Electronic Supplementary Information (ESI) for

Five new Coordination Polymers with a Y-shaped N-heterocyclic carboxylic acid: Structural Diversity, Bifunctional Luminescence Sensing and Magnetic Properties

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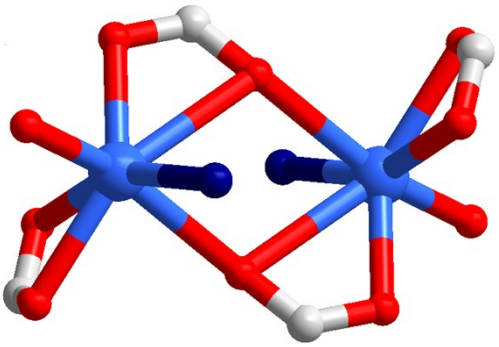

Fig. S1 The dinuclear $[Cd_2(COO)_4]$ SBUs in **1**.

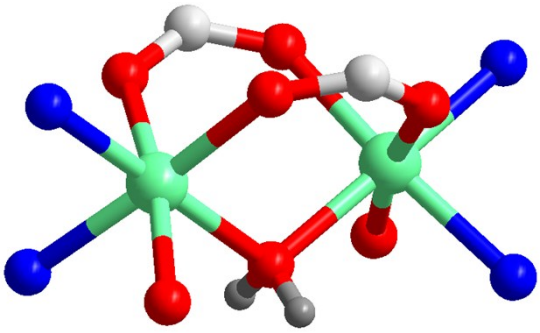

Fig. S2 The dinuclear $\{Ni_2(COO)_2(\mu_2\text{-}H_2O)\}$ SBUs in **4**.

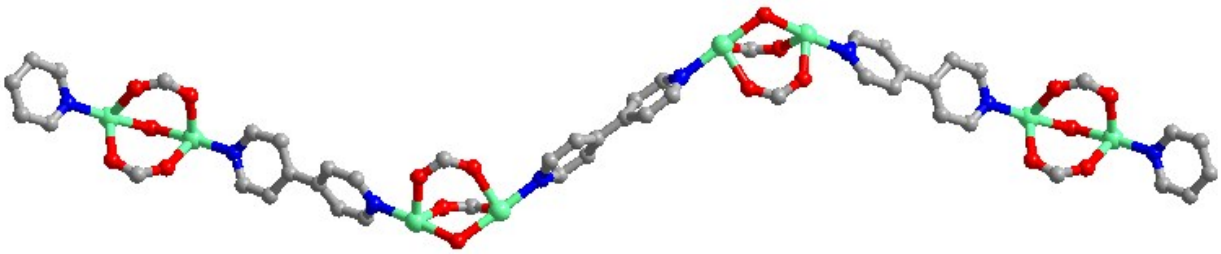

Fig. S3 The 4,4'-bipy linked the $\{Ni_2(COO)_2(\mu_2\text{-}H_2O)\}$ SBUs to form a 1D chain along *a* axis in **4**.

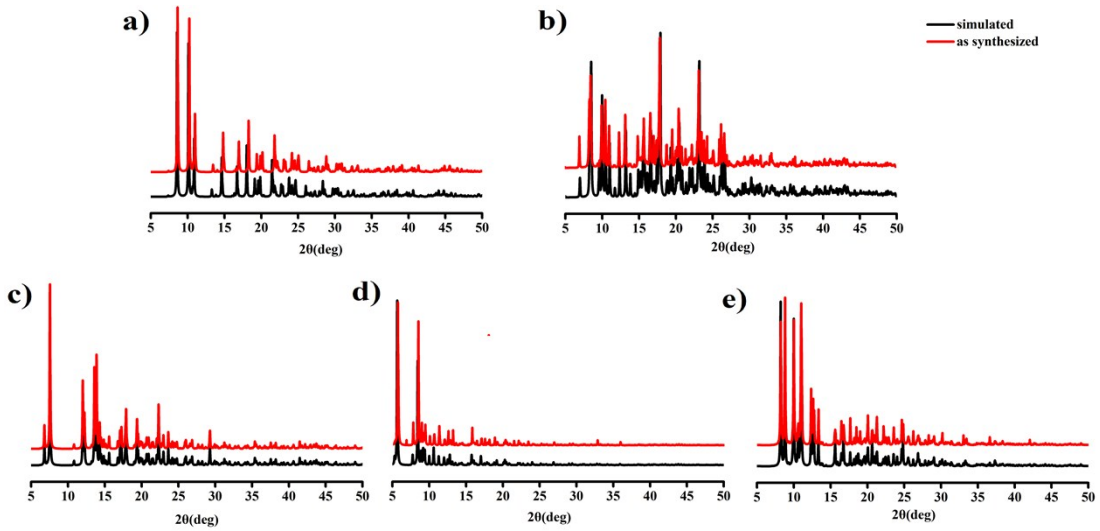

Fig. S4 PXRD patterns of **1-5**.

