Electronic Supplementary Material (ESI) for CrystEngComm.

Table S1: Crystallographic table for CP-**1a-1f**

Parameters	CP-**1a**	CP-**1b**	CP-**1c**	CP-**1d**	CP-**1e**	CP-**1f**
Emperical formula	$C_{46}H_{40}N_7O_7S_2Zn$	$C_{30}H_{17}N_4O_7SZn$	$C_{66}H_{64}CdN_{14}O_{14}S_4$	$C_{38}H_{38}CdN_6O_8S_2$	$C_{35}H_{32}CdN_5O_8S2$	$C_{36}H_{37}CdN_6NaO_{10}S$
Formula weight	932.34	642.90	1517.96	883.27	827.17	881.16
Crystal System	Monoclinic	Monoclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space Group	*P* 21/*c*	*P* 21/*m*	*P* -1	*P* -1	*P* -1	*P* -1
***a*/ Å**	18.304(3)	10.1841(19) Å	11.3999(3)	9.6261(10)	10.134(2)	10.304(3) Å
***b*/ Å**	12.325(2)	21.484(4)	11.8133(3)	9.6647(9)	11.560(2)	10.679(3)
***c*/ Å**	21.955(4)	10.4012(17)	13.5392(4)	10.2254(10)	17.570(4)	18.996(4)
***α*/ º**	90	90.00	102.517(1)	81.045(5)	99.98(3)	79.775(15)
***β*/ º**	107.923(7)	100.300(6)	99.513(1)	87.123(5)	104.00(3)	76.308(15)
***γ* / º**	90	90.00	106.844(1)	85.792(5)	108.19(3)	70.154(14)
***V* / Å³**	4712.5(14)	2239.1(7)	1652.09(8)	936.45(16)	1826.9(8)	1899.5(8)
Z	4	2	1	1	2	2
D_{calc} **/ g cm^{-3}**	1.314	0.954	1.526	1.573	1.504	1.541
***F*(000)**	1932	654	782.0	454.0	842	900
μ/mm^{-1}	0.666	0.630	0.535	0.756	0.769	0.706
Crystal size/mm³	0.31 x 0.23 x 0.16	0.27 x 0.17 x 0.12	0.32 x 0.21 x 0.18	0.28 x 0.16 x 0.10	0.21 x 0.16 x 0.11	0.21 x 0.17 x 0.12
θ range/ º	1.918-26.141	1.896 - 28.352	28.384	2.018- 28.325	2.230 - 29.141	2.141-25.252
Reflections collected	57146	33961	8153	4603	12661	19673
Independent reflections	9286	5661	5948	3577	7284	6566

Ranges (h,k,l)	-22<=h<=22 -12<=k<=15 -27<=l<=26	-13<=h<=13 -28<=k<=28 -12<=l<=13	-15<=h<=14 -15<=k<=14 -18<=l<=14	-12<=h<=8 -12<=k<=12 -12<=l<=13	-8<=h<=13 -15<=k<=12 -23<=l<=21	-12<=h<=6 -12<=k<=10 -22<=l<=21
Complete to 2θ	99.8	98.6	98.3	98.5	78.7	95.2
Data / restraints / parameters	9286 / 513 / 570	5661 / 575 / 298	5948/0/ 450	3577/0/252	7284 / 12 / 478	6566 / 47 / 522
GOF(F^2)	1.017	1.061	0.983	0.985	0.929	0.985
***R*1; w*R*2 [$I > 2\sigma(I)$]**	0.0439, 0.1012	0.0686; 0.1743	0.0501; 0.1726	0.0455; 0.1561	0.0576; 0.1431	0.0548; 0.0943
***R*1; w*R*2 (all data)**	0.0797, 0.1194	0.1188; 0.1950	0.0778; 0.1726	0.0713; 0.1561	0.0985; 0.1635	0.1054; 0.1127

Table S2. Hydrogen bonds for CP-**1a** [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(11)-H(11A)...O(5)#4	0.95	2.29	3.200(4)	160.5
C(14)-H(14A)...O(6)	0.99	2.42	3.328(4)	152.3
C(29)-H(29A)...O(6)#5	0.99	2.65	3.593(4)	159.8
C(29)-H(29B)...O(4)#6	0.99	2.47	3.317(3)	143.8
C(31)-H(31A)...O(4)#6	0.95	2.39	3.165(4)	138.5
C(33)-H(33A)...O(11S)#2	0.95	2.10	3.007(4)	160.3
C(32)-H(32A)...O(11S)#7	0.95	2.37	3.199(4)	146.1
C(36)-H(36A)...O(3)#8	0.99	2.43	3.312(4)	147.9
C(12S)-H(12D)...O(3)	0.98	2.66	3.255(5)	119.7

