Electronic Supplementary Information (ESI) for

An Exceptionally Stable Luminescent Cadmium(II) Metal-Organic Framework as Dual-functional Chemoensor for Detecting Cr(VI) Anions and Nitro-containing Antibiotics in Aqueous Media

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Table of Contents

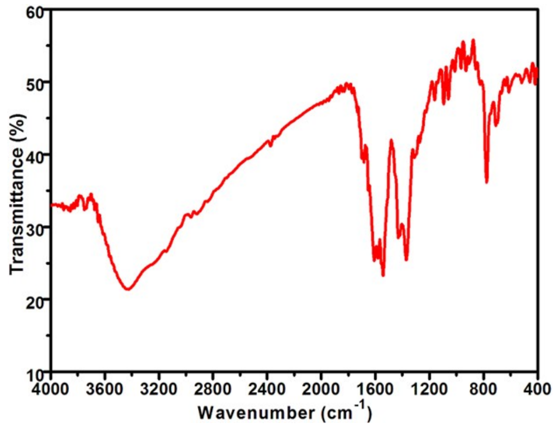

Fig. S1 The IR spectrum of **1**.

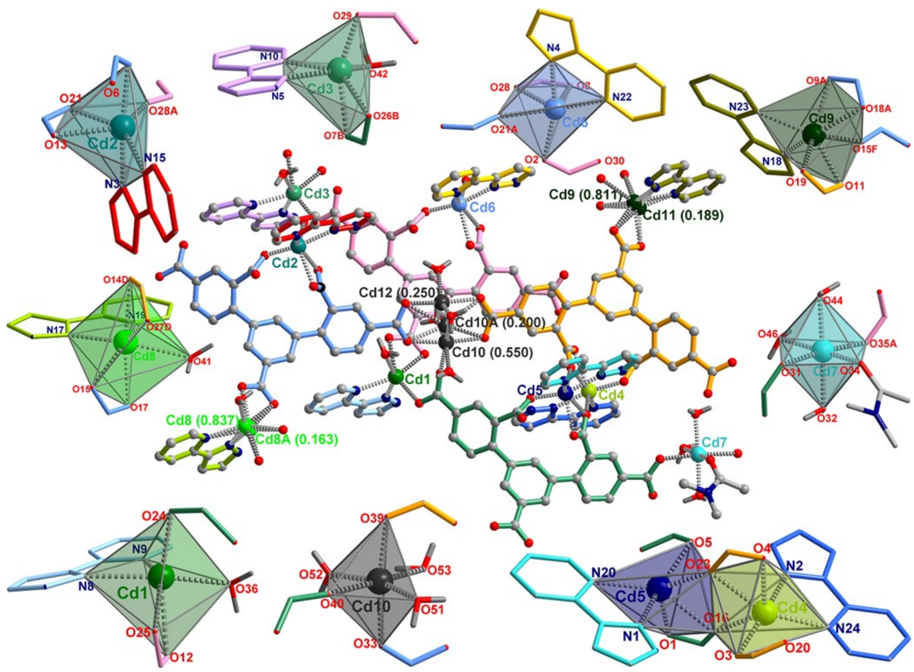

Fig. S2 The asymmetric unit of **1** with the coordination environments of ten crystallography independent Cd(II) cations (Symmetry codes: A –*x*, 1–*y*, –*z*; B *x*, *y*, –1+*z*; D –*x*, 1–*y*, 1–*z*; F *x*, 1+*y*, *z*.).

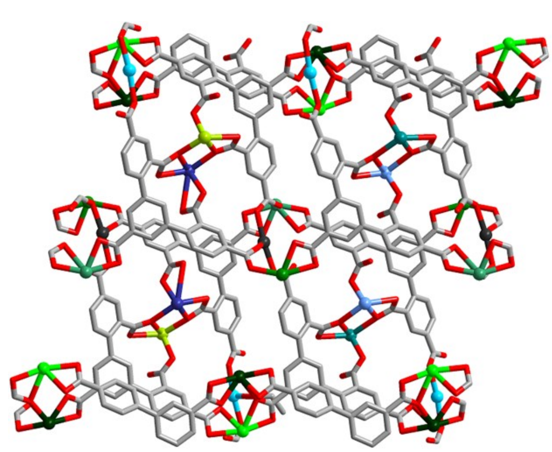

Fig. S3 The 3D $[Cd_{10}(DDB)_4]_n$ network in **1**.