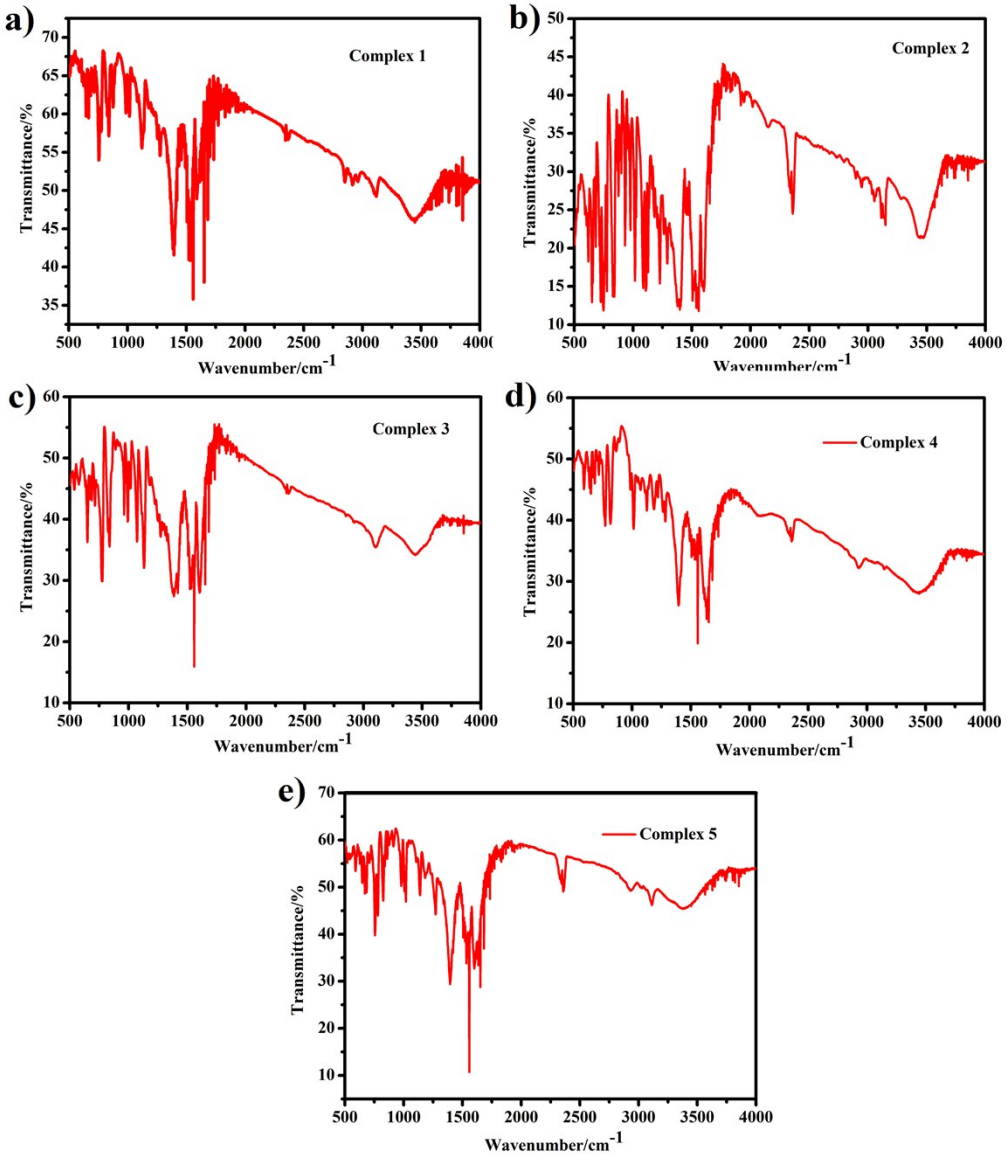

Fig. S5. The IR spectra of **1-5**.

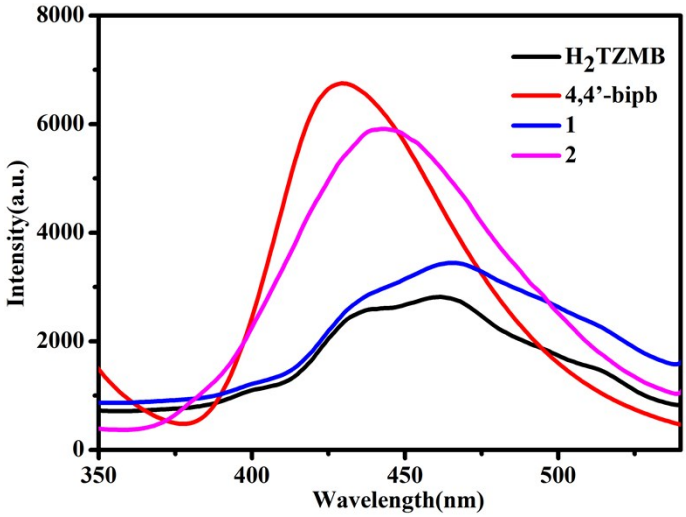

Fig. S6 The luminescence spectrum of organic linkers, complexes **1** and **2** in the solid state at room temperature.

