Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for New Journal of Chemistry

Pyrene – N-phenylparaphenylene diamine-Based Imine Conjugate as a Chemodosimeter for the Detection of Trace Amounts of Water in Organic Solvents: Real-Time Application in Honey Samples

Ramakrishnan AbhijnaKrishna, Natarajan Vijay and Sivan Velmathi*

Organic and Polymer Synthesis Laboratory, Department of Chemistry, National Institute of Technology, Tiruchirappalli, 620015, India
Corresponding author: velmathis@nitt.edu

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SUPPLIMENTARY FIGURES

1. POWDER X-RAY DIFFRACTION (PXRD) STUDY

Crystallite size of PNPD was evaluated and was found to be 142.8 nm. The high intensity peak at 20.462^{o} (2Θ) shows a uniform orientation of crystals at that angle. The uniformity in crystal orientation was then found to be in the following angle of orientations (2Θ), 24.288^{o}, 21.264^{o} and 27.567^{o}. At lower angles, there is not much high intensity peaks evidencing lack of uniform orientation however moderate peaks are observed at 10.18^{o} and 14.58^{o} (Fig. S1).

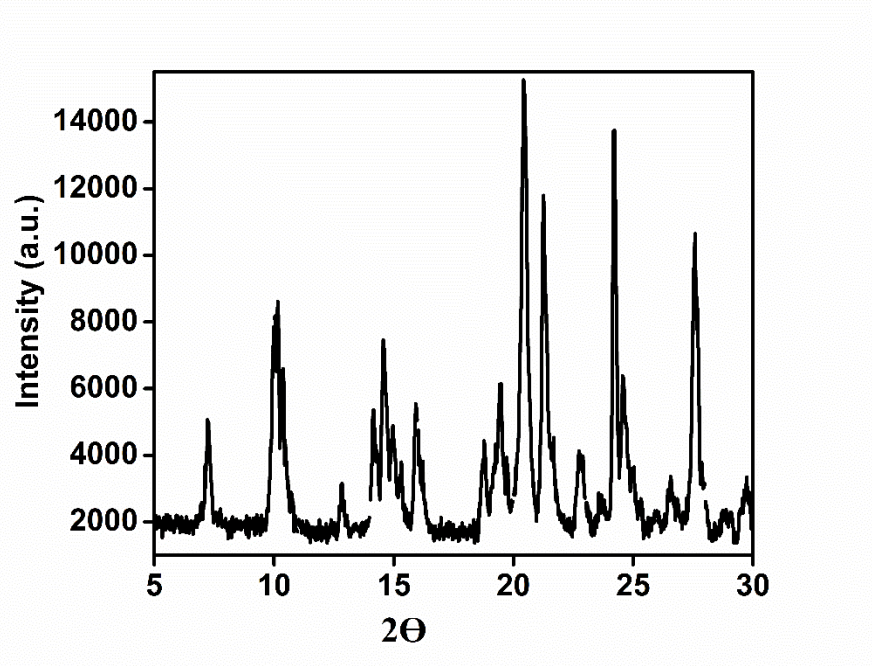


Figure S1. PXRD pattern of PNPD

