Supporting information for the manuscript entitled

Facile construction of anthracene-decorated highly luminescent coordination polymer for selective detection of explosive nitroaromatics and mutagenic pollutant TNP

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Table S1 Crystal data and refinement parameters for compound **1**.

Formula	$C_{50}H_{36}N_2O_5Zn$
fw	810.20
cryst syst	Triclinic
space group	$P\bar{1}$
a (Å)	6.011(3)
b (Å)	15.789(8)
c (Å)	21.392(11)
α (deg)	73.242(6)
β (deg)	83.793(7)
γ (deg)	86.176(6)
V (Å^3)	1931.3(17)
Z	2
D_{calcd} (g/cm^3)	1.393
μ (mm^{-1})	0.690
F(000)	840.0
λ (Å)	0.71073
GOF on F^2	1.032
Final*R* indices $[I > 2\sigma(I)]^{a,b}$	$R1$ = 0409 $wR2$ = 0967
Temperature(K)	293

$^aR1 = \Sigma||F_o| \quad |F_c||/ \Sigma|F_o|$, $^bwR2 = [\Sigma w(F_o^2 \quad F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths and bond angles **1**.

Bond length (Å)	
Zn(1)-N(1)	2.189(3)
Zn(1)-N(2)	2.224(3)
Zn(1)-O(1)	2.132(3)
Zn(1)-O(2)	2.287(3)
Zn(1)-O(3)	2.004(3)
Zn(1)-O(5)	2.049(3)
Bond angle (°)	
N(1)-Zn(1)-N(2)	176.02(11)
N(1)-Zn(1)-O(1)	93.35(11)
N(1)-Zn(1)-O(2)	90.40(10)
N(1)-Zn(1)-O(3)	87.40(11)
N(1)-Zn(1)-O(5)	88.91(12)
N(2)-Zn(1)-O(1)	90.63(11)
N(2)-Zn(1)-O(2)	91.53(11)
N(2)-Zn(1)-O(3)	88.66(11)
N(2)-Zn(1)-O(5)	91.10(12)
O(1)-Zn(1)-O(2)	59.10(8)
O(1)-Zn(1)-O(3)	170.86(15)
O(1)-Zn(1)-O(5)	91.79(12)
O(2)-Zn(1)-O(3)	111.81(14)
O(2)-Zn(1)-O(5)	150.79(12)
O(3)-Zn(1)-O(5)	97.33(10)

Table S3 Hydrogen bonding in compound **1**.

D—H···A	Distance (Å) D—H	Distance (Å) H···A	Distance (Å) D··A	Angle (°) ∠D—H···A
O(5)-H(5)···O(4)	0.853	1.813(2)	2.612(3)	155.0(1)
O(5)-H(5)···O(2)	0.787	1.92(3)	2.694(3)	167(3)

Table S4 Geometric features (distances, Å and angles,°) of the π···π stacking interactions in compound **1**.

Compound	**Cg(Ring I)···Cg(Ring J)**	**Cg···Cg (Å)**	**Cg(I)···Perp (Å)**	**Cg(J)···Perp (Å)**
1	Cg(4)···Cg(5)	3.664(3)	3.648	3.648
	Cg(9)···Cg(10)	3.629(3)	3.602	3.591

Cg(I)···Perp = Perpendicular distance of Cg(I) on ring J. Cg(J)···Perp = Perpendicular distance of Cg(J) on ring I.

For Compound **1:**

Cg(4) = Centre of gravity of the ring [C(9)-C(10)-C(11)-C(12)-C(13)-C(14)];

Cg(5) = Centre of gravity of the ring [C(16)-C(17)-C(18)-C(19)-C(20)-C(21)].

Cg(9) = Centre of gravity of the ring[C(38)-C(39)-C(40)-C(41)-C(42)-C(43)].

Cg(10) = Centre of gravity of the ring[C(45)-C(46)-C(47)-C(48)-C(49)-C(50)].

