Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

## Transition-Metal-Free Decarboxylative Thiolation of Stable Aliphatic Carboxylates

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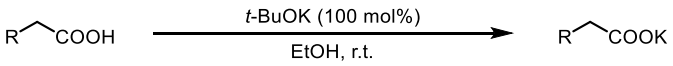
## 1. General Information

All reactions were carried out in oven-dried Schlenk tubes under argon atmosphere (purity≥99.999%) unless otherwise mentioned. Commercial reagents were purchased from Adamas-beta, TCI and Aldrich. Organic solutions were concentrated under reduced pressure on Buchi rotary evaporator. Flash column chromatographic purification of products was accomplished using forced-flow chromatography on Silica Gel (200-300 mesh).

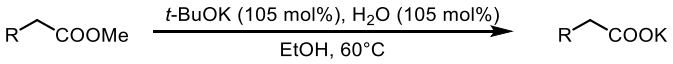
$^{1}$H-NMR and $^{13}$C-NMR spectra were recorded on a Bruker Avance 400 spectrometer at ambient temperature. Data for $^{1}$H-NMR are reported as follows: chemical shift (ppm, scale), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet and/or multiplet resonances, br = broad), coupling constant (Hz), and integration. Data for $^{13}$C- NMR are reported in terms of chemical shift (ppm, scale), multiplicity, and coupling constant (Hz). HRMS analysis was performed on Finnigan LCQ advantage Max Series MS System. ESI/EI-mass data were acquired using a Thermo LTQ Orbitrap XL Instrument equipped with an ESI/EI source and controlled by Xcalibur software.

## 2. Preparation of Substrates

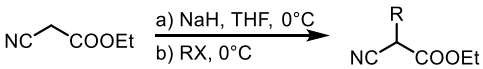
### 2.1 Preparation of Potassium Carboxylates [1]




**General procedure for the synthesis of potassium carboxylates from corresponding carboxylic acids:** A 100 mL, round-bottomed flask was charged with the substituted carboxylic acids (10.0 mmol) and ethanol (10 mL). To this, a solution of potassium tert-butoxide (10 mmol) in ethanol (10 mL) was added dropwise over 10 min. After completion of addition, the reaction mixture was stirred for another 1 h at room temperature. After removing the ethanol solvent by evaporation, 20 mL diethyl ether was added. The resulting solid was collected by filtration, washed sequentially with ethanol (1 mL x 2) and diethyl ether (10 mL x 2), transferred to a round-bottomed flask and dried under vacuum at 30°C for 2 h to provide the corresponding potassium carboxylates.

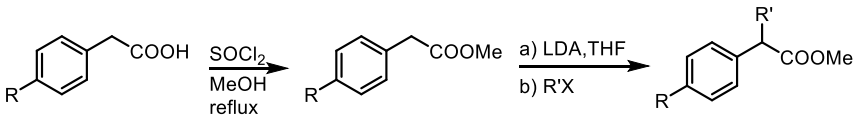



**General procedure for the synthesis of potassium carboxylates from corresponding methyl carboxylates:** A 100 mL, two-necked, round-bottomed flask was charged with the substituted methyl carboxylates (10.0 mmol), $H_2O$ (10.5 mmol) and ethanol (20 mL), the reaction mixture was stirred in 60°C oil bath. To this, a solution of potassium tert-butoxide (1.18g, 10.5 mmol) in ethanol (10 mL) was added dropwise over 30 min. After completion of addition, the reaction mixture was kept in 60°C oil bath until consumption of the starting material (monitored by TLC analysis). After cooling, the ethanol solvent was removed by evaporation and 20 mL diethyl ether was added. The resulting solid was collected by filtration, washed sequentially with ethanol (1 mL x 2) and diethyl ether (10 mL x 2), transferred to a round-bottomed flask and dried under vacuum at 30°C for 2 h to provide the corresponding potassium carboxylates.




**General procedure for the synthesis of 2-substituted cyanoacetate:** To an oven dried round

bottom flask charged with a stirring bar containing sodium hydride (60% dispersion in mineral oil, 19.9 mmol) was added ethyl cyanoacetate (6.8 g, 60 mmol) and THF (20 mL) under $N_2$, and the suspension was then cooled to 0 °C. To the suspension was slowly added sodium hydride (60% dispersion in mineral oil, 19.9 mmol) portion by portion. After 15 min, RX (20 mmol) were added dropwise via syringe to the solution. The resulting reaction mixture was allowed to stir at 0 °C for 3 h. The mixture was then quenched with $H_2O$ (30 mL) and diluted with $Et_2O$. The aqueous layer was removed and the organic layer was washed twice with brine. The combined aqueous layers were then extracted three times with $Et_2O$. The combined organic extracts were then dried over anhydrous $Na_2SO_4$ and the solvent was removed in vacuo. The residue was purified by silica gel column chromatography (petroleum ether /EtOAc = 15/1) to give 2-substituted ethyl cyanoacetate.

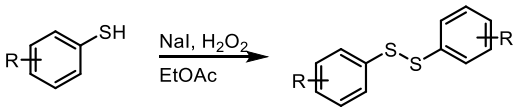



**General procedure for the synthesis of 2-substituted arylacetate:** To a solution of aryl acetic acid (15 mmol) in MeOH (30 mL) was added $SOCl_2$ (30 mmol). This mixture was heated to reflux for 3 h before evaporation. The residue was dissolved in DCM (30 mL), washed with aqueous $NaHCO_3$, water and brine, dried over anhydrous $Na_2SO_4$, and concentrated concentrated in vacuo. The residue was purified by silica gel column chromatography (petroleum ether /EtOAc 10/1) to give methyl arylacetate.

To a solution of diisopropylamine (0.5 mL, 3.6 mmol) in tetrahydrofuran (4 mL) was added n-butyllithium (1.52 M in hexane, 2.4 mL) at −78 °C under Ar, and the mixture was stirred for 30 min. Then a solution of methyl arylacetate (0.50 g, 3.0 mmol) in tetrahydrofuran (5 mL) was added dropwise, and the mixture was stirred for 20 min at the same temperature. The mixture was then allowed to warm to 0 °C. Methyl iodide (0.3 mL, 4.8 mmol) was added and the mixture was stirred for 30 min. The reaction mixture was acidified by 2 M hydrochloric acid and extracted with EtOAc. The organic layer was washed with brine, dried over anhydrous sodium sulfate, and concentrated in vacuo. The residue was purified by silica gel column chromatography (petroleum ether /EtOAc 10/1) to give 2-substituted arylacetate.

All potassium acetates shown in text are known compounds.

### 2.2 Preparation of disulfides[2]

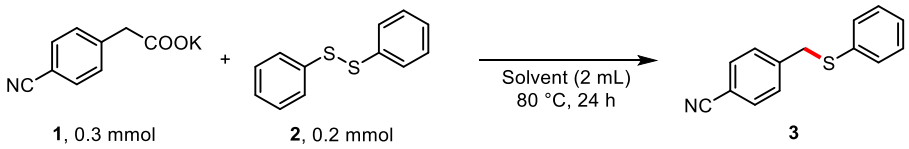



To a stirred solution of thiol (1.0 equiv.) in EtOAc (15 mL) at 0 °C was added sodium iodide (0.1 equiv.) and hydrogen peroxide (1.0 equiv.). The mixture was stirred at room temperature for 30 minutes. Saturated aqueous $Na_2S_2O_3$ (15 mL) was added, and the resulting mixture was extracted with EtOAc (3 x 15 mL). The combined organic phases were washed with brine (15 mL) and dried ($MgSO_4$). Subsequently the solvent was evaporated and the residue was purified by silica gel column chromatography (petroleum ether) to give disulfides.

All disulfides shown in text are known compounds.

## 3. Investigation of the Key Reaction Parameters

**Table S1: Screening of different solvents.**



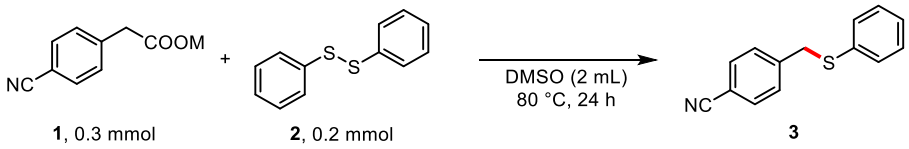

**1**, 0.3 mmol **2**, 0.2 mmol **3**

| Entry | Solvent | Yield of **3** (%)[a] |
|---|---|---|
| 1 | DMSO | 97 (95[b]) |
| 2 | DMF | 81 |
| 3 | DMA | 81 |
| 4 | MeCN | 7 |
| 5 | 1,4-dioxane | 0 |
| 6 | glyme | 0 |
| 7 | Diglyme | 0 |
| 8 | Mesitylene | 0 |
| 9 | DCE | 0 |

Reaction condition: Carboxylates (0.3 mmol), diphenyl disulfide (0.2 mmol), solvent (2 mL), 80 ℃, 24 h, under Ar.

[a] Determined by GC using diphenylmethane as internal standard. [b] Isolated yield.

**Table S2: Screening of different cation.**



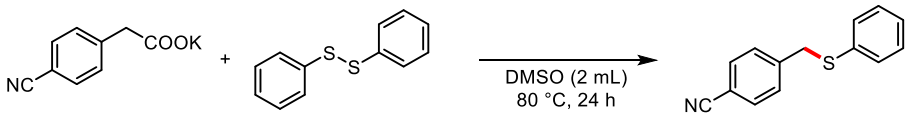

**1**, 0.3 mmol **2**, 0.2 mmol **3**

| Entry | M | Yield of **3** (%)[a] |
|---|---|---|
| 1 | H | 0 |
| 2 | Li | 72 |
| 3 | Na | 81 |
| 4 | K | 97 |
| 5 | Rb | 84 |
| 6 | Cs | 87 |
| 7[b] | Ca | 28 |

Reaction condition: Carboxylates (0.3 mmol), diphenyl disulfide (0.2 mmol), DMSO (2 mL), 80 ℃, 24 h, under Ar.

[a] Determined by GC using diphenylmethane as internal standard. [b] 0.15 mmol ($p$-$CNC_6H_5CH_2CO_2)_2Ca$ instead of **1**

**Table S3: Screening of other parameters.**




**1**, 0.3 mmol **2**, 0.2 mmol **3**

| entry | variations from above conditions | Yield of **3** (%)[a] |
|---|---|---|
| 1 | carried out at 25 ℃ | 14 |
| 2 | carried out at 40 ℃ | 27 |
| 3 | carried out at 60 ℃ | 52 |
| 4 | carried out at 80 ℃ | 97 |
| 5 | carried out at 100 ℃ | 81 |
| 6 | carried out at 120 ℃ | 56 |
| 7 | carried out at 150 ℃ | 17 |
| 8 | added 0.2 mmol $H_2O$ | 65 |
| 9 | added 20 mol% $NBu_4^+PF_6^-$ | 85 |
| 10 | added 20 mol% $NBu_4^+I^-$ | 77 |
| 11 | added 20 mol% $NBu_4^+Br^-$ | 89 |
| 12 | added 20 mol% $NBu_4^+F^-$ | 83 |
| 13 | 0.2 mmol **1** | 74 |
| 14 | 0.4 mmol **1** | 98 |
| 15 | 0.2 mmol **1** + 0.3 mmol **2** | 69 |

Reaction condition: Carboxylates (0.3 mmol), diphenyl disulfide (0.2 mmol), DMSO (2 mL), 80 ℃, 24 h, under Ar.

[a] Determined by GC using diphenylmethane as internal standard.

## 4. Experimental Procedures and Spectral Data

### 4.1 General procedure for C–S coupling of potassium carboxylates and disulfides.

**General procedure A:** Potassium carboxylates (0.3 mmol, 1.5 equiv.) and disulfides (0.2 mmol, 1.0 equiv.) were placed in a transparent Schlenk tube equipped with a stirring bar. The tube was evacuated and filled with argon (repeated for three times). To these solids, anhydrous DMSO (2.0 mL) were added via a gastight syringe under argon atmosphere. The reaction mixture was stirred at 80°C for 24 h. The mixture was then quenched with saturated NaCl solution and extracted with ethyl acetate (3 × 10 mL). The organic layers were combined and concentrated by evaporation. The product was purified by flash column chromatography on silica gel (petroleum ether : ethyl acetate = 30:1~3:1).

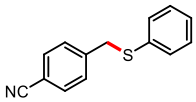
**General procedure B:** Potassium carboxylates (0.3 mmol, 1.5 equiv.) and disulfides (0.2 mmol, 1.0 equiv.) were placed in a transparent Schlenk tube equipped with a stirring bar. The tube was evacuated and filled with argon (repeated for three times). To these solids, anhydrous DMF (2.0 mL) were added via a gastight syringe under argon atmosphere. The reaction mixture was stirred at 150°C for 24 h. The mixture was then quenched with saturated NaCl solution and extracted with ethyl acetate (3 × 10 mL). The organic layers were combined and concentrated by evaporation. The product was purified by flash column chromatography on silica gel (petroleum ether : ethyl acetate = 30:1~3:1).

**General procedure C:** Potassium carboxylates (0.3 mmol, 1.5 equiv.), disulfides (0.2 mmol, 1.0 equiv.) and 18-crown-6 (0.3 mmol, 1.5 equiv.) were placed in a transparent Schlenk tube equipped with a stirring bar. The tube was evacuated and filled with argon (repeated for three times). To these solids, anhydrous DMF (2.0 mL) were added via a gastight syringe under argon atmosphere. The reaction mixture was stirred at 150 °C for 24 h. The mixture was then quenched with saturated NaCl solution and extracted with ethyl acetate (3 × 10 mL). The organic layers were combined and concentrated by evaporation. The product was purified by flash column chromatography on silica gel (petroleum ether : ethyl acetate = 30:1~3:1).

### 4.2 General procedure for C–Se coupling of potassium carboxylates and diselenides.

**General procedure D:** Potassium carboxylates (0.3 mmol, 1.5 equiv.) and diselenides (0.2 mmol, 1.0 equiv.) were placed in a transparent Schlenk tube equipped with a stirring bar. The tube was evacuated and filled with argon (repeated for three times). To these solids, anhydrous DMSO (2.0 mL) were added via a gastight syringe under argon atmosphere. The reaction mixture was stirred at 80 °C for 24 h. The mixture was then quenched with saturated NaCl solution and extracted with ethyl acetate (3 × 10 mL). The organic layers were combined and concentrated by evaporation. The product was purified by flash column chromatography on silica gel (petroleum ether : ethyl acetate = 30:1~3:1).

## 4.3 Spectral Data.

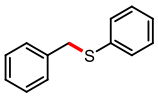


**4-((phenylthio)methyl)benzonitrile (3):** Following the general procedure A, obtained in 95% yield as a colorless oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 7.28 – 7.16 (m, 5H), 4.09 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 143.4, 134.8, 132.3, 130.9, 129.5, 129.1, 127.2, 118.8, 111.0, 39.2.

**HRMS** (EI) Calcd for $C_{14}H_{11}NS^+$ $[M]^+$: 225.0607, found: 225.0605.

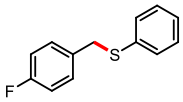


**benzyl(phenyl)sulfane (4):** Following the general procedure B, obtained in 76% yield as a colorless oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.34 – 7.19 (m, 9H), 7.19 – 7.13 (m, 1H), 4.10 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 137.5, 136.4, 129.9, 128.9, 128.9, 128.5, 127.2, 126.4, 39.1.

**HRMS** (EI) Calcd for $C_{13}H_{12}S^+$ $[M]^+$: 200.0654, found: 200.0654.



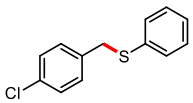
**(4-fluorobenzyl)(phenyl)sulfane (5):** Following the general procedure C, obtained in 74% yield as a colorless oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.17 (m, 7H), 7.00 – 6.90 (m, 2H), 4.06 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 162.0 (d, *J* = 245.5 Hz), 135.9, 133.3 (d, *J* = 2.9 Hz), 130.4 (d, *J* = 8.0 Hz), 130.2, 128.9, 126.6, 115.4 (d, *J* = 21.3 Hz), 38.5.

**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -115.38 (s).

**HRMS** (EI) Calcd for $C_{13}H_{11}FS^+$ $[M]^+$: 218.0560, found: 218.0559.

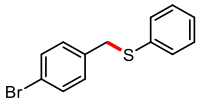


**(4-chlorobenzyl)(phenyl)sulfane (6):** Following the general procedure B, obtained in 83% yield as a colorless oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.41 – 7.06 (m, 9H), 4.05 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 136.2, 135.7, 133.0, 131.3, 130.1, 128.9, 128.6, 126.7, 38.6.

**HRMS** (EI) Calcd for $C_{13}H_{11}ClS^+$ $[M]^+$: 234.0265, found: 234.0264.

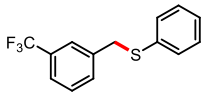


**(4-bromobenzyl)(phenyl)sulfane (7):** Following the general procedure B, obtained in 75% yield as a colorless oil.

**$^1$H NMR** (500 MHz, $CDCl_3$) δ 7.41 – 7.36 (m, 2H), 7.30 – 7.24 (m, 4H), 7.22 – 7.16 (m, 1H), 7.13 (d, *J* = 8.3 Hz, 2H), 4.04 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 136.7, 135.6, 131.6, 130.5, 130.3, 128.9, 126.7, 121.1, 38.6.

**HRMS** (EI) Calcd for $C_{13}H_{11}BrS^+$ $[M]^+$: 277.9759, found: 277.9761.



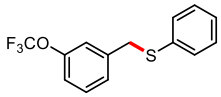

**phenyl(3-(trifluoromethyl)benzyl)sulfane (8):** Following the general procedure B, obtained in 81% yield as a colorless liquid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.51 – 7.41 (m, 3H), 7.40 – 7.35 (m, 1H), 7.30 – 7.18 (m, 5H), 4.11 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 138.7, 135.2, 132.1, 130.8 (q, *J* = 32.1 Hz), 130.8, 129.0, 128.9, 127.0, 125.6 (q, *J* = 3.8 Hz), 124.0 (q, *J* = 272.2 Hz), 124.0 (q, *J* = 3.7 Hz), 39.1.

**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -62.66 (s).

**HRMS** (EI) Calcd for $C_{14}H_{11}F_3S^+$ $[M]^+$: 268.0528, found: 268.0529.



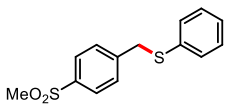

**phenyl(3-(trifluoromethoxy)benzyl)sulfane (9):** Following the general procedure B, obtained in 79% yield as a light yellow liquid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.18 (m, 7H), 7.12 – 7.04 (m, 2H), 4.08 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 138.7, 135.2, 132.1, 130.8 (q, *J* = 32.1 Hz), 130.8, 129.0, 128.9, 127.0, 125.6 (q, *J* = 3.8 Hz), 124.0 (q, *J* = 272.2 Hz), 124.0 (q, *J* = 3.7 Hz), 39.1.

**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -62.66 (s).

**HRMS** (EI) Calcd for $C_{14}H_{11}F_3S^+$ $[M]^+$: 268.0528, found: 268.0529.

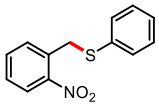



**(4-(methylsulfonyl)benzyl)(phenyl)sulfane (10):** Following the general procedure A, obtained in 82% yield as a light yellow solid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.3 Hz, 2H), 7.44 (d, *J* = 8.3 Hz, 2H), 7.30 – 7.21 (m, 5H), 4.14 (s, 2H), 3.03 (s, 3H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 144.4, 139.2, 134.8, 130.7, 129.7, 129.1, 127.6, 127.4 (d, *J* = 56.9 Hz), 44.5, 38.9.

**HRMS** (EI) Calcd for $C_{14}H_{14}O_2S_2^+$ $[M]^+$: 278.0430, found: 278.0428.

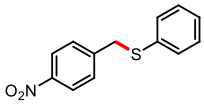


**(2-nitrobenzyl)(phenyl)sulfane (11):** Following the general procedure A, obtained in 75% yield as a colorless liquid.

**$^1$H NMR** (500 MHz, $CDCl_3$) δ 7.97 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.43 (td, *J* = 7.5, 1.3 Hz, 1H), 7.37 (td, *J* = 7.9, 1.4 Hz, 1H), 7.30 – 7.19 (m, 6H), 4.43 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 148.5, 134.7, 133.5, 133.0, 131.9, 131.8, 129.0, 128.2, 127.4, 125.2, 37.2.

**HRMS** (EI) Calcd for $C_{13}H_{11}NO_2S^+$ $[M]^+$: 245.0505, found: 245.0505.

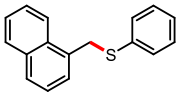


**(4-nitrobenzyl)(phenyl)sulfane (12):** Following the general procedure A, obtained in 73% yield as a colorless liquid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.16 – 8.05 (m, 2H), 7.41 – 7.35 (m, 2H), 7.30 – 7.21 (m, 5H), 4.13 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 147.1, 145.6, 134.5, 131.0, 129.6, 129.1, 127.3, 123.7, 39.0.

**HRMS** (EI) Calcd for $C_{13}H_{11}NO_2S^+$ $[M]^+$: 245.0505, found: 245.0506.

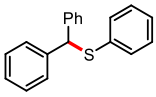


**(naphthalen-1-ylmethyl)(phenyl)sulfane (13):** Following the general procedure B, obtained in 72% yield as a colorless liquid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.2 Hz, 1H), 7.89 – 7.81 (m, 1H), 7.79 – 7.71 (m, 1H), 7.59 – 7.45 (m, 2H), 7.37 – 7.29 (m, 4H), 7.28 – 7.22 (m, 2H), 7.21 – 7.16 (m, 1H), 4.54 (d, *J* = 0.9 Hz, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 136.7, 134.0, 132.8, 131.5, 130.2, 128.9, 128.8, 128.3, 127.4, 126.5, 126.3, 125.9, 125.3, 123.9, 37.2.

**HRMS** (EI) Calcd for $C_{17}H_{14}S^+$ $[M]^+$: 250.0811, found: 250.0810.

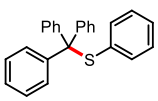


**benzhydryl(phenyl)sulfane (14):** Following the general procedure A, obtained in 93% yield as a colorless liquid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.44 – 7.36 (m, 4H), 7.31 – 7.25 (m, 4H), 7.24 – 7.18 (m, 4H), 7.18 – 7.08 (m, 3H), 5.53 (s, 1H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 141.1, 136.2, 130.6, 128.8, 128.6, 128.5, 127.3, 126.6, 57.5.

**HRMS** (EI) Calcd for $C_{19}H_{16}S^+$ $[M]^+$: 276.0967, found: 276.0969.



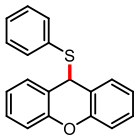
**phenyl(trityl)sulfane (15):** Following the general procedure A, obtained in 97% yield as a colorless oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.43 – 7.38 (m, 6H), 7.24 – 7.15 (m, 9H), 7.12 – 7.05 (m, 1H), 7.00 –

6.92 (m, 4H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 144.6, 134.6, 134.5, 130.1, 128.1, 128.0, 127.7, 126.7, 70.8.

**HRMS** (EI) Calcd for $C_{25}H_{20}S^+$ $[M]^+$: 352.1280, found: 352.1282.

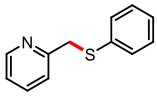


**9-(phenylthio)-9H-xanthene (16):** Following the general procedure C, obtained in 98% yield as a colorless oil. (obtained in 52% yield following the general procedure A)

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.29 – 7.23 (m, 3H), 7.21 – 7.15 (m, 2H), 7.13 – 7.06 (m, 2H), 7.06 – 7.00 (m, 2H), 6.97 – 6.82 (m, 4H), 5.48 (s, 1H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 152.2, 136.4, 131.4, 129.6, 128.9, 128.5, 128.4, 123.2, 121.3, 116.3, 47.7.

**HRMS** (EI) Calcd for $C_{19}H_{14}OS^+$ $[M]^+$: 290.0760, found: 290.0760.

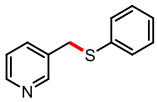


**2-((phenylthio)methyl)pyridine (17):** Following the general procedure A, obtained in 81% yield as a light yellow liquid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.53 (d, $J$ = 4.5 Hz, 1H), 7.58 (td, $J$ = 7.7, 1.7 Hz, 1H), 7.32 (t, $J$ = 7.2 Hz, 3H), 7.27 – 7.20 (m, 2H), 7.19 – 7.09 (m, 2H), 4.26 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 157.7, 149.3, 136.7, 135.8, 129.7, 128.9, 126.4, 123.0, 122.1, 40.5.

**HRMS** (ESI) Calcd for $C_{12}H_{12}NS^+$ $[M+H]^+$: 202.0685, found: 202.0681.

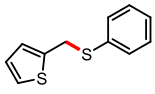


**3-((phenylthio)methyl)pyridine (18):** Following the general procedure B, obtained in 86% yield as a light yellow liquid. (obtained in 60% yield following the general procedure A)

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.49 – 8.42 (m, 2H), 7.58 (d, $J$ = 7.8 Hz, 1H), 7.35 – 7.12 (m, 6H), 4.07 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 149.9, 148.5, 136.3, 134.9, 133.5, 130.8, 129.0, 127.1, 123.4, 36.6.

**HRMS** (ESI) Calcd for $C_{12}H_{12}NS^+$ $[M+H]^+$: 202.0685, found: 202.0686.

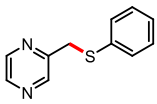


**2-((phenylthio)methyl)thiophene (19):** Following the general procedure A, obtained in 98% yield as a yellow oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.36 – 7.31 (m, 2H), 7.28 – 7.22 (m, 2H), 7.22 – 7.18 (m, 1H), 7.18 – 7.12 (m, 1H), 6.89 – 6.82 (m, 2H), 4.29 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 140.9, 135.7, 130.4, 129.0, 126.8, 126.8, 126.3, 125.0, 33.8.

**HRMS** (EI) Calcd for $C_{11}H_{10}S_2^+$ $[M]^+$: 206.0218, found: 206.0216.

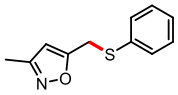


**2-((phenylthio)methyl)pyrazine (20):** Following the general procedure A, obtained in 85% yield as a brown oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.55 – 8.36 (m, 3H), 7.40 – 7.15 (m, 5H), 4.24 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 153.8, 144.7, 144.0, 143.0, 134.5, 130.7, 129.1, 127.1, 38.4.

**HRMS** (ESI) Calcd for $C_{11}H_{11}N_2S^+$ $[M+H]^+$: 203.0638, found: 203.0636.

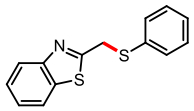


**3-methyl-5-((phenylthio)methyl)isoxazole (21):** Following the general procedure A, obtained in 88% yield as a light yellow liquid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.37 – 7.20 (m, 5H), 5.90 (s, 1H), 4.09 (s, 2H), 2.22 (s, 3H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 169.0, 160.0, 134.5, 130.5, 129.1, 127.3, 103.4, 29.5, 11.5.

**HRMS** (ESI) Calcd for $C_{11}H_{12}ONS^+$ $[M+H]^+$: 206.0634, found: 206.0632.

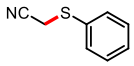


**2-((phenylthio)methyl)benzo[d]thiazole (22):** Following the general procedure A, obtained in 78% yield as a brown oil.

**$^1$H NMR** (500 MHz, $CDCl_3$) δ 7.95 (d, $J$ = 8.1 Hz, 1H), 7.82 (dd, $J$ = 8.0, 0.5 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.40 (dd, $J$ = 8.3, 1.1 Hz, 2H), 7.38 – 7.33 (m, 1H), 7.29 – 7.23 (m, 3H), 7.22 – 7.17 (m, 1H), 4.52 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 170.1, 153.1, 135.7, 134.5, 129.9, 129.2, 127.1, 126.1, 125.2, 122.9, 121.7, 36.9.

**HRMS** (ESI) Calcd for $C_{14}H_{12}NS_2^+$ $[M+H]^+$: 258.0406, found: 258.0403.

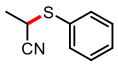


**2-(phenylthio)acetonitrile (23):** Following the general procedure A, obtained in 72% yield as a light yellow liquid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.60 – 7.51 (m, 2H), 7.43 – 7.34 (m, 3H), 3.57 (s, 2H).

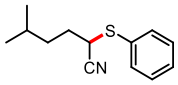
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 132.5, 132.1, 129.6, 129.0, 116.5, 21.4.

**HRMS** (EI) Calcd for $C_8H_7NS^+$ $[M]^+$: 149.0294, found: 149.0293.

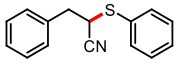


**2-(phenylthio)propanenitrile (24):** Following the general procedure A, obtained in 81% yield as a light yellow oil.

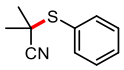
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.66 – 7.57 (m, 2H), 7.44 – 7.36 (m, 3H), 3.80 (q, *J* = 7.3 Hz, 1H), 1.60 (d, *J* = 7.3 Hz, 3H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 136.8, 130.3, 129.9, 129.3, 122.5, 39.8, 27.6.
**HRMS** (EI) Calcd for $C_9H_9NS^+$ $[M]^+$: 163.0450, found: 163.0449.



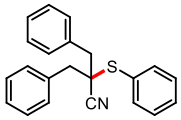

**5-methyl-2-(phenylthio)hexanenitrile (25):** Following the general procedure A, obtained in 77% yield as a colorless liquid.
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.69 – 7.53 (m, 2H), 7.47 – 7.33 (m, 3H), 3.66 (t, *J* = 7.3 Hz, 1H), 1.88 – 1.80 (m, 2H), 1.63 – 1.55 (m, 1H), 1.50 – 1.43 (m, 2H), 0.91 (dd, *J* = 6.6, 1.6 Hz, 6H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 134.5, 130.9, 129.4, 119.4, 37.4, 36.0, 30.5, 27.6, 22.4, 22.3. (one carbon signal is overlapped)
**HRMS** (EI) Calcd for $C_{13}H_{17}NS^+$ $[M]^+$: 219.1076, found: 219.1075.



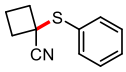

**3-phenyl-2-(phenylthio)propanenitrile (26):** Following the general procedure A, obtained in 93% yield as a light yellow liquid.
**$^1$H NMR** (500 MHz, $CDCl_3$) δ 7.65 – 7.56 (m, 2H), 7.42 – 7.37 (m, 3H), 7.36 – 7.31 (m, 2H), 7.31 – 7.27 (m, 1H), 7.26 – 7.22 (m, 2H), 3.88 (dd, *J* = 9.1, 6.1 Hz, 1H), 3.10 (ddd, *J* = 23.0, 13.9, 7.6 Hz, 2H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 135.7, 134.7, 130.6, 129.7, 129.6, 129.2, 128.9, 127.8, 118.6, 38.9. (one carbon signal is overlapped)
**HRMS** (EI) Calcd for $C_{15}H_{13}NS^+$ $[M]^+$: 239.0763, found: 239.0761.




**2-methyl-2-(phenylthio)propanenitrile (27):** Following the general procedure B, obtained in 83% yield as a light yellow liquid.
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.81 – 7.60 (m, 2H), 7.53 – 7.37 (m, 3H), 1.61 (s, 6H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 136.8, 130.3, 129.9, 129.3, 122.5, 39.8, 27.6.
**HRMS** (EI) Calcd for $C_{10}H_{11}NS^+$ $[M]^+$: 177.0607, found: 177.0604.




**2-benzyl-3-phenyl-2-(phenylthio)propanenitrile (28):** Following the general procedure A, obtained in 95% yield as a colorless oil.
**$^1$H NMR** (500 MHz, $CDCl_3$) δ 7.67 – 7.62 (m, 2H), 7.47 – 7.42 (m, 1H), 7.41 – 7.37 (m, 2H), 7.35 – 7.28 (m, 10H), 3.04 (dd, *J* = 47.9, 13.9 Hz, 4H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 137.1, 134.3, 130.6, 130.3, 129.3, 129.2, 128.5, 127.8, 120.3, 50.3, 44.6.
**HRMS** (EI) Calcd for $C_{22}H_{19}NS^+$ $[M]^+$: 329.1233, found: 329.1232.

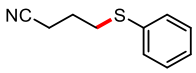


**1-(phenylthio)cyclobutane-1-carbonitrile (29):** Following the general procedure A, obtained in 69% yield as a yellow oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.63 – 7.56 (m, 2H), 7.43 – 7.35 (m, 3H), 2.76 – 2.65 (m, 2H), 2.40 – 2.31 (m, 3H), 2.24 – 2.11 (m, 1H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 134.4, 131.1, 129.5, 129.3, 122.0, 40.4, 34.2, 17.2.

**HRMS** (EI) Calcd for $C_{11}H_{11}NS^+$ $[M]^+$: 189.0607, found: 189.0603.

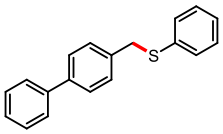


**1-(phenylthio)cyclobutane-1-carbonitrile (30):** Following the general procedure B, obtained in 81% yield as a brown oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.38 – 7.34 (m, 2H), 7.34 – 7.27 (m, 2H), 7.25 – 7.20 (m, 1H), 3.03 (t, J = 6.9 Hz, 2H), 2.51 (t, J = 7.1 Hz, 2H), 1.95 (p, J = 7.0 Hz, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 134.8, 130.2, 129.2, 126.9, 119.1, 32.6, 24.8, 15.9.

**HRMS** (EI) Calcd for $C_{11}H_{11}NS^+$ $[M]^+$: 177.0607, found: 177.0608.

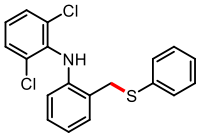


**([1,1'-biphenyl]-4-ylmethyl)(phenyl)sulfane (31):** Following the general procedure C, obtained in 84% yield as a colorless oil. (obtained in 21% yield following the general procedure A)

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.59 – 7.54 (m, 2H), 7.51 (d, $J$ = 8.2 Hz, 2H), 7.42 (t, $J$ = 7.6 Hz, 2H), 7.39 – 7.29 (m, 5H), 7.28 – 7.23 (m, 2H), 7.22 – 7.14 (m, 1H), 4.15 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 140.8, 140.1, 136.6, 136.4, 129.9, 129.3, 128.9, 128.8, 127.3, 127.3, 127.1, 126.4, 38.8.

**HRMS** (EI) Calcd for $C_{19}H_{16}S^+$ $[M]^+$: 276.0967, found: 276.0968.

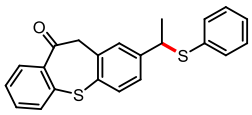


**2,6-dichloro-N-(2-((phenylthio)methyl)phenyl)aniline (32):** Following the general procedure C, obtained in 71% yield as a yellow oil. (obtained in 35% yield following the general procedure B)

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.40 – 7.36 (m, 3H), 7.34 – 7.29 (m, 4H), 7.27 – 7.17 (m, 3H), 7.08 (t, $J$ = 7.5 Hz, 1H), 7.04 (dd, $J$ = 8.1, 0.8 Hz, 1H), 6.45 (d, $J$ = 7.8 Hz, 1H), 3.71 (d, $J$ = 4.0 Hz, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 173.9, 143.6, 141.3, 134.7, 134.0, 132.1, 130.4, 129.6, 128.8, 128.6, 127.9, 127.9, 124.7, 124.4, 122.9, 109.4, 35.7.

**HRMS** (ESI) Calcd for $C_{19}H_{15}Cl_2NSNa^+$ $[M+Na]^+$: 382.0194, found: 382.0195.

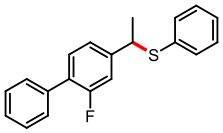


**2-(1-(phenylthio)ethyl)dibenzo[b,f]thiepin-10(11H)-one (33):** Following the general procedure C, obtained in 84% yield as a light yellow oil. (obtained in 53% yield following the general procedure B)

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.22 – 8.16 (m, 1H), 7.60 – 7.55 (m, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.43 – 7.36 (m, 1H), 7.32 – 7.17 (m, 7H), 7.13 (dd, *J* = 8.0, 2.0 Hz, 1H), 4.35 – 4.26 (m, 3H), 1.58 (d, *J* = 7.0 Hz, 3H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 191.3, 145.6, 140.3, 137.6, 136.2, 134.4, 133.0, 132.8, 132.5, 131.5, 131.3, 130.9, 128.8, 128.3, 127.5, 126.8, 126.1, 51.0, 47.6, 22.1.

**HRMS** (EI) Calcd for $C_{22}H_{18}O_2S^+$ $[M]^+$: 362.0794, found: 362.0796.



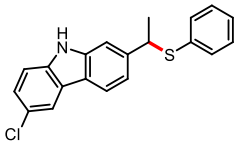
**(1-(2-fluoro-[1,1'-biphenyl]-4-yl)ethyl)(phenyl)sulfane (34):** Following the general procedure B, obtained in 81% yield as a colorless oil.

**$^1$H NMR** (500 MHz, $CDCl_3$) δ 7.59 – 7.48 (m, 2H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.37 – 7.29 (m, 4H), 7.26 – 7.22 (m, 3H), 7.21 – 7.05 (m, 2H), 4.34 (q, *J* = 7.0 Hz, 1H), 1.64 (d, *J* = 7.0 Hz, 3H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 159.6 (d, *J* = 248.1 Hz), 145.0 (d, *J* = 7.3 Hz), 135.6, 134.6, 132.7, 130.6 (d, *J* = 3.6 Hz), 130.1, 129.0, 128.8, 128.5, 127.6 (d, *J* = 23.3 Hz), 126.6, 123.3 (d, *J* = 2.7 Hz), 114.9 (d, *J* = 23.7 Hz), 47.5, 22.2.

**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -117.92 (s).

**HRMS** (EI) Calcd for $C_{20}H_{17}FS^+$ $[M]^+$: 308.1030, found: 308.1027.

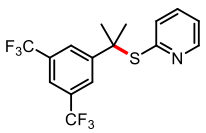


**6-chloro-2-(1-(phenylthio)ethyl)-9H-carbazole (35):** Following the general procedure C, obtained in 77% yield as a light gray oil. (obtained in 24% yield following the general procedure B)

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.02 – 7.68 (m, 3H), 7.25 – 7.17 (m, 5H), 7.14 – 7.10 (m, 3H), 4.42 (q, *J* = 7.0 Hz, 1H), 1.63 (d, *J* = 7.0 Hz, 3H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 142.2, 140.2, 138.0, 135.2, 132.4, 128.8, 127.2, 125.8, 125.0, 124.4, 121.7, 120.4, 120.0, 119.6, 111.5, 109.4, 48.6, 22.8.

**HRMS** (EI) Calcd for $C_{20}H_{16}ClNS^+$ $[M]^+$: 337.0687, found: 337.0688.



**2-((2-(3,5-bis(trifluoromethyl)phenyl)propan-2-yl)thio)pyridine (36):** Following the general

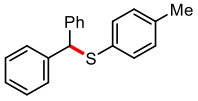
procedure B, obtained in 79% yield as a light yellow oil.

**$^1$H NMR** (500 MHz, $CDCl_3$) δ 8.31 (d, *J* = 4.2 Hz, 1H), 7.97 (s, 2H), 7.66 (s, 1H), 7.39 (td, *J* = 7.7, 1.8 Hz, 1H), 7.04 – 6.94 (m, 2H), 1.96 (s, 6H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 156.7, 149.4, 136.2, 130.9 (q, *J* = 33.1 Hz), 127.0, 126.3, 123.5 (q, *J* = 272.8 Hz), 121.2, 120.3 – 120.2 (m), 51.2, 30.0. (one carbon signal is overlapped)

**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -62.74 (s).

**HRMS** (ESI) Calcd for $C_{16}H_{14}NF_6S^+$ $[M+H]^+$: 366.0746, found: 366.0742.

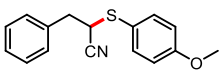



**benzhydryl(p-tolyl)sulfane (37):** Following the general procedure A, obtained in 94% yield as a light yellow oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.4 Hz, 4H), 7.31 – 7.22 (m, 4H), 7.18 (t, *J* = 7.3 Hz, 2H), 7.13 (d, *J* = 8.1 Hz, 2H), 6.96 (d, *J* = 8.0 Hz, 2H), 5.46 (s, 1H), 2.23 (s, 3H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 141.3, 136.9, 132.3, 131.4, 129.6, 128.5, 128.5, 127.2, 58.1, 21.1.

**HRMS** (EI) Calcd for $C_{20}H_{18}S^+$ $[M]^+$: 290.1124, found: 290.1125.

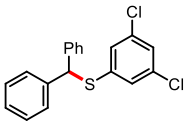



**2-((4-methoxyphenyl)thio)-3-phenylpropanenitrile (38):** Following the general procedure A, obtained in 81% yield as a colorless oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.61 – 7.54 (m, 2H), 7.36 – 7.24 (m, 5H), 6.96 – 6.87 (m, 2H), 3.82 (s, 3H), 3.77 (dd, *J* = 9.2, 6.1 Hz, 1H), 3.07 (ddd, *J* = 23.1, 13.9, 7.7 Hz, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 161.2, 137.5, 135.9, 129.1, 128.9, 127.7, 120.7, 118.9, 115.1, 55.4, 39.6, 38.9.

**HRMS** (EI) Calcd for $C_{16}H_{15}NOS^+$ $[M]^+$: 269.0869, found: 269.0870.

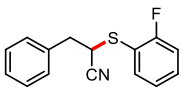



**benzhydryl(3,5-dichlorophenyl)sulfane (39):** Following the general procedure A, obtained in 91% yield as a yellow oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.4 Hz, 4H), 7.30 (t, *J* = 7.5 Hz, 4H), 7.25 – 7.21 (m, 2H), 7.12 – 7.01 (m, 3H), 5.56 (s, 1H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 139.9, 139.9, 134.9, 128.8, 128.4, 127.7, 127.7, 126.5, 57.0.

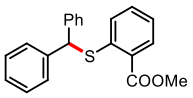
**HRMS** (ESI) Calcd for $C_{19}H_{14}Cl_2SNa^+$ $[M+Na]^+$: 367.0085, found: 367.0068.



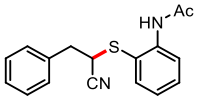

**2-((2-fluorophenyl)thio)-3-phenylpropanenitrile (40):** Following the general procedure A, obtained in 87% yield as a light yellow liquid.

**$^1$H NMR** (500 MHz, $CDCl_3$) δ 7.62 (td, *J* = 7.5, 1.7 Hz, 1H), 7.49 – 7.39 (m, 1H), 7.38 – 7.26 (m,

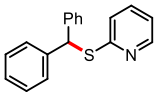
5H), 7.23 – 7.11 (m, 2H), 4.04 (dd, *J* = 9.2, 5.8 Hz, 1H), 3.15 (ddd, *J* = 23.1, 13.8, 7.5 Hz, 2H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 163.0 (d, *J* = 248.3 Hz), 136.9, 135.5, 132.2 (d, *J* = 8.0 Hz), 129.1, 128.9, 127.9, 125.1 (d, *J* = 3.9 Hz), 118.3, 117.8 (d, *J* = 18.0 Hz), 116.3 (d, *J* = 22.9 Hz), 38.9, 37.8.
**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -106.24 (s).
**HRMS** (EI) Calcd for $C_{15}H_{12}FNS^+$ $[M]^+$: 257.0669, found: 257.0668.



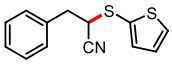

**methyl 2-(benzhydrylthio)benzoate (41):** Following the general procedure A, obtained in 83% yield as a colorless liquid.
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.44 (d, *J* = 7.4 Hz, 4H), 7.29 (t, *J* = 7.5 Hz, 4H), 7.21 (t, *J* = 7.2 Hz, 3H), 7.15 (d, *J* = 7.7 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 5.66 (s, 1H), 3.89 (s, 3H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 167.0, 141.3, 140.4, 132.2, 131.0, 128.7, 128.7, 127.9, 127.4, 127.4, 124.2, 55.4, 52.2.
**HRMS** (EI) Calcd for $C_{21}H_{18}O_2S^+$ $[M]^+$: 334.1022, found: 334.1021.




**N-(2-((1-cyano-2-phenylethyl)thio)phenyl)acetamide (42):** Following the general procedure A, obtained in 57% yield as a light gray oil.
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 8.2 Hz, 1H), 8.17 (s, 1H), 7.64 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.47 – 7.42 (m, 1H), 7.40 – 7.30 (m, 3H), 7.28 – 7.23 (m, 2H), 7.10 (td, *J* = 7.6, 1.2 Hz, 1H), 3.74 (t, *J* = 7.6 Hz, 1H), 3.14 (ddd, *J* = 35.3, 14.1, 7.6 Hz, 2H), 2.06 (s, 3H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 168.5, 140.7, 137.3, 135.2, 132.2, 129.1, 129.0, 128.0, 124.5, 120.9, 118.8, 117.6, 39.1, 38.6, 24.9.
**HRMS** (ESI) Calcd for $C_{17}H_{17}ON_2S^+$ $[M+H]^+$: 297.1056, found: 297.1053.




**2-(benzhydrylthio)pyridine (43):** Following the general procedure A, obtained in 81% yield as a colorless liquid.
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.42 – 8.32 (m, 1H), 7.45 (d, *J* = 7.6 Hz, 4H), 7.38 (td, *J* = 7.8, 1.9 Hz, 1H), 7.27 (t, *J* = 7.5 Hz, 4H), 7.19 (t, *J* = 7.3 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 1H), 6.91 (ddd, *J* = 7.3, 4.9, 0.7 Hz, 1H), 6.33 (s, 1H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 158.4, 149.5, 141.4, 136.1, 128.6, 128.5, 127.1, 122.3, 119.8, 52.7.
**HRMS** (ESI) Calcd for $C_{18}H_{16}NS^+$ $[M+H]^+$: 278.0998, found: 278.0999.



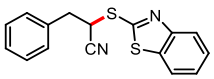

**3-phenyl-2-(thiophen-2-ylthio)propanenitrile (44):** Following the general procedure B, obtained

in 82% yield as a light yellow liquid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 5.4, 1.2 Hz, 1H), 7.41 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.38 – 7.29 (m, 3H), 7.28 – 7.23 (m, 2H), 7.10 (dd, *J* = 5.4, 3.6 Hz, 1H), 3.78 (dd, *J* = 9.0, 6.3 Hz, 1H), 3.11 (qd, *J* = 13.9, 7.7 Hz, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 138.0, 135.5, 132.8, 129.2, 128.9, 128.3, 127.8, 127.6, 118.4, 40.9, 38.7.

**HRMS** (EI) Calcd for $C_{13}H_{11}NS_2^+$ $[M]^+$: 245.0327, found: 245.0327.

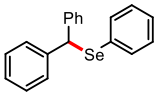



**2-(benzo[d]thiazol-2-ylthio)-3-phenylpropanenitrile (45):** Following the general procedure B, obtained in 76% yield as a yellow oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.1 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.50 – 7.42 (m, 1H), 7.41 – 7.30 (m, 6H), 5.07 (dd, *J* = 8.7, 5.8 Hz, 1H), 3.36 (ddd, *J* = 22.5, 13.8, 7.2 Hz, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 161.4, 152.7, 135.7, 135.1, 129.4, 129.0, 128.1, 126.5, 125.1, 122.2, 121.3, 118.0, 38.6, 36.3.

**HRMS** (ESI) Calcd for $C_{16}H_{13}N_2S_2^+$ $[M+H]^+$: 297.0515, found: 297.0513.

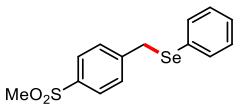



**benzhydryl(phenyl)selane (46):** Following the general procedure D, obtained in 98% yield as a colorless liquid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.5 Hz, 4H), 7.32 (d, *J* = 6.9 Hz, 2H), 7.26 (t, *J* = 7.5 Hz, 4H), 7.21 – 7.10 (m, 5H), 5.63 (s, 1H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 141.4, 134.1, 131.1, 128.9, 128.8, 128.5, 127.6, 127.1, 52.9.

**HRMS** (EI) Calcd for $C_{19}H_{16}Se^+$ $[M]^+$: 324.0412, found: 324.0422.

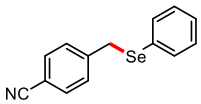



**(4-(methylsulfonyl)benzyl)(phenyl)selane (47):** Following the general procedure D, obtained in 99% yield as a light yellow oil.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 6.6 Hz, 2H), 7.33 – 7.22 (m, 5H), 4.10 (s, 2H), 3.02 (s, 3H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 145.7, 138.8, 134.3, 129.6, 129.2, 129.0, 128.0, 127.5, 44.5, 31.4.

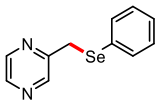
**HRMS** (EI) Calcd for $C_{14}H_{14}O_2SSe^+$ $[M]^+$: 325.9874, found: 325.9873.



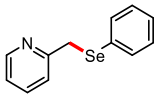

**4-((phenylselanyl)methyl)benzonitrile (48):** Following the general procedure D, obtained in 97% yield as a light yellow liquid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 2H), 7.42 – 7.37 (m, 2H), 7.29 – 7.18 (m, 5H), 4.05 (s, 2H).

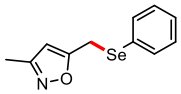
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 144.7, 134.5, 132.2, 129.5, 129.2, 128.8, 128.1, 118.9, 110.5, 31.7.
**HRMS** (EI) Calcd for $C_{14}H_{11}NSe^+$ $[M]^+$: 273.0051, found: 273.0051.



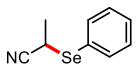
**2-((phenylselanyl)methyl)pyrazine (49):** Following the general procedure D, obtained in 87% yield as a yellow oil.
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.44 (dd, $J$ = 2.4, 1.6 Hz, 1H), 8.36 (d, $J$ = 2.5 Hz, 1H), 8.31 (d, $J$ = 1.3 Hz, 1H), 7.51 – 7.43 (m, 2H), 7.32 – 7.20 (m, 3H), 4.18 (s, 2H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 155.0, 144.4, 144.0, 142.6, 134.3, 129.2, 128.7, 128.0, 30.7.
**HRMS** (ESI) Calcd for $C_{11}H_{11}N_2Se^+$ $[M+H]^+$: 251.0082, found: 251.0081.



**2-((phenylselanyl)methyl)pyridine (50):** Following the general procedure D, obtained in 89% yield as a yellow oil.
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.50 (d, $J$ = 4.6 Hz, 1H), 7.52 (td, $J$ = 7.7, 1.8 Hz, 1H), 7.49 – 7.43 (m, 2H), 7.26 – 7.17 (m, 3H), 7.13 – 7.05 (m, 2H), 4.22 (s, 2H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 158.7, 149.4, 136.5, 133.7, 129.9, 129.0, 127.4, 123.1, 121.8, 33.8.
**HRMS** (ESI) Calcd for $C_{12}H_{12}NSe^+$ $[M+H]^+$: 250.0130, found: 250.0130.



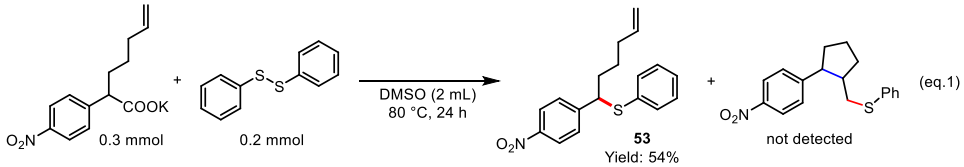
**3-methyl-5-((phenylselanyl)methyl)isoxazole (51):** Following the general procedure D, obtained in 86% yield as a yellow oil.
**$^1$H NMR** (500 MHz, $CDCl_3$) δ 7.56 – 7.40 (m, 2H), 7.33 – 7.24 (m, 3H), 5.78 (s, 1H), 4.03 (s, 2H), 2.22 (s, 3H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 169.7, 159.9, 134.0, 129.3, 129.0, 128.1, 103.0, 20.3, 11.4.
**HRMS** (ESI) Calcd for $C_{11}H_{12}ONSe^+$ $[M+H]^+$: 254.0079, found: 254.0078.

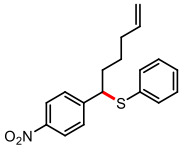


**2-(phenylselanyl)propanenitrile (52):** Following the general procedure B, obtained in 58% yield as a light yellow liquid.
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.83 – 7.66 (m, 2H), 7.47 – 7.41 (m, 1H), 7.40 – 7.35 (t, $J$ = 7.2 Hz, 2H), 3.71 (q, $J$ = 7.3 Hz, 1H), 1.66 (d, $J$ = 7.3 Hz, 3H).
**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 136.5, 129.7, 129.5, 125.9, 120.8, 19.5, 19.3.
**HRMS** (EI) Calcd for $C_9H_9NSe^+$ $[M]^+$: 210.9895, found: 210.9893.

## 5. Experimental Studies on Mechanism

### 5.1 Radical clock experiments



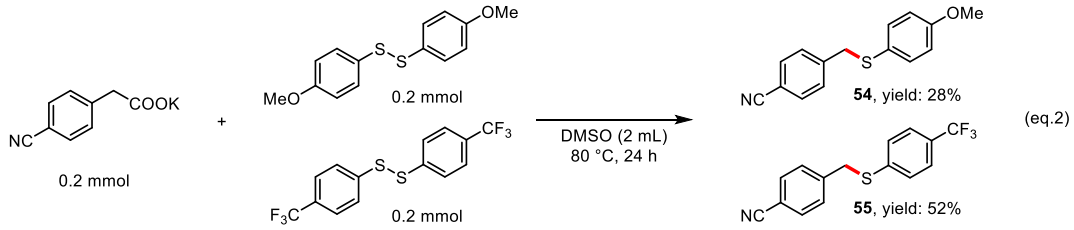

**(1-(4-nitrophenyl)hex-5-en-1-yl)(phenyl)sulfane (53):** Following the above reaction condition in equation 1, obtained in 54% yield as a colorless liquid.

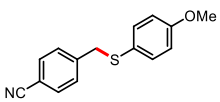
**$^1$H NMR** (500 MHz, $CDCl_3$) δ 8.16 – 8.03 (m, 2H), 7.35 – 7.29 (m, 2H), 7.25 – 7.11 (m, 5H), 5.73 (ddt, *J* = 16.9, 10.2, 6.7 Hz, 1H), 5.03 – 4.92 (m, 2H), 4.16 (dd, *J* = 8.4, 6.6 Hz, 1H), 2.14 – 1.98 (m, 3H), 1.97 – 1.86 (m, 1H), 1.59 – 1.46 (m, 1H), 1.43 – 1.32 (m, 1H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 150.3, 146.9, 137.9, 133.5, 133.1, 128.9, 128.6, 127.9, 123.6, 115.2, 53.4, 35.1, 33.3, 26.8.

**HRMS** (EI) Calcd for $C_{18}H_{19}O_2NS^+$ $[M]^+$: 313.1131, found: 313.1131.

### 5.2 Competition experiments



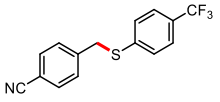




**4-(((4-methoxyphenyl)thio)methyl)benzonitrile (54):** Following the above reaction condition in equation 2, obtained in 28% yield as a colorless liquid.

