Supporting Information

For

Microwave-Assisted Pd-Catalyzed Cross-Coupling of Aryl Alkyl Selenides with Arylboronic Acids

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1. Experimental

Unless otherwise noted, all chemicals and solvents were used directly without further purification and were acquired from Sigma-Aldrich Chemicals Pvt. Limited India and Alfa-Aesar (Thermo Fischer Scientific India Pvt. Limited), as well as from local commercial sources. Solvents used in column chromatography were dried and distilled prior to use. Solvents were removed using a rotary evaporator at low pressure, and the remaining solvent was removed thereafter under high vacuum. The column chromatography method used silica gel (100-200 mesh). Using a Buchi M-560 instrument that was not adjusted, melting points were determined. The compounds were visible under UV irradiation. The R_f values of the

compounds were reported from an analytical thin layer chromatography (TLC) examination utilizing the indicated solvents and 0.25 mm silica gel 60 F254 plates. Using tetramethylsilane (TMS) as an internal standard, the ^{1}H, ^{13}C, and ^{19}F spectra were recorded on the *J*EOL alpha-400 and Bruker-Avance Neo 400 FT-NMR spectrometers. The coupling constant (*J*) is expressed in Hz while the chemical shift values are on the δ scale. Tetramethylsilane (TMS) served as internal standard for NMR analysis. All microwave assisted experiments were performed in a closed vial reaction vial applying a dedicated CEM-Discover monomode microwave apparatus operating at a frequency of 2.45 GHz with continuous irradiation power from 0 to 300 W (CEM Corporation, P.O. Box 200, Matthews, NC 28106).

1.1. General method for the synthesis of aryl methyl selenide (1a-i) from diaryl diselenide.

To an oven-dried round bottom flask equipped with a magnetic stir bar was added diaryl diselenide[1] (1 mmol), zinc dust (5 mmol) and glacial acetic acid (5 mL). The reaction mixture was stirred at room temperature for 4 h. The complete conversion of diselenide into the corresponding selenol was indicated by the discoloration of the reaction mixture. After that, MeI (2.5 mmol) was added and stirred again for 4 h at room temperature. After completion of the reaction, the reaction mixture was filtered and extracted with EtOAc (30 mL × 3). The combined organic layers were dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified through column chromatography using hexane as the eluent to give products **1a-i**.[2]

1.2. General method for the synthesis of phenyl alkyl selenide (1j-l)/ phenyl benzyl selenide (1m) from diphenyl diselenide.

A stirred solution of alkyl bromide/benzyl bromide (2.5 mmol) and diphenyl diselenide[1] (1.0 mmol) in DME (10.0 mL) was treated with $NaBH_4$ (7.5 mmol). After being left to stand at room temperature for 12 h, water was added and the mixture was extracted using EtOAc (30 mL × 3). The organic phase was treated with saturated solution of NH_4Cl and NaCl. The combined organic layers were dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified through column chromatography using hexane as eluent to yield phenyl alkyl selenide (**1j-l**) and phenyl benzyl selenide **1m** as a yellow liquid.[3]

1.3. General method for the cross-coupling of phenyl methyl selenide (1a) with organoborane (2a-y).

To an oven-dried sealed tube equipped with a magnetic stir bar was added phenyl methyl selenide **1a** (85.5 mg, 0.5 mmol), $Pd_2(dba)_3$ (22.9 mg, 0.025 mmol), CuTC (143 mg, 0.75

mmol), TFP (23.2 mg, 0.1 mmol), organoborane **2** (0.6 mmol), and 2-Me-THF (3 mL). The reaction mixture was stirred at 100 °C under microwave irradiation for 60 min, and then quenched with saturated NH_4Cl aq. Solution (2 mL). After quenching, extraction was done with EtOAc (20 mL × 3). The combined organic layers were dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified through column chromatography using hexane as eluent to give product **3**.

1.4. General method for the cross-coupling of aryl methyl selenide (1b-i) with phenylboronic acid (2a).

To an oven-dried sealed tube equipped with a magnetic stir bar was added aryl methyl selenide **1b-i** (0.5 mmol), $Pd_2(dba)_3$ (22.9 mg, 0.025 mmol), CuTC (143 mg, 0.75 mmol), TFP (23.2 mg, 0.1 mmol), phenylboronic acid **2a** (73.2 mg, 0.6 mmol), and 2-Me-THF (3 mL). The reaction mixture was stirred at 100 °C under microwave irradiation for 60 min, and then quenched with saturated NH_4Cl aq. Solution (2 mL). After quenching, extraction was done with EtOAc (20 mL × 3). The combined organic layers were dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified through column chromatography using hexane as eluent to give product **3**.

1.5. General method for the cross-coupling of phenyl alkyl selenide (1j-l) with phenylboronic acid (2a).

To an oven-dried sealed tube equipped with a magnetic stir bar was added phenyl alkyl selenide **1j-l** (0.5 mmol), $Pd_2(dba)_3$ (22.9 mg, 0.025 mmol), CuTC (143 mg, 0.75 mmol), TFP (23.2 mg, 0.1 mmol), phenylboronic acid **2a** (73.2 mg, 0.6 mmol), and 2-Me-THF (3 mL). The reaction mixture was stirred at 100 °C under microwave irradiation for 60 min, and then quenched with saturated NH_4Cl aq. Solution (2 mL). After quenching, extraction was done with EtOAc (20 mL × 3). The combined organic layers were dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified through column chromatography using hexane as eluent to give product **3**.

1.6. General method for the cross-coupling of phenyl benzyl selenide (1m) with phenylboronic acid (2a).

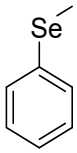
To an oven-dried sealed tube equipped with a magnetic stir bar was added phenyl benzyl selenide **1m** (0.5 mmol), $Pd_2(dba)_3$ (22.9 mg, 0.025 mmol), CuTC (143 mg, 0.75 mmol), TFP (23.2 mg, 0.1 mmol), phenylboronic acid **2a** (73.2 mg, 0.6 mmol), and 2-Me-THF (3 mL). The reaction mixture was stirred at 100 °C under microwave irradiation for 60 min, and then

quenched with saturated NH_4Cl aq. Solution (2 mL). After quenching, extraction was done with EtOAc (20 mL × 3). The combined organic layers were dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified through column chromatography using hexane as eluent to give product **3**.

1.7. Gram scale synthesis.

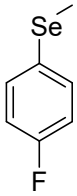
To an oven-dried sealed tube equipped with a magnetic stir bar was added phenyl methyl selenide **1a** (1.027 g, 6 mmol), $Pd_2(dba)_3$ (274.8 mg, 0.3 mmol), CuTC (1.7 g, 9.0 mmol), TFP (23.2 mg, 1.2 mmol), phenylboronic acid **2a** (0.9 g, 7.2 mmol), and 2-Me-THF (6 mL). The reaction mixture was stirred at 100 °C under microwave irradiation for 60 min, and then quenched with saturated NH_4Cl aq. Solution (20 mL). After quenching, extraction was done with EtOAc (60 mL × 3). The combined organic layers were dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified through column chromatography using hexane as eluent to give product **3a.**

Compound 1a: Methyl(phenyl)selane



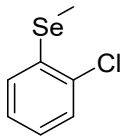
It was obtained as a yellow oil in 86% (294.2 mg) yield. R_f = 0.74 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64-7.61 (m, 1H), 7.45-7.43 (m, 1H), 7.30-7.27 (m, 2H), 7.24-7.21 (m, 1H), 2.37 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 131.51, 130.36, 129.22, 129.06, 127.75, 126.13, 7.26.

Compound 1b: (4-Fluorophenyl)(methyl)selane



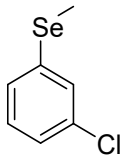
It was obtained as a yellow oil in 81% (306.3 mg) yield. R_f = 0.74 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44-7.43 (m, 1H), 7.42-7.41 (m, 1H)), 7.00-6.98 (m, 1H), 6.97-6.95 (m, 1H), 2.34 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 162.51 (d, J = 247.7 Hz), 161.90 (d, J = 247.7 Hz), 134.98 (d, J = 7.9 Hz), 132.96 (d, J = 7.9 Hz), 116.62 (d, J = 21.6 Hz), 116.20 (d, J = 21.2 Hz), 8.31.

Compound 1c: (2-Chlorophenyl)(methyl)selane



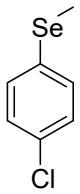
It was obtained as a yellow oil in 78% (320.6 mg) yield. R_f = 0.74 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29-7.28 (m, 1H), 7.22-7.21 (m, 1H), 7.19-7.18 (m, 1H), 7.17-7.16 (m, 1H), 2.24 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 137.20, 133.02, 130.11, 127.78, 21.13.

Compound 1d: (3-Chlorophenyl)(methyl)selane



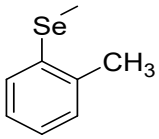
It was obtained as a yellow oil in 82% (337.1 mg) yield. R_f = 0.74 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33 (d, J = 2.5 Hz, 1H), 7.31 (s, 1H), 7.24-7.21 (m, 2H), 2.29 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 134.61, 132.60, 132.06, 132.00, 7.49.

Compound 1e: (4-Chlorophenyl)(methyl)selane



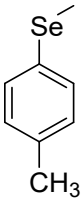
It was obtained as a yellow oil in 80% (328.8 mg) yield. R_f = 0.74 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36-7.35 (m, 1H), 7.34-7.33 (m, 1H), 7.24-7.23 (m, 1H), 7.22-7.21 (m, 1H), 2.35 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 137.21, 133.04, 130.13, 127.80, 21.16.

Compound 1f: (2-Methylphenyl)(methyl)selane



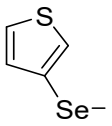
It was obtained as a yellow oil in 84% (311.0 mg) yield. R_f = 0.74 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 (d, J = 7.7 Hz, 1H), 7.25-7.22 (m, 1H), 7.22-7.19 (m, 1H), 7.10-7.08 (m, 1H), 2.46 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 133.04, 132.35, 130.98, 130.13, 129.97, 129.89, 21.07, 7.73.

Compound 1g: (4-Methylphenyl)(methyl)selane



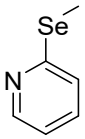
It was obtained as a yellow oil in 86% (318.4 mg) yield. R_f = 0.74 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47-7.42 (m, 1H), 7.29-7.28 (m, 1H), 7.16-7.13 (m, 1H), 7.00-6.98 (m, 1H), 2.23 (s, 3H), 1.35 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 132.51, 131.49, 129.18, 128.98,127.71, 126.68, 21.33, 15.47.

Compound 1h: 3-(methylselanyl)thiophene



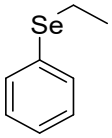
It was obtained as a yellow oil in 80% (283.4 mg) yield. R_f = 0.68 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39-7.37 (m, 1H), 7.36-7.35 (m, 1H), 7.24-7.23 (m, 1H), 2.37 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 135.39, 133.38, 132.84, 132.78, 8.27.

Compound 1i: 2-(methylselanyl)pyridine



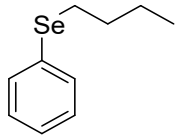
It was obtained as a yellow oil in 82% (282.2 mg) yield. R_f = 0.64 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.38-8.37 (m, 1H), 8.35-8.34 (m, 2H), 7.42-7.39 (m, 1H), 7.11-7.08 (m, 1H), 2.25 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 150.22, 146.89, 136.39, 133.05, 123.09, 18.40.

Compound 1j: Ethyl(phenyl)selane



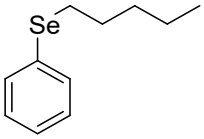
It was obtained as a yellow oil in 88% (325.8 mg) yield. R_f = 0.74 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62-7.61 (m, 1H), 7.60-7.59 (m, 1H), 7.50-7.48 (m, 1H), 7.25-7.24 (m, 2H), 2.92 (q, J = 7.5 Hz, 2H), 1.43 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 132.55, 131.53, 129.22, 129.01, 127.75, 126.72, 21.37, 15.51.

Compound 1k: Butyl(phenyl)selane



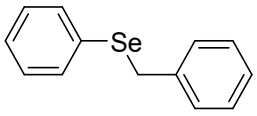
It was obtained as a yellow oil in 84% (358.1 mg) yield. R_f = 0.74 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63-7.60 (m, 1H), 7.50-7.48 (m, 2H), 7.28-7.27 (m, 1H), 7.25-7.24 (m, 1H), 2.94-2.90 (m, 2H), 1.73-1.67 (m, 2H), 1.43 (m, 2H), 0.92 (t, J = 7.3 Hz, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 132.38, 131.55, 129.22, 129.01, 127.76, 126.61, 32.27, 27.64, 22.99, 13.60.

Compound 1l: Pentyl(phenyl)selane



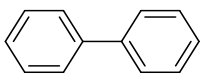
It was obtained as a yellow oil in 84% (381.7 mg) yield. R_f = 0.74 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48-7.46 (m, 2H), 7.25-7.22 (m, 2H), 7.20-7.18 (m, 1H), 2.89 (t, J = 7.5 Hz, 2H), 1.73-1.66 (m, 2H), 1.39-1.27 (m, 4H), 0.87 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 132.37, 129.22, 129.00, 126.60, 32.06, 29.88, 27.93, 22.22, 14.02.

Compound 1m: Benzyl(phenyl)selane



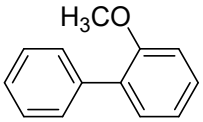
It was obtained as a yellow oil in 89% (440.0 mg) yield. R_f = 0.74 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46-7.43 (m, 2H), 7.25-7.22 (m, 5H), 7.21-7.18 (m, 3H), 4.10 (s, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 138.68, 133.61, 130.49, 129.05, 128.92, 128.49, 127.36, 126.93, 32.29.

Compound 3a: 1,1'-Biphenyl[4]



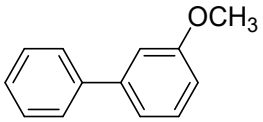
It was obtained as a white solid in 84% yield (64.8 mg). R_f = 0.74 (hexane); Melting point = 68-70 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66-7.61 (m, 4H), 7.50-7.46 (m, 4H), 7.41-7.36 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 141.30, 128.81, 127.30, 127.22.

Compound 3b: 2-Methoxy-1,1'-biphenyl[5]



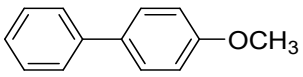
It was obtained as a colourless liquid in 78% yield (71.8 mg). R_f = 0.58 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70-7.63 (m, 2H), 7.53 (dd, J = 8.3, 6.7 Hz, 2H), 7.46-7.41 (*m*, 3H), 7.17-7.13 (m, 1H), 7.11-7.07 (m, 1H), 3.90 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 156.60, 138.70, 131.03, 130.85, 129.69, 128.76, 128.12, 127.05, 120.97, 111.36, 55.64.

Compound 3c: 3-Methoxy-1,1'-biphenyl[6]



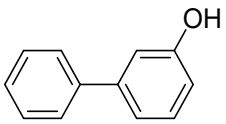
It was obtained as a white solid in 79% yield (72.8 mg). R_f = 0.59 (hexane); Melting point = 88-90 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52-7.48 (m, 2H), 7.39-7.33 (m, 2H), 7.30-7.28 (m, 2H), 7.26-7.24 (m, 1H), 6.98-6.96 (m, 1H), 6.92-6.90 (m, 1H), 3.71 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 156.80, 138.90, 131.23, 131.05, 129.90, 128.96, 128.33, 127.26, 121.17, 111.57, 55.84.

Compound 3d: 4-Methoxy-1,1'-biphenyl[6]



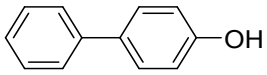
It was obtained as white solid in 80% yield (73.7 mg). R_f = 0.58 (hexane); Melting point = 98-100 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58-7.53 (m, 4H), 7.45-7.41 (m, 2H), 7.33-7.30 (m, 1H), 7.00-6.97 (m, 2H), 3.86 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 159.16, 140.85, 133.80, 128.75, 128.18, 126.77, 126.68, 114.22, 55.37.

Compound 3e: [1,1'-Biphenyl]-3-ol[7]



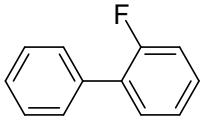
It was obtained as white solid in 83% yield (70.6 mg). R_f = 0.48 (hexane); Melting point = 75-77 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60-7.57 (m, 2H), 7.46-7.42 (m, 2H), 7.38-7.30 (m, 2H), 7.19-7.17 (m, 1H), 7.09-7.08 (m, 1H), 6.84 (dd, J = 8.1, 2.5 Hz, 1H), 3.53 (brs, 1H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 155.86, 143.05, 140.76, 130.03, 130.00, 128.78, 127.52, 127.49, 127.14, 119.82, 114.24, 114.15.

Compound 3f: [1,1'-Biphenyl]-4-ol[5]



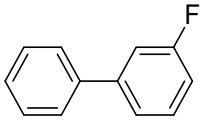
It was obtained as White solid in 81% yield (68.9 mg). R_f = 0.49 (hexane); Melting point =165-167 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 7.56-7.54 (m, 2H), 7.50-7.48 (m, 2H), 7.44-7.40 (m, 2H), 7.33-7.30 (m, 1H), 6.92-6.90 (m, 2H), 4.94 (brs, 1H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 155.07, 140.78, 134.07, 128.76, 128.43, 126.75, 115.67.

Compound 3g: 2-Fluoro-1,1'-biphenyl[8]



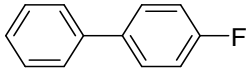
It was obtained as white solid in 76% yield (65.4 mg). R_f = 0.72 (hexane); Melting point = 74-76 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56-7.52 (m, 2H), 7.45-7.39 (m, 3H), 7.38-7.26 (m, 2H), 7.21-710 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 159.83 (d, J = 247.7 Hz), 135.89, 130.84 (d, J = 3.6 Hz), 129.21, 129.10 (d, J = 2.9 Hz), 129.01 (d, J = 8.4 Hz), 128.49, 127.71, 124.39 (d, J = 3.7 Hz), 116.14 (d, J = 22.6 Hz).

Compound 3h: 3-Fluoro-1,1'-biphenyl[9]



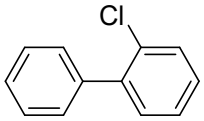
It was obtained as colourless liquid in 77% yield (66.3 mg). R_f = 0.71 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62-7.58 (m, 2H), 7.49-7.45 (m, 2H), 7.42-7.38 (m, 3H), 7.33-7.30 (m, 1H), 7.09-7.04 (m, 1H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 163.24 (d, J = 245.1 Hz), 143.55 (d, J = 7.4 Hz), 139.98 (d, J = 2.5 Hz), 130.23 (d, J = 8.2 Hz), 128.91, 127.87, 127.14, 122.79 (d, J = 2.9 Hz), 114.06 (d, J = 20.8 Hz).

Compound 3i: 4-Fluoro-1,1'-biphenyl[10]



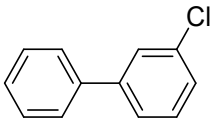
It was obtained as white solid in 82% yield (70.6 mg). R_f = 0.72 (hexane); Melting point = 75-76 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62-7.58 (m, 2H), 7.51-7.46 (m, 3H), 7.43-7.32 (m, 2H), 7.26-7.15 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 162.49 (d, J = 246.2 Hz), 140.28, 137.37 (d, J = 3.5 Hz), 128.85, 128.71 (d, J = 8.0 Hz), 127.29, 127.05, 115.64 (d, J = 21.2 Hz).

Compound 3j: 2-Chloro-1,1'-biphenyl[11]



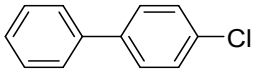
It was obtained as white solid in 83% yield (78.3 mg). R_f = 0.72 (hexane); Melting point = 32-34 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (dd, J = 8.0, 1.2 Hz, 1H), 7.46-7.33 (m, 7H), 7.08-7.04 (m, 1H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 146.68, 144.25, 139.55, 130.15, 129.33, 128.85, 128.18, 128.02, 127.70, 98.71.

Compound 3k: 3-Chloro-1,1'-biphenyl[4]



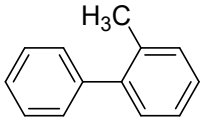
It was obtained as colourless liquid in 85% yield (80.2 mg). R_f = 0.72 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99-7.97 (m, 1H), 7.73-7.70 (m, 1H), 7.59-7.54 (m, 3H), 7.51-7.44 (m, 2H), 7.43-7.38 (m, 1H), 7.20-7.17 (m, 1H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 142.36, 138.53, 135.09, 135.06, 129.34, 127.80, 126.76, 126.03, 125.32, 93.77.

Compound 3l: 4-Chloro-1,1'-biphenyl[10]



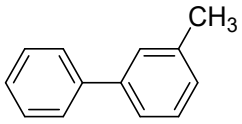
It was obtained as white solid in 86% yield (81.1 mg). R_f = 0.72 (hexane); Melting point = 77-79 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81-7.76 (m, 2H), 7.59-7.54 (m, 2H), 7.48-7.44 (m, 2H), 7.42-7.37 (m, 1H), 7.37-7.33 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 140.76, 140.09, 137.89, 129.06, 128.96, 127.75, 126.94, 93.11.

Compound 3m: 2-Methyl-1,1'-biphenyl[6]



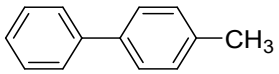
It was obtained as colourless liquid in 84% yield (70.6 mg). R_f = 0.78 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49-7.45 (m, 2H), 7.42-7.37 (m, 3H), 7.34-7.32 (m, 2H), 7.31-7.28 (m, 2H), 2.34 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 142.04, 142.01, 135.41, 130.38, 129.87, 129.27, 128.14, 127.32, 126.83, 125.84, 20.55.

Compound 3n: 3-Methyl-1,1'-biphenyl[4]



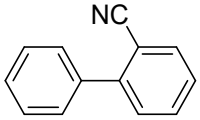
It was obtained as colourless liquid in 82% yield (69.0 mg). R_f = 0.79 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56-7.52 (m, 2H), 7.40-7.34 (m, 4H), 7.32-7.26 (m, 2H), 7.13-7.09 (m, 1H), 2.37 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 141.46, 141.34, 138.41, 128.79, 128.77, 128.10, 128.08, 127.28, 127.25, 124.38, 21.64.

Compound 3o: 4-Methyl-1,1'-biphenyl[5]



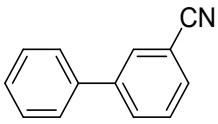
It was obtained as white solid in 88% yield (74.0 mg). R_f = 0.77 (hexane); Melting point = 46-48 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71-7.60 (m, 4H), 7.55-7.51 (m, 2H), 7.45-7.41 (m, 1H), 7.37-7.35 (m, 2H), 2.51 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 141.30, 138.49, 137.12, 129.63, 128.86, 127.13, 127.11, 21.23.

Compound 3p: [1,1'-Biphenyl]-2-carbonitrile[12]



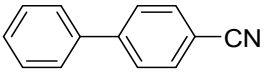
It was obtained as colourless liquid in 66% yield (59.1 mg). R_f = 0.62 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85-7.84 (m, 1H), 7.80-7.78 (m, 1H), 7.62-7.59 (m, 1H), 7.55-7.52 (m, 3H), 7.48-7.37 (m, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 142.95, 139.37, 131.97, 131.19, 131.17, 130.07, 129.61, 128.87, 127.57, 119.32, 113.46.

Compound 3q: [1,1'-Biphenyl]-3-carbonitrile[13]



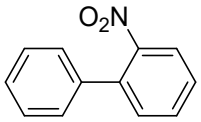
It was obtained as colourless liquid in 68% yield (60.9 mg). R_f = 0.61 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88-7.86 (m, 1H), 7.83-7.80 (m, 1H), 7.66-7.62 (m, 1H), 7.59-7.54 (m, 3H), 7.51-7.46 (m, 2H), 7.44-7.40 (m, 1H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 142.48, 138.91, 131.53, 130.74, 129.64, 129.17, 128.43, 127.12, 118.90, 112.99.

Compound 3r: [1,1'-Biphenyl]-4-carbonitrile[4]



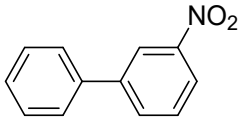
It was obtained as white solid in 72% yield (64.5 mg). R_f = 0.61 (hexane); Melting point =86-88 °C; ^{1}H NMR (400MHz, $CDCl_3$): δ 7.74-7.67 (m, 4H), 7.61-7.58 (m, 2H), 7.51-7.47 (m, 2H), 7.45-7.42 (m, 1H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 145.69, 139.19, 132.62, 129.15, 128.70, 127.76, 127.26, 118.98, 110.92.

Compound 3s: 2-Nitro-1,1'-biphenyl[13]



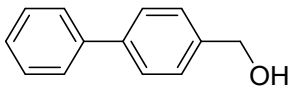
It was obtained as colourless liquid in 60% yield (59.8 mg). R_f = 0.60 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.45 (t, J = 2.0 Hz, 1 Hz, 1H), 8.20-8.17 (m, 1H), 7.92-7.89 (m, 1H), 7.63-7.62 (m, 1H), 7,61-7,60 (m, 2H), 7.51-7.47 (m, 2H), 7.45-7,40 (m, 1H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 149.18, 143.31, 139.10, 133.44, 130.11, 129.58, 128.95, 127.58, 122.44, 122.38.

Compound 3t: 3-Nitro-1,1'-biphenyl[10]



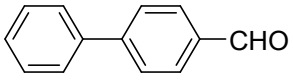
It was obtained as white solid in 64% yield (63.7 mg). R_f = 0.61 (hexane); Melting point = 58-60 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.46-8.44 (m, 1H), 8.20 (ddd, J = 8.2, 2.3, 1.1 Hz, 1H), 7.92 (dt, J = 7.7, 1.5 Hz, 1H), 7.64-7.59 (m, 3H), 7.52-7.42 (m, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 148.75, 142.89, 138.68, 133.07, 129.74, 129.19, 128.57, 127.18, 122.05, 121.97.

Compound 3u: [1,1'-Biphenyl]-4-ylmethanol[14]



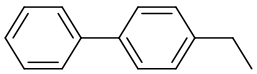
It was obtained as white solid in 75% yield (69.1 mg). R_f = 0.59 (hexane); Melting point = 97-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63-7.58 (m, 4H), 7.46-7.43 (m, 4H), 7.39-7.33 (m, 1H), 4.74 (s, 2H), 3.48 (brs, 1H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 140.86, 140.66, 139.92, 128.82, 127.49, 127.35, 127.12, 65.11.

Compound 3v: 4-Formyl [1,1'-biphenyl][15]



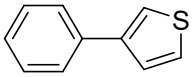
It was obtained as white solid in 58% yield (52.8 mg). R_f = 0.58 (hexane); Melting point = 56-58 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.05 (s, 1H), 7.46-7.43 (m, 2H), 7.96-7.94 (m, 2H), 7.76-7.74 (m, 2H), 7.65-7.63 (m, 2H), 7.51-7.47 (m, 2H), 7.44-7.42 (m, 1H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 191.96, 147.18, 139.72, 135.23, 130.31, 129.07, 128.53, 127.71, 127.40.

Compound 3w: 4-Ethyl-1,1'-biphenyl[16]



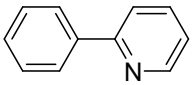
It was obtained as white solid in 82% yield (74.7 mg). R_f = 0.61 (hexane); Melting point = 34-36 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62-7.59 (m, 2H), 7.56-7.54 (m, 2H), 7.45 (t, J=7.7 Hz, 2H), 7.38-7.33 (m, 1H), 7.32-7.29 (m, 2H), 2.73 (q, J = 7.6 Hz, 2H), 1.31 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 143.43, 141.23, 138.65, 128.74, 128.32, 127.12, 127.05, 127.00, 28.56, 15.63.

Compound 3x: 3-Phenylthiophene[17]



It was obtained as white solid in 69% yield (55.3 mg). R_f = 0.62 (hexane); Melting point = 91-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62-7.61 (m, 1H), 7.60-7.59 (m, 1H), 7.46-7.45 (m, 1H), 7.42-7.39 (m, 4H), 7.32-7.27 (m, 1H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 142.41, 135.90, 128.81, 127.14. 126.47. 126.36, 126.18. 120.17.

Compound 3y: 2-Phenylpyridine[18]



It was obtained as colourless liquid in 71% yield (55.1 mg). R_f = 0.64 (hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71-8.69 (m, 1H), 8.02-7.99 (m, 2H), 7.73-7.70 (m, 2H), 7.50-7.46 (m, 2H), 7.44-7.39 (m, 1H), 7.22-7.19 (m, 1H). ^{13}C NMR (100.6 MHz, $CDCl_3$): 157.50, 149.69, 139.45, 136.74, 128.97, 128.76, 126.94, 122.10, 120.56.

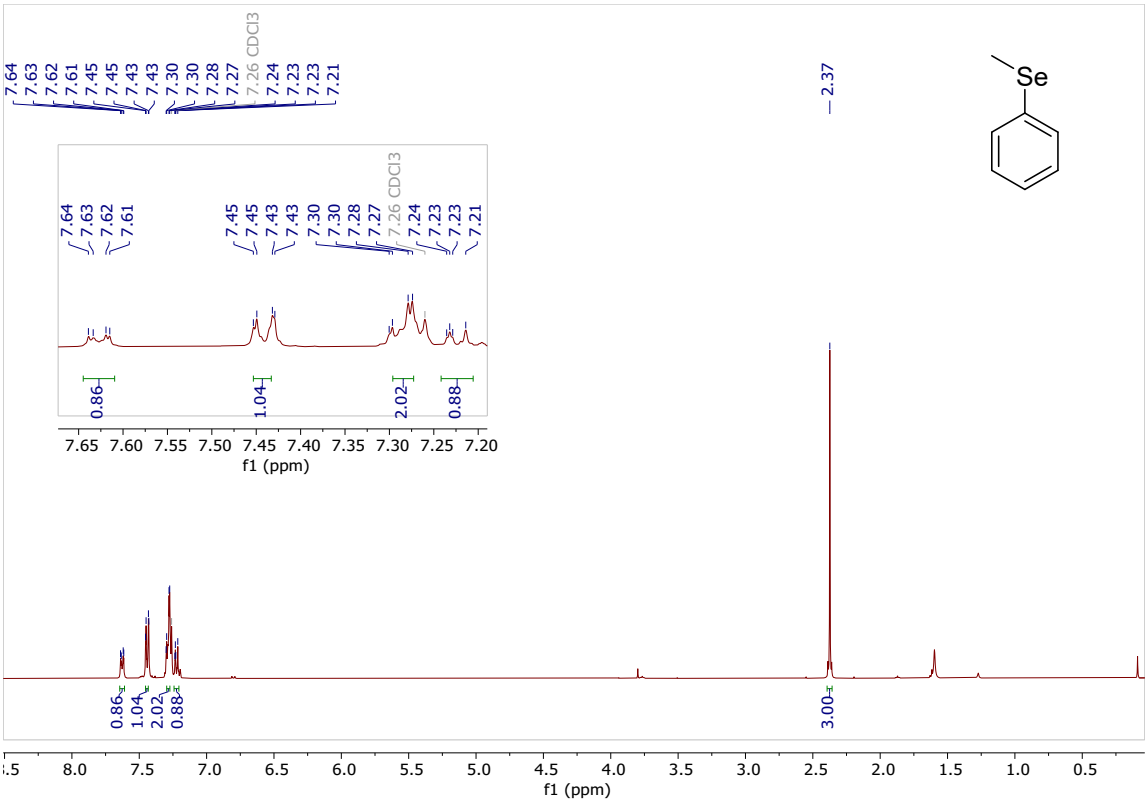


Figure 1: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1a.**

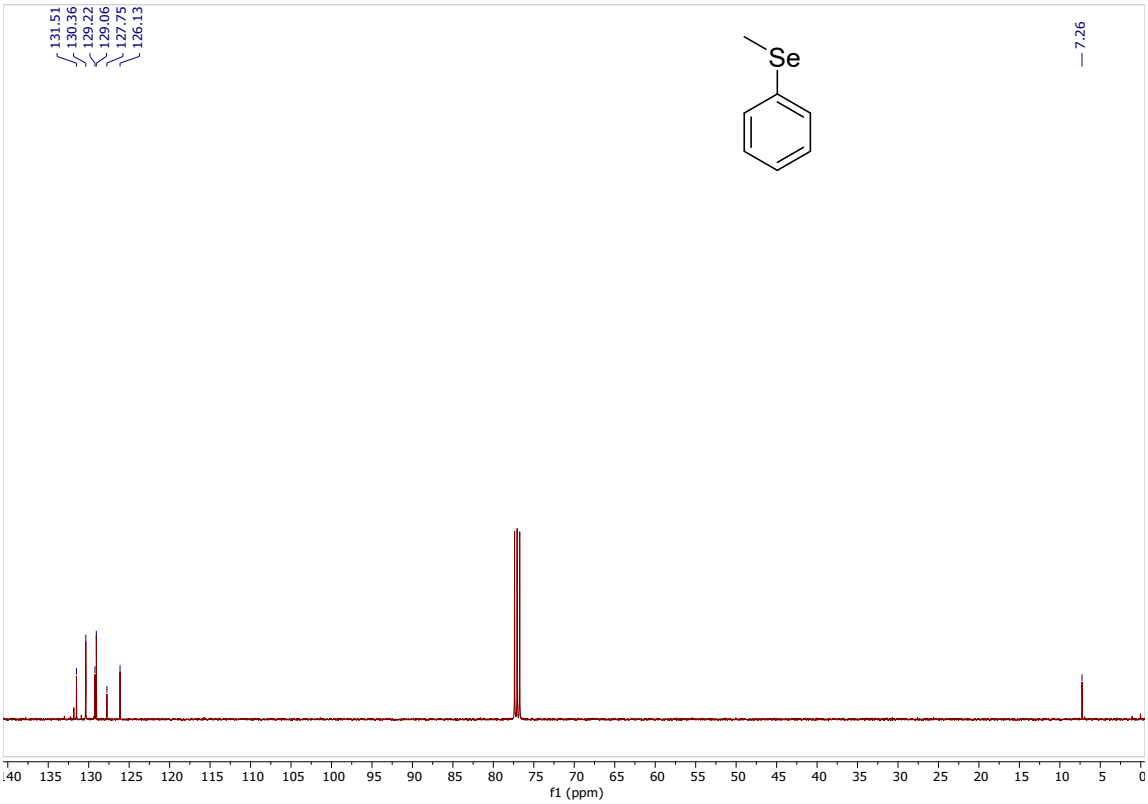


Figure 2: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1a**.

