Construction of functional coordination polymers derived from designed flexible bis(4-carboxybenzyl)amine: syntheses, structural diversities and luminescence sensing properties in aqueous solution

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Table S1. Selected bond lengths and bond angles for compounds **1**-**4.**

Compound **1**					
N(4)-Zn(1)	2.023(2)	N(5)-Zn(1)$^{\#3}$	2.002(2)	O(1)-Zn(1)	1.977(2)
O(3)-Zn(1)	1.934(2)	Zn(1)-N(5)$^{\#3}$	2.002(2)		
C(17)-N(4)-Zn(1)	129.1(2)	C(19)-N(4)-Zn(1)	125.3(2)	C(27)-N(5)-Zn(1)$^{\#3}$	124.1(2)
C(28)-N(5)-Zn(1)$^{\#3}$	130.6(2)	C(1)-O(1)-Zn(1)	110.3(2)	C(8)-O(3)-Zn(1)	127.0(2)
O(3)-Zn(1)-O(1)	105.90(10)	O(3)-Zn(1)-N(5)$^{\#3}$	120.65(10)	O(1)-Zn(1)-N(5)$^{\#3}$	108.71(10)
O(3)-Zn(1)-N(4)	95.35(10)	O(1)-Zn(1)-N(4)	112.41(10)	N(5)$^{\#3}$-Zn(1)-N(4)	113.21(10)
Symmetry transformations used to generate equivalent atoms: #1 x-3/2,-y+1/2, z-1/2. #2 x+3/2,-y+1/2, z+1/2. #3 -x+1,-y,-z+2.					
Compound **2**					
N(2)-Pb(1)	2.511(9)	O(1)-Pb(1)	2.599(7)	O(2)-Pb(1)	2.404(9)
O(4)-Pb(1)	2.346(8)	O(5)-Pb(1)	2.671(12)		
C(1)-N(2)-Pb(1)	123.4(7)	C(3)-N(2)-Pb(1)	129.9(8)	C(14)-O(1)-Pb(1)	88.8(6)
C(14)-O(2)-Pb(1)	97.3(7)	C(7)-O(4)-Pb(1)	101.1(8)	C(7)-O(5)-Pb(1)	86.3(9)
O(4)-Pb(1)-O(2)	77.5(3)	O(2)-Pb(1)-N(2)	80.9(3)	O(4)-Pb(1)-O(1)	82.9(3)
O(2)-Pb(1)-O(1)	52.2(2)	N(2)-Pb(1)-O(1)	131.1(3)	O(4)-Pb(1)-O(5)	50.7(3)
O(2)-Pb(1)-O(5)	126.6(4)	N(2)-Pb(1)-O(5)	107.6(4)	O(1)-Pb(1)-O(5)	92.8(4)
Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1. #2 x-1/2,-y+1/2, z+1/2. #3 x+1/2, -y+1/2, z-1/2.					
Compound **3**					
Cd(1)-O(5)	2.267(4)	Cd(1)-N(9)	2.271(5)	Cd(1)-N(8)	2.286(5)
Cd(1)-O(6)$^{\#7}$	2.320(4)	Cd(1)-O(7)	2.445(5)	Cd(1)-O(8)	2.449(4)
Cd(2)-N(3)	2.281(4)	Cd(2)-N(5)	2.283(4)	Cd(2)-O(2)	2.324(4)
Cd(2)-O(4)$^{\#8}$	2.324(4)	Cd(2)-O(3)	2.383(4)	Cd(2)-O(1)	2.513(4)
Cd(2)-O(4)	2.539(4)	O(4)-Cd(2)$^{\#8}$	2.324(4)	O(6)-Cd(1)$^{\#7}$	2.320(4)
O(5)-Cd(1)-N(9)	90.61(18)	O(5)-Cd(1)-N(8)	99.34(18)	N(9)-Cd(1)-N(8)	168.92(18)
O(5)-Cd(1)-O(6)$^{\#7}$	121.52(17)	N(9)-Cd(1)-O(6)$^{\#7}$	83.21(17)	N(8)-Cd(1)-O(6)$^{\#7}$	87.40(17)
O(5)-Cd(1)-O(7)	139.04(17)	N(9)-Cd(1)-O(7)	86.64(17)	N(8)-Cd(1)-O(7)	88.98(17)
O(6)$^{\#7}$-Cd(1)-O(7)	98.73(16)	O(5)-Cd(1)-O(8)	86.12(16)	N(9)-Cd(1)-O(8)	92.72(16)
N(8)-Cd(1)-O(8)	92.81(16)	O(6)$^{\#7}$-Cd(1)-O(8)	151.98(16)	O(7)-Cd(1)-O(8)	53.28(15)
N(3)-Cd(2)-N(5)	171.38(17)	N(3)-Cd(2)-O(2)	92.39(16)	N(5)-Cd(2)-O(2)	90.25(16)
N(3)-Cd(2)-O(4)$^{\#8}$	88.57(16)	N(5)-Cd(2)-O(4)$^{\#8}$	85.32(15)	O(2)-Cd(2)-O(4)$^{\#8}$	152.66(15)
N(3)-Cd(2)-O(3)	100.20(17)	N(5)-Cd(2)-O(3)	88.37(18)	O(2)-Cd(2)-O(3)	78.80(14)
O(4)$^{\#8}$-Cd(2)-O(3)	127.89(14)	N(3)-Cd(2)-O(1)	87.13(16)	N(5)-Cd(2)-O(1)	87.82(16)

