

Design of Pyrene Scaffold Multifunctional Material: Real Time Turn-On Chemo Sensor for Nitric Oxide, AIEE Behavior and Detection of TNP Explosive

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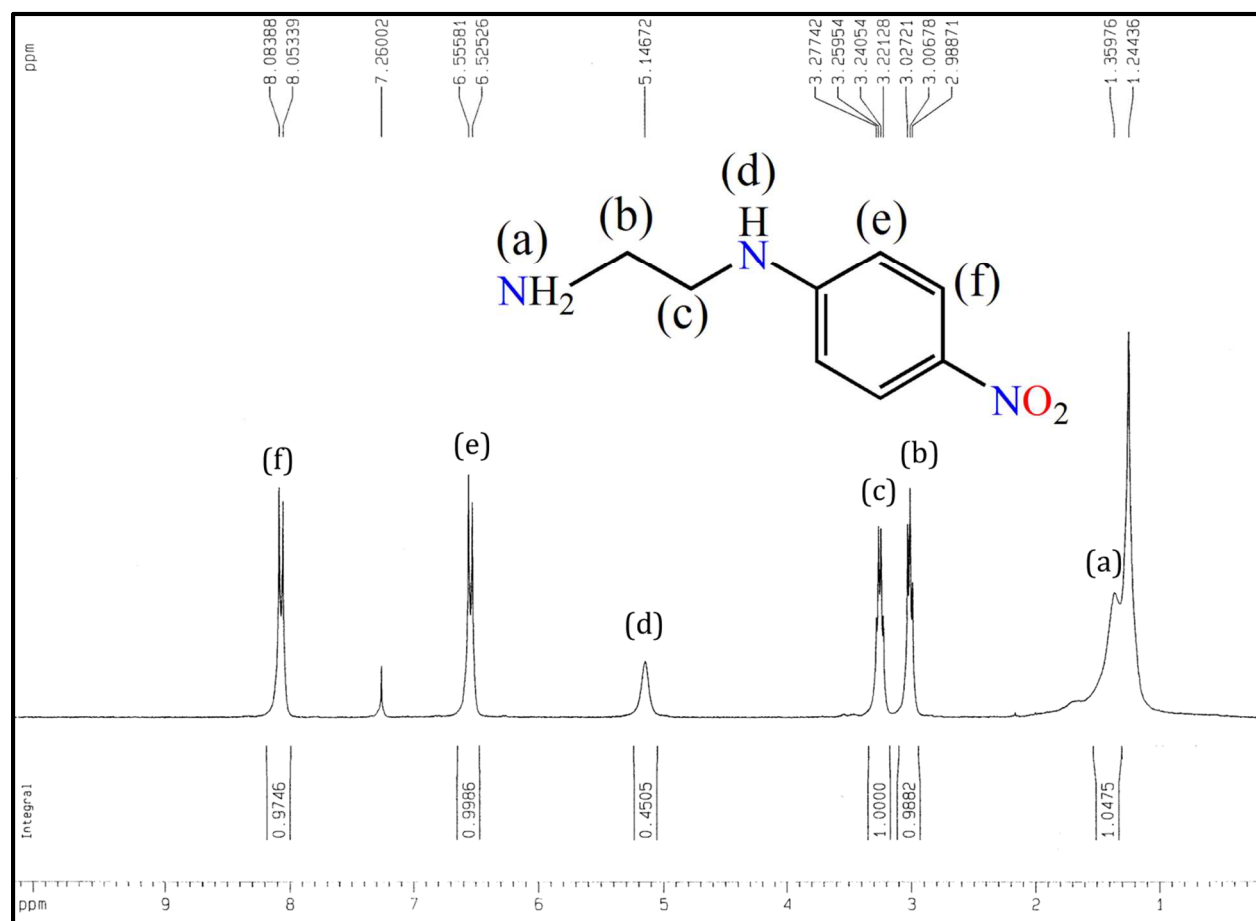


Figure S1. 1H -NMR spectrum of L^1 in DMSO- d_6 .

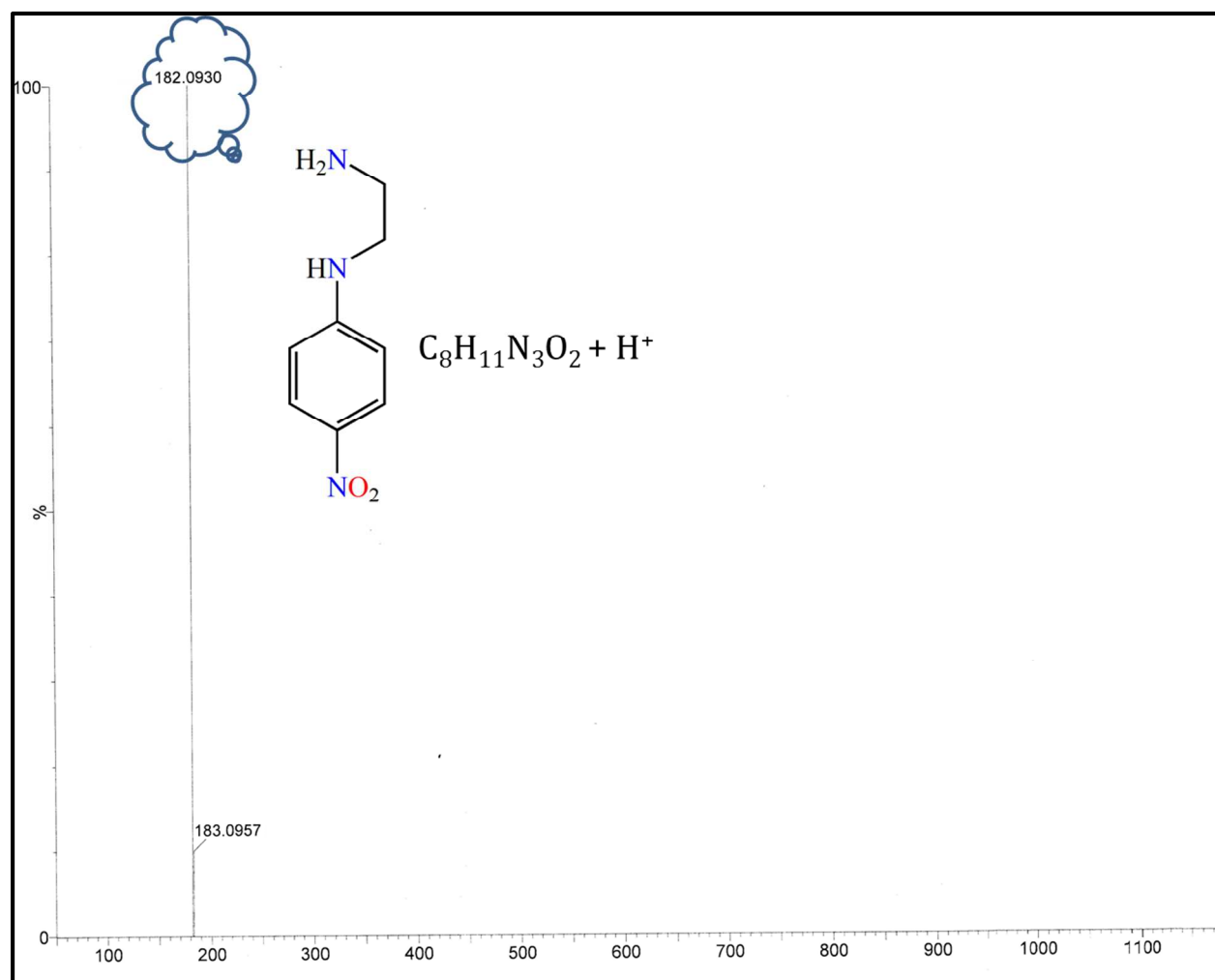


Figure S2. Mass spectra of L^1 in CH_3CN .

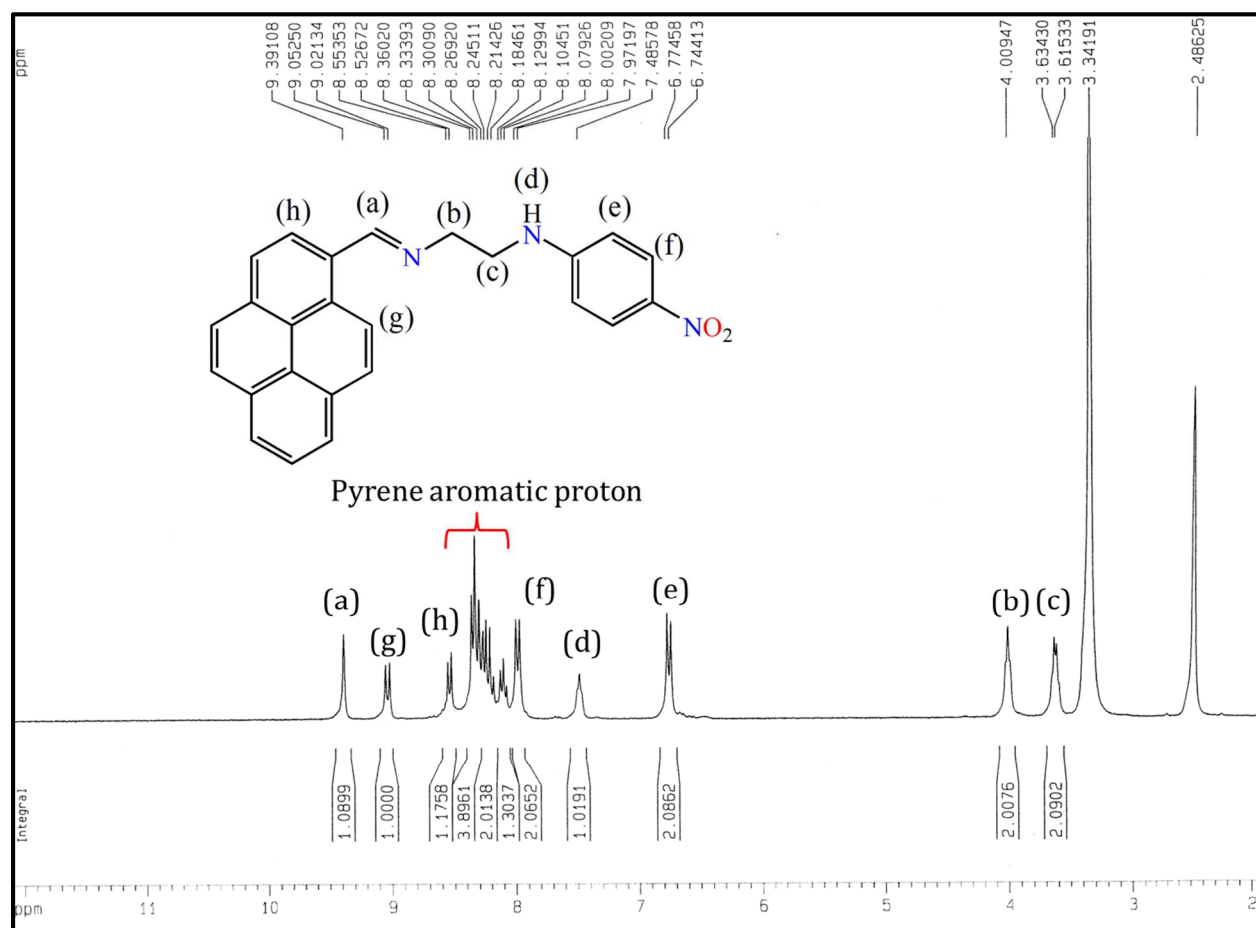


Figure S3. ^1H -NMR spectrum of PyDA-NP in DMSO- d_6 .