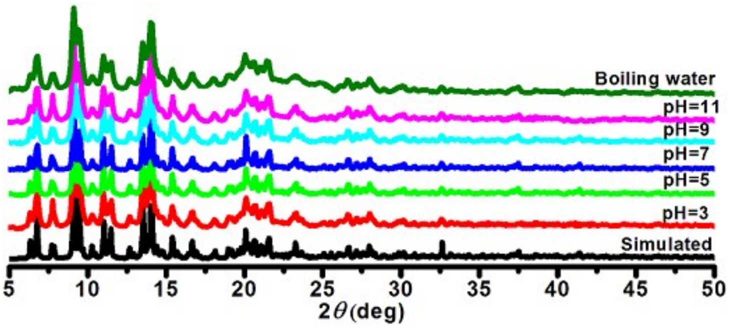

Fig. S4 The PXRD patterns of **1** after immersing into the acidic/basic aqueous solutions with the pH range from 3 to 11 for 6 h, or the boiling water for 6 h.

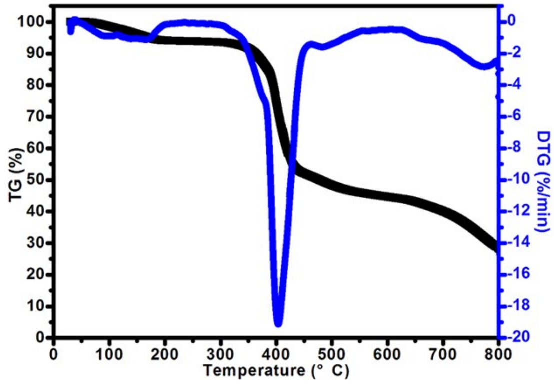

Fig. S5 TG-DTG curves for **1**.

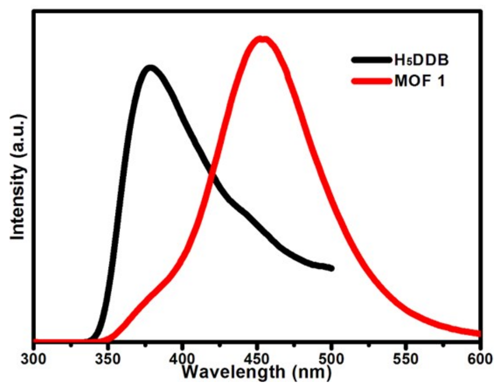

Fig. S6 The fluorescence spectra of free H_5DDB and **1** in solid state at room temperature.

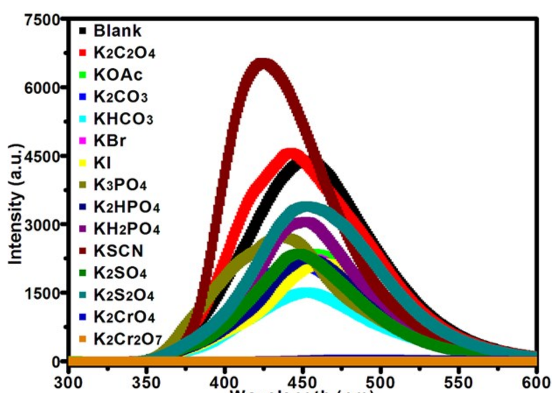

Fig. S7 The luminescence intensities of **1** dispersed in the 0.01M K_nX aqueous solutions.

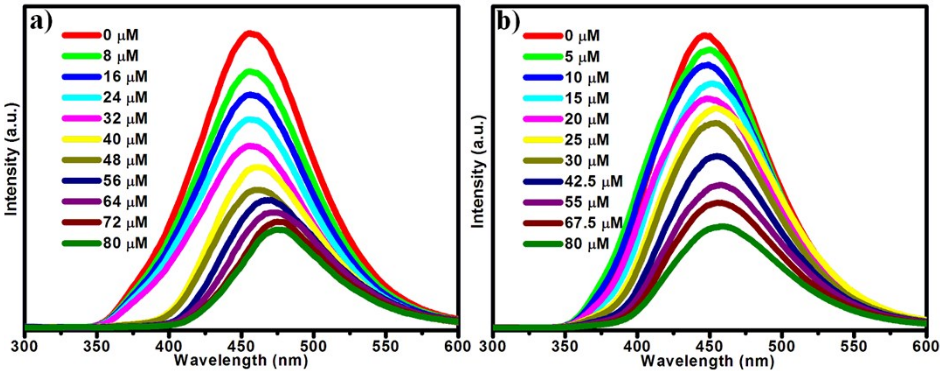

Fig. S8 The effect on the emission spectra of **1** in aqueous solutions with incremental addition of CrO_4^{2-} anion (a) and $Cr_2O_7^{2-}$ anion (b).