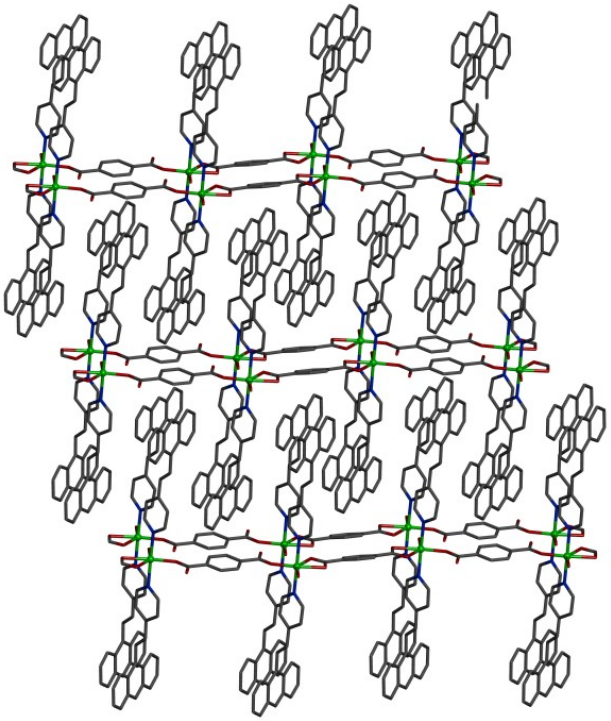

Fig. S1 3D supramolecular architecture of CP **1** based on π···π and hydrogen bonding interactions.

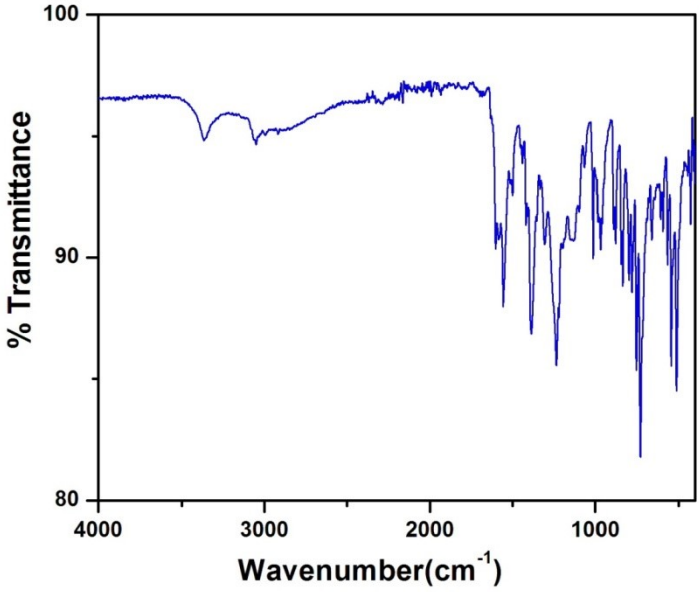

Fig. S2 IR spectrum of CP **1**.

