Supporting Information

Development of Reaction-based AIE Handy Pen for Visual Detection of Toxic Vapors

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Supplementary Figures:

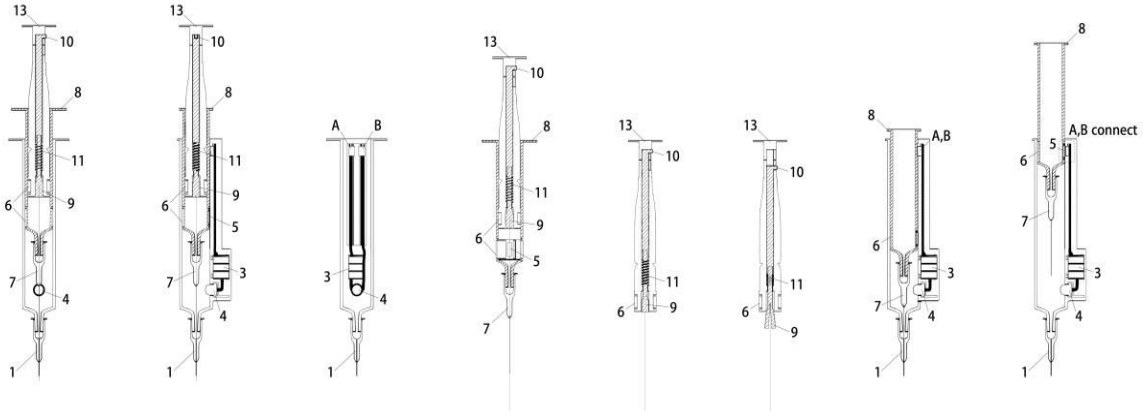

Figure S1. The structure of AIE handy pen

1. Outer needle；2. Observation window；3. power；4. UV light；5.Metal sheets; 6. Buffer zone；7. Inner needle；8. Lug；9. Chuck; 10. Slider；11. Spring；12. Cover；13. Piston；A、B-Metal contact; C、D-Sliding slot