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.52 (d, J = 8.2 Hz, 2H), 7.24 – 7.16 (m, 4H), 6.81 – 6.75 (m, 2H), 3.95 (s, 2H), 3.78 (s, 3H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 159.7, 144.0, 134.9, 132.1, 129.6, 124.4, 118.9, 114.6, 110.7, 55.3, 41.2.

**HRMS** (EI) Calcd for $C_{10}H_{13}N^+$ $[M]^+$: 255.0712, found: 255.0717.



**4-(((4-(trifluoromethyl)phenyl)thio)methyl)benzonitrile (55):** Following the above reaction condition in equation 2, obtained in 52% yield as a colorless liquid.

**$^1$H NMR** (500 MHz, $CDCl_3$) δ 7.59 (d, $J$ = 8.2 Hz, 2H), 7.50 (d, $J$ = 8.3 Hz, 2H), 7.43 (d, $J$ = 8.5 Hz, 2H), 7.33 (d, $J$ = 8.1 Hz, 2H), 4.19 (s, 2H).

**$^{13}$C NMR** (126 MHz, $CDCl_3$) δ 142.3, 140.5, 132.5, 129.5, 128.7, 128.5 (q, $J$ = 32.9 Hz), 125.8 (q, $J$ = 3.7 Hz), 124.0 (q, $J$ = 272.0 Hz), 118.6, 111.5, 37.7.

**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -62.52 (s).

**HRMS** (EI) Calcd for $C_{15}H_{10}NF_3S^+$ $[M]^+$: 293.0481, found: 293.0481.

### 5.3. DFT Calculations

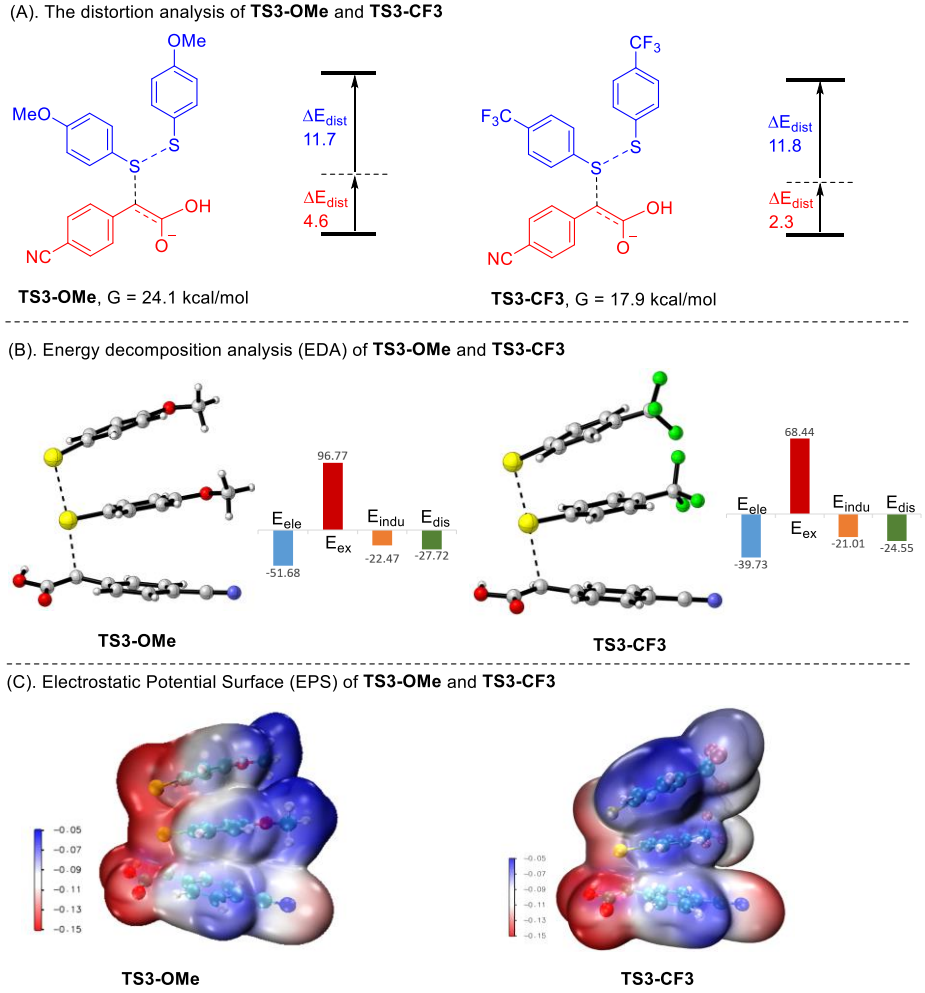
#### 5.3.1 Computational Methods

All calculations were performed with Gaussian 16, Rev. C01.[3] The DFT functional of B3LYP,[4] associated with the Grimme empirical dispersion correction (GD3BJ),[5] was used for geometry optimization of all intermediates and transition states. The 6-31G(d)[6] basis set was employed on all elements. Frequency analysis was performed at the same level of theory with the geometry optimization to confirm that the optimized structures are local minima or transition states, and to gain the thermal correction to Gibbs free energy. Single-point energy calculations were conducted on the basis of optimized structures, and with the M06-2X[7] functional, including Grimme empirical dispersion correction (GD3), and the 6-311++G(d,p)[8] basis set was employed. The solvent effects were taken into account in all calculations by employing the SMD[9] (DMSO) solvation model. The intrinsic reaction coordinate (IRC)[10] calculations were performed to ensure that the transition state connects the correct reactants and products. Symmetry adapted perturbation theory (SAPT)[11] was applied with the level recommended by C. David Sherrill[12] (sSAPT0/jun-cc-pVDZ) via the Psi4 Package.[13] This method decomposes the interaction energy to electrostatic ($E_{ele}$), exchange ($E_{ex}$), dispersion ($E_{dis}$) and induction ($E_{indu}$) terms. All energies in this study are corrected Gibbs free energy, and are given in kcal/mol. The geometries of the optimized structures were drawn with CYLview.[14]

#### 5.3.2 Calculation Discussions of Reaction Details

This proposal also gives a reasonable explanation for the difference in reaction rate of substituted aryl disulfide. The calculation results of the energy barriers of the electrophilic attack step are shown in Scheme S1-A. The disparity of Gibbs free energy ($G_{\mathbf{TS3\text{-}OMe}}$ = 24.1 kcal/mol vs $G_{\mathbf{TS3\text{-}CF3}}$ = 17.9 kcal/mol) is in line with the conclusions of our mechanism experiments. In order to explore the origin of the disparity, we took the methoxy and trifluoromethyl substituted substrates (**IN2-OMe** and **IN2-CF$_3$**) as examples to conduct the distortion model analysis first, and the results indicated that the distortion of **TS3-OMe** and **TS3-CF$_3$** are not much different ($\Delta E_{\text{dist-}\mathbf{TS3\text{-}OMe}}$ = 16.3 vs $\Delta E_{\text{dist-}\mathbf{TS3\text{-}CF3}}$ = 14.1 kcal/mol). In order to further investigate the contribution of each component in the interaction energy, symmetry adapted perturbation theory (SAPT) was carried out for energy decomposition analysis (Scheme S1-B). Among them, the contribution of interaction energy is broken down into four parts: electrostatic ($E_{ele}$), exchange ($E_{ex}$), dispersion ($E_{dis}$) and induction ($E_{indu}$). Unexpectedly, the electrostatic interaction we thought before is not the dominant factor, and the exchange term is an important source of the gap. In addition, we also give the electrostatic potential surface of the two transition states (Scheme S1-C). Due to the different electronic effects of the substituents, the charge distributions of the two are obviously different, which also explains

the electrostatic potential and the difference of electrostatic and exchange items.




**Scheme S1**. Energy analysis of diphenyl disulfide nucleophilic attack.

A plausible mechanism involving dienol formation and proton transfer was proposed (Figure S1). First, the benzyl carboxylate ion substrate **IN1** undergoes benzyl C–H proton migration with the assistance of additional **IN1**, to deliver an electrostatic-dominated dimer intermediate **IN1**-dimer. Due to the inhomogeneity of the charge distribution, the migrated proton is easily transferred to the original carboxyl anion with a free-energy decrease of 11.7 kcal/mol, and the corresponding dienol anion **IN3** is obtained. This strategy is more advantageous than the intramolecular proton migration (**TS1**, 23.2 kcal/mol vs. **TS2**, 44.1 kcal/mol). Subsequently, the disulfide substrate **IN2** electrophilically attacks the dienol anion **IN3** to deliver the corresponding sulfurized product **IN4**. At the same time, the released thiophenol anion binds to the carboxyl O–H bond through electrostatic interaction. After abstracting the proton of the carboxyl group, the generated thiophenol **IN6** leaves briefly, and the decarboxylation of the remaining species **IN5** becomes achievable (**TS5**, 18.4 kcal/mol); this is easier than the direct decarboxylation of benzyl carboxylate ion (**TS7**, 21.1 kcal/mol, see SI for details). When the new benzyl carbanion intermediate **IN7** forms after decarboxylation, the thiophenol **IN6** "returns" the previously captured proton to **IN7**. Thereby, the formation of the product **P0** is exergonic by 24.5 kcal/mol, and the energy barrier of this step is 7.1 kcal/mol.

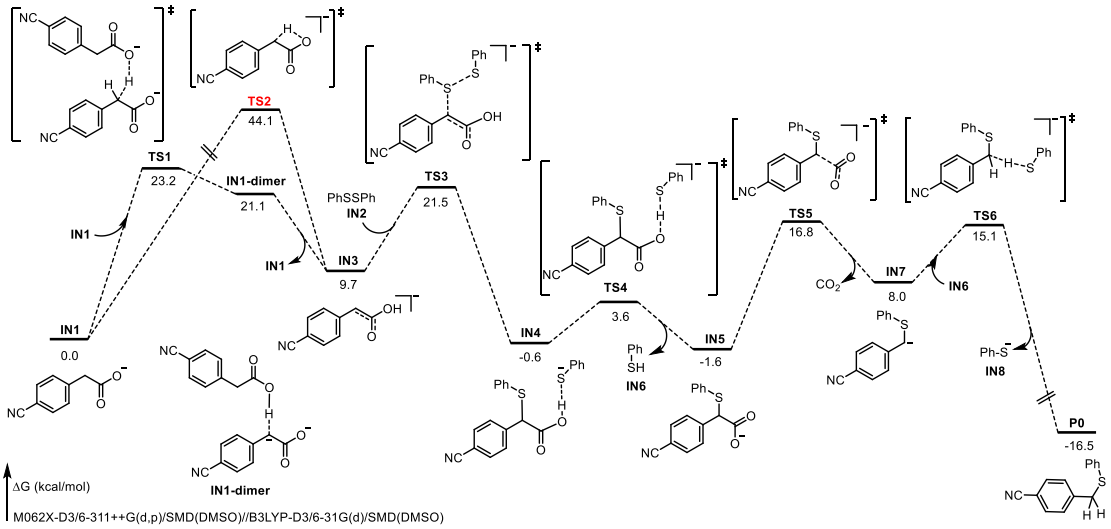



**Figure S1.** The Gibbs free energies of the feasible mechanism.

In addition, we also calculated the dienolate process assisted by benzyl carbanion (Figure S2, **Path II**), the classical carbanion decarboxylation pathway (Figure S2, **Path III**) and a coordinated electrophilic attack-decarboxylation pathway (Figure S2, **Path IV**). The higher energy barrier of the two process also illustrated that the proposal involved dienol formation and proton-transfer is the dominant path (25.6 kcal/mol in **Path III** and 28.2 kcal/mol in **Path IV** vs 23.2 kcal/mol in Figure S1).

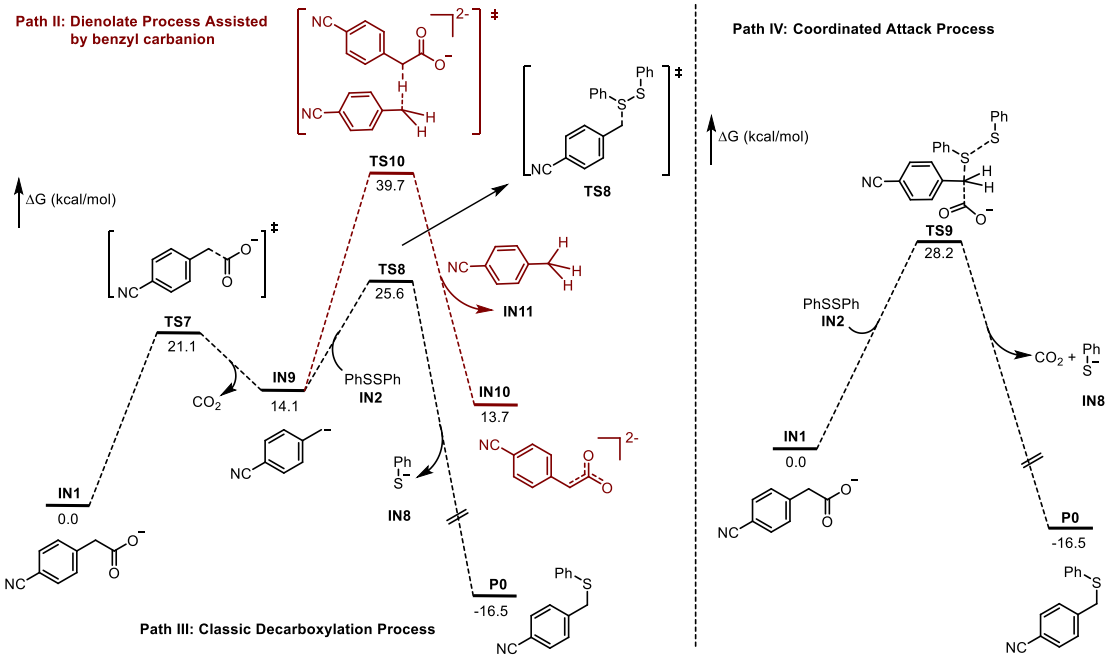



**Figure S2.** The Gibbs free energies of classic decarboxylation process and coordinated process.

### 5.3.3 Calculation Discussions of Reaction Details

$\Delta G_{sol} = \Delta E_{sol} + \Delta G_{corr}$

$\Delta E_{sol}$ refers to the solvation single point energy by M06-2X/6–311++G(d,p).

$\Delta G_{corr}$ refers to the thermal correction to the Gibbs free energy calculated at B3LYP-D3(BJ)/6–

31G(d) level of theory.

$\Delta G_{sol}$ refers to the sum of the solvation single point energy and the thermal correction to the Gibbs free energy.

**Table S4.** The $\Delta G_{corr}$, $\Delta E_{sol}$ and $\Delta G_{sol}$ of Optimized Structures

| Number | $\Delta E_{sol}$ (Hartree) | $\Delta G_{corr}$ (Hartree) | $\Delta G_{sol}$ (kcal/mol) |
|---|---|---|---|
| **IN1** | -551.8590476 | 0.09192 | -346239.0592 |
| **IN1-dimer** | -1103.699357 | 0.198727 | -692457.0185 |
| **IN2** | -1259.598424 | 0.142508 | -790320.4261 |
| **IN2-CF3** | -1933.701164 | 0.139033 | -1213328.413 |
| **IN2-OMe** | -1488.630631 | 0.202199 | -934002.8323 |
| **IN3** | -551.844408 | 0.092666 | -346229.4046 |
| **IN4** | -1811.482442 | 0.258465 | -1136560.071 |
| **IN5** | -1181.066232 | 0.164064 | -741027.2111 |
| **IN6** | -630.3928709 | 0.069477 | -395533.8547 |
| **IN7** | -992.454789 | 0.153207 | -622678.5703 |
| **IN8** | -629.9303541 | 0.060582 | -395249.2028 |
| **IN9** | -363.2400321 | 0.080668 | -227885.9147 |
| **IN10** | -551.3445926 | 0.079017 | -345924.3306 |
| **IN11** | -363.756543 | 0.095235 | -228200.8892 |
| **P0** | -992.9607284 | 0.1666 | -622987.6478 |
| **TS1** | -1103.695801 | 0.198589 | -692454.8737 |
| **TS2** | -551.7840445 | 0.087145 | -346194.9904 |
| **TS3** | -1811.447498 | 0.258692 | -1136538.001 |
| **TS3-CF3** | -2485.555384 | 0.254576 | -1559549.619 |
| **TS3-OMe** | -2040.477321 | 0.320197 | -1280217.773 |
| **TS4** | -1811.471984 | 0.254613 | -1136555.926 |
| **TS5** | -1181.032728 | 0.159786 | -741008.8715 |
| **TS6** | -1622.857911 | 0.244315 | -1018205.284 |
| **TS7** | -551.8192562 | 0.085765 | -346217.952 |
| **TS8** | -1622.844938 | 0.247929 | -1018194.876 |
| **TS9** | -1811.427698 | 0.249618 | -1136531.27 |
| **TS10** | -915.0763974 | 0.190888 | -574099.2571 |

**The Cartesian coordinates of all stationary points.**

**IN1**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 2.16836900 | 0.01072000 | 0.02372600 |
| C | 1.39829300 | -1.10104700 | -0.37034800 |
| C | 0.04981900 | -0.94054400 | -0.65190800 |
| C | -0.57080900 | 0.32019500 | -0.55666600 |
| C | 0.21228100 | 1.41654900 | -0.15714200 |
| C | 1.56446200 | 1.27545700 | 0.13177000 |
| H | 1.86778800 | -2.07643900 | -0.45223600 |

| | | | |
|---|---|---|---|
| H | -0.55243600 | -1.79641000 | -0.93230600 |
| H | -0.24941500 | 2.39699600 | -0.07557900 |
| H | 2.15732700 | 2.13250200 | 0.43530700 |
| C | 3.55757200 | -0.14608600 | 0.30820700 |
| N | 4.69201500 | -0.27511200 | 0.54038500 |
| C | -2.03253500 | 0.47324900 | -0.82265900 |
| H | -2.29402000 | -0.03172600 | -1.76209900 |
| H | -2.29857600 | 1.52940700 | -0.91566500 |
| C | -2.93516800 | -0.19921100 | 0.30152400 |
| O | -2.67320300 | -1.40107900 | 0.54807300 |
| O | -3.82035700 | 0.54054800 | 0.78703400 |

**IN1-dimer**

| Atom | X | Y | Z |
|---|---|---|---|
| C | -1.58477600 | -2.17563400 | -0.20263100 |
| C | -0.91972300 | -1.73976900 | 0.97452200 |
| C | 0.43789600 | -1.50678900 | 0.98624600 |
| C | 1.25664700 | -1.69358900 | -0.18402900 |
| C | 0.55707300 | -2.16274500 | -1.35424800 |
| C | -0.80107600 | -2.38552900 | -1.36997300 |
| H | -1.50294200 | -1.57200300 | 1.87710900 |
| H | 0.92950100 | -1.15301500 | 1.88459000 |
| H | 1.13060200 | -2.32995300 | -2.26444000 |
| H | -1.28654900 | -2.72144800 | -2.28338700 |
| C | -2.98266900 | -2.35277300 | -0.22386600 |
| N | -4.14811100 | -2.48942600 | -0.24212600 |
| C | 2.64414300 | -1.42991000 | -0.25392600 |
| H | 2.60947900 | 0.19882400 | -1.00242200 |
| H | 3.14349500 | -1.80072500 | -1.15184600 |
| C | 3.56362200 | -1.08716200 | 0.86475000 |
| O | 3.07395500 | -0.62116000 | 1.95322600 |
| O | 4.81287200 | -1.24577900 | 0.64829000 |
| C | -2.77084900 | 1.40986900 | 0.22852200 |
| C | -2.15318600 | 1.84492500 | 1.41496700 |
| C | -0.77489400 | 2.02012500 | 1.44468000 |
| C | 0.01417700 | 1.76043000 | 0.31271600 |
| C | -0.61606500 | 1.33299600 | -0.86464400 |
| C | -1.99500600 | 1.15506000 | -0.91436300 |
| H | -2.75328400 | 2.04208300 | 2.29779700 |
| H | -0.29843300 | 2.35321300 | 2.36277600 |
| H | -0.03230300 | 1.11595000 | -1.75349200 |
| H | -2.47134300 | 0.81219500 | -1.82701000 |
| C | -4.18700700 | 1.22414000 | 0.18786300 |
| N | -5.34235200 | 1.07639900 | 0.15806200 |

| | | | |
|---|---|---|---|
| C | 1.51843600 | 1.90231600 | 0.42656700 |
| H | 1.92914100 | 1.01130400 | 0.92492400 |
| H | 1.74635400 | 2.76331800 | 1.06259600 |
| C | 2.19791900 | 2.13657900 | -0.91411900 |
| O | 2.27583400 | 3.24918300 | -1.41899600 |
| O | 2.69503200 | 1.07478300 | -1.54413900 |

**IN2**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 2.76574100 | -0.52723900 | 0.43045800 |
| C | 1.67505500 | -0.45308400 | -0.44642200 |
| C | 1.32893900 | 0.76775400 | -1.04115100 |
| C | 2.07800500 | 1.91151200 | -0.75966100 |
| C | 3.16343500 | 1.83899900 | 0.11490600 |
| C | 3.50633500 | 0.62023400 | 0.70879100 |
| H | 3.02454500 | -1.47479400 | 0.89266400 |
| H | 0.47945000 | 0.81836200 | -1.71414000 |
| H | 1.80887900 | 2.85780600 | -1.21994300 |
| H | 3.74336200 | 2.73071000 | 0.33509500 |
| H | 4.35224700 | 0.56398200 | 1.38791000 |
| S | 0.69157800 | -1.90282000 | -0.80812400 |
| S | -0.69157800 | -1.90282000 | 0.80812400 |
| C | -1.67505500 | -0.45308400 | 0.44642200 |
| C | -1.32893900 | 0.76775400 | 1.04115100 |
| C | -2.76574100 | -0.52723900 | -0.43045800 |
| C | -2.07800500 | 1.91151200 | 0.75966100 |
| H | -0.47945000 | 0.81836200 | 1.71414000 |
| C | -3.50633500 | 0.62023400 | -0.70879100 |
| H | -3.02454500 | -1.47479400 | -0.89266400 |
| C | -3.16343500 | 1.83899900 | -0.11490600 |
| H | -1.80887900 | 2.85780600 | 1.21994300 |
| H | -4.35224700 | 0.56398200 | -1.38791000 |
| H | -3.74336200 | 2.73071000 | -0.33509500 |

**IN2-CF3**

| Atom | X | Y | Z |
|---|---|---|---|
| C | -2.69470800 | 1.74795200 | 0.20098400 |
| C | -1.55479500 | 1.72406200 | -0.61480800 |
| C | -1.13357700 | 0.52860500 | -1.20686000 |
| C | -1.85266000 | -0.64663000 | -0.98779800 |
| C | -2.98286700 | -0.61899900 | -0.17327900 |
| C | -3.40728700 | 0.57578800 | 0.42193700 |
| H | -3.01362500 | 2.67602800 | 0.66352000 |
| H | -0.24516500 | 0.51363700 | -1.82848200 |

| | | | |
|---|---|---|---|
| H | -1.52530700 | -1.57434800 | -1.44255800 |
| H | -4.29033600 | 0.58698700 | 1.05328200 |
| S | -0.58730800 | 3.20537100 | -0.88327600 |
| S | 0.61496200 | 3.21326700 | 0.87005700 |
| C | 1.58115200 | 1.72873200 | 0.61455300 |
| C | 1.15529600 | 0.53684700 | 1.21258300 |
| C | 2.72406600 | 1.74557200 | -0.19542500 |
| C | 1.87250800 | -0.63972000 | 1.00219000 |
| H | 0.26578300 | 0.52780300 | 1.83275100 |
| C | 3.43648000 | 0.57028100 | -0.40739600 |
| H | 3.04843900 | 2.67062600 | -0.66022000 |
| C | 3.00800500 | -0.61933900 | 0.19207200 |
| H | 1.54310200 | -1.56454900 | 1.46248400 |
| H | 4.32336600 | 0.57880500 | -1.03206200 |
| C | -3.77248800 | -1.86745800 | 0.09369100 |
| C | 3.74968400 | -1.89282600 | -0.09405800 |
| F | 5.08268300 | -1.68997700 | -0.20629800 |
| F | 3.56624100 | -2.82304800 | 0.86880600 |
| F | 3.34712100 | -2.45620900 | -1.26094200 |
| F | -3.27456900 | -2.94829100 | -0.54255000 |
| F | -3.80435000 | -2.16417500 | 1.41642200 |
| F | -5.06396800 | -1.73501100 | -0.29627600 |

**IN2-OMe**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 2.82694900 | 1.18874100 | -0.08395000 |
| C | 1.62762600 | 1.12137700 | 0.63475400 |
| C | 1.20762400 | -0.11556200 | 1.15436500 |
| C | 1.97506500 | -1.25495500 | 0.96042200 |
| C | 3.17701000 | -1.18163600 | 0.23728700 |
| C | 3.60352000 | 0.04970500 | -0.28525600 |
| H | 3.15660100 | 2.13776400 | -0.49548600 |
| H | 0.27699000 | -0.17962700 | 1.70827600 |
| H | 1.65930800 | -2.21490600 | 1.35665600 |
| H | 4.52845000 | 0.12803300 | -0.84355100 |
| S | 0.61540100 | 2.56502200 | 0.87646500 |
| S | -0.61541600 | 2.56502600 | -0.87649600 |
| C | -1.62764700 | 1.12138600 | -0.63476900 |
| C | -1.20766700 | -0.11553500 | -1.15443000 |
| C | -2.82691800 | 1.18872300 | 0.08402500 |
| C | -1.97509300 | -1.25493900 | -0.96047900 |
| H | -0.27705900 | -0.17958000 | -1.70838900 |
| C | -3.60345400 | 0.04967300 | 0.28537400 |
| H | -3.15655100 | 2.13773300 | 0.49560800 |

| | | | |
|---|---|---|---|
| C | -3.17697800 | -1.18164900 | -0.23724300 |
| H | -1.65936500 | -2.21487500 | -1.35677000 |
| H | -4.52833400 | 0.12797300 | 0.84375500 |
| O | 3.85434100 | -2.34661800 | 0.09668700 |
| O | -3.85428300 | -2.34664000 | -0.09659600 |
| C | 5.08280500 | -2.32599000 | -0.63322400 |
| H | 5.44943600 | -3.35376800 | -0.62478000 |
| H | 4.92488700 | -2.00322400 | -1.66885500 |
| H | 5.81989700 | -1.67182100 | -0.15328300 |
| C | -5.08285100 | -2.32596100 | 0.63313600 |
| H | -5.44957100 | -3.35370700 | 0.62455800 |
| H | -4.92505200 | -2.00329200 | 1.66881600 |
| H | -5.81981500 | -1.67168700 | 0.15314300 |

**IN3**

| Atom | X | Y | Z |
|---|---|---|---|
| C | -2.31064800 | -0.02292300 | -0.00004200 |
| C | -1.39415000 | -1.10369100 | 0.00004300 |
| C | -0.03295200 | -0.88724400 | 0.00006300 |
| C | 0.52201400 | 0.43631900 | -0.00001500 |
| C | -0.42895900 | 1.51065900 | -0.00003500 |
| C | -1.78848400 | 1.29510400 | -0.00005900 |
| H | -1.77808600 | -2.12078800 | 0.00007400 |
| H | 0.65555500 | -1.72286800 | 0.00012100 |
| H | -0.05487100 | 2.53218100 | -0.00001800 |
| H | -2.47323700 | 2.13899700 | -0.00009200 |
| C | -3.70592800 | -0.25202800 | 0.00001800 |
| N | -4.86054900 | -0.44192700 | 0.00007200 |
| C | 1.90506300 | 0.72313100 | -0.00009700 |
| H | 2.18117700 | 1.77654400 | -0.00023600 |
| C | 2.95490700 | -0.23885500 | -0.00003000 |
| O | 2.87676400 | -1.47318600 | -0.00014200 |
| O | 4.24568900 | 0.28232500 | 0.00009300 |
| H | 4.18850100 | 1.25347200 | 0.00096300 |

**IN4**

| Atom | X | Y | Z |
|---|---|---|---|
| C | -5.30735200 | -0.52264800 | 0.26689700 |
| C | -4.91025000 | 0.58291500 | -0.50401900 |
| C | -3.55902300 | 0.87880500 | -0.63470500 |
| C | -2.59192000 | 0.08263100 | -0.00384100 |
| C | -2.99818900 | -1.01602700 | 0.76501300 |
| C | -4.34619400 | -1.32561400 | 0.90270400 |
| H | -5.65847200 | 1.19738400 | -0.99321800 |

| | | | |
|---|---|---|---|
| H | -3.24388100 | 1.72296000 | -1.23727100 |
| H | -2.25117000 | -1.63157700 | 1.25659300 |
| H | -4.65905700 | -2.17872100 | 1.49519600 |
| C | -6.69685300 | -0.83243400 | 0.40334300 |
| N | -7.82753900 | -1.08404600 | 0.51447600 |
| C | -1.11926000 | 0.40286400 | -0.11450100 |
| H | -0.54083000 | -0.41123500 | 0.32706800 |
| C | -0.69676200 | 0.58909800 | -1.58165200 |
| O | -0.97290500 | 1.57663600 | -2.23718700 |
| O | -0.04509300 | -0.43687500 | -2.11827300 |
| H | 0.22291300 | -1.15534200 | -1.43386500 |
| C | 3.56229800 | -2.31694500 | 0.84933800 |
| C | 2.65506700 | -1.95330600 | -0.16977200 |
| C | 3.15291800 | -1.14155000 | -1.21239500 |
| C | 4.48722300 | -0.73780800 | -1.24320200 |
| C | 5.37451200 | -1.12092900 | -0.23333300 |
| C | 4.89621900 | -1.90999800 | 0.81663500 |
| H | 3.20834500 | -2.93266900 | 1.67226900 |
| H | 2.48120400 | -0.82540800 | -2.00452400 |
| H | 4.83471100 | -0.11303400 | -2.06306200 |
| H | 6.41379200 | -0.80521000 | -0.26009500 |
| H | 5.56629100 | -2.21364200 | 1.61810400 |
| S | 0.97559800 | -2.52725600 | -0.14071500 |
| S | -0.76654700 | 1.91406600 | 0.89996900 |
| C | 1.02617600 | 1.91583900 | 0.80880300 |
| C | 1.77782100 | 1.21203100 | 1.75878100 |
| C | 1.67483500 | 2.63992900 | -0.19975300 |
| C | 3.17125700 | 1.24293700 | 1.70518200 |
| H | 1.27141500 | 0.64472100 | 2.53344800 |
| C | 3.06931000 | 2.66885400 | -0.24632200 |
| H | 1.08738300 | 3.17105100 | -0.94113000 |
| C | 3.81749000 | 1.97649500 | 0.70790600 |
| H | 3.75095800 | 0.69136700 | 2.43887000 |
| H | 3.57024400 | 3.23184500 | -1.02883100 |
| H | 4.90215900 | 1.99793300 | 0.66807700 |

**IN5**

| Atom | X | Y | Z |
|---|---|---|---|
| C | -2.98139000 | -0.45800100 | 0.08007600 |
| C | -2.62537900 | 0.55251000 | -0.83469500 |
| C | -1.40565900 | 1.19783200 | -0.70070200 |
| C | -0.52161800 | 0.86323100 | 0.33937800 |
| C | -0.88987100 | -0.14106100 | 1.24439200 |
| C | -2.10783400 | -0.80260300 | 1.12366600 |

| | | | |
|---|---|---|---|
| H | -3.30659100 | 0.81653200 | -1.63703700 |
| H | -1.11501500 | 1.97548600 | -1.39979000 |
| H | -0.20790000 | -0.41501000 | 2.04370800 |
| H | -2.38361200 | -1.58445200 | 1.82369000 |
| C | -4.23192000 | -1.13479700 | -0.05539000 |
| N | -5.25114100 | -1.68682100 | -0.16644900 |
| C | 0.81425100 | 1.54196200 | 0.44316000 |
| H | 1.27942200 | 1.28936200 | 1.39835800 |
| C | 0.68415000 | 3.10636900 | 0.32595900 |
| O | 0.32351100 | 3.65982200 | 1.38771800 |
| O | 0.91650200 | 3.60078800 | -0.80422800 |
| C | 1.16305900 | -3.07991300 | -0.77121400 |
| C | 1.16243600 | -1.73151000 | -1.13343800 |
| C | 1.98014900 | -0.81627800 | -0.45655400 |
| C | 2.79602600 | -1.26925900 | 0.58972200 |
| C | 2.78995300 | -2.61627000 | 0.95486800 |
| C | 1.97440700 | -3.52451400 | 0.27454000 |
| H | 0.52403200 | -3.78058900 | -1.30188900 |
| H | 0.51896500 | -1.38195600 | -1.93499800 |
| H | 3.43106500 | -0.56392000 | 1.11809800 |
| H | 3.42412300 | -2.95700400 | 1.76893200 |
| H | 1.97166400 | -4.57308900 | 0.55888500 |
| S | 1.94357300 | 0.92320800 | -0.90520900 |

**IN6**

| Atom | X | Y | Z |
|---|---|---|---|
| C | -1.59974900 | -1.20008700 | 0.00000800 |
| C | -0.20515200 | -1.21408100 | -0.00014300 |
| C | 0.50396300 | -0.00573900 | -0.00011500 |
| C | -0.18968400 | 1.21071000 | 0.00001000 |
| C | -1.58522900 | 1.21170000 | 0.00001500 |
| C | -2.29648300 | 0.01034300 | 0.00006800 |
| H | -2.14135100 | -2.14191000 | 0.00001100 |
| H | 0.32709400 | -2.16136400 | -0.00040200 |
| H | 0.35249600 | 2.15197700 | 0.00004900 |
| H | -2.11514600 | 2.16023300 | 0.00002100 |
| H | -3.38245400 | 0.01703500 | 0.00018300 |
| S | 2.29256000 | -0.08438200 | 0.00016500 |
| H | 2.51240300 | 1.24707000 | -0.00156300 |

**IN7**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 3.48106900 | 0.42258100 | -0.12896500 |
| C | 2.37277400 | 0.57319100 | -1.00665600 |

| | | | |
|---|---|---|---|
| C | 1.21013500 | -0.13514200 | -0.82108900 |
| C | 1.04878700 | -1.07634500 | 0.26008600 |
| C | 2.18741800 | -1.20385600 | 1.14008200 |
| C | 3.34561300 | -0.49162800 | 0.95375600 |
| H | 2.44998100 | 1.27209900 | -1.83619100 |
| H | 0.38015900 | 0.01511800 | -1.50468600 |
| H | 2.11510300 | -1.89482700 | 1.97740500 |
| H | 4.17781100 | -0.62299700 | 1.64110900 |
| C | 4.66839700 | 1.15613300 | -0.32025000 |
| N | 5.65734000 | 1.76547300 | -0.47943300 |
| C | -0.10913100 | -1.81780600 | 0.49125900 |
| H | -0.16900400 | -2.45609500 | 1.36892100 |
| C | -4.40130900 | 1.06876700 | -0.54328000 |
| C | -3.64485000 | -0.06706800 | -0.83133800 |
| C | -2.46081400 | -0.32416300 | -0.12411900 |
| C | -2.04497200 | 0.57060800 | 0.86718600 |
| C | -2.80595900 | 1.70664200 | 1.14950700 |
| C | -3.98664200 | 1.96309800 | 0.44842300 |
| H | -5.31841500 | 1.25580900 | -1.09645300 |
| H | -3.97454200 | -0.75509100 | -1.60692700 |
| H | -1.12763900 | 0.36596400 | 1.41146400 |
| H | -2.47214900 | 2.39476500 | 1.92248800 |
| H | -4.57622000 | 2.84822100 | 0.67022500 |
| S | -1.51559800 | -1.80321000 | -0.54993400 |

**IN8**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 1.55951700 | -1.20166600 | 0.00001600 |
| C | 0.16527800 | -1.20211700 | 0.00004600 |
| C | -0.58608400 | -0.00036800 | -0.00003000 |
| C | 0.16433900 | 1.20155400 | -0.00007000 |
| C | 1.55896500 | 1.20199700 | -0.00010000 |
| C | 2.27527000 | 0.00051700 | -0.00006800 |
| H | 2.09330400 | -2.15028800 | 0.00006300 |
| H | -0.36994400 | -2.14881900 | 0.00012100 |
| H | -0.37088800 | 2.14823100 | -0.00008600 |
| H | 2.09182600 | 2.15113900 | -0.00014900 |
| H | 3.36201900 | 0.00063200 | -0.00008900 |
| S | -2.35187600 | -0.00002500 | 0.00008600 |

**IN9**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 1.08803800 | -0.00004600 | 0.00039400 |
| C | 0.34130500 | 1.21984900 | 0.00034000 |

| | | | |
|---|---|---|---|
| C | -1.02696500 | 1.22419500 | 0.00014600 |
| C | -1.81710900 | 0.00003700 | -0.00025100 |
| C | -1.02698300 | -1.22419700 | 0.00016400 |
| C | 0.34127200 | -1.21995700 | 0.00033500 |
| H | 0.88270300 | 2.16379300 | 0.00052400 |
| H | -1.55756200 | 2.17486900 | 0.00023900 |
| H | -1.55767900 | -2.17481700 | 0.00028100 |
| H | 0.88264600 | -2.16391100 | 0.00054200 |
| C | 2.49000900 | -0.00005000 | -0.00018100 |
| N | 3.66592800 | 0.00009300 | -0.00052600 |
| C | -3.18953500 | 0.00002900 | -0.00063800 |
| H | -3.75576800 | 0.92865700 | 0.00024800 |
| H | -3.75602800 | -0.92839800 | -0.00000100 |

**IN10**

| Atom | X | Y | Z |
|---|---|---|---|
| C | -2.27510200 | -0.03096800 | -0.00001600 |
| C | -1.32454500 | -1.10292900 | -0.00008200 |
| C | 0.02546900 | -0.87665000 | -0.00015000 |
| C | 0.59074200 | 0.46644400 | -0.00016400 |
| C | -0.40069600 | 1.53388100 | -0.00024800 |
| C | -1.74922300 | 1.30007600 | -0.00017700 |
| H | -1.69843900 | -2.12600500 | 0.00000500 |
| H | 0.74495700 | -1.68846300 | -0.00026400 |
| H | -0.04208200 | 2.56280400 | -0.00040300 |
| H | -2.44394100 | 2.13811400 | -0.00023600 |
| C | -3.65484400 | -0.27315100 | 0.00022800 |
| N | -4.81400800 | -0.47723300 | 0.00034100 |
| C | 1.94604400 | 0.74647400 | -0.00006100 |
| H | 2.22326400 | 1.80403700 | -0.00000400 |
| C | 3.11359300 | -0.19463800 | 0.00006500 |
| O | 2.90253000 | -1.45217700 | -0.00034500 |
| O | 4.25817900 | 0.35704100 | 0.00061400 |

**IN11**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 1.11678800 | 0.00000000 | 0.00101200 |
| C | 0.41454700 | 1.21708300 | -0.00313700 |
| C | -0.97516300 | 1.20620700 | -0.01031000 |
| C | -1.69195400 | 0.00000000 | -0.01087800 |
| C | -0.97516300 | -1.20620700 | -0.01031000 |
| C | 0.41454700 | -1.21708300 | -0.00313700 |
| H | 0.96008800 | 2.15496000 | -0.00420100 |
| H | -1.51587000 | 2.14844000 | -0.01691900 |

| | | | |
|---|---|---|---|
| H | -1.51587000 | -2.14844000 | -0.01691900 |
| H | 0.96008800 | -2.15496000 | -0.00420100 |
| C | 2.54580500 | 0.00000000 | 0.00480800 |
| N | 3.70991000 | 0.00000000 | 0.00840600 |
| C | -3.19686800 | 0.00000000 | 0.01367500 |
| H | -3.56527800 | 0.00000000 | 1.04835000 |
| H | -3.60388500 | -0.88946700 | -0.47764400 |
| H | -3.60388500 | 0.88946700 | -0.47764400 |

**CO2**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| O | 0.00000000 | 0.00000000 | 1.16899300 |
| O | 0.00000000 | 0.00000000 | -1.16899300 |

**P0**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 2.80822600 | 0.17447900 | 0.13126300 |
| C | 2.64703700 | -1.01820400 | -0.59686800 |
| C | 1.52139000 | -1.80229300 | -0.38326800 |
| C | 0.54814200 | -1.42259700 | 0.55267100 |
| C | 0.72292600 | -0.23427400 | 1.27490800 |
| C | 1.84175000 | 0.56564100 | 1.07135800 |
| H | 3.40010200 | -1.31602400 | -1.31862500 |
| H | 1.38829700 | -2.71790500 | -0.95228000 |
| H | -0.03064100 | 0.07072900 | 1.99396700 |
| H | 1.97038400 | 1.48733200 | 1.62874000 |
| C | 3.96064300 | 0.99167300 | -0.08741700 |
| N | 4.89844600 | 1.65742800 | -0.26605300 |
| C | -0.70076500 | -2.23158500 | 0.72828400 |
| H | -1.16198200 | -2.04793000 | 1.70116800 |
| C | -1.43049800 | 2.14844000 | -1.06402700 |
| C | -1.36826100 | 0.76563100 | -1.24396600 |
| C | -2.08662000 | -0.08345800 | -0.39345900 |
| C | -2.86865800 | 0.45770300 | 0.63489900 |
| C | -2.92123600 | 1.84032500 | 0.81551700 |
| C | -2.20289700 | 2.68669300 | -0.03311300 |
| H | -0.86819800 | 2.80283100 | -1.72415100 |
| H | -0.75269200 | 0.34260500 | -2.03134000 |
| H | -3.42594000 | -0.20194700 | 1.29328400 |
| H | -3.52511500 | 2.25610400 | 1.61720500 |
| H | -2.24570200 | 3.76272100 | 0.10966700 |
| S | -1.95973600 | -1.86038500 | -0.59509200 |

| | | | |
|---|---|---|---|
| H | -0.50893300 | -3.30340500 | 0.62551800 |

**TS1**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 1.85614800 | 2.06219800 | -0.12638800 |
| C | 1.11476300 | 1.67156200 | 1.01686100 |
| C | -0.25186600 | 1.50761900 | 0.95490700 |
| C | -0.98958200 | 1.72055400 | -0.25388400 |
| C | -0.21912200 | 2.15400000 | -1.38068200 |
| C | 1.14977300 | 2.30751300 | -1.32941500 |
| H | 1.64248200 | 1.48776700 | 1.94942100 |
| H | -0.82507800 | 1.19558900 | 1.82040400 |
| H | -0.73688400 | 2.34756600 | -2.31820400 |
| H | 1.69873500 | 2.61677900 | -2.21516600 |
| C | 3.26515200 | 2.16489400 | -0.07615500 |
| N | 4.43236900 | 2.23837700 | -0.03297000 |
| C | -2.39568000 | 1.47778100 | -0.38959700 |
| H | -2.50065900 | 0.08678200 | -0.95567400 |
| H | -2.83730900 | 1.99033700 | -1.25214800 |
| C | -3.36417500 | 1.36365000 | 0.77175700 |
| O | -2.95204200 | 0.80855200 | 1.84790200 |
| O | -4.53584000 | 1.78048300 | 0.56714700 |
| C | 2.55054800 | -1.59060600 | 0.13493700 |
| C | 1.96036900 | -1.98031100 | 1.34973400 |
| C | 0.57812700 | -2.07411600 | 1.44038700 |
| C | -0.24820500 | -1.77292700 | 0.34554900 |
| C | 0.35749500 | -1.39289800 | -0.86203900 |
| C | 1.73905200 | -1.30114500 | -0.97458700 |
| H | 2.58647100 | -2.20476500 | 2.20715900 |
| H | 0.12549200 | -2.37365600 | 2.38159300 |
| H | -0.26154800 | -1.14156900 | -1.71548900 |
| H | 2.19431600 | -0.99404100 | -1.91013900 |
| C | 3.96992300 | -1.47277000 | 0.03323700 |
| N | 5.12724300 | -1.37385300 | -0.04956800 |
| C | -1.74923600 | -1.82551000 | 0.52261400 |
| H | -2.08575500 | -0.90339000 | 1.03274400 |
| H | -1.99721000 | -2.67152300 | 1.17169500 |
| C | -2.51552500 | -2.00199900 | -0.78905700 |
| O | -2.88409400 | -3.11680400 | -1.15335800 |
| O | -2.72403400 | -0.92128900 | -1.50512900 |

**TS2**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 2.25410900 | -0.06152800 | -0.02658300 |

| | | | |
|---|---|---|---|
| C | 1.29642500 | -1.08964800 | -0.17380800 |
| C | -0.05433900 | -0.80216200 | -0.13063100 |
| C | -0.53545600 | 0.52502900 | 0.05995100 |
| C | 0.45099500 | 1.54042800 | 0.21828400 |
| C | 1.80276500 | 1.26361300 | 0.17385000 |
| H | 1.63122900 | -2.11323300 | -0.31620000 |
| H | -0.77264600 | -1.61025900 | -0.22842700 |
| H | 0.12356300 | 2.56506200 | 0.37752900 |
| H | 2.52898400 | 2.06164300 | 0.29926900 |
| C | 3.64153700 | -0.35439700 | -0.06884700 |
| N | 4.78412600 | -0.59465000 | -0.10359800 |
| C | -1.93708600 | 0.84526700 | 0.02647400 |
| H | -2.81226500 | 0.82072400 | -1.13426000 |
| H | -2.21234700 | 1.76193700 | 0.55683800 |
| C | -3.00681600 | -0.23841300 | 0.12356500 |
| O | -3.18086400 | -1.12913400 | 0.94792300 |
| O | -3.75016200 | -0.00742300 | -0.95330900 |

**TS3**

| Atom | X | Y | Z |
|---|---|---|---|
| C | -3.79043300 | 1.51894100 | -0.04052300 |
| C | -3.82499200 | 0.41037200 | -0.91205800 |
| C | -3.14505500 | -0.75278400 | -0.59743000 |
| C | -2.39601900 | -0.86670700 | 0.60323700 |
| C | -2.39454700 | 0.25400000 | 1.47466700 |
| C | -3.06511200 | 1.42158600 | 1.16563400 |
| H | -4.38331900 | 0.48003700 | -1.84089700 |
| H | -3.17006200 | -1.59626100 | -1.27470000 |
| H | -1.83120600 | 0.19467200 | 2.40081500 |
| H | -3.03348300 | 2.26855200 | 1.84383500 |
| C | -4.46810300 | 2.72204800 | -0.37776300 |
| N | -5.02165300 | 3.71104900 | -0.65533900 |
| C | -1.57828700 | -2.00405500 | 0.92978000 |
| H | -1.10950300 | -1.96736500 | 1.90977500 |
| C | -1.79391700 | -3.33196500 | 0.38421500 |
| O | -2.58779600 | -3.66926800 | -0.48630100 |
| O | -0.97656700 | -4.31026000 | 0.90076800 |
| H | -0.33691700 | -3.89826900 | 1.50901700 |
| C | 4.12901500 | -0.48462100 | 0.60122300 |
| C | 3.51555000 | -0.22350000 | -0.63713000 |
| C | 3.50133700 | 1.09972300 | -1.11340700 |
| C | 4.08078700 | 2.12967500 | -0.37305600 |
| C | 4.68122300 | 1.85998100 | 0.85946500 |
| C | 4.70415000 | 0.54789500 | 1.34144200 |

| | | | |
|---|---|---|---|
| H | 4.13861700 | -1.50065000 | 0.98477400 |
| H | 3.01563100 | 1.31667900 | -2.05945200 |
| H | 4.05305000 | 3.14701400 | -0.75470500 |
| H | 5.12586600 | 2.66375400 | 1.43966100 |
| H | 5.16928300 | 0.32818100 | 2.29912900 |
| S | 2.71282000 | -1.50951300 | -1.55626700 |
| S | 0.58881900 | -1.69518700 | -0.30097800 |
| C | 0.45224600 | 0.06287700 | -0.07797200 |
| C | 0.88729800 | 0.65026700 | 1.11721000 |
| C | -0.08332600 | 0.87236100 | -1.08889400 |
| C | 0.78790300 | 2.03027000 | 1.29983900 |
| H | 1.30666700 | 0.02466500 | 1.89783500 |
| C | -0.18320700 | 2.25070700 | -0.90329700 |
| H | -0.41880800 | 0.41802400 | -2.01514900 |
| C | 0.25238900 | 2.83295900 | 0.29082700 |
| H | 1.13234400 | 2.47679000 | 2.22851500 |
| H | -0.60540400 | 2.87078500 | -1.68936300 |
| H | 0.17410500 | 3.90728400 | 0.43242200 |

**TS3-CF3**

| Atom | X | Y | Z |
|---|---|---|---|
| C | -2.11174700 | 3.16624100 | -0.95556700 |
| C | -2.48140700 | 2.23947100 | -1.95183100 |
| C | -3.10924500 | 1.05210600 | -1.60932300 |
| C | -3.40114400 | 0.73716900 | -0.25610500 |
| C | -3.03805400 | 1.69659600 | 0.72703200 |
| C | -2.40380500 | 2.87948100 | 0.39535500 |
| H | -2.25721100 | 2.45426600 | -2.99280800 |
| H | -3.37146800 | 0.34044700 | -2.38169500 |
| H | -3.24589900 | 1.48099200 | 1.77125900 |
| H | -2.11959000 | 3.58526100 | 1.17007400 |
| C | -1.43310500 | 4.36635200 | -1.30447200 |
| N | -0.87139500 | 5.34958300 | -1.58991600 |
| C | -3.96305100 | -0.51441500 | 0.18393000 |
| H | -4.21904100 | -0.55120900 | 1.23936000 |
| C | -4.68339700 | -1.42718800 | -0.67624400 |
| O | -4.77951000 | -1.39568300 | -1.90240800 |
| O | -5.31210300 | -2.47283600 | -0.03361500 |
| H | -5.13979400 | -2.42721500 | 0.92525200 |
| C | 1.98599700 | -2.29786700 | 1.17552000 |
| C | 1.10064300 | -3.01172500 | 0.34422100 |
| C | 1.31252100 | -2.98531100 | -1.04607500 |
| C | 2.35841500 | -2.24563300 | -1.59454300 |
| C | 3.21434200 | -1.52527100 | -0.75481700 |

| | | | |
|---|---|---|---|
| C | 3.03263800 | -1.56028500 | 0.63390000 |
| H | 1.83057500 | -2.30153900 | 2.24918900 |
| H | 0.63672800 | -3.52608800 | -1.70145800 |
| H | 2.49385200 | -2.22186600 | -2.67082000 |
| H | 3.69108000 | -0.99569500 | 1.28765800 |
| S | -0.30104700 | -3.82998900 | 1.04813900 |
| S | -2.04961600 | -2.14908900 | 0.56464300 |
| C | -0.95190400 | -0.78015500 | 0.83482700 |
| C | -0.68096000 | -0.31131800 | 2.12818200 |
| C | -0.33227500 | -0.17150000 | -0.26426700 |
| C | 0.20083900 | 0.74889700 | 2.31935000 |
| H | -1.15678800 | -0.78097500 | 2.98319500 |
| C | 0.54505800 | 0.89409900 | -0.08022400 |
| H | -0.53567400 | -0.53390800 | -1.26437200 |
| C | 0.81062000 | 1.35150900 | 1.21213100 |
| H | 0.40950600 | 1.10513900 | 3.32359100 |
| H | 1.01749300 | 1.35756400 | -0.93908600 |
| C | 1.79354700 | 2.45957100 | 1.43143500 |
| C | 4.29366300 | -0.65611100 | -1.31673400 |
| F | 2.01811300 | 3.20151400 | 0.31809400 |
| F | 1.39631100 | 3.32778000 | 2.40297300 |
| F | 3.01796800 | 1.99527700 | 1.83009700 |
| F | 4.50693300 | -0.85019400 | -2.64252000 |
| F | 4.01506200 | 0.67640600 | -1.16832800 |
| F | 5.49676700 | -0.84490900 | -0.70035400 |

**TS3-OMe**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 2.84528300 | 2.80067100 | -0.01924100 |
| C | 3.46015900 | 1.93638200 | 0.90801800 |
| C | 3.58931300 | 0.58631800 | 0.62748100 |
| C | 3.11318100 | 0.04197500 | -0.59075000 |
| C | 2.53561700 | 0.93755400 | -1.52443200 |
| C | 2.39307000 | 2.28465700 | -1.25052900 |
| H | 3.81237200 | 2.33222100 | 1.85560500 |
| H | 4.04535200 | -0.07582700 | 1.35145700 |
| H | 2.16630100 | 0.54529100 | -2.46698200 |
| H | 1.91998500 | 2.94513400 | -1.97016300 |
| C | 2.62844500 | 4.16952700 | 0.30221600 |
| N | 2.42558500 | 5.28699000 | 0.56853900 |
| C | 3.07463200 | -1.37385400 | -0.87921500 |
| H | 2.79198000 | -1.61342300 | -1.90132700 |
| C | 3.97313800 | -2.33874700 | -0.24897200 |
| O | 4.75493200 | -2.14392400 | 0.67081900 |

| | | | |
|---|---|---|---|
| O | 3.88142100 | -3.61505100 | -0.74181100 |
| H | 3.18260700 | -3.64773500 | -1.42030600 |
| C | -3.03307200 | -2.51429400 | -0.63260000 |
| C | -2.38273200 | -2.35498400 | 0.60985700 |
| C | -2.74795200 | -1.24044400 | 1.38483700 |
| C | -3.68039300 | -0.30350700 | 0.94030700 |
| C | -4.28345400 | -0.46467600 | -0.31341000 |
| C | -3.96964200 | -1.59338300 | -1.08564800 |
| H | -2.77747300 | -3.36488500 | -1.25816400 |
| H | -2.26771800 | -1.08755500 | 2.34615900 |
| H | -3.90811100 | 0.55450800 | 1.56224700 |
| H | -4.44903100 | -1.71539800 | -2.05293800 |
| S | -1.10272200 | -3.45115300 | 1.13859500 |
| S | 1.05369500 | -2.24769400 | 0.09216700 |
| C | 0.22121000 | -0.69486600 | -0.00780500 |
| C | -0.49904800 | -0.33927300 | -1.16169800 |
| C | 0.27956000 | 0.22209400 | 1.04884800 |
| C | -1.13310200 | 0.89091000 | -1.25557000 |
| H | -0.55857300 | -1.03794200 | -1.98939000 |
| C | -0.34603000 | 1.46578200 | 0.96600400 |
| H | 0.82616300 | -0.03734400 | 1.94911100 |
| C | -1.05763000 | 1.80430400 | -0.19262600 |
| H | -1.69514900 | 1.16505700 | -2.14294800 |
| H | -0.27342300 | 2.15474400 | 1.79877700 |
| O | -1.71008400 | 2.98443700 | -0.37634700 |
| O | -5.17205200 | 0.41451100 | -0.86072100 |
| C | -1.63588300 | 3.95561900 | 0.66724800 |
| H | -0.59991400 | 4.26911300 | 0.84522700 |
| H | -2.21879800 | 4.81041900 | 0.31975500 |
| H | -2.06986600 | 3.57456200 | 1.59914300 |
| C | -5.33937600 | 1.66937100 | -0.20464000 |
| H | -4.38197900 | 2.19776100 | -0.11150200 |
| H | -6.01517000 | 2.24991400 | -0.83611600 |
| H | -5.78969800 | 1.55139700 | 0.78877400 |

