

Supporting Information

GENERAL CONSIDERATIONS

Reagents. Unless otherwise indicated, all reactions were carried out in resealable screw-cap test tubes under an argon atmosphere with dry solvents. Dry toluene was obtained by passing through successive alumina and Q5 reactant-packed columns on a solvent purification system. $(\text{AllylPdCl})_2$ was purchased from Strem and used as received. Anhydrous Cs_2CO_3 was purchased from Alfa Aesar and stored in a glovebox. Small portions were removed and stored in a desiccator for up to two weeks (all reactions were set-up outside of the glovebox). Tributylamine was distilled from CaH_2 and stored under argon. Cyclohexanol was distilled from CaH_2 and stored under argon over 3\AA molecular sieves. All other reagents were purchased from commercial sources and used as received. Flash chromatography was performed using Silicycle SiliaFlaP60 (230-400 mesh) silica gel.

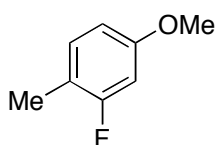
Analytical Methods. All new compounds were characterized by ^1H NMR, ^{13}C NMR, ^{31}P NMR (where applicable), IR spectroscopy and in most cases, elemental analysis. ^1H NMR and ^{13}C NMR spectra, and IR spectroscopy are included for all known compounds. NMR spectra were recorded on a Varian 300 MHz instrument and calibrated using residual solvent as an internal reference (CDCl_3 : 7.26 ppm for ^1H NMR and 77.0 ppm for ^{13}C NMR). IR spectra were recorded on a Perkin-Elmer Model 2000 FT-IR using KBr

plates (thin film). Melting points were obtained on a Mel-Temp capillary melting point apparatus. Gas chromatographic analyses were performed on Agilent 6890 gas chromatography. Elemental analyses were performed by Atlantic Microlab Inc., Norcross, GA. Reactions were monitored by GC and thin-layer chromatography (TLC) carried out on 0.25 mm E. Merck silica gel plates (60F-254) using UV light as a visualizing agent. All yields stated are the average of at least two experiments.

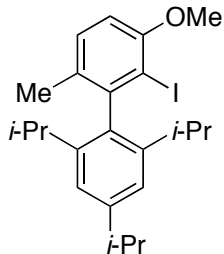
SYNTHESIS OF LIGANDS.

Ligands **L1** and **L5** were purchased from Strem. Ligand **L3** was prepared as previously described by our group.¹

Synthesis of Ligand L4 (RockPhos).



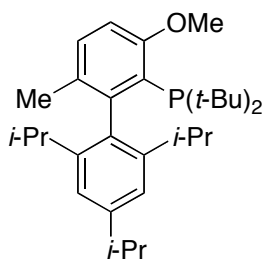
2-Fluoro-4-methoxy-1-methylbenzene: A two-necked 500 mL round bottom flask, which was equipped with a magnetic stir bar and charged with anhydrous K_2CO_3 (22.1 g, 160 mmol), was fitted with a reflux condenser and rubber septum. The flask was purged with argon and then anhydrous acetone (250 mL), 3-fluoro-4-methylphenol (10.1 g, 80 mmol), and Me_2SO_4 (10.6 mL, 112 mmol) were added via syringe. The reaction mixture was stirred at reflux for 3 h and 2 M aqueous KOH (100 mL) was added. The reaction mixture was then heated to 80 °C for 15 min to quench the excess Me_2SO_4 . The mixture was cooled to room temperature and acetone was removed by rotary evaporator. The aqueous layer was extracted with ether (3 × 150 mL) and the combined organic layers were washed with brine (100 mL), dried over $MgSO_4$, and concentrated in vacuo. The crude product was purified with flash chromatography (silica gel, hexanes) to afford 2-fluoro-4-methoxy-1-methylbenzene as a colorless oil (10.3 g, 92% yield): 1H NMR (300 MHz, $CDCl_3$) δ 7.11-7.03 (m, 1H), 6.63-6.57 (m, 2H), 3.78 (s, 3H), 2.22-2.20 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.2, 160.0, 158.9, 158.8, 131.45, 131.36, 116.5, 116.3, 109.4, 109.3, 101.5, 101.1, 55.4, 13.71, 13.66 (observed complexity is due to F-C splitting); ^{19}F NMR (282 MHz, $CDCl_3$) δ -112.0 (t, $J = 9.2$ Hz); IR (neat, cm^{-1}) 2958, 2934, 1627, 1589, 1512, 1268, 1153, 1121, 1035, 944, 834; Anal Calcd. for C_8H_9FO : C, 68.56; H, 6.47. Found: C, 68.25; H, 6.63.



2-Iodo-2',4',6'-triisopropyl-3-methoxy-6-methyl-1,1'-biphenyl: An

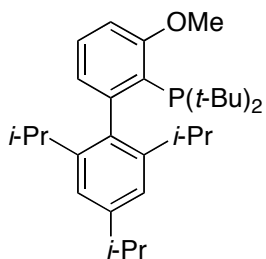
oven-dried three-neck 500 mL round bottom flask, which was equipped with a magnetic stir bar and charged with magnesium shavings (1.75 g, 72 mmol), was fitted with a reflux condenser, glass stopper, and rubber septum. The flask was purged with argon and then THF (120 mL) and 2,4,6-triisopropylbromobenzene (15.04 mL, 60 mmol) were added via syringe. The reaction was heated to reflux and 1,2-dibromomethane (50 μ L) was added via syringe. The reaction mixture was allowed to stir at reflux for 1 h and was then cooled to room temperature. A separate oven-dried 500 mL round bottom flask, which was equipped with a magnetic stir bar and fitted with a septum, was purged with argon and then THF (160 mL) and 2-fluoro-4-methoxy-1-methylbenzene (4.21 g, 30 mmol) were added to the flask via syringe. The reaction vessel was cooled via a -78 $^{\circ}$ C bath and *n*-BuLi (2.5 M in Hexane, 13.2 mL, 33 mmol) was added by a syringe pump over a 1 h period. The solution was stirred for an additional 2 h and the Grignard reagent, which was prepared in the first reaction vessel, was added via cannula over a 30 min period and the reaction mixture was allowed to stir at -78 $^{\circ}$ C for 1 h. The reaction mixture was slowly warmed to room temperature where it was stirred overnight. The mixture was then cooled to 0 $^{\circ}$ C and a solution of iodine (16.75 g, 66 mmol) in THF (66 mL) was added via syringe over a 30 min period and then the dark red solution was warmed to room temperature and stirred for 1 h. Saturated aqueous Na₂SO₃ (200 mL) was added to quench excess iodine. The two layers were separated and the aqueous layer was extracted with ether (2 \times 200 mL). The combined organic layers were washed with brine, dried over MgSO₄, filtered, and the solvent was removed with the aid of a rotary evaporator. The crude material was purified by flash chromatography (silica gel, gradient from pure hexanes to 30:1 hexanes:EtOAc) to yield a white solid (11.05 g, 82% yield): m.p. 147 – 148 $^{\circ}$ C; ¹H NMR (300 MHz, CDCl₃) δ 7.19 (d, 1H, J = 8.3 Hz), 7.06 (s, 2H), 6.74 (d, 1H, J = 8.3 Hz), 3.92 (s, 3H), 2.96 (septet, 1H, J = 6.9 Hz), 2.34 (septet, 2H, J = 6.9 Hz), 1.98 (s, 3H), 1.31 (d, 6H, J = 6.9 Hz), 1.19 (d, 6H, J = 6.9 Hz), 1.05 (d, 6H, J = 6.9 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 156.4, 148.4, 146.6, 145.1, 138.5, 130.6, 130.1, 121.1, 109.0, 94.9, 56.3, 34.1, 30.6, 24.51, 24.48, 24.1, 21.3; IR (neat, cm⁻¹): 2960, 1461, 1434, 1289, 1271, 1077, 876, 799, 755; Anal. Calcd. for C₂₃H₃₁IO: C, 61.33;

H, 6.94. Found: C, 61.43; H, 6.79.



di-tert-Butyl-(2',4',6'-triisopropyl-3-methoxy-6-methyl-[1,1'-biphenyl]-2-yl)phosphine (L4, RockPhos): An oven-dried 200 mL round-bottom Schlenk flask, which was equipped with a magnetic stir bar, fitted with a rubber septum, and charged with 2-iodo-2',4',6'-triisopropyl-3-methoxy-6-methyl-1,1'-biphenyl (4.0 g, 8.96 mmol), was evacuated and backfilled with argon (this process was repeated a total of three times). Toluene (45 mL) was added via syringe, the reaction mixture was cooled to $-78\text{ }^{\circ}\text{C}$, and *t*-BuLi (1.7 M in pentane, 10.5 mL, 17.92 mmol) was added in a dropwise fashion over a 10 min period. The solution was stirred for 30 min and then under a positive pressure of argon the septum was removed from the Schlenk flask and anhydrous CuCl (890 mg, 8.96 mmol), which was weighed out in nitrogen filled glovebox, was added rapidly. The flask was refitted with the rubber septum and $\text{ClP}(t\text{-Bu})_2$ (2.55 mL, 13.44 mmol) was added in a dropwise fashion over a 5 min period. The reaction mixture was warmed from $-78\text{ }^{\circ}\text{C}$ to room temperature at which point the flask was sealed with a Teflon screw cap and heated to $140\text{ }^{\circ}\text{C}$ (bath temperature) for 20 h. The solution was cooled to room temperature, diluted with ethyl acetate, washed with NH_4OH 28% in water (this process was repeated a total of three times), washed with brine, dried over MgSO_4 , and concentrated in vacuo. The crude material was recrystallized from hot methanol to afford 3.02 g (72% yield) of desired product as white crystals: m.p. $129 - 130\text{ }^{\circ}\text{C}$; ^1H NMR (300 MHz, CDCl_3) δ 7.19 (d, 1H, $J = 8.6\text{ Hz}$), 6.98 (s, 2H), 6.79 (d, 1H, $J = 8.6\text{ Hz}$), 3.79 (s, 3H), 2.92 (septet, 1H, $J = 6.9\text{ Hz}$), 2.47 (septet, 2H, $J = 6.7\text{ Hz}$), 1.77 (s, 3H), 1.29 (d, 6H, $J = 6.9\text{ Hz}$), 1.21 (d, 6H, $J = 6.7\text{ Hz}$), 1.16 (s, 9H), 1.12 (s, 9H), 0.96 (d, 6H, $J = 6.7\text{ Hz}$); ^{13}C NMR (75 MHz, CDCl_3) δ 160.01, 159.98, 151.0, 150.5, 147.3, 145.67, 145.65, 136.5, 136.4, 131.88, 131.86, 130.5, 130.4, 125.5, 124.9, 120.7, 108.1, 53.6, 34.2, 33.9, 33.8, 32.0, 31.8, 30.8, 30.7, 25.3, 24.63, 24.60, 24.1, 22.2, 22.1 (observed complexity is due to P-C splitting); ^{31}P NMR (121.5 Hz, CDCl_3) δ 35.84; IR (neat, cm^{-1}): 2960, 2925, 1564, 1459, 1427, 1360, 1263, 1168, 1024, 803; Anal. Calcd. for $\text{C}_{31}\text{H}_{49}\text{OP}$: C, 79.44; H, 10.54. Found: C, 79.44; H, 10.36.

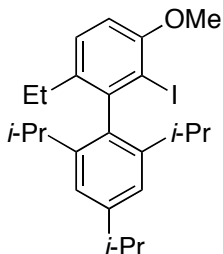
Synthesis of Ligand L6.



di-tert-Butyl-(2',4',6'-triisopropyl-3-methoxy-[1,1'-biphenyl]-2-yl)phosphine (L6):

An oven-dried Schlenk tube, which was equipped with a magnetic stir bar, fitted with a rubber septum, and charged with 2-iodo-2',4',6'-triisopropyl-3-methoxy-1,1'-biphenyl² (1.31 g, 3.0 mmol), was evacuated and backfilled with argon (this process was repeated a total of three times). THF (15 mL) was added via syringe, the reaction mixture was cooled to $-78\text{ }^{\circ}\text{C}$, and *t*-BuLi (1.7 M in pentane, 4.06 mL, 6.9 mmol) was added in a dropwise fashion over a 10 min period. The solution was stirred for 30 min and then under a positive pressure of argon the septum was removed from the Schlenk tube and anhydrous CuCl (357 mg, 3.6 mmol), which was weighed out in nitrogen filled glovebox, was added rapidly. The flask was refitted with the rubber septum and $\text{ClP}(t\text{-Bu})_2$ (0.68 mL, 3.6 mmol) was added in a dropwise fashion over a 5 min period. The reaction mixture was warmed from $-78\text{ }^{\circ}\text{C}$ to room temperature at which point the flask was sealed with a Teflon screw cap and heated to $70\text{ }^{\circ}\text{C}$ (bath temperature) for 7 days. The solution was cooled to room temperature, diluted with ethyl acetate, washed with NH_4OH 28% in water (this process was repeated a total of three times), washed with brine, dried over MgSO_4 , and concentrated in vacuo. The crude material was recrystallized from hot methanol to afford 1.02 mg (75% yield) of desired product as white crystals: m.p. $168 - 170\text{ }^{\circ}\text{C}$; ^1H NMR (300 MHz, CDCl_3) δ 7.29 (dd, 1H, $J = 8.2, 7.6\text{ Hz}$), 6.97 (s, 2H), 6.87 (d, 1H, $J = 8.2\text{ Hz}$), 6.83 (dd, 1H, $J = 7.6, 3.7\text{ Hz}$), 3.83 (s, 3H), 2.93 (septet, 1H, $J = 6.9\text{ Hz}$), 2.59 (septet, 2H, $J = 6.7\text{ Hz}$), 1.31 (d, 6H, $J = 6.9\text{ Hz}$), 1.21 (d, 6H, $J = 6.8\text{ Hz}$), 1.16 (s, 9H), 1.12 (s, 9H), 0.96 (d, 6H, $J = 6.7\text{ Hz}$); ^{13}C NMR (75 MHz, CDCl_3) δ 161.71, 161.67, 151.4, 150.9, 147.2, 145.92, 145.90, 137.65, 137.57, 128.77, 128.75, 125.8, 125.7, 125.3, 124.7, 120.1, 108.4, 53.8, 33.94, 33.93, 33.6, 31.6, 31.4, 30.8, 30.7, 26.4, 24.1, 22.69, 22.68 (observed complexity is due to P-C splitting); ^{31}P NMR (121.5 Hz, CDCl_3) δ 34.10; IR (neat, cm^{-1}): 2957, 2924, 2885, 2862, 1560, 1458, 1430, 1360, 1264, 1248, 1169, 1090, 1020, 793, 740; Anal. Calcd. for $\text{C}_{30}\text{H}_{47}\text{OP}$: C, 79.25; H, 10.42. Found: C, 79.39; H, 10.21.

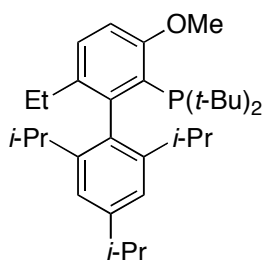
Synthesis of Ligand L7.



2-Iodo-2',4',6'-triisopropyl-3-methoxy-6-ethyl-1,1'-biphenyl: An oven-dried 500 mL round bottom flask, which was equipped with a magnetic stir bar and charged with Pd(OAc)₂ (336.8 mg, 1.5 mmol) and DavePhos (1.18 g, 3.0 mmol), was evacuated and backfilled with argon (this process was repeated a total of three times). THF (100 mL) and 1-bromo-2-fluoro-4-methoxybenzene (10.26 g, 50 mmol) were added via syringe. A solution of EtMgCl (2 M in THF, 37.5 mL, 75 mmol) was added by syringe pump over 1 h at room temperature. The reaction solution was stirred at 40 °C for 5 h and allowed to cool to room temperature. Saturated aqueous NH₄Cl (80 mL) was added and THF was removed by rotary evaporator. The aqueous layer was extracted with ether (3 × 100 mL) and the combined organic layers were washed with brine (100 mL), dried over MgSO₄, and concentrated in vacuo. Flash chromatography (silica gel, hexanes) afforded 4.46 g (58%, ~85% pure) of 2-fluoro-4-methoxy-1-ethylbenzene contaminated with 1-fluoro-3-methoxybenzene.

An oven-dried three-neck 500 mL round bottom flask, which was equipped with a magnetic stir bar and charged with magnesium shavings (1.28 g, 52.8 mmol), was fitted with a reflux condenser, glass stopper, and rubber septum. The flask was purged with argon and then THF (90 mL) and 2,4,6-triisopropylbromobenzene (11.15 mL, 44 mmol) were added via syringe. The reaction was heated to reflux and 1,2-dibromomethane (40 μL) was added via syringe. The reaction mixture was allowed to stir at reflux for 1 h and was then cooled to room temperature. A separate oven-dried 500 mL round bottom flask, which was equipped with a magnetic stir bar and fitted with a septum, was purged with argon and then THF (120 mL) and 2-fluoro-4-methoxy-1-ethylbenzene (3.4 g, 22 mmol) were added to the flask via syringe. The reaction vessel was cooled via a -78 °C bath and *n*-BuLi (2.5 M in Hexane, 9.3 mL, 23.1 mmol) was added by a syringe pump over a 1 h period. The solution was stirred for an additional 4 h and the Grignard reagent, which was prepared in the first reaction vessel, was added via cannula over a 30 min period and the reaction mixture was allowed to stir at -78 °C for 1 h. The reaction mixture was slowly warmed to room temperature where it was stirred overnight. The mixture was then cooled to 0 °C and a solution of iodine (12.29 g, 48.4 mmol) in THF (48 mL) was added via syringe over a 30 min period and then the dark red solution was warmed to room

temperature and stirred for 1 h. Saturated aqueous Na₂SO₃ (100 mL) was added to quench excess iodine and THF was removed by rotary evaporator. The aqueous layer was extracted with ether (3 × 150 mL) and the combined organic layers were washed with brine, dried over MgSO₄, and concentrated in vacuo. Flash chromatography (silica gel, gradient from pure hexanes to 30:1 hexanes:EtOAc) afforded a light yellow solid. The yellow solid was recrystallized from hot methanol (25 mL) to yield 6.35 g (62% yield) of desired product as white solid: m.p. 125 – 126 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.29 (d, 1H, J = 8.5 Hz), 7.05 (s, 2H), 6.83 (d, 1H, J = 8.5 Hz), 3.92 (s, 3H), 2.96 (septet, 1H, J = 6.9 Hz), 2.33 (septet, 2H, J = 6.9 Hz), 2.27 (q, 2H, J = 7.6 Hz), 1.31 (d, 6H, J = 6.9 Hz), 1.19 (d, 6H, J = 6.9 Hz), 1.14 (t, 3H, J = 7.6 Hz), 1.03 (d, 6H, J = 6.9 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 156.2, 148.3, 146.2, 145.3, 138.3, 136.2, 127.3, 121.0, 109.2, 95.0, 56.3, 34.1, 30.5, 26.1, 24.53, 24.51, 24.1, 13.8; IR (neat, cm⁻¹): 2961, 2931, 2869, 1555, 1461, 1433, 1287, 1269, 1054, 1018, 877, 809, 742; Anal. Calcd. for C₂₄H₃₃IO: C, 62.07; H, 7.16. Found: C, 61.92; H, 7.17.

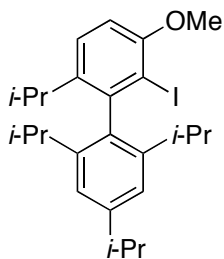


di-*tert*-Butyl-(2',4',6'-triisopropyl-3-methoxy-6-ethyl-[1,1'-biphenyl]-2-yl)phosphine (L7): An oven-dried Schlenk tube,

which was equipped with a magnetic stir bar, fitted with a rubber septum, and charged with 2-iodo-2',4',6'-triisopropyl-3-methoxy-6-ethyl-1,1'-biphenyl (1.39 g, 3.0 mmol), was evacuated and backfilled with argon (this process was repeated a total of three times). THF (13 mL) was added via syringe, the reaction mixture was cooled to –78 °C, and *t*-BuLi (1.7 M in pentane, 3.9 mL, 6.6 mmol) was added in a dropwise fashion over a 10 min period. The solution was stirred for 30 min and then under a positive pressure of argon the septum was removed from the Schlenk flask and anhydrous CuCl (356 mg, 3.6 mmol), which was weighed out in nitrogen filled glovebox, was added rapidly. The flask was refitted with the rubber septum and ClP(*t*-Bu)₂ (0.74 mL, 3.9 mmol) was added in a dropwise fashion over a 5 min period. The reaction mixture was warmed from –78 °C to room temperature at which point the flask was sealed with a Teflon screw cap and heated to 70 °C (bath temperature) for 7 d. The solution was cooled to room temperature, diluted with ethyl acetate, washed with NH₄OH 28% in water (this process was repeated a total of three times), washed with brine, dried over MgSO₄, and concentrated in vacuo. The

crude material was recrystallized from hot methanol to afford 862.1 mg (60% yield) of desired product as white crystals: m.p. 92 – 94 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.29 (d, 1H, J = 8.5 Hz), 6.97 (s, 2H), 6.85 (d, 1H, J = 8.5 Hz), 3.80 (s, 3H), 2.92 (septet, 1H, J = 6.9 Hz), 2.42 (septet, 2H, J = 6.7 Hz), 2.07 (q, 2H, J = 7.5 Hz), 1.29 (d, 6H, J = 6.9 Hz), 1.22 (d, 6H, J = 6.7 Hz), 1.14 (s, 9H), 1.10 (s, 9H), 1.09 (t, 3H, J = 7.5 Hz), 0.95 (d, 6H, J = 6.7 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 159.92, 159.89, 150.7, 150.2, 147.2, 145.93, 145.91, 136.1, 136.0, 135.8, 135.7, 128.55, 128.53, 125.5, 124.9, 120.7, 108.1, 53.5, 34.1, 33.9, 33.7, 32.0, 31.8, 30.52, 30.49, 25.59, 25.55, 24.80, 24.77, 24.1, 13.8 (observed complexity is due to P-C splitting); ³¹P NMR (121.5 Hz, CDCl₃) δ 35.67; IR (neat, cm⁻¹): 2959, 2867, 1562, 1457, 1427, 1382, 1361, 1264, 1020, 877, 811; Anal. Calcd. for C₃₂H₅₁OP: C, 79.62; H, 10.65. Found: C, 79.44; H, 10.53.

Synthesis of Ligand L8.

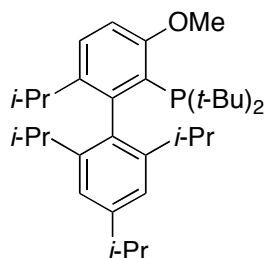


2-Iodo-2',4',6'-triisopropyl-3-methoxy-6-isopropyl-1,1'-biphenyl:

An oven-dried 200 mL round bottom flask, which was equipped with a magnetic stir bar and charged with Pd(OAc)₂ (33.7 mg, 0.15 mmol) and CPhos (131.0 mg, 0.3 mmol),³ was evacuated and backfilled with argon (this process was repeated a total of three times). THF (20 mL) and 1-bromo-2-fluoro-4-methoxybenzene (3.08 g, 15 mmol) were added via syringe. The solution was cooled to 0 °C and a solution of ⁱPrZnBr (1.1 M in THF, 16.4 mL, 18 mmol) was added over 20 min by syringe pump. The ice bath was removed and the reaction solution was stirred at room temperature for 30 min. Brine (20 mL) was added and THF was removed by rotary evaporator. The aqueous layer was extracted with ethyl acetate (3 × 30 mL) and the combined organic layers were washed with brine (30 mL), dried over MgSO₄, and concentrated in vacuo. Flash chromatography (silica gel, 50:1 Hexanes/EtOAc) afforded a 7:1 mixture of 2-fluoro-1-isopropyl-4-methoxybenzene and 2-fluoro-4-methoxy-1-propylbenzene (2.28 g, 90%).

An oven-dried three-neck 300 mL round bottom flask, which was equipped with a magnetic stir bar and charged with magnesium shavings (0.73 g, 30.0 mmol), was fitted with a reflux condenser, glass stopper, and rubber septum. The flask was purged with argon and then THF (50 mL) and 2,4,6-triisopropylbromobenzene (6.33 mL, 25 mmol)

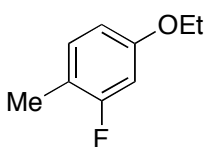
were added via syringe. The reaction was heated to reflux and 1,2-dibromethane (25 μ L) was added via syringe. The reaction mixture was allowed to stir at reflux for 1 h and was then cooled to room temperature. A separate oven-dried 300 mL round bottom flask, which was equipped with a magnetic stir bar and fitted with a septum, was purged with argon and then THF (60 mL) and 2-fluoro-1-isopropyl-4-methoxybenzene (2.1 g, 12.5 mmol) were added to the flask via syringe. The reaction vessel was cooled via a -78 $^{\circ}$ C bath and *n*-BuLi (2.5 M in Hexane, 5.5 mL, 13.75 mmol) was added by a syringe pump over a 1 h period. The solution was stirred for an additional 4 h and the Grignard reagent, which was prepared in the first reaction vessel, was added via cannula over a 30 min period and the reaction mixture was allowed to stir at -78 $^{\circ}$ C for 1 h. The reaction mixture was slowly warmed to room temperature where it was stirred overnight. The mixture was then cooled to 0 $^{\circ}$ C and a solution of iodine (6.98 g, 27.5 mmol) in THF (28 mL) was added via syringe over a 30 min period and then the dark red solution was warmed to room temperature and stirred for 1 h. Saturated aqueous Na₂SO₃ (100 mL) was added to quench excess iodine and THF was removed by rotary evaporator. The aqueous layer was extracted with ether (3 \times 150 mL) and the combined organic layers were washed with brine, dried over MgSO₄, and concentrated in vacuo. Flash chromatography (silica gel, gradient from pure hexanes to 50:1 hexanes:EtOAc) afforded a light yellow solid. The yellow solid was recrystallized from hot methanol (4 mL) to yield 3.19 g (53% yield) of desired product as white solid: m.p. 143 – 145 $^{\circ}$ C; ¹H NMR (300 MHz, CDCl₃) δ 7.32 (d, 1H, J = 8.6 Hz), 7.05 (s, 2H), 6.87 (d, 1H, J = 8.6 Hz), 3.91 (s, 3H), 2.96 (septet, 1H, J = 6.9 Hz), 2.63 (septet, 1H, J = 6.9 Hz), 2.36 (septet, 2H, J = 6.9 Hz), 1.31 (d, 6H, J = 6.9 Hz), 1.21 (d, 6H, J = 6.9 Hz), 1.11 (d, 6H, J = 6.9 Hz), 1.09 (d, 6H, J = 6.9 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 156.1, 148.3, 145.8, 145.0, 141.7, 138.3, 126.2, 121.1, 109.2, 95.0, 56.4, 34.0, 30.6, 30.4, 25.0, 24.91, 24.87, 24.1; IR (neat, cm⁻¹): 2963, 2930, 2868, 1589, 1555, 1463, 1435, 1381, 1361, 1283, 1270, 1070, 1015, 878, 808, 732; Anal. Calcd. for C₂₅H₃₅IO: C, 62.76; H, 7.37. Found: C, 62.99; H, 7.41.



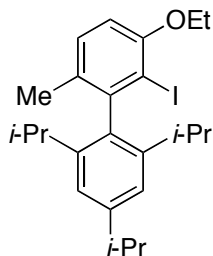
di-*tert*-Butyl-(2',4',6'-triisopropyl-3-methoxy-6-isopropyl-[1,1'-biphenyl]-2-yl)phosphine (L8):

An oven-dried Schlenk tube, which was equipped with a magnetic stir bar, fitted with a rubber septum, and charged with 2-iodo-2',4',6'-triisopropyl-3-methoxy-6-isopropyl-1,1'-biphenyl (478.4 mg, 1.0 mmol), was evacuated and backfilled with argon (this process was repeated a total of three times). THF (5 mL) was added via syringe, the reaction mixture was cooled to $-78\text{ }^{\circ}\text{C}$, and *t*-BuLi (1.7 M in pentane, 1.3 mL, 2.2 mmol) was added in a dropwise fashion over a 5 min period. The solution was stirred for 30 min and then under a positive pressure of argon the septum was removed from the Schlenk flask and anhydrous CuCl (109 mg, 1.1 mmol), which was weighed out in nitrogen filled glovebox, was added rapidly. The flask was refitted with the rubber septum and $\text{CIP}(t\text{-Bu})_2$ (0.25 mL, 1.3 mmol) was added in a dropwise fashion over a 5 min period. The reaction mixture was warmed from $-78\text{ }^{\circ}\text{C}$ to room temperature at which point the flask was sealed with a Teflon screw cap and heated to $70\text{ }^{\circ}\text{C}$ (bath temperature) for 7 d. The solution was cooled to room temperature, diluted with ethyl acetate, washed with NH_4OH 28% in water (this process was repeated a total of three times), washed with brine, dried over MgSO_4 , and concentrated in vacuo. The crude material was recrystallized from hot methanol to afford 264.5 mg (53% yield) of desired product as white crystals: m.p. $100 - 101\text{ }^{\circ}\text{C}$; ^1H NMR (300 MHz, CDCl_3) δ 7.31 (d, 1H, $J = 8.6\text{ Hz}$), 6.93 (s, 2H), 6.85 (d, 1H, $J = 8.6\text{ Hz}$), 3.76 (s, 3H), 2.90 (septet, 1H, $J = 6.9\text{ Hz}$), 2.60 (septet, 1H, $J = 6.7\text{ Hz}$), 2.42 (septet, 2H, $J = 6.7\text{ Hz}$), 1.27 (d, 6H, $J = 6.9\text{ Hz}$), 1.25 (d, 6H, $J = 6.7\text{ Hz}$), 1.12 (d, 6H, $J = 6.7\text{ Hz}$), 1.04 (s, 9H), 1.02 (d, 6H, $J = 6.7\text{ Hz}$), 1.00 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ 160.15, 160.12, 149.0, 148.5, 147.2, 147.08, 147.07, 141.7, 141.6, 134.7, 134.6, 127.03, 127.00, 126.1, 125.4, 120.3, 108.5, 53.5, 34.0, 33.8, 33.4, 31.8, 31.6, 30.20, 30.17, 29.15, 29.13, 27.0, 26.1, 24.8, 24.7, 24.1 (observed complexity is due to P-C splitting); ^{31}P NMR (121.5 Hz, CDCl_3) δ 37.47; IR (neat, cm^{-1}): 2961, 2874, 1578, 1561, 1459, 1426, 1384, 1362, 1310, 1264, 1164, 1054, 1020, 876, 807; Anal. Calcd. for $\text{C}_{33}\text{H}_{53}\text{OP}$: C, 79.79; H, 10.75. Found: C, 79.49; H, 10.78.

Synthesis of Ligand L9.

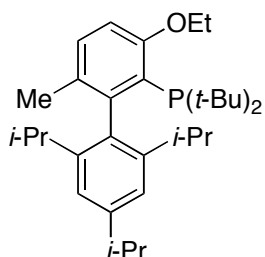


2-Fluoro-4-ethoxy-1-methylbenzene: An oven-dried 100 mL round bottom flask, which was equipped with a magnetic stir bar and charged with anhydrous K_2CO_3 (5.53 g, 40 mmol), was evacuated and backfilled with argon (this process was repeated a total of three times). Anhydrous DMF (20 mL), 3-fluoro-4-methylphenol (2.16 mL, 20 mmol), and EtI (4.8 mL, 60 mmol) were added via syringe. The reaction mixture was stirred at 80 °C overnight and was allowed to cooled to room temperature. H_2O (40 mL) was added and the mixture was extracted with ether (3 × 70 mL). The combined organic layers were washed with brine (4 × 40 mL), dried over $MgSO_4$, and concentrated in vacuo. The crude product was purified with flash chromatography (silica gel, hexanes) to afford 2-fluoro-4-ethoxy-1-methylbenzene as a colorless oil (2.74 g, 89% yield): 1H NMR (300 MHz, $CDCl_3$) δ 7.09-7.02 (m, 1H), 6.62-6.56 (m, 2H), 3.99 (q, 2H, $J = 7.0$), 2.22-2.19 (m, 3H), 1.41 (t, 3H, $J = 7.0$); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.2, 160.0, 158.3, 158.1, 131.4, 131.3, 116.4, 116.1, 109.94, 109.90, 102.0, 101.6, 63.7, 14.7, 13.72, 13.68 (observed complexity is due to F-C splitting); ^{19}F NMR (282 MHz, $CDCl_3$) δ -112.1 (t, $J = 9.1$ Hz); IR (neat, cm^{-1}) 2983, 2931, 1630, 1587, 1512, 1311, 1283, 1159, 1121, 1103, 1045, 847, 823; Anal Calcd. for $C_9H_{11}FO$: C, 70.11; H, 7.19. Found: C, 69.93; H, 7.40.



2-Iodo-2',4',6'-triisopropyl-3-ethoxy-6-methyl-1,1'-biphenyl: An oven-dried three-neck 250 mL round bottom flask, which was equipped with a magnetic stir bar and charged with magnesium shavings (0.95 g, 39.1 mmol), was fitted with a reflux condenser, glass stopper, and rubber septum. The flask was purged with argon and then THF (53 mL) and 2,4,6-triisopropylbromobenzene (8.26 mL, 32.6 mmol) were added via syringe. The reaction was heated to reflux and 1,2-dibromomethane (27 μ L) was added via syringe. The reaction mixture was allowed to stir at reflux for 1 h and was then cooled to room temperature. A separate oven-dried 500 mL round bottom flask, which was equipped with a magnetic stir bar and fitted with a septum, was purged with argon and then THF (160 mL) and 2-fluoro-4-methoxy-1-methylbenzene (2.51 g, 16.3 mmol) were added to the flask via syringe. The reaction vessel was cooled via a -78 °C bath and *n*-BuLi (2.5 M in Hexane, 6.52 mL, 16.3 mmol) was added by a syringe pump over a

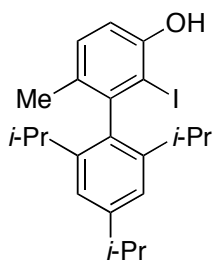
1 h period. The solution was stirred for an additional 2 h and the Grignard reagent, which was prepared in the first reaction vessel, was added via cannula over a 30 min period and the reaction mixture was allowed to stir at $-78\text{ }^{\circ}\text{C}$ for 1 h. The reaction mixture was slowly warmed to room temperature where it was stirred overnight. The mixture was then cooled to $0\text{ }^{\circ}\text{C}$ and a solution of iodine (8.69 g, 34.2 mmol) in THF (34 mL) was added via syringe over a 30 min period and then the dark red solution was warmed to room temperature and stirred for 1 h. Saturated aqueous Na_2SO_3 (200 mL) was added to quench excess iodine. The two layers were separated and the aqueous layer was extracted with ether ($2 \times 200\text{ mL}$). The combined organic layers were washed with brine, dried over MgSO_4 , filtered, and the solvent was removed with the aid of a rotary evaporator. Flash chromatography (silica gel, gradient from pure hexanes to 30:1 hexanes:EtOAc) afforded a light yellow solid. The yellow solid was recrystallized from hot methanol (30 mL) to yield 2.39 g (32% yield) of desired product as white solid: m.p. $122 - 123\text{ }^{\circ}\text{C}$; $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.16 (d, 1H, $J = 8.3\text{ Hz}$), 7.06 (s, 2H), 6.71 (d, 1H, $J = 8.3\text{ Hz}$), 4.12 (q, 2H, $J = 7.0\text{ Hz}$), 2.96 (septet, 1H, $J = 6.9\text{ Hz}$), 2.35 (septet, 2H, $J = 6.9\text{ Hz}$), 1.97 (s, 3H), 1.51 (t, 3H, $J = 7.0\text{ Hz}$), 1.31 (d, 6H, $J = 6.9\text{ Hz}$), 1.19 (d, 6H, $J = 6.9\text{ Hz}$), 1.04 (d, 6H, $J = 6.9\text{ Hz}$); $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 155.9, 148.3, 146.5, 145.1, 138.6, 130.5, 130.1, 121.1, 110.4, 95.8, 65.0, 34.1, 30.6, 24.51, 24.50, 24.1, 21.3, 14.9; IR (neat, cm^{-1}): 2961, 2928, 2868, 1457, 1428, 1289, 1268, 1256, 1069, 946, 875, 796, 761; Anal. Calcd. for $\text{C}_{24}\text{H}_{33}\text{IO}$: C, 62.07; H, 7.16. Found: C, 61.99; H, 7.18.



di-*tert*-Butyl-(2',4',6'-triisopropyl-3-ethoxy-6-methyl-[1,1'-biphenyl]-2-yl)phosphine (L9): An oven-dried Schlenk tube, which was equipped with a magnetic stir bar, fitted with a rubber septum, and charged with 2-iodo-2',4',6'-triisopropyl-3-ethoxy-6-methyl-1,1'-biphenyl (1.04 g, 2.24 mmol), was evacuated and backfilled with argon (this process was repeated a total of three times). THF (10 mL) was added via syringe, the reaction mixture was cooled to $-78\text{ }^{\circ}\text{C}$, and *t*-BuLi (1.7 M in pentane, 3.03 mL, 5.15 mmol) was added in a dropwise fashion over a 10 min period. The solution was stirred for 30 min and then under a positive pressure of argon the septum was removed from the Schlenk tube and anhydrous CuCl (266 mg, 2.69 mmol),

which was weighed out in nitrogen filled glovebox, was added rapidly. The flask was refitted with the rubber septum and $\text{CIP}(t\text{-Bu})_2$ (0.51 mL, 2.69 mmol) was added in a dropwise fashion over a 5 min period. The reaction mixture was warmed from $-78\text{ }^\circ\text{C}$ to room temperature at which point the flask was sealed with a Teflon screw cap and heated to $70\text{ }^\circ\text{C}$ (bath temperature) for 7 days. The solution was cooled to room temperature, diluted with ethyl acetate, washed with NH_4OH 28% in water (this process was repeated a total of three times), washed with brine, dried over MgSO_4 , and concentrated in vacuo. The crude material was recrystallized from hot methanol to afford 484.8 mg (45% yield) of desired product as white crystals: m.p. $119 - 120\text{ }^\circ\text{C}$; ^1H NMR (300 MHz, CDCl_3) δ 7.16 (d, 1H, $J = 8.6\text{ Hz}$), 6.97 (s, 2H), 6.78 (d, 1H, $J = 8.6\text{ Hz}$), 4.16 (q, 2H, $J = 7.1\text{ Hz}$), 2.92 (septet, 1H, $J = 6.9\text{ Hz}$), 2.47 (septet, 2H, $J = 6.7\text{ Hz}$), 1.76 (s, 3H), 1.51 (t, 3H, $J = 7.1\text{ Hz}$), 1.29 (d, 6H, $J = 6.9\text{ Hz}$), 1.21 (d, 6H, $J = 6.7\text{ Hz}$), 1.18 (s, 9H), 1.14 (s, 9H), 0.95 (d, 6H, $J = 6.7\text{ Hz}$); ^{13}C NMR (75 MHz, CDCl_3) δ 159.63, 159.60, 151.3, 150.8, 147.2, 145.7, 136.8, 136.7, 131.82, 131.80, 130.2, 130.1, 125.3, 124.7, 120.7, 108.8, 62.8, 33.95, 33.93, 33.5, 32.2, 31.9, 30.8, 30.7, 25.3, 24.62, 24.60, 24.1, 22.14, 22.11, 14.7 (observed complexity is due to P-C splitting); ^{31}P NMR (121.5 Hz, CDCl_3) δ 35.86; IR (neat, cm^{-1}): 2959, 2891, 2868, 1561, 1461, 1382, 1362, 1253, 1145, 1036, 876, 802; Anal. Calcd. for $\text{C}_{32}\text{H}_{51}\text{IOP}$: C, 79.62; H, 10.65. Found: C, 79.77; H, 10.53.

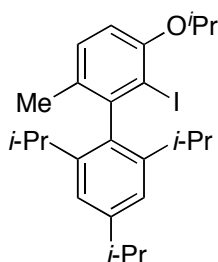
Synthesis of Ligand L10.



2-Iodo-2',4',6'-triisopropyl-3-hydroxy-6-methyl-1,1'-biphenyl: An oven-dried 50 mL round bottom flask, which was equipped with a magnetic stir bar and charged with 2-Iodo-2',4',6'-triisopropyl-3-methoxy-6-methyl-1,1'-biphenyl (2.25 g, 5 mmol), was evacuated and backfilled with argon (this process was repeated a total of three times). Dry CH_2Cl_2 (20 mL), was added via syringe and the solution

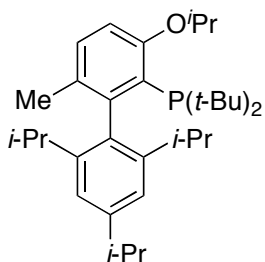
was cooled to $-78\text{ }^\circ\text{C}$. A solution of BBr_3 (1 M in Hexanes, 6.0 mL, 6 mmol) was added slowly via syringe. The reaction solution was warmed to room temperature over 2 h and stirred at room temperature for 2 h. Brine (20 mL) was added and the layers were separated. The aqueous layer was extracted with EtOAc ($3 \times 20\text{ mL}$). The combined organic layers were washed with brine (40 mL), dried over MgSO_4 , and concentrated in

vacuo. The crude product was purified with flash chromatography (silica gel, 20:1 Hexanes/EtOAc) to afford 2-Iodo-2',4',6'-triisopropyl-3-hydroxy-6-methyl-1,1'-biphenyl as white solids (2.16 g, 99% yield): m.p. 164 – 165 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.14 (d, 1H, J = 8.2 Hz), 7.06 (s, 2H), 6.93 (d, 1H, J = 8.2 Hz), 5.34 (s, 1H), 2.95 (septet, 1H, J = 6.9 Hz), 2.35 (septet, 2H, J = 6.9 Hz), 1.98 (s, 3H), 1.31 (d, 6H, J = 6.9 Hz), 1.17 (d, 6H, J = 6.9 Hz), 1.05 (d, 6H, J = 6.9 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 153.0, 148.7, 145.2, 138.3, 130.9, 130.2, 121.2, 112.9, 95.6, 34.1, 30.5, 24.5, 24.4, 24.1, 21.2; IR (neat, cm⁻¹) 3466, 2963, 2924, 2868, 1588, 1453, 1194, 881, 810, 761; Anal Calcd. for C₂₂H₂₉I₂O: C, 60.55; H, 6.70. Found: C, 60.79; H, 6.72.



2-Iodo-2',4',6'-triisopropyl-3-isopropoxy-6-methyl-1,1'-biphenyl:

An oven-dried 50 mL round bottom flask, which was equipped with a magnetic stir bar and charged with anhydrous K₂CO₃ (1.29 g, 9.35 mmol), was evacuated and backfilled with argon (this process was repeated a total of three times). Anhydrous DMF (10 mL), 2-Iodo-2',4',6'-triisopropyl-3-hydroxy-6-methyl-1,1'-biphenyl (2.04 g, 4.67 mmol), and ^tPrBr (1.32 mL, 14.03 mmol) were added via syringe. The reaction mixture was stirred at 80 °C overnight and was allowed to cooled to room temperature. H₂O (20 mL) was added and the mixture was extracted with ether (3 × 50 mL). The combined organic layers were washed with brine (4 × 30 mL), dried over MgSO₄, and concentrated in vacuo. The crude product was purified with flash chromatography (silica gel, hexanes) to afford 2-Iodo-2',4',6'-triisopropyl-3-isopropoxy-6-methyl-1,1'-biphenyl as a white solid (2.19 g, 98% yield): m.p. 74 – 76 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.15 (d, 1H, J = 8.3 Hz), 7.05 (s, 2H), 6.75 (d, 1H, J = 8.3 Hz), 4.56 (septet, 1H, J = 6.1 Hz), 2.95 (septet, 1H, J = 6.9 Hz), 2.35 (septet, 2H, J = 6.9 Hz), 1.97 (s, 3H), 1.42 (d, 6H, J = 6.1 Hz), 1.30 (d, 6H, J = 6.9 Hz), 1.19 (d, 6H, J = 6.9 Hz), 1.04 (d, 6H, J = 6.9 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 155.2, 148.3, 146.6, 145.0, 138.7, 130.8, 130.0, 121.0, 113.3, 98.2, 72.7, 34.0, 30.5, 24.5, 24.4, 24.1, 22.3, 21.3; IR (neat, cm⁻¹): 2963, 2924, 2863, 1607, 1590, 1567, 1462, 1383, 1288, 1267, 1205, 1177, 1138, 1111, 1050, 968, 877, 802, 758; Anal. Calcd. for C₂₅H₃₅I₂O: C, 62.76; H, 7.37. Found: C, 63.02; H, 7.42.

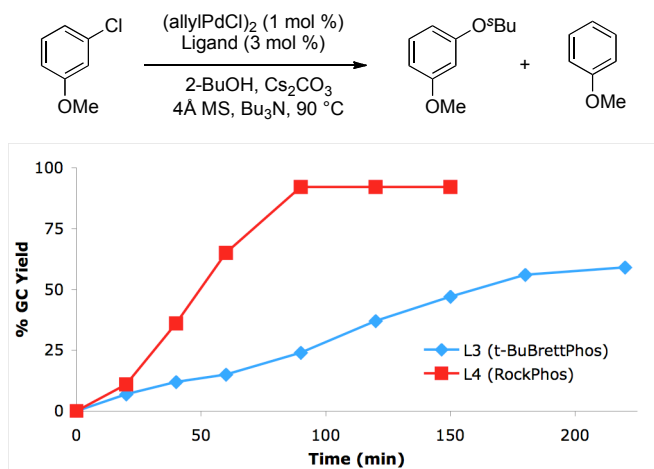


di-*tert*-Butyl-(2',4',6'-triisopropyl-isopropoxy-6-methyl-[1,1'-biphenyl]-2-yl)phosphine (L10):

An oven-dried Schlenk tube, which was equipped with a magnetic stir bar, fitted with a rubber septum, and charged with 2-iodo-2',4',6'-triisopropyl-3-isopropoxy-6-methyl-1,1'-biphenyl (478.4 mg, 1 mmol), was evacuated and backfilled with argon (this process was repeated a total of three times). THF (5 mL) was added via syringe, the reaction mixture was cooled to $-78\text{ }^{\circ}\text{C}$, and *t*-BuLi (1.7 M in pentane, 1.3 mL, 2.2 mmol) was added in a dropwise fashion over a 5 min period. The solution was stirred for 30 min and then under a positive pressure of argon the septum was removed from the Schlenk tube and anhydrous CuCl (109 mg, 1.1 mmol), which was weighed out in nitrogen filled glovebox, was added rapidly. The flask was refitted with the rubber septum and $\text{ClP}(t\text{-Bu})_2$ (0.25 mL, 1.3 mmol) was added in a dropwise fashion over a 5 min period. The reaction mixture was warmed from $-78\text{ }^{\circ}\text{C}$ to room temperature at which point the flask was sealed with a Teflon screw cap and heated to $70\text{ }^{\circ}\text{C}$ (bath temperature) for 7 days. The solution was cooled to room temperature, diluted with ethyl acetate, washed with NH_4OH 28% in water (this process was repeated a total of three times), washed with brine, dried over MgSO_4 , and concentrated in vacuo. The crude material was recrystallized from hot methanol to afford 290.9 mg (59% yield) of desired product as white crystals: m.p. $142 - 143\text{ }^{\circ}\text{C}$; ^1H NMR (300 MHz, CDCl_3) δ 7.14 (d, 1H, $J = 8.5\text{ Hz}$), 6.96 (s, 2H), 6.77 (d, 1H, $J = 8.5\text{ Hz}$), 4.75 (septet, 1H, $J = 6.1\text{ Hz}$), 2.92 (septet, 1H, $J = 6.9\text{ Hz}$), 2.46 (septet, 2H, $J = 6.7\text{ Hz}$), 1.75 (s, 3H), 1.46 (d, 6H, $J = 6.1\text{ Hz}$), 1.28 (d, 6H, $J = 6.9\text{ Hz}$), 1.21 (d, 6H, $J = 6.7\text{ Hz}$), 1.19 (s, 9H), 1.15 (s, 9H), 0.95 (d, 6H, $J = 6.7\text{ Hz}$); ^{13}C NMR (75 MHz, CDCl_3) δ 158.71, 158.67, 151.8, 151.3, 147.2, 145.7, 137.1, 137.0, 131.71, 131.69, 129.6, 129.5, 125.5, 124.8, 120.6, 109.3, 68.9, 34.0, 33.8, 33.4, 32.3, 32.0, 30.81, 30.78, 25.3, 24.60, 24.57, 24.2, 22.14, 22.11, 21.9 (observed complexity is due to P-C splitting); ^{31}P NMR (121.5 Hz, CDCl_3) δ 36.94; IR (neat, cm^{-1}): 2958, 1578, 1559, 1456, 1383, 1274, 1254, 1117, 963, 802, 735; Anal. Calcd. for $\text{C}_{33}\text{H}_{53}\text{OP}$: C, 79.79; H, 10.75. Found: C, 79.77; H, 10.82.

Further Studies on the Effect of the Substituent in the 6-Position of the Ligand:

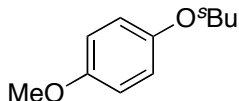
In order to gain additional insight into this effect we compared catalysts based on **L3** and **L4** for the reaction of 3-chloranisole and 2-butanol. As shown in figure 3 the reaction utilizing **L3** as the supporting ligand went to completion in ~3.5 hours and led to only 59% of the desired coupling product and 20% of the undesired reduced arene. When the same reaction was carried out employing a catalyst based on **L4** the reaction went to completion in ~1.5 hours and gave 92% of the desired product and only 7% reduction. These results indicate that replacing the 6-methoxy with a 6-methyl in the ligand not only leads to a decrease in the amount of b-H elimination but also significantly accelerates the rate of product formation.



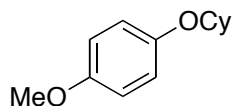
General Procedure A: Cs₂CO₃ (489 mg, 1.5 mmol, 1.5 equiv.) and 4Å Molecular sieves (200 mg, where applicable) were added to an oven-dried resealable screw-cap test tube and dried with flame under vacuum. The Pd source (1 – 4 mol%), Ligand (1.5 – 4.8 mol%), and aryl halide (if it is a solid) (1.0 mmol, 1.0 equiv.) were added under a positive pressure of argon. The tube was evacuated and backfilled with argon (this process was repeated a total of 3 times). The aryl halide (if it is a liquid) (1.0 mmol, 1.0 equiv.) and alcohol (2.0 mmol, 2.0 equiv.) were added through the septum via syringe, followed by solvent (1 mL). The sealed tube was placed into a pre-heated 90 °C oil bath and the mixture was stirred vigorously for the indicated time. After the reaction was allowed to cool to room temperature, it was filtered through a layer of Celite eluting with EtOAc. In the cases where toluene or NEt₃ was used as the solvent, the filtrate was concentrated *in vacuo* and the crude product was purified by flash chromatography. In

the cases where NBu_3 was used as the solvent, the filtrate was washed with 10% aqueous HCl. The organic layer was separated and the aqueous layer was back extracted with EtOAc twice. The combined organic extracts were dried over MgSO_4 and concentrated. The crude product was purified via flash chromatography.

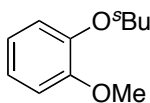
General Procedure B: Cs_2CO_3 (489 mg, 1.5 mmol, 1.5 equiv.) was added to an oven-dried resealable screw-cap test tube and dried with flame under vacuum. To the tube were added $(\text{allylPdCl})_2$ (1 – 2.5 mol%) and RockPhos (2.4 – 6 mol%) under argon. The tube was evacuated and backfilled with argon (this process was repeated a total of 3 times). Toluene and the alcohol were added through the septum via syringe and the mixture was stirred at 90 °C in a pre-heated oil bath for 3 min. Aryl halide was added and the mixture was stirred vigorously for the indicated time. After the reaction was allowed to cool to room temperature, it was filtered through a layer of Celite eluting with EtOAc. The filtrate was concentrated *in vacuo* and the crude product was purified by flash chromatography.



