Supporting Information

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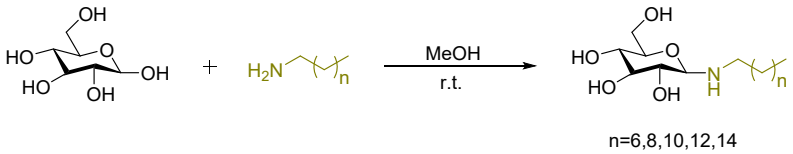
General Information

All solvents and reagents were purchased at the highest commercial quality grade and used without further purification, unless otherwise stated. All reactions were carried out under an atmosphere of nitrogen, unless otherwise stated. Reactions were monitored by GC, HPLC, and thin layer chromatography (TLC). Column chromatography was performed using E. Merck silica (60, particle size 0.040 – 0.045 mm). TLC analysis was performed using 0.25 mm E. Merck silica plates (60F-254), using 254 nm UV light as the visualizing agent. HPLC analysis was performed on a 1220 Infinity II, Agilent with silica column (Supersil ODS2 5μm, 4.6 mm × 250 mm). GC analysis was recorded on an Agilent 7890A. Melting points were determined using a digital melting point apparatus (Shanghai INESA Physico-Optical Instrument Co., Ltd. SGW ® X-4B) and were uncorrected. ^{1}H NMR spectra was recorded at ambient temperature on 400 MHz NMR spectrometers (Bruker AVANCE III) using deuterated chloroform ($CDCl_3$) or deuterated dimethyl sulfoxide (DMSO-d_6) as solvent and tetramethylsilane (TMS, $\delta = 0$) as internal reference. Chemical shifts are reported in parts per million (ppm) downfield and quoted to the nearest 0.01 ppm relative to the residual protons in in the NMR solvent ($CHCl_3$ = δ 7.26, DMSO-d_6 = δ 2.62), and coupling constants (J) are quoted in Hertz. Data are reported as follows: chemical shift, multiplicity, coupling constants, number of protons. Coupling constants were quoted to the nearest 0.1 Hz and multiplicity reported according to the following convention: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad singlet, and associated combinations for example: dd=doublet of doublet, dt=doublet of triplet, tt=triplet of triplet. ^{13}C NMR spectra were measured at ambient temperature on 101 MHz NMR spectrometers (Bruker AVANCE III). Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$ = δ 77.16, DMSO-d_6 = δ 39.52). IR spectra were measured on Nicolet IS50 FT-IR Spectrometers. GC-MS analysis was recorded on an Agilent 5977B MSD Series spectrometer. HRMS (high-resolution mass spectra) were recorded on a Shimadzu LCMS-IT-TOF mass spectrometer by electrospray ionization time of flight reflectron experiments. The surface tension (γ) was measured at 25 °C by the pendant method using an OCA 40 optical contact angle instrument (Dataphysics, Germany). The size and distribution of aggregates were measured by the ALV / DLS / SLS-5022F laser light scattering system under the condition of He-Ne laser (λ=632.8 nm) 90 °C, and the autocorrelation function is analyzed by CONTIN software.

Synthesis and Characterization of N-alkyl Glucosamine (AGA)

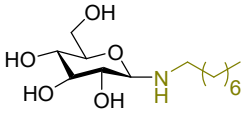
General Procedure



A mixture of glucose (0.1 mol) and N-alkylamine (0.1 mol) in CH_3OH (200 mL) were stirred for 24 hours at room temperature. Then the final mixture was suction filtered to remove solvent CH_3OH, washed the filter cake three times with cyclohexane, once with water, twice with ethanol, recrystallized twice with ethanol, and dried in vacuum to give solid powder.

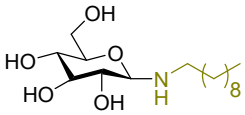
Characterization Data

N-Octyl glucosamine (AGA8)



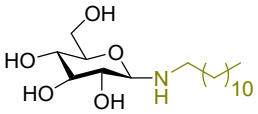
White solid powder (26.8g, 92%), **mp.** 106.5 – 109.6 °C. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 4.84 – 4.63 (m, 2H), 4.46 – 4.24 (m, 2H), 4.06 – 3.42 (m, 5H), 3.03 (d, J = 12.2 Hz, 2H), 2.91 – 2.77 (m, 1H), 2.80 – 2.67 (m, 1H), 1.34 (s, 2H), 1.21 (s, 10H), 0.82 (s, 3H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 91.32, 78.05 (d, J = 16.5 Hz), 74.04, 71.06, 61.92, 46.08, 31.82, 30.50, 29.52 (d, J = 8.7 Hz), 29.28, 27.39, 22.64, 14.48. **IR** (film) 3399.48, 2916.72, 2849.23, 1467.30, 1380.83, 1330.73, 1145.12, 1079.72, 1015.08, 992.36, 720.04 cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{14}H_{30}NO_5$ 292.2124, found 292.2122; $[M + Na]^+$ calcd. for $C_{14}H_{29}NNaO_5$ 314.1943, found 314.1925.

N-Decyl glucosamine (AGA10)



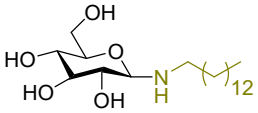
White solid powder (27.5g, 86%), **mp.** 109.9 – 110.4 °C. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 4.84 – 4.62 (m, 2H), 4.46 – 4.21 (m, 2H), 3.55 (dd, J = 37.6, 8.0 Hz, 5H), 3.03 (d, J = 43.0 Hz, 2H), 2.82 (t, J = 8.6 Hz, 1H), 2.75 (dd, J = 11.4, 7.0 Hz, 1H), 1.34 (s, 2H), 1.20 (s, 14H), 0.81 (t, J = 6.2 Hz, 3H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 91.31, 78.05 (d, J = 16.9 Hz), 74.04, 71.07, 61.92, 46.09, 31.83, 30.50, 29.59 (d, J = 6.3 Hz), 29.26, 27.39, 22.63, 14.48. **IR** (film) 3398.67, 2916.02, 2848.27, 1467.83, 1381.70, 1330.83, 1145.61, 1079.66, 1016.66, 992.84, 719.90 cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{16}H_{34}NO_5$ 320.2437, found 320.2423; $[M + Na]^+$ calcd. for $C_{16}H_{33}NNaO_5$ 342.2256, found 342.2220.

N-Dodecyl glucosamine (AGA12) [1]



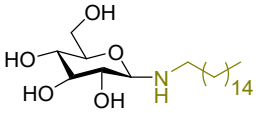
White solid powder (28.1g, 81%), **mp.** 111.7 – 112.5 ℃. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 4.84 – 4.63 (m, 2H), 4.45 – 4.22 (m, 2H), 3.66 – 3.37 (m, 5H), 3.10 – 2.95 (m, 2H), 2.82 (td, *J* = 8.6, 3.0 Hz, 1H), 2.73 (dd, *J* = 11.4, 7.2 Hz, 1H), 1.40 – 1.30 (m, 2H), 1.20 (s, 18H), 0.81 (t, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 91.32 , 78.05 (d, *J* = 16.6 Hz), 74.04, 71.07, 61.92, 46.09, 31.83, 30.51 , 29.59 (d, *J* = 6.9 Hz), 29.25, 27.38, 22.63, 14.48. **IR** (film) 3397.78, 2915.54, 2847.86, 1468.23, 1381.60, 1330.44, 1145.77, 1079.68, 1014.47, 992.25, 719.81 cm^{-1}. **HRMS** (ESI-TOF) m/z: [M + H]$^+$ calcd. for $C_{18}H_{38}NO_5$ 348.2750, found 348.2746; [M + Na]$^+$ calcd. for $C_{18}H_{37}NNaO_5$ 370.2569, found 370.2552.

N-Tetradecyl glucosamine (AGA14) [1]



White solid powder (29.3g, 78%), **mp.** 112.7 – 113.6 ℃. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 4.87 – 4.64 (m, 2H), 4.45 – 4.24 (m, 2H), 3.65 – 3.38 (m, 5H), 3.14 – 2.92 (m, 2H), 2.82 (td, *J* = 9.2, 8.6, 3.6 Hz, 1H), 2.74 (dt, *J* = 11.4, 7.2 Hz, 1H), 1.43 – 1.24 (m, 2H), 1.20 (s, 22H), 0.81 (t, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 91.31, 78.05 (d, *J* = 17.0 Hz), 74.04, 71.07, 61.92, 46.09, 31.83, 30.51, 29.57 (d, *J* = 4.5 Hz), 29.24, 27.39, 22.63, 14.48. **IR** (film) 3400.05, 2915.30, 2848.49, 1470.86, 1344.56, 1330.50, 1145.53, 1081.76, 1014.94, 992.56, 716.17 cm^{-1}. **HRMS** (ESI-TOF) m/z: [M + H]$^+$ calcd. for $C_{20}H_{42}NO_5$ 376.3063, found 376.3053; [M + Na]$^+$ calcd. for $C_{20}H_{41}NNaO_5$ 398.2882, found 398.2862.

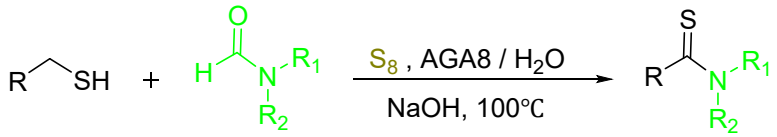
N-Hexadecyl glucosamine (AGA16) [1]



White solid powder (29.1g, 72%), **mp.** 116.1 – 116.5 ℃. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 4.90 – 4.62 (m, 2H), 4.49 – 4.21 (m, 2H), 3.73 – 3.42 (m, 5H), 3.14 – 2.91 (m, 2H), 2.86 – 2.77 (m, 1H), 2.73 (dd, *J* = 12.2, 6.8 Hz, 1H), 1.34 (s, 2H), 1.20 (s, 26H), 0.81 (t, *J* = 6.4 Hz, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 91.26, 78.06 (d, *J* = 20.6 Hz), 74.03, 71.06, 61.91, 46.07, 31.82, 30.46, 29.55 (d, *J* = 4.2 Hz), 29.23, 27.37, 22.62, 14.48. **IR (film)** 3400.25, 2915.97, 2847.72, 1468.77, 1376.68, 1329.83, 1146.26, 1080.18, 1017.75, 991.36, 720.45 cm^{-1}. **HRMS** (ESI-TOF) m/z: [M + H]$^+$ calcd. for $C_{22}H_{46}NO_5$ 404.3376, found 404.3376; [M + Na]$^+$ calcd. for $C_{22}H_{45}NNaO_5$ 426.3195, found 426.3165.

Synthesis of Thioamides from Mercaptans

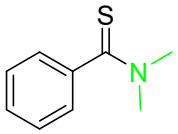
General Procedure A



To a Schlenk tube were added mercaptans (3.0 mmol), elemental sulfur (0.14 g, 4.5 mmol), NaOH (0.24 g, 6.0 mmol) and formamide (6.0 mmol) in 1.5 wt% AGA8 aqueous solution (6 mL). The mixture was stirred at 100℃ for 6 h, and monitored by TLC and HPLC. When the reaction was finished, the mixture was cooled to rt, quenched by H_2O (6 mL) and extracted with ethyl acetate (6 mL×3). Then the combined extract was washed with saturated aqueous NaCl (6 mL×3), dried over anhydrous sodium sulfate and concentrated under vacuum. Purification by column chromatography on silica gel affords product thioamide.

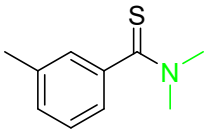
Characterization Data

N,N-Dimethylbenzothioamide（1a）[2]



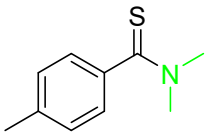
Following general **procedure A** on 3.0 mmol scale. The title compound (0.40 g, 81 %) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a yellow solid, **mp.** 66.8 – 68.7 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 – 7.19 (m, 5H), 3.54 (s, 3H), 3.10 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.14, 143.35, 128.57, 128.32, 125.71, 44.19, 43.25. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_9H_{12}NS$ 166.0685, found 166.0673.

N,N,3-Trimethylbenzothioamide（1b）[2]



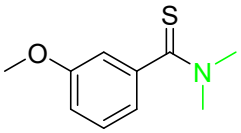
Following general **procedure A** on 3.0 mmol scale. The title compound (0.40 g, 72%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1: 20) as bright yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.26 (m, 1H), 7.17 (d, J = 5.8 Hz, 2H), 7.11 (d, J = 7.6 Hz, 1H), 3.64 (s, 3H), 3.21 (s, 3H), 2.39 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.53, 142.32, 137.16, 128.29, 127.17, 125.34, 121.58, 43.11, 42.15, 20.36. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_{10}H_{14}NS$ 180.0841, found 180.0825.

N,N,4-Trimethylbenzothioamide（1c）[2]



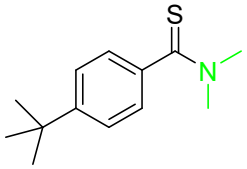
Following general **procedure A** on 3.0 mmol scale. The title compound (0.37 g, 68%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a bright yellow solid, **mp.** 50.5 – 51.3 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 – 6.97 (m, 4H), 3.51 (s, 3H), 3.10 (s, 3H), 2.27 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.50, 140.55, 138.69, 128.89, 125.88, 44.24, 43.36, 21.28. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_{10}H_{14}NS$ 180.0841, found 180.0828.

3-Methoxy-N,N-dimethylbenzothioamide（1d）[3]



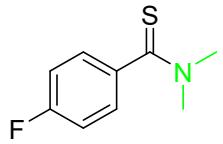
Following general **procedure A** on 3.0 mmol scale. The title compound (0.38 g, 65%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as bright yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.25 (t, J = 8.2 Hz, 1H), 6.95 – 6.72 (m, 3H), 3.80 (s, 3H), 3.59 (s, 3H), 3.16 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 200.93, 159.41, 144.56, 129.51, 117.83, 114.41, 111.29, 55.36, 44.11, 43.14. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_{10}H_{14}NOS$ 196.0791, found 196.0783.

4-*tert*-Butyl-N,N-dimethylbenzothioamide（1e）[4]



Following general **procedure A** on 3.0 mmol scale. The title compound (0.53 g, 73%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:10) as a brown yellow solid, **mp.** 101.5 – 102.8 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 – 7.32 (m, 2H), 7.28 – 7.20 (m, 2H), 3.58 (s, 3H), 3.17 (s, 3H), 1.29 (s, 9H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.67, 151.85, 140.55, 125.76, 125.29, 44.36, 43.39, 34.77, 31.31. **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ calcd. for $C_{13}H_{19}NNaS$ 244.1136, found 245.1125.

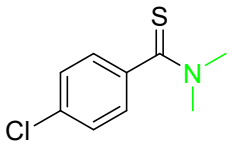
4-Fluoro-N,N-dimethylbenzothioamide（1f）[5]



Following general **procedure A** on 3.0 mmol scale. The title compound (0.34 g, 62%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a yellow solid, **mp.** 84.3 – 85.7 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.26 – 7.21 (m, 2H), 6.97 (t, J = 8.8 Hz, 2H),

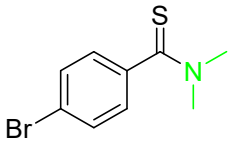
3.52 (s, 3H), 3.11 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 200.17, 163.89, 139.40 (d, *J* = 3.6 Hz), 127.98 (d, *J* = 8.5 Hz), 115.33 (d, *J* = 22.1 Hz), 44.25, 43.45. **^{19}F NMR** (376 MHz, $CDCl_3$): δ -112.24. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_9H_{11}FNS$ 184.0591, found 184.0589.

4-Chloro-N,N-dimethylbenzothioamide（1g）[2]



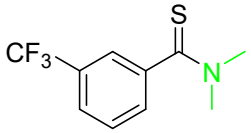
Following general **procedure A** on 3.0 mmol scale. The title compound (0.45 g, 75%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a yellow solid, **mp.** 78.4 – 79.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.6 Hz, 2H), 7.18 (d, *J* = 8.6 Hz, 2H), 3.52 (s, 3H), 3.10 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.90, 141.69, 134.64, 128.63, 127.35, 44.26, 43.39. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_9H_{11}ClNS$ 200.0295, found 200.0285.

4-Bromo-N,N-dimethylbenzothioamide（1h）[2]



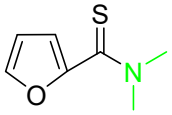
Following general **procedure A** on 3.0 mmol scale. The title compound (0.52 g, 72%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a yellow solid, **mp.** 117.6 – 118.5 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 – 7.44 (m, 2H), 7.18 – 7.14 (m, 2H), 3.55 (s, 3H), 3.14 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.81, 142.19, 131.62, 127.54, 122.80, 44.30, 43.37. **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_9H_{11}BrNS$ 243.9796, found 243.9778.

N,N-Dimethyl-3-(trifluoromethyl)benzothioamide（1i）[2]



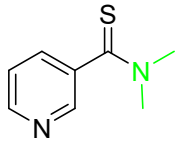
Following general **procedure A** on 3.0 mmol scale. The title compound (0.52 g, 75 %) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1: 20) as bright yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.53 – 7.41 (m, 4H), 3.54 (s, 3H), 3.10 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 198.12, 142.83, 129.48 (dd, *J* = 64.7, 32.4 Hz), 128.02 (d, *J* = 4.2 Hz), 127.90, 124.26 (q, *J* = 3.6 Hz), 123.25 (q, *J* = 3.9 Hz), 121.63 (q, *J* = 4.0 Hz), 43.14, 42.23. **^{19}F NMR** (376 MHz, $CDCl_3$): δ -62.75. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_{10}H_{11}F_3NS$ 234.0559, found 234.0540.

N,N-Dimethylfuran-2-carbothioamide（1j）[4]



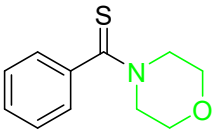
Following general **procedure A** on 3.0 mmol scale. The title compound (0.27 g, 57%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a black solid, **mp.** 35.8 – 37.2 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 – 7.45 (m, 1H), 7.09 (dd, *J* = 3.4, 0.8 Hz, 1H), 6.45 (dd, *J* = 3.6, 1.8 Hz, 1H), 3.55 (s, 3H), 3.43 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 185.76, 152.42, 143.21, 117.73, 111.92, 44.44, 44.22. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_7H_{10}NOS$ 156.0478, found 156.0473.

N,N-Dimethylpyridine-3-carbothioamide（1k）[4]



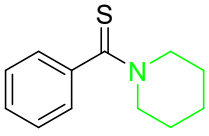
Following general **procedure A** on 3.0 mmol scale. The title compound (0.41 g, 83%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1: 3) as yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.63 – 8.50 (m, 2H), 7.70 – 7.67 (m, 1H), 7.31 (dd, *J* = 7.8, 4.8 Hz, 1H), 3.61 (s, 3H), 3.21 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 197.51, 149.51, 146.08, 139.18, 133.83, 123.22, 44.25, 43.38. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_8H_{11}N_2S$ 167.0637, found 167.0641.

Thiobenzmorpholid（1l）[2]



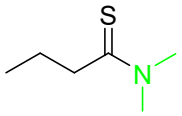
Following general **procedure A** on 3.0 mmol scale. The title compound (0.50 g, 80%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a bright yellow solid, **mp.** 142.0 – 143.1 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 – 7.25 (m, 3H), 7.23 – 7.19 (m, 2H), 4.43 – 4.33 (m, 2H), 3.86 – 3.79 (m, 2H), 3.60 – 3.51 (m, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.46, 128.89, 128.56, 125.87, 66.76, 66.54, 52.52, 49.55. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_{11}H_{14}NOS$ 208.0791, found 208.0784.

N-Thiobenzoylpiperidine（1m）[2]



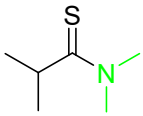
Following general **procedure A** on 3.0 mmol scale. The title compound (0.42 g, 68%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a brown yellow solid, **mp.** 65.5 – 66.5 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (q, *J* = 8.2, 7.8 Hz, 3H), 7.21 – 7.17 (m, 2H), 4.40 – 4.14 (m, 2H), 3.55 – 3.33 (m, 2H), 1.75 (q, *J* = 6.0 Hz, 2H), 1.70 – 1.64 (m, 2H), 1.49 (dd, *J* = 11.6, 5.6 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.60, 128.41, 128.36, 125.42, 53.18, 50.63, 26.90, 25.51, 24.18. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_{12}H_{16}NS$ 206.0998, found 206.0981.

N,N-Dimethylbutanethioamide（1n）[6]



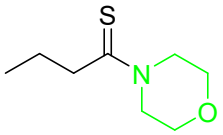
Following general **procedure A** on 3.0 mmol scale. The title compound (0.25 g, 63%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether =1: 20) as light yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.49 (s, 3H), 3.30 (s, 3H), 2.84 – 2.74 (m, 2H), 1.83 – 1.83 (m, 2H), 1.01 (t, J = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 204.34, 45.60, 44.56, 41.59, 22.50, 13.89. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_6H_{14}NS$ 132.0841, found 132.0856.

N,N,2-Trimethylpropanethioamide（1o）[7]



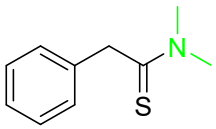
Following general **procedure A** on 3.0 mmol scale. The title compound (0.23 g, 58%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether =1: 20) as light yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.51 (s, 3H), 3.36 (s, 3H), 3.16 (p, J = 6.6 Hz, 1H), 1.23 (d, J = 6.5 Hz, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 211.10, 45.15, 41.25, 37.08, 23.20. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_6H_{14}NS$ 132.0841, found 132.0861.

4-Thiobutyryl-morpholine（1p）



Following general **procedure A** on 3.0 mmol scale. The title compound (0.34 g, 66%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether =1: 20) as brown black oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.37 – 4.31 (m, 2H), 3.79 – 3.76 (m, 2H), 3.74 (s, 4H), 2.87 – 2.80 (m, 2H), 1.74 (m, 2H), 1.01 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 203.81, 66.57, 66.53, 50.12, 49.92, 45.52, 22.67, 13.89. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_8H_{16}NOS$ 174.0947, found 174.0951.

N,N-Dimethyl-2-phenylethanethioamide（1q）[8]

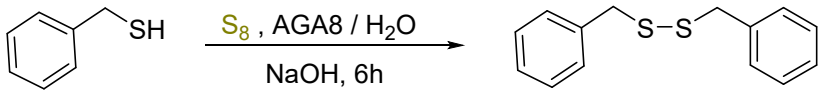


Following general **procedure A** on 3.0 mmol scale. The title compound (0.37 g, 70%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether =1: 10) as a light yellow solid, **mp.** 75.2 – 76.4 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36 – 7.22 (m, 5H), 4.32 (s, 2H), 3.50 (s, 3H), 3.20 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.62, 135.67, 128.81, 128.08, 126.96, 50.95, 44.84, 42.30. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_{10}H_{14}NS$ 180.0841, found 180.0828.

Synthesis of Disulfides from Mercaptans

Conditions Optimization

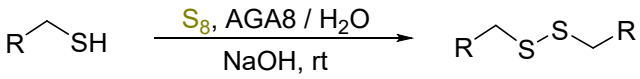
Table S1 Optimization of reaction conditions



Entry	S_8 (equiv.)	Temp (℃)	Yield [a]
1	1.5	100	95%
2	1.5	75	96%
3	1.5	50	95%
4	1.5	rt	94%
5	1.0	rt	96%
6	**0.5**	**rt**	**96%**
7	0.1	rt	45%
8	0	rt	11%

Typical conditions: Benzyl mercaptan (1.0 mmol), NaOH (2.0 mmol), 1.5wt% AGA8, H_2O (2 mL). [a] Determined by HPLC (Hypersil ODS C18, 35 ℃, λ=254 nm, MeOH, 1 mL/min) analysis: Benzyl mercaptan (3.3 min), dibenzyl disulfide (4.1 min).

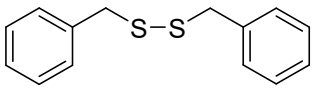
General Procedure B



To a Schlenk tube were added mercaptans (3.0 mmol), elemental sulfur (0.05 g, 1.5 mmol), and NaOH (0.24 g, 6.0 mmol) in 1.5 wt% AGA8 aqueous solution (6 mL). The mixture was stirred at room temperature for 6 h, and monitored by TLC and HPLC/ GC. When the reaction was finished, the mixture was quenched by H_2O (6 mL) and extracted with ethyl acetate (6 mL×3). Then the combined extract was washed with saturated aqueous NaCl (6 mL×3), dried over anhydrous sodium sulfate and concentrated under vacuum.

Characterization Data

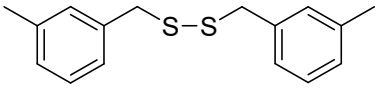
Dibenzyl disulfide (2a) [9]



Following general **procedure B** on 3.0 mmol scale. The title compound (0.35 g, 96%) was obtained through silica gel column chromatography (100% petroleum ether) as a white solid, **mp.** 68.9 – 70.3 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36 – 7.20 (m, 10H), 3.59 (s, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 137.37, 129.44, 128.50, 127.45, 43.28. **GC-MS** (EI) m/z: [M] calcd. for $C_{14}H_{14}S_2$ 246.05, found

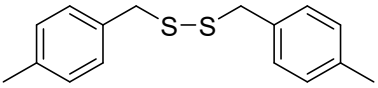
246.04.

Bis(3-methylbenzyl) disulfide (2b) [10]



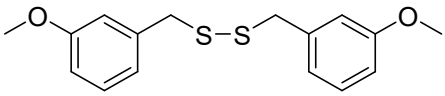
Following general **procedure B** on 3.0 mmol scale. The title compound (0.36 g, 88%) was obtained through silica gel column chromatography (100% petroleum ether) as yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 – 7.27 (m, 2H), 7.17 (dd, *J* = 13.2, 6.2 Hz, 6H), 3.68 (s, 4H), 2.44 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.25, 137.50, 130.41, 128.62, 128.41, 126.71, 43.53, 21.61. **GC-MS** (EI) m/z: [M] calcd. for $C_{16}H_{18}S_2$ 274.08, found 274.05.

Bis(4-methylbenzyl) disulfide (2c) [9]



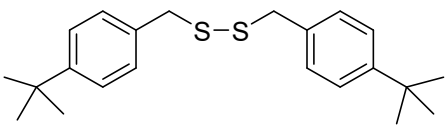
Following general **procedure B** on 3.0 mmol scale. The title compound (0.37 g, 91%) was obtained through silica gel column chromatography (100% petroleum ether) as a yellow solid, **mp.** 45.3 – 46.2 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.12 (s, 8H), 3.58 (s, 4H), 2.32 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 137.16, 134.34, 129.36, 129.22, 43.05, 21.25. **GC-MS** (EI) m/z: [M] calcd. for $C_{16}H_{18}S_2$ 274.08, found 274.04.

Bis(3-methoxybenzyl) disulfide (2d) [11]



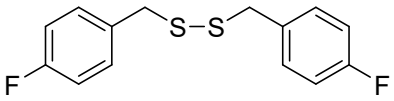
Following general **procedure B** on 3.0 mmol scale. The title compound (0.42 g, 91%) was obtained through silica gel column chromatography (100% petroleum ether) as a yellow solid, **mp.** 80.2 – 80.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 (t, J = 7.2 Hz, 2H), 6.91 – 6.77 (m, 6H), 3.81 (s, 6H), 3.61 (s, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.78, 139.01, 129.61, 121.85, 115.03, 113.16, 55.31, 43.44. **GC-MS** (EI) m/z: [M] calcd. for $C_{16}H_{18}O_2S_2$ 306.07, found 306.05.

Bis(4-*tert*-butylbenzyl) disulfide (2e) [9]



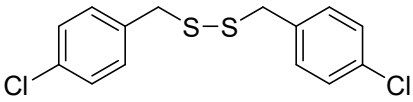
Following general **procedure B** on 3.0 mmol scale. The title compound (0.46 g, 86%) was obtained through silica gel column chromatography (100% petroleum ether) as a yellow solid, **mp.** 66.2 – 67.1 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.2 Hz, 4H), 7.18 (d, *J* = 8.2 Hz, 4H), 3.61 (s, 4H), 1.32 (s, 18H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 150.57, 134.31, 129.20, 125.50, 43.07, 34.64, 31.45. **GC-MS** (EI) m/z: [M] calcd. for $C_{22}H_{30}S_2$ 358.18, found 358.04.

Bis(4-fluorobenzyl) disulfide (2f) [9]



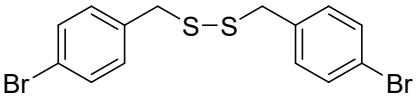
Following general **procedure B** on 3.0 mmol scale. The title compound (0.38 g, 90%) was obtained through silica gel column chromatography (100% petroleum ether) as a white solid, **mp.** 55.3 – 56.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.22 (dd, *J* = 8.6, 5.6 Hz, 4H), 7.06 – 7.00 (m, 4H), 3.61 (s, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.37 (d, *J* = 246.2 Hz), 133.32 (d, *J* = 3.3 Hz), 131.11 (d, *J* = 8.0 Hz), 115.54 (d, *J* = 21.5 Hz), 42.50; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -114.30. **GC-MS** (EI) m/z: [M] calcd. for $C_{14}H_{12}F_2S_2$ 282.03, found 282.00.

Bis(4-chlorobenzyl) disulfide (2g) [9]



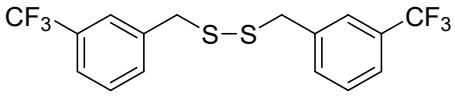
Following general **procedure B** on 3.0 mmol scale. The title compound (0.43 g, 91%) was obtained through silica gel column chromatography (100% petroleum ether) as a white solid, **mp.** 61.5 – 63.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 6.4 Hz, 4H), 7.18 (d, *J* = 8.0 Hz, 4H), 3.61 (s, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 135.80, 133.26, 130.64, 128.61, 42.36. **GC-MS** (EI) m/z: [M] calcd. for $C_{14}H_{12}Cl_2S_2$ 313.98, found 313.97.

Bis(4-bromobenzyl) disulfide (2h) [9]



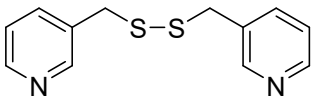
Following general **procedure B** on 3.0 mmol scale. The title compound (0.57 g, 94%) was obtained through silica gel column chromatography (100% petroleum ether) as a reddish solid, **mp.** 77.9 – 80.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.2 Hz, 4H), 7.09 (d, *J* = 8.4 Hz, 4H), 3.56 (s, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 136.36, 131.69, 131.08, 121.54, 42.56. **GC-MS** (EI) m/z: [M] calcd. for $C_{14}H_{12}Br_2S_2$ 403.87, found 403.79.

Bis(3-trifluoromethylbenzyl) disulfide (2i) [12]



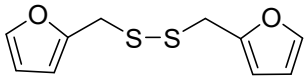
Following general **procedure B** on 3.0 mmol scale. The title compound (0.49 g, 85%) was obtained through silica gel column chromatography (100% petroleum ether) as yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.6 Hz, 2H), 7.50 – 7.38 (m, 6H), 3.61 (s, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.31, 132.69, 131.10, 130.78, 129.05, 126.07 (q, *J* = 3.8 Hz), 125.35, 124.34 (q, *J* = 3.8 Hz), 122.64, 119.93, 42.48; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.55. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_{16}H_{13}F_6S_2$ 383.0363, found 383.0336.

Bis(3-pyridylmethyl) disulfide (2j)



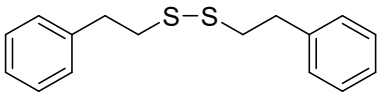
Following general **procedure B** on 3.0 mmol scale. The title compound (0.35 g, 95%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:2) as brown oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.48 (d, J = 3.2 Hz, 2H), 8.40 (d, J = 2.2 Hz, 2H), 7.52 (dt, J = 7.8, 1.8 Hz, 2H), 7.25 – 7.21 (m, 2H), 3.53 (s, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 150.30, 148.86, 136.84, 133.03, 123.60, 40.10. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_{12}H_{13}N_2S_2$ 249.0520, found 249.0482.

Difurfuryl disulfide (2k) [13]



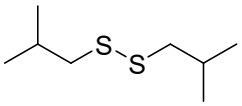
Following general **procedure B** on 3.0 mmol scale. The title compound (0.29 g, 87%) was obtained through silica gel column chromatography (100% petroleum ether) as light yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 (dd, J = 1.8, 1.0 Hz, 2H), 6.35 (dd, J = 3.2, 1.8 Hz, 2H), 6.24 (d, J = 3.2 Hz, 2H), 3.69 (s, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 150.21, 142.52, 110.85, 109.06, 35.65. **GC-MS** (EI) m/z: [M] calcd. for $C_{10}H_{10}O_2S_2$ 226.01, found 225.98.

Bis(2-phenylethyl) disulfide (2l) [14]



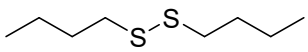
Following general **procedure B** on 3.0 mmol scale. The title compound (0.37 g, 90%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:100) as colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38 (t, J = 7.2 Hz, 4H), 7.34 – 7.22 (m, 6H), 3.15 – 3.05 (m, 4H), 3.05 – 2.95 (m, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 140.21, 128.81, 128.71, 126.61, 40.39, 35.92. **GC-MS** (EI) m/z: [M] calcd. for $C_{16}H_{18}S_2$ 274.08, found 274.06.

Diisobutyl disulfide (2m) [15]



Following general **procedure B** on 3.0 mmol scale. The title compound (0.21 g, 78%) was obtained through vacuum distillation as colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.56 (d, J = 6.8 Hz, 4H), 1.96 – 1.86 (m, 2H), 0.97 (d, J = 6.8 Hz, 12H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 48.60, 28.24, 21.84. **GC-MS** (EI) m/z: [M] calcd. for $C_8H_{18}S_2$ 178.08, found 178.11.

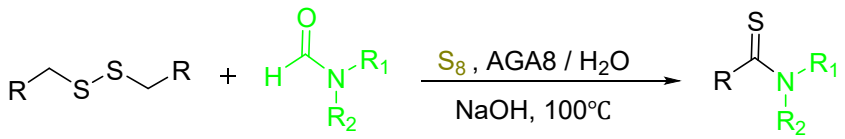
Butyl disulfide (2n) [9]



Following general **procedure B** on 3.0 mmol scale. The title compound (0.22 g, 82%) was obtained through vacuum distillation as colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.69 – 2.63 (m, 4H), 1.64 (dt, J = 15.2, 7.2 Hz, 4H), 1.39 (dq, J = 14.6, 7.2 Hz, 4H), 0.93 – 0.86 (m, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 38.92 (s, 1H), 31.38 (s, 1H), 21.73 (s, 0H), 13.76 (s, 0H). **GC-MS** (EI) m/z: [M] calcd. for $C_8H_{18}S_2$ 178.08, found 178.11.

Synthesis of Thioamides from Disulfides

General Procedure C



To a Schlenk tube were added the synthesized disulfides (1.0 mmol), elemental sulfur (0.05 g, 1.5 mmol), NaOH (0.08 g, 2.0 mmol) and formamide (2.0 mmol) in 1.5 wt% AGA8 aqueous solution (2 mL). The mixture was stirred at 100℃ for 6 h, and monitored by TLC and HPLC. When the reaction was finished, the mixture was cooled to rt, quenched by H_2O (2 mL) and extracted with ethyl acetate (2 mL×3). Then the combined extract was washed with saturated aqueous NaCl (2 mL×3), dried over anhydrous sodium sulfate and concentrated under vacuum. Purification by column chromatography on silica gel affords product thioamide.

