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A triphenylamine derived fluorescent probe for efficient detection of H_2S based on Aggregation-induced Emission

Jiaojiao Li,[a] Keli Zhong,[a] Lijun Tang*[a] and Xiaomei Yan*[b]

[a] *College of Chemistry and Materials Engineering, Bohai University, Jinzhou, 121013, China.*

[a] *College of Laboratory Medicine, Dalian Medical University, Dalian, 116044, China.*

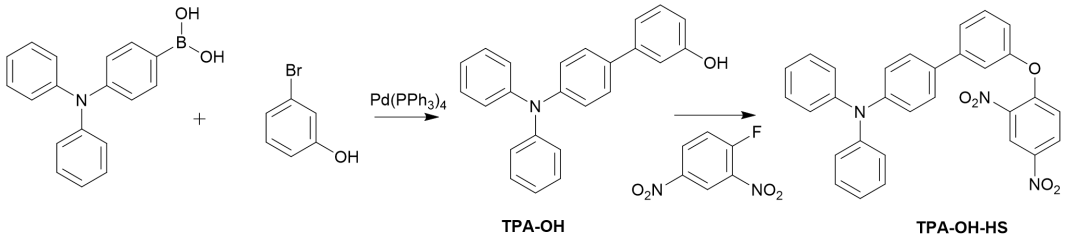
[*] *Corresponding author. E-mail: ljtang@bhu.edu.cn*

1. Synthesis of compound TPA-OH

4-(diphenylamino)phenylboronic acid (3.007 g, 10.4 mmol), 3-bromophenol (1.284 g, 8 mmol), anhydrous potassium carbonate (3.317 g, 24 mmol) and tetrakis(triphenylphosphine) palladium (0.074 g, 0.064 mmol) was dissolved in a methanol-toluene (1:1, v:v) mixed solution, and heated to 75°C under the protection of nitrogen to react overnight. After the reaction is complete, the solvent is removed under reduced pressure. It was washed three times with ethyl acetate and saturated brine, and the organic phase was collected and dried over anhydrous magnesium sulfate. Finally, the crude product was purified by silica gel column chromatography (eluent: EA/PE =1/30, v/v) to obtain a white powder compound **TPA-OH** (1.827 g, yield 67.89%). m.p. 75.4-75.6°C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.46 (s, 1H), 7.49 (d, J = 8.4 Hz, 2H), 7.29 (t, J = 12.2 Hz, 4H), 7.21 (d, J = 8 Hz, 1H), 7.06-6.94 (m, 10H), 6.71 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 157.84, 147.13, 146.72, 141.06, 134.31, 129.92, 129.66, 127.58, 124.17, 123.37, 123.26, 117.04, 114.05, 113.00. HRMS (ESI-): *m/z* Calcd for $C_{25}H_{19}NO_2[M-H]^-$ 336.1394; Found: 336.1656.

2. Synthesis of compound TPA-OH-HS

The synthesis of control compound **TPA-OH-HS** refers to probe **TPA-HS**. Purify the crude product by silica gel column chromatography (eluent: EA/PE=1/50, v/v) to obtain orange powder **TPA-OH-HS** (0.897 g, yield 89.08%). m.p. 82.6-82.8°C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.95 (s, 1H), 8.47 (d, J = 2.4 Hz, 1H), 7.65-7.53 (m, 5H), 7.32 (s, 4H), 7.25-7.22 (m, 2H), 7.10-7.01 (m, 8H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 155.12, 154.39, 147.43, 146.95, 142.36, 141.45, 139.48, 132.26, 131.29, 129.72, 127.89, 124.42, 123.91, 123.55, 122.93, 121.96, 119.49, 118.68, 117.86. HRMS (ESI+): *m/z* Calcd for $C_{30}H_{21}N_3O_5[M+H]^+$ 504.16; Found:504.30.



Scheme S1. Synthesis of probe **TPA-OH-HS**.

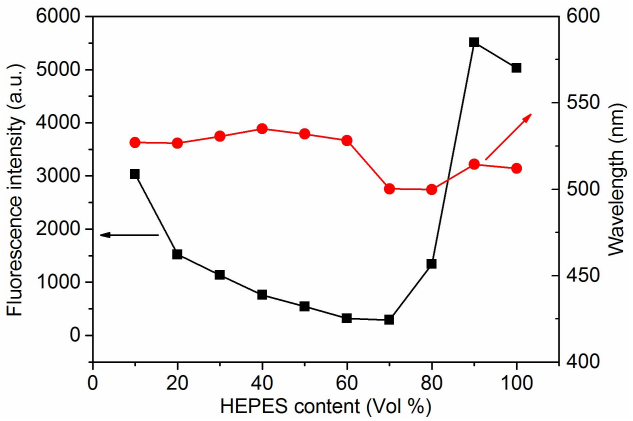


Fig. S1 The maximum fluorescence intensity and maximum emission wavelength of compound **TPA-CHO** at different HEPES content (f_w).

