Support Information

A novel fluorescent probe for the detection of oxalyl chloride in air

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1. General information

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1,2-Diamino anthraquinone, 2-hydroxy-4-methoxybenzaldehyde, trifluoroacetic acid, ethanol, formaldehyde， phosgene, acetone, phenol, isocyanate, benzenesulfonyl chloride, acetylacetone, benzene, styrene, carbon disulfide, oxalyl chloride, toluene, and phosphorus oxychloride;. Due to the highly toxic nature of phosgene, triethylamine was used to prepare with triphosgene and all other reagents were purchased from McLean Reagent Company. The water used in this experiment was distilled water prepared by secondary distillation.

The fluorescence spectra and UV-visible spectra were recorded using a Hitachi F-7000 fluorescence spectrophotometer and a Hitachi U-3010 UV-visible spectrophotometer, respectively.

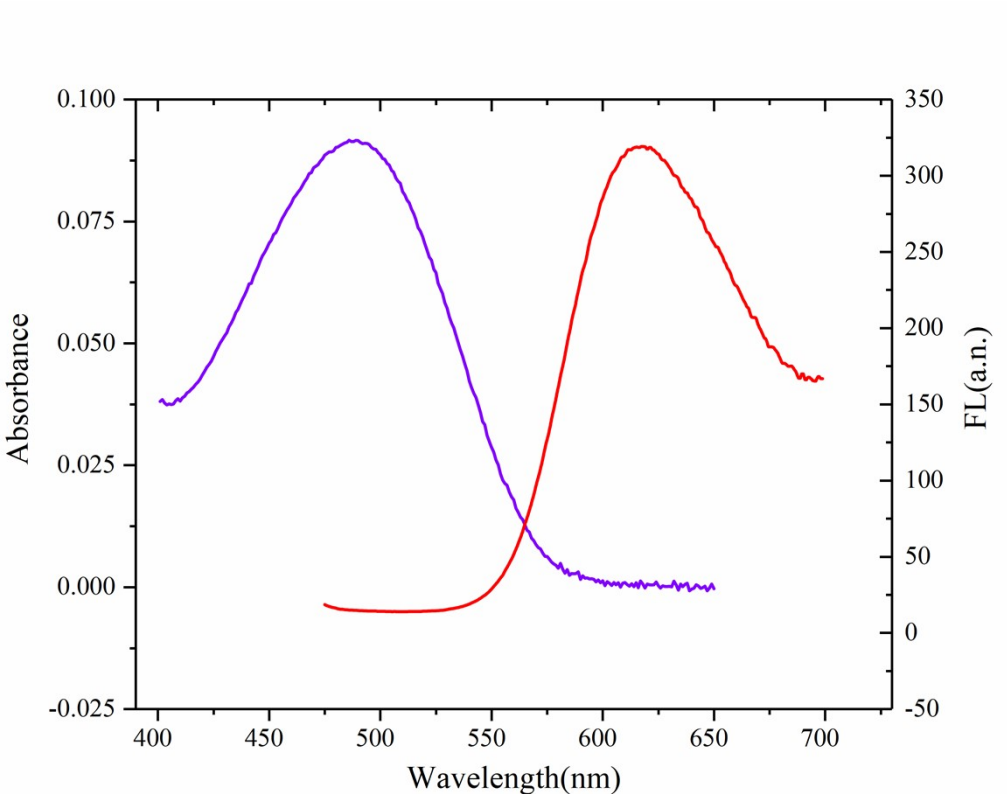

Fig. S1 UV absorption spectrum and fluorescence emission spectrum of HHD

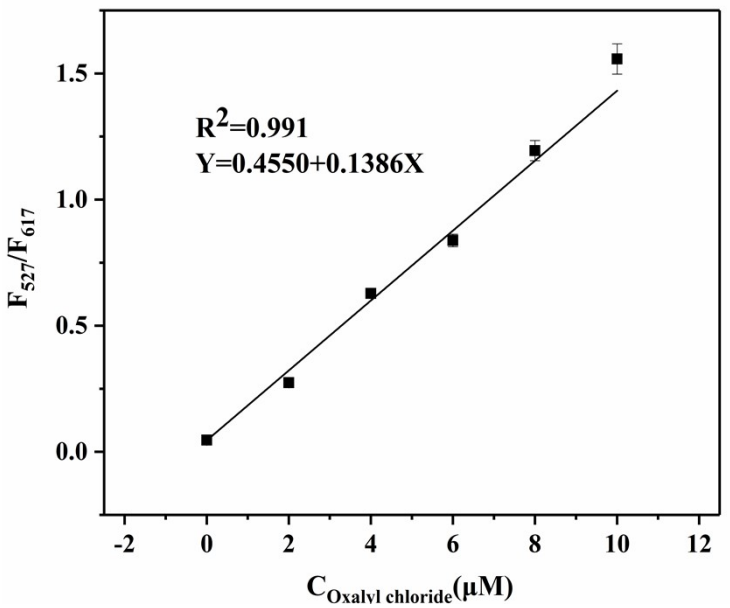

Fig. S2 Plot of F_{617}/F_{527} and oxalyl chloride (0-10 μM)

