Supporting information

D-π-A azine based AIEgen with solvent dependent response towards the nerve agent

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Materials and methods

All the chemicals were directly used for the synthesis without further purification. 4-Cynobenzaldehyde was purchased from Avra synthesis India. 4-Dipropylaminobenzaldehyde prepared by previous report.[41] Hydrazine hydrate was purchased from Spectro Chem, India. All the solvents were of HPLC grade and purchased from Merck, India. Hydrochloric acid and sodium hydroxide were purchased from Merck, India. Thionyl chloride(SOCl2), triethyl phosphate(TEP) and triethyl phosphite(TEPH) were purchased from Alfa Aesar India. Diethyl chlorophosphate(DCP) and quinine sulphate were purchased from Sigma Aldrich, India.^{1}H and ^{13}C-NMR spectra were recorded on a Bruker Seoul 400 at 400 MHz instrument. The residual solvent peaks were used as internal standards. Chemical shifts are reported in ppm. Mass spectra were obtained with Thermo scientific exactive plus, HESI mode.Absorption spectra were recorded using Varian Cary Bio 100 UV-Vis spectrophotometer.Fluorescence spectral measurements were carried out using JASCO FP-6500 fluorescence spectrophotometer. To gain theoretical insight to understand the sensing mechanism, DFT calculations were conducted. We used Gaussian 09 and the B3LYP functional was employed. The basis set used was 6–31 G*.

Limit of detection:

The detection limit of DCP was calculated based on the fluorescence titration. To determine the S/N ratio, the fluorescence intensity of DPBN without DCP was measured by 5 times and the standard deviation of blank measurements was taken for calculation. The limit of detection was then calculated using the equation ref : LOD = 3σ/k, where σ is the standard deviation of blank measurements, k is the slope between [I/I_o -1] verses DCP concentration.