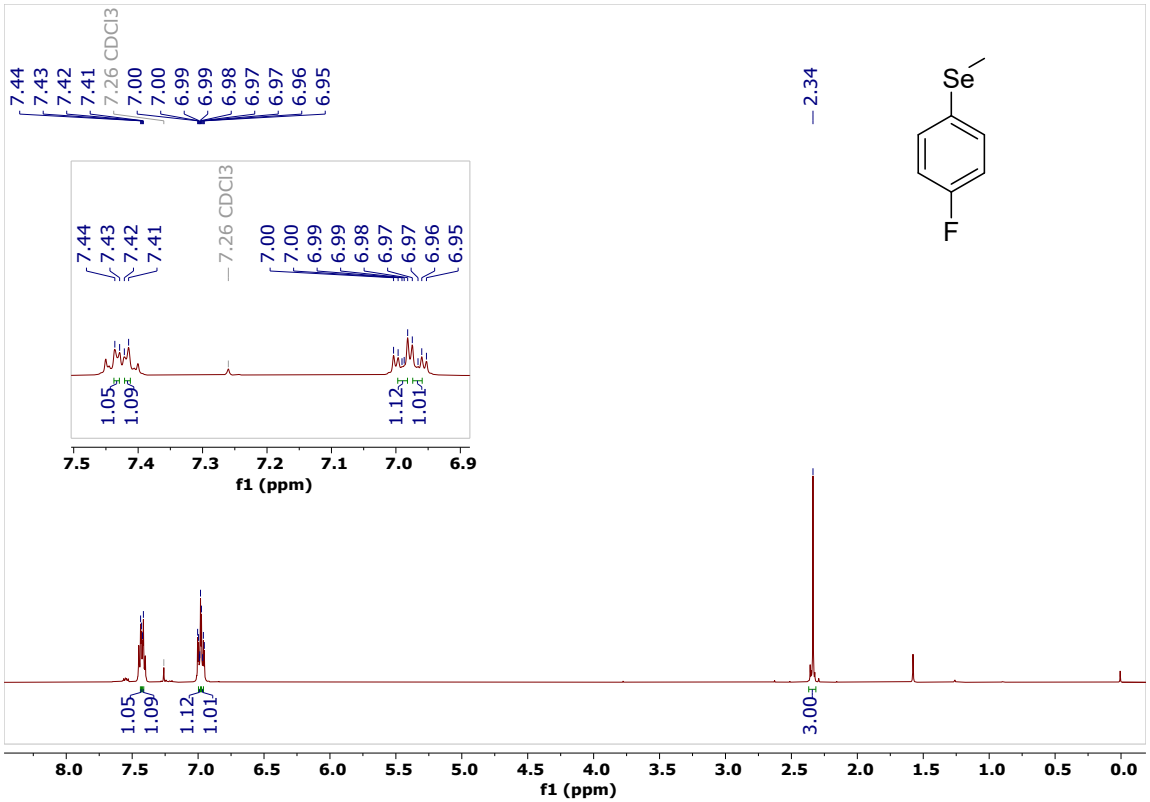


Figure 3: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1b.**

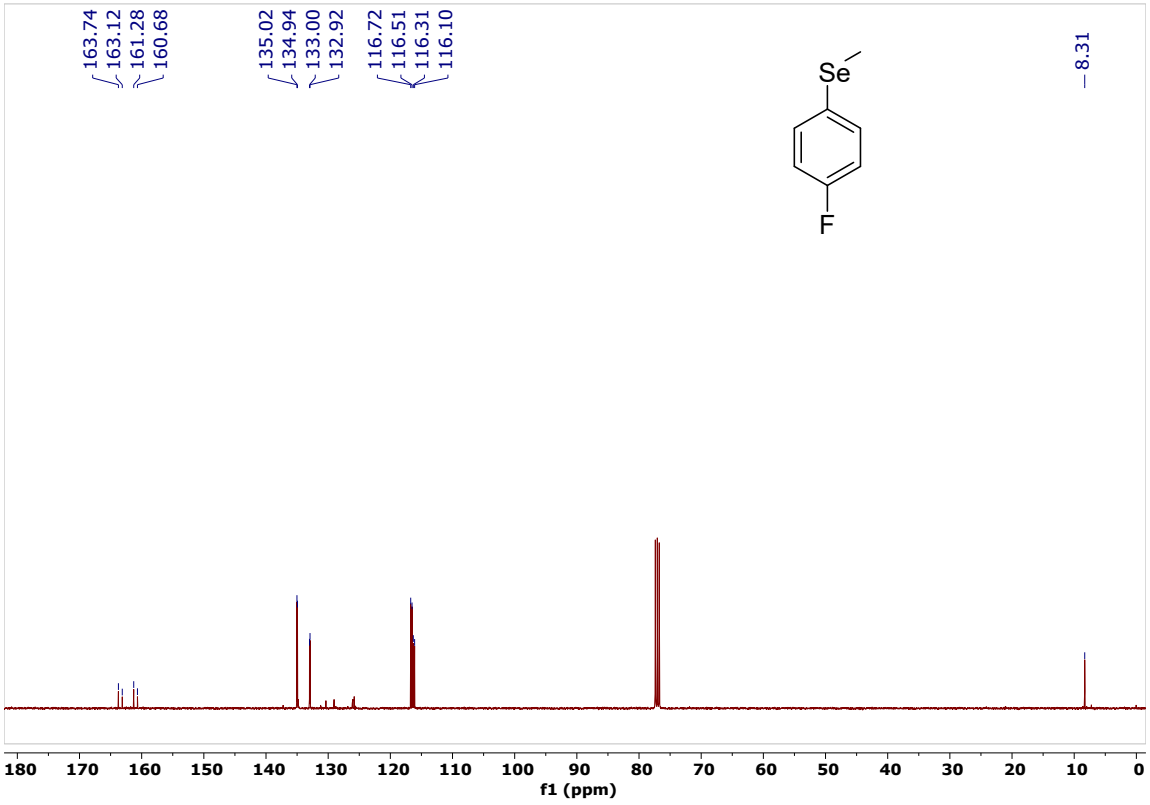


Figure 4: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1b**.

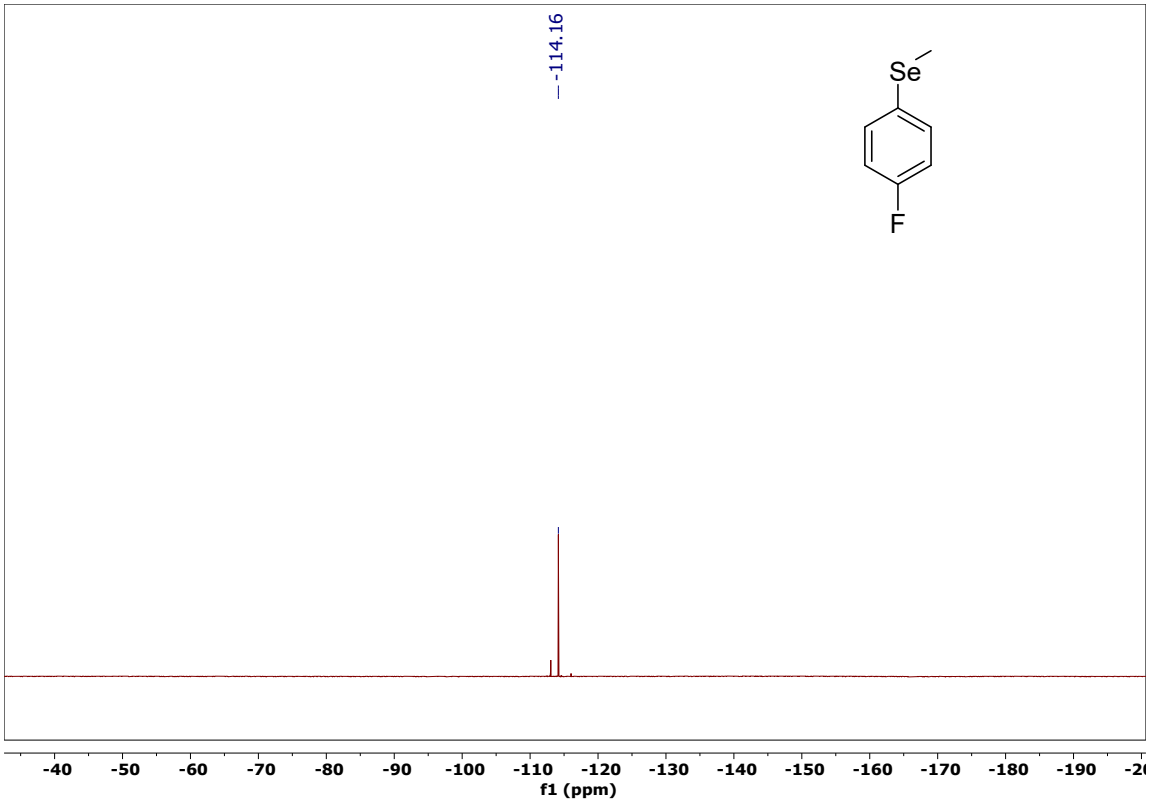


Figure 5: ^{19}F NMR (377 MHz, $CDCl_3$) of compound **1b**.

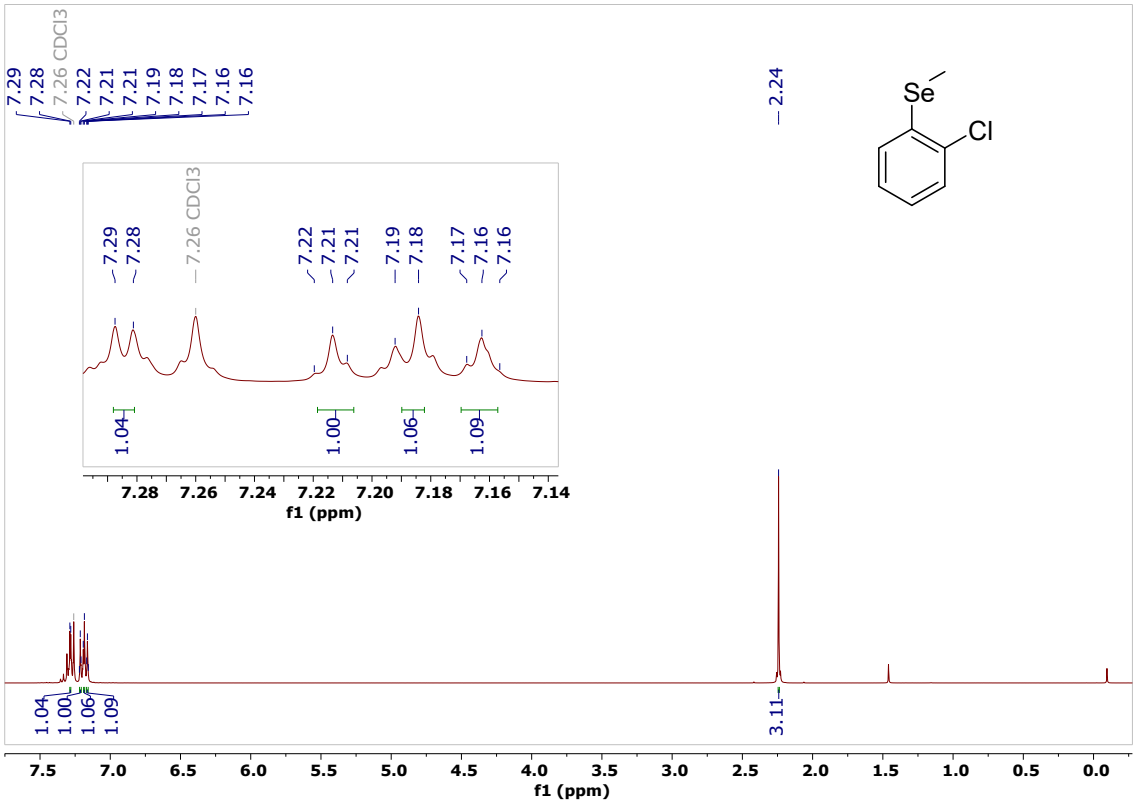


Figure 6: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1c.**

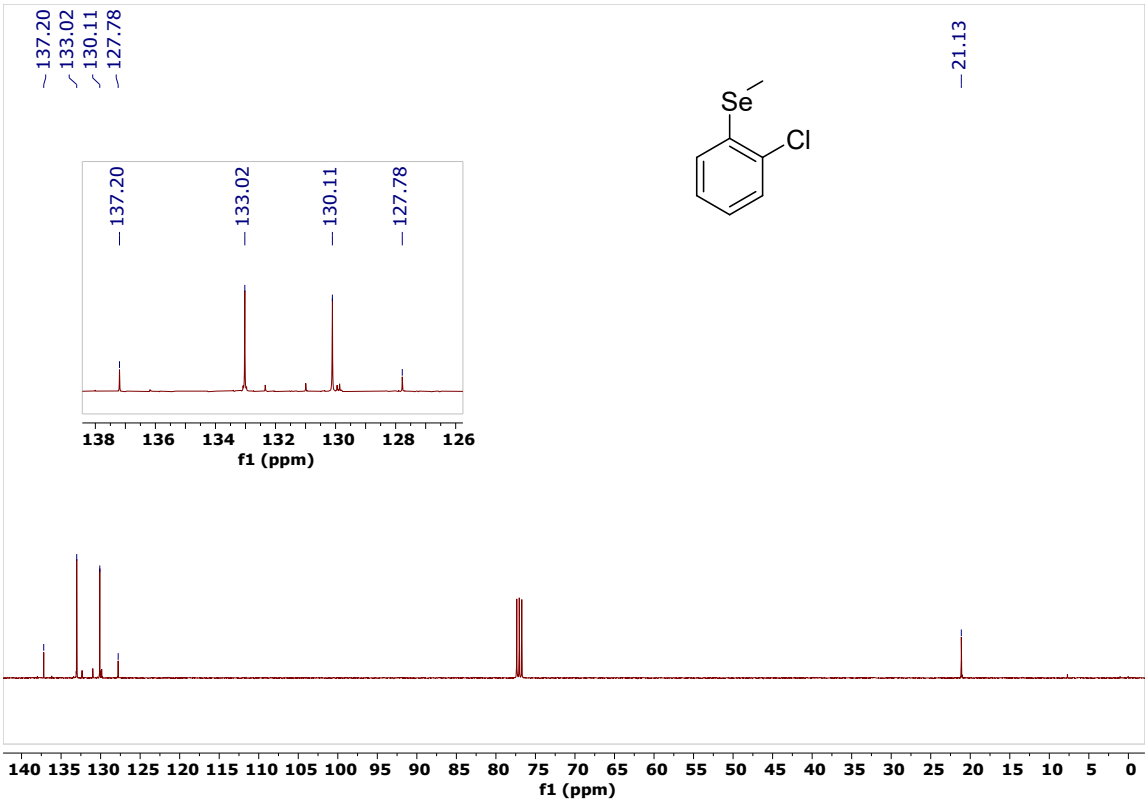


Figure 7: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1c**.

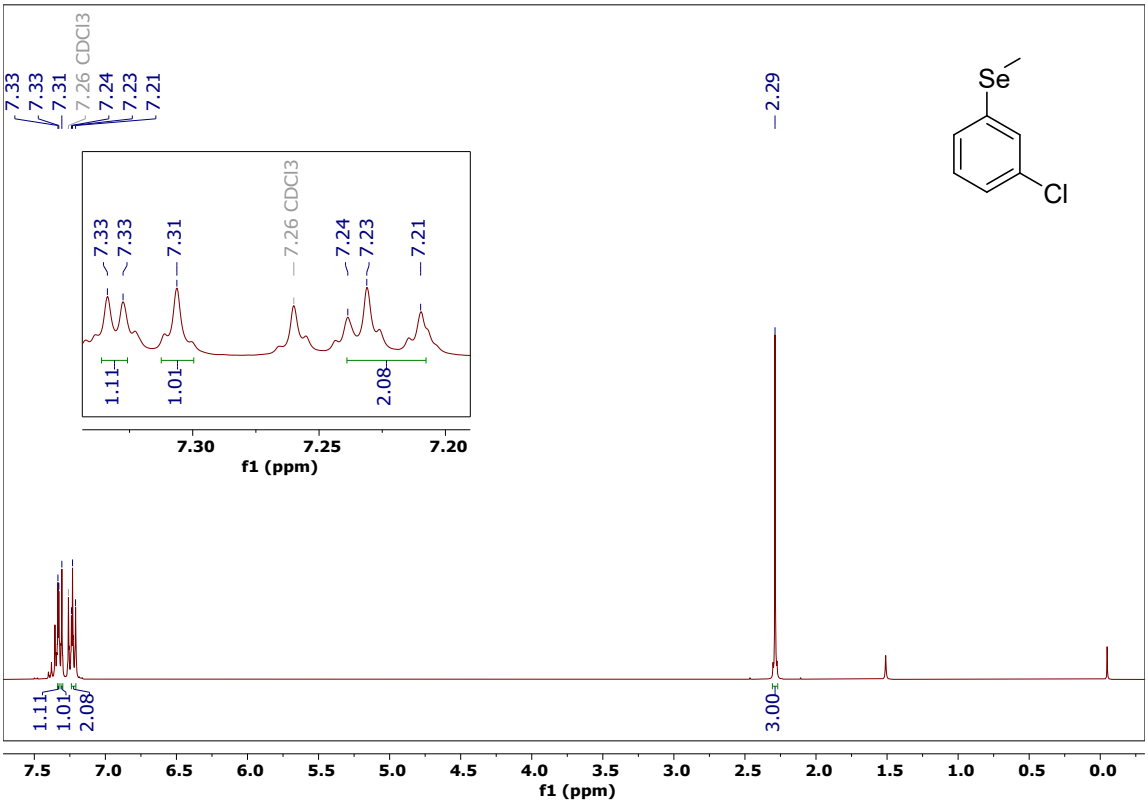


Figure 8: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1d.**

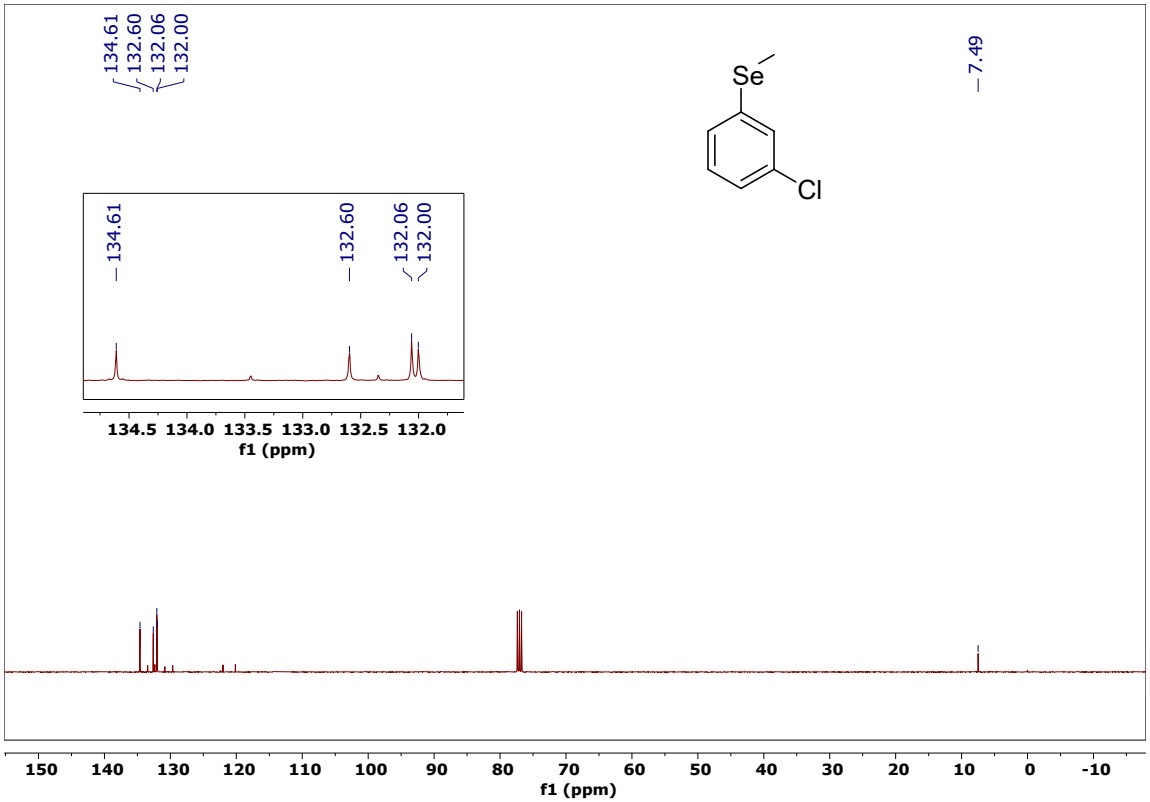


Figure 9: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1d**.

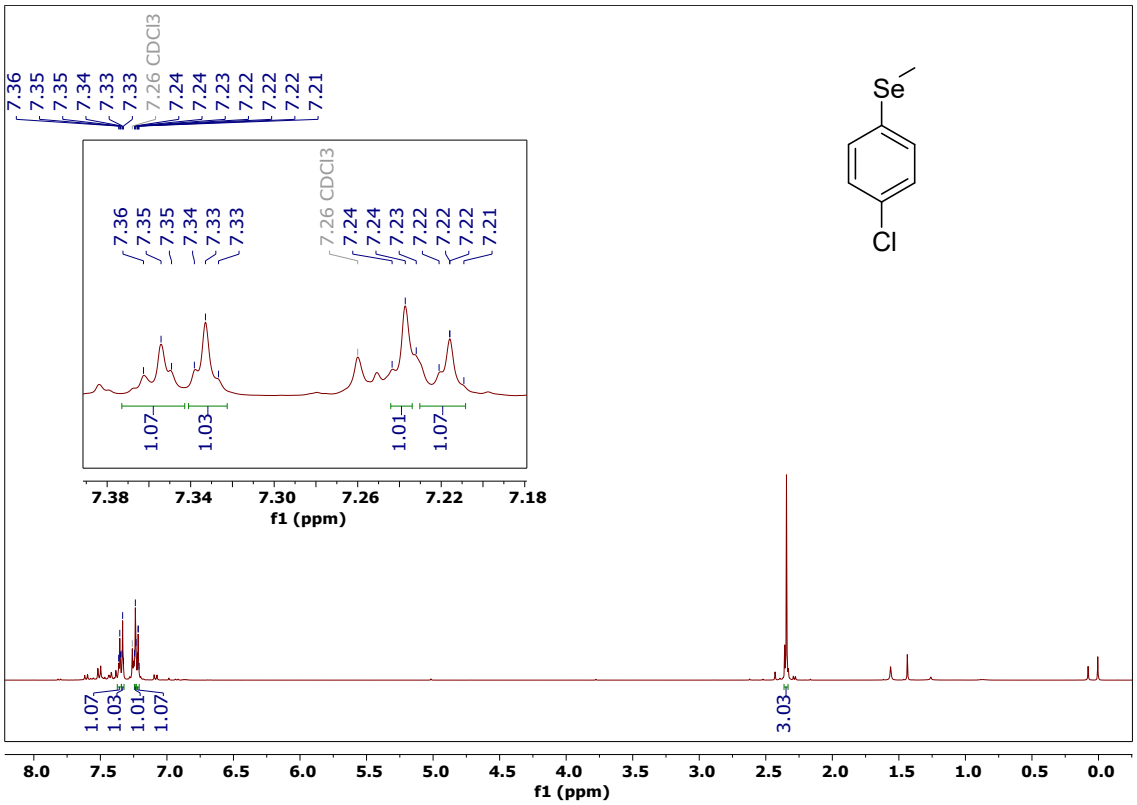


Figure 10: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1e.**

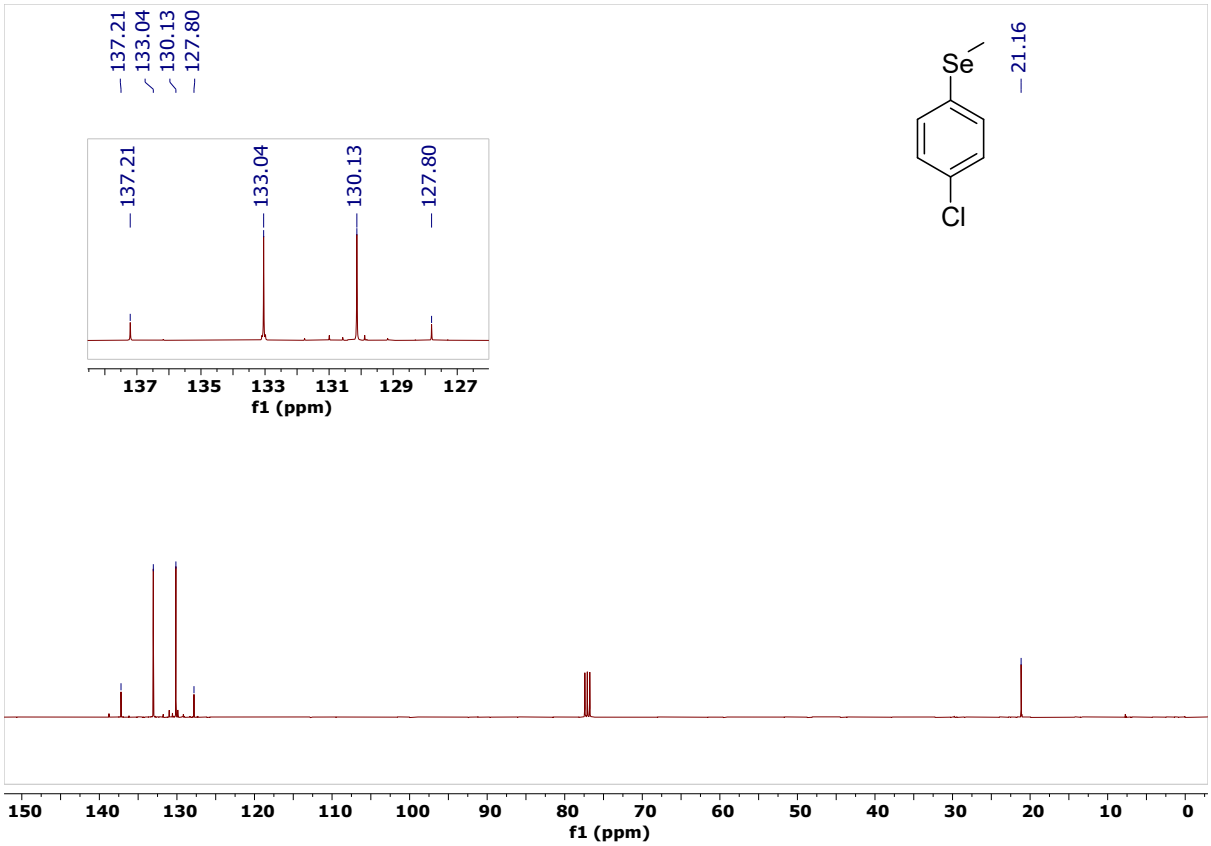


Figure 11: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1e**.

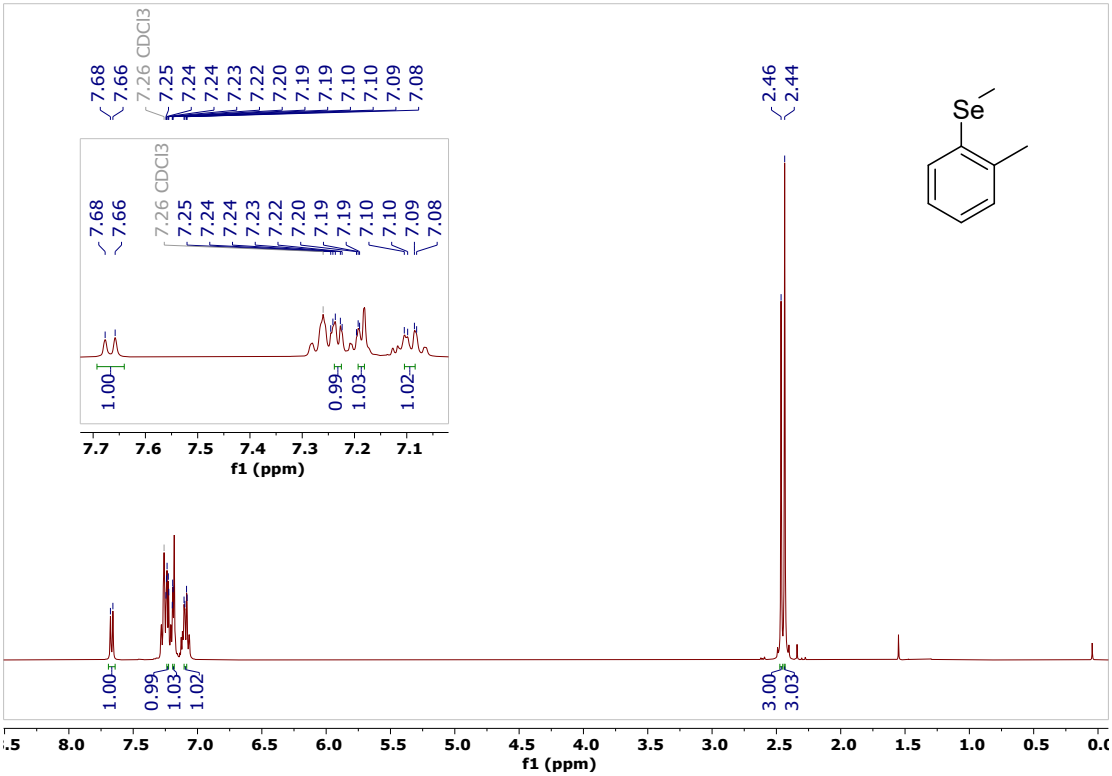


Figure 12: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1f.**

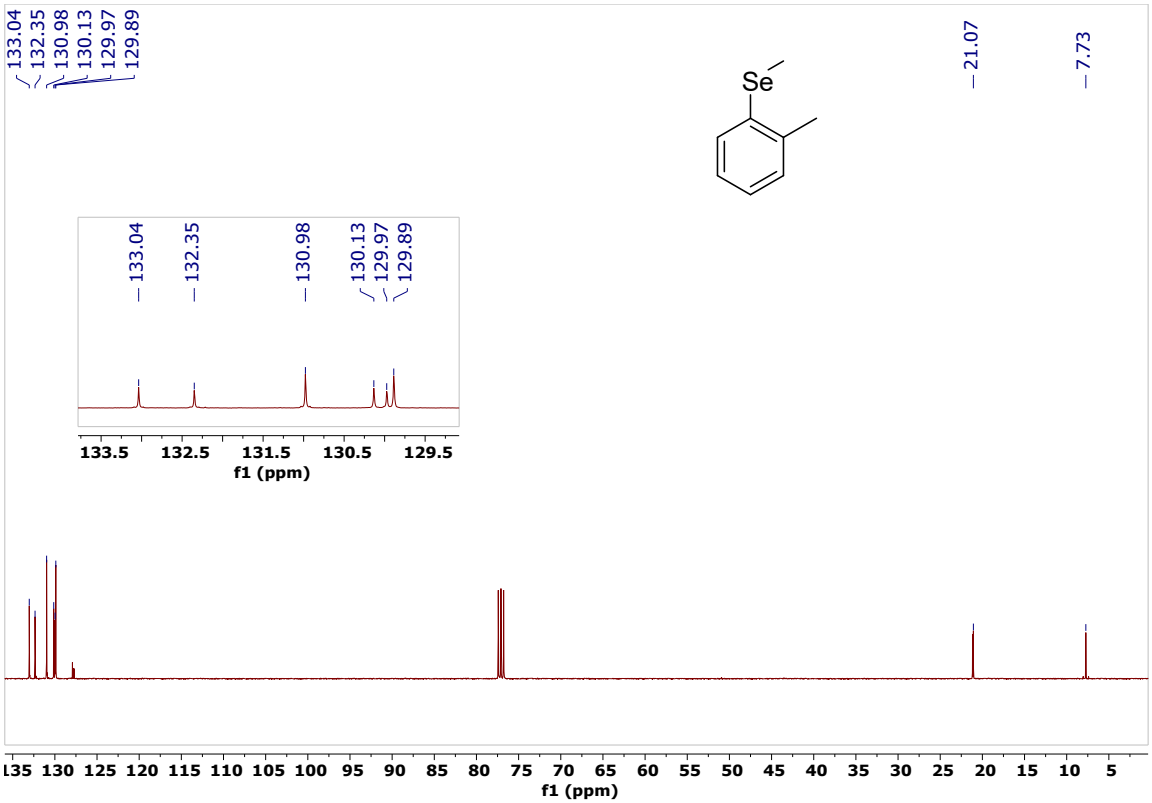


Figure 13: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1f**.

