Nickel-Catalyzed Cross Couplings of Benzylic Ammonium Salts and Boronic Acids: Stereospecific Formation of Diarylethanes via C–N Bond Activation

Prantik Maity, Danielle M. Shacklady-McAtee, Glenn P. A. Yap, Eric R. Sirianni, Mary P. Watson*

Department of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716

mpwatson@udel.edu

Supporting Information

General Information

Reactions were performed either in a N_2-atmosphere glovebox in oven-dried 1-dram vials with Teflon-lined caps or in oven-dried round-bottomed flasks unless otherwise noted. Flasks were fitted with rubber septa, and reactions were conducted under a positive pressure of N_2. Stainless steel syringes or cannulae were used to transfer air- and moisture-sensitive liquids. Flash chromatography was performed on silica gel 60 (40-63 μm, 60Å) unless otherwise noted. Select compounds were purified by flash chromatography on silica gel (5-20 μm) as needed. Thin layer chromatography (TLC) was performed on glass plates coated with silica gel 60 with F254 indicator. Commercial reagents were purchased from Sigma Aldrich, Acros, Fisher, Strem, TCI, Combi Blocks, Alfa Aesar, or Cambridge Isotopes Laboratories and used as received with the following exceptions: toluene, CH_2Cl_2, dioxane, and Et_2O were dried by passing through drying columns.[1] Toluene was then degassed by sparging with N_2 and stored over activated 4Å MS in a N_2-atmosphere glovebox. Anhydrous K_3PO_4 was purchased from Acros and used as received. MeOTf was purchased from TCI, America, and used as received. $CDCl_3$ was stored over oven-dried potassium carbonate. Proton nuclear magnetic resonance (^{1}H NMR) spectra and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on both 400 MHz and 600 MHz spectrometers. Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and are referenced to residual protium in the NMR solvent ($CHCl_3$ = δ 7.28; $(CD_3)_2CO$ = δ 2.07). Chemical shifts for carbon are reported in parts per million downfield from tetramethylsilane and are referenced to the carbon resonances of the solvent ($CDCl_3$ = δ 77.07; $(CD_3)_2CO$ = δ 28.94) Data are represented as follows: chemical shift, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet, dd = doublet of doublets, h = heptet), coupling constants in Hertz (Hz), integration. Infrared (IR) spectra were obtained using FTIR spectrophotometers with material loaded onto a NaCl plate. The mass spectral data were obtained at the University of Illinois, Urbana–Champagne, mass spectrometry facility and the University of Delaware mass spectrometry facility. Optical rotations were measured using a 2.5 mL cell with a 1 dm path length. Melting points were taken on a Stuart SMP10 instrument.

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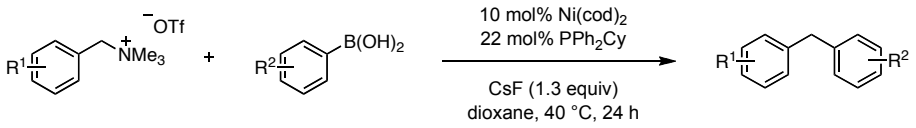
[1] Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518.

Dimethyl benzyl amines were prepared either from the benzyl amines using Escheweiler–Clarke conditions[2] or via reductive amination of the benzaldehyde or acetophenone derivative.[3] It has been reported that epimerization does not occur under the Escheweiler–Clarke conditions.[4] Precursors for racemic ammonium triflates were synthesized via reductive amination of the corresponding acetophenone derivatives.

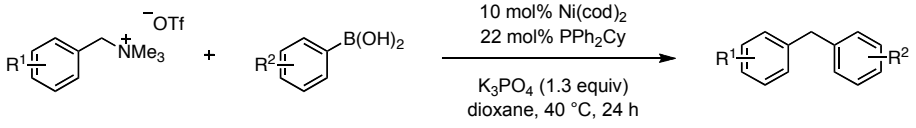
Cross-Coupling of Benzyl Ammonium Triflates to Give Diaryl Methanes

General Procedure A: CsF as Base



In a N_2-atmosphere glovebox, $Ni(cod)_2$ (10 mol %), PPh_2Cy (22 mol %), and CsF (1.3 equiv) were weighed into a 1-dram vial. Ammonium triflate (1.0 equiv) and boronic acid (1.2 equiv) were added, followed by dioxane (0.33 M). The vial was capped with a Teflon-lined cap and removed from the glovebox. The mixture was stirred for 24 h at 40 °C. The reaction mixture was then diluted with Et_2O (1.5 mL) and filtered through a plug of silica gel, which was rinsed with Et_2O (10 mL). The filtrate was concentrated and then purified by silica gel chromatography to give the diarylmethane product.

General Procedure B: K_3PO_4 as Base



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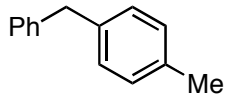
[2] Icke, R. N.; Wisegarver, B. B.; Alles, G. A. *Org. Synth.* **1955**, *Coll. Vol. 3*, 723.

[3] The reductive aminations were carried out according to literature procedure, except that Me_2NH was formed in situ from $Me_2N{\cdot}HCl$ and Et_3N. See: Bhattacharyya, S. *Synth. Commun.* **2000**, *30*, 2001.

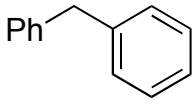
[4] Sunman, C. J.; Farkas, E. *J. Org. Chem.* **1985**, *50*, 1110.

General Procedure B is the same as General Procedure A, except that K_3PO_4 replaces CsF as base. In a N_2-atmosphere glovebox, $Ni(cod)_2$ (10 mol %), PPh_2Cy (22 mol %), and K_3PO_4 (1.3 equiv) were weighed into a 1-dram vial. Ammonium triflate (1.0 equiv) and boronic acid (1.2 equiv) were added, followed by dioxane (0.33 M). The vial was capped with a Teflon-lined cap and removed from the glovebox. The mixture was stirred for 24 h at 40 °C. The reaction mixture was diluted with Et_2O (1.5 mL) and filtered through a plug of silica gel, which was rinsed with Et_2O (10 mL). The filtrate was concentrated and then purified by silica gel chromatography to give the diarylmethane product.



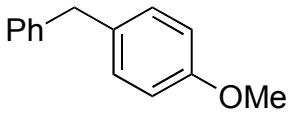
1-Benzyl-4-methylbenzene (2). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **2** (run 1: 43.0 mg, 79%; run 2: 41.0 mg, 81%) as a colorless oil.

Diarylmethane **2** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified as described above to give compound **2** (run 1: 45.0 mg, 84%; run 2: 46.0 mg, 84%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.32 (m, 2H), 7.32 – 7.22 (m, 3H), 7.22 – 7.12 (m, 4H), 4.03 (s, 2H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.5, 138.1, 135.6, 129.2, 128.9, 128.9, 128.5, 126.1, 41.6, 21.1. The spectral data for this compound matches that reported in the literature.[5]



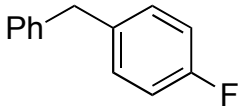
Diphenylmethane (3). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **3** (run 1: 35.0 mg, 70%; run 2: 41.0 mg, 81%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.30 (m, 4H), 7.27 – 7.20 (m, 6H), 4.03 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.1, 129.0, 128.5, 126.1, 42.0. The spectral data for this compound matches that reported in the literature.[6]

[5] Schmink, J. R.; Leadbeater, N. E. *Org. Lett.* **2009**, *11*, 2575.
[6] Kuwano, R.; Yokogi, M. *Org. Lett.* **2005**, *7*, 945.

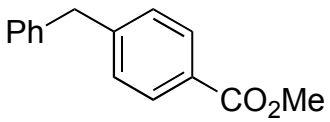


1-Benzyl-4-methoxybenzene (4). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **4** (50.0 mg, 85%) as a colorless oil.

Diarylmethane **4** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified as described above to give compound **4** (run 1: 44.0 mg, 75%; run 2: 33.0 mg, 56%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.30 (m, 2H), 7.27 – 7.21 (m, 3H), 7.18 – 7.11 (m, 2H), 6.92 – 6.84 (m, 2H), 3.98 (s, 2H), 3.83 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.0, 141.6, 133.3, 129.9, 128.8, 128.5, 126.0, 113.9, 55.3, 41.1. The spectral data for this compound matches that reported in the literature.[7]



1-Benzyl-4-fluorobenzene (5). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et3N) to give compound 5 (run 1: 40.0 mg, 71%; run 2: 36.0 mg, 65%; run 3: 44.0 mg, 78%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.30 (m, 2H), 7.30 – 7.13 (m, 5H), 7.07 – 6.95 (m, 2H), 4.00 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.4 (d, $J_{C–F}$ = 245.4 Hz), 141.0, 136.8 (q, $J_{C–F}$ = 3.0 Hz), 130.3 (q, $J_{C–F}$ = 8.1 Hz), 128.9, 128.6, 126.3, 115.3 (q, $J_{C–F}$ = 21.2 Hz), 41.1). The spectral data for this compound matches that reported in the literature.[8]

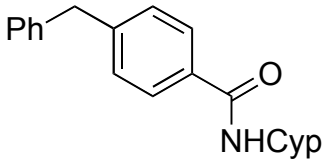


1-Methyl 4-benzylbenzoate (6). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (5% acetone/hexanes with 0.5% Et_3N) to give compound **6** (48.0 mg, 71%) as a colorless oil.

Diarylmethane **6** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified as described above to give compound **6** (15.0 mg, 22%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 7.96 (m, 2H), 7.39 – 7.17 (m, 7H),

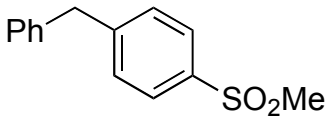
[7] Henry, N.; Enguehard-Gueiffier, C.; Thery, I.; Gueiffier, A. *Eur. J. Org. Chem.* **2008**, *28*, 4824.
[8] Chen, C. R; Biradar, D. B; Gau, H. M; Zhou, S. *Adv. Synth. Cat.* **2010**, *352*, 1718.

4.07 (s, 2H), 3.93 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 146.6, 140.2, 129.9, 129.0, 128.6, 128.1, 126.4, 52.1, 41.9; ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 166.2, 147.1, 140.6, 129.5, 129.0, 128.9, 128.5, 128.1, 126.2, 51.4, 41.4.[9] The spectral data for this compound matches that reported in the literature.[10]



4-Benzyl-*N*-cyclopentylbenzamide (7). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (10:15:75 acetone/dichloromethane/hexanes with 0.5% Et_3N) to give compound **7** (run 1: 39.4 mg, 47%; run 2: 42.8 mg, 51%) as a white solid.

Diarylmethane **7** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified as described above to give compound **7** (57 mg, 67%) as a white solid (mp 145–149 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.66 (m, 2H), 7.35 – 7.27 (m, 2H), 7.27 – 7.20 (m, 3H), 7.20 – 7.15 (m, 2H), 6.25 – 6.08 (m, 1H), 4.40 (h, *J* = 7.0 Hz, 1H), 4.03 (s, 2H), 2.17 – 2.02 (m, 2H), 1.82 – 1.57 (m, 4H), 1.49 (ddt, *J* = 12.9, 6.3, 1.8 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 144.6, 140.4, 132.8, 129.1, 128.9, 128.6, 127.1, 126.3, 51.65, 41.7, 33.2, 23.8; FTIR (NaCl/thin film) 3446, 2959, 2867, 2360, 2339, 1635, 1540 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{19}H_{21}ON$: 279.1623, found: 279.1631.

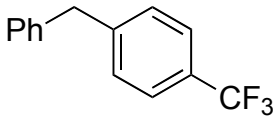


1-Benzyl-4-(methylsulfonyl)benzene (8). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (10:20:70 acetone/dichloromethane/hexanes with 0.5% Et_3N) to give compound **8** (run 1: 53.0 mg, 72%; run 2: 59.0 mg, 79%) as a white crystalline solid.

Diarylmethane **8** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified as described above to give compound **8** (run 1 74.0 mg, quantitative; run 2: 73.9 mg, quantitative) as a white crystalline solid (mp

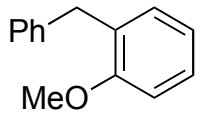
[9] Although two ^{13}C NMR peaks are coincident when $CDCl_3$ is used as solvent, all eleven ^{13}C NMR peaks are seen when $(CD_3)_2CO$ is used as solvent.
[10] Srimani, D.; Bej, A.; Sarkar, A. *J. Org. Chem.* **2010**, *75,* 4296.

67–72 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.83 (m, 2H), 7.46 – 7.38 (m, 2H), 7.38 – 7.30 (m, 2H), 7.30 – 7.23 (m, 1H), 7.23 – 7.18 (m, 2H), 4.09 (s, 2H), 3.05 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.8, 139.5, 138.3, 129.8, 129.0, 128.8, 127.6, 126.7, 44.6, 41.8; FTIR (NaCl/thin film) 3442, 3027, 2926, 1647, 1596, 1303, 1148, 1090, 957 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{14}H_{14}O_2S$: 246.0715, found: 246.0717.



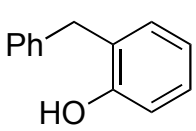
1-Benzyl-4-(trifluoromethyl)benzene (9). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **9** (59.0 mg, 83%) as a colorless oil. Diarylmethane **9** was also prepared via General Procedure A (CsF as base) on a 0.40 mmol scale. The crude material was purified as described above to give compound **9** (89.0 mg, 94%) as a colorless oil.

Diarylmethane **9** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified as described above to give compound **9** (run 1: 59.0 mg, 83%; run 2: 52.0 mg, 73%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.1 Hz, 2H), 7.39 – 7.31 (m, 4H), 7.31 – 7.25 (m, 1H), 7.25 – 7.20 (m, 2H), 4.08 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.2 (q, $J_{C–F}$ = 1.0 Hz), 140.0, 129.2, 129.0, 128.7, 128.5 (q, $J_{C–F}$ = 32.3 Hz), 126.5, 125.4 (q, $J_{C–F}$ = 4.0 Hz), 124.3 (q, $J_{C–F}$ = 272.7 Hz), 41.7. The spectral data for this compound matches that reported in the literature.[11]

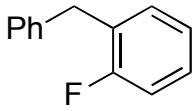


1-Benzyl-2-methoxybenzene (10). Prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **10** (49 mg, 83%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.20 (m, 6H), 7.15 (dd, J = 7.4, 1.7 Hz, 1H), 7.02 – 6.88 (m, 2H), 4.06 (s, 2H), 3.88 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.4, 141.1, 130.4, 129.7, 129.0, 128.3, 127.5, 125.8, 120.5, 110.4, 55.4, 35.9. The spectral data for this compound matches that reported in the literature.[7]

[11] Bedford, R. B.; Huwe, M.; Wilkinson, M. C. *Chem. Comm.* **2009**, *5*. 600.

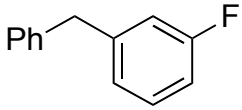


2-Benzylphenol (11). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (15–100% dichloromethane/hexanes with 0.5% Et_3N) to give compound **10** (30.0 mg, 65%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.22 (m, 5H), 7.21 – 7.13 (m, 2H), 6.94 (td, *J* = 7.5, 1.2 Hz, 1H), 6.85 – 6.78 (m, 1H), 4.83 (s, 1H), 4.05 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.7, 139.9, 131.0, 128.7, 128.7, 127.9, 127.0, 126.4, 121.0, 115.7, 36.4. The spectral data for this compound matches that reported in the literature.[1]



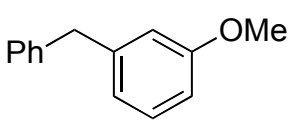
1-Benzyl-2-fluorobenzene (12). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **12** (51.0 mg, 91%) as a colorless oil.

Diarylmethane **12** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified as described above to give compound **12** (run 1: 54.0 mg, 98%; run 2: 51.2 mg, 91%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.31 (m, 2H), 7.31 – 7.16 (m, 5H), 7.15 – 7.04 (m, 2H), 4.07 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.0 (d, $J_{C–F}$ = 245.4 Hz), 139.9, 131.1 (d, $J_{C–F}$ = 4.0 Hz), 128.8, 128.6, 128.2, 128.0 (d, $J_{C–F}$ = 8.1 Hz), 126.3, 124.1 (d, $J_{C–F}$ = 4.0 Hz), 115.4 (d, $J_{C–F}$ = 22.2 Hz), 34.9 (d, $J_{C–F}$ = 3.0 Hz); ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 160.9 (d, $J_{C–F}$ = 245.4 Hz), 140.1, 131.3 (d, $J_{C–F}$ = 4.0 Hz), 128.6 (d, $J_{C–F}$ = 1.0 Hz), 128.4, 128.20 (d, $J_{C–F}$ = 8.1 Hz), 128.19 (d, $J_{C–F}$ = 15.2 Hz), 126.1, 124.3 (d, $J_{C–F}$ = 2.0 Hz), 115.2 (d, $J_{C–F}$ = 22.2 Hz), 34.4 (d, $J_{C–F}$ = 3.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ –117.8; LRMS (EI+) $[M]^+$ calculated for $C_{13}H_{11}F$: 186.1, found: 186.1.

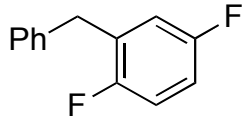


1-Benzyl-3-fluorobenzene (13). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **13** (run 1: 39 mg, 70%; run 2: 43 mg, 77%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.21 (m, 6H), 7.03 (ddd, *J* = 7.6, 2.0, 1.0 Hz, 1H), 6.98 – 6.89 (m, 2H), 4.02 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0 (d, $J_{C–F}$ = 246.4 Hz), 143.7 (d, $J_{C–F}$ = 7.1 Hz), 140.3, 129.9 (d, $J_{C–F}$ = 8.1 Hz), 129.0, 128.6, 126.4, 124.6 (d, $J_{C–F}$ = 3.0 Hz), 115.8 (d, $J_{C–F}$ = 21.2 Hz), 113.0 (d, $J_{C–F}$ = 20.2 Hz), 41.7 (d, $J_{C–F}$ = 2.0 Hz); FTIR (NaCl/thin film) 3027, 2926, 1647, 1596, 1494, 1408,

1303, 1148, 1090, 957 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{13}H_{11}F$: 186.0845, found: 186.0846.

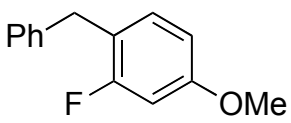


1-Benzyl-3-methoxybenzene (14). Prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **14** (49.0 mg, 83%) as a colorless oil: ^1H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.31 (m, 2H), 7.31 – 7.21 (m, 4H), 6.85 (dt, *J* = 7.5, 1.2 Hz, 1H), 6.83 – 6.79 (m, 2H), 4.02 (s, 2H), 3.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 142.8, 141.0, 129.5, 129.0, 128.5, 126.2, 121.4, 114.8, 111.3, 55.2, 42.0. The spectral data for this compound matches that reported in the literature.[10]



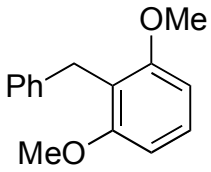
2-Benzyl-1,4-difluorobenzene (15). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **15** (run 1: 55.0 mg, 90%; run 2: 58.6 mg, 96%) as a colorless oil.

Diarylmethane **15** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified as described above to give compound **15** (run 1: 61.5 mg, quantitative; run 2: 60.0 mg, 98%) as a colorless oil: ^1H NMR (400 MHz, $CDCl_3$) δ 7.34 (dd, *J* = 8.0, 6.6 Hz, 2H), 7.30 – 7.22 (m, 3H), 7.02 (td, *J* = 9.0, 4.5 Hz, 1H), 6.94 – 6.79 (m, 2H), 4.00 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9 (dd, J_{C-F} = 184.8, 3.0 Hz), 156.5 (dd, J_{C-F} = 180.8, 2.0 Hz), 139.0, 129.9 (dd, J_{C-F} = 19.2, 8.1 Hz), 128.9, 128.7, 126.6, 117.2 (dd, J_{C-F} = 24.2, 5.1 Hz), 116.2 (dd, J_{C-F} = 25.3, 9.1 Hz), 114.2 (dd, J_{C-F} = 24.2, 8.1 Hz), 34.8 (dd, J_{C-F} = 2.0, 2.0 Hz); FTIR (NaCl/thin film) 3064, 3030, 2926, 2360, 2342, 1496, 1455, 1212, 957 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{13}H_{10}F_2$: 204.0751, found: 204.0754.



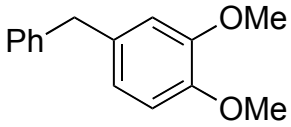
1-Benzyl-2-fluoro-4-methoxybenzene (16). Prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **16** (51.2 mg, 79%) as a colorless oil: ^1H NMR (400 MHz, $CDCl_3$) δ 7.28

(s, 2H), 7.26 – 7.16 (m, 3H), 7.06 (t, J = 8.4 Hz, 1H), 6.69 – 6.60 (m, 2H), 3.95 (s, 2H), 3.80 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.3 (d, J_{C-F} = 245.4 Hz), 159.3 (d, J_{C-F} = 11.1 Hz), 140.3, 131.2 (d, J_{C-F} = 7.1 Hz), 128.7, 128.5, 126.1, 119.9 (d, J_{C-F} = 16.2 Hz), 109.8 (d, J_{C-F} = 3.0 Hz), 101.6 (d, J_{C-F} = 26.3 Hz), 55.5, 34.2 (d, J_{C-F} = 2.0 Hz); FTIR (NaCl/thin film) 3028, 2931, 2837, 1627, 1587, 1508, 1453, 1283, 1151, 1105, 1032, 954 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{14}H_{13}OF$: 216.0950, found: 216.0952.



2-Benzyl-1,3-dimethoxybenzene (17). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (15% dichloromethane/hexanes with 0.5% Et_3N) to give compound **17** (run 1: 61.0 mg, 90%; run 2: 64.0 mg, 94%) as a white solid.

Diarylmethane **17** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified as described above to give compound **17** (run 1: 60.0 mg, 88%; run 2: 63.7 mg, 94%) as a white solid (67–71 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.07 (m, 6H), 6.62 (d, J = 8.3 Hz, 2H), 4.09 (s, 2H), 3.86 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3, 141.9, 128.6, 128.0, 127.3, 125.4, 117.7, 103.8, 55.8, 28.7. The spectral data for this compound matches that reported in the literature.[12]

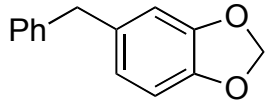


4-Benzyl-1,2-dimethoxybenzene (18). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (15% dichloromethane/hexanes with 0.5% Et_3N) to give compound **18** (66.8 mg, 98%) as a colorless oil.

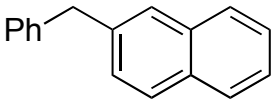
Diarylmethane **18** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified as described above to give compound **18** (run 1: 66.0 mg, 97%; run 2: 68.3 mg, quantitative) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.30 (m, 2H), 7.29 – 7.20 (m, 3H), 6.84 (d, J = 8.0 Hz, 1H), 6.82 – 6.73 (m, 2H), 3.98 (s, 2H), 3.90 (s, 3H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.9, 147.4, 141.4,

[12] Ramachary, D. B.; Kishor, M. *J. Org. Chem.* **2007**, *72*, 5056.

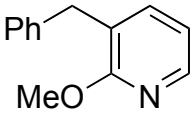
133.7, 128.8, 128.5, 126.1, 120.9, 112.2, 111.1, 55.9, 55.8, 41.5. The spectral data for this compound matches that reported in the literature.[13]



5-Benzylbenzo[*d*][1,3]dioxole (19). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (5% dichloromethane/hexanes with 0.5% Et_3N) to give compound **19** (run 1: 56.7 mg, 83%; run 2: 60.0 mg, 87%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.31 (m, 2H), 7.31 – 7.18 (m, 3H), 6.84 – 6.77 (m, 1H), 6.76 – 6.67 (m, 2H), 5.96 (s, 2H), 3.95 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.8, 145.9, 141.3, 135.0, 128.8, 128.5, 126.2, 121.8, 109.5, 108.2, 100.9, 41.7; FTIR (NaCl/thin film) 3062, 2897, 1488, 1442, 1246, 1188, 1040, 930 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{14}H_{12}O_2$: 212.0837, found: 212.0836.



2-Benzylnaphthalene (20). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **20** (run 1: 51.0 mg, 81%; run 2: 41.0 mg, 63%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.76 (m, 3H), 7.76 – 7.66 (m, 1H), 7.50 (ddd, *J* = 7.1, 4.8, 1.7 Hz, 2H), 7.43 – 7.22 (m, 6H), 4.21 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0, 138.7, 133.6, 132.1, 129.1, 128.6, 128.1, 127.70, 127.68, 127.6, 127.2, 126.2, 126.0, 125.4, 42.2. The spectral data for this compound matches that reported in the literature.[10]

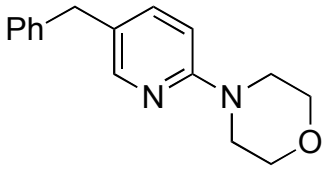


3-Benzyl-2-methoxypyridine (21). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (20% dichloromethane/hexanes with 0.5% Et_3N) to give compound **21** (run 1: 56.0 mg, 93%; run 2: 54.0 mg, 91%) as a colorless oil.

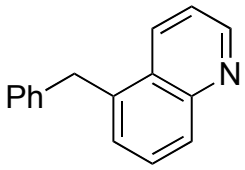
Diarylmethane **21** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified as described above to give compound **21** (run 1: 58.0 mg, 97%; run 2: 61.0 mg, quantitative) as a colorless oil: ^{1}H NMR (400 MHz,

[13] Schmink, J. R.; Leadbeater, N. E. *Org. Lett.* **2009**, *11*, 2575.

$CDCl_3$) δ 8.07 (dd, *J* = 5.0, 1.9 Hz, 1H), 7.38 – 7.18 (m, 6H), 6.82 (dd, *J* = 7.2, 5.0 Hz, 1H), 4.00 (s, 3H), 3.95 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.0, 144.6, 139.6, 138.0, 129.1, 128.5, 126.2, 124.03, 116.8, 53.4, 35.6. The spectral data for this compound matches that reported in the literature.[14]



4-(5-Benzylpyridin-2-yl)morpholine (22). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (30:5:65 dichloromethane/acetone/hexanes with 0.5% Et_3N) to give compound **22** (run 1: 39.0 mg, 51%; run 2: 35.6 mg, 48%; run 3: 37.5 mg, 49%) as a white solid (84–89 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 2.4 Hz, 1H), 7.41 – 7.25 (m, 3H), 7.25 – 7.10 (m, 3H), 6.61 (d, *J* = 8.7 Hz, 1H), 3.94 – 3.77 (m, 6H), 3.54 – 3.43 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.4, 147.8, 141.0, 138.3, 128.7, 128.5, 126.3, 126.2, 107.0, 66.8, 45.9, 38.1; FTIR (NaCl/thin film) 2960, 2919, 2852, 1744, 1607, 1492, 1451, 1403, 1244, 1221, 1120, 1070, 1029, 944 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{16}H_{18}ON_2$: 254.1419, found: 254.1413.

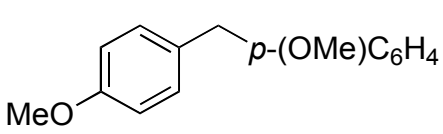


5-Benzylquinoline (23). Prepared via General Procedure A (CsF as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (15:5:5:75 dichloromethane/acetone/Et_3N/hexanes) to give compound **23** (run 1: 38.0 mg, 53%; run 2: 50.8 mg, 77%) as a colorless oil.

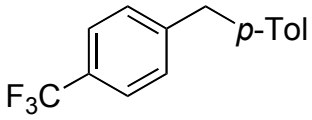
Diarylmethane **23** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified as described above to give compound **23** (run 1: 34.0 mg, 52%; run 2: 34.0 mg, 52%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 – 8.85 (m, 1H), 8.41 – 8.27 (m, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 7.69 (dd, *J* = 8.5, 7.0 Hz, 1H), 7.39 (ddd, *J* = 12.7, 7.8, 2.6 Hz, 2H), 7.33 – 7.26 (m, 2H), 7.26 – 7.15 (m, 3H), 4.47 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.0, 148.9, 140.1, 137.0, 132.7, 129.2, 128.61, 128.57, 128.5, 127.8,

[14] Nagaradja, E.; Chevallier, F.; Roisnel, T.; Jouikov, V.; Mongin, F. *Tetrahedron* **2012**, *14*, 3063.

127.2, 126.3, 120.9, 38.5; FTIR (NaCl/thin film) 3061, 3027, 2922, 2852, 1595, 1559, 1498, 1455, 821, 708; HRMS (EI+) $[M]^+$ calculated for $C_{16}H_{13}N$: 219.1048, found: 219.1048.



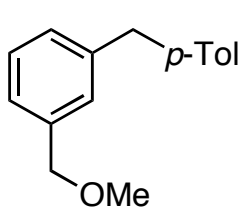
Bis(4-methoxyphenyl)methane (24). Prepared via General Procedure B (K_3PO_4 as base) on a 0.20 mmol scale. The crude material was purified by silica gel chromatography (15% dichloromethane/hexanes with 0.5% Et_3N) to give compound **24** (run 1: 45.0 mg, 98%; run 2: 40.0 mg, 87%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.05 (m, 4H), 6.92 – 6.80 (m, 4H), 3.91 (s, 2H), 3.82 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 133.8, 129.8, 113.9, 55.3, 40.1. The spectral data for this compound matches that reported in the literature.[15]



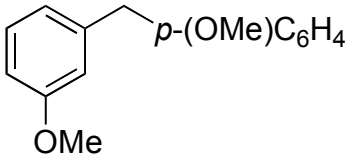
1-Methyl-4-(4-(trifluoromethyl)benzyl)benzene (25). Prepared via General Procedure A (CsF as base) on a 0.20 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **25** (run 1: 43.3 mg, 87%; run 2: 45.0 mg, 90%) as a colorless oil.

Diarylmethane **25** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.20 mmol scale. The crude material was purified as described above to give compound **25** (run 1: 42.0 mg, 84%; run 2: 50.0 mg, quantitative) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, J = 8.1 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.16 (d, J = 8.0 Hz, 2H), 7.11 (d, J = 8.1 Hz, 2H), 4.03 (s, 2H), 2.37 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.6 (q, J_{C-F} = 1.0 Hz), 137.0, 136.1, 129.4, 129.1, 128.8, 128.4 (q, J_{C-F} = 32.3), 125.4 (q, J_{C-F} = 4.0 Hz), 124.3 (q, J_{C-F} = 272.7 Hz), 41.3, 21.1. The spectral data for this compound matches that reported in the literature.[16]

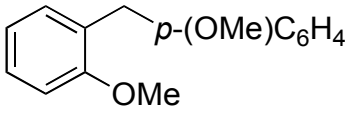
[15] Wilsily, A.; Nguyen, Y.; Fillion, E. *J. Am. Chem. Soc.* **2009**, *131*, 15606.
[16] Bedford, R. B.; Huwe, M.; Wilkinson, M. C. *Chem. Commun*. **2009**, *5*, 600.



1-(methoxymethyl)-3-(4-methylbenzyl)benzene (26). Prepared via General Procedure B (K_3PO_4 as base) on a 0.30 mmol scale. The crude material was purified by silica gel chromatography (10:5:85 dichloromethane/acetone/hexanes) to give compound **26** (60.0 mg, 94%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 7.8 Hz, 1H), 7.24 (d, *J* = 7.8 Hz, 2H), 7.21 – 7.12 (m, 5H), 4.49 (s, 2H), 4.02 (s, 2H), 3.45 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.6, 138.4, 138.1, 135.6, 129.2, 128.9, 128.6, 128.3, 128.3, 125.5, 74.8, 58.2, 41.5, 21.1; FTIR (NaCl/thin film) 3020, 2980, 2921, 2846, 2830, 2734, 1608, 1513, 1488, 1447, 1379, 1193, 1153, 1105, 1022; HRMS (EI+) $[M]^+$ calculated for $C_{16}H_{18}O$: 226.1358, found 226.1351.



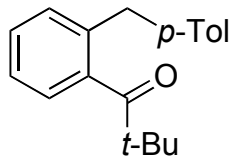
1-Methoxy-3-(4-methoxybenzyl)benzene (27). Prepared via General Procedure B (K_3PO_4 as base) on a 0.20 mmol scale. The crude material was purified by silica gel chromatography (15% dichloromethane/hexanes with 0.5% Et_3N) to give compound **27** (run 1: 46.0 mg, 96%; run 2: 46.0 mg, 96%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.20 (m, 1H), 7.19 – 7.12 (m, 2H), 6.91 – 6.84 (m, 2H), 6.84 – 6.72 (m, 3H), 3.94 (s, 2H), 3.82 (s, 3H), 3.81 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 158.0, 143.2, 133.1, 129.9, 129.4, 121.3, 114.7, 113.9, 111.2, 55.3, 55.2, 41.1. The spectral data for this compound matches that reported in the literature.[17]



1-Methoxy-2-(4-methoxybenzyl)benzene (28). Prepared via General Procedure B (K_3PO_4 as base) on a 0.20 mmol scale. The crude material was purified by silica gel chromatography (15% dichloromethane/hexanes with 0.5% Et_3N) to give compound **28** (run 1: 41.0 mg, 89%; run 2: 44.0 mg, 96%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.15 (m, 3H), 7.10 (dd, *J* = 7.3, 1.7 Hz, 1H), 6.96 – 6.82 (m, 4H), 3.96 (s, 2H), 3.86 (s, 3H), 3.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ

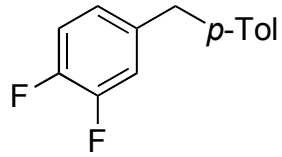
[17] Bedford, R. B.; Gower, N. J.; Haddow, M. F.; Harvey, J. N.; Nunn, J.; Okopie, R. A.; Sankey, R. F. *Angew. Chem. Int. Ed.* **2012**, *51*, 5435.

157.8, 157.3, 133.1, 130.2, 130.1, 129.9, 127.3, 120.5, 113.7, 110.4, 55.4, 55.3, 35.0. The spectral data for this compound matches that reported in the literature.[18]



2,2-Dimethyl-1-(2-(4-methylbenzyl)phenyl)propan-1-one (29). Prepared via General Procedure A (CsF as base) on a 0.20 mmol scale. The crude material was purified by silica gel chromatography (15% dichloromethane/hexanes with 0.5% Et_3N) to give compound **29** (run 1: 53.0 mg, quantitative; run 2: 44.0 mg, 83%) as a colorless oil.

Diarylmethane **29** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.20 mmol scale. The crude material was purified as described above to give compound **29** (run 1: 53.0 mg, quantitative; run 2: 55.3 mg, quantitative) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.14 (m, 4H), 7.09 (m, 4H), 3.89 (s, 2H), 2.34 (s, 3H), 1.23 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 214.7, 140.7, 137.8, 137.3, 135.7, 130.7, 129.2, 129.1, 128.8, 125.3, 124.8, 44.9, 38.6, 27.6, 21.1; FTIR (NaCl/thin film) 2968, 2930, 2869, 1687, 1514, 1477, 1365, 1274, 1194, 964 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{19}H_{22}O$: 266.1671, found: 266.1668.

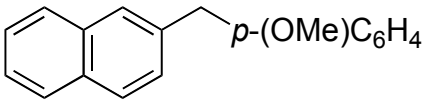


1,2-Difluoro-4-(4-methylbenzyl)benzene (30). Prepared via General Procedure A (CsF as base) on a 0.20 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **30** (run 1: 36.0 mg, 82%; run 2: 34.0 mg, 77%) as a colorless oil.

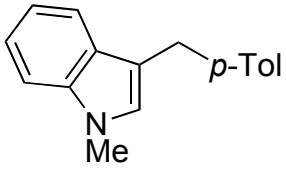
Diarylmethane **30** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.20 mmol scale. The crude material was purified as described above to give compound **30** (run 1: 36.0 mg, 82%; run 2: 42.1 mg, 96%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (d, J = 8.0 Hz, 2H), 7.14 – 7.05 (m, 3H), 6.99 (ddd, J = 11.3, 7.7, 2.2 Hz, 1H), 6.95 – 6.90 (m, 1H), 3.93 (s, 2H), 2.37 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.8 (dd, J_{C-F} = 136.4, 13.1 Hz), 148.3 (dd, J_{C-F} = 135.3, 13.1 Hz), 138.4 (dd, J_{C-F} = 4.0, 4.0 Hz), 137.1, 136.1, 129.4, 128.7, 124.6 (dd, J_{C-F} = 3.0, 3.0 Hz), 117.6 (d, J_{C-F} = 17.2 Hz), 117.0 (d, J_{C-F} = 17.2 Hz), 40.7

[18] Podder, S.; Choudhury, J.; Roy, U. K.; Roy, S. *J. Org. Chem.* **2007**, *72*, 3100.

(d, J_{C-F} = 1.0 Hz), 21.1; FTIR (NaCl/thin film) 3022, 2923, 2858, 1607, 1515, 1434, 1282, 1209, 1115, 956 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{14}H_{12}F_2$: 218.0907, found: 218.0901.



2-(4-Methoxybenzyl)naphthalene (31). Prepared via General Procedure B (K_3PO_4 as base) on a 0.20 mmol scale. The crude material was purified by silica gel chromatography (100% hexanes with 0.5% Et_3N) to give compound **31** (49.0 mg, 99%) as a colorless oil: ^1H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.77 (m, 3H), 7.69 (s, 1H), 7.58 – 7.45 (m, 2H), 7.38 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.24 – 7.17 (m, 2H), 6.95 – 6.87 (m, 2H), 4.15 (s, 2H), 3.85 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 139.2, 133.7, 133.1, 132.1, 130.0, 128.1, 127.69, 127.66, 127.6, 127.0, 126.0, 125.4, 114.0, 55.3, 41.3. The spectral data for this compound matches that reported in the literature.[19]



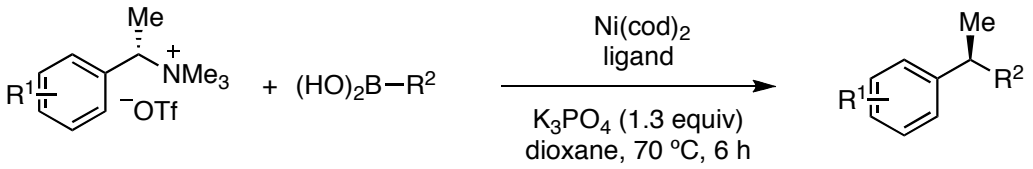
1-Methyl-3-(4-methylbenzyl)-1*H*-indole (32). Prepared via General Procedure A (CsF as base) on a 0.20 mmol scale. The crude material was purified by silica gel chromatography (15% dichloromethane/hexanes with 0.5% Et_3N) to give compound **32** (run 1: 30.5 mg, 65%; run 2: 27.0 mg, 57%) as a colorless oil.

Diarylmethane **32** was also prepared via General Procedure B (K_3PO_4 as base) on a 0.20 mmol scale. The crude material was purified as described above to give compound **32** (40.2 mg, 86%) as a colorless oil: ^1H NMR (400 MHz, $CDCl_3$) δ 7.58 (dt, *J* = 7.9, 1.0 Hz, 1H), 7.37 – 7.32 (m, 1H), 7.31 – 7.20 (m, 3H), 7.20 – 7.07 (m, 3H), 6.79 (s, 1H), 4.12 (s, 2H), 3.77 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.4, 137.2, 135.3, 129.0, 128.6, 127.9, 127.1, 121.6, 119.2, 118.8, 114.6, 109.2, 32.6, 31.1, 21.1; FTIR (NaCl/thin film) 3047, 3021, 2917, 1514, 1473, 1423, 1374, 1327, 1251, 1153, 1012 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{17}H_{17}N$: 235.1361, found: 235.1363.

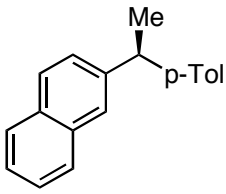
[19] Inés, B.; Moreno, I.; SanMartin, R.; Domínguez, E. *J. Org. Chem.* **2008**, *73*, 8448.

Stereospecific Cross Coupling of Benzyl Ammonium Triflates to Give Diarylethanes

General Procedure C



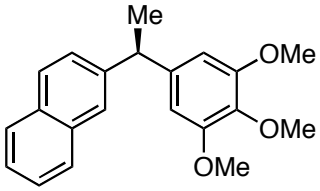
In a N_2-atmosphere glovebox, $Ni(cod)_2$, ligand, and K_3PO_4 (1.3 equiv) were weighed into a 1-dram vial. Benzyl ammonium triflate (1.0 equiv) and boronic acid (1.2 equiv) were added, followed by dioxane (0.33 M). The vial was capped with a Teflon-lined cap and removed from the glovebox. The mixture was stirred for 6 h at 70 °C. The reaction mixture was then diluted with Et_2O (1.5 mL) and filtered through a plug of silica gel, which was rinsed with Et_2O (10 mL). The filtrate was concentrated and purified by silica gel chromatography to give the diarylethane product.



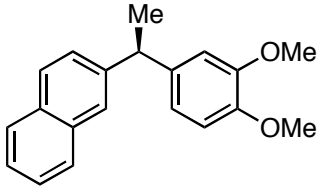
(*S*)-2-(1-*p*-Tolylethyl)naphthalene (34). Diarylethane **34** was prepared via General Procedure C on a 0.26 mmol scale using $Ni(cod)_2$ (3 mol %) and P(*o*-Tol)$_3$ (7 mol %). The crude material was purified by silica gel chromatography (100% hexanes) to give compound **34** (run 1: 39.0 mg, 61%; run 2: 37.0 mg, 58%) as a colorless oil. The enantiomeric excess was determined to be 99% ee (run 1: 99% ee; run 2: 99% ee) by chiral HPLC analysis (CHIRALPAK IB, 0.4 mL/min, 100% hexane, λ=254 nm); t_R(major)=21.70 min, t_R(minor)=23.30 min. $[\alpha]_D^{24}$ = +65.7° (c 1.20, $CHCl_3$).

Diarylethane **34** was also prepared on a 0.2 mmol scale using $Ni(cod)_2$ (10 mol%) and P(*o*-Tol)$_3$ (22 mol%). The crude material was purified as described above to give compound **34** (35.4 mg, 72%) as a colorless oil. The enantiomeric excess was determined to be 97% ee by chiral HPLC analysis as described above: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.70 (m, 4H), 7.56 – 7.45 (m, 2H), 7.37 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.21 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 4.34 (q, *J* = 7.2 Hz, 1H), 2.38 (s, 3H), 1.78 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz,

$CDCl_3$) δ 144.0, 143.3, 135.6, 133.6, 132.1, 129.1, 128.0, 127.8, 127.7, 127.6, 126.9, 126.0, 125.4, 125.3, 44.5, 21.9, 21.1; FTIR (NaCl/thin film) 3052, 3019, 2966, 2928, 2872, 1511, 1452, 1375, 1020 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{19}H_{18}$: 246.1409, found: 246.1405.



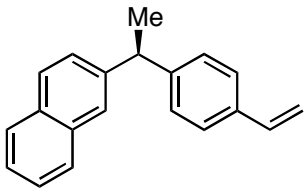
(*R*)-2-(1-(3,4,5-Trimethoxyphenyl)ethyl)naphthalene (35). Diarylethane **35** was prepared via General Procedure C on a 0.26 mmol scale using $Ni(cod)_2$ (3 mol %) and P(*o*-Tol)$_3$ (7 mol %). The crude material was purified by silica gel chromatography (10% acetone/hexanes) to give compound **35** (run 1: 70.0 mg, 83%; run 2: 68.0 mg, 81%) as a colorless oil. The enantiomeric excess was determined to be 99% ee (run 1: 99% ee; run 2: 99%) by chiral HPLC analysis (CHIRALPAK IA, 0.8 mL/min, 3% *i*-PrOH/hexane, λ=254 nm); t_R(minor)=12.60 min, t_R(major)=13.98 min. $[\alpha]_D^{24}$ = +37.6° (c 1.88, $CHCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.77 (m, 3H), 7.77 – 7.69 (m, 1H), 7.49 (m, 2H), 7.37 (dd, *J* = 8.5, 1.8 Hz, 1H), 6.52 (s, 2H), 4.30 (q, *J* = 7.2 Hz, 1H), 3.88 (s, 3H), 3.84 (s, 6H), 1.77 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.1, 143.6, 142.0, 136.2, 133.5, 132.1, 128.0, 127.8, 127.6, 126.7, 126.0, 125.5, 125.3, 104.8, 60.9, 56.1, 45.1, 22.0. The spectral data for this compound matches that reported in the literature.[20] The positive sign of the optical rotation enables assignment of the absolute configuration of **35** as *R*.[20]



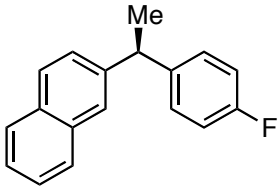
(*R*)-2-(1-(3,4-Dimethoxyphenyl)ethyl)naphthalene (36). Diarylethane **36** was prepared via General Procedure C on a 0.26 mmol scale using $Ni(cod)_2$ (3 mol %) and P(*o*-Tol)$_3$ (7 mol %). The crude material was purified by silica gel chromatography (9% diethyl ether/hexanes) to give compound **36** (run 1: 39.0 mg, 51%; run 2: 38.0 mg, 50%) as a white solid (mp 65–70 °C). The enantiomeric excess was determined to be 95% ee (run 1: 94% ee; run 2: 95% ee) by chiral HPLC analysis (CHIRALPAK IC, 0.8 mL/min, 3% *i*-PrOH/hexane, λ=254 nm); t_R(minor)=17.21 min, t_R(major)=17.94 min. $[\alpha]_D^{24}$ = +32.8° (c 1.52, $CHCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.75 (m, 3H), 7.76 – 7.70 (m, 1H), 7.48 (m,, 2H), 7.35 (dd, *J* = 8.5, 1.8 Hz, 1H), 6.90 – 6.83 (m, 2H), 6.80 (d, *J* = 1.6 Hz, 1H), 4.30 (q, *J* = 7.2 Hz, 1H), 3.89 (s, 3H), 3.84 (s, 3H), 1.76 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.8, 147.3, 144.1, 138.8,

[20] Taylor, B. L. H.; Swift, E. C.; Waetzig, J. D.; Jarvo, E. R. *J. Am. Chem. Soc.* **2011**, *133*, 389.

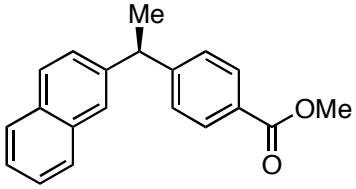
133.5, 132.1, 128.0, 127.8, 127.6, 126.8, 126.0, 125.4, 125.2, 119.5, 111.3, 111.0, 55.9, 55.8, 44.4, 22.0; FTIR (NaCl/thin film) 3051, 2962, 2931, 2833, 1516, 1458, 1251, 1235, 1143, 1028 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{20}H_{20}O_2$: 292.1463, found: 292.1467.



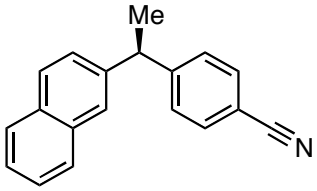
(*S*)-2-(1-(4-vinylphenyl)ethyl)naphthalene (37). Diarylethane **37** was prepared via General Procedure C on a 0.26 mmol scale using $Ni(cod)_2$ (3 mol %) and P(*o*-Tol)$_3$ (7 mol %). The crude material was purified by silica gel chromatography (100% hexanes) to give compound **37** (run 1: 45.0 mg, 67%; run 2: 47.0 mg, 69%) as a clear oil. The enantiomeric excess was determined to be 98% ee (run 1: 99% ee; run 2: 97% ee) by chiral HPLC analysis (CHIRALCEL IB, 0.8 mL/min, 100% hexane, λ =254 nm); t_R(major)=13.46 min, t_R(minor) =14.81 min. $[\alpha]_D^{24}$ = +44.8° (c 1.47, $CHCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.70 (m, 4H), 7.50 (m, 2H), 7.46 – 7.34 (m, 3H), 7.34 – 7.21 (m, 2H), 6.75 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.77 (dd, *J* = 17.6, 1.0 Hz, 1H), 5.26 (dd, *J* = 10.9, 1.0 Hz, 1H), 4.37 (q, *J* = 7.2 Hz, 1H), 1.79 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.0, 143.7, 136.6, 135.6, 133.6, 132.1, 128.04, 127.98, 127.8, 127.6, 126.9, 126.3, 126.0, 125.5, 125.4, 113.4, 44.6, 21.8. FTIR (NaCl/thin film) 3051, 2966, 2928, 841, 817, 746 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{20}H_{18}$: 258.1409, found: 258.1412.



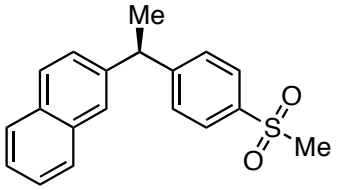
(*S*)-2-(1-(4-fluorophenyl)ethyl)naphthalene ((*S*)-38). Diarylethane **38** was prepared from ammonium triflate **33** and 4-fluorophenyl boronic acid via General Procedure C on a 0.26 mmol scale using $Ni(cod)_2$ (10 mol %) and P(*o*-Tol)$_3$ (22 mol %), except that CsF was used in place of K_3PO_4. The crude material was purified by silica gel chromatography (100% hexanes) to give compound (*S*)-**38** (61.0 mg, 94%) as a white solid. The enantiomeric excess was determined to be 98% ee by chiral HPLC analysis (CHIRALCEL OD-H, 0.8 mL/min, 100% hexane, λ =254 nm); t_R(major)=24.40 min, t_R(minor)=31.78 min. The spectral data for (*S*)-**38** matches that of (*R*)-**38** reported below.



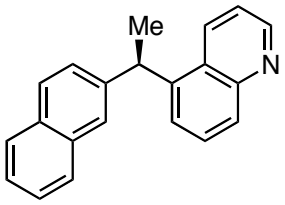
(*S*)-methyl 4-(1-(naphthalen-2-yl)ethyl)benzoate (39). Diarylethane **39** was prepared via General Procedure C on a 0.26 mmol scale using $Ni(cod)_2$ (10 mol %) and P(*o*-Tol)$_3$ (22 mol %), except that CsF was used in place of K_3PO_4. The crude material was purified by silica gel chromatography (15-19% Et_2O/hexanes) to give compound **39** (run 1: 51.0 mg, 68%, run 2: 56.0 mg, 74%) as a white solid (mp 75–78 °C). The enantiomeric excess was determined to be 98% ee (run 1: 98% ee; run 2: 97% ee) by chiral HPLC analysis (CHIRALCEL IB, 0.6 mL/min, 1% *i*-PrOH/hexane, λ =254 nm); t_R (major)=17.22 min, t_R (minor)=19.57 min. $[\alpha]_D^{24}$ = +12.5° (c 1.03, $CHCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 7.97 (m, 2H), 7.87 – 7.81 (m, 2H), 7.79 (d, *J* = 8.5 Hz, 1H), 7.75 – 7.70 (m, 1H), 7.55 – 7.44 (m, 2H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 13.1 Hz, 1H), 4.40 (q, *J* = 7.2 Hz, 1H), 3.93 (s, 3H), 1.78 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, CDCl3) δ 167.1, 151.6, 142.8, 133.5, 132.2, 129.8, 128.2, 128.1, 127.8, 127.8, 127.6, 126.6, 126.1, 125.6, 125.5, 52.1, 44.9, 21.6; FTIR (NaCl/thin film) 3054, 2968, 2361, 2338, 1718, 1280, 1110 cm^{-1}; LRMS (EI+) [M]+ calculated for $C_{20}H_{18}O_2$: 290.1, found: 290.2.



(*S*)-4-(1-(naphthalen-2-yl)ethyl)benzonitrile (40). Diarylethane **40** was prepared via General Procedure C on a 0.5 mmol scale using $Ni(cod)_2$ (1 mol %) and P(*o*-Tol)$_3$ (3 mol %). The crude material was purified by silica gel chromatography (10% Et_2O/hexanes) to give compound **40** (95.0 mg, 76%) as a pale yellow solid (mp 84–90 °C). The enantiomeric excess was determined to be 95% ee by chiral HPLC analysis (CHIRALCEL IC, 0.5 mL/min, 3% *i*-PrOH/hexane, λ =254 nm); t_R(major)=32.79 min, t_R(minor)=34.15 min. $[\alpha]_D^{24}$ = +42.8° (c 3.03, $CHCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.78 (m, 3H), 7.74 – 7.70 (m, 1H), 7.63 – 7.58 (m, 2H), 7.56 – 7.46 (m, 2H), 7.41 – 7.35 (m, 2H), 7.31 – 7.25 (m, 1H), 4.39 (q, *J* = 7.2 Hz, 1H), 1.78 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.8, 142.1, 133.5, 132.32, 132.26, 128.6, 128.4, 127.8, 127.7, 126.4, 126.3, 125.8, 125.6, 119.1, 110.0, 45.0, 21.4; FTIR (NaCl/thin film) 3053, 2968, 2929, 2226, 1605, 1502, 840, 820, 751 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{19}H_{15}N$: 257.1205, found: 257.1209.

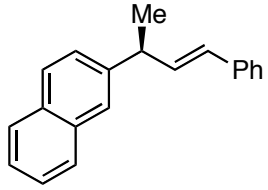


(*S*)-4-(1-(naphthalen-2-yl)ethyl)benzonitrile (41). Diarylethane **41** was prepared via General Procedure C on a 0.26 mmol scale using $Ni(cod)_2$ (3 mol %) and P(*o*-Tol)$_3$ (7 mol %). The crude material was purified by silica gel chromatography (8% acetone/ 0.5% Et_3N/hexanes) to give compound **41** (run 1: 77.0 mg, 97%, run 2: 72.0 mg, 91%) as a white solid (mp 123–126 °C). The enantiomeric excess was determined to be 97% ee (run 1: 97% ee, run 2: 96% ee) by chiral HPLC analysis (CHIRALCEL IB, 1.0 mL/min, 8% *i*-PrOH/hexane, λ =254 nm); t_R(major)=26.71 min, t_R(minor)=29.51 min. $[\alpha]_D^{24}$ = +29.4° (c 1.76, $CHCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.77 (m, 5H), 7.75 – 7.70 (m, 1H), 7.55 – 7.44 (m, 4H), 7.29 (d, *J* = 7.2 Hz, 1H), 4.43 (q, *J* = 7.2 Hz, 1H), 3.06 (s, 3H), 1.79 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.8, 142.1, 138.3, 133.5, 132.3, 128.8, 128.4, 127.8, 127.7, 127.6, 126.4, 126.3, 125.8, 125.6, 44.9, 44.6, 21.5; FTIR (NaCl/thin film) 3054, 2969, 2928, 1595, 1306, 1150, 1090, 955, 763 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{19}H_{18}O_2S$: 310.1028, found: 310.1023.

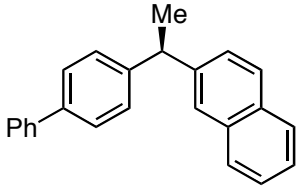


(*R*)-5-(1-(naphthalen-2-yl)ethyl)quinoline (42). Diarylethane **42** was prepared via General Procedure C on a 0.1 mmol scale using $Ni(cod)_2$ (10 mol %) and P(*o*-Tol)$_3$ (22 mol %). The crude material was purified by silica gel chromatography (7% acetone/11% dichloromethane/3% Et_3N/hexanes) to give compound **42** (15.0 mg, 53%) as a clear oil. The enantiomeric excess was determined to be 52% ee by chiral HPLC analysis (CHIRALCEL IB, 1.0 mL/min, 5% *i*-PrOH/hexane, λ =254 nm); t_R(minor)=12.59 min, t_R(major)=14.51 min. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.88 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.45 – 8.38 (m, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.84 – 7.72 (m, 4H), 7.70 – 7.66 (m, 1H), 7.59 (d, *J* = 7.2 Hz, 1H), 7.46 (pd, *J* = 6.9, 1.5 Hz, 2H), 7.38 – 7.29 (m, 2H), 5.05 (q, *J* = 7.1 Hz, 1H), 1.89 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.8, 148.9, 143.7, 141.8, 133.6, 132.4, 132.1, 129.1, 128.5, 128.3, 127.7, 127.6, 126.9, 126.4, 126.1, 125.5, 125.0, 120.8, 40.6, 22.5; ^{13}C NMR (151 MHz, $(CD_3)_2CO$) δ 149.8, 149.1, 144.1, 142.2, 133.7, 132.3, 132.1, 128.8, 128.4, 128.1, 127.6, 127.5, 126.7, 126.4, 126.0, 125.5, 125.4,

124.7, 120.9, 40.1, 21.9;[21] FTIR (NaCl/thin film) 3054, 2966, 2927, 2361, 2341, 1501, 802 cm^{-1}; LRMS (EI+) $[M]^+$ calculated for $C_{21}H_{17}N$: 283.1, found: 283.2.



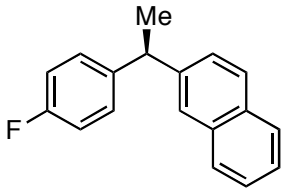
(*S*,*E*)-2-(4-Phenylbut-3-en-2-yl)naphthalene (43). Diarylethane **43** was prepared via General Procedure C on a 1.36 mmol scale using $Ni(cod)_2$ (2 mol %) and P(*o*-Tol)$_3$ (5 mol %). The crude material was purified by silica gel chromatography (100% hexanes) to give compound **43** (run 1: 334 mg, 96%, run 2: 335 mg, 96%) as a white solid (mp 81–86 °C). The enantiomeric excess was determined to be 99% ee (run 1: 99% ee; run 2: 99% ee) by chiral HPLC analysis (CHIRALCEL OD-H, 0.8 mL/min, 100% hexane, λ=254 nm); t_R(major)=34.24 min, t_R(minor)=37.38 min. $[\alpha]_D^{24}$ = –21.0° (c 8.40, $CHCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.82 (m, 3H), 7.77 – 7.74 (m, 1H), 7.55 – 7.45 (m, 3H), 7.45 – 7.40 (m, 2H), 7.38 – 7.31 (m, 2H), 7.31 – 7.22 (m, 1H), 6.54 – 6.50 (m, 2H), 3.86 (m, 1H), 1.61 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.1, 137.5, 135.1, 133.7, 132.3, 128.8, 128.6, 128.1, 127.7, 127.6, 127.1, 126.4, 126.2, 126.0, 125.4, 125.3, 42.7, 21.2. The spectral data for this compound matches that reported in the literature.[22]



(*R*)-2-(1-(Biphenyl-4-yl)ethyl)naphthalene (44). Diarylethane **44** was prepared via General Procedure C on a 0.20 mmol scale using $Ni(cod)_2$ (10 mol %) and t-Bu-XantPhos (12 mol %). The crude material was purified by silica gel chromatography (100% hexanes) to give compound **44** (29.0 mg, 46%) as a white solid (mp 83–85 °C). The enantiomeric excess was determined to be 98% ee by chiral HPLC analysis (CHIRALPAK IB, 0.8 mL/min, 2% *i*-PrOH/hexane, λ=254 nm); t_R(major)=8.60 min, t_R(minor)=10.0 min. $[\alpha]_D^{24}$ = –24.0° (c 1.44, $CHCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.76 (m, 4H), 7.63 – 7.53 (m, 4H), 7.53 – 7.41 (m, 4H), 7.41 – 7.32 (m, 4H), 4.40 (q, *J* = 7.2 Hz, 1H), 1.81 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.4, 143.7, 141.0, 139.0, 133.5, 132.1, 128.7, 128.2, 128.0, 127.8, 127.6, 127.2, 127.1, 127.0, 126.9, 126.0, 125.4, 125.4, 44.6, 21.8; FTIR (NaCl/thin film) 3053, 3026,

[21] We observe coincident peaks in the ^{13}C NMR spectrum when $CDCl_3$ is used as solvent. However, all 21 peaks are distinct when $(CD_3)_2CO$ is used as solvent.
[22] Li, C.; Xing, J., Zhao, J.; Huynh, P.; Zhang, W.; Jiang, P.; Zhang, Y. J. *Org. Lett.* **2012**, *14*, 390.

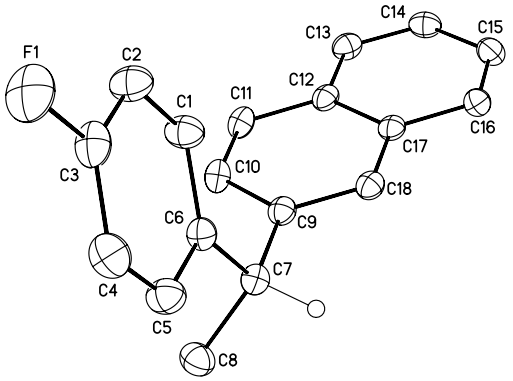
2965, 2927, 1600, 1486, 1449, 1008 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{24}H_{20}$: 308.1565, found: 308.1561.

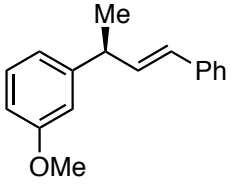


(*R*)-2-(1-(4-Fluorophenyl)ethyl)naphthalene ((*R*)-38). Diarylethane (*R*)-**38** was prepared from (R)-1-(4-fluorophenyl)-N,N,N-trimethylethanaminium trifluoromethanesulfonate and 2-naphthyl boronic acid via General Procedure C on a 0.20 mmol scale using $Ni(cod)_2$ (10 mol %) and t-Bu-XantPhos (12 mol %). The crude material was purified by silica gel chromatography (100% hexanes) to give compound (*R*)-**38** (run 1: 18.0 mg, 36%; run 2: 20.0 mg, 38%) as a pale green solid (mp 54–58 °C). The enantiomeric excess was determined to be 95% ee (run 1: 95% ee; run 2: 95% ee) by chiral HPLC analysis (CHIRALCEL OD-H, 0.8 mL/min, 100% hexane, λ=254 nm); t_R(minor)=25.96 min, t_R(major)=33.26 min. $[\alpha]_D^{24}$ = –25.2° (c 1.88, $CHCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.74 (m, 3H), 7.73 – 7.67 (m, 1H), 7.54 – 7.41 (m, 2H), 7.34 – 7.19 (m, 3H), 7.04 – 6.95 (m, 2H), 4.32 (q, J = 7.2 Hz, 1H), 1.74 (d, J = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.3 (d, $J_{C–F}$ = 245.4 Hz), 143.6, 141.9 (d, $J_{C–F}$ = 4.0 Hz), 133.5, 132.1, 129.1 (d, $J_{C–F}$ = 7.1 Hz), 128.1, 127.7, 127.6, 126.7, 126.1, 125.5, 125.3, 115.1 (d, $J_{C–F}$ = 21.2 Hz), 44.1, 21.9; FTIR (NaCl/thin film) 3054, 2966, 2924, 2851, 1507, 1221, 1158 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{18}H_{15}F$: 250.1158, found: 250.1160.

X-ray quality crystals were prepared by slow evaporation from pentane. The crystal structure demonstrated that the absolute configuration is *R* (Fig S1).

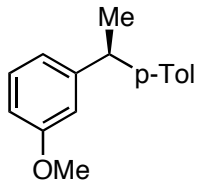
Figure S1. Molecular diagram of (*R*)-**38** with ellipsoids at 30% probability. Tertiary H-atom depicted with arbitrary radius. All other H-atoms and a second symmetry-unique compound molecule are omitted for clarity. (CCDC-899360)



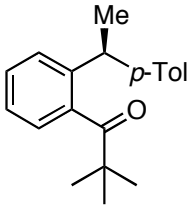


(*S*,*E*)-1-Methoxy-3-(4-phenylbut-3-en-2-yl)benzene (45). Aryl vinyl ethane **45** was prepared via General Procedure C on a 0.20 mmol scale using $Ni(cod)_2$ (15 mol %) and P(*o*-Tol)$_3$ (32 mol %). The crude material was purified by silica gel chromatography (100% hexanes) to give compound **45** (run 1: 26.0 mg, 55%; run 2: 27.0 mg, 56%) as a colorless oil. The enantiomeric excess was determined to be 98% ee (run 1: 98% ee; run 2: 97% ee) by chiral HPLC analysis (CHIRALPAK IB, 1.0 mL/min, 100% hexane, λ=254 nm); t_R(major)=15.46 min, t_R(minor)=18.19 min. $[\alpha]_D^{24}$ = –25.2° (c 1.00, $CHCl_3$)[23]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.19 (m, 6H), 6.95 – 6.77 (m, 3H), 6.52 – 6.36 (m, 2H), 3.85 (s, 3H), 3.66 (q, *J* = 6.8 Hz, 1H), 1.50 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 147.4, 137.5, 135.0, 129.5, 128.6, 128.5, 127.1, 126.2, 119.8, 113.3, 111.3, 55.2, 42.6, 21.2. The spectral data for this compound matches that reported in the literature.[22]

[23] Based on the optical rotation of diarylethane **35** and the crystal structure of diarylethane (*R*)-**38**, we are confident that these Suzuki reactions proceed with inversion of configuration and have thus assigned the absolute configuration of compound **45** as *S*. However, we note that the sign of the optical rotation is in disagreement with the previously reported value (see ref 22). The reasons for this discrepancy are unclear. We have obtained a negative optical rotation for this compound on two polarimeters and at two different concentrations.

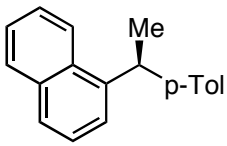


(*S*)-1-Methoxy-3-(1-*p*-tolylethyl)benzene (46). Diarylethane **46** was prepared via General Procedure C on a 0.20 mmol scale using $Ni(cod)_2$ (15 mol %) and P(*o*-Tol)$_3$ (32 mol %). The crude material was purified by silica gel chromatography (100% hexanes) to give compound **46** (run 1: 22.0 mg, 49%; run 2: 26 mg, 58%) as a colorless oil. The enantiomeric excess was determined to be 91% ee (run 1: 90% ee, run 2: 92% ee) by chiral HPLC analysis (CHIRALPAK IA, 0.8 mL/min, 1% *i*-PrOH/hexane, λ=254 nm); t_R(minor)=5.73 min, t_R(major)=6.17 min. $[\alpha]_D^{24}$ = +15.4° (c 0.96, $CHCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (t, *J* = 7.9 Hz, 1H), 7.19 – 7.10 (m, 4H), 6.88 – 6.80 (m, 2H), 6.76 (ddd, *J* = 8.1, 2.6, 0.9 Hz, 1H), 4.13 (q, *J* = 7.2 Hz, 1H), 3.81 (s, 3H), 2.35 (s, 3H), 1.65 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 148.3, 143.2, 135.5, 129.3, 129.1, 127.4, 120.1, 113.7, 110.8, 55.1, 44.4, 21.9, 21.0. The spectral data for this compound matches that reported in the literature.[24]



(*S*)-2,2-dimethyl-1-(2-(1-*p*-tolylethyl)phenyl)propan-1-one (50). Diarylethane **50** was prepared via General Procedure C on a 0.10 mmol scale using $Ni(cod)_2$ (10 mol %) and PPh_2Cy (22 mol %). The crude material was purified by silica gel chromatography (100% hexanes) to give compound **50** (17.0 mg, 64%) as a colorless oil. The enantiomeric excess was determined to be 33% ee by chiral HPLC analysis (CHIRALPAK IA, 1.0 mL/min, 3% *i*-PrOH/hexane, λ =254 nm); t_R(major)=5.70 min, t_R(minor)=6.39 min. $[\alpha]_D^{24}$ = +15.4° (c 0.96, $CHCl_3$): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.21 (ddd, *J* = 8.4, 5.2, 3.3 Hz, 1H), 7.19 – 7.16 (m, 1H), 7.11 – 7.08 (m, 2H), 7.06 – 7.04 (m, 2H), 7.01 – 6.99 (m, 2H), 3.97 (q, *J* = 7.1 Hz, 1H), 2.22 (s, 3H), 1.52 (d, *J* = 7.1 Hz, 3H), 1.15 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 215.0, 143.3, 142.5, 140.4, 135.6, 128.97, 128.95, 128.2, 127.6, 125.0, 124.6, 44.9, 40.6, 27.8, 22.4, 21.0; FTIR (NaCl/thin film) 2968, 2931, 2871, 1685, 1513, 1477, 1460, 1392, 1365, 1277, 1184, 1109, 1041, 1020, 963, 943, 821, 765 cm^{-1}; LRMS (EI+) $[M–(t\text{-Bu})]^+$ calculated for $C_{16}H_{15}O$: 223.11, found: 223.20.

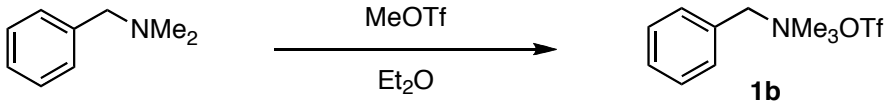
[24] Nakamura, R.; Obora, Y.; Ishii, Y. *Chem. Commun.* **2008**, *29*, 3417.



(*S*)-1-(1-*p*-Tolylethyl)naphthalene (S1). Diarylethane **S1** was prepared via General Procedure C on a 0.26 mmol scale using $Ni(cod)_2$ (3 mol %) and P(*o*-Tol)$_3$ (7 mol %). The crude material was purified by silica gel chromatography (100% hexanes) to give compound **S1** (34.0 mg, 70%) as a colorless oil. The enantiomeric excess was determined to be 67% ee by chiral HPLC analysis (CHIRALPAK IB, 0.4 mL/min, 100% hexane, λ=254 nm); t_R(major)=30.70 min, t_R(minor)=38.65 min. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 – 8.04 (m, 1H), 7.97 – 7.86 (m, 1H), 7.84 – 7.73 (m, 1H), 7.59 – 7.44 (m, 4H), 7.22 – 7.15 (m, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 4.94 (q, *J* = 7.1 Hz, 1H), 2.34 (s, 3H), 1.80 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7, 141.8, 135.5, 134.0, 131.7, 129.2, 128.8, 127.5, 126.9, 125.9, 125.5, 125.3, 124.3, 124.0, 40.2, 22.7, 21.1; FTIR (NaCl/thin film) 3047, 2966, 2931, 2871, 1510, 1449, 1396, 1373, 1020 cm^{-1}; HRMS (EI+) $[M]^+$ calculated for $C_{19}H_{18}$: 246.1409, found: 246.1407.

Preparation of Benzyl Ammonium Triflates

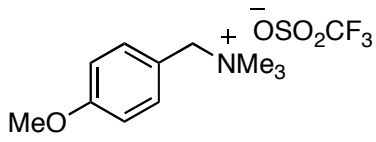
General Procedure for the Preparation of Benzyl Ammonium Triflates: Preparation of *N,N,N*-Trimethyl-1-phenylmethanaminium trifluoromethanesulfonate (1b)



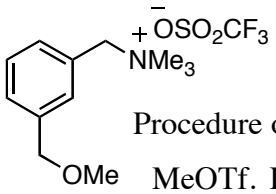
Dimethylbenzylamine (2.5 g, 18.5 mmol, 1.0 equiv) was dissolved in Et_2O (15 mL, 4.0 M). MeOTf (2.7 mL, 23.9 mmol, 1.3 equiv) was added dropwise at 0 °C. White precipitate formed immediately. After complete addition the reaction mixture was stirred for an additional 15 minutes at 0 °C. The precipitate was isolated by filtration and washed with Et_2O (2 x 20 mL). The resulting solid was dried under vacuum to give salt **1b** (5.34 g, 97%) as a white solid (mp 97–99 °C): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57 – 7.46 (m, 5H), 4.64 (s, 2H), 3.22 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 132.9, 131.0, 129.4, 127.1, 120.7 (q, $J_{C–F}$ = 320.1 Hz), 69.6, 52.5; ^{19}F NMR (565 MHz, $CDCl_3$) δ –78.5; FTIR (NaCl/thin film) 3038, 2968, 2254, 1653, 1480, 1457, 1259, 1155, 1031, 920 cm^{-1}; LRMS (APCI+) [M–OTf]$^+$ calculated for [$C_{10}H_{16}N$]$^+$: 150.1, found: 150.1.

The ammonium triflate salts were used as prepared without further purification. The ^{1}H and ^{13}C NMR spectra for all salts are included below.

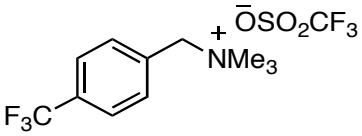
Please note: Salts have been observed to decompose in solution over the course of 1 week, but can be stored indefinitely in the solid form.



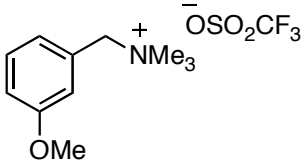
1-(4-Methoxyphenyl)-*N,N,N*-trimethylmethanaminium trifluoromethanesulfonate (S2). Prepared according to the General Procedure on 5.10 mmol scale to give salt **S3** (1.55 g, 94%) as a light pink solid (mp 96–99 °C): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.48 – 7.39 (m, 2H), 7.06 – 6.88 (m, 2H), 4.52 (s, 2H), 3.83 (s, 3H), 3.13 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.5, 134.3, 120.7 (q, $J_{C–F}$ = 320.1 Hz), 119.0, 114.7, 69.3, 55.4, 52.1; ^{19}F NMR (565 MHz, $CDCl_3$) δ –78.4; FTIR (NaCl/thin film) 3040, 2967, 2843, 1614, 1517, 1481, 1257, 1225, 1160, 1030 cm^{-1}; LRMS (APCI+) [M–OTf]$^+$ calculated for [$C_{11}H_{18}NO$]$^+$: 180.1, found: 180.1.



1-(3-(Methoxymethyl)phenyl)-*N*,*N*,*N*-trimethylmethanaminium trifluoromethanesulfonate (S3). Prepared according to the General Procedure on 8.50 mmol scale. In this case, a precipitate did not form upon addition of MeOTf. Instead, two distinct layers formed. The top layer was decanted off. The bottom layer was washed with Et_2O (2 x 10 mL) and then dried under vacuum to give salt **S3** (2.92 g, 99%) as a light yellow viscous oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.35 (m, 4H), 4.53 (s, 2H), 4.44 (s, 2H), 3.37 (s, 3H), 3.11 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.7, 132.1, 131.8, 130.1, 129.4, 127.3, 120.5 (q, $J_{C–F}$ = 321.2 Hz), 73.8, 69.3, 58.4, 52.40, 52.36, 52.3;[25] ^{19}F NMR (376 MHz, $CDCl_3$) δ –78.5; FTIR (NaCl/thin film) 1653, 1490, 1257, 1226, 1165, 1089, 1030; LRMS (APCI+) $[M–OTf]^+$ calculated for $[C_{12}H_{20}NO]^+$: 194.2, found: 194.1.



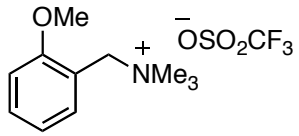
***N*,*N*,*N*-Trimethyl-1-(4-(trifluoromethyl)phenyl)methanaminium trifluoromethanesulfonate (S4).** Prepared according to the General Procedure on 2.83 mmol scale to give salt **S4** (2.61 g, 97%) as a white solid (mp 158–161 °C): ^{1}H NMR (600 MHz, $(CD)_3CO$) δ 7.99 (d, J = 8.1 Hz, 2H), 7.91 (d, J = 8.1 Hz, 2H), 4.93 (s, 2H), 3.41 (s, 9H); ^{13}C NMR (151 MHz, Acetone) δ 134.0, 132.6, 131.8 (q, $J_{C–F}$ = 33.2 Hz), 125.9 (q, $J_{C–F}$ = 4.5 Hz), 124.1 (q, $J_{C–F}$ = 271.8 Hz), 121.3 (q, $J_{C–F}$ = 321.6 Hz), 68.0, 52.4; ^{19}F NMR (565 MHz, $(CD)_3CO$) δ –63.5, –78.9; FTIR (NaCl/thin film) 3042, 1698, 1482, 1424, 1277, 1262, 1165, 1107, 1035 cm^{-1}; LRMS (APCI+) $[M–OTf]^+$ calculated for $[C_{11}H_{15}F_3NO]^+$: 218.1, found: 218.1.



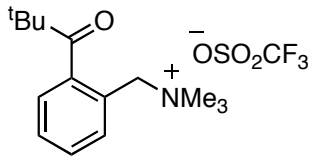
1-(3-Methoxyphenyl)-*N*,*N*,*N*-trimethylmethanaminium trifluoromethanesulfonate (S5). Prepared according to the General Procedure on 3.50 mmol scale. In this case, a precipitate did not form upon addition of MeOTf. Instead, two distinct layers formed. The top layer was decanted off. The bottom layer was washed with Et_2O (2 x 10 mL) and then dried under vacuum to give salt **S5** (1.13 g, 95%) as a light brown solid (mp 57–60 °C): ^{1}H NMR (600

[25] In several of the ammonium triflates, the methyl groups of the NMe_3 fragment appear as three, nearly coincident peaks. We hypothesize that this may be due to hindered rotation about the benzylic C–N bond.

MHz, $CDCl_3$) δ 7.36 (d, J = 7.9 Hz, 1H), 7.13 – 7.06 (m, 2H), 7.06 – 6.99 (m, 1H), 4.58 (s, 2H), 3.84 (s, 3H), 3.20 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.2, 130.4, 128.4, 124.8, 120.7 (q, $J_{C–F}$ = 320.1 Hz), 118.1, 116.8, 69.6, 55.5, 52.6; ^{19}F NMR (565 MHz, $CDCl_3$) δ –78.4; FTIR (NaCl/thin film) 3042, 2971, 2843, 1653, 1603, 1489, 1457, 1259, 1225, 1160, 1030 cm^{-1}; LRMS (APCI+) [M–OTf]$^+$ calculated for [$C_{11}H_{18}NO$]$^+$: 180.1, found: 180.1.