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+3/2,z-1/2 #2 x,-y+3/2,z+1/2 #3 -x+1,-y+2,-z+1
#4 -x,y+1/2,-z+1/2 #5 -x,-y+1,-z+1 #6 x,-y+1/2,z+1/2
#7 x,y,z+1 #8 -x+1,y+1/2,-z+1/2

Table S3. Hydrogen bonds for CP-**1f** [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(1W1)...S(1)#3	0.822(19)	2.91(3)	3.690(4)	159(4)
O(1W)-H(1W1)...O(7)#3	0.822(19)	1.940(19)	2.759(5)	174(5)
O(1W)-H(1W2)...O(2)	0.816(19)	1.92(2)	2.715(5)	165(6)
C(9A)-H(9AA)...O(4)#1	0.95	2.54	3.16(2)	122.5
C(9B)-H(9BA)...O(4)#1	0.95	2.59	3.17(3)	120.0
C(10B)-H(10B)...O(2)#7	0.95	2.66	3.45(2)	140.9
C(21)-H(21A)...O(6)#8	0.95	2.29	3.220(7)	165.8
C(23)-H(23B)...O(6)#3	0.99	2.47	3.370(6)	150.3
C(13S)-H(13A)...O(3)#2	0.98	2.40	3.172(9)	134.8
C(13S)-H(13C)...O(7)#4	0.98	2.49	3.463(8)	171.1

Symmetry transformations used to generate equivalent atoms:
#1 x,y+1,z #2 x-1,y,z #3 x+1,y,z #4 x,y-1,z

#5 -x,-y+2,-z+1 #6 -x+2,-y+2,-z #7 -x+1,-y+1,-z+1
#8 -x+1,-y+1,-z

Table. S4. Photophysical properties for CP-**1a-1c** and CP-**1f** in DMF

Compound	**Stokes Shift** $\Delta\nu(cm^{-1})$	λ_{max} **Em**	λ_{max} **Ex**	Φ_f	$\langle\tau\rangle$ **(ns)**	χ
Anthracene	8300	409	302	0.27	-	-
BIA	9000	429	306	0.46	-	-
CP-1a	11290	429	295	0.77	1.63	1
CP-1b	10880	428	295	0.51	0.96	1.1
CP-1c	10300	426	295	0.24	0.80	1
CP-1f	14478	426	315	0.37	0.84	1

Table S5. Frontier molecular orbital composition (%) in the ground state for BIA

MO	**Energy**	**Contribution**	
		Anthracene	**CH_2Imidazole**
L+5	0.6	2	98
L+4	0.59	4	95
L+3	0.4	85	15
L+2	-0.33	98	2
L+1	-0.83	99	1
LUMO	-2.38	95	5
HOMO	-5.82	93	7
H-1	-6.26	3	99
H-2	-6.29	3	97
H-3	-6.79	1	99
H-4	-6.83	3	97
H-5	-7.06	88	12

Table S6. Frontier molecular orbital composition (%) in the ground state for SIA

MO	Energy	Contribution		
		Benzene ring	COOH	SO_3H
L+5	-15.52	26	28	46
L+4	-16.48	8	14	77
L+3	-16.74	48	27	25
L+2	-17.01	61	38	1
L+1	-17.81	0	99	0
LUMO	-17.83	0	99	0
HOMO	-21.94	34	2	64
H-1	-22.43	85	14	1
H-2	-22.65	52	11	37
H-3	-22.77	2	97	1
H-4	-22.8	4	94	2
H-5	-23.32	15	1	84

Table S7. Frontier molecular orbital composition (%) in the ground state for PA

MO	Energy	Contribution	
		Phenol	NO_2
L+5	-1.11	68	32
L+4	-1.26	25	75
L+3	-3.11	20	80
L+2	-3.53	5	95
L+1	-3.76	33	67
LUMO	-3.92	40	60
HOMO	-8.47	81	19
H-1	-8.61	14	86
H-2	-8.86	3	97
H-3	-8.99	8	92
H-4	-9.04	21	79

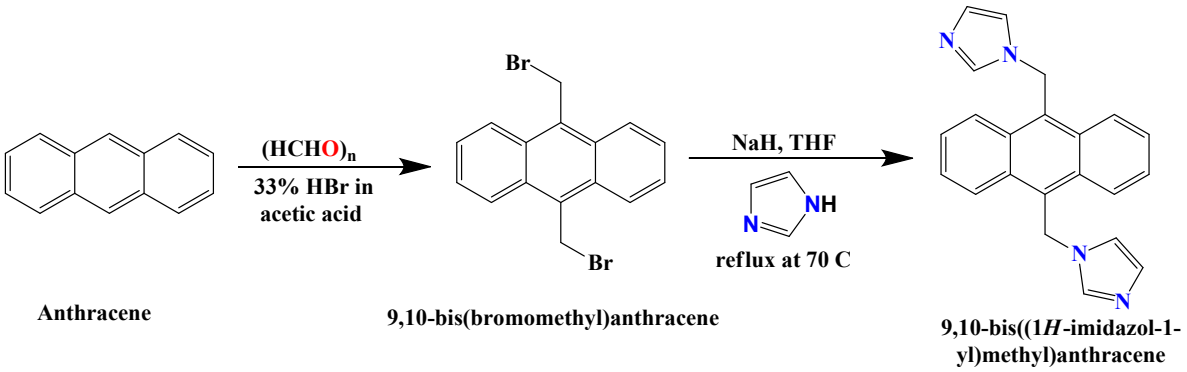
Table S8. Summary of Detection Limit for CPs with Various Nitroaromatics