O(2)-Cd(2)-O(1)	53.78(14)	O(4)$^{\#8}$-Cd(2)-O(1)	99.03(14)	O(3)-Cd(2)-O(1)	132.39(13)
N(3)-Cd(2)-O(4)	93.72(15)	N(5)-Cd(2)-O(4)	90.71(16)	O(2)-Cd(2)-O(4)	131.14(14)
O(4)$^{\#8}$-Cd(2)-O(4)	75.97(14)	O(3)-Cd(2)-O(4)	52.41(13)	O(1)-Cd(2)-O(4)	174.89(12)
Symmetry transformations used to generate equivalent atoms: #1 -x+1, y-1/2,-z-1/2. #2 -x+1, y-1/2,-z+3/2. #3 -x+1, y+1/2,-z-1/2. #4 -x+1, y+1/2,-z+3/2. #5 x+1,y+1,z. #6 x-1,y-1,z. #7 -x+2,-y+1,-z+1. #8 -x+1,-y,-z+1.					
Compound **4**					
Zn(1)-O(1)	1.944(7)	Zn(1)-N(5)$^{\#1}$	1.977(8)	Zn(1)-O(5)	1.987(7)
Zn(1)-N(2)	2.000(7)	Zn(2)-O(8)	1.950(7)	Zn(2)-O(4)$^{\#2}$	1.983(6)
Zn(2)-N(10)$^{\#3}$	1.989(8)	Zn(2)-N(7)	2.003(7)	O(4)-Zn(2)$^{\#4}$	1.983(6)
N(5)-Zn(1)$^{\#1}$	1.977(8)	N(10)-Zn(2)$^{\#3}$	1.989(8)		
O(1)-Zn(1)-N(5)$^{\#1}$	112.5(3)	O(1)-Zn(1)-O(5)	105.3(3)	N(5)$^{\#1}$-Zn(1)-O(5)	113.6(3)
O(1)-Zn(1)-N(2)	95.1(3)	N(5)$^{\#1}$-Zn(1)-N(2)	113.4(3)	O(5)-Zn(1)-N(2)	115.2(3)
O(8)-Zn(2)-O(4)$^{\#2}$	105.0(3)	O(8)-Zn(2)-N(10)$^{\#3}$	112.5(3)	O(4)$^{\#2}$-Zn(2)-N(10)$^{\#3}$	113.8(3)
O(8)-Zn(2)-N(7)	95.7(3)	O(4)$^{\#2}$-Zn(2)-N(7)	114.9(3)	N(10)$^{\#3}$-Zn(2)-N(7)	113.2(3)
C(16)-O(4)-Zn(2)$^{\#4}$	104.4(6)	C(49)-N(7)-Zn(2)	129.3(7)	C(47)-N(7)-Zn(2)	125.8(6)
C(1)-O(1)-Zn(1)	123.3(6)	C(46)-O(8)-Zn(2)	124.2(6)	C(19)-N(2)-Zn(1)	129.1(7)
C(17)-N(2)-Zn(1)	125.7(7)	C(31)-O(5)-Zn(1)	104.6(6)		
Symmetry transformations used to generate equivalent atoms: #1 -x-1, y,-z. #2 x+1/2, y+3/2,z. #3 -x-1,y,-z-1. #4 x-1/2,y-3/2,z.					