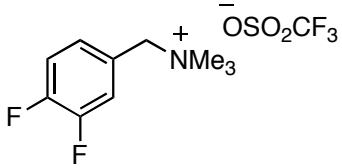


1-(2-Methoxyphenyl)-*N*,*N*,*N*-trimethylmethanaminium trifluoromethanesulfonate (S6). Prepared according to the General Procedure on 4.91 mmol scale. In this case, a precipitate did not form upon addition of MeOTf. Instead, two distinct layers formed. The top layer was decanted off. The bottom layer was washed with Et_2O (2 x 10 mL) and then dried under vacuum to give salt **S6** (1.58 g, 98%) as a brown solid (mp 123–125 °C): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 – 7.45 (m, 2H), 7.07 (t, J = 7.5 Hz, 1H), 7.02 (d, J = 8.2 Hz, 1H), 4.59 (s, 2H), 3.91 (s, 3H), 3.20 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.7, 135.1, 133.0, 121.4, 120.7 (q, $J_{C–F}$ = 320.1 Hz), 115.6, 111.6, 64.4, 55.7, 52.8; ^{19}F NMR (565 MHz, $CDCl_3$) δ –78.4; FTIR (NaCl/thin film) 1653, 1636, 1489, 1473, 1255, 1159, 1030 cm^{-1}; LRMS (APCI+) [M–OTf]$^+$ calculated for [$C_{11}H_{18}NO$]$^+$: 180.1, found: 180.1.

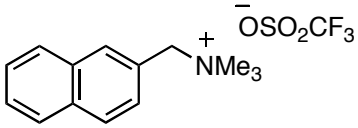


***N*,*N*,*N*-Trimethyl-1-(2-pivaloylphenyl)methanaminium trifluoromethanesulfonate (47).** Prepared according to the General Procedure on 7.06 mmol scale to give salt **47** (2.53 g, 96%) as a white solid (mp 117–120 °C): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, J = 5.9 Hz, 1H), 7.65 – 7.55 (m, 2H), 7.55 – 7.47 (m, 1H), 4.50 (s, 2H), 3.23 (s, 9H), 1.25 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 213.6, 141.8, 134.1, 130.3, 126.8, 124.2, 120.6 (q, $J_{C–F}$ = 320.1 Hz), 67.0, 53.8, 45.6, 27.6; ^{13}C NMR (101 MHz, $(CD)_3CO$) δ 213.2, 142.5, 134.4, 130.3, 129.7, 126.8, 124.4, 121.3 (q, $J_{C–F}$ = 322.2 Hz), 66.7, 53.2, 53.21, 53.17,[25] 45.1, 26.8;[26] ^{19}F NMR (565 MHz, $CDCl_3$) δ –78.5; FTIR (NaCl/thin film) 3042, 2973, 2873, 2253, 1684, 1653, 1488, 1475, 1254, 1224, 1154, 1029, 954 cm^{-1}; LRMS (APCI+) [M–OTf]$^+$ calculated for [$C_{15}H_{24}NO$]$^+$: 234.2, found: 234.2.

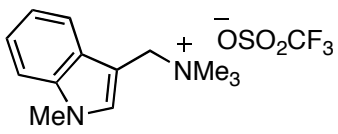
[26] Although two ^{13}C NMR peaks are coincident when $CDCl_3$ is used as solvent, all twelve ^{13}C NMR peaks are seen when $(CD_3)_2CO$ is used as solvent.



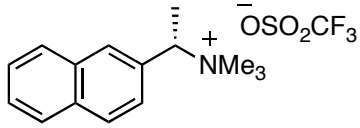
1-(3,4-Difluorophenyl)-*N*,*N*,*N*-trimethylmethanaminium trifluoromethanesulfonate (S7). Prepared according to the General Procedure on 5.42 mmol scale to give salt **S7** (1.75 g, 96%) as a white solid (mp 119–122 °C): ^{1}H NMR (600 MHz, $(CD_3)_2CO$) δ 7.81 – 7.74 (m, 1H), 7.64 – 7.58 (m, 1H), 7.55 – 7.47 (m, 1H), 4.82 (s, 2H), 3.35 (s, 9H); ^{13}C NMR (151 MHz, $(CD_3)_2CO$) δ 151.7 (dd, $J_{C–F}$ = 237.1, 12.1 Hz), 150.0 (dd, $J_{C–F}$ = 235.6, 12.1 Hz), 130.5 (dd, $J_{C–F}$ = 6.0, 3.0 Hz), 125.7 (dd, $J_{C–F}$ = 6.0, 3.0 Hz), 122.2 (d, $J_{C–F}$ = 18.1 Hz), 121.3 (q, $J_{C–F}$ = 321.6 Hz), 118.1 (d, $J_{C–F}$ = 18.1 Hz), 67.5, 52.2; ^{19}F NMR (565 MHz, $(CD_3)_2CO$) δ –79.0, –137.0 (d, $J_{F–F}$ = 17.0 Hz), –138.3 (d, $J_{F–F}$ = 22.6 Hz); FTIR (NaCl/thin film) 3044, 2286, 2059, 1915, 1614, 1524, 1478, 1442, 1257, 1164, 1128, 1033, 959 cm^{-1}; LRMS (APCI+) [M–OTf]$^+$ calculated for $[C_{10}H_{14}F_2N]^+$: 186.1, found: 186.1.



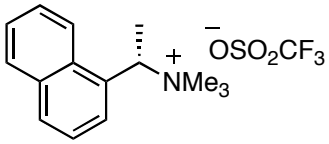
***N*,*N*,*N*-Trimethyl-1-(naphthalen-2-yl)methanaminium trifluoromethanesulfonate (S8).** Prepared according to the General Procedure on 1.12 mmol scale to give salt **S8** (365 mg, 95%) as an off-white solid (mp 107–110 °C): ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.96 – 7.75 (m, 3H), 7.63 – 7.46 (m, 3H), 4.81 (s, 2H), 3.25 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 133.8, 133.5, 132.8, 129.1, 128.6, 128.5, 127.9, 127.7, 127.1, 124.4, 120.7 (q, $J_{C–F}$ = 320.1 Hz), 69.6, 52.5; ^{19}F NMR (565 MHz, $CDCl_3$) δ –78.4; FTIR (NaCl/thin film) 3041, 1635, 1601, 1490, 1479, 1257, 1226, 1162, 1030 cm^{-1}; LRMS (APCI+) [M–OTf]$^+$ calculated for $[C_{14}H_{18}N]^+$: 200.1, found: 200.1.



***N*,*N*,*N*-Trimethyl-1-(1-methyl-1*H*-indol-3-yl)methanaminium trifluoromethanesulfonate (S9)** Prepared according to the General Procedure on 3.50 mmol scale to give salt **S9** (1.22 g, 97%) as a pale brown solid (mp 128–133 °C decomp): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 1H), 7.53 (s, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 7.32 – 7.27 (m, 1H), 7.24 (t, *J* = 7.4 Hz, 1H), 4.77 (s, 2H), 3.77 (s, 3H), 3.17 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 136.9, 134.1, 127.9, 122.6, 121.1, 120.8 (q, $J_{C–F}$ = 320.1 Hz), 118.6, 110.0, 100.5, 61.8, 51.9, 33.0; ^{19}F NMR (565 MHz, $CDCl_3$) δ –78.4; FTIR (NaCl/thin film) 2085, 1642, 1547, 1482, 1267, 1033 cm^{-1}; LRMS (APCI+) [M–OTf]$^+$ calculated for $[C_{13}H_{19}N_2]^+$: 203.2, found: 203.1.



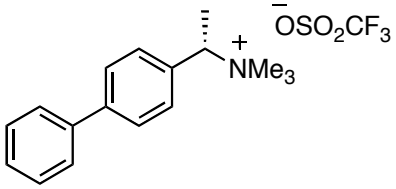
(*S*)-*N*,*N*,*N*-Trimethyl-1-(naphthalen-2-yl)ethanaminium trifluoromethanesulfonate (33). Prepared according to the General Procedure on 9.05 mmol scale starting from (*S*)-*N*,*N*-dimethyl-1-(naphthalen-2-yl)ethanamine, which was prepared using Escheweiler–Clarke conditions[2] from (*S*)-(-)-1-(2-naphthyl)ethylamine purchased in 99.6% ee. In this case, a precipitate did not form upon addition of MeOTf. Instead, two distinct layers formed. The top layer was decanted off. The bottom layer was washed with Et_2O (2 x 10 mL) and then dried under vacuum to give salt **33** (3.25 g, 99%) as a light brown solid (mp 65–70 °C): ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.96 (d, *J* = 8.2 Hz, 2H), 7.90 (d, *J* = 7.7 Hz, 1H), 7.66 – 7.49 (m, 3H), 5.08 (q, *J* = 6.9 Hz, 1H), 3.23 (s, 9H), 1.95 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 133.9, 132.8, 129.6, 129.2, 128.6, 127.9, 127.7, 127.2, 120.8 (q, $J_{C–F}$ = 320.1 Hz), 74.2, 51.2, 51.13, 51.10,[25] 15.0;[27] ^{19}F NMR (565 MHz, $CDCl_3$) δ –78.4; FTIR (NaCl/thin film) 1642, 1479, 1252, 1029 cm^{-1}; LRMS (APCI+) $[M–OTf]^+$ calculated for $[C_{15}H_{20}N]^+$: 214.2, found: 214.1.



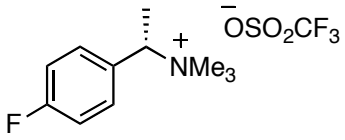
(*S*)-*N*,*N*,*N*-Trimethyl-1-(naphthalen-1-yl)ethanaminium trifluoromethanesulfonate (S10). Prepared according to the General Procedure on 1.90 mmol scale starting from (*S*)-*N*,*N*-dimethyl-1-(naphthalen-1-yl)ethanamine, which was prepared using Escheweiler–Clarke conditions[2] from (*S*)-(-)-α-(1-naphthyl)ethylamine purchased in ≥99% ee. In this case, a precipitate did not form upon addition of MeOTf. Instead, two distinct layers formed. The top layer was decanted off. The bottom layer was washed with Et_2O (2 x 10 mL) and then dried under vacuum to give salt **S10** (647 mg, 93%) as a brown solid (mp 56–63 °C): ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.7 Hz, 1H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.78 – 7.69 (m, 2H), 7.65 – 7.49 (m, 2H), 5.82 (q, *J* = 6.9 Hz, 1H), 3.20 (s, 9H), 1.97 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 134.0, 132.4, 131.7, 129.4, 128.7, 128.4, 127.6, 126.8, 124.8, 122.7, 120.6 (q, $J_{C–F}$ = 320.1 Hz), 67.5, 51.39, 51.36, 51.3,[25] 16.1; ^{19}F NMR (565 MHz,

[27] Although this compound should have 16 distinct ^{13}C NMR signals, only 14 were observed in both $CDCl_3$ and $(CD_3)_2CO$. The ^{1}H, IR and LRMS confirm this structure.

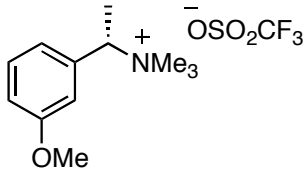
$CDCl_3$) δ –78.4; FTIR (NaCl/thin film) 3054, 1635, 1599, 1515, 1489, 1416, 1392, 1252, 1225, 1160, 1029, 955 cm^{-1}; LRMS (APCI+) $[M–OTf]^+$ calculated for $[C_{15}H_{20}N]^+$: 214.2, found: 214.1.



(*S*)-1-(Biphenyl-4-yl)-*N*,*N*,*N*-trimethylethanaminium trifluoromethanesulfonate (S11). Prepared according to the General Procedure on 2.32 mmol scale starting from (*S*)-1-(biphenyl-4-yl)-*N*,*N*-dimethylethanamine, which was prepared using Escheweiler–Clarke conditions[2] from (*S*)-(-)-1-(4-bromophenyl)ethylamine (see preparation below) purchased in 98% ee, to give salt **S11** (846 mg, 94%) as an off-white solid (mp 195 °C decomp): ^{1}H NMR (600 MHz, $(CD_3)_2CO$) δ 7.84 (s, 4H), 7.74 (d, *J* = 7.7 Hz, 2H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 1H), 5.08 (q, *J* = 7.1 Hz, 1H), 3.33 (s, 9H), 2.00 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (151 MHz, $(CD_3)_2CO$) δ 142.9, 139.6, 132.3, 131.2, 129.0, 128.0, 127.4, 126.9, 121.5 (q, $J_{C–F}$ = 321.6 Hz), 73.7, 50.94, 50.92, 50.89,[25] 14.4; ^{19}F NMR (565 MHz, Acetone) δ –78.9; FTIR (NaCl/thin film) 3032, 1488, 1457, 1419, 1256, 1227, 1030, 954, 841; LRMS (APCI+) $[M–OTf]^+$ calculated for $[C_{17}H_{22}N]^+$: 240.2, found: 240.2.

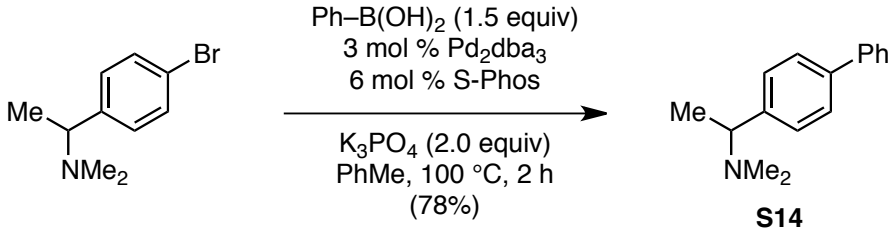


(*S*)-1-(4-Fluorophenyl)-*N*,*N*,*N*-trimethylethanaminium trifluoromethanesulfonate (S12). Prepared according to the General Procedure on 4.1 mmol scale starting from (*S*)-1-(4-fluorophenyl)-*N*,*N*-dimethylethanamine, which was prepared using Escheweiler–Clarke conditions[2] from (*S*)-1-4(fluorophenyl)ethylamine purchased in 99% ee, to give salt **S12** (1.31 g, 95%) as a light white solid (mp 75–78 °C): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 8.6, 5.1 Hz, 2H), 7.19 (t, *J* = 8.4 Hz, 2H), 4.94 (q, *J* = 7.0 Hz, 1H), 3.15 (s, 9H), 1.82 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.9 (d, $J_{C–F}$ = 253.7 Hz), 163.1, 128.3 (d, $J_{C–F}$ = 3.0 Hz), 120.7 (q, $J_{C–F}$ = 320.1 Hz), 116.6, 116.5, 73.2, 51.0, 50.97, 50.94,[25] 15.1; ^{19}F NMR (565 MHz, $CDCl_3$) δ –78.5, –108.7; FTIR (NaCl/thin film) 2090, 1647, 1508, 1260, 1033 cm^{-1}; LRMS (APCI+) $[M–OTf]^+$ calculated for $[C_{11}H_{17}FN]^+$: 182.1, found: 182.1.



(*S*)-1-(3-Methoxyphenyl)-*N*,*N*,*N*-trimethylethanaminium trifluoromethanesulfonate (S13). Prepared according to the General Procedure on 2.91 mmol scale starting from (*S*)-1-(3-methoxyphenyl)-*N*,*N*-dimethylethamine, which was prepared using Escheweiler–Clarke conditions[2] from (*S*)-(-)-1-(3-methoxyphenyl)ethylamine purchased in ≥99%, to give salt **S13** (947 mg, 95%) as a brown solid (mp 51–55 °C): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 (t, *J* = 8.0 Hz, 1H), 7.07 (d, *J* = 7.1 Hz, 2H), 7.02 (d, *J* = 6.2 Hz, 1H), 4.85 – 4.79 (m, 1H), 3.85 (s, 3H), 3.16 (s, 9H), 1.82 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.1, 133.8, 130.4, 120.5 (q, J_{C-F} = 320.1 Hz), 116.3, 74.1, 55.6, 51.2, 51.19, 51.16,[25] 15.0;[28] ^{19}F NMR (565 MHz, $CDCl_3$) δ –78.5; FTIR (NaCl/thin film) 2081, 1636, 1491, 1261, 1168, 1032 cm^{-1}; LRMS (APCI+) [M–OTf]$^+$ calculated for $[C_{12}H_{20}NO]^+$: 194.2, found: 194.1.

Cross Coupling of Aryl Bromide in Presence of Benzylic Dimethylamino Group: Preparation of 1-(Biphenyl-4-yl)-*N*,*N*-dimethylethanamine[29]



S14

In a N_2-atmosphere glovebox, Pd_2dba_3 (3 mol %, 0.145 mmol, 132.4 mg), S-Phos (6 mol %, 0.289 mmol, 118.7 mg), K_3PO_4 (2.0 equiv, 9.64 mmol, 2.20 g), $PhB(OH)_2$ (1.5 equiv, 7.23 mmol, 883 mg), and [1-(4-bromophenyl)ethyl]dimethylamine (1.0 equiv, 4.82 mmol, 1.10 g) were combined in a oven-dried Schlenk tube. The tube was sealed and then removed from the glovebox. Under positive N_2 pressure, PhMe (20 mL, 0.24 M) was added. The N_2-inlet was removed, and the reaction mixture was heated at 100 °C for 2 h. The mixture was cooled to room temperature and filtered through a pad of Celite, which was then rinsed with Et_2O (2 x 10 mL). The solution was concentrated. The crude material was purified by silica gel chromatography

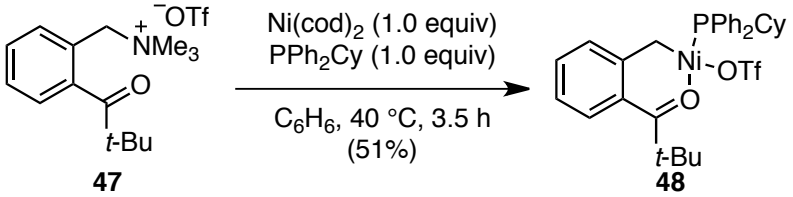
[28] Although this compound should have 13 distinct ^{13}C NMR signals, only 11 were observed in both $CDCl_3$ and C_6D_6. The ^{1}H, IR and LRMS confirm this structure.

[29] This procedure is adapted from literature procedure. See: Barder, T. E.; Walker, S. D.; Martinelli, J. R.; Buchwald, S. L. *J. Am. Chem. Soc.* **2005**, *127*, 4685.

(20:2:1:78 acetone/CH_2Cl_2/Et_3N/hexanes) to give compound **S14** (847 mg, 78%) as a colorless oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65–7.56 (m, 4H), 7.49–7.43 (m, 2H), 7.42–7.33 (m, 3H), 3.33 (q, *J* = 6.8 Hz, 1H), 2.26 (s, 6H), 1.44 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.2, 141.0, 139.8, 128.8, 128.0, 127.13, 127.06, 127.0, 65.7, 43.3, 20.3. HRMS (EI+) $[M]^+$ calculated for $C_{16}H_{19}N$: 225.1518, found: 225.1521.

Preparation and Activity of Alkylnickel(II) Triflate 48

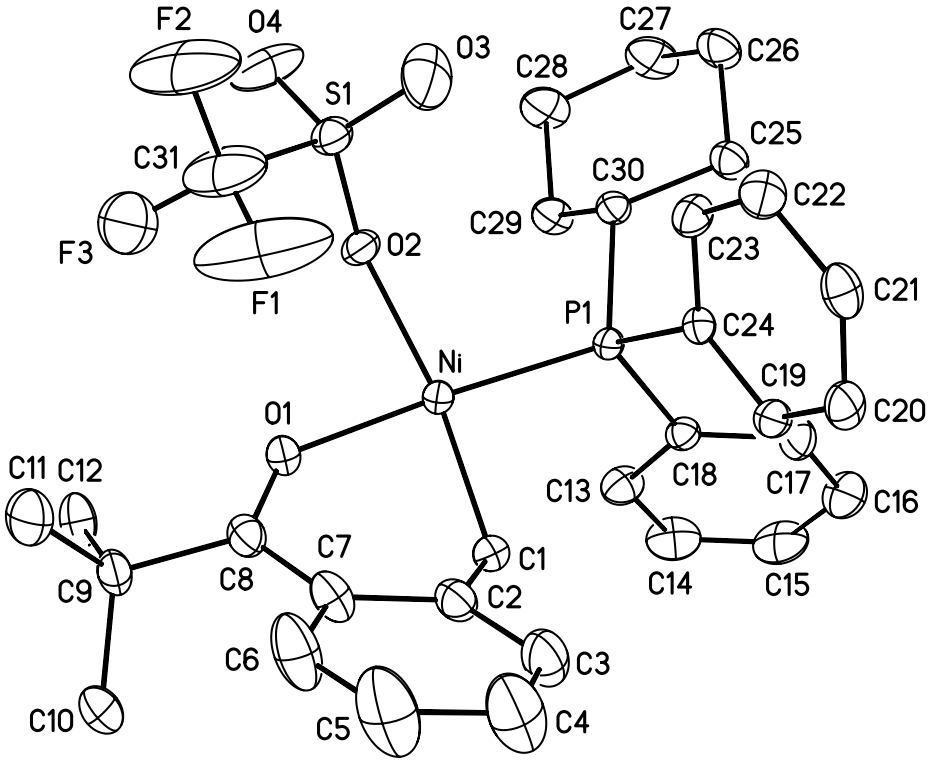
Preparation of Alkylnickel(II) Triflate 48



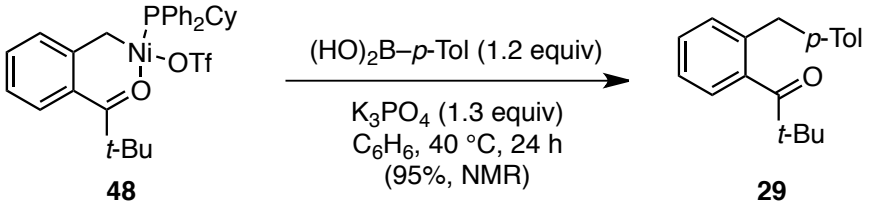
In a N_2-atmosphere glovebox, $Ni(cod)_2$ (55 mg, 0.20 mmol, 1.0 equiv), PPh_2Cy (59 mg, 0.20 mmol, 1.0 equiv), and benzene (0.2 M, 1.0 mL) were combined in a 1-dram vial. Ammonium triflate **47** (76 mg, 0.20 mmol, 1.0 equiv) was added. The vial was capped with a Teflon-lined cap and heated at 40 ºC for 3.5 h. The vial was then cooled to room temperature. The reaction mixture was filtered through a Kimwipe plug to remove insoluble material. Pentane (5 mL) was added, and the solution was stored overnight at –35 ºC. A purple precipitate formed. The supernatant was decanted off, and the obtained solid was washed with pentane (2 x 1 mL). The purple solid was recrystallized from benzene/pentane to give X-ray quality crystals (Fig S2) of compound **48** (66 mg, 51%) (mp 106 °C sinters; 120-125 °C dec. red film): ^{1}H NMR (600 MHz, C_6D_6) δ 7.75 (s, 4H), 7.36 (d, *J* = 7.8 Hz, 1H), 7.21 – 7.07 (m, 6H), 6.80 (t, *J* = 7.6 Hz, 1H), 6.69 (t, *J* = 7.5 Hz, 1H), 6.13 (d, *J* = 7.6 Hz, 1H), 2.02 (s, 2H), 1.49 (s, 2H), 1.44 – 1.31 (m, 6H), 1.19 (s, 9H), 0.82 – 0.62 (m, 3H); ^{13}C NMR (101 MHz, C_6D_6, 60 °C) δ 217.2, 145.6, 137.8, 134.2, 130.6, 129.4, 129.1, 128.7, 128.5, 128.3, 124.4, 44.7, 29.2, 28.0, 27.1, 23.2, 14.7, 14.0;[30] ^{31}P NMR (162.0 MHz, C_6D_6): δ 35.3; ^{19}F NMR (376.5 MHz, C_6D_6): δ –77.6.

[30] The quartet for the CF_3 group was not apparent in the ^{13}C NMR spectrum, despite long acquisition times and an extended relaxation delay. However, the ^{19}F NMR spectrum and crystal structure clearly indicate the presence of the triflate group.

Figure S2. Molecular diagram of **48** with ellipsoids at 30% probability. H-atoms omitted for clarity. (CCDC-899359)



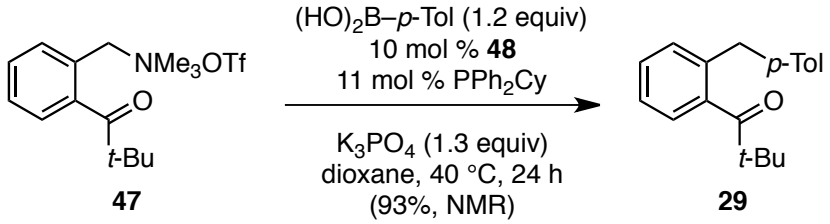
Reaction of Alkylnickel(II) Triflate 48 with *p*-Tolylboronic Acid



In a N_2-atmosphere glovebox, complex **48** (62 mg, 0.1 mmol, 1.0 equiv) *p*-tolylboronic acid (15 mg, 0.12 mmol, 1.2 equiv), and K_3PO_4 (28 mg, 0.13 mmol, 1.3 equiv) were weighed into a 1-dram vial. Dioxane (0.3 mL, 0.33 M) was added. The vial was capped with a Teflon-lined cap and removed from the glovebox. The mixture was heated at 40 °C for 24 h. The reaction mixture was then diluted with Et_2O (1.0 mL) and filtered through a plug of silica gel, which was rinsed with Et_2O (5 mL). The filtrate was concentrated, and 1,3,5-trimethoxybenzene (16.7 mg,

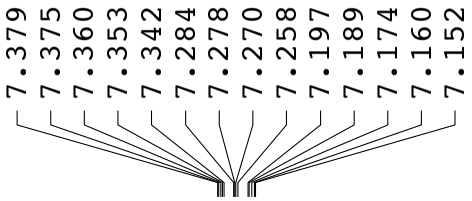
0.10 mmol, 1.0 equiv) was added as an internal standard. ^{1}H NMR analysis of the crude material showed 95% yield of diarylmethane **29**. The spectral data for this compound matches that reported above.

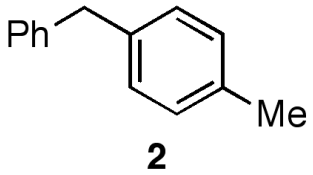
Catalytic Activity of Alkylnickel(II) Triflate 48



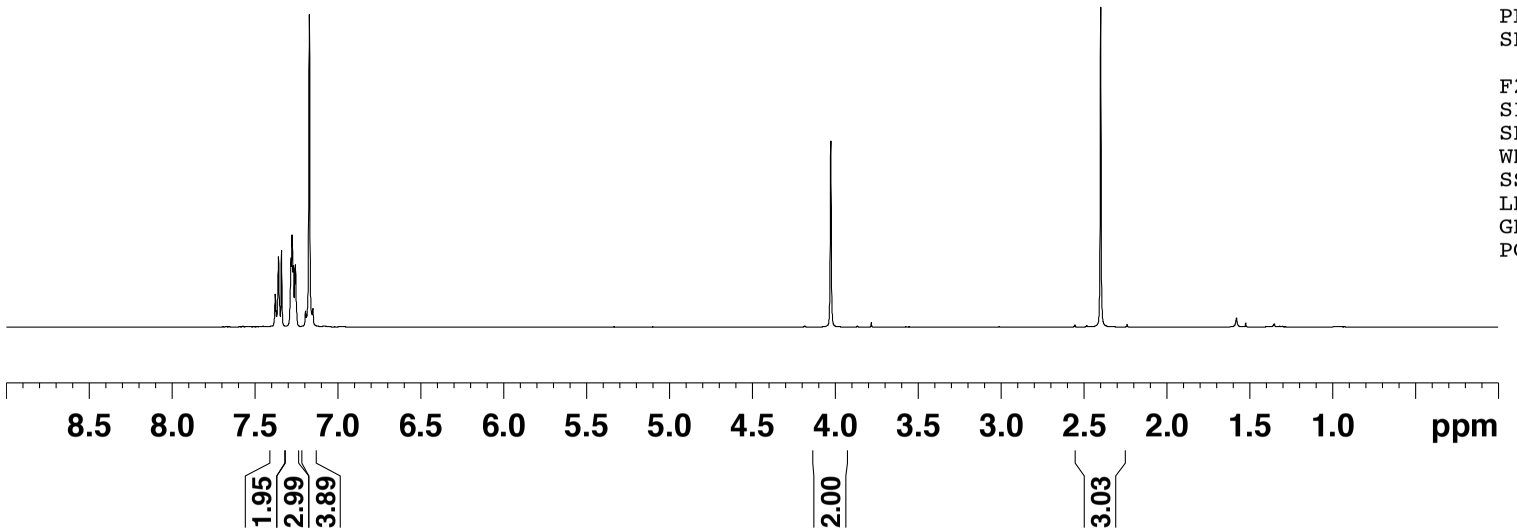
In a N_2-atmosphere glovebox, complex **48** (6.3 mg, 0.01 mmol, 10 mol %) *p*-tolylboronic acid (15 mg, 0.12 mmol, 1.2 equiv), K_3PO_4 (28 mg, 0.13 mmol, 1.3 equiv) and PPh_2Cy (4 mg, 0.01 mmol, 11 mol %) were weighed into a 1-dram vial, followed by dioxane (0.3 mL, 0.33 M). The vial was capped with a Teflon-lined cap and removed from the glovebox. The mixture was heated at 40 °C for 24 h. The reaction mixture was then diluted with Et_2O (1.0 mL) and filtered through a plug of silica gel, which was rinsed with Et_2O (5 mL). The filtrate was concentrated, and 1,3,5-trimethoxybenzene (16.8 mg, 0.10 mmol, 1.0 equiv) was added as an internal standard. ^{1}H NMR analysis of the crude material showed 98% yield of diarylmethane **29**. The reaction of complex **48** was included in the calculation of the maximum theoretical yield. Thus, 1.1 equiv of product **29** are possible in this reaction. The spectral data for this compound matches that reported above.

Compound 2, 1HNMR





2



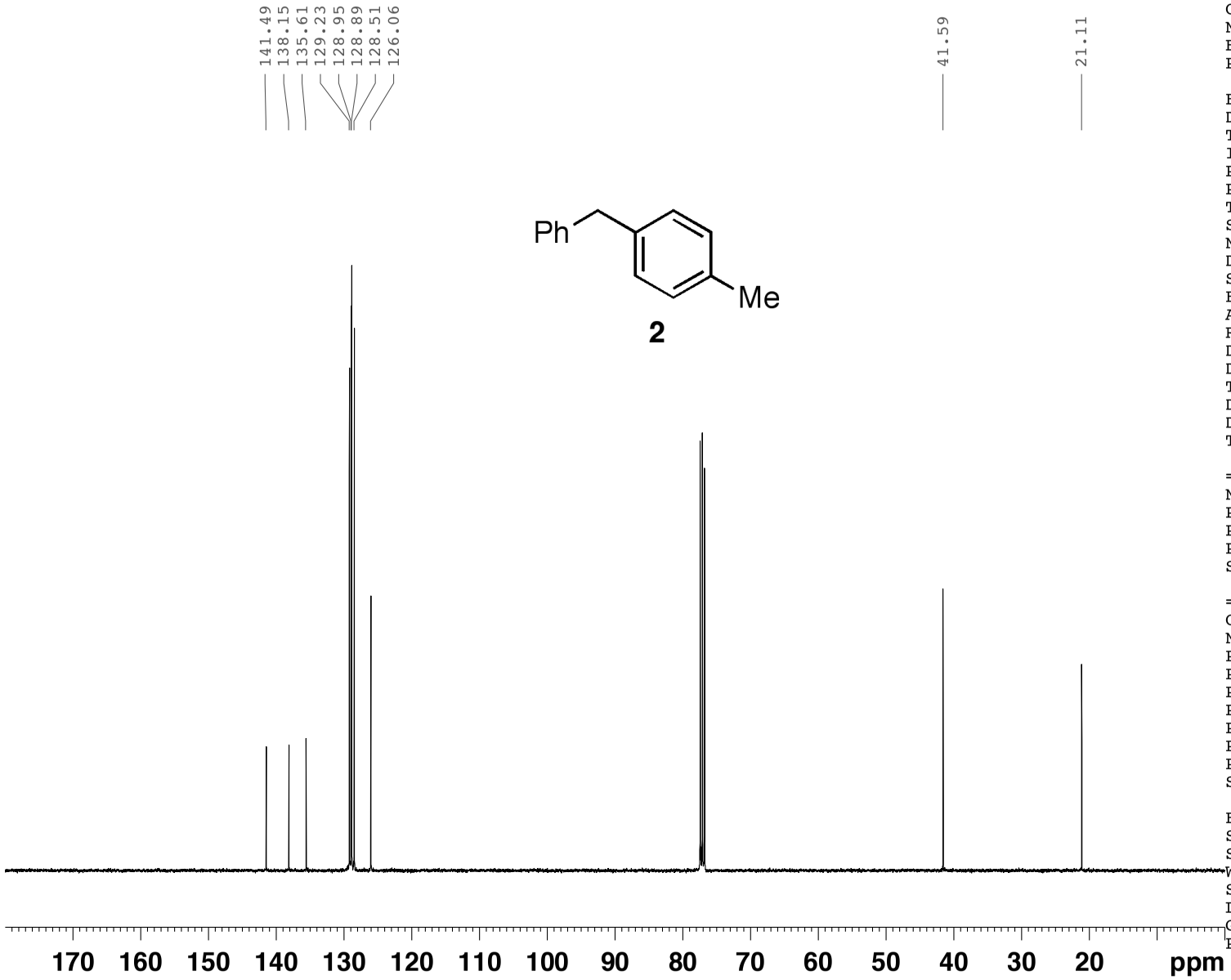

```
Current Data Parameters
NAME      PM-3-291-1-1H
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20120711
Time              12.17
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8278.146 Hz
FIDRES        0.126314 Hz
AQ            3.9584243 sec
RG                14.3
DW              60.400 usec
DE               6.00 usec
TE              298.1 K
D1          1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1              15.00 usec
PL1              4.90 dB
PL1W        3.30822015 W
SFO1      400.1324710 MHz

F2 - Processing parameters
SI                32768
SF        400.1300000 MHz
WDW                 EM
SSB                  0
LB              0.30 Hz
GB                   0
PC               1.00
```

Compound 2, 13CNMR

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Current Data Parameters
NAME      PM-3-291-1-13C
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20120711
Time              12.20
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
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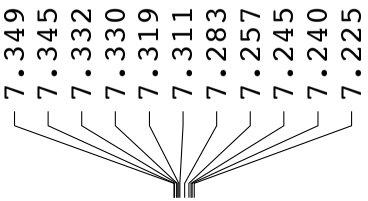
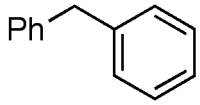
Compound 3, 1HNMR





3

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Current Data Parameters
NAME        DMM3-077-1-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120522
Time               17.47
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  12.7
DW                60.400 usec
DE                 6.00 usec
TE                298.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
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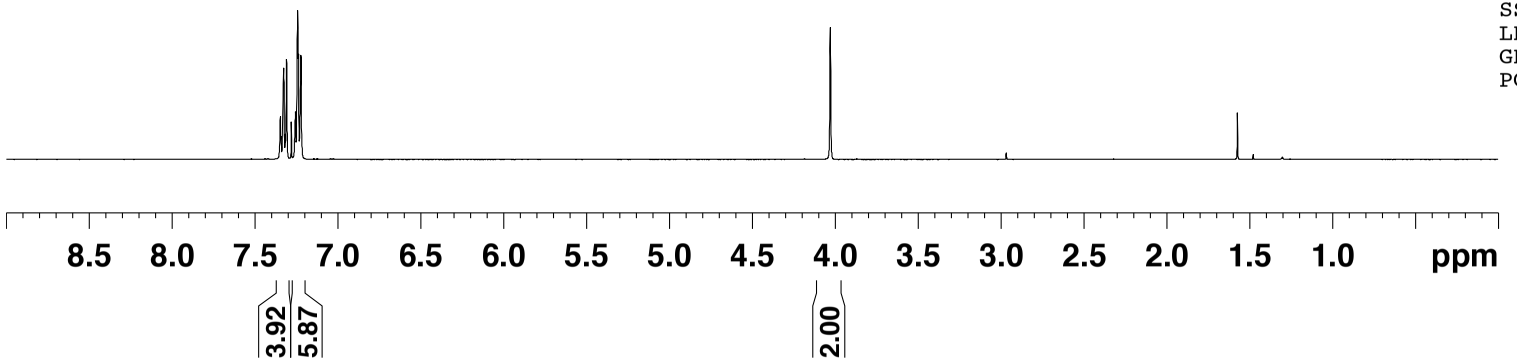
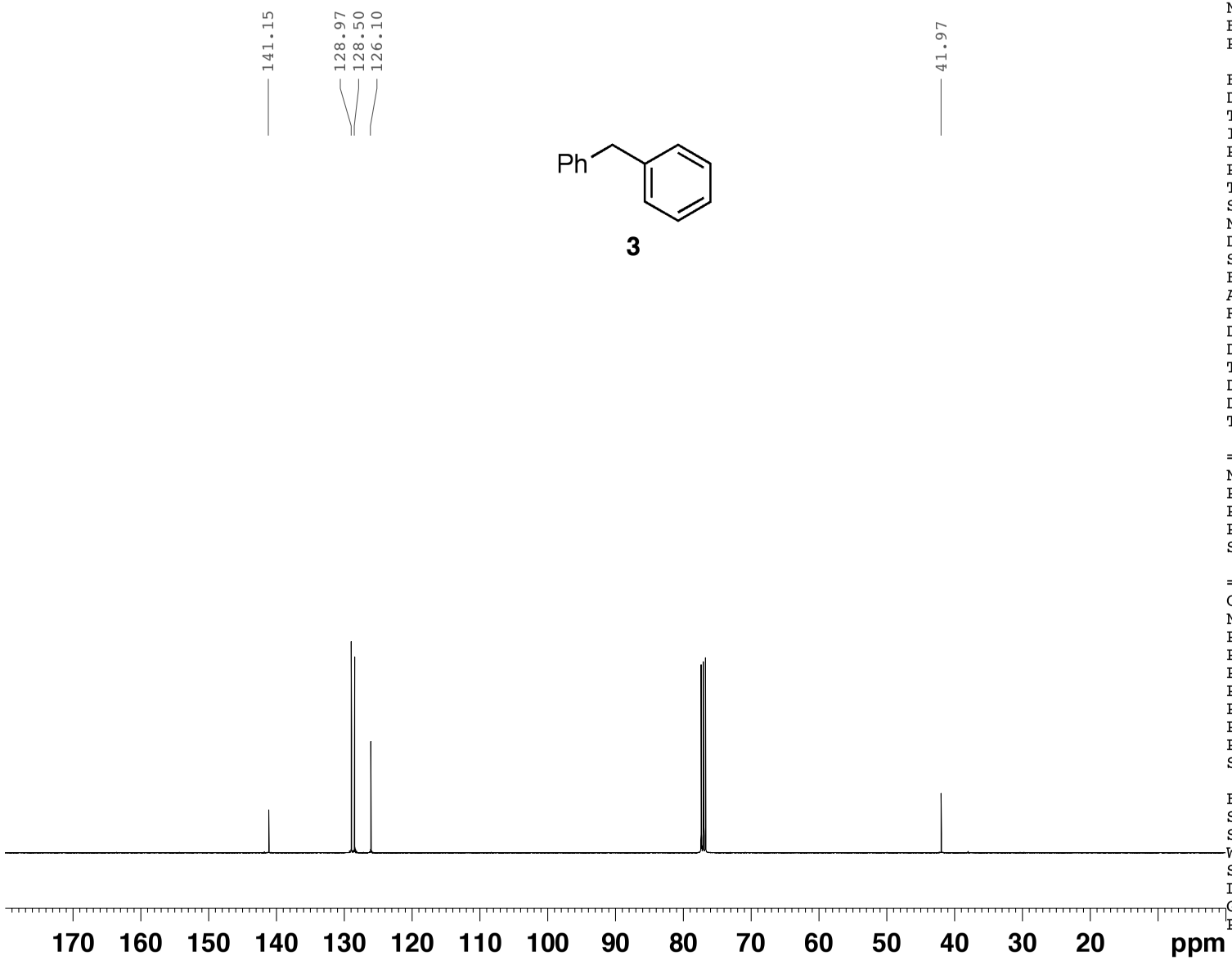


Compound 3, 13CNMR




```
Current Data Parameters
NAME        DMM3-077-1-2
EXPNO                  2
PROCNO                 1

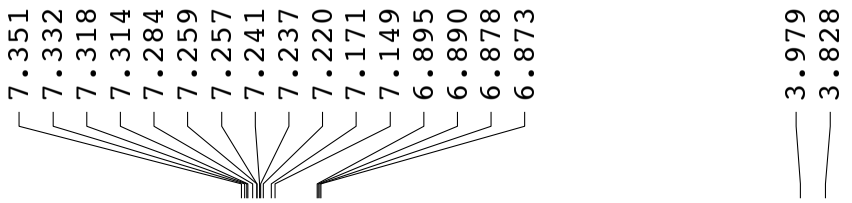
F2 - Acquisition Parameters
Date_           20120522
Time              23.05
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

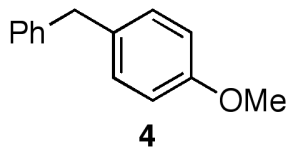
======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1                0.55 dB
PL1W        35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2       400.1316005 MHz

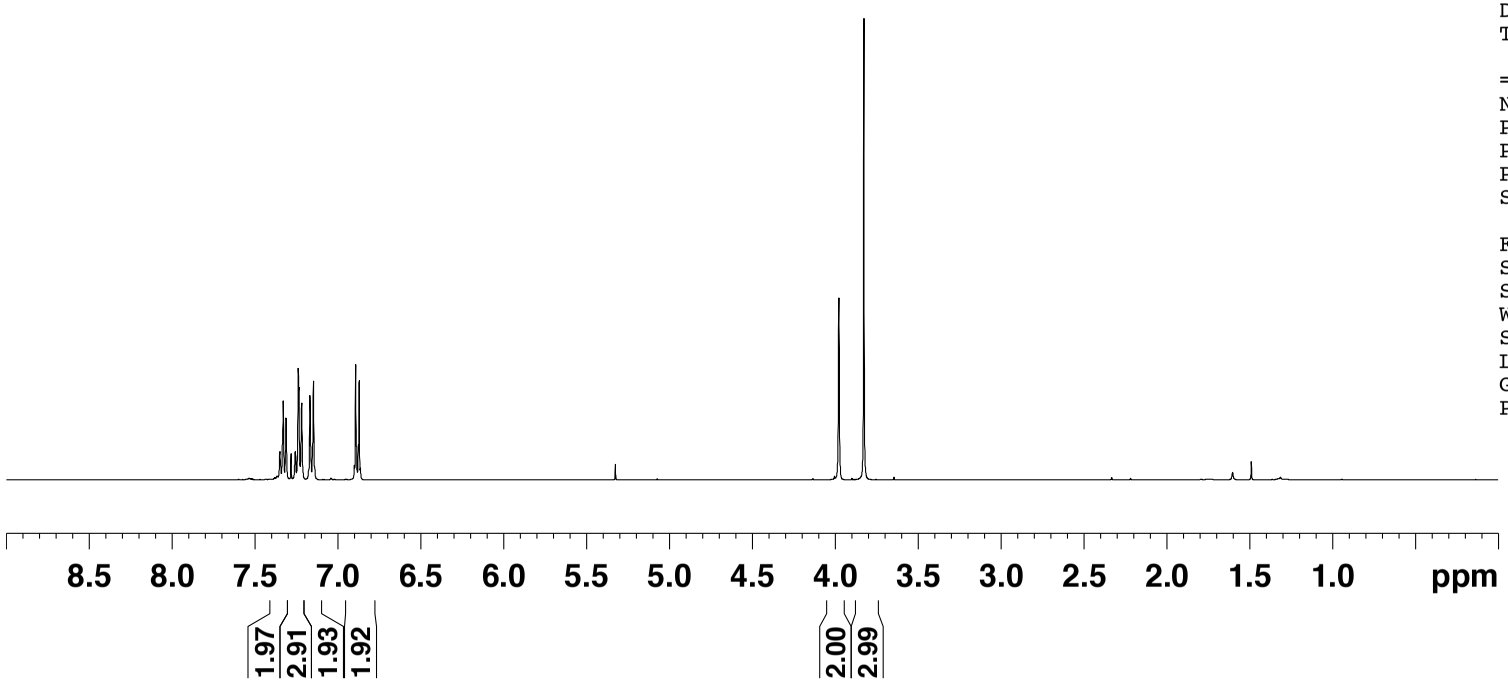
F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 4, 1HNMR





4

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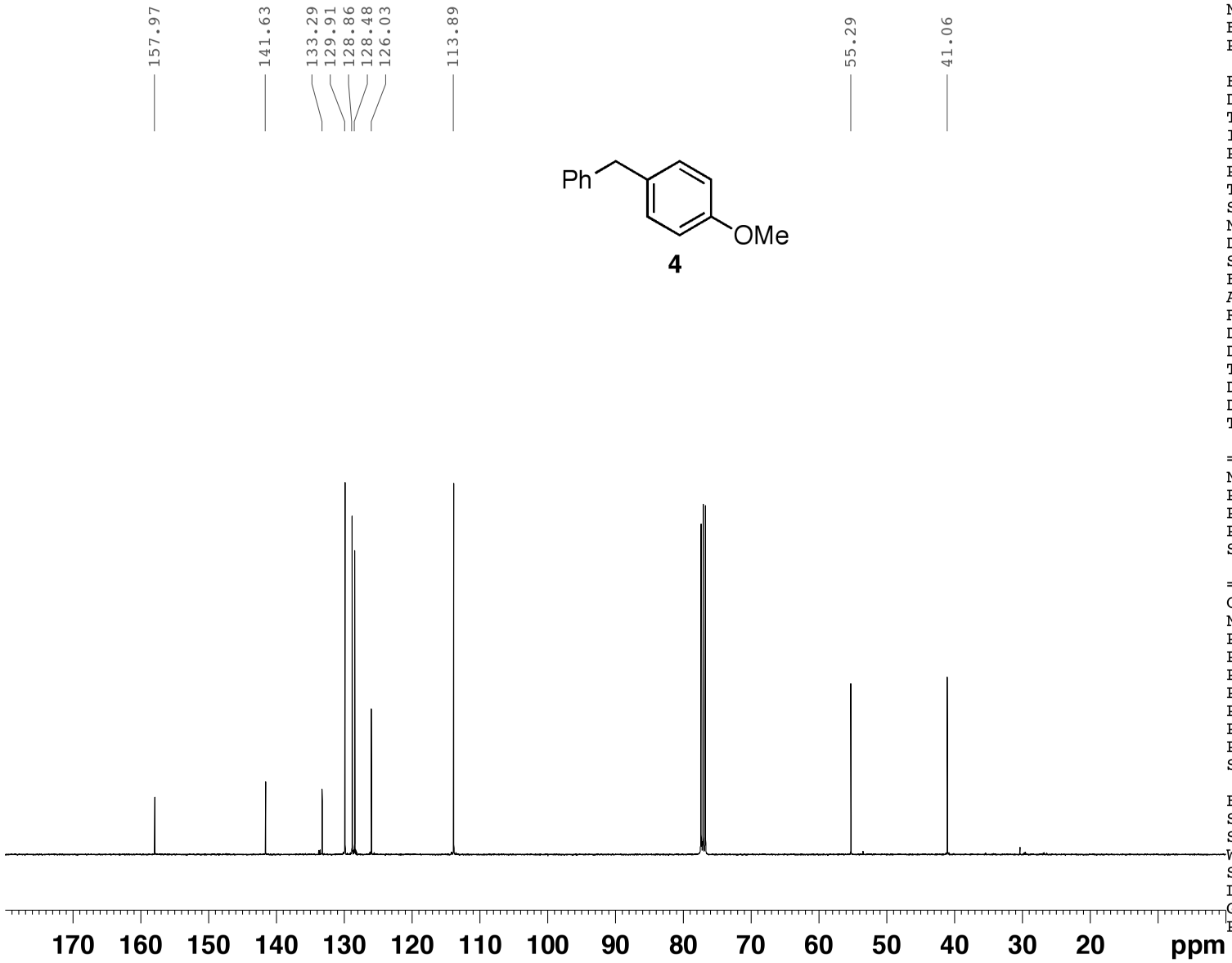
Current Data Parameters
NAME          DMM3-104-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120706
Time              16.35
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                 10.1
DW               60.400 usec
DE                6.00 usec
TE                298.1 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

Compound 4, 13CNMR




```
Current Data Parameters
NAME          DMM3-104-1
EXPNO                  2
PROCNO                 1

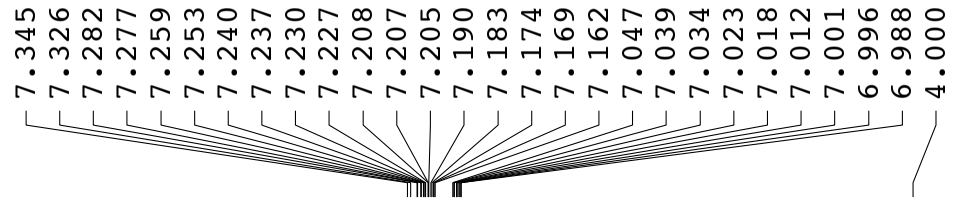
F2 - Acquisition Parameters
Date_           20120706
Time              16.51
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

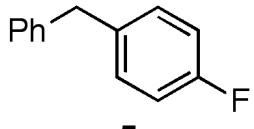
======== CHANNEL f1 ========
NUC1                13C
P1                9.25 usec
PL1               0.55 dB
PL1W       35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2               4.90 dB
PL12             20.46 dB
PL13             21.00 dB
PL2W        3.30822015 W
PL12W       0.09195905 W
PL13W       0.08120718 W
SFO2       400.1316005 MHz

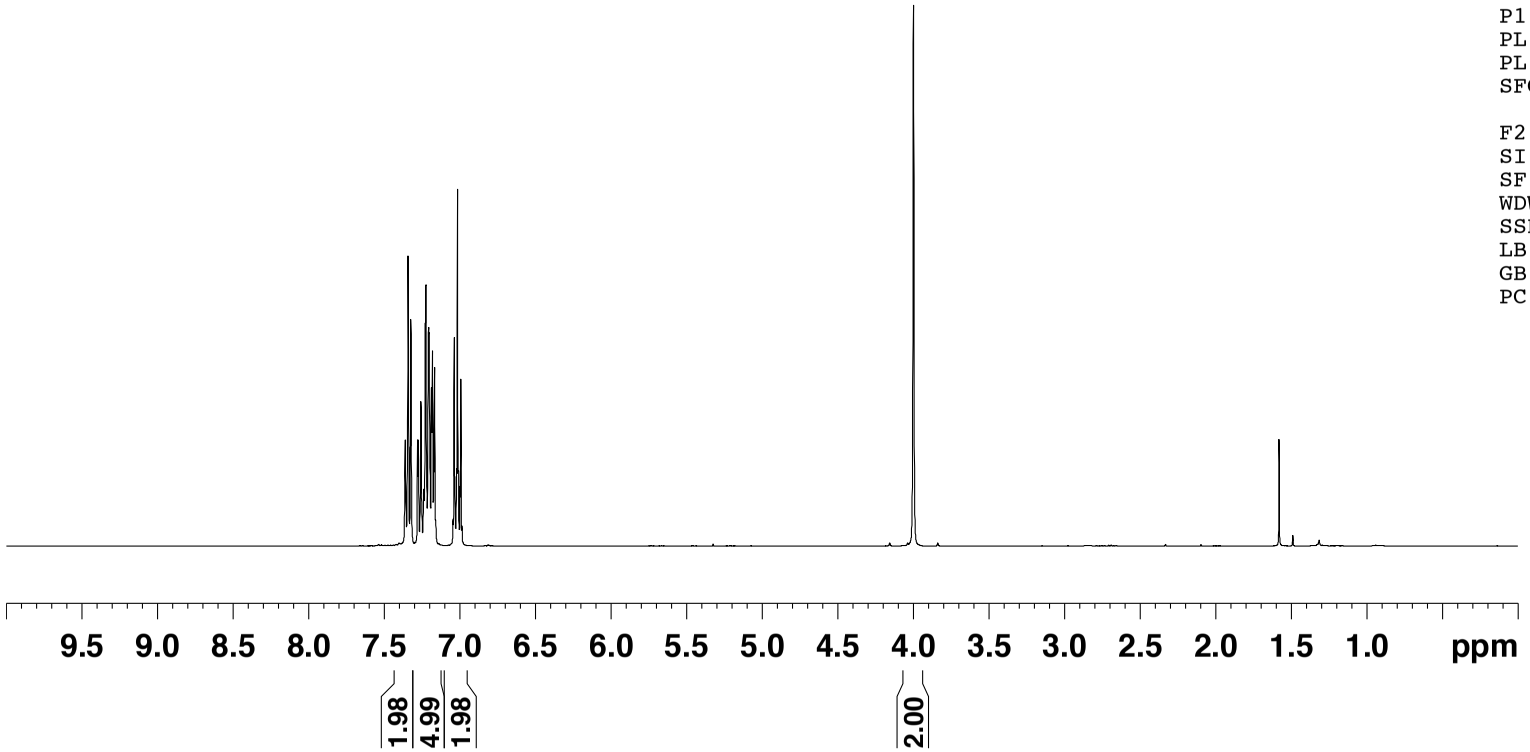
F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC                1.40
```

Compound 5, 1HNMR





5



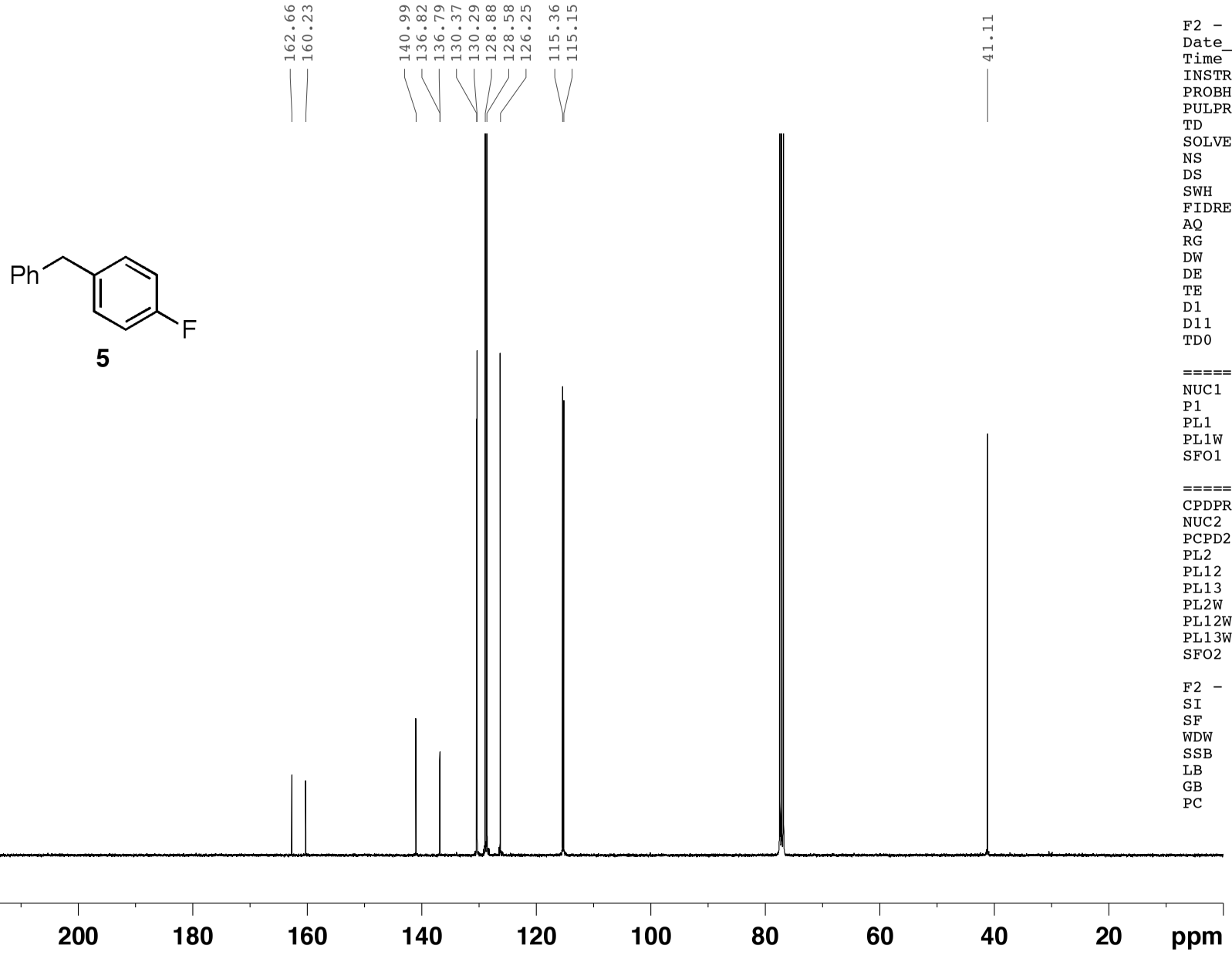

```
Current Data Parameters
NAME          DMM3-077-3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120522
Time              21.40
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES        0.126314 Hz
AQ            3.9584243 sec
RG                 28.5
DW               60.400 usec
DE                6.00 usec
TE                298.2 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                 1.00
```

Compound 5, 13CNMR

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Current Data Parameters
NAME          DMM3-077-3
EXPNO                  2
PROCNO                 1

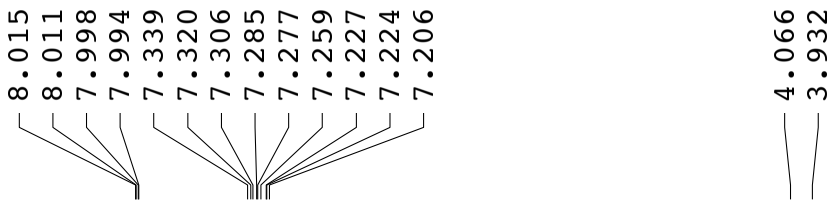
F2 - Acquisition Parameters
Date_           20120522
Time               21.37
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

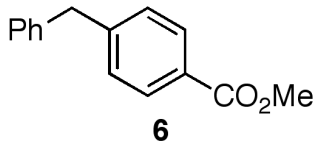
======== CHANNEL f1 ========
NUC1                 13C
P1                9.25 usec
PL1               0.55 dB
PL1W        35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            90.00 usec
PL2               4.90 dB
PL12             20.46 dB
PL13             21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2       400.1316005 MHz

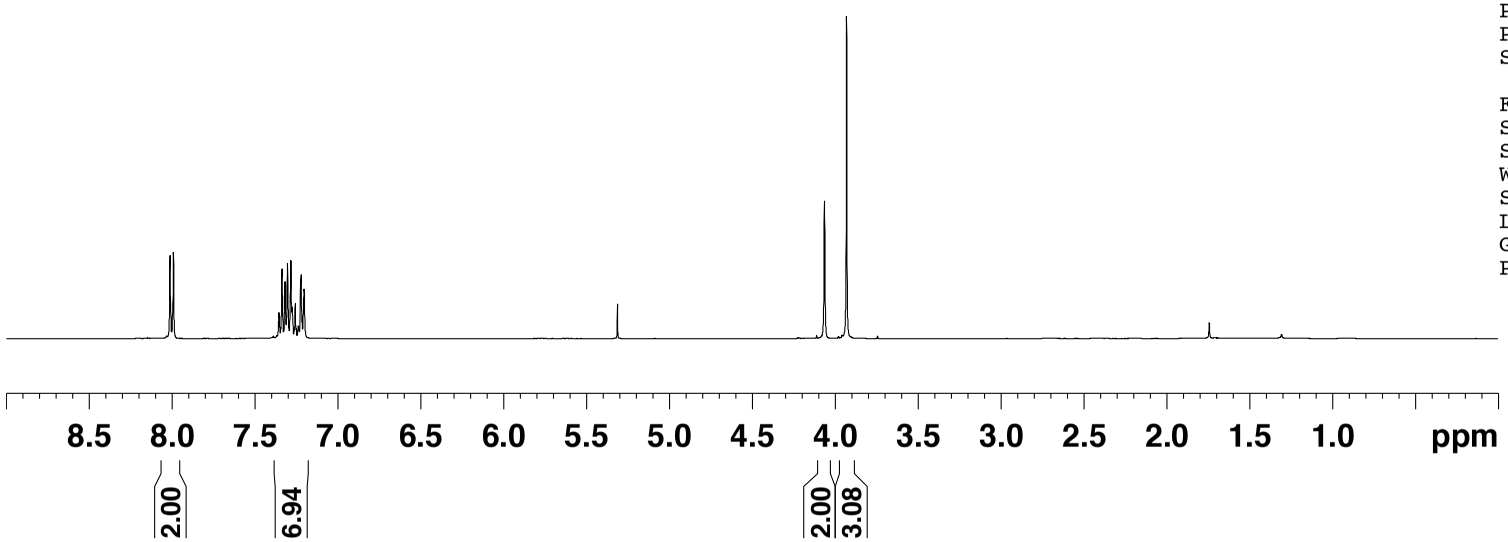
F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

Compound 6, 1HNMR





6



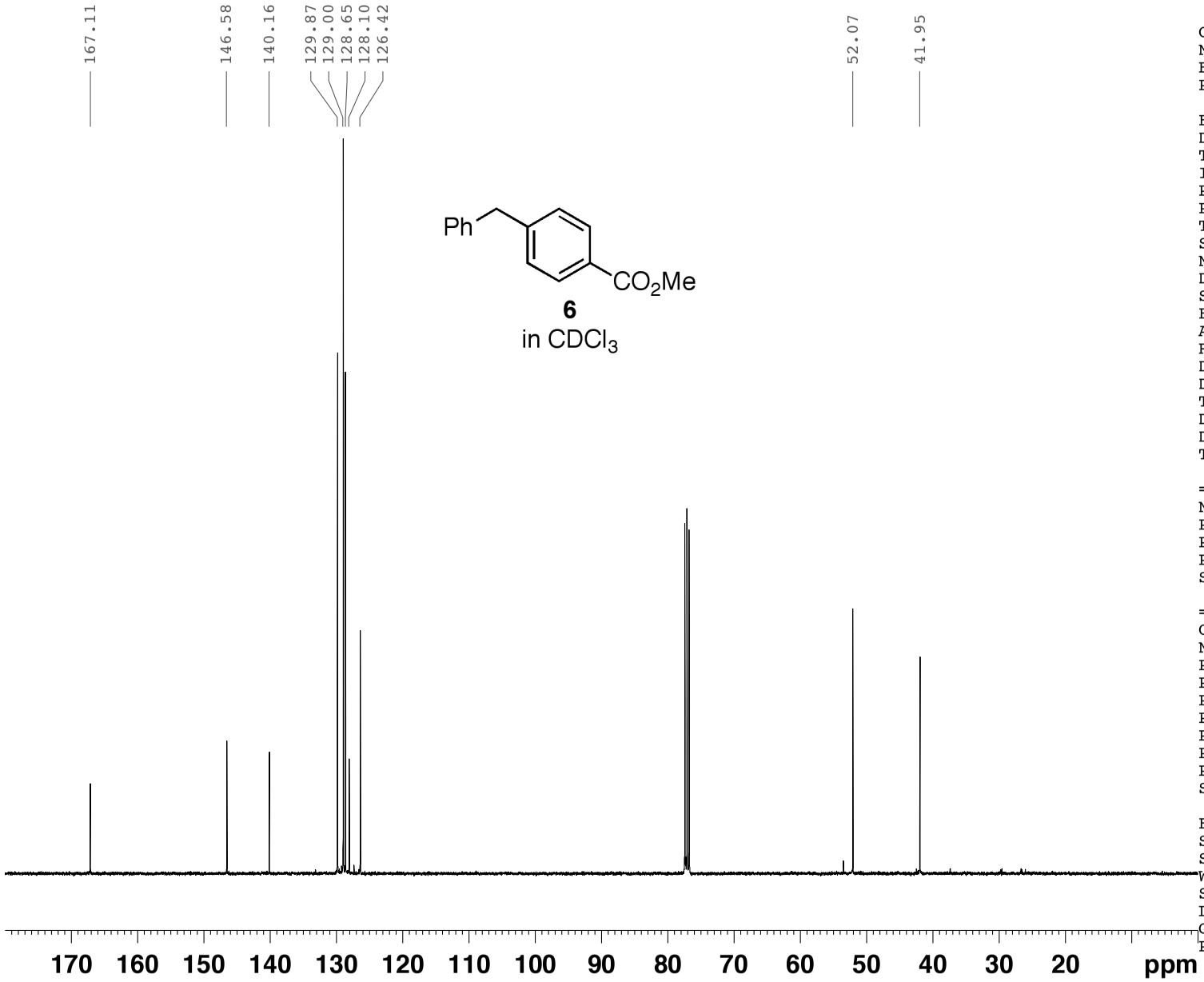

```
Current Data Parameters
NAME        PM-3-Ester-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120717
Time               12.14
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  11.3
DW                60.400 usec
DE                 6.00 usec
TE                298.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

Compound 6, 13CNMR



Current Data Parameters
NAME PM-3-Ester-2
EXPNO 2
PROCNO 1

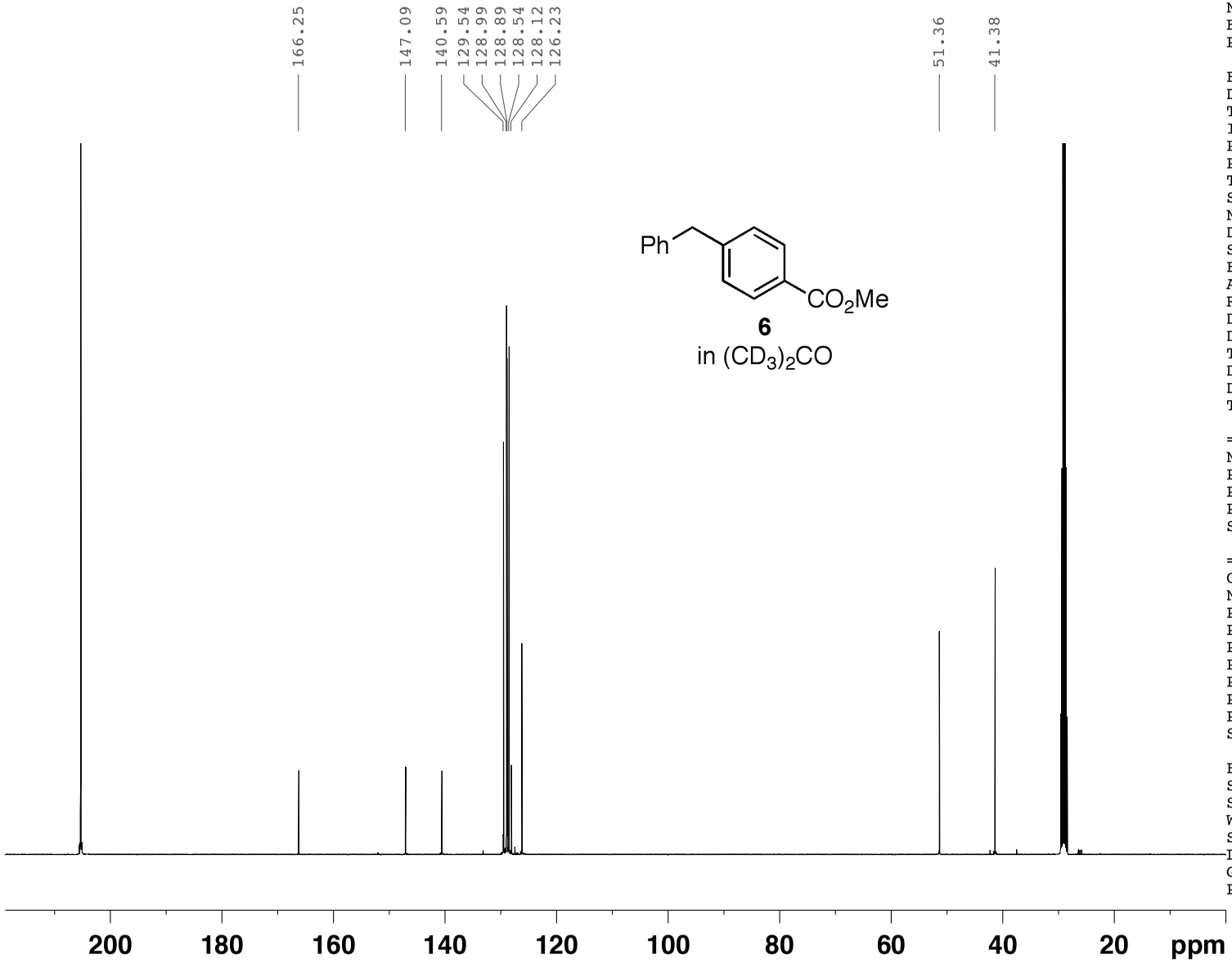
F2 - Acquisition Parameters
Date_ 20120717
Time 12.17
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 512
DW 20.850 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PL1 0.55 dB
PL1W 35.18820572 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 4.90 dB
PL12 20.46 dB
PL13 21.00 dB
PL2W 3.30822015 W
PL12W 0.09195905 W
PL13W 0.08120718 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 6, 13CNMR in Acetone-D




```
Current Data Parameters
NAME      PM-4-Methylester-rerun
EXPNO                  1
PROCNO                 1

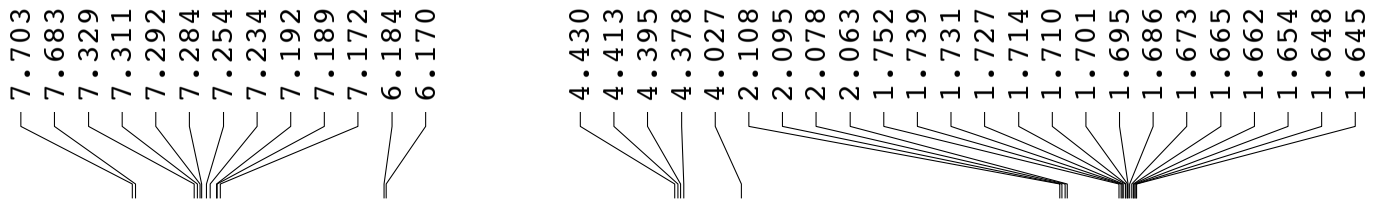
F2 - Acquisition Parameters
Date_           20120816
Time                2.30
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG           zgpg30
TD                65536
SOLVENT          Acetone
NS                 1024
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                  512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

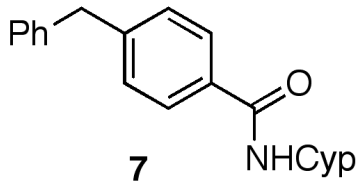
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12                20.46 dB
PL13                21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

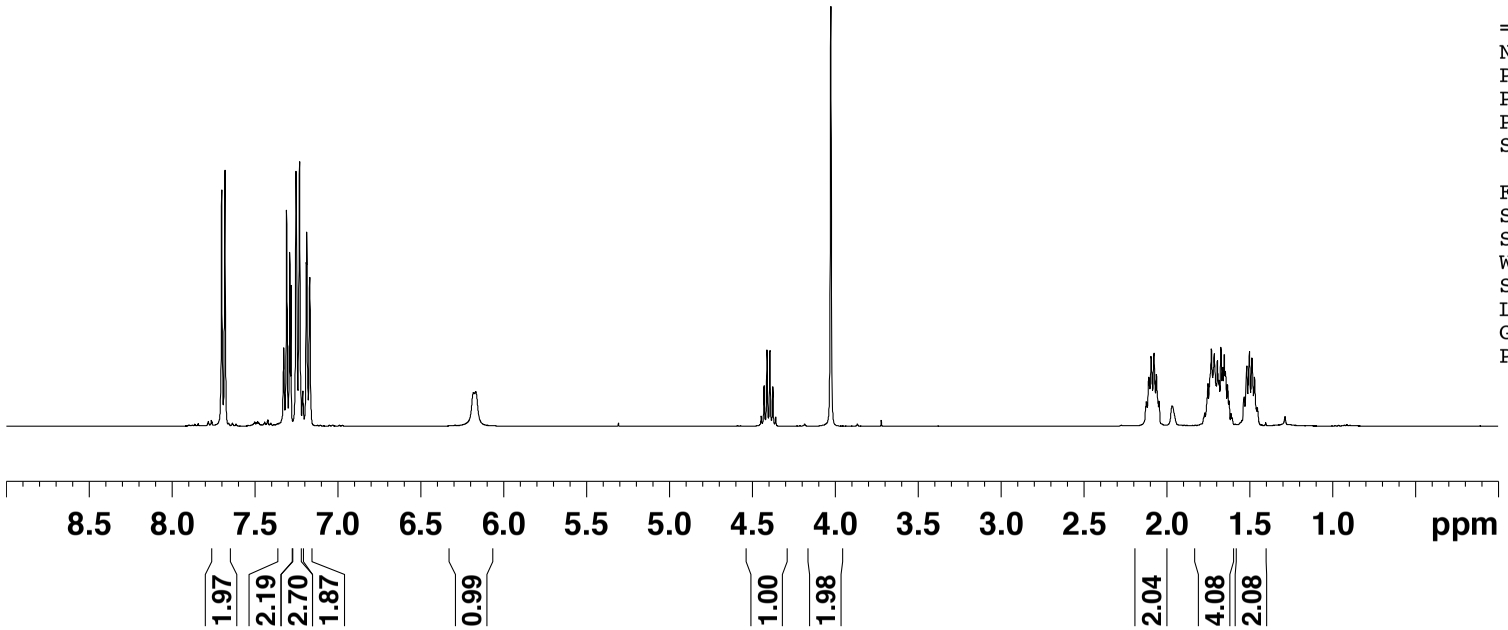
F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 7, 1HNMR





7



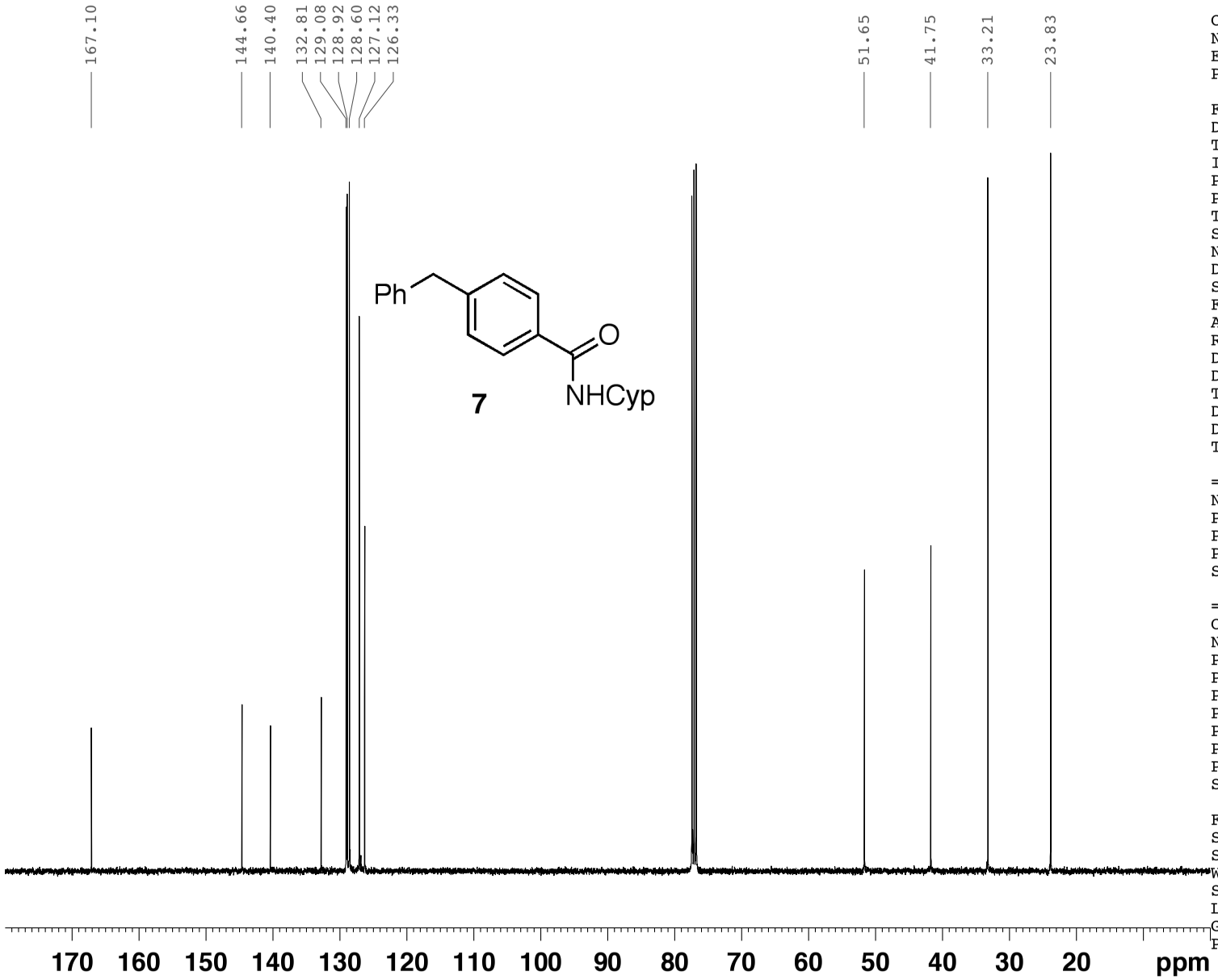
Current Data Parameters
NAME PM-4-17-4
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120711
Time 11.39
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 7.1
DW 60.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 4.90 dB
PL1W 3.30822015 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 7, 13NMR

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Current Data Parameters
NAME          PM-4-17-4
EXPNO                 4
PROCNO                1

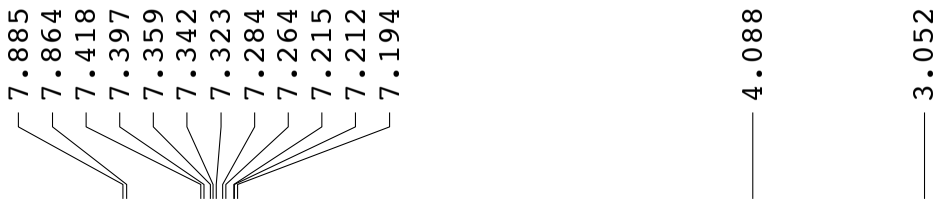
F2 - Acquisition Parameters
Date_          20120711
Time              11.43
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

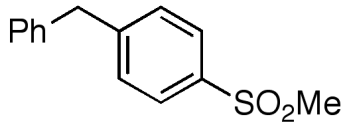
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

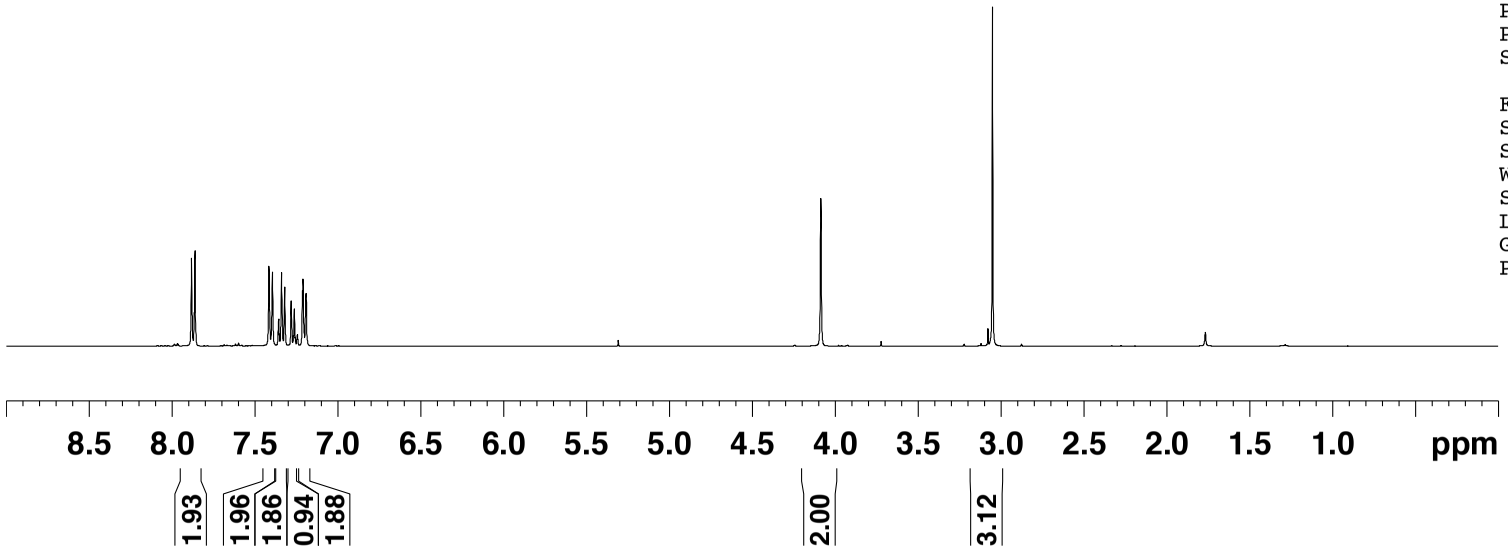
F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 8, 1HNMR





8



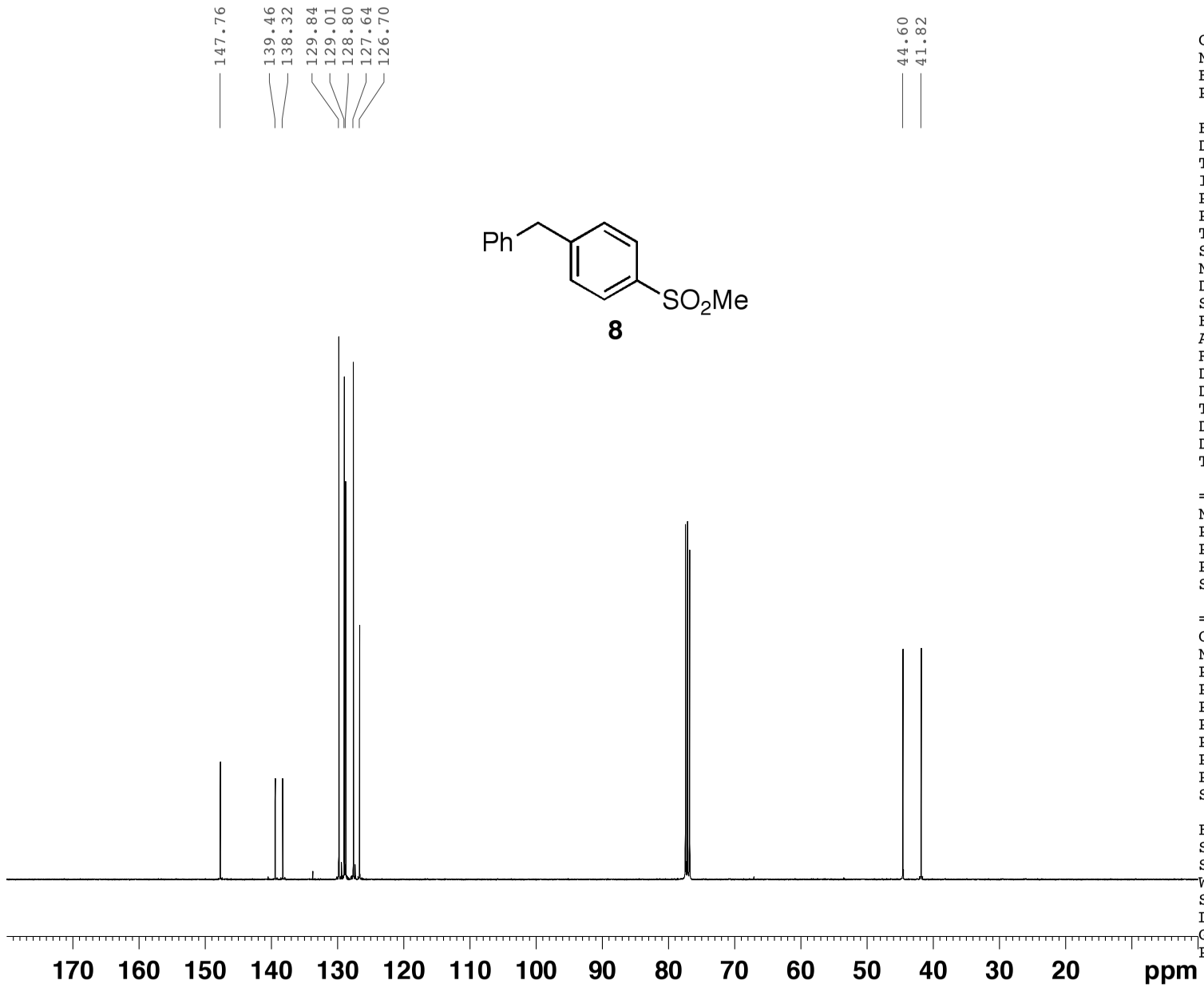

