Various Cd(II) Coordination Polymers Induced by Carboxylates: Multi-functional Detections for Fe^{3+}, Anions, Aspartic Acids and Bovine Serum Albumin

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Supporting information

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

1			
Cd(1)–O(1)	2.301(3)	Cd(1)–O(3)	2.316(3)
Cd(1)–O(4)A	2.305(3)	Cd(1)–N(1)	2.337(3)
Cd(1)–O(2)B	2.308(3)	Cd(1)–N(2)C	2.342(3)
O(1)–Cd(1)–O(4)A	174.63(10)	O(2)B–Cd(1)–N(1)	80.81(11)
O(1)–Cd(1)–O(2)B	92.19(9)	O(3)–Cd(1)–N(1)	77.53(10)
O(4)A–Cd(1)–O(2)B	86.39(9)	O(1)–Cd(1)–N(2)C	89.98(10)
O(1)–Cd(1)–O(3)	86.66(9)	O(4)A–Cd(1)–N(2)C	95.35(10)
O(4)A–Cd(1)–O(3)	92.74(9)	O(2)B–Cd(1)–N(2)C	98.45(10)
O(2)B–Cd(1)–O(3)	158.33(10)	O(3)–Cd(1)–N(2)C	103.19(10)
O(1)–Cd(1)–N(1)	88.44(11)	N(1)–Cd(1)–N(2)C	178.23(11)
O(4)A–Cd(1)–N(1)	86.22(11)		

Symmetry codes: A: $-x+2, -y, -z$; B: $-x+1, -y, -z$; C: $x, y+1, z$

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Table S2 Selected bond distances (Å) and angles (°) for **2**.

2			
Cd(1)–O(1W)	2.322(4)	Cd(2)–O(2W)	2.337(4)
Cd(1)–N(3)	2.327(4)	Cd(2)–N(2)	2.313(4)
Cd(1)–N(4)	2.347(4)	Cd(2)–O(8)A	2.443(4)
Cd(1)–O(2)	2.381(3)	Cd(2)–O(4)	2.454(3)
Cd(1)–O(6)	2.427(4)	Cd(2)–N(1)	2.349(5)
Cd(1)–O(7)	2.429(4)	Cd(2)–O(3)	2.397(3)
Cd(1)–O(1)	2.459(3)	Cd(2)–O(5)	2.413(4)
O(1W)–Cd(1)–N(3)	88.05(14)	N(2)–Cd(2)–O(2W)	88.80(15)
O(1W)–Cd(1)–N(4)	85.47(13)	N(2)–Cd(2)–N(1)	170.48(16)
N(3)–Cd(1)–N(4)	165.64(14)	O(2W)–Cd(2)–N(1)	84.98(16)
O(1W)–Cd(1)–O(2)	150.24(12)	N(2)–Cd(2)–O(3)	93.50(14)
N(3)–Cd(1)–O(2)	90.35(15)	O(2W)–Cd(2)–O(3)	150.73(12)
N(4)–Cd(1)–O(2)	88.95(14)	N(1)–Cd(2)–O(3)	88.46(14)
O(1W)–Cd(1)–O(6)	130.05(15)	N(2)–Cd(2)–O(5)	94.64(17)
N(3)–Cd(1)–O(6)	90.18(15)	O(2W)–Cd(2)–O(5)	131.06(14)
N(4)–Cd(1)–O(6)	103.80(14)	N(1)–Cd(2)–O(5)	94.89(18)
O(2)–Cd(1)–O(6)	79.65(13)	O(3)–Cd(2)–O(5)	77.88(13)
O(1W)–Cd(1)–O(7)	78.12(15)	N(2)–Cd(2)–O(8)A	98.16(15)
N(3)–Cd(1)–O(7)	99.98(17)	O(2W)–Cd(2)–O(8)A	77.49(13)
N(4)–Cd(1)–O(7)	91.21(16)	N(1)–Cd(2)–O(8)A	87.54(16)
O(2)–Cd(1)–O(7)	131.28(14)	O(3)–Cd(2)–O(8)A	130.76(12)
O(6)–Cd(1)–O(7)	53.12(16)	O(5)–Cd(2)–O(8)A	53.67(14)
O(1W)–Cd(1)–O(1)	96.82(13)	N(2)–Cd(2)–O(4)	90.50(14)
N(3)–Cd(1)–O(1)	84.90(14)	O(2W)–Cd(2)–O(4)	97.05(13)
N(4)–Cd(1)–O(1)	83.17(14)	N(1)–Cd(2)–O(4)	83.13(15)
O(2)–Cd(1)–O(1)	53.46(11)	O(3)–Cd(2)–O(4)	53.79(12)
O(6)–Cd(1)–O(1)	132.71(14)	O(5)–Cd(2)–O(4)	131.63(13)
O(7)–Cd(1)–O(1)	172.76(16)	O(8)A–Cd(2)–O(4)	169.60(15)

Symmetry codes: A: $x, y + 1, z + 1$

Table S3 Selected bond distances (Å) and angles (°) for **3**.

3			
Cd(1)–N(1)	2.324(3)	Cd(1)–O(4)A	2.392(3)
Cd(1)–O(3)A	2.351(3)	Cd(1)–O(1)	2.500(3)
Cd(1)–N(3)B	2.358(3)	Cd(1)–O(5)C	2.559(3)
Cd(1)–O(2)	2.363(3)		
N(1)–Cd(1)–O(3)A	100.28(12)	O(3)A–Cd(1)–O(1)	84.38(10)
N(1)–Cd(1)–N(3)B	167.60(11)	N(3)B–Cd(1)–O(1)	87.30(11)
O(3)A–Cd(1)–N(3)B	91.59(12)	O(2)–Cd(1)–O(1)	53.44(9)
N(1)–Cd(1)–O(2)	86.92(10)	O(4)A–Cd(1)–O(1)	138.26(9)
O(3)A–Cd(1)–O(2)	137.42(10)	N(1)–Cd(1)–O(5)C	89.84(10)
N(3)B–Cd(1)–O(2)	81.89(10)	O(3)A–Cd(1)–O(5)C	136.34(10)
N(1)–Cd(1)–O(4)A	90.19(10)	N(3)B–Cd(1)–O(5)C	83.93(9)
O(3)A–Cd(1)–O(4)A	54.54(10)	O(2)–Cd(1)–O(5)C	85.01(9)
N(3)B–Cd(1)–O(4)A	99.68(10)	O(4)A–Cd(1)–O(5)C	83.37(9)
O(2)–Cd(1)–O(4)A	168.04(9)	O(1)–Cd(1)–O(5)C	138.37(8)
N(1)–Cd(1)–O(1)	90.31(11)		

