Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Ratiometric chemosensor for differentiation of TNP from other NACs by distinct blue fluorescence and visualization of latent fingerprints

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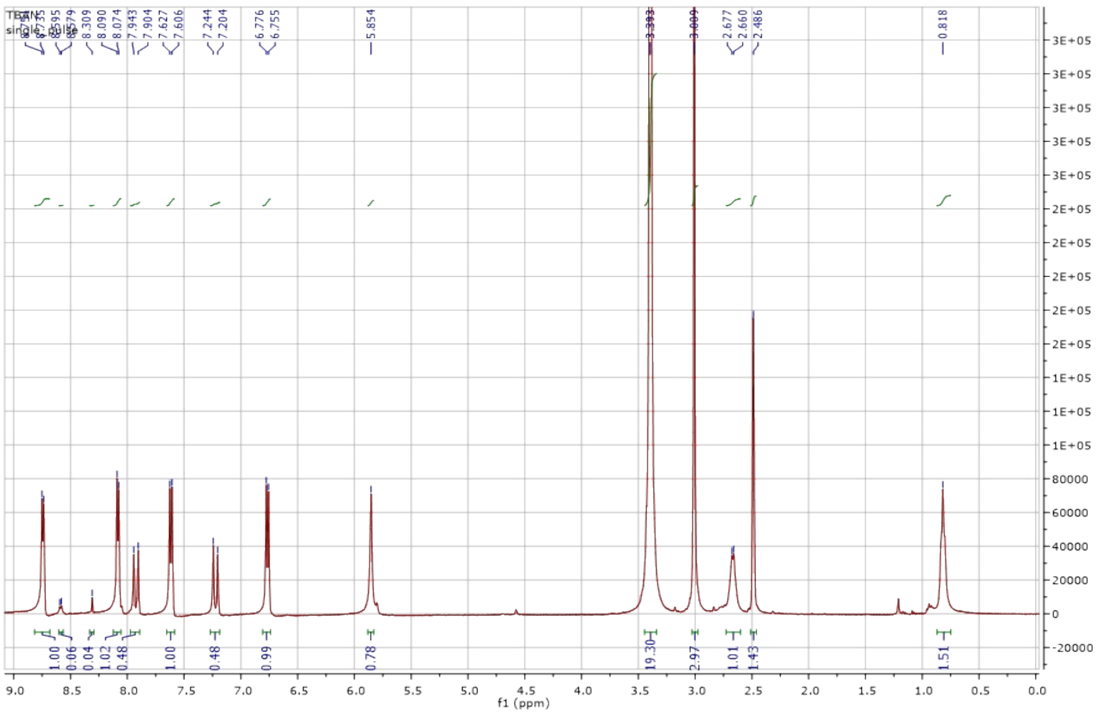

