

Negishi Coupling of Secondary Alkylzinc Halides with Aryl Bromide and Chloride

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Supporting Information

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I. General Information.

General Analytical Information. Nuclear Magnetic Resonance spectra were recorded on a Varian 300 MHz instrument at ambient temperature. All ^1H NMR spectra were measured in parts per million (ppm) relative to the signals for residue chloroform in the deuterated solvent, unless otherwise stated. Data for ^1H NMR are reported as follows: chemical shift, multiplicity (app = apparent, br = broad, ovrlp = overlapping, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants, and integration. All ^{13}C NMR spectra are reported in ppm relative to deuteriochloroform (77.23 ppm), unless otherwise stated, and were obtained with complete ^1H decoupling. All ^{31}P NMR spectra are reported in ppm relative to H_3PO_4 (0 ppm – external standard). All GC analyses were performed on an Agilent 6890 gas chromatograph with an FID detector using a J & W DB-1 column (10 m, 0.1 mm I.D.). Tetradecane was used as an internal standard to determine the GC yields if necessary. IR spectra were recorded on a Perkin-Elmer System 2000 FT-IR instrument (KBr disc). Melting points (uncorrected) were obtained on a Mel-Temp II capillary melting point apparatus. Elemental analyses were performed by Atlantic Microlabs, Inc., Norcross, GA.

General Reagent Information. THF, Et_2O , CH_2Cl_2 and toluene were purchased from J.T. Baker in CYCLE-TAINER[®] solvent-delivery kegs and vigorously purged with argon for 1 h. The solvents were further purified by passing them under argon pressure through two packed columns of neutral alumina (for THF and Et_2O) or through neutral alumina and copper (II) oxide (for toluene and CH_2Cl_2). $\text{Pd}(\text{OAc})_2$ was received as a gift from BASF and aryl halides were purchased from Aldrich, Alfa Aesar, Acros, or TCI America. SPhos and XPhos were received as gifts from Shasun. RuPhos and DavePhos were purchased from Strem. Dimethylamine (2.0 M solution in THF), LiHMDS (1.0 M solution in THF), *n*-butyllithium (2.5 M solution in hexanes), and 2-bromopropane- d_7 were purchased from Aldrich. 2-bromopropane-1,1,1- d_3 was purchased from CDN isotope. ClPCy₂ was received as a gift from Nippon Chemical. Zinc powder (325 mesh) and LiCl were purchased from Strem. LiCl was stored and weighed out in a nitrogen-filled glovebox. Cyclopropyl zinc bromide solution in THF was purchased from Rieke Metals. Commercially obtained materials were used as received unless otherwise noted. *t*-BuXPhos precatalyst,¹ $\text{PdCl}_2(\text{dppf})$,² *tert*-butyl 4-iodopiperidine-1-carboxylate,³ and 6-iodo-2-methylhept-2-ene⁴ were prepared according to literature procedures.

¹ Biscoe, M. R.; Fors, B. P.; Buchwald, S. L. *J. Am. Chem. Soc.* **2008**, *130*, 6686.

² Hayashi, T.; Konishi, M.; Kobori, Y.; Kumada, M.; Higuchi, T.; Hirotsu, K. *J. Am. Chem. Soc.* **1984**, *106*, 158.

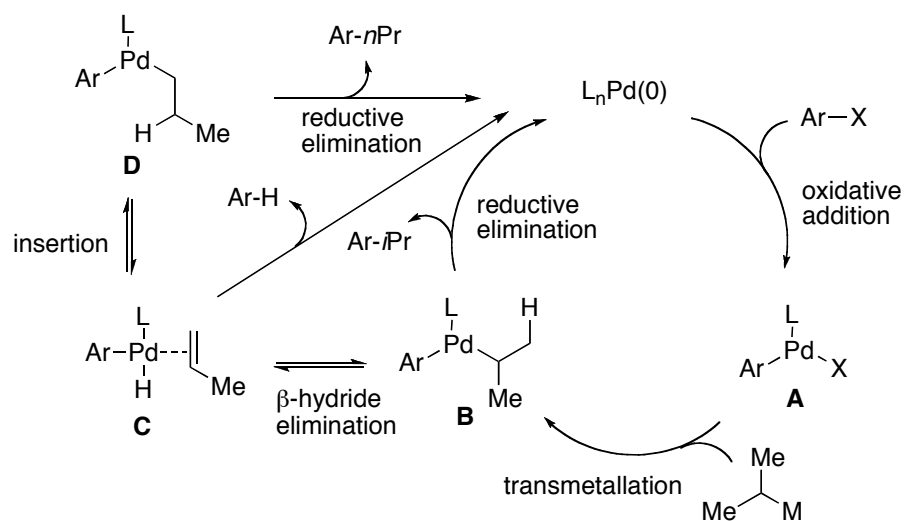
³ Corley, E. G.; Conrad, K.; Murry, J. A.; Savarin, C.; Holko, J.; Boice, G. *J. Org. Chem.* **2004**, *69*, 5120.

⁴ Vyvyan, J. R.; Loitz, C.; Looper, R. E.; Mattingly, C. S.; Peterson, E. A.; Staben, S. T. *J. Org. Chem.* **2004**, *69*, 2461.

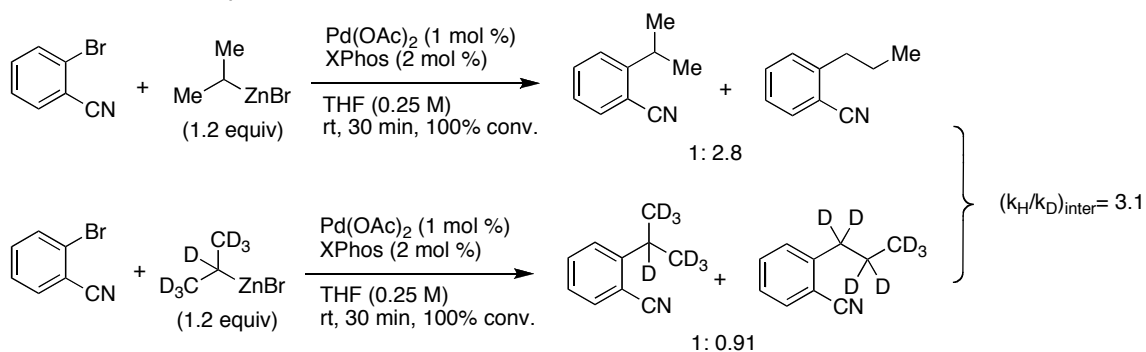
General Considerations. All reactions were carried out in resealable test tubes with Teflon septa under an argon or nitrogen atmosphere. Flash column chromatography was performed using a) Silicycle silica gel (ultra pure grade) or b) a Biotage SP4 instrument with pre-packed silica cartridges. Yields reported in the publication are of isolated material and represent an average of at least two independent runs. Compounds previously described in the literature were characterized by comparing their ^1H NMR and ^{13}C NMR spectra, and melting points (m.p.) to the previously reported data. All new compounds were characterized by ^1H NMR, ^{13}C NMR, and IR spectroscopy; their purity was confirmed by gas chromatography (GC) or elemental analysis. Copies of the ^1H , ^{13}C , and ^{31}P NMR spectra can be found at the end of the Supporting Information.

II. Experimental Procedures and Characterization Data.

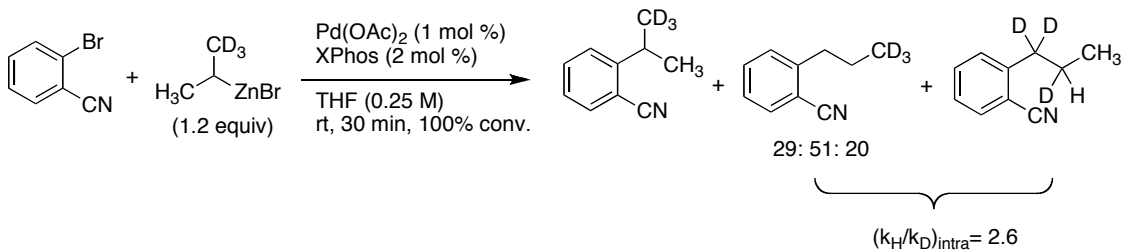
A) Deuterium-Labeling Experiments.



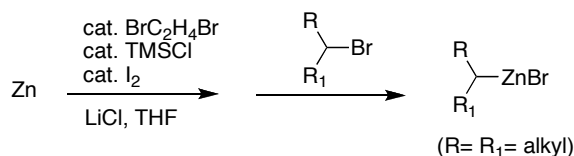
Intermolecular isotope effect:



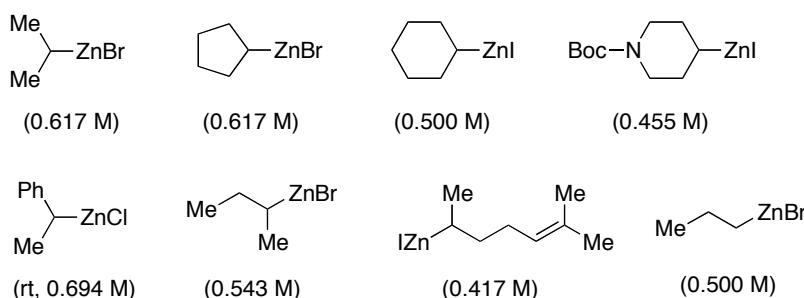
Intramolecular isotope effect:



B) Preparation of Secondary Alkylzinc Halides Using Knochel's Protocol.⁵



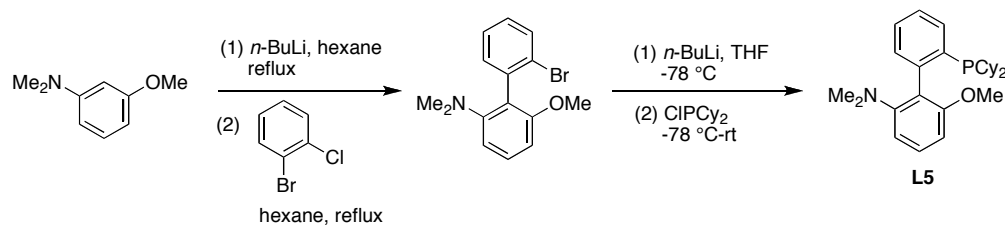
General Procedure: An oven-dried 250 mL round-bottom flask equipped with a magnetic stir bar and a rubber septum was charged with LiCl (8.48 g, 200 mmol). The vessel was heated with a heat gun for 10 min under high vacuum and backfilled with argon after cooling to room temperature. Zinc dust (13.1 g, 200 mmol) was added. The vessel was again heated with a heat gun for 10 min under high vacuum and backfilled with argon after cooling to room temperature. THF (100 mL) and 1,2-dibromoethane (431 μL , 5.00 mmol) were added via syringe and the reaction mixture was heated at 60 °C until bubbling occurred. After cooling to room temperature, trimethylsilyl chloride (126 μL , 1.00 mmol) and a solution of iodine (127 mg, 0.500 mmol) in THF (1 mL) were added via syringe. The reaction mixture was heated at 60 °C for 20 min and then cooled to room temperature. Alkyl halides (100 mmol) was added and the reaction was stirred at 50 °C for 18 h. The reaction mixture was allowed to stand at room temperature for 1 h and the supernatant solution was carefully transferred to a dry vessel via cannula. The concentration of the organozinc solution was determined by iodometric titration using Knochel's procedure.⁶



⁵ Krasovskiy, A.; Malakhov, V.; Gavryushin, A.; Knochel, P. *Angew. Chem., Int. Ed.* **2006**, 45, 6040.

⁶ Krasovskiy, A.; Knochel, P. *Synthesis* **2006**, 890.

C) Preparation of Biarylphosphine Ligands L5 and L6 (CPhos).

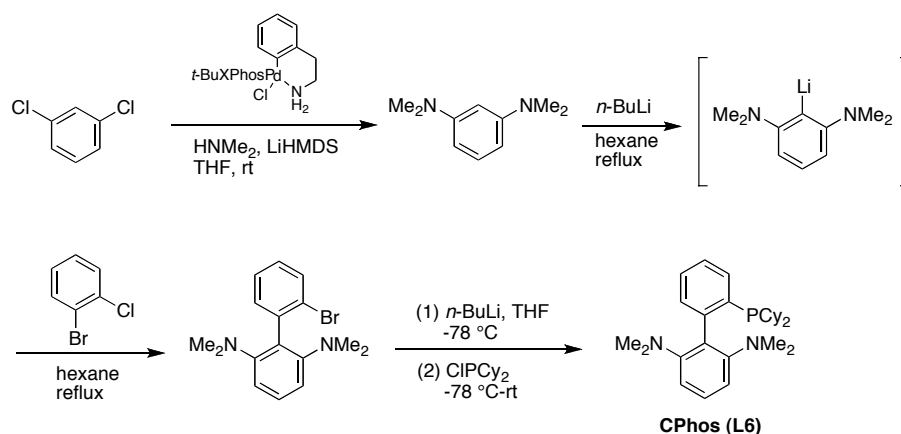


2'-(Dicyclohexylphosphino)-6-methoxy-*N,N*-dimethylbiphenyl-2-amine (L5). An oven-dried 500 mL three-neck round-bottom flask equipped with a magnetic stir bar and a reflux condenser was capped with rubber septa, fitted with an argon inlet adapter. The flask was then evacuated and backfilled with argon (this sequence was repeated three times). The reaction vessel was charged with 3-methoxy-*N,N*-dimethylaniline (8.07 mL, 55.0 mmol), anhydrous hexane (125 mL), and *n*-butyllithium (24.0 mL, 60.0 mmol, 2.5 M solution in hexanes). The reaction mixture was heated under reflux for 1 h (oil bath temperature at 80 °C) and cooled to room temperature. 2-bromochlorobenzene (5.81 mL, 50.0 mmol) was then added dropwise over 15 min with vigorous stirring (CAUTION: EXOTHERMIC!). The reaction mixture was heated at reflux for another 2 h and then cooled to room temperature (GC analysis of a reaction aliquot which was quenched by addition of ethanol indicated that complete consumption of the 2-bromochlorobenzene and clean conversion to 2'-bromo-6-methoxy-*N,N*-dimethylbiphenyl-2-amine had occurred). The reaction mixture was quenched by slow addition of water. The aqueous layer was extracted with ether (3×). The combined organic layer was dried over Na₂SO₄, filtered, and concentrated in vacuo. The resulting crude was purified by recrystallization from methanol/diethyl ether to afford 2'-bromo-6-methoxy-*N,N*-dimethylbiphenyl-2-amine as a brown solid (7.72 g, 50% yield), which was used directly for the next step.

An oven-dried 250 mL round-bottom flask, which was equipped with a magnetic stir bar and fitted with a Teflon septum, was charged with 2'-bromo-6-methoxy-*N,N*-dimethylbiphenyl-2-amine (6.12 g, 20.0 mmol). The vessel was evacuated and backfilled with argon (this process was repeated a total of 3 times). THF (80.0 mL) was added via syringe and the solution was cooled to -78 °C. *n*-Butyllithium (8.40 mL, 21.0 mmol, 2.5 M solution in hexanes) was added dropwise via syringe over 15 min. The resulting mixture was stirred at -78 °C for 30 min (periodic swirling of the reaction flask by hand was required as magnetic stirring became difficult). Chlorodicyclohexylphosphine (4.64 mL, 21.0 mmol) was then added dropwise via syringe over 15 min. The reaction mixture was stirred at -78 °C for 1 h and then allowed to slowly warm to room temperature. The reaction was quenched by addition of methanol and filtered through a pad of silica gel topped with a layer of Celite, eluting with ethyl acetate (400 mL). The filtrate was concentrated in vacuo to afford a yellow solid. Recrystallization from

dichloromethane and methanol provided the title compound as a pale-yellow solid (first crop: 7.24 g; second crop: 0.95 g; 96% combined yield).

^1H NMR (300 MHz, CDCl_3) δ : 7.20 (d, J = 8.7 Hz, 2H), 6.90 (d, J = 8.7 Hz, 2H), 3.83 (s, 3H), 2.92 (septet, J = 6.9 Hz, 1H), 1.28 (d, J = 6.9 Hz, 6H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 158.0, 153.2, 145.3, 144.9, 136.2, 135.9, 133.0, 133.0, 132.9, 132.8, 128.8, 128.1, 125.9, 124.4, 124.3, 110.8, 104.2, 55.4, 43.8 (2C), 36.0, 35.8, 33.2, 33.0, 30.7, 30.4, 30.1, 30.0, 29.9, 29.8, 28.6, 28.5, 28.2, 28.0, 27.9, 27.8, 27.8, 27.7, 27.6, 27.5, 27.0, 26.7 ppm (observed complexity due to P-C splitting; definitive assignments have not been made). ^{31}P NMR (121 MHz, CDCl_3) δ : -8.75 ppm. IR (neat, cm^{-1}): 2920, 2850, 1592, 1576, 1468, 1448, 1427, 1252, 1080, 1003, 979, 910, 850, 791, 761, 729.



2'-Bromo- N^2,N^2,N^6,N^6 -tetramethylbiphenyl-2,6-diamine. An oven-dried flask was charged with *t*-BuXPhos precatalyst¹ (275 mg, 0.400 mmol). The flask was then evacuated and backfilled with argon (this process was repeated a total of 3 times). 1,3-dichlorobenzene (2.28 mL, 20.0 mmol) and dimethylamine (30.0 mL, 60.0 mmol, 2.0 M solution in THF) were added via syringe. The solution was cooled to 0 °C in an ice bath and LiHMDS (60.0 mL, 60.0 mmol, 1.0 M solution in THF) was added slowly via syringe. The ice bath was removed after the addition and the reaction was stirred at room temperature for 16 h. The reaction mixture was then quenched by the addition of water and extracted with ethyl acetate (3 $\times$). The combined organic layer was dried over Na_2SO_4 , filtered, and concentrated in vacuo. The resulting residue was purified via flash chromatography on silica gel (hexanes: ethyl acetate = 6: 1) to afford N^1,N^1,N^3,N^3 -tetramethylbenzene-1,3-diamine as a pale-yellow oil (3.10 g, 94% yield).

An oven-dried 250 mL three-neck round-bottom flask equipped with a magnetic stir bar and a reflux condenser was capped with rubber septa, fitted with an argon inlet adapter. The flask was then evacuated and backfilled with argon (this sequence was repeated three times). The reaction vessel was charged with N^1,N^1,N^3,N^3 -tetramethylbenzene-1,3-diamine (3.29 g, 20.0 mmol), anhydrous hexane (50.0 mL), and *n*-butyllithium (8.80 mL, 22.0 mmol, 2.5 M solution in hexanes). The reaction mixture was heated at reflux for 1 h (oil bath temperature at 80 °C) and

cooled to room temperature. 2-bromochlorobenzene (2.55 mL, 22.0 mmol) was then added dropwise over 15 min with vigorous stirring (CAUTION: EXOTHERMIC!). The reaction mixture was heated at reflux for another 2 h and then cooled to room temperature (GC analysis of a reaction aliquot which was quenched by addition of ethanol indicated that complete consumption of the 2-bromochlorobenzene and clean conversion to 2'-bromo- N^2,N^2,N^6,N^6 -tetramethylbiphenyl-2,6-diamine had occurred). The reaction mixture was quenched by slow addition of water. The aqueous layer was extracted with ether (3 $\times$). The combined organic layer was dried over Na_2SO_4 , filtered, and concentrated in vacuo. The resulting crude was washed with cold methanol to afford the title compound as a pale-yellow solid (3.20 g). The filtrate was concentrated and purified using column chromatography on silica gel (hexanes: ethyl acetate = 20: 1) to provide the title compound as a yellow solid (2.76 g, 93% combined yield). m.p. 68-71 $^\circ\text{C}$. ^1H NMR (300 MHz, CDCl_3) δ : 7.71 (d, J = 8.1 Hz, 1H), 7.40-7.34 (m, 3H), 7.22-7.16 (m, 1H), 6.95 (d, J = 8.1 Hz, 2H), 2.50 (s, 12H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 153.4, 140.3, 133.4, 132.8, 130.4, 129.1, 127.8, 127.0, 126.4, 114.0, 44.1 ppm. IR (neat, cm^{-1}): 2941, 2827, 2783, 1576, 1473, 1427, 1296, 1161, 1048, 1009, 945, 879, 805, 759, 744, 668. Anal. Calcd. for $\text{C}_{16}\text{H}_{19}\text{BrN}_2$: C, 60.20; H, 6.00. Found: C, 60.32; H, 5.85.

2'-(Dicyclohexylphosphino)- N^2,N^2,N^6,N^6 -tetramethylbiphenyl-2,6-diamine (L6). An oven-dried 250 mL round-bottom flask, which was equipped with a magnetic stir bar and fitted with a Teflon septum, was charged with 2'-bromo- N^2,N^2,N^6,N^6 -tetramethylbiphenyl-2,6-diamine (3.20 g, 10.0 mmol). The vessel was evacuated and backfilled with argon (this process was repeated a total of 3 times). THF (40.0 mL) was added via syringe and the solution was cooled to -78 $^\circ\text{C}$. *n*-Butyllithium (4.20 mL, 10.5 mmol, 2.5 M solution in hexanes) was added dropwise via syringe over 15 min. The resulting mixture was stirred at -78 $^\circ\text{C}$ for 30 min (periodic swirling of the reaction flask by hand was required as magnetic stirring became difficult). Chlorodicyclohexylphosphine (2.32 mL, 10.5 mmol) was then added dropwise via syringe over 15 min. The reaction mixture was stirred at -78 $^\circ\text{C}$ for 1 h and then allowed to slowly warm to room temperature. The reaction was quenched by addition of methanol and filtered through a pad of silica gel topped with a layer of Celite, eluting with ethyl acetate (200 mL). The filtrate was concentrated in vacuo. Recrystallization from dichloromethane and methanol provided the title compound as a white solid (first crop: 3.62 g; second crop: 0.18 g; 87% combined yield). m.p. 111-113 $^\circ\text{C}$. ^1H NMR (300 MHz, CDCl_3) δ : 7.69 (d, J = 7.2 Hz, 1H), 7.41-7.31 (m, 4H), 6.91 (d, J = 8.1 Hz, 2H), 3.49 (s, 12H), 2.02-1.58 (m, 12H), 1.38-0.60 (m, 10H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 153.5, 146.6, 146.1, 137.0, 136.8, 133.2, 133.1, 132.7, 132.7, 132.2, 132.1, 128.6, 127.6, 125.8, 114.0, 44.9, 44.8, 35.3, 35.1, 31.4, 31.2, 29.7, 29.6, 28.1, 27.9, 27.7, 27.6, 27.0 ppm (observed complexity due to P-C splitting; definitive assignments have not been made). ^{31}P NMR (121 MHz, CDCl_3) δ : -8.63 ppm. IR (neat, cm^{-1}): 2922, 2849, 2778, 1576, 1448, 1299, 1164, 1050, 1011, 910, 851, 802, 738. Anal. Calcd. for $\text{C}_{28}\text{H}_{41}\text{N}_2\text{P}$: C, 77.02; H, 9.47. Found: C, 77.24; H, 9.52.

