Supporting Information for

A Benzoxazole-triphenylamine Conjugated Fluorogenic Probe for Specific Detection of Sarin gas Mimic, Diethylchlorophosphate

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Table of contents

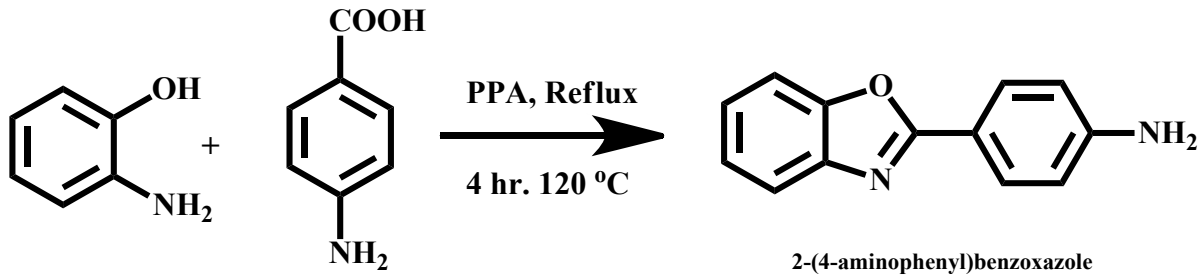
1. Materials and instrumentations

All reagents used in the synthetic procedure are purchased from Sigma-Aldrich, India, and TCI, India, respectively. All organophosphates used in the present study are purchased from Sigma-Aldrich, India, and TCI, India. HPLC-grade solvents are used for synthesis and spectroscopic studies purpose. For nuclear magnetic resonance (NMR) spectral analysis, deuterated chloroform ($CDCl_3$) is used and obtained from Sigma Aldrich-India. ^1H NMR and ^{13}C NMR spectra are recorded on a Bruker 400 MHz instrument

at ambient conditions using tetramethylsilane (TMS) as a standard reference with chemical shifts (δ) in ppm unit. On an Agilent 6545XT AdvanceBio LC/Q-TOF spectrometer, high-resolution mass spectra (HRMS) have been performed. The UV-visible absorption spectrum study and photoluminescence experiments have been carried out on a HITACHI U-2910 and HITACHI F-7100 fluorimeter with 2.5 nm excitation and emission slit, respectively, under ambient environments. Excitation and emission wavelengths during the photoluminescence experiment are kept at 320 nm and 340-600 nm, respectively.

2. Synthesis of 2-(4-aminophenyl) benzoxazole (L)

2-(4-aminophenyl) benzoxazole is prepared by following the literature procedure. A mixture of 2-aminophenol (1 g, 9.17 mmol) and polyphosphoric acid (PPA) (20 g) is refluxed for 30 min at 120 ℃, then added 4-aminobenzoic acid (1.3 g, 9.17 mmol) and again refluxed 4 hours at 120℃ temperature, then poured the reaction mixture into an ice-cold water bath. The purified product was collected by column chromatography, and finally, the brownish solid of L was isolated (**Scheme S1**). Yield 85% ^{1}H NMR (400 MHz, DMSO-d_6, 25 ℃) δ(ppm): 6.01(s,2H), 6.68 (d, 2H), 7.35 (d, 2H), 7.66 (d, 2H), and 7.85 (d, 2H).



Scheme S1 Synthetic route for preparing 2-(4-aminophenyl) benzoxazole.