Characterization Data

N,N-Dimethylbenzothioamide（1a）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.30 g, 90 %) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a yellow solid.

N,N,3-Trimethylbenzothioamide（1b）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.28 g, 78%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1: 20) as bright yellow oil.

N,N,4-Trimethylbenzothioamide（1c）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.30 g, 78%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a bright yellow solid.

3-Methoxy-N,N-dimethylbenzothioamide（1d）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.31 g, 80%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as bright yellow oil.

4-*tert*-Butyl-N,N-dimethylbenzothioamide（1e）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.34 g, 76%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:10) as a brown yellow solid.

4-Fluoro-N,N-dimethylbenzothioamide（1f）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.25 g, 68%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a yellow solid.

4-Chloro-N,N-dimethylbenzothioamide（1g）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.32 g, 81%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a yellow solid.

4-Bromo-N,N-dimethylbenzothioamide（1h）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.40 g, 83%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a yellow solid.

N,N-Dimethyl-3-(trifluoromethyl)benzothioamide（1i）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.38 g, 81 %) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1: 20) as bright yellow oil.

N,N-Dimethylfuran-2-carbothioamide（1j）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.20 g, 65%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a black solid.

N,N-Dimethylpyridine-3-carbothioamide（1k）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.31 g, 92%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1: 3) as yellow oil.

Thiobenzmorpholid（1l）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.37 g, 89%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a bright yellow solid.

N-Thiobenzoylpiperidine（1m）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.33 g, 81%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether = 1:15) as a brown yellow solid.

N,N-Dimethylbutanethioamide（1n）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.18 g, 69%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether =1: 20) as light yellow oil.

N,N,2-Trimethylpropanethioamide（1o）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.17 g, 64%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether =1: 20) as light yellow oil.

4-Thiobutyryl-morpholine（1p）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.24 g, 69%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether =1: 20) as brown black oil.

N,N-Dimethyl-2-phenylethanethioamide（1q）

Following general **procedure C** on 1.0 mmol scale. The title compound (0.28 g, 78%) was obtained through silica gel column chromatography (ethyl acetate: petroleum ether =1: 10) as a light yellow solid.

Optimized Coordinates of Key Structures

R0 (frequency: 1 (24.99); single-point energy: -669.384391 Hartree)

0 1

C	0.65411800	1.20723100	0.26136000
C	-0.02465800	0.00016800	0.48365600
C	0.65389000	-1.20707900	0.26163700
C	1.98544700	-1.20875000	-0.15855400
C	2.65543100	-0.00018100	-0.36922300
C	1.98568600	1.20855700	-0.15882300
H	0.12977700	2.15361700	0.41828200
H	0.12935900	-2.15332200	0.41879200
H	2.50240800	-2.15738200	-0.32253700
H	3.69776200	-0.00033700	-0.69691100
H	2.50280800	2.15706800	-0.32299500
C	-1.47011400	0.00033300	0.90219400
H	-1.70130100	0.89392500	1.49940900
H	-1.70130500	-0.89285700	1.49999800
S	-2.52977400	-0.00014100	-0.61597200
H	-3.72191900	-0.00012600	0.02803300

IM1 (frequency: 1 (-60.67); single-point energy: -1337.569866 Hartree)

0 1

C	-4.11473200	1.20778400	-0.27803100
C	-3.44586000	-0.00056000	-0.52303600
C	-4.11489800	-1.20846400	-0.27634100
C	-5.43130500	-1.20912500	0.18878600
C	-6.09298200	0.00028500	0.42079900

C	-5.43113400	1.20928000	0.18709500
H	-3.59425500	2.15284600	-0.45366200
H	-3.59455900	-2.15384600	-0.45065600
H	-5.94287900	-2.15721000	0.37139400
H	-7.12357300	0.00061000	0.78371600
H	-5.94257600	2.15769100	0.36837300
C	-2.01445600	-0.00098200	-0.98588900
H	-1.78408400	0.89337400	-1.58355200
H	-1.78404700	-0.89644200	-1.58187500
C	2.01449300	0.00110400	0.98599100
H	1.78438500	0.89645200	1.58226000
H	1.78381400	-0.89336700	1.58336200
C	3.44589100	0.00040100	0.52312100
C	4.11546800	1.20819000	0.27733500
C	4.11417900	-1.20805900	0.27707700
C	5.43182800	1.20861500	-0.18792800
H	3.59559300	2.15367400	0.45248000
C	5.43053300	-1.20979100	-0.18817900
H	3.59327800	-2.15301900	0.45199700
C	6.09291700	-0.00091400	-0.42098400
H	5.94382200	2.15660900	-0.36982700
H	5.94151600	-2.15829300	-0.37027400
H	7.12346900	-0.00142700	-0.78401300
S	-0.94195400	0.00050400	0.51073300
S	0.94198300	0.00048200	-0.51064700

IM2 (frequency: 1 (14.80); single-point energy: -1413.356281 Hartree)

-1 1

C	-1.57483900	-1.35504700	0.44252100
H	-1.96725100	-2.38279300	0.49048900
H	-1.05669500	-1.01507000	1.37412200
C	-2.64450400	-0.35037600	0.11437100
C	-3.70102100	-0.63419100	-0.76476700
C	-2.55861400	0.92788300	0.69970000
C	-4.66708500	0.33457800	-1.05533100
H	-3.76364900	-1.62533000	-1.22538400
C	-3.52804800	1.88973700	0.40769700
H	-1.71106300	1.07743400	1.39859600
C	-4.58161000	1.60157400	-0.46957400
H	-5.48749600	0.10118000	-1.74119500
H	-3.46389700	2.88047600	0.86947000

H	-5.33537900	2.36219700	-0.69668100
S	-0.29730100	-1.28858700	-0.90189100
O	-0.12967200	0.29378800	2.30833500
H	-0.22981900	0.41316200	3.26513200
C	2.08964400	-1.17961400	1.05976800
H	2.86673300	-1.80169000	1.53874800
C	2.67439400	0.01923300	0.36890900
C	3.79325900	-0.06736700	-0.47425000
C	2.05395300	1.26559100	0.56742000
C	4.29971800	1.07056300	-1.10549100
H	4.25979400	-1.04266500	-0.64656200
C	2.56485500	2.40124100	-0.07020000
H	1.18306600	1.27337900	1.25272800
C	3.68340400	2.31189000	-0.90508900
H	5.17390800	0.99105300	-1.75953500
H	2.07908300	3.37022800	0.08377800
H	4.07539800	3.20469100	-1.40274100
S	1.27683200	-2.38252400	-0.09530000
H	1.32110100	-0.83294100	1.79330200

TS2/3 (Number of imaginary frequency: 1 (-106.59); single-point energy: -1413.345144 Hartree)

-1 1

C	0.96975600	-1.70677100	0.36781400
H	1.41312500	-2.68898800	0.60321900
H	0.59472600	-1.76499900	-0.78082200
C	2.02217100	-0.64207500	0.33217400
C	2.13404600	0.42733800	1.23659700
C	2.93243600	-0.68774400	-0.74698700
C	3.12790100	1.40047700	1.08680900
H	1.41782200	0.50691600	2.05711600
C	3.92955200	0.27617900	-0.88986300
H	2.78594100	-1.46884100	-1.49771700
C	4.03854100	1.32794900	0.02936200
H	3.18849500	2.22356900	1.80579700
H	4.61785900	0.22139200	-1.73942200
H	4.81654100	2.08838000	-0.08636200
S	-0.40642700	-1.36196600	1.50896800
O	0.30708900	-1.74801800	-2.25537800
H	0.67727800	-0.94459200	-2.64866400
C	-2.27080300	-0.98238200	-0.98278200
H	-3.27975200	-1.22869200	-1.35462800
C	-2.12816200	0.46965900	-0.65320100

C	-3.17124900	1.23545200	-0.11039200
C	-0.87276700	1.07260000	-0.83456200
C	-2.96959600	2.57391900	0.23332300
H	-4.14593300	0.76668900	0.05670800
C	-0.66508900	2.40742900	-0.48177300
H	-0.08029000	0.45435000	-1.25983100
C	-1.71276000	3.16418900	0.05130700
H	-3.79334000	3.15998600	0.65264000
H	0.32640900	2.84931300	-0.61242500
H	-1.55213400	4.20973900	0.33099100
S	-2.10354900	-2.08226300	0.51453700
H	-1.46771900	-1.30972000	-1.68661300

IM3 (frequency: 1 (16.06); single-point energy: -1413.385041 Hartree)

-1 1

C	-1.77575900	-1.23778300	-1.10068900
H	-2.58976000	-1.97555900	-1.04152500
H	-0.85054600	-2.75815800	1.47927300
C	-2.11476600	0.09158500	-0.61925300
C	-1.17632400	1.15333000	-0.56821600
C	-3.43333100	0.38262800	-0.18669000
C	-1.53577000	2.41543500	-0.11073300
H	-0.15508500	0.94971800	-0.89200600
C	-3.79093400	1.65198400	0.26686600
H	-4.18058800	-0.41706000	-0.20736200
C	-2.84711500	2.68438900	0.31186400
H	-0.77590100	3.20219400	-0.07591600
H	-4.81864400	1.83650000	0.59638400
H	-3.12452100	3.67813500	0.67430700
S	-0.27141700	-1.74236000	-1.59599000
O	-1.66209400	-2.38840400	1.88757000
H	-1.96551800	-1.80269500	1.17787600
C	1.28334300	-1.09761200	1.30889800
H	1.82533000	-1.35931400	2.23738300
C	1.97246300	0.09099300	0.67544900
C	2.83566200	-0.03470200	-0.42047700
C	1.74553300	1.37436100	1.19828100
C	3.46231300	1.08638900	-0.97055300
H	2.97764800	-1.03184100	-0.84253000
C	2.36949500	2.49819000	0.65242600
H	1.04646200	1.49145600	2.03097500
C	3.23414400	2.35896100	-0.43809200

H	4.12472400	0.96695100	-1.83319200
H	2.16780600	3.48886800	1.07054300
H	3.71593900	3.23753300	-0.87681600
S	1.16237800	-2.63860200	0.33190500
H	0.27029800	-0.81298700	1.63291600

IM4 (frequency: 1 (43.38); single-point energy: -802.62624 Hartree)

-1 1

C	0.92554800	0.83729900	0.77943100
C	0.45428000	0.13307800	-0.34416900
C	1.39079900	-0.59226200	-1.09712600
C	2.75009400	-0.61036800	-0.75605200
C	3.19794400	0.07986900	0.37090900
C	2.27099400	0.80189500	1.14026900
H	0.19889900	1.45803400	1.30963400
H	1.04444300	-1.14526500	-1.97672400
H	3.46055500	-1.16856300	-1.37533200
H	4.25770000	0.06815500	0.64472300
H	2.61211300	1.35604000	2.02130300
C	-1.03598800	0.11229400	-0.69324000
H	-1.10420900	-0.28156600	-1.72675700
S	-1.77350200	1.76475100	-0.61054400
C	-1.29893600	-2.26915600	-0.07987100
H	-1.20042600	-2.48001500	-1.15972200
H	-0.31085600	-2.50575900	0.38816800
H	-2.03252100	-2.98534400	0.33861700
C	-1.99747300	-0.59405600	1.49604800
H	-2.29616000	0.46712400	1.52909700
H	-2.81427600	-1.22437600	1.89928900
H	-1.11168900	-0.74088200	2.16274300
N	-1.75301500	-0.92073800	0.11663900

IM5(S_1) (frequency: 1 (27.22); single-point energy: -1200.733269 Hartree)

-1 1

C	-2.01488900	0.96236200	-0.47232800
C	-1.09747800	-0.06357900	-0.18462500
C	-1.60788100	-1.33190800	0.13519400
C	-2.98584500	-1.56393000	0.17100000
C	-3.88748700	-0.53412900	-0.11229500
C	-3.39202200	0.73296400	-0.43638600

H	-1.61229900	1.94463800	-0.72631400
H	-0.89066400	-2.12315400	0.36302100
H	-3.35777500	-2.56129500	0.42510300
H	-4.96593300	-0.71643400	-0.08158500
H	-4.08451800	1.54940500	-0.66491200
C	0.40245700	0.19804300	-0.29962700
N	0.69928200	1.61173800	-0.09445100
C	0.54387300	2.04108500	1.28283100
H	0.66757300	3.13624400	1.34498900
H	-0.46409700	1.79048200	1.64929800
H	1.27787600	1.55572500	1.95865000
C	1.98979000	2.01309000	-0.63412100
H	2.84380900	1.53265600	-0.11972800
H	2.06251800	1.70946500	-1.68951000
H	2.08180800	3.11342100	-0.57035200
S	1.43950600	-0.99928100	0.71462700
S	3.13067900	-1.30558900	-0.50225500
H	0.72065200	-0.05939800	-1.32332100

IM5(S_2) (frequency: 1 (33.61); single-point energy: -1598.840482 Hartree)

-1 1

C	1.56338400	-1.35454800	0.35986500
C	1.34789000	-0.01207600	0.00283500
C	2.44110000	0.77043600	-0.39011800
C	3.72983900	0.22714400	-0.42113200
C	3.94072600	-1.10563600	-0.05727800
C	2.84930200	-1.89341200	0.33330400
H	0.69499200	-1.95990500	0.63892400
H	2.25318400	1.81112500	-0.66265100
H	4.57503800	0.84942700	-0.73178600
H	4.94836100	-1.53125500	-0.07942900
H	3.00465900	-2.93895500	0.61579800
C	-0.06492600	0.52921700	0.02163300
N	-0.09561100	1.98522400	0.23466400
C	0.26331600	2.28935900	1.60865200
H	1.23751000	1.84360000	1.85941100
H	0.34521500	3.38177300	1.74334800
H	-0.48214800	1.90782900	2.34291600
C	-1.34253600	2.63654400	-0.12470300
H	-1.22611500	3.72654500	0.00771500
H	-1.58070000	2.42668500	-1.17478500

H	-2.20752600	2.29509700	0.48304700
S	-0.88916200	-0.08492200	-1.49645100
S	-2.85225900	-0.62706200	-0.59230800
S	-2.42351700	-1.67671900	1.11934700
H	-0.62274700	-0.01145900	0.82707900

IM5(S_3) (frequency: 1 (16.05); single-point energy: -1996.945763 Hartree)

-1 1

C	2.80577900	0.39224700	0.78201100
C	1.75208500	-0.13644000	0.01967100
C	1.99087500	-1.31183900	-0.71348200
C	3.24698100	-1.92151600	-0.70044600
C	4.29534300	-1.37197800	0.04404300
C	4.06502500	-0.21320800	0.78990400
H	2.60782700	1.27832900	1.38637100
H	1.17285300	-1.74117700	-1.29342900
H	3.40635100	-2.83740000	-1.27674500
H	5.28014800	-1.84779800	0.04912700
H	4.86985900	0.22089700	1.39075200
C	0.36843800	0.49564800	0.07499800
N	0.36938200	1.80754600	0.65166900
C	0.91924700	2.86228200	-0.17024500
H	1.10548400	3.75719800	0.44856300
H	1.87542200	2.54894600	-0.61622700
H	0.24143800	3.14646600	-1.00261500
C	-0.84675500	2.20523200	1.34416300
H	-1.60550000	2.63584500	0.66068700
H	-1.31150200	1.33017100	1.82452400
H	-0.60221100	2.96426800	2.11117300
S	-0.42092900	0.37060200	-1.66293600
H	-0.27499600	-0.15638000	0.69200800
S	-2.50034500	0.42772100	-1.14297800
S	-2.94239500	-1.37649900	-0.13723100
S	-2.31964100	-1.29399700	1.83317100

IM5(S_4) (frequency: 1 (22.49); single-point energy: -2395.051366 Hartree)

-1 1

C	3.15718400	-0.22495400	-0.71389900
C	2.03254900	0.11631500	0.04897600
C	2.17635300	1.08753900	1.05588400
C	3.41680000	1.67302700	1.31002900

C	4.54038400	1.30343700	0.56209100
C	4.40220800	0.35665300	-0.45557200
H	3.03230600	-0.93117700	-1.53542000
H	1.29522700	1.38626900	1.62654700
H	3.50556000	2.43158300	2.09284100
H	5.51298700	1.76143200	0.76324700
H	5.26794600	0.07414500	-1.06203400
C	0.66109000	-0.46664600	-0.24276000
N	0.62280900	-1.38631300	-1.33768000
C	1.03445300	-2.74566800	-1.07923600
H	1.93770700	-2.76602000	-0.45135400
H	0.25743700	-3.33885100	-0.55182100
H	1.26441500	-3.25291700	-2.03316600
C	-0.51754200	-1.27557100	-2.23545400
H	-0.24309900	-1.68482900	-3.22554800
H	-1.40968900	-1.81871700	-1.86930000
H	-0.79001800	-0.21504800	-2.34903700
S	0.04964300	-1.14926100	1.42709700
H	-0.01378200	0.38653100	-0.47201300
S	-1.97084200	-1.51936400	1.09687400
S	-2.98557400	0.40350000	1.20912800
S	-1.35684300	2.22872400	-1.20113100
S	-3.07373000	1.20683900	-0.72381500

IM5(S_5) (frequency: 1 (20.61); single-point energy: -2793.145183 Hartree)

-1 1

C	-2.95762600	-0.74682300	-1.13608400
C	-2.29272500	-0.10639500	-0.08436300
C	-2.91739500	0.99173400	0.53414100
C	-4.17618800	1.42410900	0.11843600
C	-4.83918300	0.76943400	-0.92592700
C	-4.22256900	-0.31530800	-1.55149700
H	-2.46997000	-1.58628700	-1.63350300
H	-2.38606300	1.49614000	1.34166900
H	-4.64112900	2.28476600	0.60786400
H	-5.82684500	1.10796400	-1.25187500
H	-4.72559000	-0.83342300	-2.37313800
C	-0.89582900	-0.46517000	0.39864100
N	-0.81193300	-0.46966900	1.82775700
C	0.53895400	-0.33619900	2.34349300
H	1.01507100	0.55042300	1.90237700

H	0.49695100	-0.20518400	3.43748000
H	1.17142600	-1.21885600	2.11448000
C	-1.58546000	-1.49734800	2.48992900
H	-1.63817100	-1.28404400	3.57063500
H	-2.61270200	-1.51427000	2.09413900
H	-1.15190000	-2.51389800	2.36576100
H	-0.21925000	0.32477400	0.02759200
S	3.48810000	0.92154000	0.24140800
S	2.14441600	1.96350300	-0.83574600
S	-0.23564600	-2.06915900	-0.38188600
S	1.50878500	-1.45568700	-1.42402700
S	3.10430900	-1.51575200	-0.17427700
S	0.53752500	2.67876600	0.19212800

IM5(S_6) (frequency: 1 (10.63); single-point energy: -3191.243165 Hartree)

-1 1

C	-2.97284200	0.64799200	-1.05940900
C	-2.64599300	-0.12687700	0.06534600
C	-3.62261800	-0.30890800	1.05568500
C	-4.90403600	0.23053400	0.90890800
C	-5.22606900	0.97978700	-0.22477100
C	-4.24897800	1.19391200	-1.20230900
H	-2.20657700	0.82433600	-1.81369800
H	-3.35325400	-0.85726200	1.95903200
H	-5.65059300	0.07168300	1.69259400
H	-6.22717600	1.40448600	-0.34125600
H	-4.47950500	1.79872800	-2.08366200
C	-1.23059000	-0.63593500	0.26659200
N	-1.08942000	-1.56509400	1.34170700
C	0.25974800	-1.64773200	1.86945800
H	0.67116800	-0.63973200	2.01781000
H	0.24945700	-2.18190300	2.83486700
H	0.94867400	-2.18155600	1.18435000
C	-1.66859200	-2.87604400	1.12020500
H	-1.72354600	-3.42496100	2.07546000
H	-2.68746200	-2.78795000	0.71621900
H	-1.07099000	-3.48342600	0.40799600
H	-0.59929000	0.25360300	0.43482400
S	3.44513200	-0.74559800	0.68302000
S	3.35768000	1.37644200	0.61163900
S	1.42099100	2.09340800	1.22187800

S	-0.55065800	-1.29623700	-1.40791000
S	1.20797800	-0.20712800	-1.71459100
S	2.88381700	-1.42017200	-1.26128100
S	0.19223900	2.53798700	-0.33742500

IM5(S_7) (frequency: 1 (20.77); single-point energy: -3589.336257 Hartree)

-1 1

C	-4.01829700	-0.90622000	0.01662100
C	-2.94777600	-0.00142800	0.04113200
C	-3.20674600	1.36011900	-0.18459000
C	-4.51043600	1.80047600	-0.42332200
C	-5.57437700	0.89284100	-0.43691600
C	-5.32363300	-0.46438200	-0.21848700
H	-3.83053400	-1.97148000	0.17064400
H	-2.36226300	2.05491400	-0.21060100
H	-4.69449500	2.86240900	-0.60868000
H	-6.59422600	1.24033500	-0.62528700
H	-6.14589300	-1.18528500	-0.23462400
C	-1.51628900	-0.39386700	0.34553300
N	-1.19597100	-0.28988400	1.72764100
C	0.22752400	-0.29794200	2.00435400
H	0.73468300	0.43634500	1.36743900
H	0.40375000	-0.01376200	3.05433200
H	0.69338800	-1.28953200	1.82741400
C	-1.96471200	-1.10073000	2.64436200
H	-1.73286600	-0.80099800	3.67904500
H	-3.04262000	-0.95618400	2.48193600
H	-1.74267200	-2.18723600	2.55046400
H	-0.84407300	0.26479000	-0.23751900
S	3.59417000	0.34282500	1.01777300
S	3.13701300	2.25200700	0.08294100
S	1.11045100	2.80075500	0.17974400
S	-1.16628000	-2.14700700	-0.40021600
S	0.52608200	-1.93960600	-1.56504500
S	0.06579300	2.23132300	-1.47514300
S	2.19088800	-2.53887200	-0.34076200
S	3.70051300	-1.11132100	-0.50180300

IM5(S_8) (frequency: 1 (10.06); single-point energy: -3987.428744 Hartree)

-1 1

C	4.31731800	0.82788000	-0.34942800

C	3.31428500	-0.02200700	0.12865900
C	3.64417600	-1.35643800	0.42793200
C	4.94769500	-1.82051400	0.25752000
C	5.94878500	-0.96041300	-0.20935600
C	5.62800900	0.36344500	-0.51276600
H	4.07187600	1.85942000	-0.60682100
H	2.84979100	-2.01644700	0.78032400
H	5.18391300	-2.86394700	0.48397200
H	6.97165200	-1.32432300	-0.34104200
H	6.39938600	1.04448000	-0.88323200
C	1.86065800	0.35983900	0.34523100
N	1.45230800	0.14222400	1.68747400
C	0.01625800	0.04409600	1.85457300
H	-0.21817800	-0.32961400	2.86364800
H	-0.50147200	1.01735400	1.71611300
H	-0.38488700	-0.66996600	1.12690800
C	2.11632500	0.93590200	2.69573400
H	3.20720200	0.90106100	2.55242000
H	1.80027000	2.00235500	2.68104700
H	1.88701400	0.53189100	3.69529700
H	1.24683400	-0.28347100	-0.31443700
S	-2.99877100	-1.53361700	1.41156900
S	-2.99903600	-2.31261300	-0.56408700
S	1.51235200	2.15333400	-0.26793400
S	-0.11333400	1.98844800	-1.53494500
S	-1.28134700	-1.53294400	-1.54410200
S	-1.83209200	2.68089600	-0.47633700
S	-3.38671600	1.25168700	-0.57413100
S	0.41423300	-2.54287300	-1.04355200
S	-3.90532800	0.40423800	1.25632600

TS5/6(S_1) (Number of imaginary frequency: 1 (-1117.82); single-point energy: -1200.692858 Hartree)

-1 1

C	1.84167900	1.00762000	0.55519500
C	0.93898300	0.03669600	0.03240400
C	1.52598000	-1.17267900	-0.43459900
C	2.89817900	-1.39223100	-0.36740700
C	3.76908300	-0.42381600	0.15524800
C	3.21438700	0.77823400	0.61437300
H	1.42022700	1.94215100	0.93006500
H	0.86316100	-1.93247700	-0.85203400

H	3.30219300	-2.34173200	-0.73654900
H	4.84758400	-0.60087100	0.19992000
H	3.86746400	1.55635400	1.02640100
C	-0.49815200	0.25966200	0.07404100
N	-0.91635700	1.62475500	0.17717000
C	-0.77444200	2.40700500	-1.03680100
H	-0.96051100	3.47931200	-0.83732500
H	0.25007700	2.30311600	-1.42606600
H	-1.48090200	2.08098600	-1.83449700
C	-2.20393500	1.81943200	0.80610600
H	-3.04577900	1.42878900	0.19306800
H	-2.23081800	1.28319300	1.76565400
H	-2.37956900	2.89617800	0.98707000
S	-1.55432300	-0.81634400	-1.02043900
S	-2.26201900	-1.84684500	0.75780100
H	-1.24773100	-0.77681600	1.15494300

TS5/6(S_2) (Number of imaginary frequency: 1 (-961.72); single-point energy: -1598.826864 Hartree)

-1 1

C	1.48252500	-1.34798200	-0.18484900
C	1.26850200	0.04598100	-0.20121000
C	2.38579500	0.88827100	-0.05615400
C	3.67302700	0.35948000	0.08421100
C	3.87349600	-1.02274300	0.09580300
C	2.76458500	-1.87114600	-0.03868400
H	0.61534500	-2.00272200	-0.29007700
H	2.22109500	1.96718800	-0.07491200
H	4.52747800	1.03717600	0.18233100
H	4.87918400	-1.43768200	0.21072100
H	2.90420200	-2.95649500	-0.02468400
C	-0.11828500	0.59007800	-0.35889200
N	-0.25826700	1.97338900	0.06260400
C	-0.20906500	2.16088700	1.50397600
H	0.64639000	1.61268600	1.92563700
H	-0.07419200	3.23173300	1.73744700
H	-1.12529800	1.79534500	2.01186800
C	-1.32098700	2.73804800	-0.55024100
H	-1.24555700	3.78603200	-0.20993000
H	-1.23011300	2.70533900	-1.64491700
H	-2.33423000	2.35866400	-0.30026100
S	-1.04752300	-0.03553600	-1.65312000
S	-2.76298600	-1.49384200	-0.25050900
S	-1.81442900	-1.03283400	1.50115300
H	-0.77498900	-0.16083700	0.71441400

TS5/6(S_3) (Number of imaginary frequency: 1 (-644.38); single-point energy: -1996.914091 Hartree)

-1 1

C	2.51956200	0.44567400	0.64156500
C	1.43370300	0.07384400	-0.19423500
C	1.62536900	-1.07970600	-0.99929000
C	2.82199600	-1.78774400	-0.98412000
C	3.89176100	-1.39350900	-0.16604700
C	3.71646100	-0.27118100	0.64933100
H	2.38511600	1.30624700	1.29811300
H	0.79996300	-1.41318500	-1.62968500
H	2.92242900	-2.67302200	-1.62123900
H	4.83094500	-1.95382300	-0.15958400
H	4.52704800	0.05405600	1.31094000
C	0.17140400	0.81322900	-0.13844400
N	0.20335400	2.07786100	0.55602700
C	0.75926700	3.17163300	-0.21721500
H	0.89474600	4.06514600	0.41997700
H	1.74459500	2.88257100	-0.61482600
H	0.11179000	3.46090800	-1.07649700
C	-1.03267700	2.44981100	1.21250400
H	-1.83334600	2.73691000	0.49403900
H	-1.41687000	1.60708100	1.80287500
H	-0.85908300	3.31076000	1.88430300
S	-0.89770500	0.70550900	-1.54995500
H	-0.41604700	-0.25930100	1.02388300
S	-2.77570100	-0.17211700	-0.78382900
S	-2.09417500	-1.93597200	0.08988100
S	-1.14215900	-1.23502400	1.87835500

TS5/6(S_4) (Number of imaginary frequency: 1 (-304.52); single-point energy: -2395.02176 Hartree)

-1 1

C	-2.89463400	-0.05510700	0.66878600
C	-1.81158200	-0.02966600	-0.24762800
C	-1.87254900	0.95214700	-1.27128600
C	-2.95166600	1.82281100	-1.38061800
C	-4.02339800	1.76901000	-0.47775700
C	-3.97332500	0.82129100	0.54951100
H	-2.85016800	-0.77498600	1.48674500
H	-1.04139200	1.02027700	-1.97464700
H	-2.95355400	2.56703400	-2.18387900
H	-4.86928800	2.45599000	-0.56905800
H	-4.78869200	0.76422900	1.27885500

C	-0.66910900	-0.92884300	-0.06469800
N	-0.80389400	-1.94269600	0.94757500
C	-1.44691000	-3.16350500	0.50334300
H	-2.40200800	-2.92043800	0.01159000
H	-0.82635600	-3.74009700	-0.21917500
H	-1.66218600	-3.82059600	1.36608100
C	0.38742500	-2.19538500	1.73199800
H	0.13307600	-2.81065300	2.61507000
H	1.18110100	-2.72776400	1.16361100
H	0.81693900	-1.24533300	2.07861700
S	0.29870700	-1.28676300	-1.47713100
H	0.09952200	0.42084400	0.78068800
S	2.44592600	-0.98613100	-1.01851500
S	2.93491400	1.05620900	-0.83082000
S	0.51184400	1.70729500	1.33389600
S	2.57890600	1.41275400	1.20898100

TS5/6(S_5) (Number of imaginary frequency: 1 (-602.13); single-point energy: -2793.117451 Hartree)

-1 1

C	-2.62104900	0.11581300	-1.47044400
C	-2.21787300	-0.19731400	-0.14996700
C	-3.04755900	0.26965600	0.89953500
C	-4.21665400	0.98579300	0.63821800
C	-4.60606400	1.27227200	-0.67313000
C	-3.78814000	0.83021600	-1.72277000
H	-1.98941500	-0.21653600	-2.29605700
H	-2.73786700	0.06129800	1.92417200
H	-4.83047100	1.33011500	1.47715900
H	-5.52226900	1.83364700	-0.87619500
H	-4.06540600	1.05048200	-2.75883700
C	-0.95316600	-0.87809900	0.16144100
N	-0.82875300	-1.38787500	1.51043300
C	0.52083200	-1.43510100	2.03957600
H	1.00050700	-0.45190200	1.95564200
H	0.48713300	-1.71109800	3.10829400
H	1.16608400	-2.17011600	1.51258000
C	-1.54112200	-2.63388600	1.72682600
H	-1.56108300	-2.88040100	2.80387200
H	-2.58119000	-2.53361000	1.37944100
H	-1.08086900	-3.49393800	1.18942300
H	-0.27391800	0.58949400	0.37204600
S	3.32436300	0.90936900	0.79982200
S	1.94759900	2.17498400	-0.01263100

S	-0.13334500	-1.76695000	-1.09199900
S	1.66597900	-0.57644600	-1.81317000
S	3.26654100	-0.90950800	-0.62467300
S	0.09228800	1.93927500	0.92638300

TS5/6(S_6) (Number of imaginary frequency: 1 (-531.23); single-point energy: -3191.217858 Hartree)

-1 1

C	-2.95703200	-0.10927700	-1.38583700
C	-2.57029500	-0.22605000	-0.02848500
C	-3.42687500	0.36602600	0.93217900
C	-4.60741600	1.00580800	0.55786200
C	-4.98189500	1.09671600	-0.78748700
C	-4.13646200	0.53551200	-1.75239800
H	-2.30879300	-0.54177700	-2.14968600
H	-3.12348900	0.32192700	1.97868800
H	-5.24306900	1.44896700	1.33164900
H	-5.90660800	1.60212000	-1.07926800
H	-4.39847900	0.60416300	-2.81315900
C	-1.29549700	-0.83124000	0.38221200
N	-1.10895800	-1.02450300	1.80035600
C	0.25167100	-0.85828900	2.26514100
H	0.65342700	0.11263800	1.94825400
H	0.27886000	-0.90007800	3.36849700
H	0.94141200	-1.63803500	1.87582500
C	-1.72289700	-2.23492400	2.31558000
H	-1.69272100	-2.23755900	3.42031000
H	-2.77769400	-2.27930900	2.00239500
H	-1.21973800	-3.16183800	1.95879000
H	-0.54563200	0.62377300	0.05014900
S	3.47568200	-0.27530700	0.66556700
S	3.25450600	1.67679300	-0.05829300
S	1.44621900	2.41542200	0.78242100
S	-0.54547300	-1.98723300	-0.68965500
S	1.17387400	-0.96704000	-1.75468200
S	2.97584500	-1.56179600	-0.98838300
S	-0.16906400	1.99608800	-0.42494800

TS5/6(S_7) (Number of imaginary frequency: 1 (-588.77); single-point energy: -3589.311594 Hartree)

-1 1

C	-3.44161400	-0.67853800	-1.06421800
C	-2.81192800	-0.16749600	0.09373100
C	-3.40451200	0.96497300	0.70019600
C	-4.56951600	1.53543900	0.18866300
C	-5.18600200	1.00987700	-0.95171600

C	-4.60266100	-0.10095600	-1.57328700
H	-2.99671600	-1.54333300	-1.55957800
H	-2.90818000	1.39461900	1.57100400
H	-4.99748900	2.41266900	0.68466700
H	-6.09791500	1.46034900	-1.35315000
H	-5.05985700	-0.52526900	-2.47291000
C	-1.54237900	-0.70737500	0.61554600
N	-1.16883300	-0.27155800	1.94223300
C	0.25702600	-0.22576300	2.19260300
H	0.76256000	0.35545100	1.41480400
H	0.45178100	0.26871300	3.16010600
H	0.72876500	-1.23140600	2.21422700
C	-1.88688000	-0.95362700	3.00363100
H	-1.67908600	-0.47001900	3.97479400
H	-2.97082700	-0.89739400	2.81866100
H	-1.60815200	-2.02828900	3.09077000
H	-0.70842000	0.27835500	-0.35453800
S	3.49404100	0.88601100	0.80575000
S	2.72175400	2.52912300	-0.25625500
S	0.62128300	2.64995600	-0.03920600
S	-1.04719000	-2.30313200	0.14108300
S	0.67907700	-2.19788500	-1.33759600
S	-0.22461800	1.31035900	-1.35433300
S	2.43504900	-2.29889100	-0.22816900
S	3.72036500	-0.67758900	-0.60723500

TS5/6(S_8) (Number of imaginary frequency: 1 (-646.22); single-point energy: -3987.400317 Hartree)

-1 1

C	3.68661300	0.73368300	-1.04269100
C	3.20403100	0.14836400	0.15073800
C	3.96931800	-0.90512300	0.70433900
C	5.15956300	-1.32749900	0.11093400
C	5.63054100	-0.72515900	-1.05940200
C	4.87534200	0.30792000	-1.62959200
H	3.10463100	1.53437400	-1.50182700
H	3.59230000	-1.38640300	1.60723300
H	5.72467500	-2.14536900	0.56963100
H	6.56215300	-1.05843300	-1.52484700
H	5.21610800	0.78667600	-2.55303800
C	1.91146700	0.52020000	0.75917600
N	1.67365600	0.00472200	2.08681700
C	0.30109600	-0.35702500	2.36001200
H	0.22504600	-0.83478200	3.35219500
H	-0.39248800	0.51222200	2.34303400

