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Electronic Supplementary Information

Handy ratiometric detection of gaseous nerve agents with AIE-fluorophore-based solid test strips

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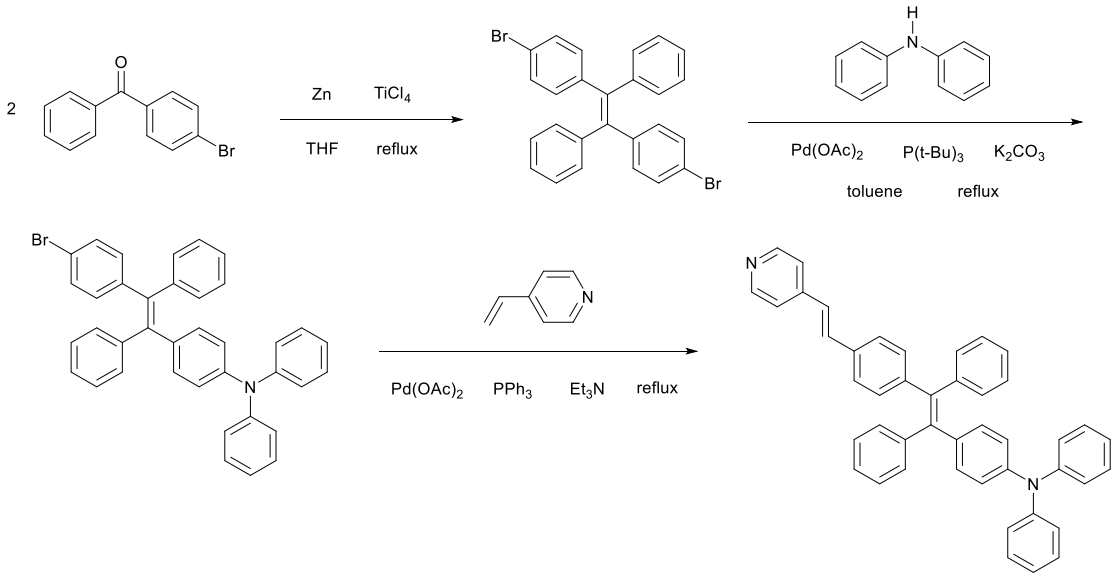

Scheme S1. Synthesis and structure of DPA-TPE-Py.

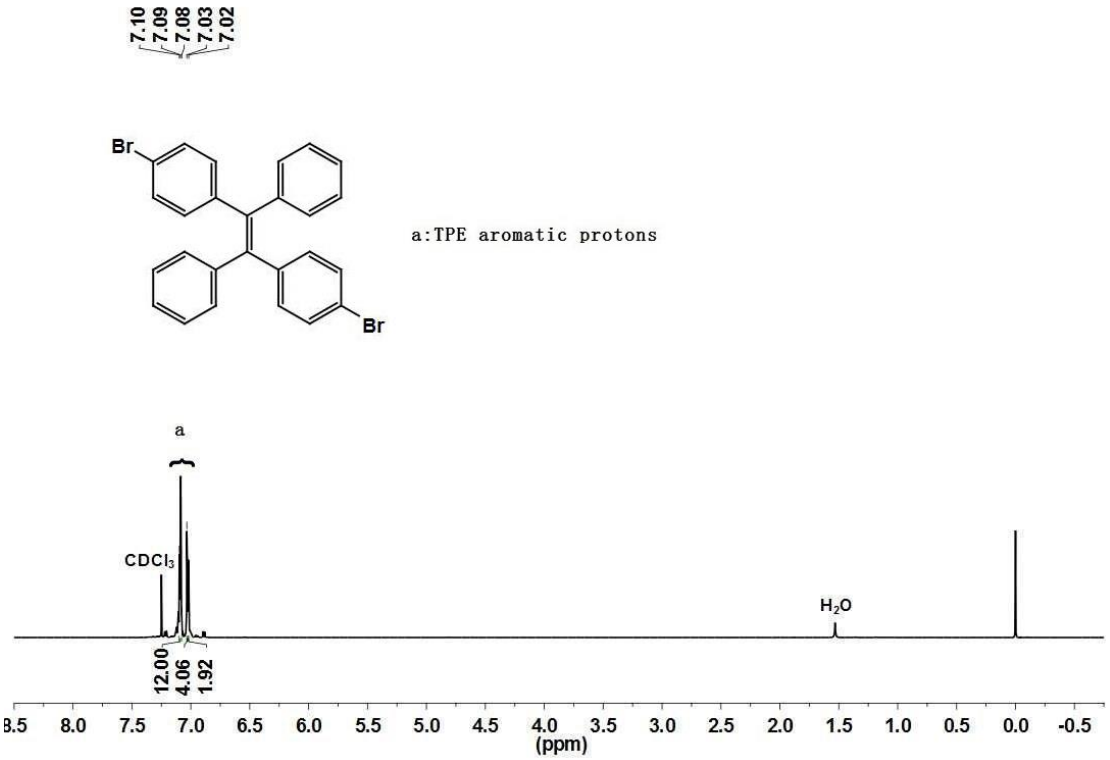

Fig. S1. ^{1}H NMR spectrum of Br-TPE-Br in $CDCl_3$.