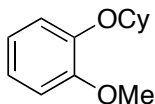
1-sec-Butoxy-4-methoxybenzene: Following general procedure A, 4-chloroanisole (122 μL , 1 mmol), 2-butanol (184 μL , 2 mmol), $(\text{allylPdCl})_2$ (3.66 mg, 1 mol%), RockPhos (14.06 mg, 3 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), and 4Å molecular sieves (200 mg), with NBu_3 as solvent were heated at 90 °C for 21 h. The crude product was purified by flash column chromatography (silica gel, gradient from 100:1 to 50:1 hexanes:EtOAc) to afford the title compound as a colorless liquid (119.1 mg, 66% yield): ^1H NMR (300 MHz, CDCl_3) δ 6.87-6.79 (m, 4H), 4.17 (sextet, 1H, $J = 6.1$ Hz), 3.77 (s, 3H), 1.81-1.66 (m, 1H), 1.66-1.52 (m, 1H), 1.27 (d, 3H, $J = 6.1$ Hz), 0.98 (t, 3H, $J = 7.5$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 153.7, 152.2, 117.4, 114.6, 76.2, 55.7, 29.2, 19.3, 9.8; IR (neat, cm^{-1}) 2971, 2935, 1507, 1465, 1230, 1040, 825; Anal. Calcd. for $\text{C}_{11}\text{H}_{16}\text{O}_2$: C, 73.30; H, 8.95. Found: C, 73.40; H, 9.10. The ^1H NMR and ^{13}C NMR spectral data were consistent with those of the previously reported compound.⁴



1-Cyclohexyloxy-4-methoxybenzene: Following general procedure A, 4-chloroanisole (122 μL , 1 mmol), cyclohexanol (190 μL , 2 mmol), (allylPdCl)₂ (3.66 mg, 1 mol%), RockPhos (14.06 mg, 3 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), and 4 \AA molecular sieves (200 mg) with NBU₃ as solvent were heated at 90 $^{\circ}\text{C}$ for 21 h. The crude product was purified by flash column chromatography (silica gel, gradient from 100:1 to 50:1 hexanes:EtOAc) to afford the title compound as a colorless liquid (131.5 mg, 64% yield): ¹H NMR (300 MHz, CDCl₃) δ 6.88-6.79 (m, 4H), 4.11 (septet, 1H, J = 4.2 Hz), 3.77 (s, 3H), 2.03-1.91 (m, 2H), 1.86-1.72 (m, 2H), 1.64-1.22 (m, 6H); ¹³C NMR (75 MHz, CDCl₃) δ 153.8, 151.7, 117.6, 114.5, 76.6, 55.6, 31.9, 25.6, 23.8; IR (neat, cm⁻¹) 2935, 2858, 1505, 1465, 1450, 1229, 1040, 968, 825, 747; Anal. Calcd. for C₁₃H₁₈O₂: C, 75.69; H, 8.80. Found: C, 75.84; H, 8.74. The ¹H NMR and ¹³C NMR spectral data were consistent with those of the previously reported compound.⁵

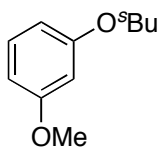


1-sec-Butoxy-2-methoxybenzene: Following procedure A, 4-chloroanisole (127 μL , 1 mmol), 2-butanol (184 μL , 2 mmol), (allylPdCl)₂ (3.66 mg, 1 mol%), RockPhos (14.06 mg, 3 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), 4 \AA molecular sieves (200 mg), and NBU₃ were heated at 90 $^{\circ}\text{C}$ for 21 h. The crude product was purified by flash column chromatography (silica gel, gradient from 100:1 to 20:1 hexanes:EtOAc) to afford the title compound as a colorless liquid (77.7 mg, 43% yield): ¹H NMR (300 MHz, CDCl₃) δ 6.93-6.87 (m, 4H), 4.27 (sextet, 1H, J = 6.1 Hz), 3.85 (s, 3H), 1.90-1.75 (m, 1H), 1.71-1.56 (m, 1H), 1.33 (d, 3H, J = 6.1 Hz), 0.99 (t, 3H, J = 7.5 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 150.5, 147.7, 121.1, 120.7, 116.0, 112.1, 76.7, 55.9, 29.2, 19.3, 9.9; IR (neat, cm⁻¹) 2970, 2930, 1592, 1505, 1456, 1253, 1226, 1126, 1030, 743.

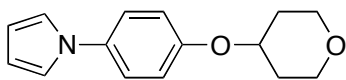


1-Cyclohexyloxy-2-methoxybenzene: Following procedure A, 4-chloroanisole (127 μL , 1 mmol), cyclohexanol (190 μL , 2 mmol), (allylPdCl)₂ (3.66 mg, 1 mol%), RockPhos (14.06 mg, 3 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), 4 \AA molecular sieves (200 mg), and NBU₃ were heated at 90 $^{\circ}\text{C}$ for 21 h. The crude product was purified by flash column chromatography (silica gel, gradient from

100:1 to 20:1 hexanes:EtOAc) to afford the title compound as a colorless oil (80.9 mg, 39% yield): ^1H NMR (300 MHz, CDCl_3) δ 6.96-6.85 (m, 4H), 4.18 (septet, 1H, $J = 4.5$ Hz), 3.85 (s, 3H), 2.11-2.00 (m, 2H), 1.90-1.78 (m, 2H), 1.66-1.48 (m, 3H), 1.42-1.20 (m, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 150.5, 147.1, 121.3, 120.6, 116.4, 112.1, 77.2, 55.9, 32.0, 25.6, 24.1; IR (neat, cm^{-1}) 2936, 2857, 1592, 1505, 1455, 1252, 1224, 1179, 1124, 1046, 1029, 964, 745; Anal. Calcd. for $\text{C}_{13}\text{H}_{18}\text{O}_2$: C, 75.69; H, 8.80. Found: C, 75.48; H, 8.78.

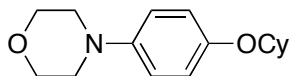


1-sec-Butoxy-3-methoxybenzene: Following procedure A, 3-chloroanisole (123 μL , 1 mmol), 2-butanol (184 μL , 2 mmol), (allylPdCl) $_2$ (1.83 mg, 0.5 mol%), RockPhos (7.03 mg, 1.5 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), 4 \AA molecular sieves (200 mg), and NBu_3 were heated at 90 $^\circ\text{C}$ for 21 h. The crude product was purified by flash column chromatography (silica gel, 50:1 hexanes:EtOAc) to afford the title compound as a colorless oil (155.1 mg, 86% yield): ^1H NMR (300 MHz, CDCl_3) δ 7.17 (t, 1H, $J = 7.9$ Hz), 6.53-6.45 (m, 3H), 4.29 (sextet, 1H, $J = 6.1$ Hz), 3.79 (s, 3H), 1.83-1.68 (m, 1H), 1.68-1.54 (m, 1H), 1.30 (d, 3H, $J = 6.1$ Hz), 0.98 (t, 3H, $J = 7.5$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 160.8, 159.4, 129.8, 107.9, 105.9, 102.2, 75.0, 55.2, 29.2, 19.3, 9.8; IR (neat, cm^{-1}) 2972, 2937, 1600, 1492, 1455, 1286, 1265, 1201, 1150, 1043, 1001, 837, 763, 688. The ^1H NMR and ^{13}C NMR spectral data were consistent with those of the previously reported compound.⁶

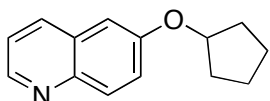


1-(4-((Tetrahydro-2H-pyran-4-yl)oxy)phenyl)-1H-pyrrole: Following procedure A, 1-(4-chlorophenyl)-1H-pyrrole (177.6 mg, 1 mmol), tetrahydro-4-pyranol (191 μL , 2 mmol), (allylPdCl) $_2$ (3.66 mg, 1 mol%), RockPhos (14.06 mg, 3 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), 4 \AA molecular sieves (200 mg), and NBu_3 were heated at 90 $^\circ\text{C}$ for 21 h. The crude product was purified by flash column chromatography (silica gel, 10:1 hexanes:EtOAc) to afford the title compound as a off-white solid (173.9 mg, 72% yield): m.p. 80 –81 $^\circ\text{C}$; ^1H NMR (300 MHz, CDCl_3) δ 7.34-7.28 (m, 2H), 7.03-6.99 (m, 2H), 7.00-6.94 (m, 2H), 6.35-6.31 (m, 2H), 4.49 (septet, 1H), 4.06-3.96 (m, 2H), 3.65-3.55 (m, 2H), 2.10-1.99 (m, 2H), 1.88-1.75 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 155.1, 134.7, 122.2, 119.6, 116.9, 109.9,

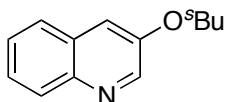
72.1, 65.1, 31.7; IR (neat, cm^{-1}) 2955, 2865, 1520, 1260, 1239, 1152, 1092, 1071, 989, 836, 730; Anal Calcd. for $\text{C}_{15}\text{H}_{17}\text{NO}_2$: C, 74.05; H, 7.04. Found: C, 73.78; H, 7.05.



4-(4-Cyclohexyloxyphenyl)morpholine: Following procedure A, 4-(4-bromophenyl)morpholine (242.1 mg, 1 mmol), cyclohexanol (159 μL , 1.5 mmol), (allylPdCl)₂ (3.66 mg, 1 mol%), RockPhos (14.06 mg, 3 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), 4 Å molecular sieves (200 mg), and toluene were heated at 90 °C for 21 h. The crude product was purified by flash column chromatography (silica gel, 15:1 hexanes:EtOAc) to afford the title compound as a white solid (136.4 mg, 52% yield): m.p. 68–69 °C; ¹H NMR (300 MHz, CDCl_3) δ 6.86 (s, 4H), 4.12 (septet, 1H, J = 4.2), 3.88–3.82 (m, 4H), 3.08–3.02 (m, 4H), 2.03–1.90 (m, 2H), 1.86–1.70 (m, 2H), 1.63–1.20 (m, 6H); ¹³C NMR (75 MHz, CDCl_3) δ 151.9, 145.5, 117.6, 117.2, 76.2, 67.0, 50.7, 31.9, 25.6, 23.8; IR (neat, cm^{-1}) 2934, 2855, 2812, 1511, 1450, 1259, 1236, 1122, 1048, 969, 929, 825; Anal Calcd. for $\text{C}_{16}\text{H}_{23}\text{NO}_2$: C, 73.53; H, 8.87. Found: C, 73.69; H, 8.69.

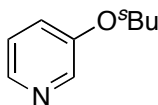


6-Cyclopentyloxyquinoline: Following procedure A, 6-chloroquinoline (163.6 mg, 1 mmol), cyclopentanol (182 μL , 2 mmol), (allylPdCl)₂ (3.66 mg, 1 mol%), RockPhos (11.25 mg, 2.4 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), and Et_3N were heated at 90 °C for 21 h. The crude product was purified by flash column chromatography (silica gel, 5:1 hexanes:EtOAc) to afford the title compound as a colorless oil (131.4 mg, 62% yield): ¹H NMR (300 MHz, CDCl_3) δ 8.74 (dd, 1H, J = 1.5, 4.3 Hz), 8.01 (d, 1H, J = 8.1 Hz), 7.97 (d, 1H, J = 9.1 Hz), 7.32 (dd, 1H, J = 2.7, 9.1 Hz), 7.31 (dd, 1H, J = 8.1, 4.3 Hz), 7.16 (d, 1H, J = 2.7 Hz), 4.88 (septet, 1H), 2.05–1.54 (m, 8H); ¹³C NMR (75 MHz, CDCl_3) δ 156.1, 147.7, 144.1, 134.6, 130.7, 129.2, 123.1, 121.2, 107.0, 79.5, 32.8, 24.1; IR (neat, cm^{-1}) 2961, 2874, 1616, 1594, 1496, 1465, 1435, 1378, 1325, 1226, 1167, 1114, 1035, 988, 833, 789, 771, 617.

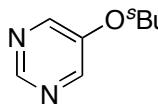


3-sec-Butoxyquinoline: Following procedure A, 3-bromoquinoline (136 μL , 1 mmol), 2-butanol (184 μL , 2 mmol), (allylPdCl)₂ (3.66 mg,

1 mol%), RockPhos (11.25 mg, 2.4 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), and toluene were heated at 90 °C for 21 h. The crude product was purified by flash column chromatography (silica gel, 10:1 hexanes:EtOAc) to afford the title compound as a colorless oil (164.7 mg, 82% yield): ¹H NMR (300 MHz, CDCl₃) δ 8.65 (d, 1H, J = 2.8 Hz), 8.05-8.00 (m, 1H), 7.72-7.67 (m, 1H), 7.58-7.45 (m, 2H), 7.36 (br d, 1H, J = 2.8 Hz), 4.45 (sextet, 1H, J = 6.1 Hz), 1.91-1.63 (m, 2H), 1.38 (d, 3H, J = 6.1 Hz), 1.02 (t, 3H, J = 7.5 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 151.5, 145.6, 143.3, 129.0, 128.8, 126.9, 126.5, 126.4, 114.2, 75.5, 28.9, 18.8, 9.7; IR (neat, cm⁻¹) 2973, 2935, 1603, 1496, 1464, 1423, 1379, 1345, 1274, 1211, 1189, 1140, 1121, 995, 924, 782, 751, 615; Anal Calcd. for C₁₃H₁₅NO: C, 77.58; H, 7.51. Found: C, 77.05; H, 7.61.

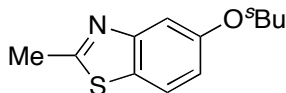


3-sec-Butoxypyridine: Following procedure B, 3-chloropyridine (94 μL, 1 mmol), 2-butanol (184 μL, 2 mmol), (allylPdCl)₂ (7.32 mg, 2 mol%), RockPhos (22.50 mg, 4.8 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), and toluene were heated at 90 °C for 21 h. The crude product was purified by flash column chromatography (silica gel, 4:1 hexanes:EtOAc) to afford the title compound as a colorless oil (105.2 mg, 70% yield): ¹H NMR (300 MHz, CDCl₃) δ 8.27 (dd, 1H, J = 2.3, 1.1 Hz), 8.16 (dd, 1H, J = 2.3, 3.9 Hz), 7.20-7.15 (m, 2H), 4.31 (sextet, 1H, J = 6.1 Hz), 1.81-1.54 (m, 2H), 1.29 (d, 3H, J = 6.1 Hz), 0.96 (t, 3H, J = 7.5 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 154.3, 141.7, 139.3, 123.8, 122.3, 75.6, 29.0, 19.0, 9.7; IR (neat, cm⁻¹) 2974, 2936, 1583, 1573, 1475, 1424, 1379, 1279, 1228, 1124, 1094, 988, 921, 800, 709, 601.

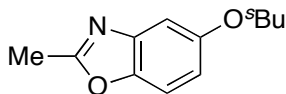


5-sec-Butoxypyrimidine: Following procedure B, 5-bromopyrimidine (159.0 mg, 1 mmol), 2-butanol (184 μL, 2 mmol), (allylPdCl)₂ (9.15 mg, 2 mol%), RockPhos (28.12 mg, 6.0 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), and toluene were heated at 90 °C for 24 h. The crude product was purified by flash column chromatography (silica gel, 4:1 hexanes:EtOAc) to afford the title compound as a colorless oil (115.7 mg, 76% yield): ¹H NMR (300 MHz, CDCl₃) δ 8.76 (s, 1H), 8.34 (s, 2H), 4.35 (sextet, 1H, J = 6.1 Hz), 1.82-1.55 (m, 2H), 1.30 (d, 3H, J = 6.1 Hz), 0.95 (t, 3H, J = 7.5 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 152.3, 151.0, 144.6, 76.2, 28.9, 18.8, 9.5;

IR (neat, cm^{-1}) 2975, 2937, 1573, 1557, 1419, 1382, 1275, 1182, 1114, 1096, 919, 887, 723, 630, 615; Anal Calcd. for $\text{C}_8\text{H}_{12}\text{N}_2\text{O}$: C, 63.13; H, 7.95. Found: C, 62.86; H, 8.14.

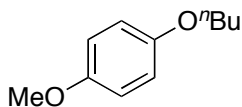


5-(*sec*-Butoxy)-2-methylbenzothiazole: Following procedure A, 5-chloro-2-methylbenzothiazole (183.7 mg, 1 mmol), 2-butanol (183 μL , 2 mmol), $(\text{allylPdCl})_2$ (3.66 mg, 1 mol%), RockPhos (11.25 mg, 2.4 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), and toluene were heated at 90 $^\circ\text{C}$ for 21 h. The crude product was purified by flash column chromatography (silica gel, gradient from 4:1 CH_2Cl_2 :hexanes to CH_2Cl_2) to afford the desired product, proceeded a mixture of 2-methylbenzothiazole and the product. The mixture was further purified by flash column chromatography (silica gel, gradient from 4:1 CH_2Cl_2 :hexanes to CH_2Cl_2) to afford a total 138.6 mg (63% yield) of the desired product: ^1H NMR (300 MHz, CDCl_3) δ 7.63 (d, 1H, $J = 8.8$ Hz), 7.44 (d, 1H, $J = 2.4$ Hz), 6.96 (dd, 1H, $J = 8.8, 2.4$ Hz), 4.34 (sextet, 1H, $J = 6.1$ Hz), 2.80 (s, 3H), 1.89-1.56 (m, 2H), 1.33 (d, 3H, $J = 6.1$ Hz), 0.99 (t, 3H, $J = 7.5$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 168.0, 157.3, 154.6, 127.1, 121.6, 116.2, 107.4, 75.6, 29.0, 20.1, 19.1, 9.8; IR (neat, cm^{-1}) 2972, 2933, 1601, 1557, 1524, 1456, 1376, 1320, 1276, 1163, 988, 806, 645; Anal Calcd. for $\text{C}_{12}\text{H}_{15}\text{NOS}$: C, 65.12; H, 6.83. Found: C, 64.96; H, 6.94.

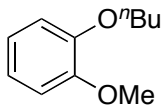


5-(*sec*-Butoxy)-2-methylbenzoxazole: Following procedure A, 5-chloro-2-methylbenzoxazole (167.6 mg, 1 mmol), 2-butanol (184 μL , 2 mmol), $(\text{allylPdCl})_2$ (7.32 mg, 2 mol%), RockPhos (28.12 mg, 6 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), 4 \AA molecular sieves (200 mg), and toluene were heated at 90 $^\circ\text{C}$ for 21 h. The crude product was purified by flash column chromatography (silica gel, gradient from 4:1 CH_2Cl_2 :hexanes to CH_2Cl_2) to afford the desired product, proceeded a mixture of 2-methylbenzoxazole and the product. The mixture was further purified by flash column chromatography (silica gel, gradient from 4:1 CH_2Cl_2 :hexanes to CH_2Cl_2) to afford a total 124.4 mg (61% yield) of the desired product: ^1H NMR (300 MHz, CDCl_3) δ 7.32 (d, 1H, $J = 8.8$ Hz), 7.14 (d, 1H, $J = 2.5$ Hz), 6.86 (dd, 1H, $J = 8.8, 2.5$ Hz), 4.26 (sextet, 1H, $J = 6.1$ Hz), 2.60 (s, 3H), 1.84-1.54 (m, 2H), 1.30 (d, 3H, $J = 6.1$ Hz), 0.98 (t, 3H, $J = 7.5$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 164.5, 155.4, 145.5, 142.2, 114.7,

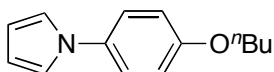
110.2, 105.5, 76.3, 29.0, 19.1, 14.6, 9.8; IR (neat, cm^{-1}) 2973, 2934, 2880, 1576, 1476, 1438, 1381, 1272, 1178, 1151, 989, 952, 928, 908, 847, 805, 664; Anal Calcd. for $\text{C}_{12}\text{H}_{15}\text{NO}_2$: C, 70.22; H, 7.37. Found: C, 70.03; H, 7.37.



1-Butoxy-4-methoxybenzene: Following procedure A, 4-bromoanisole (125 μL , 1 mmol), 1-butanol (183 μL , 2 mmol), (allylPdCl)₂ (1.83 mg, 0.5 mol%), RockPhos (7.03 mg, 1.5 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), 4 \AA molecular sieves (200 mg), and toluene were heated at 90 $^\circ\text{C}$ for 21 h. The crude product was purified by flash column chromatography (silica gel, gradient from 100:1 to 50:1 hexanes:EtOAc) to afford the title compound as a colorless liquid (144.0 mg, 80% yield): ^1H NMR (300 MHz, CDCl_3) δ 6.84 (s, 4H), 3.91 (t, 2H, $J = 6.5$ Hz), 3.77 (s, 3H), 1.80-1.69 (m, 2H), 1.55-1.42 (m, 2H), 0.97 (t, 3H, $J = 7.4$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 153.6, 153.3, 115.4, 114.6, 68.3, 55.7, 31.4, 19.2, 13.9; IR (neat, cm^{-1}) 2958, 2935, 2873, 1508, 1466, 1231, 1042, 825, 744. The ^1H NMR and ^{13}C NMR spectral data were consistent with those of the previously reported compound.⁷

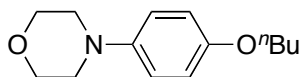


1-Butoxy-2-methoxybenzene: Following procedure A, 2-bromoanisole (125 μL , 1 mmol), 1-butanol (183 μL , 2 mmol), (allylPdCl)₂ (1.83 mg, 0.5 mol%), RockPhos (7.03 mg, 1.5 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), 4 \AA molecular sieves (200 mg), and toluene were heated at 90 $^\circ\text{C}$ for 21 h. The crude product was purified by flash column chromatography (silica gel, gradient from 100:1 to 20:1 hexanes:EtOAc) to afford the title compound as a colorless oil (150.9 mg, 84% yield): ^1H NMR (300 MHz, CDCl_3) δ 6.90 (s, 4H), 4.03 (t, 2H, $J = 6.5$ Hz), 3.87 (s, 3H), 1.89-1.78 (m, 2H), 1.57-1.43 (m, 2H), 0.98 (t, 3H, $J = 7.4$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 149.4, 148.6, 120.8, 120.7, 112.9, 111.7, 68.6, 55.9, 31.2, 19.2, 13.9; IR (neat, cm^{-1}) 2958, 2935, 2873, 1593, 1506, 1456, 1253, 1228, 1180, 1125, 1030, 740. The ^1H NMR and ^{13}C NMR spectral data is in agreement with those reported in the literature.⁸



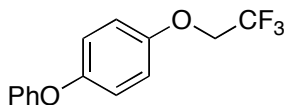
1-(4-Butoxyphenyl)-1H-pyrrole: Following procedure A, 1-(4-

chlorophenyl)-1*H*-pyrrole (177.6 mg, 1 mmol), 1-butanol (183 μ L, 2 mmol), (allylPdCl)₂ (7.32 mg, 2 mol%), RockPhos (22.50 mg, 4.8 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), and toluene were heated at 90 °C for 21 h. The crude product was purified by flash column chromatography (silica gel, 50:1 hexanes:EtOAc) to afford the title compound as a off-white solid (187.7 mg, 87% yield): m.p. 75 –76 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.35-7.28 (m, 2H), 7.04-7.01 (m, 2H), 6.99-6.92 (m, 2H), 6.37-6.32 (m, 2H), 4.00 (t, 2H, J = 6.5 Hz), 1.81 (pentet, 2H, J = 7.0 Hz), 1.54 (sextet, 2H, J = 6.2 Hz), 1.02 (t, 3H, J = 7.4 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 157.2, 134.2, 122.1, 119.6, 115.1, 109.7, 68.0, 31.3, 19.2, 13.8; IR (neat, cm⁻¹) 2956, 2937, 1527, 1260, 1129, 827, 718; Anal Calcd. for C₁₄H₁₇NO: C, 78.10; H, 7.96. Found: C, 77.82; H, 7.93.



4-(4-Butoxyphenyl)morpholine: Following procedure A, 4-(4-bromophenyl)morpholine (242.1 mg, 1 mmol), cyclohexanol

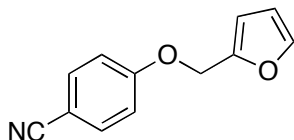
(159 μ L, 1.5 mmol), (allylPdCl)₂ (1.83 mg, 0.5 mol%), RockPhos (7.03 mg, 1.5 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), and toluene were heated at 90 °C for 15 h. The crude product was purified by flash column chromatography (silica gel, gradient from 10:1 hexanes:EtOAc) to afford the title compound as a white solid (169.1 mg, 72% yield): m.p. 59 –60 °C; ¹H NMR (300 MHz, CDCl₃) δ 6.91-6.83 (m, 4H), 3.92 (t, 2H, J = 6.5 Hz), 3.89-3.83 (m, 4H), 3.09-3.02 (m, 4H), 1.80-1.69 (m, 2H), 1.55-1.41 (m, 2H), 0.97 (t, 3H, J = 7.4 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 153.5, 145.5, 117.8, 115.2, 68.1, 67.0, 50.8, 31.4, 19.2, 13.9; IR (neat, cm⁻¹) 2915, 2857, 1514, 1466, 1449, 1261, 1225, 1124, 1070, 1029, 975, 919, 828; Anal Calcd. for C₁₄H₂₁NO₂: C, 71.46; H, 8.99. Found: C, 71.47; H, 9.08.



1-Phenoxy-4-(2,2,2-trifluoroethoxy)benzene: Following procedure A, 4-chlorodiphenyl ether (172 μ L, 1 mmol), 2,2,2-trifluoroethanol (144 μ L, 2 mmol), (allylPdCl)₂ (1.83 mg, 0.5 mol%), RockPhos (7.03 mg,

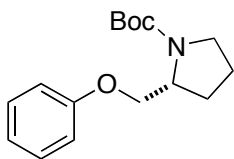
1.5 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), and toluene were heated at 90 °C for 5 h. The crude product was purified by flash column chromatography (silica gel, 50:1 hexanes:EtOAc) to afford the title compound as a colorless liquid (223.2 mg, 83% yield): ¹H NMR (300 MHz, CDCl₃) δ 7.36-7.29 (m, 2H), 7.12-7.05 (m, 1H), 7.04-6.90 (m, 6H),

4.34 (q, 2H, J = 8.2 Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 157.9, 153.5, 151.9, 129.7, 123.4 (q, J = 278.0 Hz), 122.9, 120.6, 118.0, 116.3, 66.5 (q, J = 35.5 Hz); ^{19}F NMR (282 MHz, CDCl_3) δ -74.3 (t, J = 8.0 Hz); IR (neat, cm^{-1}) 3045, 2945, 1592, 1504, 1488, 1459, 1285, 1217, 1165, 1079, 974, 860, 842, 692; Anal Calcd. for $\text{C}_{14}\text{H}_{11}\text{F}_3\text{O}_2$: C, 62.69; H, 4.13. Found: C, 62.40; H, 4.23.



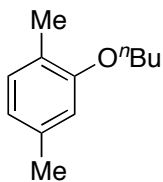
2-((4-Cyanophenoxy)methyl)furan: Following procedure A, 4-bromobenzonitrile (182.0 mg, 1 mmol), furfuryl alcohol (173 μL , 2 mmol), $(\text{allylPdCl})_2$ (1.83 mg, 0.5 mol%), RockPhos (7.03 mg,

1.5 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), and toluene were heated at 90 $^\circ\text{C}$ for 5 h. The crude product was purified by flash column chromatography (silica gel, 5:1 hexanes:EtOAc) to afford the title compound as a white solid (152.0 mg, 76% yield): m.p. 71–72 $^\circ\text{C}$; ^1H NMR (300 MHz, CDCl_3) δ 7.62–7.56 (m, 2H), 7.46 (dd, 1H, J = 1.8, 0.7 Hz), 7.6–7.01 (d, 2H, J = 9.0 Hz), 6.47 (br d, 1H, J = 3.3 Hz), 6.40 (dd, 1H, J = 3.3, 1.8 Hz), 5.05 (s, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 161.5, 148.9, 143.5, 134.0, 119.1, 115.5, 110.7, 110.6, 104.4, 62.4; IR (neat, cm^{-1}) 2221, 1605, 1506, 1254, 1176, 994, 926, 834, 770; Anal Calcd. for $\text{C}_{12}\text{H}_9\text{NO}_2$: C, 72.35; H, 4.55. Found: C, 72.26; H, 4.44.

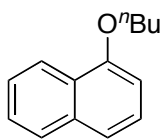


(R)-tert-Butyl 2-(Phenoxy)methylpyrrolidine-1-carboxylate:

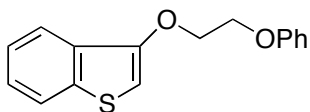
Following procedure A, bromobenzene (107 μL , 1 mmol), *N*-Boc-D-prolinol (250 μL , 2 mmol), $(\text{allylPdCl})_2$ (1.83 mg, 0.5 mol%), RockPhos (7.03 mg, 1.5 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), and toluene were heated at 90 $^\circ\text{C}$ for 10 h. The crude product was purified by flash column chromatography (silica gel, 4:1 hexanes:EtOAc) to afford the title compound as a colorless liquid (237.8 mg, 86% yield): ^1H NMR (300 MHz, CDCl_3) δ 7.27 (br t, 2H, J = 8.0 Hz), 6.93 (br d, 3H, J = 8.0 Hz), 4.24–4.04 (m, 2H), 4.00–3.70 (m, 1H), 3.48–3.24 (m, 2H), 2.14–1.72 (m, 4H), 1.48 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ 158.7, 154.6, 154.4, 129.3, 120.7, 120.5, 114.4, 79.6, 79.2, 68.0, 67.7, 55.9, 55.8, 46.9, 46.5, 28.6, 28.5, 27.9, 23.7, 22.7 (observed complexity is due to the presence of two rotamers); IR (neat, cm^{-1}) 2975, 1695, 1497, 1394, 1245, 1171, 1107, 755; Anal Calcd. for $\text{C}_{16}\text{H}_{23}\text{NO}_3$: C, 69.29; H, 8.36. Found: C, 69.16; H, 8.45.



1-Butoxy-2,5-dimethylbenzene: Following procedure A, 1-bromo-2,5-dimethylbenzene (138 μL , 1 mmol), 1-butanol (183 μL , 2 mmol), $\text{Pd}(\text{OAc})_2$ (4.49 mg, 2 mol%), *t*-BuBrettPhos (11.63 mg, 2.4 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), 4 \AA molecular sieves (200 mg), and toluene were heated at 90 $^\circ\text{C}$ for 21 h. The crude product was purified by flash column chromatography (silica gel, 100:1 hexanes:EtOAc) to afford the title compound as a colorless oil (144.8 mg, 81% yield): ^1H NMR (300 MHz, CDCl_3) δ 7.02 (d, 1H, $J = 7.7$ Hz); 6.67 (d, 1H, $J = 7.7$ Hz); 6.66 (s, 1H), 3.96 (t, 2H, $J = 6.5$ Hz), 2.33 (s, 3H), 2.20 (s, 3H), 1.85-1.74 (m, 2H), 1.60-1.44 (m, 2H), 1.00 (t, 3H, $J = 7.4$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 157.1, 136.4, 130.2, 123.6, 120.5, 111.9, 67.5, 31.5, 21.4, 19.4, 15.8, 13.9; IR (neat, cm^{-1}) 2959, 2933, 2872, 1614, 1586, 1509, 1459, 1414, 1266, 1159, 1132, 1041, 1030, 802. The ^1H NMR and ^{13}C NMR spectral data were consistent with those of the previously reported compound.⁶

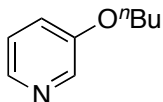


1-Butoxynaphthalene: Following procedure A, 1-bromo-naphthalene (139 μL , 1 mmol), 1-butanol (183 μL , 2 mmol), $\text{Pd}(\text{OAc})_2$ (4.49 mg, 2 mol%), *t*-BuBrettPhos (11.63 mg, 2.4 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), 4 \AA molecular sieves (200 mg), and toluene were heated at 90 $^\circ\text{C}$ for 21 h. The crude product was purified by flash column chromatography (silica gel, 100:1 hexanes:EtOAc) to afford the title compound as a colorless oil (173.1 mg, 86% yield): ^1H NMR (300 MHz, CDCl_3) δ 8.38-8.30 (m, 1H), 7.87-7.79 (m, 1H), 7.56-7.37 (m, 4H), 6.83 (dd, 1H, $J = 7.1, 1.5$ Hz); 4.17 (t, 2H, $J = 6.5$ Hz), 2.01-1.90 (m, 2H), 1.72-1.58 (m, 2H), 1.07 (t, 3H, $J = 7.4$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 154.9, 134.4, 127.4, 126.3, 125.9, 125.7, 125.0, 122.1, 119.9, 104.4, 67.7, 31.4, 19.5, 13.9; IR (neat, cm^{-1}) 3053, 2958, 2933, 2872, 1596, 1581, 1509, 1460, 1405, 1390, 1271, 1240, 1156, 1100, 1073, 1020, 962, 790, 770. The ^1H NMR and ^{13}C NMR spectral data were consistent with those of the previously reported compound.⁶

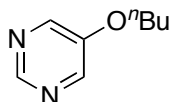
**3-(2-Phenoxyethoxy)benzo[*b*]thiophene:**

Following

procedure A, 3-bromothiophene (131 μL , 1 mmol), 2-phenoxyethanol (250 μL , 2 mmol), (allylPdCl)₂ (1.83 mg, 0.5 mol%), RockPhos (7.03 mg, 1.5 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), and toluene were heated at 90 °C for 10 h. The crude product was purified by flash column chromatography (silica gel, 15:1 hexanes:EtOAc) to afford the title compound as a off-white solid (220.4 mg, 82% yield): m.p. 91 –93 °C ¹H NMR (300 MHz, CDCl₃) δ 7.89-7.81 (m, 1H), 7.81-7.74 (m, 1H), 7.42-7.30 (m, 4H), 7.06-7.98 (m, 3H), 6.37 (s, 1H), 4.51-4.45 (m, 2H), 4.45-4.39 (m, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 158.6, 150.6, 137.6, 132.0, 129.5, 125.2, 123.7, 122.7, 121.12, 121.10, 114.7, 96.6, 68.5, 66.3; IR (neat, cm⁻¹) 2934, 1600, 1572, 1530, 1498, 1455, 1355, 1251, 1189, 934, 758, 716; Anal Calcd. for C₁₆H₁₄O₂S: C, 71.08; H, 5.22. Found: C, 70.96; H, 5.07.

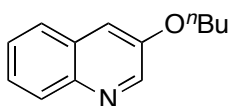
**3-Butoxypyridine:** Following procedure B, 3-chloropyridine (94 μL , 1 mmol), 1-butanol (183 μL , 2 mmol), (allylPdCl)₂ (1.83 mg, 0.5 mol%),

RockPhos (7.03 mg, 1.5 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), and toluene were heated at 90 °C for 5 h. The crude product was purified by flash column chromatography (silica gel, 4:1 hexanes:EtOAc) to afford the title compound as a colorless oil (136.9 mg, 91% yield): ¹H NMR (300 MHz, CDCl₃) δ 8.31-8.26 (m, 1H), 8.18 (dd, 1H, J = 2.3, 3.9 Hz), 7.21-7.12 (m, 2H), 3.98 (t, 2H, J = 6.5 Hz), 1.82-1.70 (m, 2H), 1.55-1.40 (m, 2H), 0.96 (t, 3H, J = 7.4 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 155.2, 141.8, 138.0, 123.7, 120.9, 67.9, 31.1, 19.1, 13.7; IR (neat, cm⁻¹) 2960, 2935, 2874, 1583, 1576, 1473, 1426, 1280, 1264, 1231, 1049, 798, 707; Anal Calcd. for C₉H₁₃NO: C, 71.49; H, 8.67. Found: C, 71.26; H, 8.79. The ¹H NMR and ¹³C NMR spectral data were consistent with those of the previously reported compound.⁹

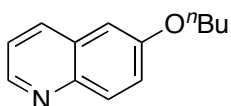
**5-Butoxypyrimidine:** Following procedure B, 5-bromopyrimidine (159.0 mg, 1 mmol), 1-butanol (183 μL , 2 mmol), (allylPdCl)₂ (1.83 mg,

0.5 mol%), RockPhos (7.03 mg, 1.5 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), and toluene were heated at 90 °C for 10 h. The crude product was purified by flash column chromatography (silica gel, 4:1 hexanes:EtOAc) to afford the title compound as a

colorless oil (140.1 mg, 92% yield): ^1H NMR (300 MHz, CDCl_3) δ 8.79 (s, 1H), 8.35 (s, 2H), 4.03 (t, 2H, $J = 6.5$ Hz), 1.82-1.70 (m, 2H), 1.54-1.39 (m, 2H), 0.94 (t, 3H, $J = 7.4$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 153.0, 151.2, 143.4, 68.3, 30.9, 18.9, 13.6; IR (neat, cm^{-1}) 2960, 2936, 2875, 1569, 1560, 1419, 1387, 1276, 1182, 1113, 966, 886, 722, 615; Anal Calcd. for $\text{C}_8\text{H}_{12}\text{N}_2\text{O}$: C, 63.13; H, 7.95. Found: C, 62.86; H, 8.16.

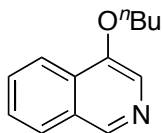


3-Butoxyquinoline: Following procedure A, 3-bromoquinoline (136 μL , 1 mmol), 1-butanol (183 μL , 2 mmol), (allylPdCl) $_2$ (1.83 mg, 0.5 mol%), RockPhos (7.03 mg, 1.5 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), and toluene were heated at 90 $^\circ\text{C}$ for 5 h. The crude product was purified by flash column chromatography (silica gel, 10:1 hexanes:EtOAc) to afford the title compound as a colorless oil (188.5 mg, 94% yield): ^1H NMR (300 MHz, CDCl_3) δ 8.67 (d, 1H, $J = 2.8$ Hz), 8.06-8.01 (m, 1H), 7.73-7.68 (m, 1H), 7.57-7.46 (m, 2H), 7.37 (br d, 1H, $J = 2.8$ Hz), 4.08 (t, 2H, $J = 6.5$ Hz), 1.91-1.79 (m, 2H), 1.62-1.48 (m, 2H), 1.01 (t, 3H, $J = 7.4$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 152.5, 144.9, 143.3, 129.1, 128.8, 126.9, 126.6, 126.5, 112.8, 68.0, 31.0, 19.2, 13.8; IR (neat, cm^{-1}) 2960, 2873, 1604, 1496, 1464, 1427, 1380, 1347, 1275, 1213, 1184, 1141, 1067, 1026, 874, 851, 781, 750, 615; Anal Calcd. for $\text{C}_{13}\text{H}_{15}\text{NO}$: C, 77.58; H, 7.51. Found: C, 77.45; H, 7.59.

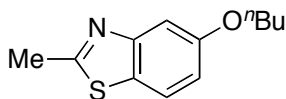


6-Butoxyquinoline: Following procedure A, 6-chloroquinoline (163.6 mg, 1 mmol), 1-butanol (183 μL , 2 mmol), (allylPdCl) $_2$ (1.83 mg, 0.5 mol%), RockPhos (7.03 mg, 1.5 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), and toluene were heated at 90 $^\circ\text{C}$ for 5 h. The crude product was purified by flash column chromatography (silica gel, 5:1 hexanes:EtOAc) to afford the title compound as a colorless oil (188.4 mg, 94% yield): ^1H NMR (300 MHz, CDCl_3) δ 8.74 (dd, 1H, $J = 1.5, 4.3$ Hz), 8.01 (d, 1H, $J = 8.1$ Hz), 7.98 (d, 1H, $J = 9.1$ Hz), 7.36 (dd, 1H, $J = 2.7, 9.1$ Hz), 7.32 (dd, 1H, $J = 8.1, 4.3$ Hz), 7.04 (d, 1H, $J = 2.7$ Hz), 4.06 (t, 2H, $J = 6.5$ Hz), 1.88-1.77 (m, 2H), 1.60-1.46 (m, 2H), 0.99 (t, 3H, $J = 7.4$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 157.2, 147.8, 144.3, 134.7, 130.8, 129.3, 122.5, 121.3, 105.7, 67.9, 31.2, 19.3, 13.8; IR (neat, cm^{-1}) 2959, 2936, 2873, 1623, 1596, 1501, 1464, 1379, 1324,

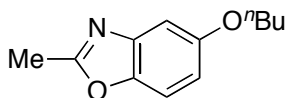
1262, 1226, 1171, 1113, 1035, 977, 923, 834, 618; Anal Calcd. for C₁₃H₁₅NO: C, 77.58; H, 7.51. Found: C, 77.33; H, 7.58.



4-Butoxyisoquinoline: Following procedure A, 4-bromoisoquinoline (208.1 mg, 1 mmol), *n*-BuOH (275 μ L, 3 mmol), (allylPdCl)₂ (1.83 mg, 0.5 mol%), RockPhos (7.03 mg, 1.5 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), and toluene were heated at 90 °C for 10 h. The crude product was purified by flash column chromatography (silica gel, 4:1 hexanes:EtOAc) to afford the title compound as a yellow liquid (161.8 mg, 80% yield): ¹H NMR (300 MHz, CDCl₃) δ 8.88 (s, 1H), 8.22 (d, 1H, J = 8.4 Hz), 8.07 (s, 1H), 7.92 (d, 1H, J = 7.0 Hz), 7.72-7.57 (m, 2H), 4.22 (t, 2H, J = 6.5 Hz), 1.92 (pentet, 2H, J = 7.0 Hz), 1.60 (sextet, 2H, J = 6.2 Hz), 1.03 (t, 3H, J = 7.4 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 149.9, 144.9, 129.3, 129.0, 128.2, 127.4, 126.7, 123.6, 121.1, 68.2, 31.3, 19.3, 13.8; IR (neat, cm⁻¹) 2959, 2935, 2872, 1580, 1502, 1459, 1400, 1327, 1283, 1158, 1123, 1093, 962, 852, 781, 754, 591.

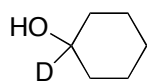


5-Butoxy-2-methylbenzothiazole: Following procedure A, 5-chloro-2-methylbenzothiazole (183.7 mg, 1 mmol), 1-butanol (183 μ L, 2 mmol), (allylPdCl)₂ (1.83 mg, 0.5 mol%), RockPhos (7.03 mg, 1.5 mol%), Cs₂CO₃ (489 mg, 1.5 mmol), and toluene were heated at 90 °C for 15 h. The crude product was purified by flash column chromatography (silica gel, 7:1 hexanes:EtOAc) to afford the title compound as brown solids (193.1 mg, 87% yield): m.p. 40–42 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.64 (d, 1H, J = 8.8 Hz), 7.43 (d, 1H, J = 2.4 Hz), 6.98 (dd, 1H, J = 8.8, 2.4 Hz), 4.02 (t, 2H, J = 6.5 Hz), 2.80 (s, 3H), 1.85-1.74 (m, 2H), 1.58-1.44 (m, 2H), 0.98 (t, 3H, J = 7.4 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 168.0, 158.2, 154.6, 127.1, 121.5, 115.0, 105.8, 68.0, 31.2, 20.1, 19.2, 13.8; IR (neat, cm⁻¹) 2957, 2930, 2868, 1602, 1558, 1521, 1457, 1323, 1279, 1169, 1068, 1009, 840, 643; Anal Calcd. for C₁₂H₁₅NOS: C, 65.12; H, 6.83. Found: C, 65.32; H, 6.75.



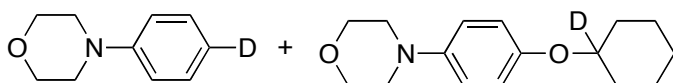
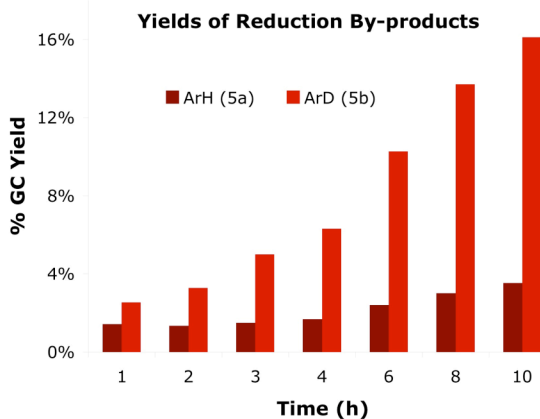
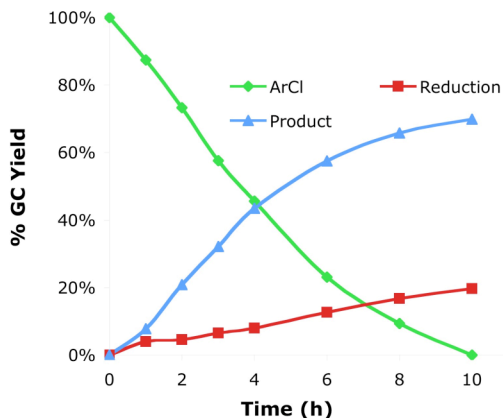
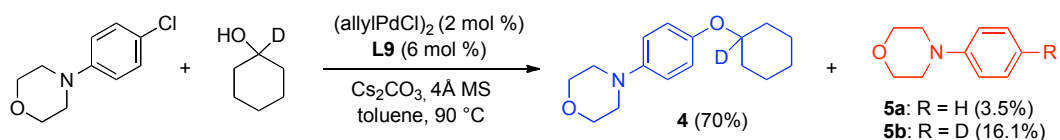
5-Butoxy-2-methylbenzoxazole: Following procedure A, 5-chloro-2-methylbenzoxazole (167.6 mg, 1 mmol), 1-butanol (183 μ L, 2 mmol), (allylPdCl)₂ (3.66 mg, 1 mol%), RockPhos (11.25 mg, 2.4 mol%),

Cs₂CO₃ (489 mg, 1.5 mmol), and toluene were heated at 90 °C for 21 h. The crude product was purified by flash column chromatography (silica gel, 5:1 hexanes:EtOAc) to afford the title compound as a colorless oil (180.2 mg, 88% yield): ¹H NMR (300 MHz, CDCl₃) δ 7.32 (d, 1H, J = 8.9 Hz), 7.12(d, 1H, J = 2.5 Hz), 6.87 (dd, 1H, J = 8.9, 2.5 Hz), 3.98 (t, 2H, J = 6.5 Hz), 2.60 (s, 3H), 1.83-1.72 (m, 2H), 1.57-1.43 (m, 2H), 0.98 (t, 3H, J = 7.4 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 164.5, 156.5, 145.5, 142.3, 113.2, 110.2, 103.5, 68.5, 31.3, 19.2, 14.6, 13.8; IR (neat, cm⁻¹) 2960, 2930, 2873, 1576, 1472, 1438, 1382, 1283, 1172, 1158, 927, 846, 804, 664; Anal Calcd. for C₁₂H₁₅NO₂: C, 70.22; H, 7.37. Found: C, 70.06; H, 7.45.



1-Deuteriocyclohexanol was prepared according the literature procedure.¹⁰ To a suspension of LiAlD₄ (4.20 g, 100 mmol) in ether (250 mL) was added a solution of cyclohexanone (10.36 mL, 100 mmol) in ether (50 mL) by syringe pump over 1 h at room temperature under argon. The reaction mixture was stirred at room temperature overnight and quenched by sequentially adding H₂O (4.2 mL), 15% aqueous NaOH (4.2 mL), and then H₂O (12.6 mL) at 0 °C with caution. The mixture was stirred at room temperature for 1 h. The white precipitate was filtered off and rinsed with hot CHCl₃ (4 × 150 mL). H₂O (100 mL) was added and the two layers were separated. The organic layer was washed with brine, dried over MgSO₄, and concentrated in vacuo. The crude product was purified by distillation (bp 79-82 °C/35 torr) to give the deuterio alcohol as a colorless oil (7.8 g, 77% yield): ¹H NMR (300 MHz, CDCl₃) δ 2.05-1.05 (m, 10H); ¹³C NMR (75 MHz, CDCl₃) δ 69.7 (t, J = 21.5 Hz), 35.3, 25.4, 24.1. The ¹H NMR and ¹³C NMR spectral data were consistent with those of the previously reported compound.¹¹

Deuterium Labeling Studies.



4-(4-Deuteriophenyl)morpholine and

4-(4-((1-deuteriocyclohexyl)oxy)phenyl)morpholine: Following procedure A, 4-(4-bromophenyl)morpholine (242.1 mg, 1 mmol), 1-deuteriocyclohexanol (160 μL , 1.5 mmol), $(\text{allylPdCl})_2$, (3.66 mg, 1 mol%), RockPhos (14.06 mg, 3 mol%), Cs_2CO_3 (489 mg, 1.5 mmol), 4 \AA molecular sieves (200 mg), and toluene were heated at 90 $^\circ\text{C}$ for 21 h. The crude product was purified by flash column chromatography (silica gel, 15:1 hexanes:EtOAc) to afford 4-(4-deuteriophenyl)morpholine (35.2 mg, 17% yield) as a white solid, followed by 4-(4-((1-deuteriocyclohexyl)oxy)phenyl)morpholine (166.8 mg, 64% yield) as a white solid.

Data for 4-(4-deuteriophenyl)morpholine: ^1H NMR (300 MHz, CDCl_3) δ 7.29 (br d, 2H, $J = 8.7$ Hz), 6.96-6.91 (m, 2H), 3.90-3.85 (m, 4H), 3.19-3.14 (m, 4H); ^{13}C NMR (75 MHz, CDCl_3) δ 151.2, 129.0, 120.0 (s, from H-incorporated), 119.7 (t, $J = 24.5$ Hz, from D-incorporated), 115.7, 66.9, 49.3; IR (neat, cm^{-1}) 2962, 2855, 2826, 1596, 1496, 1449, 1259, 1232, 1116, 927; Anal Calcd. for $\text{C}_{10}\text{H}_{12}\text{DN}_2\text{O}$: C, 73.59; H, 8.03. Found: C, 73.38; H, 7.90.

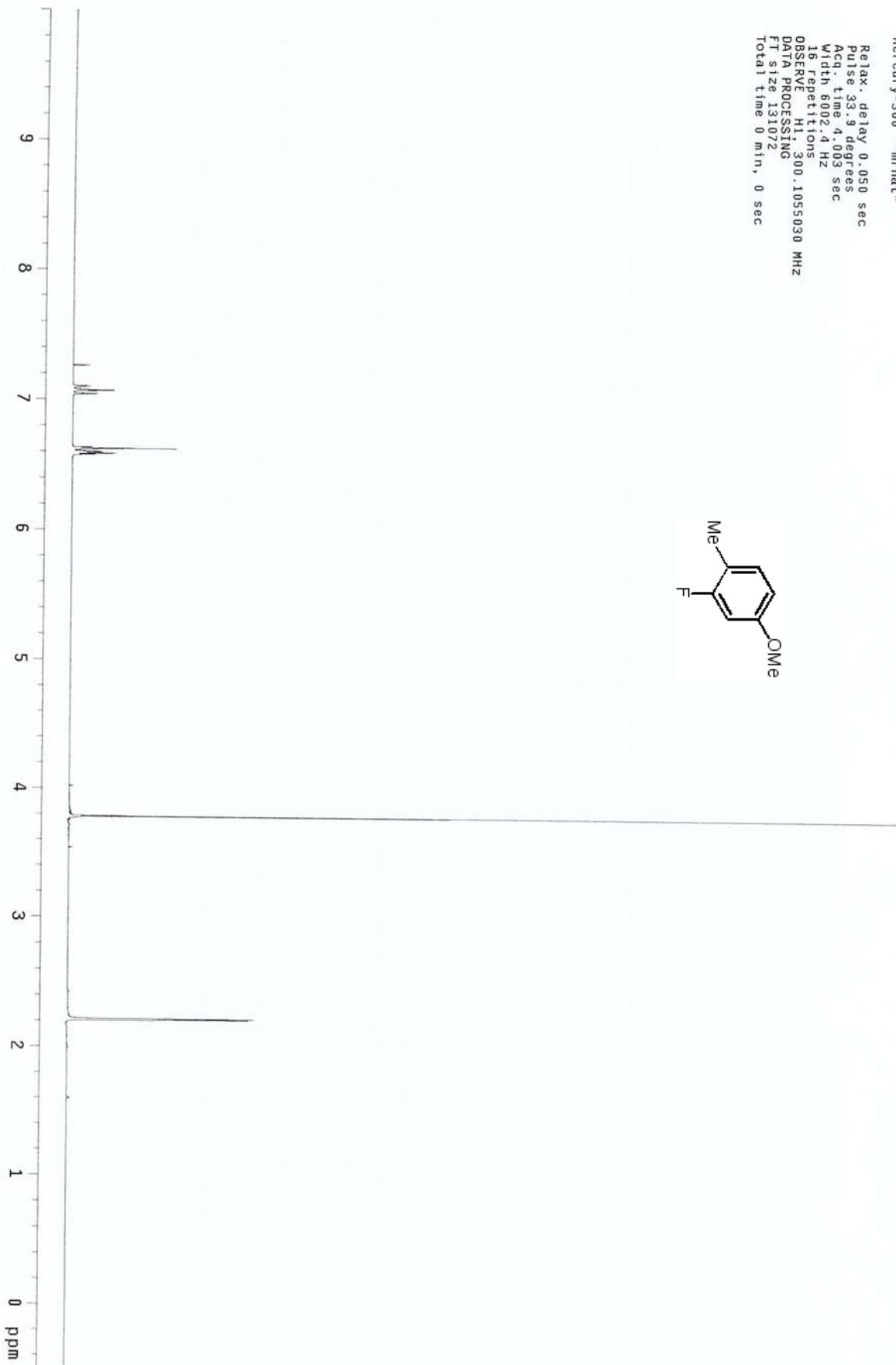
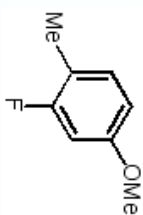
Data for 4-(4-((1-deuteriocyclohexyl)oxy)phenyl)morpholine: m.p. 67-68 °C; ¹H NMR (300 MHz, CDCl₃) δ 6.86 (s, 4H), 3.88-3.82 (m, 4H), 3.08-3.02 (m, 4H), 2.03-1.90 (m, 2H), 1.86-1.70 (m, 2H), 1.63-1.20 (m, 6H); ¹³C NMR (75 MHz, CDCl₃) δ 151.9, 145.5, 117.6, 117.2, 75.7 (t, J = 21.5 Hz), 67.0, 50.7, 31.8, 25.6, 23.8; IR (neat, cm⁻¹) 2934, 2855, 1510, 1450, 1260, 1238, 1122, 1089, 959, 930, 824; Anal Calcd. for C₁₆H₂₂DNO₂: C, 73.53; H + D, 8.87. Found: C, 73.31; H + D, 8.86.

