Supporting Information for

A Turn-On Fluorescent Organic Nano-Optode Derived From Pyrene-Coupled Phenanthroimidazolate Room Temperature Ionic Liquid for Ultrasensitive Detection of Dextran Sulphate

Sabbir Ahamed and Sudhir Kumar Das*

Department of Chemistry, University of North Bengal, Raja Rammohunpur, Darjeeling, West Bengal-734013, India

Corresponding author: (Dr. S. K. Das; E-mail: sudhirkumardas@nbu.ac.in)

S1. Methods and materials

S1.1 General Remarks

All chemicals, including glacial acetic acid (CH3COOH) and ammonium acetate (NH_4OAc), are obtained from standard suppliers (Aldrich, Spectrochem, etc.) and used without further purification. **[PPIP]** was synthesized using simple ion exchange methods, and ^{1}H and ^{13}C NMR spectra were recorded on a Bruker-400 instrument, with the resonance of solvents and TMS used as an internal standard. Chemical shifts are reported in parts per million (ppm). High-resolution mass spectrometry (HRMS) analysis is performed on an Advanced Bio LC/Q-TOF spectrometer. A set of four Micro API (MICROMASS, UK) instruments, coupled to a LC-WATERS 2695 system equipped with a PDA2998 detector, is used for liquid chromatography-mass spectrometry (LC-MS) analysis. UV-Vis and fluorescence studies of compounds are analysed using HITACHI U-2910 and HITACHI F-7100 instruments, respectively. The morphological characteristics and particle size of n**[PPIP]** were examined using field-emission scanning electron microscopy (FE-SEM, ZEISS) at an accelerating voltage of 50 kV. For imaging, a 20 µg/mL suspension of **[PPIP]** was drop-cast onto carbon-coated grids. The average particle size was determined by analyzing more than 100 individual particles. The hydrodynamic diameter of the

nanoparticles was assessed using dynamic light scattering (DLS) on an Anton Paar Litesizer 500. The same instrument, equipped with a capillary cell, was also used to measure the particles' zeta potential. All experiments were conducted under standard laboratory conditions, and data analysis was performed using Origin software.

2.2 Synthesis of PDPI

In a 100 mL round-bottom flask, 300 mg (1.4408 mmol) of 9,10-phenanthrenequinone is dissolved in glacial acetic acid (AcOH), and then ammonium acetate (NH_4OAc) is added to the reaction mixture. Then, the reaction mixture is stirred for 90 minutes at 120 ℃ after the addition of 498 mg (2.1612 mmol) of 1-pyrenecarboxaldehyde. After completing the reaction, the reaction mixture is poured into ice-cold water, yielding a precipitate (ppt), which is washed thoroughly with cold water. The product is then dried in air. The light-yellow imidazole-based pyrene pendant molecule is purified by column chromatography using ethyl acetate/petroleum ether as the eluent.

1H NMR, 13C NMR, and HRMS spectral analysis confirm the structure of the product.

Characterization: (^{1}H NMR, DMSO-d_6, 400 MHz, in ppm units): 13.83 (1H, S), 8.95-8.91 (2H, m), 8.75-8.70 (2H, m), 8.66-8.64 (1H, d), 8.55-8.53 (1H, d), 8.41-8.39 (3H, d), 8.32 (1H, S), 8.18-8.15 (1H, t), 7.81-7.78 (2H, t), 7.71-7.68 (2H, t) (**Fig. S1**). (^{13}C NMR, DMSO-d_6, 100 MHz, in ppm units): 149.91, 137.84, 131.86, 131.45, 130.88, 129.04, 128.93, 128.82, 128.29, 128.18, 128.09, 127.89, 127.85, 127.77, 127.64, 127.59, 127.16, 126.32, 126.23, 125.99, 125.74, 125.35, 125.30, 124.91, 124.64, 124.31, 124.28, 122.93, 122.72, 122.51 (**Fig. S2**). From the high-resolution mass spectrum, the calculated molecular ion peak of **PDPI** ($m/z + H^+$) is 419.1563, whereas the obtained m/z value is 419.1556 (**Fig. S3**).

