Electronic Supplementary Information for

Construction of novel pyrene-based two-dimensional supramolecular organic framework and its selective regulation of reactive oxygen species for photocatalysis

Man Jiang,[‡a] Ying Wang,[‡b] Hui Liu,[b] Shengsheng Yu,[b] Kai-Kai Niu,*[b] Ling-Bao Xing*[b]

[a]School of Resources and Environmental Engineering, Shandong University of Technology, Zibo, Shandong 255000, P. R. China

[b]School of Chemistry and Chemical Engineering, Shandong University of Technology, Zibo 255000, P. R. China

*Corresponding authors: Tel./fax: +86 533 2781664. E-mail: kkai007@126.com; lbxing@sdut.edu.cn.

‡These authors contributed equally to this work.

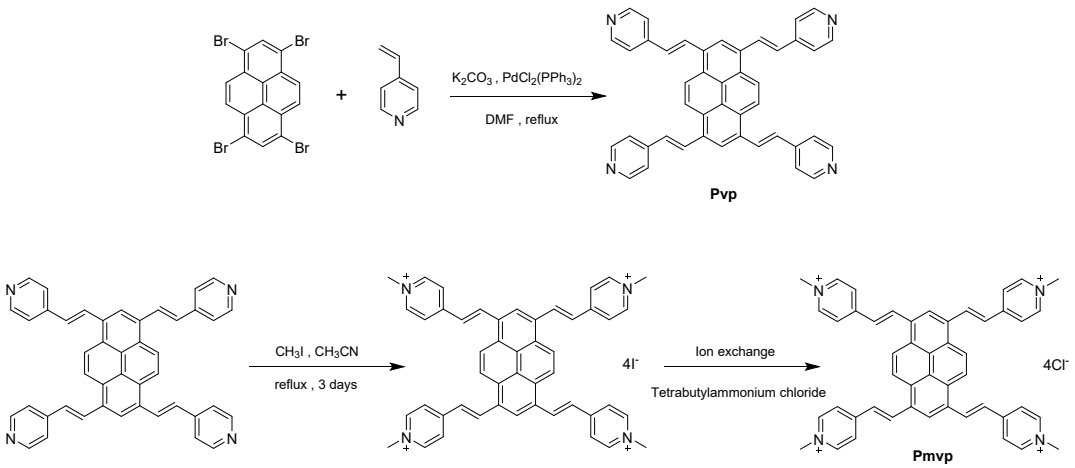
Experimental

Materials: Unless specifically mentioned, all chemicals are commercially available and were used as received.

Characterizations: ^{1}H NMR spectra was recorded on a Bruker Advance 400 spectrometer (400 MHz) at 298 K, and the chemical shifts (δ) were expressed in ppm and J values were given in Hz. UV-vis spectra were obtained on a Shimadzu UV-1601PC spectrophotometer in a quartz cell (light path 10 mm) at 298 K. Steady-state fluorescence measurements were carried out using a Hitachi 4500 spectrophotometer. Dynamic light scattering (DLS) and zeta potential are measured on Malvern Zetasizer Nano ZS90. Transmission electron microscopy (TEM) images were obtained on a JEM 2100 operating at 120 kV. Samples for TEM measurements were prepared by dropping the mixture aqueous solution on carbon-coated copper grid (300 mesh) and drying by slow evaporation. The photocatalytic reaction was performed on WATTCAS Parallel Photocatalytic Reactor (WP-TEC-HSL) with 10W COB LED.

General procedure for the aerobic oxidation of sulfides: Sulfides (0.1 mmol, 14 μL) was added in the newly produced solution of SOF (1.0 mol%, 3 mL, [Pmvp]=5.0 × 10^{-5} M, [CB[8]]= 1.0 × 10^{-4} M). The reaction was irradiated with blue LED (10 W, 450 nm - 455 nm) at room temperature under the ambient air condition for 2 h. Then the mixture was extracted with dichloromethane, and the combined organic layer was dried with anhydrous Na_2SO_4. Then the organic solvent was removed in vacuo and purified by flash column chromatography with petroleum ether/ethyl acetate to afford the products.

General procedure for the oxidative hydroxylation of arylboronic acid: arylboronic acid (0.1 mmol) was added in the newly produced solution of SOF (1.0 mol%, 3 mL, [Pmvp]=5.0 × 10^{-5} M, [CB[8]]= 1.0 × 10^{-4} M). Then *N,N*-Diisopropylethylamine (0.3 mmol, 53 μL) was added and the mixture was irradiated with blue LED (10 W, 450 nm - 455 nm) at room temperature under the ambient air condition for 10 h. Then the solvent was removed in vacuo and purified by flash column chromatography with petroleum ether/ethyl acetate to afford the products.



Scheme. S1 Synthetic route of Pmvp.

Synthesis of Pmvp: The synthesis of Pmvp was as shown in Scheme S1. 4-vinyl pyridine (1.06 mL, 10.0 mmol) was added into the solution of 1,3,6,8-tetrabromopyrene (1.04 g, 2.0 mmol) in DMF (60.0 mL), then $PdCl_2(PPh_3)_2$ (0.14 g, 0.2 mmol) and potassium carbonate (1.66 g, 12.0 mmol) were added. The mixed solution was refluxed for 3 days. Then the reaction solution was cooled down to room temperature and 100 mL water was added. The generated precipitate was collected by filtration and washed with H_2O to offer the Pvp as a red solid (0.78 g, 63%).

Pvp (0.1 g, 0.163 mmol) was added in 20 mL of CH_3CN, and CH_3I (0.71 g, 5.0 mmol) was then added. The mixed solution was refluxed for 3 days. The resulting precipitate was collected by filtration and washed with CH_2Cl_2 several times. The crude product was then dissolved in water and ammonium hexafluorophosphate was added. The resulting precipitate was collected through filtration and dried under a vacuum. After that, the solid was re-dissolved in CH_3CN, and tetrabutyl ammonium chloride was added. The resulting precipitation was collected through filtration and dried under vacuum to obtain Pmvp as purple black precipitate (0.12 g, 89%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.24 - 9.10 (m, 8H), 9.10 - 8.91 (m, 10H), 8.56 (d, J = 6.3 Hz, 8H), 8.02 (d, J = 16.0 Hz, 4H), 4.34 (s, 12H). HRMS (ESI): m/z $[M\text{-}4Cl]^{4+}$ calculated for

$C_{48}H_{42}N_4$: 168.5847; found: 168.5849.

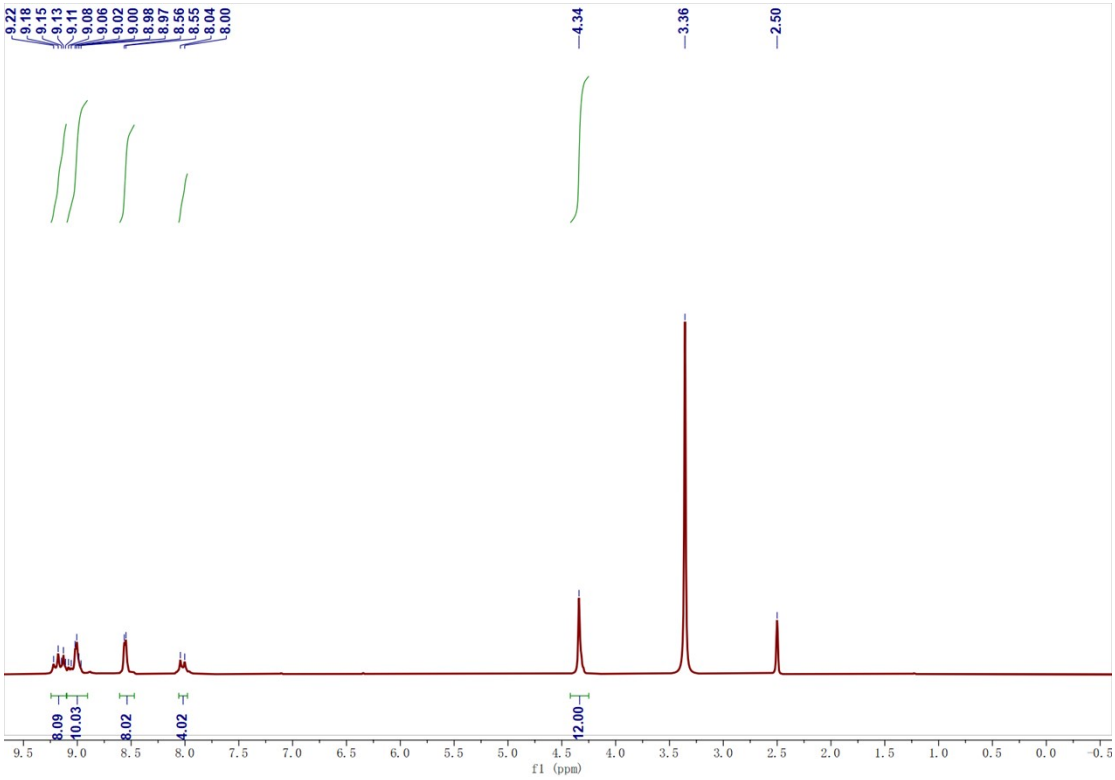


Fig. S1 ^{1}H NMR spectrum of compound **Pmvp** in DMSO-d_6.

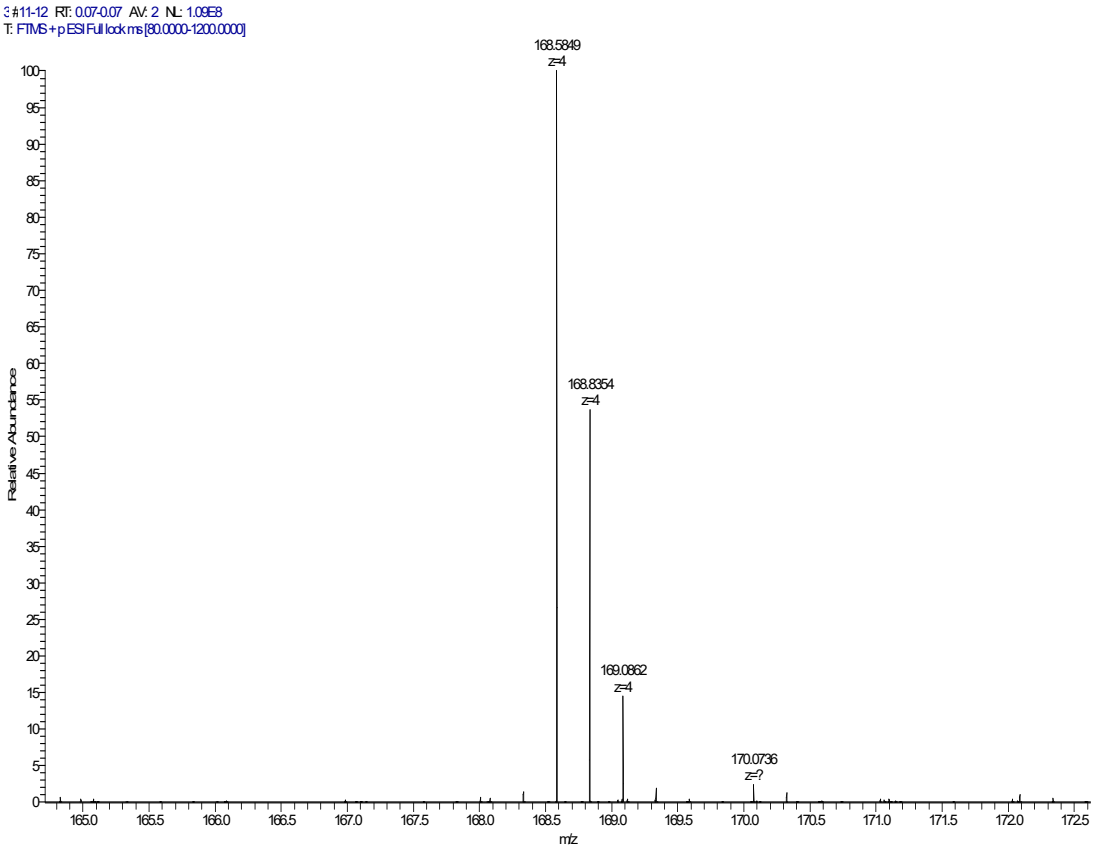


Fig. S2 HR-ESI-MS spectra of Pmvp.

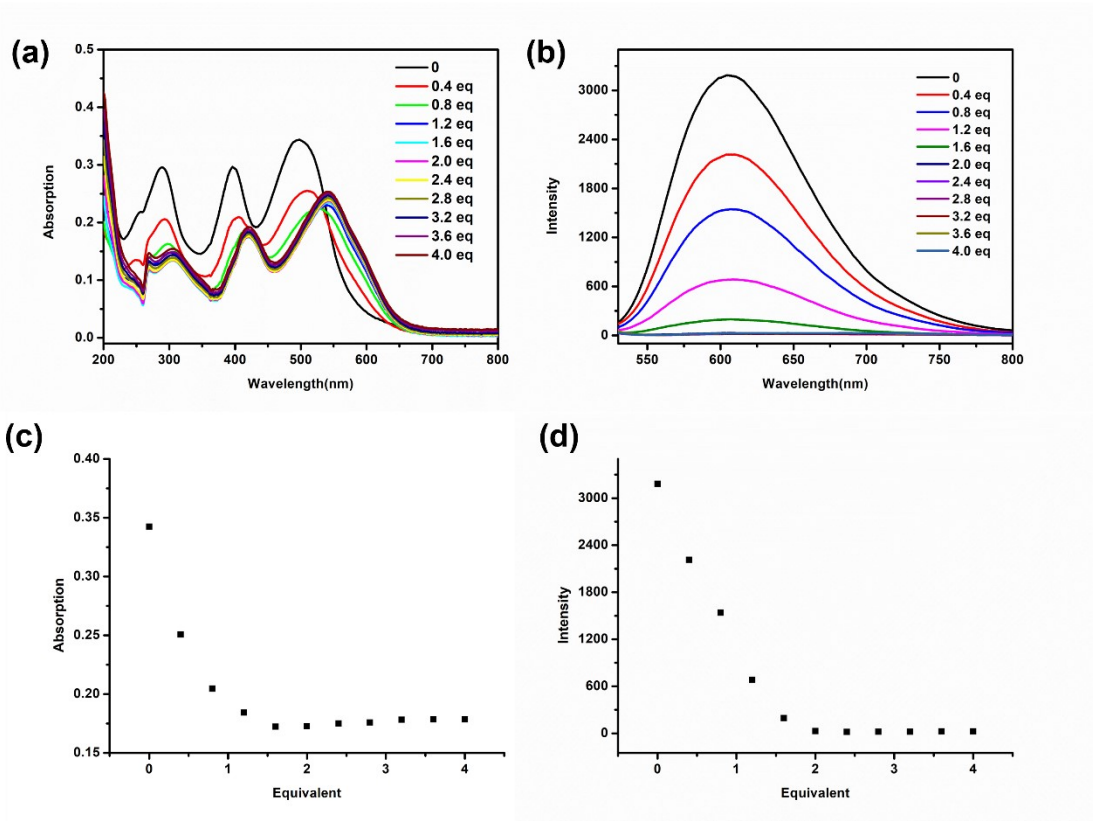


Fig. S3 (a) UV-vis absorption spectra and (b) fluorescence emission spectra of Pmvp in the presence of an excess CB[8] (1:4); (c) The UV-vis absorption and (d) fluorescence emission curve of Pmvp in the presence of an excess CB[8] (1:4).

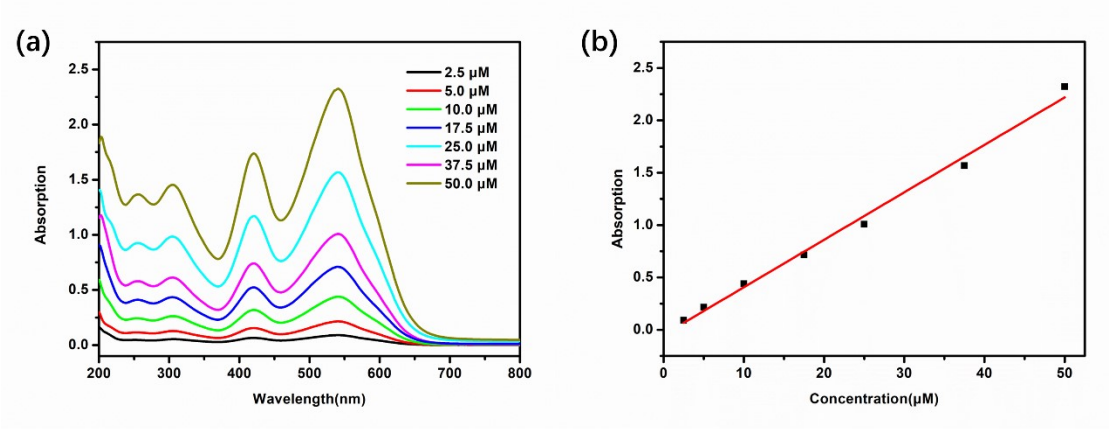


Fig. S4 (a) UV-vis absorption spectra of SOF at different concentrations; (b) The plot of the absorption of SOF at 540 nm vs [Pmvp].

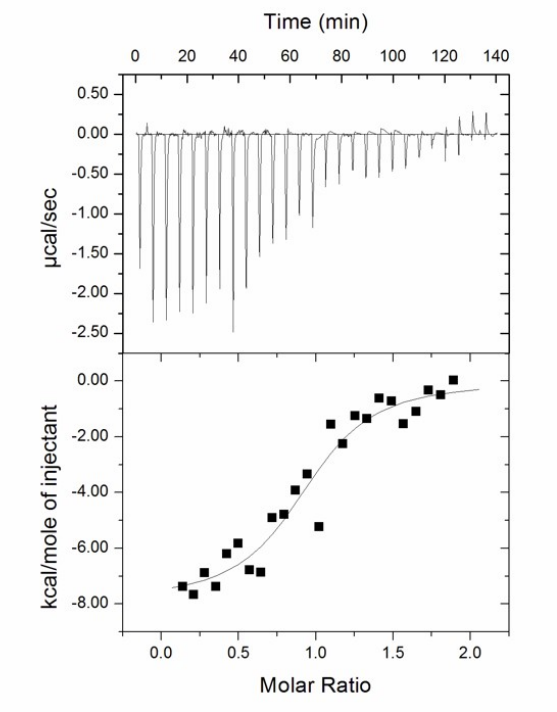


Fig. S5 ITC data for the titration of CB[8] with Pmvp in water at 298 K.

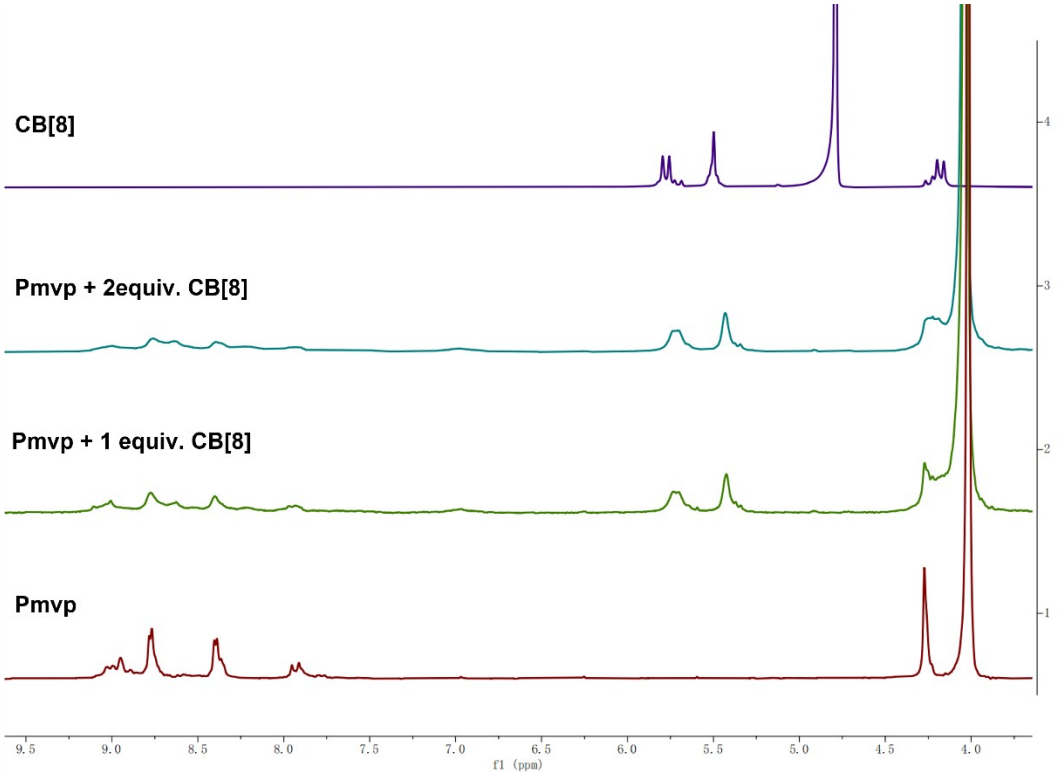


Fig. S6 ^{1}H NMR spectra (400 MHz) of Pmvp, Pmvp + 1.0 equiv. CB[8], Pmvp + 2.0 equiv. CB[8] and CB[8].

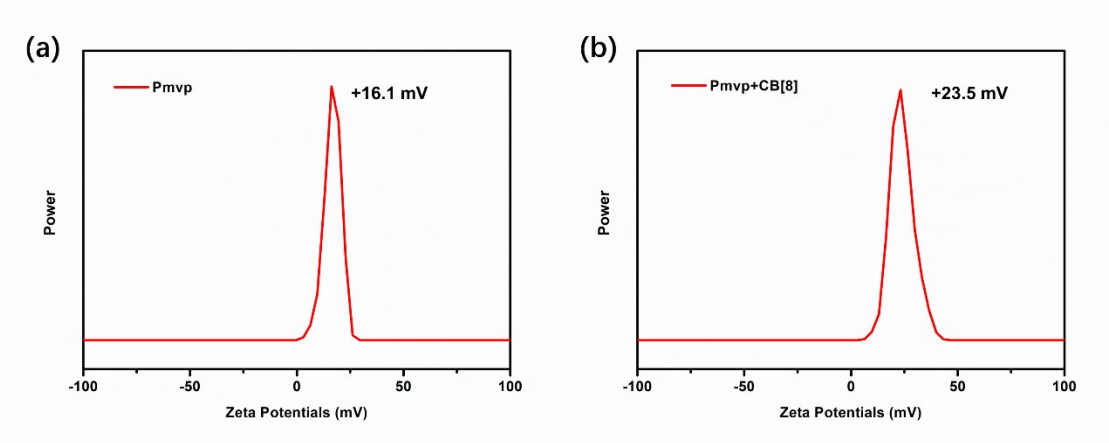


Fig. S7 Zeta potential of (a) Pmvp and (b) Pmvp + CB[8] (1 : 2).