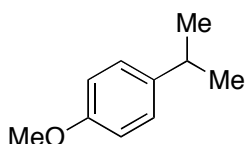
D) Experimental Procedures and Characterization Data for Examples Described in Table 1 and 2.

General Procedure A: Pd-Catalyzed Negishi Coupling of Aryl Halides with Secondary Alkylzinc Halides.

An oven-dried screw-cap test tube, which was equipped with a magnetic stir bar and fitted with a Teflon septum, was charged with Pd(OAc)₂ (2.25 mg, 0.0100 mmol) and biarylphosphine ligand **L6** (8.73 mg, 0.0200 mmol). The vessel was evacuated and backfilled with argon (this process was repeated a total of 3 times) and then the aryl bromide or chloride (1.00 mmol, if liquid) and THF or toluene (1.50-2.50 mL which makes the total volume of the reaction 4.00 mL) were added via syringe (aryl chlorides or amines that were solids at room temperature were added with the palladium catalyst and ligand). The solution was cooled to 0 °C in an ice bath and a THF solution of alkyl zinc halide (1.20 mmol, 1.50-2.50 mL) was added slowly via syringe. The ice bath was removed after the addition and the reaction was stirred at room temperature for indicated time until the starting material was completely consumed as monitored by GC. The reaction mixture was then quenched by addition of hydrochloric acid (1N) and extracted with ethyl acetate (3×). The combined organic layer was dried over Na₂SO₄, filtered, and concentrated in vacuo. The resulting residue was purified by flash chromatography using the Biotage SP4 (SNAP 10g or 25 g cartridges) to afford the desired product.

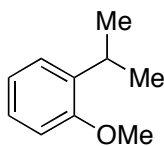
General Procedure B: Pd-Catalyzed Negishi Coupling of Aryl Halides with Secondary Alkylzinc Halides.

Procedure A was used with the following changes: A THF solution of alkyl zinc halide (1.20 mmol, 1.50-2.50 mL) was slowly added via syringe at room temperature instead of at 0 °C.

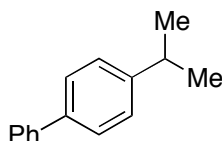


4-Isopropylanisole [CAS # 2944-47-0].⁷ (Table 1, Entry 1) Following general procedure **A** with 4-bromoanisole (125 μL, 1.00 mmol), isopropyl zinc bromide solution (1.94 mL, 1.20 mmol, 0.617 M in THF), and THF (2.06 mL) at room temperature for 30 min, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-6% ethyl acetate/hexanes) to provide a mixture of products as a light brown oil (138 mg, 92% yield). The ratio of the branched to the linear cross-coupled product was determined to be 37:1 by GC and ¹H NMR analysis. ¹H NMR (300 MHz, CDCl₃) δ: 7.20 (d, *J* = 8.7 Hz, 2H), 6.90 (d, *J* = 8.7 Hz, 2H), 3.83 (s, 3H), 2.92 (septet, *J* = 6.9 Hz, 1H), 1.28 (d, *J* = 6.9 Hz, 6H) ppm. ¹³C NMR (75 MHz, CDCl₃) δ: 157.8, 141.2, 127.4 (2C), 113.8 (2C), 55.4, 33.5, 24.4 (2C) ppm.

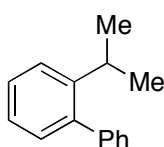
⁷ Dreher, S. D.; Dormer, P. G.; Sandrock, D. L.; Molander, G. A. *J. Am. Chem. Soc.* **2008**, *130*, 9257.



2-Isopropylanisole [CAS # 2944-47-0].⁷ (Table 1, Entry 7) Following general procedure **A** with 2-bromoanisole (125 μ L, 1.00 mmol), isopropyl zinc bromide solution (1.94 mL, 1.20 mmol, 0.617 M in THF), and THF (2.06 mL) at room temperature for 30 min, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-6% ethyl acetate/hexanes) to provide a mixture of products as a colorless oil (146 mg, 97% yield). The ratio of the branched to the linear cross-coupled product was determined to be 27:1 by GC and ¹H NMR analysis. ¹H NMR (300 MHz, CDCl₃) δ : 7.24 (d, J = 7.5 Hz, 1H), 7.19 (dd, J = 8.1, 7.5 Hz, 1H), 6.95 (t, J = 7.5 Hz, 1H), 6.87 (d, J = 8.1 Hz, 1H), 3.85 (s, 3H), 3.34 (septet, J = 6.9 Hz, 1H), 1.23 (d, J = 6.9 Hz, 6H) ppm. ¹³C NMR (75 MHz, CDCl₃) δ : 156.9, 137.1, 126.7, 126.2, 120.7, 110.4, 55.5, 26.8, 22.9 (2C) ppm.



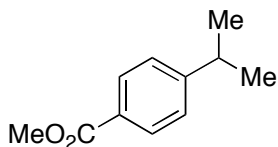
4-Isopropylbiphenyl [CAS # 7116-95-2].⁸ (Table 1, Entry 2) Following general procedure **A** with 4-bromobiphenyl (233 mg, 1.00 mmol), isopropyl zinc bromide solution (1.94 mL, 1.20 mmol, 0.617 M in THF), and THF (2.06 mL) at room temperature for 30 min, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-2% ethyl acetate/hexanes) to provide a mixture of products as a colorless oil (187 mg, 95% yield). The ratio of the branched to the linear cross-coupled product was determined to be 39:1 by GC and ¹H NMR analysis. ¹H NMR (300 MHz, CDCl₃) δ : 7.76-7.45 (9H, m), 3.11 (septet, J = 6.9 Hz, 1H), 1.45 (d, J = 6.9 Hz, 6H) ppm. ¹³C NMR (75 MHz, CDCl₃) δ : 148.1, 141.4, 138.9, 128.9 (2C), 127.3 (2C), 127.2 (2C), 127.1 (2C), 127.0, 34.0, 24.2 (2C) ppm.



2-Isopropylbiphenyl [CAS # 19486-60-3].⁹ (Table 1, Entry 8) Following general procedure **A** with 2-bromobiphenyl (172 μ L, 1.00 mmol), isopropyl zinc bromide solution (1.94 mL, 1.20 mmol, 0.617 M in THF), and THF (2.06 mL) at room temperature for 3 h, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-2% ethyl acetate/hexanes) to provide a mixture of products as a colorless oil (190 mg, 97% yield). The ratio of the branched to the linear cross-coupled product was determined to be 22:1 by GC and ¹H NMR analysis. ¹H NMR (300 MHz, CDCl₃) δ : 7.45-7.18 (9H, m), 3.07 (septet, J = 6.9 Hz, 1H), 1.18 (d, J = 6.9 Hz, 6H) ppm. ¹³C NMR (75 MHz, CDCl₃) δ : 146.5, 142.3, 141.3, 130.1, 129.5 (2C), 128.2 (2C), 127.9, 126.9, 125.7, 125.5, 29.5, 24.5 (2C) ppm.

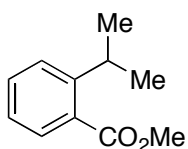
⁸ Smith, R. C.; Bodner, C. R.; Earl, M. J.; Sears, N. C.; Hill, N. E.; Bishop, L. M.; Sizemore, N.; Hehemann, D. T.; Bohn, J. J.; Protasiewicz, J. D. *J. Organomet. Chem.* **2005**, 690, 477.

⁹ Autio, J.; Vuoti, S.; Haukka, M.; Pursiainen, J. *Inorg. Chim. Acta* **2008**, 361, 1372.



Methyl 4-isopropylbenzoate [CAS # 20185-55-1].¹⁰ (Table 1, Entry 3) Following general procedure **A** with methyl 4-bromobenzoate (215 mg, 1.00 mmol), isopropyl zinc bromide solution (2.00 mL, 1.20 mmol, 0.600 M in THF), and toluene (2.00 mL) at room temperature for 30 min, the crude product was

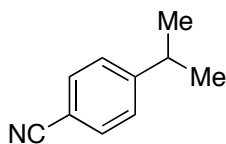
purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-6% ethyl acetate/hexanes) to provide a mixture of products as a light yellow oil (167 mg, 94% yield). The ratio of the branched to the linear cross-coupled product was determined to be 46:1 by GC and ¹H NMR analysis. Or following general procedure **B** with methyl 4-chlorobenzoate (171 mg, 1.00 mmol) and isopropyl zinc bromide solution (2.40 mL, 1.20 mmol, 0.500 M in THF), and toluene (1.60 mL) at room temperature for 3 h, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-6% ethyl acetate/hexanes) to provide a mixture of products as a light yellow oil (174 mg, 98% yield). The ratio of the branched to the linear cross-coupled product was determined to be 45:1 by GC and ¹H NMR analysis. ¹H NMR (300 MHz, CDCl₃) δ: 7.97 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.4 Hz, 2H), 3.91 (3H, s), 2.97 (septet, *J* = 6.9 Hz, 1H), 1.27 (d, *J* = 6.9 Hz, 6H) ppm. ¹³C NMR (75 MHz, CDCl₃) δ: 167.3, 154.4, 129.9 (2C), 127.9, 126.6 (2C), 52.1, 34.4, 23.8 (2C) ppm. IR (neat, cm⁻¹): 2962, 1725, 1611, 1465, 1437, 1418, 1311, 1278, 1181, 1113, 1019, 775, 708.



Methyl 2-isopropylbenzoate [CAS # 6623-98-9]. (Table 1, Entry 9) Following general procedure **A** with methyl 2-bromobenzoate (140 μL, 1.00 mmol), isopropyl zinc bromide solution (2.40 mL, 1.20 mmol, 0.500 M in THF), and toluene (1.60 mL) at room temperature for 30 min, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g;

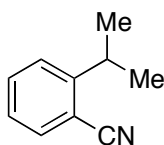
0-6% ethyl acetate/hexanes) to provide a mixture of products as a colorless oil (163 mg, 91% yield). The ratio of the branched to the linear cross-coupled product was determined to be 37:1 by GC and ¹H NMR analysis. Or following general procedure **B** with methyl 2-chlorobenzoate (143 μL, 1.00 mmol) and isopropyl zinc bromide solution (2.40 mL, 1.20 mmol, 0.500 M in THF), and toluene (1.60 mL) at room temperature for 6 h, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-6% ethyl acetate/hexanes) to provide a mixture of products as a colorless oil (172 mg, 97% yield). The ratio of the branched to the linear cross-coupled product was determined to be 30:1 by GC and ¹H NMR analysis. ¹H NMR (300 MHz, CDCl₃) δ: 7.74 (d, *J* = 8.1 Hz, 1H), 7.47 (t, *J* = 8.1 Hz, 1H), 7.43 (d, *J* = 8.1 Hz, 1H), 7.23 (t, *J* = 8.1 Hz, 1H), 3.90 (3H, s), 3.75 (septet, *J* = 6.9 Hz, 1H), 1.28 (d, *J* = 6.9 Hz, 6H) ppm. ¹³C NMR (75 MHz, CDCl₃) δ: 168.9, 149.8, 131.9, 130.0, 129.9, 126.3, 125.6, 52.1, 29.7, 24.1 (2C) ppm. IR (neat, cm⁻¹): 2966, 1718, 1457, 1437, 1288, 1251, 1125, 1074, 761, 716. Anal. Calcd. for C₁₁H₁₄O₂: C, 74.13; H, 7.92. Found: C, 73.91; H, 8.09.

¹⁰ Arnold, D. R.; de P. Nicholas, A. M.; Snow, M. S. *Can. J. Chem.* **1985**, 63, 1150.



4-Isopropylbenzonitrile [CAS # 13816-33-6].¹⁰ (Table 1, Entry 4)

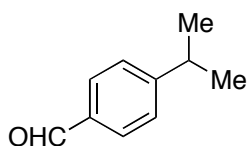
Following general procedure **A** with 4-bromobenzonitrile (182 mg, 1.00 mmol), isopropyl zinc bromide solution (2.40 mL, 1.20 mmol, 0.500 M in THF), and toluene (1.60 mL) at room temperature for 30 min, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-6% ethyl acetate/hexanes) to provide a mixture of products as a colorless oil (126 mg, 87% yield). The ratio of the branched to the linear cross-coupled product was determined to be 59:1 by GC and ¹H NMR analysis. Or following general procedure **B** with 4-chlorobenzonitrile (138 mg, 1.00 mmol) and isopropyl zinc bromide solution (2.40 mL, 1.20 mmol, 0.500 M in THF), and toluene (1.60 mL) at room temperature for 30 min, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-6% ethyl acetate/hexanes) to provide a mixture of products as a colorless oil (137 mg, 94% yield). The ratio of the branched to the linear cross-coupled product was determined to be 43:1 by GC and ¹H NMR analysis. ¹H NMR (300 MHz, CDCl₃) δ: 7.57 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 2.96 (septet, *J* = 6.9 Hz, 1H), 1.25 (d, *J* = 6.9 Hz, 6H) ppm. ¹³C NMR (75 MHz, CDCl₃) δ: 154.5, 132.3 (2C), 127.4 (2C), 119.3, 109.7, 34.5, 23.6 (2C) ppm. IR (neat, cm⁻¹): 2965, 2228, 1609, 1506, 1457, 1419, 1055, 1019, 836.



2-Isopropylbenzonitrile [CAS # 40751-52-8].¹¹ (Table 1, Entry 10)

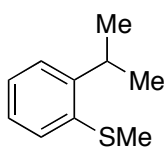
Following general procedure **A** with 2-bromobenzonitrile (182 mg, 1.00 mmol), isopropyl zinc bromide solution (2.40 mL, 1.20 mmol, 0.500 M in THF), and toluene (1.60 mL) at room temperature for 30 min, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-6% ethyl acetate/hexanes) to provide a mixture of products as a colorless oil (189 mg, 89% yield). The ratio of the branched to the linear cross-coupled product was determined to be 20:1 by GC and ¹H NMR analysis. Or following general procedure **B** with 2-chlorobenzonitrile (138 mg, 1.00 mmol) and isopropyl zinc bromide solution (2.40 mL, 1.20 mmol, 0.500 M in THF), and toluene (1.60 mL) at room temperature for 3 h, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-6% ethyl acetate/hexanes) to provide a mixture of products as a colorless oil (136 mg, 94% yield). The ratio of the branched to the linear cross-coupled product was determined to be 22:1 by GC and ¹H NMR analysis. ¹H NMR (300 MHz, CDCl₃) δ: 7.61 (d, *J* = 7.5 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.40 (d, *J* = 7.5 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 1H), 3.39 (septet, *J* = 6.9 Hz, 1H), 1.32 (d, *J* = 6.9 Hz, 6H) ppm. ¹³C NMR (75 MHz, CDCl₃) δ: 152.4, 133.1, 132.9, 126.4, 126.0, 118.3, 111.7, 32.5, 23.3 (2C) ppm. IR (neat, cm⁻¹): 2967, 2874, 2223, 1600, 1484, 1465, 1448, 1388, 1367, 1082, 1032, 762, 526.

¹¹ Schareina, T.; Zapf, A.; Mägerlein, W.; Müller, N.; Beller, M. *Chem. Eur. J.* **2007**, *13*, 6249.



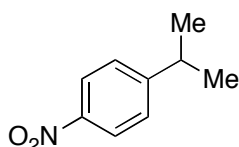
4-Isopropylbenzaldehyde [CAS # 122-03-2]. (Table 1, Entry 5)

Following general procedure **A** with 4-bromobenzaldehyde (185 mg, 1.00 mmol), isopropyl zinc bromide solution (2.40 mL, 1.20 mmol, 0.500 M in THF), and toluene (1.60 mL) at room temperature for 30 min, the reaction was quenched by saturated ammonium chloride solution instead of hydrochloric acid (1N). The crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-6% ethyl acetate/hexanes) to provide a mixture of products as a colorless oil (132 mg, 89% yield). The ratio of the branched to the linear cross-coupled product was determined to be 43:1 by GC and ^1H NMR analysis. Or following general procedure **B** with 4-chlorobenzaldehyde (141 mg, 1.00 mmol) and isopropyl zinc bromide solution (2.40 mL, 1.20 mmol, 0.500 M in THF), and toluene (1.60 mL) at room temperature for 30 min, the reaction was quenched by saturated ammonium chloride solution instead of hydrochloric acid (1N). The crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-6% ethyl acetate/hexanes) to provide a mixture of products as a colorless oil (138 mg, 93% yield). The ratio of the branched to the linear cross-coupled product was determined to be 47:1 by GC and ^1H NMR analysis. ^1H NMR (300 MHz, CDCl_3) δ : 9.98 (s, 1H), 7.83 (d, J = 8.4 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 3.00 (septet, J = 6.9 Hz, 1H), 1.29 (d, J = 6.9 Hz, 6H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 192.0, 156.2, 134.6, 130.0 (2C), 127.2 (2C), 34.5, 23.7 (2C) ppm. IR (neat, cm^{-1}): 2964, 2872, 2826, 2733, 1701, 1608, 1576, 1306, 1213, 1170, 1055, 840, 829, 730, 541.



2-Isopropylthioanisole [CAS # 2976-66-1].¹² (Table 1, Entry 11)

Following general procedure **A** with 2-bromothioanisole (133 μL , 1.00 mmol), isopropyl zinc bromide solution (1.94 mL, 1.20 mmol, 0.617 M in THF), and THF (2.06 mL) at room temperature for 1 h, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-2% ethyl acetate/hexanes) to provide a mixture of products as a colorless oil (158 mg, 95% yield). The ratio of the branched to the linear cross-coupled product was determined to be 30:1 by GC and ^1H NMR analysis. ^1H NMR (300 MHz, CDCl_3) δ : 7.26-7.15 (m, 4H), 3.39 (septet, J = 6.9 Hz, 1H), 2.47 (3H, s), 1.26 (d, J = 6.9 Hz, 6H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 146.6, 136.6, 126.5, 125.7, 125.4, 125.2, 30.1, 23.3 (2C), 16.2 ppm.



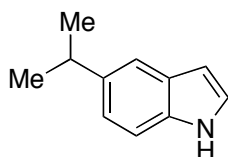
1-Isopropyl-4-nitrobenzene [CAS # 1817-47-6].¹³ (Table 1, Entry 6)

Following general procedure **A** with 1-bromo-4-nitrobenzene (185 mg, 1.00 mmol), isopropyl zinc bromide solution (2.40 mL, 1.20 mmol, 0.500 M in THF), and toluene (1.60 mL) at 0 $^\circ\text{C}$ for 30 min, the reaction was quenched by water instead of hydrochloric acid (1N).

¹² Ruff, F.; Kucsman, A. *J. Chem. Soc., Perkin Trans. II* **1988**, 1123.

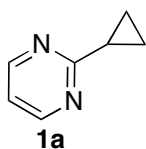
¹³ Shi, M.; Cui, S.-C. *Adv. Synth. Catal.* **2003**, 345, 1329.

The crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-2% ethyl acetate/hexanes) to provide a mixture of products as a yellow oil (83 mg, 50% yield). The ratio of the branched to the linear cross-coupled product was determined to be 28:1 by ^1H NMR analysis. ^1H NMR (300 MHz, CDCl_3) δ : 8.14 (d, J = 8.7 Hz, 2H), 7.37 (d, J = 8.7 Hz, 2H), 3.02 (septet, J = 6.9 Hz, 1H), 1.28 (d, J = 6.9 Hz, 6H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 156.7, 127.4 (2C), 124.4, 123.8 (2C), 34.4, 23.7 (2C) ppm. IR (neat, cm^{-1}): 3078, 2966, 2932, 2873, 1606, 1521, 1347, 1112, 1055, 854, 757, 700.



5-Isopropyl-1H-indole [CAS # 97820-51-4].¹⁴ (Table 1, Entry 12)

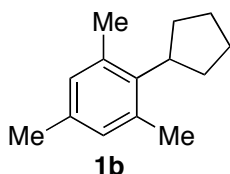
Following general procedure **A** with 5-bromoindole (196 mg, 1.00 mmol), isopropyl zinc bromide solution (2.09 mL, 1.20 mmol, 0.575 M in THF), and THF (1.91 mL) at room temperature for 30 min, the reaction was quenched by saturated ammonium chloride solution instead of hydrochloric acid (1N). The crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-32% ethyl acetate/hexanes) to provide a mixture of products as a brown oil (153 mg, 96% yield). The ratio of the branched to the linear cross-coupled product was determined to be 58:1 by GC and ^1H NMR analysis. ^1H NMR (300 MHz, CDCl_3) δ : 8.05 (br s, 1H), 7.52 (m, 1H), 7.34 (d, J = 8.4 Hz, 1H), 7.19 (dd, J = 3.0, 2.7 Hz, 1H), 7.13 (dd, J = 8.4, 1.8 Hz, 1H), 6.54-6.52 (m, 1H), 3.04 (septet, J = 6.9 Hz, 1H), 1.34 (d, J = 6.9 Hz, 6H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 140.7, 134.5, 128.1, 124.5, 121.4, 117.7, 111.0, 102.4, 34.4, 24.9 (2C) ppm. IR (neat, cm^{-1}): 3586, 2958, 2868, 1576, 1476, 1457, 1415, 1351, 1308, 1092, 878, 806, 765, 724, 607.



2-Cyclopropylpyrimidine [CAS # 58173-74-3]. (Scheme 2, **1a**)

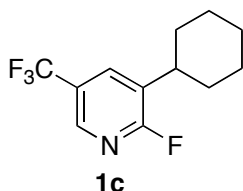
Following general procedure **A** with 2-bromopyrimidine (196 mg, 1.00 mmol), cyclopropyl zinc bromide solution (3.00 mL, 1.20 mmol, 0.400 M in THF), and THF (1.00 mL) at room temperature for 30 min, the reaction was quenched by saturated ammonium chloride solution instead of hydrochloric acid (1N). The crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-60% ethyl acetate/hexanes) to provide the title compound as a light yellow oil (90 mg, 75% yield). ^1H NMR (300 MHz, CDCl_3) δ : 8.50 (d, J = 4.8 Hz, 2H), 6.98 (t, J = 4.8 Hz, 1H), 2.19 (tt, J = 8.1, 4.8 Hz, 1H), 1.07 (dt, J = 4.8, 2.7 Hz, 2H), 1.02 (dt, J = 8.1, 2.7 Hz, 2H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 172.3, 156.9, 156.8, 118.0, 18.3, 11.0 (2C) ppm. IR (neat, cm^{-1}): 3042, 3008, 1559, 1443, 1371, 1230, 1104, 1047, 1027, 910, 794, 635, 586, 537. Anal. Calcd. for $\text{C}_7\text{H}_8\text{N}_2$: C, 69.97; H, 6.71. Found: C, 69.16; H, 7.04.