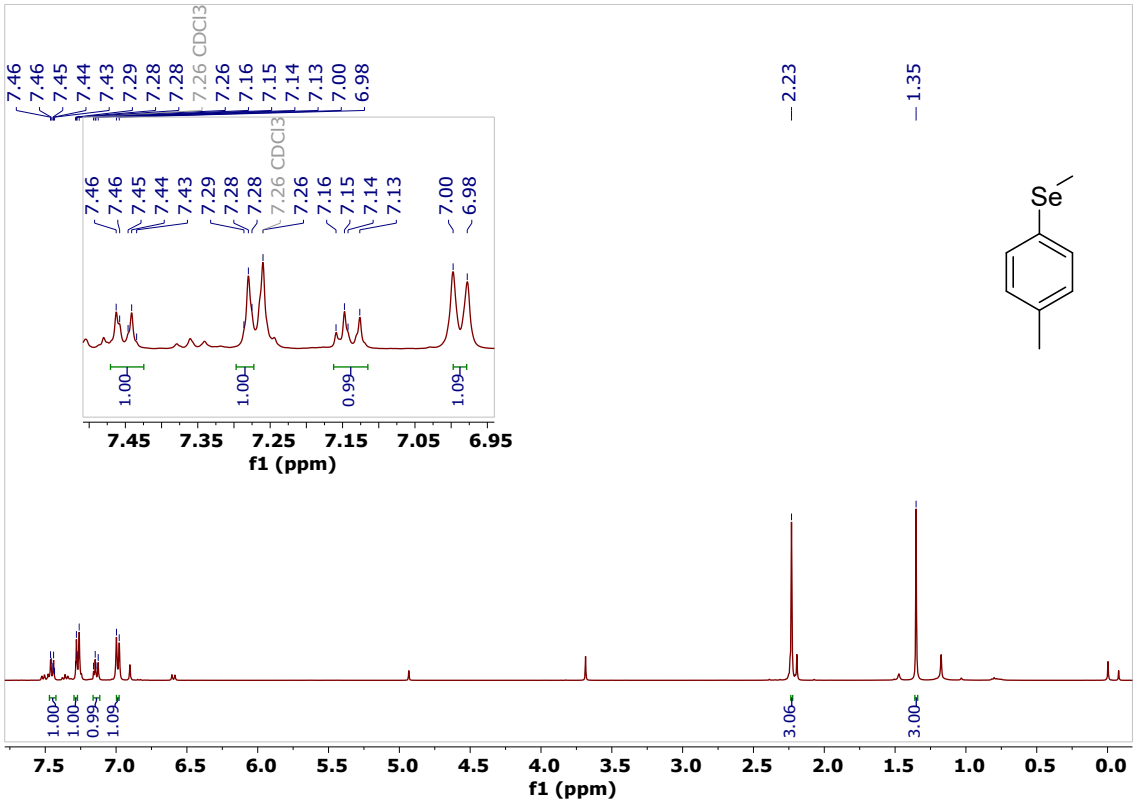


Figure 14: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1g.**

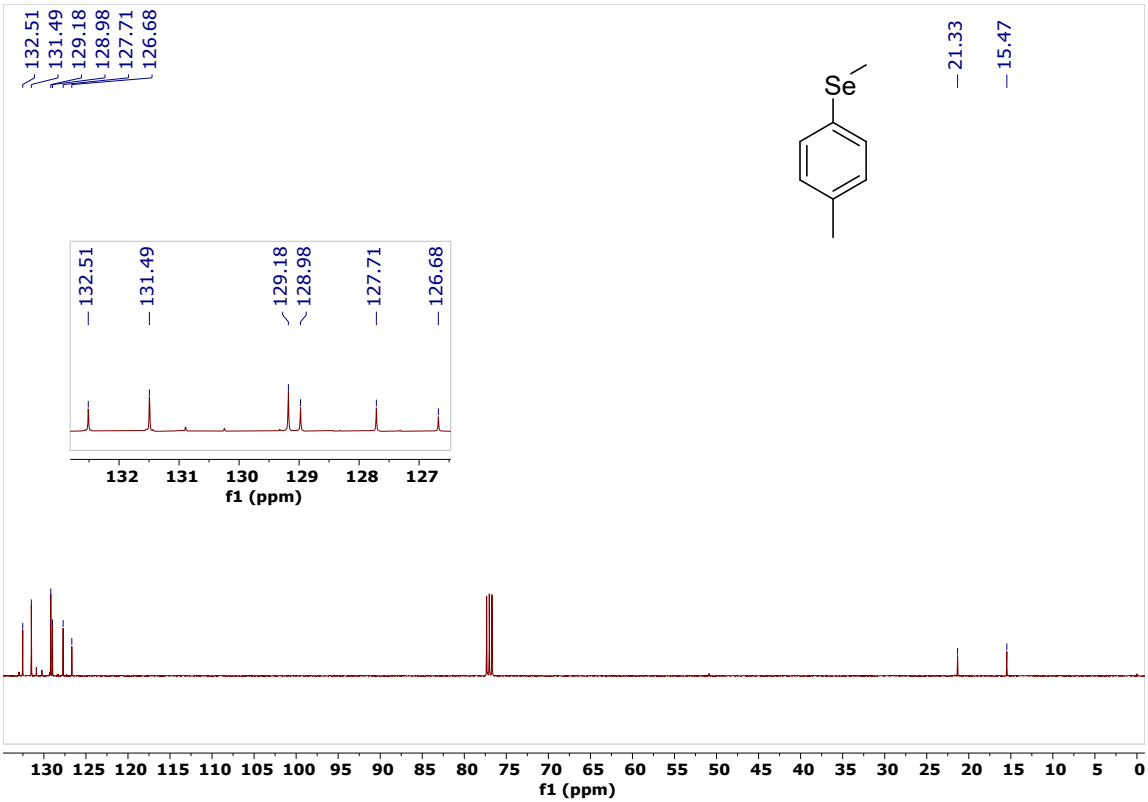


Figure 15: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1g**.

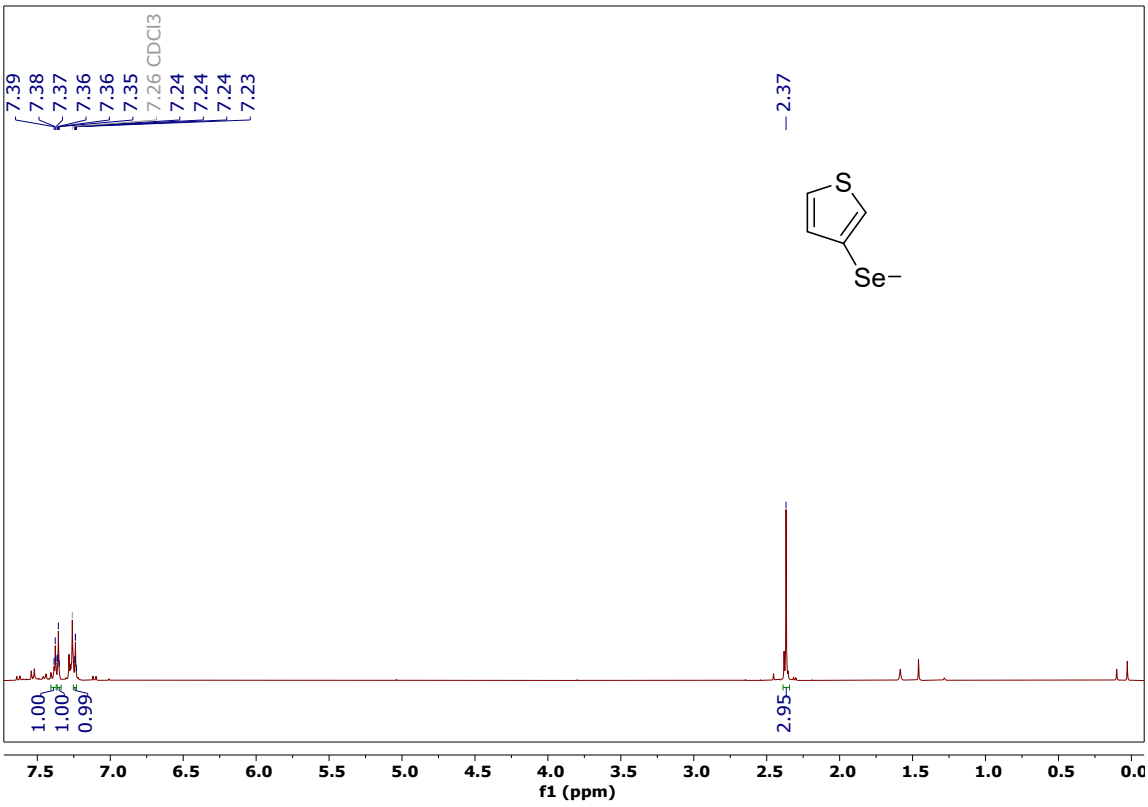


Figure 16: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1h.**

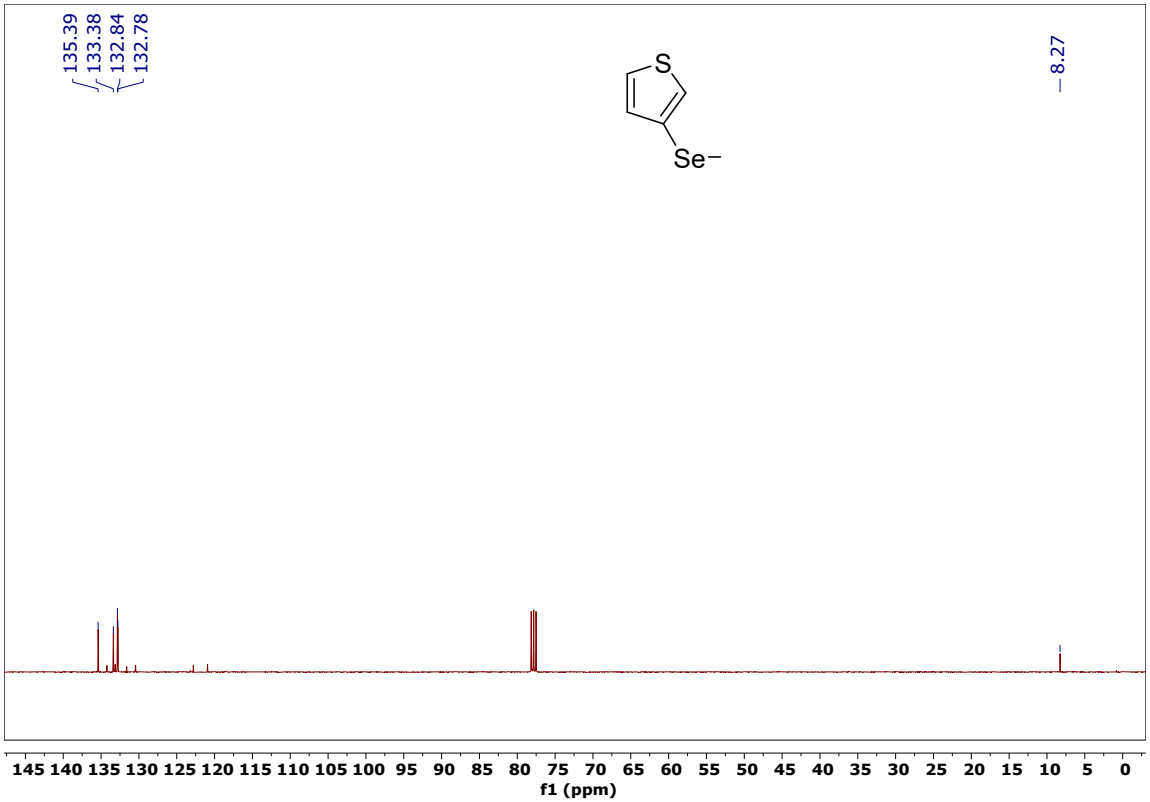


Figure 17: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1h**.

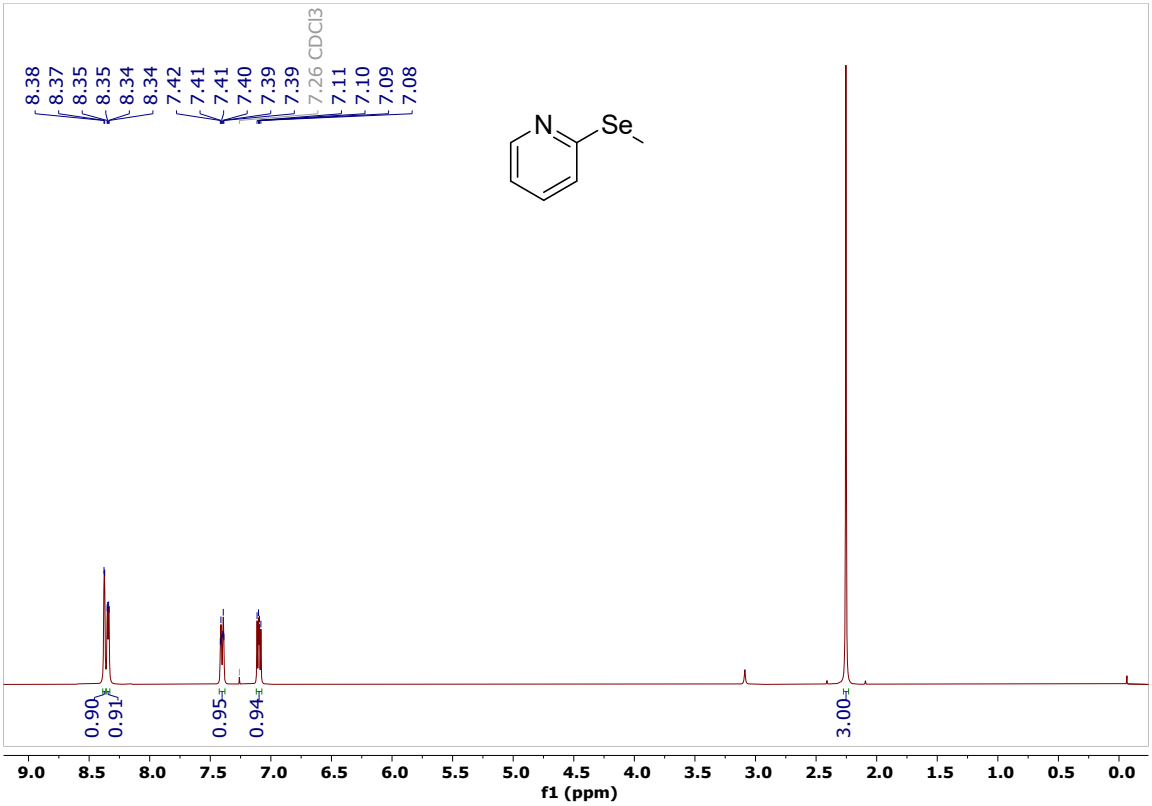


Figure 18: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1i.**

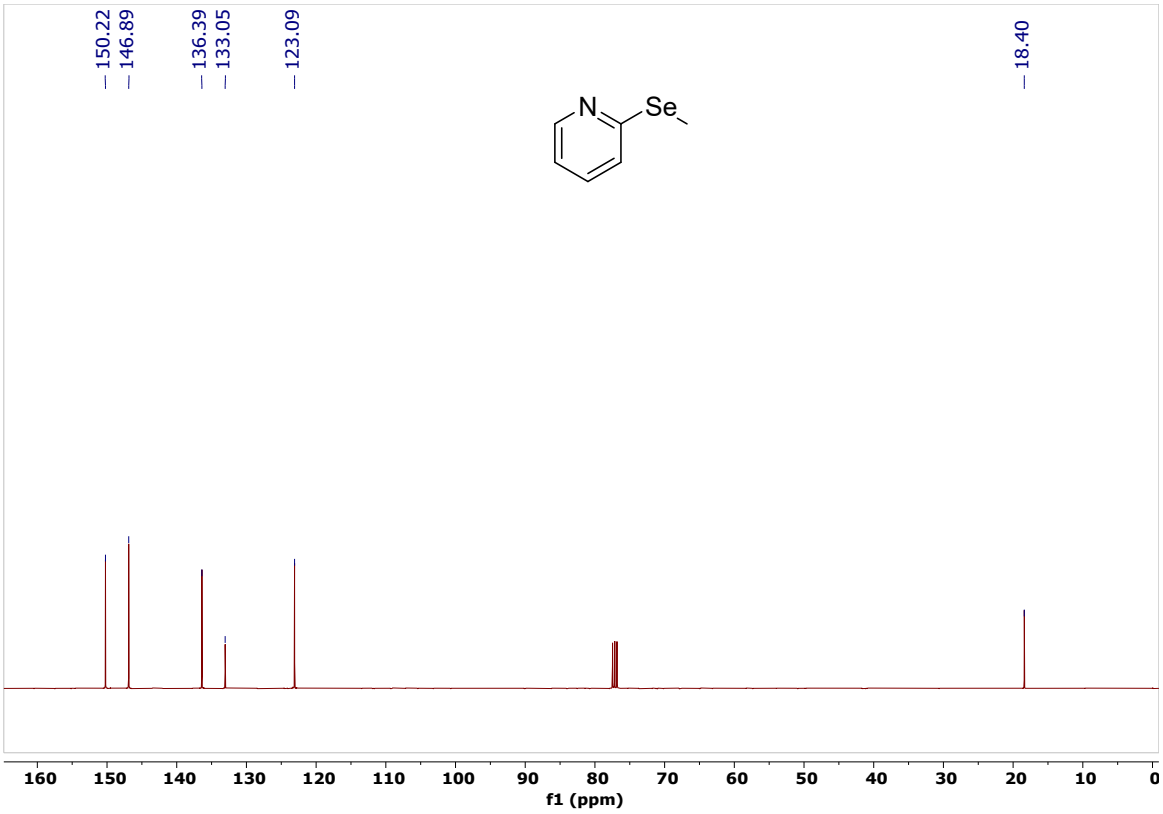


Figure 19: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1i**.

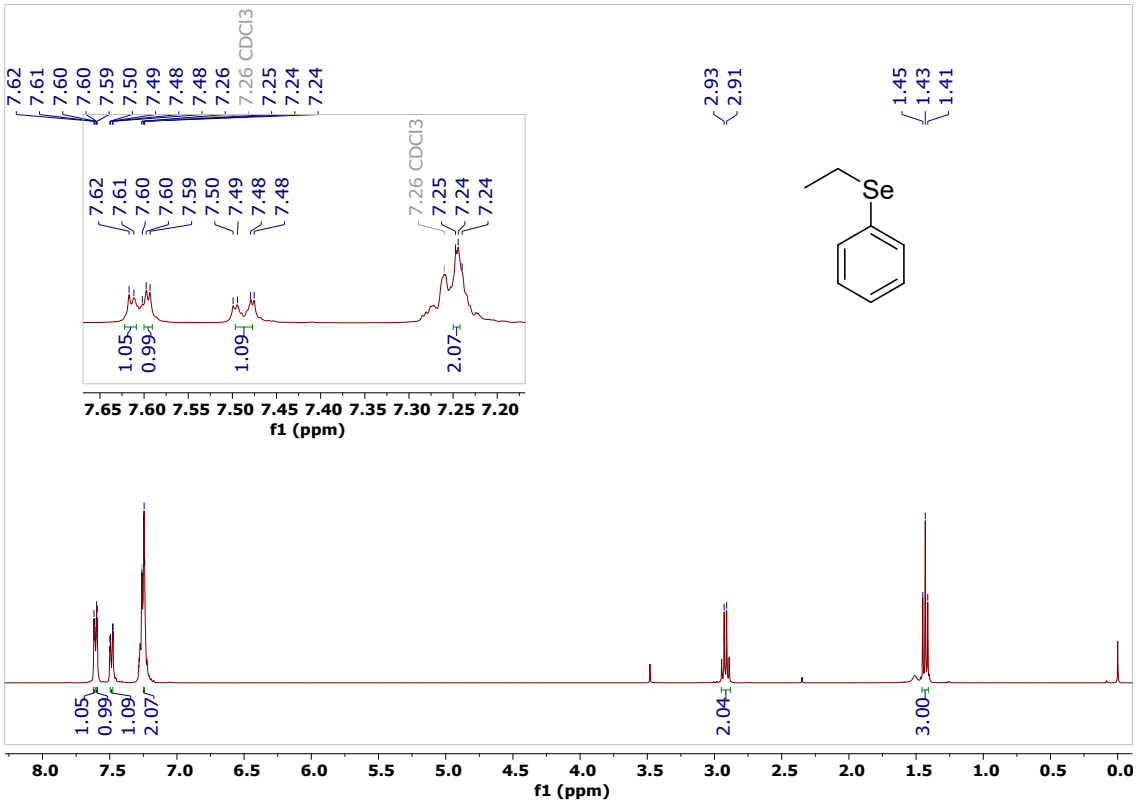


Figure 20: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1j.**

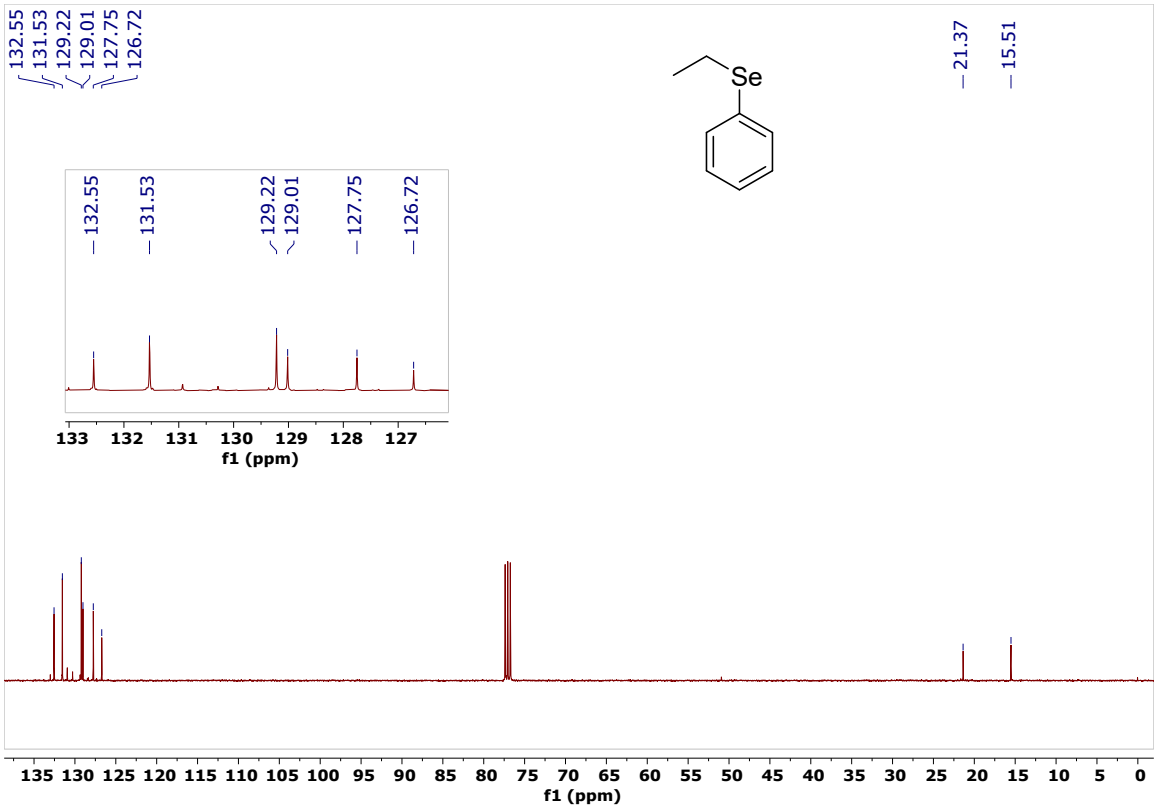


Figure 21: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1j**.

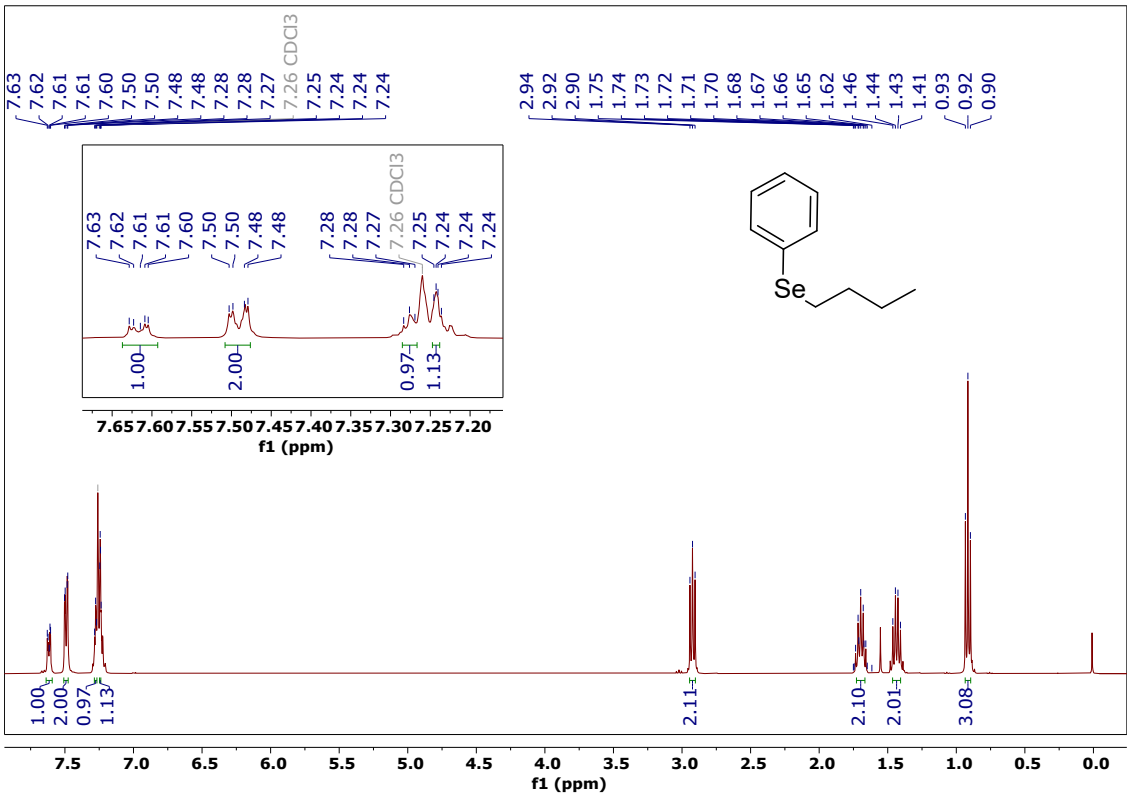


Figure 22: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1k.**

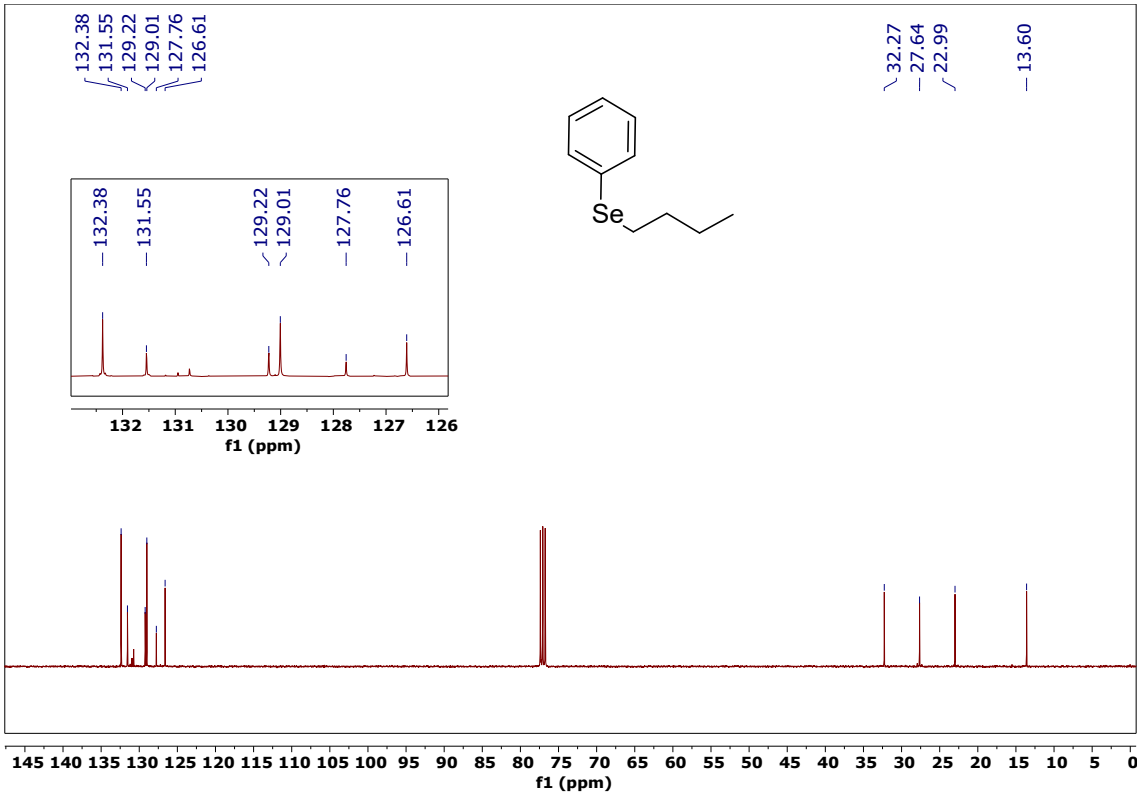


Figure 23: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1k**.

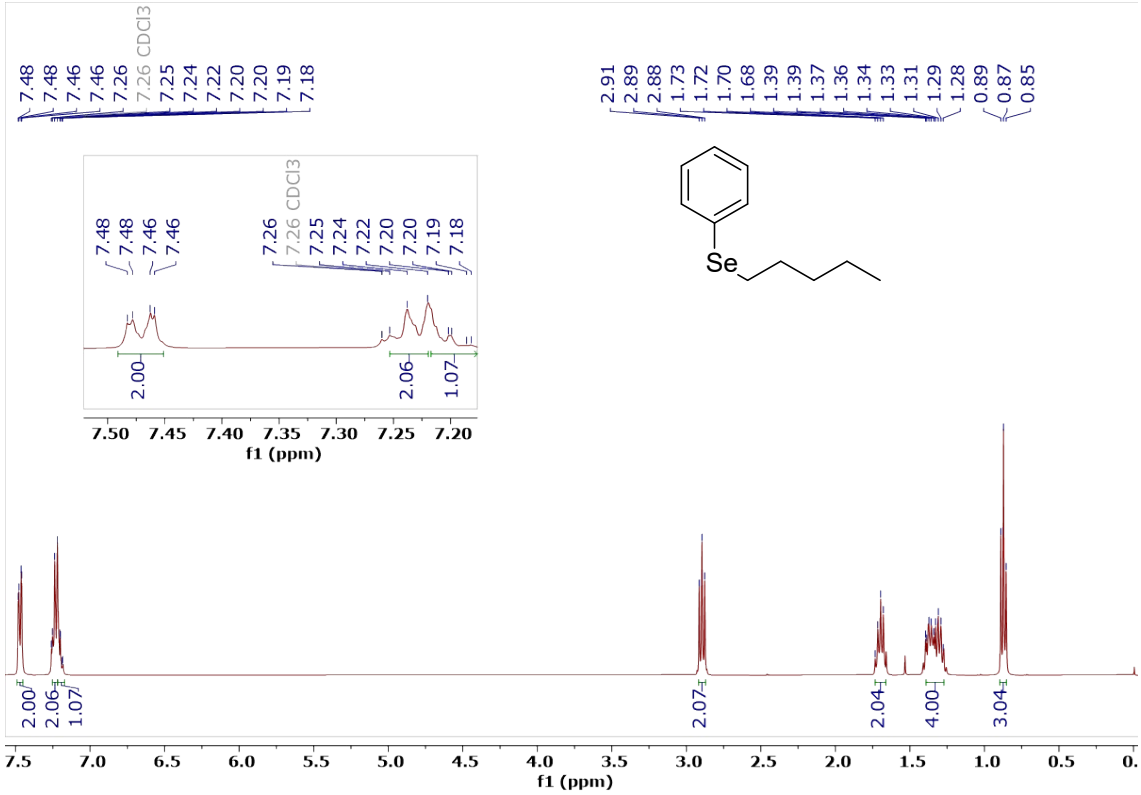


Figure 24: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1l.**

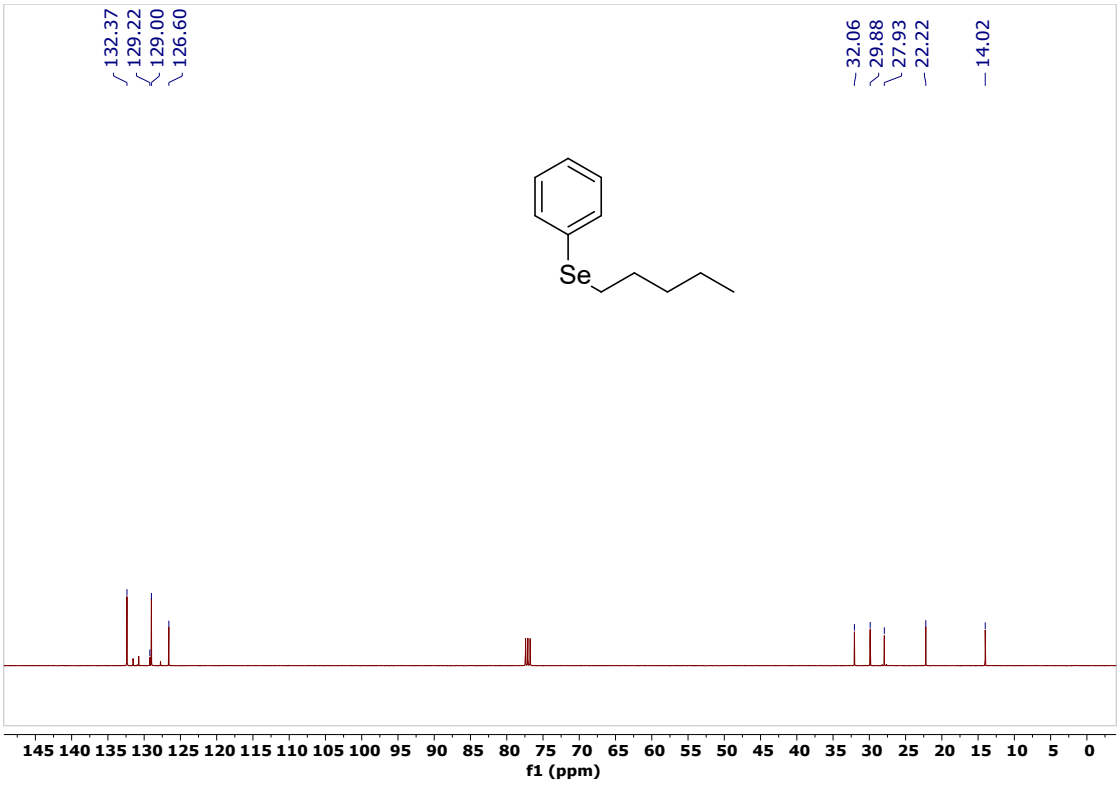


Figure 25: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1l**.