2.3 Synthesis of sodium salt of PDPI (Na-PDPI)

The sodium salt of PDPI is synthesized by a simple method: **PDPI** is dissolved in methanol. Then, sodium hydroxide (NaOH) is added to the solution, and stirring is

maintained for 2 hours. The reaction mixture is then evaporated to dryness. The solid product, a sodium salt of PDPI, is then collected.

Characterization: (^{1}H NMR, DMSO-d_6, 400 MHz, in ppm units): 8.93 -8.89 (2H, d), 8.59 (1H, s), 8.40 (1H, s), 8.32 (3H, s), 8.26-8.24 (2H, d), 7.83 (1H, s), 7.73-7.63 (4H, m), 7.62-7.59 (2H, t), 7.55-7.52 (2H, t) (**Fig. S4**). Here, the calculated m/z value is 441.1374, whereas the measured m/z value is 441.1350 (**Fig. S5**).

2.4 Determination of fluorescence quantum yield

For the determination of the fluorescence quantum yield (Φ_f) for **[PPIP]** in DMSO in DMSO and for increasing the fraction of water percentage to explored the ACQ mechanism, we have considered the quinine sulfate as a standard in 0.1(N) H_2SO_4 (Φ=0.55)[1] and used equation : $\Phi = \Phi_s\left(\frac{F_x}{F_s}\right)\left(\frac{A_s}{A_x}\right)\left(\frac{{\eta_x}^2}{{\eta_s}^2}\right)$, where Φ stands for quantum yield, F denotes the integrated photoluminescence intensity, A is defined as absorbance, η= solvent refractive index.

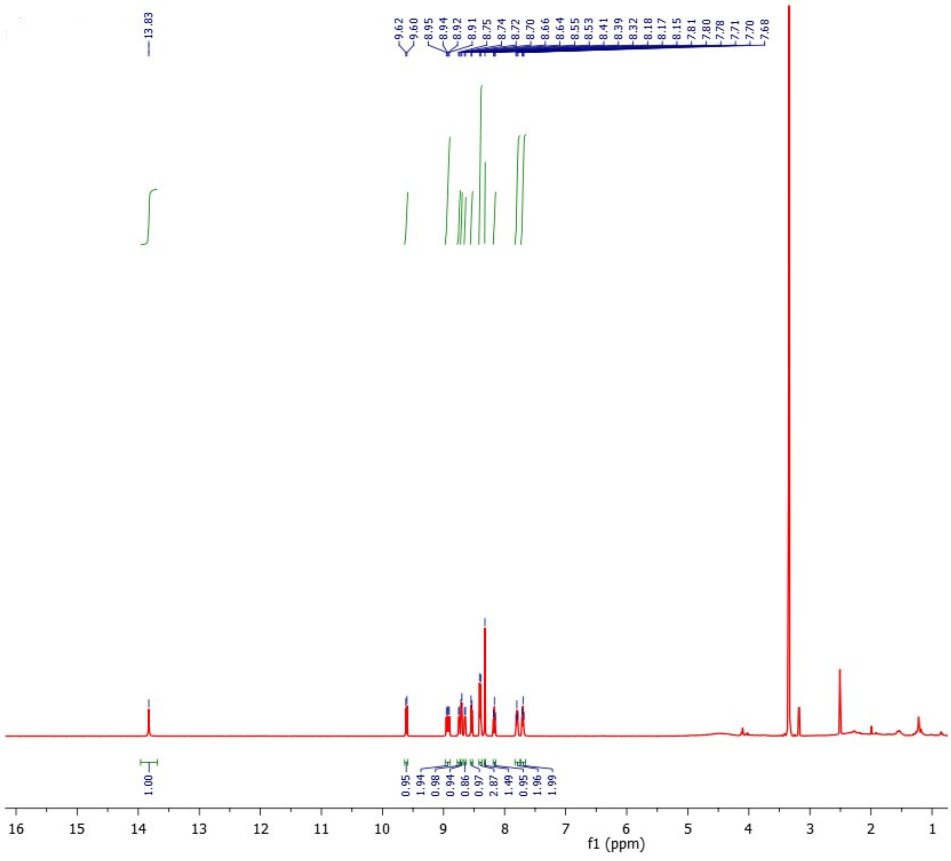


Fig. S1: ^{1}H NMR spectra of the **PDPI** in DMSO-d_6.