H	-0.05265600	-1.07069600	1.60824200
C	2.27005500	0.79304600	3.14923400
H	3.33076000	0.98049900	2.92011400
H	1.77083800	1.77712600	3.29543800
H	2.21733800	0.24316500	4.10616100
H	1.15447600	-0.56559800	-0.18401900
S	-2.75603000	-1.43749100	1.31275400
S	-2.41122400	-2.57604900	-0.41057200
S	1.26762000	2.10309000	0.40362300
S	-0.27963600	2.01077600	-1.21710000
S	-1.08630400	-1.44845500	-1.61414500
S	-2.16005600	2.52288000	-0.46342800
S	-3.58537200	1.01105900	-0.89520400
S	0.86334200	-1.79696500	-1.02947900
S	-4.24089800	-0.00986100	0.80964400

IM6 (frequency: 1 (41.77); single-point energy: -1598.836898 Hartree)

-1 1

C	1.30312000	-1.25305000	-0.44710800
C	1.25903100	0.15480100	-0.31693500
C	2.44986300	0.81962500	0.05256400
C	3.63383200	0.11319800	0.26995400
C	3.66314200	-1.27947700	0.13874900
C	2.48560700	-1.95275100	-0.21806400
H	0.37684100	-1.77165300	-0.71209300
H	2.43174900	1.90818800	0.14039900
H	4.54587900	0.65633000	0.53840400
H	4.58940300	-1.83418000	0.31447200
H	2.48917000	-3.04311100	-0.31178300
C	0.01057100	0.89085400	-0.59140500
N	-0.16124200	2.10164100	0.12061800
C	-0.07714000	2.04136500	1.57365000
H	0.77733500	1.42712000	1.88453300
H	0.06188800	3.05782300	1.98330400
H	-0.98916500	1.58583600	2.00990800
C	-1.23026200	2.96751100	-0.32319000
H	-1.13079800	3.94767800	0.17554300
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H	-2.23366700	2.55188500	-0.09852800
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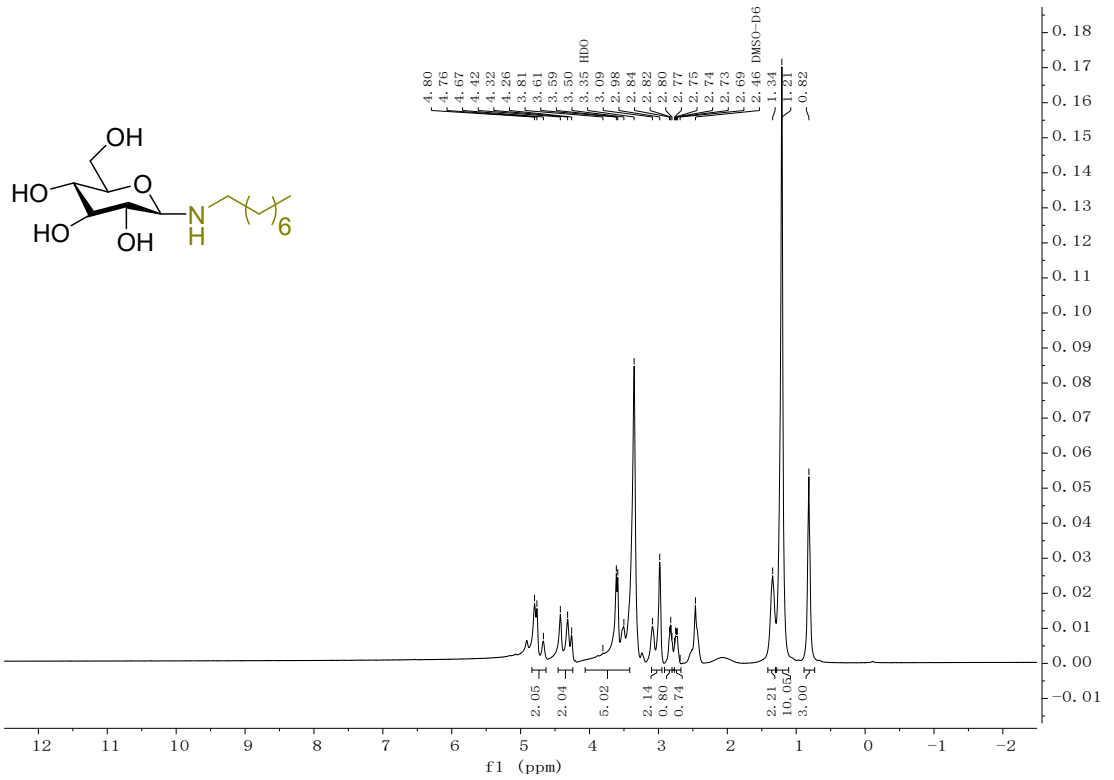
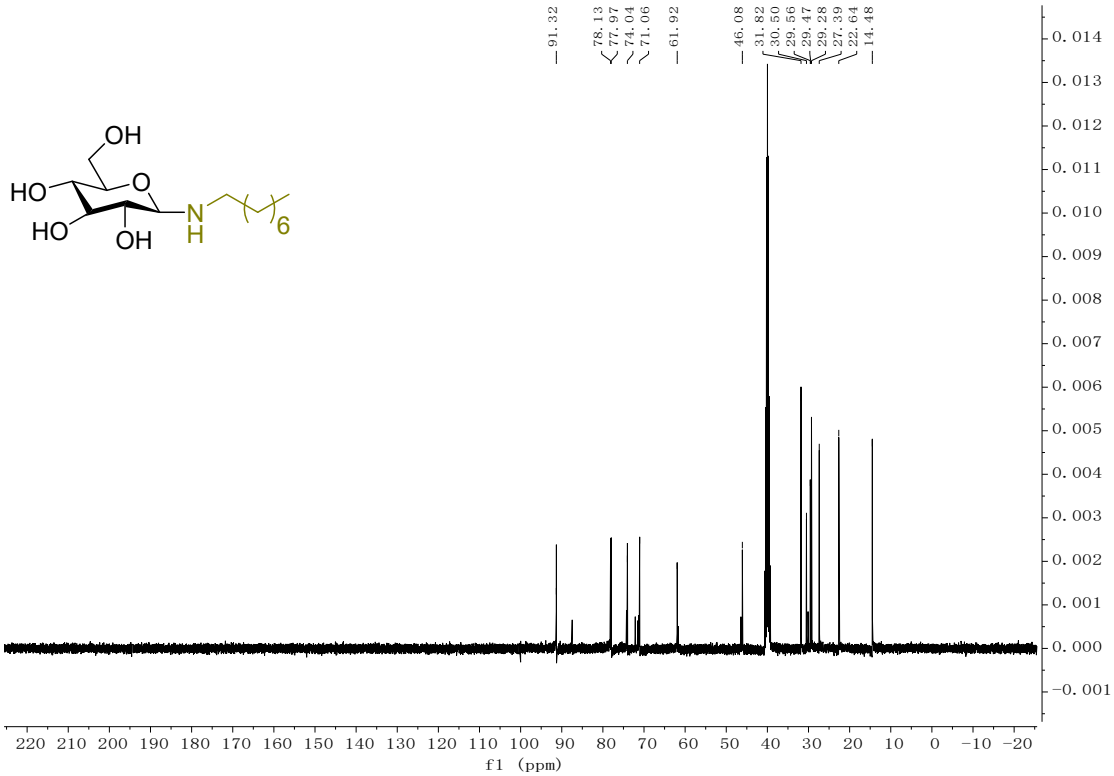
NMR Spectra

N-Octyl glucosamine (AGA8)

^{1}H NMR

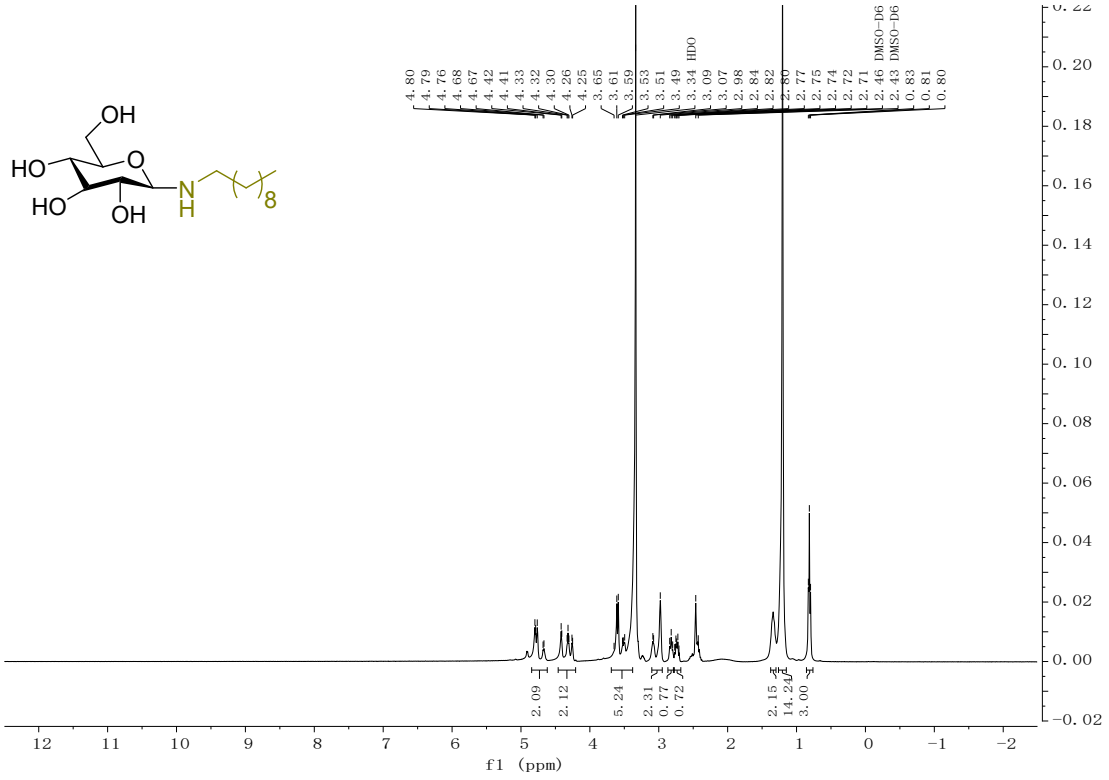


^{13}C NMR

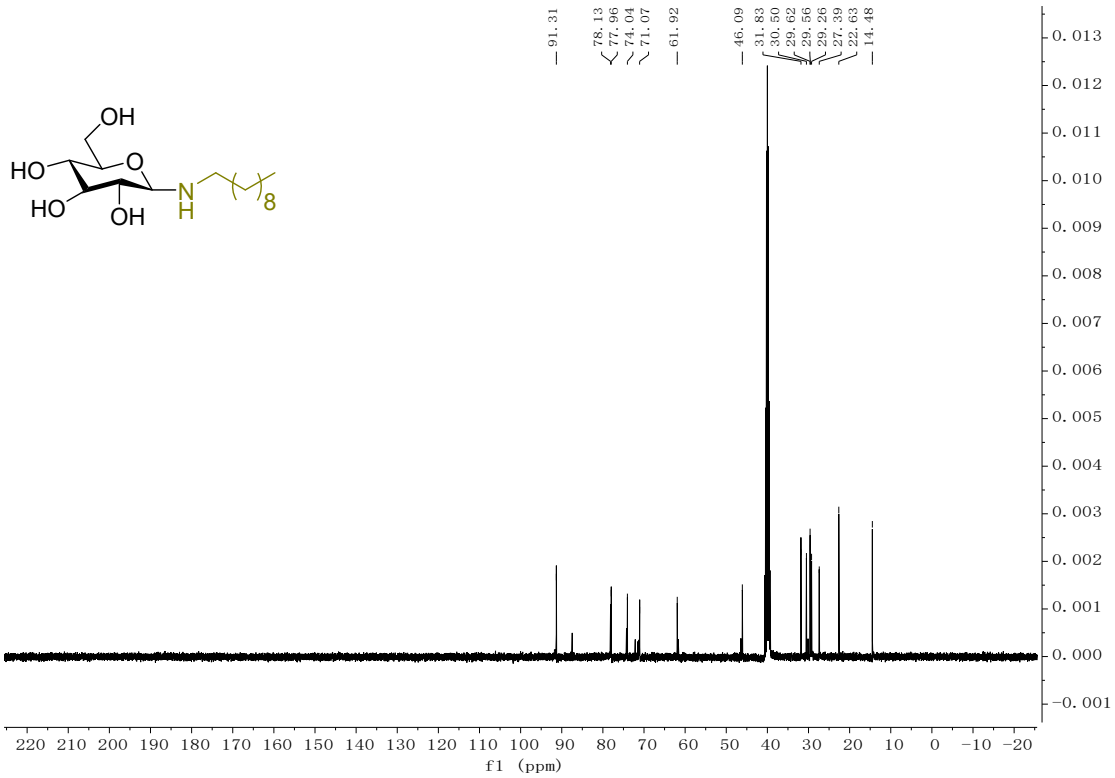


N-Decyl glucosamine (AGA10)

^{1}H NMR



^{12}C NMR



N-Dodecyl glucosamine (AGA12)

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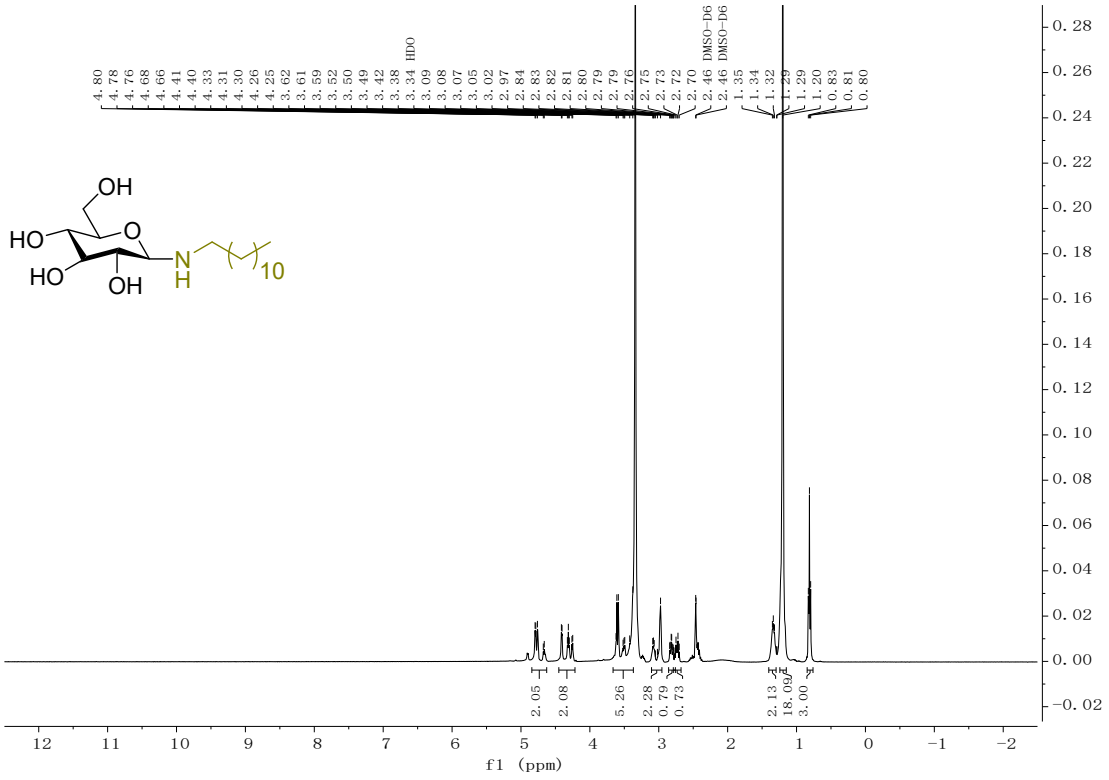

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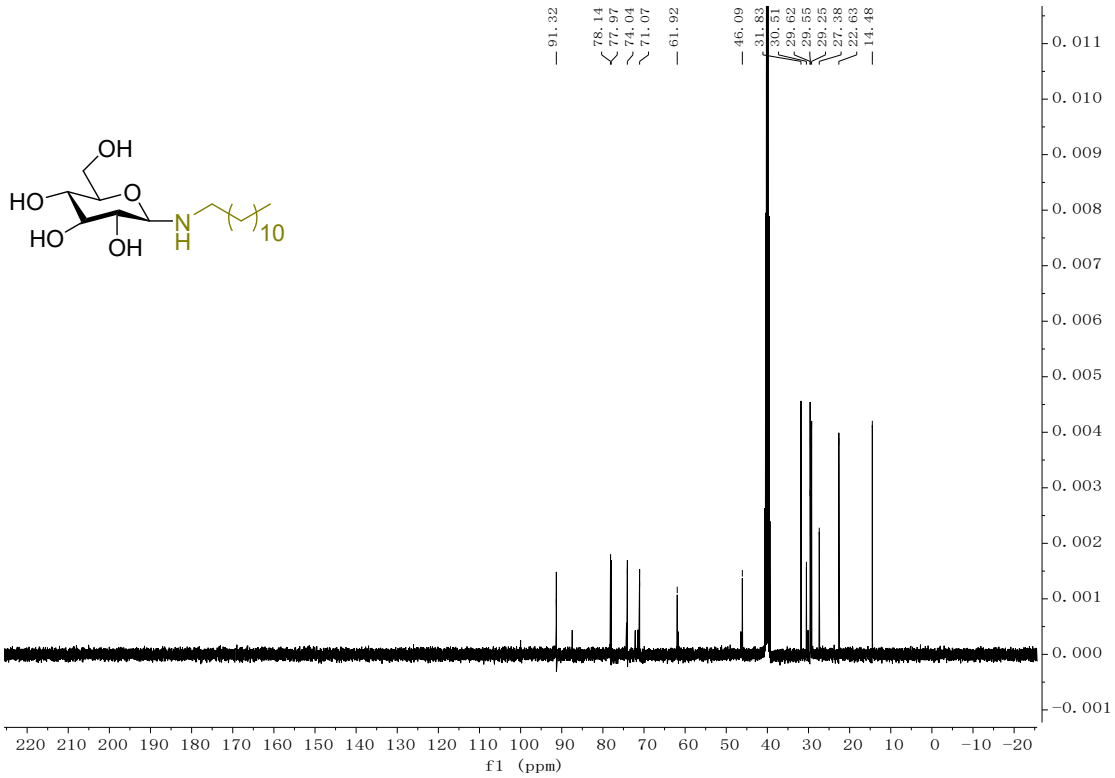

N-Tetradecyl glucosamine (AGA14)

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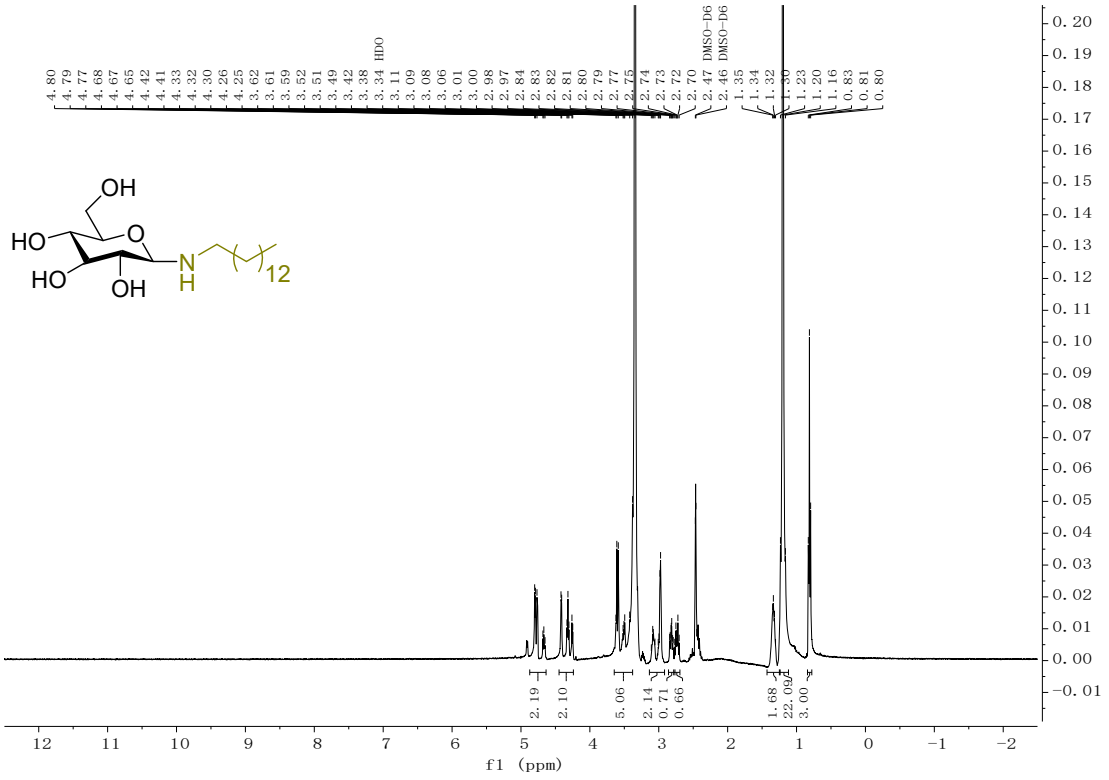

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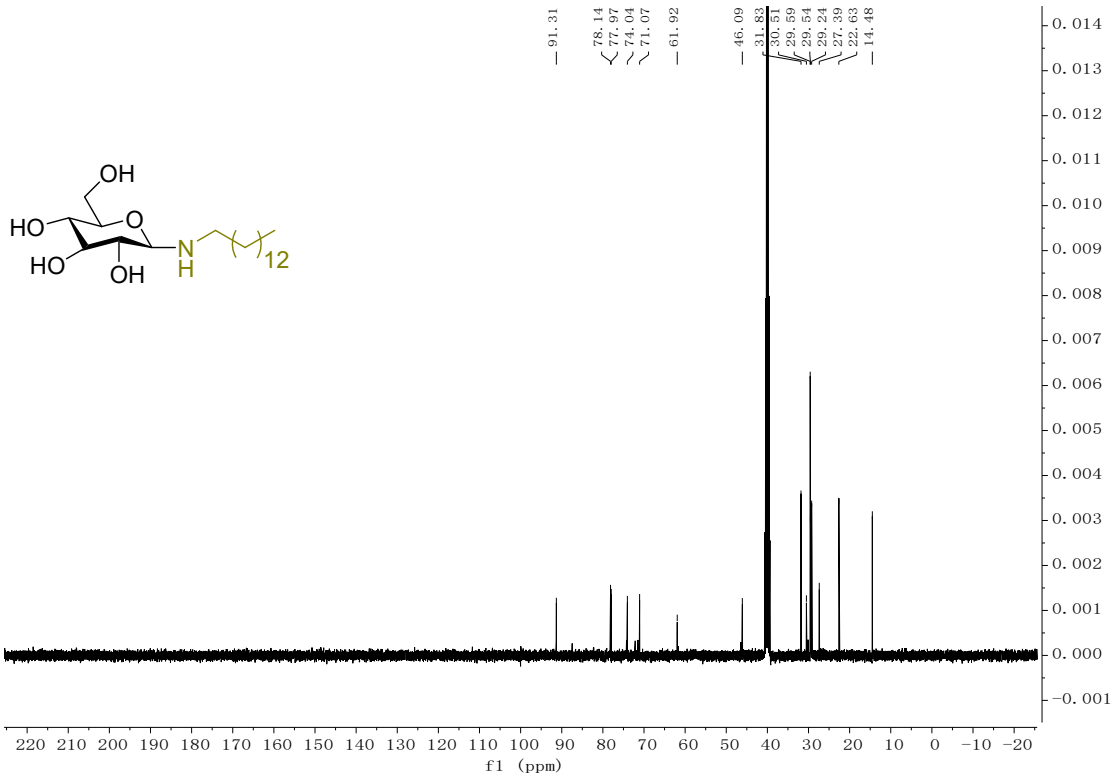

N-hexadecyl glucosamine (AGA16)

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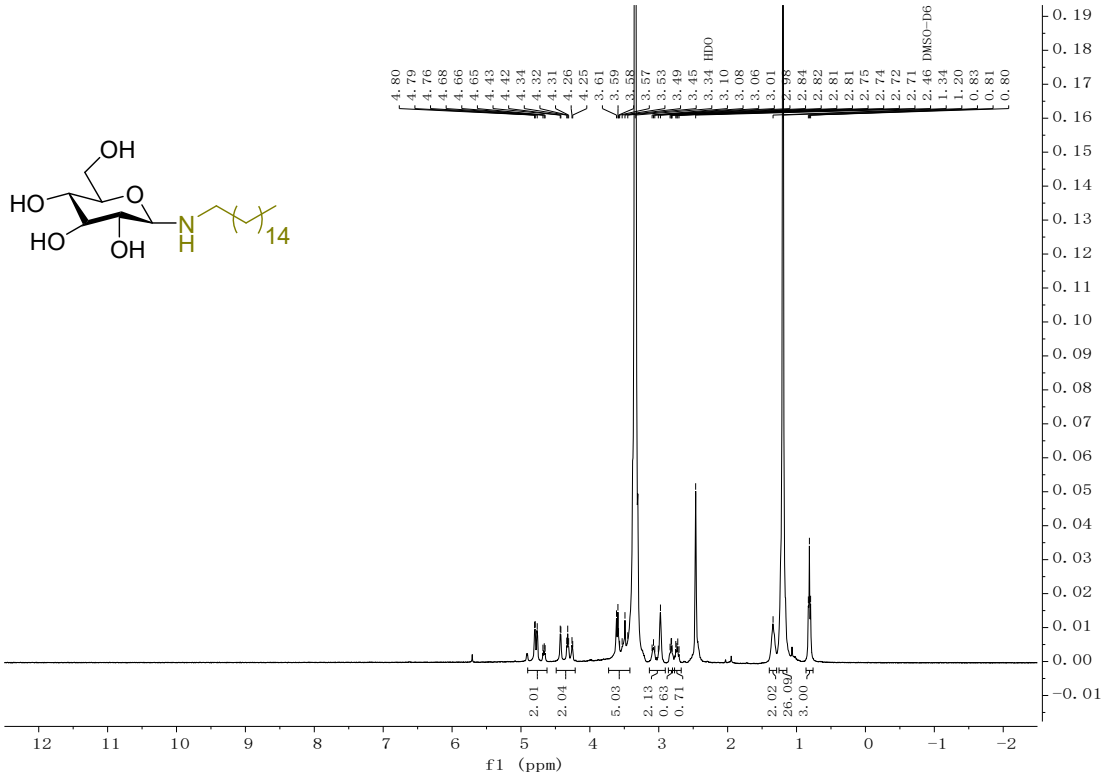

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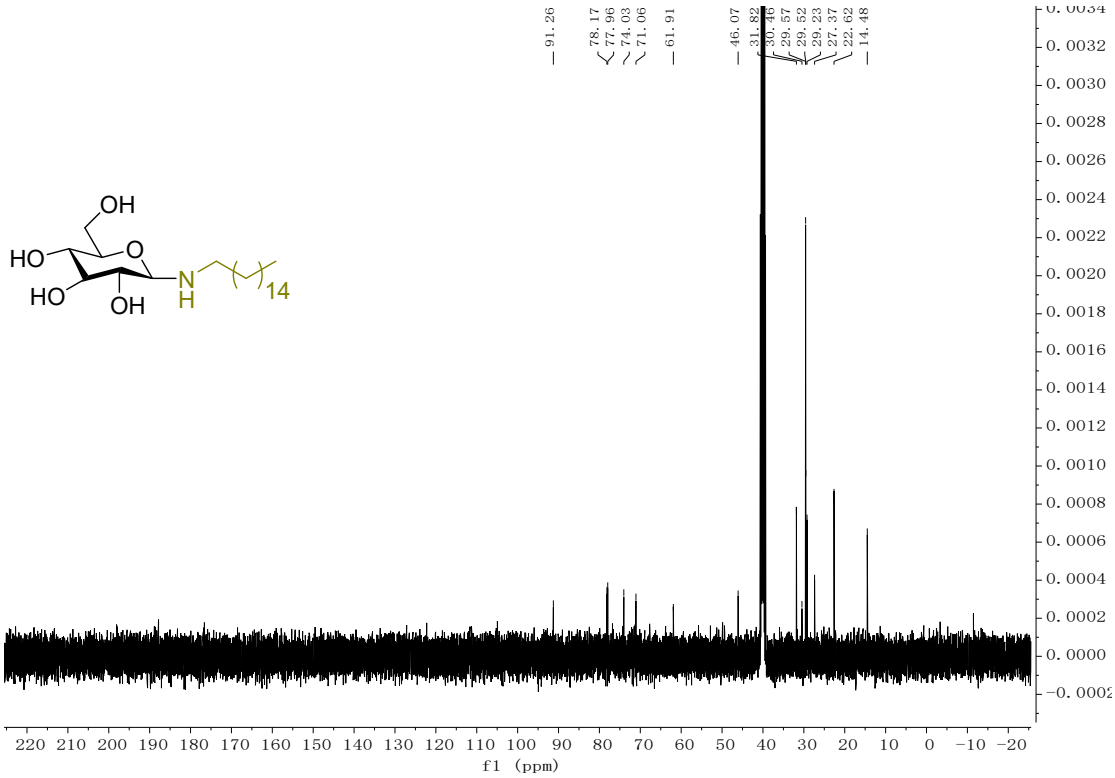
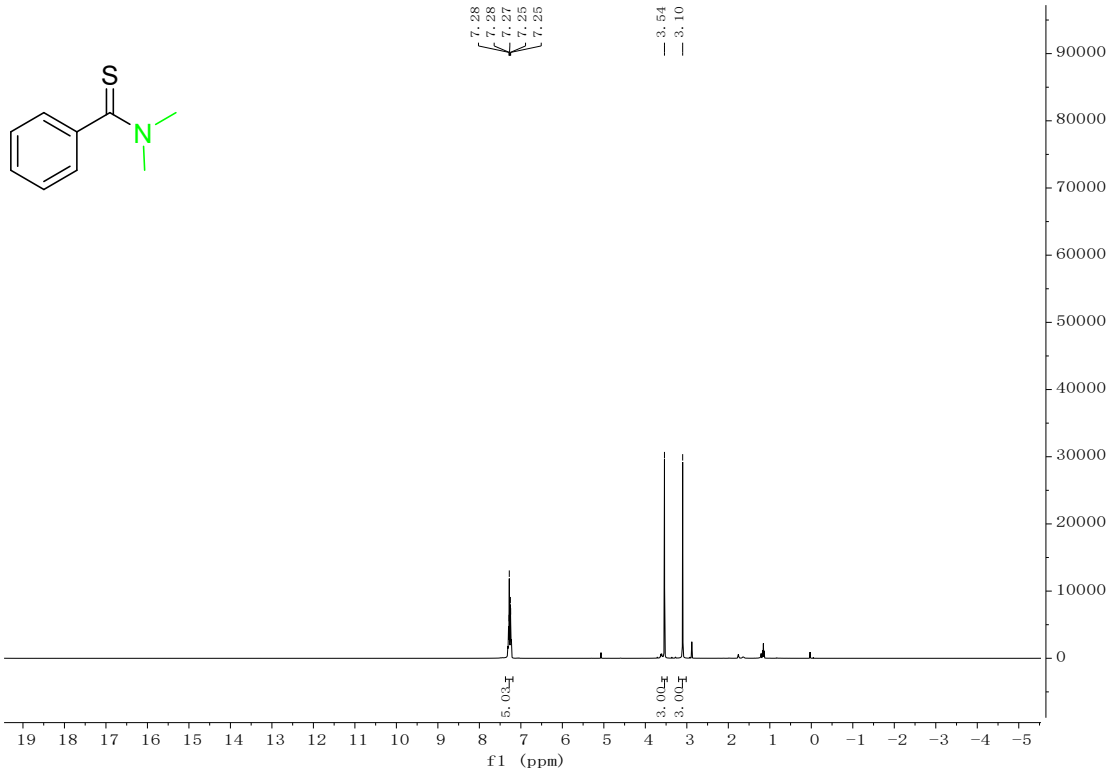


N,N-Dimethylbenzothioamide

^{1}H NMR



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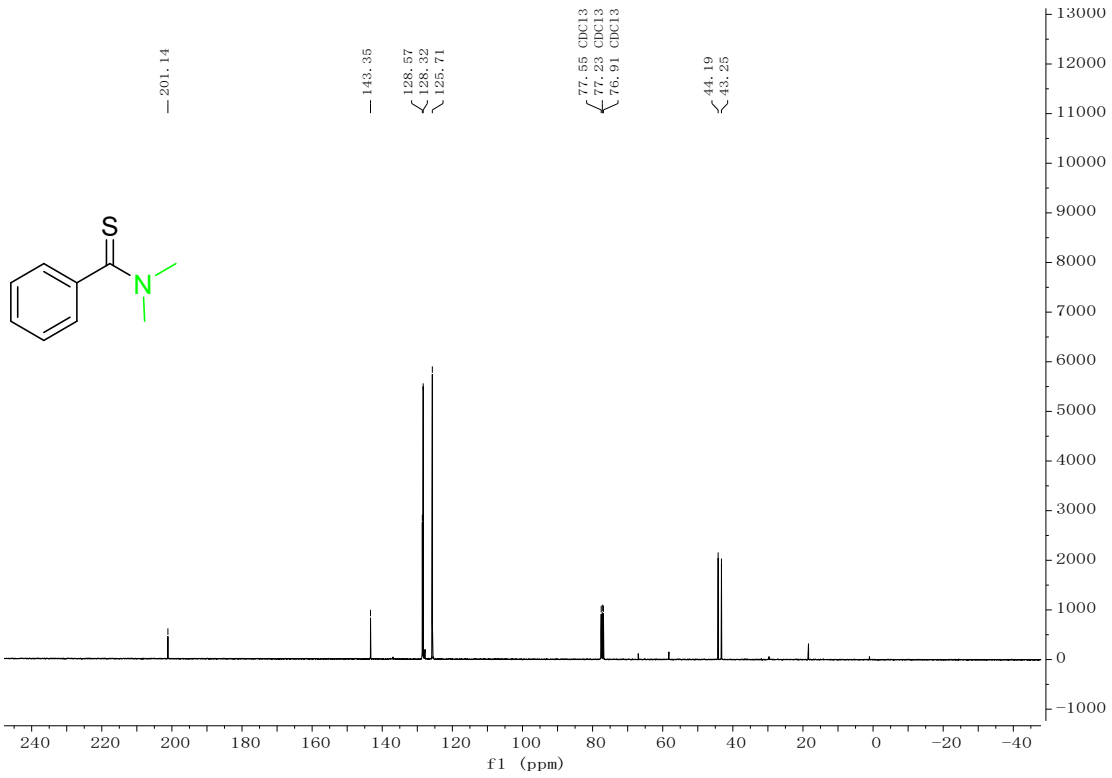