**TS4**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 5.46209700 | -0.45057600 | -0.15698200 |
| C | 4.94644600 | 0.54420400 | 0.69243500 |
| C | 3.57540300 | 0.75899100 | 0.74612500 |
| C | 2.69993500 | -0.00875700 | -0.03847100 |
| C | 3.22601500 | -0.99692400 | -0.88204600 |
| C | 4.59576200 | -1.22561700 | -0.94540000 |
| H | 5.62201200 | 1.13600200 | 1.30124200 |

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|---|---|---|---|
| H | 3.16084900 | 1.50824200 | 1.41028100 |
| H | 2.55344300 | -1.59169100 | -1.49314800 |
| H | 4.99827400 | -1.99332400 | -1.59775700 |
| C | 6.87260500 | -0.67506600 | -0.21743700 |
| N | 8.02114600 | -0.85740500 | -0.26640600 |
| C | 1.21060000 | 0.22288900 | 0.00437100 |
| H | 0.71459300 | -0.53593800 | -0.60010100 |
| C | 0.66126000 | 0.17003700 | 1.46019500 |
| O | 0.91525100 | 1.08898800 | 2.24556400 |
| O | 0.00379300 | -0.89882200 | 1.74633700 |
| H | -0.54188900 | -1.64330200 | 0.69576100 |
| C | -3.96147700 | -1.99587800 | -0.90579500 |
| C | -2.90986700 | -1.79035300 | 0.00407300 |
| C | -3.18048300 | -1.10508200 | 1.20168400 |
| C | -4.47053300 | -0.65397900 | 1.48013000 |
| C | -5.51438200 | -0.87032900 | 0.57691200 |
| C | -5.24893900 | -1.54142900 | -0.61933200 |
| H | -3.76743500 | -2.51402500 | -1.84125500 |
| H | -2.37286800 | -0.92049100 | 1.90268500 |
| H | -4.65831700 | -0.12355800 | 2.41055800 |
| H | -6.51738100 | -0.51686400 | 0.79893900 |
| H | -6.04716200 | -1.71209200 | -1.33752300 |
| S | -1.28573600 | -2.42198500 | -0.36941800 |
| S | 0.86490000 | 1.84939900 | -0.82683000 |
| C | -0.92634500 | 1.88375600 | -0.72264600 |
| C | -1.70238100 | 1.38662000 | -1.77721300 |
| C | -1.55224300 | 2.44407400 | 0.39939000 |
| C | -3.09491600 | 1.46097300 | -1.71470800 |
| H | -1.21602600 | 0.94481900 | -2.64136500 |
| C | -2.94415400 | 2.52038700 | 0.45350800 |
| H | -0.94479200 | 2.80138700 | 1.22344200 |
| C | -3.71637600 | 2.03614000 | -0.60480500 |
| H | -3.69278800 | 1.06978900 | -2.53270500 |
| H | -3.42609700 | 2.95569200 | 1.32456700 |
| H | -4.79956600 | 2.09276800 | -0.55796400 |

**TS5**

| Atom | X | Y | Z |
|---|---|---|---|
| C | -3.00448900 | -1.51795700 | -0.15612100 |
| C | -1.96084300 | -1.32366600 | -1.09396200 |
| C | -0.94067300 | -0.43079600 | -0.84709800 |
| C | -0.88912200 | 0.34661400 | 0.35414300 |
| C | -1.95127100 | 0.12331000 | 1.29277900 |
| C | -2.96995500 | -0.76866000 | 1.04828500 |

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|---|---|---|---|
| H | -1.96591200 | -1.89612300 | -2.01782100 |
| H | -0.14958300 | -0.30987600 | -1.57988200 |
| H | -1.94552200 | 0.68533900 | 2.22290100 |
| H | -3.75755100 | -0.90879500 | 1.78382700 |
| C | -4.04576300 | -2.44009500 | -0.40868000 |
| N | -4.90879800 | -3.20208600 | -0.61790500 |
| C | 0.10769400 | 1.31130100 | 0.63154900 |
| H | 0.17393700 | 1.69429900 | 1.64546700 |
| C | -1.27040000 | 3.22256000 | -0.09667400 |
| O | -1.73350500 | 3.50707400 | 0.95482500 |
| O | -1.05215100 | 3.25945500 | -1.25909400 |
| C | 4.58370800 | -1.20104100 | -0.59334700 |
| C | 3.76187400 | -0.09052200 | -0.78224400 |
| C | 2.57253800 | 0.04271300 | -0.04880600 |
| C | 2.21985200 | -0.95218600 | 0.87039200 |
| C | 3.04515900 | -2.06412600 | 1.05065400 |
| C | 4.22966800 | -2.19621200 | 0.32282200 |
| H | 5.50284400 | -1.29023900 | -1.16702300 |
| H | 4.04334600 | 0.67478300 | -1.50220800 |
| H | 1.30148300 | -0.85165900 | 1.43980400 |
| H | 2.75800300 | -2.83080800 | 1.76612500 |
| H | 4.86896200 | -3.06278800 | 0.46587100 |
| S | 1.55556000 | 1.50067700 | -0.34748300 |

**TS6**

| Atom | X | Y | Z |
|---|---|---|---|
| C | -4.02412000 | -0.38535000 | -0.45125700 |
| C | -3.06903300 | 0.18665400 | -1.32676000 |
| C | -2.03670400 | 0.96169200 | -0.84256100 |
| C | -1.87953400 | 1.22818900 | 0.55552900 |
| C | -2.86360700 | 0.64285800 | 1.41902500 |
| C | -3.89250200 | -0.13529700 | 0.93864200 |
| H | -3.15507000 | 0.00730700 | -2.39519200 |
| H | -1.31576700 | 1.38209700 | -1.53615700 |
| H | -2.78570900 | 0.82142200 | 2.48878700 |
| H | -4.61815300 | -0.56147700 | 1.62618300 |
| C | -5.07850400 | -1.18496000 | -0.94923600 |
| N | -5.95109900 | -1.84633700 | -1.36168700 |
| C | -0.78021800 | 1.92775200 | 1.11089000 |
| H | -0.87204600 | 2.25692500 | 2.14449700 |
| C | 2.84647200 | 0.89537400 | -2.21058900 |
| C | 1.77183600 | 1.67401200 | -1.77450900 |
| C | 1.62670000 | 1.97999700 | -0.41592400 |
| C | 2.57880900 | 1.51446700 | 0.49920500 |

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|---|---|---|---|
| C | 3.64252200 | 0.72380400 | 0.06378200 |
| C | 3.77827400 | 0.40983500 | -1.29118600 |
| H | 2.94503500 | 0.65543200 | -3.26598100 |
| H | 1.03682700 | 2.03693800 | -2.48732400 |
| H | 2.47475200 | 1.75644800 | 1.55153600 |
| H | 4.36598300 | 0.35140300 | 0.78393900 |
| H | 4.60443000 | -0.21055200 | -1.62684300 |
| S | 0.23697700 | 3.00207400 | 0.11899800 |
| C | 1.10649700 | -2.15110800 | -1.28544500 |
| C | 0.59714500 | -1.44683700 | -0.19487100 |
| C | 1.18696700 | -1.58356500 | 1.07132400 |
| C | 2.27900900 | -2.45157800 | 1.22411700 |
| C | 2.77204900 | -3.16514600 | 0.13104500 |
| C | 2.19371800 | -3.01465700 | -1.13137600 |
| H | 0.64617700 | -2.02176100 | -2.26163000 |
| H | -0.25410700 | -0.78915400 | -0.32975700 |
| H | 2.74981900 | -2.55869000 | 2.19745400 |
| H | 3.61980800 | -3.83175500 | 0.26697100 |
| H | 2.58590200 | -3.56189200 | -1.98389800 |
| S | 0.57722900 | -0.69108400 | 2.48930700 |
| H | 0.06785300 | 0.45904000 | 1.78728300 |

**TS7**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 2.06216100 | 0.00007400 | 0.02376700 |
| C | 1.37323600 | -1.22013100 | -0.24648800 |
| C | 0.09923100 | -1.22435800 | -0.75170800 |
| C | -0.62886900 | -0.00354500 | -1.03841800 |
| C | 0.09879500 | 1.21919600 | -0.75893800 |
| C | 1.37278500 | 1.21841200 | -0.25366400 |
| H | 1.87806900 | -2.16283900 | -0.04693800 |
| H | -0.39579500 | -2.17382100 | -0.94474200 |
| H | -0.39654500 | 2.16732400 | -0.95763200 |
| H | 1.87728700 | 2.16246100 | -0.05969600 |
| C | 3.37057800 | 0.00180700 | 0.53564100 |
| N | 4.46417000 | 0.00322400 | 0.96361600 |
| C | -1.92734700 | -0.00522400 | -1.51239400 |
| H | -2.41930000 | 0.92081800 | -1.79624600 |
| C | -2.87950300 | 0.00325000 | 0.93474800 |
| O | -2.93794500 | 1.17124500 | 1.07481300 |
| O | -2.93961200 | -1.16376400 | 1.08208200 |
| H | -2.41885800 | -0.93324400 | -1.79050200 |

**TS8**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 4.10473700 | -0.61336200 | -0.19819200 |
| C | 4.03726700 | 0.54809300 | -0.98948000 |
| C | 3.30515600 | 1.63824600 | -0.54297000 |
| C | 2.63629600 | 1.60203600 | 0.69415700 |
| C | 2.72740400 | 0.43947300 | 1.48023800 |
| C | 3.44744500 | -0.66336400 | 1.04286000 |
| H | 4.54880400 | 0.57997500 | -1.94553100 |
| H | 3.23186600 | 2.52738600 | -1.16212700 |
| H | 2.21257800 | 0.40028200 | 2.43420100 |
| H | 3.50045200 | -1.56264600 | 1.64694000 |
| C | 4.83471500 | -1.75022100 | -0.66215500 |
| N | 5.42695400 | -2.67815300 | -1.04092100 |
| C | 1.77464600 | 2.70874900 | 1.11431400 |
| H | 1.53434500 | 2.73694700 | 2.17379800 |
| C | -4.13007500 | 0.14934700 | 0.72884400 |
| C | -3.64663700 | 0.22342800 | -0.60147500 |
| C | -3.29826800 | -1.00900800 | -1.20743900 |
| C | -3.44599500 | -2.22507900 | -0.54288000 |
| C | -3.93846000 | -2.27086900 | 0.76589400 |
| C | -4.27406200 | -1.06732700 | 1.39468800 |
| H | -4.39806800 | 1.07286300 | 1.23638200 |
| H | -2.90882700 | -0.99705100 | -2.22221200 |
| H | -3.16611600 | -3.14657800 | -1.04968500 |
| H | -4.05172400 | -3.21930100 | 1.28403300 |
| H | -4.65236900 | -1.07516000 | 2.41522200 |
| S | -3.49161800 | 1.75598500 | -1.45510900 |
| S | -0.20431300 | 2.38850500 | 0.19342000 |
| C | -0.15958600 | 0.61136100 | 0.16652400 |
| C | -0.55055400 | -0.12854600 | 1.29258800 |
| C | 0.33509500 | -0.06403000 | -0.95901800 |
| C | -0.42560400 | -1.51794400 | 1.30061900 |
| H | -0.94000200 | 0.38925400 | 2.16331600 |
| C | 0.45801100 | -1.45351500 | -0.94802800 |
| H | 0.63515000 | 0.50411700 | -1.83297200 |
| C | 0.08692400 | -2.18243100 | 0.18429200 |
| H | -0.72976500 | -2.08059800 | 2.17852000 |
| H | 0.85212600 | -1.96561700 | -1.82149600 |
| H | 0.18818800 | -3.26400300 | 0.19312000 |
| H | 2.01885100 | 3.68515500 | 0.70168200 |

**TS9**

| Atom | X | Y | Z |
|---|---|---|---|
| C | 3.70234600 | 1.59190000 | 0.03110000 |

| | | | |
|---|---|---|---|
| C | 3.67665900 | 0.76561300 | -1.12414300 |
| C | 3.00334400 | -0.43313500 | -1.12133600 |
| C | 2.29556700 | -0.91046000 | 0.03591400 |
| C | 2.35008900 | -0.06091200 | 1.19554700 |
| C | 3.01955200 | 1.13797500 | 1.19282800 |
| H | 4.19158600 | 1.09688800 | -2.02235000 |
| H | 2.99105700 | -1.04211100 | -2.02199000 |
| H | 1.82762400 | -0.37988400 | 2.09343300 |
| H | 3.02349100 | 1.75965000 | 2.08431500 |
| C | 4.36501600 | 2.83673100 | 0.01980100 |
| N | 4.91403300 | 3.87174200 | 0.01092800 |
| C | 1.61535500 | -2.13117200 | 0.04233000 |
| H | 1.01251900 | -2.42474400 | 0.89401600 |
| C | 3.56301400 | -3.37573400 | 0.80359800 |
| O | 3.41904700 | -3.31318700 | 1.97835600 |
| O | 4.05706900 | -3.66825700 | -0.23323000 |
| C | -4.84006500 | 1.42338300 | 0.88742400 |
| C | -4.13477600 | 1.00369300 | -0.24180100 |
| C | -3.99188500 | -0.36504000 | -0.51135900 |
| C | -4.55137800 | -1.30850400 | 0.36307400 |
| C | -5.24791400 | -0.88327700 | 1.49299500 |
| C | -5.39424600 | 0.48249400 | 1.75684700 |
| H | -4.94619800 | 2.48516800 | 1.09154700 |
| H | -3.68828800 | 1.73156800 | -0.91145800 |
| H | -4.43232400 | -2.36807800 | 0.15823500 |
| H | -5.67873300 | -1.61753600 | 2.16805900 |
| H | -5.93770500 | 0.80984500 | 2.63867600 |
| S | -3.05611300 | -0.87989900 | -1.94125300 |
| C | 0.29579400 | 2.49614200 | -0.88520600 |
| C | -0.01401800 | 1.21303200 | -1.33297300 |
| C | -0.67035100 | 0.31493300 | -0.48030700 |
| C | -1.01373700 | 0.71077400 | 0.81896400 |
| C | -0.70028000 | 1.99700600 | 1.26190100 |
| C | -0.04845900 | 2.89128200 | 0.41088500 |
| H | 0.81265100 | 3.18664300 | -1.54562000 |
| H | 0.25134300 | 0.90378100 | -2.33846300 |
| H | -1.52257400 | 0.01308300 | 1.47595500 |
| H | -0.96852500 | 2.29865100 | 2.27055100 |
| H | 0.19728100 | 3.89137300 | 0.75664800 |
| S | -1.10269500 | -1.32362000 | -1.03764400 |
| H | 1.52281200 | -2.71898200 | -0.86320400 |

**TS10**

| Atom | X | Y | Z |
|---|---|---|---|

| | | | |
|---|---|---|---|
| C | -0.86625700 | 2.28318700 | -0.14981800 |
| C | 0.25485400 | 2.40833900 | 0.70897400 |
| C | 1.40007200 | 1.67319900 | 0.48840200 |
| C | 1.50382600 | 0.75668700 | -0.60344600 |
| C | 0.38380200 | 0.69389500 | -1.48633000 |
| C | -0.76723100 | 1.42194300 | -1.27201100 |
| H | 0.19359300 | 3.08271300 | 1.55974400 |
| H | 2.26282900 | 1.74261200 | 1.14178900 |
| H | 0.42973900 | 0.01658200 | -2.33634800 |
| H | -1.61089200 | 1.33012600 | -1.95019900 |
| C | -2.06174400 | 2.99439500 | 0.10977800 |
| N | -3.05318800 | 3.57618700 | 0.32764100 |
| C | 2.58879400 | -0.17954500 | -0.74042400 |
| H | 2.59605500 | -0.69057700 | -1.70887000 |
| C | 4.00363600 | 0.03448000 | -0.19616300 |
| O | 4.14865100 | 0.75779300 | 0.83505500 |
| O | 4.91135700 | -0.59182200 | -0.81025200 |
| C | -1.96736600 | -0.87292300 | 1.20507100 |
| C | -0.65832600 | -1.16641600 | 1.51682300 |
| C | 0.12249800 | -2.07480400 | 0.73832500 |
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| C | -1.85662200 | -2.42575600 | -0.67245000 |
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| H | -2.52812600 | -0.16487500 | 1.80841800 |
| H | -0.18787000 | -0.66840500 | 2.36092700 |
| H | 0.00288400 | -3.43278000 | -0.95302200 |
| H | -2.33250000 | -2.91486600 | -1.51806800 |
| H | 2.11229300 | -1.20802700 | 0.09233800 |
| C | 1.52980900 | -2.22426300 | 0.93966500 |
| H | 1.91493200 | -1.94004700 | 1.92166200 |
| H | 1.98322300 | -3.13818800 | 0.54897400 |
| C | -3.92595500 | -1.15693700 | -0.25980300 |
| N | -5.02647800 | -0.88301200 | -0.54843800 |

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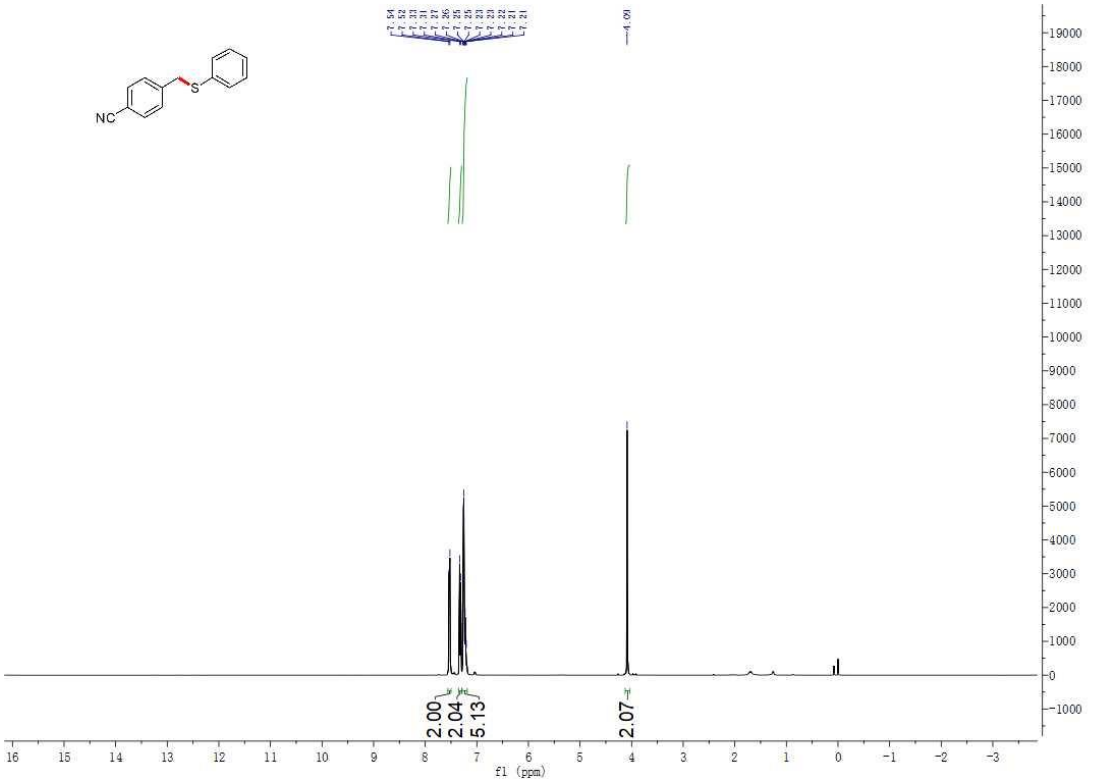
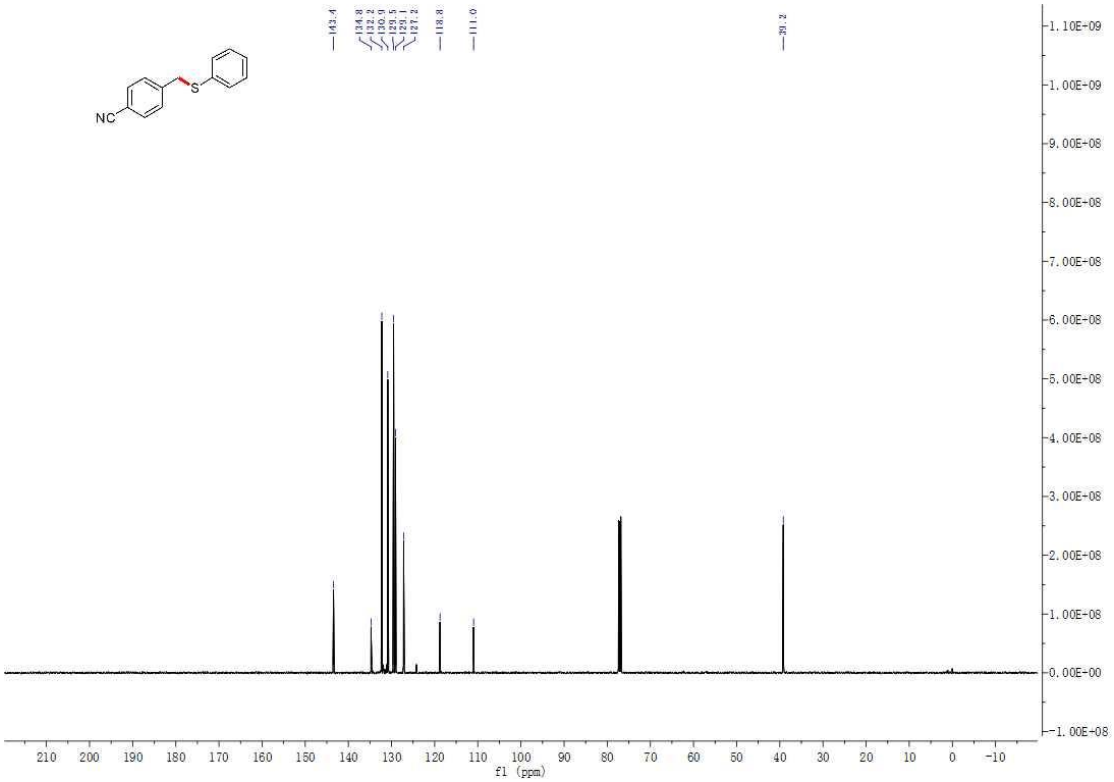
## 7. NMR Spectra

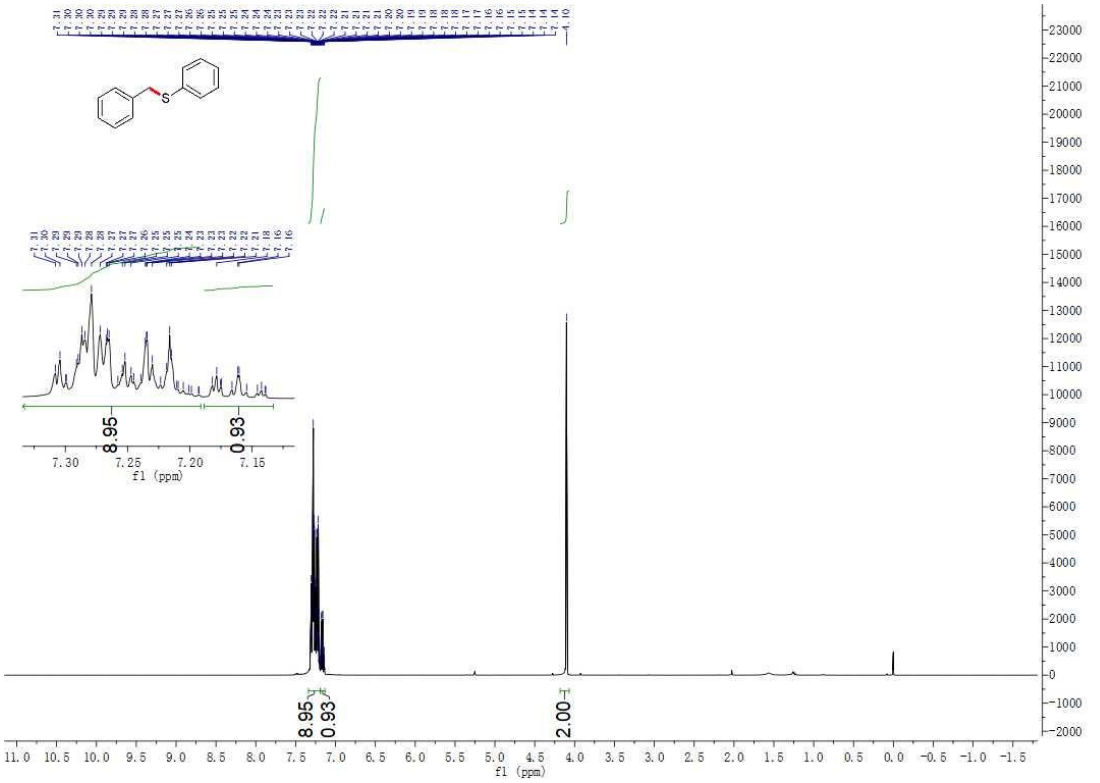
$^{1}$H NMR spectrum of **4-((phenylthio)methyl)benzonitrile (3)**




$^{13}$C NMR spectrum of **4-((phenylthio)methyl)benzonitrile (3)**



$^{1}$H NMR spectrum of **benzyl(phenyl)sulfane (4)**

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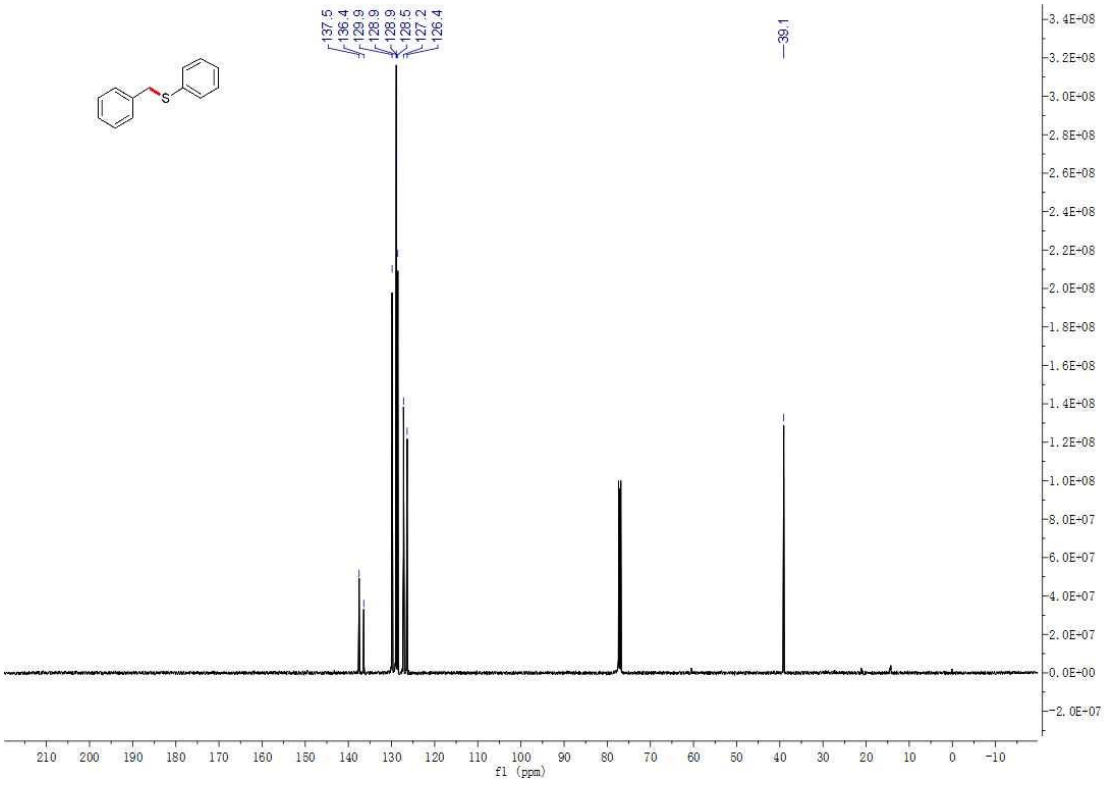
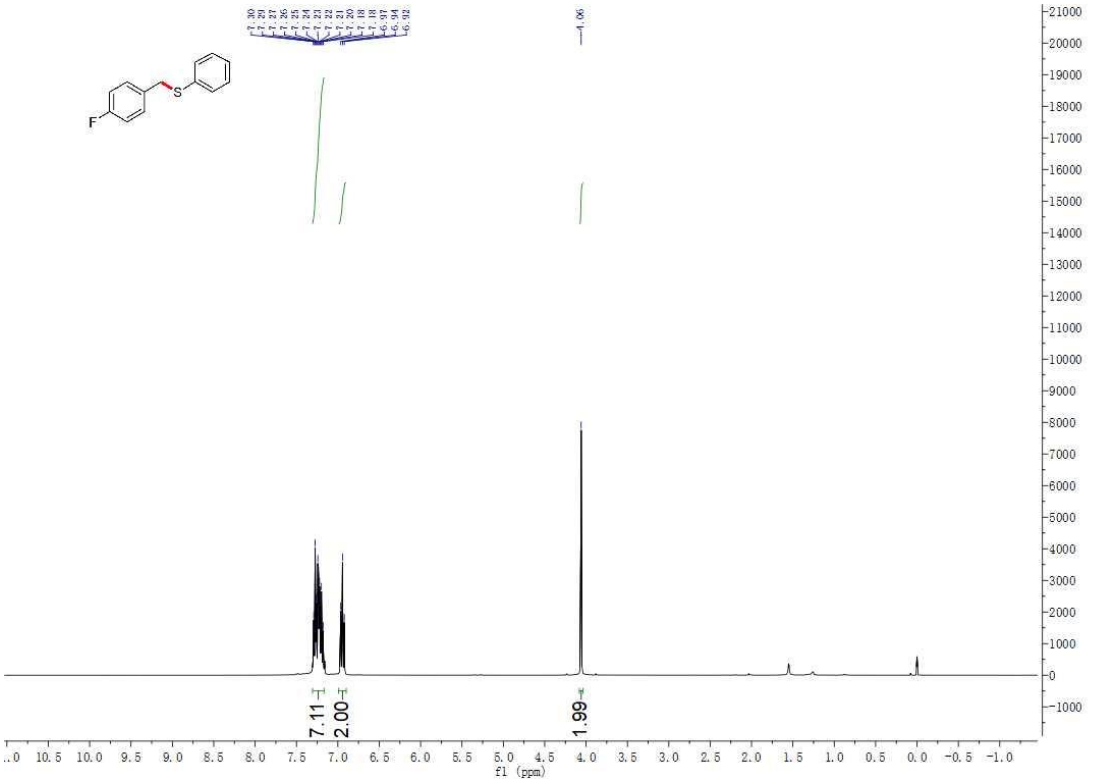


$^{1}$H NMR spectrum of **(4-fluorobenzyl)(phenyl)sulfane (5)**

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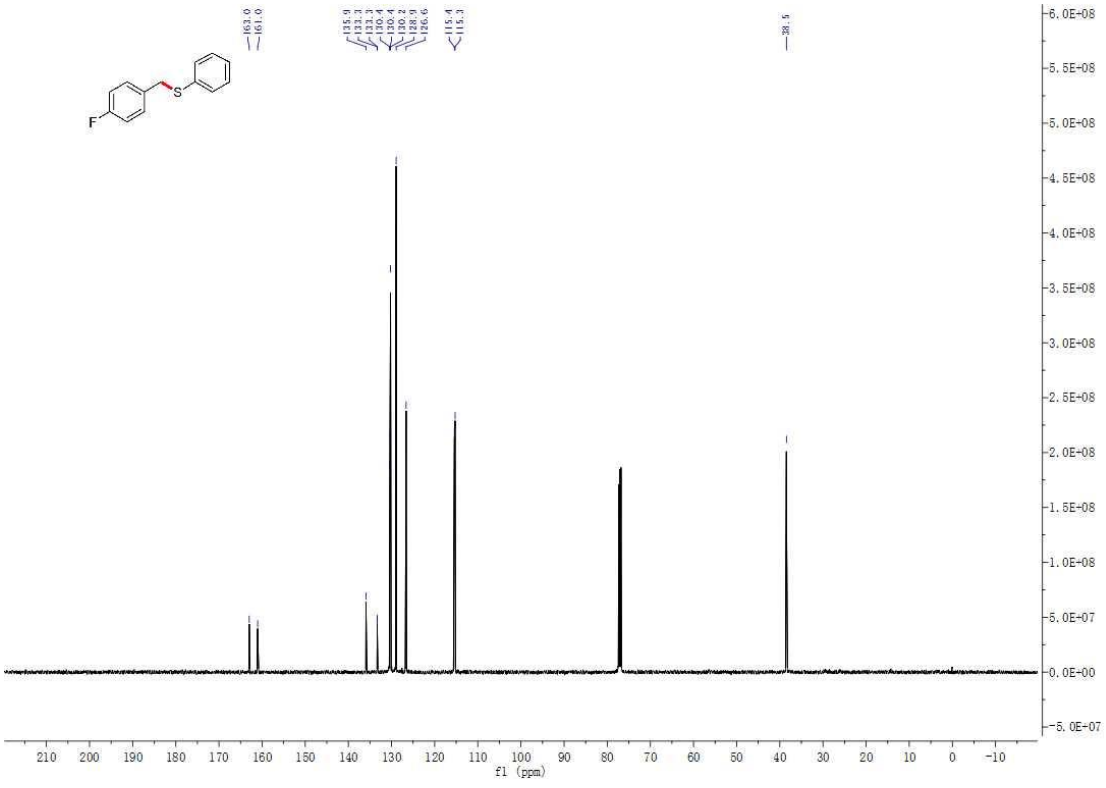

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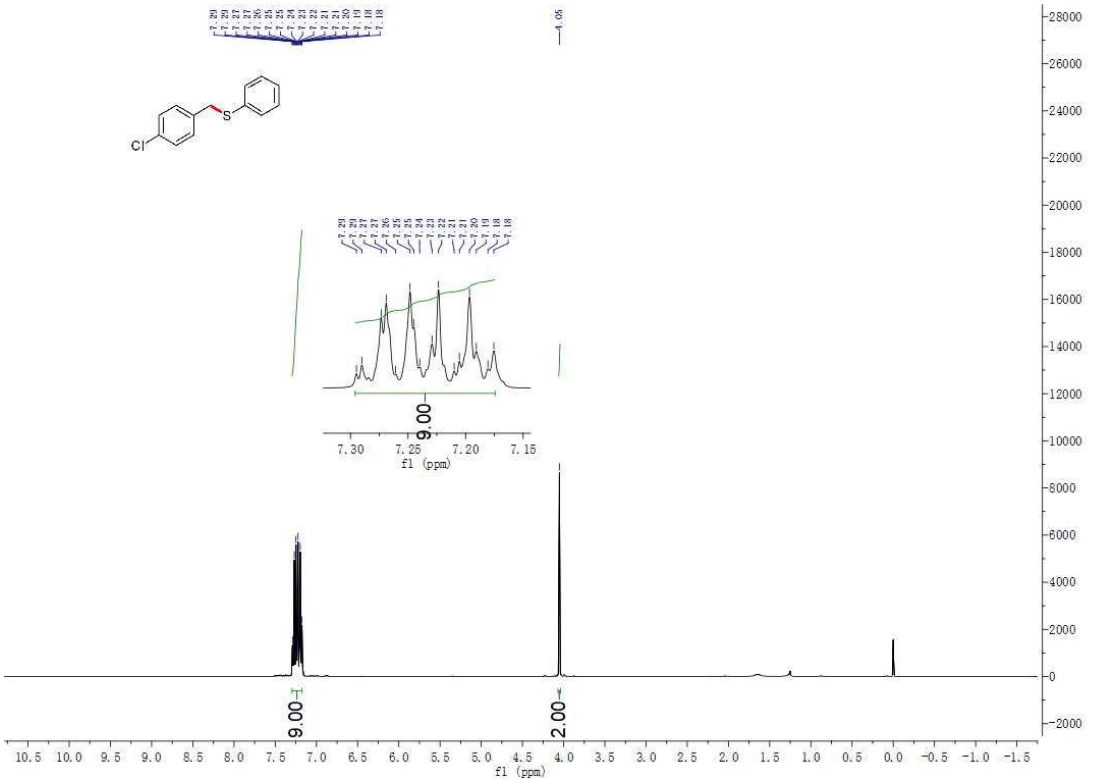


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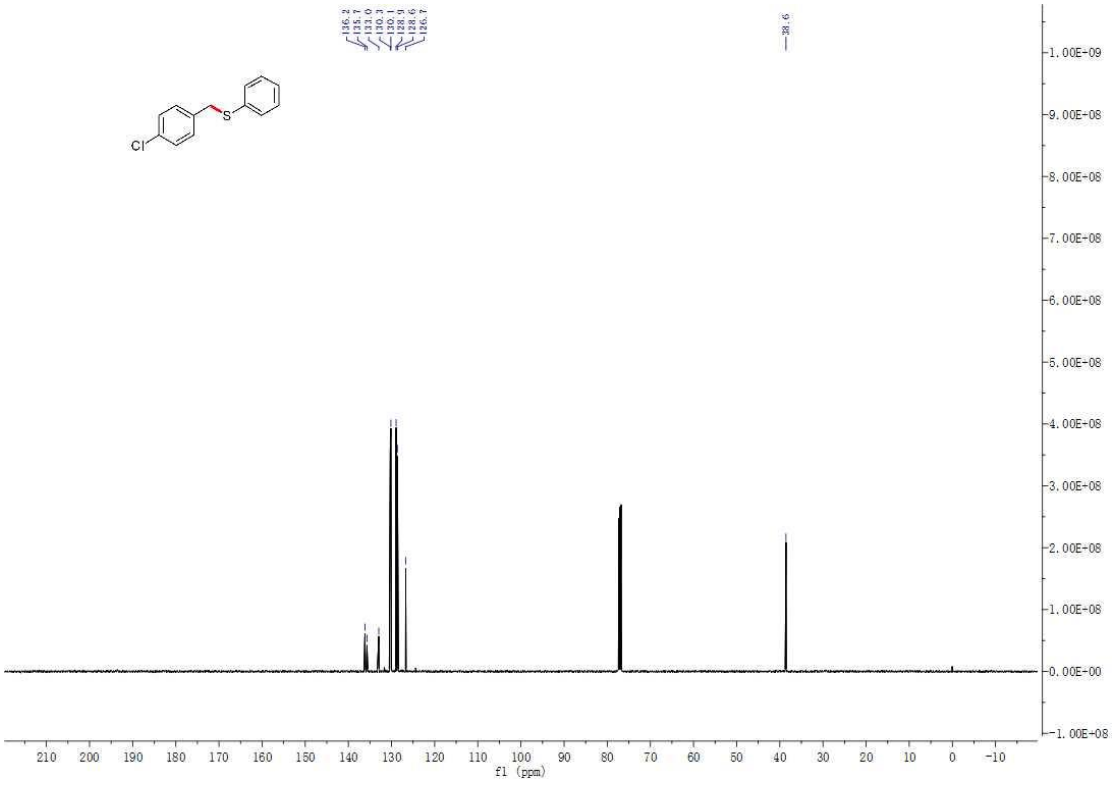
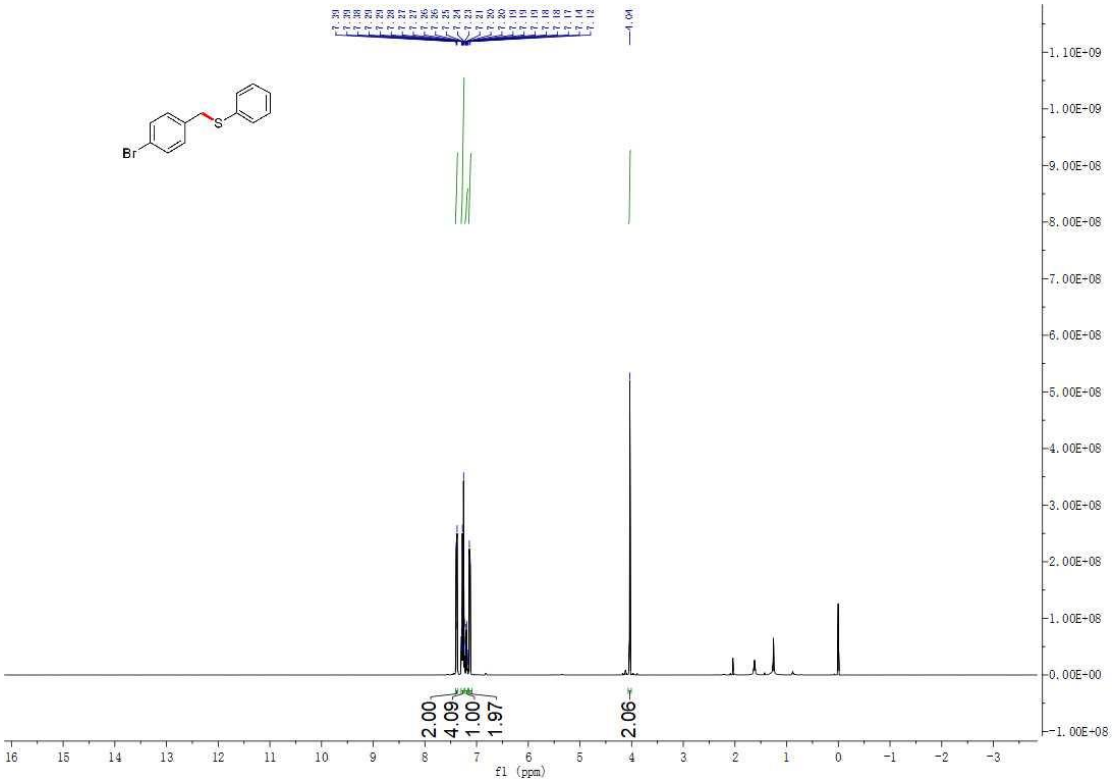


$^{1}$H NMR spectrum of **(4-bromobenzyl)(phenyl)sulfane (7)**

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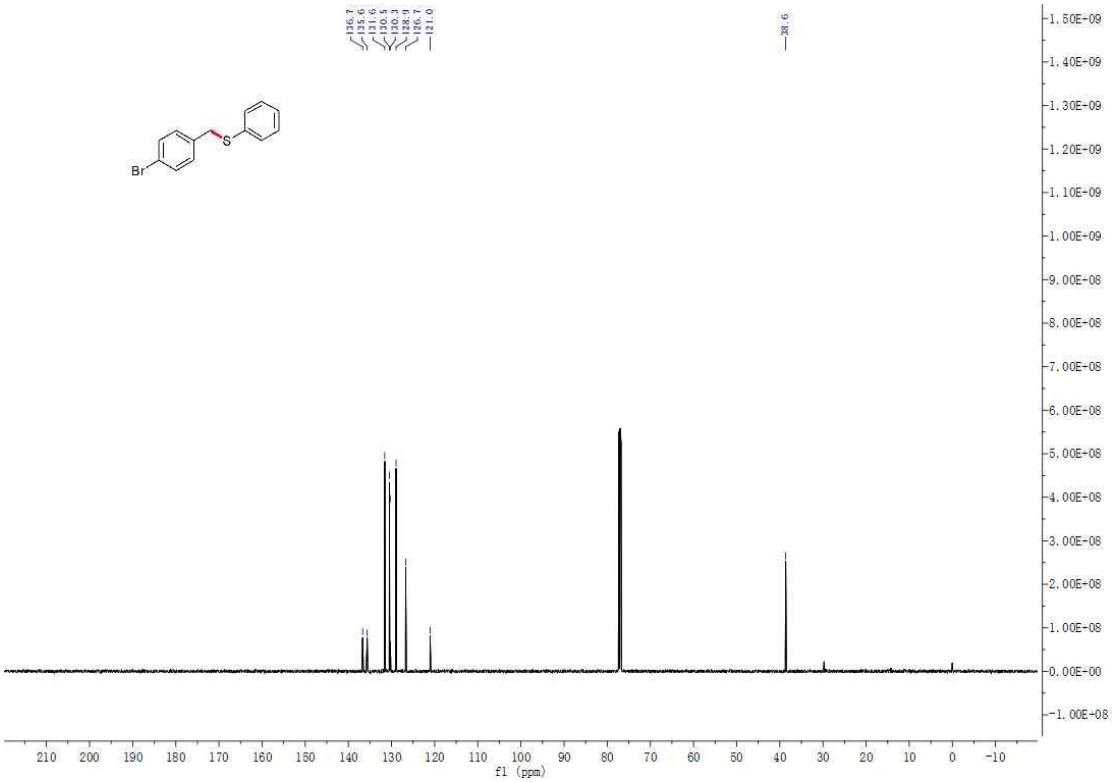
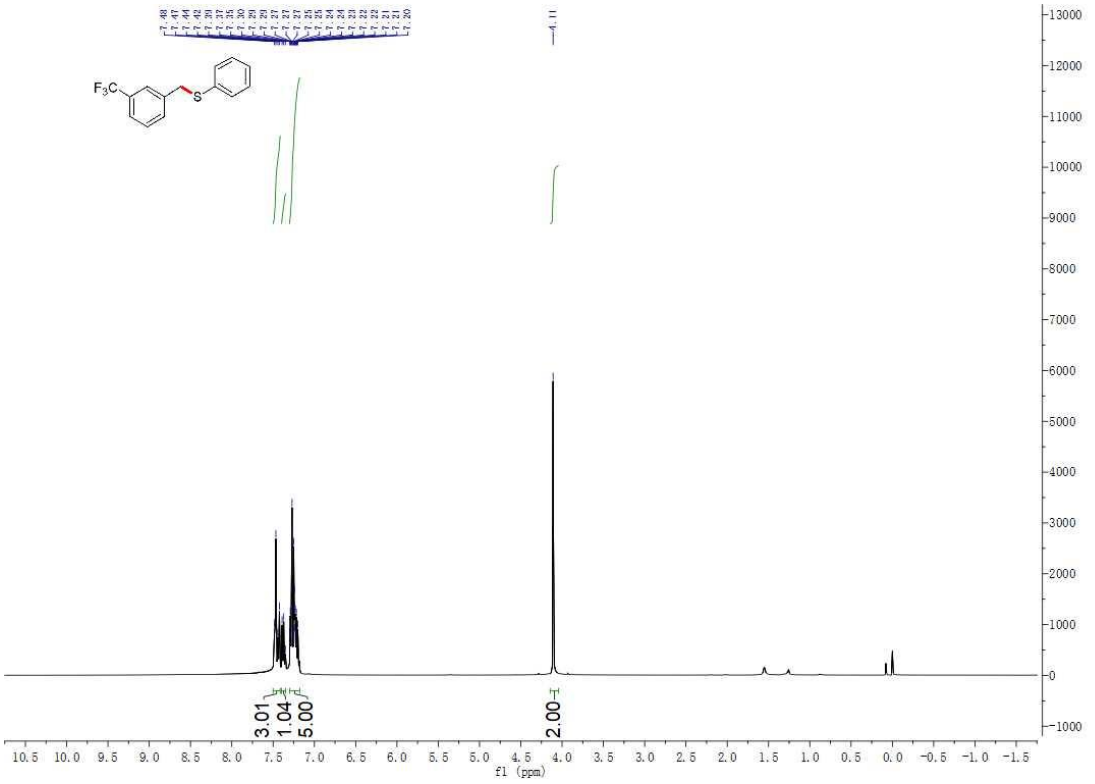
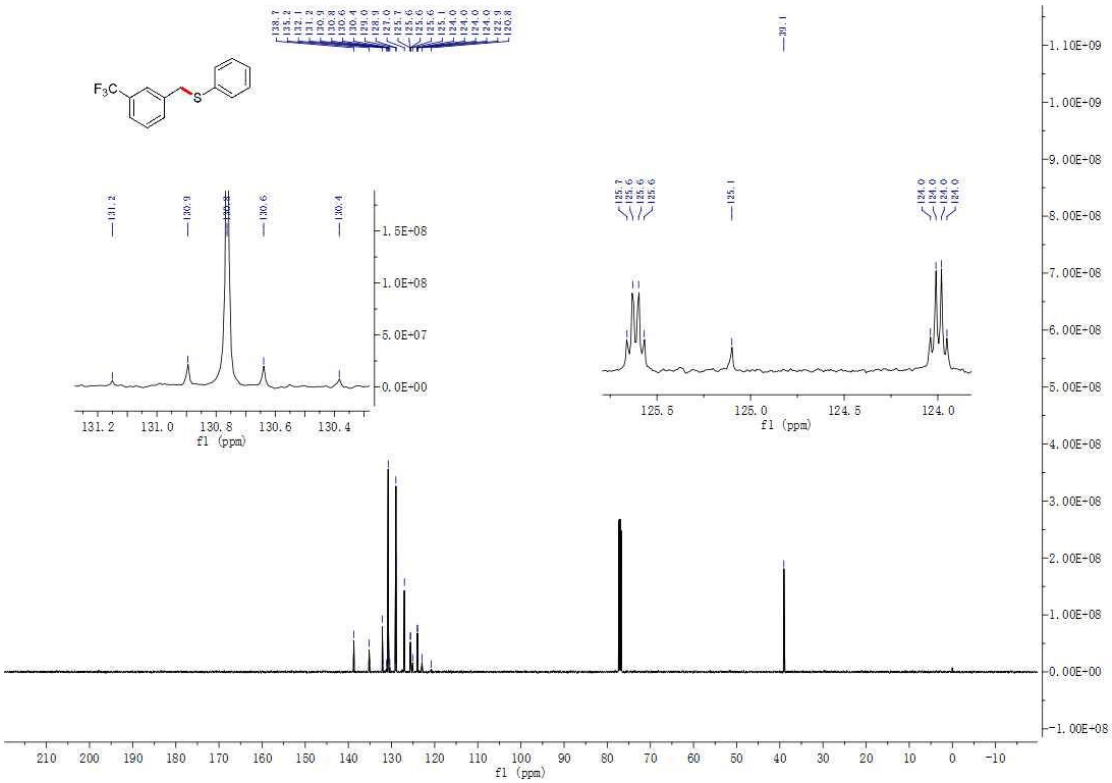


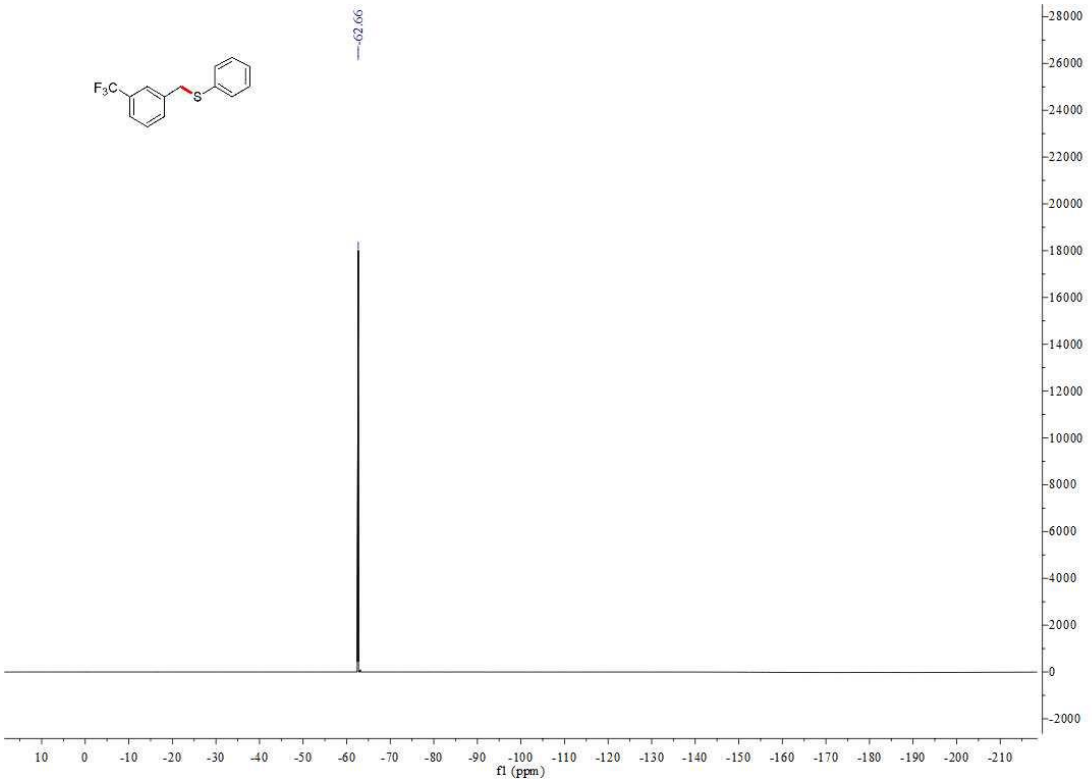
$^{1}$H NMR spectrum of **phenyl(3-(trifluoromethyl)benzyl)sulfane (8)**