```
Current Data Parameters
NAME           PM-4-10-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120705
Time                5.41
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  11.3
DW                60.400 usec
DE                 6.00 usec
TE                298.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

Compound 8, 13CNMR



Current Data Parameters
NAME PM-4-10-1
EXPNO 2
PROCNO 1

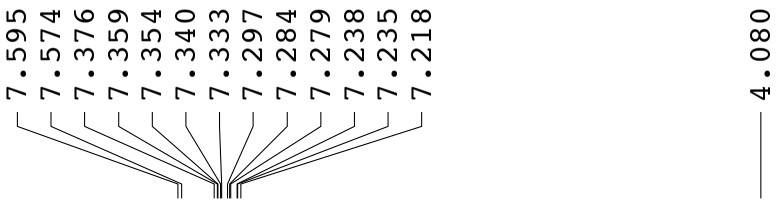
F2 - Acquisition Parameters
Date_ 20120705
Time 5.57
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 512
DW 20.850 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

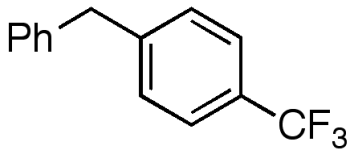
======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PL1 0.55 dB
PL1W 35.18820572 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 4.90 dB
PL12 20.46 dB
PL13 21.00 dB
PL2W 3.30822015 W
PL12W 0.09195905 W
PL13W 0.08120718 W
SFO2 400.1316005 MHz

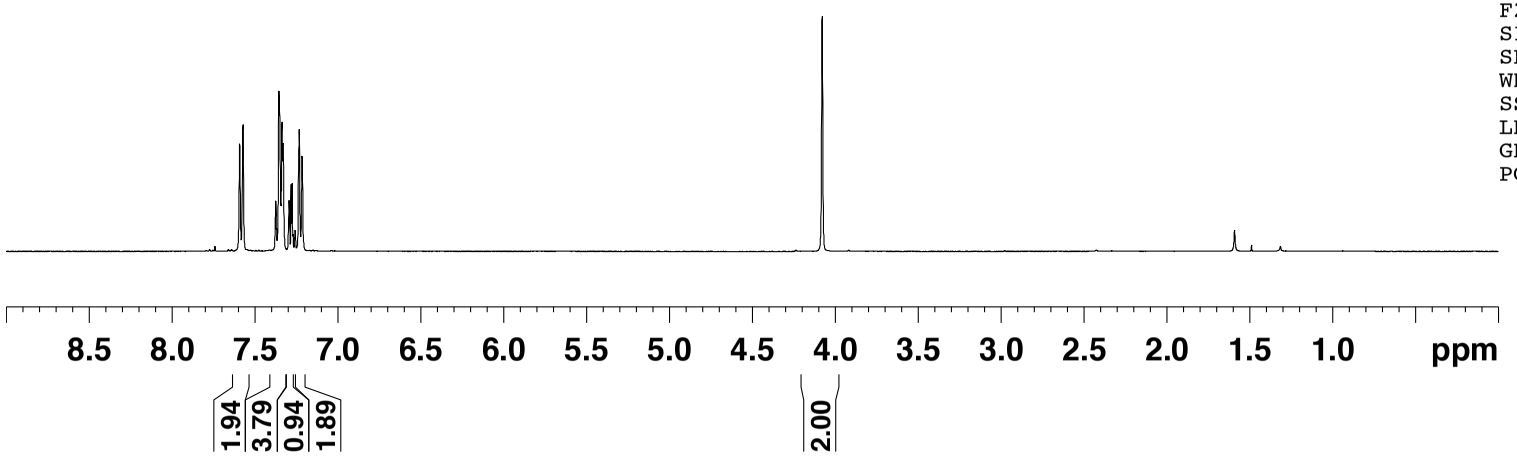
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 9, 1HNMR





9



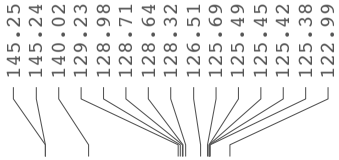

```
Current Data Parameters
NAME                  PM-4-10-2
EXPNO                         1
PROCNO                        1

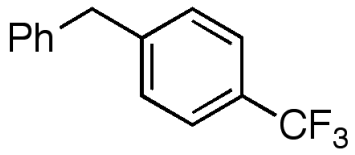
F2 - Acquisition Parameters
Date_                  20120705
Time                       6.03
INSTRUM                   spect
PROBHD    5 mm CPQNP 1H/
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                           11.3
DW                        60.400 usec
DE                         6.00 usec
TE                        298.1 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        15.00 usec
PL1                        4.90 dB
PL1W                 3.30822015 W
SFO1               400.1324710 MHz

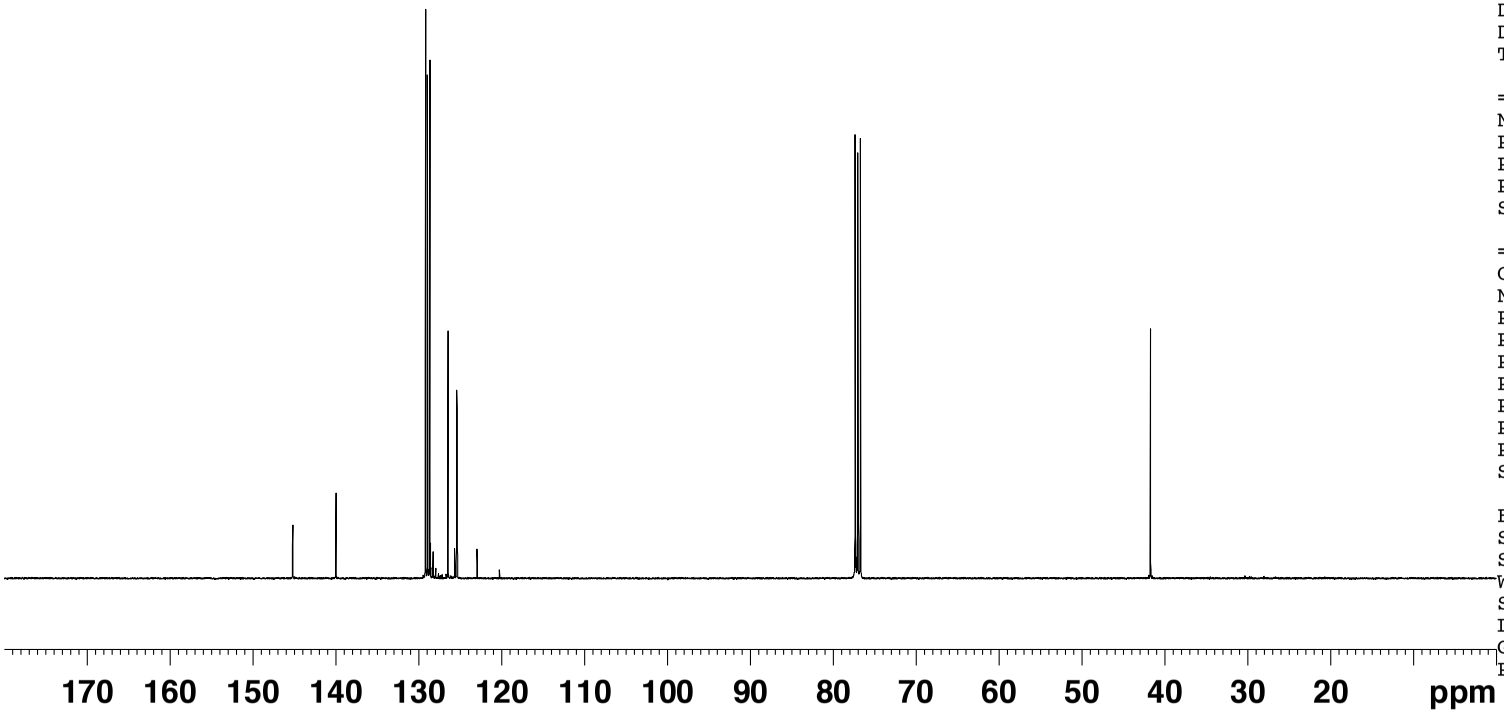
F2 - Processing parameters
SI                        32768
SF                 400.1300000 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

Compound 9, 13CNMR





9




```
Current Data Parameters
NAME          PM-4-10-2
EXPNO                 2
PROCNO                1

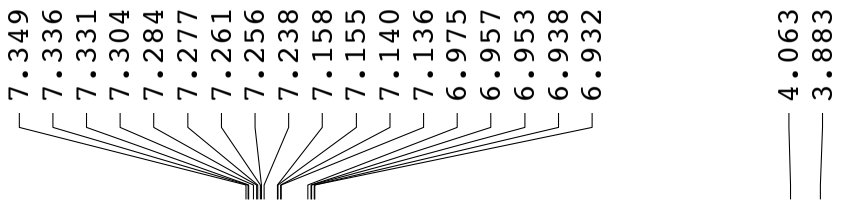
F2 - Acquisition Parameters
Date_          20120705
Time               6.19
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

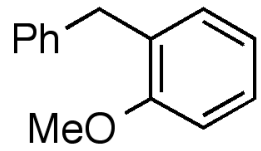
======== CHANNEL f1 ========
NUC1                13C
P1                9.25 usec
PL1               0.55 dB
PL1W        35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2               4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2       400.1316005 MHz

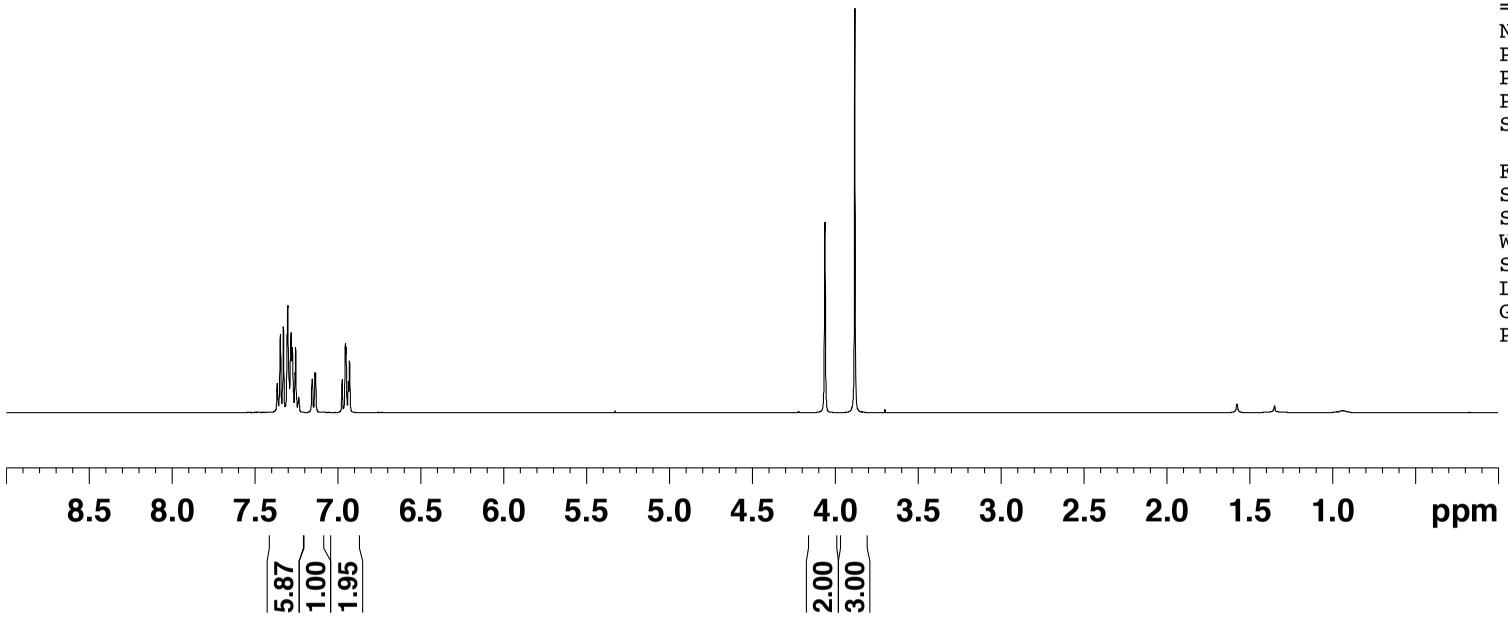
F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 10, 1HNMR





10



Current Data Parameters

NAME	PM-4-18-2
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120711
Time	12.36
INSTRUM	spect
PROBHD	5 mm CPQNP 1H/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	14.3
DW	60.400 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1

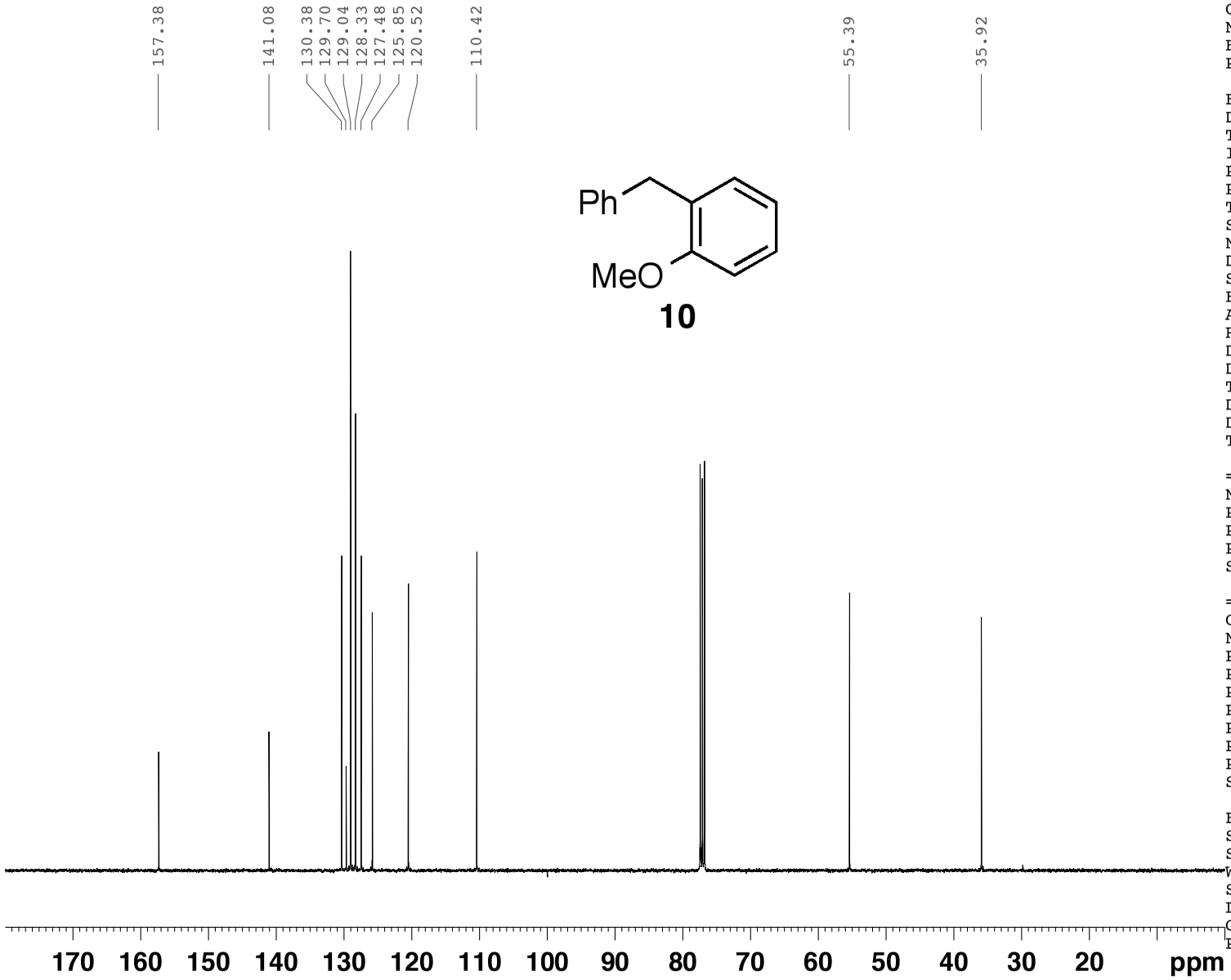
======== CHANNEL f1 ========

NUC1	1H
P1	15.00 usec
PL1	4.90 dB
PL1W	3.30822015 W
SFO1	400.1324710 MHz

F2 - Processing parameters

SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Compound 10, 13CNMR




```
Current Data Parameters
NAME          PM-4-18-2
EXPNO                 2
PROCNO                1

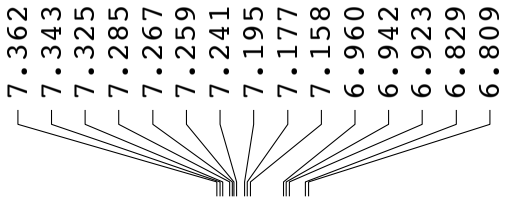
F2 - Acquisition Parameters
Date_          20120711
Time              12.39
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

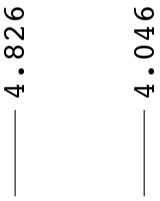
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

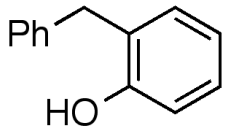
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

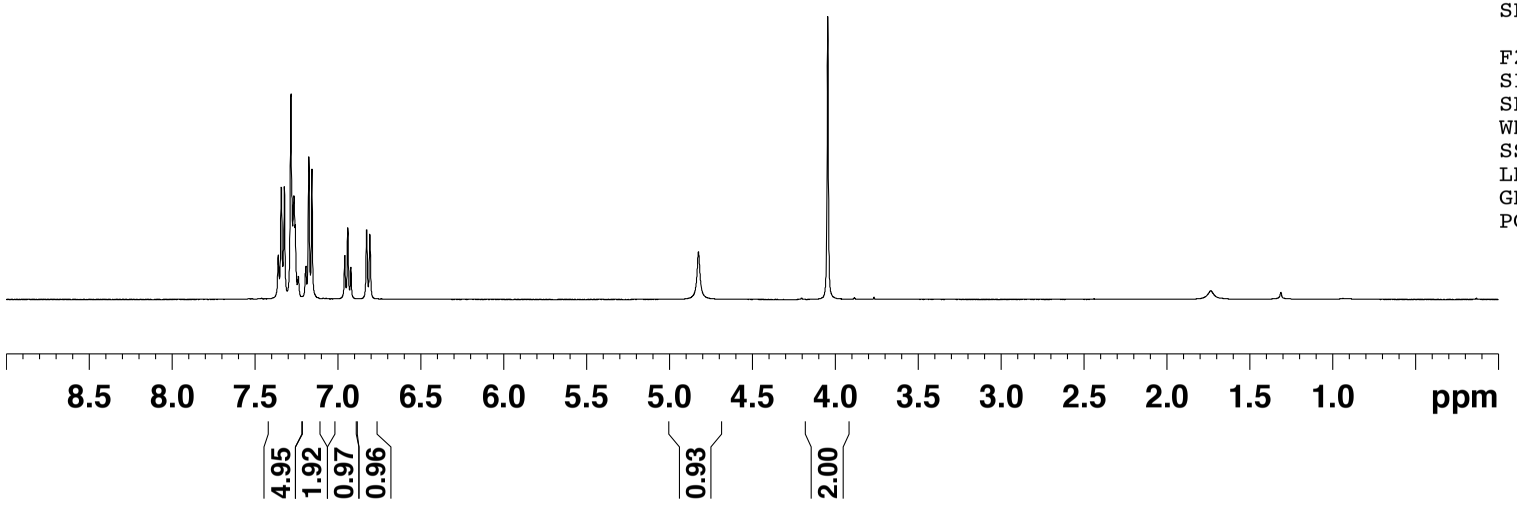
Compound 11, 1HNMR







11



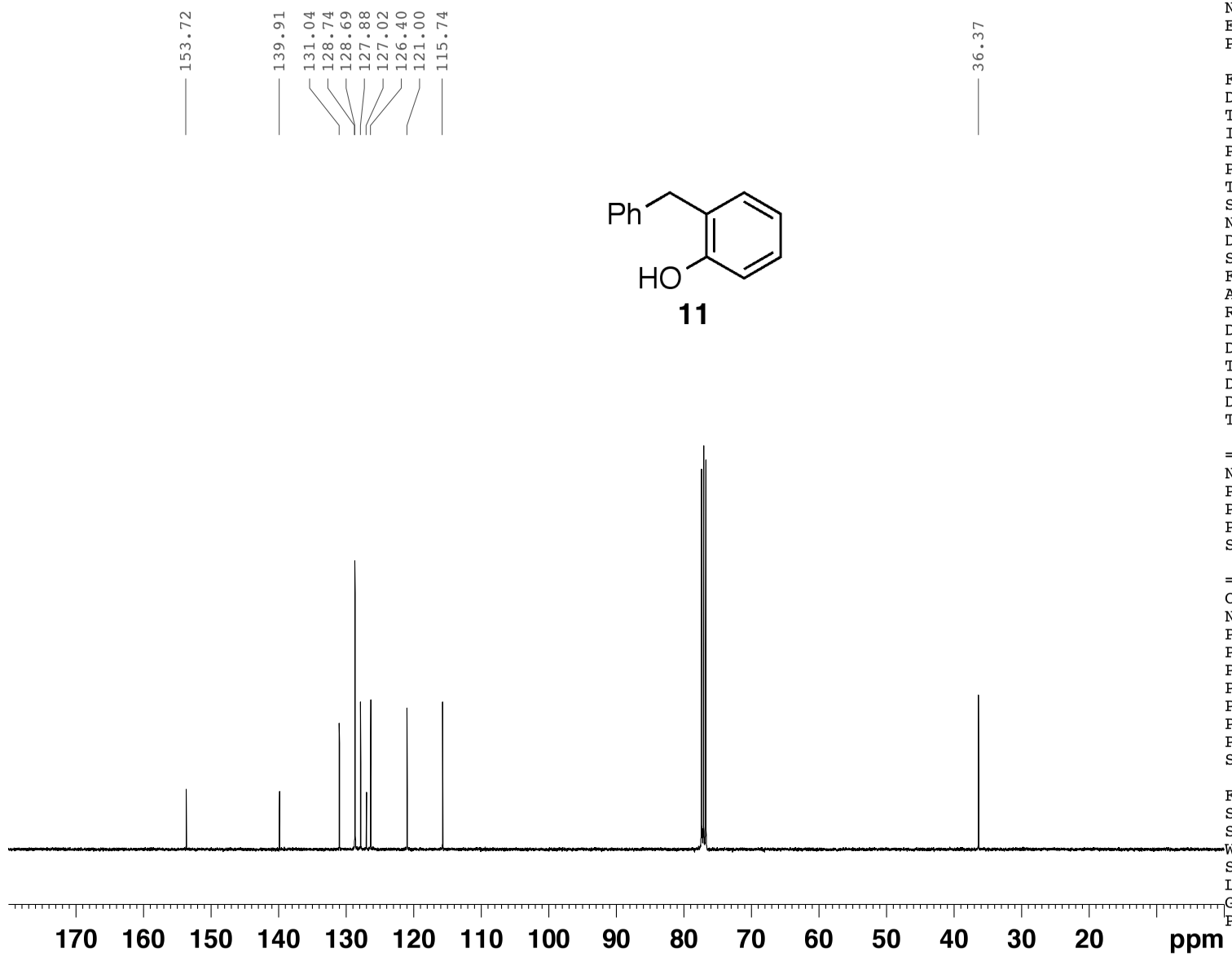

```
Current Data Parameters
NAME      PM-4-36-5, pure
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120727
Time              10.52
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                 10.1
DW               60.400 usec
DE                6.00 usec
TE                298.2 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

Compound 11, 13CNMR




```
Current Data Parameters
NAME      PM-4-36-5, pure
EXPNO                  2
PROCNO                 1

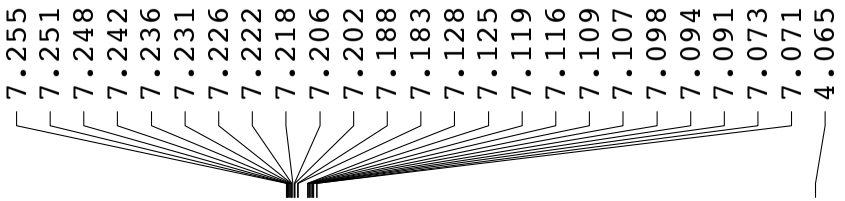
F2 - Acquisition Parameters
Date_           20120727
Time              10.55
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

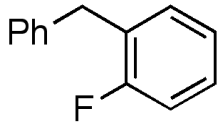
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

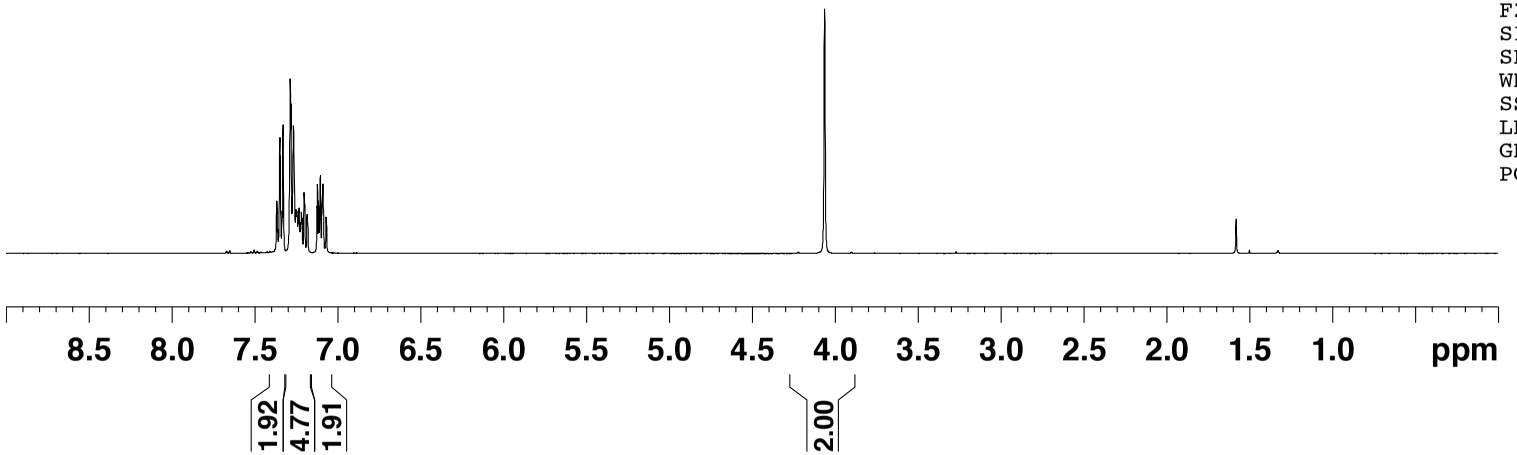
F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 12, 1HNMR





12



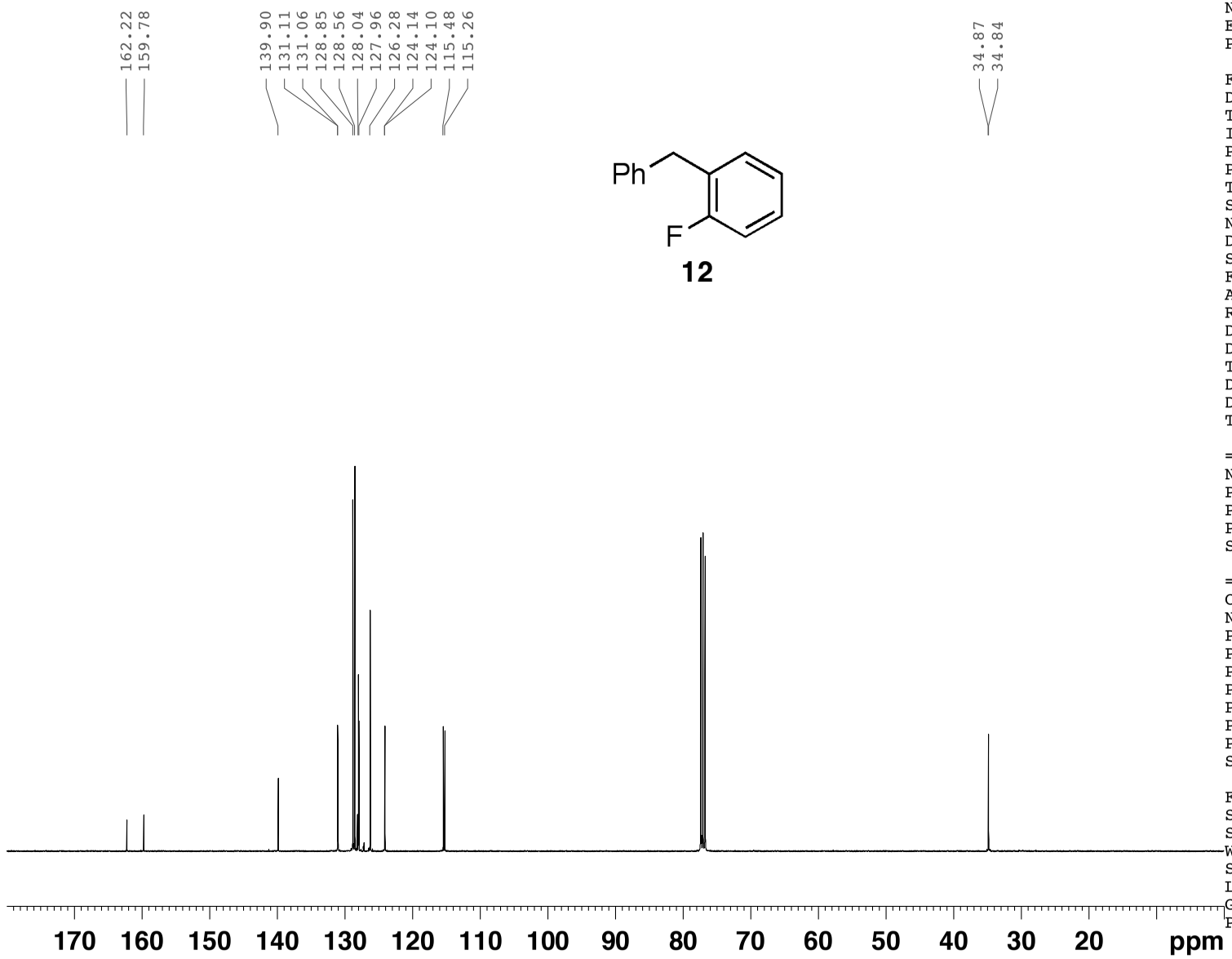

```
Current Data Parameters
NAME           PM-4-17-4
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120705
Time                6.25
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  11.3
DW                60.400 usec
DE                 6.00 usec
TE                298.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

Compound 12, 13CNMR




```
Current Data Parameters
NAME          PM-4-17-4
EXPNO                 2
PROCNO                1

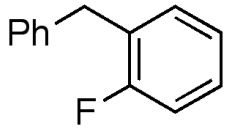
F2 - Acquisition Parameters
Date_          20120705
Time               6.41
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1                0.55 dB
PL1W        35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 12, 19FNMR



12

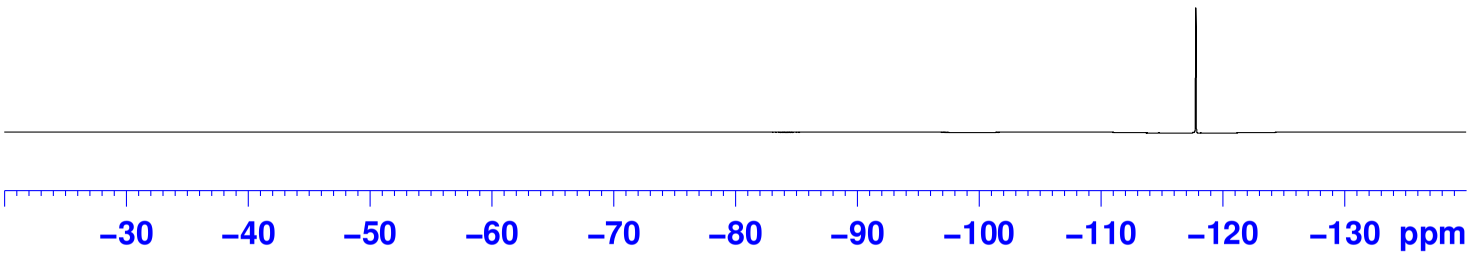
-117.78
-117.80

```
Current Data Parameters
NAME      PM-4-17-4, rerun
EXPNO                   1
PROCNO                  1

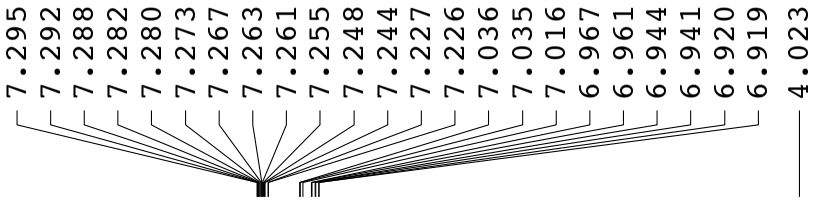
F2 - Acquisition Parameters
Date_            20120816
Time                10.37
INSTRUM             spect
PROBHD   5 mm CPQNP 1H/
PULPROG                zg
TD                 131072
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             75187.969 Hz
FIDRES          0.573639 Hz
AQ              0.8716788 sec
RG                   1024
DW                  6.650 usec
DE                 20.00 usec
TE                 298.2 K
D1             2.00000000 sec
TD0                     1

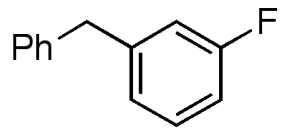
======== CHANNEL f1 ========
NUC1                  19F
P1                 15.03 usec
PL1                -4.00 dB
PL1W         25.74305916 W
SFO1         376.4607164 MHz

F2 - Processing parameters
SI                    65536
SF           376.4983660 MHz
WDW                     EM
SSB                      0
LB                  2.00 Hz
GB                       0
PC                    1.00
```

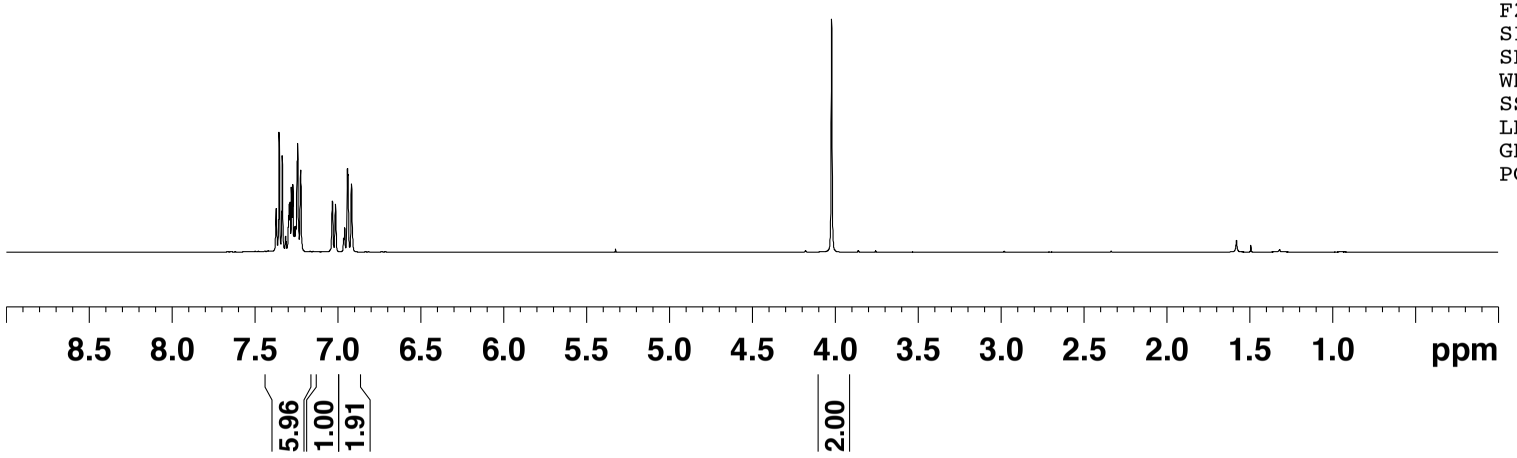


Compound 13, 1NMR





13



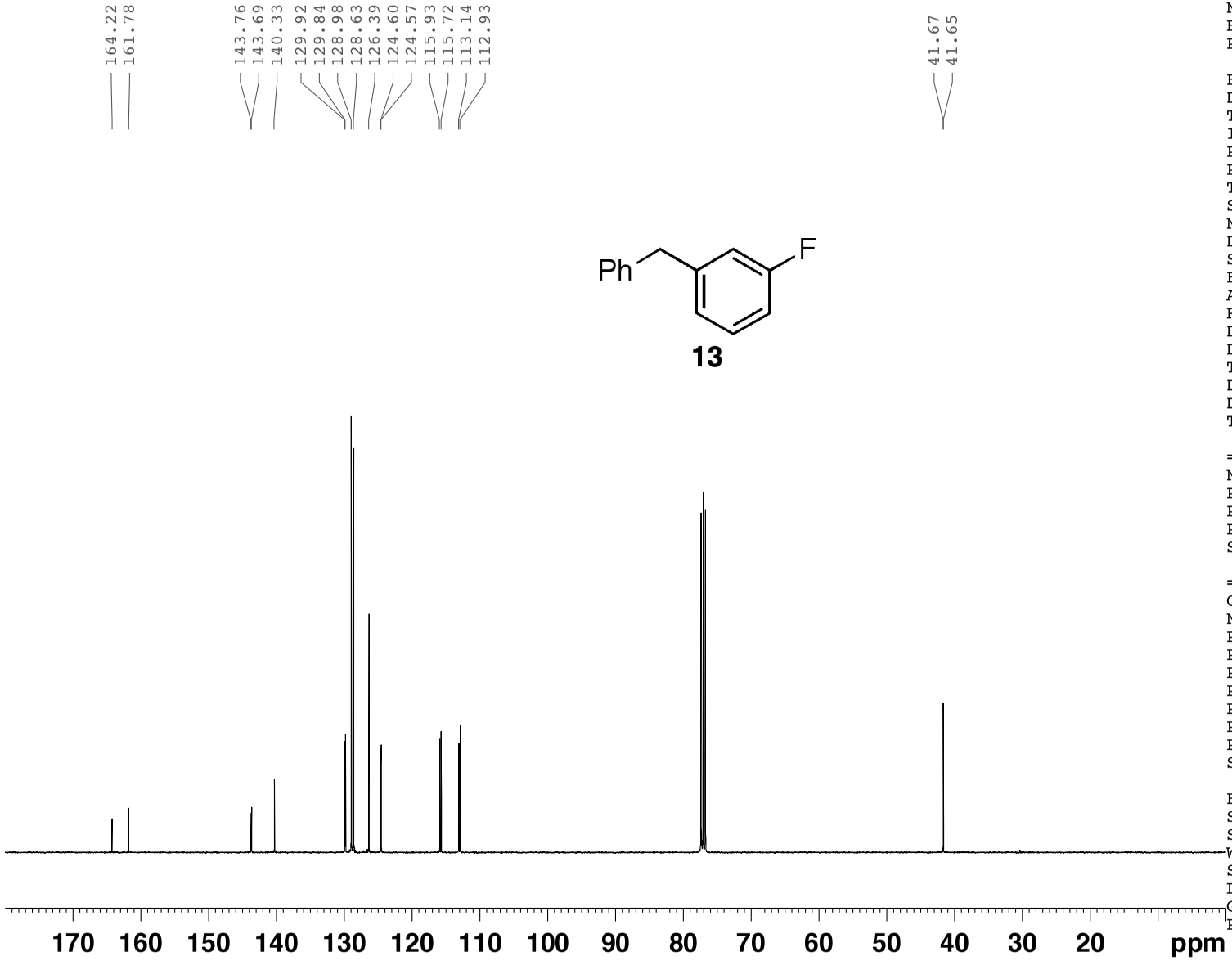
Current Data Parameters
NAME DMM3-077-4
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120525
Time 23.13
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 10.1
DW 60.400 usec
DE 6.00 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 4.90 dB
PL1W 3.30822015 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 13, 13CNMR




```
Current Data Parameters
NAME          DMM3-077-4
EXPNO                  2
PROCNO                 1

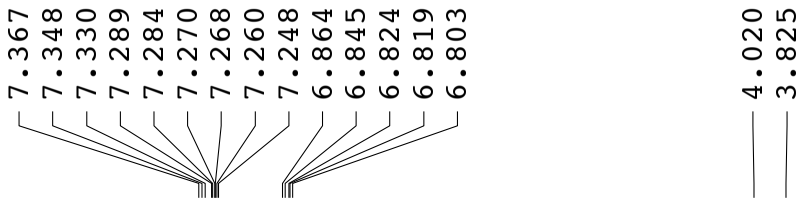
F2 - Acquisition Parameters
Date_           20120526
Time               2.31
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

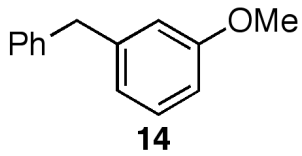
======== CHANNEL f1 ========
NUC1                13C
P1                9.25 usec
PL1               0.55 dB
PL1W       35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2               4.90 dB
PL12             20.46 dB
PL13             21.00 dB
PL2W        3.30822015 W
PL12W       0.09195905 W
PL13W       0.08120718 W
SFO2       400.1316005 MHz

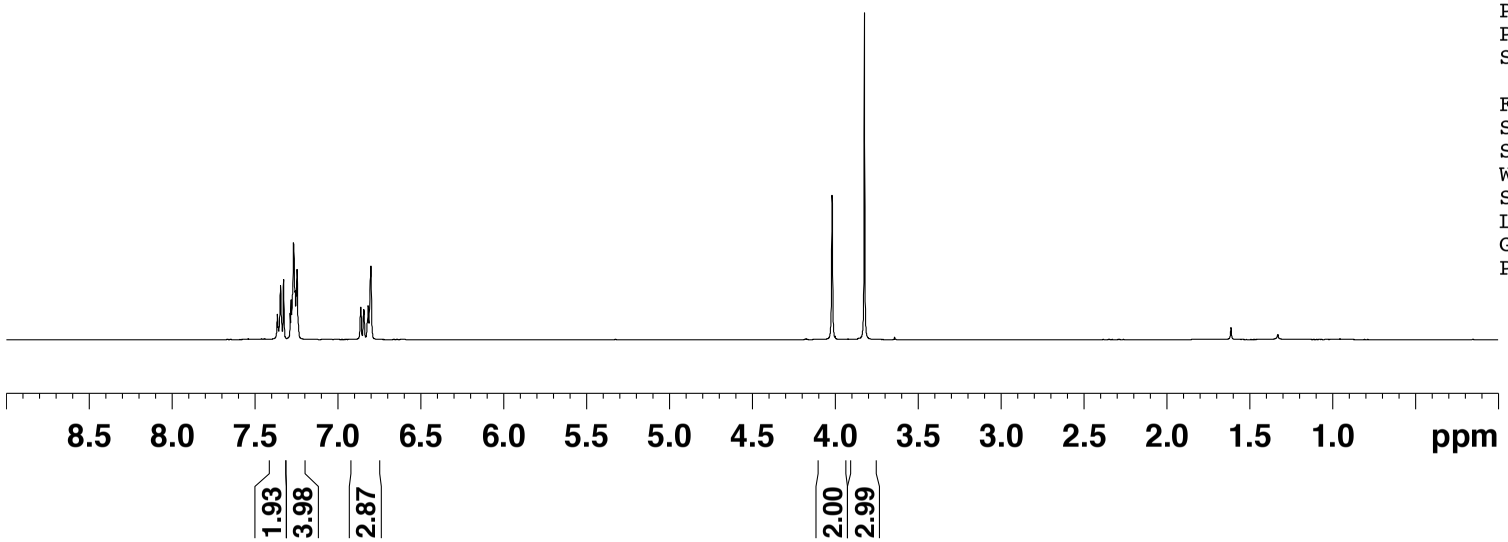
F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

Compound 14, 1HNMR





14



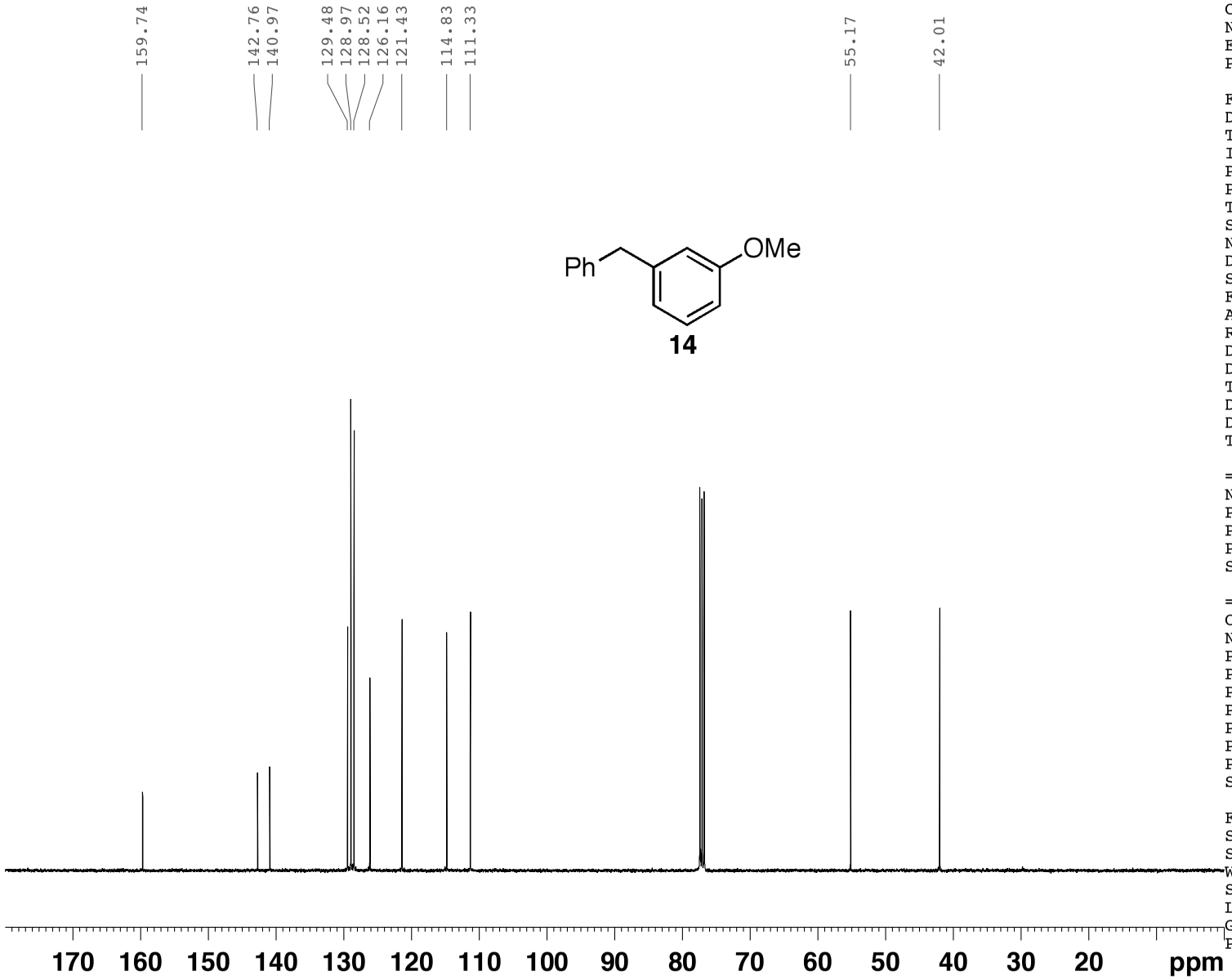

```
Current Data Parameters
NAME                  PM-4-18-1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20120711
Time                      11.58
INSTRUM                   spect
PROBHD    5 mm CPQNP 1H/
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                         14.3
DW                        60.400 usec
DE                         6.00 usec
TE                        298.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        15.00 usec
PL1                        4.90 dB
PL1W                  3.30822015 W
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF                  400.1300000 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

Compound 14, 13CNMR




```
Current Data Parameters
NAME          PM-4-18-1
EXPNO                 2
PROCNO                1

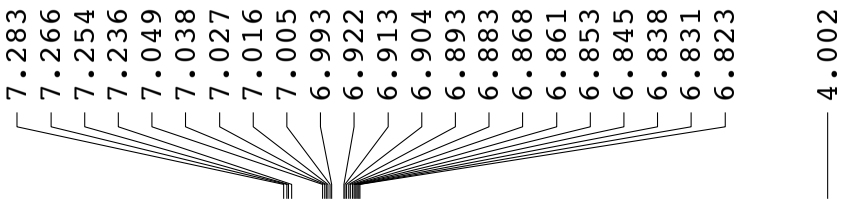
F2 - Acquisition Parameters
Date_          20120711
Time              12.01
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

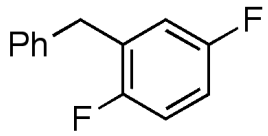
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W        35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2       400.1316005 MHz

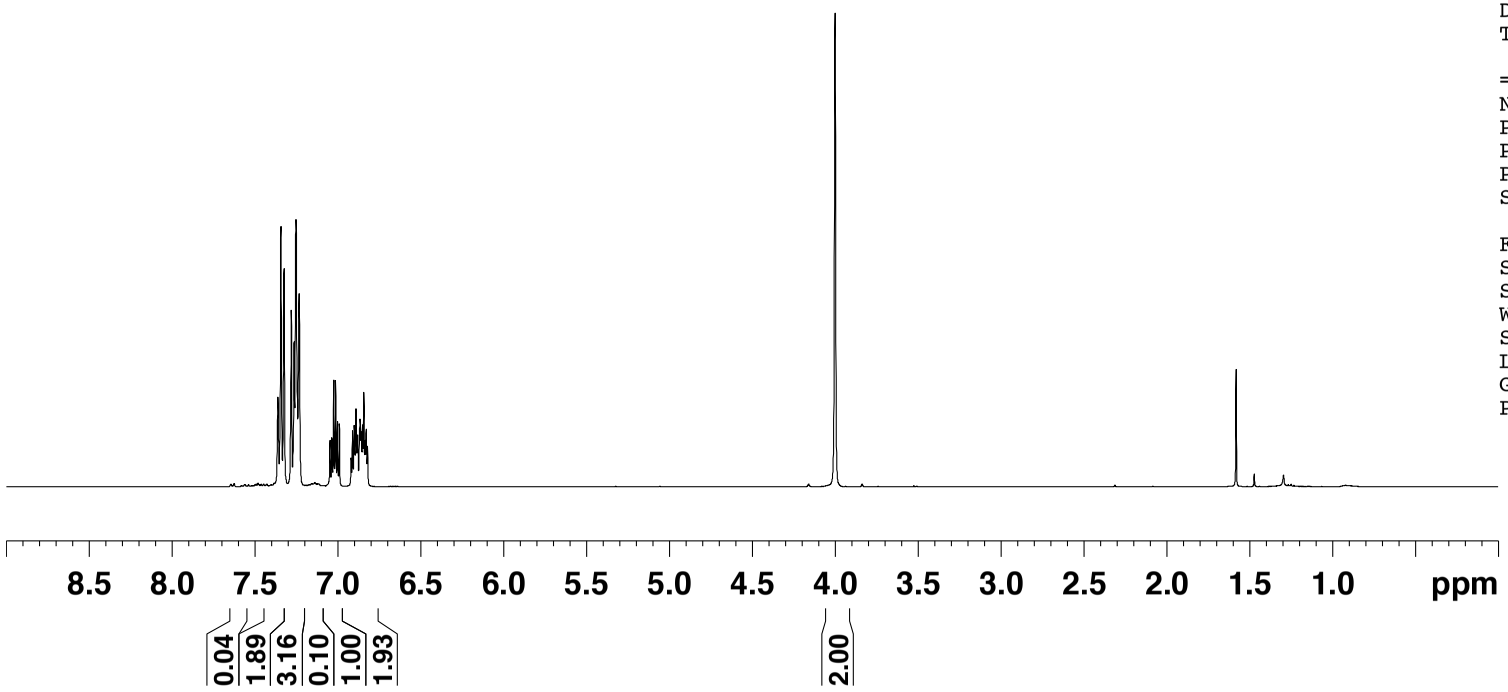
F2 - Processing parameters
SI                 32768
SF         100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 15, 1HNMR





15



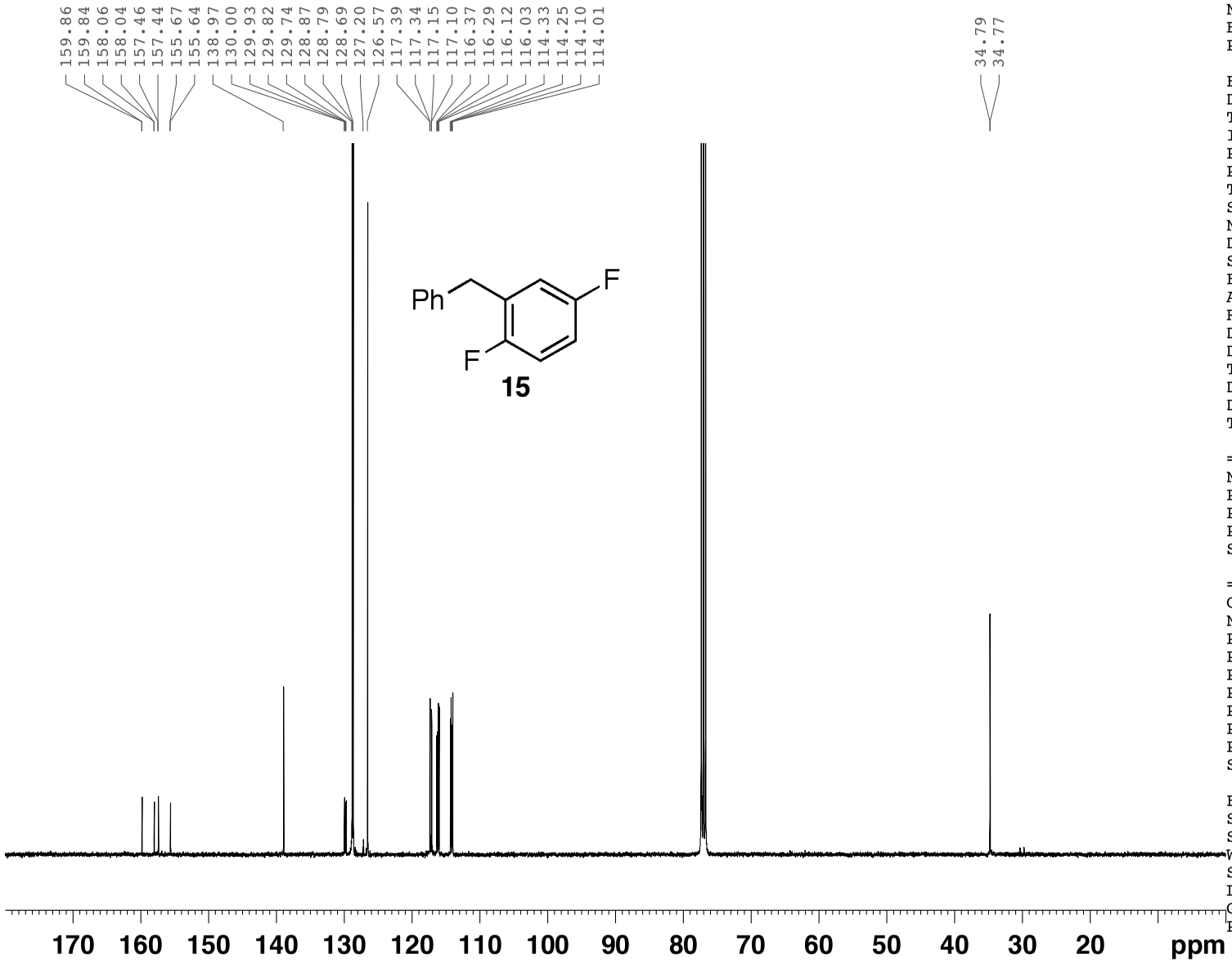

```
Current Data Parameters
NAME        DMM3-077-2-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120522
Time              18.07
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                 11.3
DW               60.400 usec
DE                6.00 usec
TE                298.1 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

Compound 15, 13CNMR



Current Data Parameters

NAME	DMM3-077-2-2
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20120522
Time	23.25
INSTRUM	spect
PROBHD	5 mm CPQNP 1H/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	512
DW	20.850 usec
DE	18.00 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	9.25 usec
PL1	0.55 dB
PL1W	35.18820572 W
SFO1	100.6228298 MHz

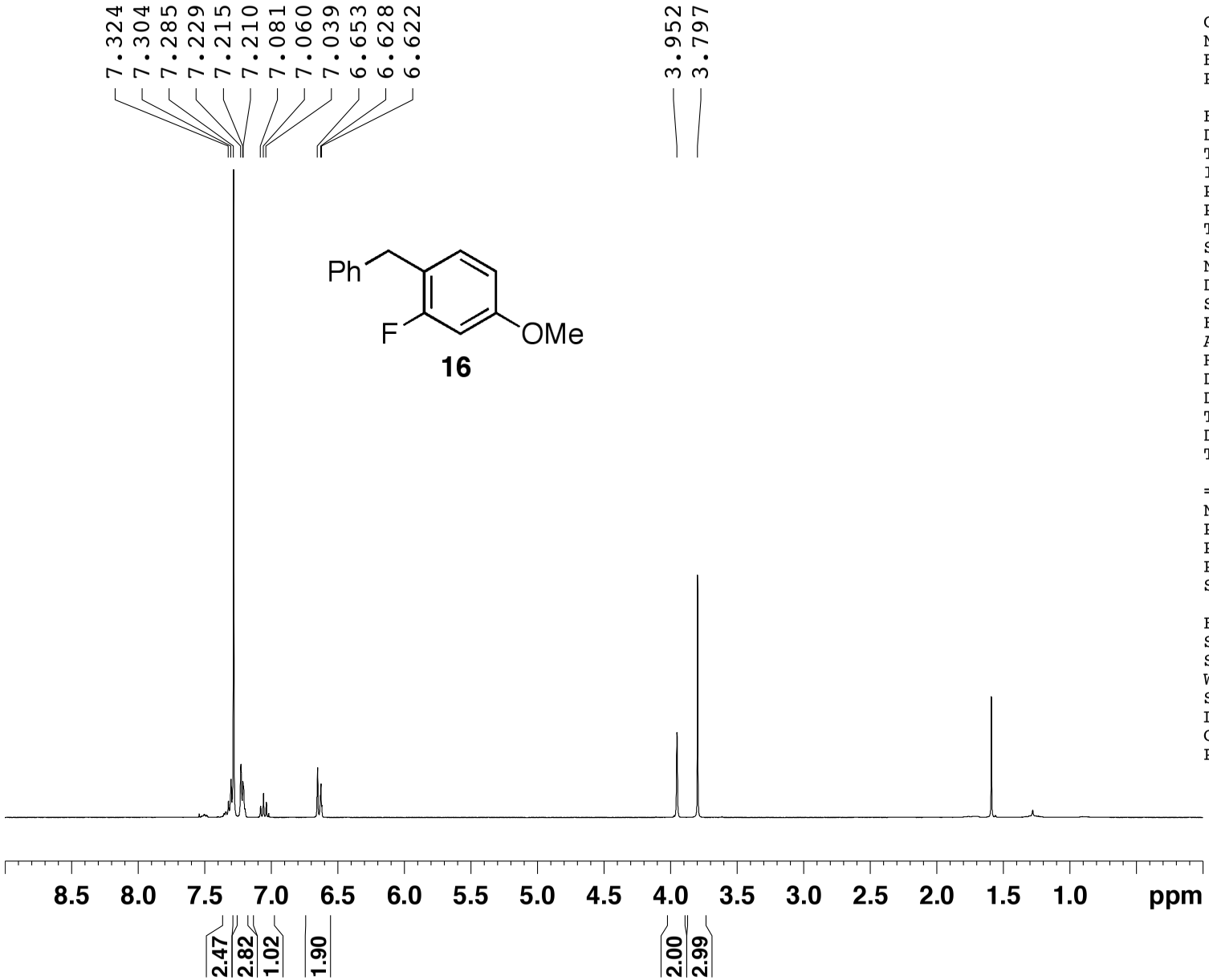
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	4.90 dB
PL12	20.46 dB
PL13	21.00 dB
PL2W	3.30822015 W
PL12W	0.09195905 W
PL13W	0.08120718 W
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Compound 16, 1HNMR



Current Data Parameters
NAME PM-4, F&OMe-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20120807
Time	11.16
INSTRUM	spect
PROBHD	5 mm CPQNP 1H/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	12.7
DW	60.400 usec
DE	6.00 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1

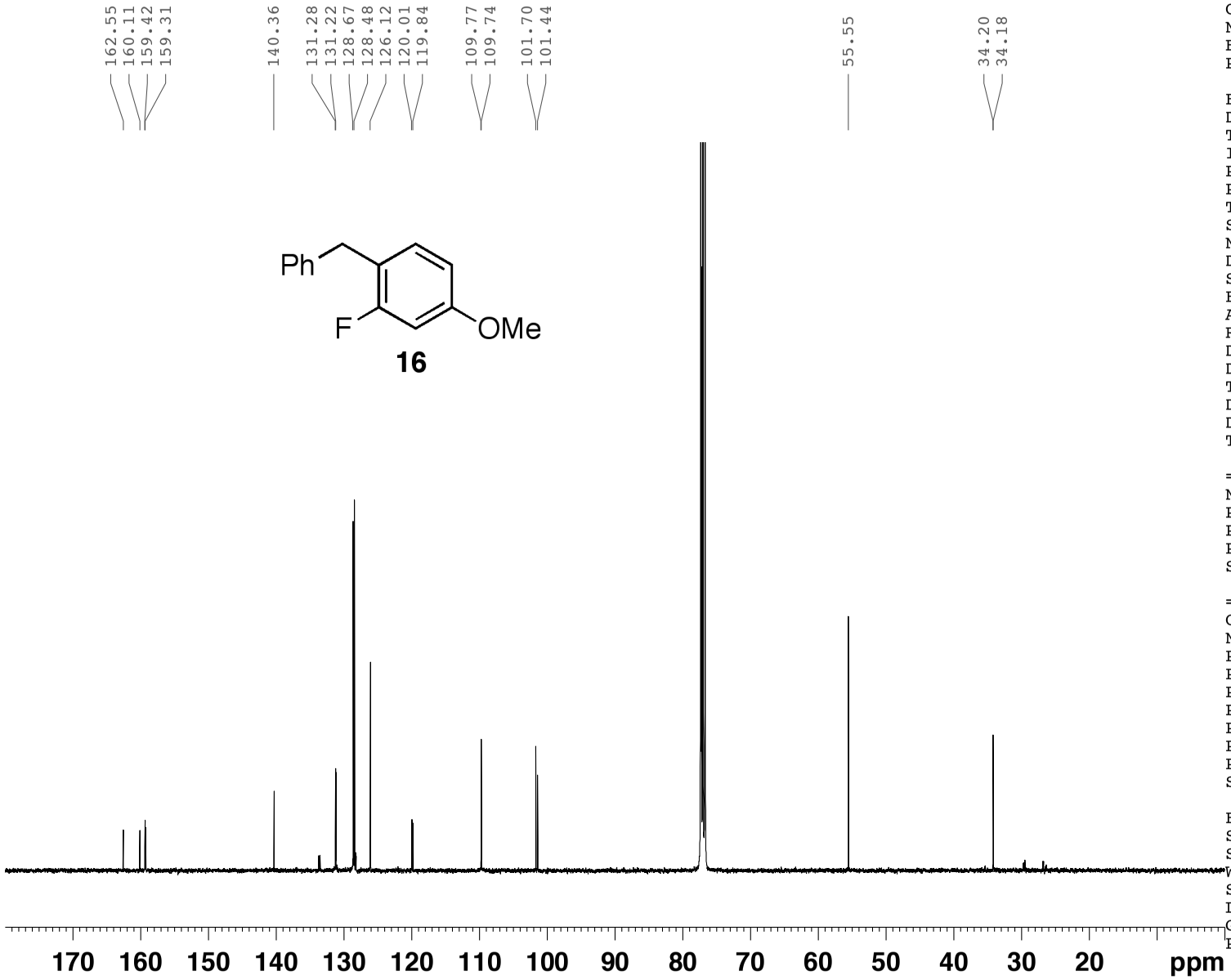
======== CHANNEL f1 ========

NUC1	1H
P1	15.00 usec
PL1	4.90 dB
PL1W	3.30822015 W
SFO1	400.1324710 MHz

F2 - Processing parameters

SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Compound 16, 13CNMR




```
Current Data Parameters
NAME      PM-4-oF, POMe
EXPNO                1
PROCNO               1

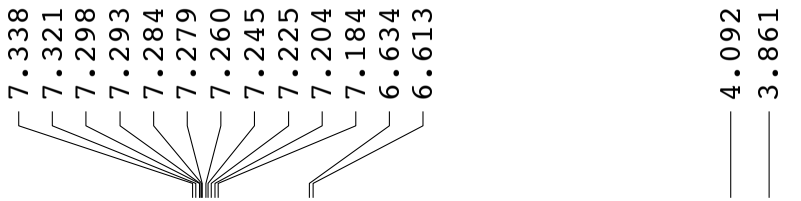
F2 - Acquisition Parameters
Date_          20120811
Time             22.24
INSTRUM          spect
PROBHD   5 mm CPQNP 1H/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                1024
DS                   4
SWH          23980.814 Hz
FIDRES        0.365918 Hz
AQ            1.3664756 sec
RG                 512
DW              20.850 usec
DE              18.00 usec
TE              298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

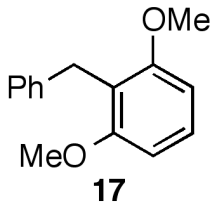
======== CHANNEL f1 ========
NUC1               13C
P1               9.25 usec
PL1              0.55 dB
PL1W       35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2        waltz16
NUC2               1H
PCPD2           90.00 usec
PL2              4.90 dB
PL12            20.46 dB
PL13            21.00 dB
PL2W        3.30822015 W
PL12W       0.09195905 W
PL13W       0.08120718 W
SFO2       400.1316005 MHz

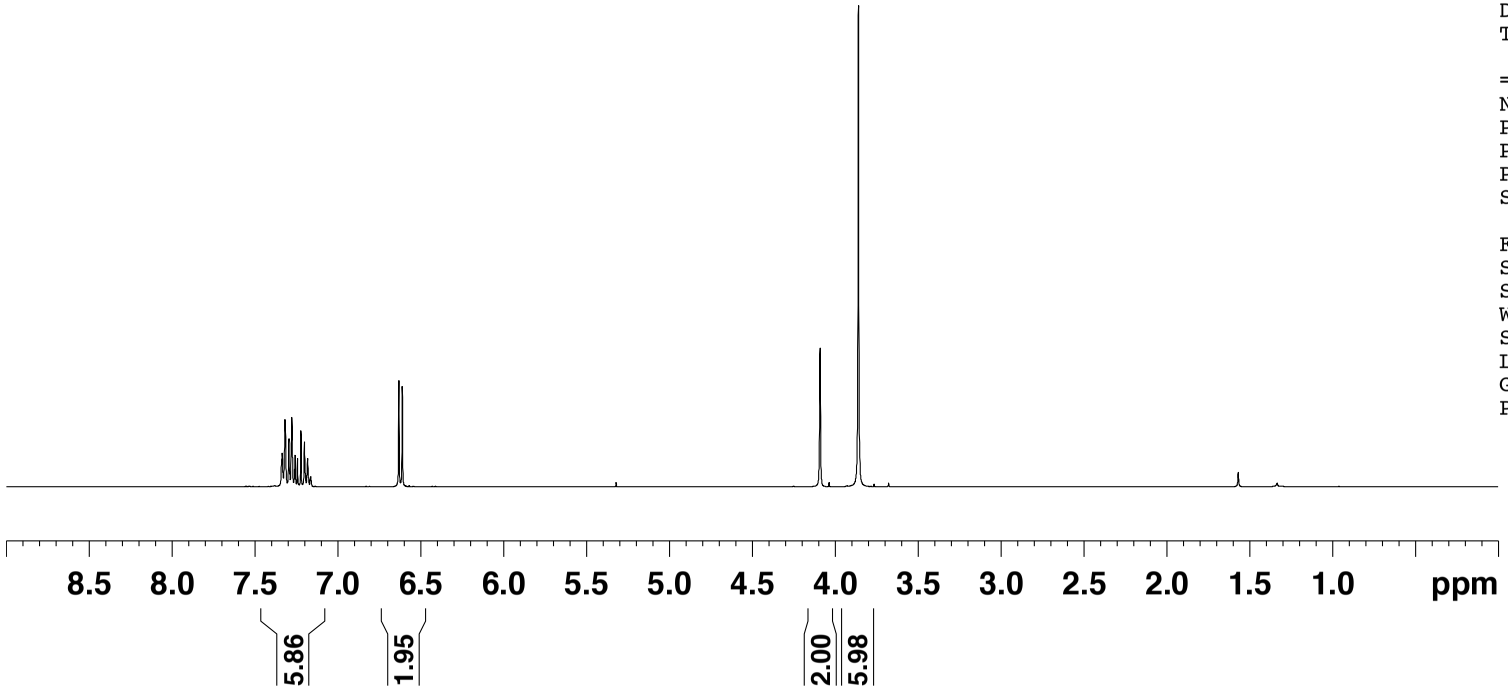
F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

Compound 17, 1HNMR





17



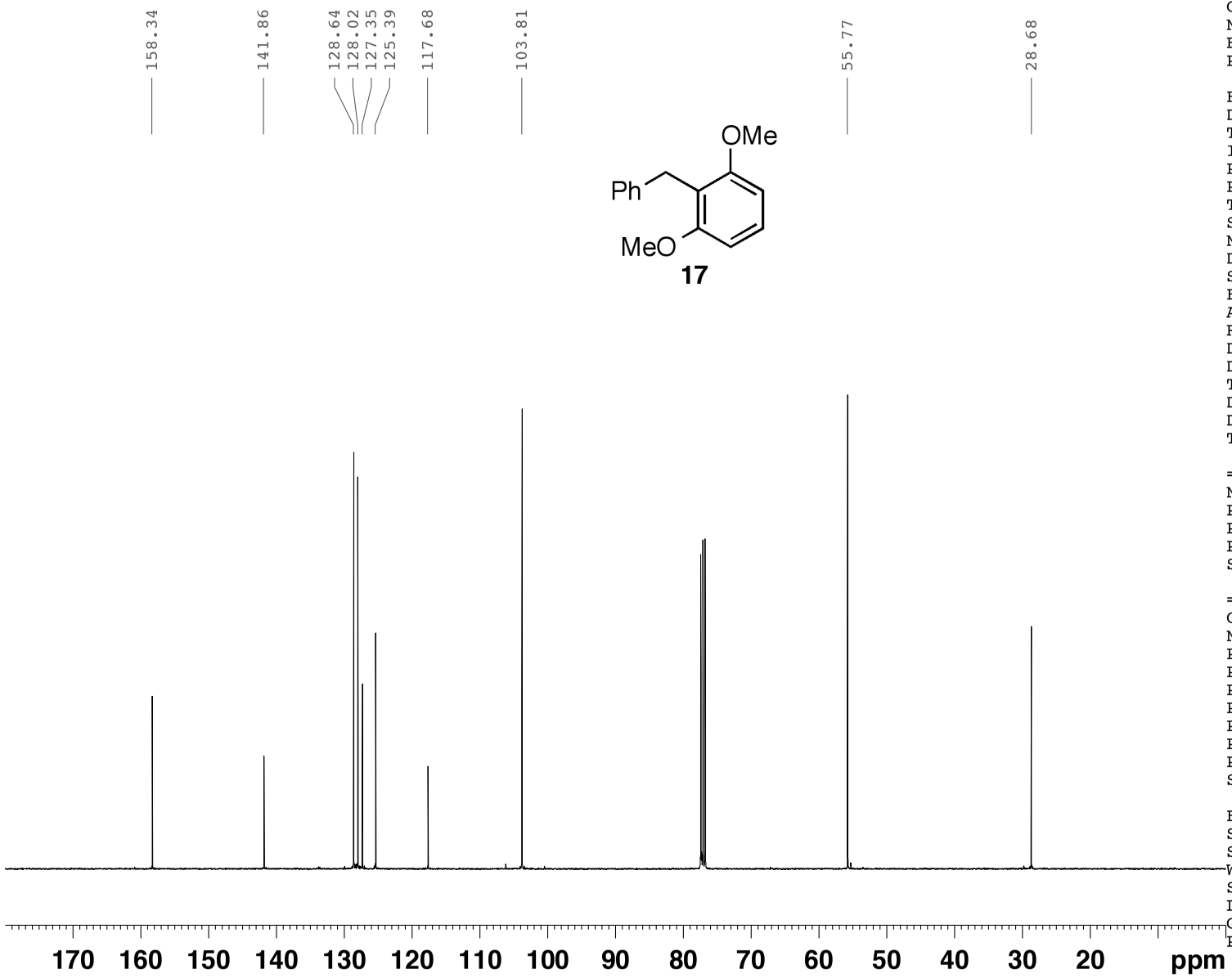

```
Current Data Parameters
NAME          PM-4-13-3
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20120705
Time               5.19
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                 11.3
DW               60.400 usec
DE                6.00 usec
TE                298.2 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

Compound 17, 13CNMR




