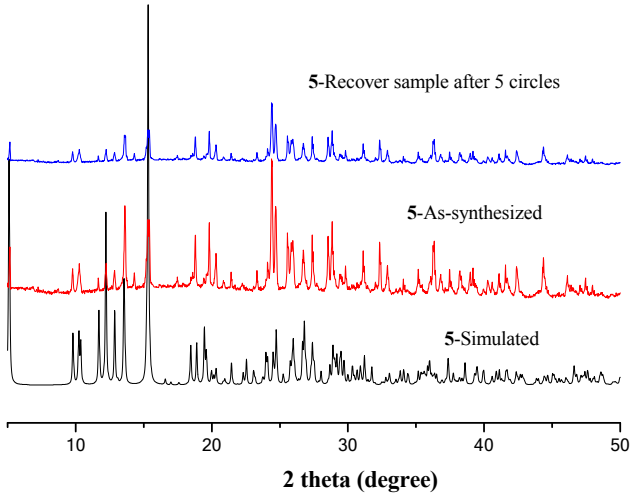


Figure S4. The X-ray powder diffraction patterns of complexes **1** - **5**.

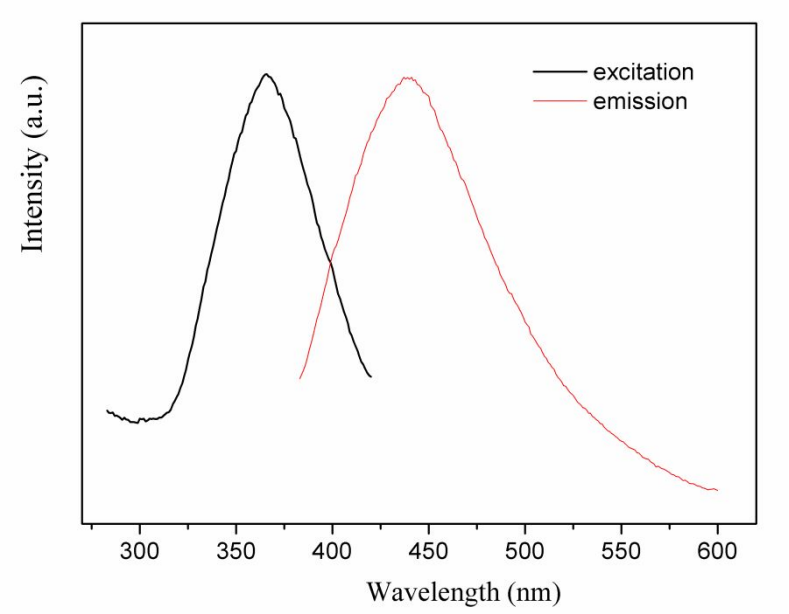
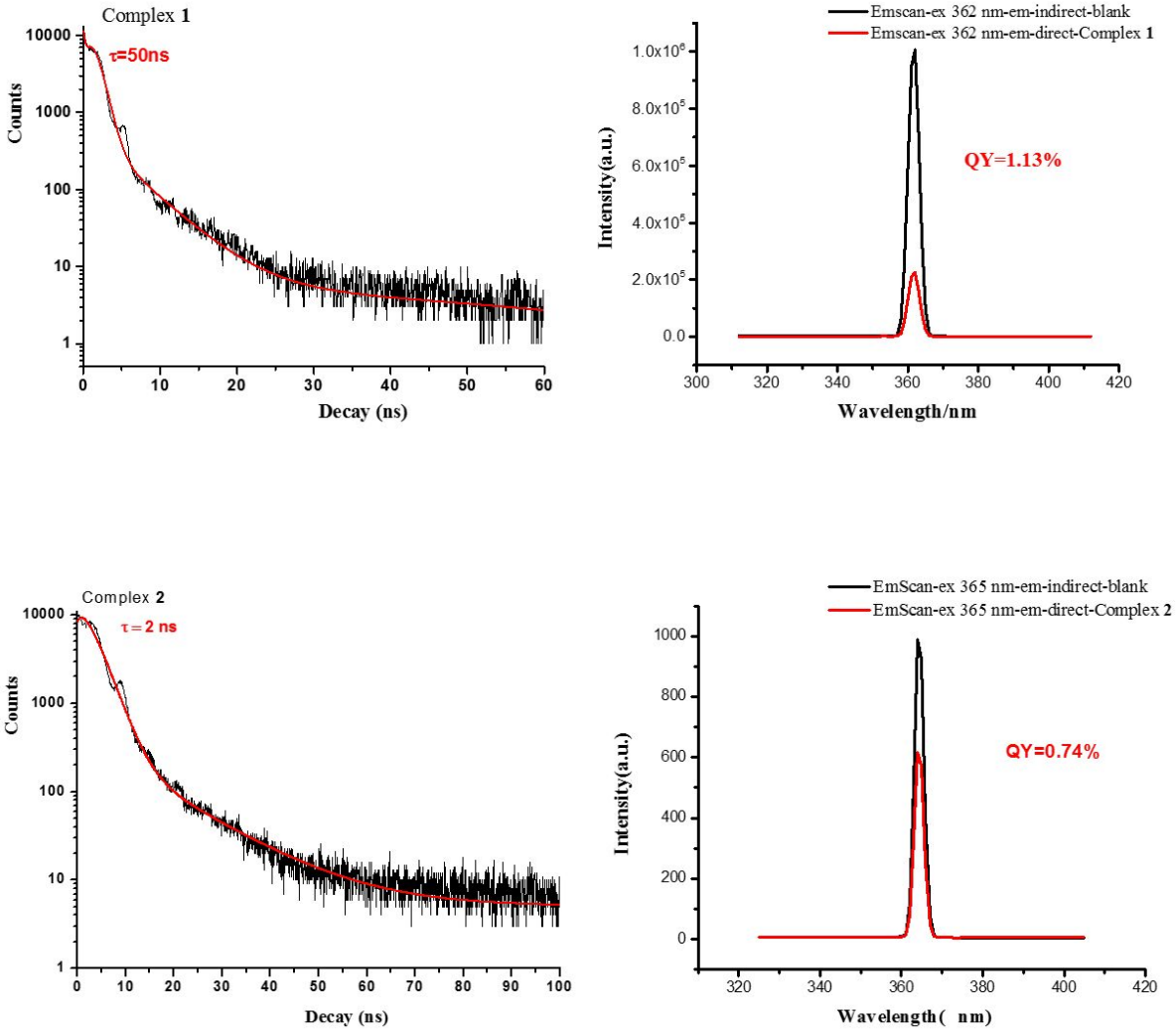


Figure S5. Photoluminescent spectra of H_2L.