Symmetry codes: A: $x, y + 1, z + 1$; B: $x - 1, y, z + 1$; C: $x, -y + 1/2, z + 1/2$

Table S4 Selected bond distances (Å) and angles (°) for **4**.

4			
Cd(1)–O(3)	2.292(3)	Cd(1)–O(5)A	2.375(3)
Cd(1)–N(2)	2.297(4)	Cd(1)–O(2)A	2.514(3)
Cd(1)–N(1)	2.324(4)	Cd(1)–O(1)	2.368(3)
O(3)–Cd(1)–N(2)	102.23(13)	O(3)–Cd(1)–O(2)A	135.59(11)
O(3)–Cd(1)–N(1)	93.32(13)	N(2)–Cd(1)–O(2)A	81.84(12)
N(2)–Cd(1)–N(1)	124.07(13)	N(1)–Cd(1)–O(2)A	88.39(12)
N(2)–Cd(1)–O(1)	83.84(14)	O(1)–Cd(1)–O(2)A	100.33(12)
O(3)–Cd(1)–O(1)	124.07(13)	O(5)A–Cd(1)–O(2)A	53.29(10)
N(1)–Cd(1)–O(1)	85.93(14)	O(4)–Cd(1)–N(2)	101.70(13)
O(3)–Cd(1)–O(5)A	82.39(11)	O(4)–Cd(1)–N(1)	86.44(13)
N(2)–Cd(1)–O(5)A	88.97(13)	O(4)–Cd(1)–O(1)	72.61(13)
N(1)–Cd(1)–O(5)A	94.98(13)	O(3)–Cd(1)–O(5)A	133.90(11)
O(1)–Cd(1)–O(5)A	153.48(12)		

Symmetry codes: A: $x - 1, y, z$

Table S5 Selected bond distances (Å) and angles (°) for **5**.

5			
Cd(1)–O(2)A	2.220(2)	Cd(1)–N(2)	2.332(2)
Cd(1)–O(1)	2.2402(18)	Cd(1)–N(1)C	2.345(2)
Cd(1)–O(3)B	2.2984(17)	Cd(1)–O(4)B	2.5239(18)
O(2)A–Cd(1)–O(1)	118.51(8)	O(3)B–Cd(1)–N(1)C	85.83(7)
O(2)A–Cd(1)–O(3)B	90.08(7)	N(2)–Cd(1)–N(1)C	167.23(8)
O(1)–Cd(1)–O(3)B	150.15(7)	O(2)A–Cd(1)–O(4)B	144.19(7)
O(2)A–Cd(1)–N(2)	98.46(9)	O(1)–Cd(1)–O(4)B	96.79(7)
O(1)–Cd(1)–N(2)	83.60(8)	O(3)B–Cd(1)–O(4)B	54.12(6)
O(3)B–Cd(1)–N(2)	101.51(7)	N(2)–Cd(1)–O(4)B	90.78(7)
O(2)A–Cd(1)–N(1)C	91.90(9)	N(1)C–Cd(1)–O(4)B	85.07(7)
O(1)–Cd(1)–N(1)C	84.90(7)		

Symmetry codes: A: $-x, -y, -z + 1$; B: $x - 1, y, z$; C: $-x + 1/2, y - 1/2, -z + 1/2$

Table S6 Selected bond distances (Å) and angles (°) for **6**.

6			
Cd(1)–O(2)	2.268(2)	Cd(1)–O(1)	2.374(2)
Cd(1)–N(2)	2.326(2)	Cd(1)–O(4)A	2.411(2)
Cd(1)–N(1)	2.345(2)	Cd(1)–O(6)A	2.468(2)
O(2)–Cd(1)–N(2)	119.19(9)	N(1)–Cd(1)–O(4)A	89.63(8)
O(2)–Cd(1)–N(1)	93.68(9)	O(1)–Cd(1)–O(4)A	81.42(7)
N(2)–Cd(1)–N(1)	103.63(9)	O(2)–Cd(1)–O(6)A	146.01(7)
O(2)–Cd(1)–O(1)	84.90(9)	N(2)–Cd(1)–O(6)A	89.36(7)
N(2)–Cd(1)–O(1)	84.93(8)	N(1)–Cd(1)–O(6)A	97.09(8)
N(1)–Cd(1)–O(1)	170.79(8)	O(1)–Cd(1)–O(6)A	79.39(8)
O(2)–Cd(1)–O(4)A	94.47(8)	O(4)A–Cd(1)–O(6)A	53.63(7)
N(2)–Cd(1)–O(4)A	142.26(8)		