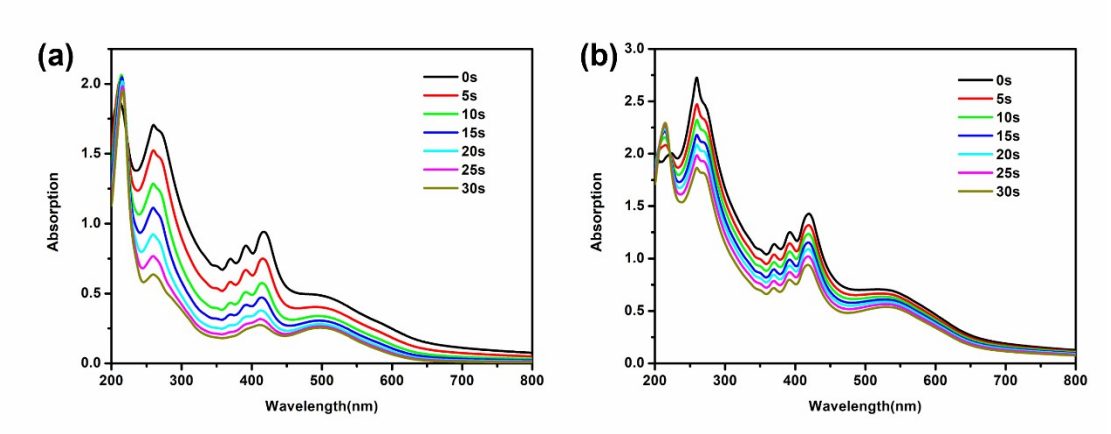


Fig. S8 (a) UV-vis absorption spectra of ABDA after the addition of Pmvp; (b) UV-vis absorption spectra of ABDA after the addition of SOF.

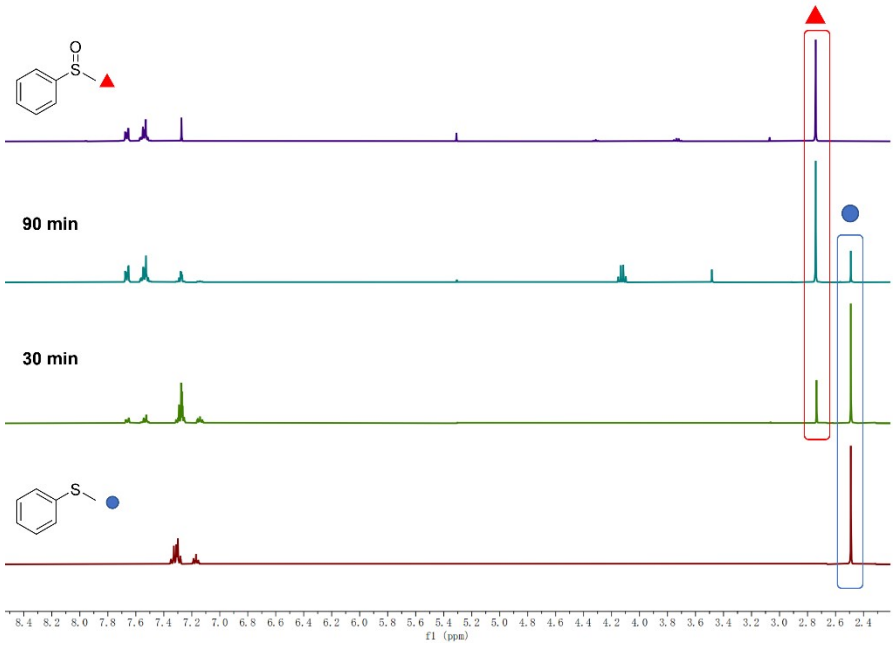


Fig. S9 Monitoring of photooxidation reaction of thioanisole by ^{1}H NMR.

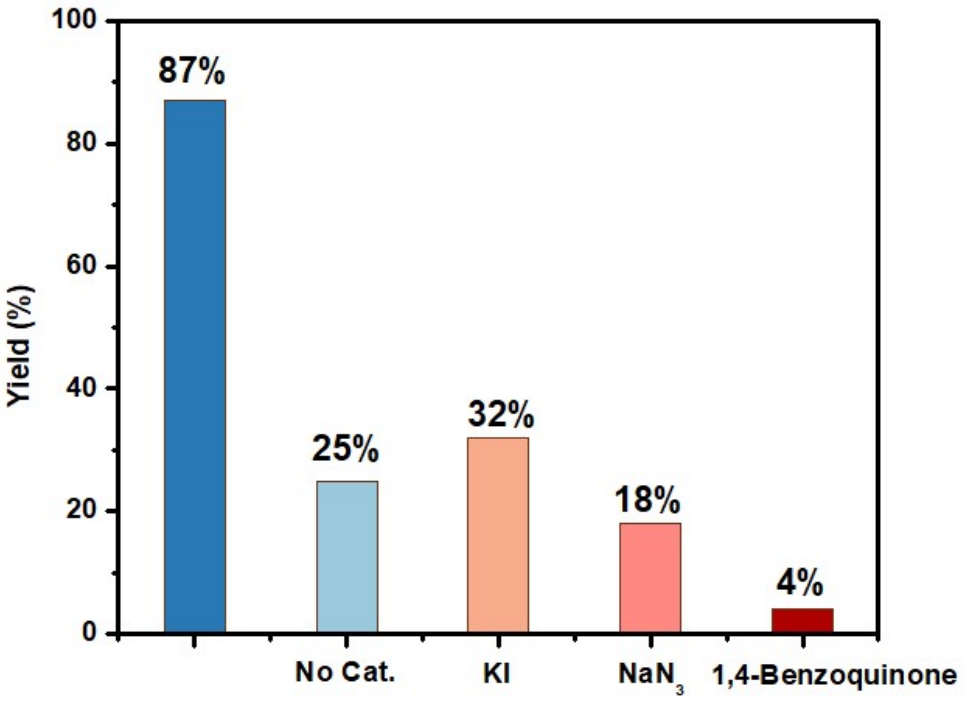


Fig. S10 Control experiments for photocatalytic aerobic oxidation of thioanisole after the addition of KI, NaN_3 and *p*-benzoquinone.

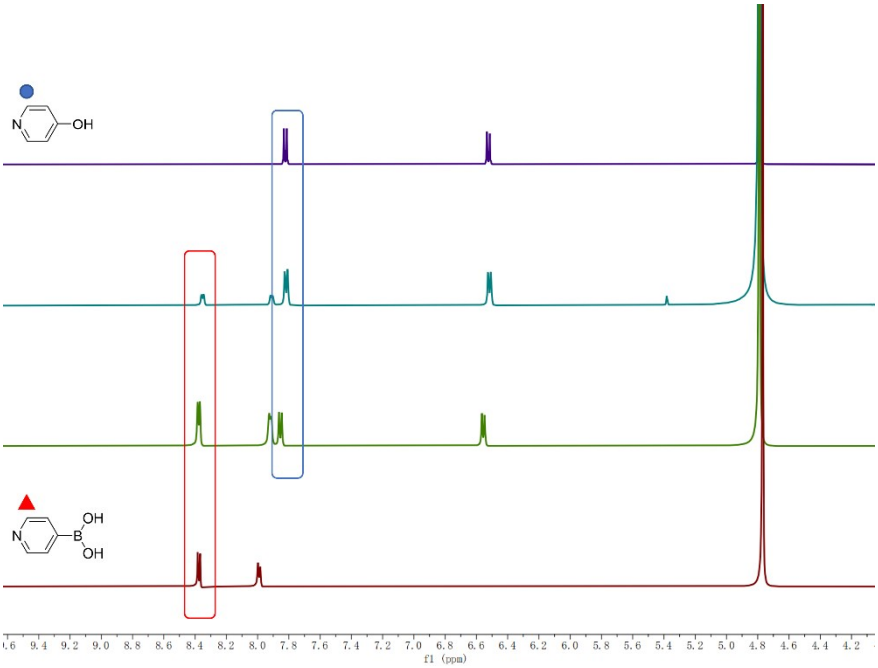


Fig. S11 Monitoring of photooxidation reaction of 4-pyridylboronic acid by ^{1}H NMR.

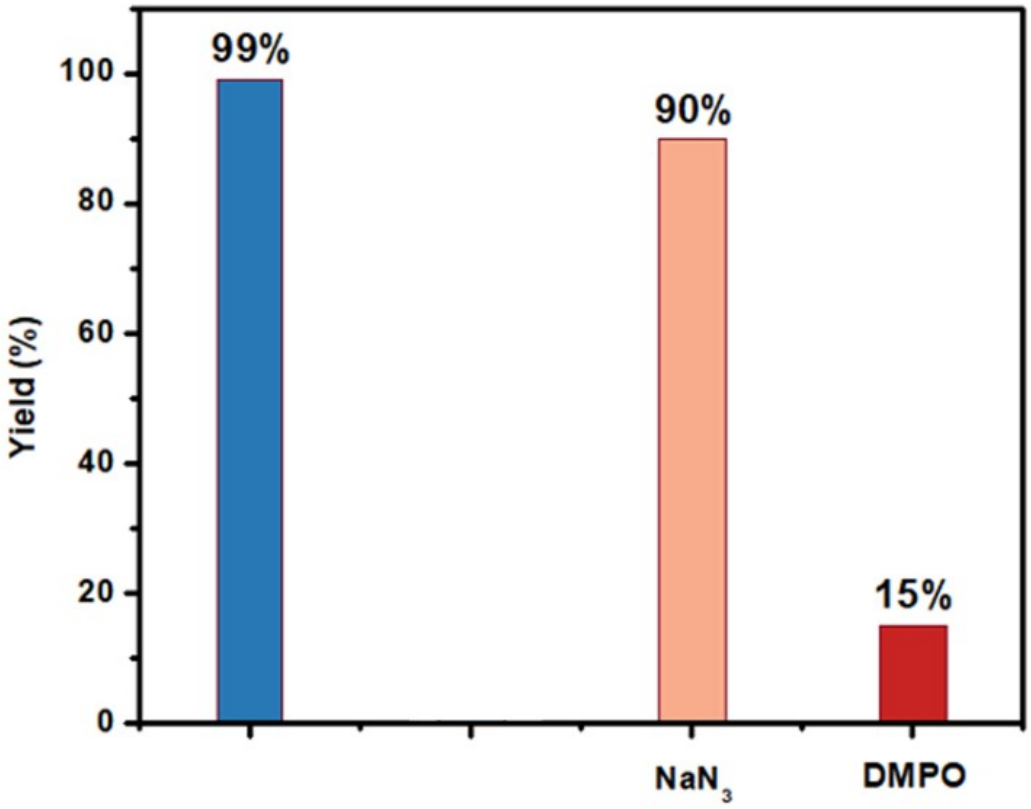


Fig. S12 Control experiments for the oxidative hydroxylation of arylboronic acid after the addition of NaN_3 and DMPO.

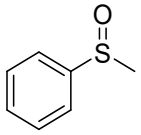
Table S1. Control experiments for the photooxidation of thioanisole and 4-pyridylboronic acid promoted by SOF.

Entry	Conditions	Light irradiation	Yield[a]/%
1[a]	H_2O	Yes	87%
2[a]	CH_3CN	Yes	99%
3[b]	H_2O	Yes	99%
4[b]	CH_3CN	Yes	99%

[a)] photooxidation of thioanisole. [b)] photooxidation of 4-pyridylboronic.

^{1}H NMR data of 2a-2n

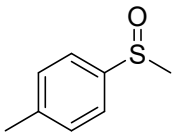
2a. Phenyl methyl sulfoxide



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 - 7.61 (m, 2H), 7.58 - 7.46 (m, 3H), 2.73 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.64, 129.34, 123.47, 43.95.

The spectral data obtained were identical with those reported in literature.[1]

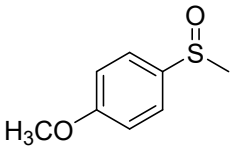
2b. 4-Me-Phenyl methyl sulfoxide



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, J = 8.2 Hz, 2H), 7.34 - 7.29 (m, 2H), 2.69 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.27, 141.48, 129.97, 43.88, 21.34.

The spectral data obtained were identical with those reported in literature.[1]

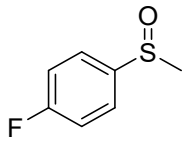
2c. 4-OMe-Phenyl methyl sulfoxide



^{1}H NMR (400 MHz, $CDCl_3$)) δ 7.58 (d, J = 8.8 Hz, 2H), 7.02 (d, J = 8.8 Hz, 2H), 3.84 (s, 3H), 2.69 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.06, 136.55, 125.58, 125.49, 114.95, 114.86, 55.64, 55.56, 44.06.

The spectral data obtained were identical with those reported in literature.[1]

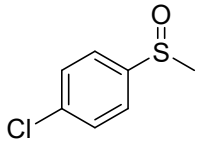
2d. 4-F-Phenyl methyl sulfoxide



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 - 7.56 (m, 2H), 7.23 - 7.14 (m, 2H), 2.68 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.42, 162.92, 140.98, 140.95, 125.77, 116.68, 116.46, 44.03, 44.01.

The spectral data obtained were identical with those reported in literature.[1]

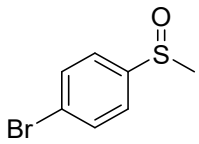
2e. 4-Cl-Phenyl methyl sulfoxide



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 - 7.49 (m, 2H), 7.46 - 7.40 (m, 2H), 2.65 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.88, 136.95, 129.40, 124.76, 43.74.

The spectral data obtained were identical with those reported in literature.[1]

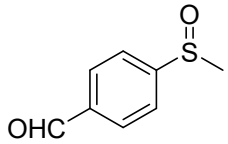
2f. 4-Br-Phenyl methyl sulfoxide



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 - 7.54 (m, 2H), 7.48 – 7.40 (m, 2H), 2.63 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.58, 132.25, 125.12, 124.88, 43.70.

The spectral data obtained were identical with those reported in literature.[1]

2g. 4-CHO-Phenyl methyl sulfoxide

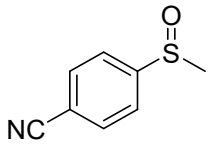


^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.00 (d, J = 8.4 Hz, 2H), 7.78 (d, J = 8.3 Hz, 2H), 2.75 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.08, 152.22, 137.97, 130.29,

124.05, 43.61.

The spectral data obtained were identical with those reported in literature.[2]

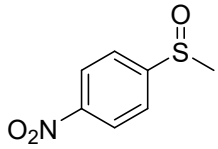
2h. 4-CN-Phenyl methyl sulfoxide



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 - 7.76 (m, 2H), 7.75 - 7.69 (m, 2H), 2.72 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.16, 132.76, 124.09, 117.53, 114.41, 43.51.

The spectral data obtained were identical with those reported in literature.[3]

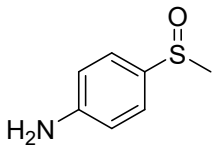
2i. 4-NO_2-Phenyl methyl sulfoxide



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.8 Hz, 2H), 7.82 (d, *J* = 8.8 Hz, 2H), 2.78 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.13, 149.37, 124.59, 124.40, 43.77.

The spectral data obtained were identical with those reported in literature.[3]

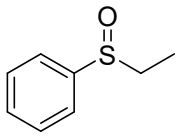
2j. 4-NH_2-Phenyl methyl sulfoxide



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.6 Hz, 2H), 6.75 (d, *J* = 8.6 Hz, 2H), 2.68 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.48, 133.19, 125.66, 115.03, 43.73.

The spectral data obtained were identical with those reported in literature.[4]

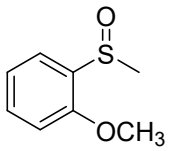
2k. Phenyl ethyl sulfoxide



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 - 7.56 (m, 2H), 7.54 - 7.44 (m, 3H), 2.82 (ddq, *J* = 54.0, 13.3, 7.4 Hz, 2H), 1.18 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.11, 130.89, 129.09, 124.11, 50.22, 5.93.

The spectral data obtained were identical with those reported in literature.[5]

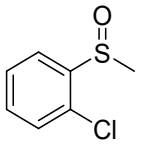
2l. 2-OMe-Phenyl methyl sulfoxide



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.43 (ddd, *J* = 8.2, 7.4, 1.7 Hz, 1H), 7.17 (td, *J* = 7.6, 1.0 Hz, 1H), 6.90 (dd, *J* = 8.2, 0.9 Hz, 1H), 3.87 (s, 3H), 2.75 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.68, 132.82, 131.89, 124.49, 121.59, 110.48, 55.62, 41.07.

The spectral data obtained were identical with those reported in literature.[6]

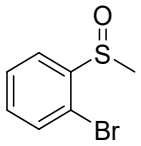
2m. 2-Cl-Phenyl methyl sulfoxide



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.46 (td, *J* = 7.5, 1.3 Hz, 1H), 7.41 - 7.28 (m, 2H), 2.75 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.22, 131.80, 129.55, 127.94, 125.02, 41.38.

The spectral data obtained were identical with those reported in literature.[4]

2n. 2-Br-Phenyl methyl sulfoxide

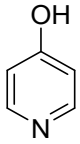


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.57 - 7.50 (m, 2H), 7.34 (ddd, *J* = 8.0, 7.3, 1.7 Hz, 1H), 2.78 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.11, 132.77, 132.15, 128.59, 125.50, 118.25, 41.72.

The spectral data obtained were identical with those reported in literature.[4]

^{1}H NMR data of 4a-4k

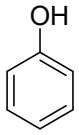
4a. 4-hydroxypyridine



^{1}H NMR (400 MHz, DMSO-d_6) δ 7.75 - 7.69 (m, 2H), 6.24 - 6.15 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 176.19, 139.72, 116.25.

The spectral data obtained were identical with those reported in literature.[7]

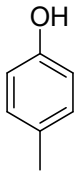
4b. Phenol



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 - 7.21 (m, 2H), 6.93 (tt, J = 7.4, 1.1 Hz, 1H), 6.89 - 6.77 (m, 2H), 5.23 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.30, 129.67, 120.81, 115.27.

The spectral data obtained were identical with those reported in literature.[8]

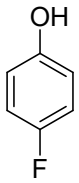
4c.4-methylphenol



^{1}H NMR (400 MHz, DMSO-d_6) δ 9.12 (s, 1H), 6.99 - 6.90 (m, 2H), 6.64 (d, J = 8.4 Hz, 2H), 2.17 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.45, 130.17, 127.59, 115.46, 20.55.

The spectral data obtained were identical with those reported in literature.[7]

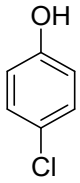
4d. 4-Fluorophenol



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 - 6.88 (m, 2H), 6.82 - 6.73 (m, 2H), 5.28 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.49, 156.12, 151.41, 151.39, 116.33, 116.25, 116.16, 115.93.

The spectral data obtained were identical with those reported in literature.[8]

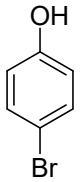
4e. 4-chlorophenol



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 - 7.16 (m, 1H), 6.80 - 6.74 (m, 1H), 5.39 - 5.33 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.89, 129.51, 125.65, 116.63.

The spectral data obtained were identical with those reported in literature.[8]

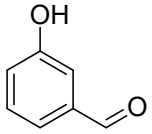
4f. 4-bromophenol



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 - 7.28 (m, 2H), 6.76 - 6.66 (m, 2H), 5.25 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.55, 132.43, 117.17, 112.81.

The spectral data obtained were identical with those reported in literature.[8]

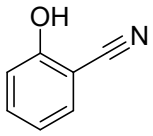
4g. 3-hydroxybenzaldehyde



^{1}H NMR (400 MHz, $CDCl_3$) δ 9.95 (s, 1H), 7.47 - 7.38 (m, 3H), 7.16 (ddd, *J* = 7.1, 2.6, 1.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.72, 156.52, 137.70, 130.39, 123.53, 122.21, 114.69.

The spectral data obtained were identical with those reported in literature.[9]

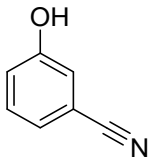
4h. 2-hydroxybenzonitrile



^{1}H NMR (400 MHz, DMSO-d_6) δ 11.08 (s, 1H), 7.58 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.48 (ddd, *J* = 8.9, 7.4, 1.7 Hz, 1H), 7.00 (dd, *J* = 8.5, 1.0 Hz, 1H), 6.91 (td, *J* = 7.5, 1.0 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 160.17, 134.76, 133.28, 119.60, 117.07, 116.18, 98.86.

The spectral data obtained were identical with those reported in literature.[10]

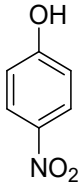
4i. 3-hydroxybenzonitrile



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (t, *J* = 7.9 Hz, 1H), 7.23 (dt, *J* = 7.7, 1.3 Hz, 1H), 7.19 - 7.12 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.43, 130.55, 124.24, 120.96, 118.71, 112.20.

The spectral data obtained were identical with those reported in literature.[11]

4j. 4-nitrophenol

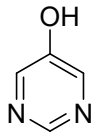


^{1}H NMR (400 MHz, DMSO-d_6) δ 11.08 (s, 1H), 8.09 (d, *J* = 9.2 Hz, 2H), 6.91 (d, *J* =

9.2 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.51, 140.15, 126.74, 116.34.

The spectral data obtained were identical with those reported in literature.[8]

4k. 5-pyrimidinol



^{1}H NMR (400 MHz, DMSO-d_6) δ 10.52 (s, 1H), 8.66 (s, 1H), 8.33 (s, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 152.47, 150.31, 144.65.

The spectral data obtained were identical with those reported in literature.[12]

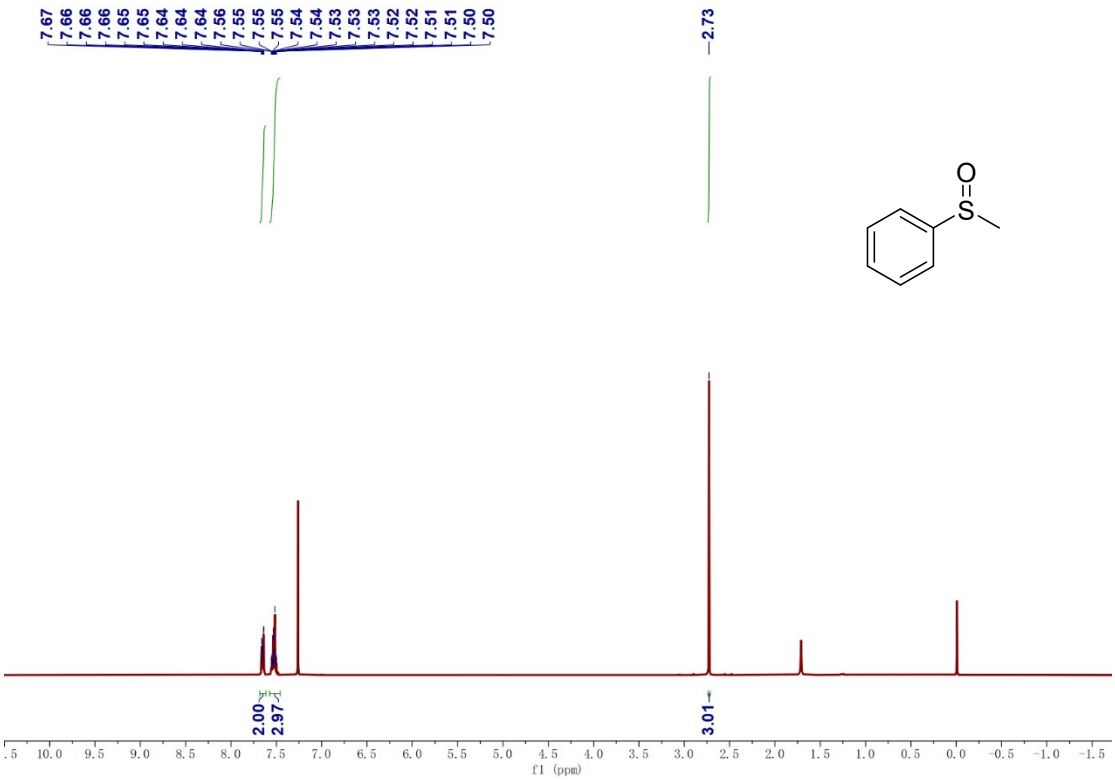


Fig. S13 ^{1}H NMR spectrum of **2a** in $CDCl_3$.