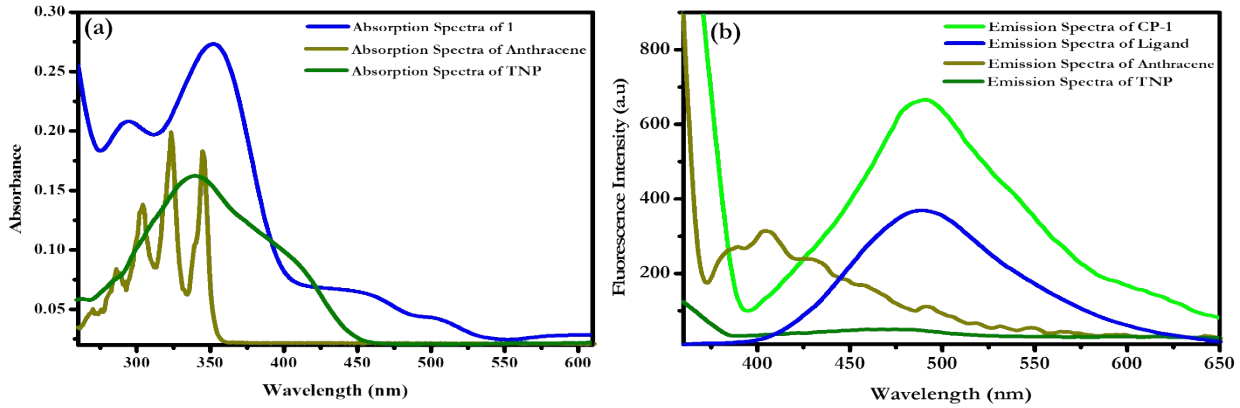

Fig. S3 (a) Absorption spectra and (b) Emission spectra of CP **1**, anthracene (10^{-4}M CAN solution), TNP (10^{-4} M ACN solution) and free avp ligand (10^{-4} M ACN solution).

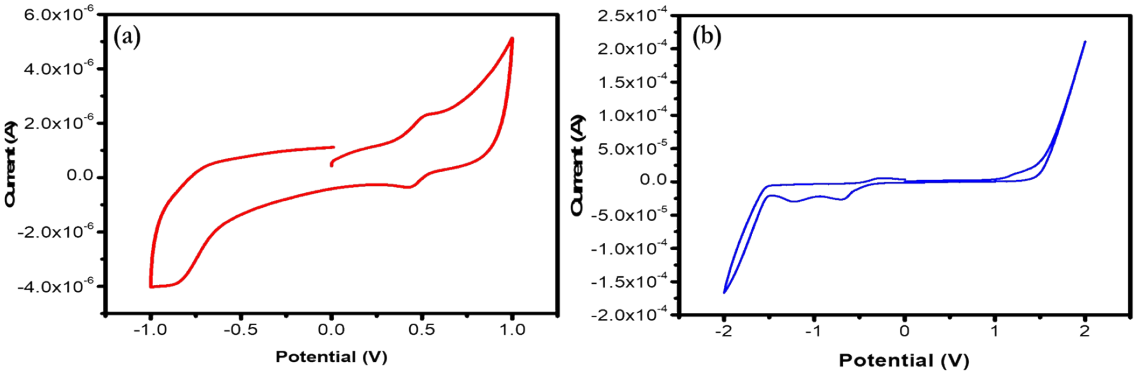

Fig. S4 Cyclic voltammogram (a) avp ligand and (b) H_2bdc.

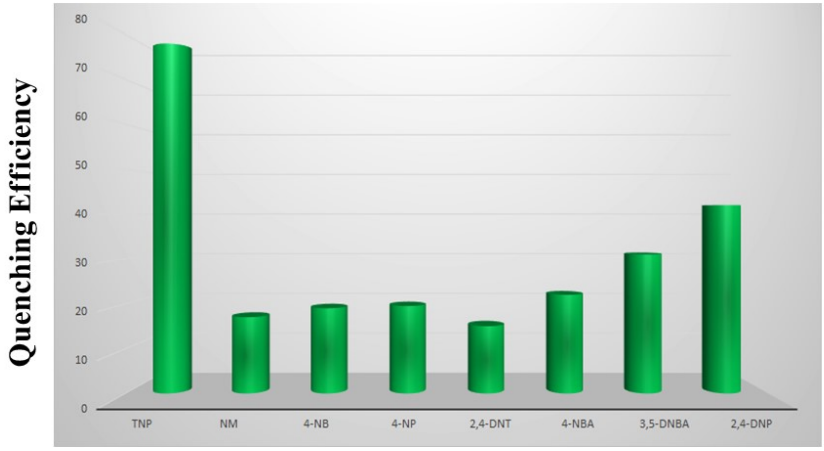

Fig. S5 Quenching efficiency of epNACs towards the fluorescence intensity of CP **1**.

