Supporting Information for

A Highly Selective Chromo-fluorogenic Probe for Specific Detection of Sarin Gas Simulant, Diethylchlorophosphate (DCP) in Liquid and Vapor Phase

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[‖]Equally contributed to this work

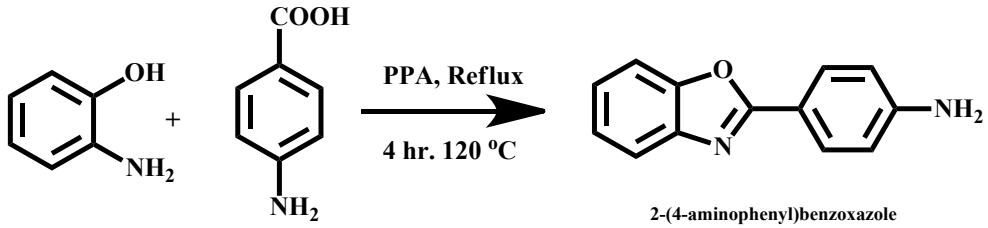
S1: Materials and instrumentations

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

S2: Synthetic pathway 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.

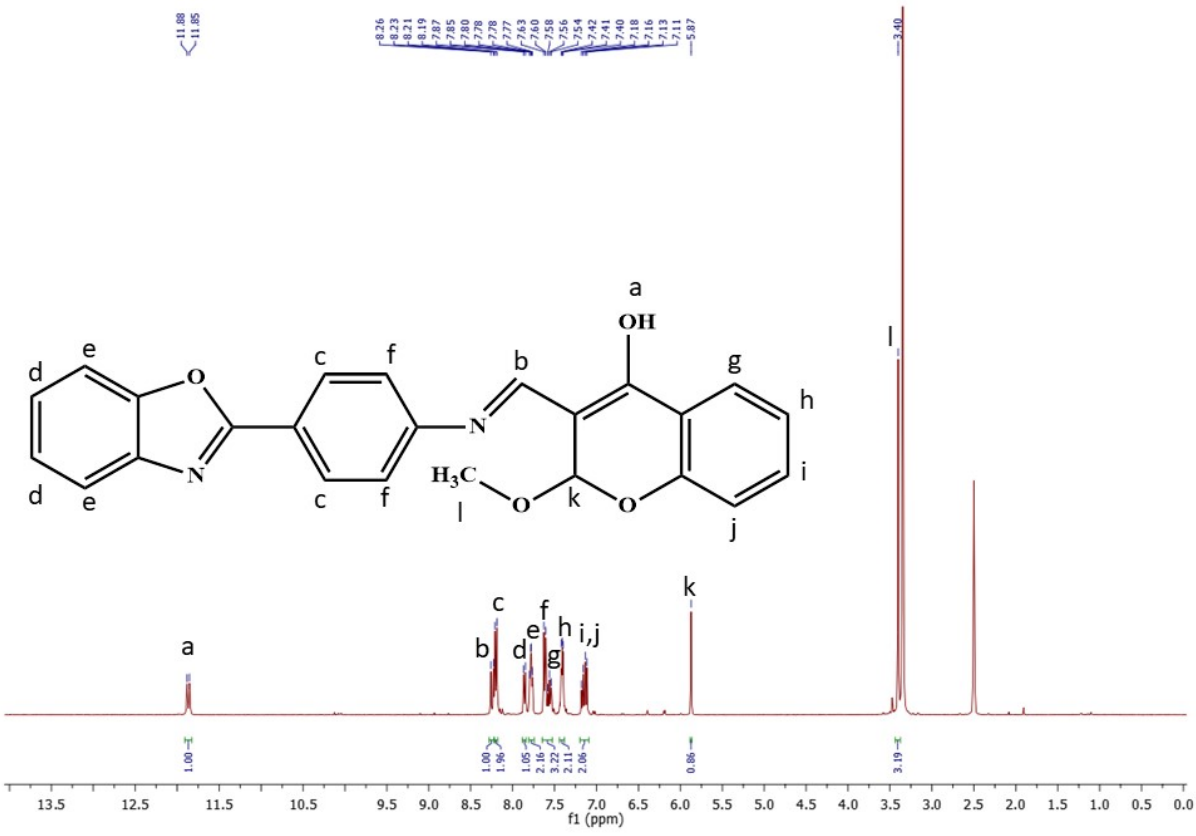


Fig. S1 ^{1}H NMR spectra of our synthesized sensor **TSB** in DMSO-d_6**.**

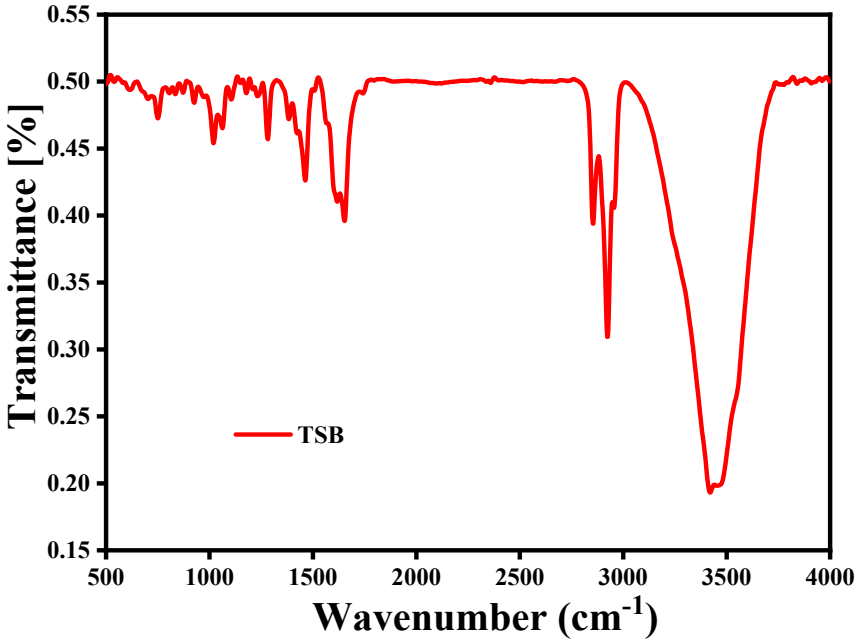


Fig. S2 IR spectra of our synthesized **TSB.**

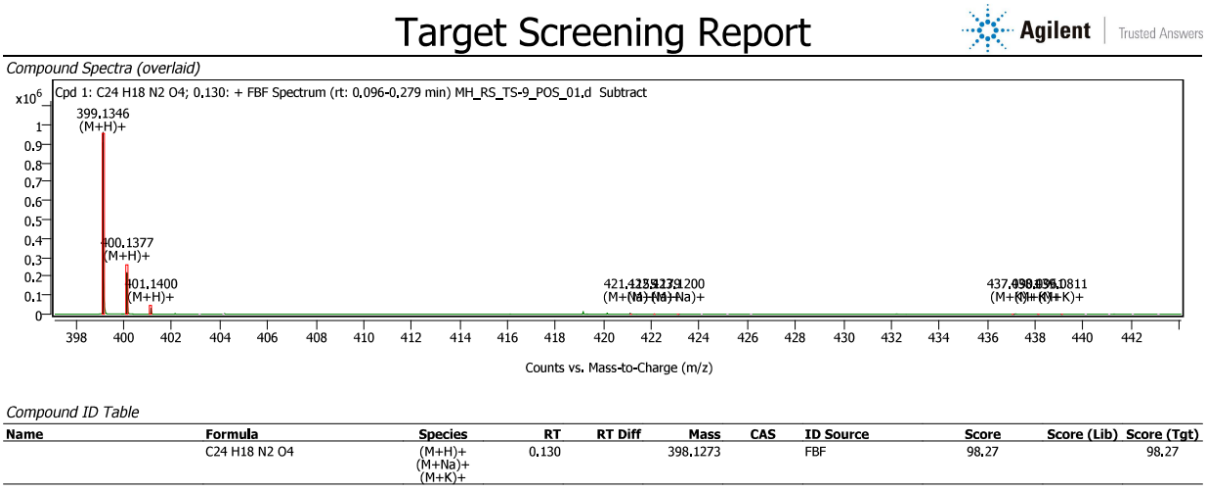
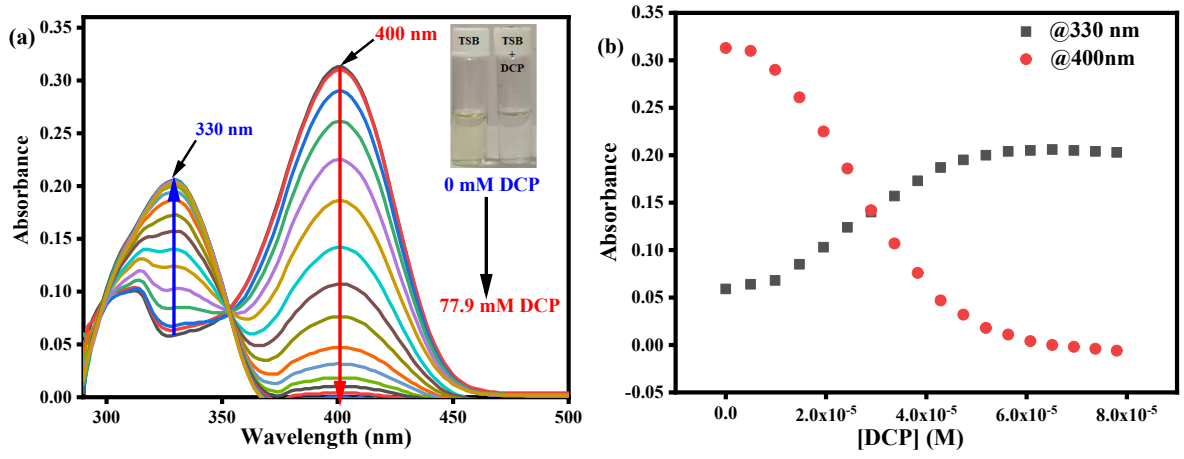


Fig. S3 HRMS spectra of our developed sensor **TSB.**



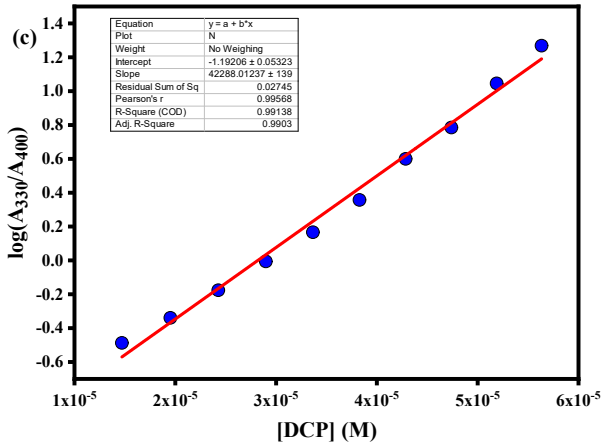


Fig. S4 **(a)** UV-visible spectrophotometric spectra of **TSB** (5.97×10^{-6} M) upon steady addition of DCP (0- 77.9 mM) in water-DMSO (50% v/v) medium and **(b)** the change of absorption behavior with increasing concentration of DCP at wavelengths 330 nm and 400 nm, respectively. **(c)** The ratiometric [DCP] vs. $\log(A_{330}/A_{400})$ calibration curve for quantifying the unknown concentration of DCP with minimal experimental error.

