Supplementary File

Water recyclable and reusable fluorescent sensor for nerve gas mimic detection

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Table of Contents

Characterization data of probes

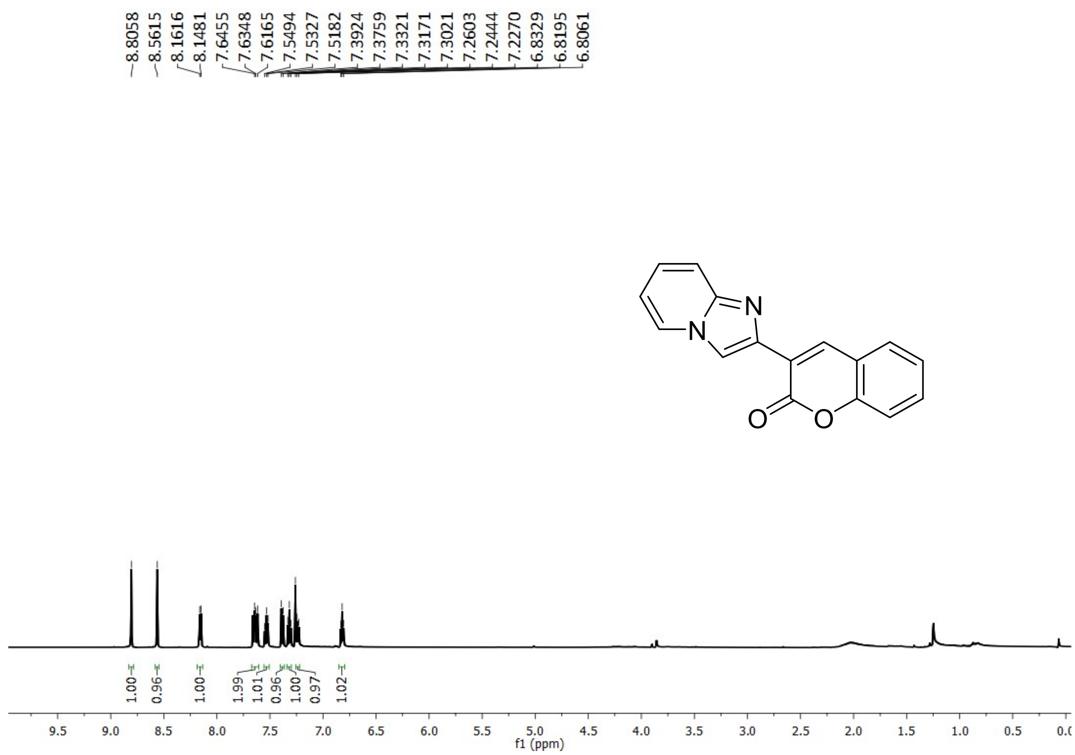


Figure S1. ^{1}H NMR spectrum of **IMPC** at 500 MHz in $CDCl_3$

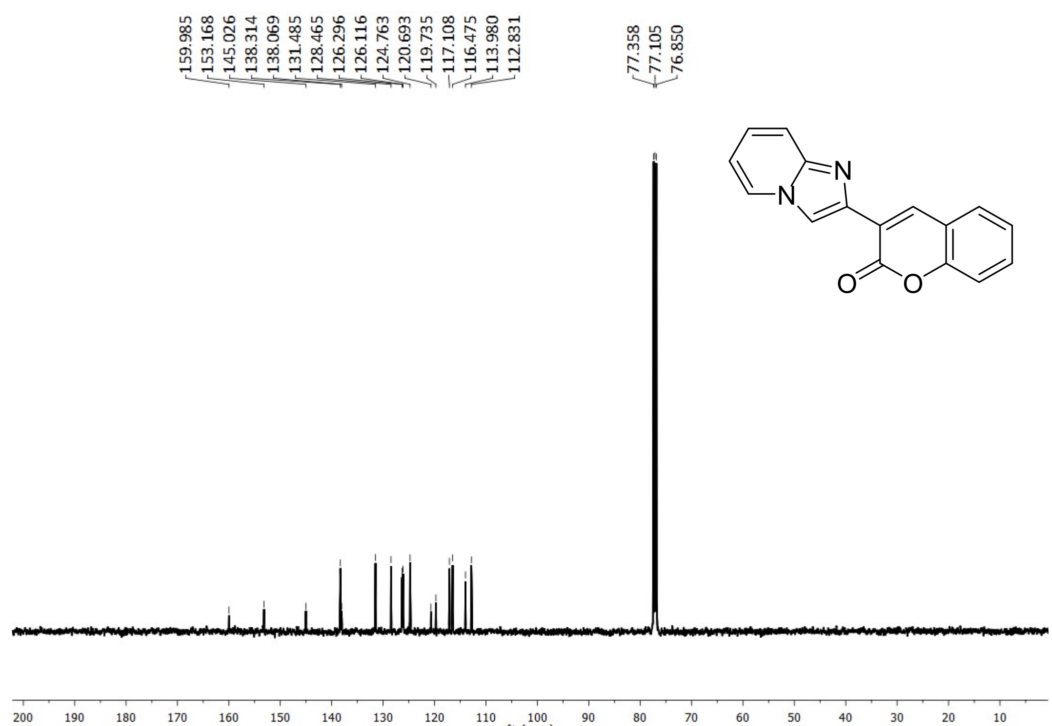


Figure S2. ^{13}C NMR spectrum of **IMPC** at 125 MHz in $CDCl_3$

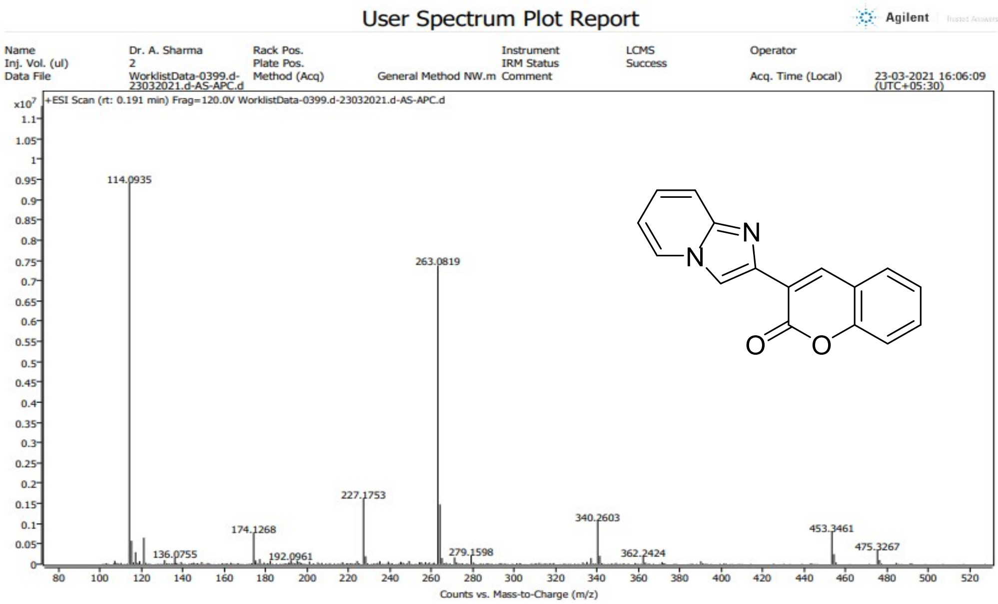


Figure S3. HRMS Data of **IMPC**

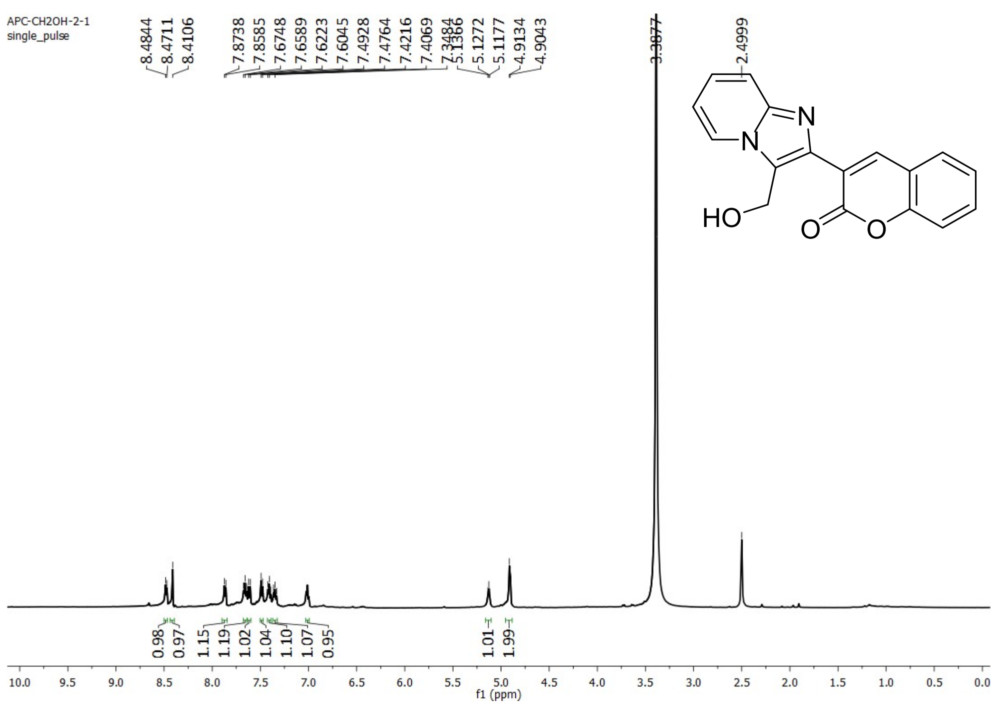


Figure S4. ^{1}H NMR spectrum of **IMPC-OH** at 500 MHz in DMSO-d_6

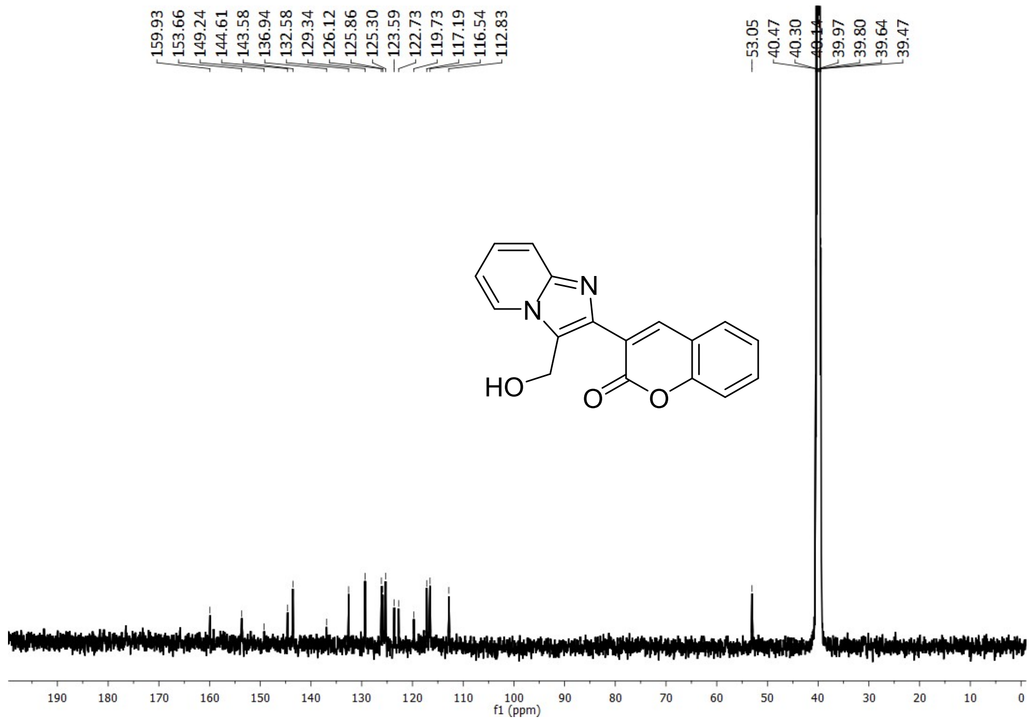


Figure S5. ^{13}C NMR spectrum of **IMPC-OH** at 125 MHz in DMSO-d_6

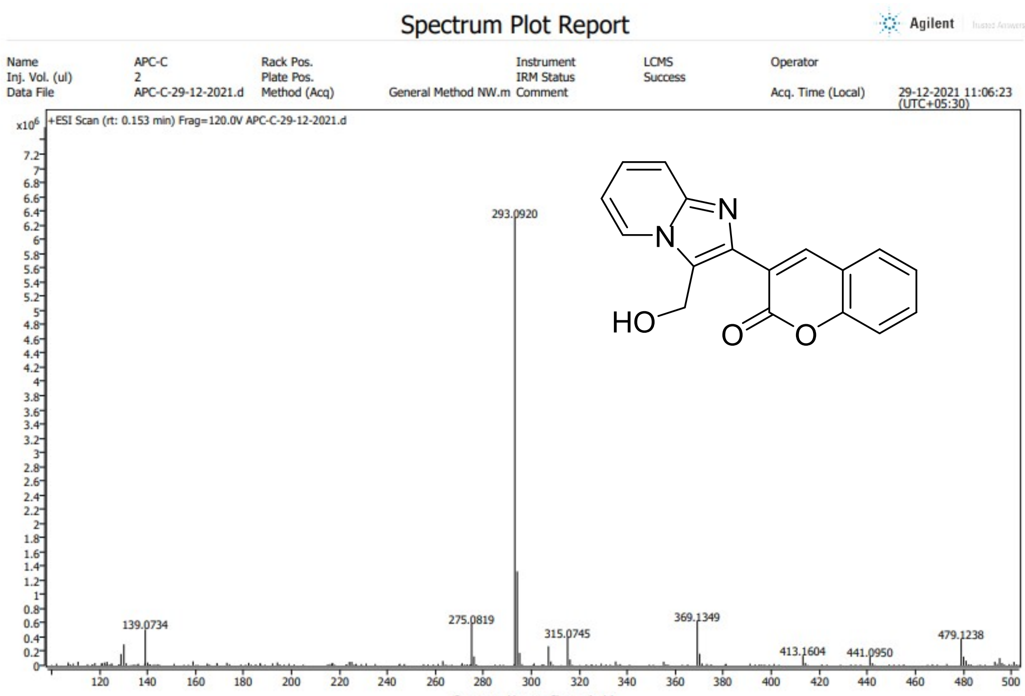


Figure S6. HRMS Data of IMPC-OH

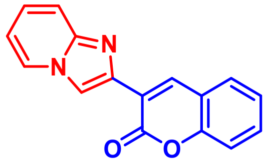
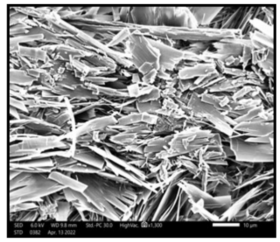
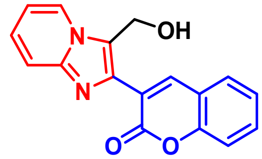
