Electronic Supporting Information

Zn(II) and Cd(II) coordination networks based on N-donor ligand: synthesis, crystal structures, and sensing of nitroaromatic explosives

Jian-Long Du,*[a] Chao-Ping Li,[a] Ju-Ping Gao,[a] Xiao-Ying Zhang,[a] Xu Jing,[a] Ya-Juan Mu,*[b] and Li-Jun Li *[a]

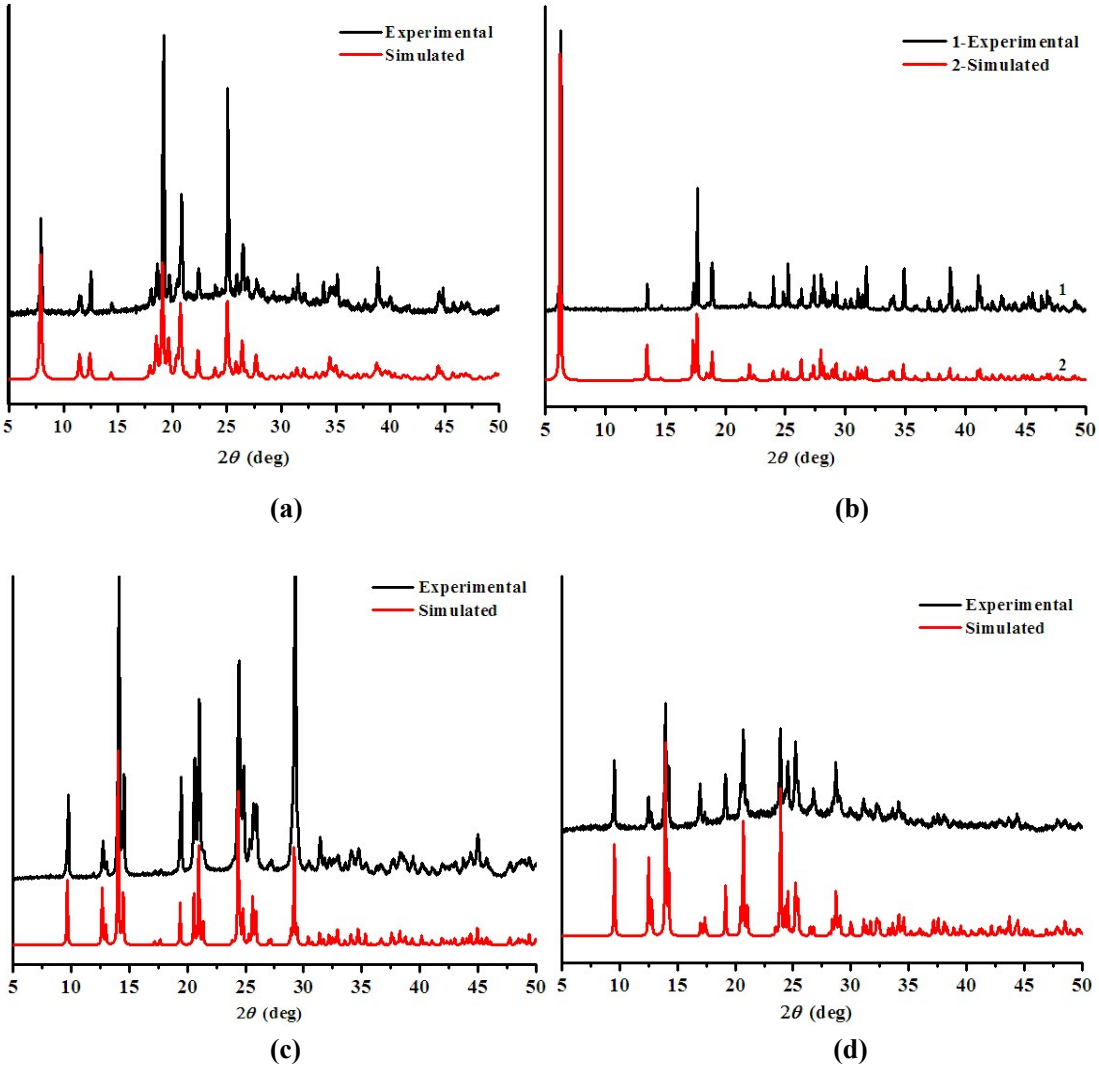
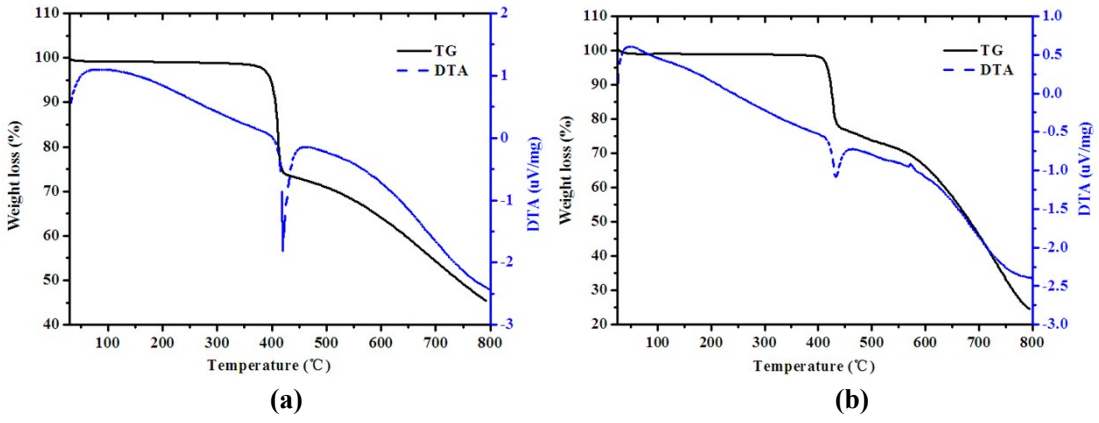
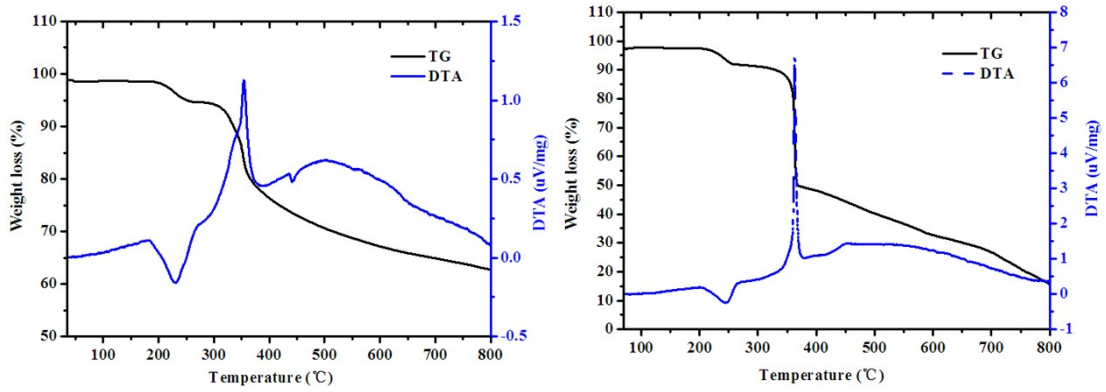


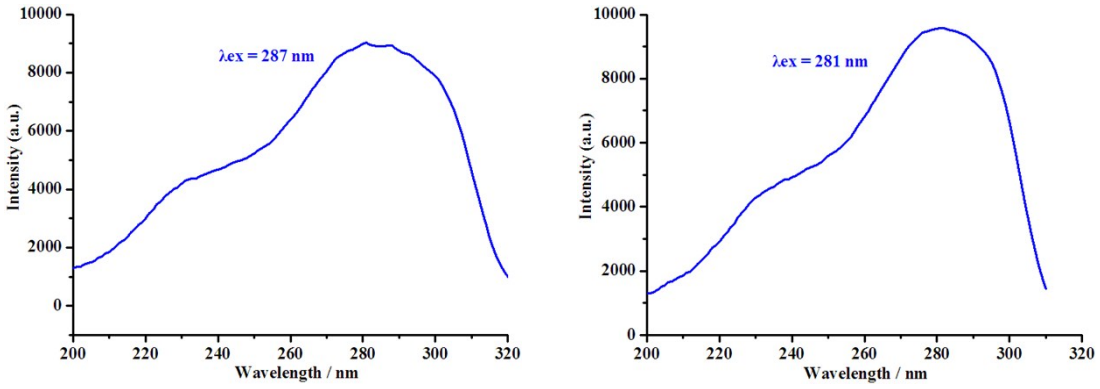
Fig. S1. PXRD patterns of the compounds (a for **1**, b for **2**, c for **3**, and d for **4**).