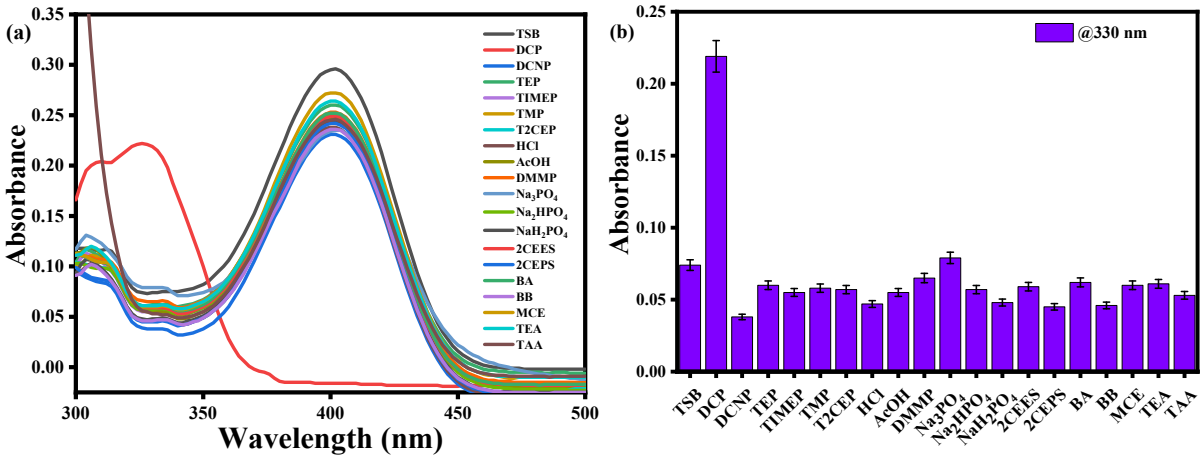
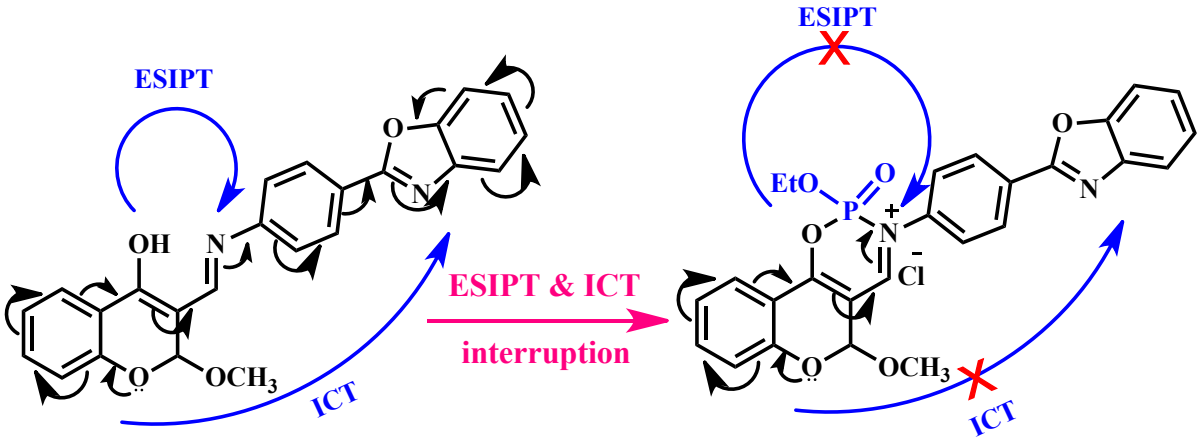


Fig. S5 (a) Selectivity spectrum profile of sensor **TSB** with various target analytes in 50% (v/v) water-DMSO mixture **(b)** corresponding selectivity bar diagram at 330 nm wavelength.



Scheme S2 Suppression of ICT and ESIPT processes due to the formation of phosphorylated **TSB**-DCP product.