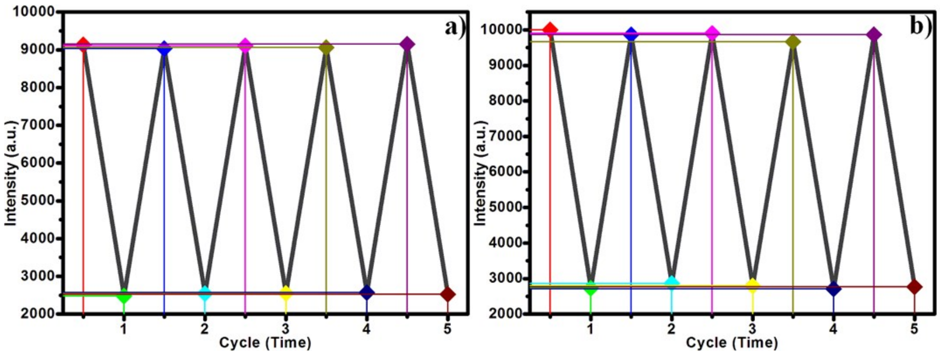

Fig. S9 Changes of the emission intensity of **1** in 5 cycles sensing of 0.1mM CrO_4^{2-} anion (a) and $Cr_2O_7^{2-}$ anion (b).

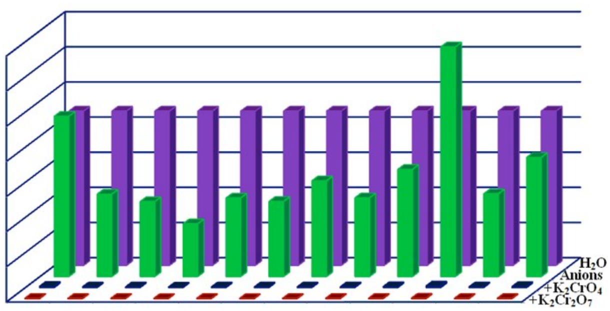

Fig. S10 The anti-interferences of **1** in sensing of Cr(VI) anions from normal anions in aqueous solutions.

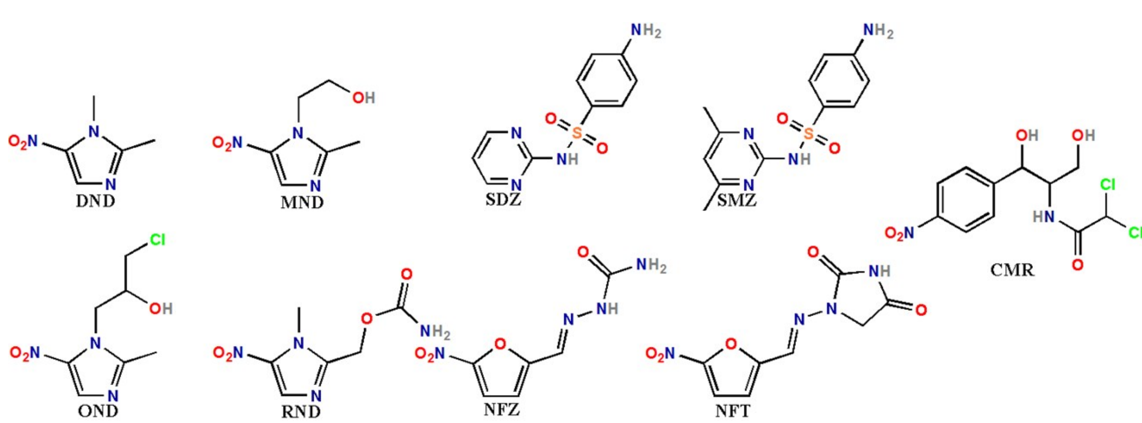

Fig. S11 The structures of selected ABXs in this work.

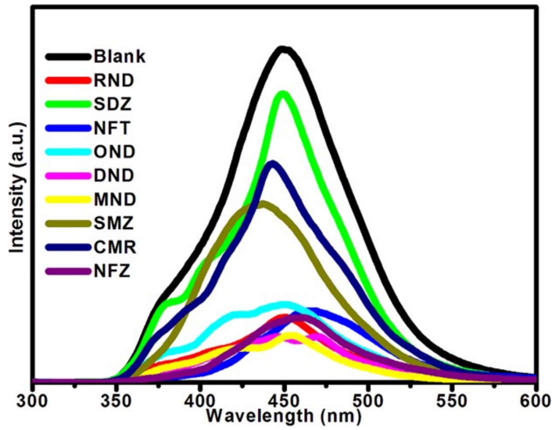

Fig. S12 The luminescence spectra of **1** as chemosensor dispersed in 0.1 mM ABXs aqueous solutions.