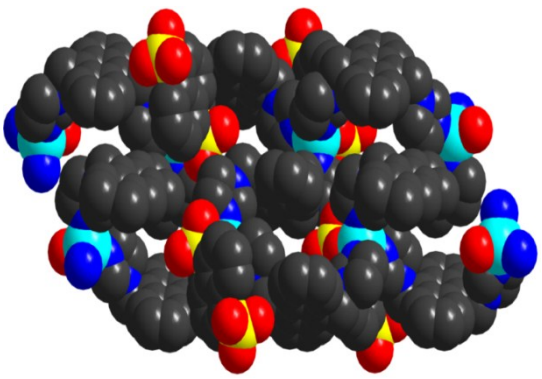
Compounds	Detection limit (μM)		
	Picric acid (PA)	3,5-Dinitrotoluene (DNT)	Nitroaniline (NA)
CP-1a	72.8	64	-
CP-1b	73.6	60	67.6
CP-1c	59.2	55.8	-

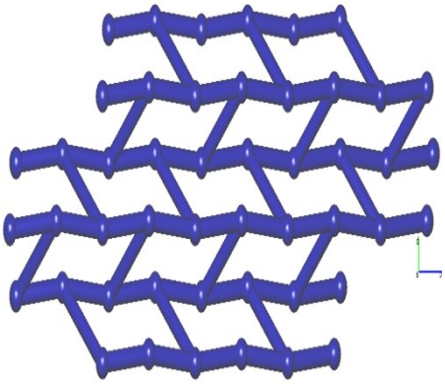
Section S1. Synthetic procedure of ligand

Synthesis of 9, 10-bis ((1H-imidazol-1-yl) methyl)anthracene (BIA)

Anthracene based flexible ligand; 9, 10-bis ((1H-imidazol-1-yl) methyl)anthracene (**BIA**) is synthesized by slow addition of NaH in the solution of imidazole (THF solvent) at 0 ˚C, stirr the mixture for 2 hrs, then 9,10-bis(bromomethyl)anthracene (2g) was added[5]. The mixture was reflux for 12 hrs at 70 ˚C, and then poured into 100 mL water. Filtered yellow precipitate, washed several times. Dried the precipitate for 24 hrs under vacuum.







a **b**

Fig. S1. (a) Space-filling model view along a-axis of 1D channel in CP-**1a**. (b) Topological representation of CP-**1a**

