Supporting Information (SI)

For

Design and synthesis of a fluorescent probe with a large Stokes shift for detecting thiophenols and its application in water sample and living cells

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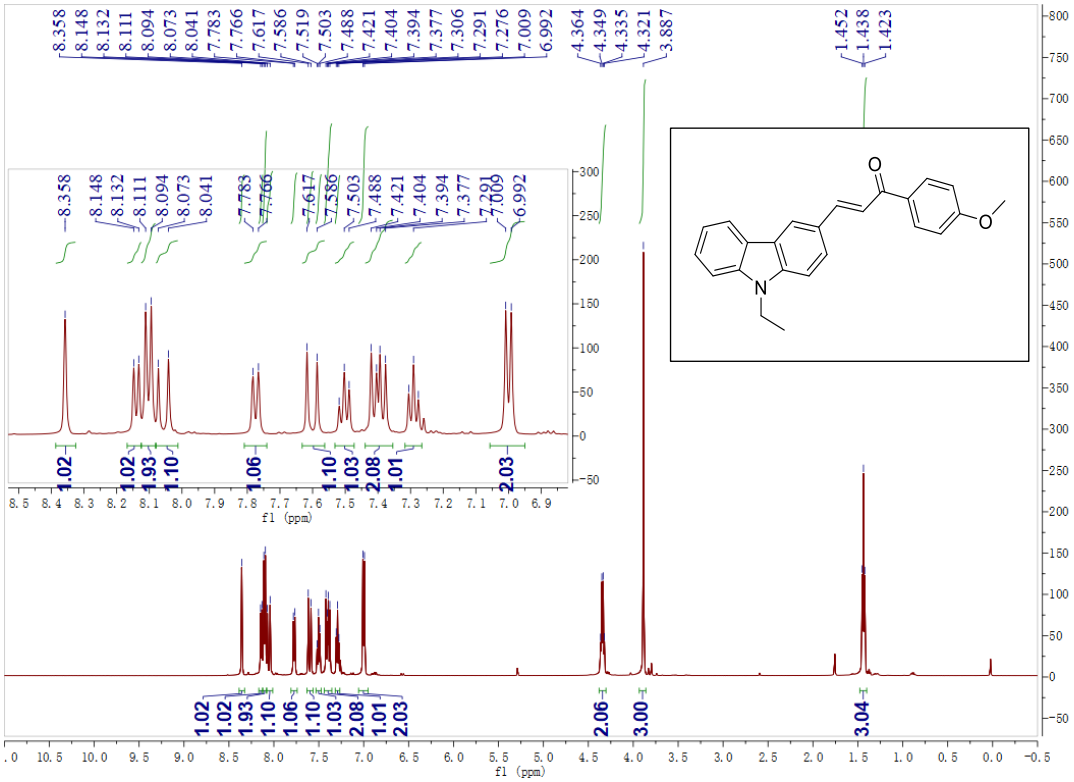
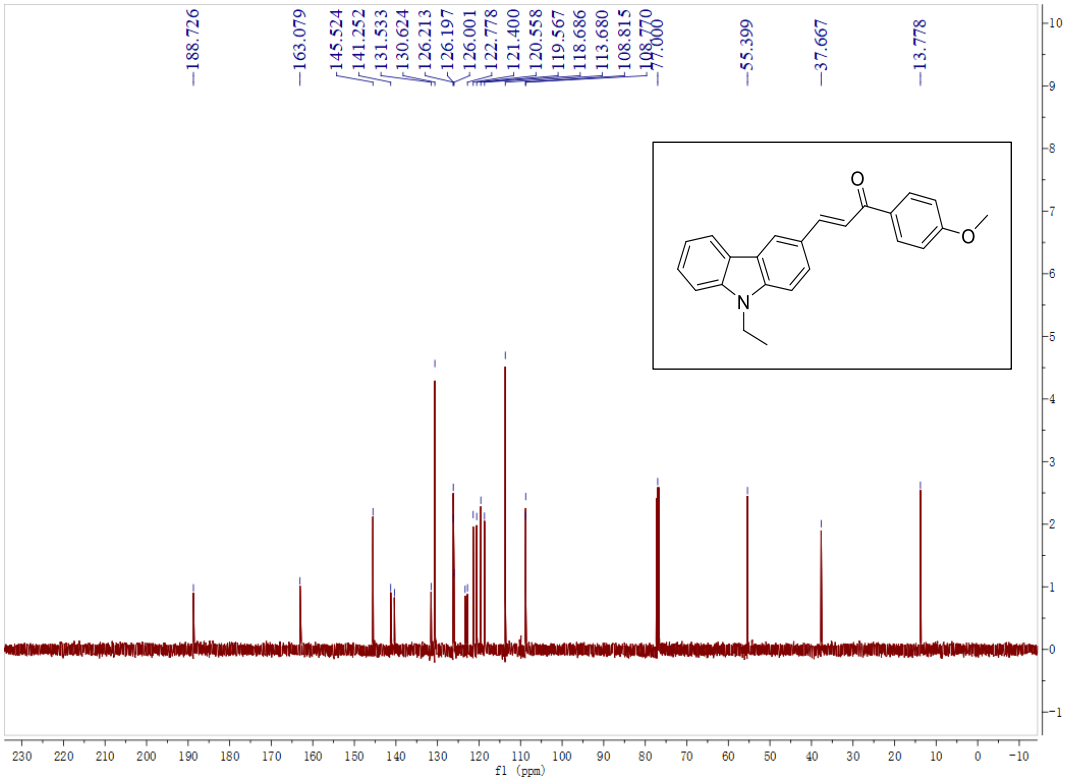
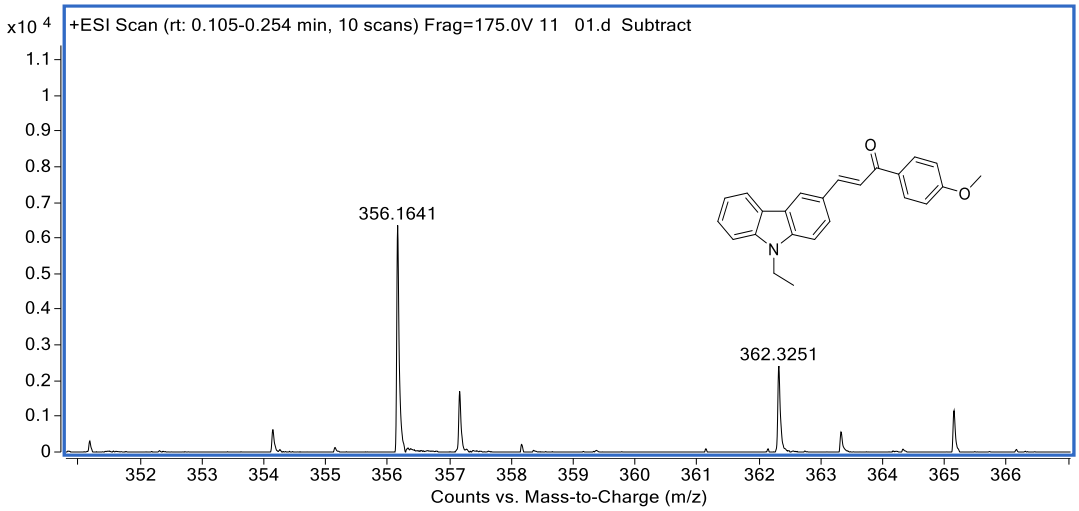
1. Structure characterization