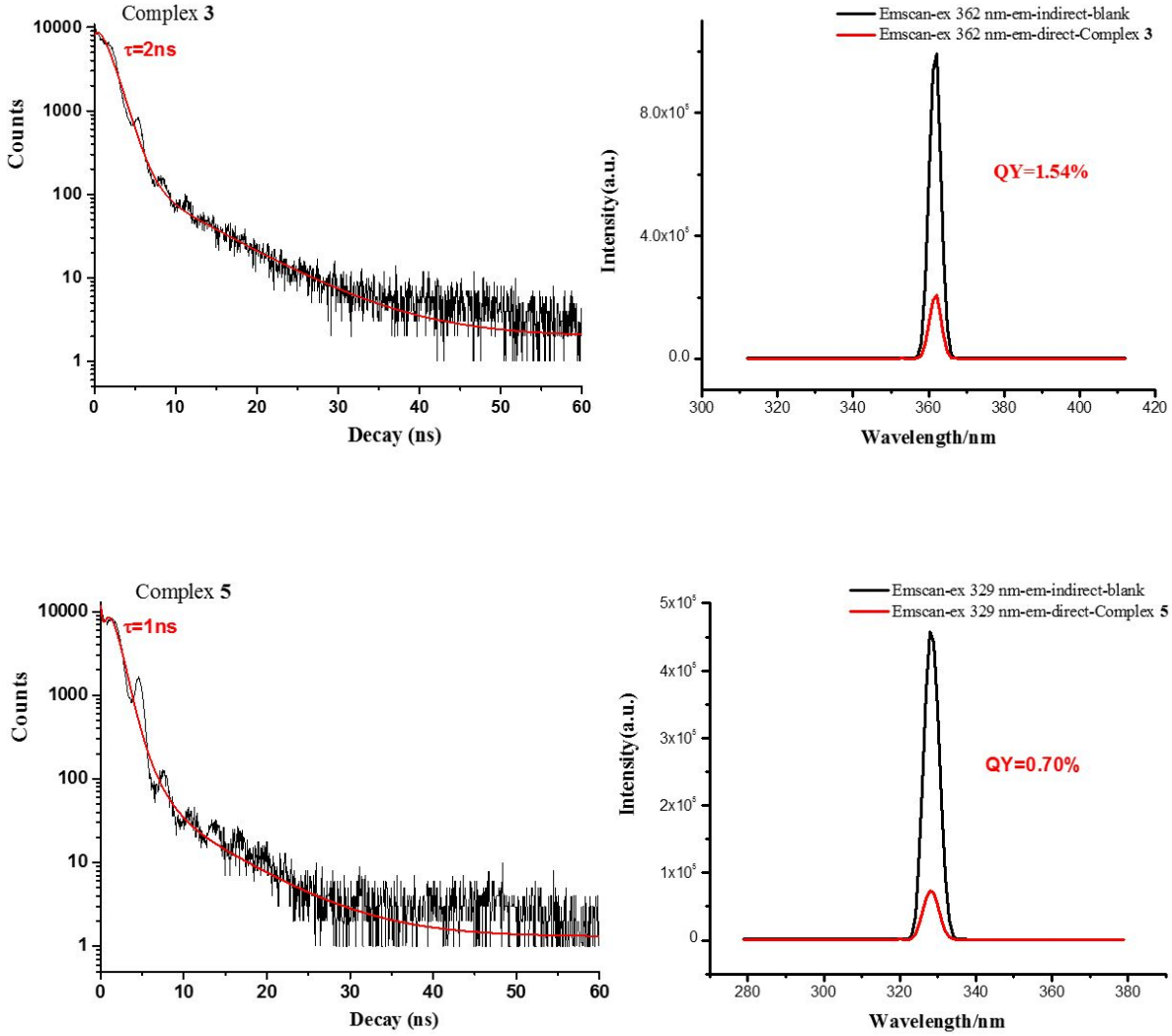


Figure S6. The decay curves and QY of compounds **1-3** and **5**.