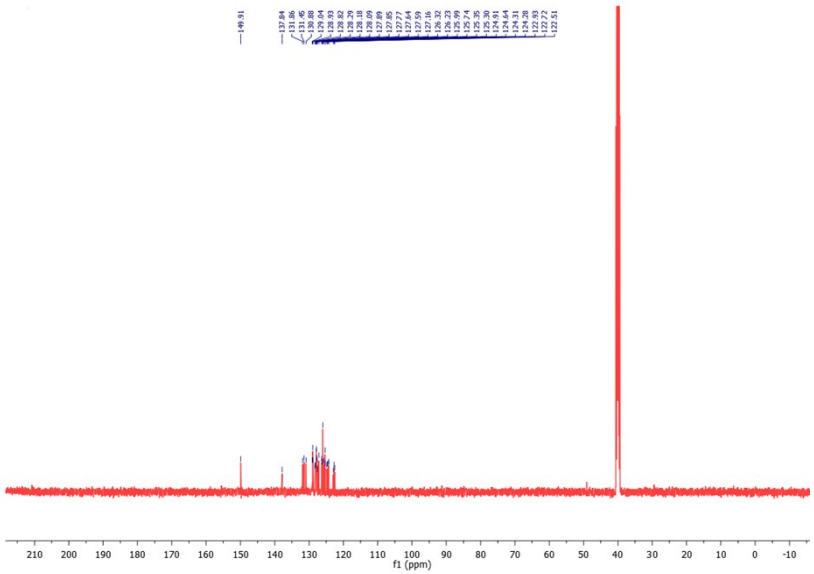


Fig. S2: ^{13}C NMR spectra of the **PDPI** in DMSO-d_6.

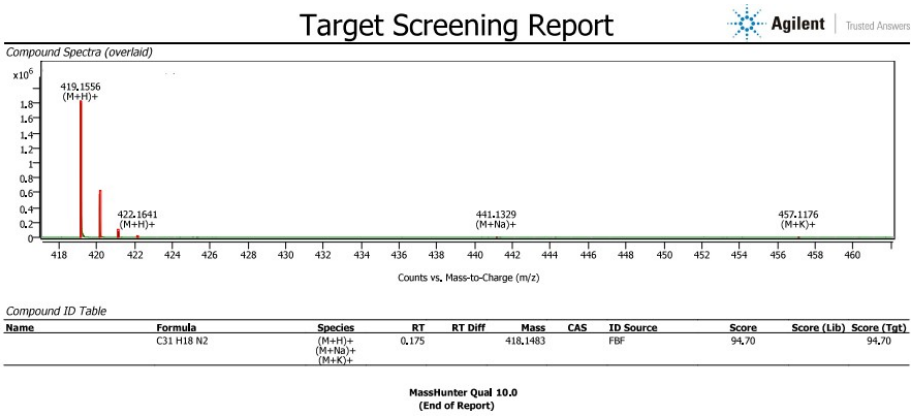


Fig. S3: HRMS spectra of **PDPI**.