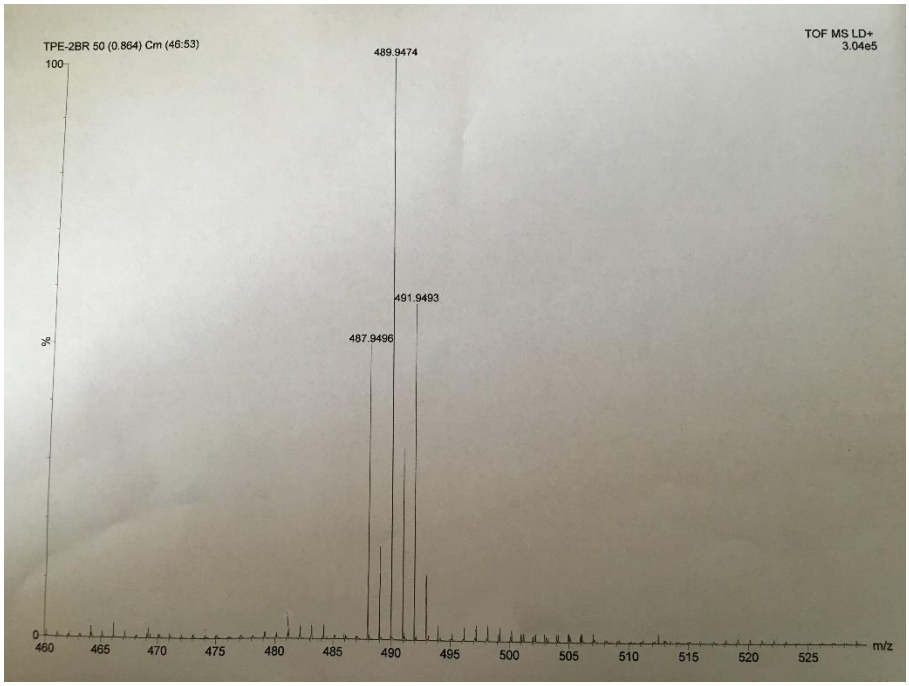

Figure S2. MALDI-TOF mass spectrum of Br-TPE-Br.

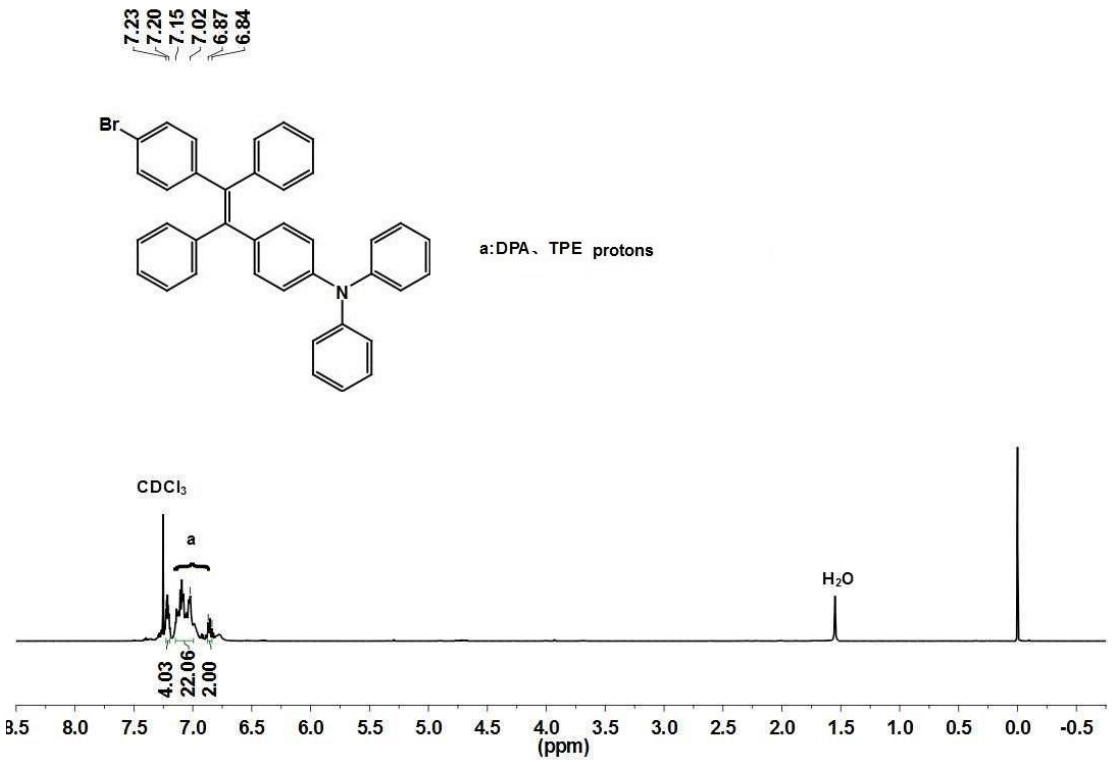

Fig. S3. ^{1}H NMR spectrum of DPA-TPE-Br in $CDCl_3$.