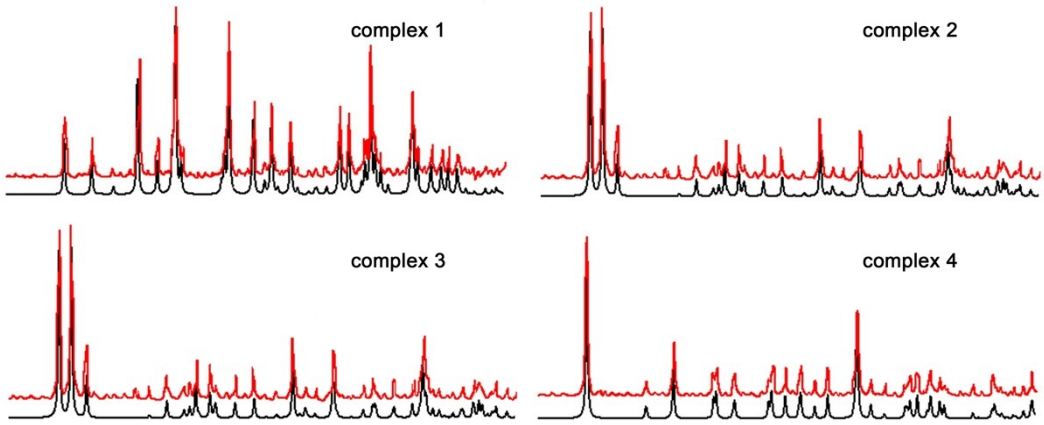

Figure S1. PXRD pattern of compounds **1–4.**

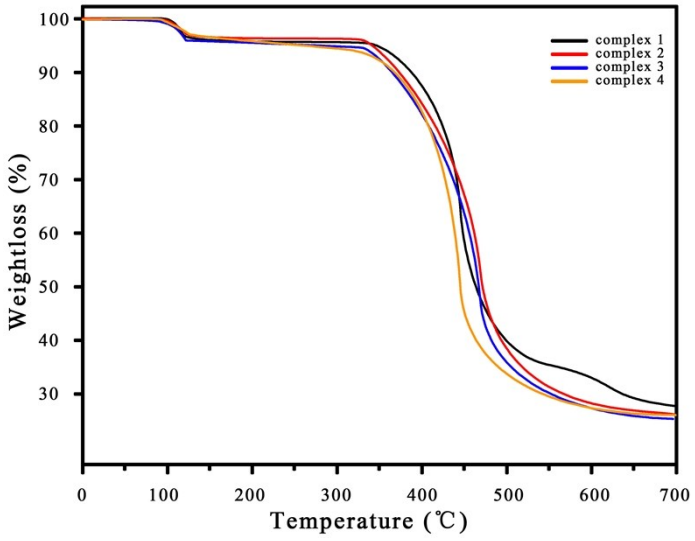

Figure S2. TGA curves for compounds **1–4**.