N,N,3-Trimethylbenzothioamide

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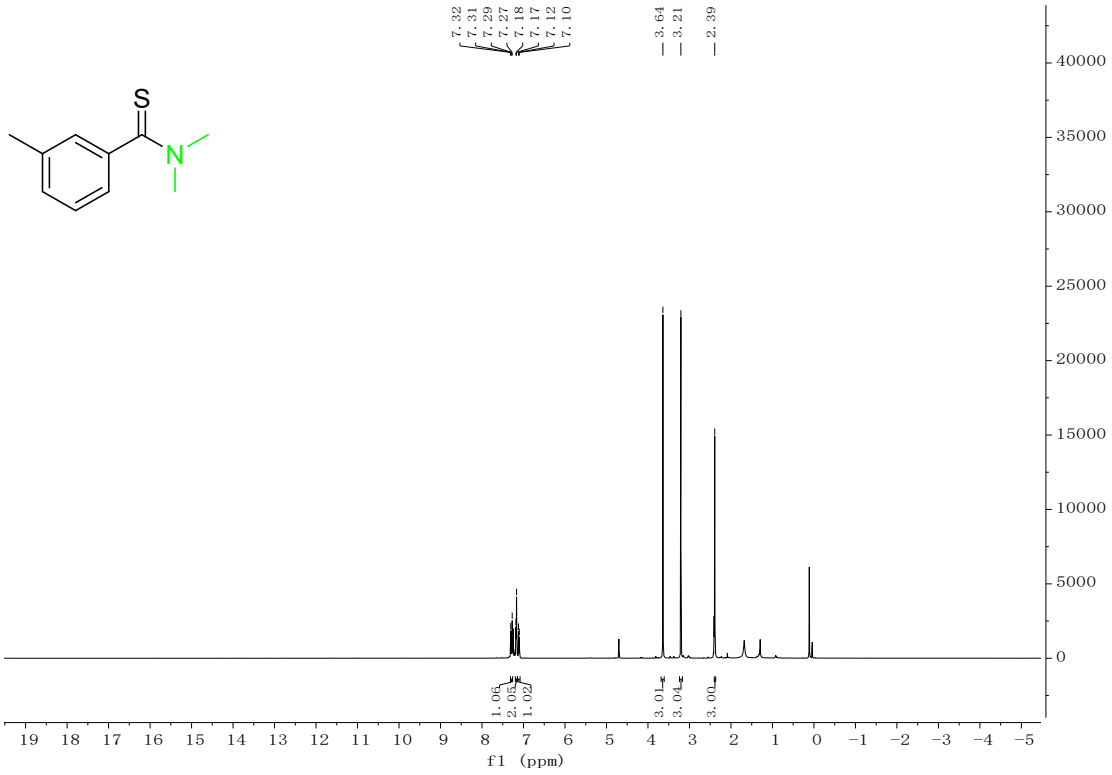
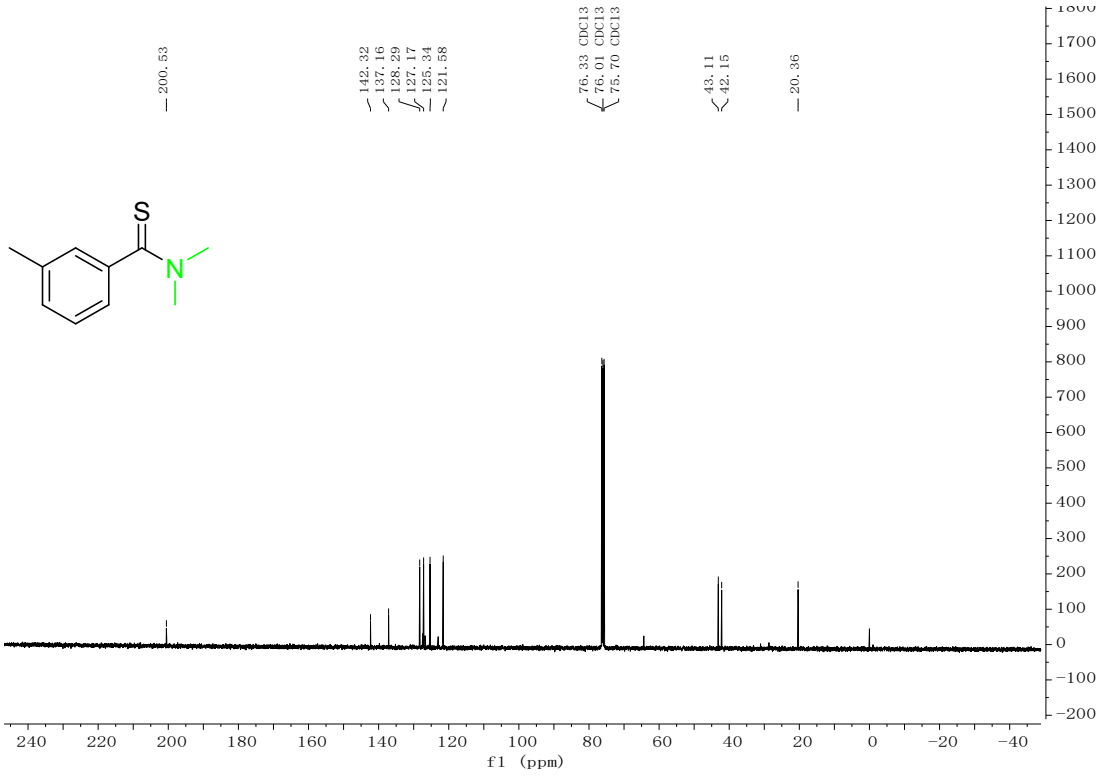
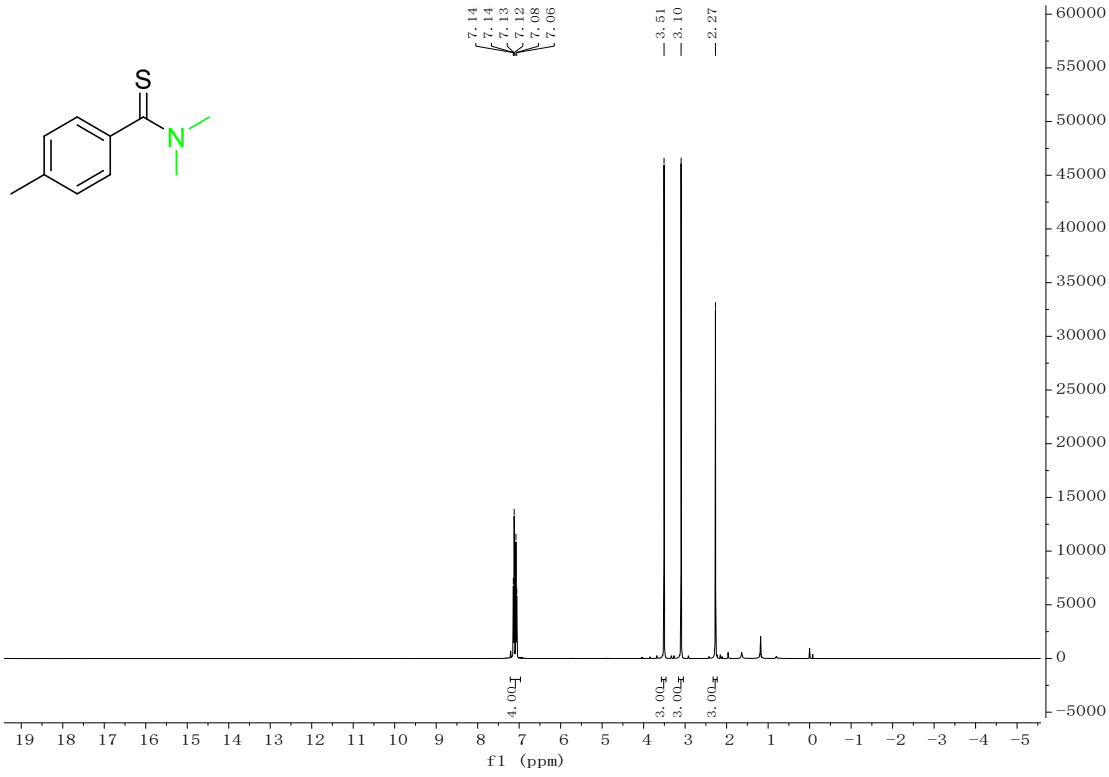


^{13}C NMR

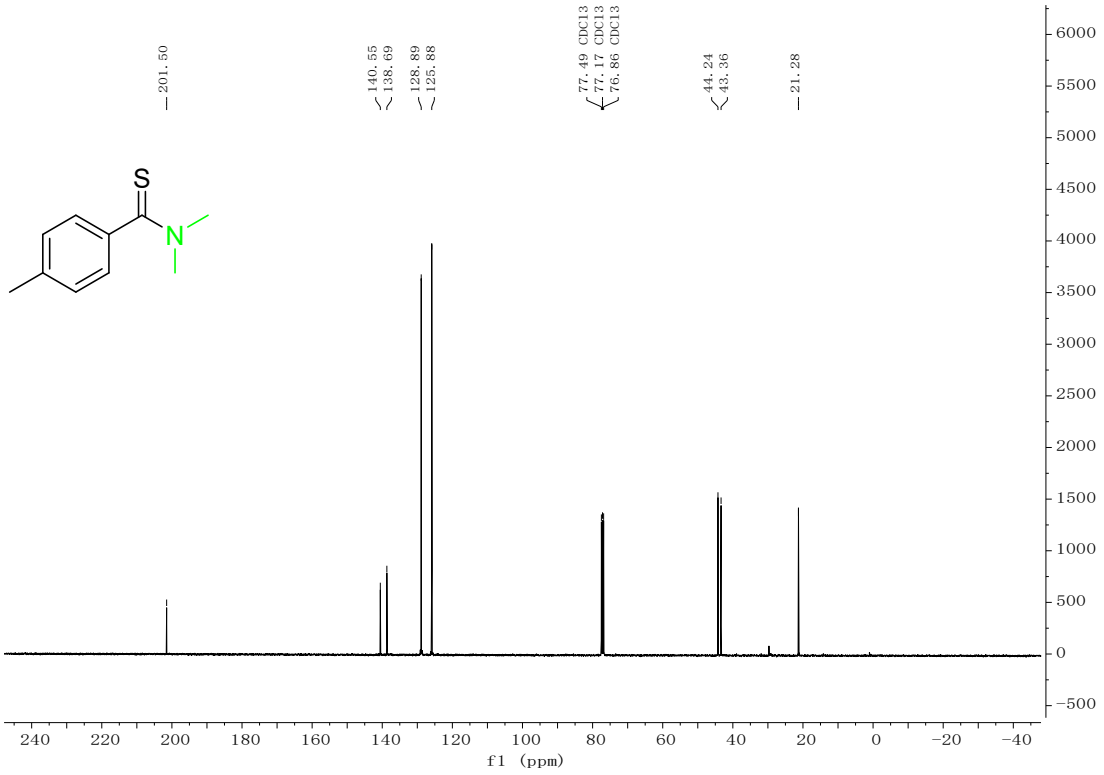


N,N,4-Trimethylbenzothioamide

^{1}H NMR

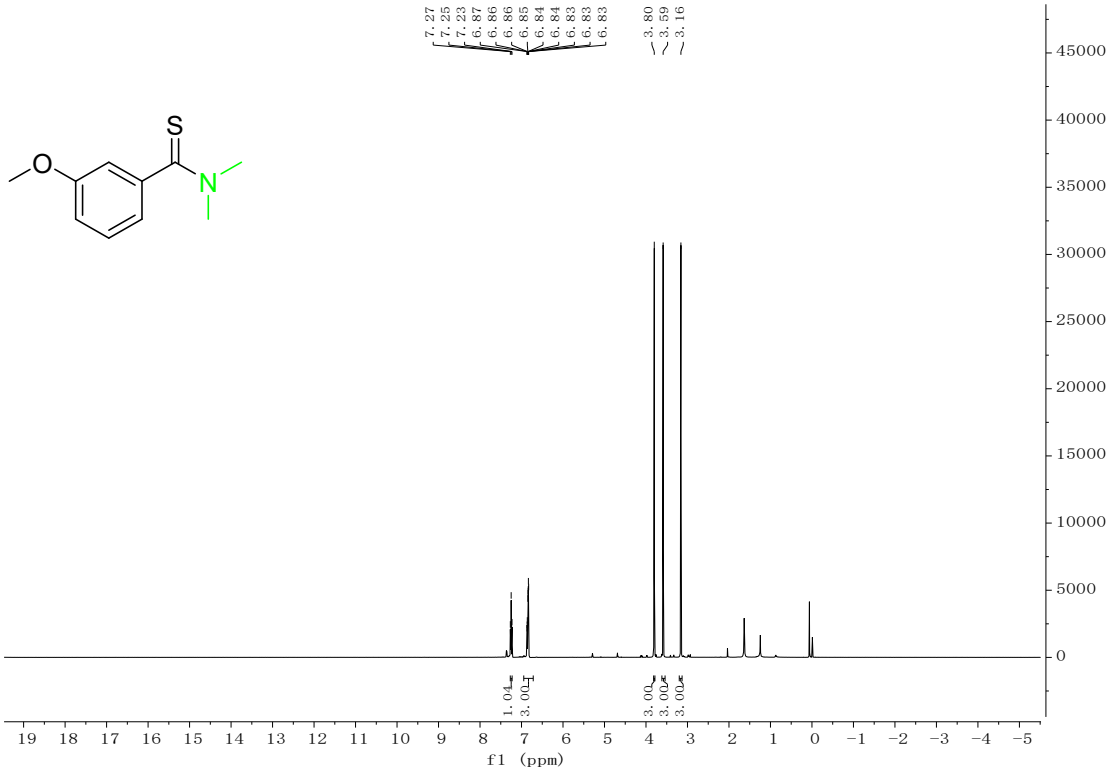


^{13}C NMR

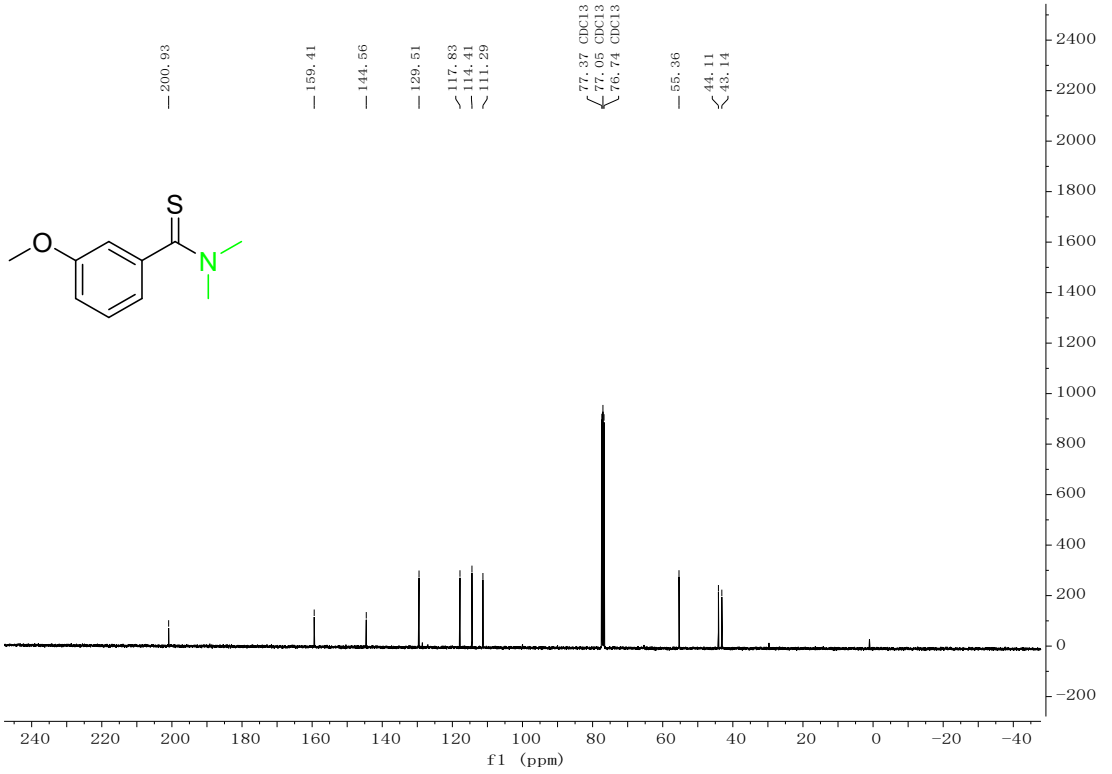


3-Methoxy-N,N-dimethylbenzothioamide

^{1}H NMR

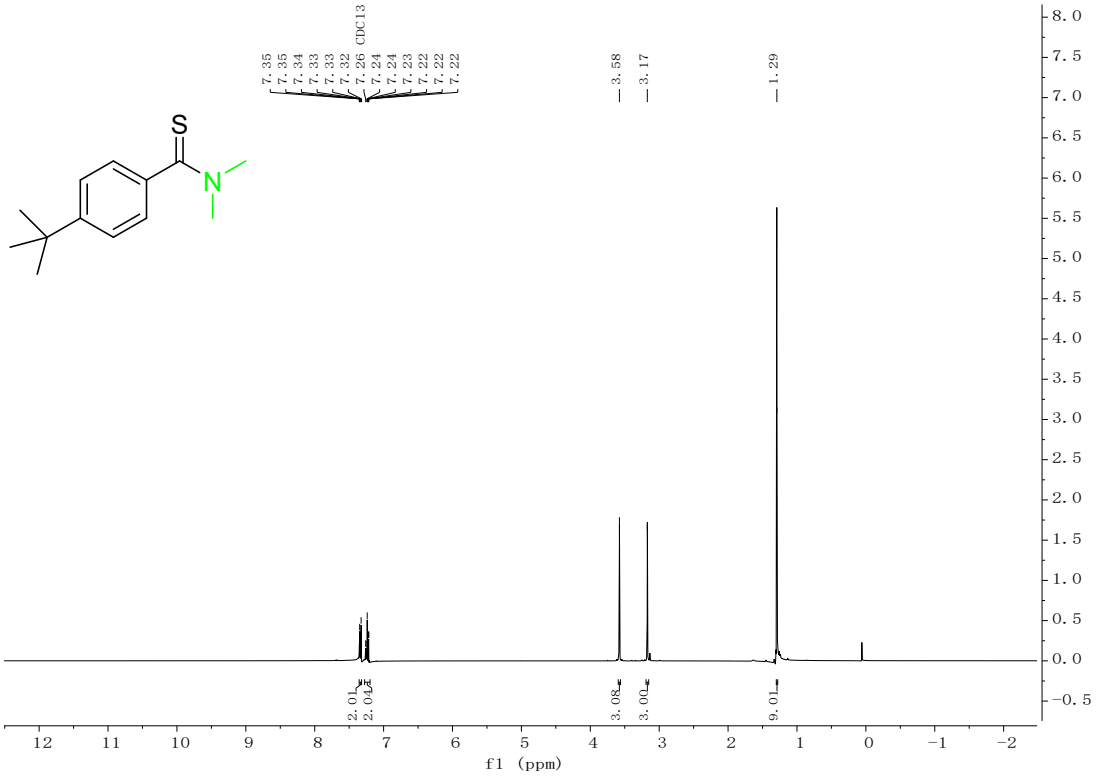


^{13}C NMR



4-*tert*-Dutyl-N,N-dimethylbenzothioamide

^{1}H NMR



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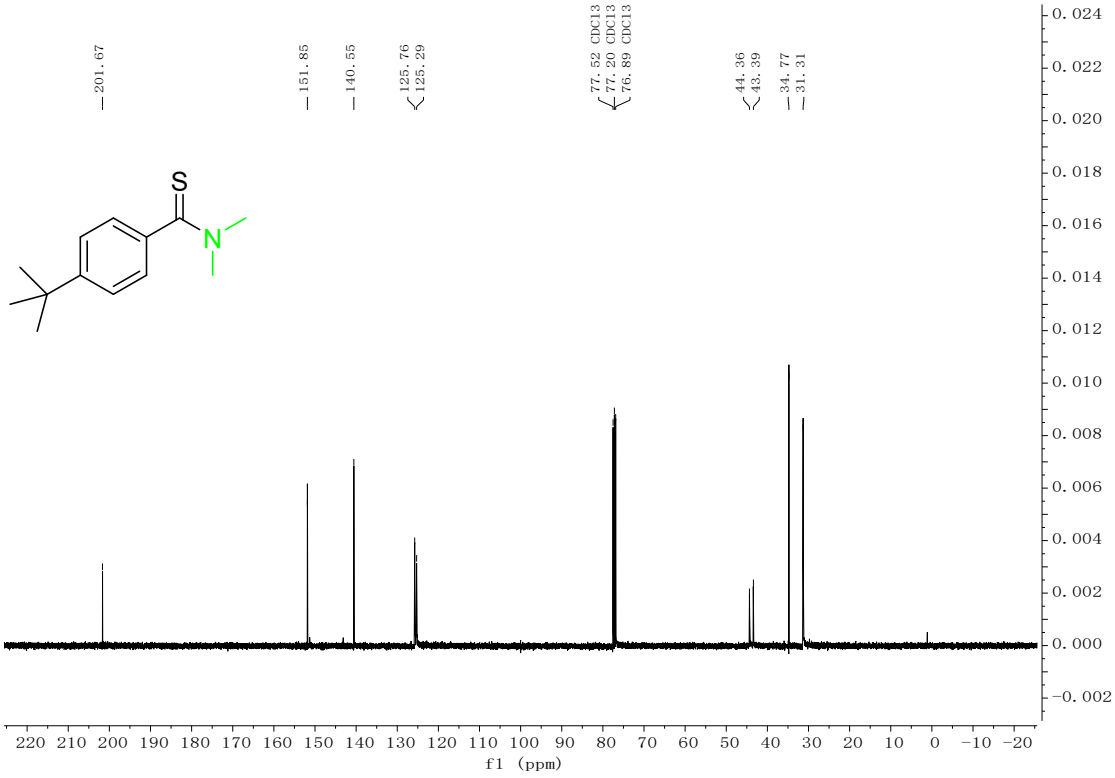
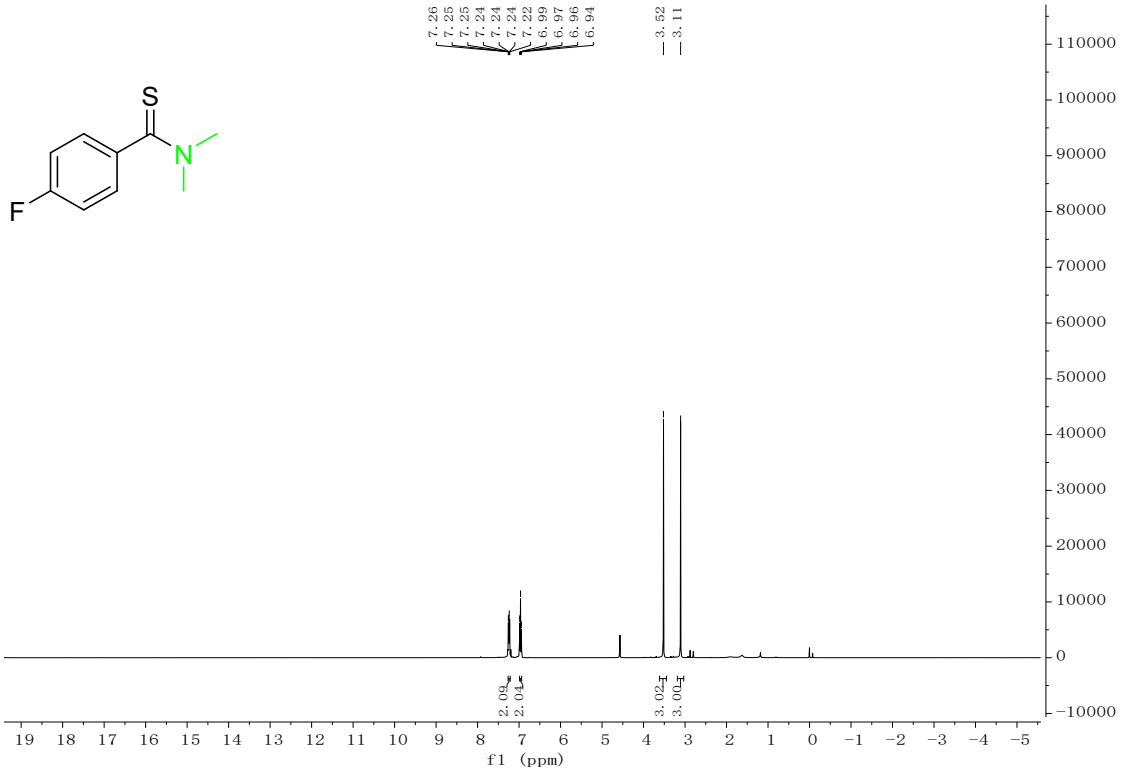


4-Fluoro-N,N-dimethylbenzothioamide

^{1}H NMR



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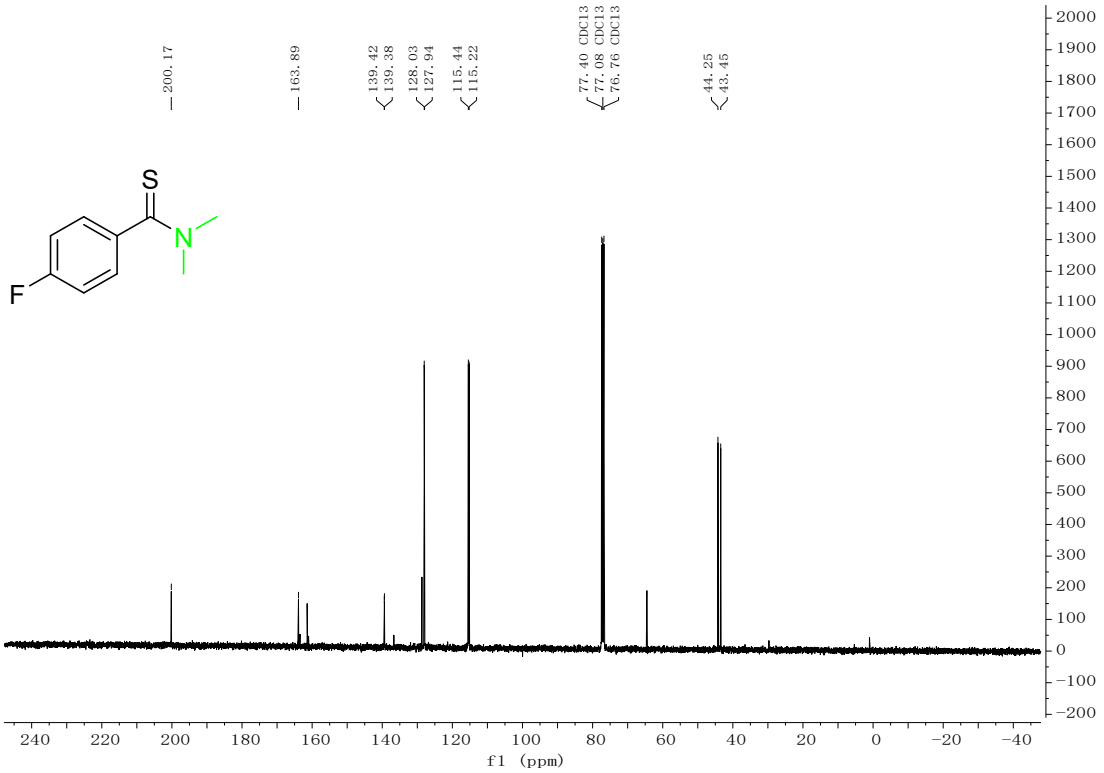
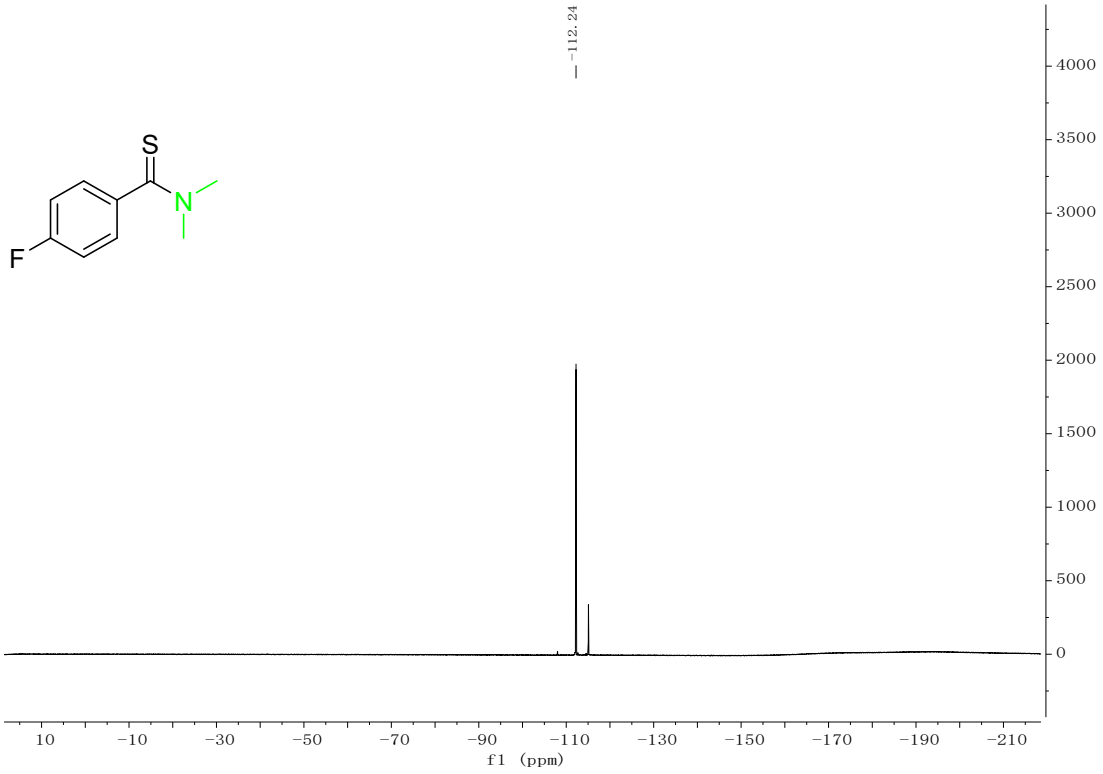


^{19}F NMR


-112.24
S
N
F
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3500
3000
2500
2000
1500
1000
500
0
10
−10
−30
−50
−70
−90
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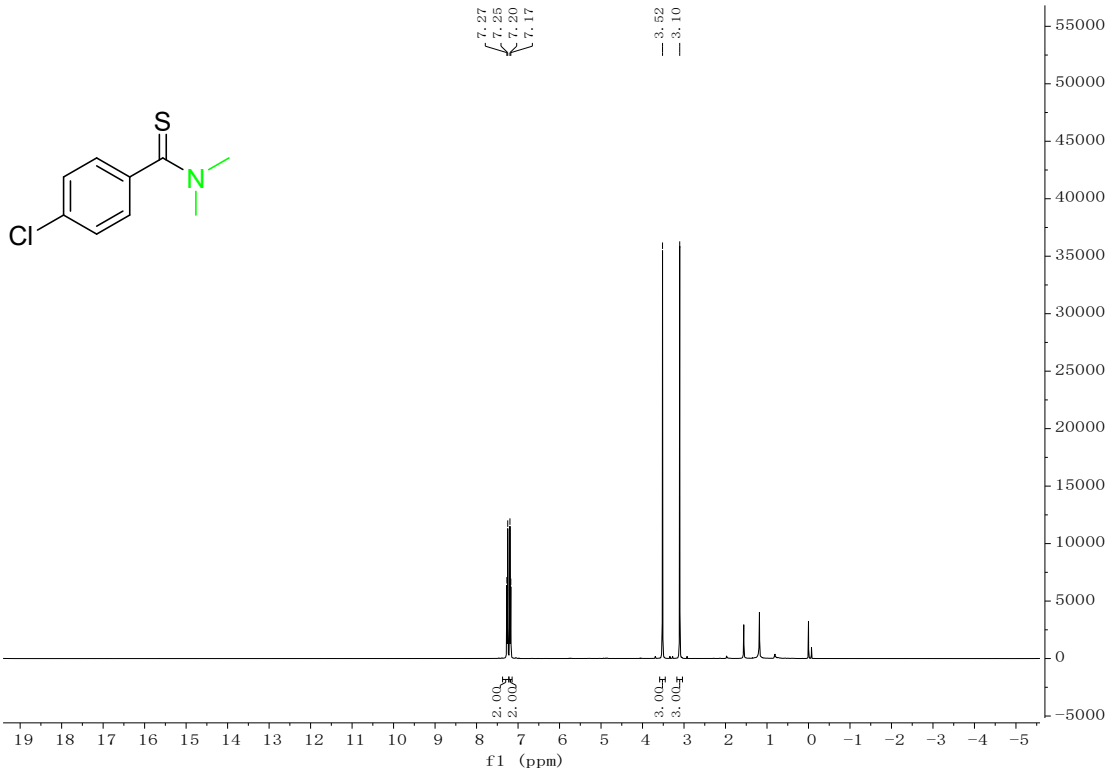
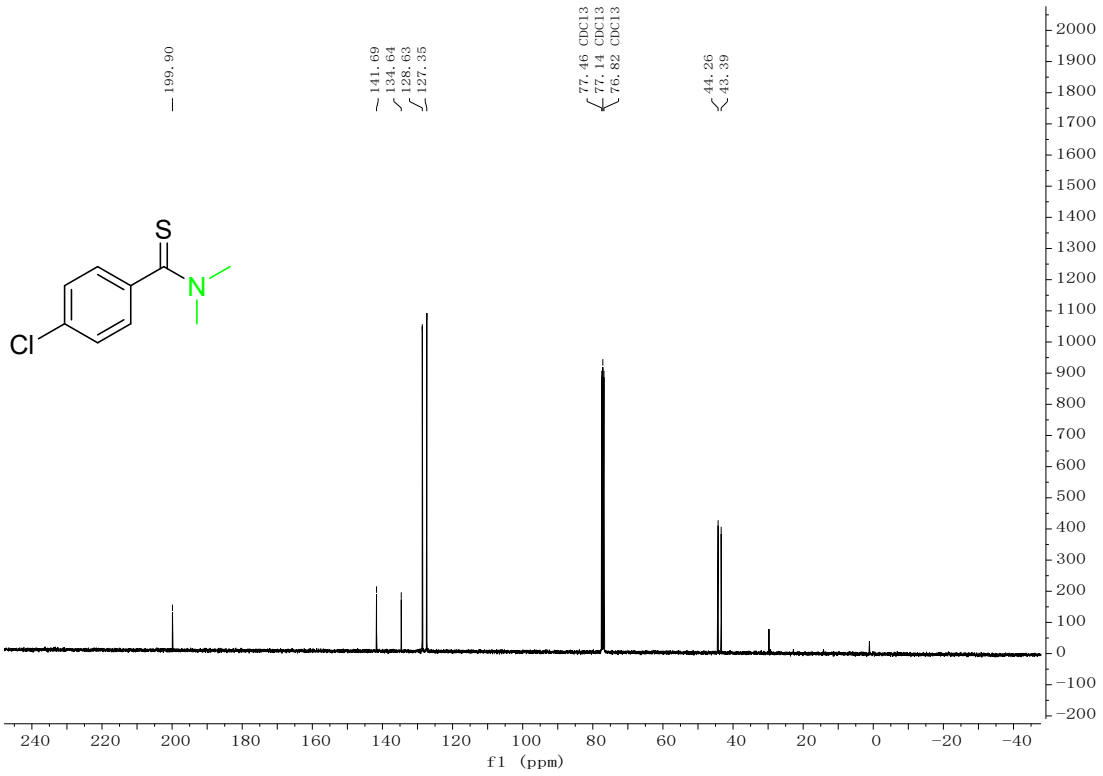
−150
−170
−190
−210
f1 (ppm)