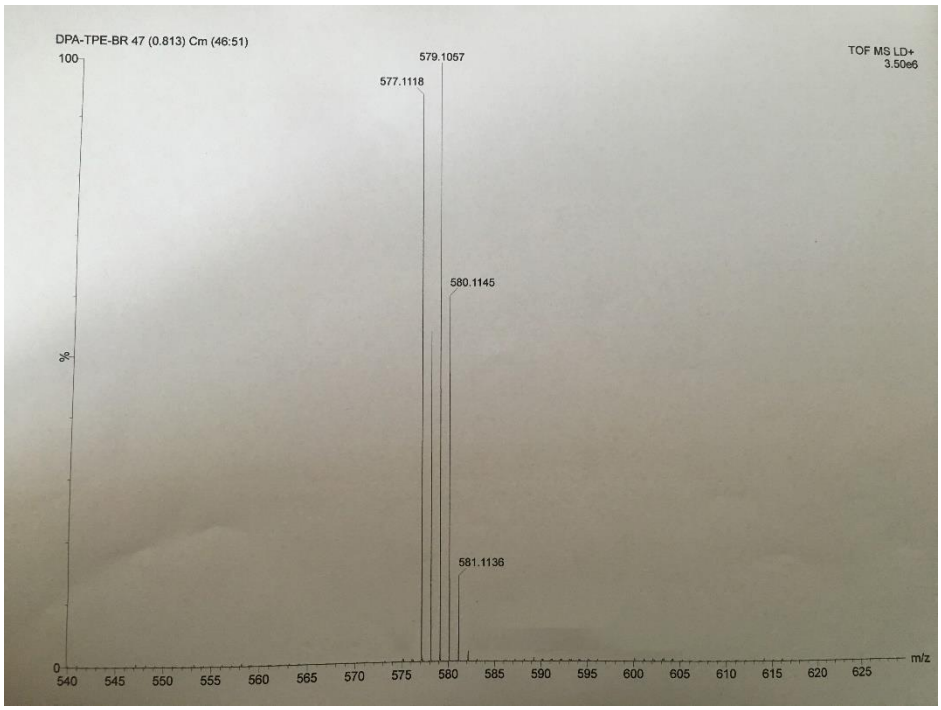

Figure S4. MALDI-TOF mass spectrum of DPA-TPE-Br.

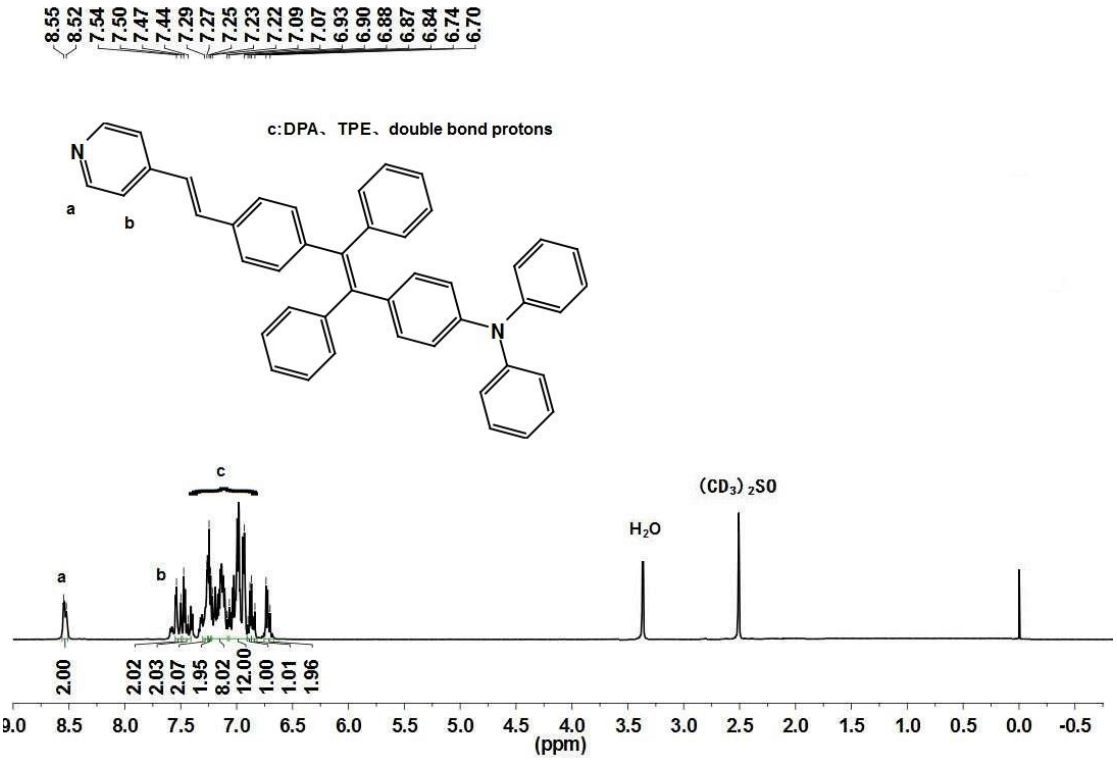

Fig. S5. ^{1}H NMR spectrum of DPA-TPE-Py in $(CD_3)_2SO$.