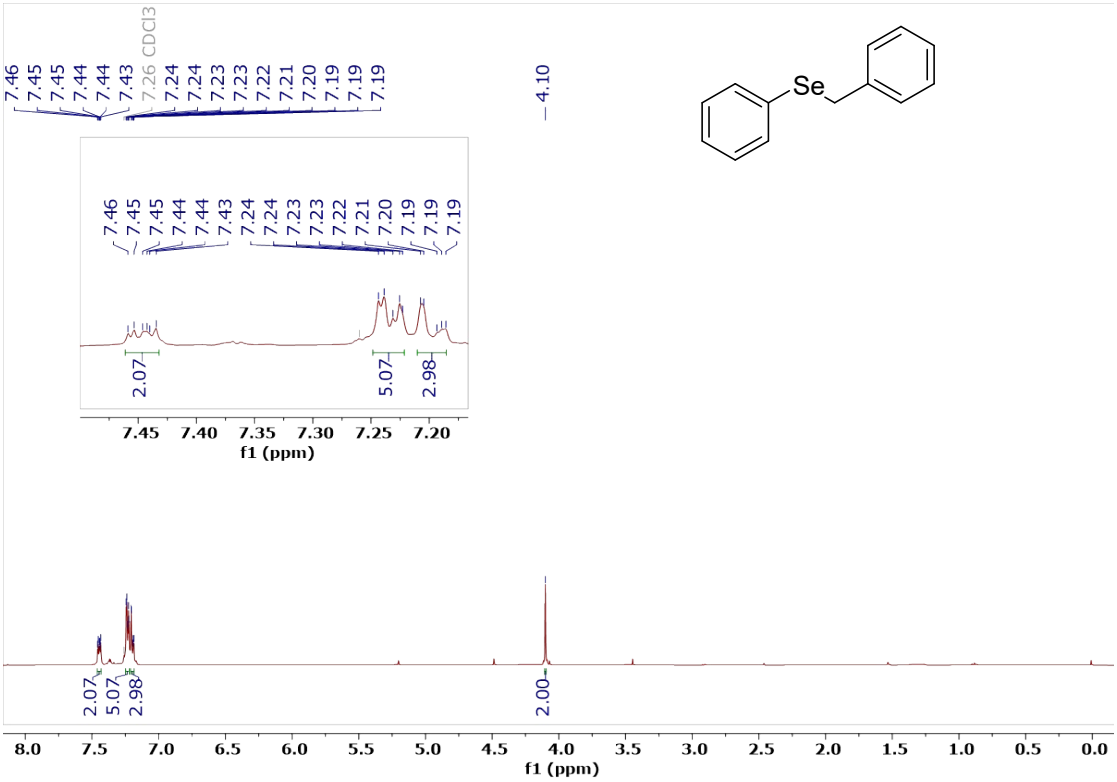


Figure 26: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1m.**

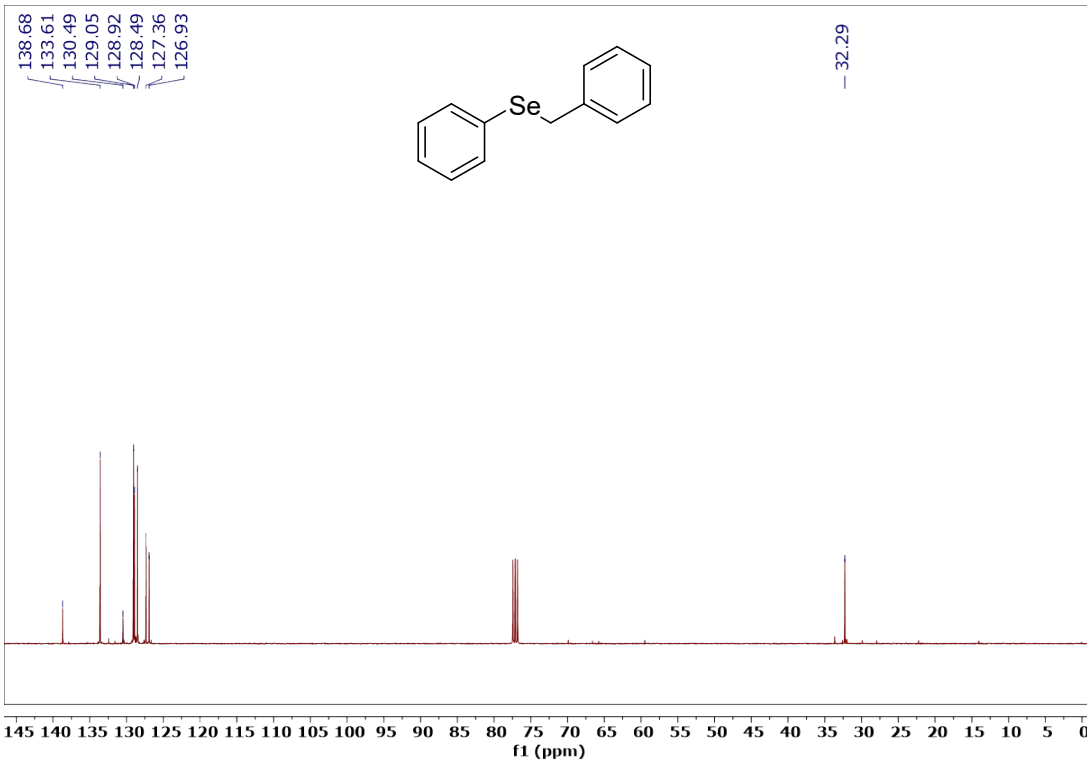


Figure 27: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **1m**.

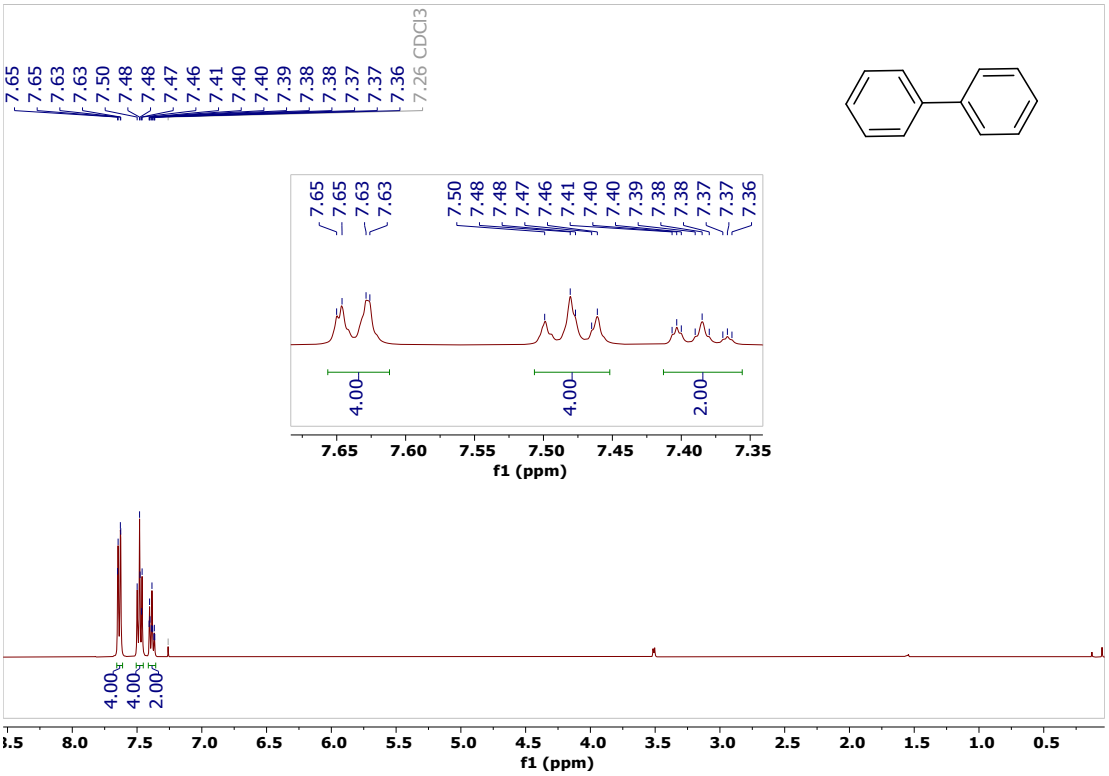


Figure 28: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3a.**

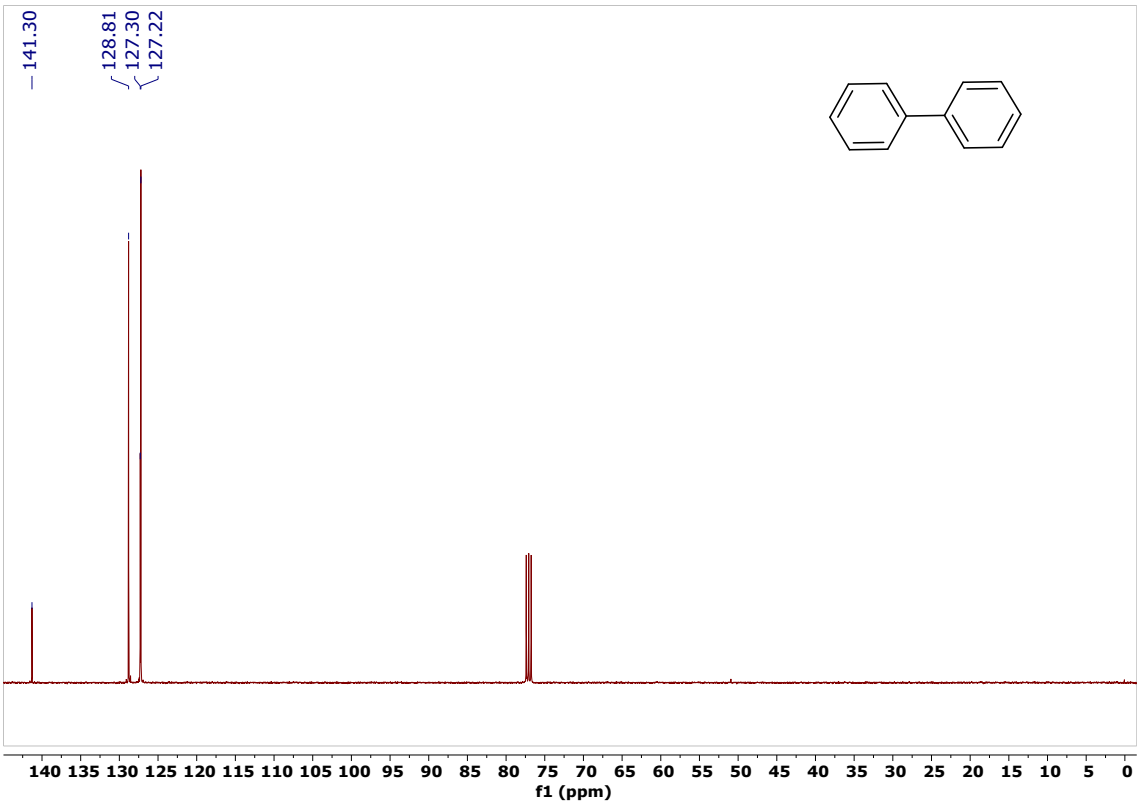


Figure 29: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3a**.

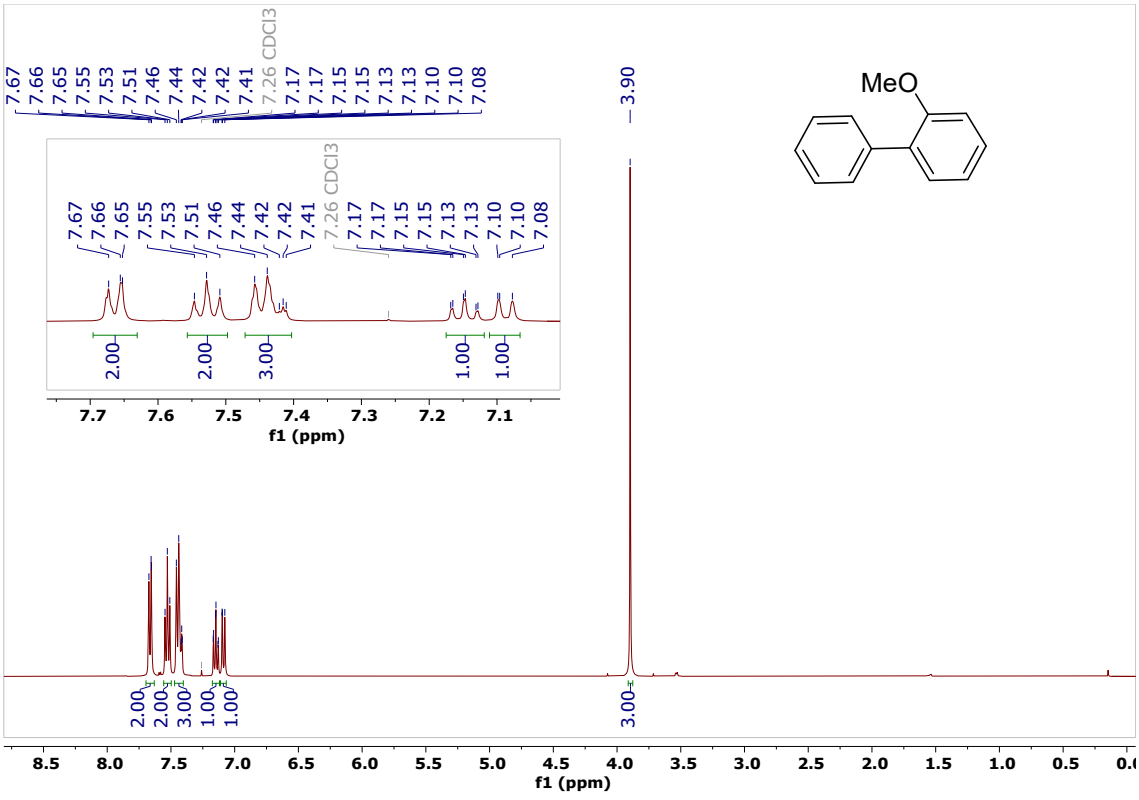


Figure 30: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3b.**

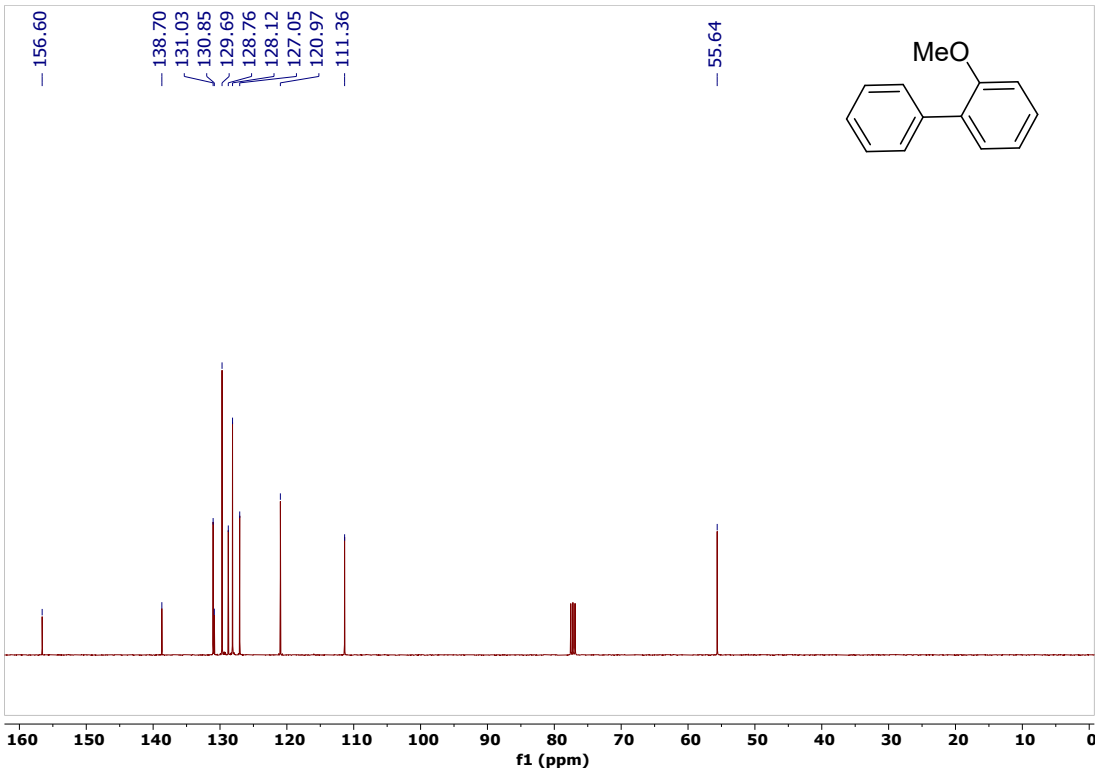


Figure 31: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3b**.

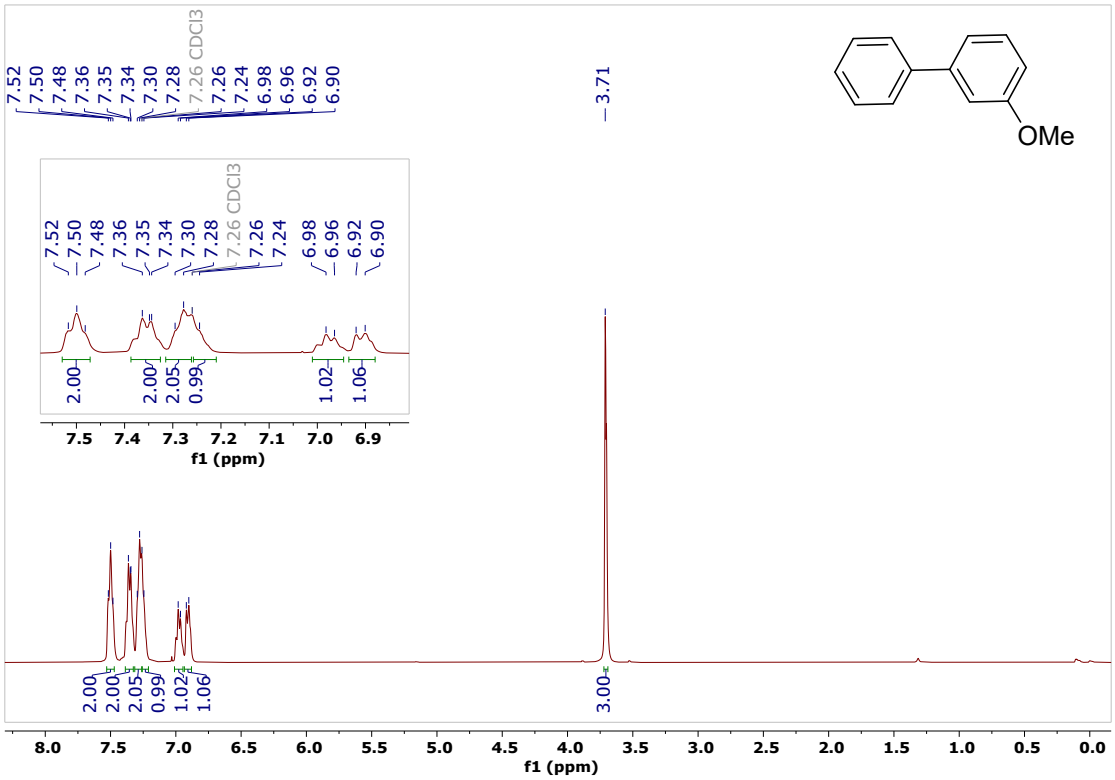


Figure 32: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3c.**

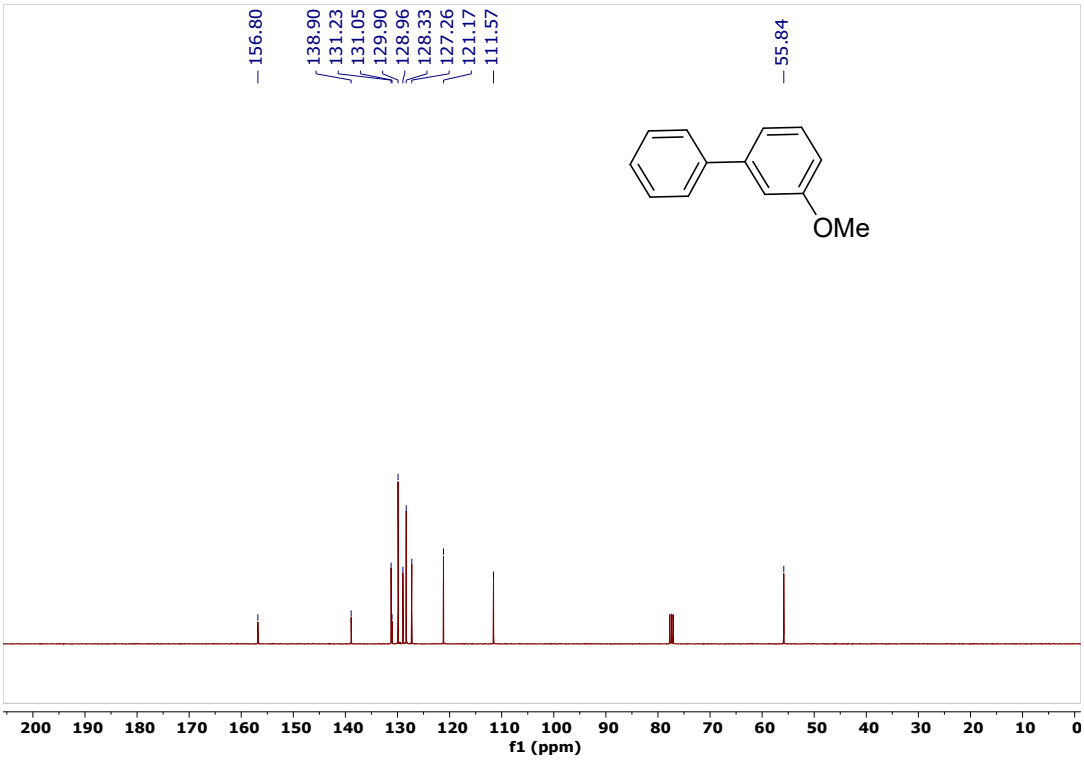


Figure 33: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3c**.

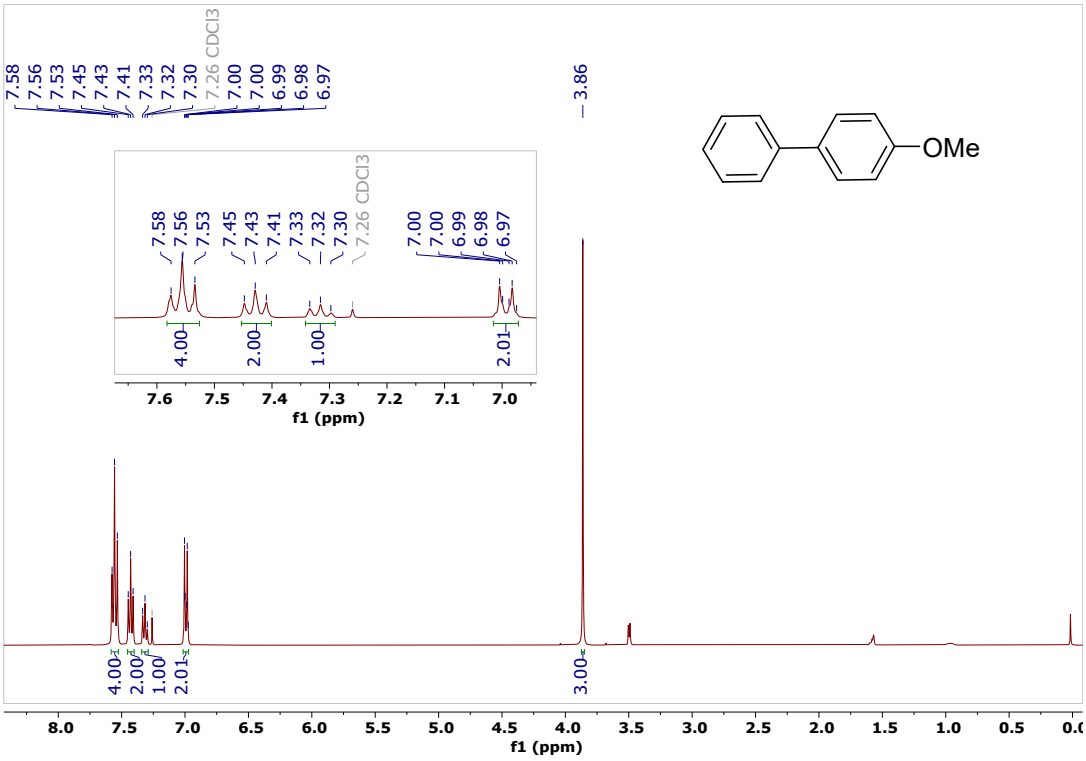


Figure 34: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3d.**

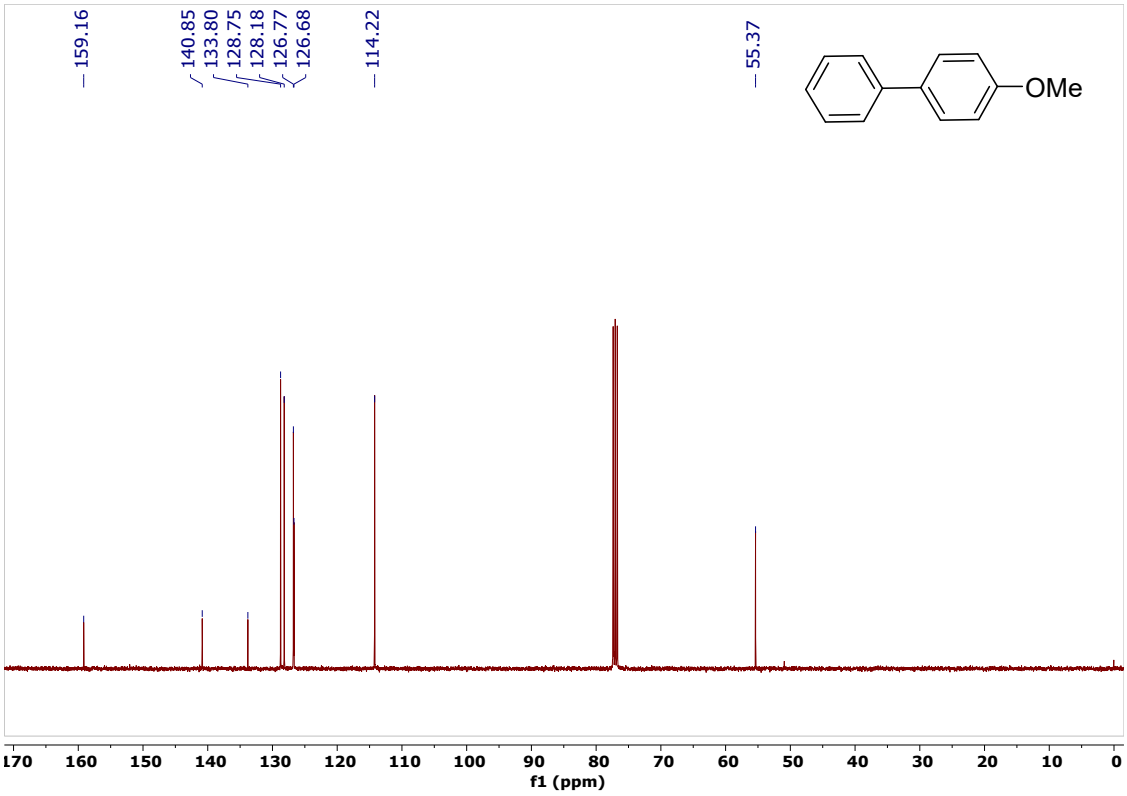


Figure 35: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3d**.

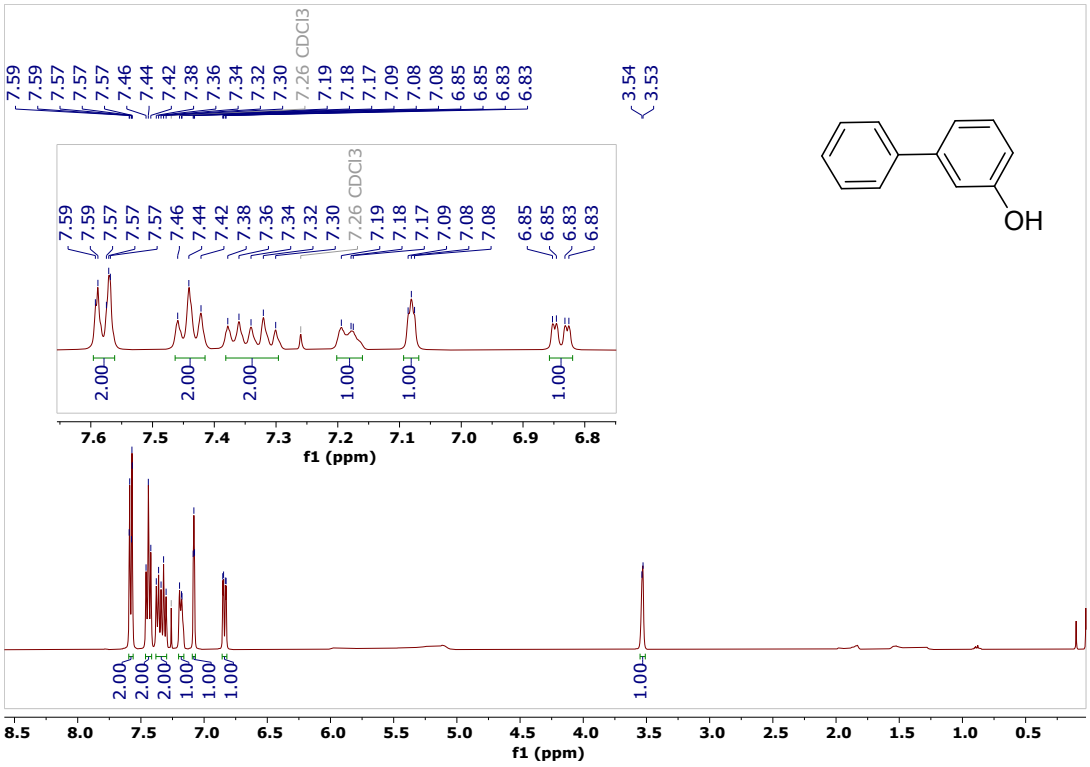


Figure 36: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3e.**

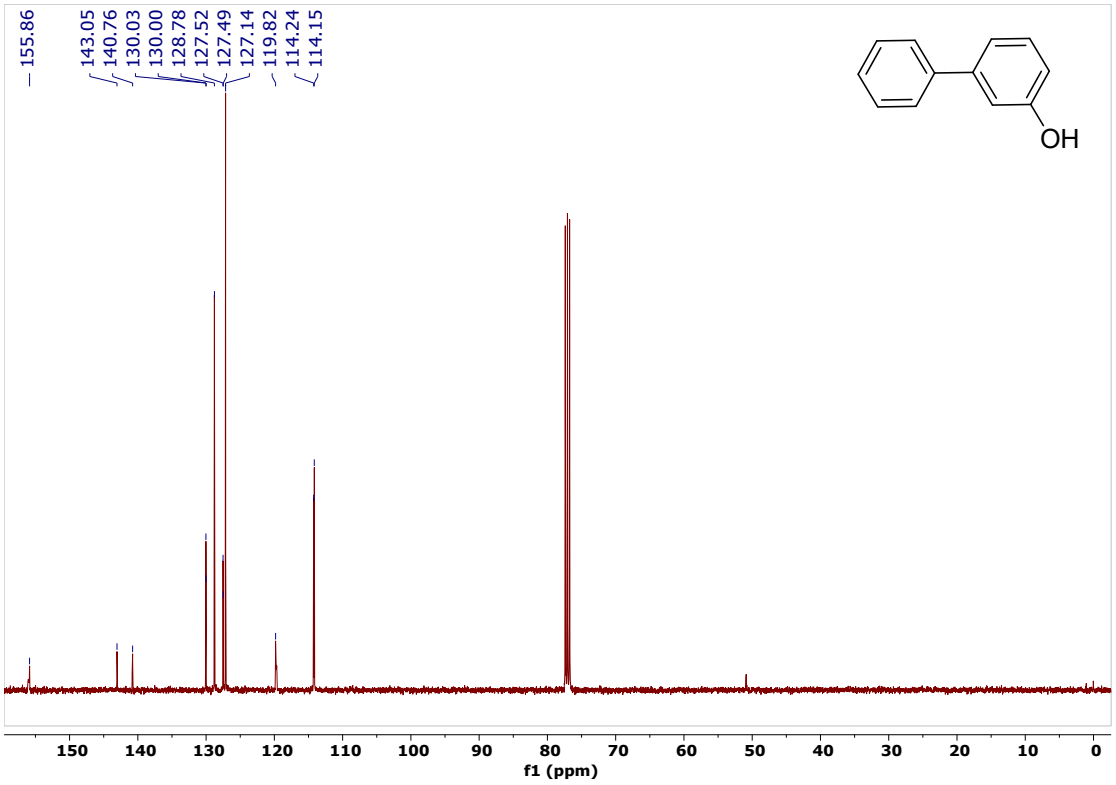


Figure 37: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3e**.