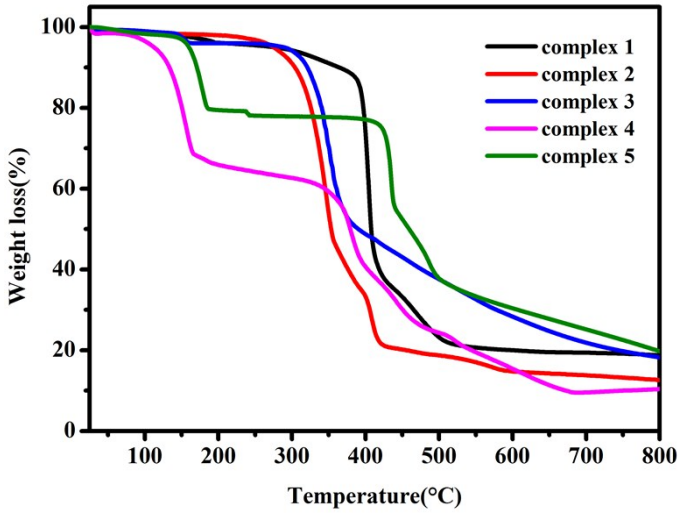

Fig. S7 TGA curves for complexes **1**-**5**.

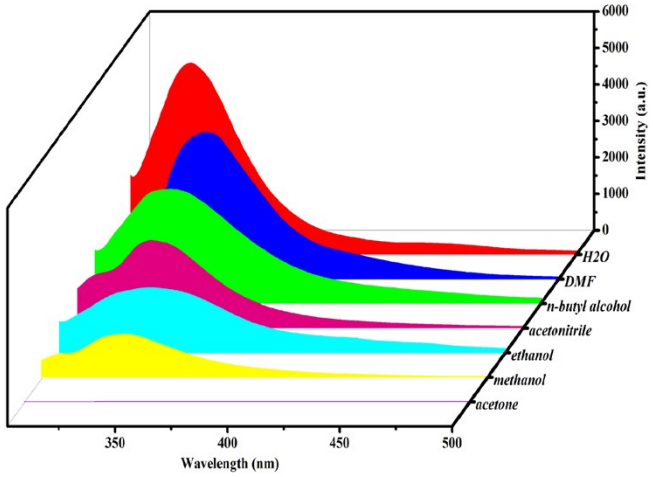

Fig. S8 The luminescence intensities of complex **1** which were dispersed in different organic solvents.

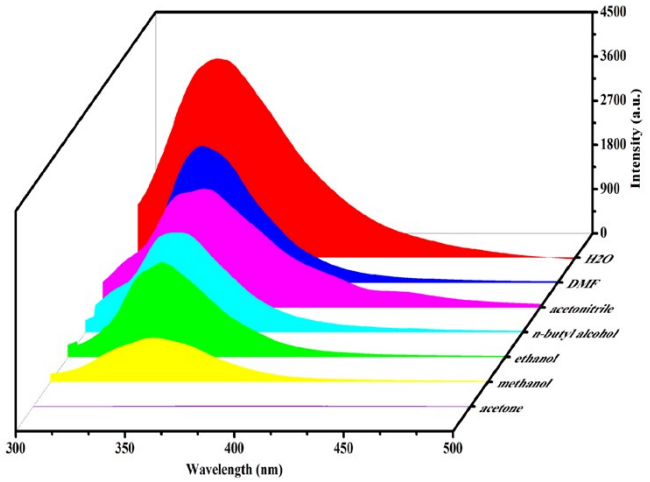

Fig. S9 The luminescence intensities of complex **2** which were dispersed in different organic solvents.

