

Dynamic fluorescence quenching by 2,4,6-trinitrophenol in voids of aggregation induced emission based fluorescent probe

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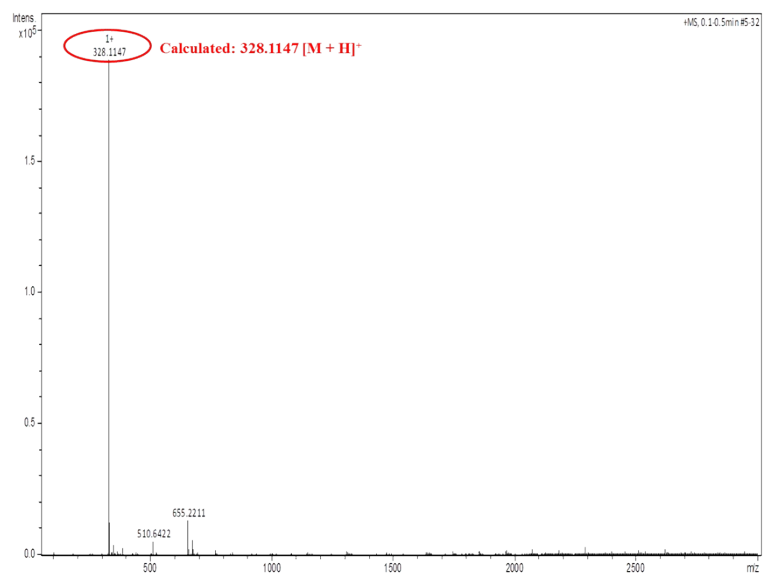
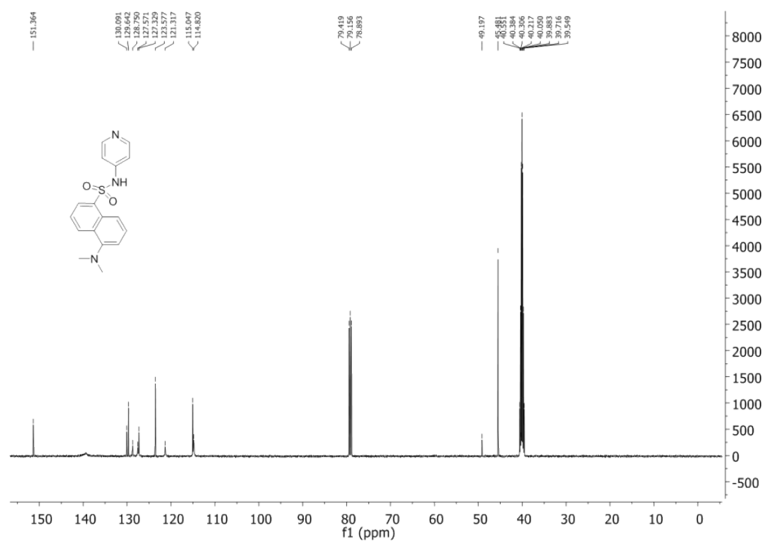
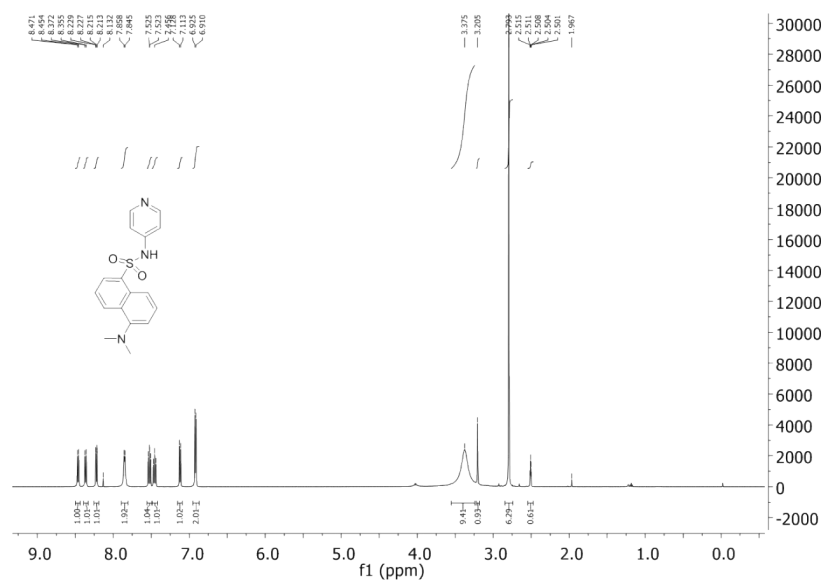