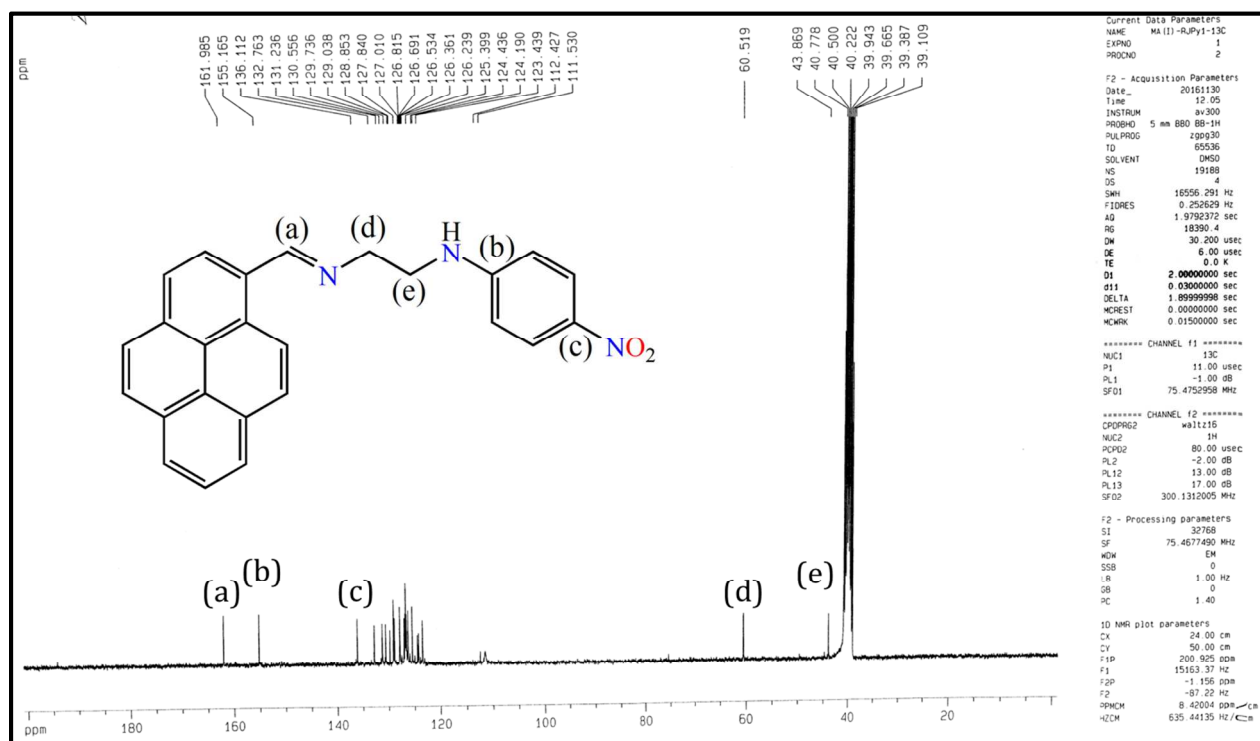


Figure S4. ^{13}C -NMR spectrum of PyDA-NP in DMSO-d_6 .

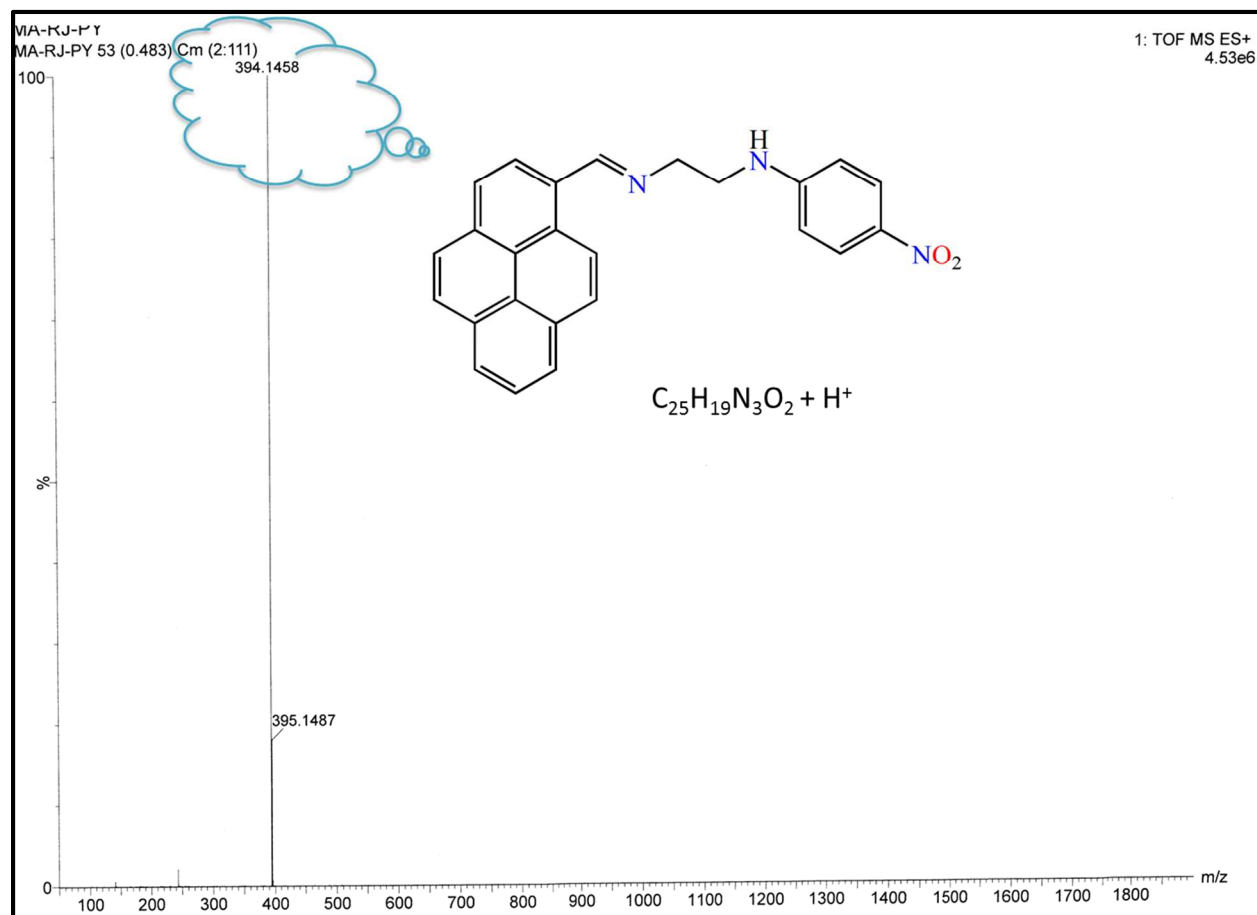


Figure S5. Mass spectra of PyDA-NP in CH₃CN.