Figure S1: ^{1}H NMR spectrum of **DMAS-TP**

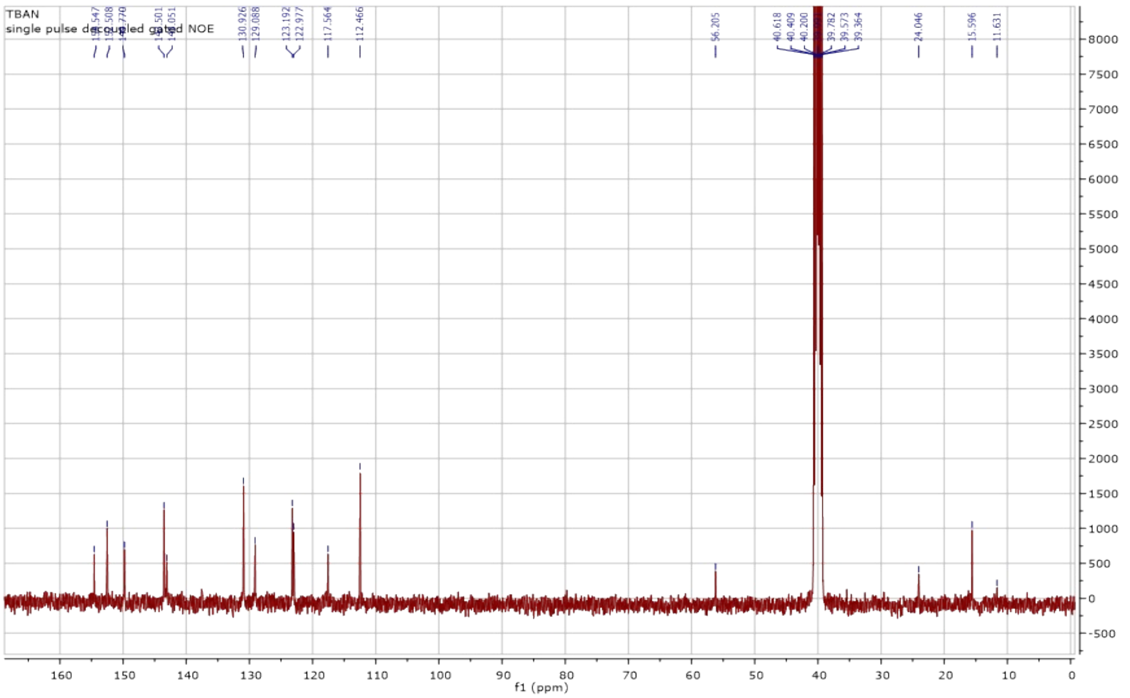

Figure S2: ^{13}C NMR spectrum of **DMAS-TP**

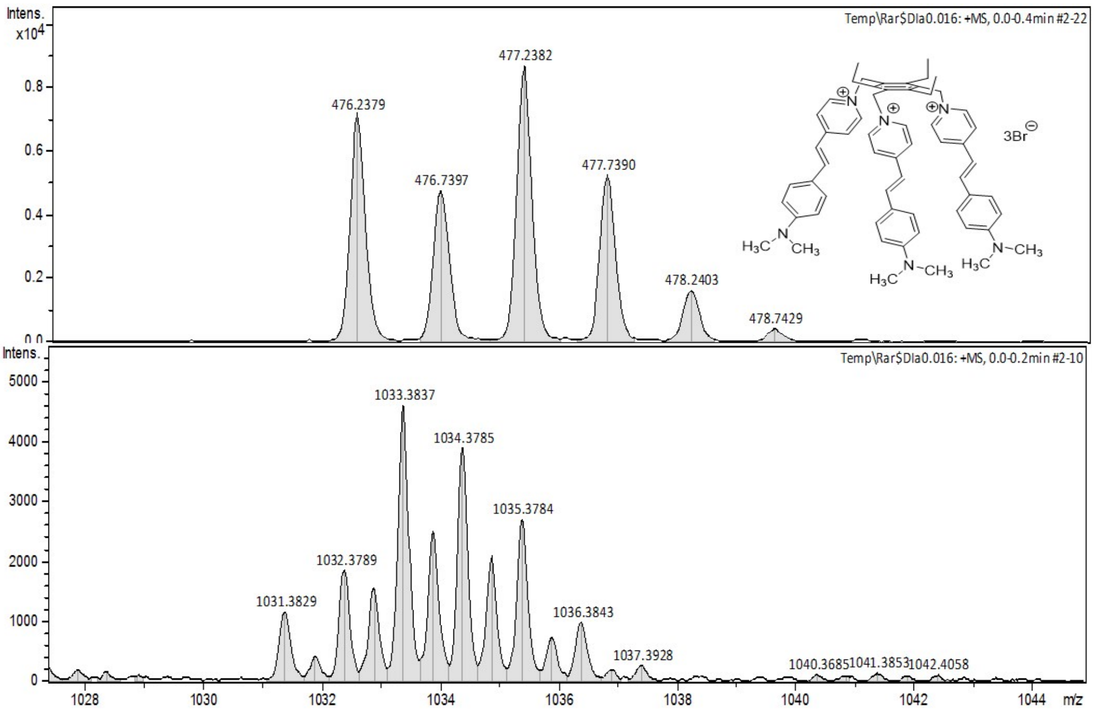

Figure S3: HRMS spectrum of **DMAS-TP**

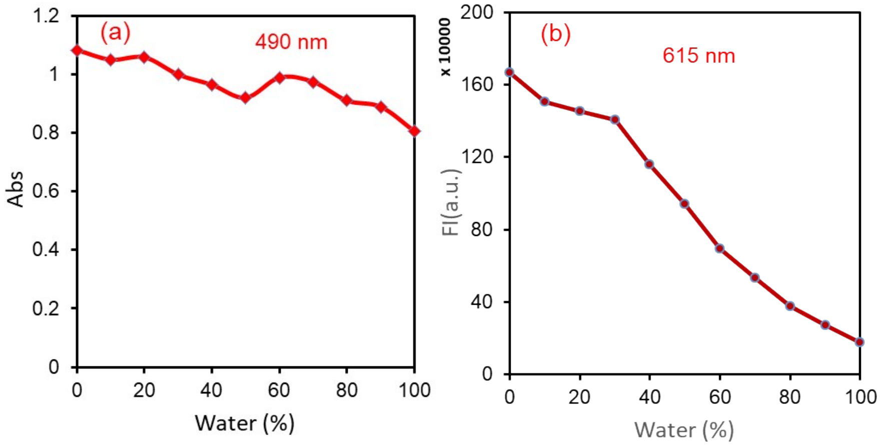

Figure S4: Change in (a) UV-Vis absorbance and (b) fluorescence intensity of **DMAS-TP** with increasing amounts of HEPES fraction.

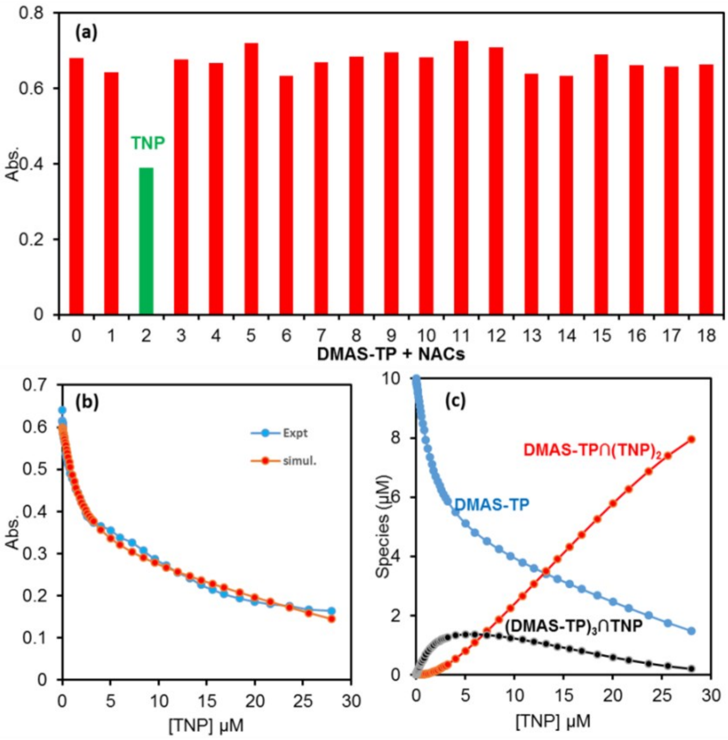

Figure S5: (a) The effect of NACs on the absorbance of DMAS-TP; NACs 0 = DMAS-TP; 1 = 2,4,6-trinitrotoluene; 2 = 2,4,6-trinitrophenol; 3 = aniline; 4 = 1-chloro-3-nitroaniline; 5 = 2-nitroaniline; 6 = 2,4-dinitroaniline; 7 = 4-nitrophenol; 8 = 1-chloro-4-nitrophenol; 9 = 1-chloro-2,4-dinitrobenzene; 10 = 1-chloro-2-nitrobenzene; 11 = 2-nitrophenol; 12 = 4-nitrophenol; 13 = 1-methyl-2-nitrobenzene; 14 = 2,4-dinitotoluene; 15 = 4-nitrobenzaldehyde; 16 = 2-nitrobenzaldehyde; 17 = 3,5-dintrobenzoic acid; 18 = 2,6-dinitrotoluene; (b-c) the formation of different stoichiometric species of DMAS-TP with [TNP]