¹⁴ Bromidge, S. M. et al. *J. Med. Chem.* **1998**, *41*, 1598.



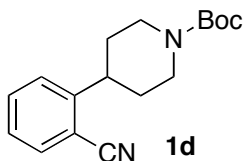
2-Cyclopentyl-1,3,5-trimethylbenzene [CAS # 30628-31-0].

(Scheme 2, **1b**) Following general procedure **A** with 2-bromo-1,3,5-trimethylbenzene (151 μ L, 1.00 mmol), cyclopentyl zinc bromide solution (1.94 mL, 1.20 mmol, 0.617 M in THF), and THF (2.06 mL) at room temperature for 2 h, the crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-1% ethyl acetate/hexanes) to provide the title compound as a colorless oil (179 mg, 95% yield). ^1H NMR (300 MHz, CDCl_3) δ : 7.04 (s, 2H), 3.69 (quintet, J = 9.6 Hz, 1H), 2.56 (s, 6H), 2.45 (s, 3H), 2.19-2.02 (m, 6H), 1.96-1.86 (m, 2H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 138.6, 136.6 (2C), 134.9, 130.2 (2C), 40.4, 31.2 (2C), 27.3 (2C), 21.5 (2C), 20.8 ppm. IR (neat, cm^{-1}): 2946, 2868, 1617, 1457, 1375, 1025, 850, 571. Anal. Calcd. for $\text{C}_{14}\text{H}_{20}$: C, 89.29; H, 10.71. Found: C, 89.53; H, 10.95.



3-Cyclohexyl-2-fluoro-5-(trifluoromethyl)pyridine. (Scheme 2, **1c**)

Following general procedure **B** with 3-chloro-2-fluoro-5-(trifluoromethyl)pyridine (131 μ L, 1.00 mmol), cyclohexyl zinc iodide solution (2.40 mL, 1.20 mmol, 0.500 M in THF), $\text{Pd}(\text{OAc})_2$ (4.50 mg, 0.0200 mmol), CPhos **L6** (17.5 mg, 0.0400 mmol), and toluene (1.60 mL) at 60 $^\circ\text{C}$ for 1 h, the reaction was quenched by saturated ammonium chloride solution instead of hydrochloric acid (1N). The crude product was purified via the Biotage SP4 (silica-packed SNAP 25 g; 0-6% ethyl acetate/hexanes) to provide the title compound as a yellow oil (208 mg, 84% yield). ^1H NMR (300 MHz, CDCl_3) δ : 8.33 (s, 1H), 7.84 (d, J = 5.7 Hz, 2H), 2.88-2.78 (m, 1H), 1.98-1.20 (m, 10H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 165.0, 161.7, 142.6, 142.5, 142.3, 142.3, 135.6, 135.6, 135.5, 135.5, 135.4, 135.4, 130.4, 130.0, 128.9, 125.9, 125.8, 125.5, 125.4, 125.2, 125.0, 124.9, 124.6, 124.5, 121.6, 118.0, 37.3, 32.5, 26.5, 25.9 ppm (observed complexity due to F-C splitting; definitive assignments have not been made). IR (neat, cm^{-1}): 2933, 2857, 1599, 1452, 1416, 1338, 1264, 1133, 1009, 927, 772, 631, 619. Anal. Calcd. for $\text{C}_{12}\text{H}_{13}\text{F}_4\text{N}$: C, 58.30; H, 5.30. Found: C, 58.50; H, 5.43.

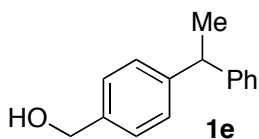


tert-Butyl 4-(2-cyanophenyl)piperidine-1-carboxylate [CAS # 256951-72-1].¹⁵ (Scheme 2, **1d**)

Following general procedure **B** with 2-chloro-benzonitrile (138 mg, 1.00 mmol), (1-(tert-butoxycarbonyl)piperidin-4-yl)zinc iodide solution (2.64 mL, 1.20 mmol, 0.455 M in THF), and toluene (1.36 mL) at 60 $^\circ\text{C}$ for 30 min, the reaction was quenched by saturated ammonium chloride solution instead of hydrochloric acid (1N). The crude product was purified via the Biotage SP4 (silica-packed SNAP 25 g; 0-50% ethyl acetate/hexanes) to provide the title compound as a light yellow solid (260 mg, 91% yield). The isomeric products were not observed by GC and ^1H NMR analysis. m.p. 83-85 $^\circ\text{C}$. ^1H NMR (300 MHz, CDCl_3) δ : 7.62 (d, J = 7.5 Hz, 1H), 7.56 (t, J = 7.5 Hz, 1H), 7.33 (d, J =

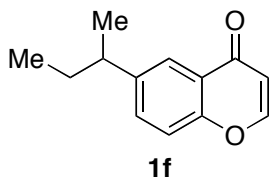
¹⁵ Barrow, J. C. et al. *J. Med. Chem.* **2000**, 43, 2703.

7.5 Hz, 1H), 7.30 (t, $J = 7.5$ Hz, 1H), 4.26 (br s, 2H), 3.12 (tt, $J = 12.0, 3.6$ Hz, 1H), 2.86 (br t, $J = 12.0$ Hz, 2H), 1.85 (br d, $J = 12.0$ Hz, 2H), 1.70-1.56 (m, 2H), 1.48 (s, 9H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 154.4, 148.9, 133.0, 132.9, 126.7, 126.3, 117.7, 111.7, 79.3, 43.8, 40.7 (2C), 32.2 (2C), 28.3 (3C) ppm. IR (neat, cm^{-1}): 2976, 2934, 2854, 2223, 1695, 1600, 1426, 1366, 1326, 1281, 1235, 1166, 1126, 1064, 1013, 986, 940, 888, 862, 764, 736, 520.



(4-(1-Phenylethyl)phenyl)methanol [CAS # 117455-21-7].

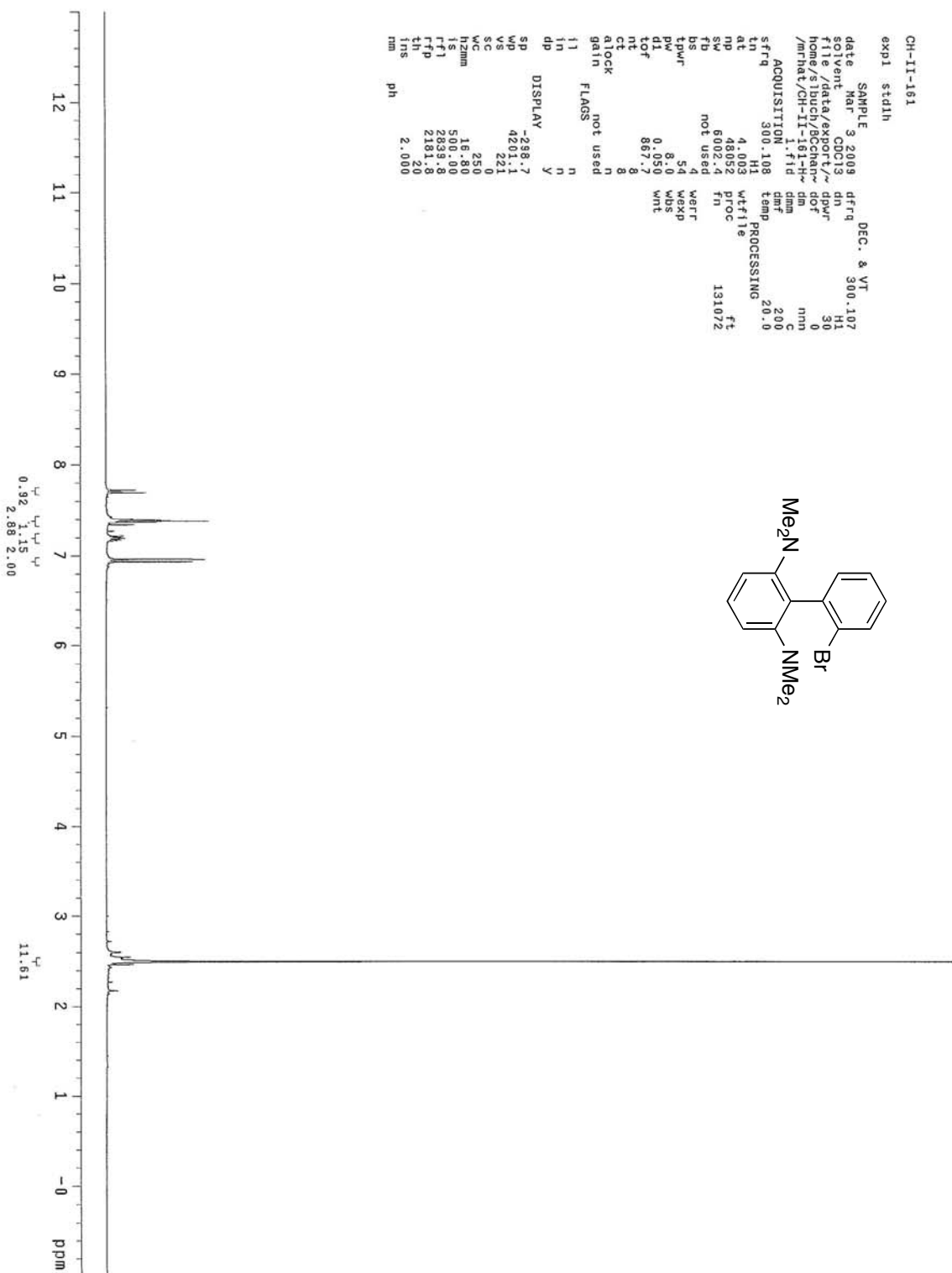
(Scheme 2, **1e**) Following general procedure **B** with 4-bromobenzyl alcohol (187 mg, 1.00 mmol), (1-phenylethyl)zinc chloride solution (2.16 mL, 1.50 mmol, 0.694 M in THF), and toluene (1.84 mL) at room temperature for 1 h, except that the alkylzinc solution was added dropwise over 30 min. The crude product was purified via the Biotage SP4 (silica-packed SNAP 10 g; 0-50% ethyl acetate/hexanes) to provide the title compound as a colorless oil (183 mg, 86% yield). The isomeric linear product was not observed by GC and ^1H NMR analysis. ^1H NMR (300 MHz, CDCl_3) δ : 7.39-7.22 (m, 9H), 4.62 (s, 2H), 4.22 (q, $J = 7.2$ Hz, 1H), 2.42 (br s, 1H), 1.71 (d, $J = 7.2$ Hz, 3H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 146.4, 145.8, 138.7, 128.5 (2C), 127.8 (2C), 127.6 (2C), 127.3 (2C), 126.1, 64.8, 44.5, 21.9 ppm. IR (neat, cm^{-1}): 3324, 3024, 2966, 2872, 1560, 1487, 1457, 1419, 1209, 1010, 794, 700.



6-sec-Butyl-4H-chromen-4-one. (Scheme 2, **1f**) Following general procedure **A** with 6-bromochromone (225 mg, 1.00 mmol), *sec*-butylzinc bromide solution (2.21 mL, 1.20 mmol, 0.543 M in THF), and toluene (1.80 mL) at room temperature for 1 h, the crude product was purified via the Biotage SP4 (silica-packed SNAP 25 g;

0-60% ethyl acetate/hexanes) to provide a mixture of products as a yellow oil (180 mg, 89% yield). The ratio of the branched to the linear cross-coupled product was determined to be 23:1 by GC and ^1H NMR analysis. ^1H NMR (300 MHz, CDCl_3) δ : 8.00 (d, $J = 2.1$ Hz, 1H), 7.84 (d, $J = 6.3$ Hz, 1H), 7.50 (dd, $J = 8.7, 2.1$ Hz, 1H), 7.39 (d, $J = 8.7$ Hz, 1H), 6.33 (d, $J = 6.3$ Hz, 1H), 2.72 (sextet, $J = 7.2$ Hz, 1H), 1.63 (dq, $J = 7.5, 7.2$ Hz, 2H), 1.27 (d, $J = 7.2$ Hz, 3H), 0.80 (d, $J = 7.5$ Hz, 3H) ppm. ^{13}C NMR (75 MHz, CDCl_3) δ : 178.1, 155.4, 145.2, 133.3, 124.8, 123.5, 118.2, 113.0, 112.9, 41.5, 31.2, 22.0, 12.3 ppm. IR (neat, cm^{-1}): 3073, 2962, 2930, 2874, 1653, 1617, 1482, 1448, 1395, 1358, 1313, 1256, 1202, 1135, 1028, 866, 833, 585, 536. Anal. Calcd. for $\text{C}_{13}\text{H}_{14}\text{O}_2$: C, 77.20; H, 6.98. Found: C, 76.37; H, 6.88.

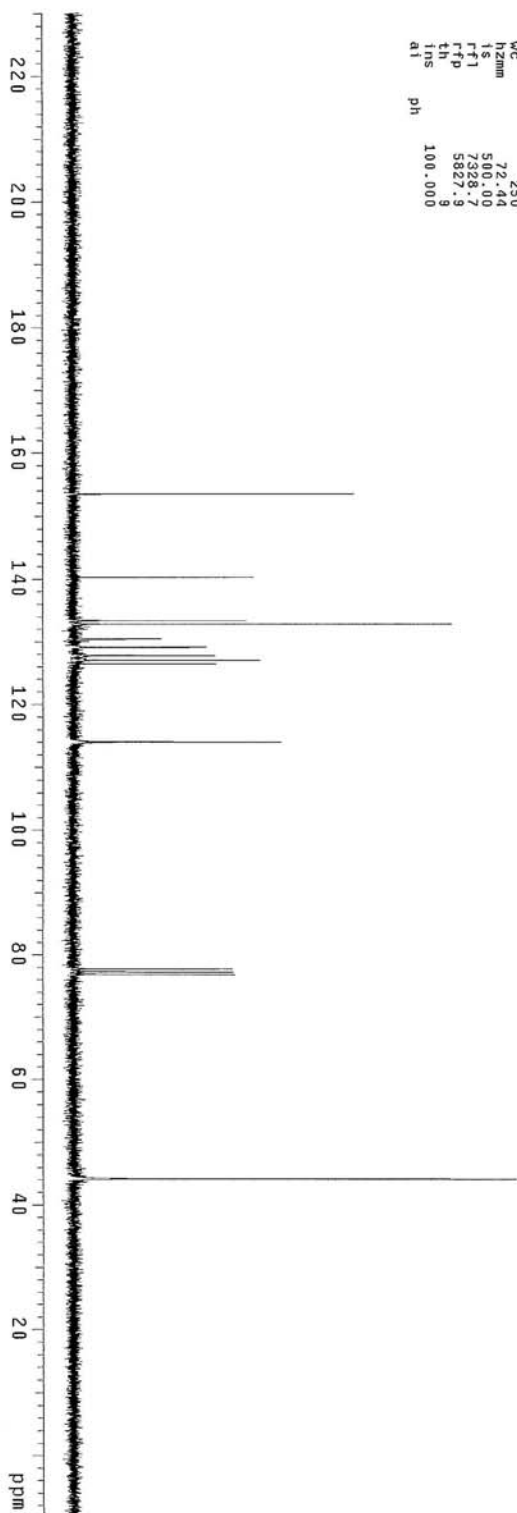
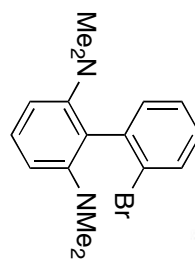
III. Attached NMR Spectra.



CH-II-161-C13

expt std13c

SAMPLE DEC. & VT
date Mar 3 2009 dfreq 300.107
solvent CDCl3 dn H1
file /data/export/~ dpwr 39
home/sibuch/Bcchan~ dof 0
/mrhat/CH-II-161-C~ dm yyy
13.fid dnm w
ACQUISITION 73.471 temp 11000
sfrq 111.111 PROCESSING 20.0
en 1.500 sp -1.500
si 67874 sbs -1.500
np 22624.4 wifile
sw 12400 proc ft
fb 16 fn 282144
bs 55
tpwr 10.0 werr
pw 0.500 wexp
di 22694.0 wds
tof 256 wnt
ct 256
clock n
gain not used
flags
i1 n
i1 n
in n
dp y
DISPLAY 748.4
sp 18110.7
vp 35
wc 0
sc 250
h2mm 72.44
is 500.00
rf1 7328.7
rfp 5827.9
th 100.000
ins
at pH



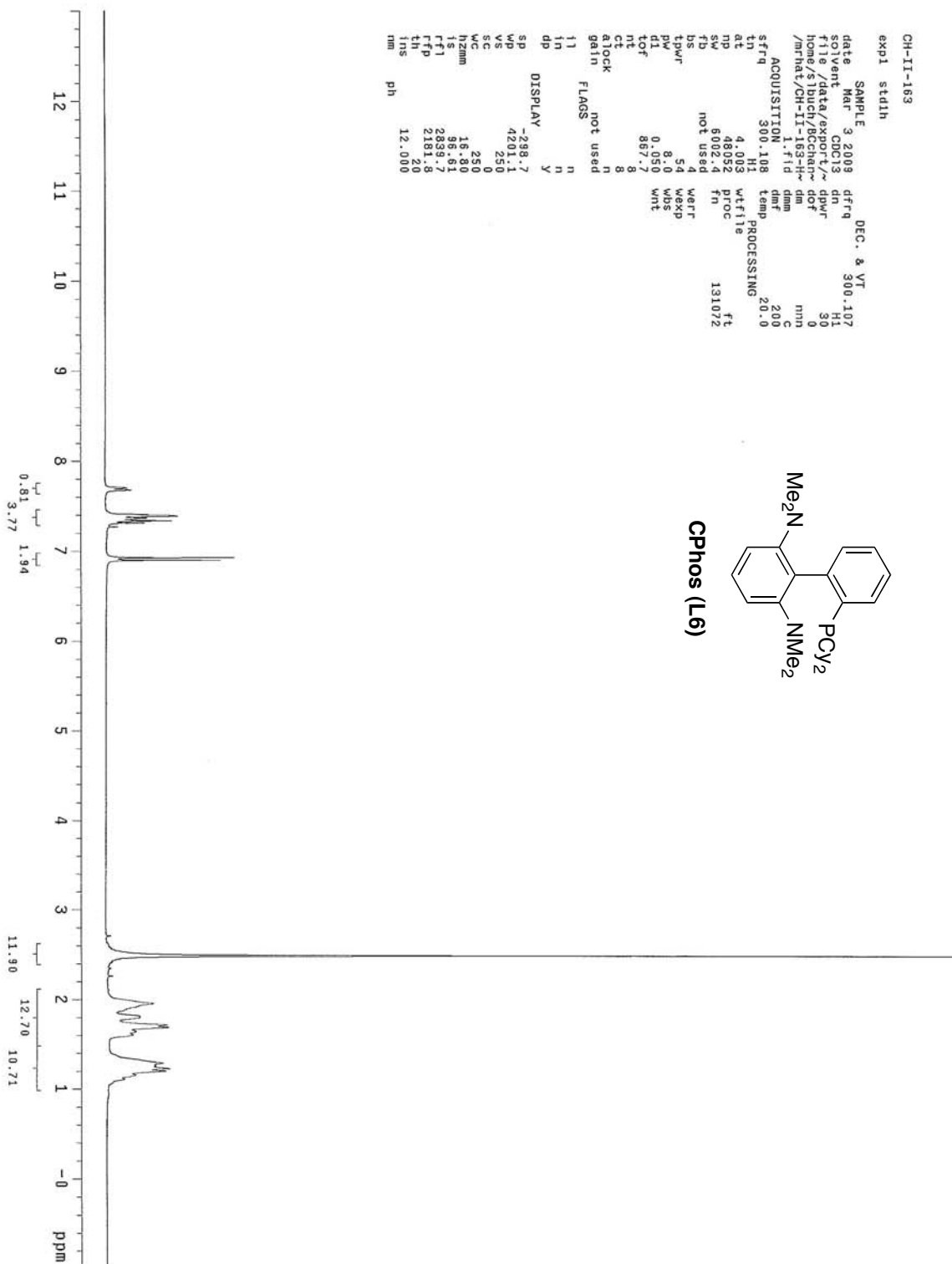
exp1	std1h
1	1
2	2
3	3
4	4
5	5
6	6
7	7
8	8
9	9
10	10
11	11
12	12
13	13
14	14
15	15
16	16
17	17
18	18
19	19
20	20
21	21
22	22
23	23
24	24
25	25
26	26
27	27
28	28
29	29
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31	31
32	32
33	33
34	34
35	35
36	36
37	37
38	38
39	39
40	40
41	41
42	42
43	43
44	44
45	45
46	46
47	47
48	48
49	49
50	50
51	51
52	52
53	53
54	54
55	55
56	56
57	57
58	58
59	59
60	60
61	61
62	62
63	63
64	64
65	65
66	66
67	67
68	68
69	69
70	70
71	71
72	72
73	73
74	74
75	75
76	76
77	77
78	78
79	79
80	80
81	81
82	82
83	83
84	84
85	85
86	86
87	87
88	88
89	89
90	90
91	91
92	92
93	93
94	94
95	95
96	96
97	97
98	98
99	99
100	100

CPHOS (L6)



The chemical structure of CPHOS (L6) is a 1,1'-bisphosphine-2,2'-biphenyl derivative. It consists of two benzene rings connected at the 1 and 1' positions. At the 2-position of the left ring, there is a dimethylamino group (NMe₂). At the 2'-position of the right ring, there is a dimethylphosphino group (PCy₂). The other phosphorus atom is located at the 2-position of the right ring, also as a dimethylphosphino group (PCy₂).

