Supplementary Material (ESI)

Fabrication of 5-R-isophthalic acid-modulated a series of cadmium-organic coordination polymers and selectivity for the efficient detection of multiple analytes

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Table S1 Crystallographic data for Cd-CP-**1**–**4**.

Cd-CP	**1**	**2**	**3**	**4**
Empirical formula	$C_{31}H_{26}Cd_2N_4O_{11}$	$C_{15.5}H_{18}CdN_2O_8$	$C_{33}H_{38}Cd_2N_4O_{15}$	$C_{23}H_{23}CdN_4O_{8.5}$
Formula weight	855.395	472.736	955.511	603.872
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	*P*2/*c*	*C*2/*c*	*P*–1	*C*2/*c*
a (Å)	10.3061(1)	11.0328(1)	10.0583(2)	27.3243(2)
b (Å)	8.9312(1)	17.1307(2)	10.1823(2)	10.2895(1)
c (Å)	16.6010(3)	19.2872(2)	20.6673(3)	17.8117(2)
α (°)	90	90	97.263(2)	90
β (°)	95.428(1)	93.281(1)	94.133(1)	105.530(1)
γ (°)	90	90	119.439(2)	90
V (Å^3)	1521.20(4)	3639.30(7)	1806.38(7)	4824.99(8)
Z	2	8	2	8
D_c (g cm^{-3})	1.867	1.726	1.757	1.663
R_{int}	0.0191	0.0232	0.0379	0.0160
GOF	1.0483	1.0708	1.0450	0.9176
$R_1{}^a$ [$I > 2\sigma(I)$]	0.0234	0.0234	0.0330	0.0576
$wR_2{}^b$ (all data)	0.0613	0.0637	0.0924	0.1449

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, [b] $wR_2 = \Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]^{1/2}$.

Table S2 Selected bond distances (Å) and angles (°) for Cd-CP-**1**.

Cd(1)–O(3)#1	2.1960(17)	Cd(1)–O(4)#2	2.2227(18)
Cd(1)–O(1)	2.3069(19)	Cd(1)–N(1)	2.368(2)
Cd(1)–O(2)	2.4157(19)	Cd(1)–O(5)#3	2.4512(18)
O(3)#1–Cd(1)–O(4)#2	124.22(7)	O(1)–Cd(1)–O(2)	55.29(7)
O(3)#1–Cd(1)–O(1)	95.88(7)	N(1)–Cd(1)–O(2)	86.76(8)
O(4)#2–Cd(1)–O(1)	137.86(7)	O(3)#1–Cd(1)–O(5)#3	92.26(7)
O(3)#1–Cd(1)–N(1)	90.04(8)	O(4)#2–Cd(1)–O(5)#3	80.61(7)
O(4)#2–Cd(1)–N(1)	89.74(8)	O(1)–Cd(1)–O(5)#3	85.91(8)
O(1)–Cd(1)–N(1)	103.91(8)	N(1)–Cd(1)–O(5)#3	169.63(8)
O(3)#1–Cd(1)–O(2)	148.94(7)	O(2)–Cd(1)–O(5)#3	96.39(7)
O(4)#2–Cd(1)–O(2)	86.68(7)		

Symmetry codes: #1 $x + 1, y, z$; #2 $-x, y, -z + 1/2$; #3 $x, y - 1, z$.

Table S3 Selected bond distances (Å) and angles (°) for Cd-CP-**2**.

Cd(1)–O(1W)	2.285(2)	Cd(1)–N(1)	2.327(3)
Cd(1)–O(2W)	2.330(2)	Cd(1)–O(4)#1	2.331(2)
Cd(1)–O(1)	2.344(2)	Cd(1)–O(2)	2.535(2)
Cd(1)–O(3)#1	2.561(2)	O(1W)–Cd(1)–O(2)	83.89(8)
O(1W)–Cd(1)–N(1)	93.88(10)	N(1)–Cd(1)–O(2)	88.09(8)
O(1W)–Cd(1)–O(2W)	178.90(8)	O(2W)–Cd(1)–O(2)	96.90(8)
N(1)–Cd(1)–O(2W)	86.92(10)	O(4)#1–Cd(1)–O(2)	133.09(7)
O(1W)–Cd(1)–O(4)#1	88.44(8)	O(1)–Cd(1)–O(2)	52.91(7)
N(1)–Cd(1)–O(4)#1	138.67(8)	O(1W)–Cd(1)–O(3)#1	95.40(8)
O(2W)–Cd(1)–O(4)#1	90.46(8)	N(1)–Cd(1)–O(3)#1	86.04(8)
O(1W)–Cd(1)–O(1)	93.51(8)	O(2W)–Cd(1)–O(3)#1	83.90(8)
N(1)–Cd(1)–O(1)	139.12(9)	O(4)#1–Cd(1)–O(3)#1	52.70(7)
O(2W)–Cd(1)–O(1)	86.37(8)	O(1)–Cd(1)–O(3)#1	133.05(7)
O(4)#1–Cd(1)–O(1)	81.66(7)	O(2)–Cd(1)–O(3)#1	174.03(7)