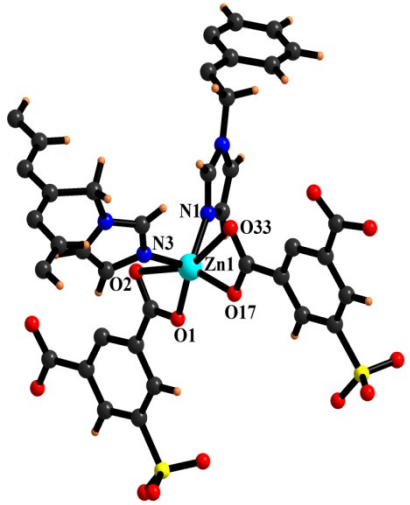


Fig. S2. Crystal structure of CP-**1b**

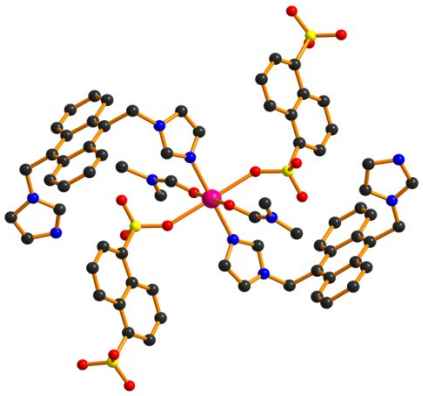


Fig. S3. Crystal structure of CP-**1c**

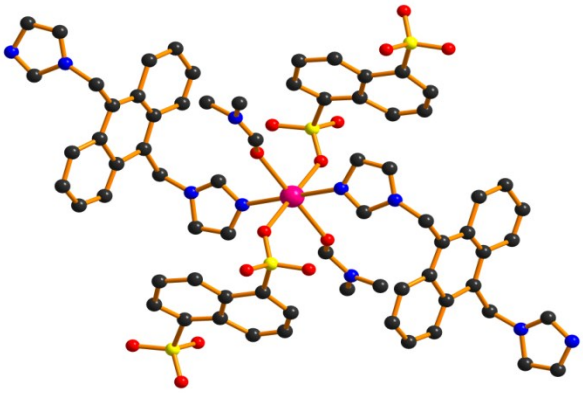


Fig. S4. Crystal structure of CP-**1d**

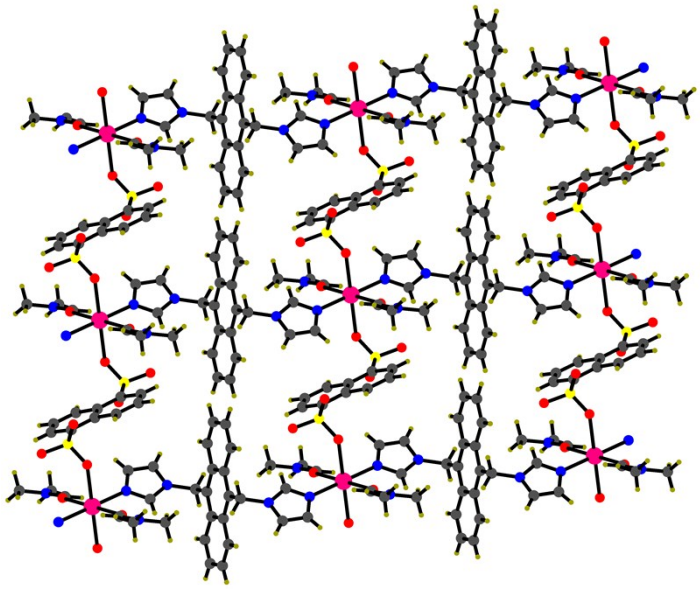


Fig. S5: 2D corrugated sheet of CP-**1d**

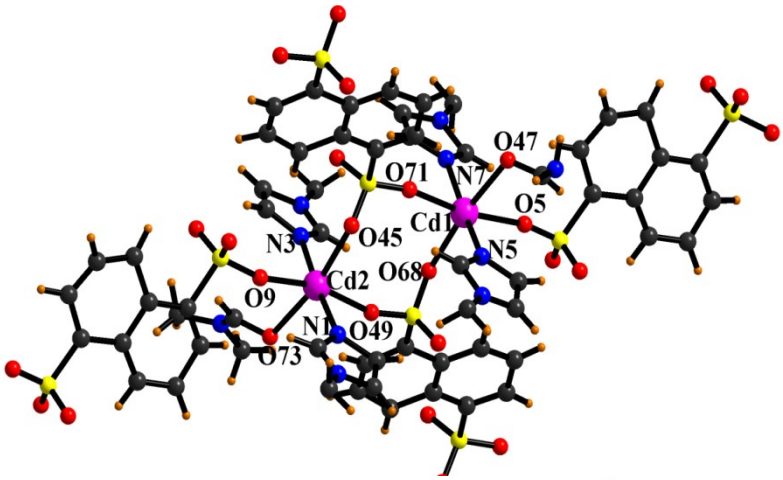


Fig. S6. Crystal structure of CP-**1e**