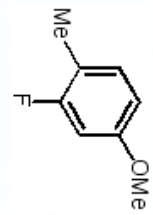
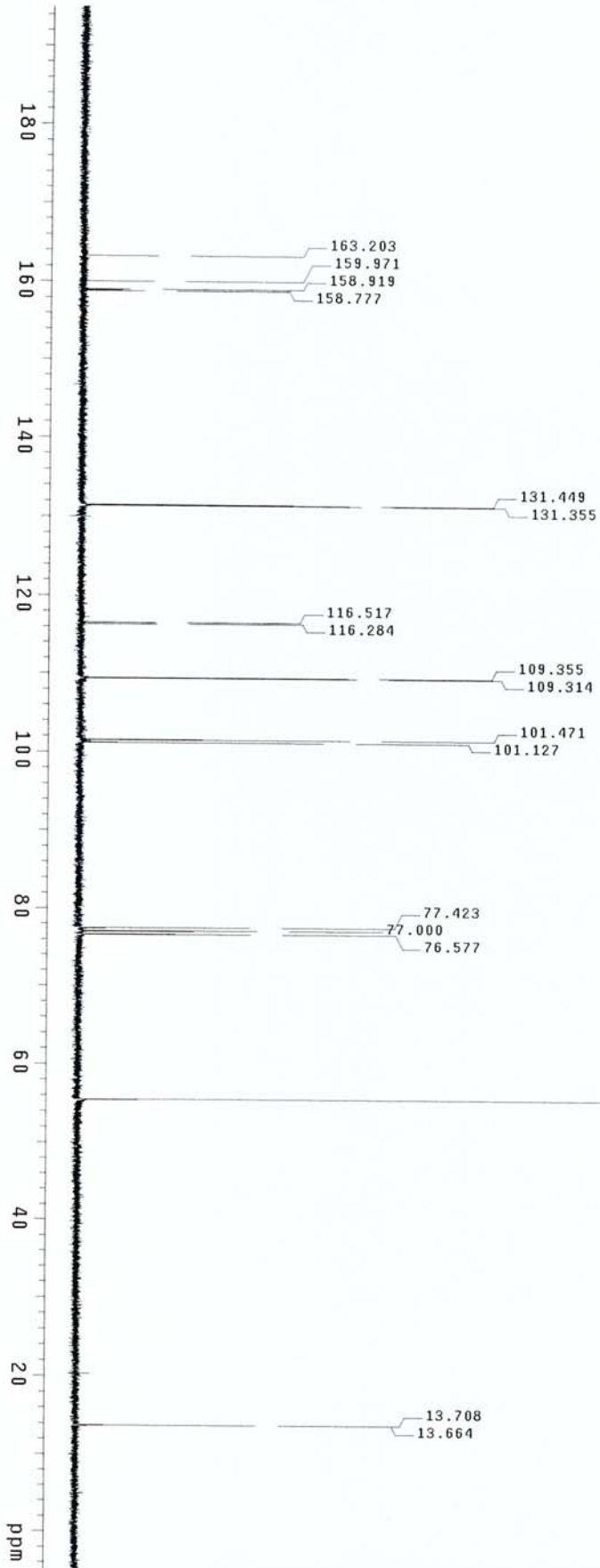
1. Fors, B. P.; Dooleweerd, K.; Zeng, Q.; Buchwald, S. L. *Tetrahedron* **2009**, *65*, 6576.
2. Hicks, J. D.; Hyde, A. M.; Cuezva, A. M.; Buchwald, S. L. *J. Am. Chem. Soc.* **2009**, *131*, 16720.
3. Han, C.; Buchwald, S. L. *J. Am. Chem. Soc.* **2009**, *131*, 7532.
4. Mattiza, J. T.; Meyer, V. J.; Duddeck, H. *Magn. Reson. Chem.* **2010**, *48*, 192.
5. Yang, C.-G.; He, C. *J. Am. Chem. Soc.* **2005**, *127*, 6966.
6. Vorogushin, A. V.; Huang, X.; Buchwald, S. L. *J. Am. Chem. Soc.* **2005**, *127*, 8146-8149.
7. Torraca, K. E.; Huang, X.; Parrish, C. A.; Buchwald, S. L. *J. Am. Chem. Soc.* **2001**, *123*, 10770-10771.
8. Boden, N.; Bushby, R. J.; Cammidge, A. N.; E1-Mansoury, A.; Martin, P. S.; Lu, Z. *J. Mater. Chem.* **1999**, *9*, 1391-1402.
9. Wolter, M.; Nordmann, G.; Job, G. E.; Buchwald, S. L. *Org. Lett.* **2002**, *4*, 973.
10. T. Hashimoto, G. K. Surya, J. G. Shih, G. A. Olah, *J. Org. Chem.* **1987**, *52*, 931.
11. A. Seifert, U. Scheffler, M. Markert, R. Mahrwald, *Org. Lett.* **2010**, *12*, 1660-1663.

wxx-1-270-2

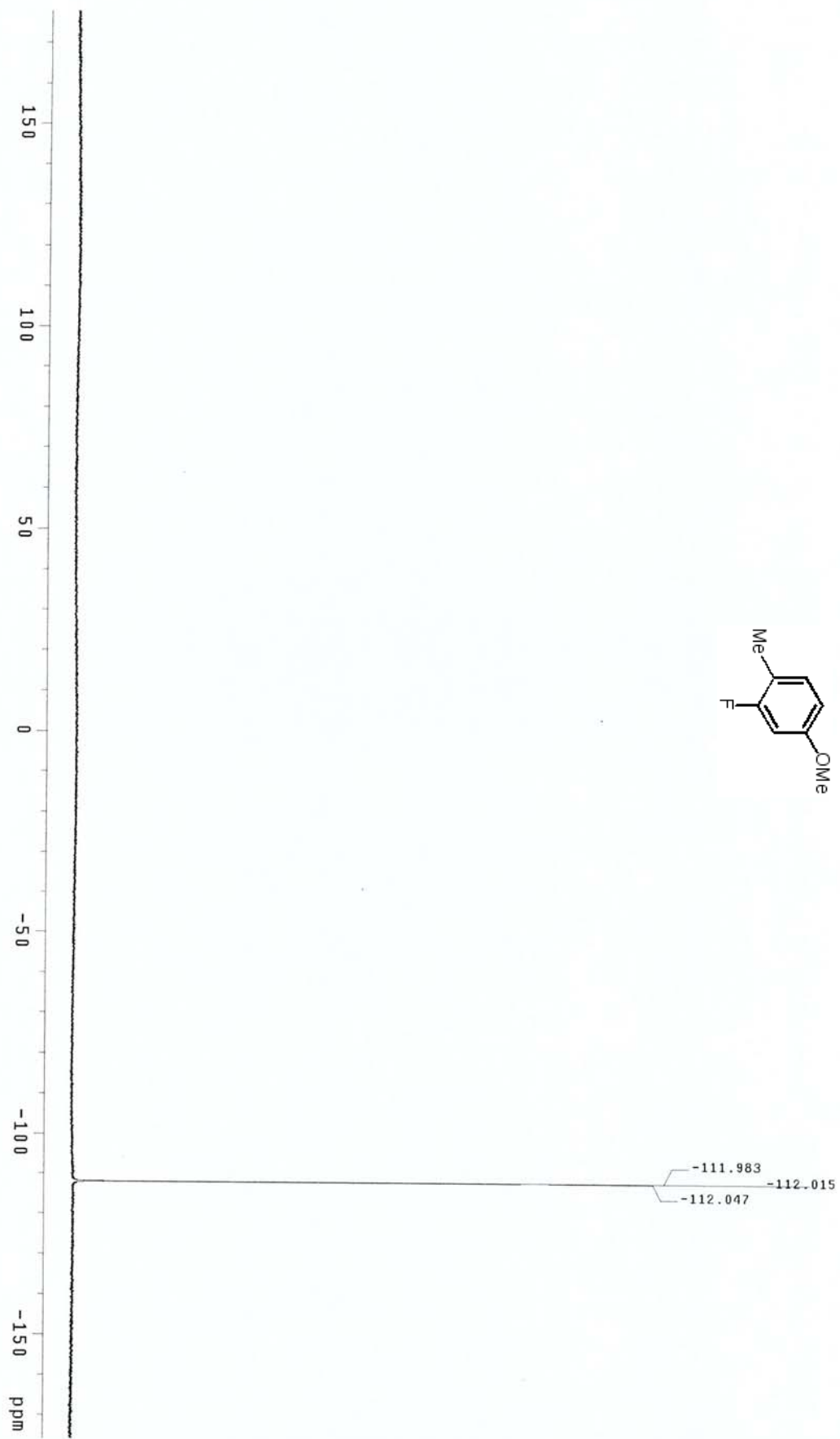
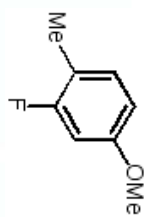
Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrat"

Relax. delay 0.050 sec
Pulse 33.9 degrees
Acq. time 4.003 sec
Width 6002.4 Hz
16 repetitions
OBSERVE HI 300.1055030 MHZ
DATA PROCESSING
FT size 131072
Total time 0 min, 0 sec





wxx-1-270-2f
Pulse Sequence: s2pu1



wxx-1-286-3

Pulse Sequence: s2pul

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

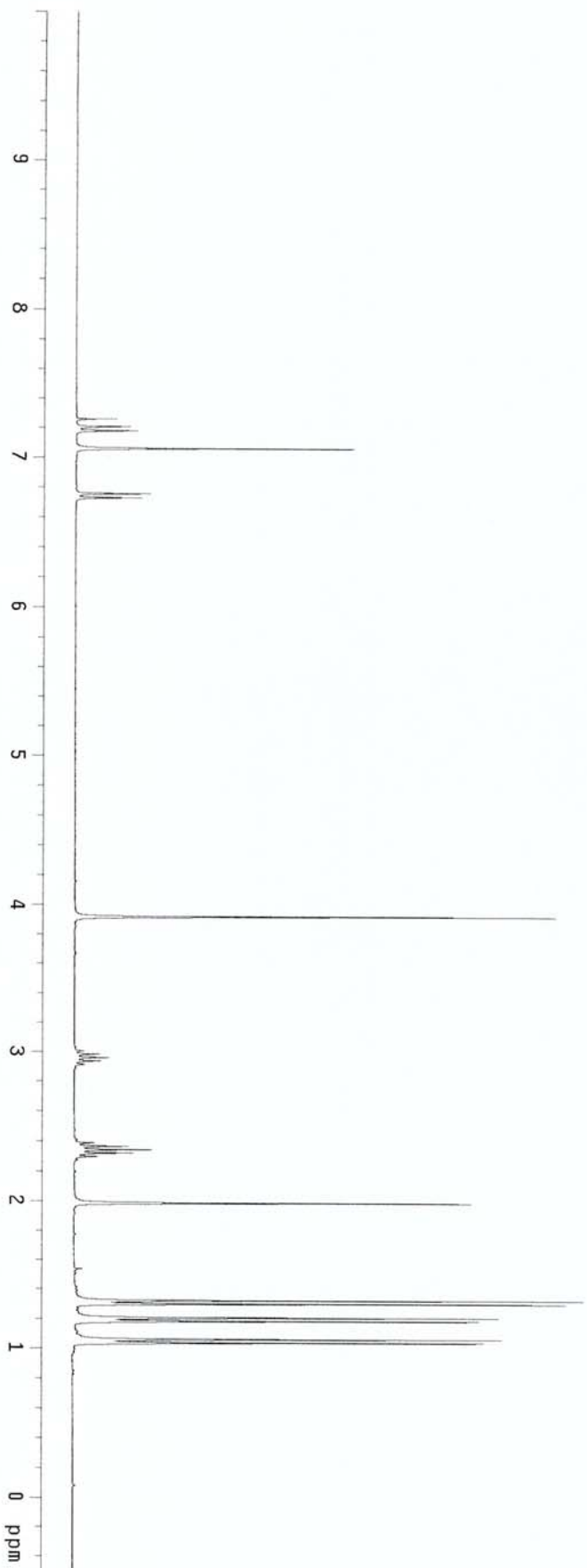
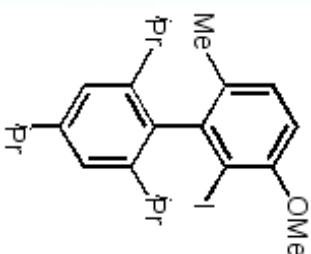
17 repetitions

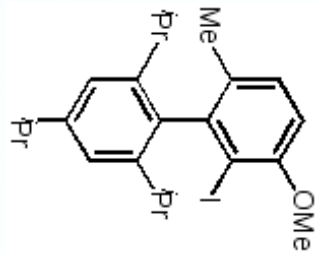
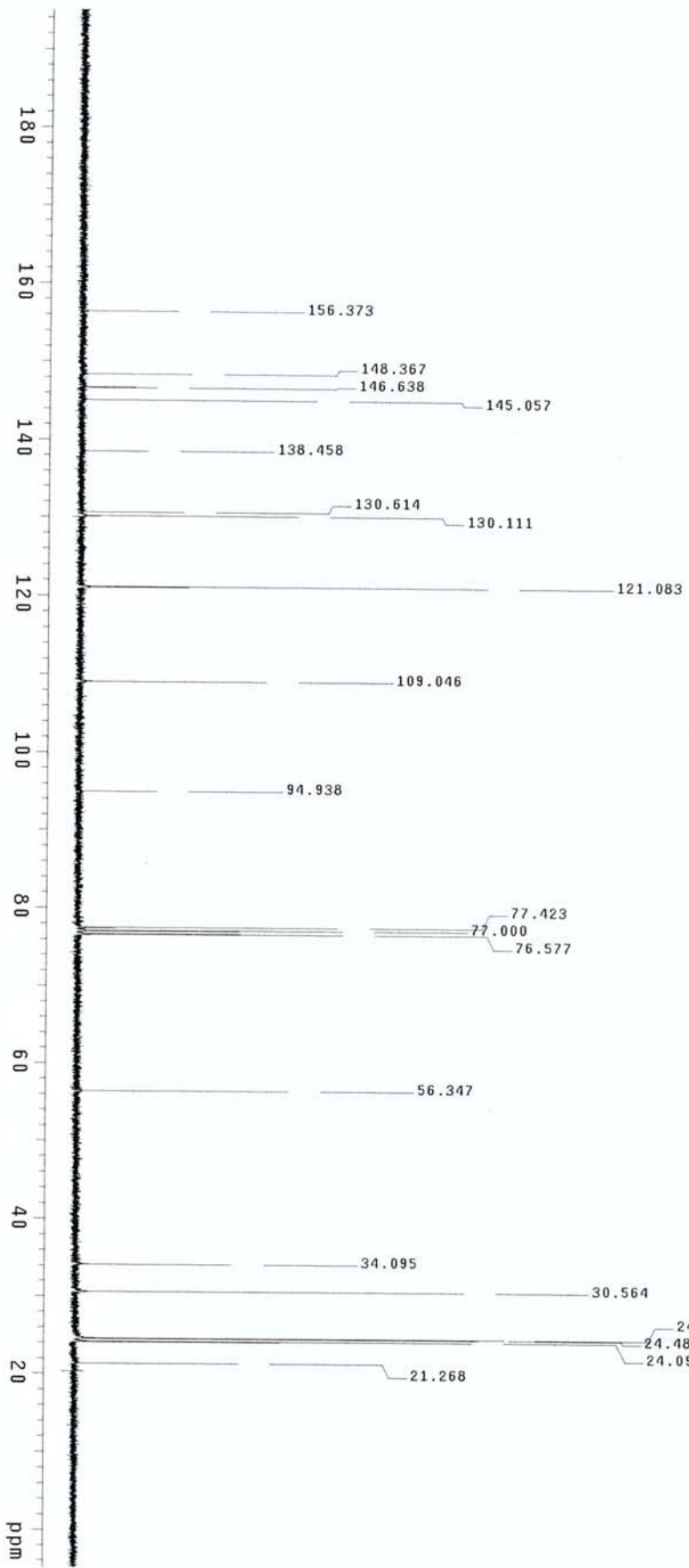
OBSERVE H1 300.1055034 MHz

DATA PROCESSING

FT size 131072

Total time 0 min, 0 sec

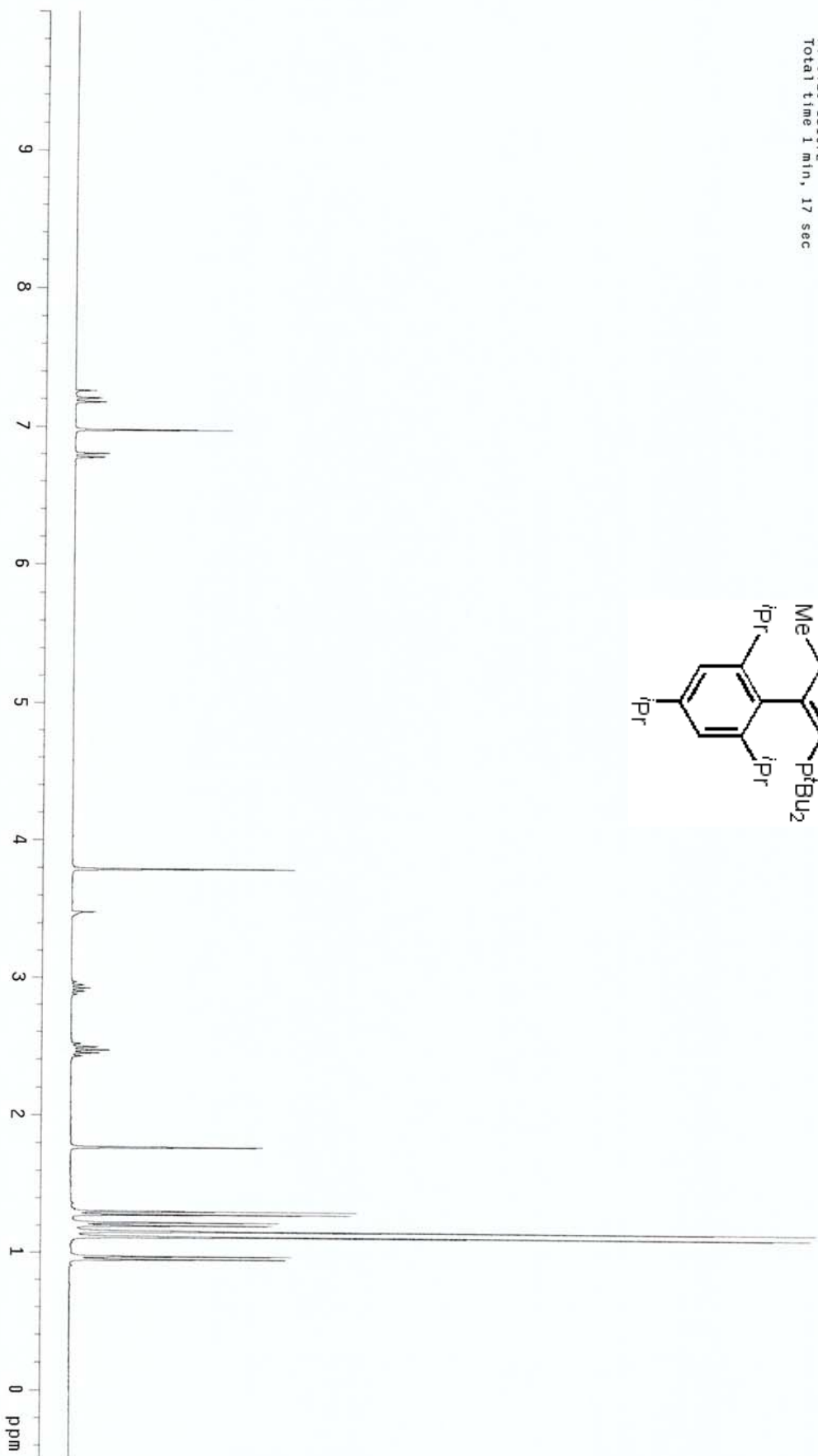
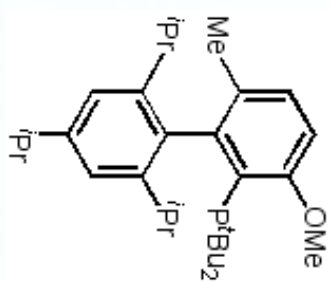


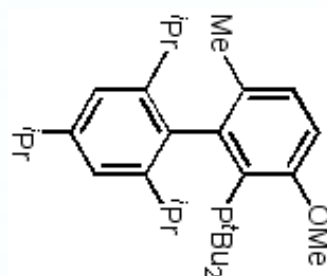
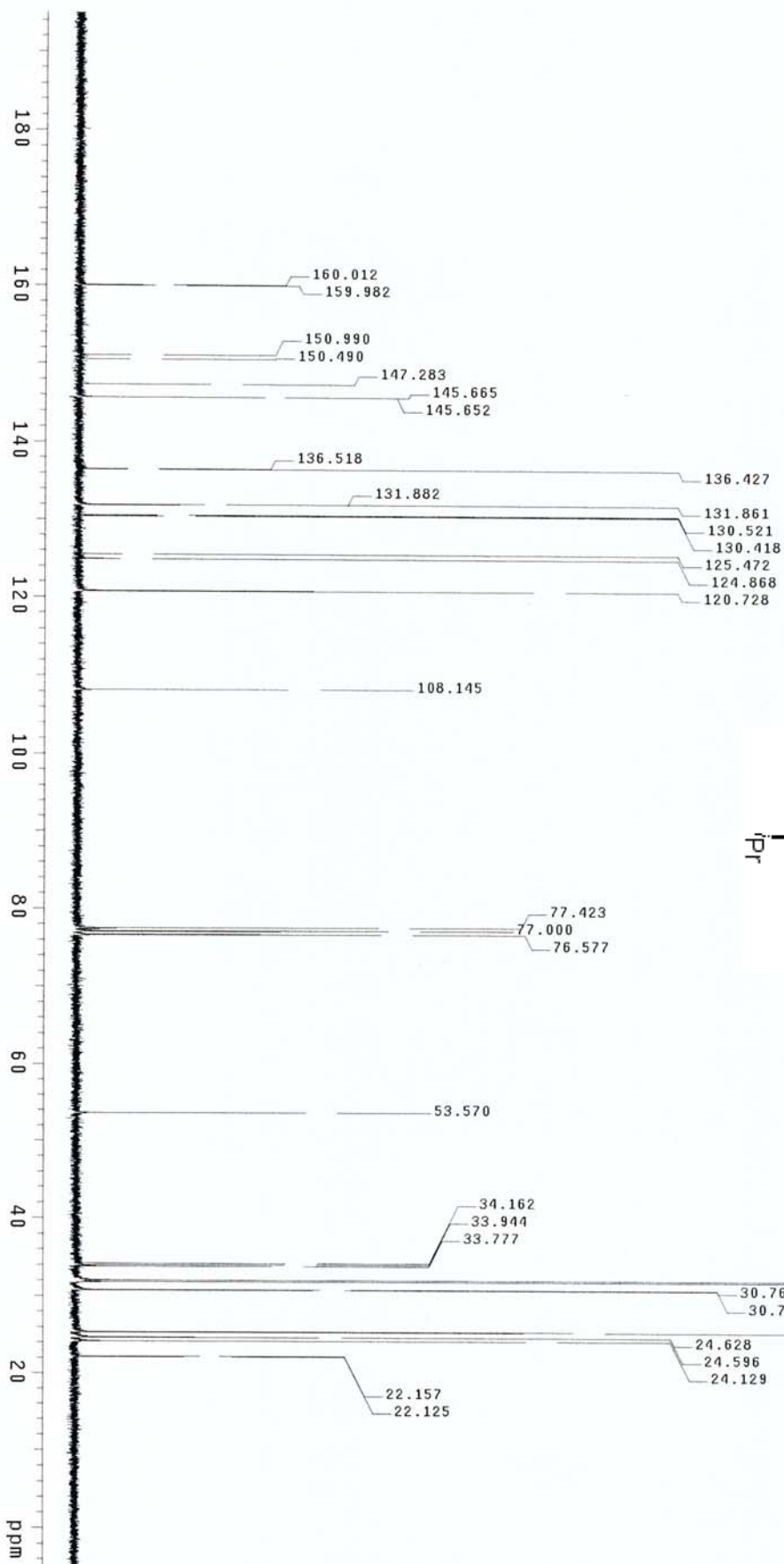


wxx-1-245-4

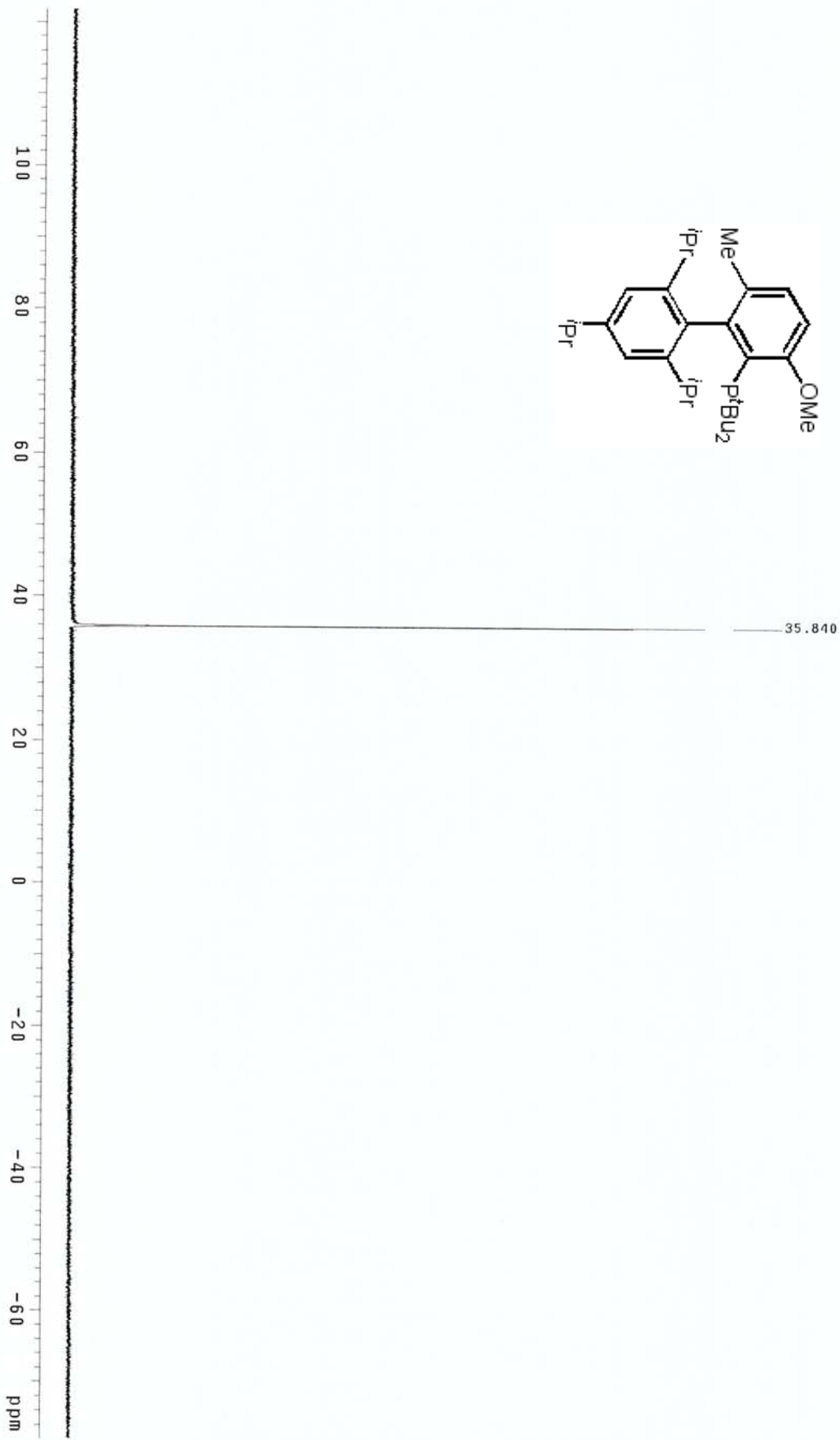
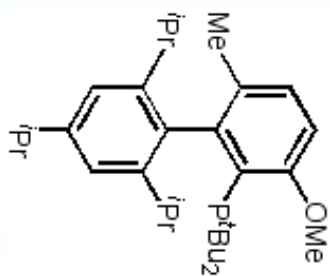
Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhlt"

Relax. delay 0.050 sec
Pulse 33.9 degrees
Acq. time 4.003 sec
Width 6002.4 Hz
16 repetitions
OBSERVE H1 300.1055033 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 17 sec





wxx-1-245-4p
Pulse Sequence: s2pu1



wxx-1-269-1

Pulse Sequence: s2pul1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse: 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

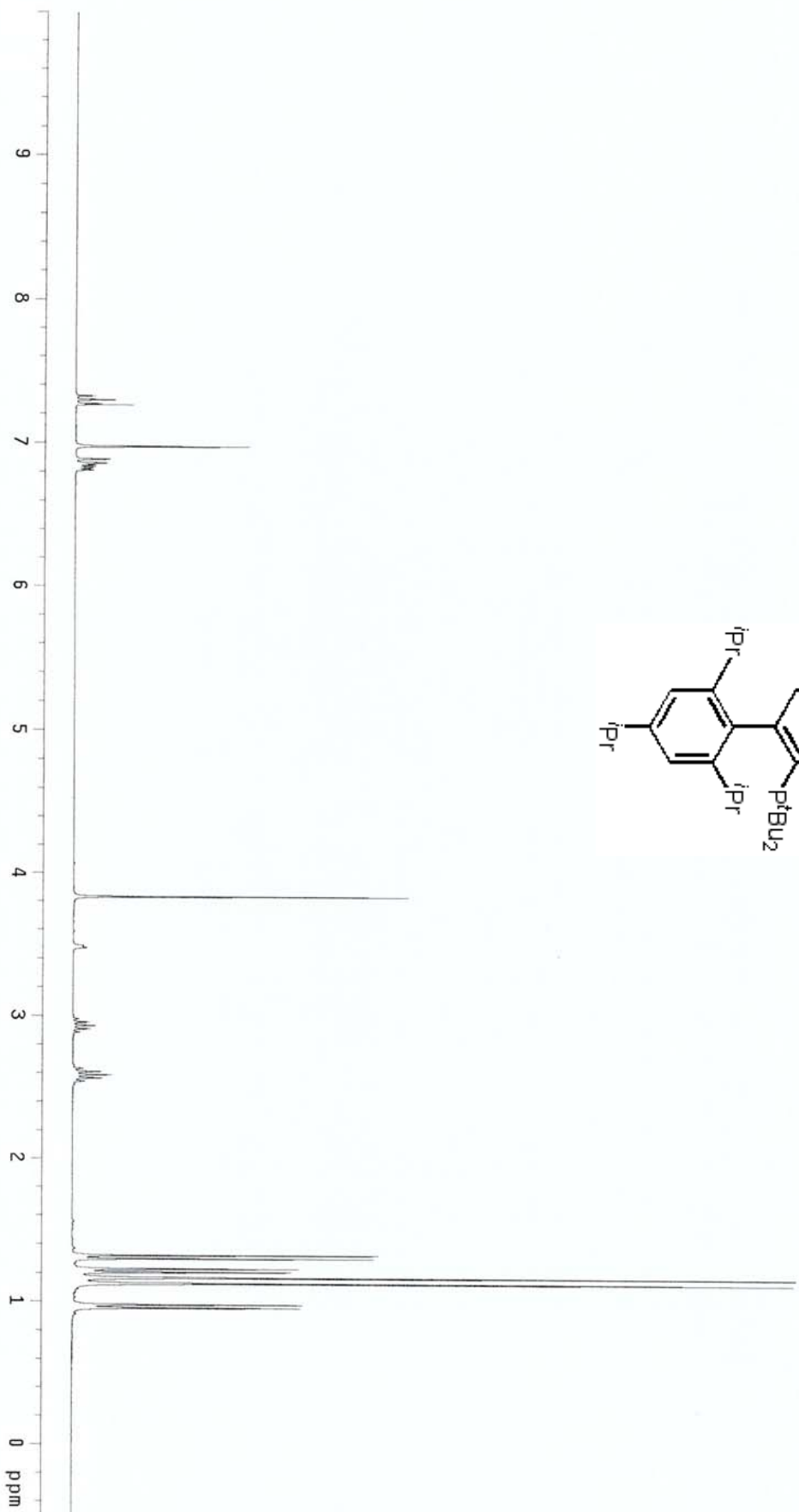
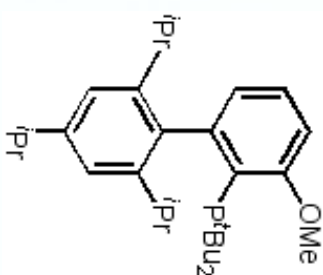
18 repetitions

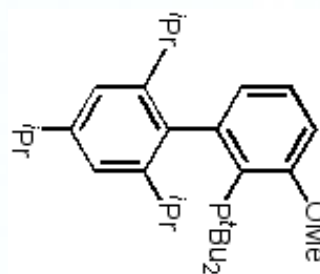
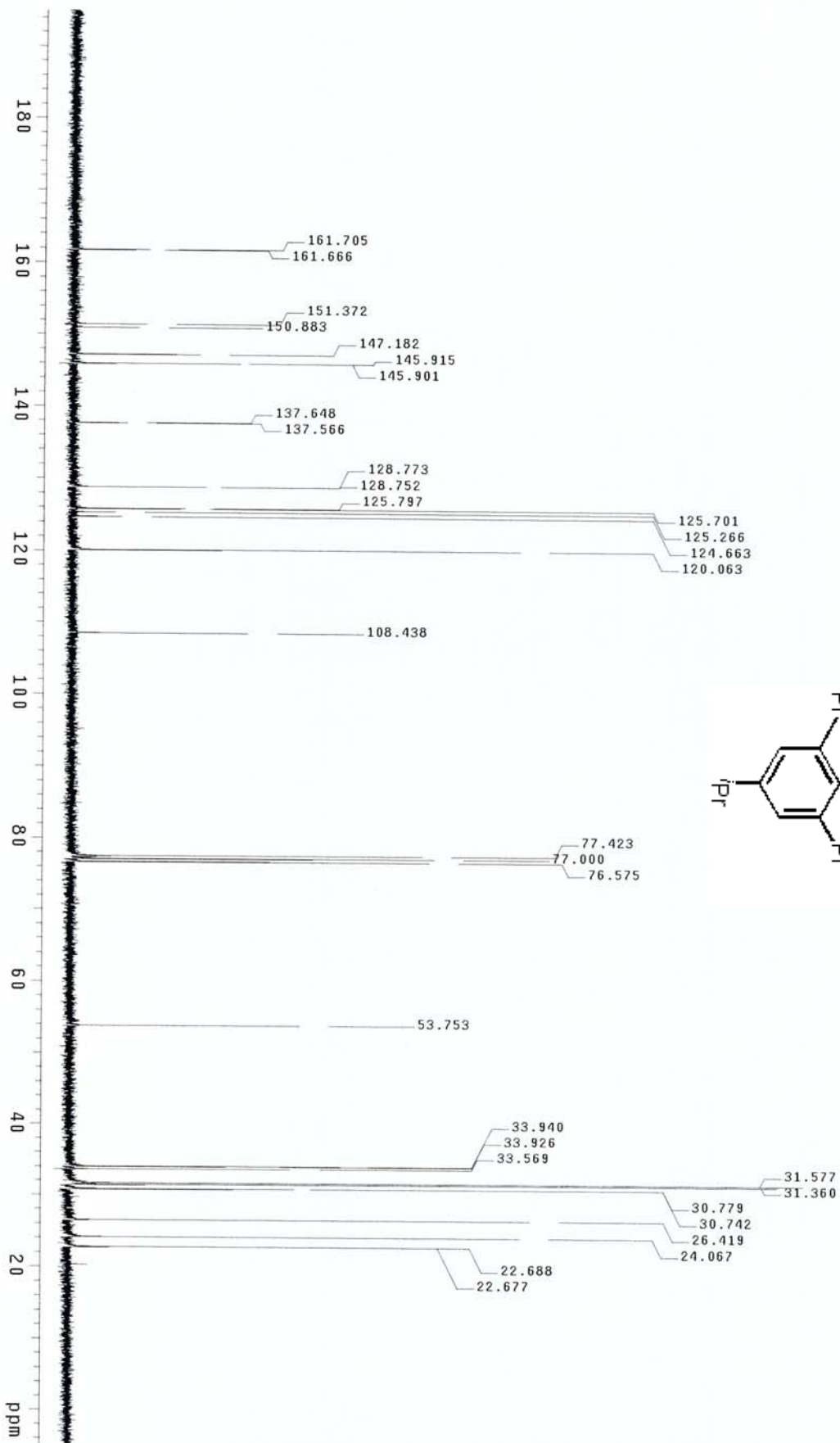
OBSERVE H1: 300.1055034 MHz

DATA PROCESSING

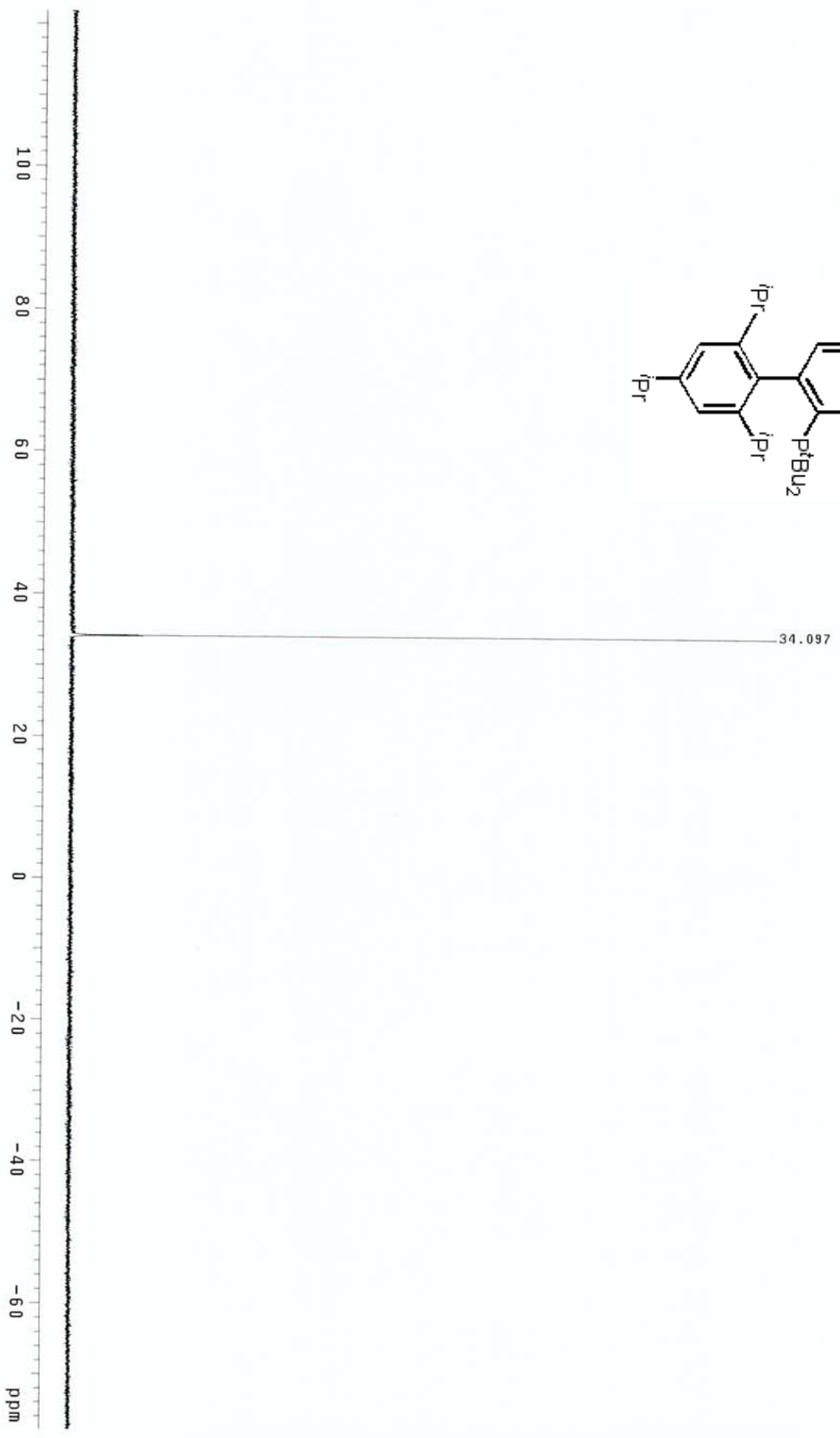
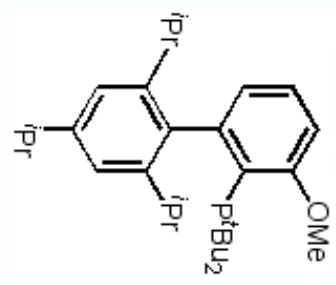
FT size 131072

Total time 1 min, 17 sec





wxx-1-269-1P
Pulse Sequence: s2pu1



wxx-2-105-3

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse: 33.9 degrees

Acq. time: 4.005 sec

Width: 6002.4 Hz

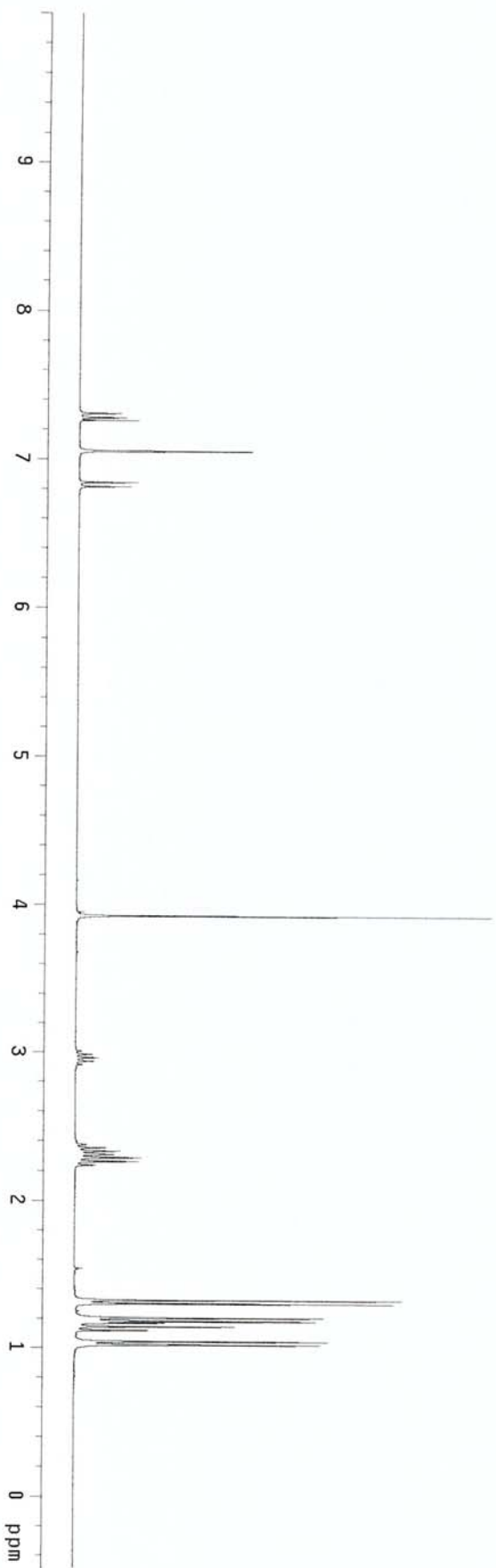
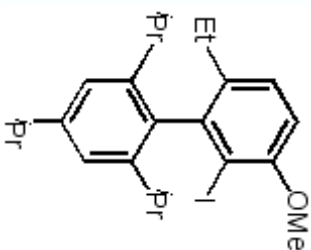
18 repetitions

OBSERVE H1: 300.1055029 MHz

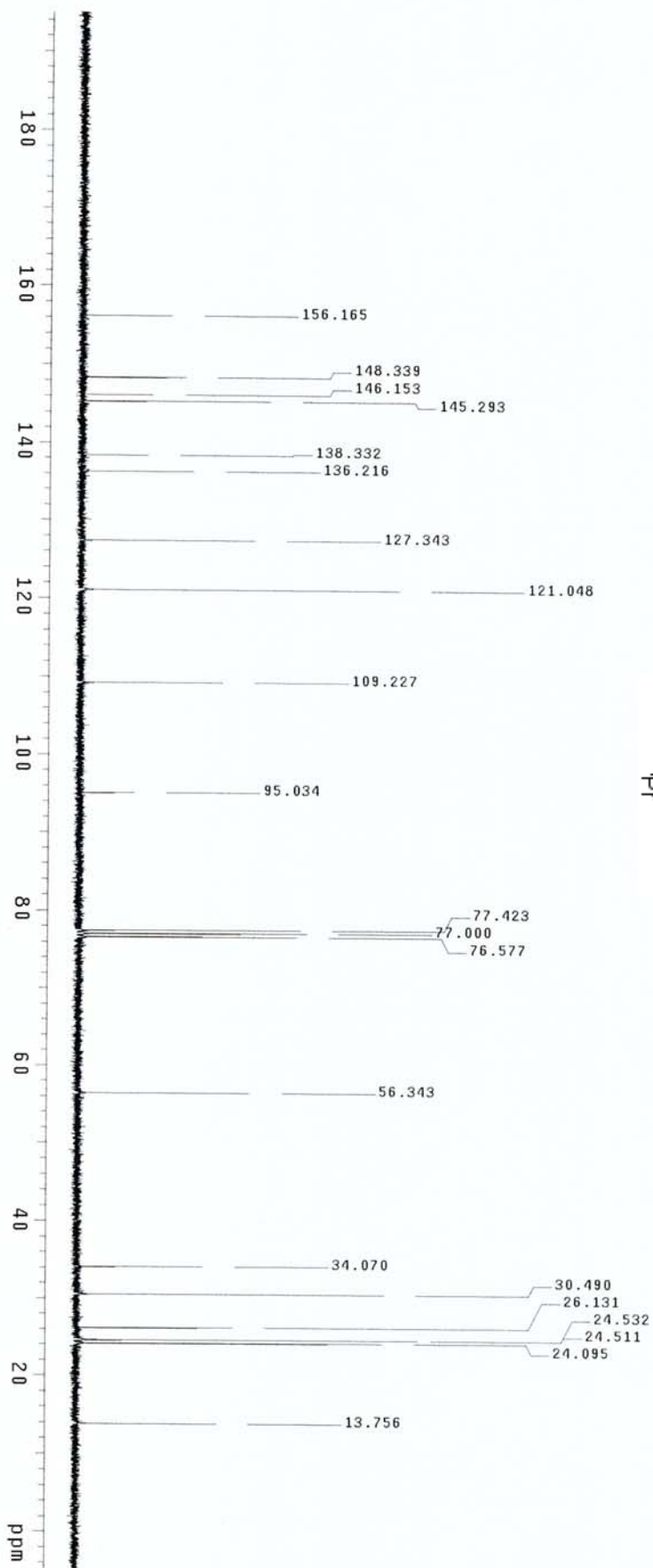
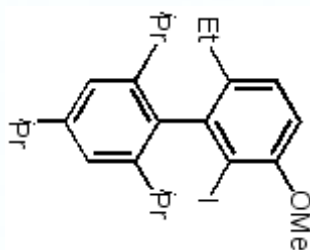
DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec



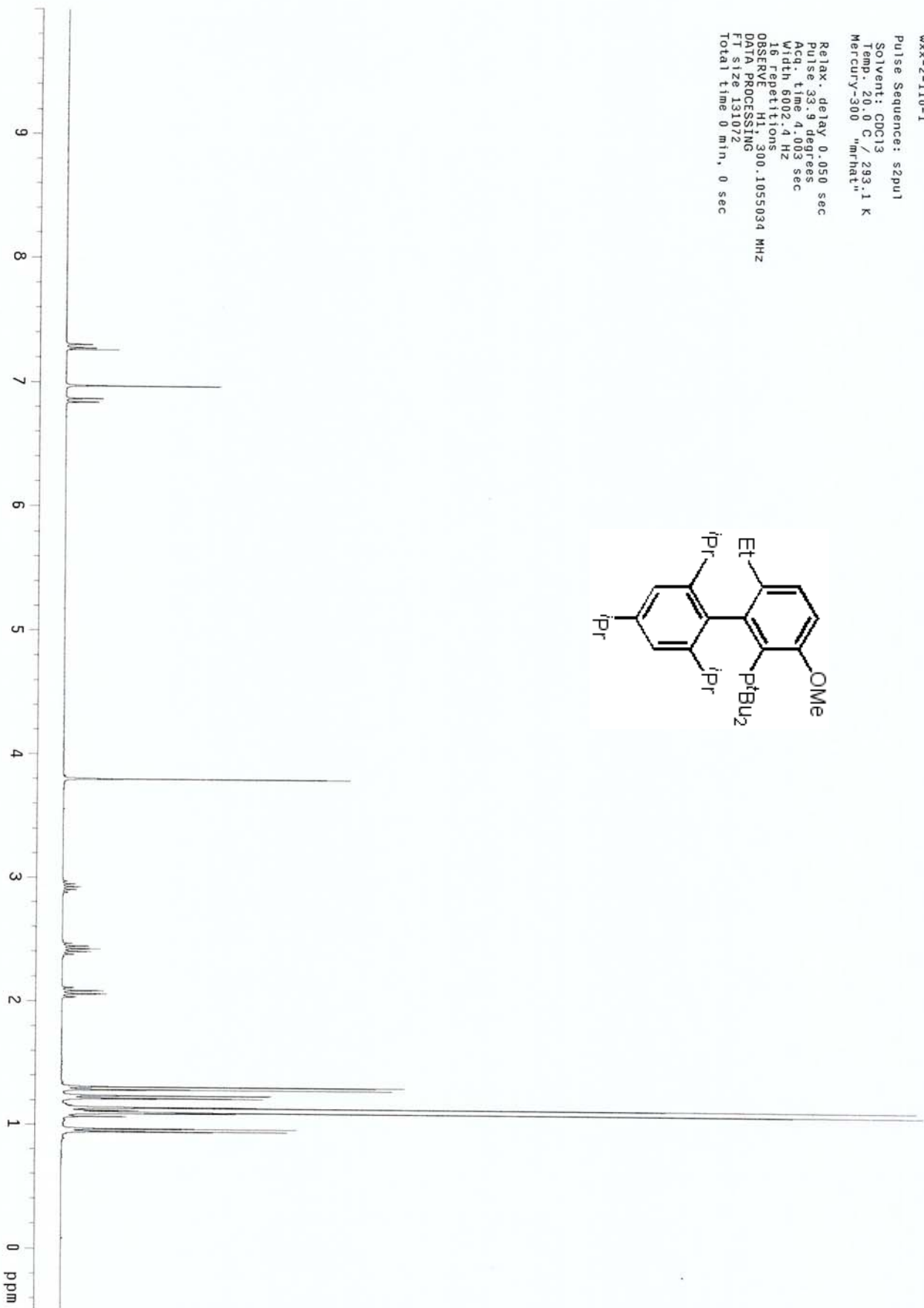
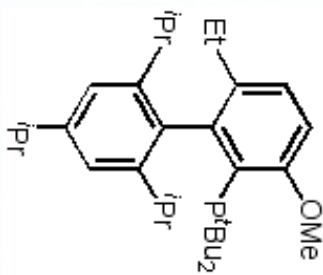
wxx-2-105-3C
Pulse Sequence: s2pu1