Symmetry code: #1 $x - 1/2, y + 1/2, z$.

Table S4 Selected bond distances (Å) and angles (°) for Cd-CP-**3**.

Cd(1)–O(4)#1	2.205(2)	Cd(2)–O(6)	2.247(2)
Cd(1)–N(1)	2.291(3)	Cd(2)–N(2)	2.252(3)
Cd(1)–O(2)	2.294(2)	Cd(2)–O(7)	2.328(3)
Cd(1)–O(1W)	2.325(2)	Cd(2)–O(3W)	2.364(3)
Cd(1)–O(2W)	2.427(2)	Cd(2)–O(8)	2.380(2)
Cd(1)–O(1)	2.500(2)	Cd(2)–O(6)#2	2.528(2)
O(4)#1–Cd(1)–N(1)	135.89(9)	O(6)–Cd(2)–N(2)	121.41(10)
O(4)#1–Cd(1)–O(2)	136.64(9)	O(6)–Cd(2)–O(7)	85.79(9)
N(1)–Cd(1)–O(2)	87.20(9)	N(2)–Cd(2)–O(7)	143.22(10)
O(4)#1–Cd(1)–O(1W)	96.28(9)	O(6)–Cd(2)–O(3W)	109.83(10)
N(1)–Cd(1)–O(1W)	85.60(9)	N(2)–Cd(2)–O(3W)	91.31(10)
O(2)–Cd(1)–O(1W)	90.79(10)	O(7)–Cd(2)–O(3W)	102.65(11)
O(4)#1–Cd(1)–O(2W)	88.15(9)	O(6)–Cd(2)–O(8)	140.73(8)
N(1)–Cd(1)–O(2W)	84.06(9)	N(2)–Cd(2)–O(8)	92.61(9)
O(2)–Cd(1)–O(2W)	93.05(10)	O(7)–Cd(2)–O(8)	55.31(8)
O(1W)–Cd(1)–O(2W)	168.78(8)	O(3W)–Cd(2)–O(8)	86.28(9)
O(4)#1–Cd(1)–O(1)	82.84(8)	O(6)–Cd(2)–O(6)#2	77.98(9)
N(1)–Cd(1)–O(1)	139.96(8)	N(2)–Cd(2)–O(6)#2	80.11(9)
O(2)–Cd(1)–O(1)	53.90(8)	O(7)–Cd(2)–O(6)#2	82.56(9)
O(1W)–Cd(1)–O(1)	102.24(8)	O(3W)–Cd(2)–O(6)#2	170.72(9)
O(2W)–Cd(1)–O(1)	88.51(8)	O(8)–Cd(2)–O(6)#2	90.55(8)

Symmetry codes: #1 $x, y + 1, z$; #2 $-x + 1, -y, -z + 1$.

Table S5 Selected bond distances (Å) and angles (°) for Cd-CP-**4**.