4-Chloro-N,N-dimethylbenzothioamide

^{1}H NMR

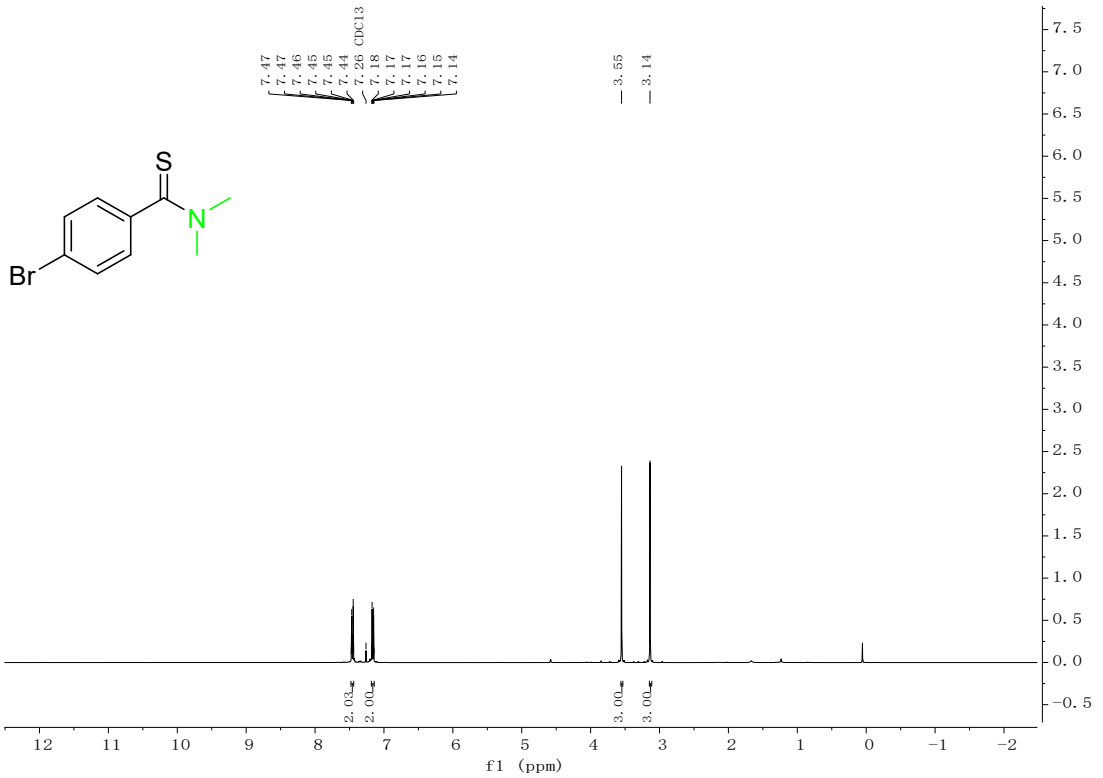


^{13}C NMR

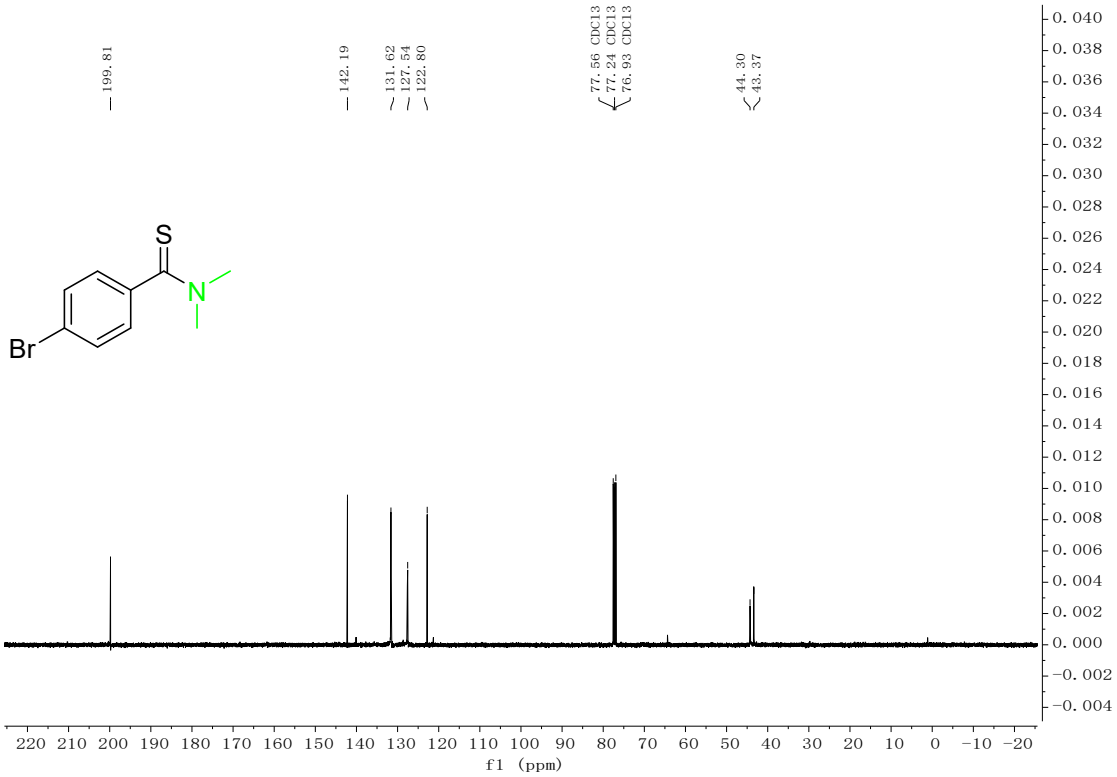


4-Bromo-N,N-dimethylbenzothioamide

^{1}H NMR

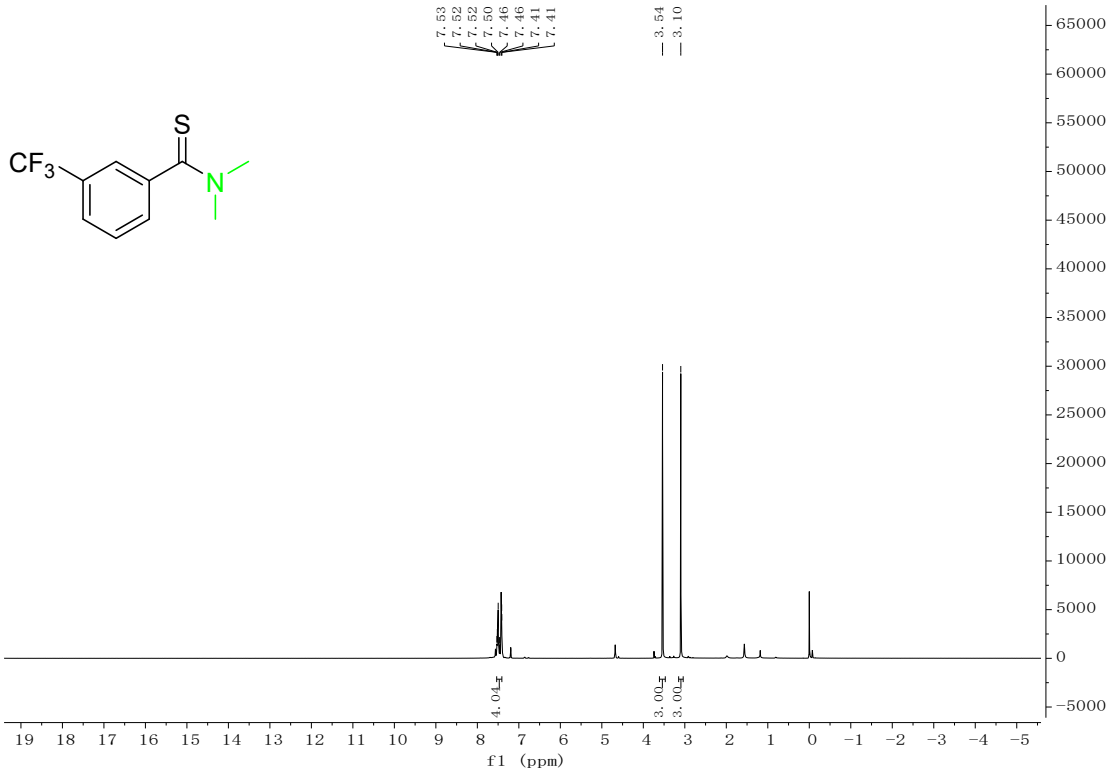


^{12}C NMR



N,N-Dimethyl-3-(trifluoromethyl)benzothioamide

^{1}H NMR



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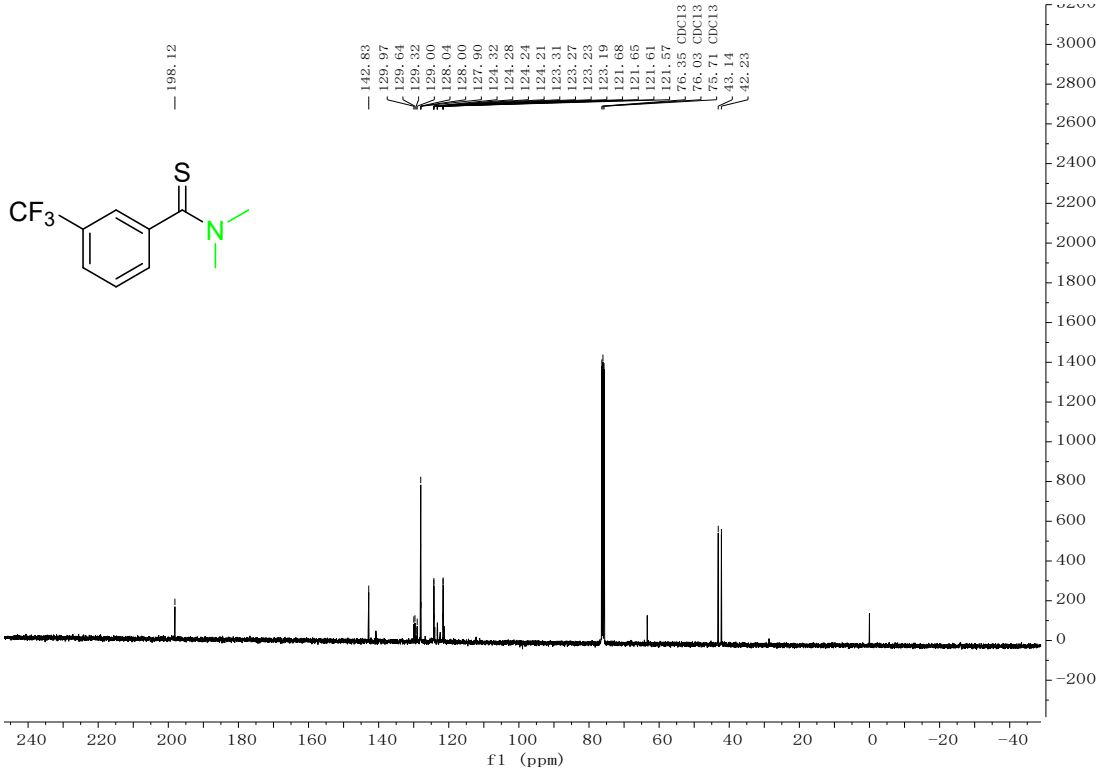
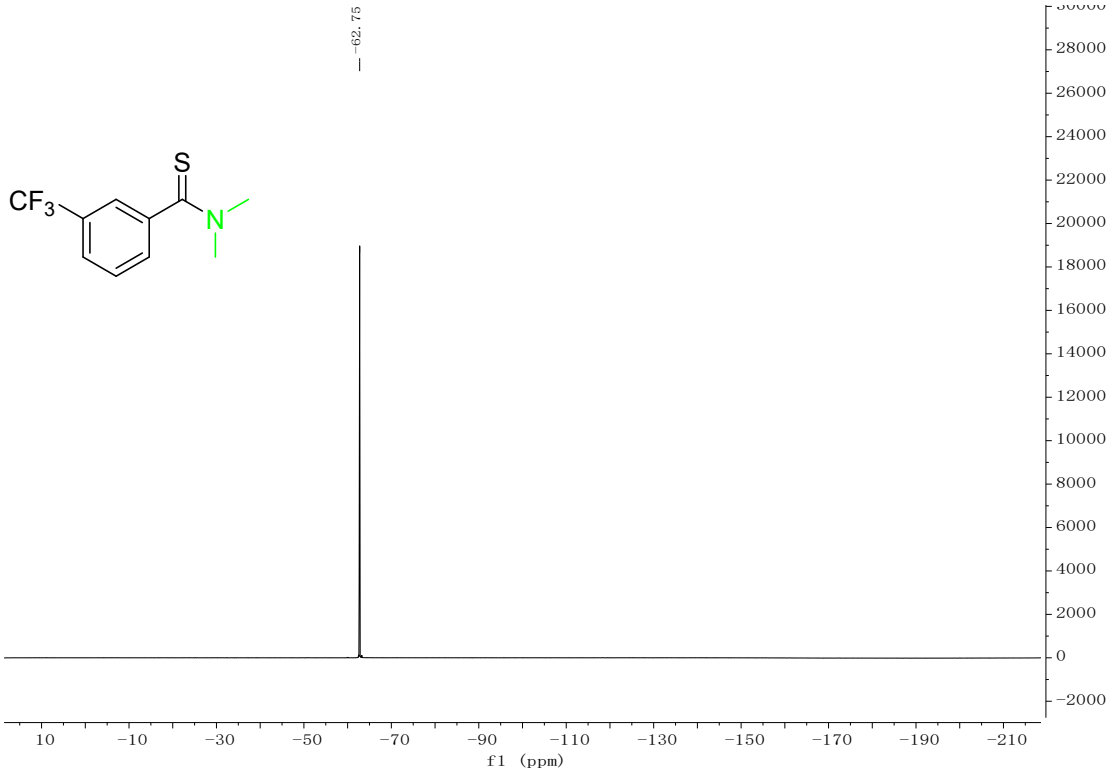
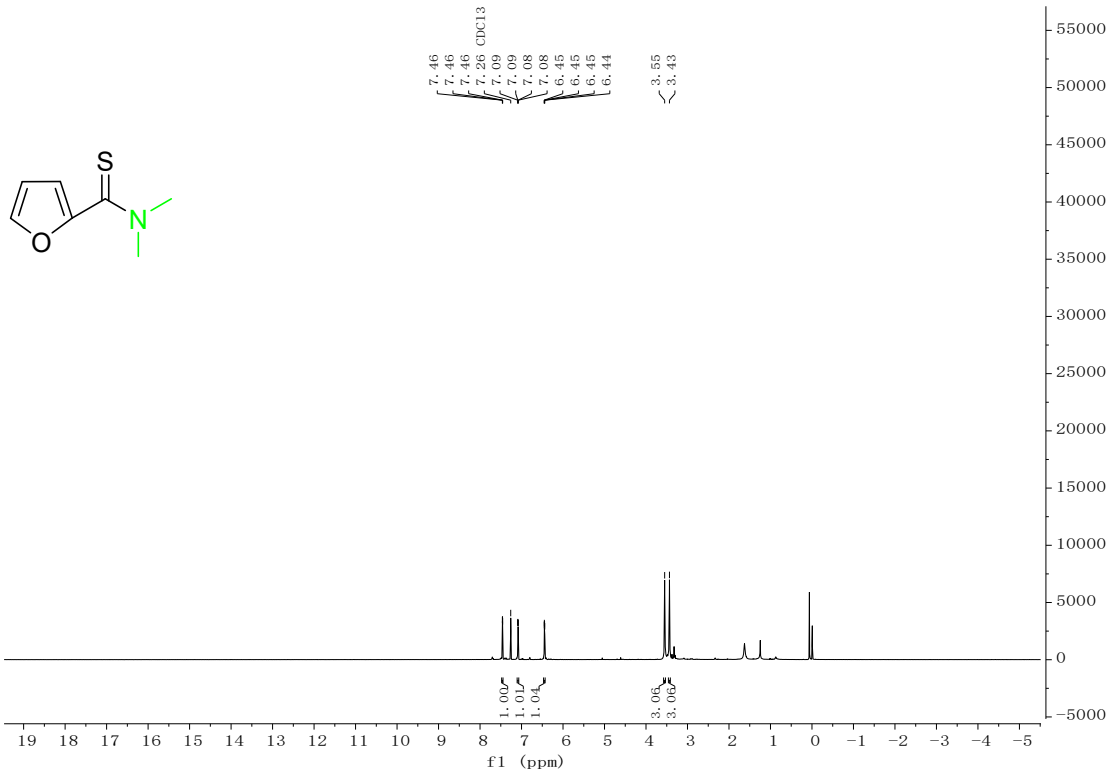