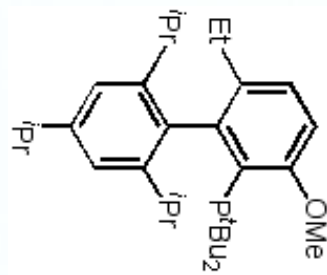
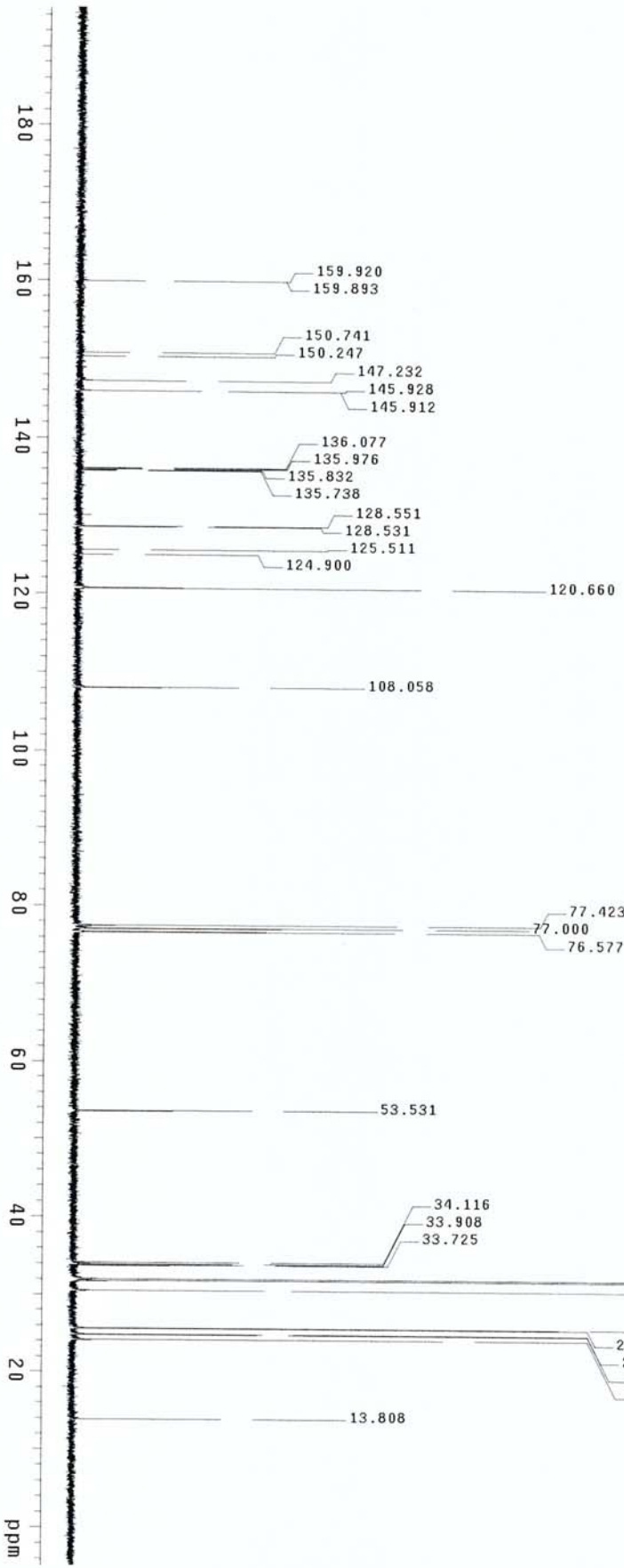


wxx-2-110-1

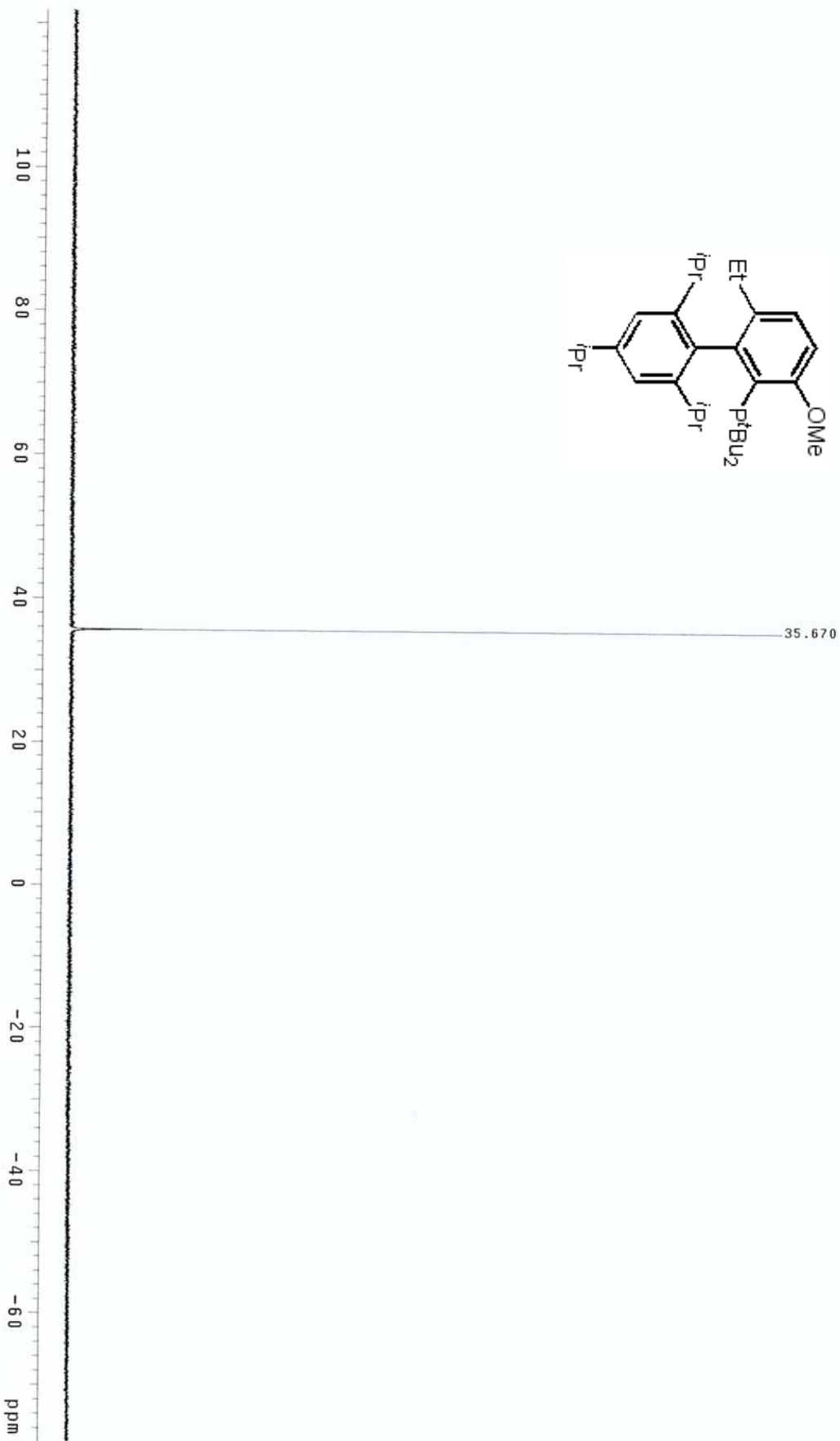
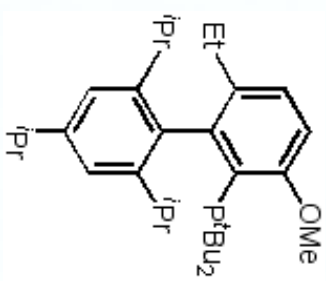
Pulse Sequence: s2pul1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhat"

Relax. delay 0.050 sec
Pulse: 33.9 degrees
Acq. time 4.003 sec
Width 6002.4 Hz
18 Repetitions
OBSERVE H1: 300.1055034 MHz
DATA PROCESSING
F1 size 131072
Total time 0 min, 0 sec





wxx-2-110-1P
Pulse Sequence: s2pu1



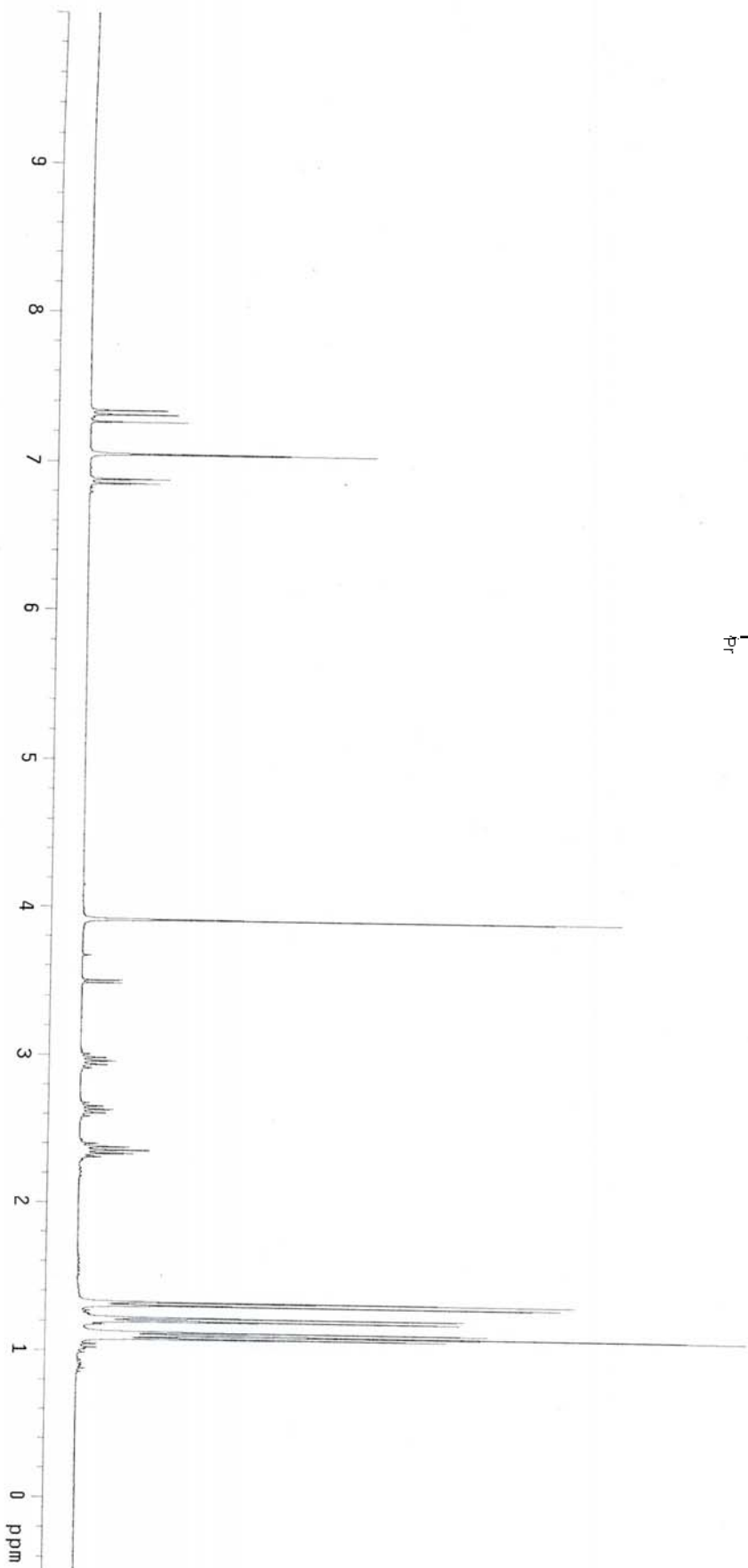
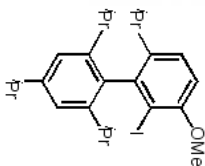
wxx-2-200-4

Pulse Sequence: szpul1

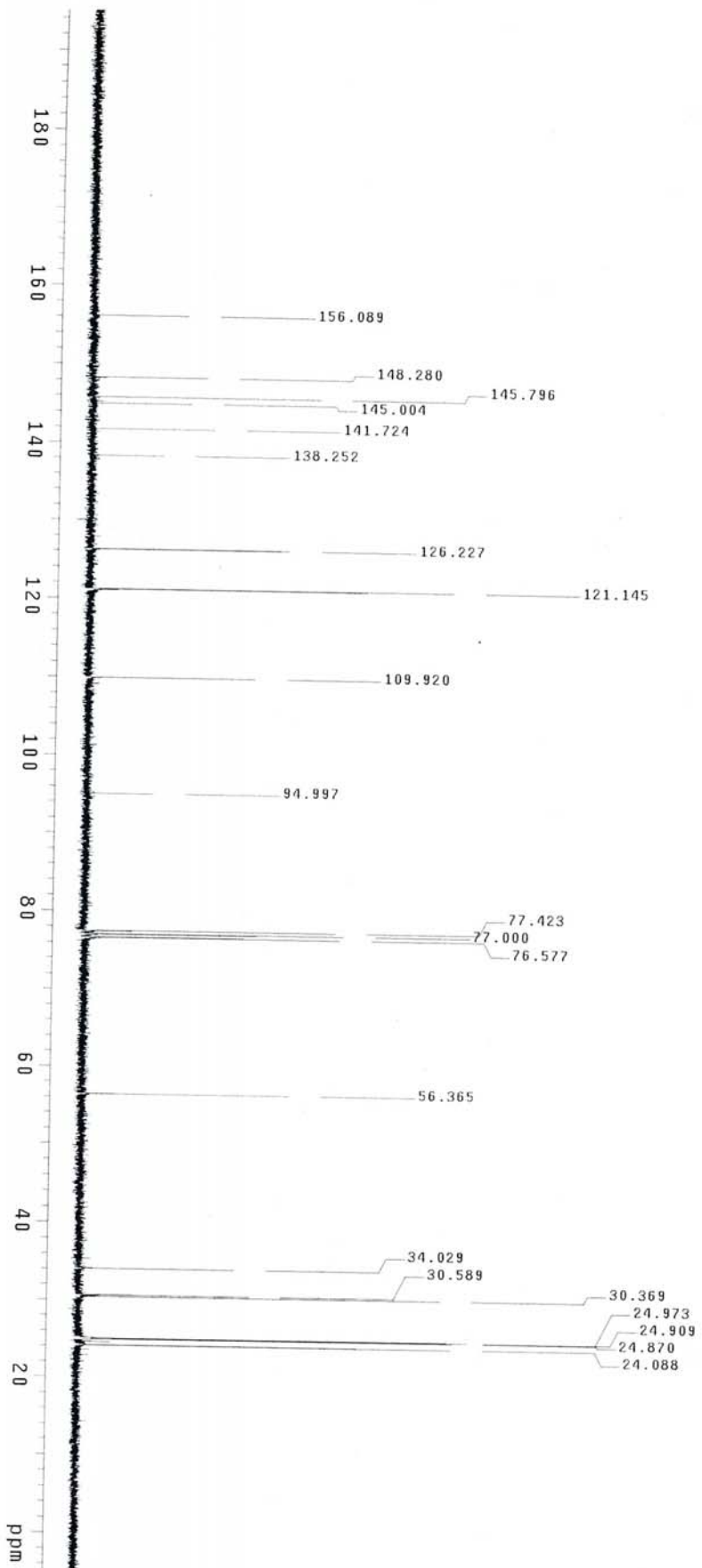
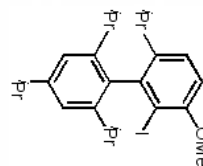
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhah"

Relax. delay: 0.050 sec
Pulse: 33.9 degrees
Acq. time: 4.003 sec
Width: 6002.4 Hz

16 repetitions
OBSERVE: H1, 300.1055032 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 17 sec



wxx-2-200-4c
Pulse Sequence: s2pu1



wxx-2-202-5

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

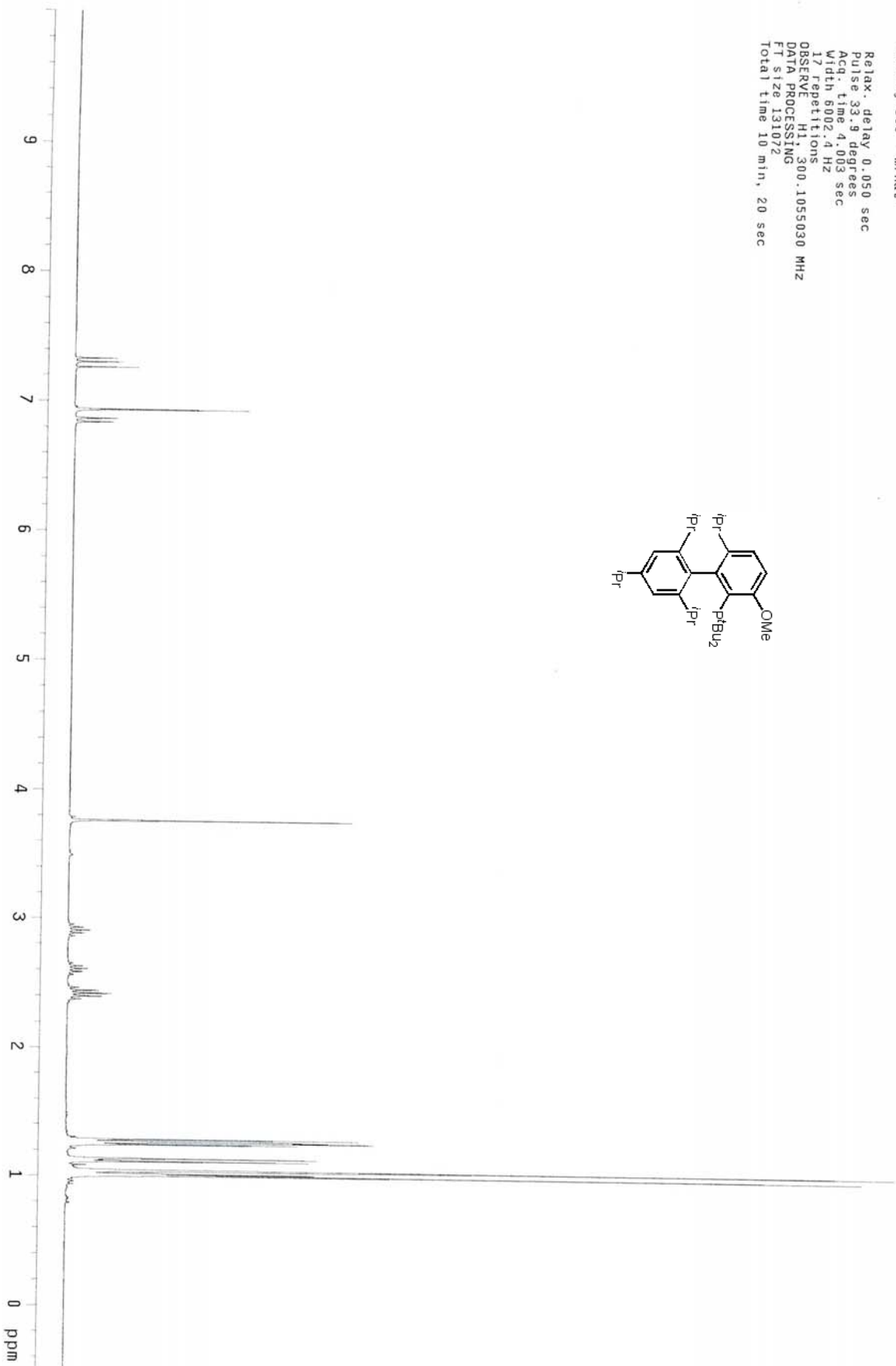
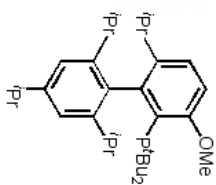
12 repetitions

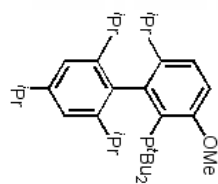
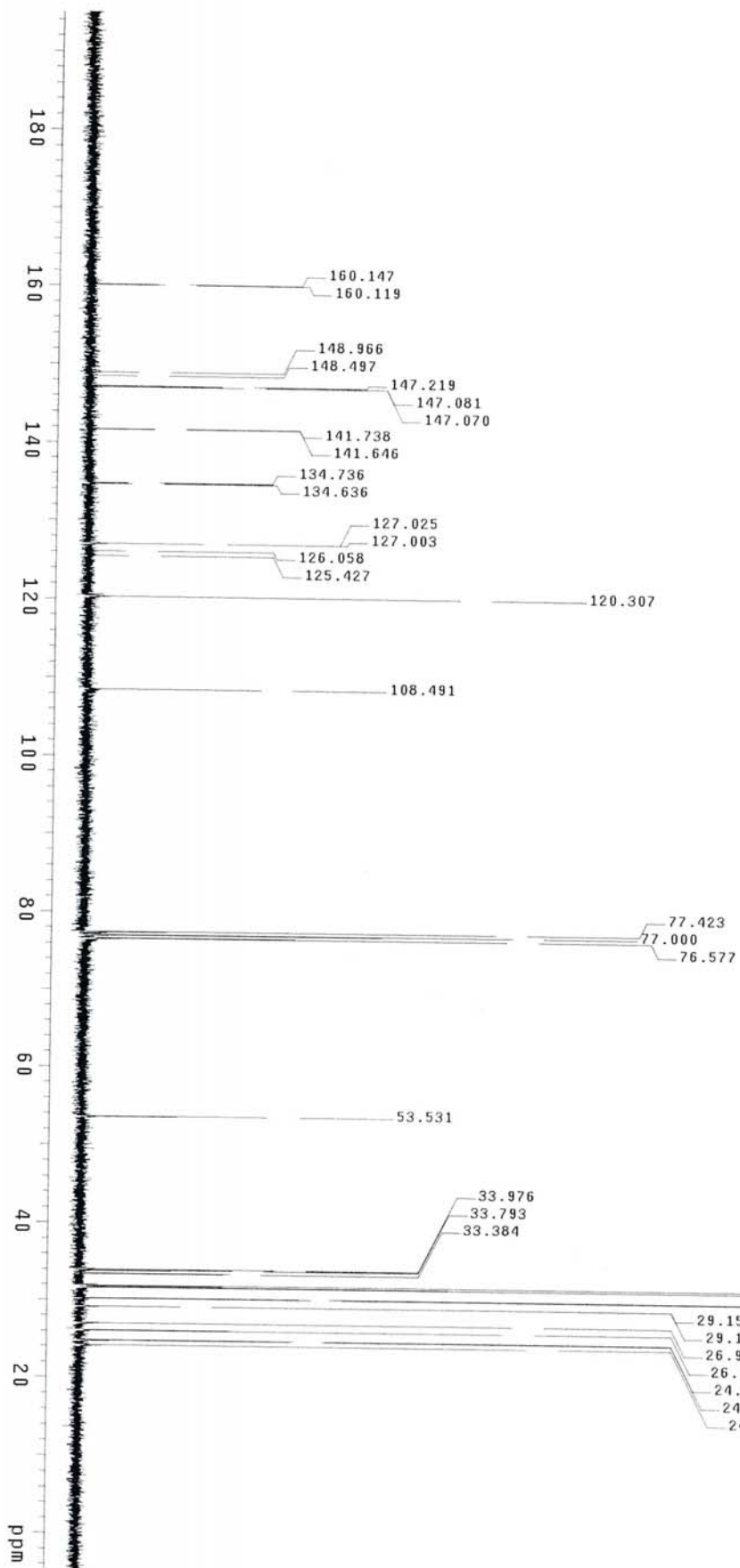
OBSERVE H1, 300.1055030 MHz

DATA PROCESSING

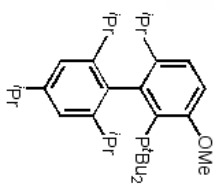
FT size 131072

Total time 10 min, 20 sec





wxx-2-202-5p
Pulse Sequence: szpu1



37.468



wxx-1-267-2

Pulse Sequence: s2pul1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

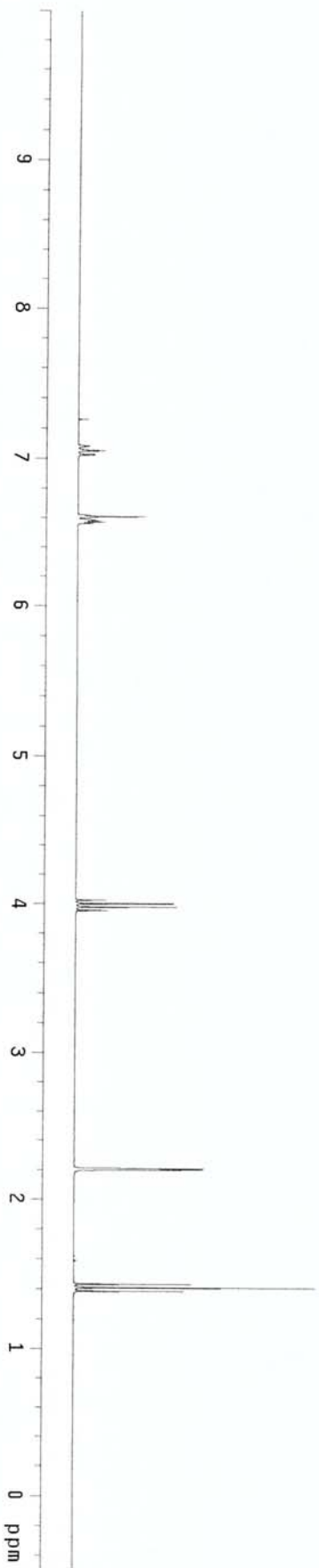
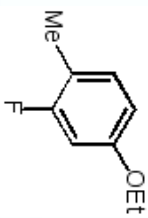
16 repetitions

OBSERVE H1, 300.1055029 MHz

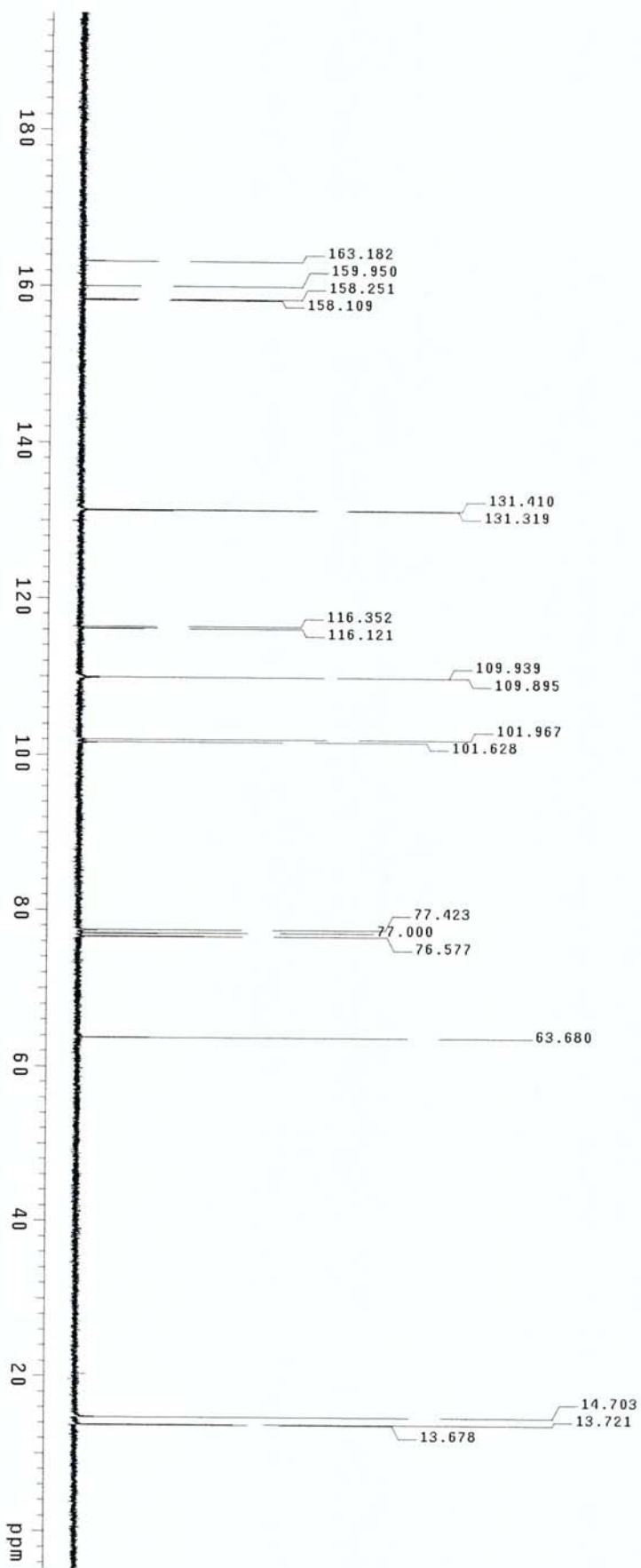
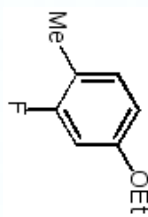
DATA PROCESSING

FT size 131072

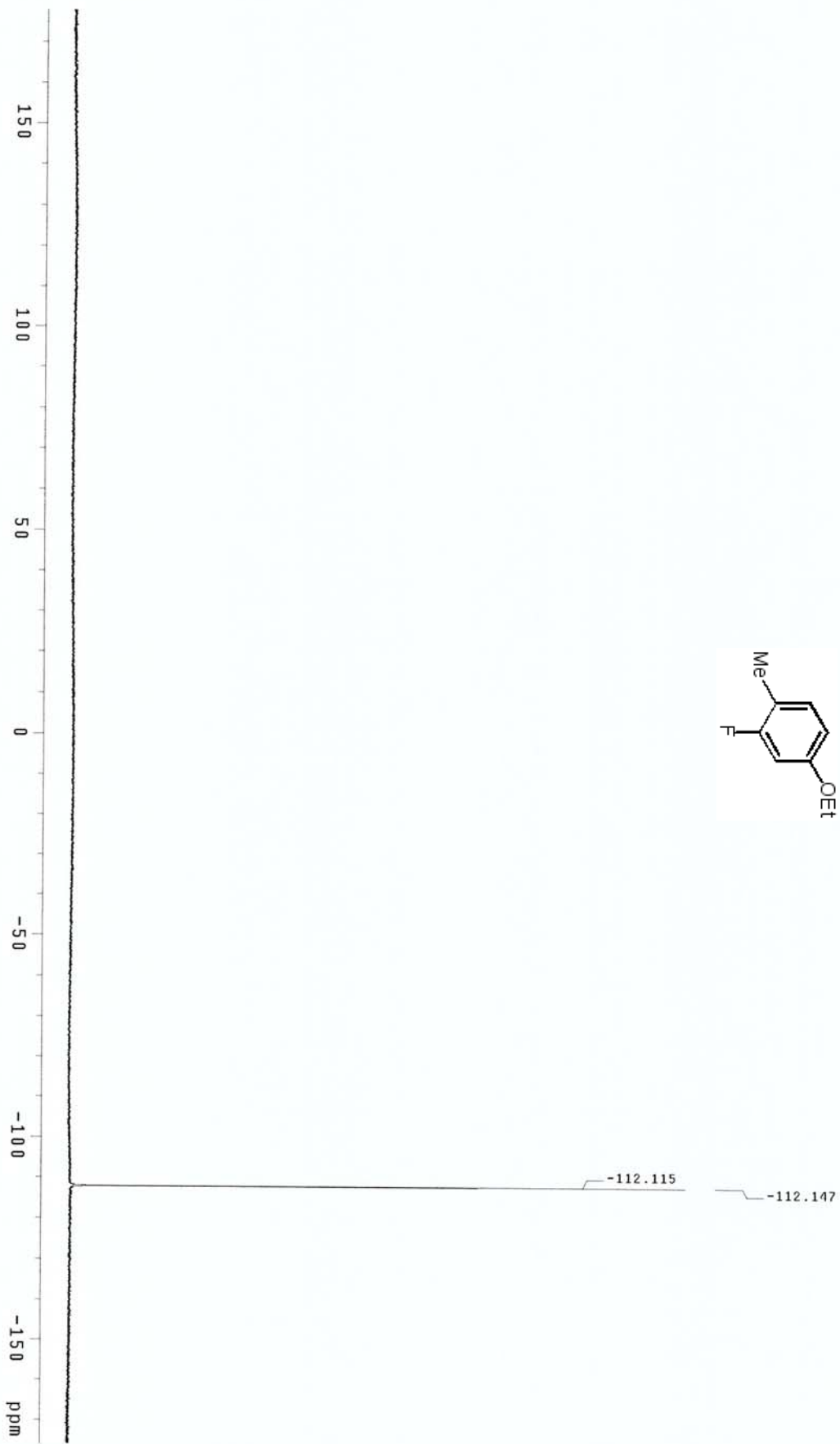
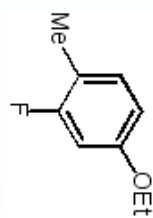
Total time 0 min, 0 sec



wxx-1-257-2C
Pulse Sequence: s2pu1



wxx-1-267-2f
Pulse Sequence: s2pu1



wxx-1-274-3

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse: 33.9 degrees

Acq. time: 4.003 sec

Width: 6002.4 Hz

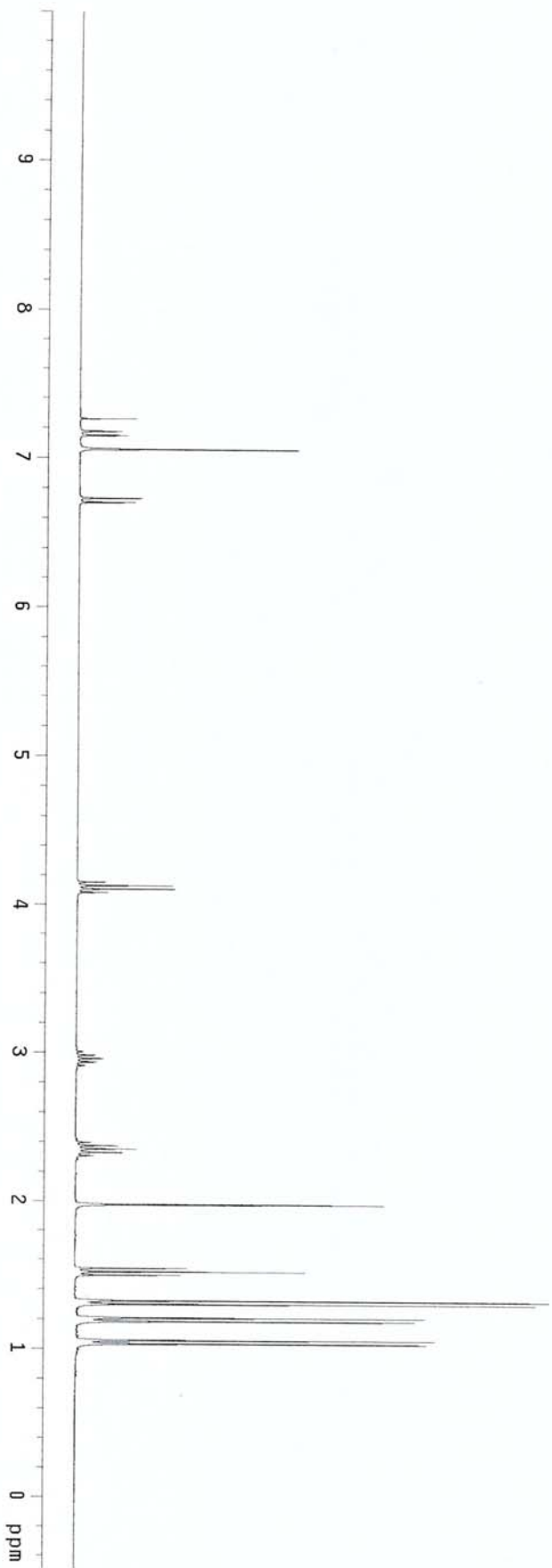
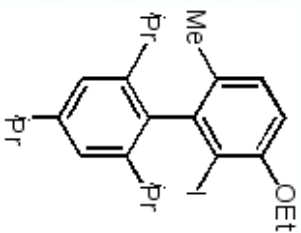
18 repetitions

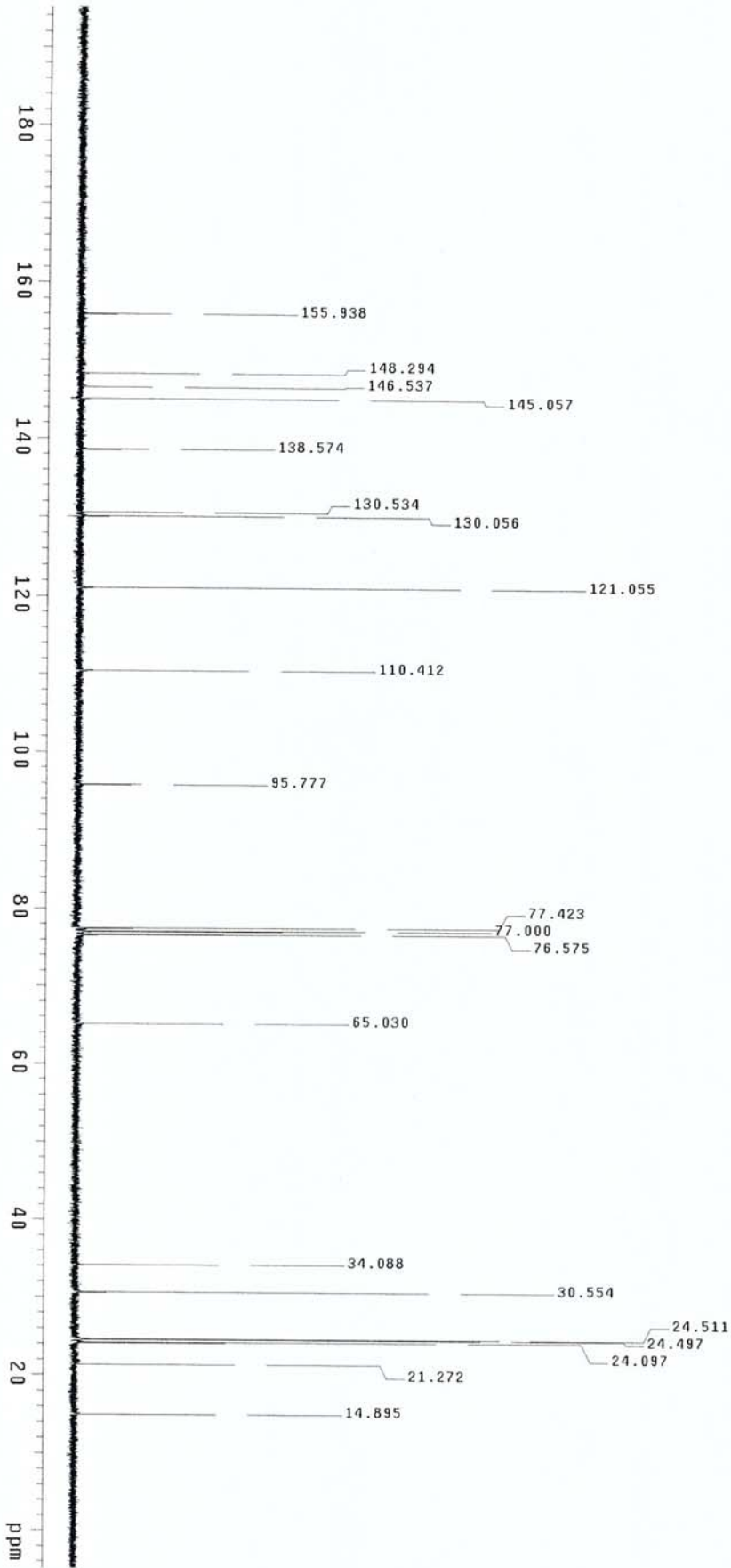
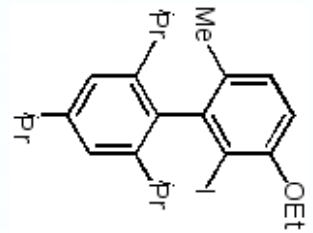
OBSERVE H1: 300.1055034 MHz

DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec





wxx-1-275-2

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse: 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

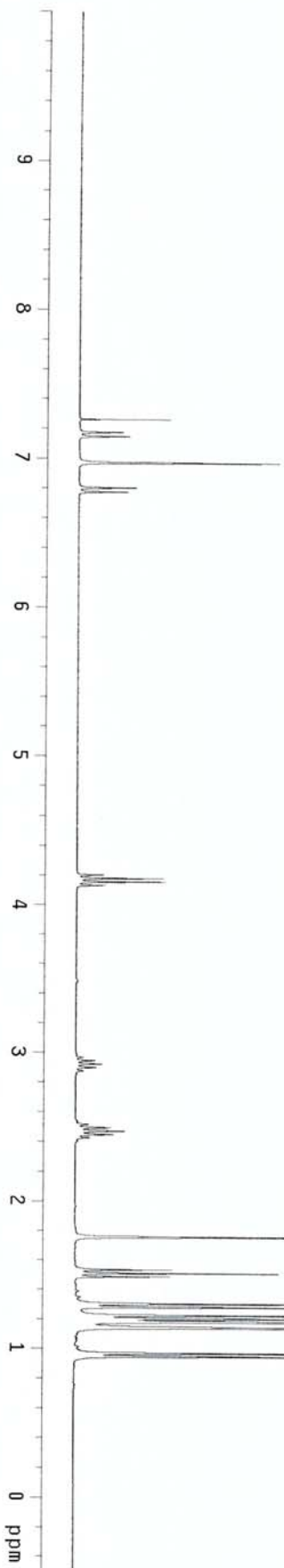
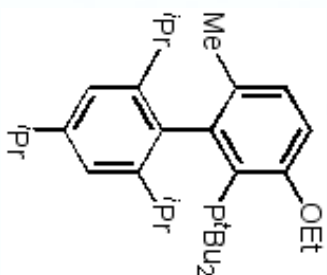
16 repetitions

OBSERVE H1: 300.1055033 MHz

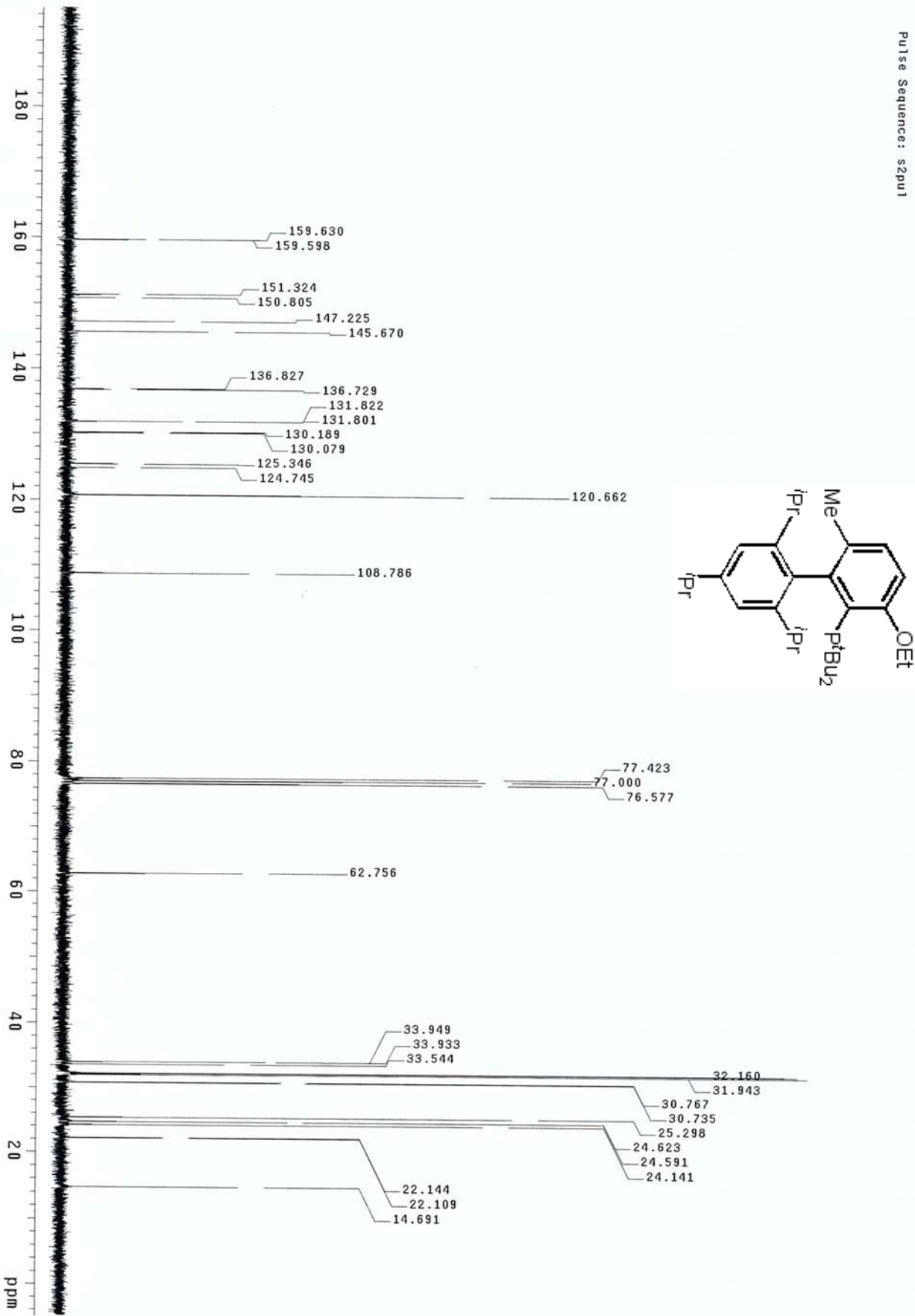
DATA PROCESSING

FT size 131072

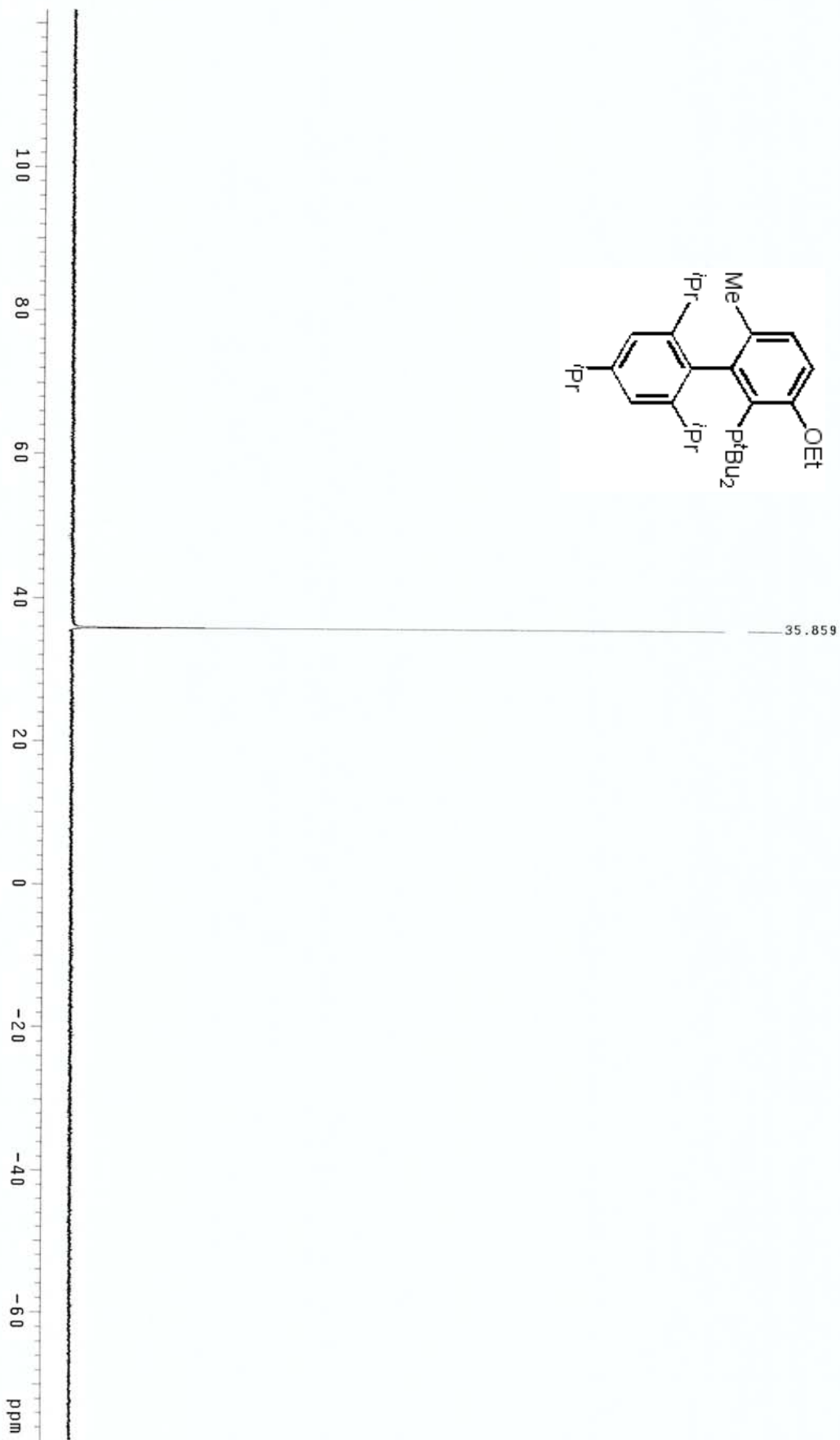
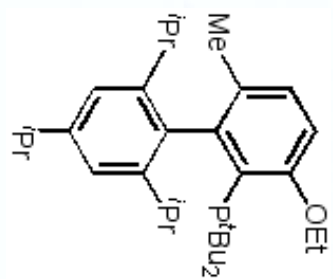
Total time 1 min, 17 sec



WXX-1-275-2C
Pulse Sequence: szpu1



wxx-1-275-2p
Pulse Sequence: s2pu1



wxx-2-195-2

Pulse Sequence: szpu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-500 "mrhnl"

Relax. delay: 0.050 sec

Pulse: 33.9 degrees

Acq. time: 4.003 sec

Width: 6002.4 Hz

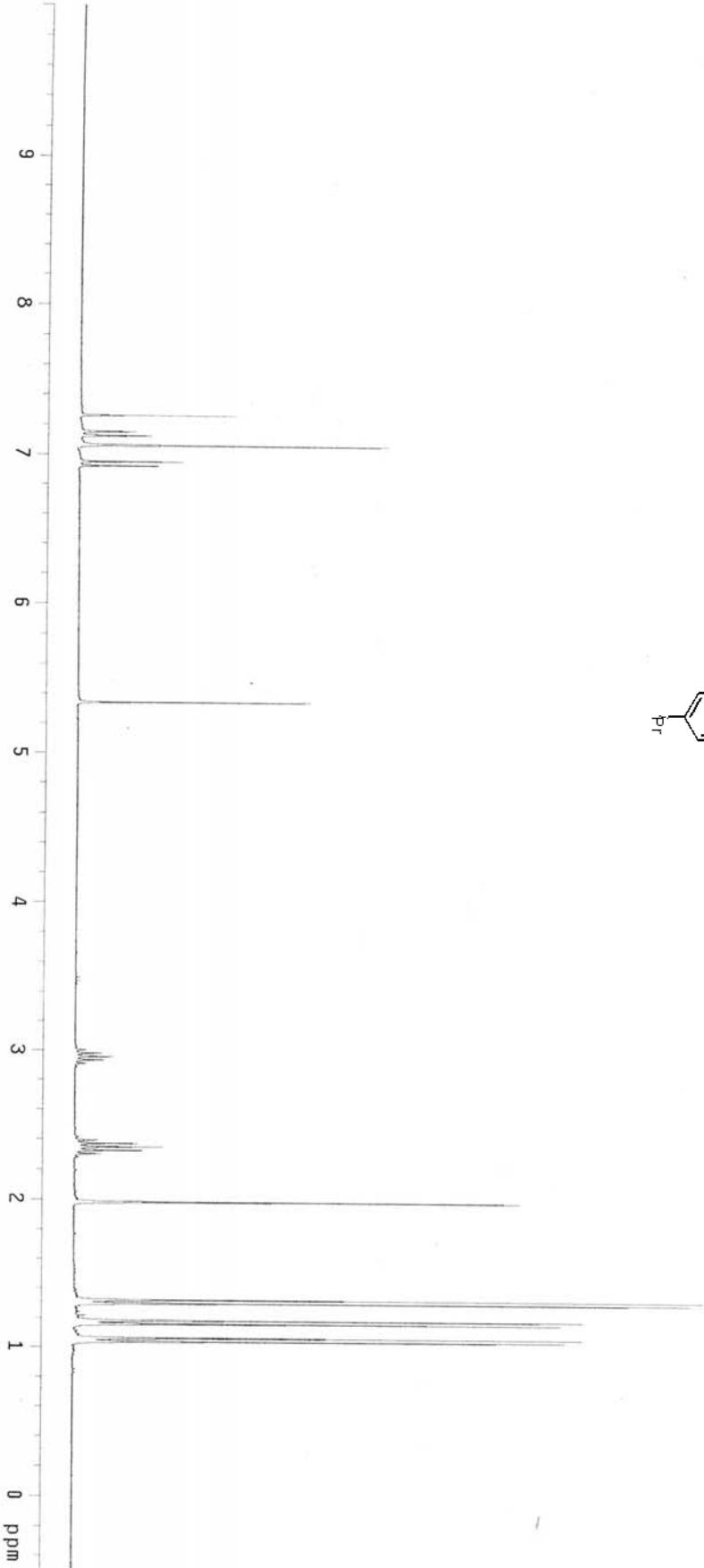
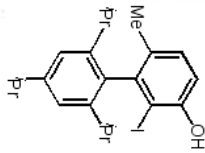
16 repetitions