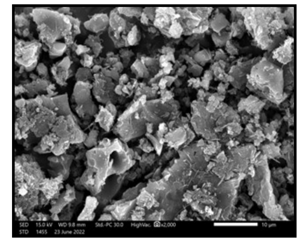
Table S1. Summary of previously reported fluoroscent probes for the detection of OPs.

Sr. No.	Analytes detection	Sensor type	Detection limit	Detection state	Response type	Recyclable	Test kit method	Reference
1	**DCNP**	**Imidazo[1,2-a]pyridine based probe**	**IMPC 0.1 µM** **IMPC-OH 0.13 µM**	**Liquid**	**Change in color**	**Yes**	**Yes**	**Present Manuscript**
	DCP	**Imidazo[1,2-a]pyridine based probe**	**IMPC 1.58 nM** **IMPC-OH 0.62 nM**	**Liquid**	**Change in color**	**Yes**	**Yes**	**Present Manuscript**
2	DCNP, DCP	Triaryl methane dye	2.1 mM - 3.2 mM	Liquid	Change in color (naked eye)	No	No	*Tetrahedron* 2012, 68, 8612-8616
4	DCNP	B-Sal-Oxime based	92.2 µM	Liquid	-	No	No	*Chem. Commun.*, 2014, 50, 7531-7534.
5	DCNP, DCP	BODIPY	2.45 µM and 2.21 µM	Liquid	Change in color	No	Yes	*Org. Biomol. Chem.* 2014, 12, 8745–8751
6	DCNP	polymeric based probe	1 mM	Liquid	Naked eye	No	Yes	*Macromolecules.*, 2016, 7, 2568-2574.