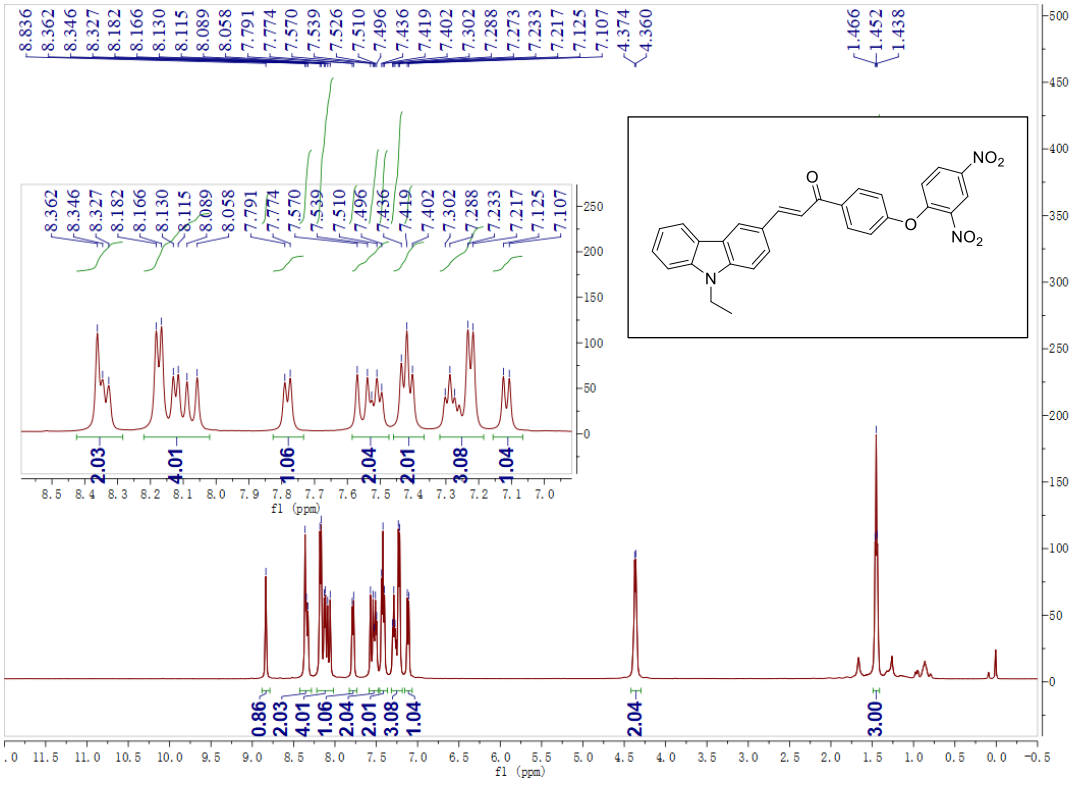
^{1}H NMR spectrum of KCP-OCH$_3$



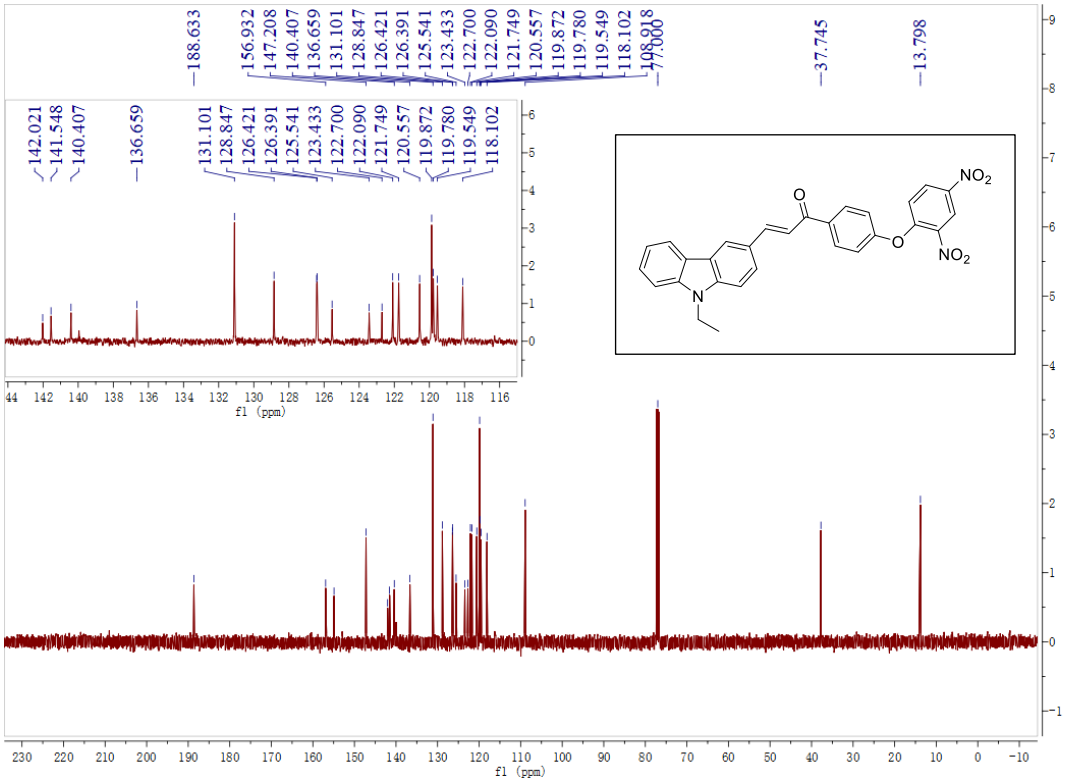
^{13}C NMR spectrum of KCP-OCH$_3$



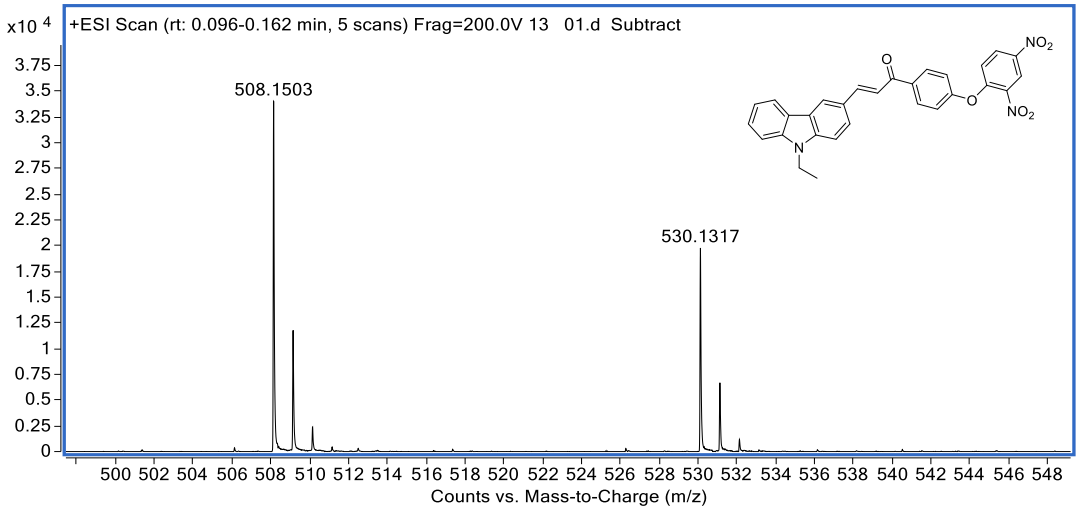