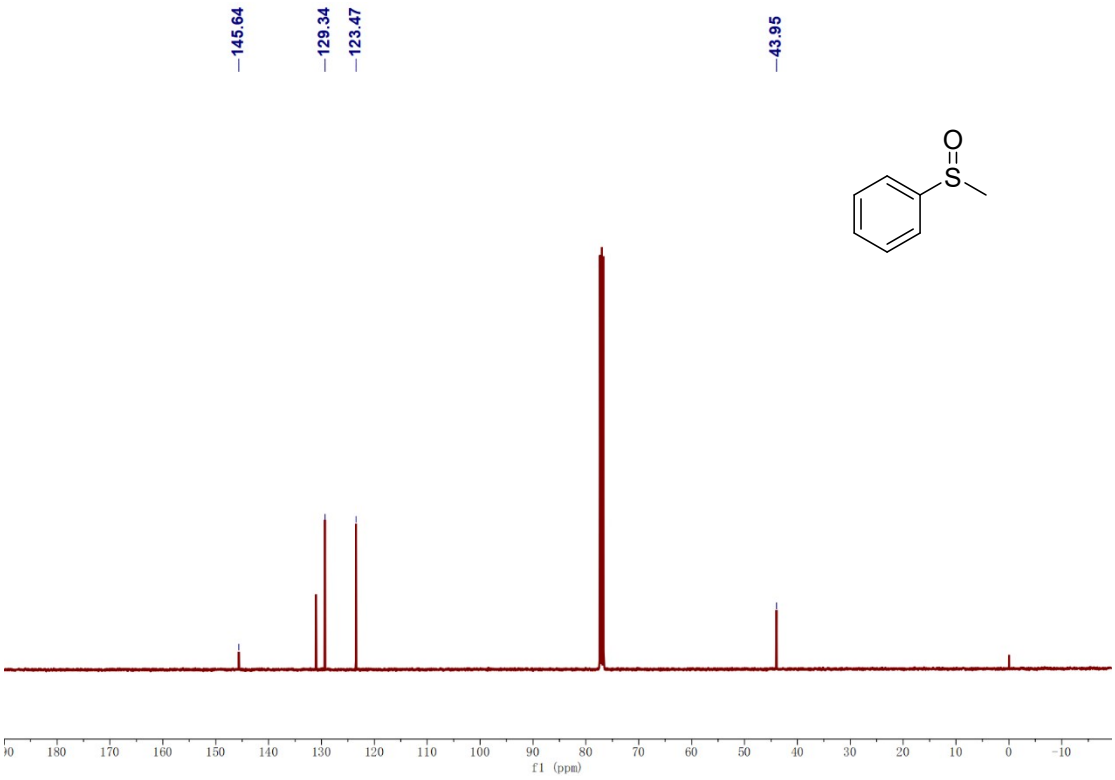


Fig. S14 ^{13}C NMR spectrum of **2a** in $CDCl_3$.

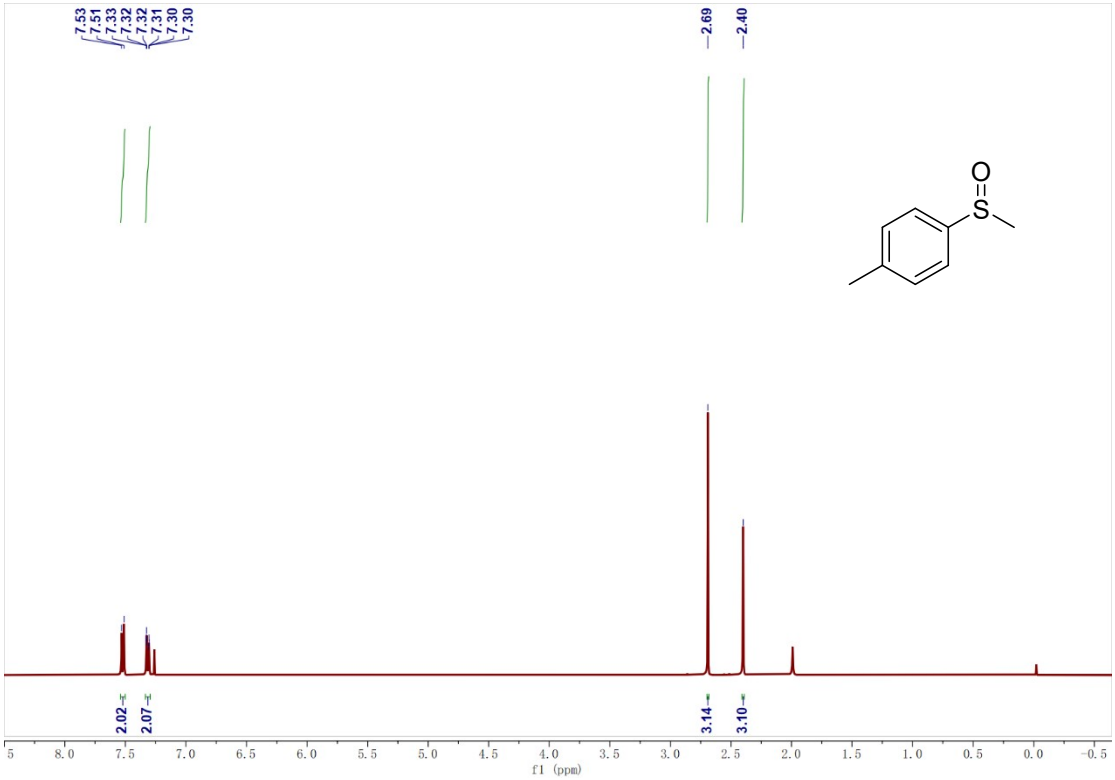


Fig. S15 ^{1}H NMR spectrum of **2b** in $CDCl_3$.

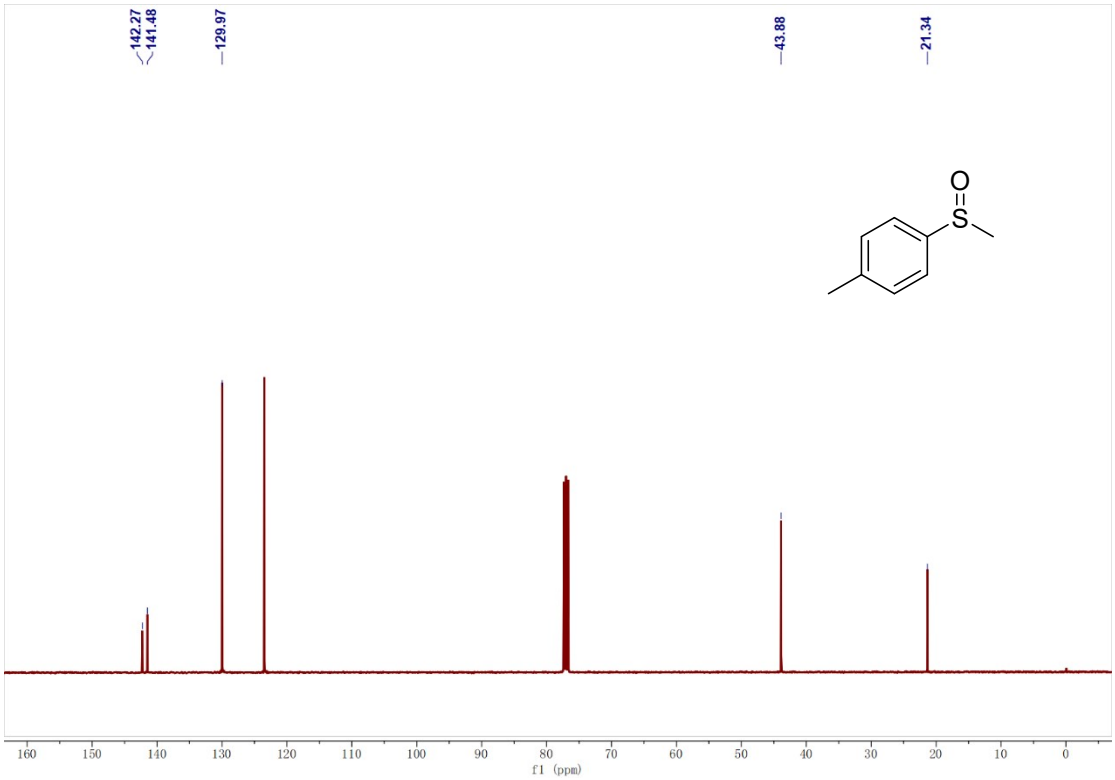


Fig. S16 ^{13}C NMR spectrum of **2b** in $CDCl_3$.

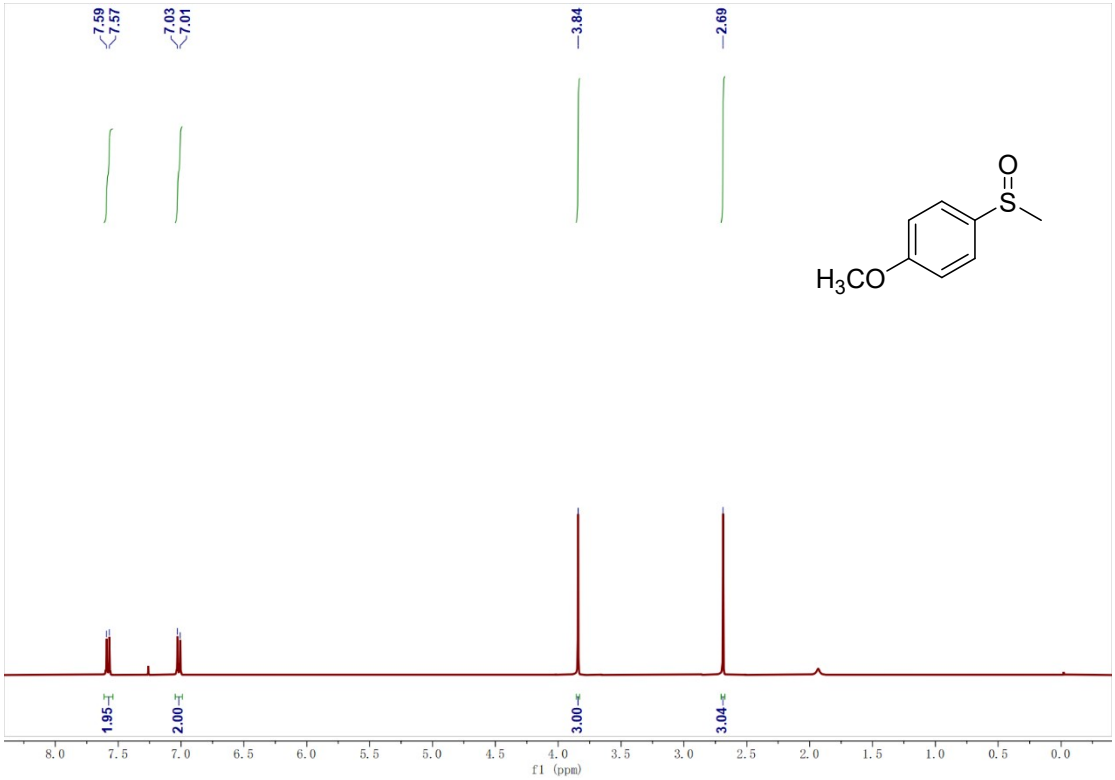


Fig. S17 ^{1}H NMR spectrum of **2c** in $CDCl_3$.

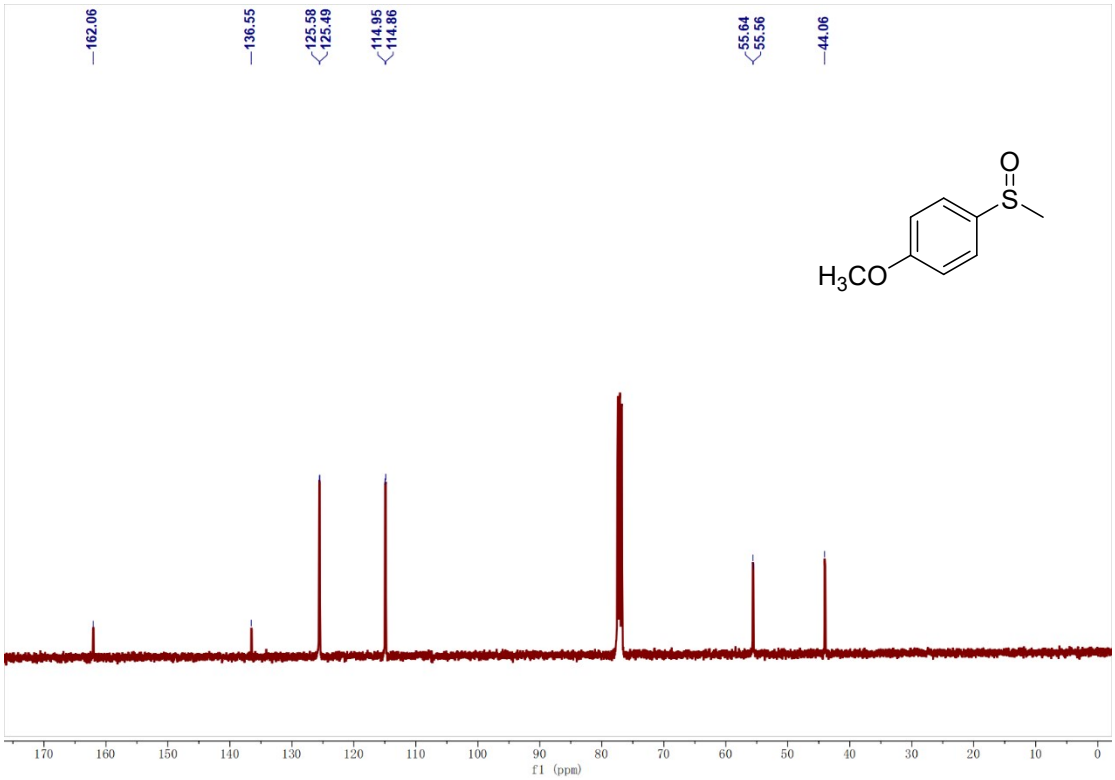


Fig. S18 ^{13}C NMR spectrum of **2c** in $CDCl_3$.

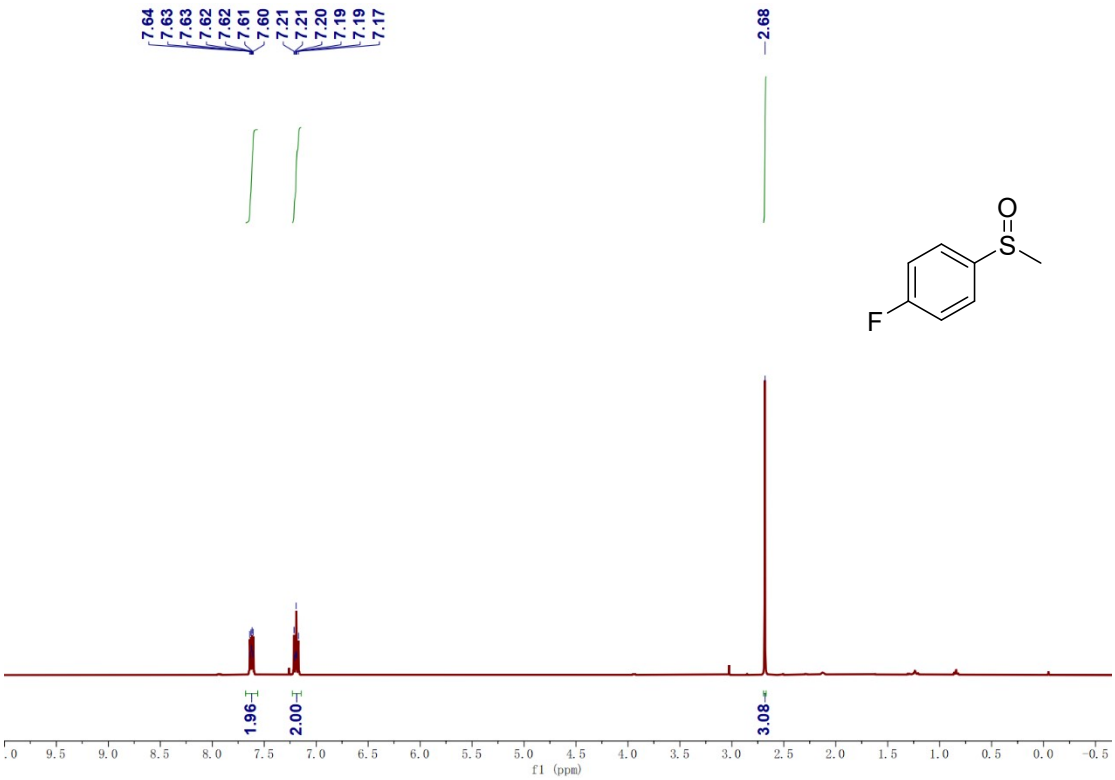


Fig. S19 ^{1}H NMR spectrum of **2d** in $CDCl_3$.

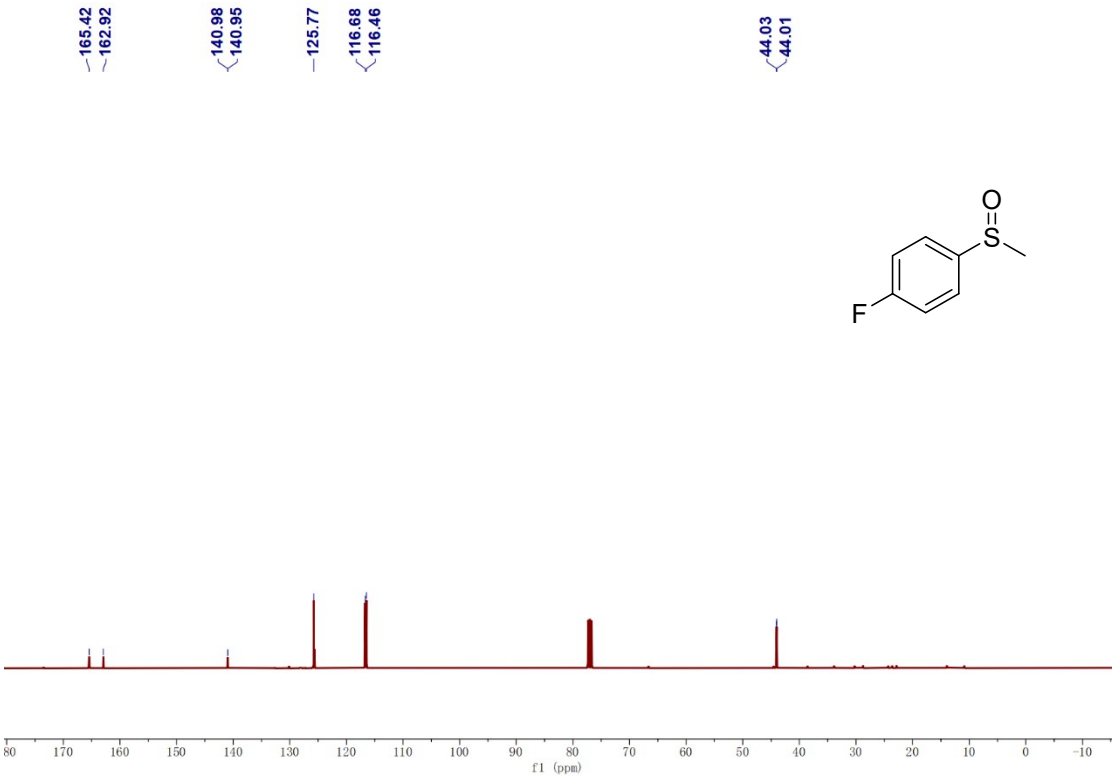


Fig. S20 ^{13}C NMR spectrum of **2d** in $CDCl_3$.

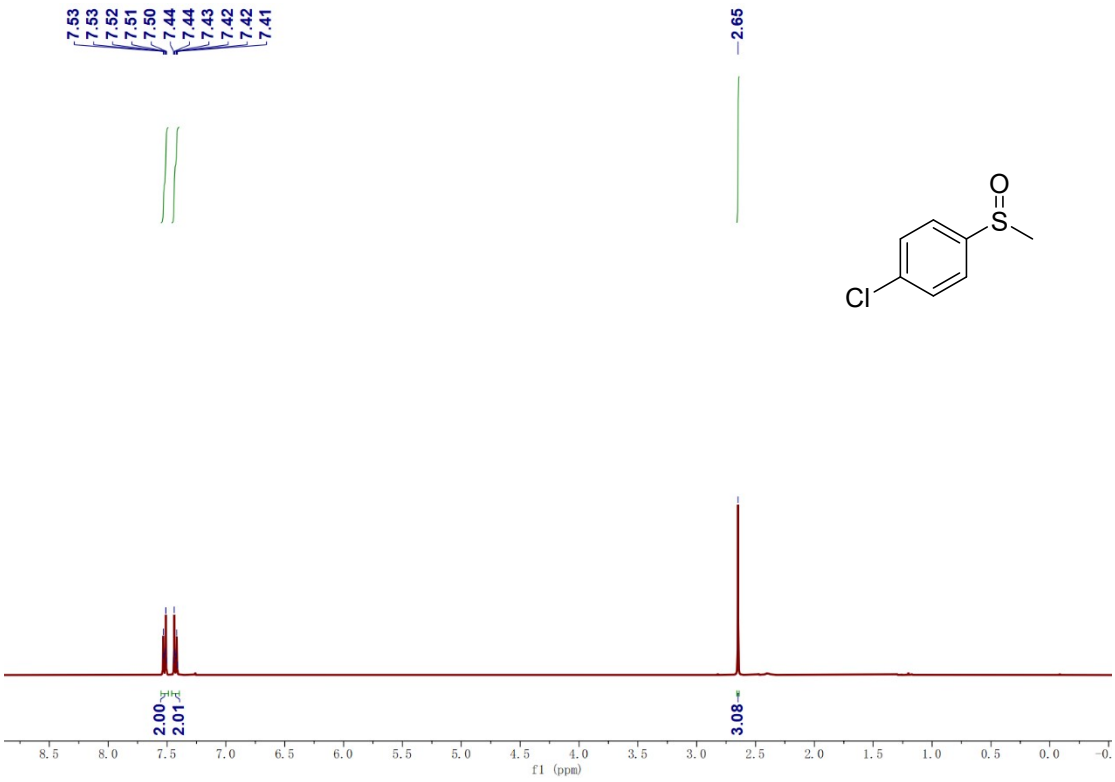


Fig. S21 ^{1}H NMR spectrum of **2e** in $CDCl_3$.