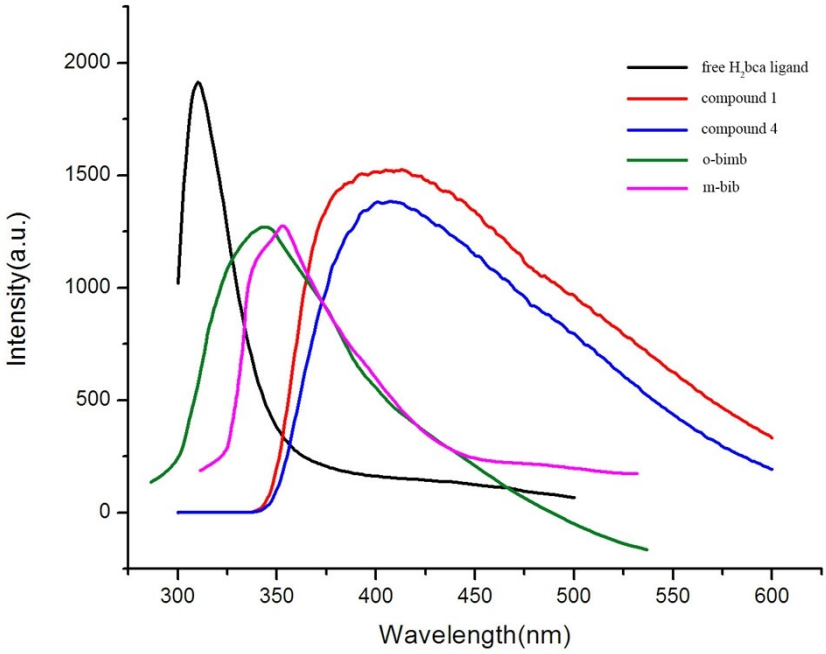

Figure S3. The fluorescence spectra of two zinc compounds (**1** and **4**), free H_2bca, o-bimb, and m-bib ligand.

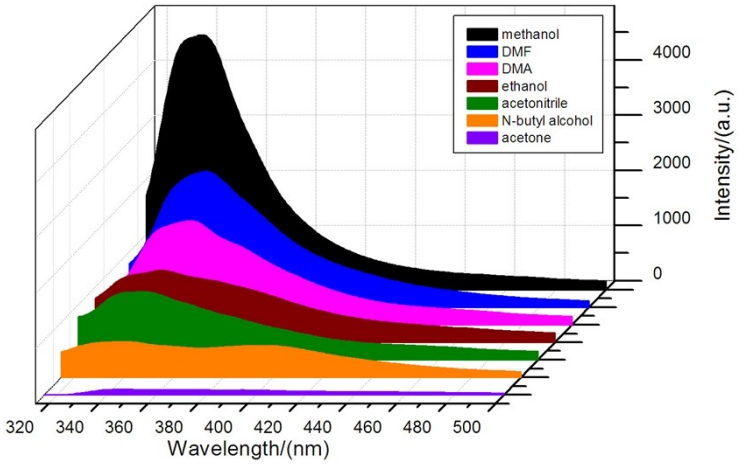

Figure S4. The luminescence intensities of compound **4** which were dispersed in different organic solvents.

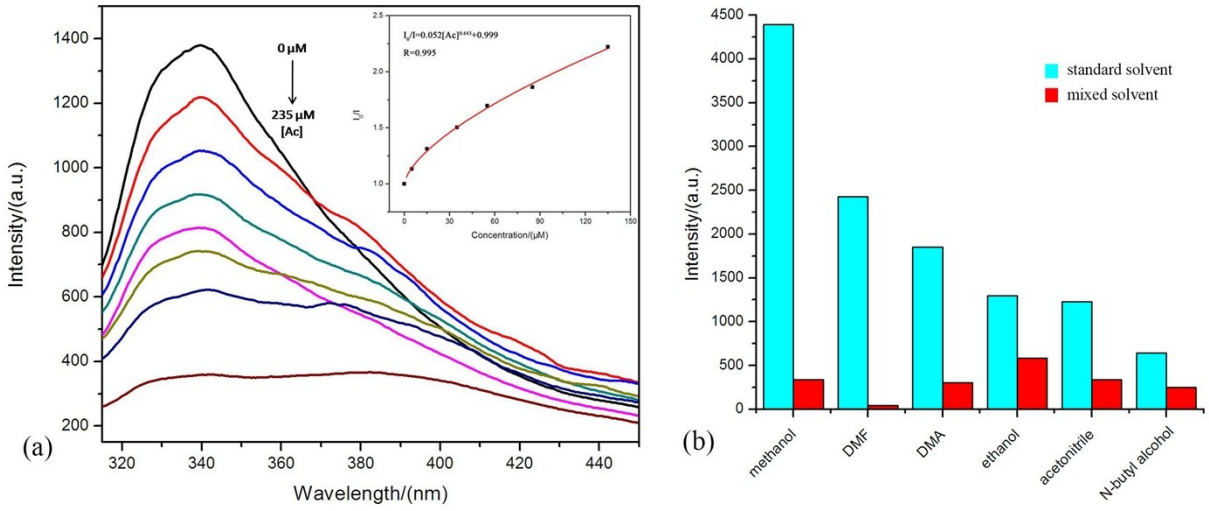

Figure S5. (a) The PL spectra of the aqueous suspension of compound **4** upon incremental addition of acetone. Inset: The luminescent intensity (I_0/I) versus the acetone concentration. (b) Luminescence intensities of **4** in six different standard solvents or mixed solvents in the presence of acetone.