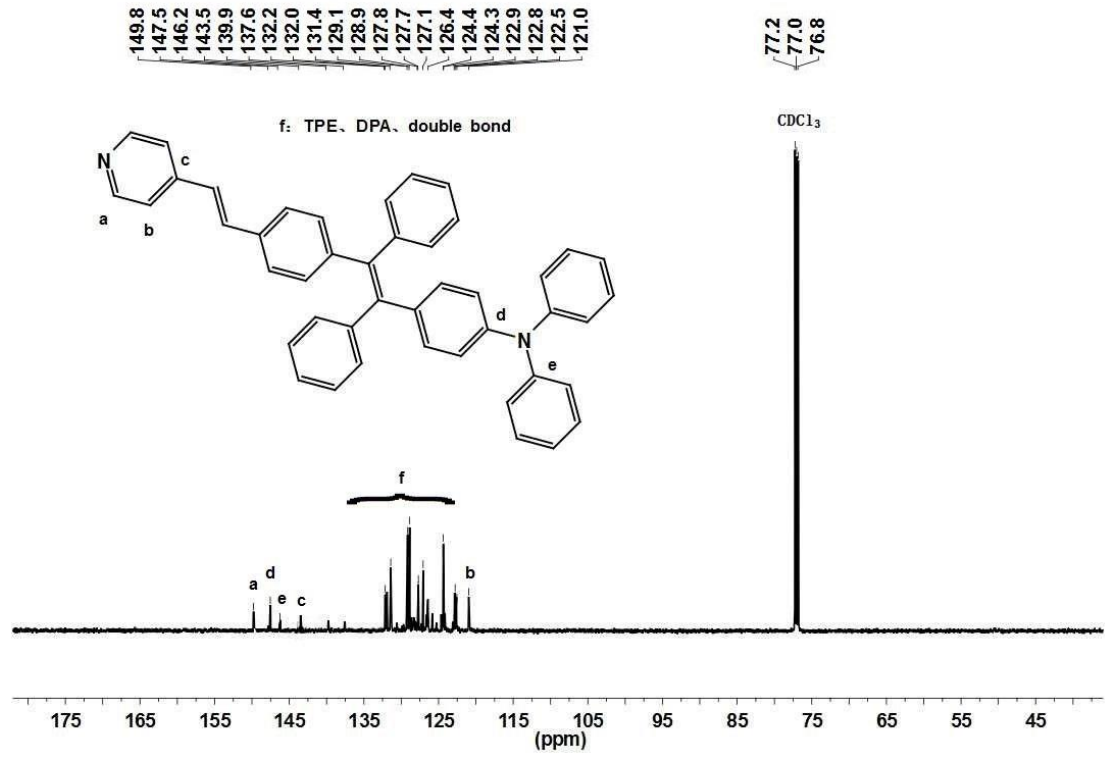

Fig. S6. ^{13}C NMR spectrum of DPA-TPE-Py in $CDCl_3$.

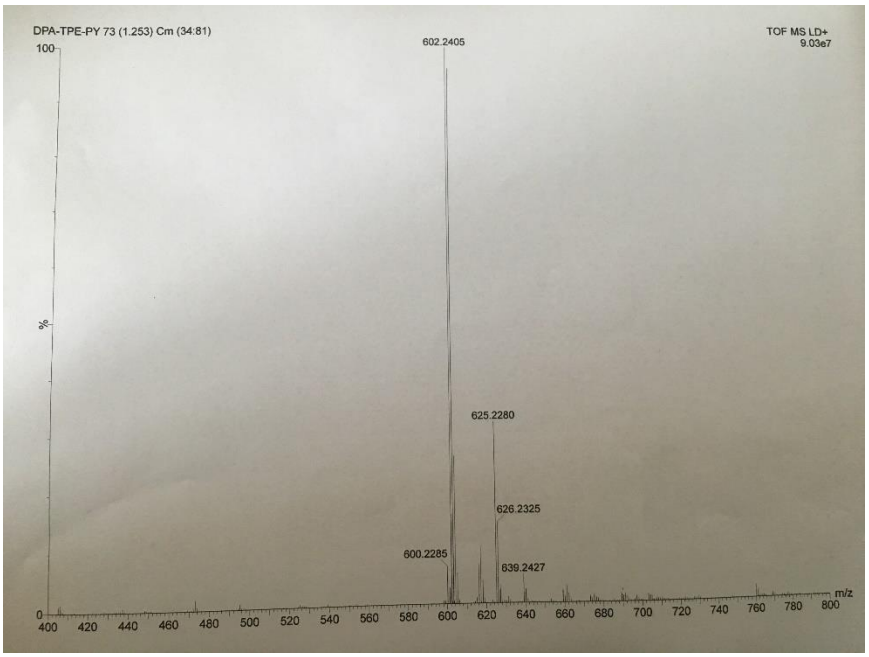

Figure S7. MALDI-TOF mass spectrum of DPA-TPE-Py.