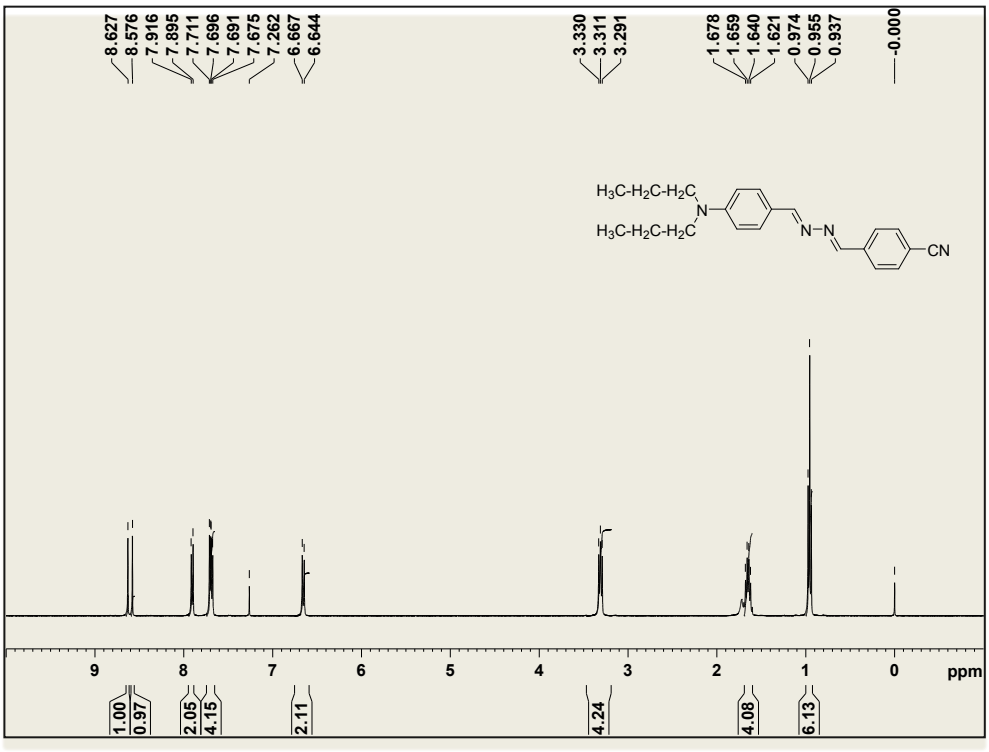


Figure S1. ^{1}H NMR spectrum of DPBN in $CDCl_3$

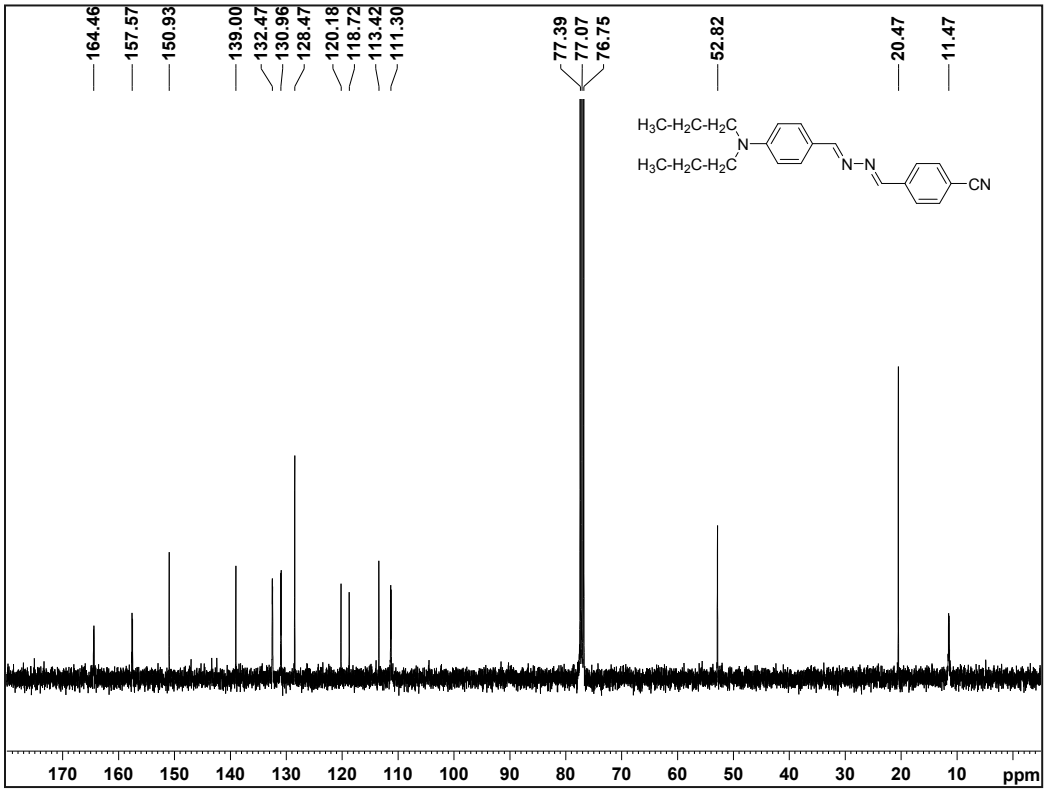


Figure S2. ^{13}C NMR spectrum of DPBN in $CDCl_3$

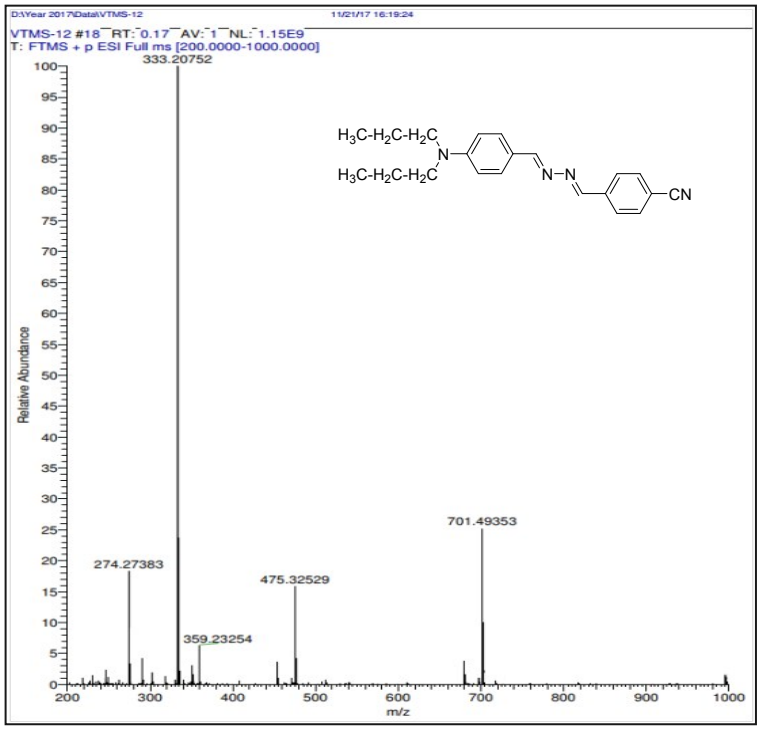


Figure S3. Mass spectrum of DPBN

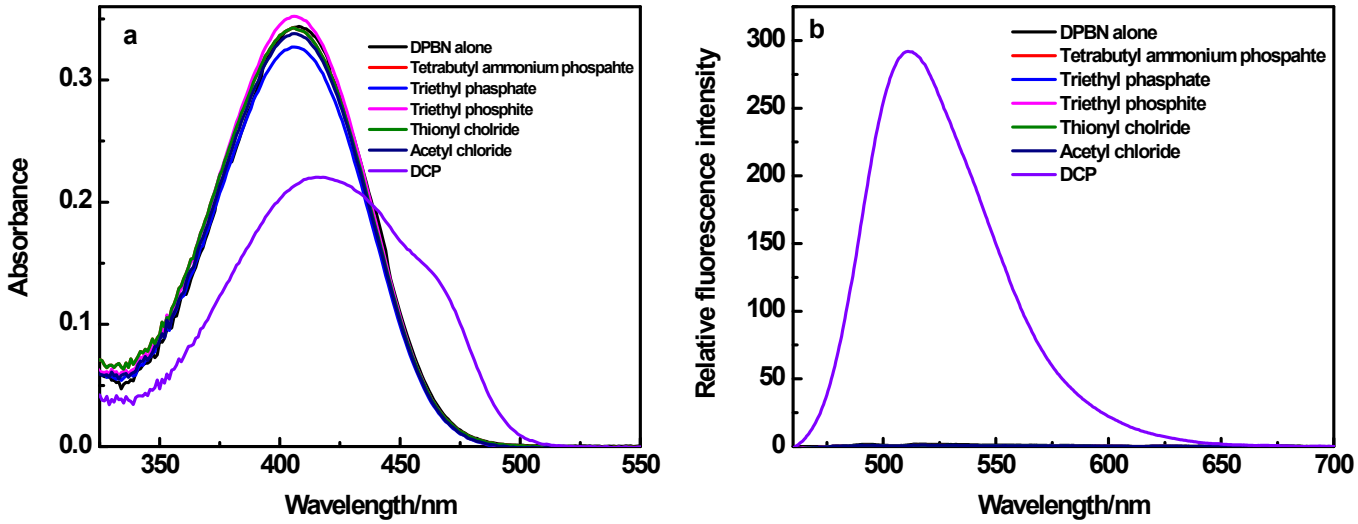