Symmetry codes: A: $-x + 1/2, y + 1/2, z$

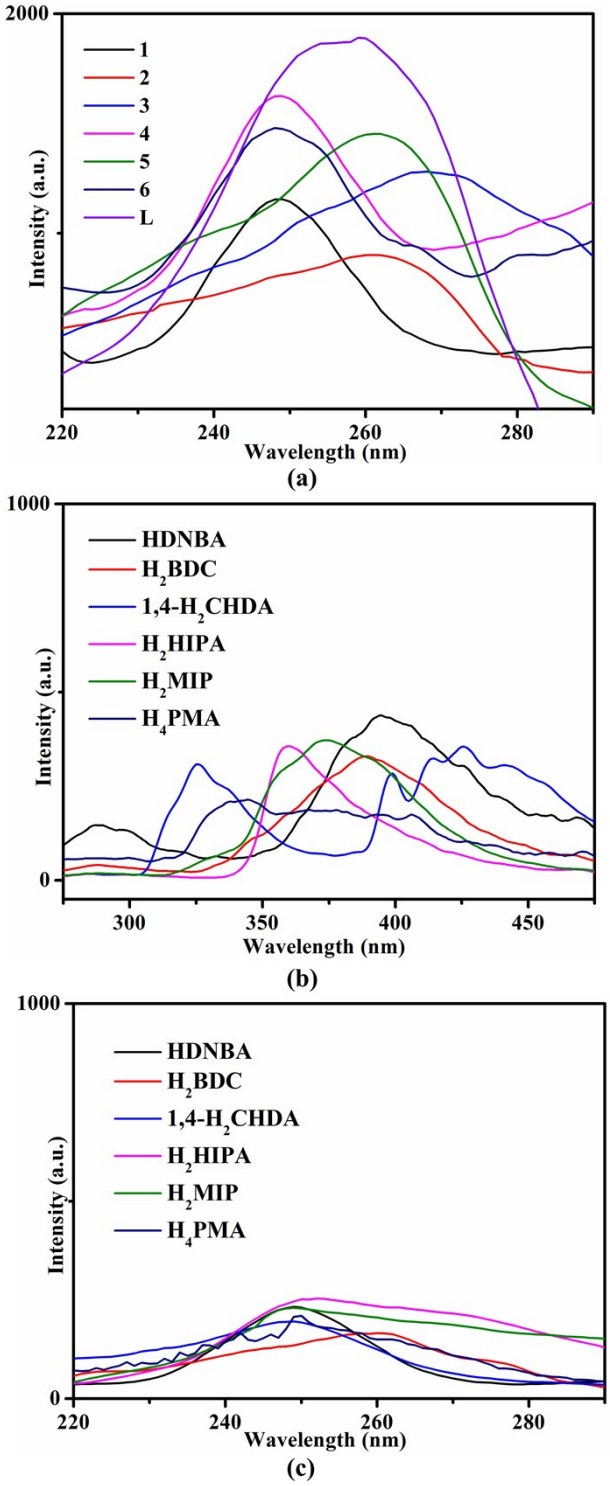

Figure S1. (a) Excitation spectra of L and **1**–**6** in the solid state. (a) The emission spectra of the organic carboxylic acids in solid state in **1**–**6**. (a) Excitation spectra of organic carboxylic acids in solid state in **1**–**6**.

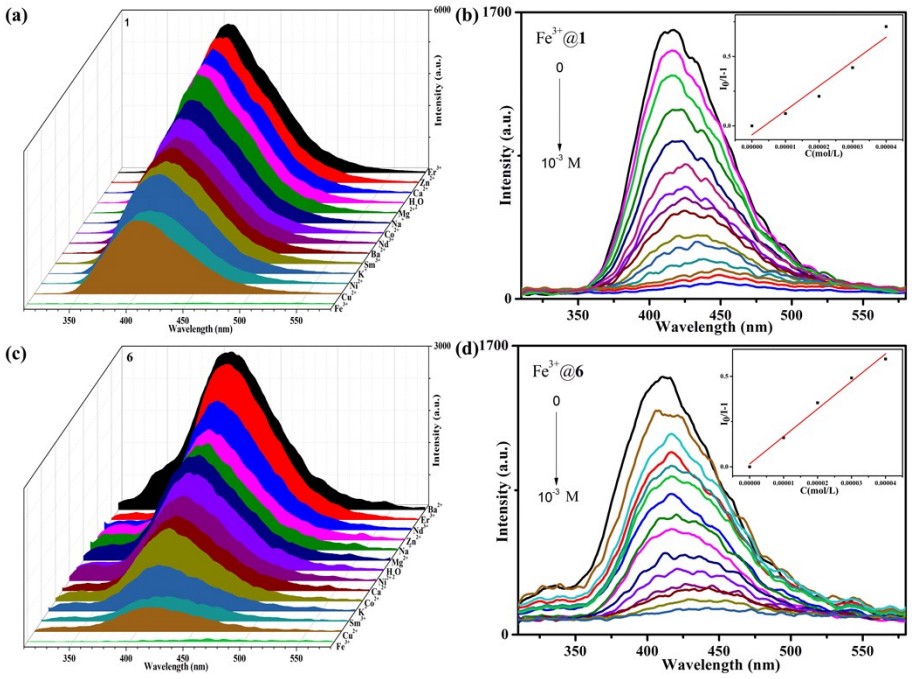

Figure S2. (a) Fluorescence emission intensities of M^{n+}@**1**. (b) The luminescence intensity of **1** upon incremental addition of Fe^{3+} ions solution in water. (c) Fluorescence emission intensities of M^{n+}@**6**. (d) The luminescence intensity of **6** upon incremental addition of Fe^{3+} ions solution in water.