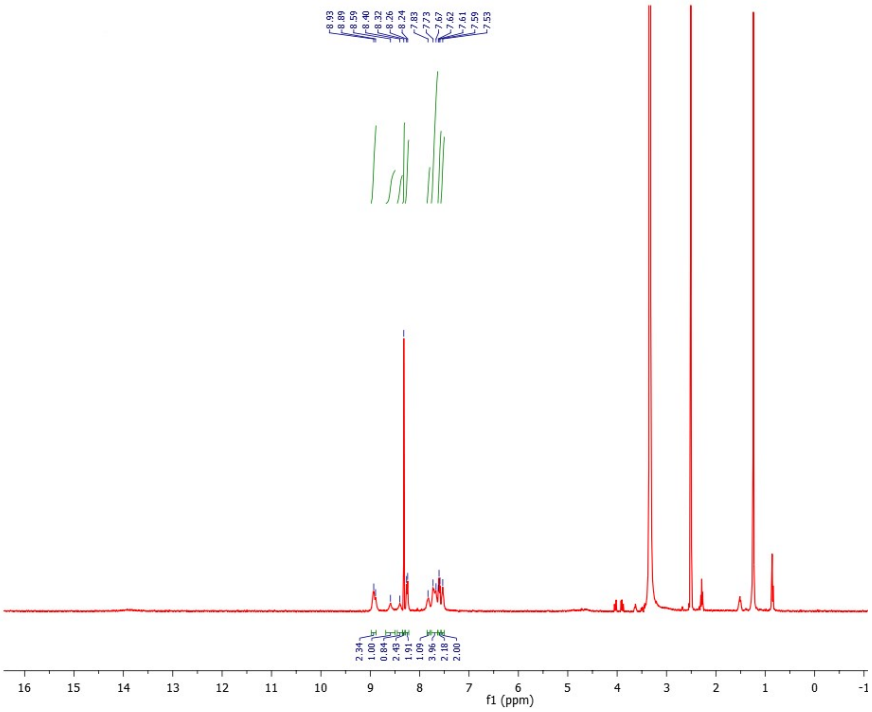


Fig. S4: ^{1}H NMR spectra of the **Na-PDPI** in DMSO-d_6.

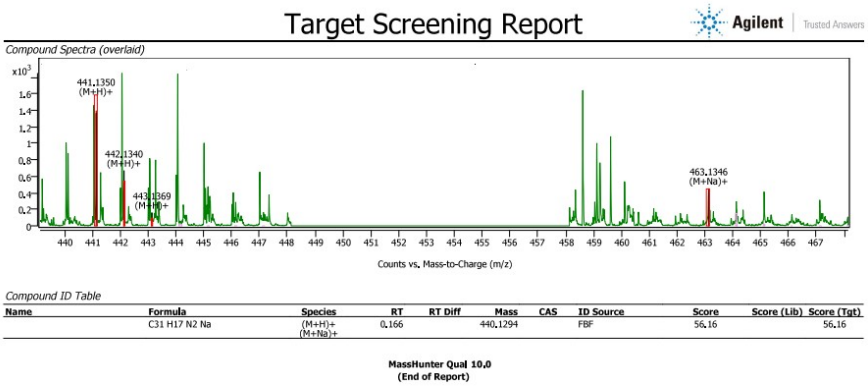


Fig. S5: HRMS spectra of **Na-PDPI**.

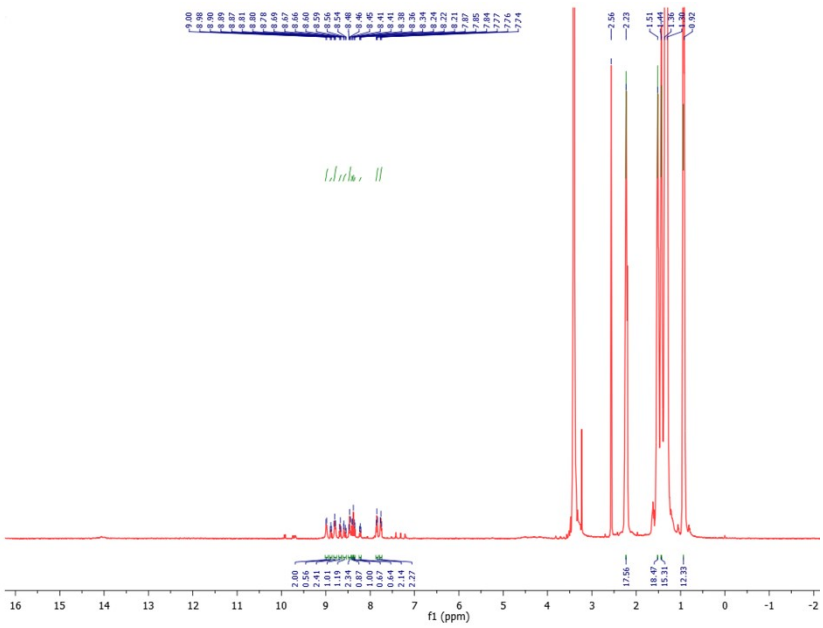
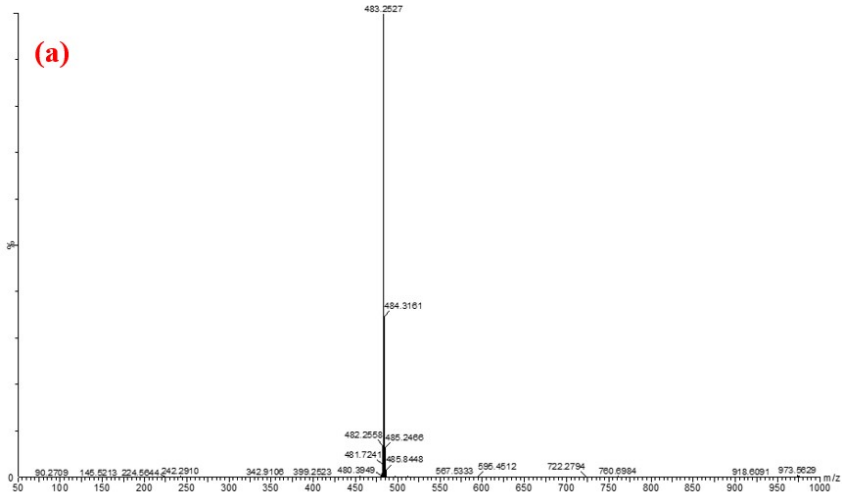