$^{13}$C NMR spectrum of **phenyl(3-(trifluoromethyl)benzyl)sulfane (8)**



$^{19}$F NMR spectrum of **phenyl(3-(trifluoromethyl)benzyl)sulfane (8)**

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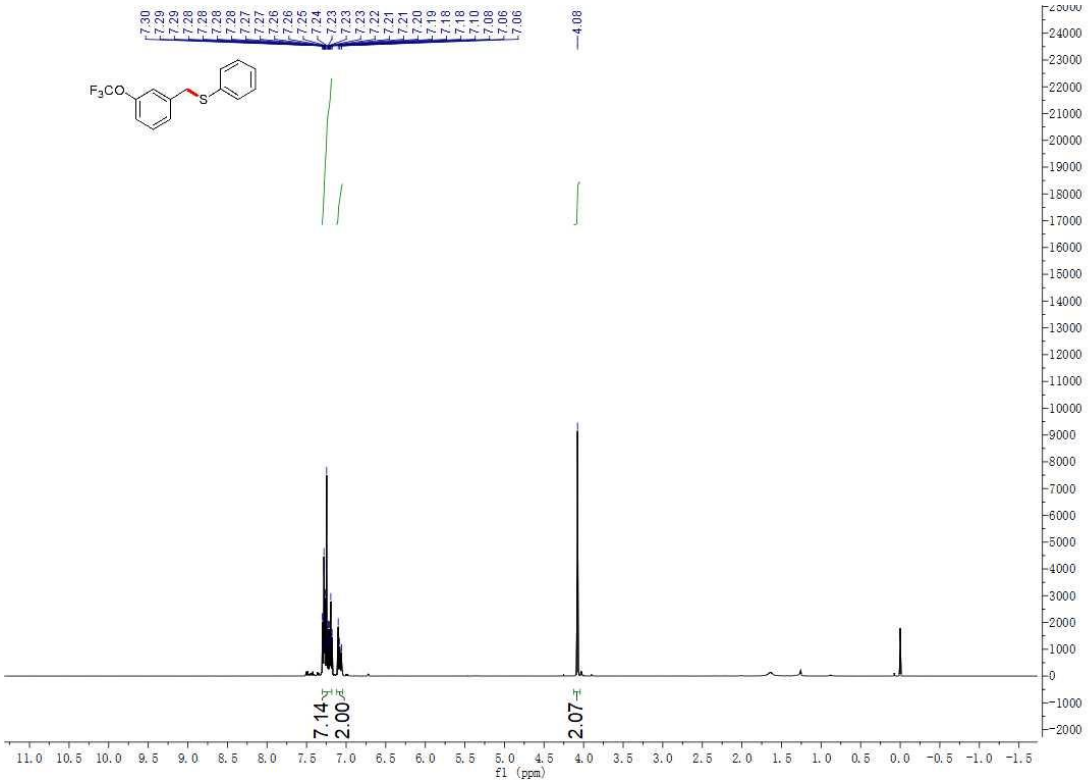
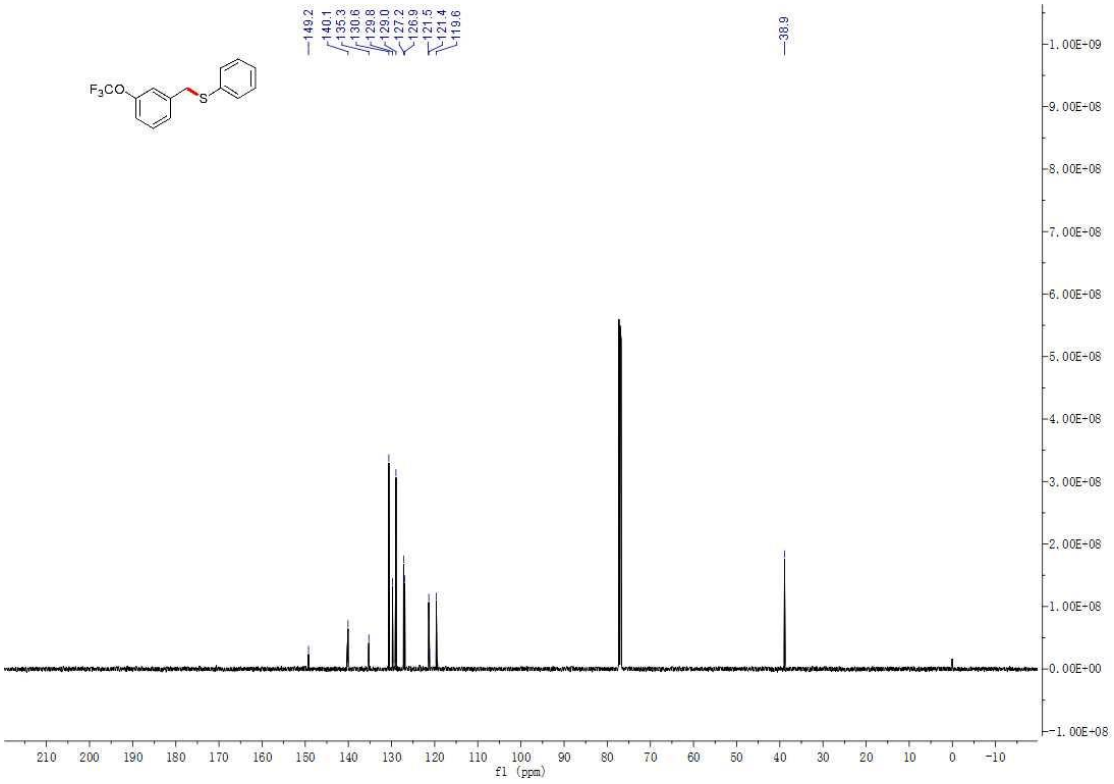
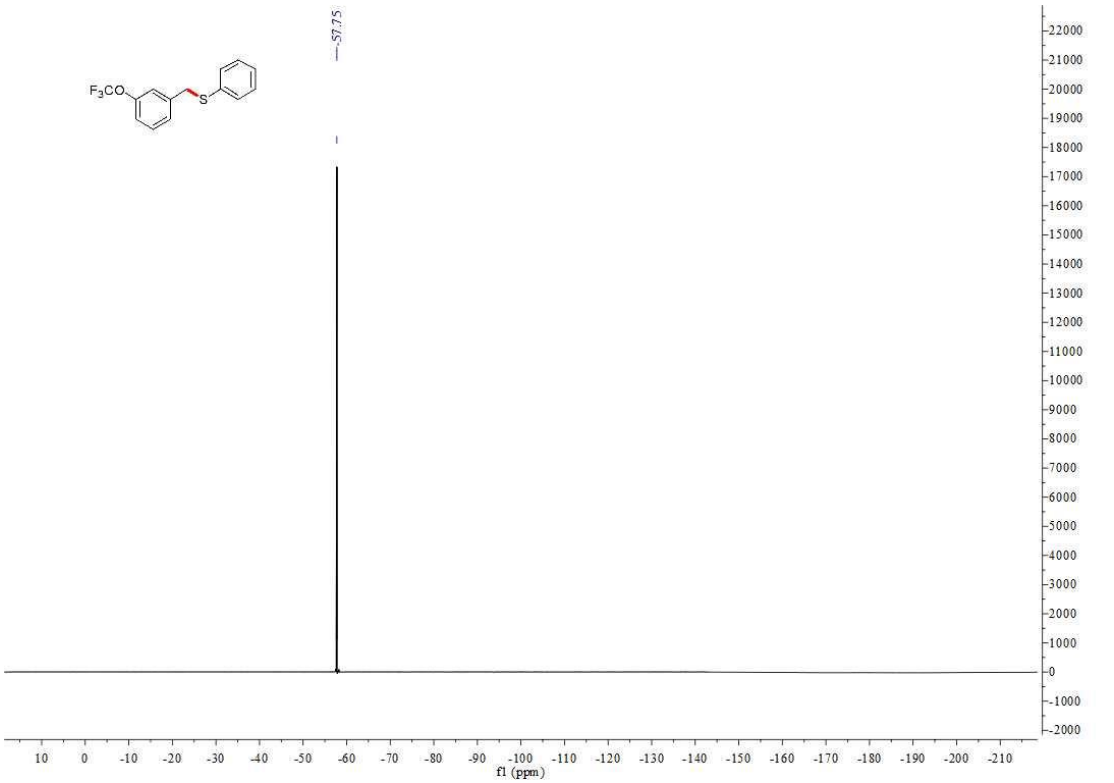


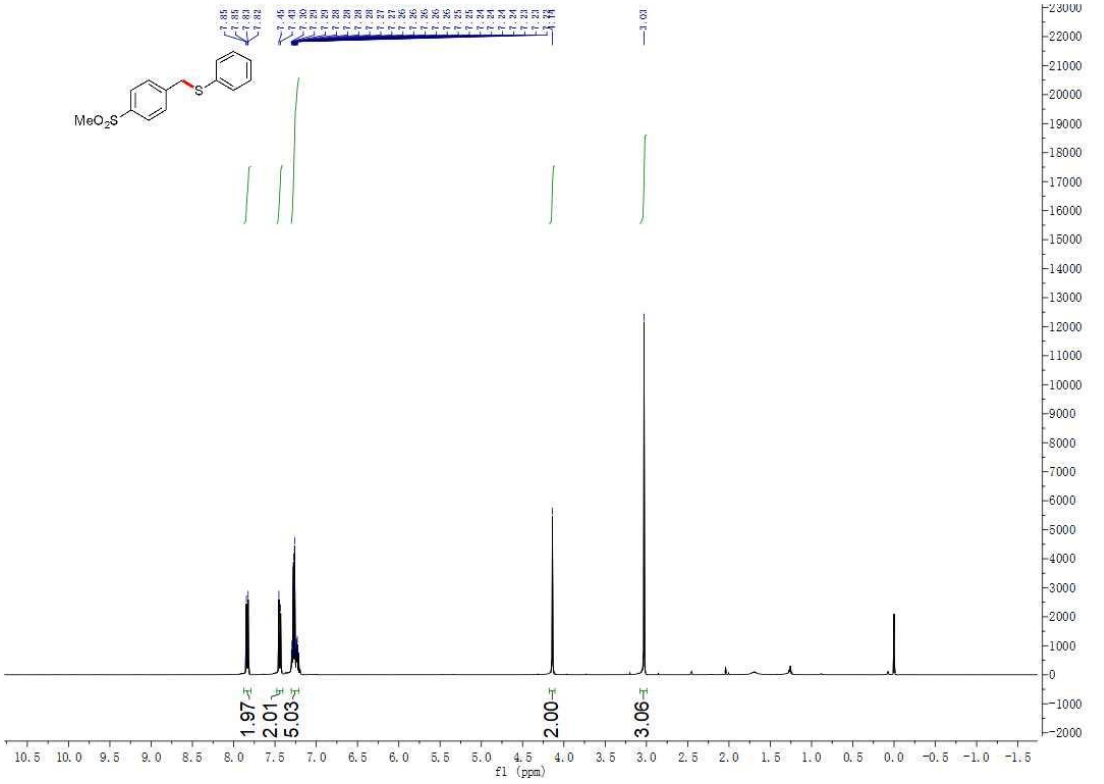
$^{13}$C NMR spectrum of **phenyl(3-(trifluoromethoxy)benzyl)sulfane (9)**



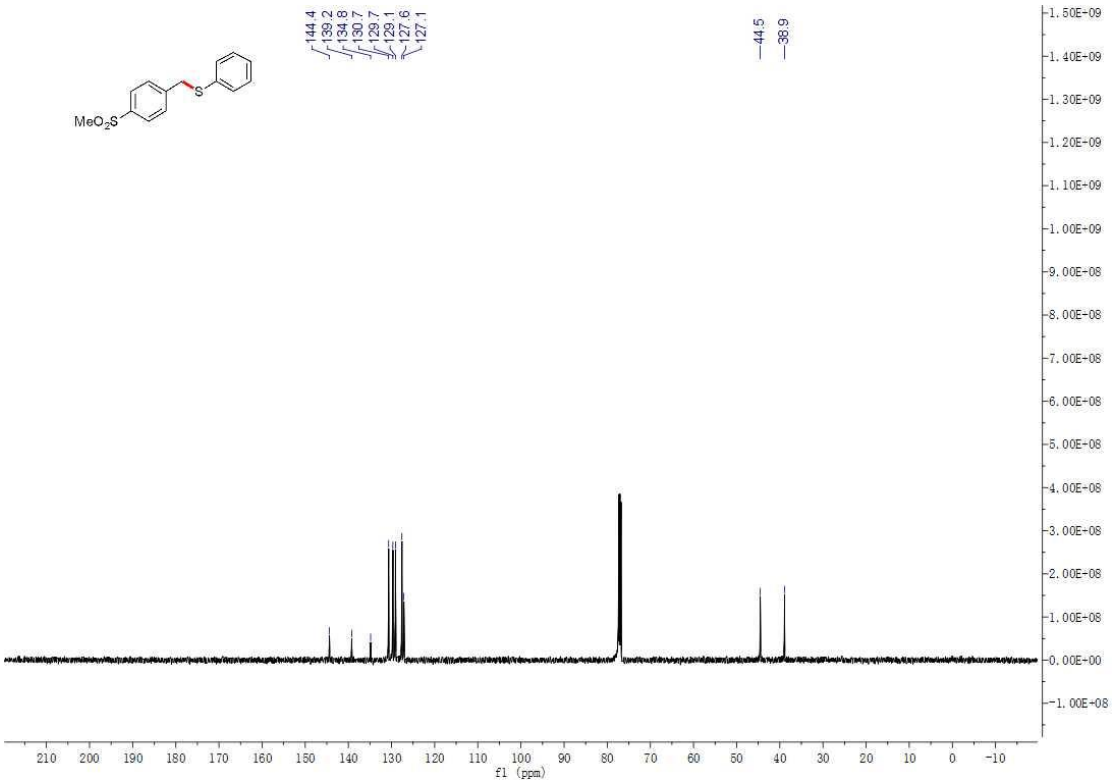

$^{19}$F NMR spectrum of **phenyl(3-(trifluoromethoxy)benzyl)sulfane (9)**



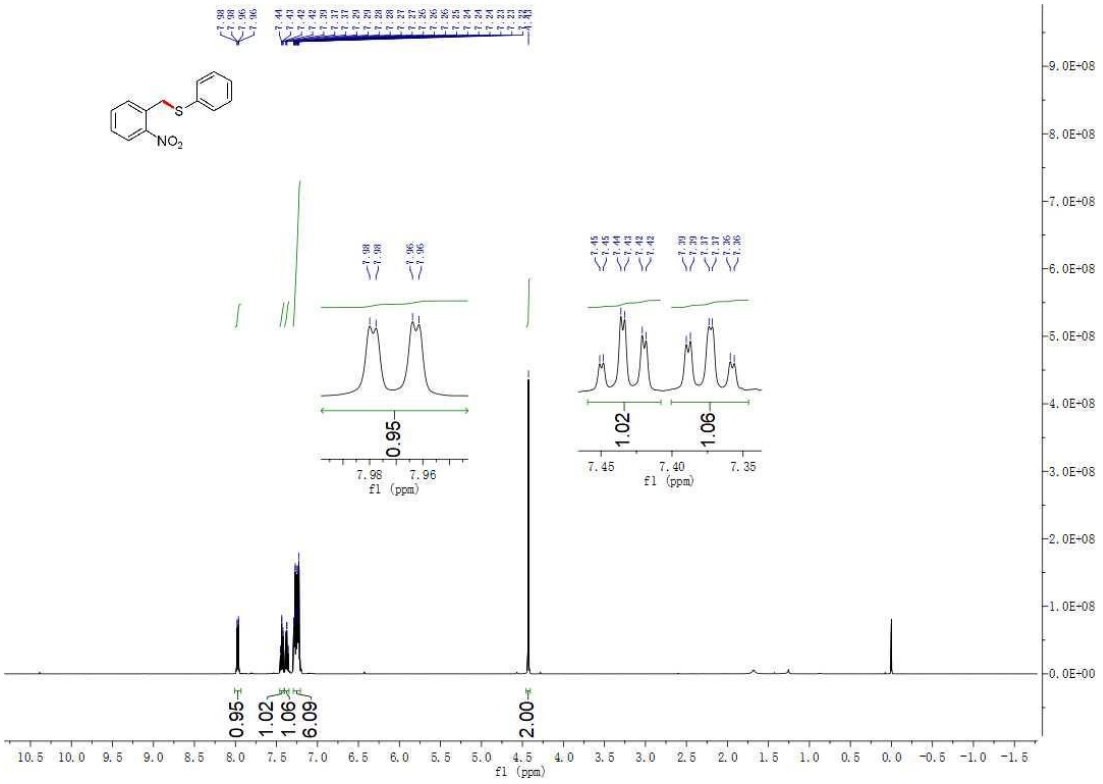
$^{1}$H NMR spectrum of **(4-(methylsulfonyl)benzyl)(phenyl)sulfane (10)**




$^{13}$C NMR spectrum of **(4-(methylsulfonyl)benzyl)(phenyl)sulfane (10)**



$^{1}$H NMR spectrum of **(2-nitrobenzyl)(phenyl)sulfane (11)**

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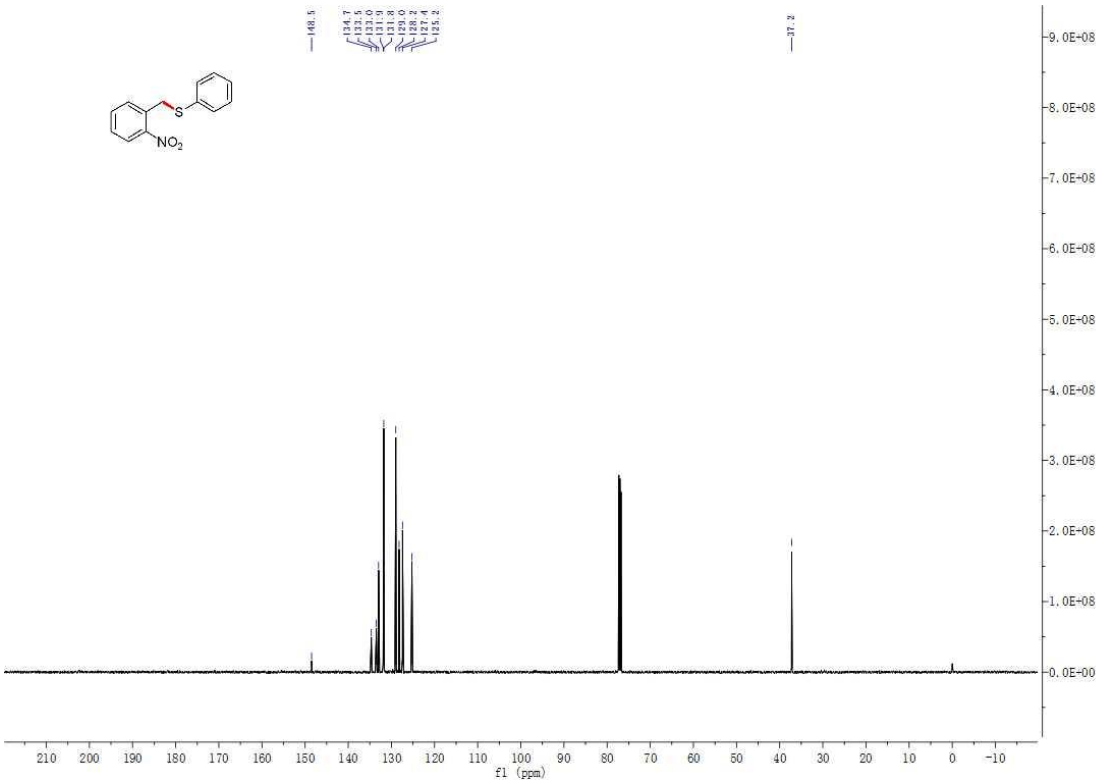

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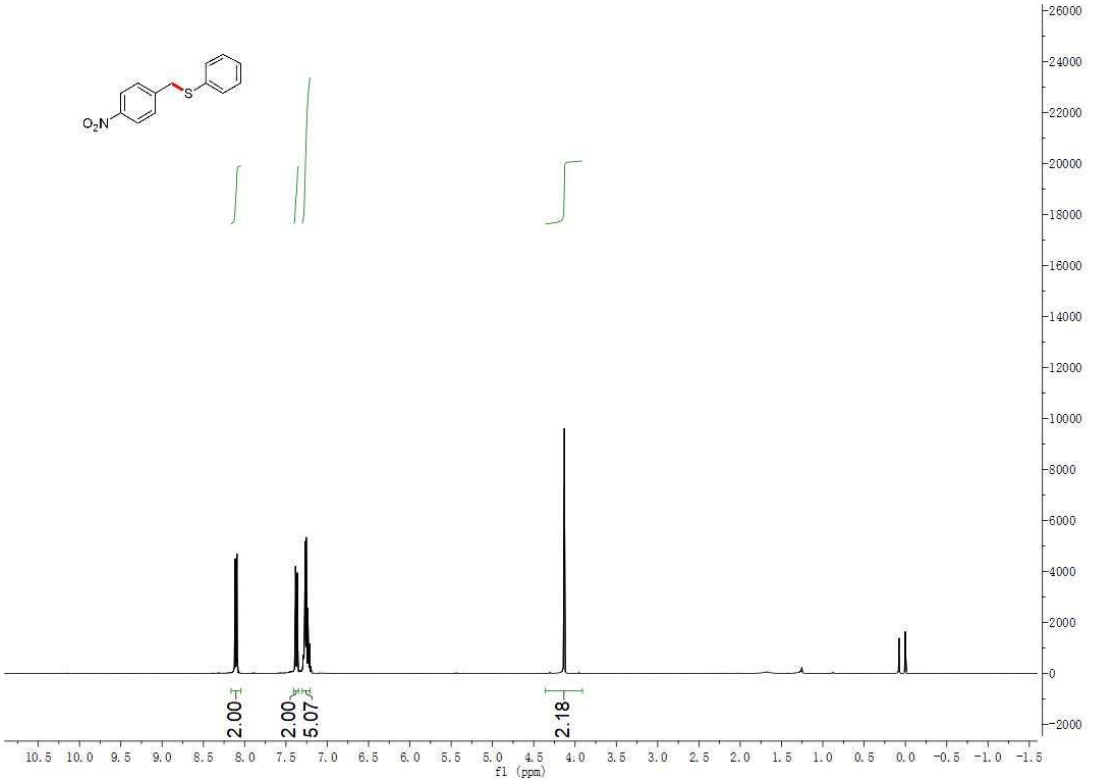


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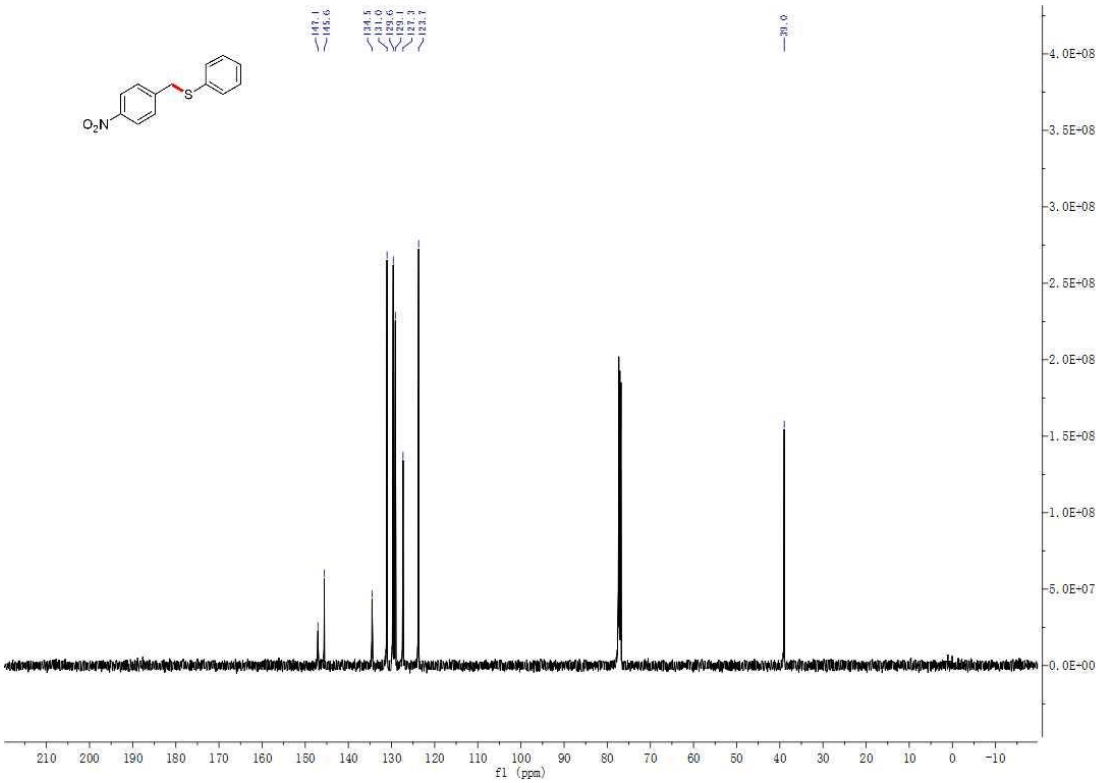
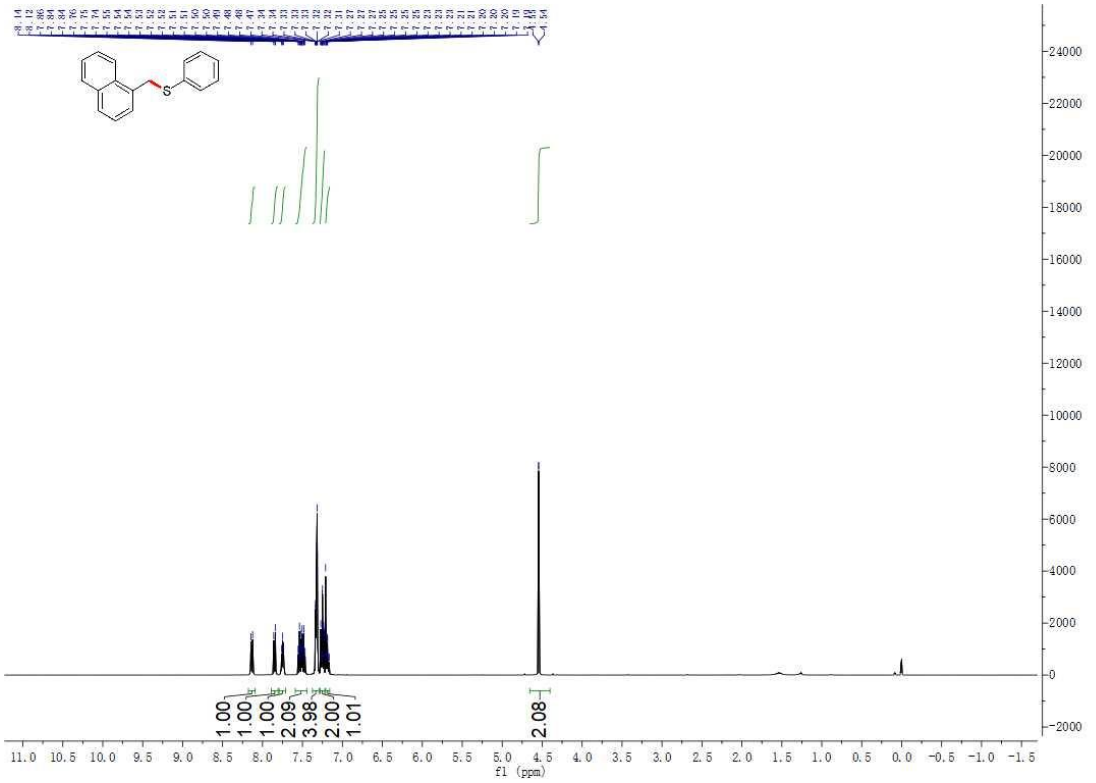


$^{1}$H NMR spectrum of **(naphthalen-1-ylmethyl)(phenyl)sulfane (13)**

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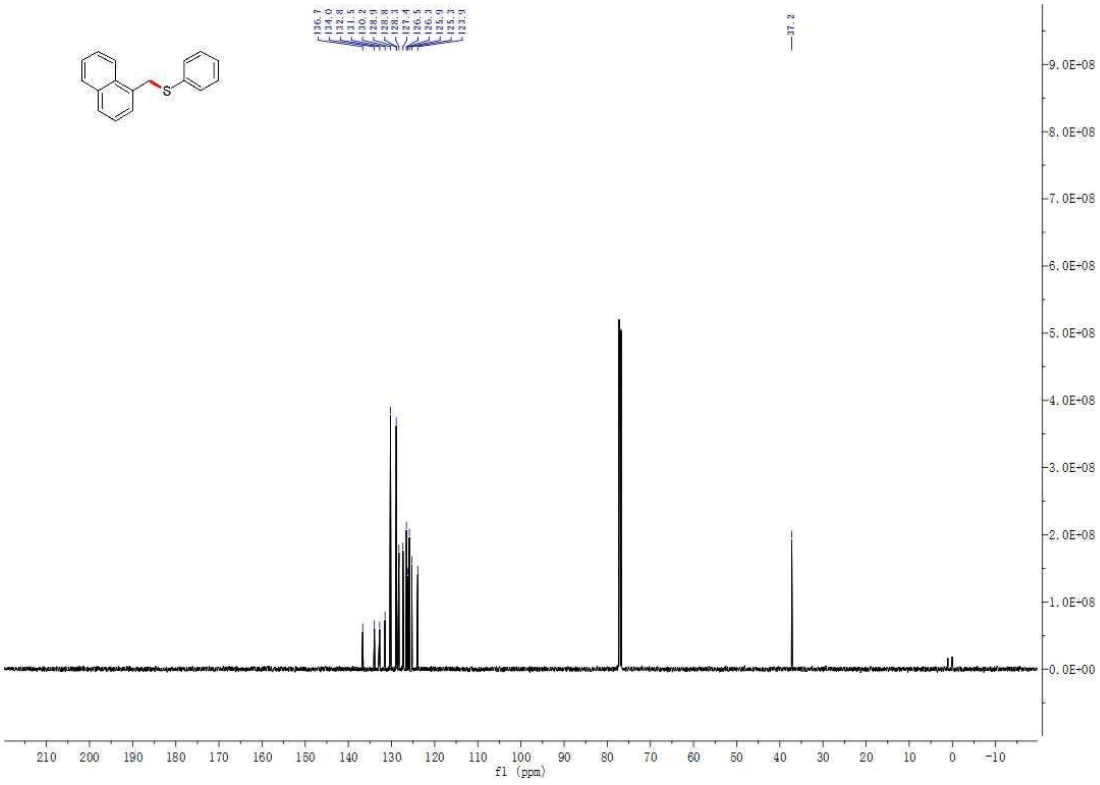

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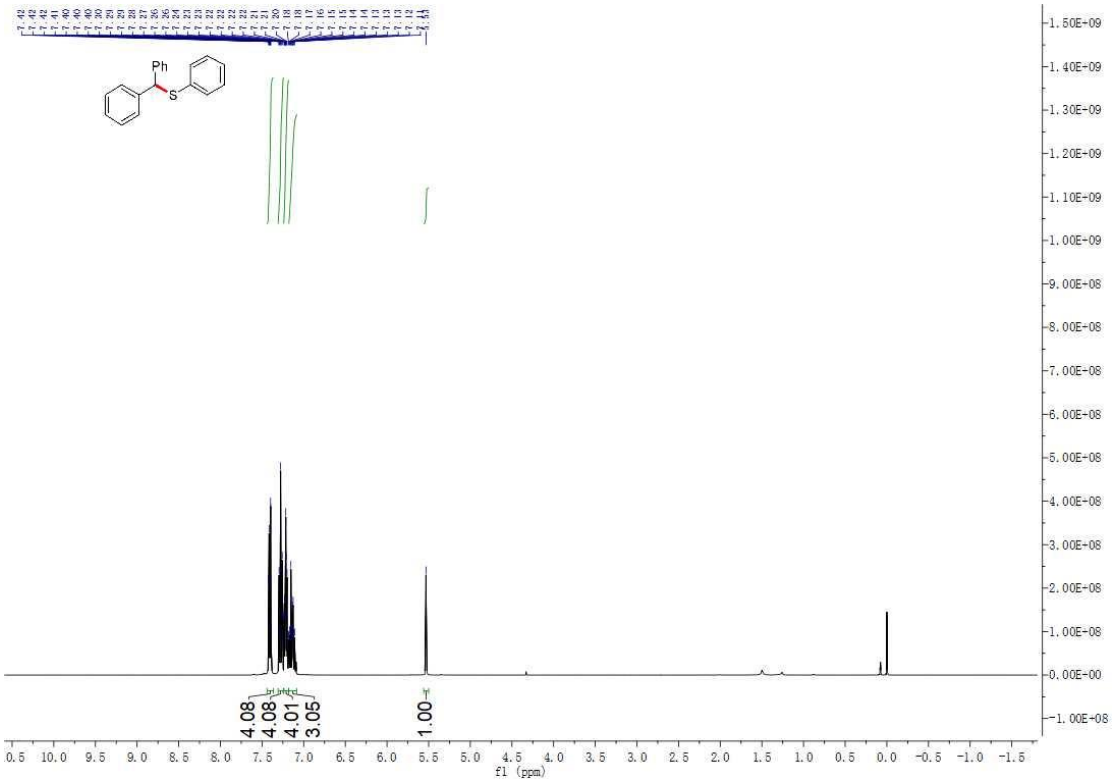


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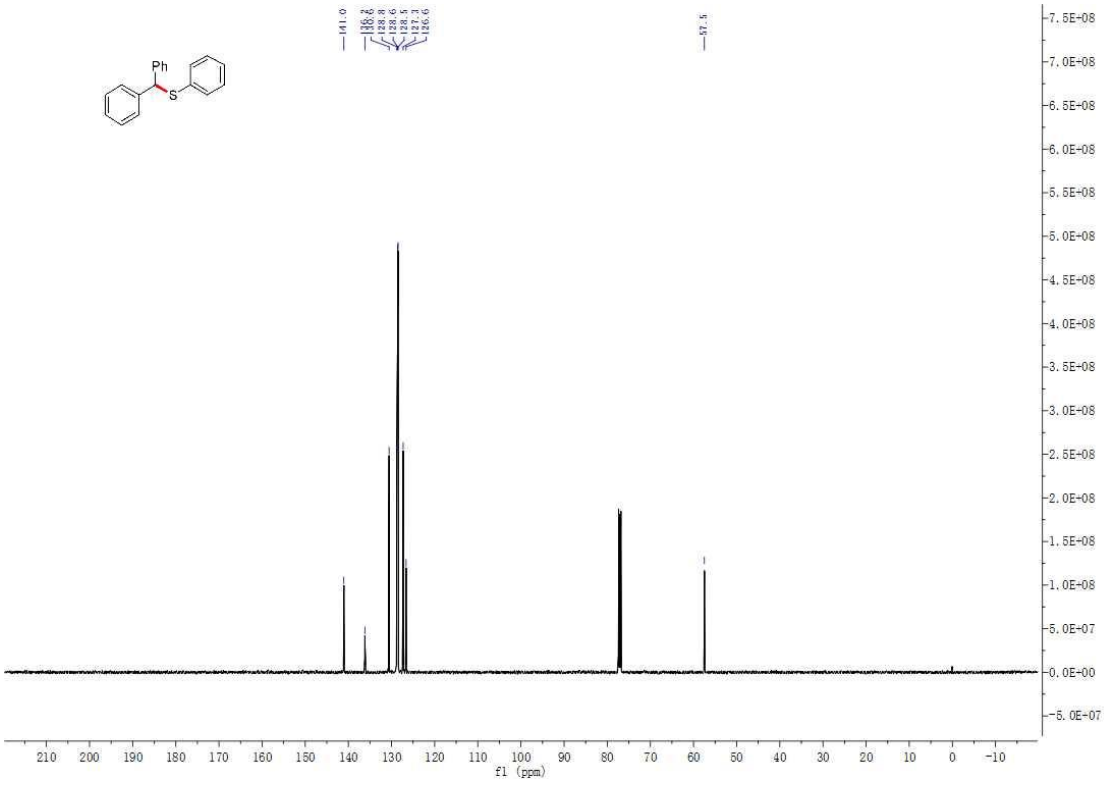

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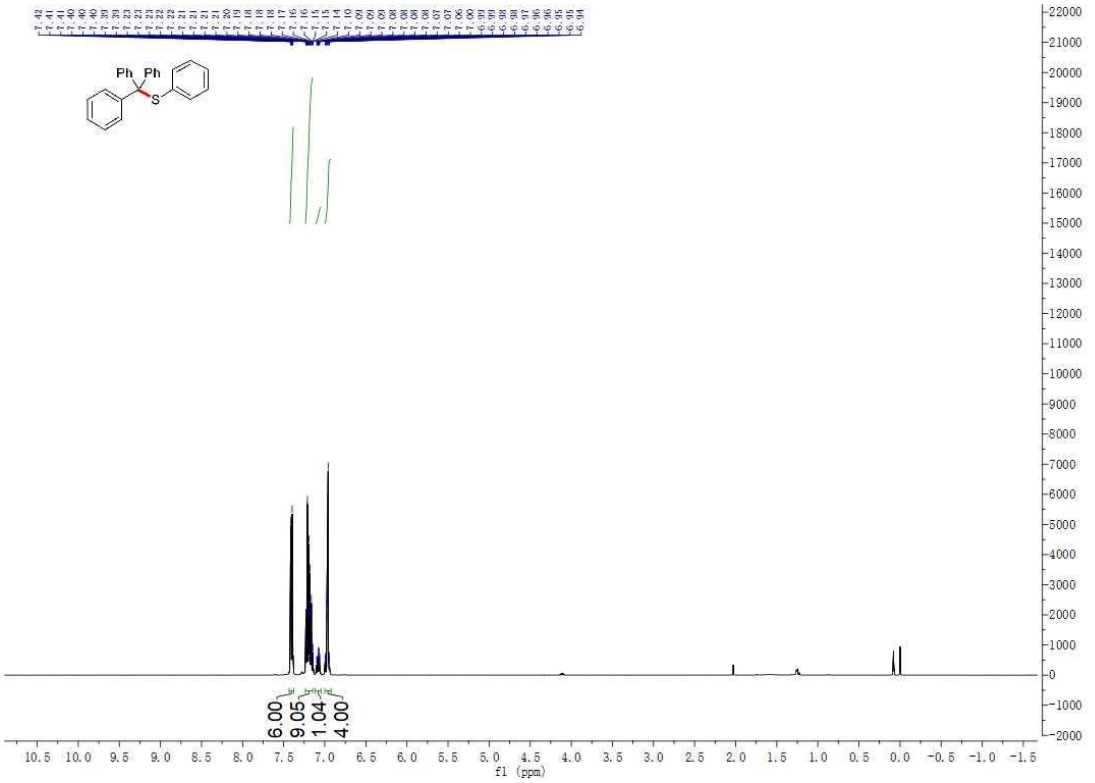


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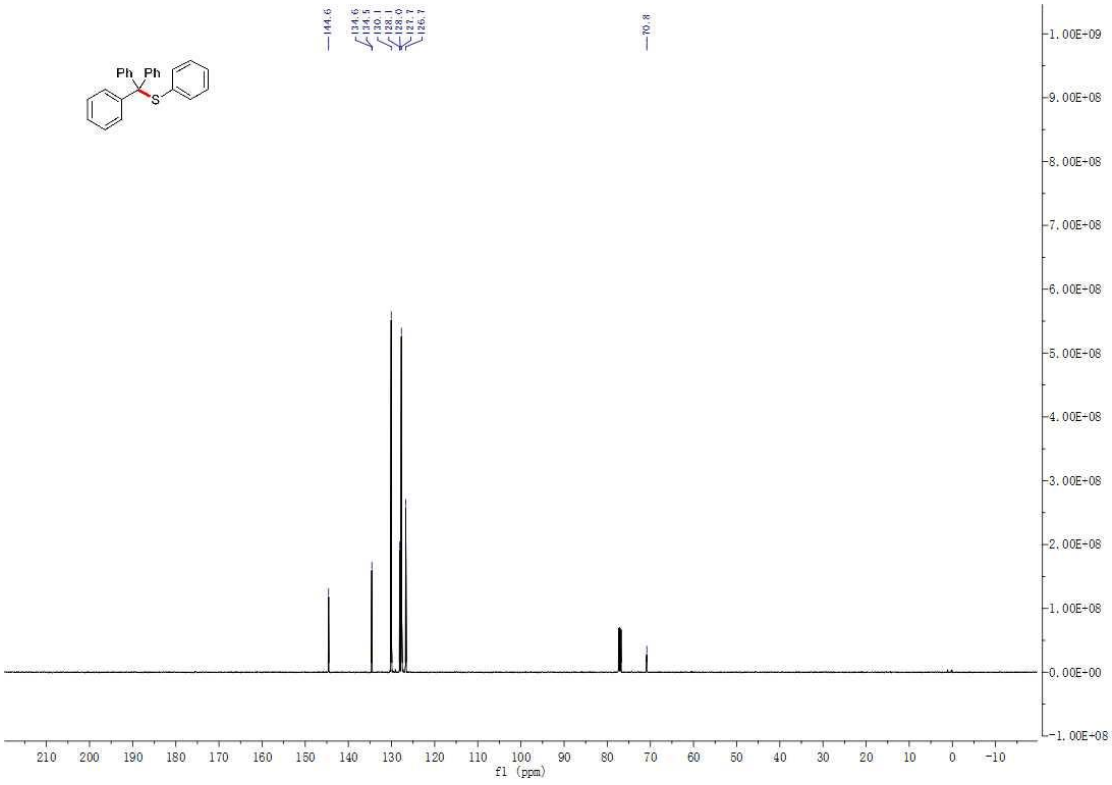

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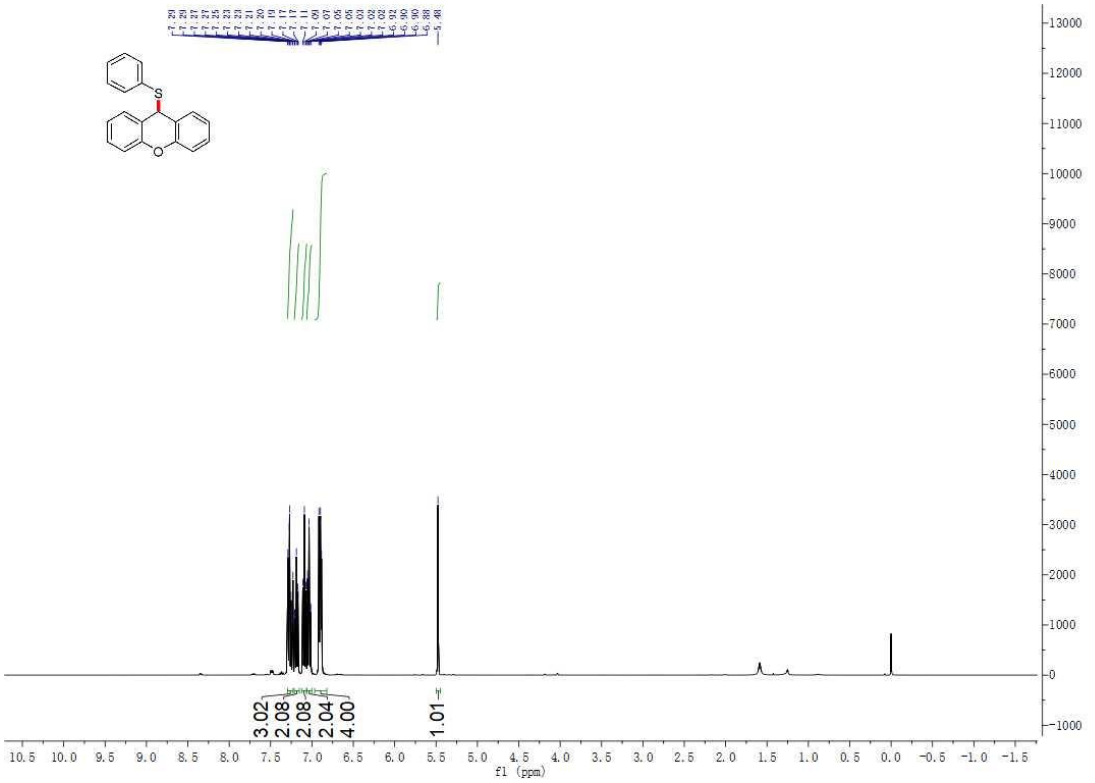


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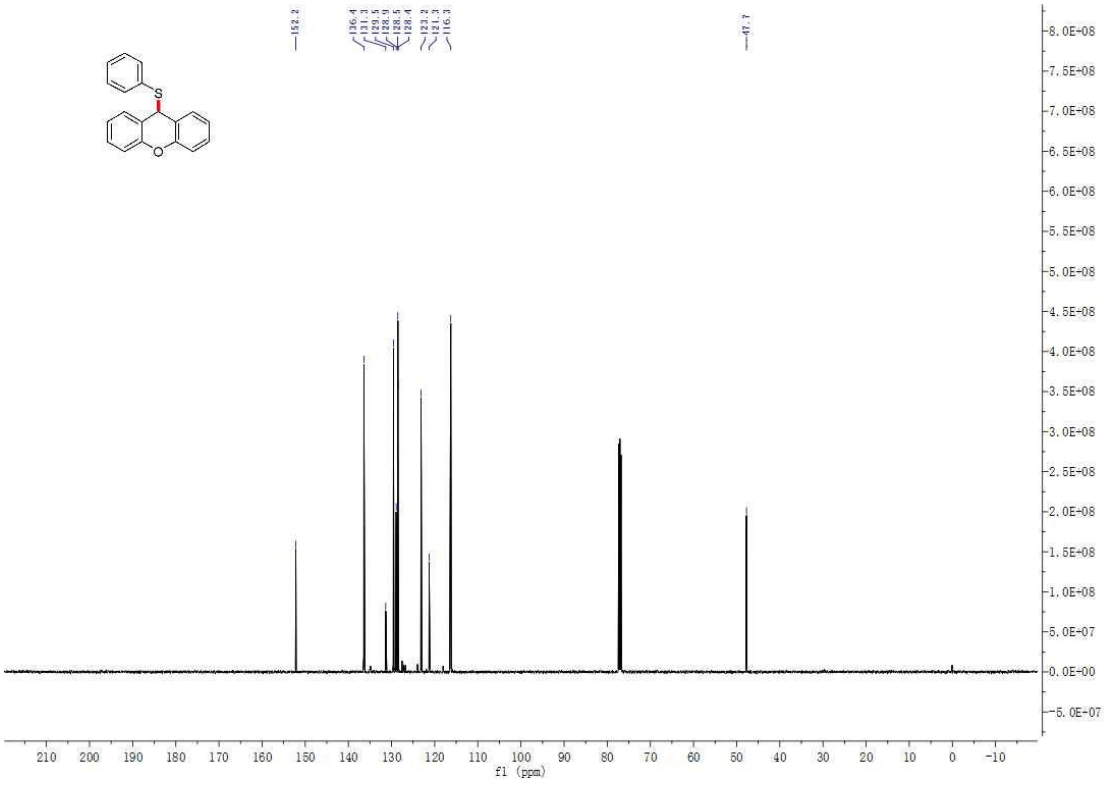

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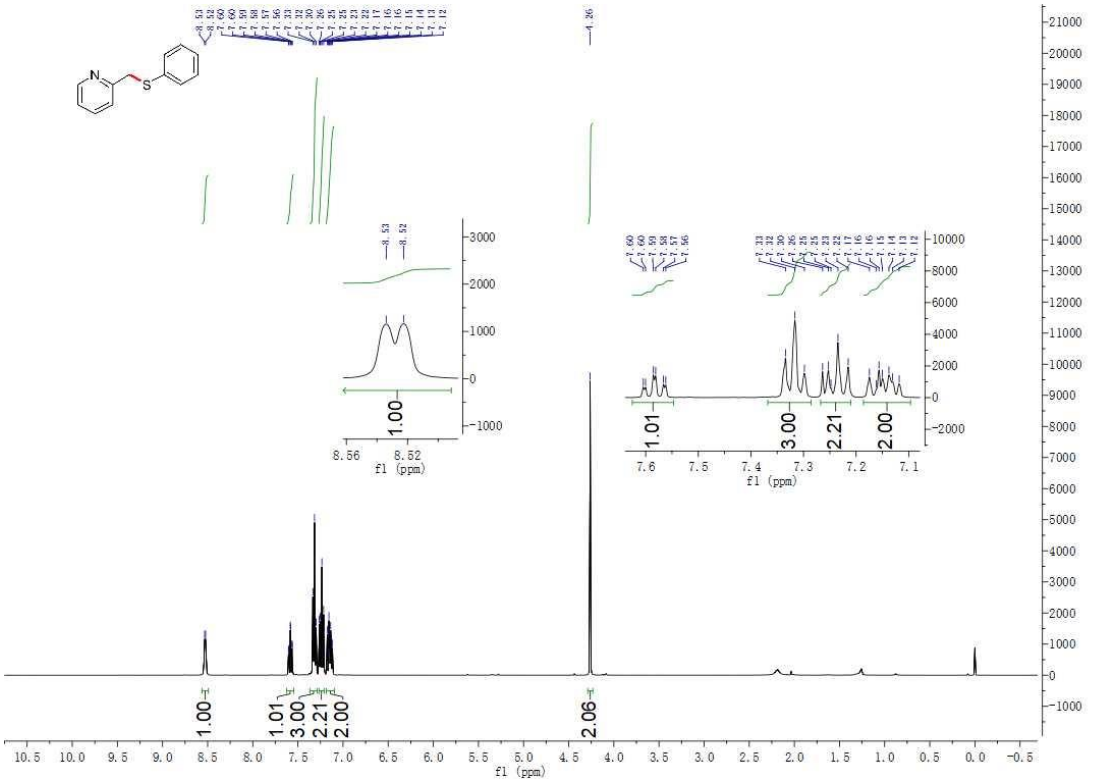


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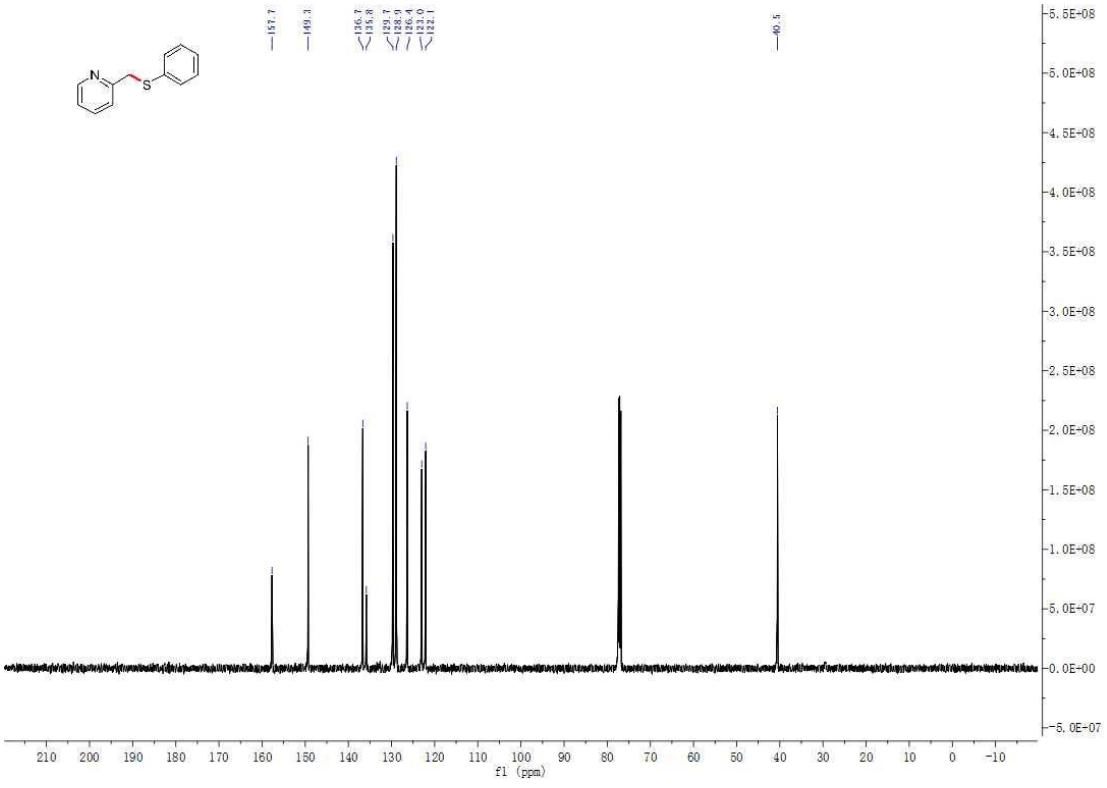

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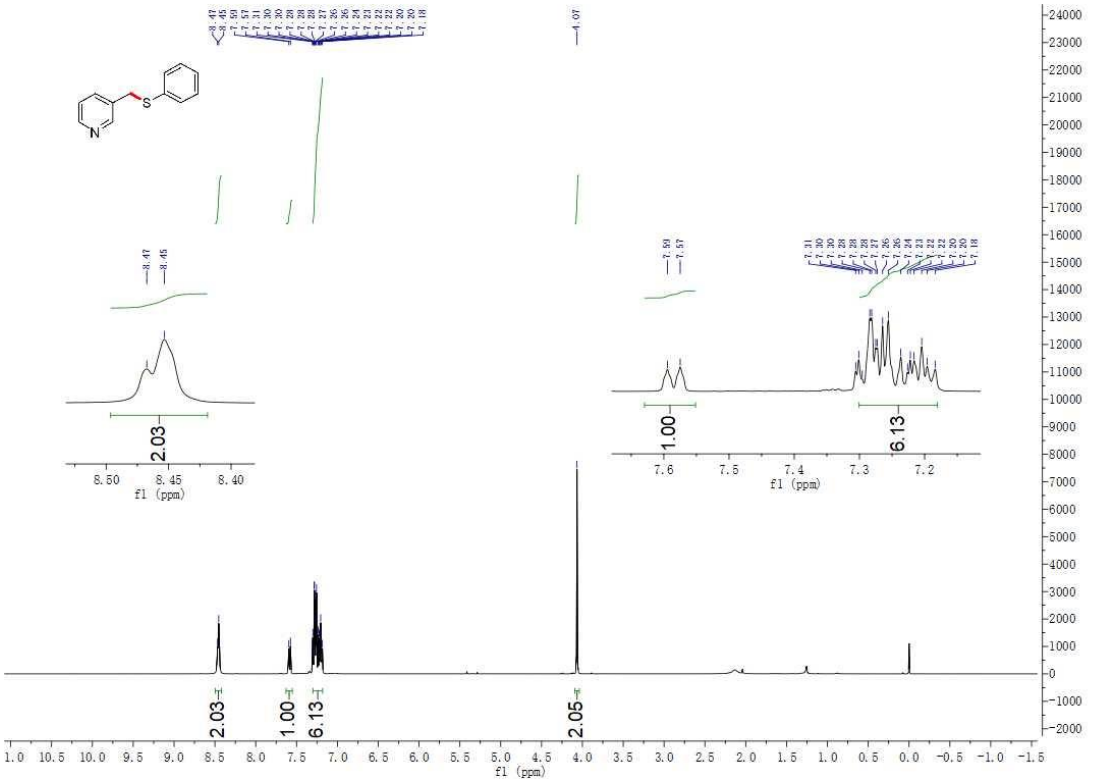