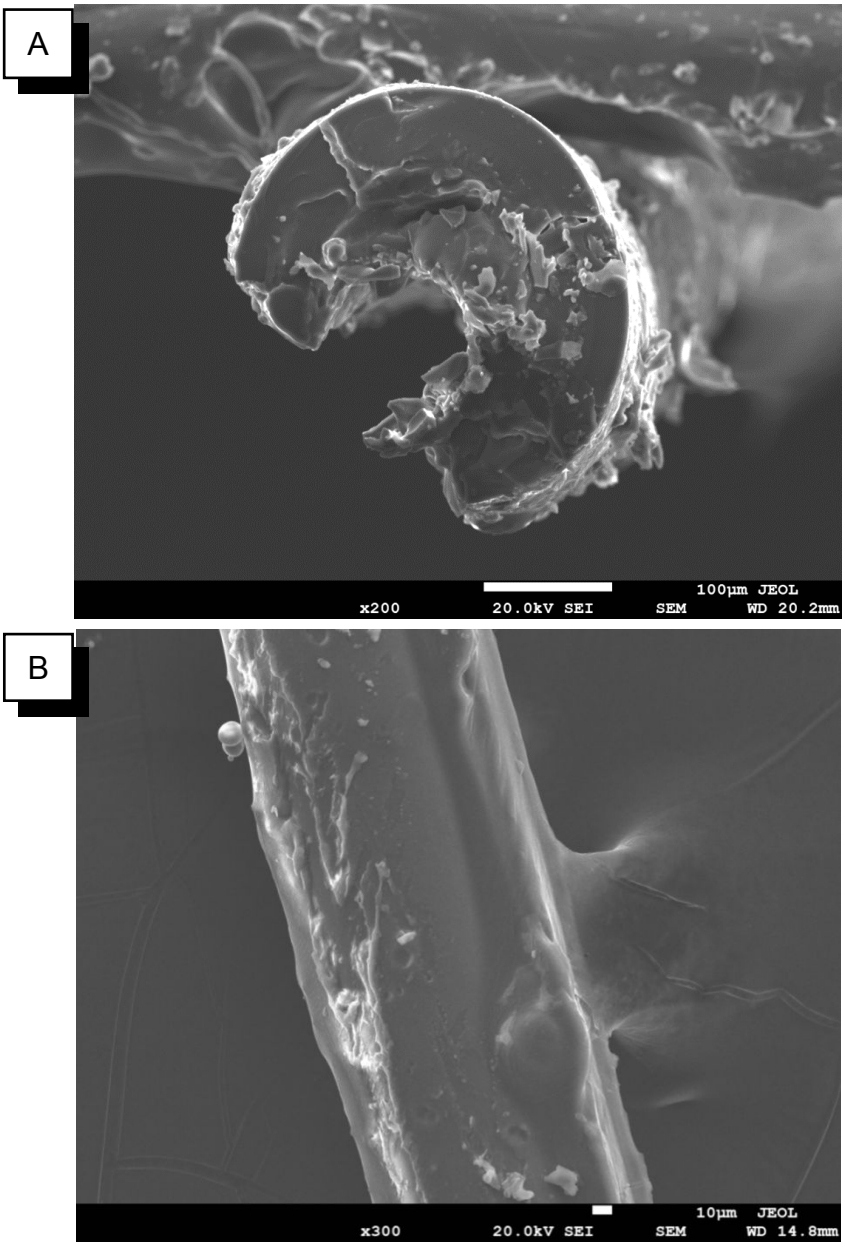

Figure S2. The SEM graphs of coated film (A) intersecting surface (B) the overall surface of fiber

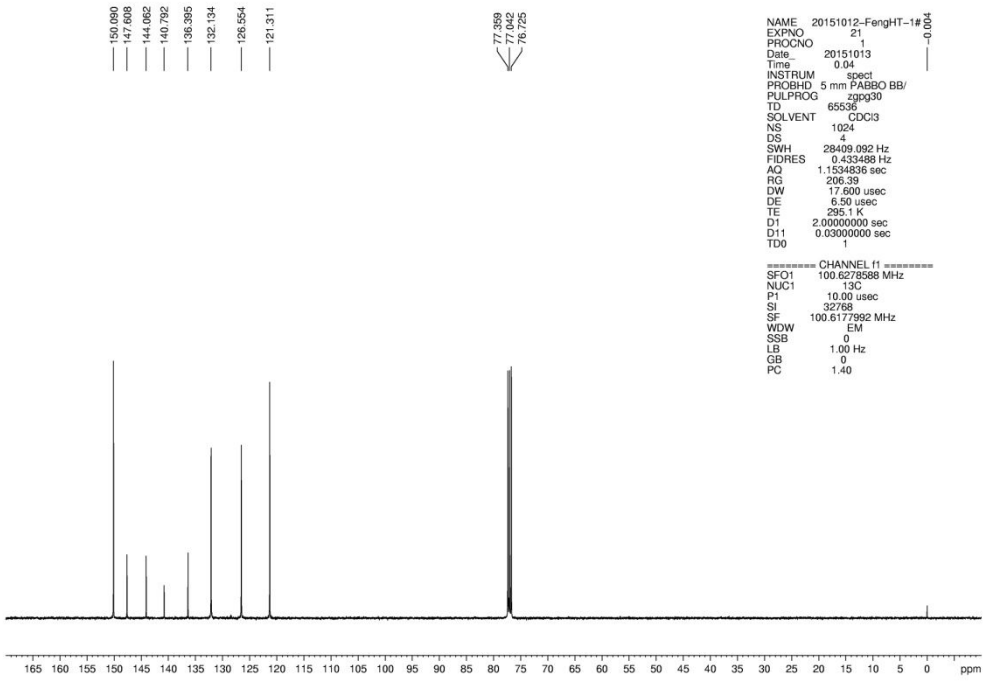

Figure S3. ^{1}H NMR spectrum of compound **TPE-Py** in $CDCl_3$.