7	DCNP, DMMP, DCP	Zn(II) bisterpyridine	0.1 µM	Liquid	-	No	Yes	*Chem. Commun.* 2012, 48, 964–966
8	DCNP, DCP	Fluorescein-hydroxamate aldehyde based probe	3 mM	Liquid	Change in color (naked eye)	No	Yes	*RSC Adv.*, 2014, 4, 24645-24648.
9	DCNP	N,N-dimethylaniline and pyridine containing dye	0.9 mM	Liquid	Change in color (naked eye)	No	Yes	*Chem. Eur. J.* 2011, 17, 6931 – 6934
10	DCP	Rhodium(II,II) Paddlewhe	0.113 µM	Liquid	Change in color (naked eye)	No	No	*Sens.*,2024, 2325-2333.

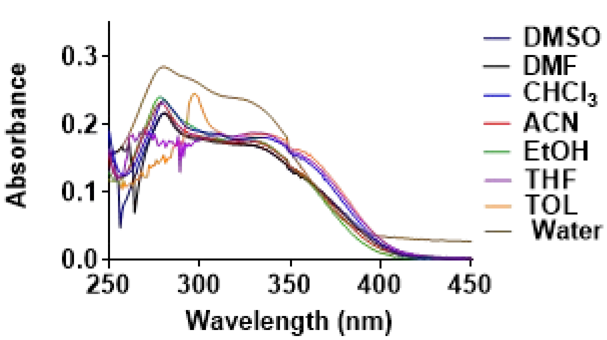
		el Complexes						
11	DCNP	Pyrene derived polymeric probe	0.1 mM	Liquid	Turn-on fluroscemce	No	Yes	*Macromolecules.*, 2017, 17, 6888-6895.
12	DCP	rhodamine-deoxylactum-based sensor	9.66 nM	Liquid & Gaseous	colorimetric and fluorimetric sensor	No	Yes	*Dyes and Pigments,* 2019, 171, 107712.
13	DCNP	Bis-indolyl based probes	10.8 µM	Liquid	Change in color (naked eye)	No	Yes	*Analyst*, 2018, 143, 528-535.