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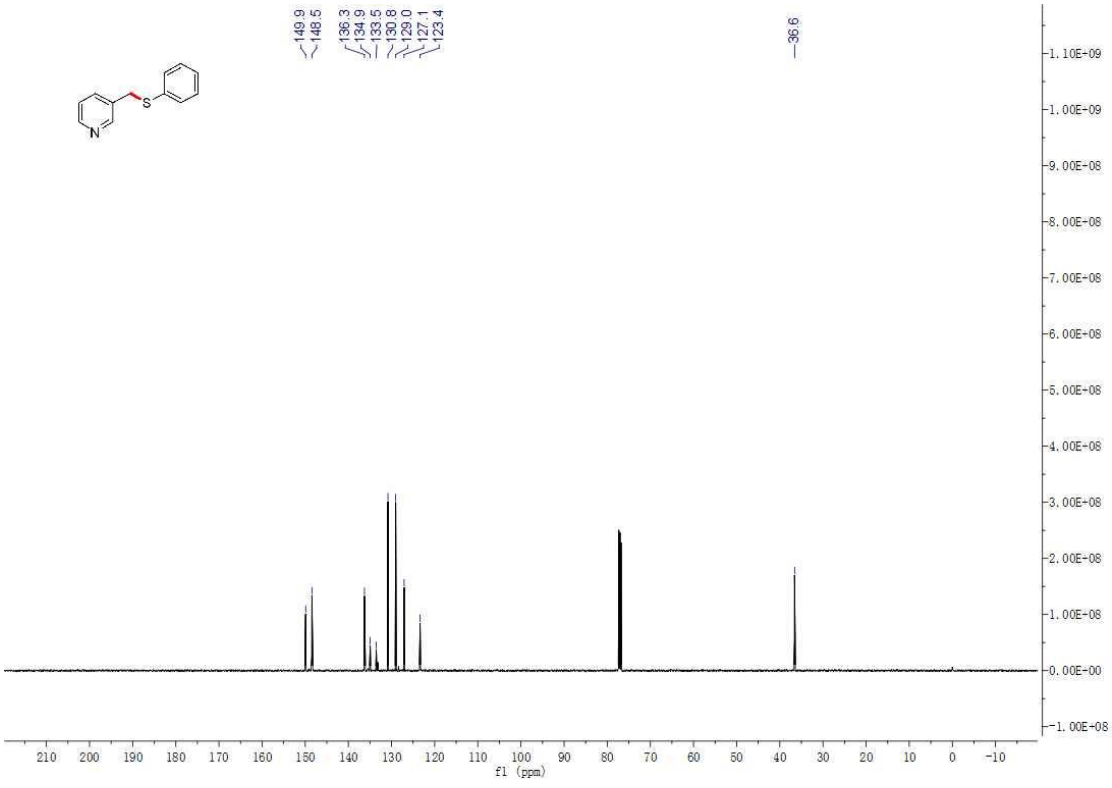

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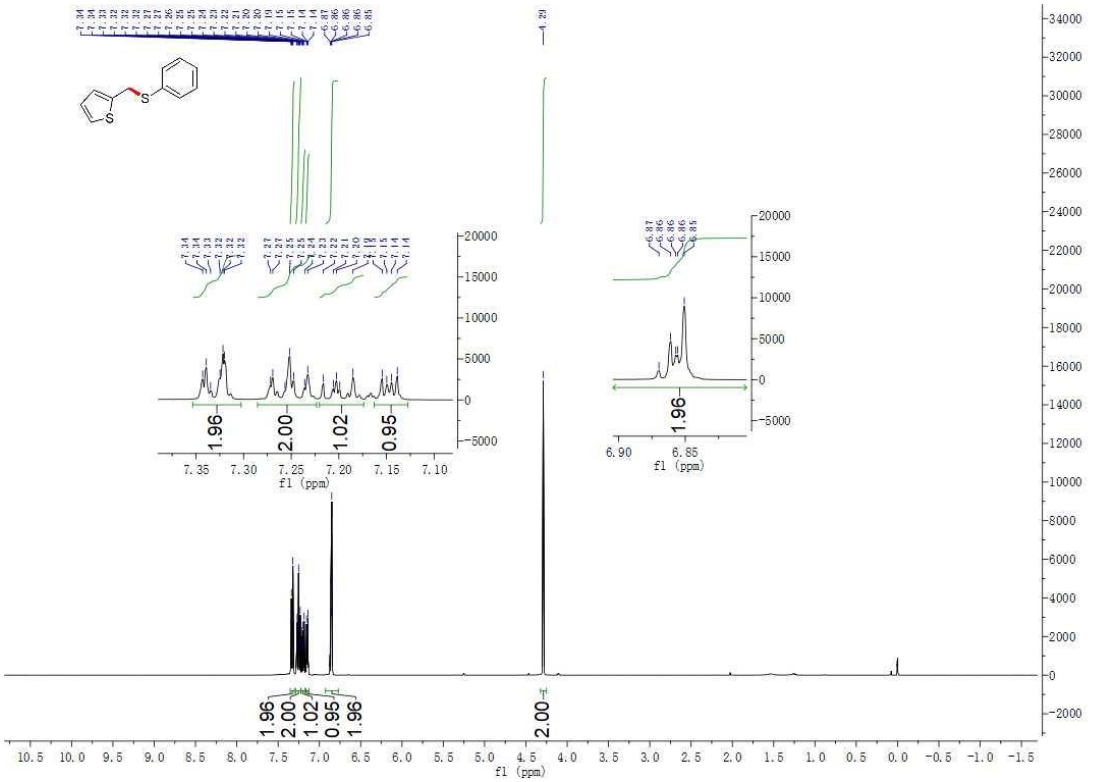
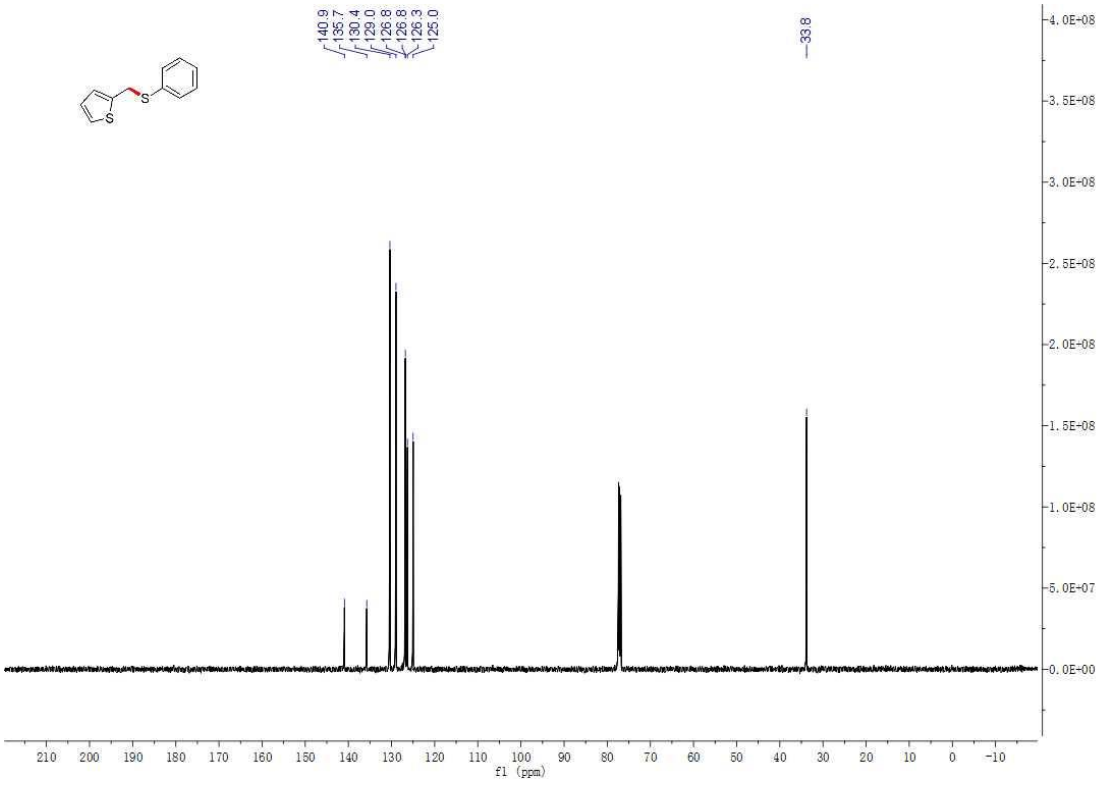
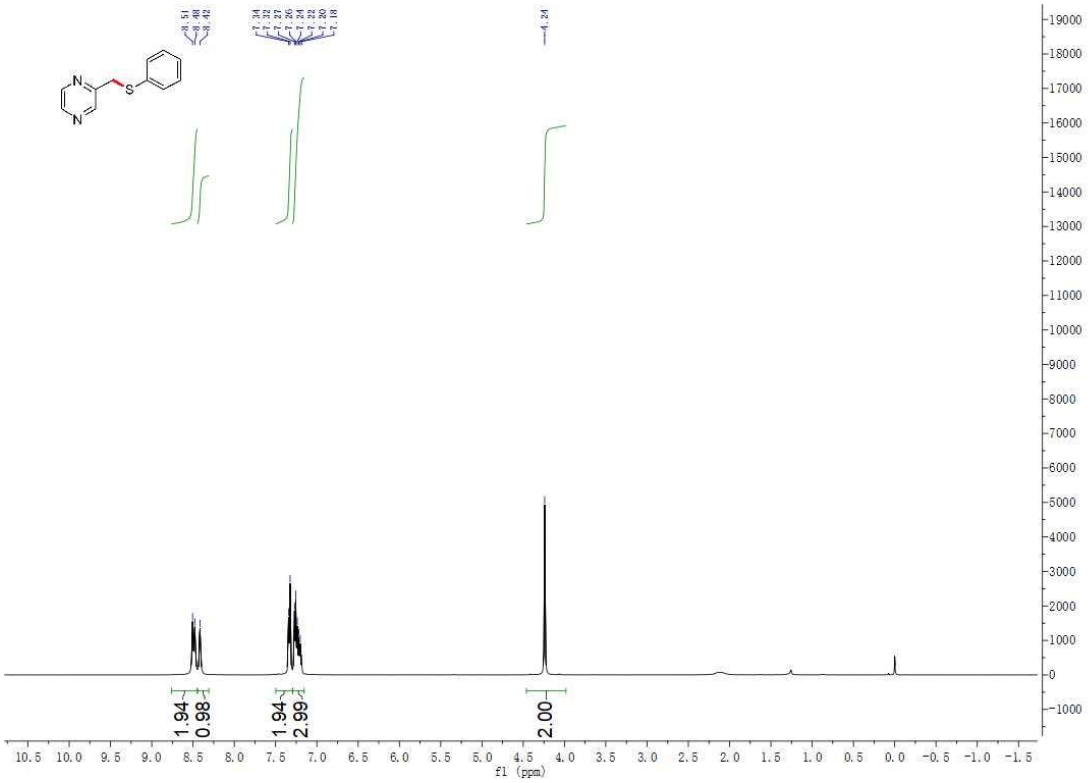


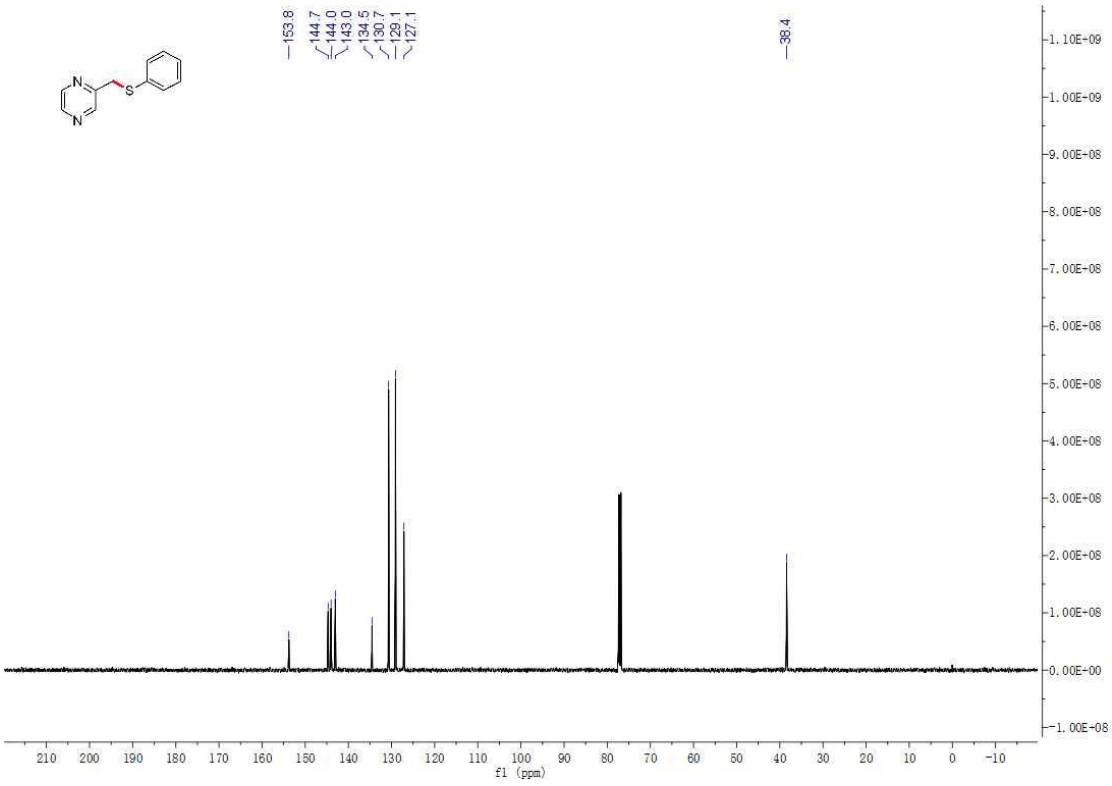
$^{13}$C NMR spectrum of **2-((phenylthio)methyl)thiophene (19)**



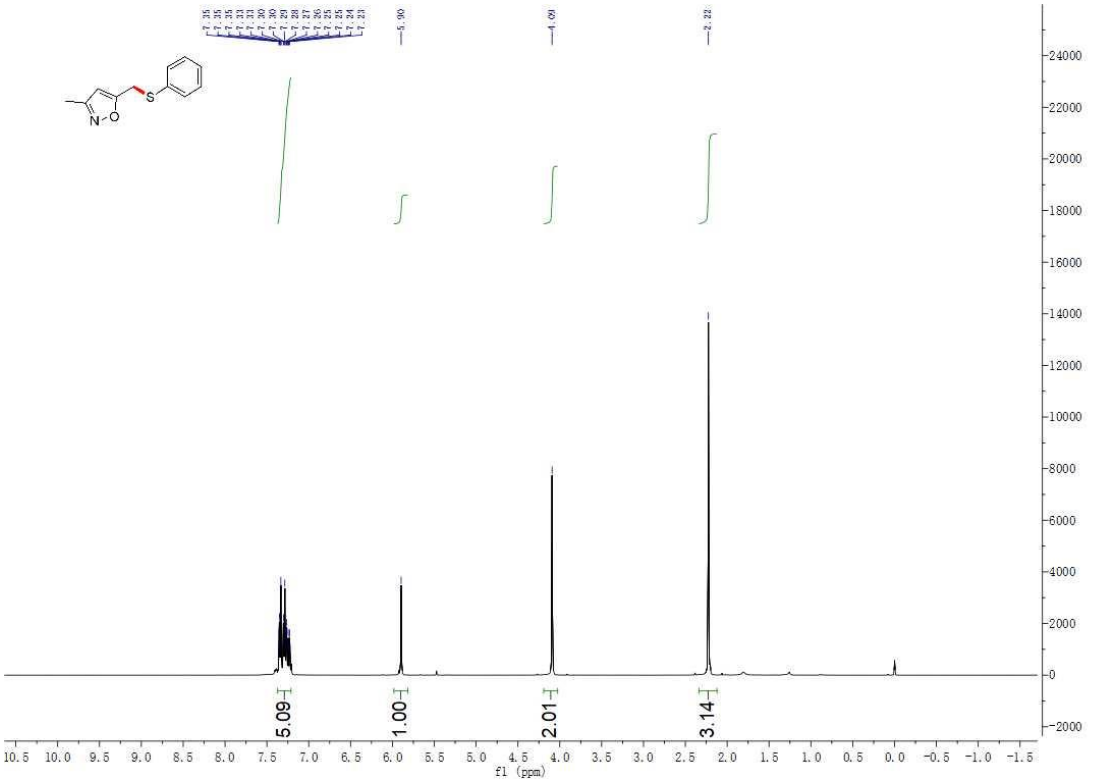
$^{1}$H NMR spectrum of **2-((phenylthio)methyl)pyrazine (20)**



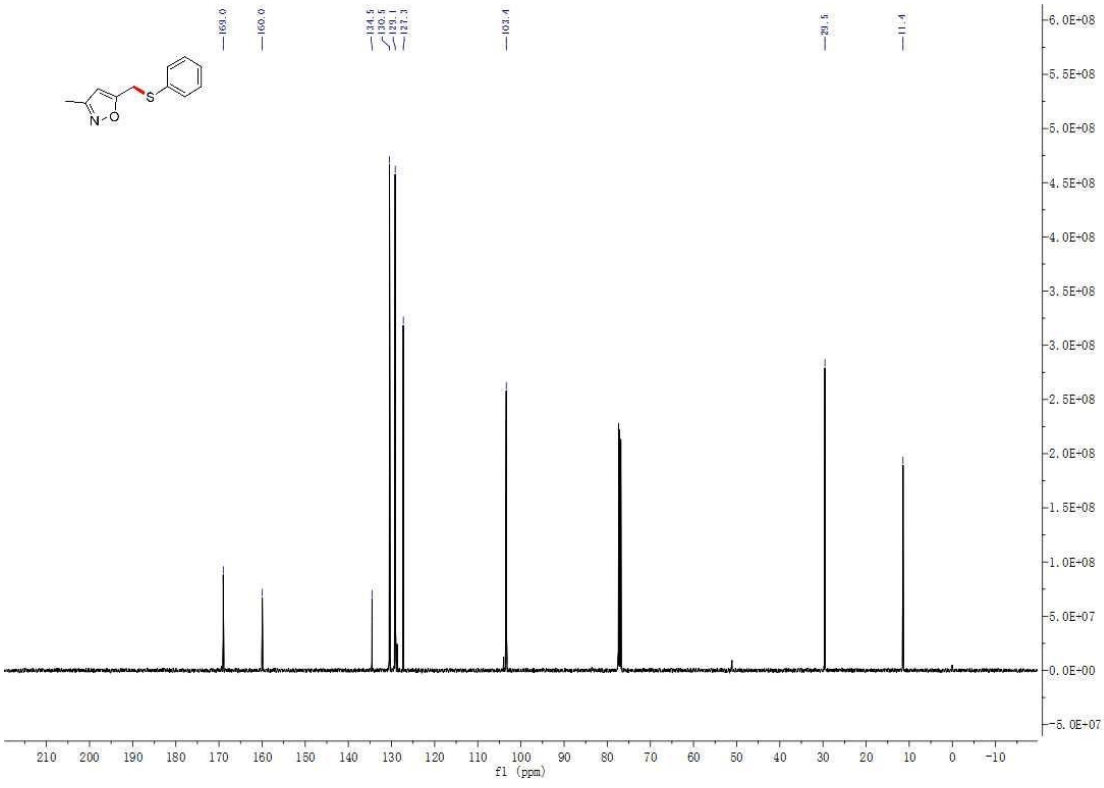

$^{13}$C NMR spectrum of **2-((phenylthio)methyl)pyrazine (20)**



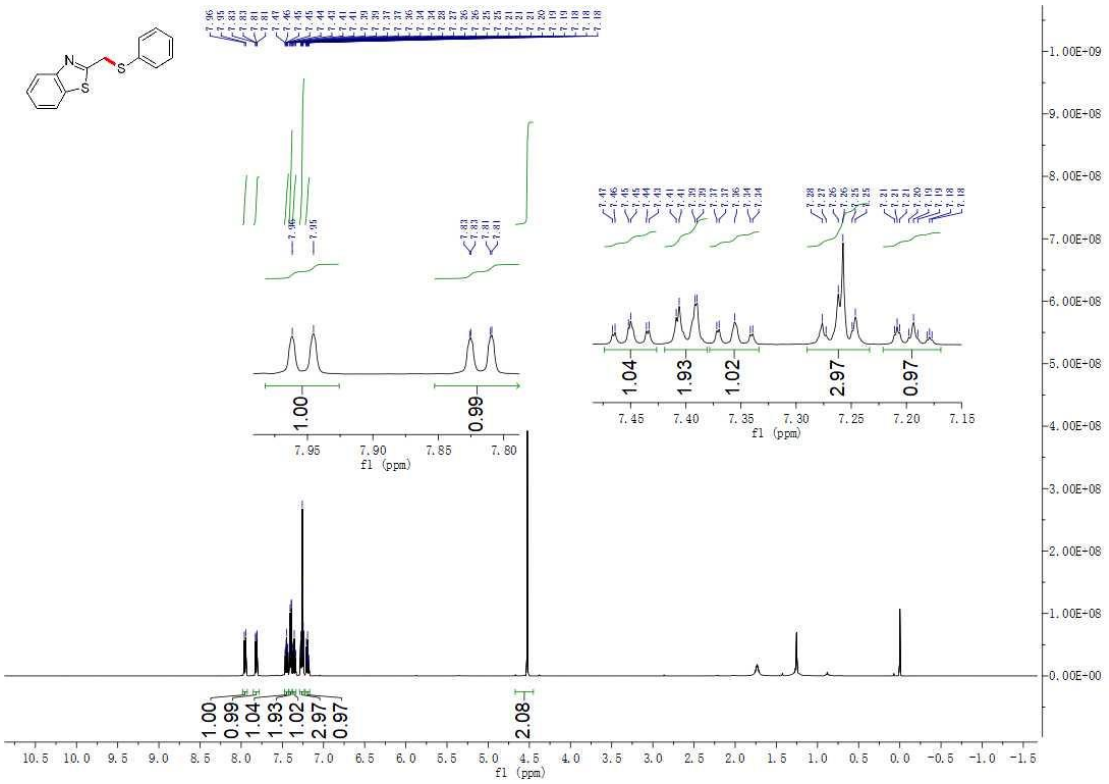
$^{1}$H NMR spectrum of **3-methyl-5-((phenylthio)methyl)isoxazole (21)**



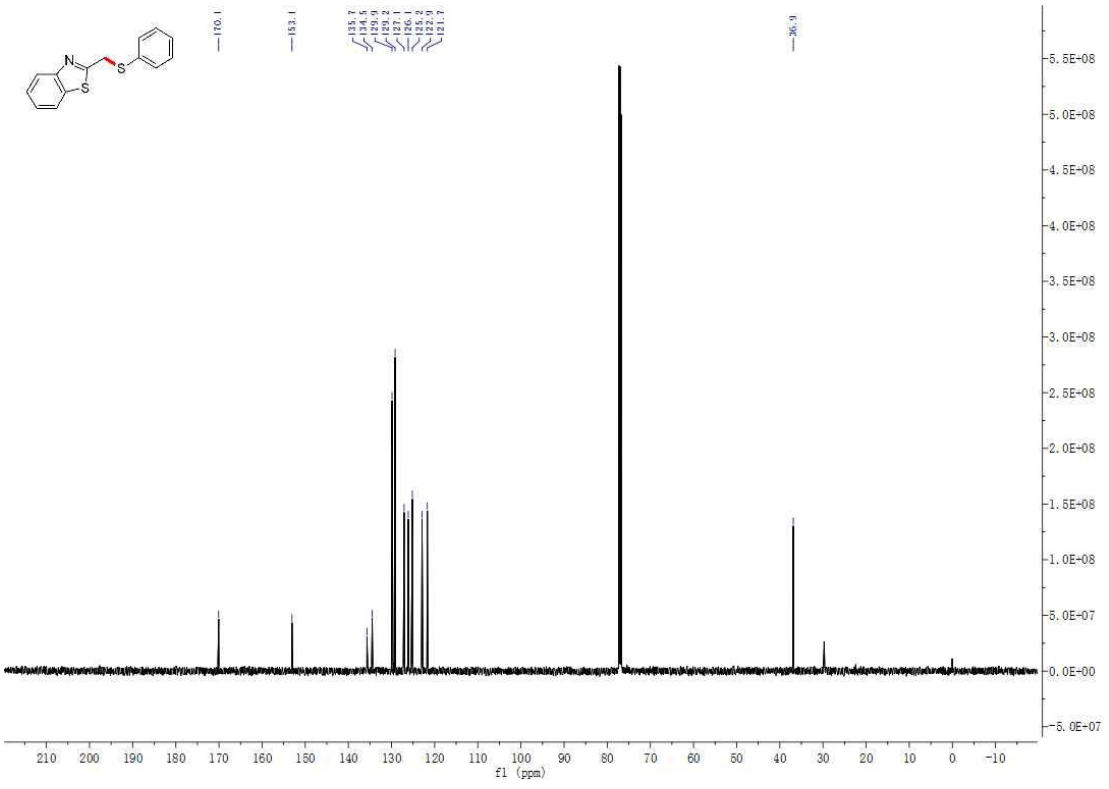

$^{13}$C NMR spectrum of **3-methyl-5-((phenylthio)methyl)isoxazole (21)**



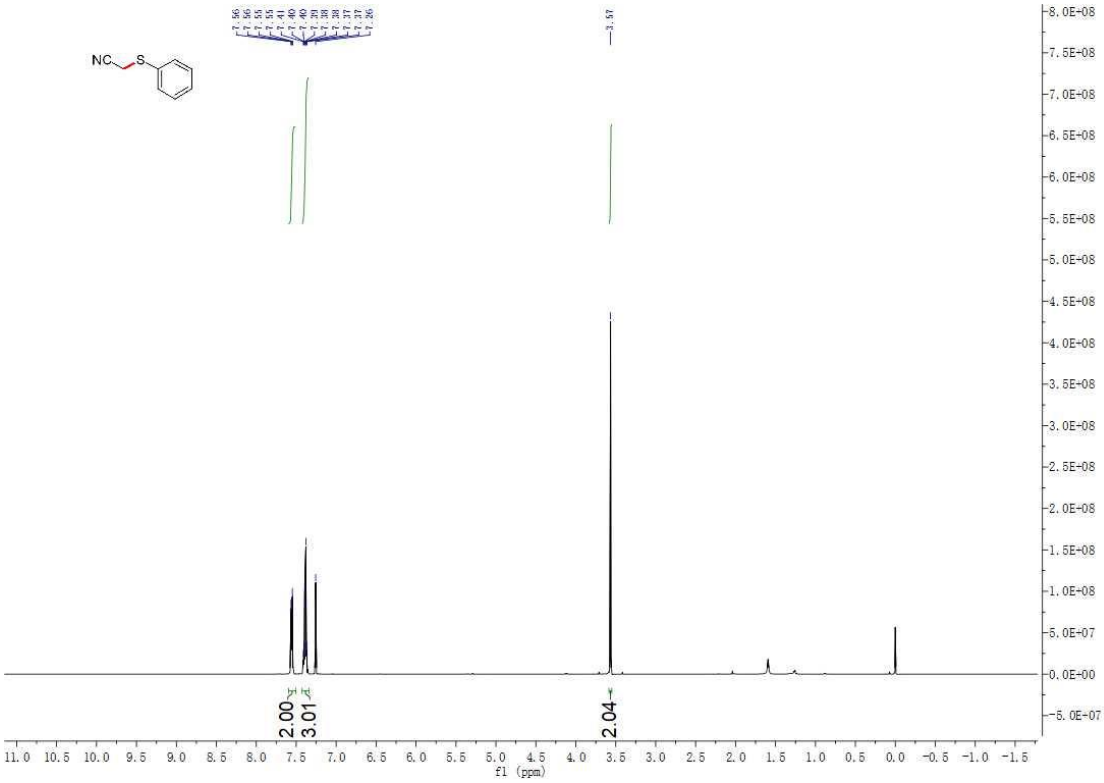
$^{1}$H NMR spectrum of **2-((phenylthio)methyl)benzo[d]thiazole (22)**



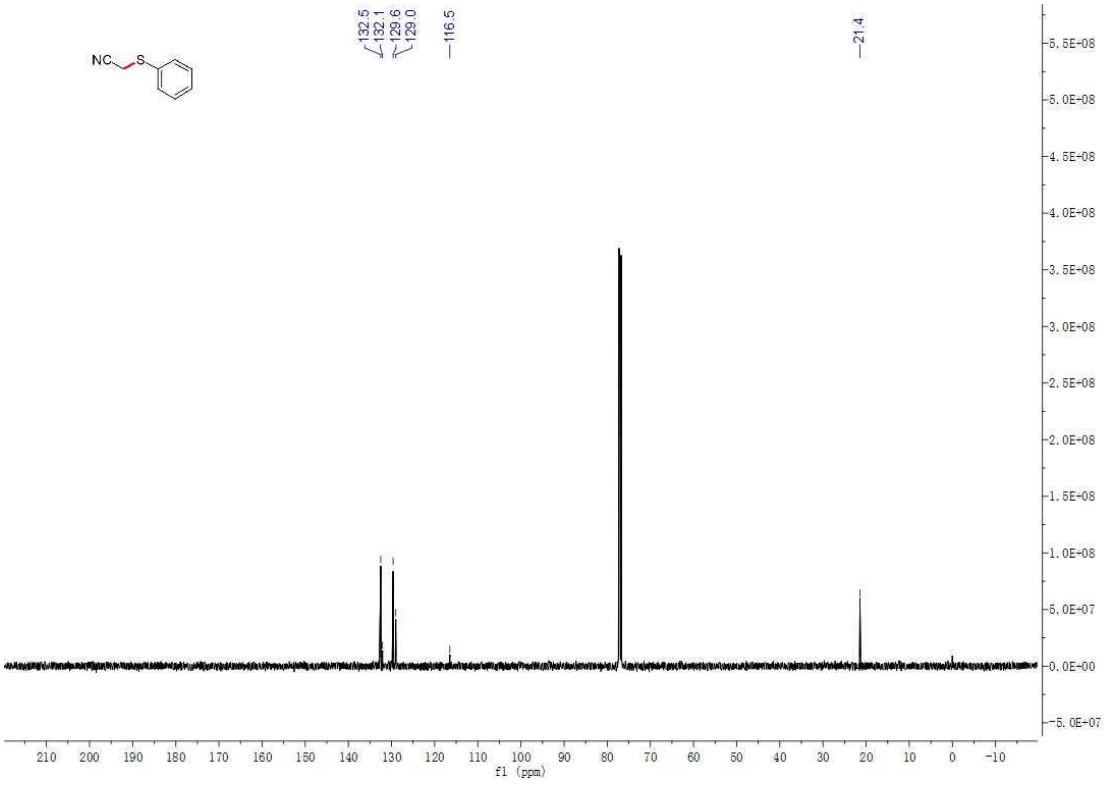

$^{13}$C NMR spectrum of **2-((phenylthio)methyl)benzo[d]thiazole (22)**



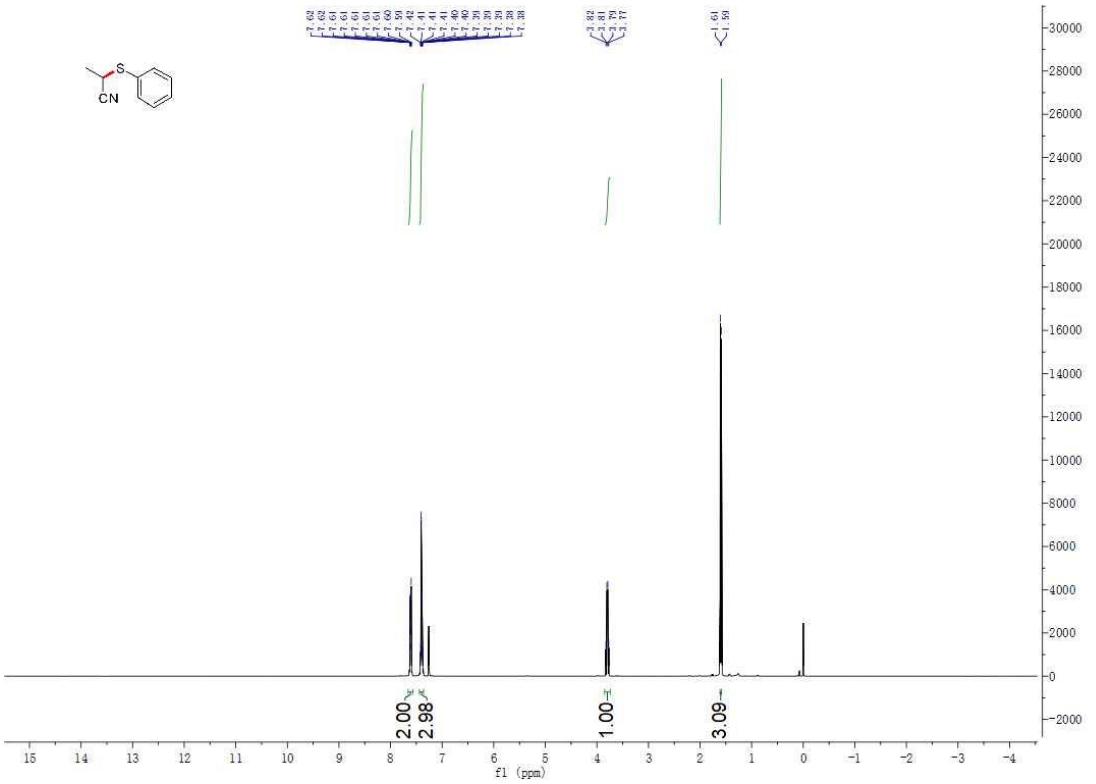
$^{1}$H NMR spectrum of **2-(phenylthio)acetonitrile (23)**



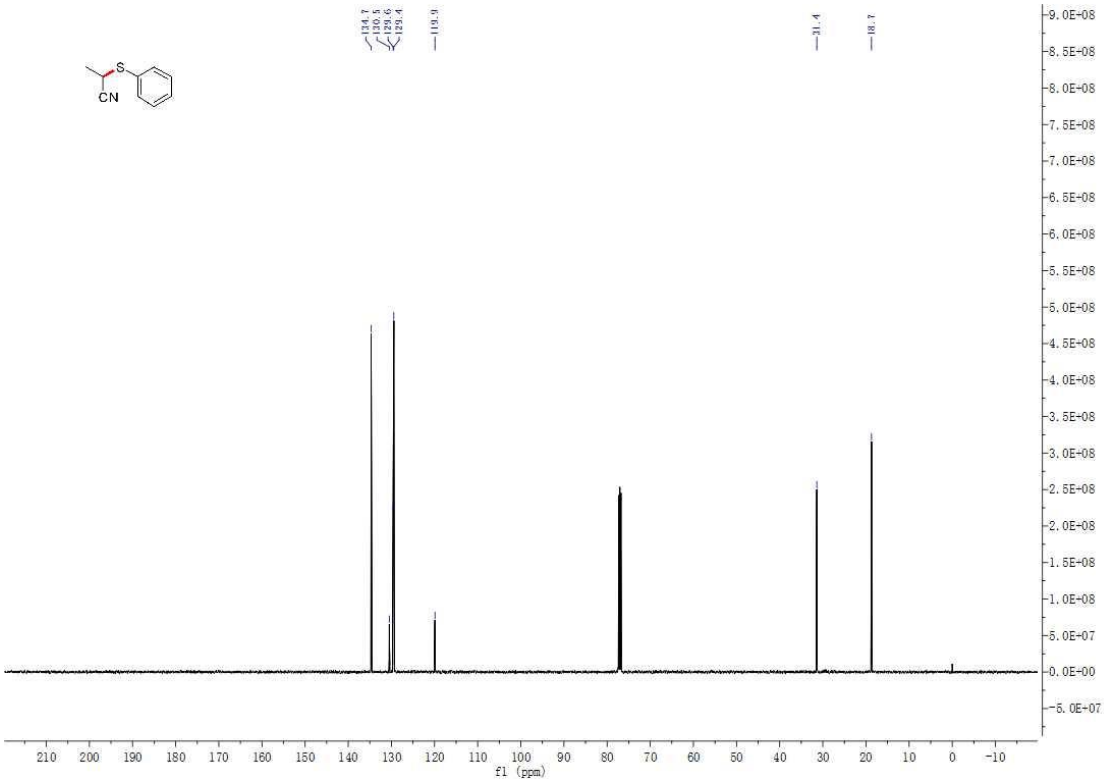

$^{13}$C NMR spectrum of **2-(phenylthio)acetonitrile (23)**



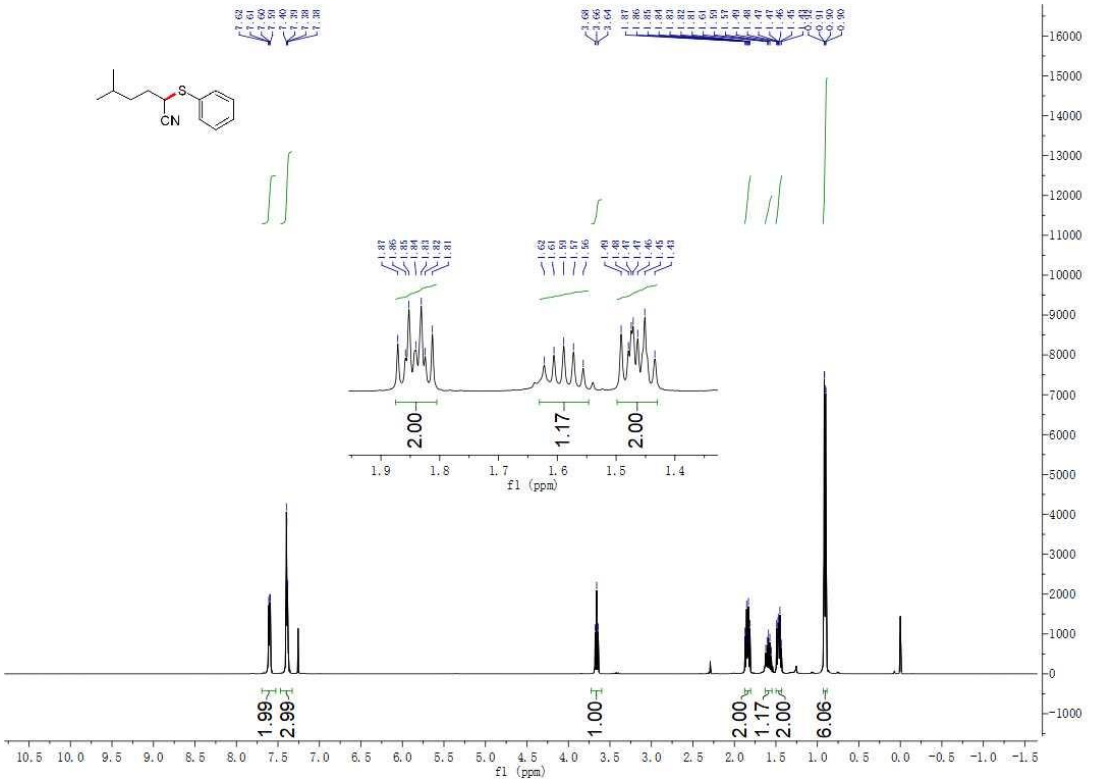
$^{1}$H NMR spectrum of **2-(phenylthio)propanenitrile (24)**



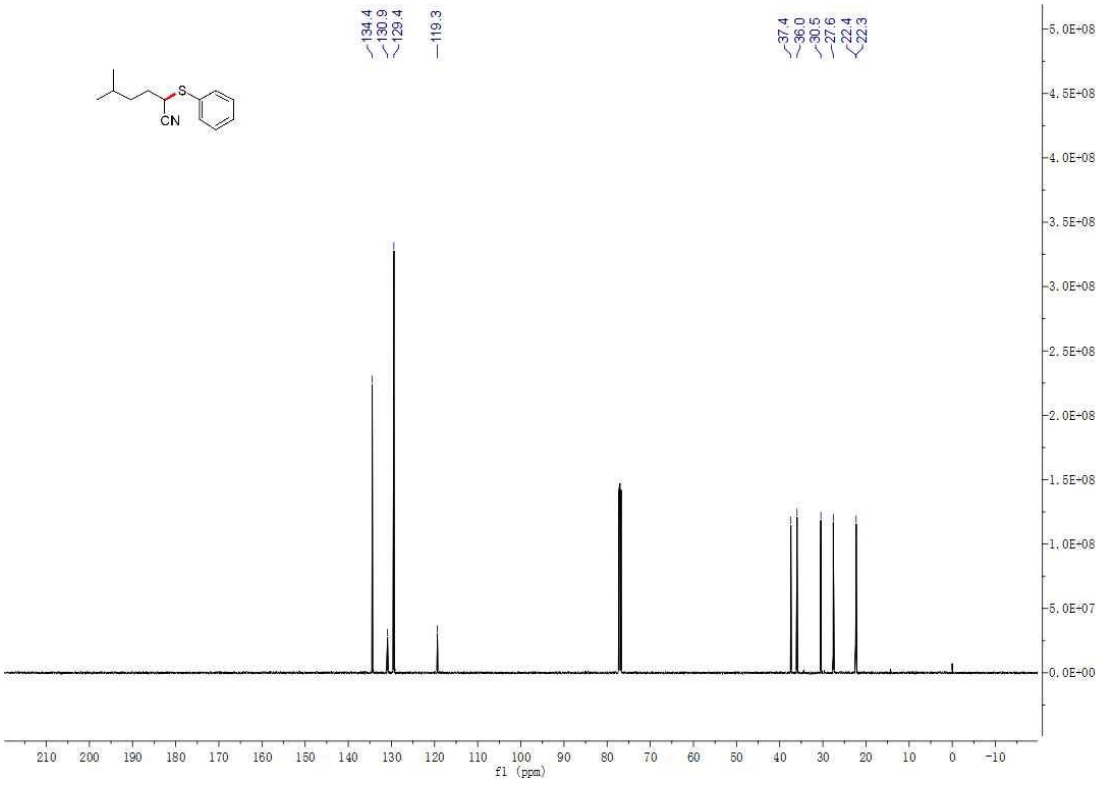

$^{13}$C NMR spectrum of **2-(phenylthio)propanenitrile (24)**



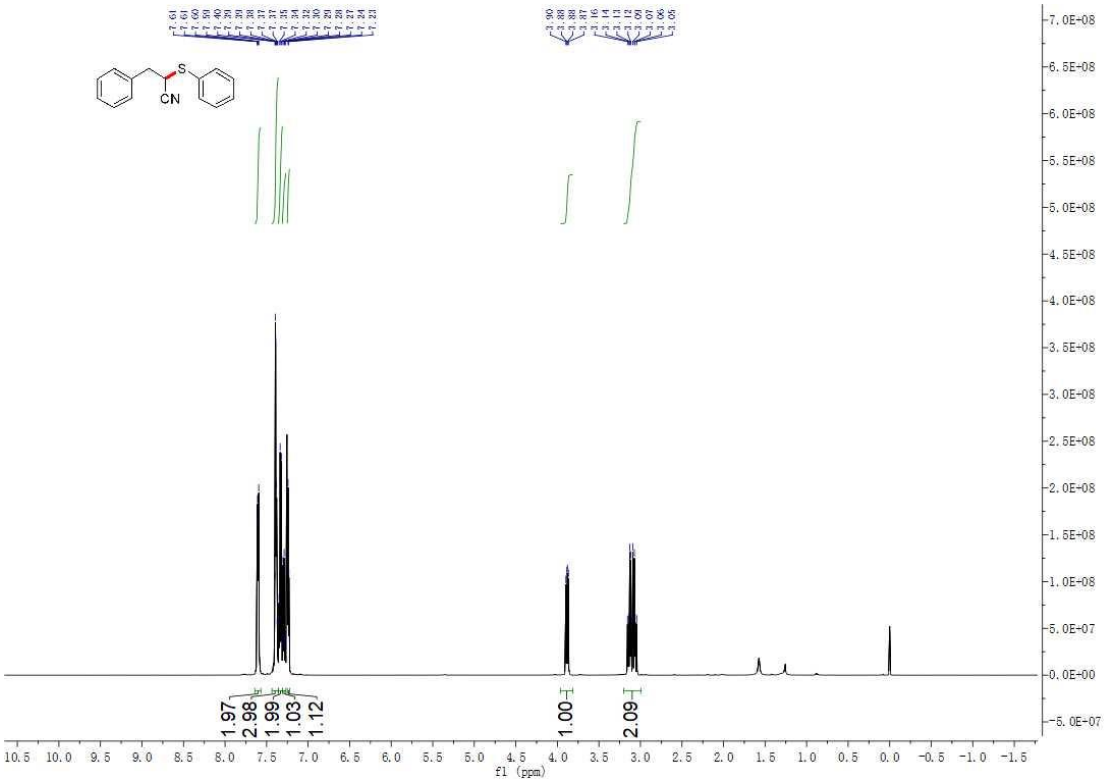
$^{1}$H NMR spectrum of **5-methyl-2-(phenylthio)hexanenitrile (25)**



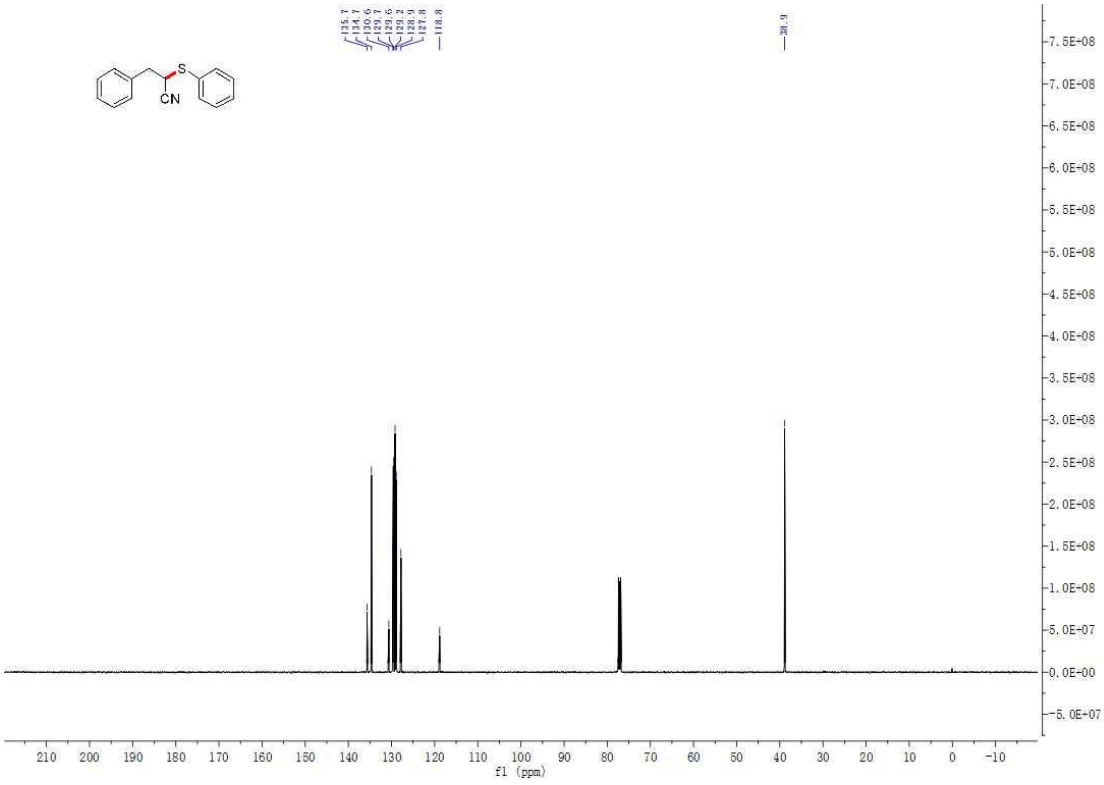

$^{13}$C NMR spectrum of **5-methyl-2-(phenylthio)hexanenitrile (25)**



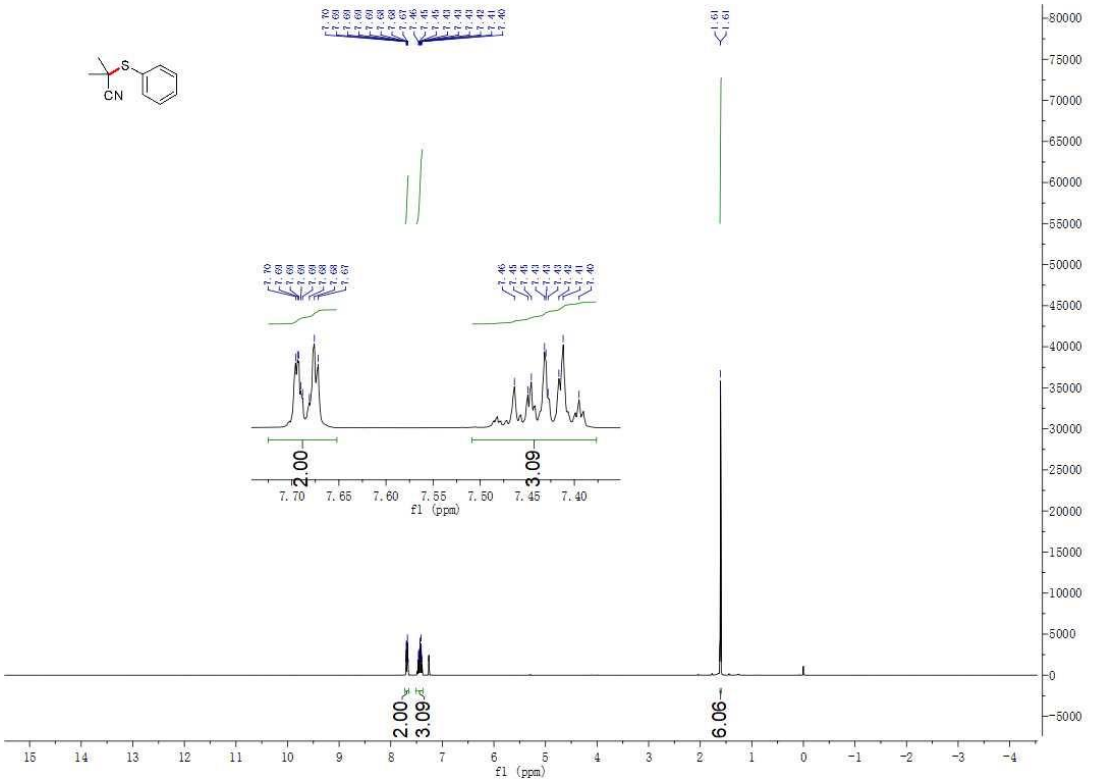
$^{1}$H NMR spectrum of **3-phenyl-2-(phenylthio)propanenitrile (26)**



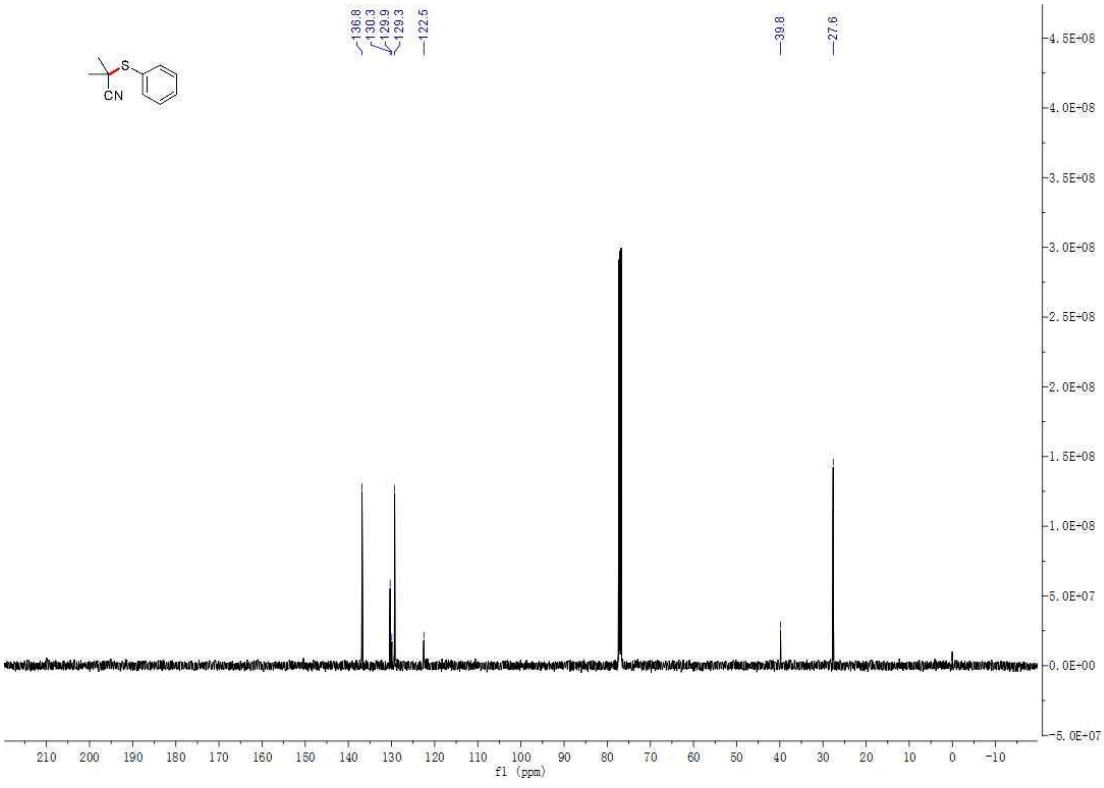

$^{13}$C NMR spectrum of **3-phenyl-2-(phenylthio)propanenitrile (26)**



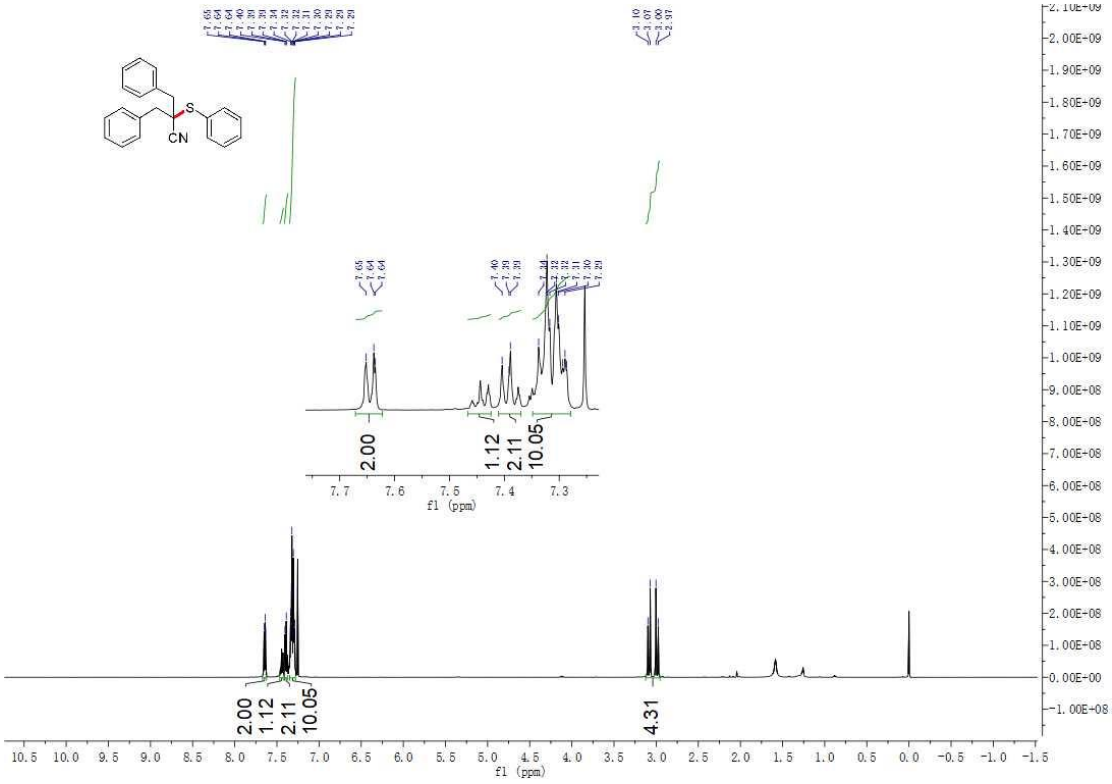
$^{1}$H NMR spectrum of **2-methyl-2-(phenylthio)propanenitrile (27)**