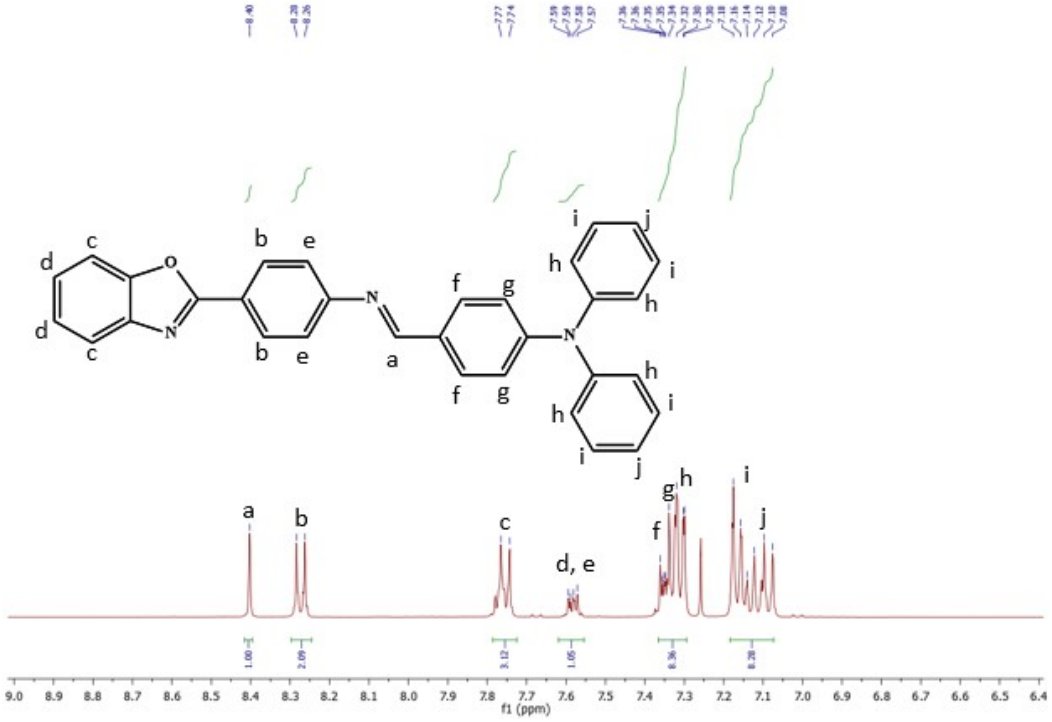


Fig. S1 ^{1}H NMR spectra of **PMPA** in $CDCl_3$.

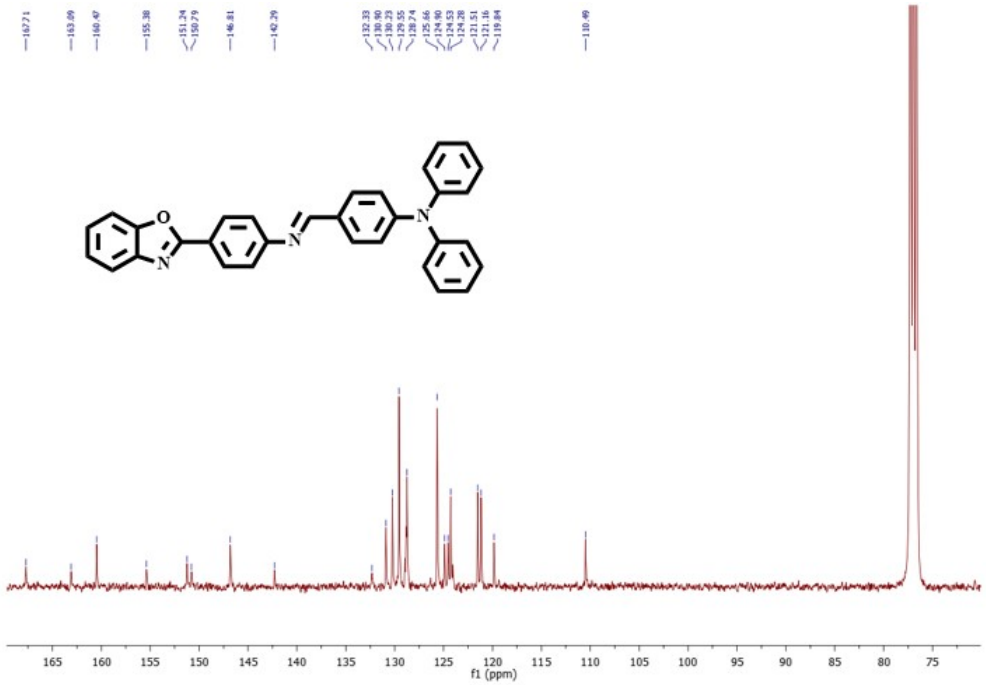


Fig. S2 ^{13}C NMR spectra of **PMPA** in $CDCl_3$.