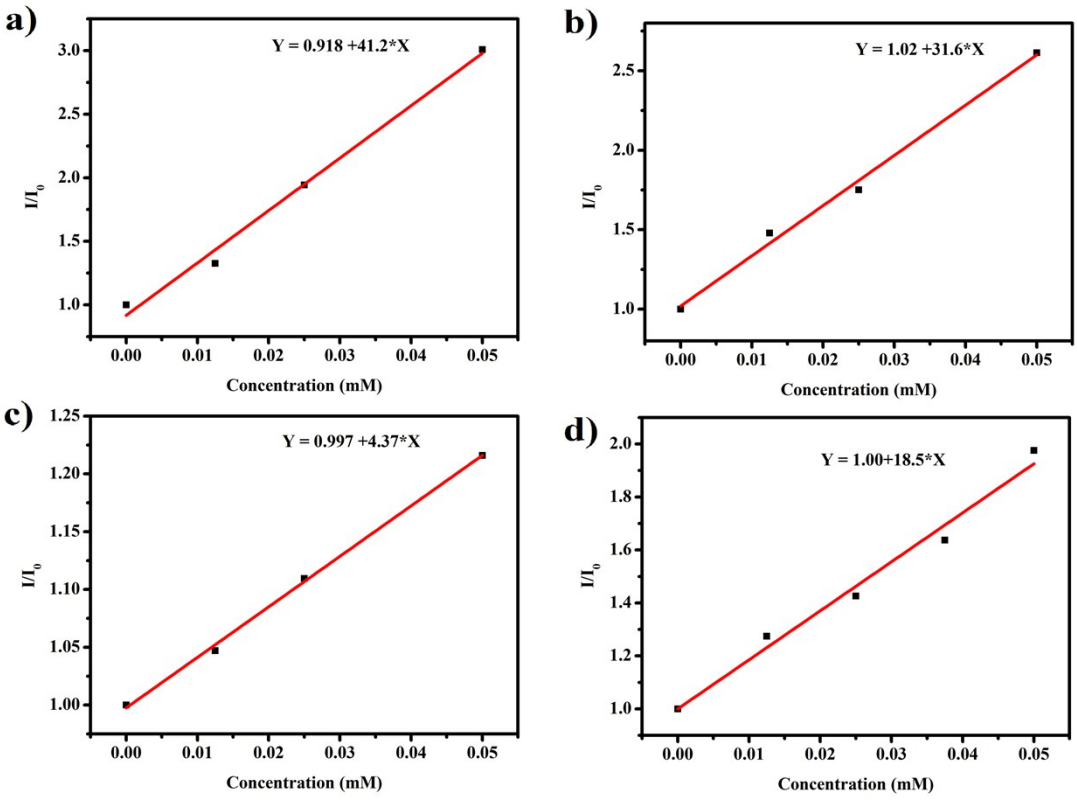

Fig. S10 The linear plots at low concentration of PNP (a), PNT (b), PNA (c) and NB (d) for **1**.

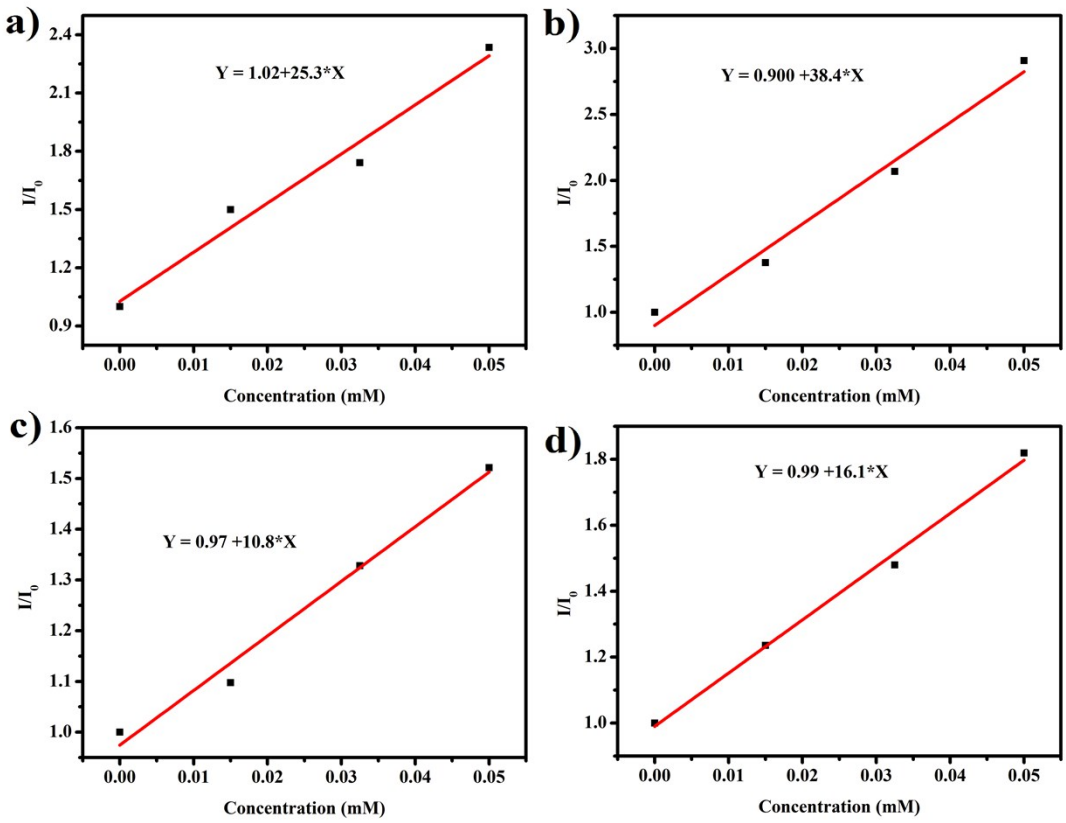

Fig. S11 The linear plots at low concentration of PNP (a), PNT (b), PNA (c) and NB (d) for **2**.