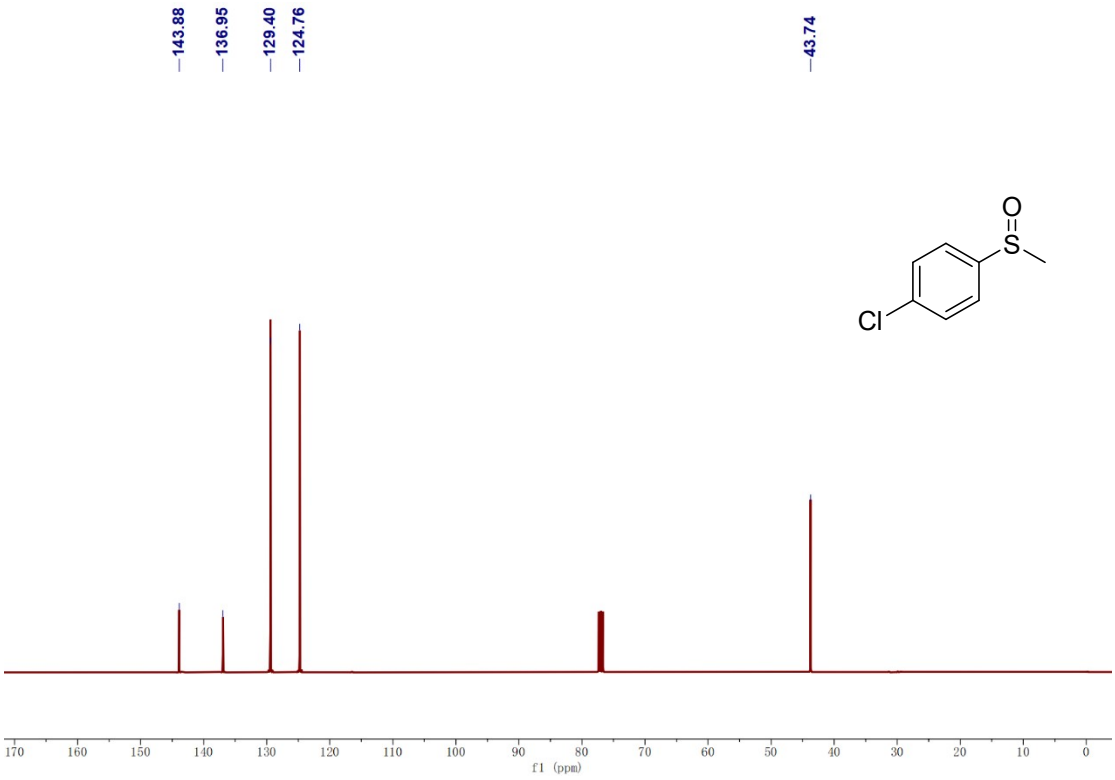


Fig. S22 ^{13}C NMR spectrum of **2e** in $CDCl_3$.

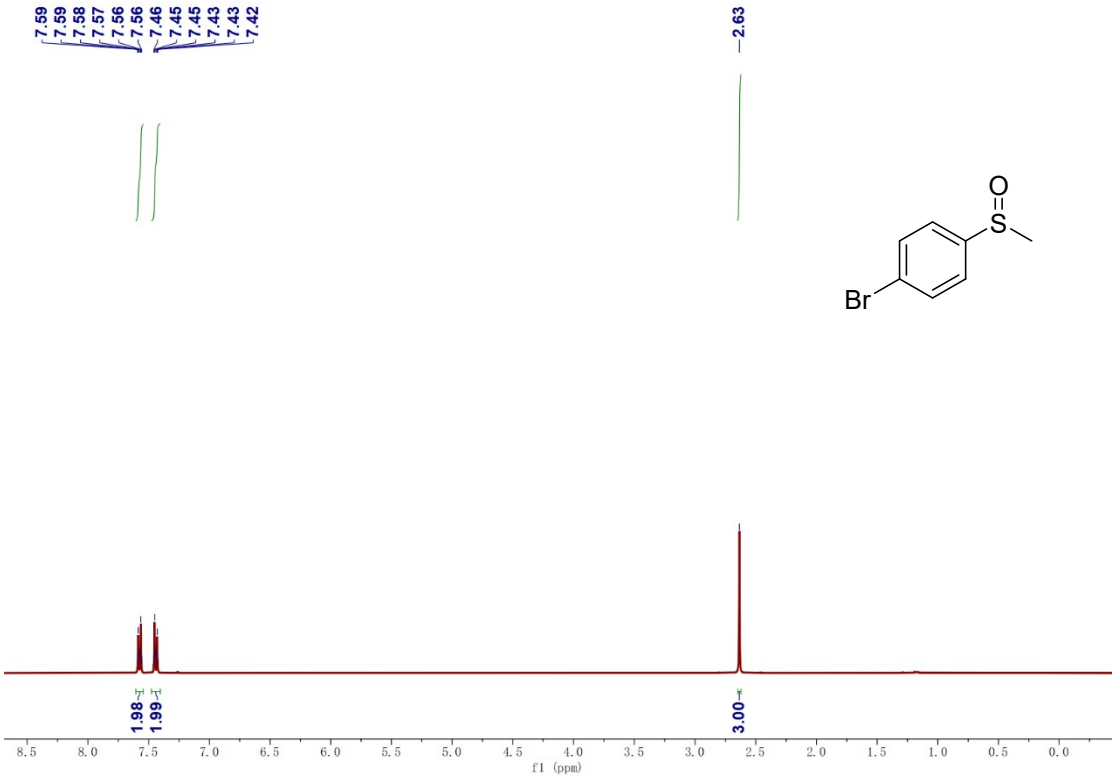


Fig. S23 ^{1}H NMR spectrum of **2f** in $CDCl_3$.

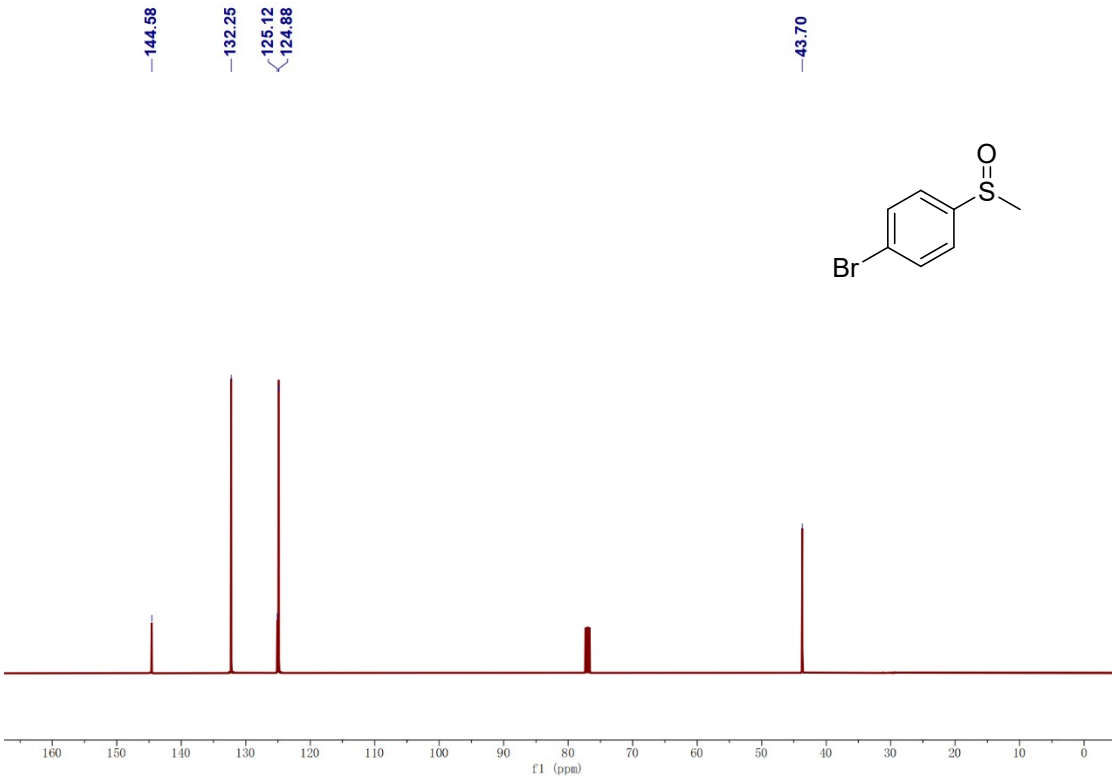


Fig. S24 ^{13}C NMR spectrum of **2f** in $CDCl_3$.

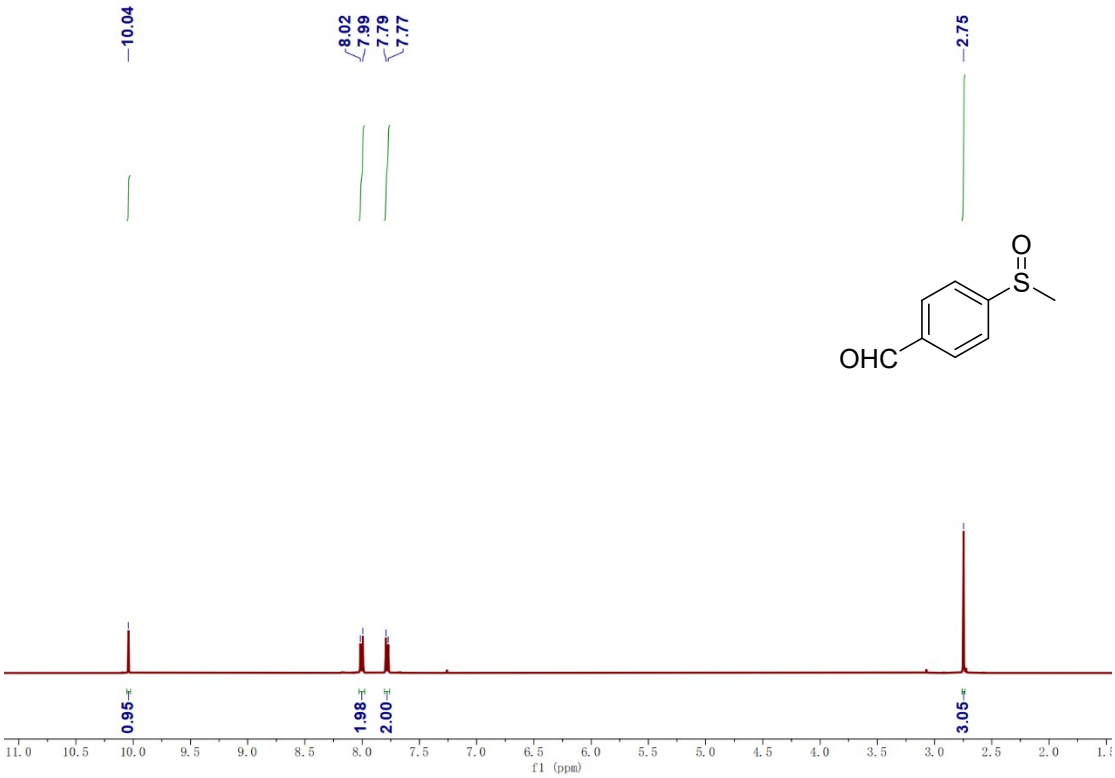


Fig. S25 ^{1}H NMR spectrum of **2g** in $CDCl_3$.

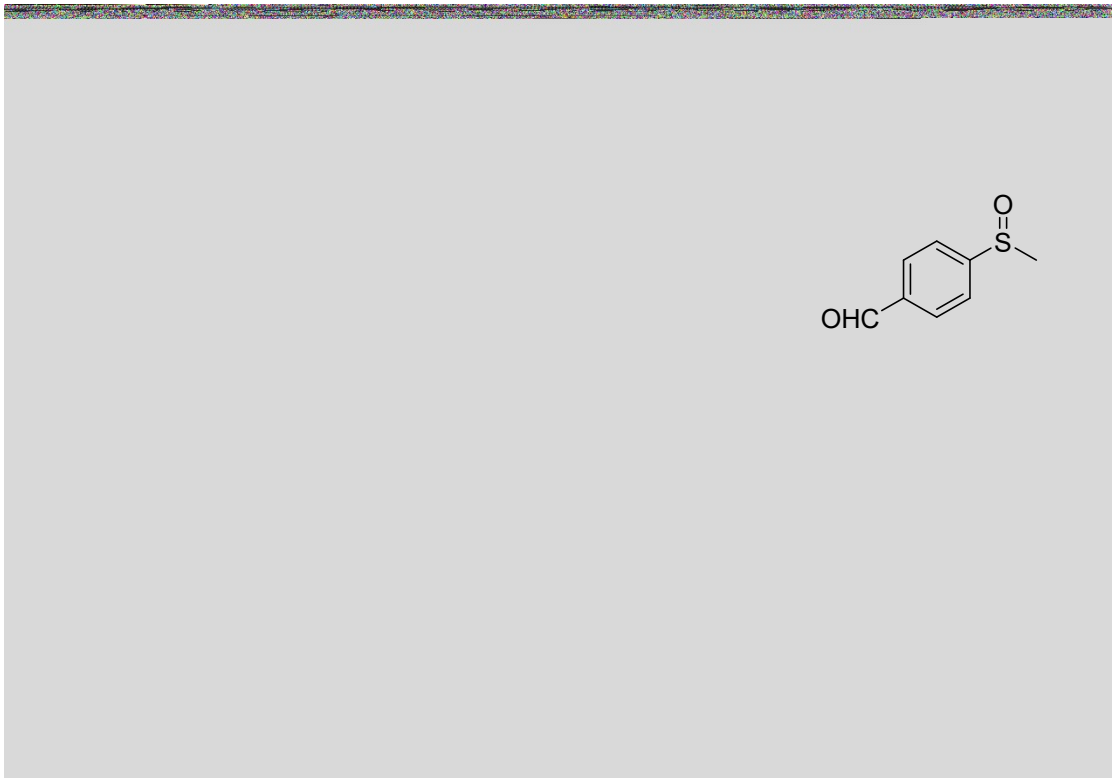


Fig. S26 ^{13}C NMR spectrum of **2g** in $CDCl_3$.

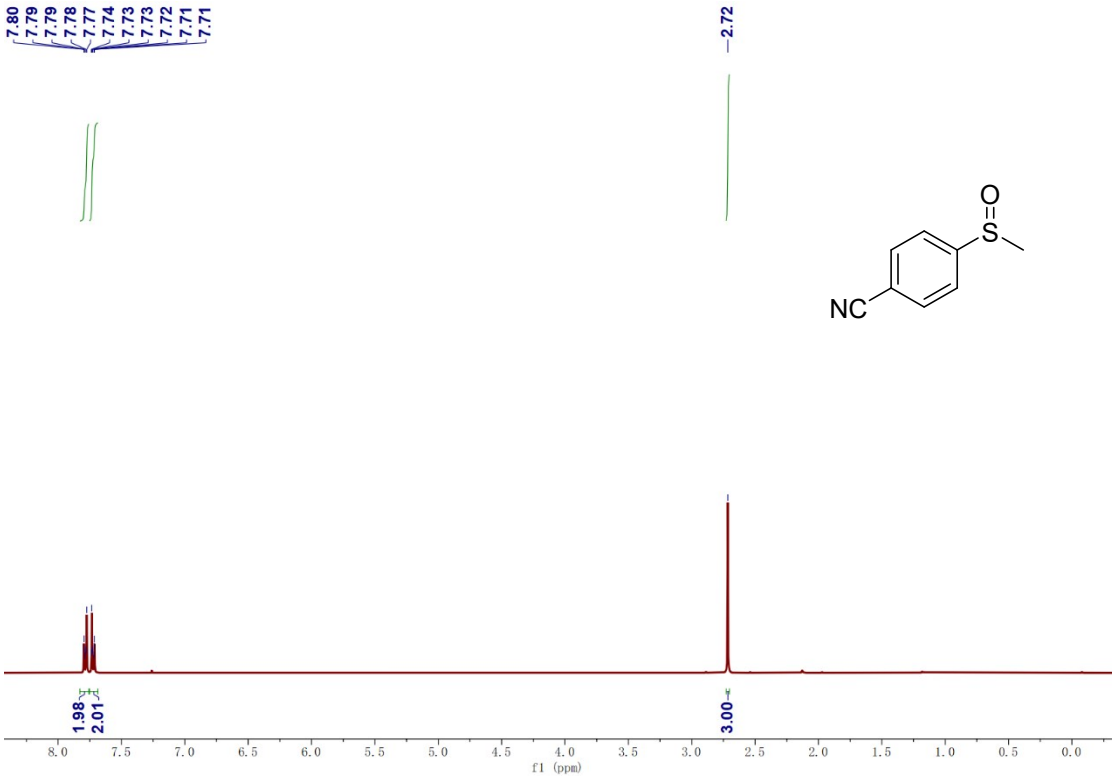


Fig. S27 ^{1}H NMR spectrum of **2h** in $CDCl_3$.

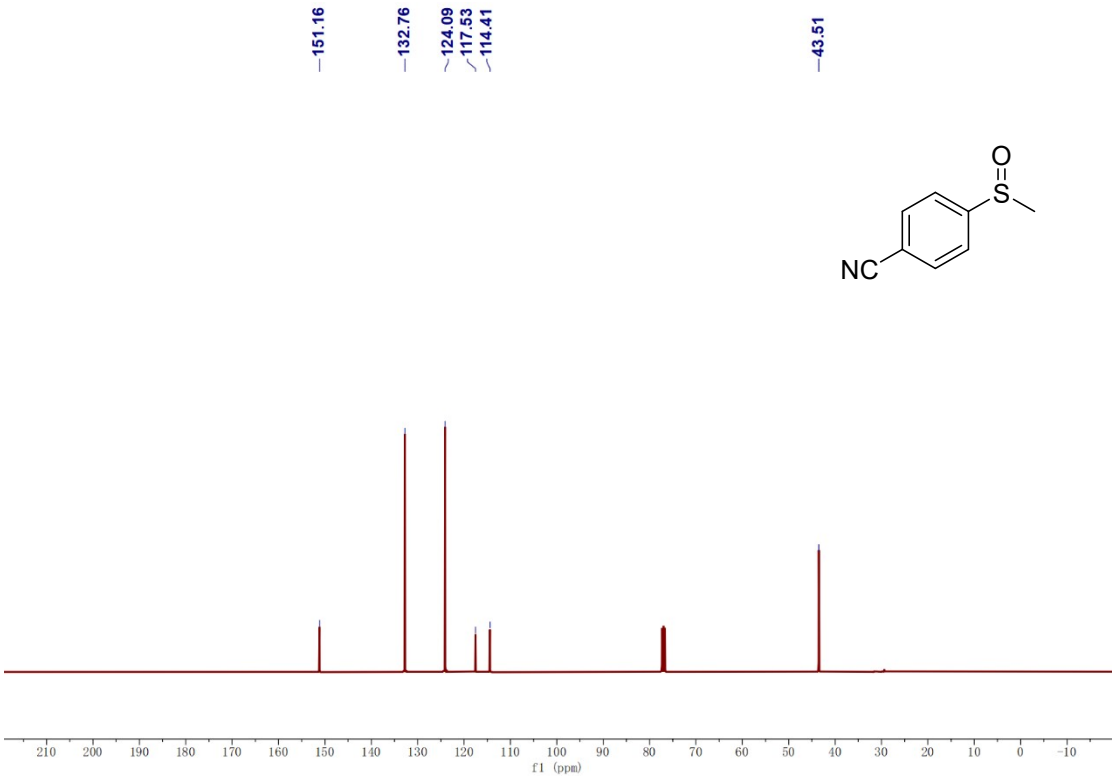


Fig. S28 ^{13}C NMR spectrum of **2h** in $CDCl_3$.

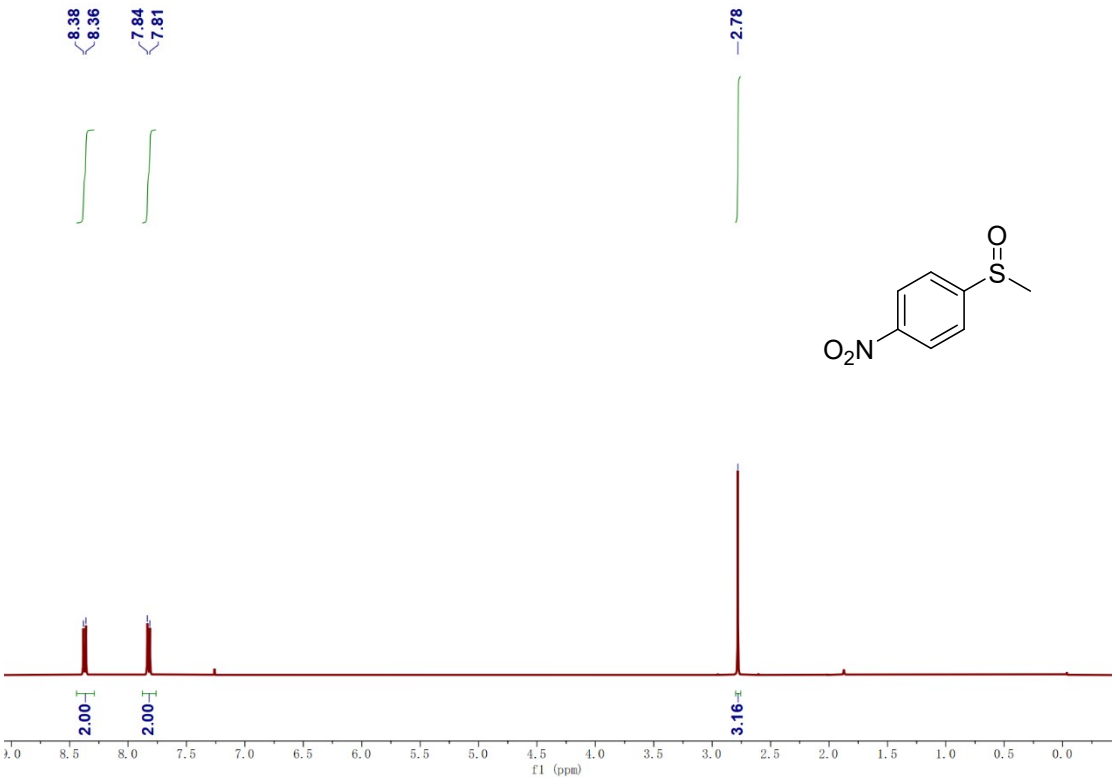


Fig. S29 ^{1}H NMR spectrum of **2i** in $CDCl_3$.