HR-MS spectrum of KCP-OCH_3



^{1}H NMR spectrum of probe-KCP

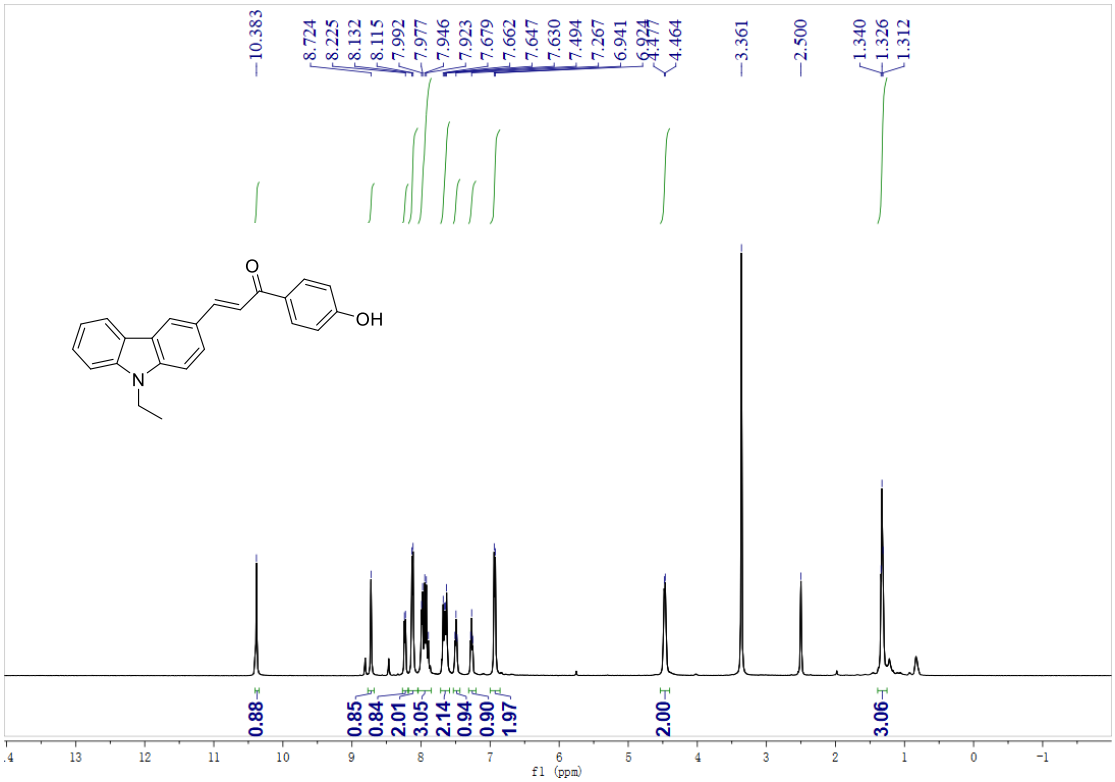


^{13}C NMR spectrum of probe-KCP

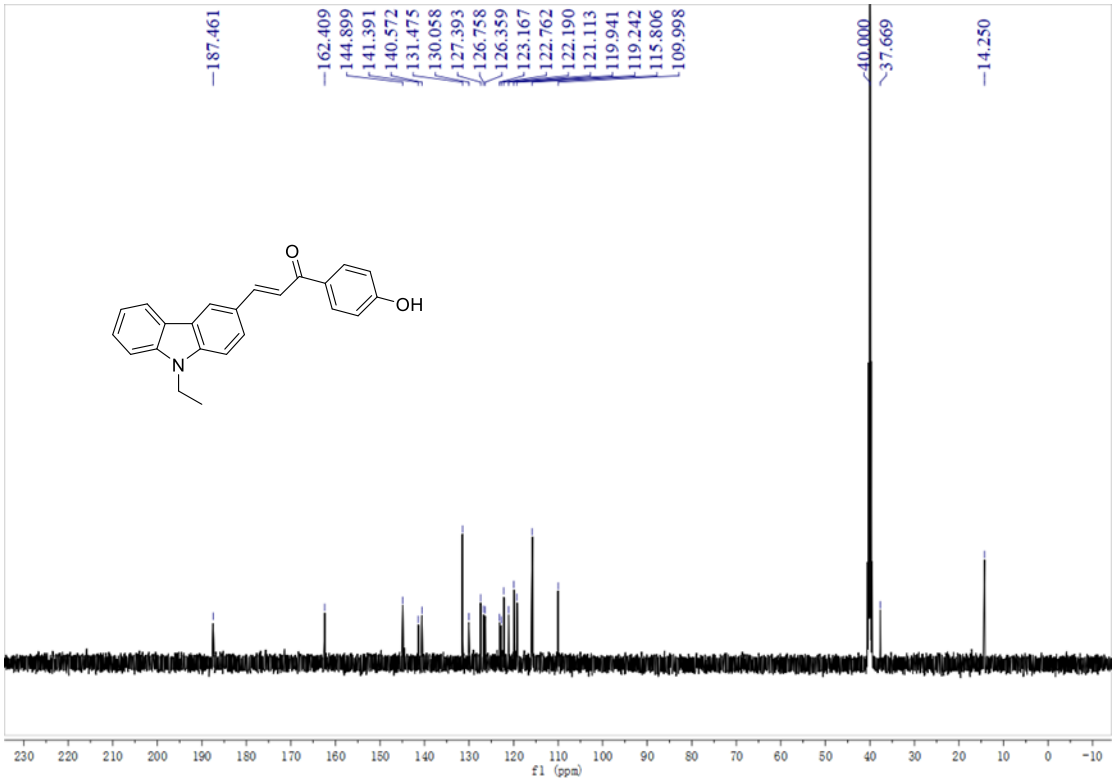


HR-MS spectrum of probe-KCP

