Comparative Study of Luminescent Cd-MOF and Cd-MOF@HNT Nanomaterial for detection of Hydroxyl-Functionalized Nitroaromatic compounds

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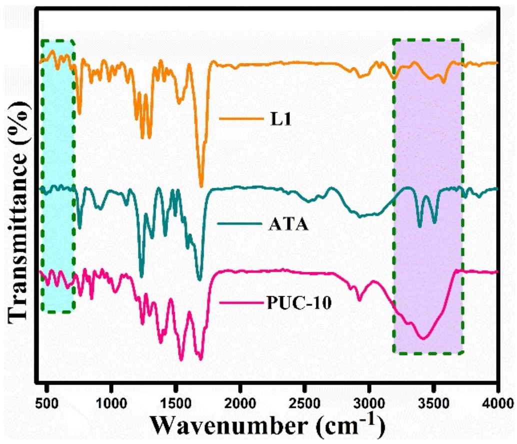

Figure S1. FTIR analysis of PUC-10 and both the ligands L1 and ATA (2-aminoterephthalic acid) which are used to synthesize PUC-10.

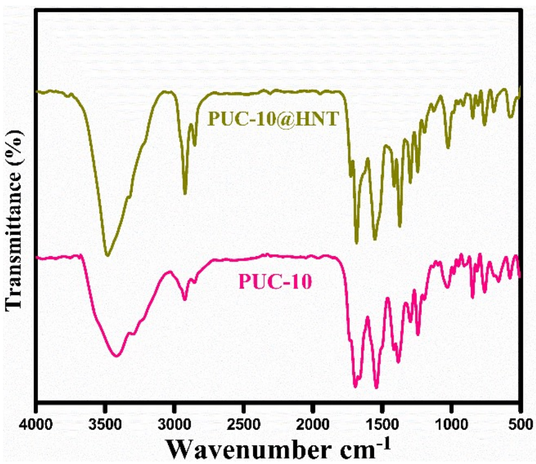

Figure S2. FTIR spectra of PUC-10 and PUC-10@HNT.

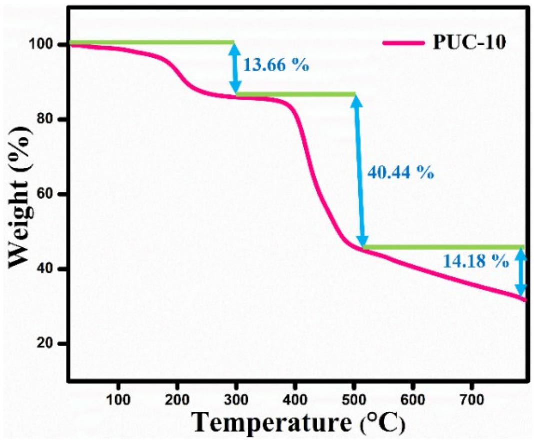

Figure S3. TGA analysis of PUC-10.

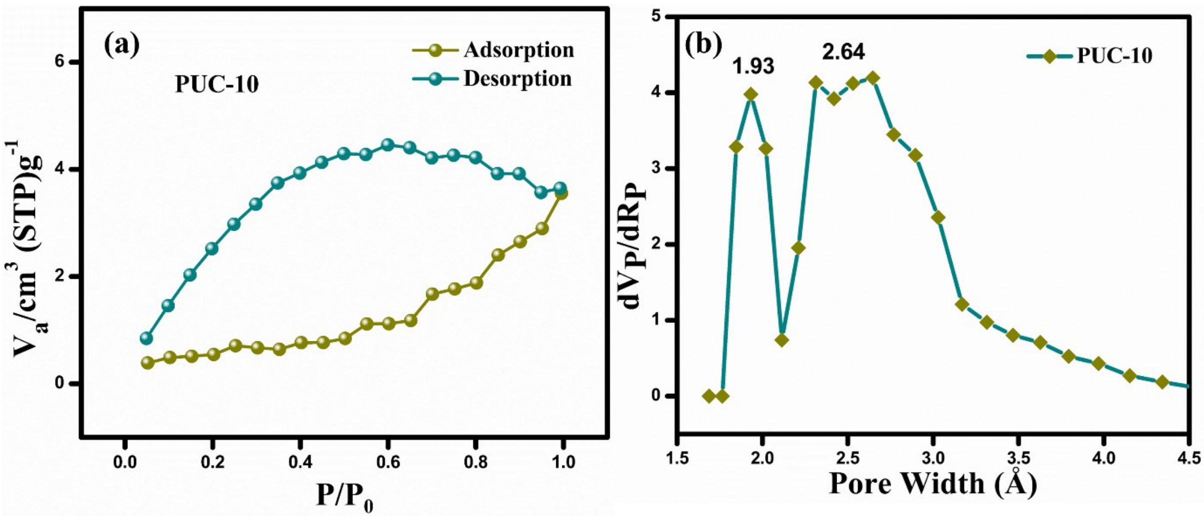

Figure S4. N_2 sorption isotherm for PUC-10 **(a)** and pore size distribution curve for PUC-10 based on adsorption isotherm **(b).**

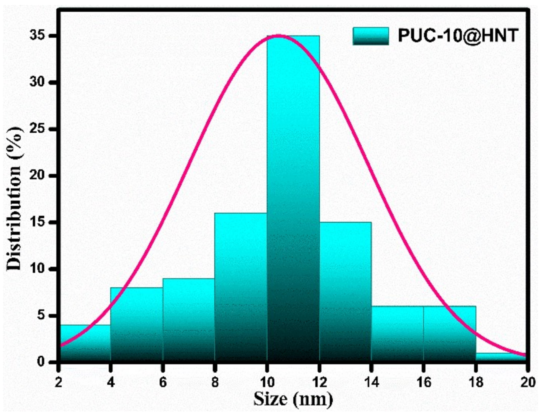

Figure S5. Size distribution histogram plot of PUC-10@HNT.

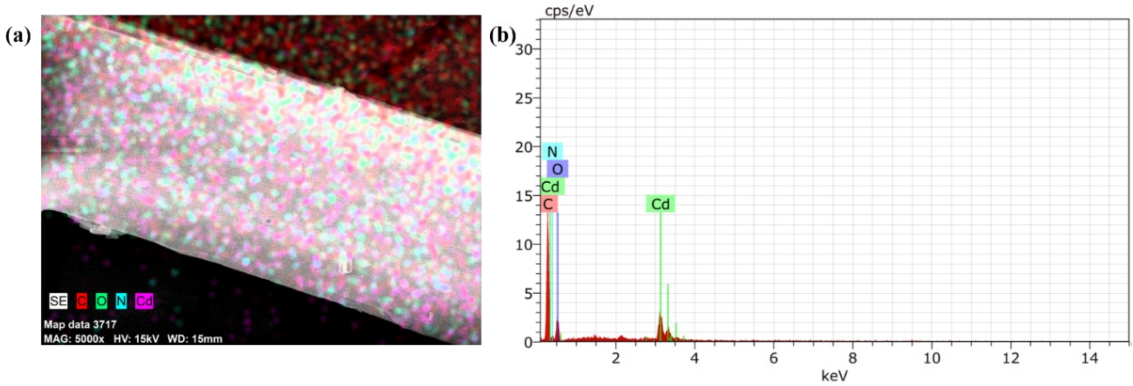

Figure S6. Elemental mapping **(a)** and EDX spectrum **(b)** of PUC-10.

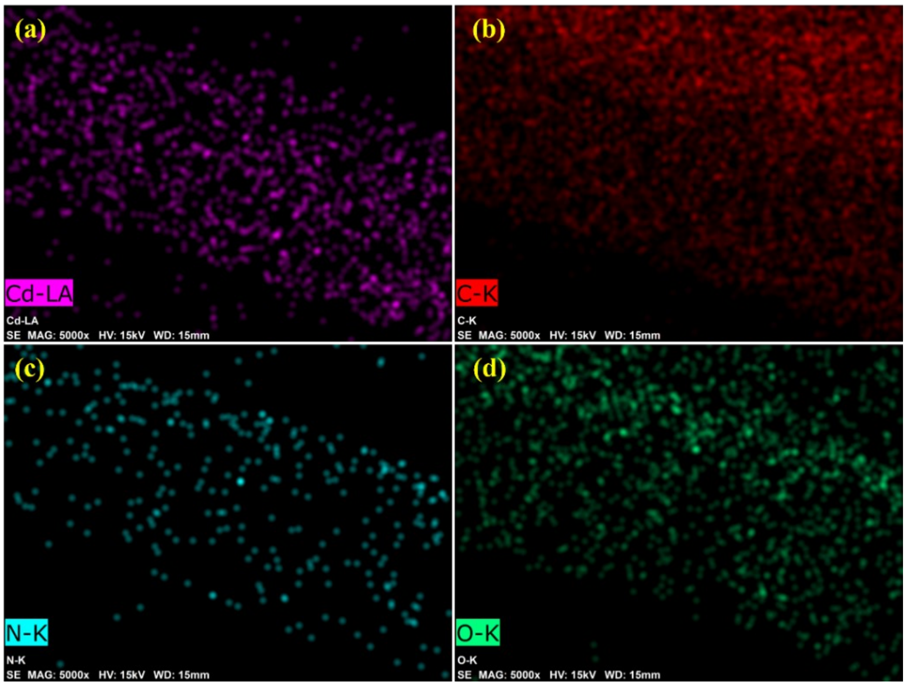

Figure S7. Mapping of elemental distribution of Cd **(a),** C **(b),** N **(c)** and O **(d)** of PUC-10.