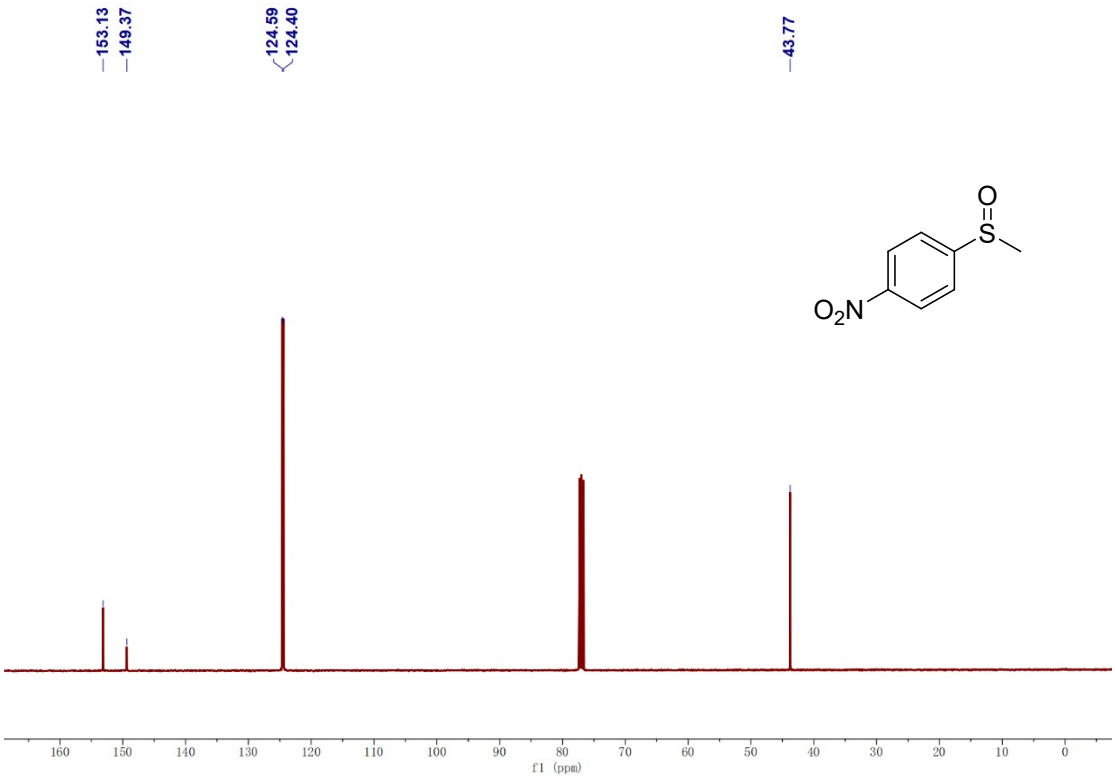


Fig. S30 ^{13}C NMR spectrum of **2i** in $CDCl_3$.

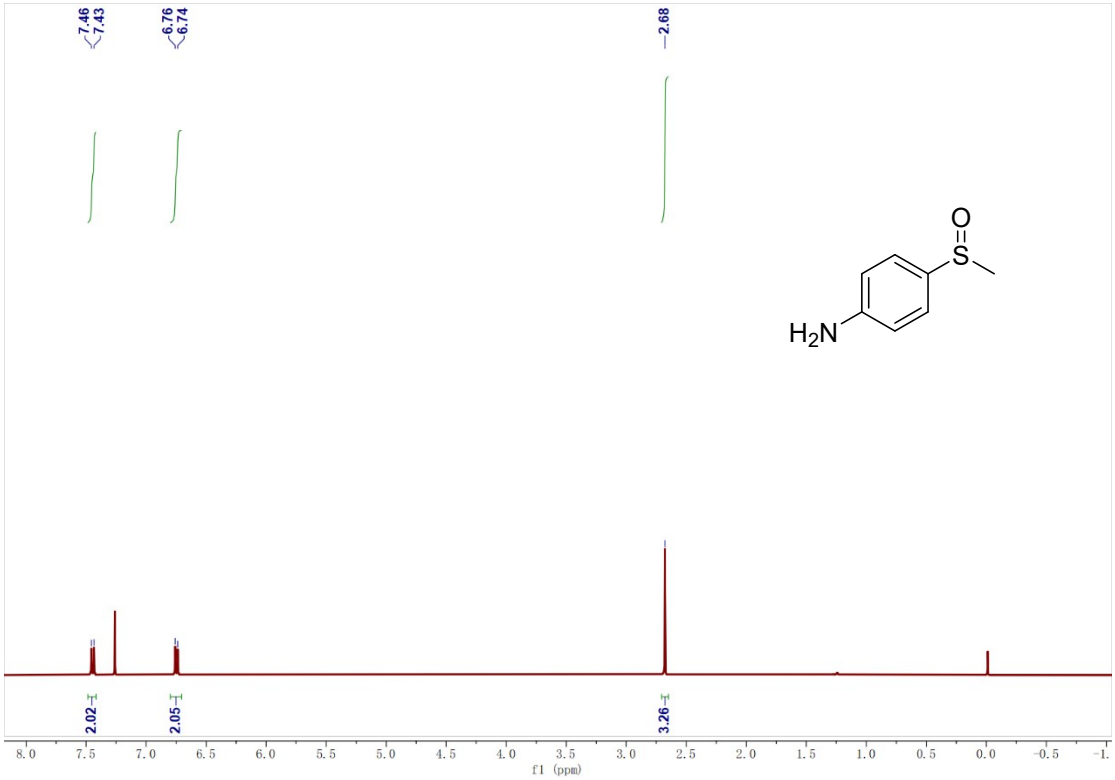


Fig. S31 ^{1}H NMR spectrum of **2j** in $CDCl_3$.

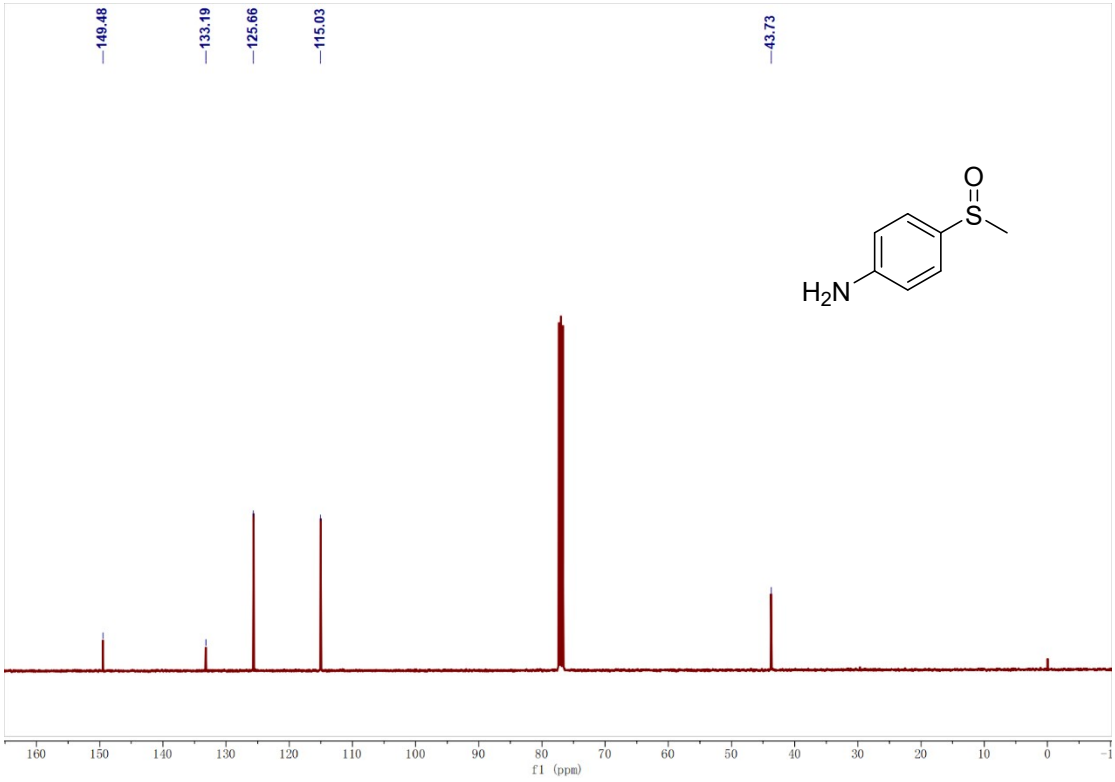


Fig. S32 ^{13}C NMR spectrum of **2j** in $CDCl_3$.

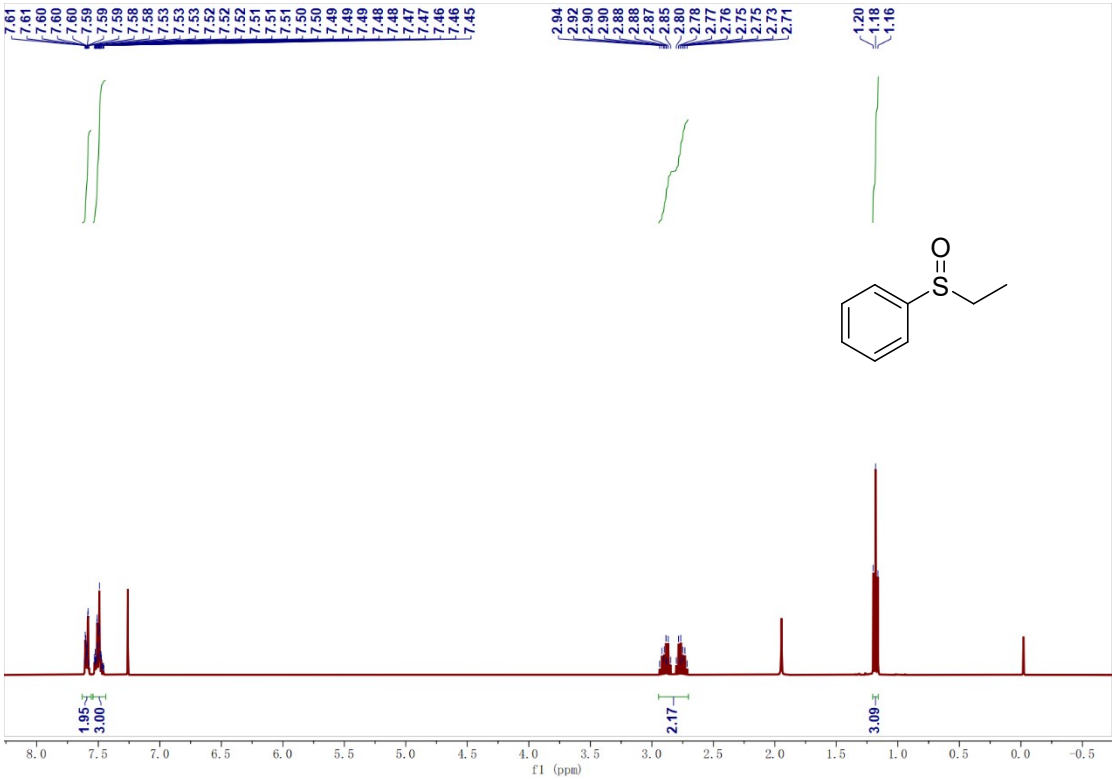


Fig. S33 ^{1}H NMR spectrum of **2k** in $CDCl_3$.

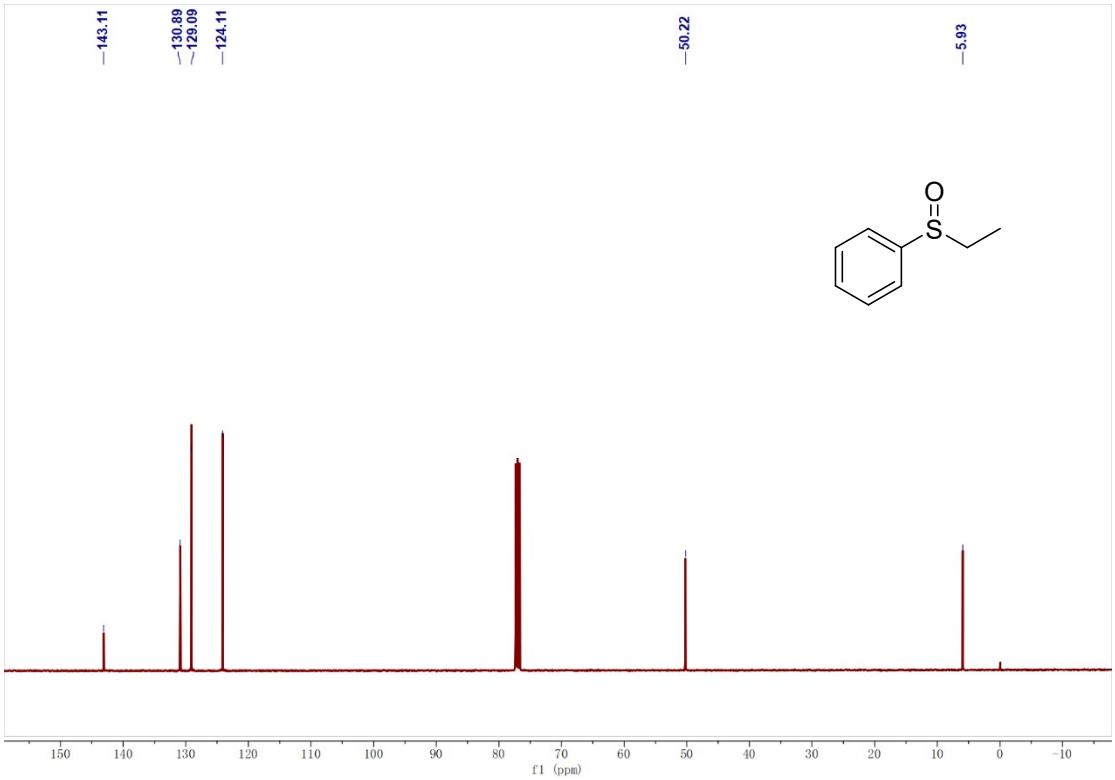


Fig. S34 ^{13}C NMR spectrum of **2k** in $CDCl_3$.

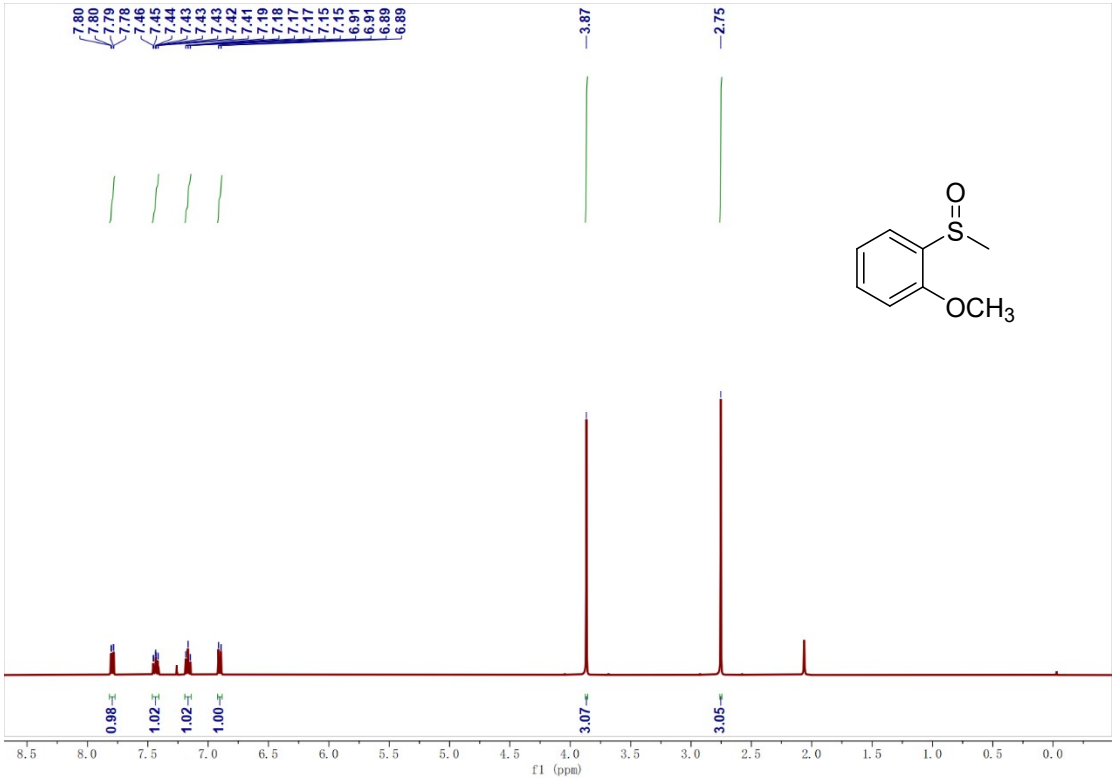


Fig. S35 ^{1}H NMR spectrum of **2l** in $CDCl_3$.

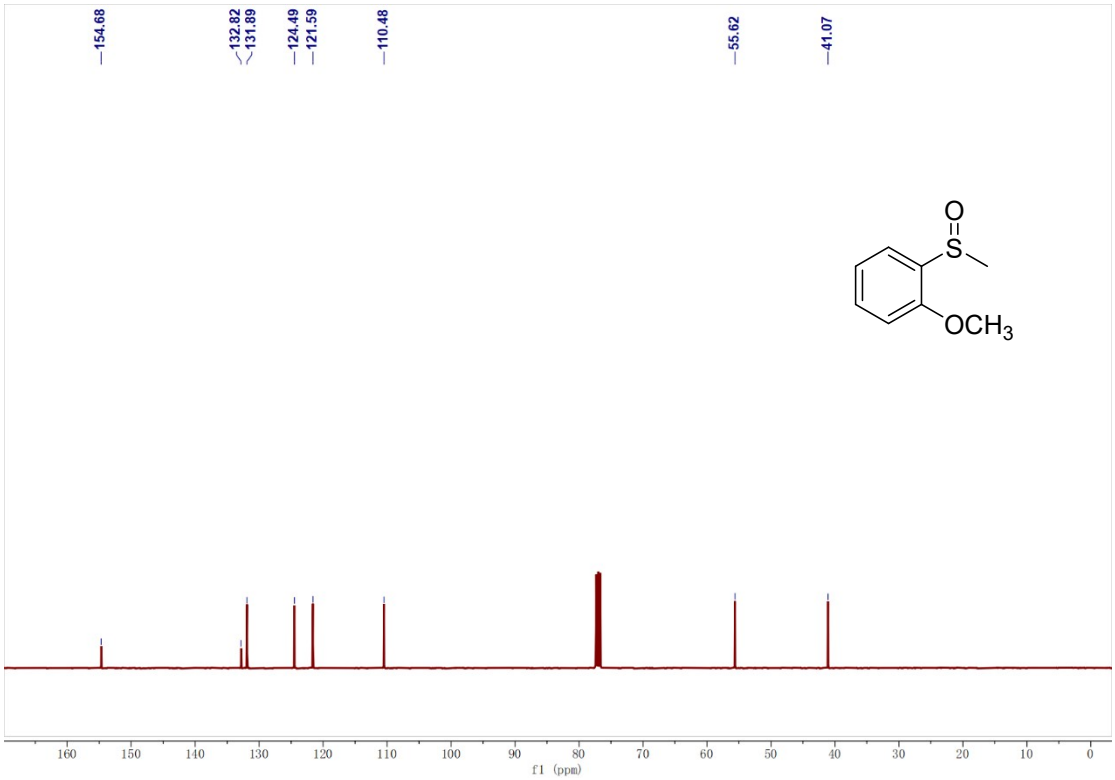


Fig. S36 ^{13}C NMR spectrum of **2l** in $CDCl_3$.

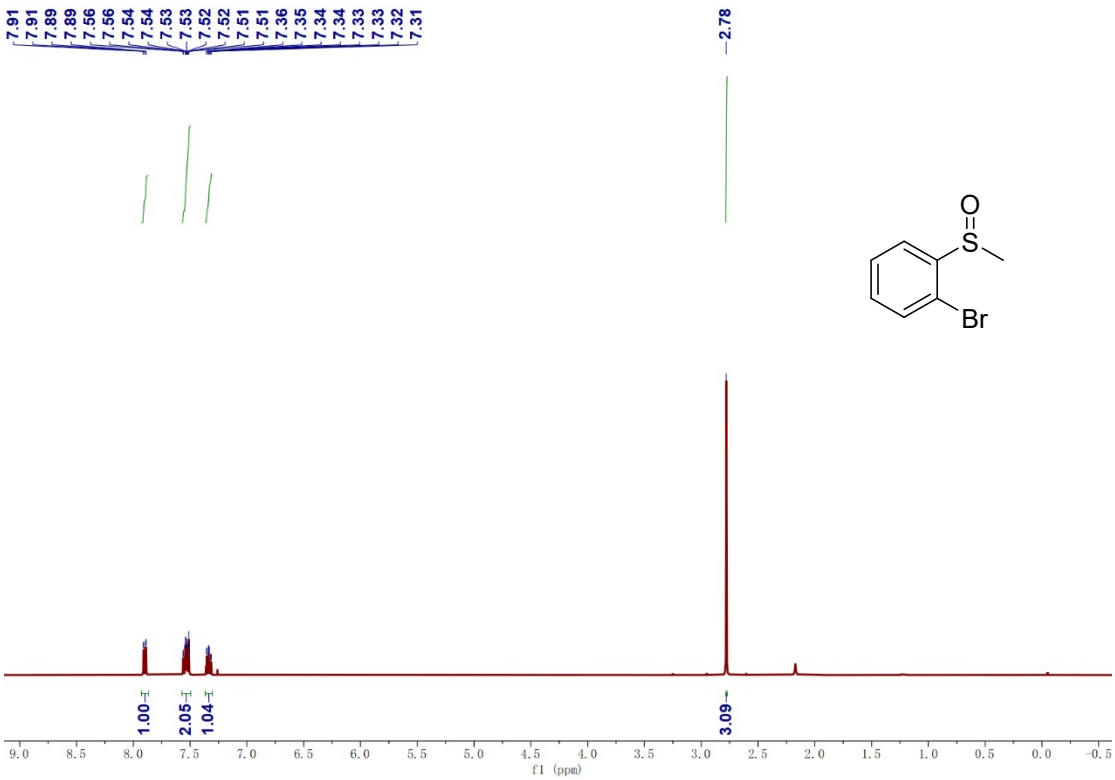


Fig. S37 ^{1}H NMR spectrum of **2m** in $CDCl_3$.