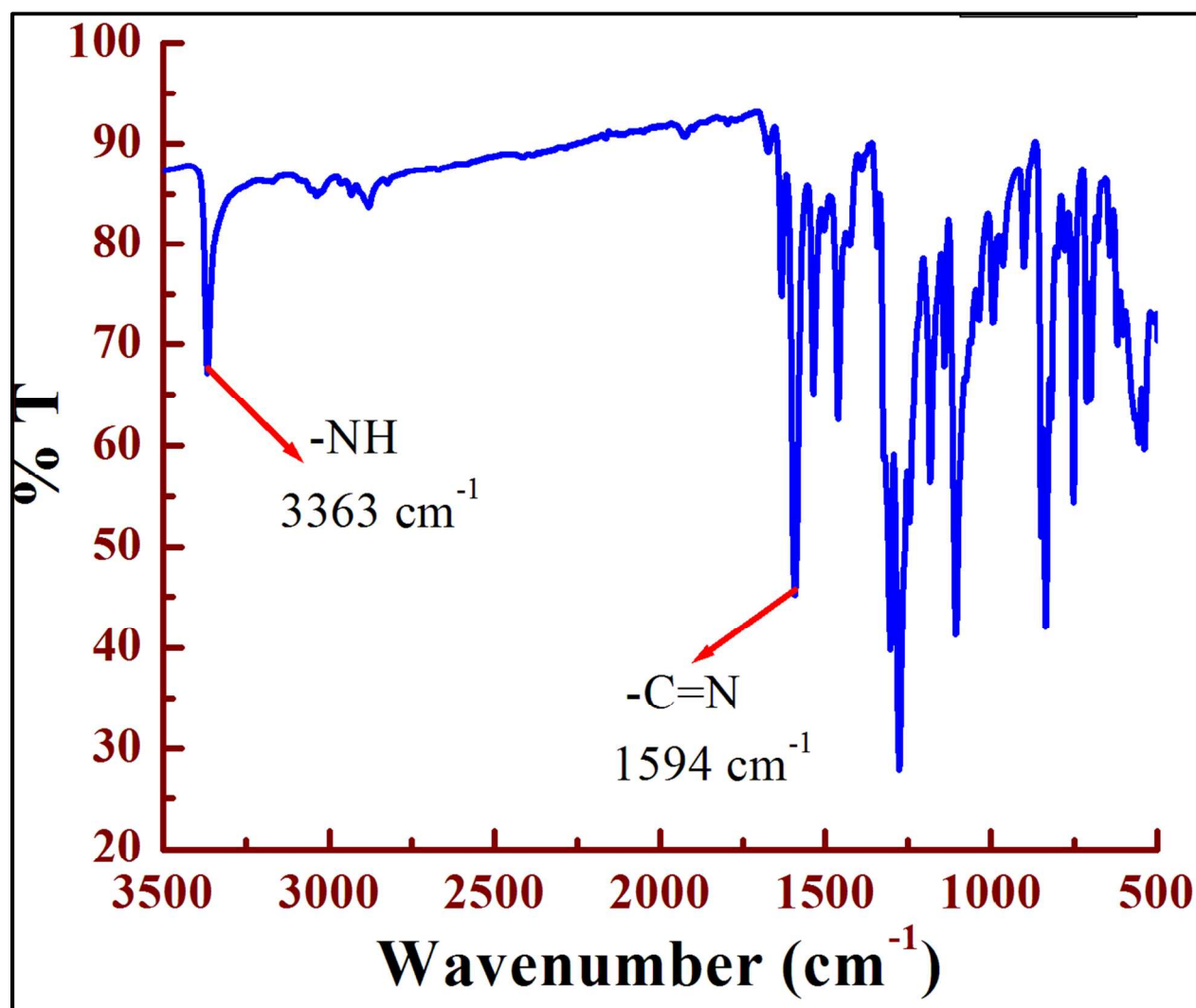


Figure S6. IR spectrum of PyDA-NP.

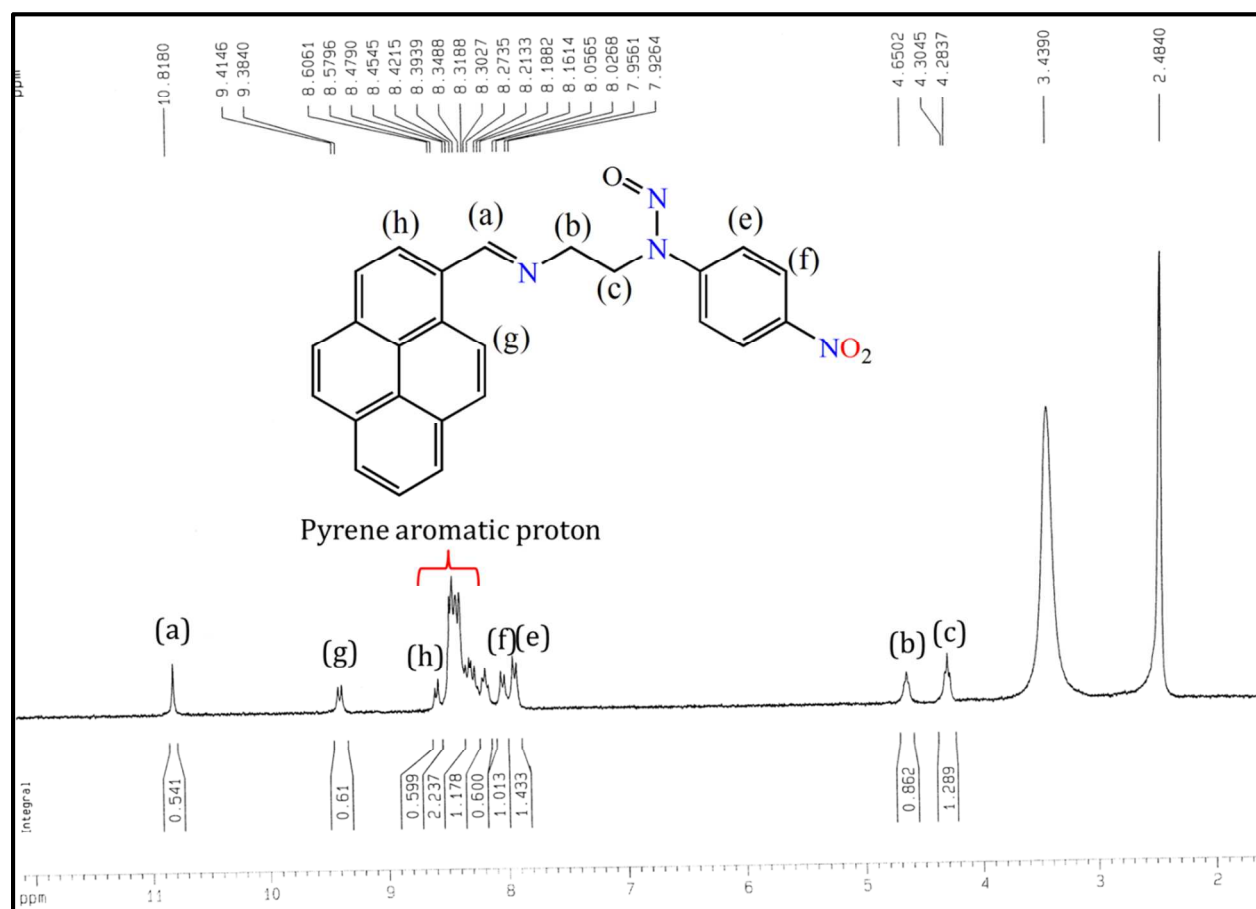
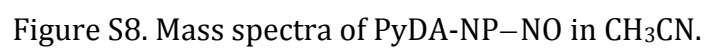


Figure S7. ^1H -NMR spectrum of PyDA-NP-NO in DMSO- d_6 .



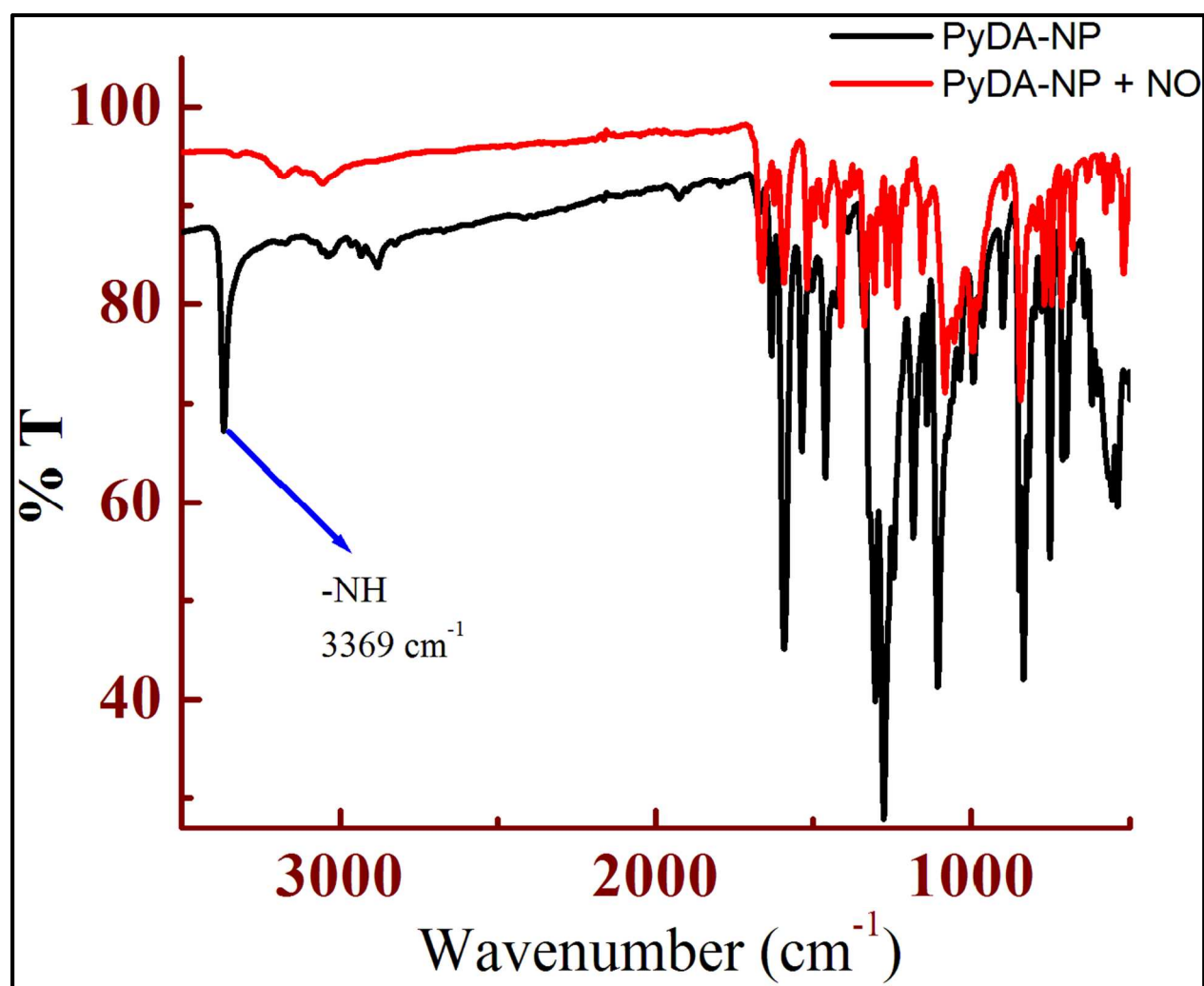


Figure S9. (a) IR spectrum of PyDA-NP–NO.