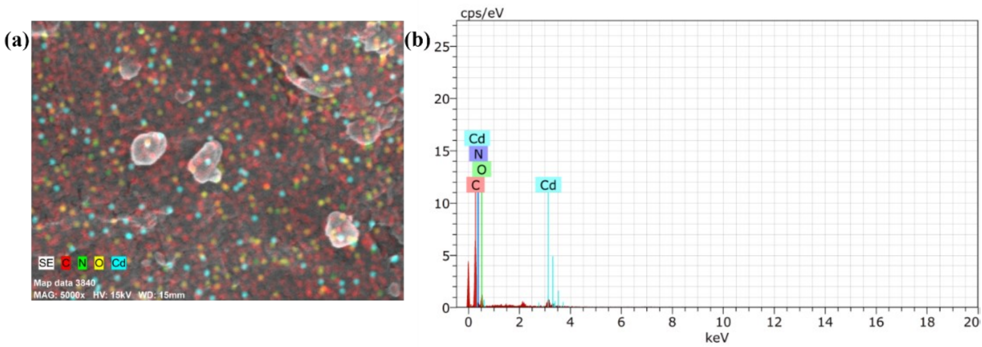

Figure S8. Elemental mapping **(a)** and EDX spectrum **(b)** of PUC-10 NPs.

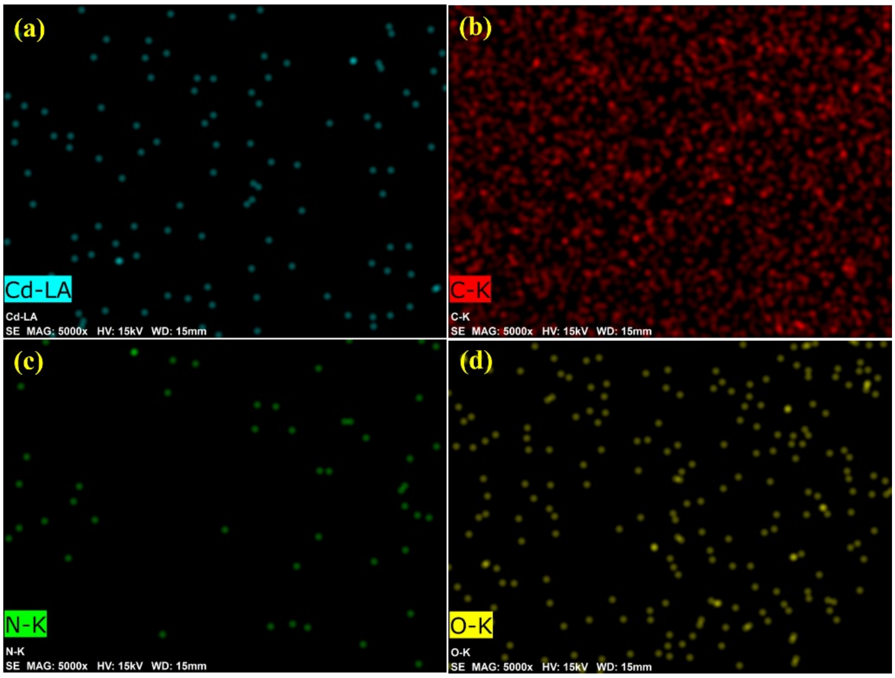

Figure S9. Mapping of elemental distribution of Cd **(a),** C **(b),** N **(c)** and O **(d)** of PUC-10 NPs.

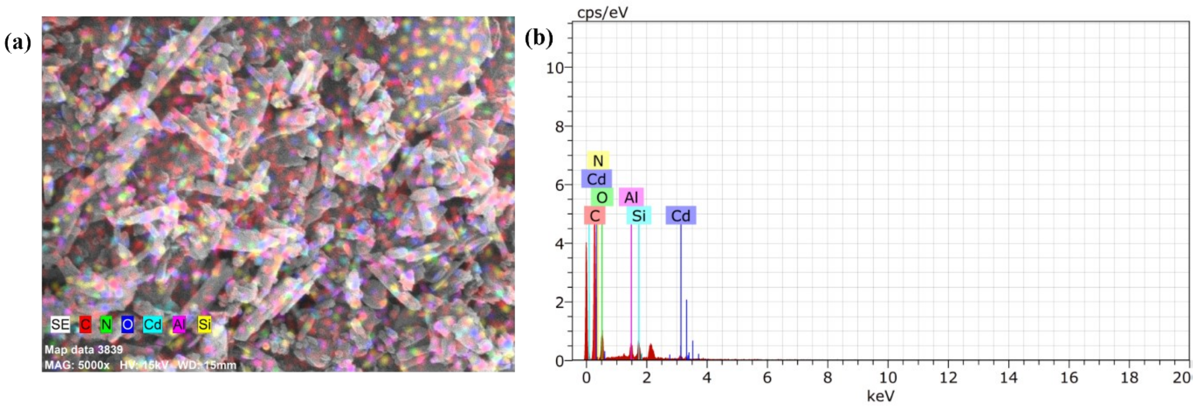

Figure S10. Elemental mapping **(a)** and EDX spectrum **(b)** of PUC-10@HNT.

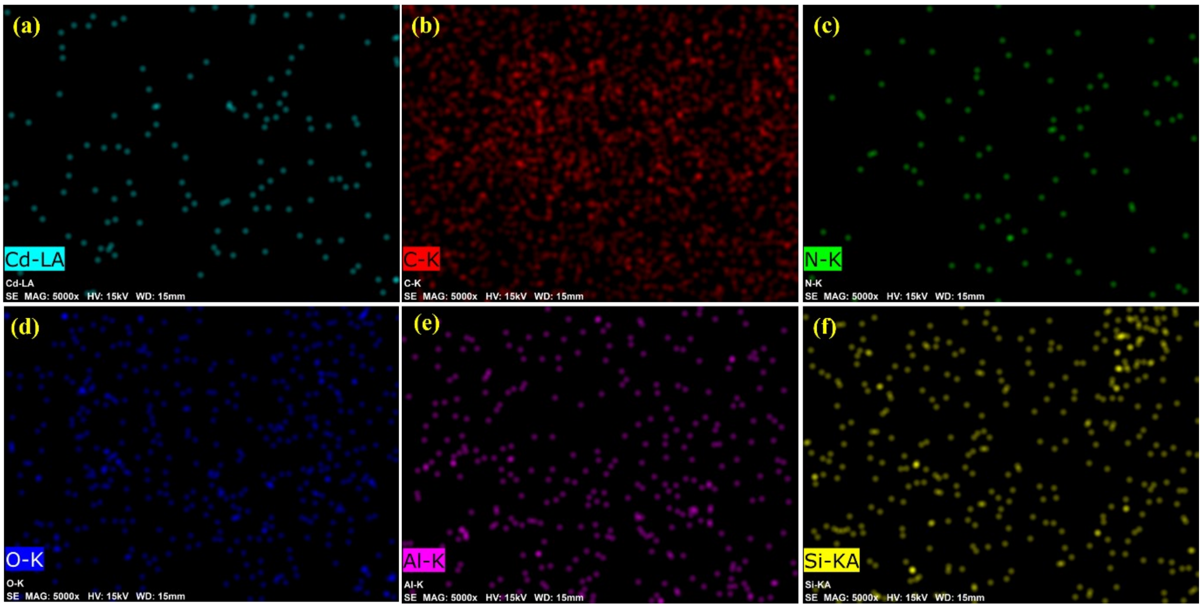

Figure S11. Mapping of elemental distribution of Cd **(a),** C **(b),** N **(c),** O **(d),** Al **(e)** and Si **(f)** of PUC-10@HNT.