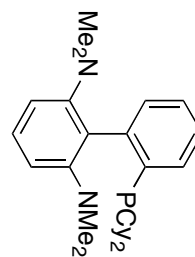
CPhos (L6)



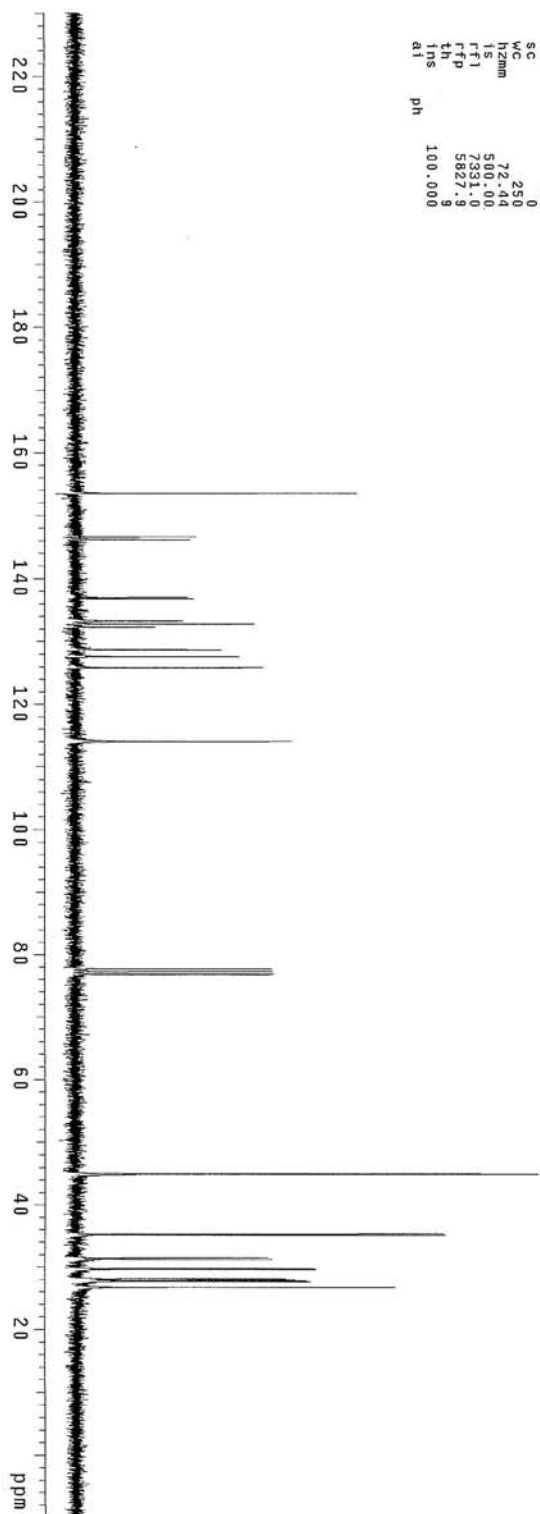
CH-II-163-C13

exp1 std13c

SAMPLE DEC. & VT
date Mar 3 2009 dfreq 300.107
solvent CDCl3 dn H1
file /data/export/~ dpwr 39
home/stbuck/Bcchan~ dof 0
/mhat/CH-II-163-C~ dm yyy
13.fid dnm w
ACQUISITION 73.413 temp 11000
sfreq 111.111 temp PROCESSING 20.0
at 1.500 sp -1.500
np 67874 sbs -1.500
sw 22624.4 wfile
fb 12400 proc ft
bs 16 fn 262144
tpwr 55
pw 10.0 werr
d1 0.500 wexp
lor 22624.0 wbs
wt 256 wnt
ct 256
a1ock n
gain not used
flags
i1 n
in n
dp y
DISPLAY
sp -750.6
vp 1810.2
vs 41
sc 0
wc 250
h2mm 72.44
ls 500.00
rftl 7331.0
rftd 5827.9
th 100.000
tms
al ph



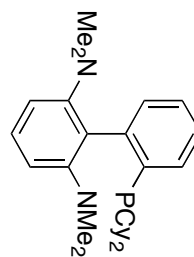
CPpos (L6)



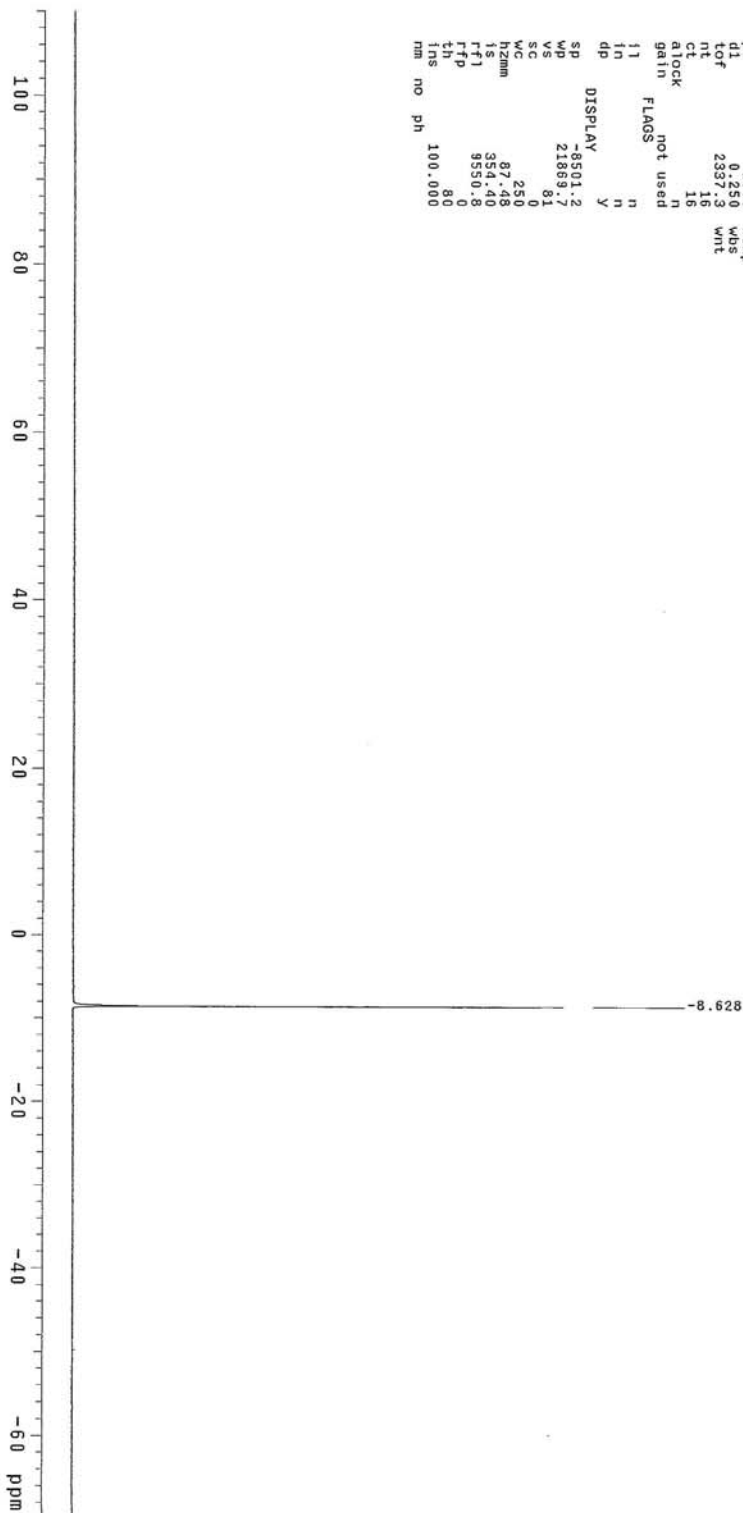
CH-II-163-P31

exp1 s2pu1

SAMPLE DEC. 8 VT
date Mar 4 2009 dfrq 300.107
solvent Mar CDC13 dn H1
file /data/export/~ dpwr 33
home/sibuch/B0chan~ dof 0
/rnat/CH-II-163-P~ dm yyy
31.1 fid 11000
ACQUISITION 121.487 temp 20.0
sfrq 121.487 temp PROCESSING 1.00
in P31 1b wtfile fl
at 1.261 1b wtfile fl
np 61204 proc not used
sw 24271.8 fn
fb 13400
ds 16
tpwr 62 weff
pw 100 wep
t1 0.250 wds
tof 233.53 WMT
nt 16
ct 16
a1ock n
gain not used
FLAGS
i1 n
i1n n
dp y
DISPLAY
SP -8501.2
WD 21889.7
VS 81
SC 0
WC 250
h2mm 87.48
h3 354.40
h4 3530.8
t1p 80
ins 100.000
mm no ph



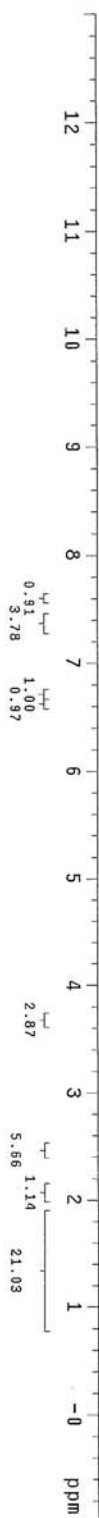
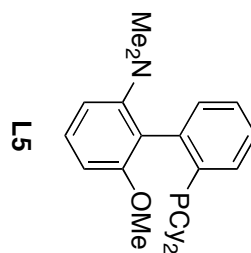
CPPhos (L6)



CH-II-103

expl stdIn

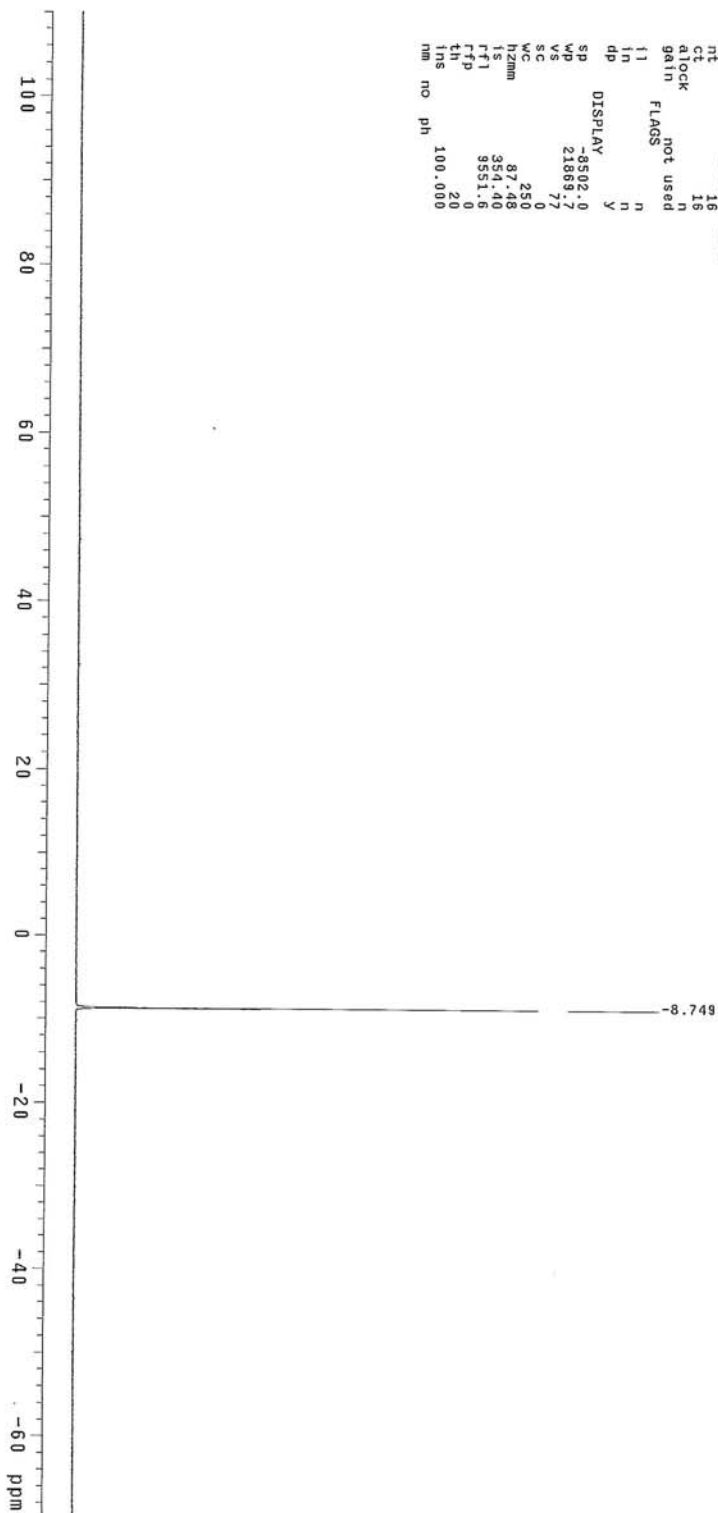
SAMPLE 4 2009 DEC. 30 VT
date Mar 4 2009 dfrq 300.107
solvent CDC13 dn H1
file /data/export/~ dpvr 30
home/sibuch/3SChan~ dof 0
/mrhat/CH-II-103-H~ dm nm
1.fid dmf 200
C
ACQUISITION 300.108 .temp 20.0
sfrq 300.108 .temp 20.0
in H1
nt 4.002 vffile
nw 48052 proc ft
sw 6002.4 fn 131072
fb not used
ds 4 weff
tpwr 54 wexp
pw 8.0 wbs
d1 0.050 wnt
lof 867.7
nt 8
scf 8
slock n
gain not used
11 n
in n
dp y
DISPLAY
sp -299.1
ap 4201.1
vp 153
wc 250
h2mm 16.80
is 146.11
rf1 2840.2
rfp 2181.8
th 20
lms 1.000
ph



exp1	std13c
------	--------

CN(C)c1ccccc1-c2ccccc2C(=O)OC

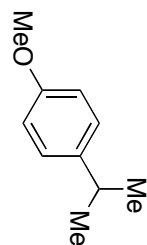
exp1 szpu1

CN(C)c1ccccc1-c2ccccc2C(=O)OC

CH-II-170

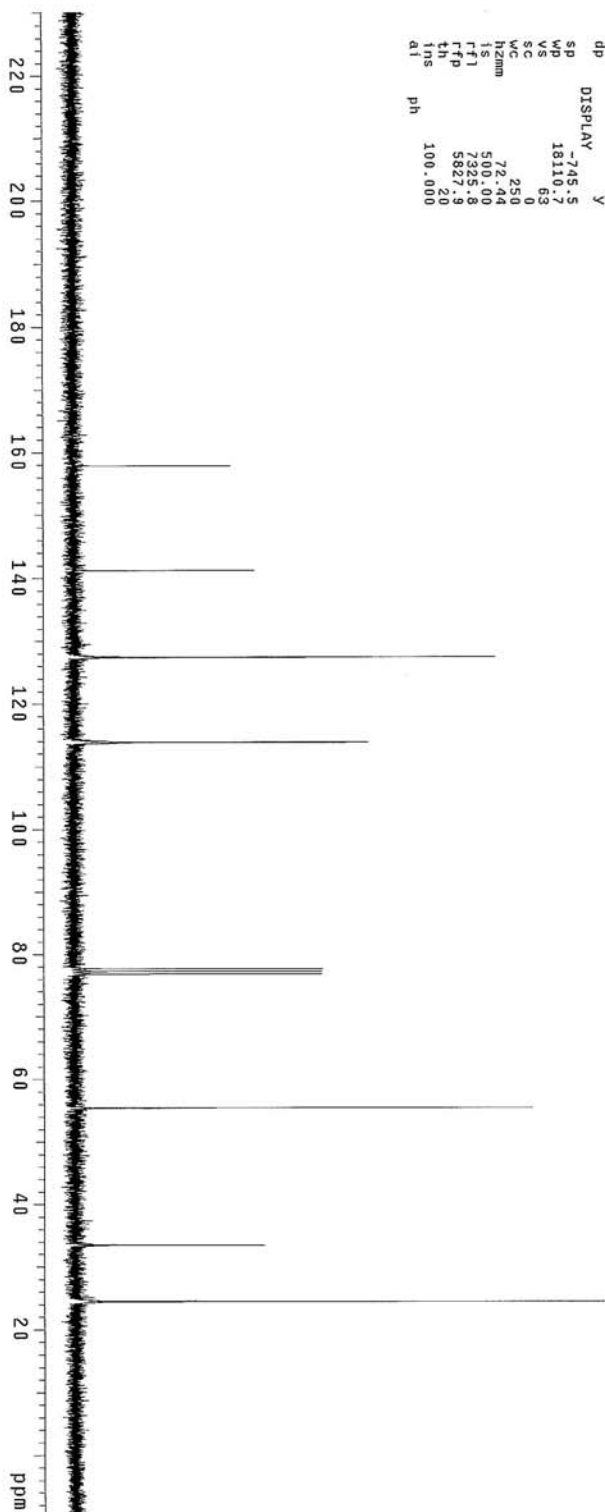
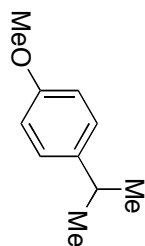
exp1 std1h

SAMPLE DEC. & VT
date Feb 22, 2009 dffrq 300.107
solvent cd 22CDCl3 dn H1
file /data/export/~ dpwr 30
home/stbuch/BCChan dof 0
/mrhat/CH-II-170-H~ dm nm
1.fid dnm 200
C
ACQUISITION
sfrq 300.108 temp PROCESSING
tn 4.001 vffile ft
at 4.002 PTOC 131072
sp 6002.4 fn
fb not used
bs 4 warr
tpwr 54 wexp
pw 8.0 wbs
dl 0.050 wnt
tof 867.7
nt 8
ct 8
stuck 8
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -301.7
wp 4201.1
vs 151
sc 0
wc 250
hzmm 16.80
is 175.94
rf1 561.0
rfp 0
th 20
ins 1.000
nm
ph



CH-II-170-C13
exp1 std13c

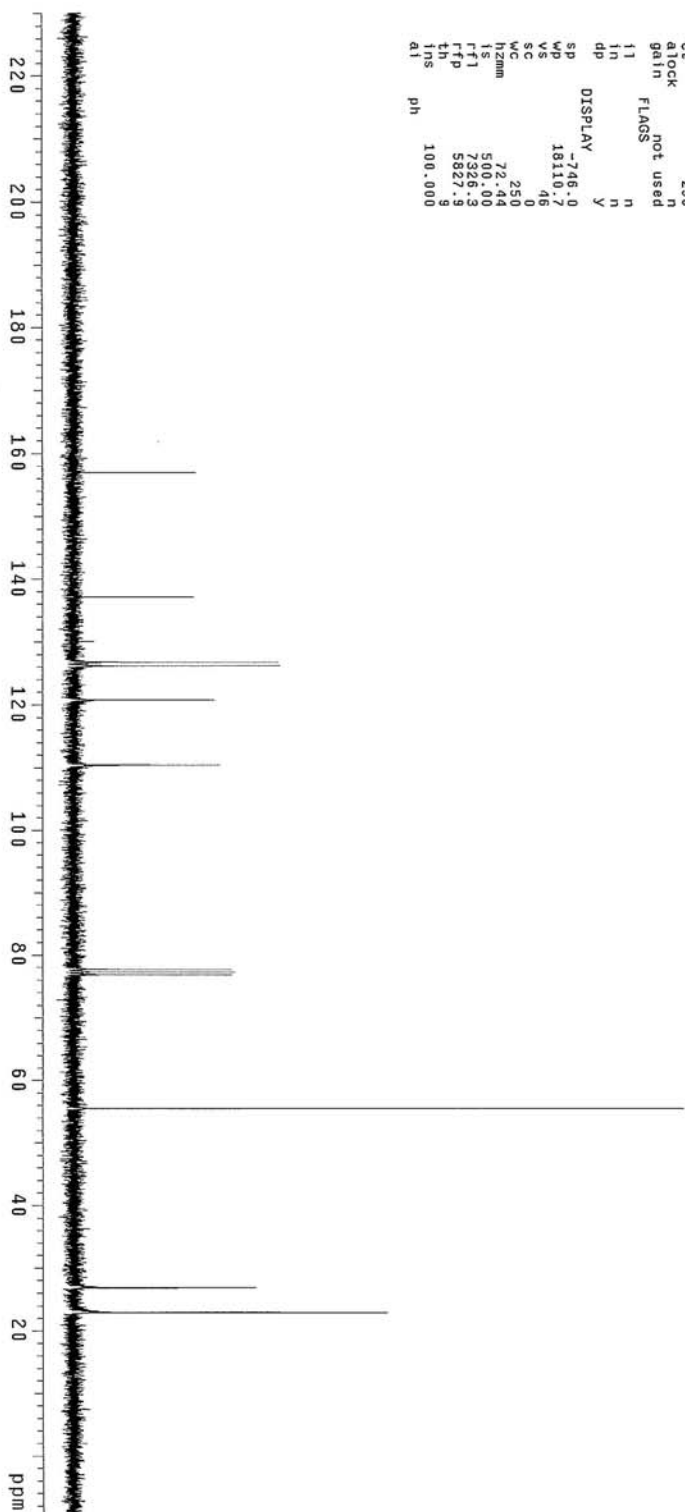
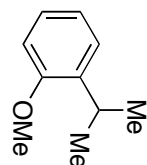
SAMPLE DEC. & VT
date 12/22/2009 dfrq 300.107
solvent eb 2cnc13 dn H1
file /data/export/~ dpwr 39
home/slbuch/Bcchan~ dof 0
/mhat/CH-II-170-C~ dm yyy
13. fid w
ACQUISITION 13. fid dnm 11000
sfrq 75.471 temp PROCESSING 20.0
tn C13 sb
at 1320 sb -1.500
dp 22624.4 wfile
fb 12400 proc
bs 8 fn 262144
tpwr 55
pw 10.0 warr
dl 0.500 wexp
tof 2264.0 wds
nt 312 wnt
rt 312
rt LOCK
gain not used
flags
il n
in n
dp y
sp DISPLAY
wp -745.5
wp 18110.7
vs 0
ss 0
wc 250
hzmm 72.44
is 500.00
rf1 7325.8
rfp 5827.9
th 20
ins 100.000
at ph



CH-II-170-C13

expt std13c

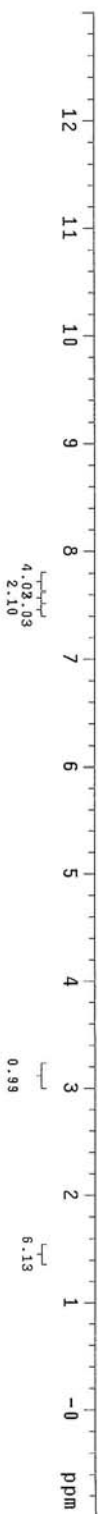
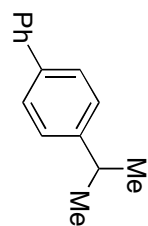
SAMPLE DEC. & VT
date Feb 22 2009 dfrq 300.107
solvent CDCl3 dn H1
file /data/export/~ dpwr 39
home/sibuch/SCchar~ dof 0
/mrhat/CH-II-165-C~ dm yyy
13.fid dnm w
ACQUISITION 13.000
sfreq 75.471 temp 20.0
in C13 sb PROCESSING
at 1.580 sb -1.580
nu 6.272 sb
sv 22624.4 wfile
fb 12400 proc
bs 32 fn 262144
tpwr 55
pw 10.0 werr
d1 0.500 wexp
tof 2264.0 wds
nt 512 wnt
clock 256
glin not used
flags
1 1 n
1 1 n
in n
dp y
DISPLAY
sp 746.0
wp 1810.7
wc 0
h2mm 72.44
ls 500.00
rf1 7326.3
rfp 5827.9
th 9
ins 100.000
at ph