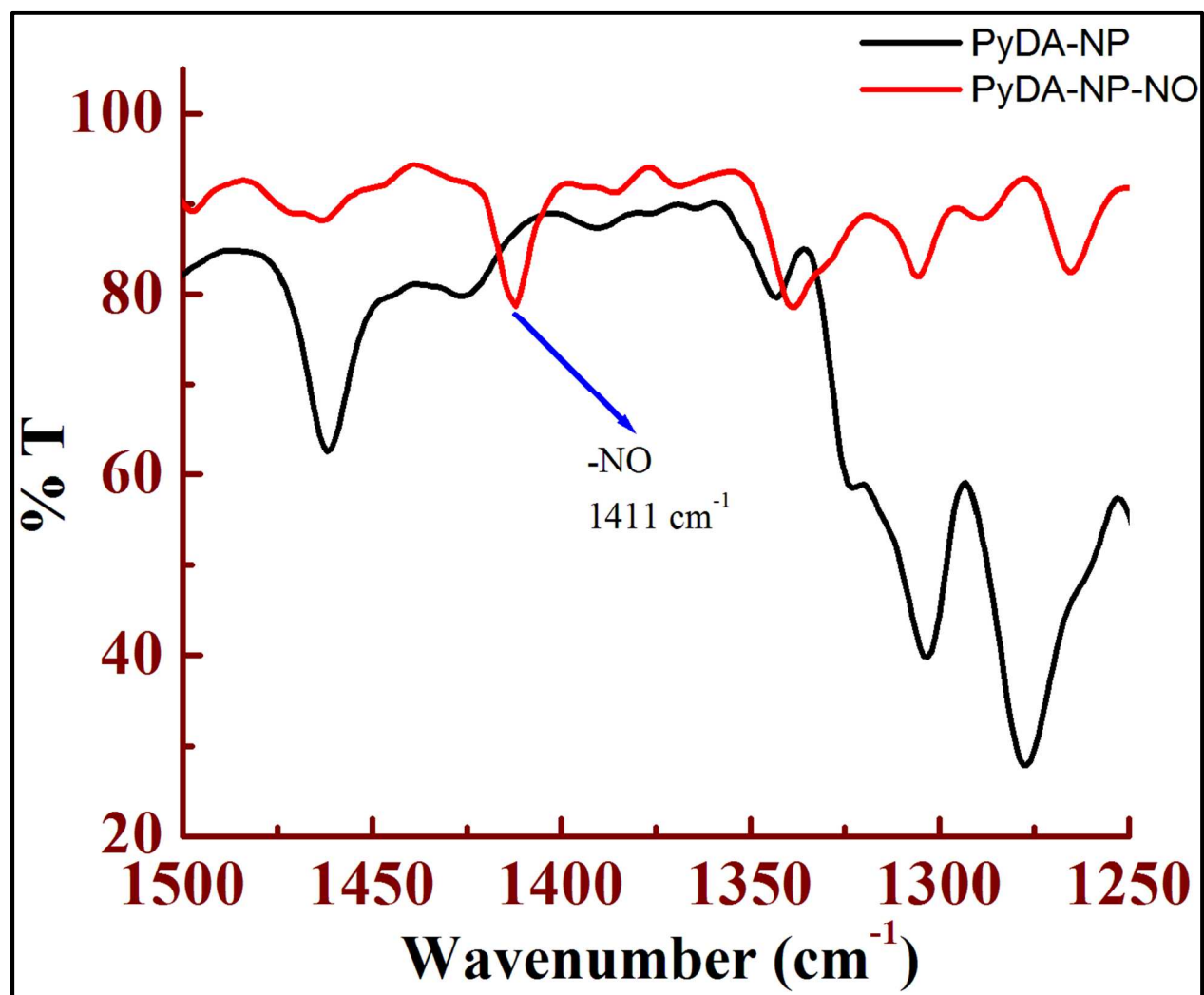


Figure S9. (b) IR spectrum of PyDA-NP-NO.

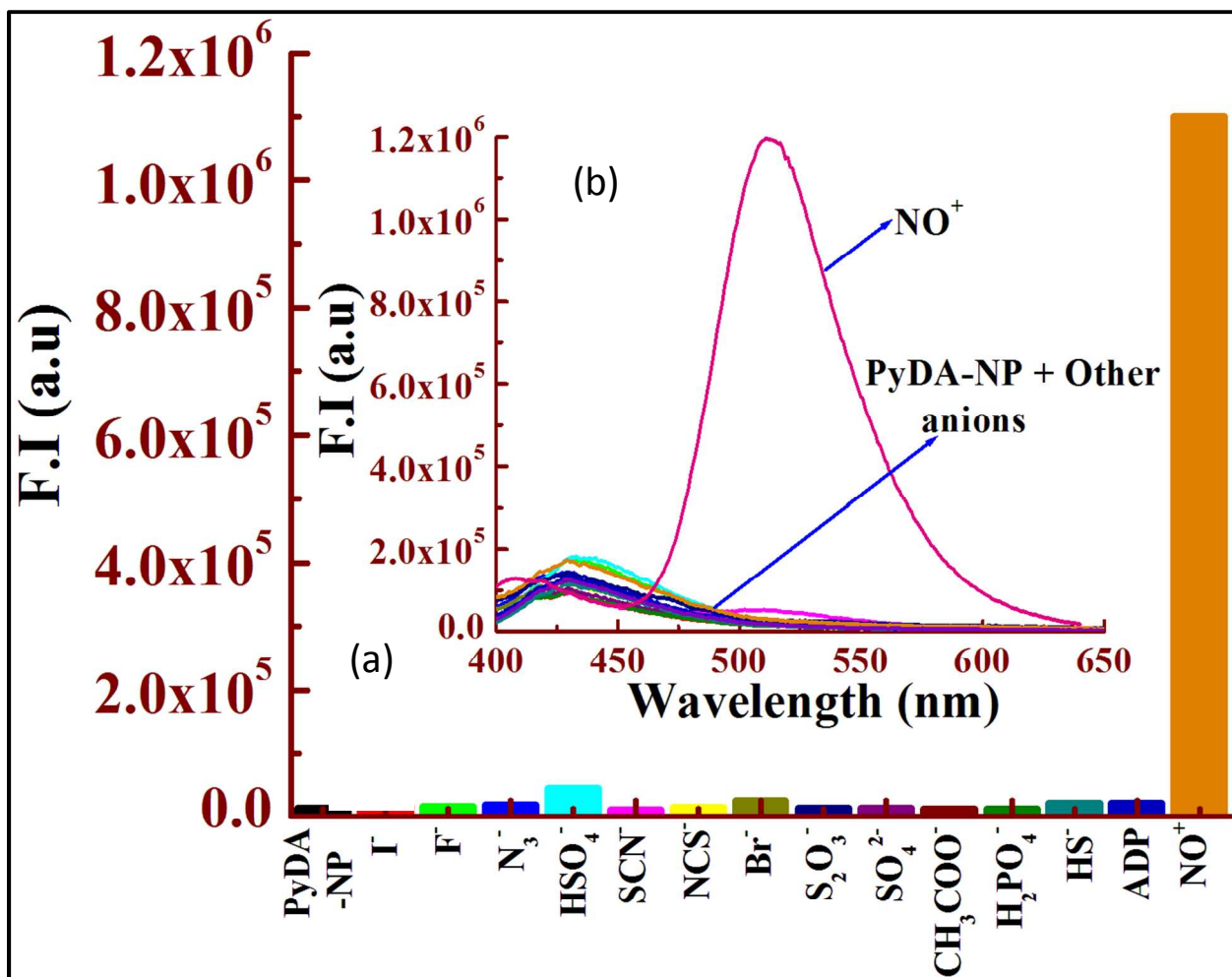


Figure S10a. (a) Bar chart illustrating fluorescence response of PyDA-NP at ~ 523 nm ($\lambda_{\text{ex}} = 390$ nm) towards different anions in 5% H₂O CH₃CN; (b) Spectral plot PyDA-NP in presence of different anions and NO. PyDA-NP = 10 μ M, Xⁿ⁻ = 100 μ M.