Table S2 Solvent-dependent photophysical properties of **IMPC** and **IMPC-OH**

#		**IMPC**		**IMPC-OH**	

								
Solvents	**Absorbance $\lambda_{abs,\ max}$ (nm)**	**Emission $\lambda_{em,max}$ (nm)**	**Stokes Shift (Δ ν cm^{-1})**	**Molar Extension coefficient (Ɛ ($M^{-1}cm^{-1}$)**	**Absorbance $\lambda_{abs,\ max}$ (nm)**	**Emission $\lambda_{em,max}$ (nm)**	**Stokes Shift (Δ ν cm^{-1})**	**Molar Extension coefficient (Ɛ , $M^{-1}cm^{-1}$)**
DMSO	358	514	8477	18000	349	535	9891	9900
DMF	348	504	8894	21000	348	514	10013	9300
$CHCl_3$	348	461	7043	22000	348	480	7902	11400
ACN	346	495	8699	27000	347	525	9734	11500
EtOH	355	498	8088	21000	336	446	4509	10900
THF	357	486	6958	25000	341	402	9365	11700
TOU	358	472	6746	20700	345	491	8281	11100
Water	353	427	7538	13000	336	393	-	10000

A



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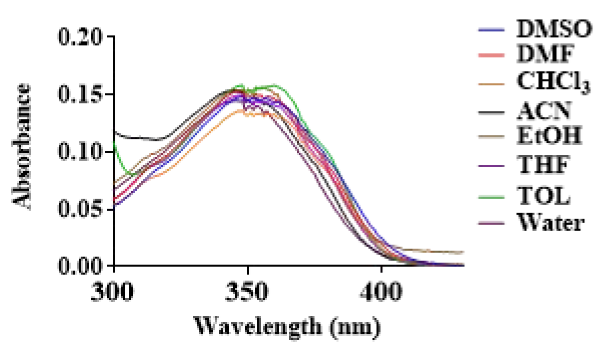

Figure S7. (A) UV-Vis. absorption of **IMPC** (20 µM) (B) UV-Vis. absorption of **IMPC-OH** (20 µM)

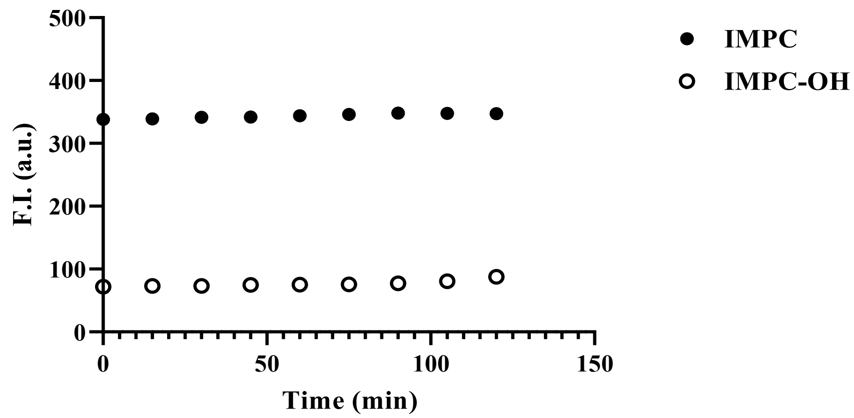

Figure S8. Photostability of (A) IMPC and (B) IMPC-OH

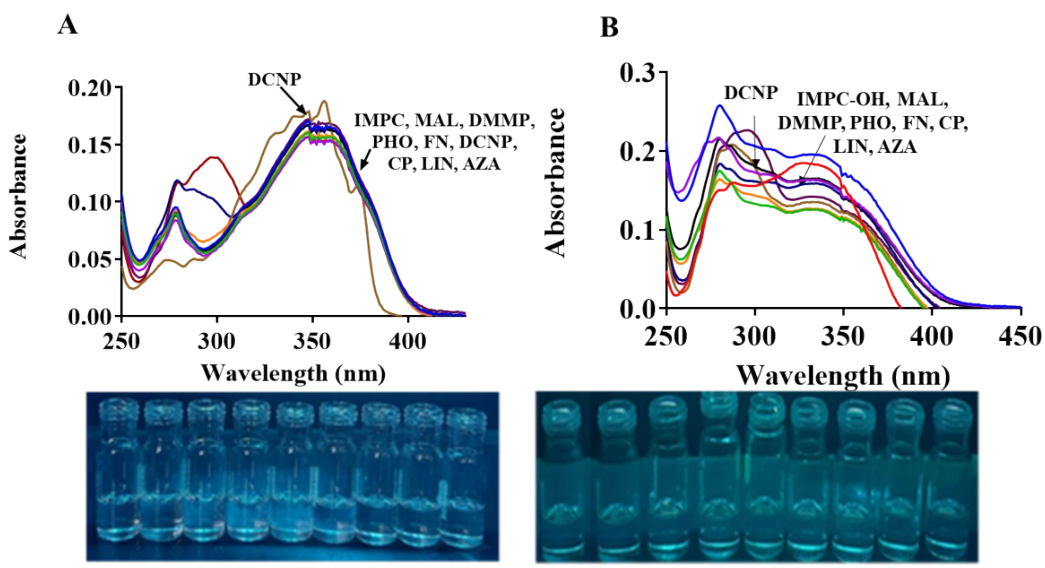

Figure S9. (A) UV-vis. Spectrum of **IMPC** (10 µM) (λ_{ex} = 348 nm, exc. slit width = 5, em. slit width= 5 and 560 V) and (B) UV-Vis. of **IMPC-OH** (20 µM) (λ_{ex} = 348 nm, exc. slit width = 10, em. slit width= 10 and 500 V) against various types of OPs compounds (10 µM) in CHCl3 and their visual changes under hand-held UV lamp at wavelength 254 nm for **IMPC**, MAl, DMMP, PHO, FN, DCNP, CP, LIN, AZA left hand side images and **IMPC-OH** followed by same sequence of OP compounds (right hand side images).

Quantum Yield Measurements

To calculate the quantum yield, a single point method was used with quinine sulphate as a reference having quantum yield of 0.54 at 360 nm. The following equation was used to calculate the quantum yield:

$$\Phi_S = \Phi_R \times \left(\frac{I_S}{I_R}\right) \times \left(\frac{1-10^{-A_R}}{1-10^{-A_S}}\right) \times \left(\frac{\eta_S}{\eta_R}\right)^2$$

where, Φ_S refers to quantum yield of sample, Φ_R refers to quantum yield of reference, I_S & I_R being the measured integrated emission intensity (area under the curve), A_R & A_S refers to the absorbance of reference & sample, η_S and η_R is the refractive index for sample and reference. In order to minimize the re-absorption effects, absorbance intensity was kept below 0.1 at the excitation wavelength in the 10 mm fluorescence cuvette. An excitation and emission slit width of 5 nm at 600 V was used.