CH-II-174

expl stdh

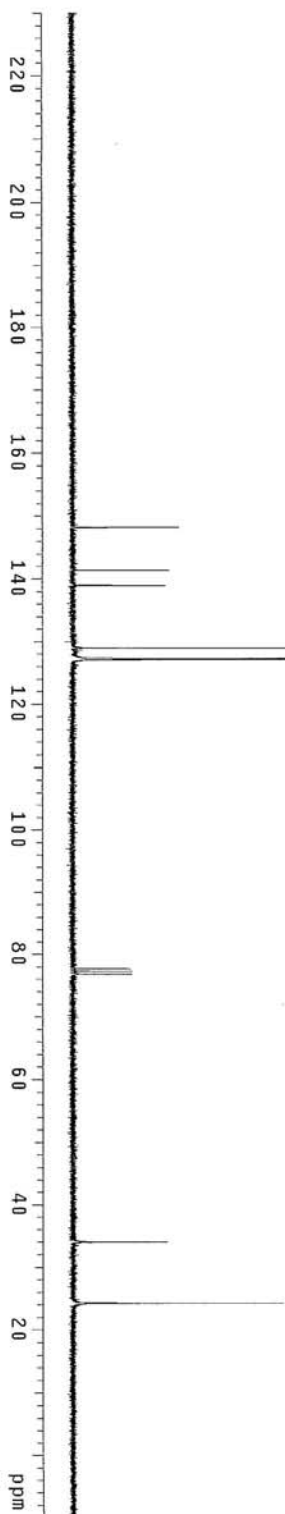
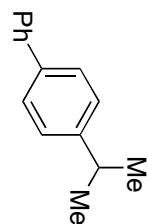
SAMPLE DEC. & VT
date Feb 22 2009 dfreq 300.107
solvent dm H1
file /data/export/~ dpwr 30
home/stbuch/Bcchan~ dof 0
/mrhat/CH-II-174b~ dm nm
H1.fid dnm 200
ACQUISITION 20.0
sfrq 300.108 temp PROCESSING
in 4.003 wfile
ns 48052 proc ft
sw 6002.4 fn 131072
bs not used
tpwr 8 werr
pw 54 wexp
di 8.0 wds
tof 0.050 wnt
nt 867.7
ct 8
clock n
gain not used
flags
il n
in n
dp y
SP DISPLAY
wp 4288.2
vp 4281.76
vs 176
sc 0
wc 250
hzmm 16.80
is 78.89
rf1 2639.3
rfp 2181.8
th 20
rms 1.000
nm
ph



CH-II-174-C13

exp1 std13c

SAMPLE DEC. & VT
date Feb 22 2009 dfrq 300.107
solvent CDC13 dn H1
file /data/export/~ dpwr 39
home/stibuch/Bcchan~ dof 0
/mhat/CH-II-174~ dm yyy
C13.fid dnm w
ACQUISITION 75.471 temp 11000
sfrq 111.111 PROCESSING 20.0
in 1.500 sb -1.500
nd 67824 sbs -1.500
sw 22624.4 wfile
fb 12400 proc 282144
bs 16 fn
tpwr 55
pw 10.0 watt
dl 0.500 wexp
tof 2264.0 wds
ct 256 wnt
cl 256
alock n
gain not used
flags
i1 n
in n
dp y
DISPLAY
sp -753.9
wp 1810.7
vp 16
wc 250
sc 0
hzmm 72.44
is 500.00
rf1 7334.2
rfp 5827.9
th 9
tms 100.000
at ph



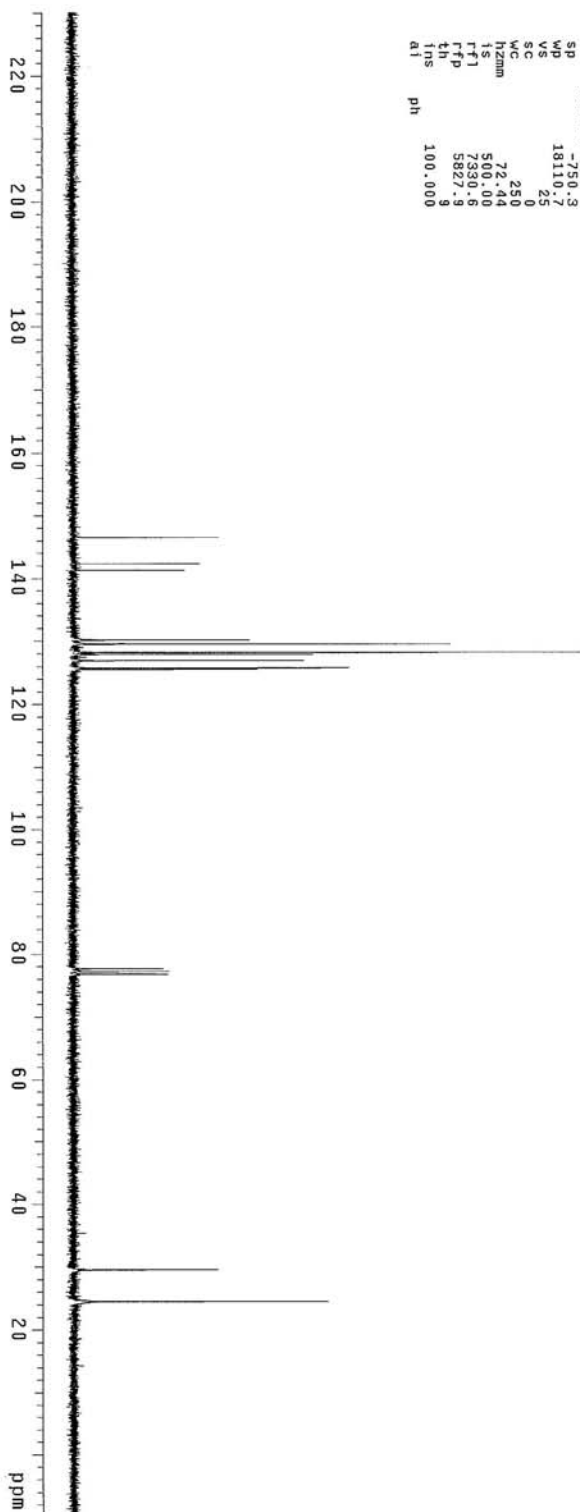
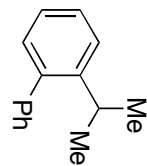
exp1	std1h
1	1
2	2
3	3
4	4
5	5
6	6
7	7
8	8
9	9
10	10
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12	12
13	13
14	14
15	15
16	16
17	17
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21	21
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43	43
44	44
45	45
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50	50
51	51
52	52
53	53
54	54
55	55
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57	57
58	58
59	59
60	60
61	61
62	62
63	63
64	64
65	65
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67	67
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73	73
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75	75
76	76
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86	86
87	87
88	88
89	89
90	90
91	91
92	92
93	93
94	94
95	95
96	96
97	97
98	98
99	99
100	100

CC(C)c1ccccc1

CH-II-173-C13

exp1 std13c

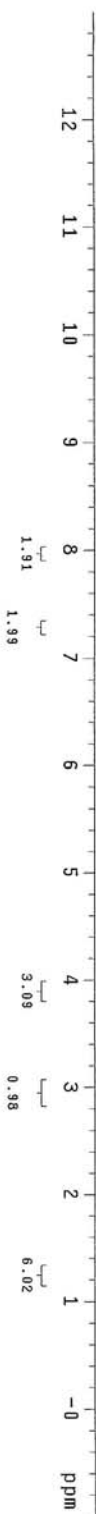
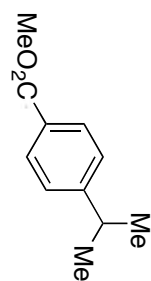
SAMPLE DEC. & VT
date Feb 22 2009 dfreq 300.107
solvent CDCl3 dn H1
file /data/export/~ dwf 39
home/s1buch/BCchar~ dof 0
/mrhat/CH-II-173C~ dm yyy
w
ACQUISITION 73.471 temp 11000
sfreq 73.471 sb 20.0
in 1.500 sb -1.500
at 67874 sbs -1.500
nd 22624.4 wf file
sw 12400 proc 262144
fb 16 fn
bs 55
tpwr 10.0 werr
pw 0.500 wexp
dl 2264.0 wos
tof 258 wte
ct 258
gain not used
alock n
gain not used
FLAGS n
il n
in n
dp y
SP DISPLAY -250.3
vpp 18110.3
vp 25
wc 0
sc 250
hzmm 72.44
ts 500.00
tfl 7330.6
tfs 5827.9
tms 100.000
at ph



CH-II-251

expt stdIn

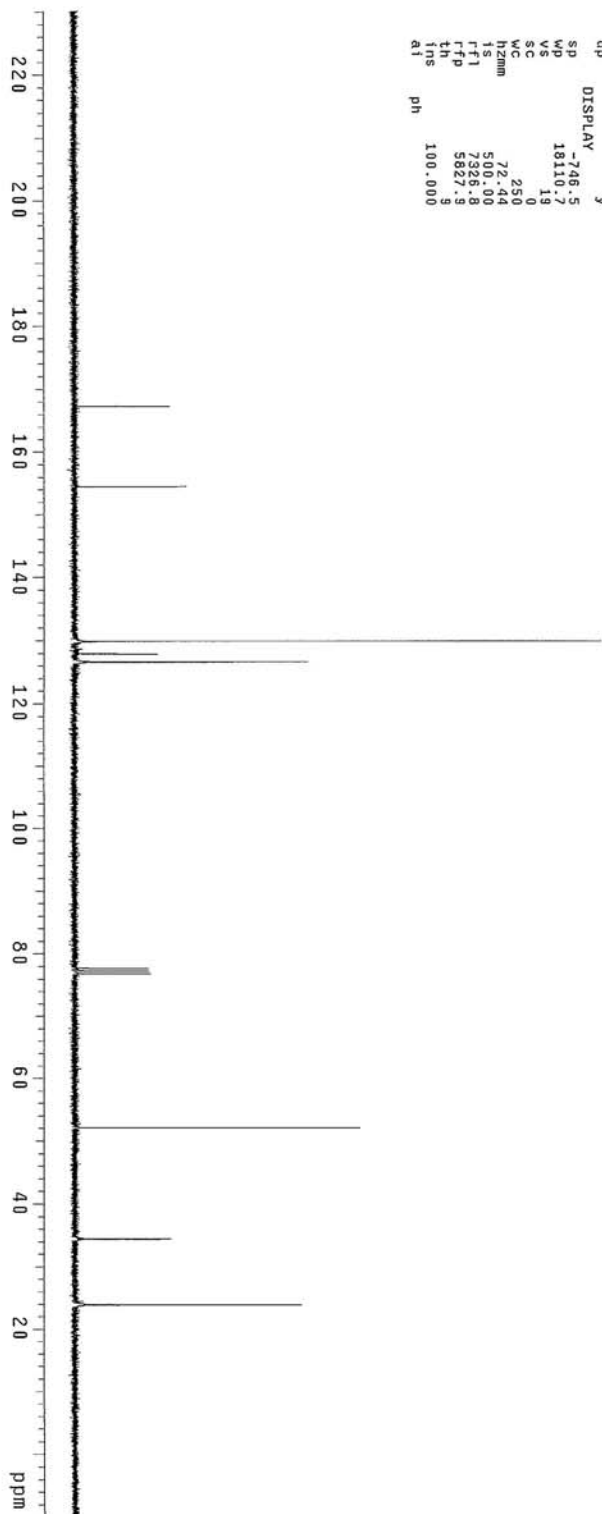
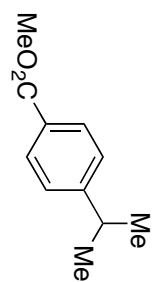
SAMPLE DEC. & VT
date Feb 22 2009 dfreq 300.107
solvent CDC13 dn H1
file /data/export/~dpwr 30
home/stibuch/Bcchan~ dof 0
/mhat/CH-II-251-H~ dm nnn
1.fid dnm 200
ACQUISITION temp PROCESSING
sfrq 300.108 20.0
in 4.003 wfile
sw 48052 proc ft
np 6002.4 fn 131072
fb not used
bs 4 warr
tpwr 54 wexp
pw 8.0 wbs
dl 0.050 wnt
tof 887.7
ct 8
cl 8
alock n
gain not used
flags
i1 n
in n
dp y
DISPLAY
sp 301.7
wp 420.7
vp 137
wc 0
sc 0
hzmm 16.80
is 125.61
rf1 661.0
rfp 0
th 20
rms 1.000
nm
ph



CH-II-251-C13

```
exp1 std13c
```

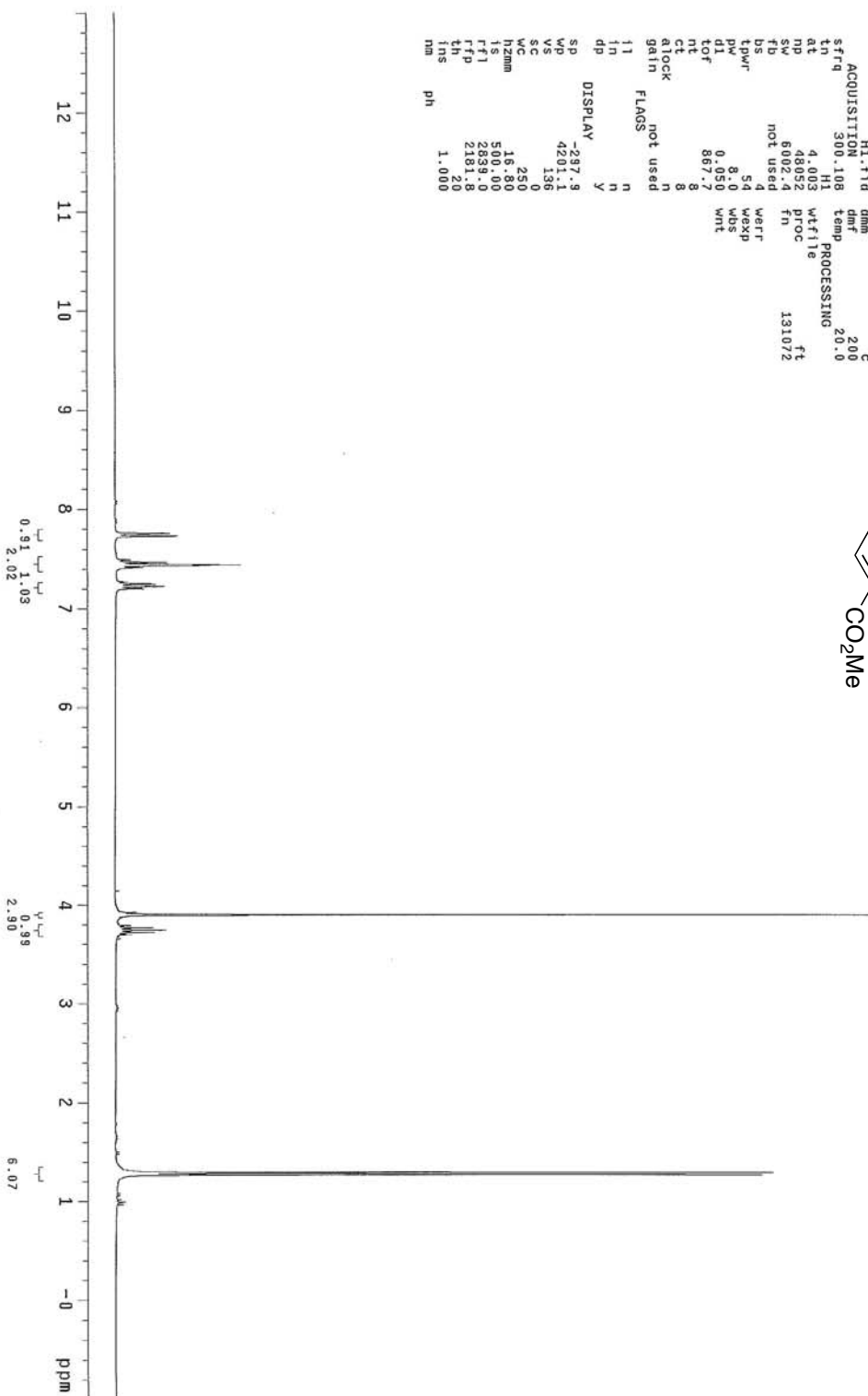
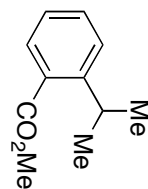
SAMPLE		DEC. & VT	
date	Feb 22 2009	dfrq	300.107
solvent	CDCl3	dn	H1
file	/data/export/~	dpwr	91
home	/sbuch/BChen	dof	3
/mha/CH-11-291-C	dm	xyy	0
ACQUSITID	3-ftid	dmf	11000
sfrq	75.471	temp	20.0
at	C13	PROCESSING	
in	1.500	sb	-1.500
np	67874	sbs	-1.500
sw	22624.4	wf1file	
fb	11400	proc	ft
bs	5	fn	262144
dpwr	10.0	verf	
d1	0.500	wexp	
tof	2284.0	wbs	
nt	256	wnt	
ct	256		
alock	n		
gain	not used		
flags			
11	n		
in	n		
dp	y		
DISPLAY			
sp	-746.5		
vc	1810.7		
vc	19		
hzm	250		
hzm	72.44		
1s	500.00		
rf1	7326.8		
rfp	5827.5		
th	5		
1s	100.000		
ph			



CH-II-223

expt stdIn

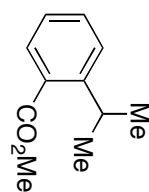
SAMPLE DEC. & VT
date Feb 22, 2009 dfrq 300.107
solvent CDC13 dn H1
file /data/export/~ dpwr 30
home/stbuck/Bcchan~ dof 0
/mrhat/CH-II-223b~ dm mn
H1.fid dnm 200
ACQUISITION temp 20.0
sfrq 300.108
in 4.003 wfile
at 48052 proc ft
sw 6002.4 fn 131072
fb not used
bs 4 werr
tpwr 54 wexp
pw 8.0 wds
d1 0.050 wnt
tof 867.7
nt 8
ct 8
alock n
gain not used
flags n
i1 n
in n
dp y
SP DISPLAY
vpp 287.9
vpe 4201.1
vpe 136
wc 250
sc 0
hzm 15.80
is 500.00
rf1 2839.0
rfp 2181.8
th 20
tms 1.000
nm
ph



CH-II-223-C13

exp1 std13c

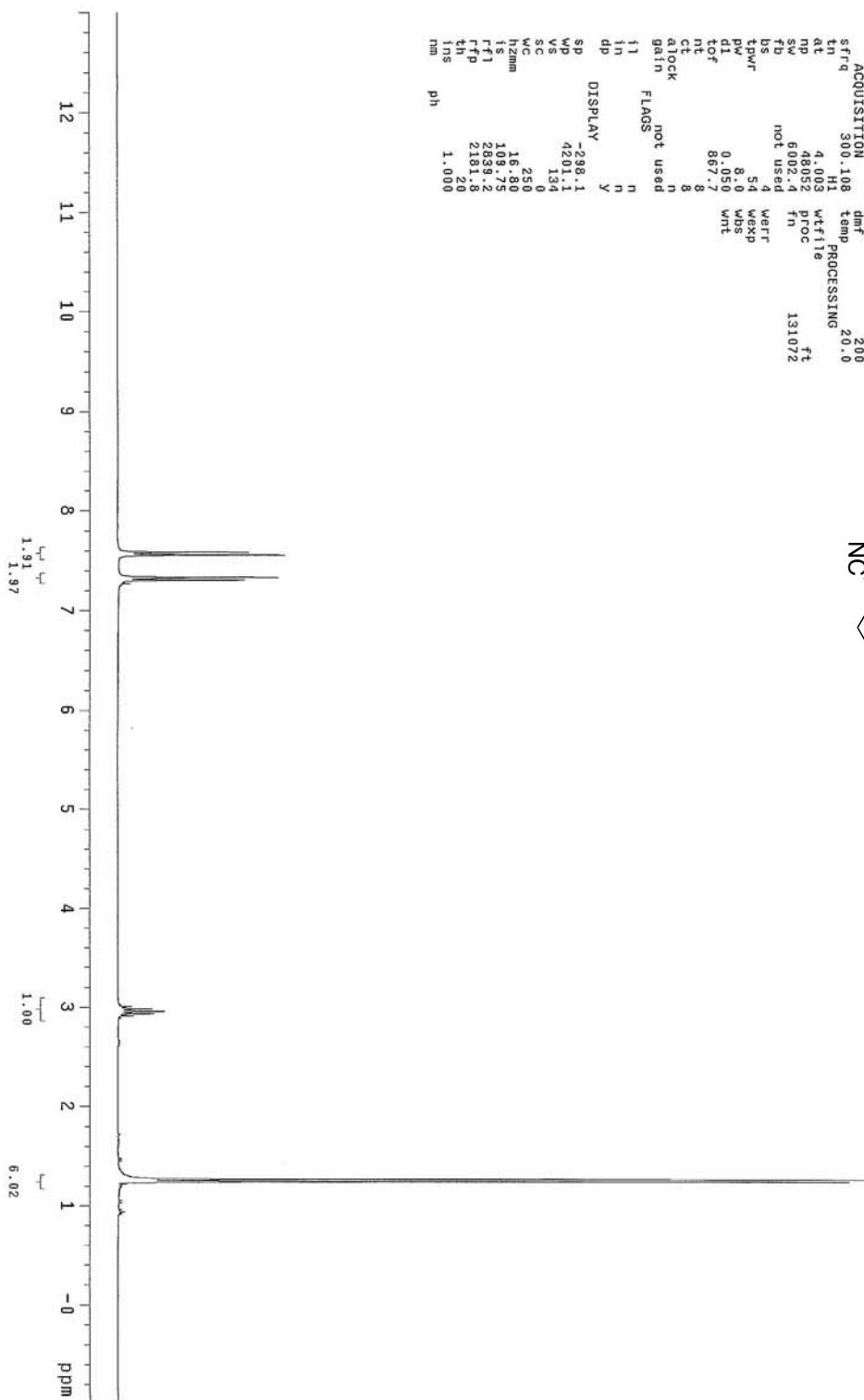
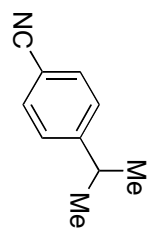
SAMPLE DEC. & VT
date Feb 22 2008 dfrq 300.107
solvent dms-dn H1
file /data/export/~ dpwr 39
home/stbuch/8Cchan~ dof 0
/mhat/CH-II-223b~ dm yyy
w
C13.fid dnm 11000
ACQUISITION 75.471 temp 20.0
sfrq 11000
tn C13 sb PROCESSING 20.0
dt 1.100 sb -1.500
sw 67874 sbs -1.500
fb 22624.4 wfile
bs 12400 proc
tpwr 16 fn 262144
pw 55
d1 10.0 wait
lof 0.500 wexp
nt 2264.9 wds
nt 258 wnt
nt 258
alock n
gain not used
FLAGS
il n
in n
dp y
SP DISPLAY
wp 747.5
vp 1810.7
vs 0
sc 0
wc 250
hzmm 72.44
is 500.00
rf1 7327.8
rfp 5827.9
th 9
tms 100.000
at pH