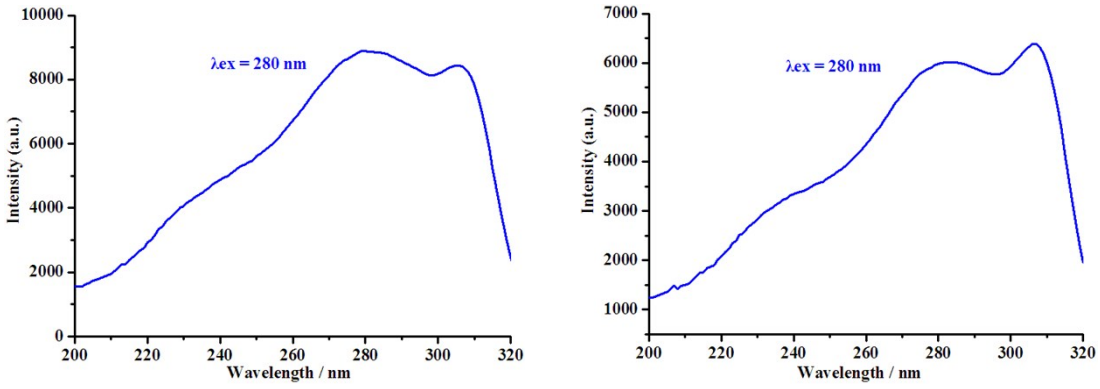


(c) **(d)**

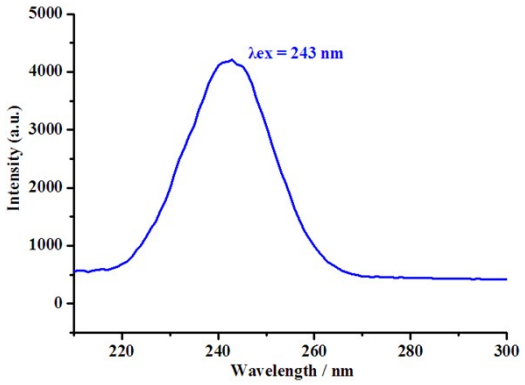
Fig. S2. TG curves of **1**–**4** (a for **1**, b for **2**, c for **3**, and d for **4**).



(a) **(b)**



(c) **(d)**



(e)

Fig. S3. Solid state excitation spectra of **1**–**4** and H**L** at ambient temperature (a for **1**, b for **2**, c for **3**, d for **4**, and e for H**L**).

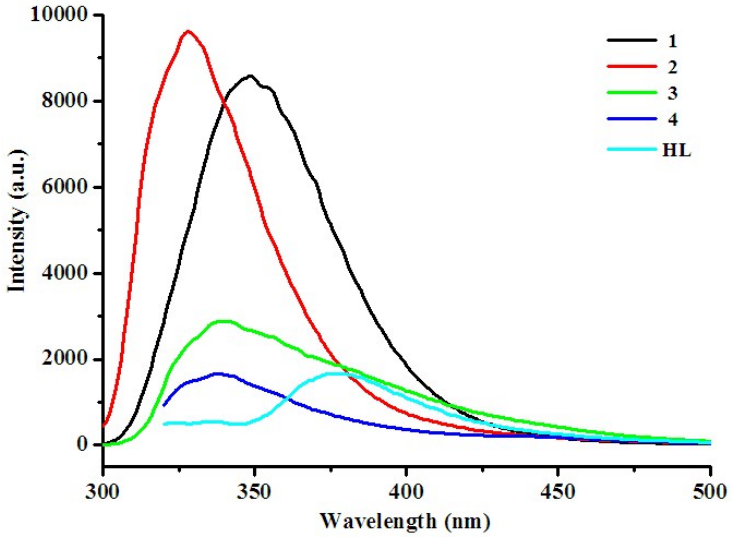


Fig. S4. Solid state emission spectra of **1**–**4** and H**L** at ambient temperature.

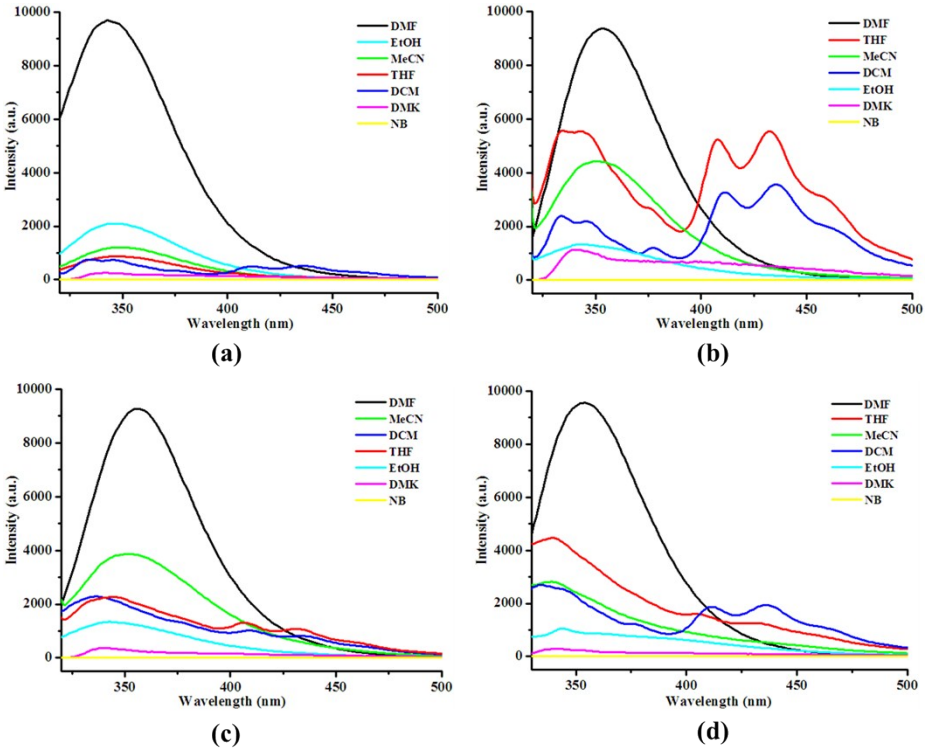
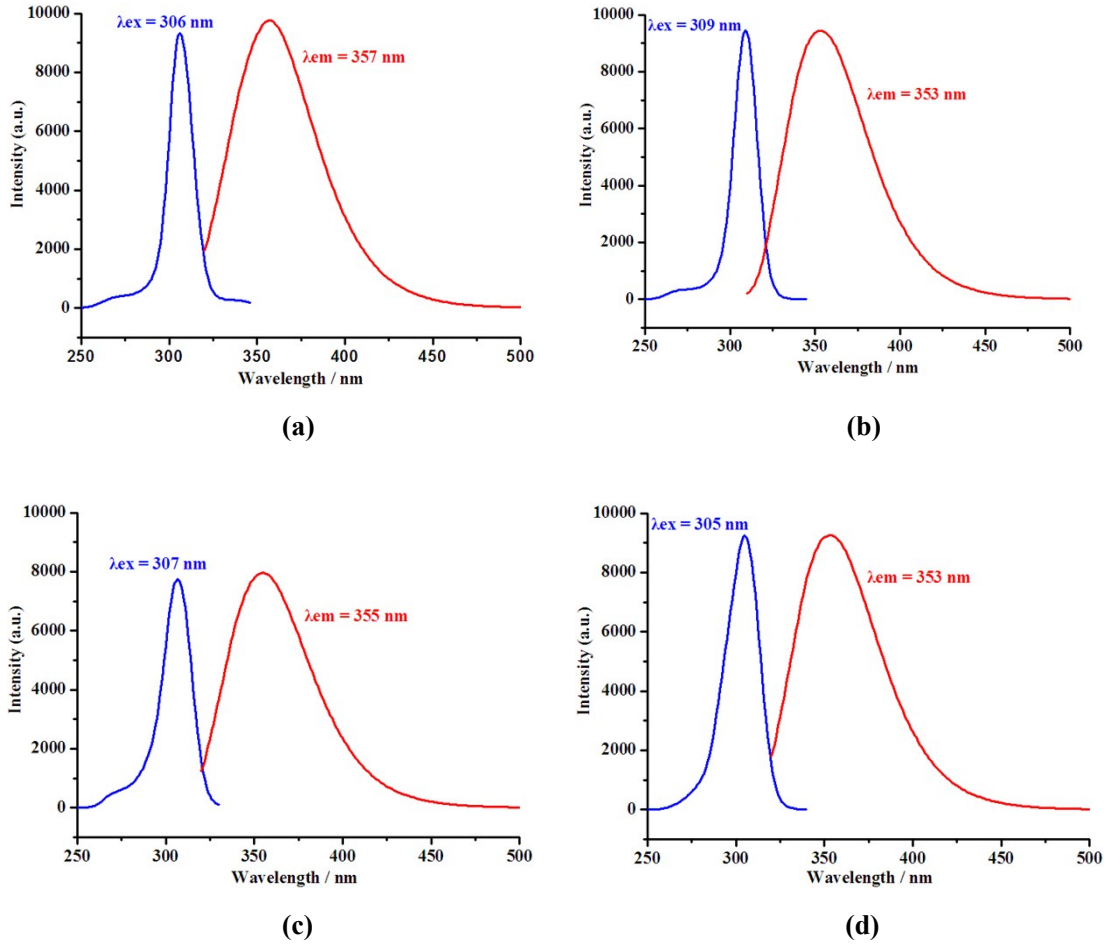
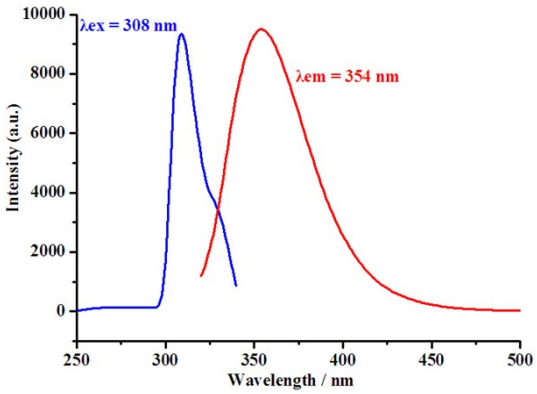