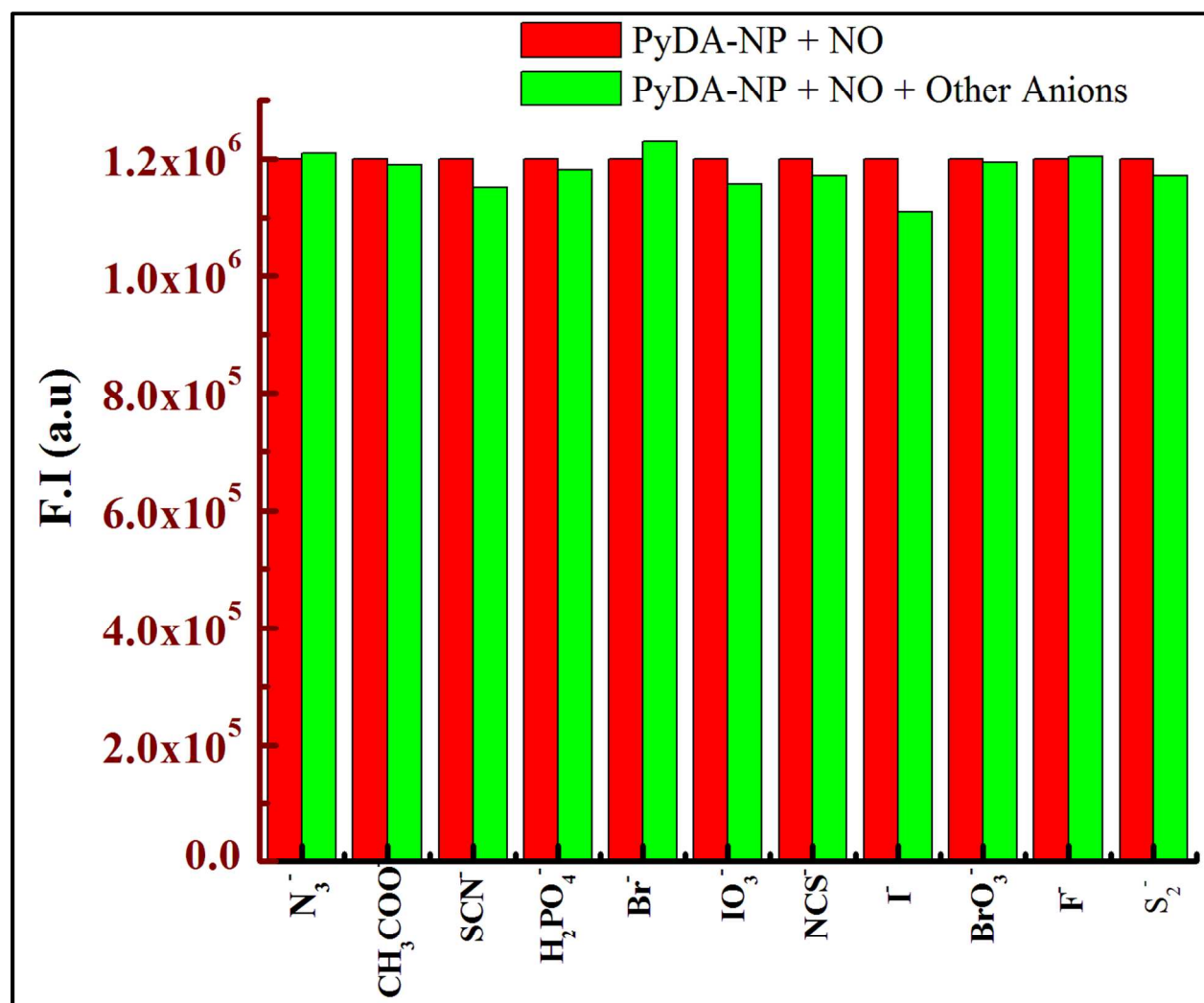


Figure S10b. Bar chart illustrating fluorescence response of PyDA-NP-NO at ~ 523 nm (λ_{ex} = 390 nm) towards different anions in 5% H_2O CH_3CN ; $X^{n+} = 100 \mu M$, $X^{n-} = 100 \mu M$.

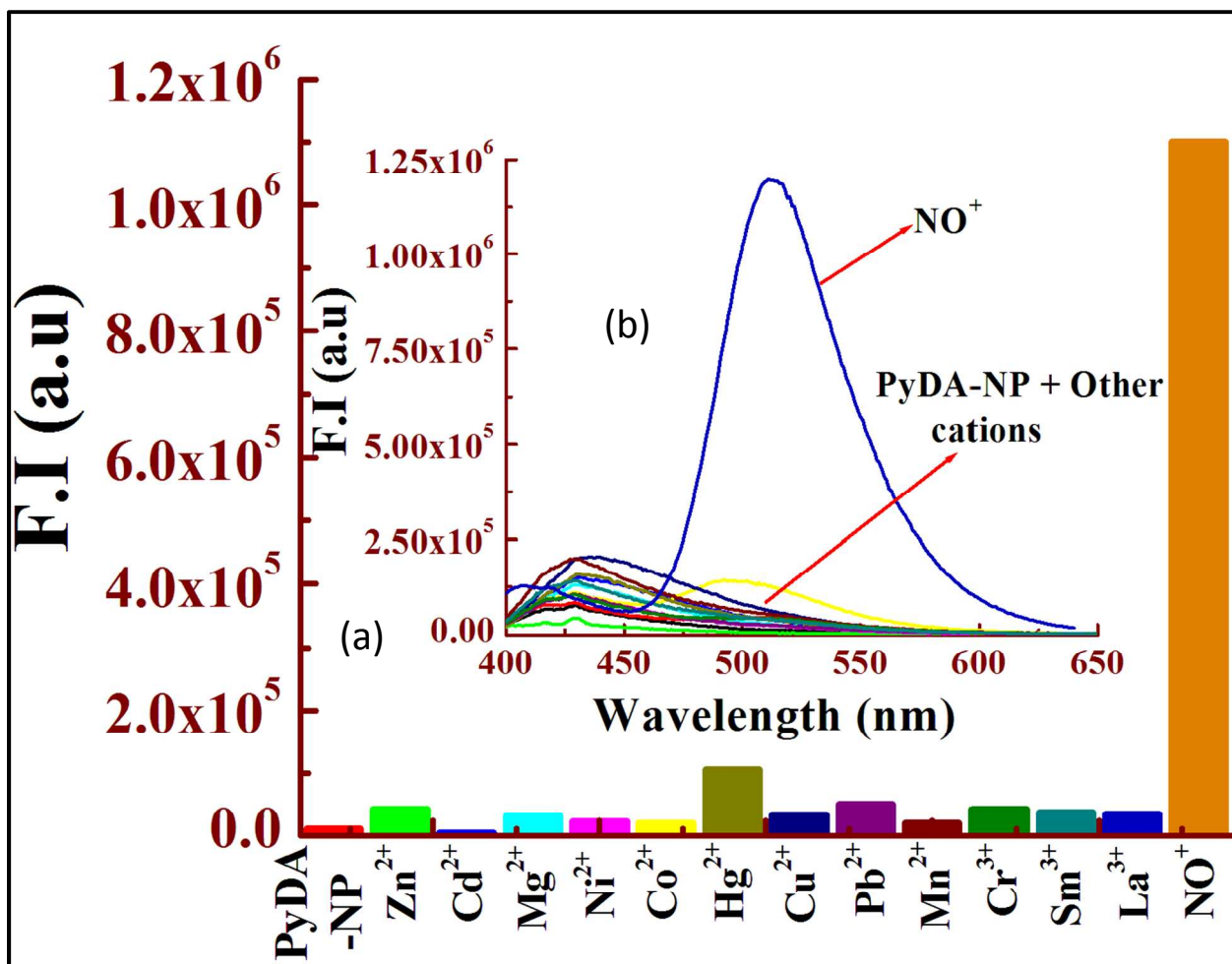


Figure S11a. (a) Bar chart illustrating fluorescence response of PyDA-NP at ~ 523 nm (λ_{ex} = 390 nm) towards different cations in 5% H_2O CH_3CN ; (b) Spectral plot PyDA-NP in presence of different cations and NO. PyDA-NP = 10 μM , X^{n+} = 100 μM .

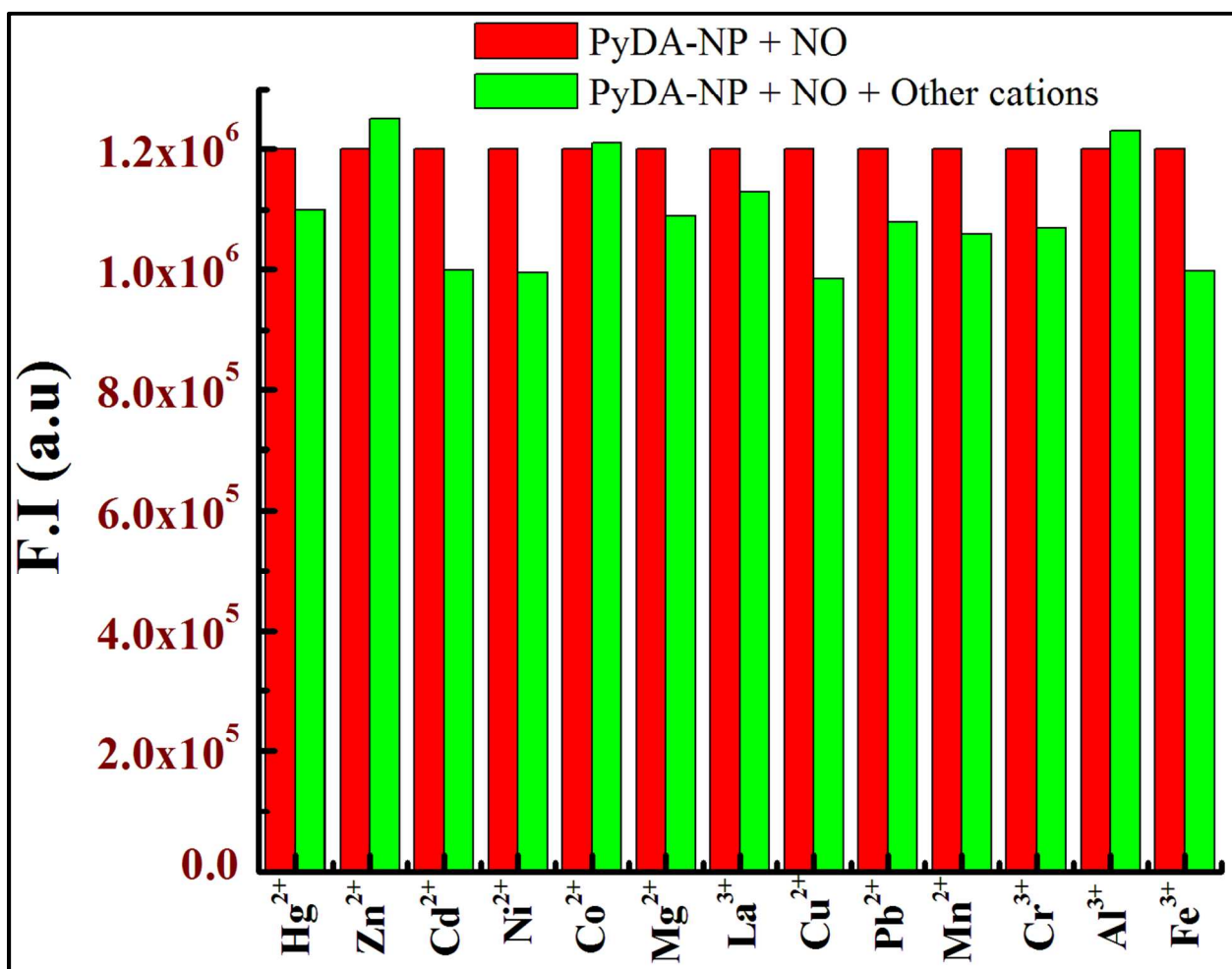


Figure S11b. Bar chart illustrating fluorescence response of PyDA-NP-NO at ~ 523 nm ($\lambda_{\text{ex}} = 390$ nm) towards different cations in 5% H₂O CH₃CN; $X^{n+} = 100$ μ M.