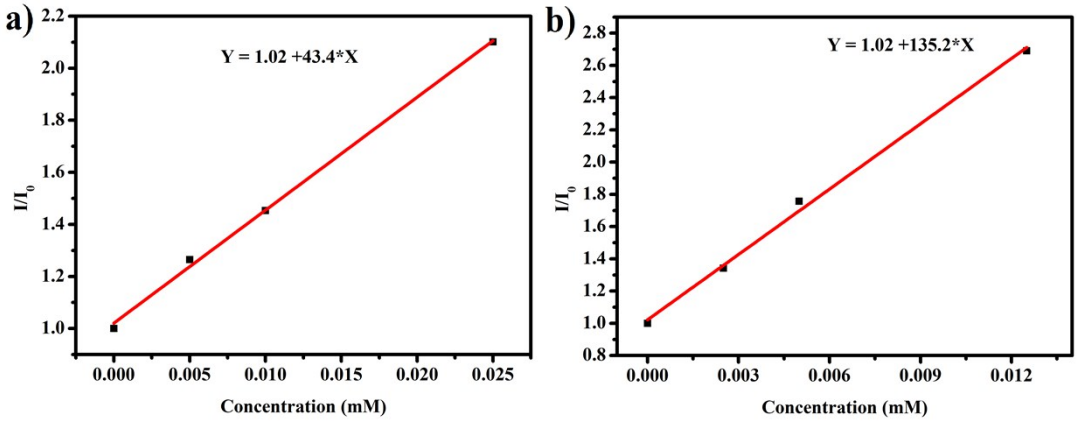

Fig. S12 The linear plots at low concentration of Fe^{3+} for **1**(a) and **2**(b).

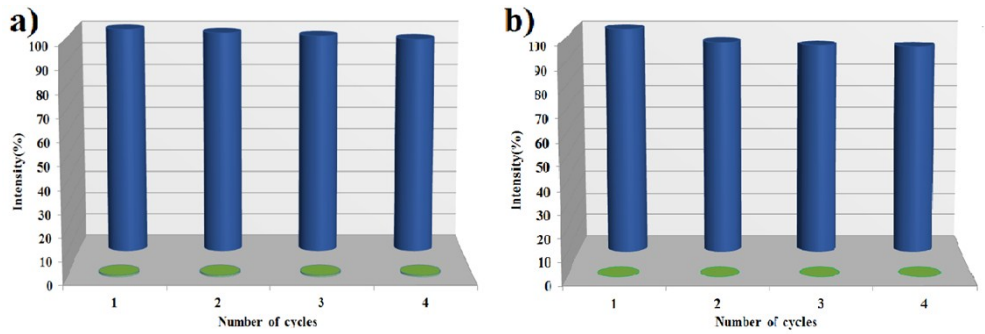

Fig. S13 Initial fluorescence intensities (blue bars) for **1**(a) and **2**(b) suspensions and those after addition of Fe^{3+} aqueous solutions (green bars) in four regeneration cycles.

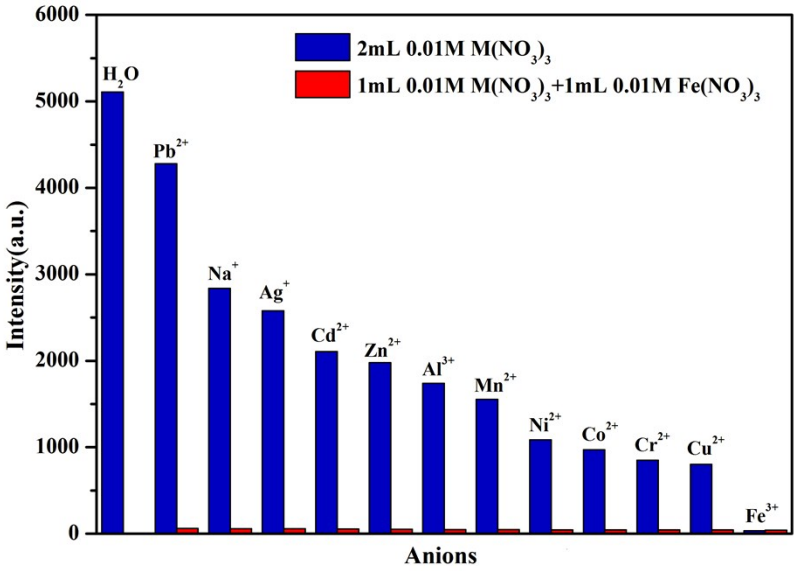

Fig. S14 The anti-interferences of **1** in sensing of Fe^{3+} ions from normal anions in aqueous solution.