CH-II-220

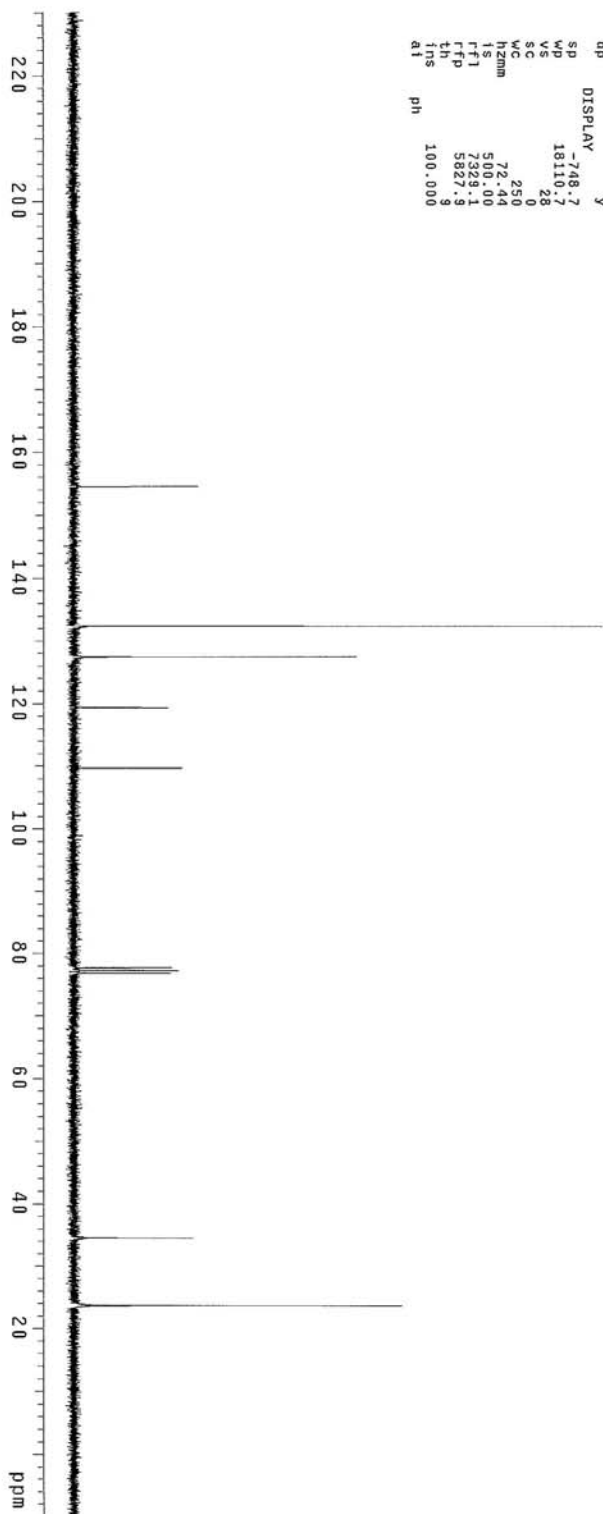
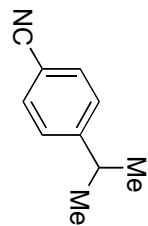
expt stdth

SAMPLE DEC. & VT
date 88 22 2009 dfrq 300.107
solvent cdcl3 dn H1
file /data/export/~ dpwr 30
home/stbush/BCchar~ dof 0
/mhat/CH-II-220b~ dm mn
H1.fid dmf 200
C
ACQUISITION
sfrq 300.108 temp 20.0
tn H1
dt 4.093 wfile
nu 48052 plog ft
sw 6002.4 fn 131072
fb not used
bs 4 warr
tpwr 54 wexp
pw 8.0 wds
d1 0.050 wnt
tof 867.7
nt 8
sc 8
atlock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -208.1
wp 4201.1
vcs 134
sc 0
wc 250
hzmm 16.80
is 109.75
rf1 2839.2
rfp 2181.8
th 20
rms 1.000
ph



CH-II-220-C13
exp1 std13c

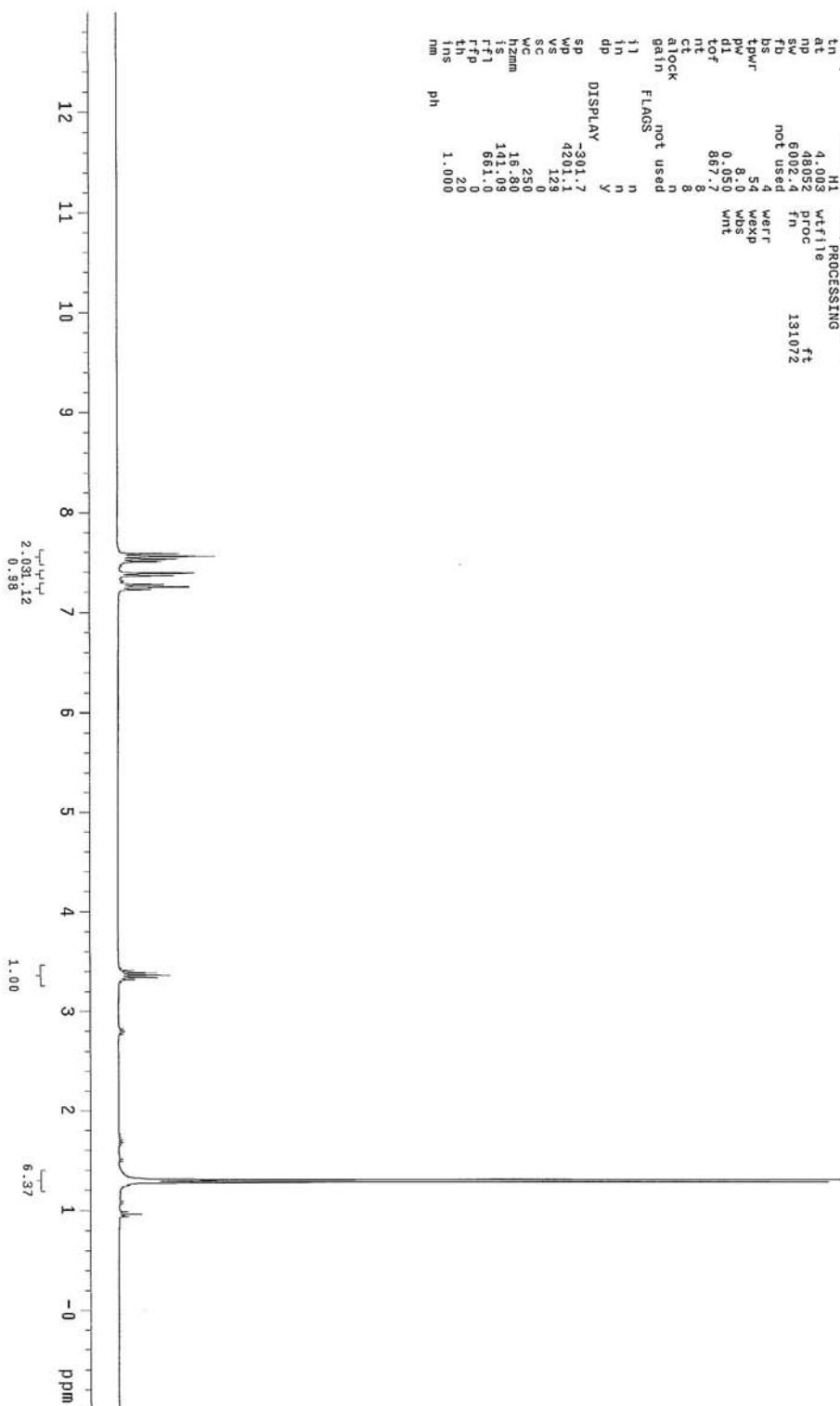
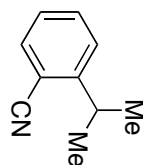
SAMPLE DEC. & VT
date Feb 22 2009 dffrq 300.107
solvent CDCl3 d1 H1
file /data/export/~ dpwr 39
home/sibuch/BChan~ dof 0
/mhat/CH-II-220D~ dm yyy
C13.fid dm w
ACQUISITION 75.471 temp 11000
sfrq 141.141 PROCESSING 20.0
ln 1.500 sb -1.500
nt 67824 sbs -1.500
sw 22624.4 wfile
fb 12400 proc
bs 16 fn 282144
tpwr 55
pw 10.0 warr
d1 0.500 wexp
tof 2264.0 wds
nt 256 wnt
atlock n
gain not used
flags
i1 n
in n
dp y
SP DISPLAY 748.7
wp 18110.28
vs 28
wc 250
sc 0
hzm 72.44
is 500.00
rfl 7329.1
rfp 5827.9
th 100.000
at pH



CH-II-238

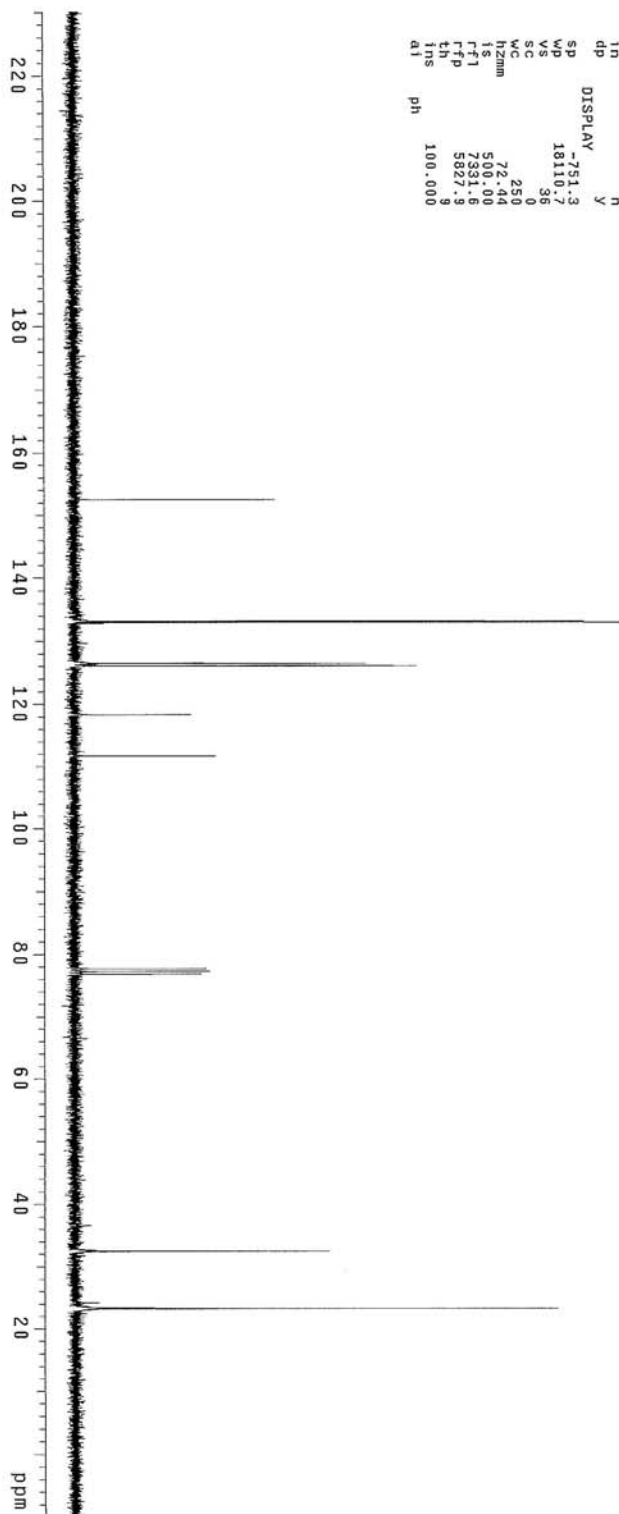
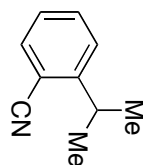
expt stdth

SAMPLE DEC. & VT
date Feb 22 2009 dfreq 300.107
solvent CDCl3 dn H1
file /data/export/~ dpwr 30
home/stbuch/BCchan~ dof 0
/mrhat/CH-II-238C~ dm mm
H1.fid dnm 200
C
ACQUISITION temp 20.0
sfrq 300.108
ln H1
dt 4.000 vfile
nu 46052 proc ft
sw 6002.4 fn 131072
fb not used
bs 4 werr
tpwr 54 wexp
pw 8.0 wds
dl 0.050 wnt
tof 867.7
nt 8
sc 3
atlock n
gain not used
flags
il n
in n
dp y
sp DISPLAY
wp -301.7
vs 4201.7
sc 124
wc 0
hzm 250
is 15.80
is 141.09
rf1 661.0
rfp 0
th 28
rms 1.000
nm
ph



CH-II-238-C13
exptl std13c

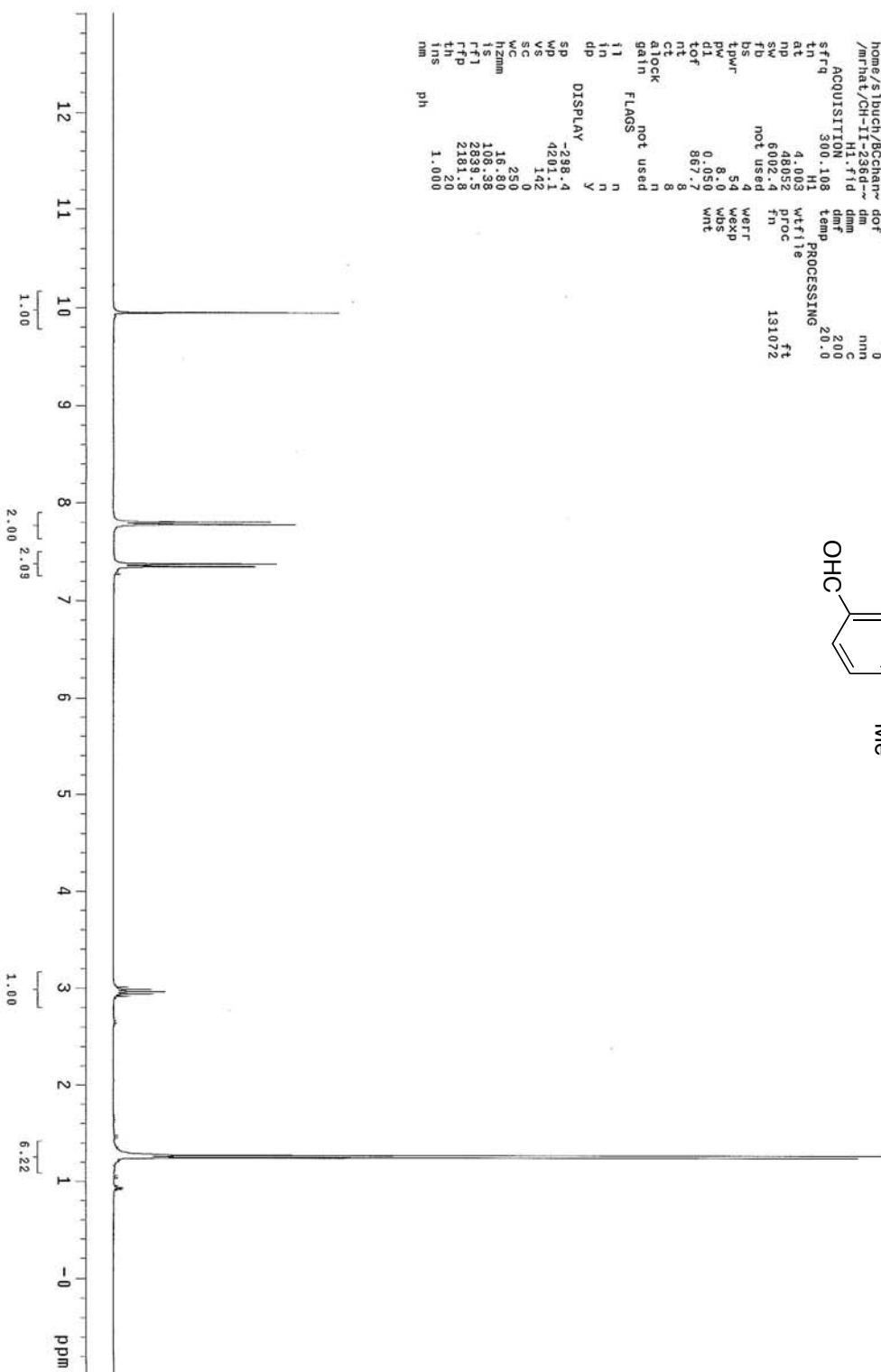
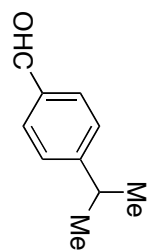
SAMPLE DEC. & VT
date Feb 22 2009 dfrq 300.107
solvent CDCl3 dn H1
file /data/export/~ dpwr 39
home/stibuch/BcChan~ dof 0
/mrhat/CH-II-238C~ dm yyy
C13.fid dmf v
ACQUISITION 75.471 temp 11000
sfrq 75.471 temp 20.0
tn 1.503 sb
at 1.503 sb -1.500
nu 67824 sbs
sw 22624.4 wf file
fb 12400 proc
bs 16 fn 262144
tpwr 55
pw 10.0 werr
d1 0.500 wexp
tof 2264.0 wbs
nt 256 wnt
sc 256
clock not used
gain not used
flags
il n
in n
dp y
sp DISPLAY
wp -751.3
vps 18110.36
vc 0
wc 250
hzmm 72.44
is 500.00
rf1 7331.6
rfp 5827.9
th 100.000
at ph



CH-II-236d

exp2 std1h

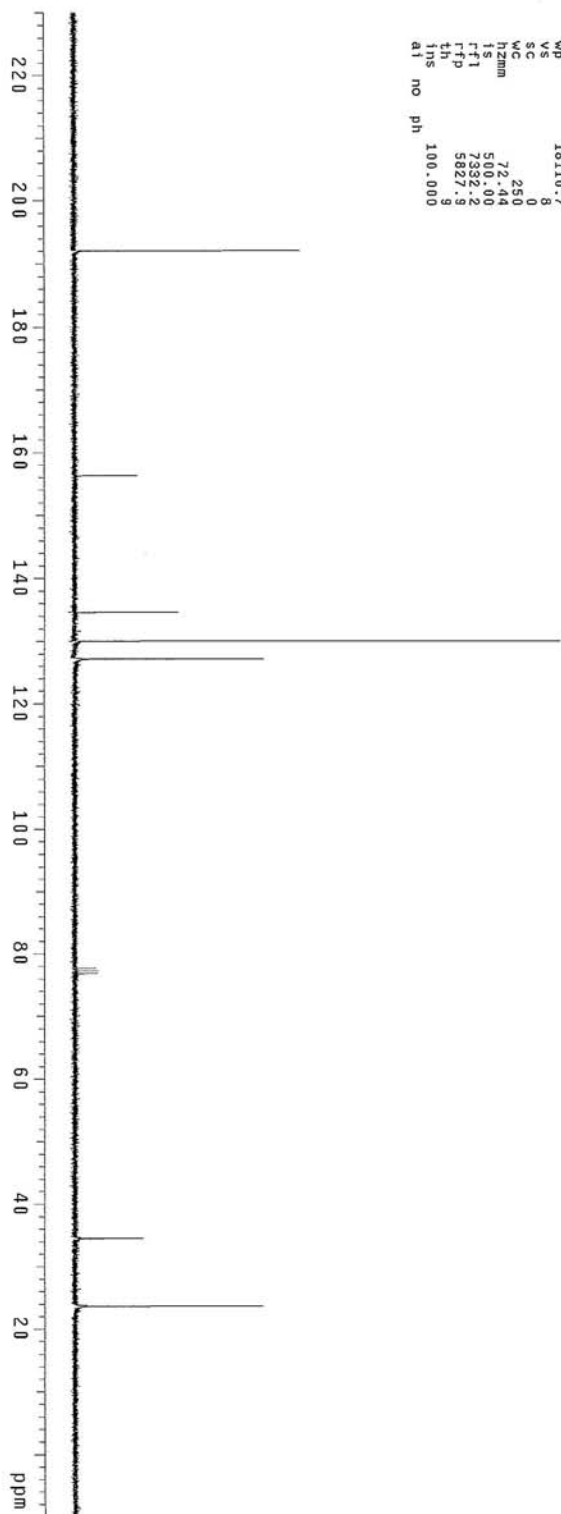
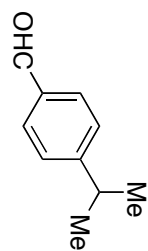
SAMPLE DEC. & VT
date Mar 17 2009 dfrq 300.107
solvent CDCl3 dn H1
file /data/export/~dpwr H1
home/sibuch/80chan~ dof 0
/mrhat/CH-II-236d~ dm nmh
H1.fid dmp c
ACQUISITION temp 20.0
sfrq 300.108
tn H1
at 4.003 wf file
np 48052 proc
sw 6002.4 fn
fb not used
bs not used
tpwr 54 weff
pw 8.0 wds
t1 0.150 wds
t2 86.7 wnt
nt 8
ct 8
ct alock n
gain not used
flags
i1 n
i1n n
dp y
display -298.4
sp 4201.1
wp 142
vs 0
sc 250
wc h2mm 16.80
is 108.38
f1 263.5
f1p 218.2
f1ns 1.000
ph nm