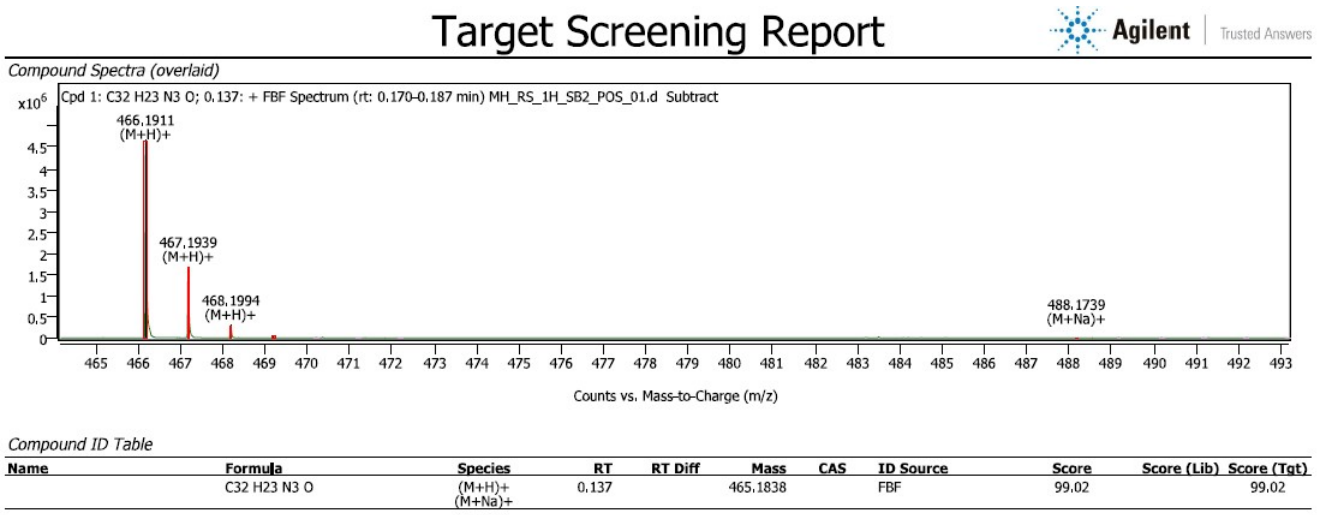


Fig. S3 High-resolution mass spectra of our synthesized **PMPA**.