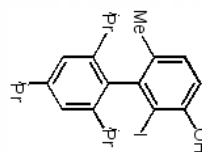
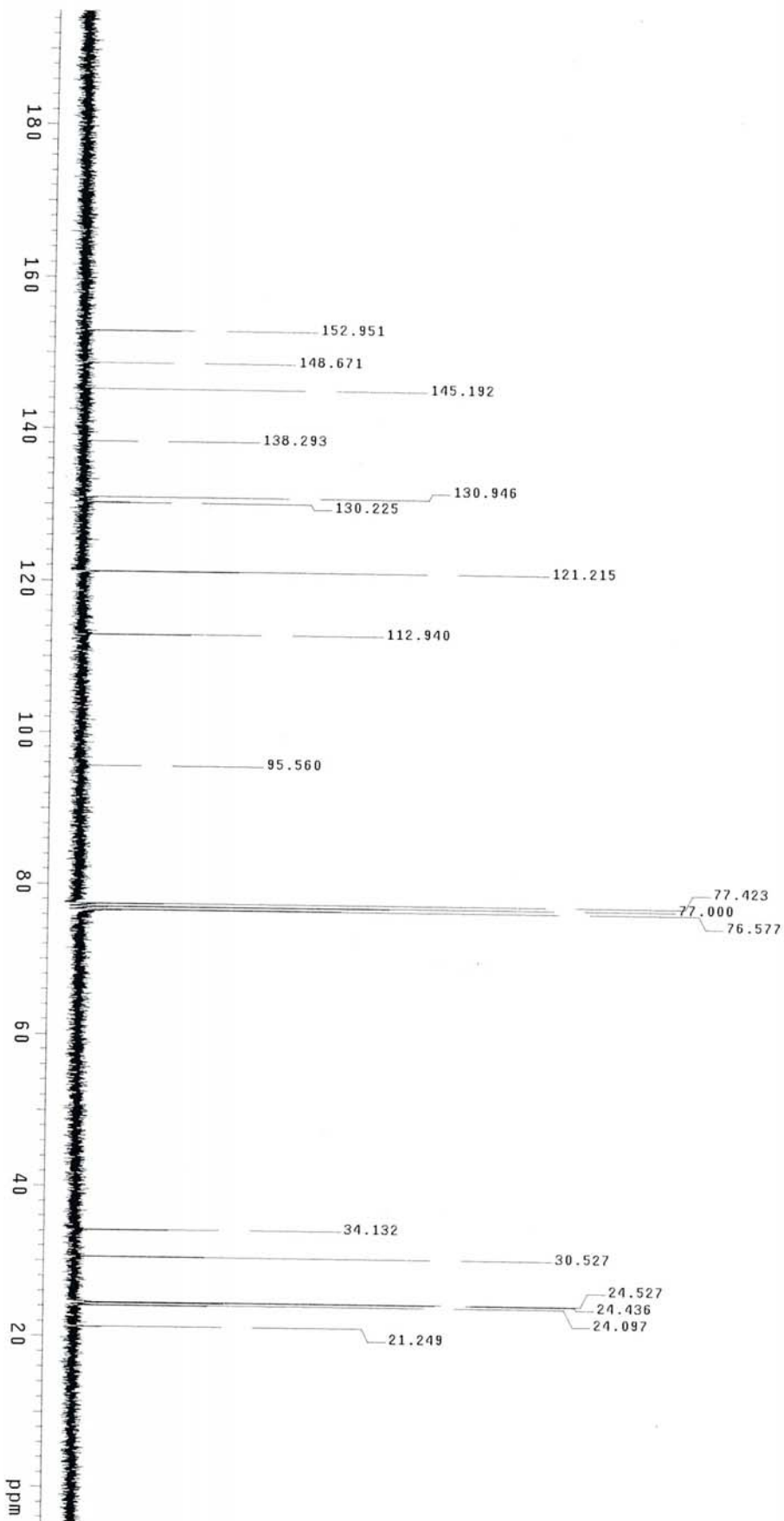
OBSERVE: H1 300.1055035 MHz

DATA PROCESSING

FT size: 131072

Total time: 1 min, 17 sec

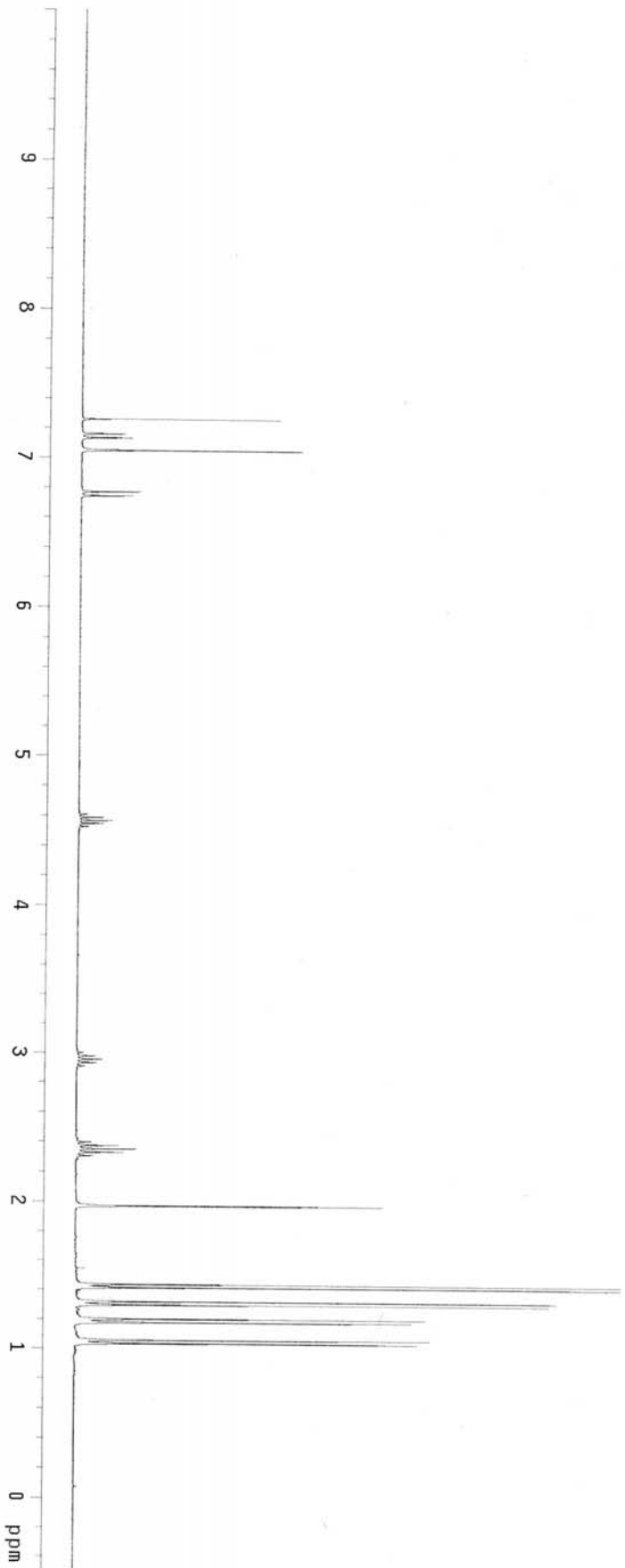
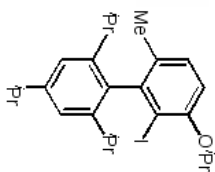




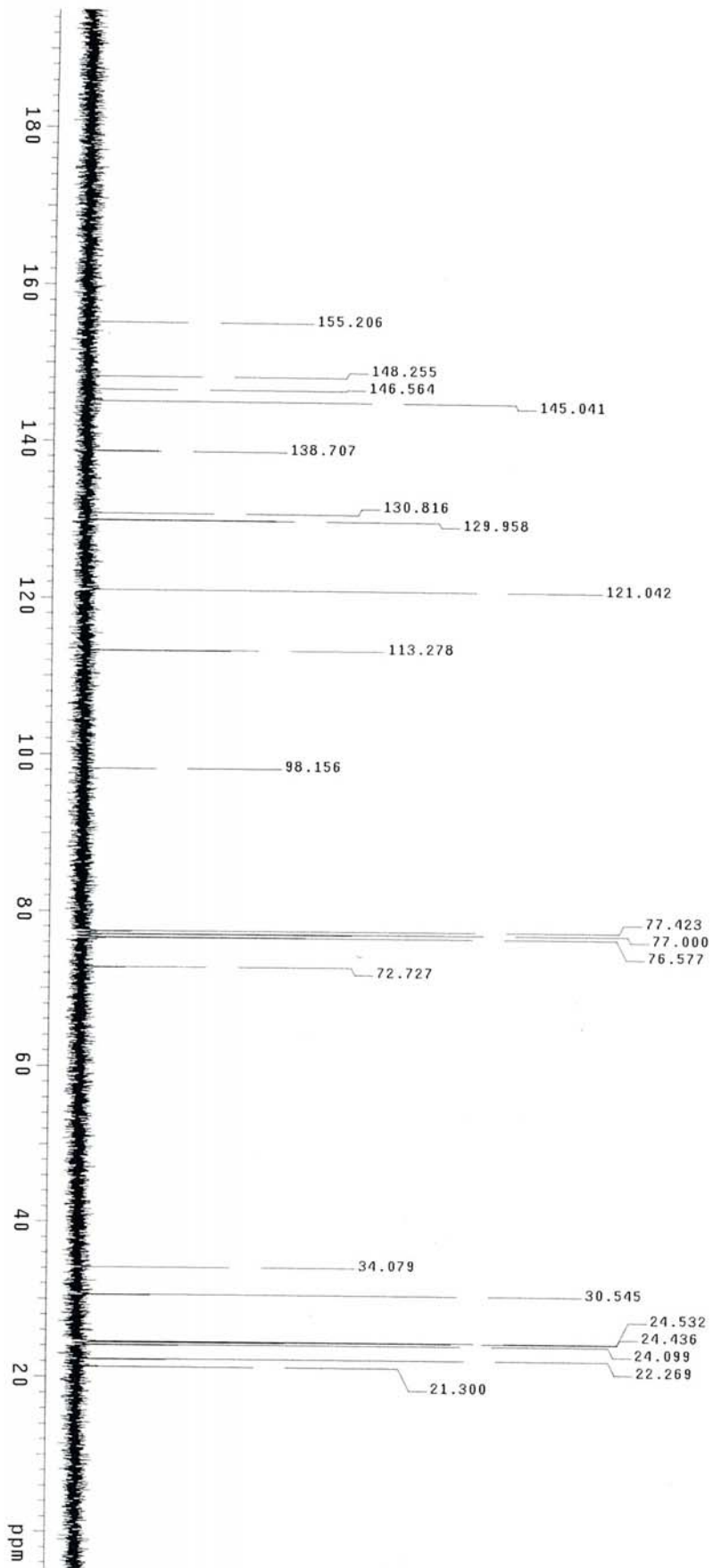
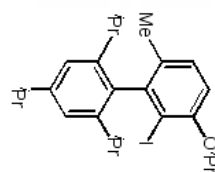
wxx-2-197-1

Pulse Sequence: szpu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-500 "mrhnl"

Relax. delay 0.050 sec
Pulse 33.9 degrees
Acq. time 4.003 sec
Width 6002.4 Hz
17 repetitions
OBSERVE HI 300.1055033 MHZ
DATA PROCESSING
FT size 131072
Total time 0 min, 0 sec



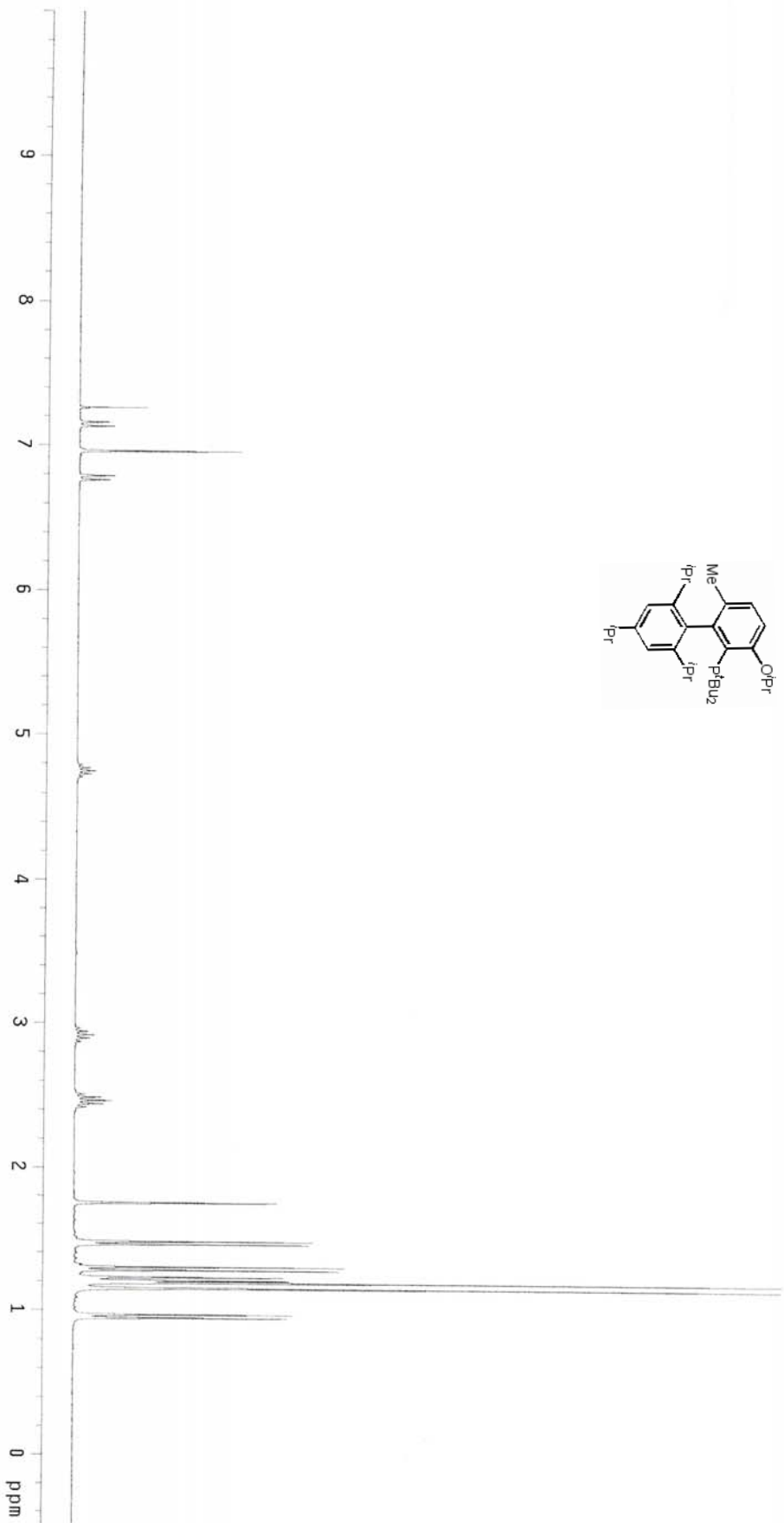
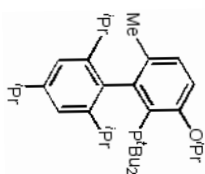
wxx-2-197-1C
Pulse Sequence: szpu1

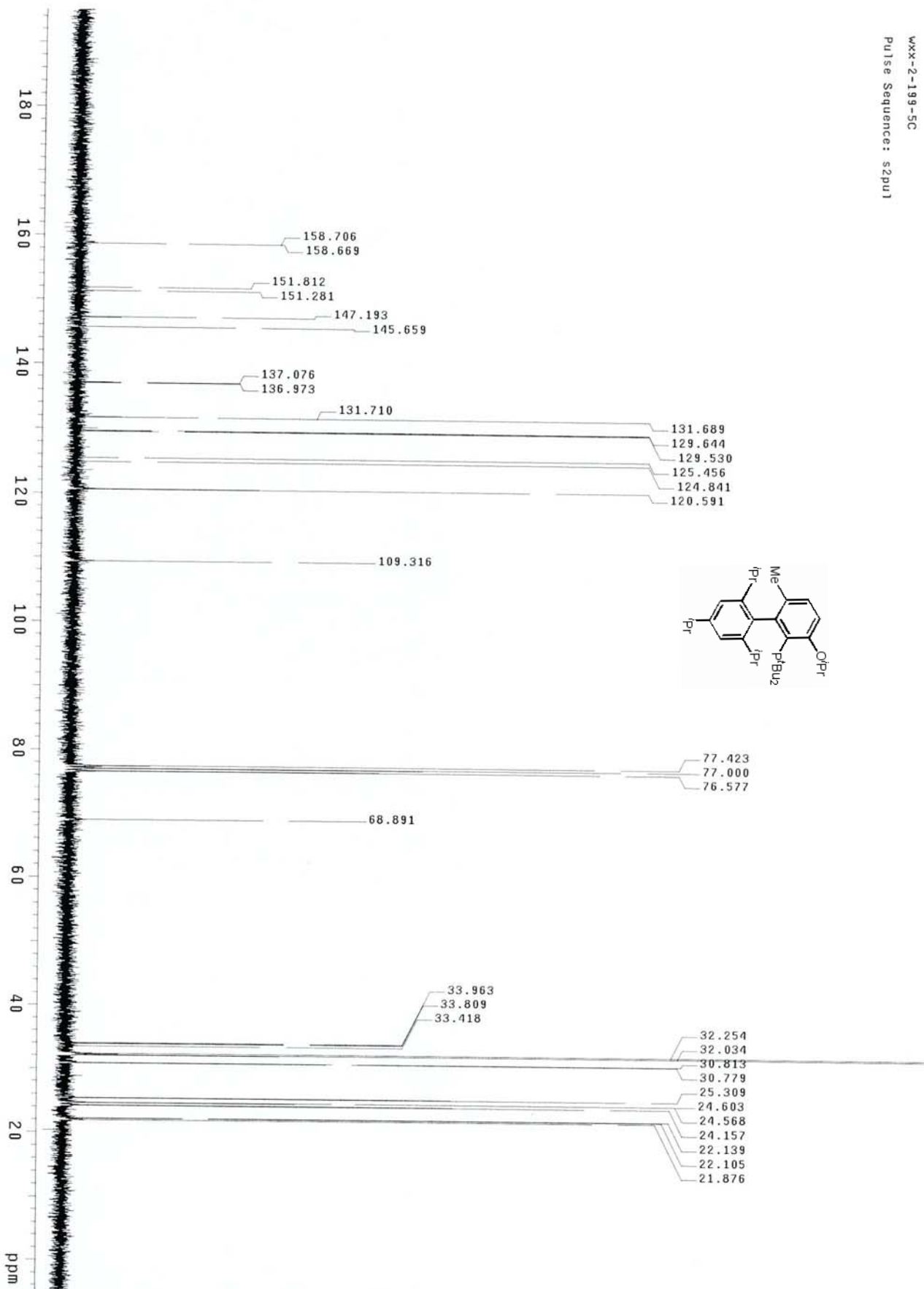


wxx-2-199-5

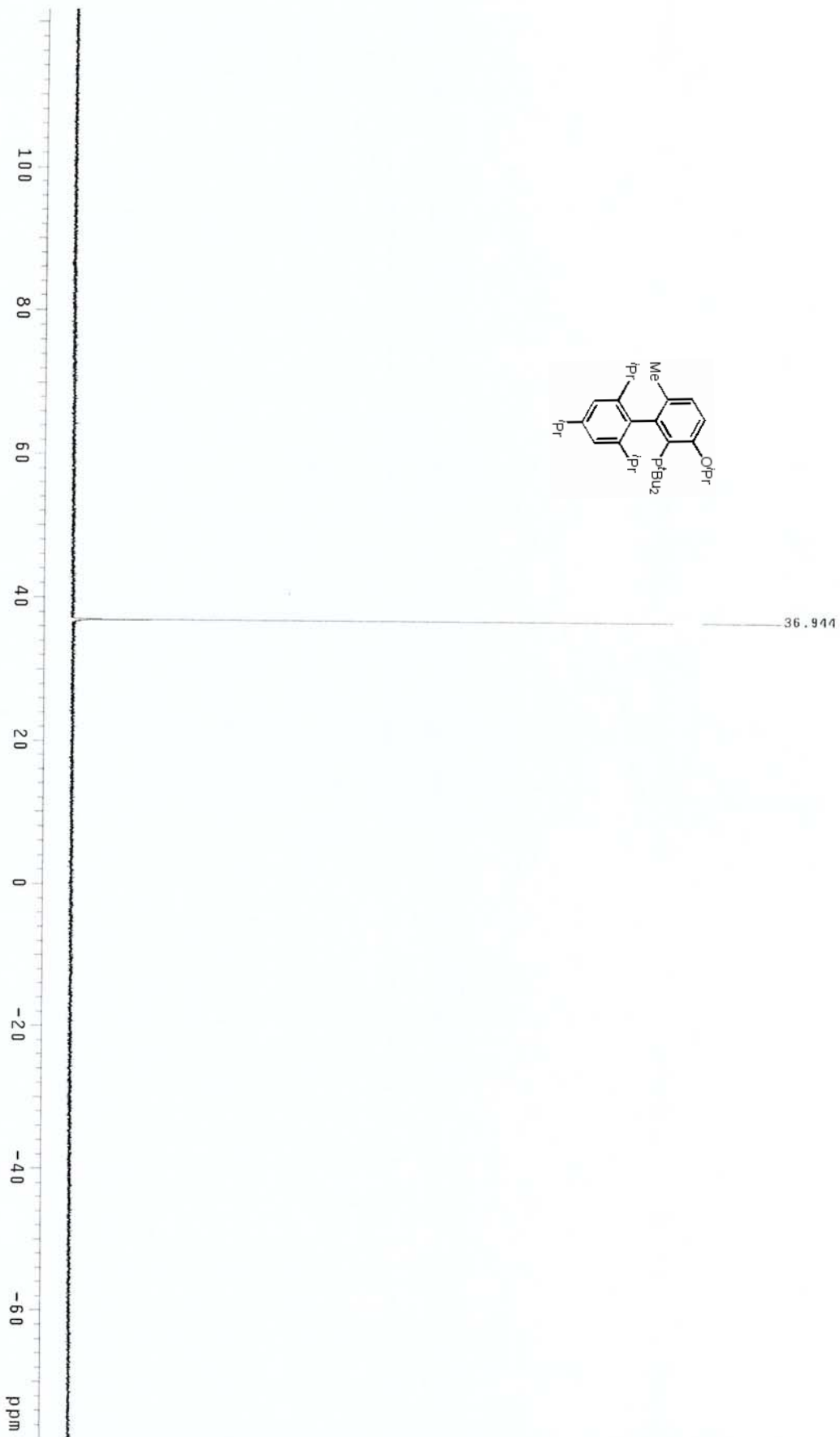
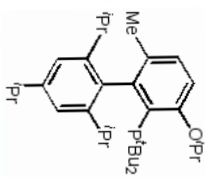
Pulse Sequence: szpu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhdt"

Relax. delay 0.050 sec
Pulse 33.9 degrees
Acq. time 4.003 sec
Width 5002.4 Hz
17 repetitions
OBSERVE H1 300.1055031 MHz
DATA PROCESSING
FT size 131072
Total time 10 min, 20 sec





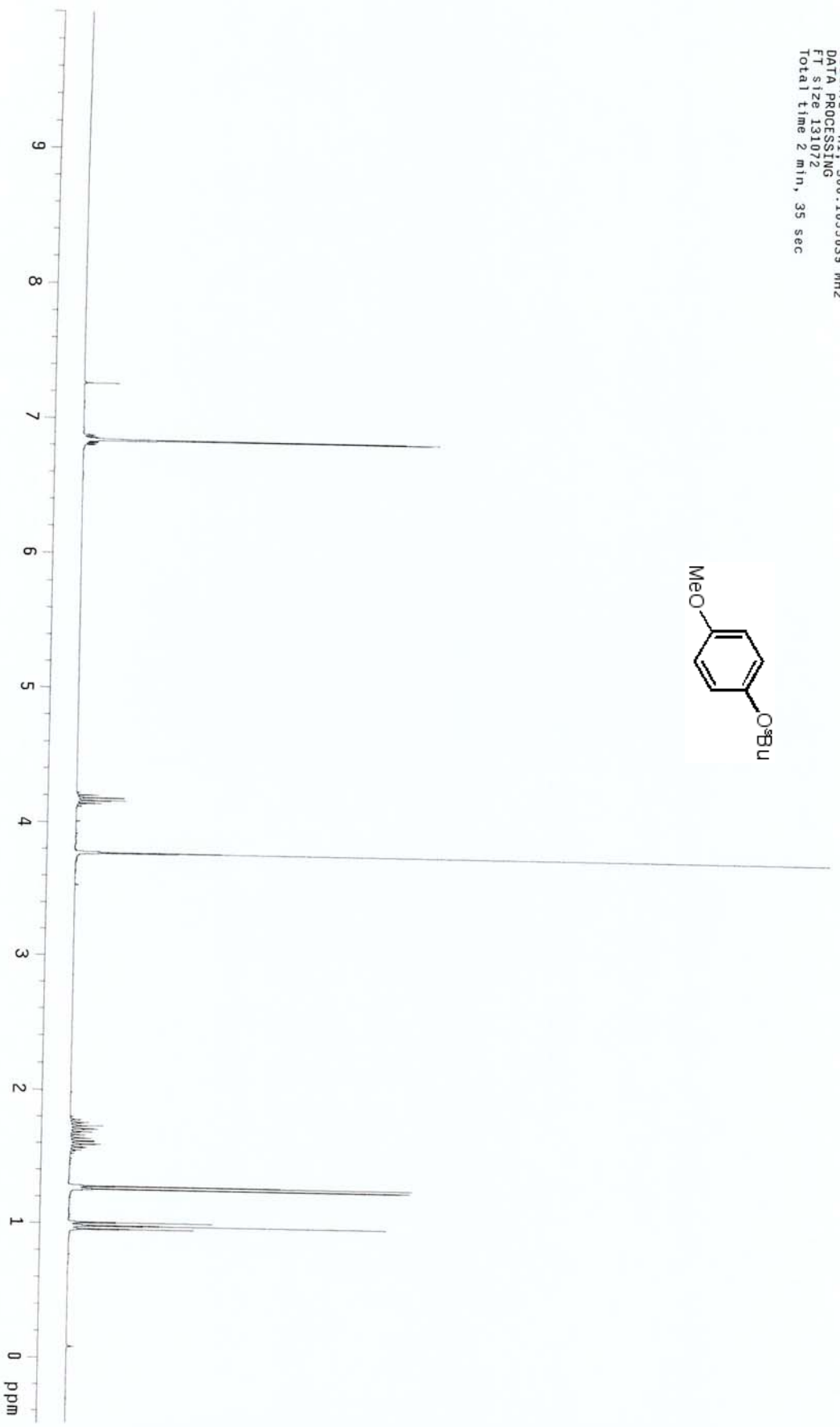
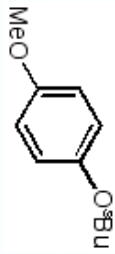
WXX-2-199-5P
Pulse Sequence: s2pu1



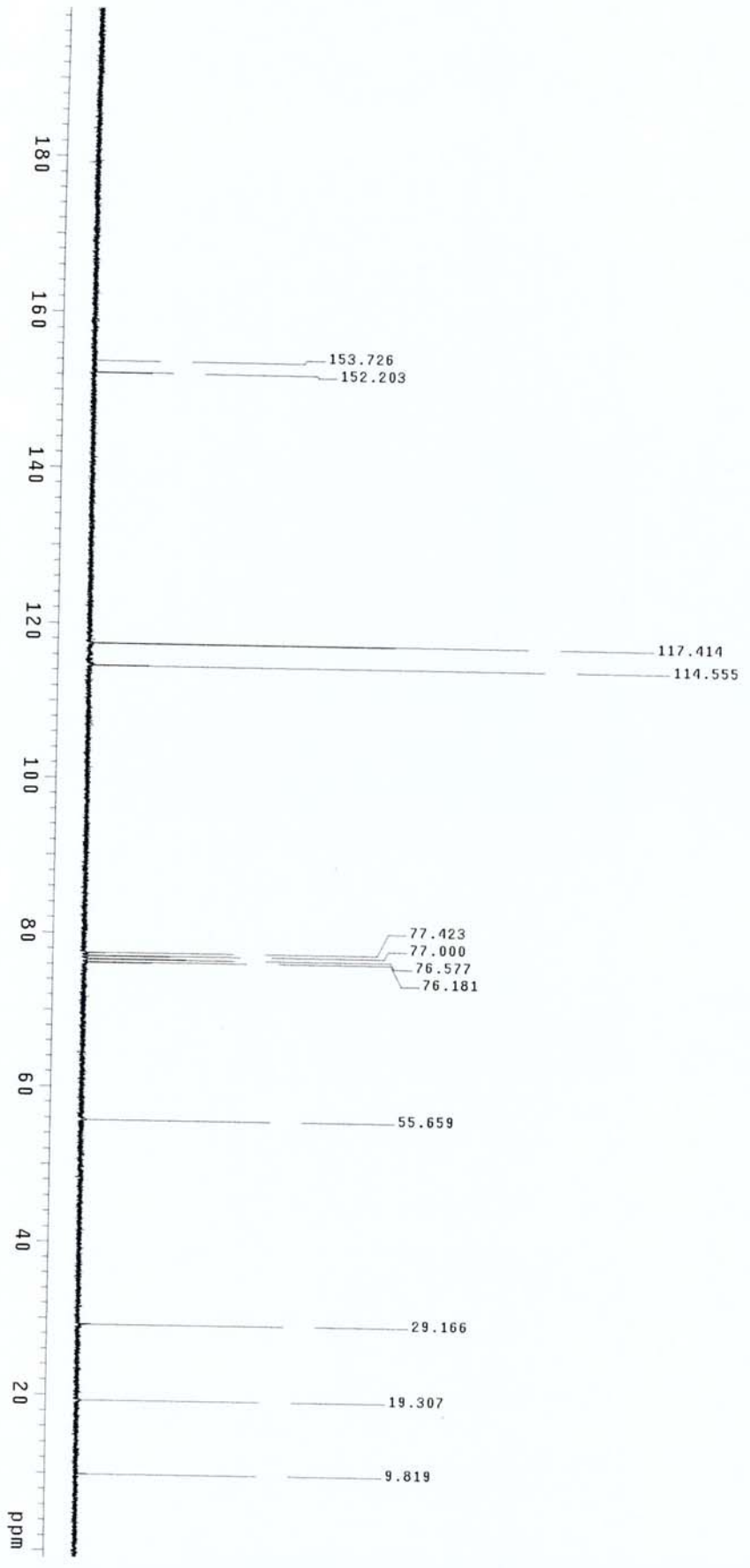
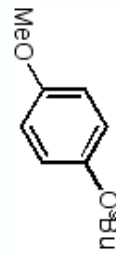
Wxx-2-34-D-2

Pulse Sequence: szpu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhat"

Relax. delay: 0.050 sec
Pulse: 33.9 degrees
Acq. time: 4.003 sec
Width: 6002.4 Hz
32 repetitions
OBSERVE: H1, 300.1055039 MHz
DATA PROCESSING
F1 size: 131072
Total time: 2 min, 35 sec



wxx-2-34-D-2C
Pulse Sequence: s2pu1



wxx-2-59-A-2

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp. 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

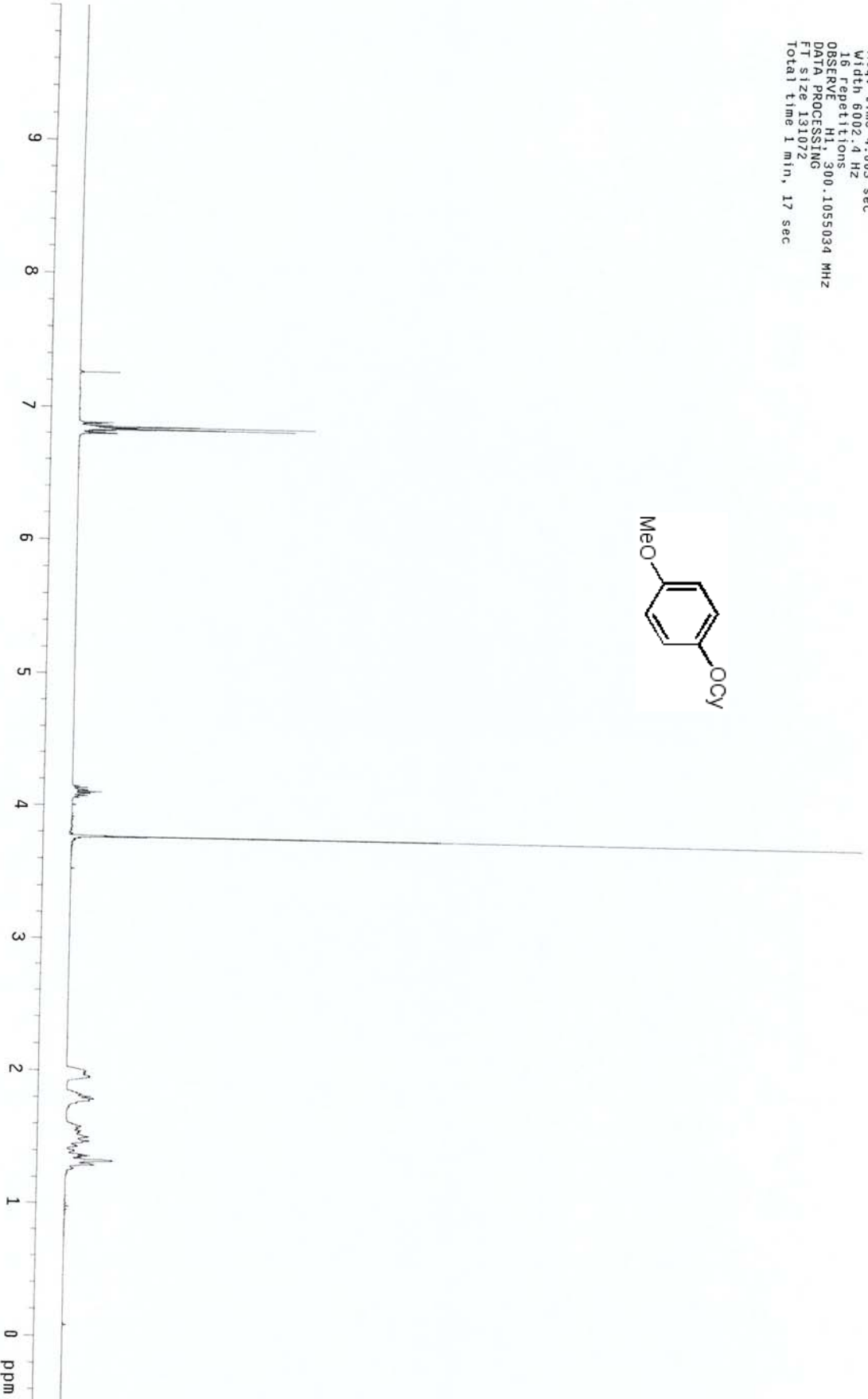
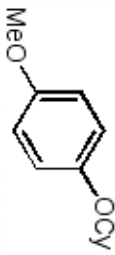
18 repetitions

OBSERVE H1, 300.1055034 MHz

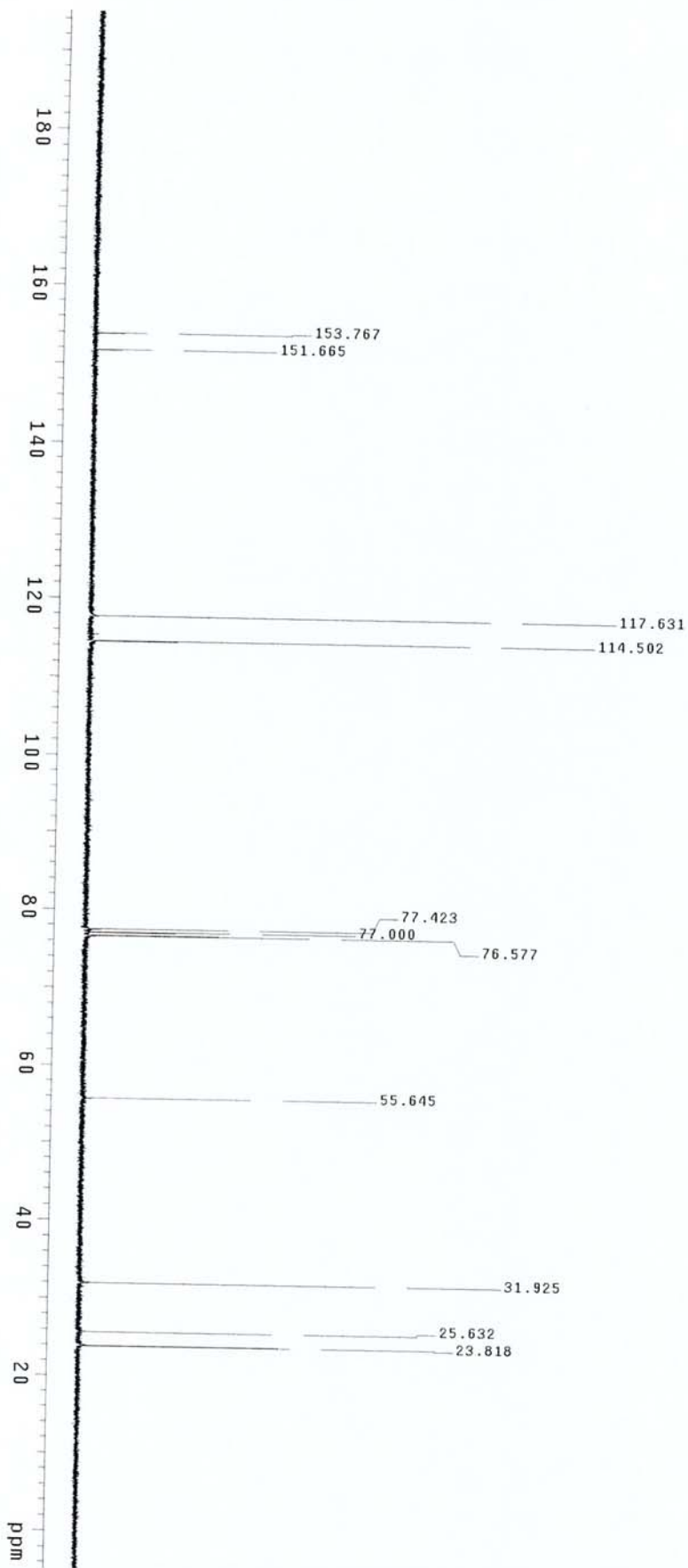
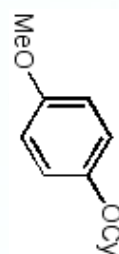
DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec



wxx-2-59-A-2C
Pulse Sequence: s2pu1



wxx-2-32-D-2

Pulse Sequence: s2pul

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

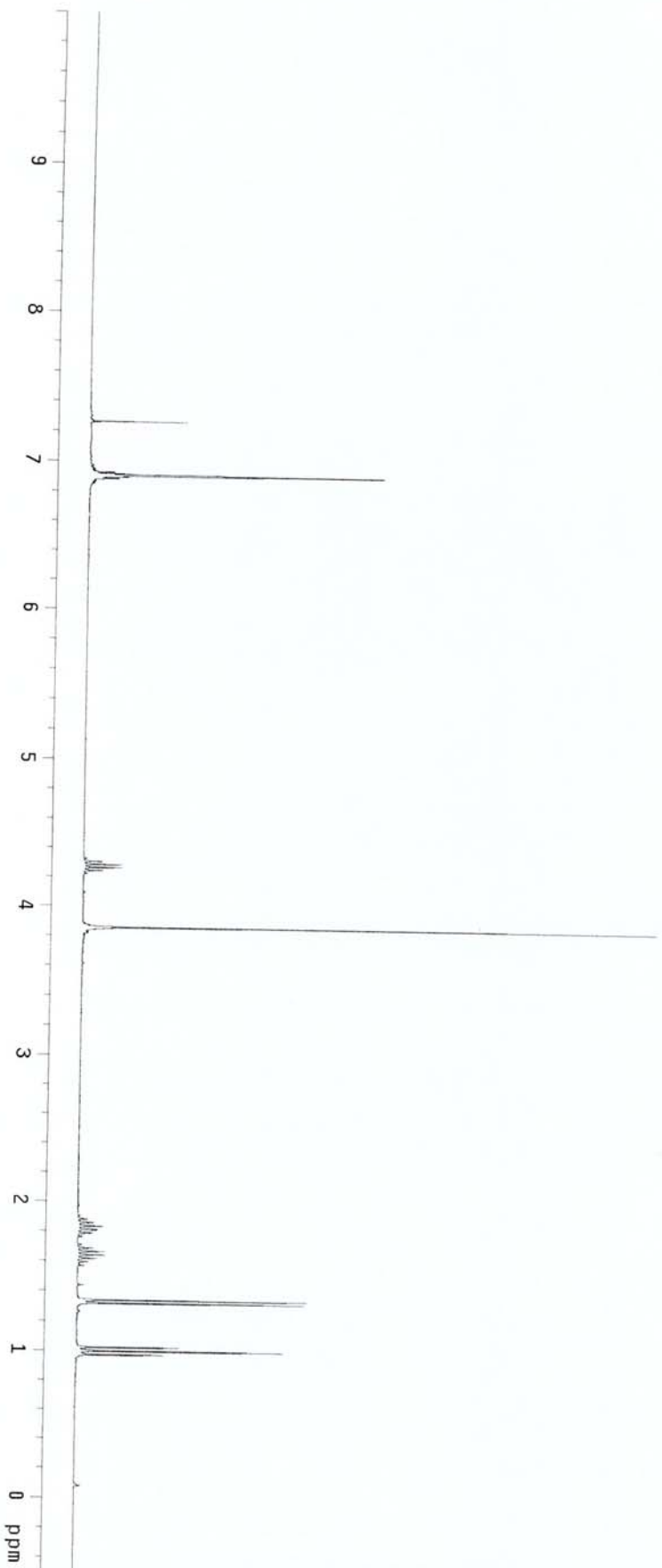
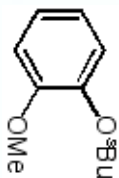
32 repetitions

OBSERVE H1, 300.1055040 MHz

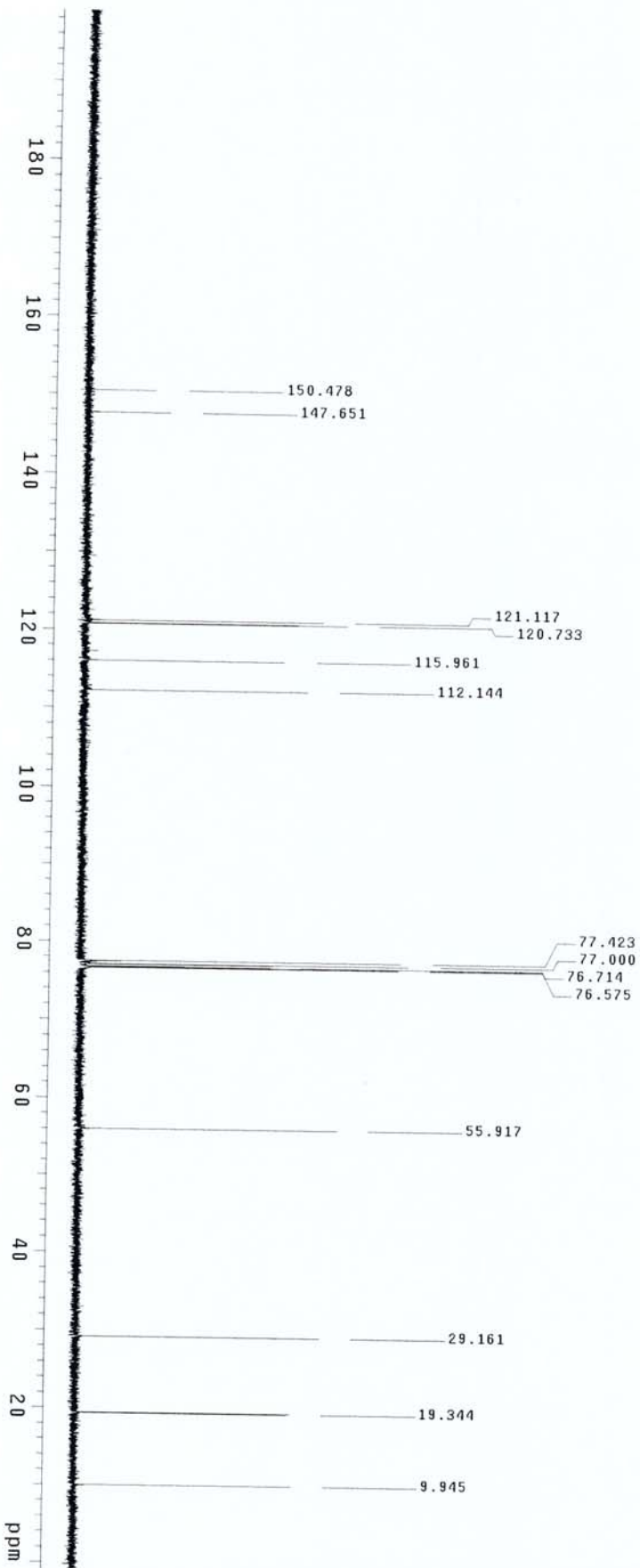
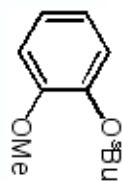
DATA PROCESSING

FT size 131072

Total time 2 min, 35 sec



wxx-2-32-D-2C
Pulse Sequence: szpu1



wxx-2-62-A-2

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

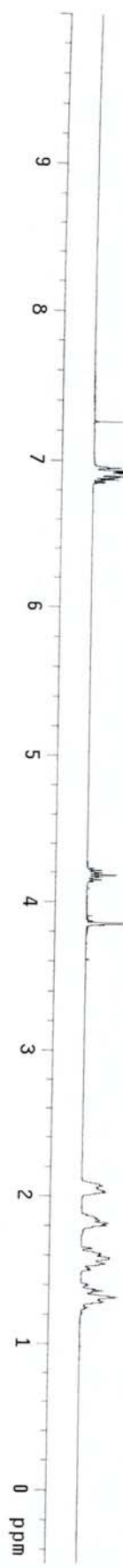
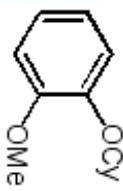
16 repetitions

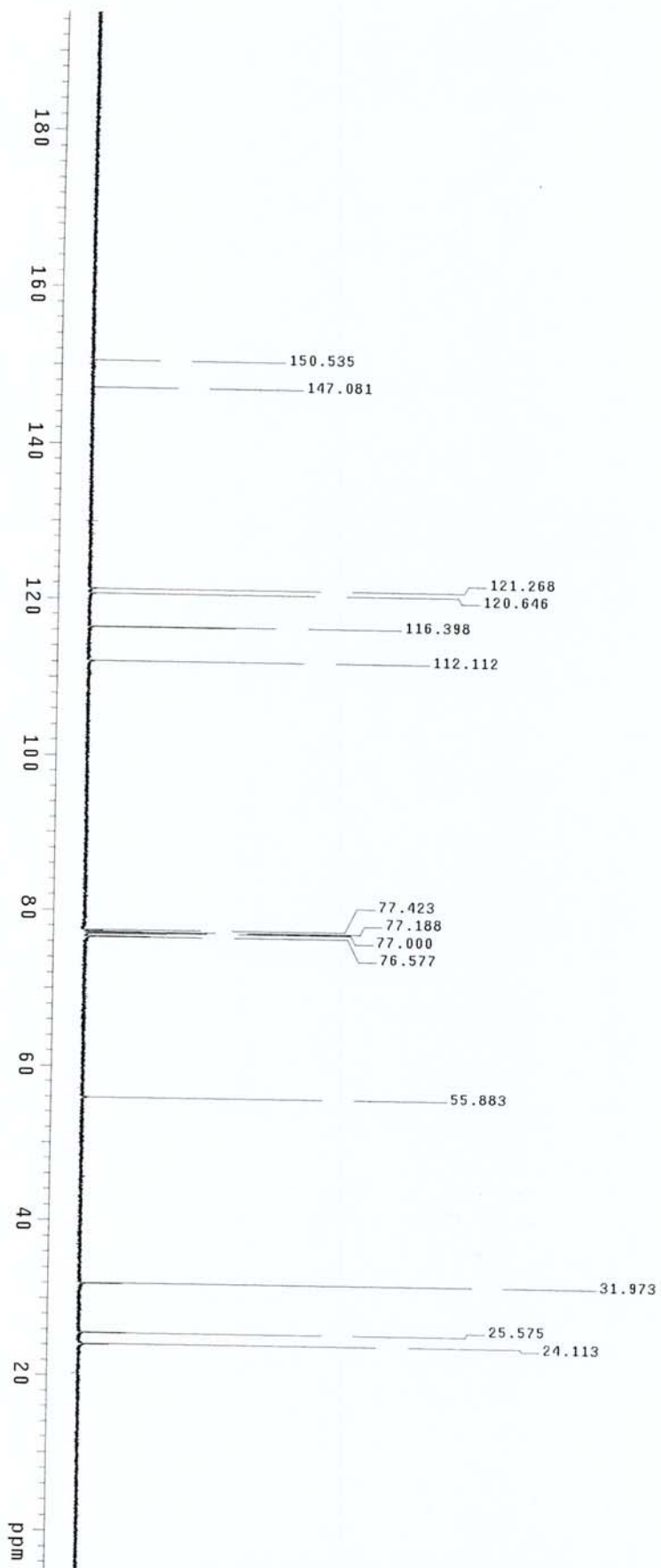
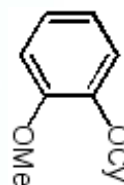
OBSERVE H1, 300.1055034 MHz