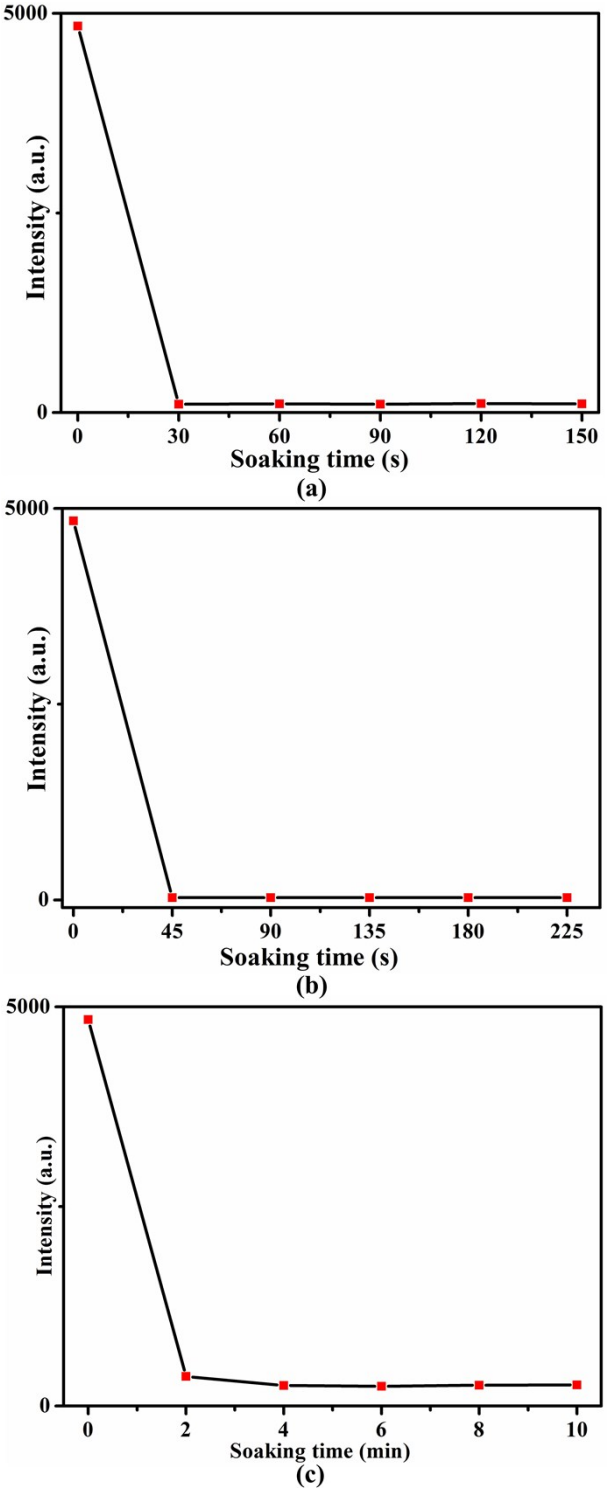

Figure S3. (a) Time-dependent emission spectra of **4** with 0.3 mL Fe^{3+} at the different reaction time. (b) Time-dependent emission spectra of **4** with 0.3 mL $Cr_2O_7^{2-}$ at the different reaction time. (c) Time-dependent emission spectra of **4** with 0.3 mL Asp at the different reaction time.

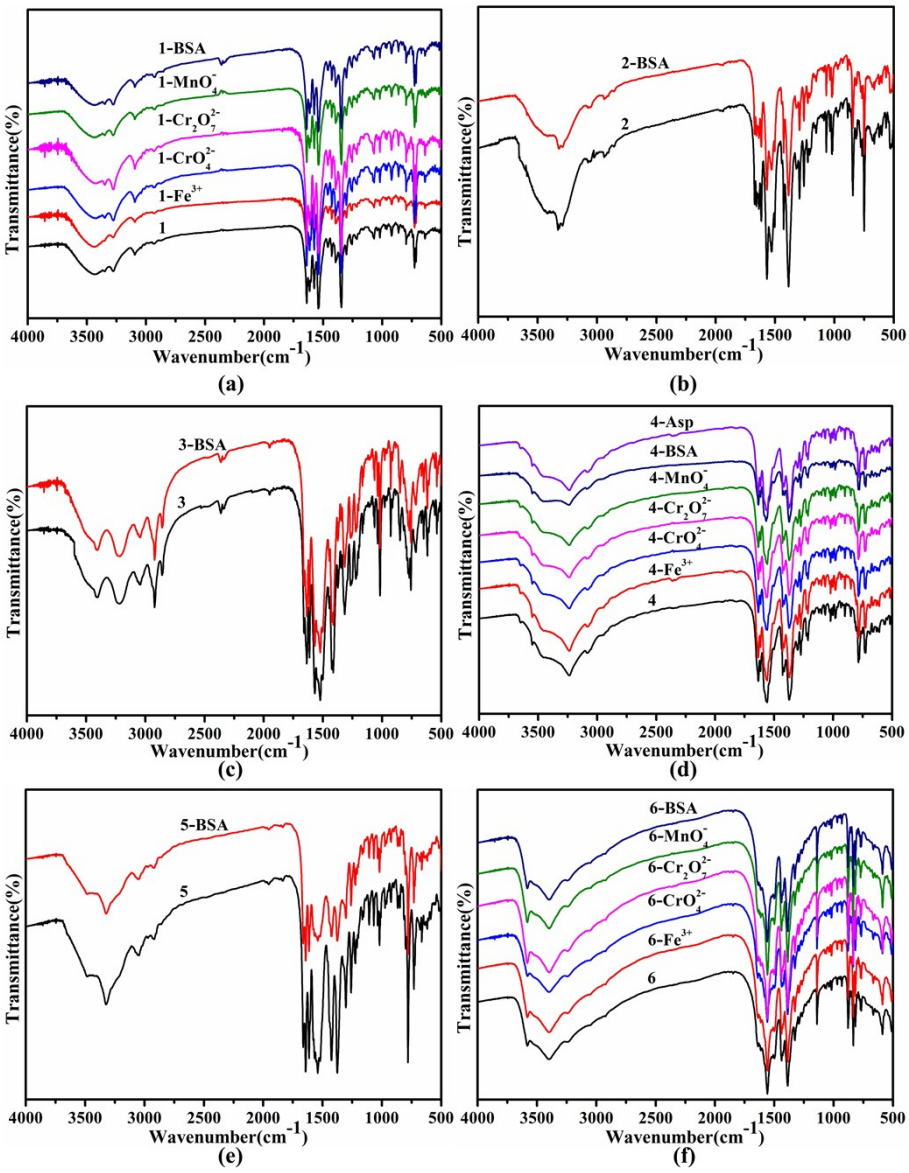

Figure S4. The IR spectra of **1**–**6**.