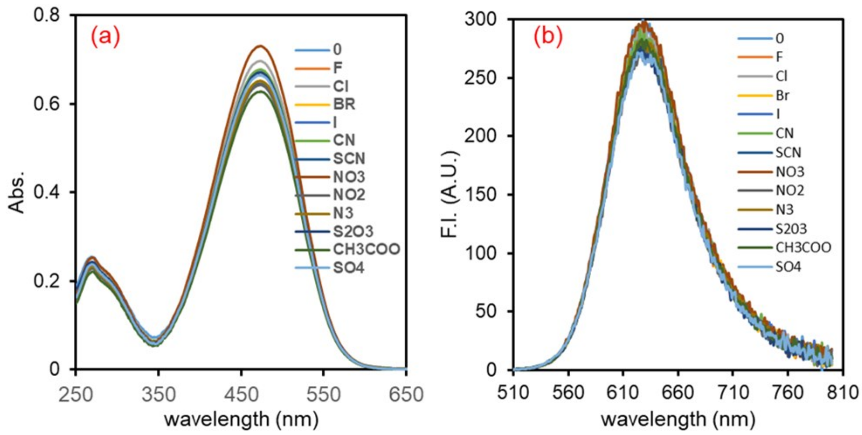

Figure S6: Effect of different inorganic anions (10 equivalents) on the (a) absorption and (b) fluorescence spectrum of **DMAS-TP**.

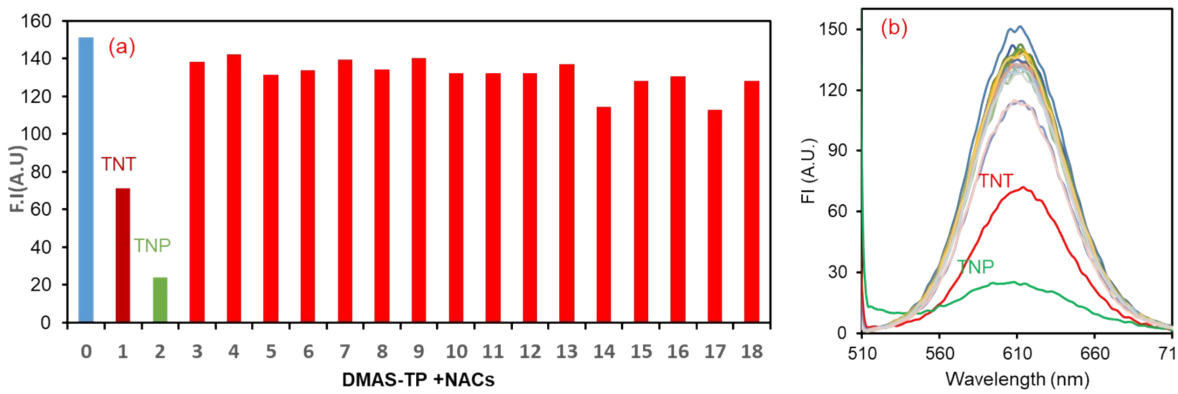

Figure S7: The effect of different NACs on the fluorescence intensity of **DMAS-TP** (10 µM, HEPES buffer pH 7.4, 0.1% DMSO). NACs 0 = DMAS-TP; 1 = 2,4,6-trinitrotoluene; 2 = 2,4,6-trinitrophenol; 3 = aniline; 4 = 1-chloro-3-nitroaniline; 5 = 2-nitroaniline; 6 = 2,4-dinitroaniline; 7 = 4-nitrophenol; 8 = 1-chloro-4-nitrophenol; 9 = 1-chloro-2,4-dinitrobenzene; 10 = 1-chloro-2-nitrobenzene; 11 = 2-nitrophenol; 12 = 4-nitrophenol; 13 = 1-methyl-2-nitrobenzene; 14 = 2,4-dinitotoluene; 15 = 4-nitrobenzaldehyde; 16 = 2-nitrobenzaldehyde; 17 = 3,5-dintrobenzoic acid; 18 = 2,6-dinitrotoluene; (a) fluorescence intensity; (b) fluorescence spectra (showing increase in fluorescence intensity between 510-540 nm only in case of TNP)

