Electronic supplementary information (ESI)

Cadmium(II) coordination polymers based on 2-(4-((E)-2-(pyridine-2-yl)vinyl)styryl)pyridine and dicarboxylate ligands as fluorescent sensor for TNP

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Table S1 Crystal data and structure refinements for **1**- **3**.

	1	**2**	**3**
Formula	$C_{28}H_{20}N_2O_4Cd$	$C_{28}H_{20}N_2O_4Cd$	$C_{29}H_{24}N_2O_5Cd$
Formula weight	560.86	560.86	592.90
T (K)	153(2)	153(2)	153(2)
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*C2/c*	*C2*	$P2_1/c$
a (Å)	17.9642(12)	21.789(3)	10.1343(5)
b (Å)	6.5854(4)	10.1900(11)	11.5821
c (Å)	20.6384(18)	10.2278(12)	20.8179
β (º)	114.147(2)	97.291(2)	93.369(2)
V (Å^3)	2227.9(3)	2252.5(4)	2439.3(2)
Z	4	4	4
D_{calc} (g cm^{-3})	1.672	1.654	1.614

$F(000)$	1128	1128	1200
θ for data collection (°)	2.541-24.996	1.88-25.01	2.673-25.008
Reflections collected	7492	2094	10594
Unique reflections	1967	2094	4289
Goodness-of-fit on F^2	1.097	1.076	0.989
R_1,	0.0227	0.0261	0.0295
wR_2 [I > 2$\sigma(I)$][a,b]	0.0646	0.0609	0.0683
R_1,	0.0251	0.0308	0.0361
wR_2 [all data]	0.0662	0.0638	0.0713

[a]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b]$wR_2 = |\Sigma w(|F_o|^2 - |F_c|^2)|/\Sigma|w(F_o)^2|^{1/2}$, where w = m= $1/[\sigma^2(F_o^2) + (aP)^2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$

Table S2 Selected bond lengths (Å) and angles (°) forassembly**1 - 3**

		1	
Cd(1)-N(1)	2.284(2)	Cd(1)-O(1)	2.295(2)
Cd(1)-O(2)	2.474(2)		
N(1)-Cd(1)-N(1)#1	120.64(10)	N(1)-Cd(1)-O(1)	118.82(6)
N(1)#1-Cd(1)-O(1)	102.67(7)	O(1)-Cd(1)-O(1)#1	89.79(8)
N(1)-Cd(1)-O(2)#1	83.03(6)	N(1)#1-Cd(1)-O(2)#1	87.78(6)
O(1)-Cd(1)-O(2)#1	143.25(6)	O(1)#1-Cd(1)-O(2)#1	55.09(6)
O(2)#1-Cd(1)-O(2)	161.39(8)		
		2	
Cd(1)-O(4)#1	2.295(4)	Cd(1)-O(3)#2	2.356(3)
Cd(1)-N(2)	2.360(5)	Cd(1)-O(1)	2.373(4)
Cd(1)-O(2)	2.453(3)	Cd(1)-N(1)#3	2.463(5)
O(4)#1-Cd(1)-O(3)#2	96.04(19)	O(4)#1-Cd(1)-N(2)	139.81(16)
O(3)#2-Cd(1)-N(2)	81.0(2)	O(4)#1-Cd(1)-O(1)	82.86(15)
O(3)#2-Cd(1)-O(1)	93.08(18)	N(2)-Cd(1)-O(1)	137.18(15)
O(4)#1-Cd(1)-O(2)	136.5(2)	O(3)#2-Cd(1)-O(2)	85.67(11)
N(2)-Cd(1)-O(2)	83.5(2)	O(1)-Cd(1)-O(2)	53.7(2)
O(4)#1-Cd(1)-N(1)#3	85.15(16)	O(3)#2-Cd(1)-N(1)#3	163.90(17)
N(2)-Cd(1)-N(1)#3	87.70(16)	O(1)-Cd(1)-N(1)#3	102.98(16)