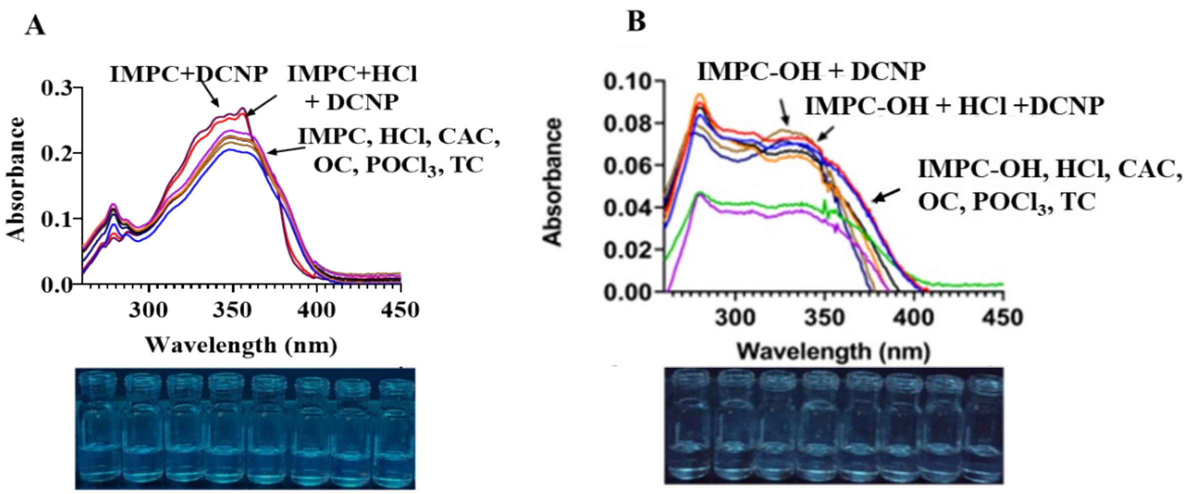

Figure S10. (A) UV spectra of **IMPC** (10 μM) (B) **IMPC-OH** (20 μM) with different interfereing analytes (λ_{ex} = 348 nm, exc. slit width = 10, em. slit width= 10 and 500 V) and their photographs under a UV lamp at 254 nm.

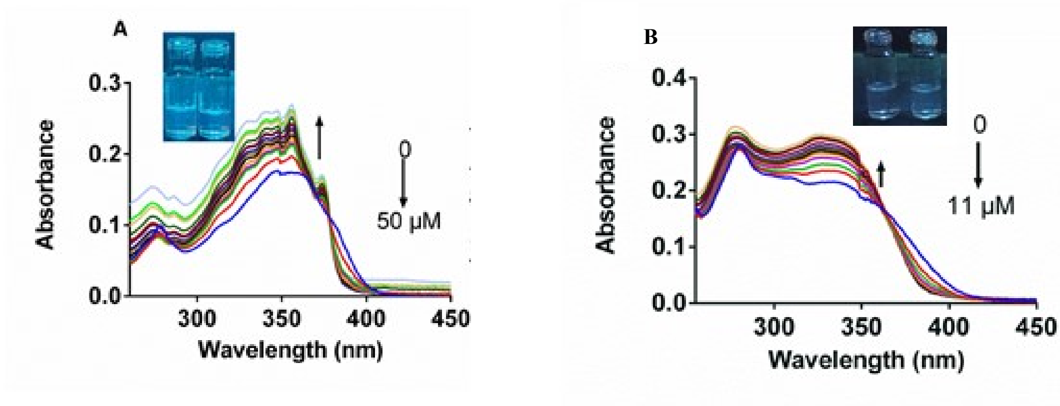

Figure S11. (A) UV-Vis. of **IMPC** (10 μM) (B) **IMPC-OH** with increasing concentration of DCNP Inset: Visible color image of **IMPC-OH** in absence and presence of DCNP under UV lamp at 254 nm.

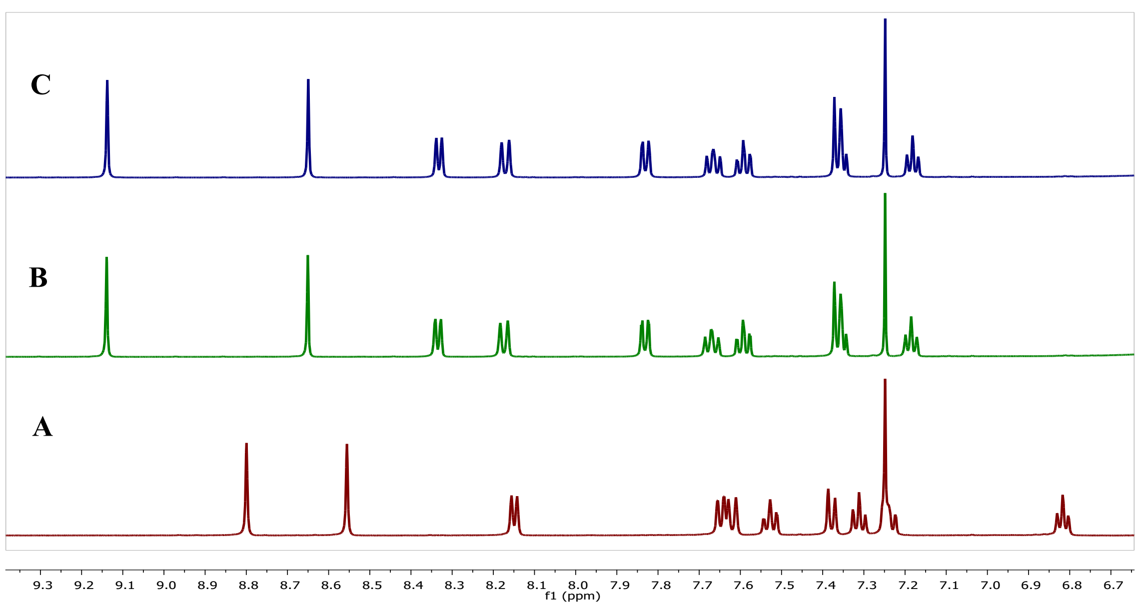

Figure S12. Partial 1H NMR of (A) **IMPC** (B) **IMPC** with DCNP just after addition (C) **IMPC** with DCNP after 1hr at 500 MHz in CDCl3.