DATA PROCESSING

FT size 131072

Total time 0 min, 0 sec





wxx-253-A-2

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

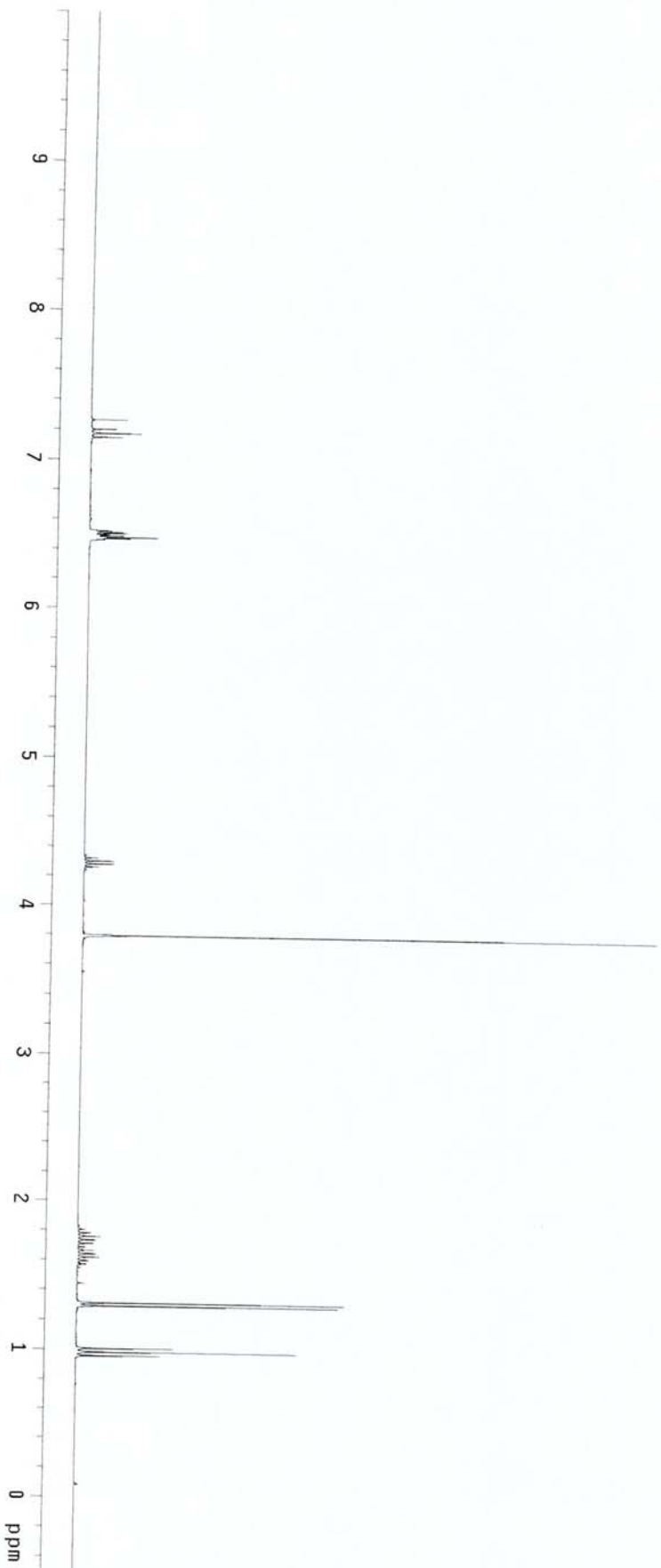
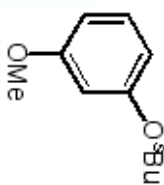
16 repetitions

OBSERVE H1: 300.1059035 MHz

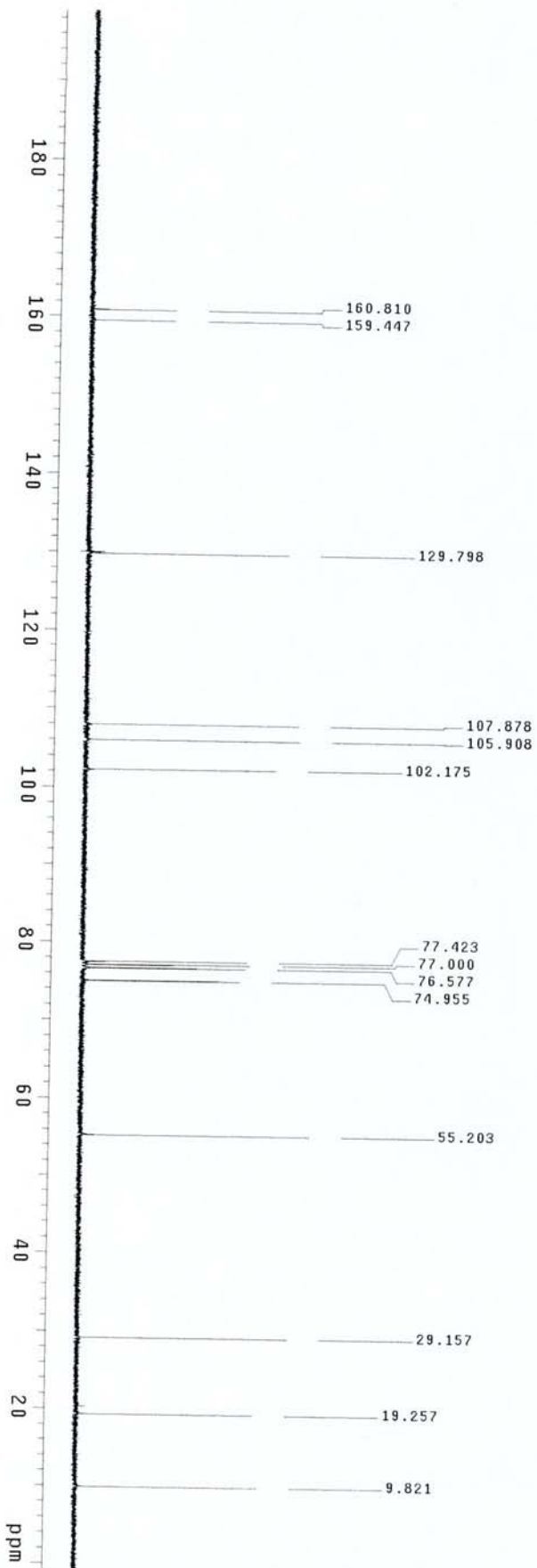
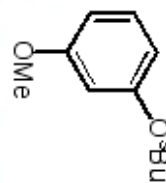
DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec



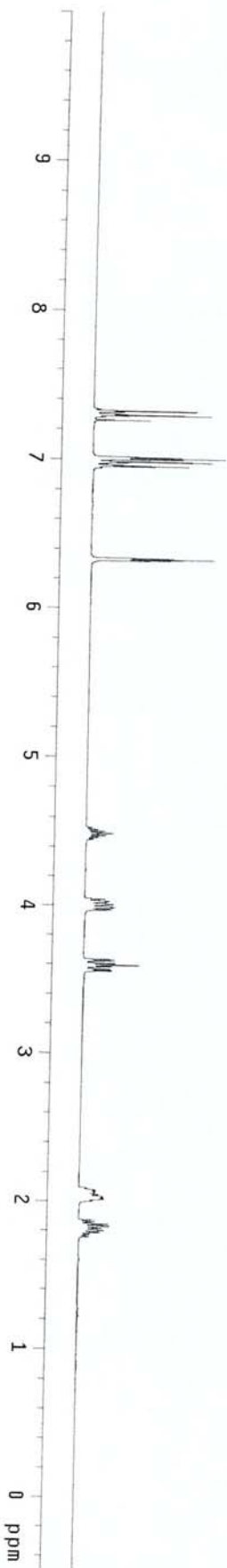
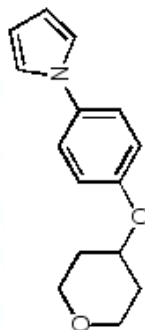
wx-253-A-2C
Pu 1se Sequence: szpu1



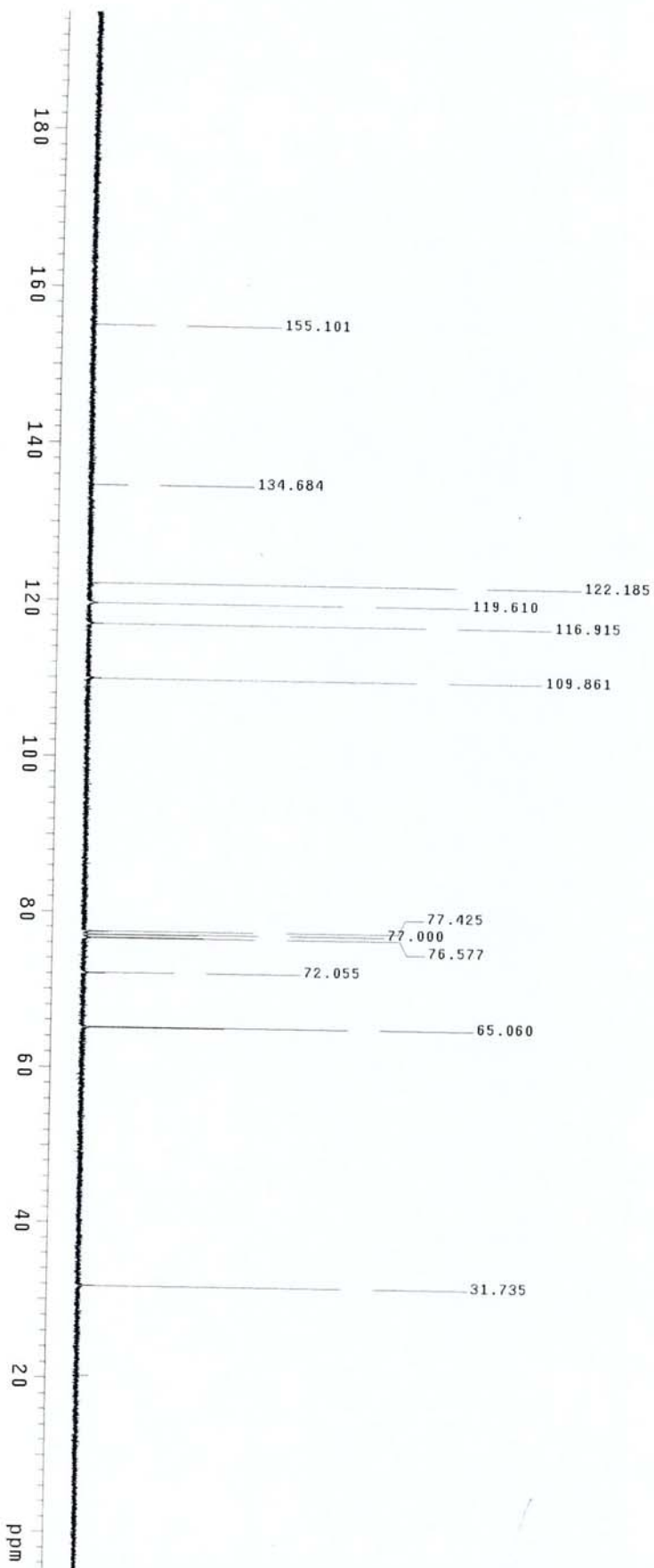
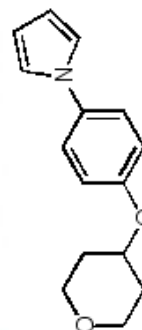
WX-2-50-C-2A

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhat"

Relax. delay 0.050 sec
Pulse 32.9 degrees
Acq. time 4.003 sec
Width 6002.4 Hz
16 repetitions
OBSERVE HI, 300.1055034 MHz
DATA PROCESSING
F1 size 131072
Total time 1 min, 17 sec



wxx-2-50-C-2C
Pulse Sequence: szpu1



wxx-2-81-A-1b

Pulse Sequence: szpu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

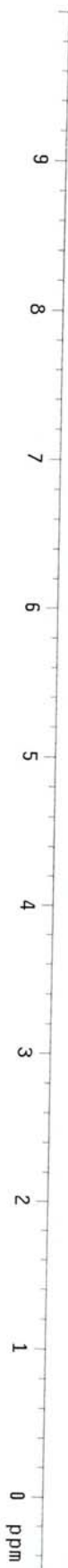
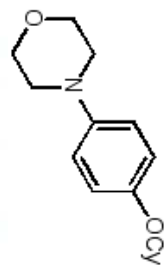
16 repetitions

OBSERVE H1, 300.1055033 MHZ

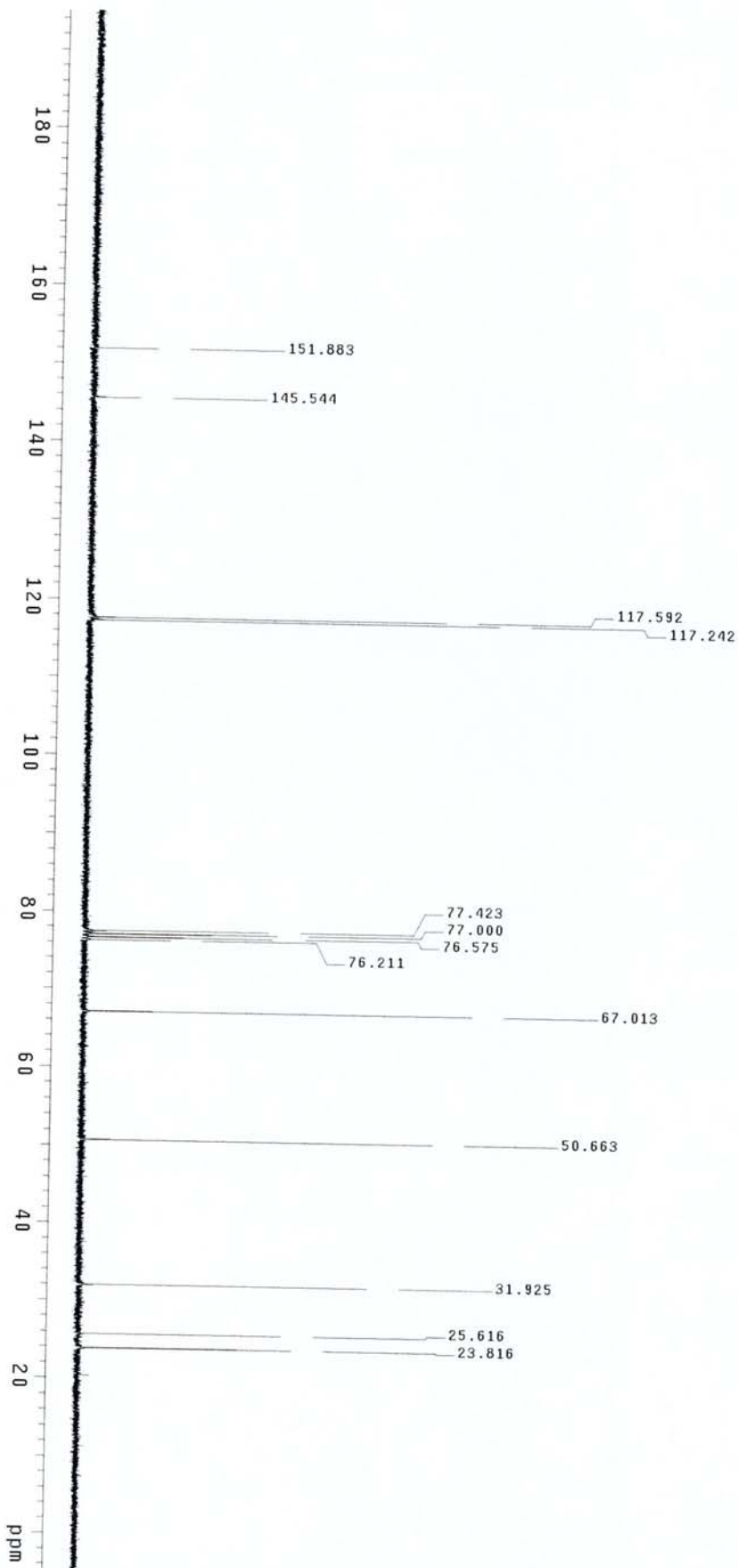
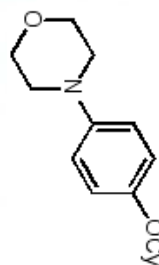
DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec



wxx-2-81-A-1b_C
Pulse Sequence: szpu1



wxx-2-42-C-2_040710

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp. 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

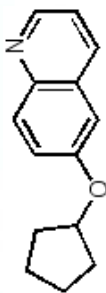
10 repetitions

OBSERVE H1, 300.1055033 MHz

DATA PROCESSING

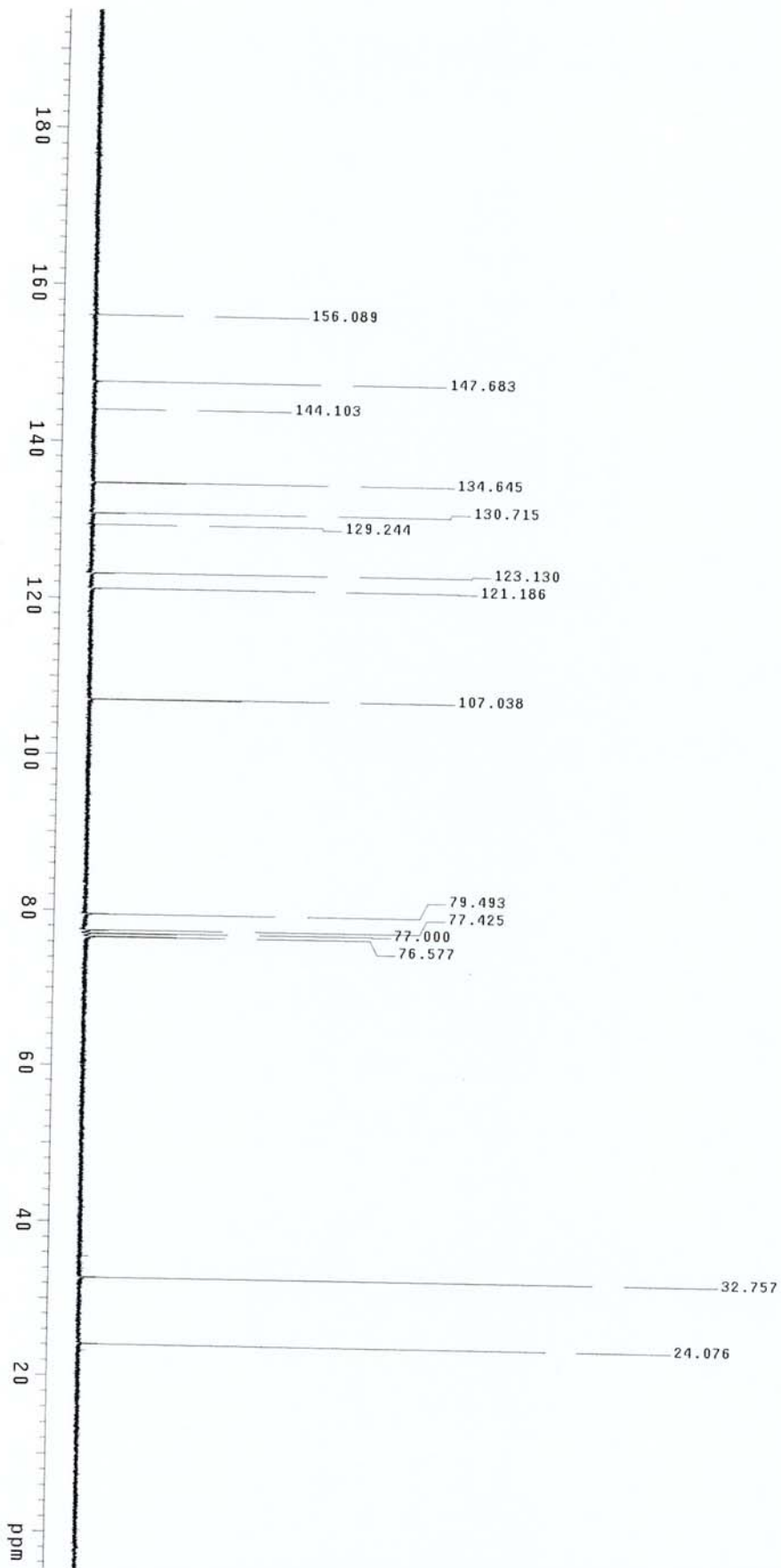
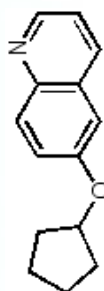
FT size 131072

Total time 1 min, 17 sec



MX-2-42-C-2C
13C OBSERVE

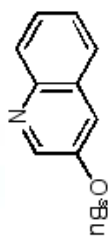
Pulse Sequence: s2pul1



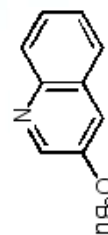
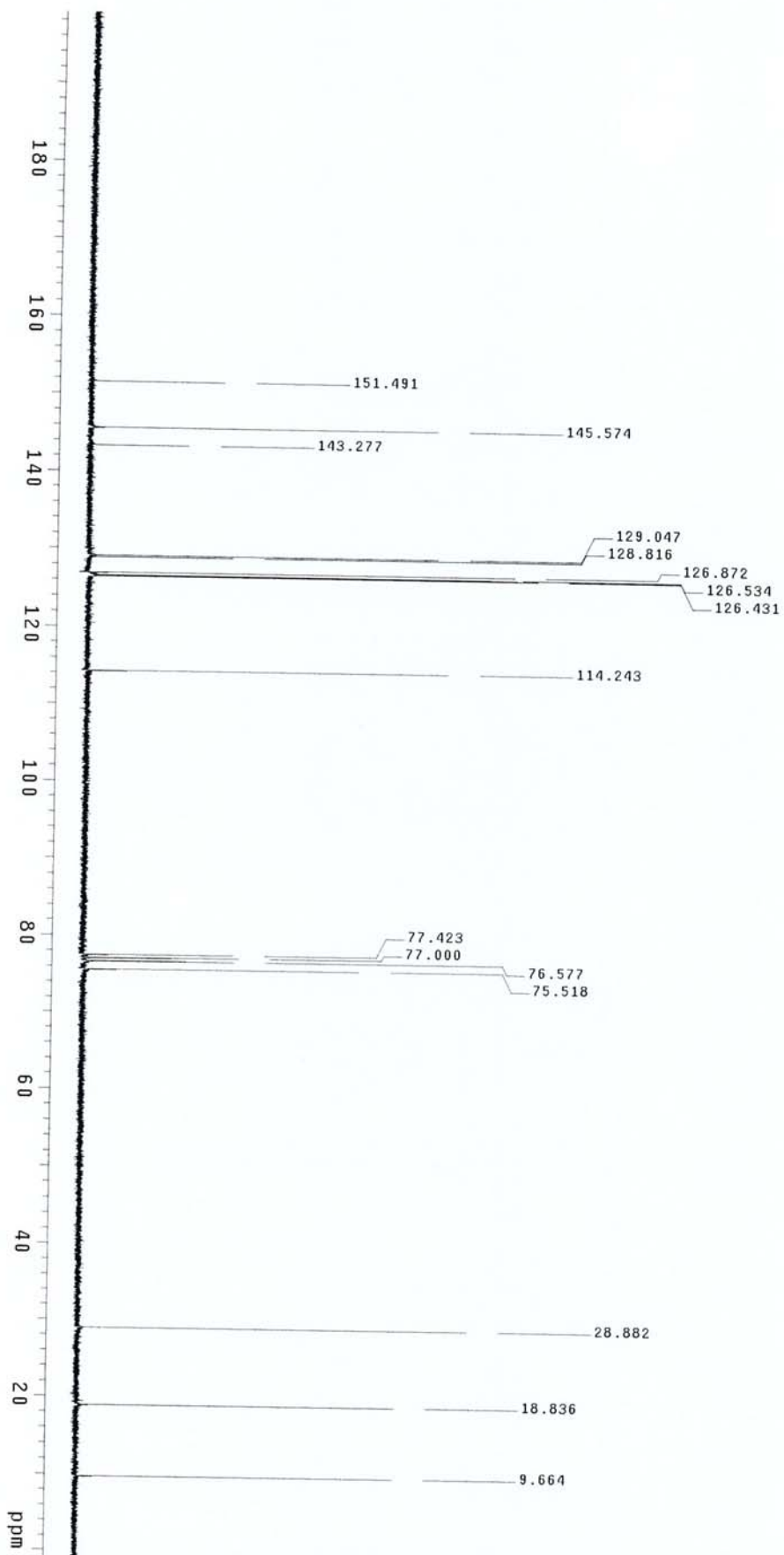
wxx-2-27-C-2

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhat"

Relax. delay 0.050 sec
Pulse 33.9 degrees
Acq. time 4.003 sec
Width 6002.4 Hz
16 repetitions
OBSERVE H1, 300.1055032 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 17 sec



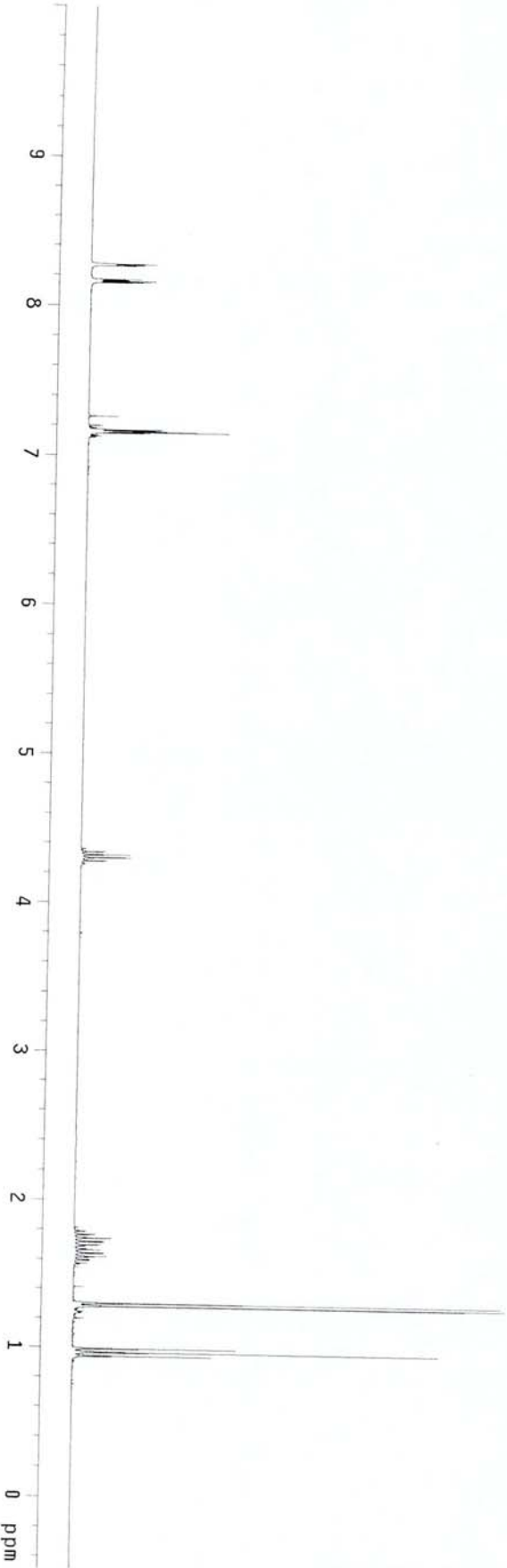
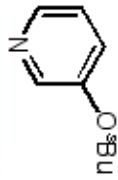
wxx-2-27-A-2C
Pulse Sequence: szpu1



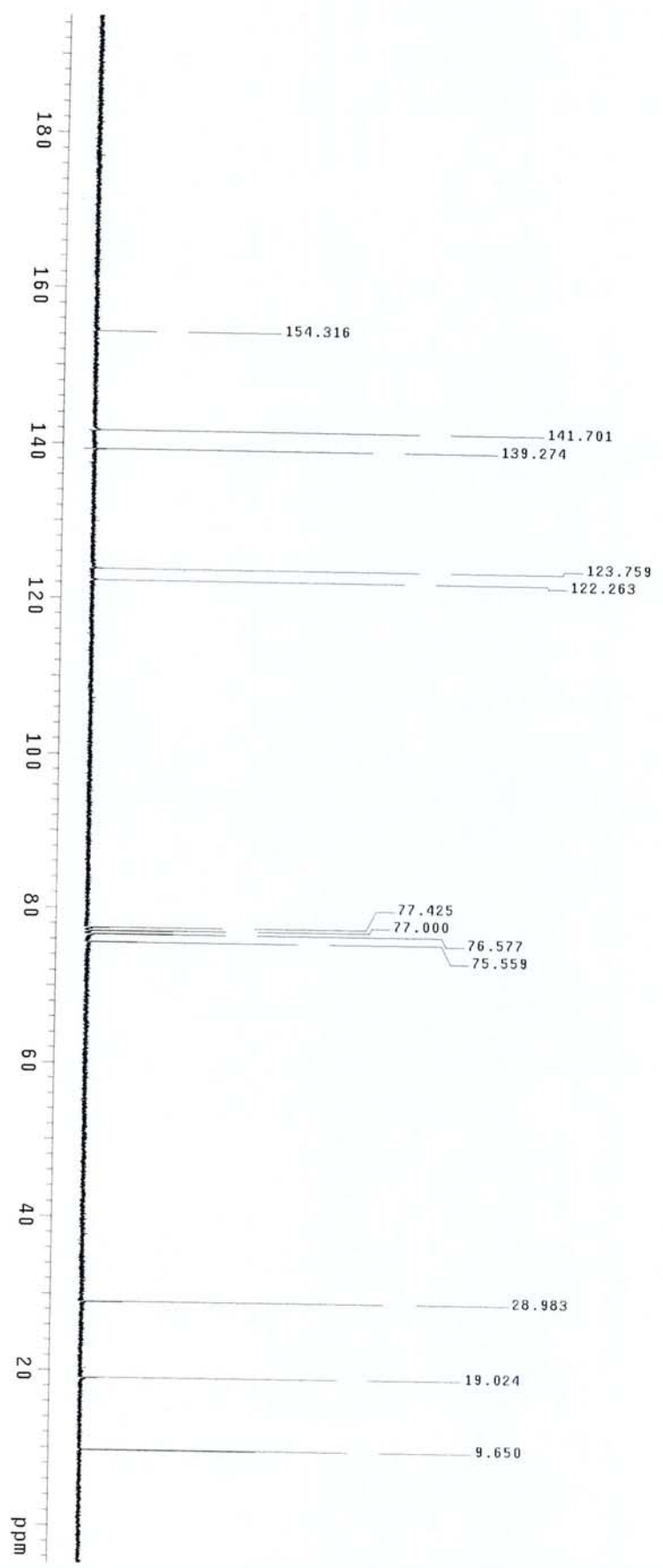
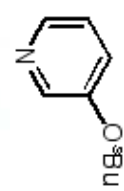
wxx-16-C-4

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhat"

Relax. delay 0.050 sec
Pulse: 33.9 degrees
Acq. time 4.003 sec
Width 6002.4 Hz
16 repetitions
OBSERVE H1: 300.1055033 MHz
DATA PROCESSING
F1 size 131072
Total time 0 min, 0 sec



wxx-2-16-C-6C
Pulse Sequence: s2pu1



wxx-2-41-B-2

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

File: wxx-2-41-B-2

INOVA-500 "zippy"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

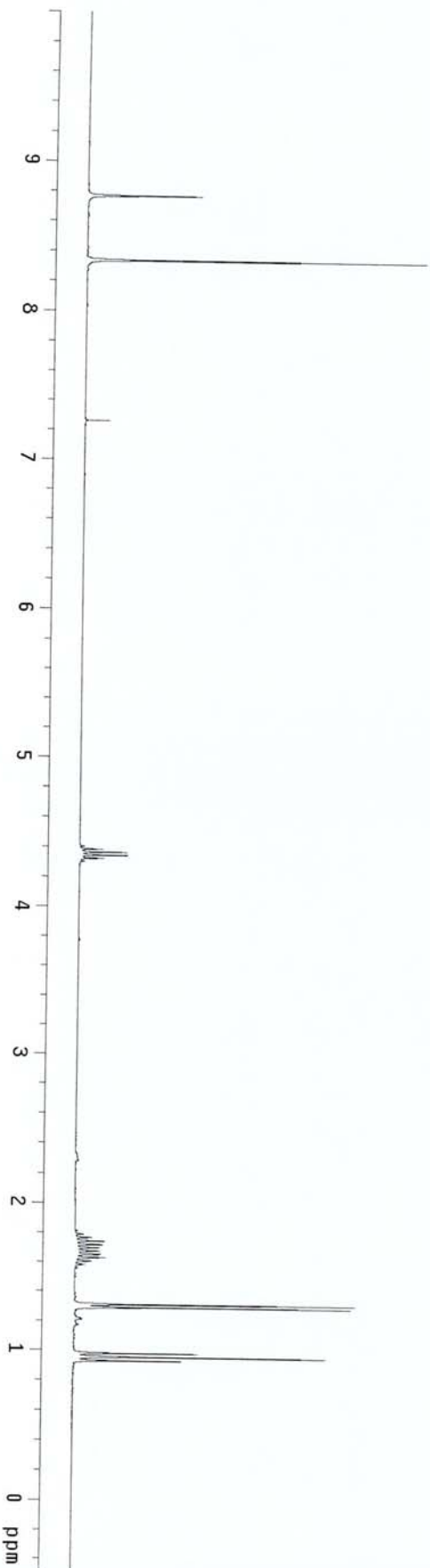
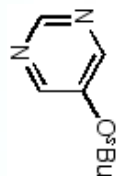
16 repetitions

OBSERVE H1, 300.1055032 MHZ

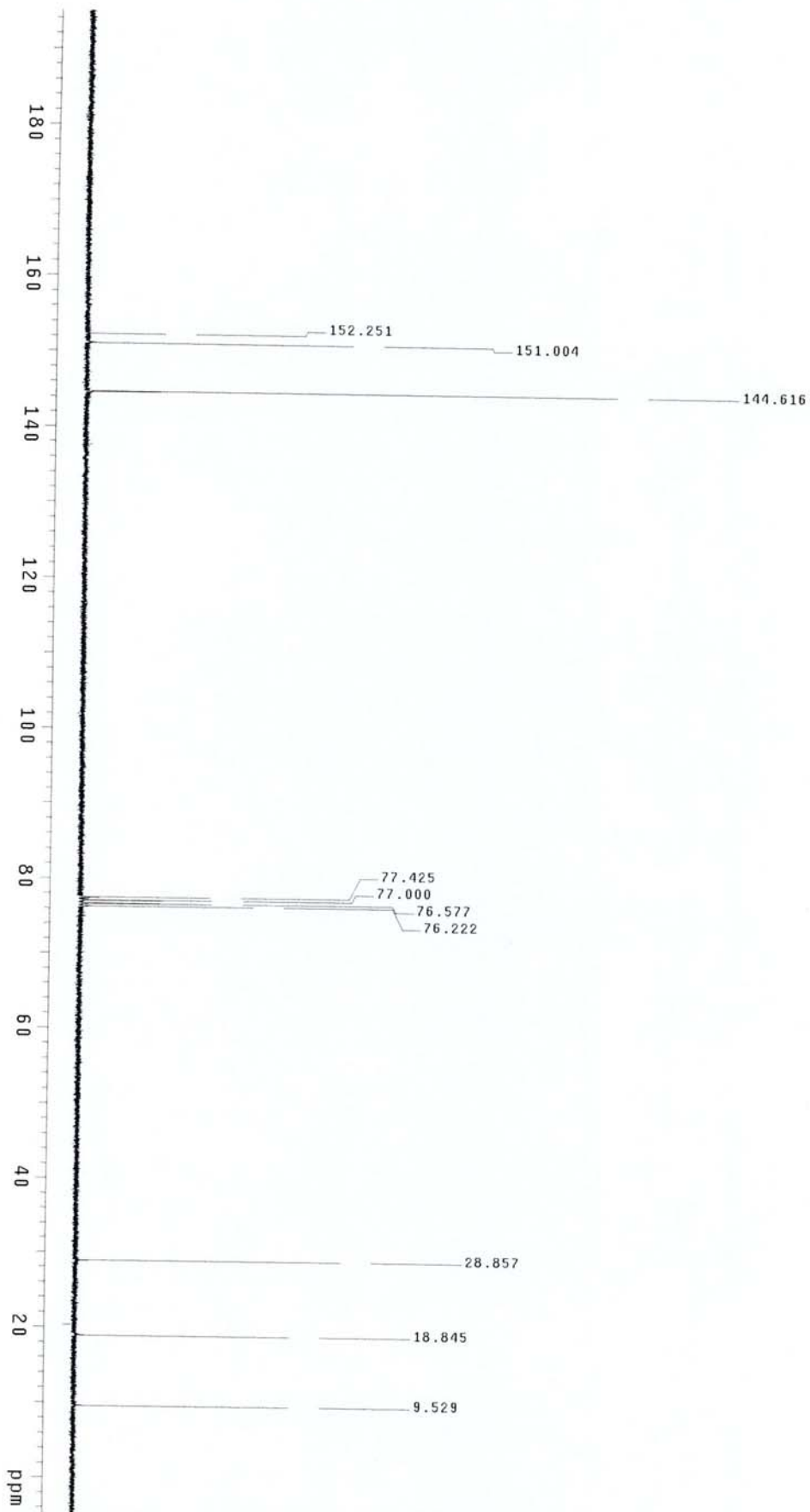
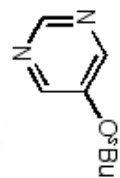
DATA PROCESSING

FT size 131072

Total time 1 min, 4 sec



wxx-2-41-C-3C
Pulse Sequence: szpu1



wxx-2-36-B-3

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

File: wxx-2-36-B-3

INOVA-500 "z1ppy"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

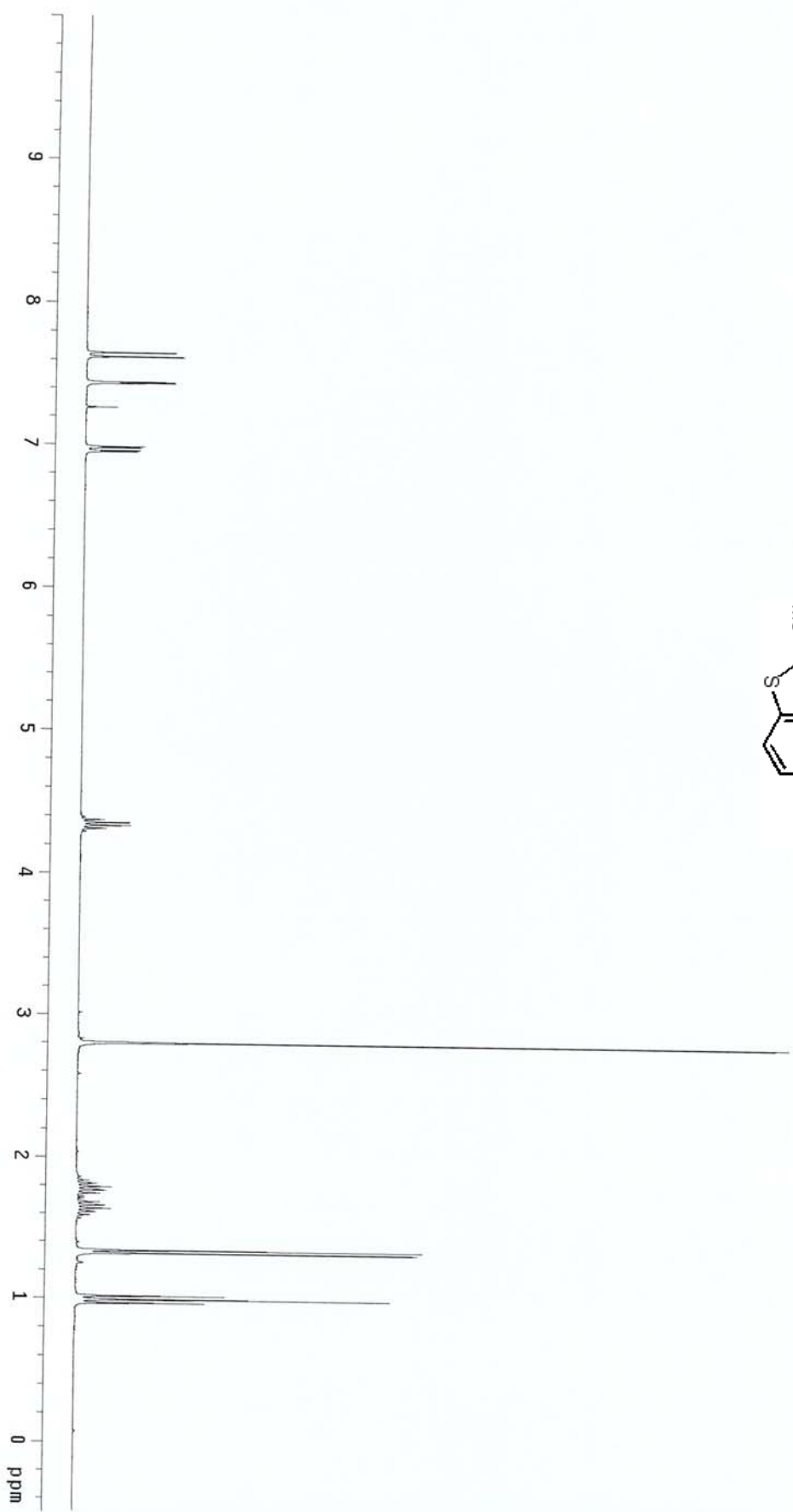
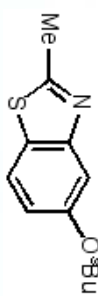
16 Repetitions

OBSERVE H1 300.1055031 MHz

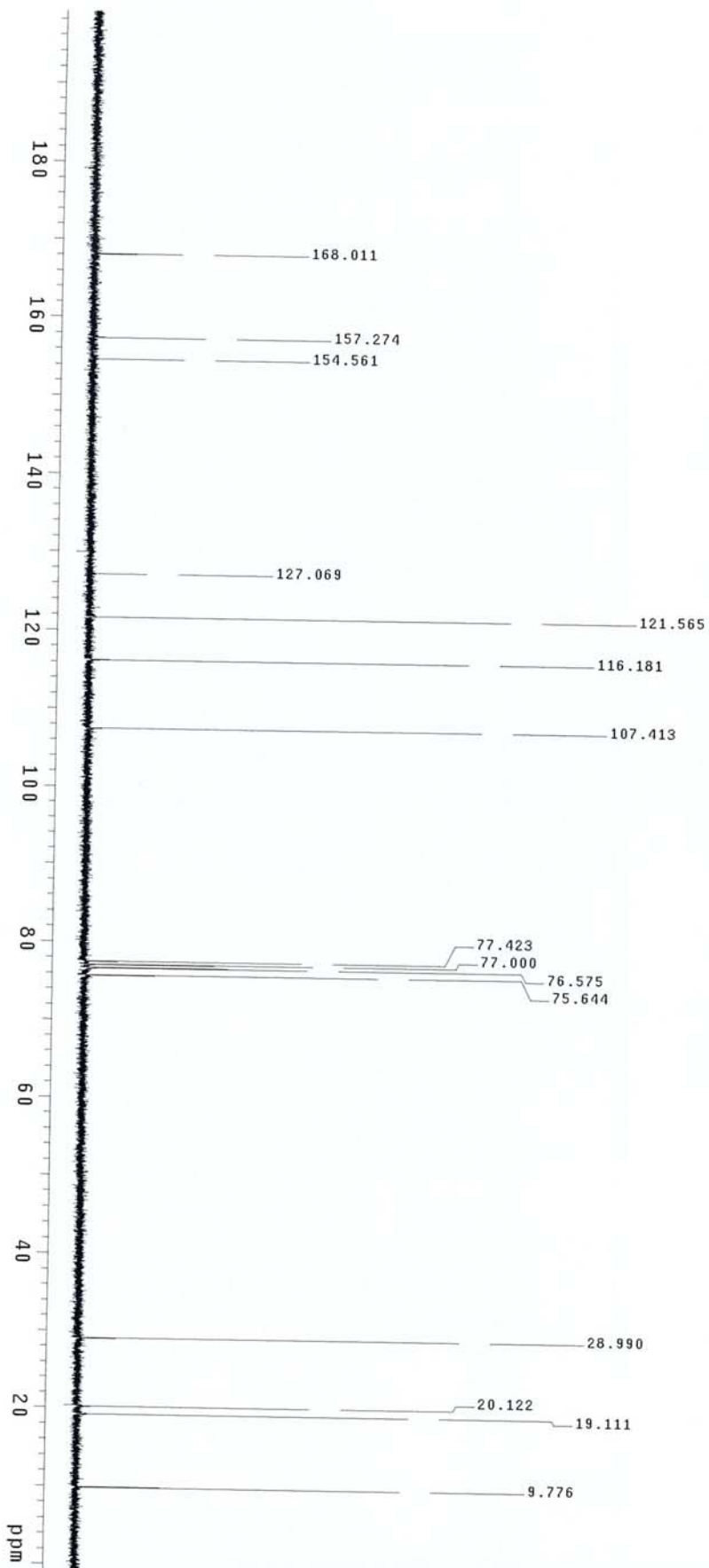
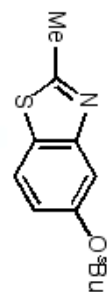
DATA PROCESSING

FT size 131072

Total time 1 min, 4 sec



wxx-2-36-b-3c
Pulse Sequence: s2pu1



wxx-2-35-D-2

Pulse Sequence: szpu1

Solvent: CDCl3

Temp. 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

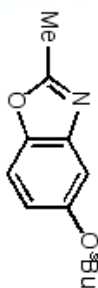
16 repetitions

OBSERVE H1, 300.1055033 MHz

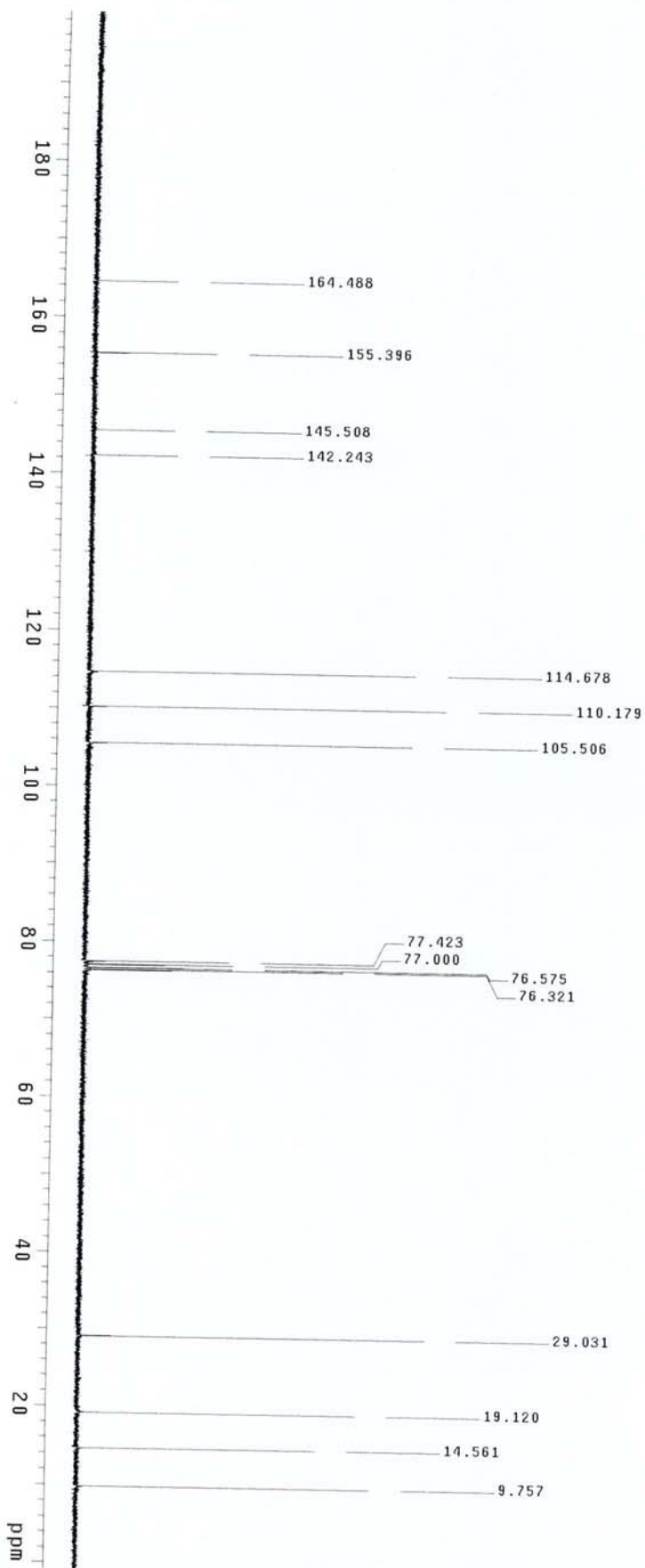
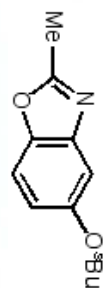
DATA PROCESSING

FT size 131072

Total time 0 min, 0 sec



wxx-2-35-D-2C
Pulse Sequence: szpu1



wxx-2-6-A-1-a

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse: 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

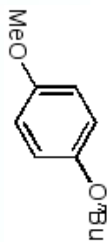
16 repetitions

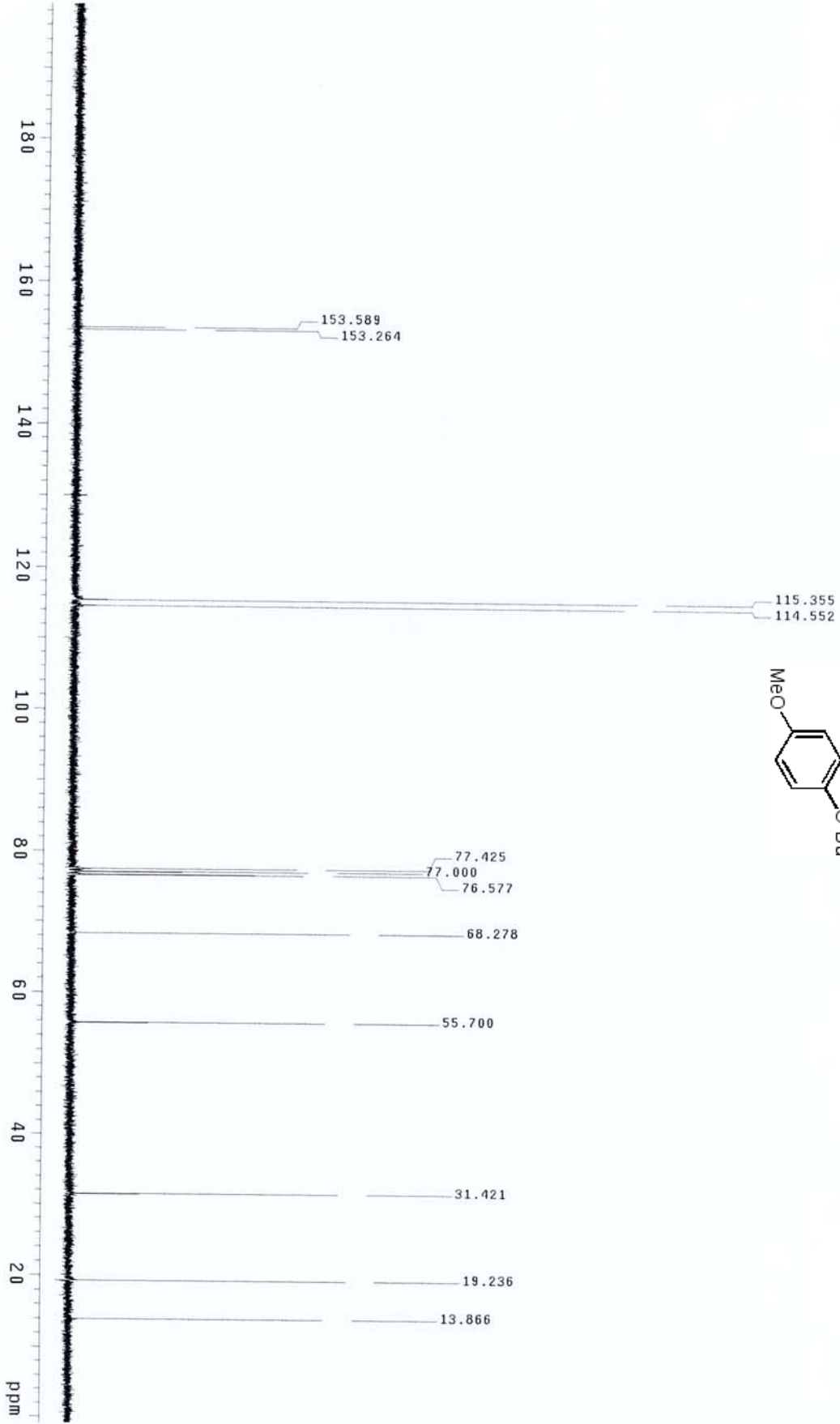
OBSERVE H1: 300.1055031 MHz

DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec





wxx-2-19-8-2

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp. 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

