

Supporting Information

An Active Catalytic System for Suzuki-Miyaura Cross-Coupling Reactions Using Low Level of Palladium Loadings

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General Considerations.....	S2
General Procedures for Reaction Condition Screenings.....	S2
General Procedure for Suzuki-Miyaura Cross-Coupling Reaction.....	S2
¹ H NMR, ¹³ C NMR and ¹⁹ F NMR Spectrum for All Isolated Products.....	S3
References.....	S59

General Considerations.

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. Phosphine ligands **1**, **2** and **3** were prepared according to the reported procedures.¹ Toluene and ⁱPrOH were degassed by sparging with nitrogen for at least 15 min before use. Water was degassed by sparging with nitrogen for at least 30 min before use. All reactions were performed in a resealable screw cap Schlenk flask (approx. 15 mL volume) in the presence of a Teflon coated magnetic stirrer bar (3 mm × 50 mm). Silica gel (70-230 and 230-400 mesh) was used for column chromatography. ¹H, ¹³C and ¹⁹F NMR spectra were recorded on a Mercury-Plus (400 MHz) spectrometer. HRMS were obtained on an IonSpec FT-ICR mass spectrometer with ESI resource. All yields reported refer to isolated yields of compounds estimated to be greater than 95% purity as determined by ¹H NMR. Compounds described in the literature were characterized by comparison of their ¹H NMR spectra to the previously reported.

General Procedures for Reaction Condition Screenings.

Stock Solution **A** (2.5×10^{-4} mmol [Pd]/0.3 mL toluene): toluene (15.0 mL) was added to the mixture of Pd(OAc)₂ (2.75 mg, 1.25×10^{-2} mmol) and phosphine (2.5×10^{-2} mmol). The resulting orange colored solution was stirred at room temperature for 1 h.

Stock Solution **B** (5.0×10^{-4} mmol [Pd]/0.3 mL toluene): toluene (7.5 mL) was added to the mixture of Pd(OAc)₂ (2.75 mg, 1.25×10^{-2} mmol) and phosphine (2.5×10^{-2} mmol). The resulting orange colored solution was stirred at room temperature for 1 h.

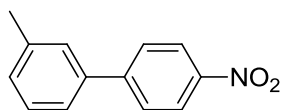
Stock Solution **C** (1.25×10^{-3} mmol [Pd]/0.3 mL toluene): toluene (3.0 mL) was added to the mixture of Pd(OAc)₂ (2.75 mg, 1.25×10^{-2} mmol) and phosphine (2.5×10^{-2} mmol). The resulting orange colored solution was stirred at room temperature for 1 h.

Aryl chlorides (2.5 mmol), Arylboronic acid (2.5 mmol), K₃PO₄ 3H₂O (5.0 mmol) were added into a Schlenk tube equipped with a Teflon-coated magnetic stir bar. The mixture was pumped and refilled with nitrogen three times, then Stock Solution **A**, **B** or **C** (0.3 mL, as indicated in Table 1), degassed toluene (1.5 mL), H₂O (1.5 mL) and ⁱPrOH (0.3 mL) were added. The reaction mixture was stirred at 90 °C under nitrogen for 16 h, and then cooled to room temperature. The reaction mixture was extracted with ethyl acetate (5 × 10 mL). The combined organic layers dried over anhydrous magnesium sulfate, filtered and concentrated in vacuo. The crude product was purified by column chromatography on silica gel to afford desired product.

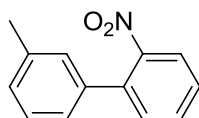
General Procedure for Suzuki-Miyaura Cross-Coupling Reaction.

A toluene solution (300 μL) containing Pd(OAc)₂ (1.25×10^{-3} mmol) and phosphine ligand **3** (2.5×10^{-3} mmol) was added to a Schlenk tube containing aryl chlorides (2.5 mmol), arylboronic acid (2.5 mmol), K₃PO₄ 3H₂O (5.0 mmol), toluene (1.5 mL), H₂O (1.5 mL) and ⁱPrOH (0.3 mL). The reaction mixture was stirred at 90 °C under nitrogen for 16 h, and then cooled to room temperature. The reaction mixture was extracted with ethyl acetate (5 × 10 mL). The combined organic layers dried over anhydrous magnesium sulfate, filtered and concentrated in vacuo. The crude product was purified by column chromatography on silica gel to afford desired product.

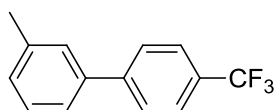
¹H NMR and ¹³C NMR Spectrum for All Isolated Products



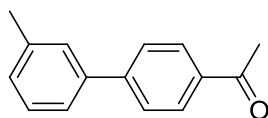
3-methyl-4'-nitro-1,1'-biphenyl.^[4] ¹H NMR (400 MHz, CDCl₃): δ 8.27 – 8.25 (m, 2 H, Ar), 7.71 – 7.69 (m, 2 H, Ar), 7.41 – 7.36 (m, 3 H, Ar), 7.24 (d, *J* = 4 Hz, 1 H, Ar), 2.24 (s, 3 H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 149.1 (s, Ar), 138.2 (s, Ar), 137.1 (s, Ar), 136.2 (s, Ar), 132.1 (s, Ar), 131.8 (s, Ar), 128.1 (s, Ar), 128.4 (s, Ar), 128.3 (s, Ar), 127.9 (s, Ar), 124.8 (s, Ar), 123.8 (s, Ar), 21.3 (s, CH₃).



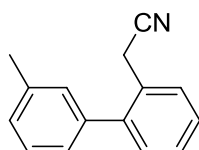
3'-methyl-2-nitro-1,1'-biphenyl.^[3] ¹H NMR (400 MHz, CDCl₃): δ 7.81 (d, *J* = 8.0 Hz, 1 H, Ar), 7.60 – 7.56 (m, 1 H, Ar), 7.44 – 7.40 (m, 2 H, Ar), 7.29 (t, *J* = 8.0 Hz, 1 H, Ar), 7.19 (d, *J* = 8.0 Hz, 1 H, Ar), 7.09 (d, *J* = 8.0 Hz, 2 H, Ar), 2.38 (s, 3 H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 147.5 (s, Ar), 146.7 (s, Ar), 138.7 (s, Ar), 138.4 (s, Ar), 129.5 (s, Ar), 128.9 (s, Ar), 127.9 (s, Ar), 127.5 (s, Ar), 124.3 (s, Ar), 123.8 (s, Ar), 21.3 (s, CH₃).



3-methyl-4'-(trifluoromethyl)-1,1'-biphenyl.^[5] ¹H NMR (400 MHz, CDCl₃): δ 7.65 (s, 4 H, Ar), 7.38 (s, 1 H, Ar), 7.35 (d, *J* = 4.0 Hz, 1 H, Ar), 7.32 (d, *J* = 8.0 Hz, 1 H, Ar), 7.20 (d, *J* = 4.0 Hz, 1 H, Ar), 2.43 (s, 3 H, CH₃). ¹⁹F NMR (376 MHz, CDCl₃): δ -64.0 (s). ¹³C NMR (100 MHz, CDCl₃): δ 144.8 (s, Ar), 139.6 (s, Ar), 138.6 (s, Ar), 129.1 (d, *J* = 2.2 Hz, CF₃), 128.9 (s, Ar), 128.8 (s, Ar), 127.9 (s, Ar), 127.3 (s, Ar), 125.5 (s, Ar), 124.3 (s, Ar), 21.3 (s, CH₃).

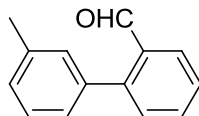


1-(3'-methyl-[1,1'-biphenyl]-4-yl)ethanone.^[4] ¹H NMR (400 MHz, CDCl₃): δ 7.99 (d, *J* = 8.0 Hz, 2 H, Ar), 7.65 (d, *J* = 8.0 Hz, 2 H, Ar), 7.40 (d, *J* = 8.0 Hz, 2 H, Ar), 7.33 (t, *J* = 8.0 Hz, 1 H, Ar), 7.19 (d, *J* = 8.0 Hz, 1 H, Ar), 2.63 (s, 3 H, COCH₃), 2.43 (s, 3 H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 197.5 (s, C=O), 147.6 (s, Ar), 139.6 (s, Ar), 138.4 (s, Ar), 135.5 (s, Ar), 128.8 (s, Ar), 128.7 (s, Ar), 127.8 (s, Ar), 127.0 (s, Ar), 124.2 (s, Ar), 26.4 (s, CH₃), 21.3 (s, CH₃).

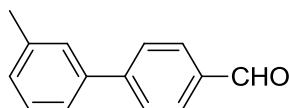


2-(3'-methyl-[1,1'-biphenyl]-2-yl)acetonitrile.^[6] ¹H NMR (400 MHz, CDCl₃): δ 7.51 (t, *J* = 8.0 Hz, 1 H, Ar), 7.37 – 7.33 (m, 2 H, Ar), 7.30 (d, *J* = 8.0 Hz, 1 H, Ar), 7.25 (t, *J* = 8.0 Hz, 1 H, Ar),

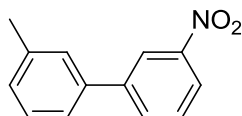
7.18 (d, $J = 8.0$ Hz, 1 H, Ar), 7.05 (t, $J = 8.0$ Hz, 2 H, Ar), 3.62 (s, 2 H, CH_2CN), 2.40 (s, 3 H, CH_3). ^{13}C NMR (100 MHz, CDCl_3): δ 141.7 (s, Ar), 139.6 (s, Ar), 138.1 (s, Ar), 130.2 (s, Ar), 129.4 (s, Ar), 128.6 (s, Ar), 128.3 (s, Ar), 128.3 (s, Ar), 127.9 (s, Ar), 127.9 (s, Ar), 127.5 (s, Ar), 125.7 (s, Ar), 118.2 (s, CN), 21.8 (s, CH_2), 21.3 (s, CH_3).



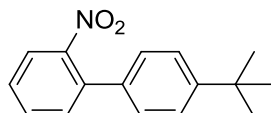
3'-methyl-[1,1'-biphenyl]-2-carbaldehyde.^[15] ^1H NMR (400 MHz, CDCl_3): δ 9.95 (s, 1 H, CHO), 7.99 (d, $J = 8.0$ Hz, 1 H, Ar), 7.62 – 7.58 (m, 2 H, Ar), 7.48 – 7.41 (m, 1 H, Ar), 7.33 (t, $J = 8.0$ Hz, 1 H, Ar), 7.16 (t, $J = 8.0$ Hz, 2 H, Ar), 2.42 (s, 3 H, CH_3). ^{13}C NMR (100 MHz, CDCl_3): δ 192.3 (s, CHO), 146.0 (s, Ar), 137.9 (s, Ar), 137.5 (s, Ar), 133.5 (s, Ar), 133.3 (s, Ar), 130.6 (s, Ar), 130.6 (s, Ar), 128.7 (s, Ar), 128.1 (s, Ar), 127.5 (s, Ar), 127.3 (s, Ar), 127.1 (s, Ar), 21.3 (s, CH_3).



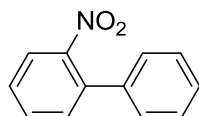
3'-methyl-[1,1'-biphenyl]-4-carbaldehyde.^[9] ^1H NMR (400 MHz, CDCl_3): δ 10.01 (s, 1 H, CHO), 7.91 (d, $J = 8.0$ Hz, 2 H, Ar), 7.71 (d, $J = 8.0$ Hz, 2 H, Ar), 7.41 (d, $J = 8.0$ Hz, 2 H, Ar), 7.34 (t, $J = 8.0$ Hz, 1 H, Ar), 7.20 (d, $J = 4.0$ Hz, 1 H, Ar), 2.43 (s, 3 H, CH_3). ^{13}C NMR (100 MHz, CDCl_3): δ 191.6 (s, CHO), 147.0 (s, Ar), 139.4 (s, Ar), 138.4 (s, Ar), 134.9 (s, Ar), 130.0 (s, Ar), 129.0 (s, Ar), 127.9 (s, Ar), 127.4 (s, Ar), 124.2 (s, Ar), 21.3 (s, CH_3).



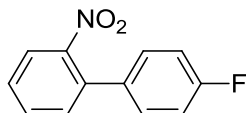
3-methyl-3'-nitro-1,1'-biphenyl.^[16] ^1H NMR (400 MHz, CDCl_3): δ 8.41 (t, $J = 4.0$ Hz, 1 H, Ar), 8.17 – 8.15 (m, 1 H, Ar), 7.88 (d, $J = 8.0$ Hz, 1 H, Ar), 7.57 (t, $J = 8.0$ Hz, 1 H, Ar), 7.41–7.35 (m, 3 H, Ar), 7.21 (s, 1 H, Ar), 2.44 (s, 3 H, CH_3). ^{13}C NMR (100 MHz, CDCl_3): δ 148.4 (s, Ar), 142.6 (s, Ar), 138.6 (s, Ar), 138.3 (s, Ar), 132.8 (s, Ar), 129.4 (s, Ar), 129.1 (s, Ar), 128.8 (s, Ar), 127.6 (s, Ar), 124.0 (s, Ar), 121.7 (s, Ar), 121.6 (s, Ar), 21.3 (s, CH_3).



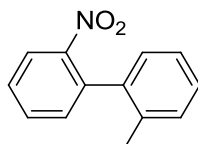
4'-(tert-butyl)-2-nitro-1,1'-biphenyl.^[2] ^1H NMR (400 MHz, CDCl_3): δ 7.80 – 7.77 (m, 1 H, Ar), 7.57 – 7.55 (m, 1 H, Ar), 7.45 – 7.40 (m, 4 H, Ar), 7.24 (t, $J = 4.0$ Hz, 1 H, Ar), 7.22 (t, $J = 4.0$ Hz, 1 H, Ar), 1.35 (s, 9 H, CMe_3). ^{13}C NMR (100 MHz, CDCl_3): δ 151.0 (s, Ar), 149.2 (s, Ar), 136.0 (s, Ar), 134.1 (s, Ar), 132.0 (s, Ar), 131.8 (s, Ar), 127.7 (s, Ar), 127.4 (s, Ar), 125.5 (s, Ar), 123.8 (s, Ar), 34.5 (s, CMe_3), 31.2 (s, CH_3).



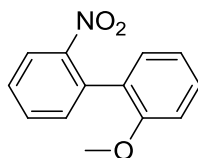
2-nitro-1,1'-biphenyl.^[2] ¹H NMR (400 MHz, CDCl₃): δ 7.83 – 7.81 (m, 1 H, Ar), 7.61 – 7.57 (m, 1 H, Ar), 7.45 – 7.38 (m, 5 H, Ar), 7.30 – 7.28 (m, 2 H, Ar). ¹³C NMR (100 MHz, CDCl₃): δ 149.0 (s, Ar), 137.3 (s, Ar), 136.0 (s, Ar), 132.2 (s, Ar), 131.7 (s, Ar), 128.5 (s, Ar), 128.0 (s, Ar), 127.7 (s, Ar), 123.8 (s, Ar).



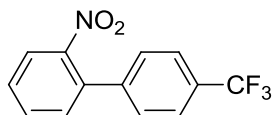
4'-fluoro-2-nitro-1,1'-biphenyl.^[2] ¹H NMR (400 MHz, CDCl₃): δ 7.85 – 7.82 (m, 1 H, Ar), 7.60 – 7.57 (m, 1 H, Ar), 7.48 (t, *J* = 4.0 Hz, 1 H, Ar), 7.40 – 7.38 (m, 1 H, Ar), 7.28 – 7.25 (m, 2 H, Ar), 7.12 – 7.07 (m, 2 H, Ar). ¹⁹F NMR (376 MHz, CDCl₃): δ -114.7 (s). ¹³C NMR (100 MHz, CDCl₃): δ 163.3 (s, Ar), 161.7 (s, Ar), 149.0 (s, Ar), 135.0 (s, Ar), 133.2 (s, Ar), 132.3 (s, Ar), 131.8 (s, Ar), 129.5 (s, Ar), 128.2 (s, Ar), 124.0 (s, Ar), 115.5 (d, *J* = 1.4 Hz, Ar).



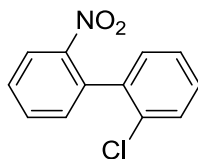
2-methyl-2'-nitro-1,1'-biphenyl.^[3] ¹H NMR (400 MHz, CDCl₃): δ 7.97 – 7.95 (m, 1 H, Ar), 7.63 – 7.59 (m, 1 H, Ar), 7.51 – 7.49 (m, 1 H, Ar), 7.32 – 7.25 (m, 3 H, Ar), 7.21 (d, *J* = 8.0 Hz, 1 H, Ar), 7.07 (d, *J* = 8.0 Hz, 1 H, Ar), 2.10 (s, 3 H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 148.9 (s, Ar), 137.3 (s, Ar), 136.3 (s, Ar), 135.4 (s, Ar), 132.4 (s, Ar), 132.0 (s, Ar), 129.8 (s, Ar), 128.1 (s, Ar), 128.1 (s, Ar), 128.0 (s, Ar), 125.6 (s, Ar), 123.9 (s, Ar), 19.7 (s, CH₃).



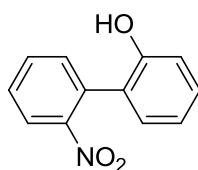
2-methoxy-2'-nitro-1,1'-biphenyl.^[8] ¹H NMR (400 MHz, CDCl₃): δ 7.90 – 7.88 (m, 1 H, Ar), 7.62 – 7.57 (m, 1 H, Ar), 7.45 – 7.41 (m, 1 H, Ar), 7.39 – 7.33 (m, 2 H, Ar), 7.29 – 7.27 (m, 1 H, Ar), 7.05 (t, *J* = 8.0 Hz, 1 H, Ar), 6.88 (d, *J* = 8.0 Hz, 1 H, Ar), 3.68 (s, 3 H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 155.6 (s, Ar), 149.5 (s, Ar), 132.8 (s, Ar), 132.6 (s, Ar), 132.3 (s, Ar), 129.7 (s, Ar), 129.5 (s, Ar), 127.9 (s, Ar), 126.8 (s, Ar), 123.7 (s, Ar), 121.1 (s, Ar), 110.4 (s, Ar), 55.0 (s, OCH₃).



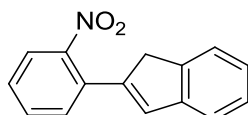
2-nitro-4'-(trifluoromethyl)-1,1'-biphenyl.^[2] ¹H NMR (400 MHz, CDCl₃): δ 7.92 (d, *J* = 8.0 Hz, 1 H, Ar), 7.67 – 7.62 (m, 3 H, Ar), 7.55 (t, *J* = 8.0 Hz, 1 H, Ar), 7.42 – 7.39 (m, 1 H, Ar). ¹⁹F NMR (376 MHz, CDCl₃): δ -64.2 (s). ¹³C NMR (100 MHz, CDCl₃): δ 148.6 (s, Ar), 141.3 (s, Ar), 134.8 (s, Ar), 132.6 (s, Ar), 131.6 (s, Ar), 130.2-129.6 (m, CF₃), 128.9 (s, Ar), 128.2 (s, Ar), 125.4 (s, Ar), 124.2 (s, Ar), 123.0 (s, Ar).



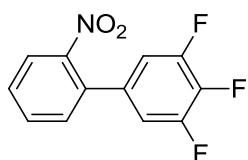
2-chloro-2'-nitro-1,1'-biphenyl.^[8] ¹H NMR (400 MHz, CDCl₃): δ 8.08 – 8.06 (m, 1 H, Ar), 7.67 – 7.63 (m, 1 H, Ar), 7.54 (t, J = 8.0 Hz, 1 H, Ar), 7.44 – 7.42 (m, 1 H, Ar), 7.36 – 7.31 (m, 3 H, Ar), 7.24 – 7.23 (m, 1 H, Ar). ¹³C NMR (100 MHz, CDCl₃): δ 148.3 (s, Ar), 136.9 (s, Ar), 134.1 (s, Ar), 132.9 (s, Ar), 132.2 (s, Ar), 129.7 (s, Ar), 129.2 (s, Ar), 128.9 (s, Ar), 126.8 (s, Ar), 124.2 (s, Ar).



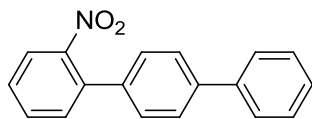
2'-nitro-[1,1'-biphenyl]-2-ol.^[14] ¹H NMR (400 MHz, CDCl₃): δ 7.95 (d, J = 8.0 Hz, 1 H, Ar), 7.63 (t, J = 6.0 Hz, 1 H, Ar), 7.49 (t, J = 8.0 Hz, 1 H, Ar), 7.41 (d, J = 8.0 Hz, 1 H, Ar), 7.26 – 7.20 (m, 2 H, Ar), 7.02 (t, J = 6.0 Hz, 1 H, Ar), 6.81 (d, J = 8.0 Hz, 1 H, Ar), 4.91 (s, 1 H, OH). ¹³C NMR (100 MHz, CDCl₃): δ 152.3 (s, Ar), 149.6 (s, Ar), 132.8 (s, Ar), 132.6 (s, Ar), 132.5 (s, Ar), 129.8 (s, Ar), 128.4 (s, Ar), 125.0 (s, Ar), 124.1 (s, Ar), 121.3 (s, Ar), 115.7 (s, Ar).



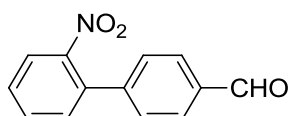
2-(2-nitrophenyl)-1H-indene. ¹H NMR (400 MHz, CDCl₃): δ 7.74 (d, J = 8.0 Hz, 1 H, Ar), 7.54 (d, J = 8.0 Hz, 1 H, Ar), 7.49 (d, J = 8.0 Hz, 1 H, Ar), 7.44 (d, J = 8.0 Hz, 1 H, Ar), 7.42 – 7.37 (m, 2 H, Ar), 7.27 (t, J = 8.0 Hz, 1 H, Ar), 7.20 (d, J = 8.0 Hz, 1 H, Ar), 6.95 (s, 1 H, =CH), 3.68 (s, 2 H, CH₂). ¹³C NMR (100 MHz, CDCl₃): δ 148.7 (s, Ar), 144.1 (s, Ar), 143.3 (s, Ar), 142.1 (s, Ar), 132.0 (s, Ar), 131.3 (s, Ar), 130.6 (s, Ar), 127.9 (s, Ar), 126.5 (s, Ar), 125.3 (s, Ar), 123.7 (s, Ar), 123.5 (s, Ar), 121.4 (s, Ar), 40.4 (s, CH₂). HRMS (ESI): $[M+H]^+$ calcd. for C₁₅H₁₂NO₂: 238.0868; Found: 238.0860.



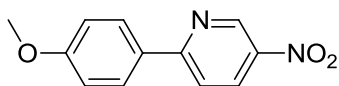
3',4',5'-trifluoro-2-nitro-1,1'-biphenyl.^[24] ¹H NMR (400 MHz, CDCl₃): δ 7.91 (d, J = 8.0 Hz, 1 H, Ar), 7.63 (t, J = 8.0 Hz, 1 H, Ar), 7.54 (d, J = 8.0 Hz, 1 H, Ar), 7.36 (d, J = 8.0 Hz, 1 H, Ar), 6.92 (t, J = 8.0 Hz, 2 H, Ar). ¹⁹F NMR (376 MHz, CDCl₃): δ -137.8 (s), -164.7 (s). ¹³C NMR (100 MHz, CDCl₃): δ 151.8 (s, Ar), 150.1 (s, Ar), 148.5 (s, Ar), 133.3 (s, Ar), 132.8 (s, Ar), 131.5 (s, Ar), 129.3 (s, Ar), 124.4 (s, Ar), 112.5 (s, Ar), 112.4 (s, Ar).



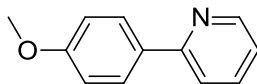
2-nitro-1,1':4',1''-terphenyl.^[13] ¹H NMR (400 MHz, CDCl₃): δ 7.84 (d, *J* = 8.0 Hz, 1 H, Ar), 7.63 – 7.58 (m, 5 H, Ar), 7.48 – 7.51 (m, 4 H, Ar), 7.36 (t, *J* = 8.0 Hz, 3 H, Ar). ¹³C NMR (100 MHz, CDCl₃): δ 149.1 (s, Ar), 140.9 (s, Ar), 140.2 (s, Ar), 136.1 (s, Ar), 135.8 (s, Ar), 132.2 (s, Ar), 131.8 (s, Ar), 128.7 (s, Ar), 128.2 (s, Ar), 128.1 (s, Ar), 127.5 (s, Ar), 127.3 (s, Ar), 127.0 (s, Ar), 124.0 (s, Ar).



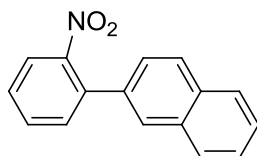
2'-nitro-[1,1'-biphenyl]-4-carbaldehyde.^[9] ¹H NMR (400 MHz, CDCl₃): δ 10.03 (s, 1 H, CHO), 7.94 – 7.91 (m, 3 H, Ar), 7.65 (t, *J* = 8.0 Hz, 1 H, Ar), 7.54 (t, *J* = 8.0 Hz, 1 H, Ar), 7.47 – 7.41 (m, 3 H, Ar). ¹³C NMR (100 MHz, CDCl₃): δ 191.6 (s, CHO), 148.5 (s, Ar), 143.6 (s, Ar), 135.5 (s, Ar), 135.0 (s, Ar), 132.6 (s, Ar), 131.5 (s, Ar), 129.7 (s, Ar), 129.0 (s, Ar), 128.5 (s, Ar), 124.3 (s, Ar).



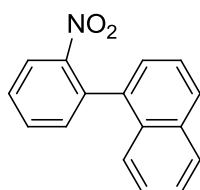
2-(4-methoxyphenyl)-5-nitropyridine.^[22] ¹H NMR (400 MHz, CDCl₃): δ 9.40 (s, 1 H, Ar), 8.45 – 8.42 (m, 1 H, Ar), 8.04 (d, *J* = 8.0 Hz, 2 H, Ar), 7.79 (d, *J* = 8.0 Hz, 1 H, Ar), 7.00 (t, *J* = 8.0 Hz, 2 H, Ar), 3.88 (s, 3 H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 161.9 (s, Ar), 161.7 (s, Ar), 145.9 (s, Ar), 142.0 (s, Ar), 131.7 (s, Ar), 129.3 (s, Ar), 129.1 (s, Ar), 118.8 (s, Ar), 114.3 (s, Ar), 55.3 (s, OCH₃).



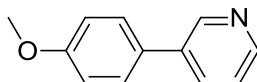
2-(4-methoxyphenyl)pyridine.^[17] ¹H NMR (400 MHz, CDCl₃): δ 8.61 (d, *J* = 4.0 Hz, 1 H, Ar), 7.92 (d, *J* = 8.0 Hz, 2 H, Ar), 7.68 – 7.64 (m, 2 H, Ar), 7.16 – 7.12 (m, 1 H, Ar), 6.97 (d, *J* = 8.0 Hz, 2 H, Ar), 3.85 (s, 3 H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 160.0 (s, Ar), 156.5 (s, Ar), 149.1 (s, Ar), 136.2 (s, Ar), 131.5 (s, Ar), 127.7 (s, Ar), 121.0 (s, Ar), 119.3 (s, Ar), 113.7 (s, Ar), 54.8 (s, OCH₃).



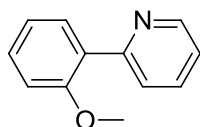
2-(2-nitrophenyl)naphthalene.^[2] ¹H NMR (400 MHz, CDCl₃): δ 7.89 – 7.78 (m, 5 H, Ar), 7.62 (d, *J* = 8.0 Hz, 1 H, Ar), 7.52 – 7.46 (m, 4 H, Ar), 7.39 – 7.36 (m, 1 H, Ar). ¹³C NMR (100 MHz, CDCl₃): δ 149.0 (s, Ar), 136.1 (s, Ar), 134.8 (s, Ar), 133.1 (s, Ar), 132.6 (s, Ar), 132.3 (s, Ar), 132.1 (s, Ar), 128.0 (s, Ar), 127.6 (s, Ar), 126.8 (s, Ar), 126.4 (s, Ar), 125.6 (s, Ar), 124.0 (s, Ar).



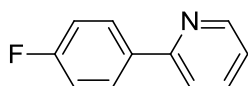
1-(2-nitrophenyl)naphthalene.^[7] ¹H NMR (400 MHz, CDCl₃): δ 8.04 (d, *J* = 8.0 Hz, 1 H, Ar), 7.87 (d, *J* = 8.0 Hz, 2 H, Ar), 7.66 (t, *J* = 8.0 Hz, 1 H, Ar), 7.57 (t, *J* = 8.0 Hz, 1 H, Ar), 7.49 (d, *J* = 8.0 Hz, 1 H, Ar), 7.44 (t, *J* = 8.0 Hz, 2 H, Ar), 7.41 – 7.37 (m, 2 H, Ar), 7.31 (d, *J* = 8.0 Hz, 1 H, Ar). ¹³C NMR (100 MHz, CDCl₃): δ 149.5 (s, Ar), 135.3 (s, Ar), 135.0 (s, Ar), 133.2 (s, Ar), 132.9 (s, Ar), 132.4 (s, Ar), 131.2 (s, Ar), 128.4 (s, Ar), 126.4 (s, Ar), 125.9 (s, Ar), 125.1 (s, Ar), 124.68 (s, Ar), 124.0 (s, Ar).



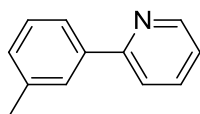
3-(4-methoxyphenyl)pyridine.^[17] ¹H NMR (400 MHz, CDCl₃): δ 8.78 (s, 1 H, Ar), 8.51 (d, *J* = 4.0 Hz, 1 H, Ar), 7.80 (d, *J* = 8.0 Hz, 1 H, Ar), 7.49 (d, *J* = 8.0 Hz, 2 H, Ar), 7.31 (t, *J* = 8.0 Hz, 1 H, Ar), 6.99 (d, *J* = 8.0 Hz, 2 H, Ar), 3.85 (s, 3 H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 159.3 (s, Ar), 147.5 (s, Ar), 135.8 (s, Ar), 133.5 (s, Ar), 133.4 (s, Ar), 129.7 (s, Ar), 127.8 (s, Ar), 123.1 (s, Ar), 114.2 (s, Ar), 54.9 (s, OCH₃).



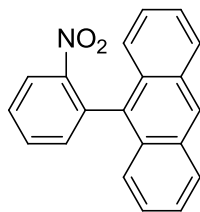
2-(2-methoxyphenyl)pyridine.^[17] ¹H NMR (400 MHz, CDCl₃): δ 8.67 (t, *J* = 8.0 Hz, 1 H, Ar), 7.79 – 7.76 (m, 1 H, Ar), 7.74 – 7.72 (m, 1 H, Ar), 7.69 – 7.65 (m, 1 H, Ar), 7.37 – 7.32 (m, 1 H, Ar), 7.19 – 7.16 (m, 1 H, Ar), 7.07 – 7.03 (m, 1 H, Ar), 6.99 – 6.97 (m, 1 H, Ar), 3.84 (s, 3 H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 156.3 (s, Ar), 155.4 (s, Ar), 148.8 (s, Ar), 135.0 (s, Ar), 130.5 (s, Ar), 129.4 (s, Ar), 128.4 (s, Ar), 124.5 (s, Ar), 121.1 (s, Ar), 120.4 (s, Ar), 110.7 (s, Ar), 54.9 (s, OCH₃).



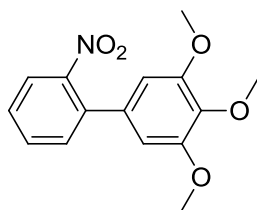
2-(4-fluorophenyl)pyridine.^[18] ¹H NMR (400 MHz, CDCl₃): δ 8.64 (d, *J* = 8.0 Hz, 1 H, Ar), 7.96 – 7.93 (m, 2 H, Ar), 7.71 (t, *J* = 8.0 Hz, 1 H, Ar), 7.65 (d, *J* = 8.0 Hz, 1 H, Ar), 7.21 – 7.18 (m, 1 H, Ar), 7.12 (d, *J* = 8.0 Hz, 2 H, Ar). ¹⁹F NMR (376 MHz, CDCl₃): δ -114.3 (s). ¹³C NMR (100 MHz, CDCl₃): δ 164.1 (s, Ar), 162.4 (s, Ar), 156.1 (s, Ar), 149.5 (s, Ar), 136.6 (s, Ar), 135.3 (s, Ar), 128.5 (s, Ar), 121.8 (s, Ar), 119.9 (s, Ar), 115.0 (d, *J* = 1.3 Hz, 1 C, Ar).



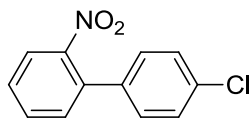
2-(m-tolyl)pyridine.^[19] ¹H NMR (400 MHz, CDCl₃): δ 8.65 (d, *J* = 4.0 Hz, 1 H, Ar), 7.81 (s, 1 H, Ar), 7.73 – 7.69 (m, 3 H, Ar), 7.33 (t, *J* = 8.0 Hz, 1 H, Ar), 7.21 – 7.17 (m, 2 H, Ar), 2.43 (s, 3 H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 156.9 (s, Ar), 149.0 (s, Ar), 138.8 (s, Ar), 137.7 (s, Ar), 136.1 (s, Ar), 129.2 (s, Ar), 128.1 (s, Ar), 127.1 (s, Ar), 123.5 (s, Ar), 120.0 (s, Ar), 21.0 (s, CH₃).



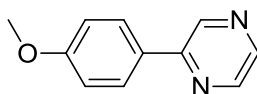
9-(2-nitrophenyl)anthracene.^[12] ¹H NMR (400 MHz, CDCl₃): δ 8.49 (s, 1 H, Ar), 8.23 – 8.21 (m, 1 H, Ar), 8.02 (d, *J* = 8.0 Hz, 2 H, Ar), 7.78 – 7.74 (m, 1 H, Ar), 7.69 (d, *J* = 8.0 Hz, 1 H, Ar), 7.46 – 7.32 (m, 7 H, Ar). ¹³C NMR (100 MHz, CDCl₃): δ 150.1 (s, Ar), 133.9 (s, Ar), 133.7 (s, Ar), 133.0 (s, Ar), 131.6 (s, Ar), 131.1 (s, Ar), 129.6 (s, Ar), 129.0 (s, Ar), 128.6 (s, Ar), 127.4 (s, Ar), 126.0 (s, Ar), 125.3 (s, Ar), 125.1 (s, Ar), 124.5 (s, Ar).



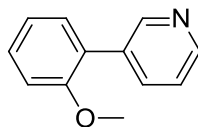
3',4',5'-trimethoxy-2-nitro-1,1'-biphenyl.^[10] ¹H NMR (400 MHz, CDCl₃): δ 7.77 (d, *J* = 8.0 Hz, 1 H, Ar), 7.58 (t, *J* = 8.0 Hz, 1 H, Ar), 7.45 (t, *J* = 8.0 Hz, 2 H, Ar), 6.50 (s, 2 H, Ar), 3.88 (s, 3 H, OMe), 3.84 (s, 6 H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 153.1 (s, Ar), 149.2 (s, Ar), 137.7 (s, Ar), 135.8 (s, Ar), 132.6 (s, Ar), 131.9 (s, Ar), 131.5 (s, Ar), 128.0 (s, Ar), 123.6 (s, Ar), 104.8 (s, Ar), 60.7 (s, OCH₃), 55.9 (s, OCH₃).



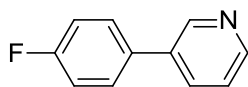
4'-chloro-2-nitro-1,1'-biphenyl.^[9] ¹H NMR (400 MHz, CDCl₃): δ 7.87 – 7.84 (m, 1 H, Ar), 7.62 – 7.58 (m, 1 H, Ar), 7.50 – 7.46 (m, 1 H, Ar), 7.39 – 7.37 (m, 3 H, Ar), 7.23 (d, *J* = 4.0 Hz, 1 H, Ar), 7.21 (s, 1 H, Ar). ¹³C NMR (100 MHz, CDCl₃): δ 148.8 (s, Ar), 135.7 (s, Ar), 134.9 (s, Ar), 134.2 (s, Ar), 132.4 (s, Ar), 131.7 (s, Ar), 129.1 (s, Ar), 128.7 (s, Ar), 128.4 (s, Ar), 124.1 (s, Ar).



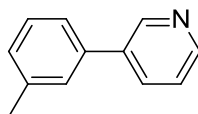
2-(4-methoxyphenyl)pyrazine.^[19] ¹H NMR (400 MHz, CDCl₃): δ 8.95 (d, *J* = 4.0 Hz, 1 H, Ar), 8.55 (t, *J* = 4.0 Hz, 1 H, Ar), 8.40 (d, *J* = 4.0 Hz, 1 H, Ar), 7.95 (d, *J* = 8.0 Hz, 2 H, Ar), 7.01 (d, *J* = 8.0 Hz, 2 H, Ar), 3.87 (s, 3 H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 160.8 (s, Ar), 152.0 (s, Ar), 143.6 (s, Ar), 141.7 (s, Ar), 141.2 (s, Ar), 128.4 (s, Ar), 127.9 (s, Ar), 114.1 (s, Ar), 55.0 (s, OCH₃).