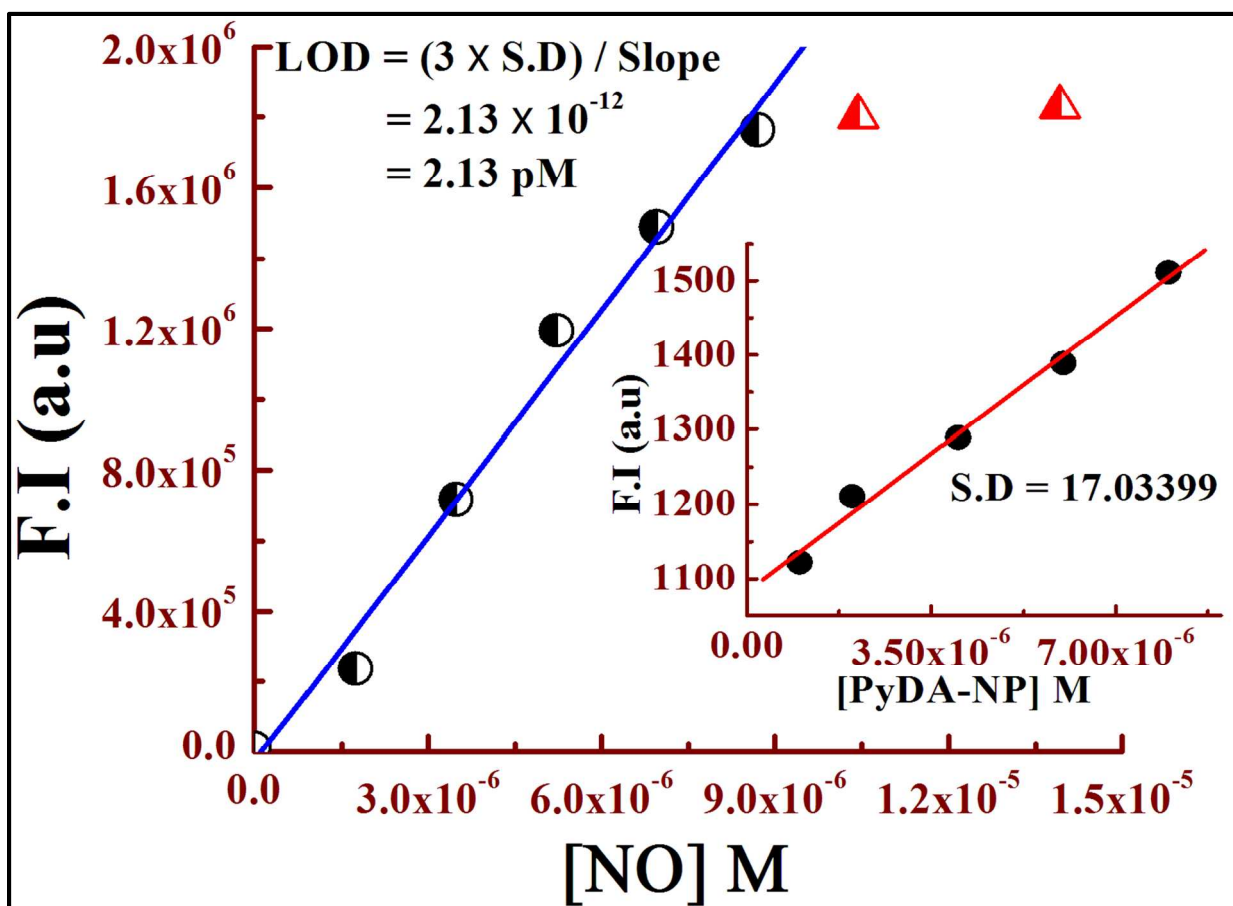


Figure S12. (a) Determination of LOD of PyDA-NH-NO.

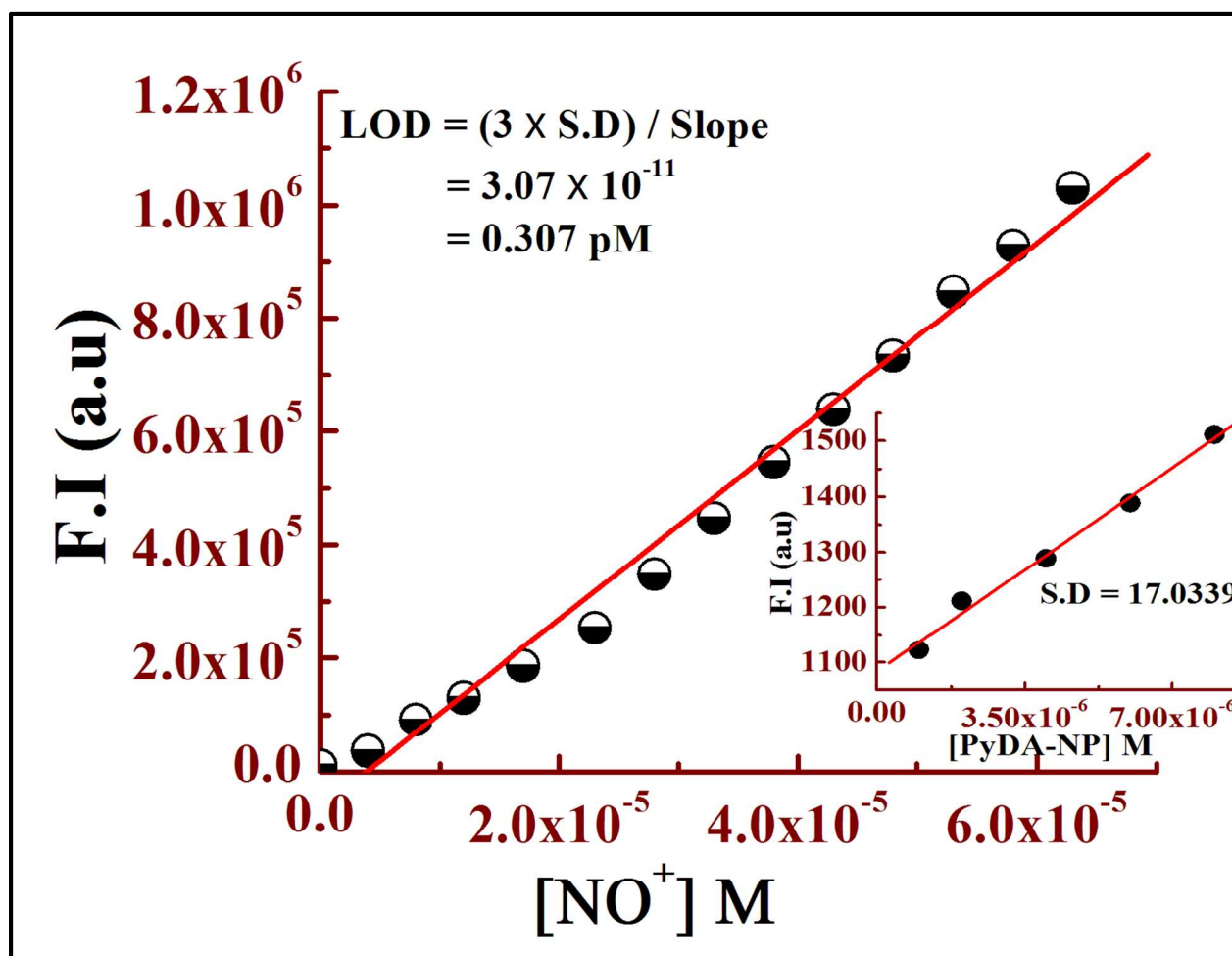


Figure S12. (b) Determination of LOD of PyDA-NH–NO⁺.

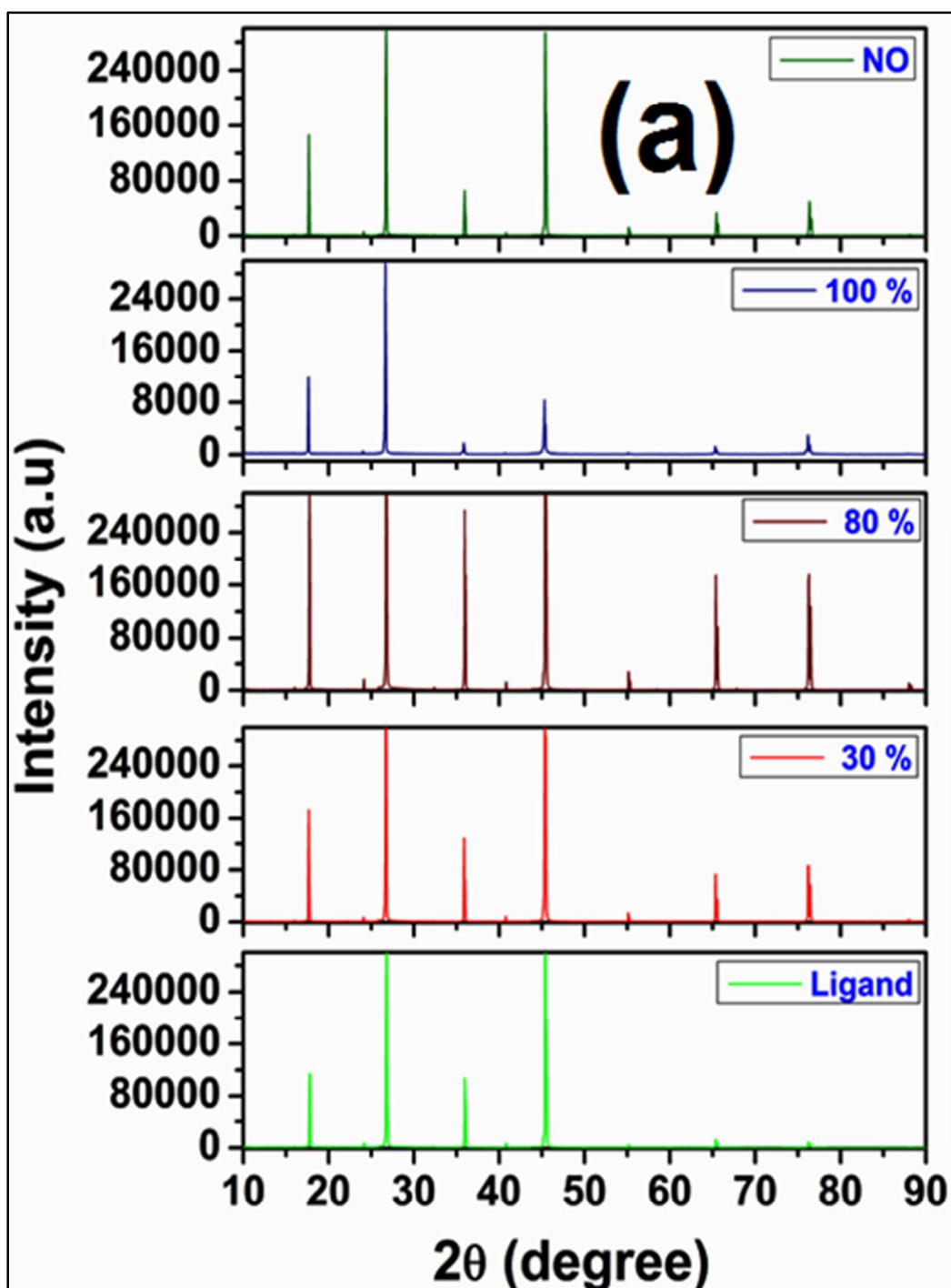


Figure S13. X-ray diffraction patterns of stack images of (a) PyDA-NP (10 μ M) in CH_3CN , PyDA-NP (10 μ M) at 30 %, 80 %, 100 % (water/ CH_3CN) and NO^+ (80 μ M) in 5 % (water/ CH_3CN).