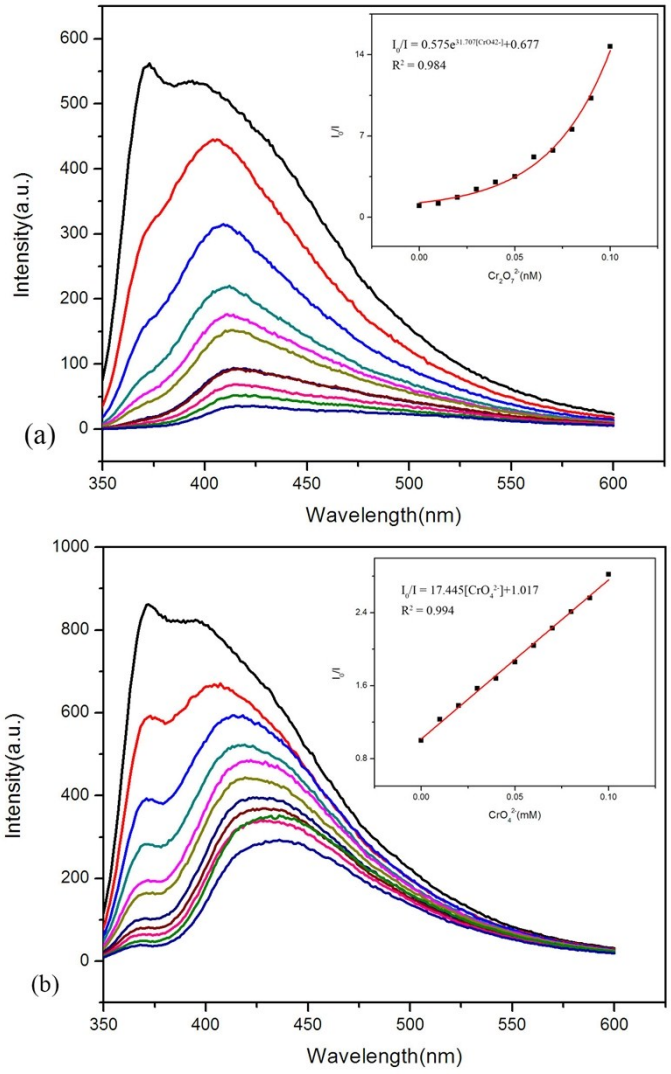

Figure S6. Luminescence spectra of **4** in a aqueous solution with different concentrations of $Cr_2O_7^{2-}$ (a) and CrO_4^{2-} (b). Inset: luminescence intensity *vs*. the $Cr_2O_7^{2-}$/CrO_4^{2-} concentrations plots.