3-(2-methoxyphenyl)pyridine.^[17] ¹H NMR (400 MHz, CDCl₃): δ 8.74 (s, 1 H, Ar), 8.53 (d, *J* = 4.0 Hz, 1 H, Ar), 7.85 (d, *J* = 8.0 Hz, 1 H, Ar), 7.36 (t, *J* = 8.0 Hz, 1 H, Ar), 7.32 (t, *J* = 8.0 Hz, 2 H, Ar), 7.05 (t, *J* = 8.0 Hz, 1 H, Ar), 6.70 (d, *J* = 4.0 Hz, 1 H, Ar), 3.83 (s, 3 H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 156.2 (s, Ar), 149.9 (s, Ar), 147.6 (s, Ar), 136.5 (s, Ar), 133.9 (s, Ar), 130.3 (s, Ar), 129.3 (s, Ar), 126.6 (s, Ar), 122.6 (s, Ar), 120.7 (s, Ar), 110.9 (s, Ar), 55.2 (s, OCH₃).

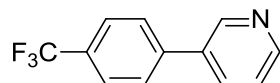


3-(4-fluorophenyl)pyridine.^[20] ¹H NMR (400 MHz, CDCl₃): δ 8.77 (d, *J* = 4.0 Hz, 1 H, Ar), 8.57 – 8.55 (m, 1 H, Ar), 7.82 – 7.79 (m, 1 H, Ar), 7.54 – 7.50 (m, 2 H, Ar), 7.35 – 7.32 (m, 1 H, Ar), 7.15 (t, *J* = 8.0 Hz, 2 H, Ar). ¹⁹F NMR (376 MHz, CDCl₃): δ -115.3 (s). ¹³C NMR (100 MHz, CDCl₃): δ 162.9 (s, Ar), 161.3 (s, Ar), 147.6 (s, Ar), 147.2 (s, Ar), 134.8 (s, Ar), 133.2 (d, *J* = 3.7 Hz, 1 C, Ar), 128.0 (s, Ar), 128.0 (s, Ar), 122.9 (s, Ar), 115.3 (d, *J* = 3.7 Hz, 1 C, Ar).

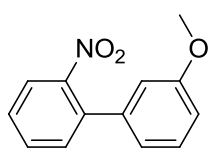


3-(m-tolyl)pyridine.^[19] ¹H NMR (400 MHz, CDCl₃): δ 8.80 (d, *J* = 0.02 Hz, 1 H, Ar), 8.55 – 8.54 (m, 1 H, Ar), 7.85 – 7.82 (m, 1 H, Ar), 7.36 – 7.31 (m, 4 H, Ar), 7.19 (d, *J* = 4.0 Hz, 1 H, Ar),

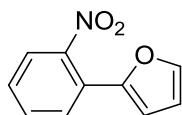
2.43 (s, 3 H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 147.7 (s, Ar), 138.2 (s, Ar), 137.2 (s, Ar), 136.2 (s, Ar), 133.8 (s, Ar), 128.5 (s, Ar), 128.4 (s, Ar), 127.3 (s, Ar), 123.7 (s, Ar), 123.0 (s, Ar), 21.0 (s, CH₃).



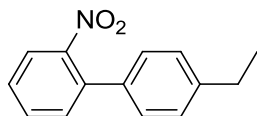
3-(4-(trifluoromethyl)phenyl)pyridine.^[21] ¹H NMR (400 MHz, CDCl₃): δ 8.83 (s, 1 H, Ar), 8.62 (t, *J* = 4.0 Hz, 1 H, Ar), 7.88 – 7.85 (m, 1 H, Ar), 7.73 – 7.66 (m, 4 H, Ar), 7.40 – 7.37 (m, 1 H, Ar). ¹⁹F NMR (376 MHz, CDCl₃): δ -64.0 (s). ¹³C NMR (100 MHz, CDCl₃): δ 148.7 (s, Ar), 147.6 (s, Ar), 140.6 (s, Ar), 134.4 (s, Ar), 133.7 (s, Ar), 129.7 – 129.0 (m, 1 C, CF₃), 126.7 (s, Ar), 125.3 (s, Ar), 124.5 (s, Ar), 123.0 (s, Ar), 21.3 (s, CH₃).



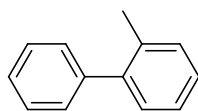
3'-methoxy-2-nitro-1,1'-biphenyl.^[2] ¹H NMR (400 MHz, CDCl₃): δ 8.05 (d, *J* = 4.0 Hz, 1 H, Ar), 7.99 (s, 1 H, Ar), 7.90 (d, *J* = 8.0 Hz, 1 H, Ar), 7.62 (t, *J* = 8.0 Hz, 1 H, Ar), 7.52 – 7.41 (m, 4 H, Ar), 3.91 (s, 3 H, OMe). ¹³C NMR (100 MHz, CDCl₃): δ 166.3 (s, Ar), 148.7 (s, Ar), 137.7 (s, Ar), 135.3 (s, Ar), 132.5 (s, Ar), 132.1 (s, Ar), 131.8 (s, Ar), 130.4 (s, Ar), 129.1 (s, Ar), 128.9 (s, Ar), 128.6 (s, Ar), 124.2 (s, Ar), 52.1 (s, OCH₃).



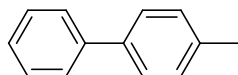
2-(2-nitrophenyl)furan.^[10] ¹H NMR (400 MHz, CDCl₃): δ 7.70 – 7.64 (m, 2 H, Ar), 7.57 – 7.49 (m, 2 H, Ar), 7.38 (t, *J* = 8.0 Hz, 1 H, Ar), 6.64 (d, *J* = 8.0 Hz, 1 H, Ar), 6.48 (t, *J* = 2.0 Hz, 1 H, Ar). ¹³C NMR (100 MHz, CDCl₃): δ 148.2 (s, Ar), 147.3 (s, Ar), 143.6 (s, Ar), 131.7 (s, Ar), 128.7 (s, Ar), 128.1 (s, Ar), 123.9 (s, Ar), 123.6 (s, Ar), 111.7 (s, Ar), 109.5 (s, Ar).



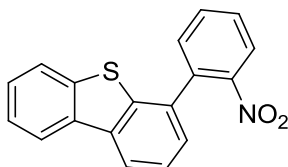
4'-ethyl-2-nitro-1,1'-biphenyl.^[11] ¹H NMR (400 MHz, CDCl₃): δ 7.80 (d, *J* = 8.0 Hz, 1 H, Ar), 7.56 (t, *J* = 8.0 Hz, 1 H, Ar), 7.42 (t, *J* = 8.0 Hz, 2 H, Ar), 7.24 – 7.20 (m, 4 H, Ar), 2.72 – 2.66 (m, 2 H, CH₂), 1.27 (t, *J* = 8.0 Hz, 3 H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 149.1 (s, Ar), 144.1 (s, Ar), 136.0 (s, Ar), 134.4 (s, Ar), 132.0 (s, Ar), 131.7 (s, Ar), 128.0 (s, Ar), 127.7 (s, Ar), 127.6 (s, Ar), 123.8 (s, Ar), 28.3 (s, CH₂), 15.2 (s, CH₃).



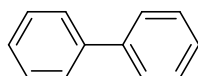
2-methyl-1,1'-biphenyl.^[26] ¹H NMR (400 MHz, CDCl₃): δ 7.40 – 7.36 (m, 2 H, Ar), 7.33 – 7.29 (m, 3 H, Ar), 7.25 – 7.23 (m, 2 H, Ar), 7.22 – 7.21 (m, 2 H, Ar), 2.27 (s, 3 H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 141.8 (s, Ar), 141.8 (s, Ar), 135.1 (s, Ar), 130.2 (s, Ar), 129.7 (s, Ar), 129.0 (s, Ar), 127.9 (s, Ar), 127.1 (s, Ar), 126.6 (s, Ar), 125.7 (s, Ar), 20.3 (s, CH₃).



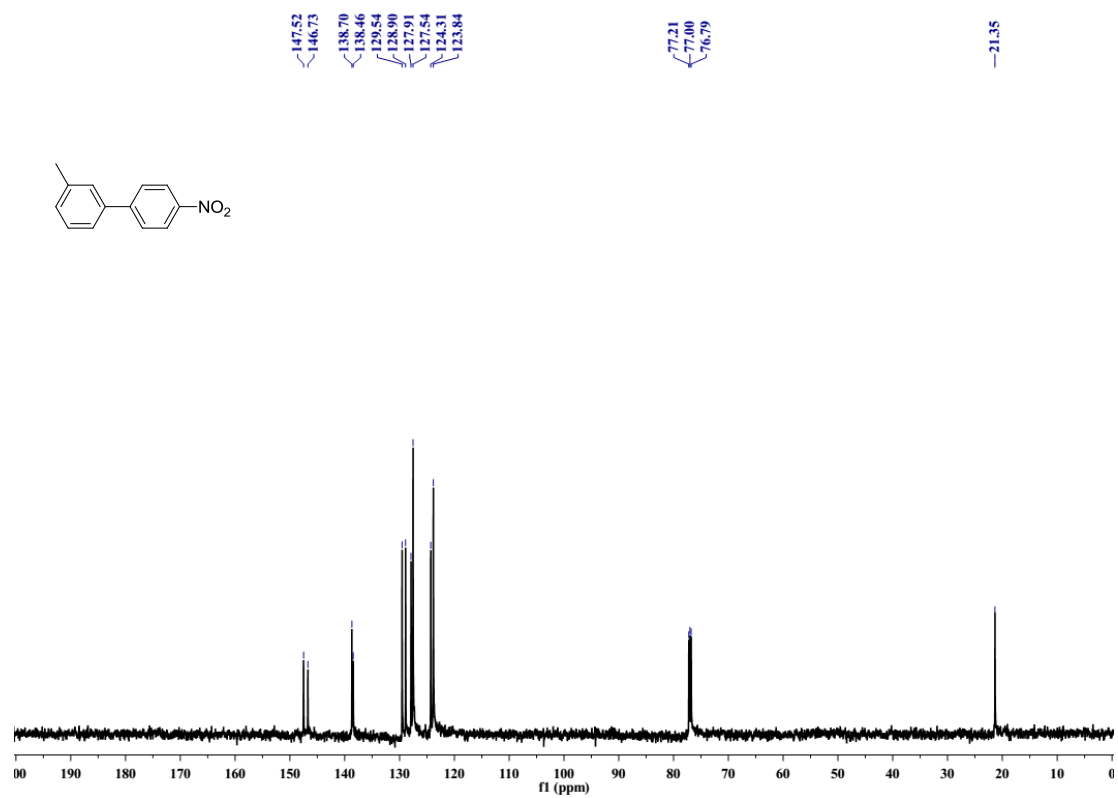
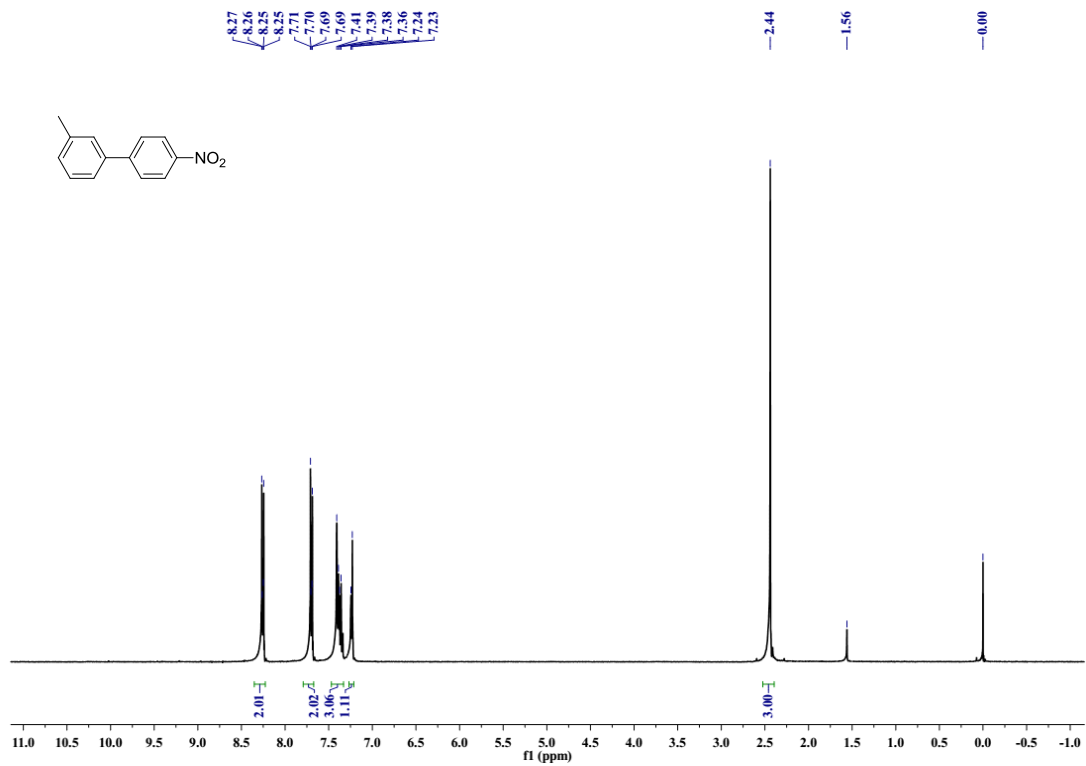
4-methyl-1,1'-biphenyl.^[7] ¹H NMR (400 MHz, CDCl₃): δ 7.54 (d, *J* = 8.0 Hz, 2 H, Ar), 7.46 (d, *J* = 8.0 Hz, 2 H, Ar), 7.39 (t, *J* = 8.0 Hz, 2 H, Ar), 7.28 (t, *J* = 8.0 Hz, 1 H, Ar), 7.21 (t, *J* = 4.0 Hz, 2 H, Ar), 2.38 (s, 3 H, CH₃). ¹³C NMR (100 MHz, CDCl₃): δ 141.0 (s, Ar), 138.2 (s, Ar), 136.8 (s, Ar), 129.4 (s, Ar), 128.6 (s, Ar), 126.8 (s, Ar), 21.0 (s, CH₃).

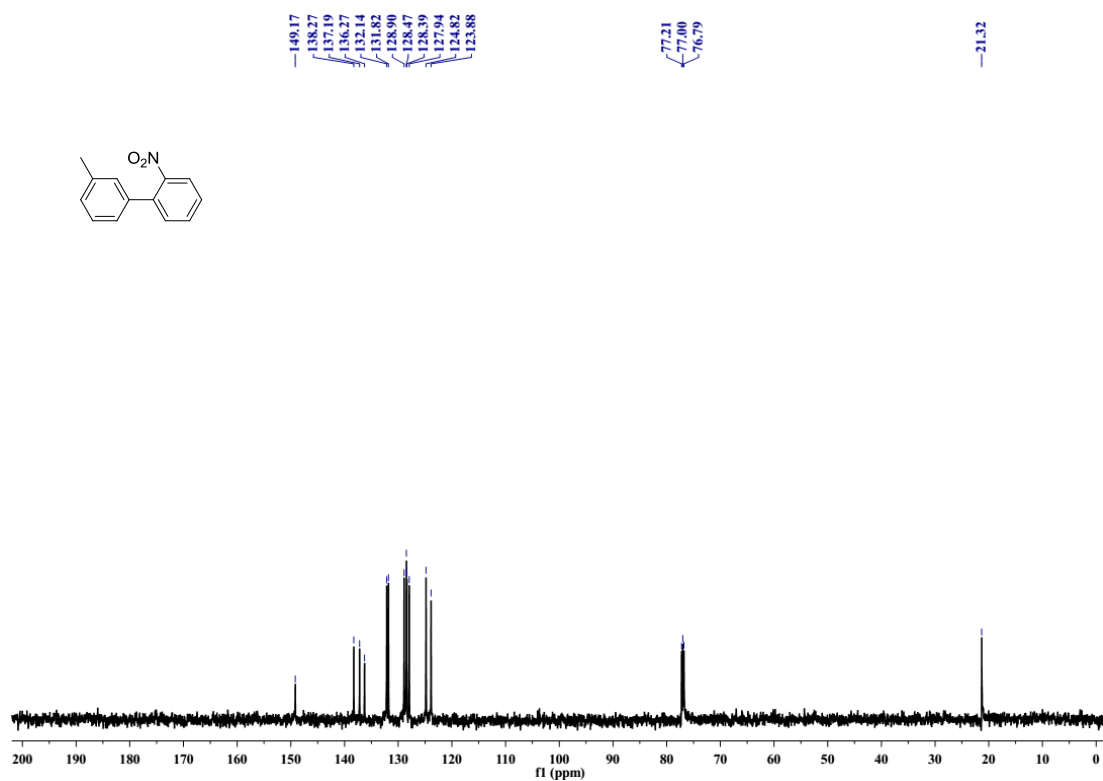
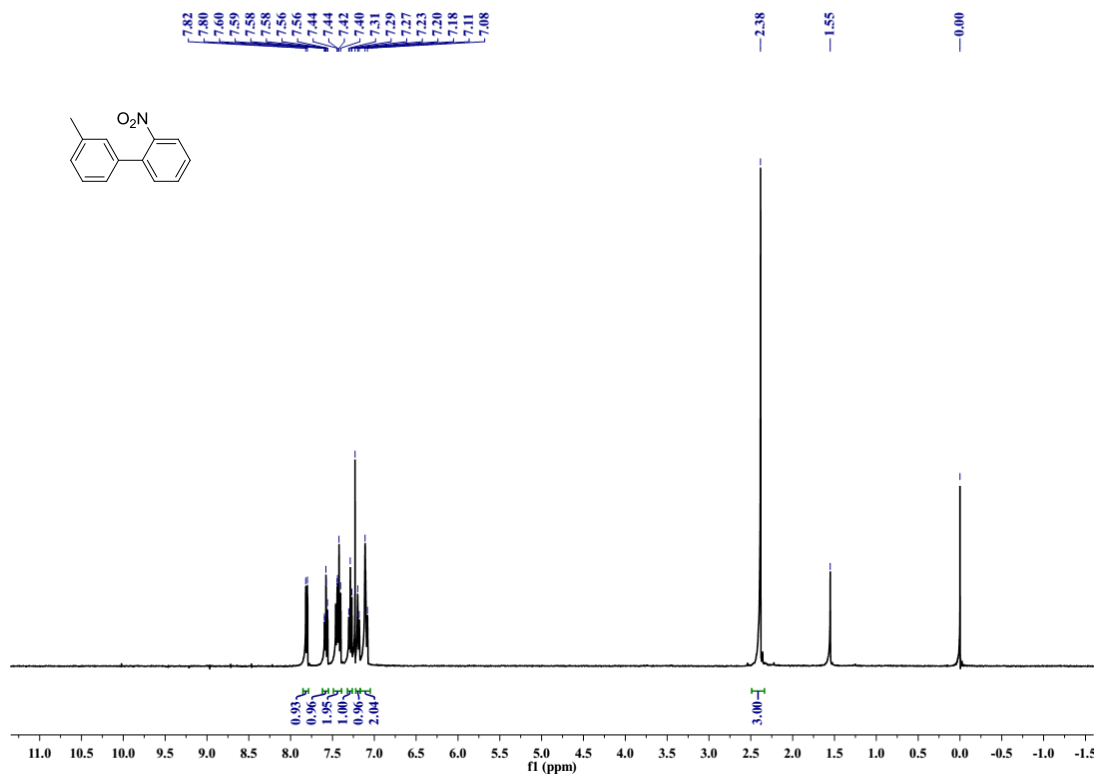


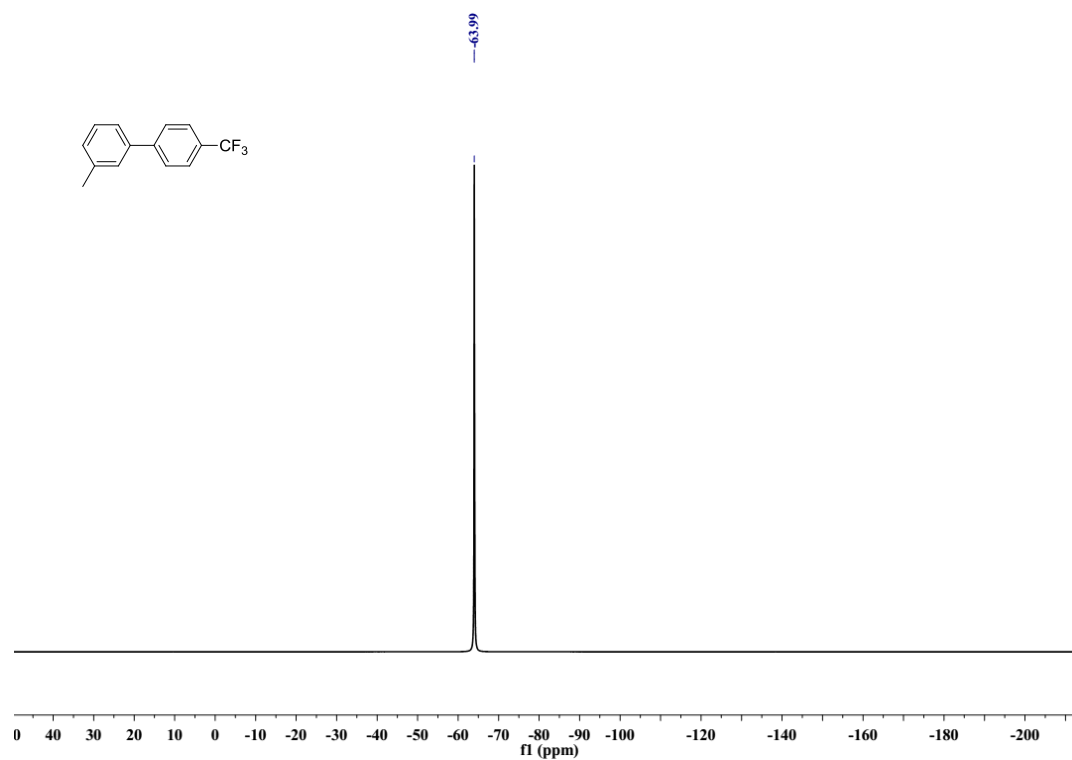
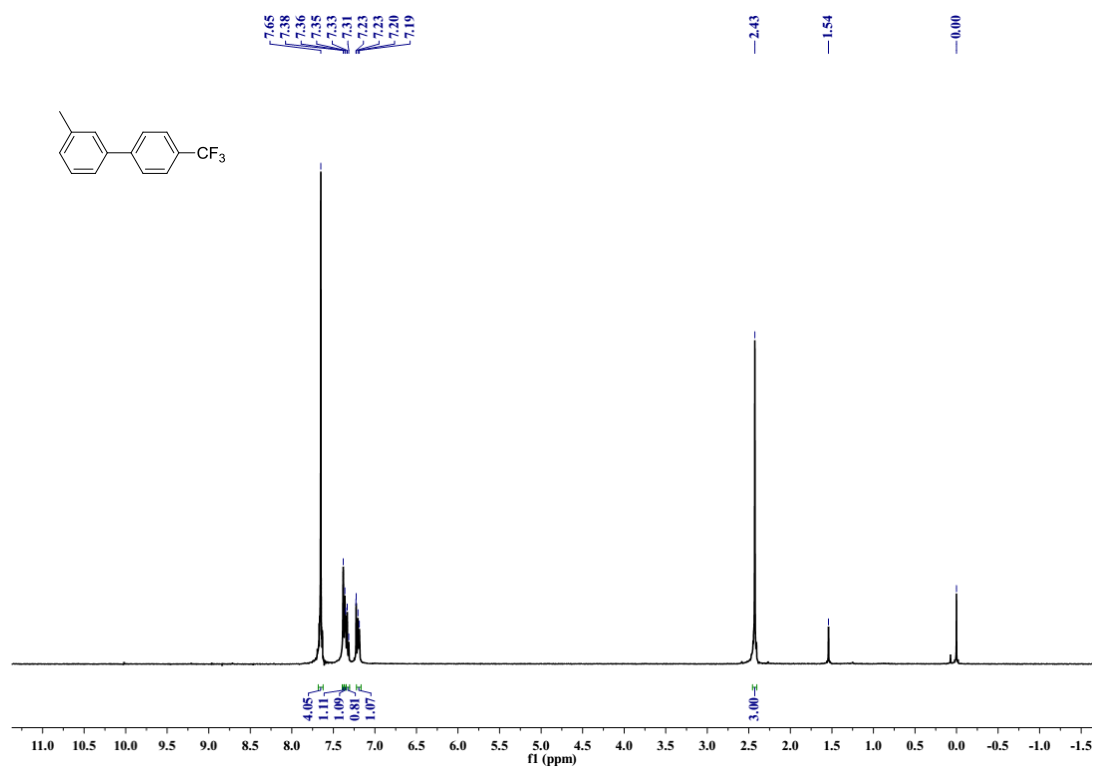
4-(2-nitrophenyl)dibenzo[b,d]thiophene.^[23] ¹H NMR (400 MHz, CDCl₃): δ 8.16 – 8.14 (m, 2 H, Ar), 8.05 (d, *J* = 8.0 Hz, 1 H, Ar), 7.74 (t, *J* = 4.0 Hz, 1 H, Ar), 7.70 – 7.66 (m, 1 H, Ar), 7.58 (t, *J* = 8.0 Hz, 2 H, Ar), 7.50 (t, *J* = 8.0 Hz, 1 H, Ar), 7.44 – 7.41 (m, 2 H, Ar), 7.30 – 7.28 (dd, *J* = 1.2 Hz, *J* = 0.8 Hz, 1 H, Ar). ¹³C NMR (100 MHz, CDCl₃): δ 148.6 (s, Ar), 139.0 (s, Ar), 138.8 (s, Ar), 135.9 (s, Ar), 135.5 (s, Ar), 134.6 (s, Ar), 133.0 (s, Ar), 132.5 (s, Ar), 131.9 (s, Ar), 129.1 (s, Ar), 126.9 (s, Ar), 126.1 (s, Ar), 124.8 (s, Ar), 124.6 (s, Ar), 124.5 (s, Ar), 122.6 (s, Ar), 121.8 (s, Ar), 121.2 (s, Ar).

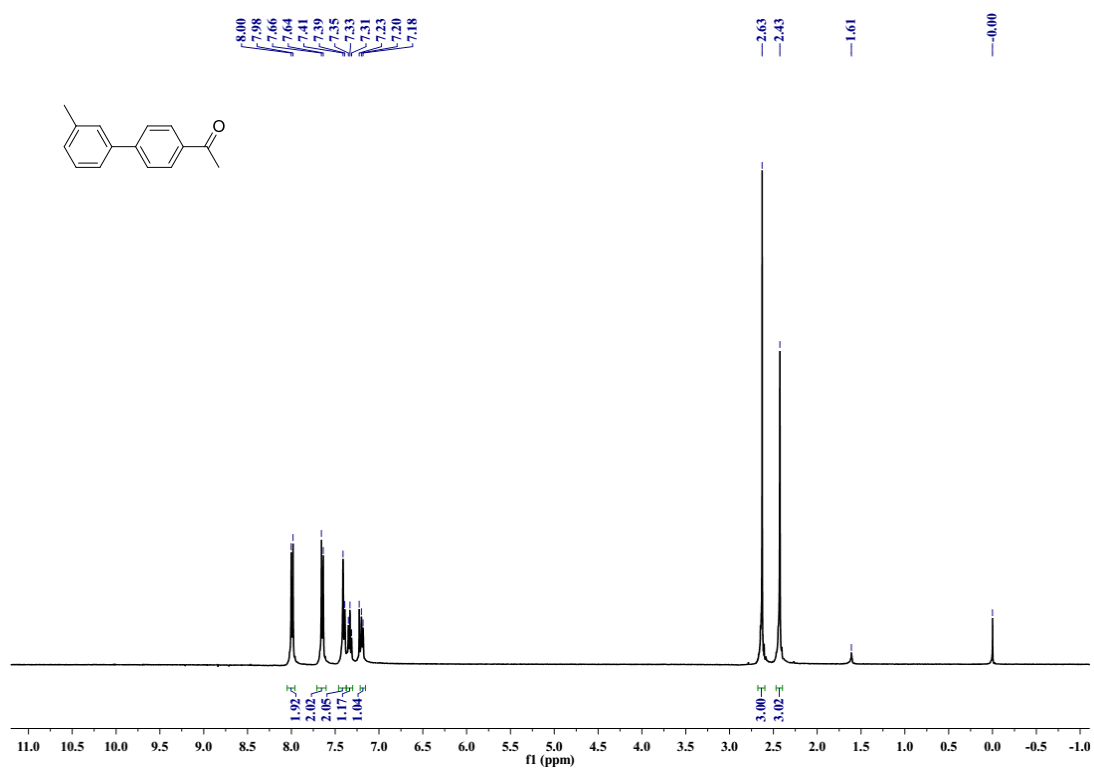
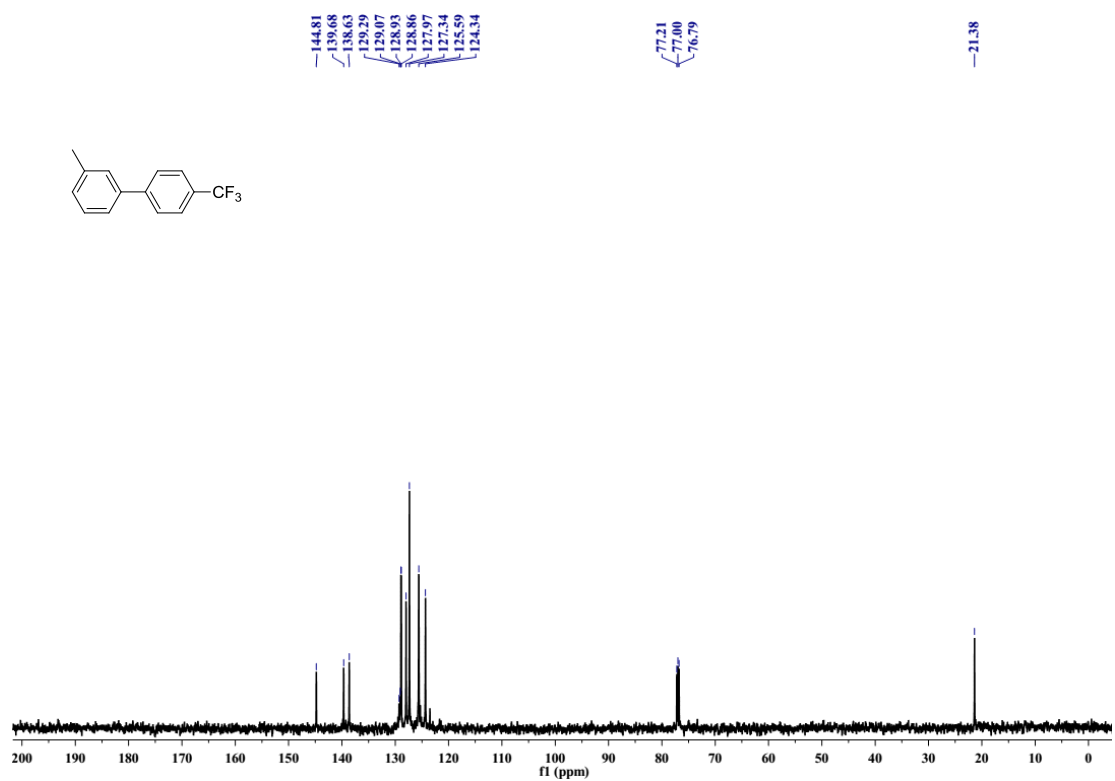


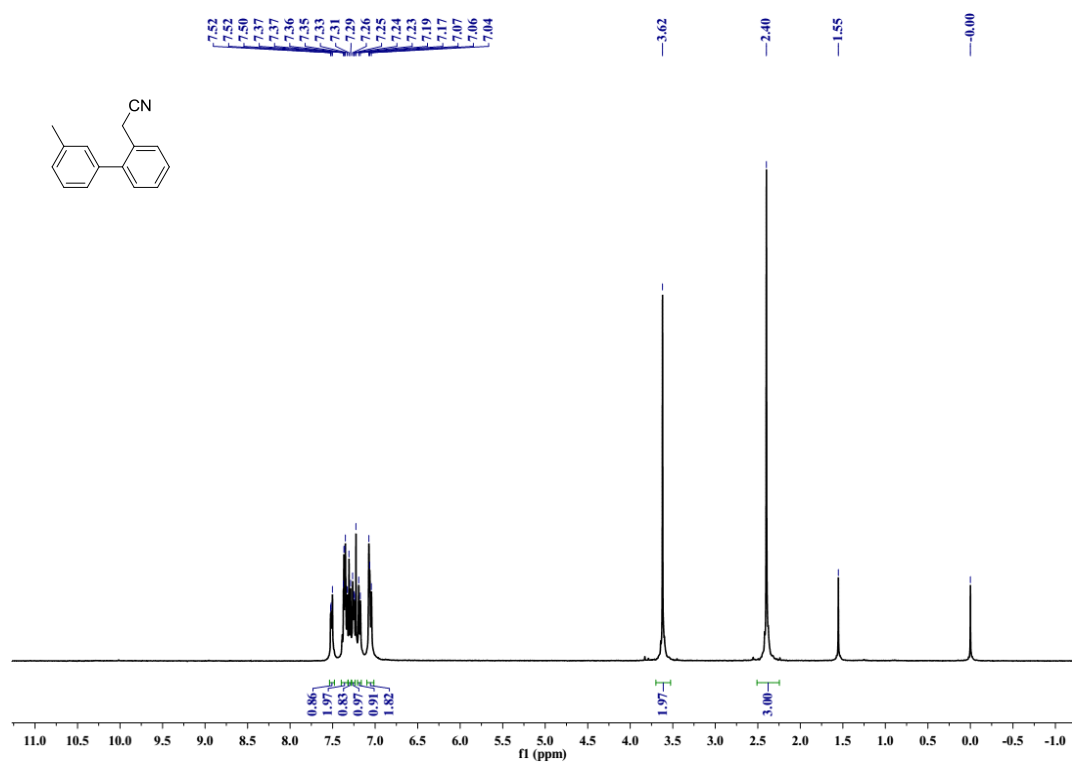
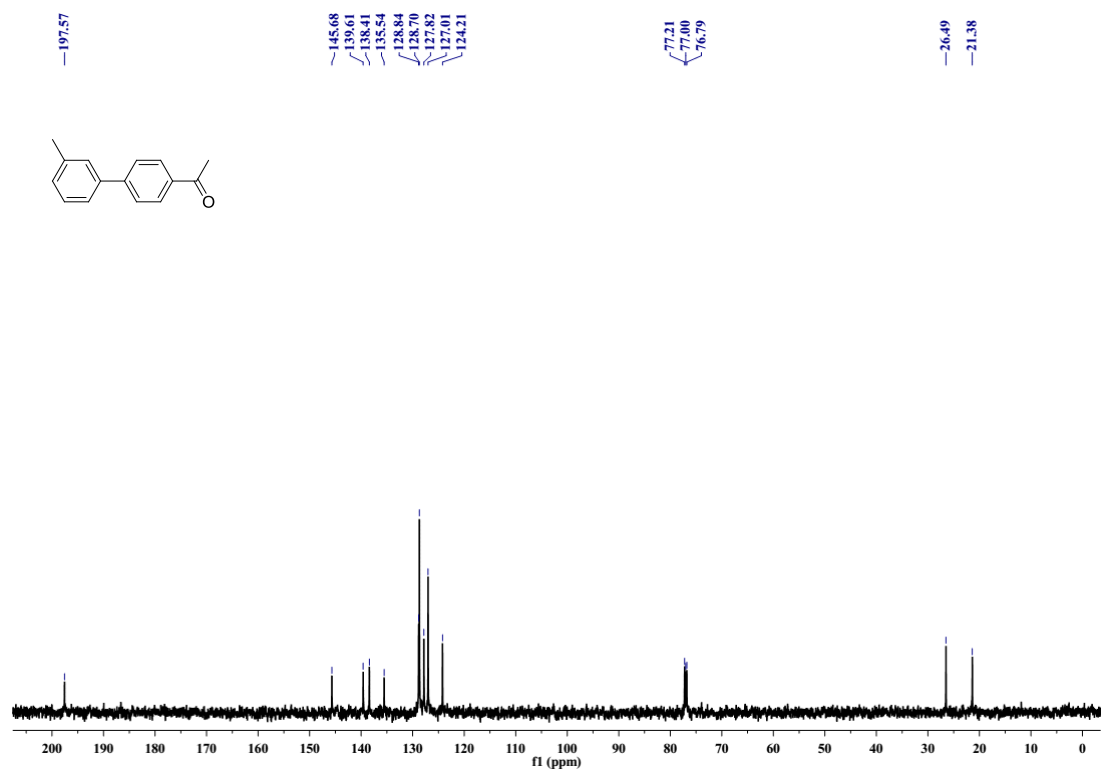
1,1'-biphenyl.^[25] ¹H NMR (400 MHz, CDCl₃): δ 7.57 (d, *J* = 8.0 Hz, 4 H, Ar), 7.41 (t, *J* = 8.0 Hz, 4 H, Ar), 7.34 – 7.29 (m, 2 H, Ar). ¹³C NMR (100 MHz, CDCl₃): δ 141.1 (s, Ar), 128.7 (s, Ar), 127.2 (s, Ar), 127.1 (s, Ar).