Calculation of detection limit

The detection limit calculated as per the standard reported method. For calculating detection limit, TNP (0-850µl, 1×10^{-4} M stock solution) was added to CPs solutions and respective fluorescence intensity was recorded. By plotting fluorescence intensity with increasing equivalent concentration of TNP, slope (k) of graph was found and Standard deviation (σ) was calculated from five blank measurements of CPs. Detection limit is calculated according to the formula: detection limit=(3σ/k).

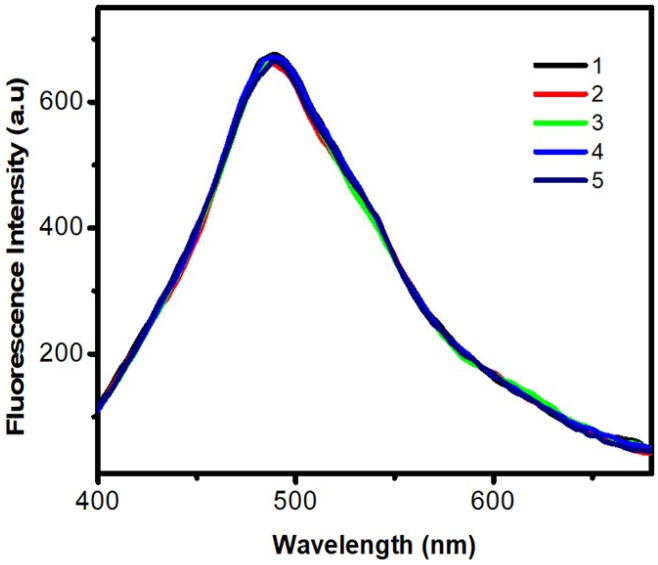

Fig. S6 Plot of blank titration of CP **1**.

Table S5 Standard deviation of CP **1**

BlankReadings	FluorescenceIntensity
1	675
2	659
3	667
4	670
5	664
Standard Deviation(σ)	**5.40**

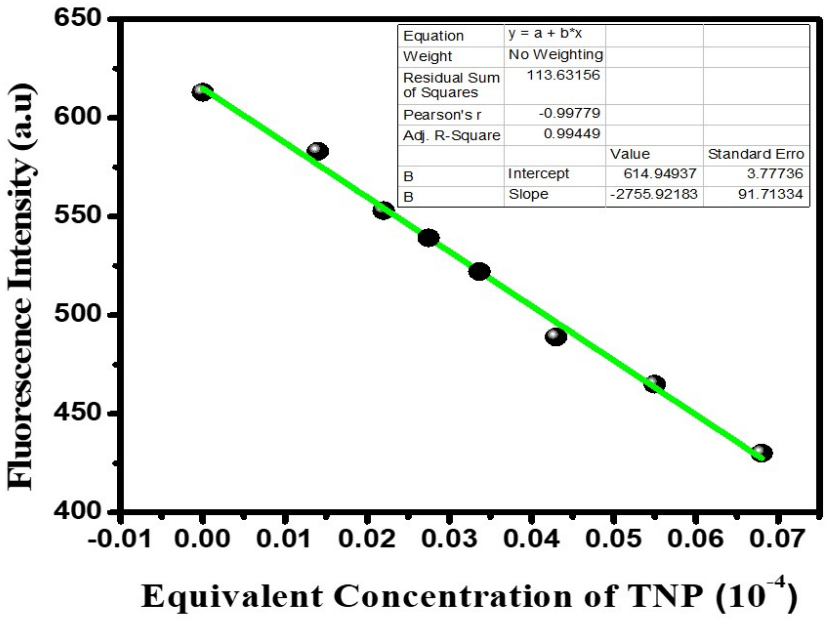

Fig. S7 Linear region of fluorescence intensity of CP **1** upon addition of TNP (10^{-4} M ACN) solution