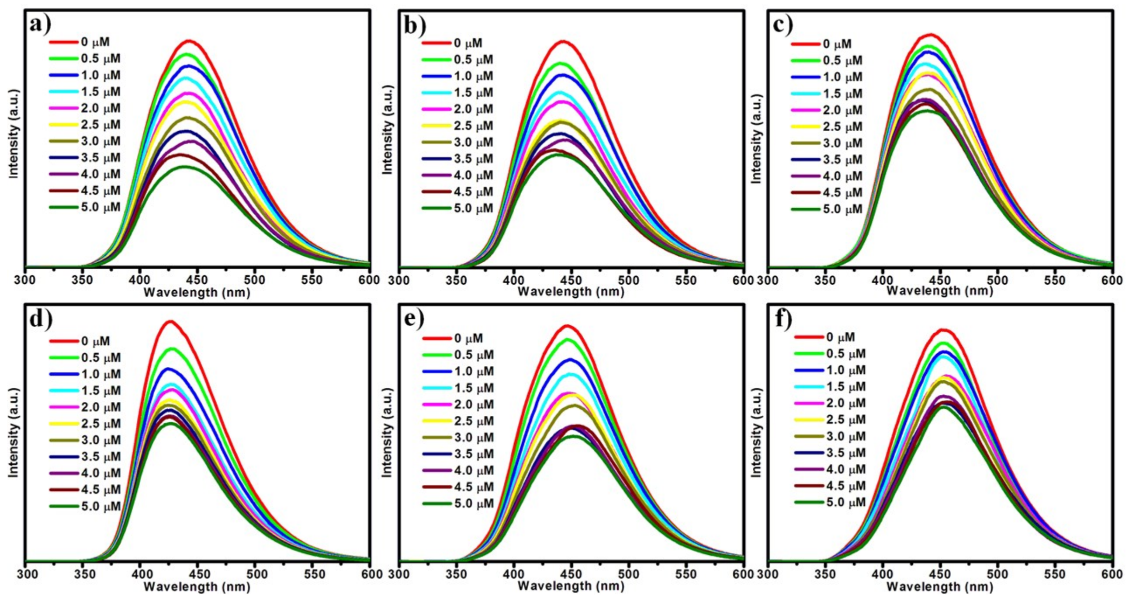

Fig. S13 The luminescence of **1** which were dispersed in the aqueous solution with different concentration of MND (a), DND (b), OND (c), RND (d), NFT (e), and NFZ (f).

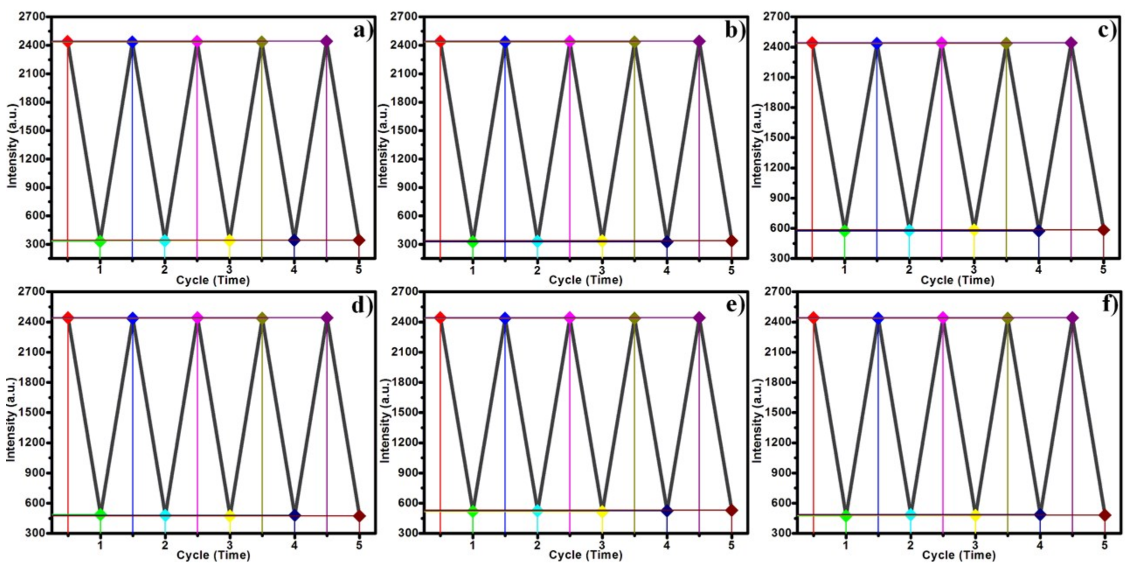

Fig. S14 The changes of the emission intensity of **1** in 5 cycles sensing of 0.1 mM MND (a), DND (b), OND (c), RND (d), NFT (e), and NFZ (f).