Fig. S6: ^{1}H NMR spectra of the sensor **[PPIP]** in DMSO-d_6.



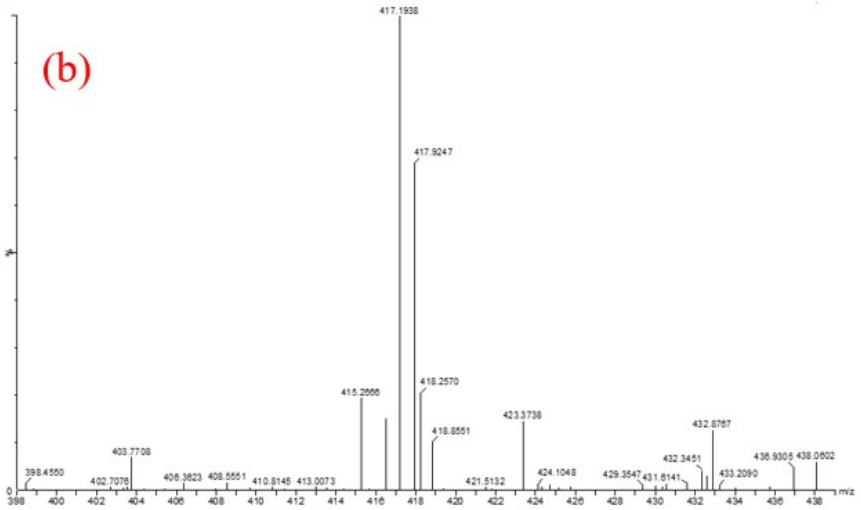


Fig. S7: LCMS spectra of **[PPIP] (a)** positive ion mode and **(b)** negative ion mode.