Slope (k) = 2755.92

Standard Deviation (σ) =5.40

Detection limit (3σ/k) = 0.58 μM

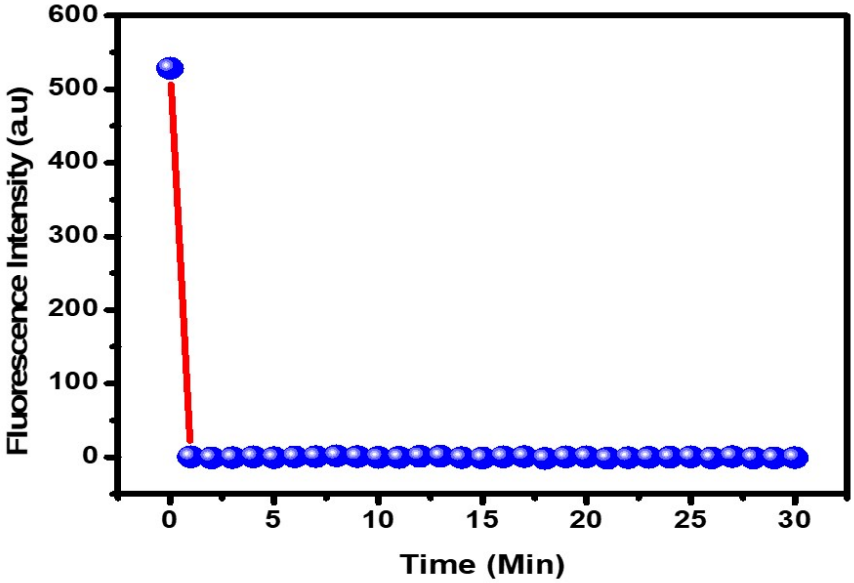

Fig. S8 Time dependent fluorescence response of the sensor probe CP **1** in presence of TNP solution.

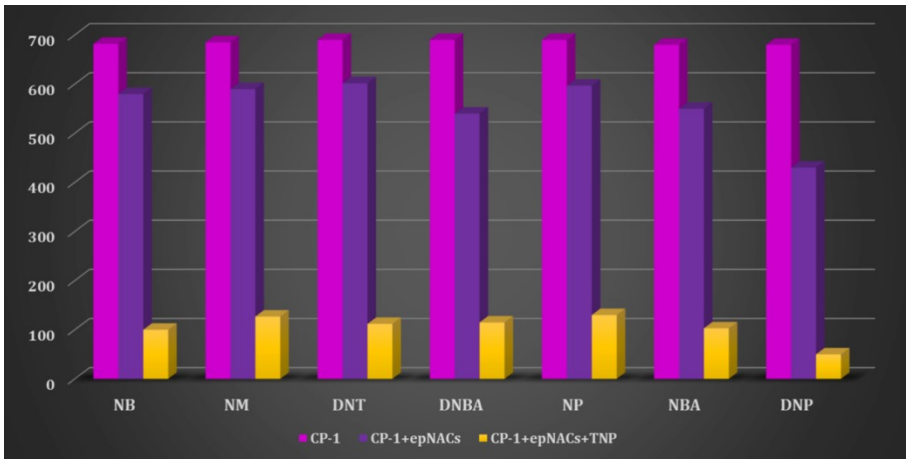

Fig. S9 Selectivity of CP **1** for TNP in presence of other epNACs.