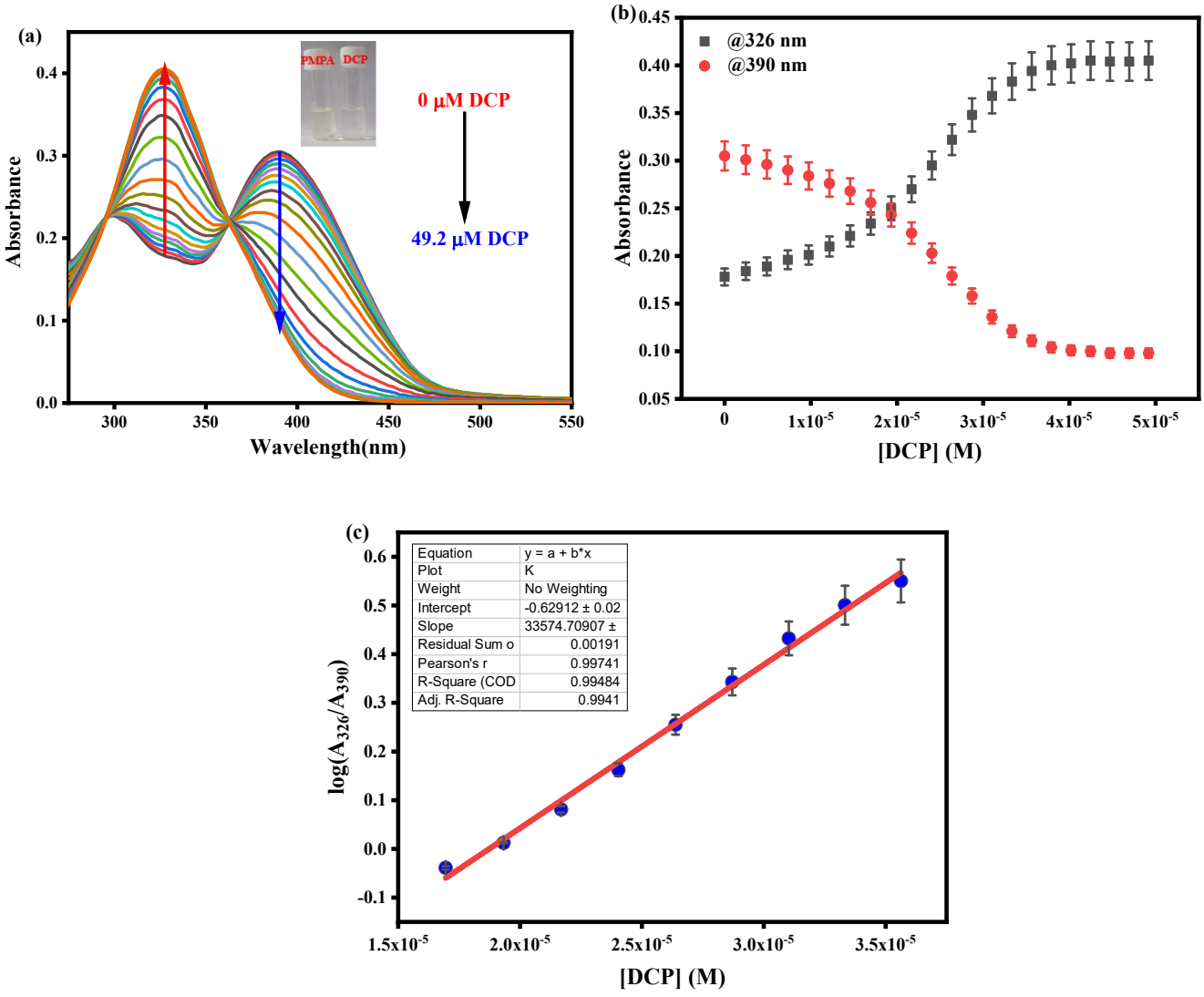


Fig. S4 **(a)** UV-visible spectrophotometric spectra of **PMPA** (22 µM) upon steady addition of DCP (0-49.2 µM) in water-DMSO (4:1) medium and **(b)** the change of absorption behavior with increasing concentration of DCP at wavelengths 326 nm and 390 nm, respectively. **(c)** The ratiometric [DCP] vs. log(A_{326}/A_{390}) calibration curve for quantifying the unknown concentration of DCP with minimal experimental error.]

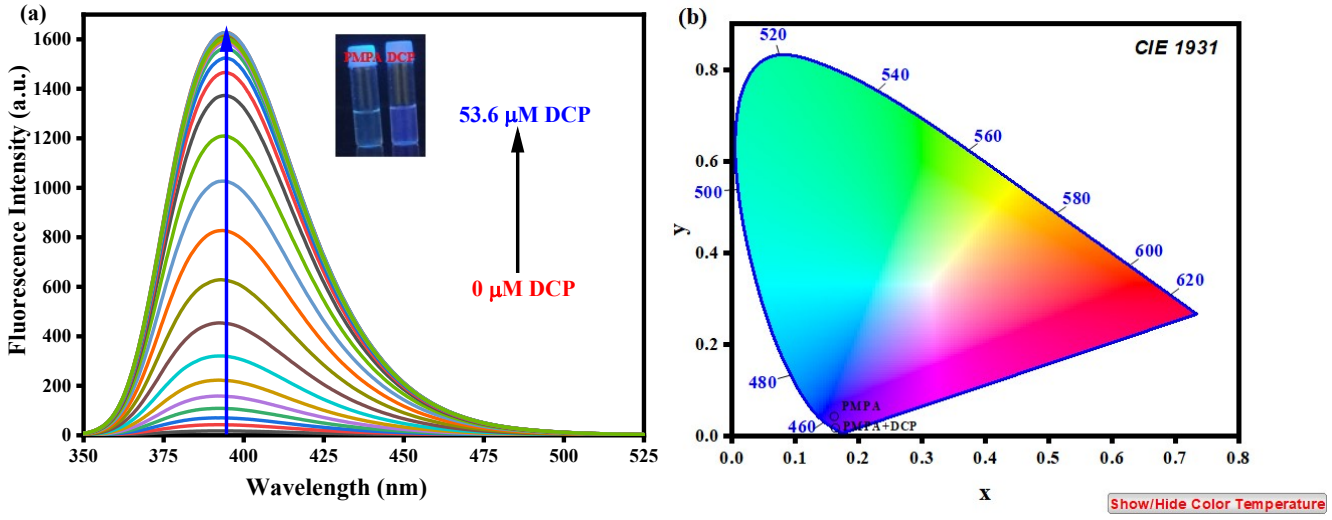


Fig. S5 (a) Fluorometric titration spectrum of **PMPA** (22 µM) upon steady accumulation of DCP (0-53.6 µM) in water-DMSO (4:1) medium. **(b)** Fluorescence color before and after phosphorylation through CIE diagram, coordinates x = 0.1612, y = 0.0429 and x = 0.1629, y = 0.0176 respectively.