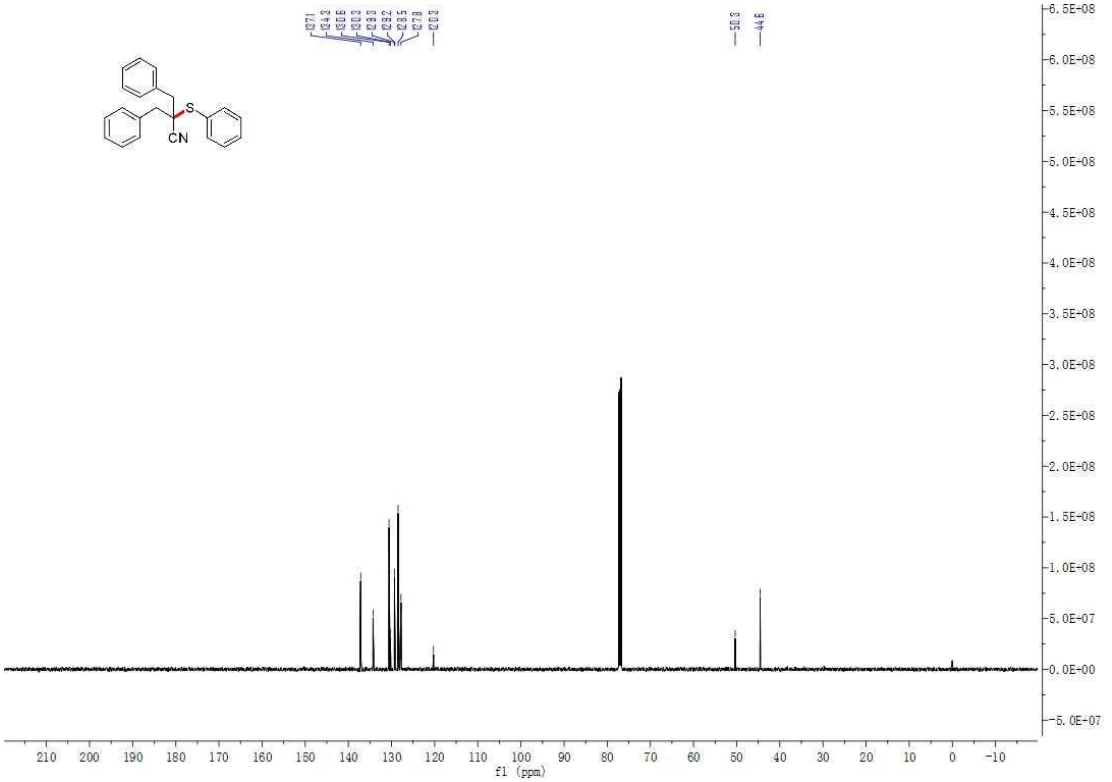

$^{13}$C NMR spectrum of **2-methyl-2-(phenylthio)propanenitrile (27)**



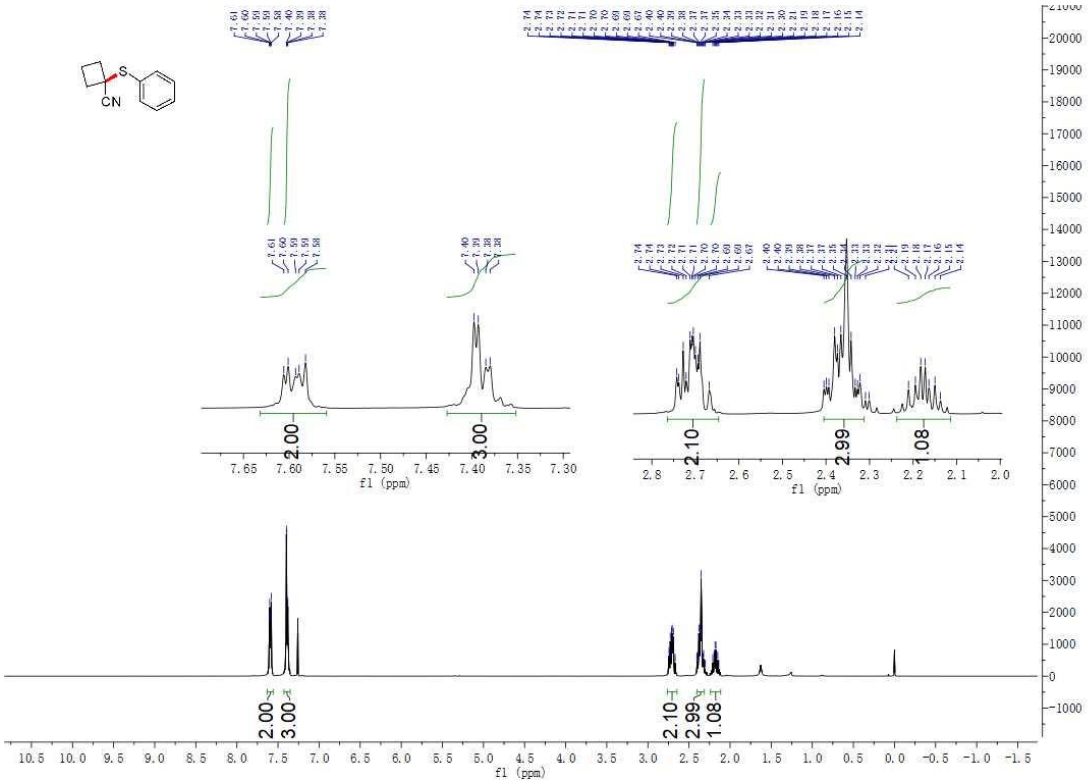
$^{1}$H NMR spectrum of **2-benzyl-3-phenyl-2-(phenylthio)propanenitrile (28)**



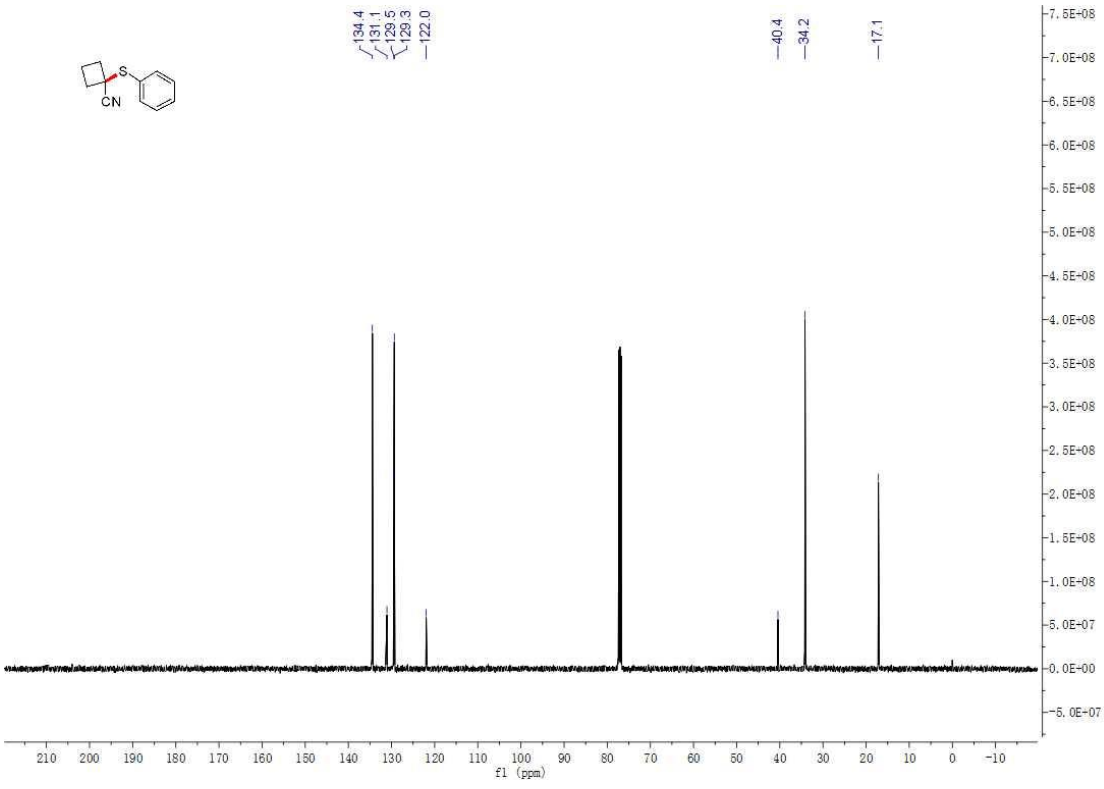

$^{13}$C NMR spectrum of **2-benzyl-3-phenyl-2-(phenylthio)propanenitrile (28)**



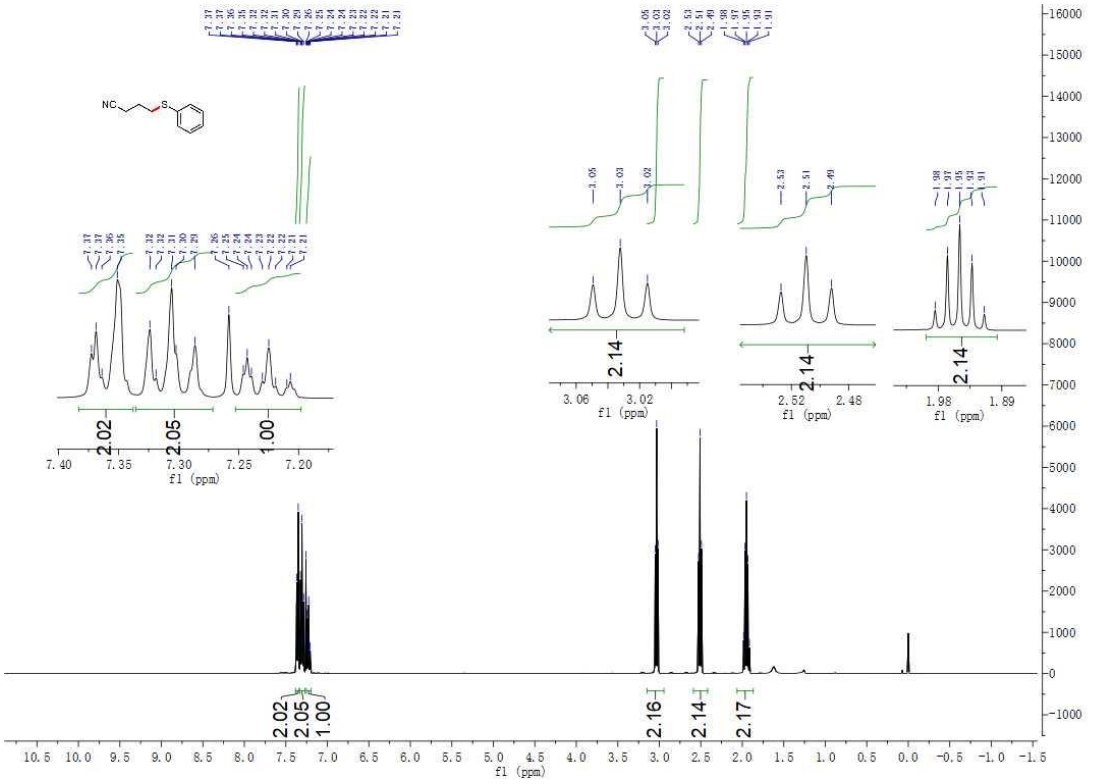
$^{1}$H NMR spectrum of **1-(phenylthio)cyclobutane-1-carbonitrile (29)**



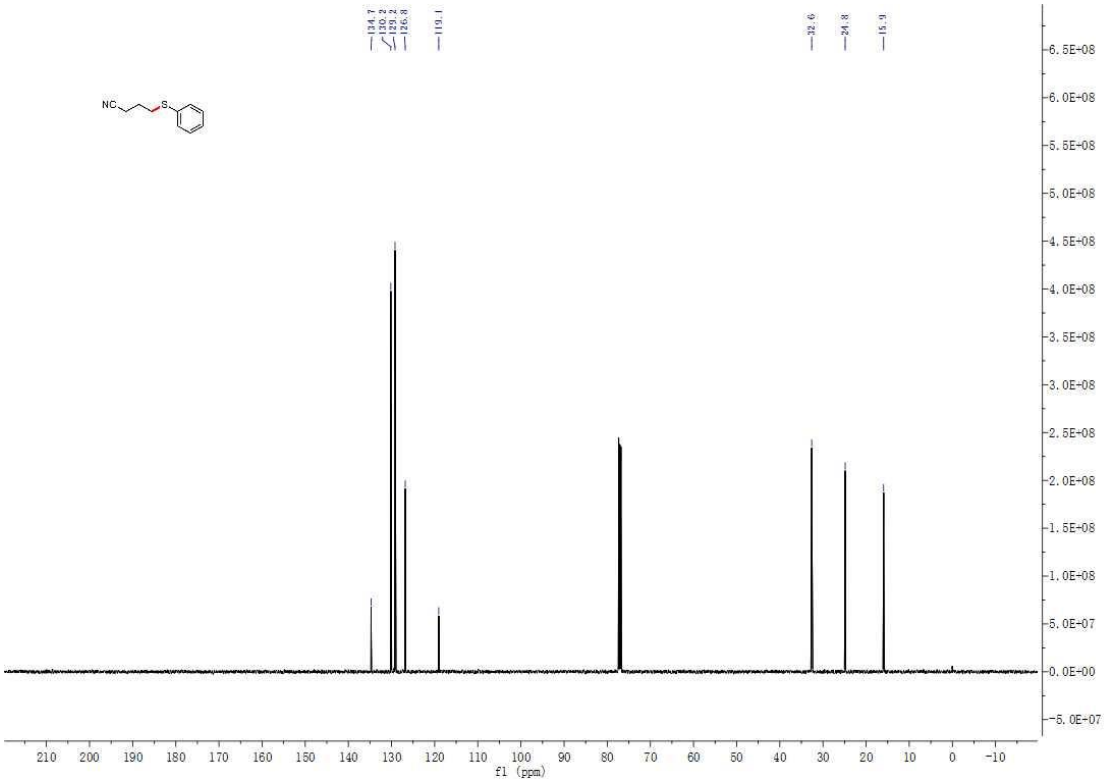
$^{13}$C NMR spectrum of **1-(phenylthio)cyclobutane-1-carbonitrile (29)**



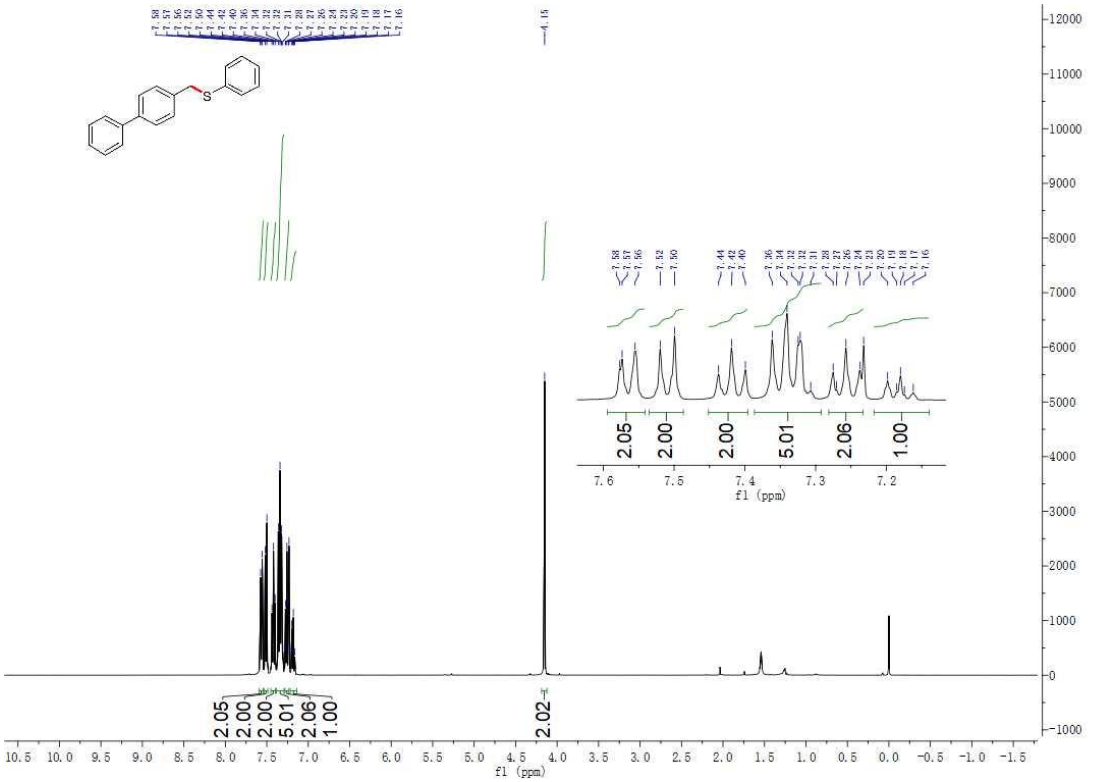
$^{1}$H NMR spectrum of **1-(phenylthio)cyclobutane-1-carbonitrile (30)**



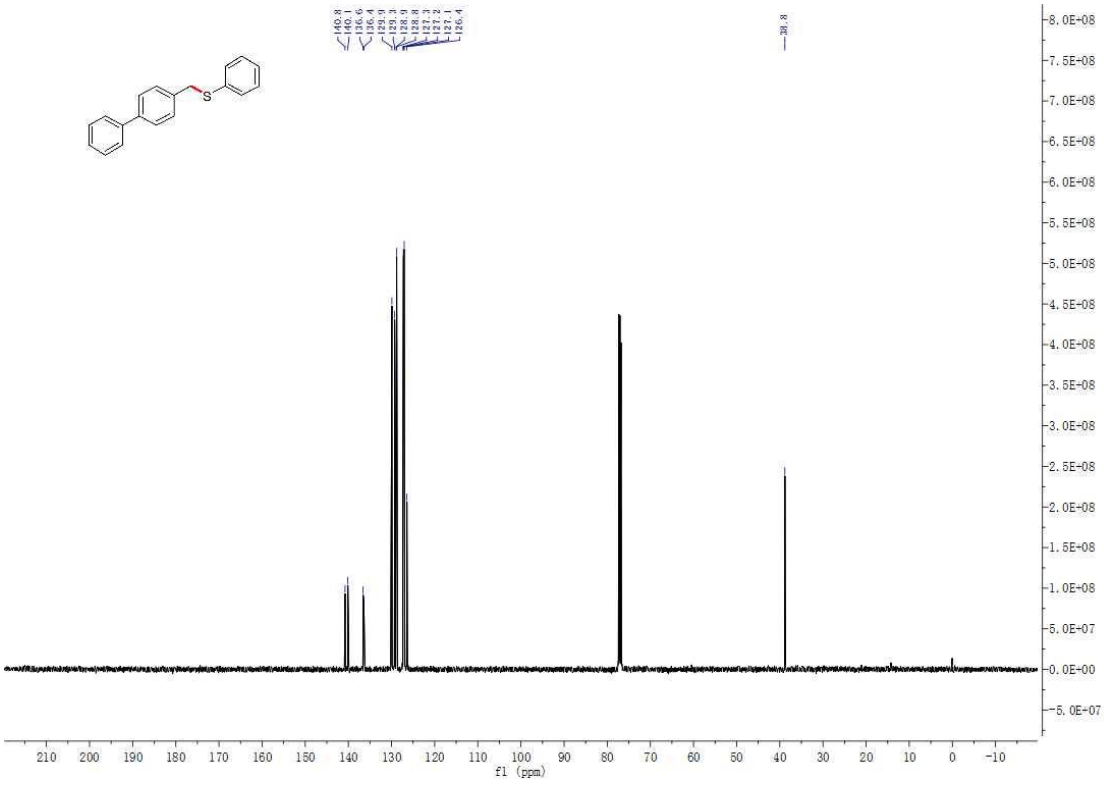
$^{13}$C NMR spectrum of **1-(phenylthio)cyclobutane-1-carbonitrile (30)**



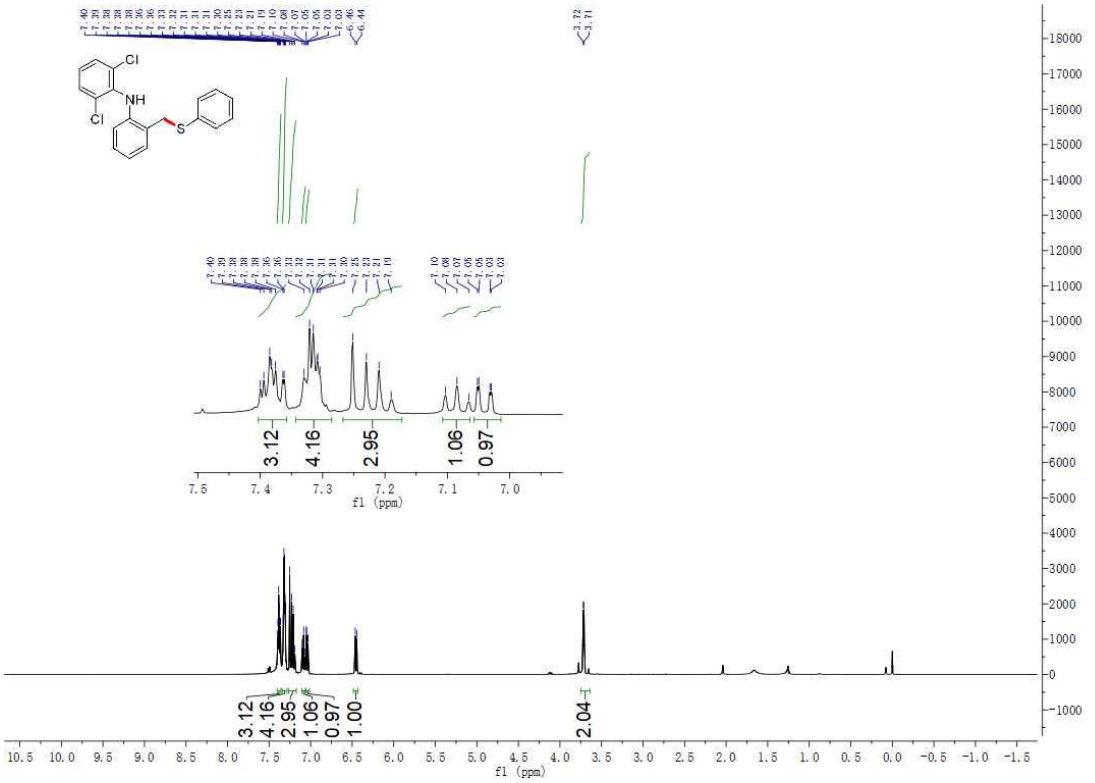
$^{1}$H NMR spectrum of **([1,1'-biphenyl]-4-ylmethyl)(phenyl)sulfane (31)**



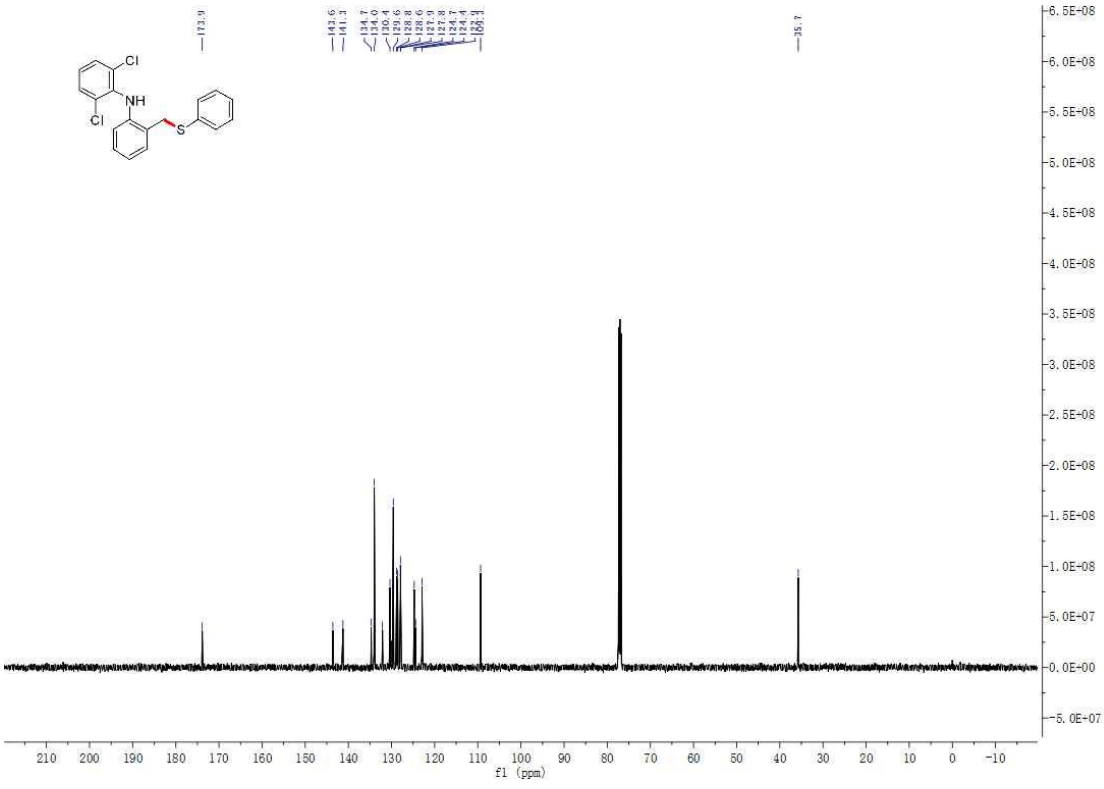

$^{13}$C NMR spectrum of **([1,1'-biphenyl]-4-ylmethyl)(phenyl)sulfane (31)**



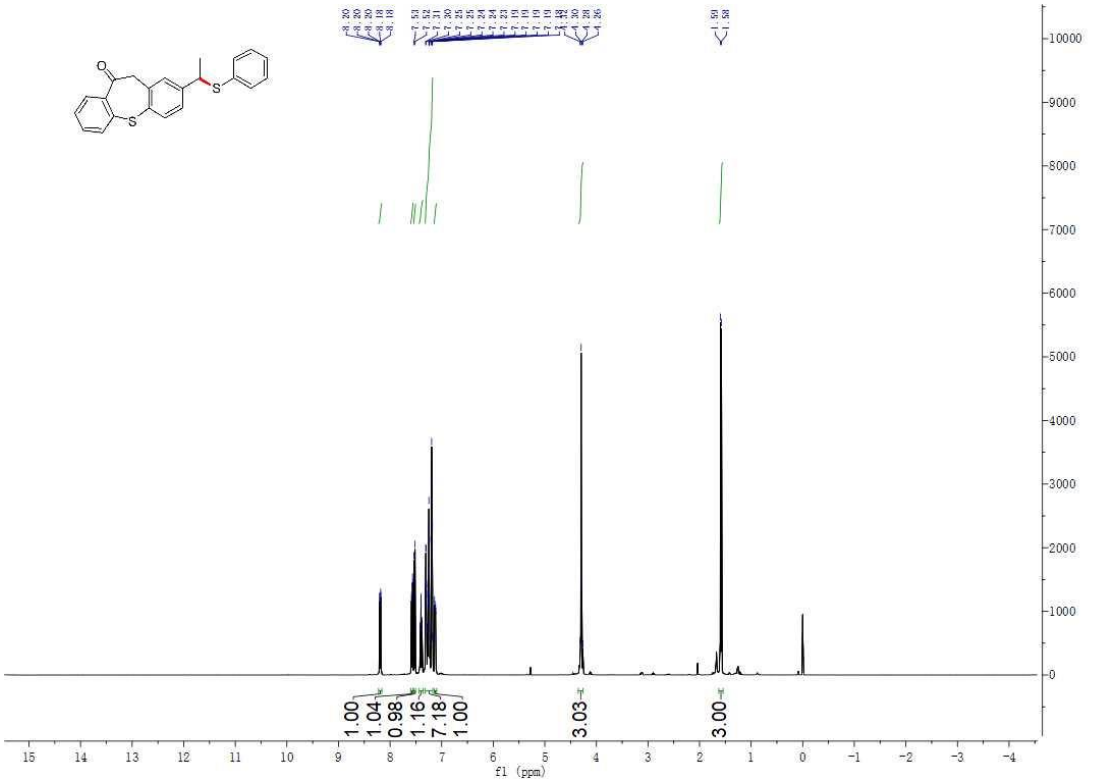
$^{1}$H NMR spectrum of **2,6-dichloro-N-(2-((phenylthio)methyl)phenyl)aniline (32)**



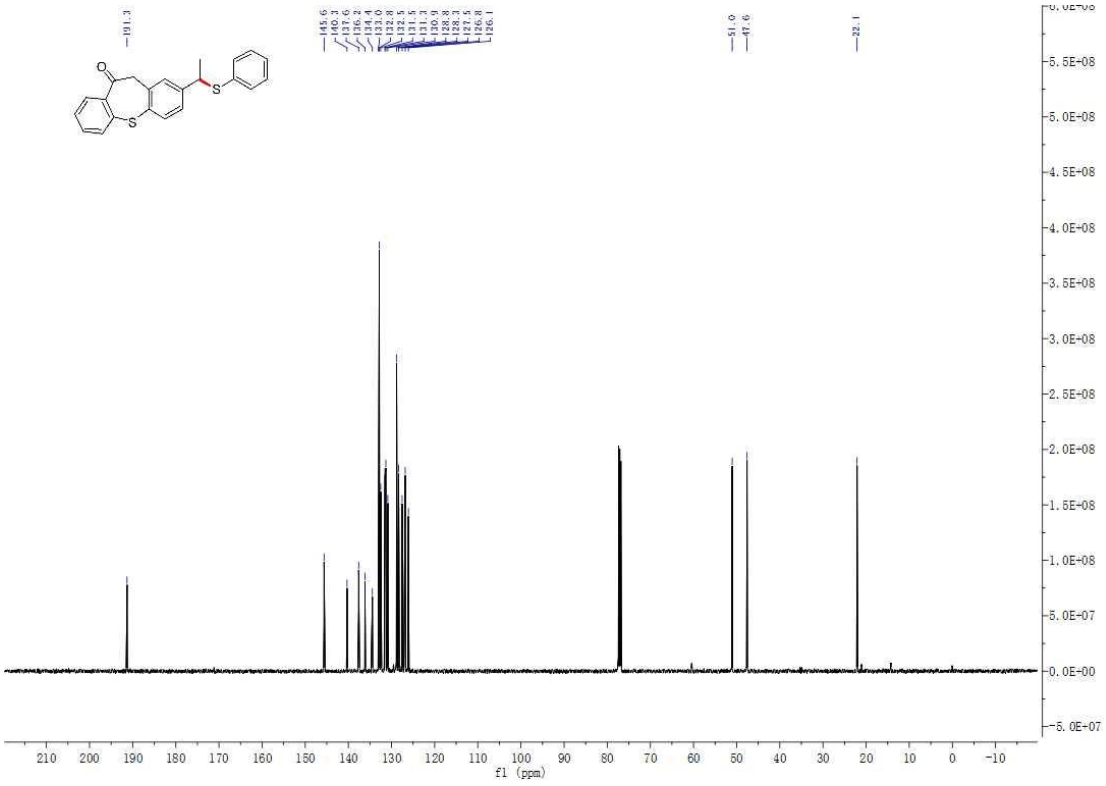

$^{13}$C NMR spectrum of **2,6-dichloro-N-(2-((phenylthio)methyl)phenyl)aniline (32)**



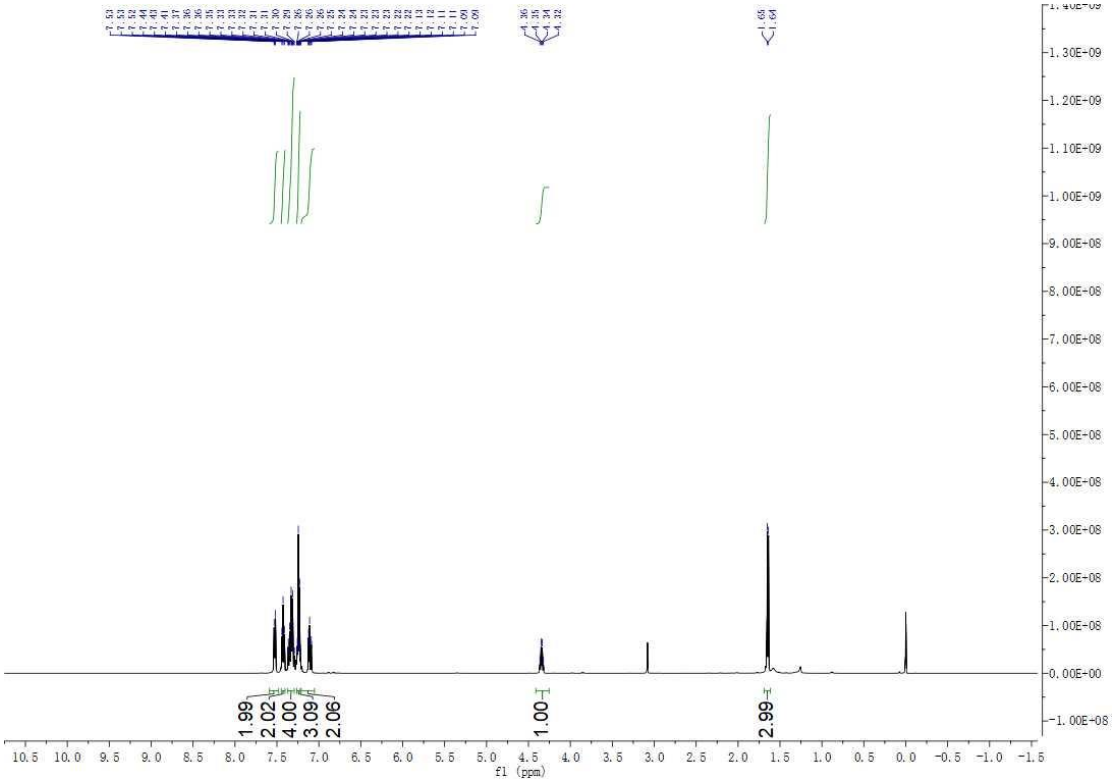
$^{1}$H NMR spectrum of **2-(1-(phenylthio)ethyl)dibenzo[b,f]thiepin-10(11H)-one (33)**



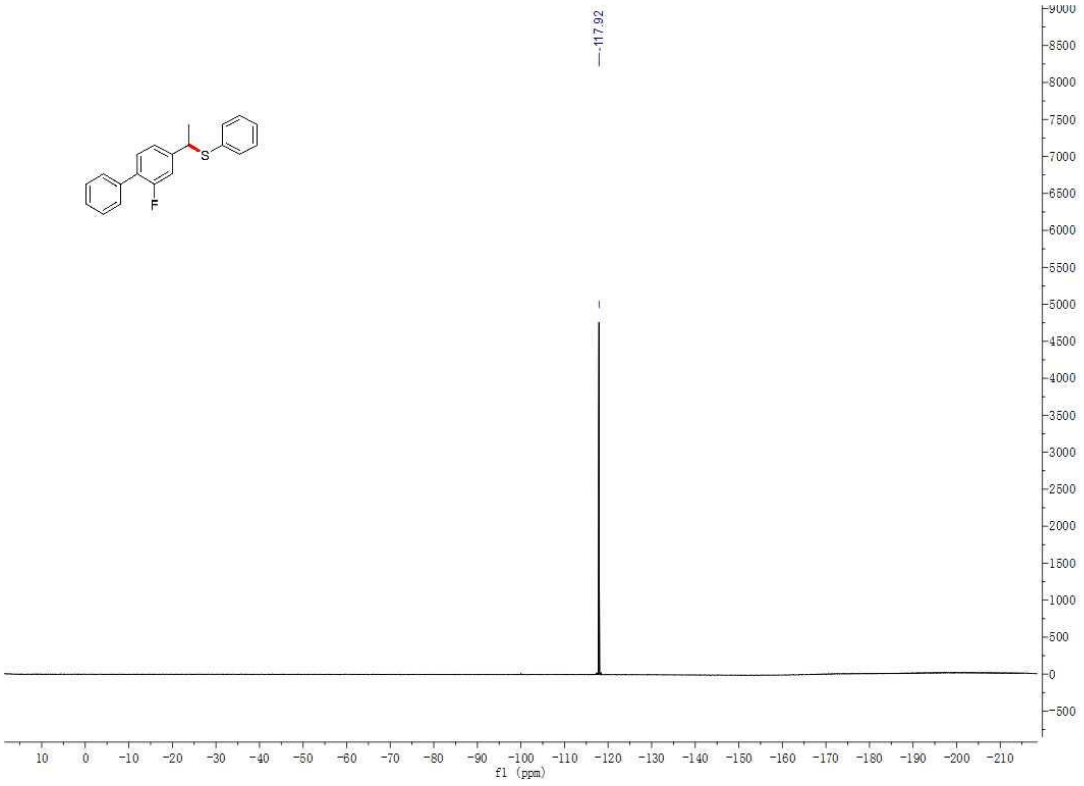

$^{13}$C NMR spectrum of **2-(1-(phenylthio)ethyl)dibenzo[b,f]thiepin-10(11H)-one (33)**



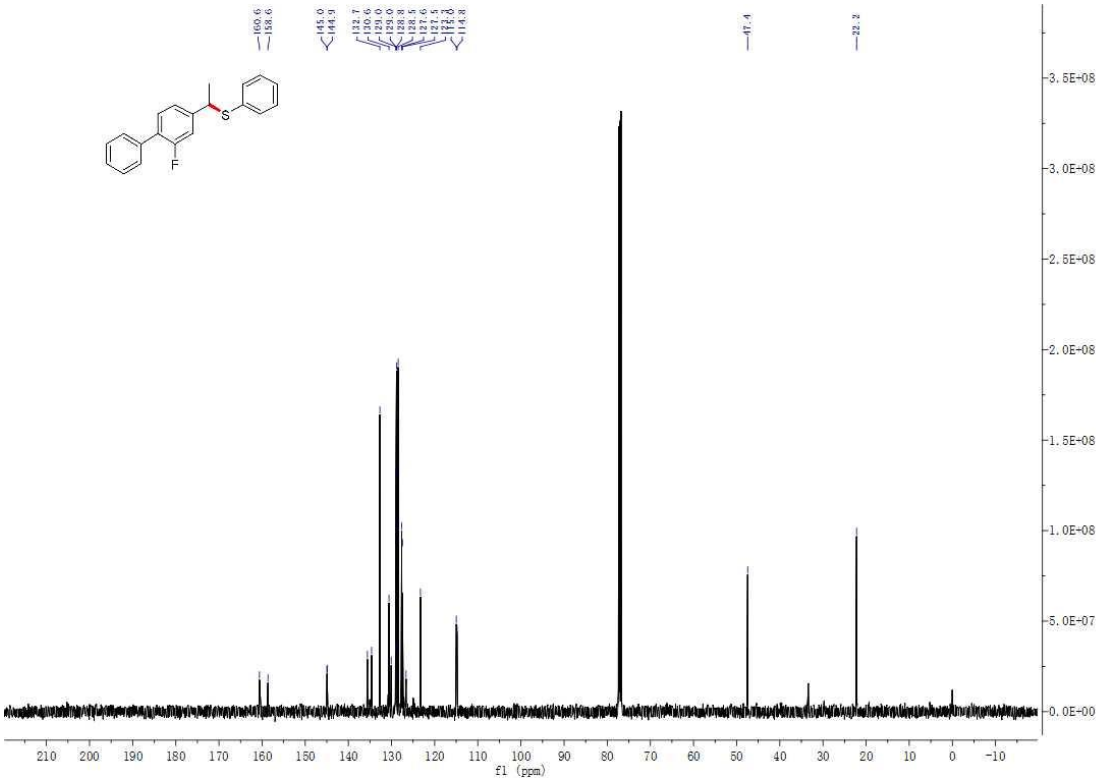
$^{1}$H NMR spectrum of **(1-(2-fluoro-[1,1'-biphenyl]-4-yl)ethyl)(phenyl)sulfane (34)**



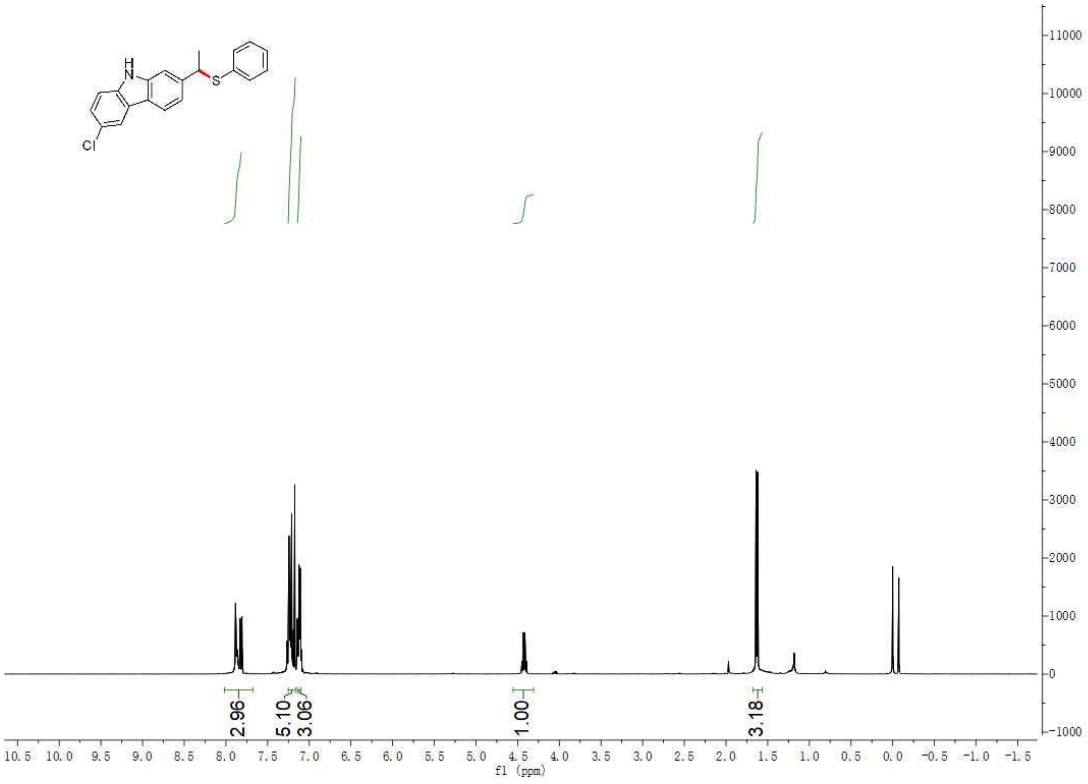

$^{19}$F NMR spectrum of **(1-(2-fluoro-[1,1'-biphenyl]-4-yl)ethyl)(phenyl)sulfane (34)**



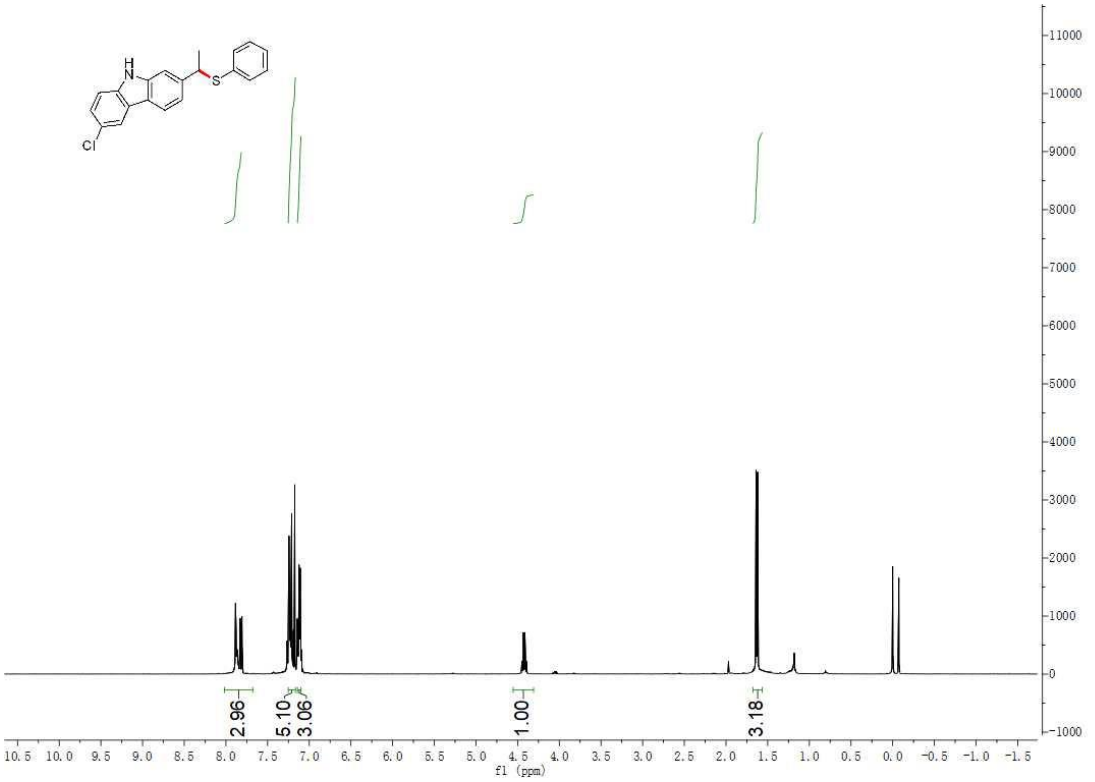
$^{13}$C NMR spectrum of **(1-(2-fluoro-[1,1'-biphenyl]-4-yl)ethyl)(phenyl)sulfane (34)**



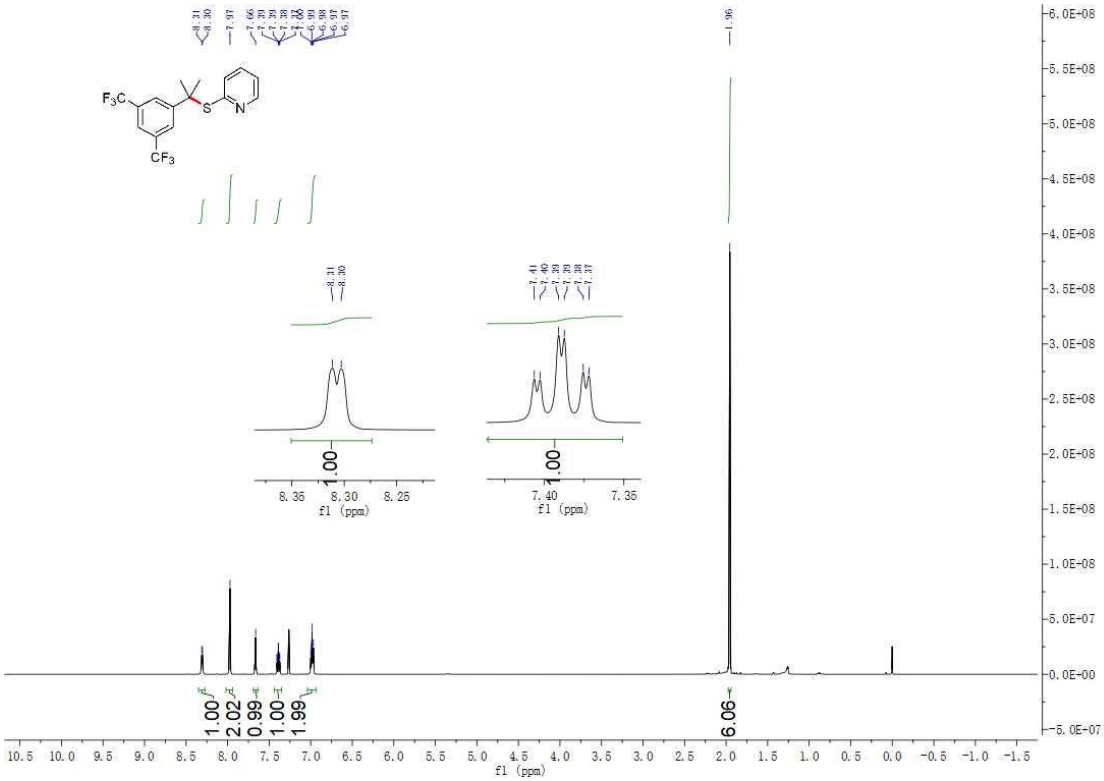

$^{1}$H NMR spectrum of **6-chloro-2-(1-(phenylthio)ethyl)-9H-carbazole (35)**



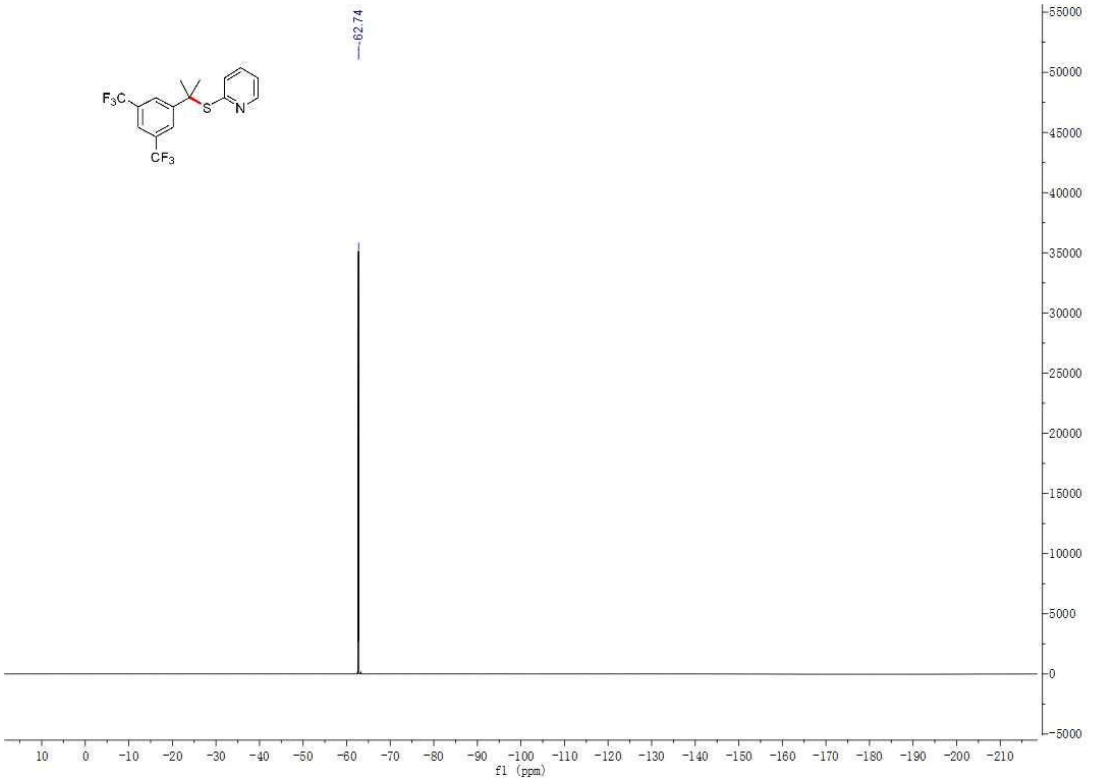
$^{13}$C NMR spectrum of **6-chloro-2-(1-(phenylthio)ethyl)-9H-carbazole (35)**



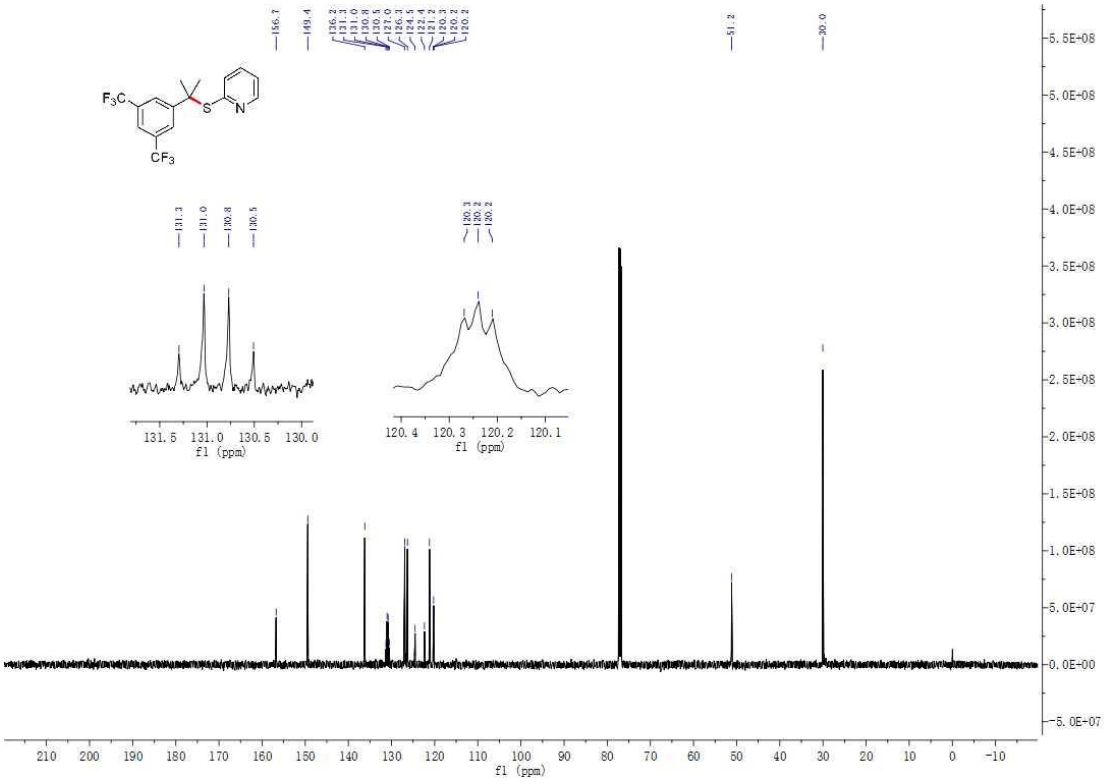

$^{1}$H NMR spectrum of **2-((2-(3,5-bis(trifluoromethyl)phenyl)propan-2-yl)thio)pyridine (36)**