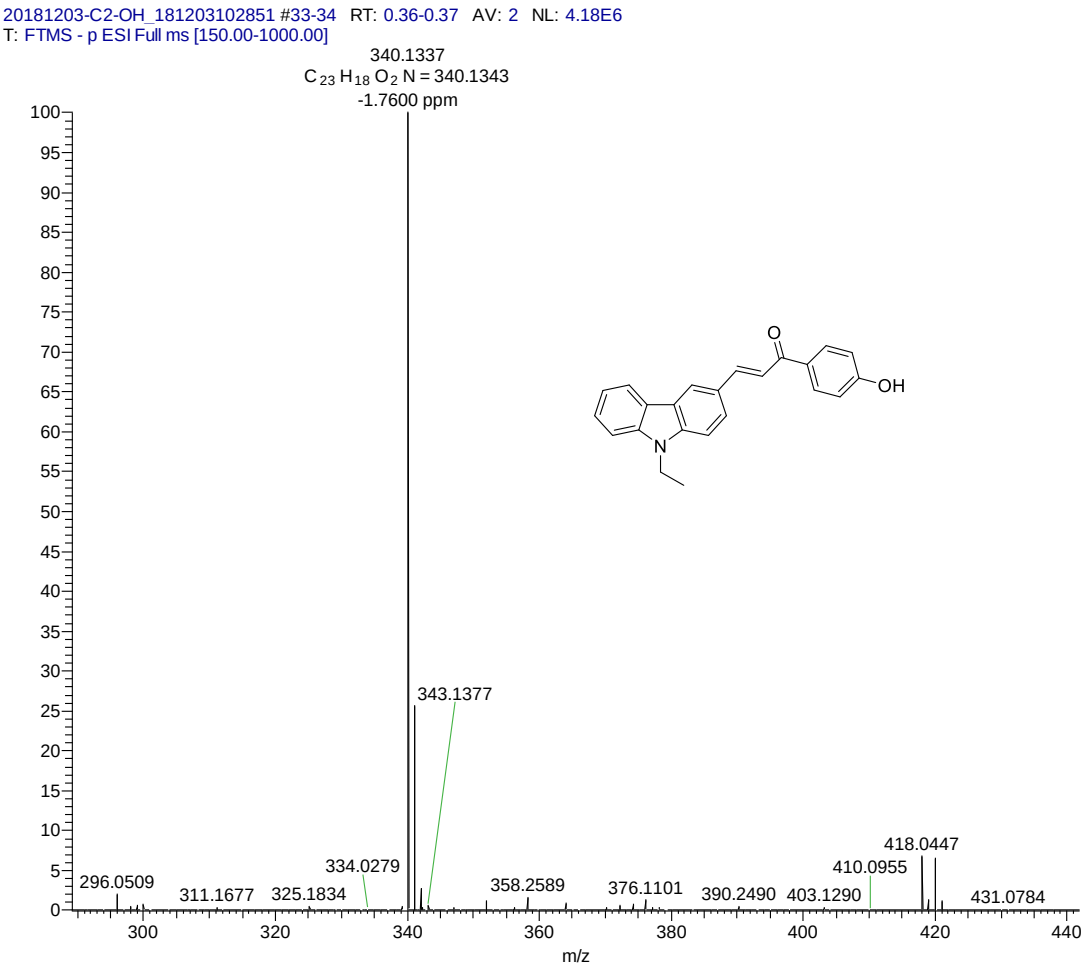
2. Additional spectra



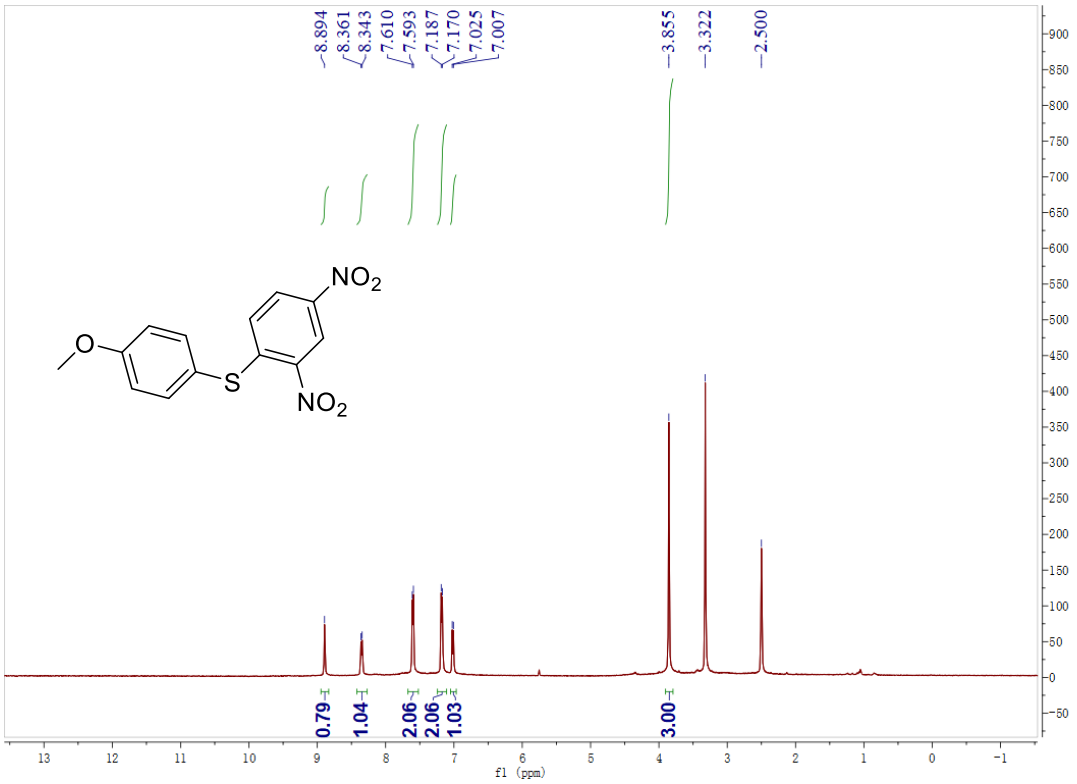
^{1}H NMR spectrum of probe-OH



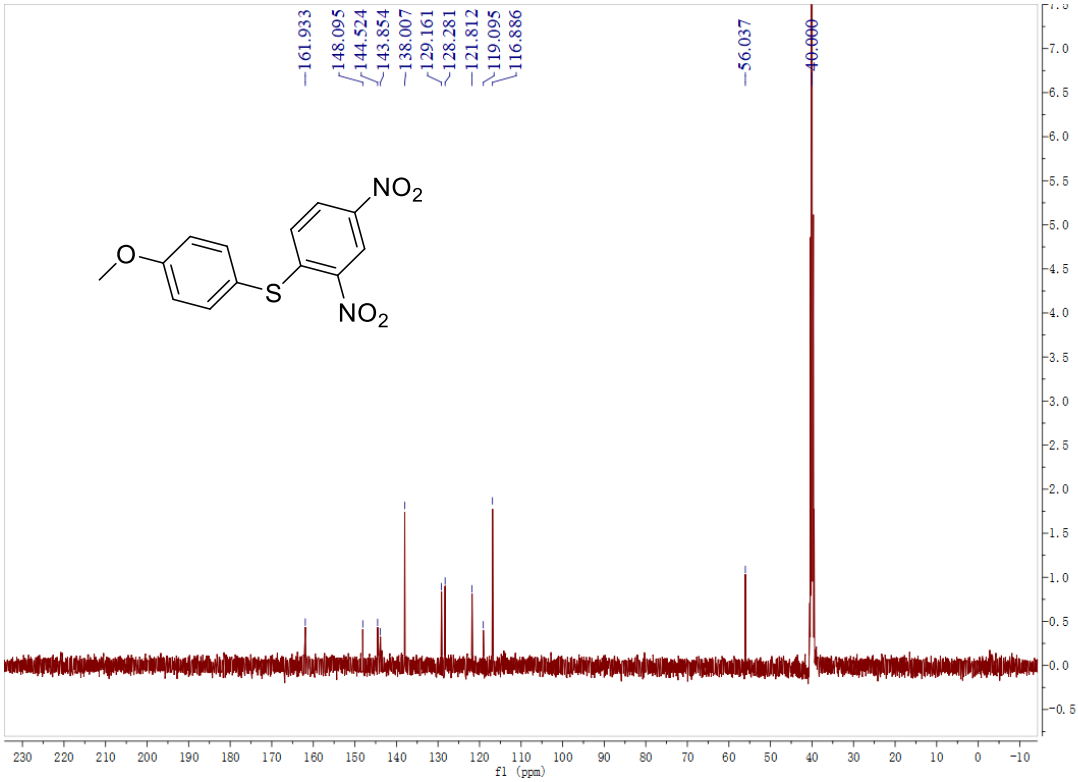
^{13}C NMR spectrum of probe-OH