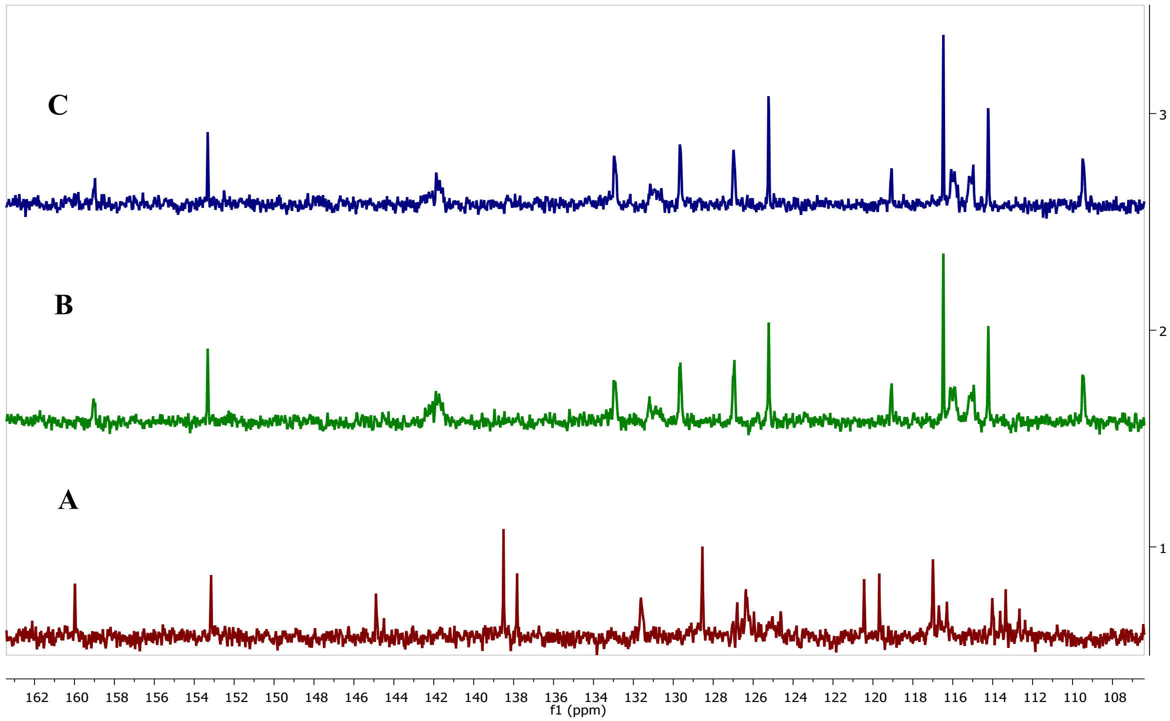

Figure S13. ^{13}C NMR of (A) **IMPC** (B) **IMPC** with DCNP just after addition (C) **IMPC** with DCNP after 1hr.

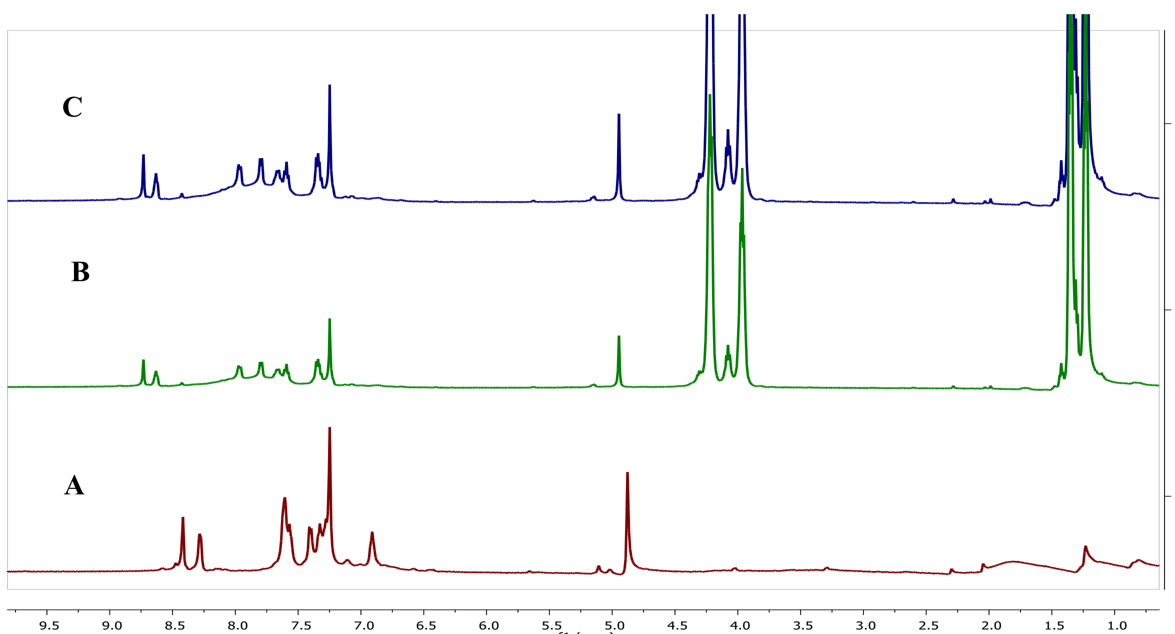

Figure S14. Partial 1H NMR of (A) **IMPC-OH** (B) **IMPC-OH** with DCNP just after addition (C) **IMPC-OH** with DCNP after 1hr at 500 MHz in CDCl3.