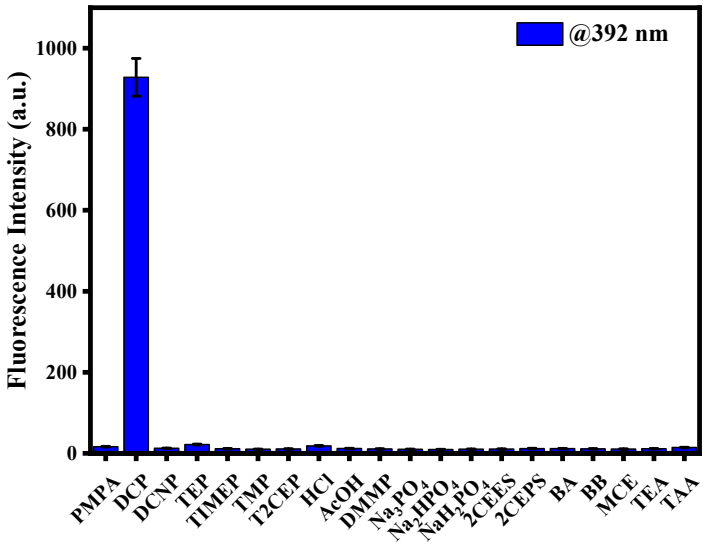


Fig. S6 Bar plot on photoluminescence intensity change at 392 nm of **PMPA** solution in pure DMSO medium in the presence of several OPs, IPs, and other toxic guest analytes.

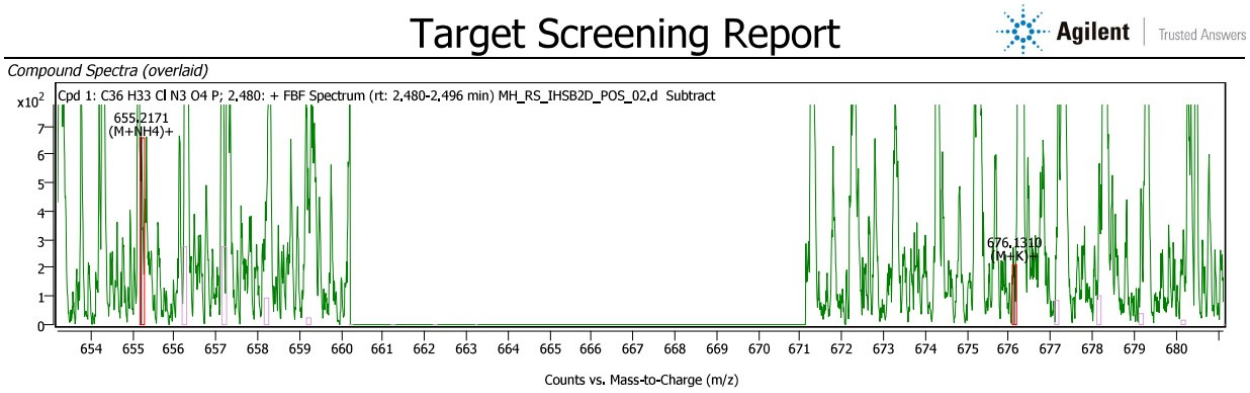


Fig. S7 HRMS of phosphorylated product **PMPA**-DCP in DMSO.

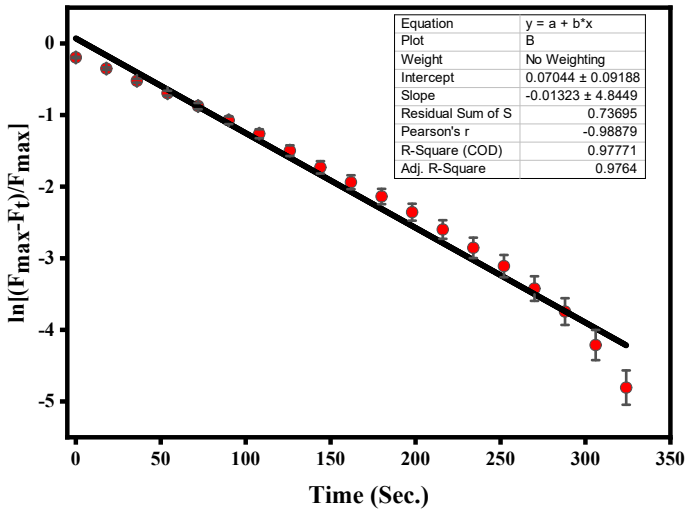


Fig. S8 Pseudo first-order rate constant plot of **PMPA** (12.6 μM) in the presence of DCP (90 μM).