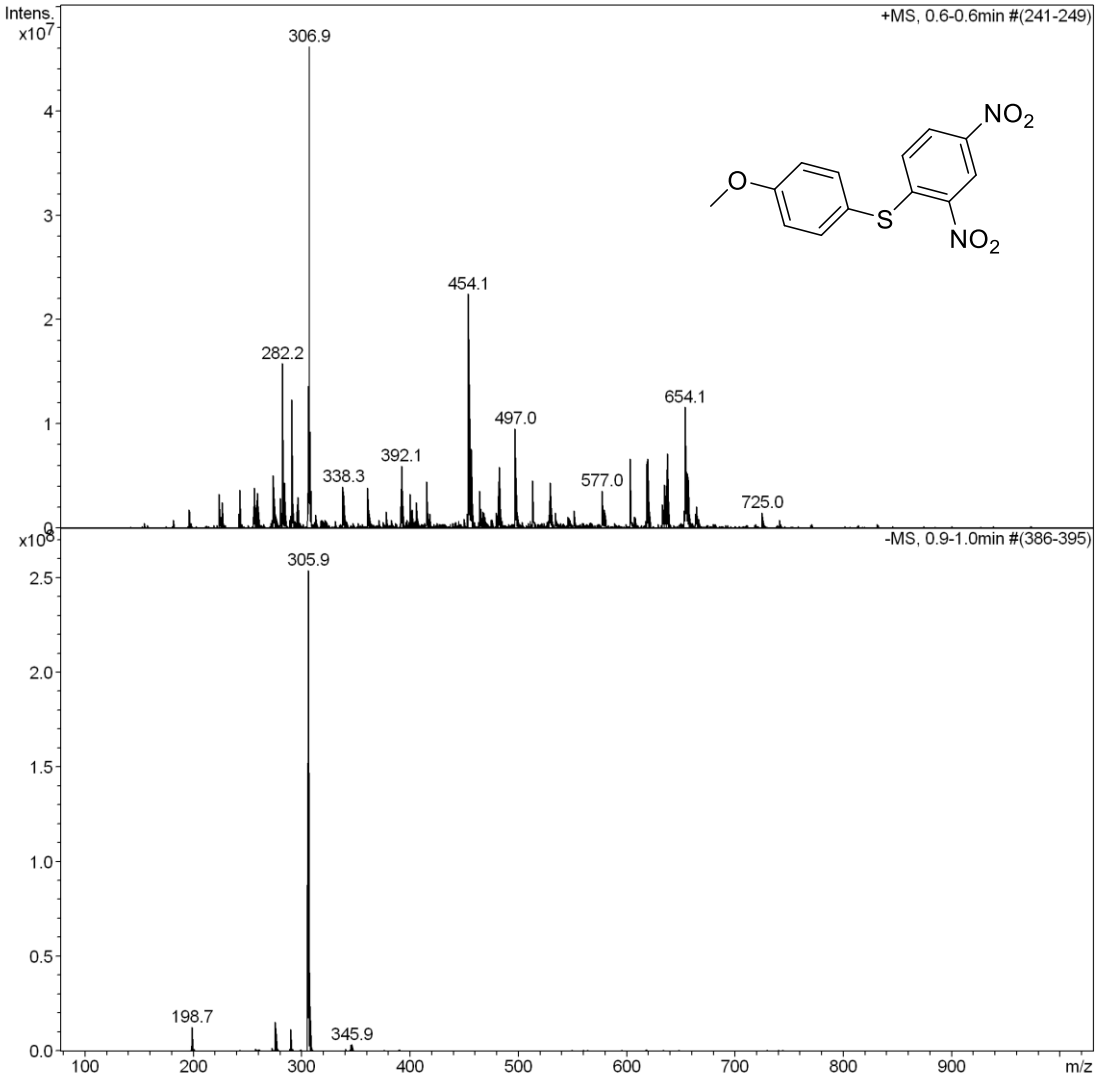
HR-MS spectrum of probe-KCN1



^{1}H NMR spectrum of S-NO_2



^{13}C NMR spectrum of S-NO_2



MS spectrum of S-NO_2

Figure S1. date for investigation of the sensing mechanism.