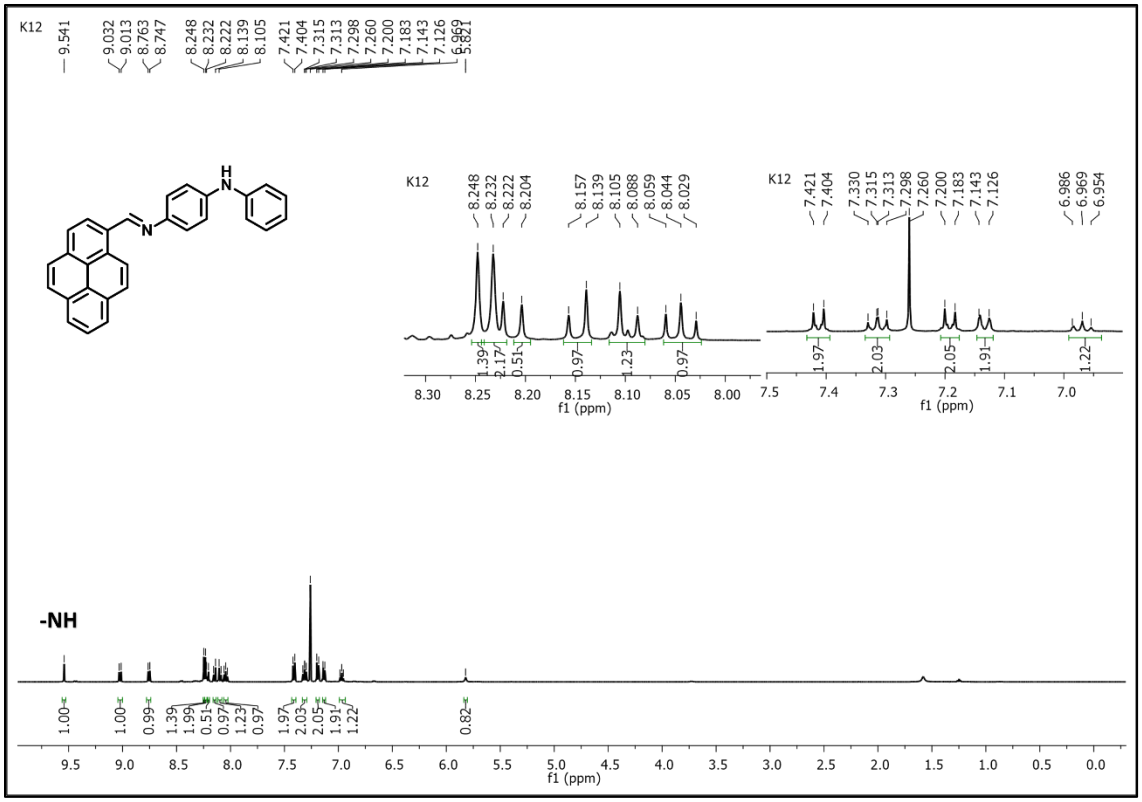


Figure S2. ^{1}H NMR spectrum ($CDCl_3$) of PNPD

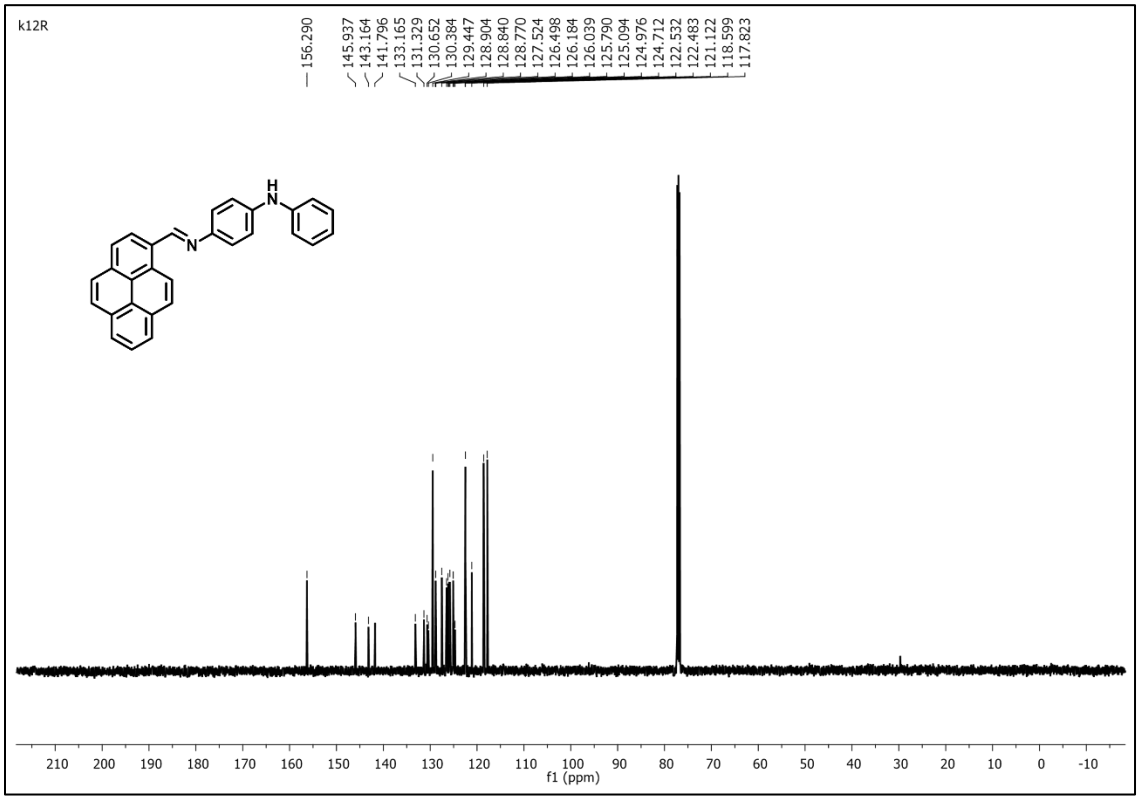


Figure S3. ^{13}C NMR spectrum ($CDCl_3$) of PNPD

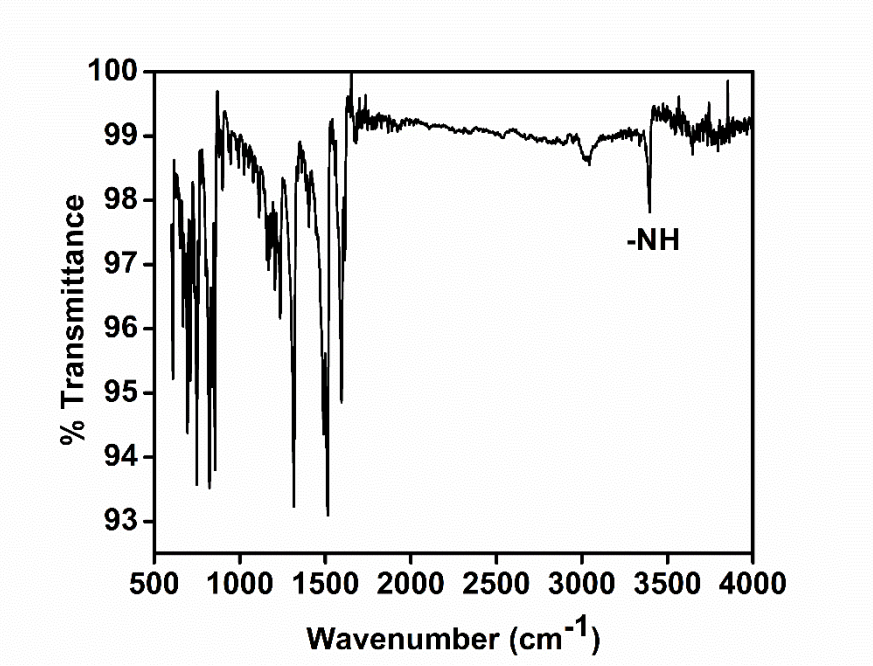


Figure S4. FT-IR spectrum of PNPD

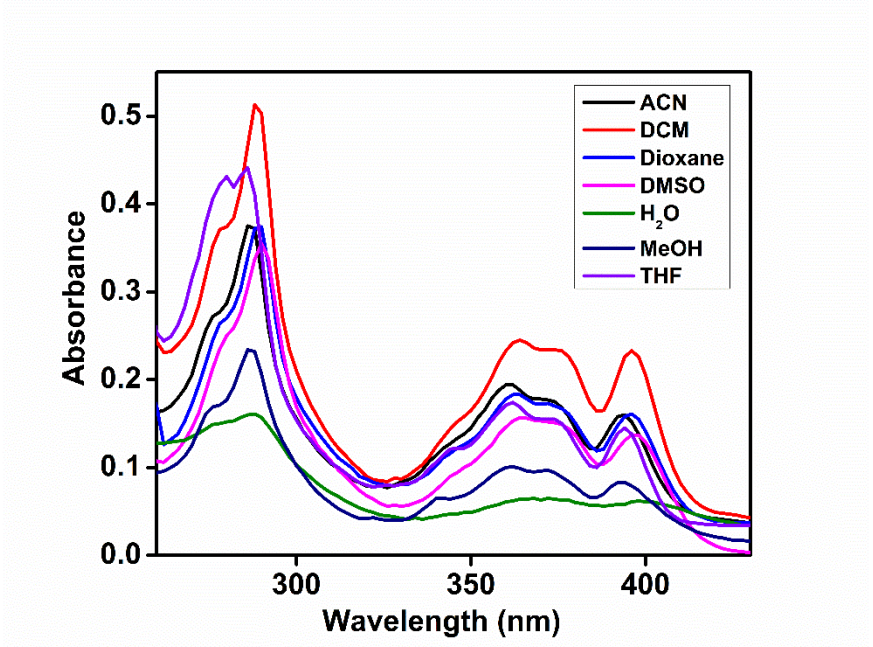


Figure S5. Absorption spectra of PNPD (10µM) in different solvents