Figure S4. (a) Absorption and (b) emission spectrum of DPBN (10 μM) in the absence and presence of 150 equivalent of different nerve agent(1.5 mM) in THF. λ_{exc} = 440 nm.

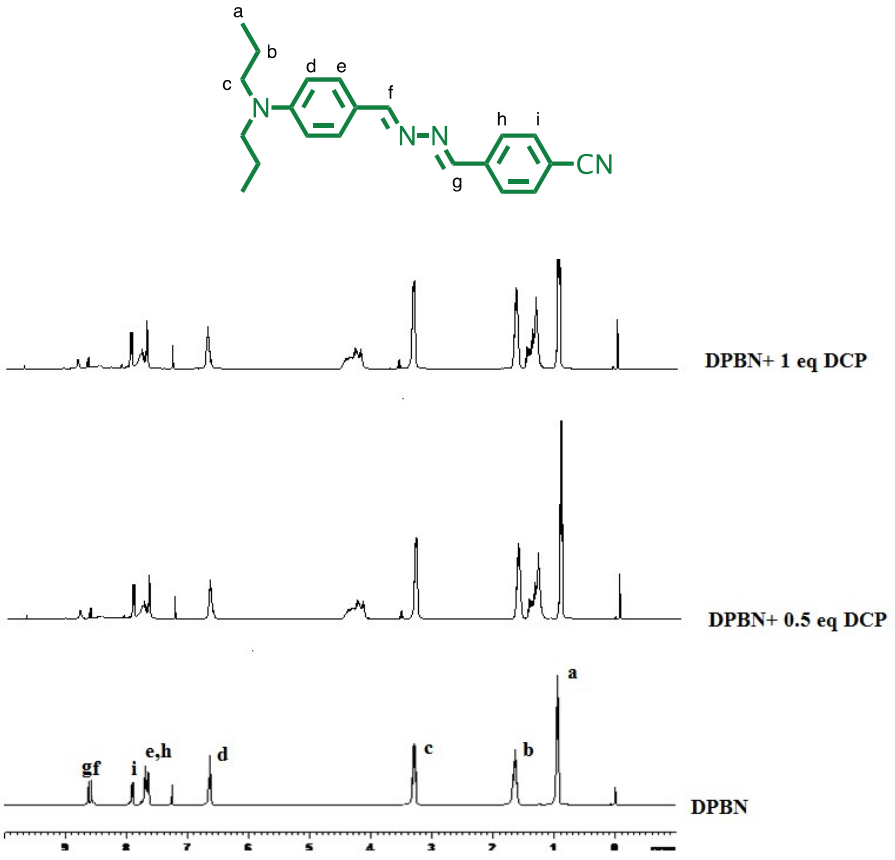
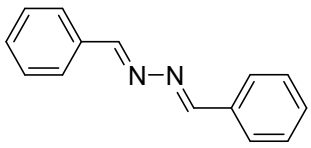


Figure S5. ^{1}H NMR spectra of DPBN in the presence and absence of DCP.