Cd(1)–O(3)#1	2.264(7)	Cd(1)–O(4)#2	2.322(8)
Cd(1)–N(2)	2.326(9)	Cd(1)–N(1)	2.334(9)
Cd(1)–O(1)	2.356(7)	Cd(1)–O(2)	2.387(9)
O(3)#1–Cd(1)–O(4)#2	132.9(3)	N(2)–Cd(1)–O(1)	86.9(3)
O(3)#1–Cd(1)–N(2)	89.0(3)	N(1)–Cd(1)–O(1)	99.4(3)
O(4)#2–Cd(1)–N(2)	88.8(3)	O(3)#1–Cd(1)–O(2)	88.8(3)
O(3)#1–Cd(1)–N(1)	87.3(3)	O(4)#2–Cd(1)–O(2)	138.3(3)
O(4)#2–Cd(1)–N(1)	89.6(3)	N(2)–Cd(1)–O(2)	94.5(4)
N(2)–Cd(1)–N(1)	173.3(3)	N(1)–Cd(1)–O(2)	91.0(4)
O(3)#1–Cd(1)–O(1)	142.5(2)	O(1)–Cd(1)–O(2)	54.5(3)
O(4)#2–Cd(1)–O(1)	84.3(3)		

Symmetry codes: #1 x, $y + 1$, z; #2 $-x$, $-y + 1$, $-z$.

Table S6 K_{sv} values and LOD of Cd-CP-**1**–**4** for different analytes.

Analyte	Cd-CP-**1**		Cd-CP-**2**		Cd-CP-**3**		Cd-CP-**4**	
	K_{sv} (M^{-1})	LOD (M)	K_{sv} (M^{-1})	LOD (M)	K_{sv} (M^{-1})	LOD (M)	K_{sv} (M^{-1})	LOD (M)
Fe^{3+}	3.18×10^3	1.42×10^{-5}	3.36×10^4	1.13×10^{-6}	4.80×10^3	9.38×10^{-6}	8.68×10^4	5.18×10^{-7}
MnO_4^-	1.34×10^5	3.37×10^{-7}	1.58×10^4	2.39×10^{-6}	1.70×10^4	2.65×10^{-6}	1.58×10^5	2.86×10^{-7}
NB	1.85×10^3	2.44×10^{-5}	2.53×10^4	1.49×10^{-6}	7.36×10^3	6.11×10^{-6}	1.20×10^5	3.75×10^{-7}

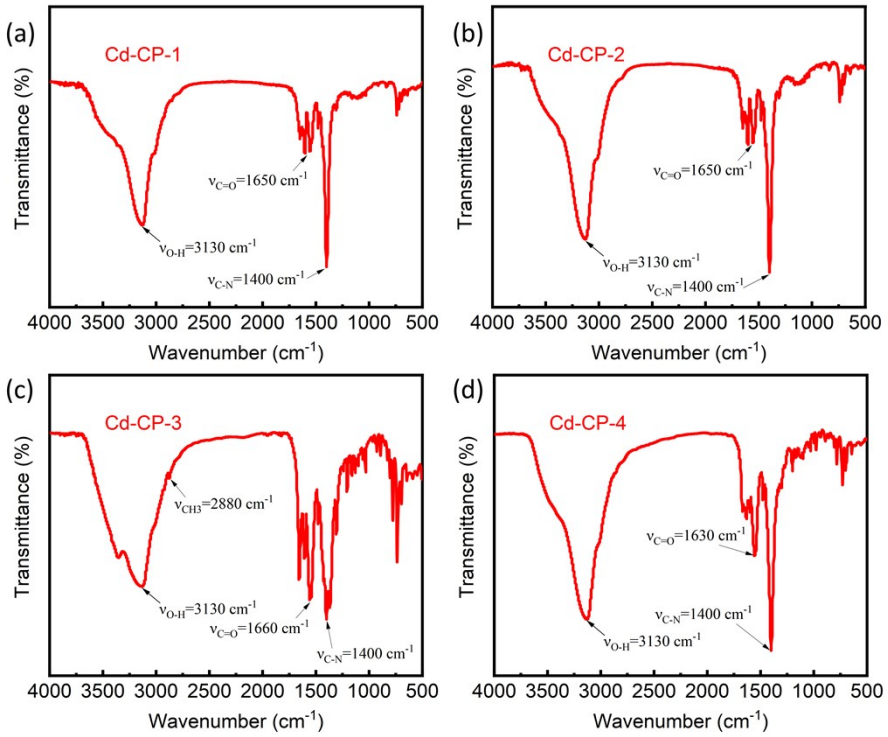

Fig. S1 The IR spectra of Cd-CP-**1**–**4**.