```
Current Data Parameters
NAME          PM-4-13-3
EXPNO                 2
PROCNO                1

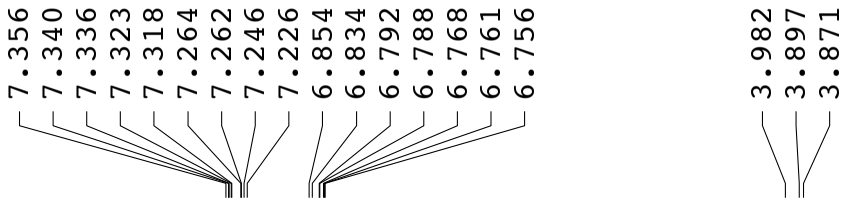
F2 - Acquisition Parameters
Date_          20120705
Time               5.35
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

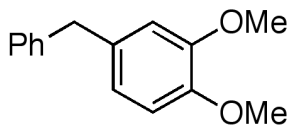
======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1                0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

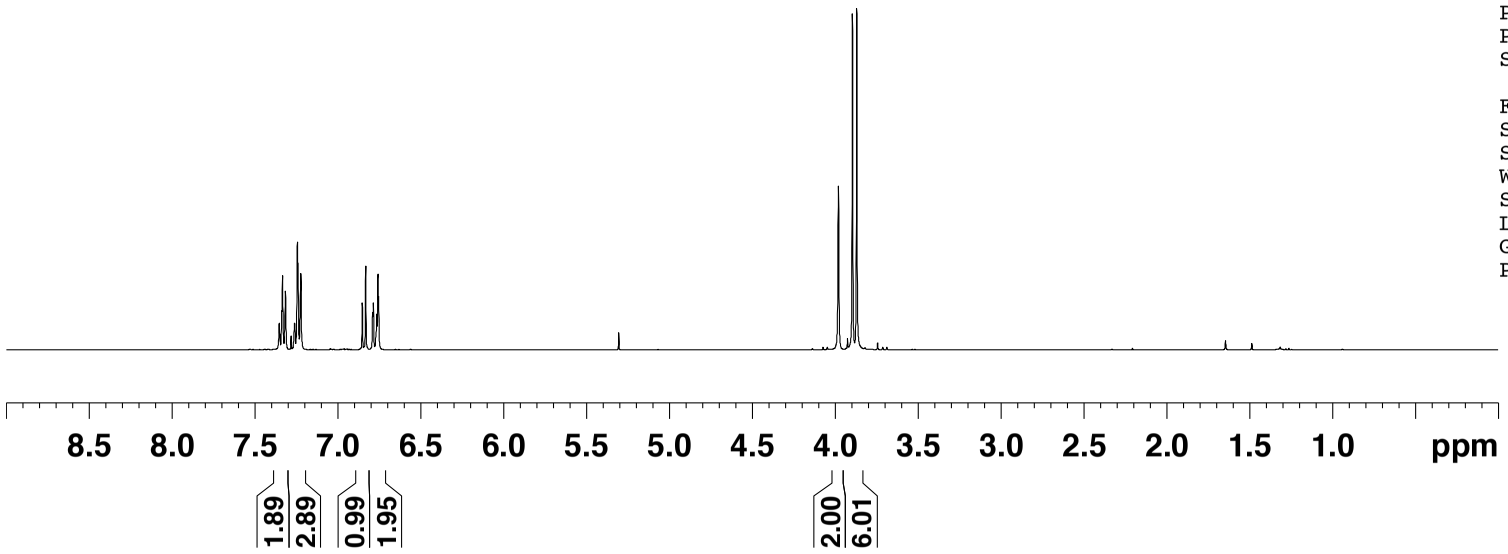
F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 18, 1HNMR





18



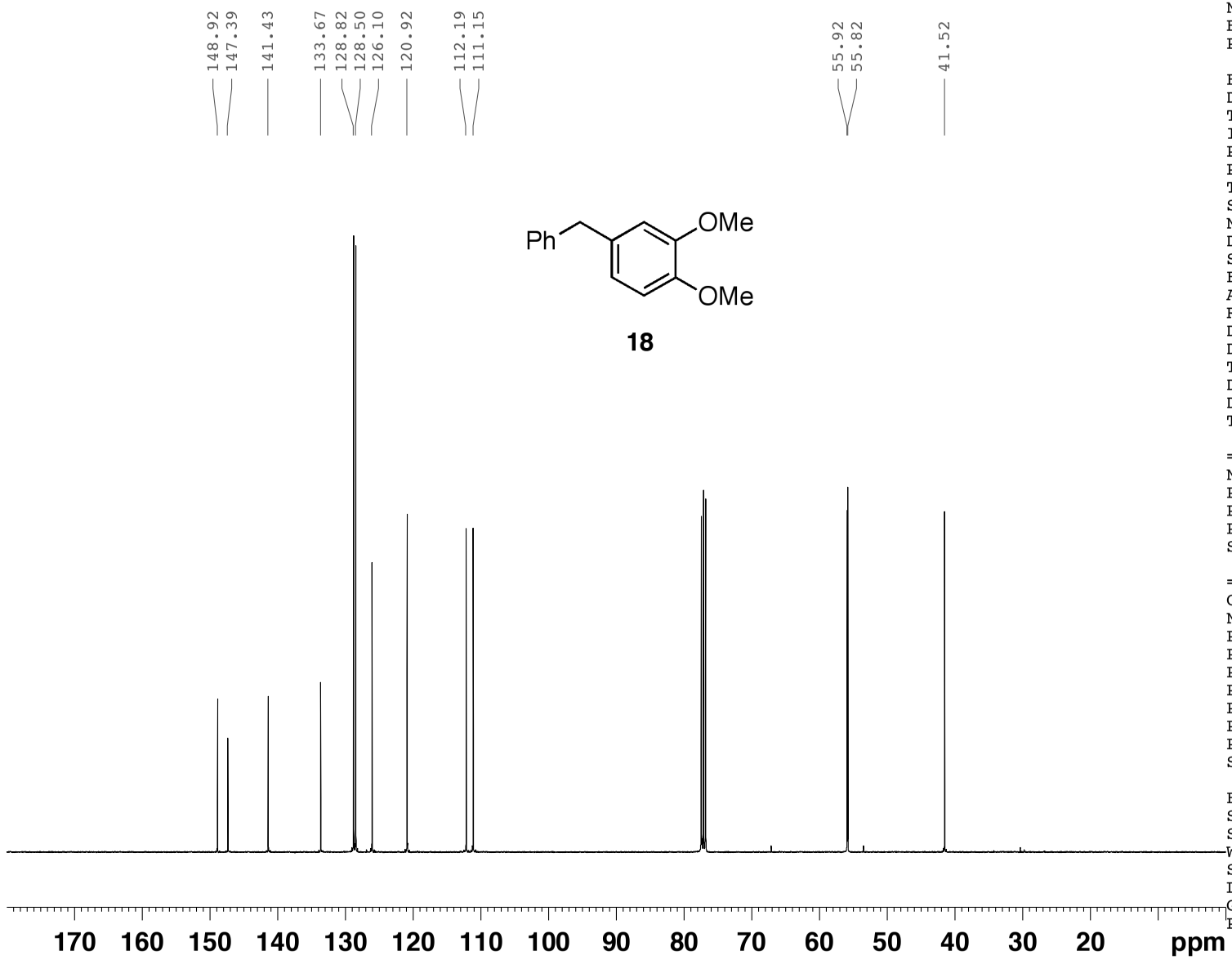

```
Current Data Parameters
NAME          DMM3-104-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120706
Time              16.57
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                 10.1
DW               60.400 usec
DE                6.00 usec
TE                298.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

Compound 18, 13CNMR




```
Current Data Parameters
NAME          DMM3-104-2
EXPNO                  2
PROCNO                 1

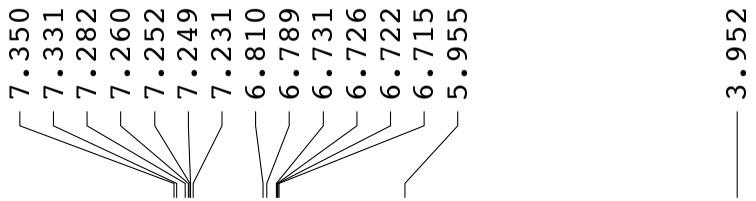
F2 - Acquisition Parameters
Date_           20120706
Time              17.13
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

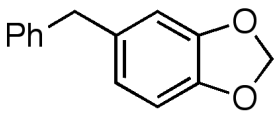
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

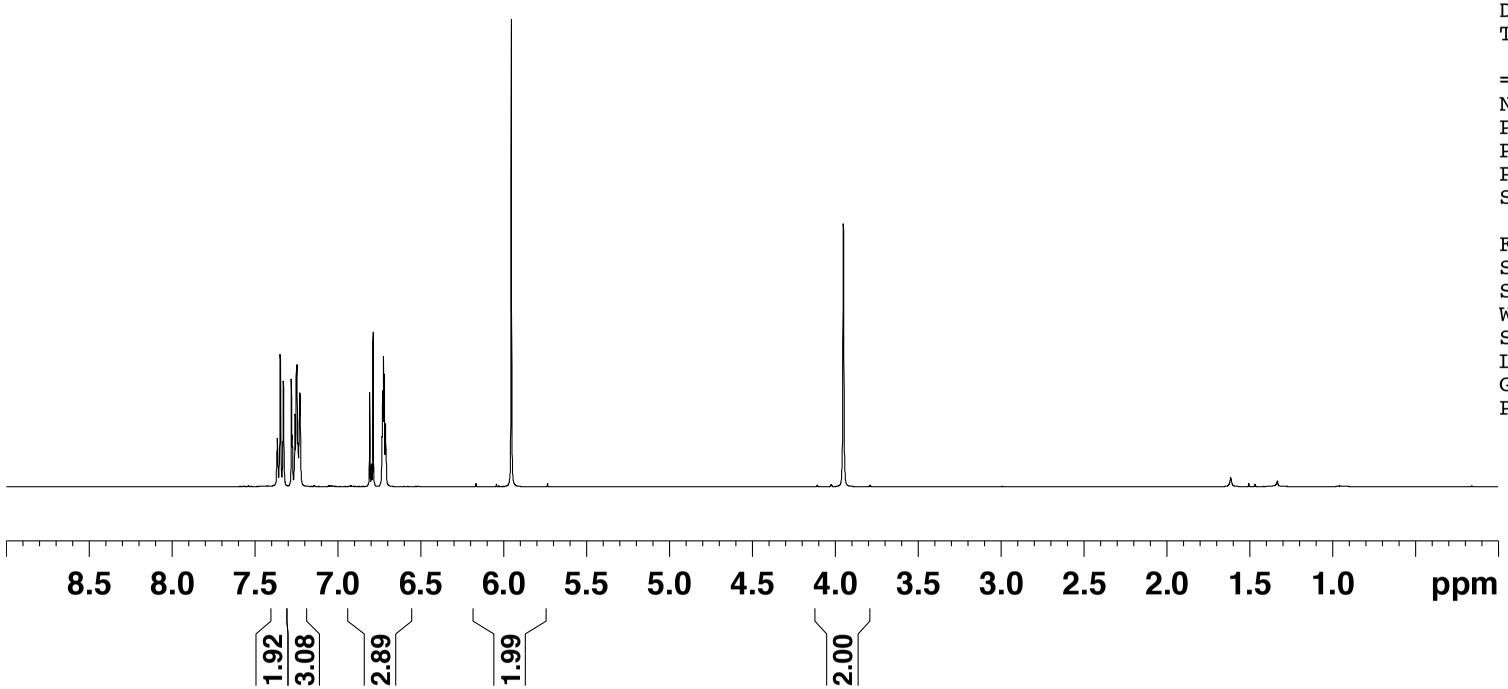
F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 19, 1HNMR





19



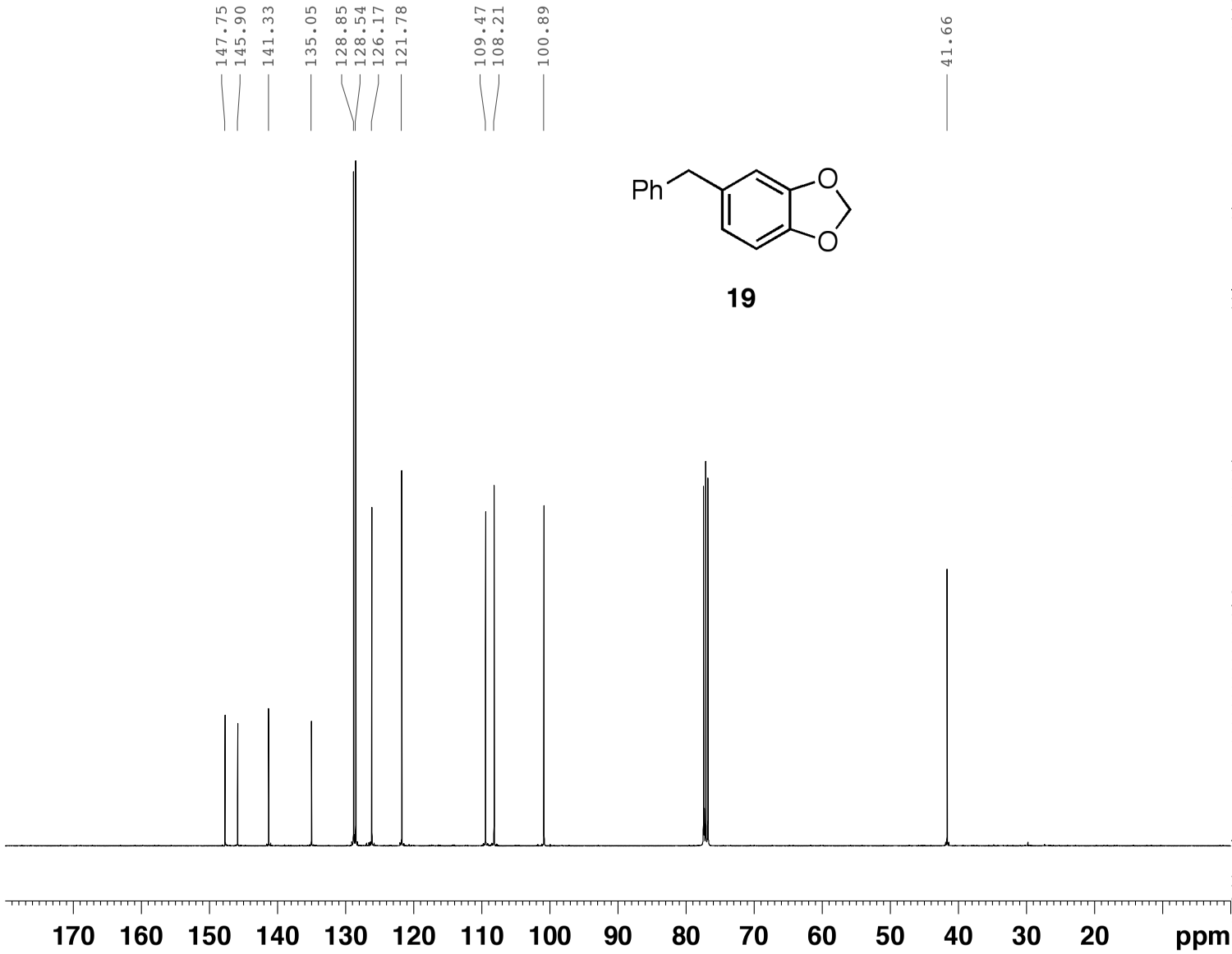

```
Current Data Parameters
NAME         PM-3-233-2A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120515
Time               23.40
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                     9
DW                60.400 usec
DE                 6.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                 4.90 dB
PL1W          3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

Compound 19, 13CNMR



19

```
Current Data Parameters
NAME         PM-3-233-2A
EXPNO                  2
PROCNO                 1

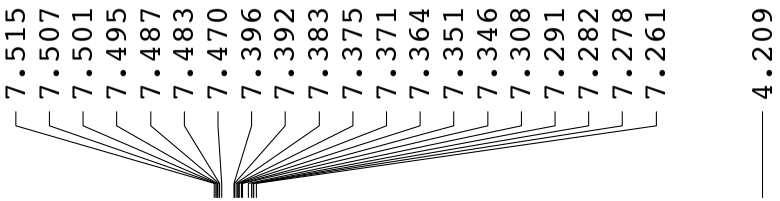
F2 - Acquisition Parameters
Date_           20120516
Time                0.40
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                   512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

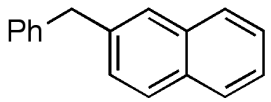
======== CHANNEL f1 ========
NUC1                  13C
P1                   9.25 usec
PL1                  0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 20, 1HNMR





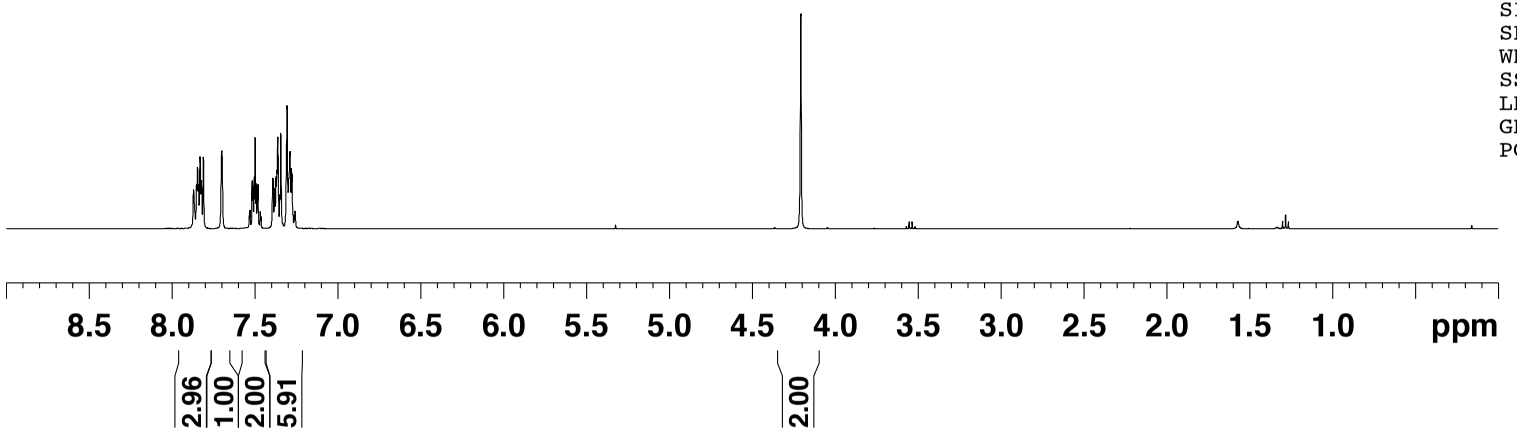
20

```
Current Data Parameters
NAME      DMM3-075-1-pure
EXPNO                  1
PROCNO                 1

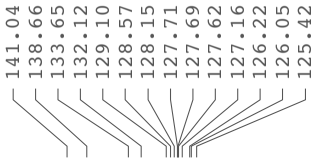
F2 - Acquisition Parameters
Date_           20120520
Time              13.43
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                 14.3
DW               60.400 usec
DE                6.00 usec
TE                298.2 K
D1           1.00000000 sec
TD0                   1

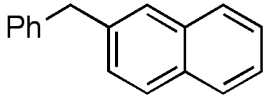
======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

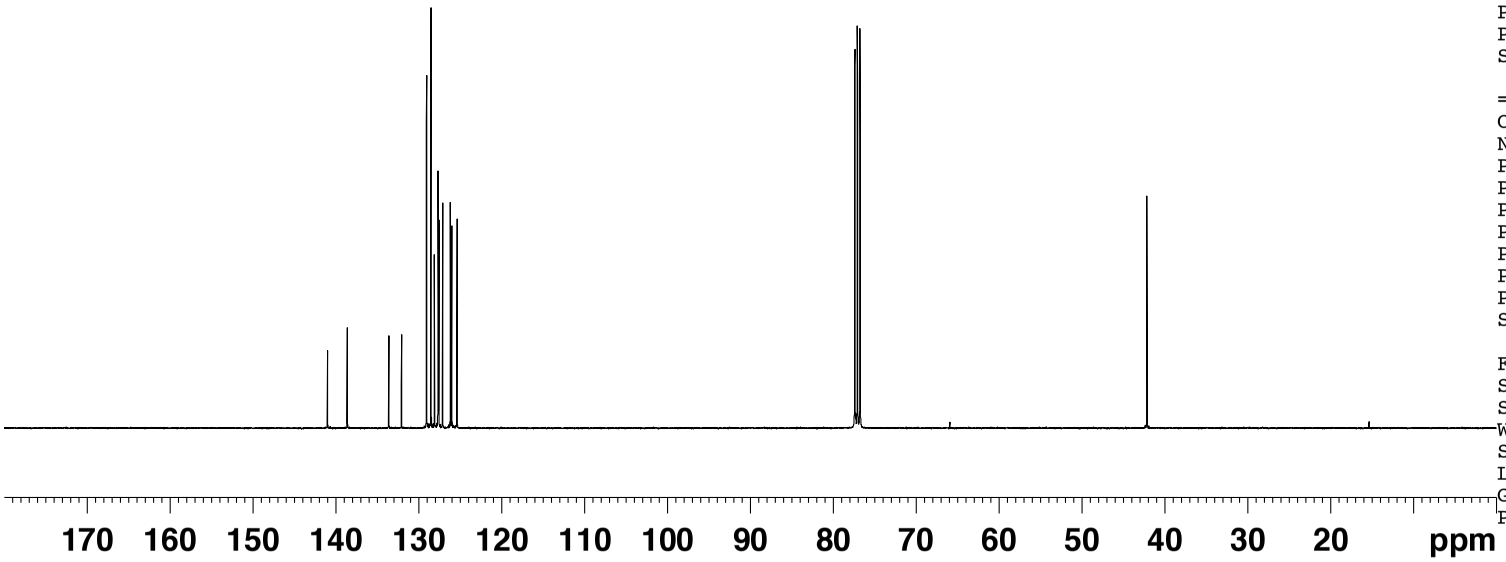


Compound 20, 13CNMR





20




```
Current Data Parameters
NAME      DMM3-075-1-pure
EXPNO                   2
PROCNO                  1

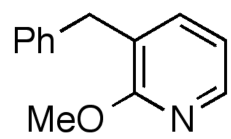
F2 - Acquisition Parameters
Date_            20120520
Time                13.59
INSTRUM             spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    256
DS                      4
SWH             23980.814 Hz
FIDRES          0.365918 Hz
AQ              1.3664756 sec
RG                    512
DW                20.850 usec
DE                18.00 usec
TE                298.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                   9.25 usec
PL1                  0.55 dB
PL1W         35.18820572 W
SFO1         100.6228298 MHz

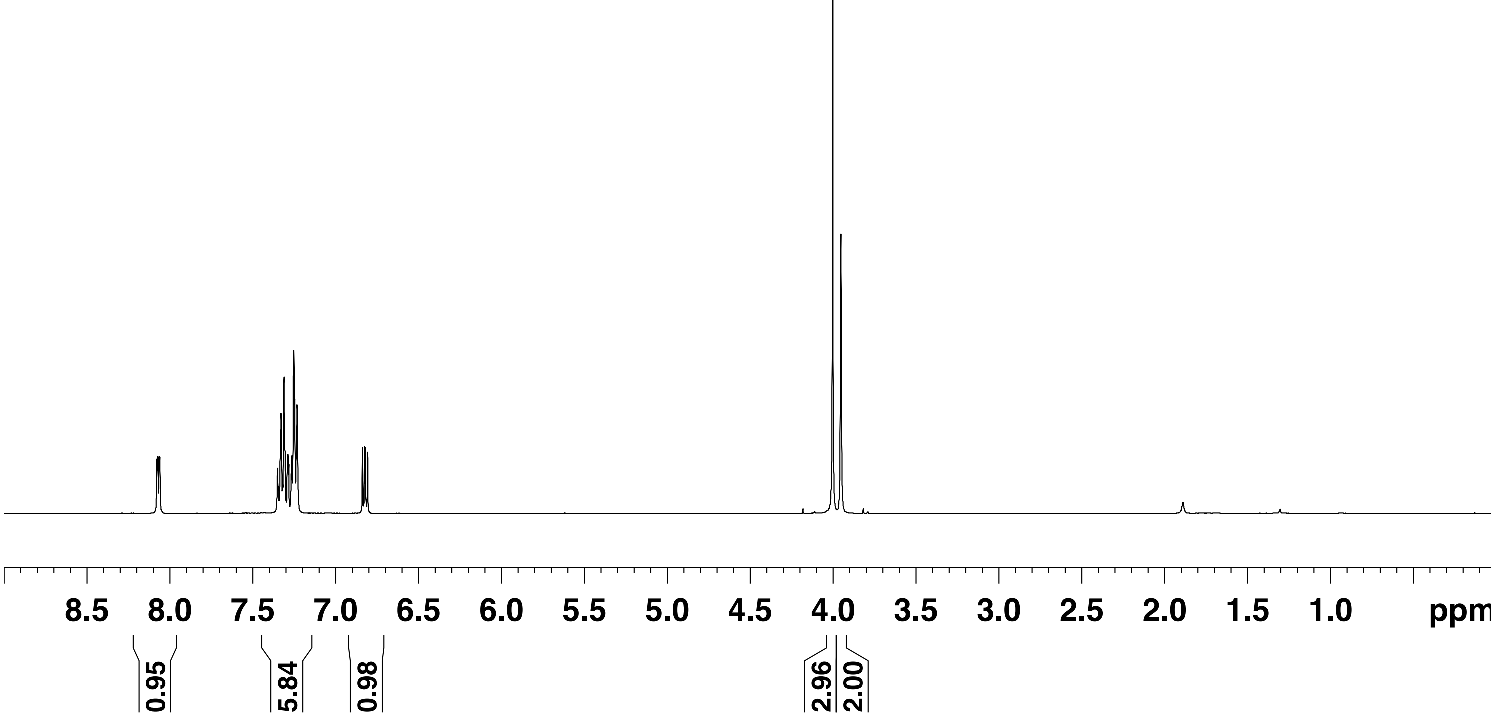
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W          3.30822015 W
PL12W         0.09195905 W
PL13W         0.08120718 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF           100.6127690 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                  1.40
```

Compound 21, 1HNMR



21



BRUKER

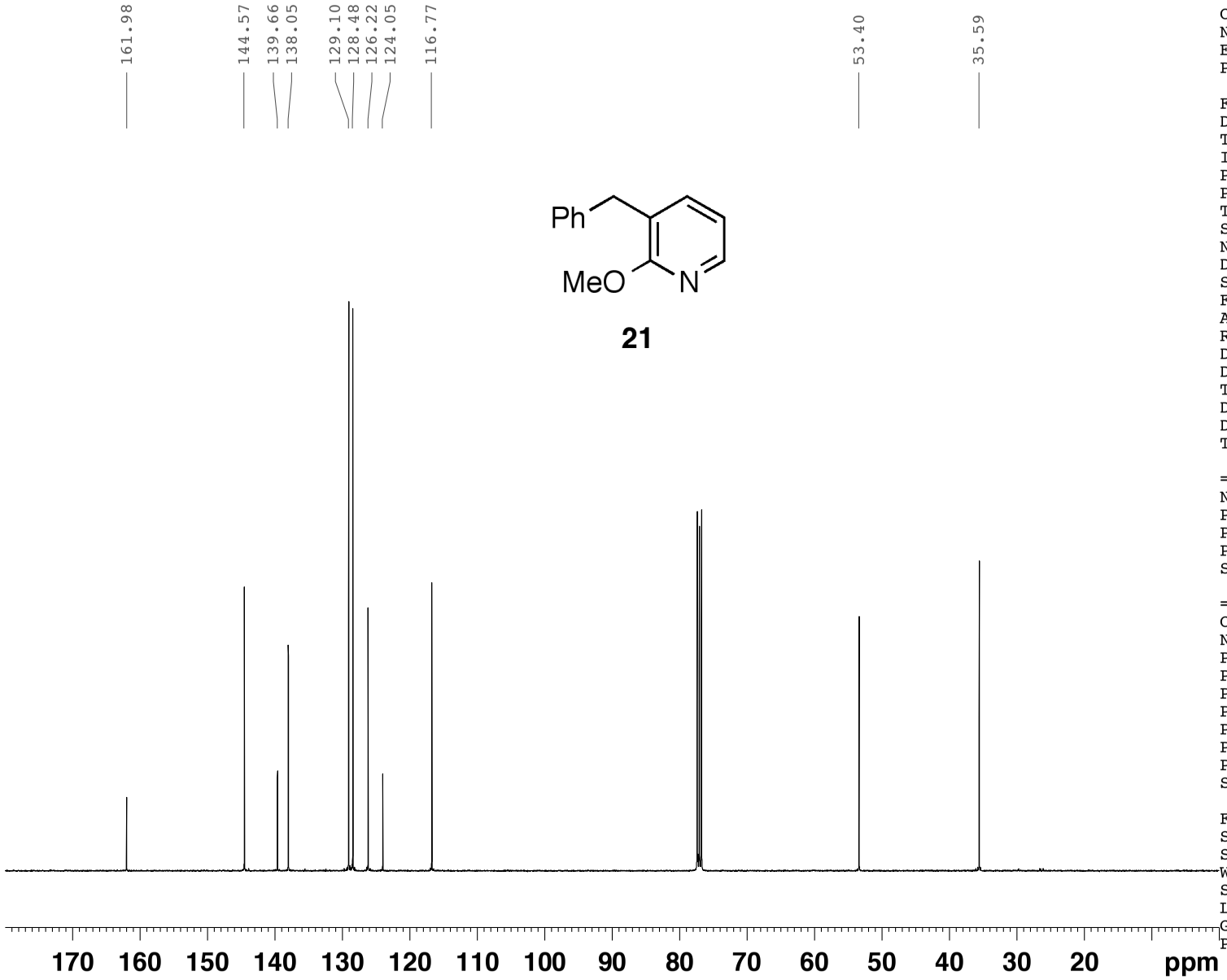
```
Current Data Parameters
NAME            PM-4-10-5
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120705
Time                 4.35
INSTRUM             spect
PROBHD   5 mm CPQNP 1H/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ              3.9584243 sec
RG                   10.1
DW                 60.400 usec
DE                   6.00 usec
TE                  298.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  15.00 usec
PL1                  4.90 dB
PL1W           3.30822015 W
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                  32768
SF            400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

Compound 21, 13CNMR




```
Current Data Parameters
NAME          PM-4-10-5
EXPNO                 2
PROCNO                1

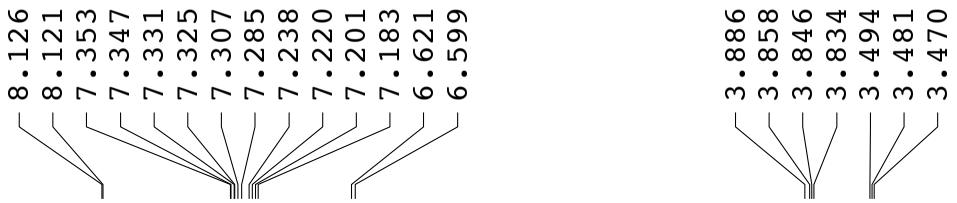
F2 - Acquisition Parameters
Date_          20120705
Time               4.51
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

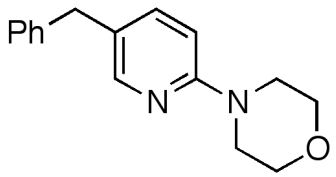
======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1                0.55 dB
PL1W        35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2       400.1316005 MHz

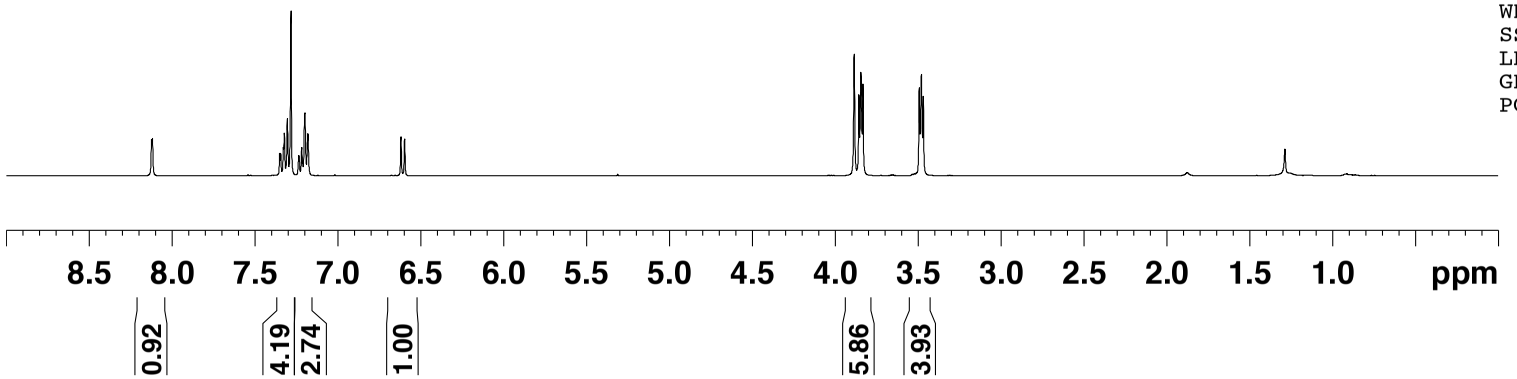
F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 22, 1HNMR





22



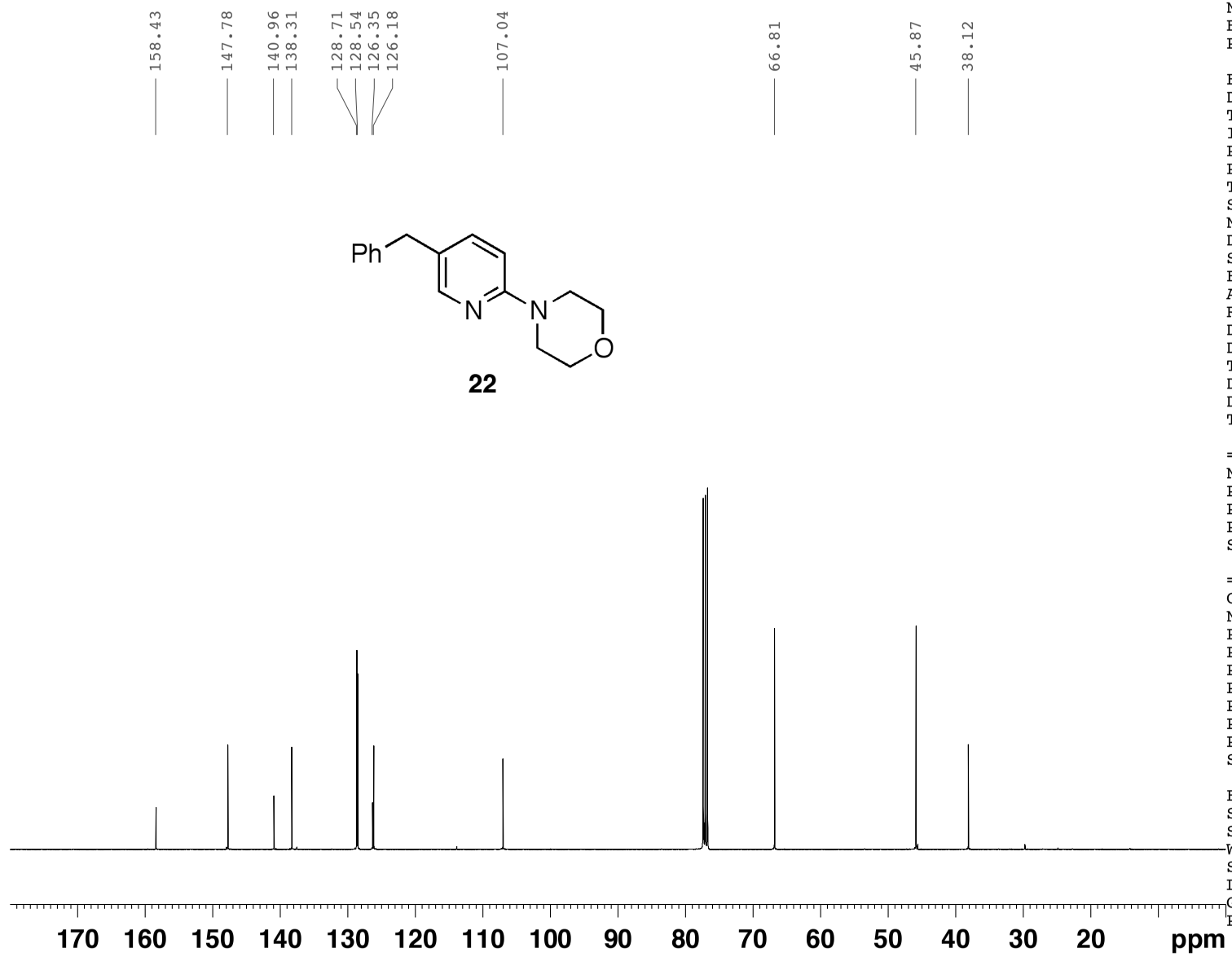

```
Current Data Parameters
NAME        PM-3-249-1-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120812
Time               13.35
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                     4
DW                60.400 usec
DE                 6.00 usec
TE                298.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

Compound 22, 13CNMR




```
Current Data Parameters
NAME          PM-3-249-1
EXPNO                  1
PROCNO                 1

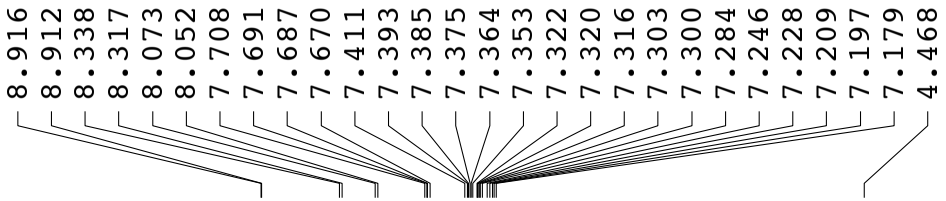
F2 - Acquisition Parameters
Date_           20120506
Time              23.56
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

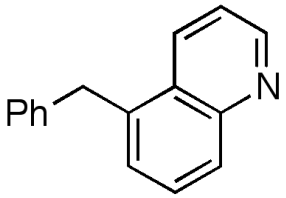
======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1                0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

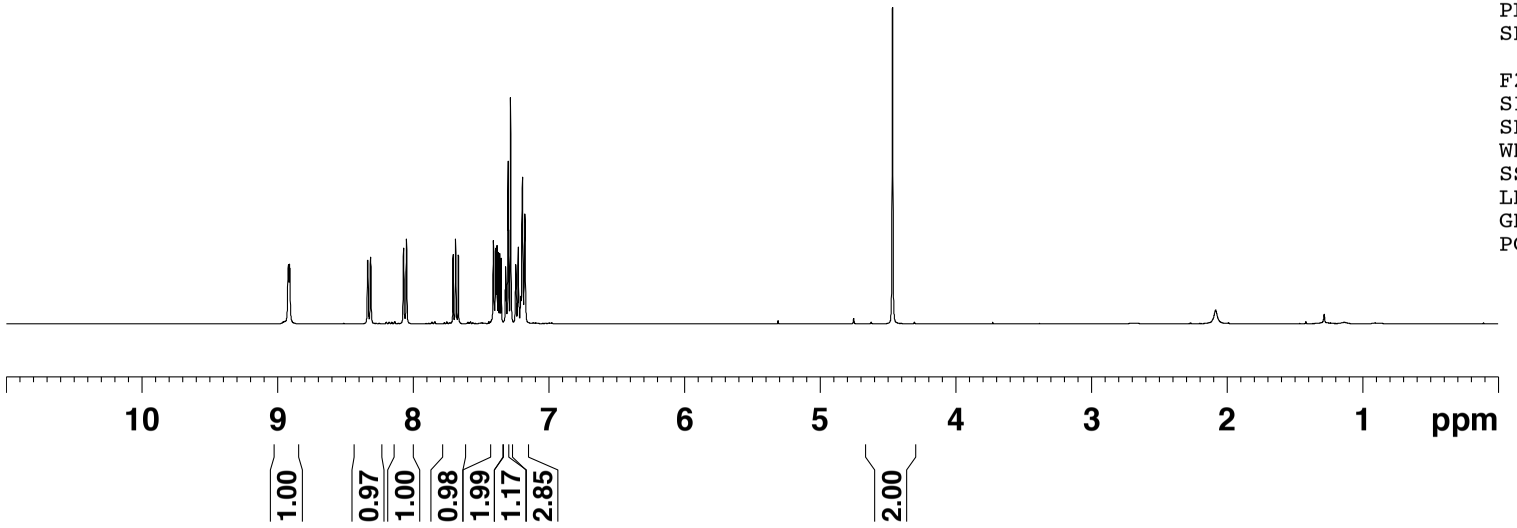
F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 23, 1HNMR





23



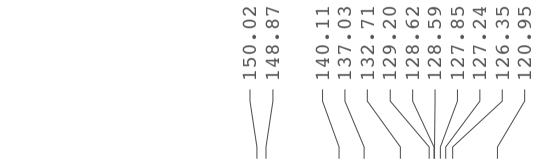

```
Current Data Parameters
NAME                  PM-4-13-1
EXPNO                         1
PROCNO                        1

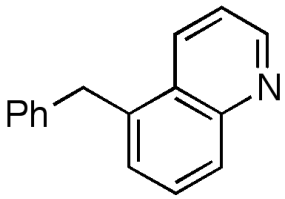
F2 - Acquisition Parameters
Date_                  20120705
Time                       4.57
INSTRUM                   spect
PROBHD    5 mm CPQNP 1H/
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8278.146 Hz
FIDRES                0.126314 Hz
AQ                    3.9584243 sec
RG                         12.7
DW                       60.400 usec
DE                        6.00 usec
TE                       298.2 K
D1                  1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       15.00 usec
PL1                       4.90 dB
PL1W                3.30822015 W
SFO1              400.1324710 MHz

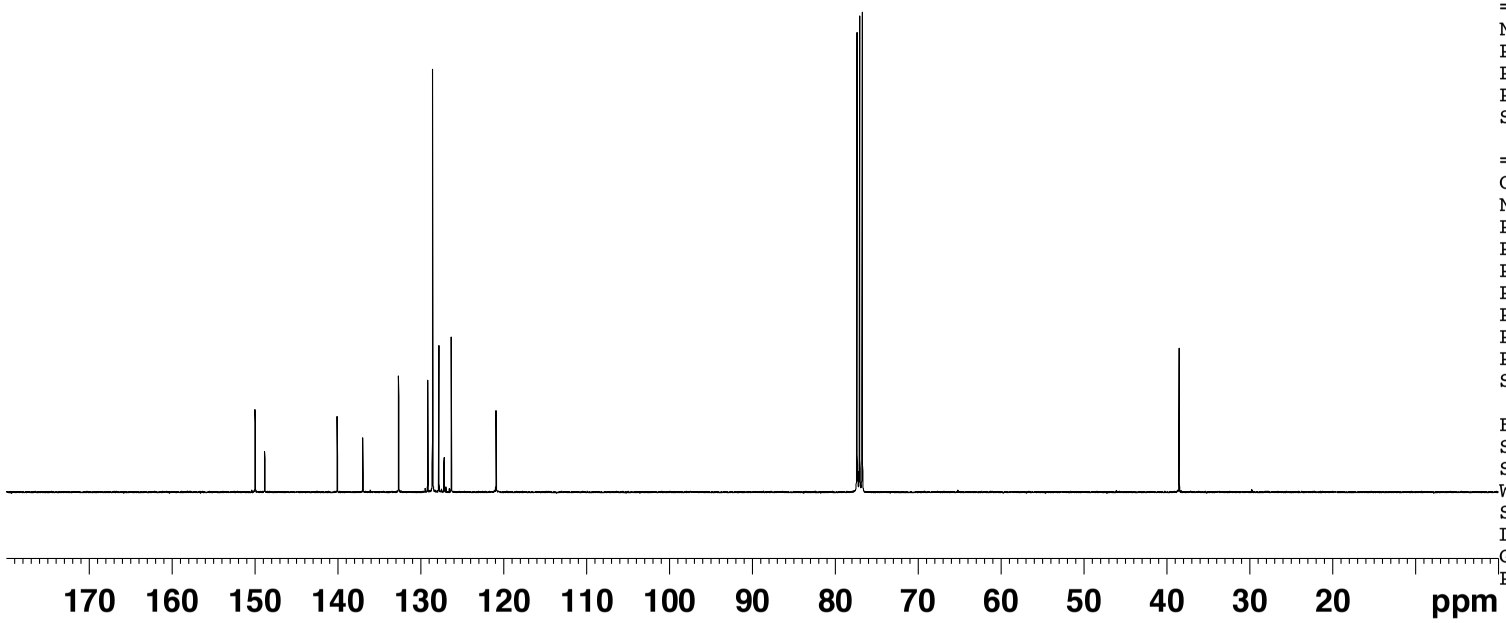
F2 - Processing parameters
SI                        32768
SF                400.1300000 MHz
WDW                          EM
SSB                           0
LB                       0.30 Hz
GB                            0
PC                         1.00
```

Compound 23, 13CNMR





23




```
Current Data Parameters
NAME          PM-4-13-1
EXPNO                 2
PROCNO                1

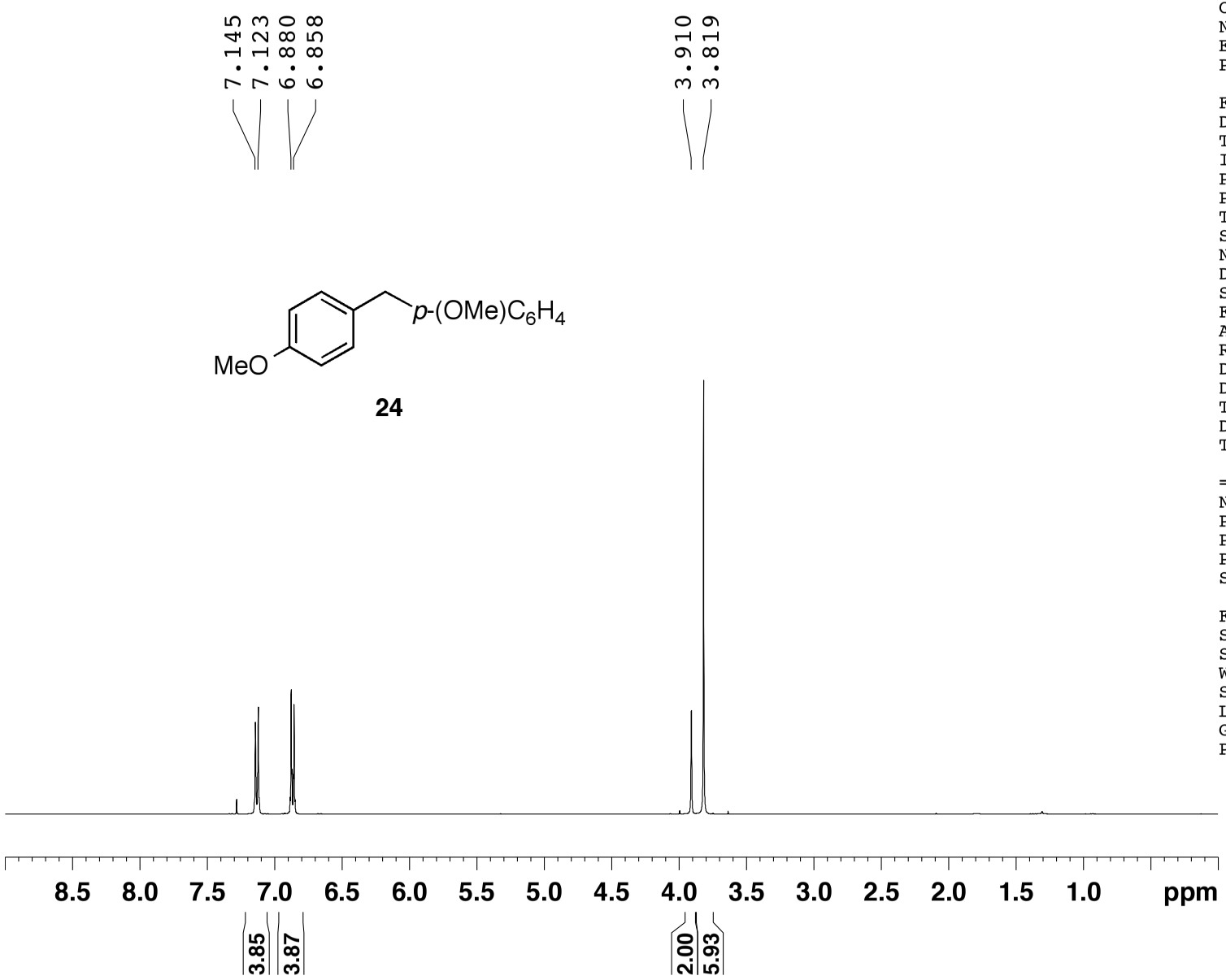
F2 - Acquisition Parameters
Date_          20120705
Time               5.13
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                9.25 usec
PL1               0.55 dB
PL1W       35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2               4.90 dB
PL12             20.46 dB
PL13             21.00 dB
PL2W        3.30822015 W
PL12W       0.09195905 W
PL13W       0.08120718 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

Compound 24, 1HNMR



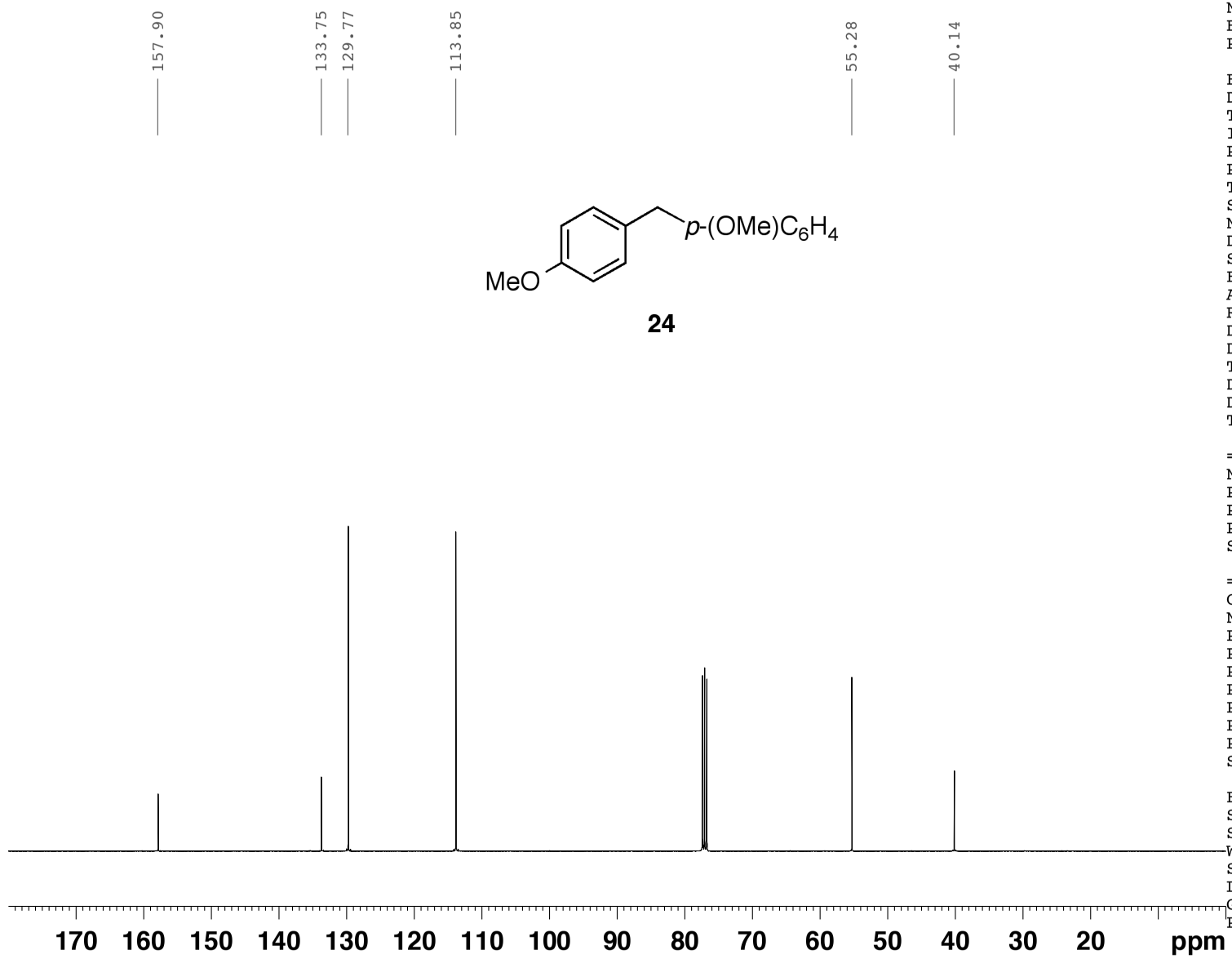

```
Current Data Parameters
NAME          DMM3-111-4
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120714
Time               12.04
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                     8
DW                60.400 usec
DE                 6.00 usec
TE                298.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                 4.90 dB
PL1W          3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

Compound 24, 13CNMR




```
Current Data Parameters
NAME          DMM3-111-4
EXPNO                  2
PROCNO                 1

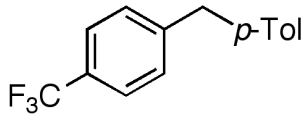
F2 - Acquisition Parameters
Date_           20120714
Time               12.20
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            23980.814 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                   512
DW                20.850 usec
DE                18.00 usec
TE                298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.25 usec
PL1                  0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

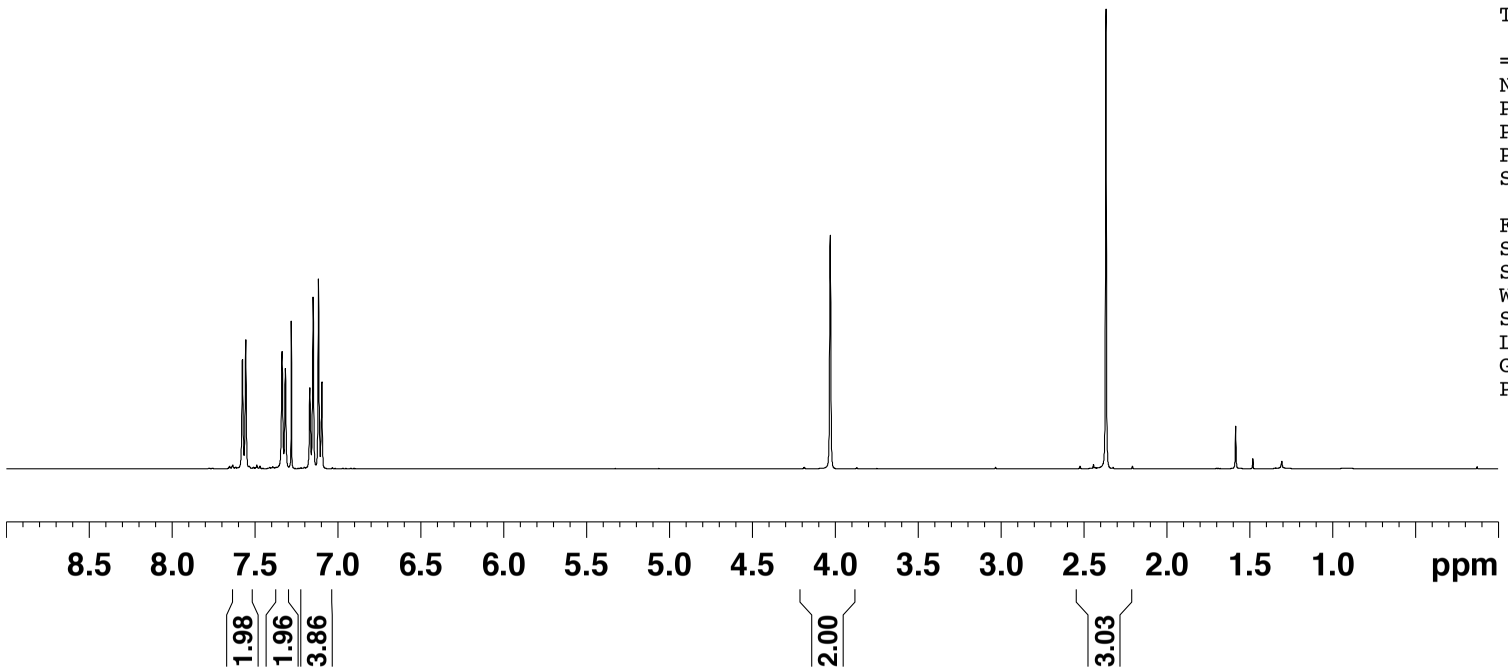
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 25, 1HNMR



25



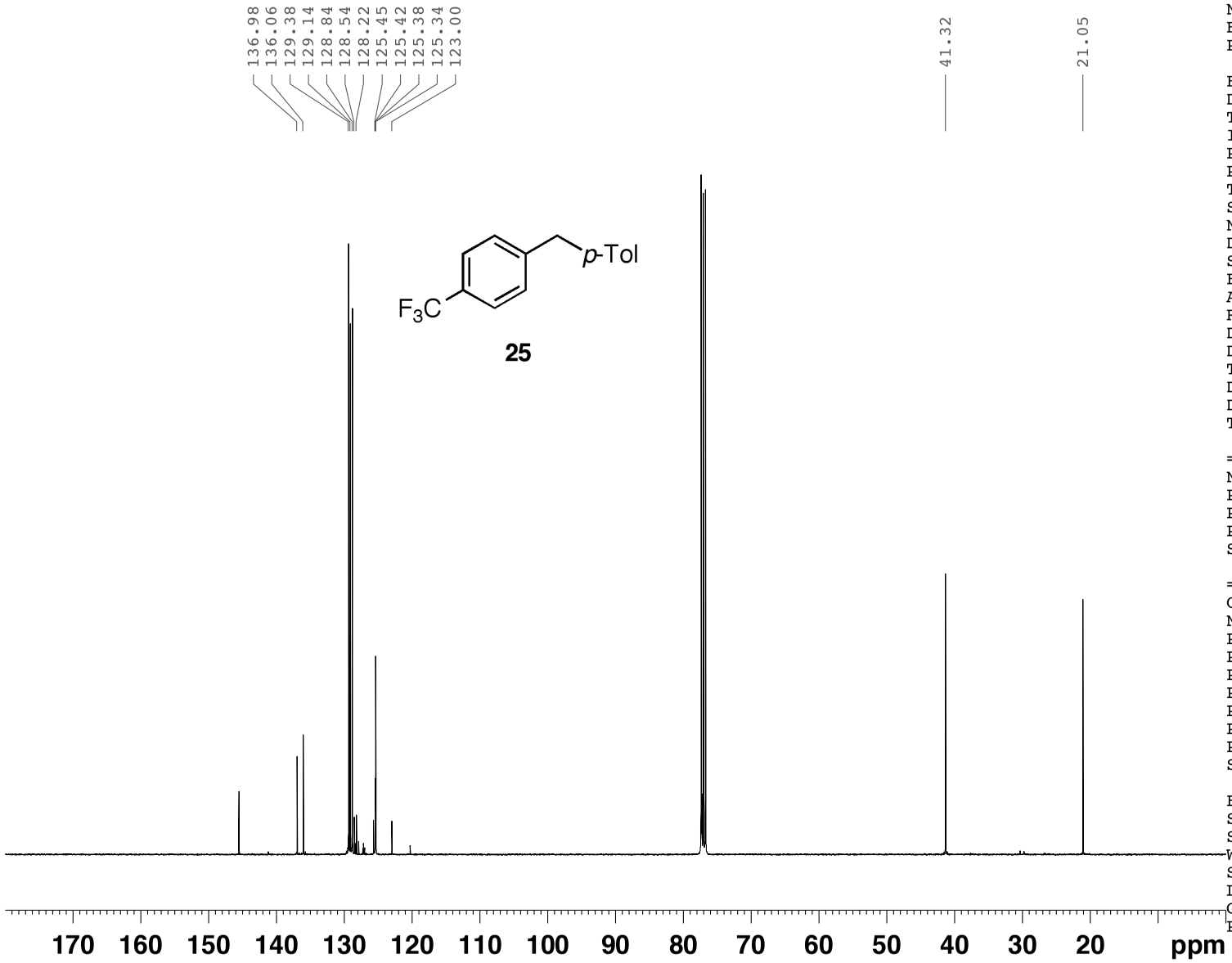

```
Current Data Parameters
NAME         PM-3-256-2A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120512
Time               14.39
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  10.1
DW                60.400 usec
DE                 6.00 usec
TE                298.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

Compound 25, 13CNMR




```
Current Data Parameters
NAME         PM-3-256-2A
EXPNO                  3
PROCNO                 1

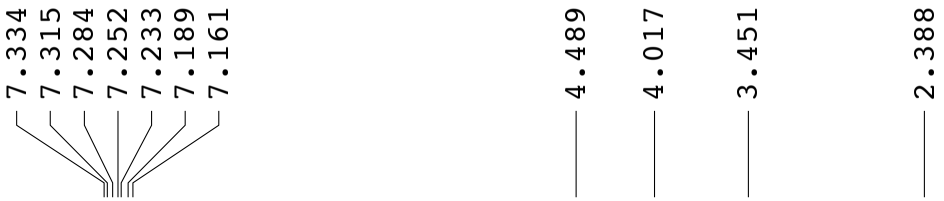
F2 - Acquisition Parameters
Date_           20120512
Time              21.04
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

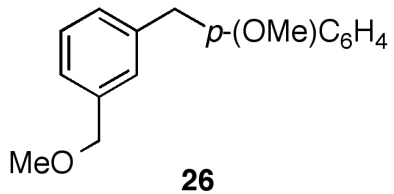
======== CHANNEL f1 ========
NUC1                13C
P1                9.25 usec
PL1               0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2               4.90 dB
PL12             20.46 dB
PL13             21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

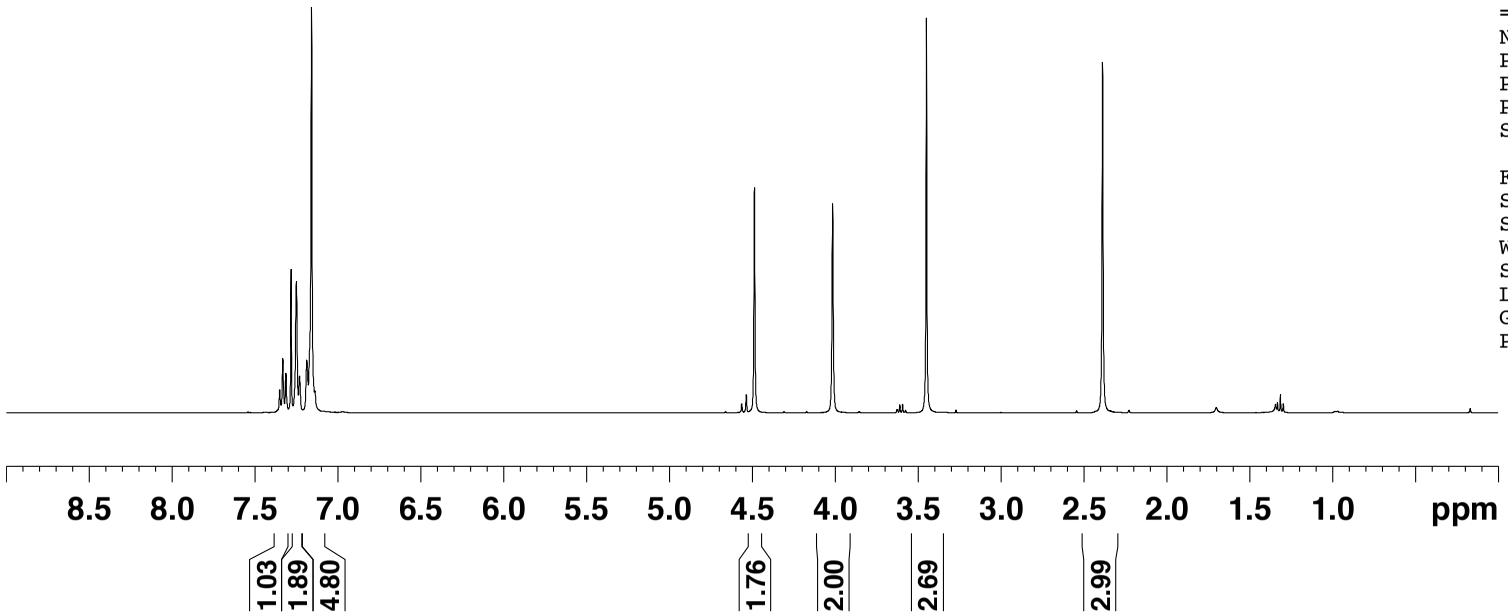
F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC                1.40
```

Compound 26, 1HNMR





26



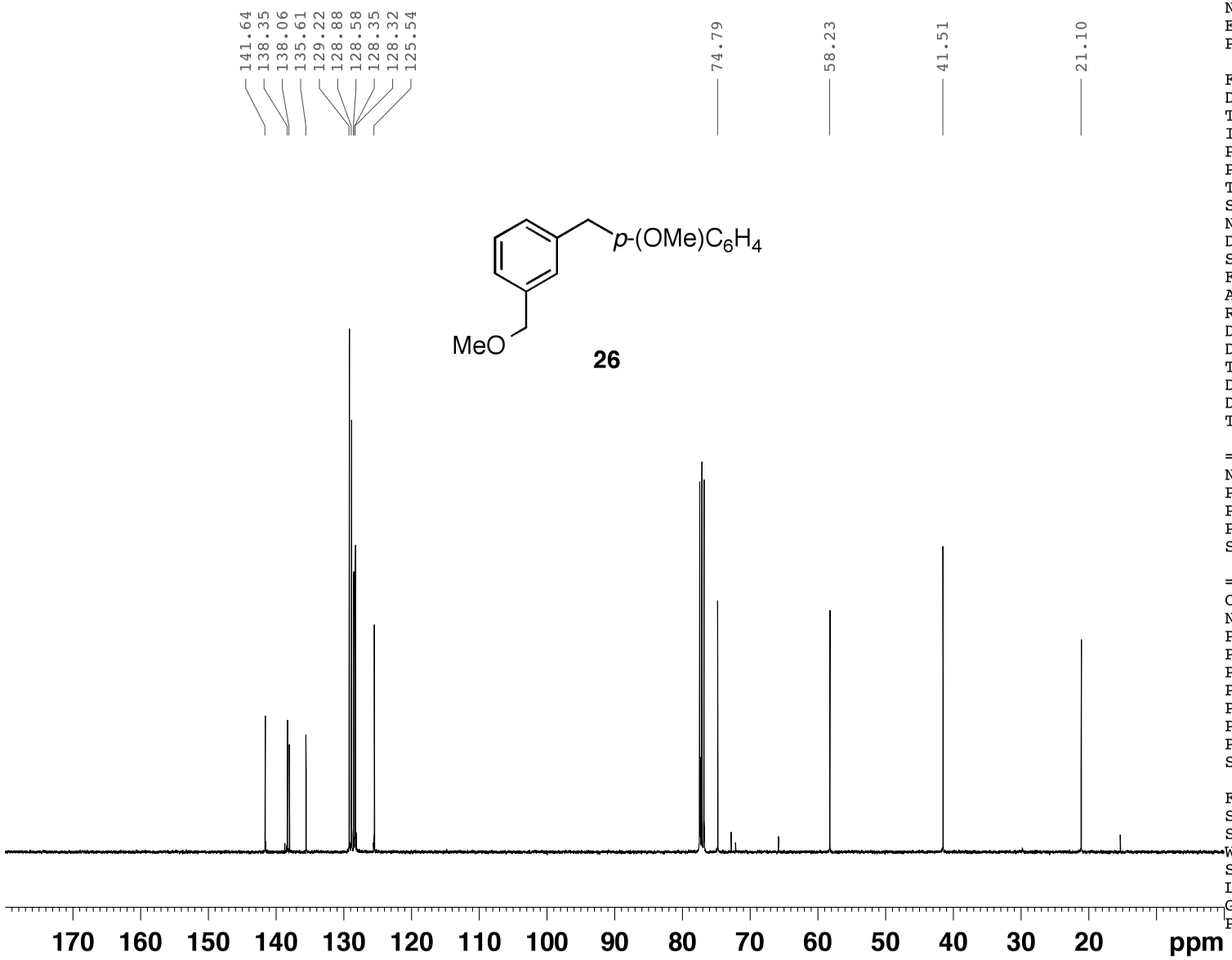

```
Current Data Parameters
NAME           PM-4-49-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120812
Time               16.02
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                     4
DW                60.400 usec
DE                 6.00 usec
TE                298.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

Compound 26, 13CNM




```
Current Data Parameters
NAME          PM-4-49-2
EXPNO                 2
PROCNO                1

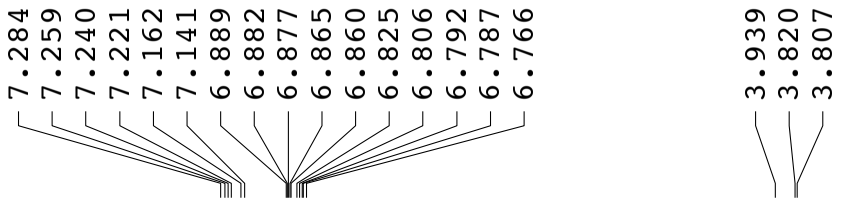
F2 - Acquisition Parameters
Date_          20120812
Time              16.05
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

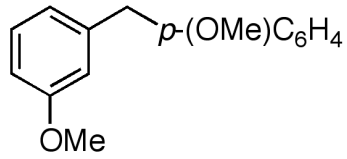
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W         0.09195905 W
PL13W         0.08120718 W
SFO2        400.1316005 MHz

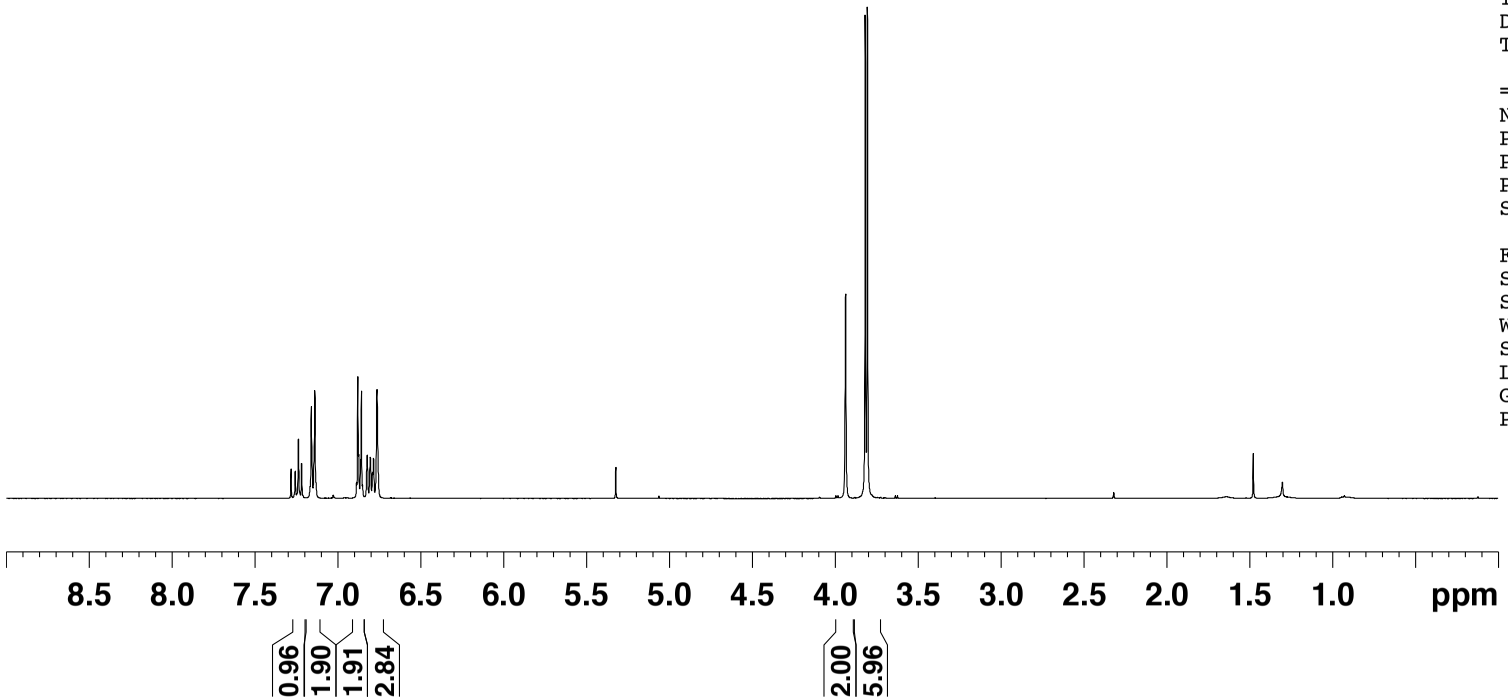
F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 27, 1HNMR





27



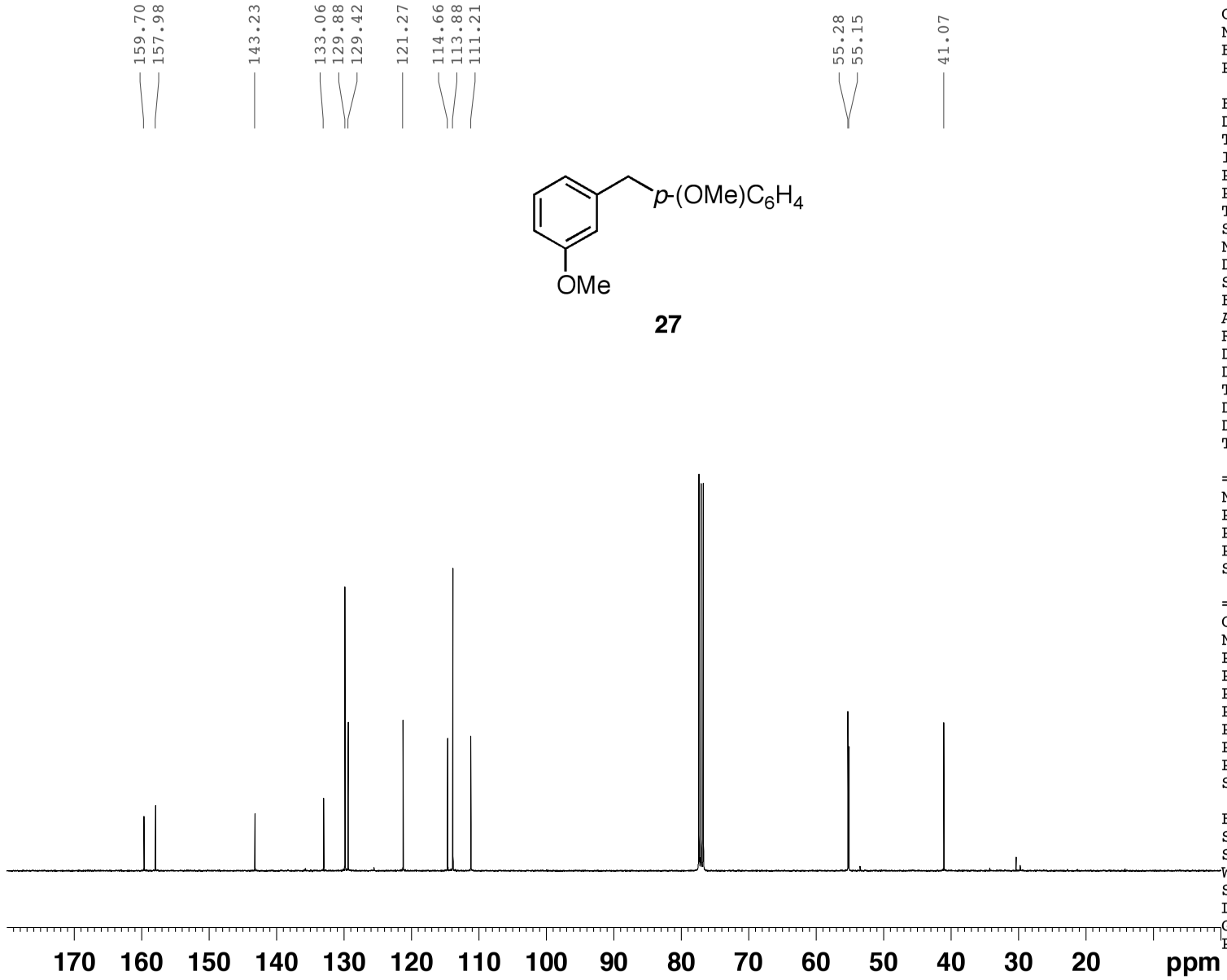