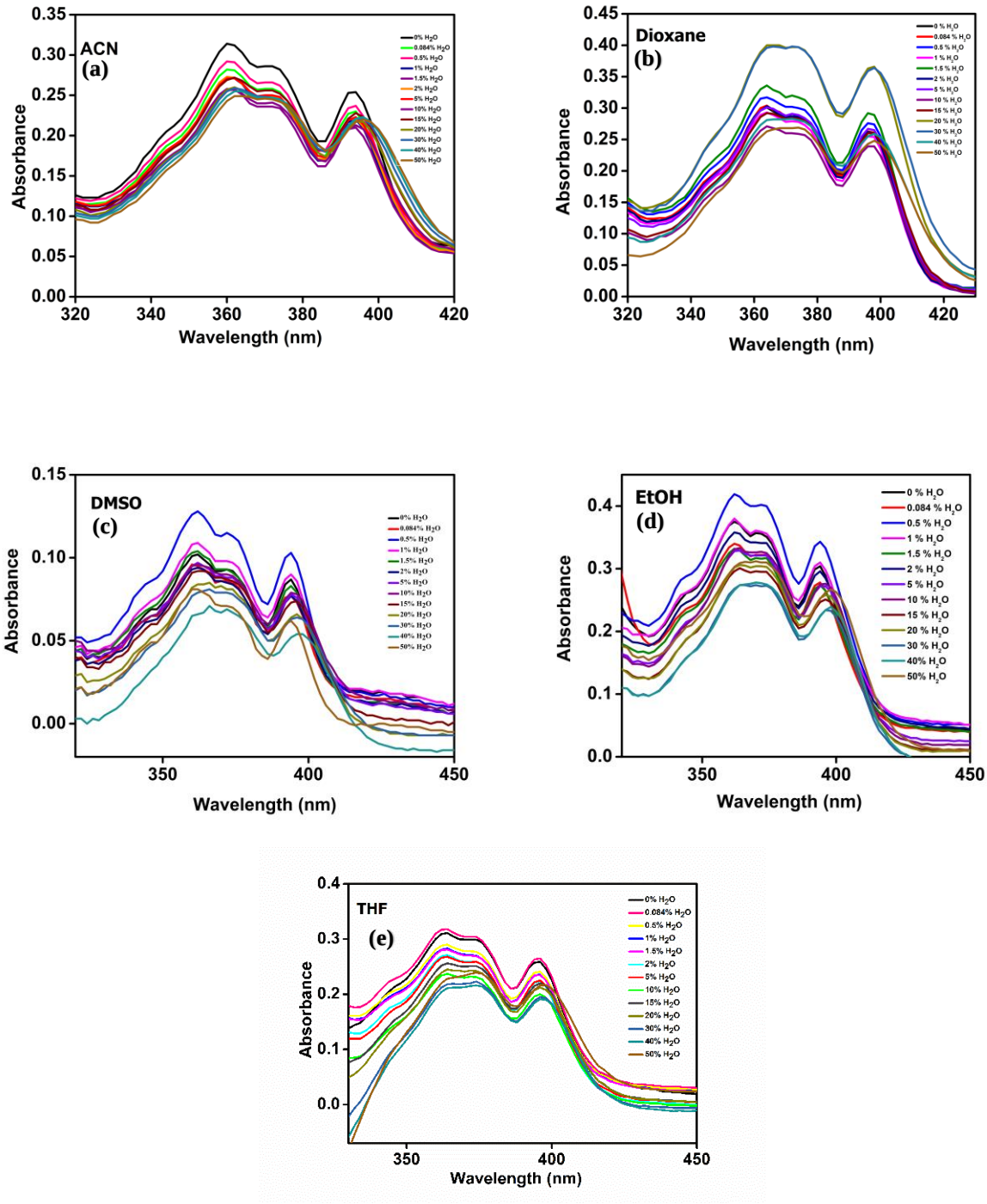


Figure S6. Absorption spectra of PNPD (10µM) with varying concentration of H_2O from 0%, 0.084%, 0.5%, 1%, 1.5%, 2%, 5%, 10%, 15%, 20%, 30%, 40%, to 50% in (a) ACN (b) Dioxane (c) DMSO (d) EtOH (e) THF

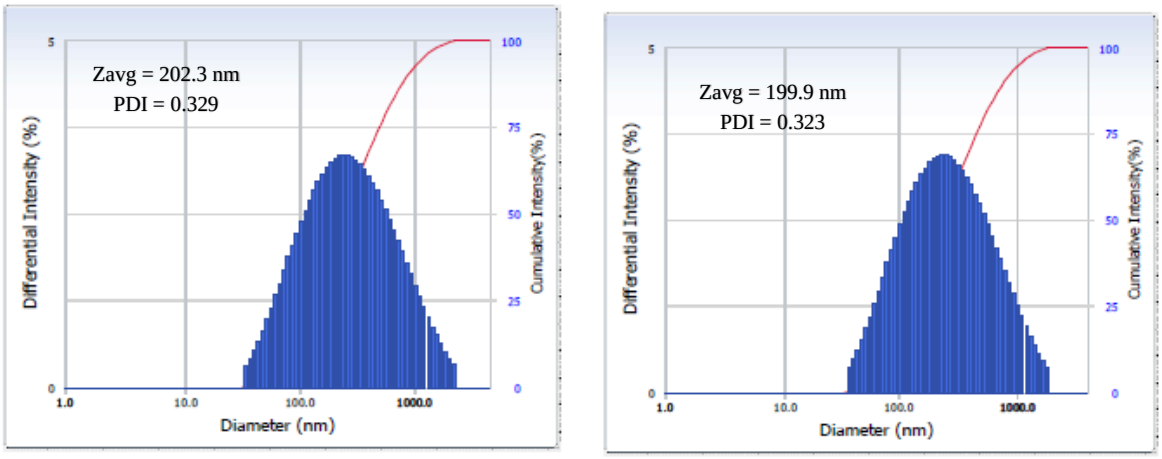


Figure S7. DLS-based particle size analysis of PNPD (10μM) in (a) 50% H_2O-DMSO and (b) 90% H_2O-DMSO