^{19}F NMR

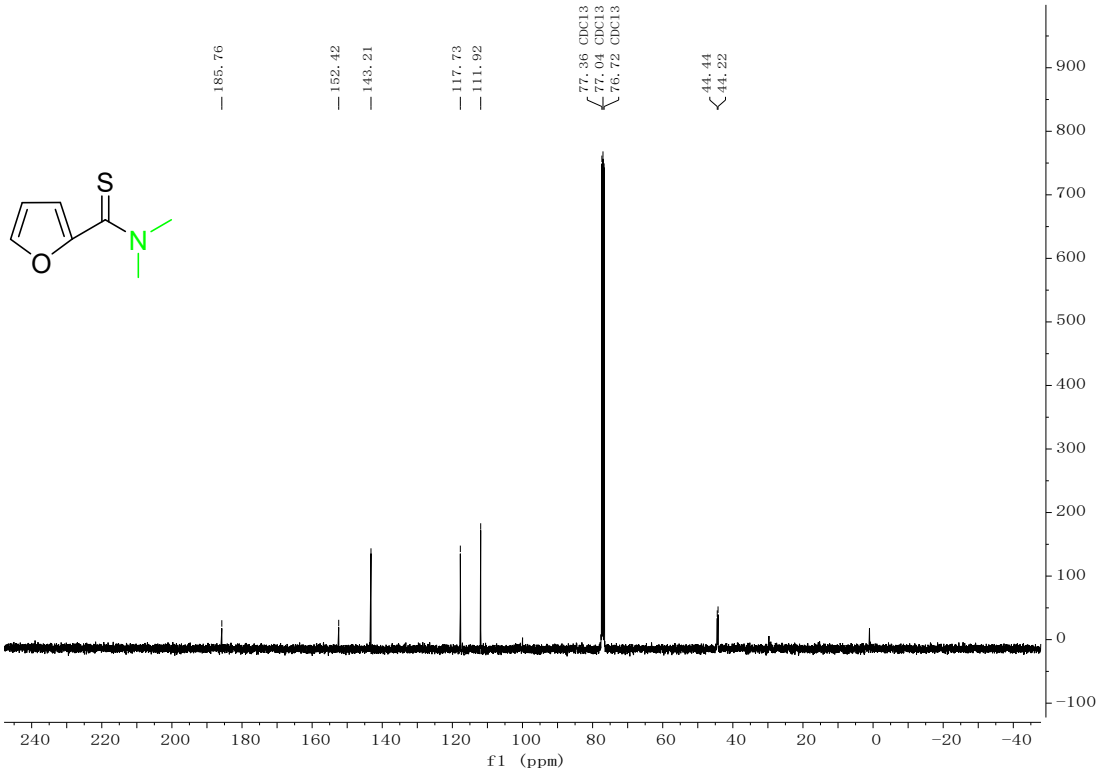


N,N-Dimethylfuran-2-carbothioamide

^{1}H NMR

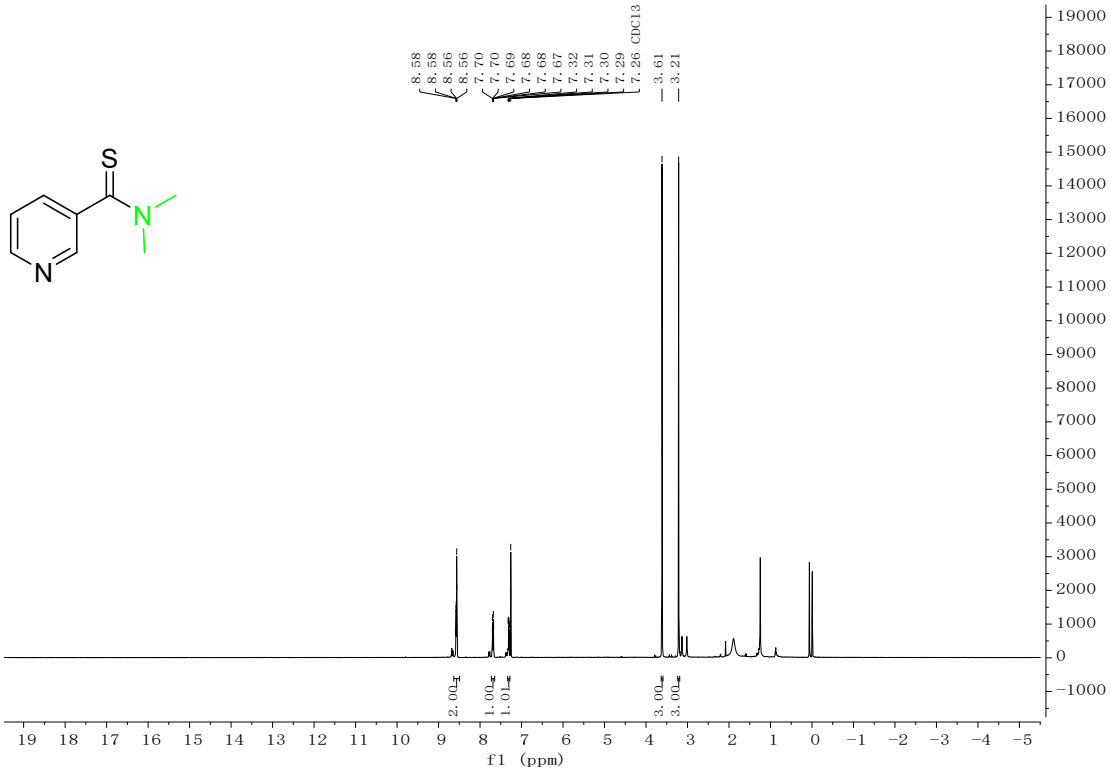


^{13}C NMR

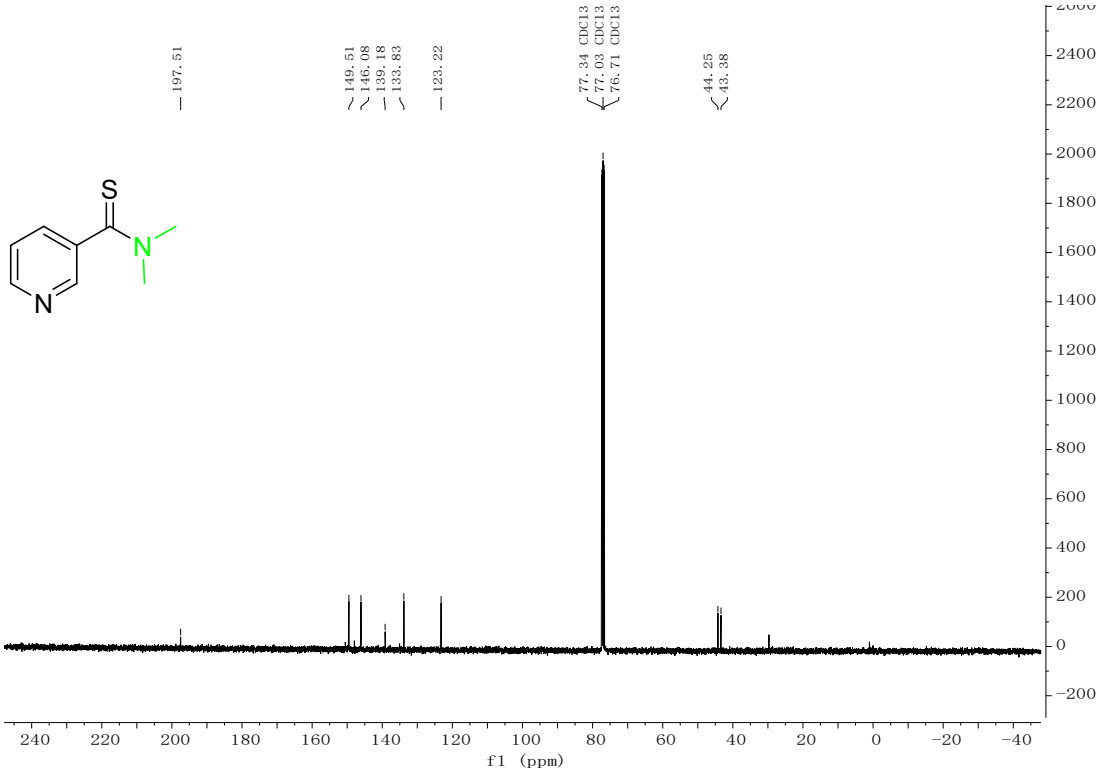


N,N-Dimethylpyridine-3-carbothioamide

^{1}H NMR

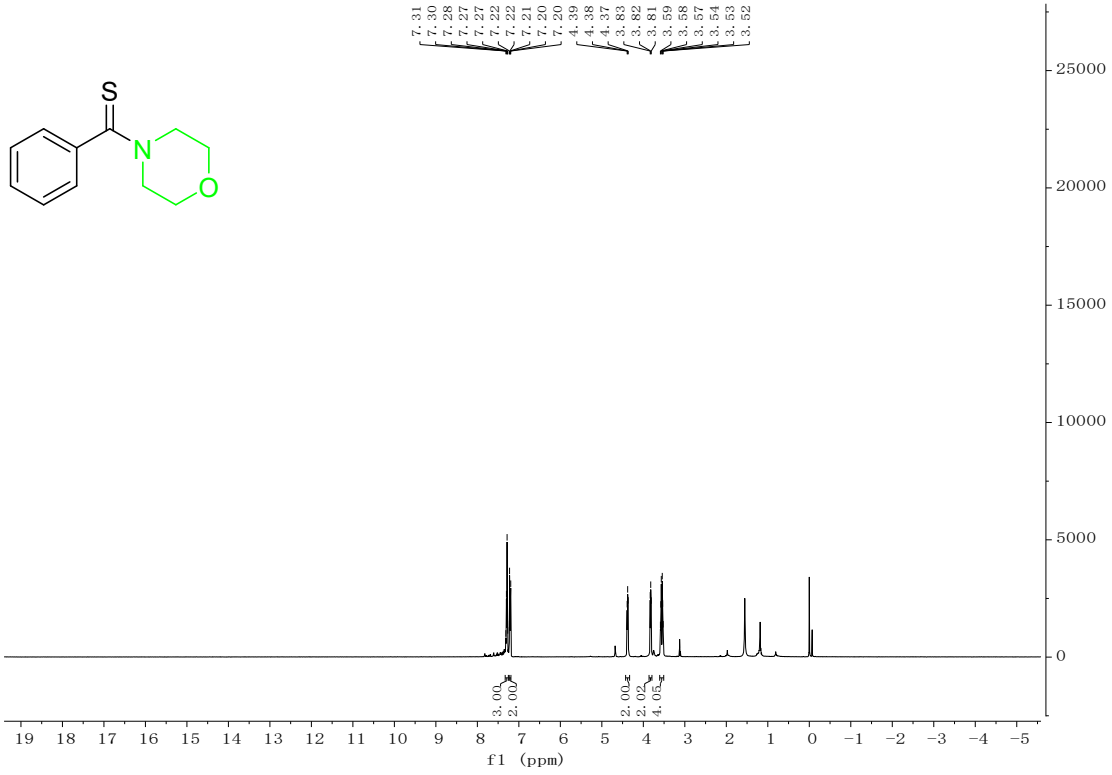


^{13}C NMR

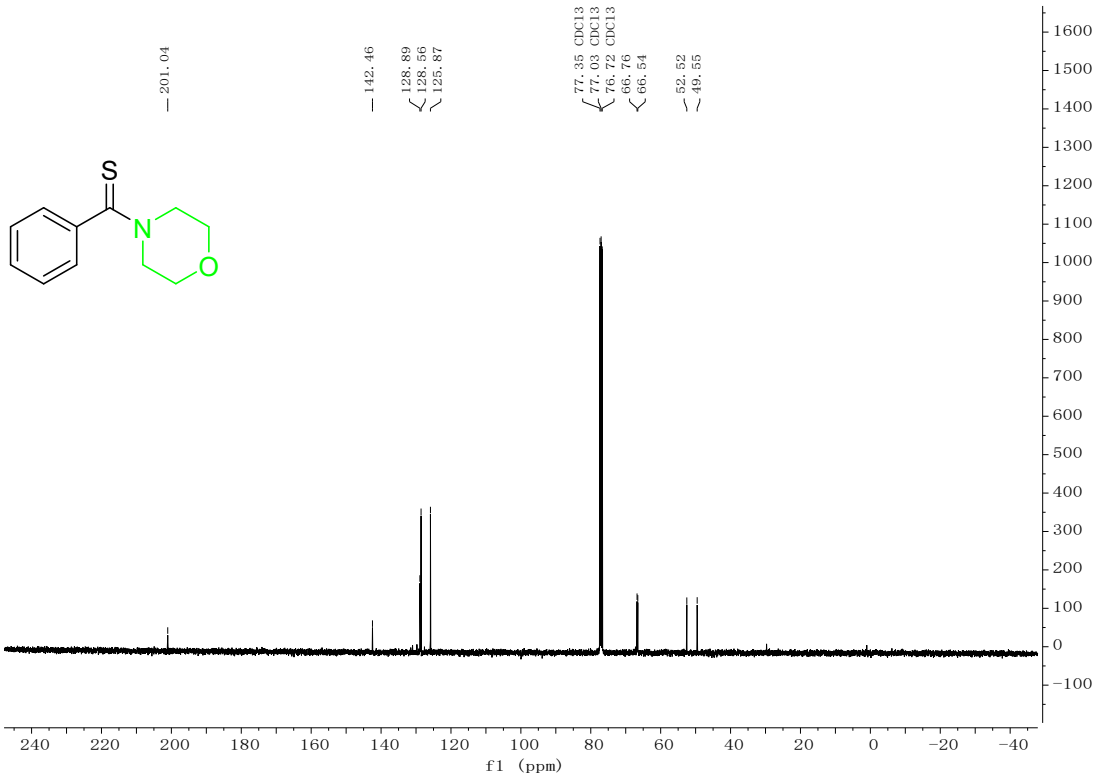


Thiobenzmorpholid

^{1}H NMR

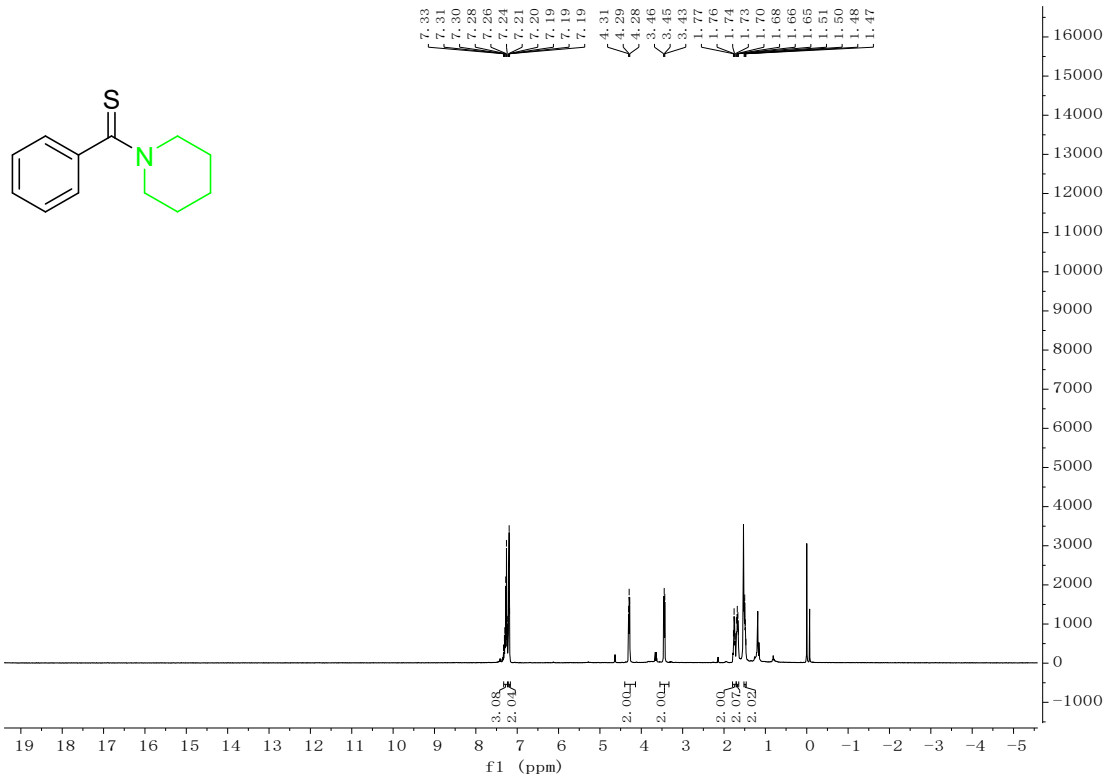


^{13}C NMR

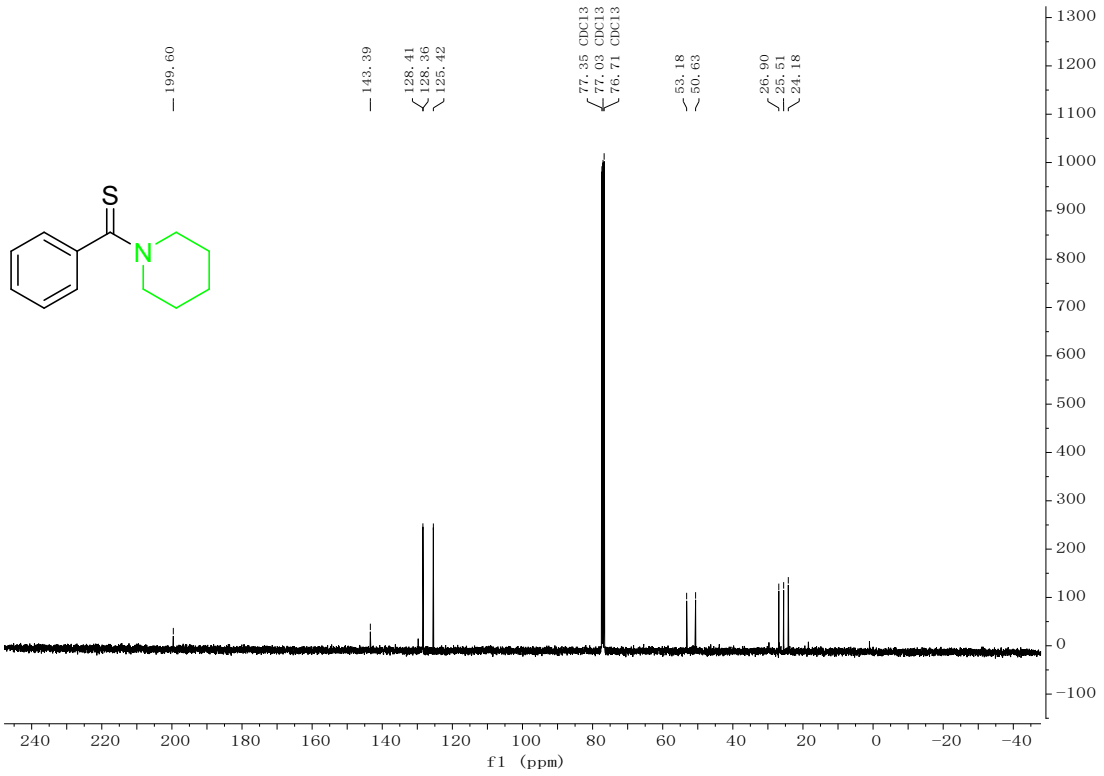


N-Thiobenzoylpiperidine

^{1}H NMR

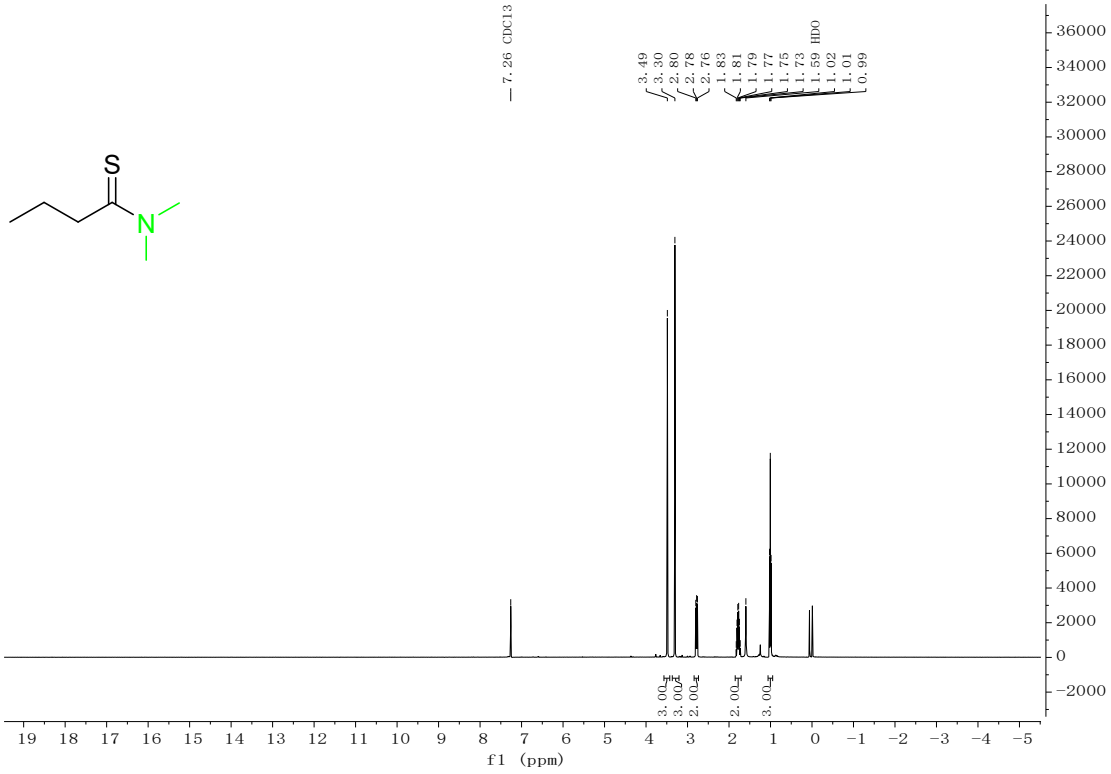


^{13}C NMR



N,N-Dimethylbutanethioamide

^{1}H NMR



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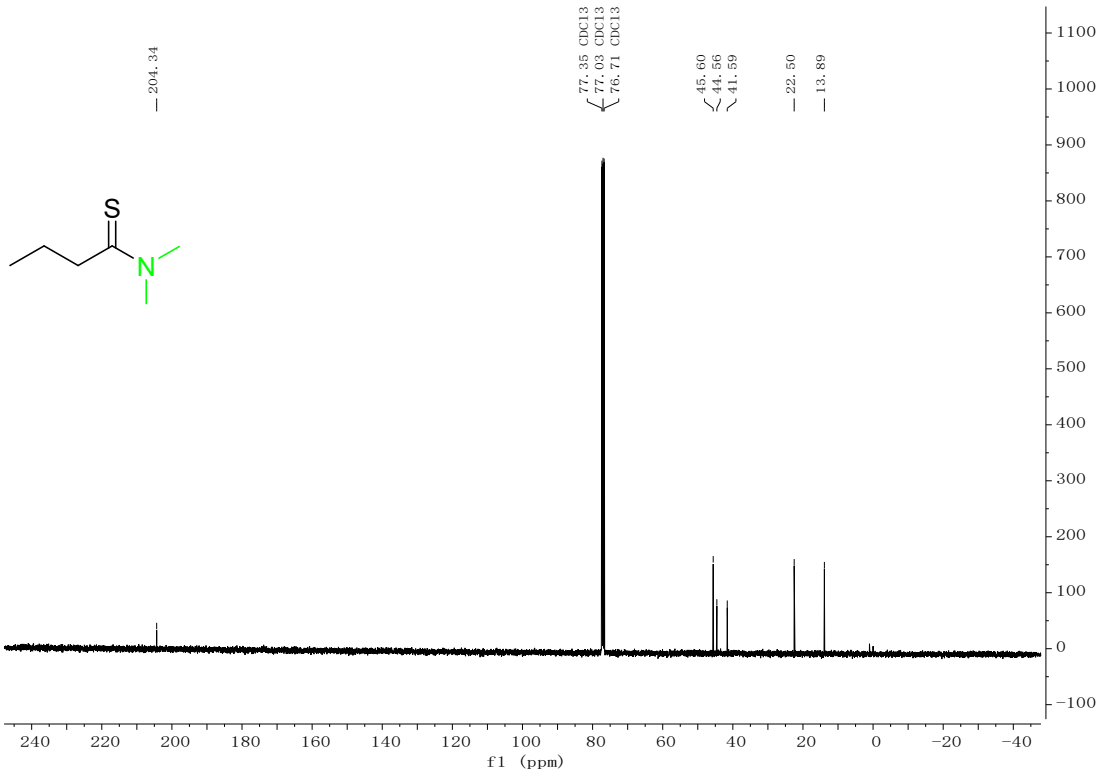
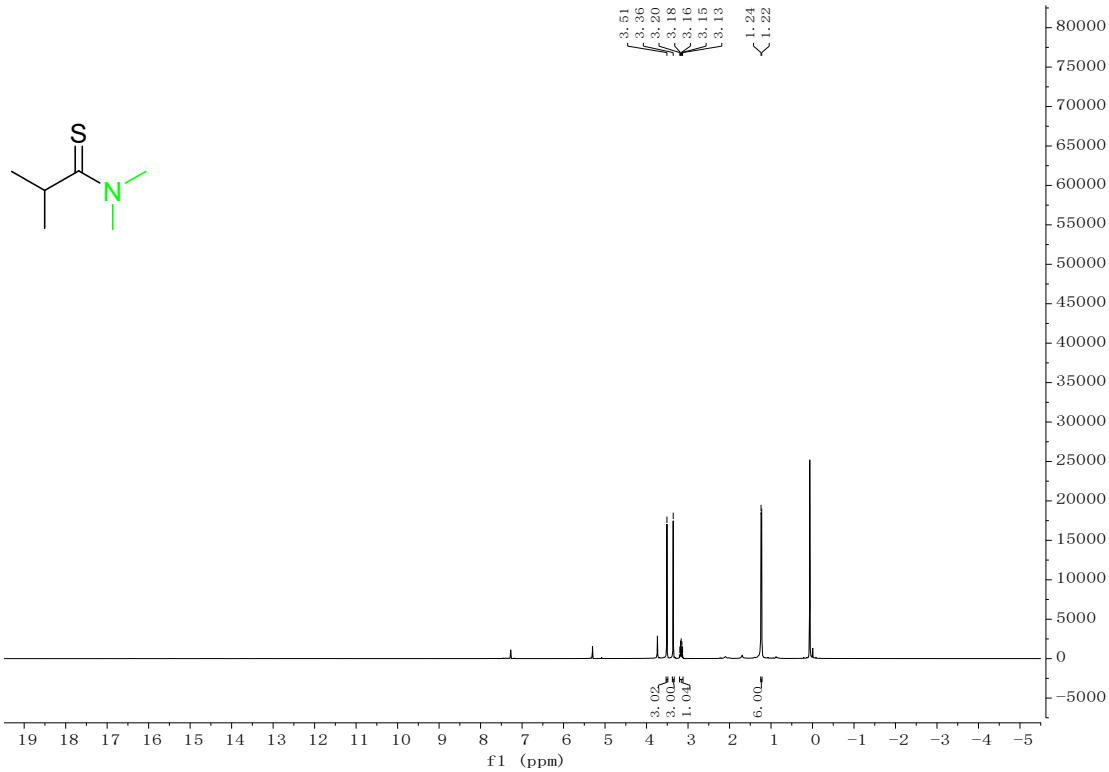


N,N,2-Trimethylpropanethioamide

^{1}H NMR



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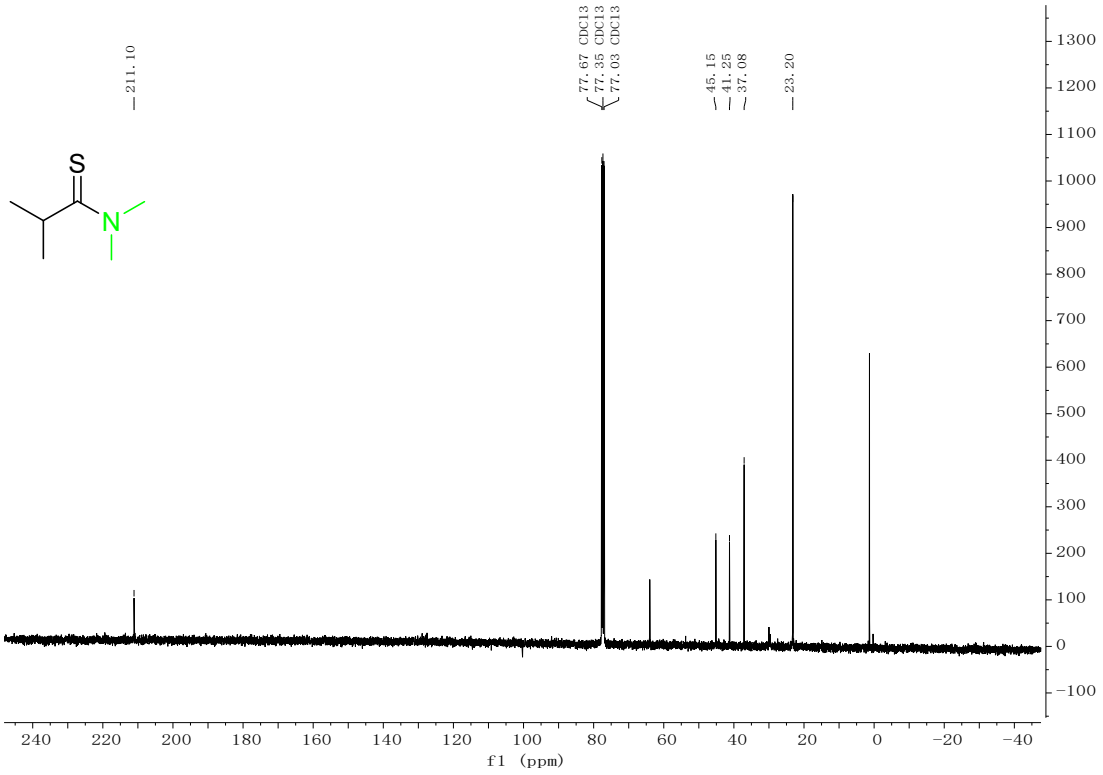
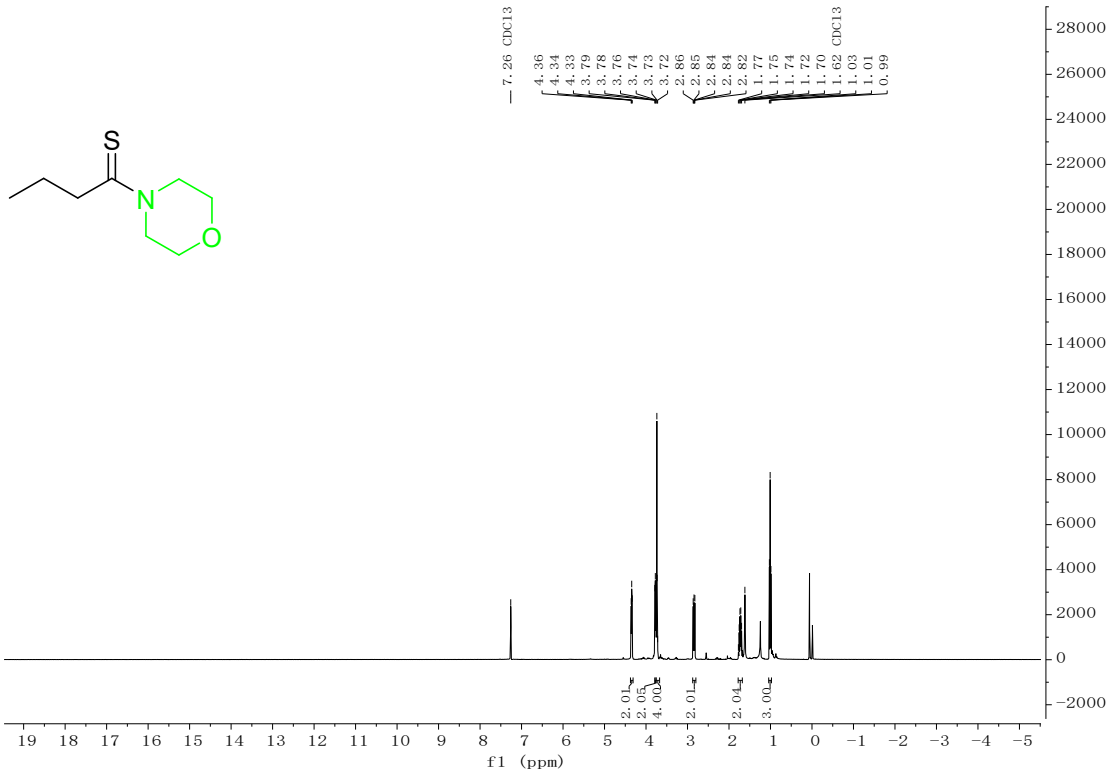
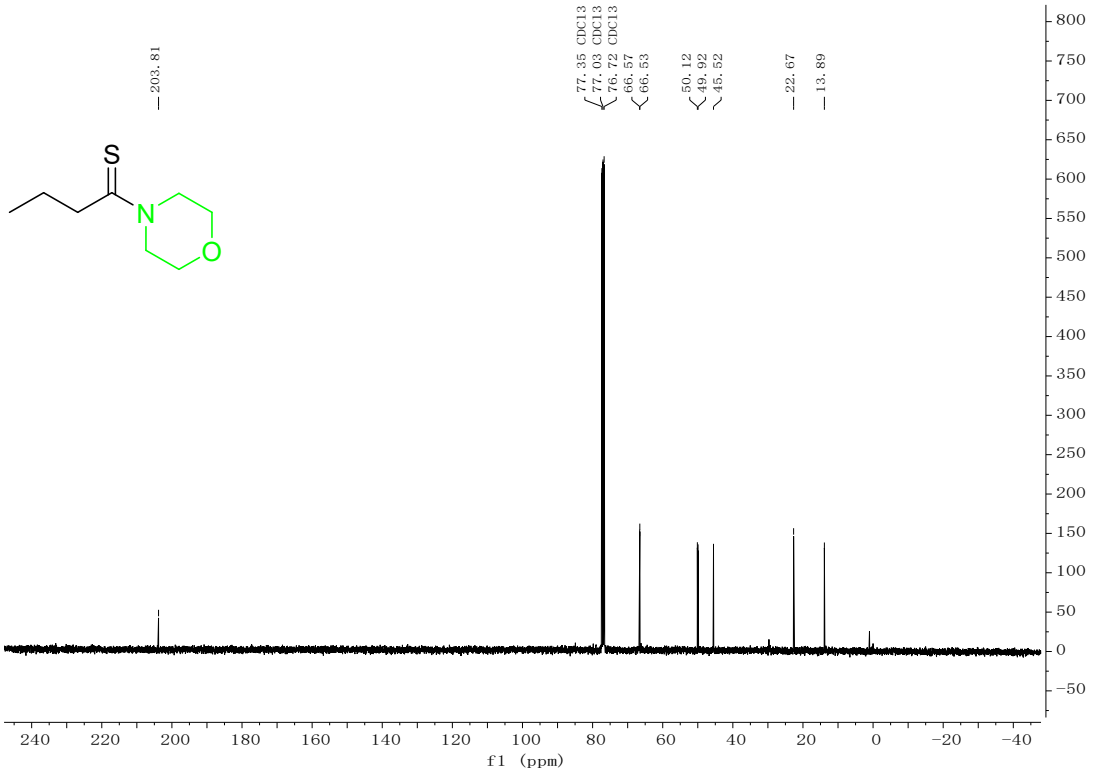