BA

Figure S6. Structure of BA

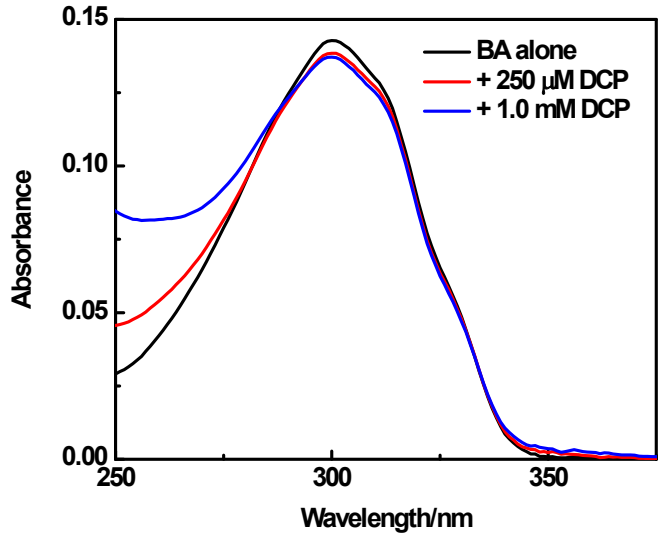


Figure S7. Absorption spectrum of BA (5 μM) in the presence and absence of DCP in THF.

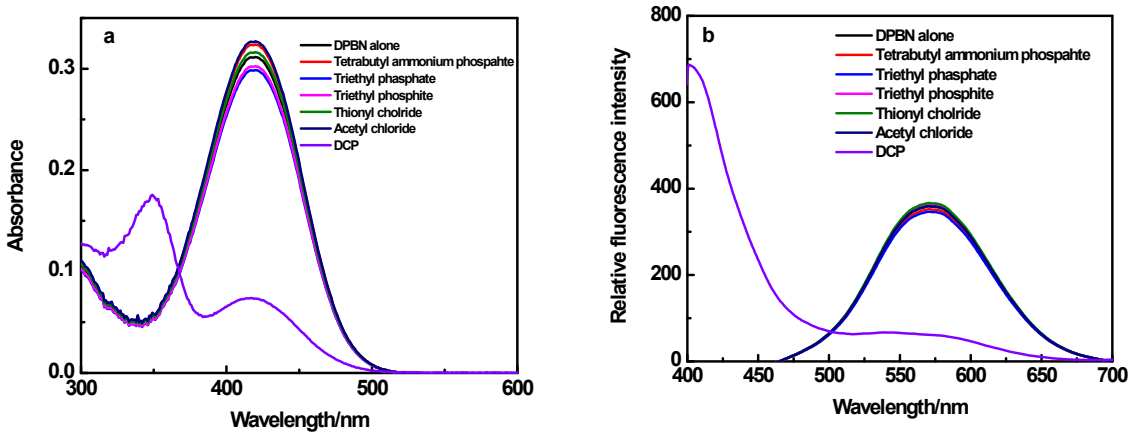


Figure S8. (a) Absorption and (b) emission spectrum of DPBN (10 μM) in the absence and presence of 150 equivalent of different nerve agent(1.5 mM) in THF/water (3:7) mixture. λ_{exc} = 368 nm.

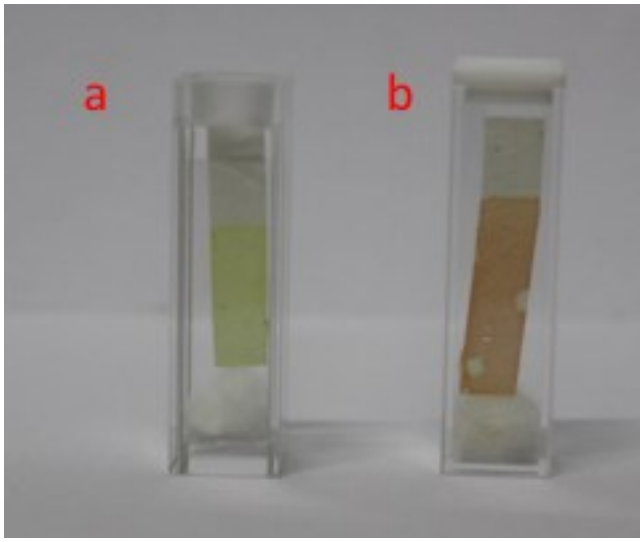


Figure S9. Whatmann filter paper treated with DPBN (10 μM) solution in THF and then air dried. (a) Fliter paper without exposed DCP vapor (b) After exposed to DCP vapor for 30 s.