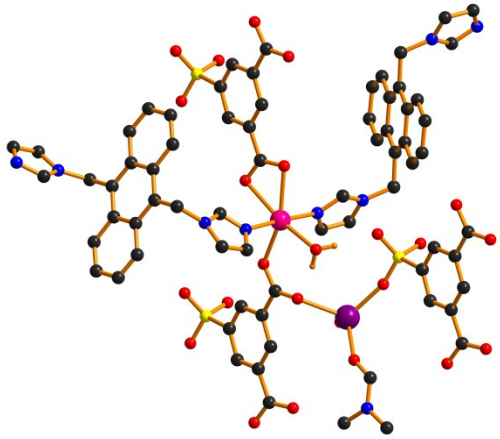


Fig. S7. Crystal structure of CP-**1f**

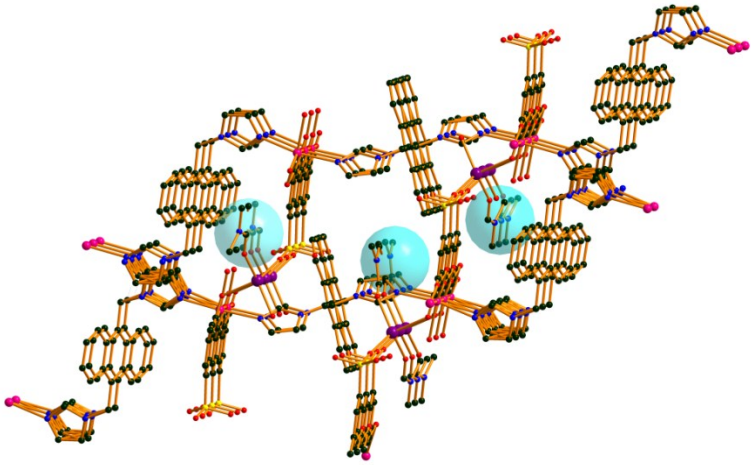
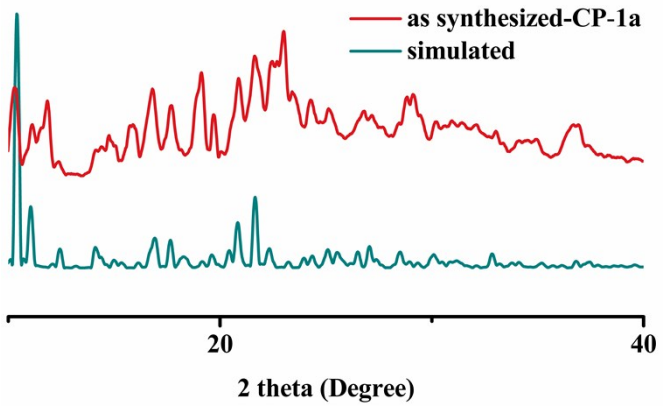
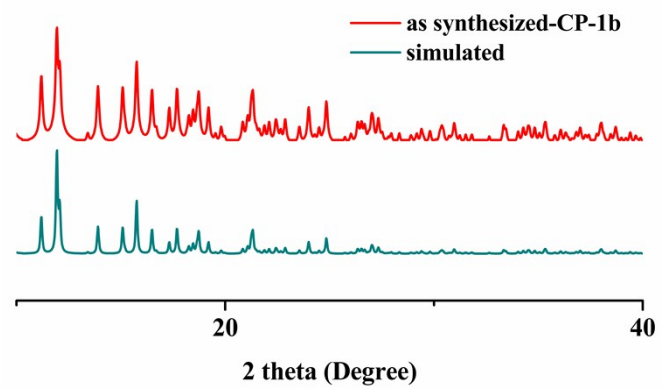
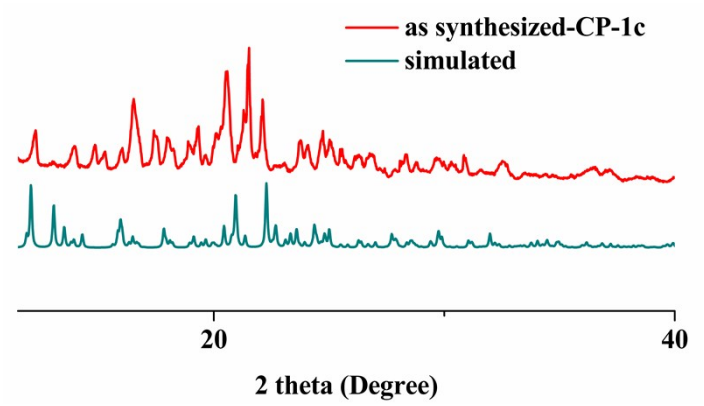


Fig. S8. 3D coordination network of CP-**1f**







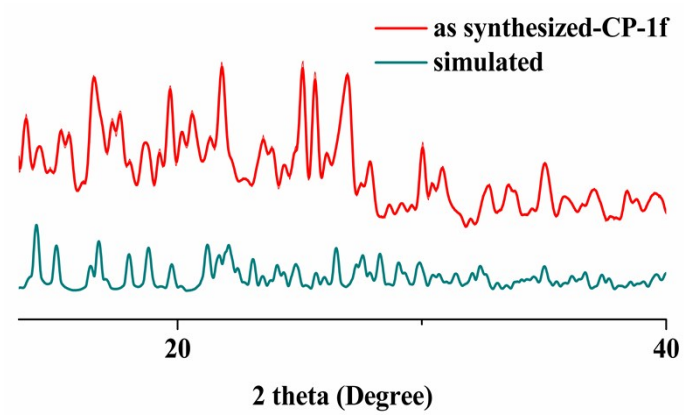


Fig. S9: Comparison of as-synthesized PXRD pattern of CP-**1a-1c** and CP-**1f** with simulated one