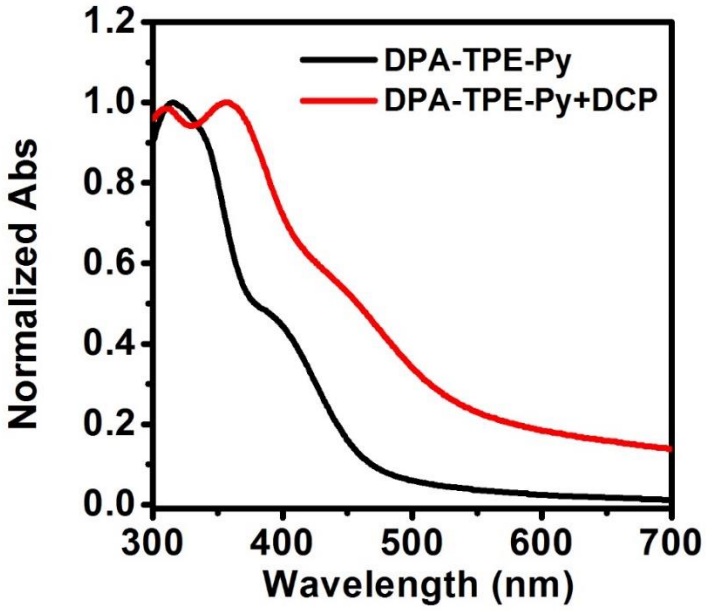

Fig. S8. Normalized UV-vis absorption spectra of DPA-TPE-Py (black) and the final reaction product of DPA-TPE-Py with DCP vapor (red).

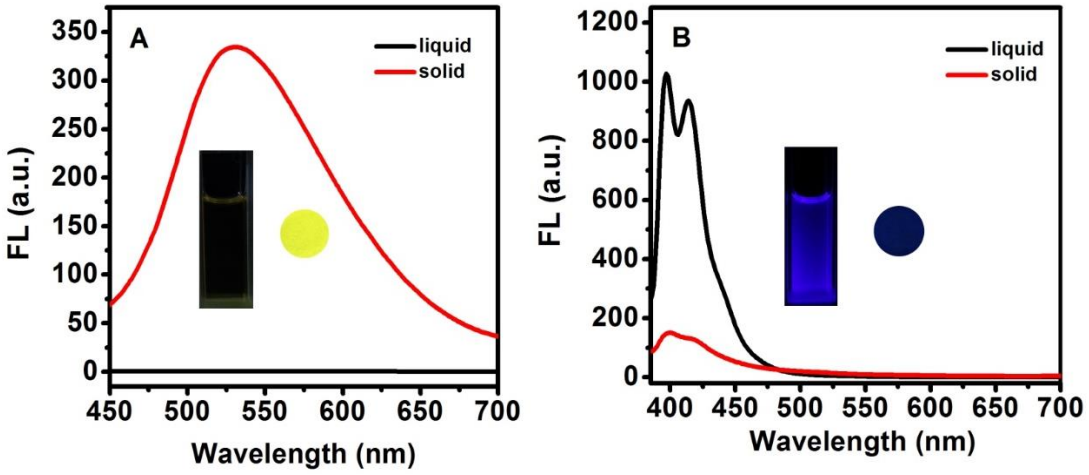

Fig. S9. (A) Fluorescence spectra of DPA-TPE-Py (10^{-3} M) in THF and DPA-TPE-Py loaded test strip; λ_{ex} =369 nm; (B) Fluorescence spectra of Py-COOH (10^{-3} M) in THF and Py-COOH loaded test strip under 369 nm excitation. Insets: photographs of solutions and test strips were taken under hand-held UV lamp (365 nm).

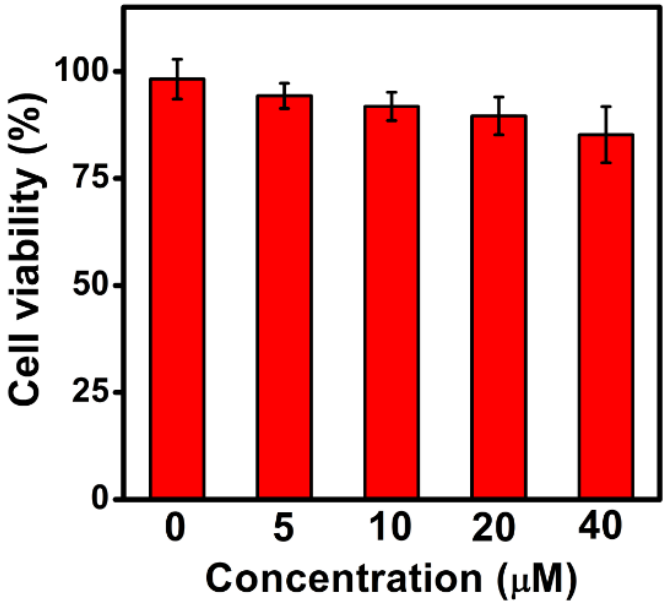

Figure S10. Cytotoxic effects against HeLa upon 24 hours of incubation with different DPA-TPE-Py concentrations (0, 5, 10, 20, 40 μM).