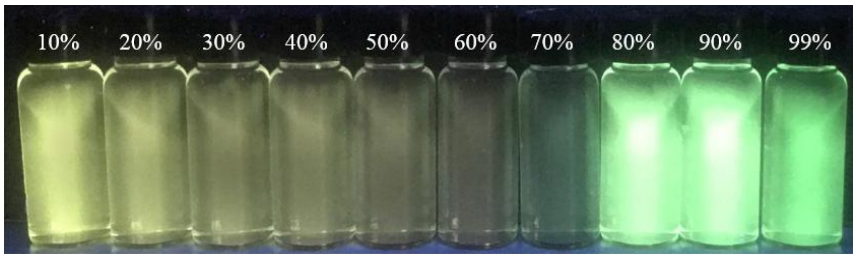


Fig. S2 Fluorescence change of compound **TPA-CHO** (10 μM) in THF/HEPES solutions with different HEPES content (f_w).

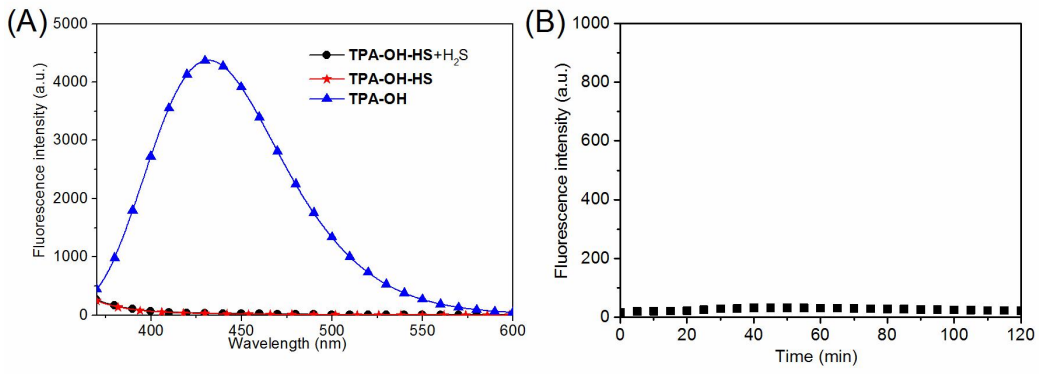


Fig. S3 (A) Fluorescence spectra of **TPA-OH-HS** (10 μM), **TPA-OH-HS** (10 μM) + H_2S (500 μM) and compound **TPA-OH** (10 μM) in THF/H_2O (2/8, v/v, HEPES 20 mM, pH = 7.12) solution; (B) The fluorescence changes (at 432 nm) of probe **TPA-OH-HS** (10 μM) over time in the presence of H_2S (500 μM). λ_{ex} = 310 nm.

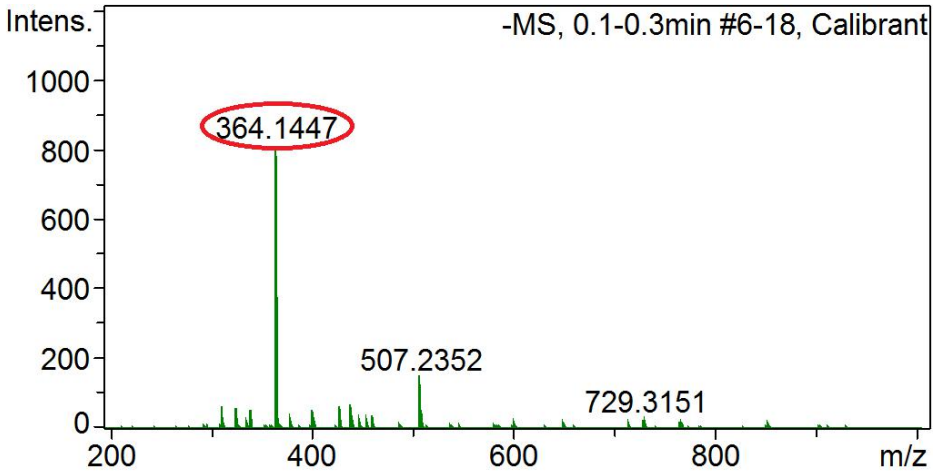


Fig. S4 High resolution mass spectroscopy of **TPA-HS** (10 μM) + H_2S (500 μM).