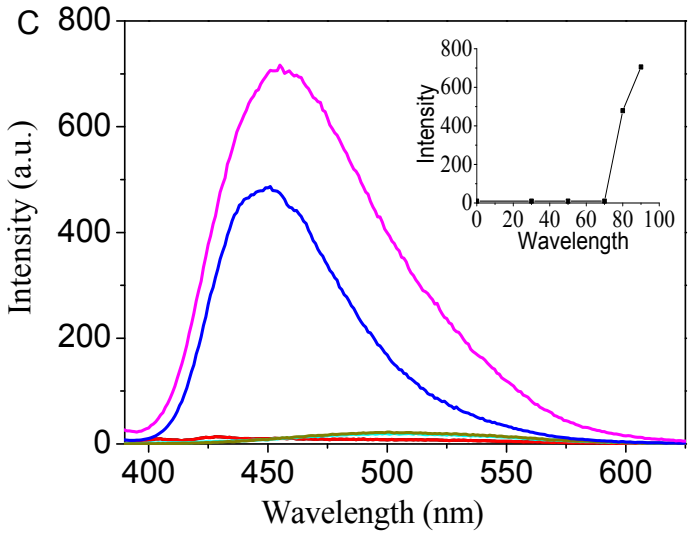

Figure S4. Fluorescence spectra of **TPE-Py** in THF after the addition of various amounts of water (excitation wavelength: 350 nm), 5.0 ×10^{-5} M.

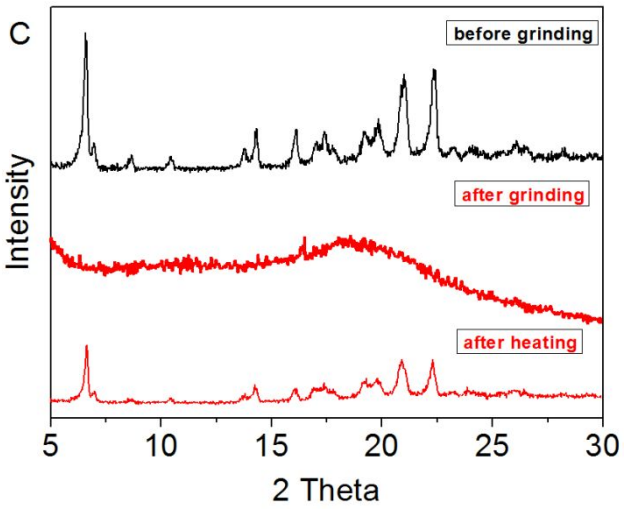

Figure S5. PXRD patterns of **TPE-Py** powders: pristine, ground and annealed sample (150 °C for 1 min).

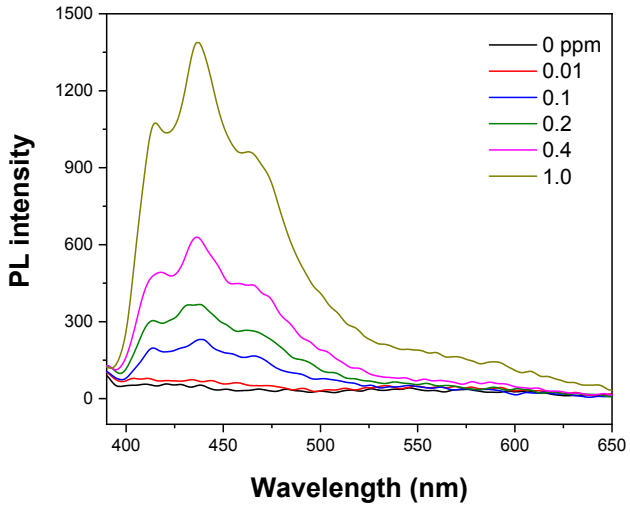

Figure S6. The PL emission spectrum of TPE-Py in the presence of DCP with different concentrations.