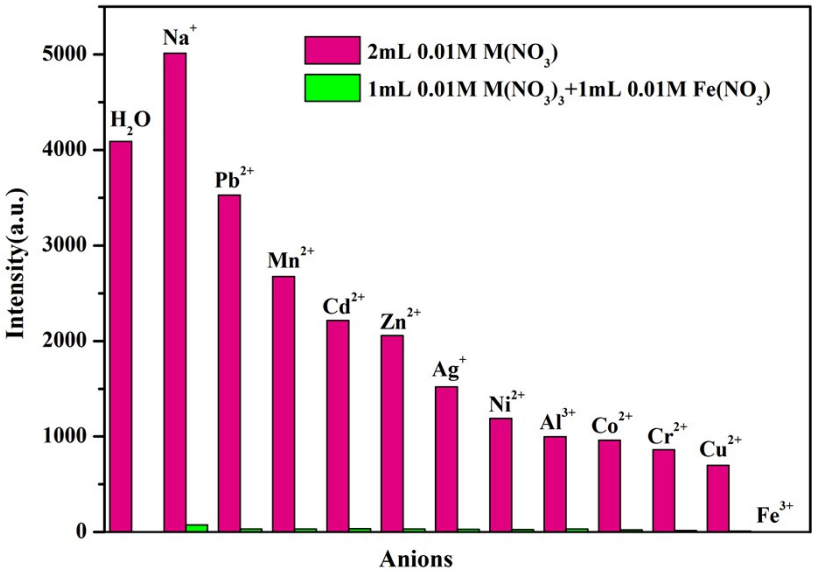

Fig. S15 The anti-interferences of **2** in sensing of Fe^{3+} ions from normal anions in aqueous solution.

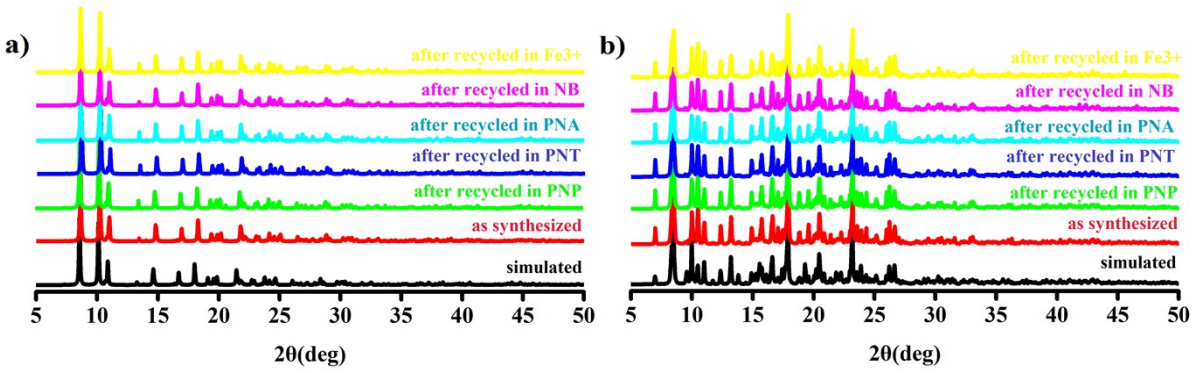

Fig. S16 The PXRD pattern of **1**(a) and **2**(b) after immerging in analytes.

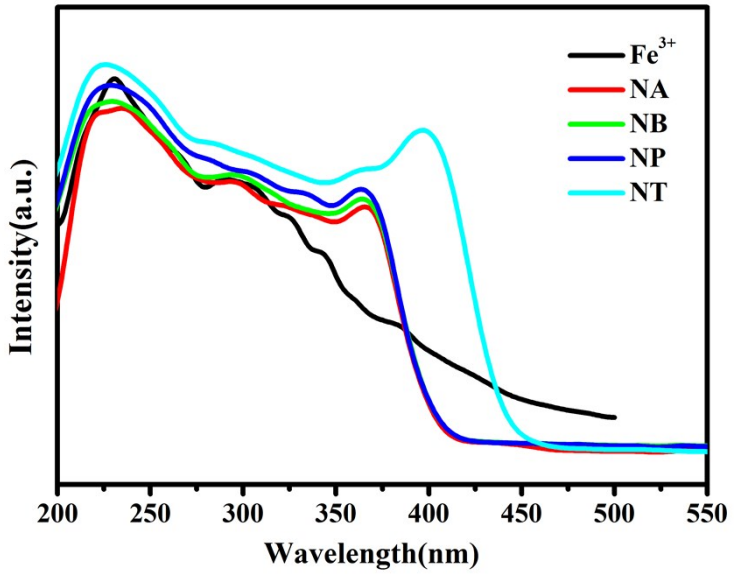

Fig. S17 The UV-Vis specrum of NACs and Fe^{3+}.