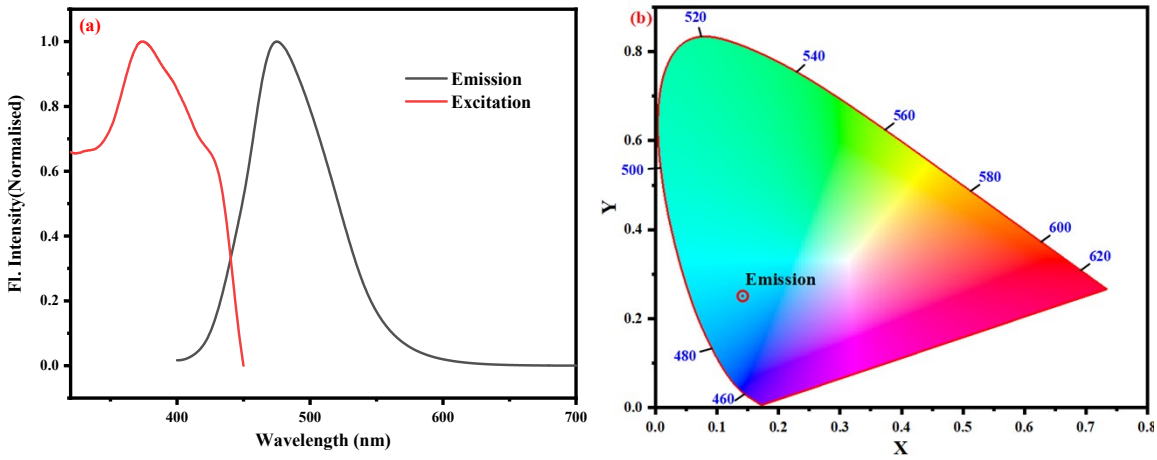


Fig. S8: (a) Excitation and emission spectra of **PDPI**. (**b**) Corresponding CIE diagram (X = 0.142, Y = 0.251).