CH-II-236-C13

exp1 std13c

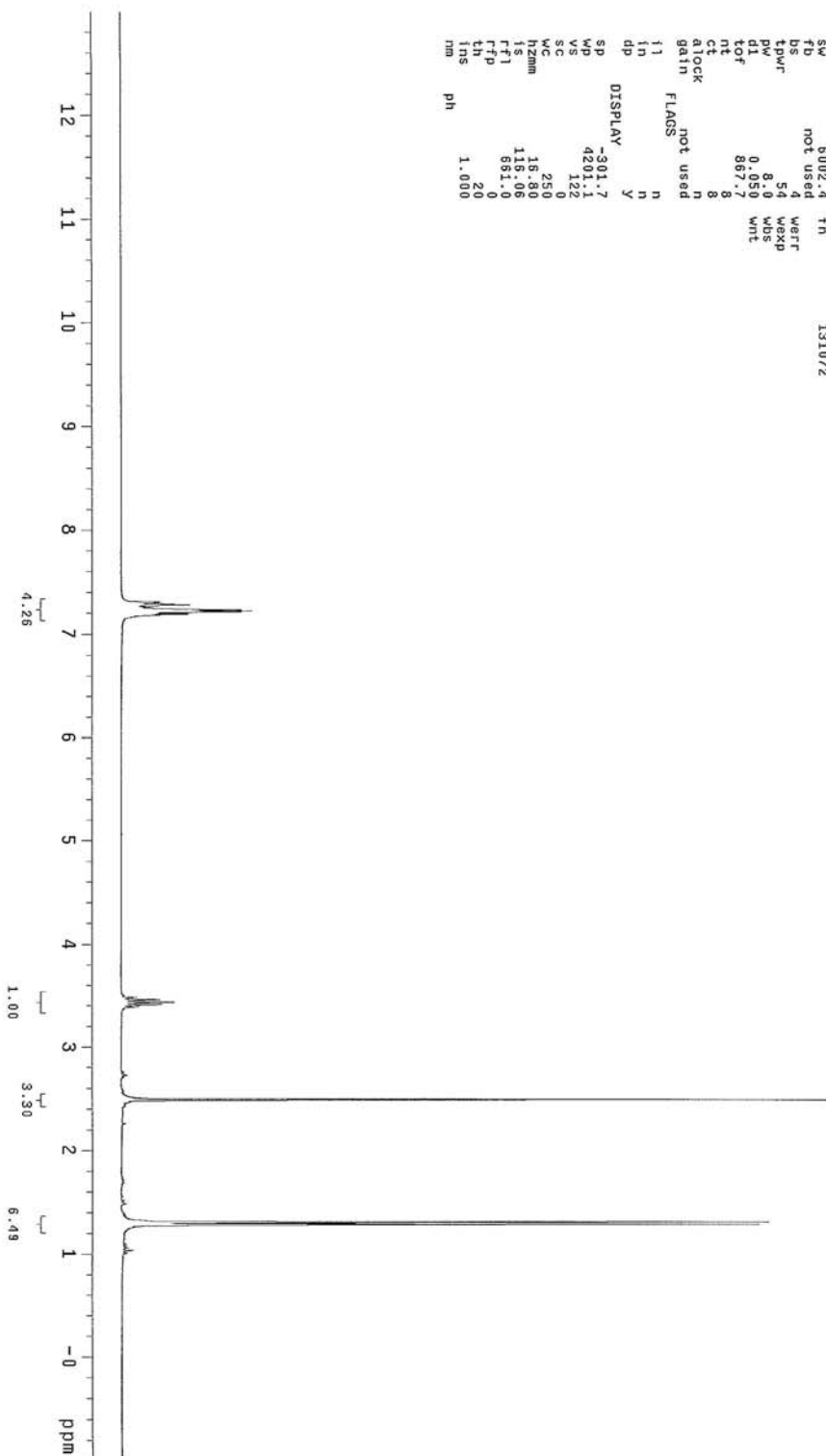
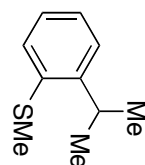
SAMPLE DEC. & VT
date Mar 2 2009 dfreq 300.107
solvent CDC13 dn H1
file /data/export/~ dpwr 39
home/stibuch/Bcchan~ dof 0
/mhat/CH-II-236C~ dm yyy
C13.fid dm w
ACQUISITION 75.471 temp 11000
sfrq 111.111 temp PROCESSING 20.0
in 1.500 sp -1.500
np 67874 sds -1.500
sw 22624.4 wfile
fb 12400 proc ft
bs 16 fn 262144
tpwr 55
pw 10.0 warr
dl 0.500 wexp
tof 22674.0 wds
nt 25.5 wnt
ct 84
atlock not used
gain flags
i1 n
in n
dp y
SP DISPLAY
sp 751.9
wpp 1810.7
wv 0
wc 250
sc 0
hzmm 72.44
is 500.00
rf1 7332.2
rfp 5827.9
th 100.000
at no ph



CH-II-177

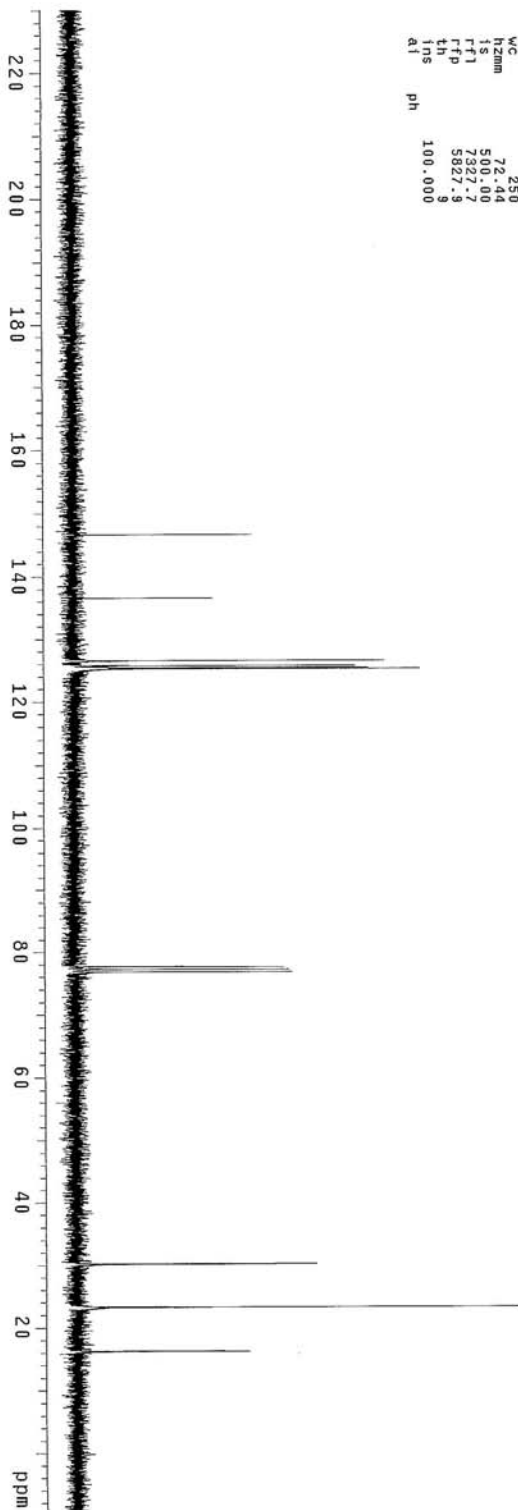
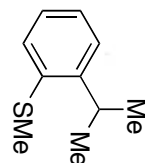
expt stdin

SAMPLE DEC. & VT
date Feb 22 2003 dfreq 300.107
solvent CDCl3 dn H1
file /data/export/~ dovr 30
home/sibuch/Bcchar~ dof 0
/mrhat/CH-II-177-H~ dm nmh
1.fid dmm 200
C
ACQUISITION 300.108 temp PROCESSING 20.0
sfrq 300.108
ln H1
dt 4.003 vfile
TD 48052 proc ft
sw 6002.4 fn 131072
fb not used
bs 4 warr
tpwr 54 wexp
pw 8.0 wds
d1 0.059 wnt
tof 867.7
nt 8
sc 8
gain alock n
gain not used
FLAGS n
i1 n
in n
dp y
SP DISPLAY
wp -301.7
wv 4201.1
vc 122
wc 250
hzmm 15.80
is 115.06
f1 651.0
f1 0
t1 20
t1 1.000
rm
ph



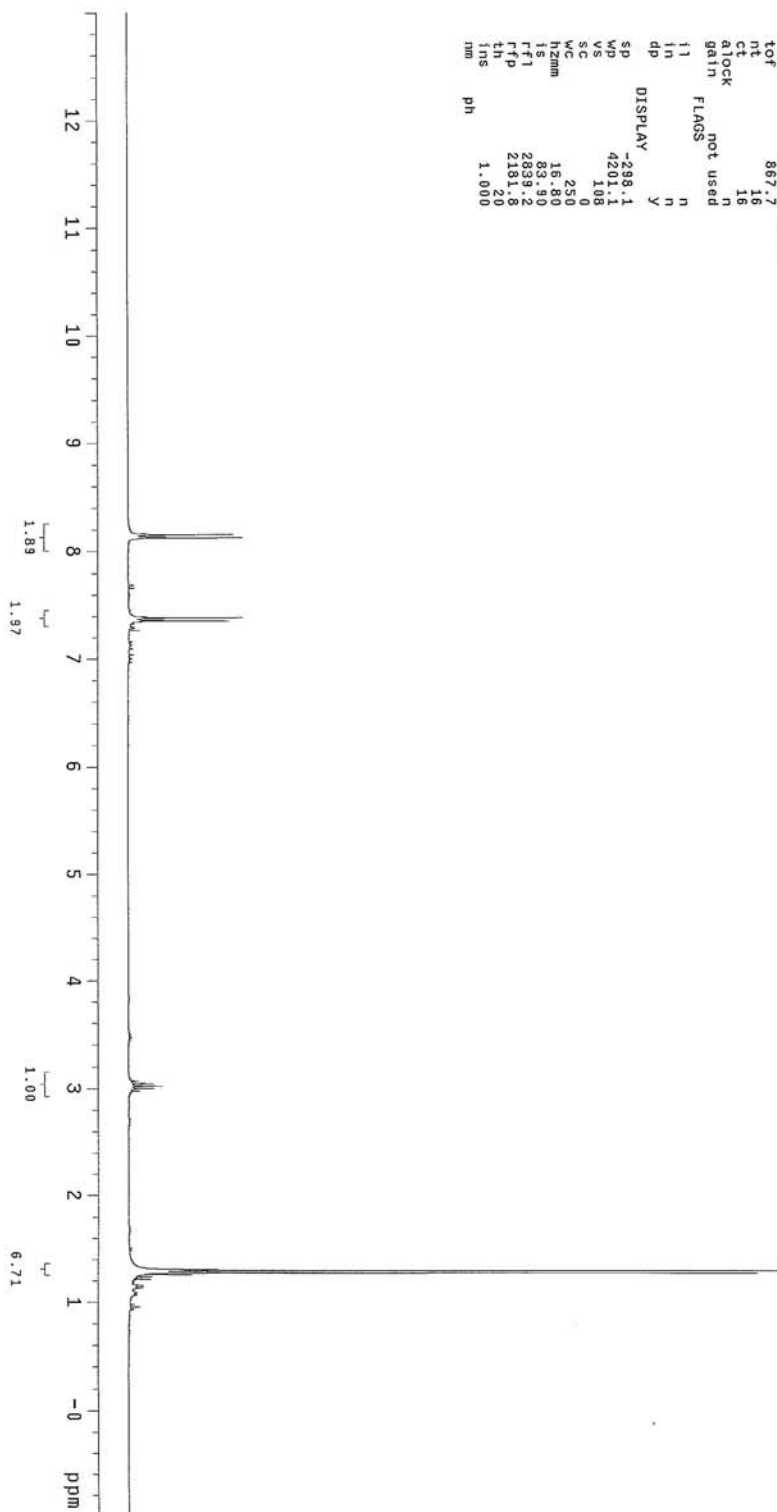
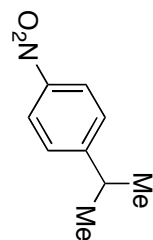
CH-II-17-C13
expt std13c

SAMPLE DEC. & VT
date Feb 22 2009 dfreq 300.107
solvent CDCl3 dn H1
file /data/export/~ dpwr 39
home/slbuch/Bcchan~ dof 0
/mhat/CH-II-17-C~ dm yyy
13.fid dmf v
ACQUISITION 13.fid temp 11000
sfreq 75.471 PROCESSING 20.0
in C13 sb
at 1300.0 sds -1.500
nu 67824 wf file
sb 22624.4 proc
fb 12400 ft
bs 16 fn 262144
tpwr 55
pw 10.0 warr
d1 0.500 wexp
tof 2264.0 wds
nt 258 wnt
cs 258
clock n
gain not used
flags
i1 n
in n
dp y
SP DISPLAY
wp -747.4
vp 18110.5
vc 0
wc 250
hzmm 72.44
is 500.00
rf1 7327.7
rfp 5827.9
th 9
ins 100.000
at ph



CH-II-221b
expl std1h

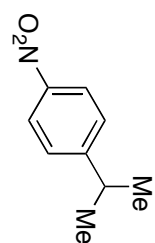
SAMPLE DEC. & VT
date Mar 2 2009 dfrq 300.107
solvent CDC13 dn H1
file /data/export/~ dwwr 30
home/stbuck/BCharr dof 0
/mrhat/CH-II-221b~ dm nmh
H1.fid dmf 200
C
ACQUISITION
sfrq 300.108 temp 20.0
ln H1
dt 4.092 wtf16
sw 48052 proc 131072
fb 6002.4 fn
bs not used
tpwr 8 warr
pw 54 wexp
d1 0.050 wds
tof 867.2 wnt
nt 16
sc 16
gain not used
alock n
FLAGS
i1 n
in n
dp y
SP DISPLAY
wp -208.1
vp 4201.1
vs 108
sc 0
wc 250
hzmm 15.80
is 83.90
rf1 2839.2
rfp 2181.8
lh 20
ins 1.000
nm
ph



CH-II-221b-C13

exptl std13c

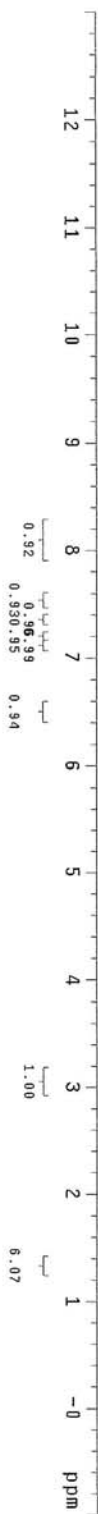
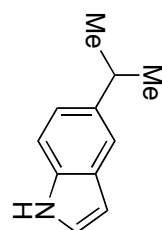
SAMPLE DEC. & VT
date Mar 2 2009 dfrq 300.107
solvent Mar CDC13 dn H1
file /data/export/~ dpwr 39
home/stibuch/BChan~ dof 0
/mhat/CH-II-221b~ dm yyy
w
C13.fid dnm 11000
sfrq 75.471 dnt
ACQUISITION temp 20.0
tn 1.500 sb PROCESSING 20.0
nt 6.7874 sbs -1.500
nd 22624.4 wfile
sw 12400 proc ft
bs 16 fn 262144
tpwr 55
pw 10.0 wprt
dl 0.500 wexp
tof 2264.8 wds
rt 258 wnt
atlock n
gain not used
flags
i1 n
in n
dp y
SP DISPLAY
wp 746.2
vp 18110.31
wc 250
sc 0
hzmm 72.44
is 500.00
rf1 7326.5
rfp 5827.9
th 9
ins 100.000
at no ph

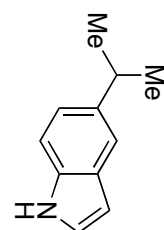


CH-II-180

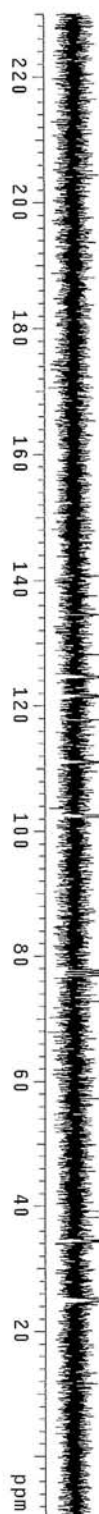
expt stdIn

SAMPLE DEC. & VT
date Mar 2 2009 dfrq 300.107
solvent CDC13 dn H1
file /data/export/~ dpwr 30
home/stbuck/Bcchan~ dof 0
/mhat/CH-II-180-H~ dm mm
1.fid dnm 200
ACQUISITION temp 20.0
sfrq 300.108
in H1
ns 4.003 wfile
np 48052 proc ft
sw 6002.4 fn 131072
fb not used
bs 8 werr
tpwr 54 wexp
pw 8.0 wbs
dl 0.050 wnt
tof 857.7
ct 16
cl 16
atlock n
gain not used
flags
i1 n
in n
dp y
DISPLAY
sp -302.8
wp 4204.8
vp 420 160
wc 0
sc 250
hzmm 16.82
is 58.68
rf1 2839.6
rfp 2181.8
th 20
tms 1.000
nm
ph





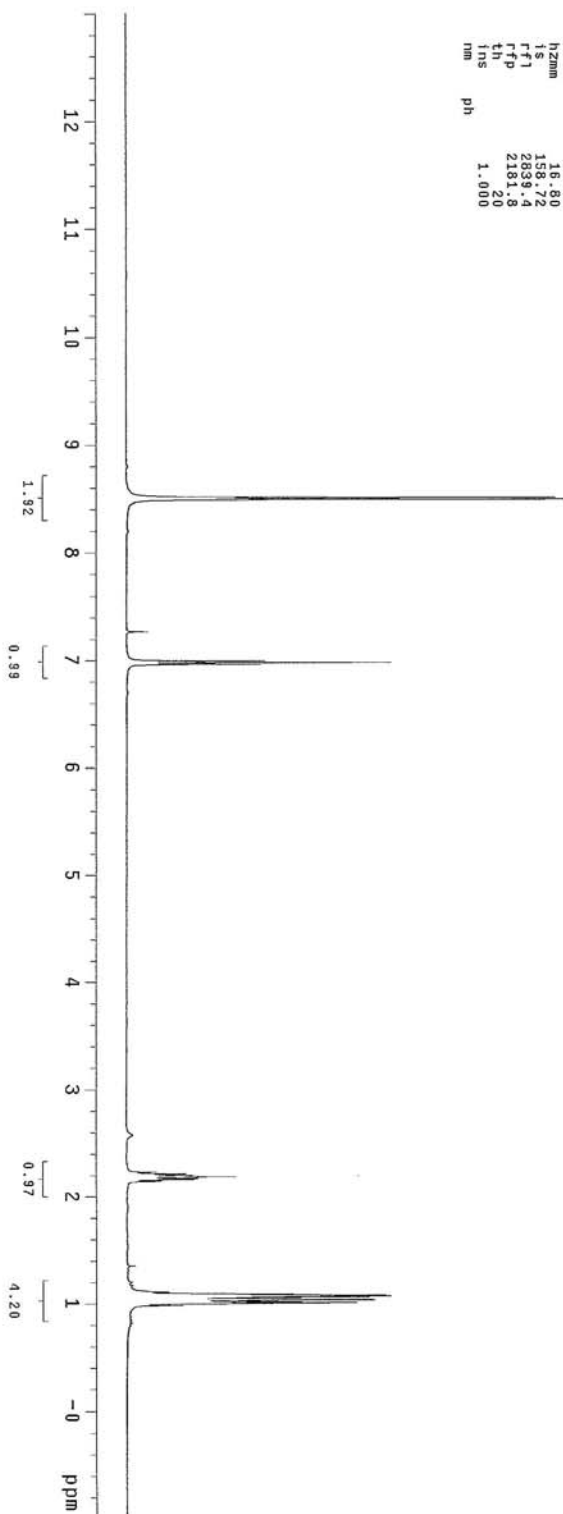
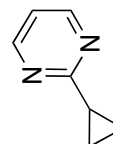
CH-II-180
 exptl std13c
 SAMPLE DEC. & VT
 date Feb 22 2003 dfrq 300.107
 solvent CDC13 dn H1
 file /data/export/~ dpwr 39
 home/sibuch/BChanw dof 0
 /mhat/CH-II-180-C~ dm yyy
 13.fid dm W
 ACQUISITION 75.471 temp 11000
 sfrq 111.111 temp PROCESSING 20.0
 an 1.500 sb -1.500
 nt 67874 sds -1.500
 sw 22624.4 wfile
 fb 12400 proc 262144
 bs 16 fn
 tpwr 55
 pw 10.0 werr
 dl 0.500 wexp
 lof 2264.8 wds
 nt 256 wnt
 gain not used
 flags
 i1 n
 in n
 dp y
 SP DISPLAY 748.8
 vpw 18110.7
 vpe 74
 wc 0
 sc 250
 hzmm 72.44
 is 500.00
 rfl 7330.1
 rfp 5827.9
 tns 100.000
 ph
 at



CH-II-196

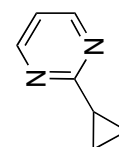
expl stdIn

SAMPLE DEC. & VT
date Feb 22 2009 dfreq 300.107
solvent CDC13 dn H1
file /data/export/~ dpwr 30
home/stbuch/Bcchanv dof 0
/mrhat/CH-II-196-Hv dm mn
1. fid dnm 200
c
ACQUISITION 300.108 temp PROCESSING 20.0
sfrq 300.108
in 4.003 wfile
at 48052
nd 6002.4
sw 131072
fb not used
bs 4 warr
tpwr 54 wexp
pw 8.0 wds
d1 0.050 wnt
tof 867.7
nt 8
ct 8
alock n
gain not used
flags
i1 n
in n
dp y
SP DISPLAY 228.3
vpp 4201.73
vc 0
wc 250
hzmm 16.60
is 158.72
rf1 2839.4
rfp 2181.8
th 20
rms 1.000
ph