```
Current Data Parameters
NAME          DMM3-111-3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120714
Time               12.26
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  14.3
DW                60.400 usec
DE                 6.00 usec
TE                298.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                 4.90 dB
PL1W          3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

Compound 27, 13CNMR




```
Current Data Parameters
NAME          DMM3-111-3
EXPNO                  2
PROCNO                 1

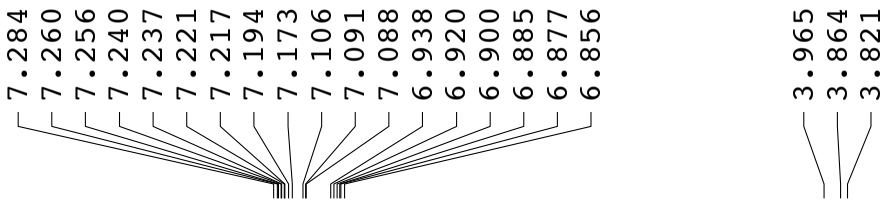
F2 - Acquisition Parameters
Date_           20120714
Time               12.42
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

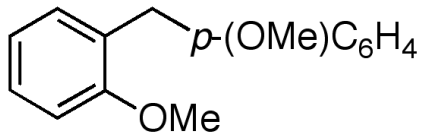
======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1                0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

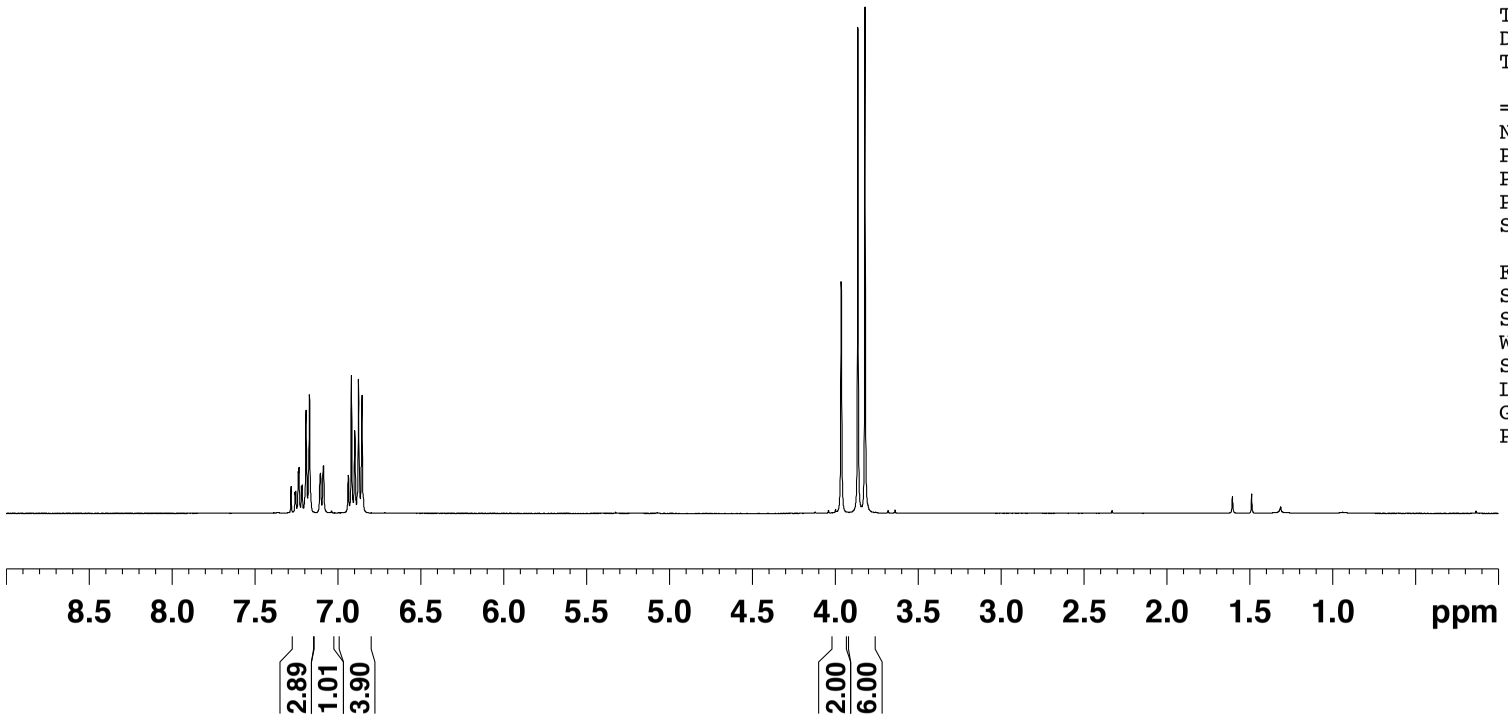
F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 28, 1HNMR





28



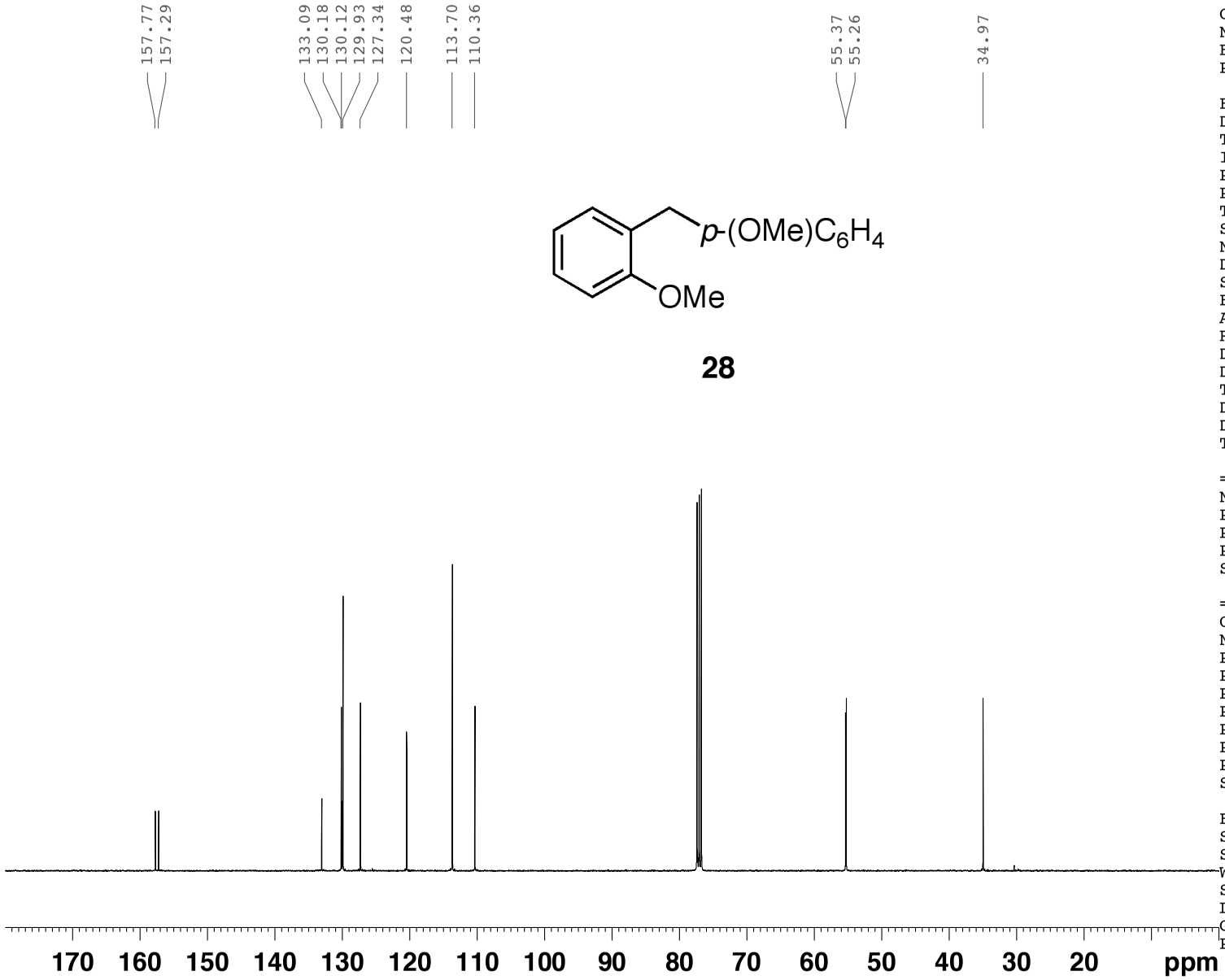

```
Current Data Parameters
NAME          DMM3-111-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120714
Time               12.49
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  14.3
DW                60.400 usec
DE                 6.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                 4.90 dB
PL1W          3.30822015 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

Compound 28, 13CNMR




```
Current Data Parameters
NAME          DMM3-111-2
EXPNO                  2
PROCNO                 1

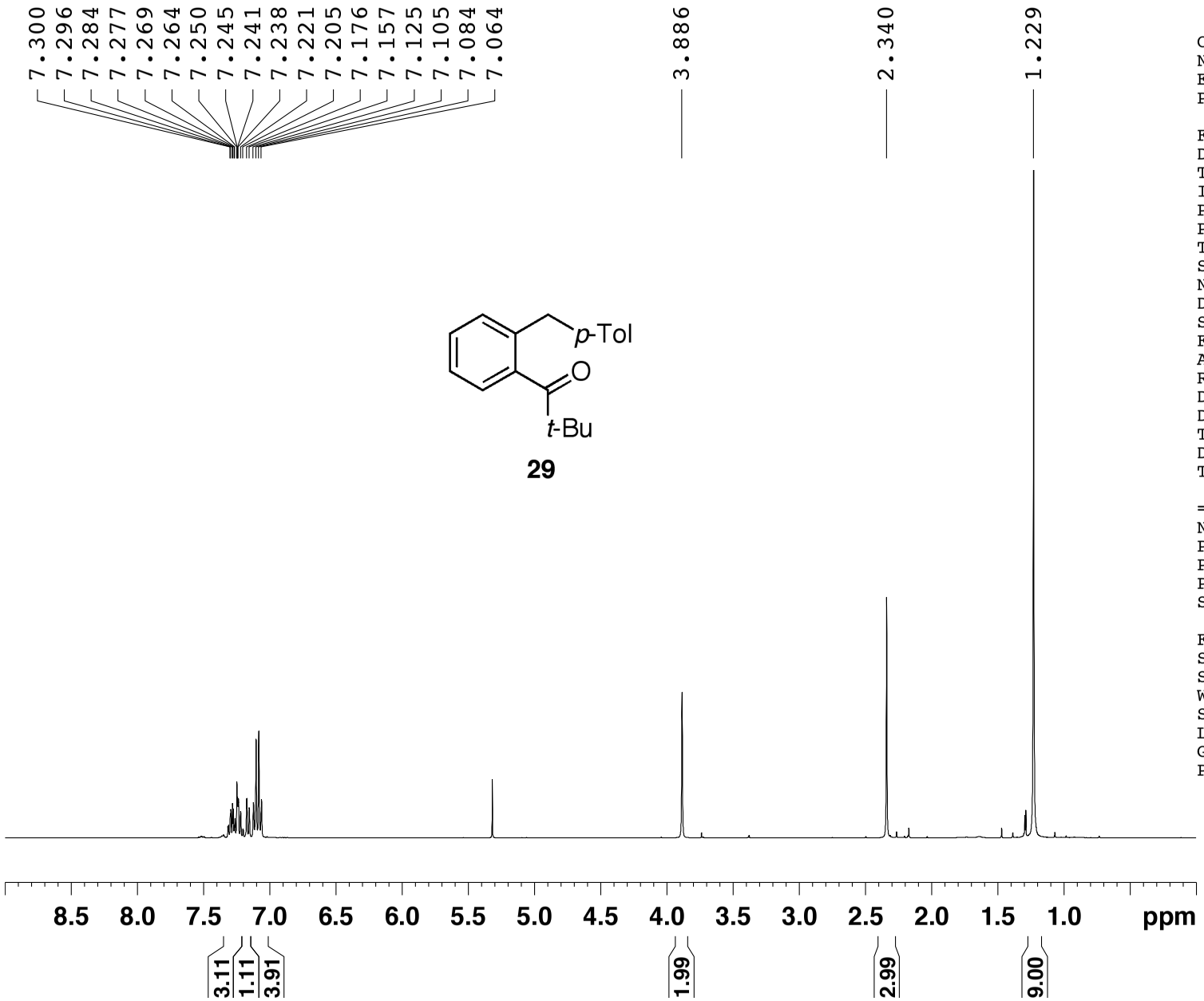
F2 - Acquisition Parameters
Date_           20120714
Time              13.05
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1                0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 29, 1HNMR



29

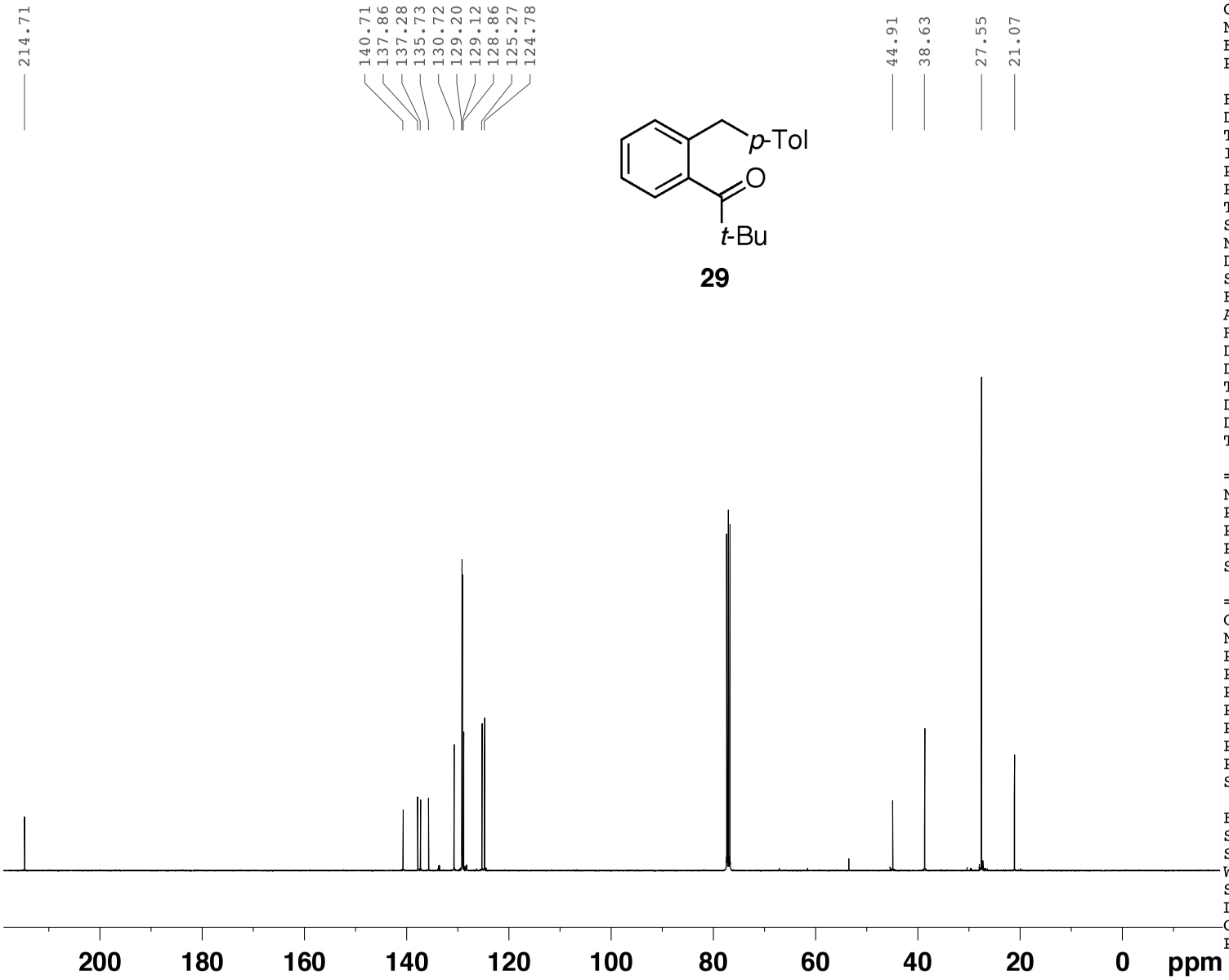

```
Current Data Parameters
NAME          DMM3-107-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120706
Time              18.05
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                 11.3
DW               60.400 usec
DE                6.00 usec
TE                298.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

Compound 29, 13CNMR



29

```
Current Data Parameters
NAME          DMM3-107-1
EXPNO                  2
PROCNO                 1

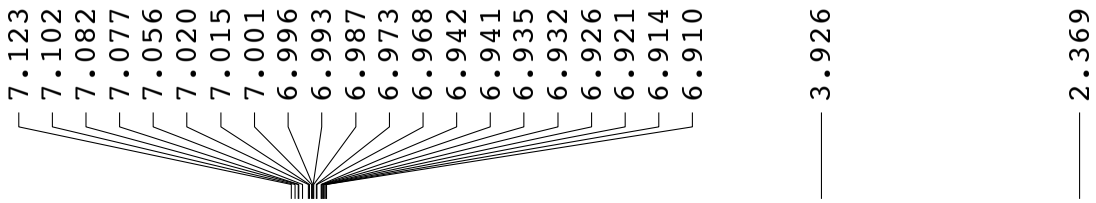
F2 - Acquisition Parameters
Date_           20120706
Time              18.21
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

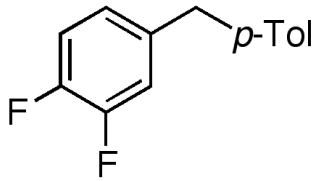
======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1                0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

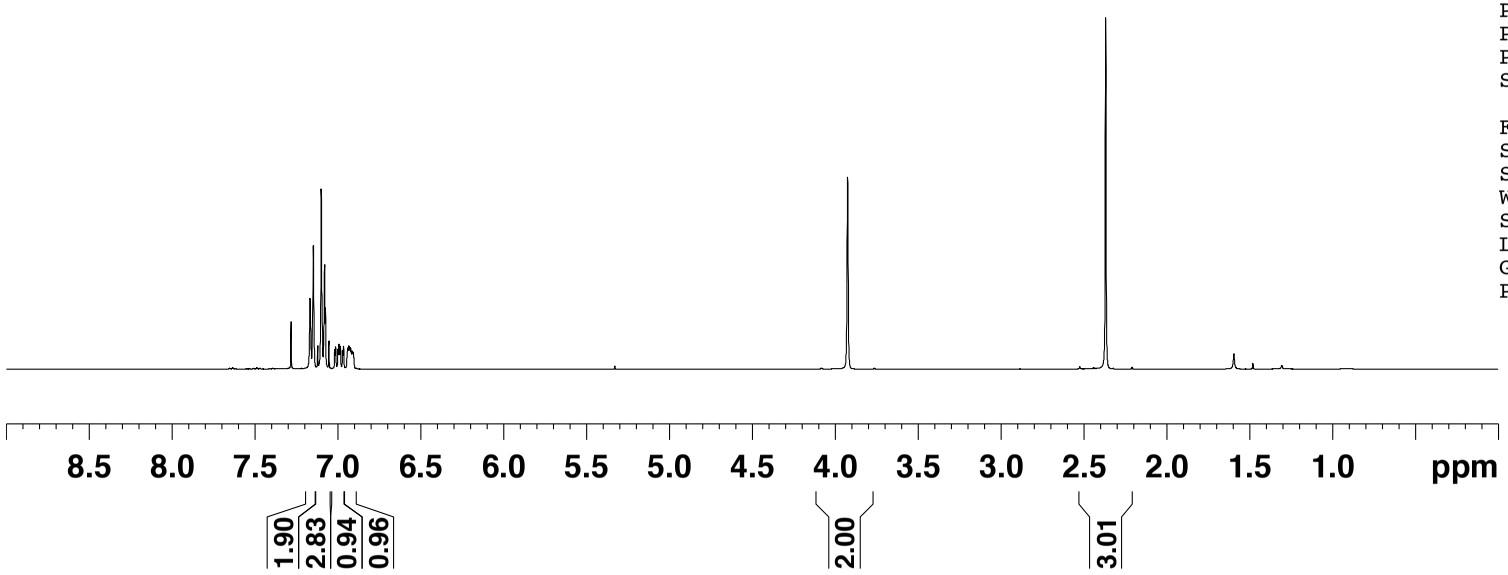
F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 30, 1HNMR





30



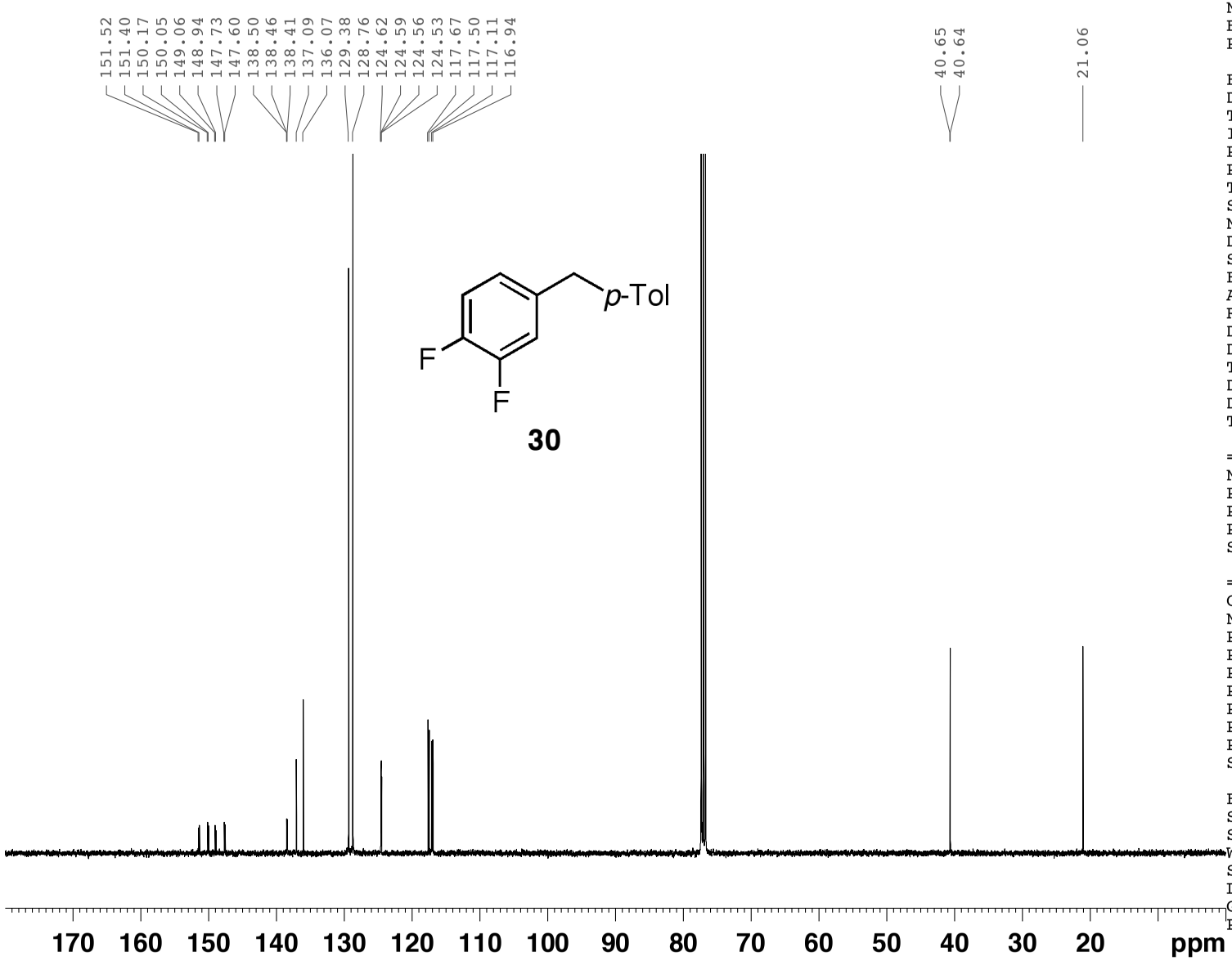

```
Current Data Parameters
NAME                  PM-4-24-1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20120717
Time                      11.17
INSTRUM                   spect
PROBHD    5 mm CPQNP 1H/
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                         12.7
DW                        60.400 usec
DE                         6.00 usec
TE                        298.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        15.00 usec
PL1                        4.90 dB
PL1W                 3.30822015 W
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF                  400.1300000 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

Compound 30, 13CNMR




```
Current Data Parameters
NAME           PM-4-24-1
EXPNO                  2
PROCNO                 1

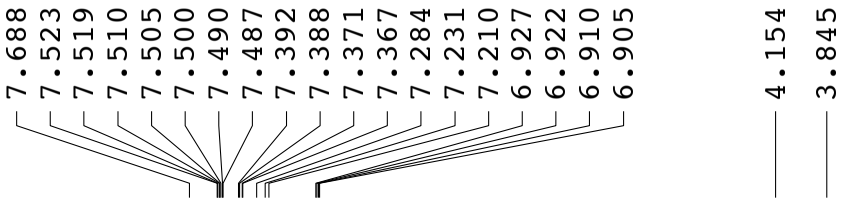
F2 - Acquisition Parameters
Date_           20120717
Time               11.21
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     4
SWH            23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                   512
DW                20.850 usec
DE                18.00 usec
TE                298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

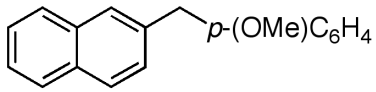
======== CHANNEL f1 ========
NUC1                  13C
P1                   9.25 usec
PL1                  0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

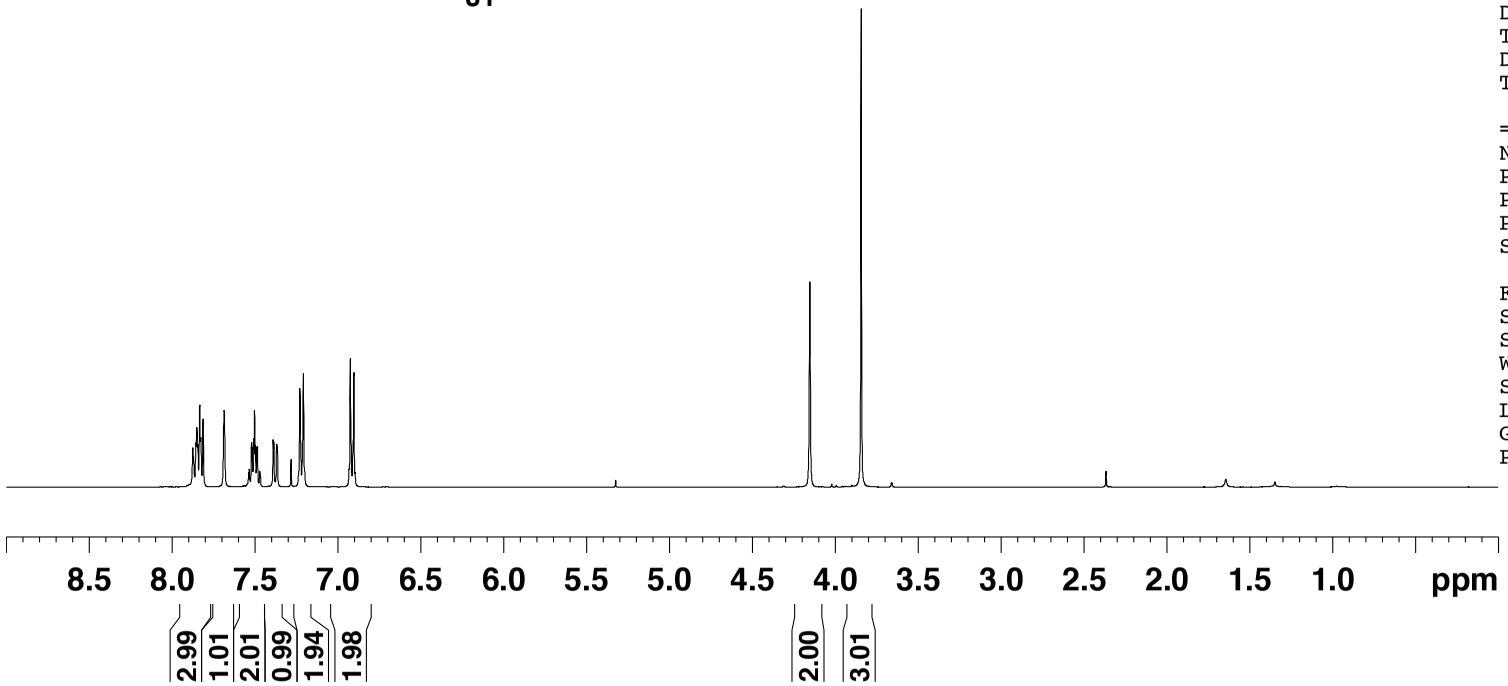
F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 31, 1HNMR





31



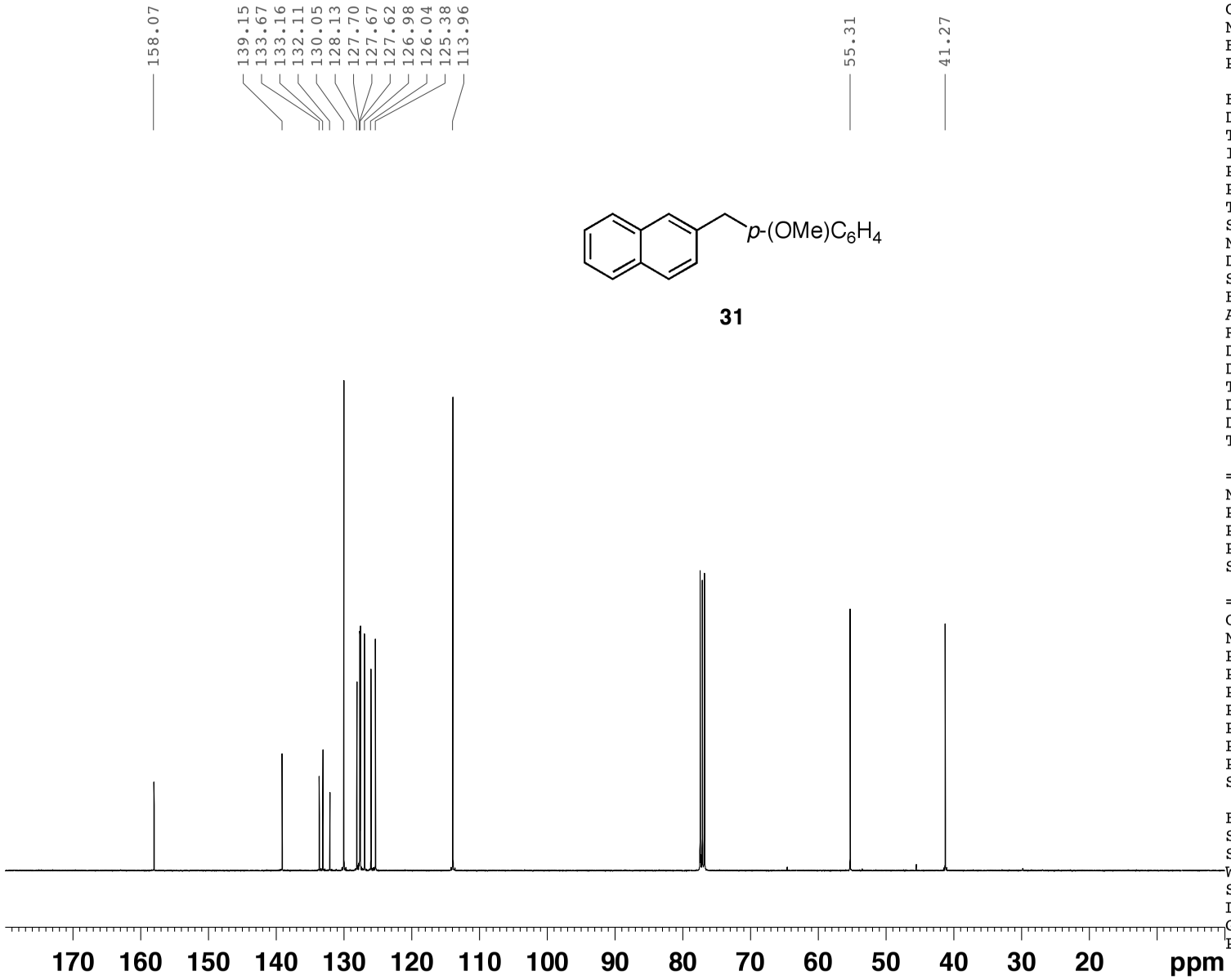

```
Current Data Parameters
NAME          PM-4-24-5
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20120718
Time               6.39
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                 10.1
DW               60.400 usec
DE                6.00 usec
TE                298.1 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

Compound 31, 13CNMR



31

```
Current Data Parameters
NAME          PM-4-24-5
EXPNO                 2
PROCNO                1

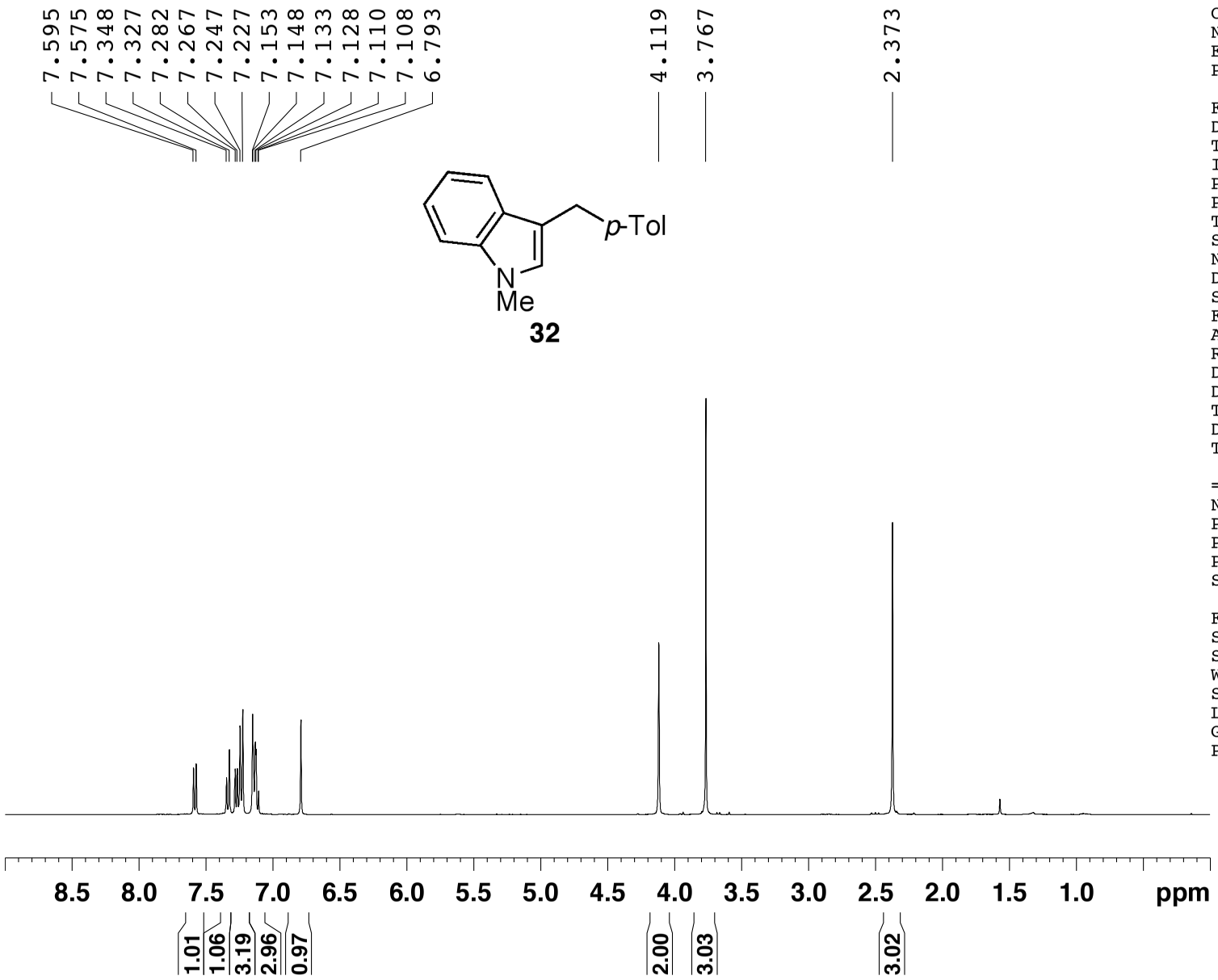
F2 - Acquisition Parameters
Date_          20120718
Time               6.55
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1                0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 32, 1HNMR



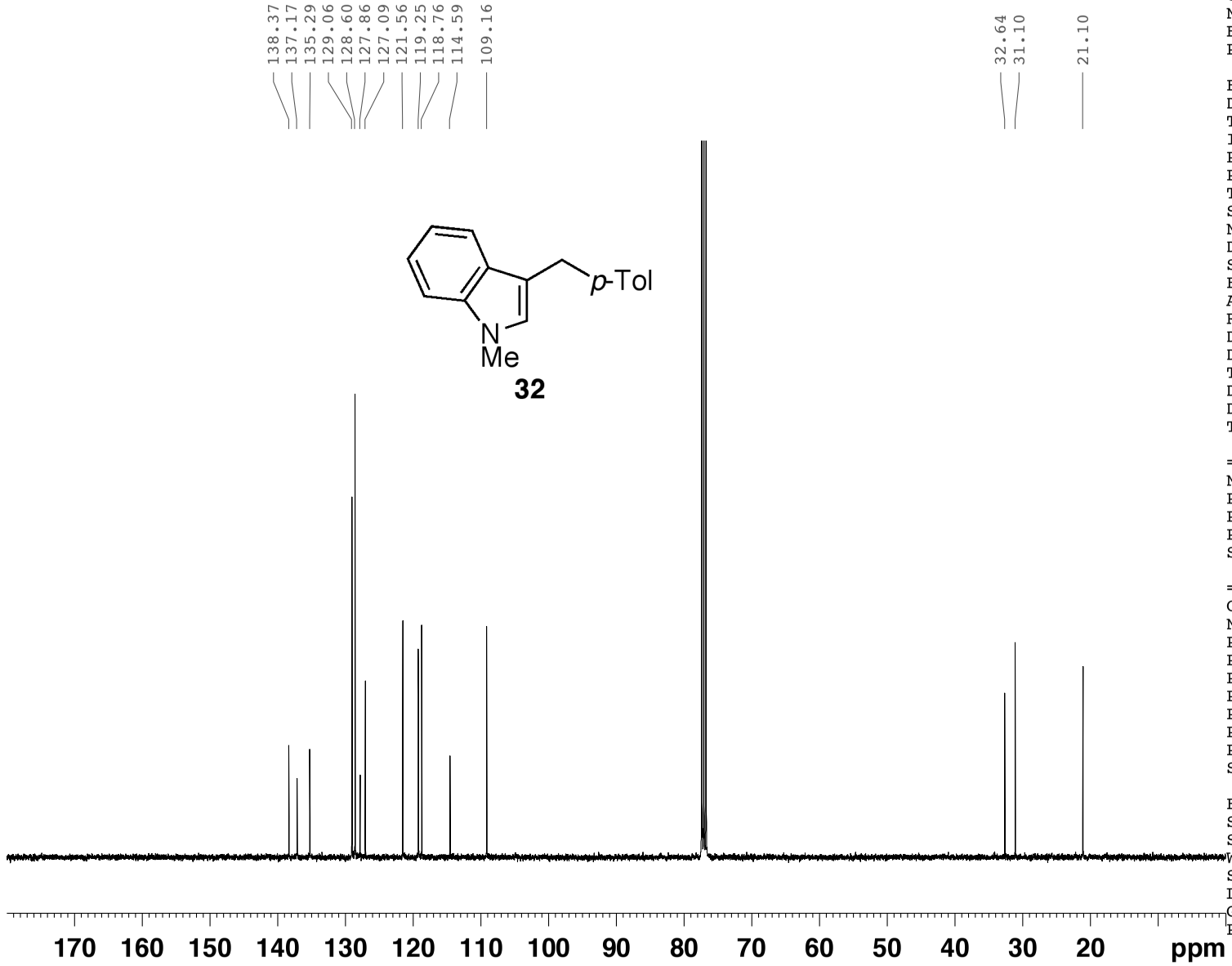

```
Current Data Parameters
NAME      DMM3-065-2-pure
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120428
Time              18.03
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                 12.7
DW               60.400 usec
DE                6.00 usec
TE                298.2 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

Compound 32, 13CNMR



Current Data Parameters
NAME DMM3-065-2-pure
EXPNO 2
PROCNO 1

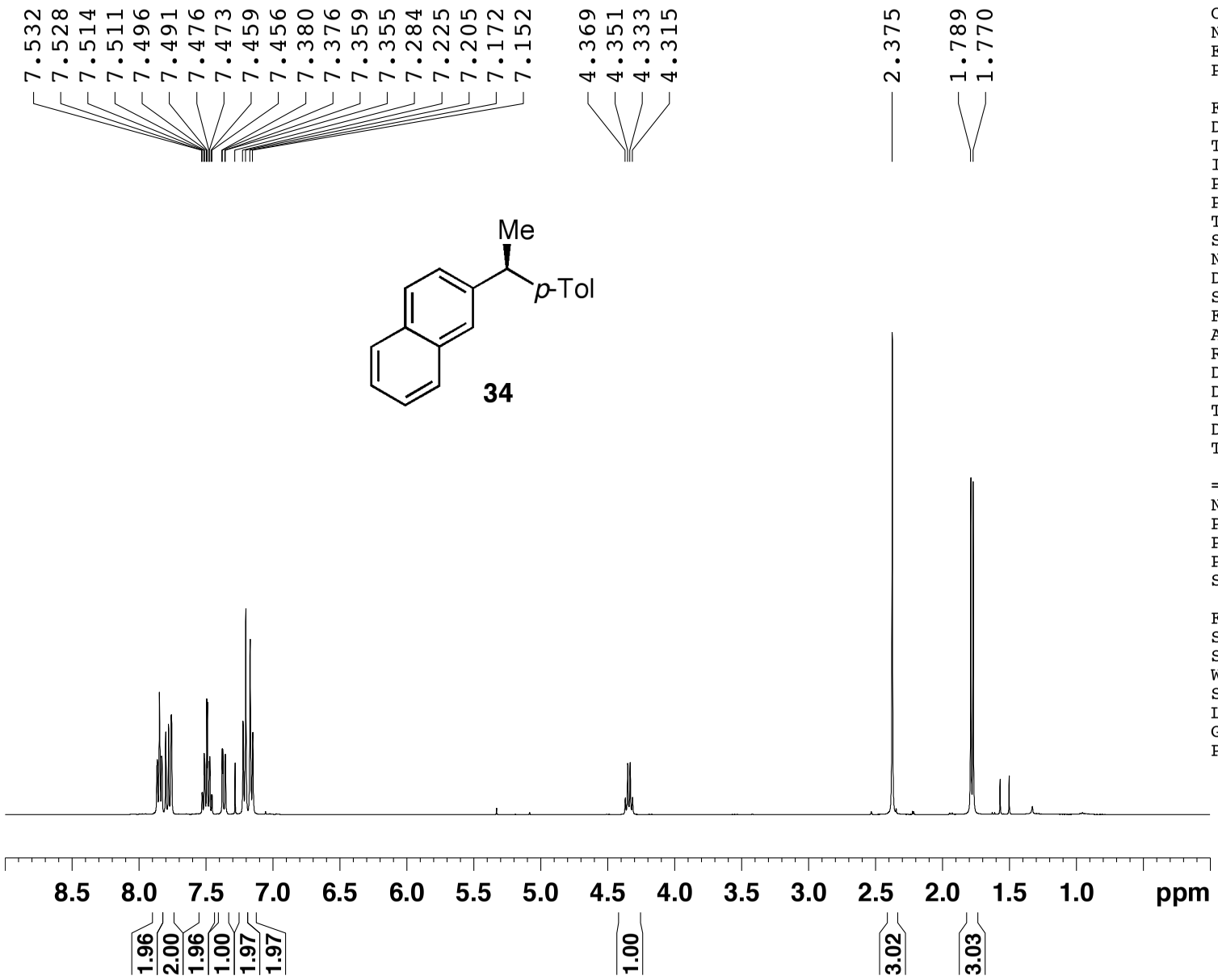
F2 - Acquisition Parameters
Date_ 20120428
Time 18.07
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 512
DW 20.850 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PL1 0.55 dB
PL1W 35.18820572 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 4.90 dB
PL12 20.46 dB
PL13 21.00 dB
PL2W 3.30822015 W
PL12W 0.09195905 W
PL13W 0.08120718 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 34, 1HNMR



BRUKER

S101

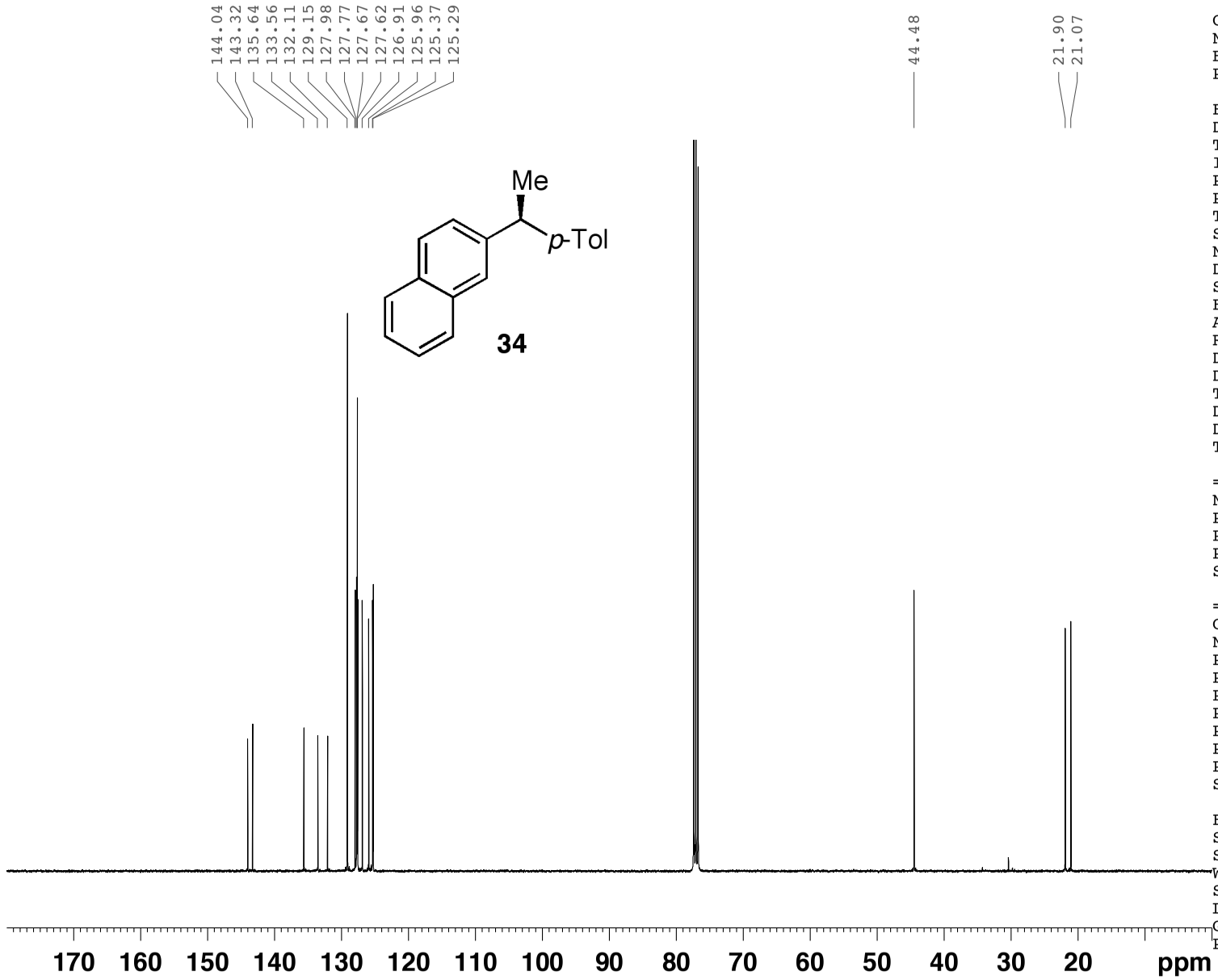
```
Current Data Parameters
NAME          DMM2-121-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120721
Time              14.47
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                 11.3
DW               60.400 usec
DE                6.00 usec
TE                298.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

Compound 34, 13CNMR




```
Current Data Parameters
NAME          DMM2-121-1
EXPNO                  2
PROCNO                 1

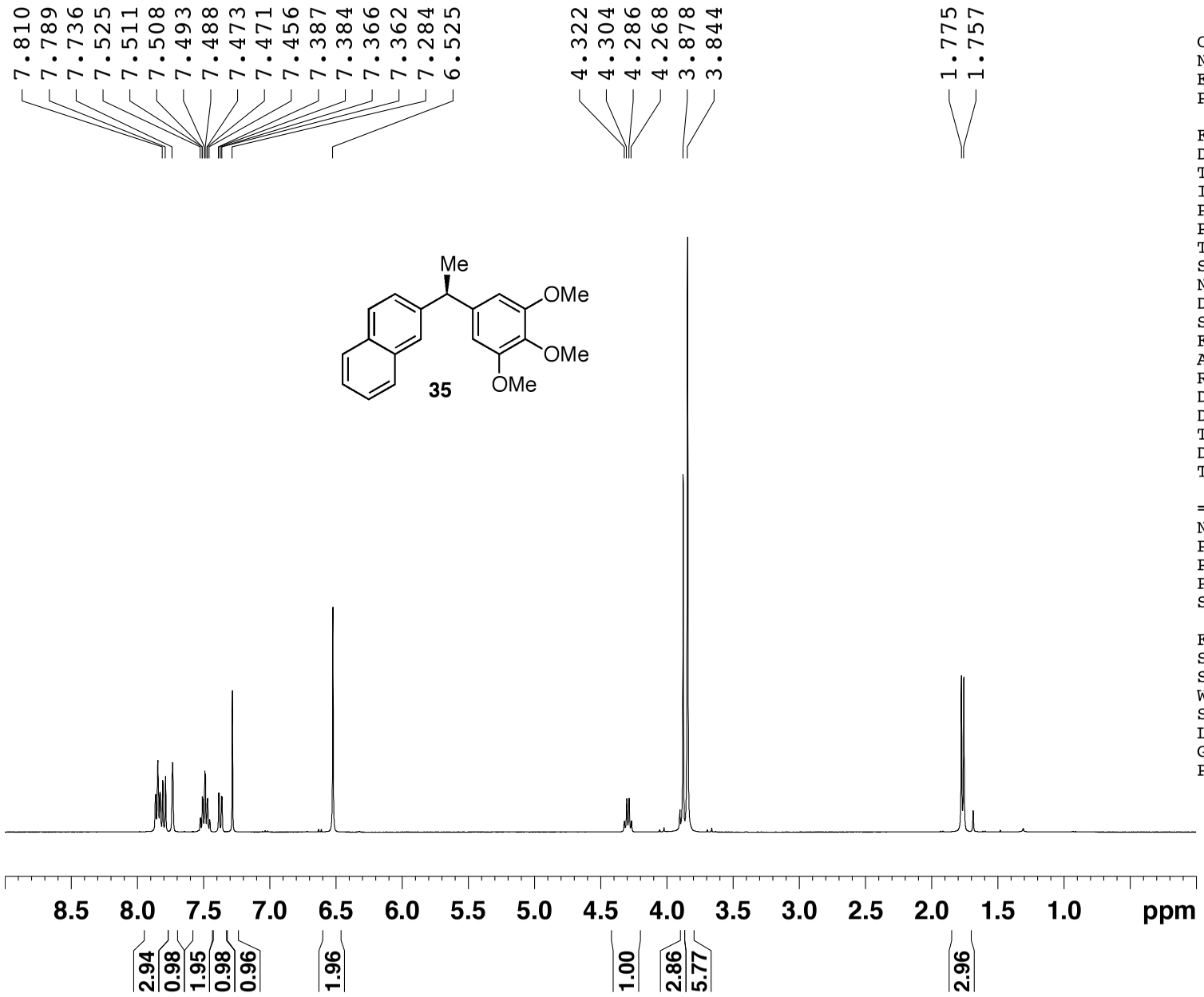
F2 - Acquisition Parameters
Date_           20120721
Time              15.03
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1                0.55 dB
PL1W        35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 35, 1HNMR



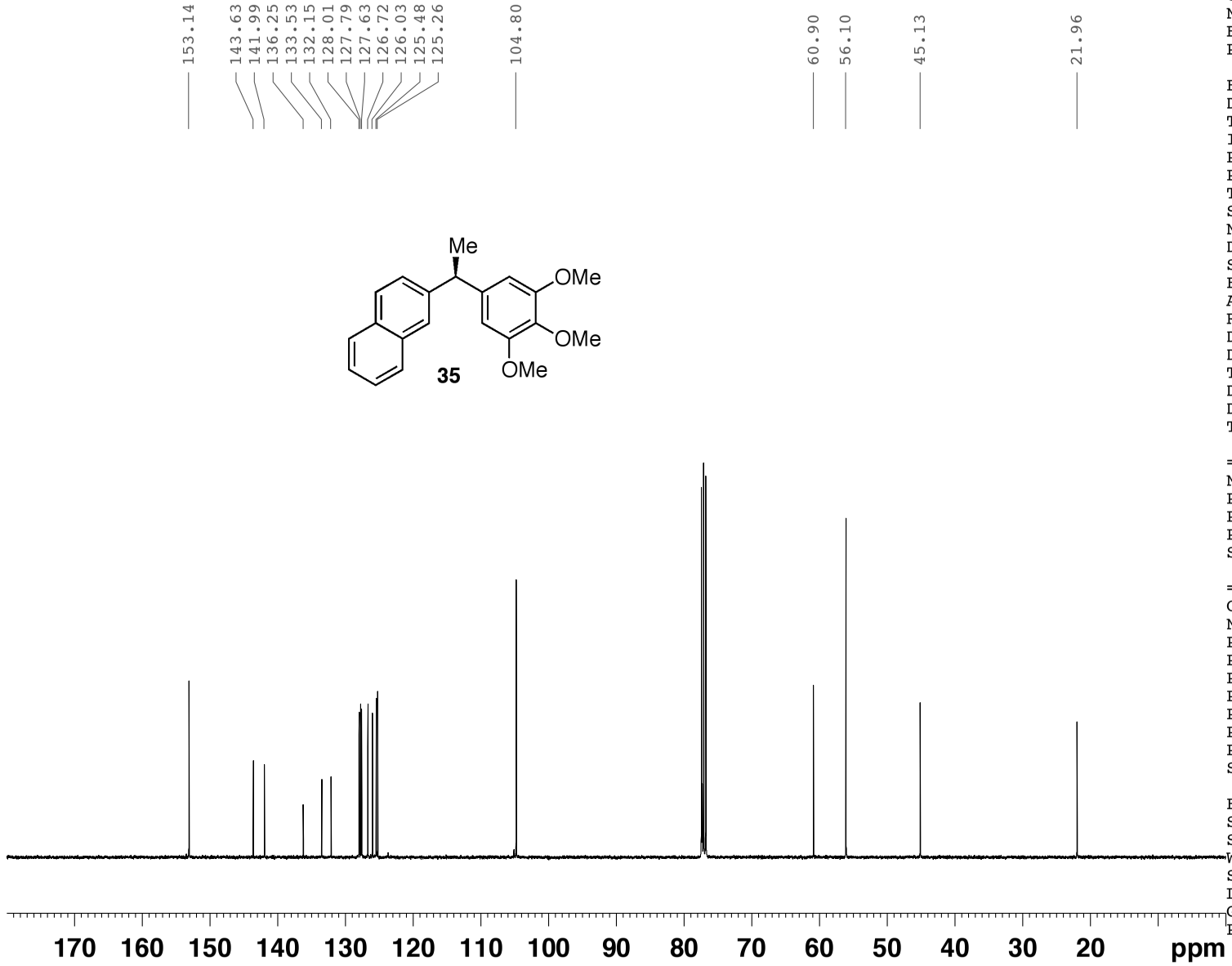

```
Current Data Parameters
NAME                  PM-4-47-3
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20120807
Time                      11.05
INSTRUM                   spect
PROBHD    5 mm CPQNP 1H/
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                            7.1
DW                       60.400 usec
DE                        6.00 usec
TE                        298.2 K
D1                   1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       15.00 usec
PL1                       4.90 dB
PL1W                 3.30822015 W
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF                 400.1300000 MHz
WDW                          EM
SSB                           0
LB                       0.30 Hz
GB                            0
PC                        1.00
```

Compound 35, 13CNMR




```
Current Data Parameters
NAME           PM-4-47-3
EXPNO                  2
PROCNO                 1

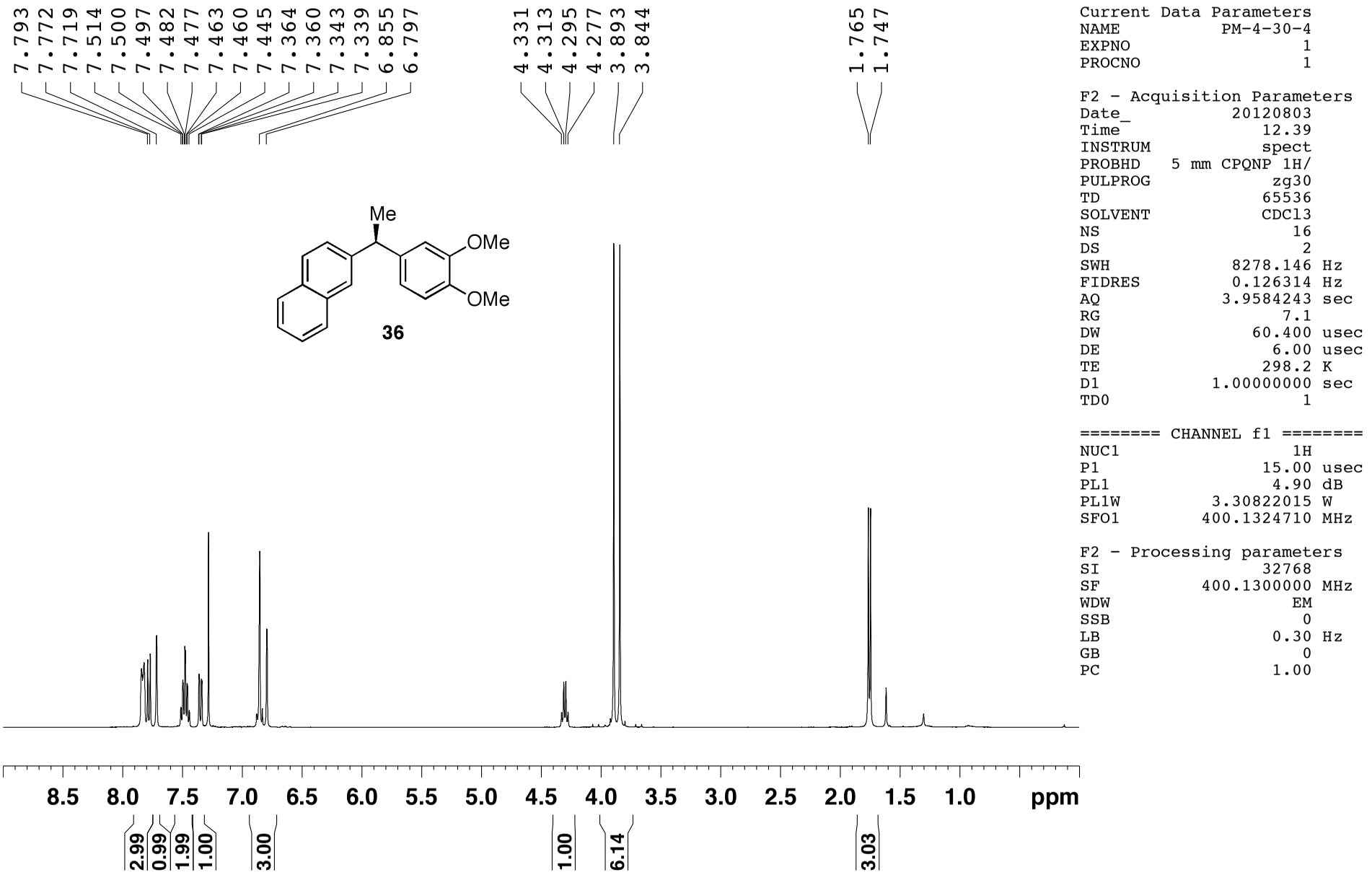
F2 - Acquisition Parameters
Date_           20120807
Time               11.08
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     4
SWH            23980.814 Hz
FIDRES          0.365918 Hz
AQ              1.3664756 sec
RG                   512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.25 usec
PL1                  0.55 dB
PL1W         35.18820572 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W          3.30822015 W
PL12W         0.09195905 W
PL13W         0.08120718 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 36, 1HNMR



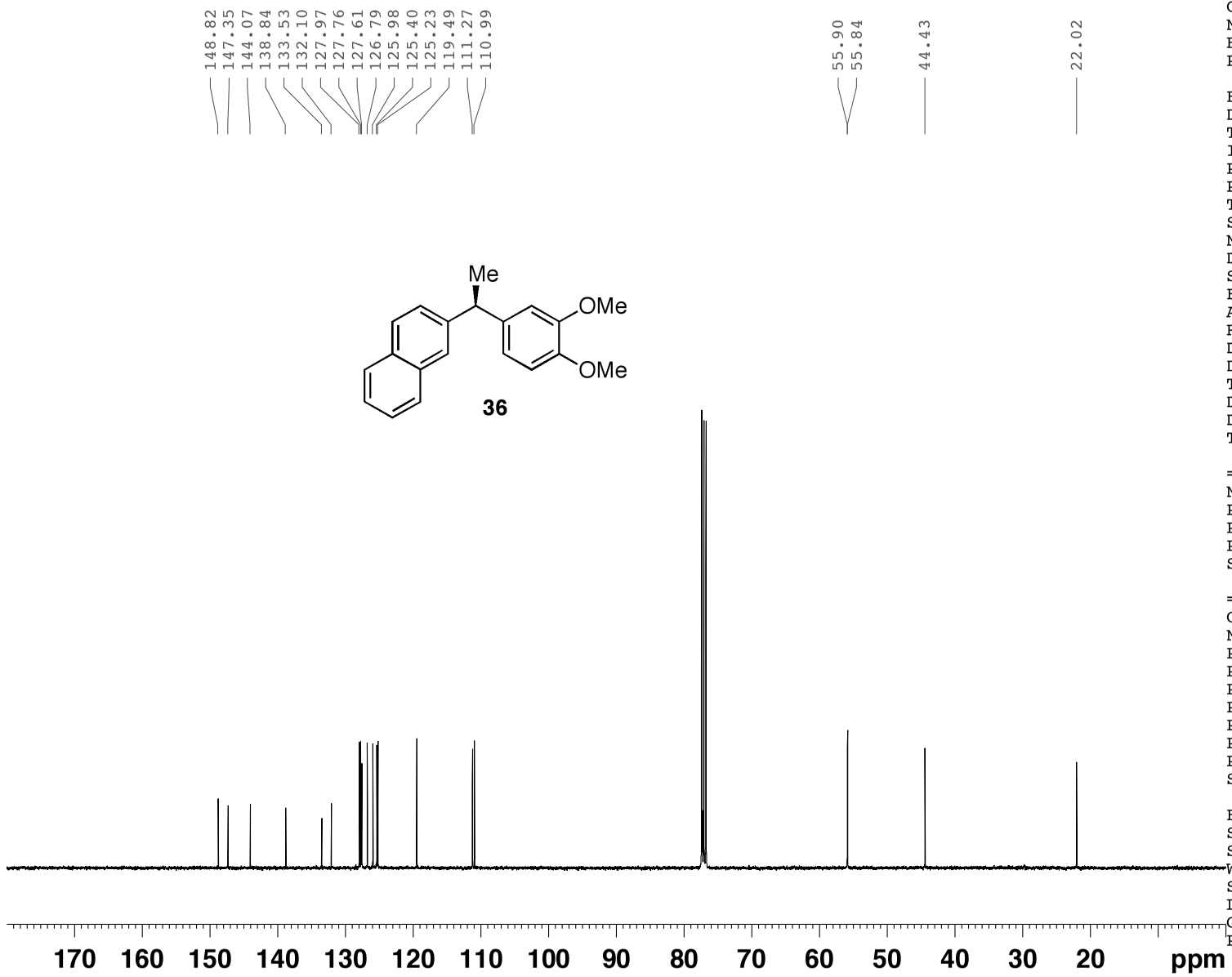
Current Data Parameters
NAME PM-4-30-4
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120803
Time 12.39
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 7.1
DW 60.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 4.90 dB
PL1W 3.30822015 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 36, 13CNMR




```
Current Data Parameters
NAME           PM-4-30-4
EXPNO                  2
PROCNO                 1

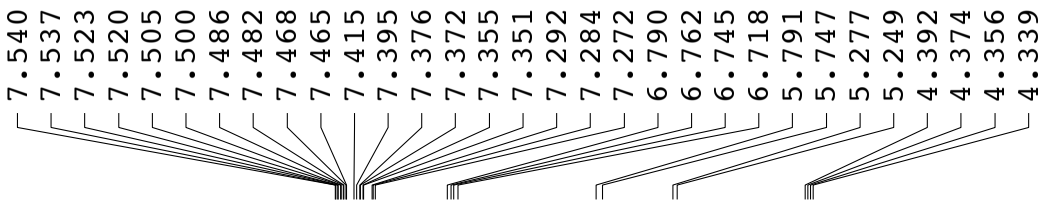
F2 - Acquisition Parameters
Date_           20120803
Time               12.42
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     4
SWH            23980.814 Hz
FIDRES          0.365918 Hz
AQ              1.3664756 sec
RG                   512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

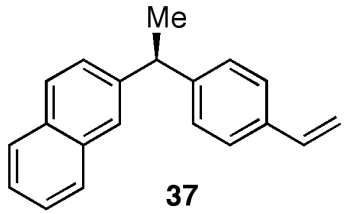
======== CHANNEL f1 ========
NUC1                  13C
P1                   9.25 usec
PL1                  0.55 dB
PL1W         35.18820572 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W          3.30822015 W
PL12W         0.09195905 W
PL13W         0.08120718 W
SFO2         400.1316005 MHz

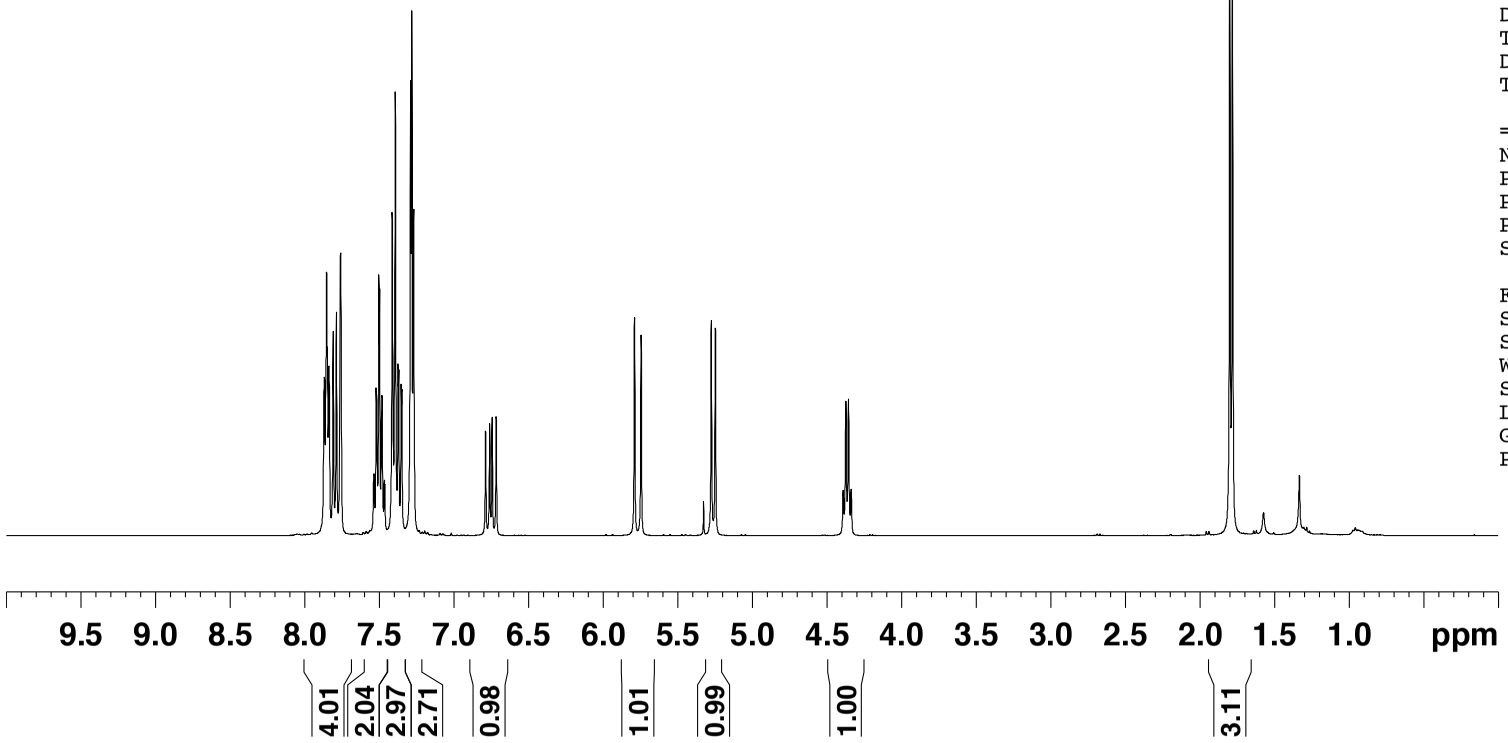
F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 37, 1HNMR





37



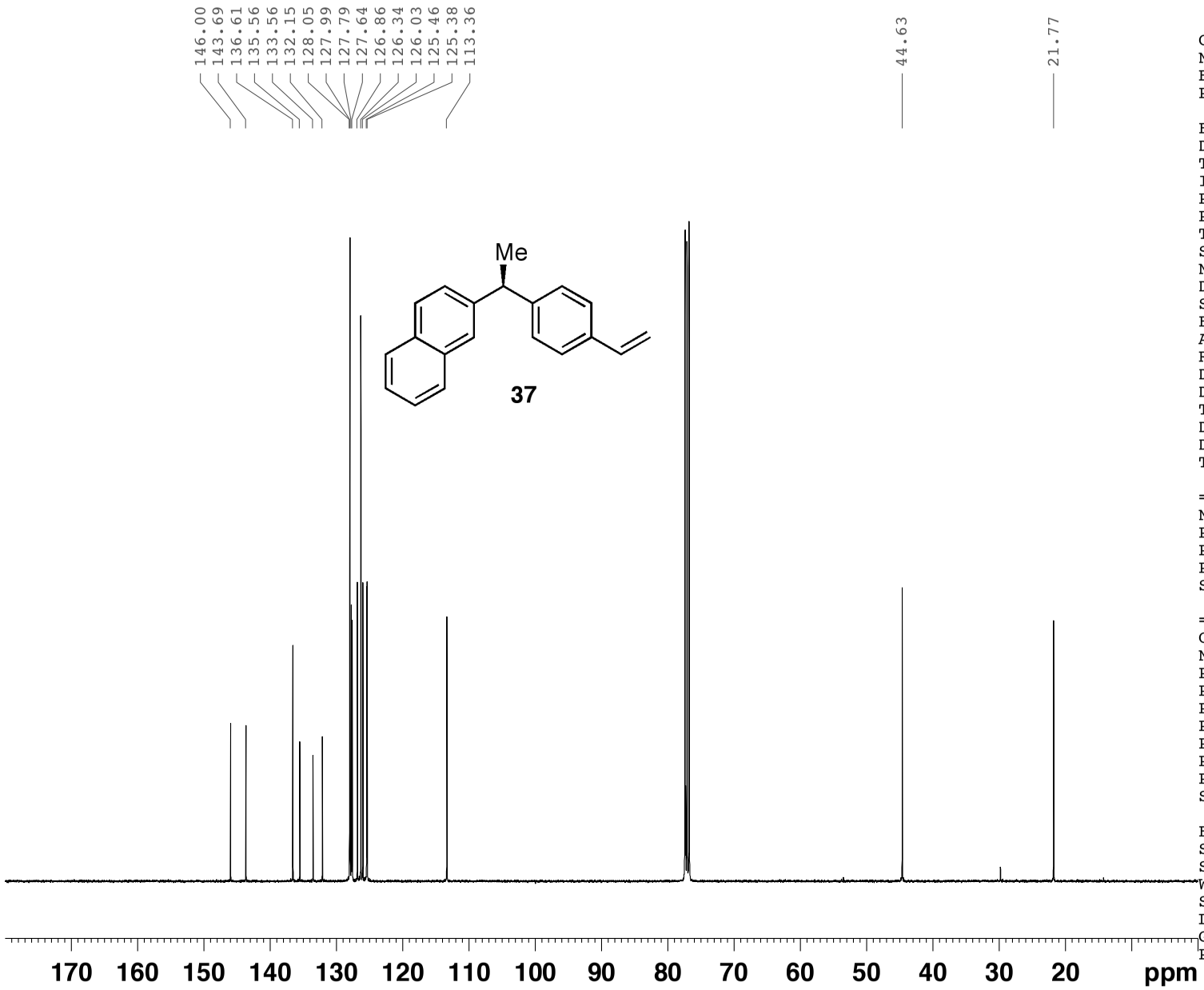
Current Data Parameters
NAME PM-4-79-3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121010
Time 1.12
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 9
DW 60.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 4.90 dB
PL1W 3.30822015 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 37, 13CNMR



Current Data Parameters

NAME	PM-4-79-3
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20121010
Time	1.28
INSTRUM	spect
PROBHD	5 mm CPQNP 1H/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	512
DW	20.850 usec
DE	18.00 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	9.25 usec
PL1	0.55 dB
PL1W	35.18820572 W
SFO1	100.6228298 MHz

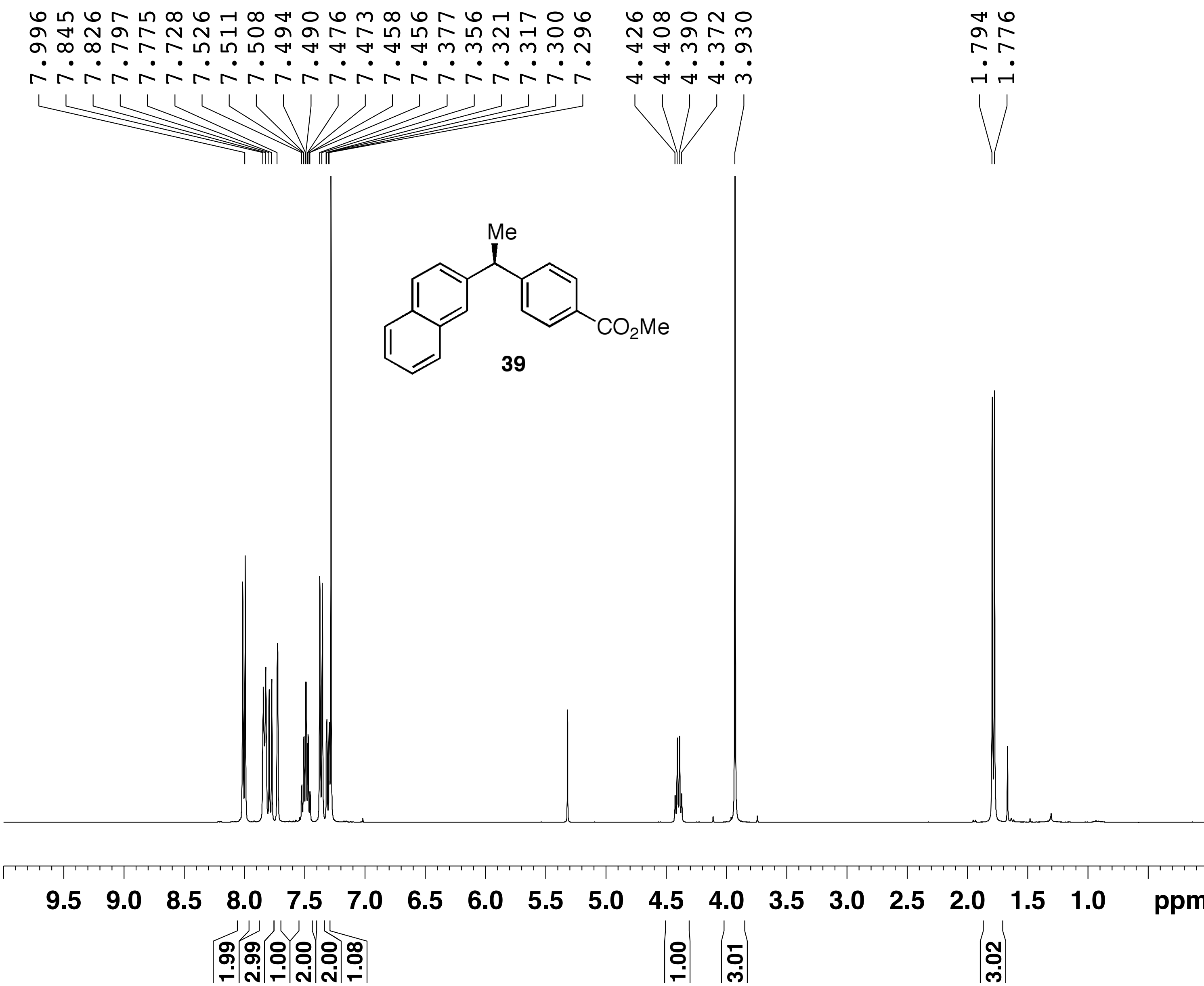
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	4.90 dB
PL12	20.46 dB
PL13	21.00 dB
PL2W	3.30822015 W
PL12W	0.09195905 W
PL13W	0.08120718 W
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Compound 39, 1HNMR