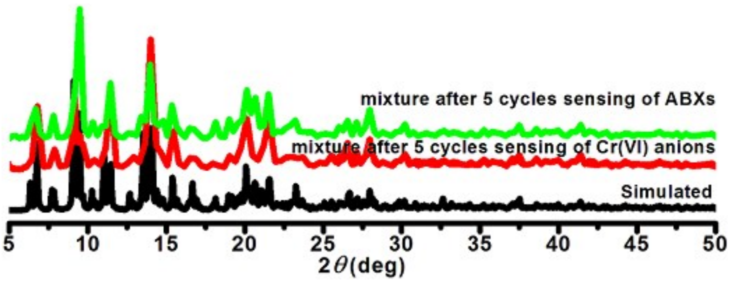

Fig. S15 PXRD patterns of the mixture of **1** after 5 cycles sensing of Cr(VI) anions and nitro-containing ABXs in aqueous solutions.

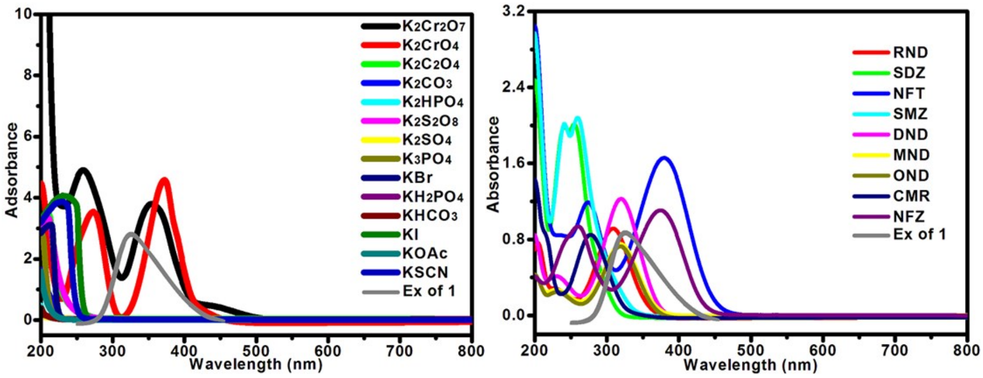

Fig. S16 The UV-Vis absorbance spectra of anions and ABXs in aqueous solution and the excitation spectra of **1**.

Table S1. Selected bond lengths (Å) and angles (º) in **1**.