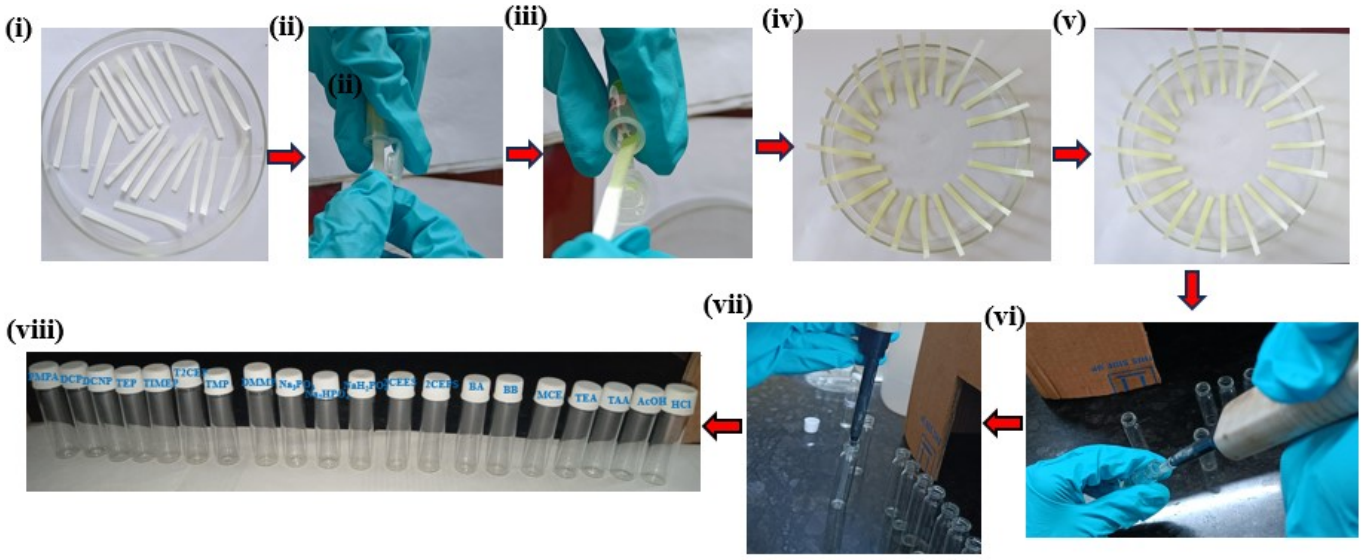
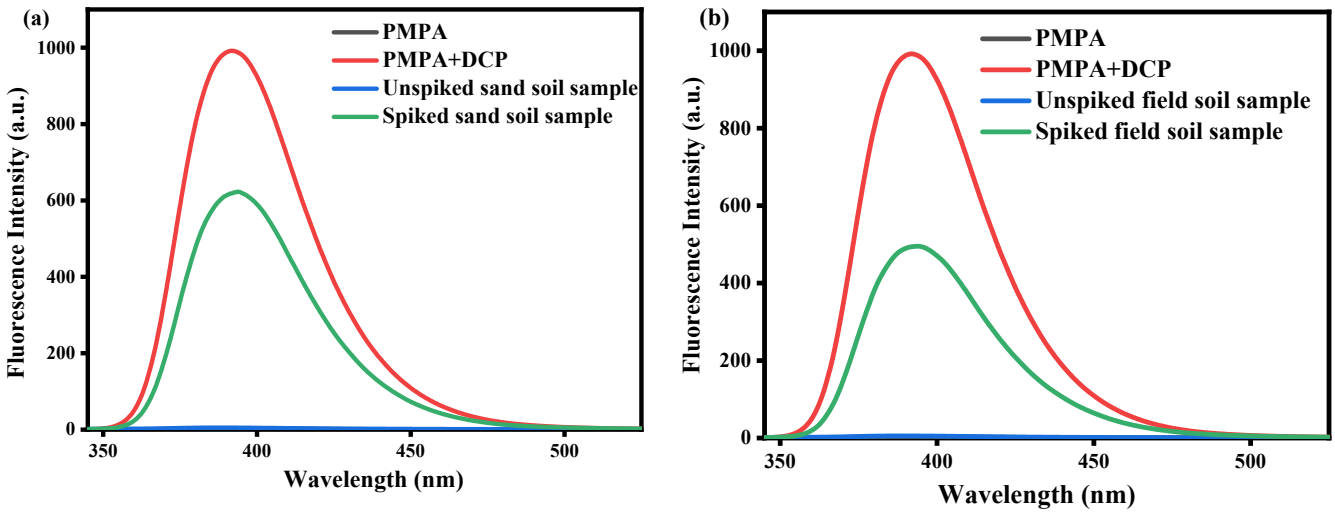