Figure SI 1: ^1H , ^{13}C NMR and HRMS spectra of 4-(dansylamino)pyridine

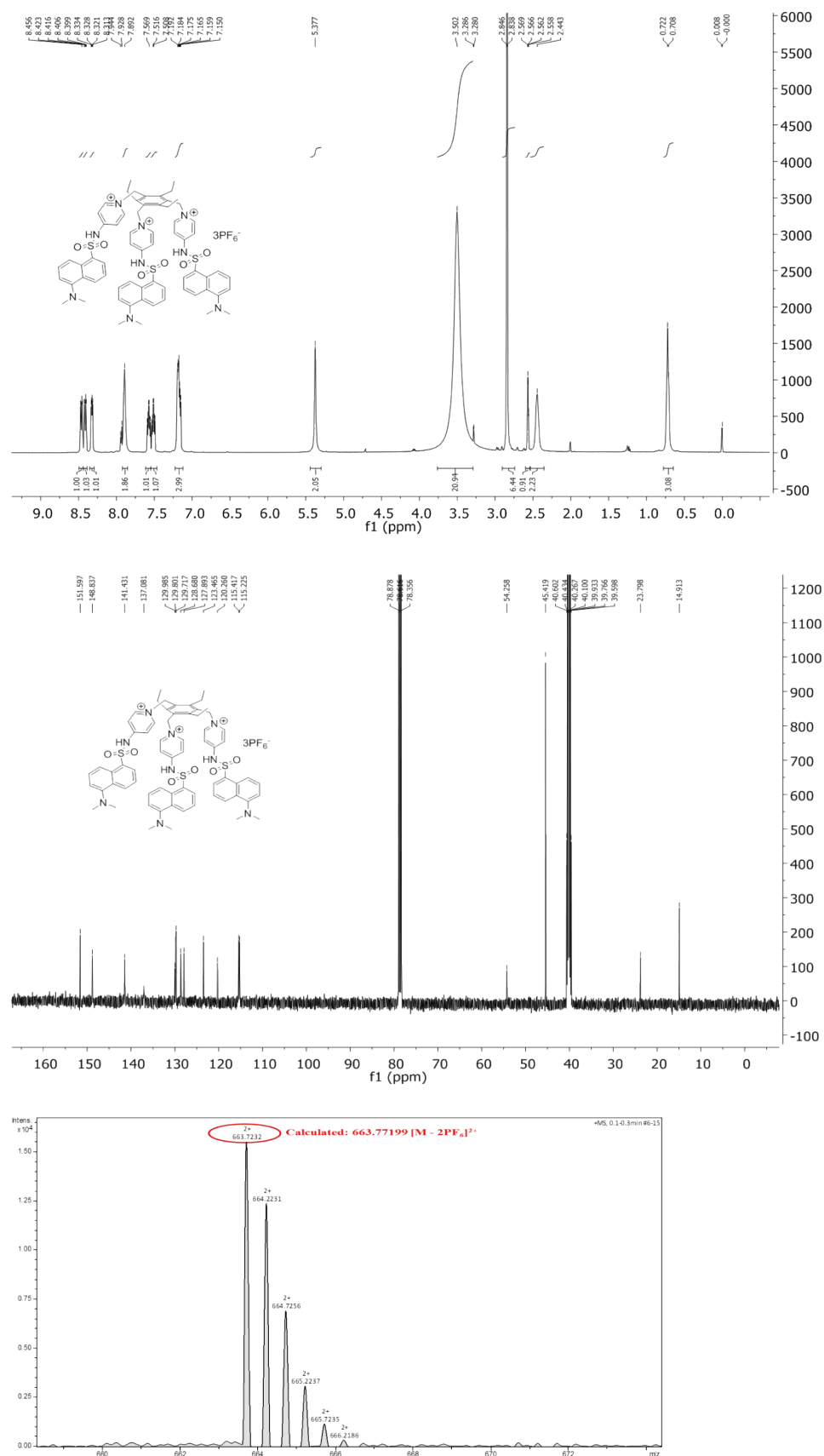


Figure SI 2: ^1H , ^{13}C NMR and HRMS spectra of PY-DNS

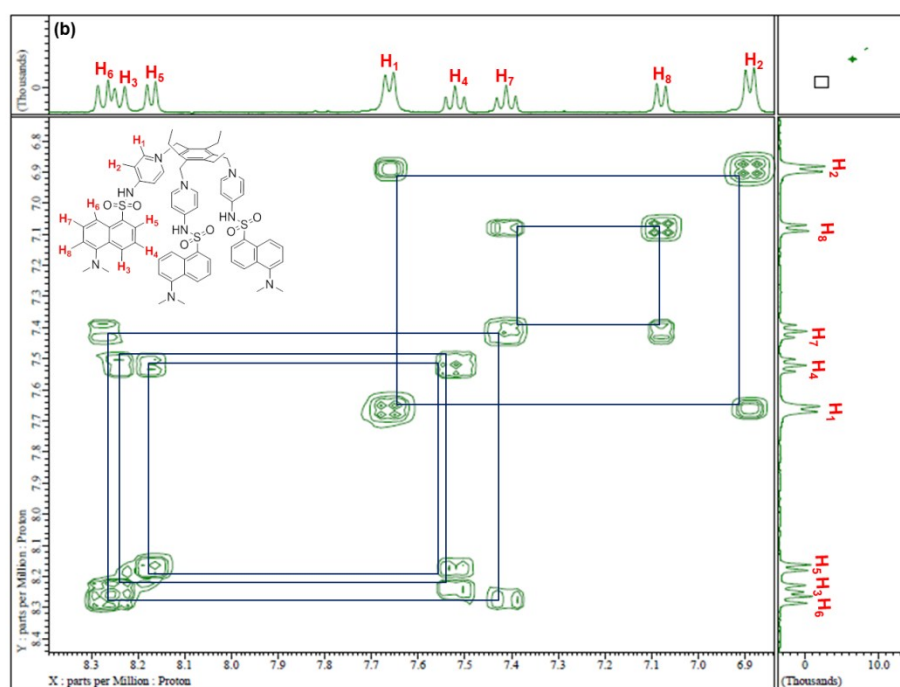


Figure SI 3: Partial COSY spectrum of **PY-DNS** showing cross peaks and assigned signals