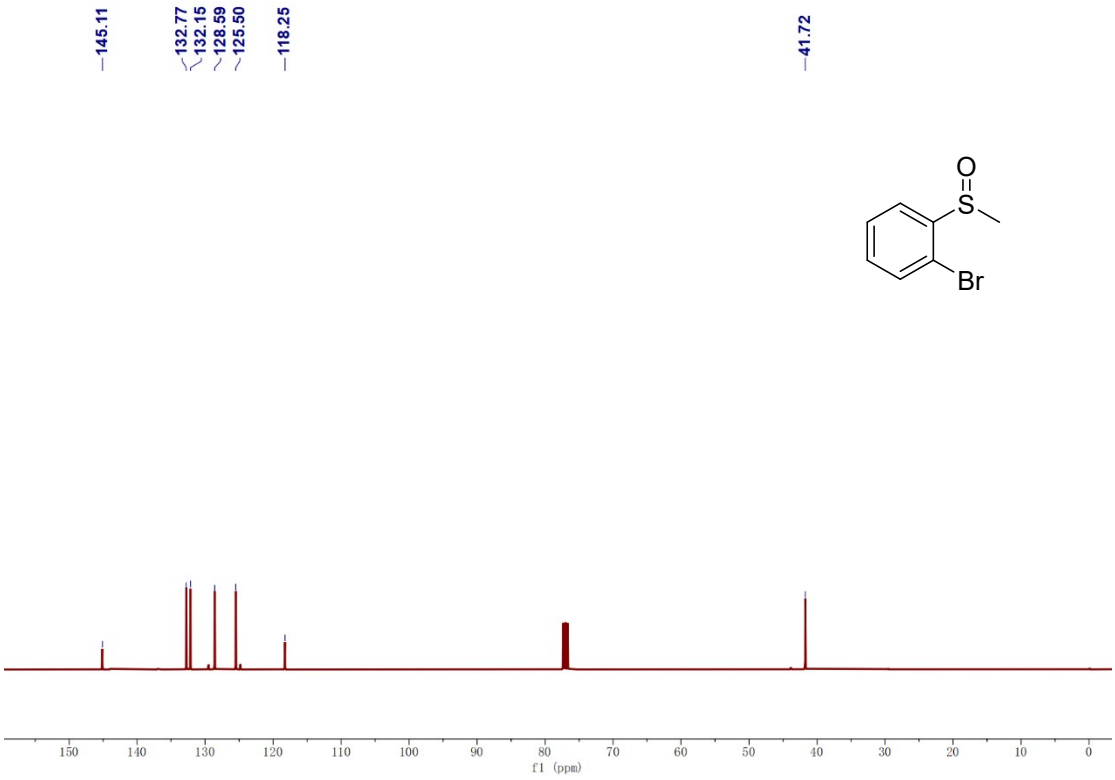


Fig. S38 ^{13}C NMR spectrum of **2m** in $CDCl_3$.

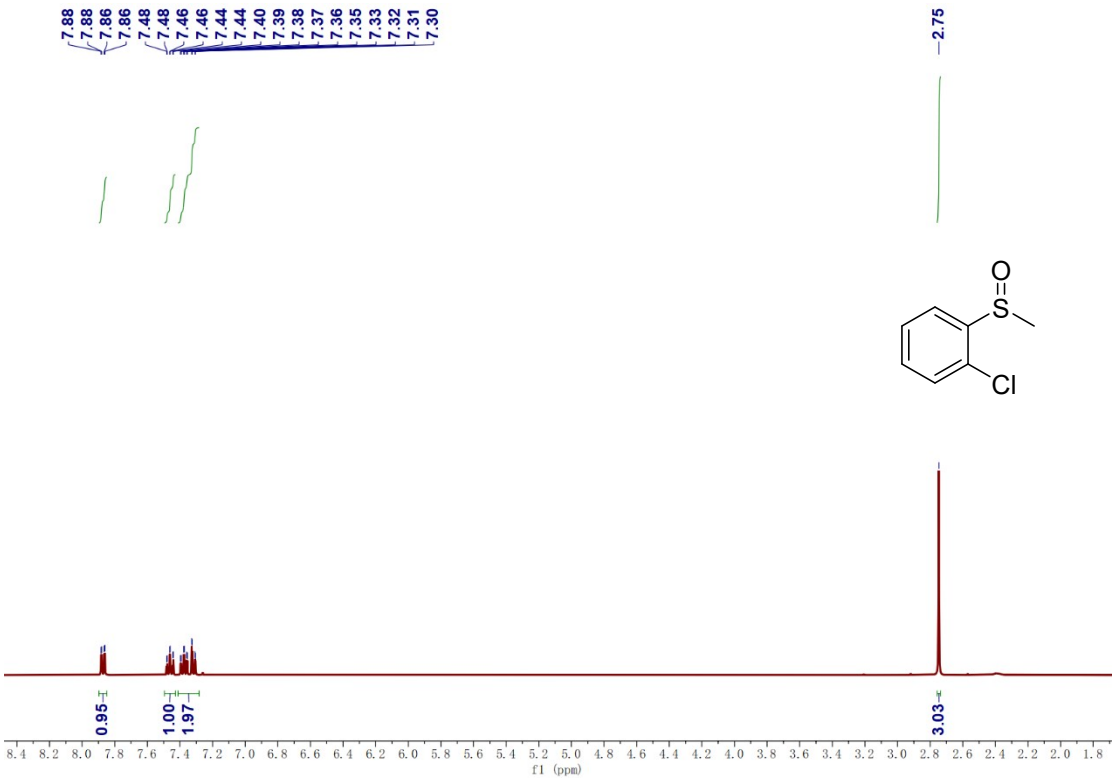


Fig. S39 ^{1}H NMR spectrum of **2n** in $CDCl_3$.

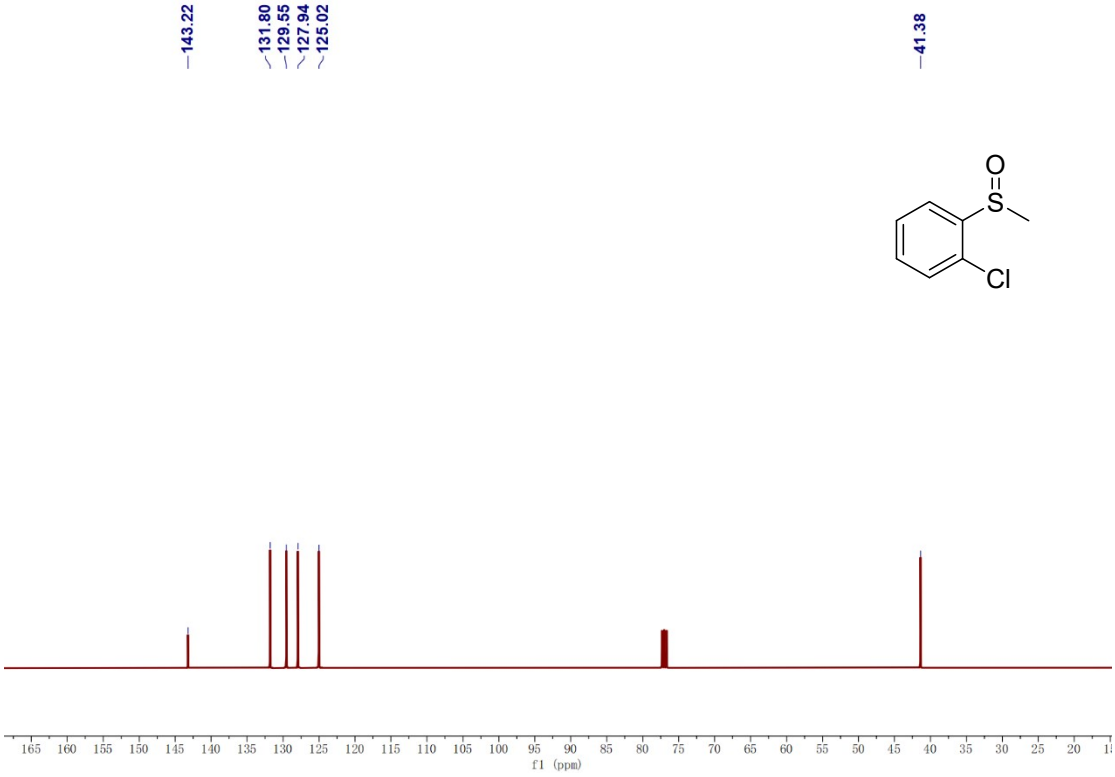


Fig. S40 ^{13}C NMR spectrum of **2n** in $CDCl_3$.

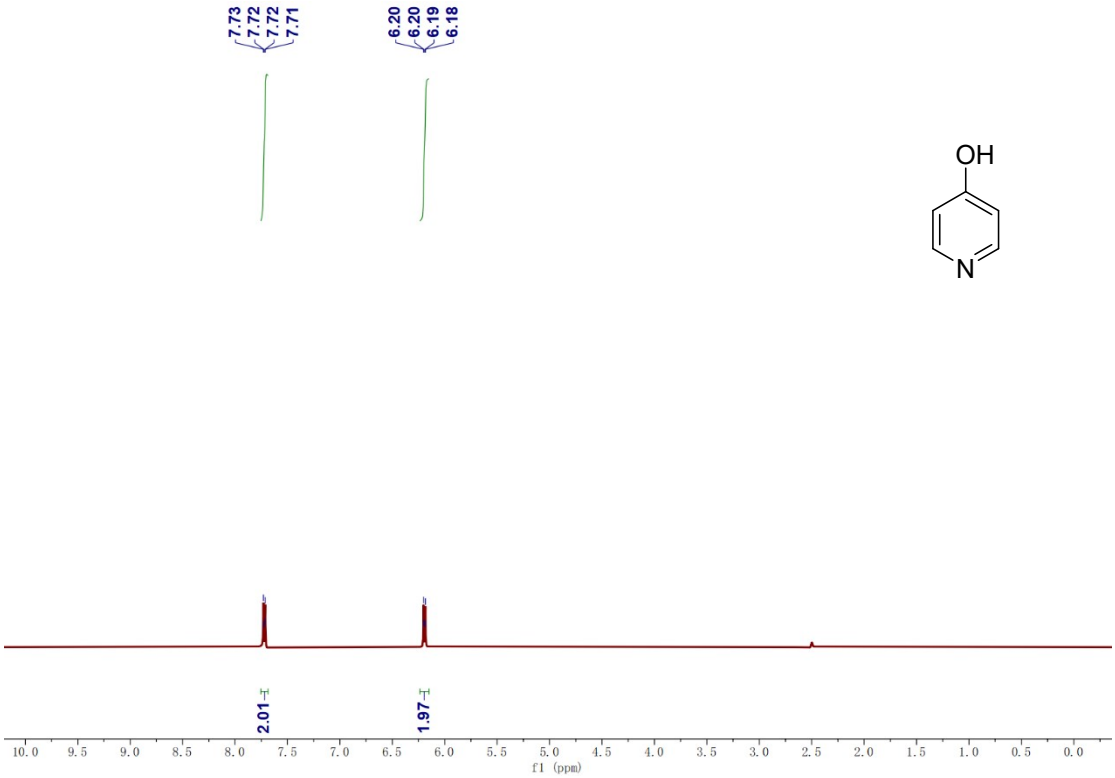


Fig. S41 ^{1}H NMR spectrum of **4a** in DMSO-d_6.

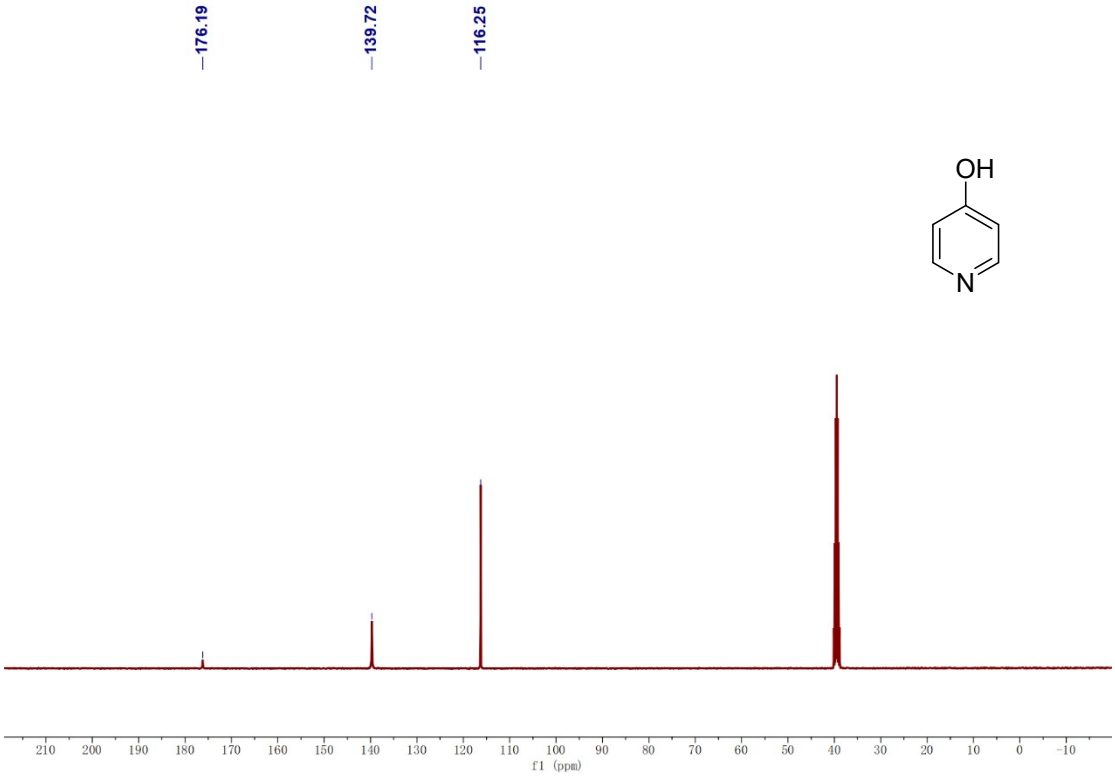


Fig. S42 ^{13}C NMR spectrum of **4a** in DMSO-d_6.

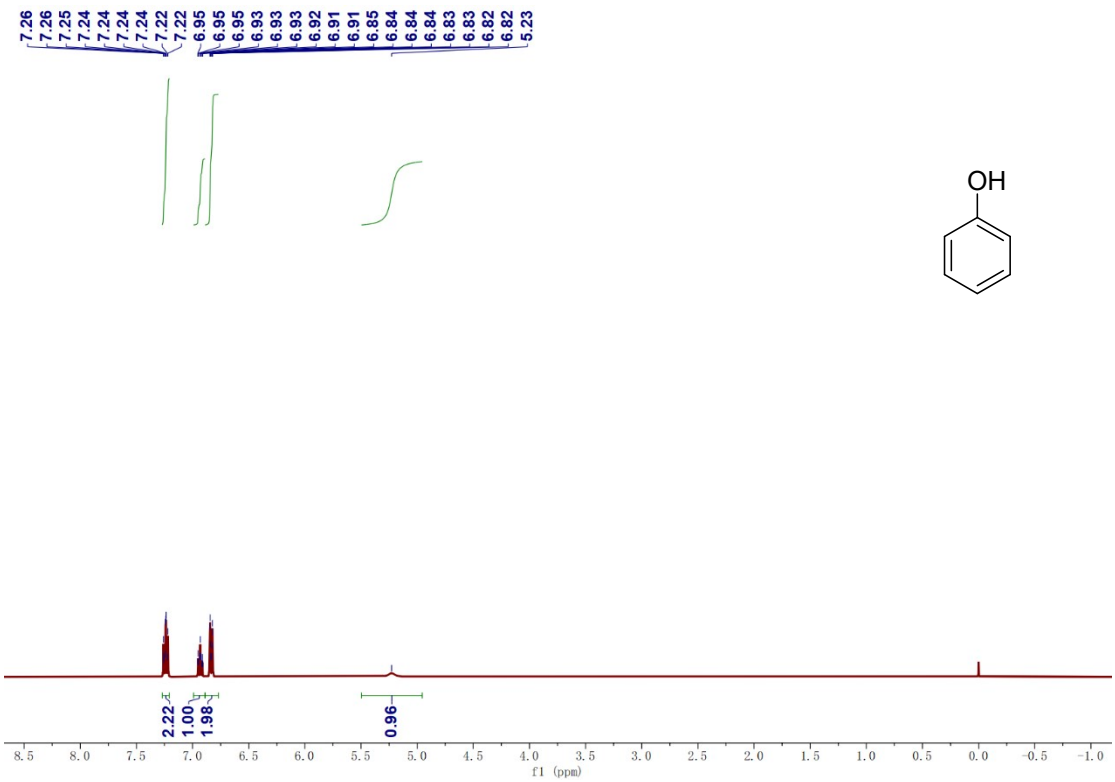


Fig. S43 ^{1}H NMR spectrum of **4b** in $CDCl_3$.

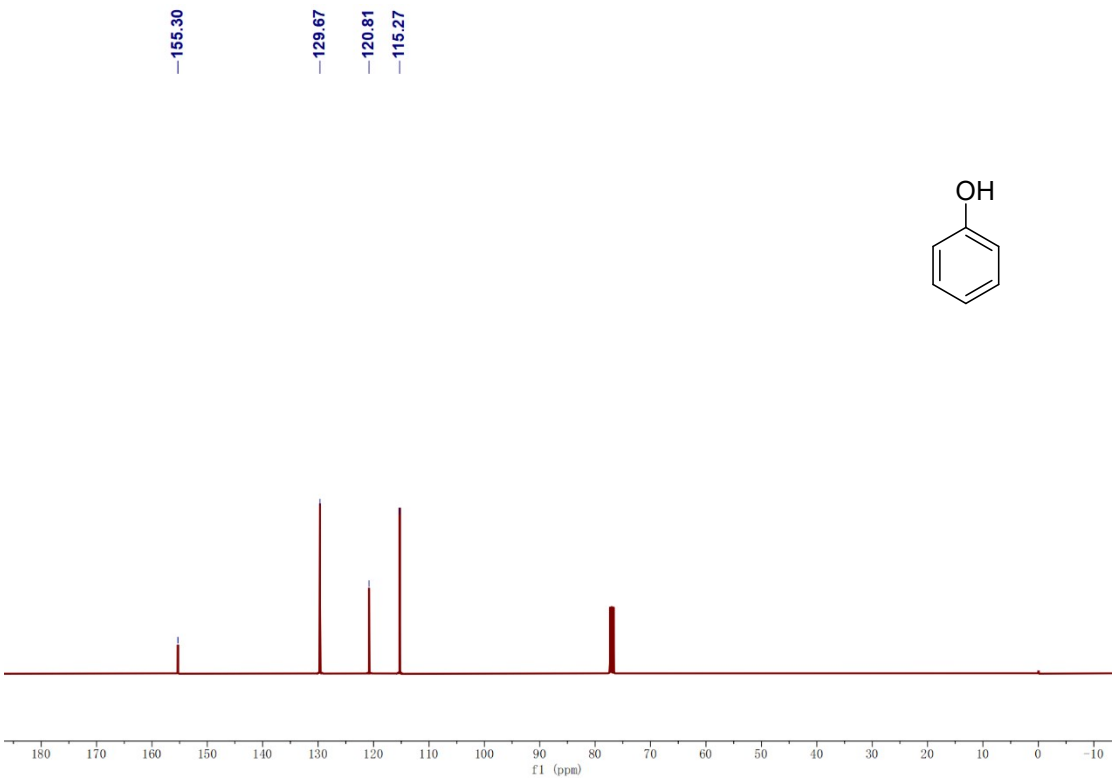


Fig. S44 ^{13}C NMR spectrum of **4b** in $CDCl_3$.

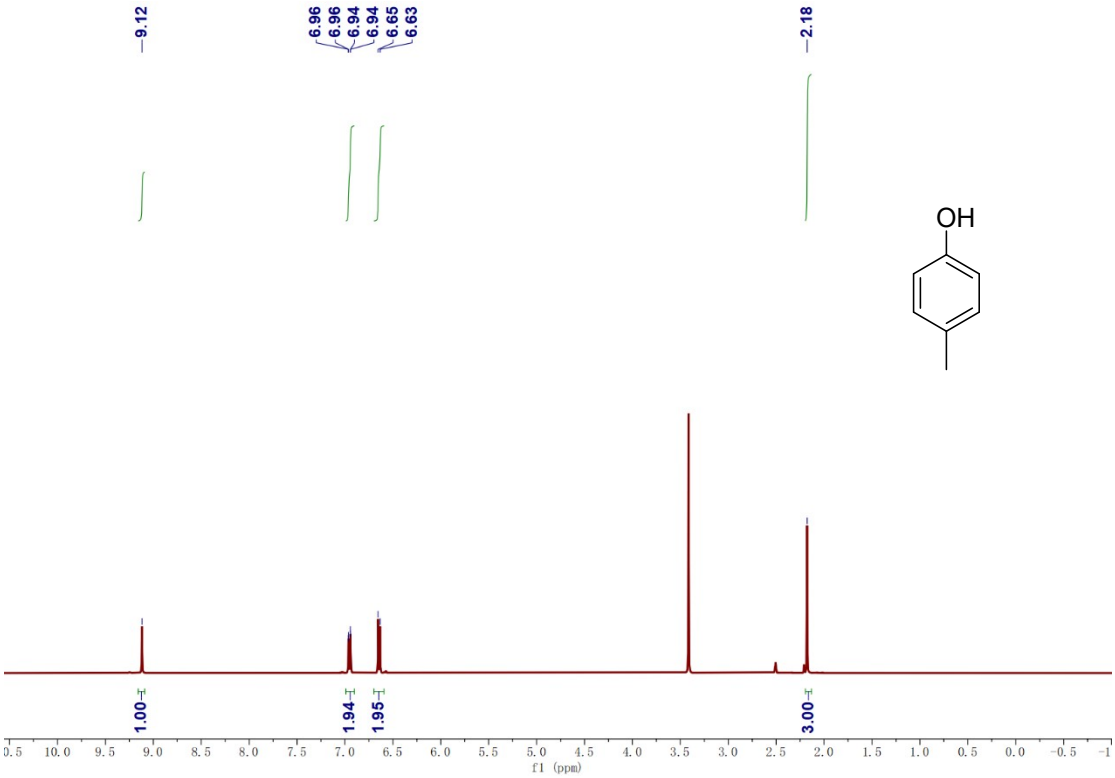


Fig. S45 ^{1}H NMR spectrum of **4c** in DMSO-d_6.

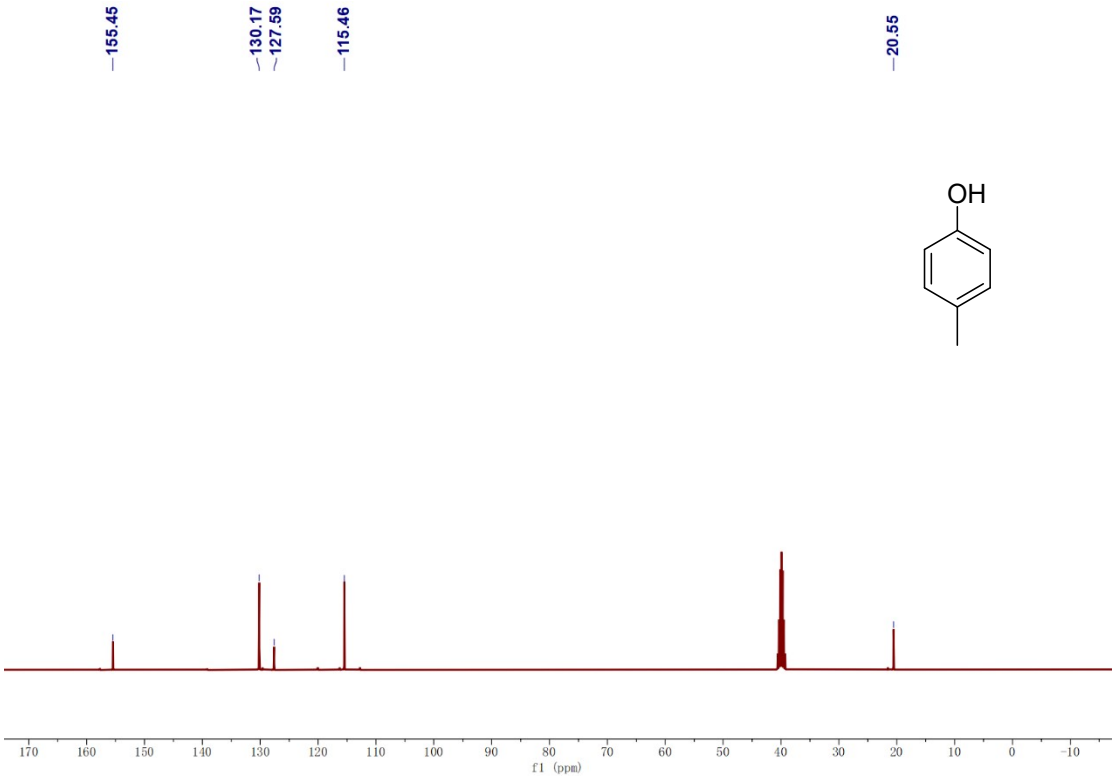


Fig. S46 ^{13}C NMR spectrum of **4c** in DMSO-d_6.