4-Thiobutyryl-morpholine

^{1}H NMR

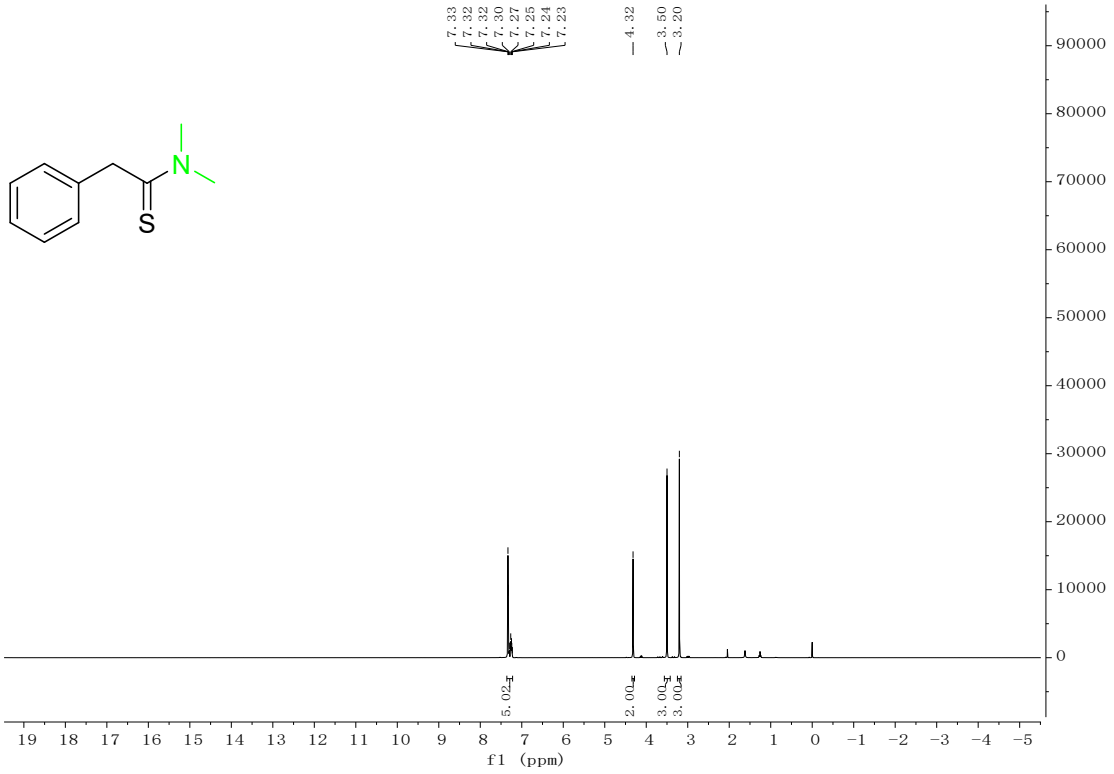


^{13}C NMR

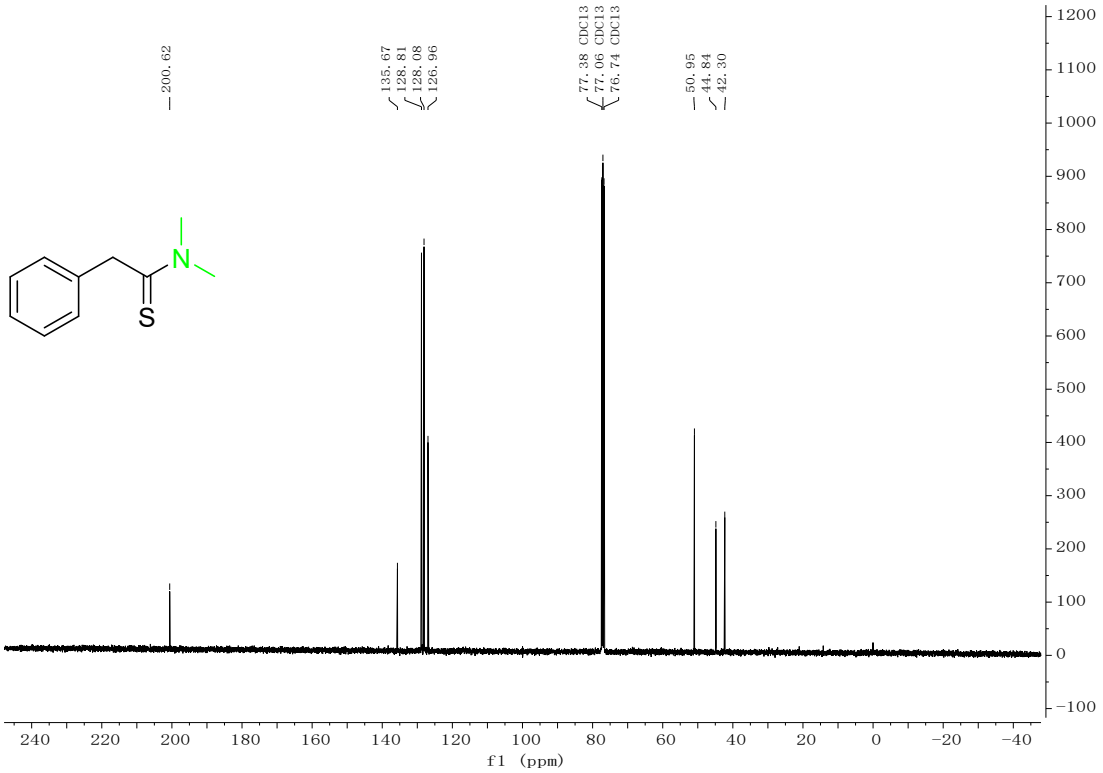


N,N-Dimethyl-2-phenylethanethioamide

^{1}H NMR

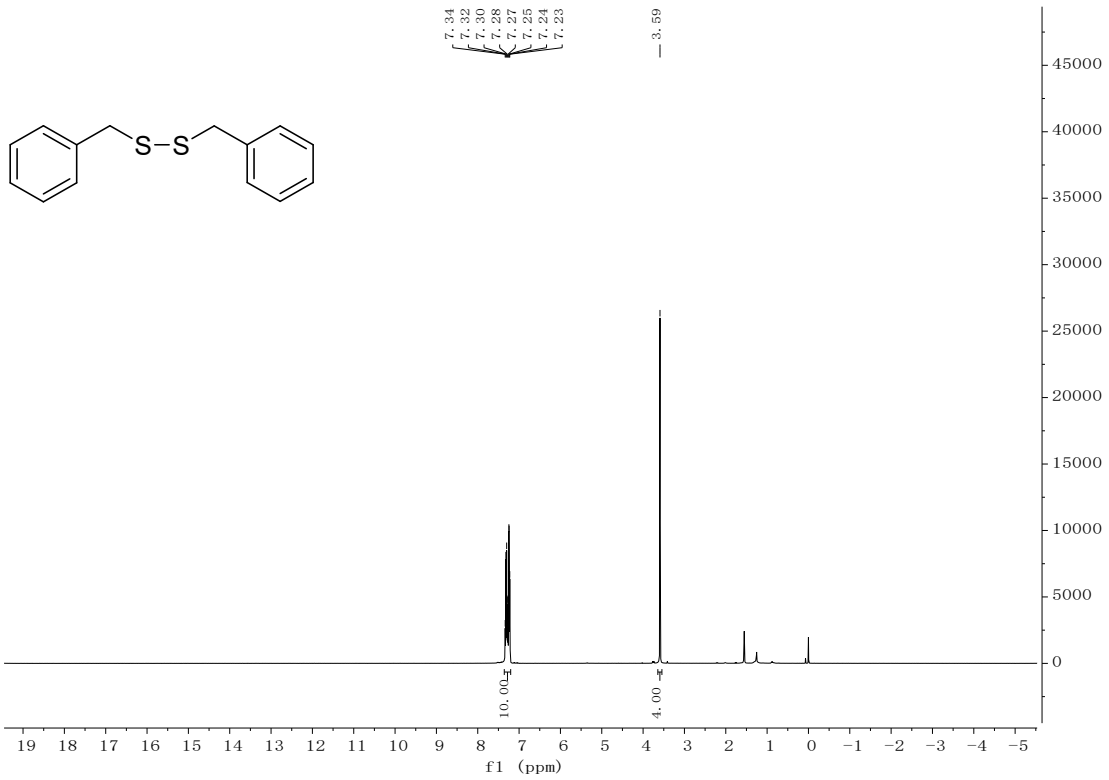


^{13}C NMR

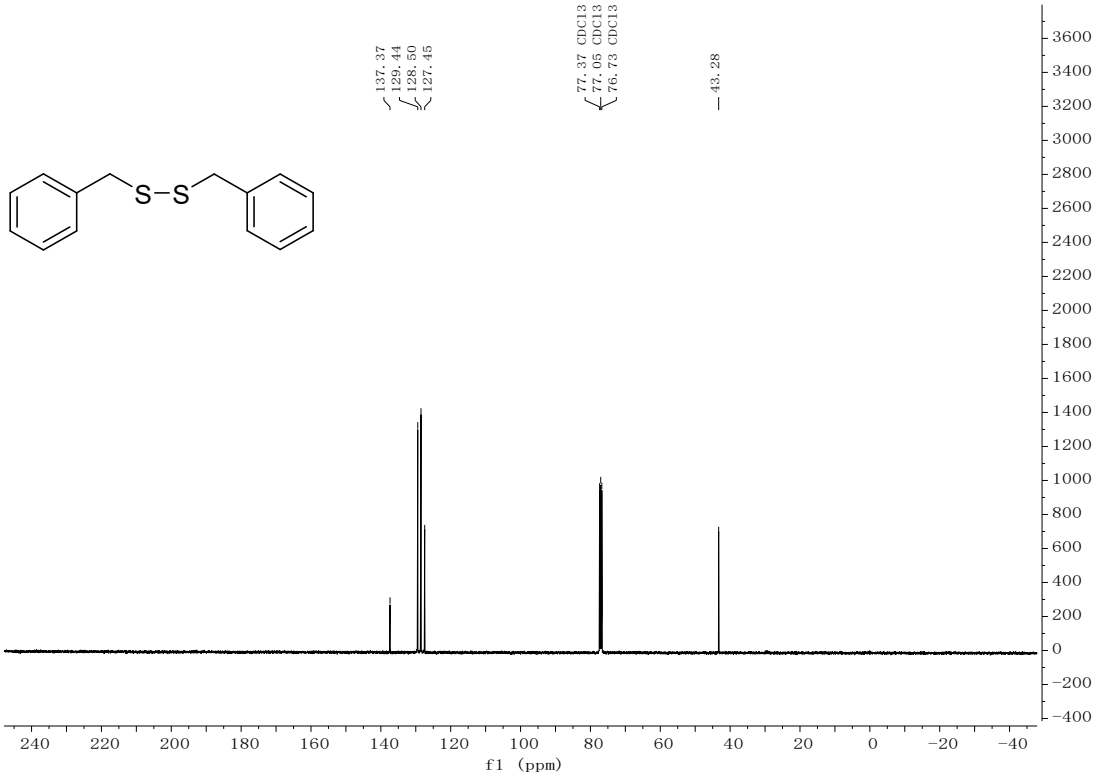


Dibenzyl disulfide

^{1}H NMR

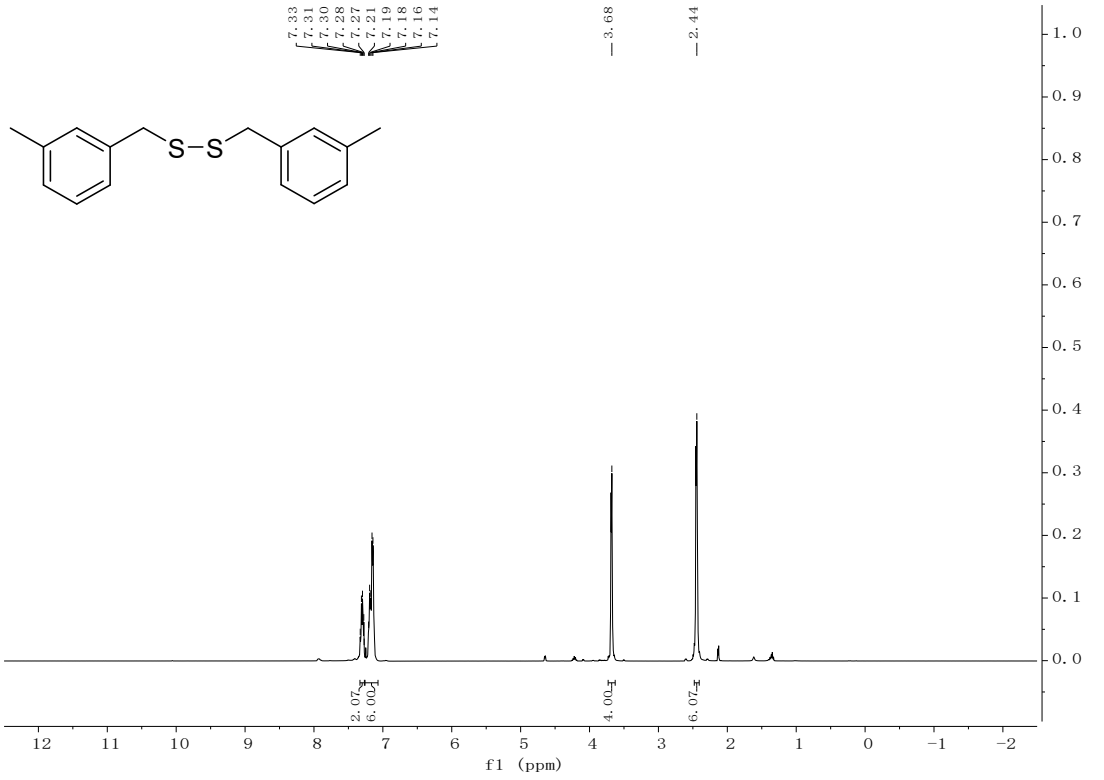


^{13}C NMR

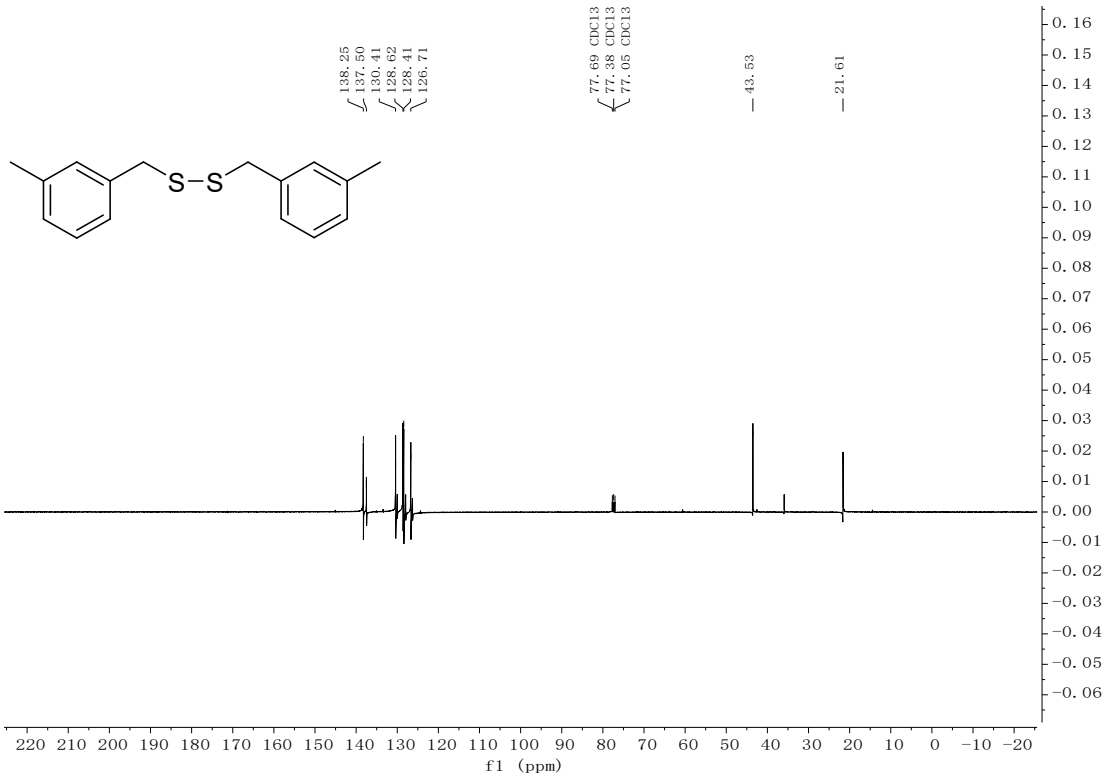


Bis(3-methylbenzyl) disulfide

^{1}H NMR

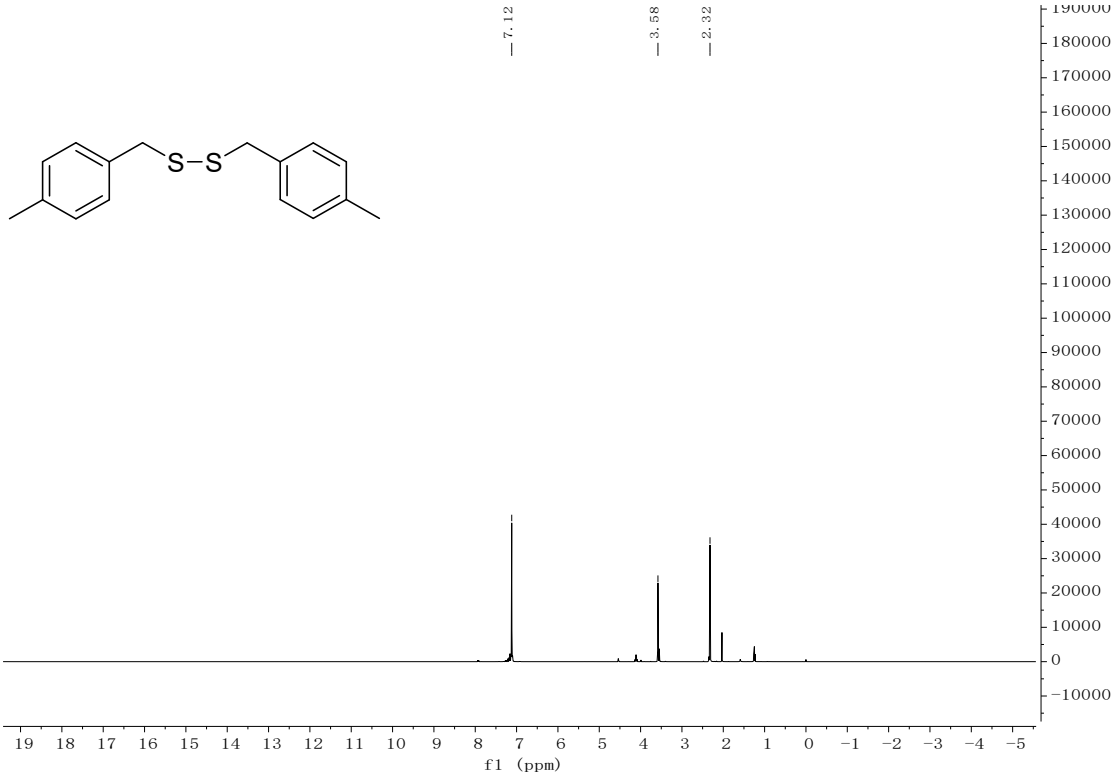


^{13}C NMR

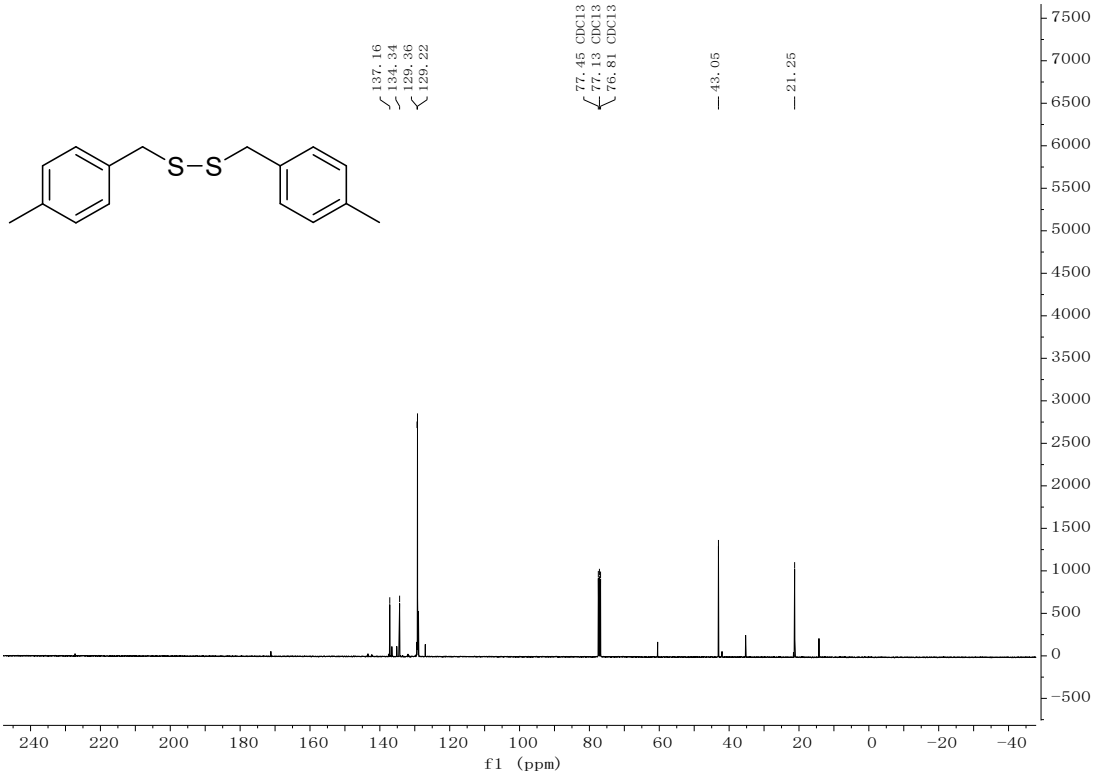


Bis(4-methylbenzyl) disulfide

^{1}H NMR

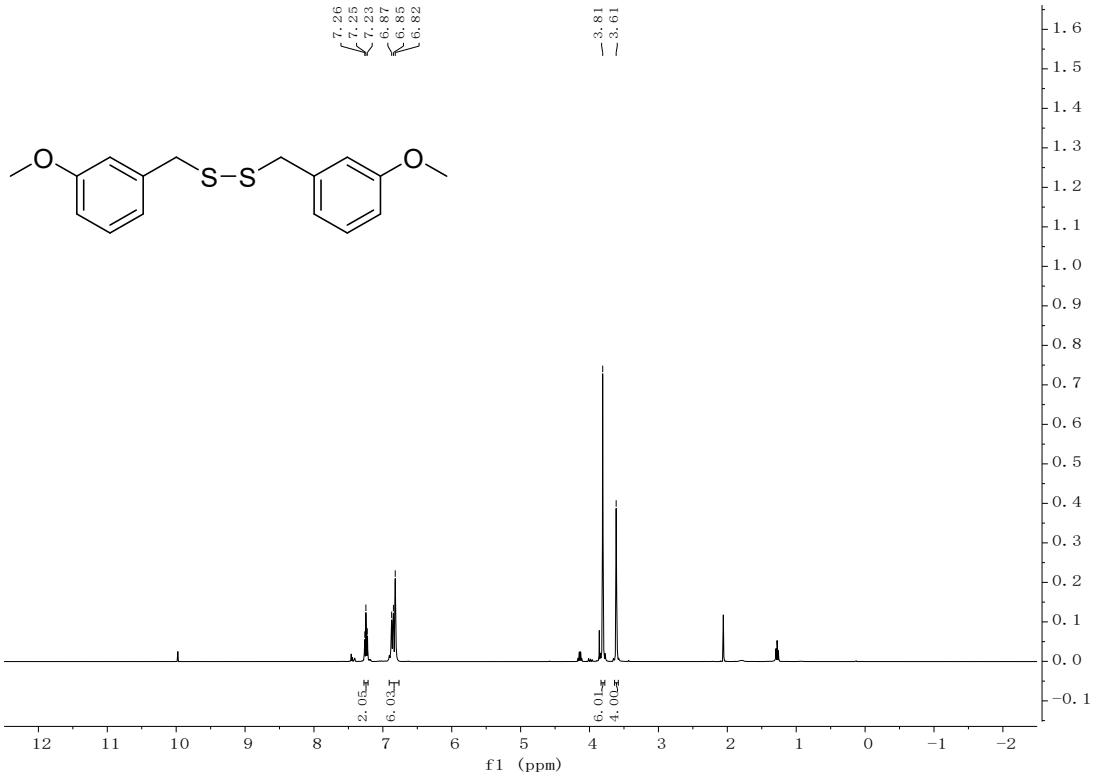


^{13}C NMR

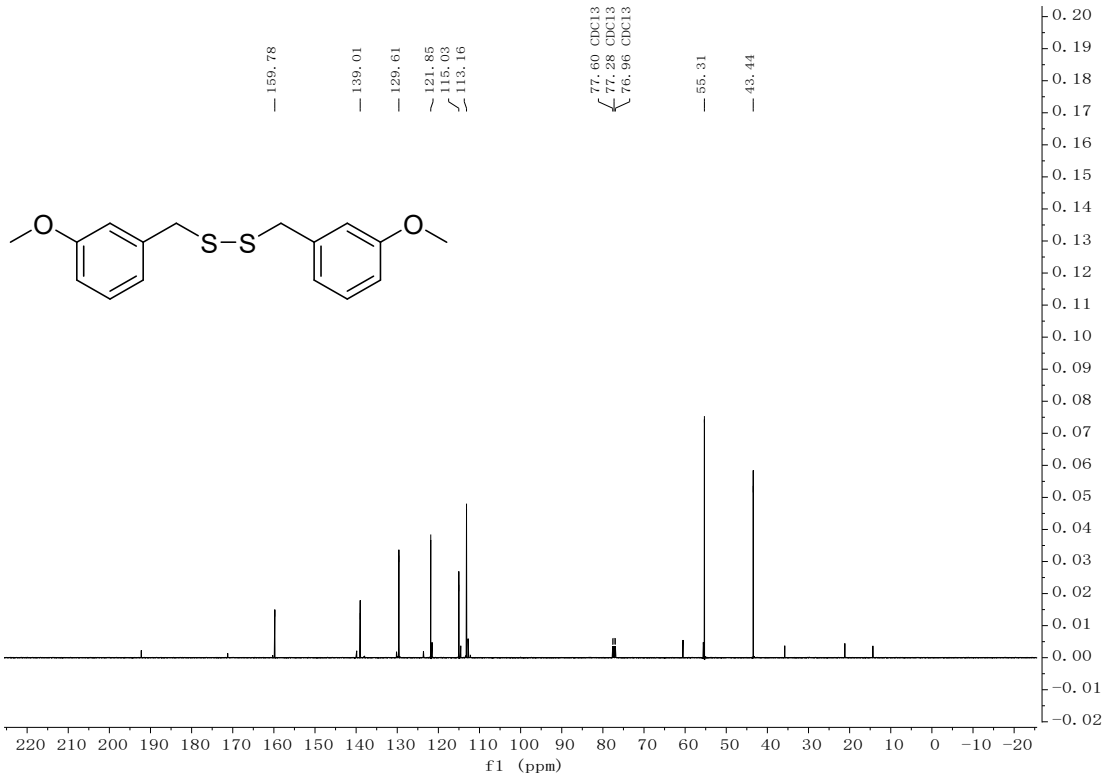


Bis(3-methoxybenzyl) disulfide

^{1}H NMR

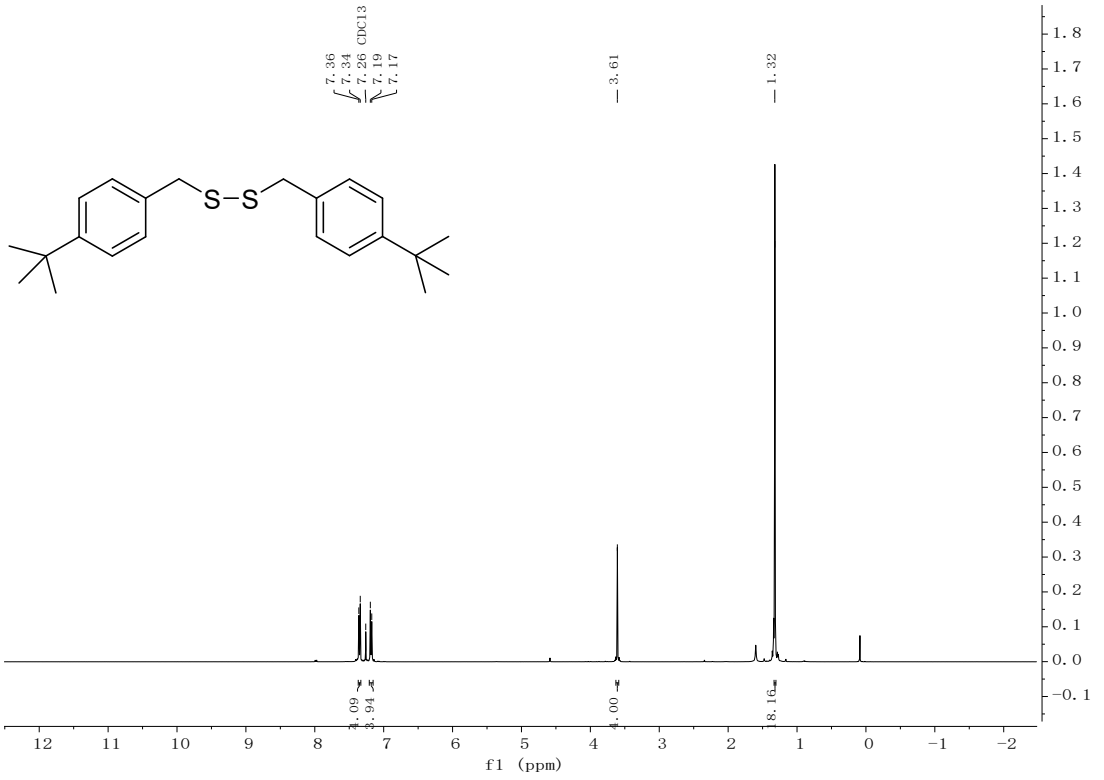


^{13}C NMR

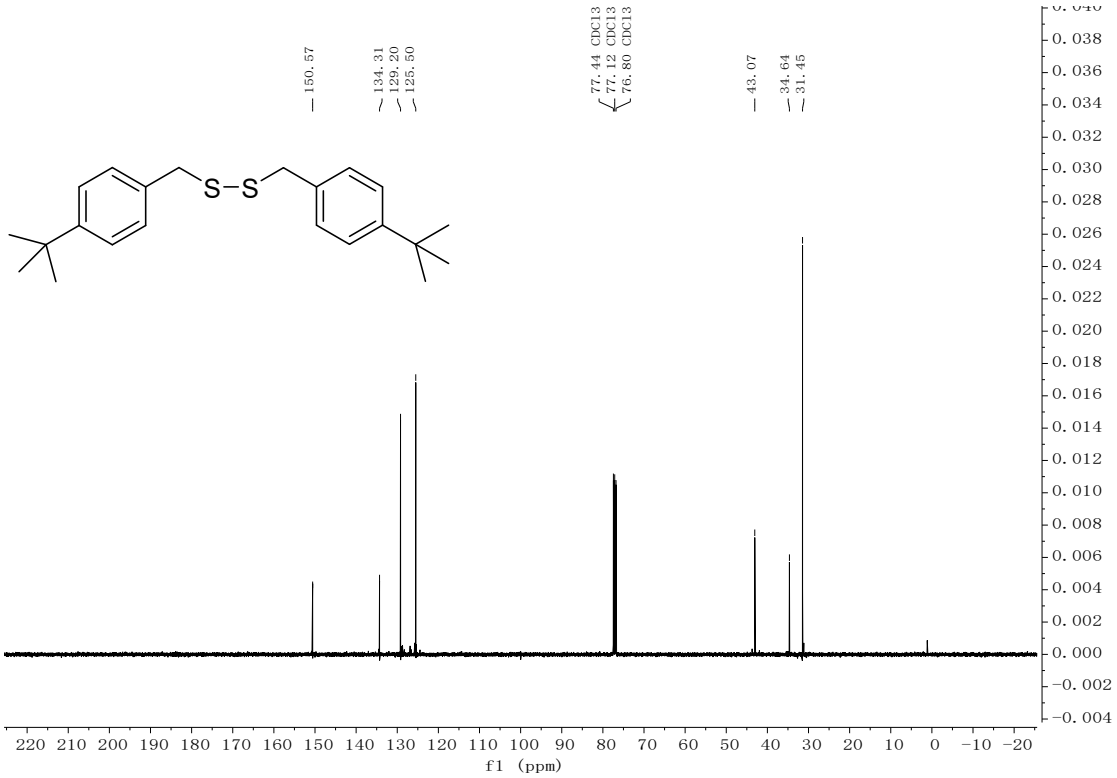


Bis(4-*tert*-butylbenzyl) disulfide

^{1}H NMR

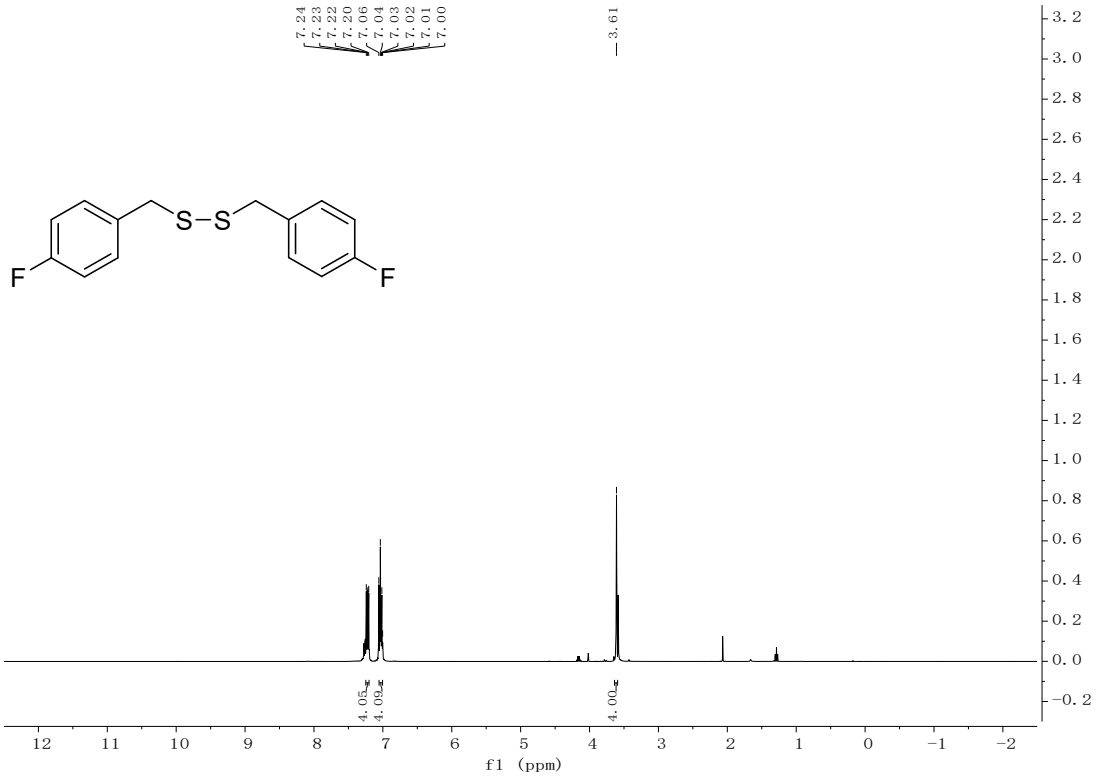


^{13}C NMR

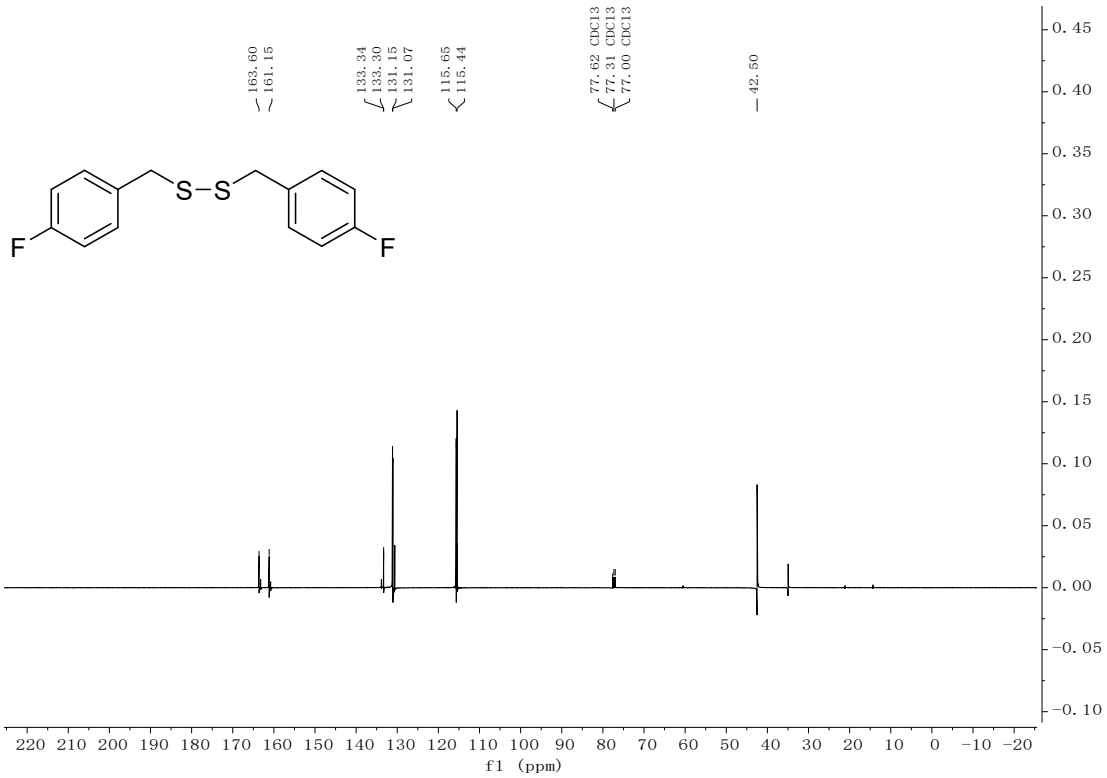


Bis(4-fluorobenzyl) disulfide

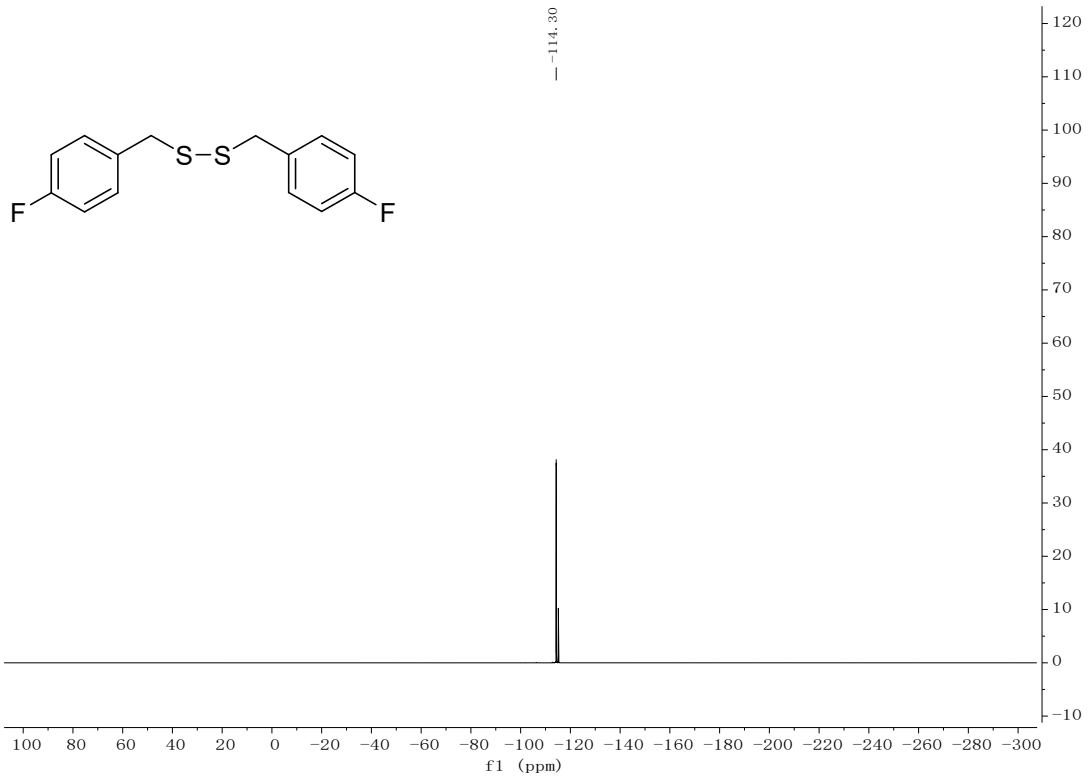
^{1}H NMR



^{13}C NMR

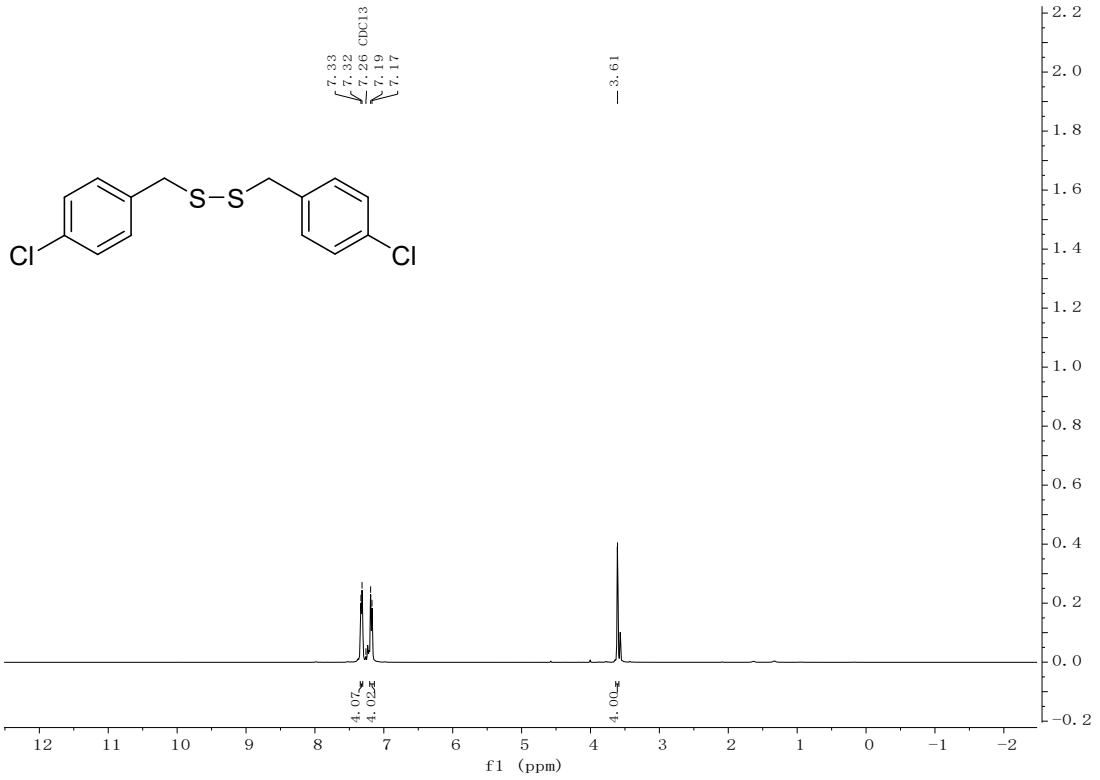


^{19}F NMR

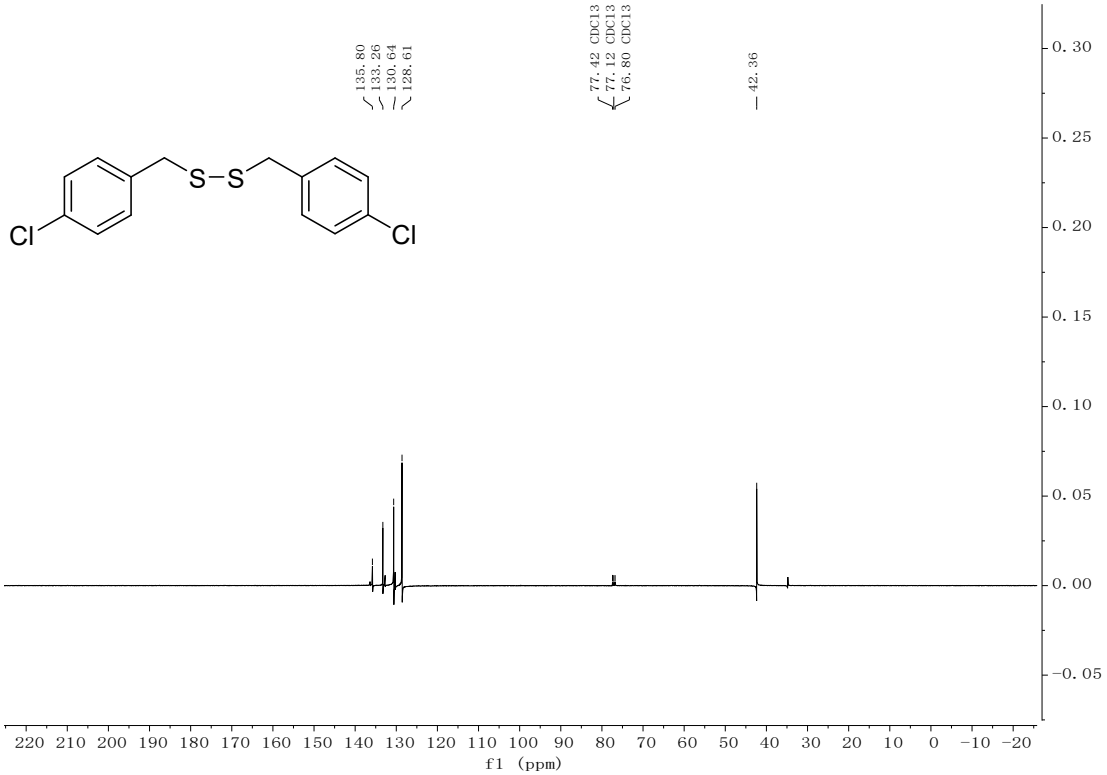


Bis(4-chlorobenzyl) disulfide

^{1}H NMR