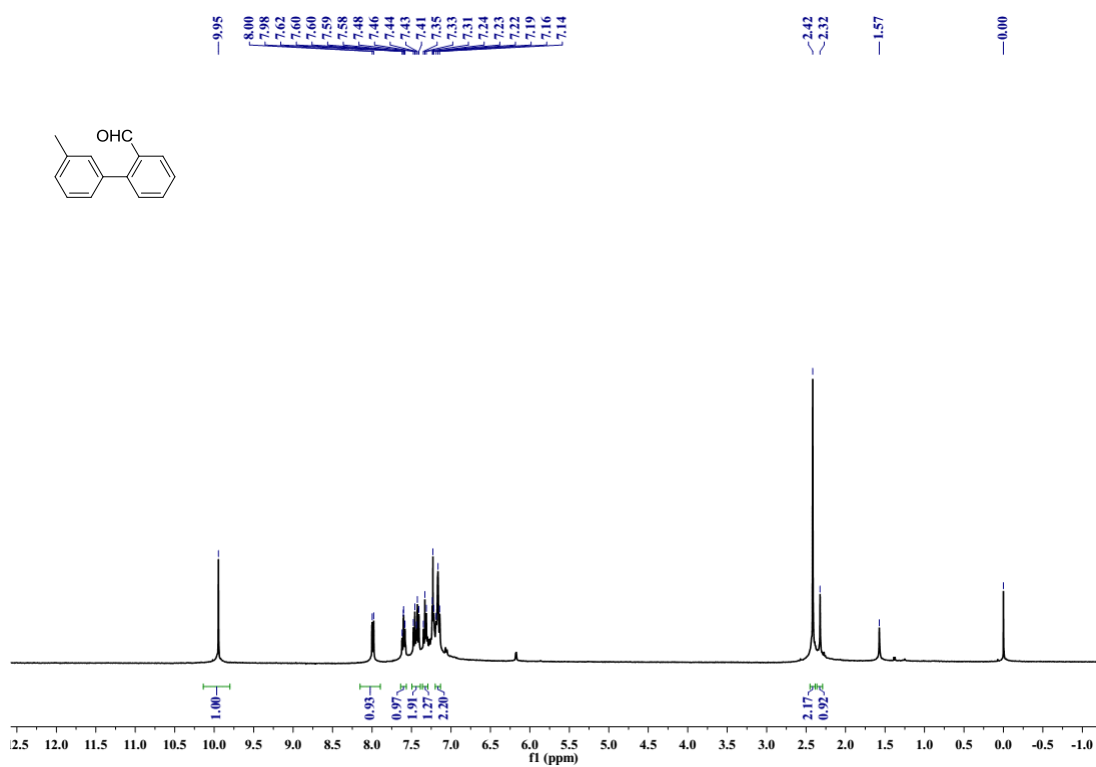
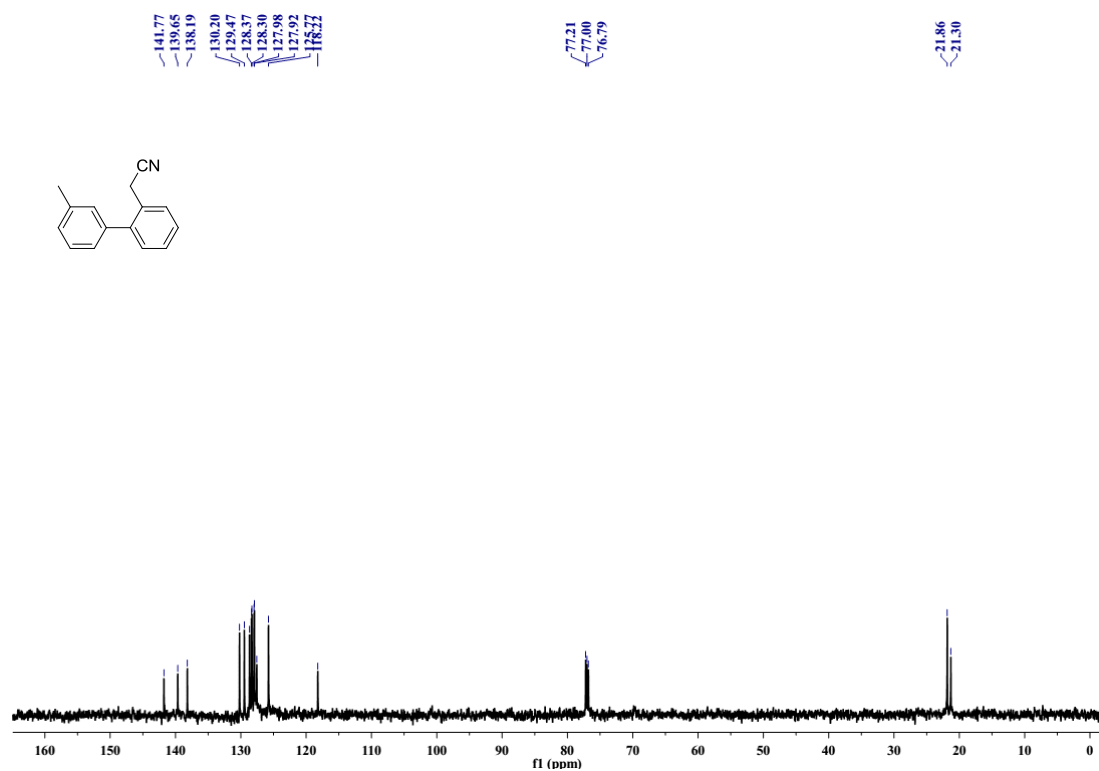


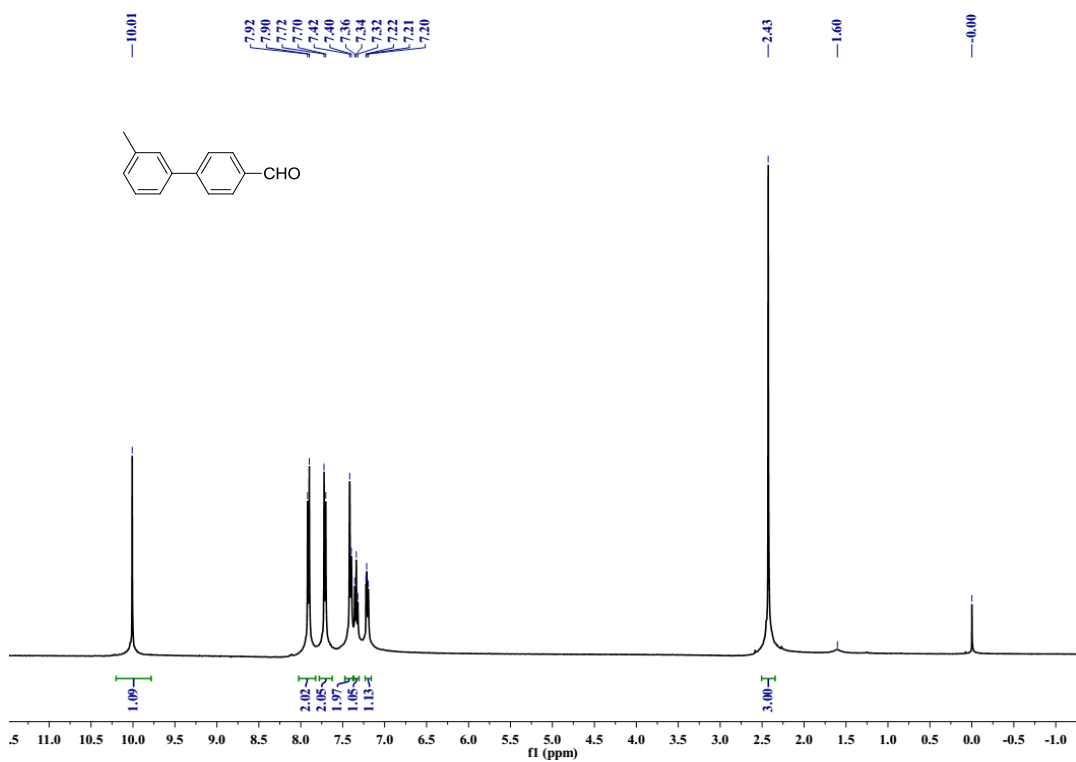
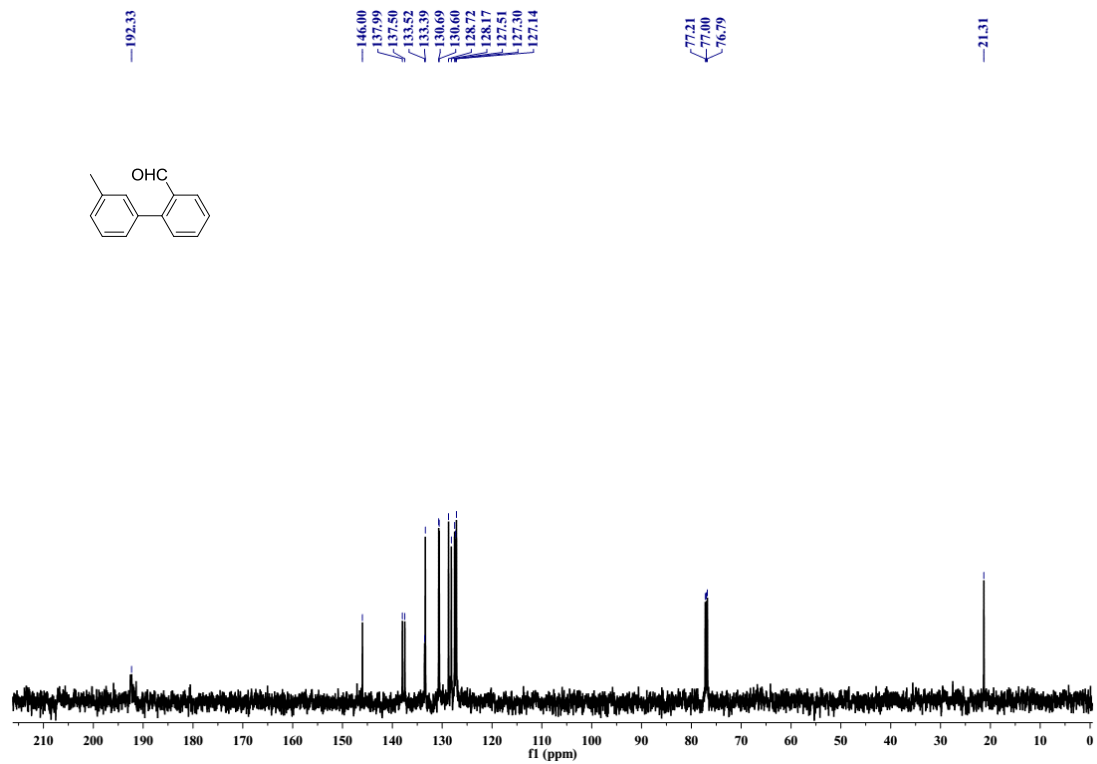


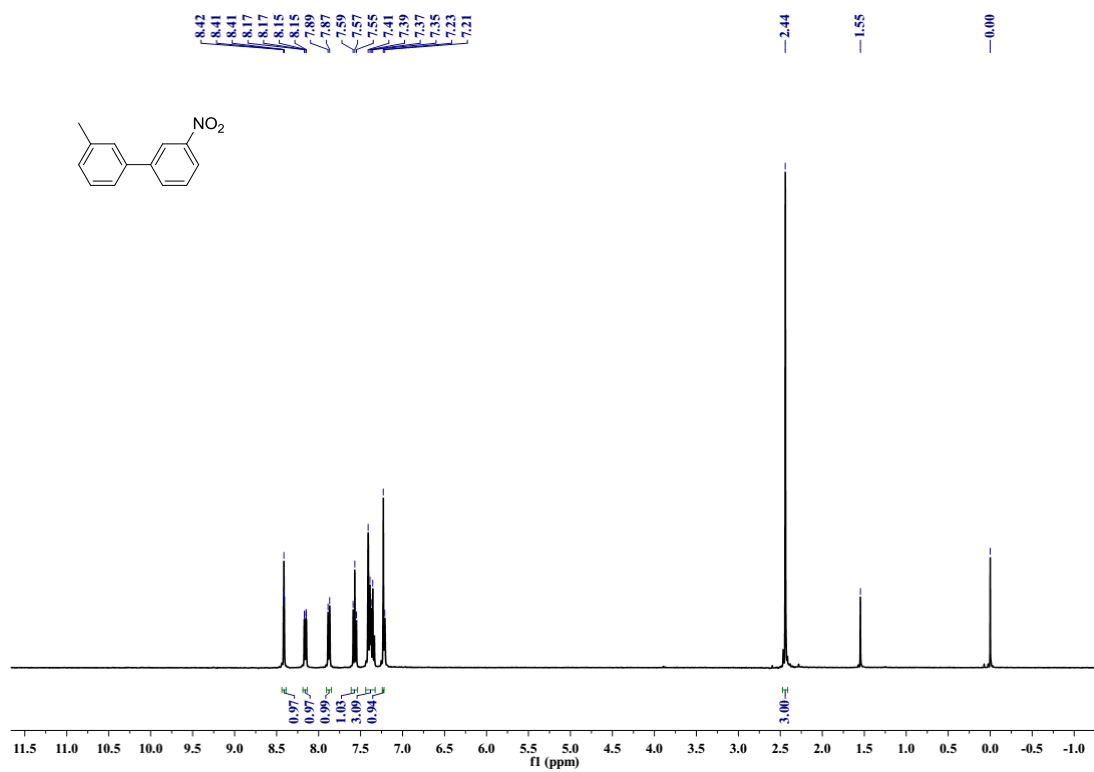
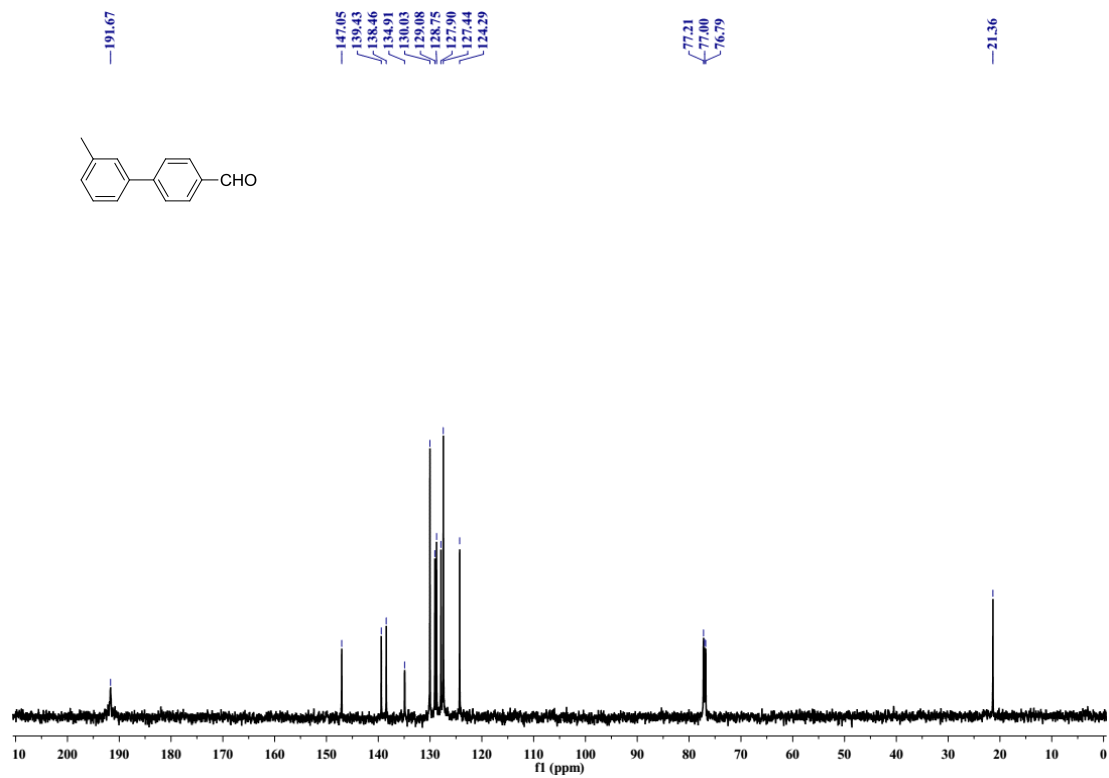


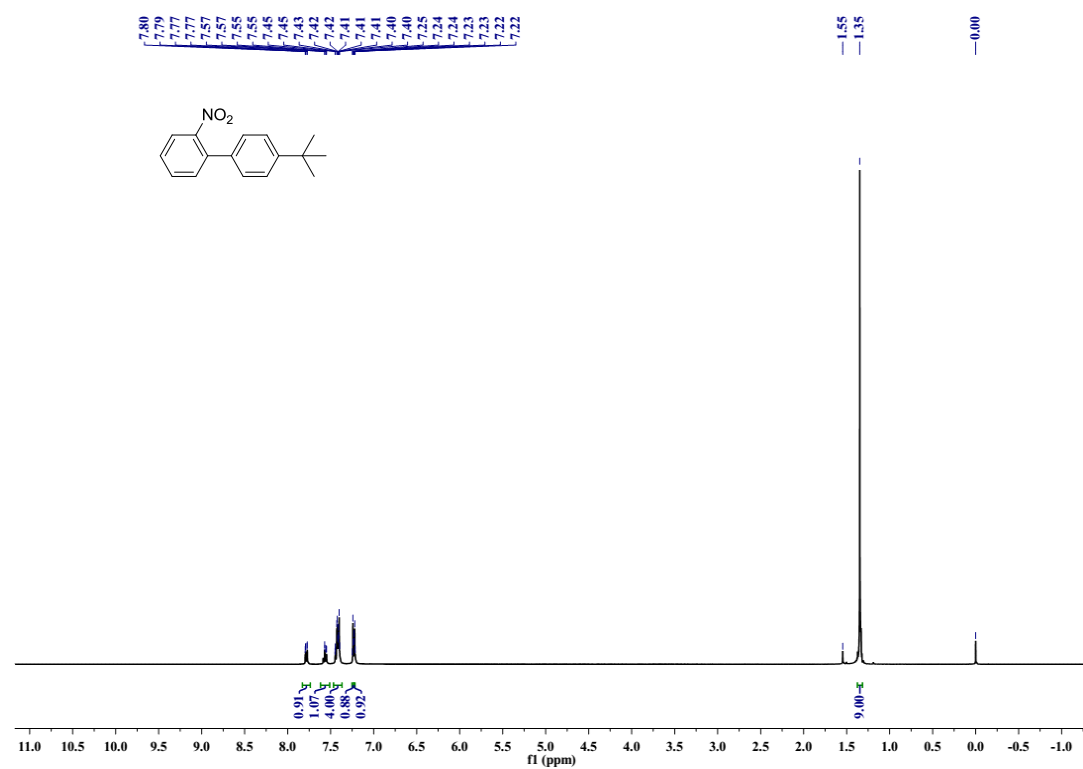
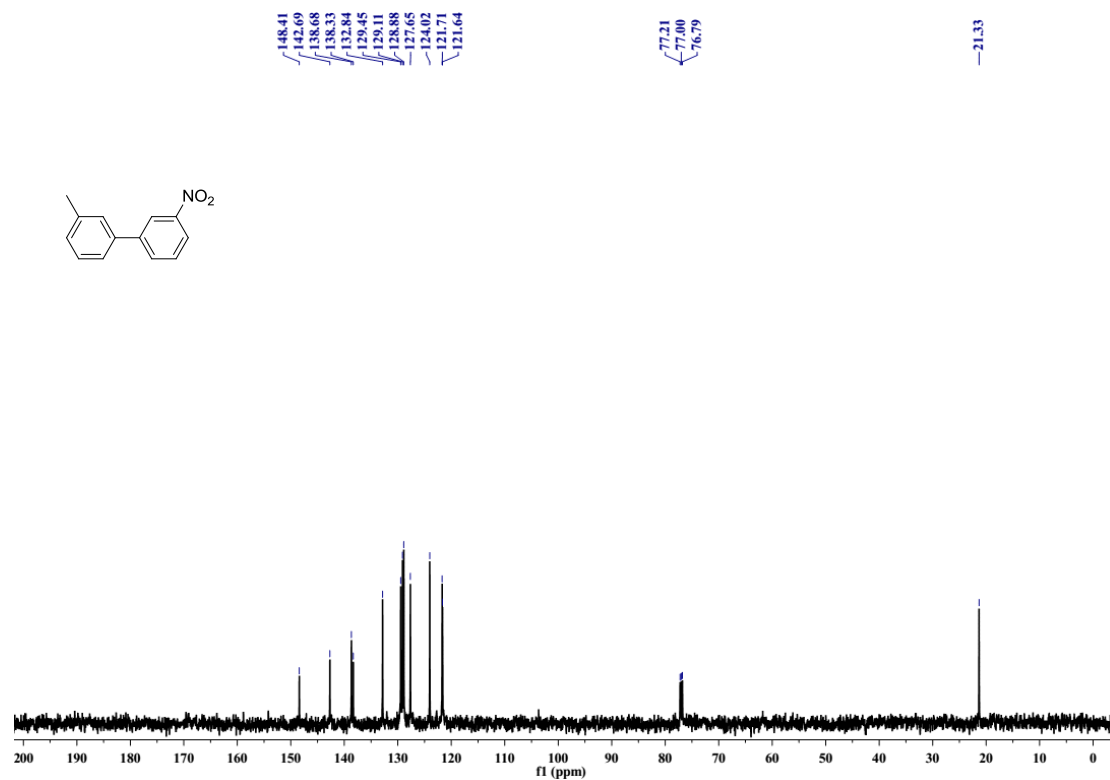


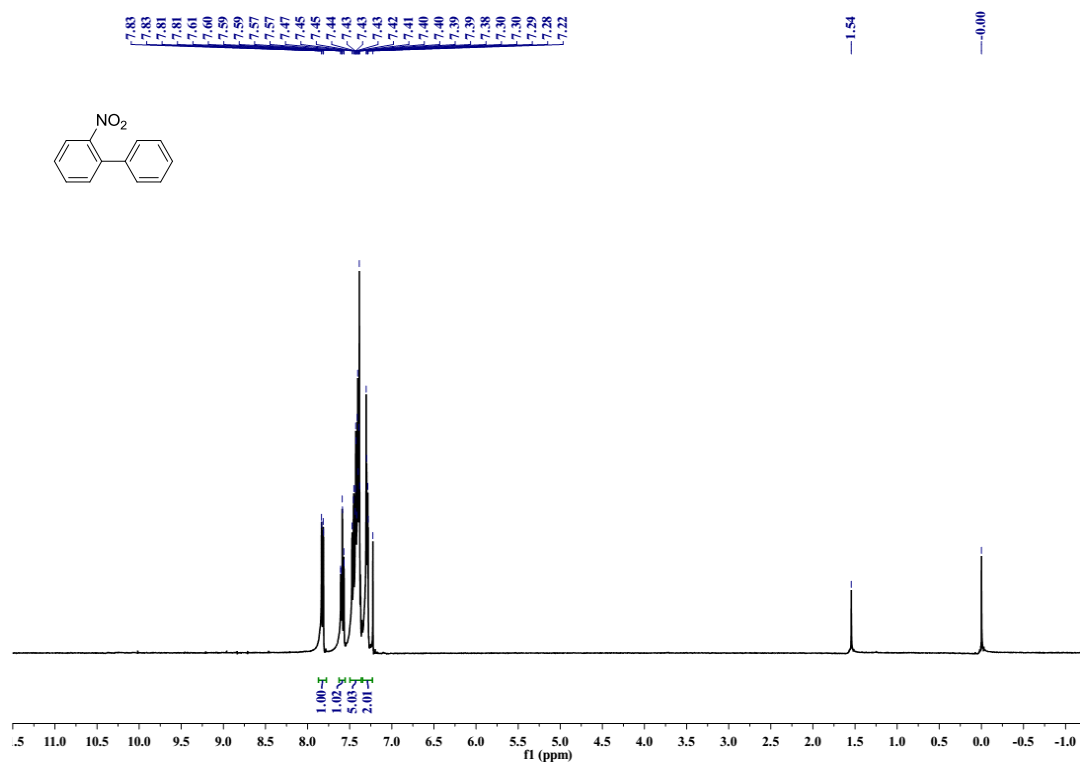
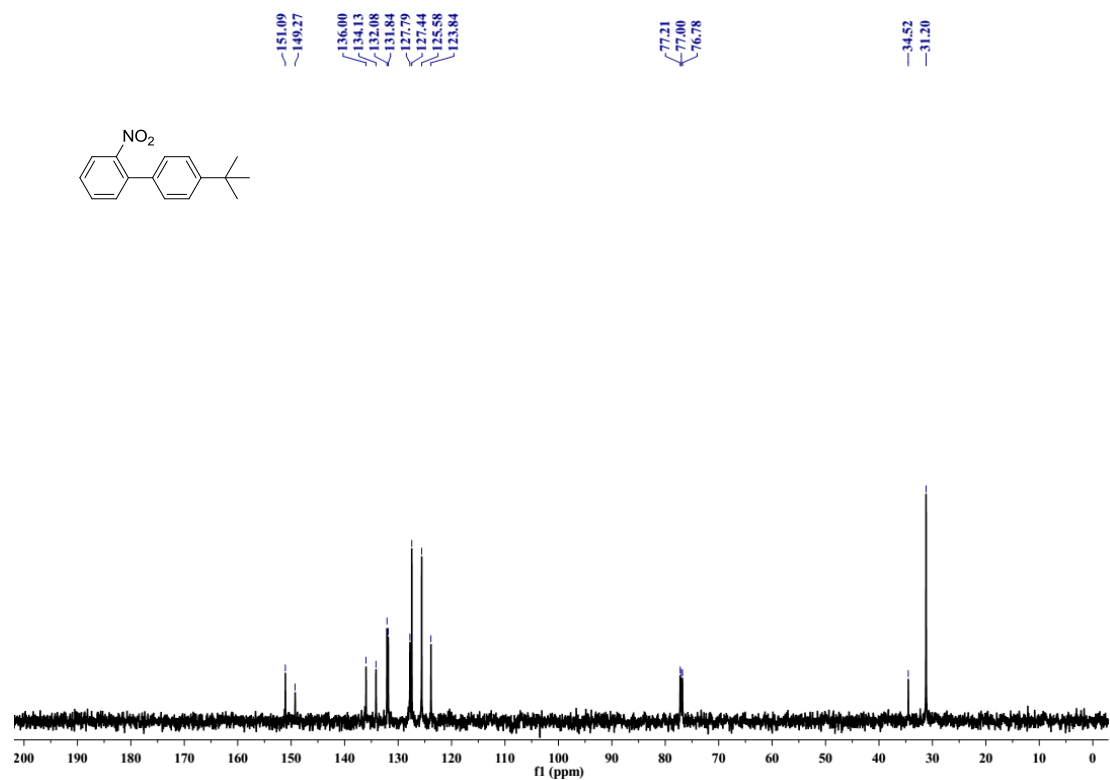


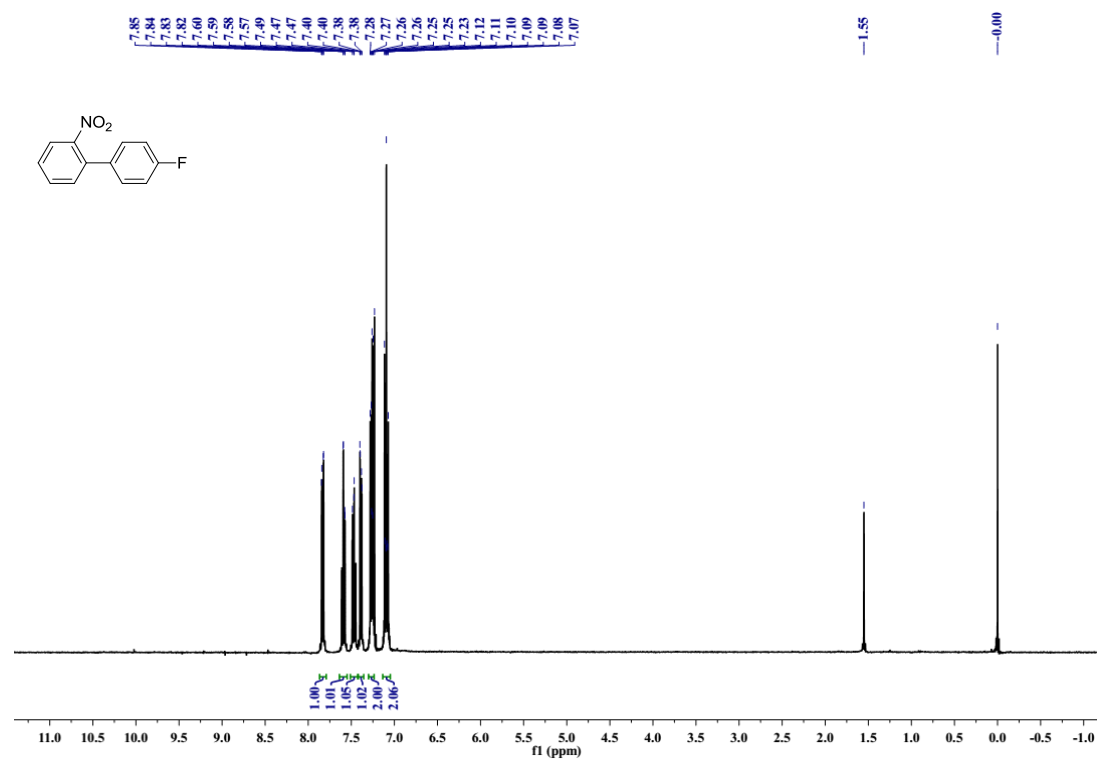
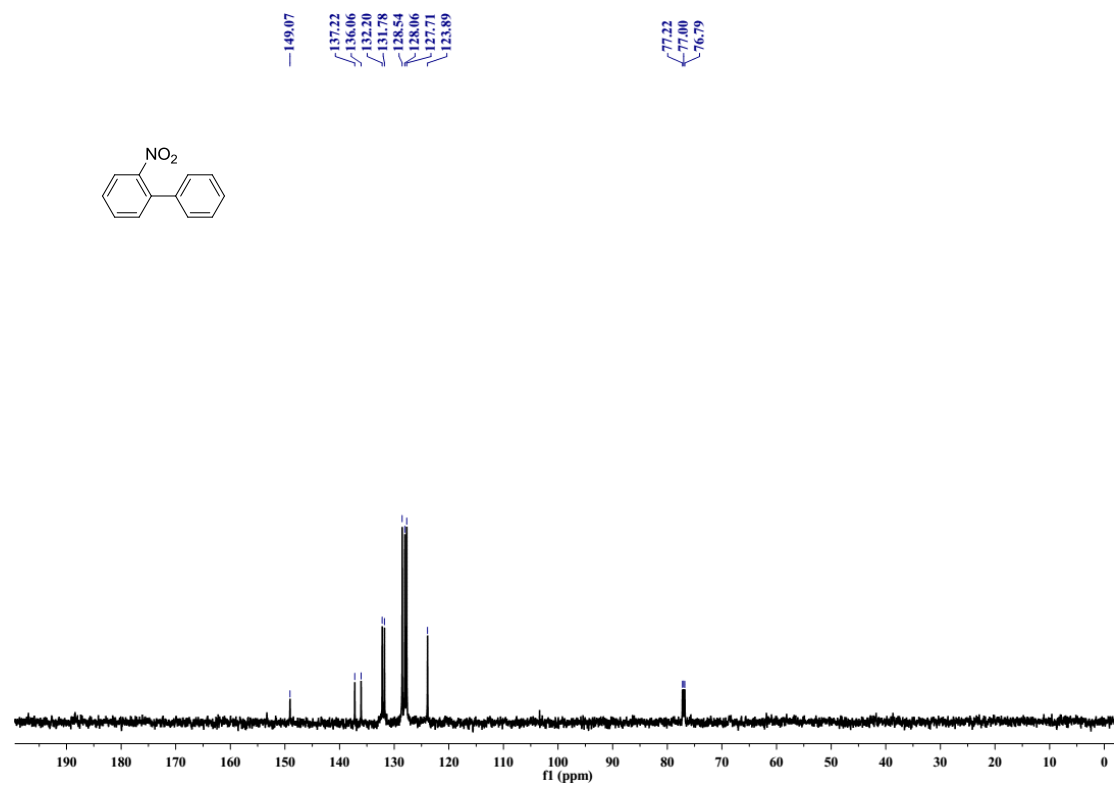


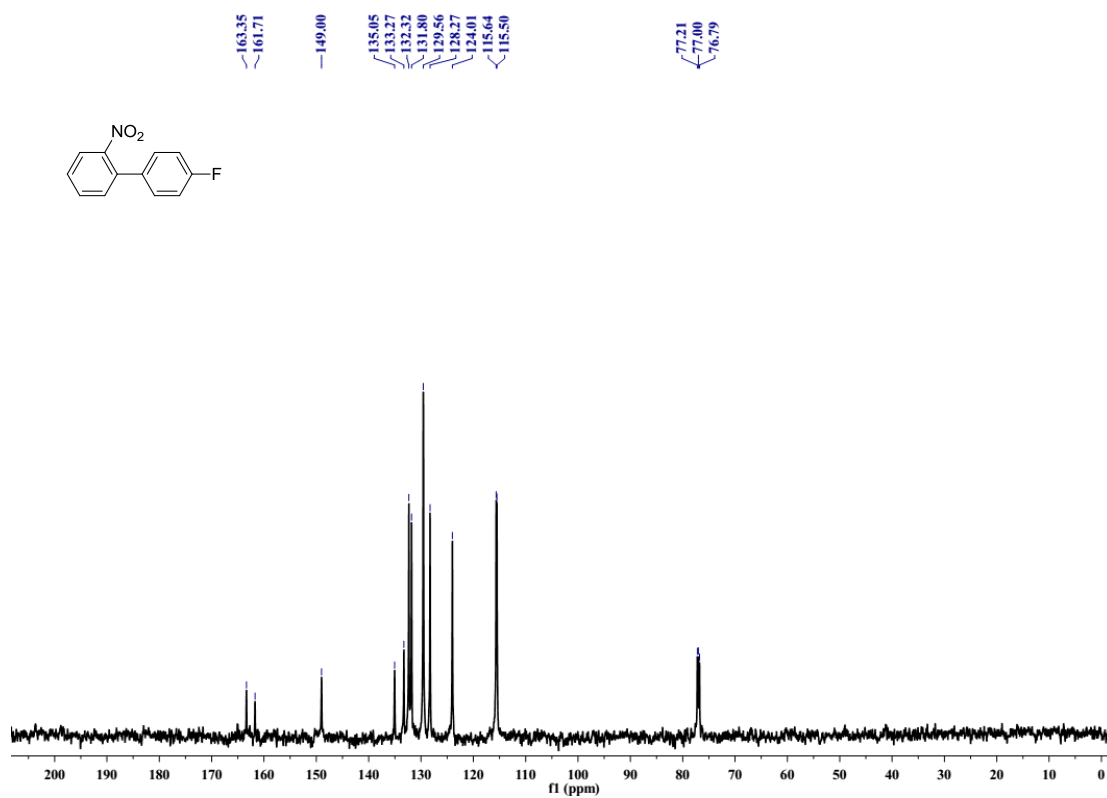
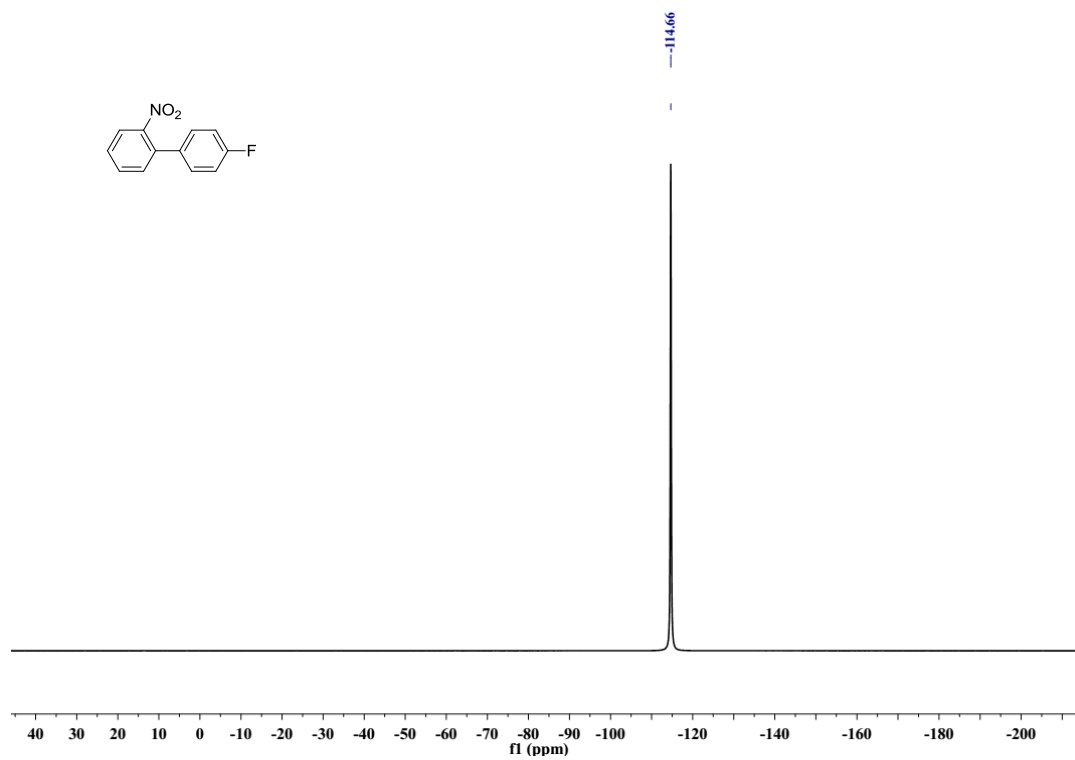