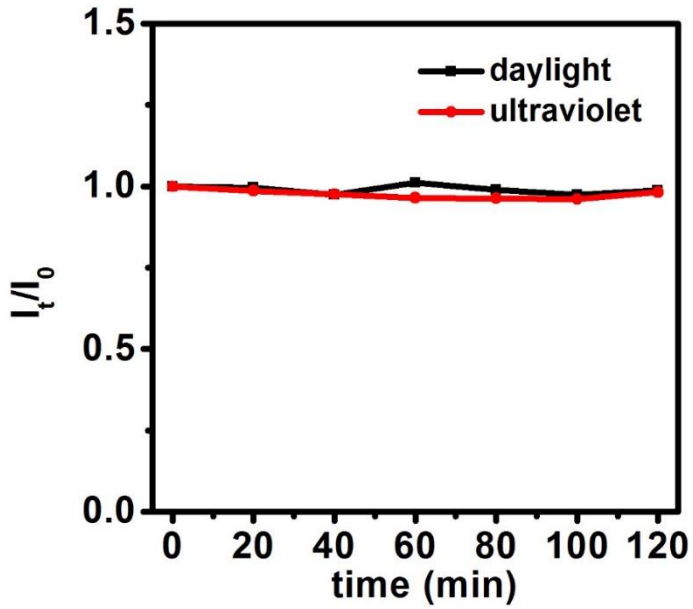

Fig. S11. Photostability of DPA-TPE-Py loaded test strips. I_0 is the original maximum fluorescence intensity excited at 465 nm before light irradiation and I_t is the fluorescence intensity (recorded at the same wavelength as I_0) excited at 465 nm after t-minute light irradiation. The ratio I_t/I_0 was calculated to be representative of the magnitude of change in fluorescence intensity. The samples were under daylight (black) or continuous light irradiation using a 15W 365 nm UV lamp (red).

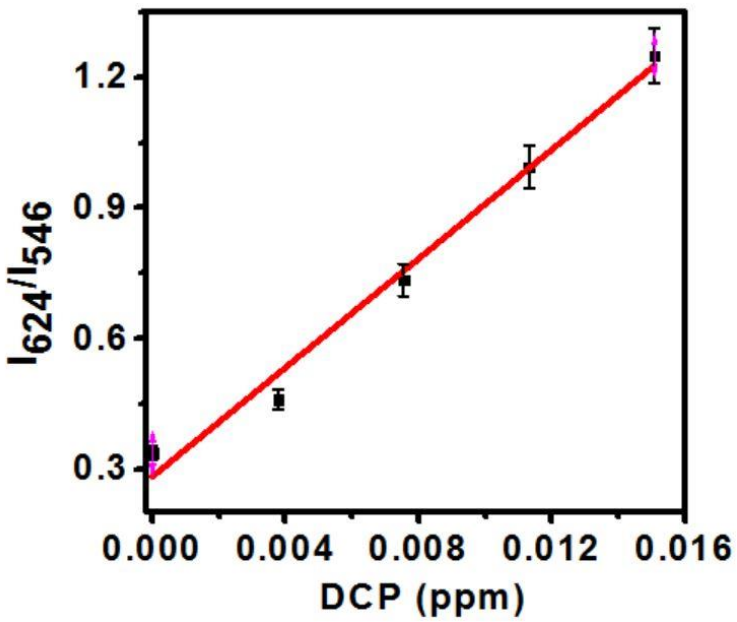

Fig. S12. Fluorescence intensity ratio as a function of DCP level.

Determination of the detection limit[1-2]**:**

The calibration curve was first obtained from the plot of fluorescence ratio I_{624}/I_{546} as a function of DCP vapor. Then the regression curve equation was obtained for the lower concentration part.

The detection limit = 3 × S.D. / k

where k is the slope of the curve equation, and S.D. represents the standard deviation for the fluorescence intensity of DPA-TPE-Py in the absence of DCP.

I_{624}/I_{546} = 0.283 + 62.62 × [DCP] (R^2 = 0.983)