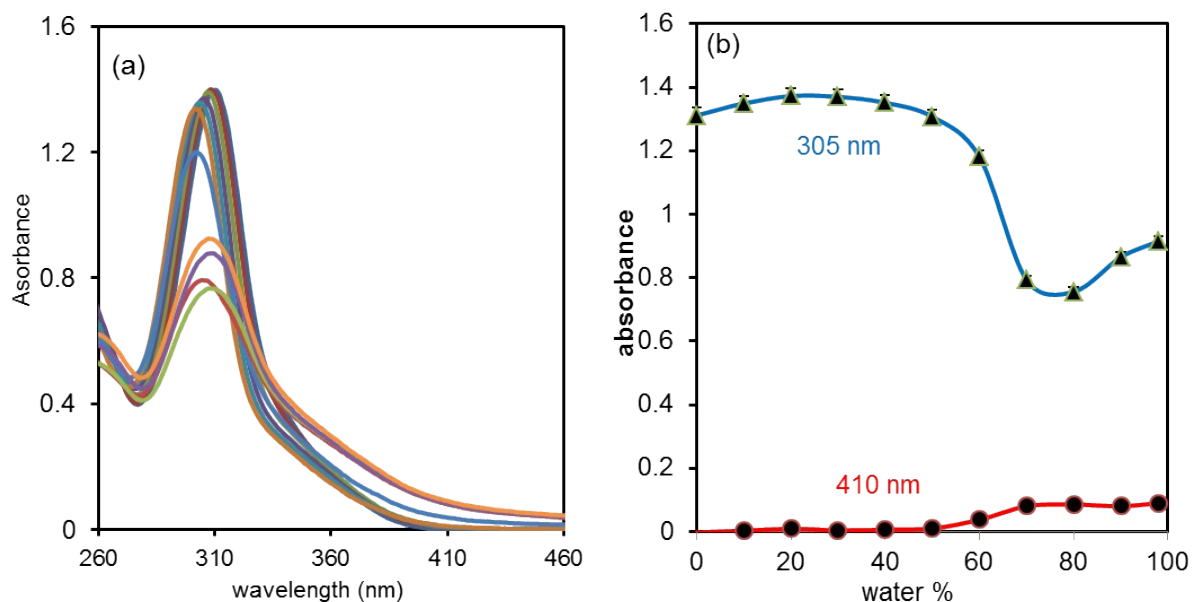


Figure SI 4. (a) The UV-Vis spectra of **PY-DNS** (1 μM) in DMSO-water binary mixtures; (b) The effect of water ratio on the absorbance of **PY-DNS** at 305 and 410 nm (error bar showing $<2\%$ error).