Table S1. Crystallite size (D) and dislocation density (δ) at different peaks of hybrid PyDA-NP films.

Materials	2θ	FWHM (rad)	D (nm)	$\delta \times 10^{-4} \text{ (nm}^{-2}\text{)}$
PyDA-NP (10 μM) in CH_3CN	26.80°	0.00222	64.23	2.4239
	45.43°	0.00342	43.97	5.1724
PyDA-NP (10 μM) at 30 % (water/ CH_3CN)	26.72°	0.00207	69.02	2.0992
	45.37°	0.00356	40.10	6.2189
PyDA-NP (10 μM) at 80 % (water/ CH_3CN)	26.79°	0.00239	59.68	2.8076
	45.43°	0.00368	40.82	6.0014
PyDA-NP (10 μM) at 100 % (water/ CH_3CN)	26.66°	0.00162	88.14	1.2872
	45.29°	0.00152	98.59	1.0288
PyDA-NP + NO^+ (80 μM) in 5 % (water/ CH_3CN)	26.75°	0.00218	65.43	2.3358
	45.42°	0.00340	44.14	5.1325

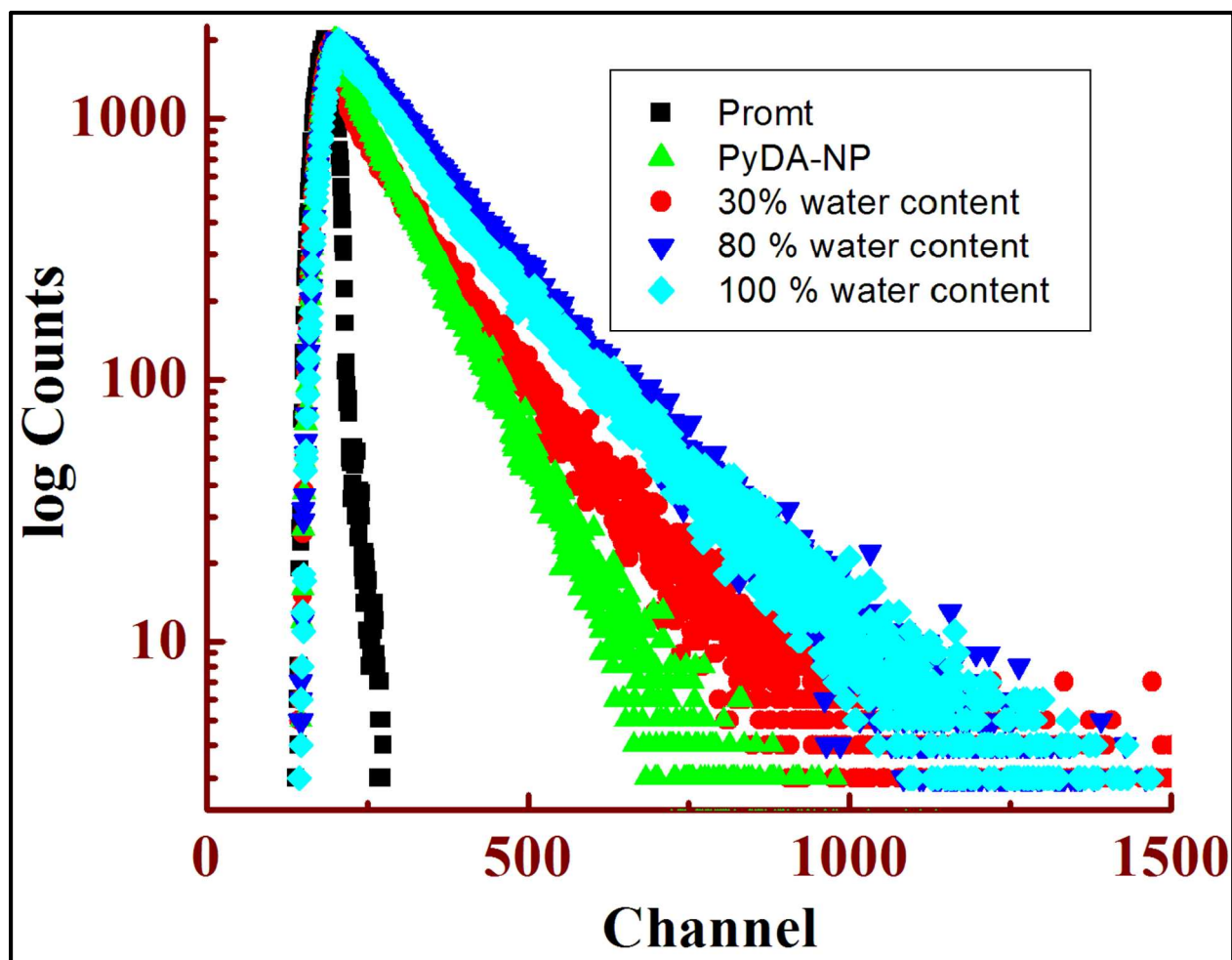


Figure S14. Fluorescence life time spectra of **PyDA-NP** at different % of water in the $\text{H}_2\text{O}/\text{CH}_3\text{CN}$ binary mixture solution.

Table S2. Different photophysical data of **PyDA-NP** at different % of water in the H₂O/CH₃CN binary mixture solution.

Sample	t_{avg} (s)	ϕ	K_r (s ⁻¹)	K_{nr} (s ⁻¹)	χ^2
PyDA-NP	8.08 E-10	0.00118	1.46E+06	1.24 E+09	1.071
PyDA-NP (30 %)	3.37 E-09	0.137	4.07 E+07	2.56 E+08	1.102
PyDA-NP (80 %)	3.76 E-09	0.79	2.10 E+08	5.59 E+07	1.089
PyDA-NP (100 %)	1.02 E-10	0.188	1.84 E+09	7.96 E+09	1.115

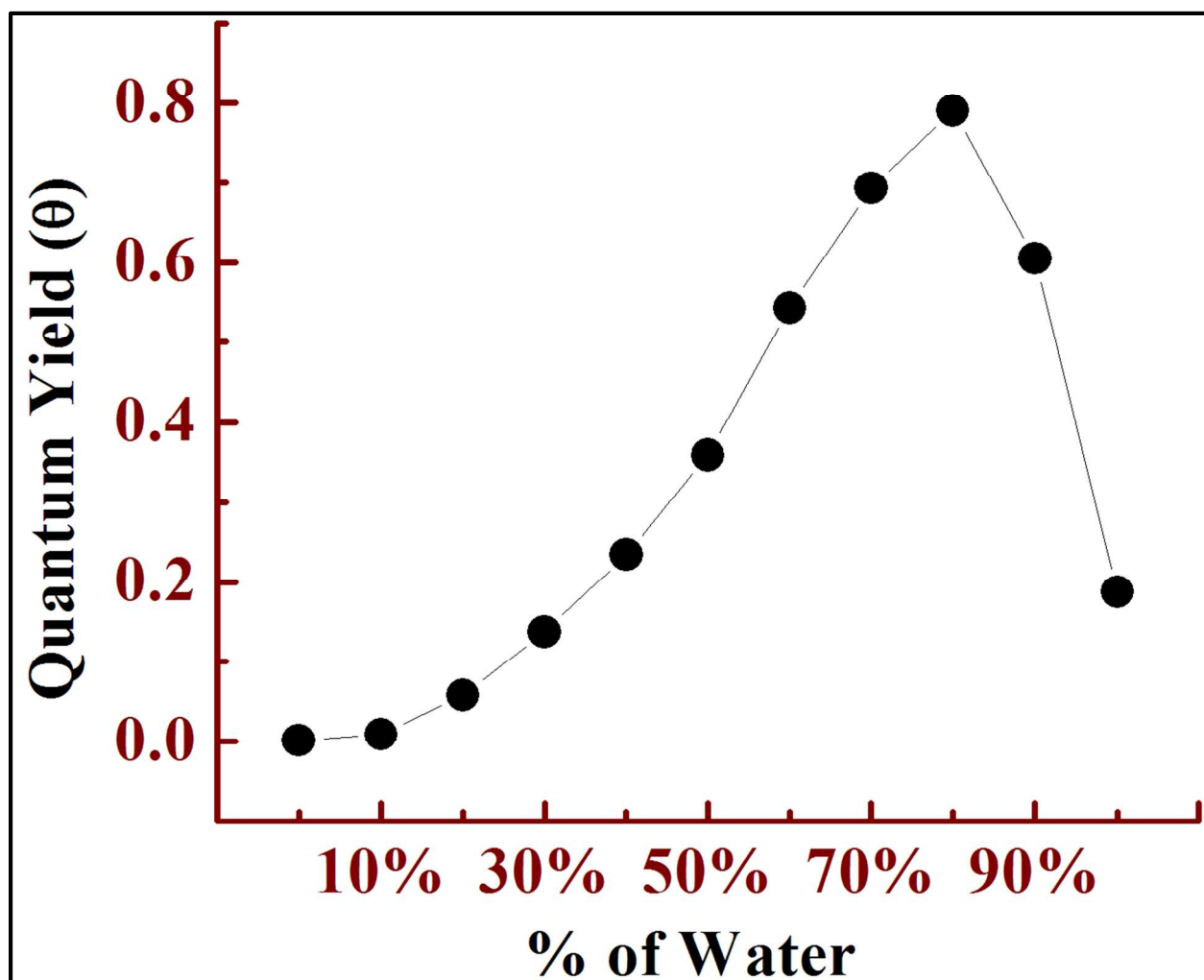


Figure S15. Plot of Quantum Yield vs % of water and CH_3CN of PyDA-NP.