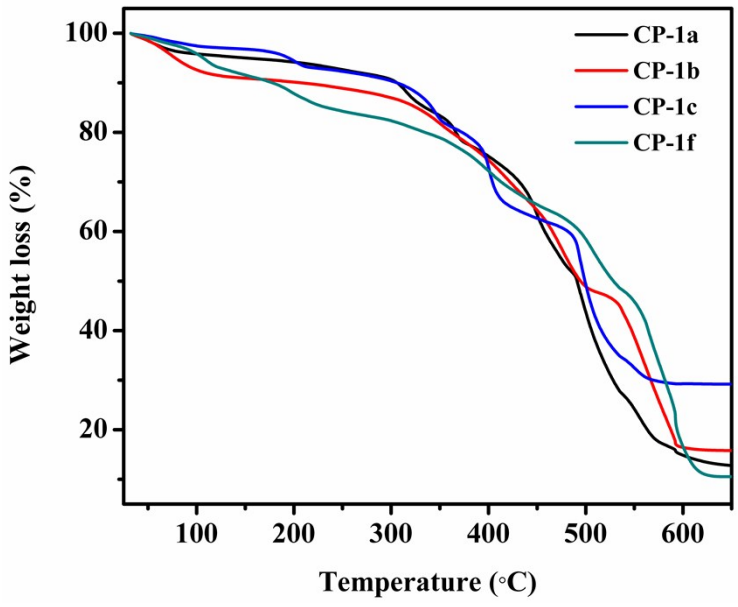


Fig. S10. Thermogravimetric analysis curve for CP-**1a-1c** and CP-**1f**

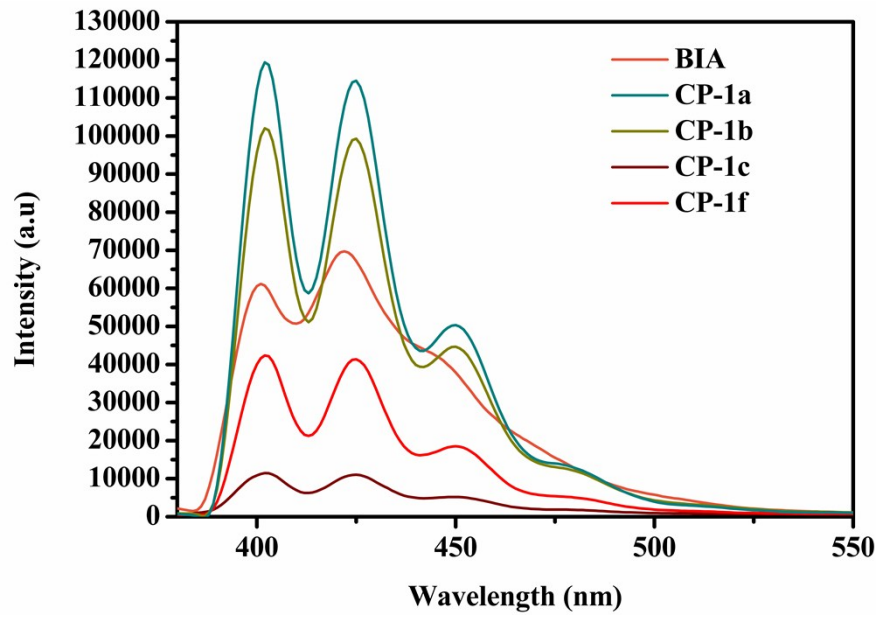


Fig. S11. Solid state emission spectra for CP-**1a-1c** and CP-**1f**

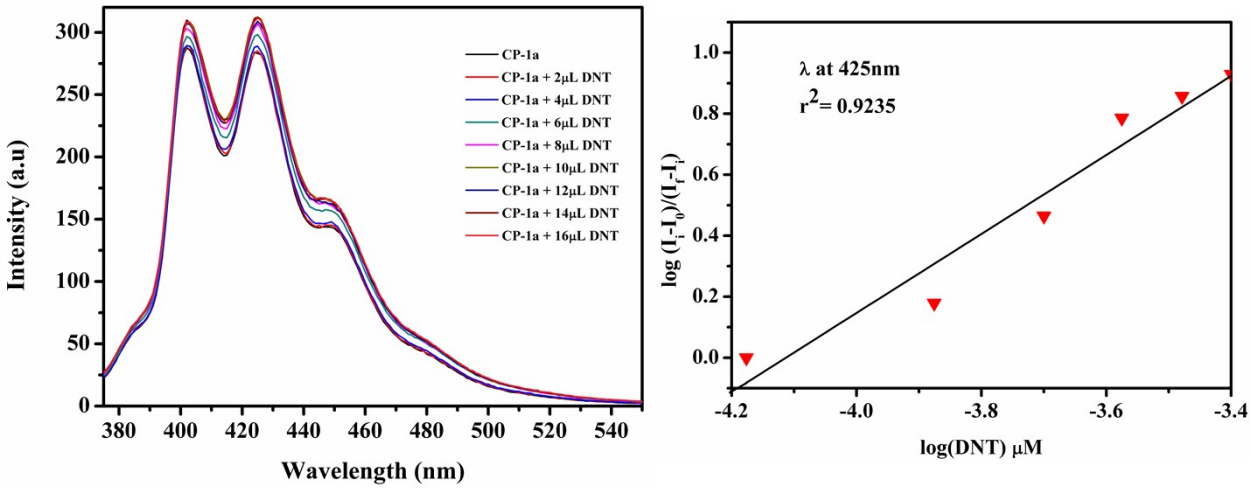


Fig. S12. Fluorescence titration of the dispersed CP-**1a** in DMF by gradual addition of 1mM solution of Dinitrotoluene (DNT) in DMF and their Hill plot