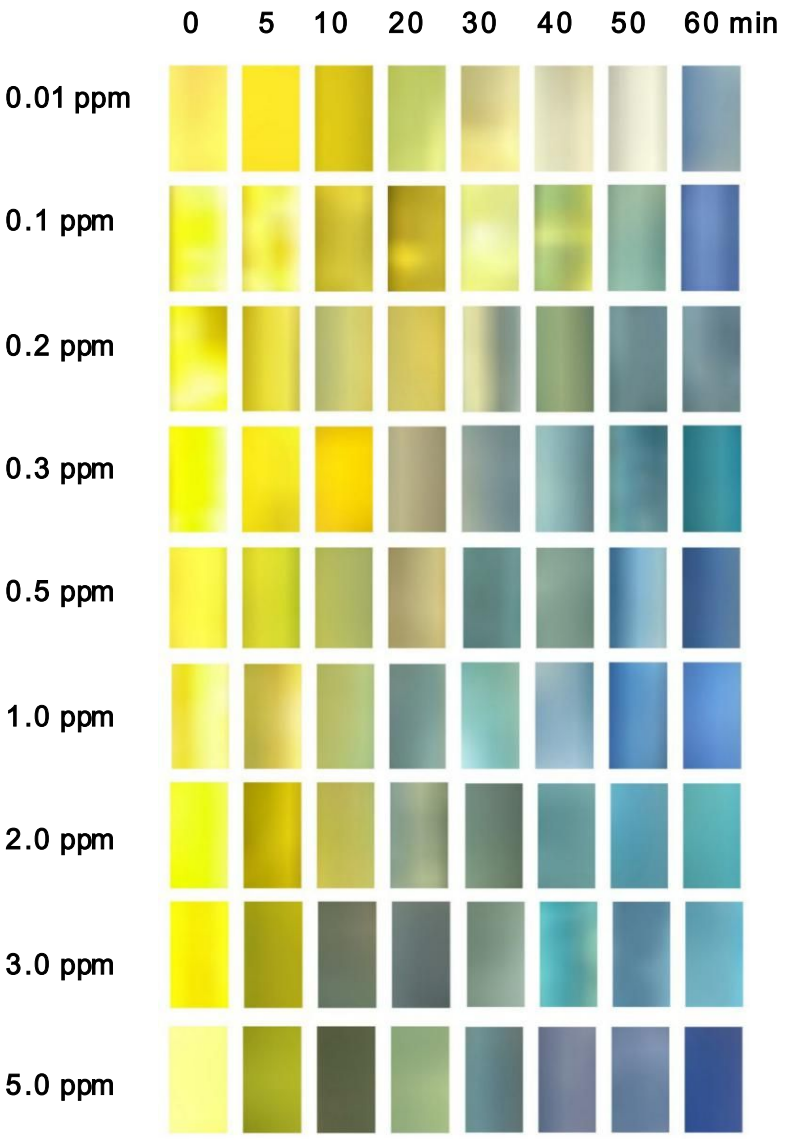

Figure S7. The emission of the TPE-Py coated fiber upon exposure to DCP vapor under UV lamp (the region of interest of the fiber was enlarged and rectangular shape was intercepted)