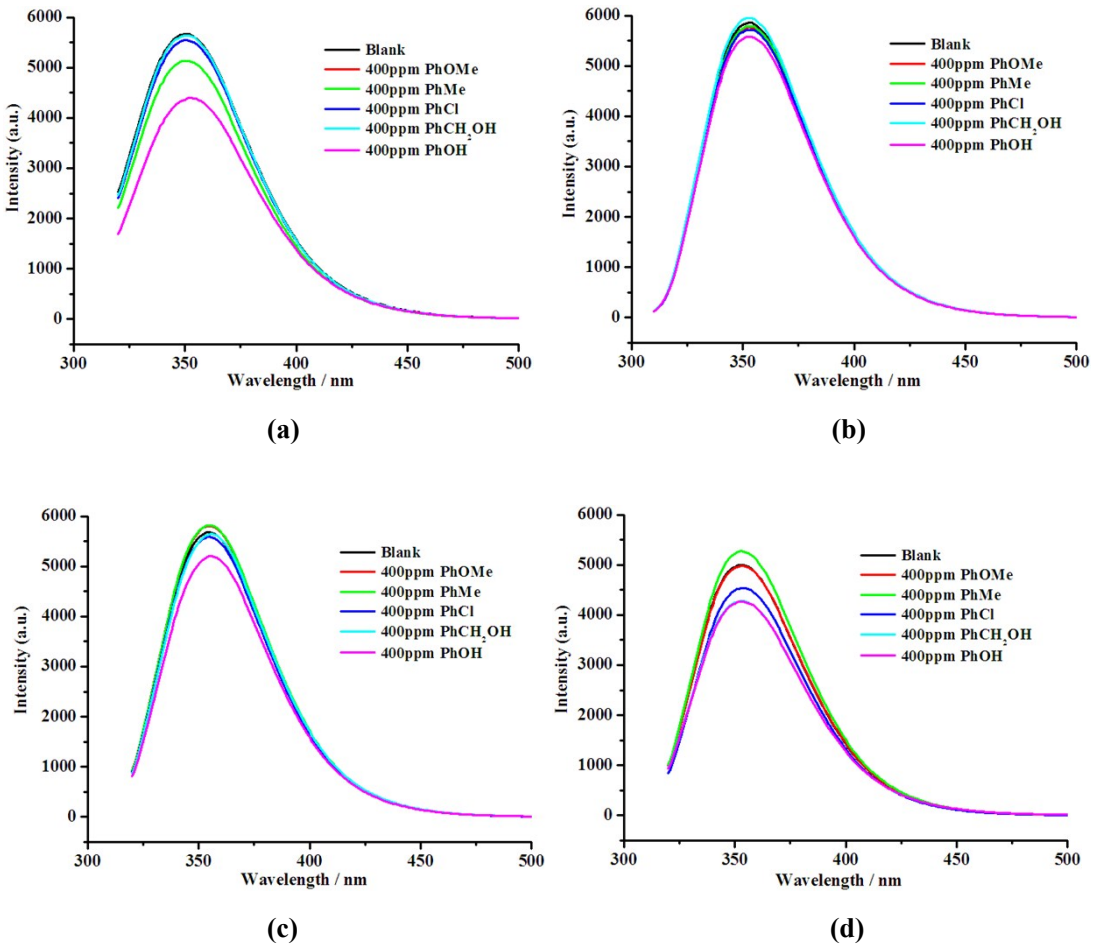
Fig. S5. Emission spectra of **1**–**4** in different solvents (a for **1**, b for **2**, c for **3**, and d for **4**).





(e)

Fig. S6. Excitation and emission spectra of **1**–**4** in DMF (a for **1**, b for **2**, c for **3**, d for **4**, and e for H**L**).



(a) **(b)**

(c) **(d)**

Fig. S7. Emission spectra of **1**–**4** at different aromatic compounds in DMF (a for **1**, b for **2**, c for **3**, and d for **4**).