O(2)-Cd(1)-N(1)#3	104.54(15)		
3			
Cd(1)-O(1)	2.267(2)	Cd(1)-O(3)#1	2.347(2)
Cd(1)-O(1W)	2.349(2)	Cd(1)-N(1)	2.379(3)
Cd(1)-N(2)#1	2.408(3)	Cd(1)-O(4)#1	2.484(2)
O(1)-Cd(1)-O(3)#1	133.12(7)	O(1)-Cd(1)-O(1W)	85.68(7)
O(3)#1-Cd(1)-O(1W)	94.56(7)	O(1)-Cd(1)-N(1)	143.96(8)
O(3)#1-Cd(1)-N(1)	82.49(8)	O(1W)-Cd(1)-N(1)	86.01(8)
O(1)-Cd(1)-N(2)#1	89.26(8)	O(3)#1-Cd(1)-N(2)#1	101.17(8)
O(1W)-Cd(1)-N(2)#1	162.39(8)	N(1)-Cd(1)-N(2)#1	88.23(9)
O(1)-Cd(1)-O(4)#1	79.59(7)	O(3)#1-Cd(1)-O(4)#1	53.78(7)
O(1W)-Cd(1)-O(4)#1	85.85(7)	N(1)-Cd(1)-O(4)#1	134.56(8)
N(2)#1-Cd(1)-O(4)#1	109.82(8)		

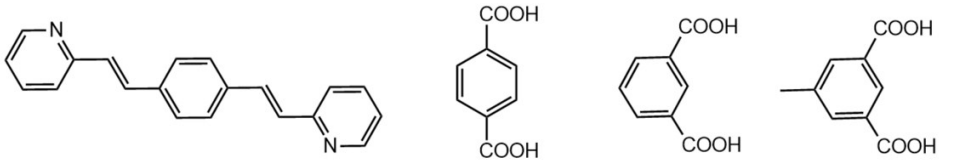
Symmetry transformations used to generate equivalent atoms: #1 -x+1, y, -z+1/2; for **1**; #1 x,y,z-1; #2 -x+1,y,-z+2; #3 x,y,z+1 for **2**; #1 x-1,y,z for **3**.

Table S3 Hydrogen bonding data of **2**and**3**.

2				
D–H···A	d(*D*–H) (Å)	d(H···A) (Å)	d(*D*···A)(Å)	*D*–H···A (°)
C(2)-H(2)···O(4)	0.9500	2.4500	3.143(8)	129
C(4)-H(4)···O(1)	0.9500	2.3500	3.267(8)	162
C(6)-H(6)···O(2)	0.9500	2.4300	3.362(8)	169
C(9)-H(9)···O(2)	0.9500	2.3500	3.295(8)	171
C(15)-H(15)···O(3)	0.9500	2.5000	3.436(9)	167
C(18)-H(18)···O(1)	0.9500	2.628	3.474(9)	148
C(20)-H(20)···O(2)	0.9500	2.3700	3.010(9)	124
3				
O(1W)-H(1WB)···O(1)	0.8400	1.9500	2.754(3)	162
O(1W)-H(1WA)···O(4)	0.8800	1.9700	2.770(3)	151
C(1)-H(1)···O(1)	0.9500	2.5000	3.208(4)	131
C(3)-H(3)···O(4)	0.9500	2.3900	3.298(4)	160
C(6)-H(6)···O(3)	0.9500	2.3400	3.279(4)	170
C(7)-H(7)···O(1)	0.9500	2.5600	3.437(4)	153
C(10)-H(10)···O(2)	0.9500	2.5300	3.432(4)	159

C(12)-H(12)···O(3)	0.9500	2.5300	3.468(4)	172
C(15)-H(15)···O(2)	0.9500	2.3400	3.277(4)	170
C(20)-H(20)···O(3)	0.9500	2.3200	2.946(4)	123

Scheme 1 The structure of ligand L and auxiliary carboxylate ligands used.