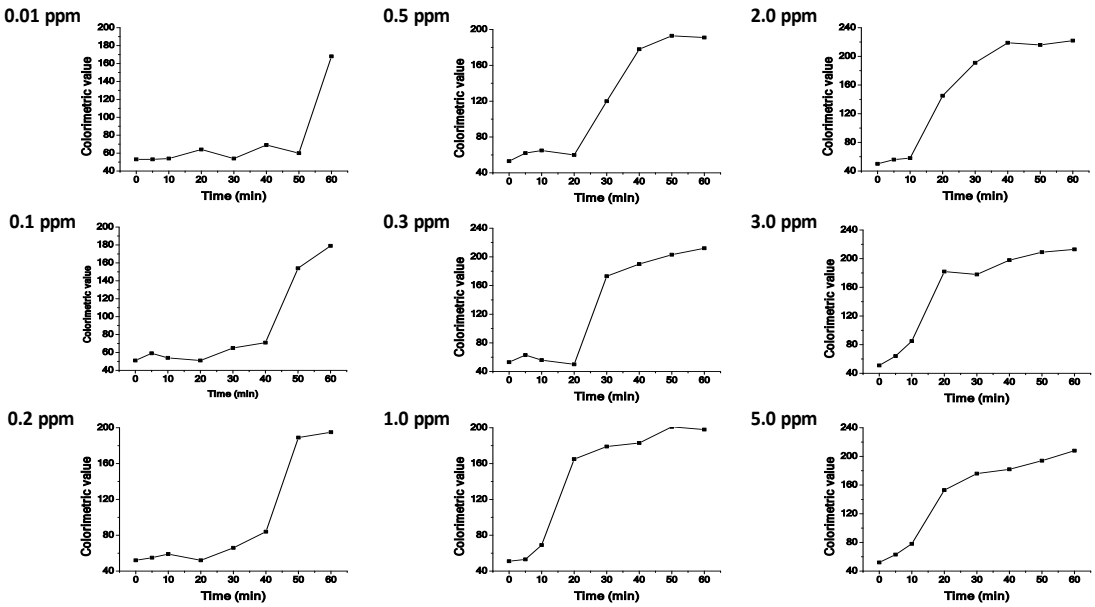

Figure S8. The colorimetric value of TPE-Py coated fiber upon exposure to DCP vapor at different time periods and different concentrations. (The colorimetric value was obtained by analyzing the region of interest of the fiber by Matalab code)

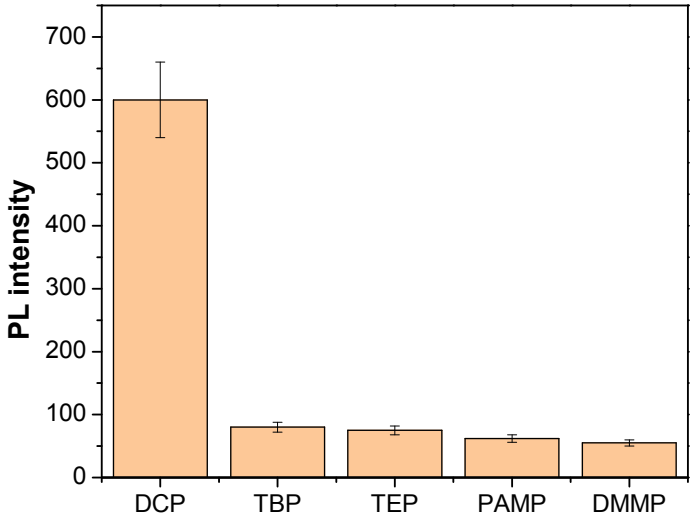

Figure S9. The photoluminescence intensity of TPE-Py loaded fiber upon exposure to 0.3 ppm DCP, TEP, TBP, DMMP or PAMP, respectively.