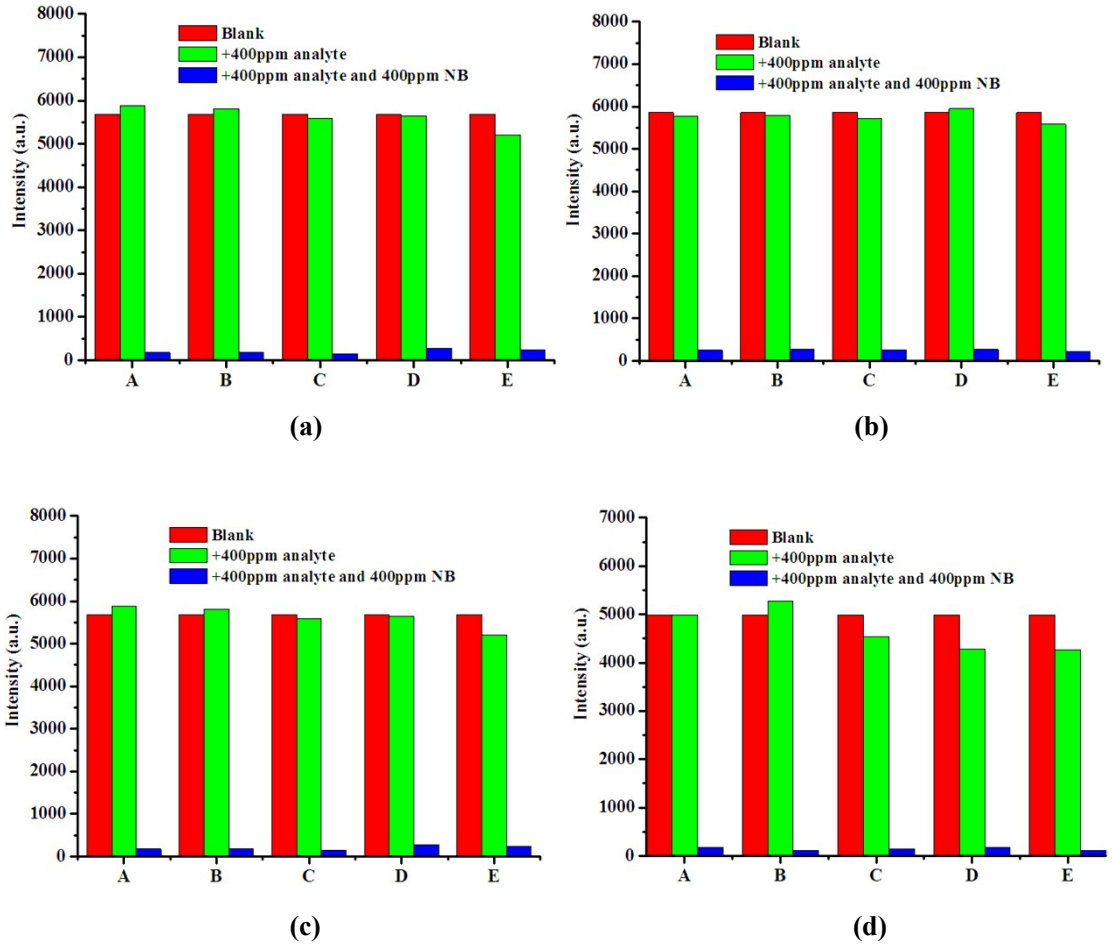
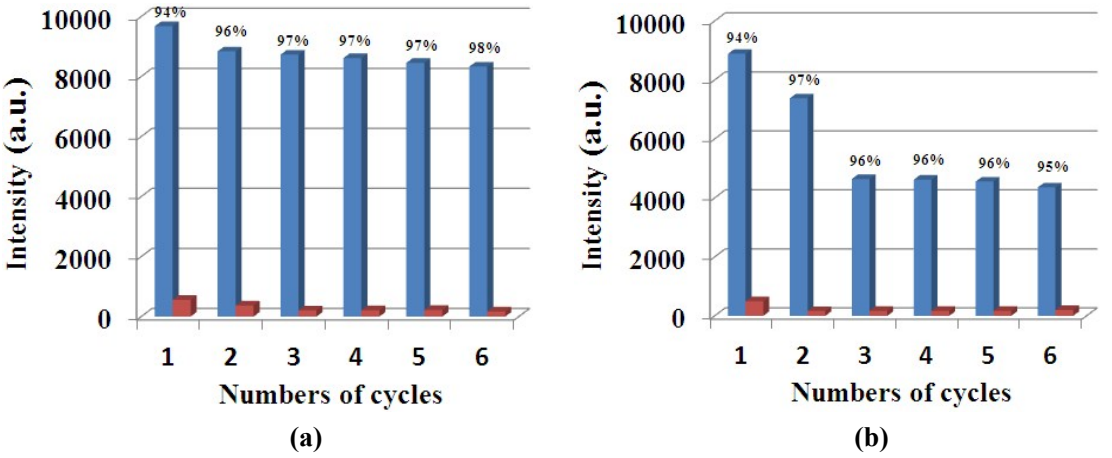


Fig. S8. Emission intensities of **1**–**4** dispersed in DMF and in the presence of 400 ppm differernt analytes (a for **1**, b for **2**, c for **3**, and d for **4**).



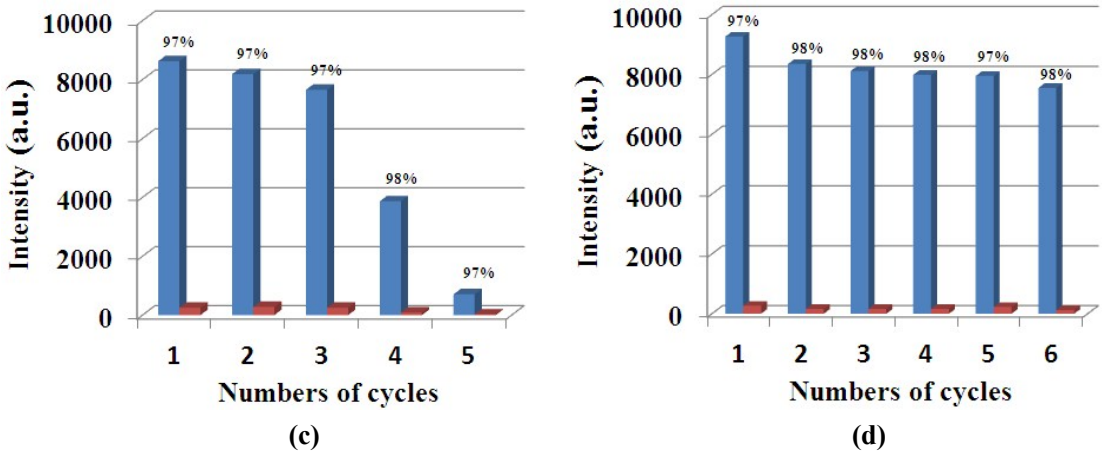


Fig. S9. Reproducibility of the quenching ablity of **1**–**4** dispersed in DMF and in the presence of 400 ppm **NB**. The percentages on the top represent quenching efficiency of every cycle (a for **1**, b for **2**, c for **3**, and d for **4**).