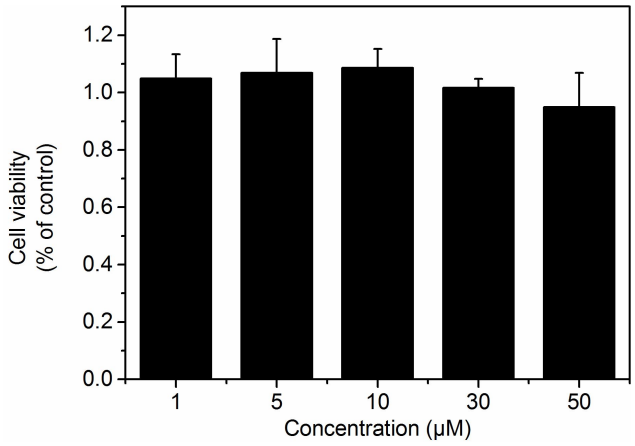


Fig.S5 The cell viability value (%) assessed by CCK-8 assay after incubating MCF-7 cells in the presence of **TPA-HS** at different concentrations (1, 5, 10, 30 and 50 μM) for 24 hours.

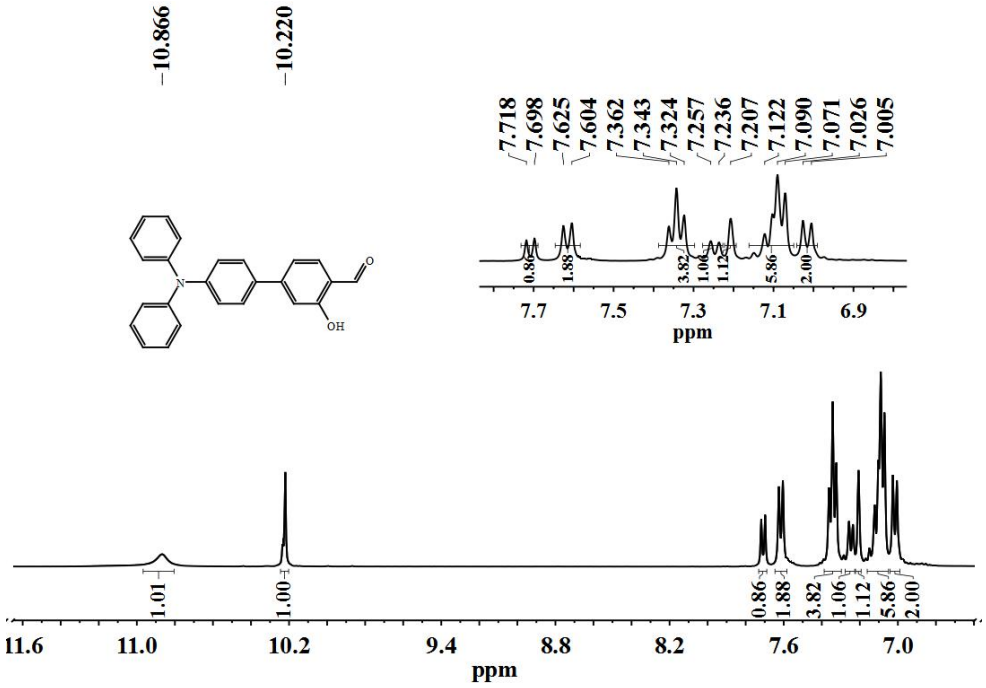


Fig. S6 [1]H NMR spectrum of compound **TPA-CHO** in DMSO-d_6.