L *p*-H_2BDC *m*-H_2BDC *m*-H_2BDC-CH_3

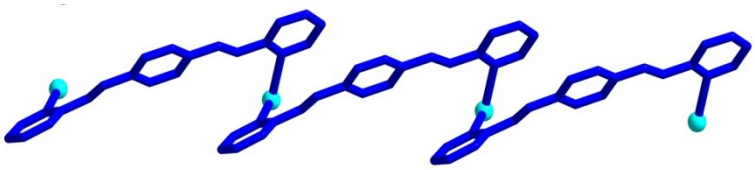


Fig. S1 The chain of Cd(II)-L in **3**.

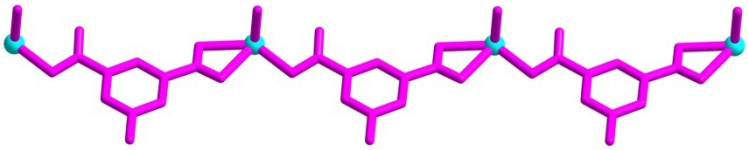


Fig. S2 The chain of Cd(II)-*m*-BDC-CH_3 in **3**.

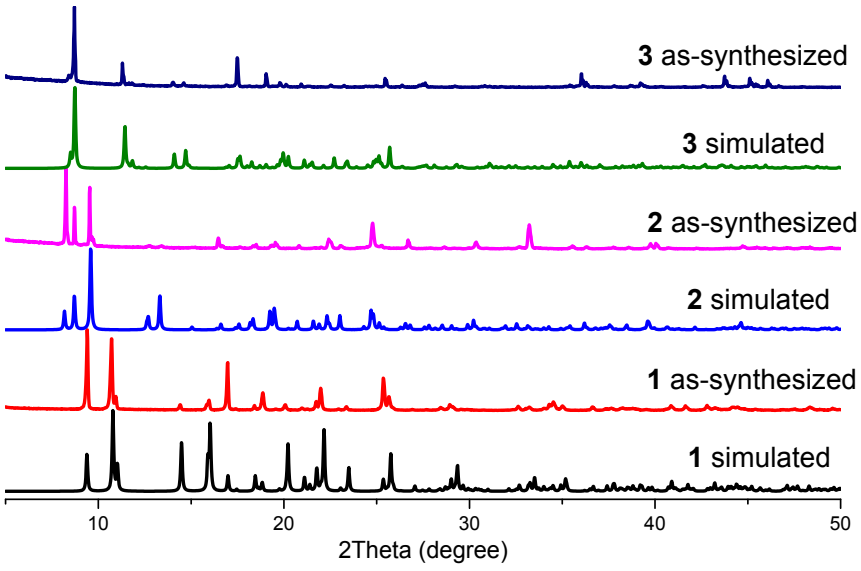


Fig. S3 PXRD patterns of complexes **1** - **3**.