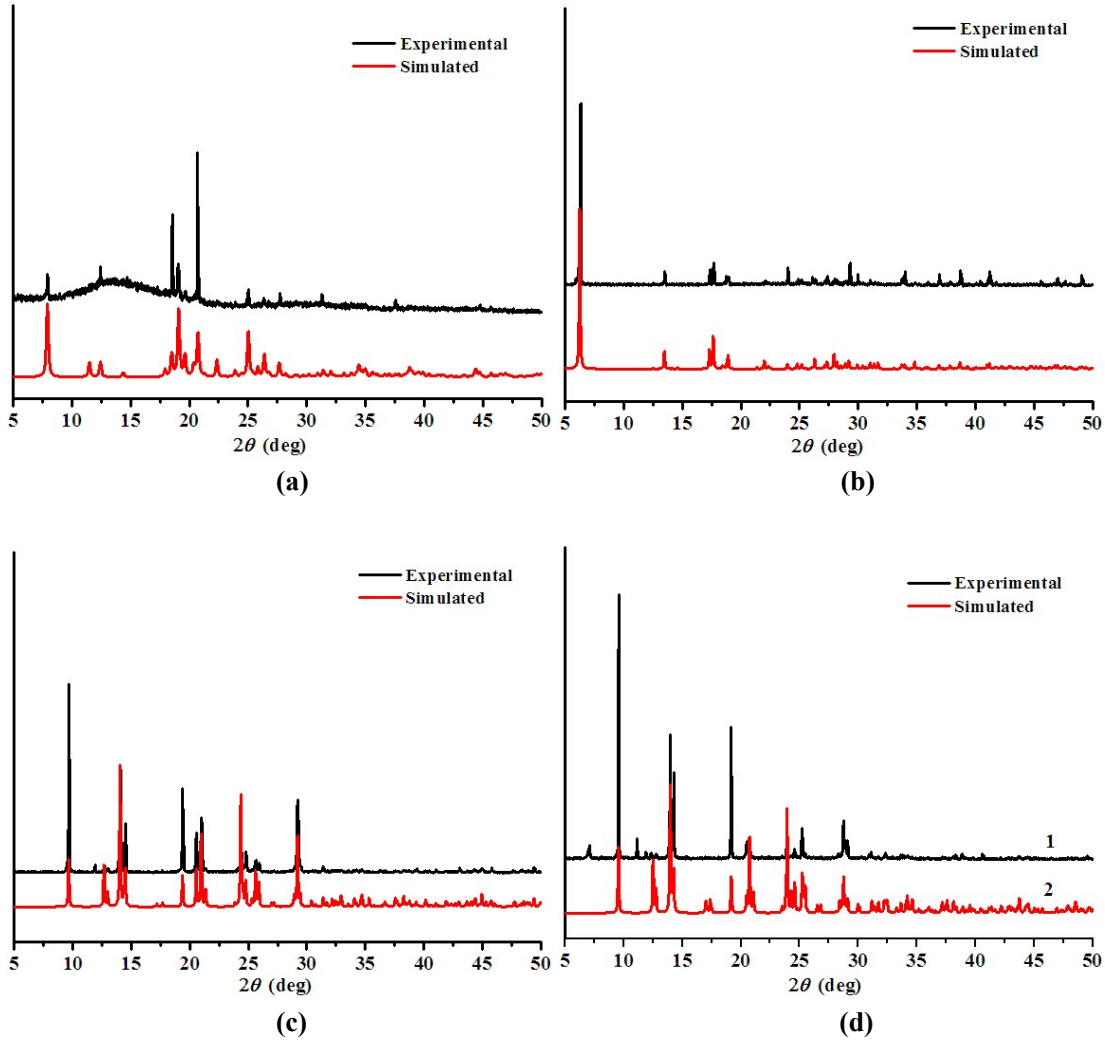


Fig. S10. PXRD patterns of the recycled compounds (a for **1**, b for **2**, c for **3**, and d for **4**).

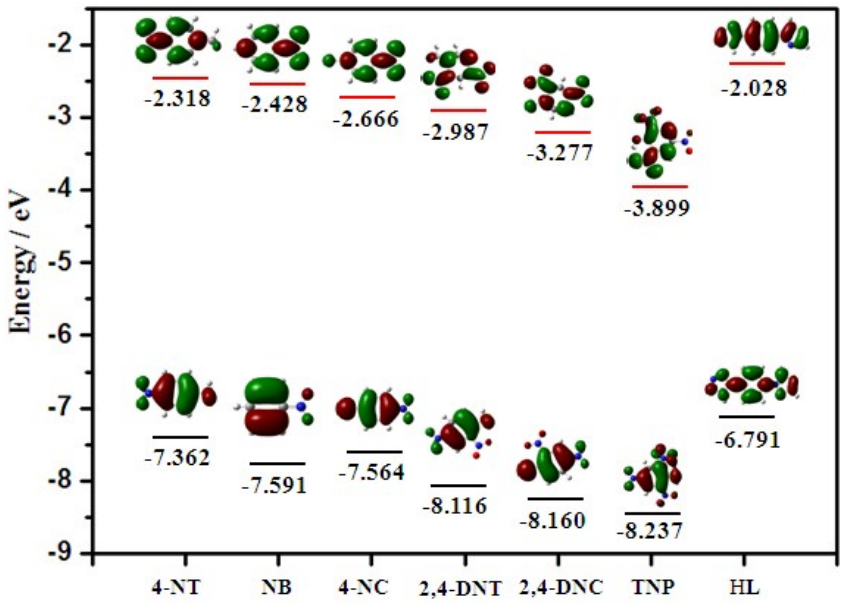
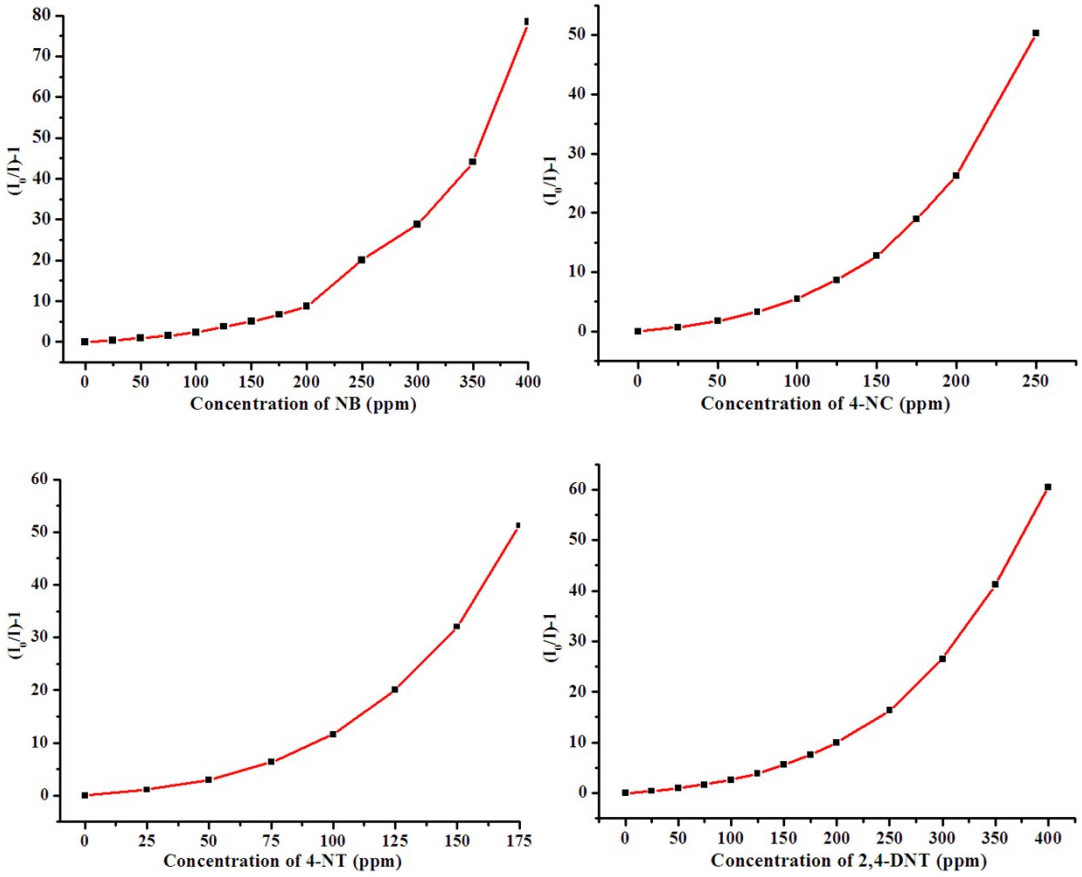


Fig. S11. HOMO and LUMO energy levels and shapes of the molecular orbitals considered for analytes and H**L** ligand. (investigated by the B3LYP/6-31G* method).