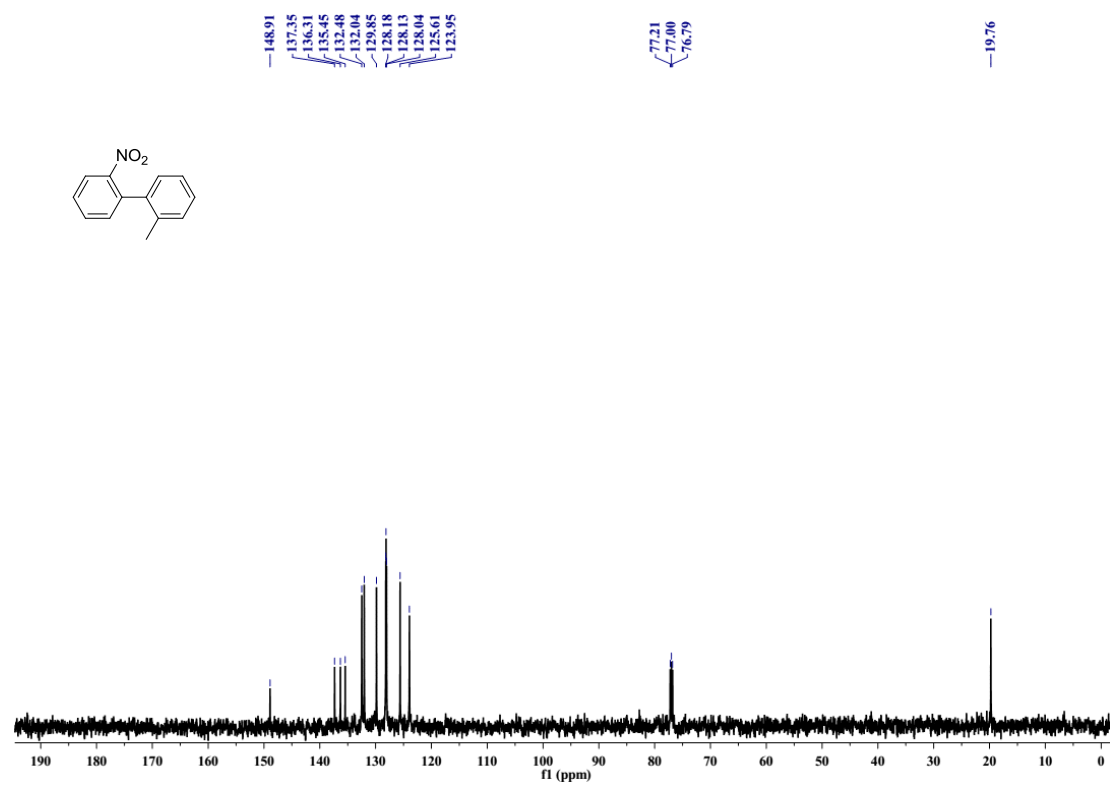
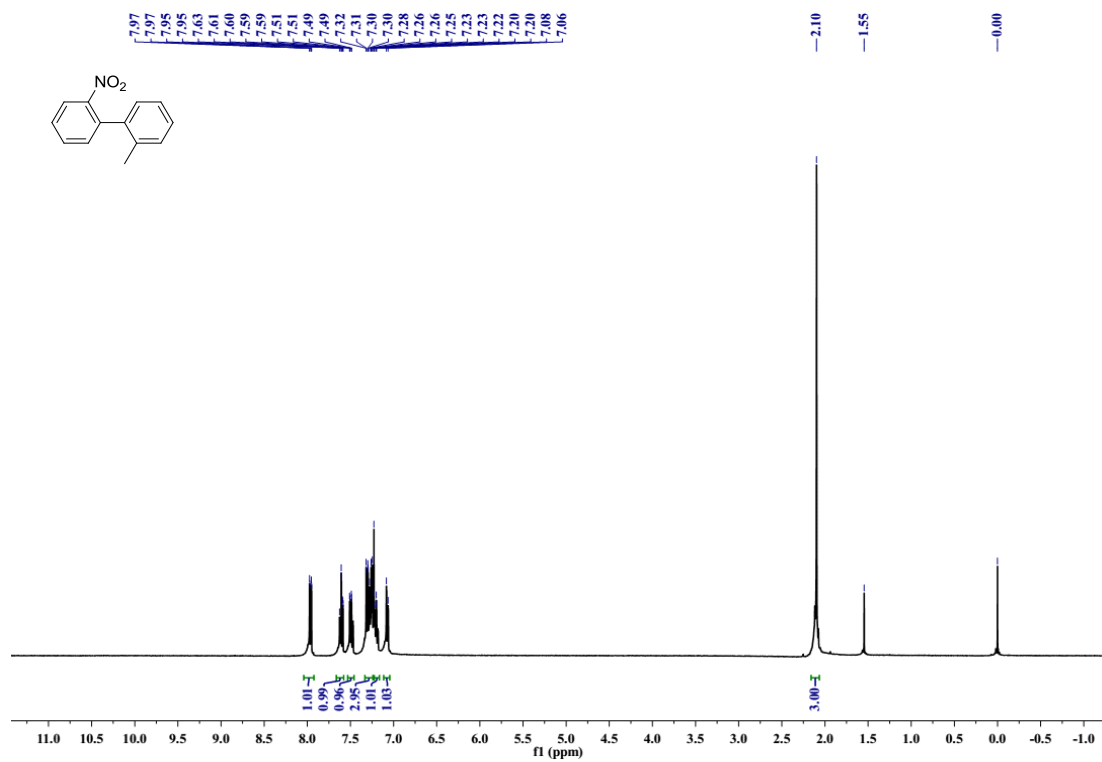


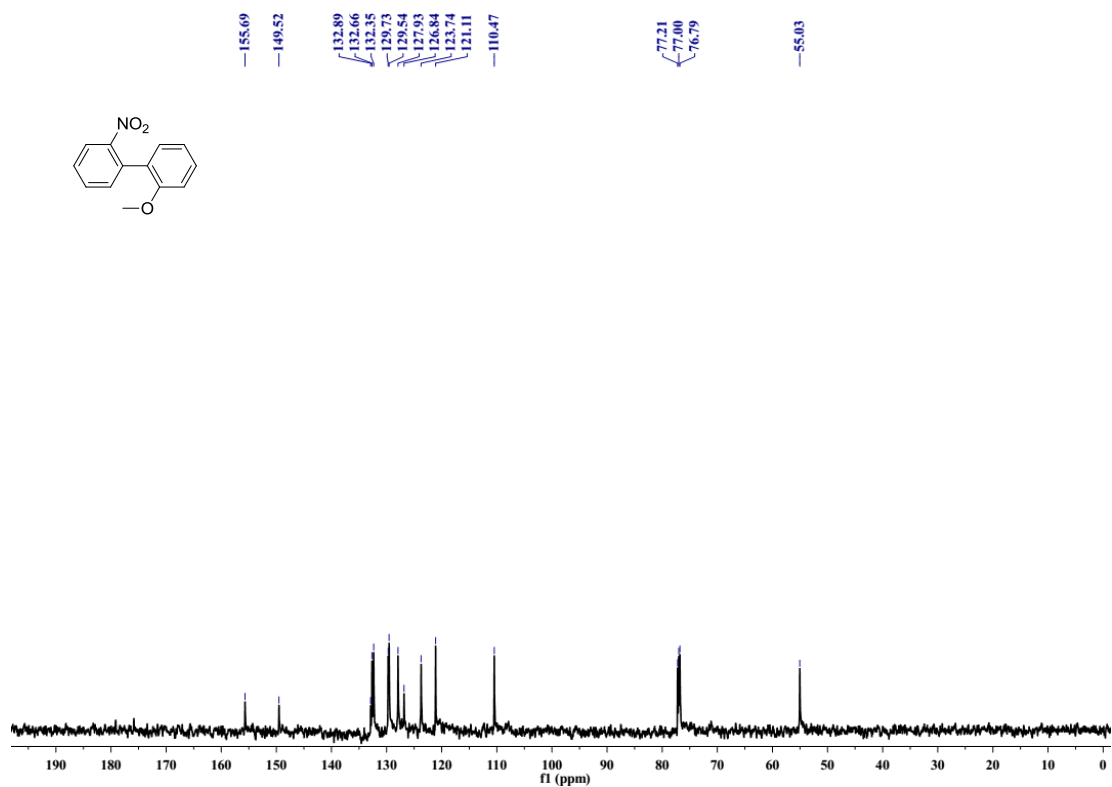
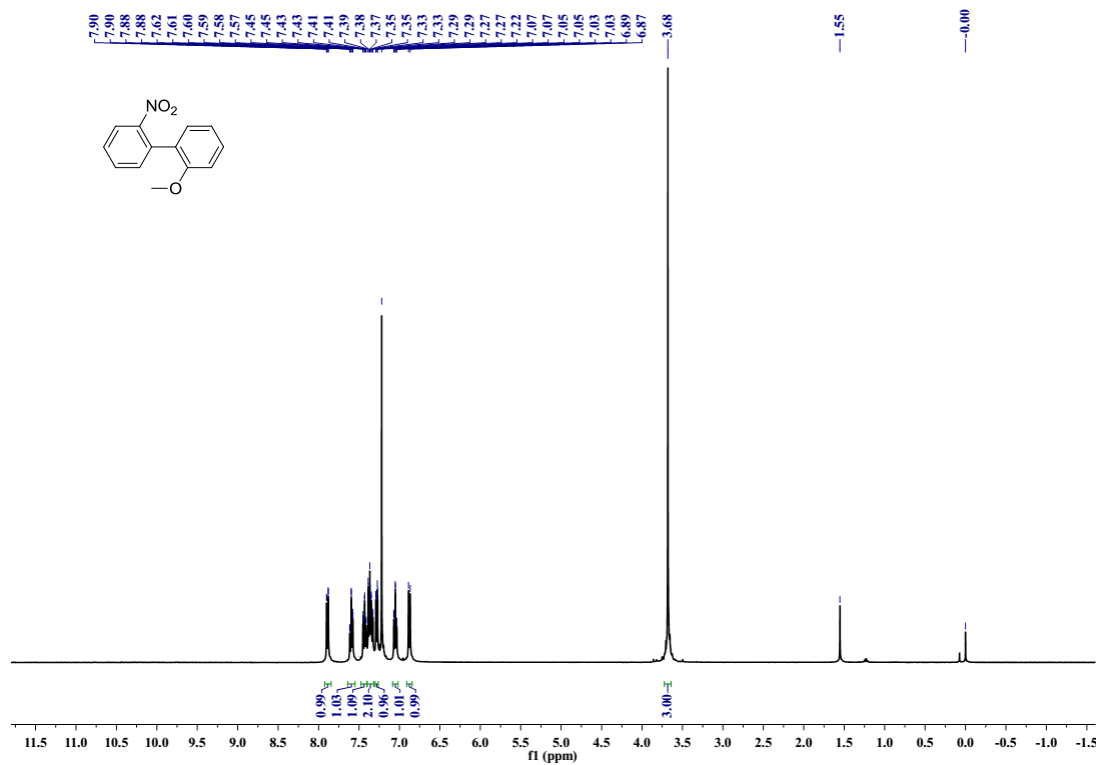


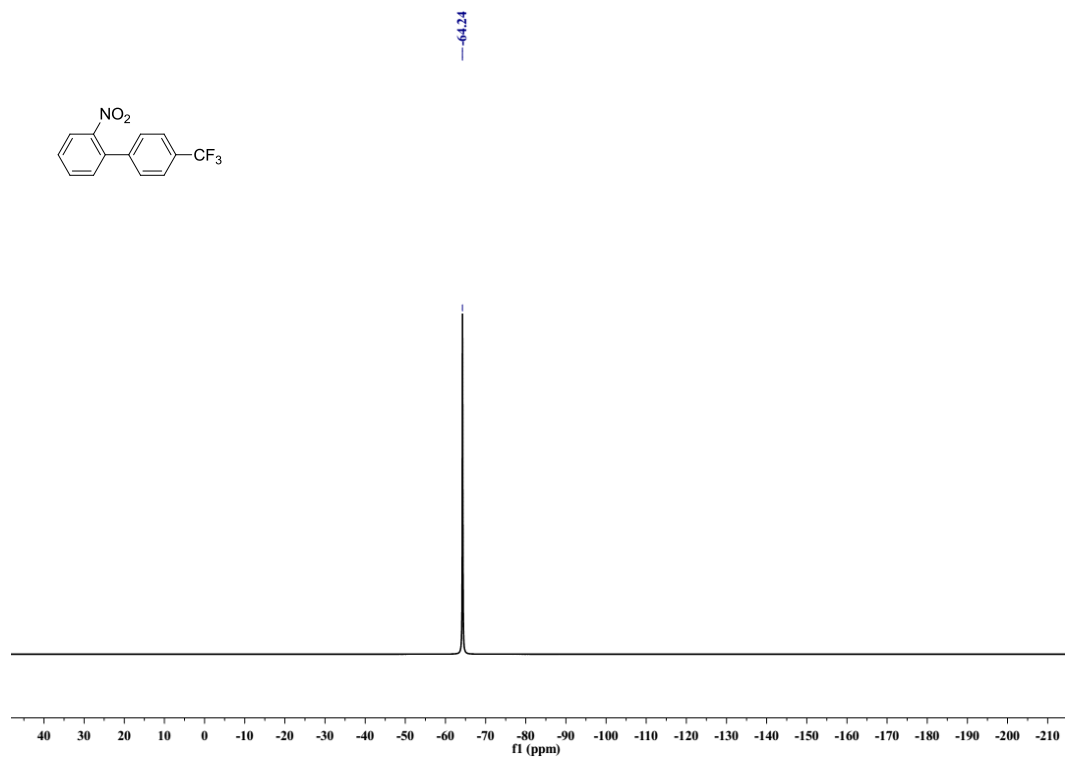
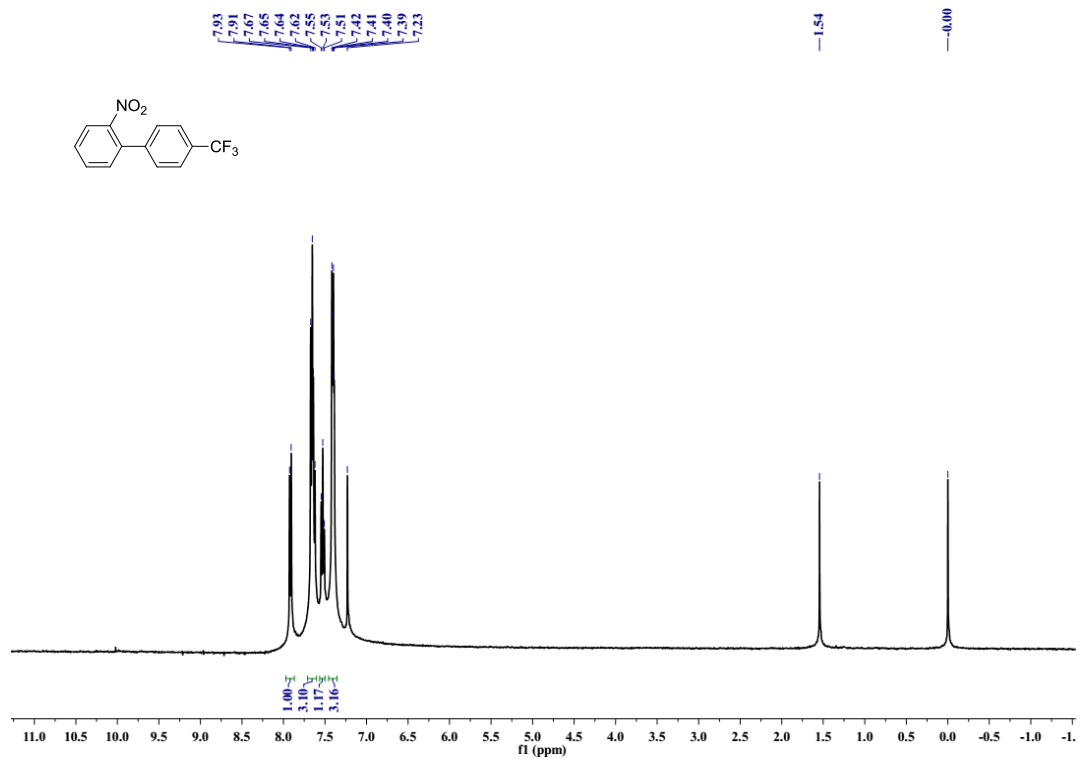


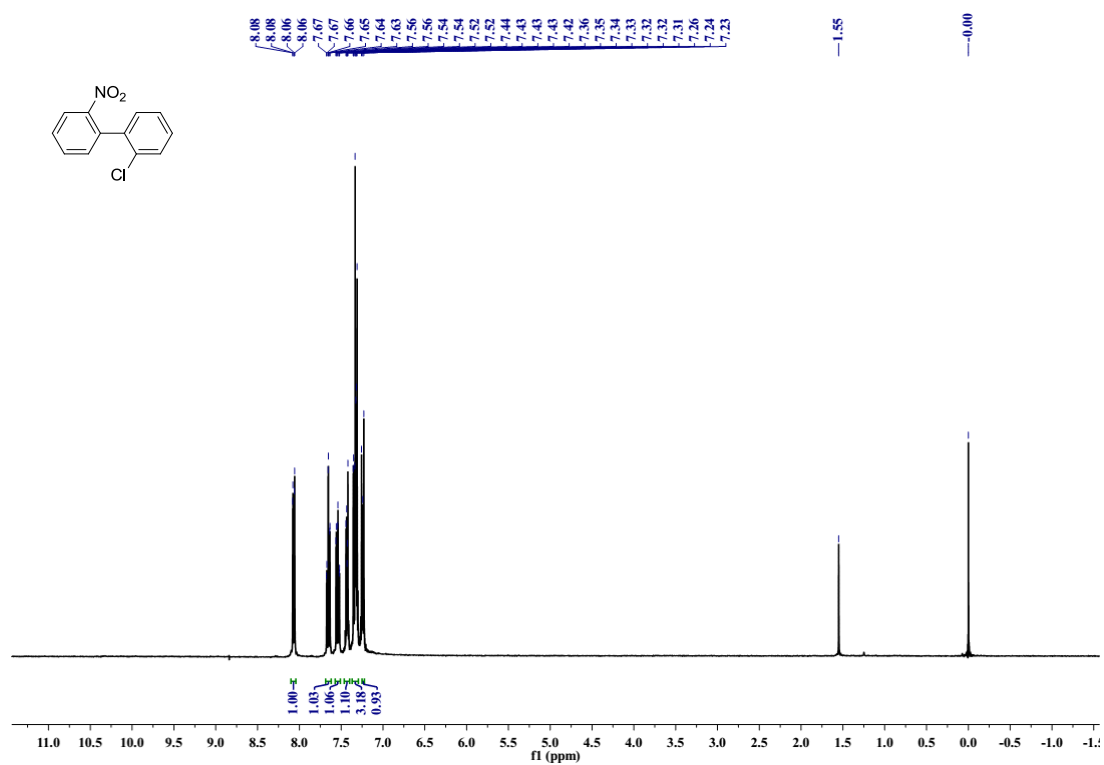
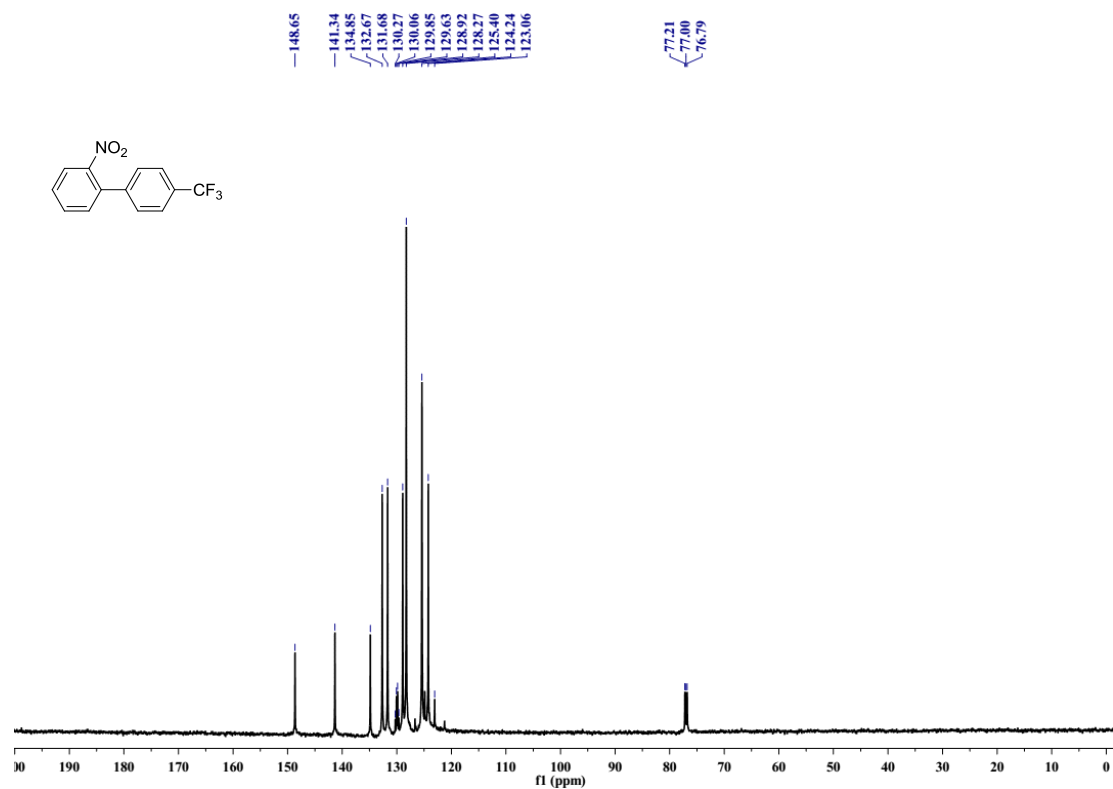


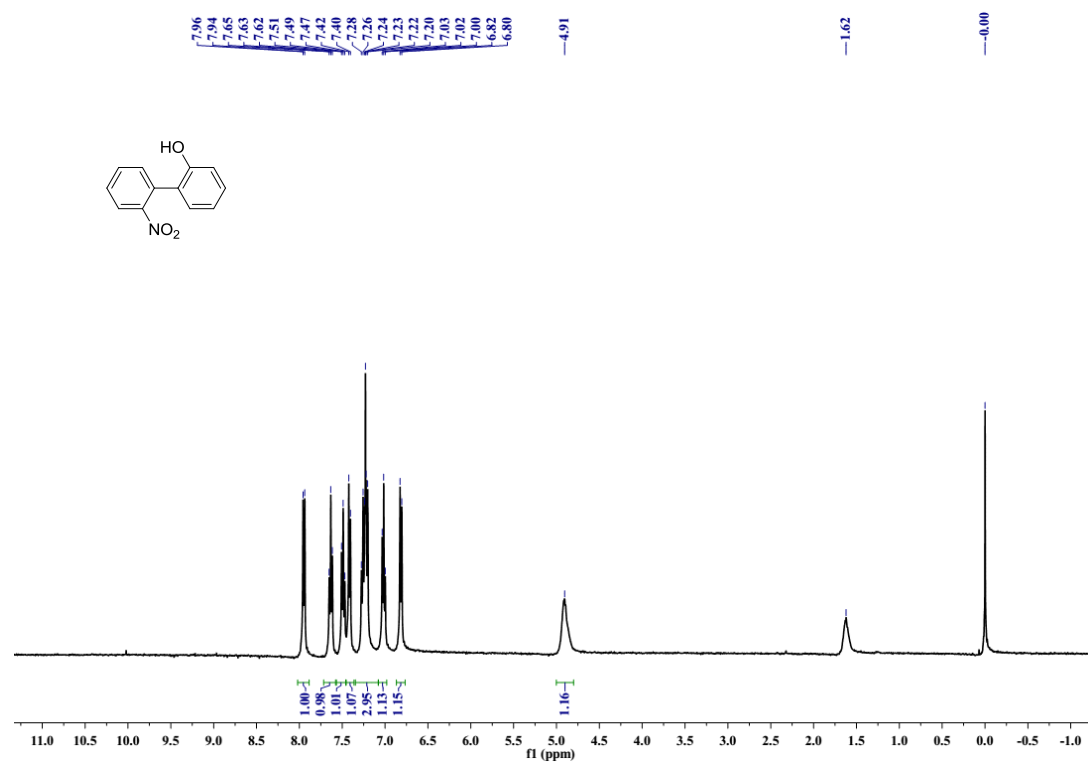
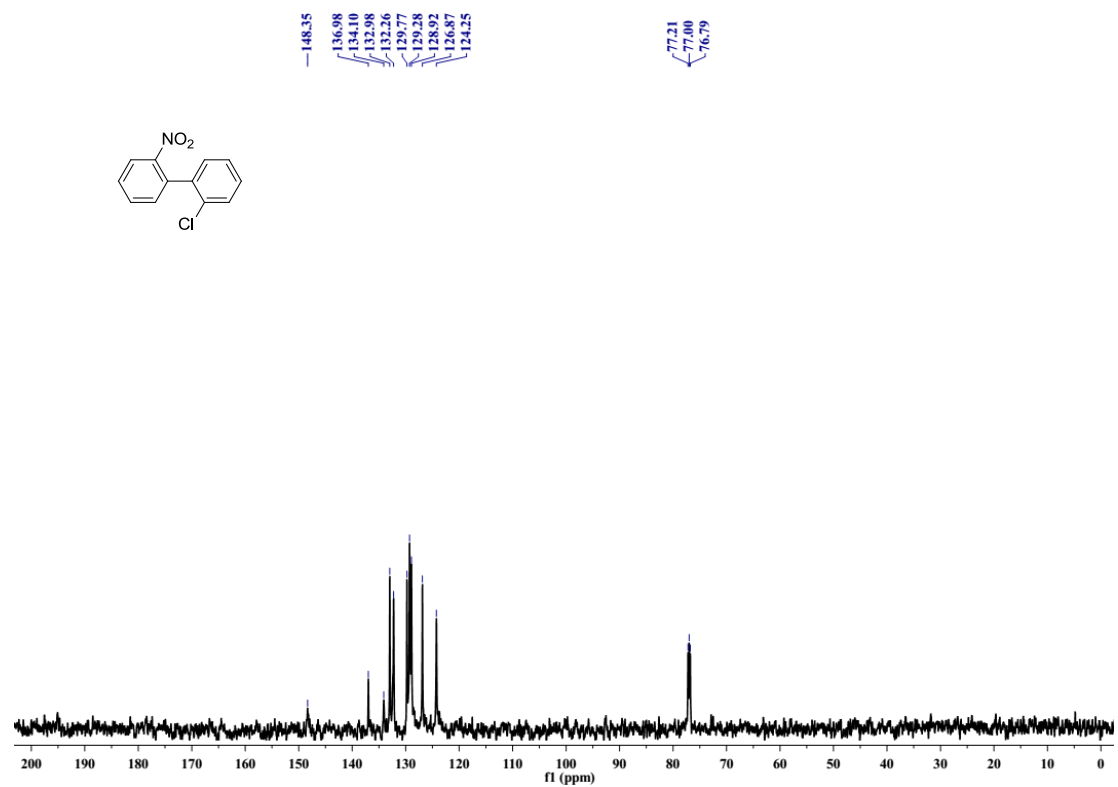


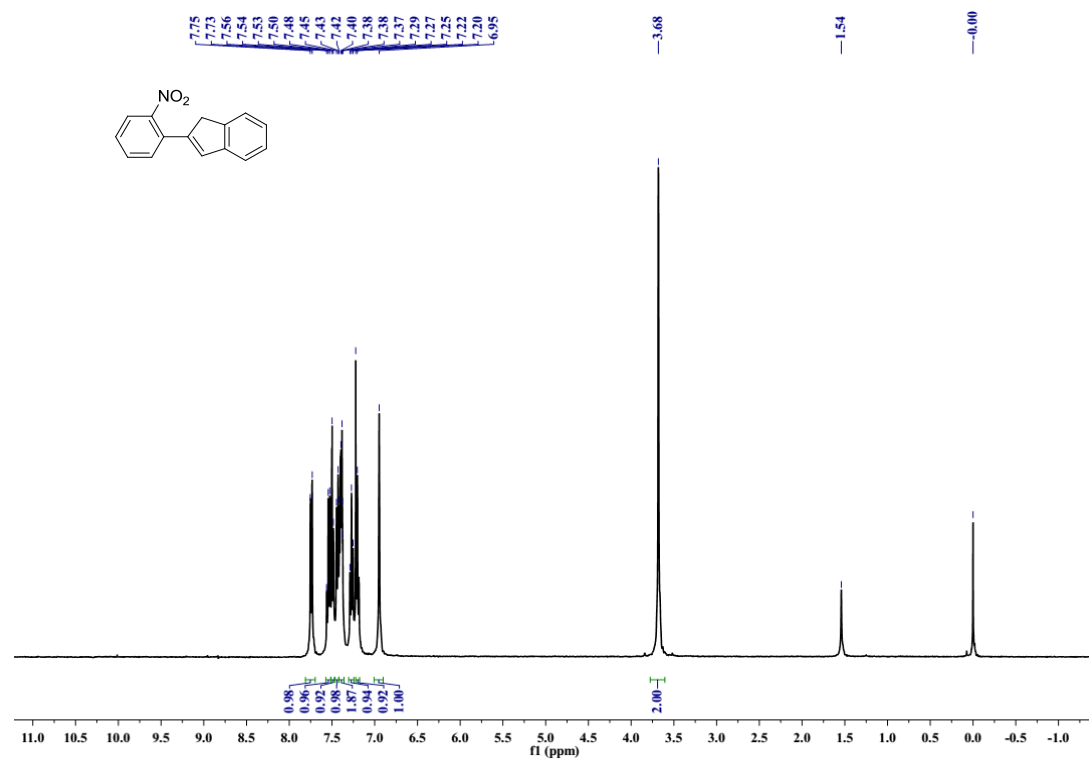
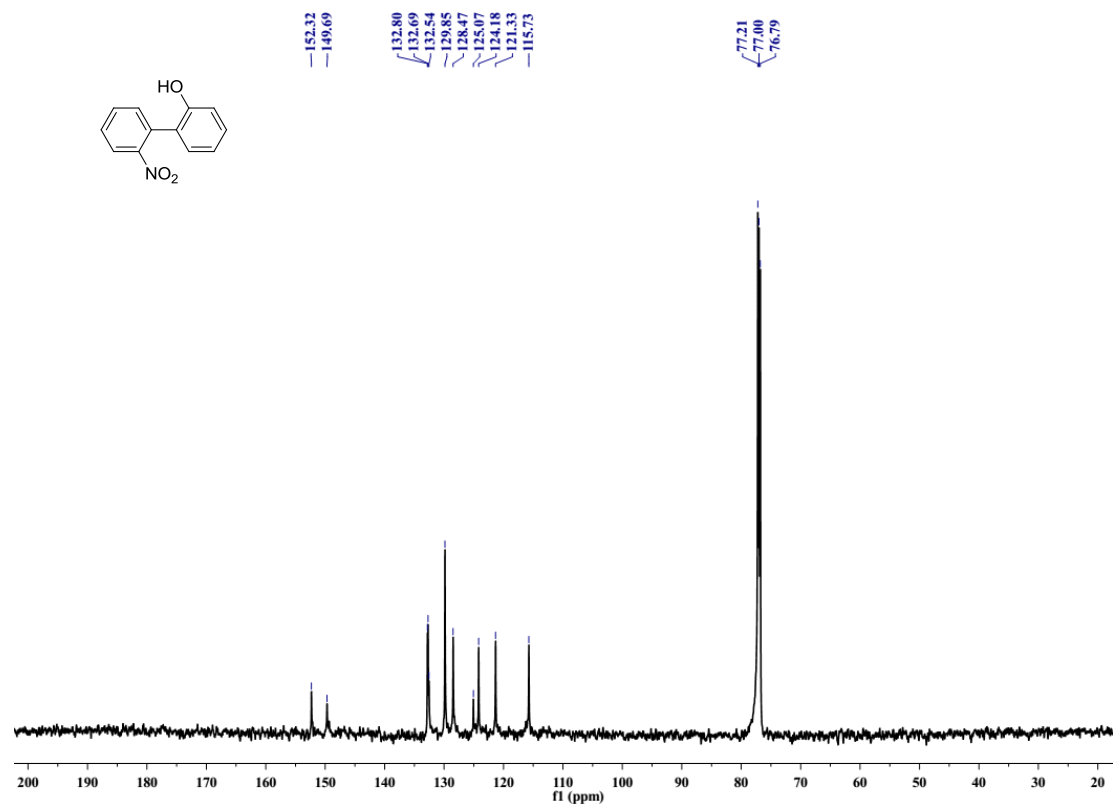


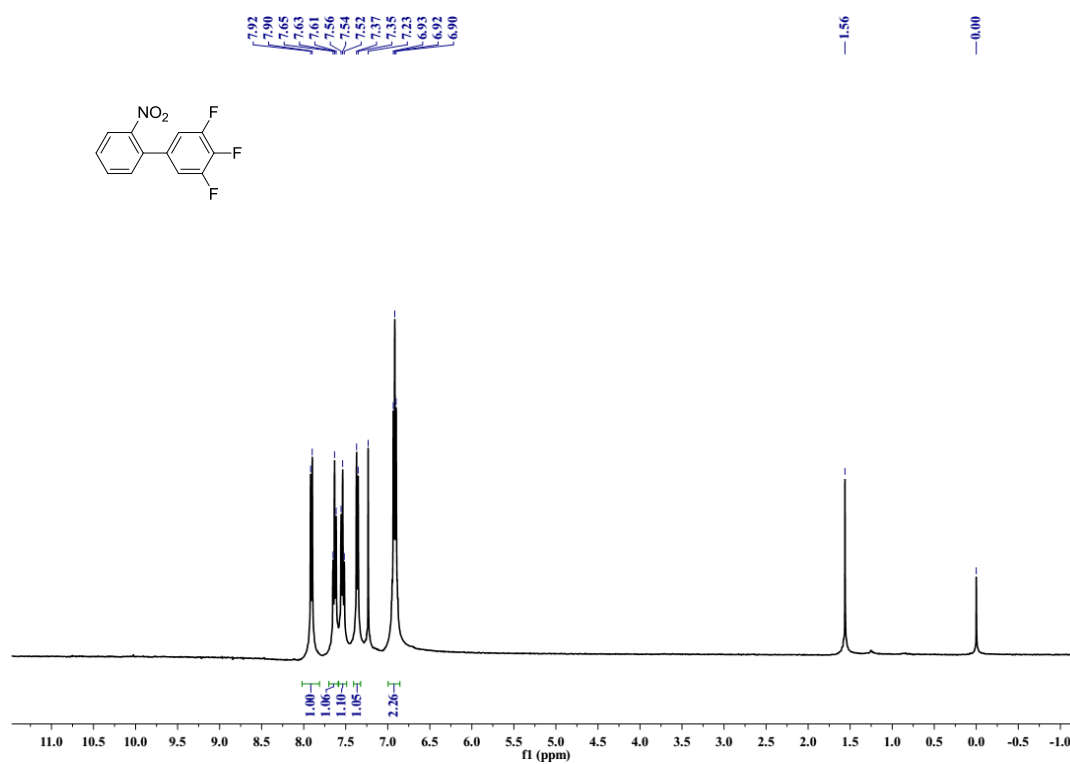
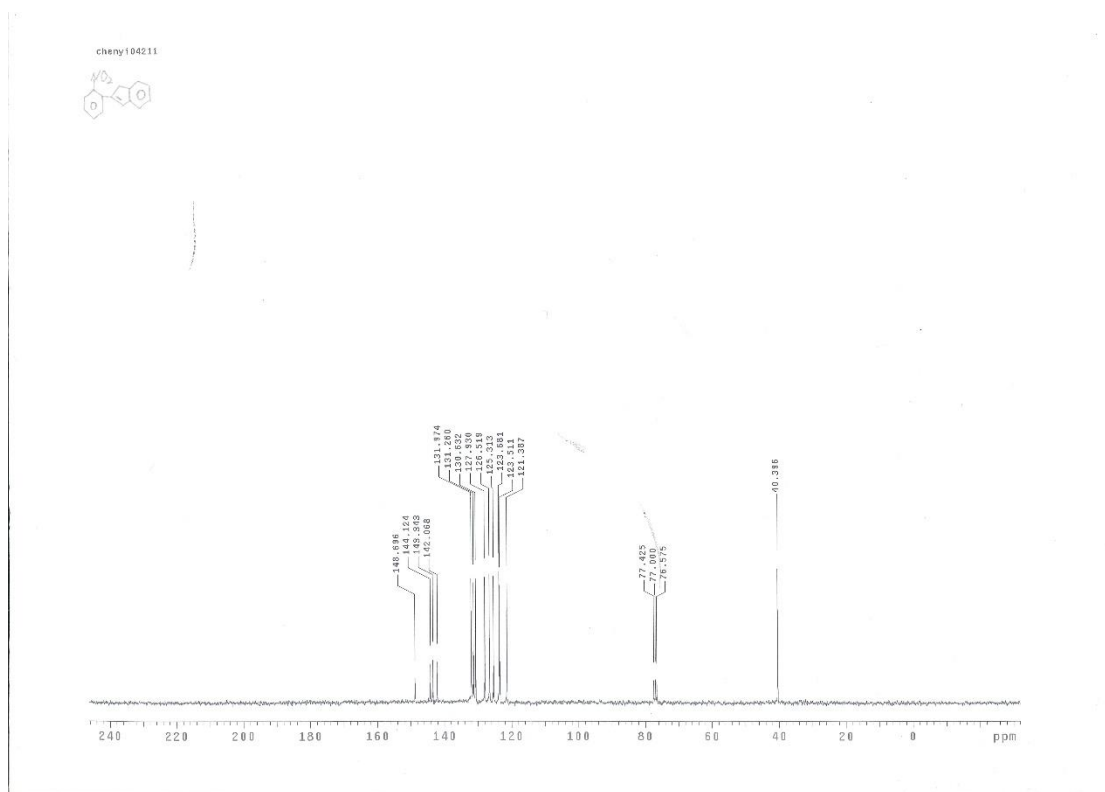