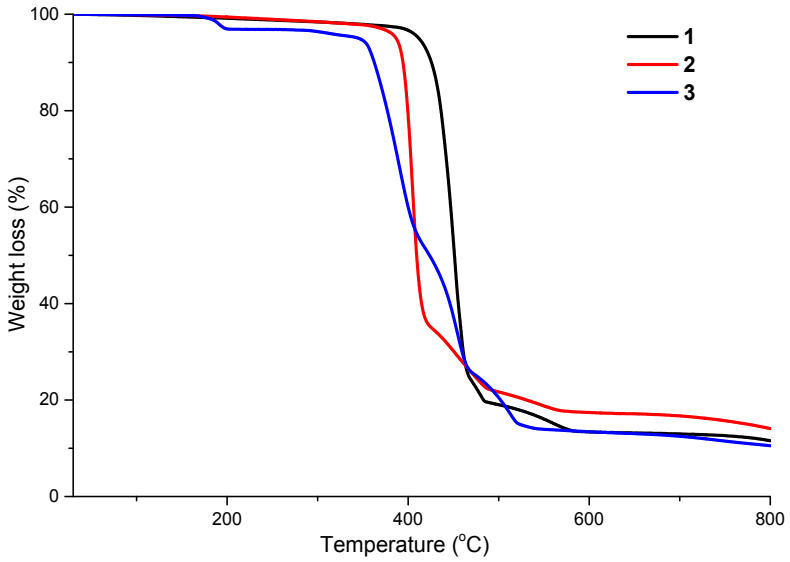


Fig. S4 TG curves of **1** - **3**.

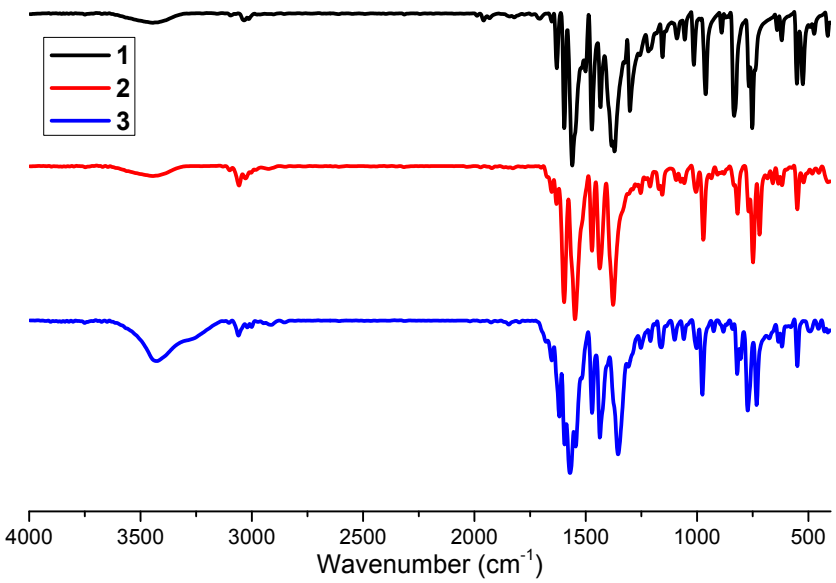
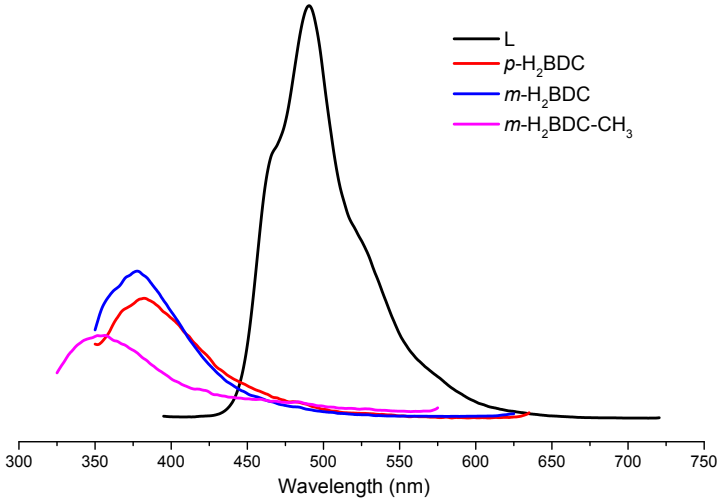
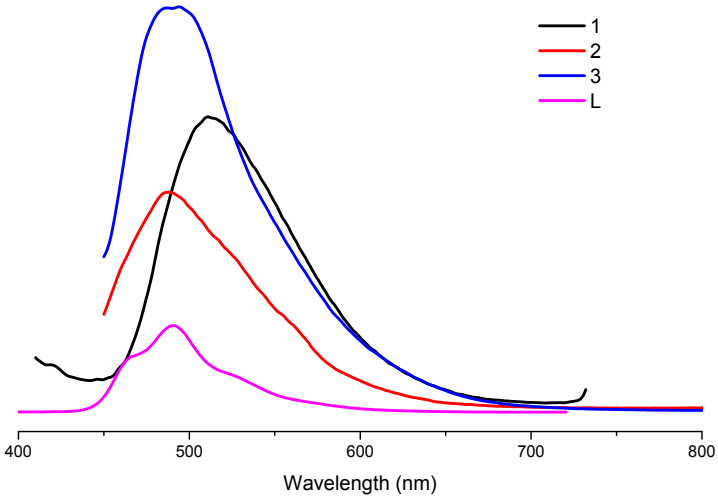