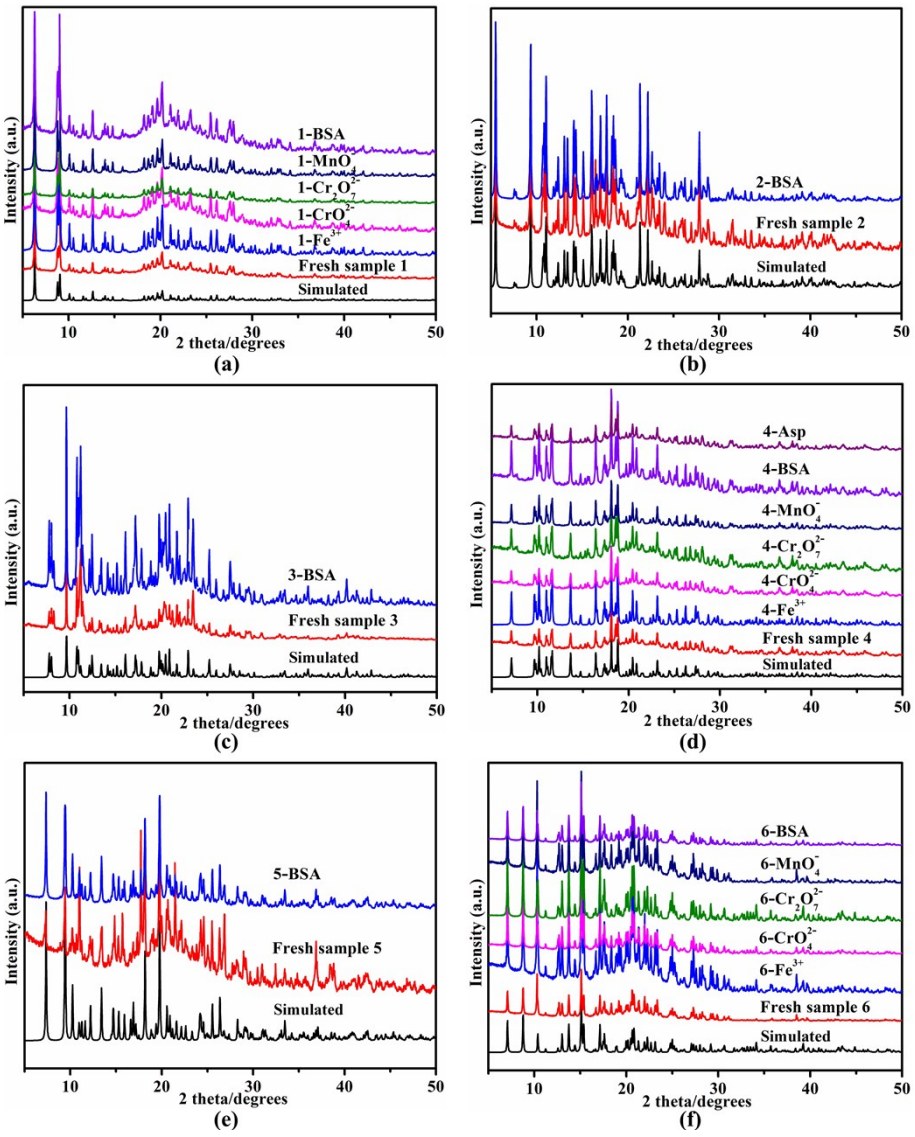

Figure S5. The PXRD patterns of **1**–**6**.

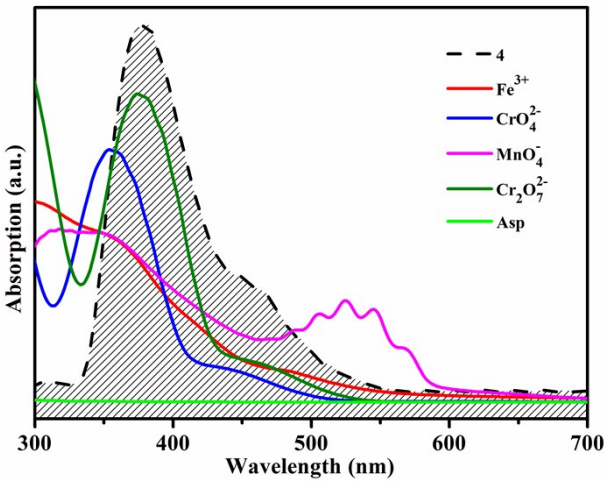

Figure S6. UV-Vis absorption spectra of Fe^{3+}, CrO_4^{2-}, $Cr_2O_7^{2-}$, MnO_4^- and Asp aqueous solution.

The emission spectrum of **4** dispersed in water upon excitation of 250 nm.

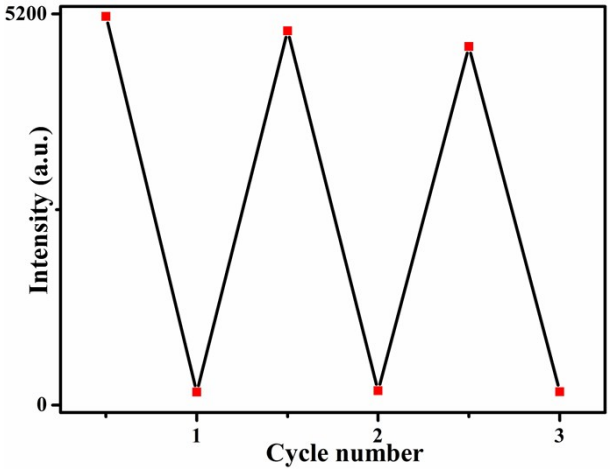

Figure S7. The cyclic response of the fluorescence intensities of **4** for detecting Fe^{3+}.