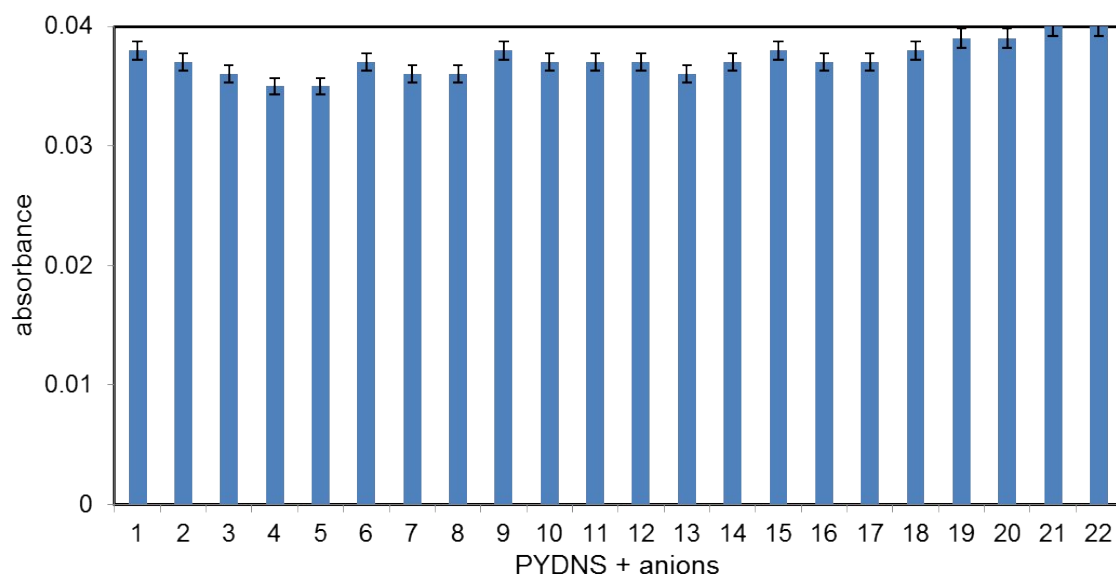


Figure SI 5: Effect of addition of various anions (6 μM) on the UV-Vis spectrum of solution of PYDNS (0.3 μM , H_2O -DMSO 98:2) 1 = PYDNS, 2 = PYDNS + F^- , 3 = PYDNS + Cl^- , 4 = PYDNS + Br^- , 5 = PYDNS + I^- , 6 = PYDNS + CN^- , 7 = PYDNS + SCN^- , 8 = PYDNS + OH^- , 9 = PYDNS + CH_3COO^- , 10 = PYDNS + NO_3^- , 11 = PYDNS + HSO_4^- , 12 = PYDNS + ClO_4^- , 13 = PYDNS + HPO_4^{2-} , 14 = PYDNS + H_2PO_4^- , 15 = PYDNS + SO_4^{2-} , 16 = PYDNS + $\text{CH}_3(\text{CH}_2)_2\text{COO}^-$, 17 = PYDNS + $\text{CH}_3(\text{CH}_2)_8\text{COO}^-$, 18 = PYDNS + $\text{CH}_3(\text{CH}_2)_{12}\text{COO}^-$, 19 = PYDNS + $\text{CH}_3(\text{CH}_2)_{11}\text{SO}_3^-$, 20 = PYDNS + Cholesterol-sulfate, 21 = PYDNS + $\text{CH}_3(\text{CH}_2)_{11}\text{O-SO}_3^-$, 22 = PYDNS + dodecylbenzene sulfonate (error bar showing $\sim 2\%$ error).