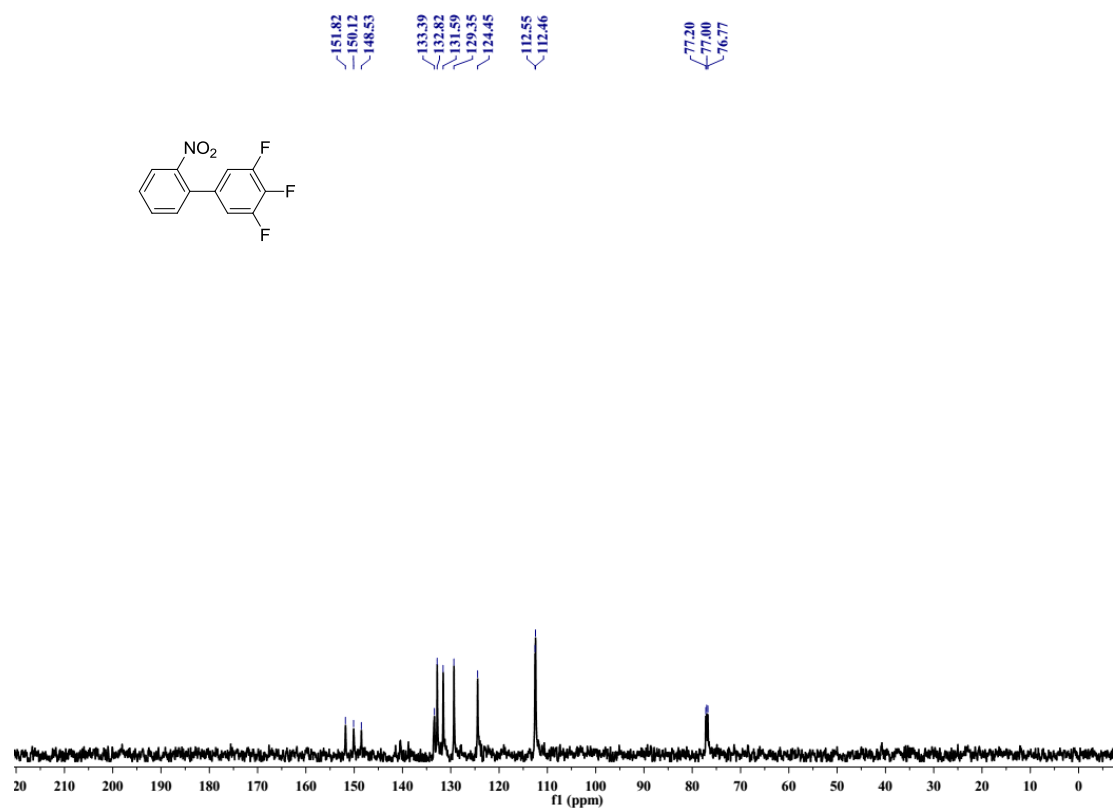
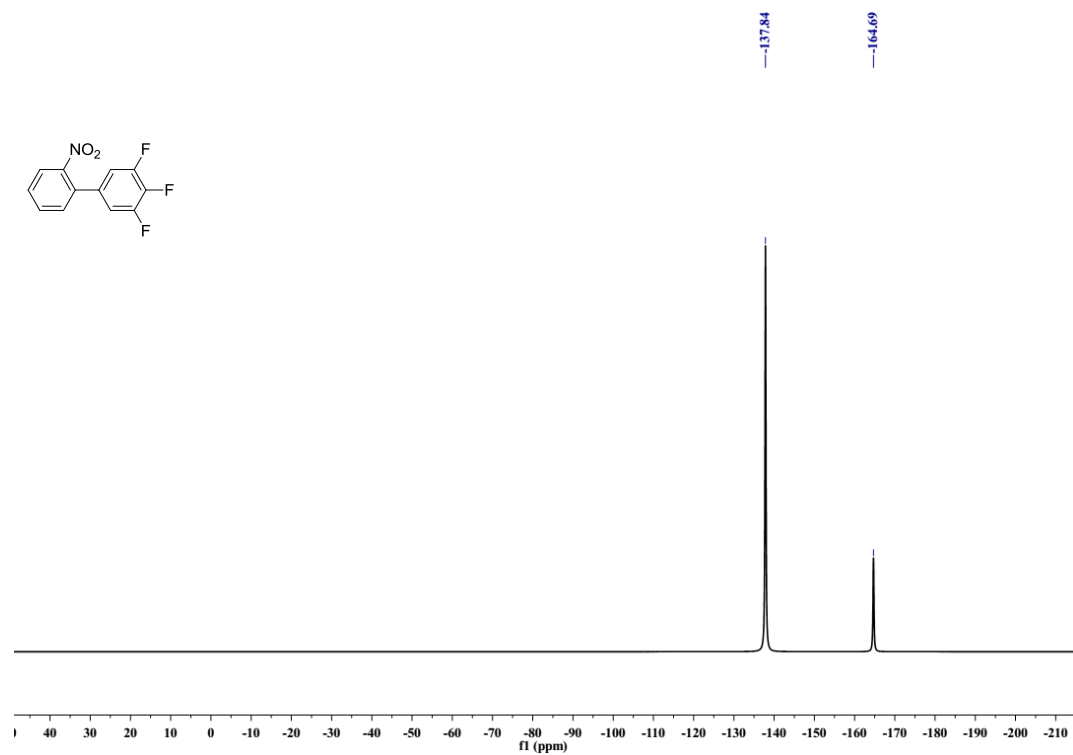


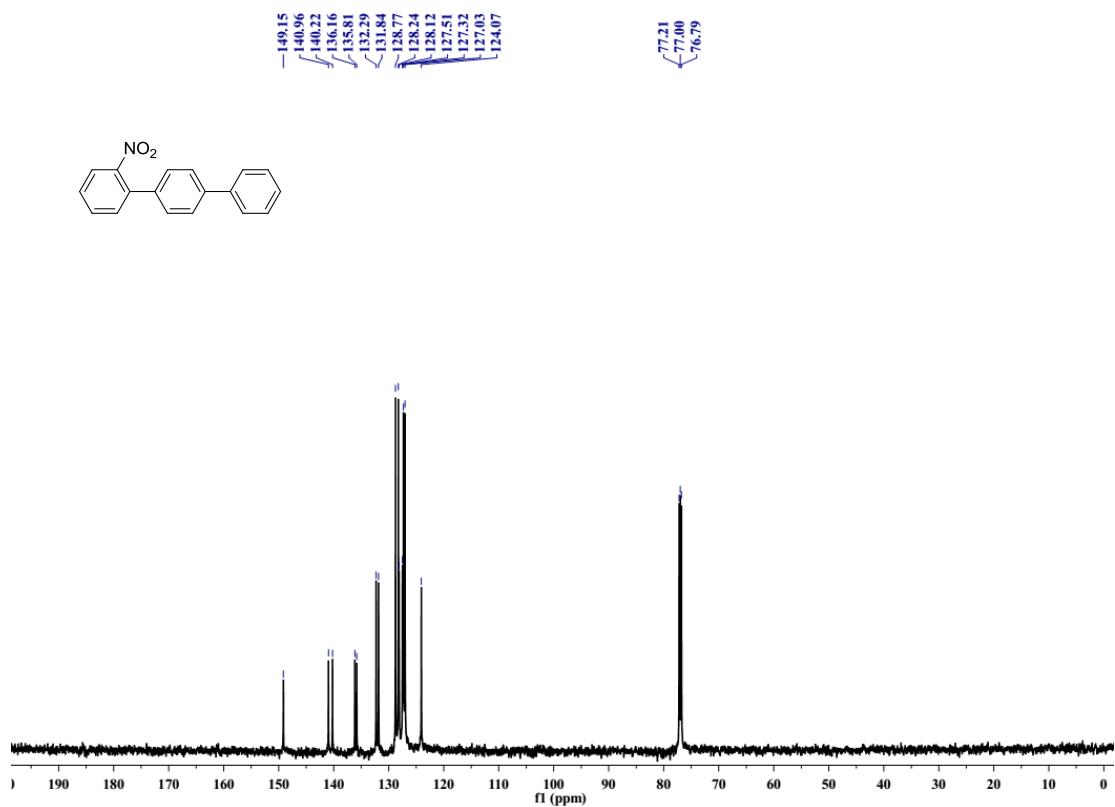
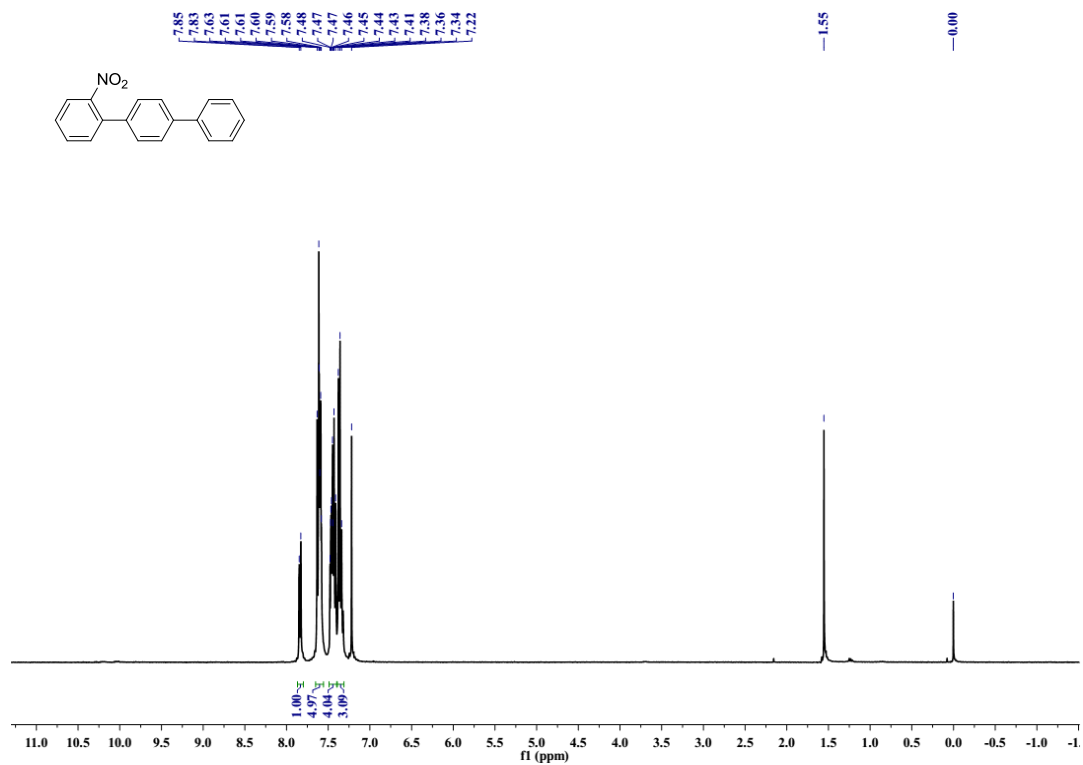


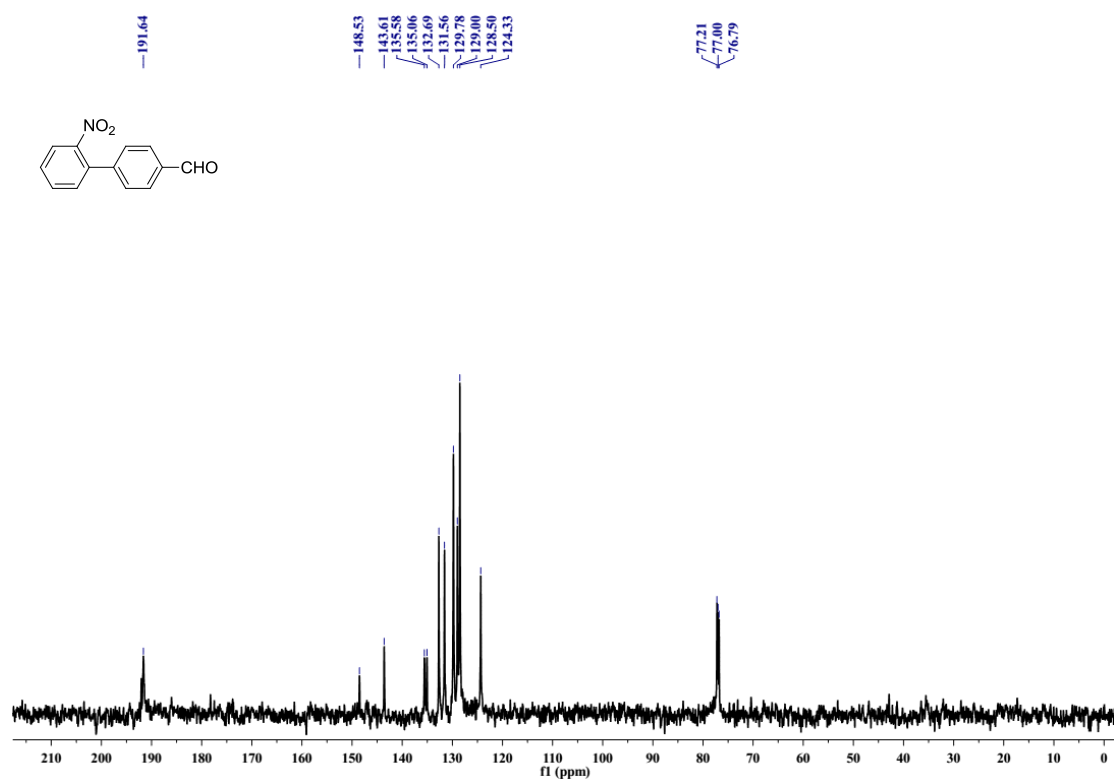
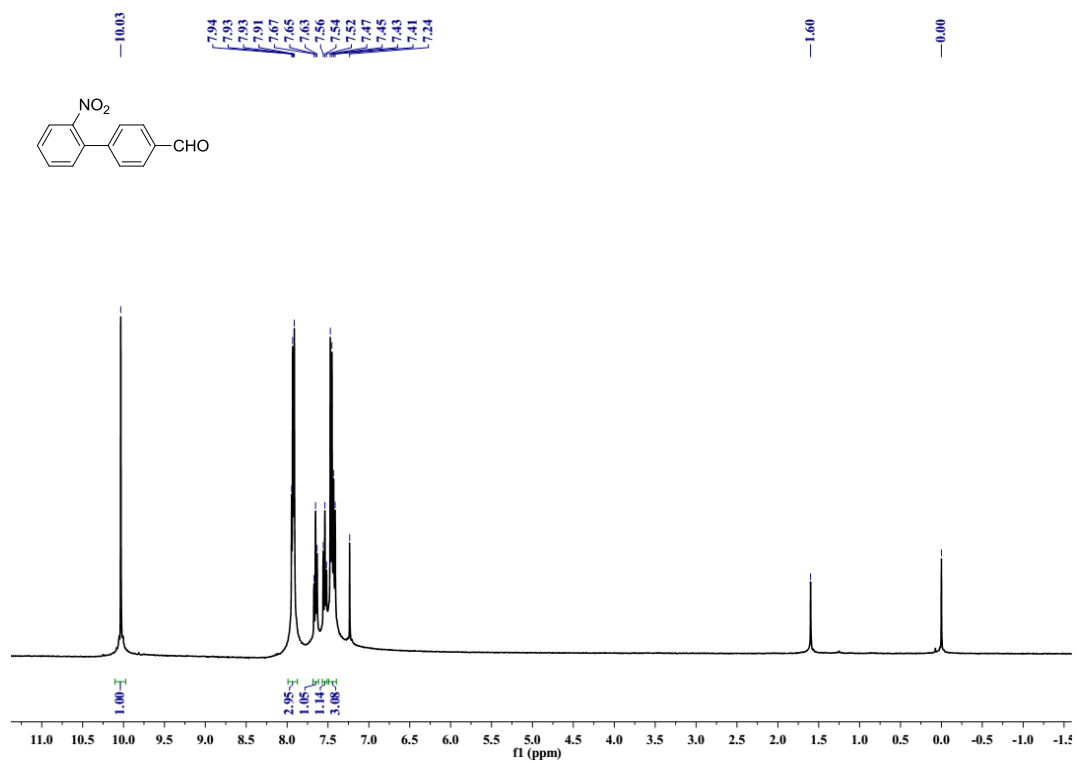


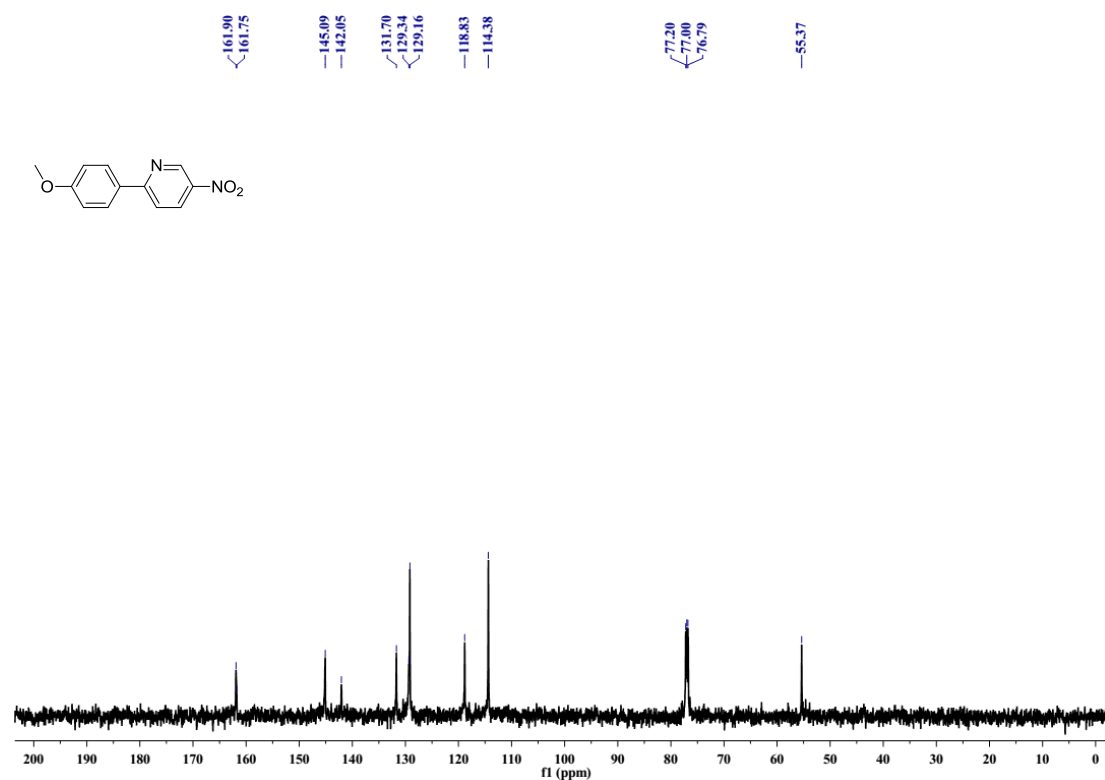
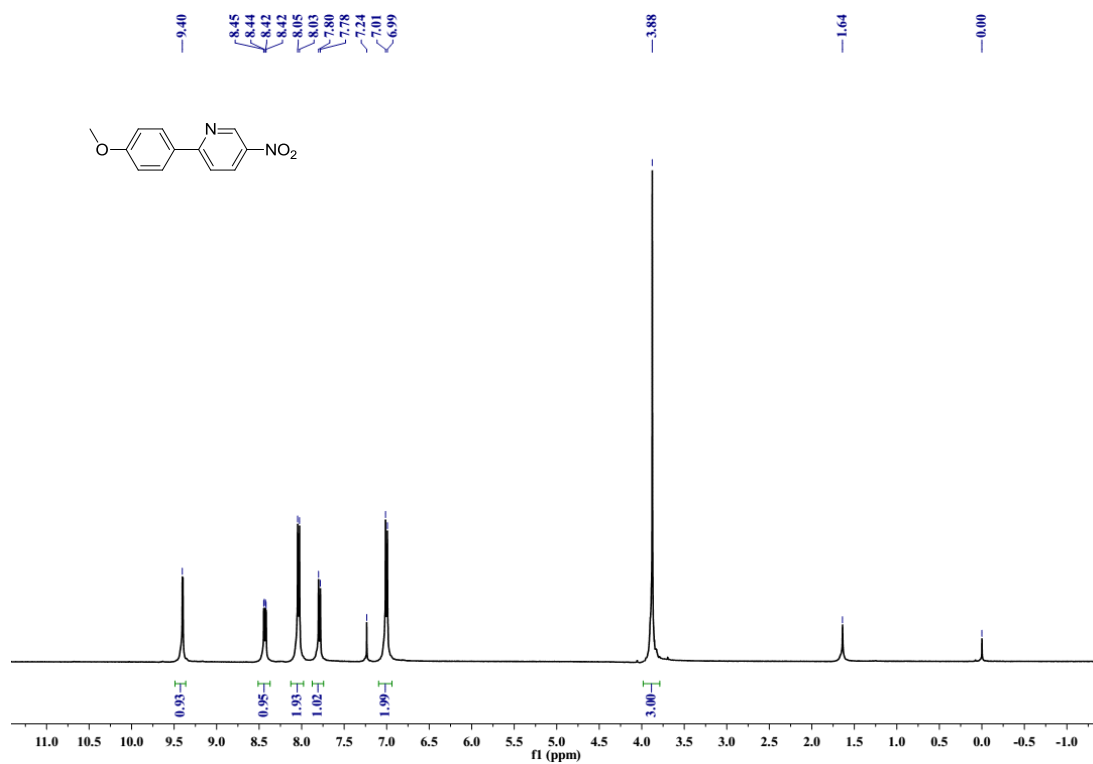


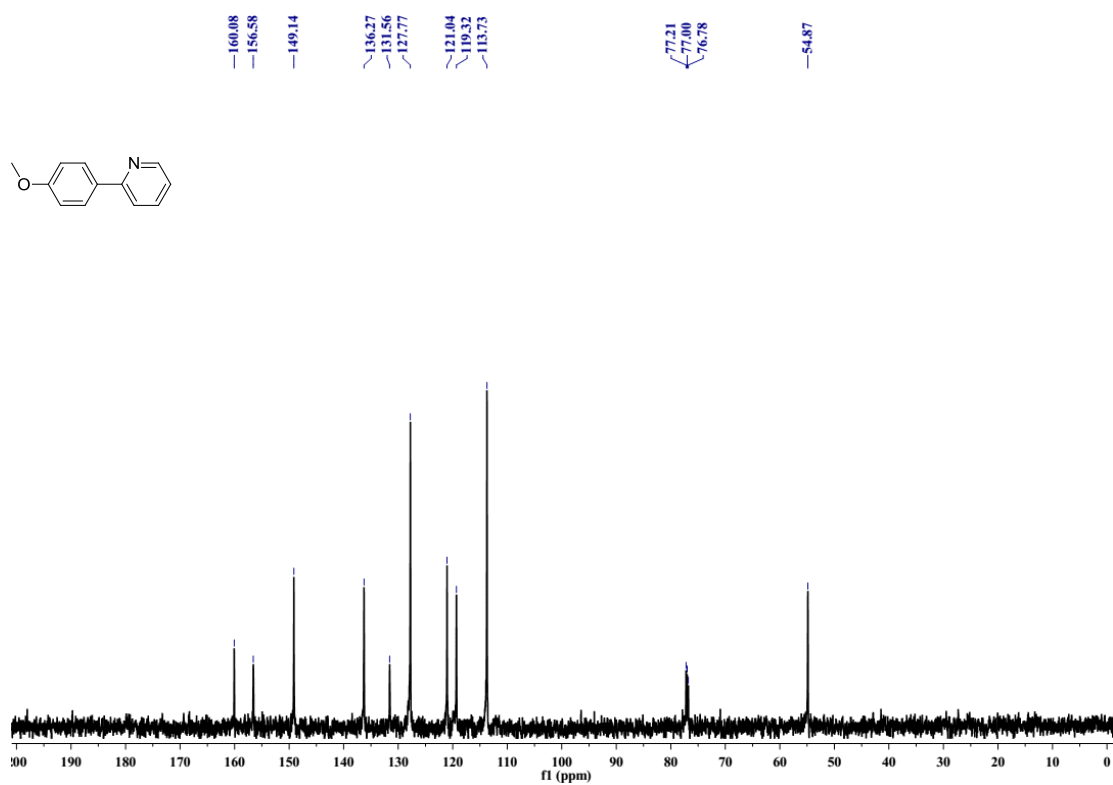
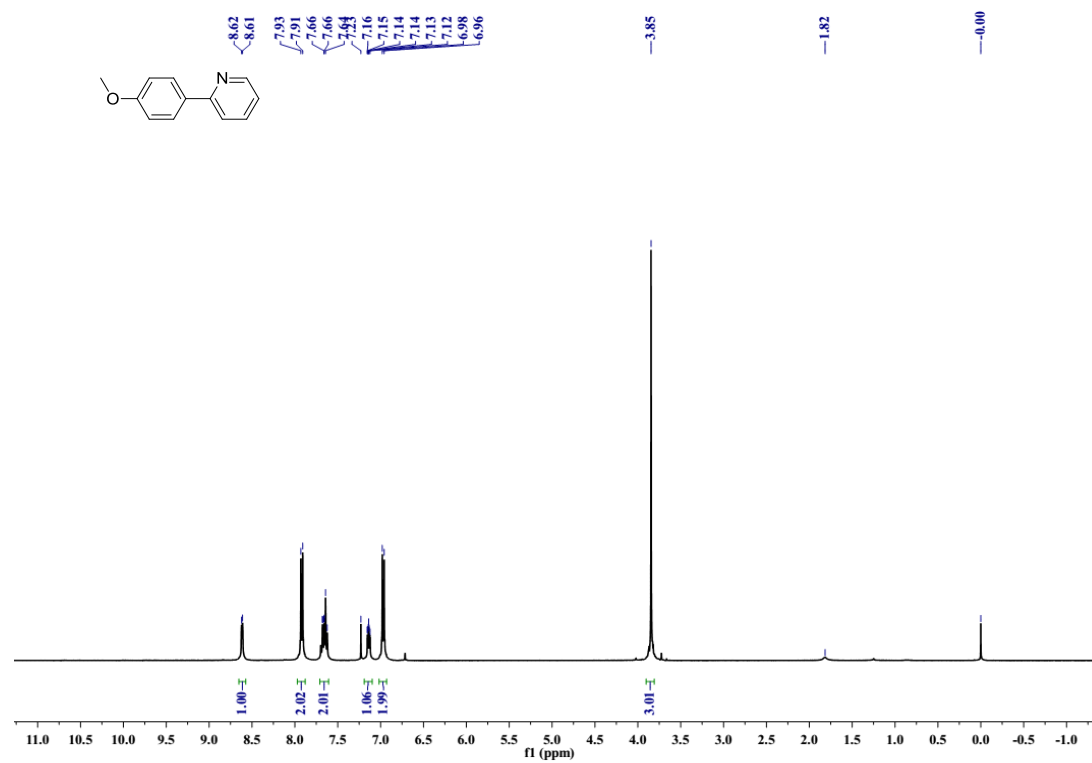


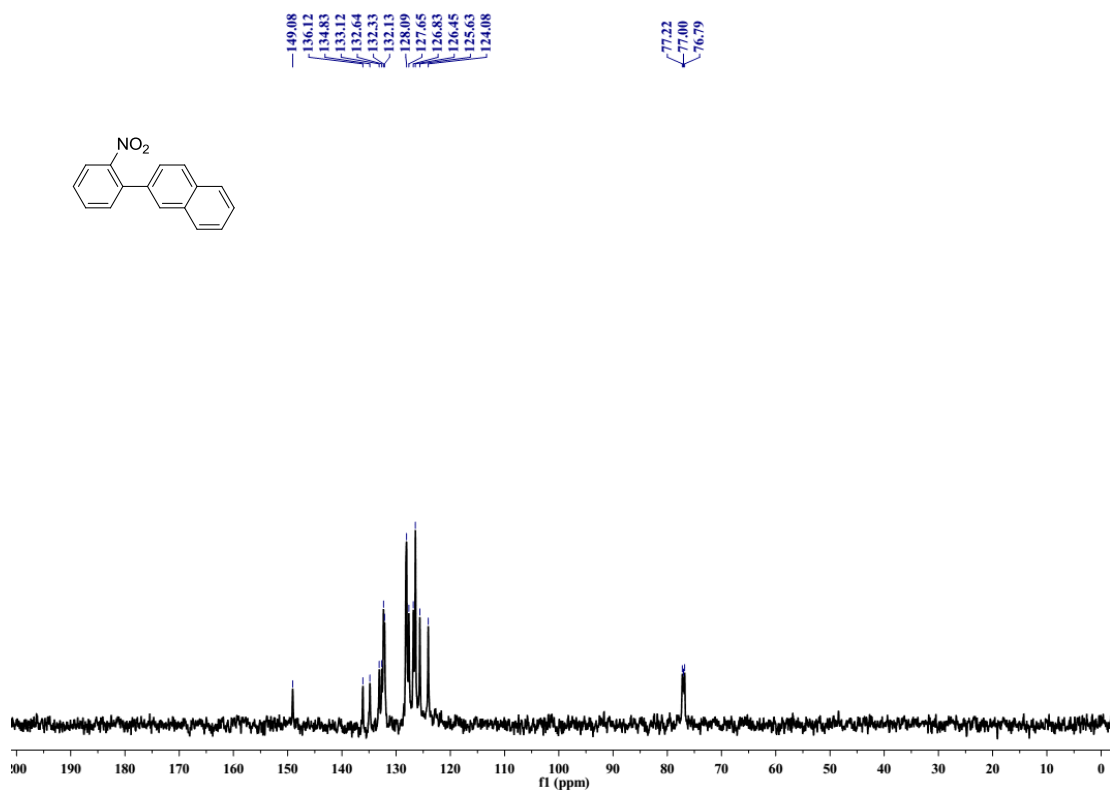
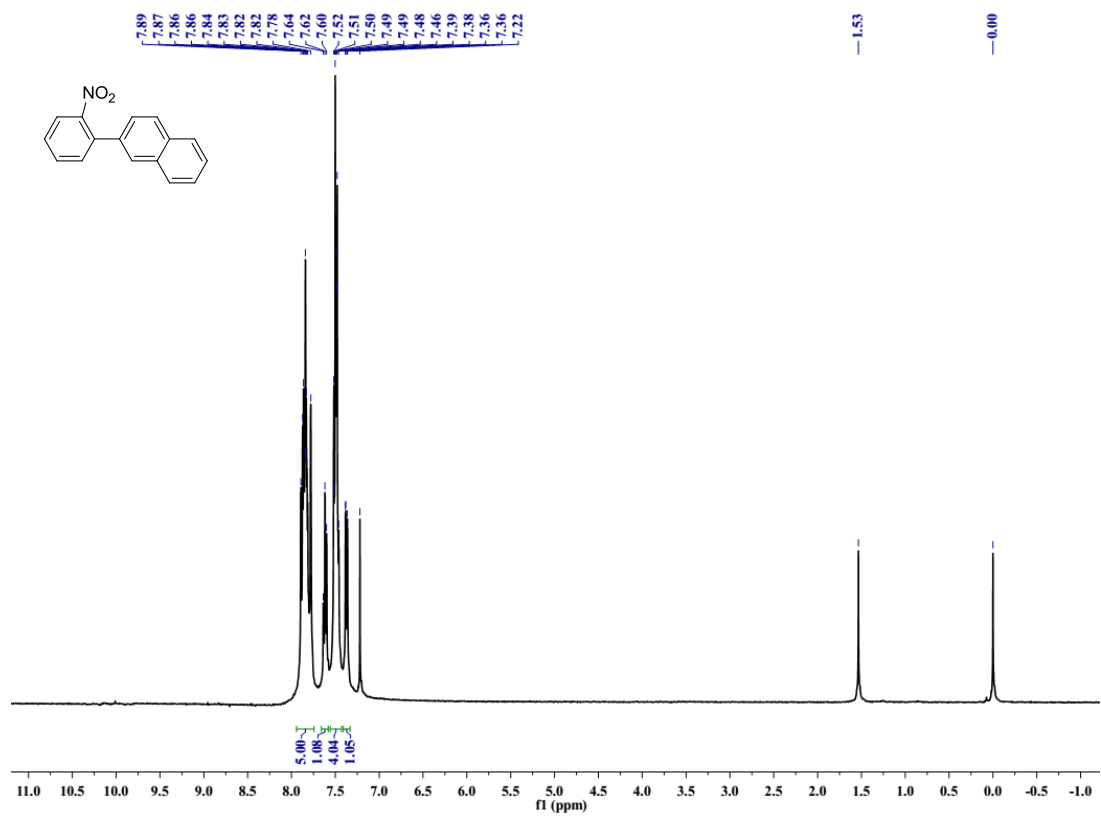


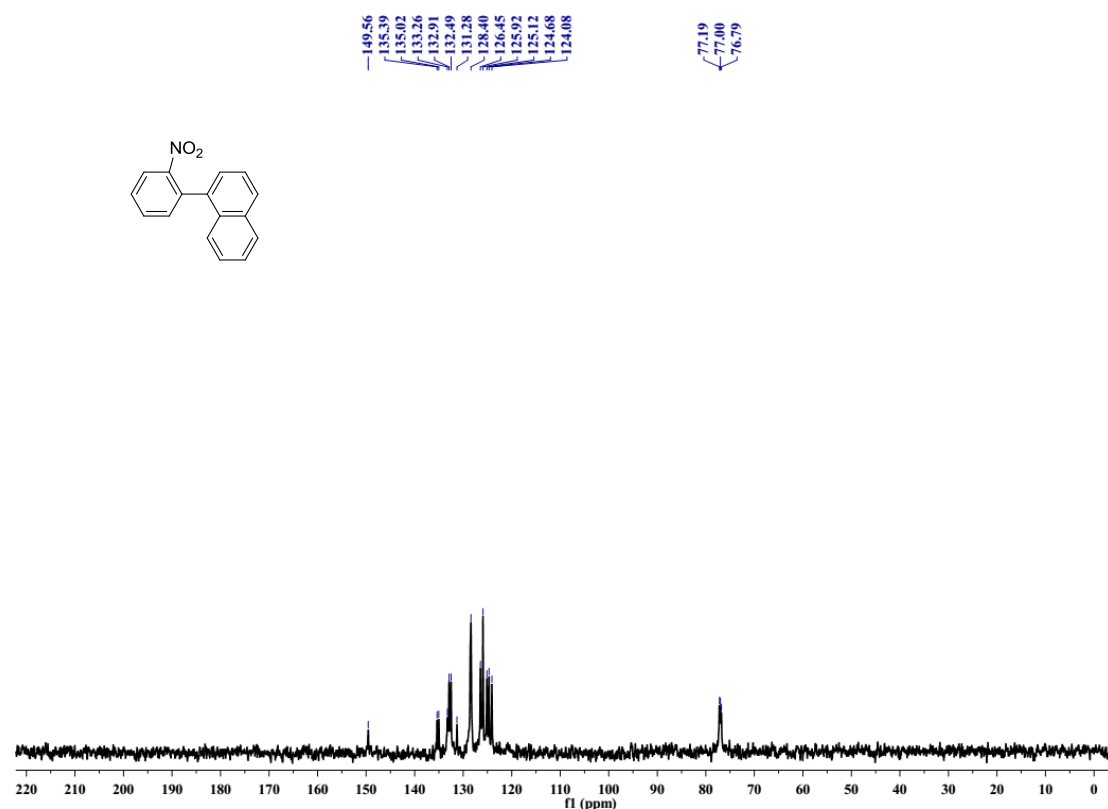
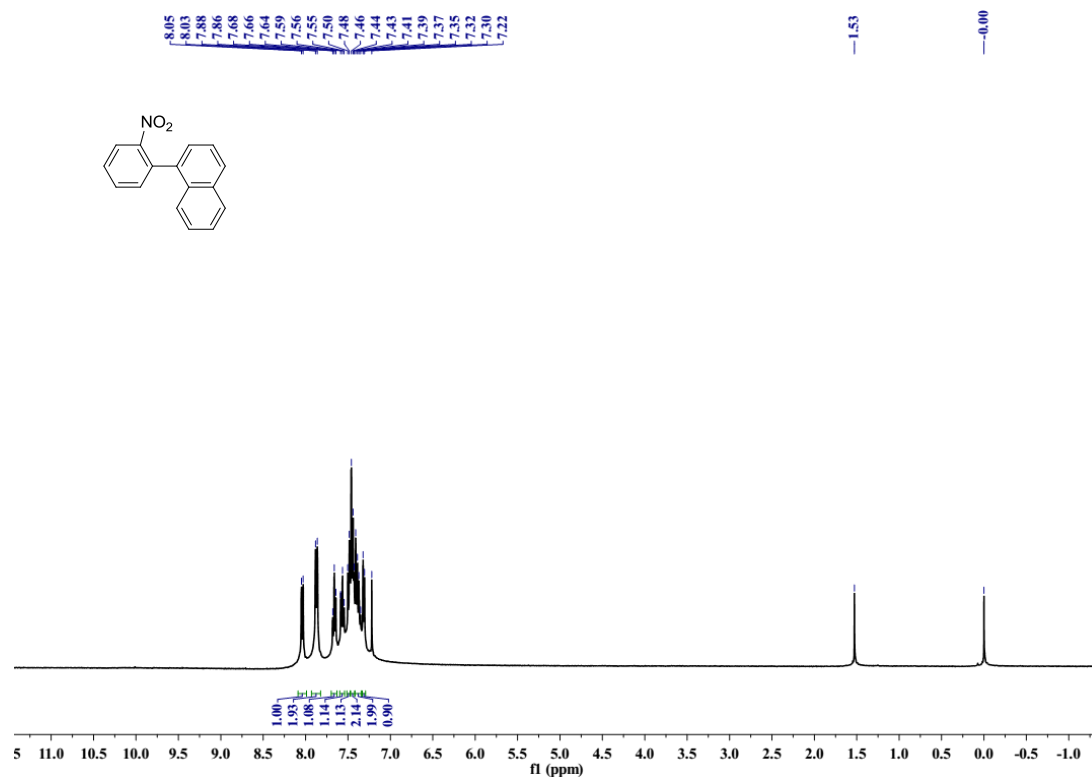