Selected bond lengths (Å)					
Cd1-O12	2.402(3)	Cd2-O6	2.215(3)	Cd3-O7^{ii}	2.364(3)
Cd1-O24	2.199(3)	Cd2-O13	2.437(3)	Cd3-O26^{ii}	2.389(3)
Cd1-O25	2.355(3)	Cd2-O21	2.361(3)	Cd3-O29	2.207(3)
Cd1-O36	2.286(5)	Cd2-O28^{i}	2.466(4)	Cd3-O42	2.330(5)
Cd1-N8	2.319(4)	Cd2-N3	2.287(4)	Cd3-N5	2.332(4)
Cd1-N9	2.380(4)	Cd2-N15	2.337(4)	Cd3-N10	2.392(4)
Cd4-O3	2.202(3)	Cd5-O1	2.418(3)	Cd6-O2	2.212(3)
Cd4-O4	2.443(3)	Cd5-O5	2.229(3)	Cd6-O8	2.359(4)
Cd4-O16	2.333(3)	Cd5-O16	2.406(4)	Cd6-O21^{i}	2.462(3)
Cd4-O23	2.357(4)	Cd5-O23	2.437(3)	Cd6-O28	2.415(4)
Cd4-N2	2.295(4)	Cd5-N1	2.289(4)	Cd6-N4	2.273(4)
Cd4-N24	2.297(5)	Cd5-N20	2.333(5)	Cd6-N22	2.358(5)
Cd7-O31	2.272(3)	Cd8-O14^{iv}	2.370(4)	Cd8A-O14^{iv}	2.308(8)
Cd7-O32	2.294(4)	Cd8-O15	2.591(4)	Cd8A-O15	2.338(16)
Cd7-O34	2.142(8)	Cd8-O17	2.288(4)	Cd8A-O17	2.432(15)
Cd7-O35^{iii}	2.303(4)	Cd8-O27^{iv}	2.404(4)	Cd8A-O27^{iv}	2.348(10)
Cd7-O44	2.267(5)	Cd8-O41	2.416(5)	Cd8A-N17	2.10(2)
Cd7-O46	2.316(6)	Cd8-N17	2.328(5)	Cd8A-N19	2.67(2)
Cd9-O9^{i}	2.284(4)	Cd8-N19	2.384(5)	Cd11-O9^{i}	2.331(7)
Cd9-O11	2.271(3)	Cd10-O33	2.221(4)	Cd11-O11	2.45(2)
Cd9-O18^{i}	2.508(4)	Cd10-O39	2.202(4)	Cd11-O18^{i}	2.479(7)
Cd9-O19	2.480(4)	Cd10-O40	2.458(5)	Cd11-O19	2.180(16)
Cd9-N18	2.247(5)	Cd10-O51	2.313(7)	Cd11-N18	2.56(3)
Cd9-N23	2.405(5)	Cd10-O52	2.227(8)	Cd11-N23	2.163(17)
Cd10A-O33	2.319(5)	Cd12-O43	2.180(5)		
Cd10A-O39	2.428(5)	Cd12-O47	2.13(3)		
Cd10A-O43	2.473(6)	Cd12-O49	2.241(6)		
Cd10A-O51	2.350(9)	Cd12-O51	2.350(9)		
Cd10A-O53	1.972(11)	Cd12-O53	2.244(10)		
Selected bond angles (º)					
O24-Cd1-O12	151.63(13)	O6-Cd2-O13	98.69(13)	O7^{ii}-Cd3-O26^{ii}	54.45(11)
O24-Cd1-O25	100.89(14)	O6-Cd2-O21	85.45(13)	O7^{ii}-Cd3-N10	96.76(13)
O24-Cd1-O36	98.82(18)	O6-Cd2-O28^{i}	79.67(13)	O26^{ii}-Cd3-N10	141.63(14)
O24-Cd1-N8	99.93(15)	O6-Cd2-N3	165.25(14)	O29-Cd3-O7^{ii}	152.59(13)
O24-Cd1-N9	107.67(14)	O6-Cd2-N15	118.91(14)	O29-Cd3-O26^{ii}	102.17(13)
O25-Cd1-O12	54.32(12)	O13-Cd2-O28^{i}	125.70(11)	O29-Cd3-O42	99.31(19)
O25-Cd1-N9	147.79(14)	O21-Cd2-O13	54.39(12)	O29-Cd3-N5	97.73(15)
O36-Cd1-O12	79.06(17)	O21-Cd2-O28^{i}	71.50(12)	O29-Cd3-N10	110.39(14)
O36-Cd1-O25	107.58(19)	N3-Cd2-O13	90.97(14)	O42-Cd3-O7^{ii}	80.46(18)
O36-Cd1-N8	150.86(16)	N3-Cd2-O21	91.24(14)	O42-Cd3-O26^{ii}	112.91(18)
O36-Cd1-N9	82.75(17)	N3-Cd2-O28^{i}	85.64(14)	O42-Cd3-N5	150.58(17)
N8-Cd1-O12	94.36(14)	N3-Cd2-N15	70.92(15)	O42-Cd3-N10	81.76(18)
N8-Cd1-O25	90.52(15)	N15-Cd2-O13	94.84(15)	N5-Cd3-O7^{ii}	94.98(14)
N8-Cd1-N9	70.40(14)	N15-Cd2-O21	144.94(15)	N5-Cd3-O26^{ii}	86.48(15)
N9-Cd1-O12	100.16(13)	N15-Cd2-O28^{i}	133.75(15)	N5-Cd3-N10	69.86(14)
O3-Cd4-O4	97.67(12)	O1-Cd5-O23	122.72(11)	O2-Cd6-O8	95.11(14)
O3-Cd4-O16	82.28(13)	O5-Cd5-O1	92.29(12)	O2-Cd6-O21^{i}	124.66(12)
O3-Cd4-O23	87.70(13)	O5-Cd5-O16	90.17(13)	O2-Cd6-O28	87.98(14)
O3-Cd4-N2	167.94(14)	O5-Cd5-O23	77.90(13)	O2-Cd6-N4	162.34(15)
O3-Cd4-N24	111.06(17)	O5-Cd5-N1	157.74(14)	O2-Cd6-N22	118.25(16)
O16-Cd4-O4	126.55(12)	O5-Cd5-N20	118.01(15)	O8-Cd6-O21^{i}	124.66(12)