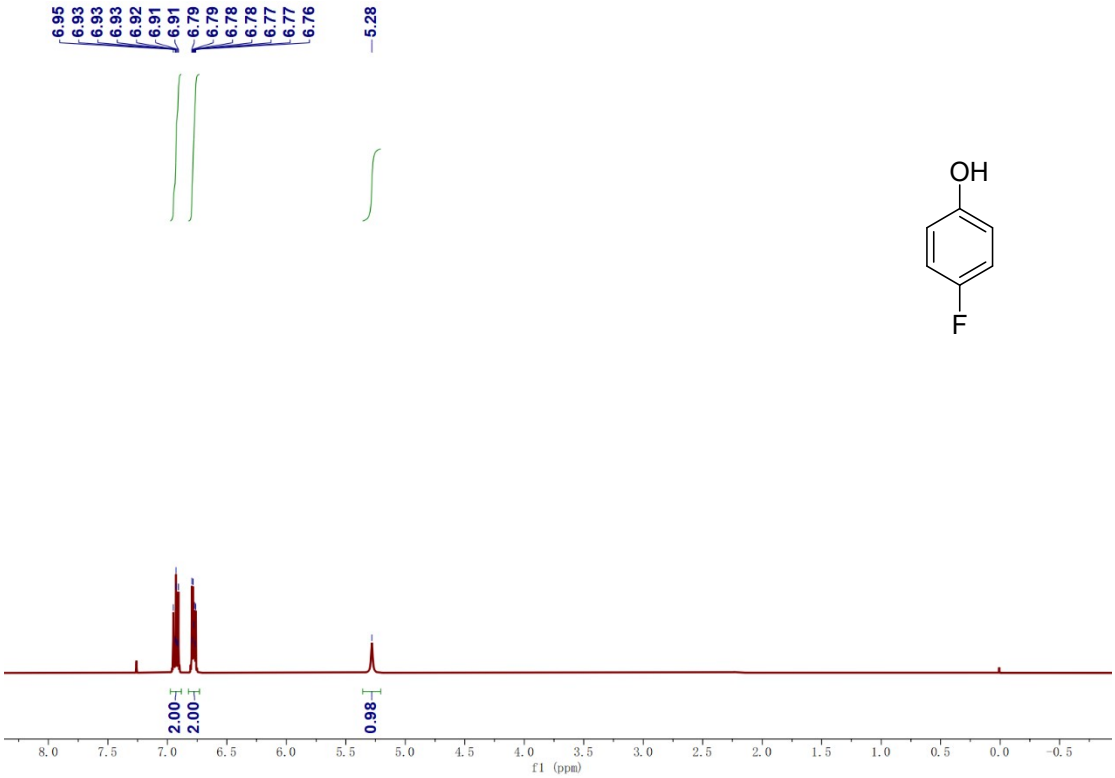


Fig. S47 ^{1}H NMR spectrum of **4d** in $CDCl_3$.

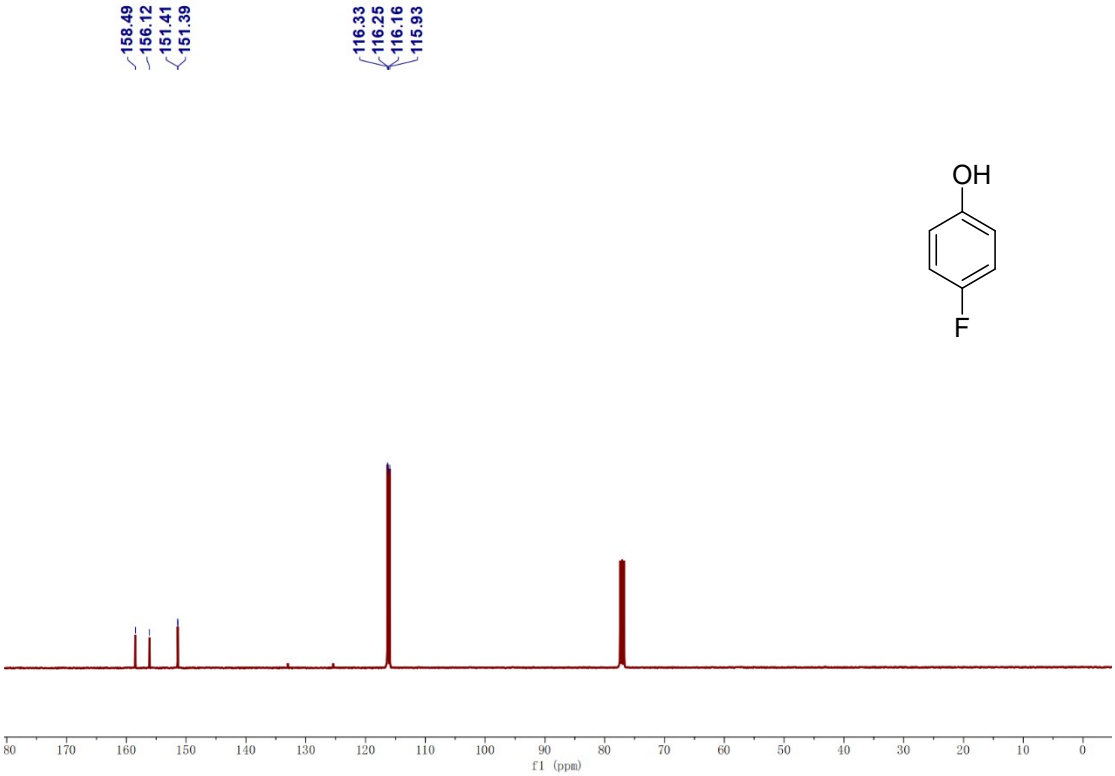


Fig. S48 ^{13}C NMR spectrum of **4d** in $CDCl_3$.

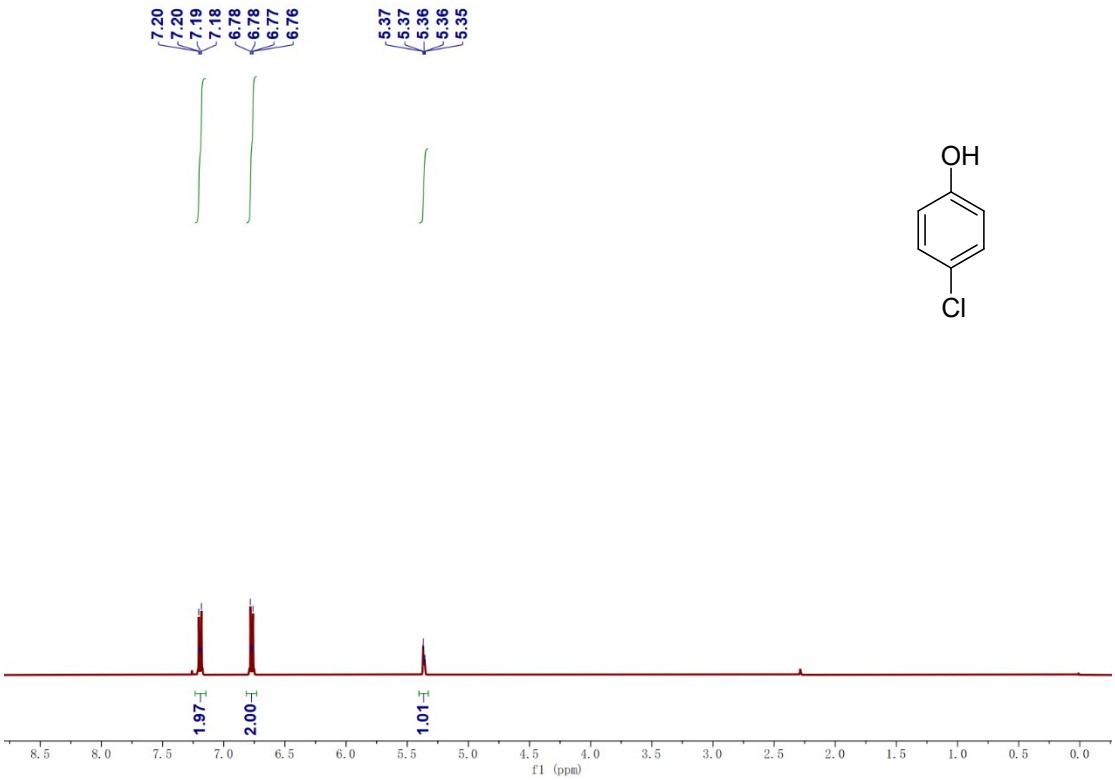


Fig. S49 ^{1}H NMR spectrum of **4e** in $CDCl_3$.

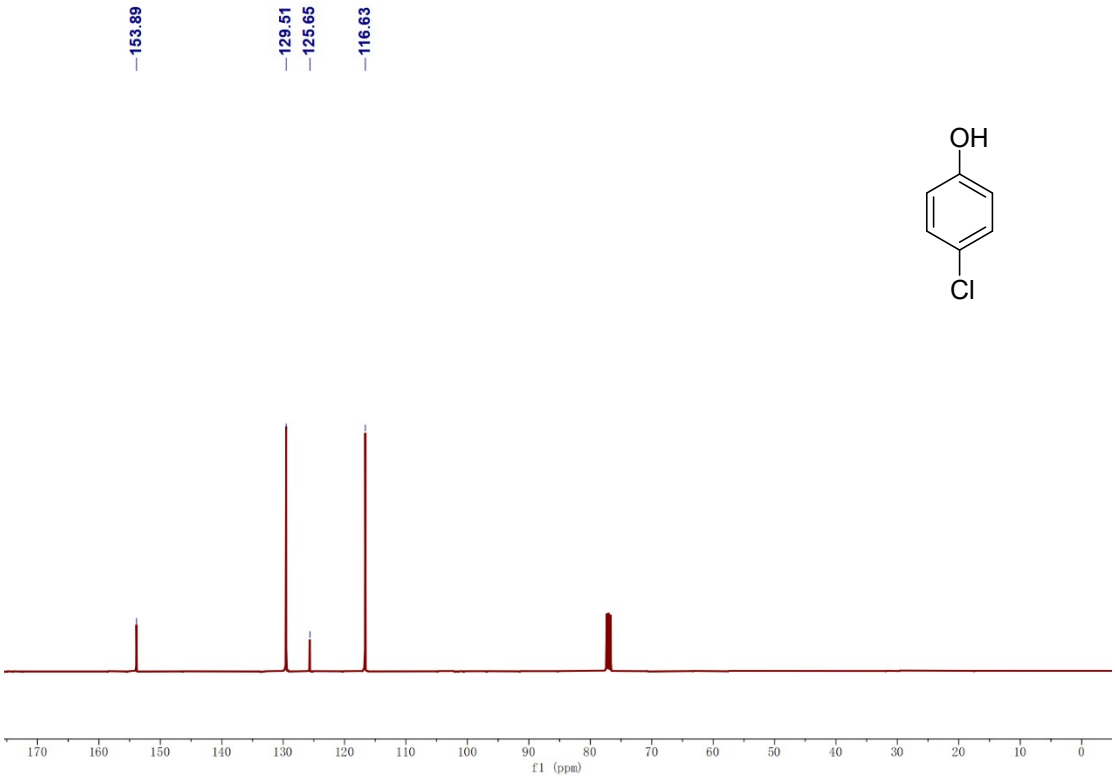


Fig. S50 ^{13}C NMR spectrum of **4e** in $CDCl_3$.

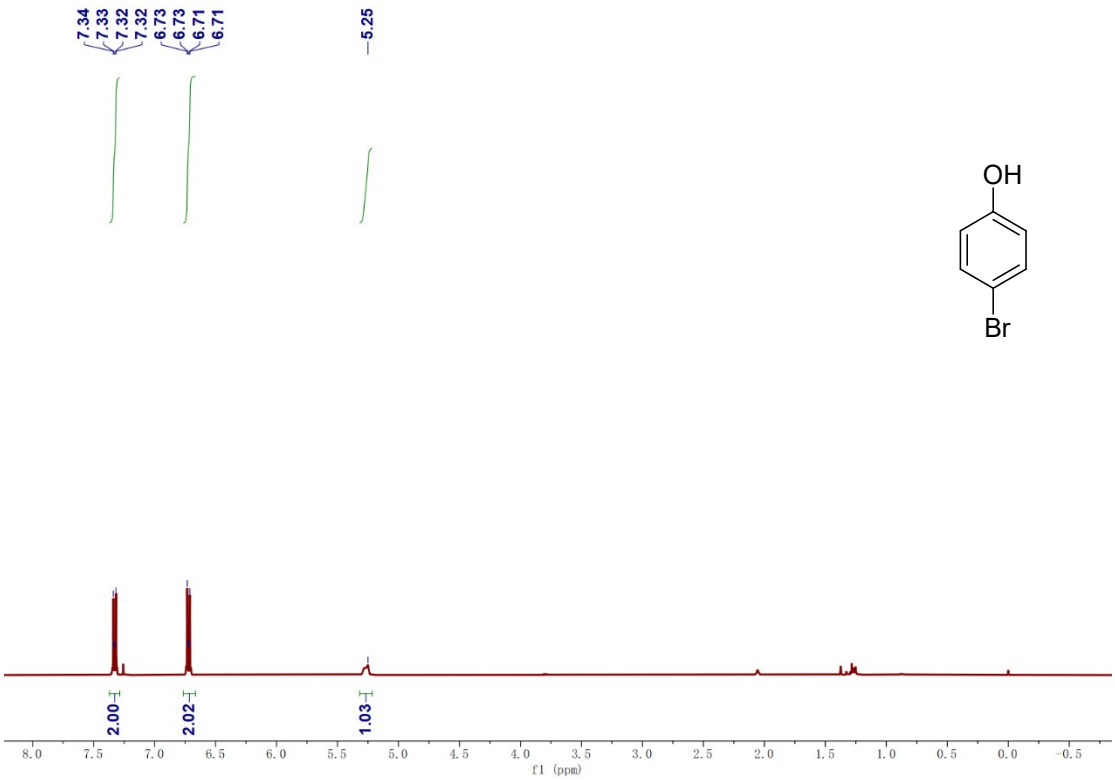


Fig. S51 ^{1}H NMR spectrum of **4f** in $CDCl_3$.

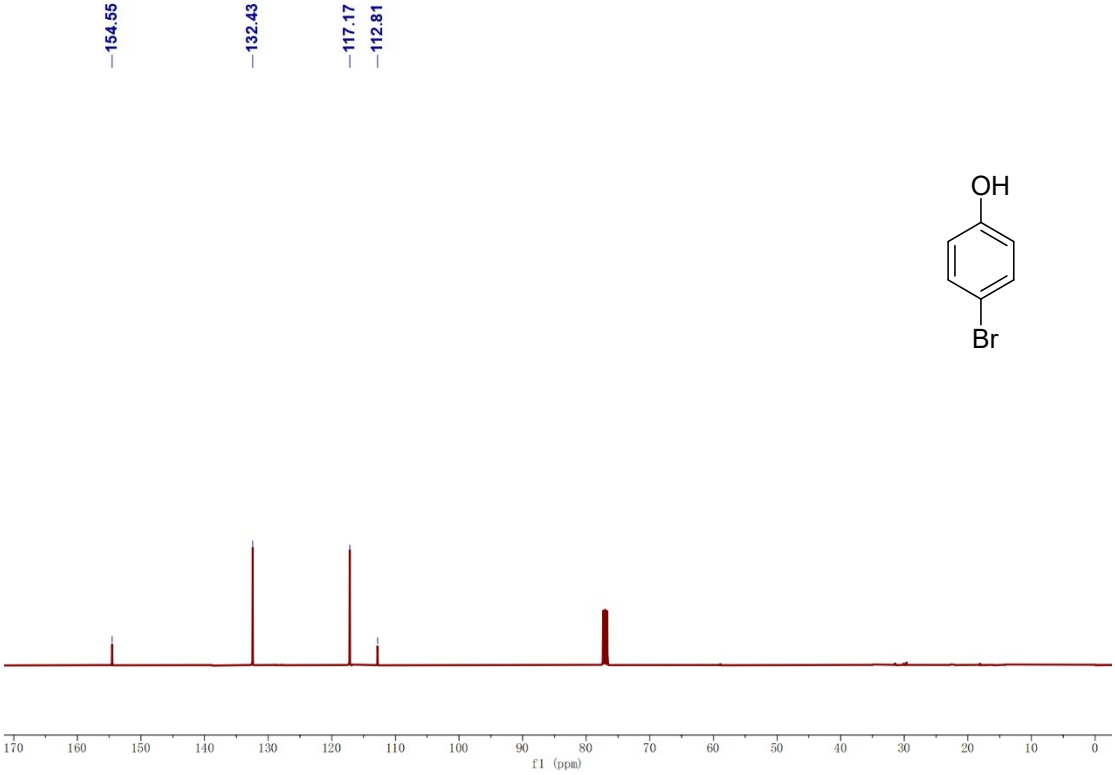


Fig. S52 ^{1}H NMR spectrum of **4f** in $CDCl_3$.

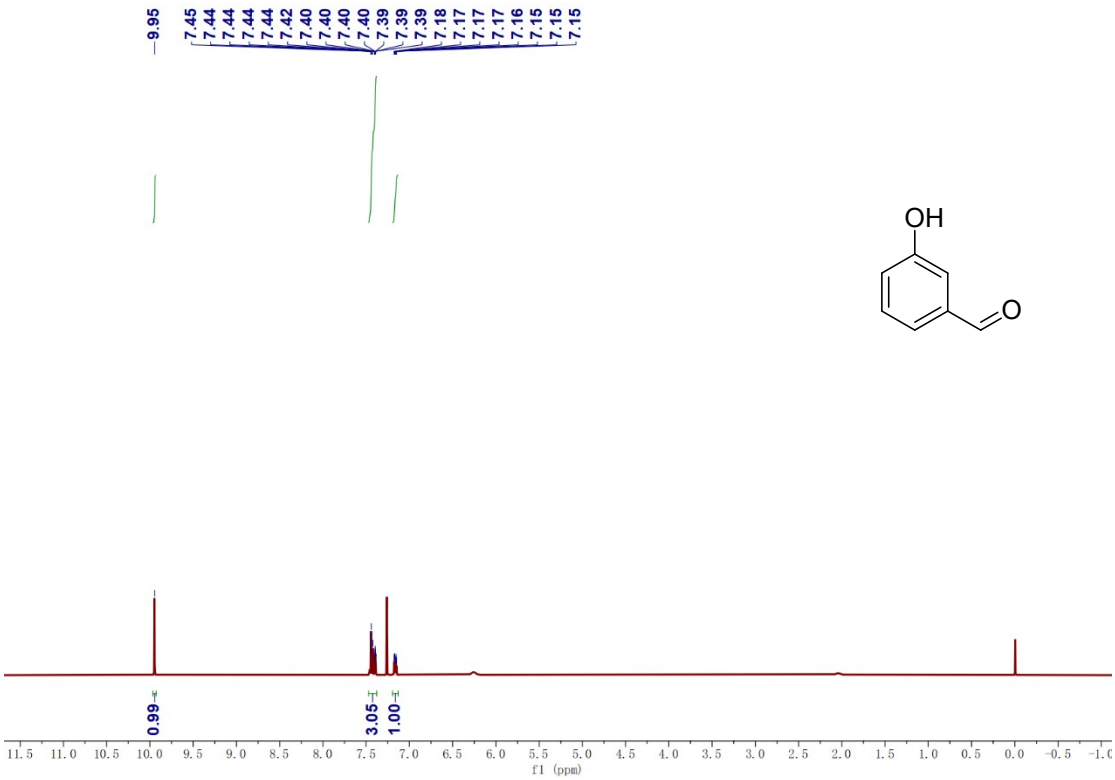


Fig. S53 ^{1}H NMR spectrum of **4g** in $CDCl_3$.

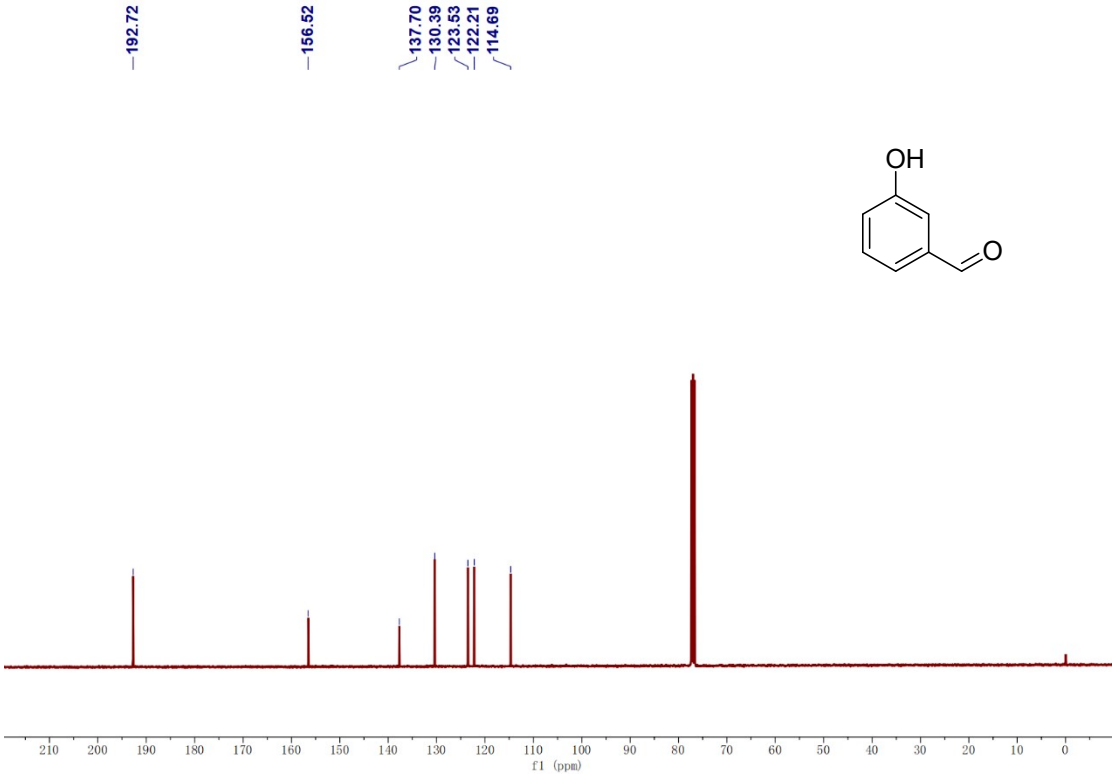


Fig. S54 ^{13}C NMR spectrum of **4g** in $CDCl_3$.