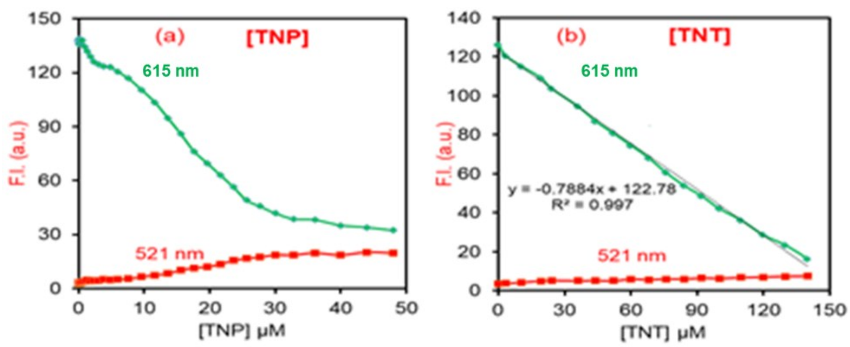

Figure S8: Plot of change in the fluorescence intensity of **DMAS-TP** at 615 nm and 521 nm (a) on gradual addition of TNP and (b) on gradual addition of TNT

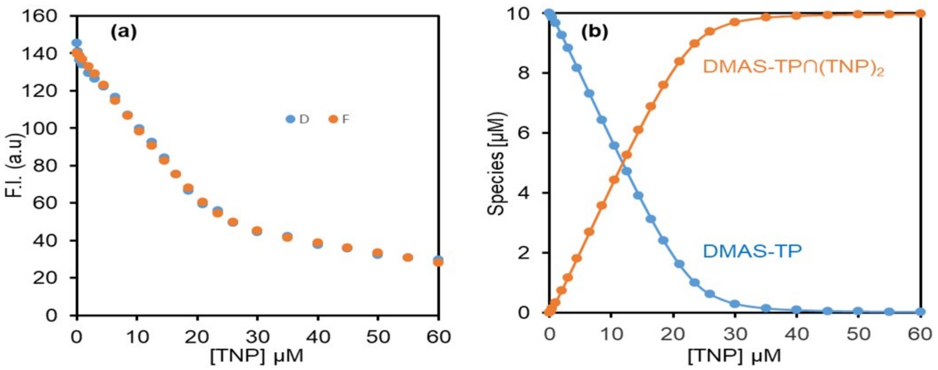

Figure S9: (a) The fit model for the titration of **DMAS-TP** with TNP; (b) The stoichiometric formation of **DMAS-TP∩(TNP)$_2$**

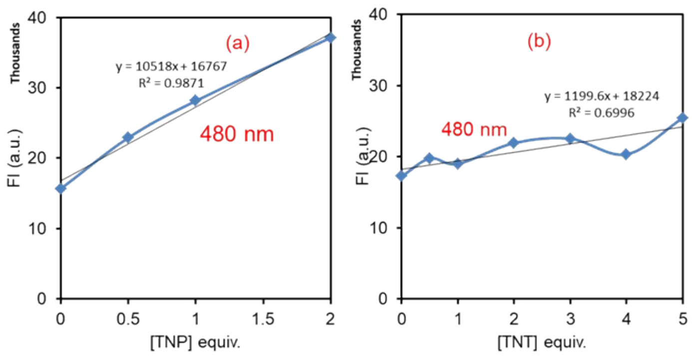

Figure S10: Change in fluorescence intensity at 480 nm on titration of **DMAS-TP** with (a) TNP and (b) with TNT using excitation wavelength 390 nm.