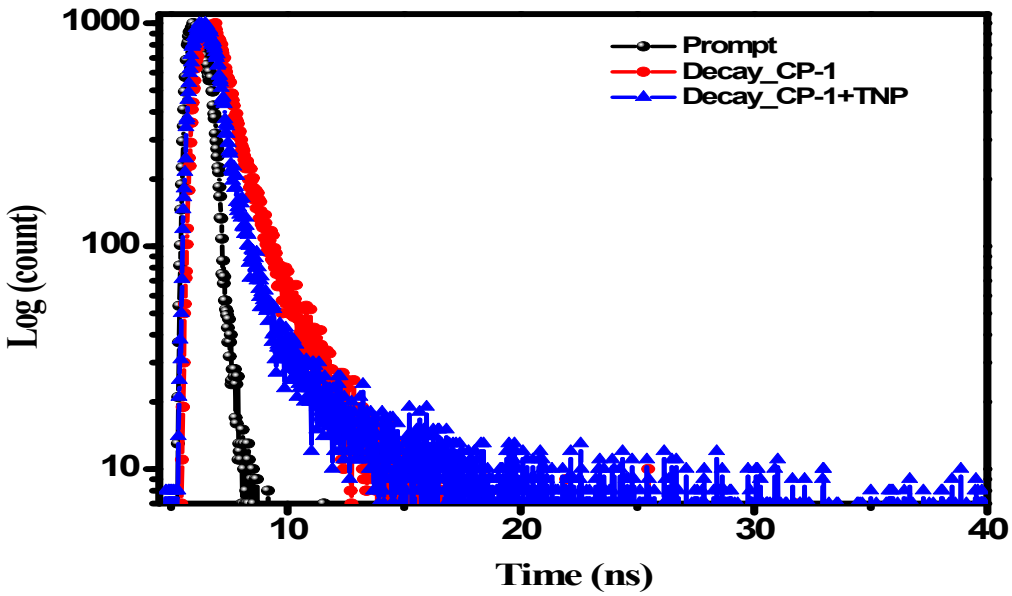

Fig. S10 Fluorescence lifetime decay profiles of CP **1** without and with TNP.

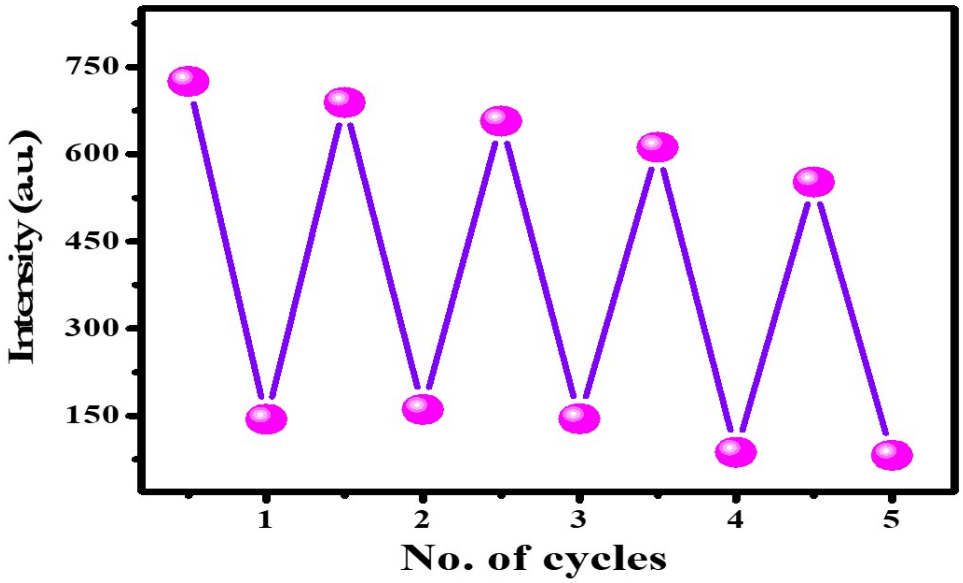

Fig. S11 Recyclability of CP **1** for luminescent quenching with TNP up to 5 times.

FESEM

The high-resolution images CP **1** captured by the FESEM revealed elongated, slender crystals resembling needles like morphology (Fig. S12a). These crystals exhibited a distinct and uniform shape (Fig. S12b) with pointed end (Fig. S12c) and a consistent width along with the length. Further resolution enabled to closely observe the fine details of the needle-shaped crystals, such as its surface features and structural nuances. The surface structural feature indicates significant smoothness (Fig. S12d), which further suggests minimal surface irregularities and the feasibility of structural homogeneity. This detailed visualization of the crystal morphology provides a comprehensive understanding of the dimension of the crystal (Fig. 5d), orientation, and potential structural homogeneity.