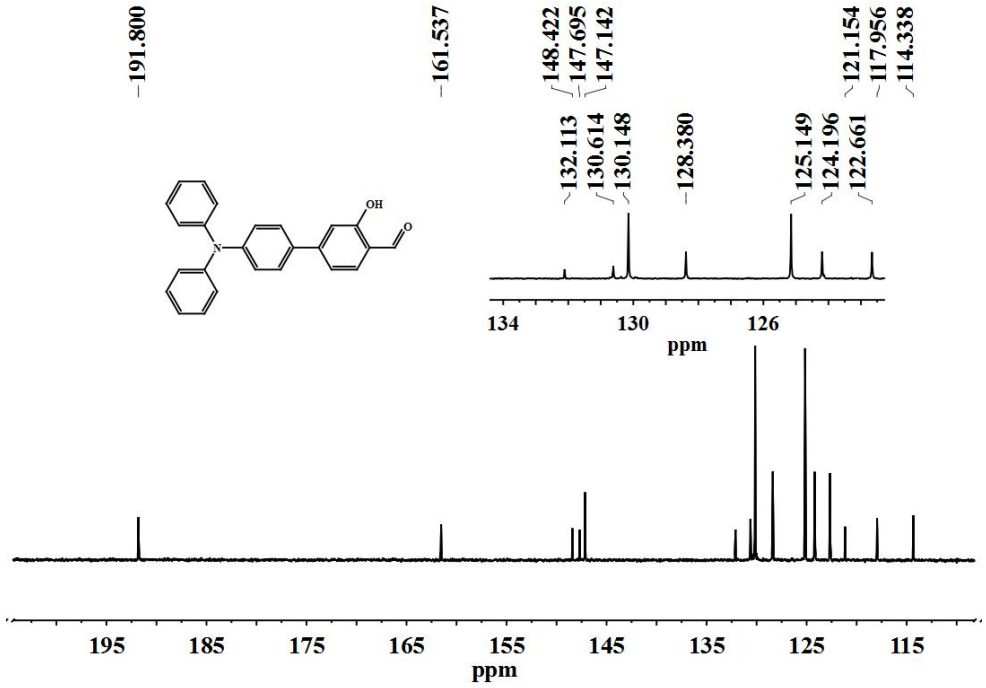


Fig. S7 [13]C NMR spectrum of compound **TPA-CHO** in DMSO-d_6.

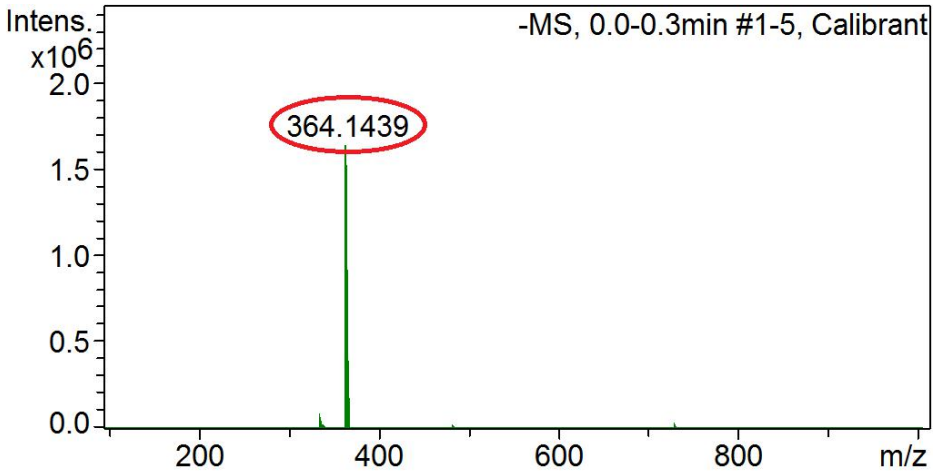


Fig. S8 HRMS spectrum of compound **TPA-CHO**.