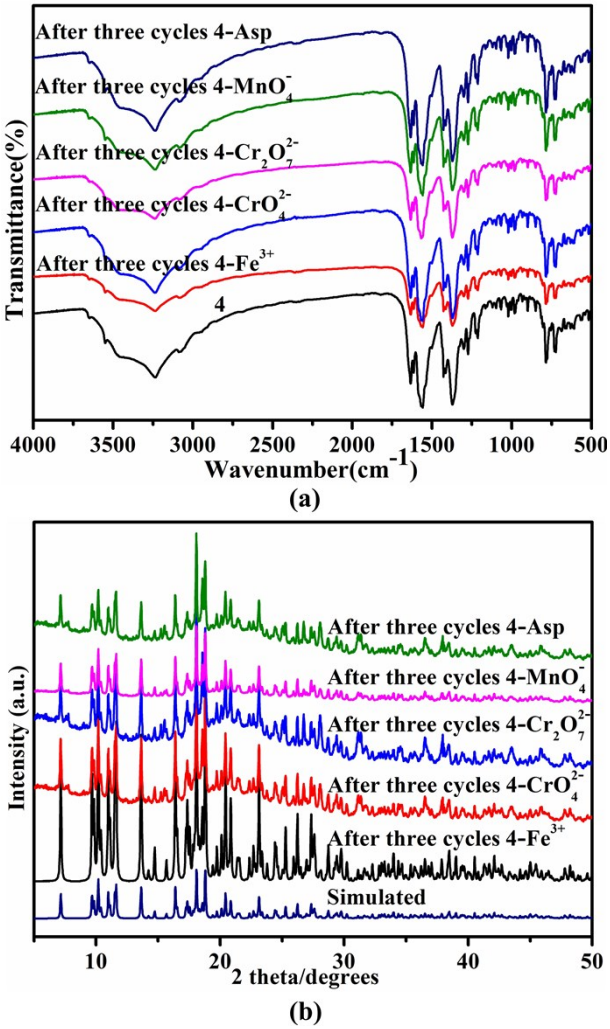

Figure S8. (a) The IR spectra of **4** after 3 cycles of fluorescence testing. (b) The PXRD spectra of **4** after 3 cycles of fluorescence testing.

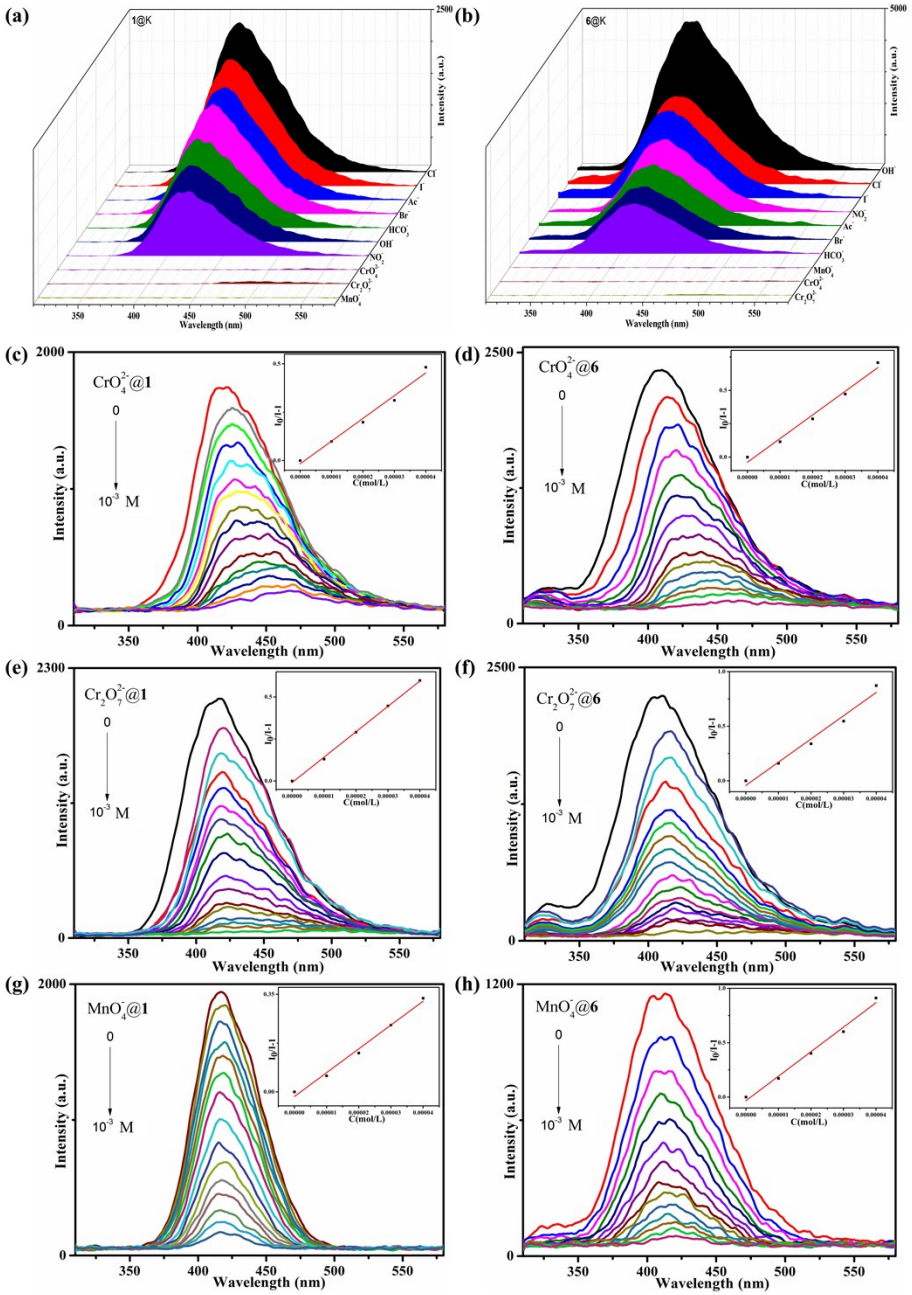

Figure S9. (a) Fluorescence emission intensities of **1** in different anion solution. (b) Fluorescence emission intensities of **6** in different anion solution. (c) The luminescence intensity of **1** upon incremental addition of CrO_4^{2-}, (e) $Cr_2O_7^{2-}$ and (g) MnO_4^- ions solution in water. (d) The luminescence intensity of **6** upon incremental addition of CrO_4^{2-}, (f) $Cr_2O_7^{2-}$ and (h) MnO_4^- ions solution in water.