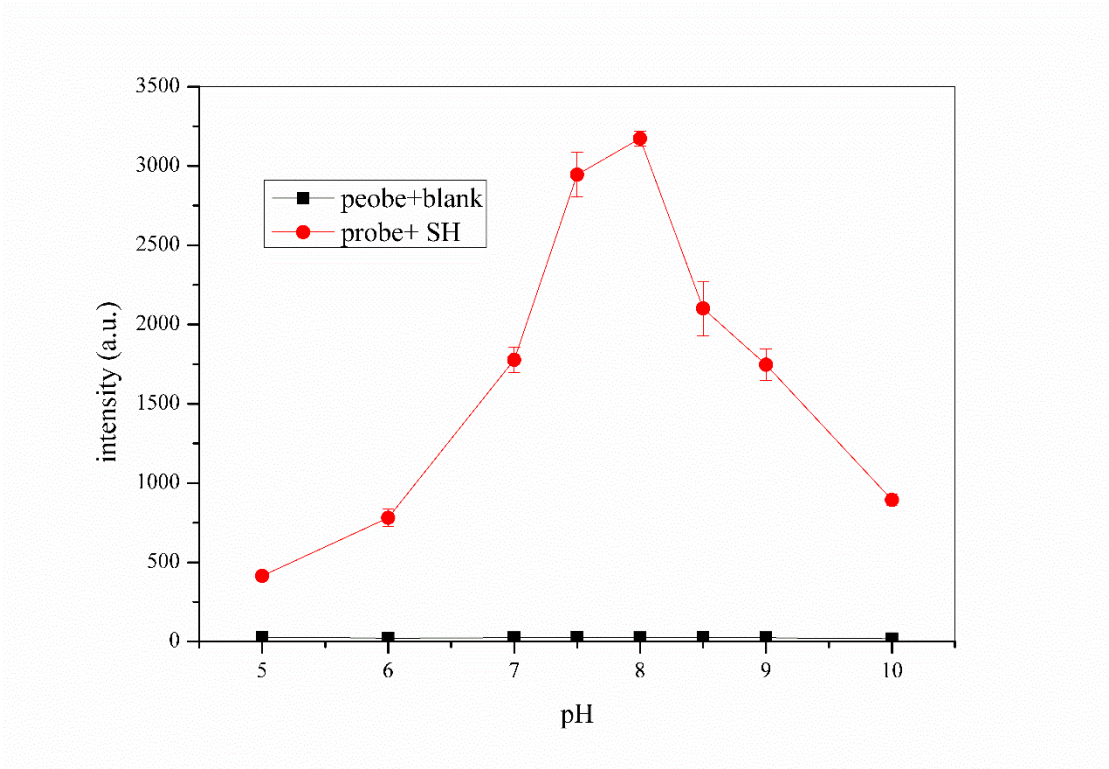


Figure S2. The effect of pH on the fluorescence intensity (λ_{em} = 540 nm) of probe-KCP (10 μM, λ_{ex} = 410 nm) in DMSO/PBS buffer (1:1, *v*/*v*, 20 mM) upon addition of 100 μM 4-Methoxy thiophenol after incubation at 37 ºC for 20 min.

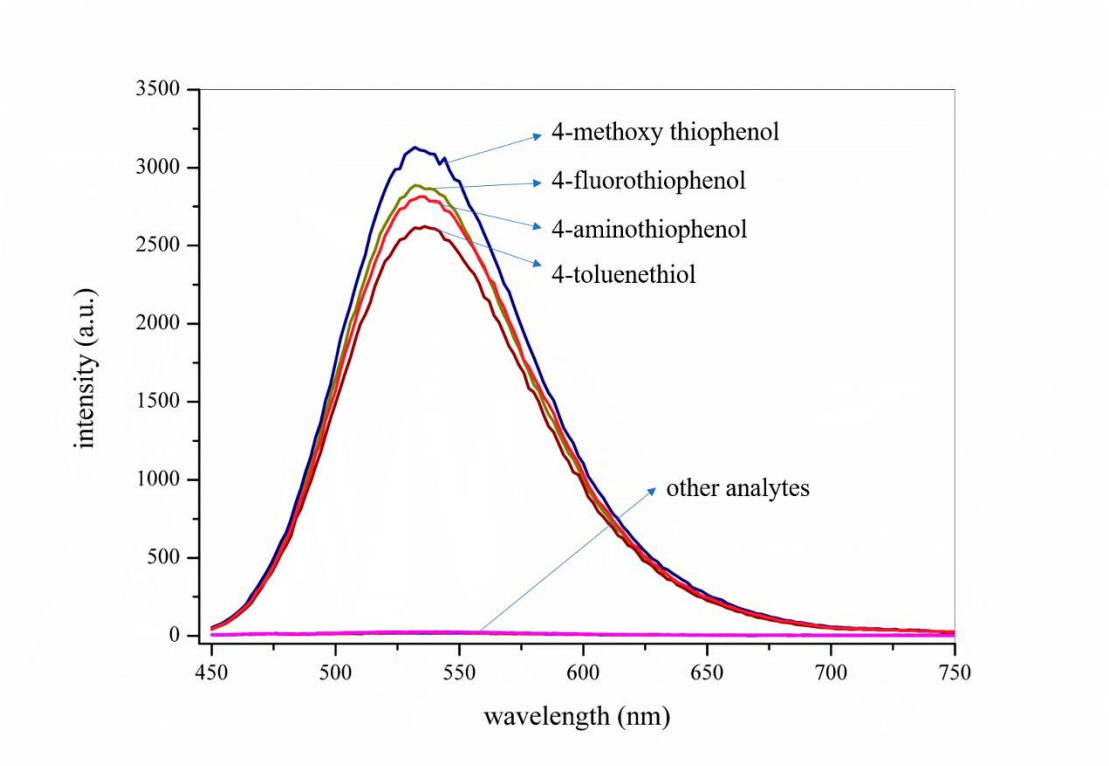


Figure S3. Fluorescence responses of probe-KCP (10 μM) to thiophenol and other

various analytes (100 μM) in PBS buffer solution (20 mM, pH = 7.4) containing 50 % DMSO.

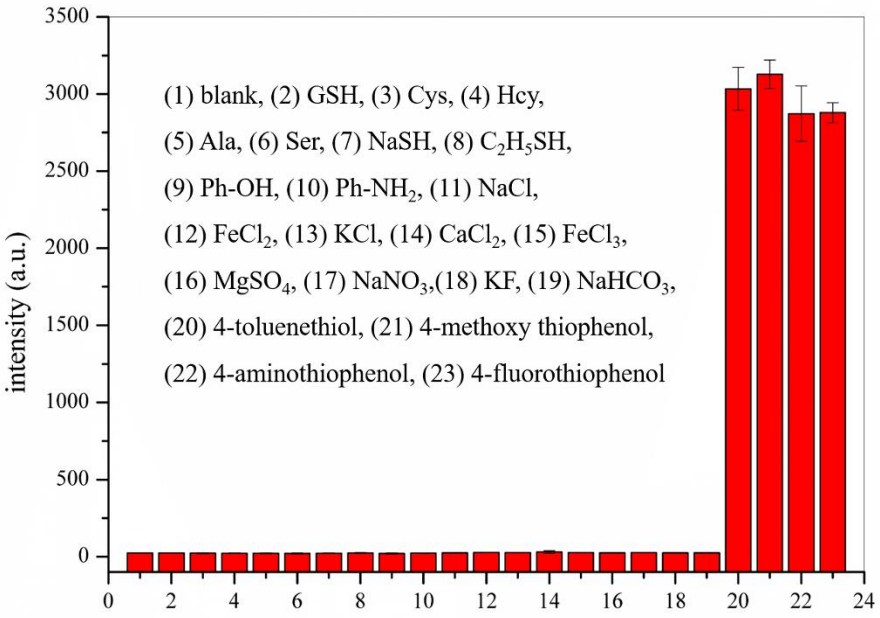


Figure S4. Enhanced fluorescence response at 540 nm of the probe-KCP (10 μM) to thiophenol and other various analytes (100 μM) in PBS buffer solution (20 mM, pH = 7.4) containing 50 % DMSO.