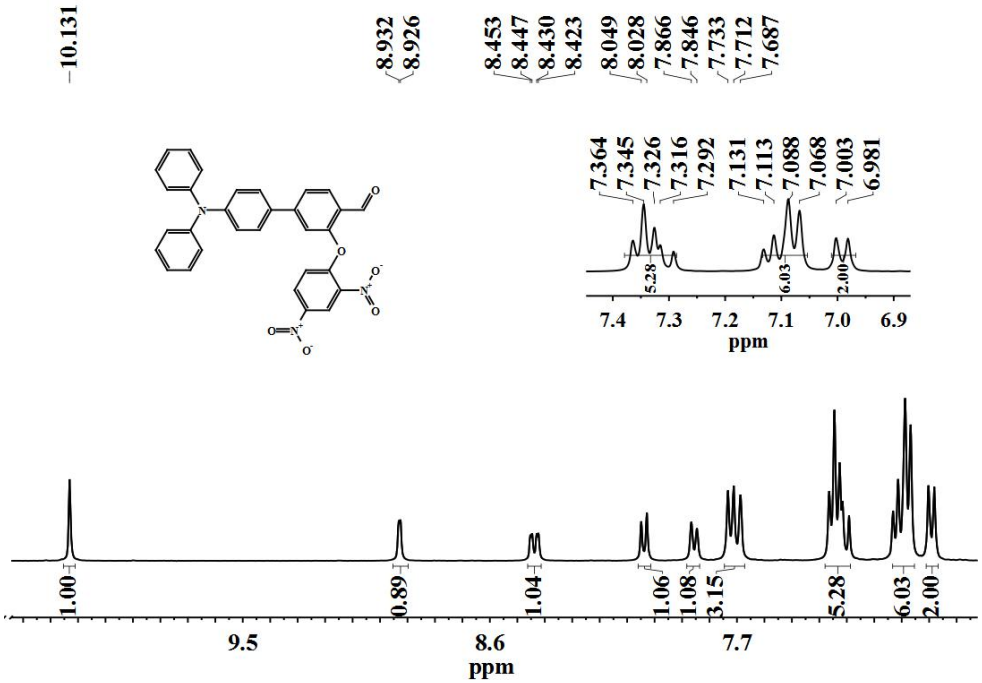


Fig. S9 ^{1}H NMR spectrum of probe **TPA-HS** in DMSO-d_6.

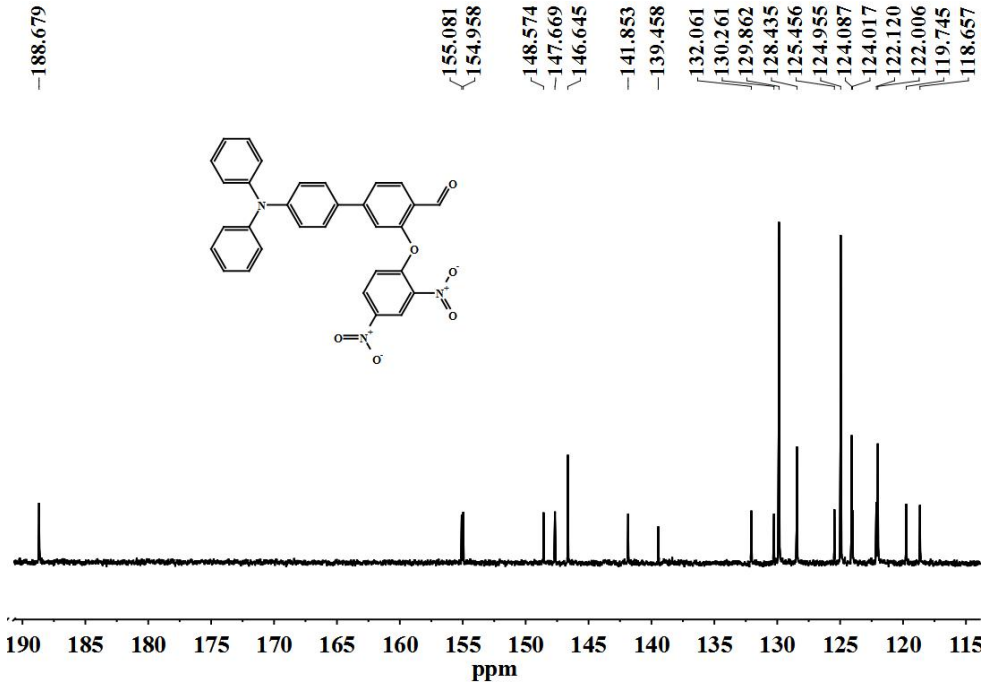


Fig. S10 ^{13}C NMR spectrum of probe **TPA-HS** in DMSO-d_6.

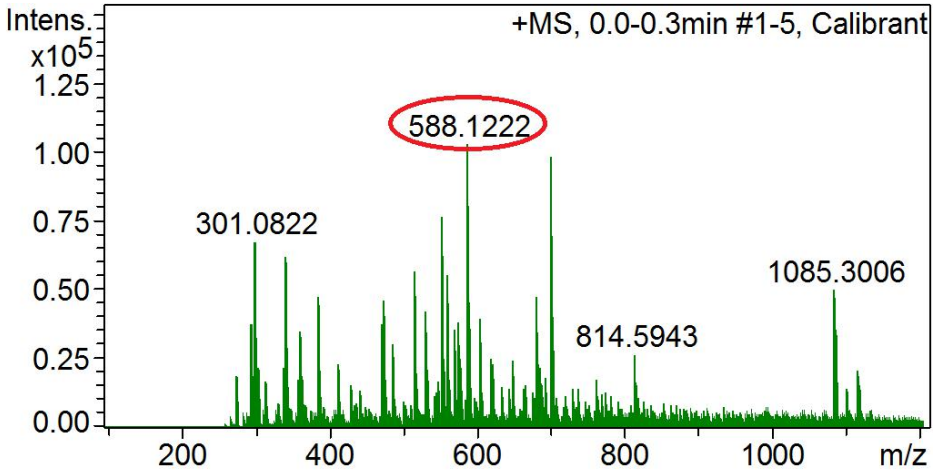


Fig. S11 HRMS spectrum of probe **TPA-HS**.