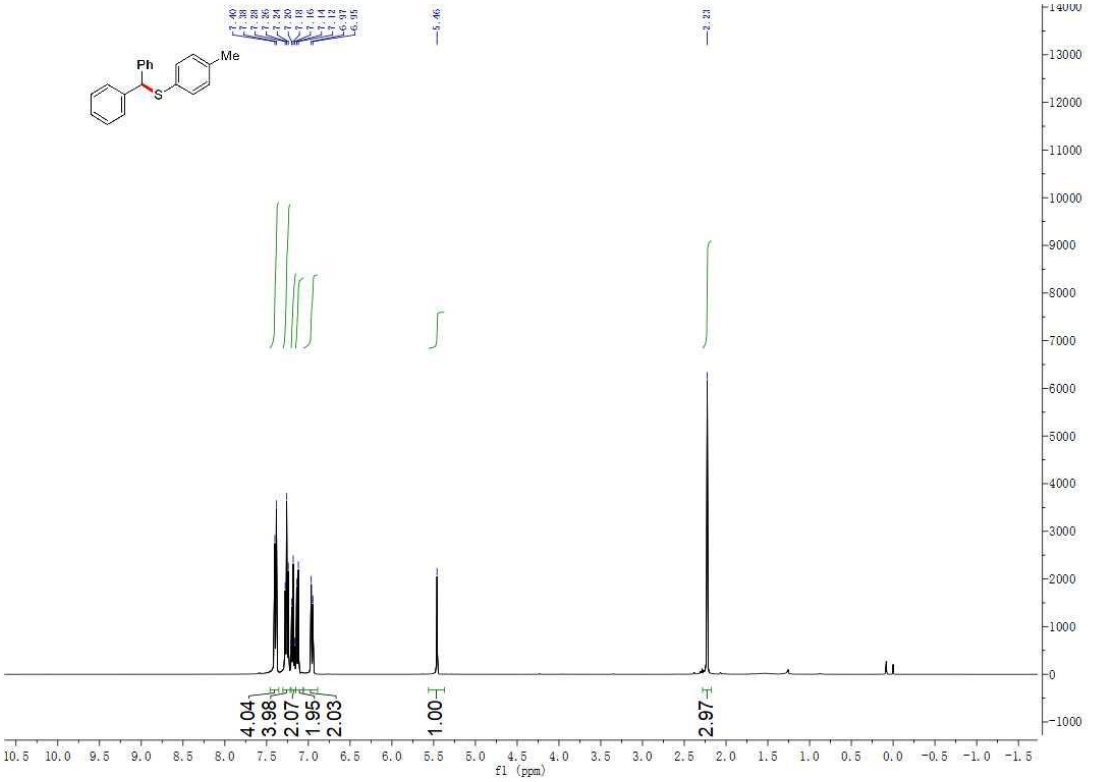
$^{19}$F NMR spectrum of **2-((2-(3,5-bis(trifluoromethyl)phenyl)propan-2-yl)thio)pyridine (36)**



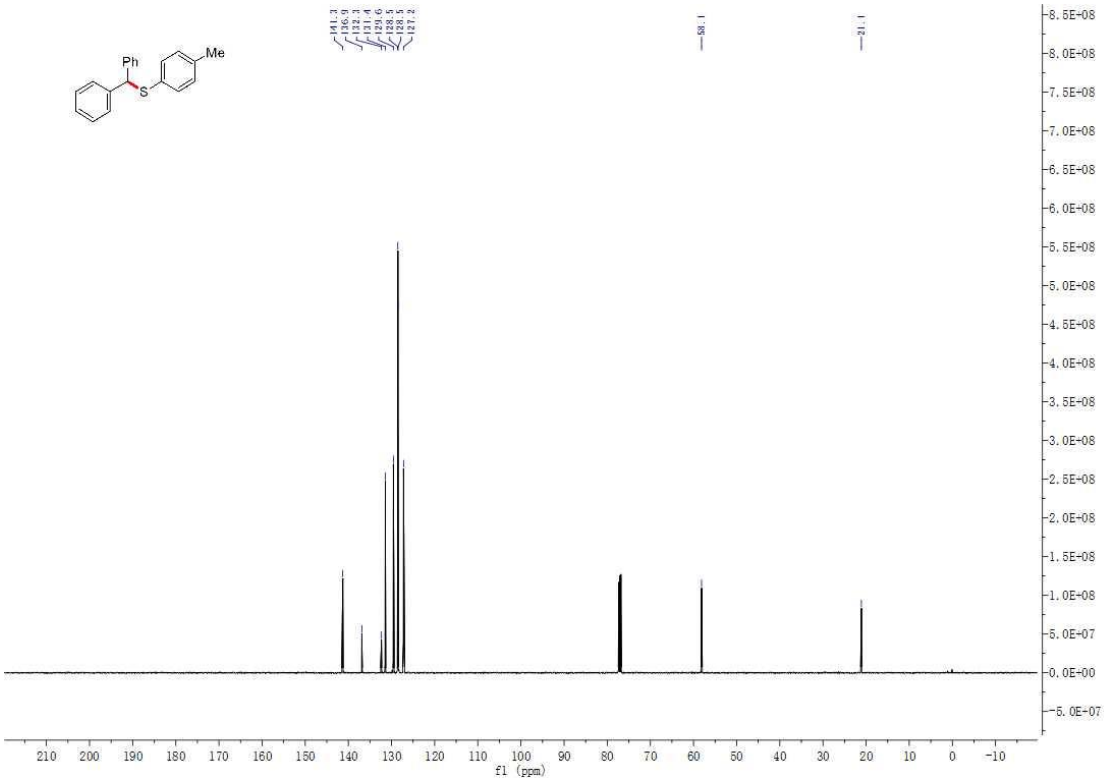

$^{13}$C NMR spectrum of **2-((2-(3,5-bis(trifluoromethyl)phenyl)propan-2-yl)thio)pyridine (36)**



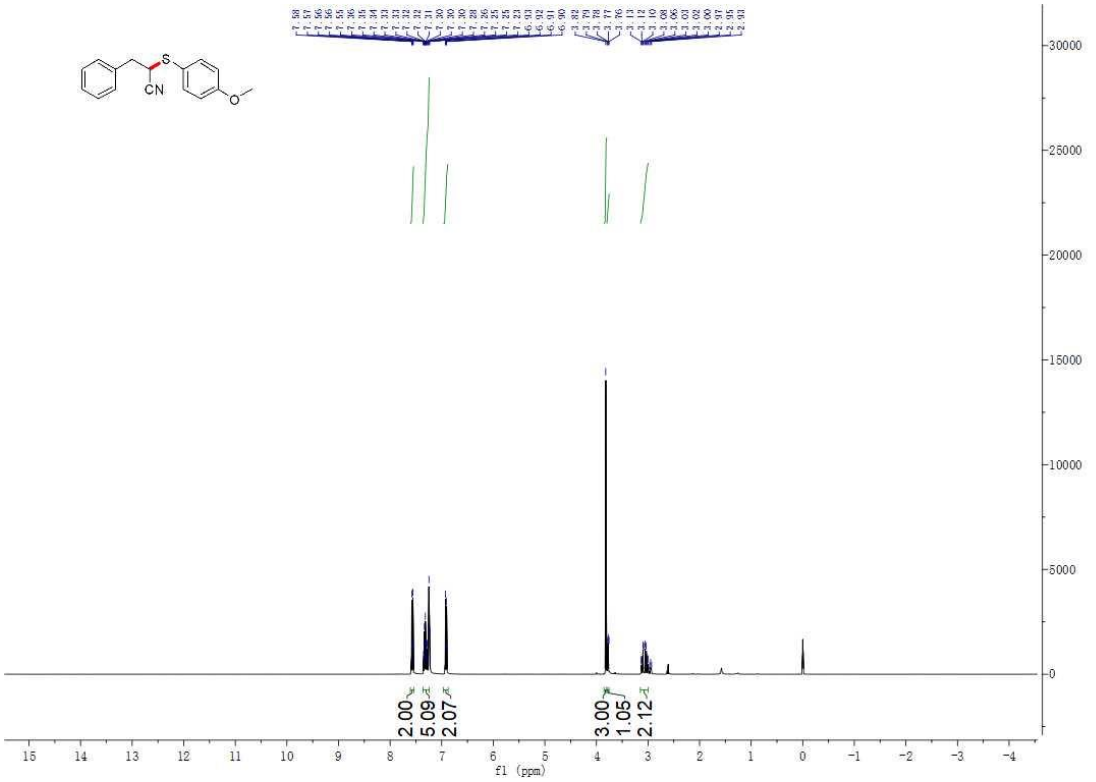
$^{1}$H NMR spectrum of **benzhydryl(p-tolyl)sulfane (37)**



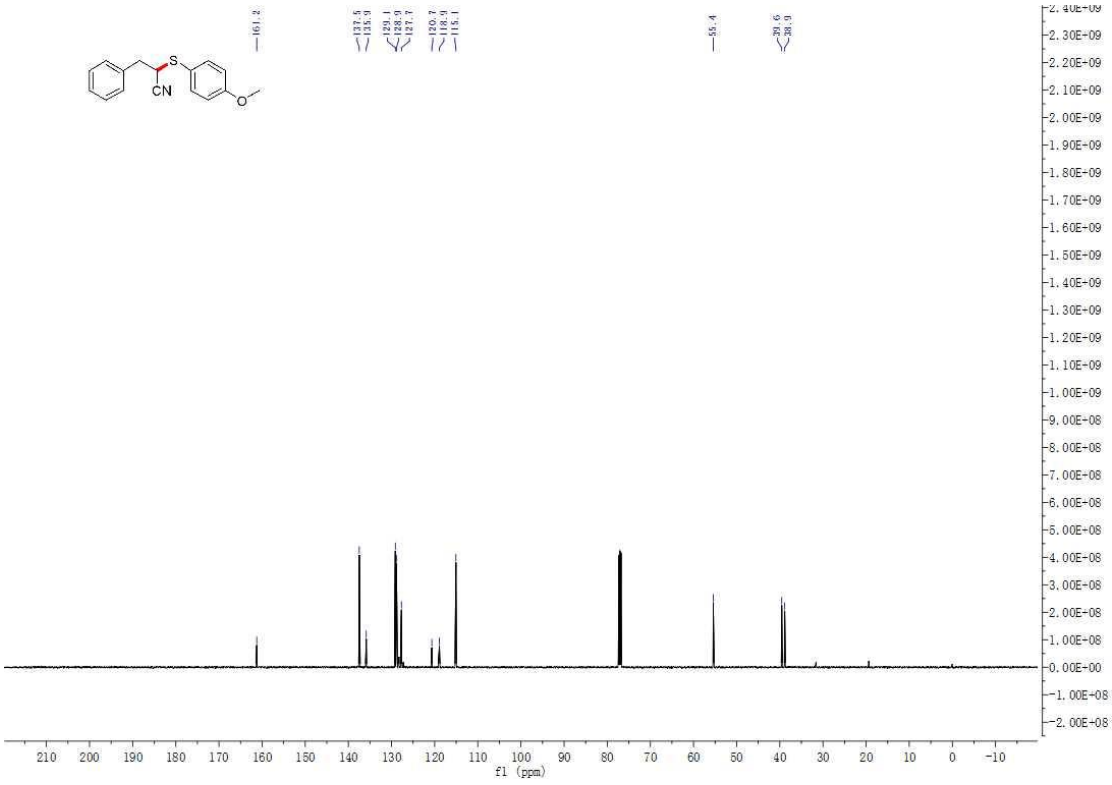

$^{13}$C NMR spectrum of **benzhydryl(p-tolyl)sulfane (37)**



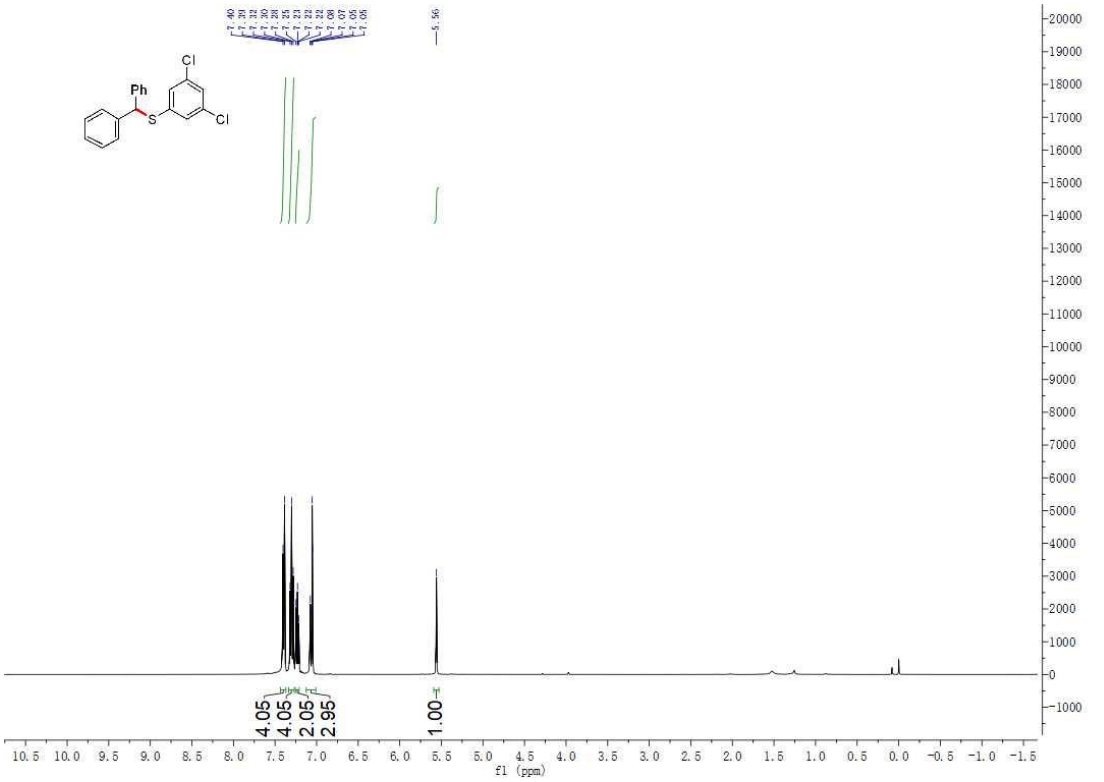
$^{1}$H NMR spectrum of **2-((4-methoxyphenyl)thio)-3-phenylpropanenitrile (38)**



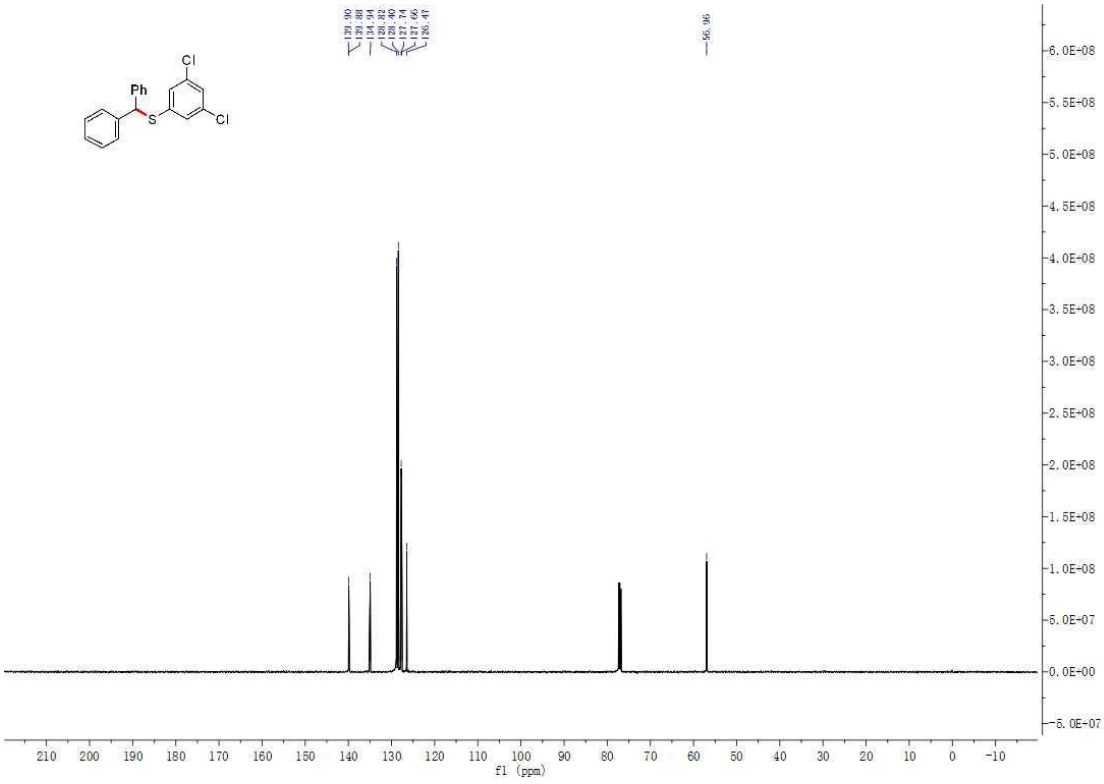

$^{13}$C NMR spectrum of **2-((4-methoxyphenyl)thio)-3-phenylpropanenitrile (38)**



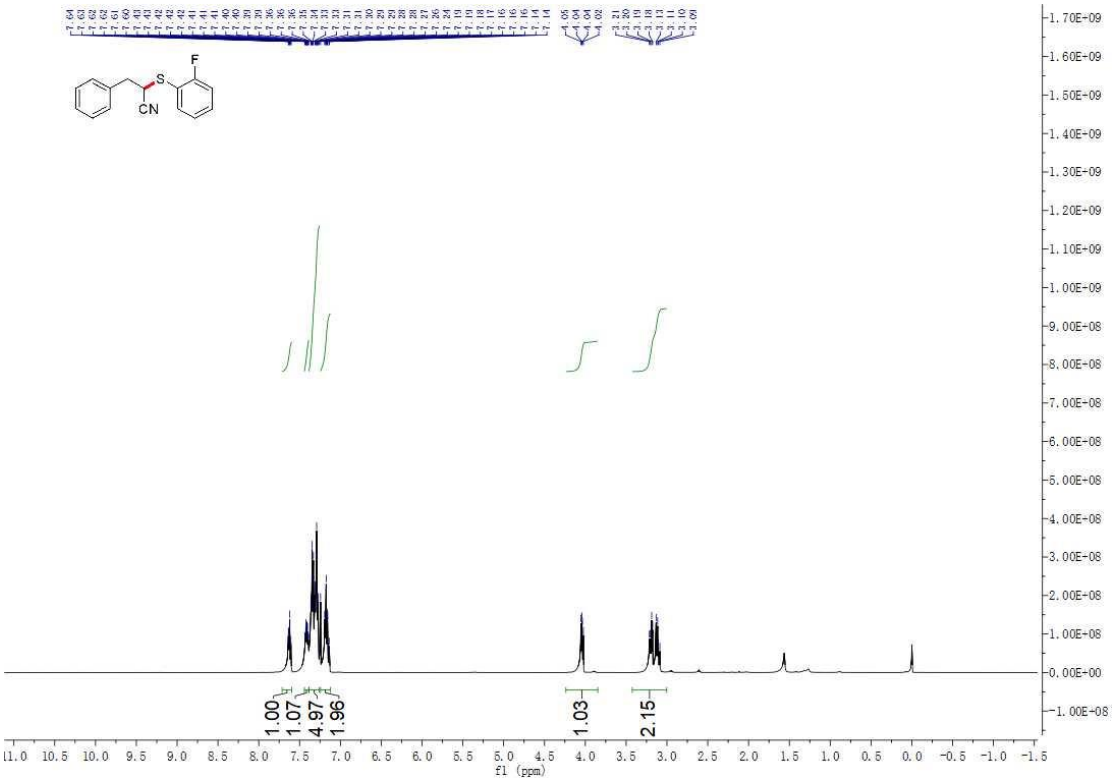
$^{1}$H NMR spectrum of **benzhydryl(3,5-dichlorophenyl)sulfane (39)**



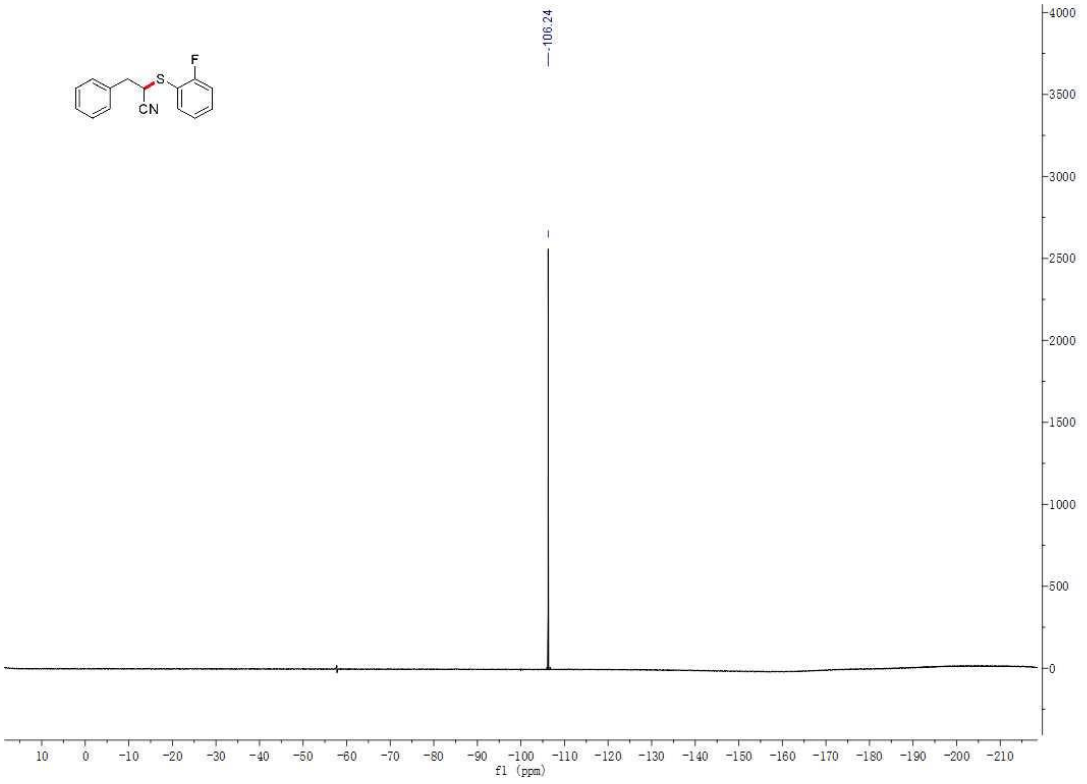

$^{13}$C NMR spectrum of **benzhydryl(3,5-dichlorophenyl)sulfane (39)**



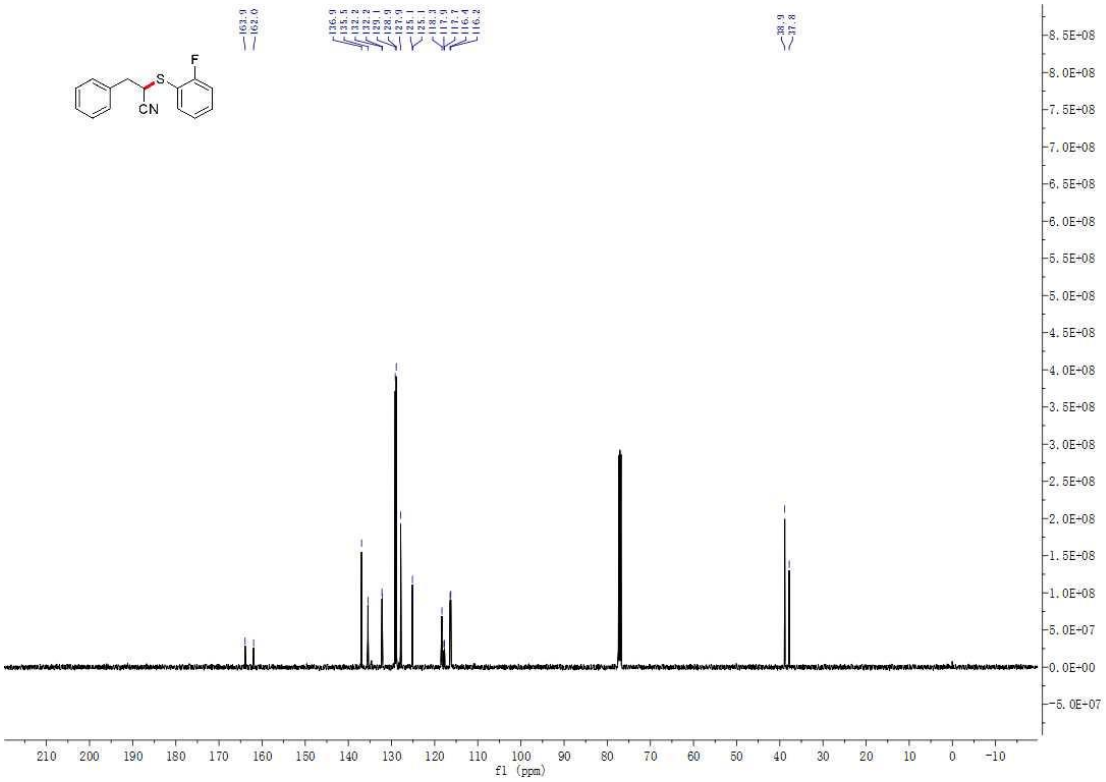
$^{1}$H NMR spectrum of **2-((2-fluorophenyl)thio)-3-phenylpropanenitrile (40)**



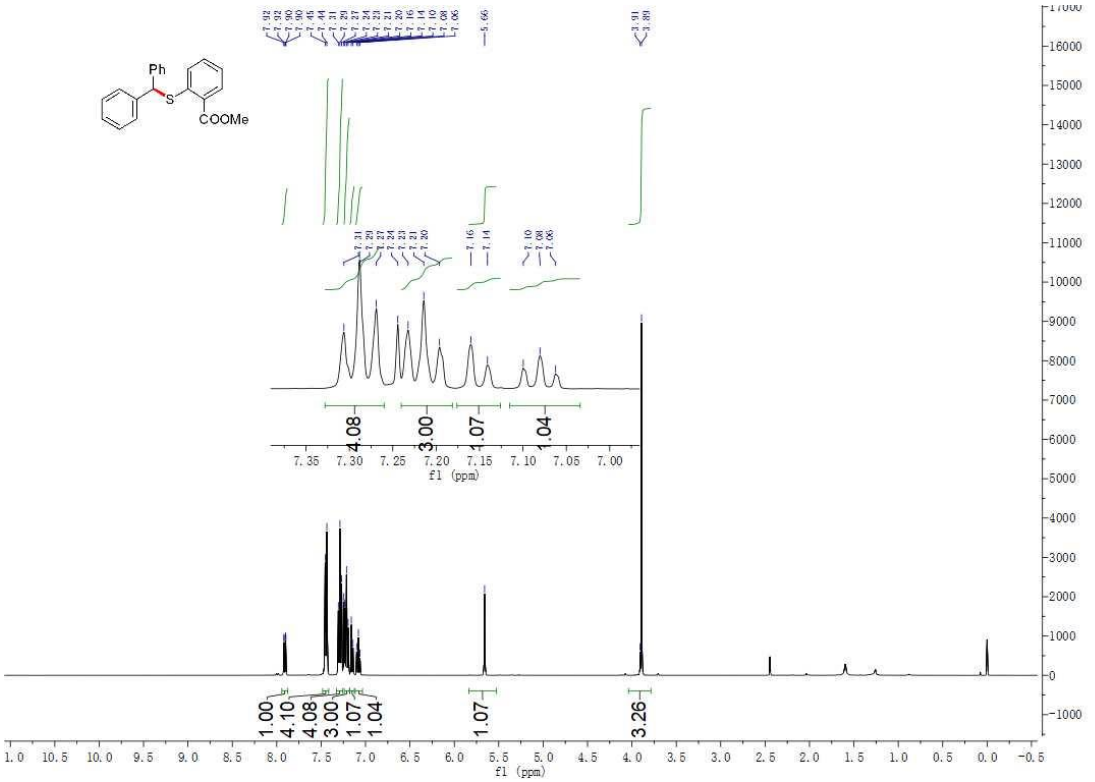

$^{13}$C NMR spectrum of **2-((2-fluorophenyl)thio)-3-phenylpropanenitrile (40)**



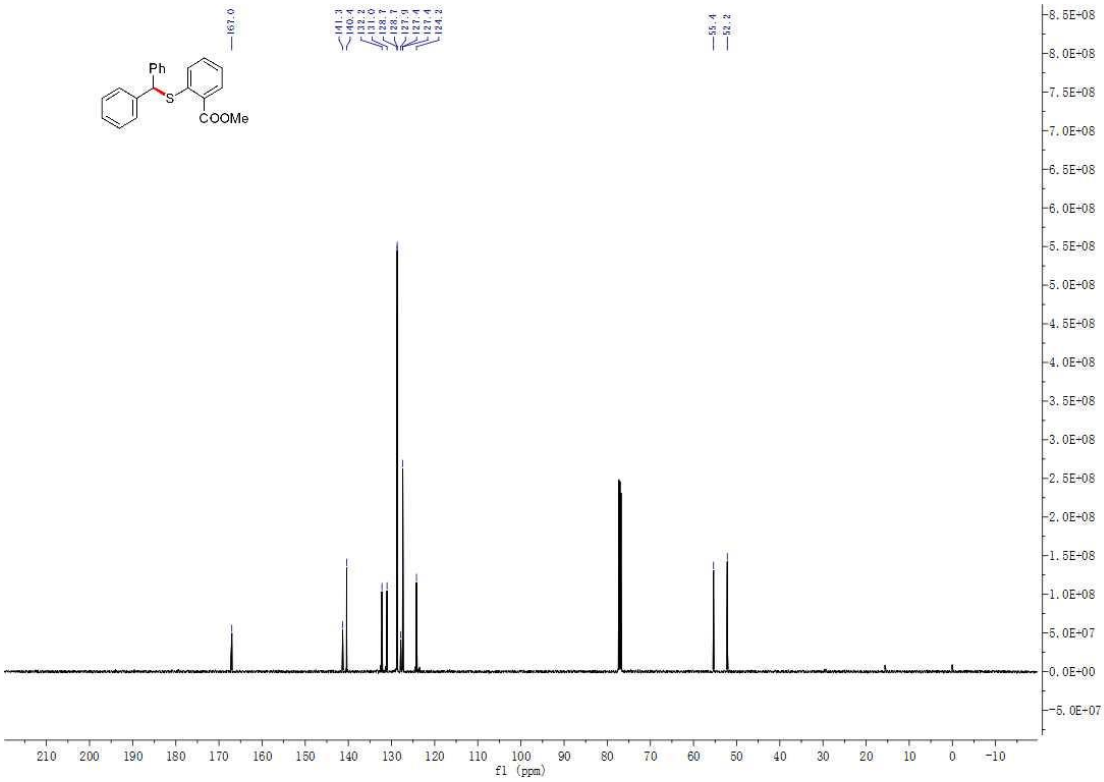
$^{13}$C NMR spectrum of **2-((2-fluorophenyl)thio)-3-phenylpropanenitrile (40)**



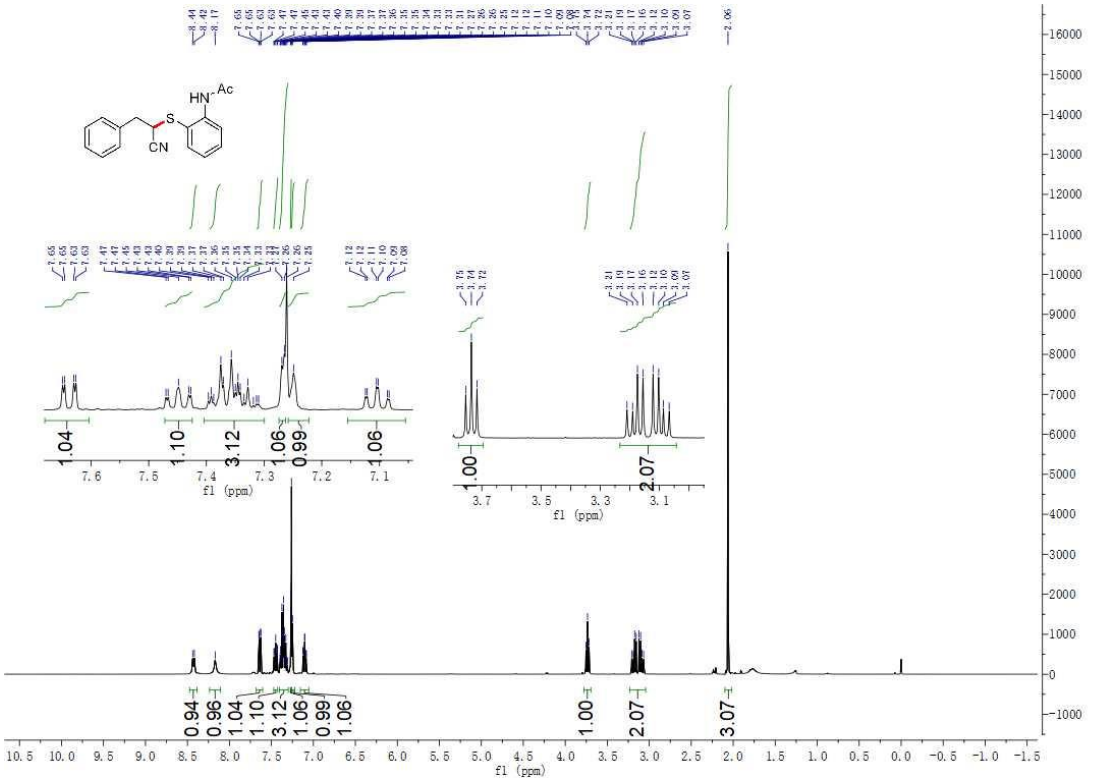

$^{1}$H NMR spectrum of **methyl 2-(benzhydrylthio)benzoate (41)**



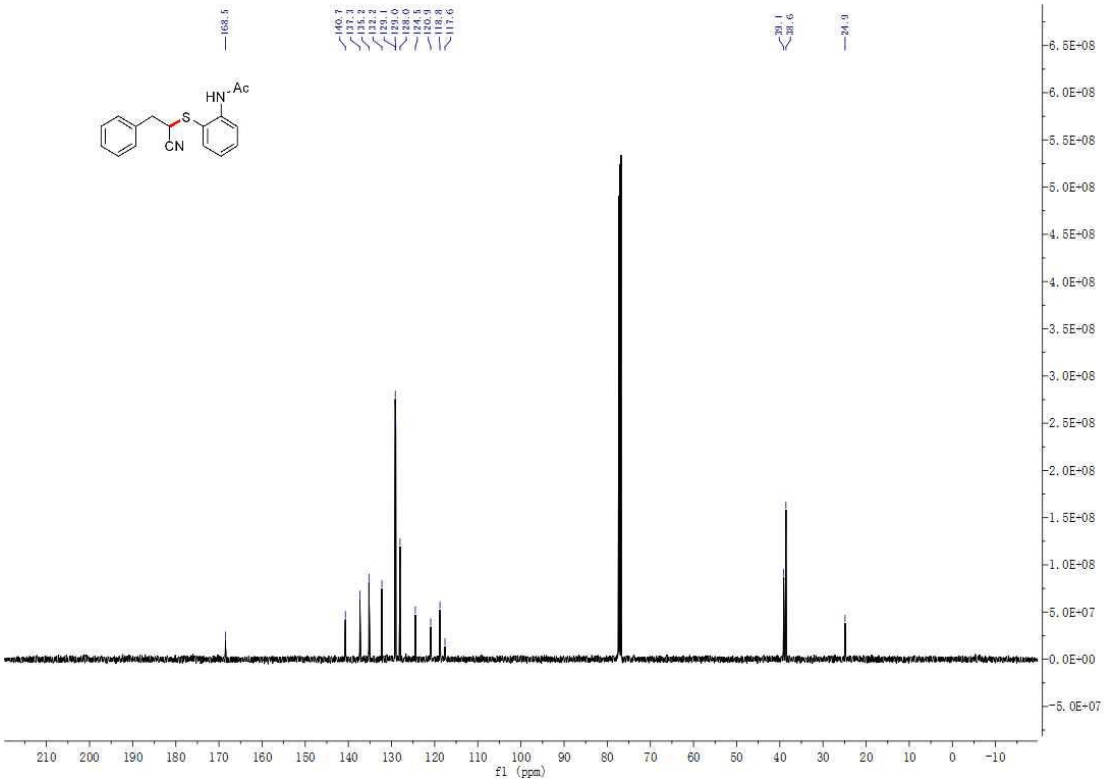
$^{13}$C NMR spectrum of **methyl 2-(benzhydrylthio)benzoate (41)**



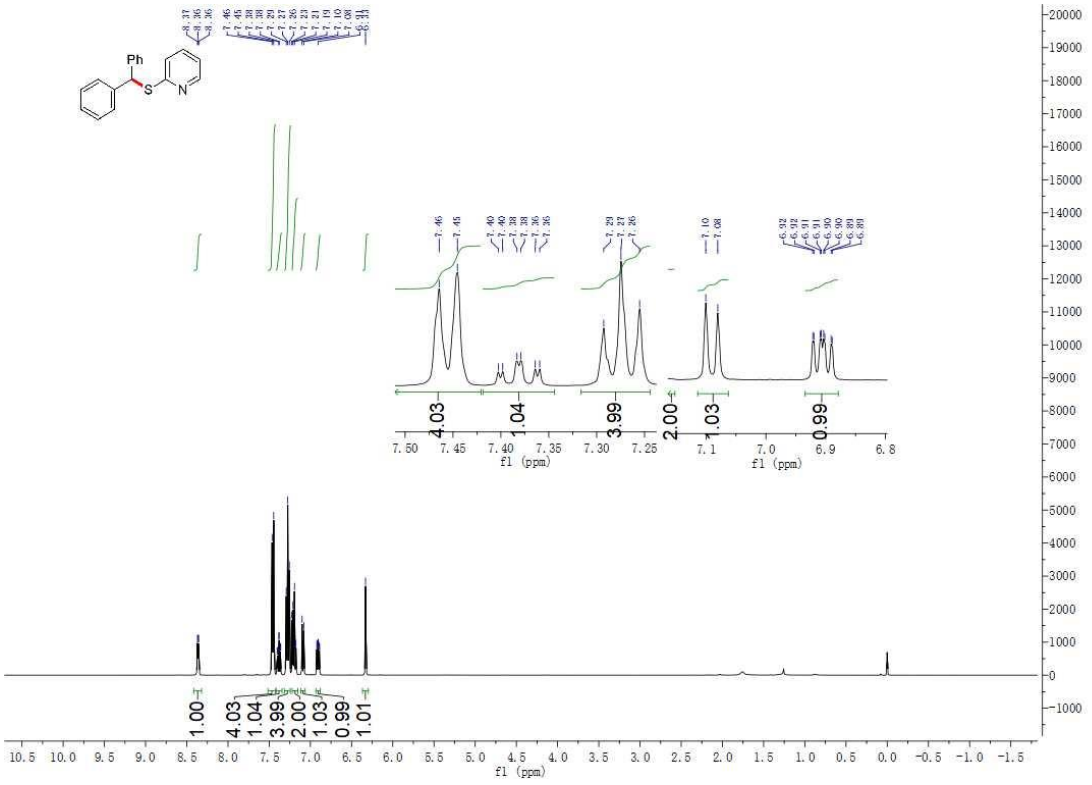

$^{1}$H NMR spectrum of **N-(2-((1-cyano-2-phenylethyl)thio)phenyl)acetamide (42)**



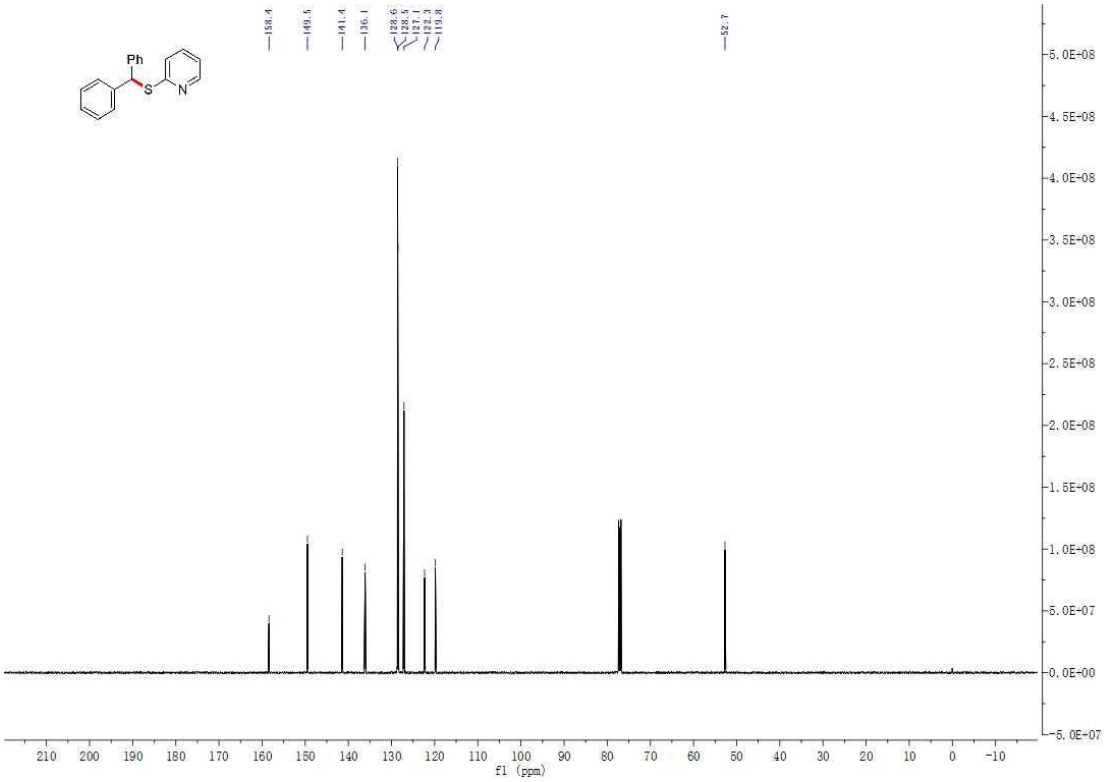
$^{13}$C NMR spectrum of **N-(2-((1-cyano-2-phenylethyl)thio)phenyl)acetamide (42)**



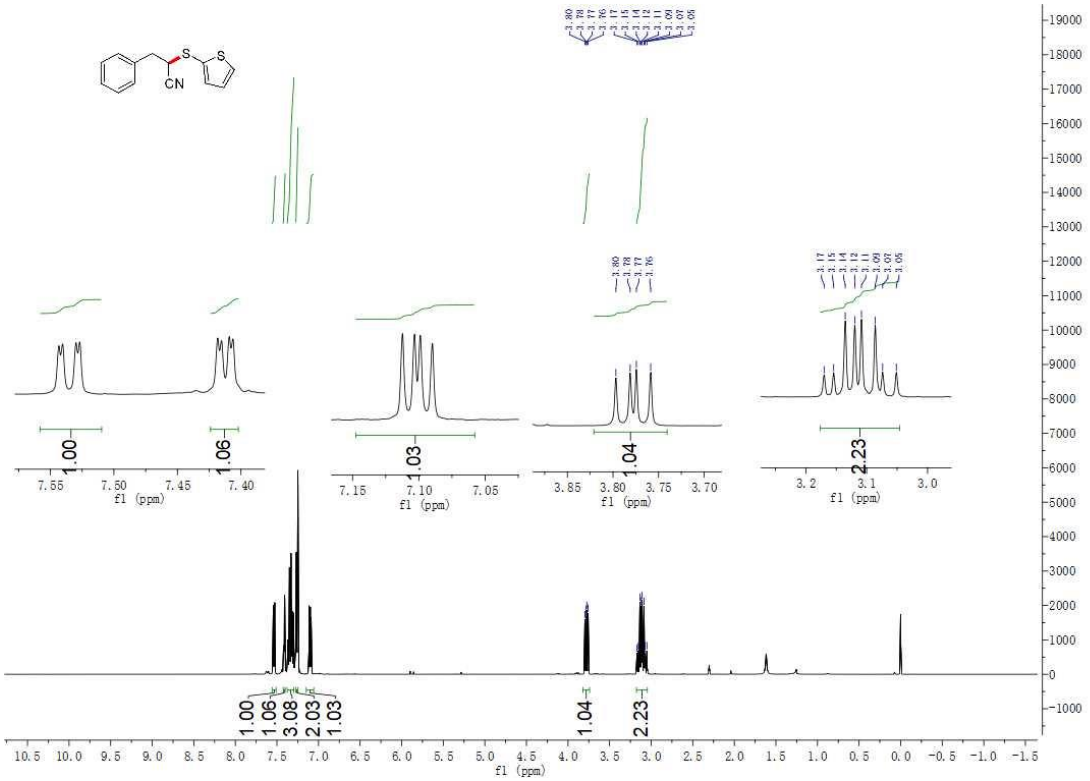

$^{1}$H NMR spectrum of **2-(benzhydrylthio)pyridine (43)**



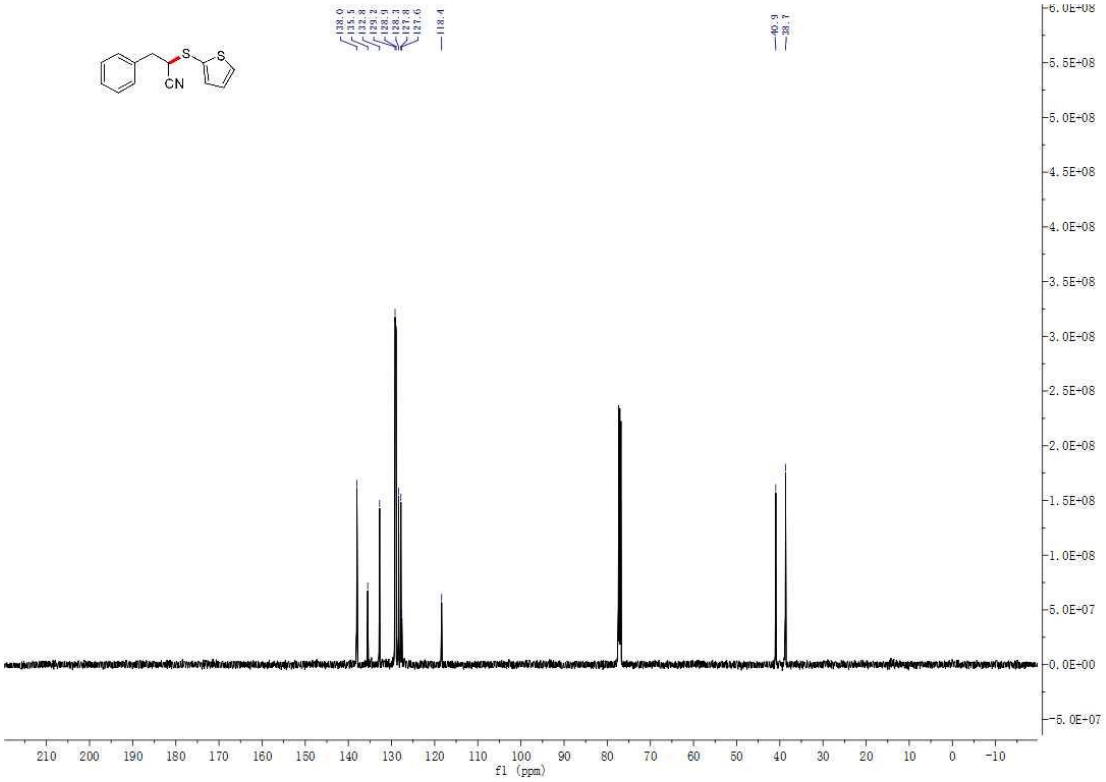
$^{13}$C NMR spectrum of **2-(benzhydrylthio)pyridine (43)**



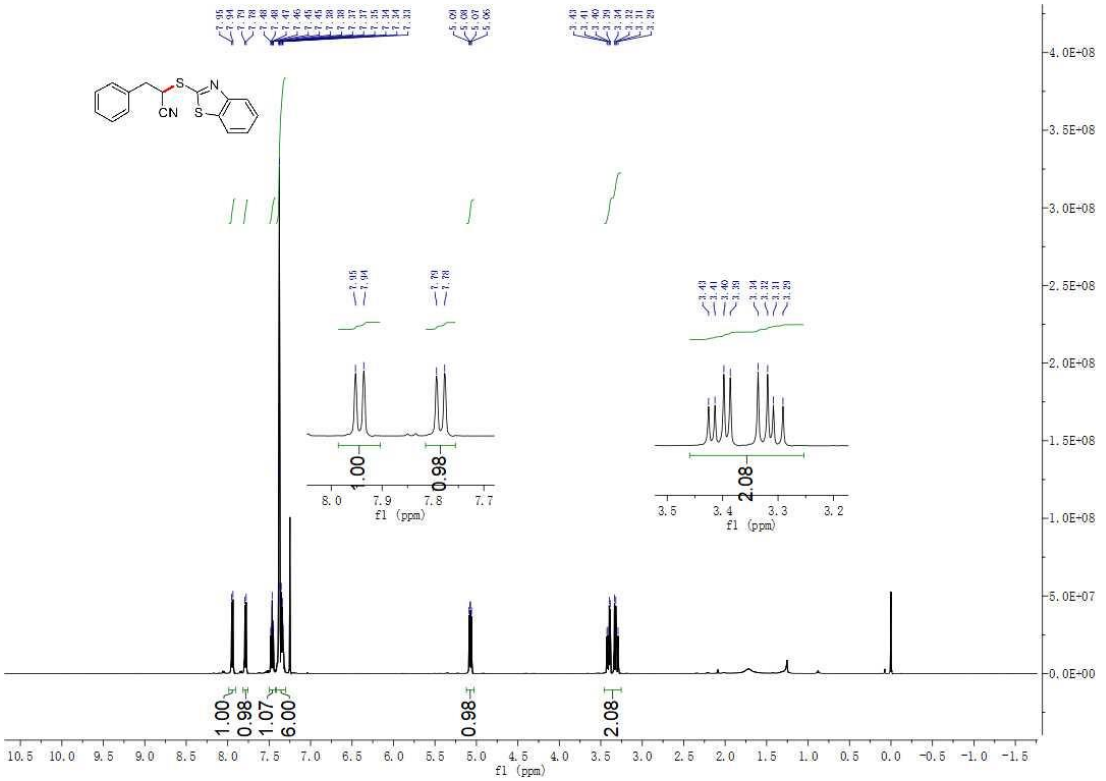
$^{1}$H NMR spectrum of **3-phenyl-2-(thiophen-2-ylthio)propanenitrile (44)**



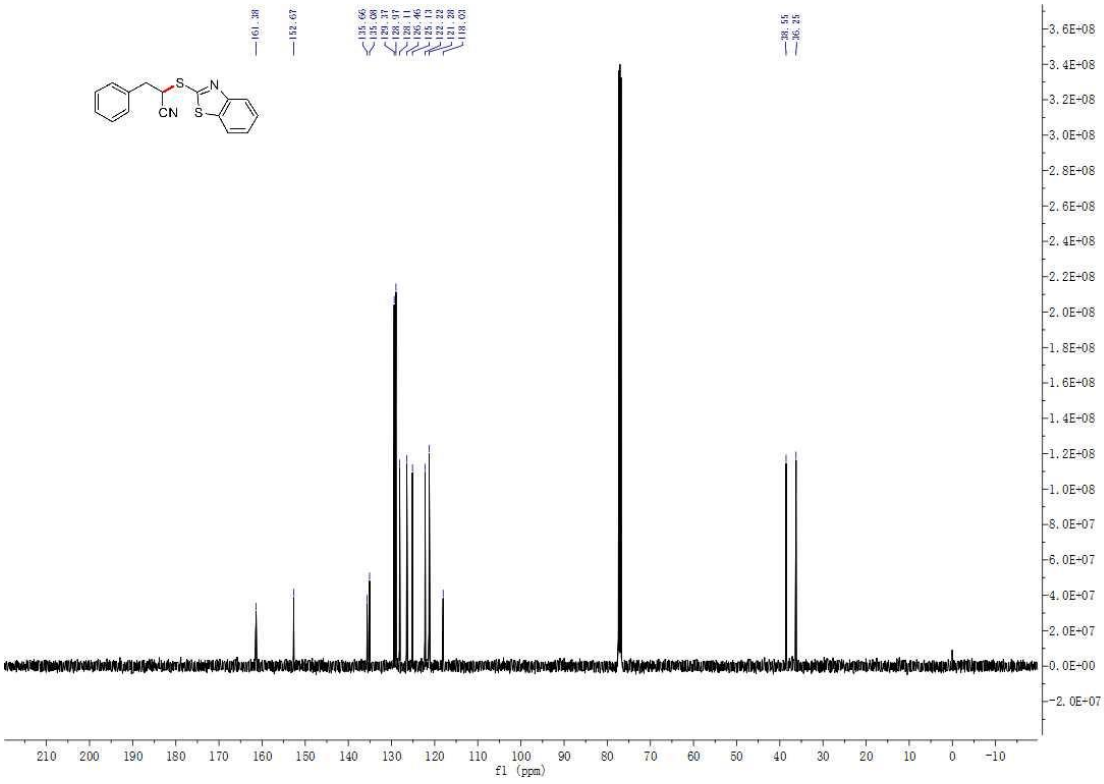
$^{13}$C NMR spectrum of **3-phenyl-2-(thiophen-2-ylthio)propanenitrile (44)**



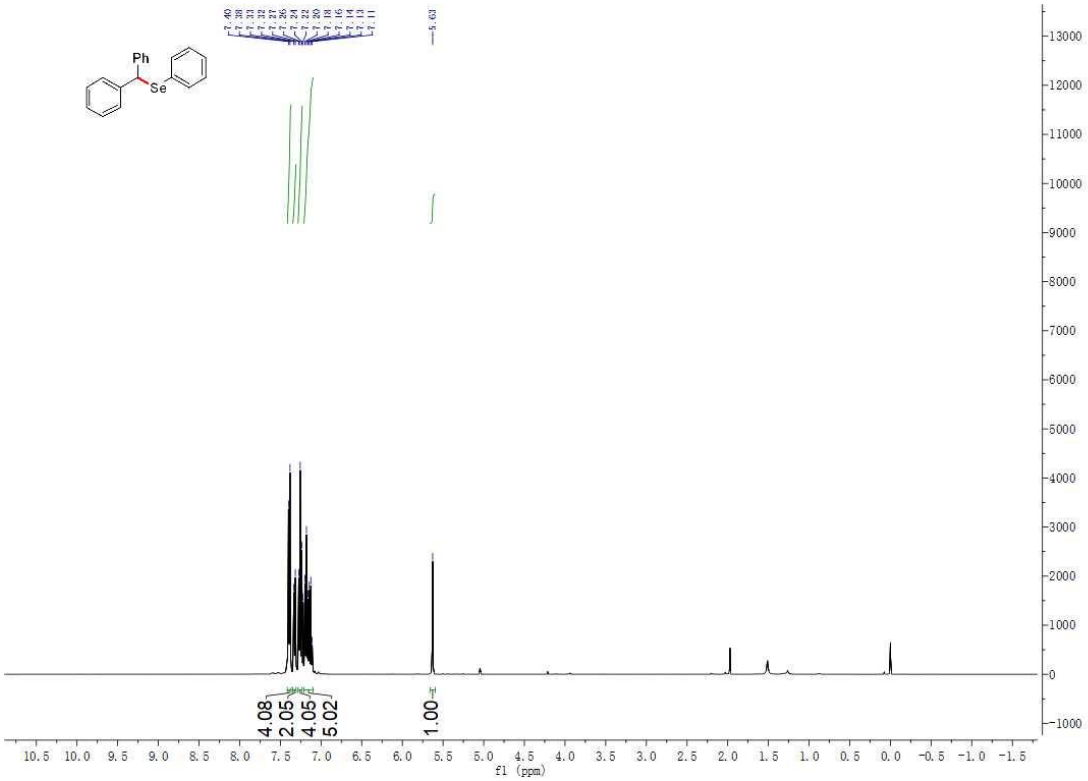
$^{1}$H NMR spectrum of **2-(benzo[d]thiazol-2-ylthio)-3-phenylpropanenitrile (45)**