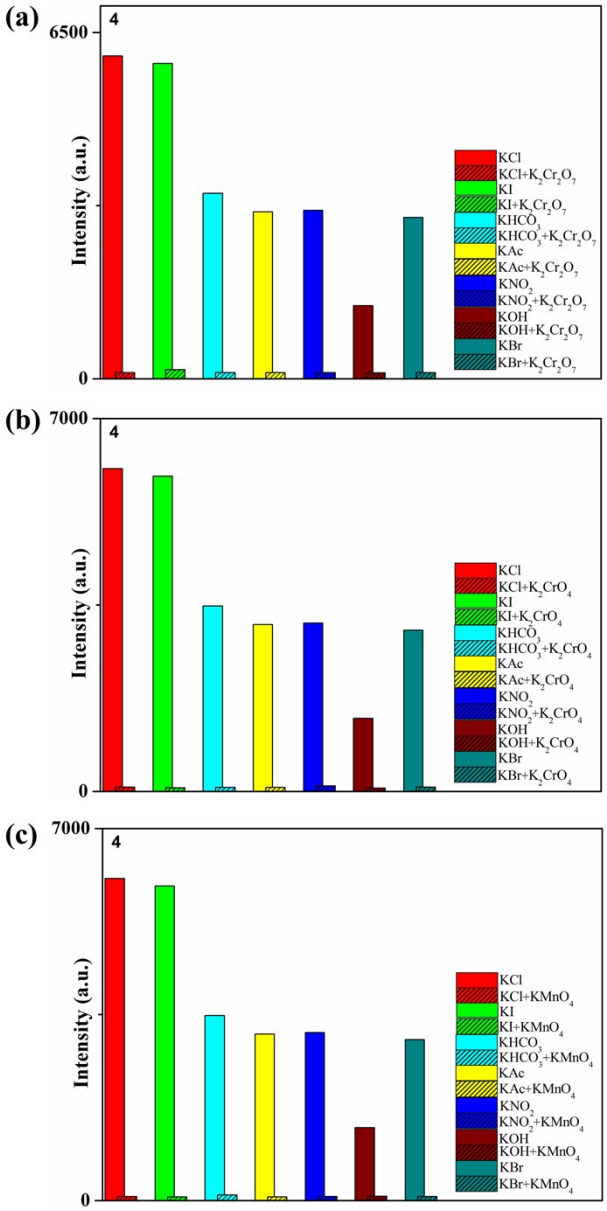

Figure S10. (a) The fluorescence selectivity of **4** for $Cr_2O_7^{2-}$, (b) CrO_4^{2-} and (c) MnO_4^- ions solution in water at room temperature.

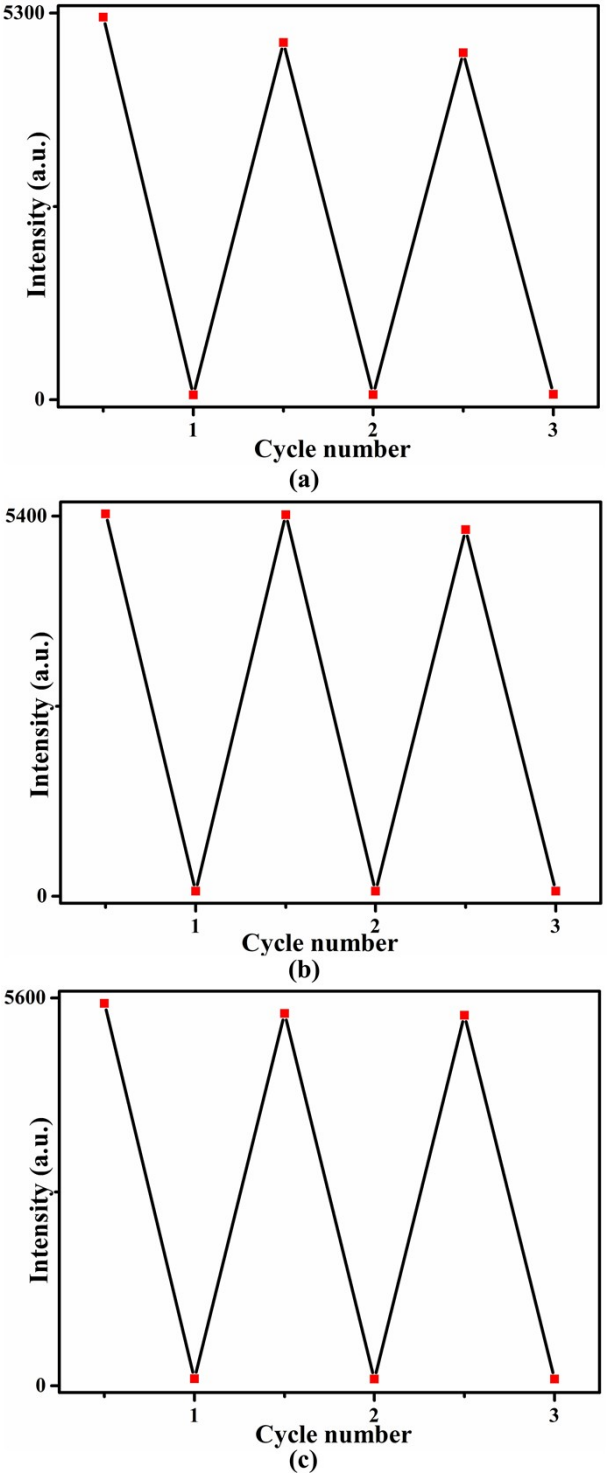

Figure S11. (a) The cyclic response of the fluorescence intensities of **4** for detecting CrO_4^{2-}, (b) $Cr_2O_7^{2-}$ and (c) MnO_4^-.