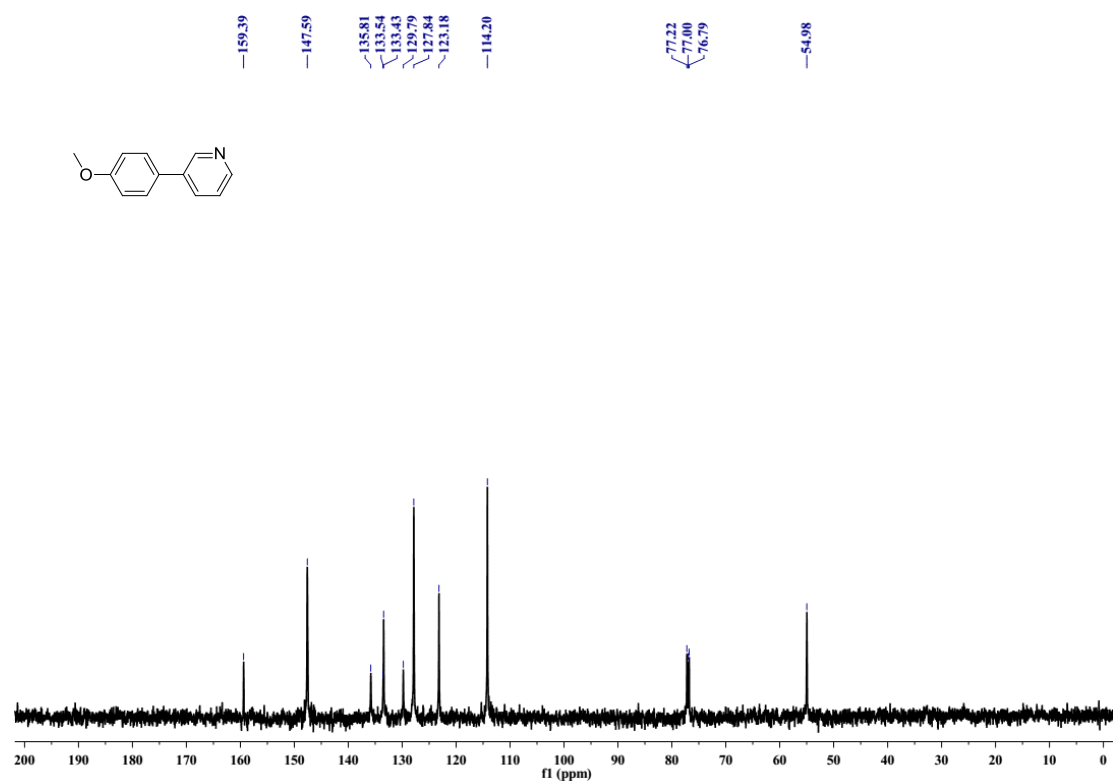
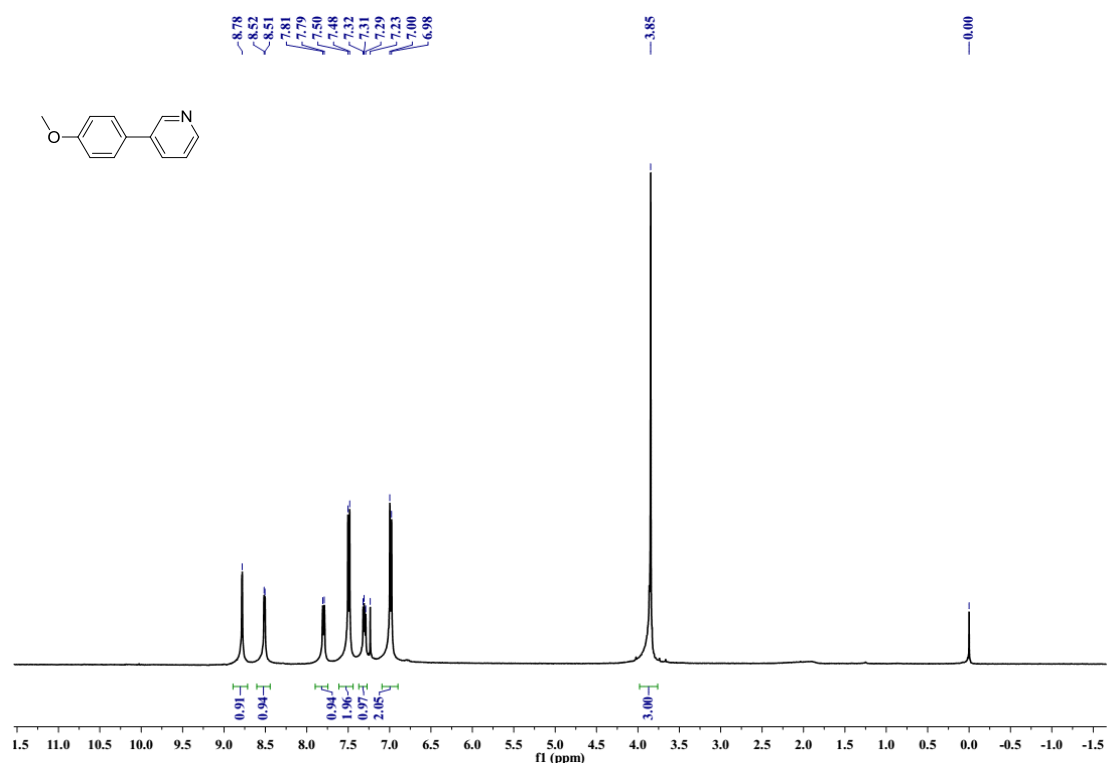


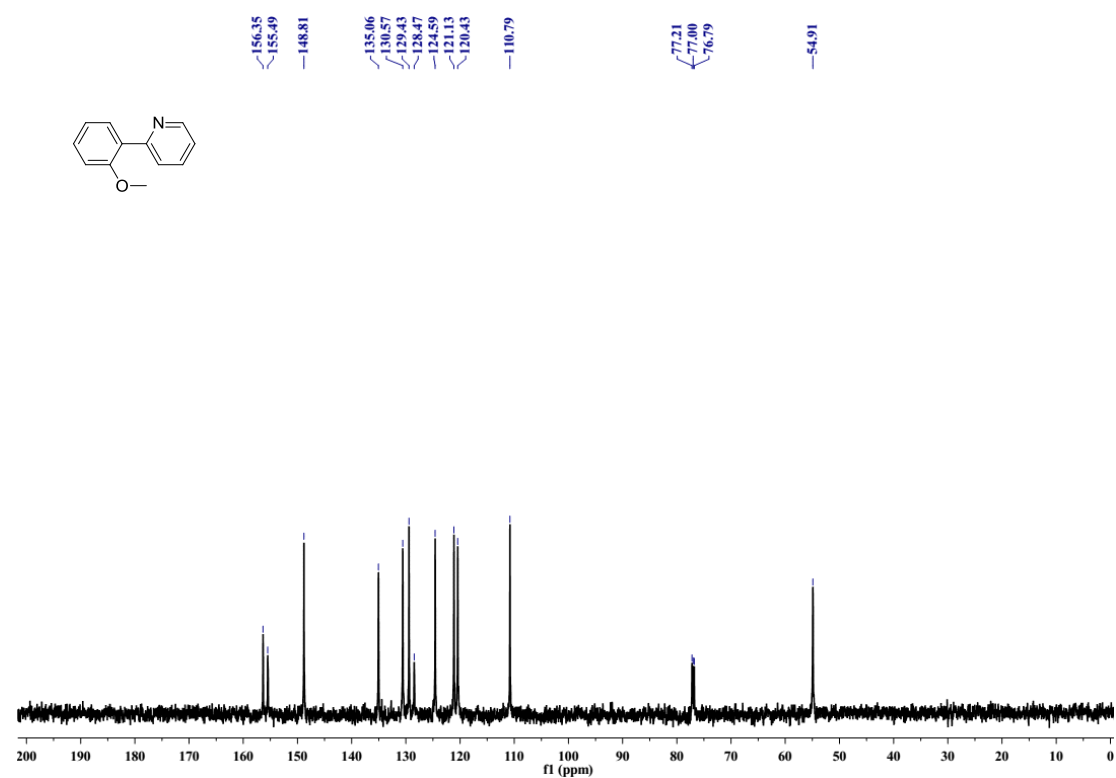
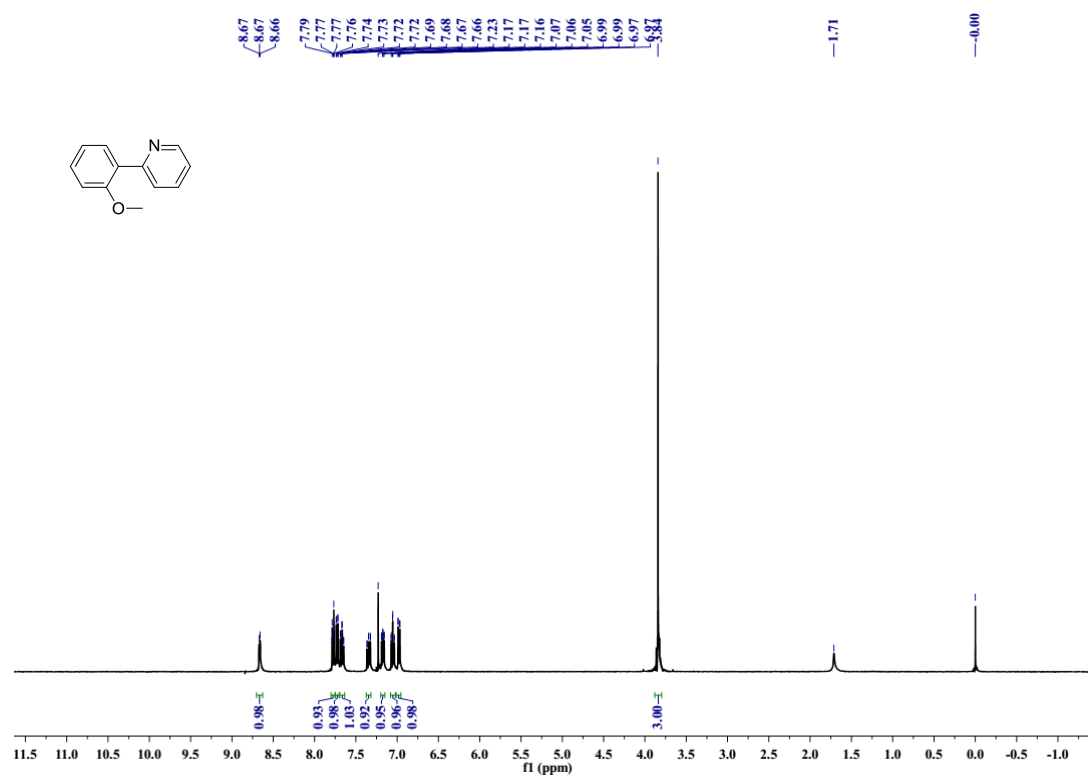


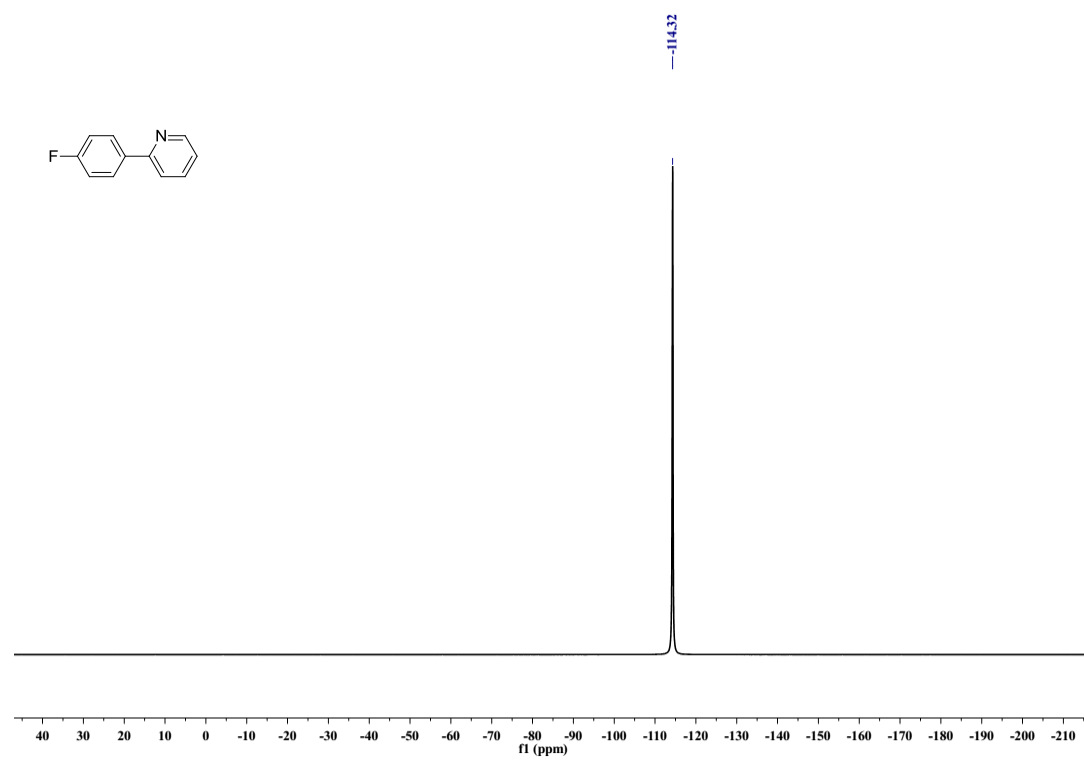
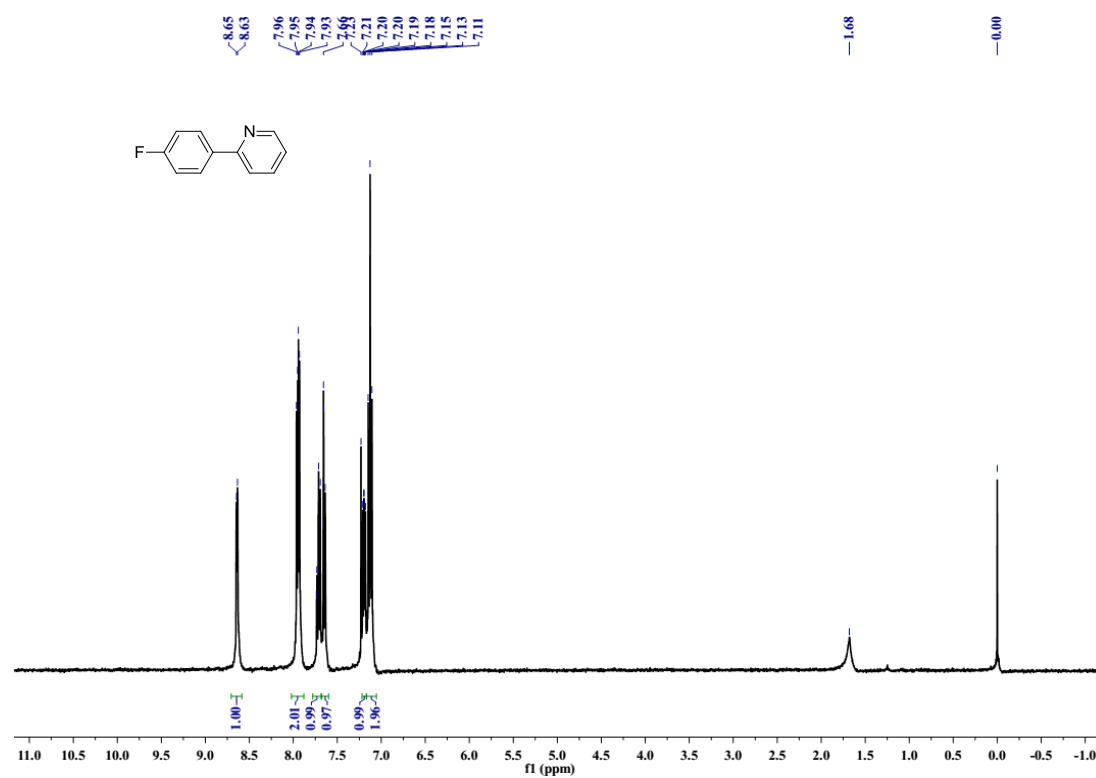


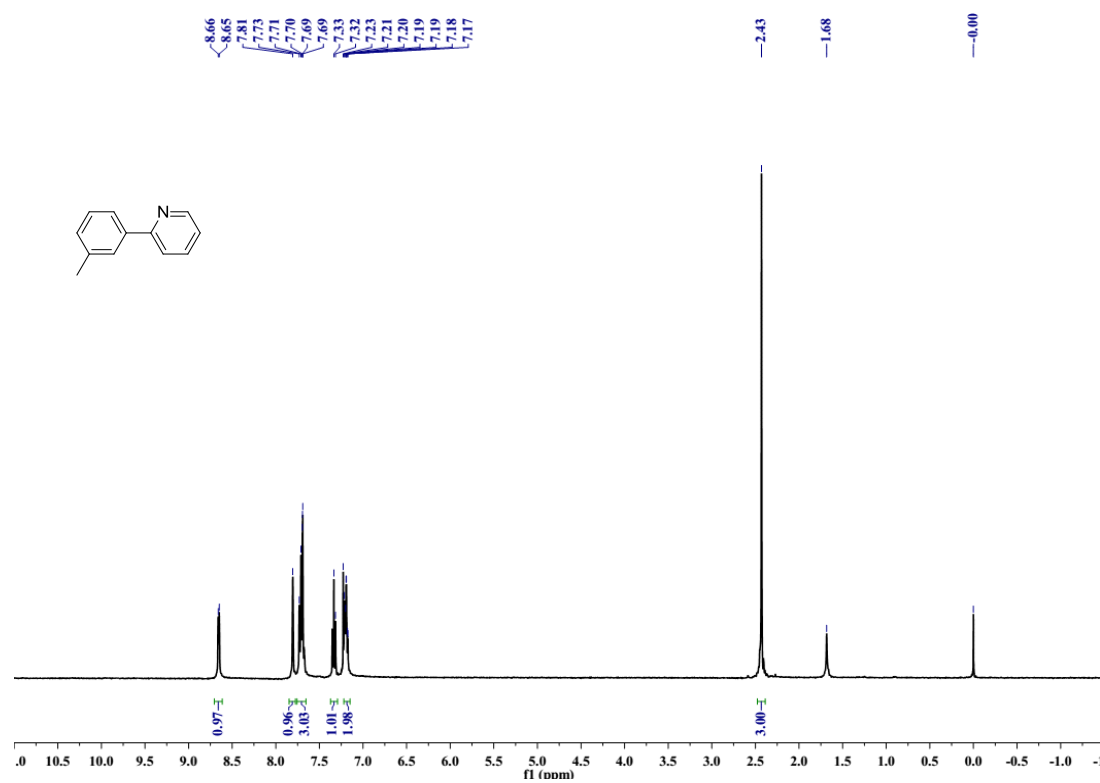
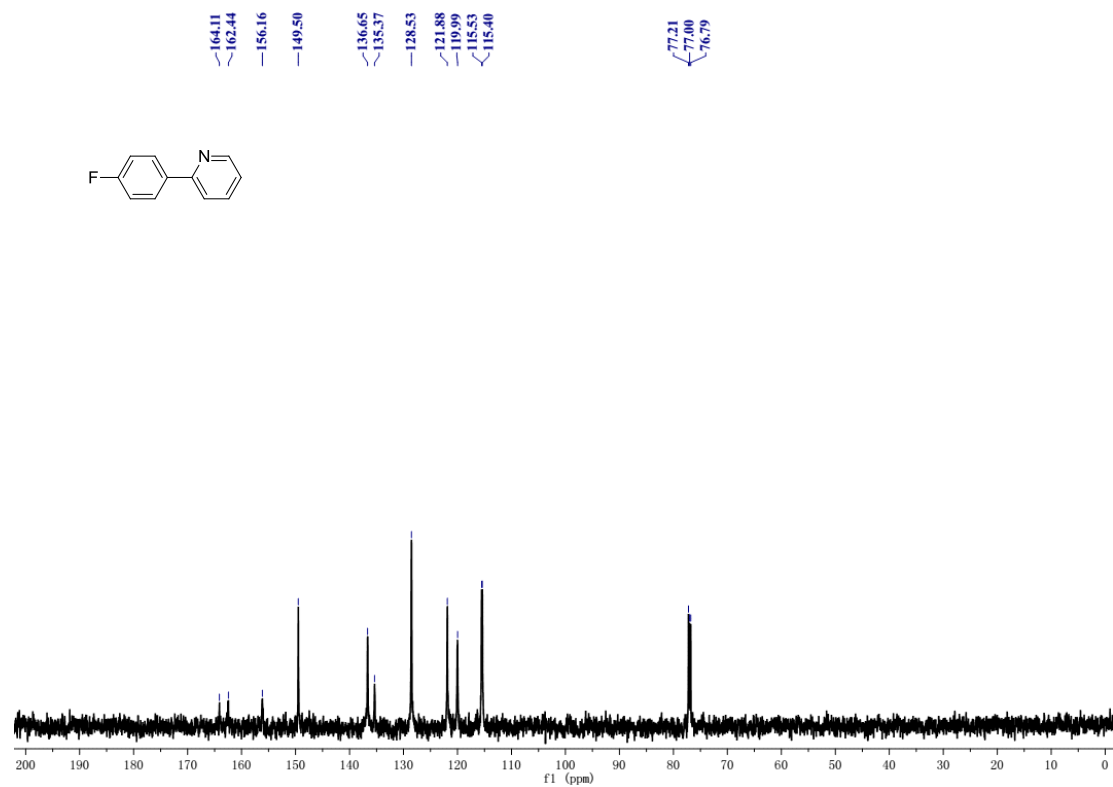


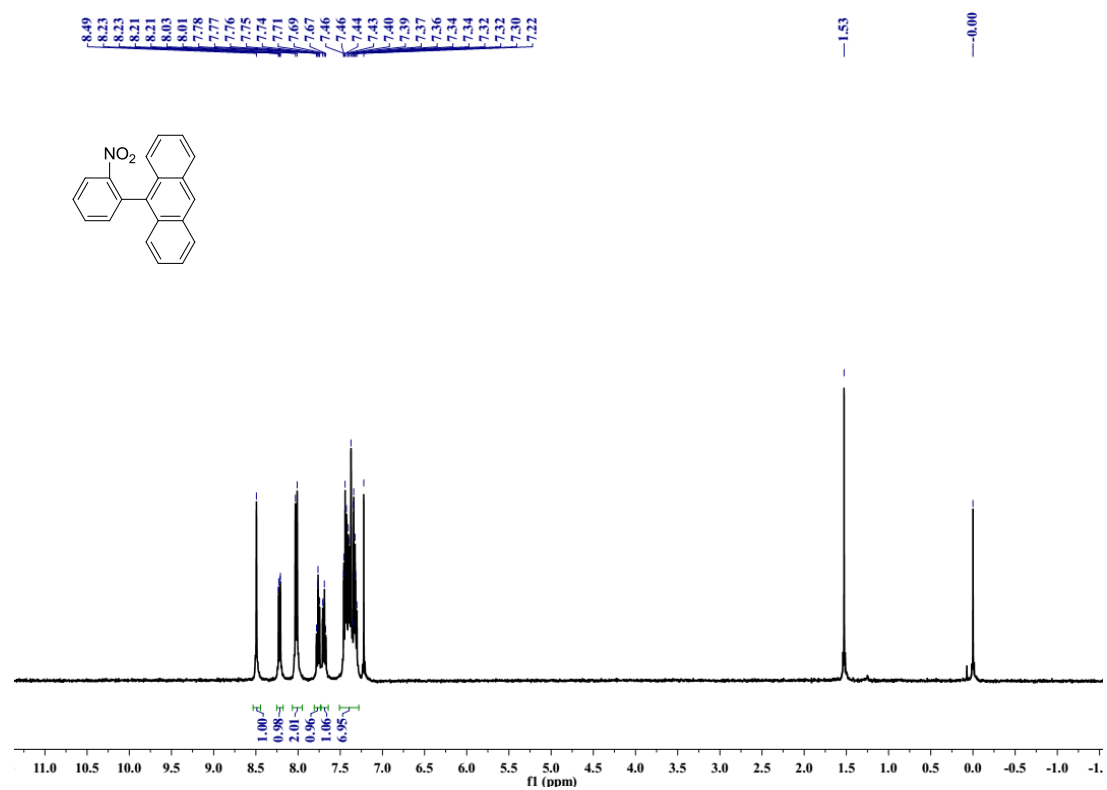
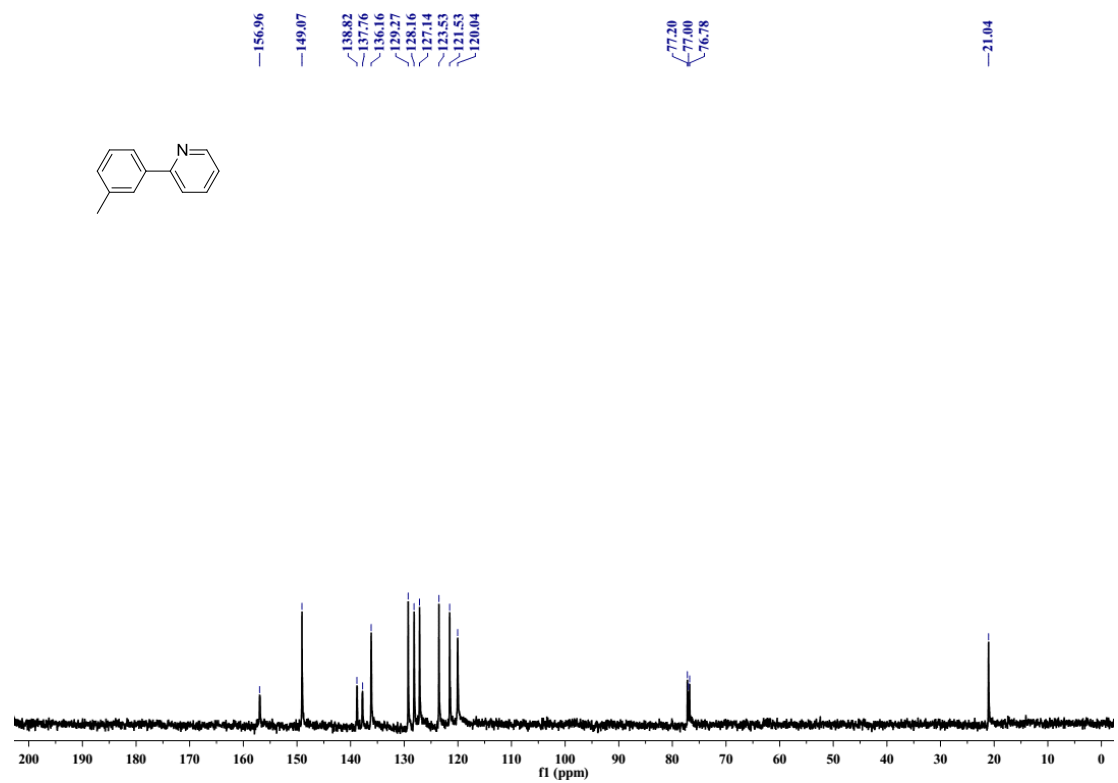


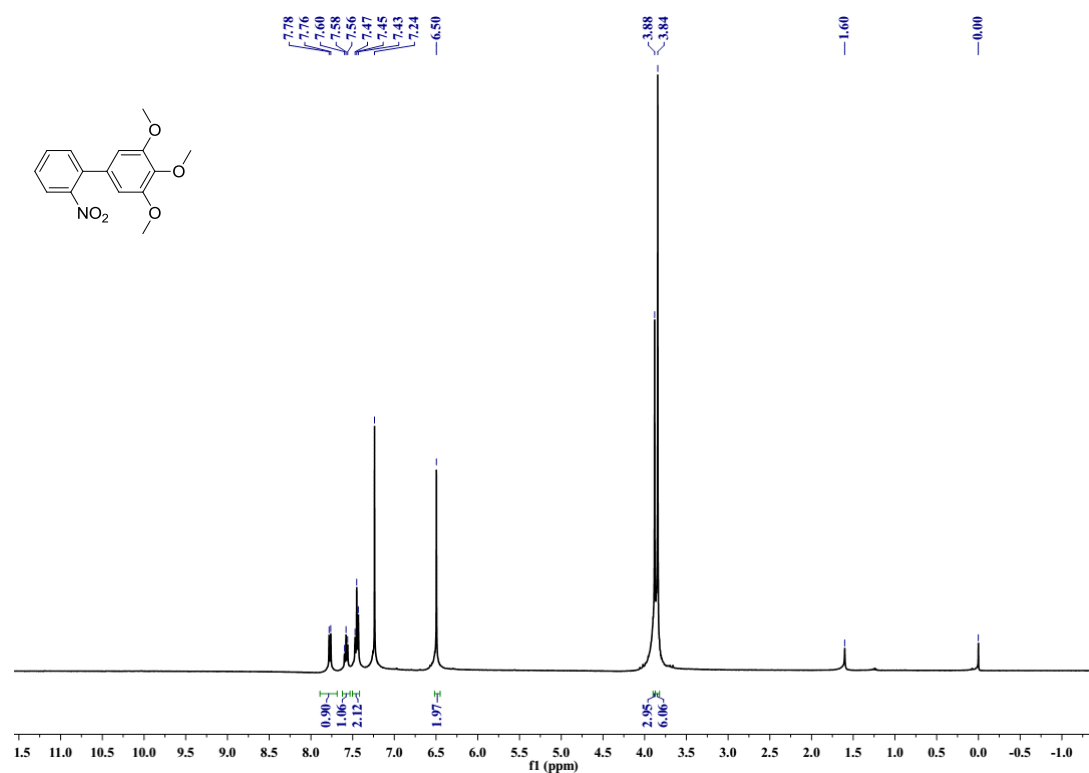
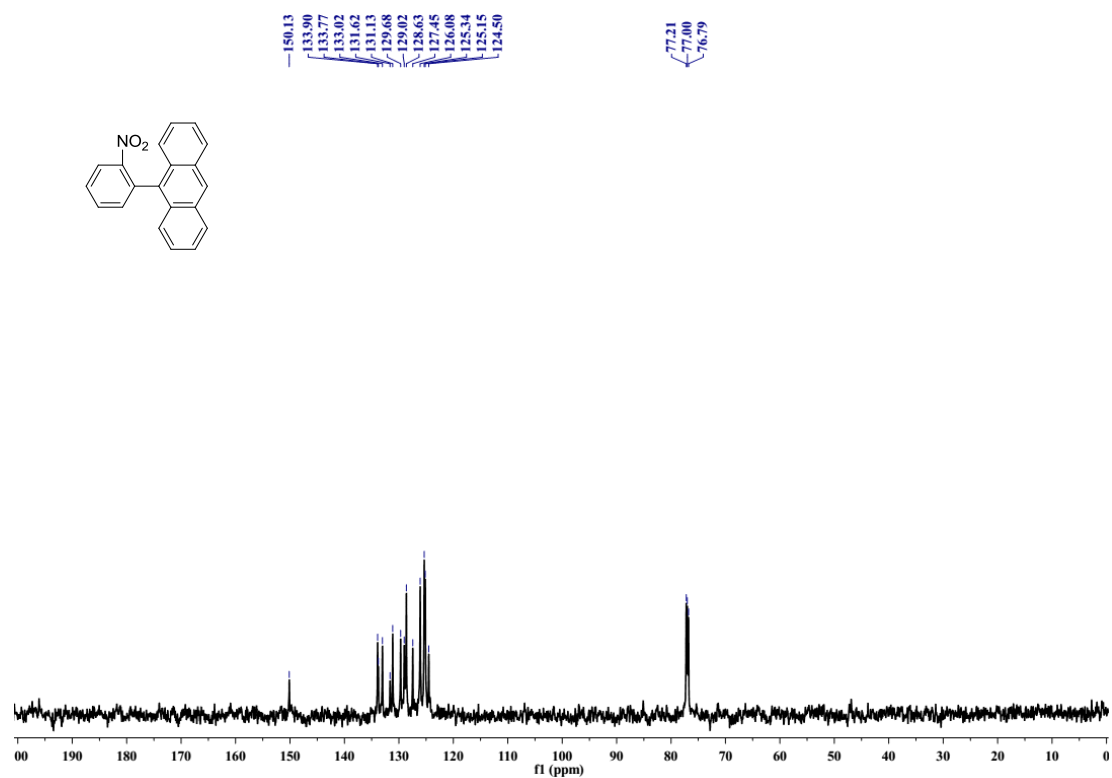


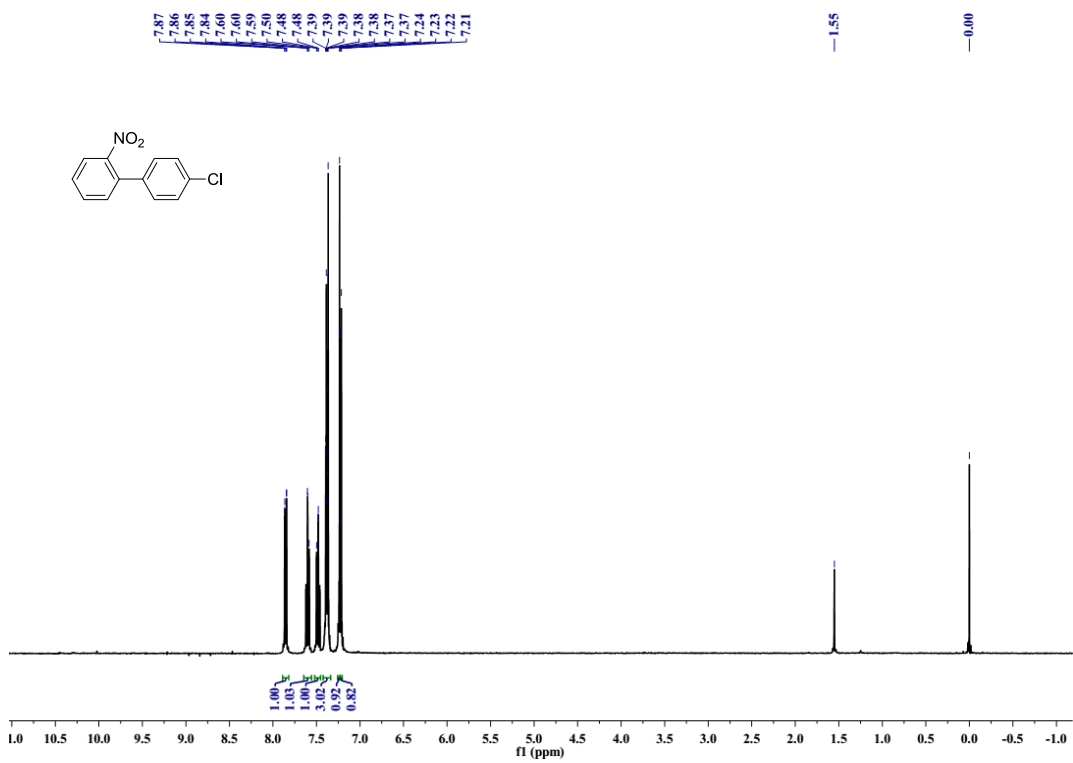
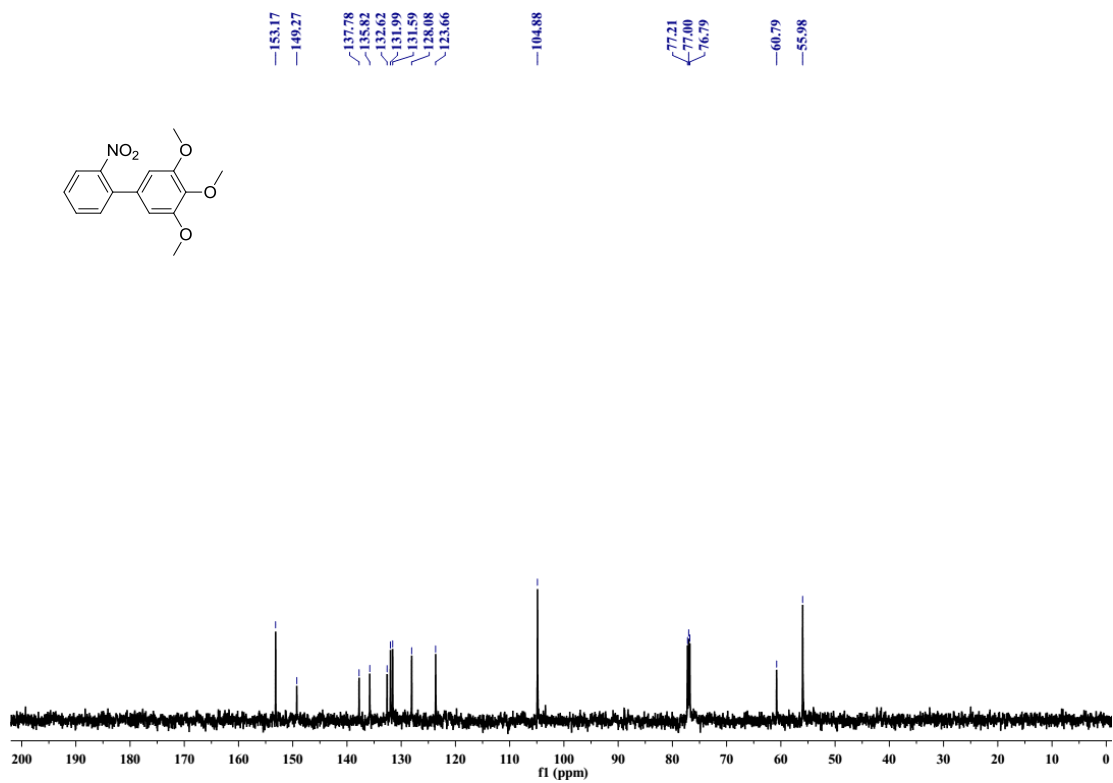