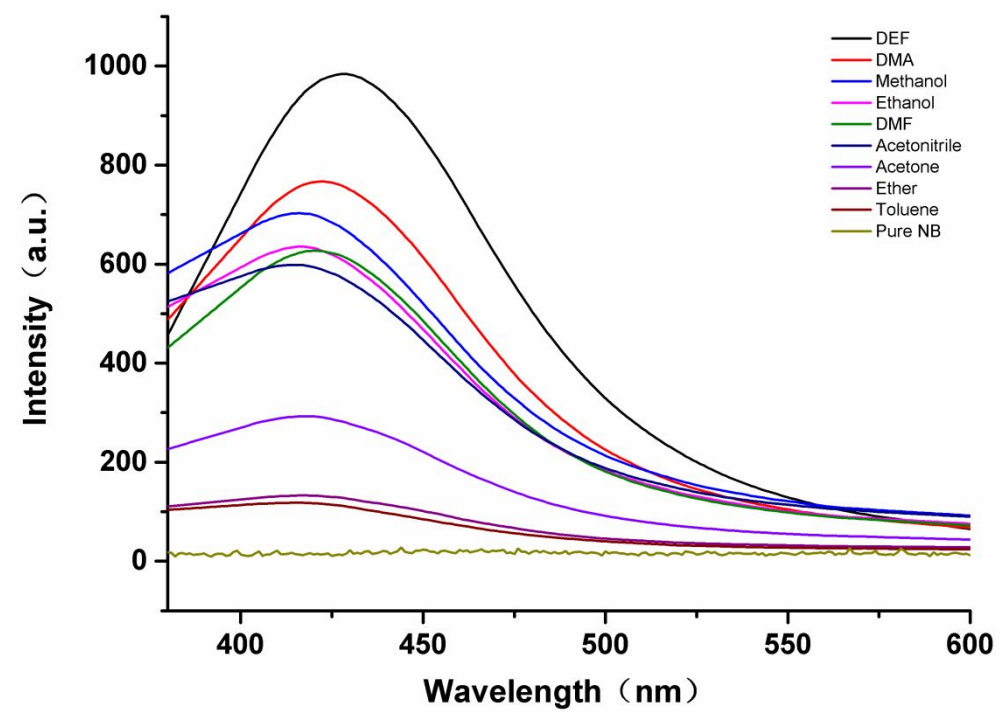


Figure S7. The fluorescent emission of complex **1** dispersed in different organic solvents.

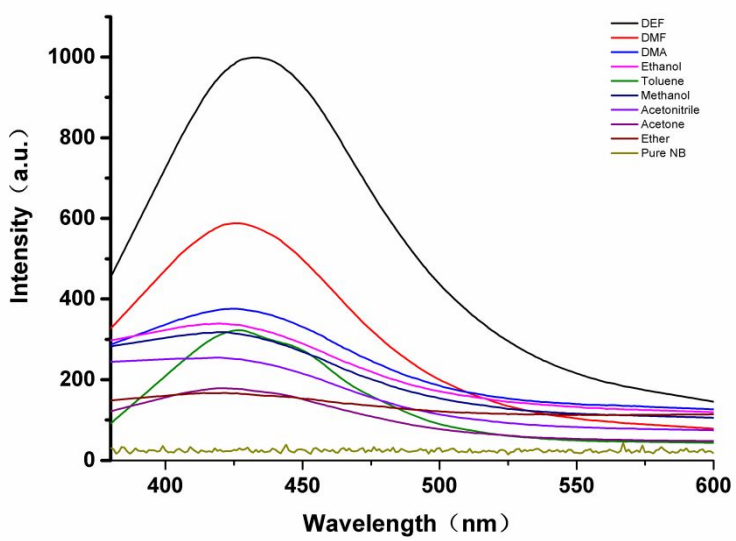


Figure S8. The fluorescent emission of complex **3** dispersed in different organic solvents.

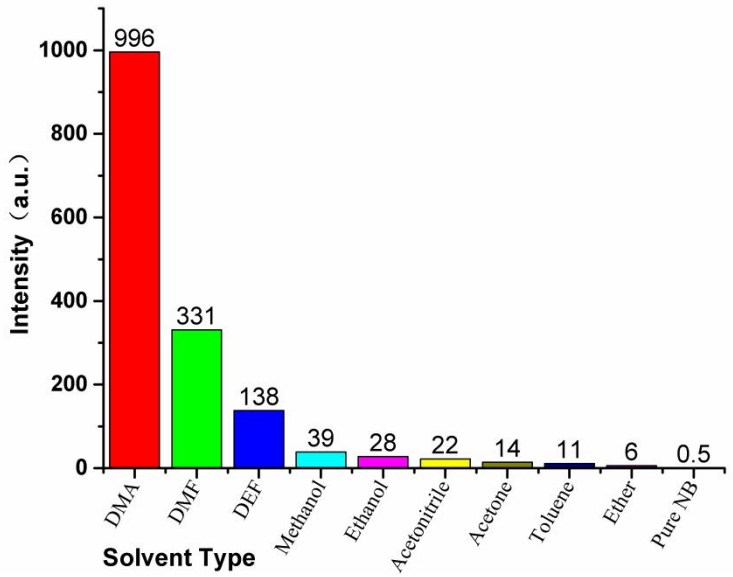


Figure S9. The fluorescent emission of complex **5** dispersed in different organic solvents.