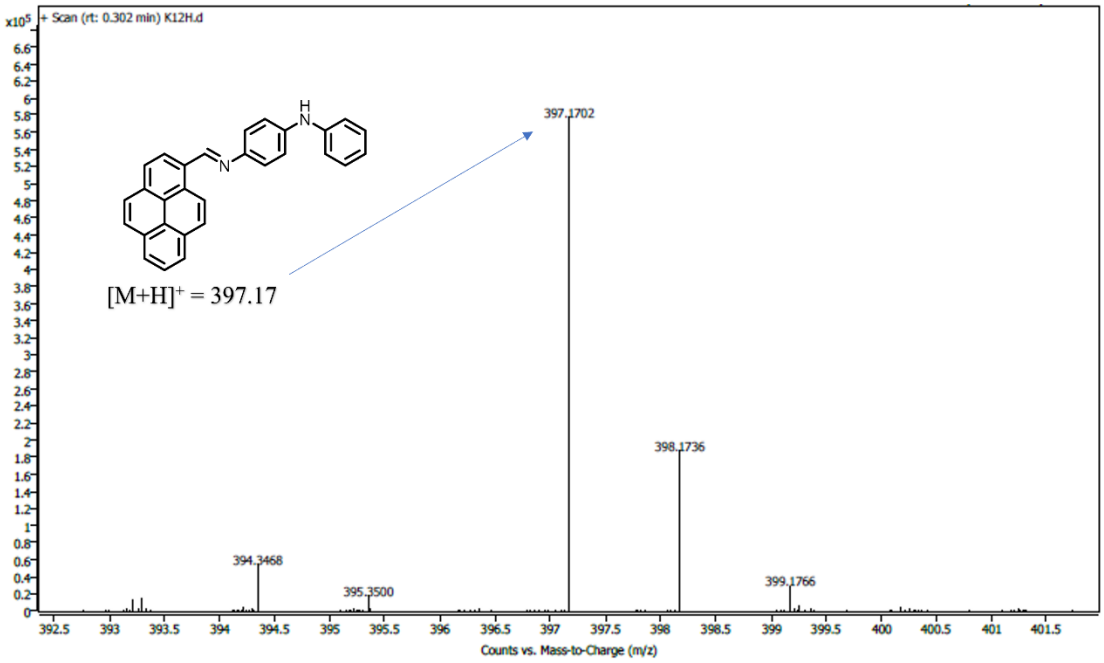


Figure S8. HRMS spectrum of PNPD in 100% acetonitrile

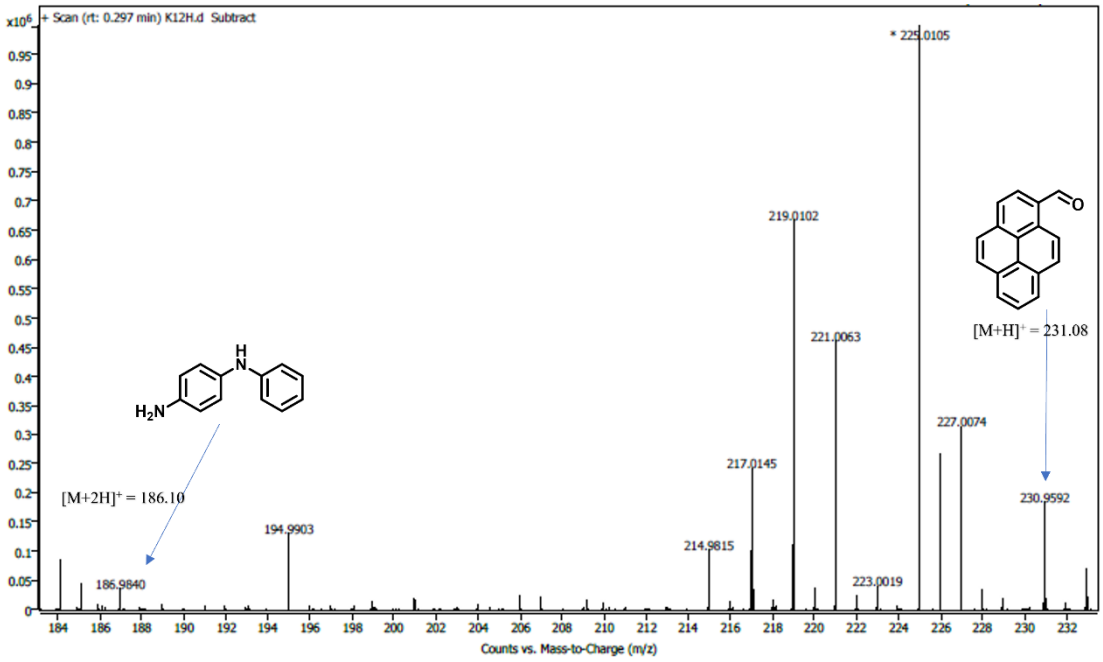
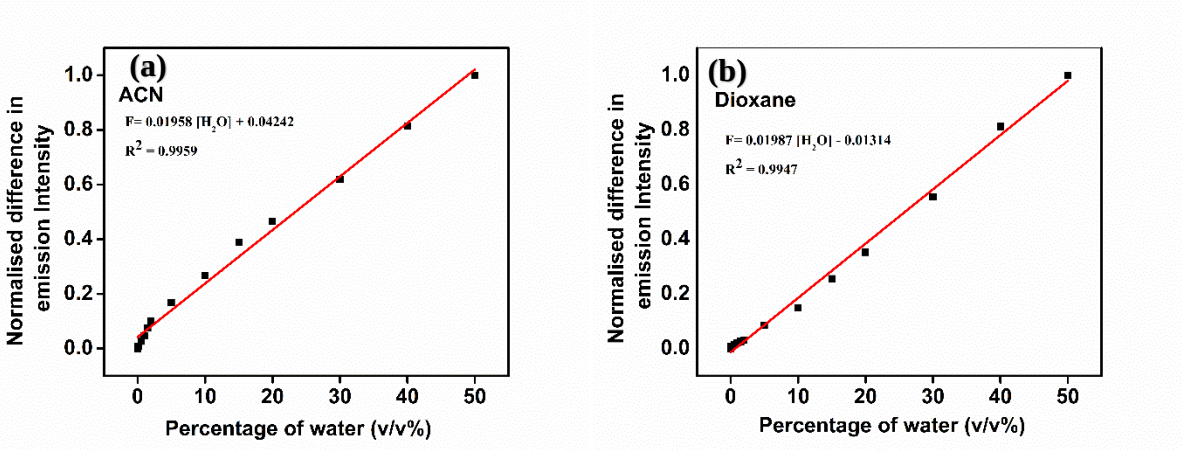