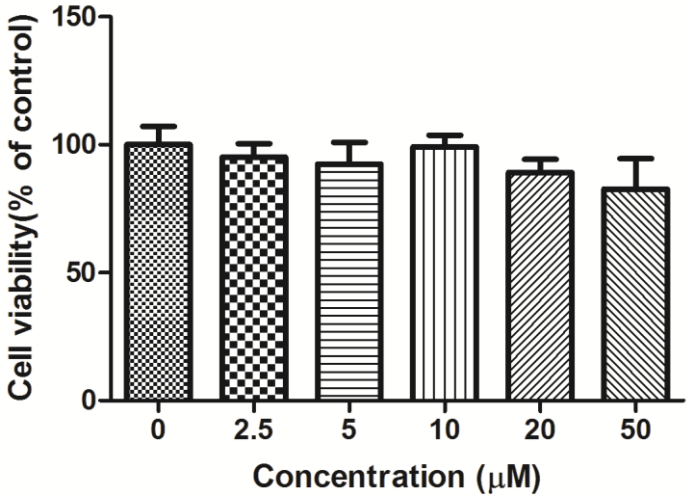


Figure S5. Percentage of viable A549 cells after treatment with different concentrations of the probe-KCP after 24 h using an MTT assay.

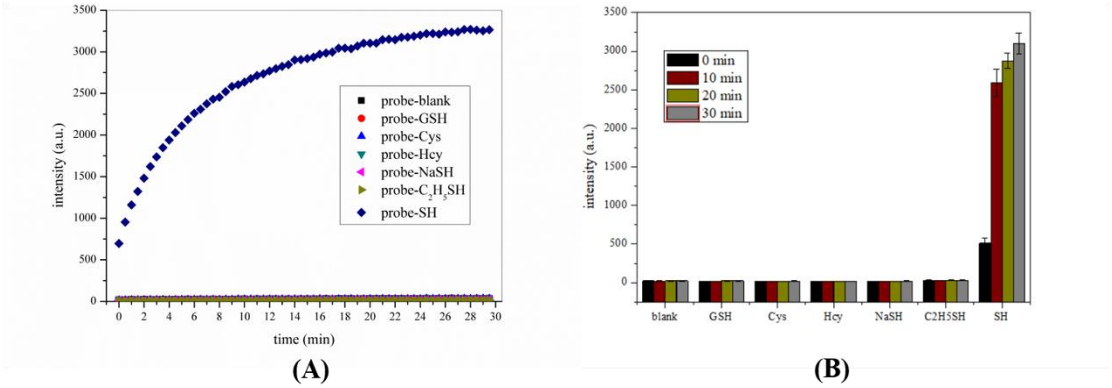


Figure S6. (A)Time-dependent the fluorescence response of probe-KCP (10 μM) in the absence (blank) and presence of 4-methoxythiophenol, GSH, Cys, Hcy, NaSH or C_2H_5SH (10 equiv) in PBS buffer solution (20 mM, pH = 7.4) containing 50 % DMSO. (B) Time-dependent the fluorescence response of probe-KCP (10 μM) in the absence (blank) and presence of 4-methoxythiophenol, GSH, Cys, Hcy, NaSH or C_2H_5SH (10 equiv) at 0 min, 10 min, 20 min, 30 min.

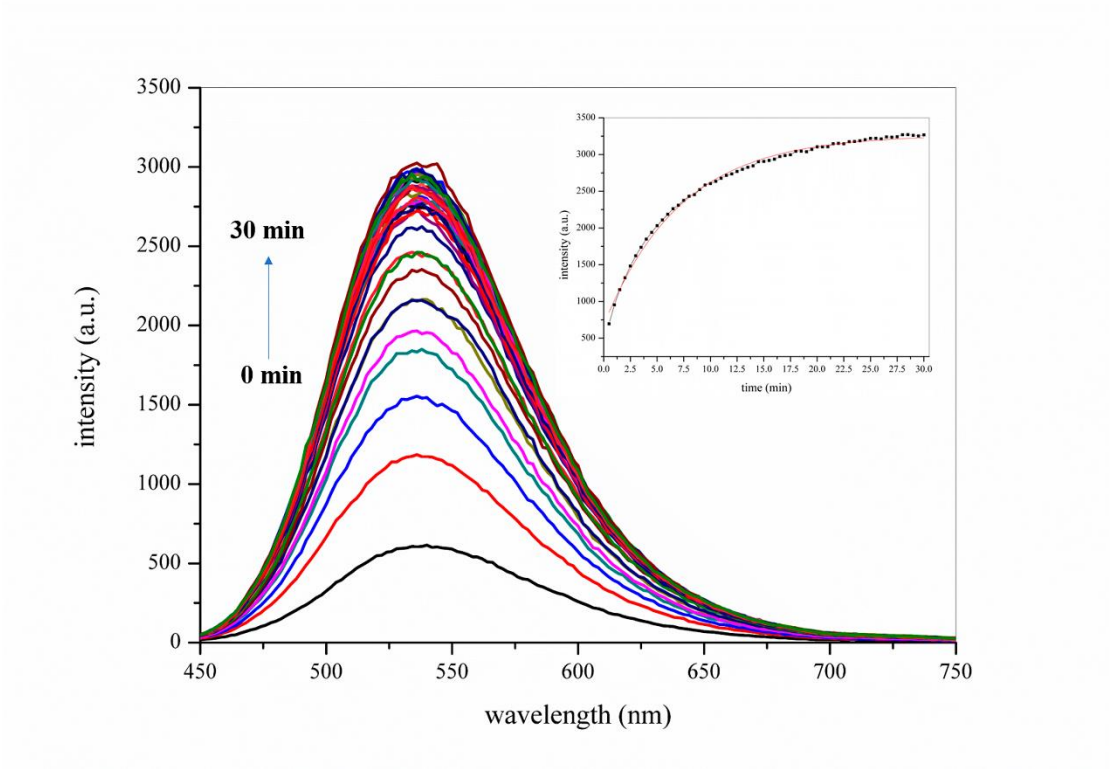


Figure S7. Time-dependent the fluorescence response of probe-KCP (10 μM) in the presence of 4-Methoxythiophenol (10 equiv) in PBS/ DMSO solution (*v*:*v* = 1:1, 20 mM, pH = 7.4).