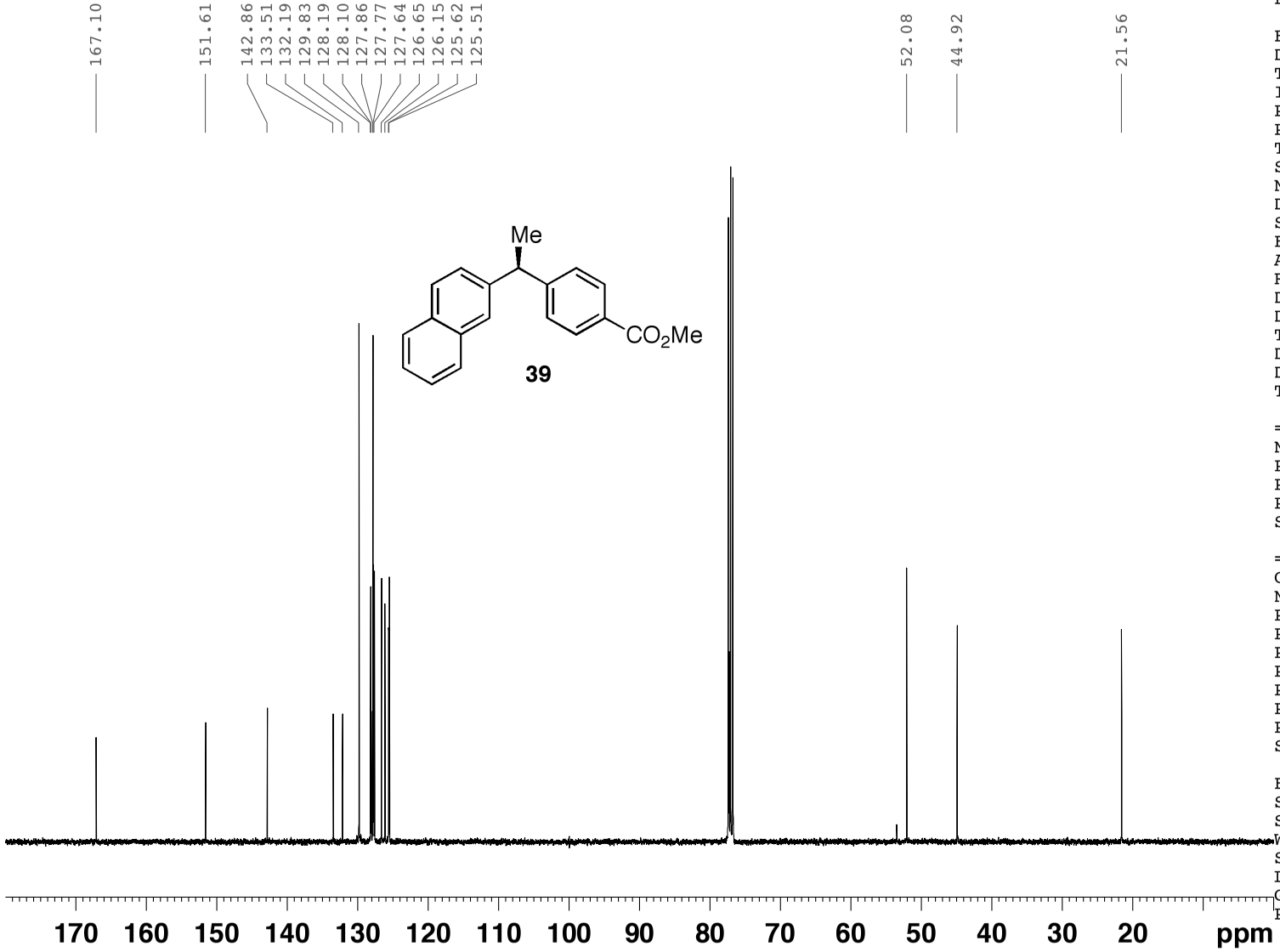

```
Current Data Parameters
NAME          DMM-3-186-1
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20121024
Time                17.39
INSTRUM             spect
PROBHD   5 mm CPQNP 1H/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ              3.9584243 sec
RG                      9
DW                 60.400 usec
DE                   6.00 usec
TE                  298.1 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  15.00 usec
PL1                  4.90 dB
PL1W           3.30822015 W
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                  32768
SF            400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

Compound 39, 13CNMR




```
Current Data Parameters
NAME         DMM-3-186-1
EXPNO                  2
PROCNO                 1

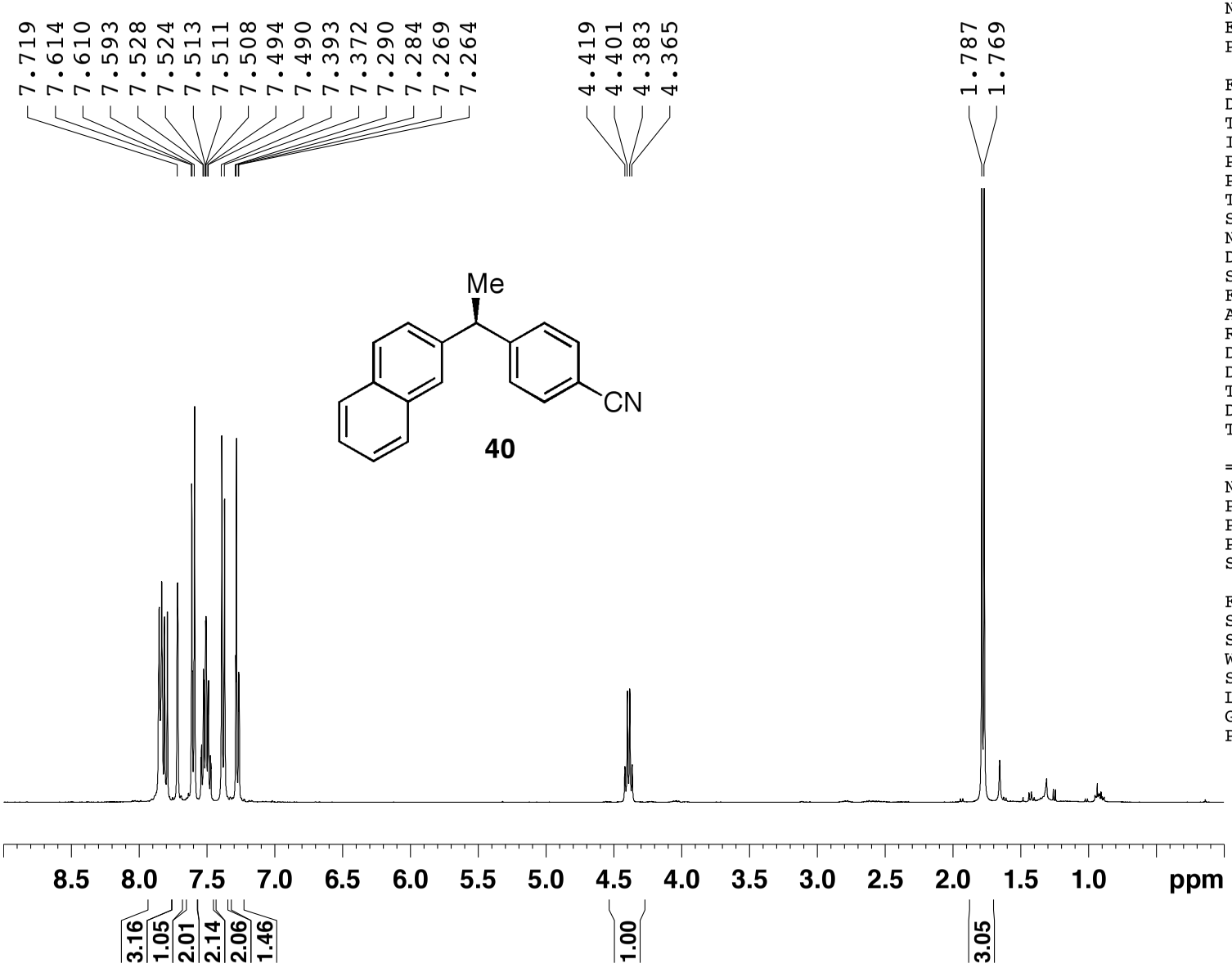
F2 - Acquisition Parameters
Date_           20121024
Time              17.43
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 40, 1HNMR



BRUKER

S111

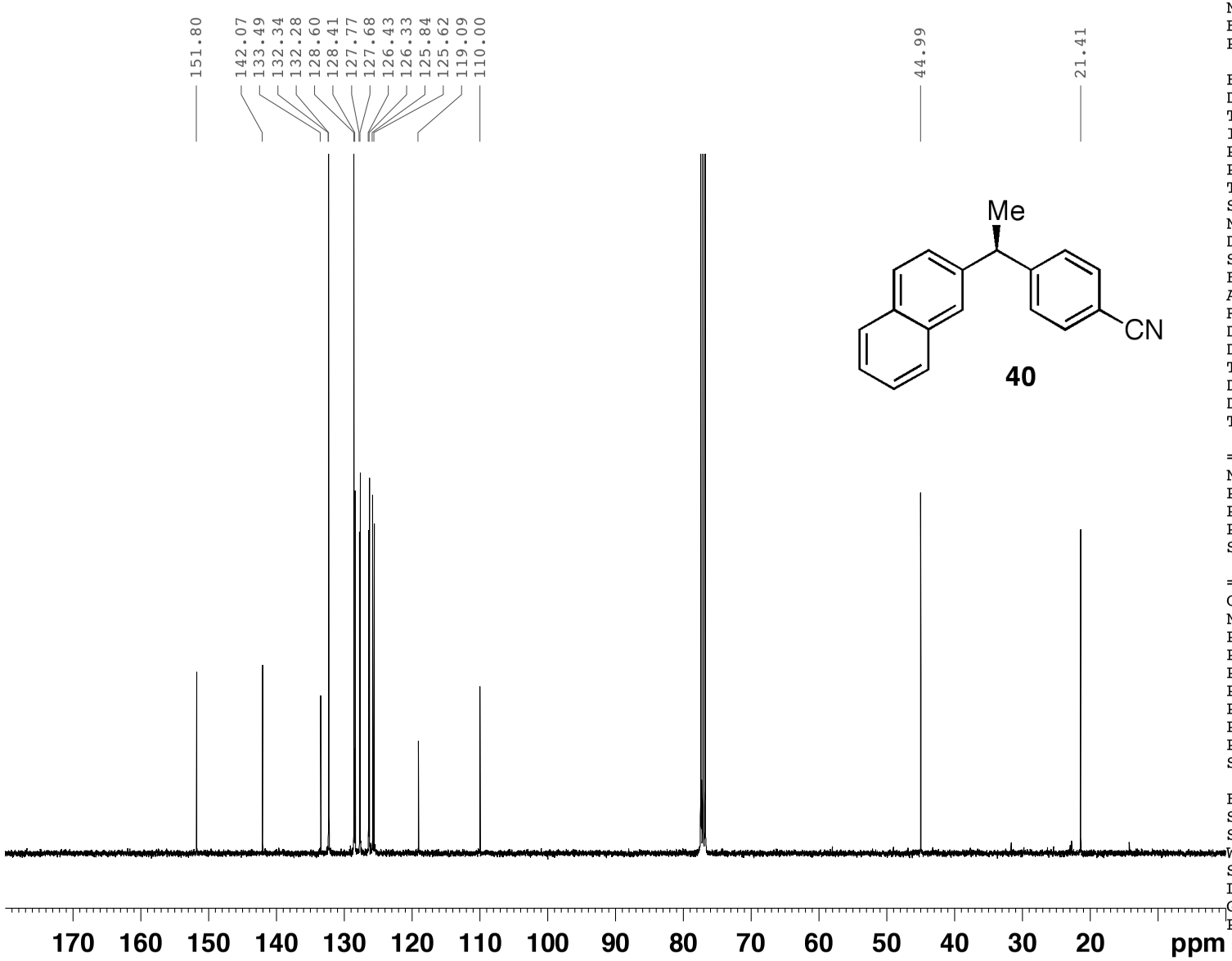
```
Current Data Parameters
NAME                  PM-4-79-1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20121003
Time                      11.49
INSTRUM                   spect
PROBHD    5 mm CPQNP 1H/
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                            4
DW                        60.400 usec
DE                         6.00 usec
TE                        298.2 K
D1                   1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        15.00 usec
PL1                        4.90 dB
PL1W                3.30822015 W
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF                400.1300000 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

Compound 40, 13CNMR



40

```
Current Data Parameters
NAME                  PM-4-79-1
EXPNO                         2
PROCNO                        1

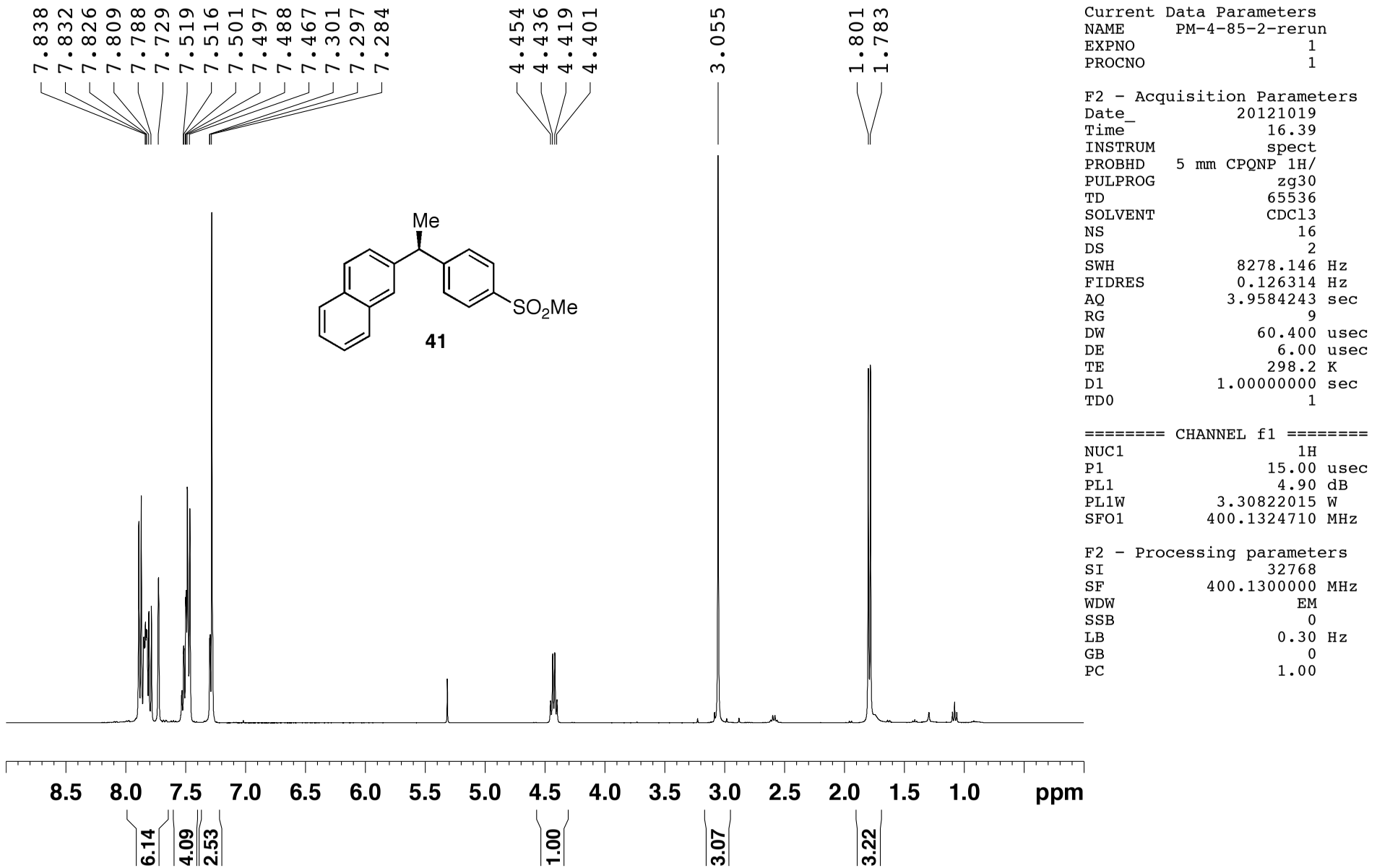
F2 - Acquisition Parameters
Date_                  20121003
Time                      11.53
INSTRUM                   spect
PROBHD    5 mm CPQNP 1H/
PULPROG                 zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                           32
DS                            4
SWH                   23980.814 Hz
FIDRES                 0.365918 Hz
AQ                     1.3664756 sec
RG                          512
DW                       20.850 usec
DE                       18.00 usec
TE                       298.2 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         13C
P1                         9.25 usec
PL1                        0.55 dB
PL1W                35.18820572 W
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     90.00 usec
PL2                        4.90 dB
PL12                      20.46 dB
PL13                      21.00 dB
PL2W                3.30822015 W
PL12W               0.09195905 W
PL13W               0.08120718 W
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6127690 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```

Compound 41, 1HNMR



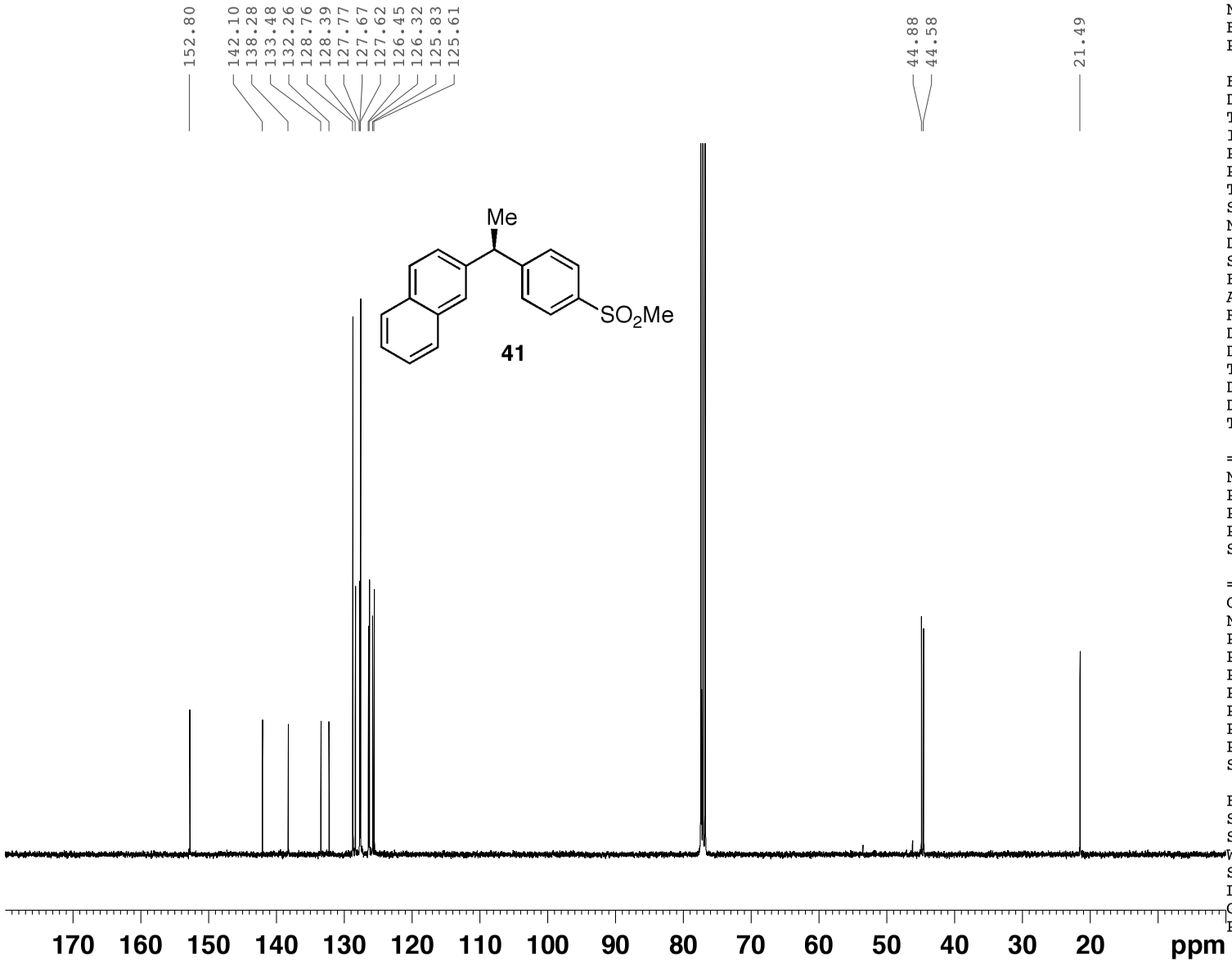

```
Current Data Parameters
NAME      PM-4-85-2-rerun
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20121019
Time                16.39
INSTRUM             spect
PROBHD   5 mm CPQNP 1H/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ               3.9584243 sec
RG                      9
DW                 60.400 usec
DE                  6.00 usec
TE                 298.2 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.00 usec
PL1                 4.90 dB
PL1W          3.30822015 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  32768
SF           400.1300000 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```

Compound 41, 13CNMR




```
Current Data Parameters
NAME      PM-4-85-2-rerun
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20121019
Time              16.42
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW                20.850 usec
DE                18.00 usec
TE                298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

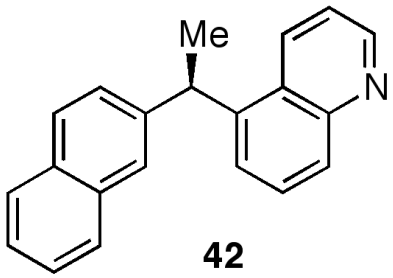
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

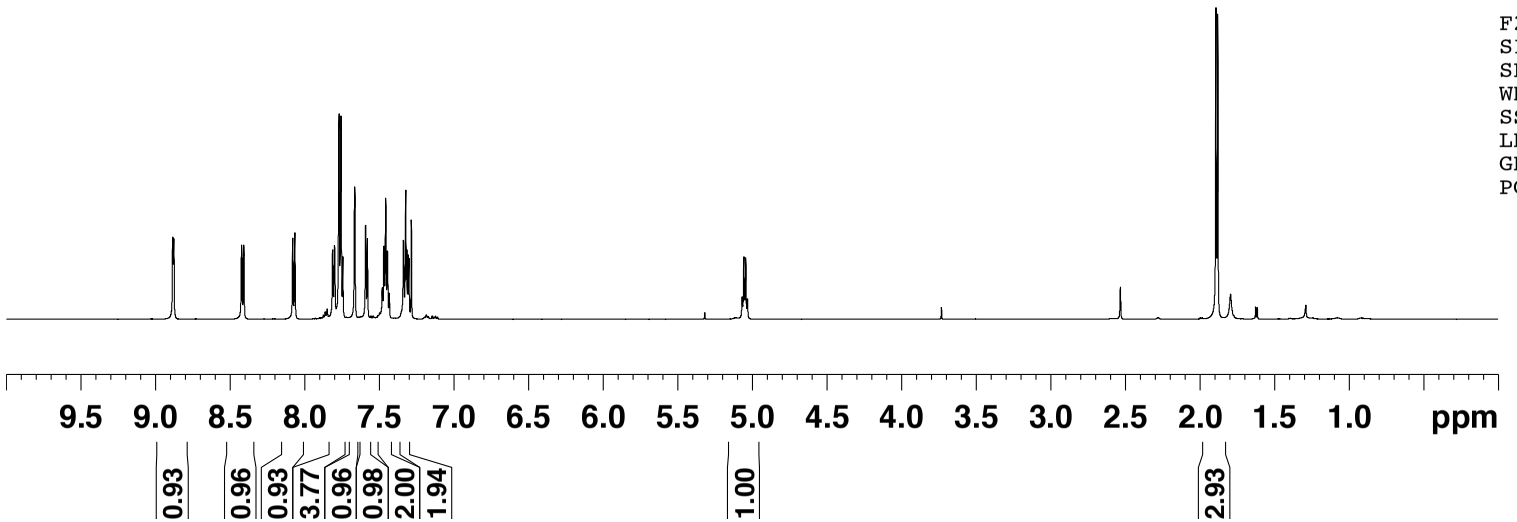
Compound 42, 1HNMR

8.068 7.815 7.802 7.772 7.759 7.746 7.667 7.594 7.582 7.481 7.472 7.470 7.460 7.457 7.448 7.446 7.341 7.338 7.324 7.317 7.310 7.303 7.287 5.069 5.058 5.046 5.034

1.893 1.881



42



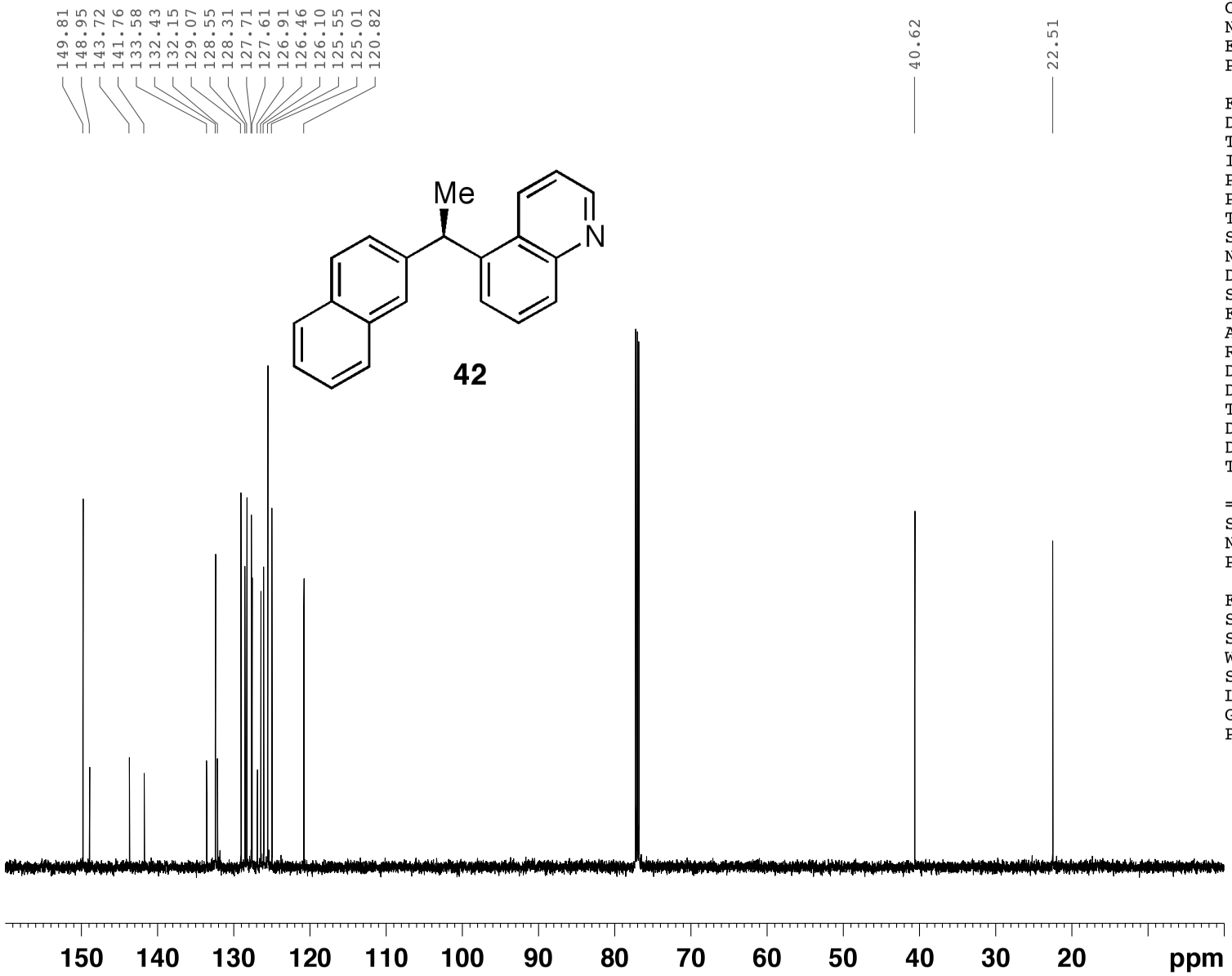

```
Current Data Parameters
NAME                  PM-4-94
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20121101
Time                     9.41
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                         8
DS                         2
SWH                 8403.361 Hz
FIDRES              0.128225 Hz
AQ                  3.8994420 sec
RG                       114
DW                    59.500 usec
DE                    17.39 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             600.3233018 MHz
NUC1                     1H
P1                    10.77 usec

F2 - Processing parameters
SI                     65536
SF               600.3200000 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                     1.00
```

Compound 42, 13CNMR



Current Data Parameters

NAME	PM-4-94
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20121101
Time	9.51
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg55
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	34722.223 Hz
FIDRES	0.529819 Hz
AQ	0.9437684 sec
RG	2050
DW	14.400 usec
DE	19.34 usec
TE	298.0 K
D1	1.10000002 sec
D11	0.03000000 sec
TD0	1

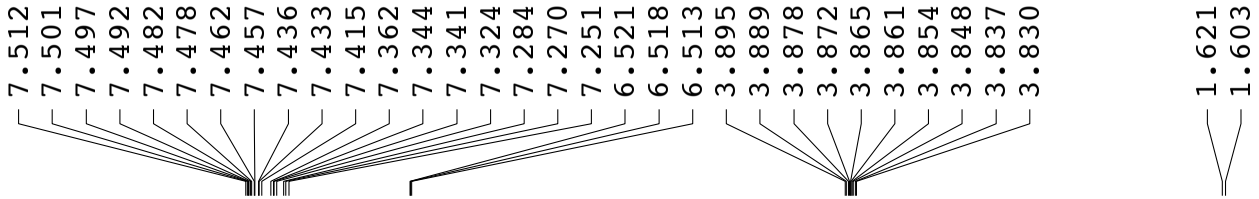
======== CHANNEL f1 ========

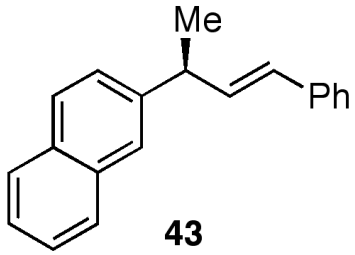
SFO1	150.9656784 MHz
NUC1	13C
P1	10.63 usec

F2 - Processing parameters

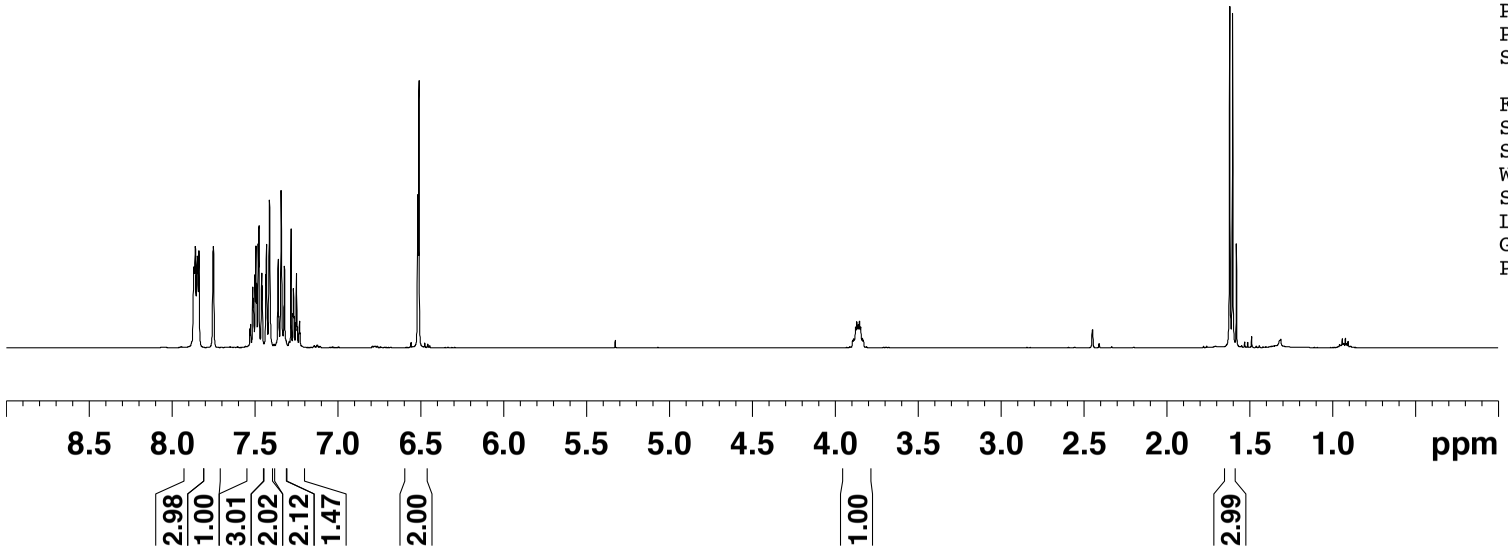
SI	32768
SF	150.9505840 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Compound 43, 1H NMR





43



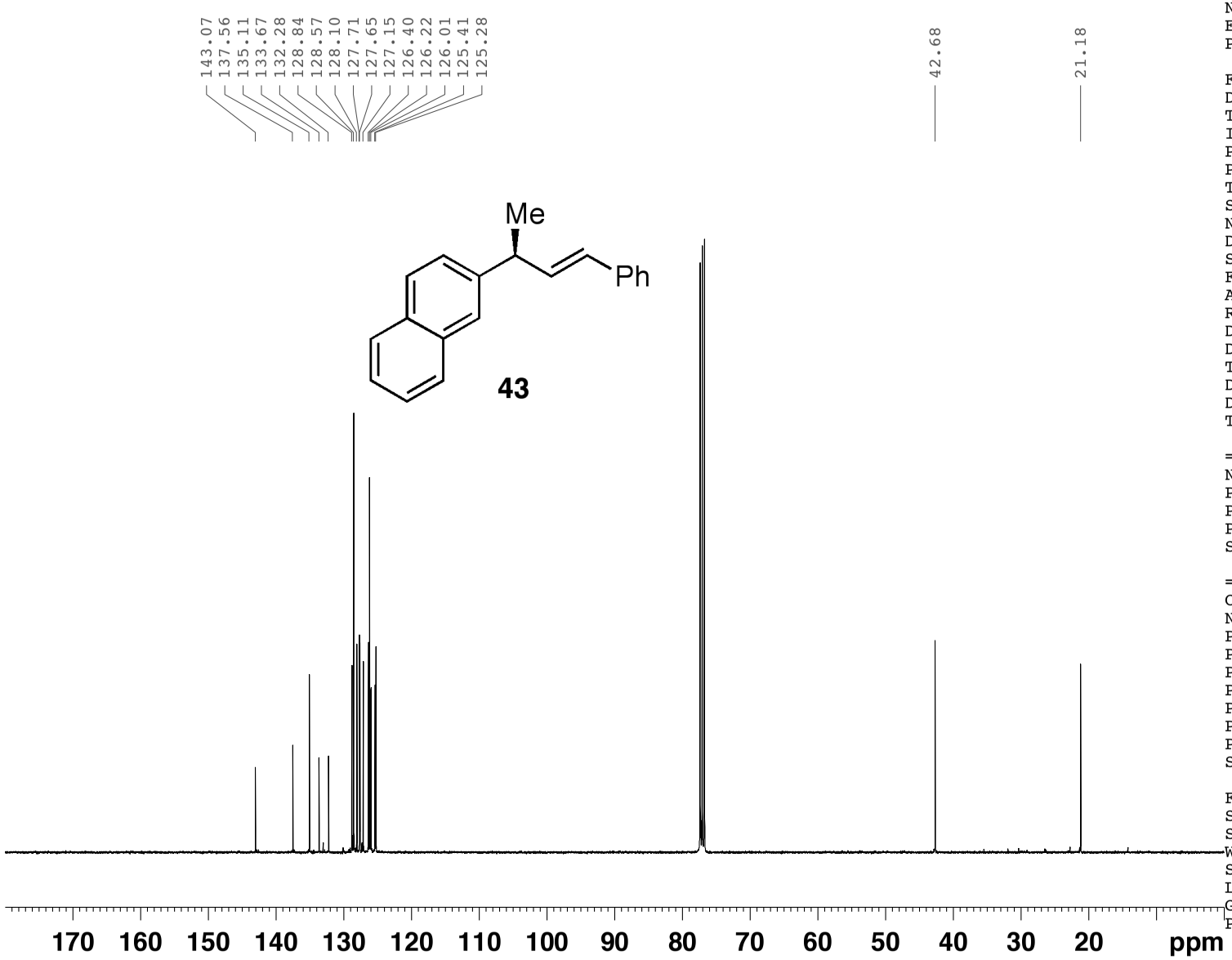

```
Current Data Parameters
NAME                 PM-4-31-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20120720
Time                   15.25
INSTRUM                spect
PROBHD    5 mm CPQNP 1H/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                  3.9584243 sec
RG                        12.7
DW                    60.400 usec
DE                     6.00 usec
TE                     298.1 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PL1                     4.90 dB
PL1W               3.30822015 W
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF               400.1300000 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                      1.00
```

Compound 43, 13C NMR




```
Current Data Parameters
NAME                 PM-4-31-1
EXPNO                        2
PROCNO                       1

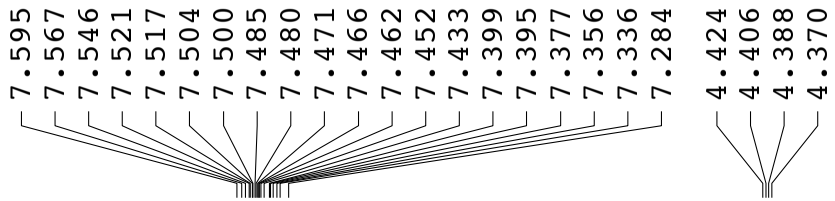
F2 - Acquisition Parameters
Date_                 20120720
Time                     21.51
INSTRUM                  spect
PROBHD    5 mm CPQNP 1H/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         256
DS                           4
SWH                  23980.814 Hz
FIDRES                0.365918 Hz
AQ                    1.3664756 sec
RG                         512
DW                      20.850 usec
DE                      18.00 usec
TE                      298.2 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

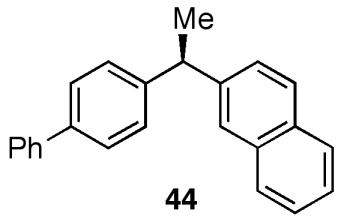
======== CHANNEL f1 ========
NUC1                       13C
P1                        9.25 usec
PL1                       0.55 dB
PL1W               35.18820572 W
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    90.00 usec
PL2                       4.90 dB
PL12                     20.46 dB
PL13                     21.00 dB
PL2W                3.30822015 W
PL12W               0.09195905 W
PL13W               0.08120718 W
SFO2              400.1316005 MHz

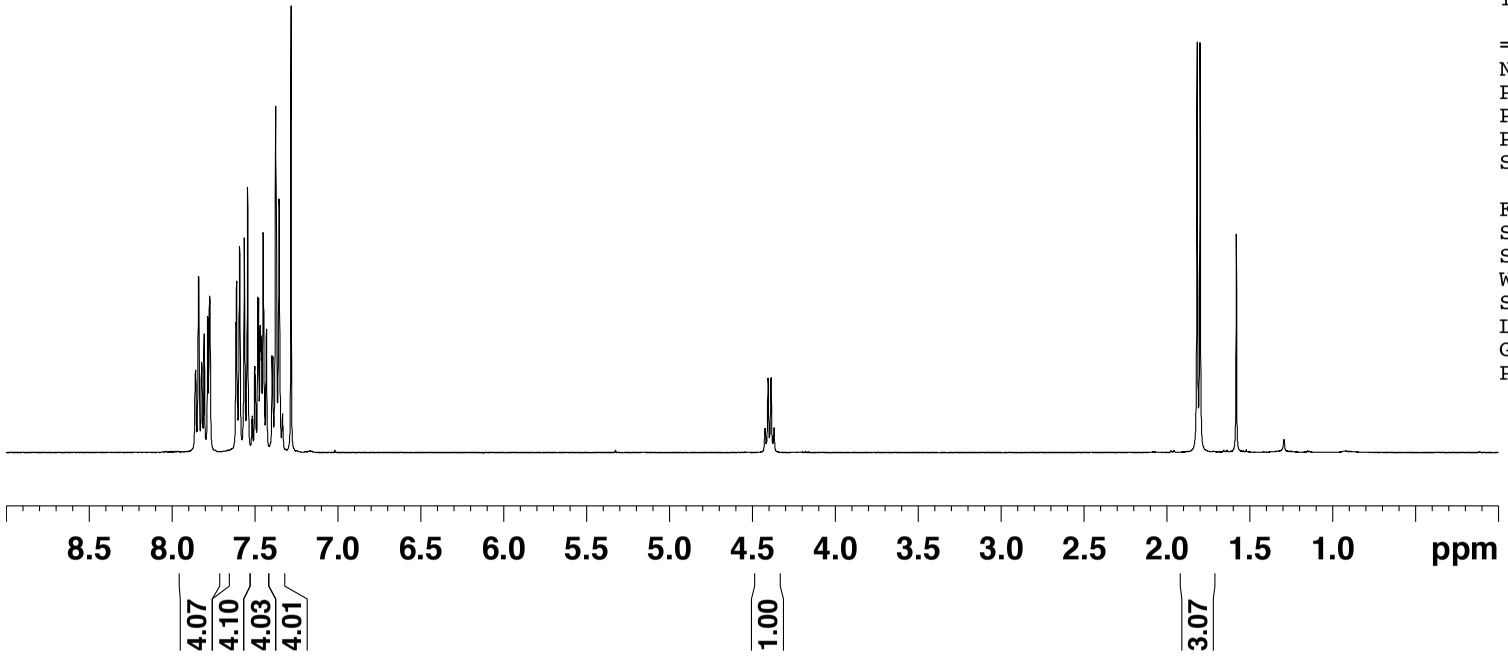
F2 - Processing parameters
SI                         32768
SF                100.6127690 MHz
WDW                           EM
SSB                            0
LB                        1.00 Hz
GB                             0
PC                        1.40
```

Compound **44**, 1H NMR





44



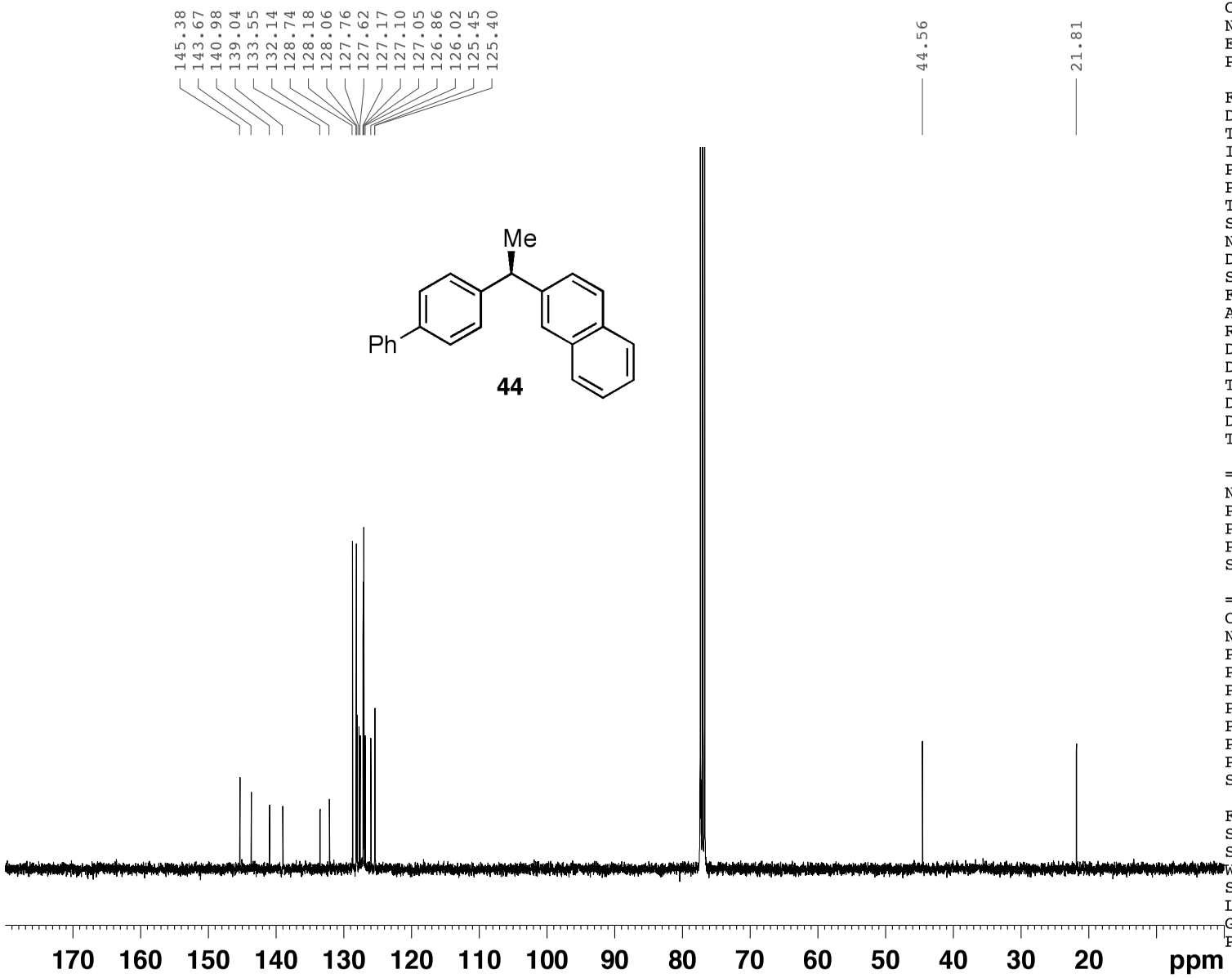

```
Current Data Parameters
NAME      PM-4-39-2-Rerun
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120730
Time                9.07
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                   6.3
DW                60.400 usec
DE                 6.00 usec
TE                298.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

Compound **44**, 13C NMR




```
Current Data Parameters
NAME      PM-4-39-2-Rerun
EXPNO                   2
PROCNO                  1

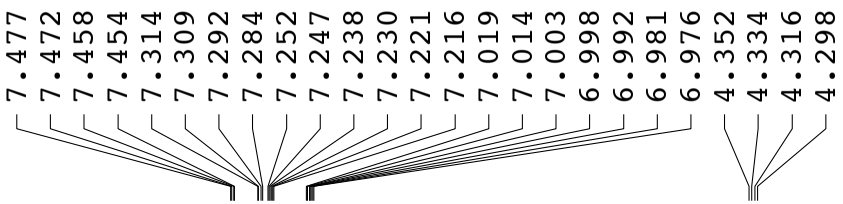
F2 - Acquisition Parameters
Date_            20120730
Time                9.10
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     4
SWH            23980.814 Hz
FIDRES          0.365918 Hz
AQ              1.3664756 sec
RG                   512
DW                20.850 usec
DE                18.00 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

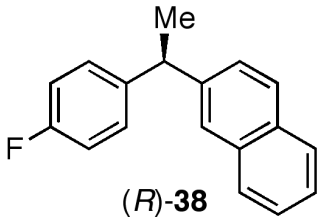
======== CHANNEL f1 ========
NUC1                  13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W        35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2       400.1316005 MHz

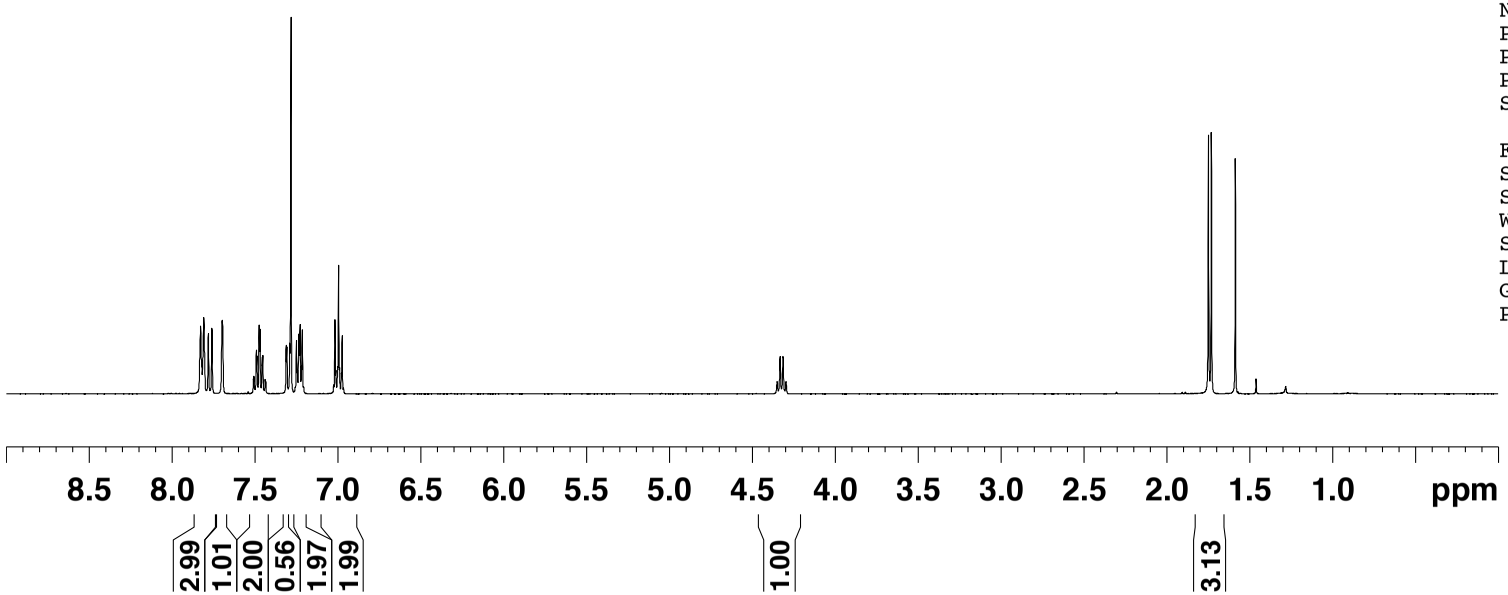
F2 - Processing parameters
SI                 32768
SF         100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound (*R*)-**38**, 1H NMR





(*R*)-**38**



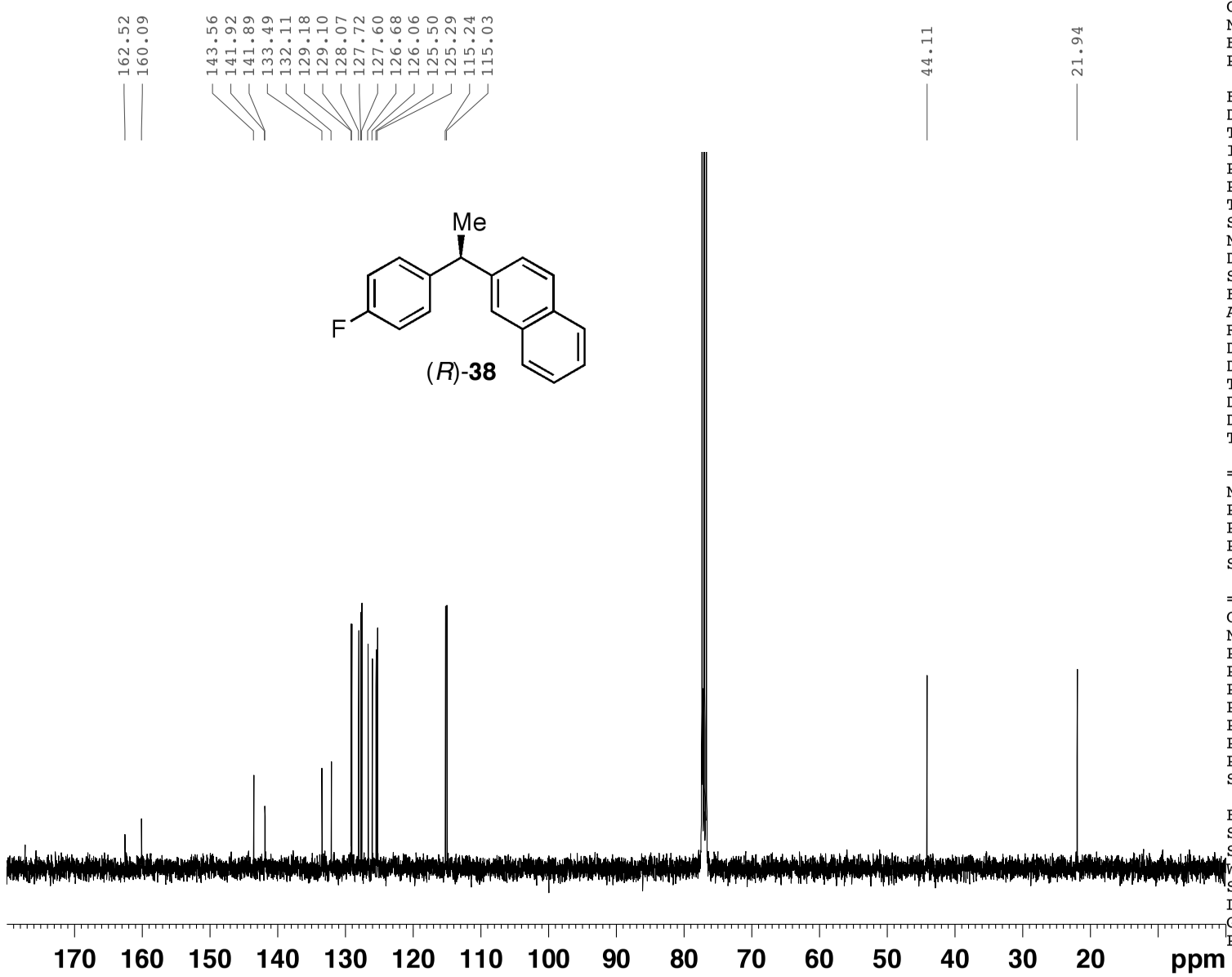

```
Current Data Parameters
NAME          PM-4-40-3
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20120730
Time              19.12
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                    4
DW               60.400 usec
DE                6.00 usec
TE                298.2 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

Compound (*R*)-**38**, 13C NMR




```
Current Data Parameters
NAME          PM-4-40-3
EXPNO                 2
PROCNO                1

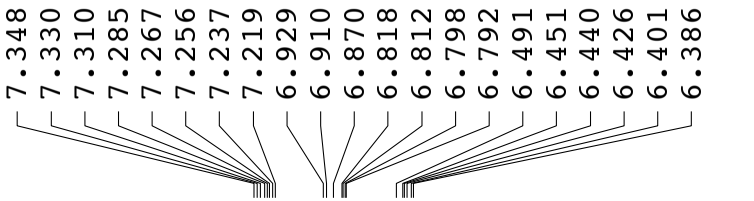
F2 - Acquisition Parameters
Date_          20120730
Time              15.16
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW                20.850 usec
DE                18.00 usec
TE                298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

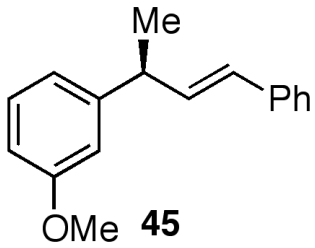
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

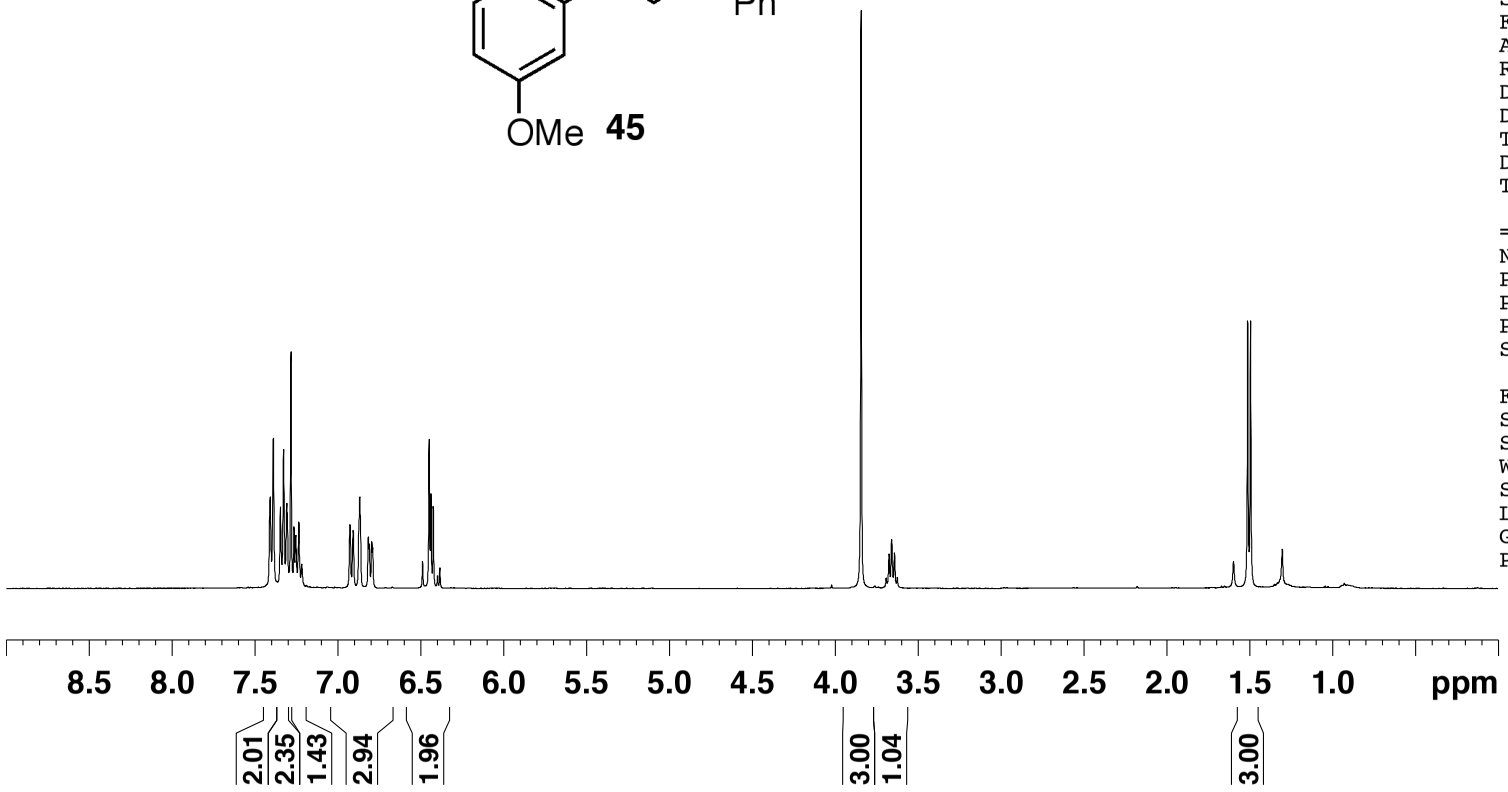
F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```

Compound **45**, 1H NMR





45



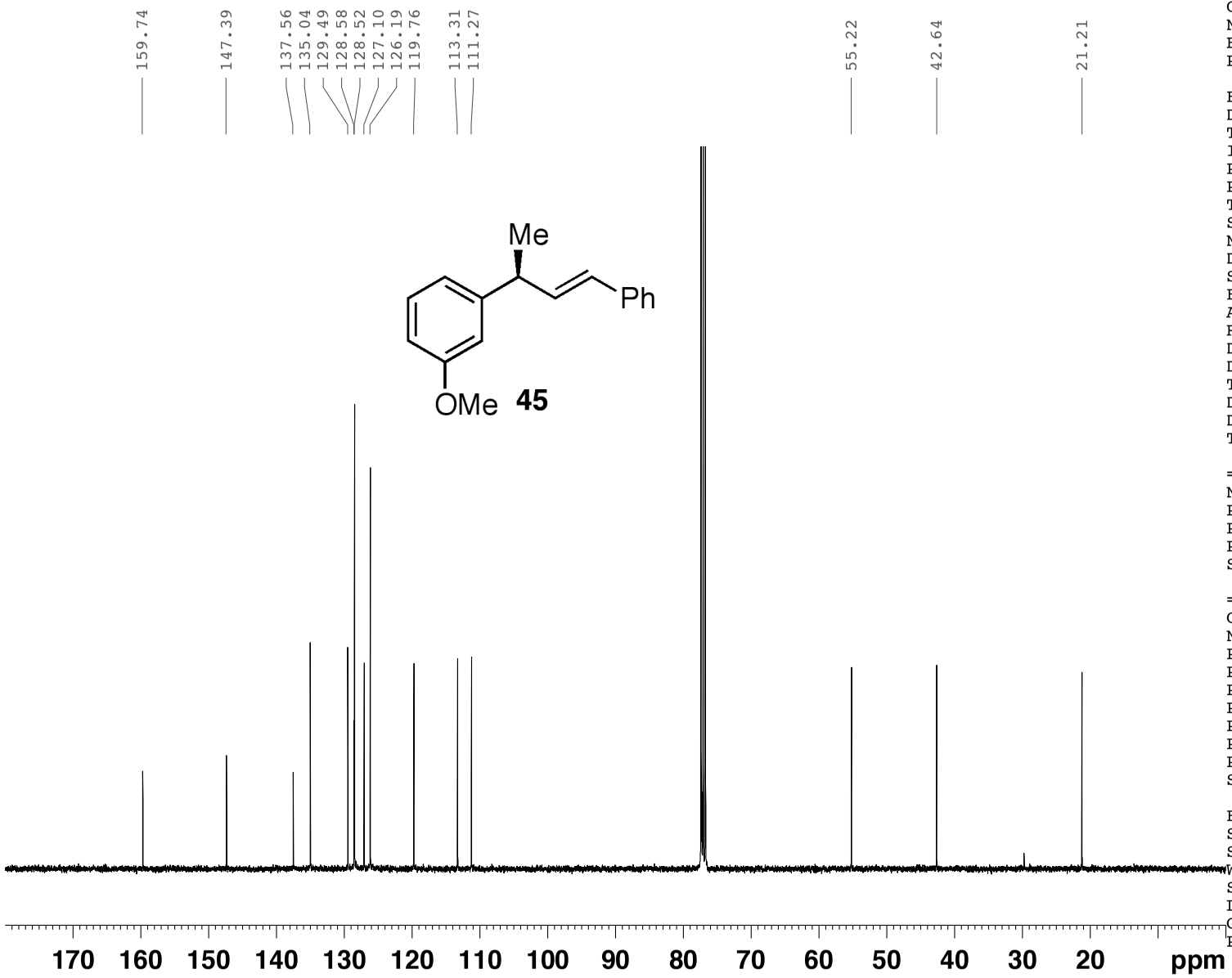

```
Current Data Parameters
NAME                  PM-4-41-1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20120801
Time                      10.19
INSTRUM                   spect
PROBHD    5 mm CPQNP 1H/
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                            7.1
DW                       60.400 usec
DE                        6.00 usec
TE                       298.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       15.00 usec
PL1                       4.90 dB
PL1W                 3.30822015 W
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF                 400.1300000 MHz
WDW                          EM
SSB                           0
LB                        0.30 Hz
GB                            0
PC                        1.00
```

Compound **45**, 13C NMR




```
Current Data Parameters
NAME          PM-4-41-1
EXPNO                 2
PROCNO                1

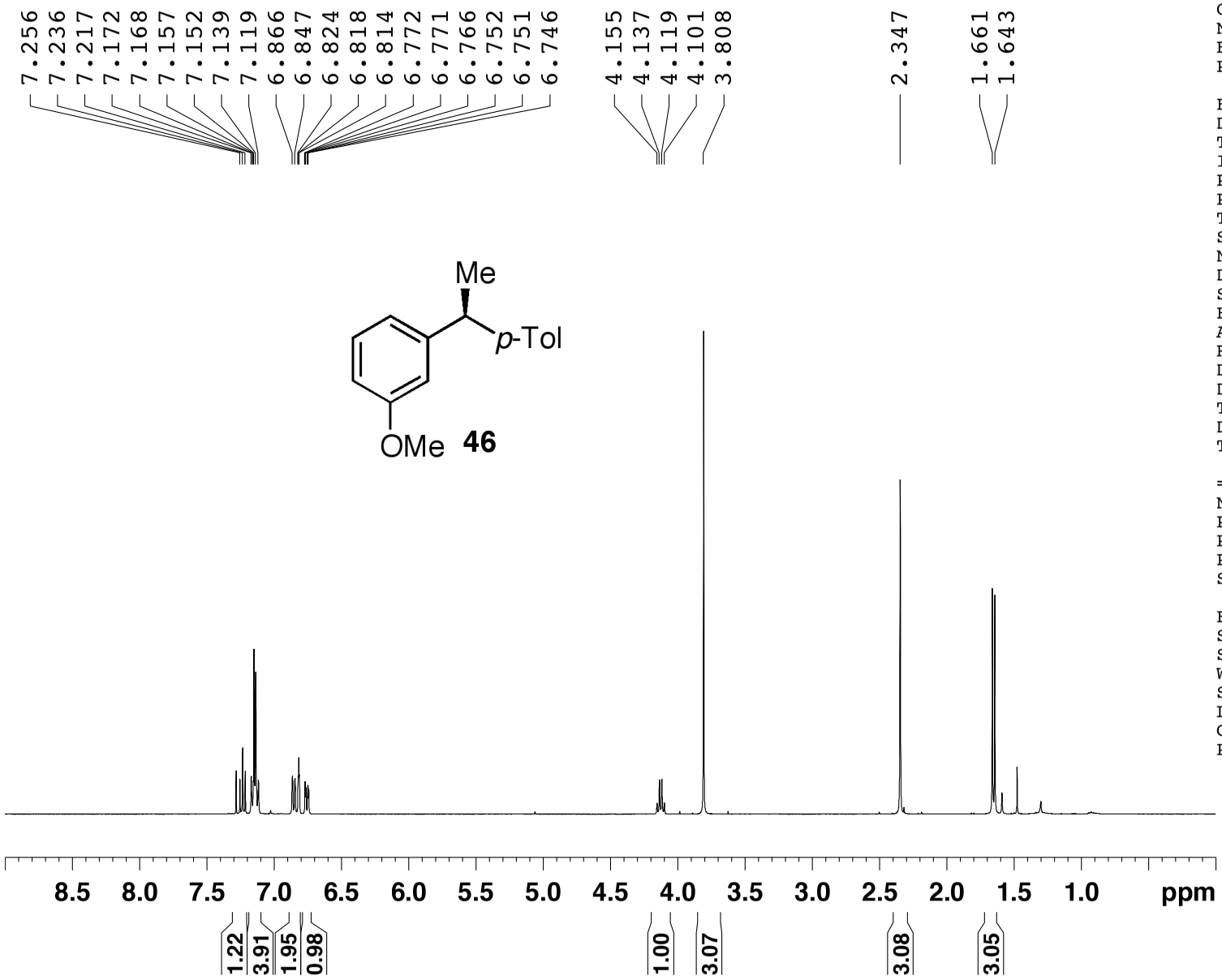
F2 - Acquisition Parameters
Date_          20120801
Time              10.22
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1                0.55 dB
PL1W        35.18820572 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound **46**, 1H NMR



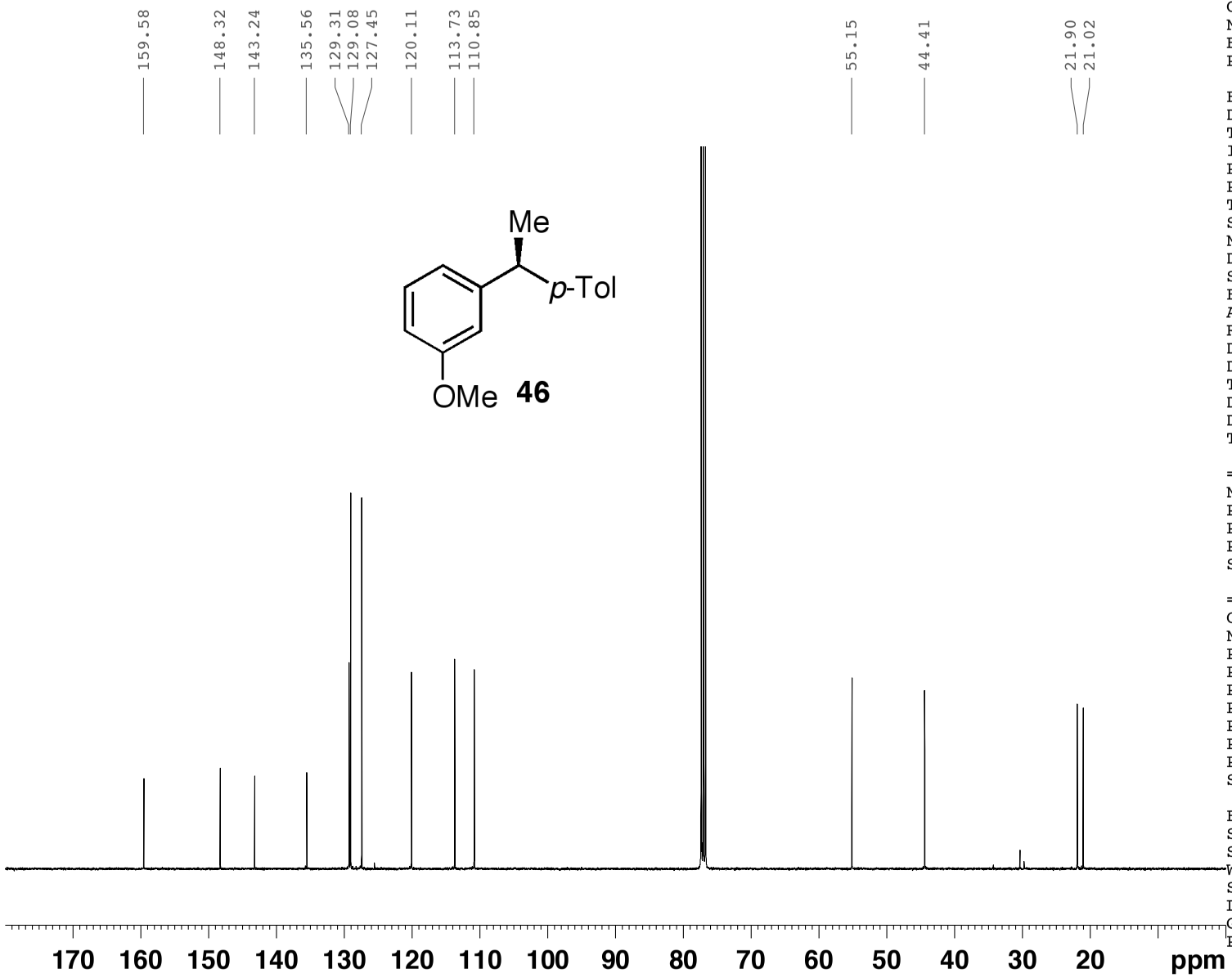
Current Data Parameters
NAME DMM3-117-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120721
Time 15.11
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 10.1
DW 60.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 4.90 dB
PL1W 3.30822015 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound **46**, 13C NMR




```
Current Data Parameters
NAME          DMM3-117-1
EXPNO                  2
PROCNO                 1

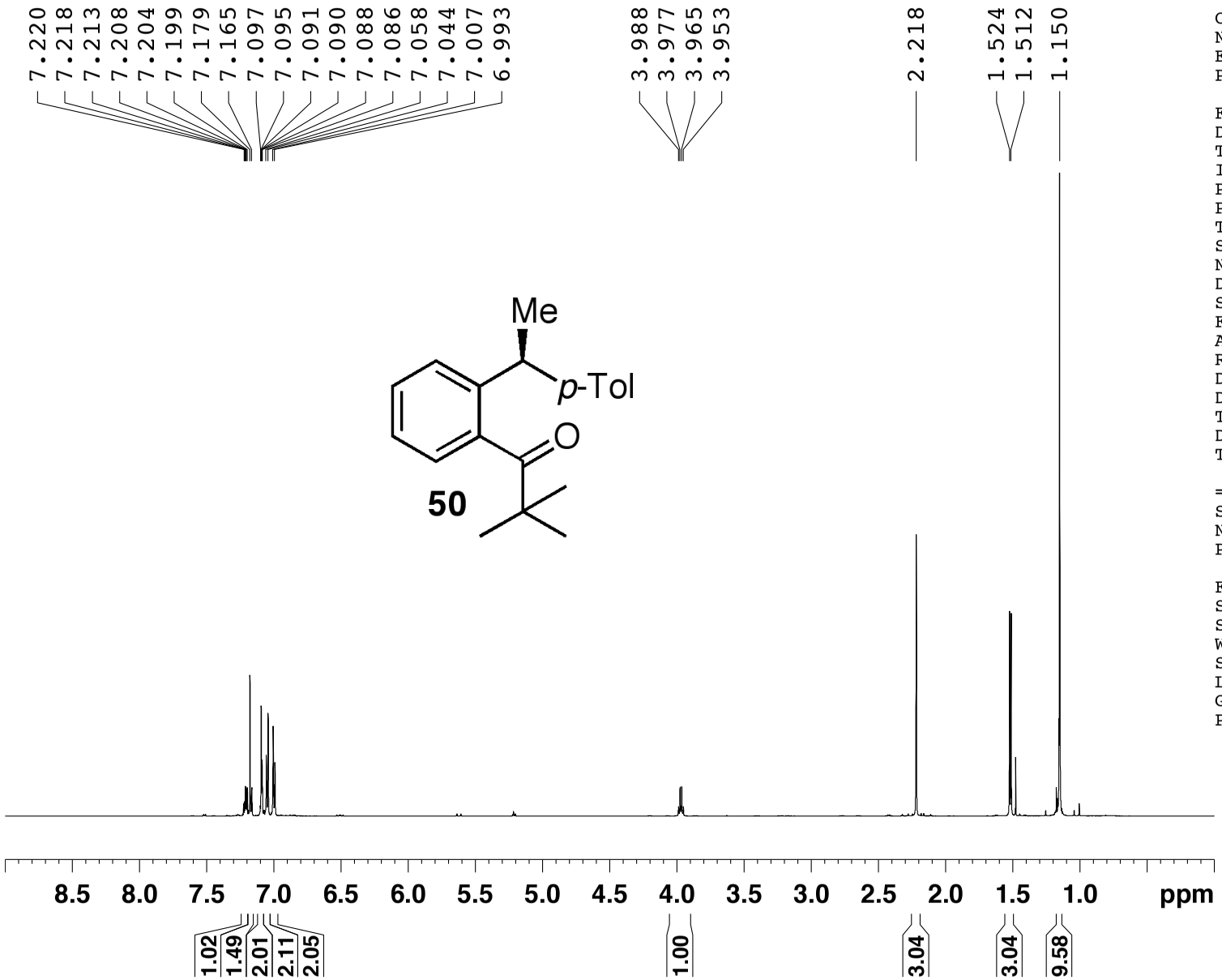
F2 - Acquisition Parameters
Date_           20120721
Time              15.27
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1                0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 50, 1HNMR



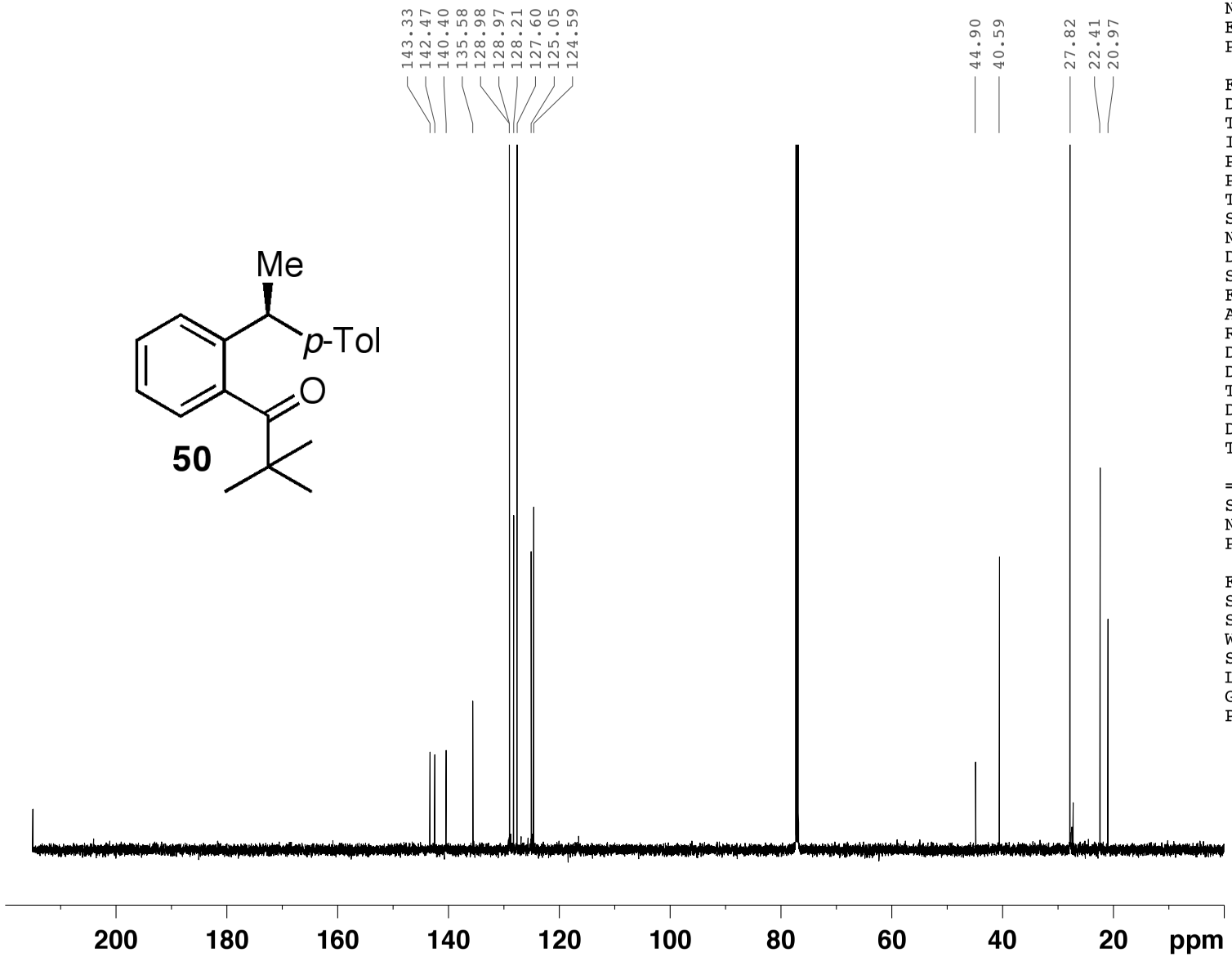
Current Data Parameters
NAME PM-4-95-1-LS
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121106
Time 15.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8403.361 Hz
FIDRES 0.128225 Hz
AQ 3.8994420 sec
RG 161
DW 59.500 usec
DE 9.10 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 600.3233018 MHz
NUC1 1H
P1 14.80 usec