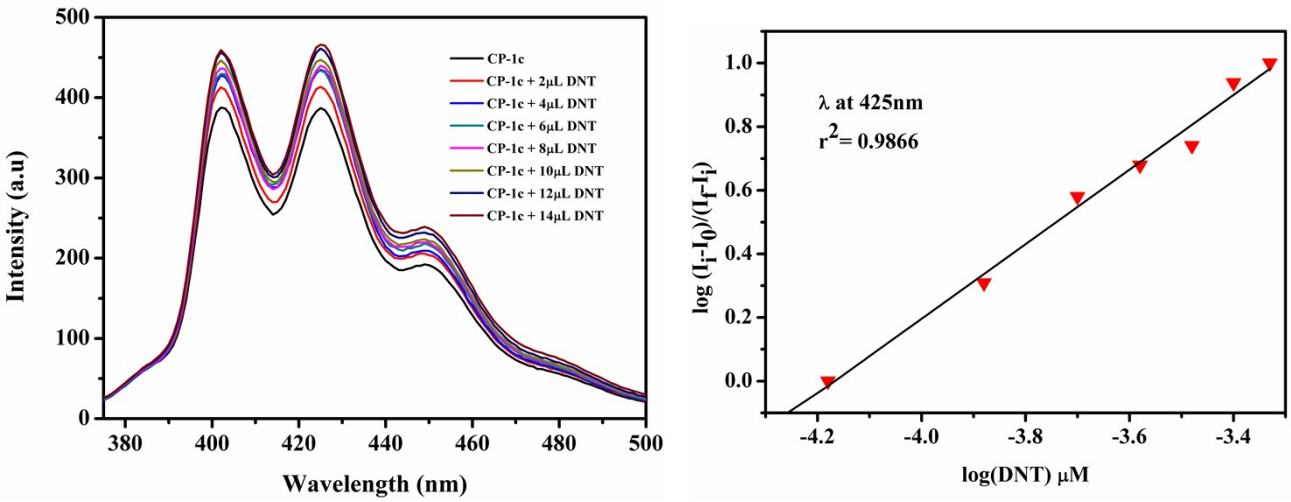


Fig. S13. Fluorescence titration of the dispersed CP-**1c** in DMF by gradual addition of 1mM solution of Dinitrotoluene (DNT) in DMF and their Hill plot

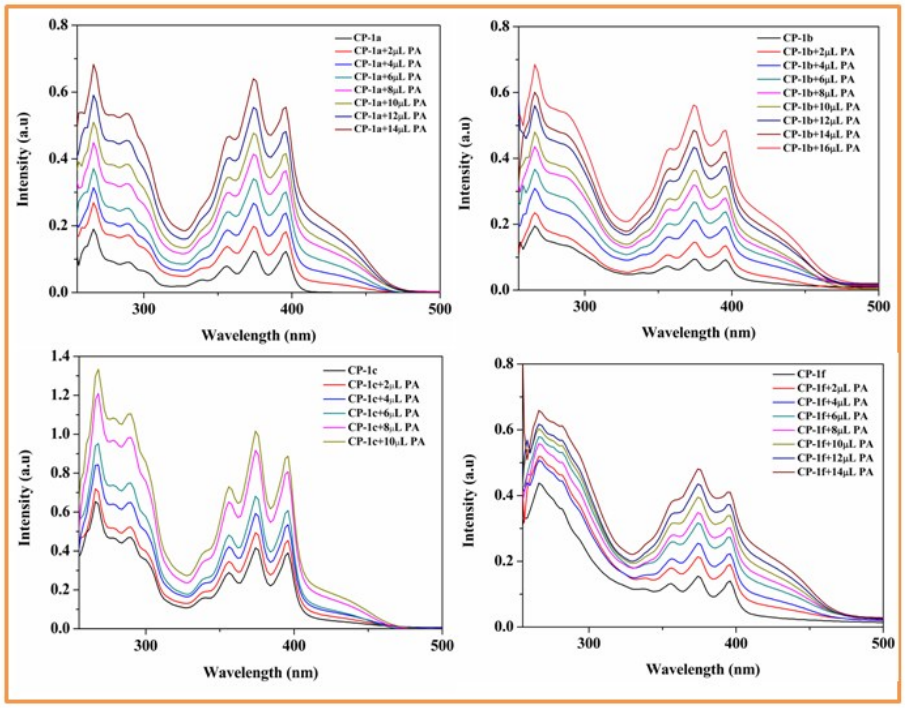


Fig. S14. UV-Vis titration of the dispersed CP-**1a** to **1c** and CP-**1f** in DMF by gradual addition of 1mM solution of Picric acid (PA) in DMF