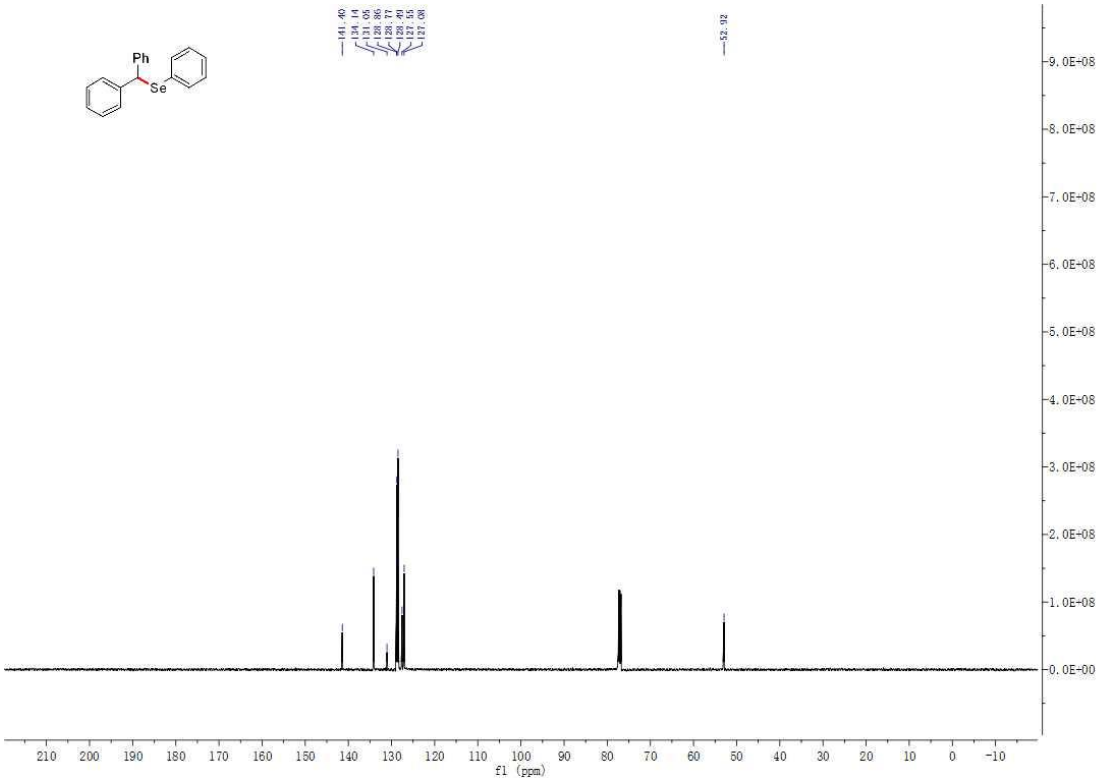
$^{13}$C NMR spectrum of **2-(benzo[d]thiazol-2-ylthio)-3-phenylpropanenitrile (45)**



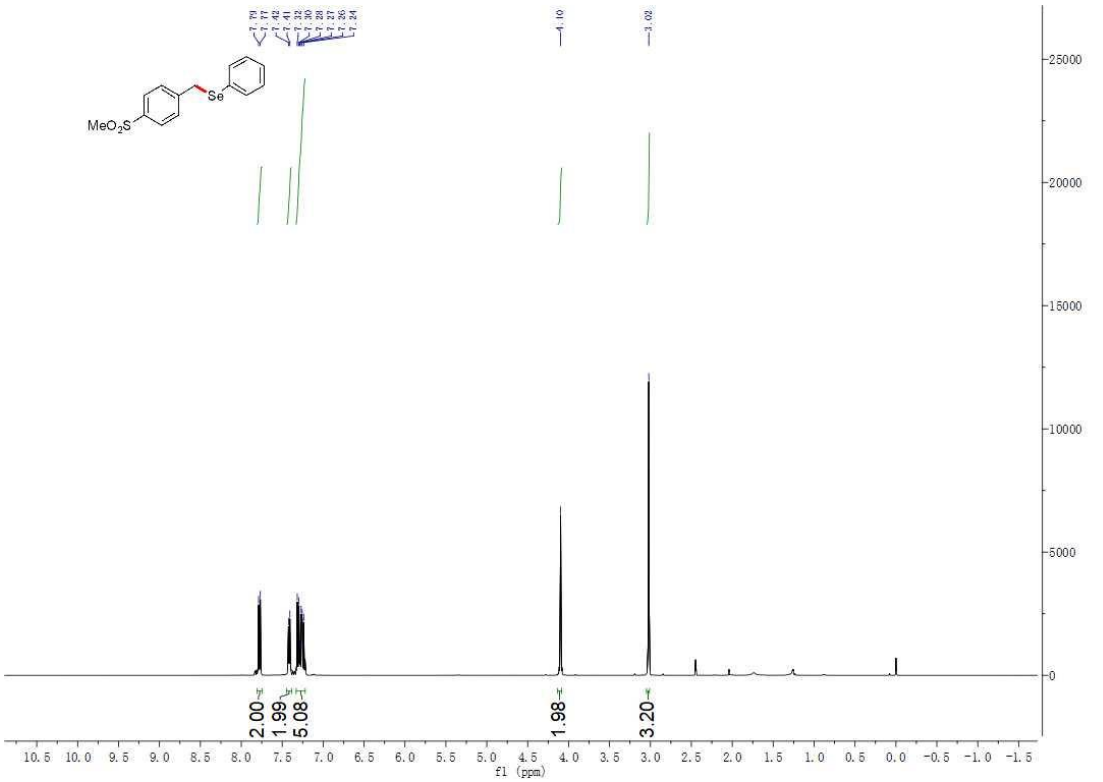

$^{1}$H NMR spectrum of **benzhydryl(phenyl)selane (46)**



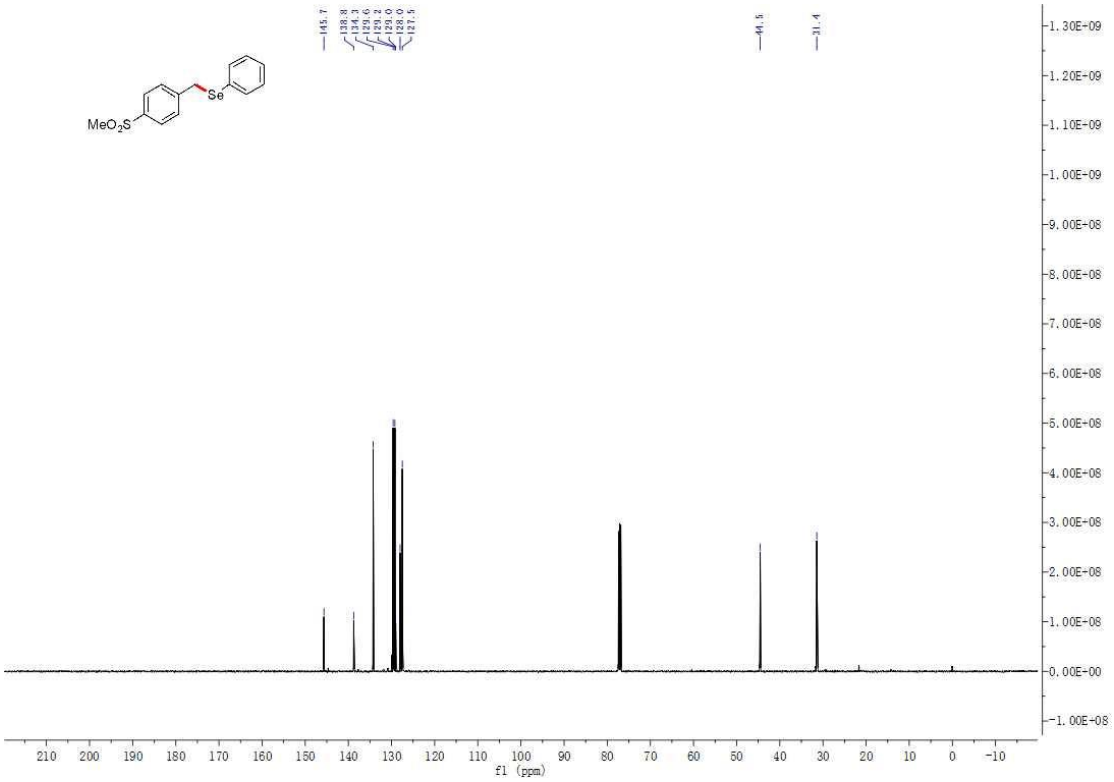
$^{13}$C NMR spectrum of **benzhydryl(phenyl)selane (46)**



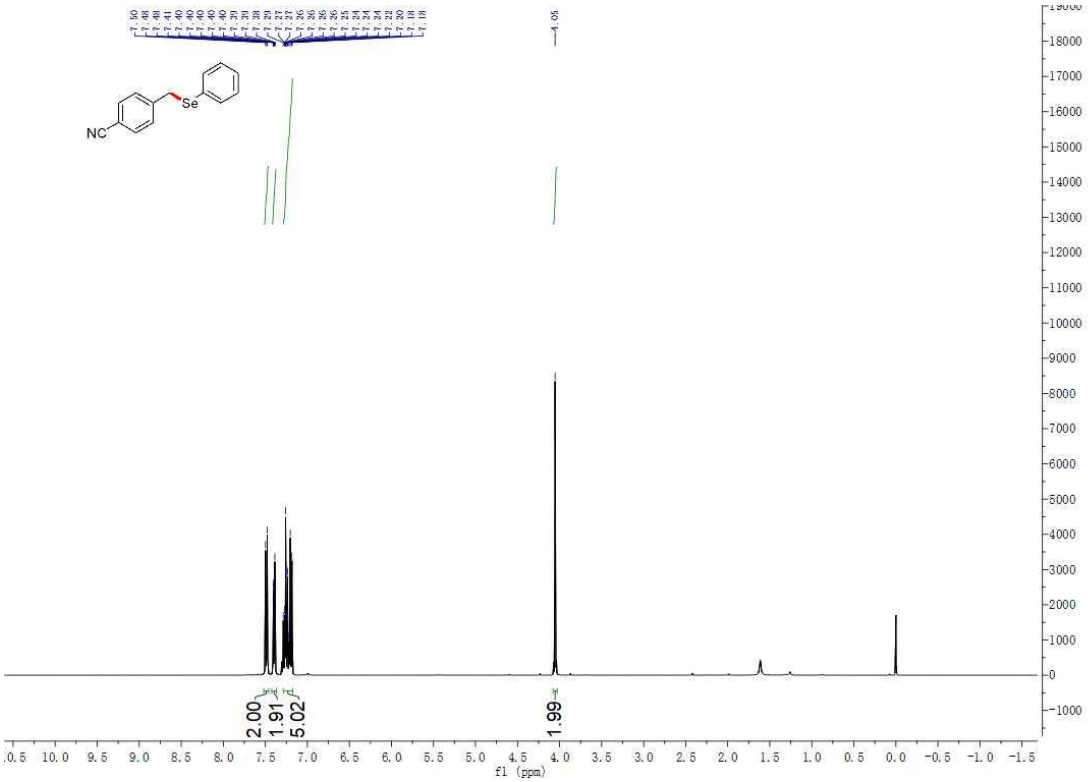

$^{1}$H NMR spectrum of **(4-(methylsulfonyl)benzyl)(phenyl)selane (47)**



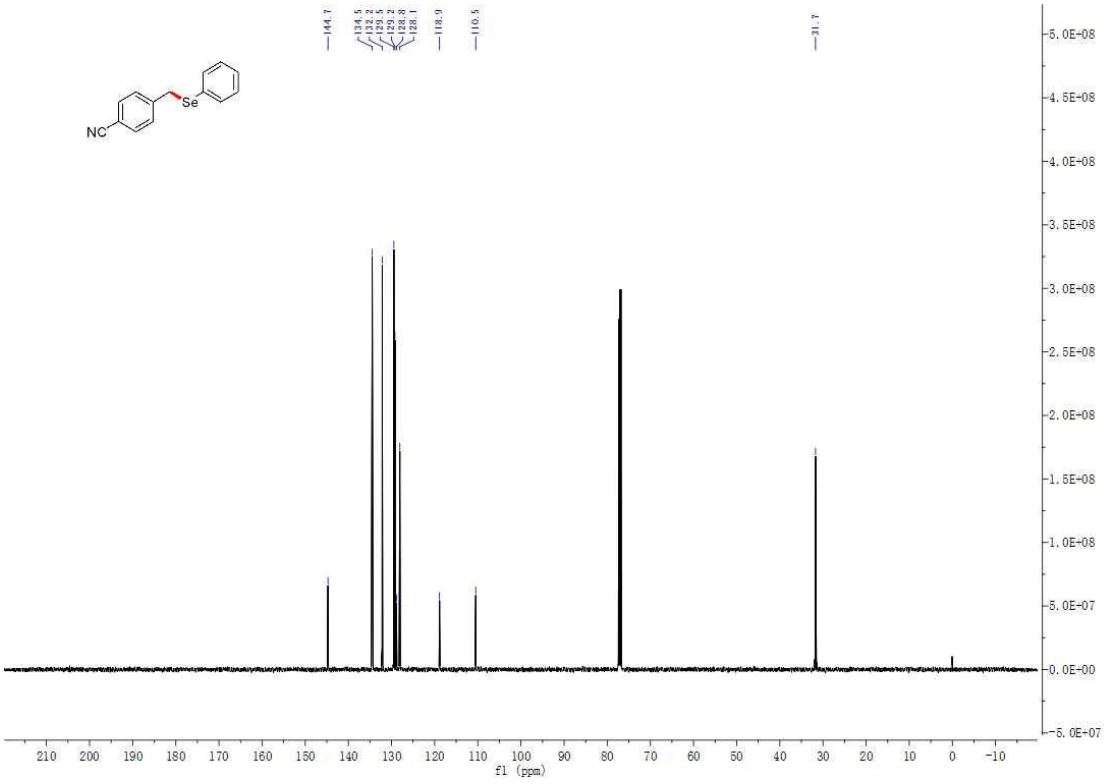
$^{13}$C NMR spectrum of **(4-(methylsulfonyl)benzyl)(phenyl)selane (47)**



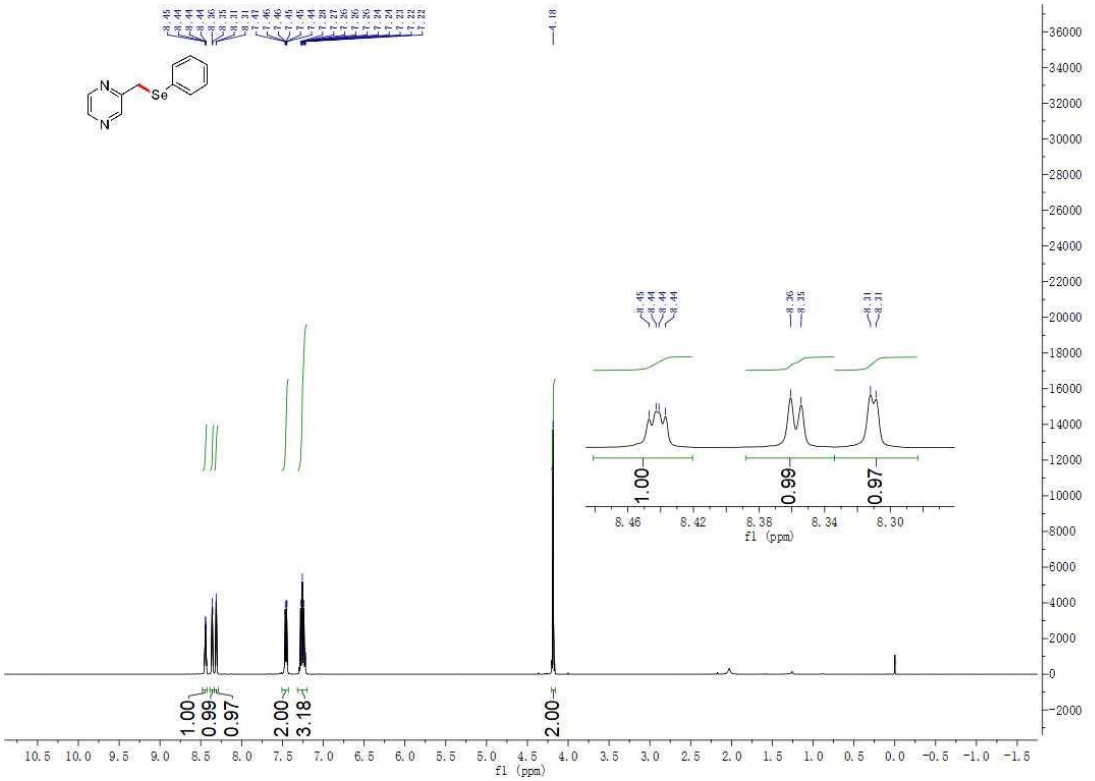

$^{1}$H NMR spectrum of **4-((phenylselanyl)methyl)benzonitrile (48)**



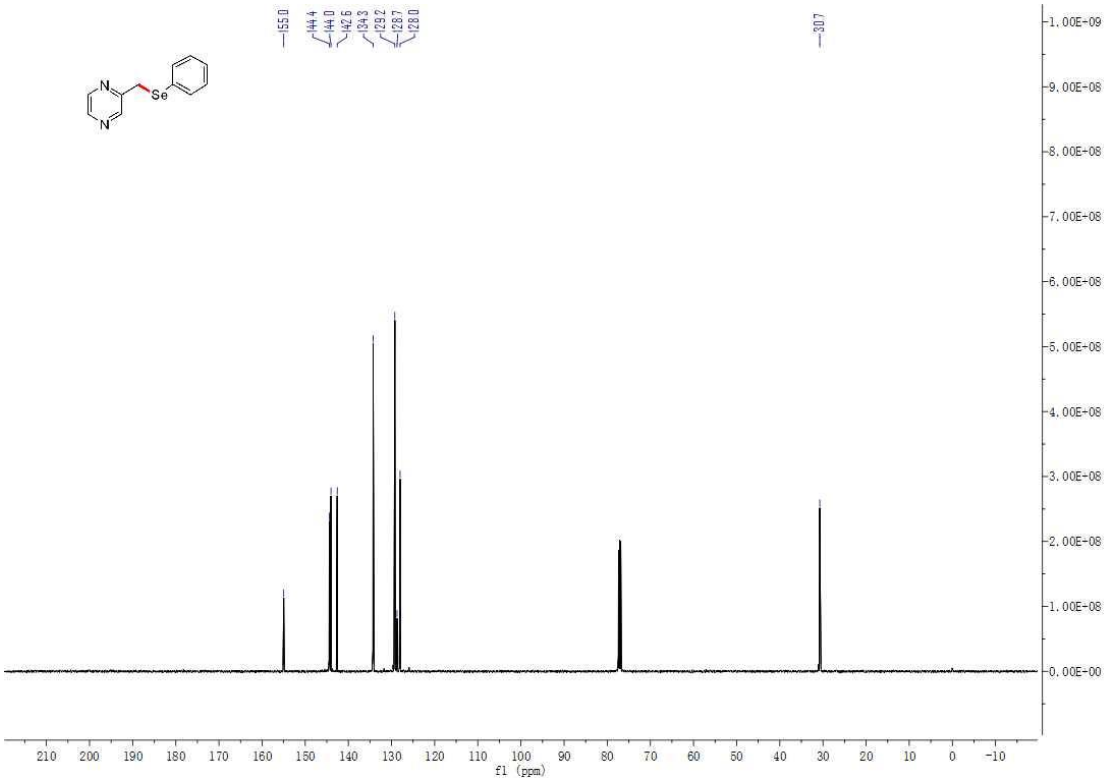
$^{13}$C NMR spectrum of **4-((phenylselanyl)methyl)benzonitrile (48)**



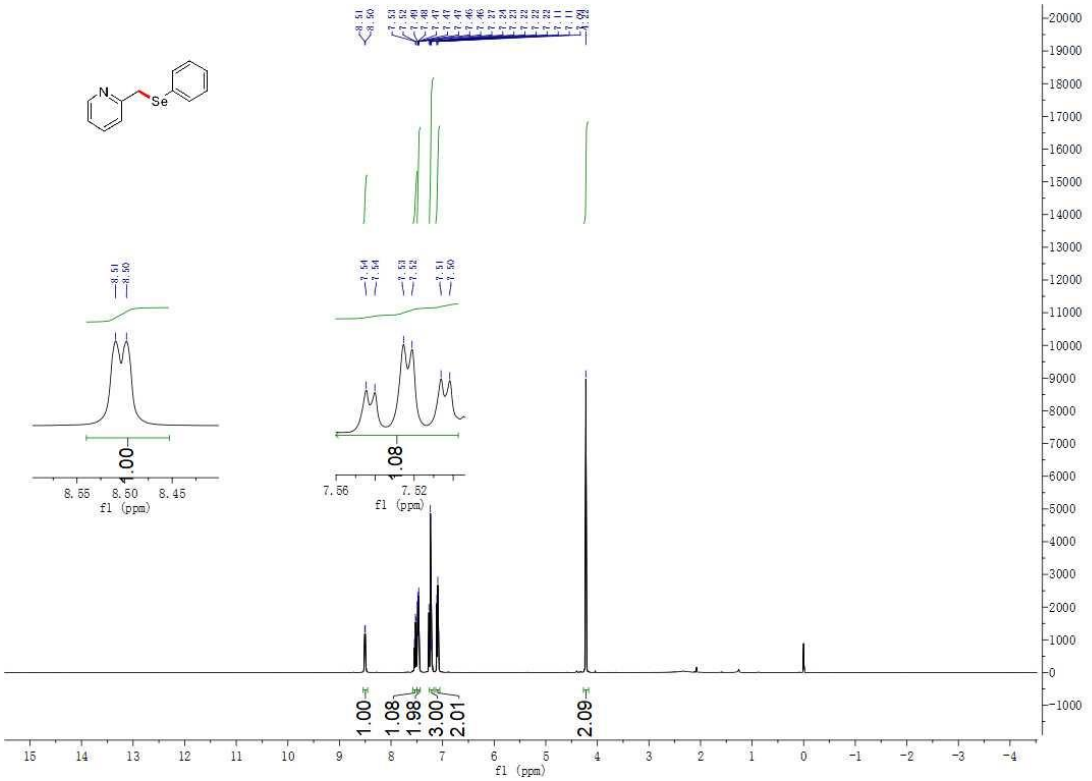

$^{1}$H NMR spectrum of **2-((phenylselanyl)methyl)pyrazine (49)**



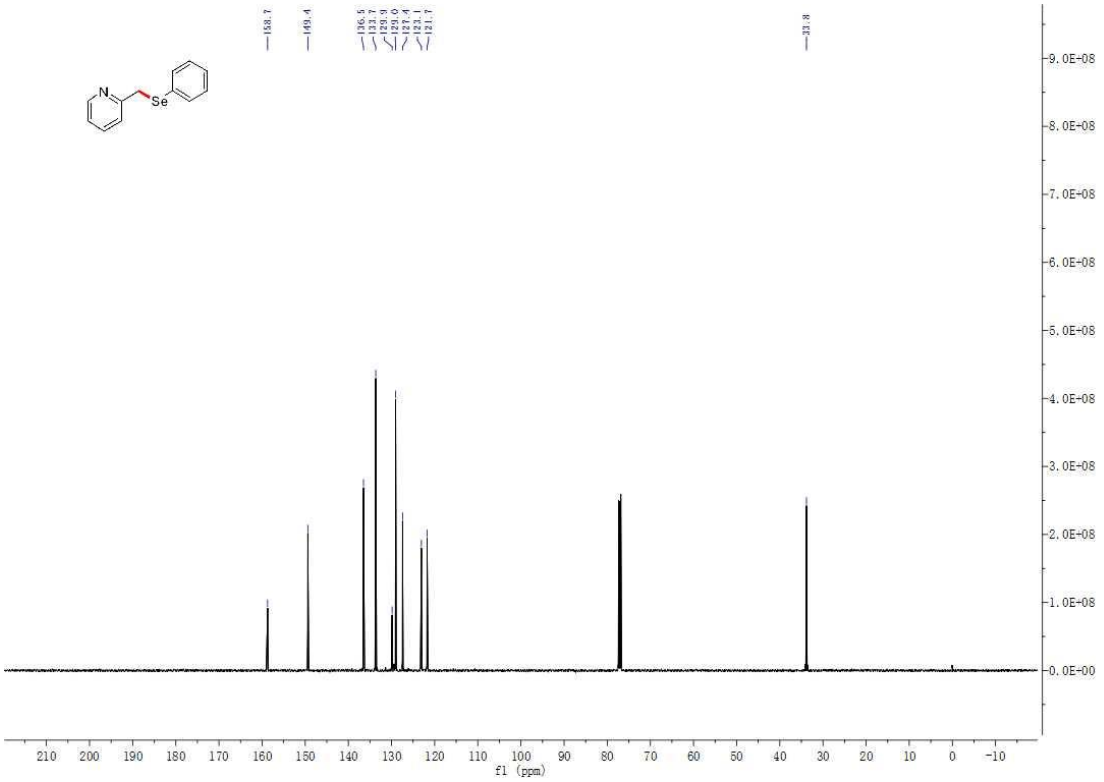
$^{13}$C NMR spectrum of **2-((phenylselanyl)methyl)pyrazine (49)**



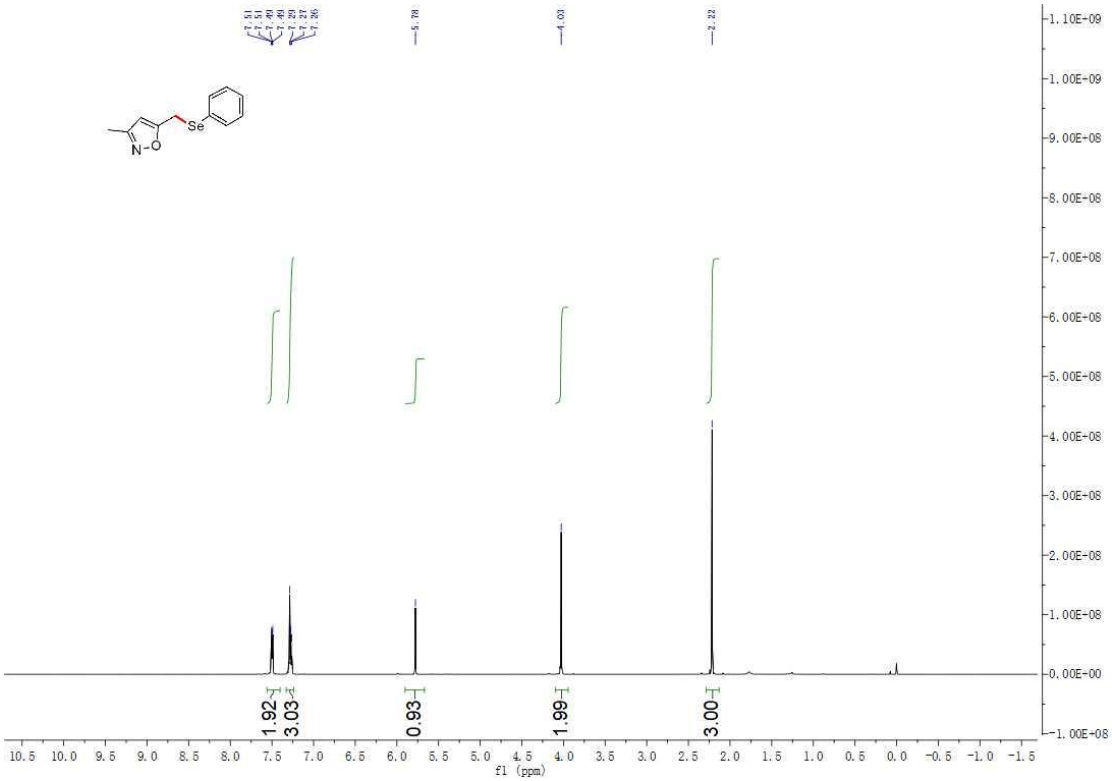

$^{1}$H NMR spectrum of **2-((phenylselanyl)methyl)pyridine (50)**



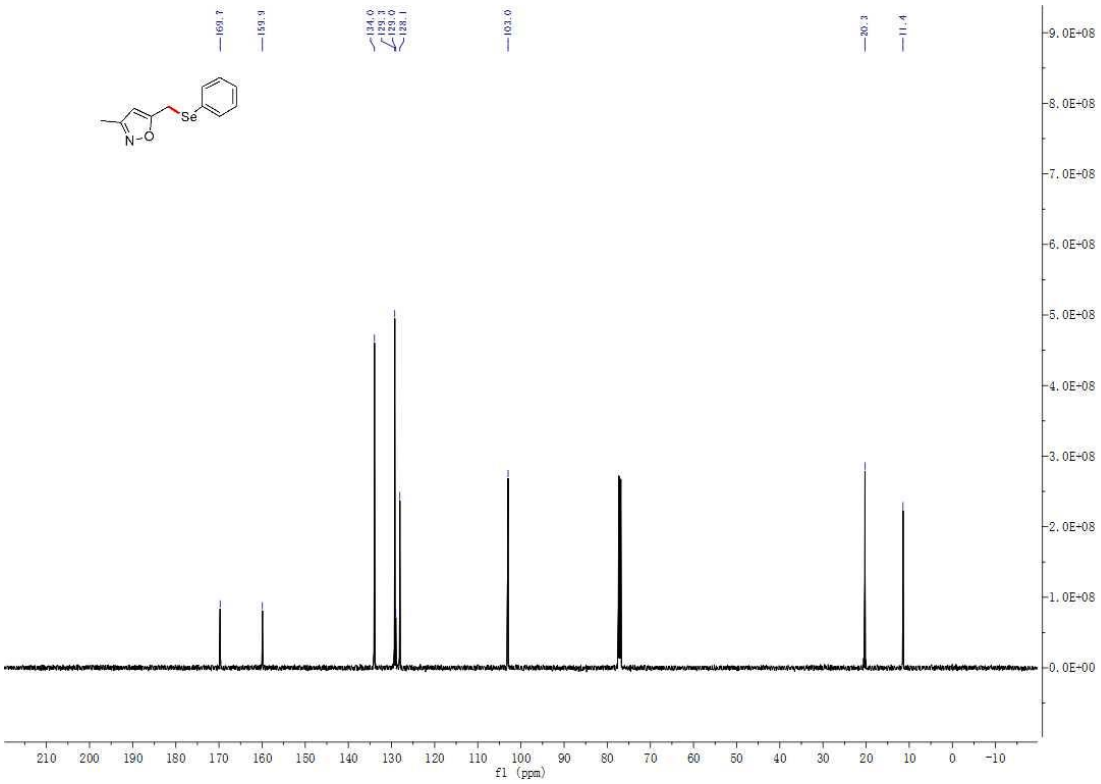
$^{13}$C NMR spectrum of **2-((phenylselanyl)methyl)pyridine (50)**



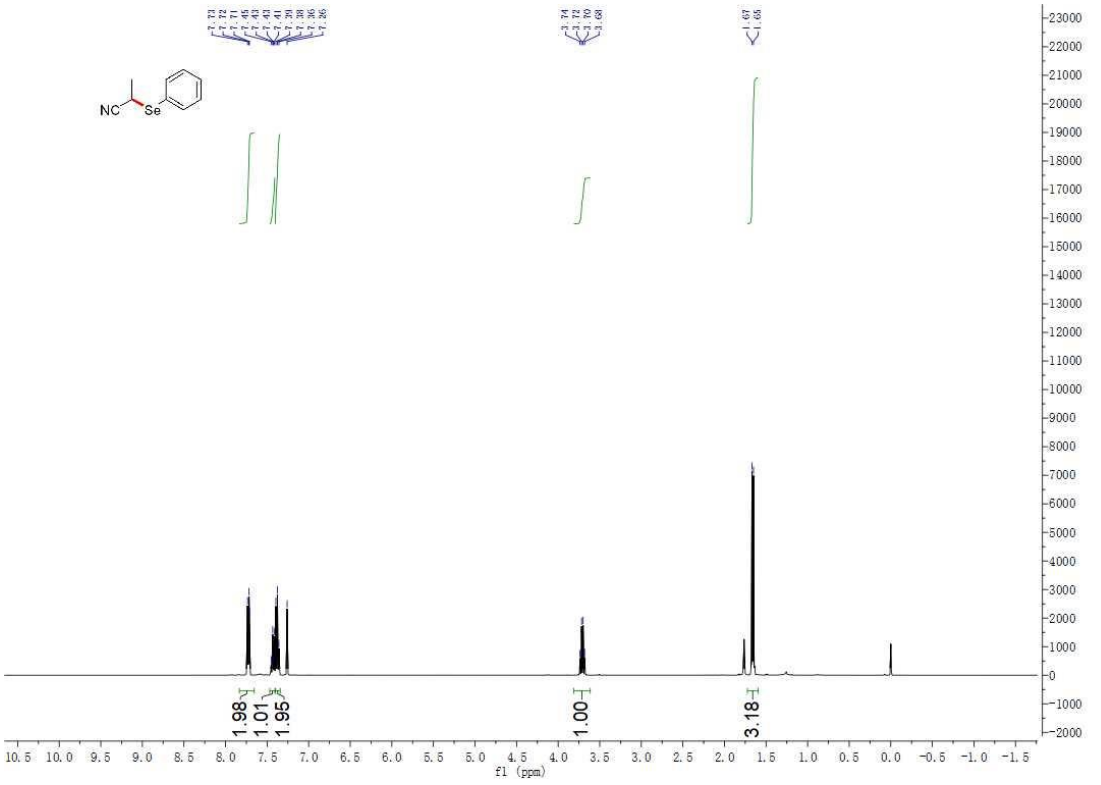

$^{1}$H NMR spectrum of **3-methyl-5-((phenylselanyl)methyl)isoxazole (51)**



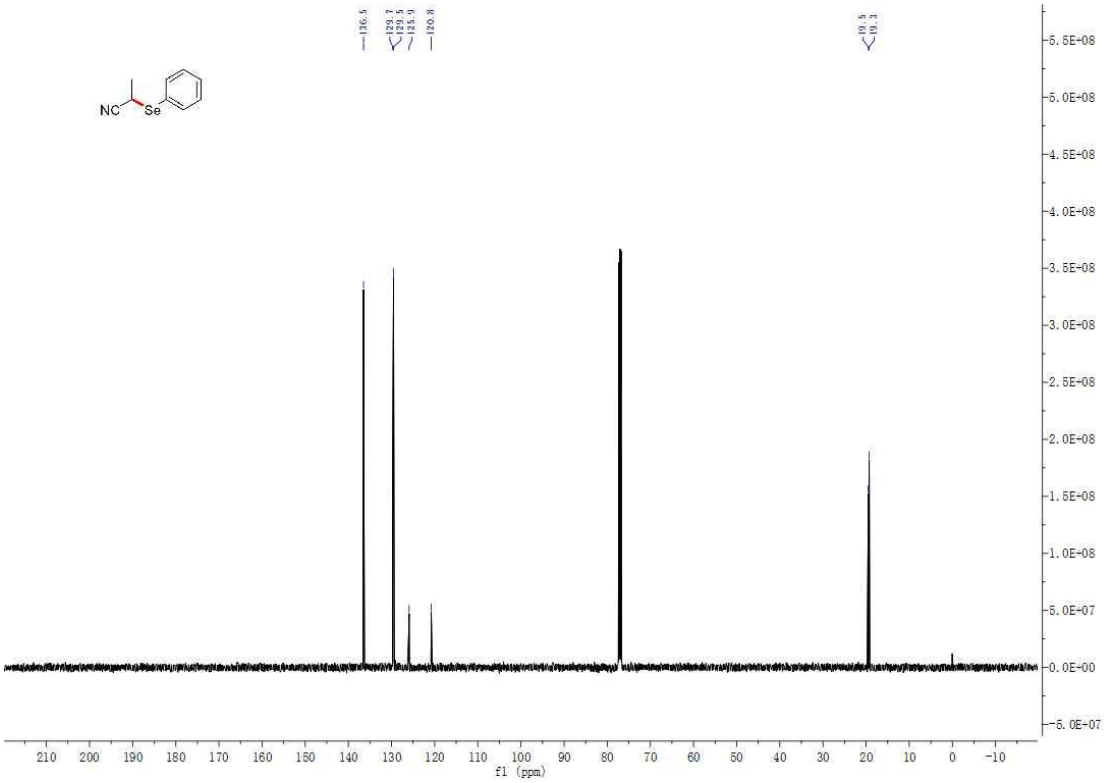
$^{13}$C NMR spectrum of **3-methyl-5-((phenylselanyl)methyl)isoxazole (51)**



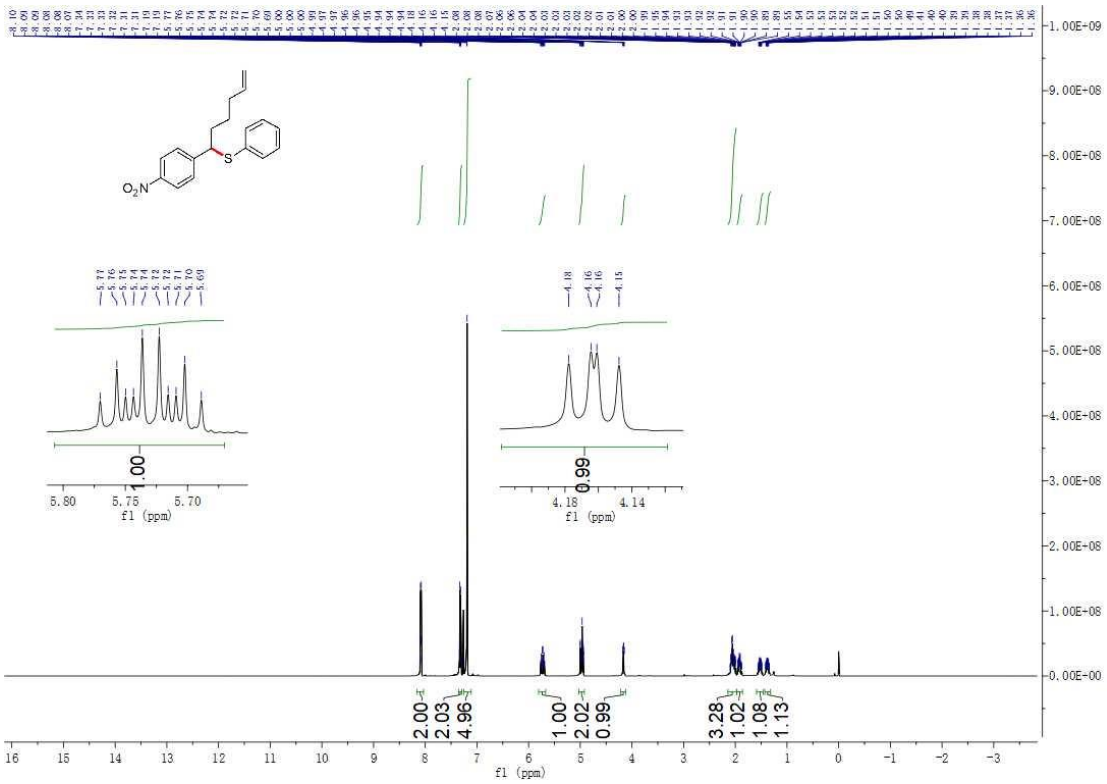

$^{1}$H NMR spectrum of **2-(phenylselanyl)propanenitrile (52)**



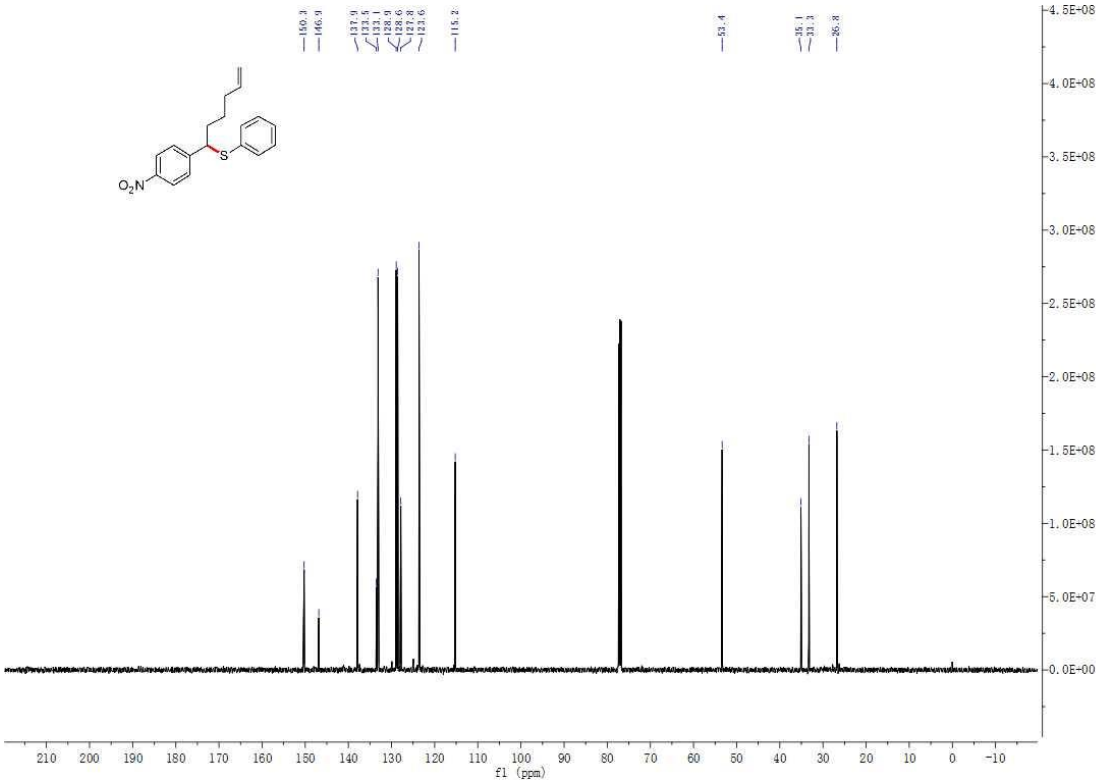
$^{13}$C NMR spectrum of **2-(phenylselanyl)propanenitrile (52)**



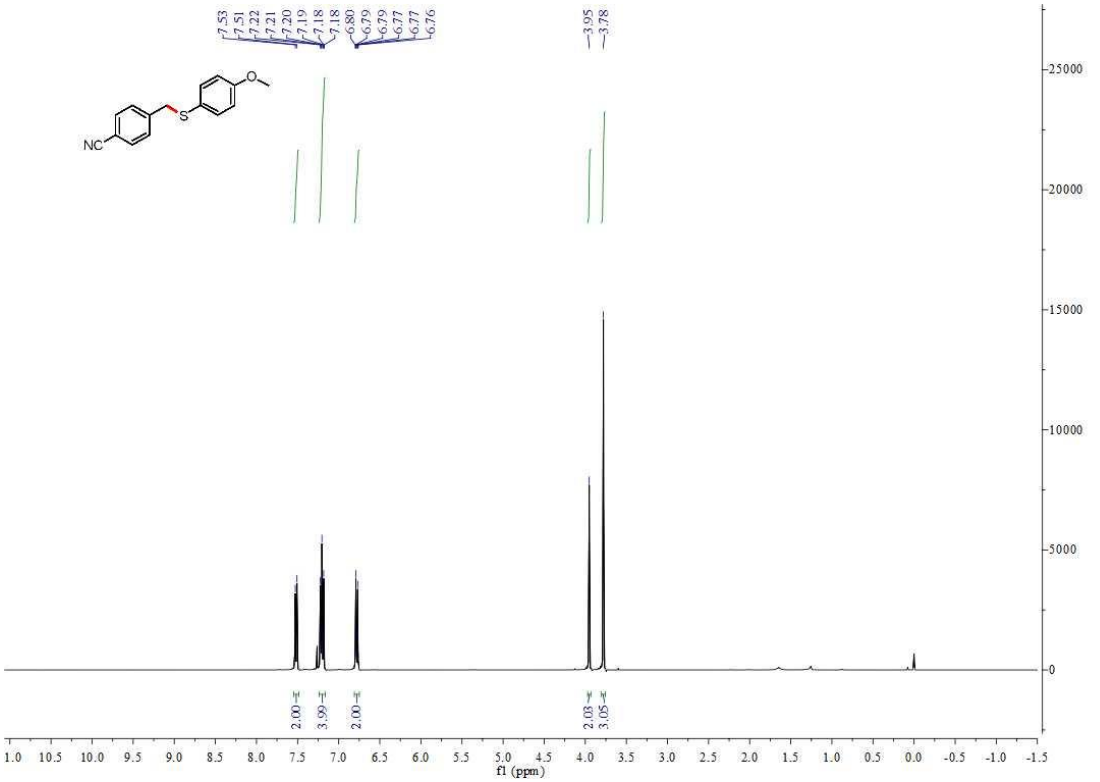

$^{1}$H NMR spectrum of **(1-(4-nitrophenyl)hex-5-en-1-yl)(phenyl)sulfane (53)**



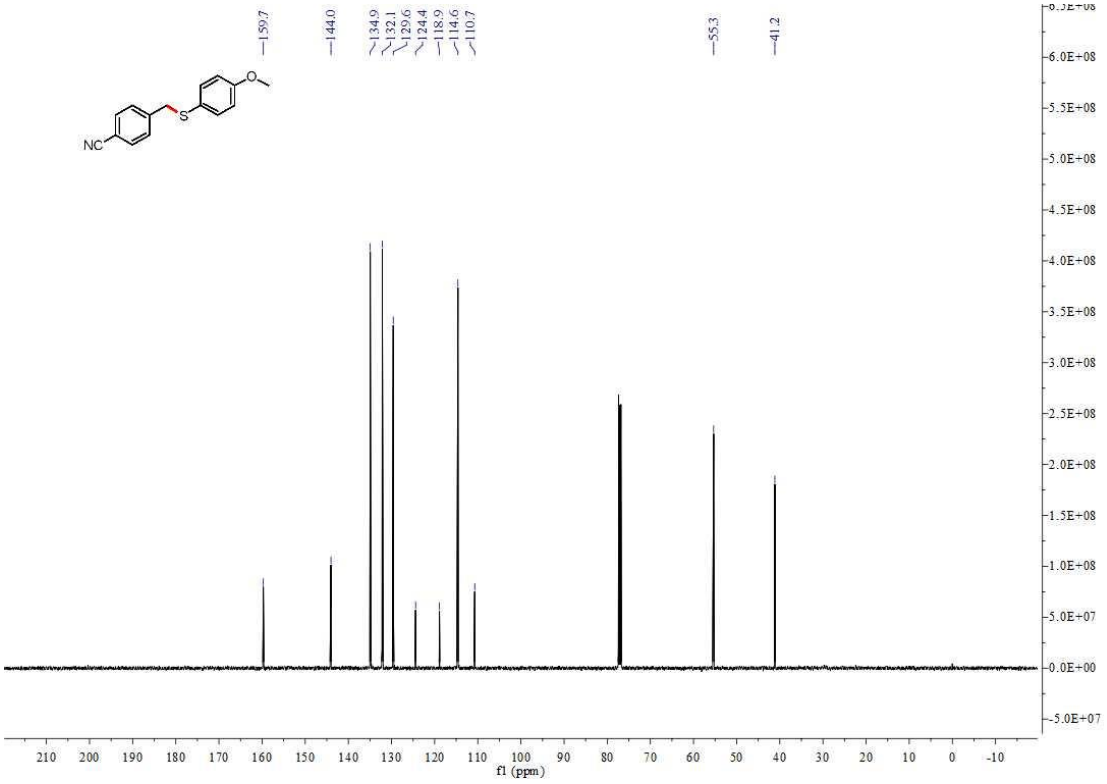
$^{13}$C NMR spectrum of **(1-(4-nitrophenyl)hex-5-en-1-yl)(phenyl)sulfane (53)**



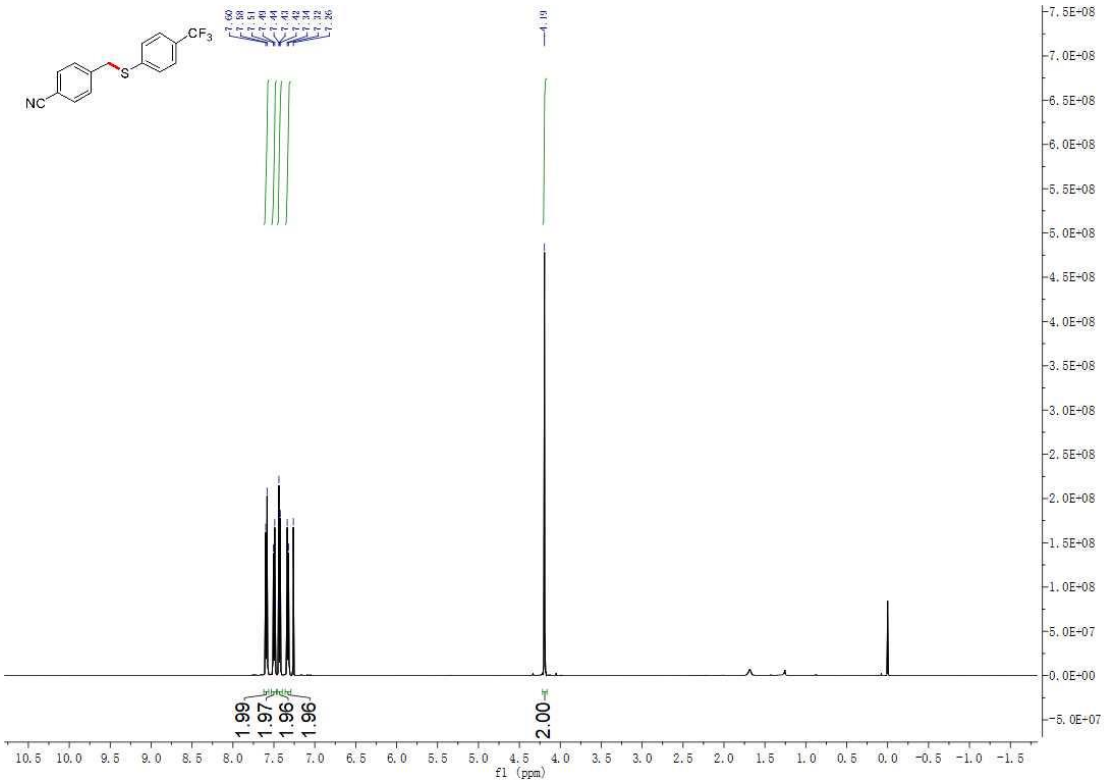

$^{1}$H NMR spectrum of **4-(((4-methoxyphenyl)thio)methyl)benzonitrile (54)**



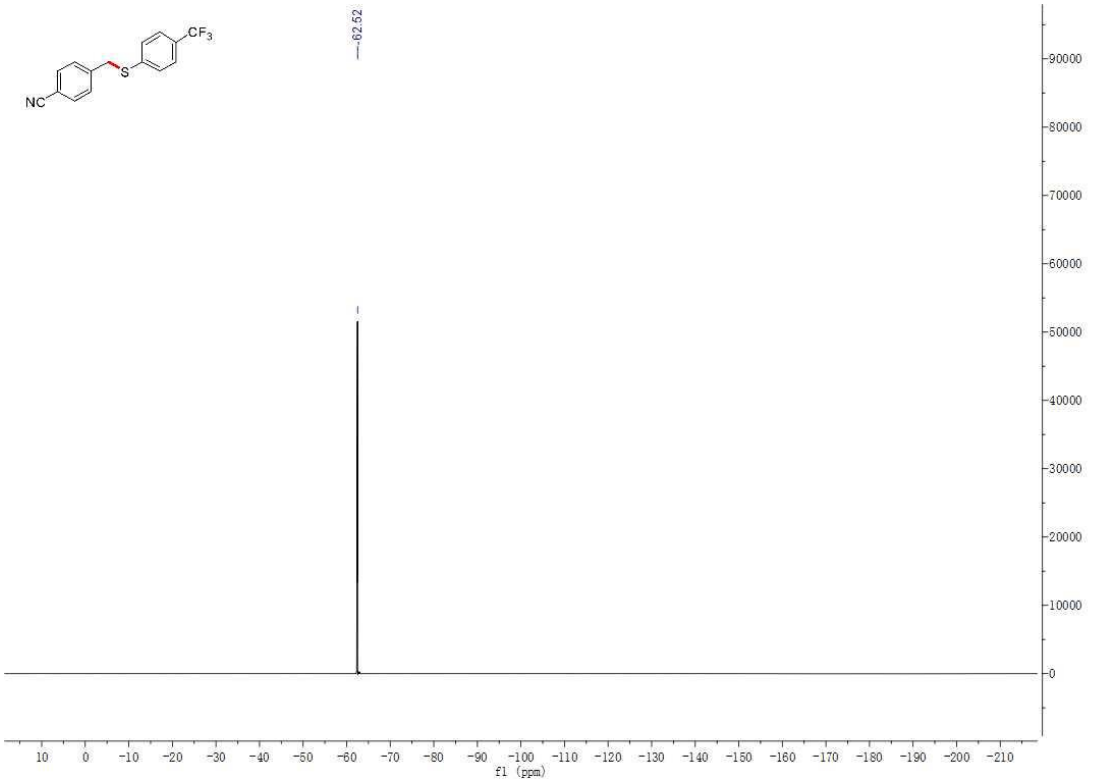
$^{13}$C NMR spectrum of **4-(((4-methoxyphenyl)thio)methyl)benzonitrile (54)**




$^{1}$H NMR spectrum of **4-(((4-(trifluoromethyl)phenyl)thio)methyl)benzonitrile (55)**



$^{19}$F NMR spectrum of **4-(((4-(trifluoromethyl)phenyl)thio)methyl)benzonitrile (55)**




$^{13}$C NMR spectrum of **4-(((4-(trifluoromethyl)phenyl)thio)methyl)benzonitrile (55)**