F2 - Processing parameters
SI 65536
SF 600.3200643 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 50, 13CNMR



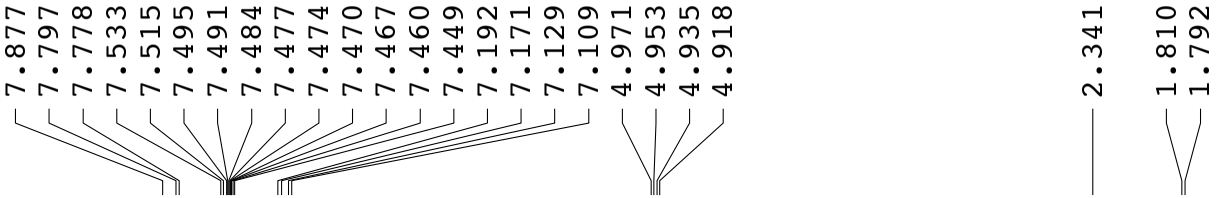

```
Current Data Parameters
NAME        PM-4-95-1-LS
EXPNO                  2
PROCNO                 1

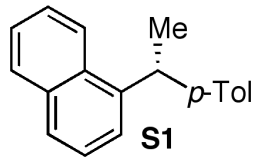
F2 - Acquisition Parameters
Date_           20121106
Time               15.25
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg55
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ            0.9437684 sec
RG                 2050
DW               14.400 usec
DE                8.88 usec
TE                298.1 K
D1           1.10000002 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        150.9656784 MHz
NUC1                13C
P1                9.00 usec

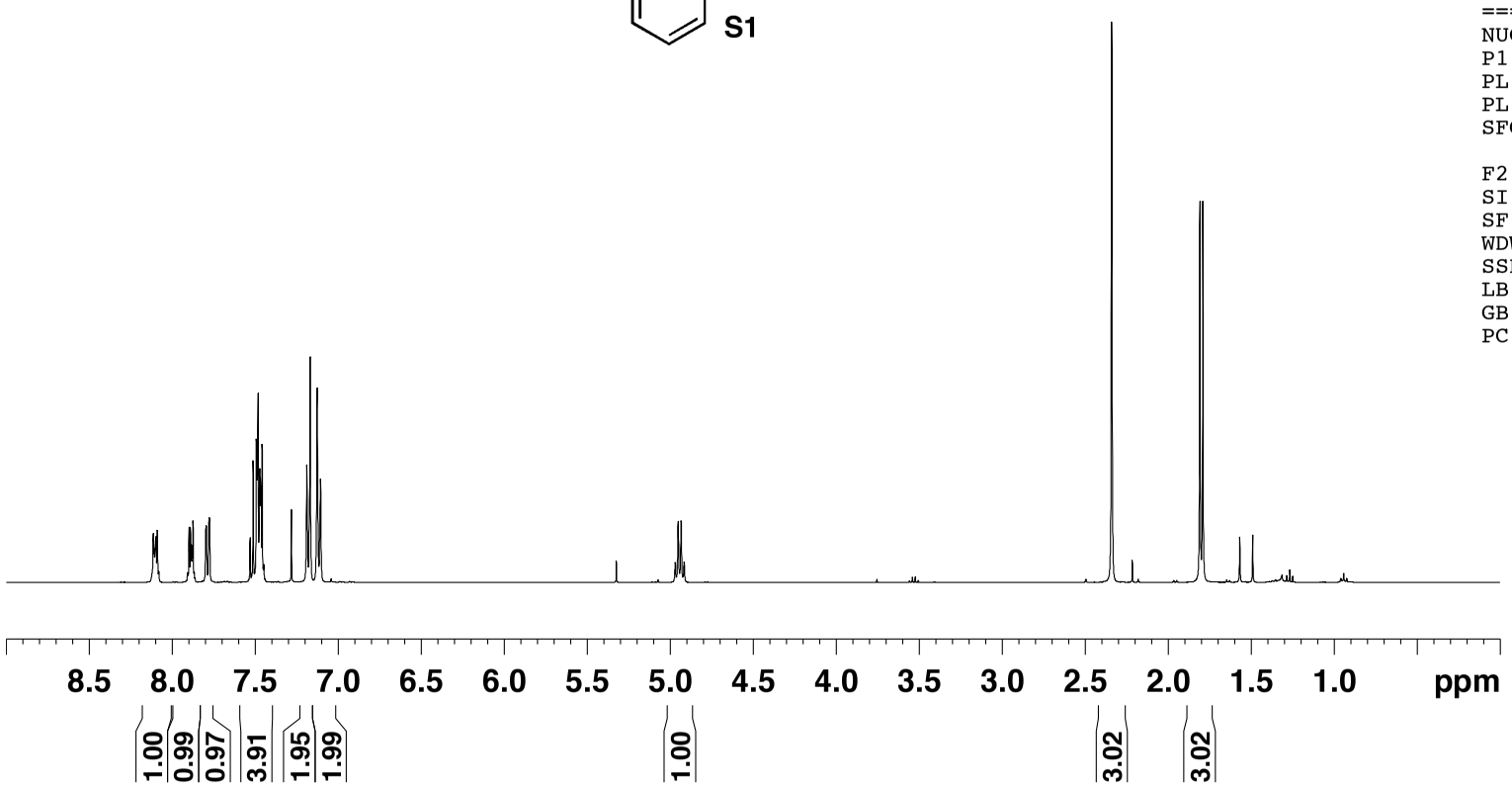
F2 - Processing parameters
SI                32768
SF          150.9505840 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound S1 1HNMR





S1




```
Current Data Parameters
NAME          DMM3-1-NAP
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120721
Time              15.55
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                12.7
DW               60.400 usec
DE                6.00 usec
TE                298.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W         3.30822015 W
SFO1        400.1324710 MHz

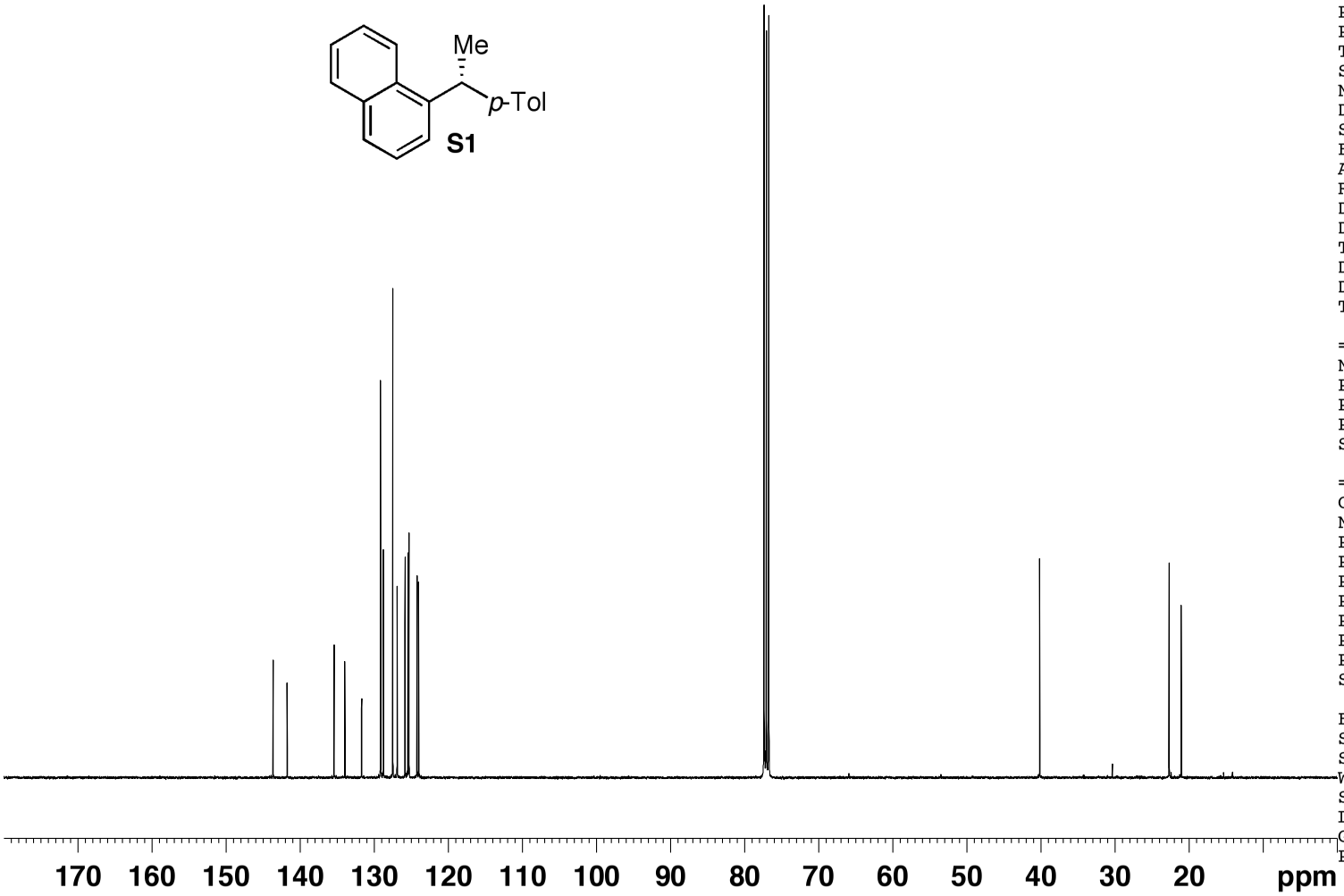
F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

Compound S1 13CNMR

143.70
141.79
135.46
134.00
131.74
129.17
128.80
127.53
126.94
125.88
125.49
125.34
124.26
124.03

40.17

22.70
21.05




```
Current Data Parameters
NAME          DMM3-1-NAP
EXPNO                  2
PROCNO                 1

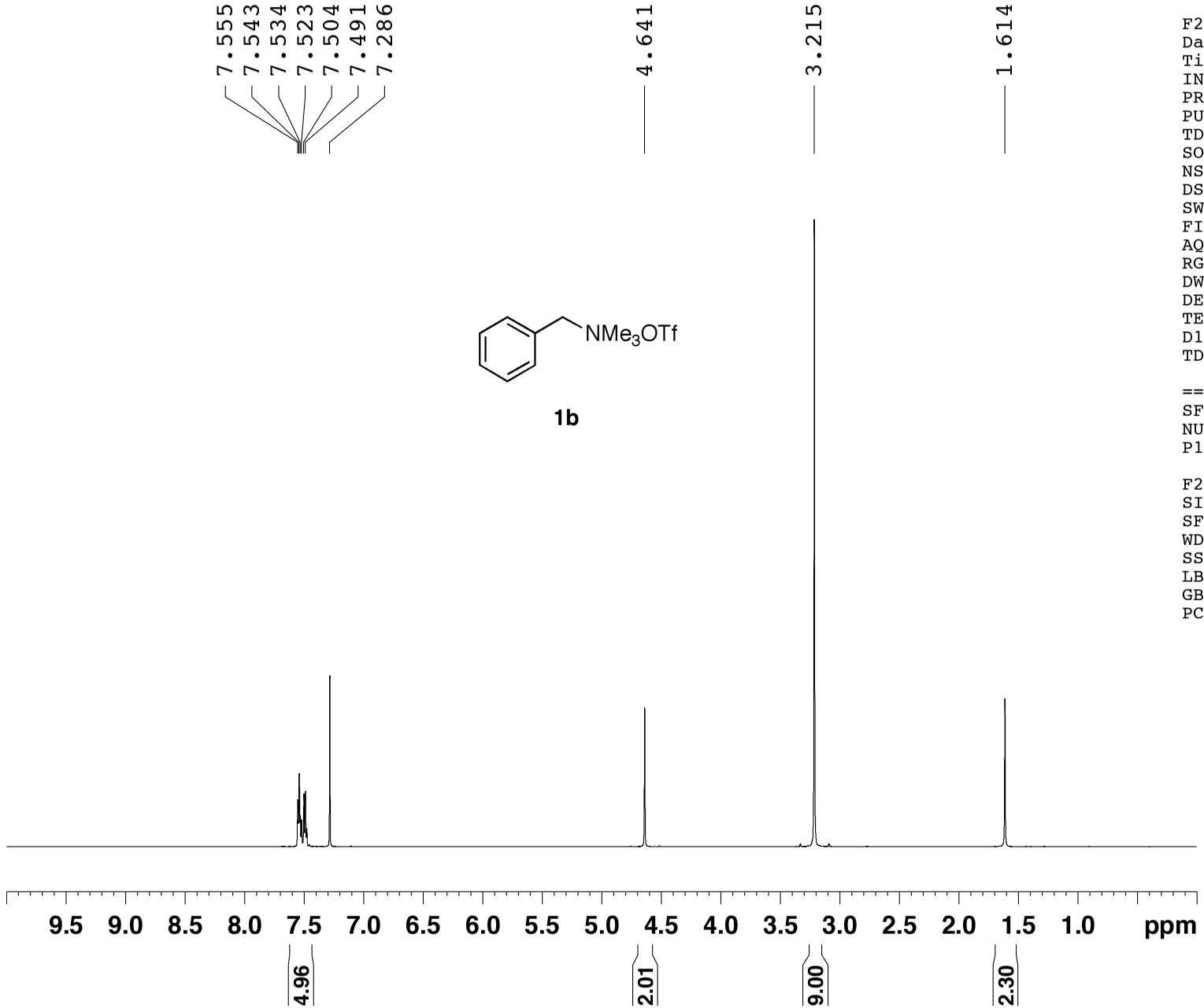
F2 - Acquisition Parameters
Date_           20120721
Time              16.11
INSTRUM           spect
PROBHD   5 mm CPQNP 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                  512
DW               20.850 usec
DE               18.00 usec
TE               298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                9.25 usec
PL1               0.55 dB
PL1W        35.18820572 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2               4.90 dB
PL12              20.46 dB
PL13              21.00 dB
PL2W         3.30822015 W
PL12W        0.09195905 W
PL13W        0.08120718 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

Compound **1b**, 1HNMR



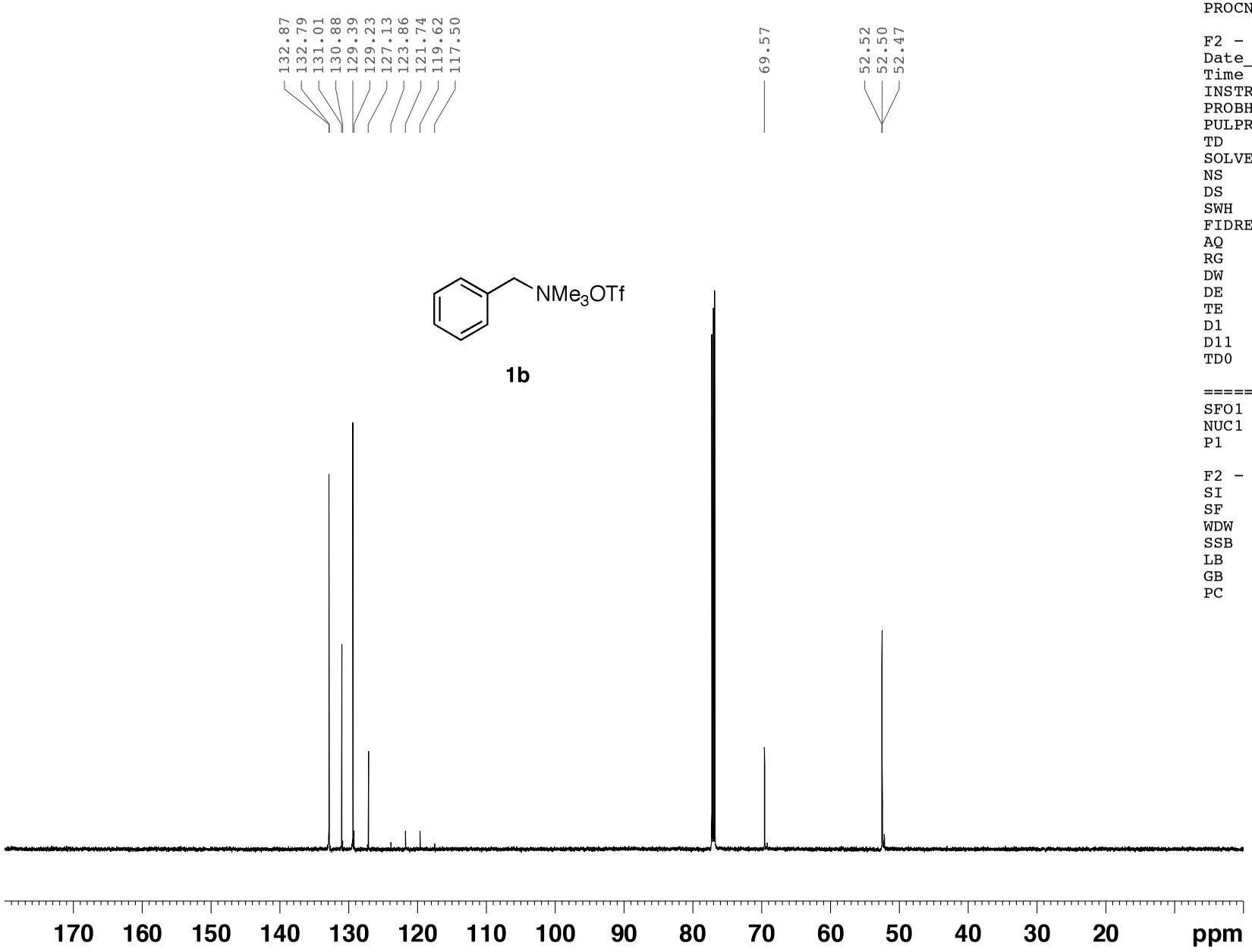

```
Current Data Parameters
NAME      DMM3-CNSI-SALT2
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120803
Time                20.14
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8403.361 Hz
FIDRES           0.128225 Hz
AQ               3.8994420 sec
RG                    287
DW                 59.500 usec
DE                 17.39 usec
TE                 300.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          600.3233018 MHz
NUC1                    1H
P1                  10.77 usec

F2 - Processing parameters
SI                    65536
SF           600.3200000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

Compound **1b** 13CNMR




```
Current Data Parameters
NAME      DMM3-CNSI-SALT-C2
EXPNO                    12
PROCNO                    1

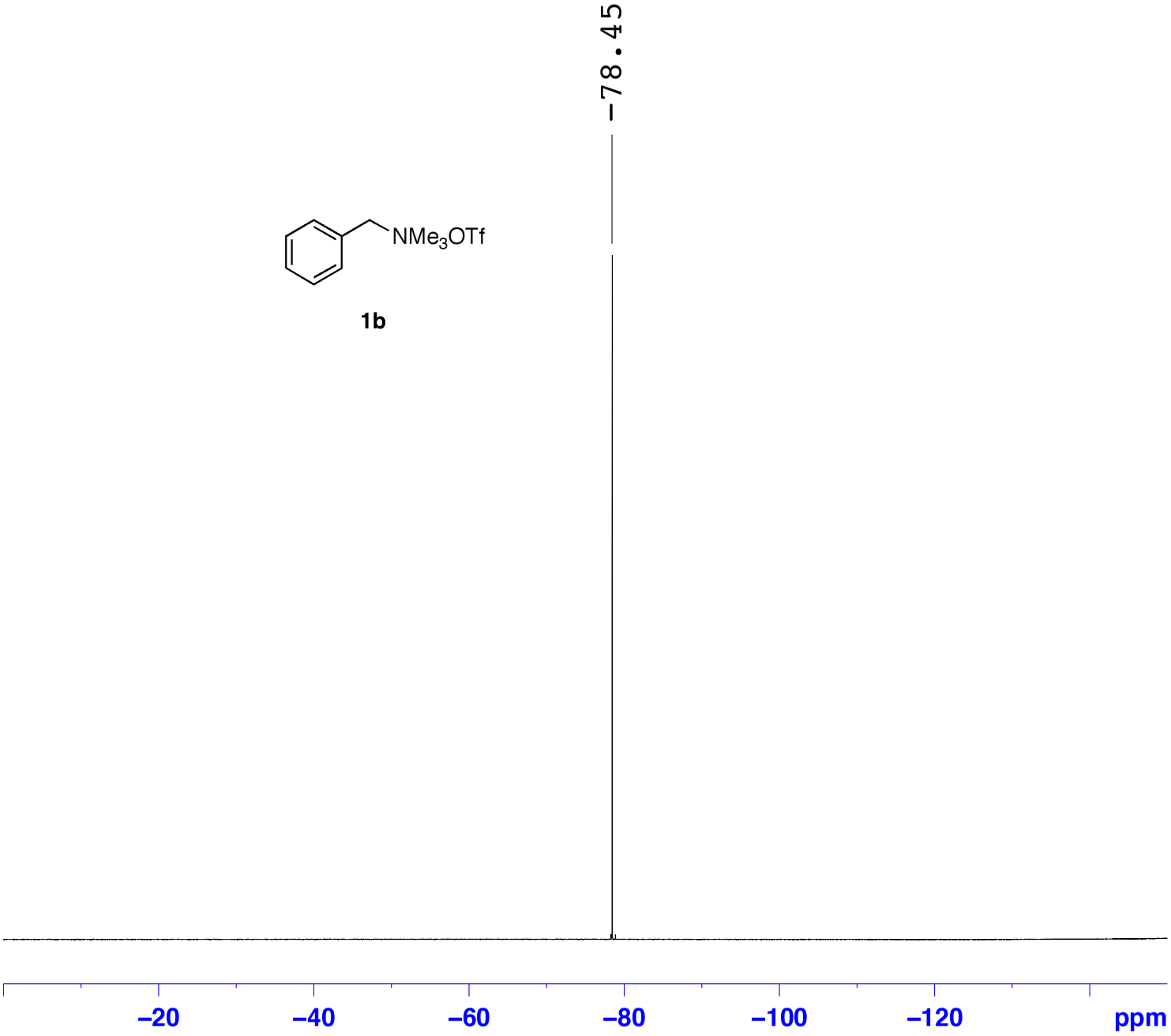
F2 - Acquisition Parameters
Date_              20120808
Time                   2.04
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg55
TD                   65536
SOLVENT              CDCl3
NS                    2048
DS                       4
SWH             34722.223 Hz
FIDRES           0.529819 Hz
AQ               0.9437684 sec
RG                    2050
DW                  14.400 usec
DE                  19.34 usec
TE                  300.2 K
D1              1.10000002 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          150.9656784 MHz
NUC1                   13C
P1                  10.63 usec

F2 - Processing parameters
SI                   32768
SF            150.9505840 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Compound **1b** 19FNMR

1b



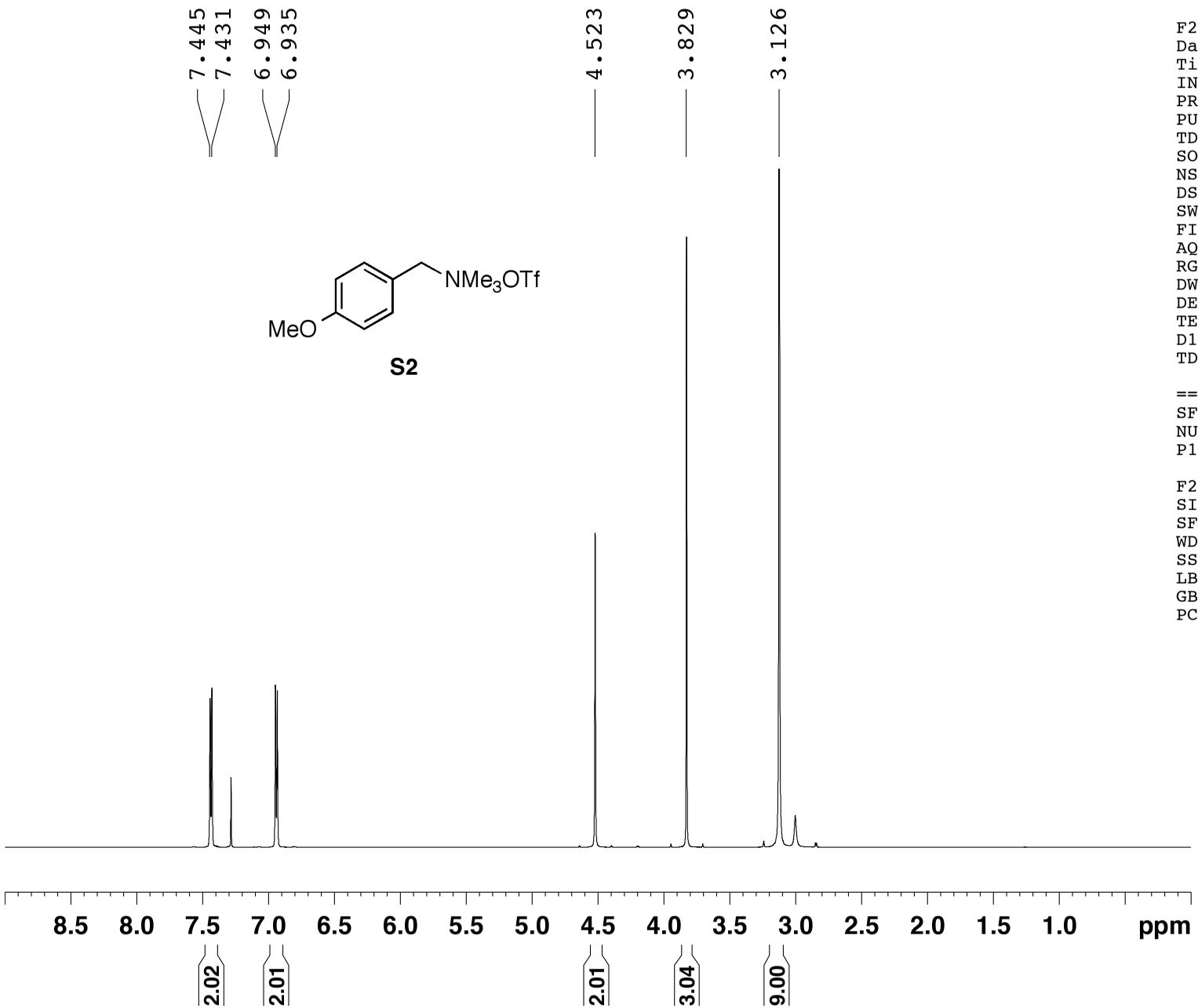

```
Current Data Parameters
NAME      DMM3-CNSI-SALT2
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_           20120803
Time              16.12
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgfhigqn
TD              131072
SOLVENT           CDCl3
NS                   16
DS                    4
SWH          133928.578 Hz
FIDRES         1.021794 Hz
AQ             0.4893855 sec
RG                  406
DW                3.733 usec
DE                8.00 usec
TE               300.2 K
D1           3.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        564.8086803 MHz
NUC1                19F
P1                11.62 usec

F2 - Processing parameters
SI                65536
SF          564.8651670 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

Compound **S2** 1HNMR



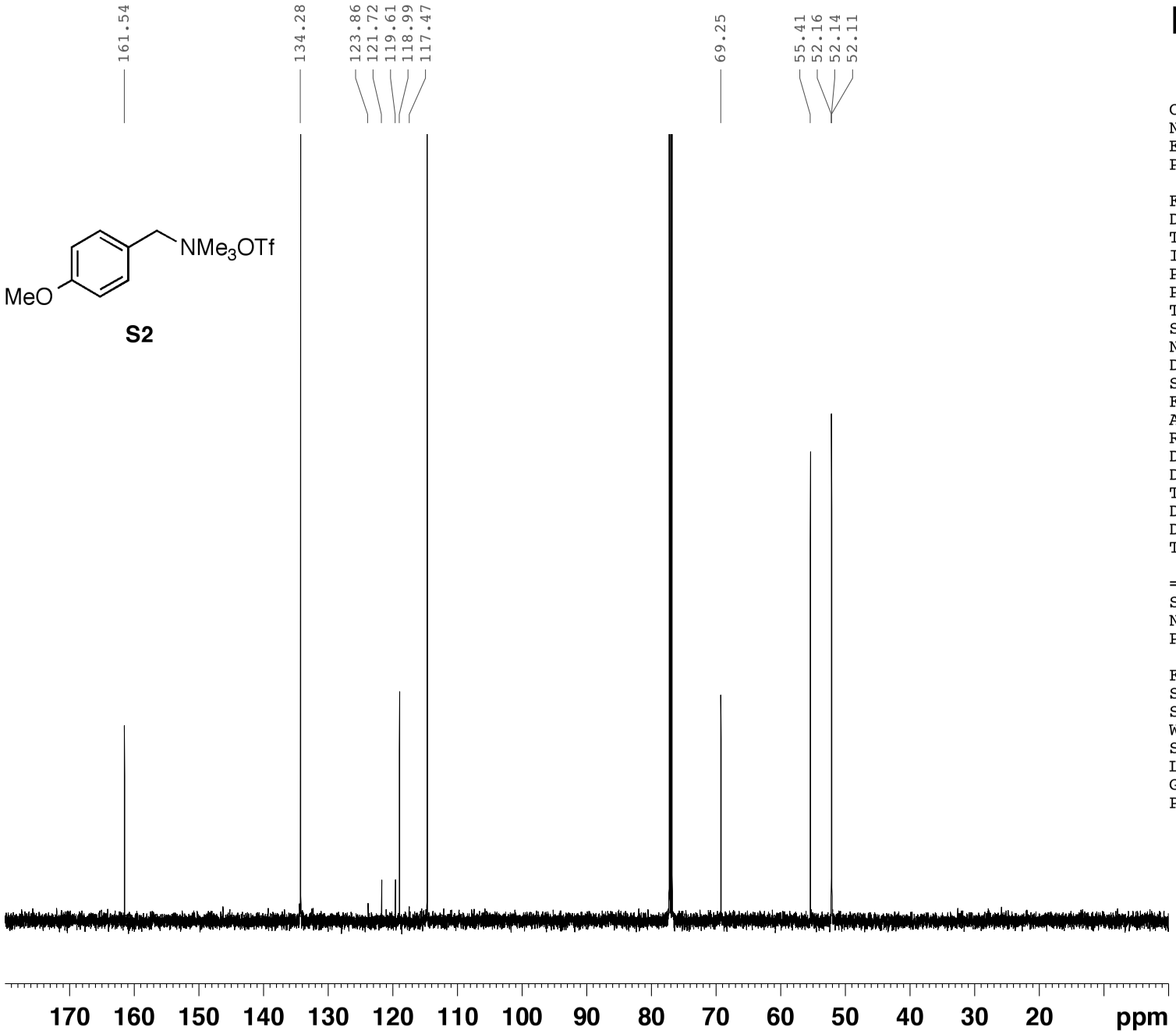

```
Current Data Parameters
NAME      DMM3-CNSI-SALT3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120803
Time                20.28
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8403.361 Hz
FIDRES           0.128225 Hz
AQ               3.8994420 sec
RG                    114
DW                 59.500 usec
DE                 17.39 usec
TE                 300.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          600.3233018 MHz
NUC1                    1H
P1                  10.77 usec

F2 - Processing parameters
SI                    65536
SF            600.3200000 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                   1.00
```

Compound S2 13CNMR




```
Current Data Parameters
NAME      DMM3-CNSI-SALT3
EXPNO                   2
PROCNO                  1

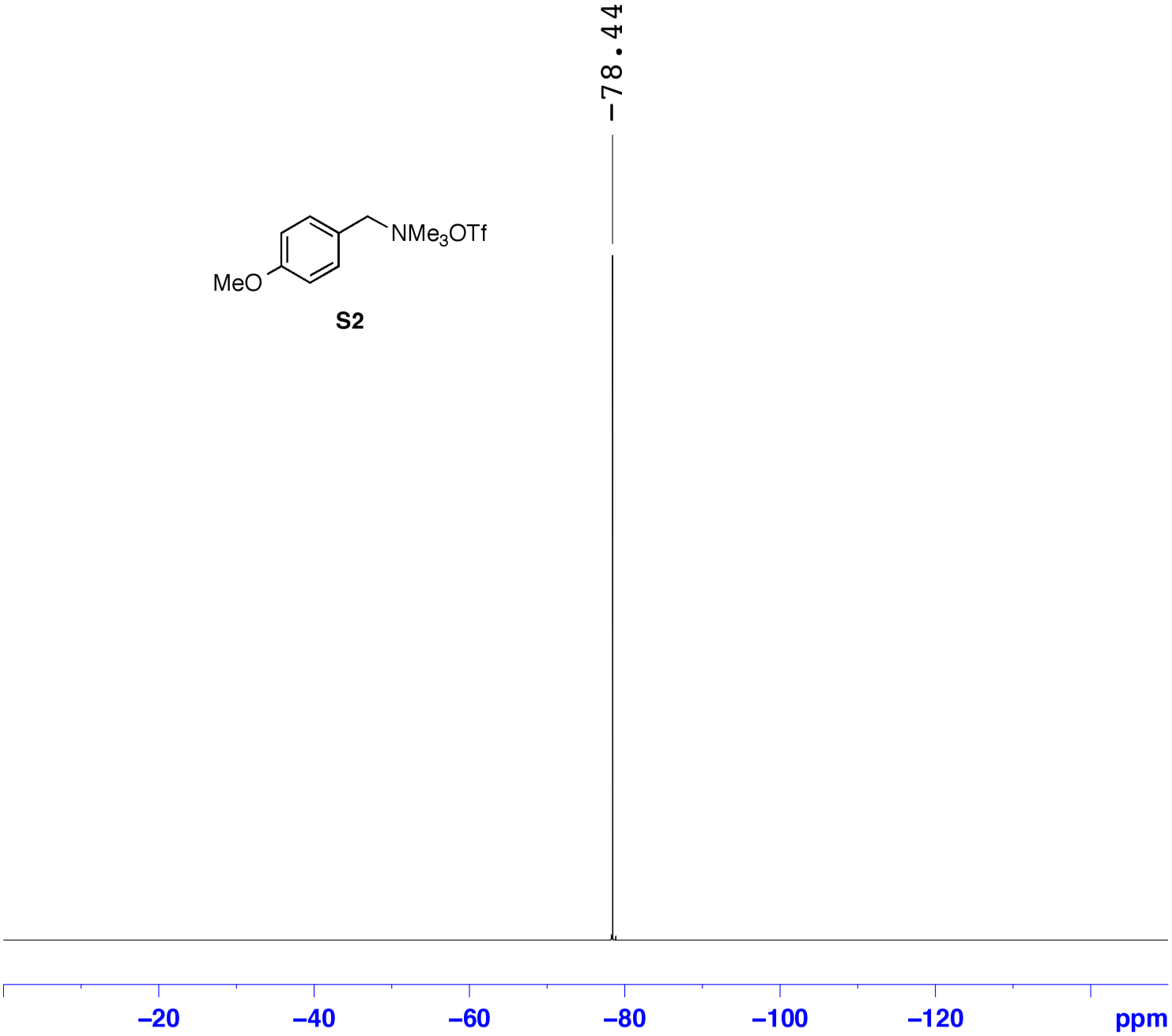
F2 - Acquisition Parameters
Date_            20120803
Time                16.38
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg55
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            34722.223 Hz
FIDRES          0.529819 Hz
AQ             0.9437684 sec
RG                  2050
DW                14.400 usec
DE                19.34 usec
TE                300.2 K
D1            1.10000002 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         150.9656784 MHz
NUC1                  13C
P1                 10.63 usec

F2 - Processing parameters
SI                 32768
SF           150.9505840 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound S2 19FNMR

S2



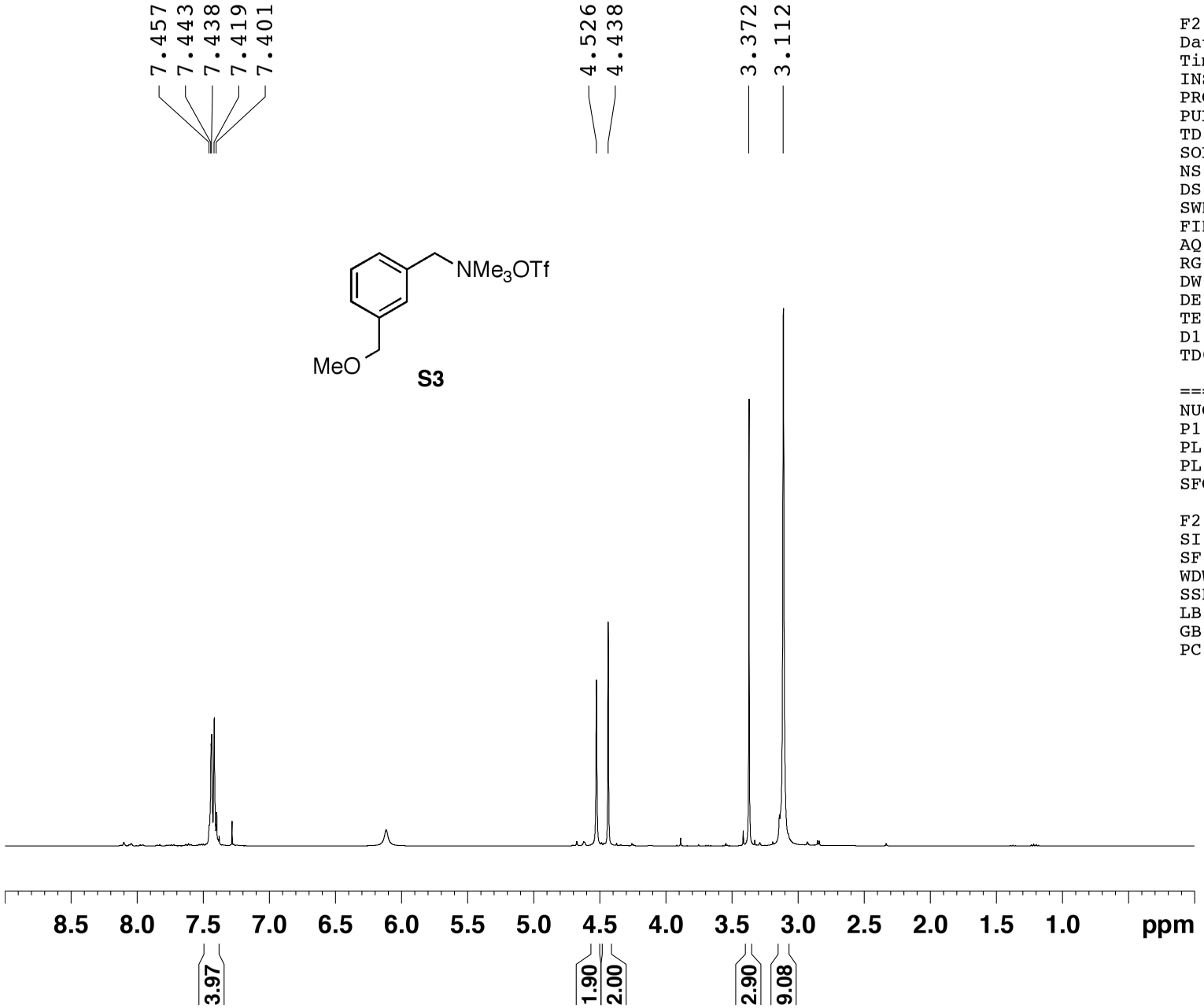

```
Current Data Parameters
NAME      DMM3-CNSI-SALT3
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_           20120803
Time              16.40
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgfhigqn
TD              131072
SOLVENT           CDCl3
NS                   16
DS                    4
SWH          133928.578 Hz
FIDRES         1.021794 Hz
AQ            0.4893855 sec
RG                  322
DW                3.733 usec
DE                8.00 usec
TE                300.2 K
D1           3.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        564.8086803 MHz
NUC1                19F
P1                11.62 usec

F2 - Processing parameters
SI                65536
SF          564.8651670 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

Compound **S3** 1HNMR



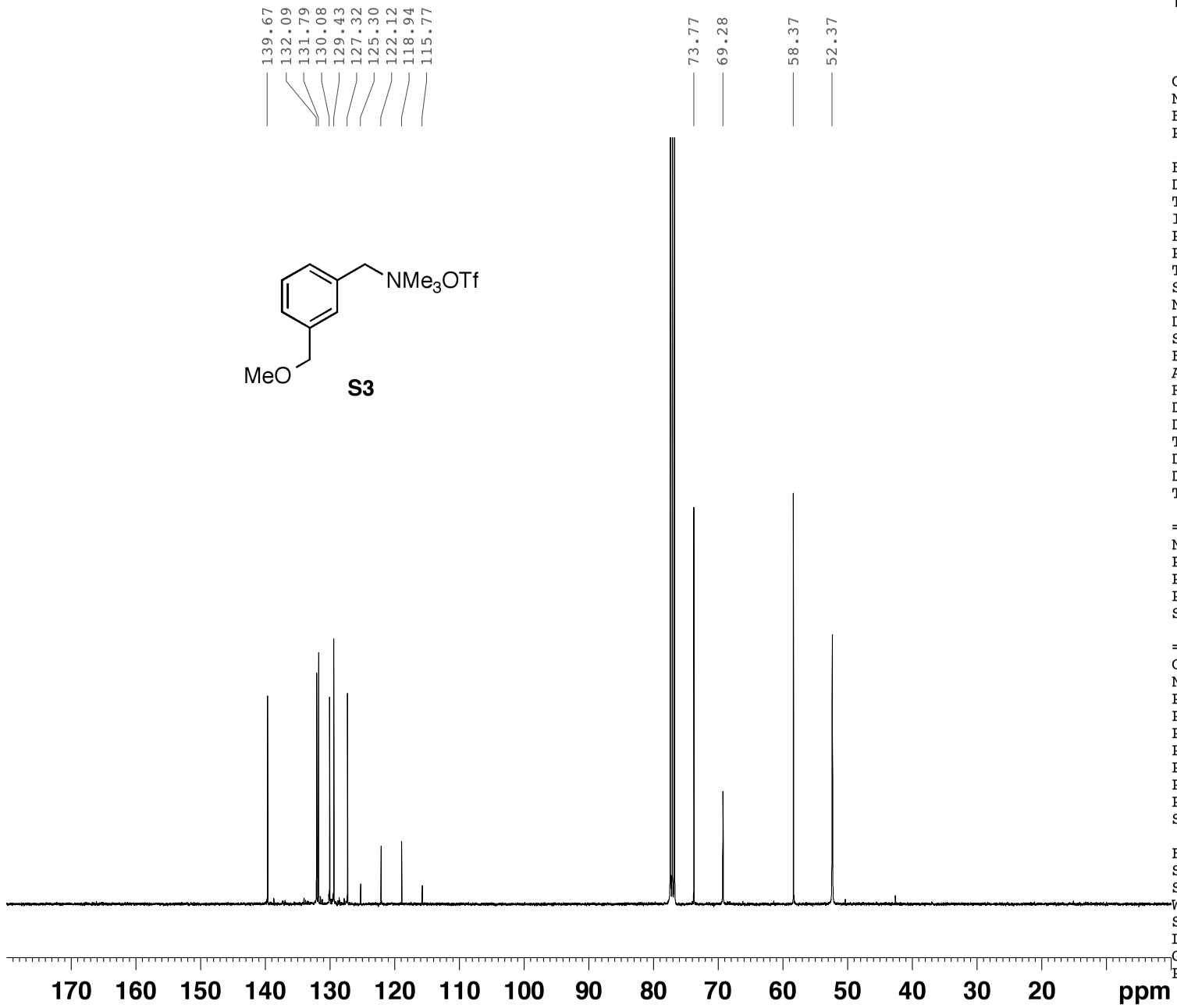

```
Current Data Parameters
NAME      DMM3-BN-OME-SALT
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120721
Time                 16.17
INSTRUM              spect
PROBHD    5 mm CPQNP 1H/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ               3.9584243 sec
RG                    11.3
DW                  60.400 usec
DE                   6.00 usec
TE                  298.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  15.00 usec
PL1                  4.90 dB
PL1W          3.30822015 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  32768
SF           400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

Compound **S3** 13CNMR




```
Current Data Parameters
NAME      DMM3-BN-OME-SALT
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120721
Time                 16.33
INSTRUM              spect
PROBHD   5 mm CPQNP 1H/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     256
DS                       4
SWH              23980.814 Hz
FIDRES           0.365918 Hz
AQ               1.3664756 sec
RG                     512
DW                20.850 usec
DE                18.00 usec
TE                298.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.25 usec
PL1                 0.55 dB
PL1W         35.18820572 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                 4.90 dB
PL12               20.46 dB
PL13               21.00 dB
PL2W          3.30822015 W
PL12W         0.09195905 W
PL13W         0.08120718 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                   1.40
```

Compound **S3** 19FNMR

S3


```
Current Data Parameters
NAME      DMM3-BN-OME-SALT
EXPNO                    3
PROCNO                   1

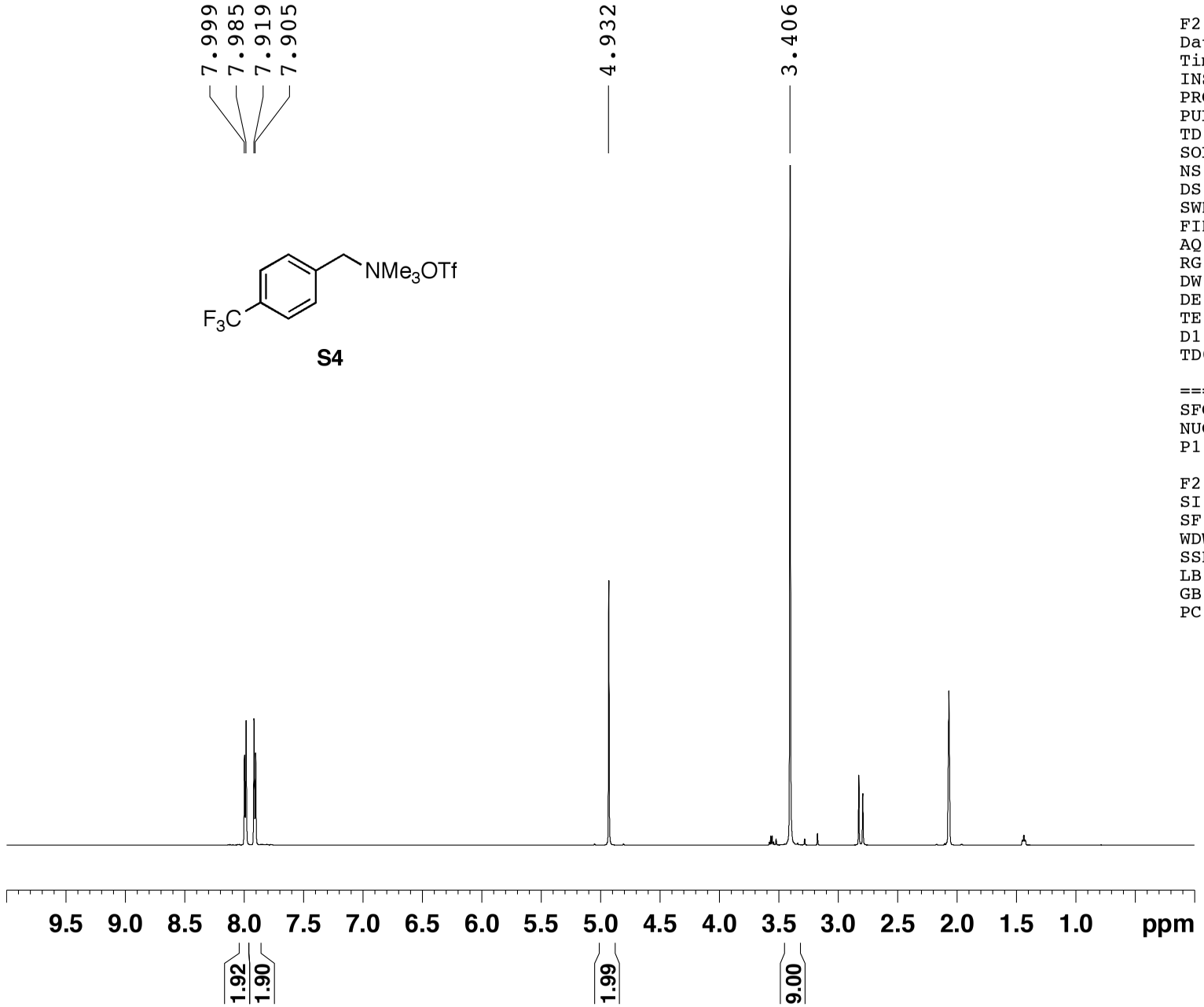
F2 - Acquisition Paramete
Date_             20120721
Time                 16.36
INSTRUM              spect
PROBHD    5 mm CPQNP 1H/
PULPROG                zgdc
TD                   131072
SOLVENT               CDCl3
NS                       16
DS                        2
SWH              75187.969 H
FIDRES           0.573639 H
AQ               0.8716788 s
RG                   322.5
DW                   6.650 u
DE                   20.00 u
TE                   298.2 K
D1             2.00000000 s
D11            0.03000000 s
TD0                      1

======== CHANNEL f1 =====
NUC1                   19F
P1                   15.03 u
PL1                  -4.00 d
PL1W          25.74305916 W
SFO1          376.4607164 M

======== CHANNEL f2 =====
CPDPRG2            waltz16
NUC2                   1H
PCPD2                90.00 u
PL2                   4.90 d
PL12                 20.46 d
PL2W           3.30822015 W
PL12W          0.09195905 W
SFO2          400.1316005 M

F2 - Processing parameter
SI                   65536
SF            376.4983660 M
WDW                    EM
SSB                     0
LB                   2.00 H
GB                      0
PC                   1.00
```

Compound **S4** 1HNMR



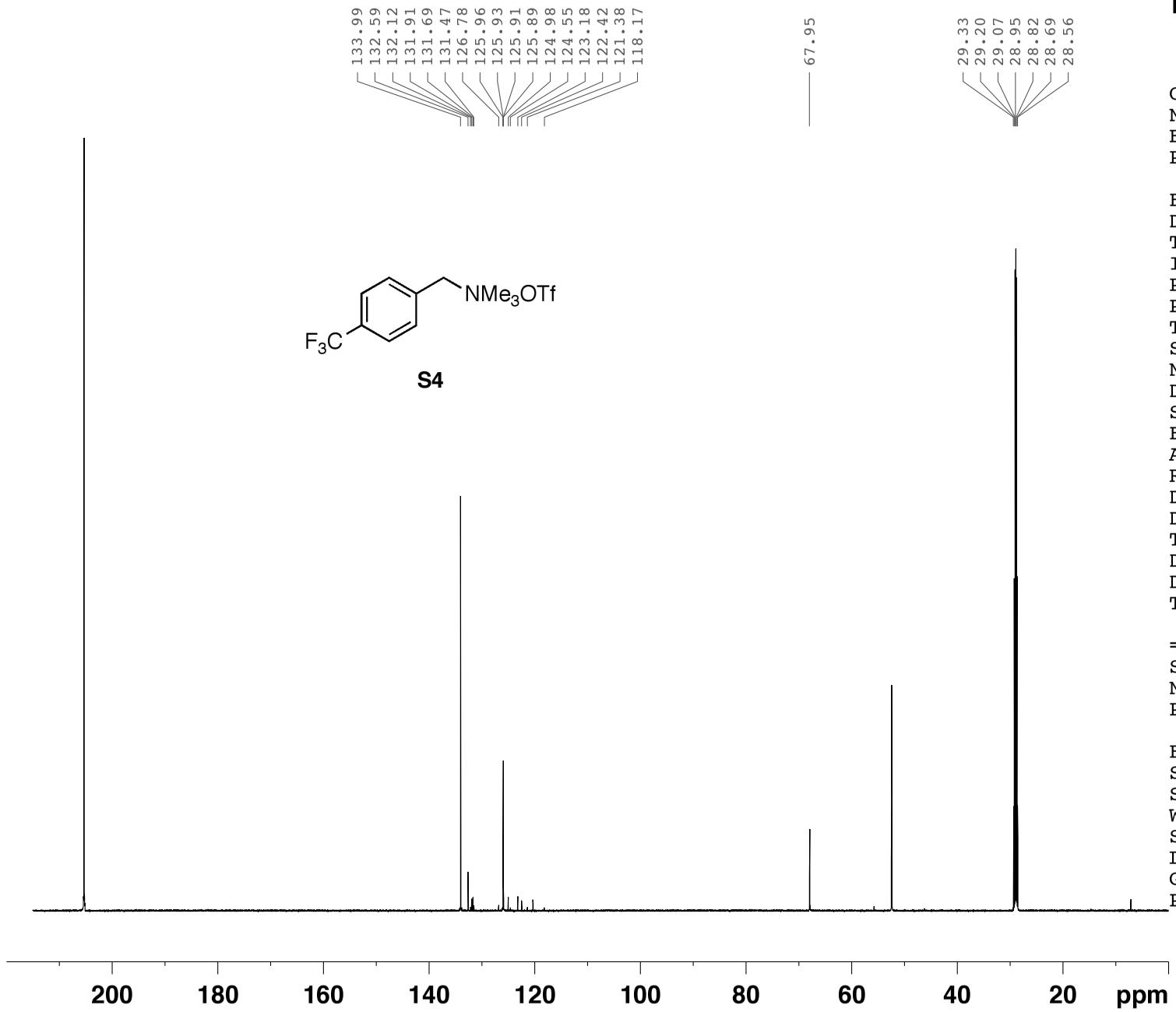

```
Current Data Parameters
NAME      DMM3-CNSI-SALT5
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20120803
Time              20.01
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                    8
DS                    2
SWH            8403.361 Hz
FIDRES        0.128225 Hz
AQ            3.8994420 sec
RG                  181
DW               59.500 usec
DE               17.39 usec
TE               300.2 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        600.3233018 MHz
NUC1                  1H
P1               10.77 usec

F2 - Processing parameters
SI                65536
SF          600.3200000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

Compound **S4** 13CNMR



S141

Current Data Parameters

NAME	DMM3-CNSI-SALT05-C2
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120807
Time	23.19
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg55
TD	65536
SOLVENT	Acetone
NS	2048
DS	4
SWH	34722.223 Hz
FIDRES	0.529819 Hz
AQ	0.9437684 sec
RG	2050
DW	14.400 usec
DE	19.34 usec
TE	300.2 K
D1	1.10000002 sec
D11	0.03000000 sec
TD0	1

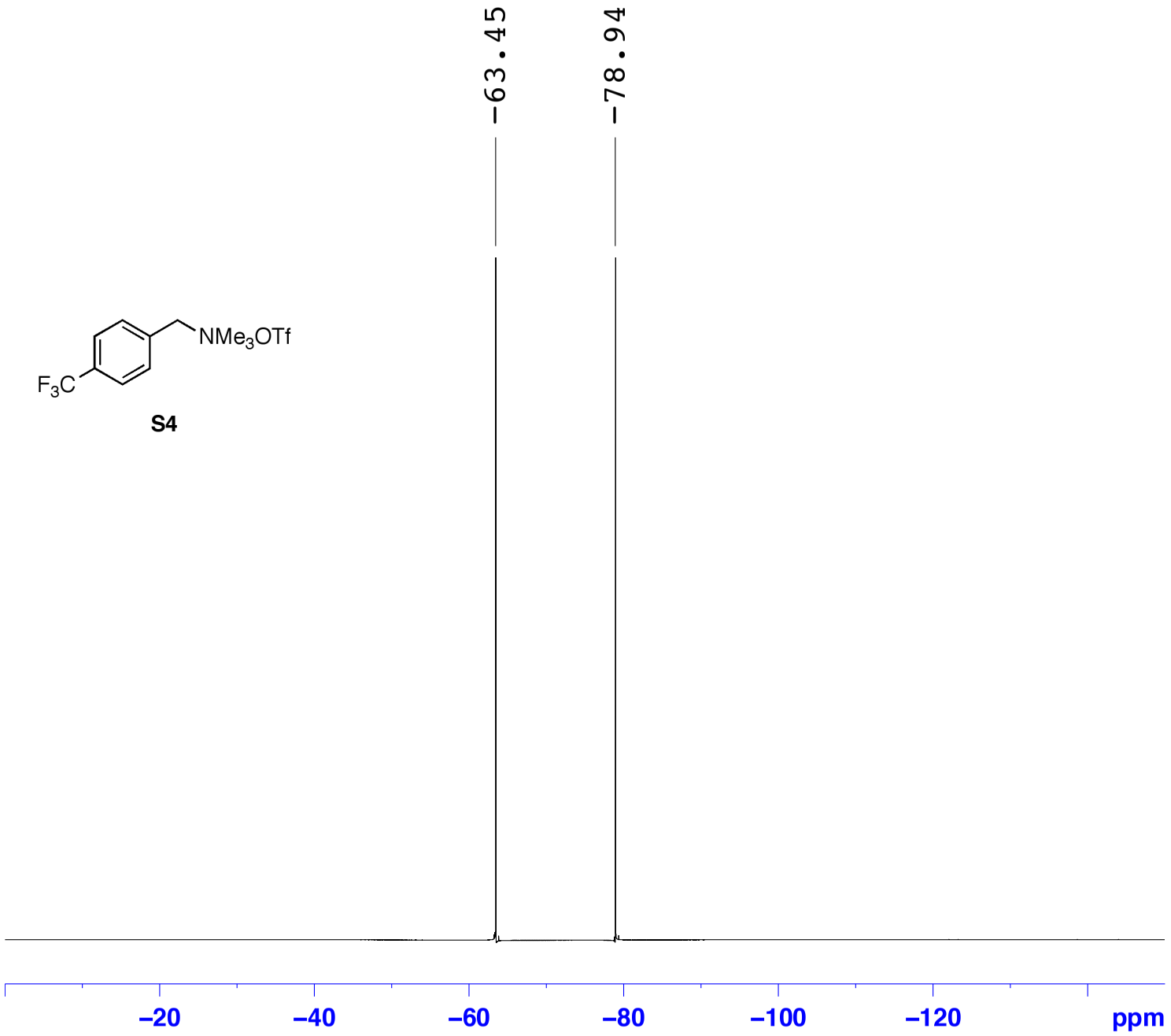
======== CHANNEL f1 ========

SFO1	150.9656784 MHz
NUC1	13C
P1	10.63 usec

F2 - Processing parameters

SI	32768
SF	150.9505840 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Compound **S4** 19FNMR



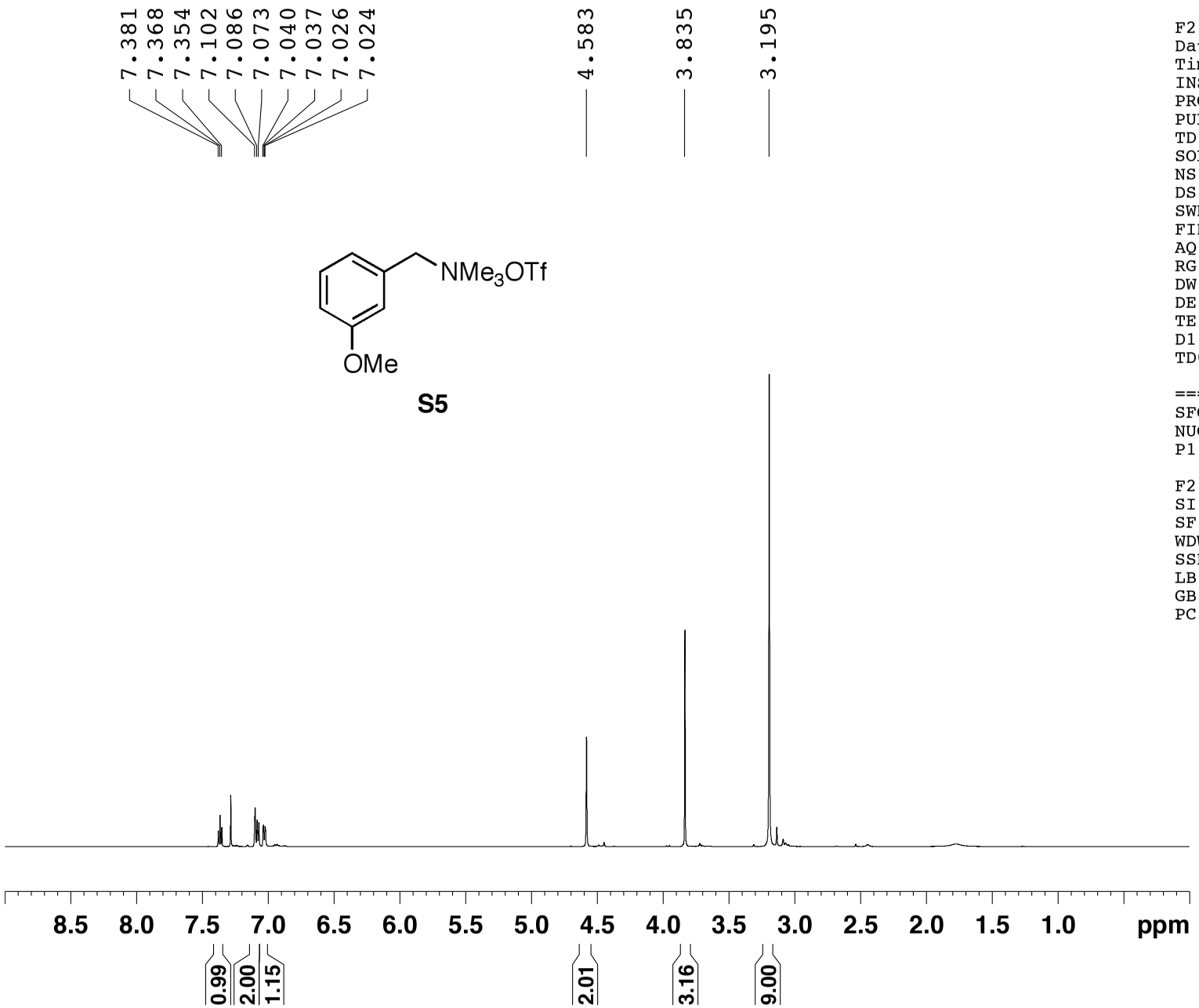

```
Current Data Parameters
NAME      DMM3-CNSI-SALT5
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_           20120803
Time              20.15
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgfhigqn
TD               131072
SOLVENT          Acetone
NS                    16
DS                     4
SWH           133928.578 Hz
FIDRES          1.021794 Hz
AQ             0.4893855 sec
RG                   456
DW                 3.733 usec
DE                 8.00 usec
TE                300.2 K
D1           3.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         564.8086803 MHz
NUC1                  19F
P1                 11.62 usec

F2 - Processing parameters
SI                 65536
SF           564.8651670 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

Compound **S5** 1HNMR



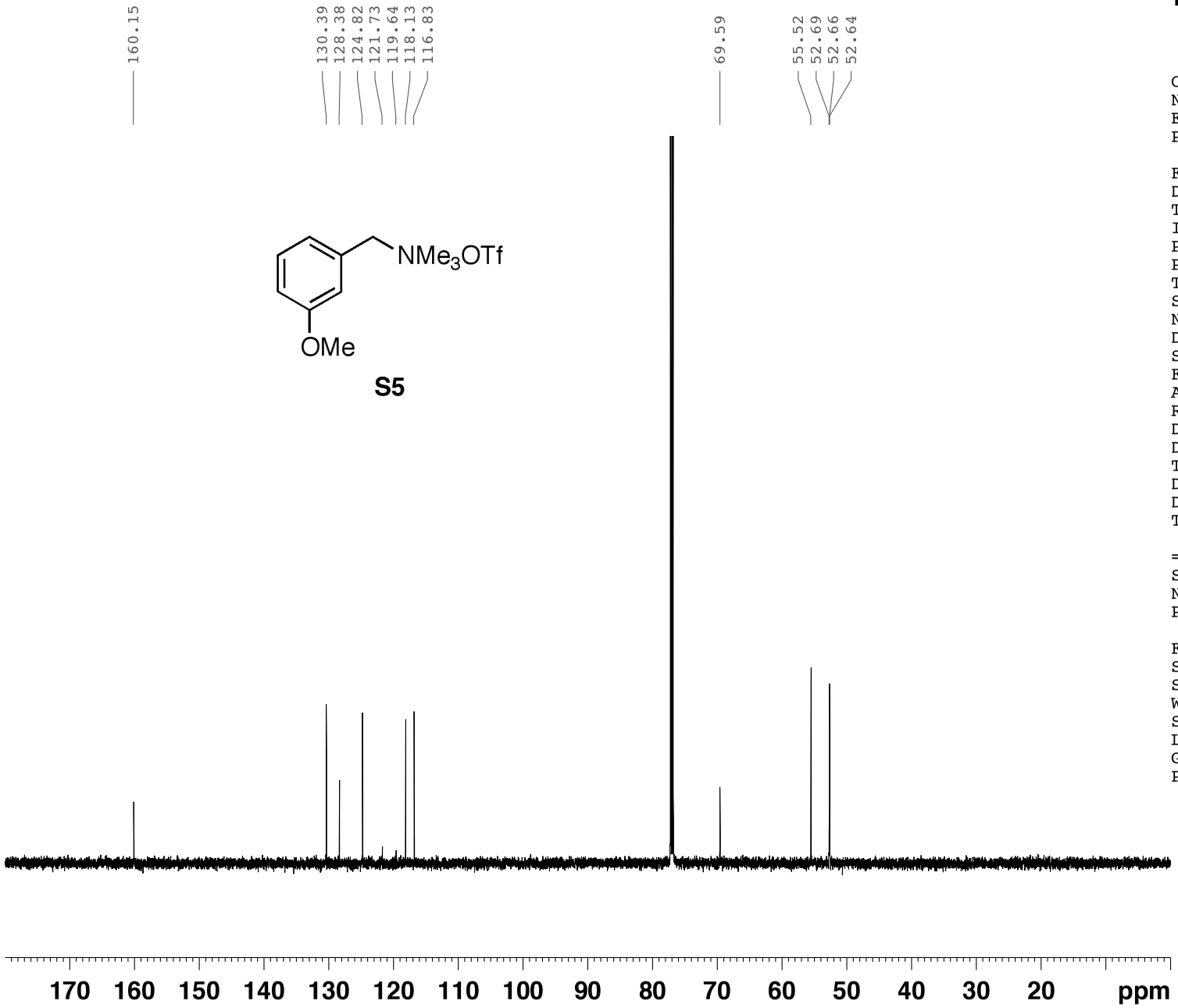

```
Current Data Parameters
NAME      DMM3-CNSI-SALT6
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120803
Time                16.44
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8403.361 Hz
FIDRES           0.128225 Hz
AQ               3.8994420 sec
RG                    161
DW                 59.500 usec
DE                 17.39 usec
TE                 300.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         600.3233018 MHz
NUC1                   1H
P1                 10.77 usec

F2 - Processing parameters
SI                  65536
SF           600.3200000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

Compound **S5** 13CNMR




```
Current Data Parameters
NAME      DMM3-CNSI-SALT6
EXPNO                   2
PROCNO                  1

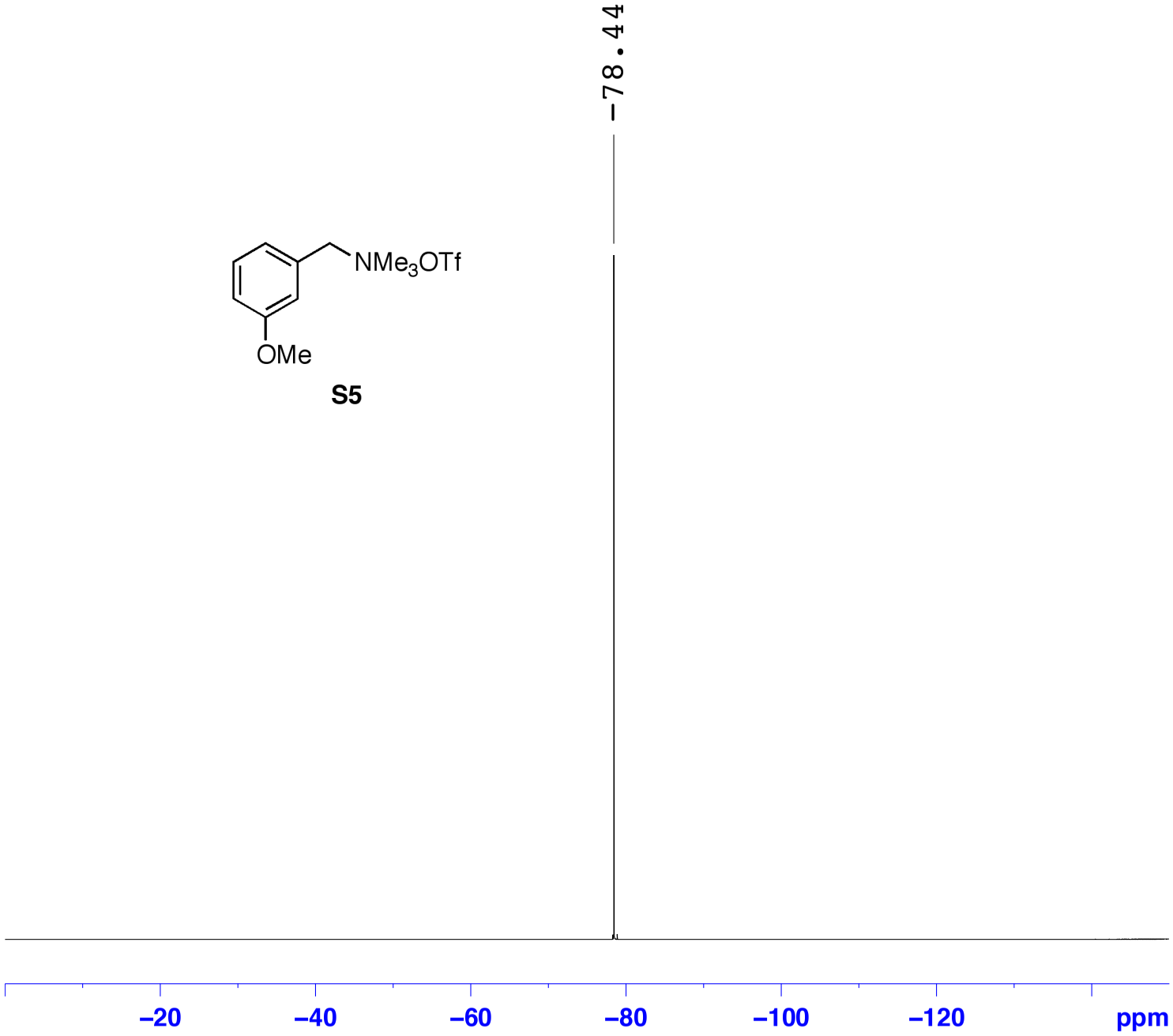
F2 - Acquisition Parameters
Date_            20120803
Time                16.55
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg55
TD                  65536
SOLVENT             CDCl3
NS                    256
DS                      4
SWH             34722.223 Hz
FIDRES           0.529819 Hz
AQ              0.9437684 sec
RG                   2050
DW                 14.400 usec
DE                 19.34 usec
TE                 300.2 K
D1             1.10000002 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         150.9656784 MHz
NUC1                  13C
P1                 10.63 usec

F2 - Processing parameters
SI                  32768
SF           150.9505840 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Compound **S5** 19FNMR

S5



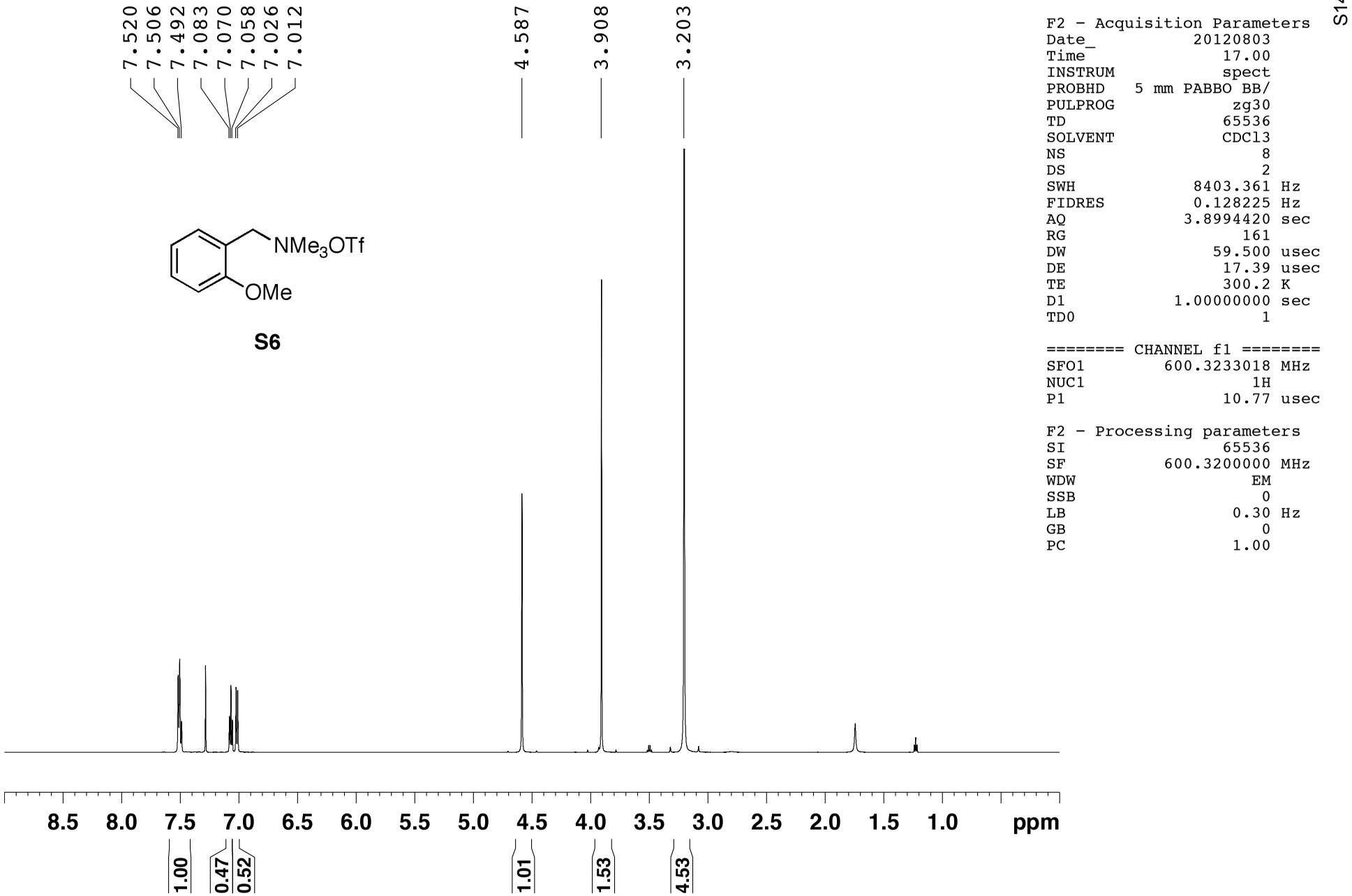

```
Current Data Parameters
NAME      DMM3-CNSI-SALT6
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120803
Time                16.57
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgfhigqn
TD                131072
SOLVENT             CDCl3
NS                     16
DS                      4
SWH           133928.578 Hz
FIDRES          1.021794 Hz
AQ             0.4893855 sec
RG                    362
DW                3.733 usec
DE                8.00 usec
TE                300.2 K
D1           3.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         564.8086803 MHz
NUC1                19F
P1                11.62 usec

F2 - Processing parameters
SI                  65536
SF           564.8651670 MHz
WDW                    EM
SSB                     0
LB                 2.00 Hz
GB                      0
PC                   1.00
```

Compound **S6** 1HNMR



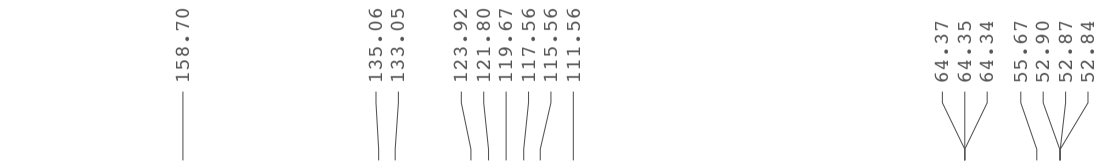

```
Current Data Parameters
NAME      DMM3-CNSI-SALT7
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20120803
Time              17.00
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            8403.361 Hz
FIDRES        0.128225 Hz
AQ            3.8994420 sec
RG                  161
DW               59.500 usec
DE               17.39 usec
TE               300.2 K
D1           1.00000000 sec
TD0                   1