LOD = 3 × 0.038 / 62.62 = 1.82 ppb

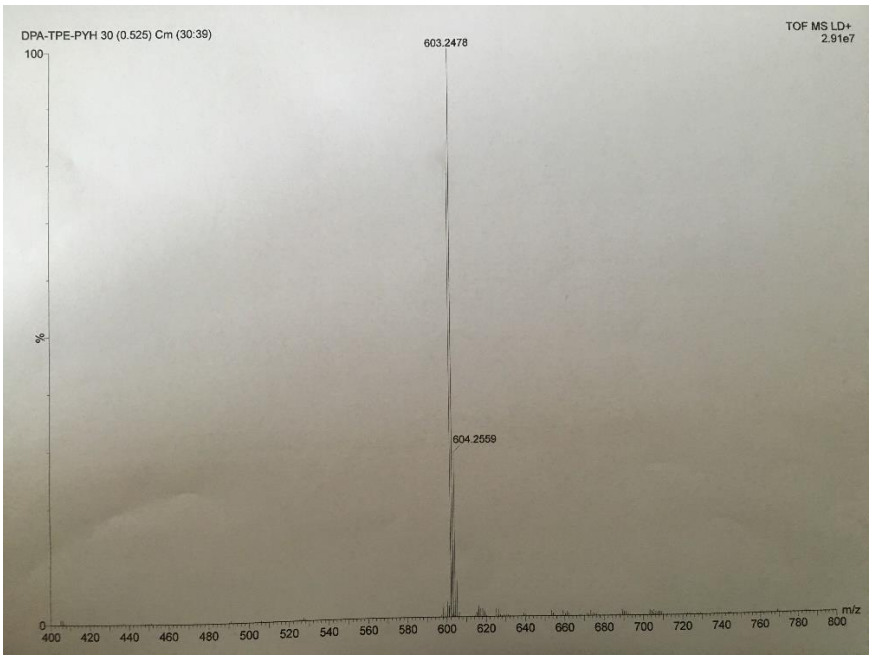

Fig. S13. MALDI-TOF mass spectrum of the reaction product (DPA-TPE-PyH) from the reaction between DPA-TPE-Py and DCP.

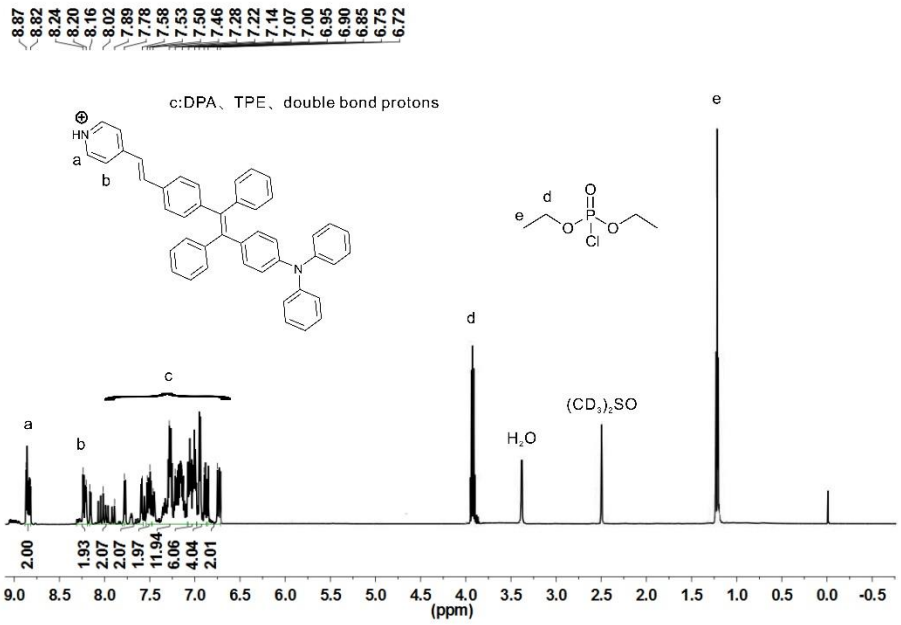

Fig. S14. ^{1}H NMR spectrum of the reaction product between DPA-TPE-Py and DCP in $(CD_3)_2SO$.