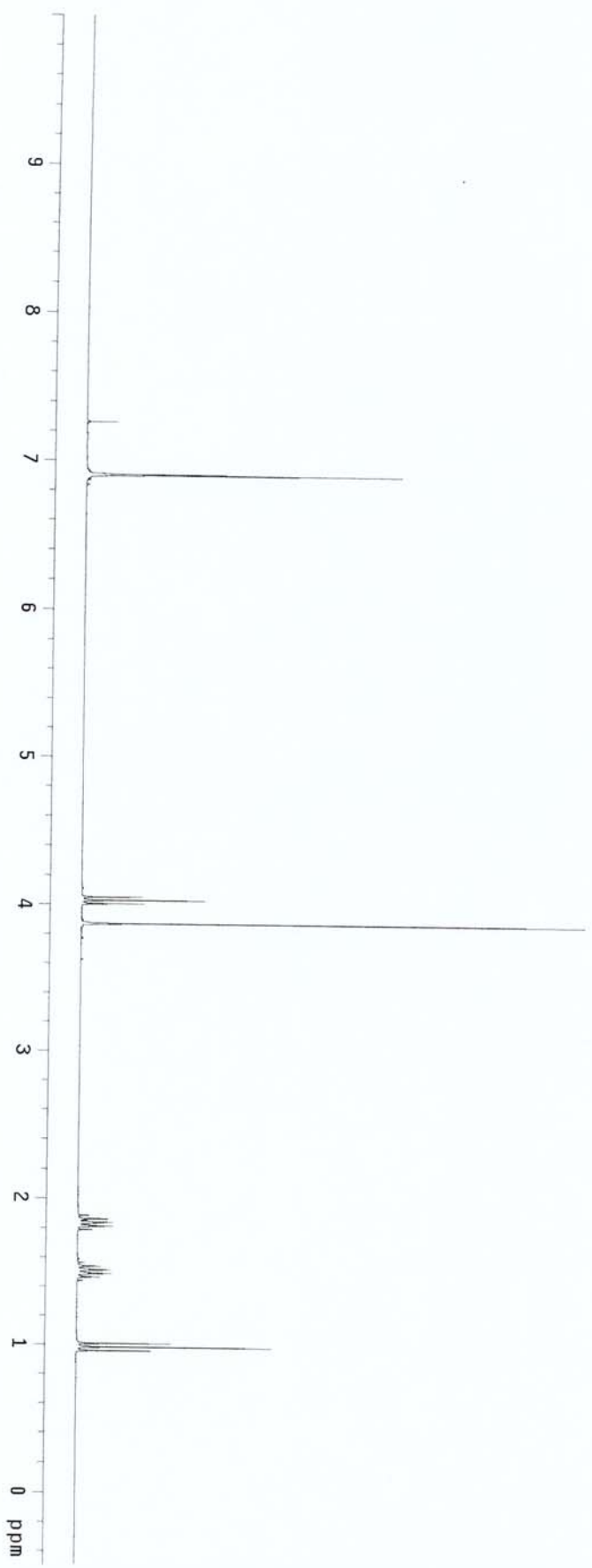
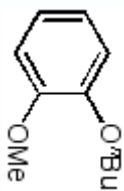
16 repetitions

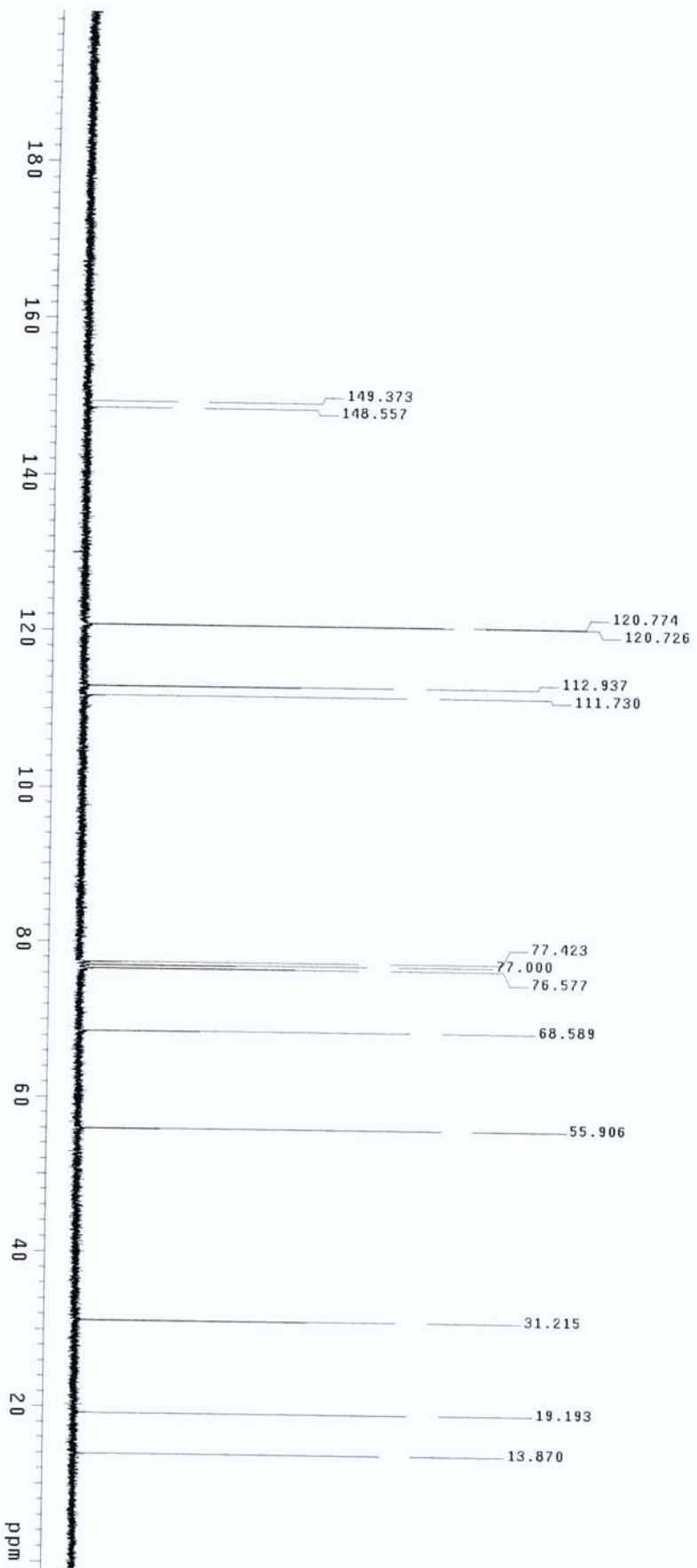
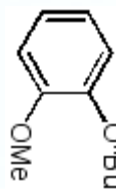
OBSERVE H1, 300.1055034 MHz

DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec





wxx-2-22-C-2

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp.: 20.0 C / 293.1 K

File: wxx-2-22-C-2

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

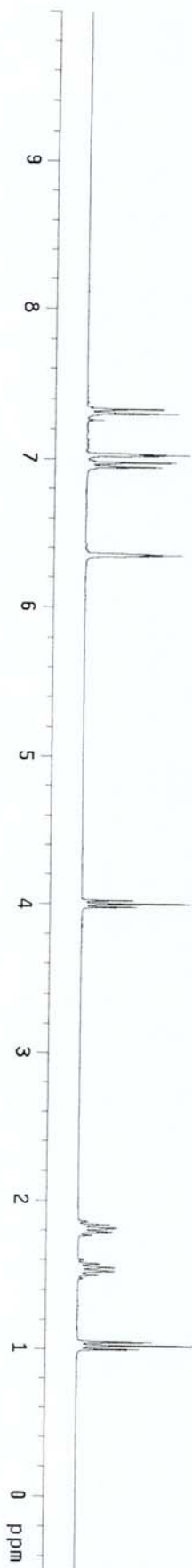
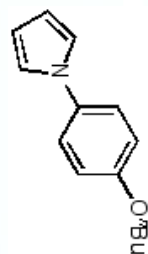
16 repetitions

OBSERVE H1, 300.1055032 MHz

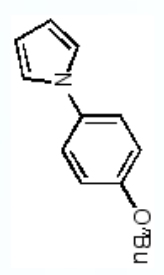
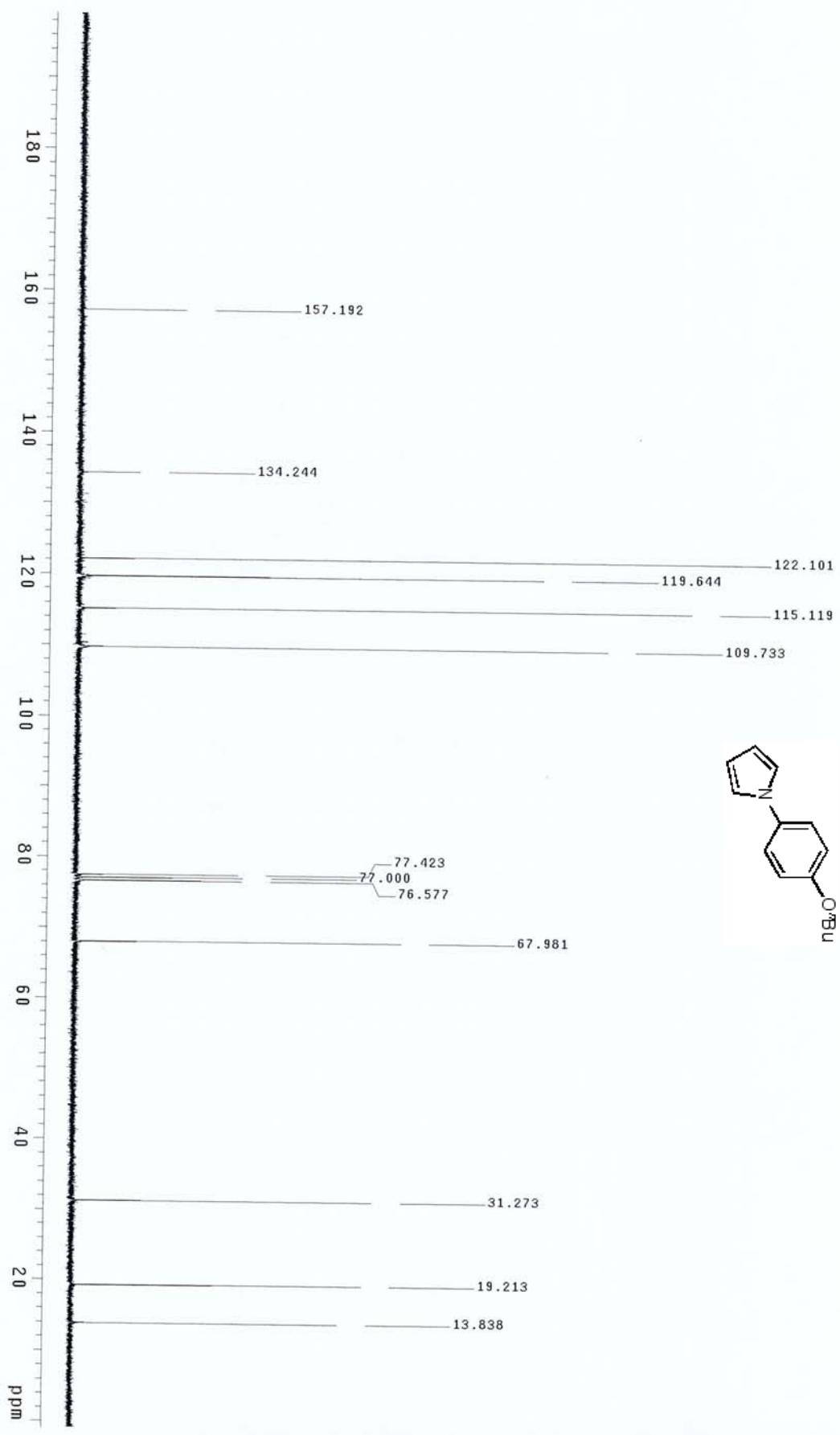
DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec



WXX-2-22-C-2C
Pulse Sequence: s2pu1



wxx-2-15-B-2

Pulse Sequence: szpu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

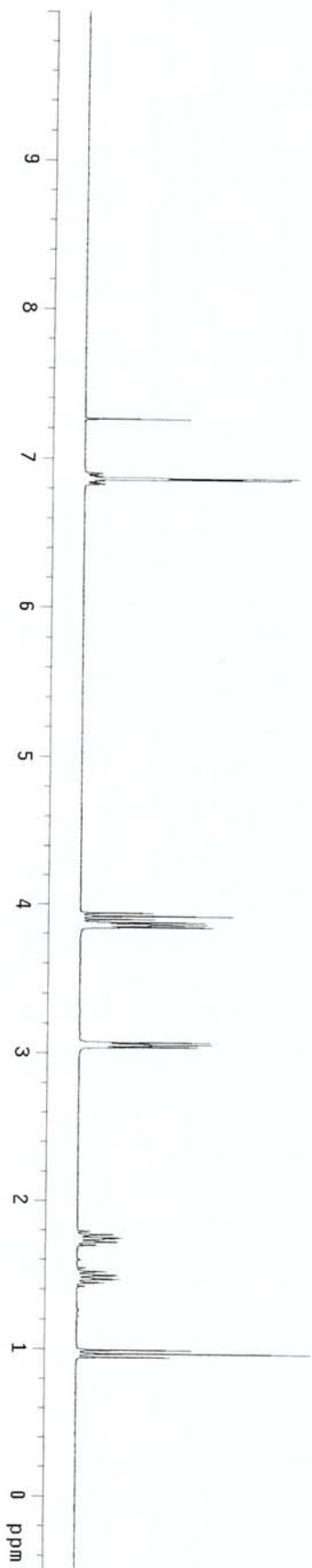
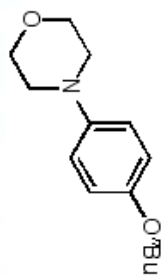
16 repetitions

OBSERVE H1, 300.1055033 MHz

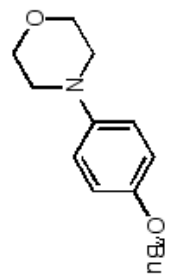
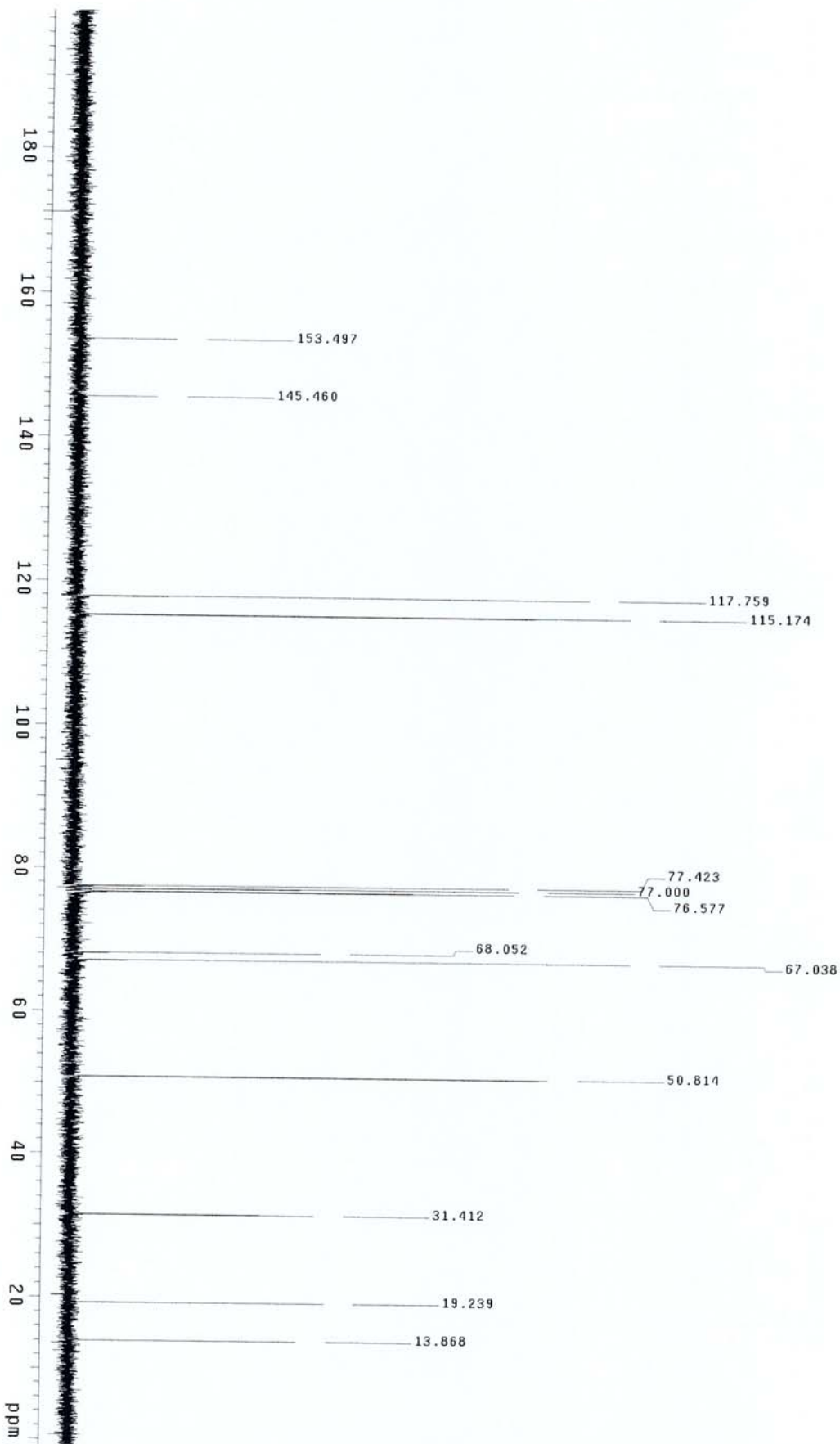
DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec



wxx-2-15-A-2C
Pulse Sequence: szpu1



wxx-2-120-B-3

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

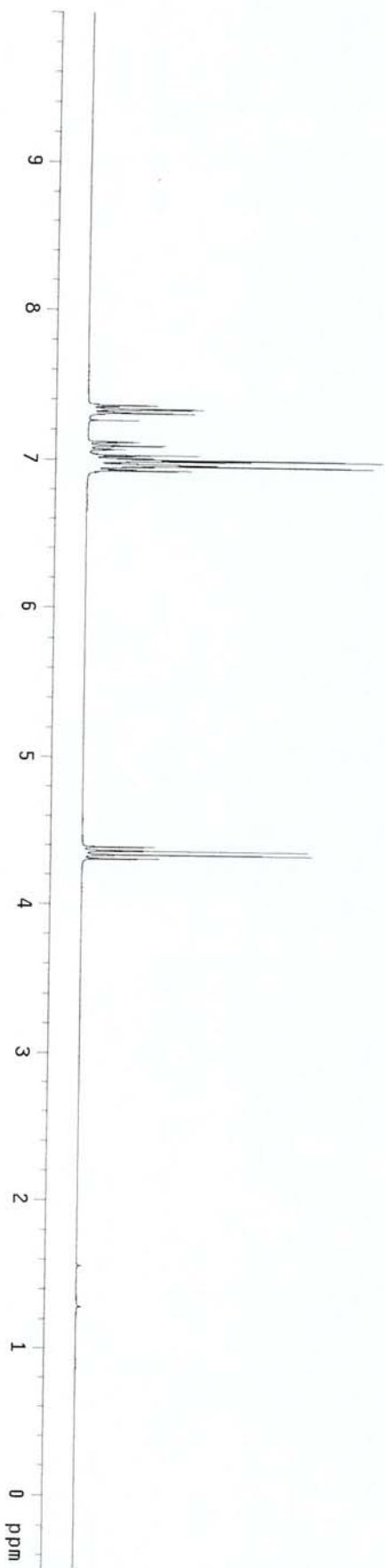
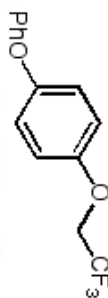
16 repetitions

OBSERVE H1, 300.1055035 MHz

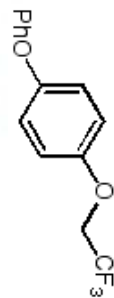
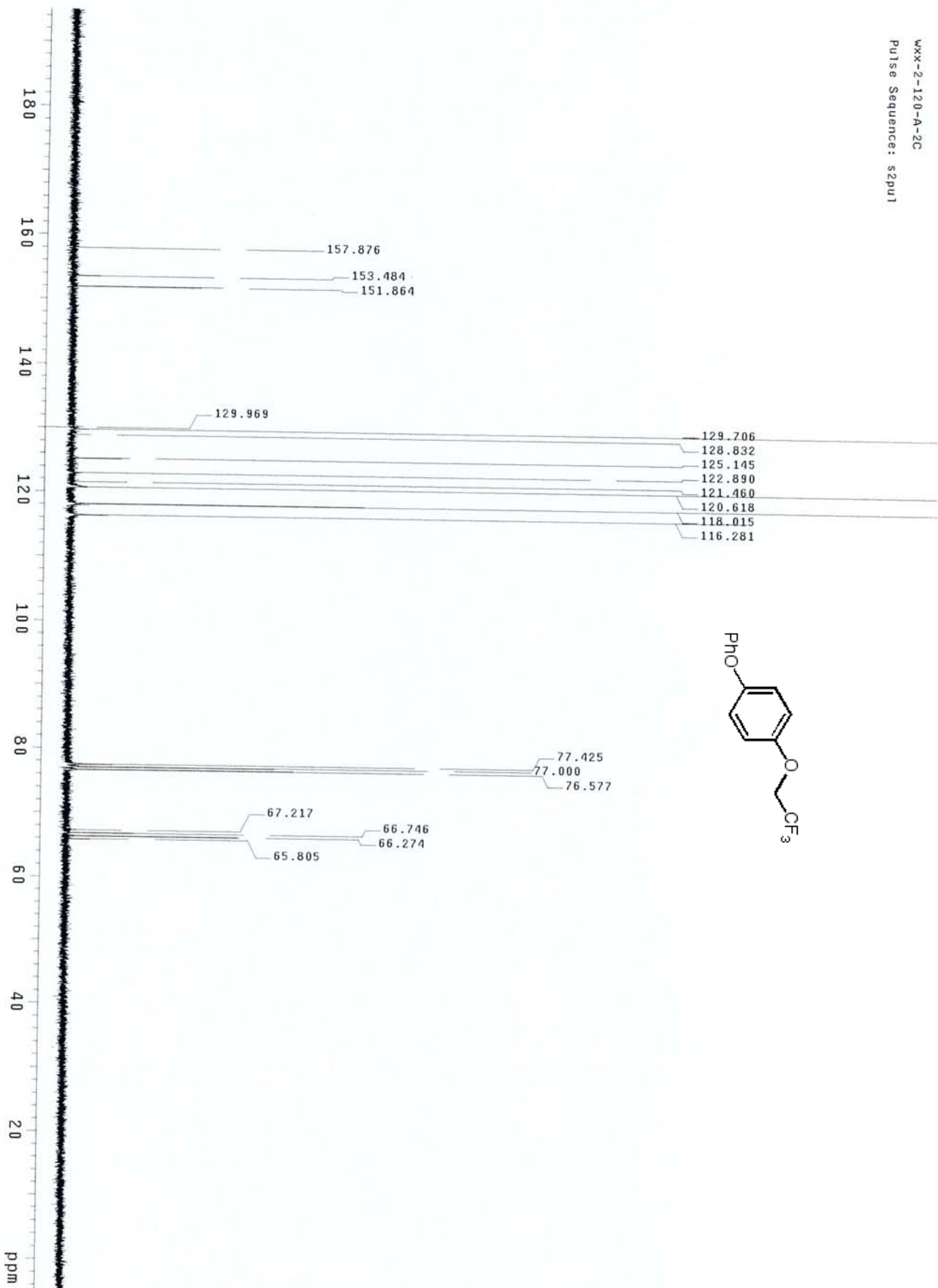
DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec



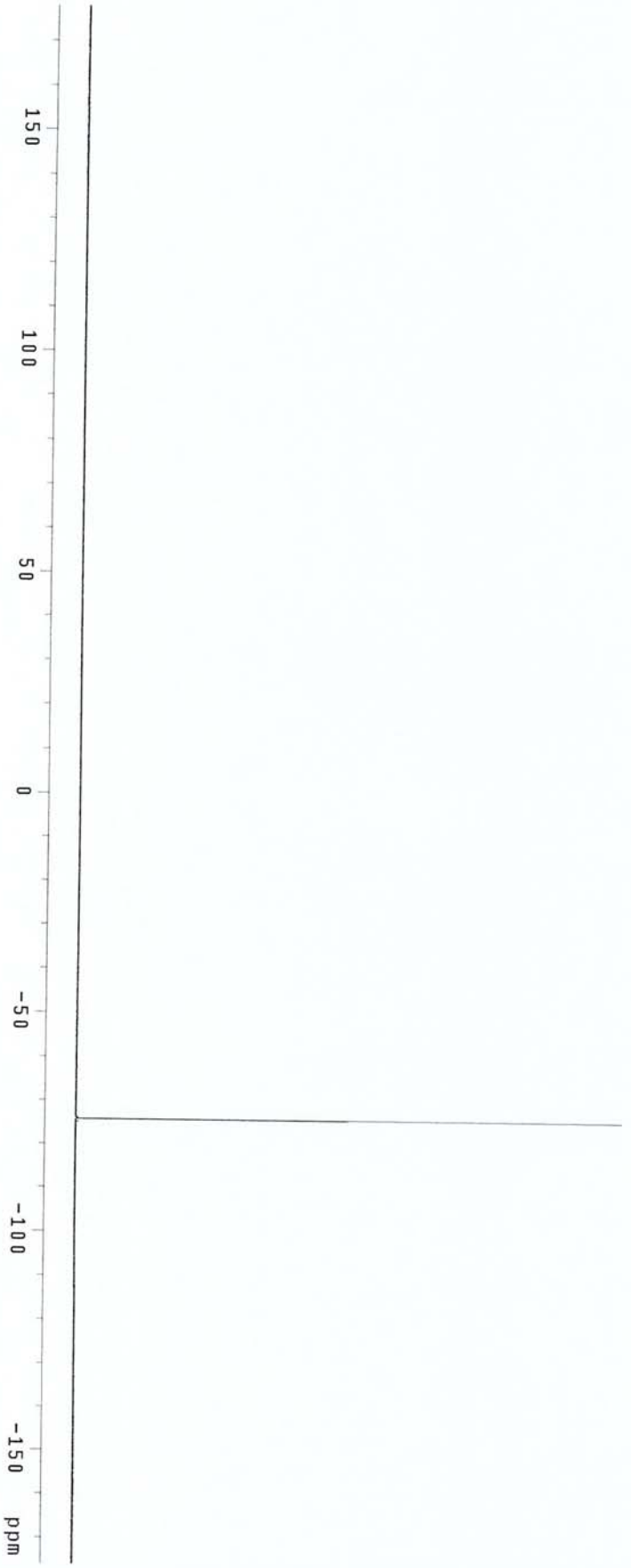
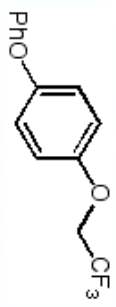
WXX-2-120-A-2C
Pulse Sequence: s2pu1



WXX-2-120-13-31-
197 OBSERVE
STANDARD PARAMETERS

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhbt"

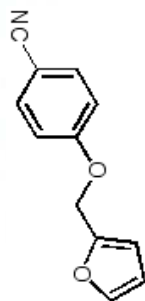
Relax. delay 4.000 sec
Pulse 45.0 degrees
Acq. time 0.300 sec
Width 100.0 KHz
16 repetitions
OBSERVE F19 282.3814158 MHz
DATA PROCESSING
Line broadening 0.3 Hz
Ft size 262144
Total time 1 min, 24 sec

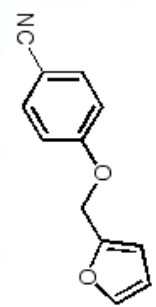
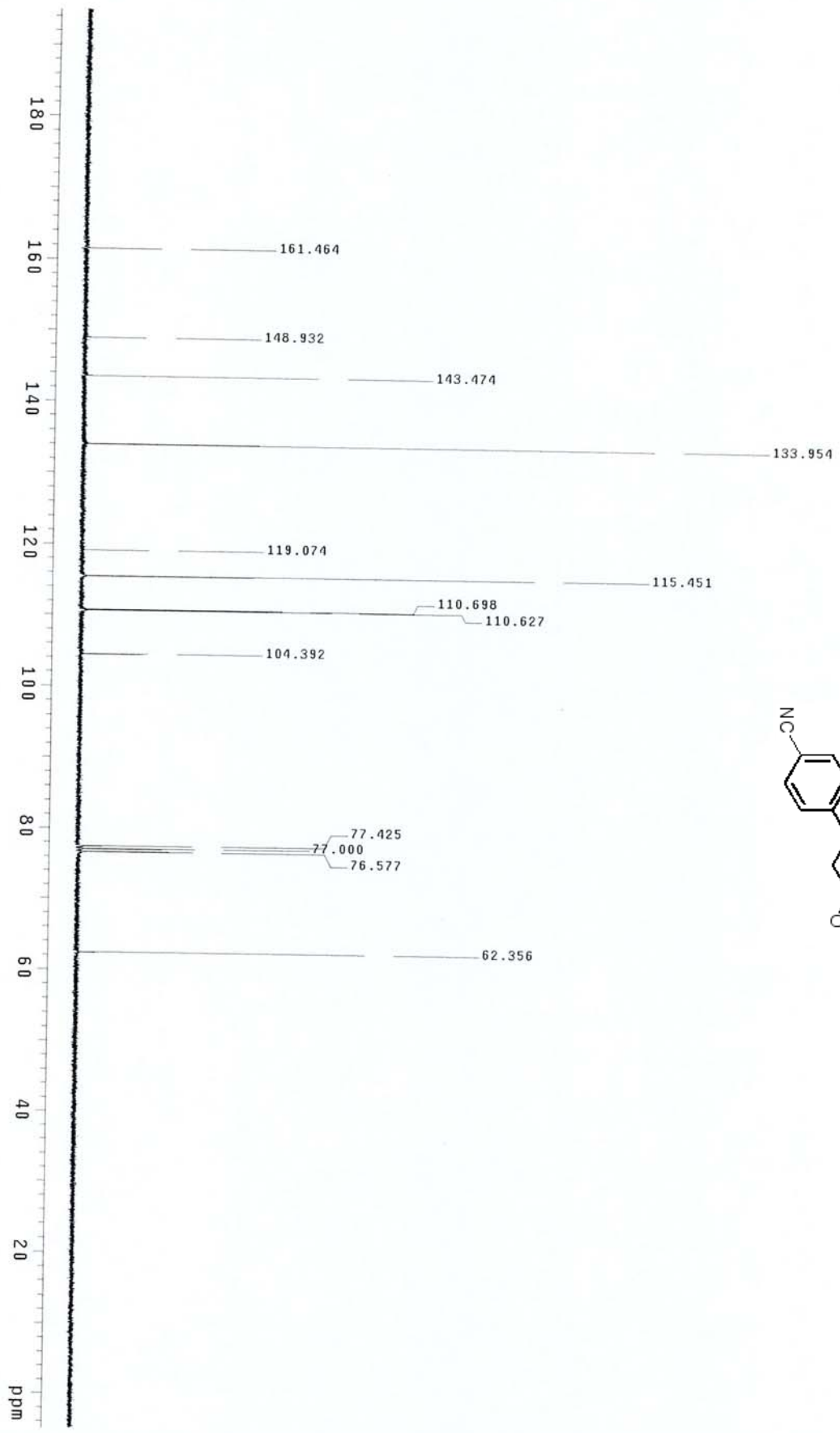


wxx-2-126-A-2

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhat"

Relax. delay 0.050 sec
Pulse 33.9 degrees
Acq. time 4.003 sec
Width 6002.4 Hz
16 repetitions
OBSERVE H1, 300.1055029 MHz
DATA PROCESSING
F1 size 131072
Total time 1 min, 17 sec





wxx-2-119-A-2

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

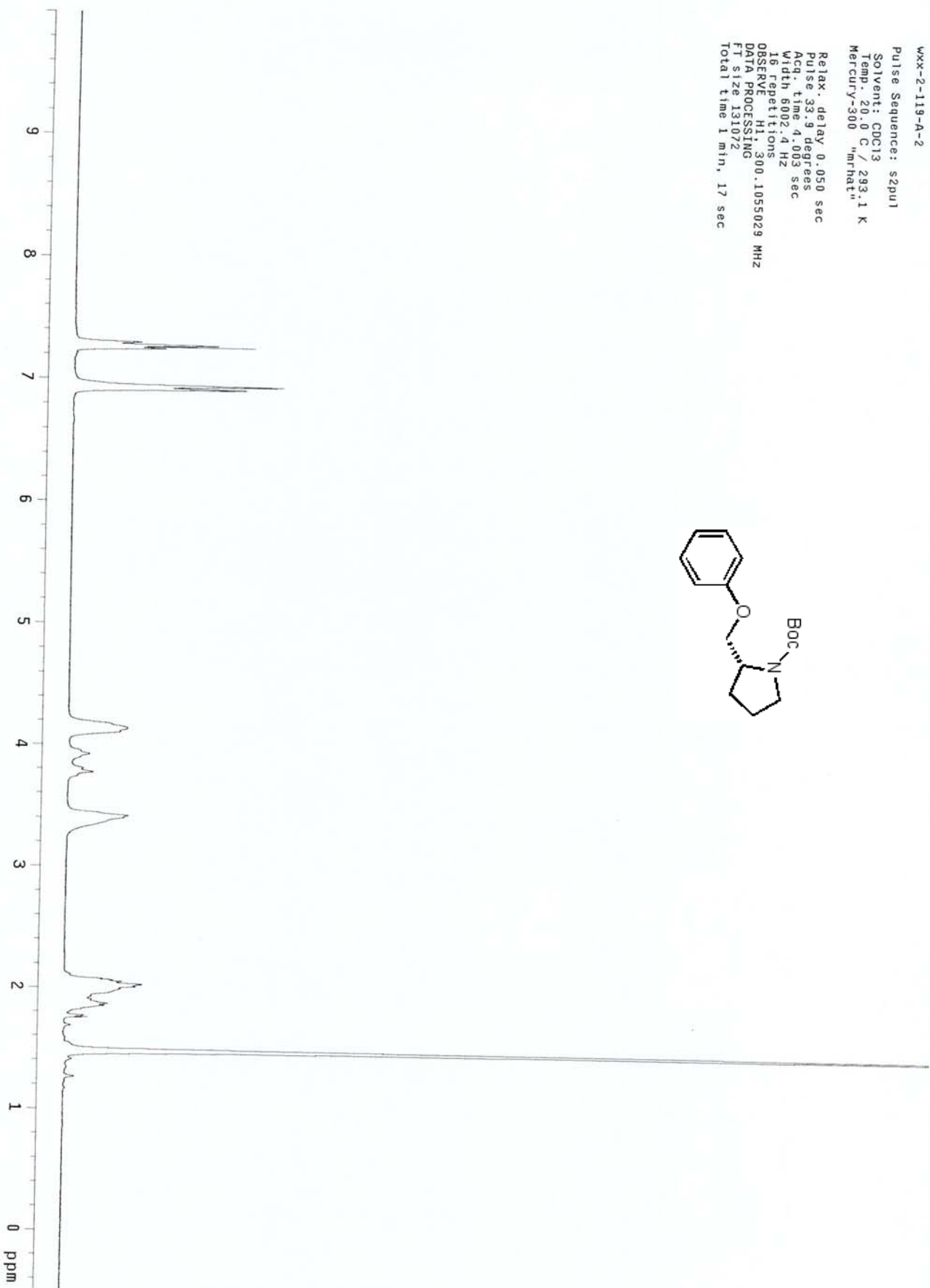
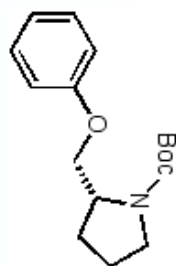
16 repetitions

OBSERVE H1, 300.1055029 MHz

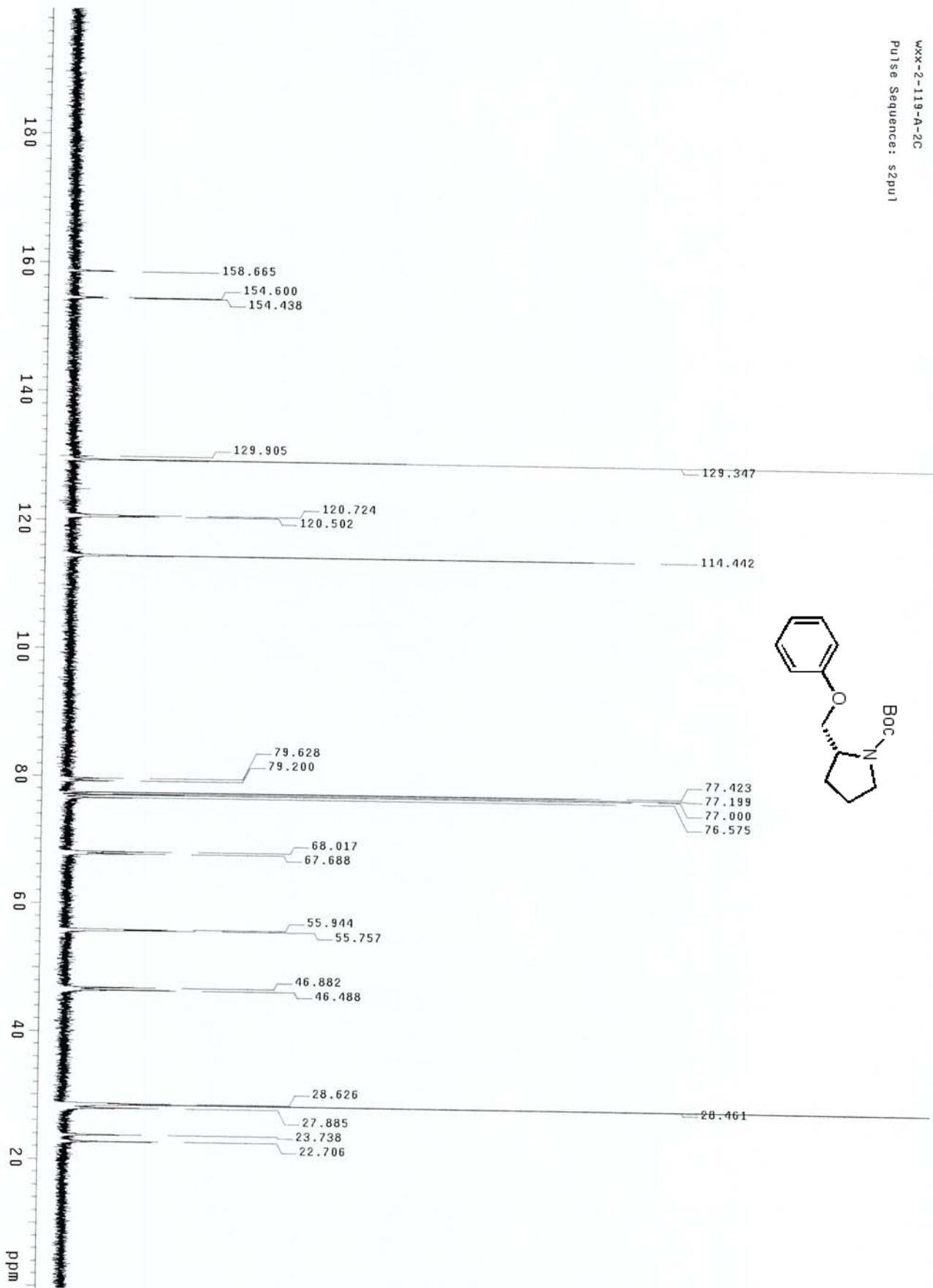
DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec



WXX-2-119-A-2C
Pulse Sequence: s2pu1



wxx-2-17-D-2

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

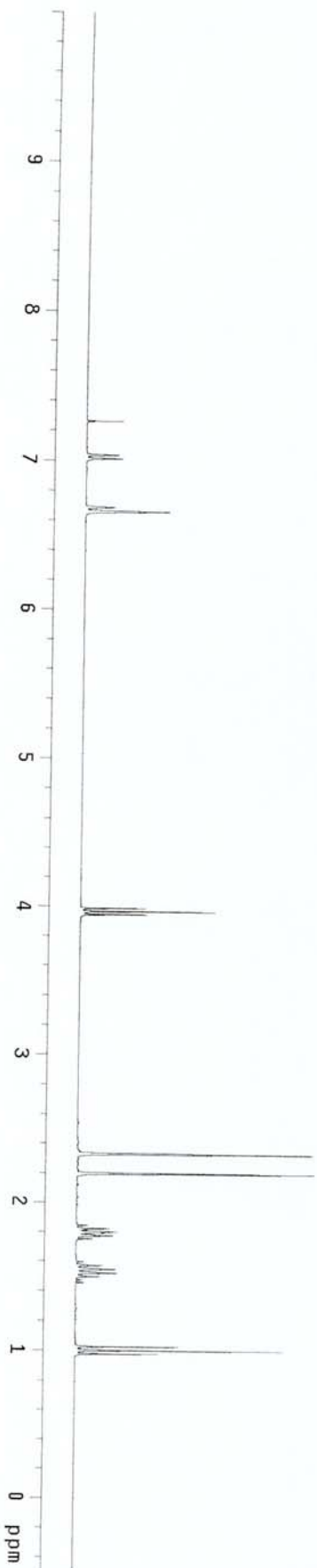
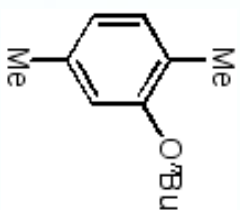
16 Repetitions

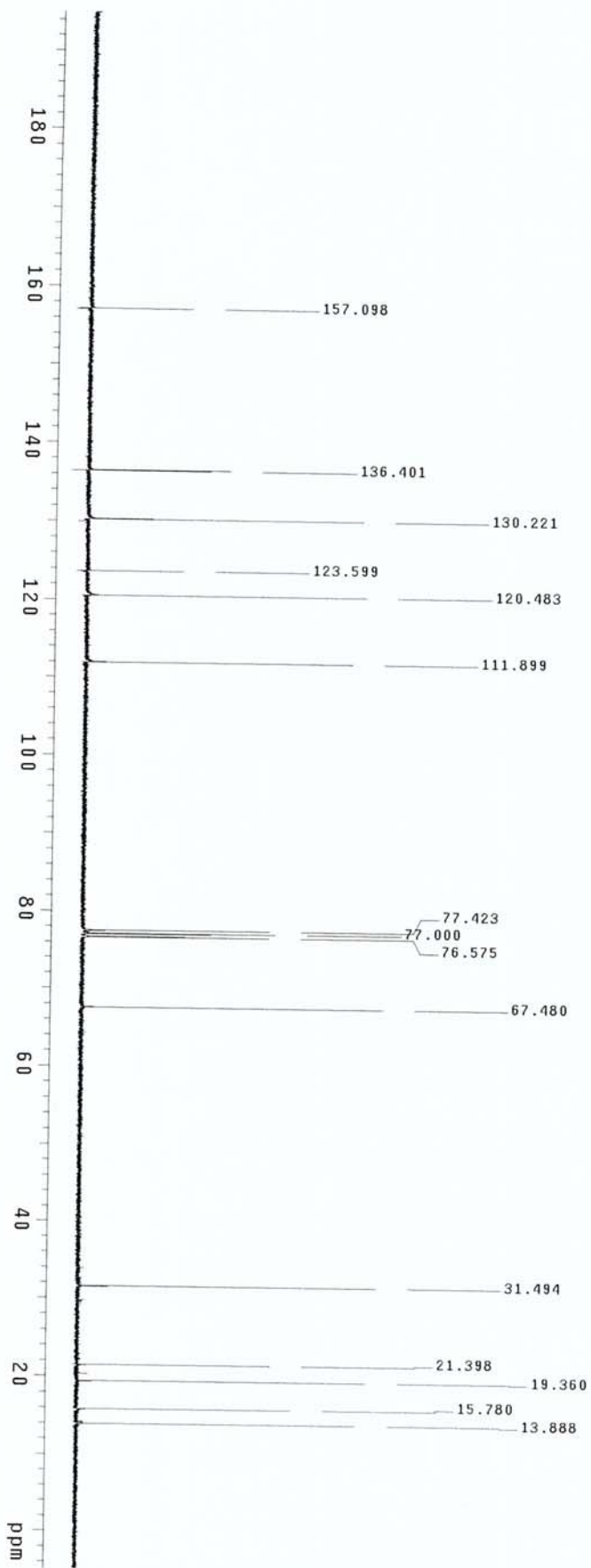
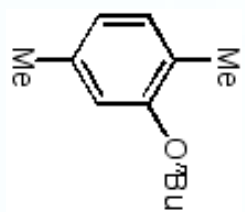
OBSERVE H1, 300.1055033 MHz

DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec

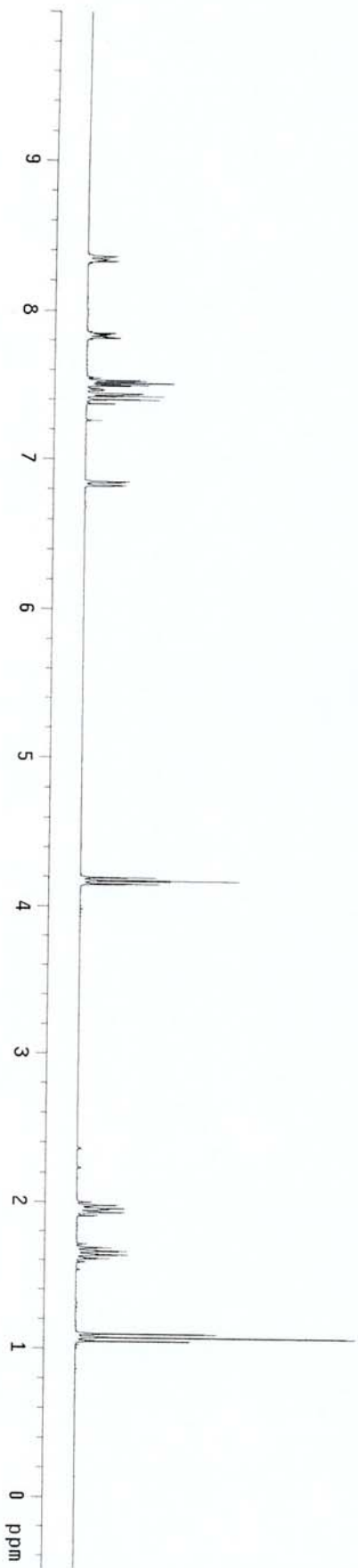
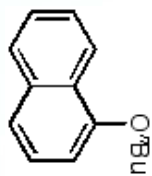




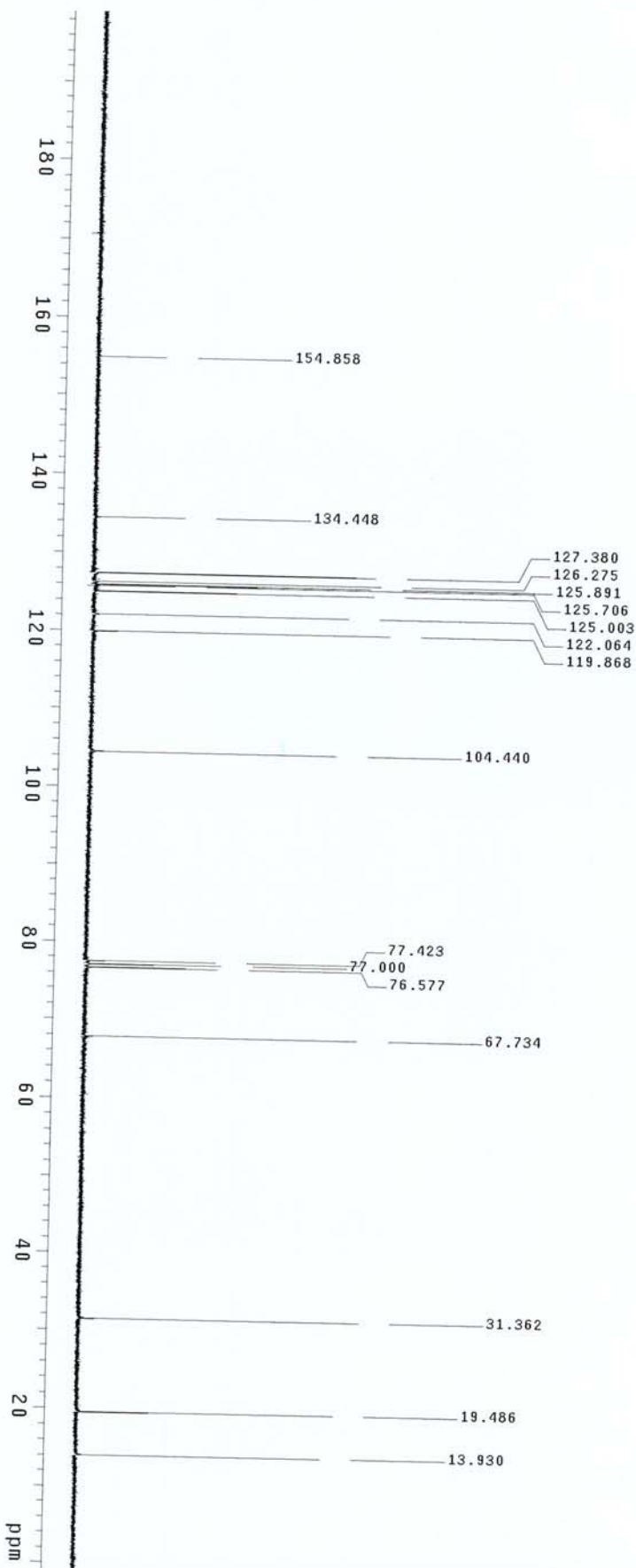
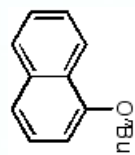
wxx-2-8-C-2

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhat"

Relax. delay 0.050 sec
Pulse 33.9 degrees
Acq. time 4.003 sec
Width 6002.4 Hz
16 repetitions
OBSERVE H1, 300.1055034 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 17 sec



wxx-2-8-C-2C
Pulse Sequence: szpu1



WXX-2-93-A-3

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

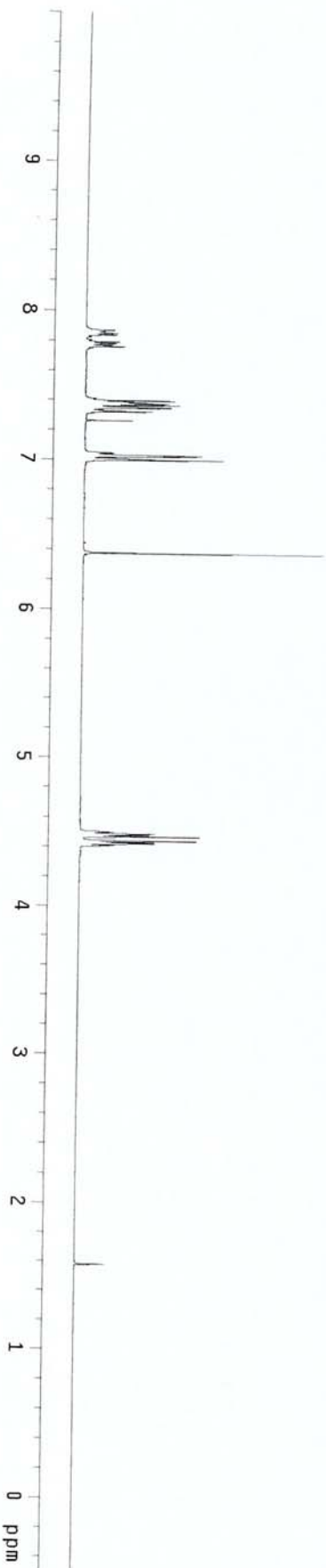
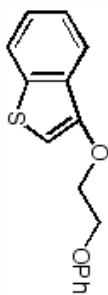
16 repetitions