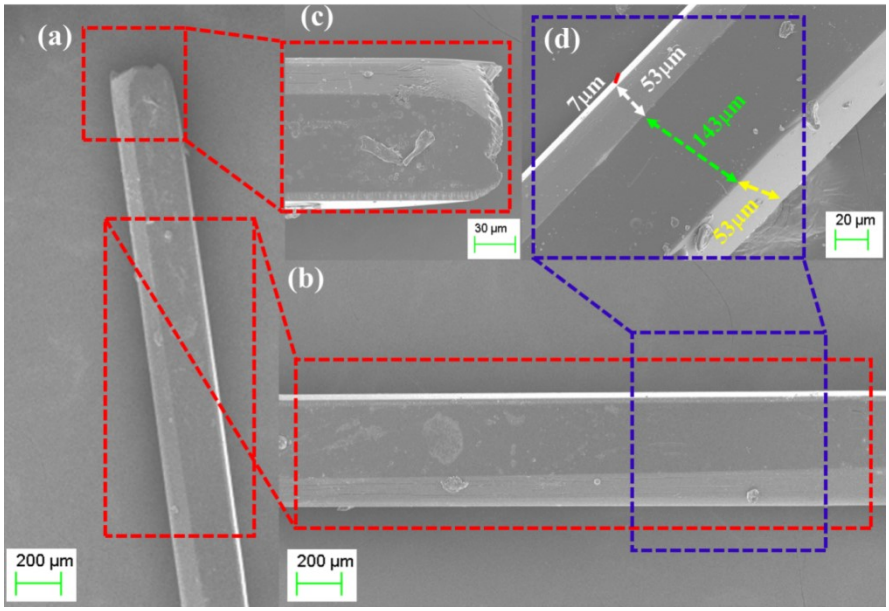

Fig. S12 FE-SEM of the luminescent probe CP **1**with different elongated section to observe its surface features.

Table S6 Comparison table with recently reported similar works

Sl. No.	Compound	Parameters		Recyclability	Reference
		LOD (M)	K_{SV} (M^{-1})		
1.	$[Cd(L_{12})(L_{13})]_n$	0.27×10^{-6}	2.68×10^4	Yes	1
2.	$[Cd_5(TCA)_4(H_2O)_2]$	6.2×10^{-6}	6.56×10^4	No	2
3.	$\{[Cd_4(L)_2(L_2)_3(H_2O)_2](8DMF)(8H_2O)\}_n$	4.9×10^{-6}	3.89×10^4	No	3
4.	$[Cd_4(\mu_3\text{-}O)(TTHA)(H_2O)_2]\cdot 3H_2O$	5.6×10^{-6}	3.83×10^4		4
5.	$[Cd(L_6)(L_7)]_2\cdot H_2O$	NA	3.7×10^4	Yes	5
6.	$[Cd_3(TPT)_2(DMF)_2]\cdot(H_2O)_{0.5}$	7.8×10^{-6}	6.56×10^4	Yes	6
7.	$[Zn_3(TPT)_2(DMF)_2]\cdot 0.5HNMe_2$	NA	6.39×10^4	Yes	7
8.	$NH_2Me_2\cdot[Zn(TPT)]\cdot DMF$	NA	7.18×10^4		
9.	$[Me_2NH_2]_4[Zn_6(qptc)_3(trz)_4]\cdot 6H_2O$	NA	2.08×10^6	Yes	8