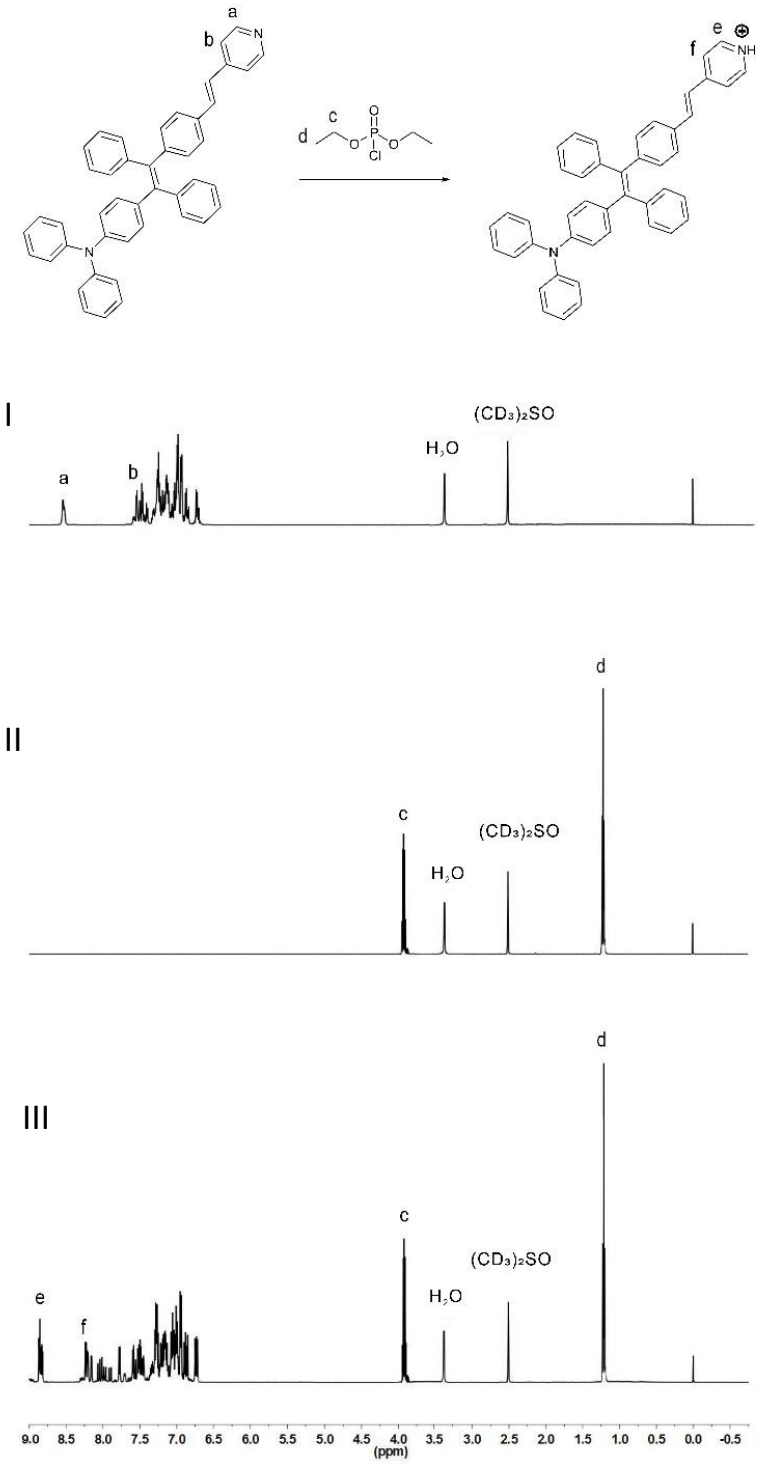

Fig. S15. ^{1}H NMR spectra for comparison of DPA-TPE-Py and its reaction product DPA-TPE- PyH in $(CD_3)_2SO$. I: DPA-TPE-Py; II: DCP; III: DPA-TPE- PyH (excessive DCP was added in the reaction).

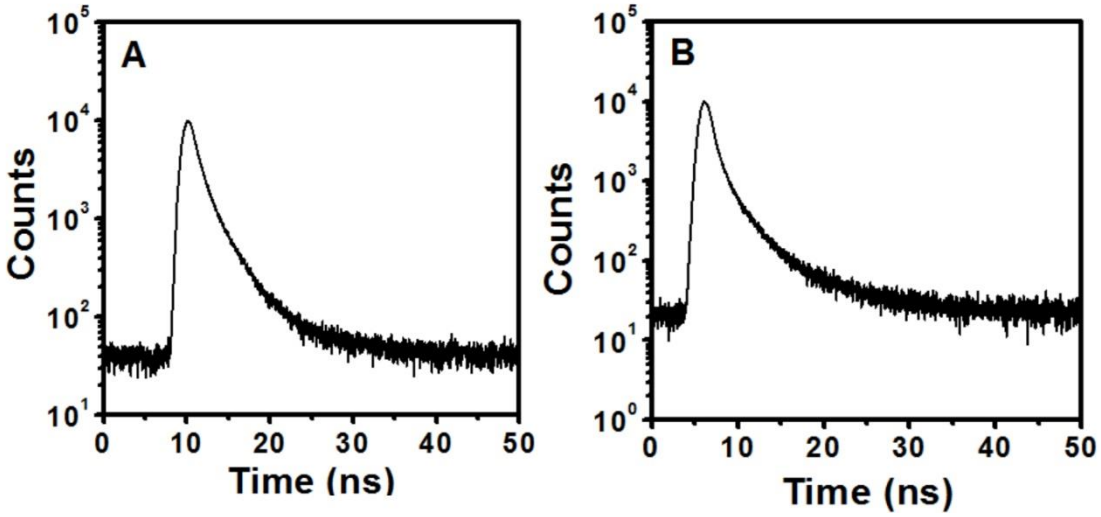

Fig. S16. (A) Fluorescence decay curve for the DPA-TPE-Py loaded test strip (recording 10000 photons measured at 465 nm excitation and 546 nm emission), Fit = $A + B_1\exp(-t/\tau_1) + B_2\exp(-t/\tau_2)$ (τ_1 = 1.10 ns, τ_2 = 3.45 ns). (B) Fluorescence decay curve for the DPA-TPE-Py loaded test strip upon exposure to DCP vapor ([DCP] = 0.377 ppm, recording 10000 photons at 465 nm excitation and 624 nm emission), Fit = $A + B_1\exp(-t/\tau_1) + B_2\exp(-t/\tau_2)$ (τ_1 = 0.80 ns, τ_2 = 3.65 ns).

References

(1) Thomsen, V.; Schatzlein, D.; Mercuro, D. Limits of Detection in Spectroscopy. *Spectroscopy*, **2003***, 18,* 112-114..

(2) McNaught, A. D.; Wilkinson, A. IUPAC Compendium of Chemical Terminology, *the "Gold Book",* **1997**.