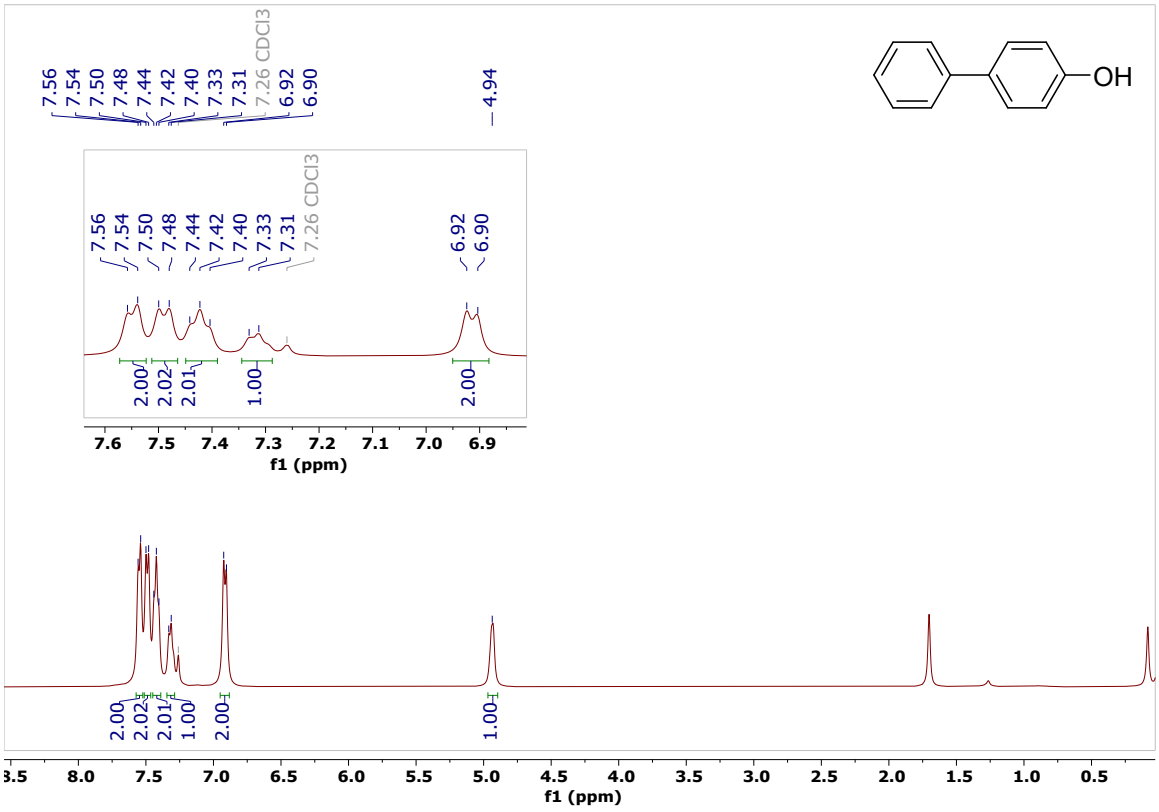


Figure 38: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3f.**

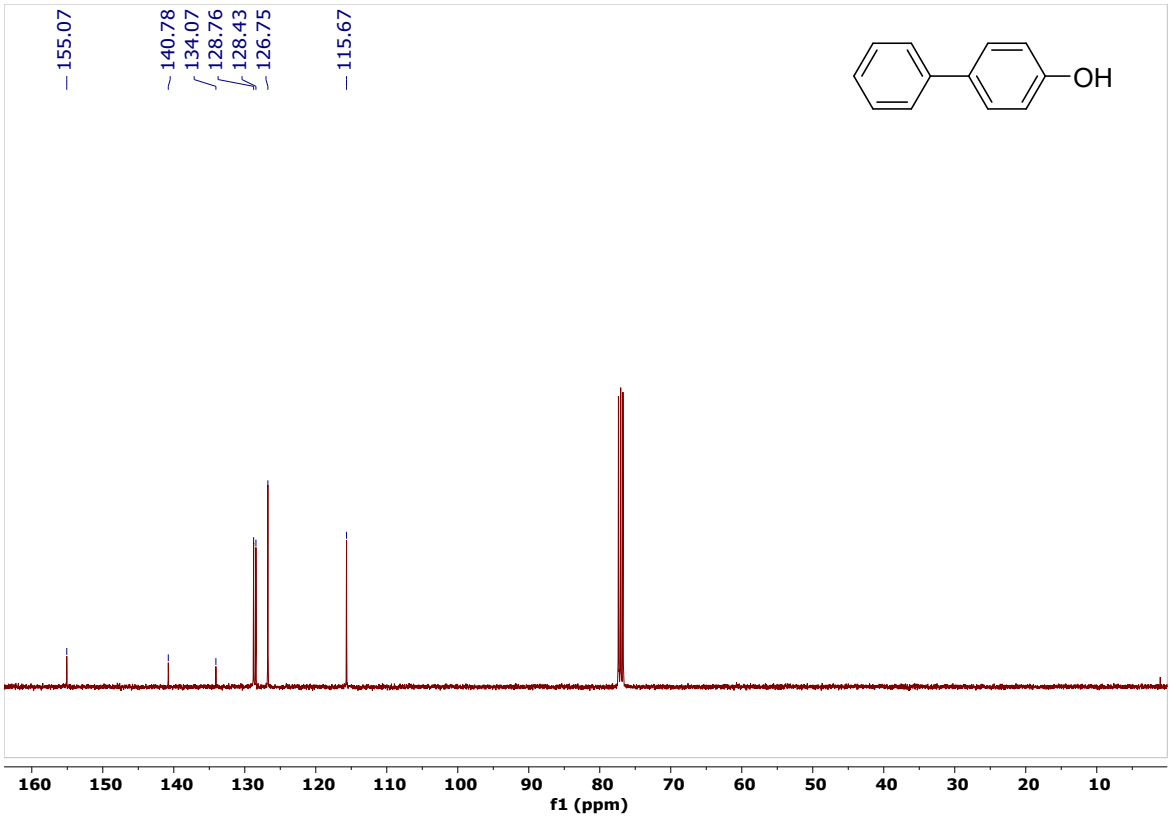


Figure 39: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3f**.

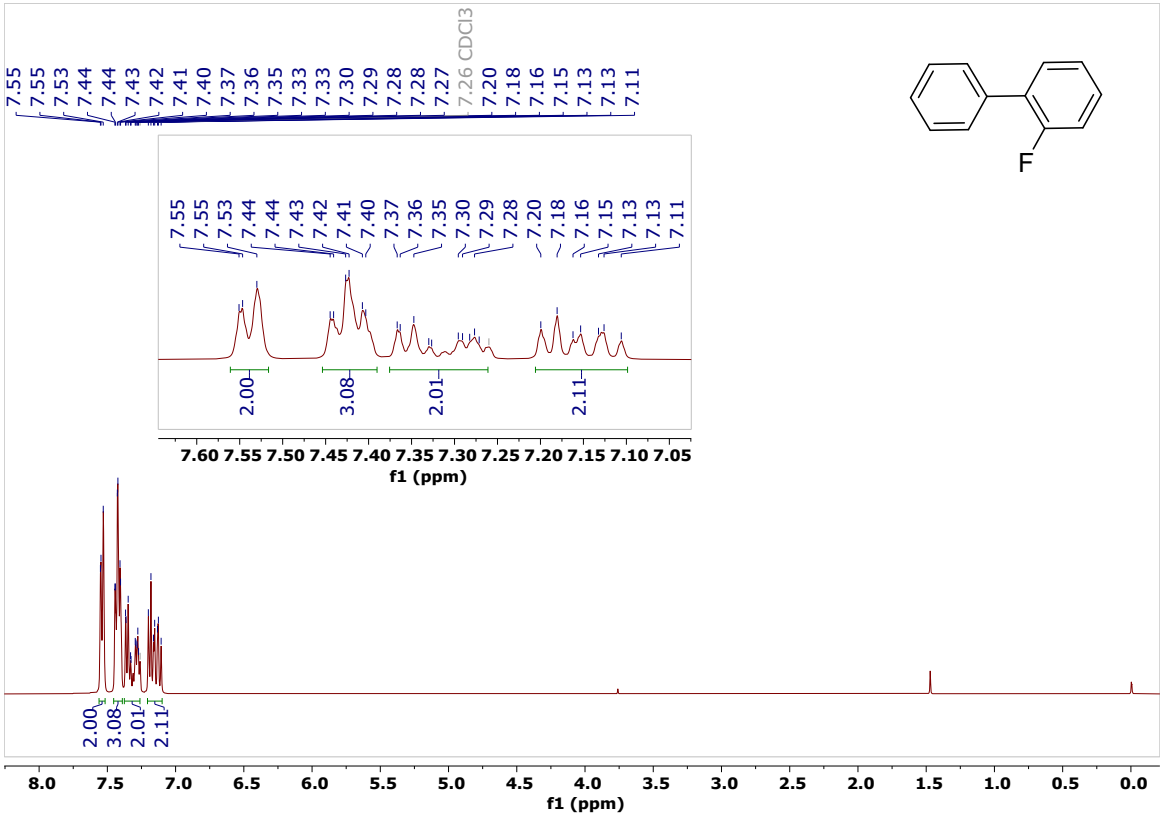


Figure 40: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3g.**

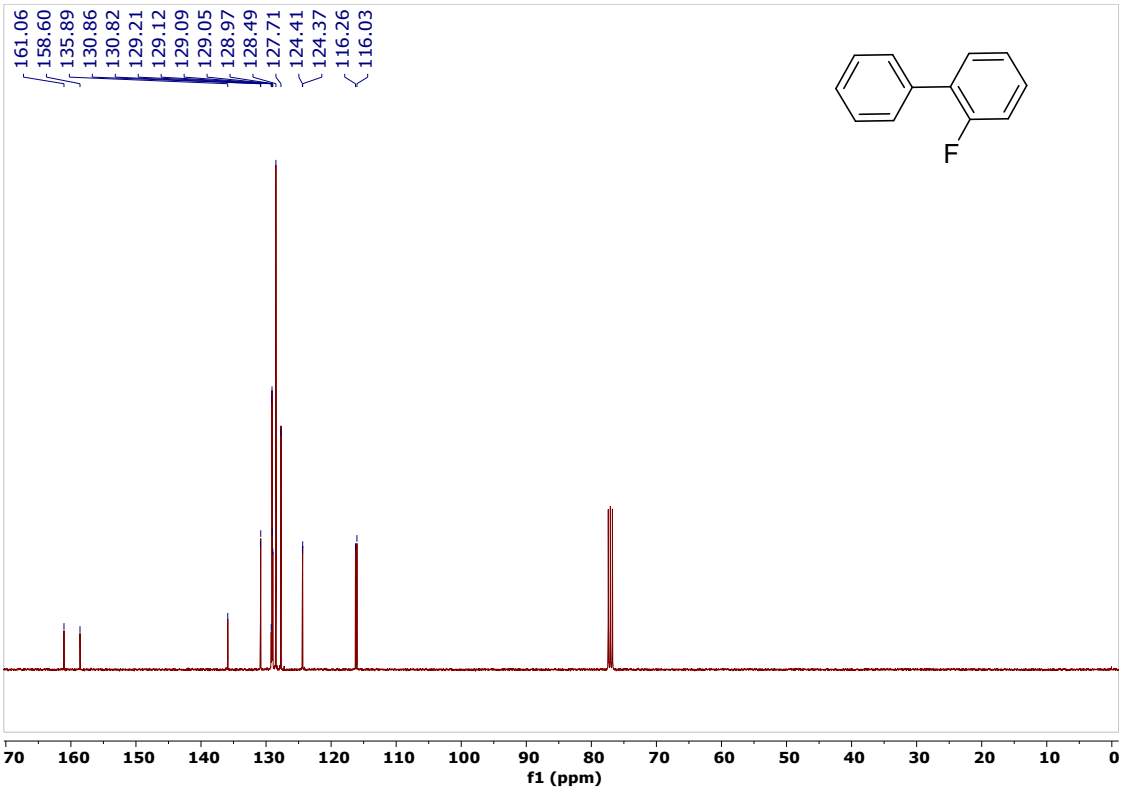


Figure 41: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3g**.

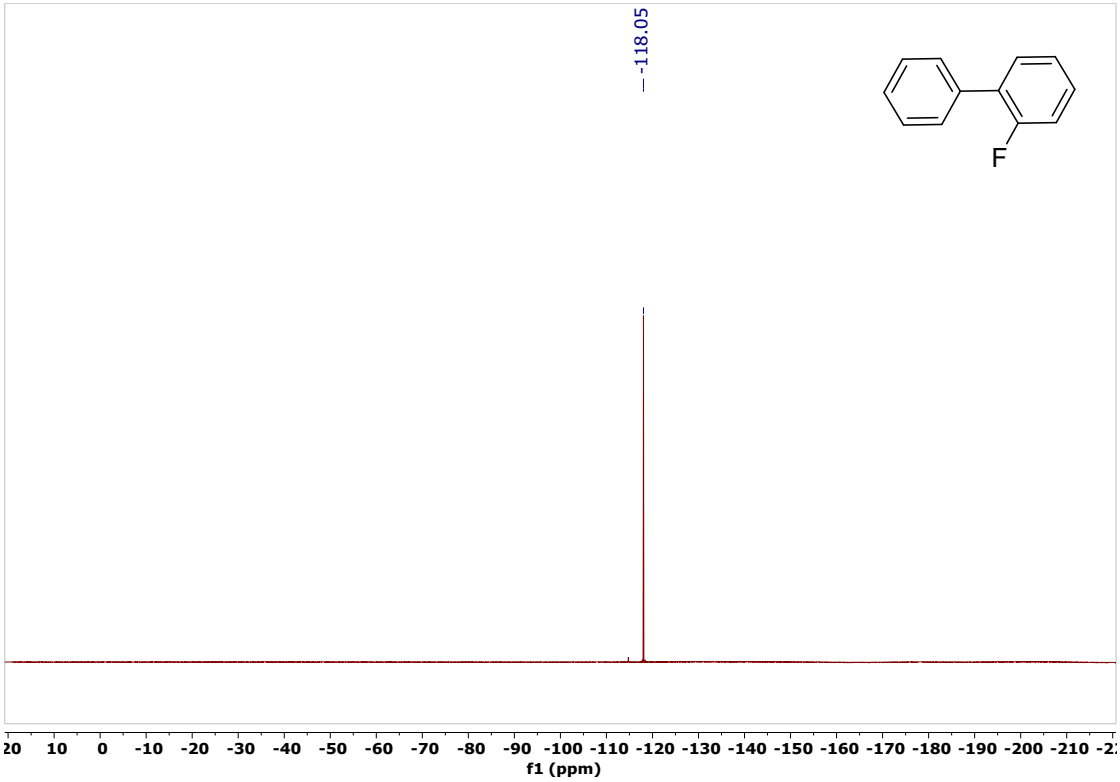


Figure 42: ^{19}F NMR (377 MHz, $CDCl_3$) of compound **3g**.

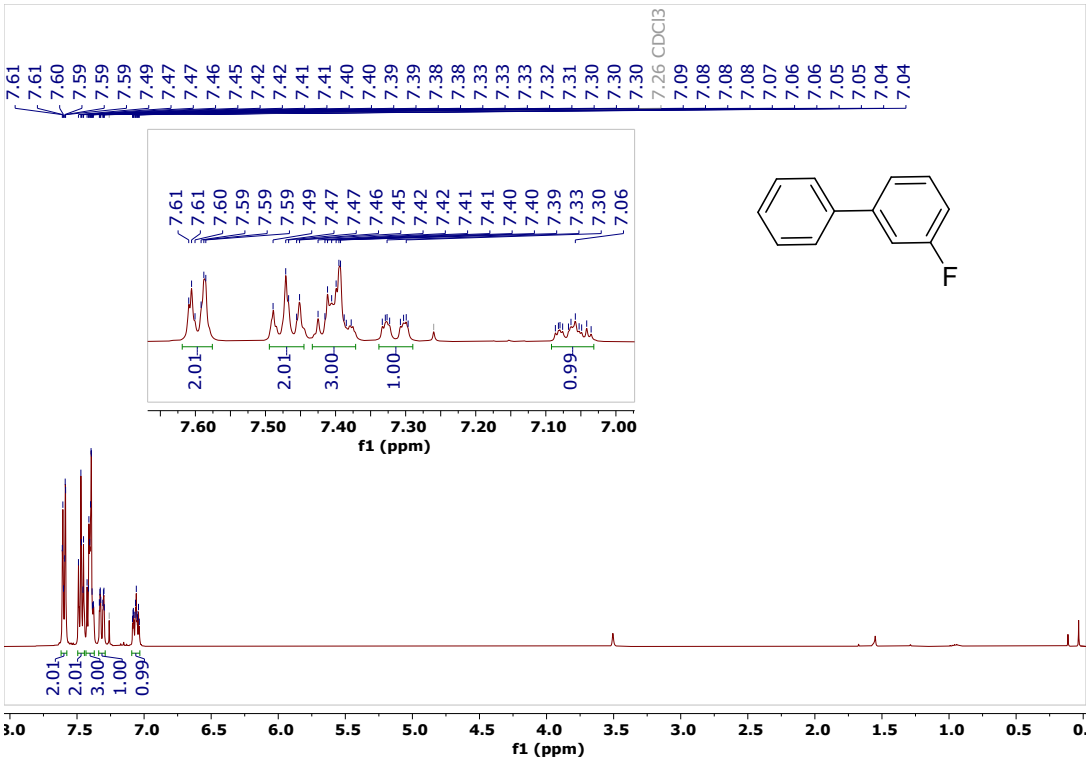


Figure 43: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3h.**

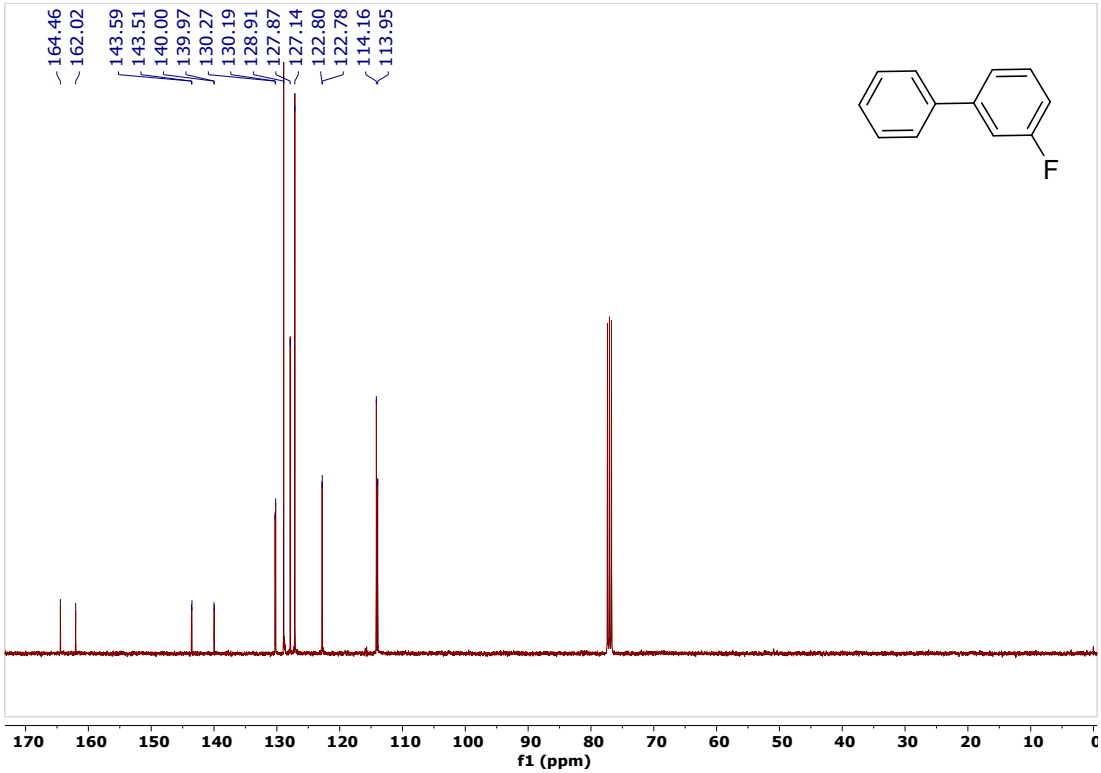


Figure 44: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3h**.

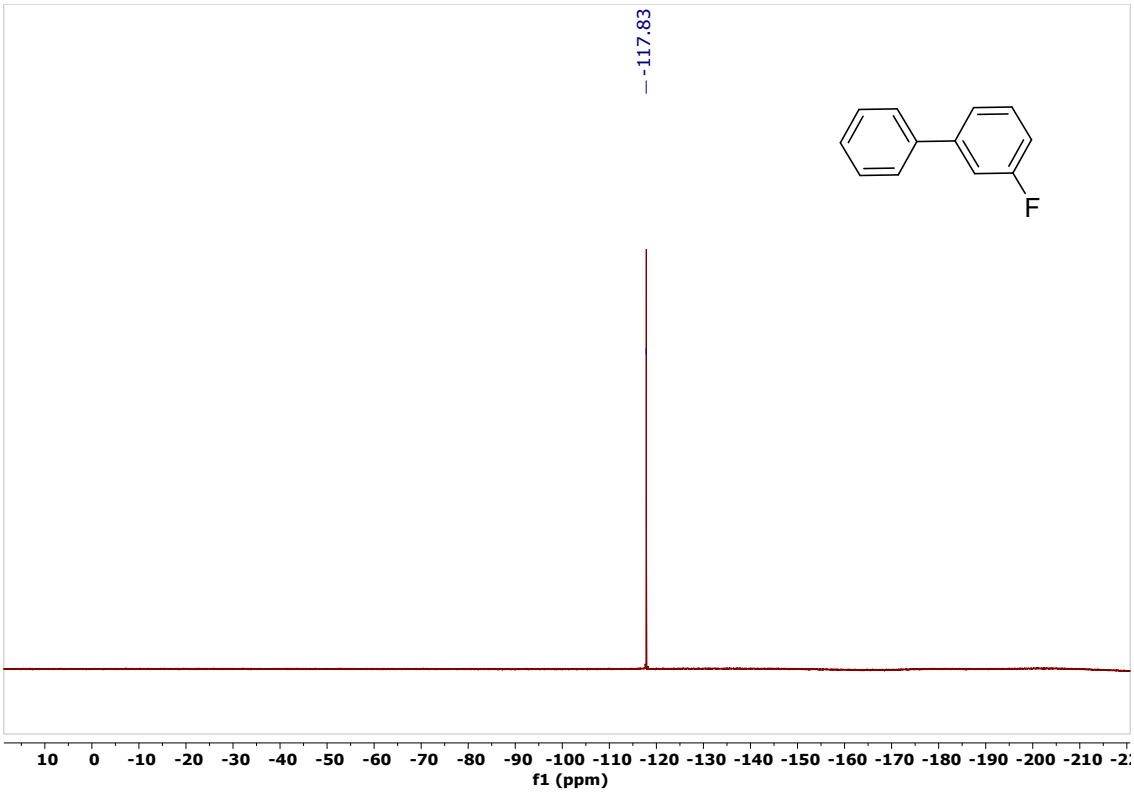


Figure 45: ^{19}F NMR (377 MHz, $CDCl_3$) of compound **3h**.

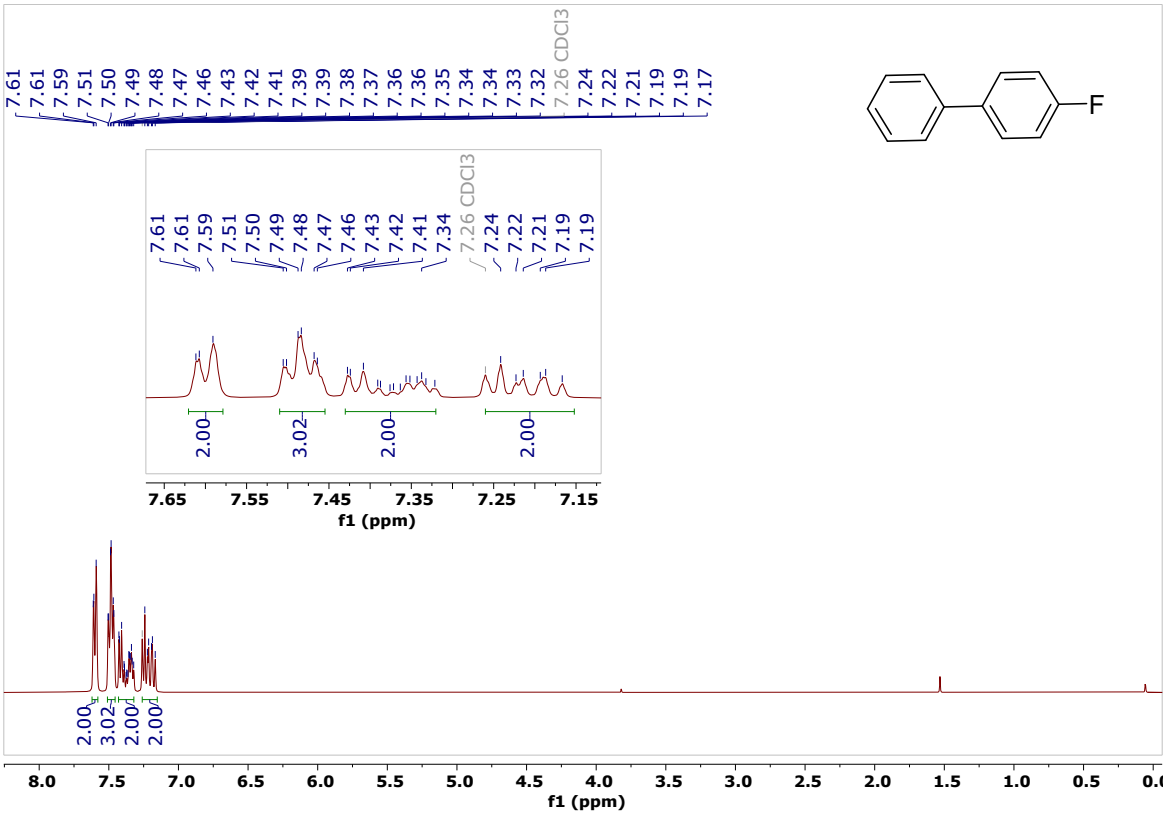


Figure 46: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3i.**

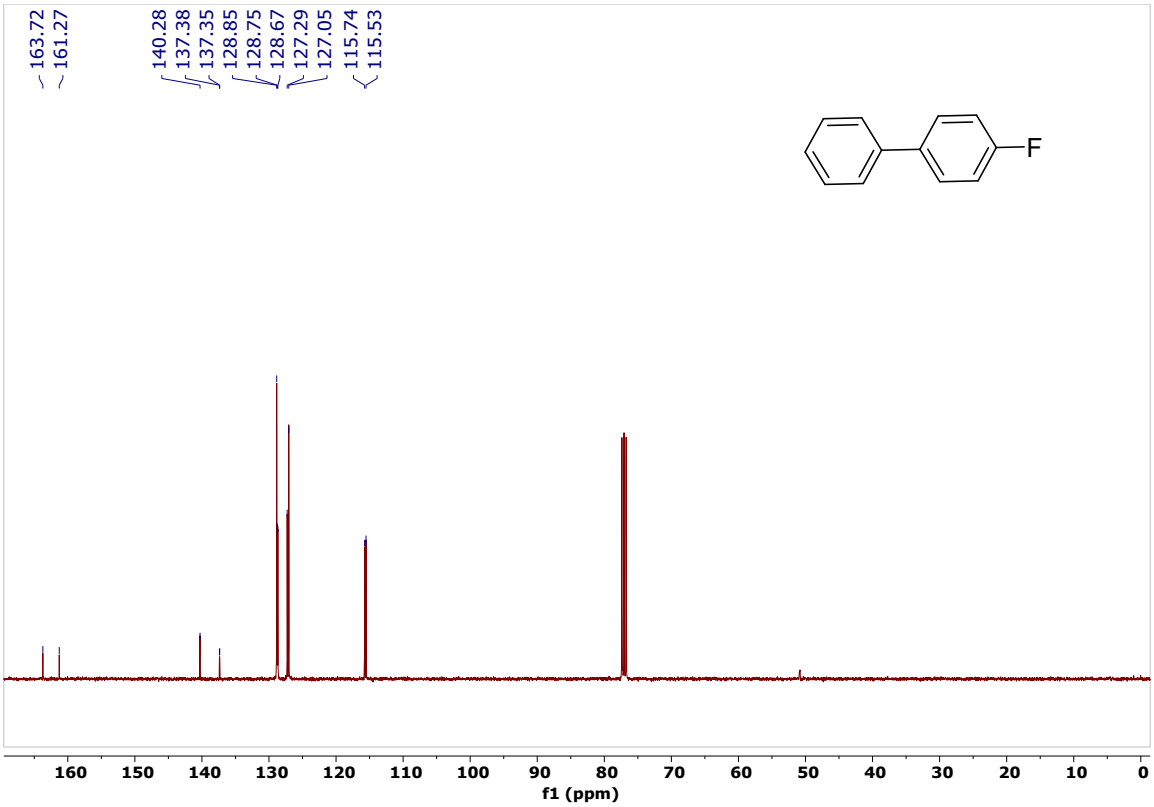


Figure 47: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3i**.

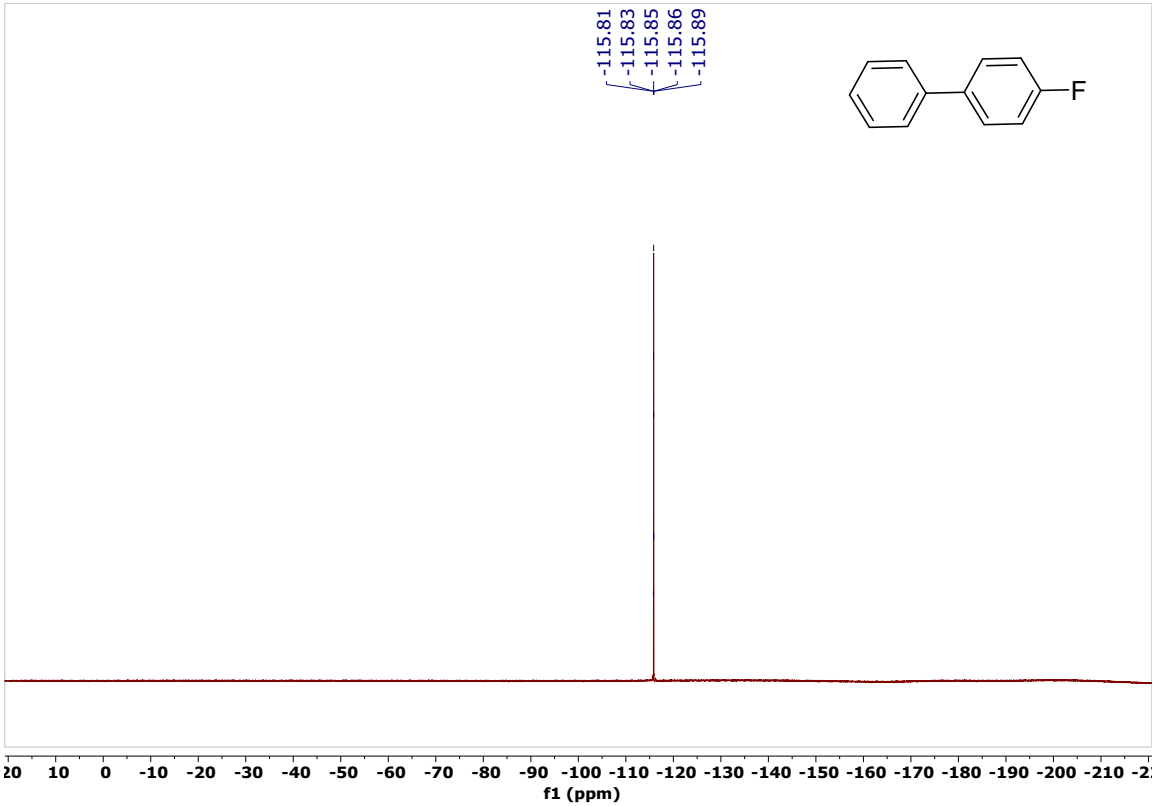


Figure 48: ^{19}F NMR (377 MHz, $CDCl_3$) of compound **3i**.