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

Cd1-O1	2.210(3)	O1-Cd1-O2A	111.20(16)
Cd1-O2A	2.617(4)	O1-Cd1-O3B	136.76(13)
Cd1-O3B	2.341(3)	O1-Cd1-O4B	86.08(12)
Cd1-O4B	2.442(4)	O1-Cd1-O5	93.57(17)
Cd1-O5	2.365(4)	O1-Cd1-N3C	113.46(13)
Cd1-N3C	2.261(3)	O3B-Cd1-O2A	82.33(12)
		O3B-Cd1-O4B	54.74(12)
		O3B-Cd1-O5	88.38(12)
		O5-Cd1-O2A	152.08(13)
		O5-Cd1-O4B	115.03(11)
		N3C-Cd1-O2A	79.32(12)
		N3C-Cd1-O3B	109.31(12)
		N3C-Cd1-O4B	155.96(11)
		N3C-Cd1-O5	79.06(12)
Symmetry codes: A: 3/2-x,1/2-y,1-z; B: +x,+y,1+z ; C: 3/2-x,1/2+y,1/2-z; D: +x,+y,-1+z; E: 3/2-x, -1/2+y,1/2-z.			

Table S2 Selected bond lengths (Å) and angles (deg) for complex 2

Cd1-O1	2.423(3)	O1-Cd1-O6	169.35(9)
Cd1-O2	2.367(3)	O2-Cd1-O1	54.29(10)
Cd1-O5	2.255(3)	O2-Cd1-O6	136.27(10)
Cd1-O6	2.749(3)	O2-Cd1-N7	90.02(10)
Cd1-N3A	2.317(3)	O5-Cd1-O1	140.48(10)
Cd1-N6B	2.304(3)	O5-Cd1-O2	86.21(10)
Cd1-N7	2.410(3)	O5-Cd1-O6	50.14(10)
		O5-Cd1-N3A	91.62(11)
		O5-Cd1-N6A	128.07(10)

		O5-Cd1-N7	88.97(11)
		N3A-Cd1-O1	91.07(10)
		N3A-Cd1-O2	91.83(10)
		N3A-Cd1-O6	87.38(12)
		N3A-Cd1-N7	178.09(11)
		N6B-Cd1-O1	91.43(10)
		N6B-Cd1-O2	145.72(11)
		N6B-Cd1-O6	77.99(10)
		N6B-Cd1-N3A	87.96(10)
		N6B-Cd1-N7	90.25(10)
		N7-Cd1-O1	89.62(10)
		N7-Cd1-O6	91.61(12)
Symmetry codes: A:-1+x,+y,+z; B: +x,1+y,+z; C:1+x,+y,+z; D: +x,-1+y,+z			

Table S3 Selected bond lengths (Å) and angles (deg) for complex **3**.

Ni1-O1	2.067(4)	O1-Ni1-O3A	85.84(17)
Ni1-O3A	2.094(5)	O1-Ni1-O5	95.32(19)
Ni1-O5	2.079(5)	O1-Ni1-N3B	88.03(19)
Ni1-N3B	2.077(5)	O1-Ni1-N4	85.6(2)
Ni1-N4	2.110(6)	O1-Ni1-N5C	172.2(2)
Ni1-N5C	2.136(5)	O3A-Ni1-N4	171.4(2)
		O3A-Ni1-N5C	86.6(2)
		O5-Ni1-O3A	92.56(19)
		O5-Ni1-N4	88.0(2)
		O5-Ni1-N5C	86.9(2)
		N3B-Ni1-O3A	86.9(2)
		N3B-Ni1-O5	176.6(2)
		N3B-Ni1-N4	93.0(2)
		N3B-Ni1-N5C	89.6(2)
		N4-Ni1-N5C	102.0(2)
Symmetry codes: A: x, 1-y, 0.5+z; B: 1-x, 1+y, 1.5-z; C: 0.5-x, 2.5-y, 0.5+z; D: x, 1-y, -0.5+z; E: 1-x, -1+y, 1.5-z; F: 0.5-x, 2.5-y, -0.5+z.			

Table S4 Selected bond lengths (Å) and angles (deg) for complex **4**.

Ni1-O1W	2.0608(14)	O1W-Ni1-N3B	91.78(8)
Ni1-O2	2.0327(18)	O2-Ni1-O1W	93.02(6)
Ni1-O1A	2.0589(19)	O1A-Ni1-O1W	92.88(7)
Ni1-O4B	2.0512(19)	O4C-Ni1-O1W	90.04(7)
Ni1-N3C	2.108(2)	N4-Ni1-O1W	177.39(7)
Ni1-N4	2.055(2)	N4-Ni1-O1A	85.76(8)
		N4-Ni1-N3B	89.48(9)
Symmetry codes:A: 1/3+x-y, 2/3-y, 7/6-z; B: 1/3+x, 2/3+x-y, 1/6+z; C: 1/3-x+y, -1/3+y, 1/6+z; D: y, x, 3/2-z; E: 2/3-x+y,			

1/3+y, -1/6+z; F: -1/3+x, 1/3+x-y, -1/6+z.