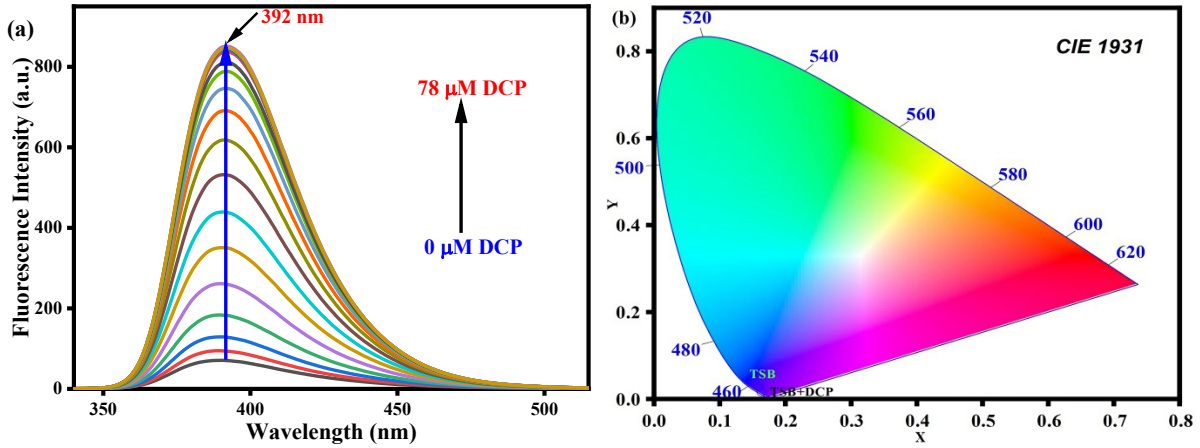


Fig. S6 (a) Emission titration of probe **TSB** solution by gradual addition of toxic analyte DCP (0 to 78 μM) in 50 % (v/v) water-DMSO medium. **(b)** Corresponding CIE diagram demonstrating its fluorogenic color.

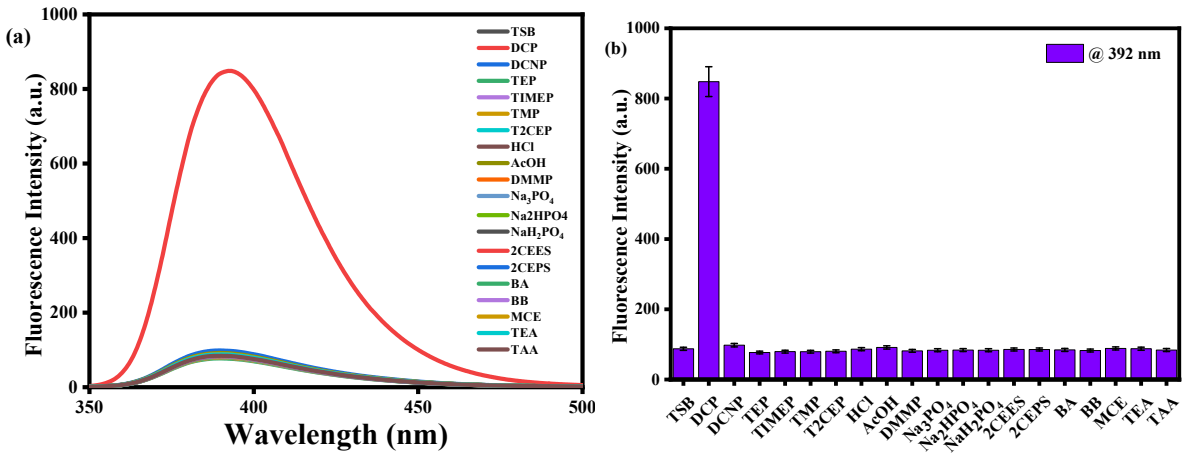


Fig. S7 (a) Selectivity emission spectra of our developed sensor **TSB** with various toxic analytes in 50 % (v/v) water-DMSO medium. **(b)** Corresponding selectivity bar diagram at 390 nm.