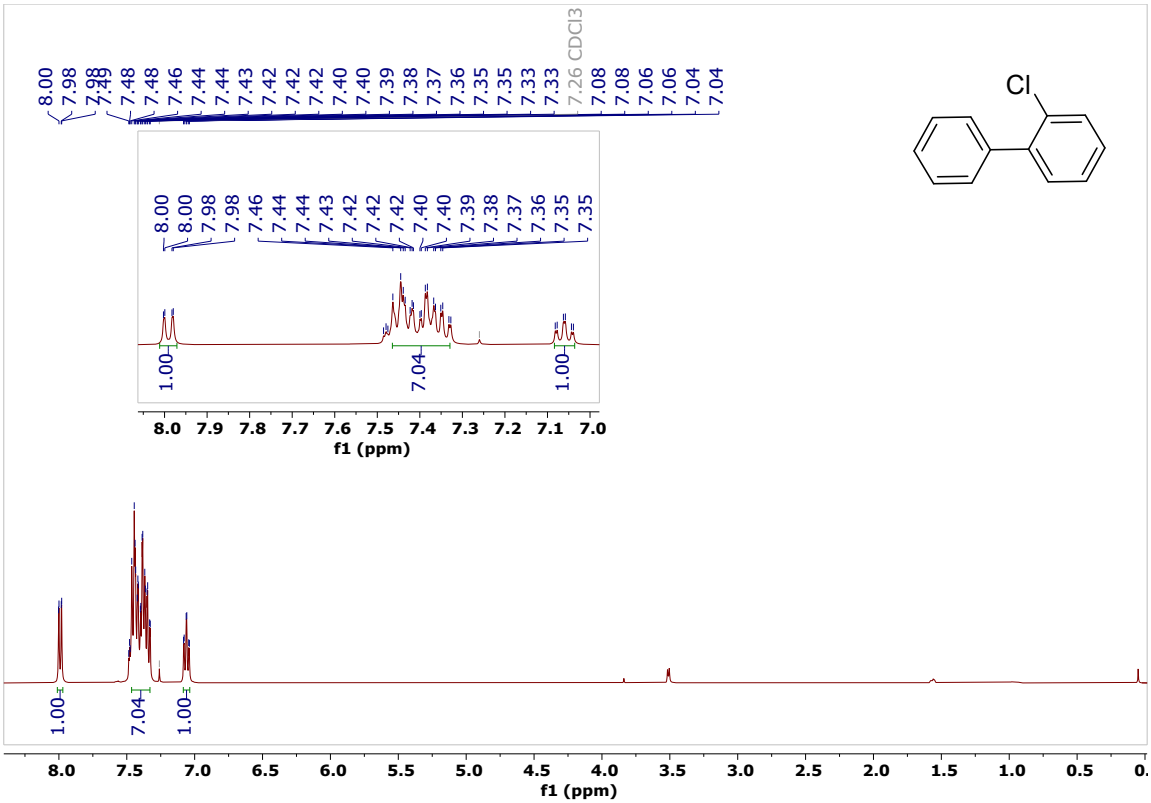


Figure 49:[1]H NMR (400 MHz, $CDCl_3$) of compound **3j.**

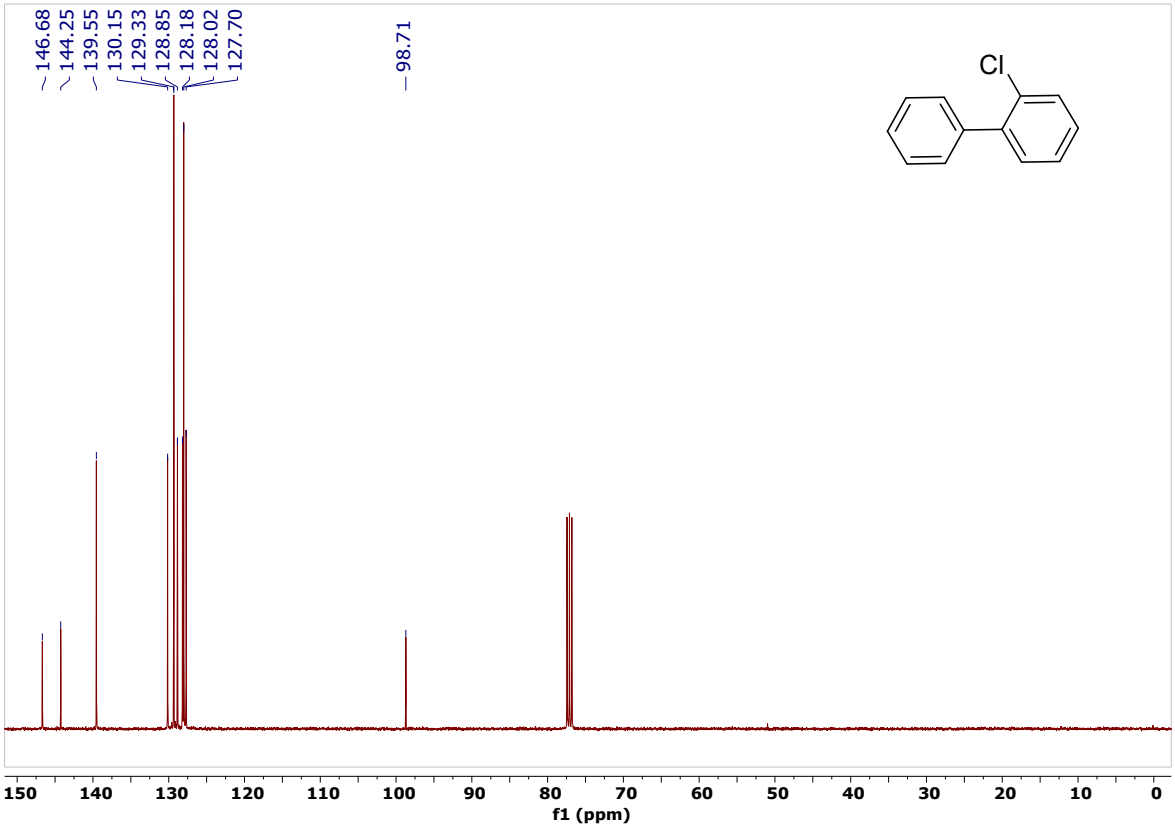


Figure 50:[13]C NMR (100.6 MHz, $CDCl_3$) of compound **3j**.

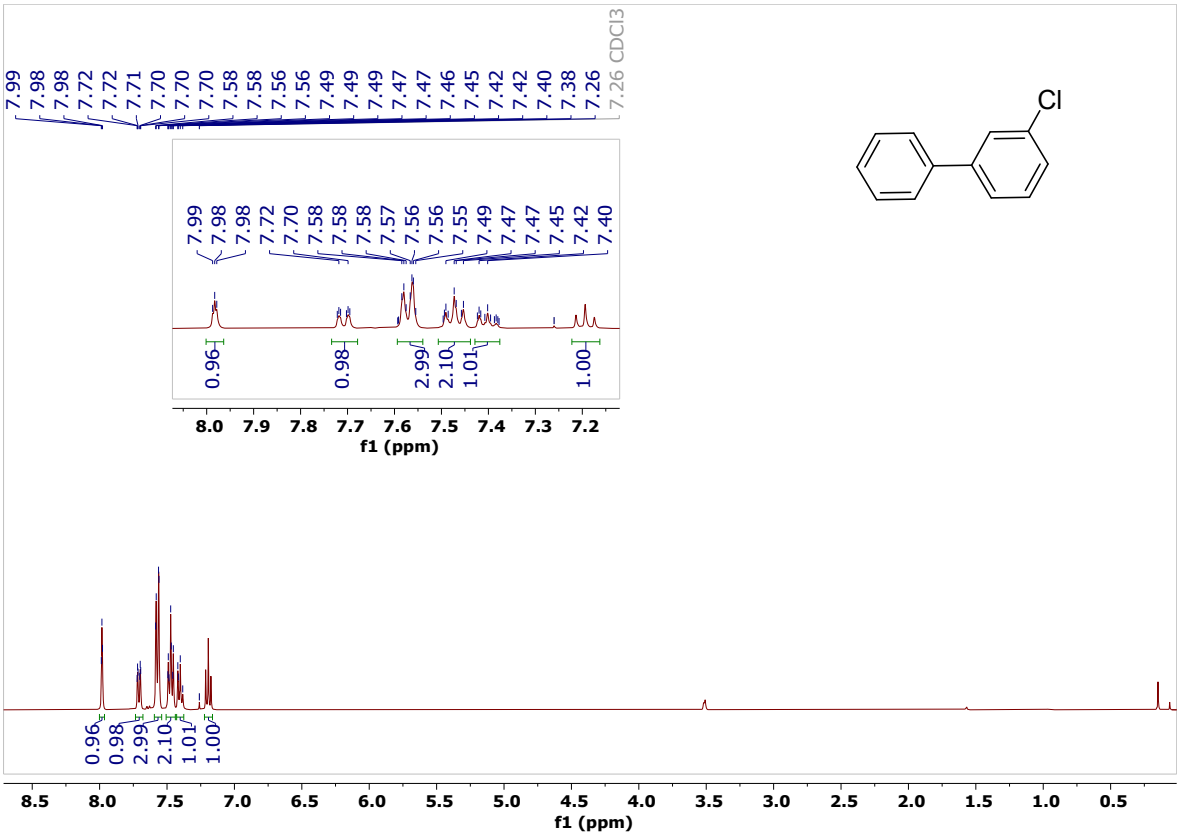


Figure 51:[1]H NMR (400 MHz, $CDCl_3$) of compound **3k.**

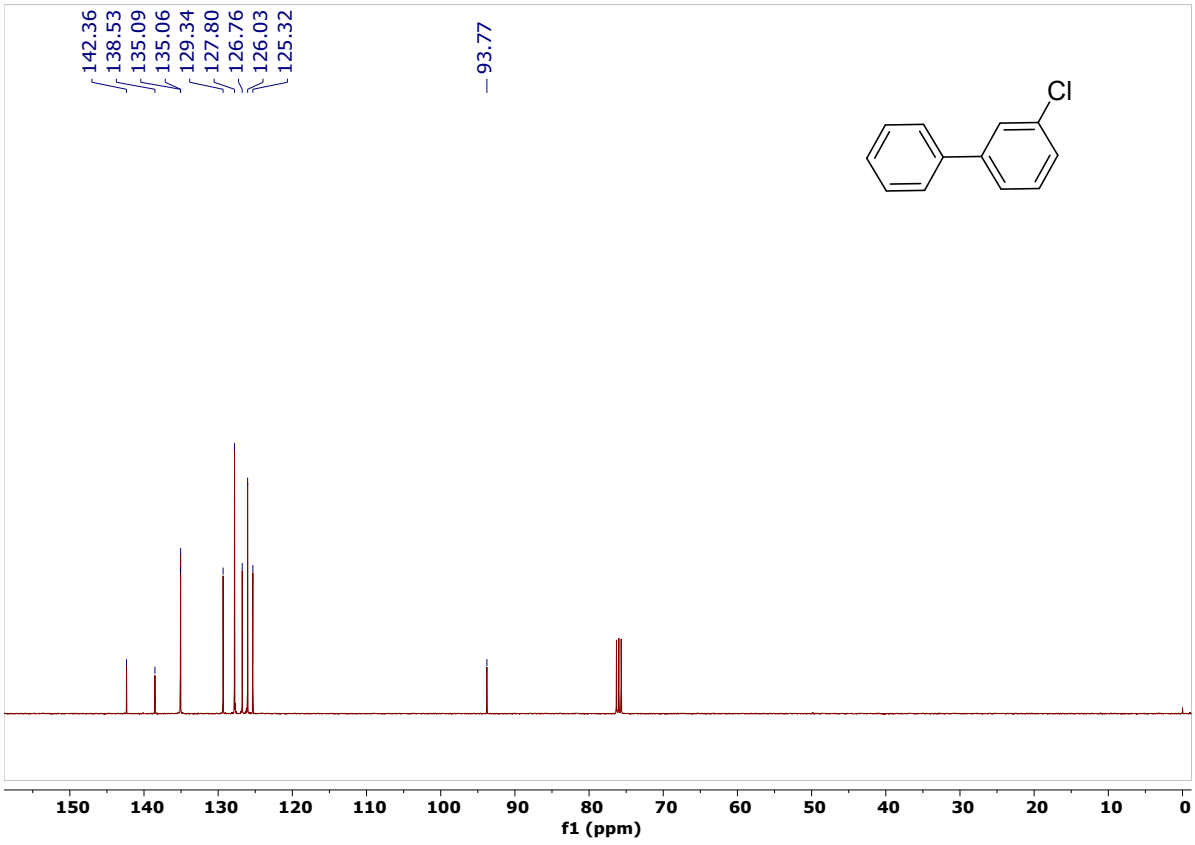


Figure 52: [13]C NMR (100.6 MHz, $CDCl_3$) of compound **3k**.

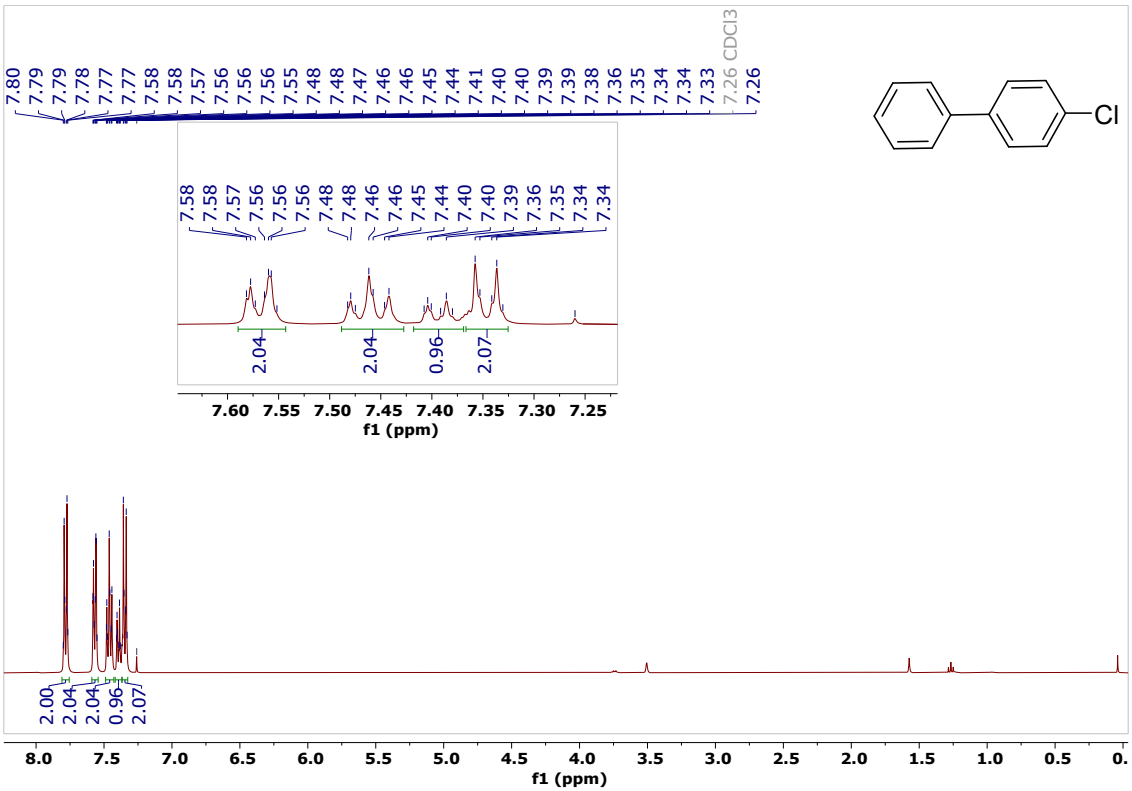


Figure 53:[1]H NMR (400 MHz, $CDCl_3$) of compound **3l.**

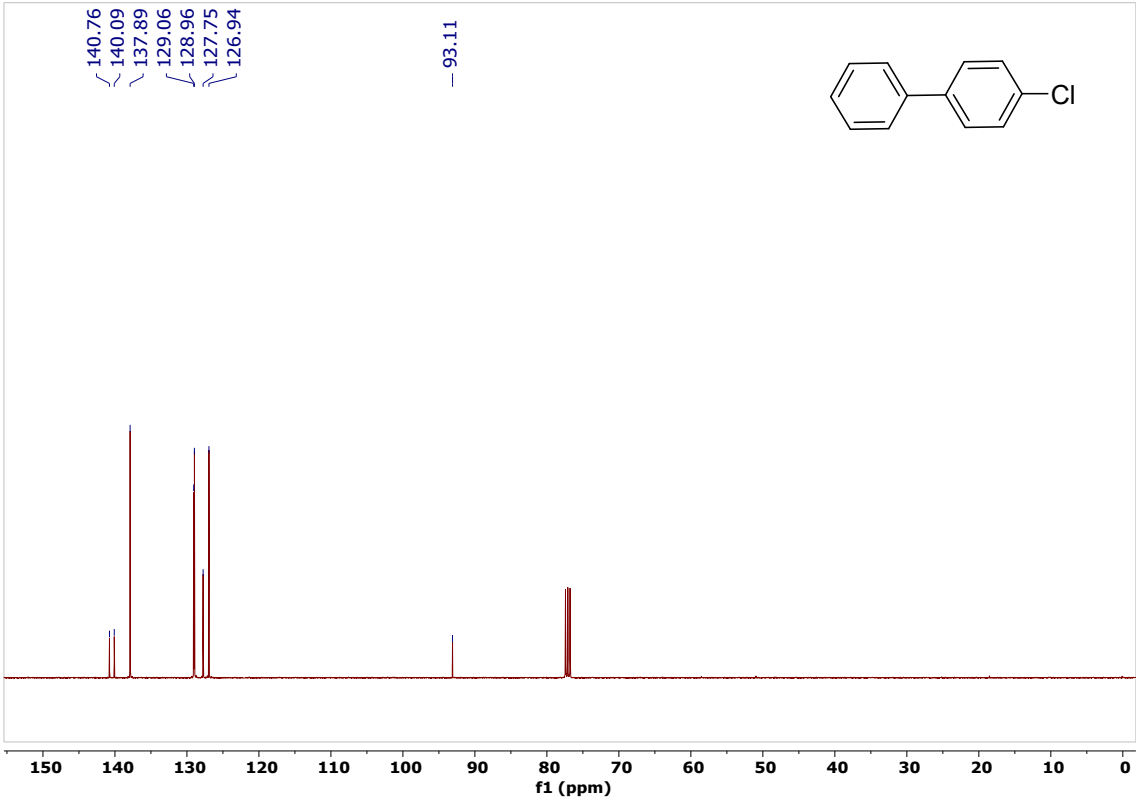


Figure 54: [13]C NMR (100.6 MHz, $CDCl_3$) of compound **3l**.

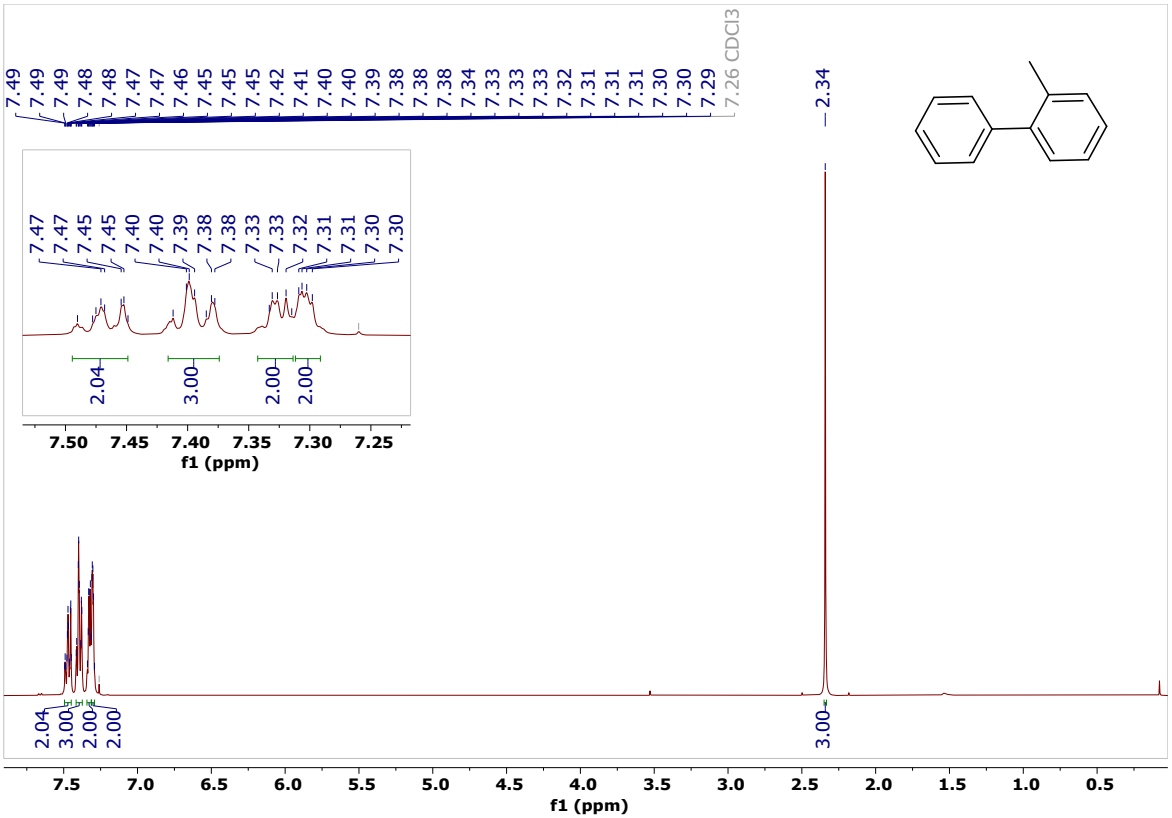


Figure 55: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3m.**

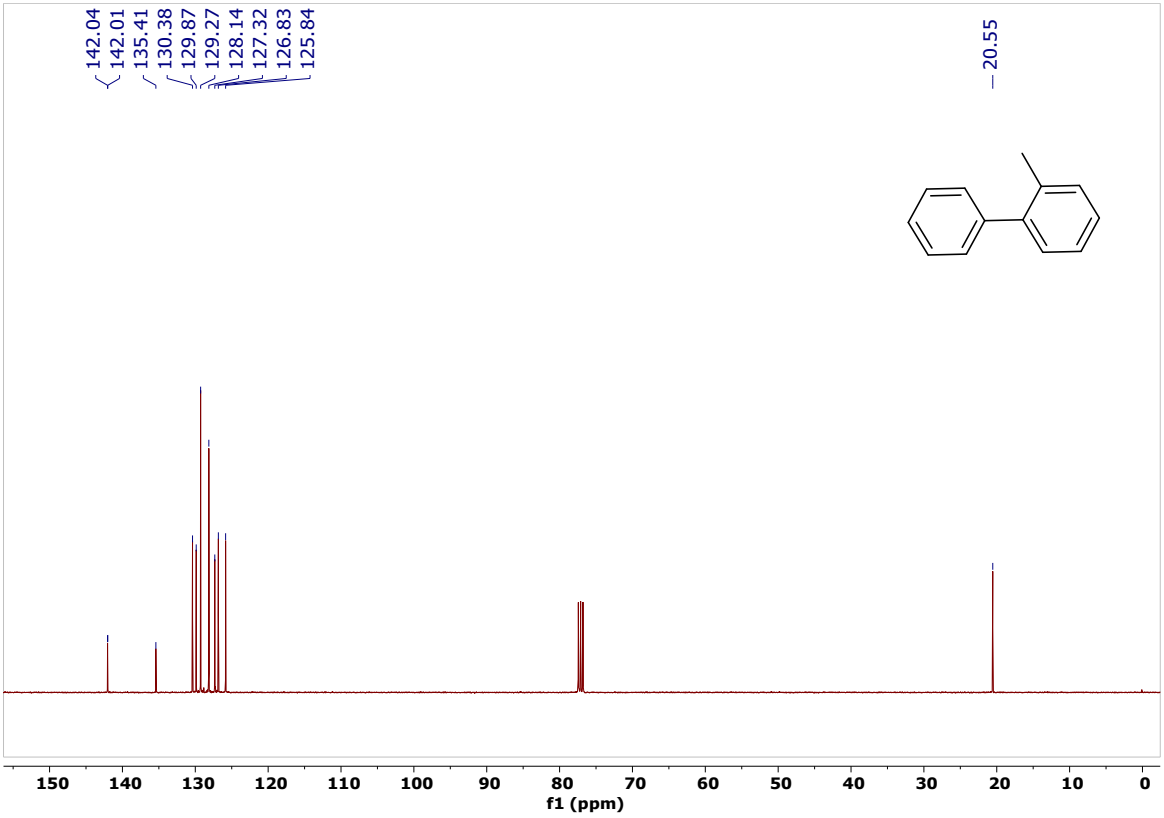


Figure 56: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3m**.

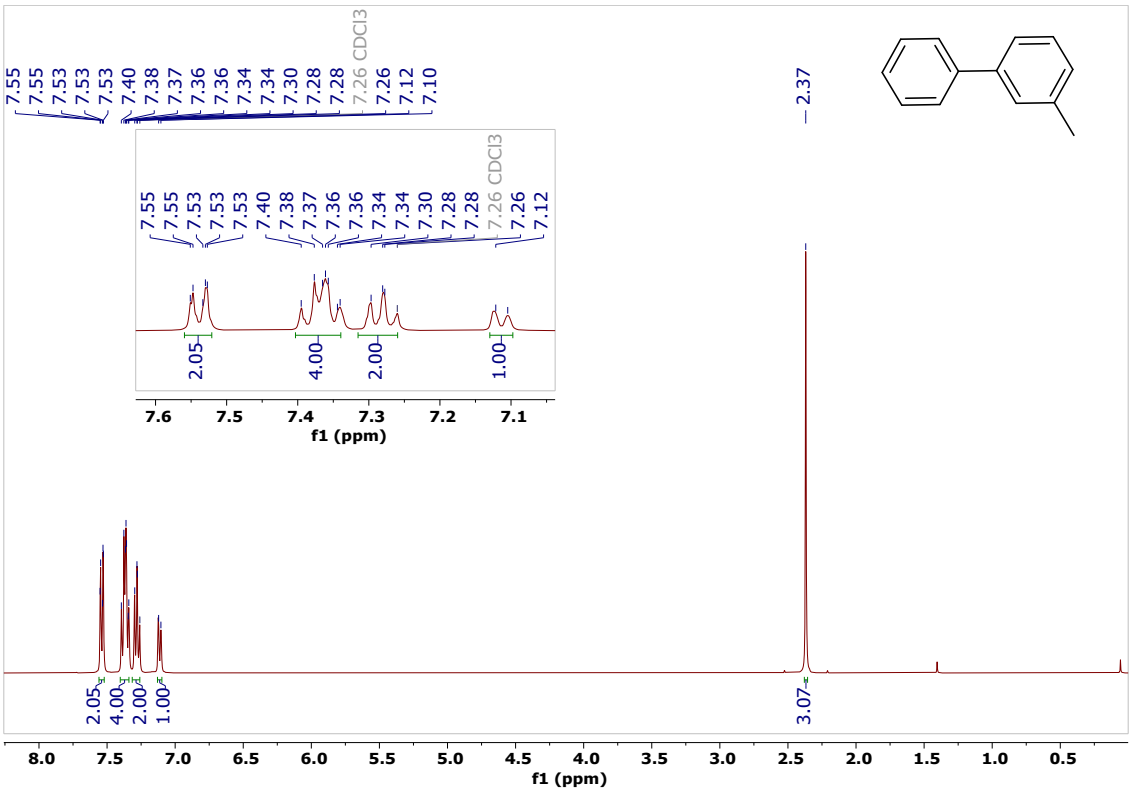


Figure 57: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3n.**

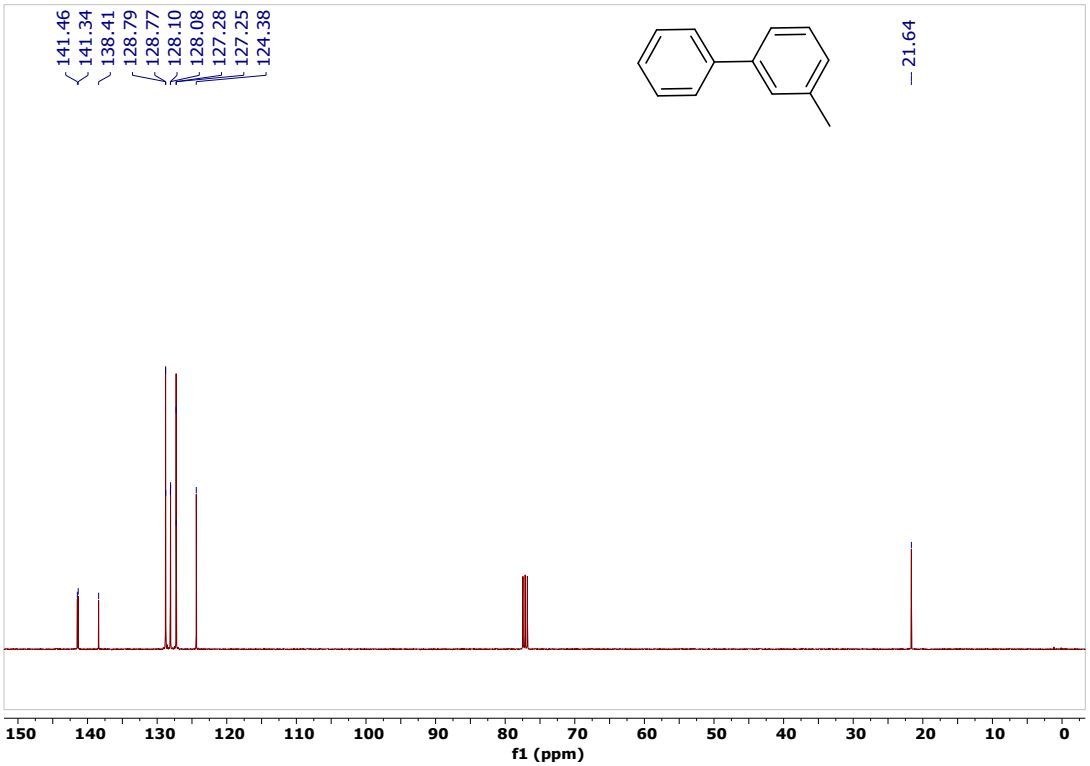


Figure 58: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3n**.