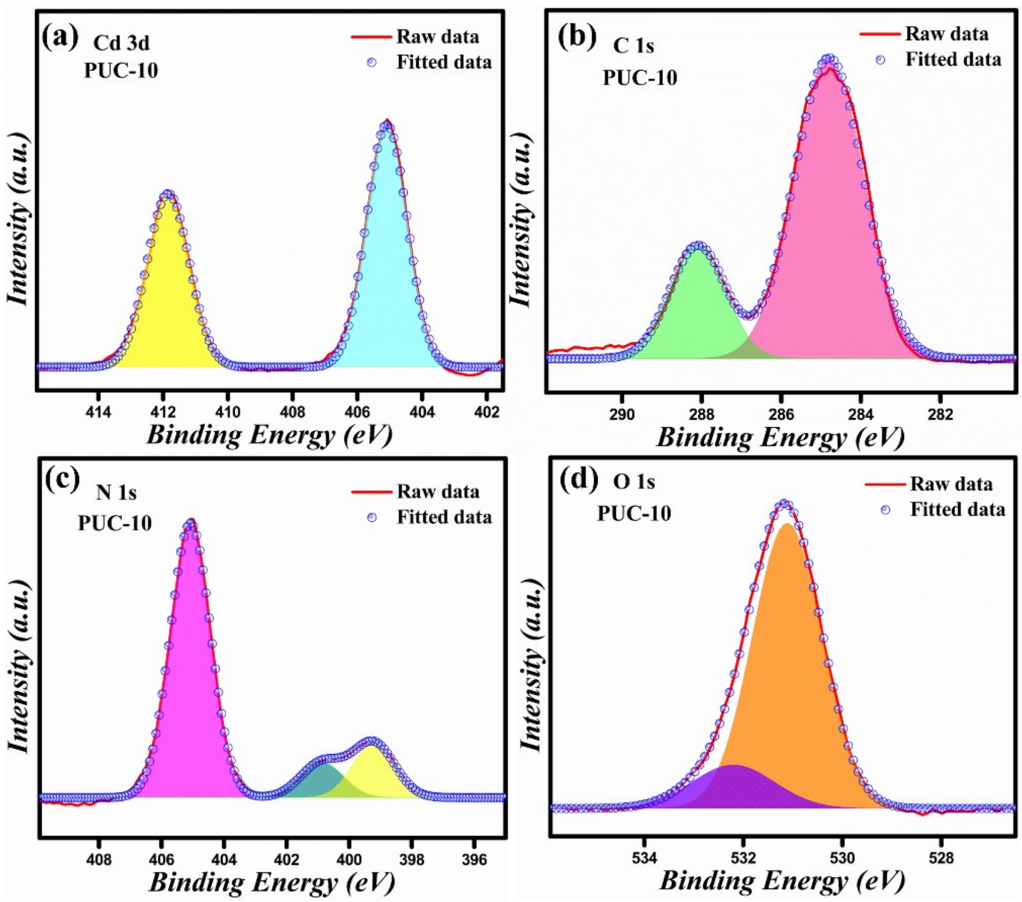

Figure S12. High-resolution XPS spectrum of Cd 3d **(a),** C 1s **(b),** N 1s **(c)** and O 1s **(d)** elements present in PUC-10.

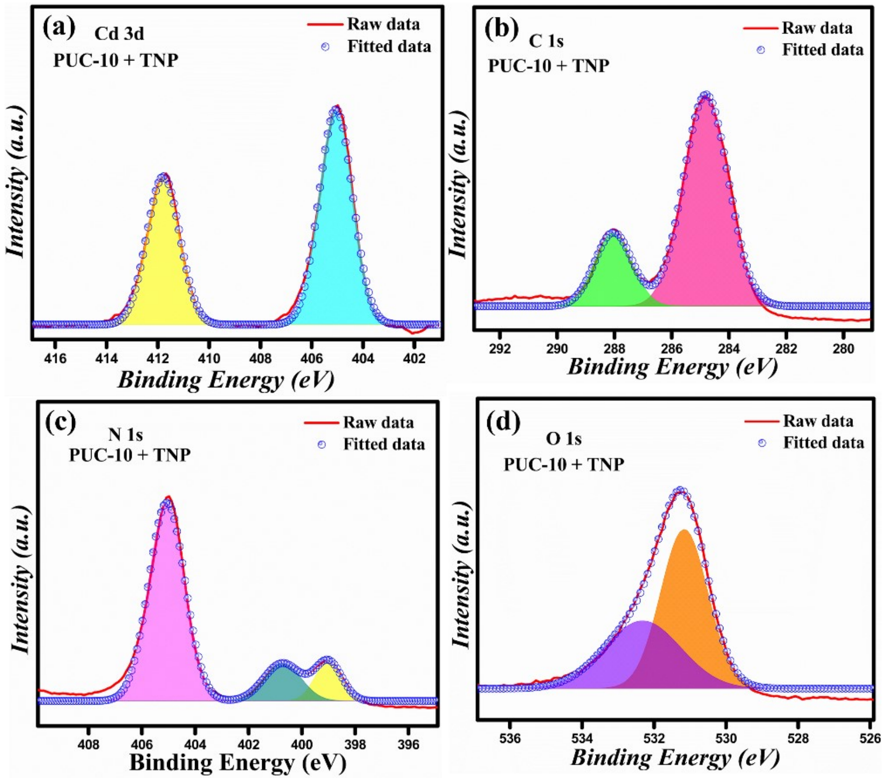

Figure S13. High-resolution XPS spectrum of Cd 3d **(a),** C 1s **(b),** N 1s **(c)** and O 1s **(d)** elements present in PUC-10 after treatment with TNP.

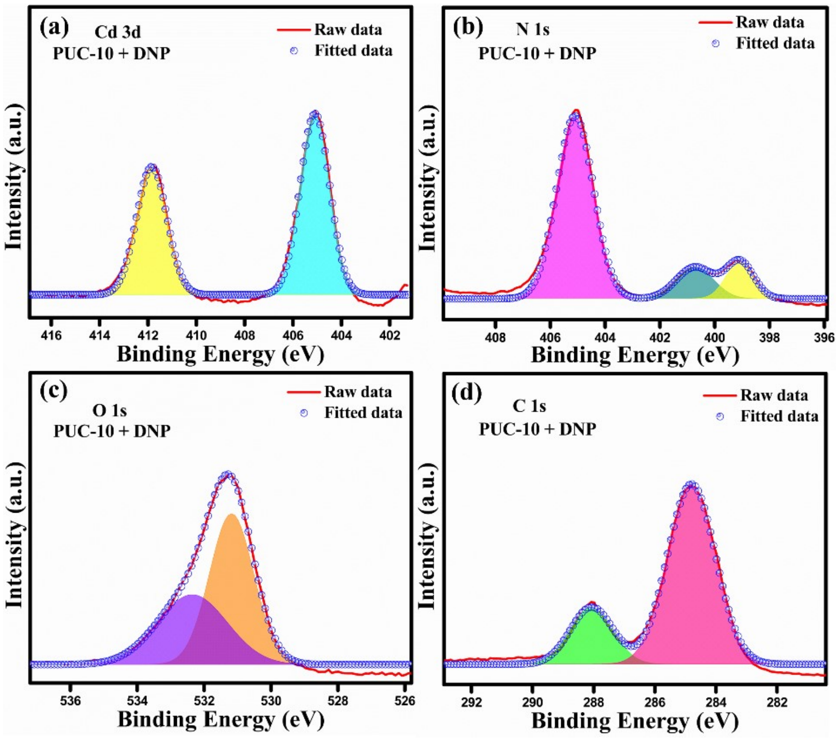

Figure S14. High-resolution XPS spectrum of Cd 3d **(a),** N 1s **(b),** O 1s **(c)** and C 1s **(d)** elements present in PUC-10 after treatment with DNP.

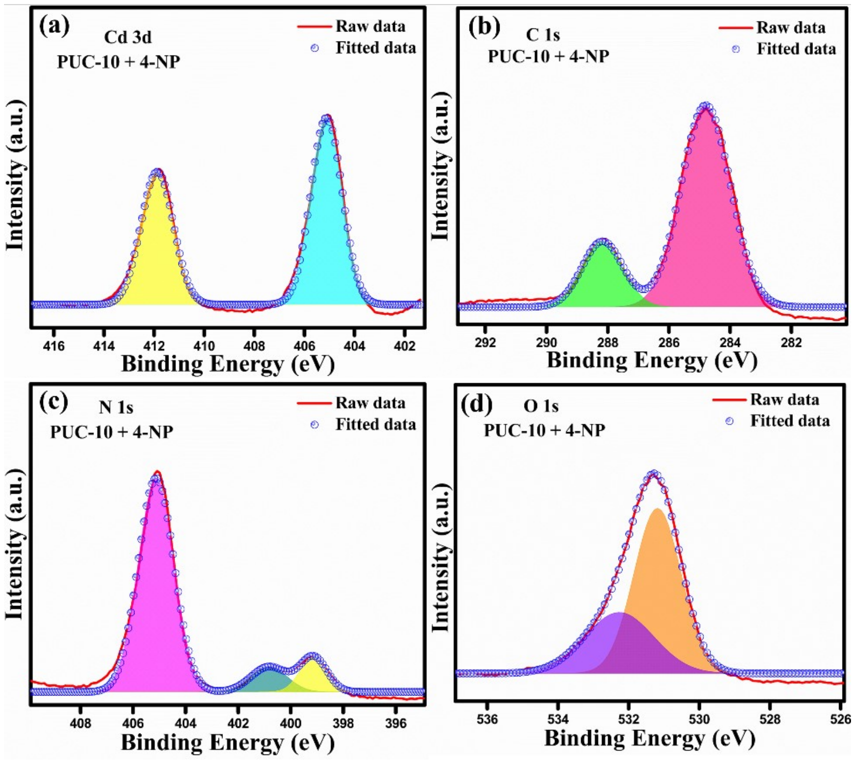

Figure S15. High-resolution XPS spectrum of Cd 3d **(a),** C 1s **(b),** N 1s **(c)** and O 1s **(d)** elements present in PUC-10 after treatment with 4-NP.