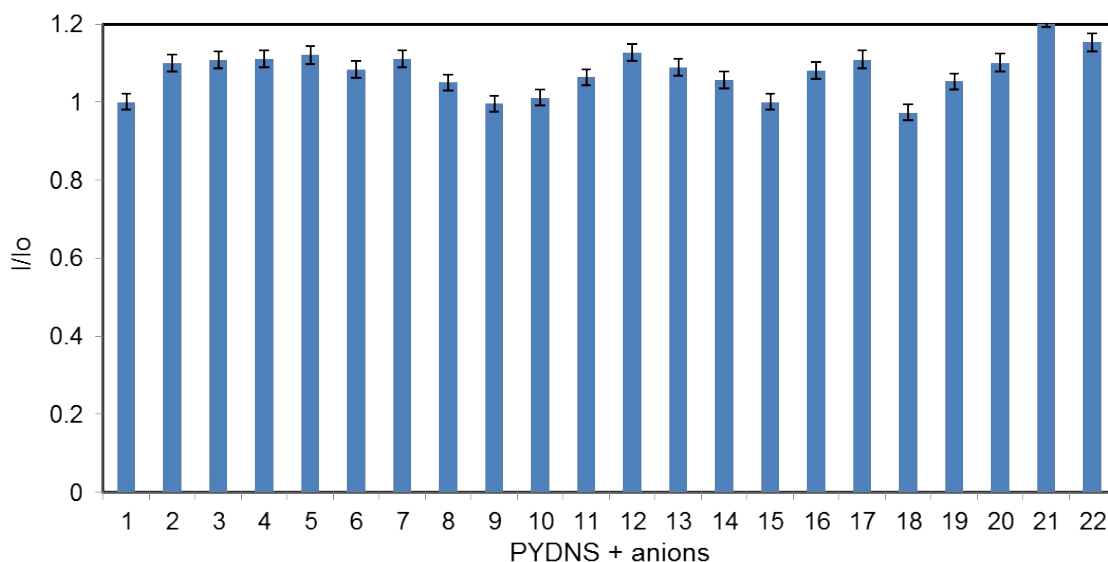


Figure SI 6: Effect of addition of various anions (6 μM) on the fluorescence intensity of solution of PYDNS (0.3 μM , H_2O -DMSO 98:2) 1 = PYDNS, 2 = PYDNS + F^- , 3 = PYDNS + Cl^- , 4 = PYDNS + Br^- , 5 = PYDNS + I^- , 6 = PYDNS + CN^- , 7 = PYDNS + SCN^- , 8 = PYDNS + OH^- , 9 = PYDNS + CH_3COO^- , 10 = PYDNS + NO_3^- , 11 = PYDNS + HSO_4^- , 12 = PYDNS + ClO_4^- , 13 = PYDNS + HPO_4^{2-} , 14 = PYDNS + H_2PO_4^- , 15 = PYDNS + SO_4^{2-} , 16 = PYDNS + $\text{CH}_3(\text{CH}_2)_2\text{COO}^-$, 17 = PYDNS + $\text{CH}_3(\text{CH}_2)_8\text{COO}^-$, 18 = PYDNS + $\text{CH}_3(\text{CH}_2)_{12}\text{COO}^-$, 19 = PYDNS + $\text{CH}_3(\text{CH}_2)_{11}\text{SO}_3^-$, 20 = PYDNS + Cholesterol-sulfate, 21 = PYDNS + $\text{CH}_3(\text{CH}_2)_{11}\text{O-SO}_3^-$, 22 = PYDNS + dodecylbenzene sulfonate (error bar showing $\sim 2\%$ error).

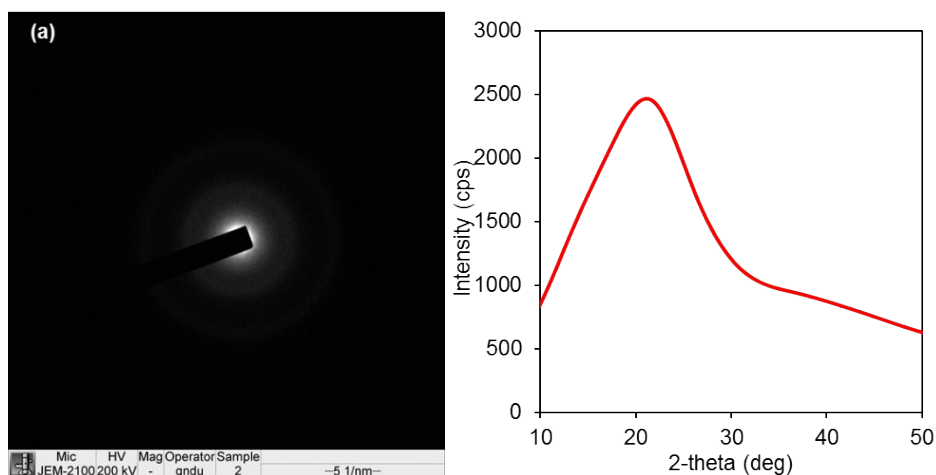


Figure SI 7. SAED pattern and X-ray powder diffraction of thin film of **PY-DNS**