Fig. S9 (i) Long-length cuts of several Whatman filter papers. **(ii)** The filter papers were immersed into the PMPA solution (1mM). **(iii)** Photo on **PMPA**-loaded filter papers. Picture of long-length cuts of filter papers **(iv)** before **(v)** after drying. **(vi)** Taking each OPs, IPs and other analytes having similar concentration by micropipette. **(vii)** Sincerely adding dropwise of each OPs, IPs and other analytes into vials. **(viii)** Arranging the vials in order to add the analytes to perform the "dipstick" experiment.



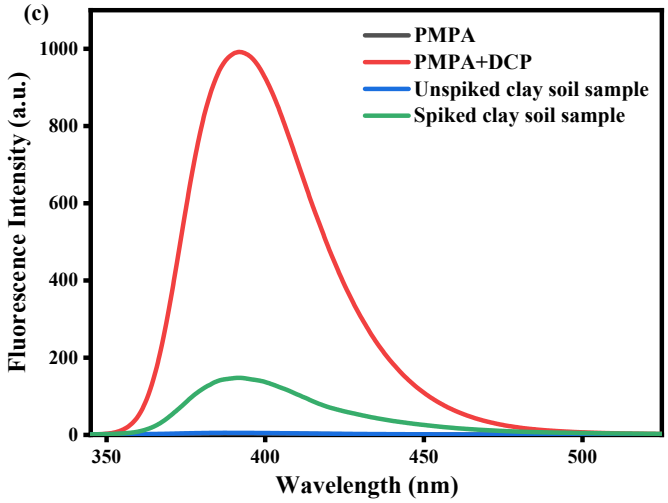


Fig. S10 Emission spectra of **PMPA** solution in different spiked and unspiked soil samples such as **(a)** sand, **(b)** field, and **(c)** clay soil, respectively.

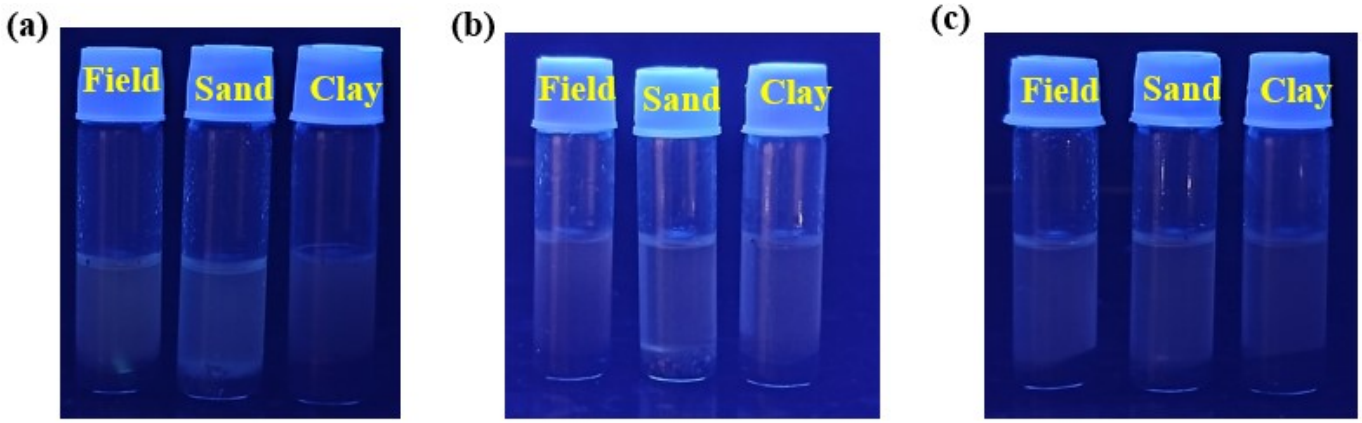


Fig. S11 The characteristic photoluminescence photos of **PMPA** solution of different pesticides-spiked soil samples **(a)** boxer biostimulant, **(b)** cypermethrin, and **(c)** bifenthrin under 365 nm UV-lamp irradiation.