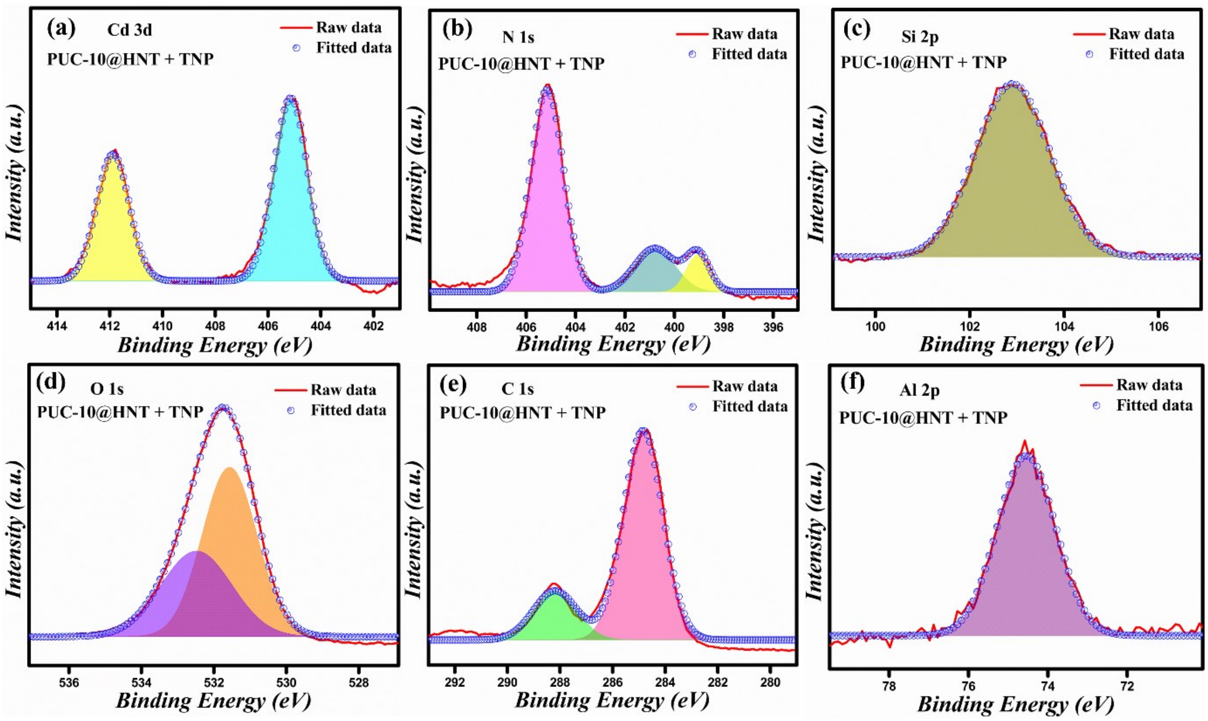

Figure S16. High resolution XPS spectrum of Cd 3d **(a),** N 1s **(b),** Si 2p **(c),** O 1s **(d),** C 1s **(e)** and Al 2p **(f)** elements present in PUC-10@HNT after treatment with TNP.

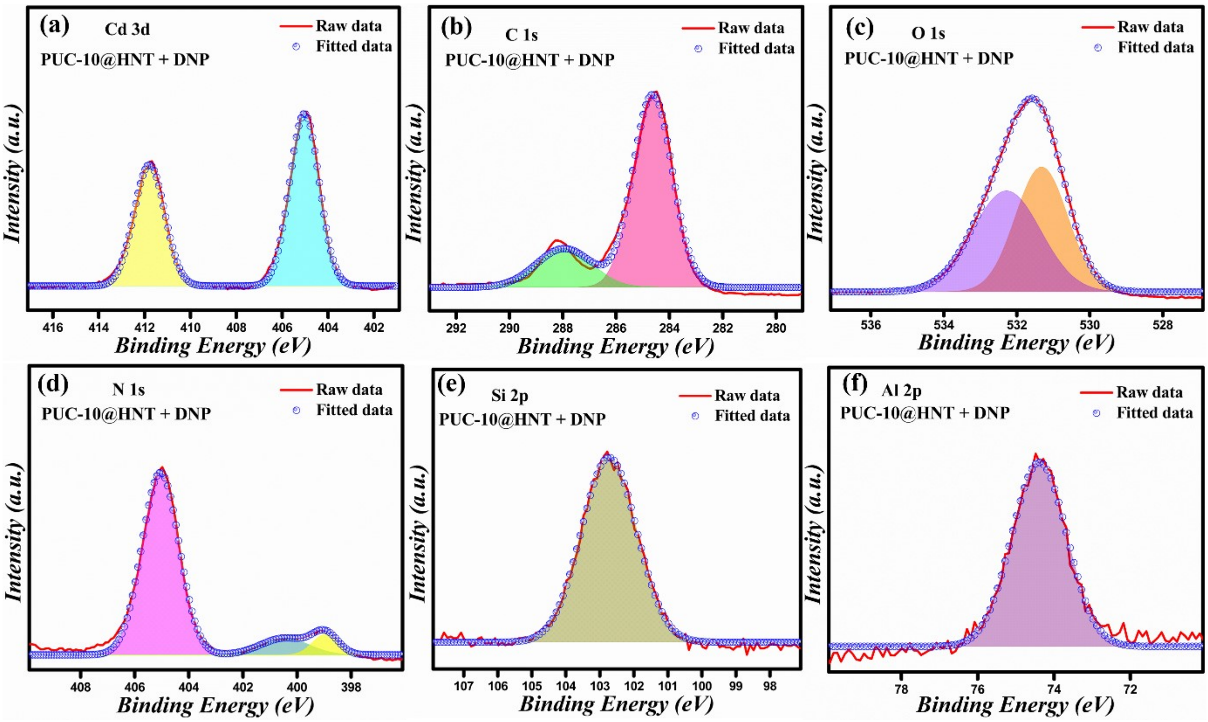

Figure S17. High-resolution XPS spectrum of Cd 3d **(a),** C 1s **(b),** O 1s **(c),** N 1s **(d),** Si 2p **(e)** and Al 2p **(f)** elements present in PUC-10@HNT after treatment with DNP.

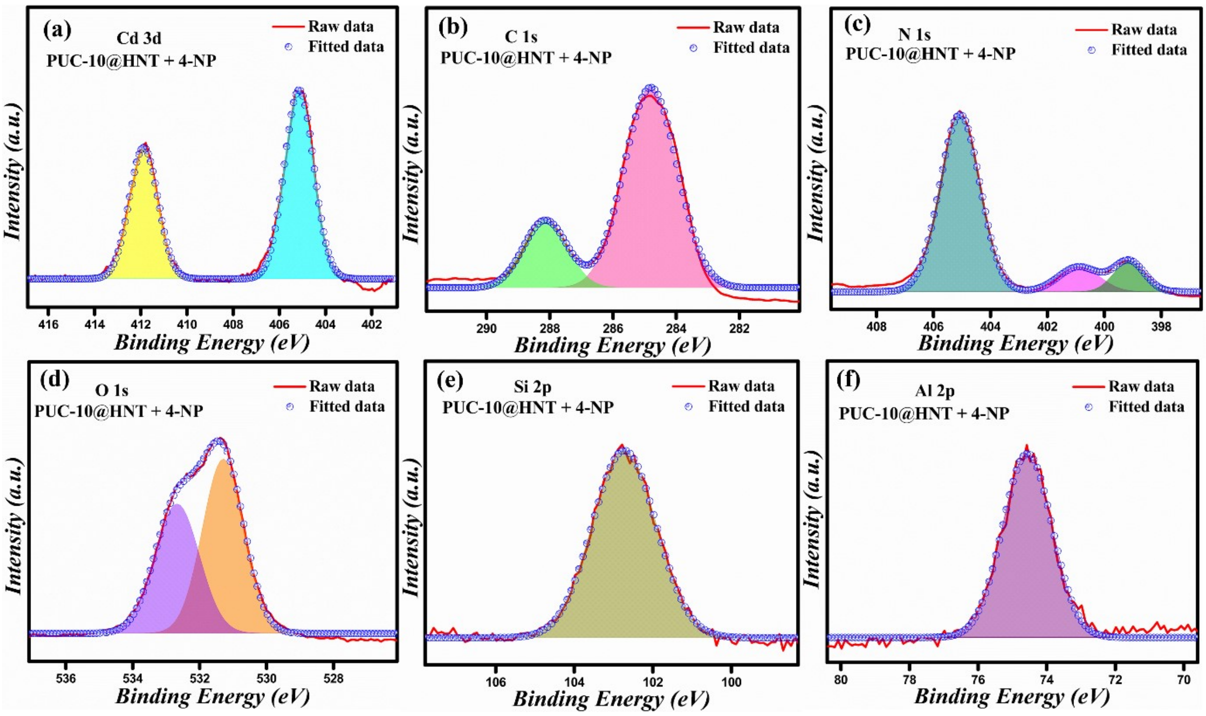

Figure S18. High-resolution XPS spectrum of Cd 3d **(a),** C 1s **(b),** N 1s **(c),** O 1s **(d),** Si 2p **(e)** and Al 2p **(f)** elements present in PUC-10@HNT after treatment with 4-NP.