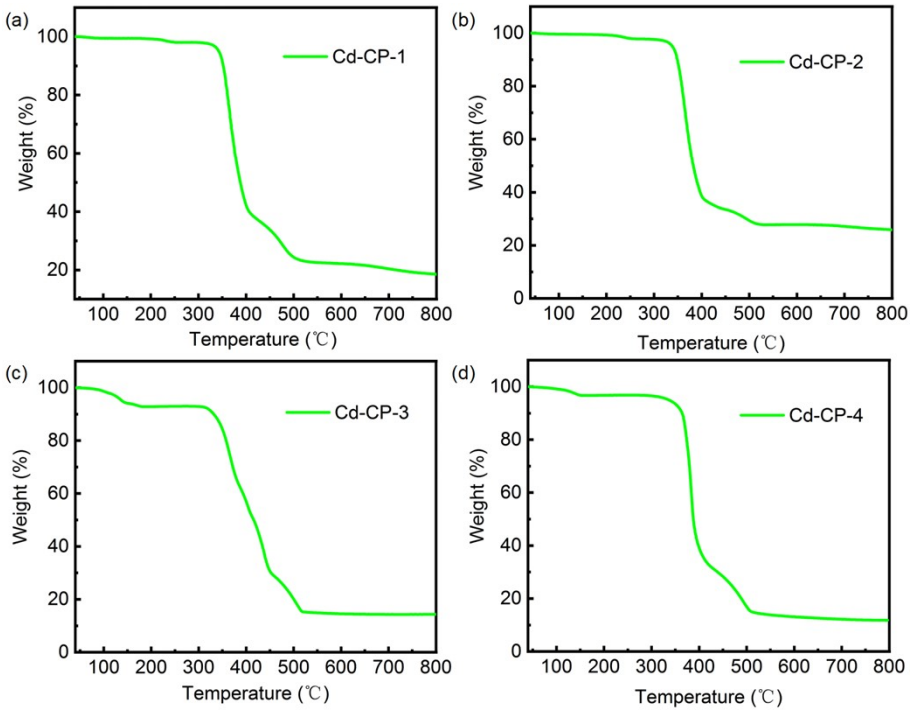

Fig. S2 The TG curves of Cd-CP-**1**–**4**.