O16-Cd4-O23	72.47(12)	O16-Cd5-O1	53.71(11)	O8-Cd6-O28	54.02(12)
O23-Cd4-O4	54.14(11)	O16-Cd5-O23	69.84(11)	O28-Cd6-O21^{i}	70.70(12)
N2-Cd4-O4	93.65(14)	N1-Cd5-O1	53.71(11)	N4-Cd6-O8	98.75(14)
N2-Cd4-O16	86.57(14)	N1-Cd5-O16	69.84(11)	N4-Cd6-O21^{i}	83.71(14)
N2-Cd4-O23	93.34(14)	N1-Cd5-O23	80.88(14)	N4-Cd6-O28	91.32(14)
N2-Cd4-N24	71.35(17)	N1-Cd5-N20	70.67(15)	N4-Cd6-N22	70.43(16)
N24-Cd4-O4	107.70(18)	N20-Cd5-O1	107.25(16)	N22-Cd6-O8	98.61(18)
N24-Cd4-O16	122.56(17)	N20-Cd5-O16	148.20(16)	N22-Cd6-O21^{i}	132.68(16)
N24-Cd4-O23	156.45(19)	N20-Cd5-O23	127.33(16)	N22-Cd6-O28	145.32(18)
O31-Cd7-O32	863.83(14)	O14^{iv}-Cd8-O15	117.98(13)	O14^{iv}-Cd8A-O15	132.6(8)
O31-Cd7-O35^{iii}	173.96(16)	O14^{iv}-Cd8-O27^{iv}	54.62(12)	O14^{iv}-Cd8A-O17	153.0(15)
O31-Cd7-O46	90.6(2)	O14^{iv}-Cd8-N19	88.36(15)	O14^{iv}-Cd8A-O27^{iv}	56.1(2)
O32-Cd7-O35^{iii}	87.95(15)	O17-Cd8-O14^{iv}	163.35(15)	O14^{iv}-Cd8A-N19	83.2(5)
O32-Cd7-O46	93.1(2)	O17-Cd8-O15	53.08(12)	O15-Cd8A-O17	54.81(19)
O34-Cd7-O31	87.63(17)	O17-Cd8-O27^{iv}	108.76(14)	O15-Cd8A-O27^{iv}	85.1(3)
O34-Cd7-O32	86.74(17)	O17-Cd8-O41	74.64(17)	O15-Cd8A-N19	144.3(5)
O34-Cd7-O35^{iii}	89.04(17)	O17-Cd8-N17	98.49(16)	O17-Cd8A-N19	93.7(8)
O34-Cd7-O44	93.5(2)	O17-Cd8-N19	105.72(16)	O27^{iv}-Cd8A-O17	105.9(7)
O34-Cd7-O46	178.2(2)	O27^{iv}-Cd8-O15	78.66(13)	O27^{iv}-Cd8A-N19	123.4(11)
O35^{iii}-Cd7-O46	92.7(2)	O27^{iv}-Cd8-O41	78.31(18)	N17-Cd8A-O14^{iv}	102.9(6)
O44-Cd7-O31	90.80(16)	O41-Cd8-O15	110.06(17)	N17-Cd8A-O15	99.0(10)
O44-Cd7-O32	177.61(16)	N17-Cd8-O14^{iv}	94.63(15)	N17-Cd8A-O17	100.6(3)
O44-Cd7-O35^{iii}	94.44(17)	N17-Cd8-O15	86.62(15)	N17-Cd8A-O27^{iv}	149.9(13)
O44-Cd7-O46	86.6(3)	N17-Cd8-O27^{iv}	130.63(15)	N17-Cd8A-N19	67.9(3)
O9^{i}-Cd9-O18^{i}	54.29(12)	N17-Cd8-O41	150.00(19)	O9^{i}-Cd11-O11	123.2(11)
O9^{i}-Cd9-O19	130.68(15)	N17-Cd8-N19	70.03(17)	O9^{i}-Cd11-O18^{i}	54.21(17)
O9^{i}-Cd9-N23	83.72(14)	N19-Cd8-O15	146.55(15)	O9^{i}-Cd11-N18	102.3(10)
O11-Cd9-O9^{i}	135.10(15)	N19-Cd8-O27^{iv}	134.74(15)	O11-Cd11-O18^{i}	81.7(5)
O11-Cd9-O18^{i}	84.77(13)	N19-Cd8-O41	83.6(2)	O11-Cd11-N18	84.6(11)
O11-Cd9-O19	54.71(13)	O33-Cd10-O40	93.38(16)	O18^{i}-Cd11-N18	135.8(16)
O11-Cd9-N23	139.12(17)	O33-Cd10-O51	88.1(2)	O19-Cd11-O9^{i}	147.4(11)
O19-Cd9-O18^{i}	88.72(14)	O33-Cd10-O52	85.3(2)	O19-Cd11-O11	56.0(3)
N18-Cd9-O9^{i}	114.41(17)	O39-Cd10-O33	172.04(19)	O19-Cd11-O18^{i}	96.7(5)
N18-Cd9-O11	96.61(17)	O39-Cd10-O40	92.99(16)	O19-Cd11-N18	109.8(6)
N18-Cd9-O18^{i}	157.73(19)	O39-Cd10-O51	88.7(2)	N23-Cd11-O9^{i}	88.2(4)
N18-Cd9-O19	110.28(17)	O39-Cd10-O52	99.6(2)	N23-Cd11-O11	143.2(6)
N18-Cd9-N23	70.58(19)	O51-Cd10-O40	76.9(2)	N23-Cd11-O18^{i}	135.1(10)
N23-Cd9-O18^{i}	121.73(16)	O52-Cd10-O40	88.5(2)	N23-Cd11-O19	108.6(11)
N23-Cd9-O19	92.42(17)	O52-Cd10-O51	163.5(3)	N23-Cd11-N18	68.9(4)
O43-Cd12-O49	160.7(3)	O33-Cd10A-O39	136.7(2)		
O43-Cd12-O51	92.5(3)	O33-Cd10A-O43	163.2(2)		
O43-Cd12-O53	86.0(3)	O33-Cd10A-O51	84.7(2)		
O47-Cd12-O43	86.4(6)	O39-Cd10A-O43	54.49(17)		
O47-Cd12-O49	99.7(6)	O51-Cd10A-O39	82.5(2)		
O47-Cd12-O51	81.2(8)	O51-Cd10A-O43	85.2(2)		
O47-Cd12-O53	142.7(9)	O53-Cd10A-O33	100.0(3)		
O49-Cd12-O51	106.5(3)	O53-Cd10A-O39	107.4(3)		
O49-Cd12-O53	78.1(3)	O53-Cd10A-O43	84.7(3)		
O53-Cd12-O51	135.5(3)	O53-Cd10A-O51	157.5(3)		
Symmetry codes: i –*x*, 1–*y*, –*z*; ii *x*, *y*, –1+*z*; iii 1-*x*, 2-*y*, 1-*z*; iv –*x*, 1–*y*, 1–*z*.					