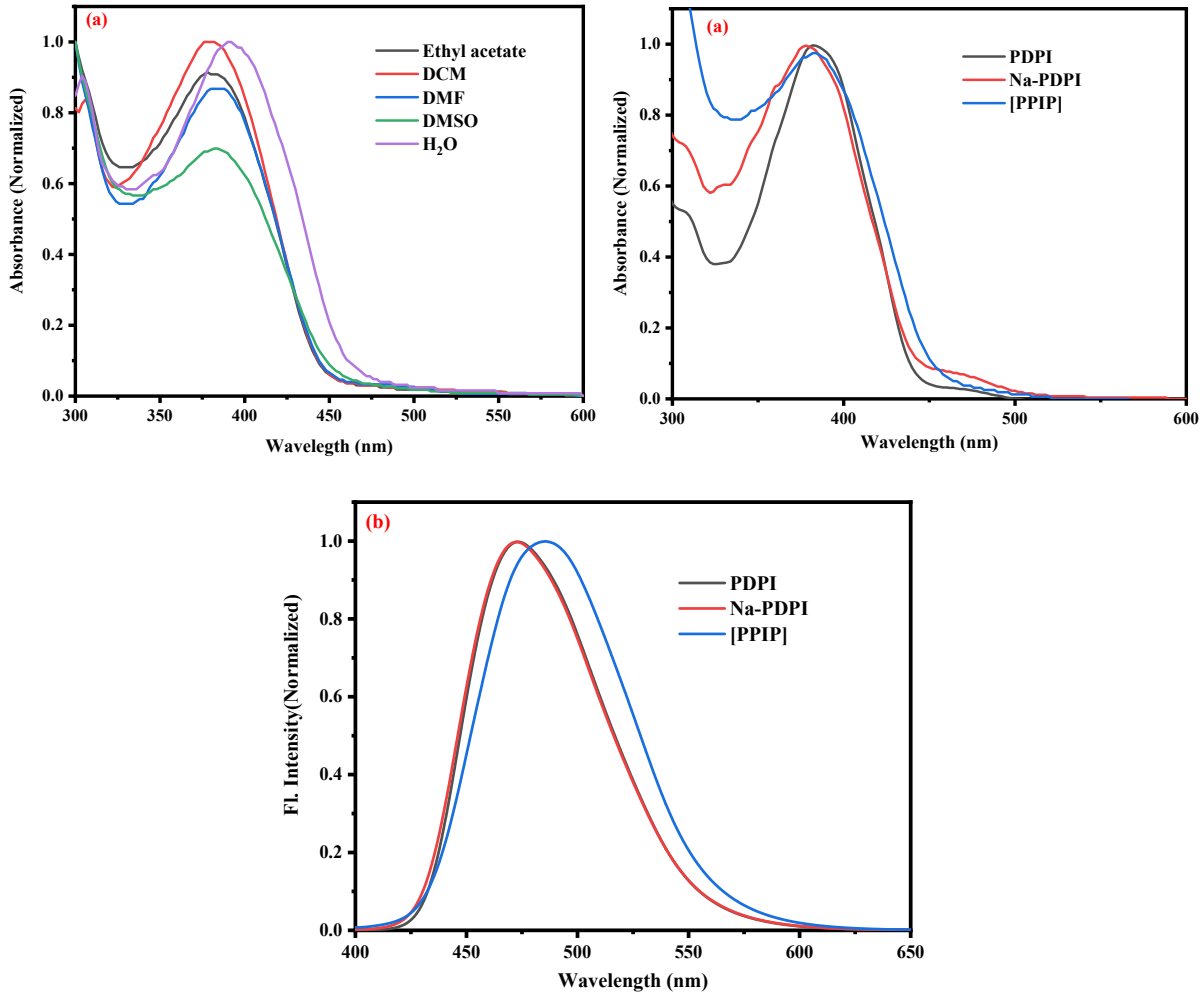


Fig. S9: (**a**) Normalized UV-visible spectra of **[PPIP]**, varying solvent polarity. (**b**) & (**c**) UV-visible and emission normalized spectra of parents' moiety **PDPI**, Na-**PDPI,** and synthesised IL, **[PPIP]** in DMSO medium, respectively.

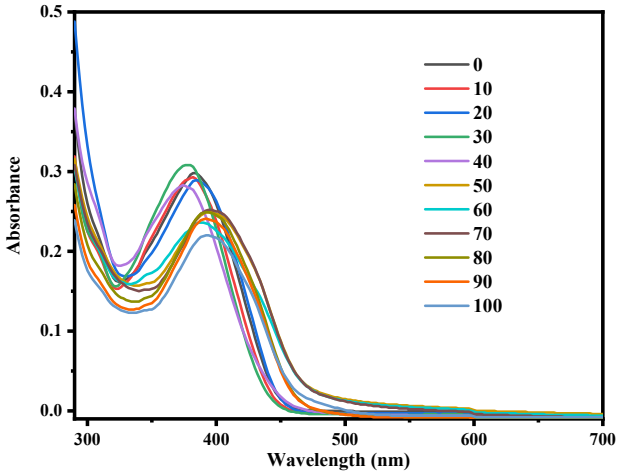


Fig. S10: UV-visible spectra of **[PPIP]**, varying the percentage of water.

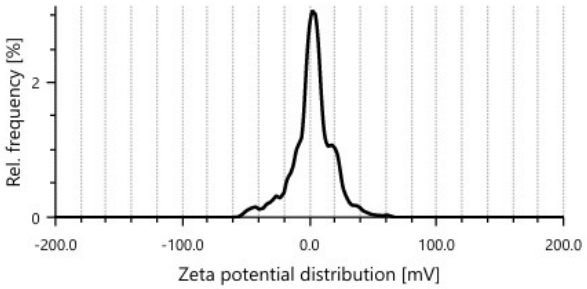


Fig. S11 Zeta potential diagram of n**[PPIP]**.

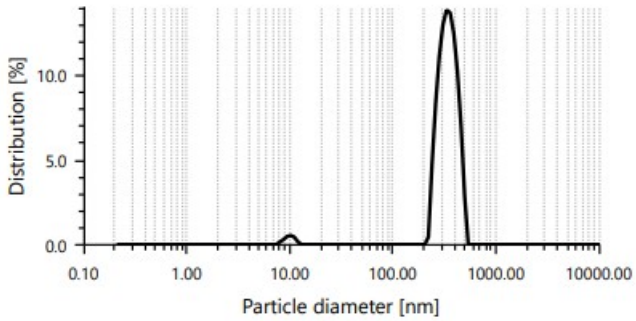


Fig. S12: DLS spectrum of n**[PPIP]** for the addition of DSS.

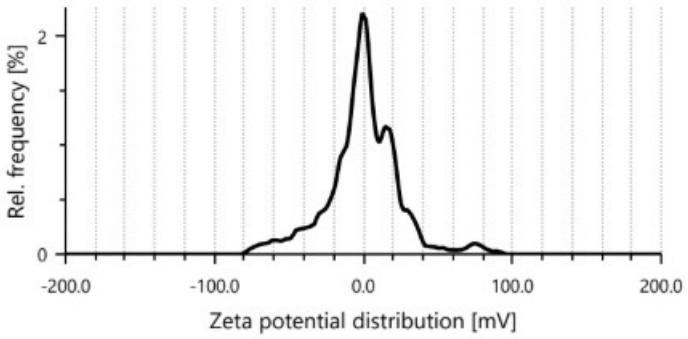


Fig. S13: Zeta potential diagram of n**[PPIP]** after interaction with DSS.