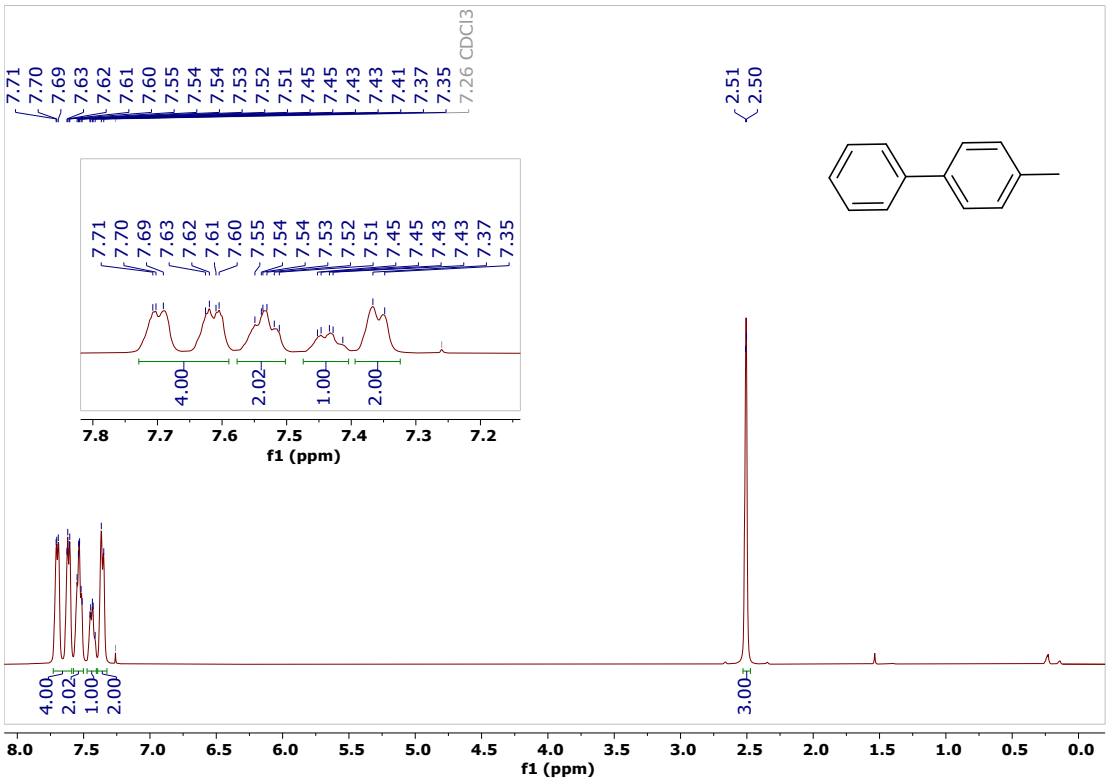


Figure 59: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3o.**

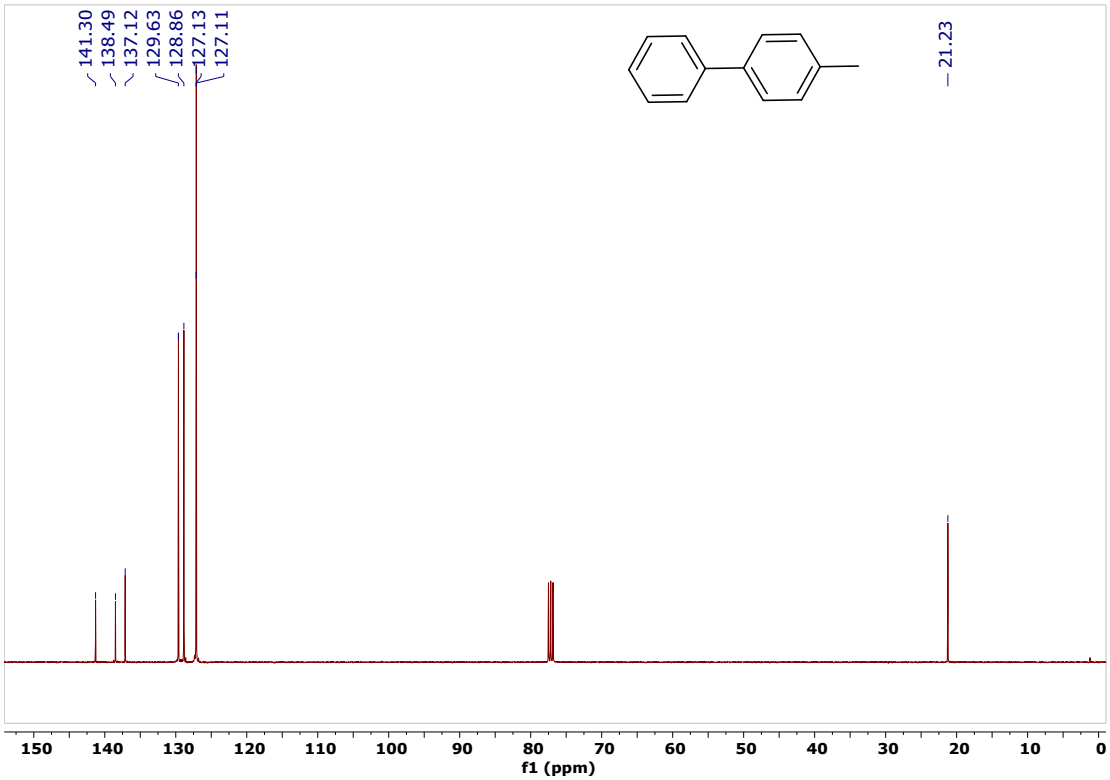


Figure 60: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3o**.

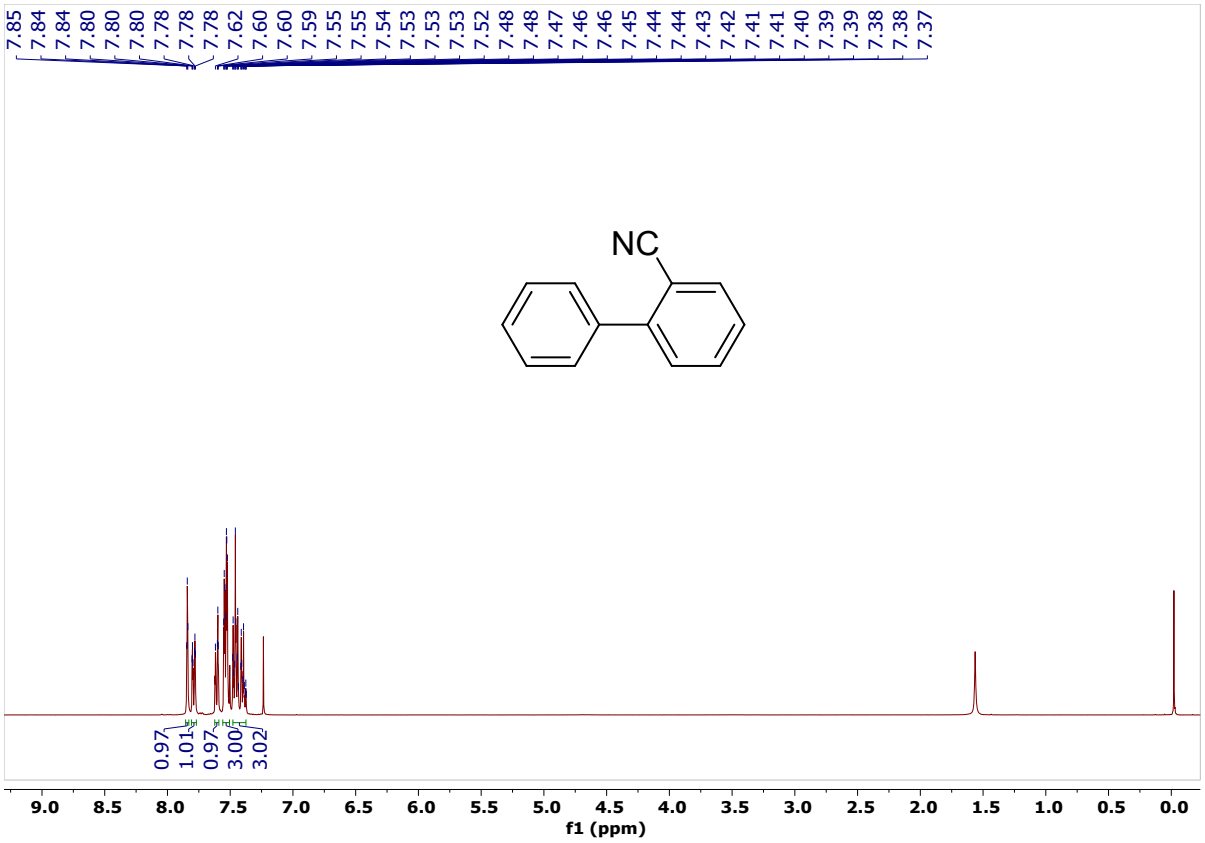


Figure 61: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3p.**

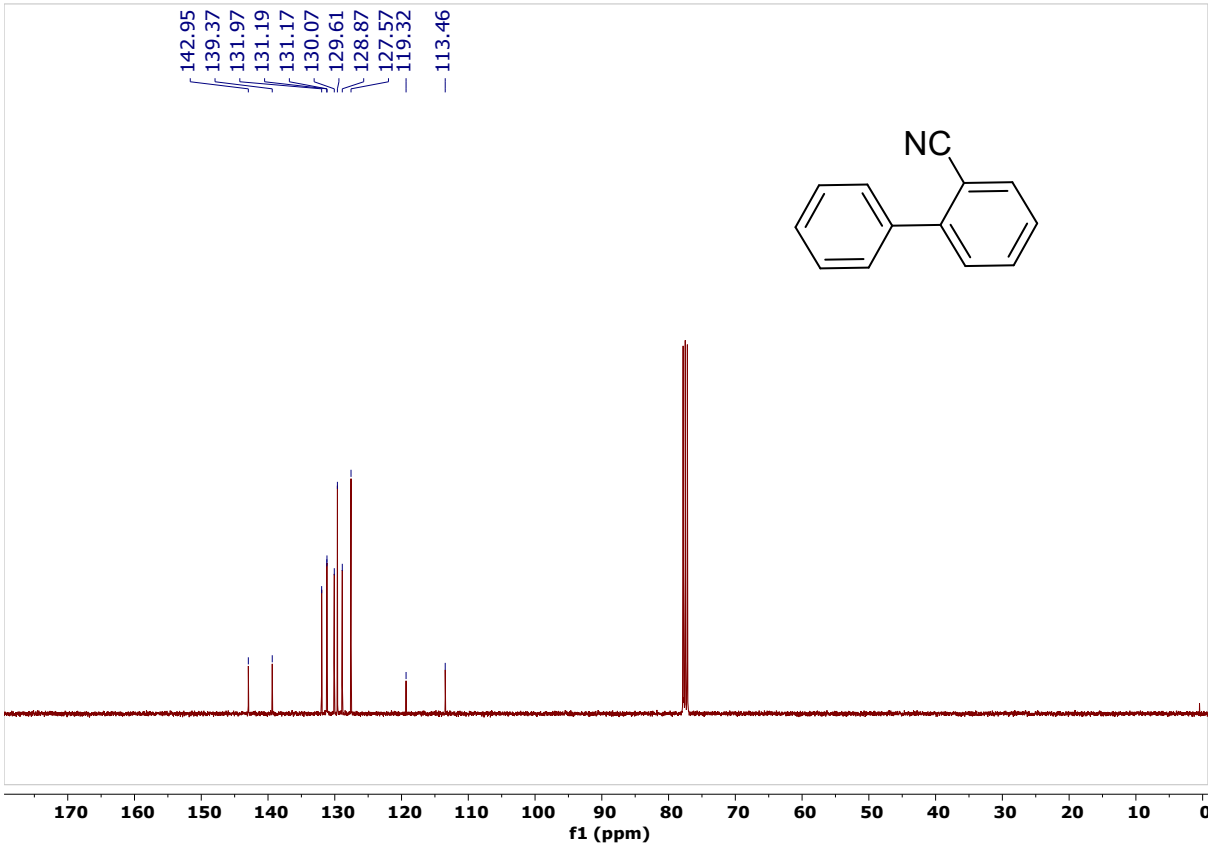


Figure 62: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3p.**

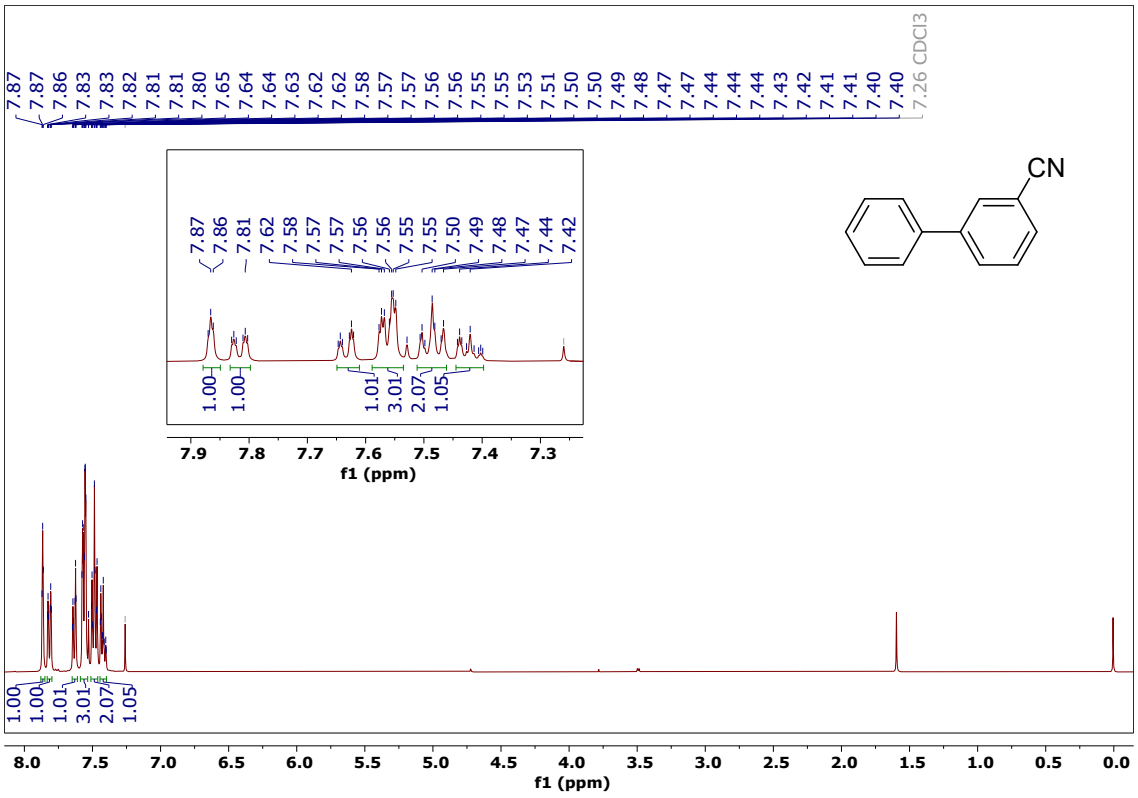


Figure 63: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3q.**

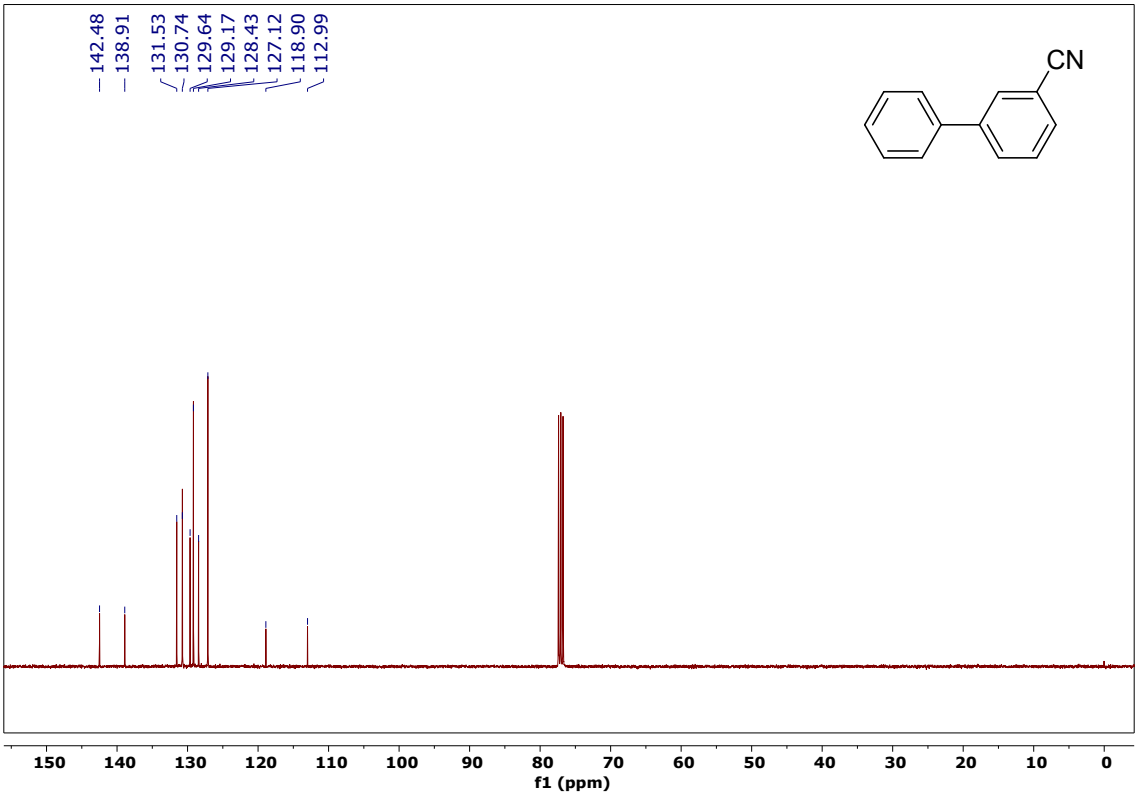


Figure 64: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3q**.

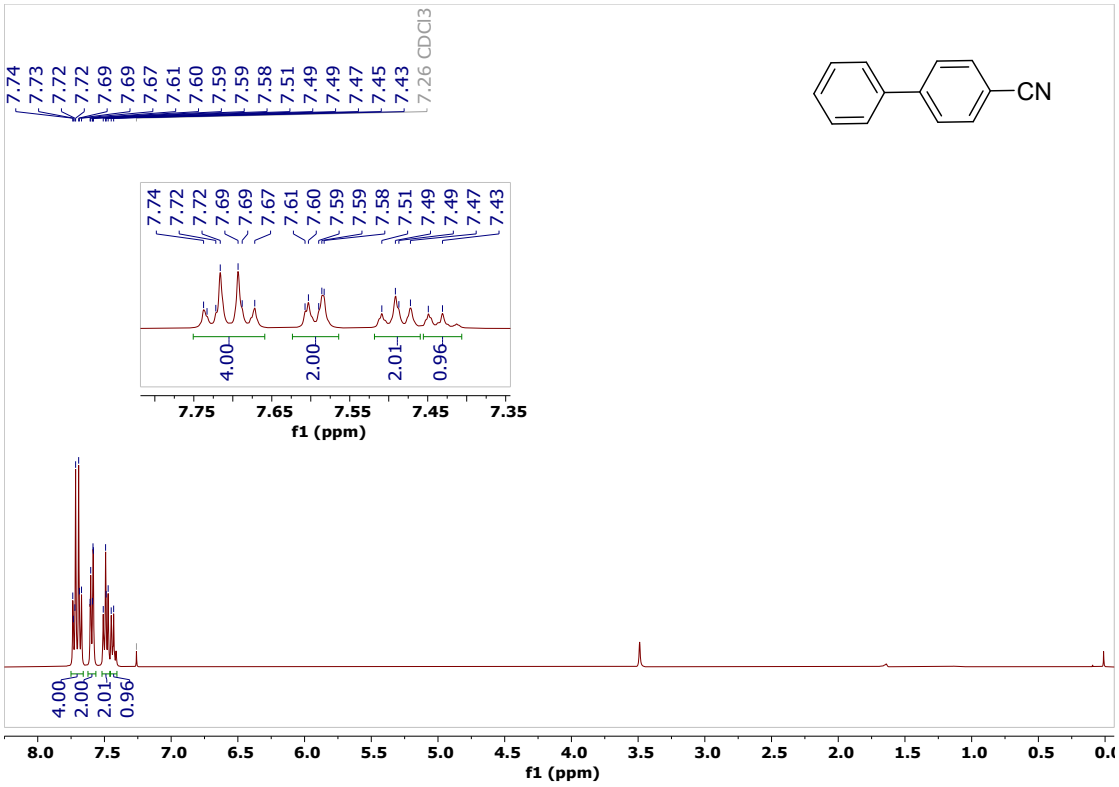


Figure 65: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3r.**

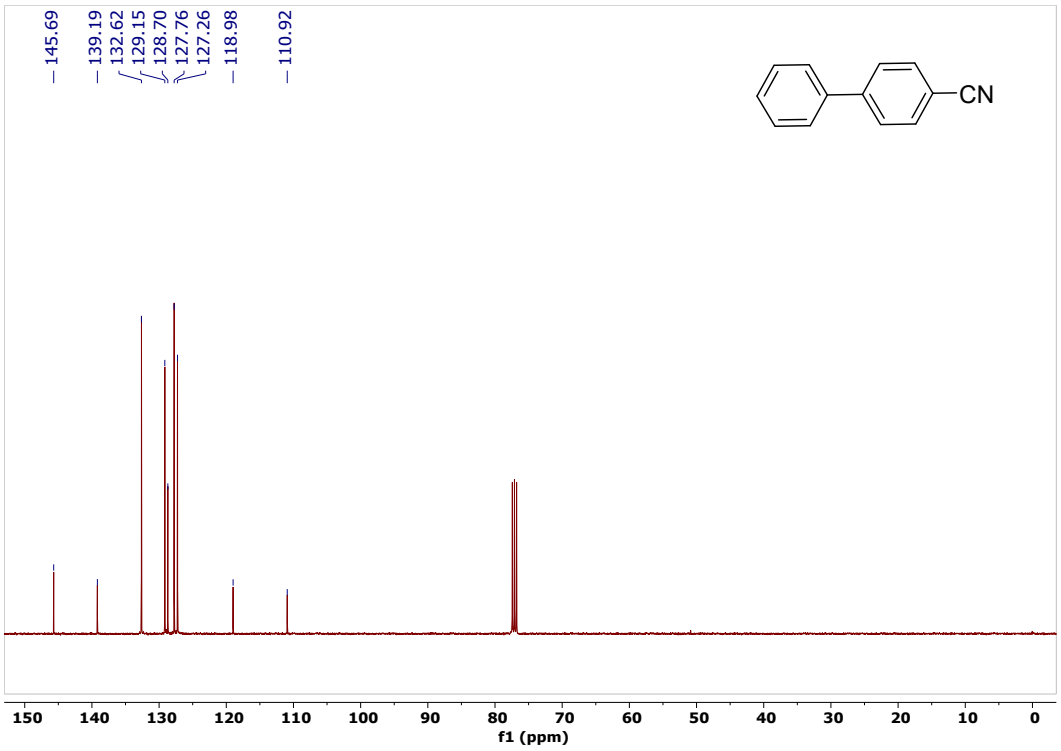


Figure 66: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3r**.

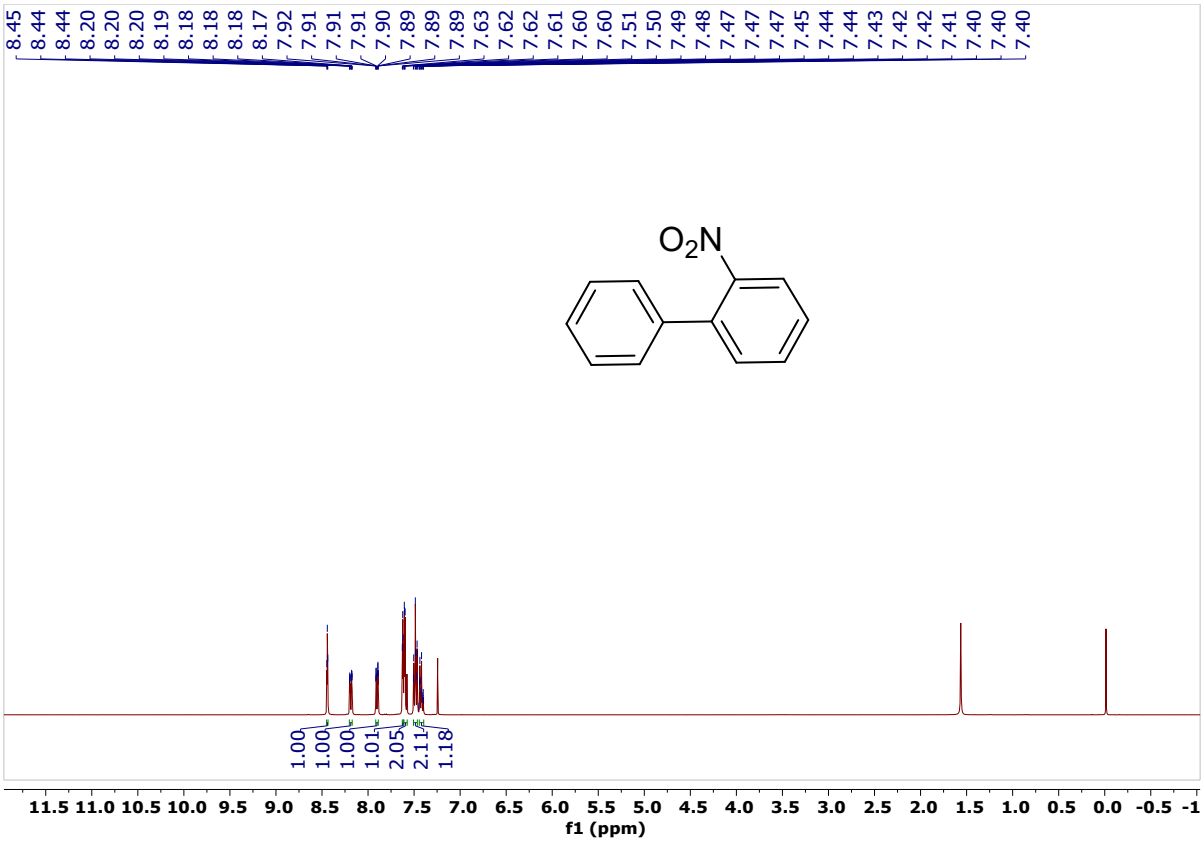


Figure 67: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3s.**

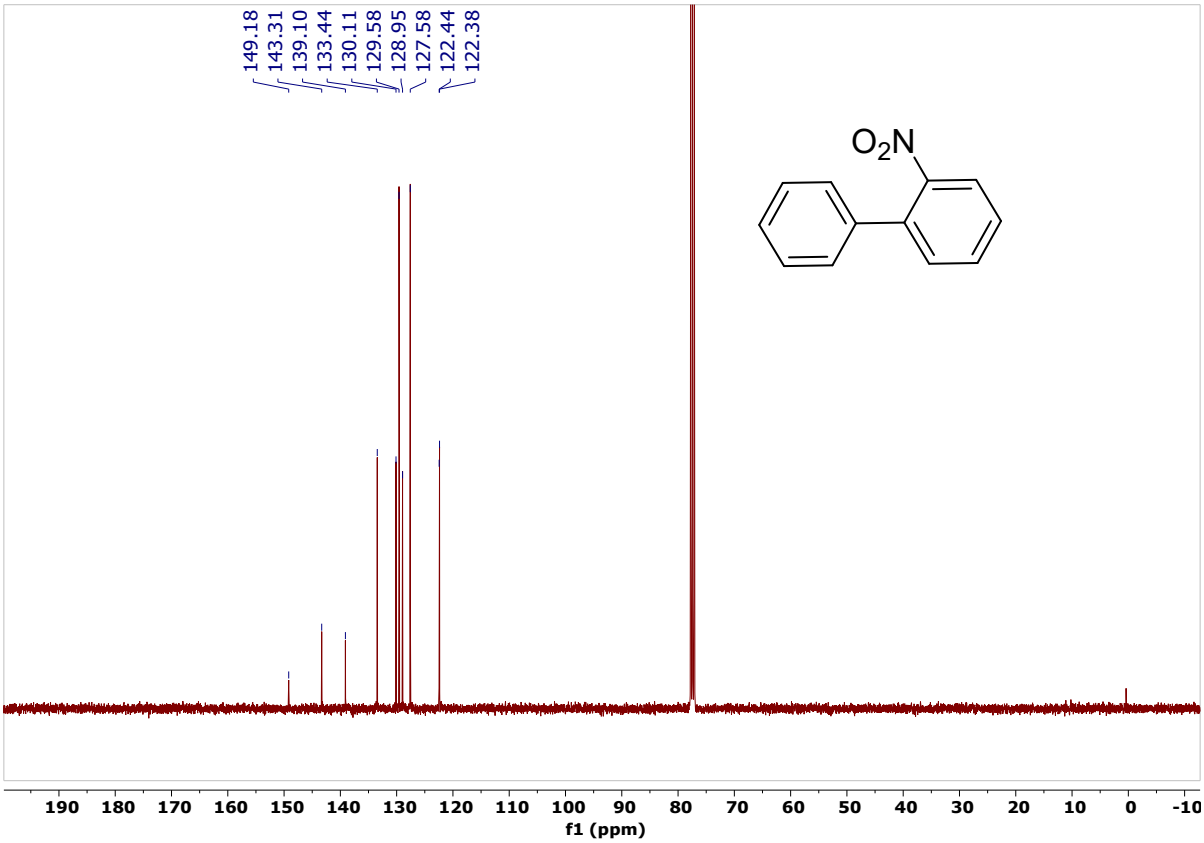


Figure 68: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3s**.

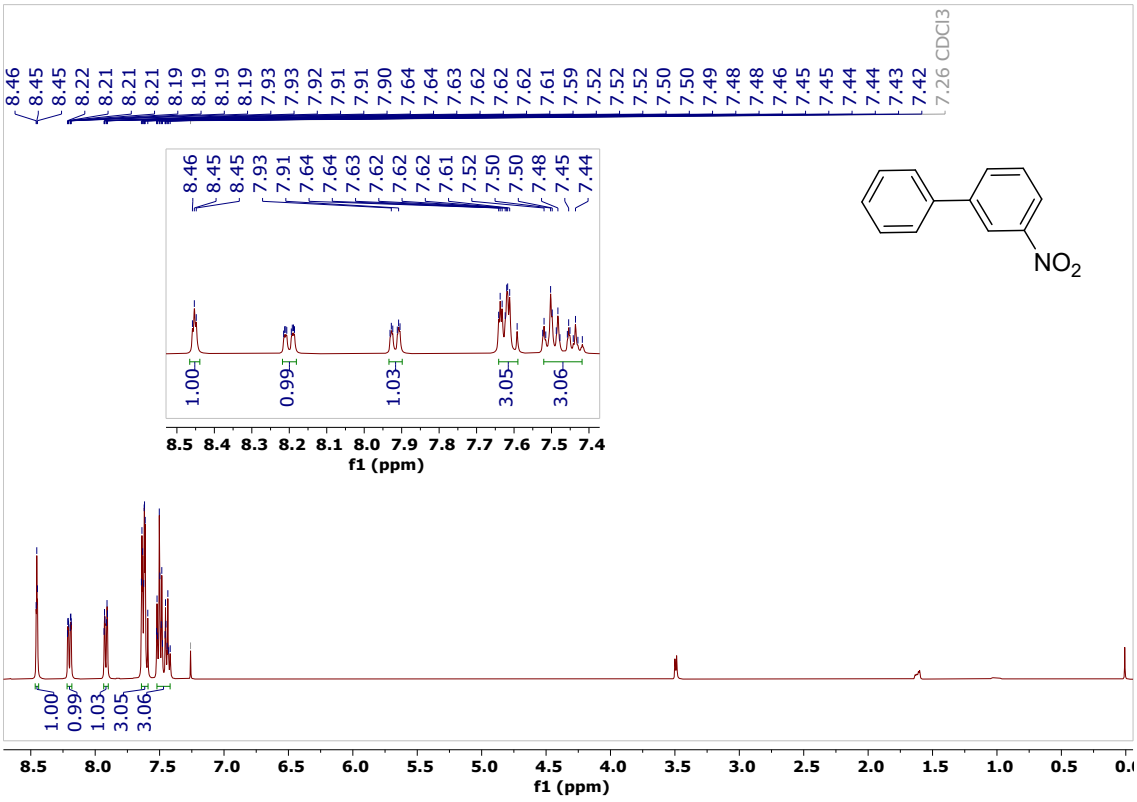


Figure 69: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3t.**

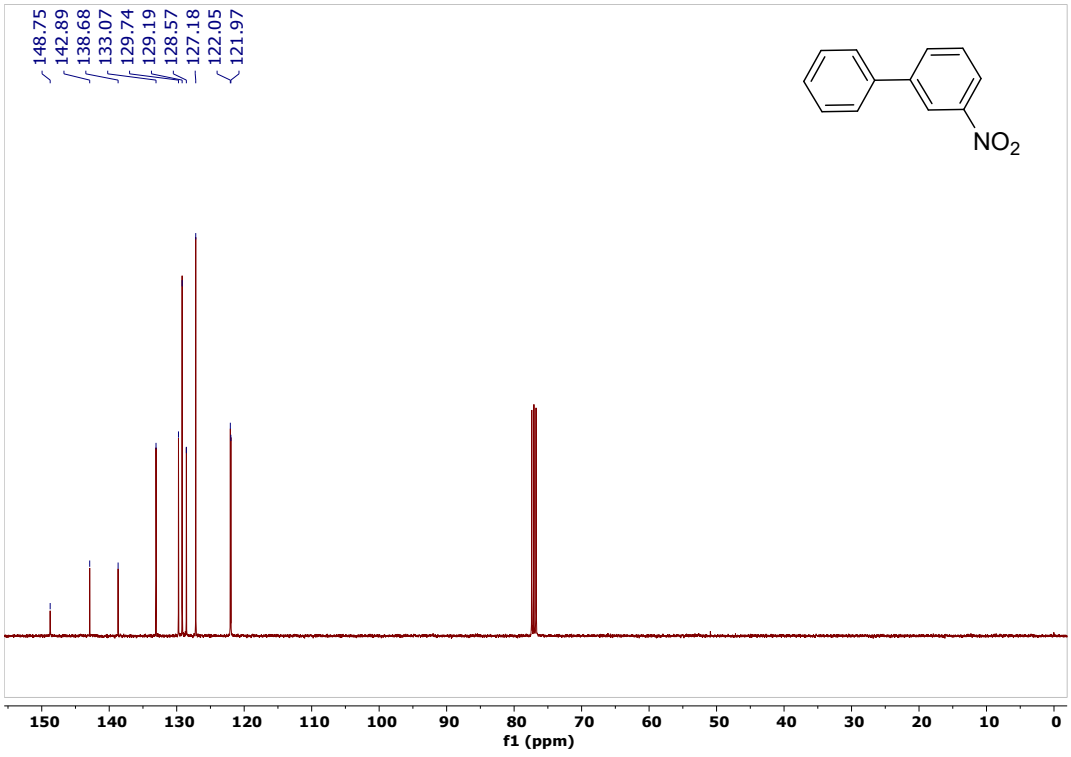


Figure 70: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3t**.