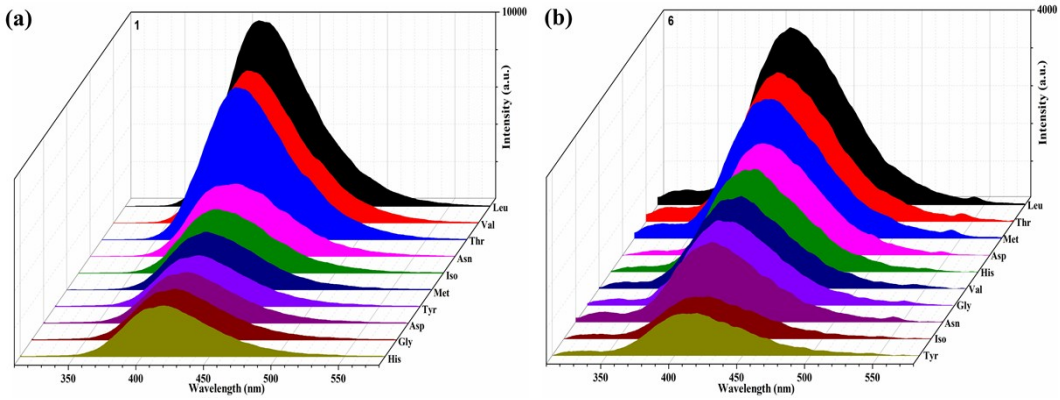

Figure S12. (a) Fluorescence emission intensity of **1** and (b) **6** in different amino acids.

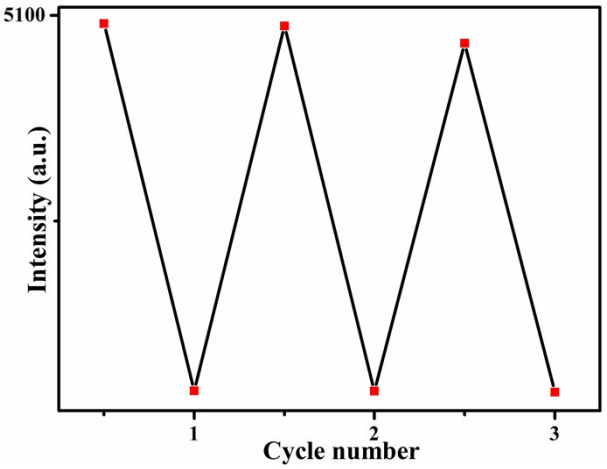

Figure S13. The cyclic response of the fluorescence intensities of **4** for detecting Asp.

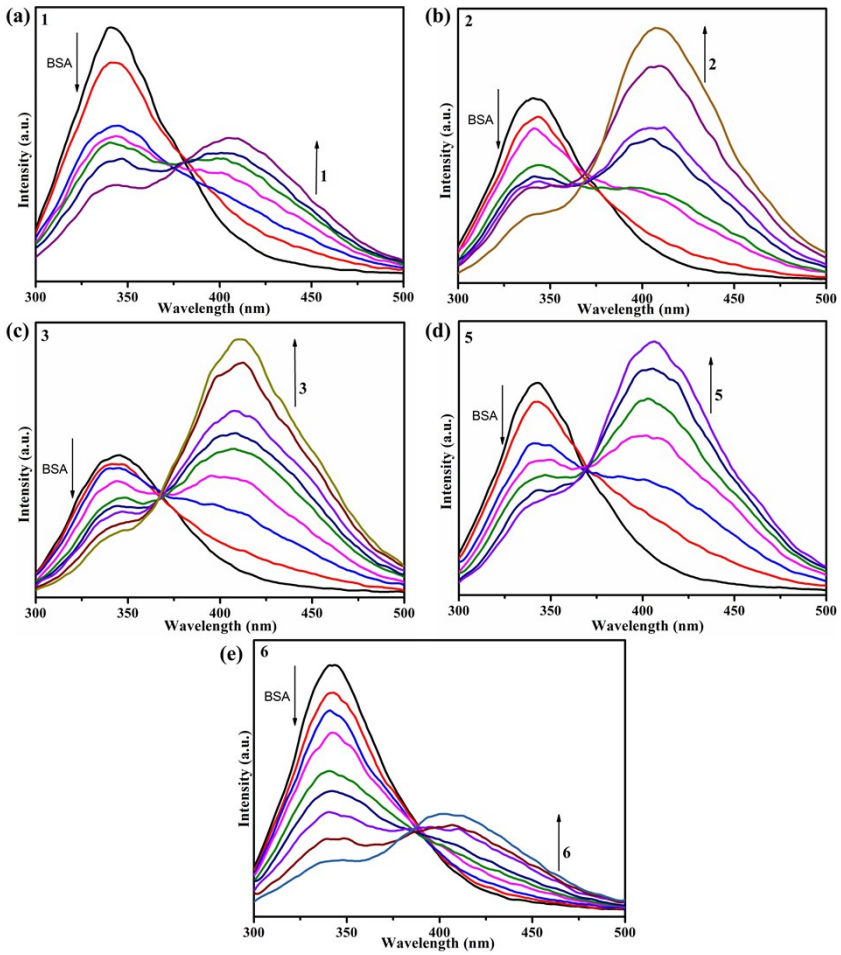

Figure S14. Fluorescence spectra of BSA@**1** (a), **2** (b), **3** (c), **5** (d) and **6** (e).

	1	**2**	**3**	**4**	**5**	**6**
(a)	HDNBA	H_2BDC	1,4-H_2CHDA	H_2HIPA	H_2MIP	H_4PMA
(b)		Cd1 Cd2				
(c)						
(d)						

Chart S1. The structural details of complexes **1**–**6**. (a) The carboxylic acids; (b) The coordination modes of Cd(II); (c) The subunits of Cd-carboxylates; (d) The subunits of Cd-L.