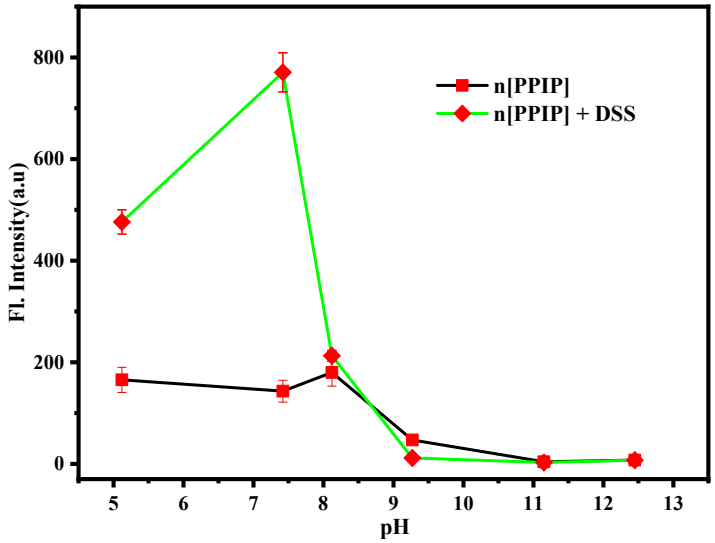


Fig. S14: pH metric analysis of free n**[PPIP]** and with the addition of DSS.

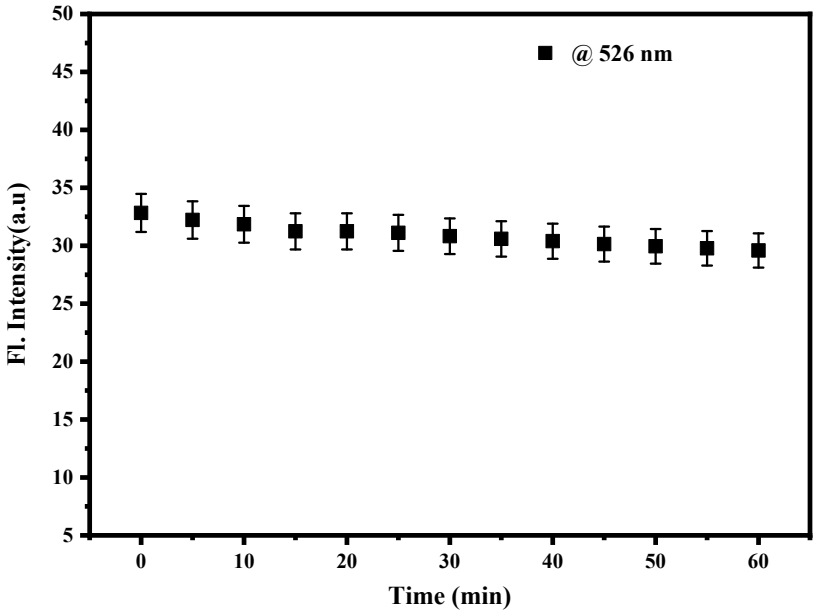


Fig. S15: Stability of the sensor n**[PPIP]** under the constant exposure of UV- irradiation.

Table S1: Comparison table of different chemosensors that have been introduced for the detection of DSS in the last few decades, with our prepared aggregates n**[PPIP]**.

Quantification Method	Matrix	Detection range	Detection limit (ng/mL)	Ref.
Competitive binding assay	plasma	1.4 to 2.5 µg/mL	1000	[2]
Size exclusion HPLC + postcolumn photometry (dimethyl methylene blue)	serum	NA	300	[3]
Strong ion exchange HPLC + postcolumn photometry (dimethyl methylene blue)	protein solution	1.0 to 10.0 µg/mL	300	[4]
Potentiometric membrane electrode	NaCl solution	0.955 - 4.467 ppm	760	[5]
phenol–sulfuric acid assay	syrup samples.	400 – 10000 mg/L	300	[6]
Rayleigh Scattering (TWO-RRS)	NA	0.1–2.5 µg/mL	13	[7]
Imidazolate-based pyrene pendant ionic liquid	**100% water,**	**9 – 79 µg/mL**	**5.5**	**This work**

References

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