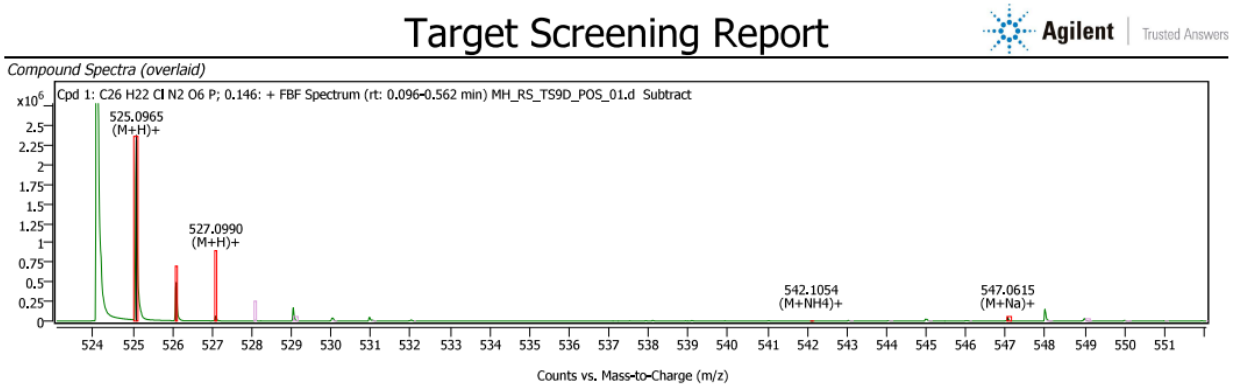


Fig. S8 High-resolution mass spectra of the **TSB**-DCP phosphorylated product.

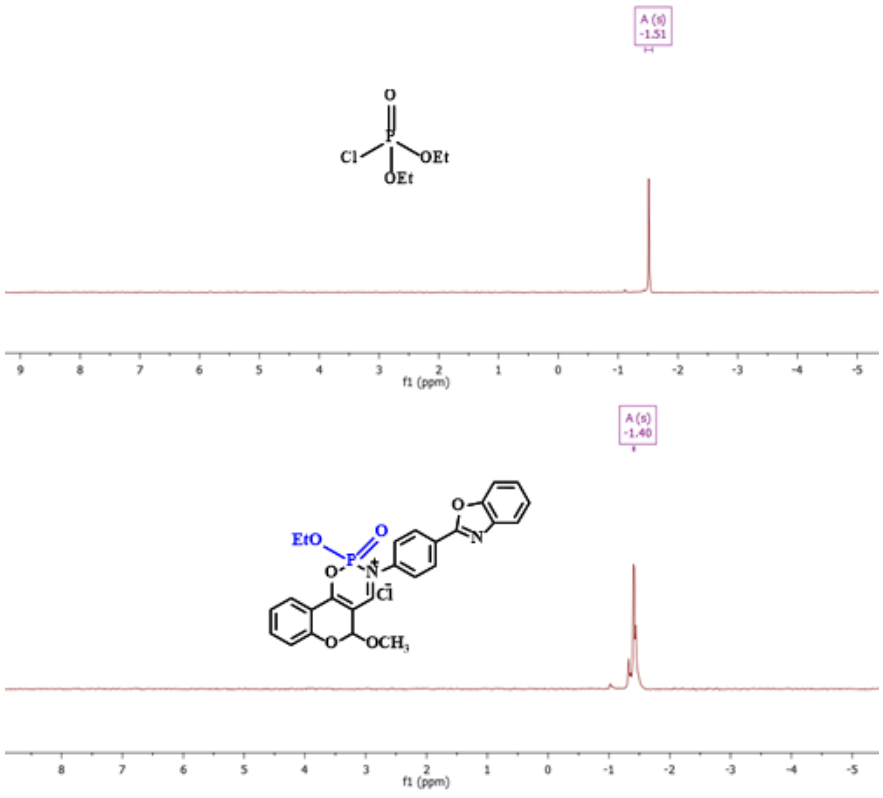


Fig. S9 ^{31}P NMR spectra of DCP and **PB**-DCP in pure DMSO-d_6.