Table S1: the comparison table of DMAS-TP with other fluorescence probes

Publication	**Fluorophore**	**solvent**	**λ_{em} (nm)**	**LOD FL**	**λ_{abs} (nm)**	**LOD abs**	**Paper strip**
Present	Single molecule	Water	615	2 nM	490	20 nM	Turn-ON
ACS Appl. Mater. Interfaces 2018, 10, 27260–27268	polymer	95 % water	501-520	473 nM	430	---	quenching
Analyst, 2019,144, 3620-3634	Single molecule	water	400-480	6000 nM	374	--	quenching
J. Mater. Chem. C, 2020,8, 8257-8267	Single molecule	H_2O/THF (9/1)	635	61.4 nM	---	---	quenching
Anal. Chem. 2019, 91, 13244–13250	Single molecule	DMSO	530	63 nM	---	no	
Dyes and Pigments, 2018, 156, 307-317.	Single molecule	water	480	0.0001 nM	340	---	quenching

RSC Adv., 2018, 8, 31658–31665	Single molecule	methanol	420 to 586	820 nM,	500	---	quenching
Sensors & Actuators: B. Chemical 280 (2019) 298–305	Single molecule	CH_3CN	550	----	520	--	---
Sensors and Actuators B 231 (2016) 293–301	Single molecule	PBS–DMSO (99.5:0.5)	494	10 nM	336	----	quenching
Sensors and Actuators B 265 (2018) 476–487	Single molecule	EtOH	518	77.5 nM	365	----	quenching
Inorg. Chem. 2019, 58, 8198–8207	MOF	EtOH	480-580	7.2 nM	380	---	---
ACS Sustainable Chem. Eng. 2019, 7, 819–830	MOF 1	aqueous suspension	437, 637	40 nM	333	--	-----

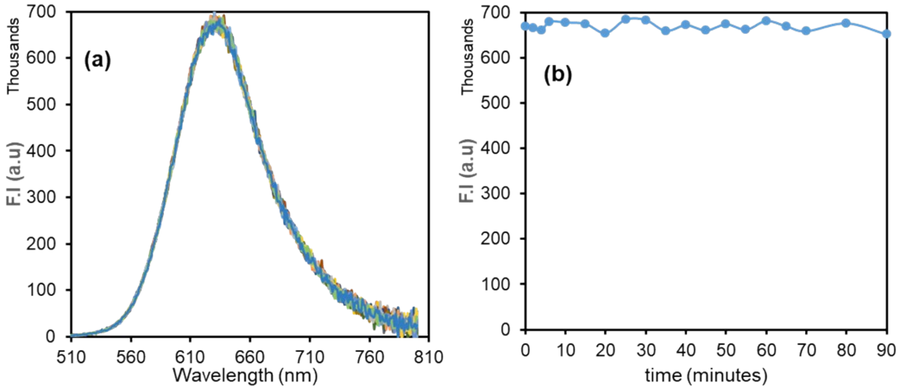

Figure **S11**- Effect of 300W xenon lamp on (a) fluorescence spectrum and (b) fluorescence intensity of **DMAS-TP** with increasing time.

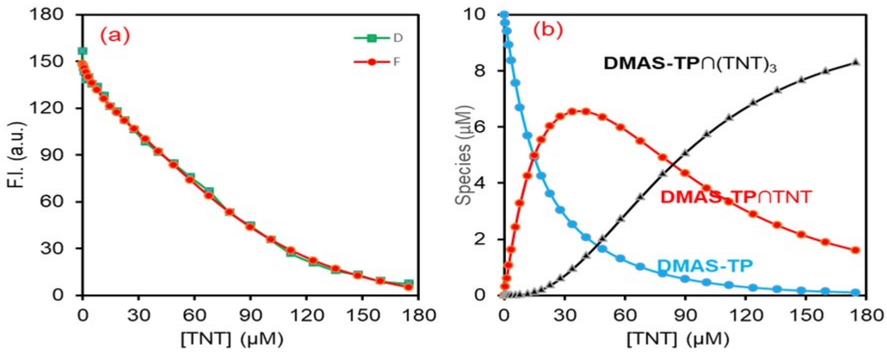

Figure S12: (a) The fit model for the titration of **DMAS-TP** with TNT; (b) The stoichiometric formation of **DMAS-TP∩TNT** and **DMAS-TP∩(TNT)$_3$**