Fig. S5 IR spectra of **1** - **3**.



(a)



(b)

Fig. S6(a)Emission spectra of **L** and dicarboxylate ligands in the solid state at room temperature. (b) Emission spectra of **1 - 3**and ligand L in the solid state at room temperature.

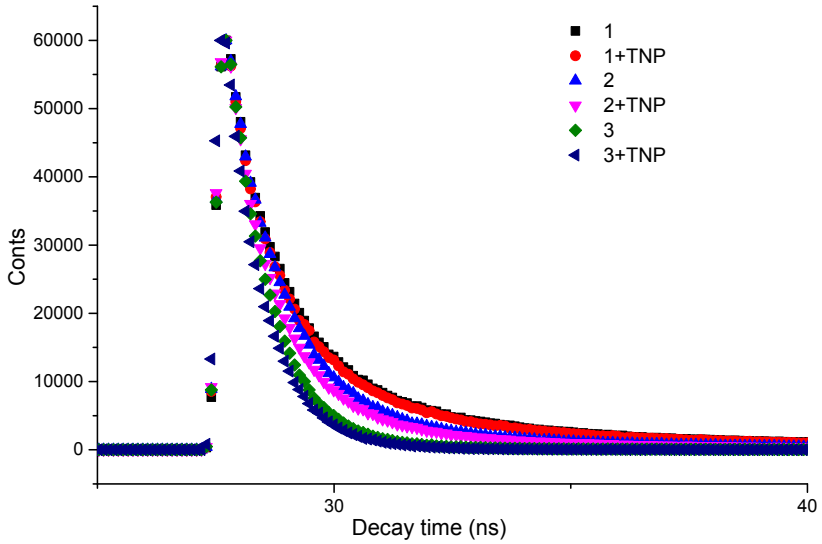


Fig. S7 Lifetimes of **1-3** dispered in DMF before and after the addition of the DMF solution of TNP.

Table S4 Comparison of the K_{SV} of **1 - 3** towards TNP with other materials.

	KSV (M^{-1})	Reference
1	5.72×10^4	This work
2	4.67×10^4	This work
3	1.86×10^5	This work
CP–C60 composite assembly	3.75×10^5	1
[CP (NH2BDC) (DMF)]	7.2×10^3	2
$\{[Zn(IPA)(L)]\}_n$/$\{[Cd(IPA)(L)]\}_n$	2.16×10^4/1.52×10^4	3
$[Zn(\mu_2\text{-}1H\text{-}ade)(\mu_2\text{-}SO4)]_n$	3.14×10^4	4
$\{(H_2pip)[Fe(pydc\text{-}2,5)_2(H_2O)]\cdot 2H_2O\}$	6.2×10^4	5
$[Ca(DMF)_4Ag_2(SCN)_4]_n$	1.74×10^4	6
$\{[Zn_3(mtrb)_3(btc)_2]\cdot 3H_2O\}_n$	3.26×10^4	7
$[Cd(NDC)L]_2\cdot H_2O$	3.7×10^4	8