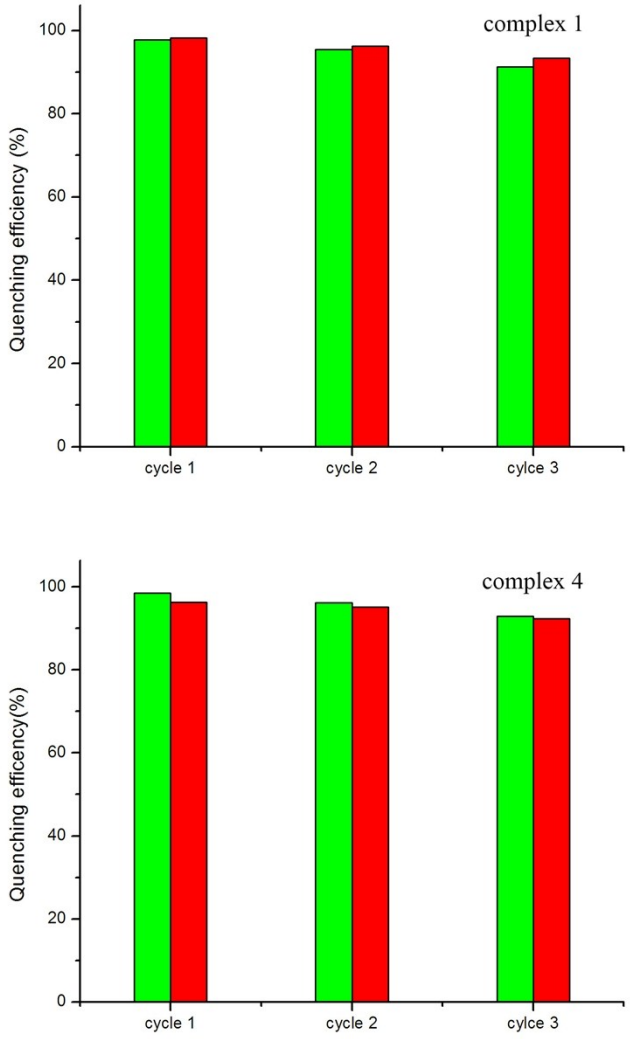

Figure S7. Recycling quenching efficiency of **1** and **4** for sensing $CrO4^{2-}$ (green) and $Cr_2O_7^{2-}$ (red) ions in aqueous solution.

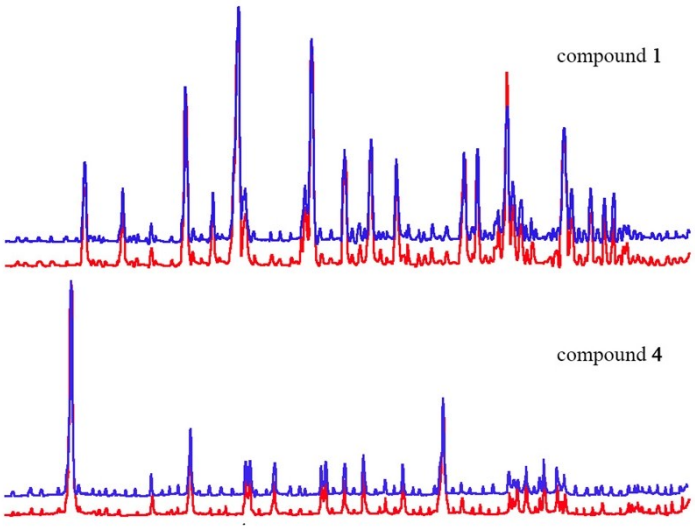

Figure S8. The PXRD plots of compounds **1** and **4** after sensing for $Cr_2O_7^{2-}$ (red) and CrO_4^{2-} (blue) anions.

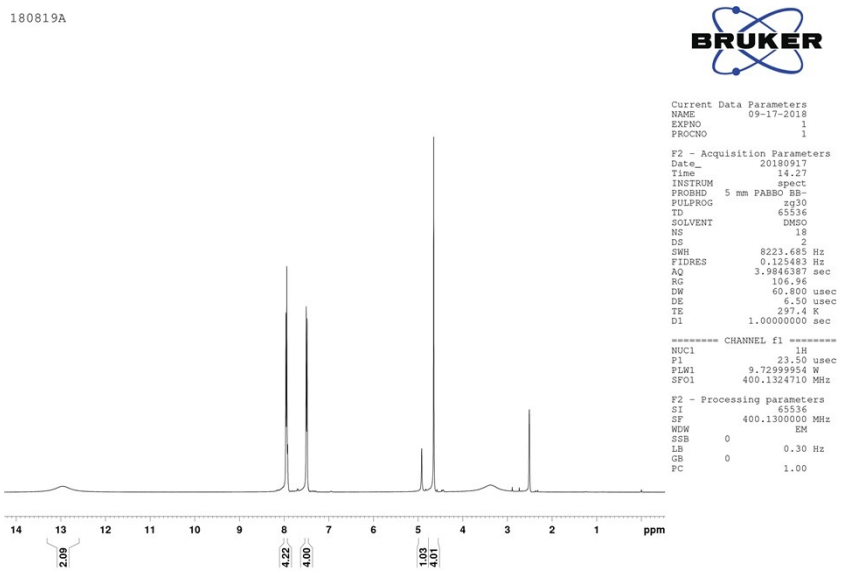

Figure S9. The 1H NMR data of the designed H_2BCA ligand.