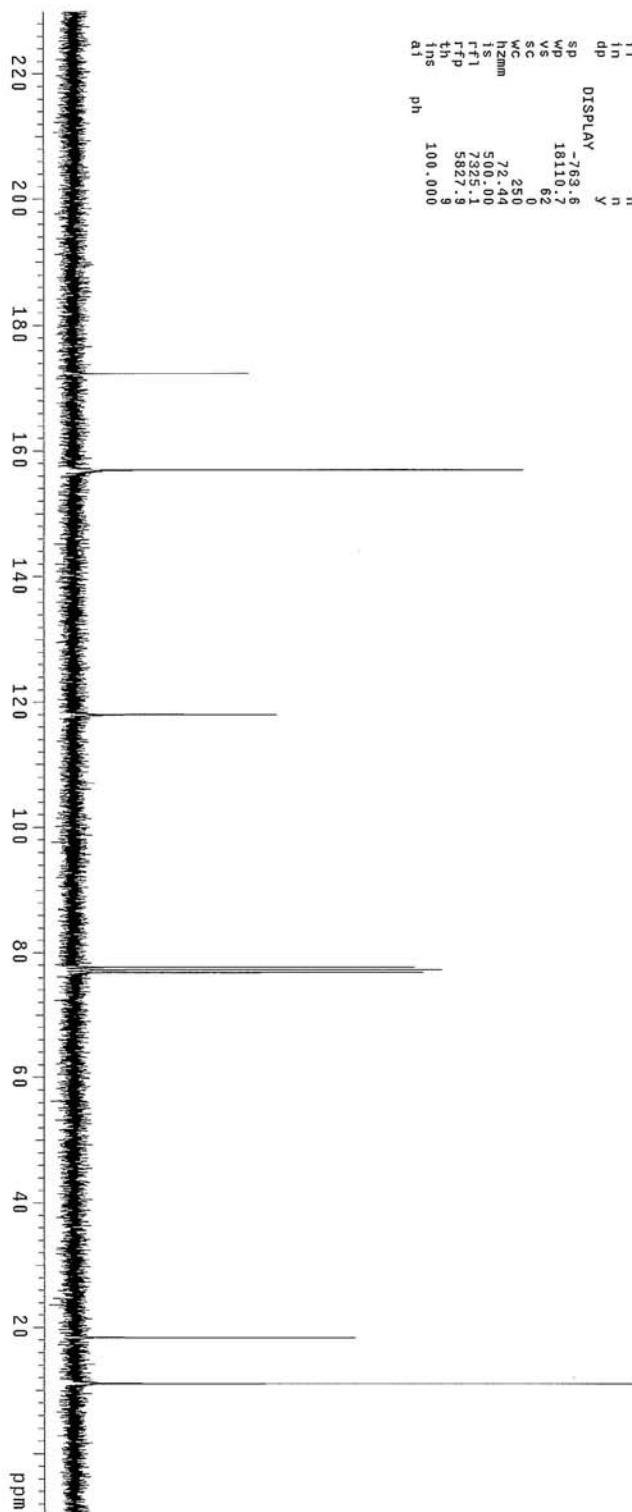


CH-II-196-C13

expl std13c



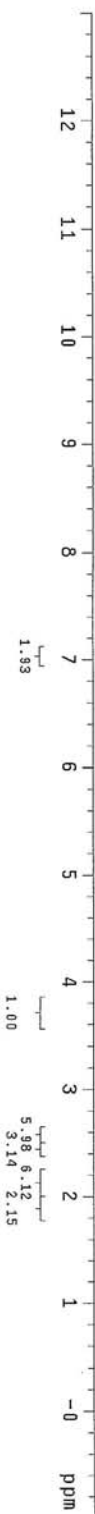
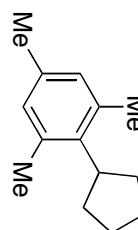
SAMPLE DEC. & VT
date Feb 22 2009 dfrq 300.107
solvent CDC13 dn H1
file /data/export/~ dpwr 39
home/stbuck/BChan~ dof 0
/mrhat/CH-II-196-C~ dm yyy
w
13.fid dnm 11000
ACQUISITION 75.471 temp 20.0
sfrq 11000
dn 1.500 sb
ns 67874 sbs -1.500
sw 22624.4 wfile
fb 12400 proc
bs 16 fn 262144
tpwr 55
pw 10.0 warr
d1 0.500 wexp
lof 2264.0 wds
te 256 wnt
ct 256
alock n
gain not used
FLAGS
i1 n
in n
dp y
SP DISPLAY 763.6
wp 18110.62
vp 0
vc 250
wc 72.44
hzmm 500.00
is 7325.1
rf1 5827.9
rfp 100.000
th
ins
at pH



CH-II-182

expl stdin

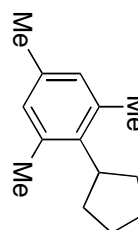
SAMPLE DEC. & VT
date Feb 23 2009 dfreq 300.107
solvent dm H1
file /data/export/~ dpwr 30
home/stbuch/Bcchanv dof 0
/mrhat/CH-II-182-Hv dm mm
1.fid dnm 200
ACQUISITION temp 20.0
sfrq 300.108
tn 4.003 vfile
nt 48052 proc ft
sw 6002.4 fn 131072
fb not used
bs 4 warr
tpwr 54 wexp
pw 8.0 wds
dl 0.050 wnt
tof 867.7
nt 8
st 8
alock n
gain not used
flags n
i1 n
in n
dp y
SP DISPLAY
wp -287.9
vp 4281.1
vs 106
sc 0
wc 250
hzmm 16.80
is 79.81
rf1 2639.0
rfp 2181.8
th 20
lms 1.000
nm
ph



CH-II-182-C13

exp1 std13c

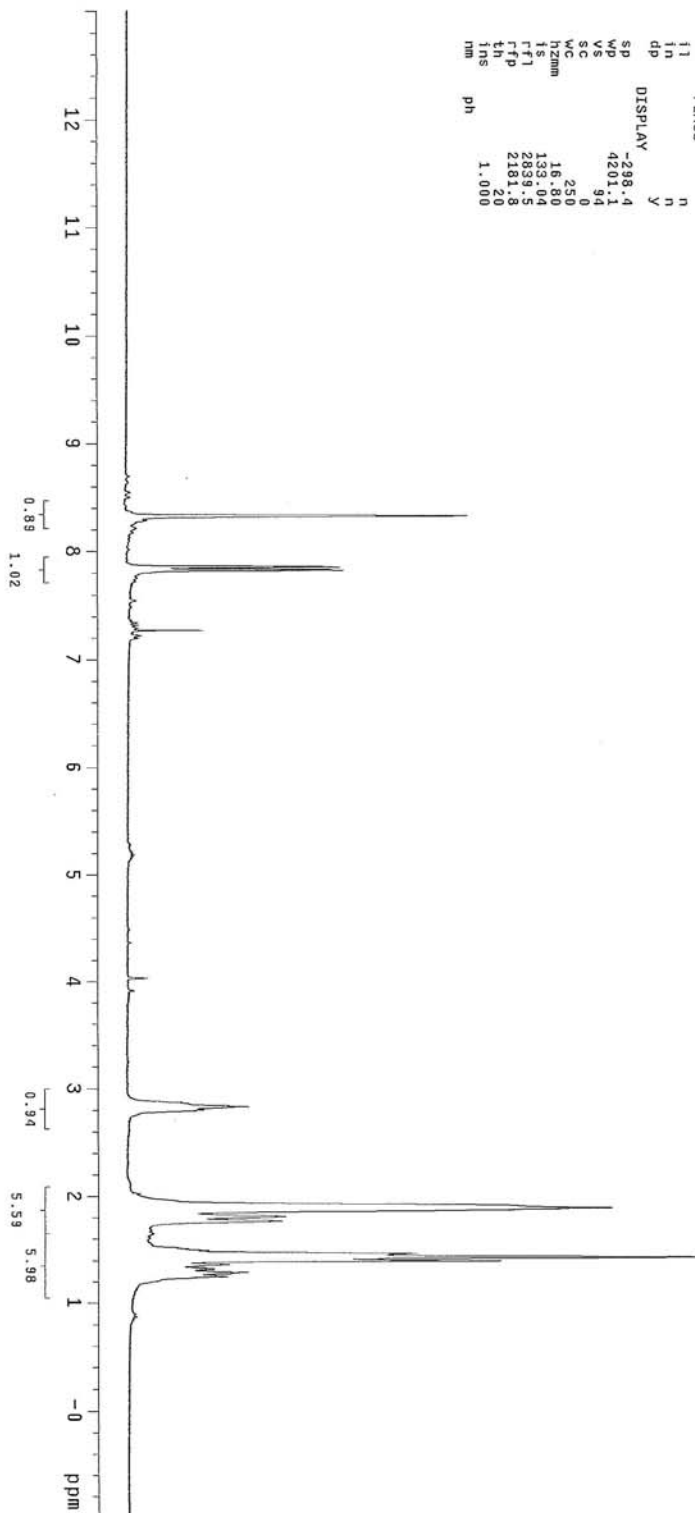
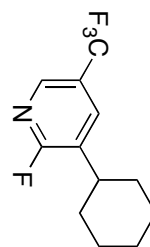
SAMPLE DEC. & VT
date Feb 23 2009 dfreq 300.107
solvent CDC13 dn H1
file /data/export/~ dpwr 39
home/stbuch/Bcchan~ dof 0
/mhat/CH-II-182-C~ dm yyy
13.fid dnm w
ACQUISITION 75.471 temp 11000
IN 1.500 sb PROCESSING 20.0
NO 67874 sbs -1.500
SW 22624.4 wfile
fb 12400 proc ft
bs 16 fn 262144
tpwr 55
pw 10.0 warr
dl 0.500 wexp
tof 2264.8 wds
nt 208 wnt
rt 208
alock n
gain not used
FLAGS
il n
in n
dp y
SP DISPLAY 756.2
wp 1810.7
vp 16
wc 250
sc 0
hzmm 72.44
is 500.00
rf1 7338.5
rfp 5827.9
th 9
tms 100.000
at1 ph



CH-II-255

expt std1h

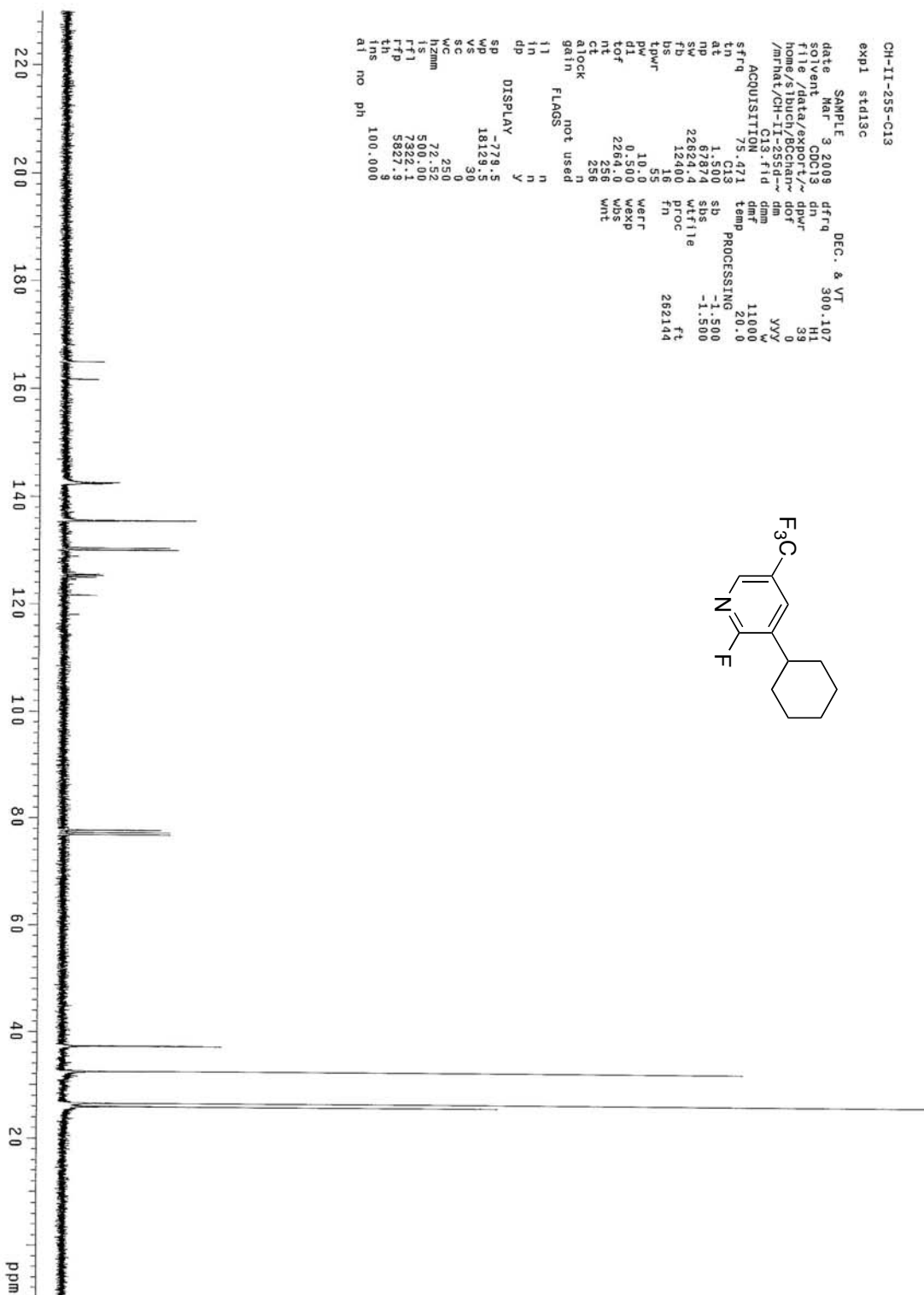
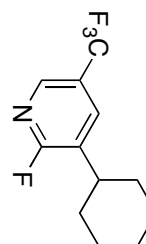
SAMPLE DEC. 8 VT
date Feb 23 2009 dfrq 300.107
solvent CDCl3 dn H1
file /data/export/~ dpvr 30
home/sibuch/bcchan~ dof 0
/mrhat/CH-II-255-H~ dm nm
1.fid dm C
ACQUISITION 300.108 temp 20.0
sfrq 300.108
t1 4.003 wfile
at 48052 proc ft
sw 6002.4 fn 131072
fb not used
bs 4 weff
tpwr 54 wbs
pw 8.0 wexp
d1 0.050 wnt
tof 867.7
nt 8
ct 8
clock n
gain not used
flags
i1 n
in n
dp y
DISPLAY
sp -298.4
ap 4201.4
vp 90
wc 250
h2mm 16.80
ls 133.04
tfl 2839.5
tff 2181.8
th 20
ins 1.000
ph



CH-II-255-C13

expl std13c

SAMPLE DEC. & VT
date Mar 3 2009 dfrq 300.107
solvent CDCl3 dh H1
file /data/export/~ dbrw 39
home/sdcl1255-11-05-08-01
/mnt/CH-11-0255-11-05-08-01
C13 fid yyy
ACQUISITION C13 fid
sfrq 75.471 temp 20.0
th C13 sb PROCESSING
at 1.500 sb -1.500
np 67874 sbs -1.500
sw 22824.4 wfile
fb 12400 proc ft
td 1.8 fn 262144
tpr 1.8
pw 10.0 werr
d1 0.500 wexp
tof 2264.0 wbs
nt 256 wnt
ct 256
atlock n
gain not used
flags
i1 n
in n
dp y
DISPLAY
sp -778.5
wp 18129.5
vs 30
sc 0
wc 250
wzmm 72.32
rfi 50.32
rfp 7922.1
th 5827.9
ins 9
al no ph 100.000



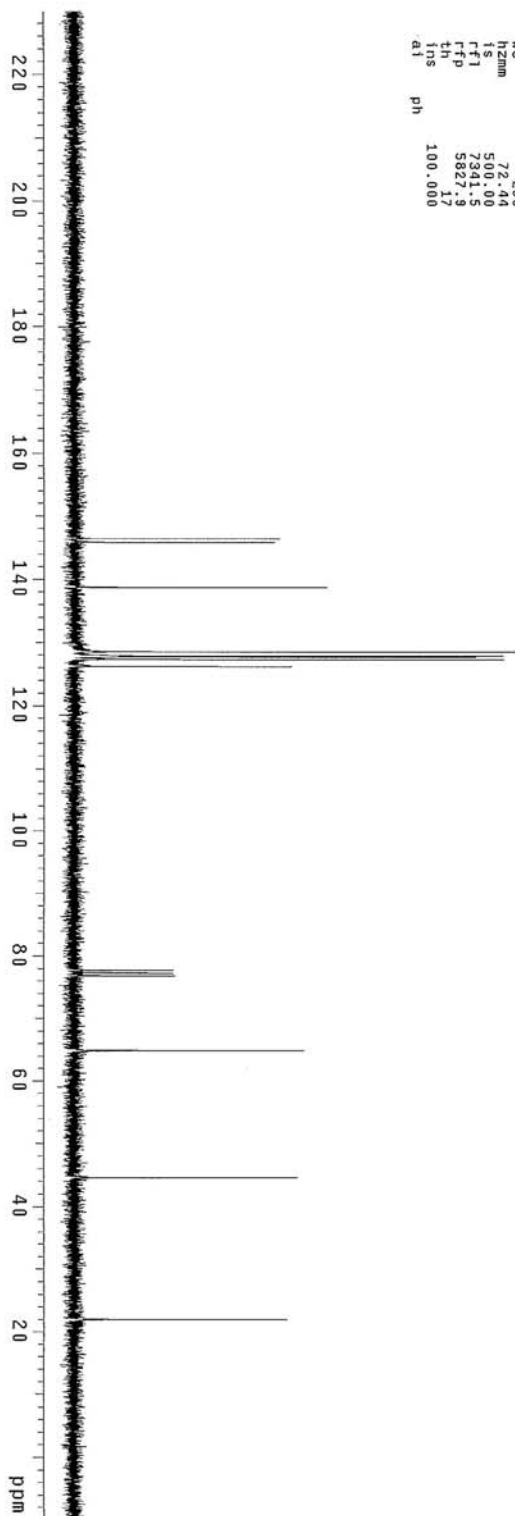
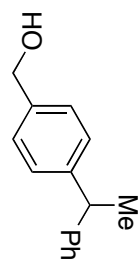
CH-III-8

exp2 stdh

SAMPLE DEC. & VT
date Mar 13 2009 dfrq 300.107
solvent CDCl3 dn H1
file /data/export/~ dpr 30
home/sibuch/BCchan- dof 0
/mha/CH-III-8-H1- dm nmh
ACQUISITION .fid nmh
sfrq 300.108 temp PROCESSING 20.0
dn H1 wtfile ft
at 4.003
np 48052 proc 131072
sw 6002.4 fn
fd not used
ds 4 weff
bwr 54 wds
pw 8.0 wnt
d1 0.050
tof 857.7
nt 32
ct 8
atlock n
gain not used
f1 n
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CH-III-8-C13
exp2 std13c

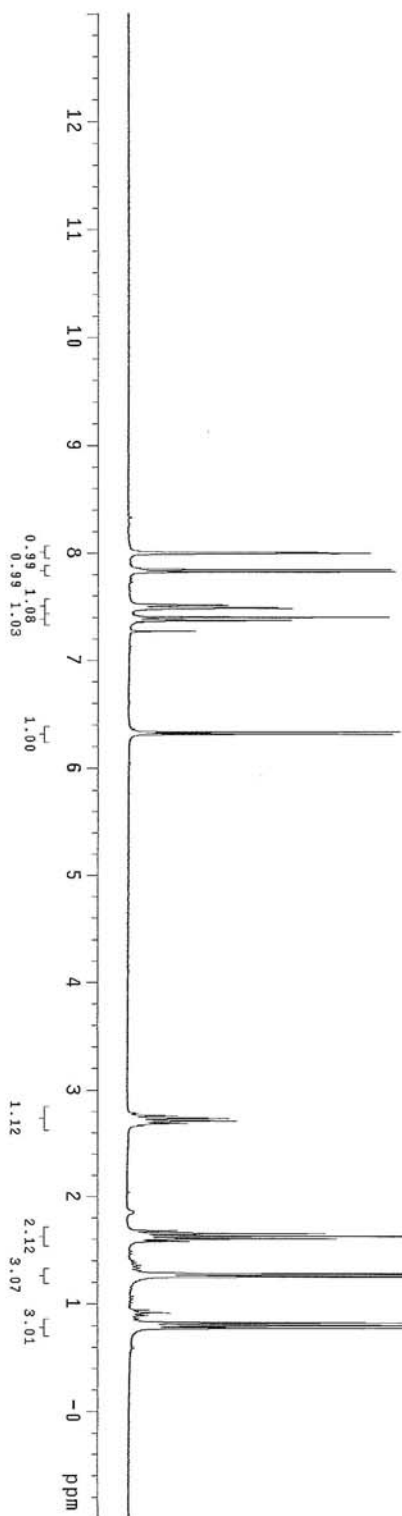
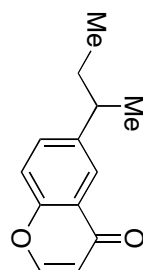
SAMPLE DEC. & VT
date Mar 13 2009 dfrq 300.107
solvent CDCl3 dn .h1
file /data/export/~ dpwr 39
home/sibuch/8Cchar~ dof 0
/mrhat/CH-III-8-C1~ dm yyy
w
ACQUISITION
sfreq 75.471 temp 11000
in C13 sb PROCESSING 20.0
at 1.500 sb -1.500
nu 4.282 sb -1.500
sp 22624.4 wtfie
fb 12400 proc ft
bs 16 fn 262144
tpwr 55
pw 10.0 weff
d1 0.500 wexp
tof 2264.0 wbs
nt 256 wnt
clock 64
gain not used
flags
i1 n
i1 n
in n
dp y
DISPLAY
sp -761.2
wp 18110.7
vc 26
sc 0
wc 250
hzmm 72.44
ts 500.00
rf1 7341.5
rfp 5827.9
th 17
ins 100.000
at ph



CH-II-224

expt std/h

SAMPLE
date Feb 23 2009 DEC. & VT
solvent CDC13 dn H1
file /data/export/~ dpwr H1
home/stbuch/Bcchanv dof 0
/mhat/CH-II-224-Hv dm mm
1.fid dnm 200
ACQUISITION 300.108 temp 20.0
sfrq 300.108 temp PROCESSING
nu 4.003 vfile
np 48052 proc ft
sw 6002.4 fn 131072
fb not used
bs 4 warr
tpwr 54 wexp
pw 8.0 wds
dl 0.050 wnt
tof 867.7
ct 8
cl 8
a1ock n
gain not used
i1 n
in n
dp y
DISPLAY
sp -288.5
vp -428.1
wc 116
sc 0
h2am 16.80
is 106.54
rf1 2839.5
rfp 2181.8
th 20
tms 1.000
nm
ph



CH-II-224-C13

exp1 std13c

SAMPLE DEC. & VT
date Feb 23 2009 dfrq 300.107
solvent CDCl3 dn H1
file /data/export/~ dnr 39
home/sibuch/8Cchar~ dm 0
/mrhat/CH-II-224-C~ yyy w
13.fid dm 11000
ACQUISITION 73.471 temp PROCESSING 20.0
sfrq 133 sb -1.500
a1 1.500 sb
nd 67874 sbs
sw 22624.4 wfile
fb 12400 proc
bs 16 fn 262144
lpwr 55
pw 10.0 werr
dl 0.500 wexp
tof 2264.0 wos
n1 3558 wnt
ct 256
atlock n
gain not used
flags
i1 n
in n
dp y
SP DISPLAY
sp -762.2
sfrq 18110.7
ve 76
wc 0
sc 250
hzmm 72.44
ls 500.00
rf1 7323.7
rfp 5827.8
th 1.000
at ph