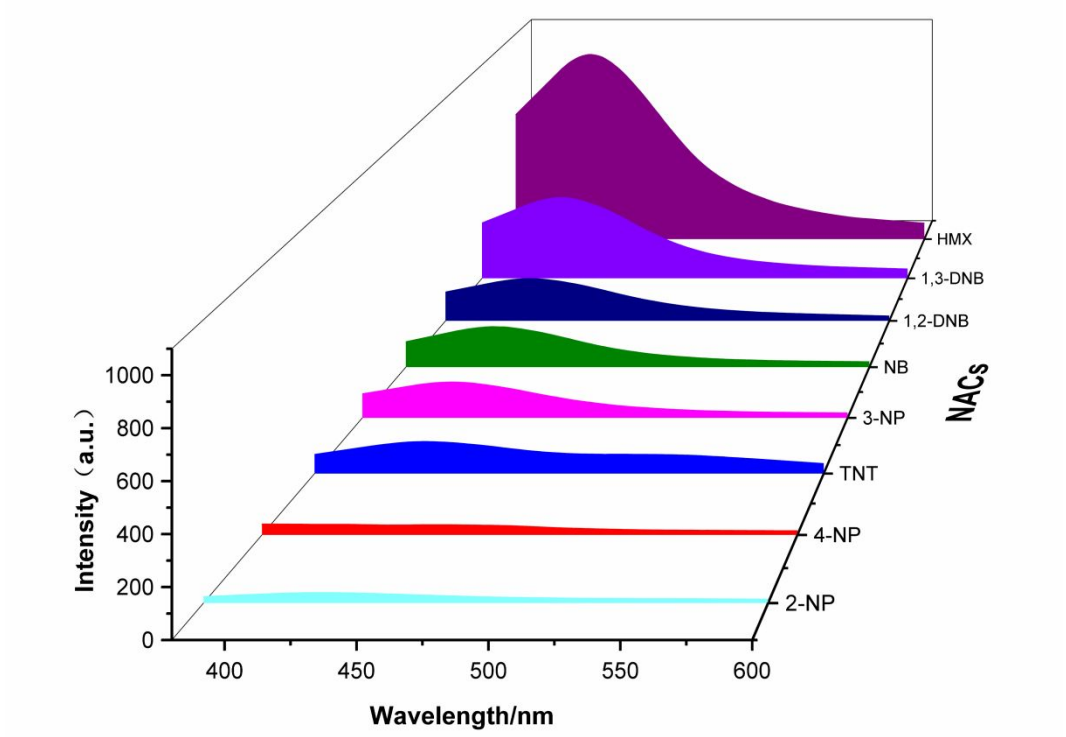


Figure S10. Fluorescence intensity curve obtained by introducing different nitrobenzene derivatives into the DMF-emulsion of complex **1**.