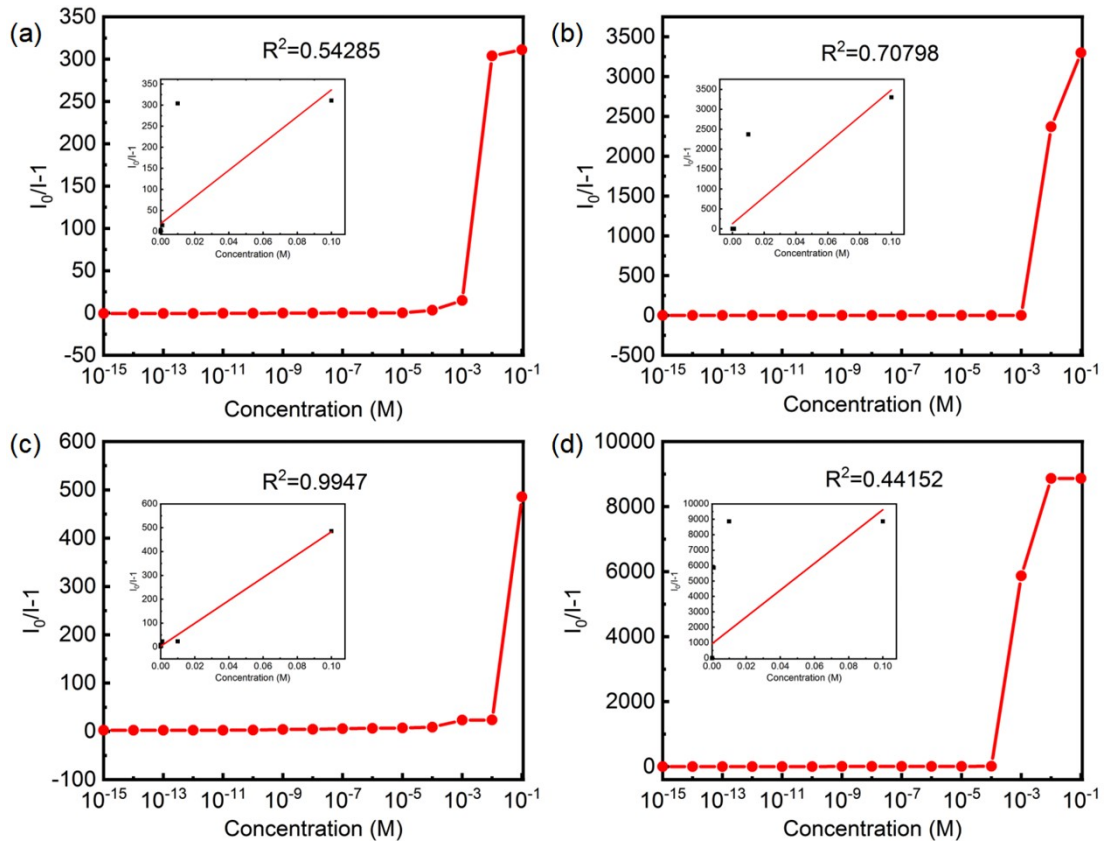

Fig. S3 K_{sv} plots of Cd-CP-**1** (a), **2** (b), **3** (c) and **4** (d) for sensing of Fe^{3+} ion.

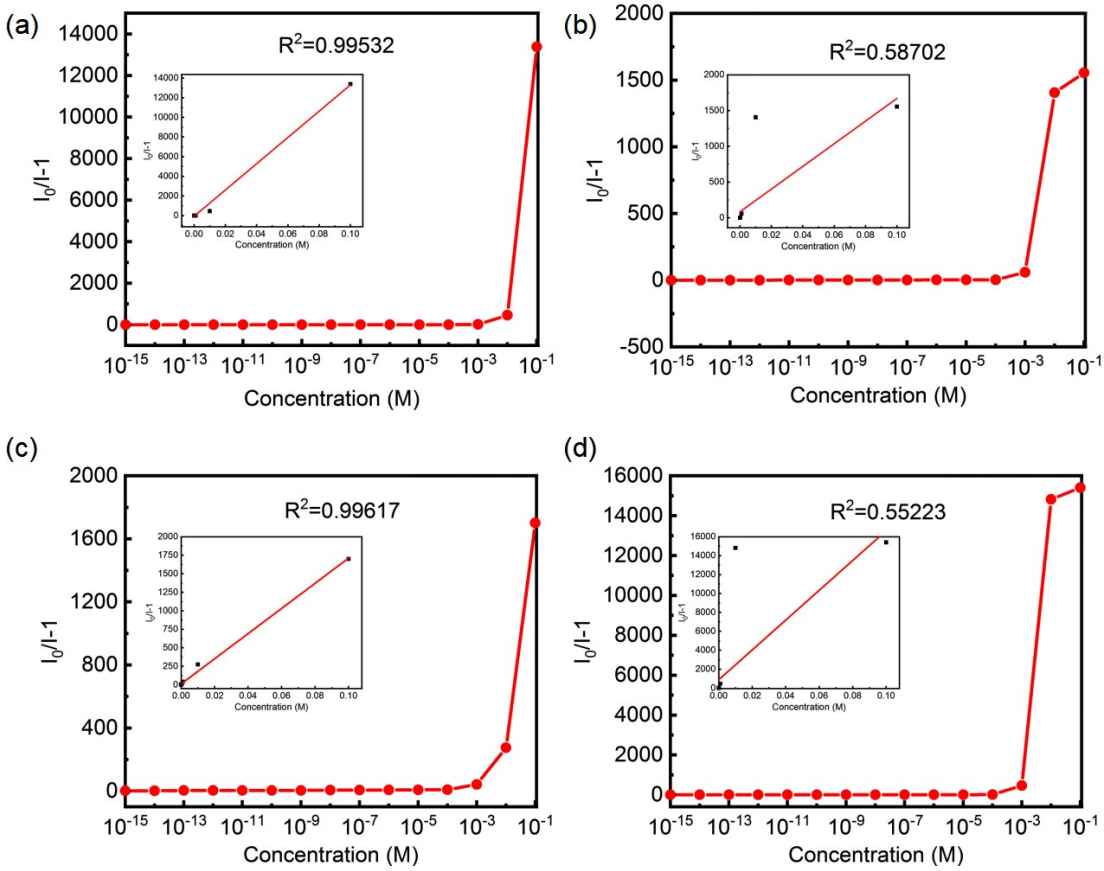

Fig. S4 K_{sv} plots of Cd-CP-**1** (a), **2** (b), **3** (c) and **4** (d) for sensing of MnO_4^- ion.