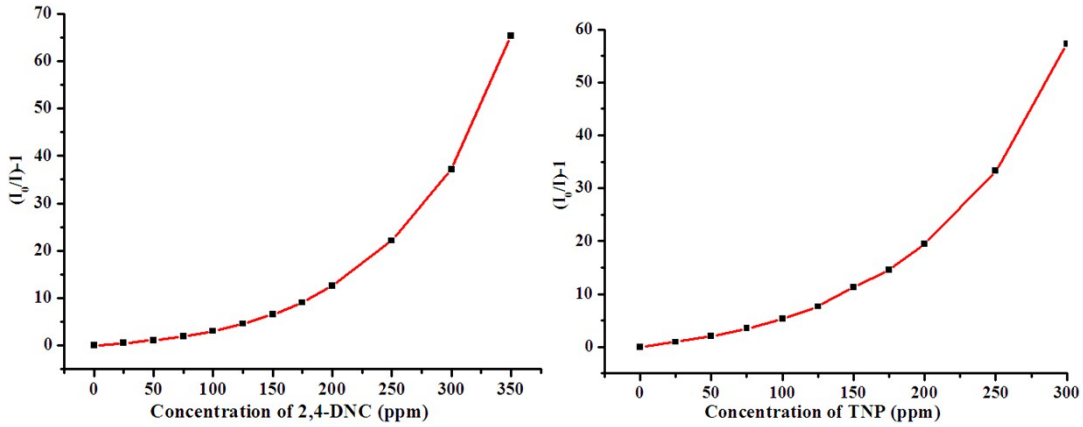
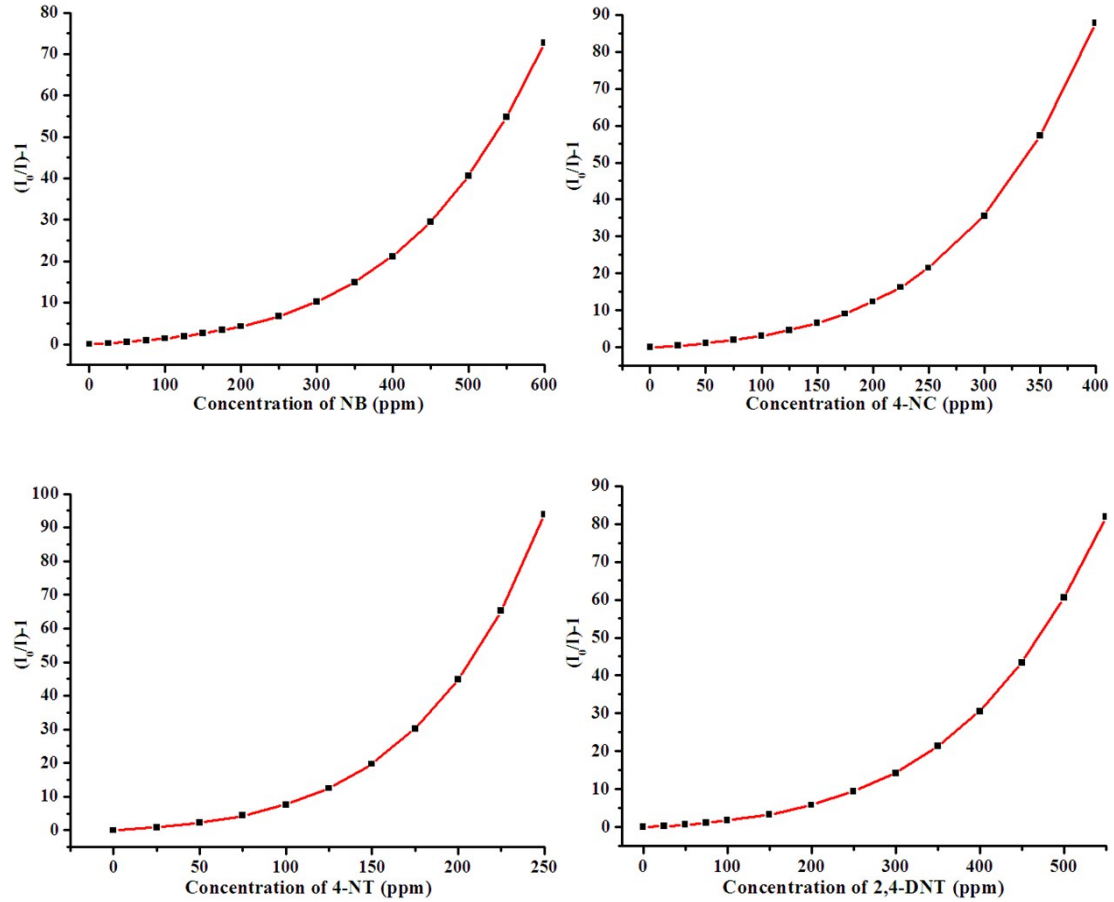


Fig. S12. Stern-Volmer plot of **1**



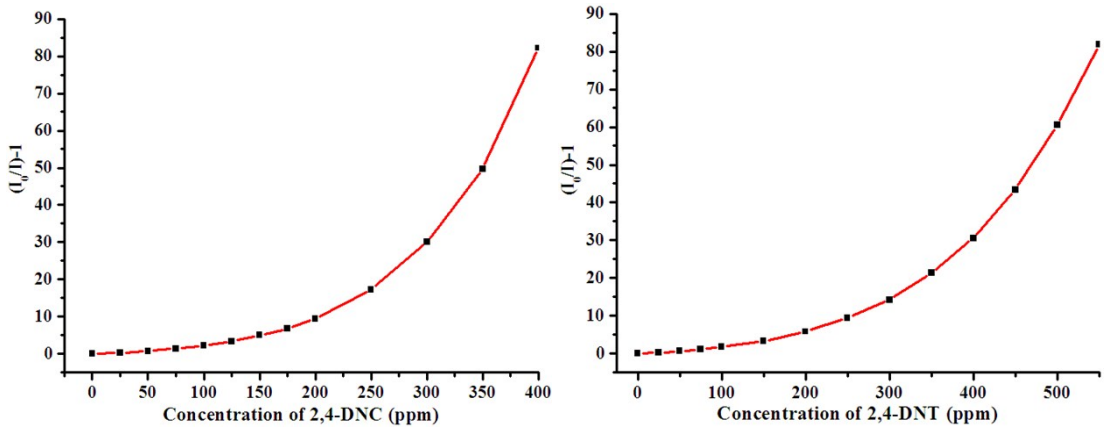
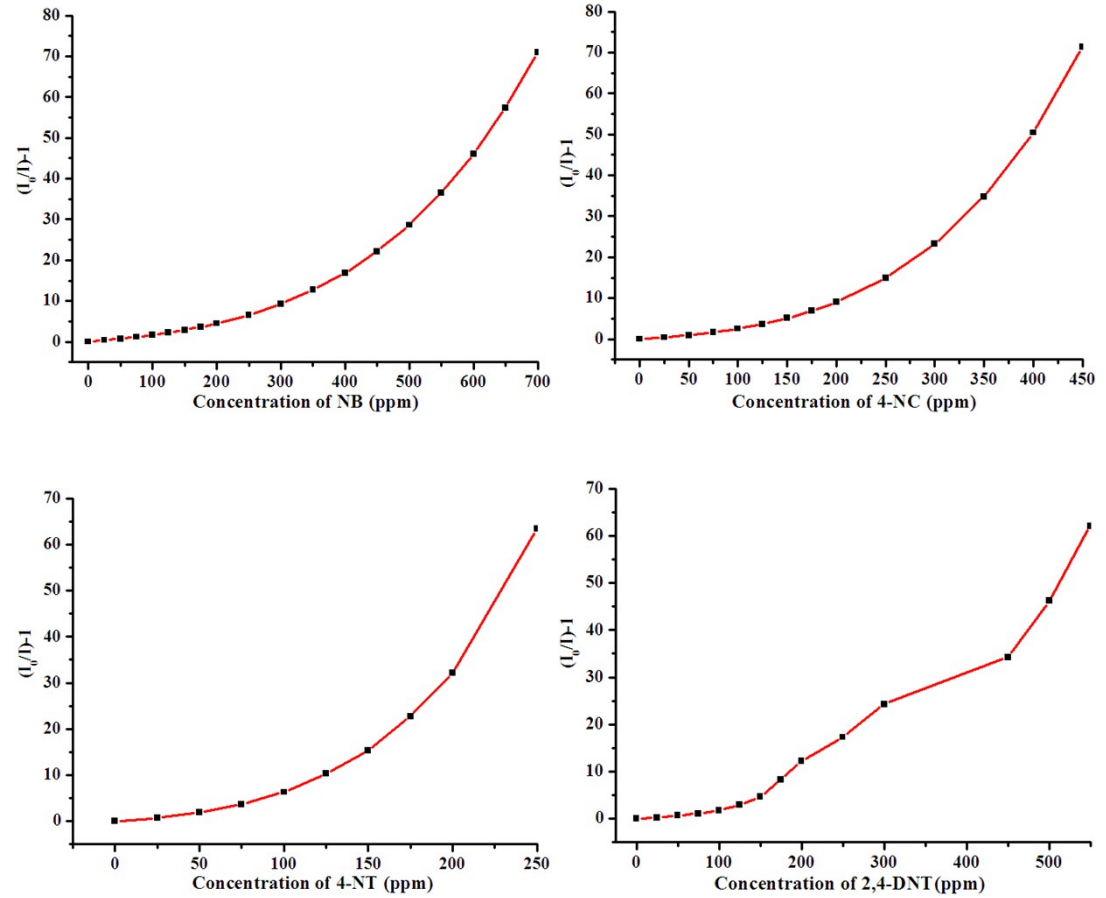