Table S2. The electronic excitation wavelength (nm), oscillator strengths and

compositions of the low-lying singlet excited states of the DMAS-TP-B and its complex DMAS-TP-B∩$(TNP)_2$				
Symmetry	**λ (nm)**	**f**	**Contributing orbitals (%)**	**Natural transition orbitals (occupancy)**
			DMAS-TP-B	
Singlet-A	**479.7**	**0.8457**	**H-2→LUMO (46 %)**	**HONTO→LUNTO (51 %)**
			H-1→L+1 (40 %)	**HONTO-1→LUNTO+1 (45 %)**
Singlet-A	**475.8**	**4.055**	**HOMO→L+2 (67 %)**	**HONTO→LUNTO (72 %)**
			H-1→L+1 (16 %)	**HONTO-1→LUNTO+1 (17 %)**
			DMAS-TP-B∩$(TNP)_2$	
Singlet-A	**478.6**	**1.5865**	**H-1→L+2 (91 %)**	**HONTO→LUNTO (96 %)**
Singlet-A	**378.3**	**2.4512**	**H-8→L+1 (79 %)**	**HONTO→LUNTO (85 %)**

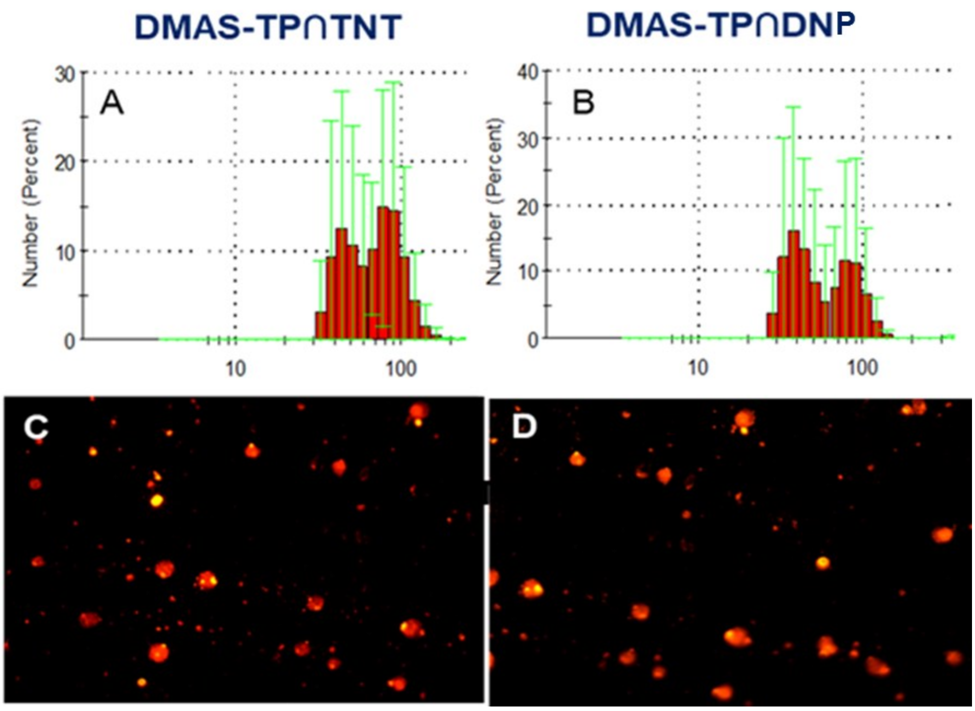

Figure S13: (A,B) DLS studies in water (0.1% DMSO) (A) **DMAS-TP** and TNT solution; (B) **DMAS-TP** and DNP solution (C, D) thin films using fluorescence microscopic (C) **DMAS-TP** and TNT (5 equiv.); (D) **DMAS-TP** and DNP (5 equiv.) solution