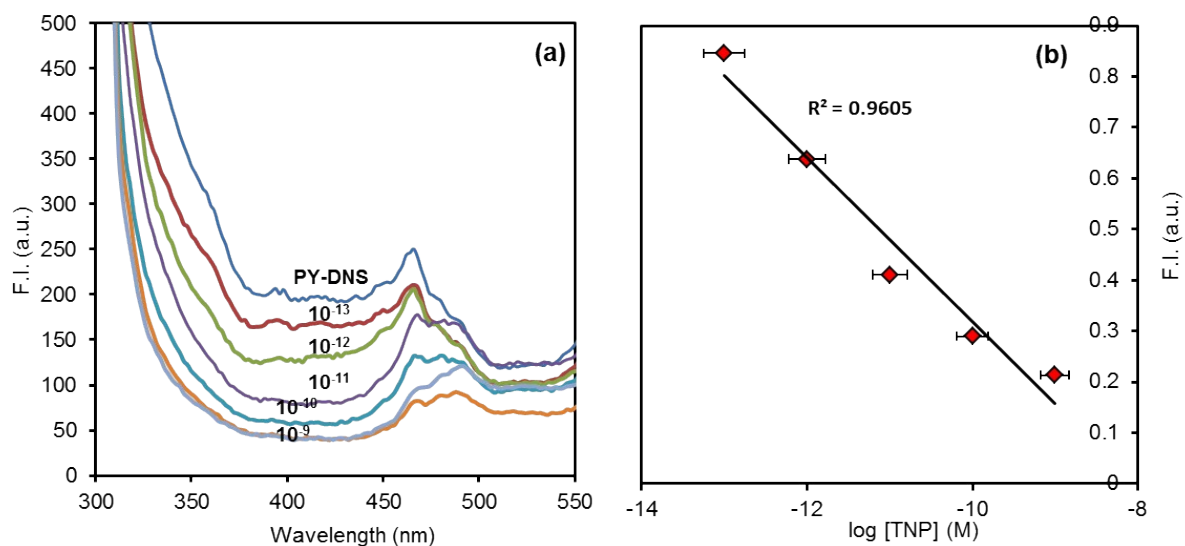


Figure SI 8. (a) Front surface steady-state fluorescence quenching of **PY-DNS** with TNP; (b) Plot of fluorescence intensity of **PY-DNS** vs $\log [TNP]$ (M) (error bar showing <2 % error).

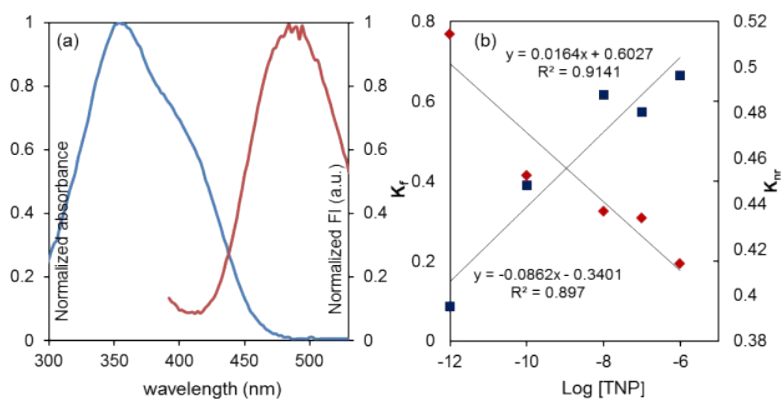


Figure SI 9. (a) the normalized UV-Vis and fluorescence spectra of TNP and **PYTR-DNS**, respectively. (b) The effect of concentration of $\log [TNP]$ on the K_f and K_{tr} values of **PYTR-DNS**.