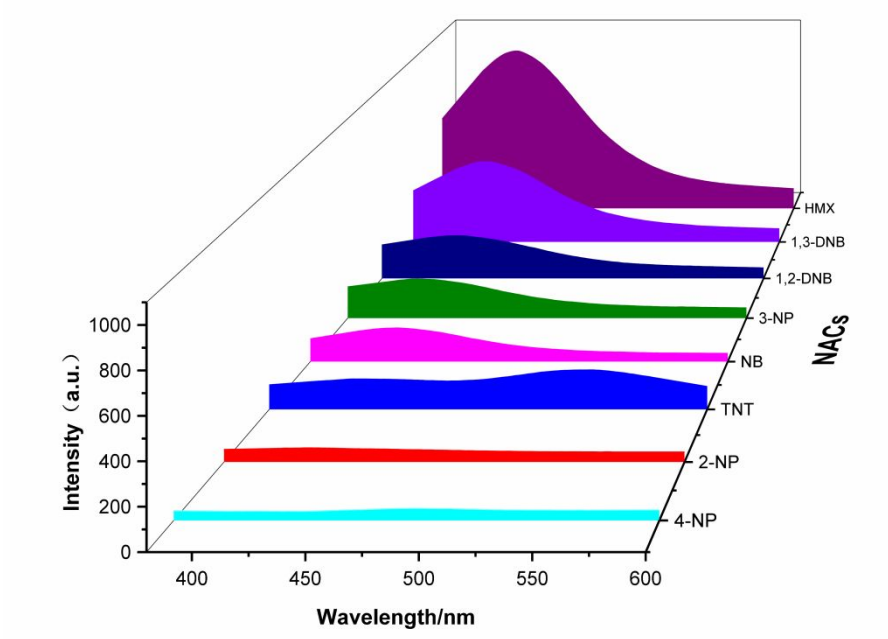
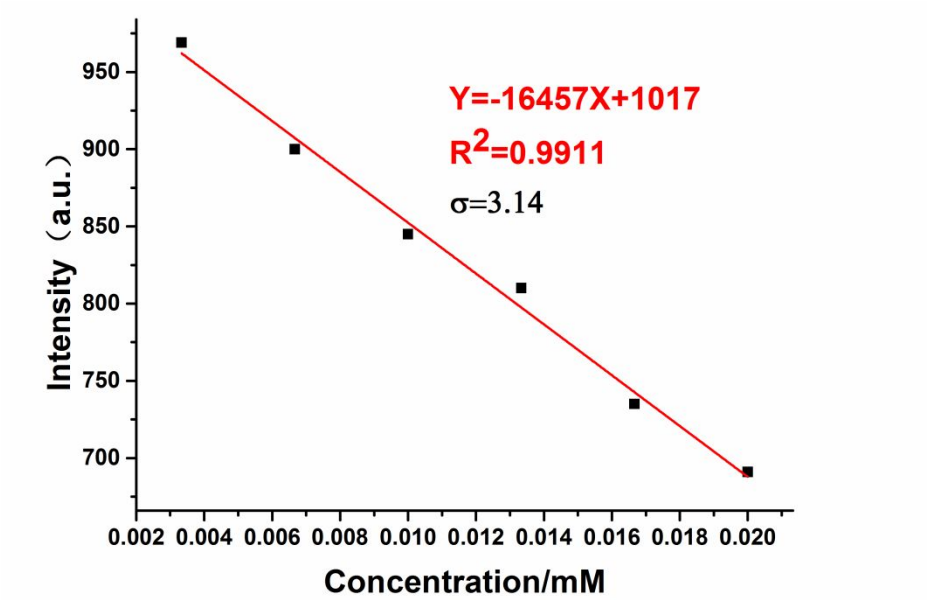


Figure S11. Fluorescence intensity curve obtained by introducing different nitrobenzene derivatives into the DMF-emulsion of complex **3**.