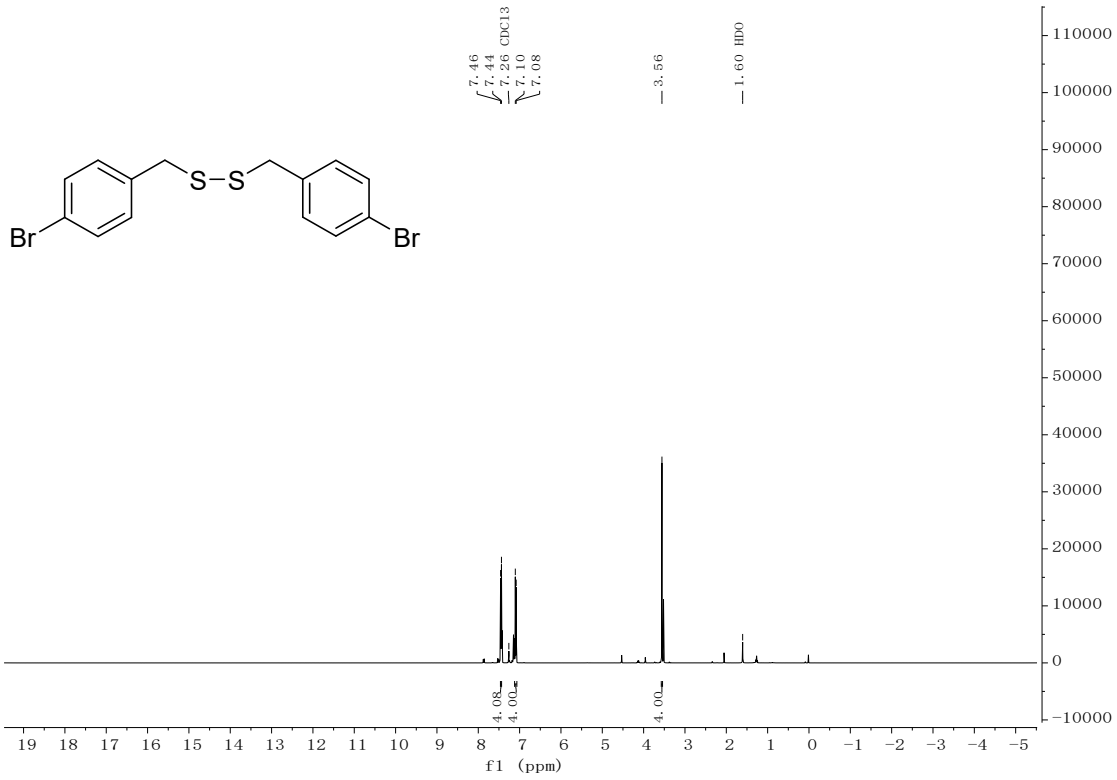


^{13}C NMR

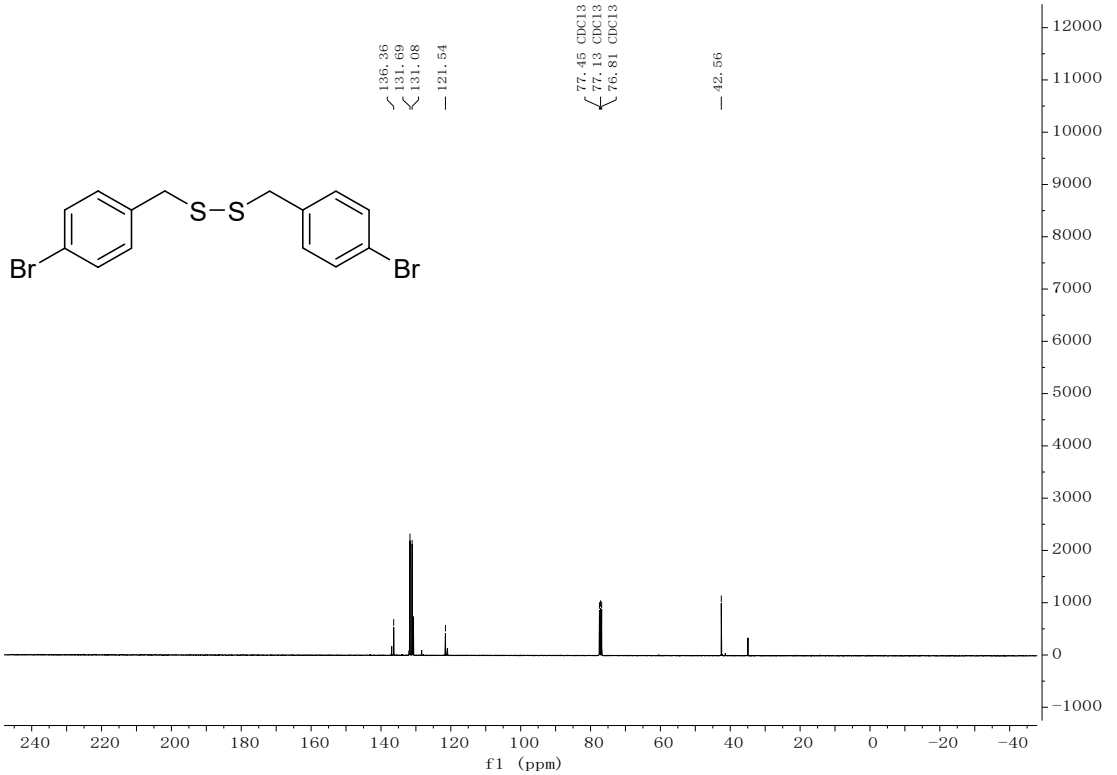


Bis(4-bromobenzyl) disulfide

^{1}H NMR

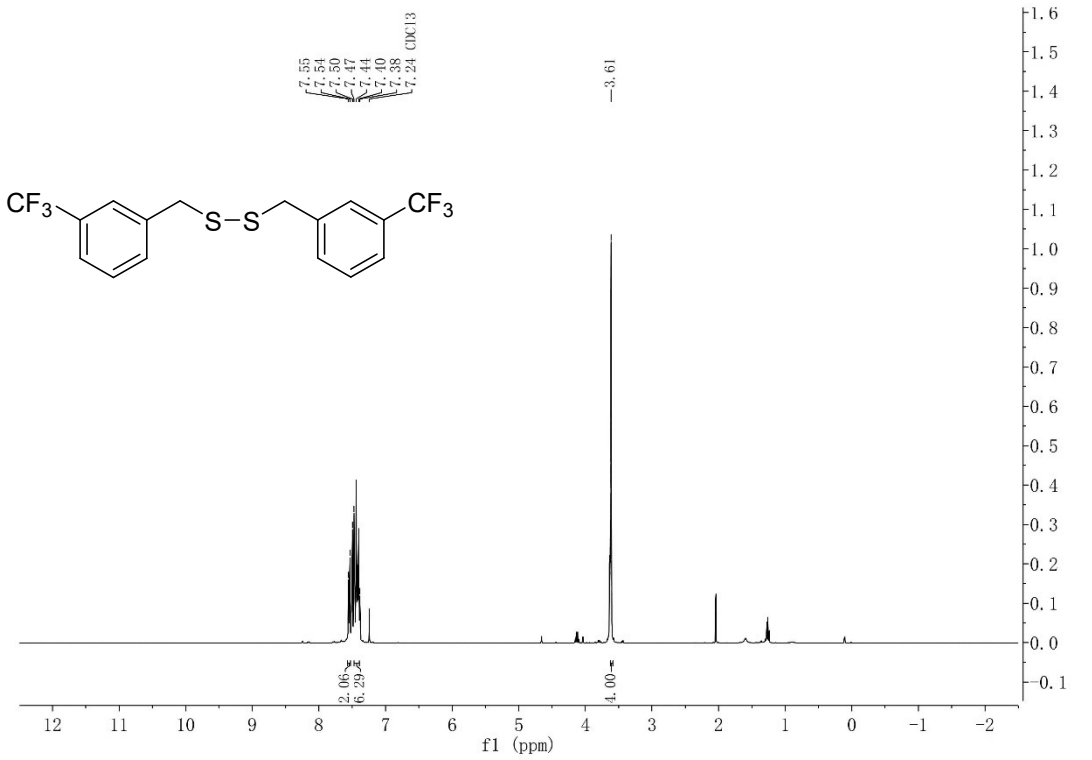


^{13}C NMR

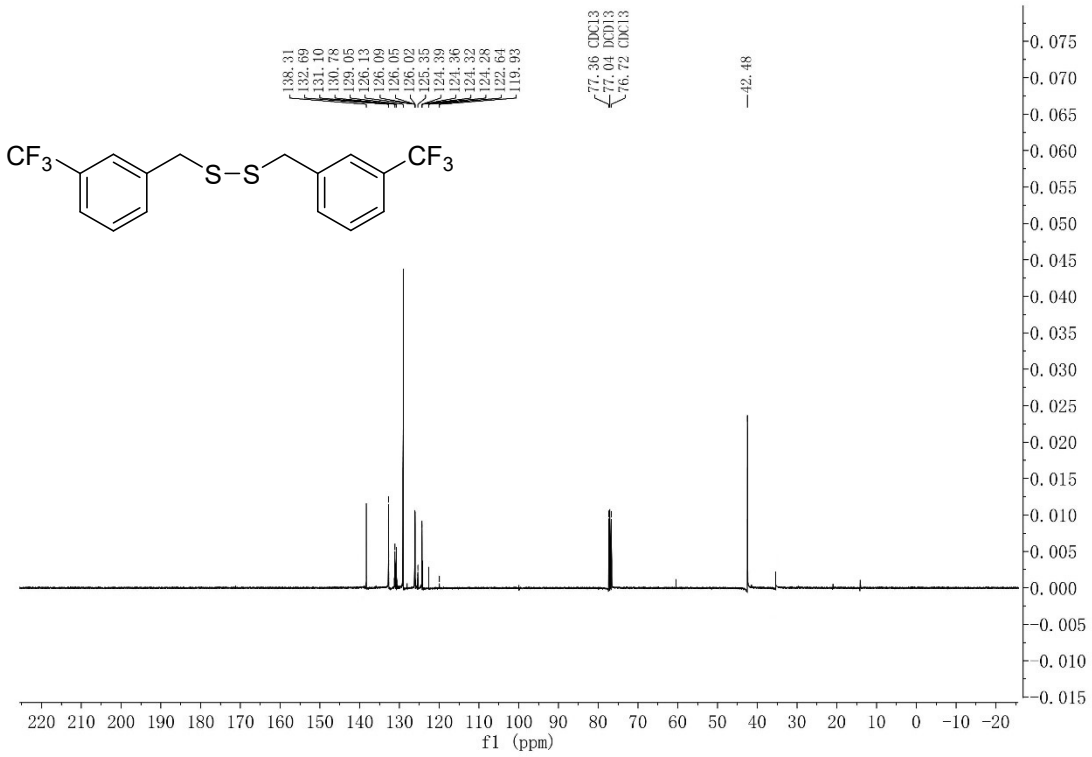


Bis(3-trifluoromethylbenzyl) disulfide

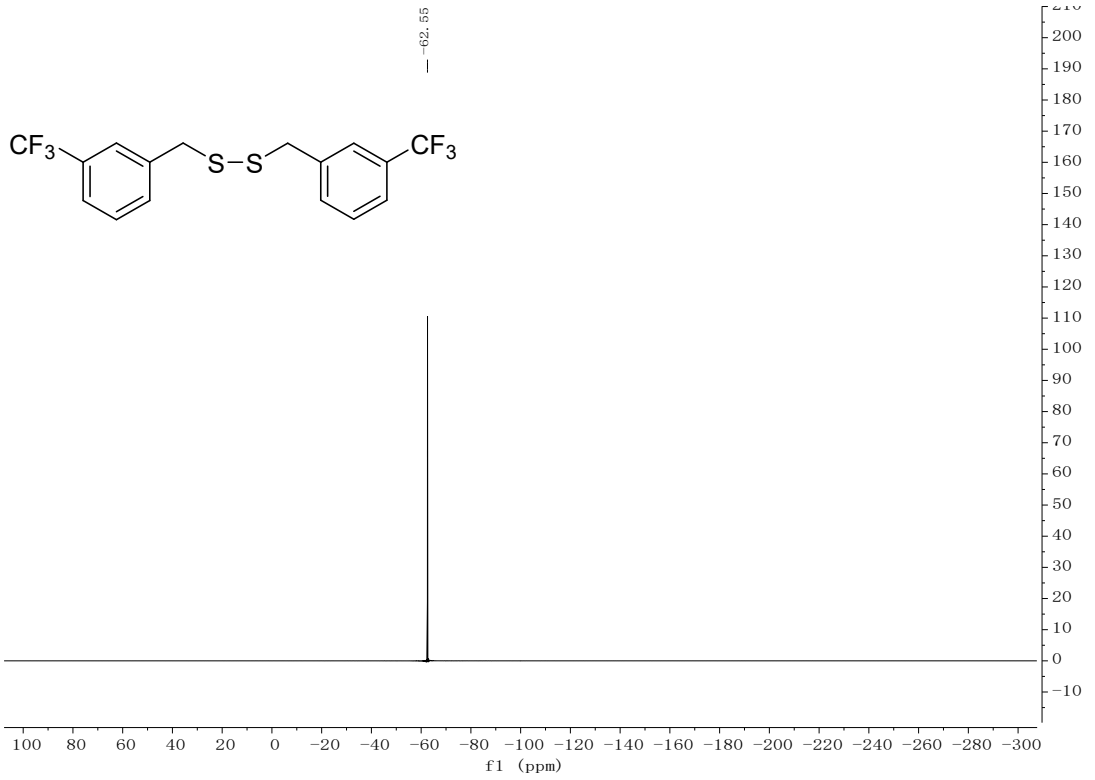
^{1}H NMR



^{13}C NMR

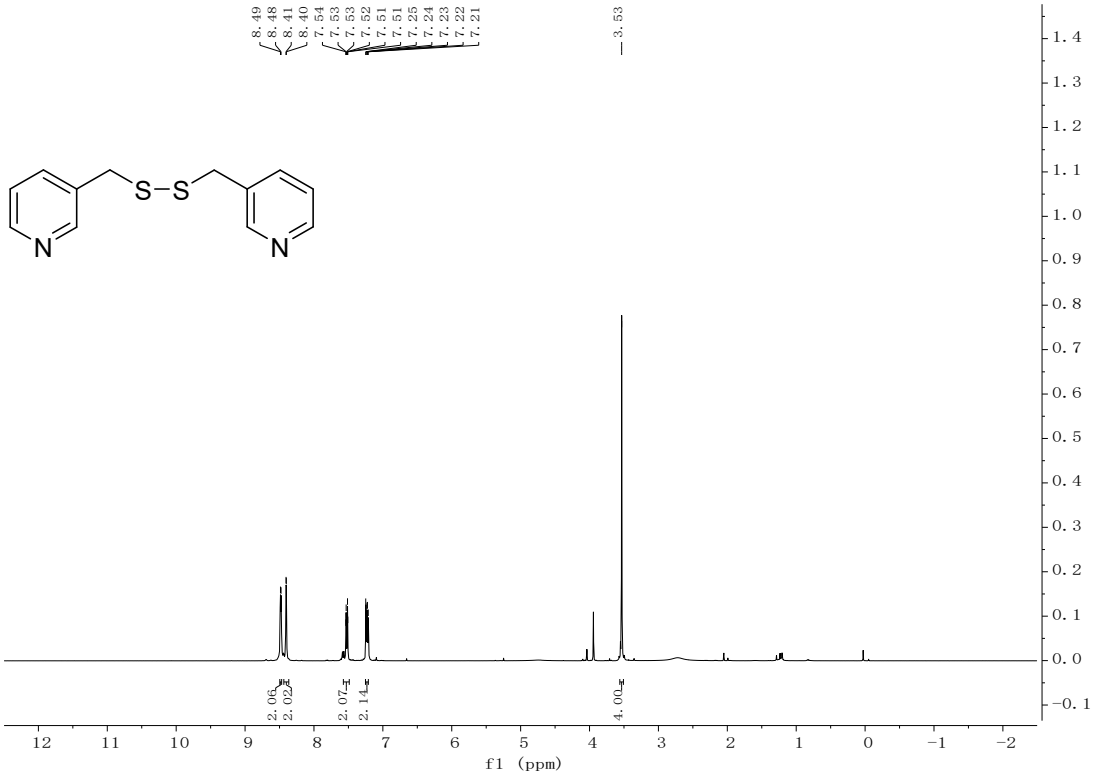


^{19}F NMR

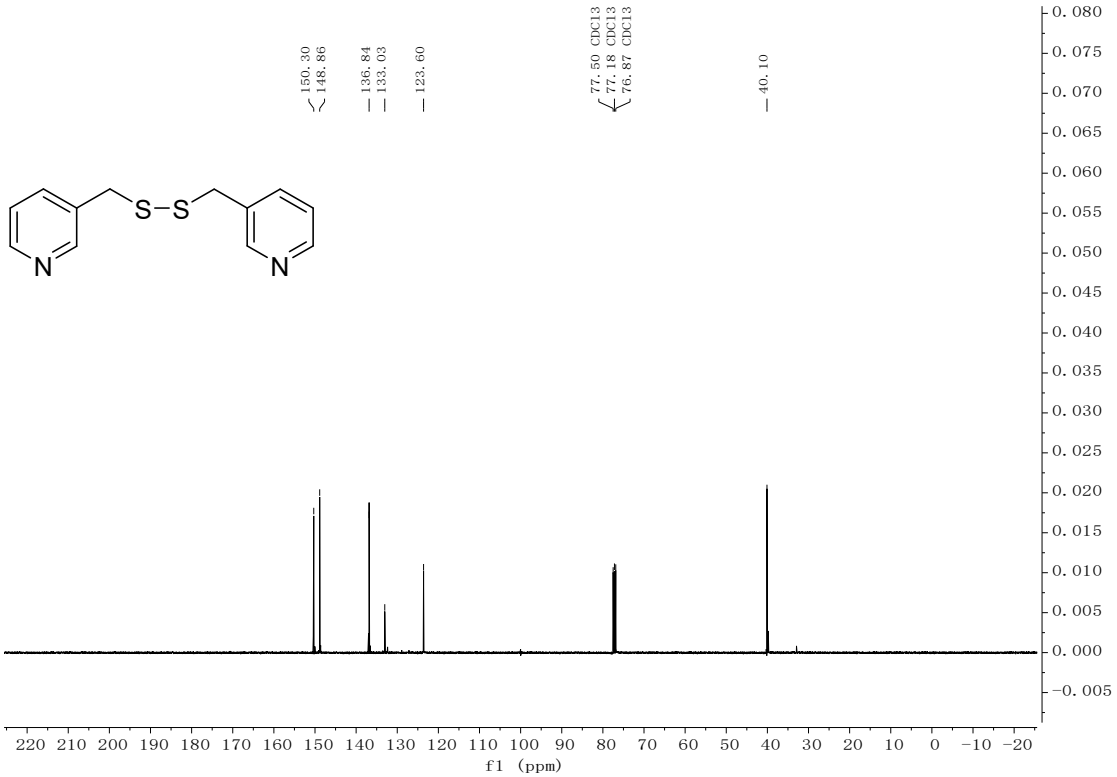


Bis(3-pyridylmethyl) disulfide

^{1}H NMR

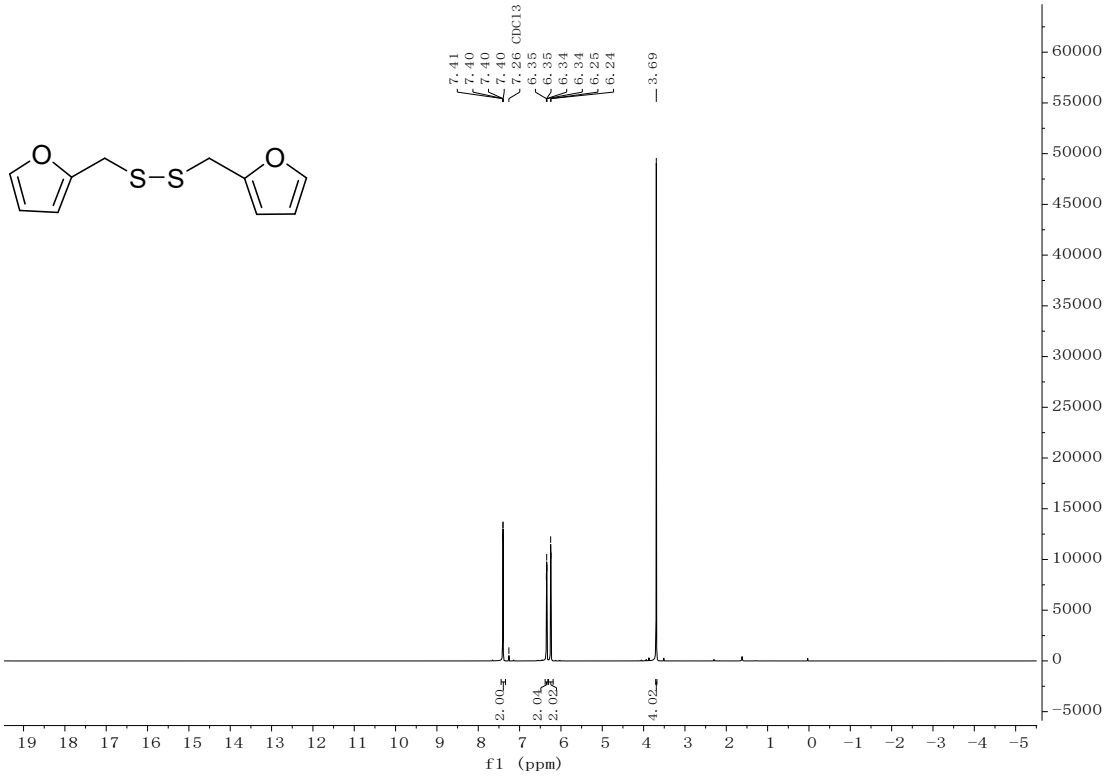


^{13}C NMR

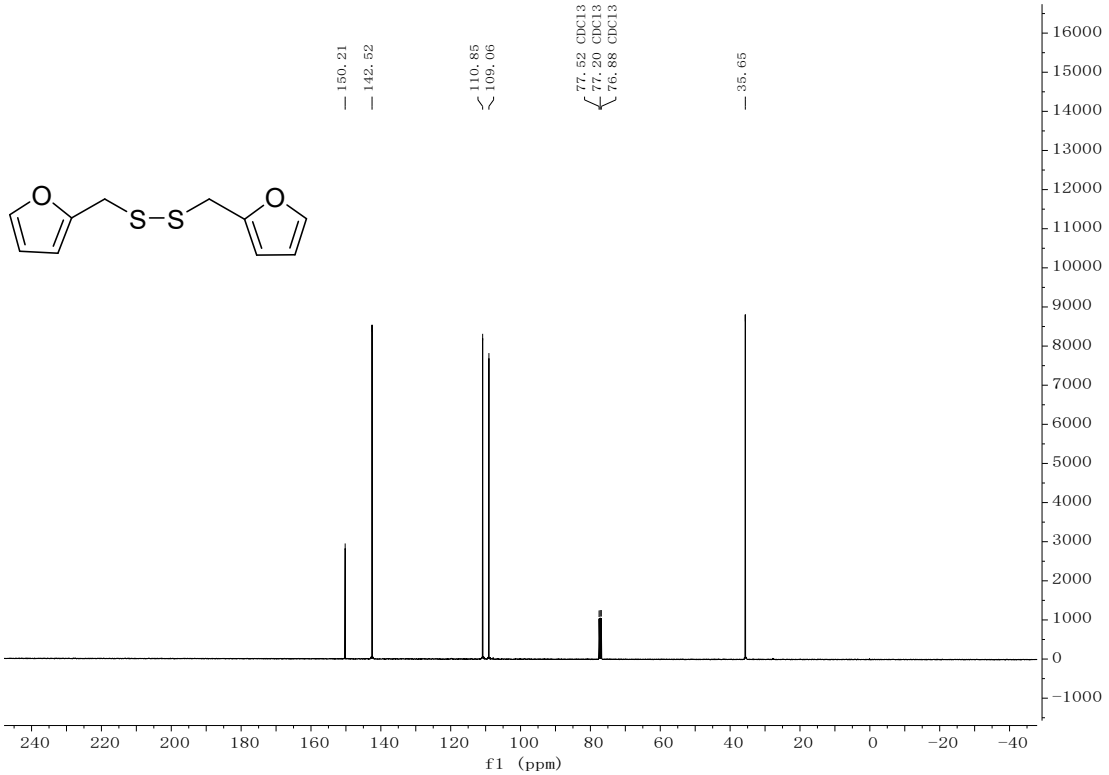


Difurfuryl disulfide

^{1}H NMR

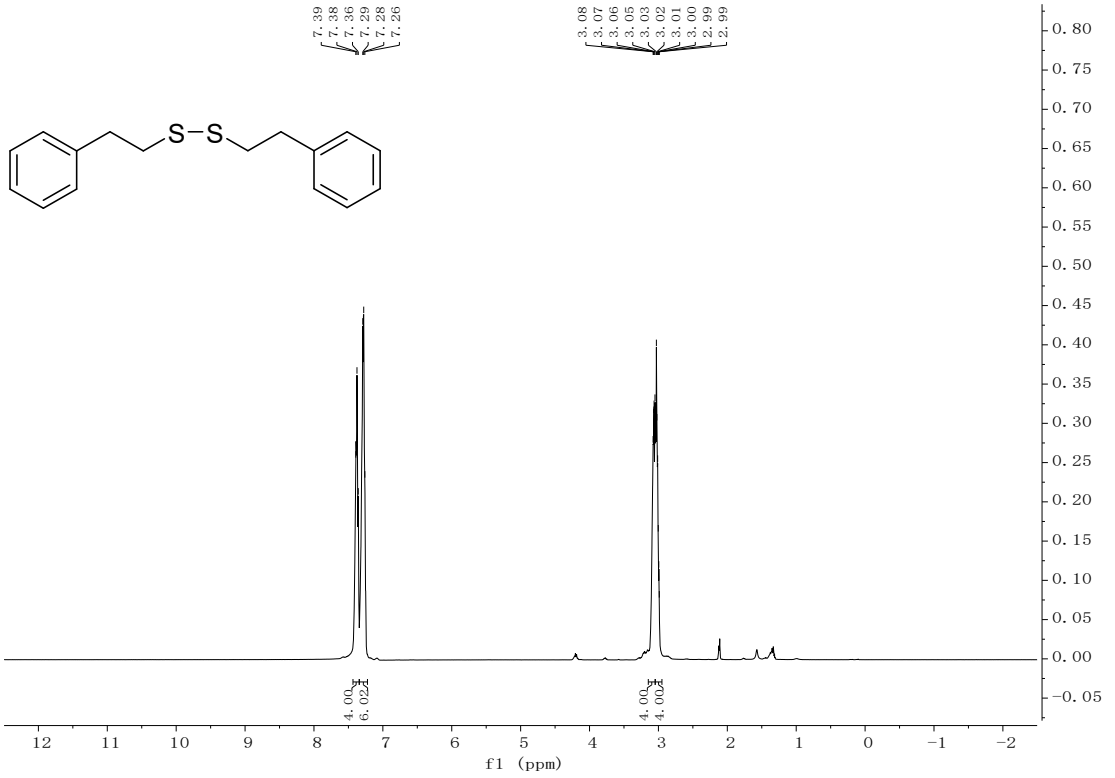


^{13}C NMR

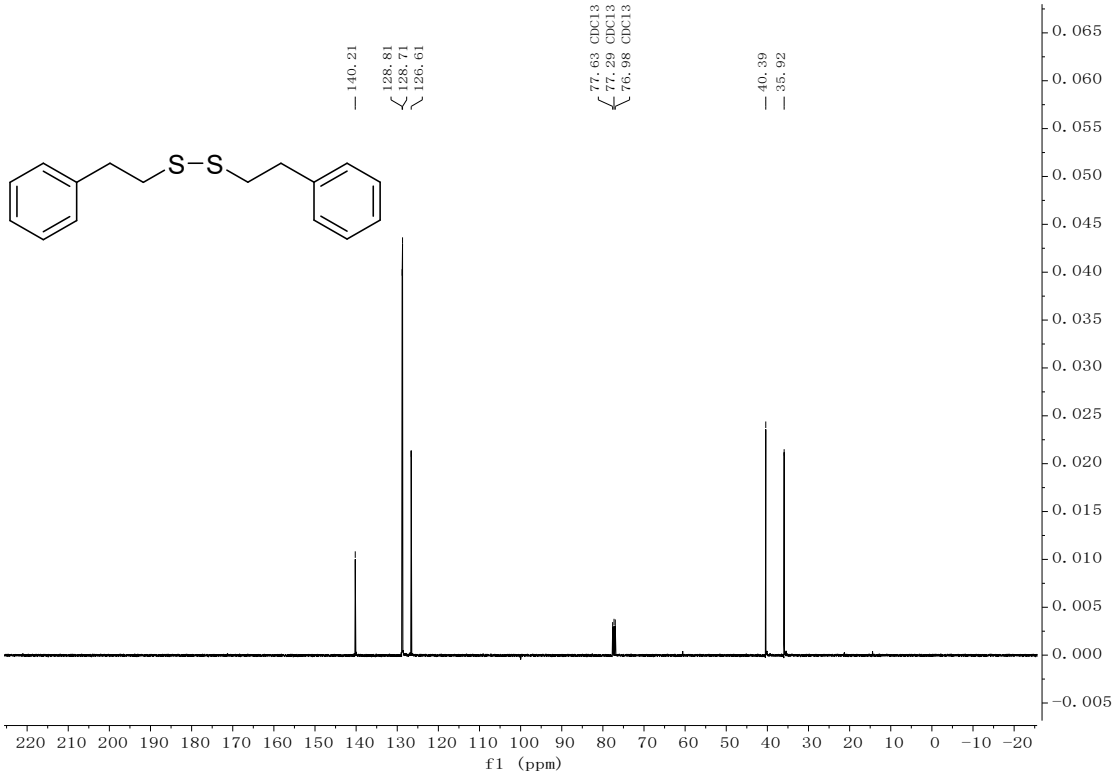


Bis(2-phenylethyl) disulfide

^{1}H NMR

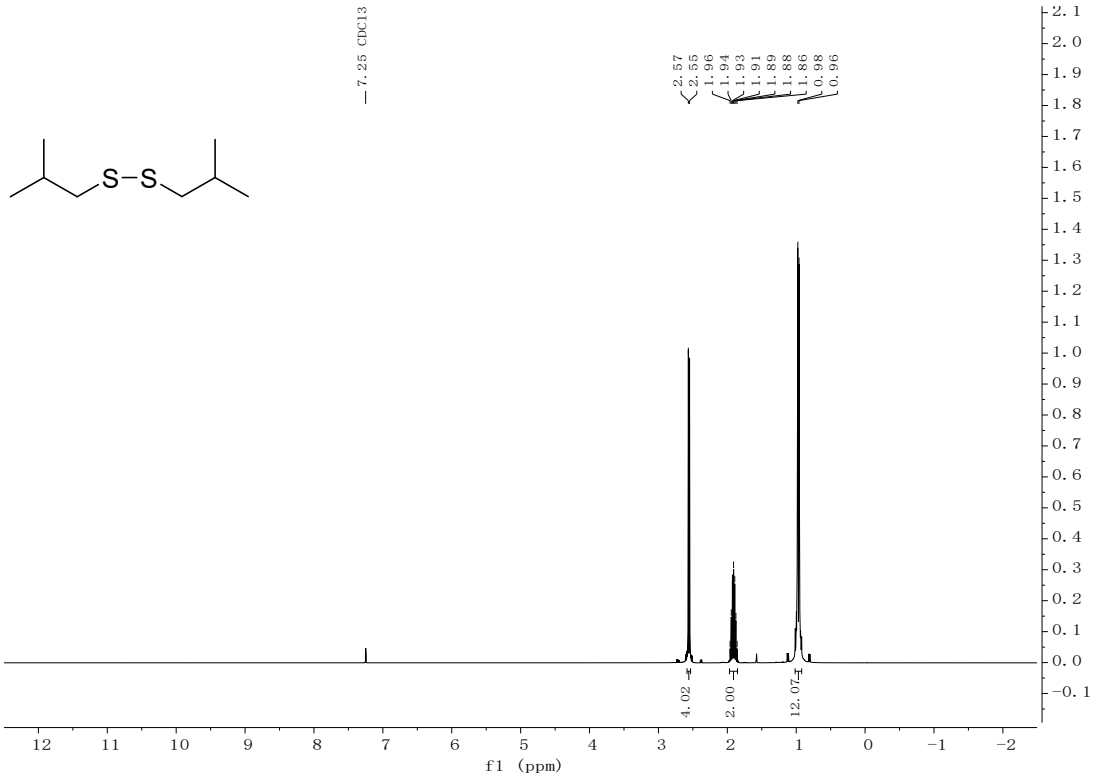


^{13}C NMR

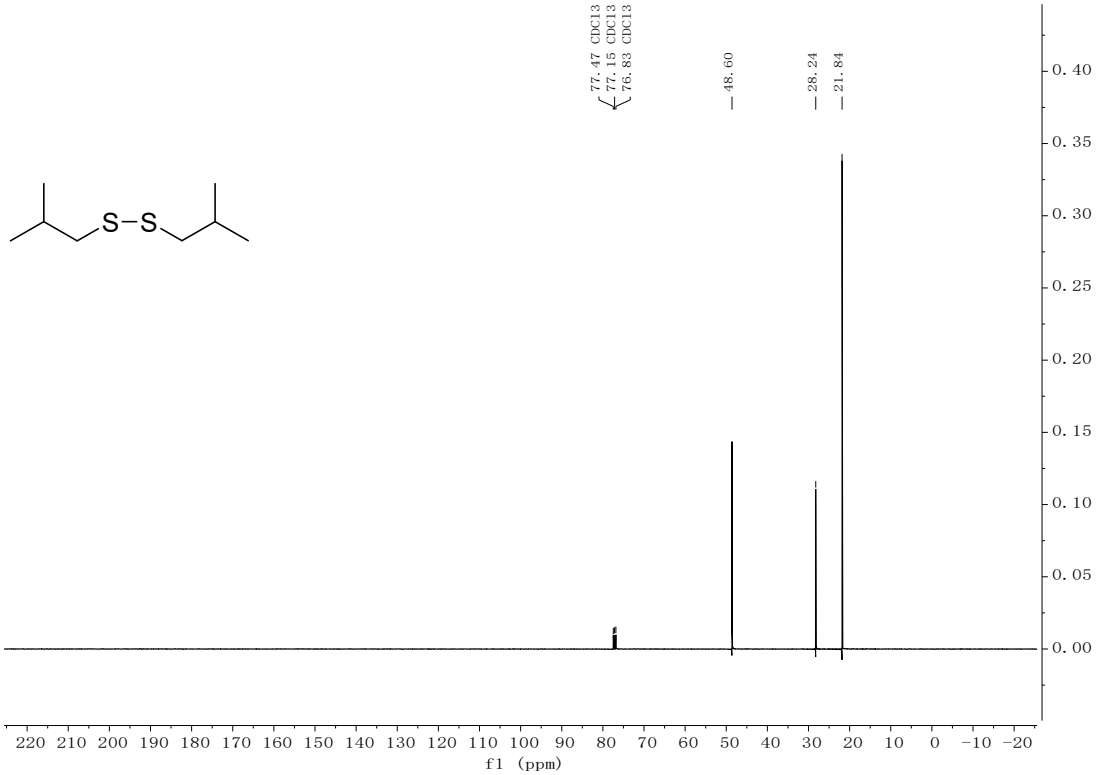


Diisobutyl disulfide

^{1}H NMR

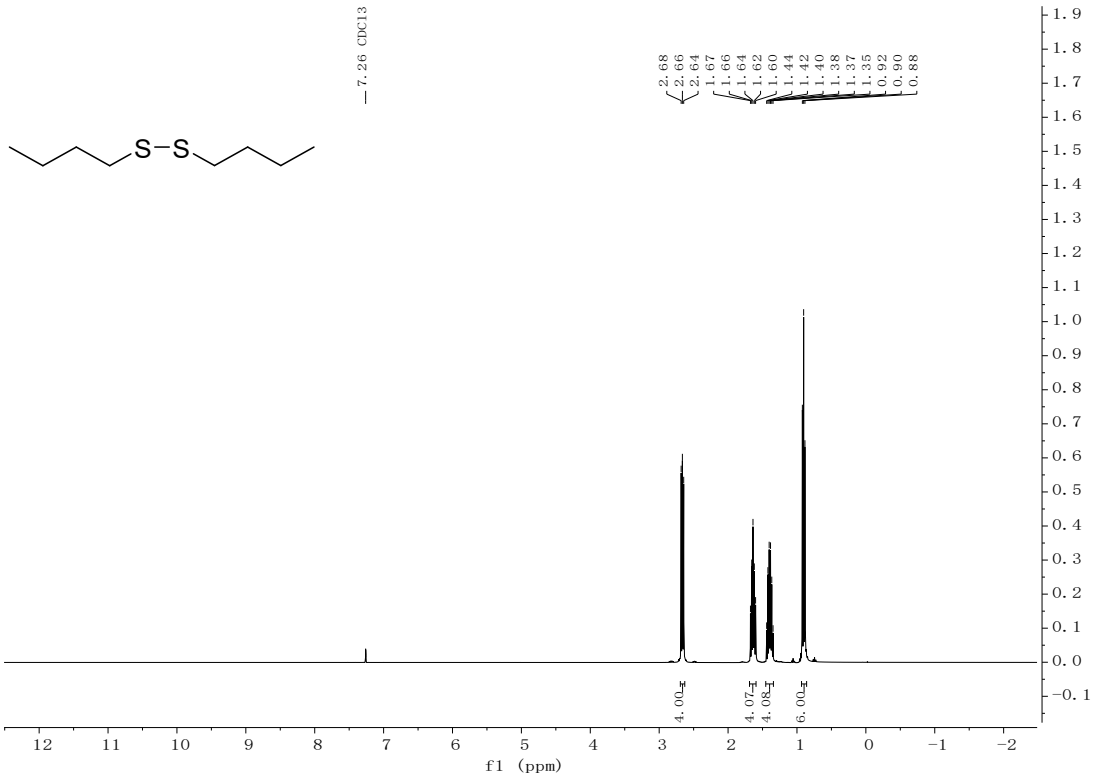


^{13}C NMR

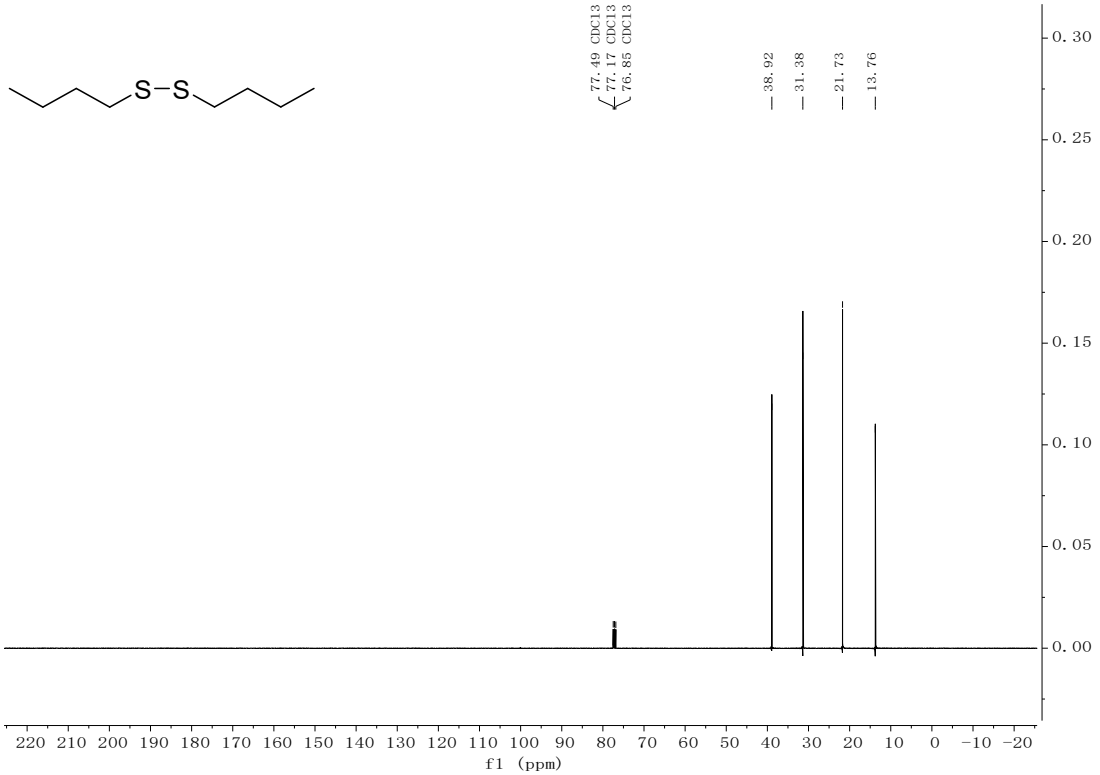


Butyl disulfide

^{1}H NMR


7.26 CDCl3
2.68
2.66
2.64
1.67
1.66
1.64
1.62
1.60
1.44
1.42
1.40
1.38
1.37
1.35
0.92
0.90
0.88
S–S
4.00
4.07
4.08
6.00
f1 (ppm)

^{13}C NMR


77.49 CDCl3
77.17 CDCl3
76.85 CDCl3
38.92
31.38
21.73
13.76
S–S
f1 (ppm)