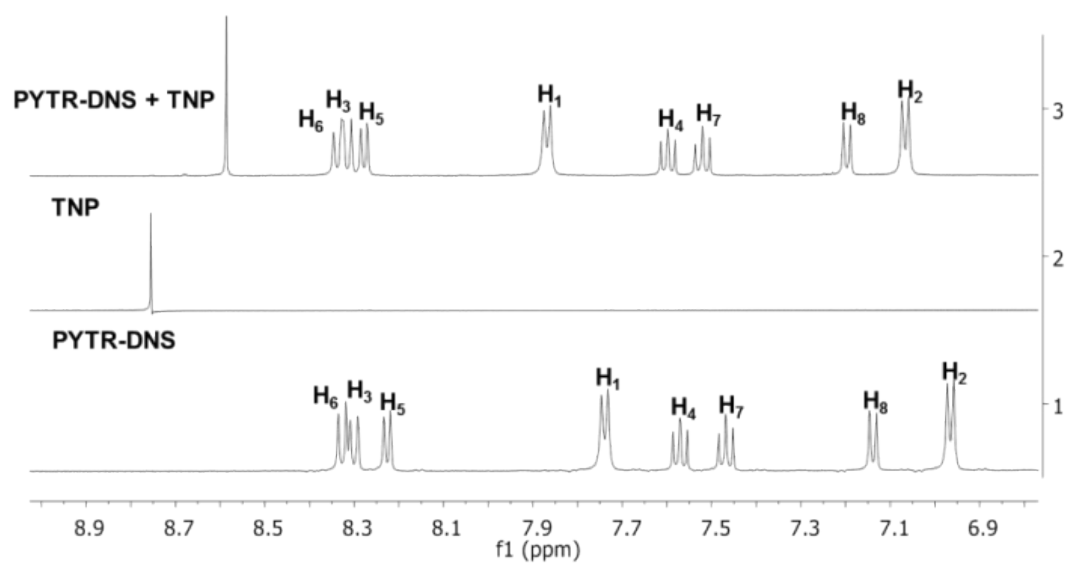


Figure SI 10. ¹H NMR spectra of **PY-DNS** (5 mM), TNP (5 mM) and **PY-DNS** + TNP (5 mM each) in DMSO-*d*₆-water 7:3.

Table SI 1: A comparison of quantum yield, linear range of detection, quenching process, Ksv and detection limits (solution and contact mode) for TNP with some of the representative reports

S. No.	Publication	Material used	Quantum yield	Linear range	Quenching process	Ksv (M^{-1})	Detection limit solution (contact mode)
1.	Present work	SOM*	0.71	10^{-13} - 10^{-5} M	dynamic	6.73×10^8	10^{-13} M (137 fg/cm ²)
2	Sensors and Actuators B, 2016, 231, 79–87	SOM	0.68	10^{-11} - 10^{-5} M	static	1.57×10^9	10^{-11} M (13.7 fg/cm ²)
3.	ACS Appl. Mater. Interfaces 2017, 9, 13415–13421	covalent organic framework	0.08	0.5-10 μ M	dynamic	1.0×10^7	0.25 μ M
4	New J. Chem., 2017, 41, 2786-792	SOM	-	-	both	1.04×10^4	0.95 μ M
5	Sensors and Actuators B 245 (2017) 665–673	SOM	0.126	-	-	8.47×10^4	576 ppb
6	Chem. Eur. J. 2016, 22, 5288 – 5294	SOM	0.12	-	static	79998	0.8 ppb
7	J. Mater. Chem. C, 2016, 4, 3523--3530	SOM	0.19	-	static	0.60×10^5	~20 ng cm ⁻²
8	J. Org. Chem. 2016, 81, 3597–3602	SOM	-	-	static	5.6×10^5	22 nM
9	Talanta 160 (2016) 133–137	SOM	-	-	static	2.66×10^4	1.2×10^{-7}
10	RSC Adv., 2015, 5, 73989-73992	SOM	-	-	both	2.82×10^4	7.0×10^{-7}
11	J. Mater. Chem. C, 2016, 4, 5578-5583	SOM	0.08	-	-	170000	-
12	Sensors and Actuators B 234 (2016) 34–45	SOM	0.43	-	Static	5.232×10^5	11.61 nM
13	RSC Adv., 2016, 6, 41340-41347	polymer	-	-	-	1.134×10^7	4.47 nM (1 x 10 ⁻⁷ M)
14	Tetrahedron Letters 56 (2015) 7094–7099	SOM	0.0649	-	-	5.95×10^3	-
15	J. Am. Chem. Soc. 2015, 137, 15276–15286	Metallacycles	0.046	-	-	2.18×10^6	0.13 ppb

*SOM= small organic molecules;