Figure S9. HRMS spectrum of PNPD in 80% acetonitrile: H_2O



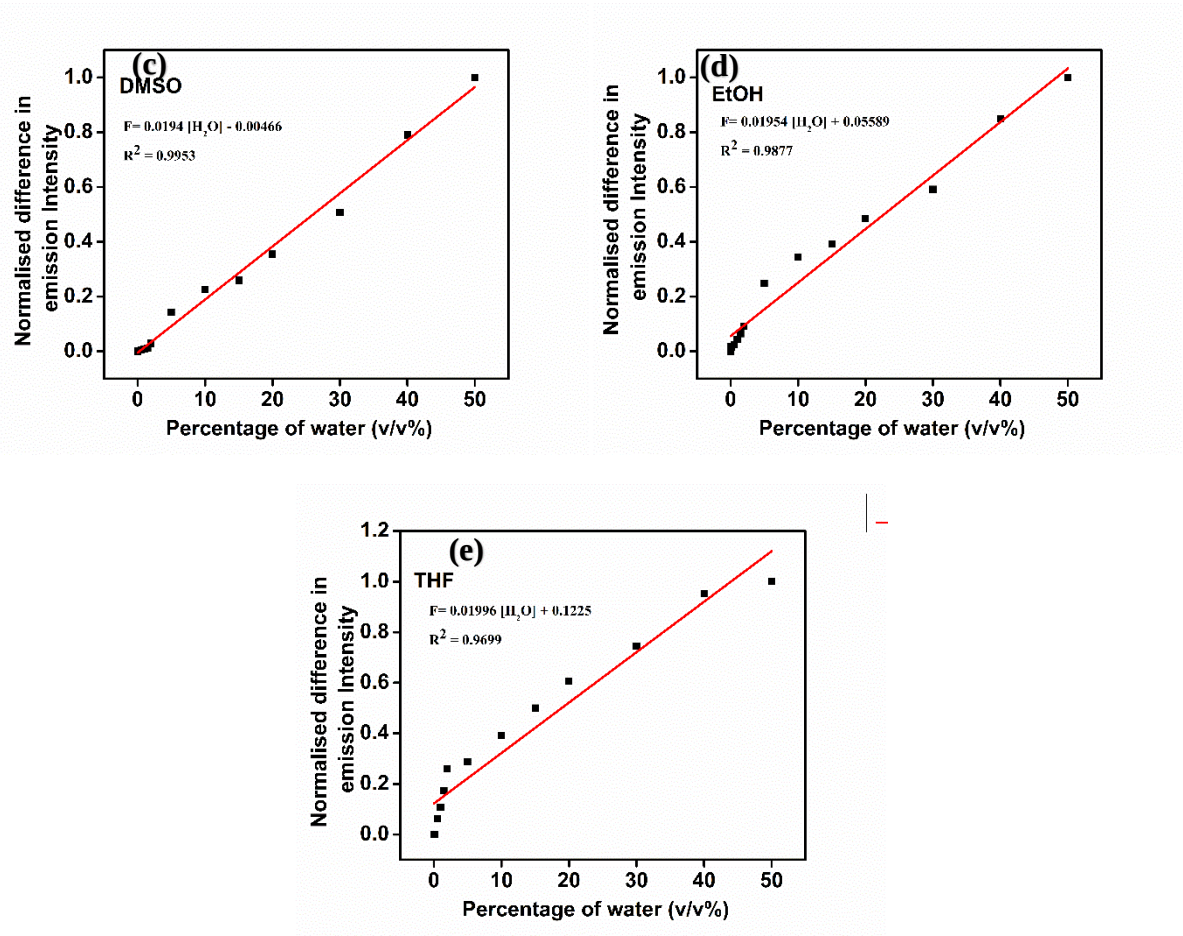


Figure S10. Normalized difference in emission intensity plot to find out the unknown water percentage in (a) ACN (b) Dioxane (c) DMSO (d) EtOH (e) THF

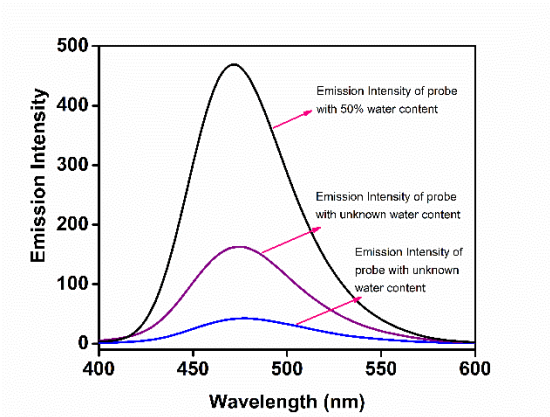
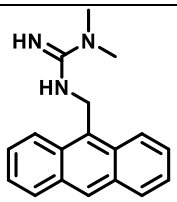
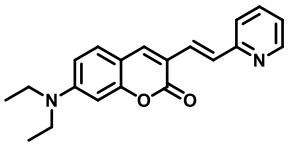
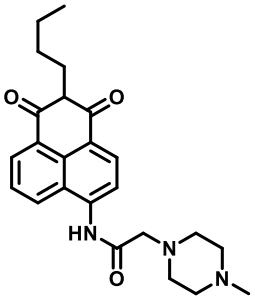
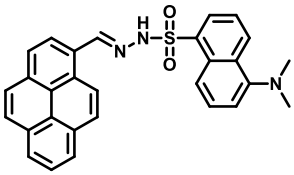
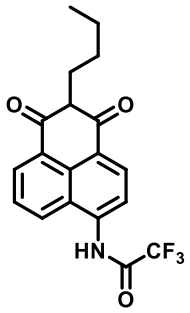
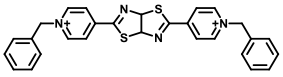
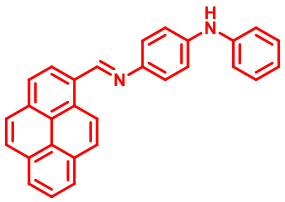


Figure S11. Emission intensity plot for the calculation of quantitative determination of water content.

Table S1: Comparison of previous reports of water sensors with PNPD

Sl. No.	Sensor molecule	Solvent	Sensing mechanism	LOD v/v%	LOQ v/v%	Reference
1		Dioxane DMF MeCN EtOH	PET	0.060 0.020 0.013 0.134	0.184 0.060 0.045 0.406	1
2		DMSO	Hydrolysis of imine bond	0.0018	0.540	2
3		MeOH EtOH	Protonation induced destabilization of excimer formation	1 2		3
4		Acetone	Monomer/excimer switching, ICT FRET	0.0165		4
5		MeCN MeOH EtOH	ICT	0.78 0.26 0.024		5
6		THF	H-bonding network	0.019		6
Present work		ACN Dioxane DMSO EtOH THF	Hydrolysis of imine bond	0.06246 0.18329 0.17478 0.39660 0.47389	0.20823 0.61097 0.58262 1.32201 1.57965	

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