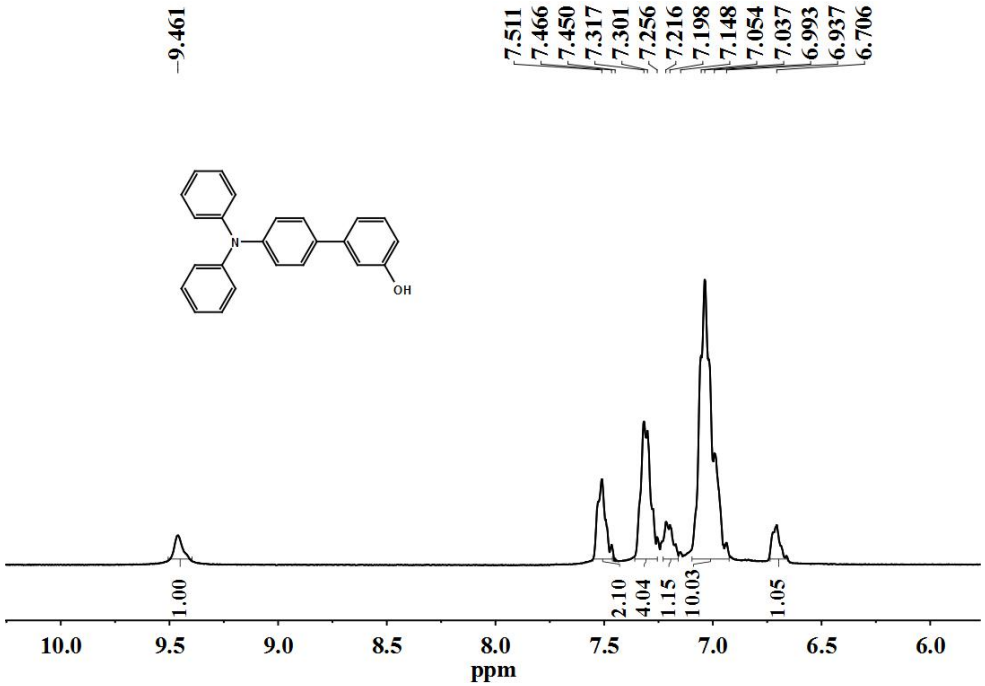


Fig. S12 ^{1}H NMR spectrum of probe **TPA-OH** in DMSO-d_6.

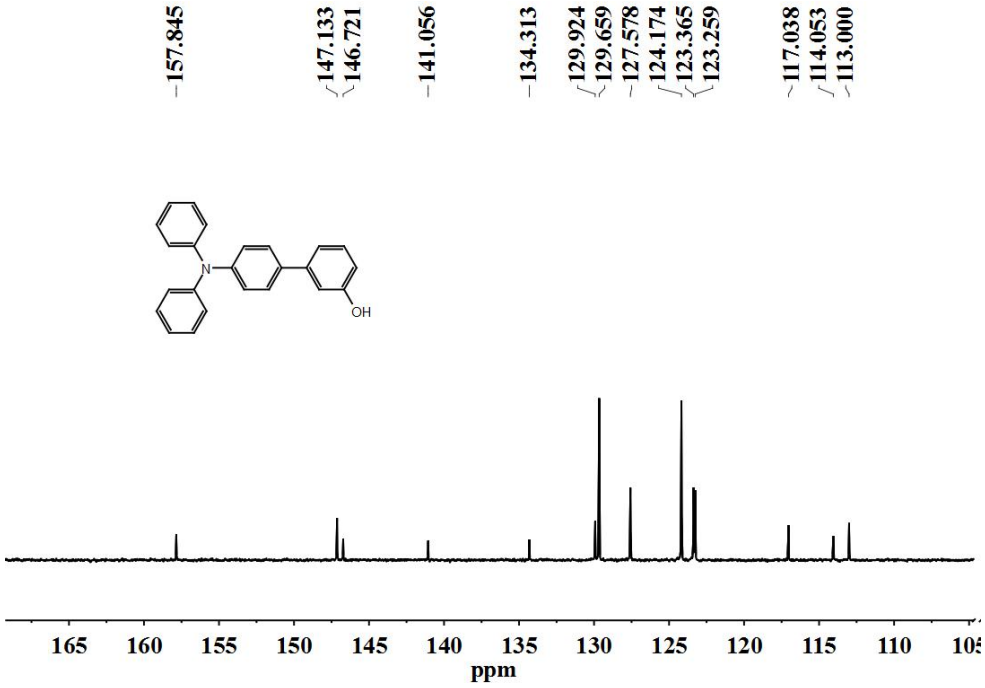


Fig. S13 ^{13}C NMR spectrum of probe **TPA-OH** in DMSO-d_6.