Table S2. Comparison of various CPs sensors for the detection of $Cr_2O_7^{2-}$ ion.

	Analyte	CPs based Fluorescent Materials	Quenching constant (K_{SV}, M^{-1})	Detection Limits (LOD)	Media	Ref
1	$Cr_2O_7^{2-}$	$[Co_{1.5}(TBIP)_{1.5}(L)]$	2.09×10^4	0.099 μM	H_2O	37
2		$[Cd_3\{Ir(ppy\text{-}COO)_3\}_2]$	3.475×10^4	145.1 ppb	H_2O	38
3		$[Zn_7(TPPE)_2(SO_4)_7]$	1.09×10^4	26.98 ppb	H_2O	39
4		$[Cd_3(L)(NTB)_2]$	3.0×10^4	5.3×10^{-5} M	H_2O	40
5		$[Cd_2(L1)(1,4\text{-}NDC)_2]$	5.86×10^4	0.031 ppm	H_2O	41
6		$[Cd(TIPA)_2(ClO_4)_2]$	7.15×10^4	8 ppb	H_2O	42

Table S3. Comparison of various CPs sensors for the detection of nitro-containing ABXs.

	Analyte	CPs based Fluorescent Materials	Quenching constant (K_{SV}, M^{-1})	Detection Limits (LOD)	Media	Ref
1	NFT	[Zn(L)(aip)]	N/A	100 ppm	H_2O	48
2		[Zn(L)(ip)]	N/A	80 ppm	H_2O	
3		[Zn(L)(HBTC)]	N/A	45 ppm	H_2O	
4		$[Mg_2(APDA)_2]$	8.82×10^4	126 ppb	H_2O	49
5		$[Cd_3(CBCD)_2]$	6.39×10^4	N/A	H_2O	51
6		$[Cd_3(TDCPB)]$	1.05×10^5	N/A	H_2O	52
1	NFZ	[Zn(L)(aip)]	N/A	80 ppm	H_2O	48
2		[Zn(L)(ip)]	N/A	40 ppm	H_2O	
3		[Zn(L)(HBTC)]	N/A	25 ppm	H_2O	
4		$[Mg_2(APDA)_2]$	9.00×10^4	108 ppb	H_2O	49
5		$[Cd_3(CBCD)_2]$	9.72×10^4	N/A	H_2O	51
6		$[Cd_3(TDCPB)]$	7.46×10^4	N/A	H_2O	52
1	OND	$[Cd_3(DBPT)_2]$	2.4×10^4	1.10 ppm	H_2O	50
1	MND	$[Cd_3(DBPT)_2]$	2.0×10^4	1.71 ppm	H_2O	50
1	DMZ	$[Cd_3(DBPT)_2]$	1.7×10^4	1.41 ppm	H_2O	50
1	2-M-5-MZ	$[Cd_3(DBPT)_2]$	1.1×10^4	1.27 ppm	H_2O	50