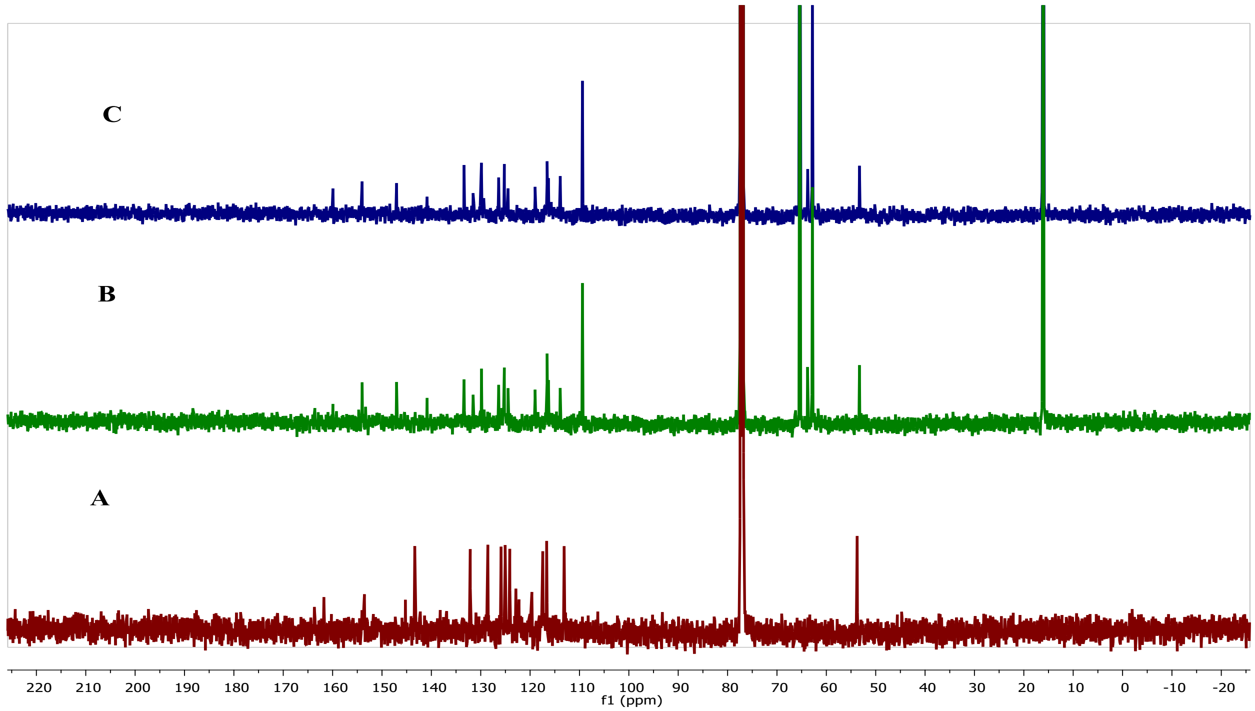

Figure S15. Partial ^{13}C NMR of (A) **IMPC-OH** (B) **IMPC-OH** + DCNP (just after addition) (C) After 1 hr. at 125 MHz in $CDCl_3$.

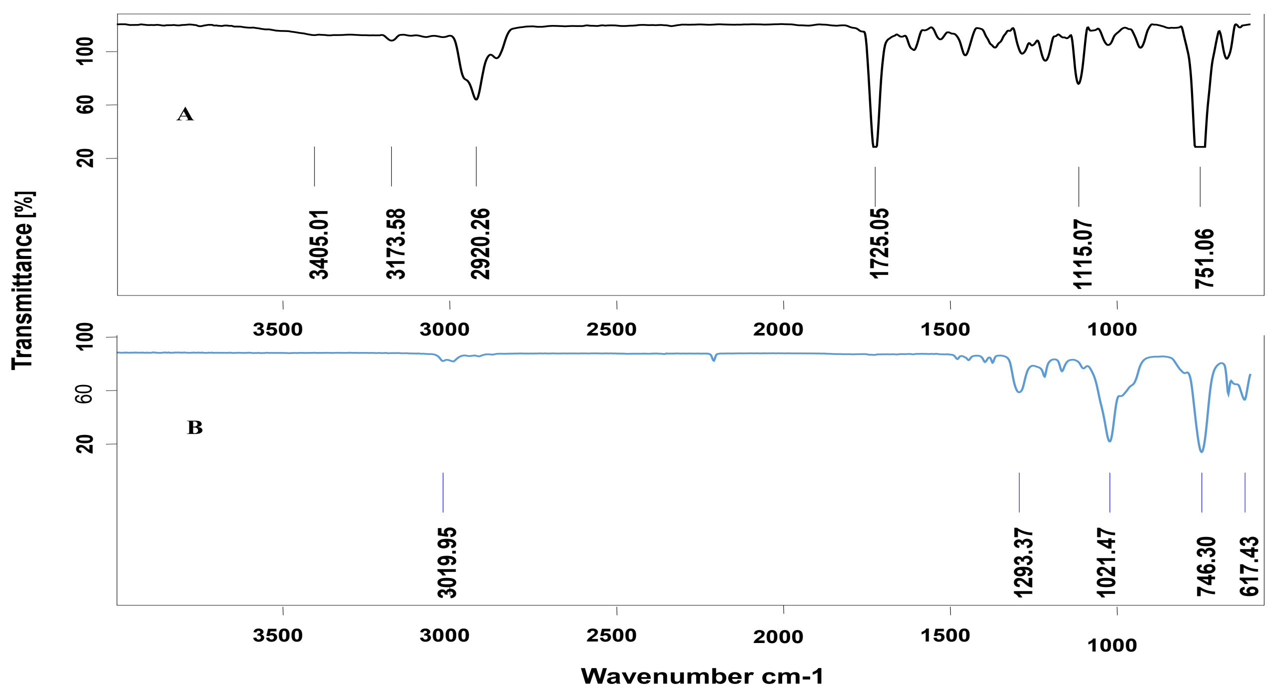

Figure S16. IR spectrum of (A) **IMPC** alone and (B) **IMPC** with DCNP.