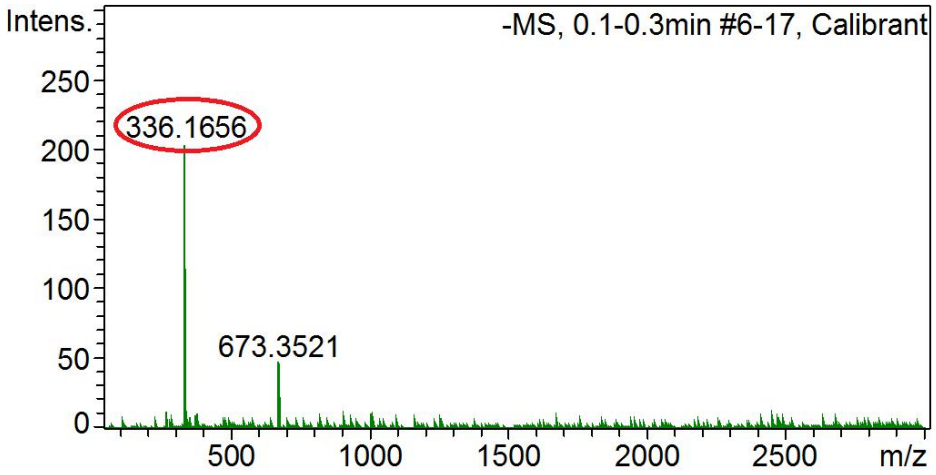


Fig. S14 HRMS spectrum of probe **TPA-OH**.

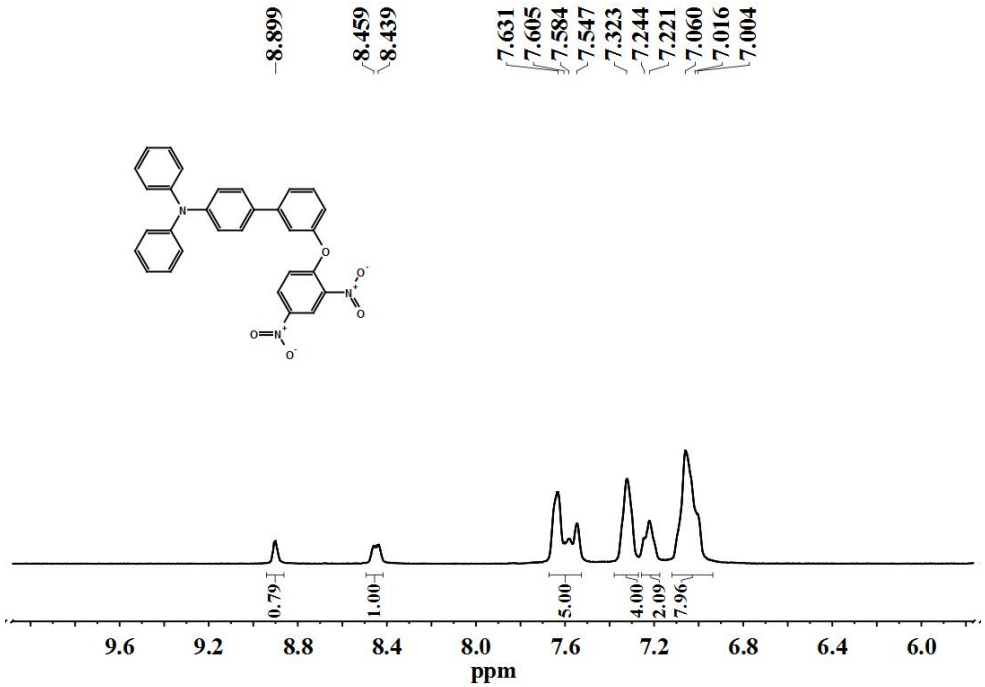


Fig. S15 ^{1}H NMR spectrum of probe **TPA-OH-HS** in DMSO-d_6.