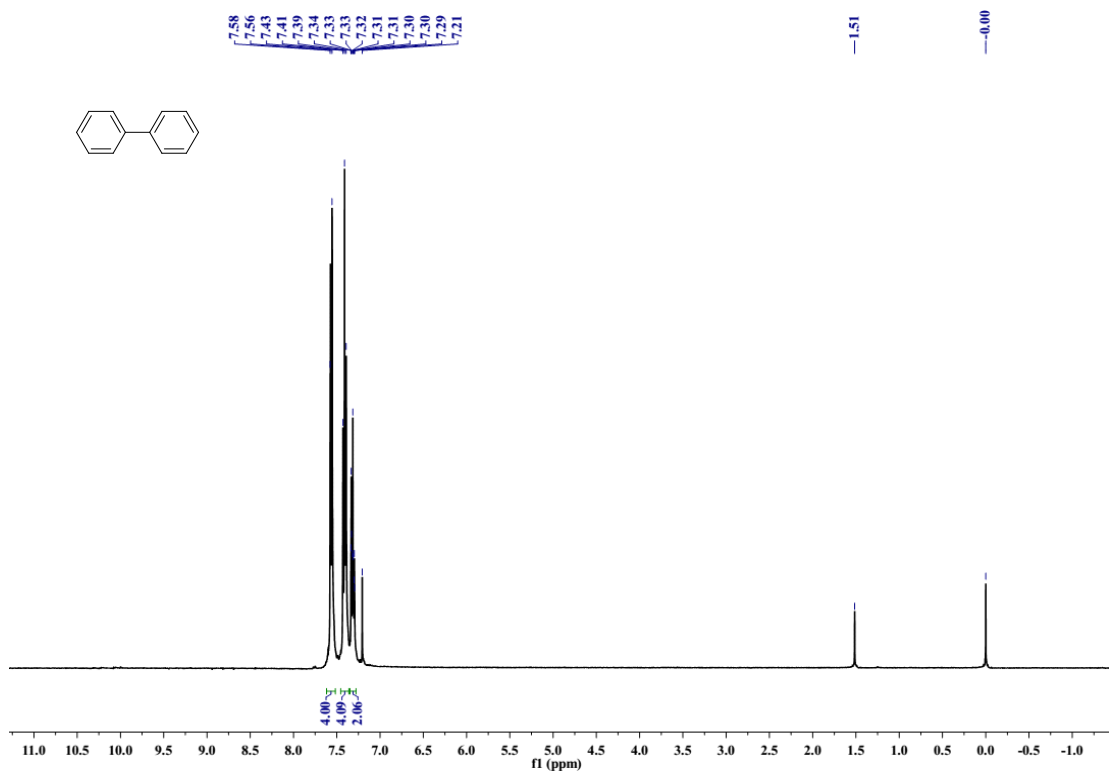
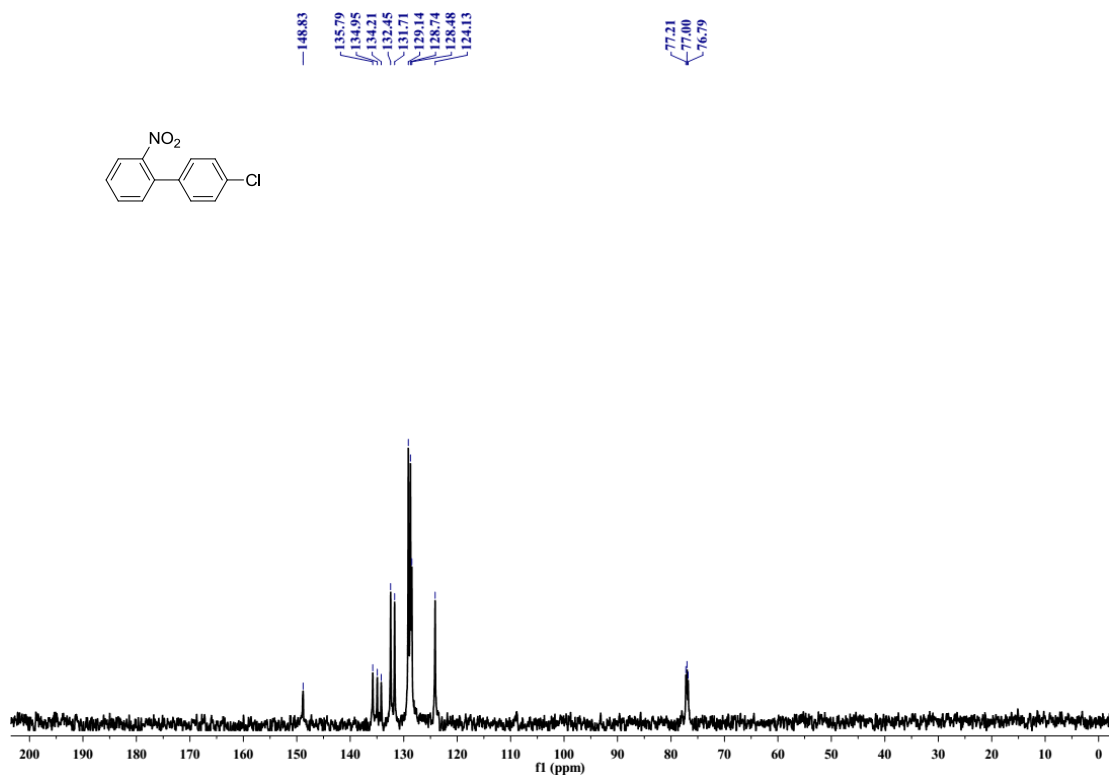


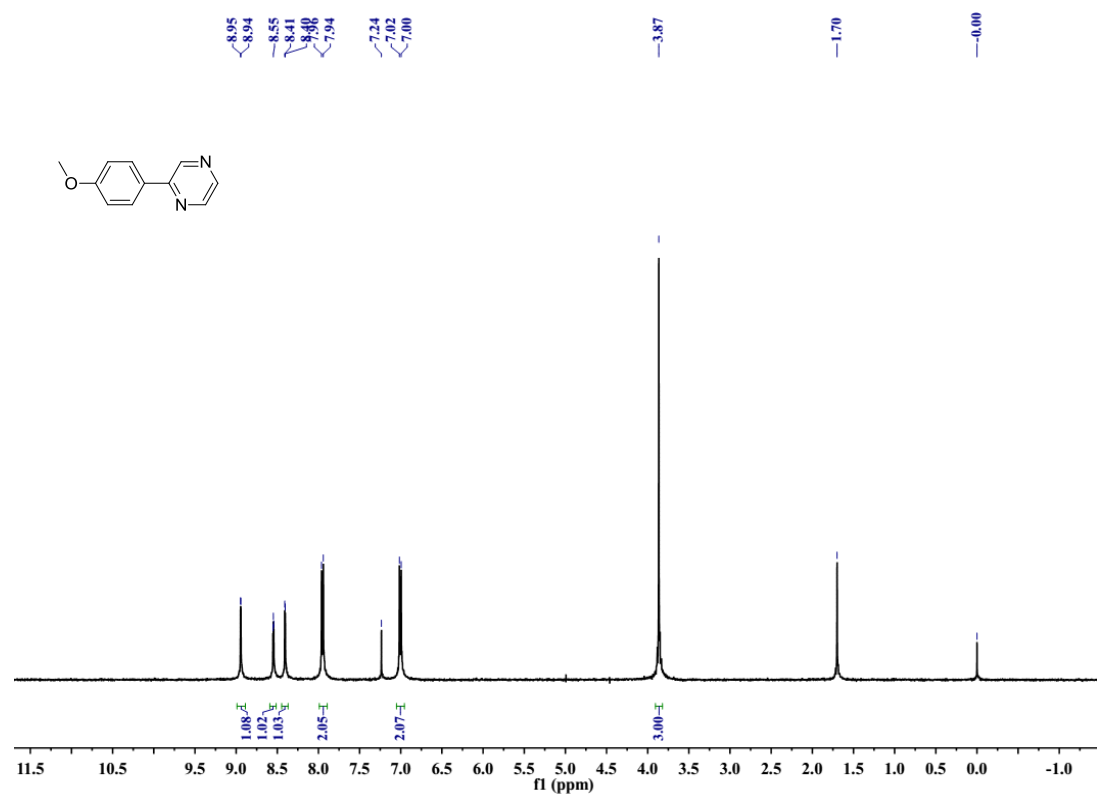
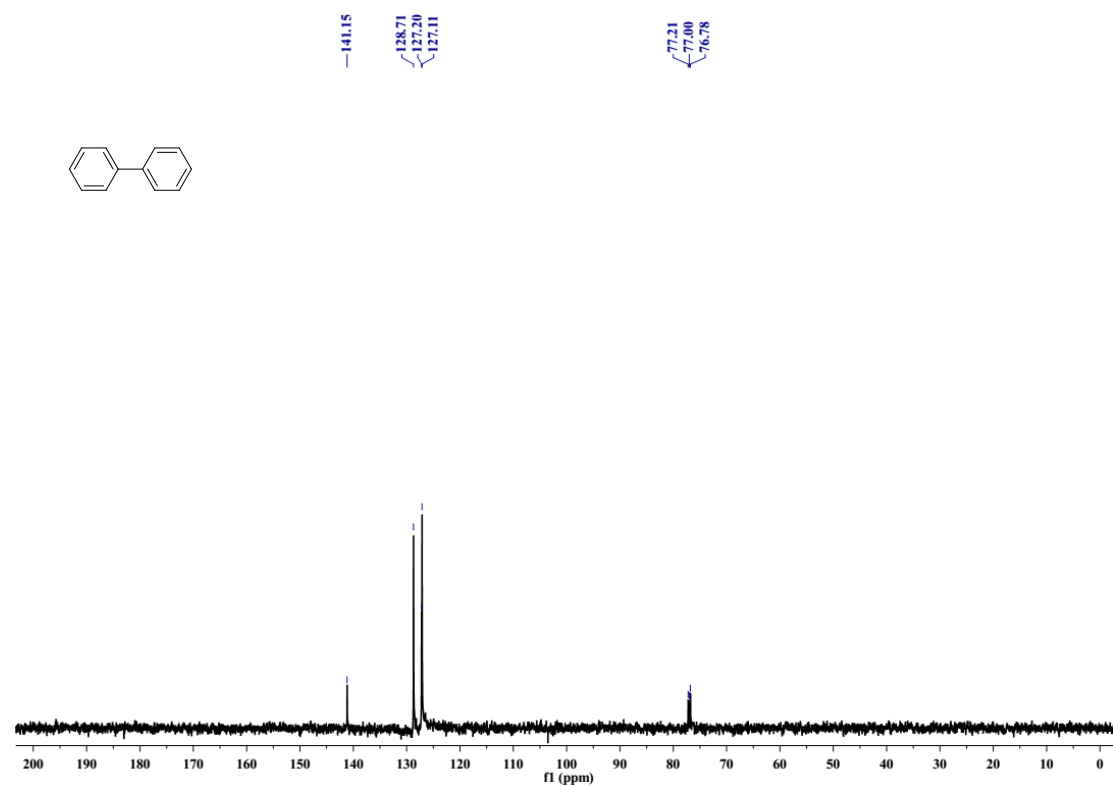


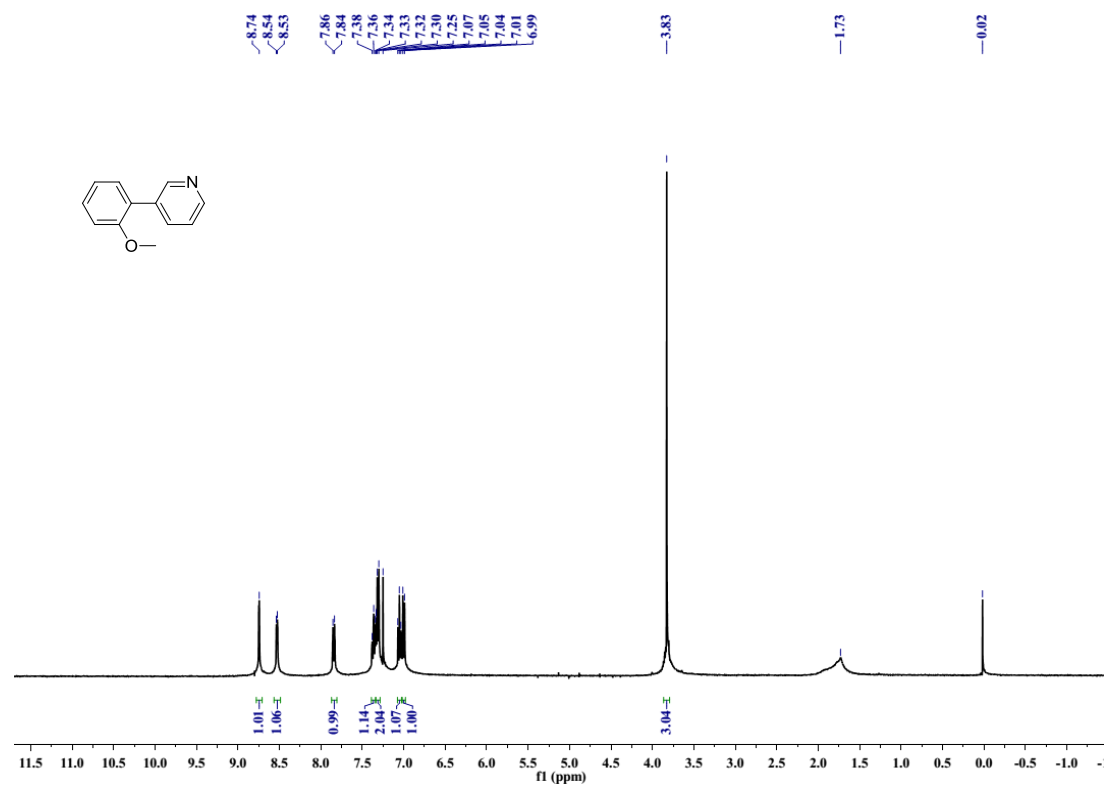
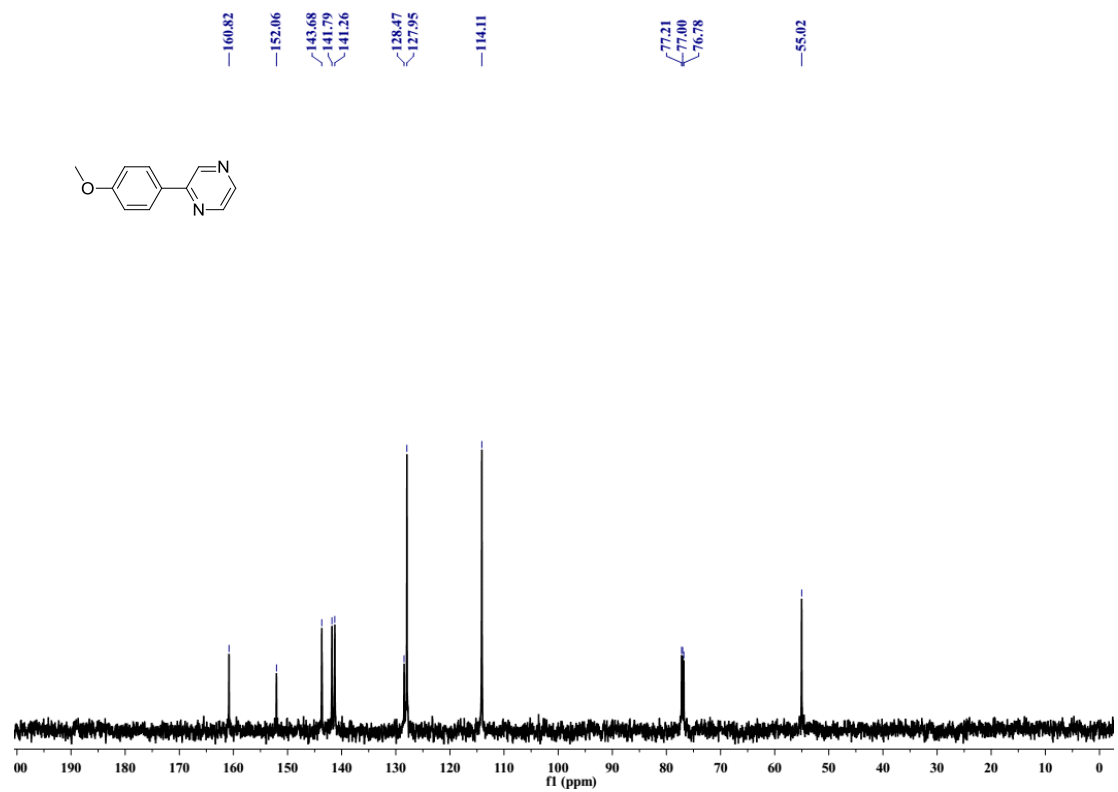


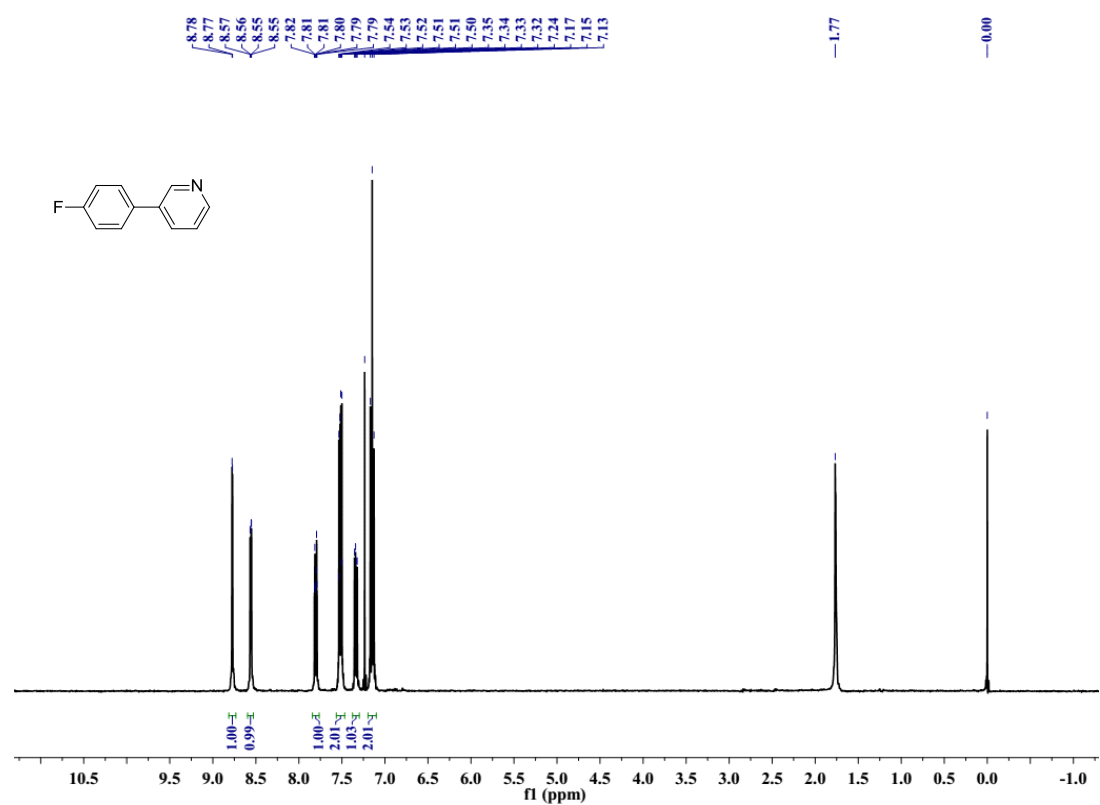
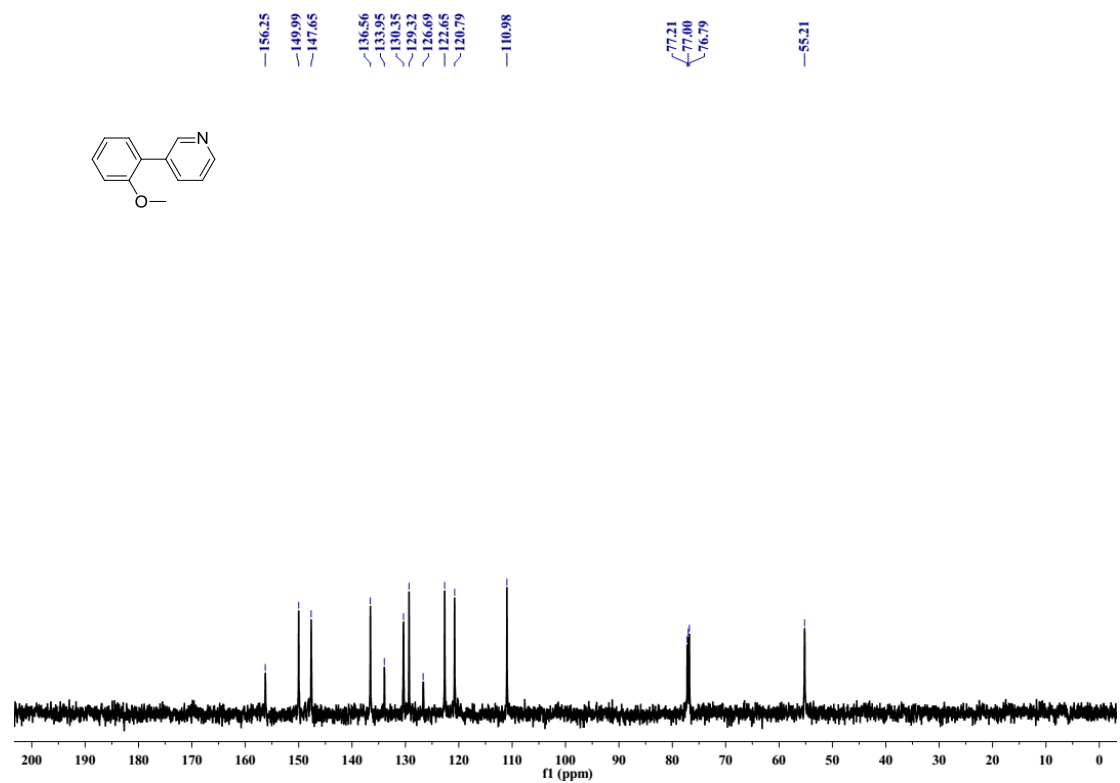


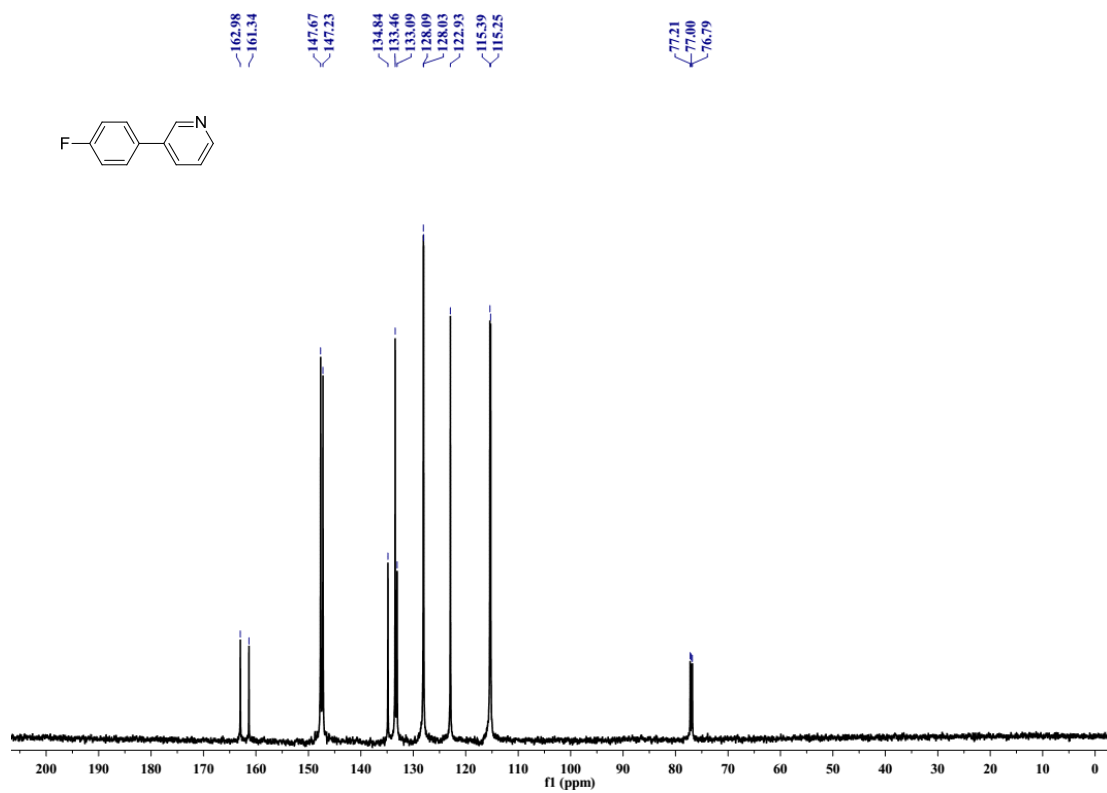
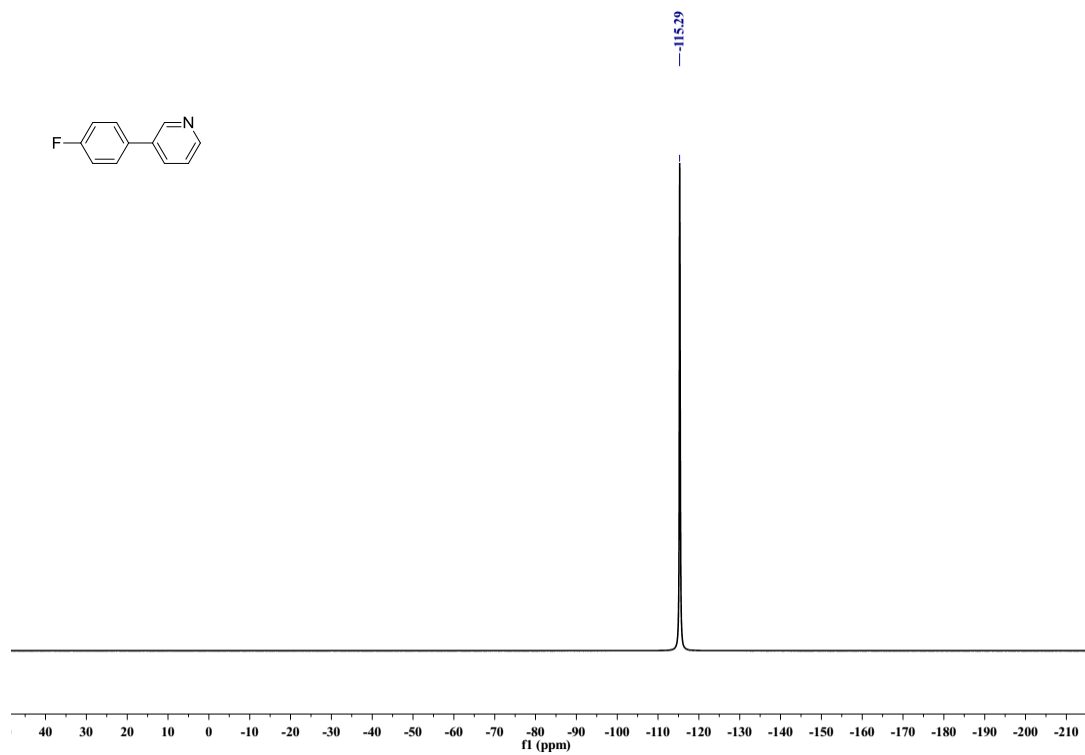


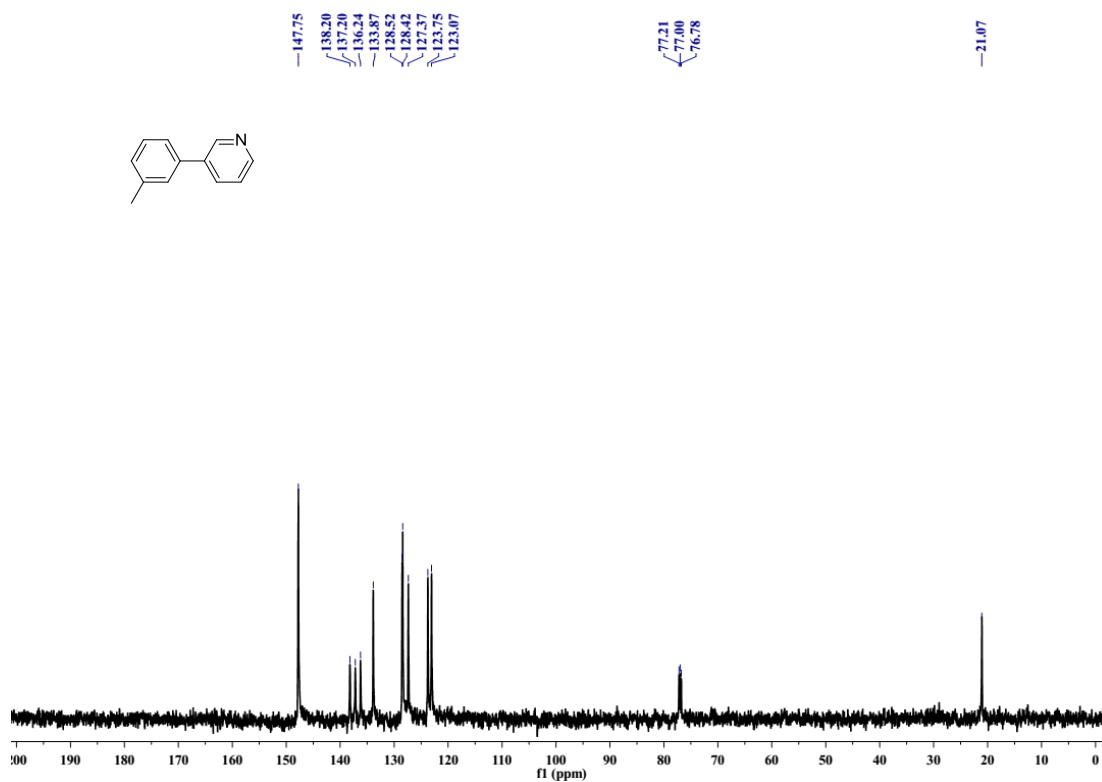
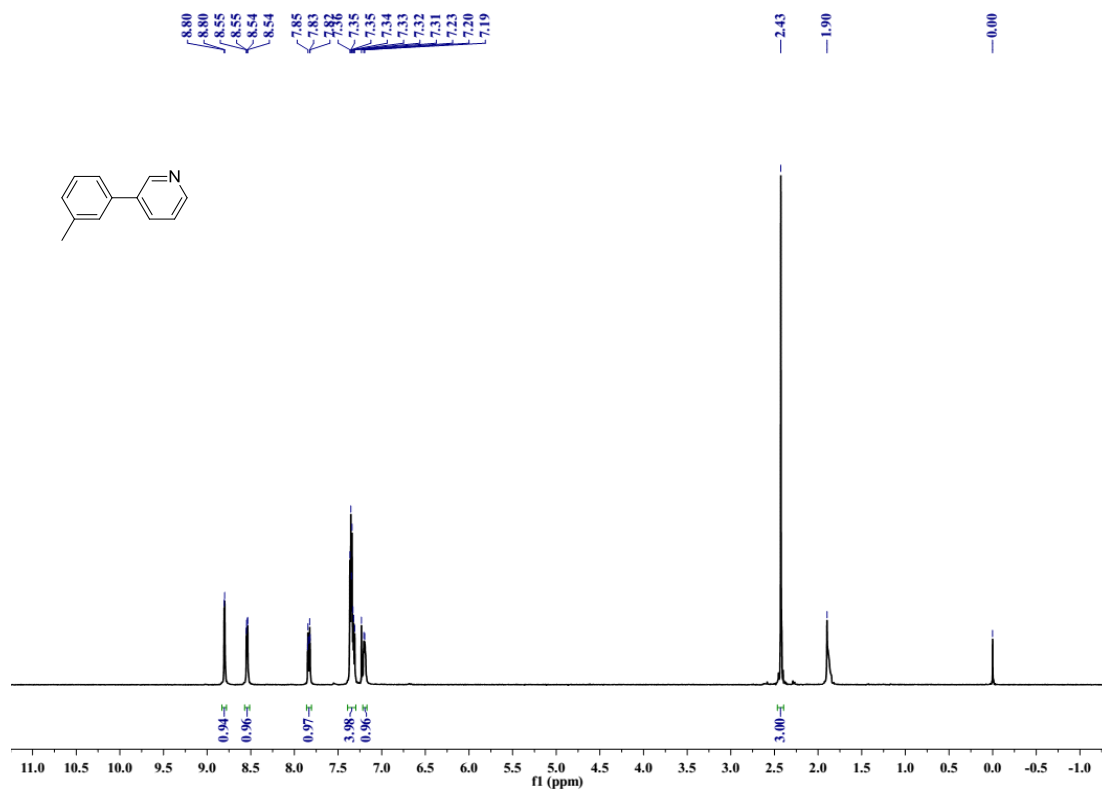


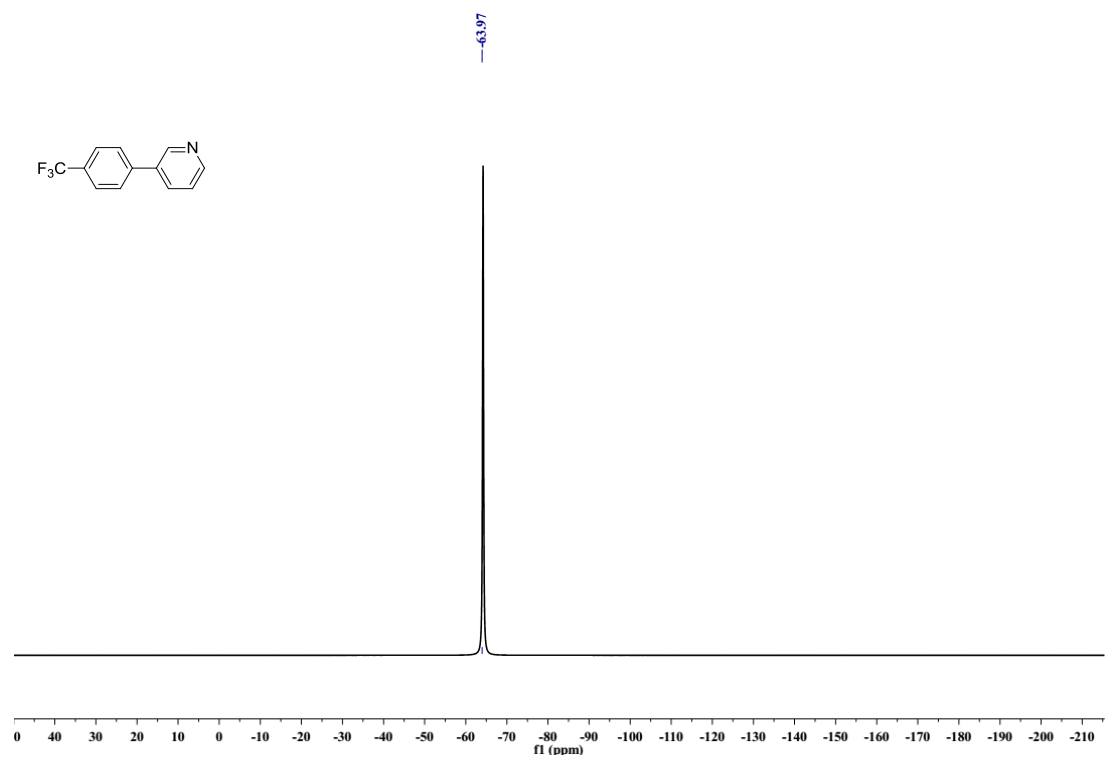
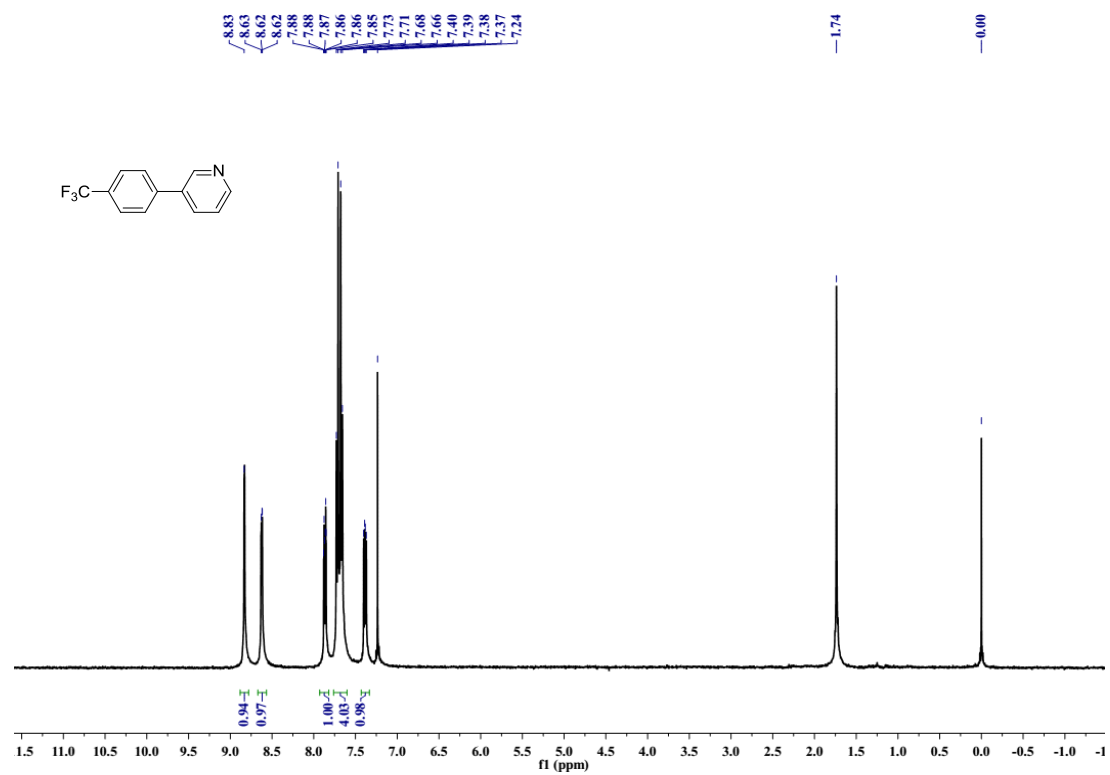