Table S5 Selected bond lengths (Å) and angles (deg) for complex **5**

Mn1-O1	2.072(4)	O1-Mn1-O5A	92.17(16)
Mn1-O5A	2.167(4)	O1-Mn1-O6B	99.08(17)
Mn1-O6B	2.267(4)	O1-Mn1-O7B	157.21(17)
Mn1-O7B	2.267(3)	O1-Mn1-O10C	91.85(17)
Mn1-O10C	2.150(4)	O1-Mn1-N3D	96.2(2)
Mn1-N3D	2.209(5)	O5A-Mn1-O6B	84.13(15)
Mn2-O2A	2.199(4)	O5[1]-Mn1-O7B	87.04(14)
Mn2-O3	2.110(4)	O5A-Mn1-N3D	87.97(16)
Mn2-O4	2.100(4)	O7B-Mn1-O6B	58.17(13)
Mn2-O8	2.210(15)	O10C-Mn1-O5A	175.76(15)
Mn2-O8A	2.250(7)	O10C-Mn1-O6B	96.57(15)
Mn2-O9	2.229(4)	O10C-Mn1-O7B	89.78(15)
Mn2-N6E	2.254(4)	O10C-Mn1-N3E	90.25(16)
		N3D-Mn1-O6B	163.03(16)
		N3D-Mn1-O7B	106.52(16)
		O2A-Mn2-O8	80.8(5)
		O2A-Mn2-O8A	101.7(2)
		O2A-Mn2-O9	175.71(17)
		O2A-Mn2-N6E	87.20(16)
		O3-Mn2-O2A	91.40(17)
		O3-Mn2-O8	81.9(4)
		O3-Mn2-O8A	86.1(2)
		O3-Mn2-O9	89.36(16)
		O3-Mn2-N6E	90.07(16)
		O4-Mn2-O2A	94.46(17)
		O4-Mn2-O3	168.82(18)
		O4-Mn2-O8	89.6(4)
		O4-Mn2-O8A	83.4(2)
		O4-Mn2-O9	85.50(16)
		O4-Mn2-N6E	99.70(18)
		O8-Mn2-O9	103.5(5)
		O8-Mn2-N6E	165.4(5)
		O8A-Mn2-N6E	170.4(2)
		O9-Mn2-O8A	82.5(2)
		O9-Mn2-N6E	88.58(16)
Symmetry codes: A: 1-x, 1-y, 1-z; B: -0.5+x, 1.5+y, -1+z; C: 1-x, 2-y, 1-z; D: x, 2-y, -0.5+z; E: x, -y, -0.5+z; F: 0.5+x, -1.5+y, 1+z; G: x, -y, 0.5+z; H: x, 2-y, 0.5+z; I: 1-x, -1-y, 1.5-z; J: x, -1+y, z; K: 1.5-x, -0.5-y, 2-z			

Table S6 Geometrical parameters of hydrogen bonds (Å) for CP **1**

D–H…A	d(D–H) (Å)	d(H…A) (Å)	d(D…A) (Å)	∠(DHA) (°)	Symmetry cod
O1W－H6A…O3	0.86	2.28	3.133(6)	174	1/2-x,1/2-y,-z
C3－H3…O1	0.93	2.54	3.413(7)	157	1-x,y,1/2-z
C7－H7…O5	0.93	2.50	2.997(6)	113	3/2-x,-1/2+y,1/2-z
C8－H8…O4	0.93	2.30	3.180(5)	157	x,-y,1/2+z
C16－H16…N1	0.93	2.55	2.876(6)	101	
C16－H16…N2	0.93	2.47	3.109(6)	126	
C17－H17…O3	0.93	2.39	3.297(6)	163	3/2-x,1/2-y,-z
C19－H19A…O5	0.96	2.40	2.790(16)	104	

Table S7 Geometrical parameters of hydrogen bonds (Å) for CP **2**

D–H…A	d(D–H) (Å)	d(H…A) (Å)	d(D…A) (Å)	∠(DHA) (°)	Symmetry cod
O4－H4…N8	0.82	1.87	2.624(5)	152	-1+x,1+y,1+z
O8－H8…N10	0.82	1.92	2.709(8)	161	2-x,-y,-z
O1W－H9A…O1	0.85	1.98	2.833(9)	179	1-x,1-y,1-z
O1W－H9…O1W	0.85	1.21	1.857(12)	127	2-x,-y,1-z
O1W－H9B…O1	0.85	2.28	2.882(9)	128	1+x,-1+y,z
C6－H6…O2	0.98	2.60	3.445(5)	145	1-x,1-y,1-z
C8－H8A…O2	0.93	2.43	3.241(5)	145	1-x,1-y,1-z
C10－H10…O5	0.93	2.58	3.485(5)	165	1-x,1-y,1-z
C14 －H14…O4	0.93	2.37	2.697(5)	100	
C16－H16…N2	0.93	2.55	3.188(6)	126	
C25－H25…N9	0.93	2.38	3.301(5)	170	x,-1+y,z
C31－H31…O3	0.93	2.47	3.368(6)	164	1-x,1-y,1-z
C76－H76…O3	0.93	2.44	3.364(6)	170	2-x,1-y,1-z
C77－H77…O3	0.93	2.43	3.360(9)	175	2-x,1-y,1-z