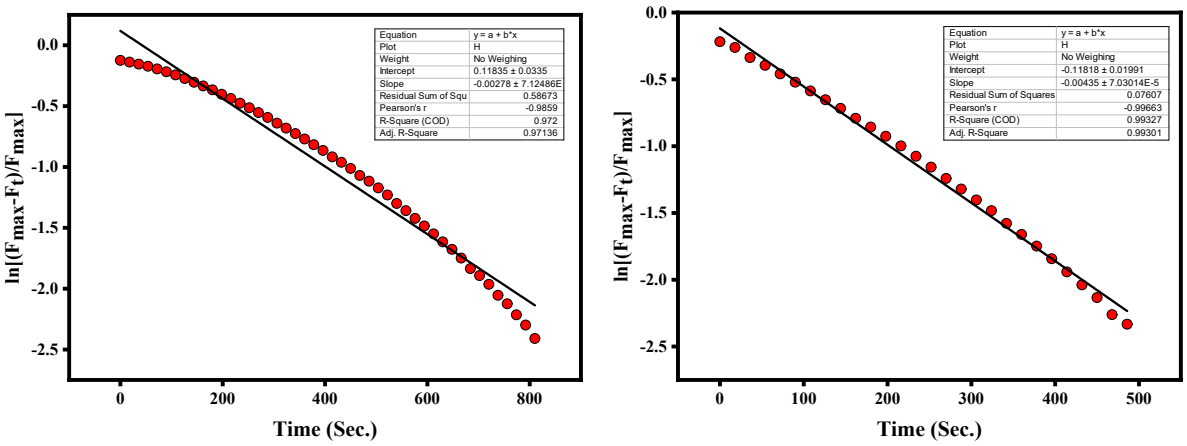


Fig. S10 Pseudo first-order rate constant plot of **TSB** in the presence of DCP in DMSO (left) and 50 % (v/v) water mixture (right).

Table S1: Comparison table of various chemosensors that have been introduced for the detection of DCP in the last few decades with our **TSB.**

Fluorophore used	**Type of response**	**Response Time (min or Sec)**	**Test kit**	**Detection limit**	**Detection in gaseous phase**	**Ref.**
No fluorophore Benzoxazole-chromone based	**Colorimetric (ratiometric), fluorometric (turn on)**	**Within few minutes**	**vapor test Paper test**	**0.64 µM (DMSO) & 0.36 µM (Water mixture)**	**Yes**	**Our work**
No fluorophore	Fluorometric (turn-off)	Almost 2 minutes	Yes (Spot Testing Device)	0.023 and 0.092 mM	Yes	[1]
fluorescein-hydroxamate aldehyde	Chromogenic	Few minutes	Not mentioned	3 mM	Not mentioned	[2]
pyridine acceptor moiety	Colorimetric	Not mentioned	Polyurethane film vapor test	0.9 mM	Yes	[3]

DASA-Derived Polymeric Probe	Colorimetric (on−off)	Within 2 minutes	vapor test	1 mM	Yes	[4]
Benzothiazole	Fluorometric (ratiometric)	Few minutes	vapor test	1.6 μM	Yes	[5]
bis-indolyl-based chromogenic probe	Colorimetric	Few minutes	vapor test Paper test	10.8 μM	Yes	[6]
pyrene-based turn-on fluorescent polymeric probe	ON/OFF reversible fluorescence	Few minutes	Quartz Plate vapour test	0.1 mM	Yes	[7]
Xanthene	Colorimetric, fluorometric (turn on)	Not mentioned	Not mentioned	1.36 μM and 26 μM	NA	[8]
thiourea-based rhodamine	Colorimetric fluorometric	Not available	No	2 μM	No	[9]
Polymer (BPAm-co-DMA-co-MPDEA)	colorimetric	Within few mins	polymeric film	18.4 μM	Yes	[10]

Reference

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