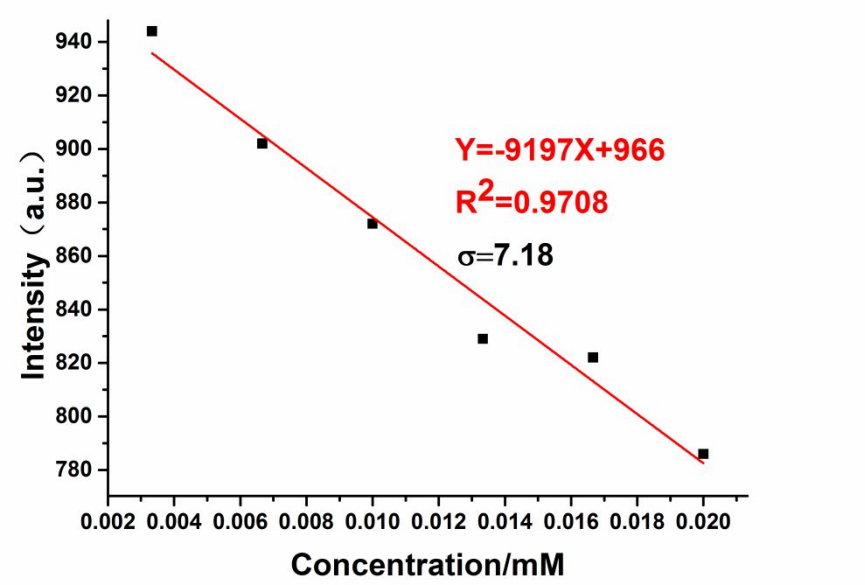


Linear Equation: $Y = -16457X + 1017$; $R^2 = 0.9911$

Slope = 1.65×10^7 M^{-1}; δ=3.14 (N=10);

Limit detection =3δ/Slope=5.75×10^{-7} M

Figure S12. The fitting curve of the luminescence intensity of **5** upon the incremental addition of 4-NP (linear range 0-0.020 mM).

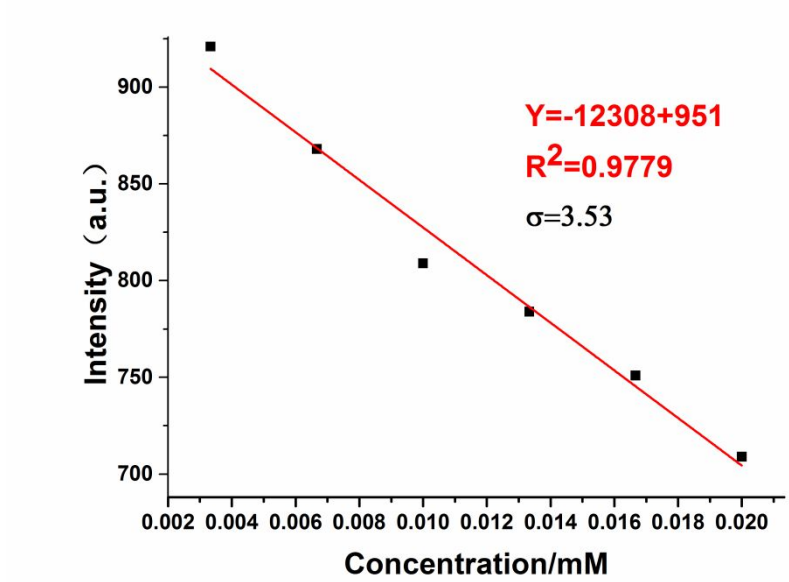


Linear Equation: Y = -9197X + 966; R^2 = 0.9708

Slope = 9.20 × 10^6 M^{-1}; δ=7.18 (N=10)

Limit detection =3δ/Slope=2.30 ×10^{-6} M

Figure S13. The fitting curve of the luminescence intensity of **1** upon the incremental addition of Fe^{3+} concentration (linear range 0-0.020 mM).



Linear Equation: Y = -12308X + 951; R^2 = 0.9779

Slope = 1.23 × 10^7 M^{-1}; δ=3.53 (N=10)

Limit detection =3δ/Slope=8.60 ×10^{-7} M

Figure S14. The fitting curve of the luminescence intensity of **3** upon the incremental addition of Fe^{3+} concentration (linear range 0-0.020 mM).