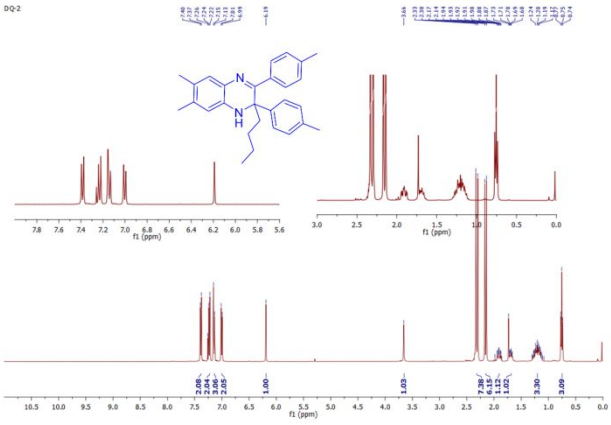

Figure S10. ^{1}H NMR spectra of DQ_2 in $CDCl_3$

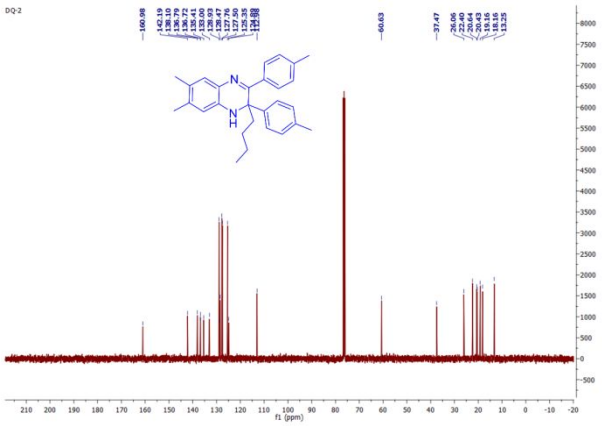

Figure S11. ^{13}C NMR spectra of DQ_2 in $CDCl_3$

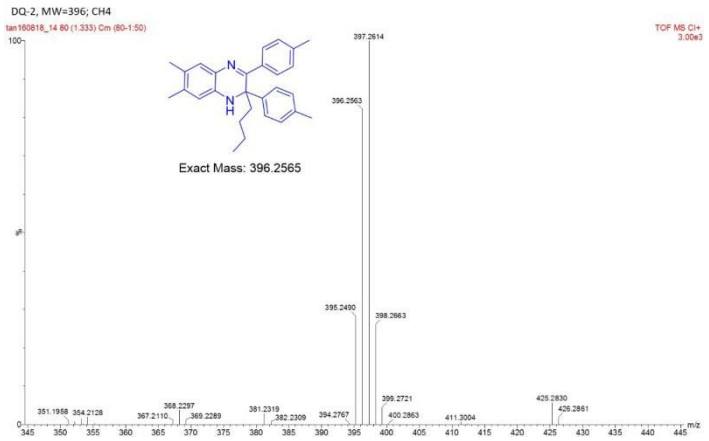

Figure S12. HRMS spectrum of DQ_2.

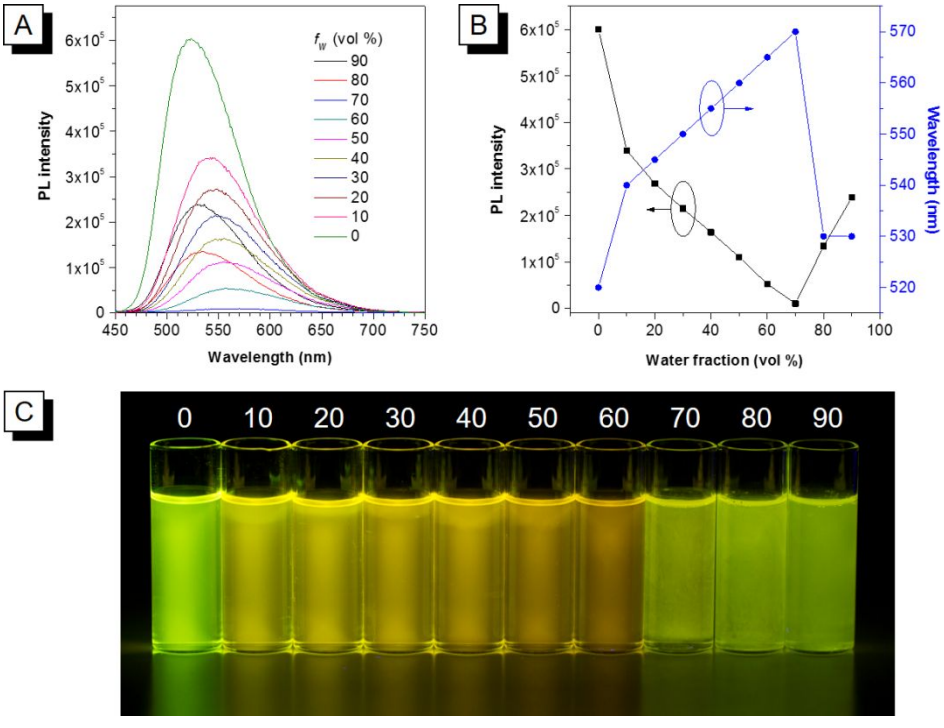

Figure S13. (A) PL spectra of DQ_2 in THF/H_2O mixtures with different water fractions (f_w). Concentration: 10 μM; λ_{ex} = 400 nm. (B) Plot of PL intensity and emission maximum versus the composition of the THF/H_2O mixtures of DQ_2. (C) Fluorescent image of DQ_2 in THF/H_2O mixtures with water fractions from 0 to 90% (left to right) taken under 365 nm UV irradiation.