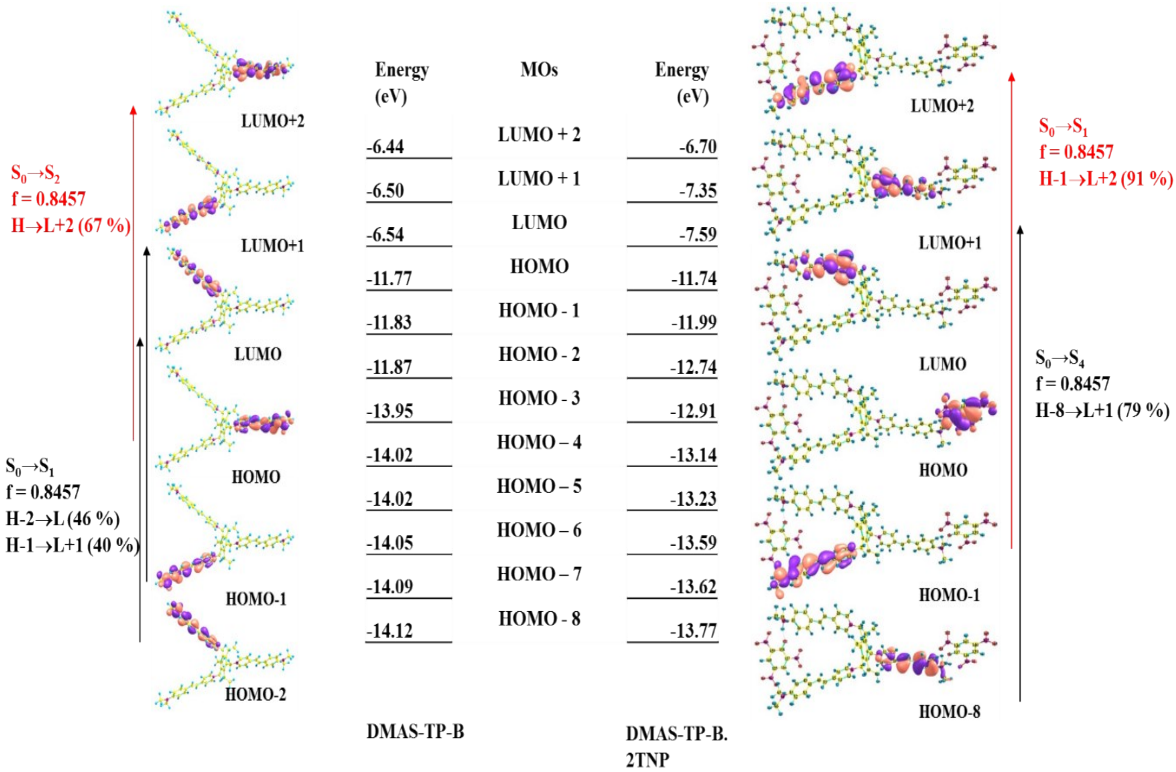

Figure S14. MOs of **DMAS-TP**-B and **DMAS-TP-B.2TNPs**

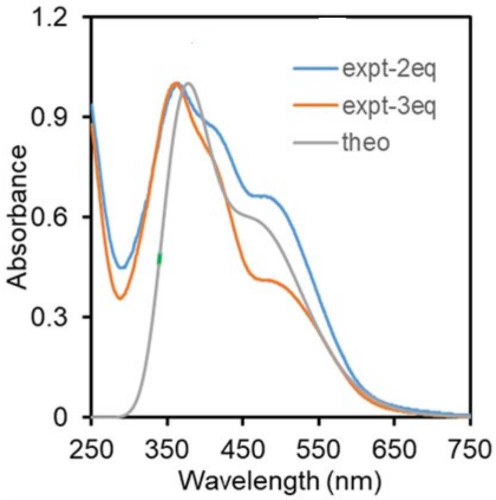

Figure S15: The comparison of UV-Vis spectrum obtained theoretically from optimized structures of **DMAS-TP∩(TNP)$_2$** with those found from addition of 2 and 3 equivalents of TNP to the solution of **DMAS-TP**