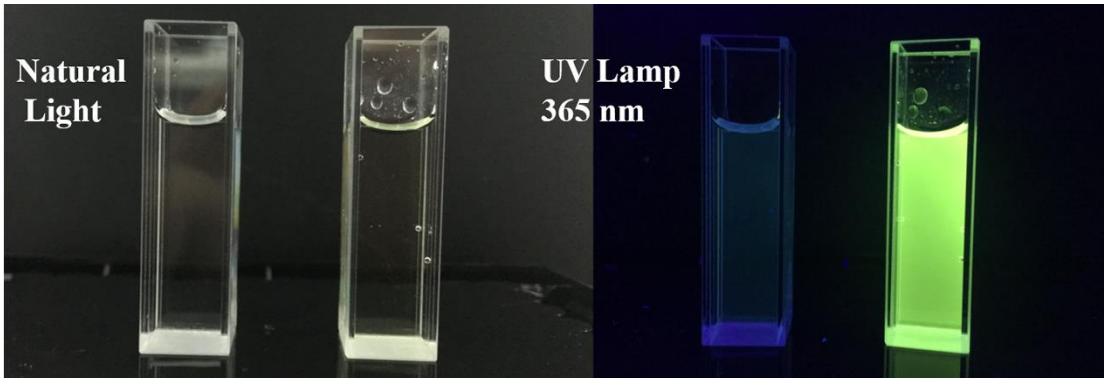


Figure S8. Photograph of probe-KCP solutions (10 μM) in the presence of 4-methoxythiophenol (10 equiv) under natrual light and UV irradiation (365 nm).

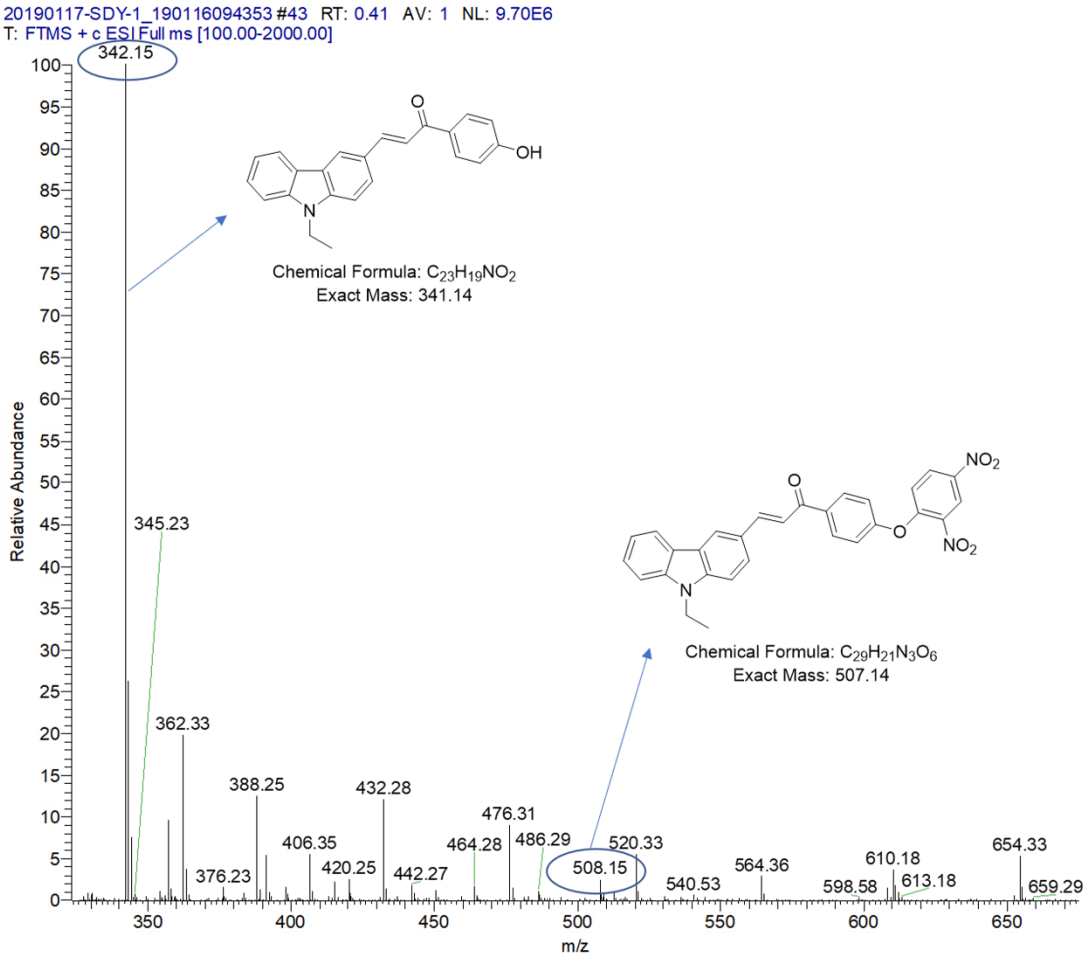


Figure S9. The ESI mass spectrum of probe-KCP in the presence of 4-methoxythiophenol.

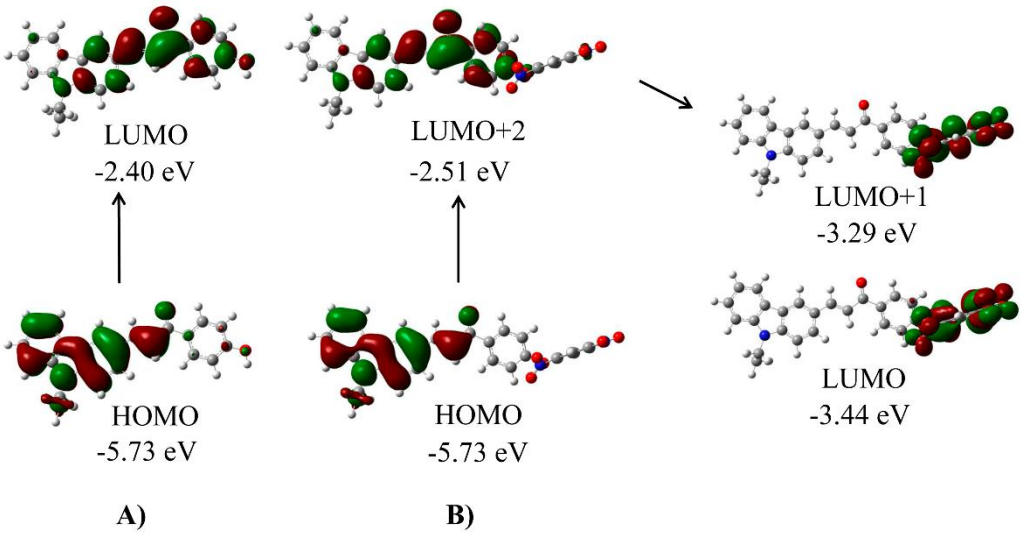


Figure S10. (A) Frontier molecular orbital plots of dye probe-OH in DMSO. (B) Frontier molecular orbital plots of probe-KCP in DMSO. The fluorescence emission of probe-KCN1 moieties is quenched by d-PET.