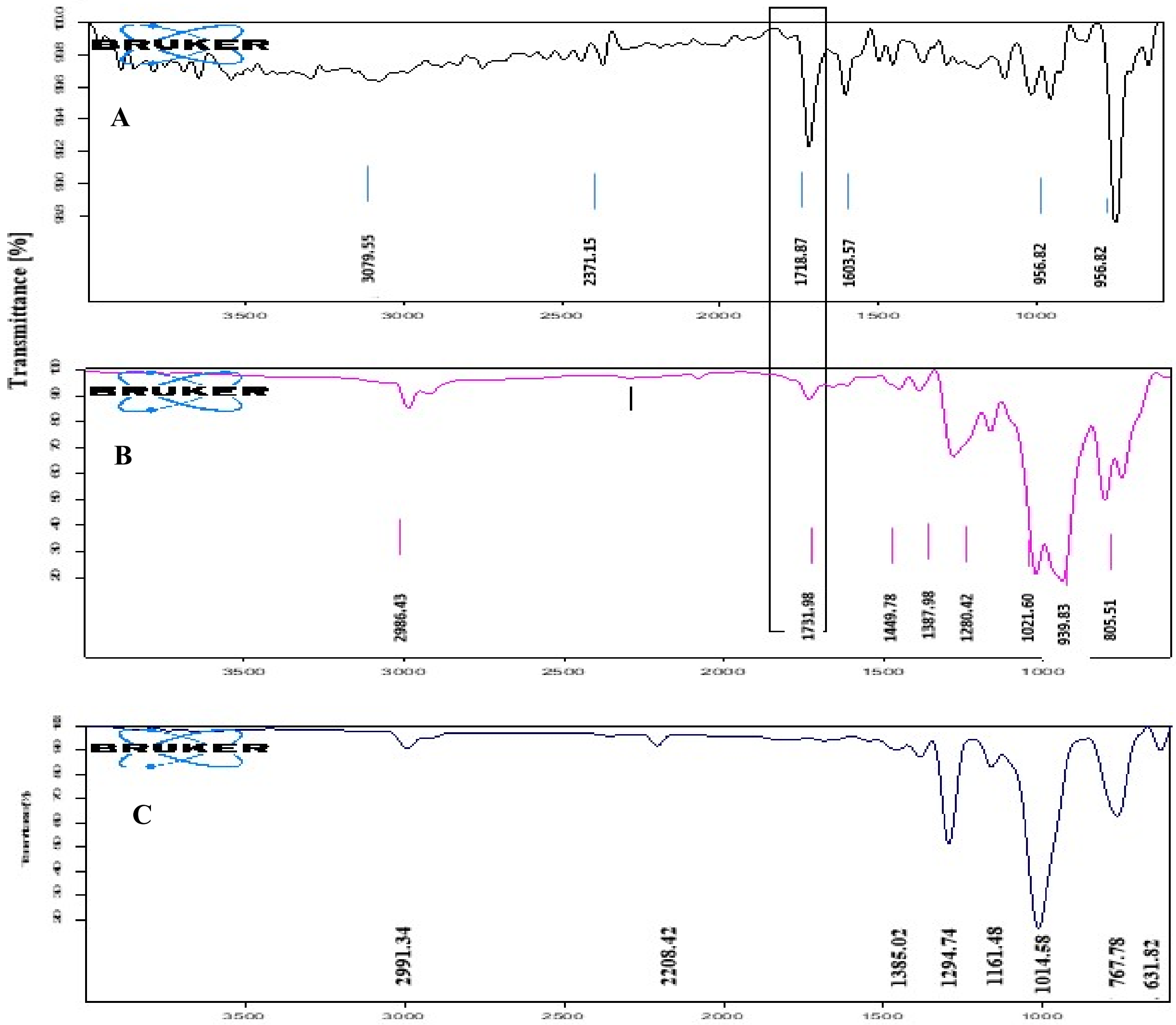

Figure S17. IR spectrum of (A) **IMPC-OH** alone and (B) **IMPC-OH** with DCNP (C) DCNP only.

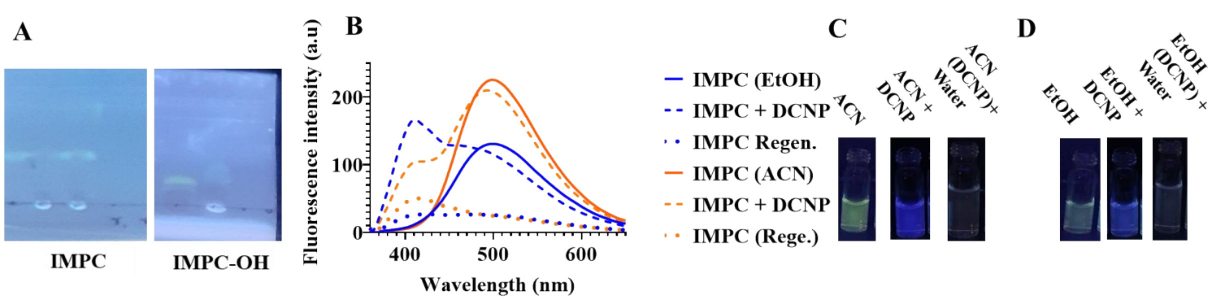

Figure S18. (A) TLC analysis of **IMPC** (left) and **IMPC-OH** (right) where probe only, probe with DCNP followed by Co are spotted from left to right (B) Fluorecence spectrum of **IMPC** in solvent EtOH and ACN, after addition of DCNP and upon dilution with water (C) Visualization of the EtOH systems (D) Visualization of the ACN systems at 365 nm.

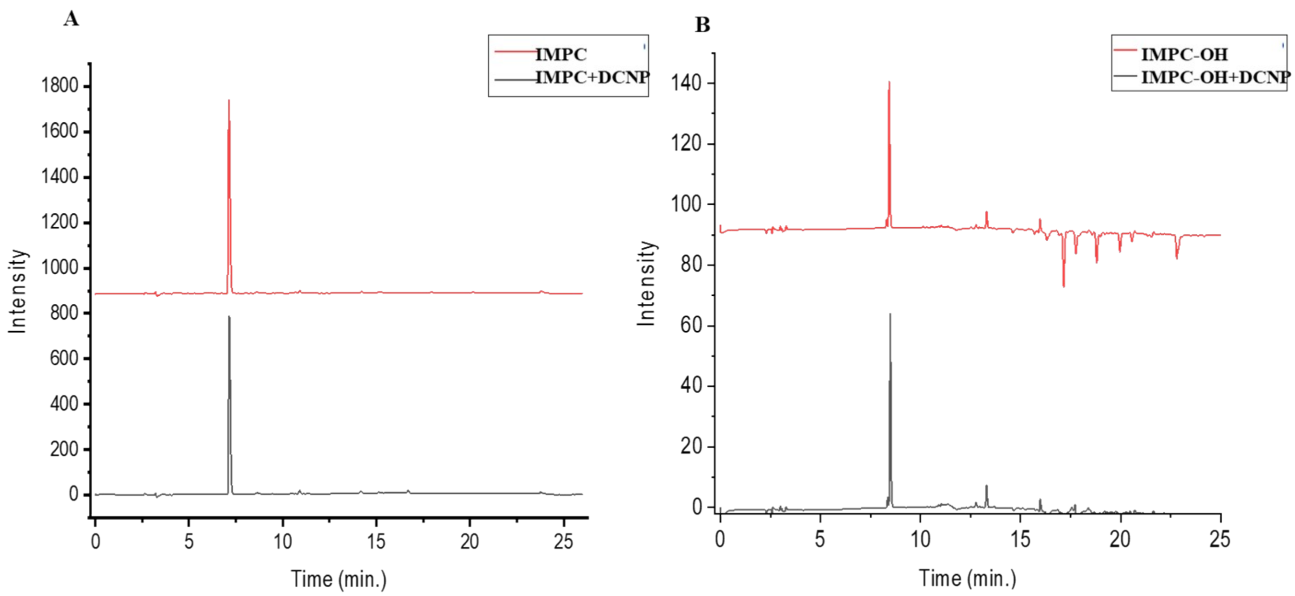

Figure S19. HPLC data of (A) **IMPC** and **IMPC** with DCNP, (B) **IMPC-OH** and **IMPC-OH** with DCNP HPLC Analysis.

High-performance liquid chromatography (HPLC) analysis was performed to prove the regeneration mechanism of both probes, which was executed on Agilent HPLC with a Eclipse Plus C18 reverse-phase column (4.6 mm x 250 mm, 5 µM, S.No.USUXA31525) at room temperature.

Time (min.)	A (0.1% Formic acid in water)	B (Acetonitrile)
2.00	90	10
20.00	10	90
20.50	10	90
23.90	10	90
24.00	90	10
27.00	90	10

Mobile phase: A (Formic acid in water (0.1%)): B (ACN)

Flow rate: 1 mL/min

Detector: UV/Vis. detector.

Data acquired were processed using Open Lab CDS Chemstation Analysis data system.