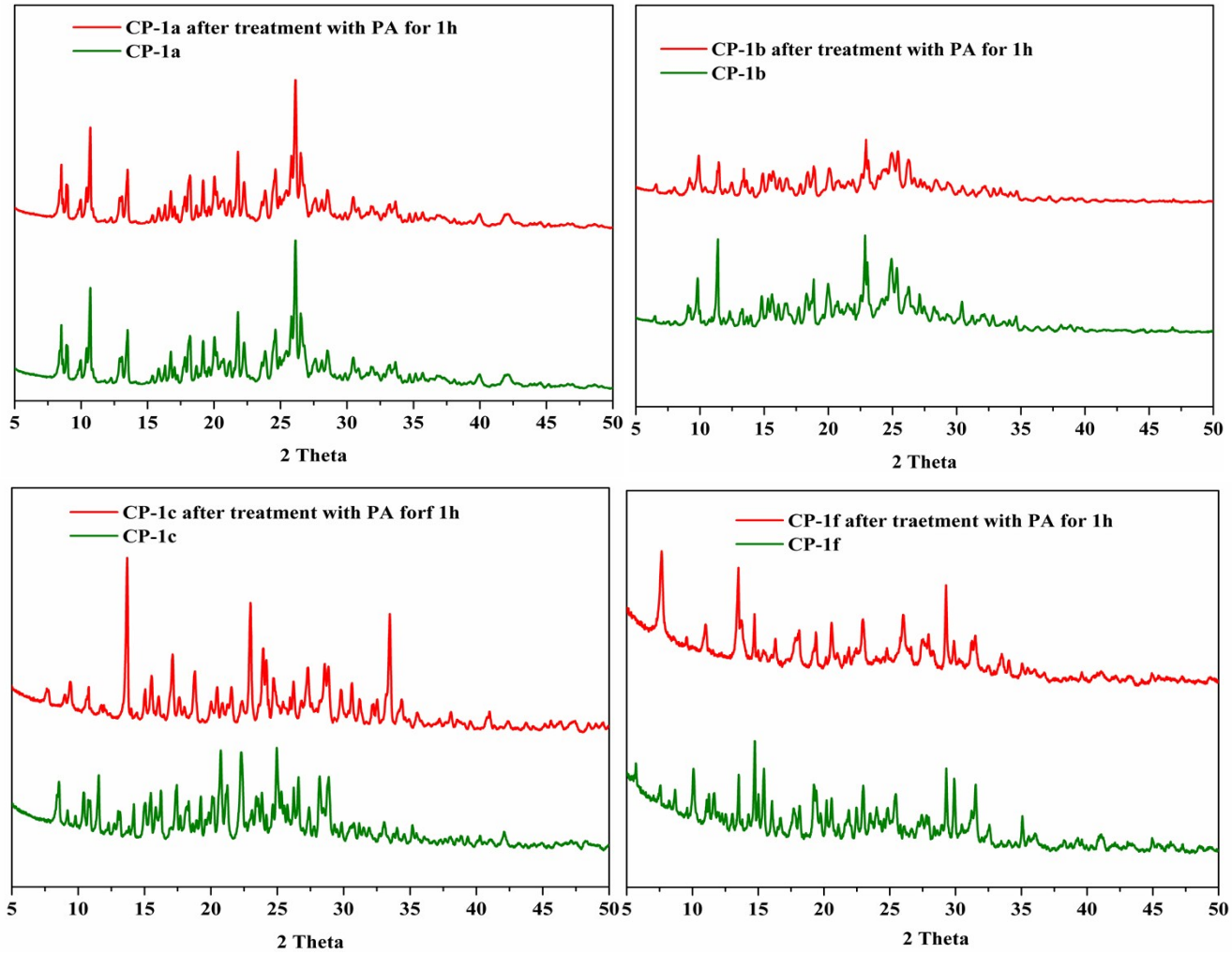


Fig. S15: Powder XRD patterns of CP-**1a-1c** and CP-**1f** (a) green color plot for fresh sample and (b) red color plot for after immersion in picric acid (PA) for 1 h

References

1. Sanjua, K. S.; Ramaiah, D. *Chem. Commun*. **2013**, 49, 11626.