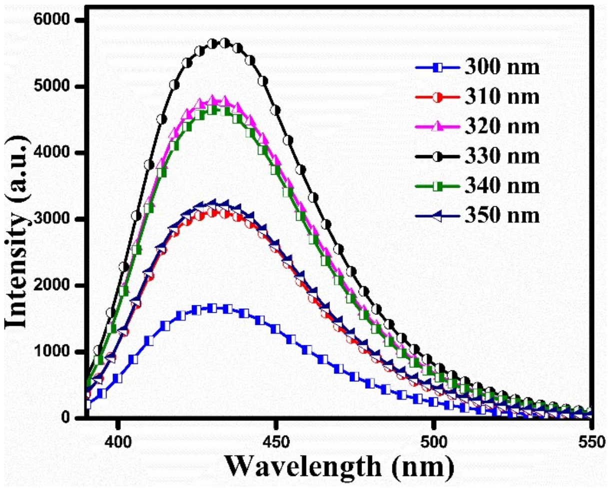

Figure S19. Emission spectra of PUC-10@HNT at different excitation wavelengths ranging from 300 to 350 nm.

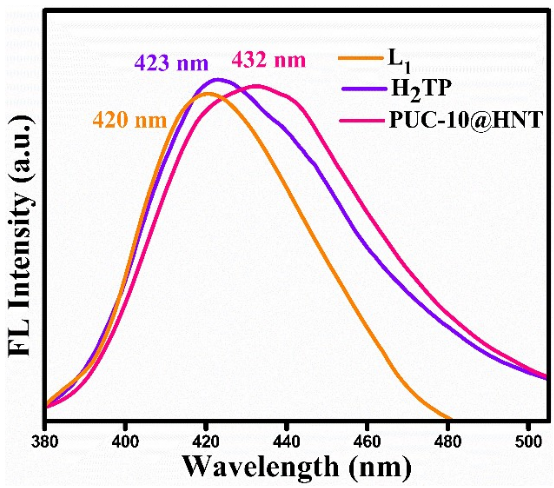

Figure S20. Emission spectra of PUC-10@HNT and both the ligands L_1 and H_2TP used in the synthesis of PUC-10

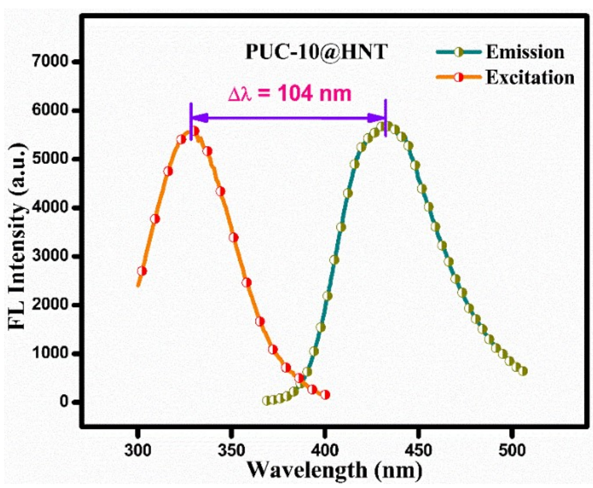

Figure S21. Excitation and emission spectra of PUC-10@HNT.

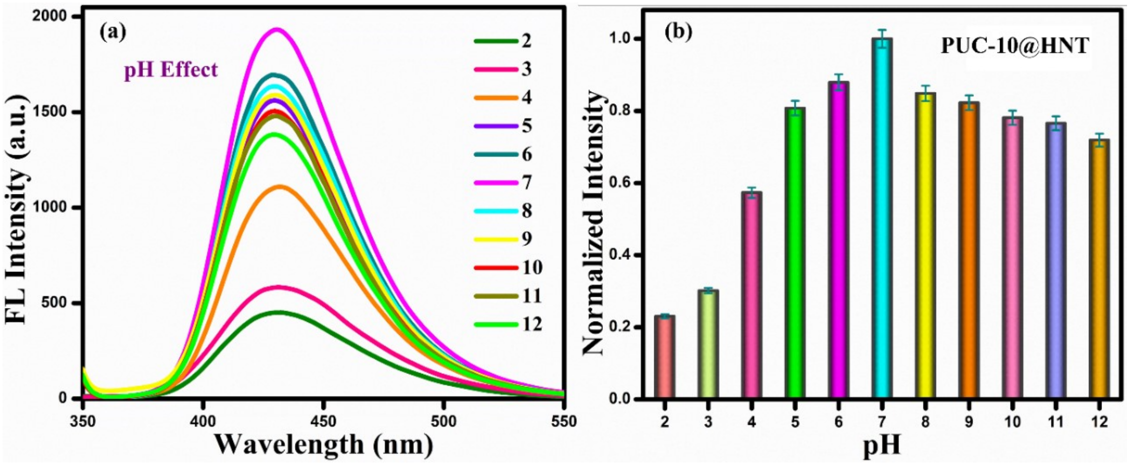

Figure S22. Emission spectra **(a)** and normalized fluorescence intensity **(b)** of PUC-10 at different pH values ranging from 2 to 12.

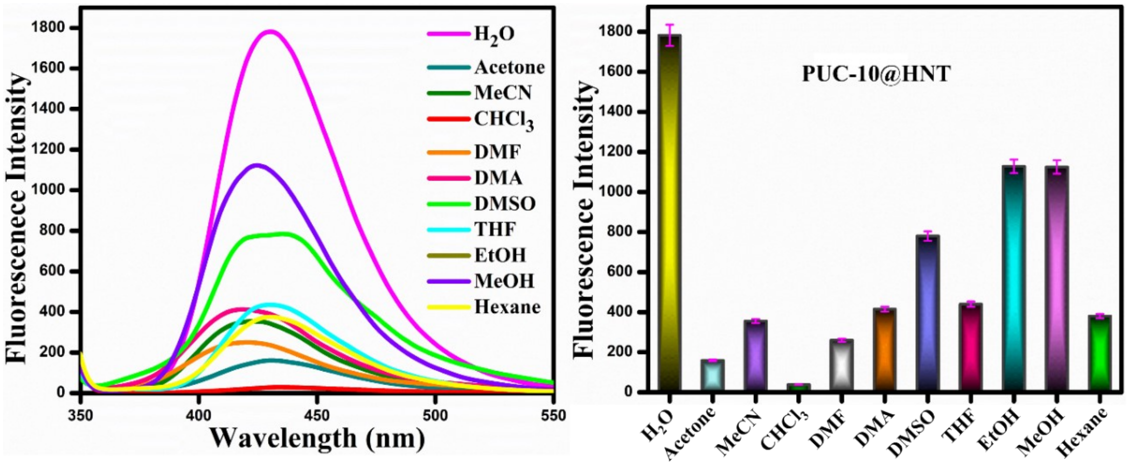

Figure S23. Emission spectra **(a)** and normalized fluorescence intensity **(b)** of PUC-10@HNT in different solvents.

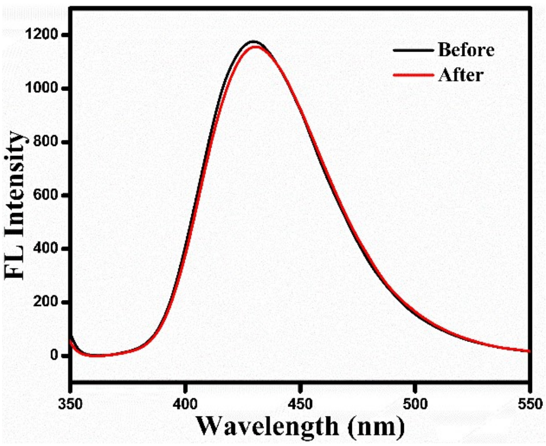

Figure S24. Fluorescenec spectra of PUC-10@HNT before and after constant illumination of light for 3 hr to check the photostability of PUC-10

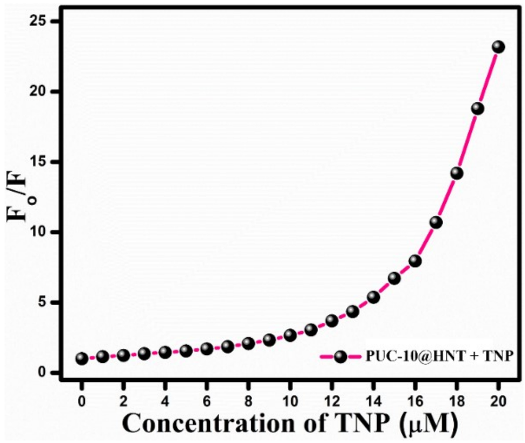

Figure S25. Stern-Volmer plot of PUC-10@HNT in the presence of 0-20 μM concentration of TNP.