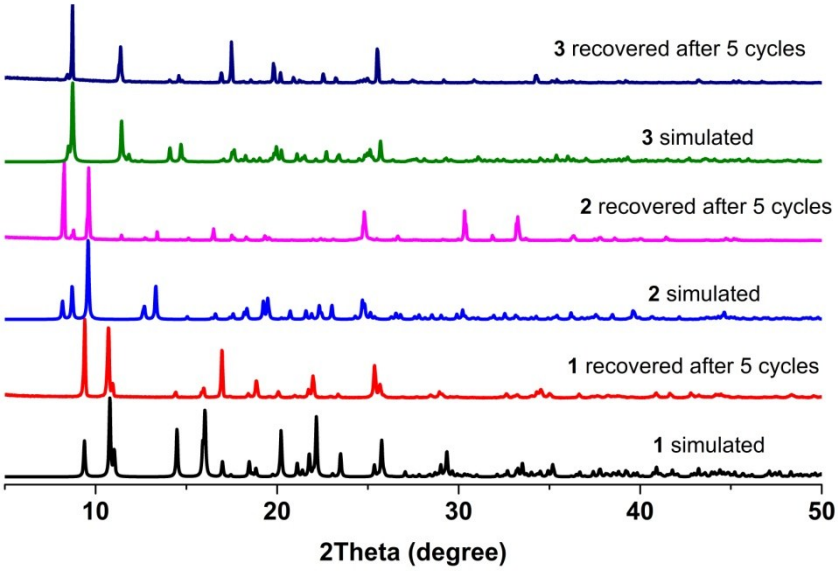


Fig. S8 PXRD patterns of complexes **1** - **3** and their recovered samples after five cycles immersed in the DMF solution of TNP. .

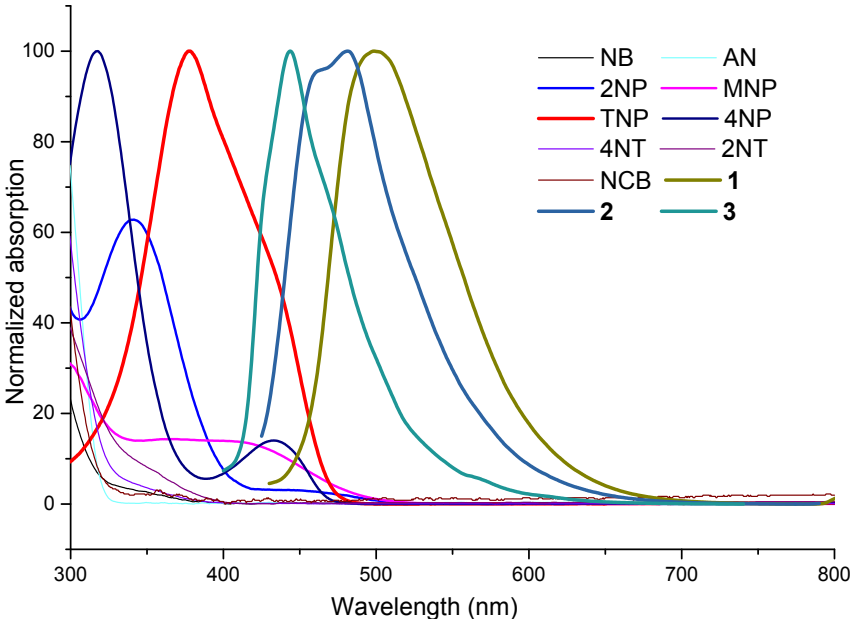


Fig. S9 The normalized emission bands of complexes **1** - **3** and UV-vis absorption of ANand selected nitroaromatic compounds (other analytes exclued due to no absorption bands in the range of 300 -800 nm).

Table S5 Frontier molecular orbital energies for complexes **1** -**3**and TNP at the genralized gradient approximation GGA-PBE level of theory.

	HOMO (eV)	LUMO (eV)	Energy gap (eV)
TNP	-6.967	-5.816	1.151
1	-6.057	-4.022	2.035
2	-5.928	-4.043	1.885
3	-5.856	-3.966	1.891

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