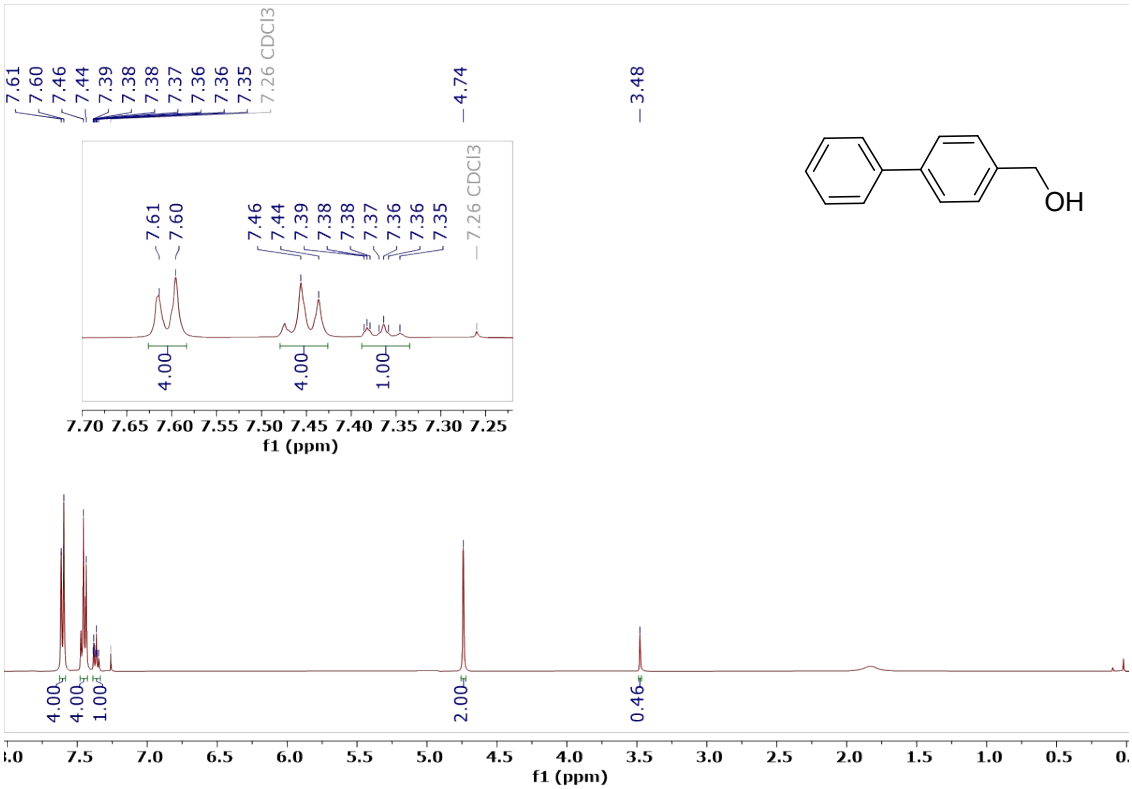


Figure 71: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3u.**

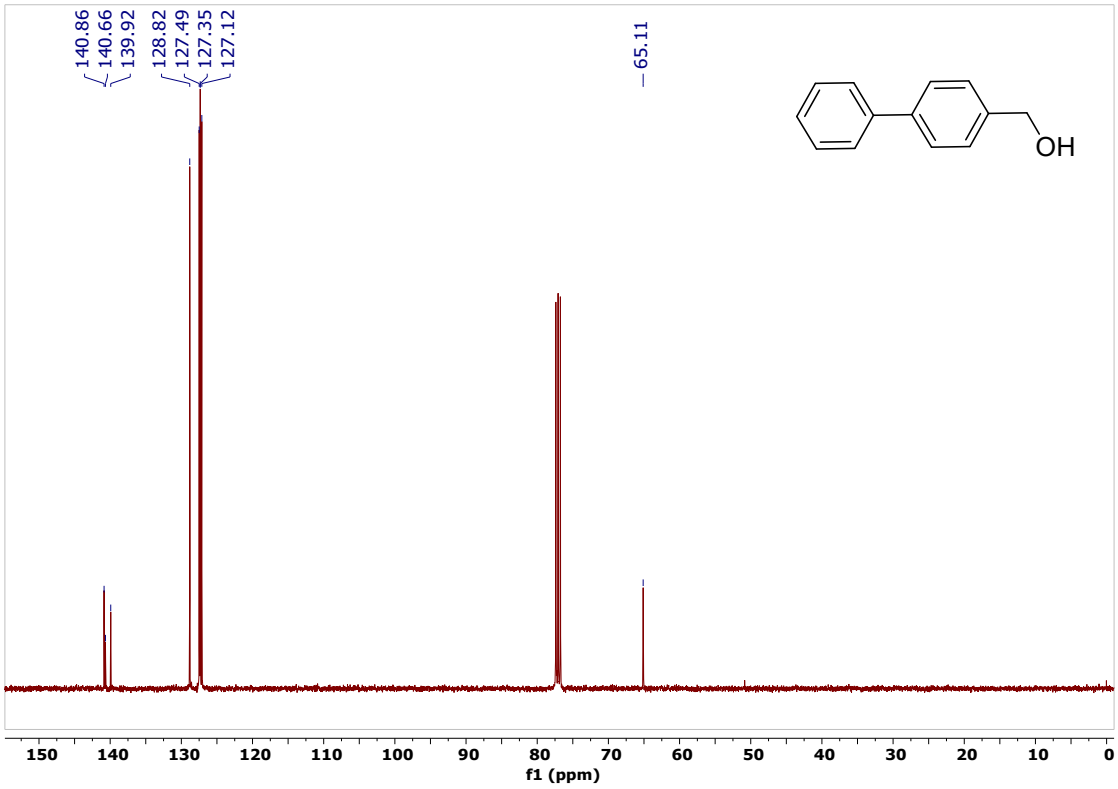


Figure 72: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3u**.

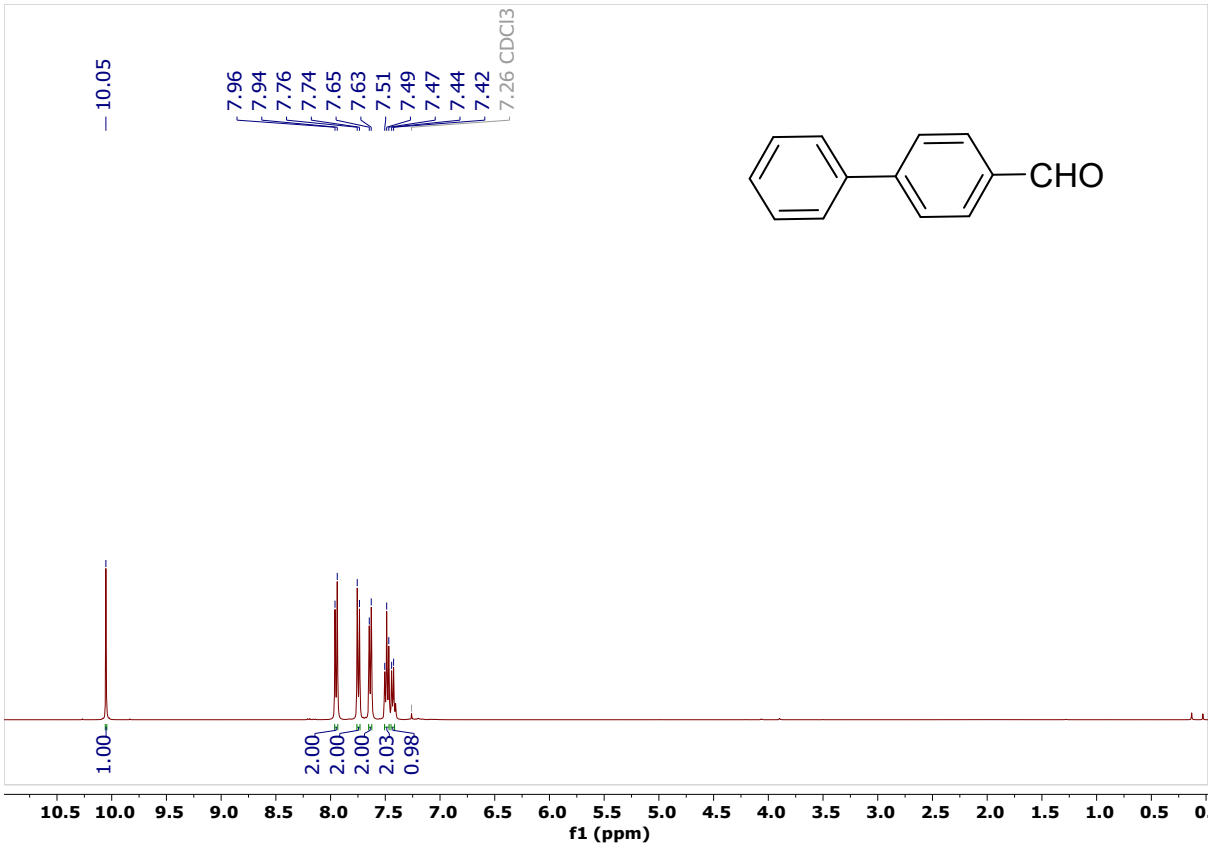


Figure 73: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3v.**

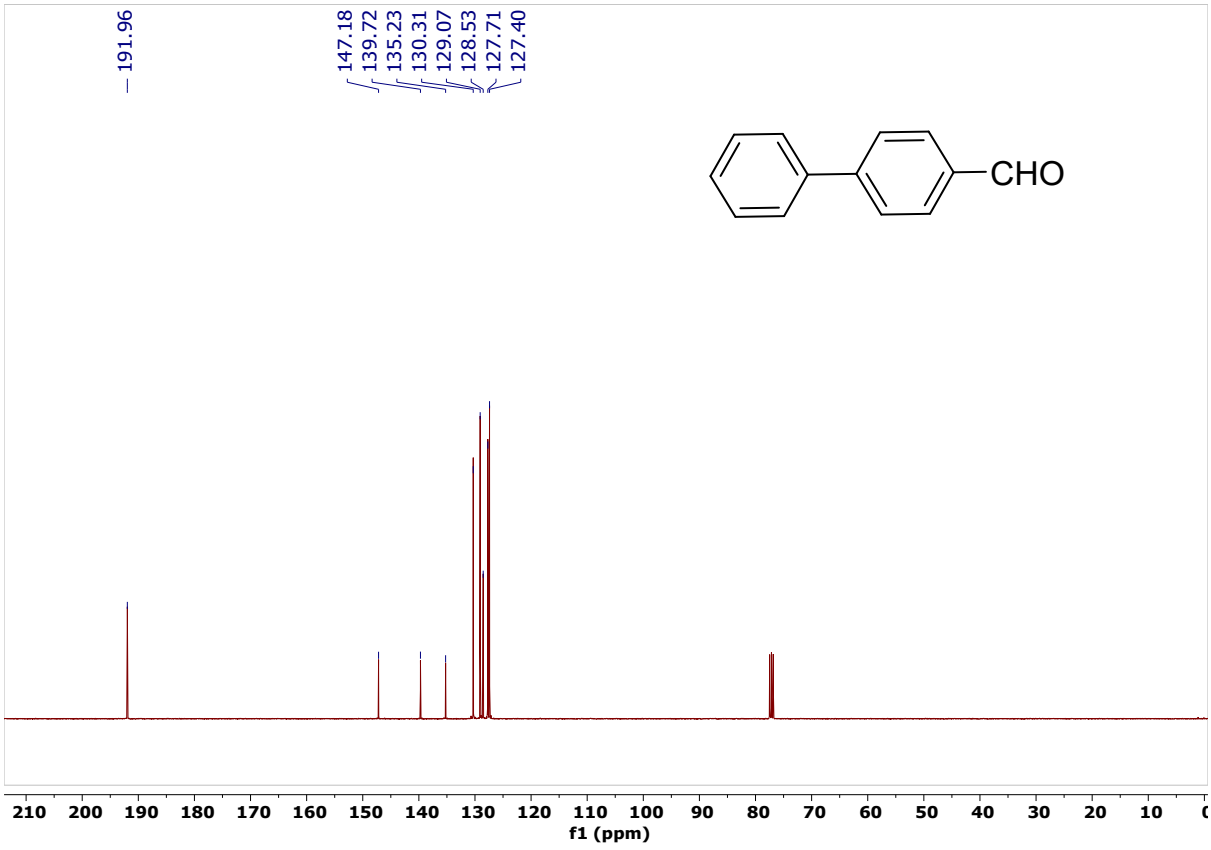


Figure 74: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3v**.

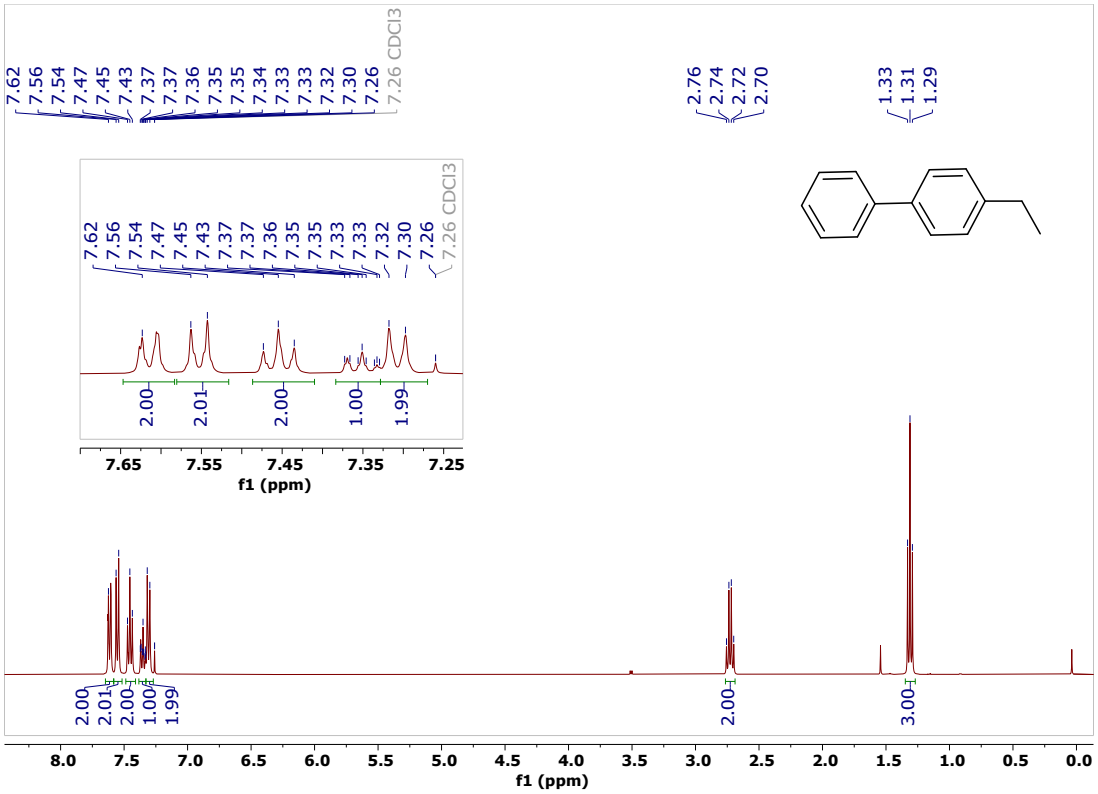


Figure 75: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3w.**

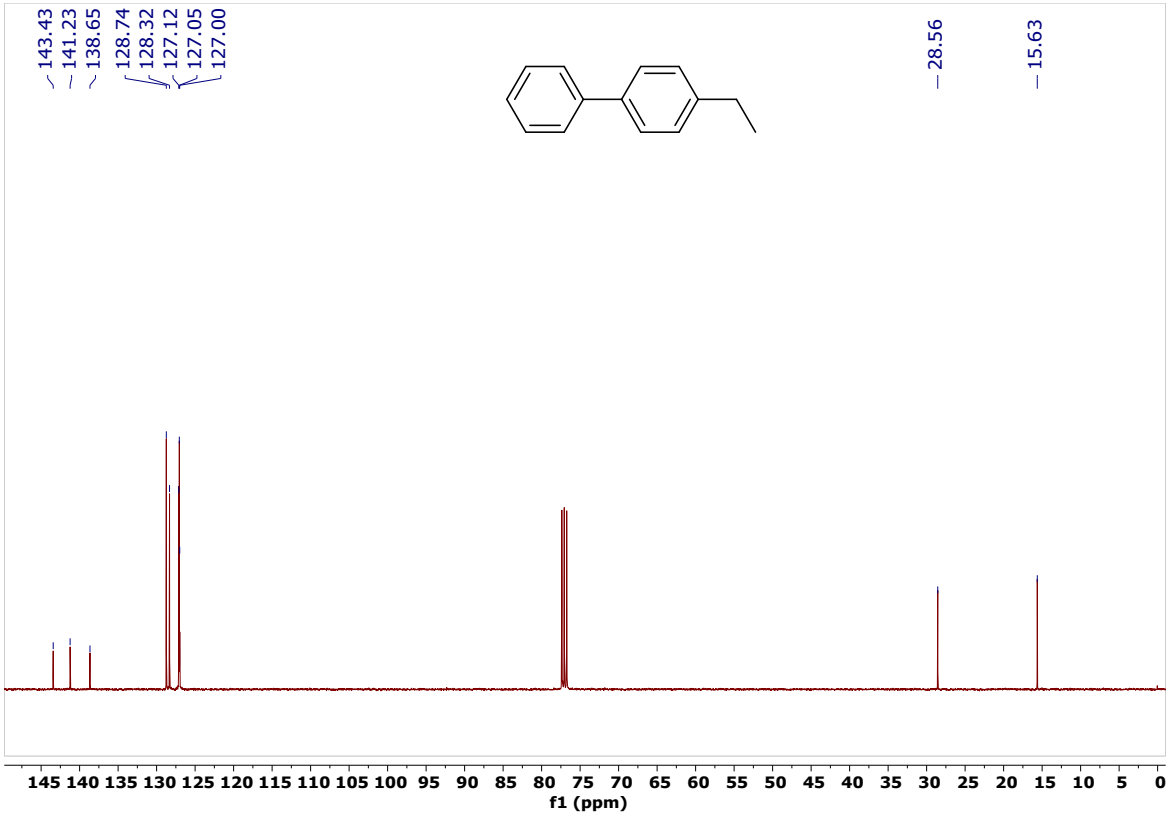


Figure 76: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3w**.

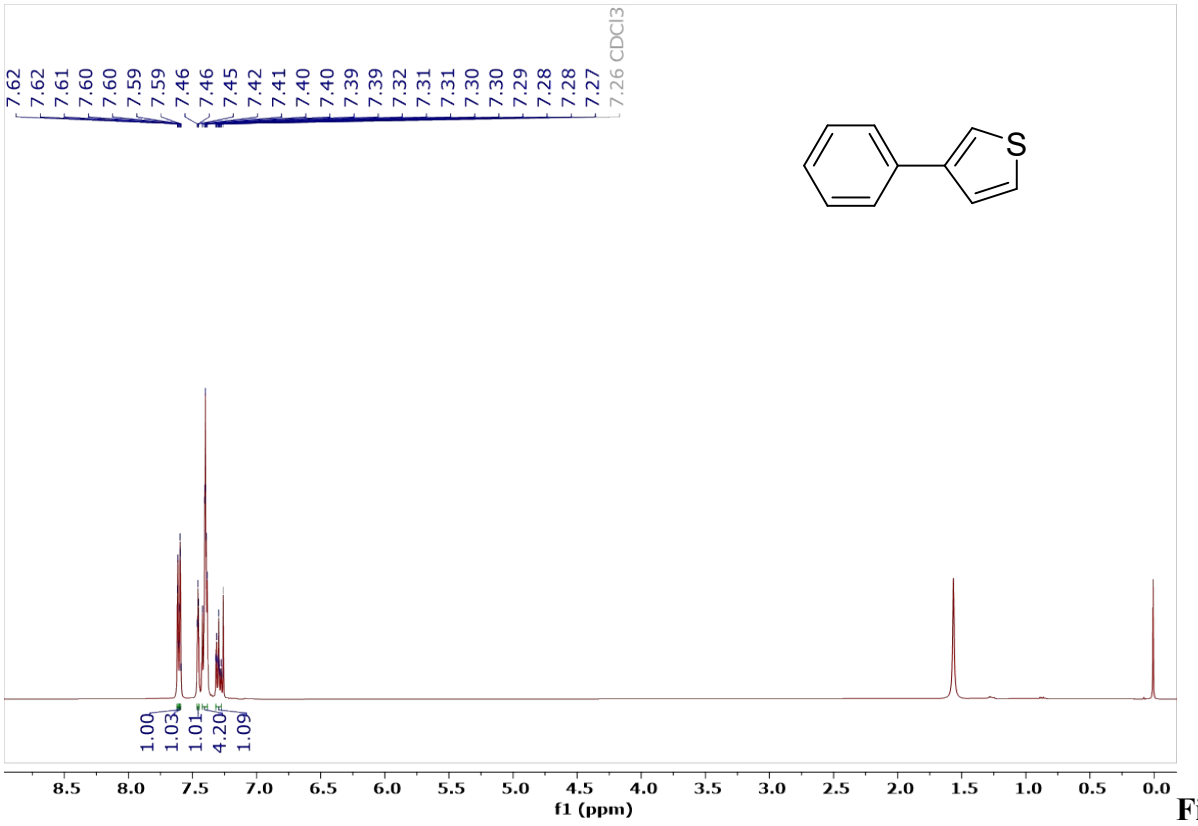


Figure 77: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3x.**

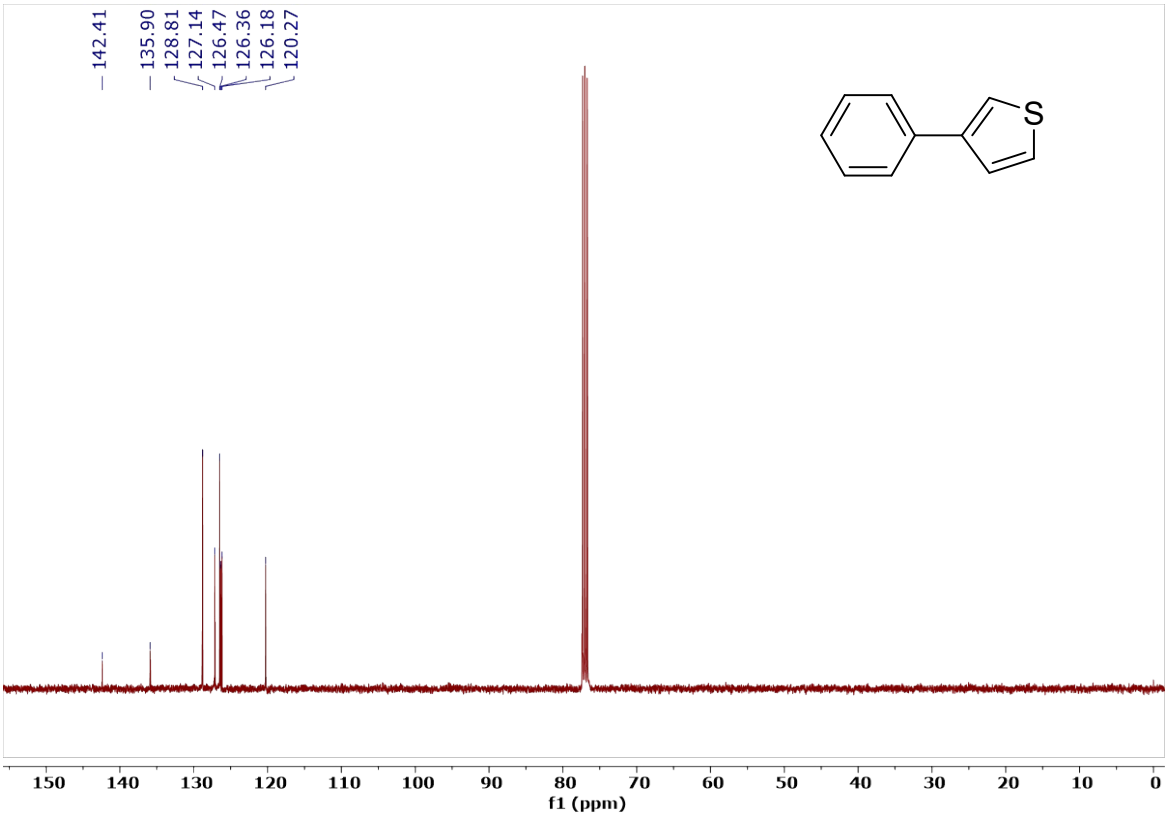


Figure 78: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3x**.

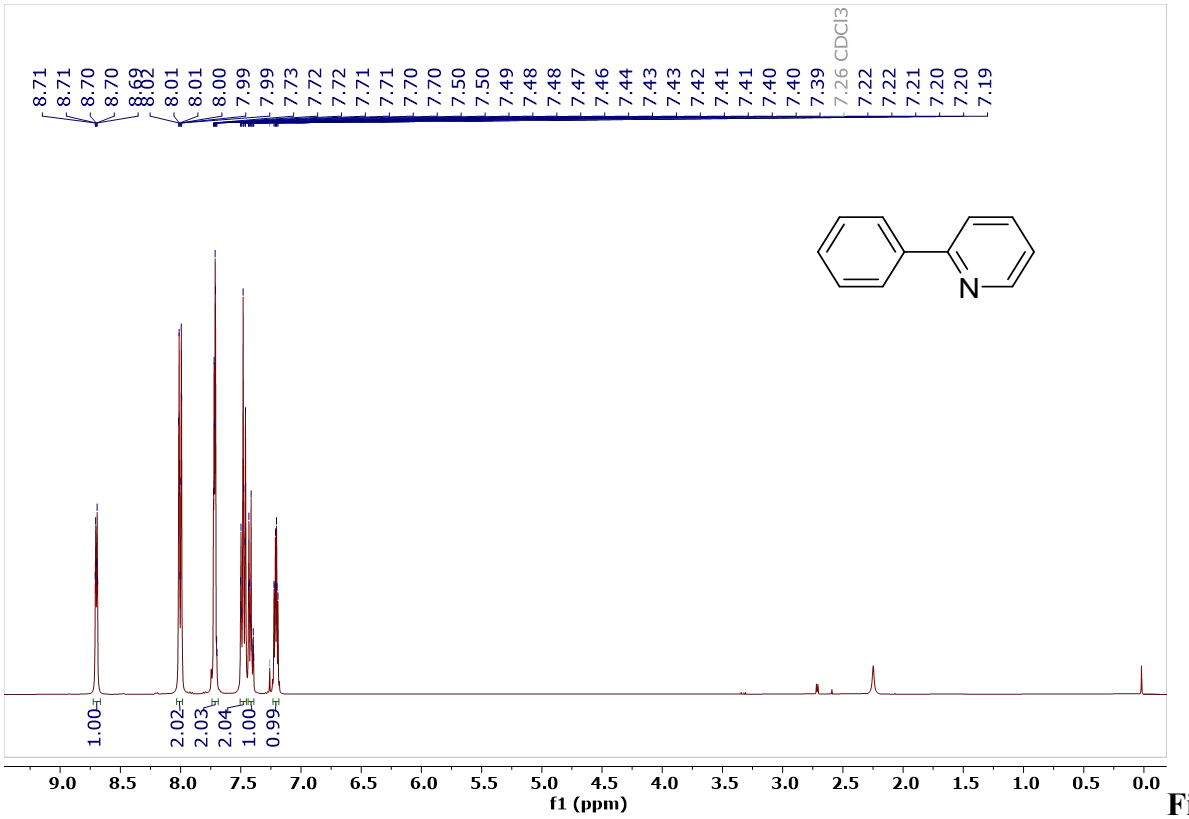


Figure 79: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3y.**

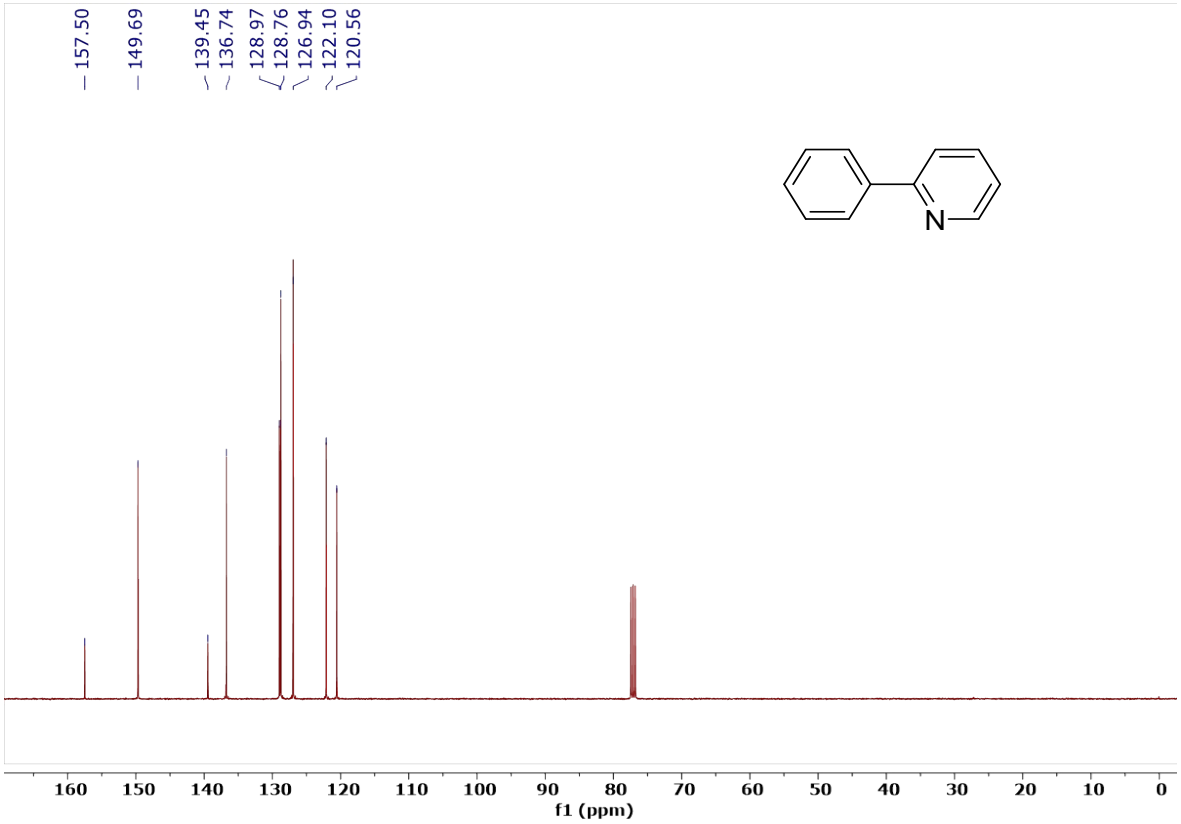
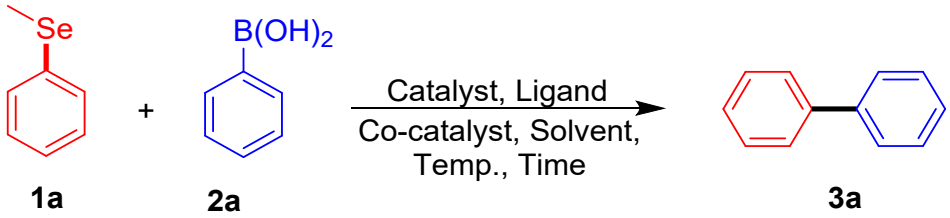


Figure 80: ^{13}C NMR (100.6 MHz, $CDCl_3$) of compound **3y**.

Table S1: Optimisation of reaction conditions[a]



Entry	Solvent	Catalyst (mol%)	Ligand (mol%)	CuTC (equiv.)	Temp. (°C)	Time (mins)	Yield (%)[b]
1	Toluene	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	15
2	CH_3CN	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	22
3	H_2O	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	NR[c]
4	DMF	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	NR[c]
5	DMSO	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	NR[c]
6	AcOH	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	NR[c]
7	1,4-Dioxane	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	NR[c]
8	DCE	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	32
9	EtOH	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	47
10	MeOH	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	41
11	MTBE	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	NR[c]
12	CPME	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	NR[c]
13	2-Me-THF	$Pd_2(dba)_3$ (10)	TFP (10)	1	80	60	63
14	2-Me-THF	$Pd(PPh_3)_4$ (10)	TFP (10)	1	80	60	36
15	2-Me-THF	$Pd(PPh_3)_2Cl_2$ (10)	TFP (10)	1	80	60	NR[c]
16	2-Me-THF	$Pd(OAC)_2$ (10)	TFP (10)	1	80	60	NR[c]
17	2-Me-THF	$PdCl_2$ (10)	TFP (10)	1	80	60	NR[c]
18	2-Me-THF	anhy. $Cu(OAc)_2$(10)	TFP (10)	1	80	60	NR[c]
19	2-Me-THF	$Ni(PPH_3)_2Cl_2$ (10)	TFP (10)	1	80	60	NR[c]
20	2-Me-THF	$NiCl_2$ (10)	TFP (10)	1	80	60	NR[c]
21	2-Me-THF	$Ni(COD)_2$ (10)	TFP (10)	1	80	60	39
22	2-Me-THF	$Pd_2(dba)_3$ (5)	TFP (20)	1.5	80	60	76
23	2-Me-THF	$Pd_2(dba)_3$ (5)	TFP (20)	2	80	60	74
24	2-Me-THF	$Pd_2(dba)_3$ (5)	TFP (20)	3	80	60	75

[a] Reaction conditions: phenyl methyl selenide (**1a**) (0.5 mmol), phenyl boronic acid (**2a**) (0.6 mmol), solvent (3 mL), catalyst, CuTC, and ligand, as indicated in table was stirred at mentioned temperature (°C) for given time (min), all the experiments were carried out in a sealed tube. [b] Isolated yields. [c] NR= No reaction.

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