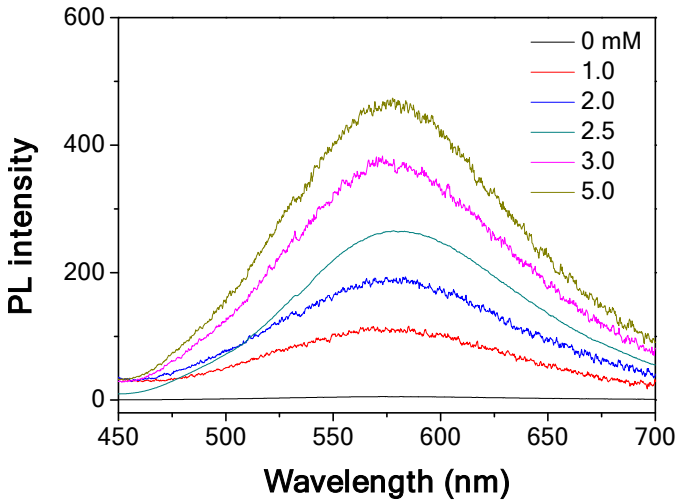

Figure S14. The PL emission spectrum of DQ_2 in the presence of amine with different concentrations.

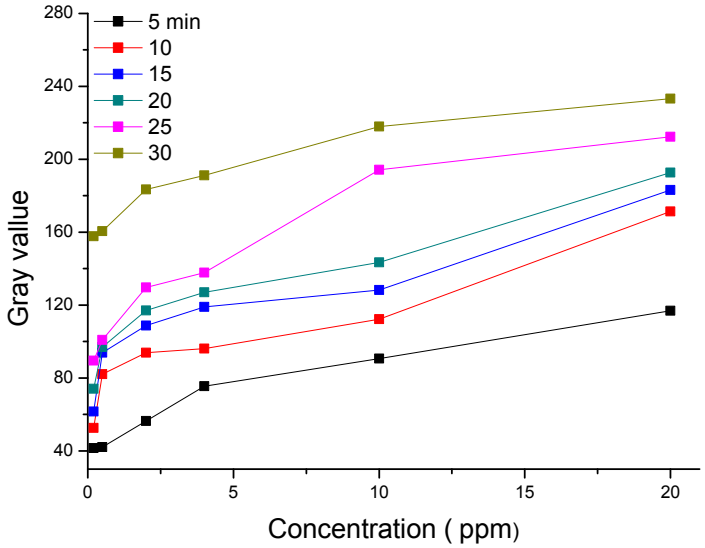

Figure S15. The gray value of DQ_2-coated fiber upon exposure to amine vapor with different concentrations and different time. (The gray value was obtained by analyzing the region of interest

of the fiber by Matalab code)

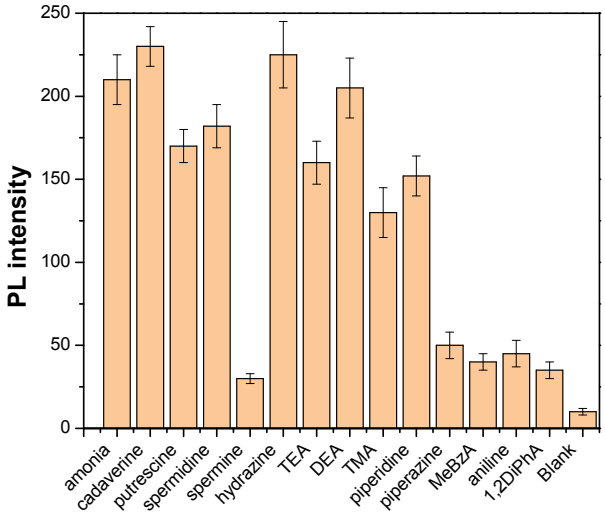

Figure S16. The PL turn-on response of DQ_2-coated fiber in the presence of various amine solutions (0.08 M). Abbreviation: TEA=triethylamine; DEA=diethylamine; TMA=trimethylamine; MeBzA=methylbenzylamine; 1,2 DiPhA=1,2-diphenylamine.