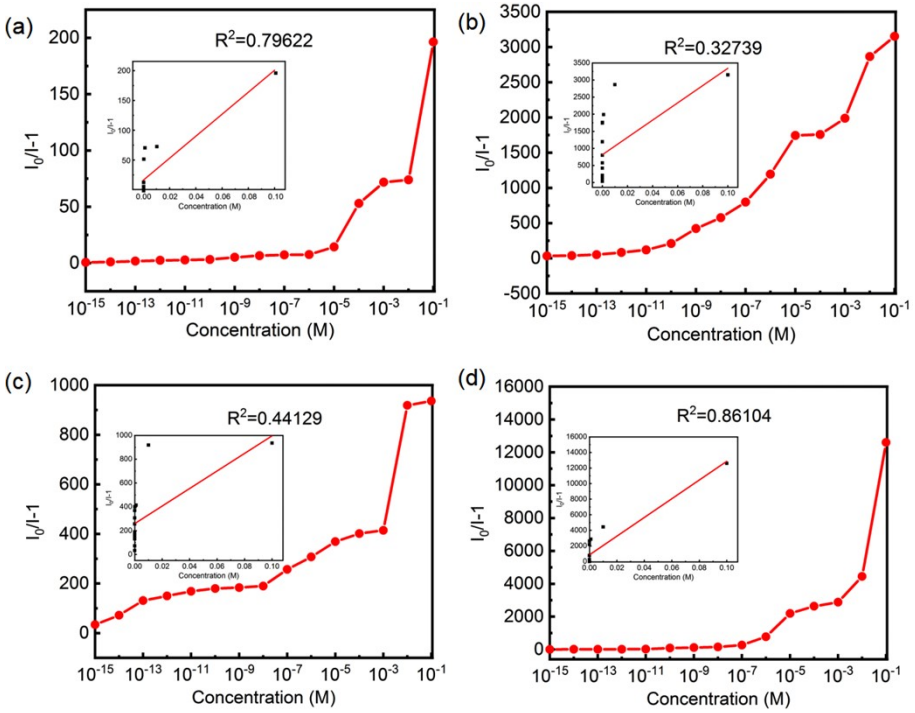

Fig. S5 K_{sv} plots of Cd-CP-**1** (a), **2** (b), **3** (c) and **4** (d) for sensing of NB.