Method to Calculate the Detection Limit

Due to the linear relation between low concentration of oxalyl chloride and the fluorescence intensity. A regression curve can be obtained from the low oxalyl chloride concentration part in plot of the fluorescence intensity as a function of oxalyl chloride concentration.

The equation of limit of detection (LOD) is:

$$\mathrm{LOD} = 3 \times \frac{S.D.}{K}$$

In this equation LOD stand for limit of detection, S.D. means the standard deviation for the fluorescence intensity ratio (F_{527}/F_{627}) without oxalyl chloride existing. And K represents the slope of the regression curve in Fig. S2.

According to the equation, the LOD of this probe is:

LOD=3×0.00258/0.1386=56 nM

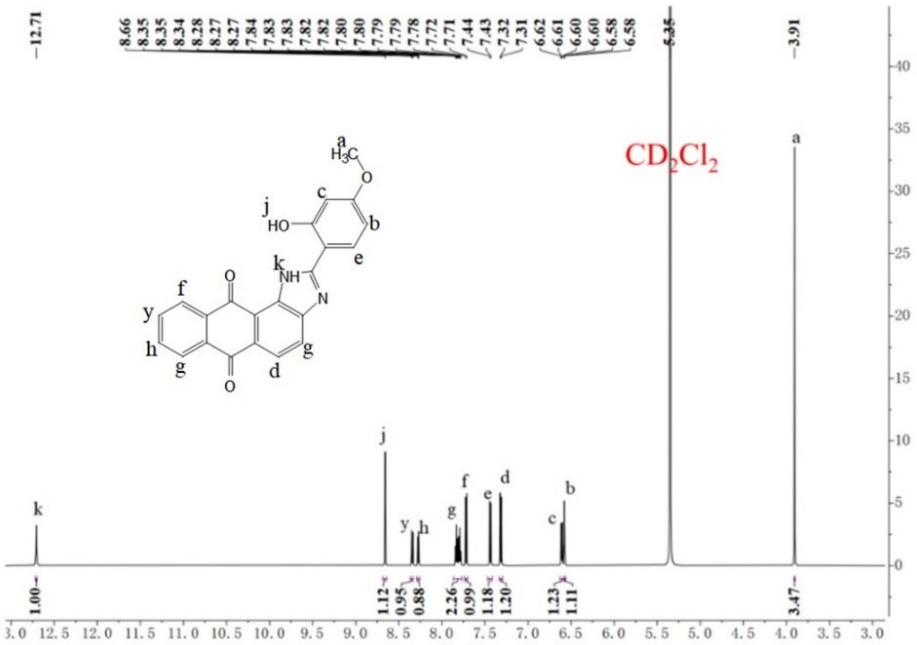

Fig. S3 ^{1}H NMR of HHD in CD_2Cl_2

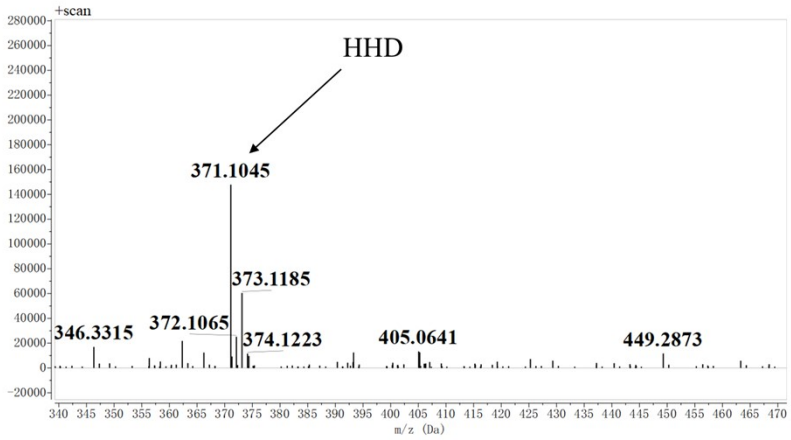

Fig. S4 HRMS for HHD

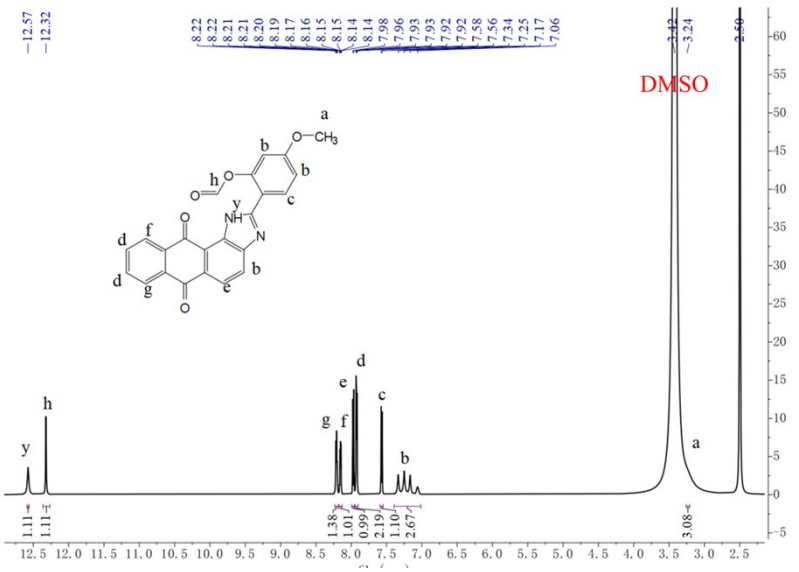

Fig. S5 ^{1}H NMR of HHD-O in DMSO

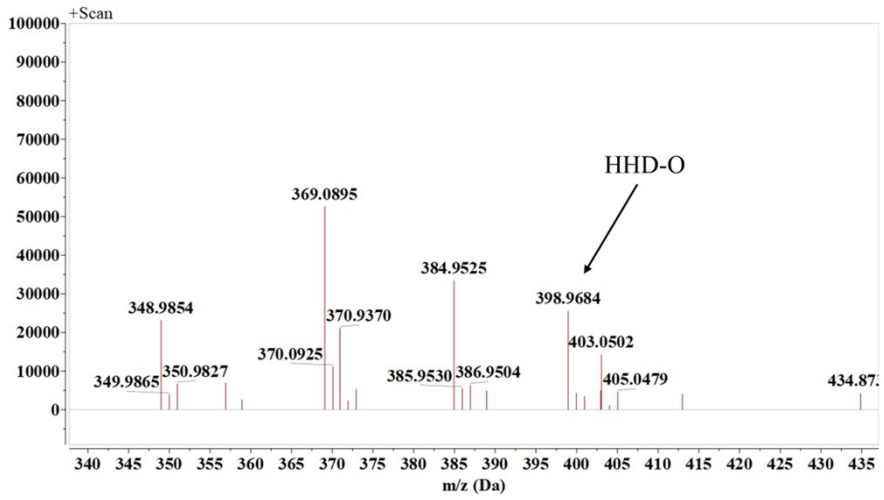

Fig. S6 HRMS for HHD-O

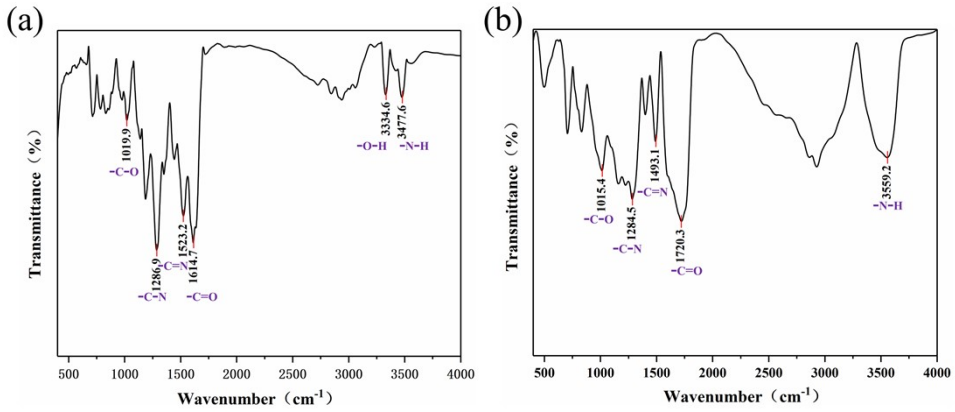

Fig. S7 IR spectra of HHD (a) and HHD-O (b)