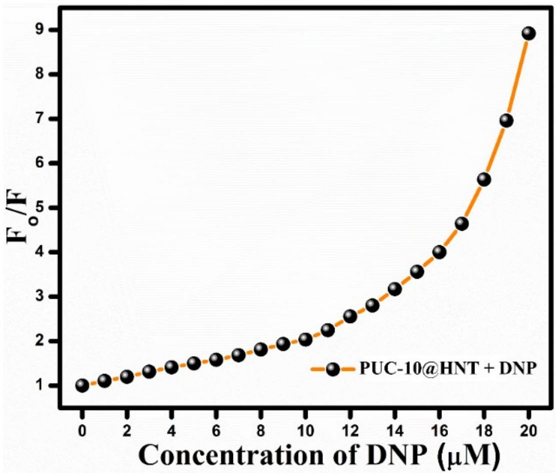

Figure S26. Stern-Volmer plot of PUC-10@HNT in presence of 0-20 μM concentration of DNP.

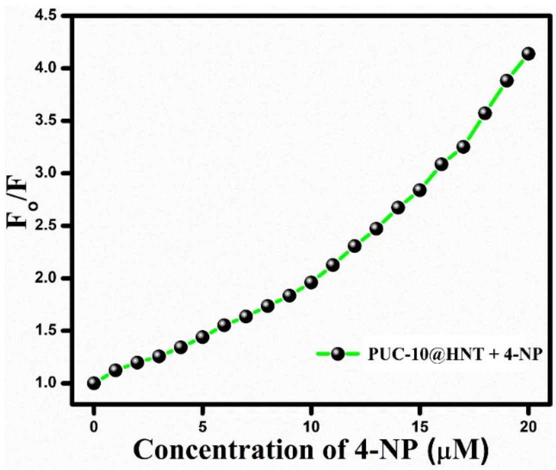

Figure S27. Stern-Volmer plot of PUC-10@HNT in the presence of 0-20 μM concentration of 4-NP.

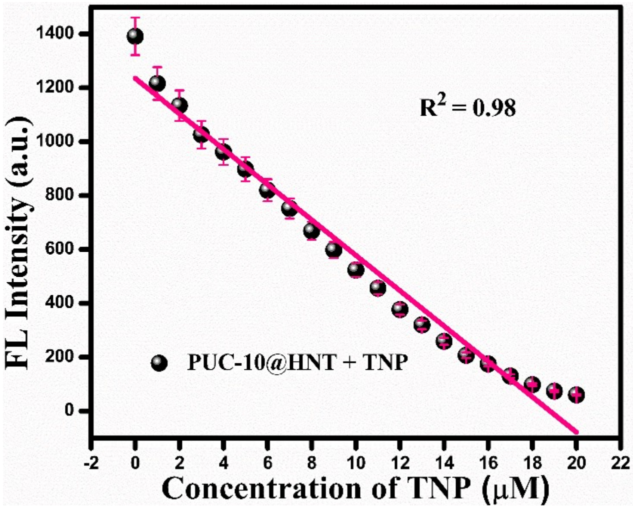

Figure S28. Calibration curve of PUC-10@HNT on addition of TNP (0-20 μM).

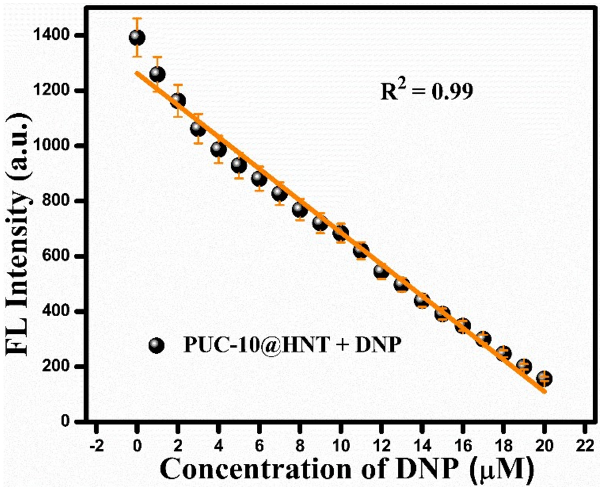

Figure S29. Calibration curve of PUC-10@HNT on the addition of DNP (0-20 μM).

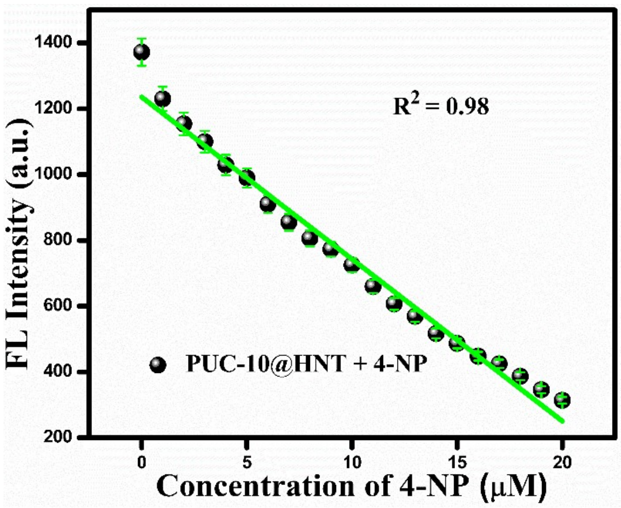

Figure S30. Calibration curve of PUC-10@HNT on the addition of 4-NP (0-20 μM)

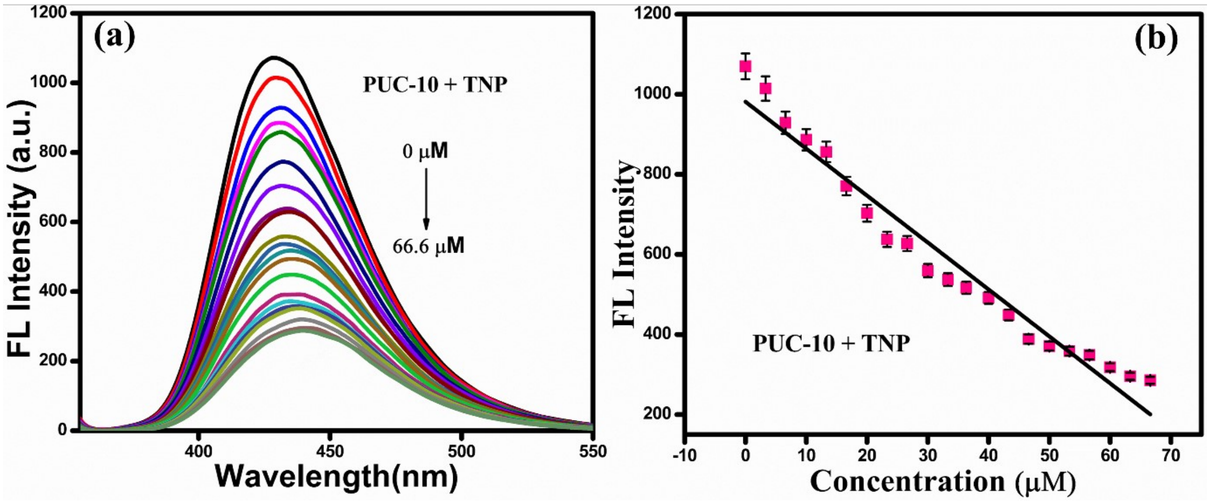

Figure S31. The emission spectrum of PUC-10 before and after incremental addition of TNP from 0 to 66.6 μM concentration **(a)** and its Calibration curve **(b).**