Fig. S13. Stern-Volmer plot of **2**



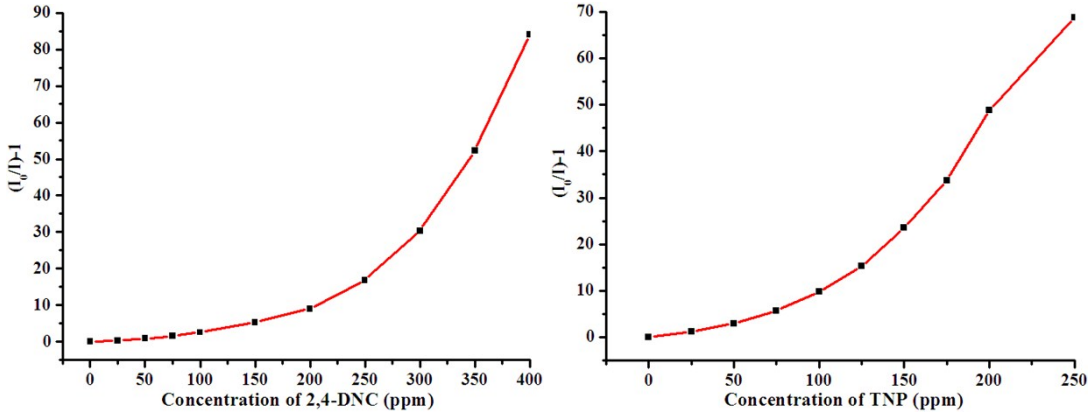


Fig. S14. Stern-Volmer plot of **3**

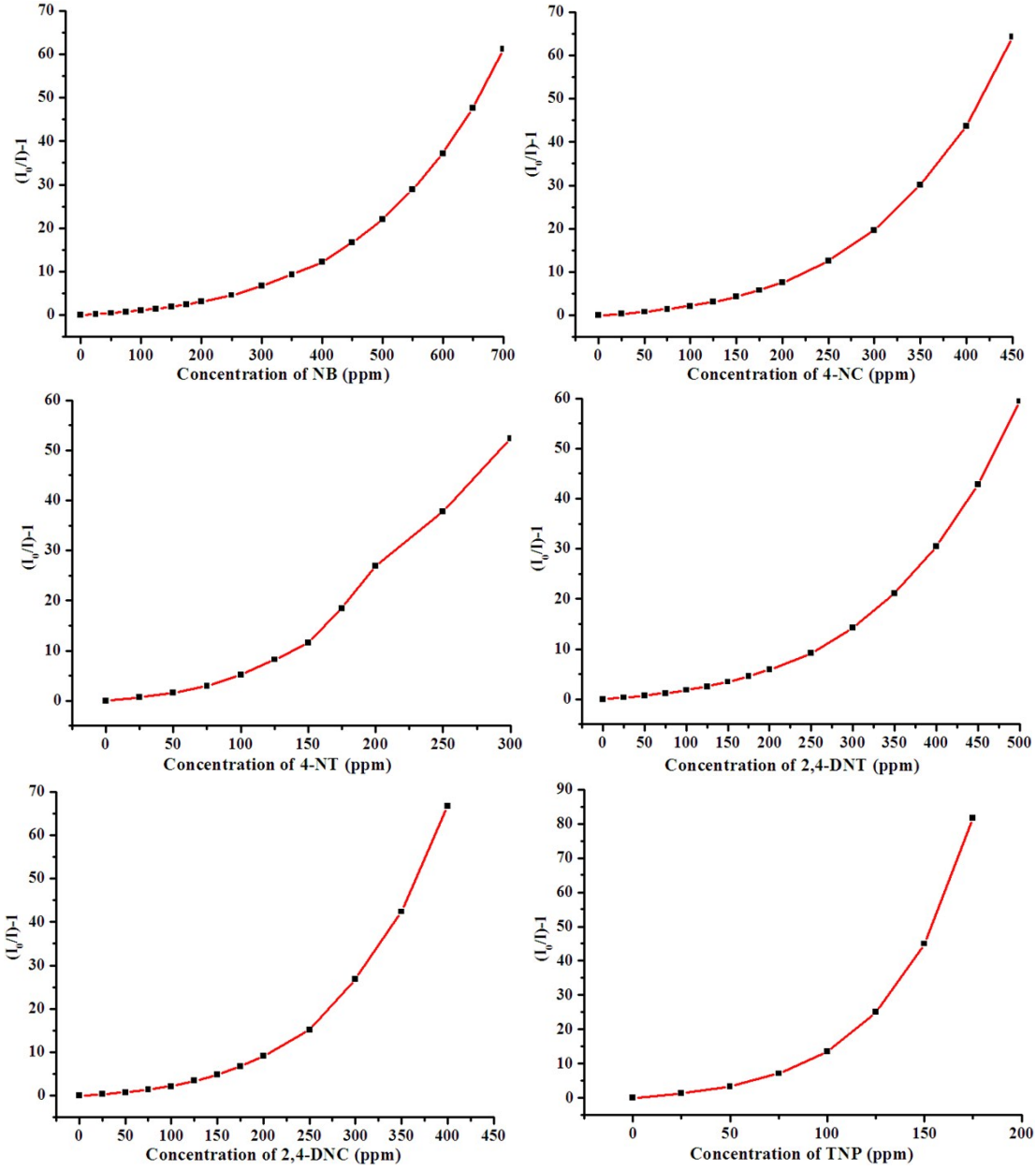


Fig. S15. Stern-Volmer plot of **4**

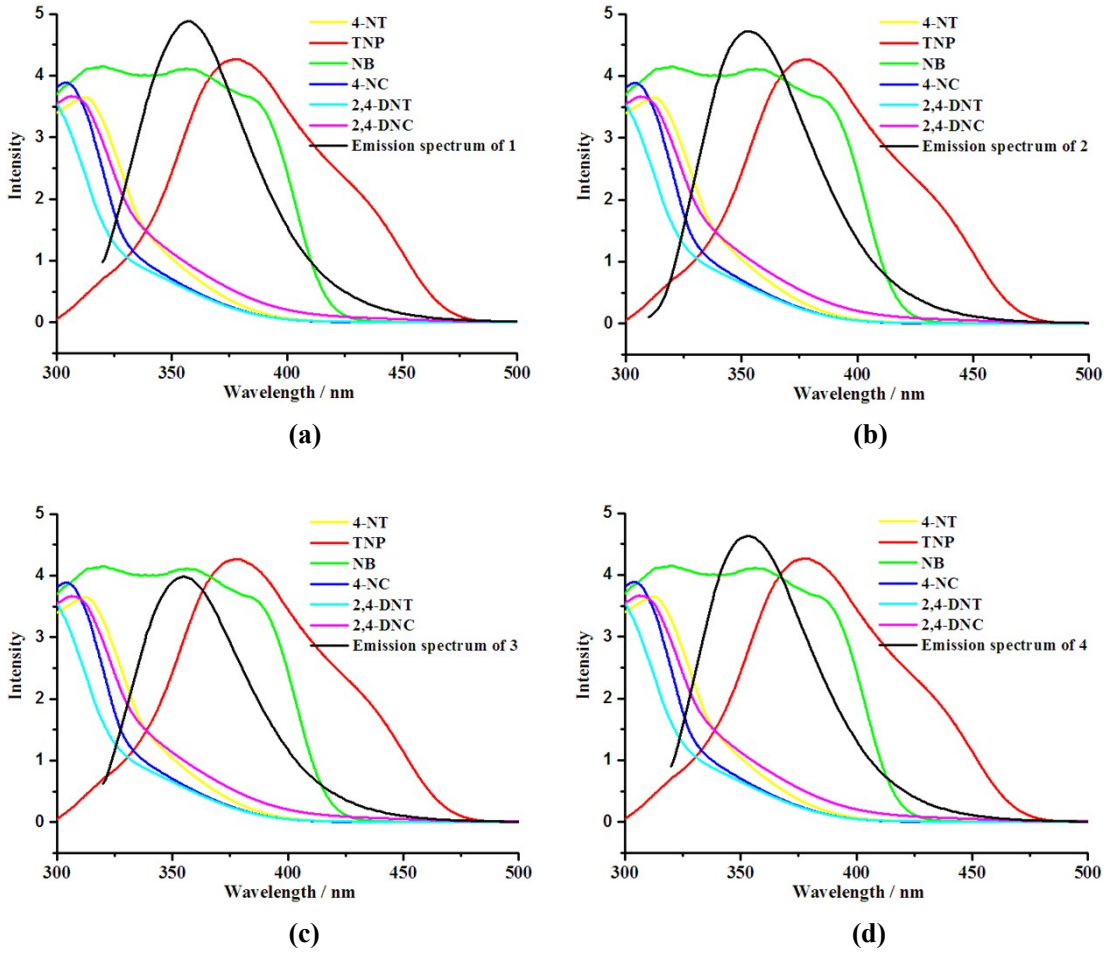


Fig. S16. Spectral overlap between the absorption spectra of analytes and the emission spectra of compounds **1**–**4** in DMF.

Table S1. Selected bond length (Å) and angles (˚) for complexes **1**–**4**.

		1	
Zn(1)-N(1)	2.000(2)	Zn(1)-N(4)#1	2.002(2)
Zn(1)-Cl(1)	2.2122(9)	Zn(1)-N(6)#2	2.030(2)
N(1)-Zn(1)-N(4)#1	112.56(10)	N(1)-Zn(1)-N(6)#2	111.64(10)
N(4)#1-Zn(1)-N(6)#2	102.40(10)	N(1)-Zn(1)-Cl(1)	104.76(7)
N(4)#1-Zn(1)-Cl(1)	117.21(7)	N(6)#2-Zn(1)-Cl(1)	108.36(8)
		2	
Cd(1)-N(7)#1	2.337(2)	Cd(1)-N(1)	2.3612(19)
Cd(1)-N(3)#2	2.480(2)	Cd(1)-Cl(3)#3	2.5632(8)
Cd(1)-Cl(1)	2.5884(8)	Cd(1)-Cl(2)	2.6270(9)
Cd(2)-N(4)#4	2.359(2)	Cd(2)-N(2)#5	2.396(2)
Cd(2)-Cl(1)	2.5303(9)	Cd(2)-Cl(3)	2.5792(9)
Cd(2)-Cl(2)	2.7953(8)	Cl(2)-Cd(2)#6	2.6468(9)
Cl(3)-Cd(1)#7	2.5631(8)		
N(7)#1-Cd(1)-N(1)	101.63(8)	N(7)#1-Cd(1)-N(3)#2	172.43(7)
N(1)-Cd(1)-N(3)#2	81.61(7)	N(7)#1-Cd(1)-Cl(3)#3	85.67(6)
N(1)-Cd(1)-Cl(3)#3	96.65(5)	N(3)#2-Cd(1)-Cl(3)#3	87.17(5)
N(7)#1-Cd(1)-Cl(1)	86.58(6)	N(7)#1-Cd(1)-Cl(2)	100.35(6)
N(1)-Cd(1)-Cl(2)	83.99(5)	N(4)#4-Cd(2)-N(2)#5	80.33(7)
Cl(1)-Cd(2)-Cl(2)#5	86.52(3)	Cl(3)-Cd(2)-Cl(2)	81.15(2)
		3	
Zn(1)-N(1)	2.1161(15)	Zn(1)-O(1)	2.1709(13)
Zn(1)-N(4)#2	2.2310(15)		
N(1)-Zn(1)-O(1)#1	95.13(6)	N(1)-Zn(1)-O(1)	84.87(6)
N(1)-Zn(1)-N(4)#2	90.58(6)	N(1)-Zn(1)-N(4)#3	89.42(6)
O(1)-Zn(1)-N(4)#2	94.29(5)	O(1)-Zn(1)-N(4)#3	85.71(5)