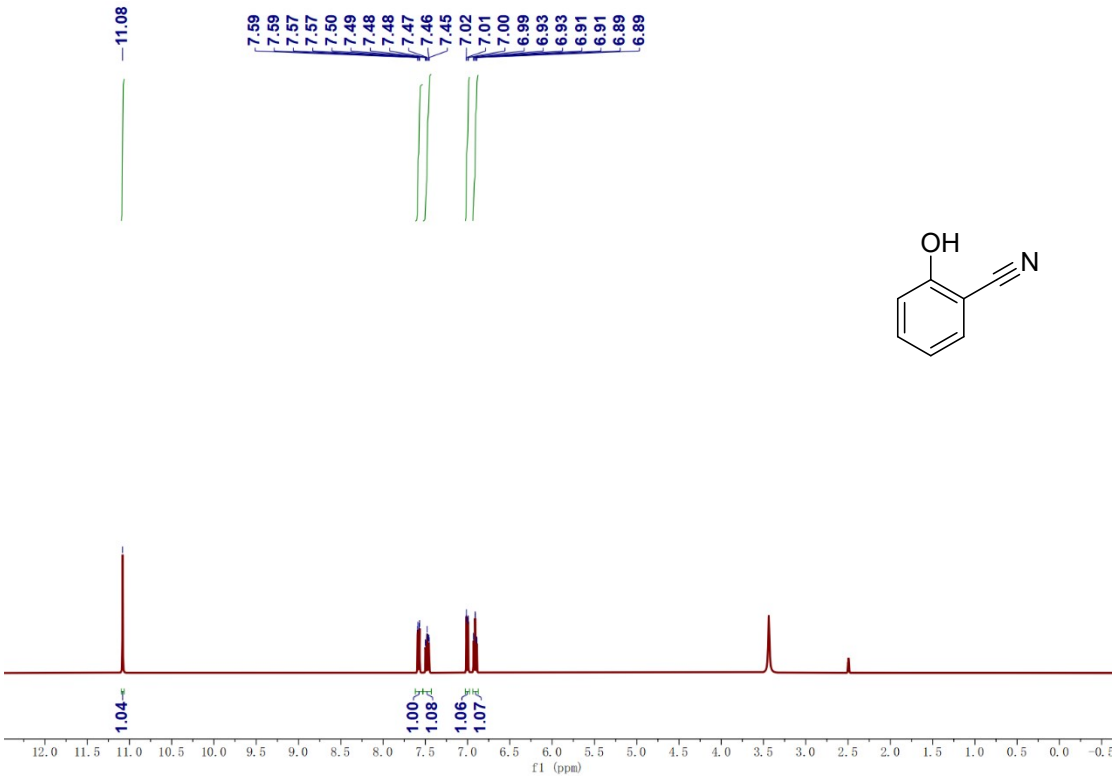


Fig. S55 ^{1}H NMR spectrum of **4h** in DMSO-d_6.

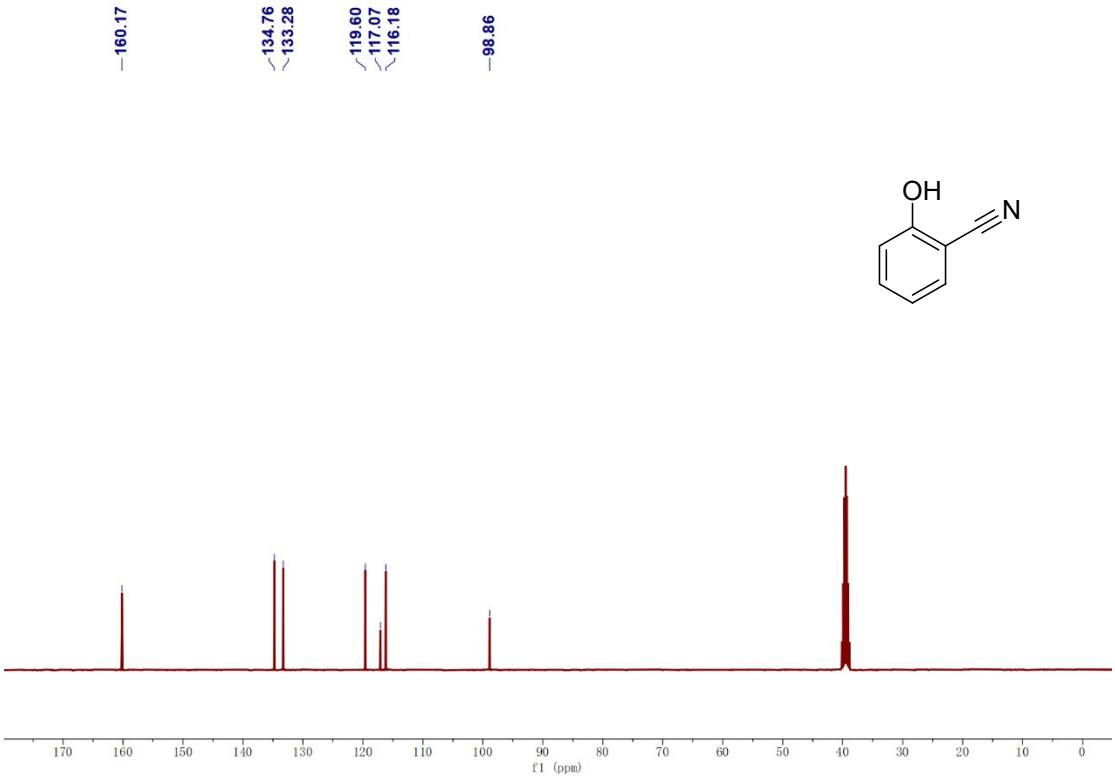


Fig. S56 ^{13}C NMR spectrum of **4h** in DMSO-d_6.

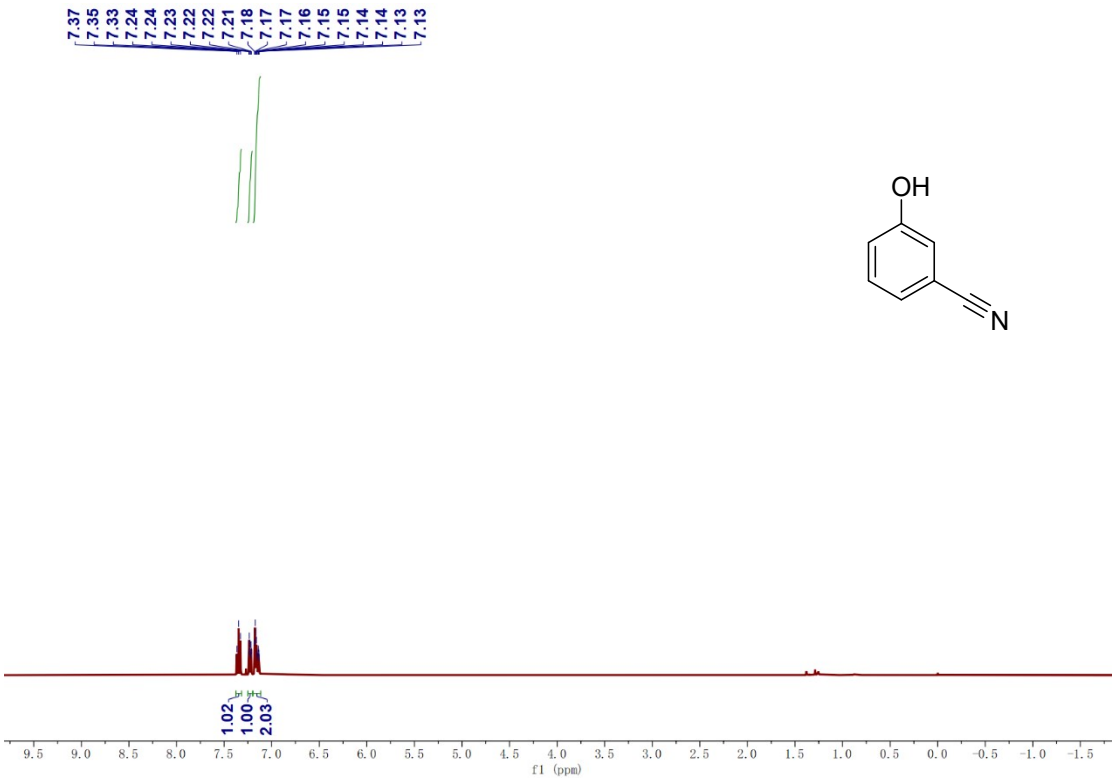


Fig. S57 ^{1}H NMR spectrum of **4i** in $CDCl_3$.

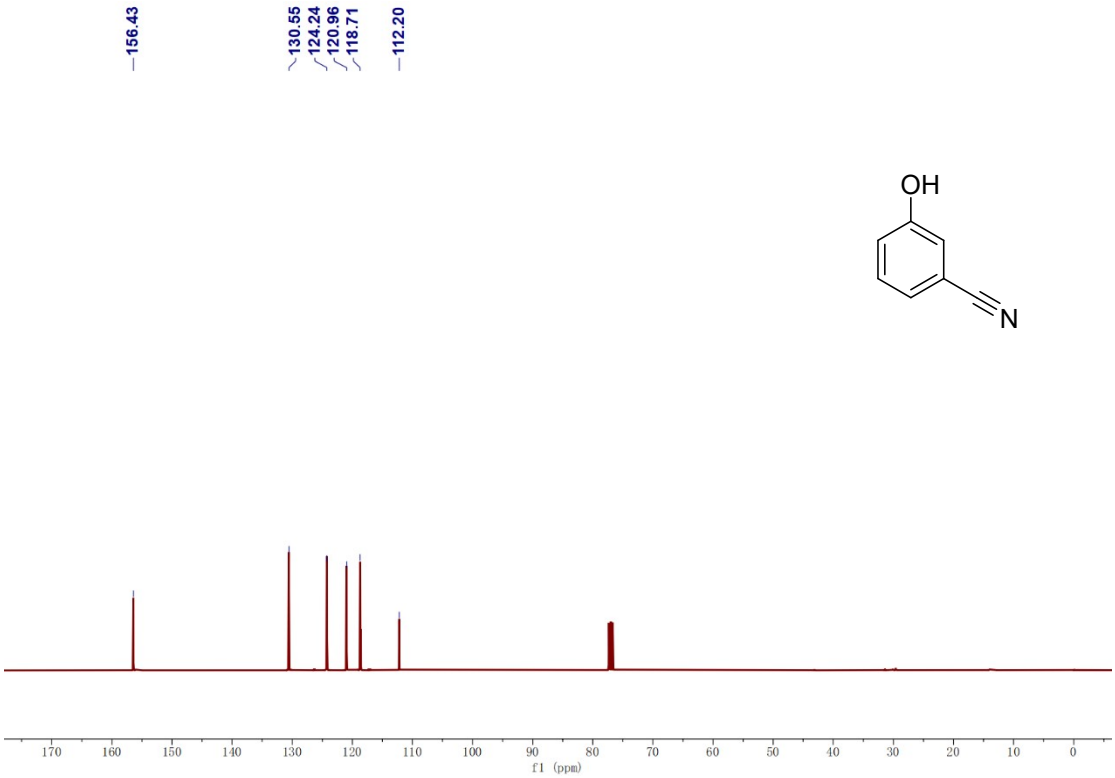


Fig. S58 ^{13}C NMR spectrum of **4i** in $CDCl_3$.

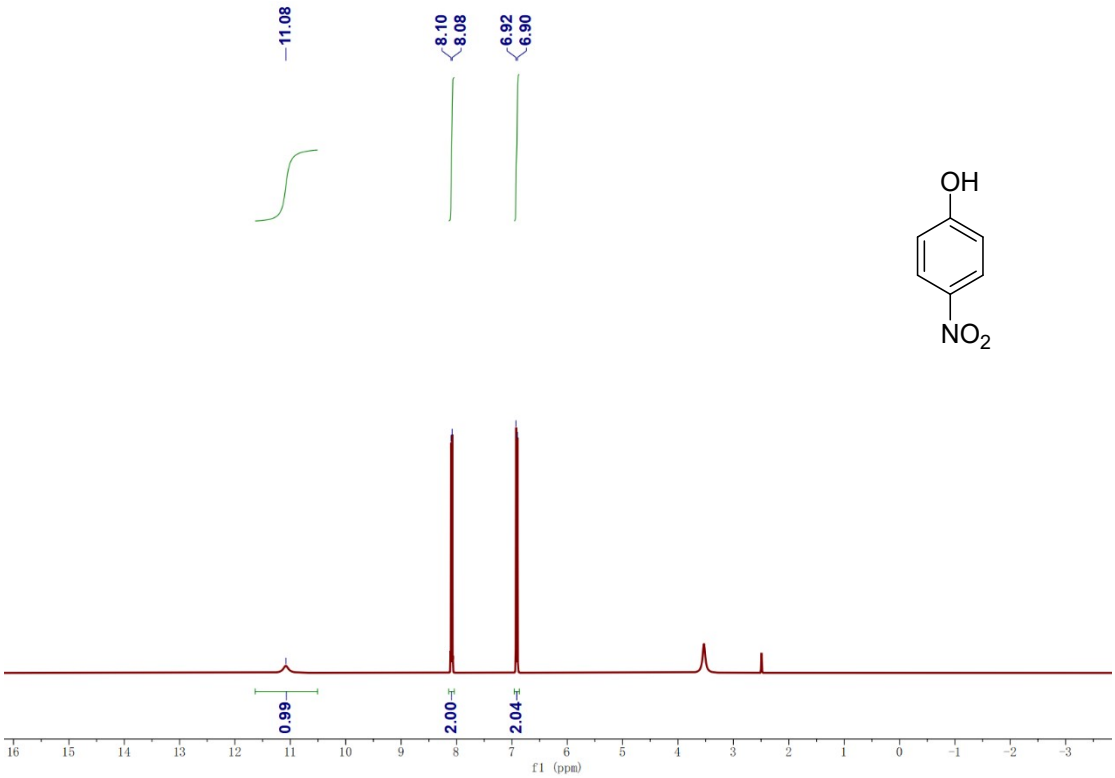


Fig. S59 ^{1}H NMR spectrum of **4j** in DMSO-d_6.

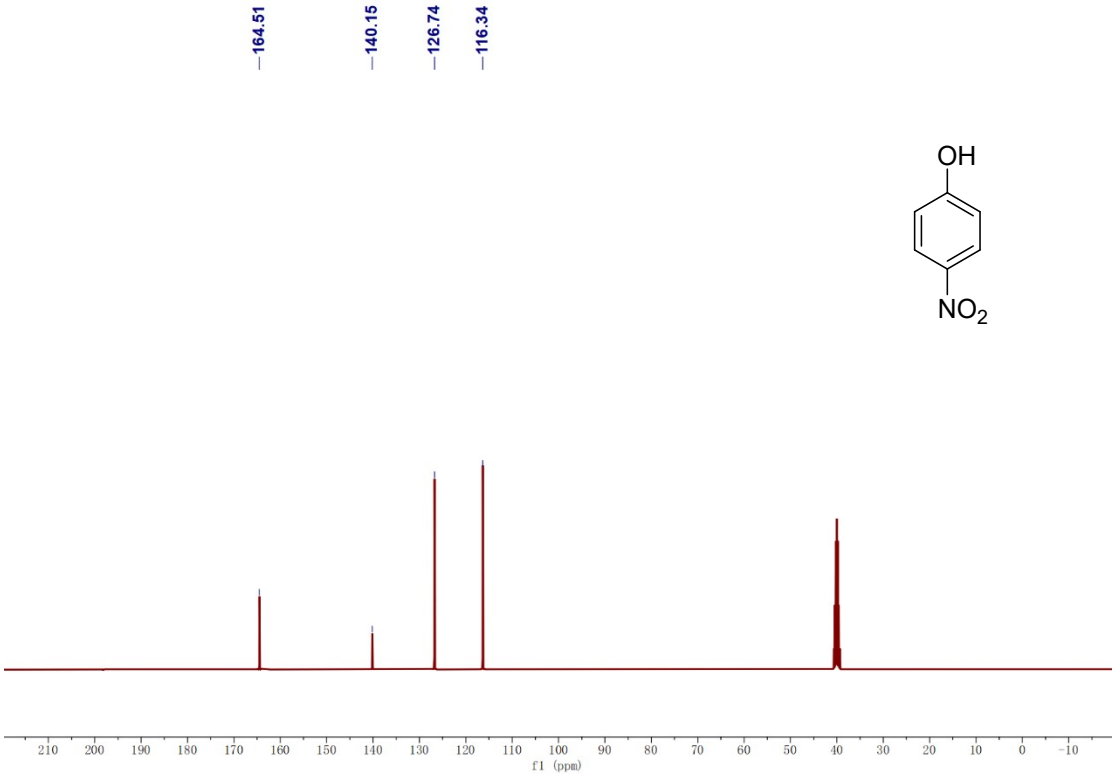


Fig. S60 ^{13}C NMR spectrum of **4j** in DMSO-d_6.

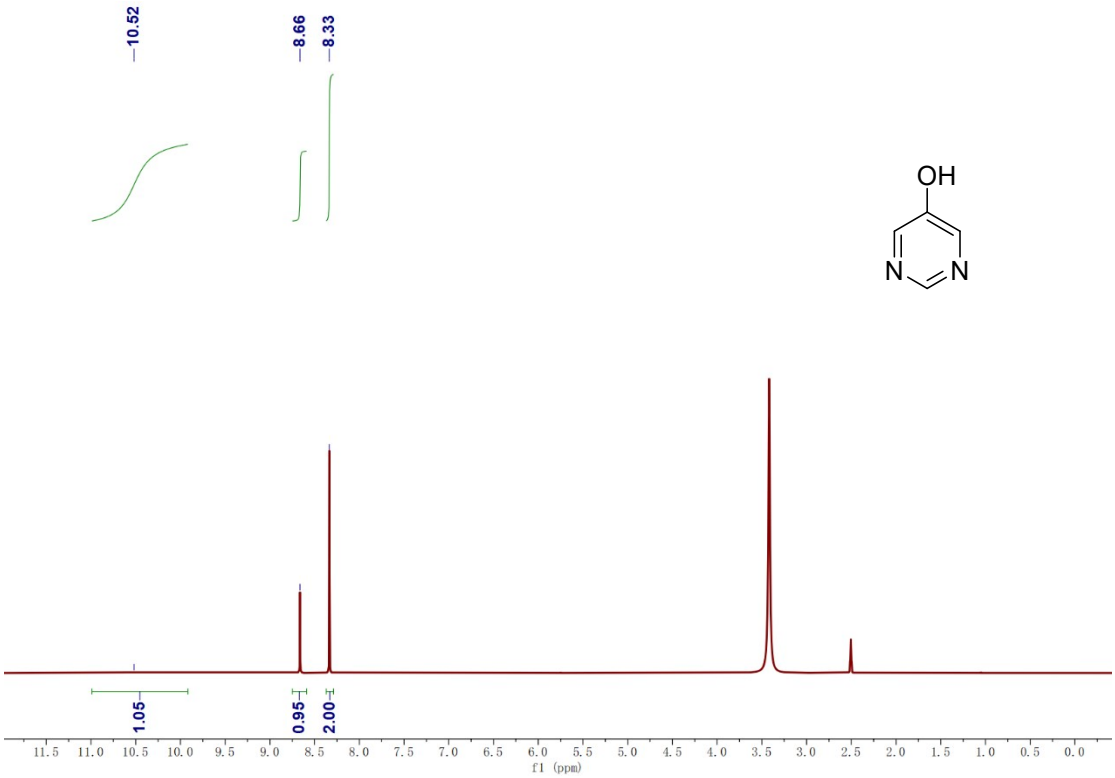


Fig. S61 ^{1}H NMR spectrum of **4k** in DMSO-d_6.

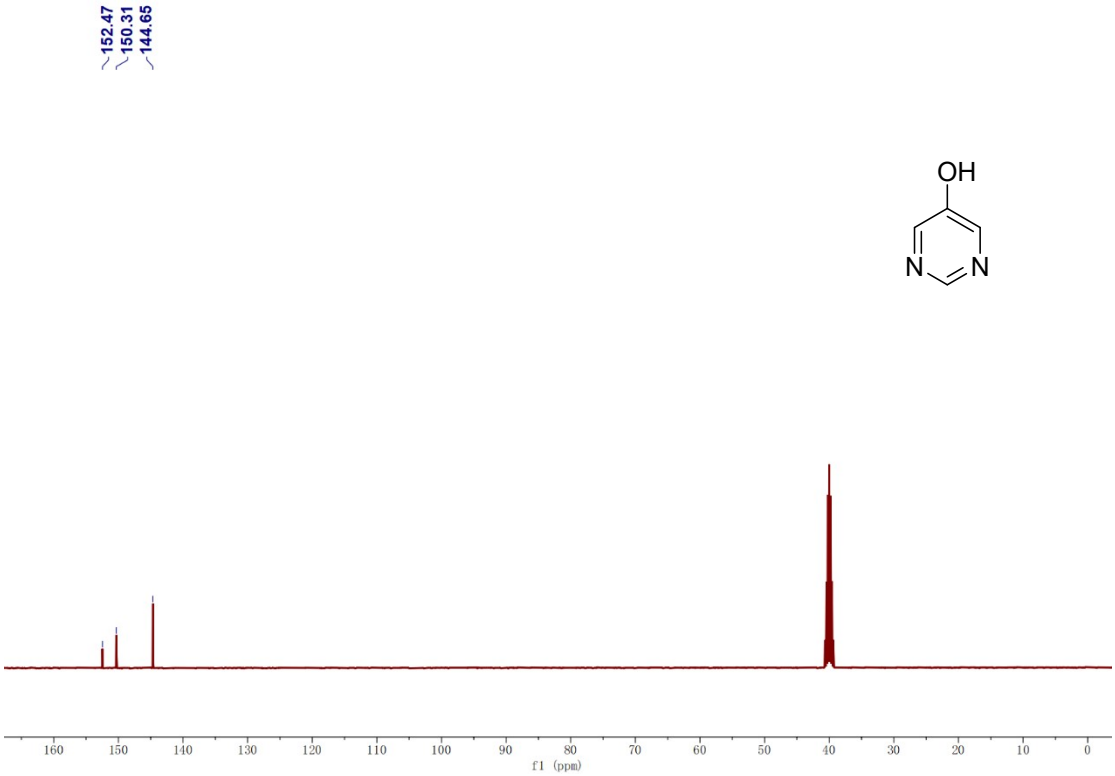


Fig. S62 ^{13}C NMR spectrum of **4k** in DMSO-d_6.

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