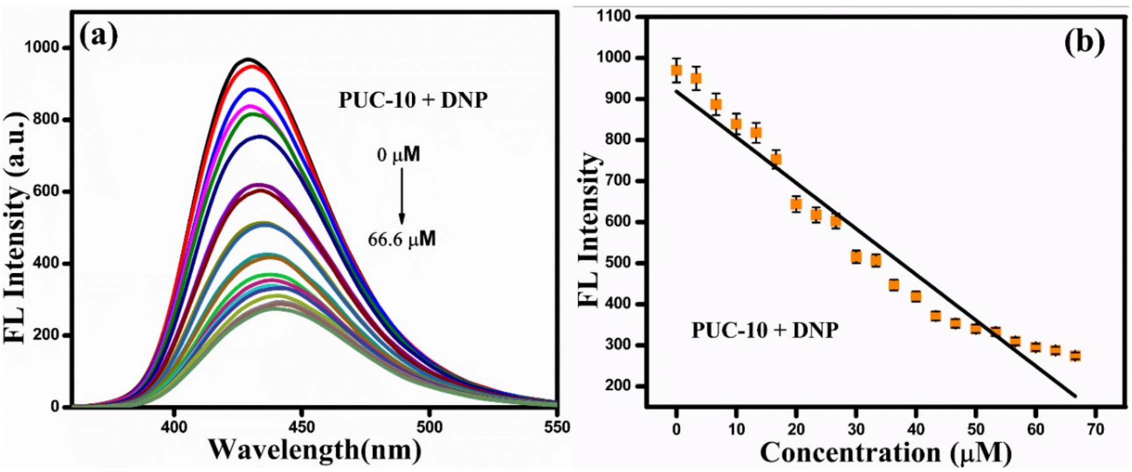

Figure S32. The emission spectrum of PUC-10 before and after incremental addition of DNP from 0 to 66.6 μM concentration **(a)** and its Calibration curve **(b).**

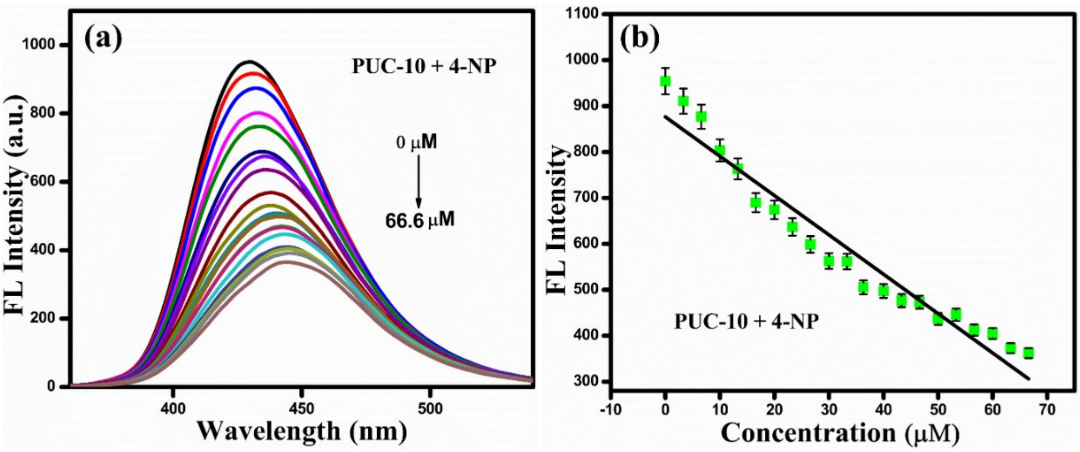

Figure S33. The emission spectrum of PUC-10 before and after incremental addition of 4-NP from 0 to 66.6 μM concentration **(a)** and its Calibration curve **(b).**

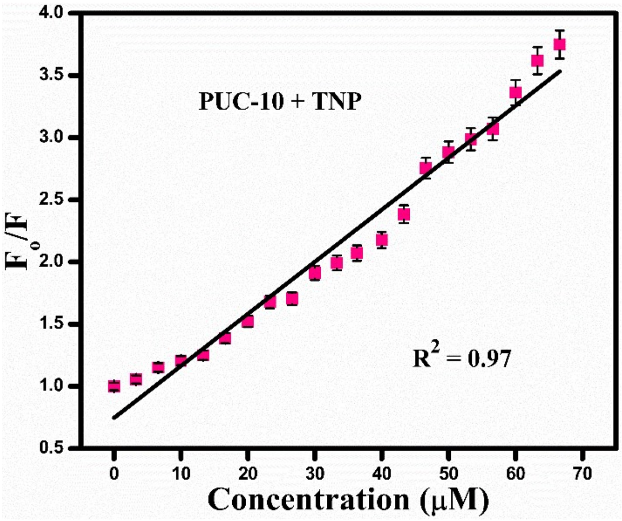

Figure S34. The stern-Volmer plot of PUC-10 in the presence of 0-66.6 μM concentration of TNP.

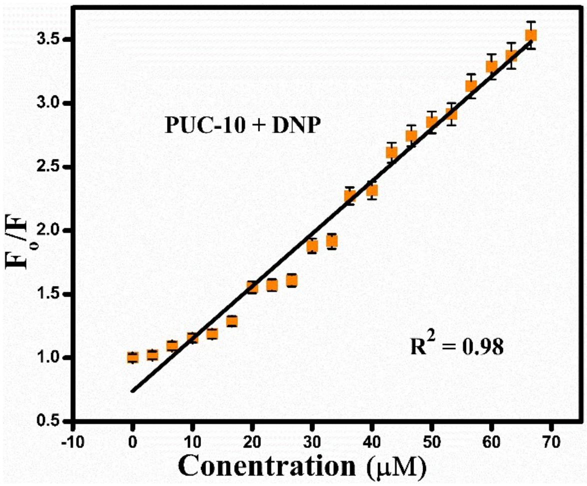

Figure S35. Stern-Volmer plot of PUC-10 in the presence of 0-66.6 μM concentration of DNP.

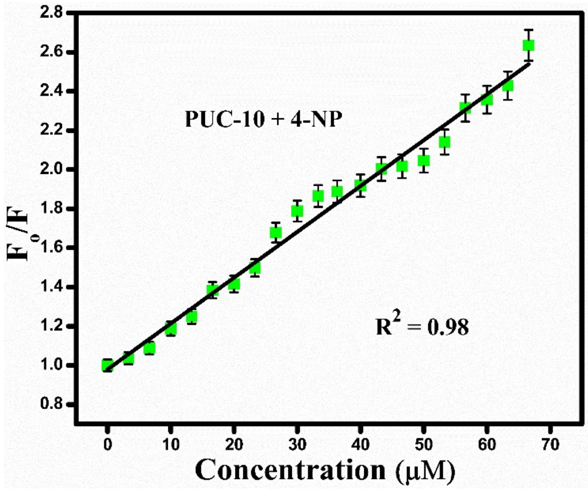

Figure S36. Stern-Volmer plot of PUC-10 in the presence of 0-66.6 μM concentration of 4-NP.

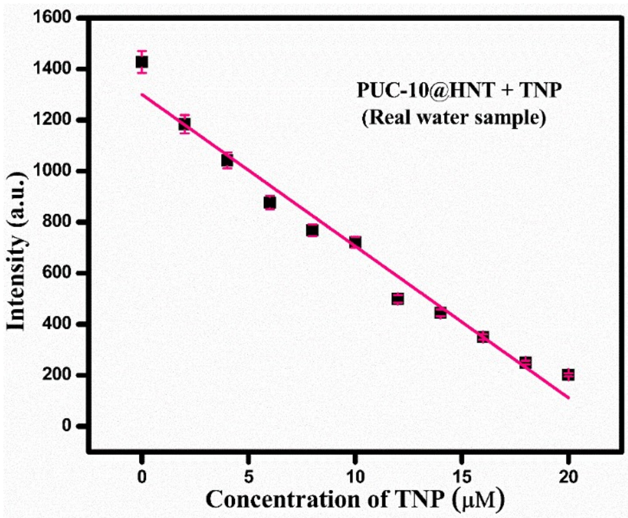

Figure S37. Calibration curve of PUC-10@HNT on addition of TNP (0-20 μM) using real water sample (tap water) as solvent.

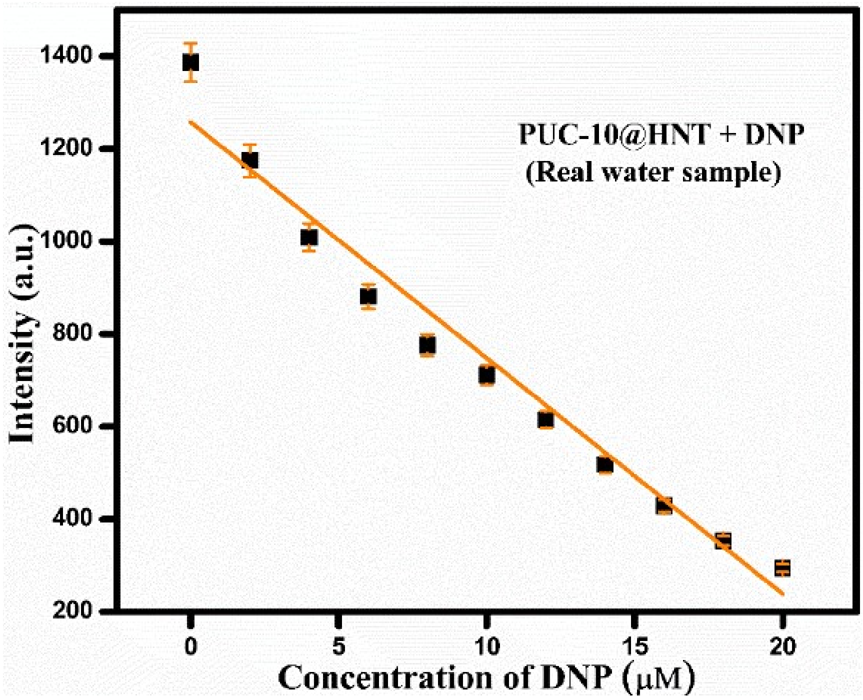

Figure S38. Calibration curve of PUC-10@HNT on the addition of DNP (0-20 μM) using real water sample (tap water) as solvent.