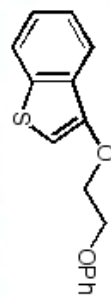
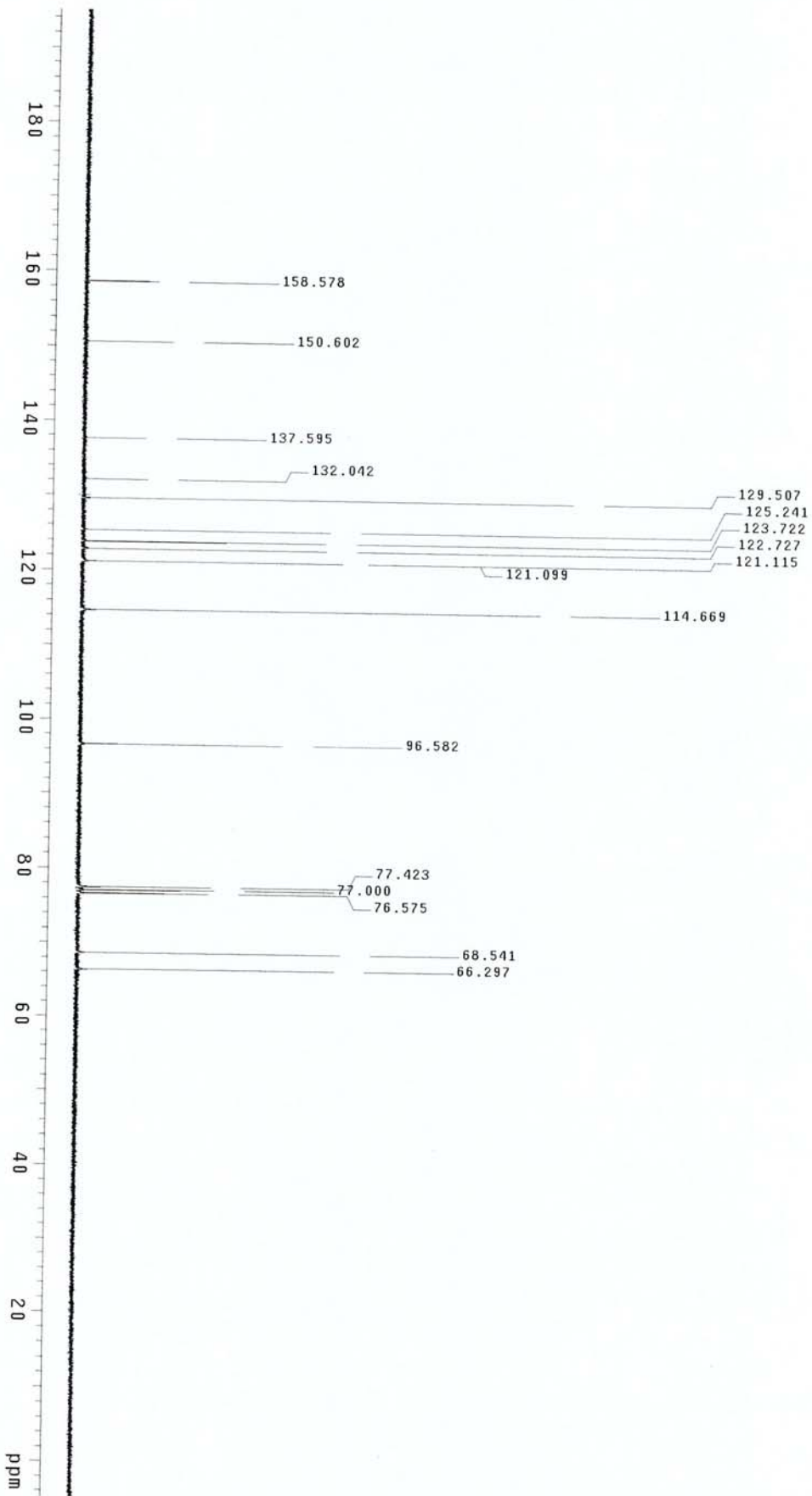
OBSERVE H1, 300.1055032 MHz

DATA PROCESSING

FT size 131072

Total time 0 min, 0 sec





wxx-2-12-E-2

Pulse Sequence: szpu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

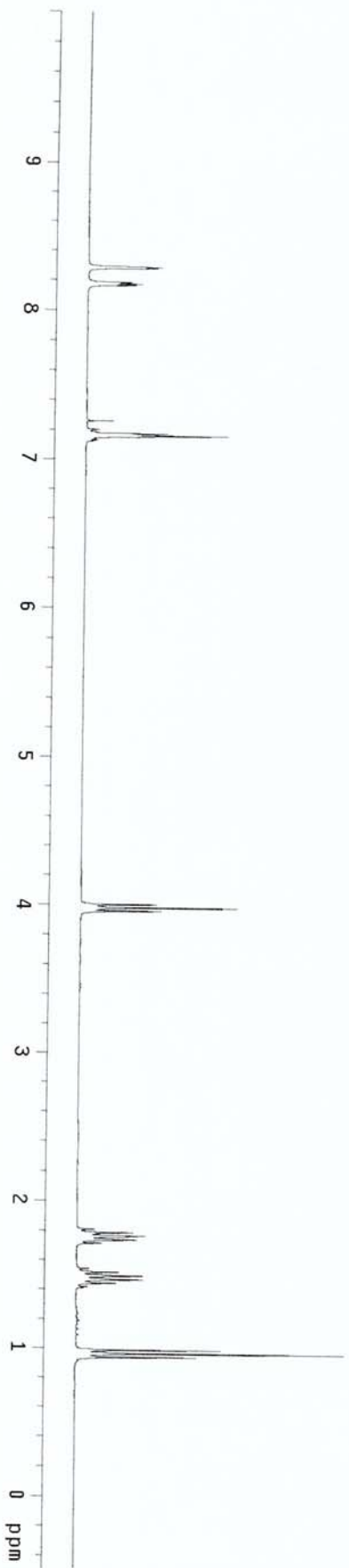
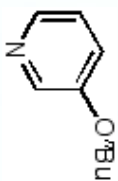
16 Repetitions

OBSERVE H1: 300.1055035 MHz

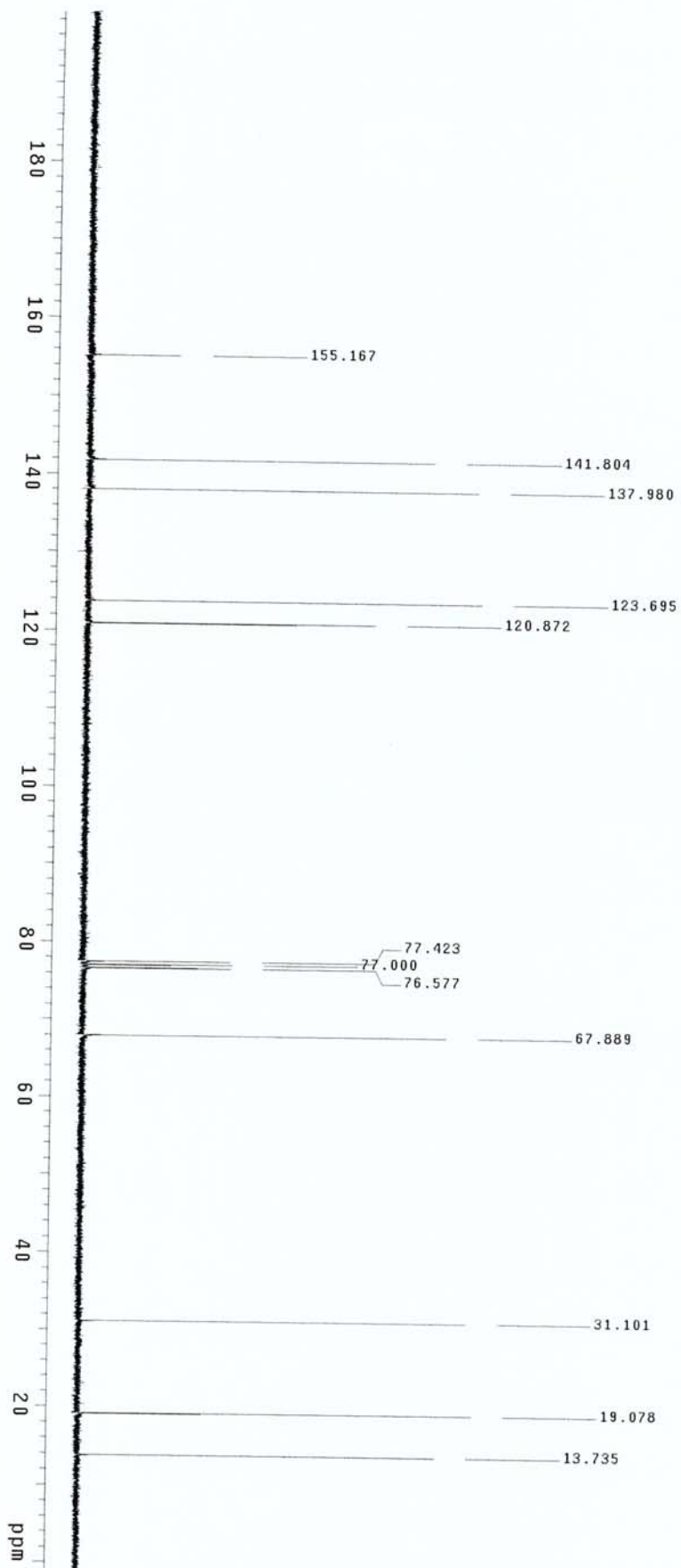
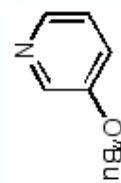
DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec



wxx-2-12-E-2C
Pulse Sequence: s2pu1



wxx-2-23-B-2

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

File: wxx-2-23-A-2

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

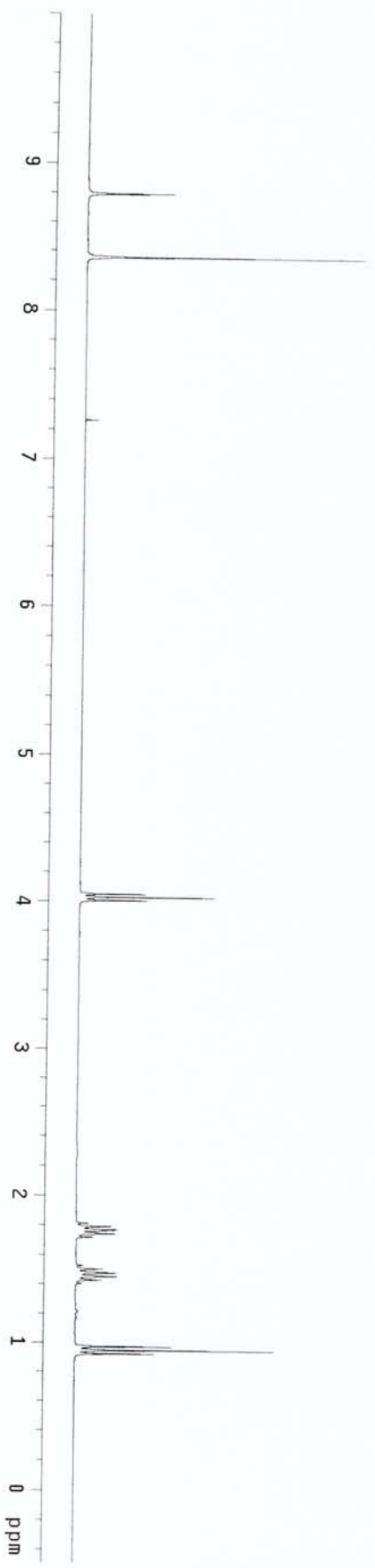
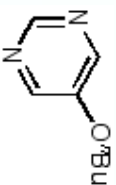
16 Repetitions

OBSERVE H1; 300.1055032 MHz

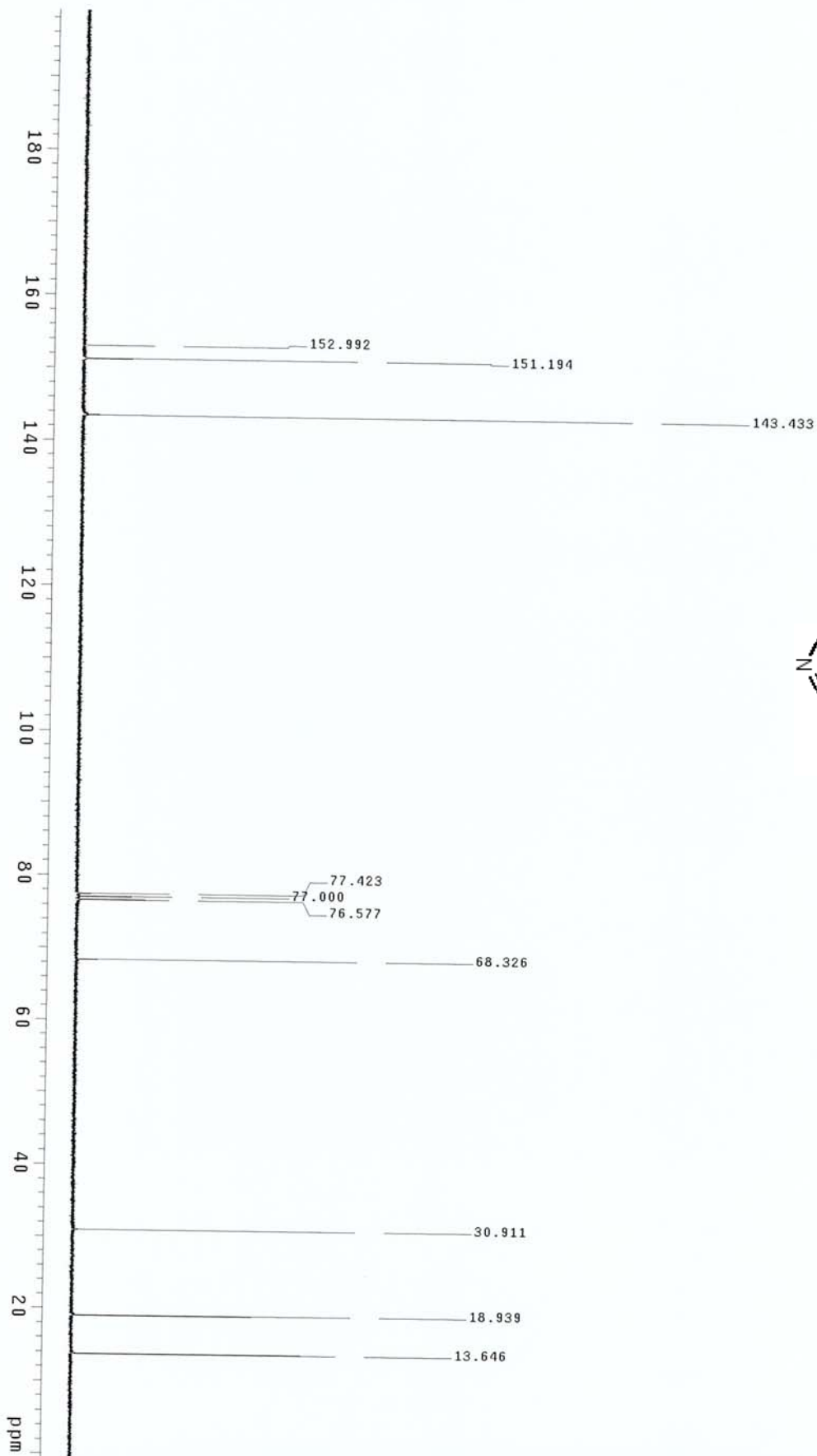
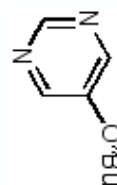
DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec



WXX-2-23-A-2C
Pulse Sequence: s2pu1



wxx-2-13-B-2

Pulse Sequence: s2pul

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

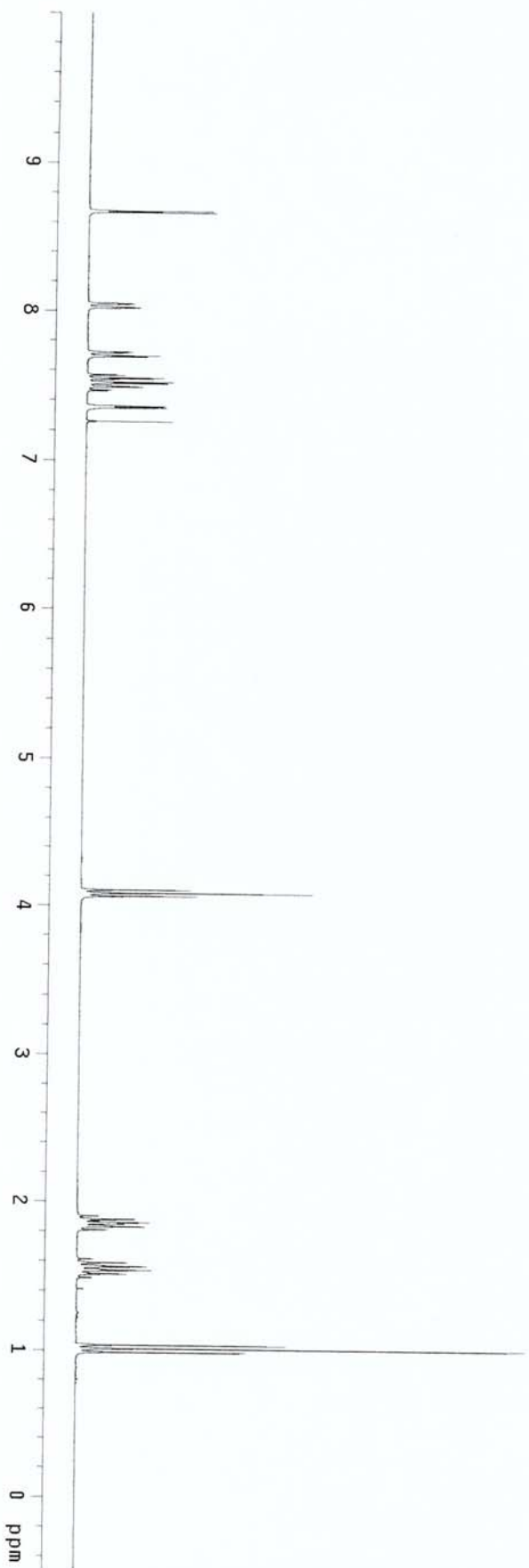
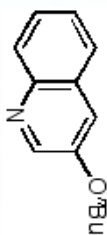
16 repetitions

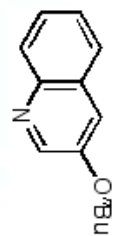
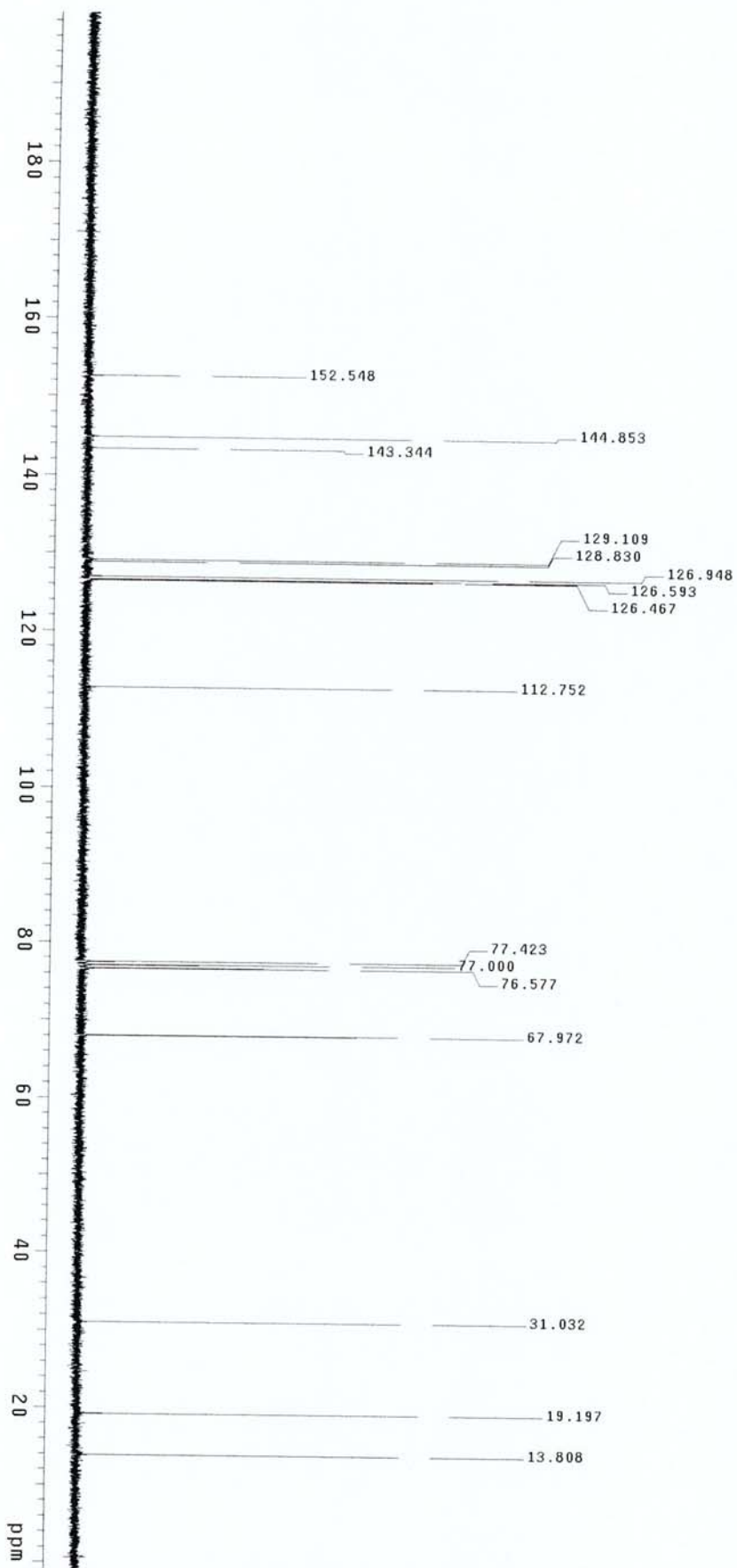
OBSERVE H1, 300.1055034 MHz

DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec





wxx-2-14-B-2

Pulse Sequence: szpu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

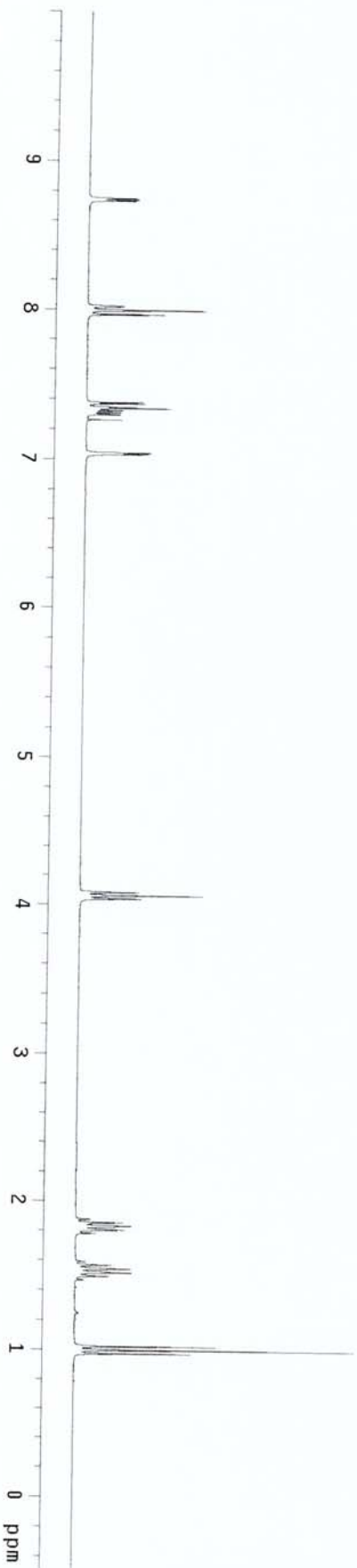
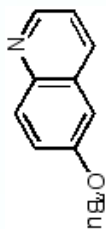
16 repetitions

OBSERVE H1, 300.1055033 MHz

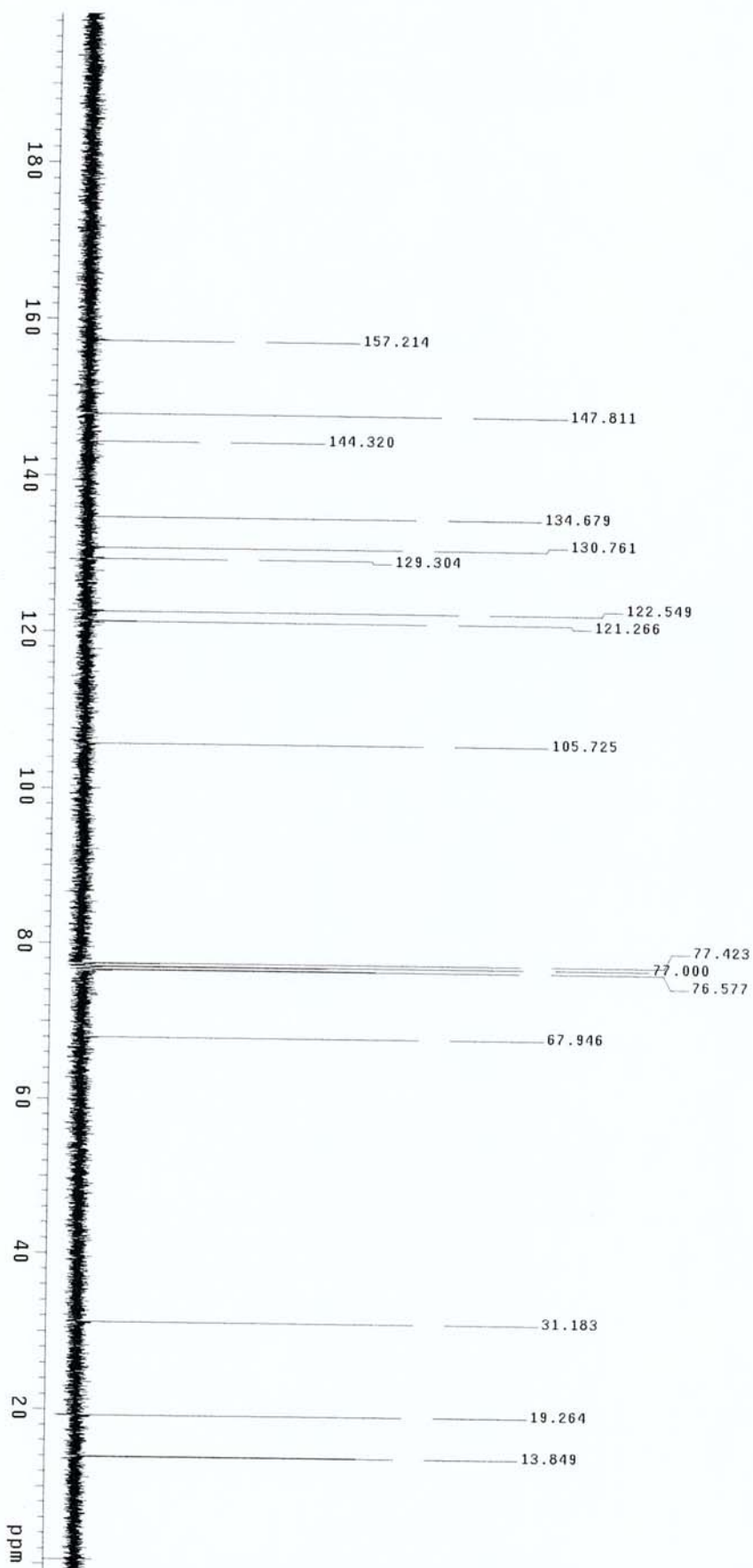
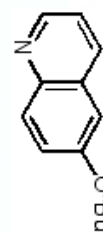
DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec



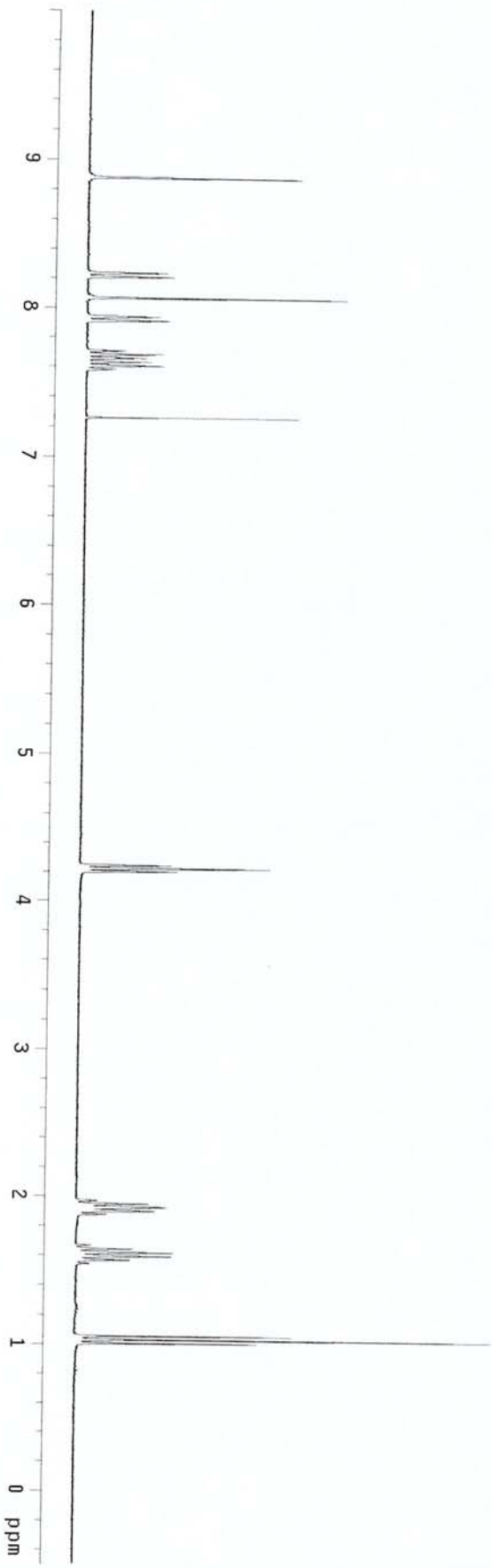
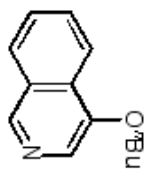
wxx-2-14-A-2C
Pulse Sequence: s2pu1

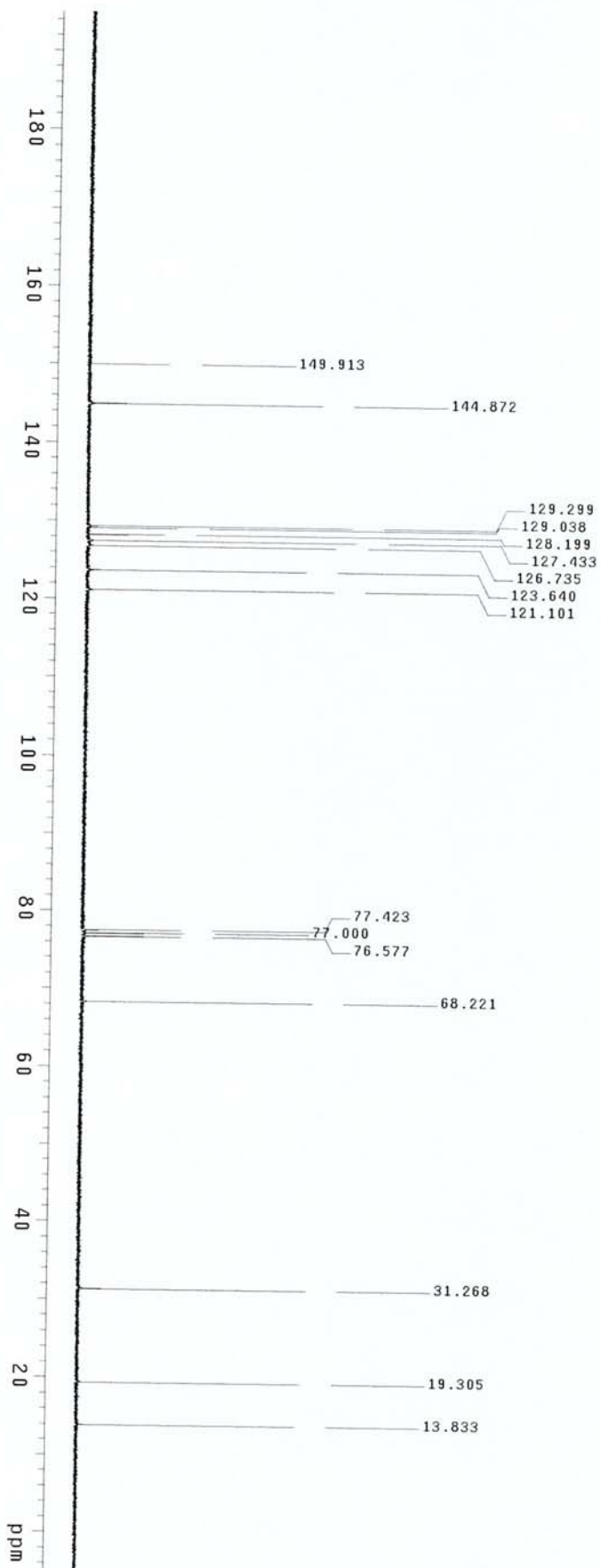
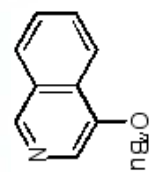


wxx-2-128-j-1

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhat"

Relax. delay 0.050 sec
Pulse 33.9 degrees
Acq. time 4.003 sec
Width 6002.4 Hz
8 repetitions
OBSERVE H1, 300.1055040 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 17 sec

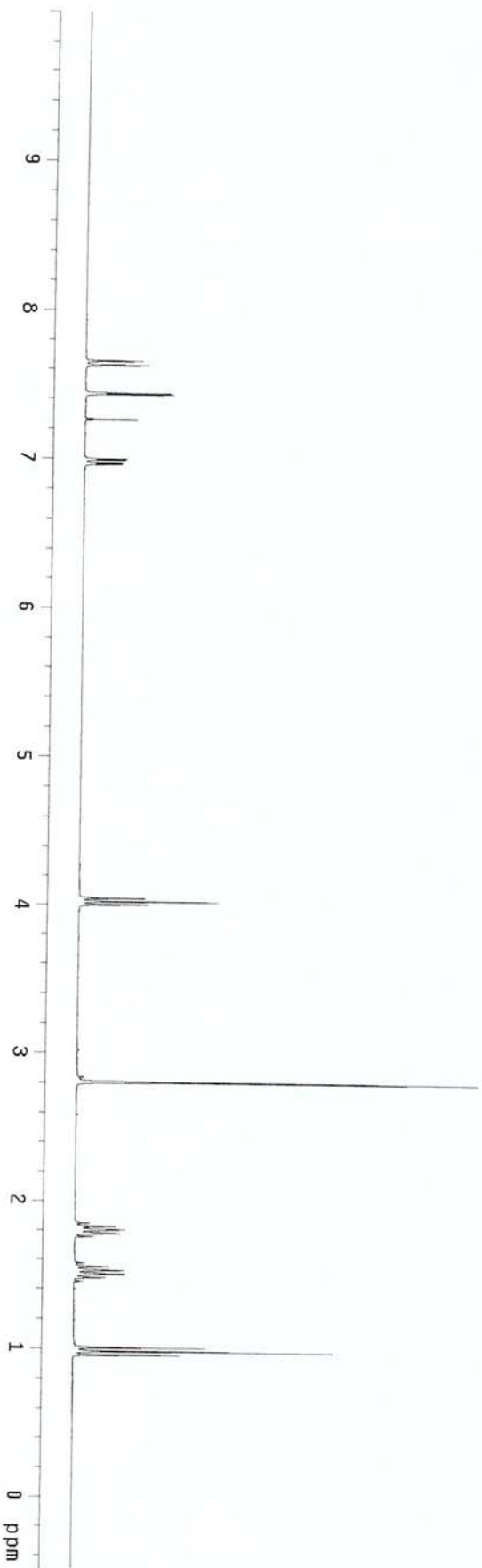




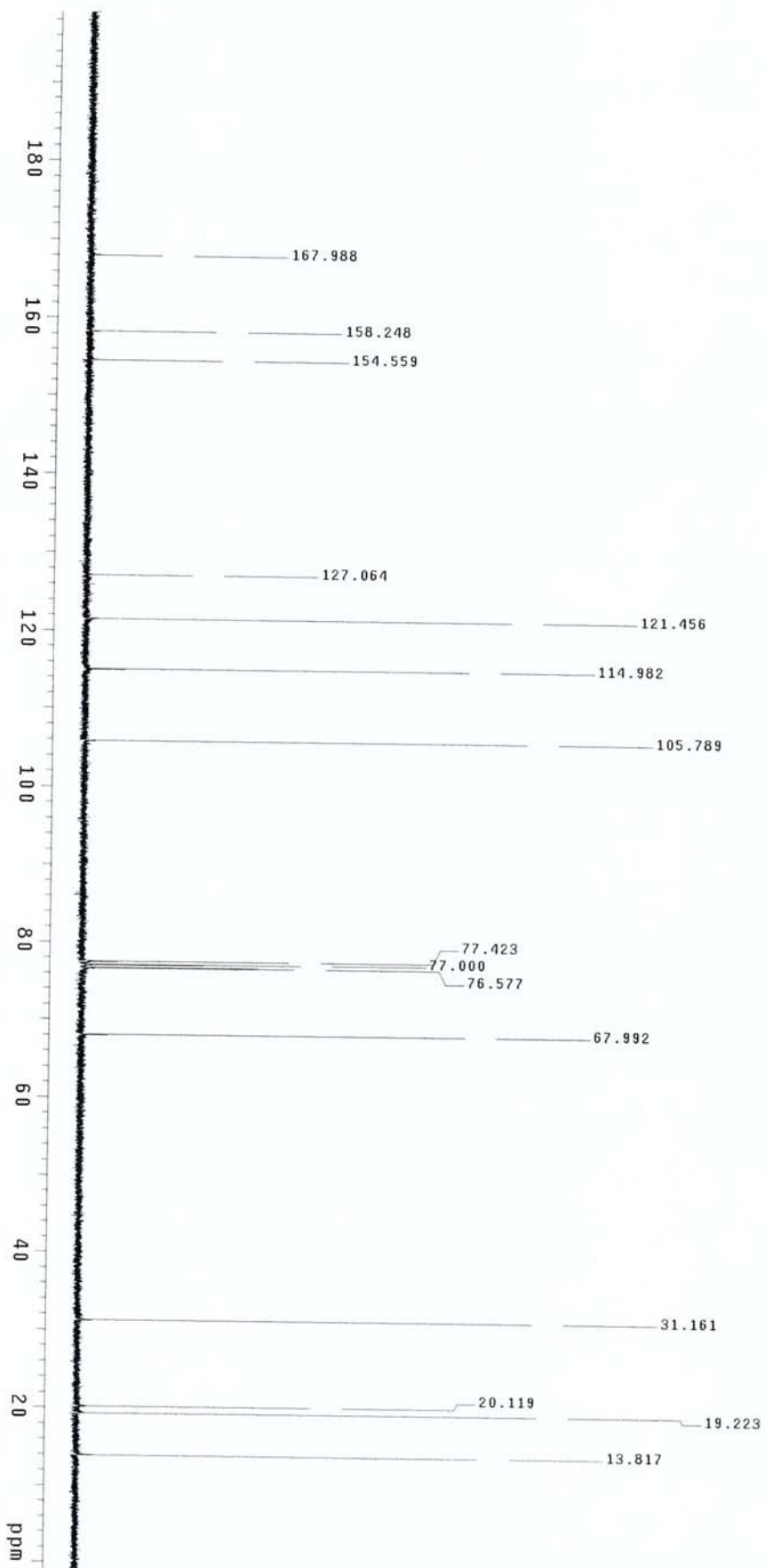
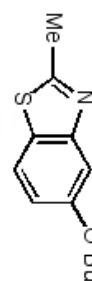
wxx-2-21-B-2

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 20.0 C / 293.1 K
Mercury-300 "mrhat"

Relax. delay 0.050 sec
Pulse 33.9 degrees
Acq. time 4.003 sec
Width 6002.4 Hz
16 Repetitions
OBSERVE H1, 300.1055034 MHz
DATA PROCESSING
FT size 131072
Total time 0 min, 0 sec



wxx-2-21-A-2C
Pulse Sequence: s2pu1



wxx-2-20-A-2

Pulse Sequence: szpu1

Solvent: CDCl3

Temp.: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

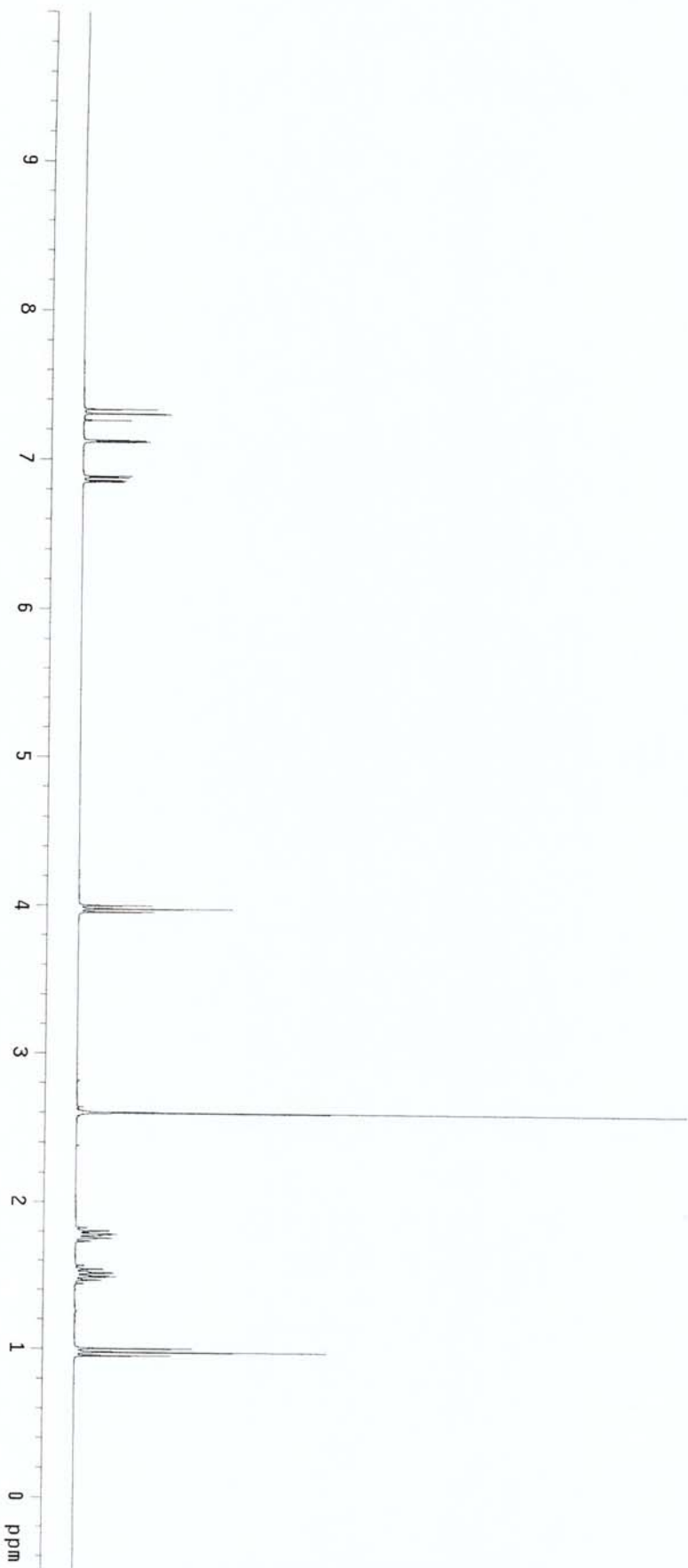
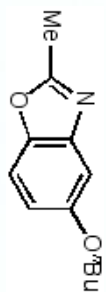
16 repetitions

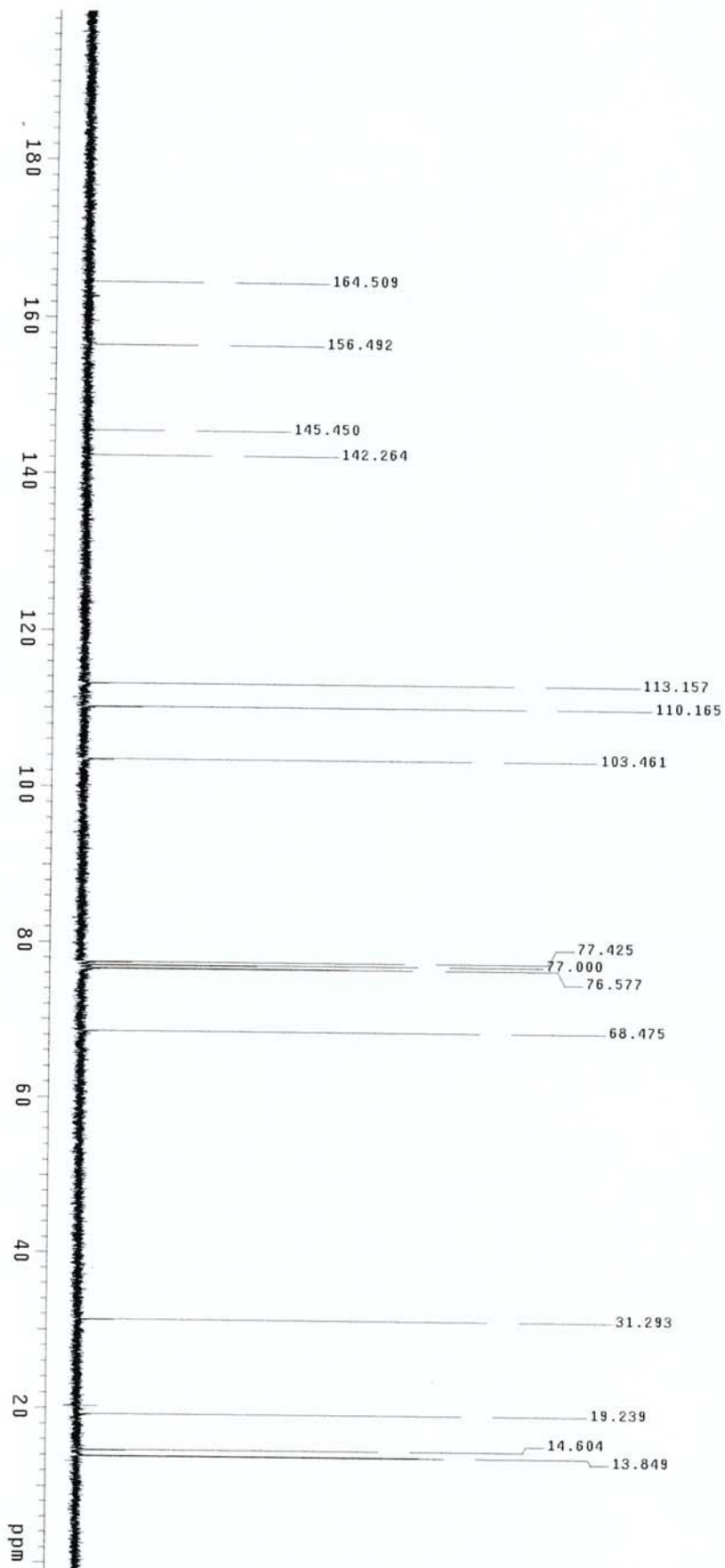
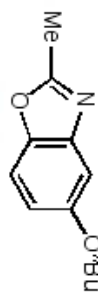
OBSERVE H1, 300.1055034 MHz

DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec





WXX-2-76-C-1a

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhat"

Relax. delay 0.050 sec

Pulse 33.9 degrees

Acq. time 4.003 sec

Width 6002.4 Hz

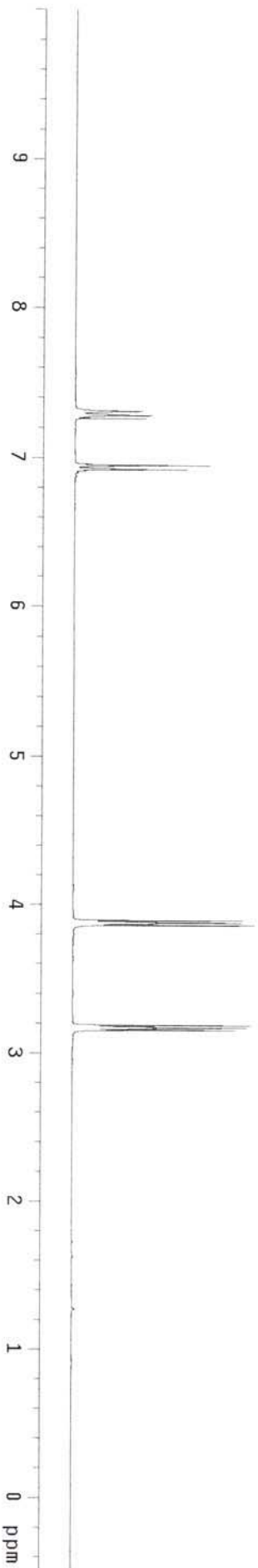
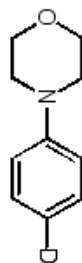
16 repetitions

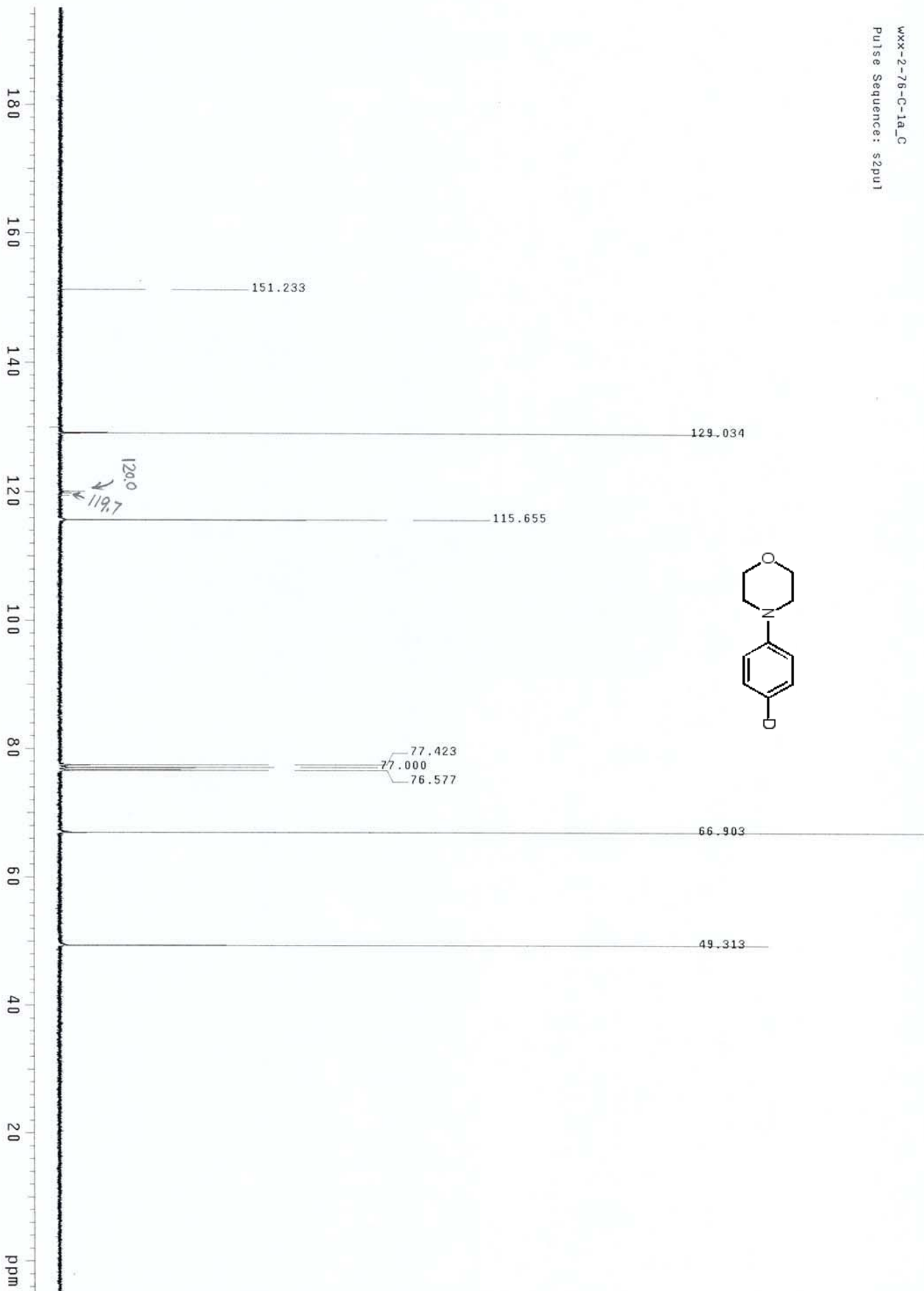
OBSERVE H1, 300.1055034 MHz

DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec





wxx-2-88-B-8b_070510

Pulse Sequence: s2pul

Solvent: CDCl3

Temp: 20.0 C / 293.1 K

Mercury-300 "mrhbt"

Relax. delay: 0.050 sec

Pulse: 33.9 degrees

Acq. time: 4.003 sec

Width: 6002.4 Hz

12 repetitions

OBSERVE H1, 300.1055034 MHz

DATA PROCESSING

FT size 131072

Total time 1 min, 17 sec