Table S1 Comparison table of various probes and technologies for detecting organophosphates.

Probe	Technology	detecting organophosphates	Ref.
Rhodamine B hydrazide (RbH) - polyvinylpyrrolidone (PVP	Optical waveguides (OWGs)	DCP	[1]
Radioactive nickel (^{63}Ni) beta emission ionization source	Time-of-flight mass spectrometer	dimethyl methylphosphonate (DMMP)	[2]

Cystamine conjugate [(BocNH)Fc(CO)CSA]2	Electrochemical Sensors	$EtSCH_2CH_2Cl$, a simulant for sulfur mustard and $(NC)(EtO)_2P(O)$, a simulant for nerve agent Tabun.	3
Self-assembled composite layer of Cu^{2+}/11-mercaptoundecanoic acid	Piezoresistive SiO_2 microcantilever	dimethyl methylphosphonate (DMMP)	4
La(III) 2-bis(carboxymethyl)amino hexadecanoic acid	Surface Acoustic Wave (SAW) sensor	Nerve agent sarin (GB)	5
Polymerized crystalline colloidal array (PCCA)	Photonic Crystal	Organophosphorus compound parathion	6
hexafluoroisopropanol functionalized polythiophene	Carbon nanotube/polythiophene chemiresistive sensors	dimethyl methylphosphonate (DMMP)	7
triphenylamine–benzaoxazole based	**Colorimetric, fluorometric**	**DCP**	**Our work**

Table S2 Comparison table of various chemosensors introduced for detecting nerve agent stimulants in the last few decades with our probe PMPA.

Sensors	Type of response	Response Time	Test kit	Detection limit	Detection in gaseous phase	Ref.
squaraine-ethanolamine adducts	Colorimetric	Not available	Not available	3.5μM	Not available	8
Terpyridine based	Colorimetric fluorometric	Few seconds	vapor test Paper test	0.35 μM and 0.30 μM	Yes	9
thiourea-based rhodamine	Colorimetric fluorometric	Not available	No	2 μM	No	10
hydroxybenzylidenemalononitrile derivative	Colorimetric, fluorometric (turn-on)	Within minutes	Yes (Test strip method)	0.10, 0.11 and 0.20 μM	Yes	11
4-diphenylamino-2-hydroxy	colorimetric and	30 s.	Not	140 nM	Yes	12

benzaldehyde oxime	ratiometric		mentioned			
DASA-Derived Polymeric Probe	Colorimetric (On−off)	Within 2 minutes	vapor test	1mM	Yes	[13]
bis-indolyl based chromogenic probe	Colorimetric	Few minutes	vapor test Paper test	10.8 µM	Yes	[14]
Bifunctional azoaniline based	colorimetric	Within 1 min	Not mentioned	0.2 mM	Not mentioned	[15]
Rhodamine based	Colorimetric and fluoremetric	Not mentioned	Vapor test	0.2 µM	Yes	[16]
Polymer (BPAm-co-DMA-co-MPDEA)	colorimetric	Within few mins	polymeric film	18.4 µM	Yes	[17]
di-methyltin derivative	Fluorometric (turn-off)	Almost 2 minutes	Yes (Spot Testing Device)	0.023 and 0.092 mM	Yes	[18]
fluorenepyrene copolymer	Fluorometric (turn-on)	Within 3 seconds	Yes (Test strip method)	132 ppb	Yes	[19]
pyrene based turn-on fluorescent polymeric probe	ON/OFF reversible fluorescence	Few minutes	Quartz Plate vapor test	0.1 mM	Yes	[20]
benzothiazole-based	Fluorometric	Not available	Not available	0.43 µM	Not available	[21]
Xanthene	Colorimetric,fluorometric (turnon)	Not mentioned	Not mentioned	1.36 µM and 26 µM	NA	[22]
BODIPY-based fluorescent probe	fluorometric	within 540 s	Test paper	20.7 ppb	Not mentioned	[23]
triphenylamine–benzoxazole-based	**Colorimetric, fluorometric**	**Within a minute**	**(Dipstick method)**	**0.42 µM**	**Yes**	**Our work**

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