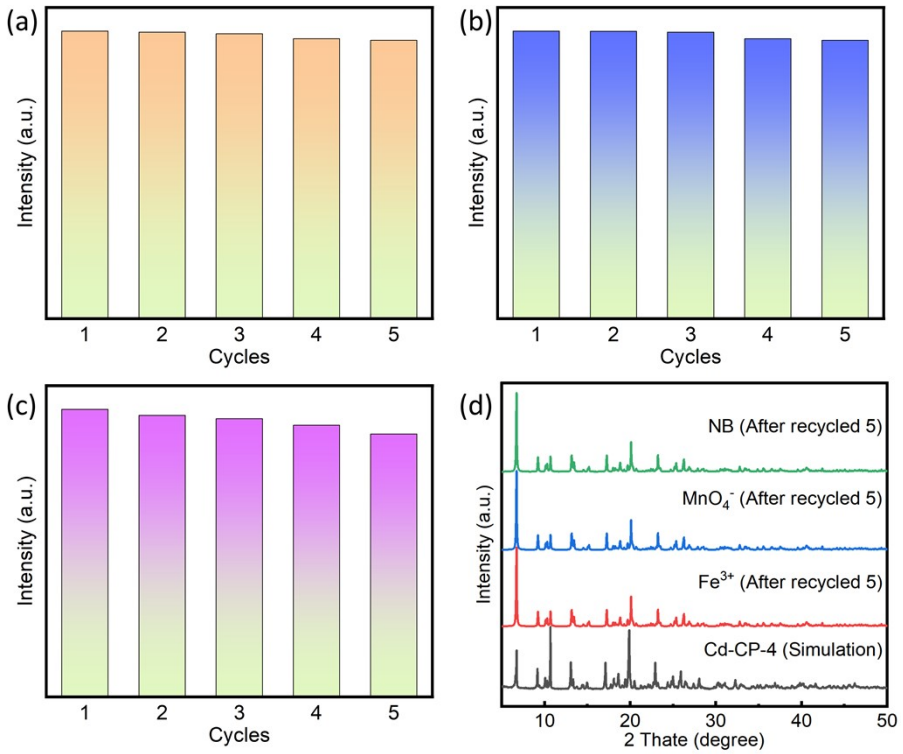

Fig. S6 The cyclic response of the fluorescence intensities of Cd-CP-**4** for detecting Fe^{3+} (a), MnO_4^- (b) and NB (c). The PXRD patterns of Cd-CP-**4** treated by Fe^{3+} (a), MnO_4^- (b) and NB before and after five cycles.

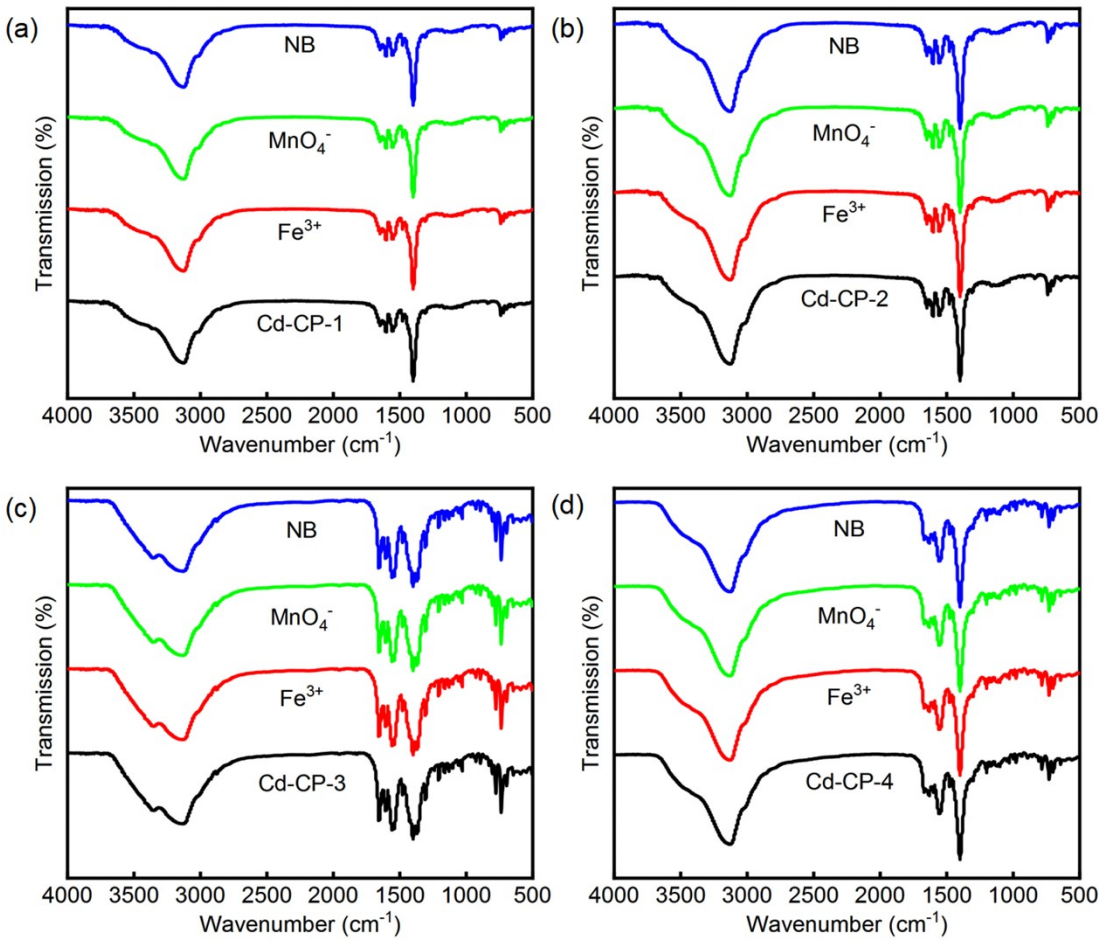

Fig. S7 The IR spectra of Cd-CP-**1**–**4** before and after being soaked in different analyzes.