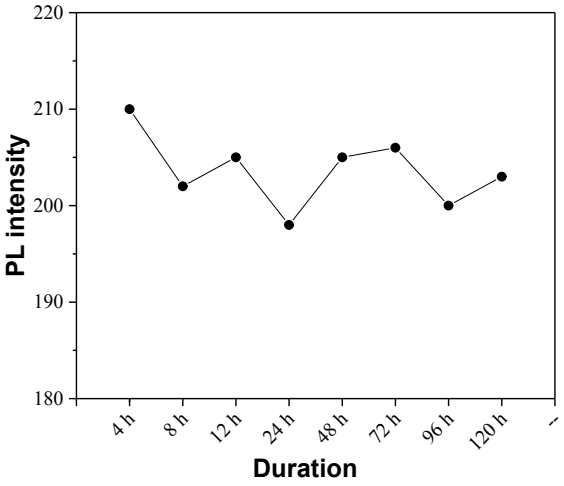

Figure S17. The emission of the DQ2-coated fiber in different time storage.

Table S1. Comparison of the LODs for detection of DCP with literatures

Methods	LODs	References
electrochemical sensors	3 ng/mL	37
reaction based fluorescence sensor	10 nM	38
nucleophilic attack fluorescence sensor	10^{-8} M	39
near Infrared colorimetric	0.136 nM	40
portable AIE handy pen	3.4 ppb	This work

Table S2. Comparison of the LODs for detection of amine with literatures

Methods	LODs	References
GC-MS	1 pg	41
HPLC	25-50 pmol/mL	42
electrochemical	0.1 (ppq) to 75000 ppm	43
colorimetric arrays	100 ppbv	44

Portable AIE handy pen	0.2 ppm	This work

MATERIALS AND METHODS

Reagents and instruments. 1, 2- dihydroquinoxaline (DQ_2), tetraphenylethylene functionalized with pyridine rings (TPE-Py) were synthesized as reported in the literature (35, 36). Silica fiber was obtained from Rui-feng chromatography instrument Co. Ltd. Trifluoroacetic acid (95%), hydroxy-terminated polydimethylsiloxane (HTPS), amine and diethyl chlorophosphate (DCP) were purchased from Sigma-Aldrich. Methyltrimethoxysilane (MTMS) and hydrogen-containing silicone were purchased from Maclin (Shanghai, China). The concentration of amine was calculated by detector tubes purchased from Gastec, Japan.

Description of the portable device. The AIE handy pen consists of a coated fiber and a light source, in this case a light emitting diode (LED), to excite the luminophore on the fiber in a syringe-like holder. The arrangement of the elements is depicted in Fig. S1. There are three layers in the device. In the outer sleeve, there is a needle (1) outside for protection of the fiber. The observe window (2), power (3), and LED light (4) were also in the outer sleeve. In the middle sleeve, the metal sheet (5) can be moved to the position of A and B to make the power on or off, the buffer zone (6) was used to make the movement smoother. The needle (7) was also used to protect the fiber. The lug (8) was used to move the second sleeve. In the third sleeve, the inner chunk (9) was used to immobilize the fiber and moved by slider (10) in the district C and D to load the fiber. The spring (11) was used to help ejecting the fiber. Outside the battery there is a cover (12). The piston (13) can be moved to control the fiber at suitable position for detection and observation.

Detection of amine/ DCP by the AIE handy pen. First, the fiber was pushed by the plunge outside, and exposed to the vapor of the target. Then the fiber was retracted inside the needle and pulled to the position of observation window. After the UV light turned on, the emission of the fiber was obtained. The video for operation was supplied in Movie.S1. The brightness of the fluorescent images was obtained by calculating the greyscale values or colormetric values of the fiber photo by using MATLAB. The values were then used to determine the limit of detection (LOD) based on 3s/m, where s is the standard deviation of the blank measurement and m is the slope of the regression line. The regression line was obtained by plotting the greyscale value or colormetric value versus the gas concentration.