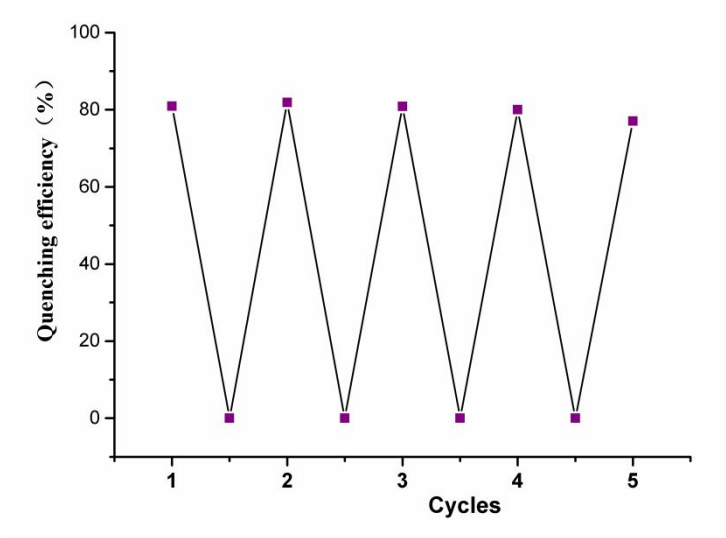


Figure S15. The quenching and recyclability test of **1**, the upper dots represent the initial luminescence intensity and the lower dots represent the intensity upon addition of 1 mM of the DMF solution of Fe^{3+}.

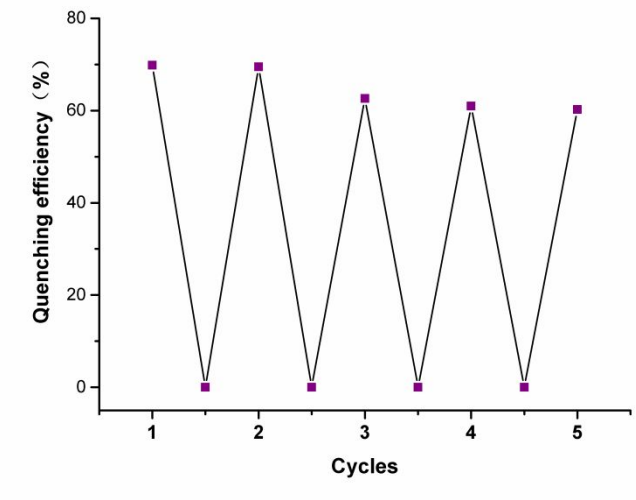


Figure S16. The quenching and recyclability test of **3**, the upper dots represent the initial luminescence intensity and the lower dots represent the intensity upon addition of 1 mM of the DMF solution of Fe^{3+}.

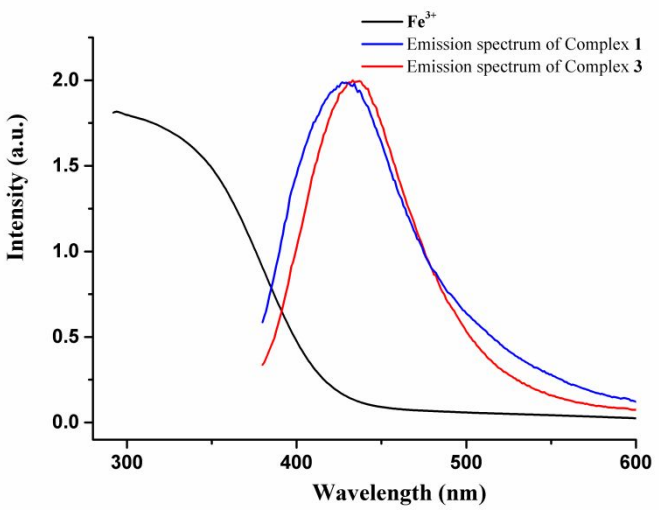


Figure S17. UV-vis spectra of Fe^{3+} and emission spectrum of complexes **1** and **3** in DMF.