10.	$Zn_2(TZBPDC)(\mu_3\text{-}OH)(H_2O)_2$	2.78×10^{-4}	4.9×10^4	No	9
11.	$[Mg_2Zn_2(OH)_2(1,4\text{-}NDC)_3(H_2O)_2]\cdot 6H_2O$	NA	1.8 × 104	No	10
12.	$[Zn_2(NH_2BDC)_2(L_{15})]_n$	1.31×10^{-6}	NA	No	11
13.	$[Zn_8(ad)_4(BPDC)_6O\cdot 2\ Me_2NH_2]\cdot G$	12.9×10^{-9}	4.6×10^4	No	12
14.	$[(CH_3)_2NH_2]_3[Zn_4Na(L_8)_3]\cdot 4CH_3OH\cdot 2$ DMF	5×10^{-6}	3.2×10^4	No	13
15.	$[Zn_4(DMF)(urotropine)_2(L_4)_4]$	7.1×10^{-6}	10.83×10^4	No	14
	AIE active material				
16.	4-((pyren-1-yl)methyleneamino)-1,2-dihydro-2,3-dimethyl-1-phenylpyrazol-5-one	16.51×10^{-9}	4.7×10^5	No	15
17.	dimethyl-5-(pyren-1-ylmethyleneamino)isophthalate	10×10^{-9}	2.03×10^4	No	16
18.	polyPhTPECz	3.8×10^{-9}	1.63×10^5	Yes	17
19.	phosphorescent cyclometalated iridium(III) complexes complex 1 complex 2 complex 3 complex 4	 0.23×10^{-6} 0.15×10^{-6} 1.05×10^{-6} 1.65×10^{-6}	 1.50×10^5 0.32×10^5 1.66×10^5 0.86×10^5	No	18
20.	Tetraphenylethene (TPE) incorporated into a UiO-isoreticular zirconium MOF	----	----	No	19
	Conjugated polymers				
21.	4'-(4-{2-[aryl]-ethenyl}phenyl)2,2':6',2"-terpyridines	$1.31–2.94\times 10^{-7}$	$\sim10^4$	No	20
22.	CP 1, CP 2, CP 3	3.2×10^{-12} 5.7×10^{-12} 6.1×10^{-12}	4.27×10^6, 3.71×10^6, 2.13×10^6	No	21
23.	poly(tetraphenylethene-co-biphenyl) (PTPEBP) nanoparticles	1.07×10^{-6}	2.50×10^4	No	22
24.	1,1,2,2-tetrakis(4-formyl-(1,10-biphenyl))-ethane (TFBE)	0.09×10^{-6}	8×10^5	No	23
25.	Fluorescein containing conjugated	7.22×10^{-7}	2.08×10^3	No	24

	microporous polymers (DTF and TTF)				
26.	**Quantum dots**				
27.	N-CDs@MIP	0.15×10^{-9}	73.5×10^{9}	No	25
28.	Oxygen containing CDs	0.0620×10^{-6}	----	No	26
29.	ZnSe quantum dots	12.4×10^{-6}	-----	No	27
30.	MoS_2 quantum dots (QDs)	95×10^{-9}	4.3×10^{4}	No	28
31.	Nitrogen doped graphene quantum dots (N-GQDs)	0.92×10^{-6}	----	No	29
32.	**CP 1**	$\mathbf{0.58 \times 10^{-6}}$	$\mathbf{18.18 \times 10^{4}}$	**Yes**	**Present work**

trz = 1,2,4- triazole; 1,4-H_2NDC = 1,4-naphthalenedicarboxylic acid; H_4qptc = terphenyl-2,5,2′5′-tetracarboxylic acid; L_1 = 4-amino-3,5-bis(4-imidazol-1-ylphenyl)-1,2,4-triazole; H_6TDPAT = 2,4,6-tris(3,5-dicarboxylphenylamino)-1,3,5-triazine; Hbpba = 4-(bis(4-(pyridin-4-yl)phenyl)amino)benzoic acid; 4-tp-3-lad = 2,3,5,6-tetra(pyridin-4-yl)-bicyclo[2.2.0]hexane; 1,4-H_2BDC = benzene-1,4-dicarboxylic acid; ppene = 4-pyrpoly-2-ene; H_3TZBPDC = 4'-(1Htetrazol-5-yl)-[1,1'-biphenyl]-3,5-dicarboxylic acid; H_3TPT = p-terphenyl-3,4",5-tricarboxylic acid; apy = aminopyridine; H_4tptc = terphenyl-3,3″,5,5″-tetracarboxylic acid; Ur = urotropin; py = pyridine; TNP= 2,4,6-trinitrophenol.

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