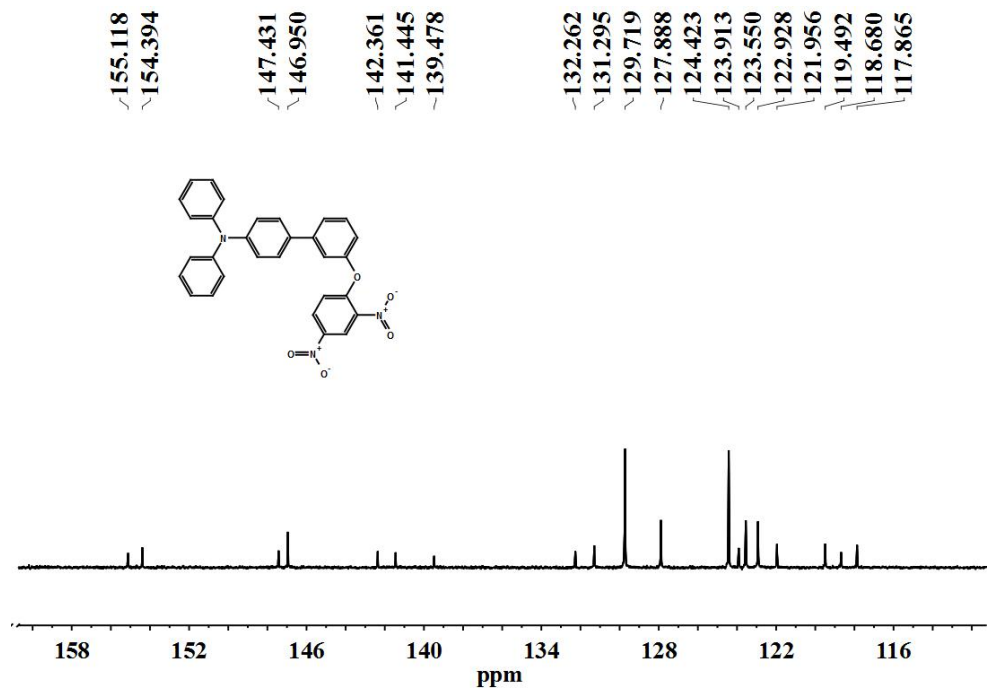


Fig. S16 ^{13}C NMR spectrum of probe **TPA-OH-HS** in DMSO-d_6.

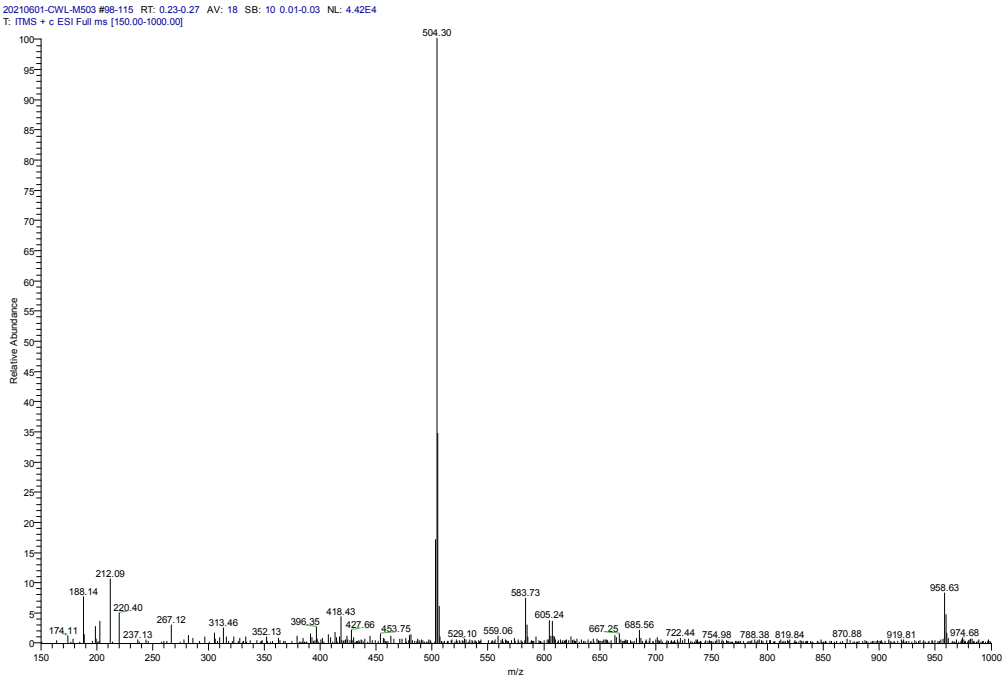


Fig. S17 HRMS spectrum of probe **TPA-OH-HS**.