		4	
Cd(1)-N(1)	2.3023(13)	Cd(1)-O(1W)	2.3456(12)
Cd(1)-N(4)#2	2.3503(13)		
N(1)#1-Cd(1)-O(1W)	83.62(5)	N(1)-Cd(1)-O(1W)	96.38(5)
N(1)#1-Cd(1)-N(4)#2	90.29(5)	N(1)-Cd(1)-N(4)#2	89.71(5)
O(1W)-Cd(1)-N(4)#2	84.75(5)	O(1W)#1-Cd(1)-N(4)#2	95.25(5)

Symmetry code for **1**: #1 x+1, y, z, #2 x+1, -y+3/2, z-1/2, #3 x-1, y, z, #4 x-1, -y+3/2, z+1/2; **2**: #1 -x+1, y+1/2, -z+1, #2 -x+1, y+1/2, -z+2, #3 x+1, y, z, #4 x-1, y+1, z, #5 -x, y+1/2, -z+2, #6 -x, y-1/2, -z+2, #7 x-1, y, z, #8 -x+1, y-1/2, -z+2, #9 x+1, y-1, z, #10 -x+1, y-1/2, -z+1; **3** (**4**): #1 -x+1, -y+3, -z+3; #2 x+1, y+1, z+1; #3 -x, -y+2, -z+2; #4 x-1, y-1,z-1.

Table S2. Percentage of fluorescence quenching obtained for different analytes at room temperature.

Quenching Percentage for 1 (%)						
Aanlystes / Concentrations	NB	TNP	4-NC	4-NT	2,4-DNC	2,4-DNT
25 ppm	30	48	42	52	32	29
50 ppm	47	67	64	75	52	49
75 ppm	60	78	77	86	66	62
100 ppm	70	84	85	92	75	73
125 ppm	79	88	90	95	82	79
150 ppm	83	92	93	97	87	85
Quenching Percentage for 2 (%)						
25 ppm	19	53	32	46	24	22
50 ppm	35	75	53	69	44	40
75 ppm	48	86	66	81	58	53
100 ppm	58	93	76	89	69	63
125 ppm	66	97	82	93	77	76
150 ppm	72	99	87	95	83	85
Quenching Percentage for 3 (%)						
25 ppm	29	54	28	40	25	21
50 ppm	43	75	48	65	46	40
75 ppm	54	85	62	78	61	53
100 ppm	62	90	72	86	72	63
125 ppm	69	93	78	91	84	75
150 ppm	74	96	84	94	90	82
Quenching Percentage for 4 (%)						
25 ppm	18	57	26	40	25	24
50 ppm	31	77	45	60	44	41
75 ppm	43	87	59	75	59	54
100 ppm	52	93	68	84	68	64
125 ppm	59	96	76	89	77	72
150 ppm	66	98	81	92	83	78