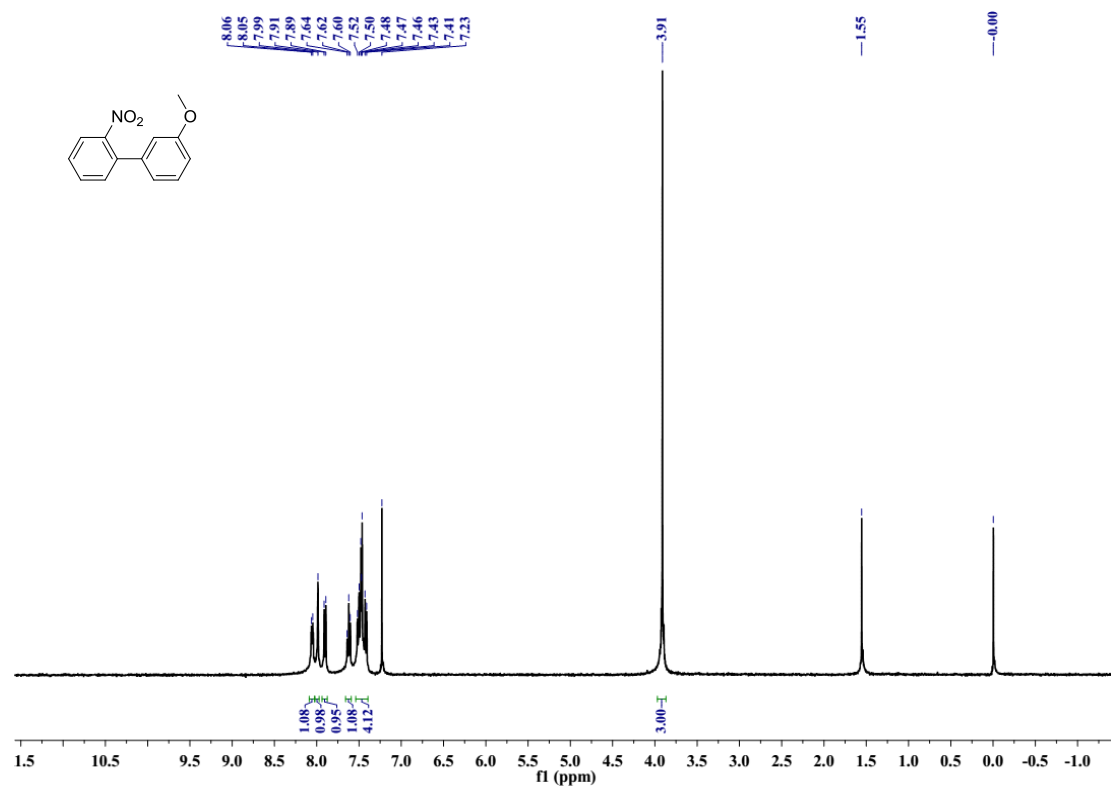
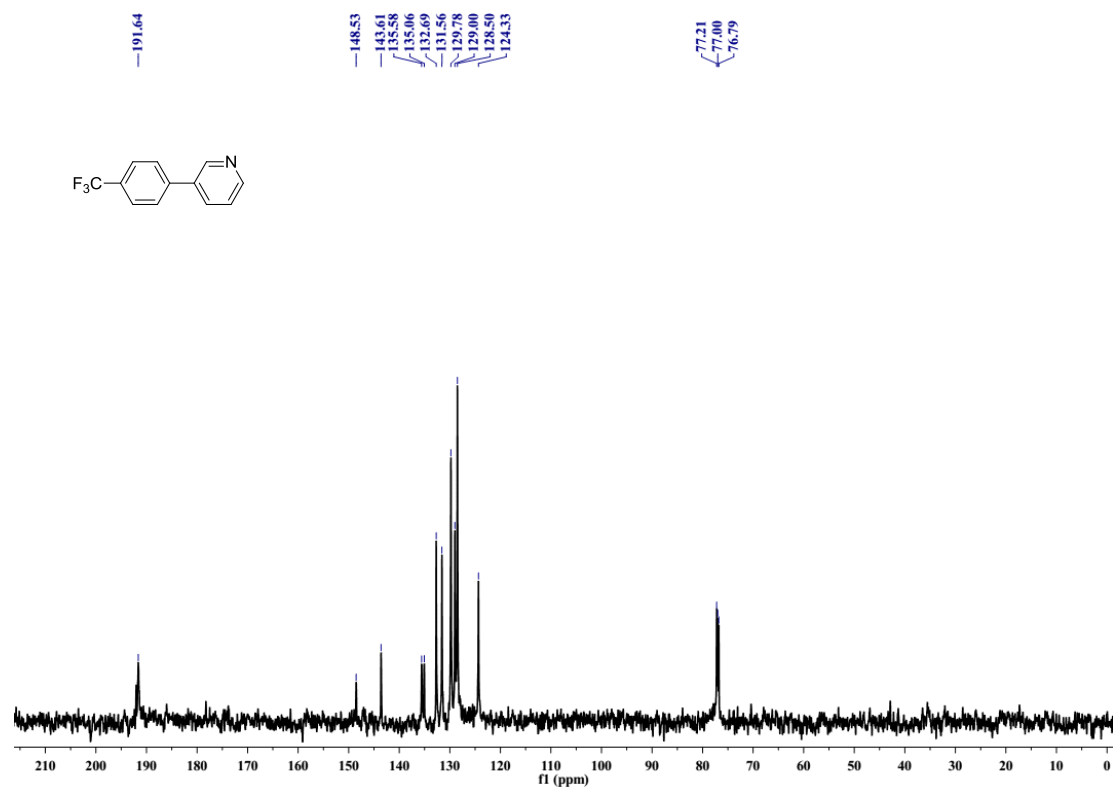


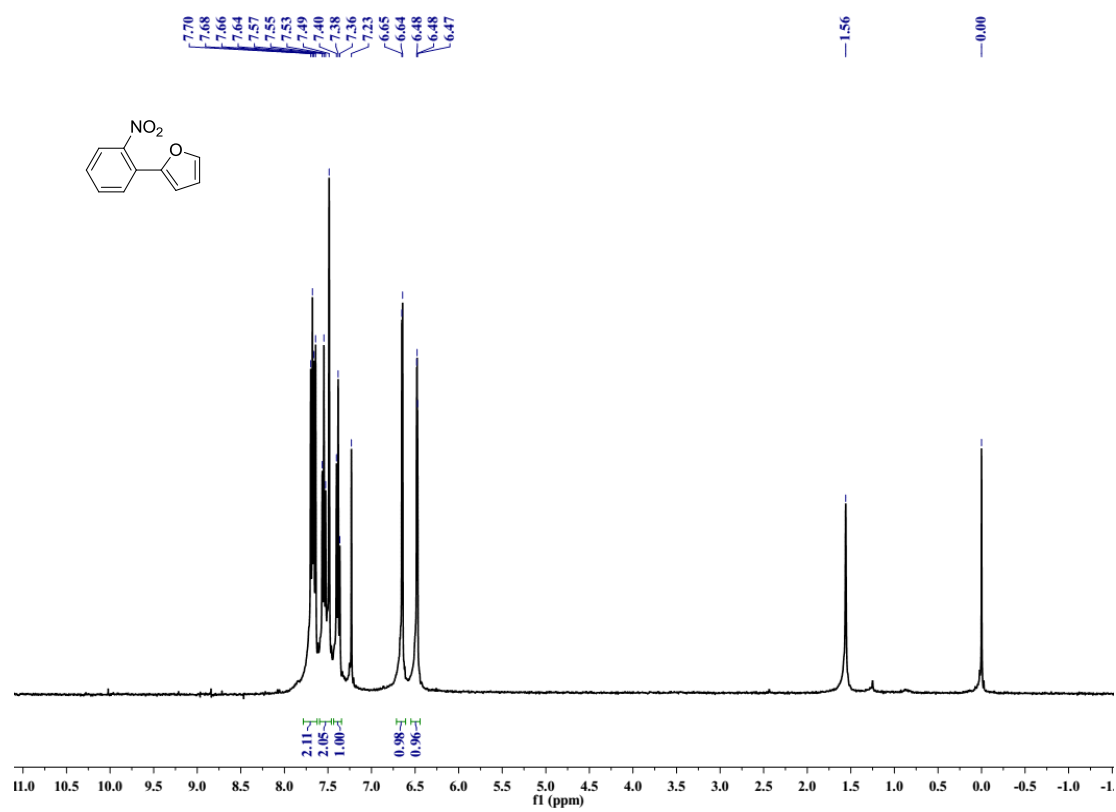
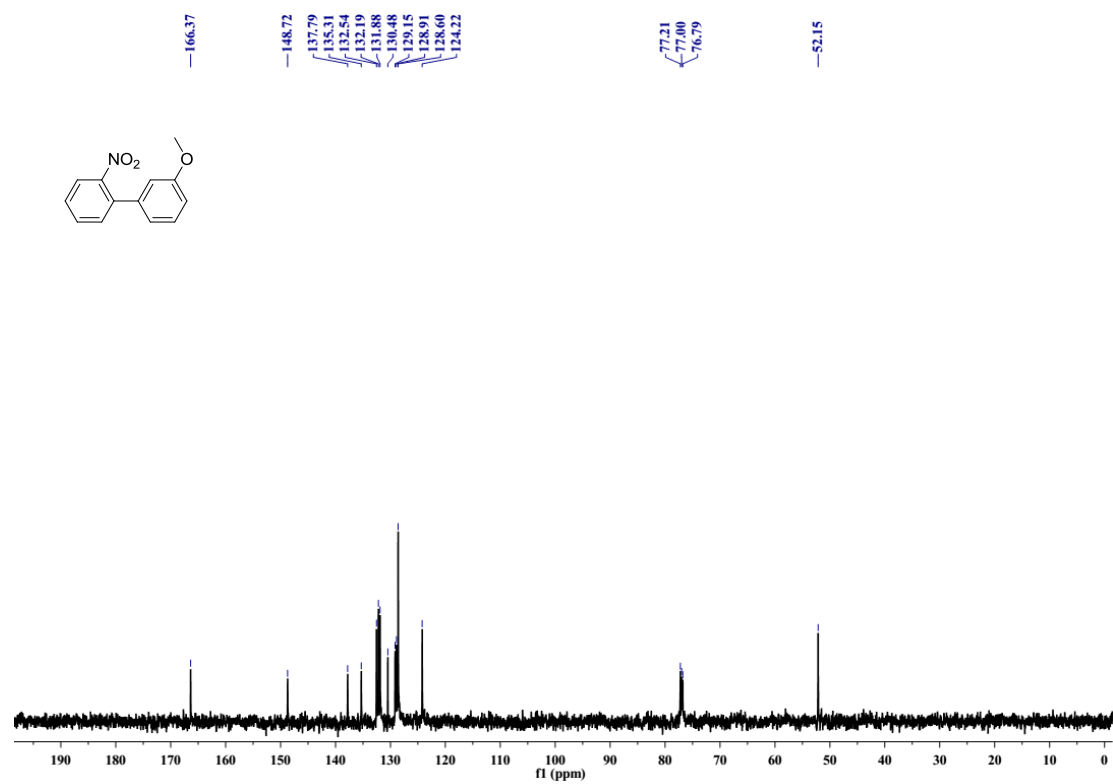


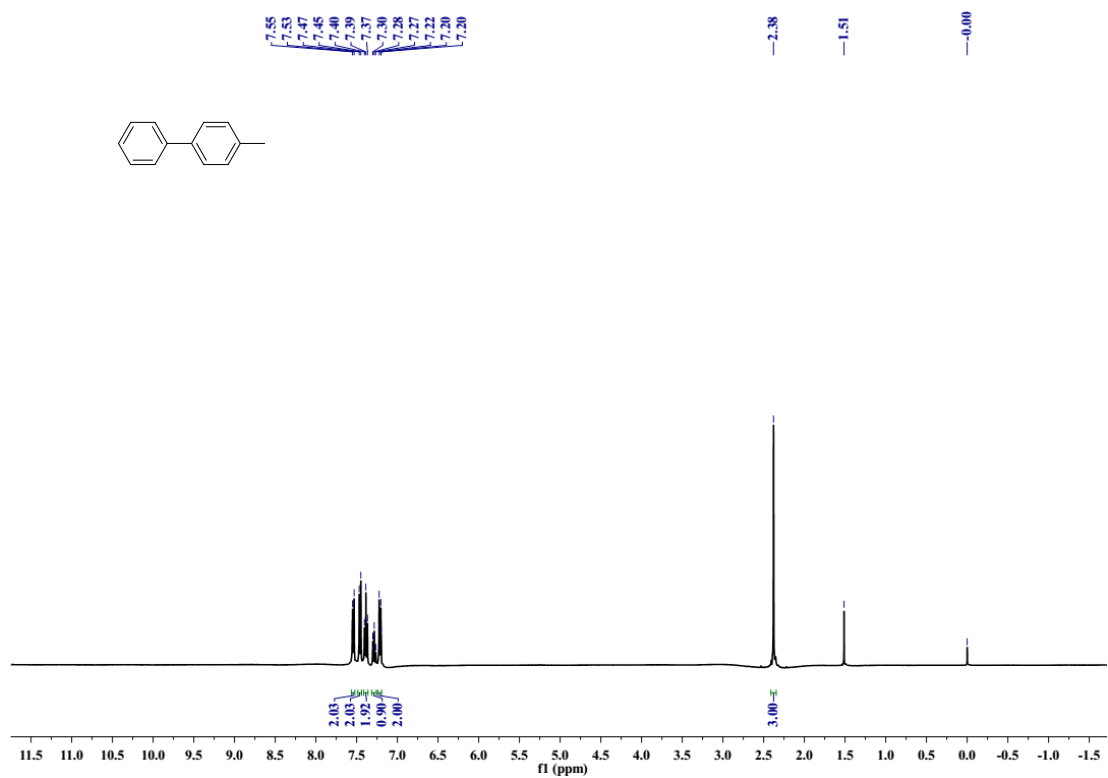
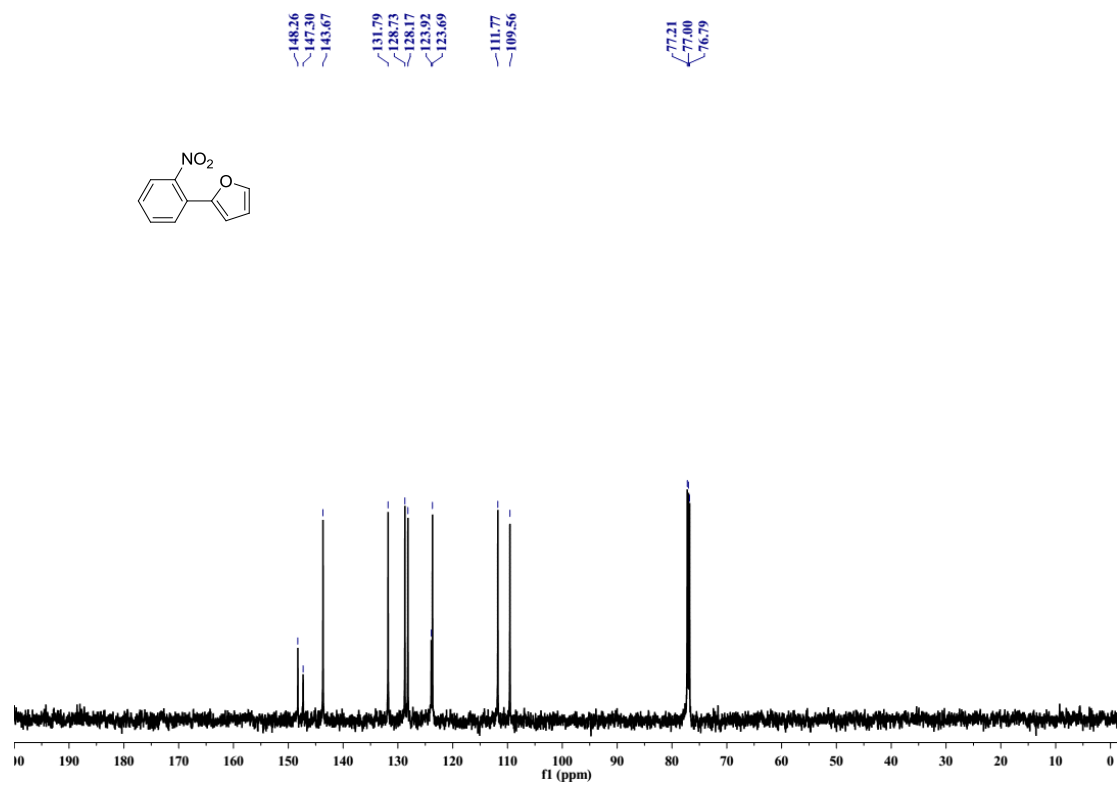


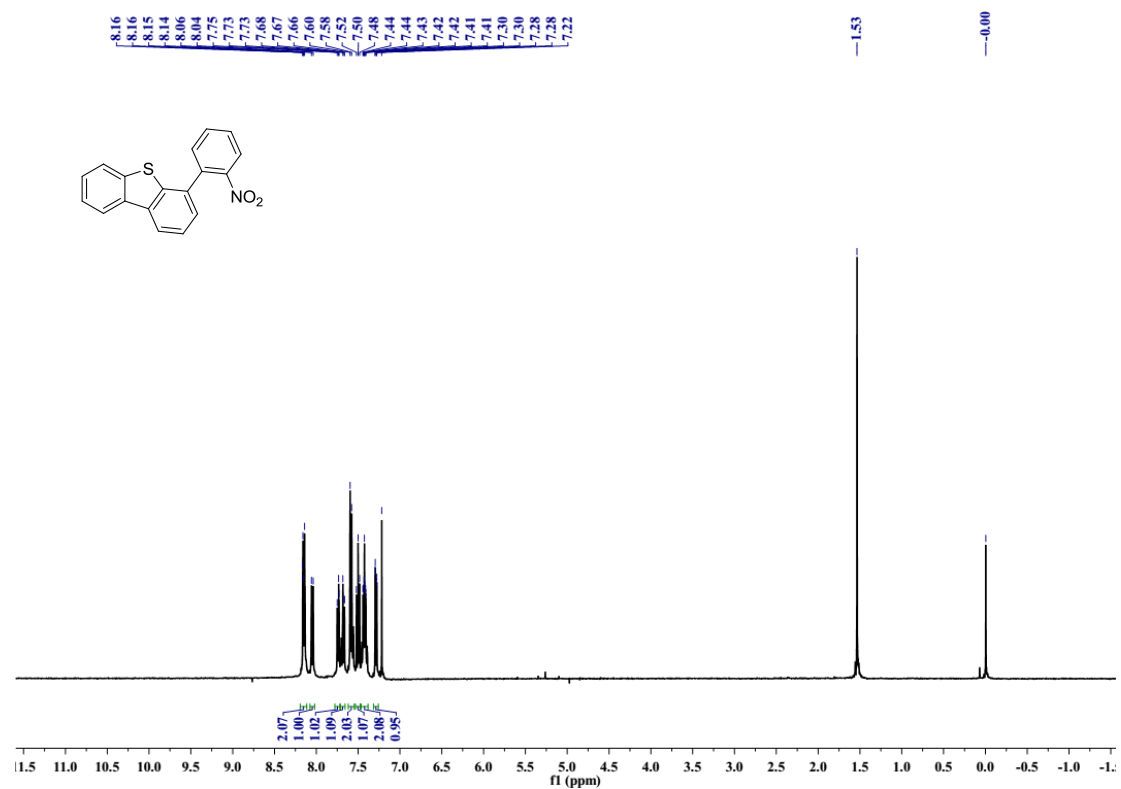
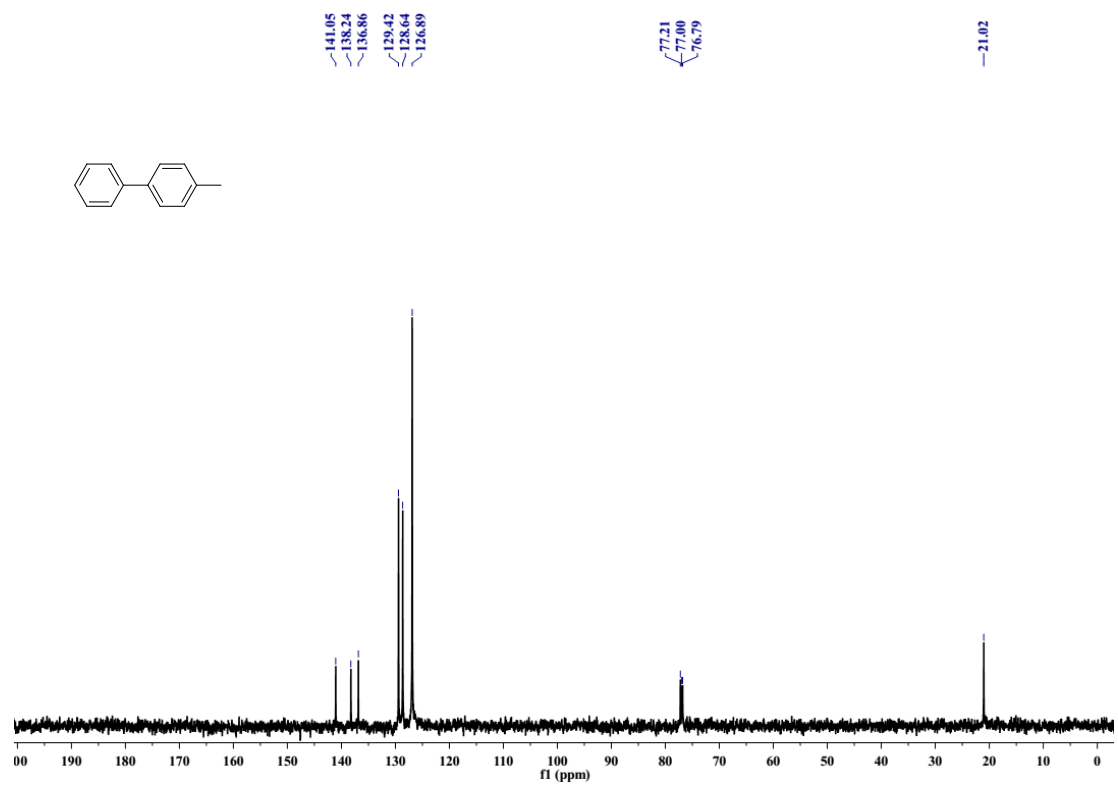


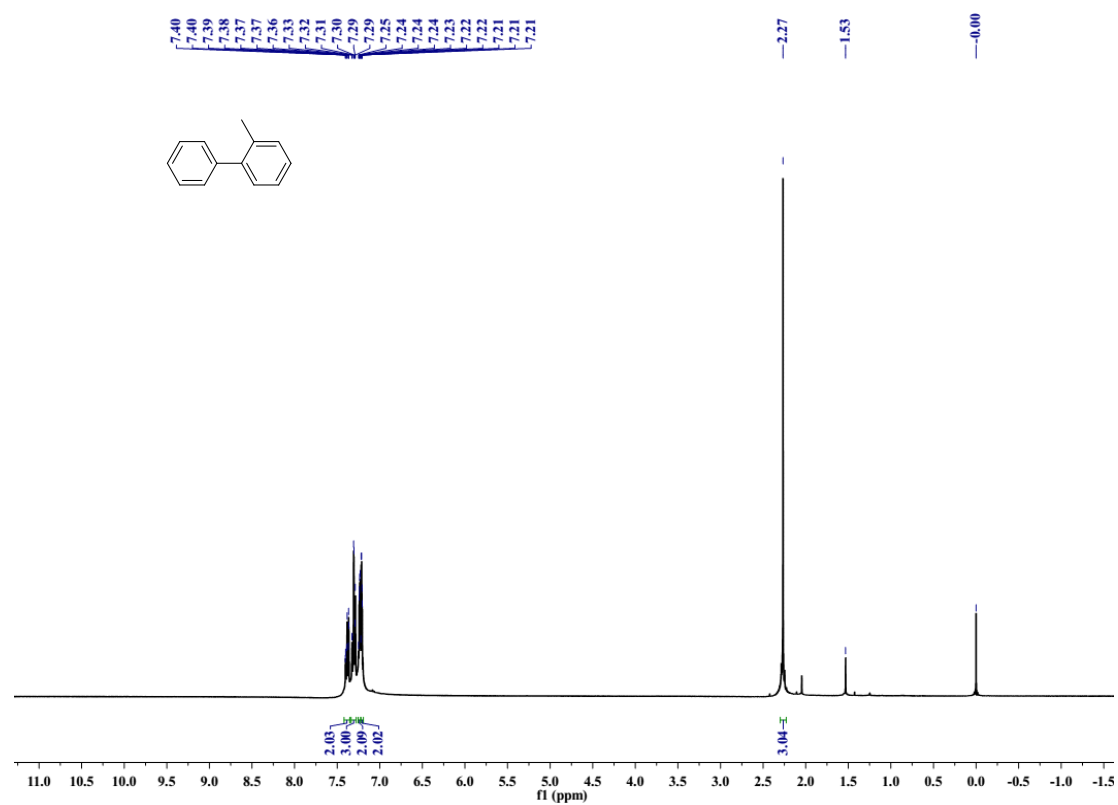
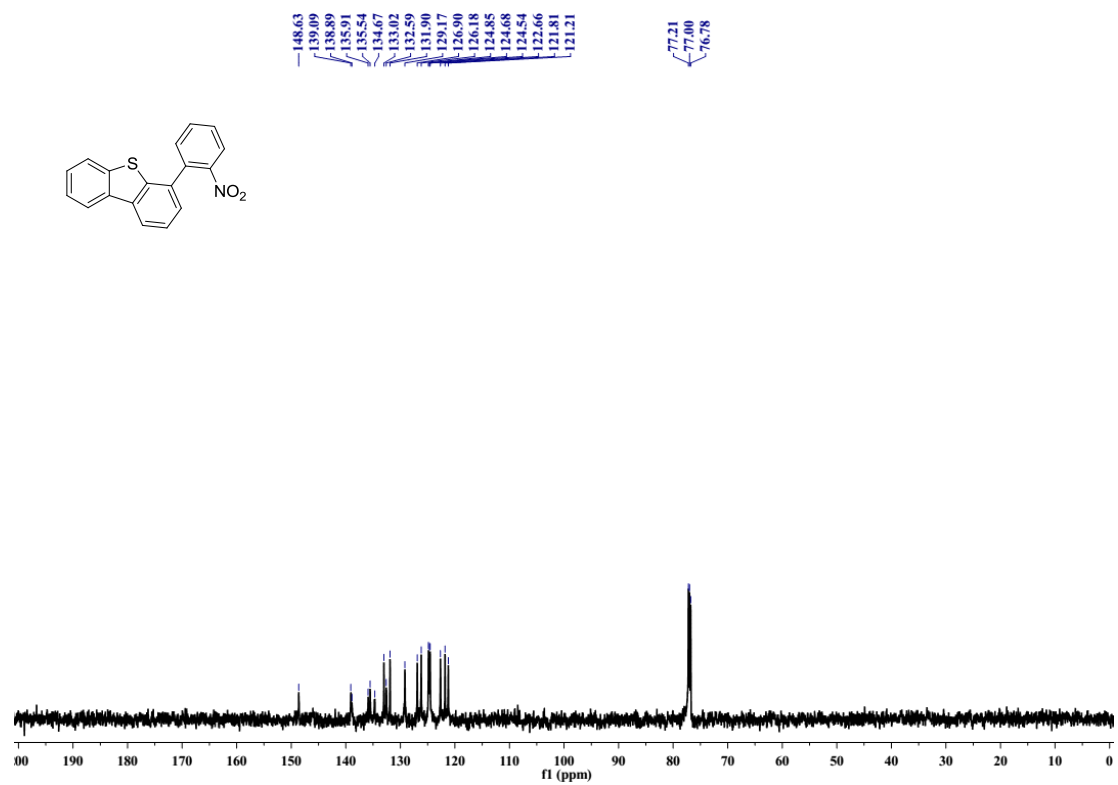


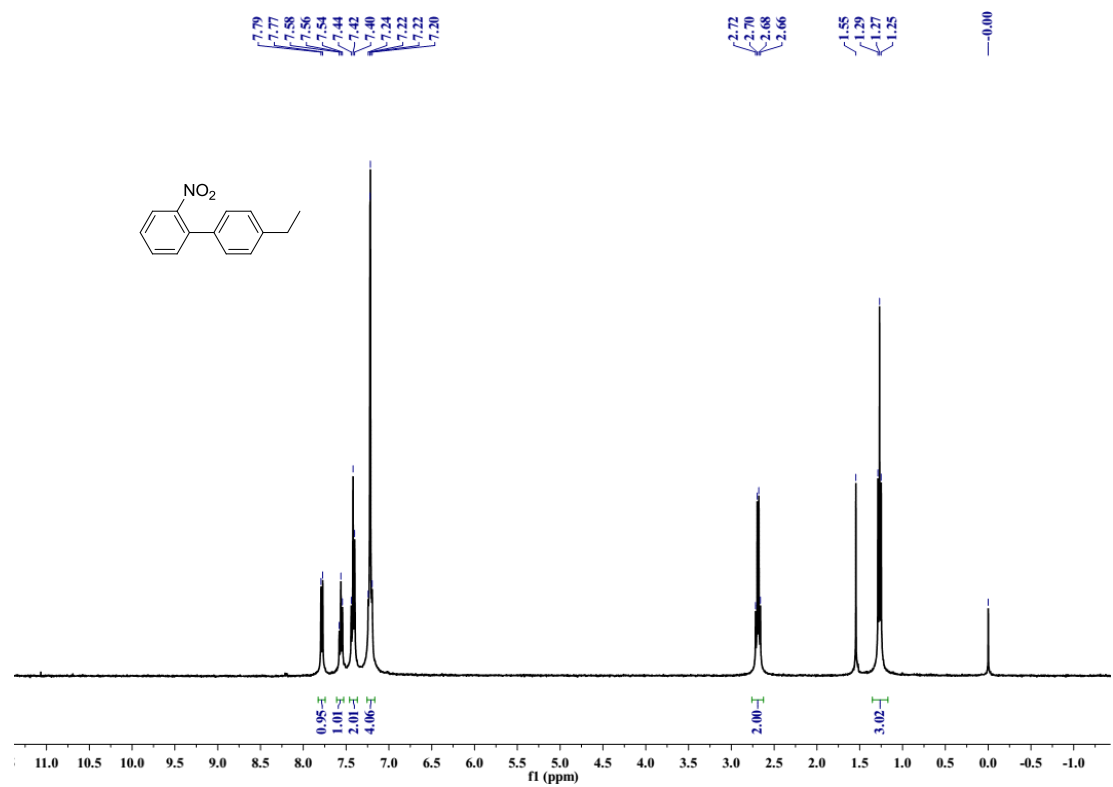
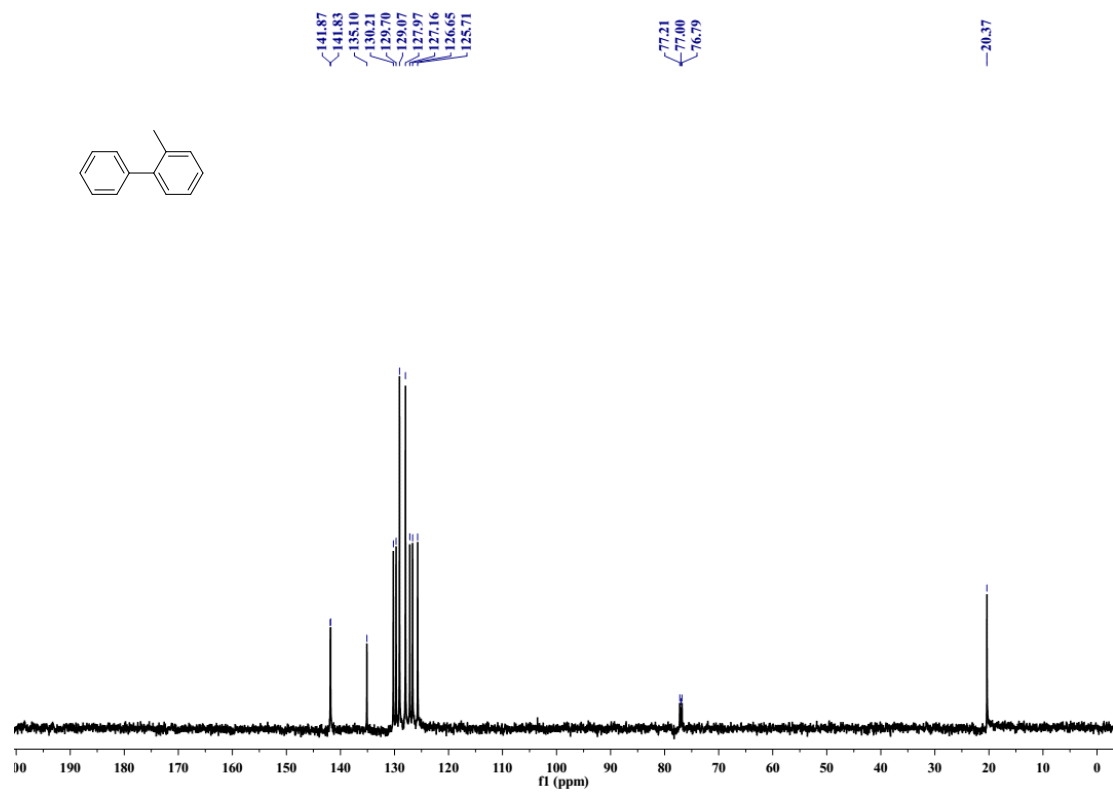


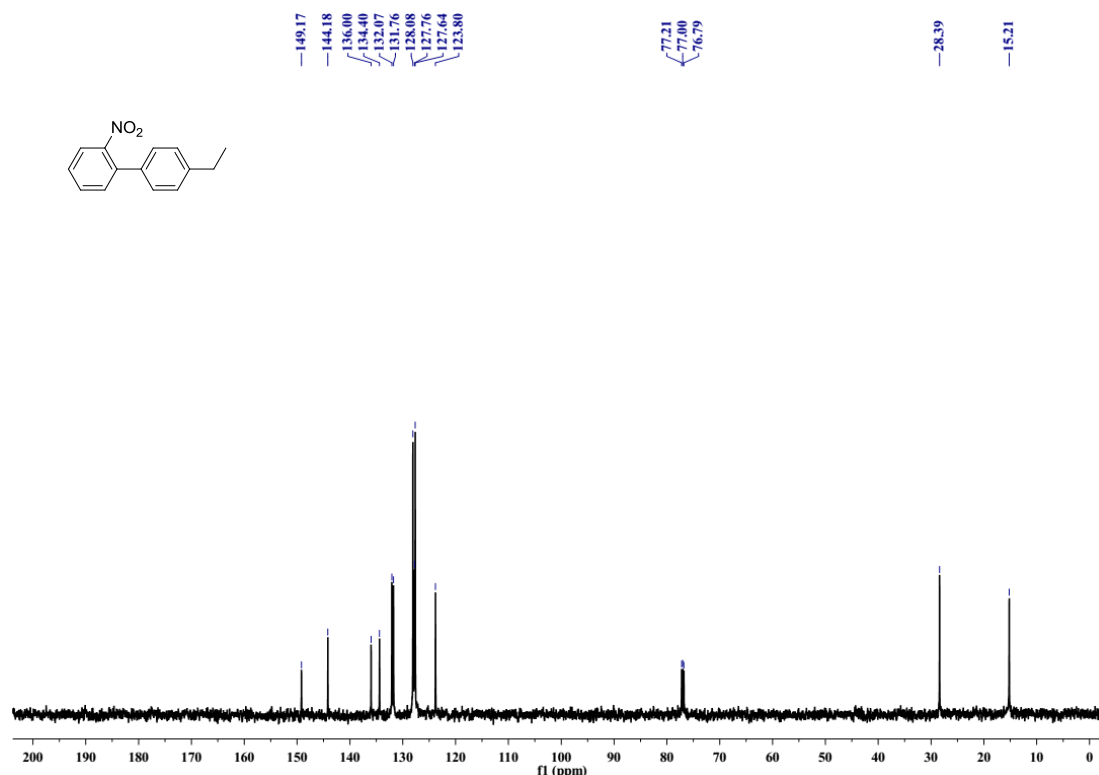












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