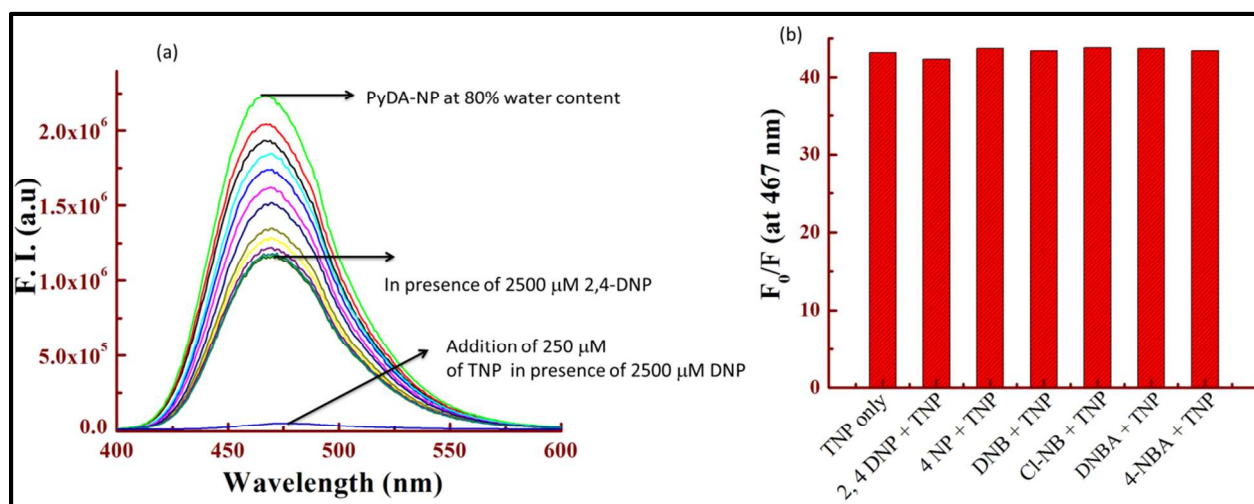


Figure S16. (a) Titration with 2,4-DNP up to 2500 μ M and then addition of 250 μ M TNP. (b) Over selectivity study for TNP.

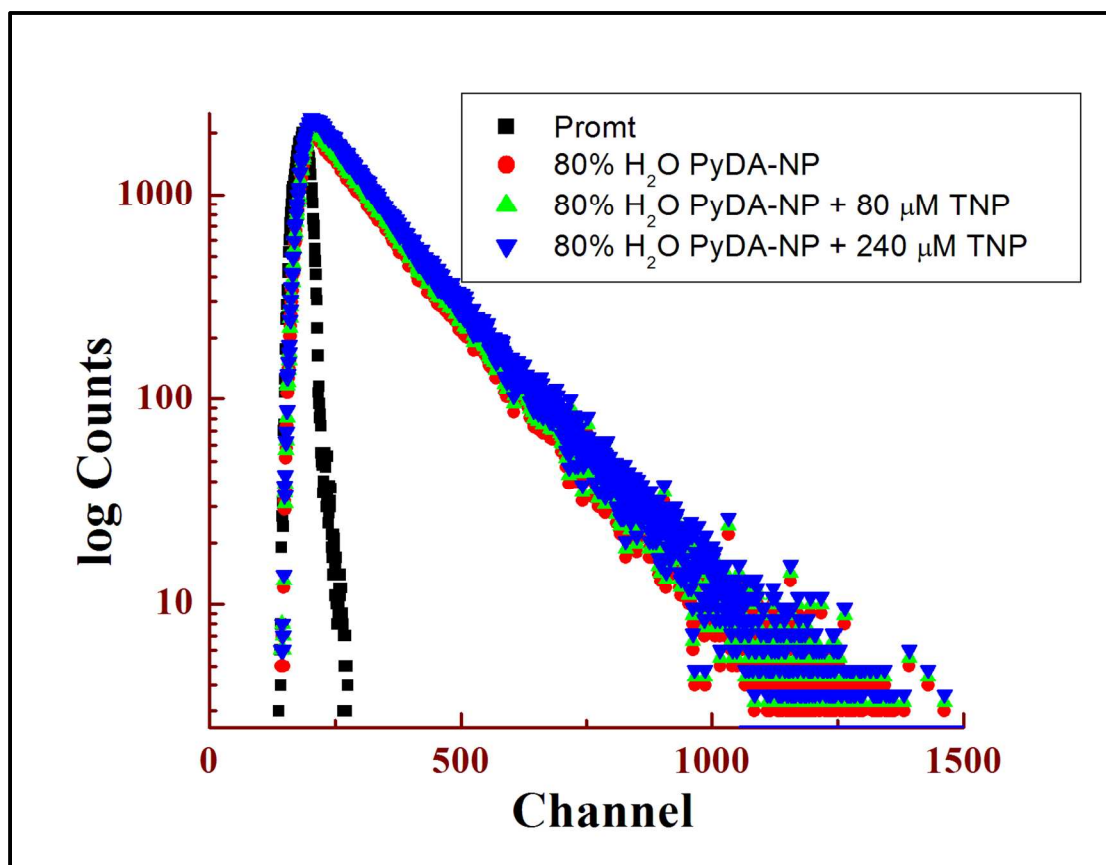


Figure S17. Fluorescence life time spectra of **PyDA-NP** at 80 % of water in the presence of different concentration of TNP.

Table S3. Fluorescence life time data of **PyDA-NP** at 80 % of water in the presence of different concentration of TNP.

Sample	t_{avg} (s)	χ^2
PyDA-NP (80 %)	3.76 E-09	1.133
PyDA-NP (80 %) + 80 μM TNP	3.79 E-09	1.048
PyDA-NP (80 %) + 240 μM TNP	3.81 E-09	1.052

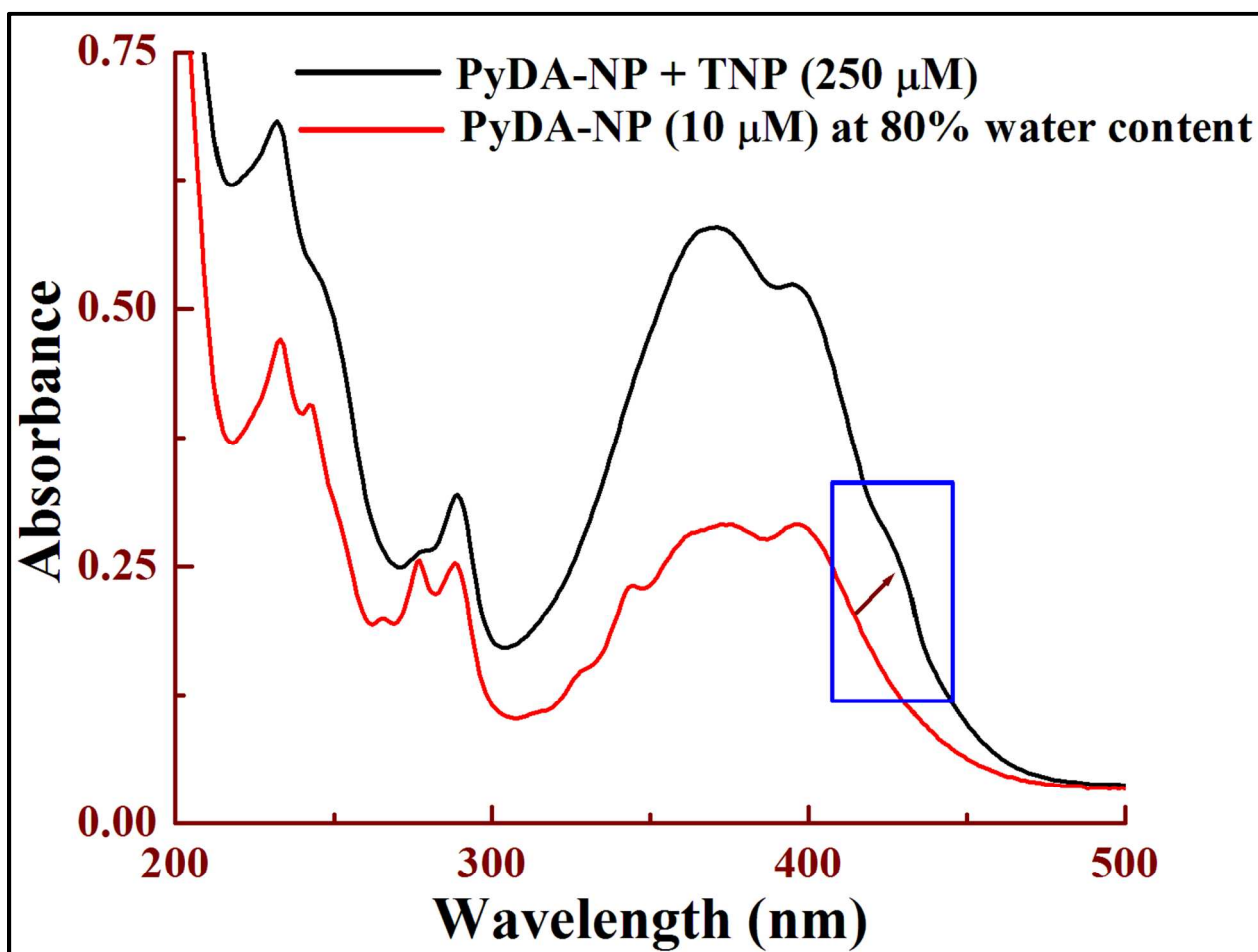


Figure S18. UV-Vis absorption spectrum of the PyDA-NP (10 μ M) at AIEE state (80% water) in the presence of TNP (240 μ M).