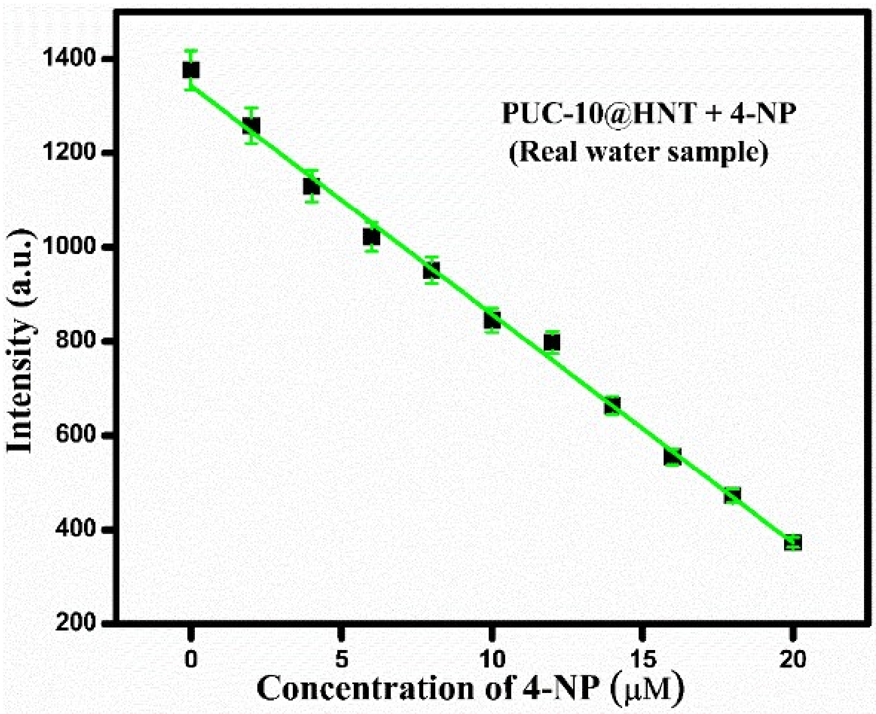

Figure S39. Calibration curve of PUC-10@HNT on the addition of 4-NP (0-20 μM) using real water sample (tap water) as solvent.

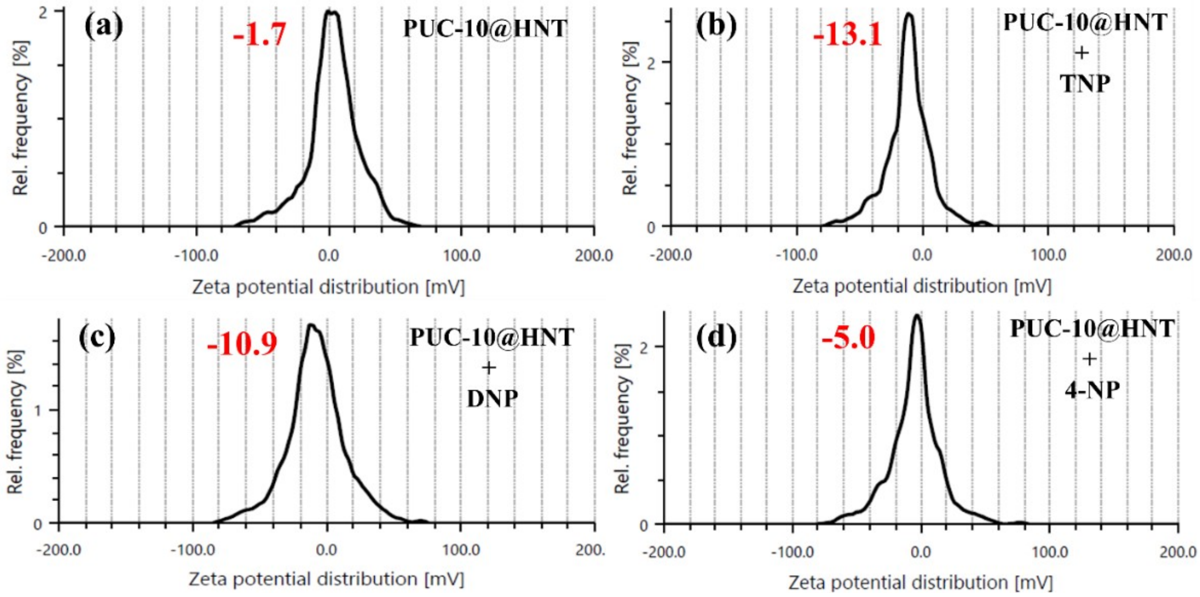

Figure S40. Zeta potential analysis curve of PUC-10@HNT before **(a)** and after the addition of TNP **(b),** DNP **(c)** and 4-NP **(d).**

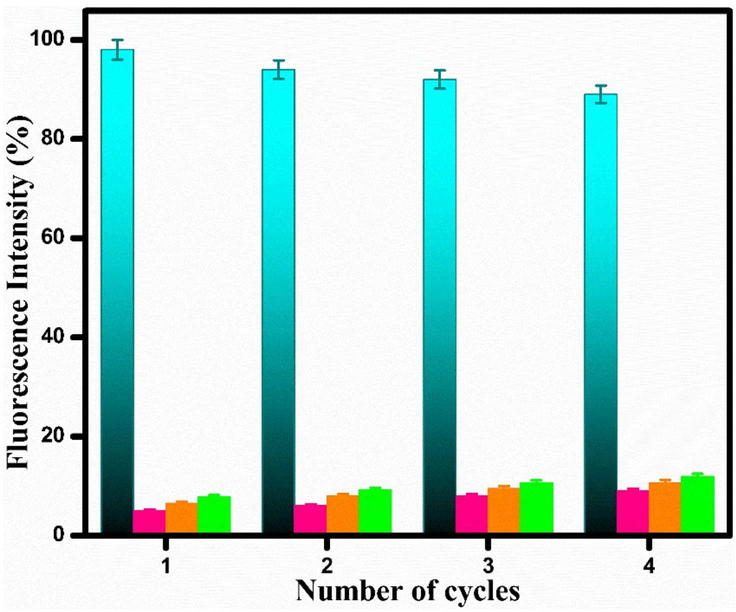

Figure S41. Recyclability of PUC-10@HNT with TNP (pink), DNP (orange) and 4-NP (green).

Table S1. Crystal data and Structure Refinement for **PUC-10.**

Identification Code	PUC-10
CCDC No.	2402328
Empirical formula	$C_{24}H_{21}CdN_5O_9$
Formula weight	635.86 g/mol
Temperature/K	293(2)
Crystal system	monoclinic
Space group	*P2/c*
a/Å	25.1793(9)
b/Å	6.27470(10)
c/Å	20.2026(5)
α/°	90
β/°	103.253(3)
γ/°	90
Volume (Å^3)	3106.85(15)
Z	4
D_{calc} (g/cm^3)	1.359
μ (mm^{-1})	0.754
F(000)	1280.0
Crystal size/mm^3	0.009×0.007×0.006
Radiation	Mo Kα (λ = 0.71073)
Reflections collected	28608
Independent reflections	67474 [R_{int} = 0.056, R_{sigma} =
Data/restraints/parameters	0.0552]
Goodness-of-fit on F^2	6474/6/355
Final R indexes [all data]	0.993

Table S2. Crystallographic features for PUC-10 and PUC-10@HNT.

	PUC-10				**PUC-10@HNT**			
Reflection number	**2θ**	**Miller Indices**	**FWHM (β)**	**Crystallite size (nm)**	**2θ**	**Miller Indices**	**FWHM (β)**	**Crystallite size (nm)**
1	7.186	(200)	0.09722	81.87549	7.186	(200)	0.19658	40.49209
2	10.769	(002)	0.11645	68.52297	10.769	(002)	0.20292	39.32338
3	17.986	(012)	0.13158	61.12753	17.986	(012)	0.21325	37.71705
4	21.621	(600)	0.13435	60.19966	21.621	(600)	0.1904	42.47807
5	25.275	(700)	0.14954	54.44381	25.275	(700)	0.19868	40.97809
	Average size = 65.2290 nm				Average size = 40.19773 nm			

Table S3. Compositional ratios of all the elements present in PUC-10 and PUC-10@HNT

Sample	**Cd (at%)**	**O (at%)**	**N (at%)**	**C (at%)**	**Si (at%)**	**Al (at%)**
PUC-10	2.11	17.21	25.59	55.09	-	-
PUC-10@HNT	2.01	18.81	20.72	56.12	2.47	0.5