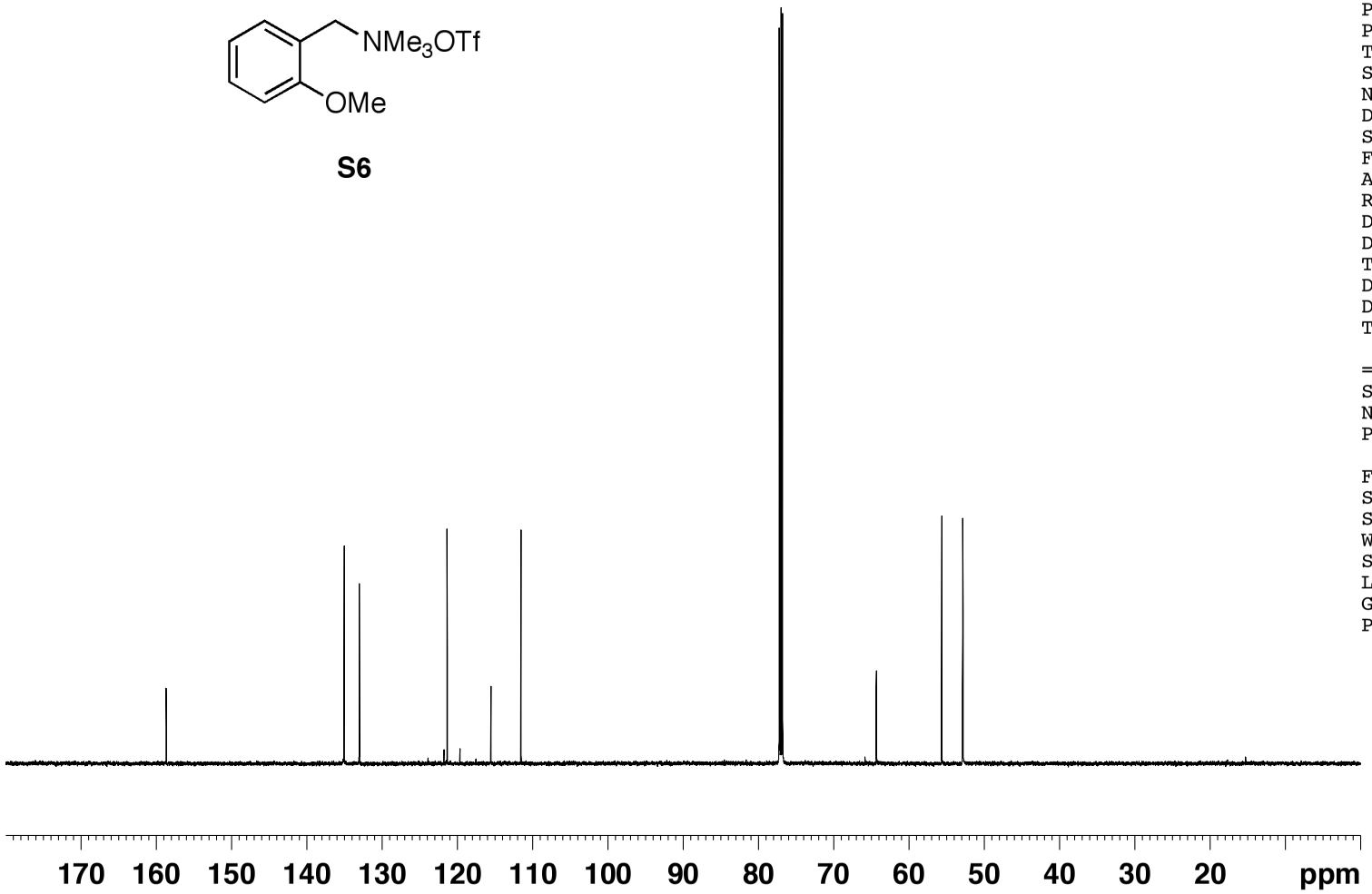
======== CHANNEL f1 ========
SFO1        600.3233018 MHz
NUC1                  1H
P1                10.77 usec

F2 - Processing parameters
SI                65536
SF          600.3200000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

Compound **S6** 13CNMR



S6




```
Current Data Parameters
NAME      DMM3-CNSI-SALT-07C
EXPNO                     1
PROCNO                    1

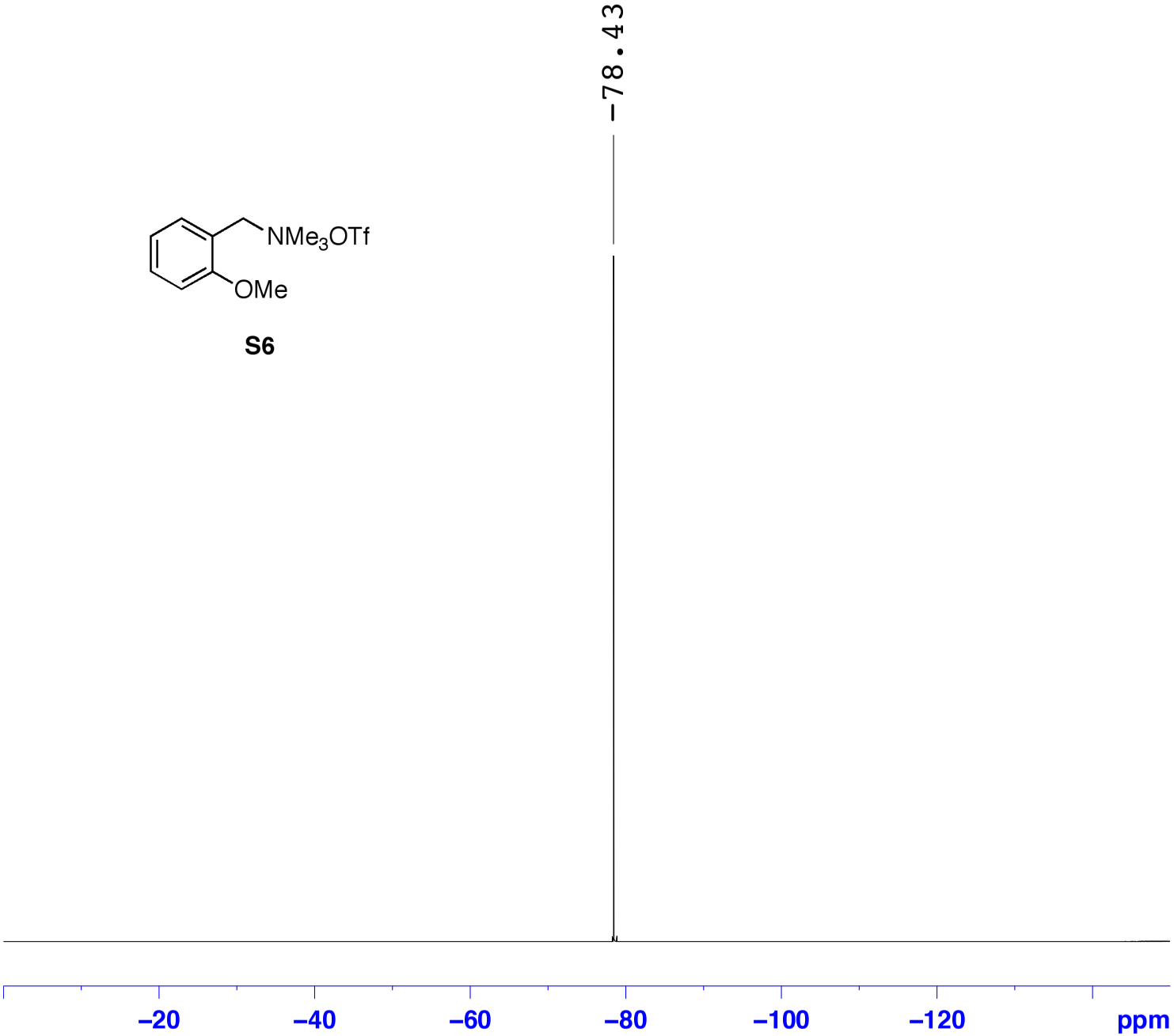
F2 - Acquisition Parameters
Date_              20120805
Time                   0.58
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg55
TD                    65536
SOLVENT               CDCl3
NS                     2048
DS                        4
SWH              34722.223 Hz
FIDRES            0.529819 Hz
AQ               0.9437684 sec
RG                     2050
DW                 14.400 usec
DE                 19.34 usec
TE                 300.2 K
D1              1.10000002 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          150.9656784 MHz
NUC1                    13C
P1                  10.63 usec

F2 - Processing parameters
SI                    32768
SF            150.9505840 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

Compound **S6** 19FNMR

S6



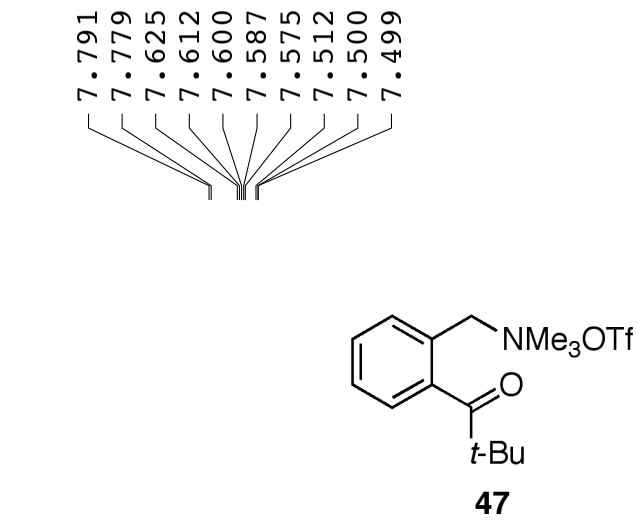

```
Current Data Parameters
NAME      DMM3-CNSI-SALT7
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120803
Time                17.14
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgfhigqn
TD                131072
SOLVENT             CDCl3
NS                     16
DS                      4
SWH           133928.578 Hz
FIDRES          1.021794 Hz
AQ             0.4893855 sec
RG                    362
DW                3.733 usec
DE                8.00 usec
TE                300.2 K
D1            3.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         564.8086803 MHz
NUC1                  19F
P1                11.62 usec

F2 - Processing parameters
SI                    65536
SF           564.8651670 MHz
WDW                      EM
SSB                       0
LB                 2.00 Hz
GB                        0
PC                 1.00
```

Compound **47**, 1H NMR



47

```
Current Data Parameters
NAME      DMM3-CNSI-SALT9
EXPNO                   1
PROCNO                  1

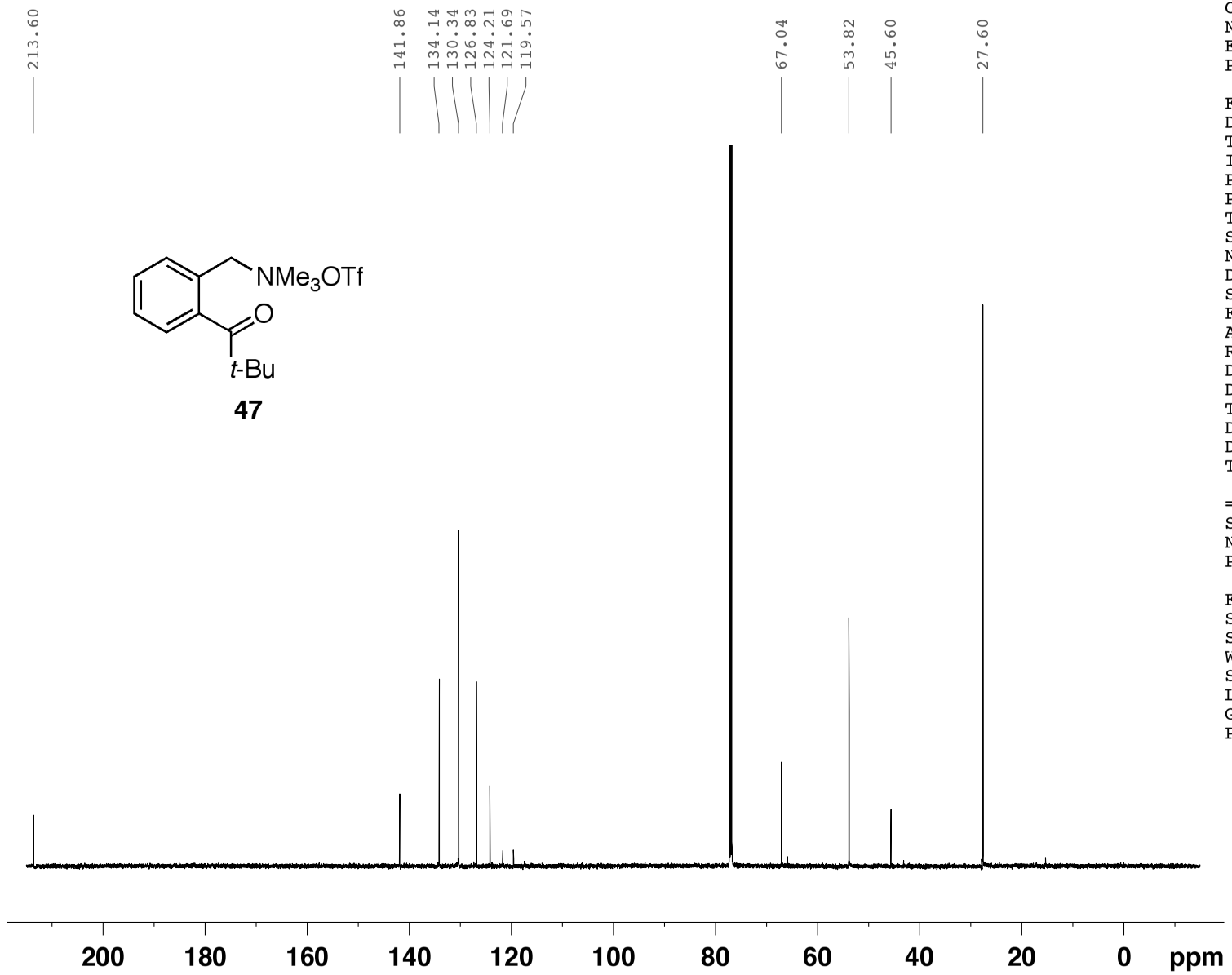
F2 - Acquisition Parameters
Date_           20120803
Time              17.34
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            8403.361 Hz
FIDRES        0.128225 Hz
AQ            3.8994420 sec
RG                  144
DW               59.500 usec
DE               17.39 usec
TE               300.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        600.3233018 MHz
NUC1                   1H
P1                10.77 usec

F2 - Processing parameters
SI                65536
SF          600.3200000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

S149

Compound **47**, 13C NMR




```
Current Data Parameters
NAME      DMM3-CNSI-SALT-09C
EXPNO                     1
PROCNO                    1

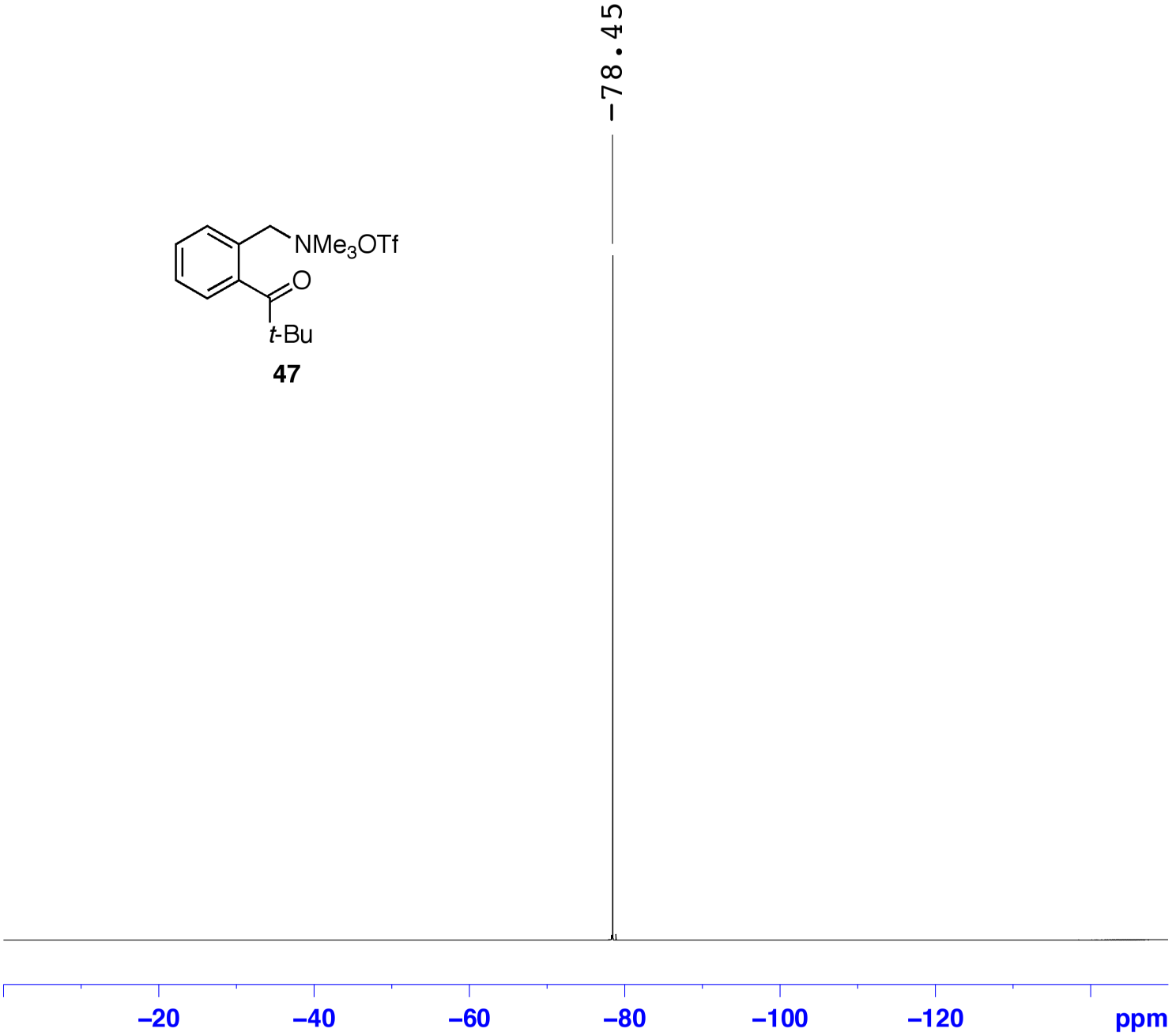
F2 - Acquisition Parameters
Date_              20120805
Time                   3.27
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg55
TD                    65536
SOLVENT               CDCl3
NS                     2048
DS                        4
SWH              34722.223 Hz
FIDRES            0.529819 Hz
AQ               0.9437684 sec
RG                     2050
DW                  14.400 usec
DE                  19.34 usec
TE                  300.2 K
D1              1.10000002 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           150.9656784 MHz
NUC1                    13C
P1                  10.63 usec

F2 - Processing parameters
SI                    32768
SF             150.9505840 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                    1.40
```

Compound **47**, 19F NMR

47



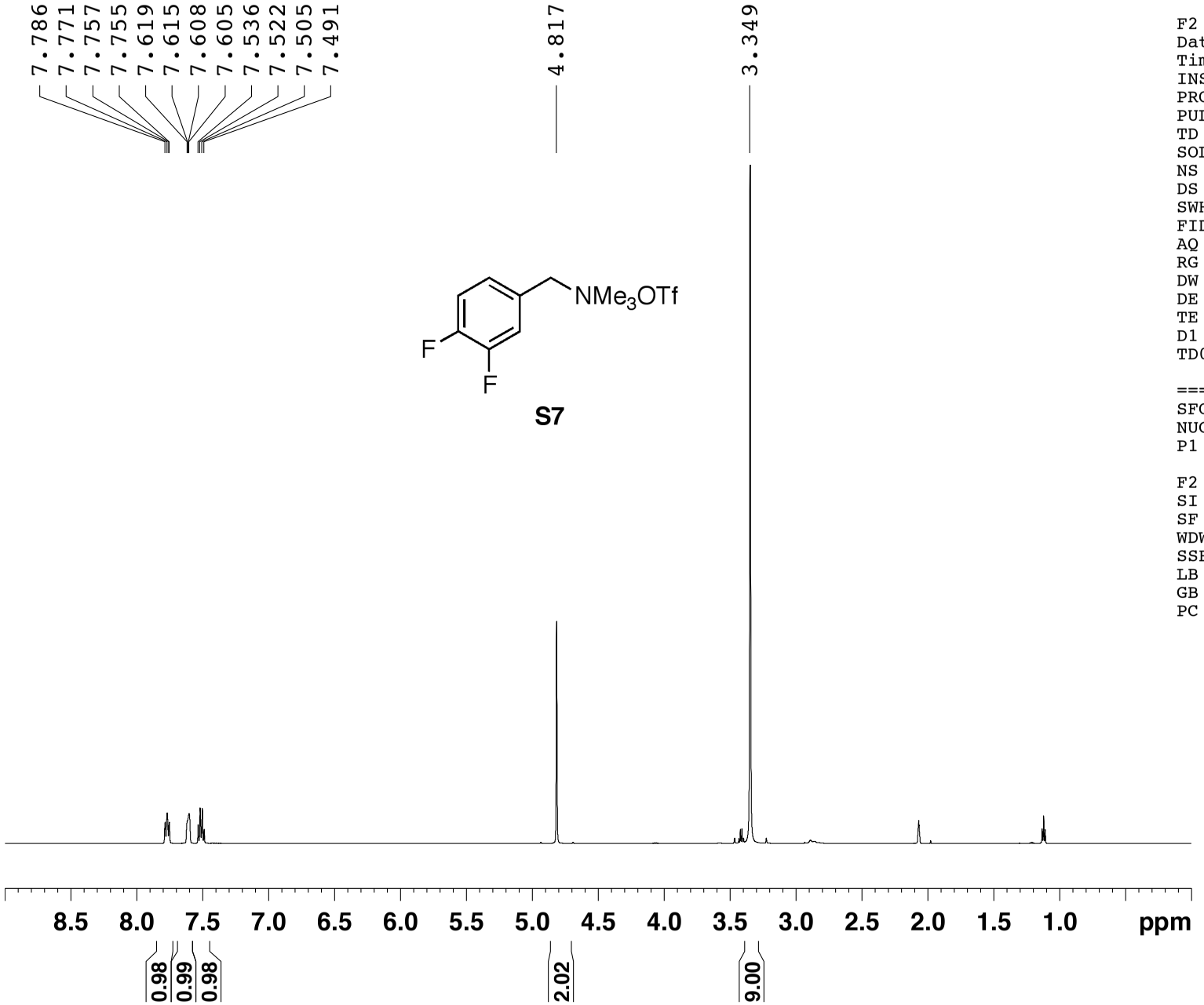

```
Current Data Parameters
NAME      DMM3-CNSI-SALT9
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120803
Time                17.47
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgfhigqn
TD                131072
SOLVENT             CDCl3
NS                     16
DS                      4
SWH           133928.578 Hz
FIDRES          1.021794 Hz
AQ             0.4893855 sec
RG                    362
DW                3.733 usec
DE                8.00 usec
TE                300.2 K
D1           3.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         564.8086803 MHz
NUC1                  19F
P1                11.62 usec

F2 - Processing parameters
SI                  65536
SF           564.8651670 MHz
WDW                    EM
SSB                     0
LB                 2.00 Hz
GB                      0
PC                 1.00
```

Compound **S7** 1HNMR



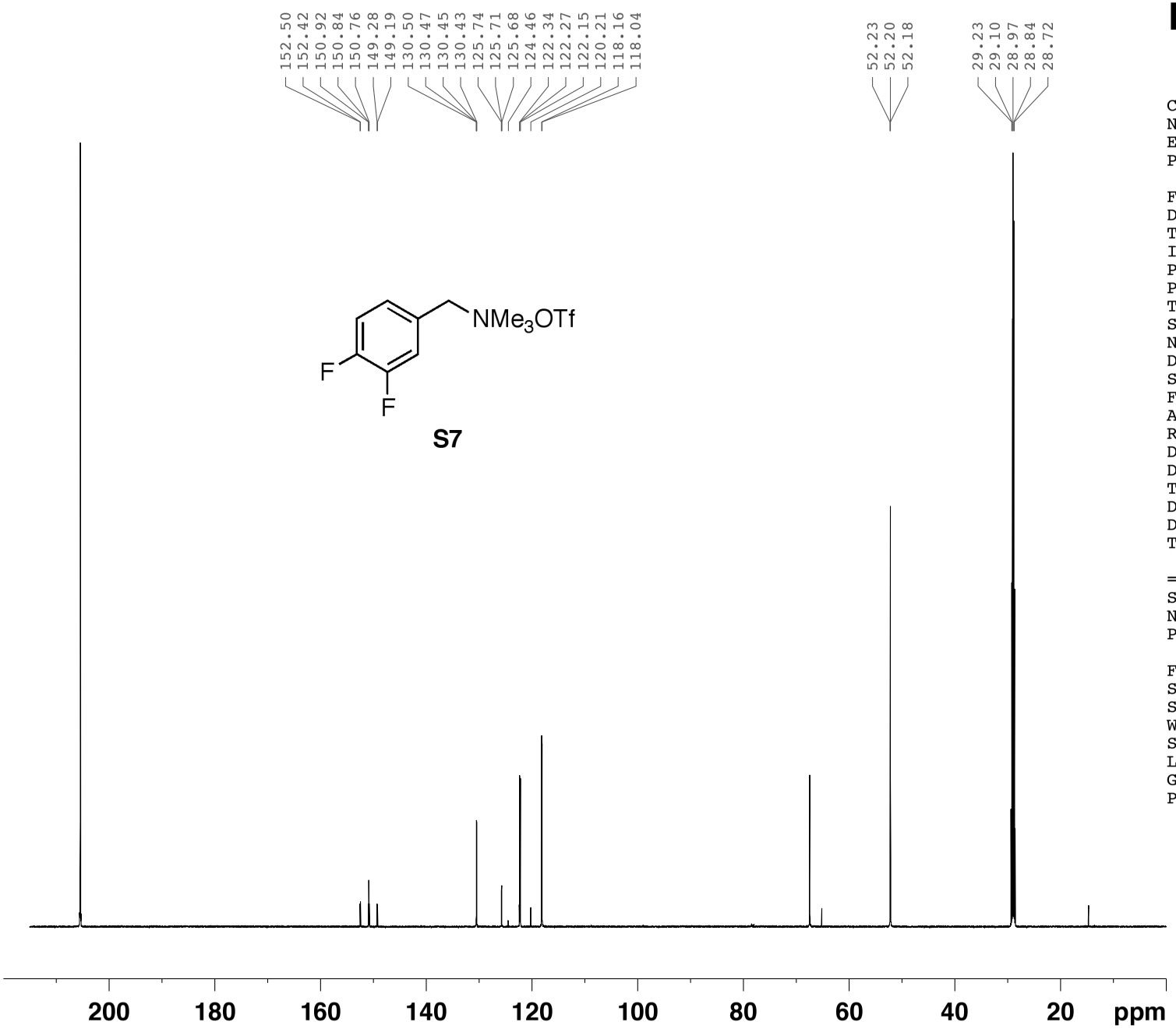

```
Current Data Parameters
NAME      DMM3-CNSI-SALT10-C2
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20120807
Time                 10.54
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT            Acetone
NS                       8
DS                       2
SWH               8403.361 Hz
FIDRES            0.128225 Hz
AQ                3.8994420 sec
RG                      57
DW                  59.500 usec
DE                  17.39 usec
TE                  300.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           600.3233018 MHz
NUC1                   1H
P1                  10.77 usec

F2 - Processing parameters
SI                   65536
SF             600.3200000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

Compound **S7** 13CNMR



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```
Current Data Parameters
NAME      DMM3-CNSI-SALT10-C2
EXPNO                      3
PROCNO                     1

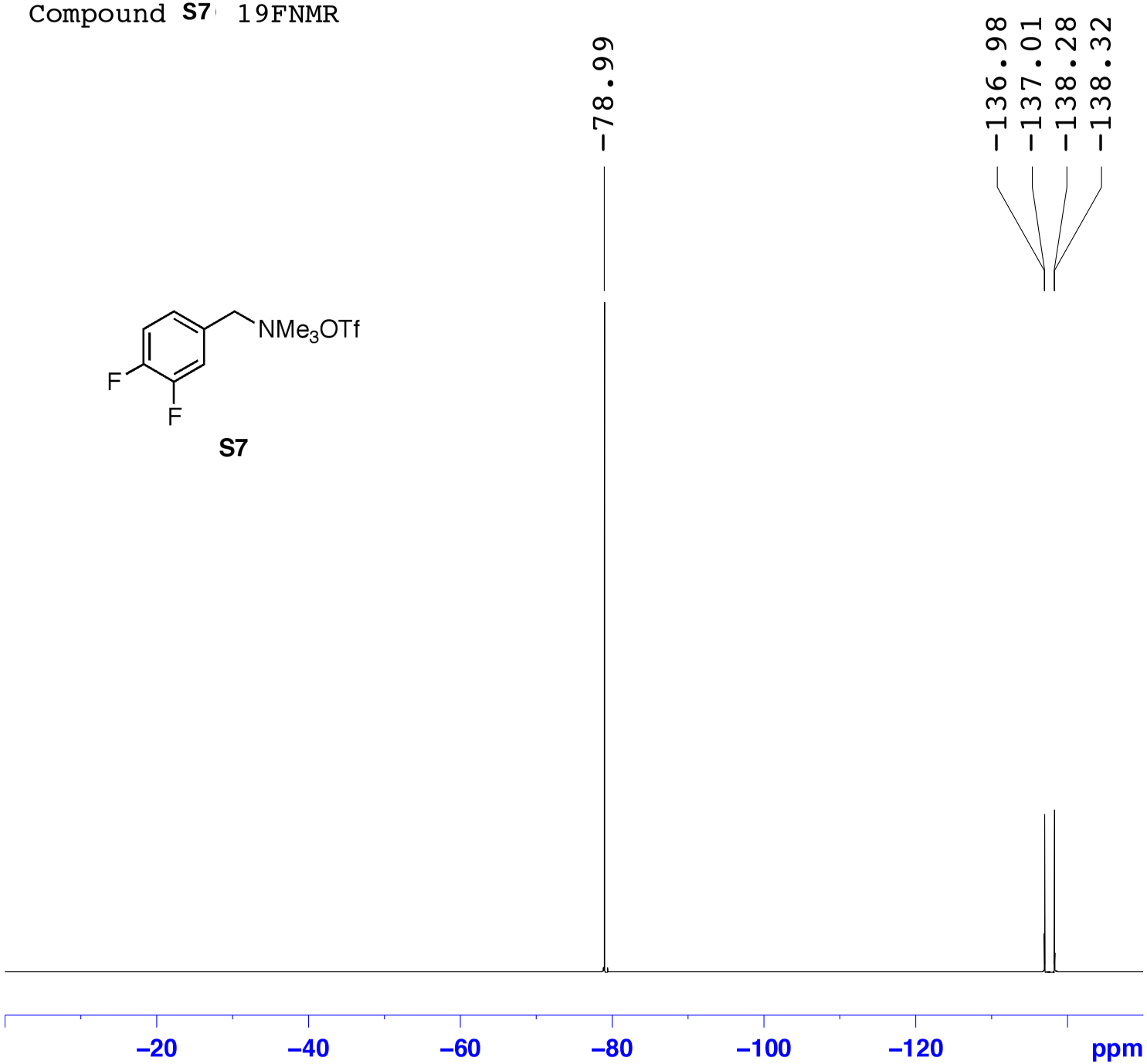
F2 - Acquisition Parameters
Date_              20120808
Time                   3.06
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg55
TD                    65536
SOLVENT           Acetone
NS                     2048
DS                        4
SWH              34722.223 Hz
FIDRES            0.529819 Hz
AQ               0.9437684 sec
RG                     2050
DW                  14.400 usec
DE                  19.34 usec
TE                  300.2 K
D1              1.10000002 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           150.9656784 MHz
NUC1                    13C
P1                  10.63 usec

F2 - Processing parameters
SI                    32768
SF             150.9505840 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

Compound **S7** 19FNMR

S7



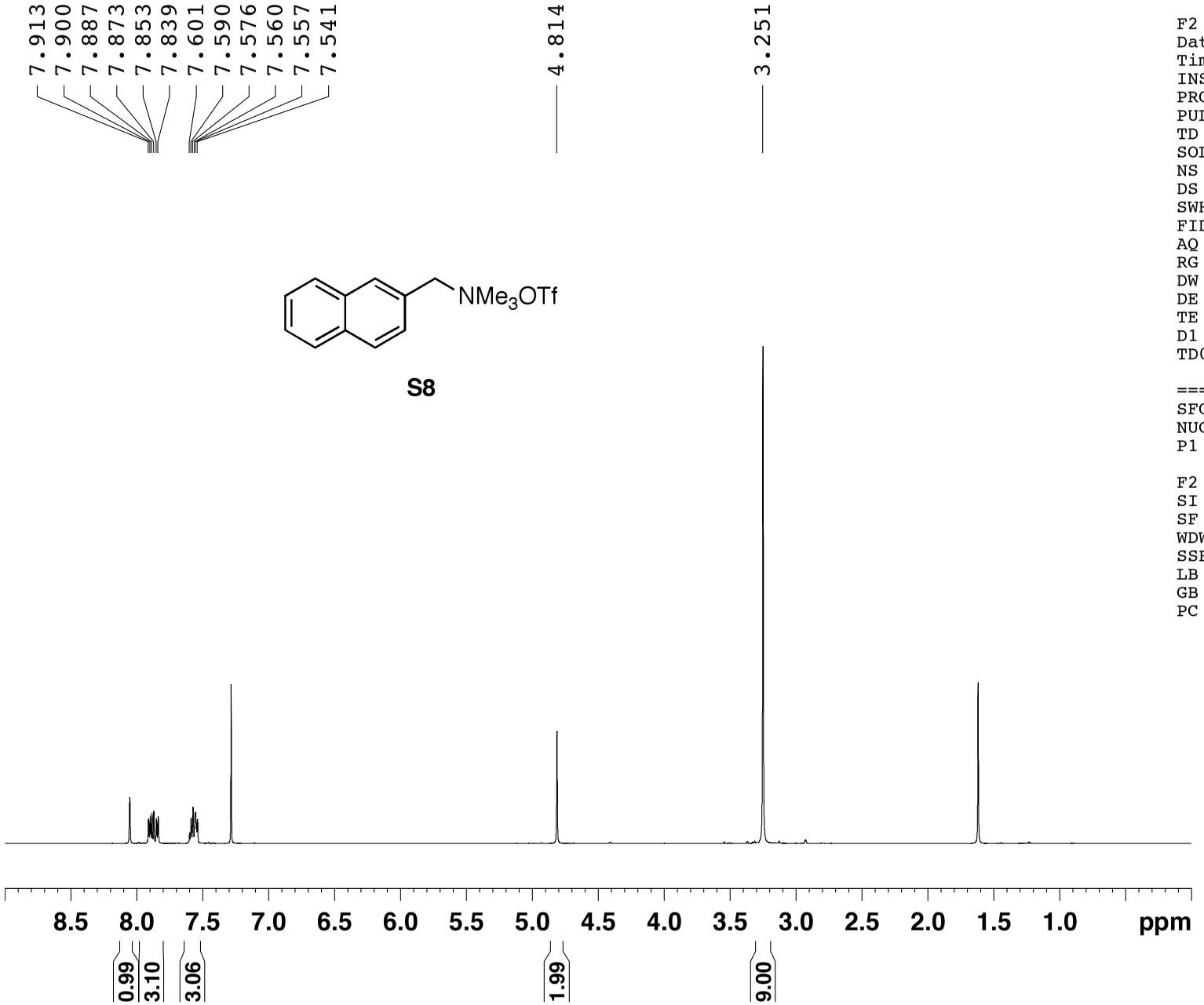

```
Current Data Parameters
NAME      DMM3-CNSI-SALT10-C2
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_           20120807
Time                10.56
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG          zgfhigqn
TD                 131072
SOLVENT           Acetone
NS                      16
DS                       4
SWH             133928.578 Hz
FIDRES            1.021794 Hz
AQ                0.4893855 sec
RG                      256
DW                  3.733 usec
DE                  8.00 usec
TE                  300.2 K
D1              3.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          564.8086803 MHz
NUC1                  19F
P1                 11.62 usec

F2 - Processing parameters
SI                    65536
SF            564.8651670 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.00
```

Compound **S8** 1HNMR



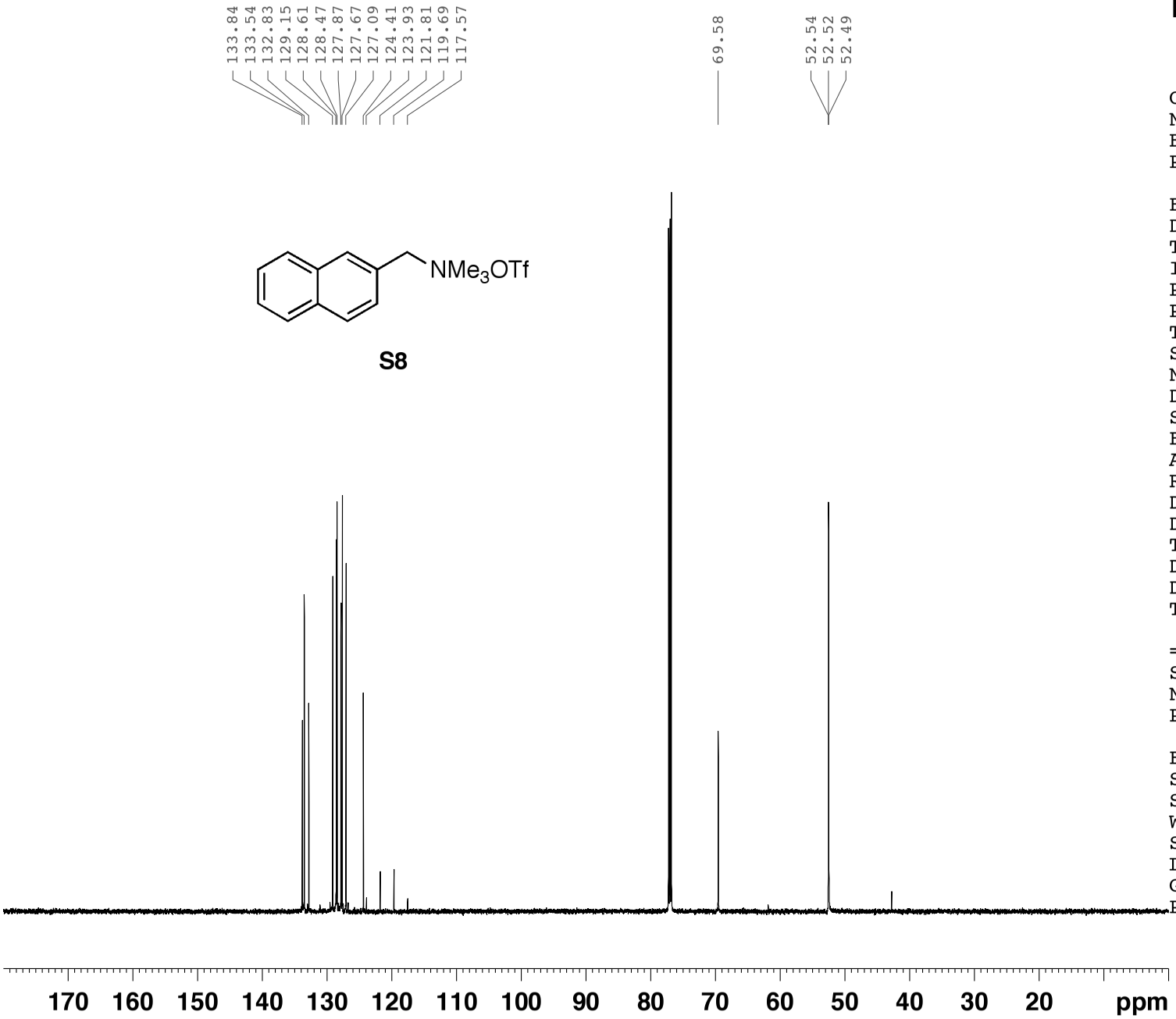

```
Current Data Parameters
NAME      DMM3-CNSI-SALT11
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120803
Time                 18.07
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8403.361 Hz
FIDRES           0.128225 Hz
AQ               3.8994420 sec
RG                     256
DW                59.500 usec
DE                17.39 usec
TE                 300.2 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          600.3233018 MHz
NUC1                    1H
P1                 10.77 usec

F2 - Processing parameters
SI                   65536
SF            600.3200000 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

Compound **S8** 13CNMR



S156

Current Data Parameters
NAME DMM3-CNSI-SALT11-C2
EXPNO 1
PROCNO 1

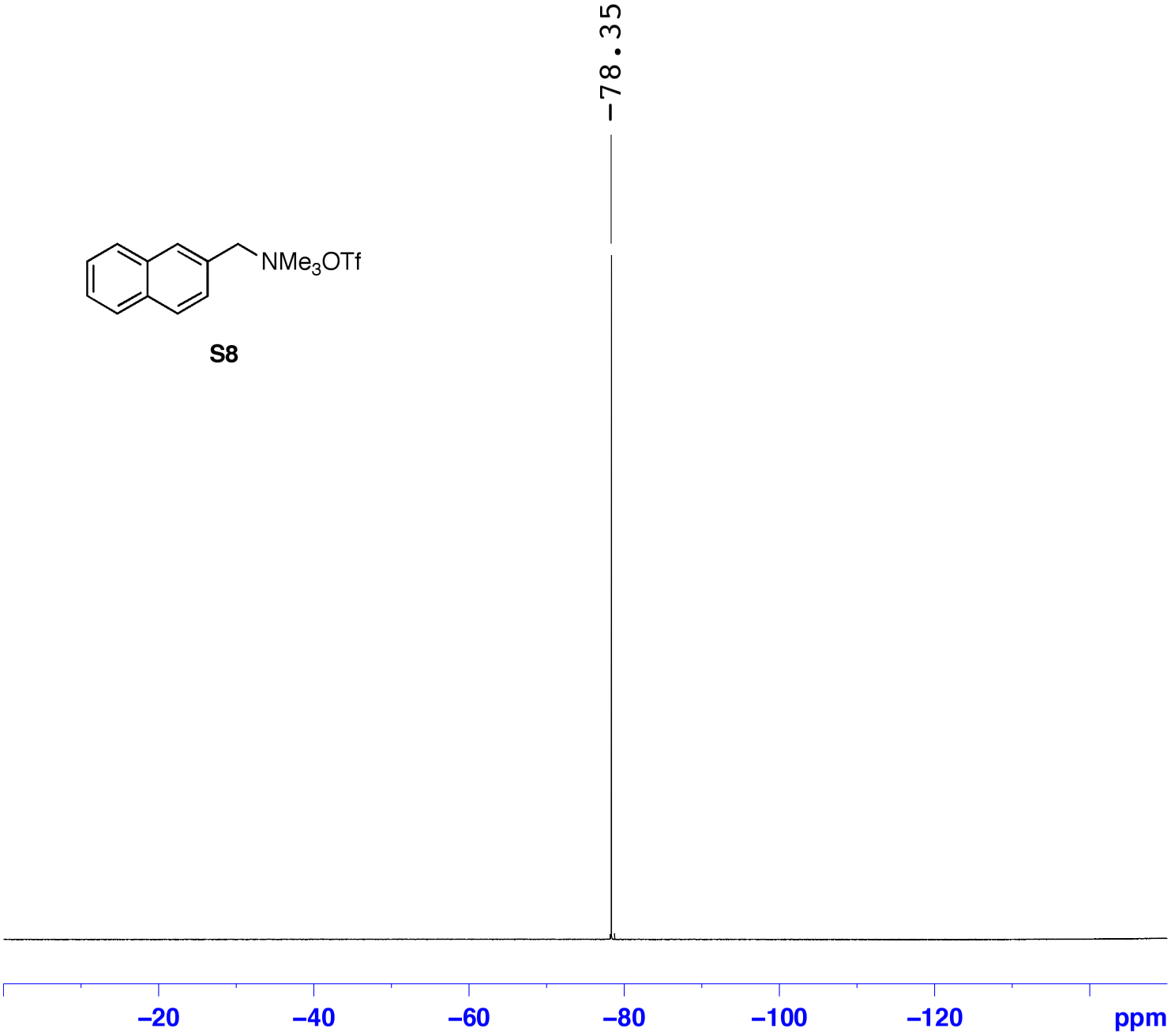
F2 - Acquisition Parameters
Date_ 20120808
Time 4.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg55
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 2050
DW 14.400 usec
DE 19.34 usec
TE 300.2 K
D1 1.10000002 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 150.9656784 MHz
NUC1 13C
P1 10.63 usec

F2 - Processing parameters
SI 32768
SF 150.9505840 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound **S8** 19FNMR

S8



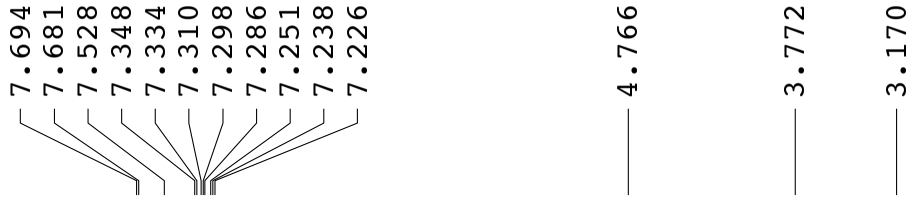

```
Current Data Parameters
NAME      DMM3-CNSI-SALT11
EXPNO                    3
PROCNO                   1

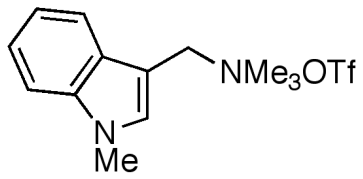
F2 - Acquisition Parameters
Date_             20120803
Time                 18.20
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                      16
DS                       4
SWH           133928.578 Hz
FIDRES          1.021794 Hz
AQ             0.4893855 sec
RG                     406
DW                 3.733 usec
DE                  8.00 usec
TE                 300.2 K
D1            3.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1         564.8086803 MHz
NUC1                   19F
P1                 11.62 usec

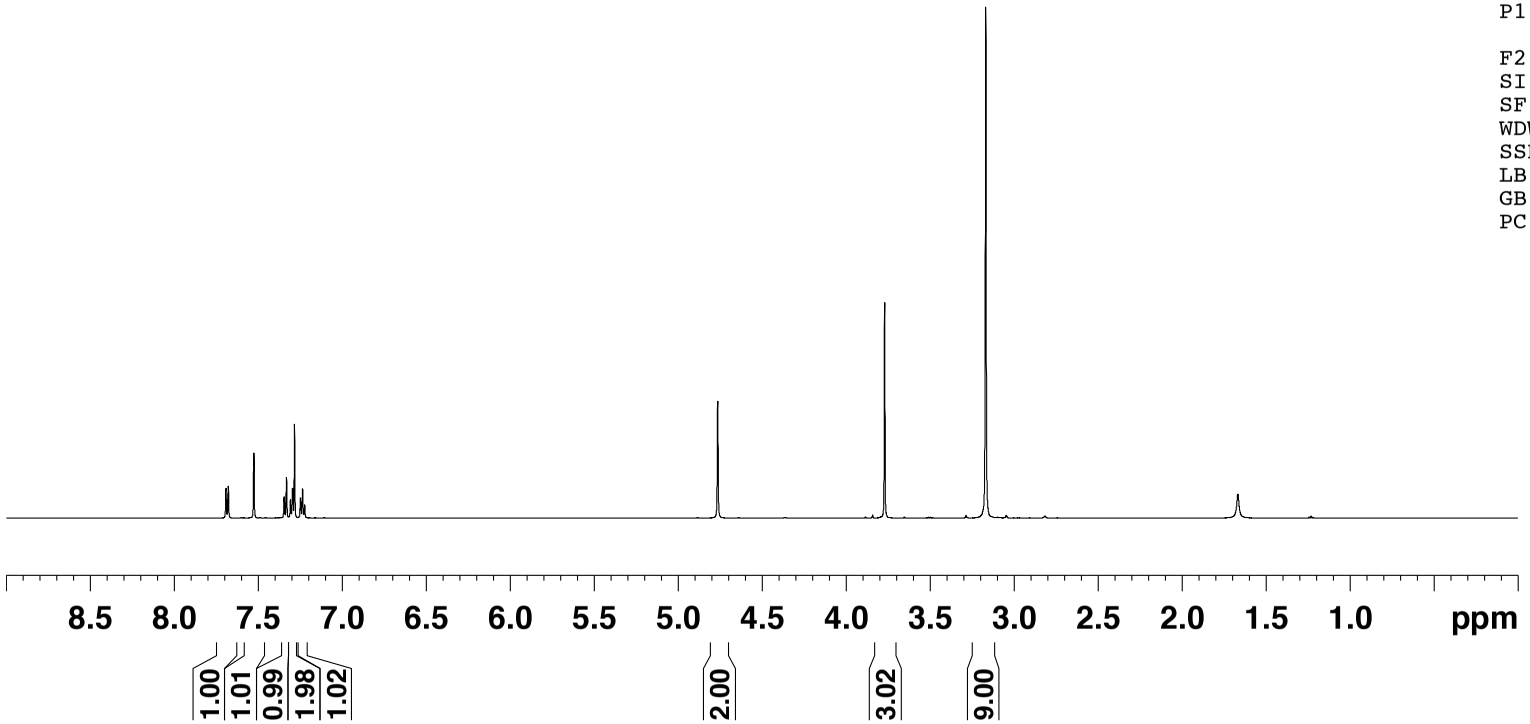
F2 - Processing parameters
SI                   65536
SF           564.8651670 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.00
```

Coompound **S9** 1HNMR





S9



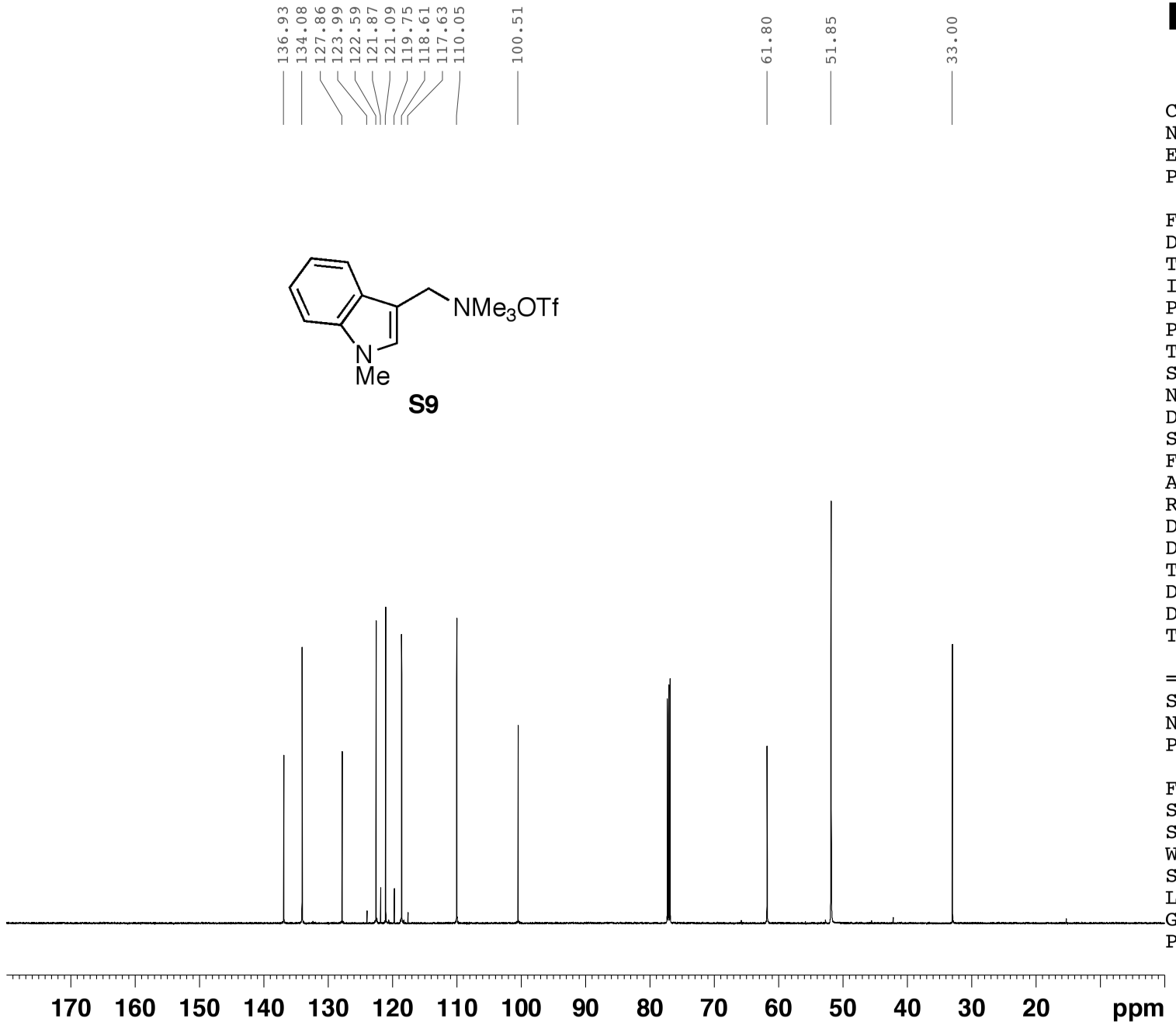

```
Current Data Parameters
NAME      DMM3-CNSI-SALT12
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120803
Time                 18.23
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8403.361 Hz
FIDRES            0.128225 Hz
AQ                3.8994420 sec
RG                     203
DW                  59.500 usec
DE                  17.39 usec
TE                  300.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          600.3233018 MHz
NUC1                    1H
P1                  10.77 usec

F2 - Processing parameters
SI                   65536
SF            600.3200000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

Compound **S9** 13CNMR



S159

Current Data Parameters

NAME	DMM3-CNSI-SALT12-C2
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120808
Time	5.36
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg55
TD	65536
SOLVENT	CDCl3
NS	2048
DS	4
SWH	34722.223 Hz
FIDRES	0.529819 Hz
AQ	0.9437684 sec
RG	2050
DW	14.400 usec
DE	19.34 usec
TE	300.2 K
D1	1.10000002 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========

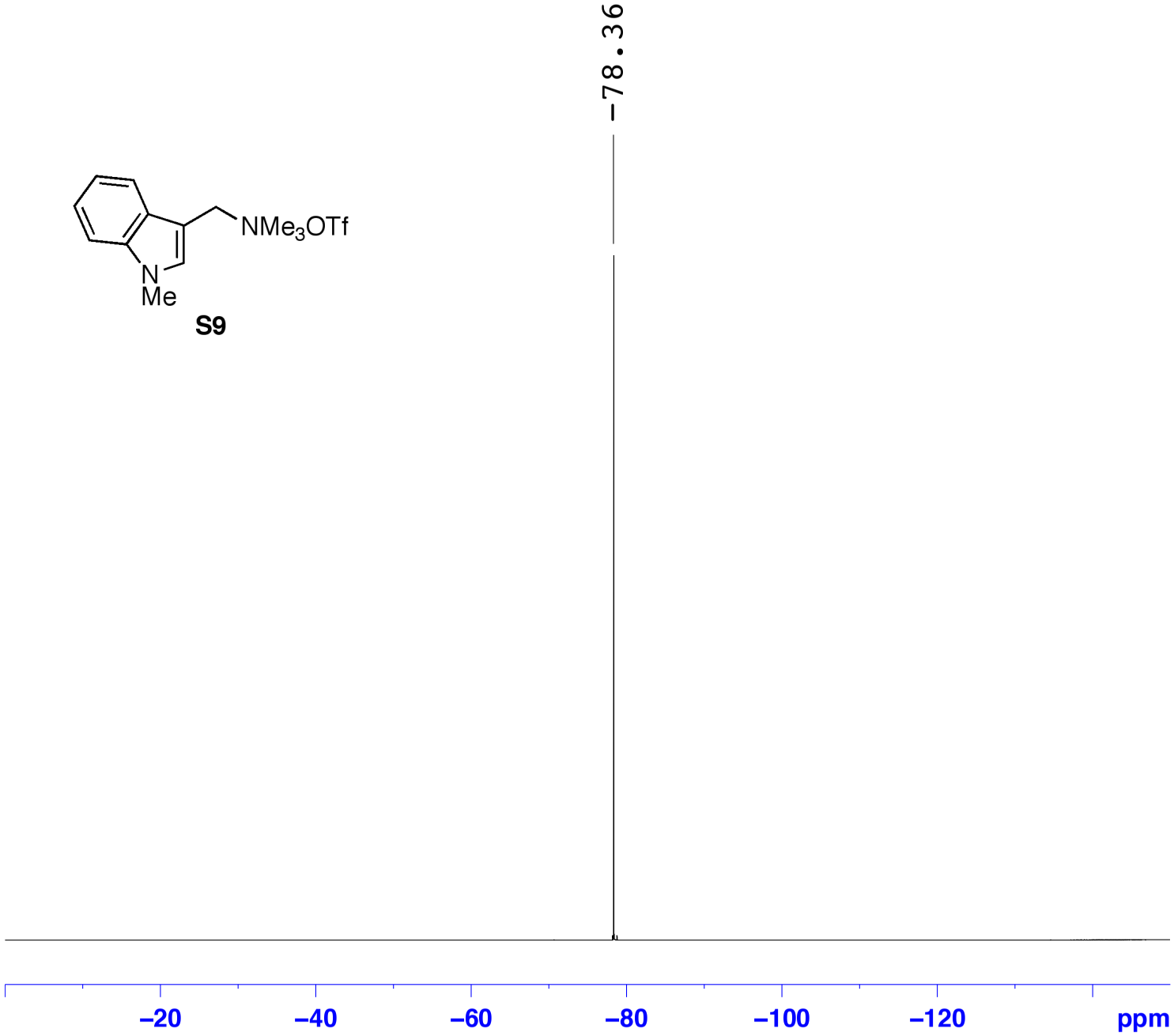
SFO1	150.9656784 MHz
NUC1	13C
P1	10.63 usec

F2 - Processing parameters

SI	32768
SF	150.9505840 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Compound **S9** 19FNMR

S9



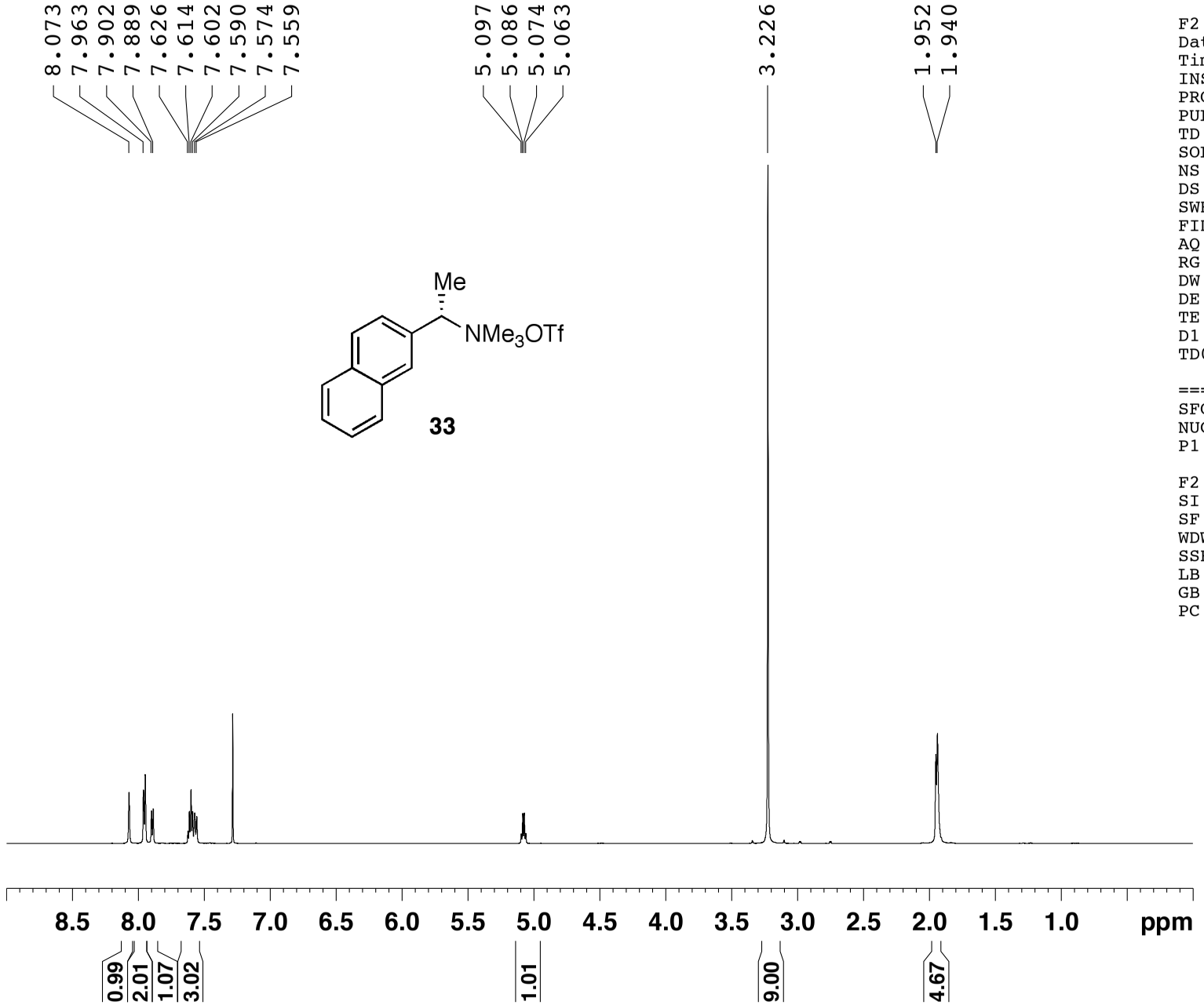

```
Current Data Parameters
NAME      DMM3-CNSI-SALT12
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120803
Time                 18.36
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                      16
DS                       4
SWH             133928.578 Hz
FIDRES            1.021794 Hz
AQ                0.4893855 sec
RG                     406
DW                   3.733 usec
DE                   8.00 usec
TE                  300.2 K
D1              3.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           564.8086803 MHz
NUC1                   19F
P1                   11.62 usec

F2 - Processing parameters
SI                   65536
SF             564.8651670 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.00
```

Compound **33** 1HNMR



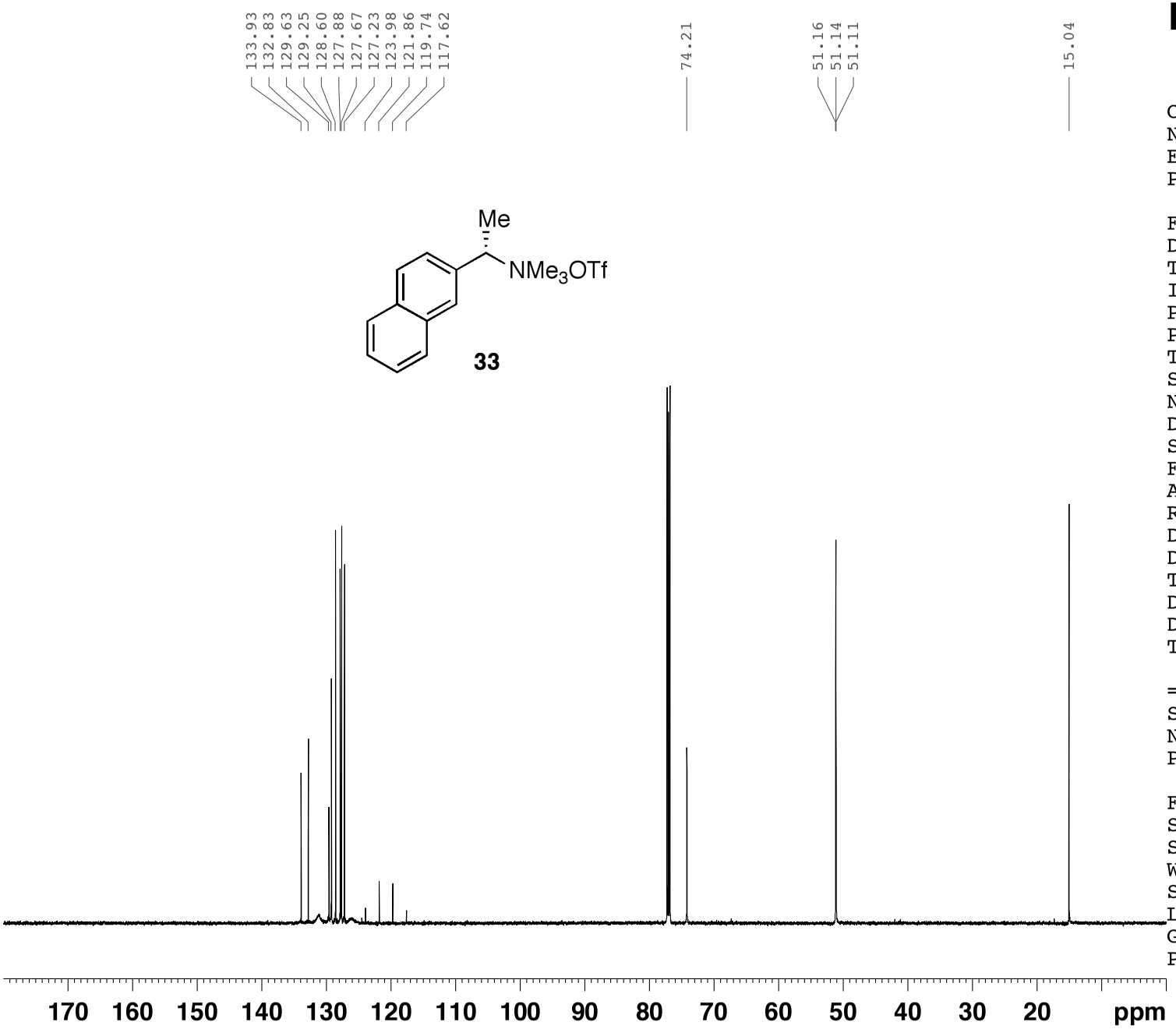

```
Current Data Parameters
NAME      DMM3-CNSI-SALT13
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120803
Time                 18.40
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8403.361 Hz
FIDRES           0.128225 Hz
AQ               3.8994420 sec
RG                     203
DW                59.500 usec
DE                17.39 usec
TE                 300.2 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          600.3233018 MHz
NUC1                     1H
P1                  10.77 usec

F2 - Processing parameters
SI                   65536
SF            600.3200000 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

Compound **33** 13CNMR



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S162

Current Data Parameters
NAME DMM3-CNSI-SALT13-C2
EXPNO 1
PROCNO 1

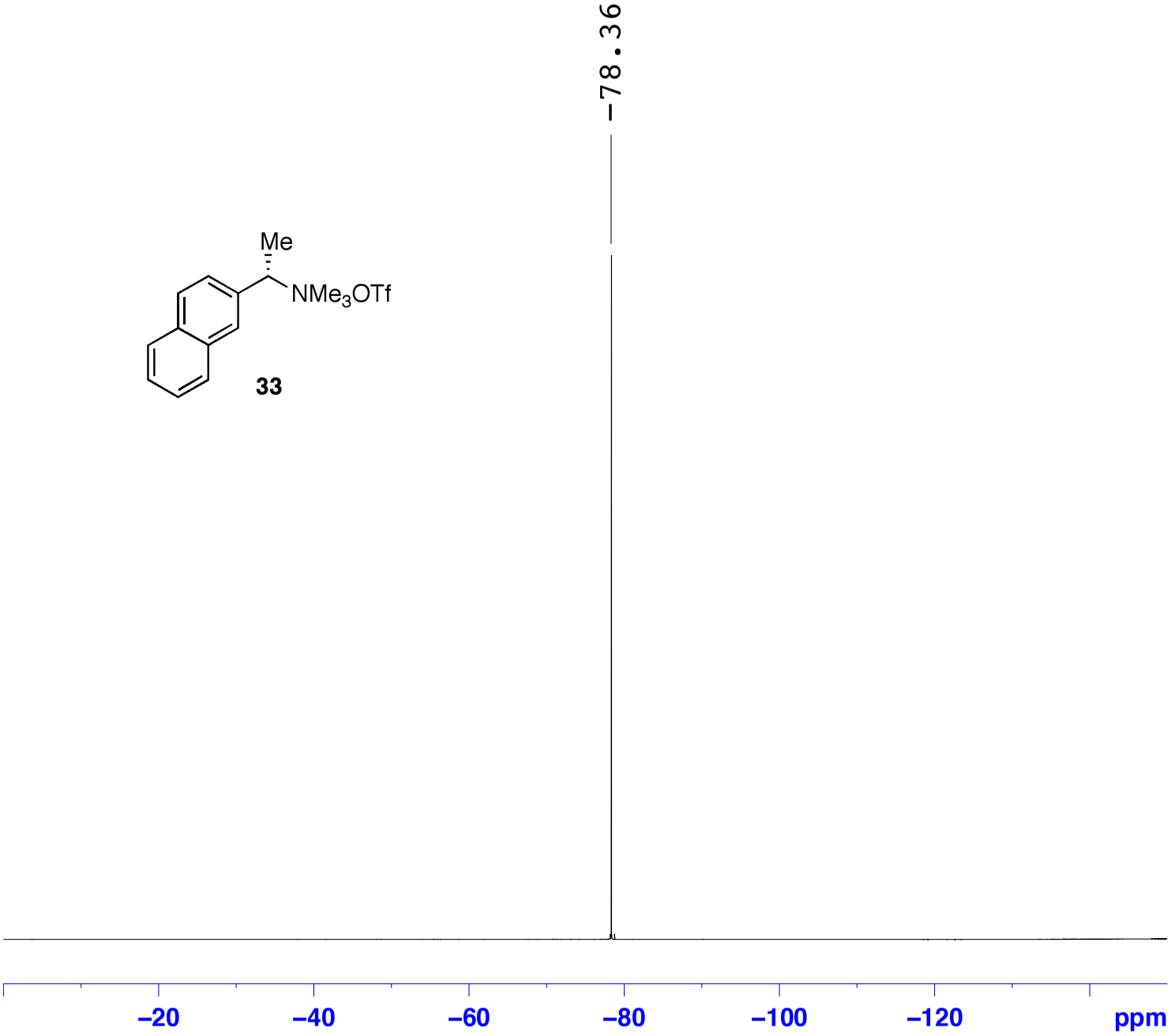
F2 - Acquisition Parameters
Date_ 20120808
Time 6.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg55
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 2050
DW 14.400 usec
DE 19.34 usec
TE 300.2 K
D1 1.10000002 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 150.9656784 MHz
NUC1 13C
P1 10.63 usec

F2 - Processing parameters
SI 32768
SF 150.9505840 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound **33** 19FNMR

33



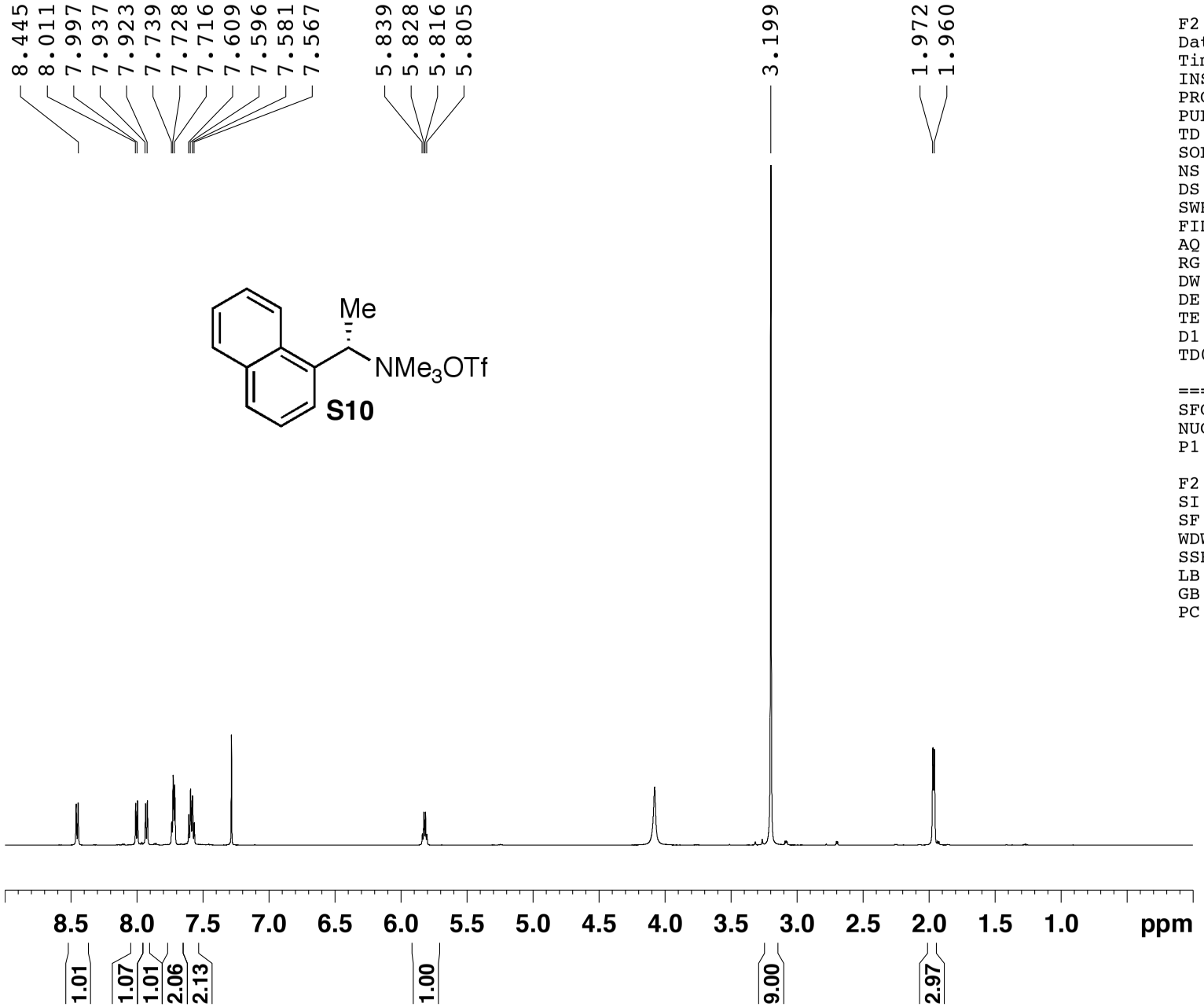

```
Current Data Parameters
NAME      DMM3-CNSI-SALT13
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120803
Time                 18.53
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                      16
DS                       4
SWH           133928.578 Hz
FIDRES          1.021794 Hz
AQ             0.4893855 sec
RG                     362
DW                 3.733 usec
DE                 8.00 usec
TE                 300.2 K
D1            3.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1         564.8086803 MHz
NUC1                   19F
P1                 11.62 usec

F2 - Processing parameters
SI                   65536
SF           564.8651670 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.00
```

Compound **S10** 1HNMR



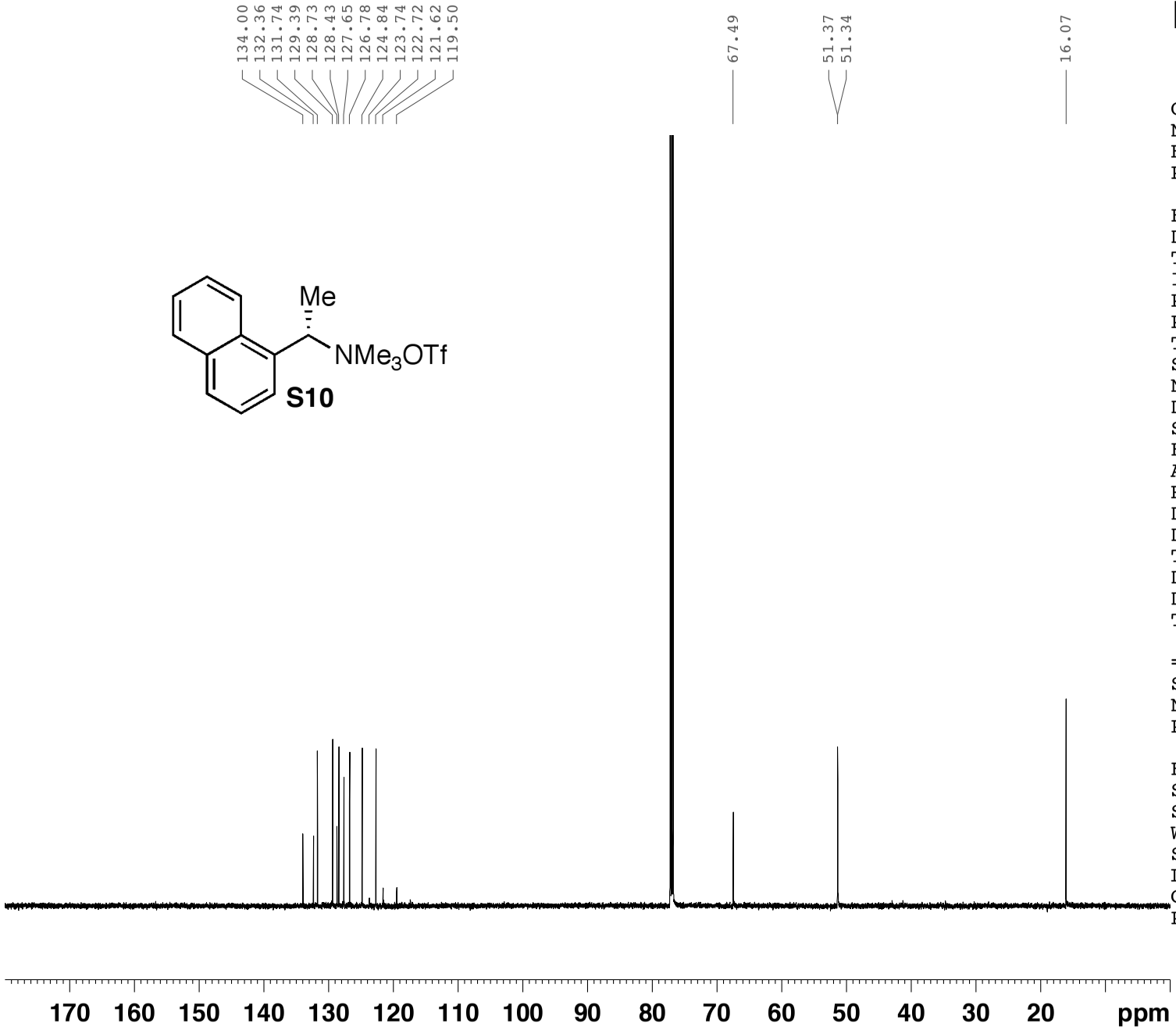

```
Current Data Parameters
NAME      DMM3-CNSI-SALT14
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120803
Time                 18.56
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8403.361 Hz
FIDRES            0.128225 Hz
AQ                3.8994420 sec
RG                     181
DW                  59.500 usec
DE                  17.39 usec
TE                  300.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          600.3233018 MHz
NUC1                    1H
P1                  10.77 usec

F2 - Processing parameters
SI                   65536
SF            600.3200000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

Compound **S10** 13CNMR



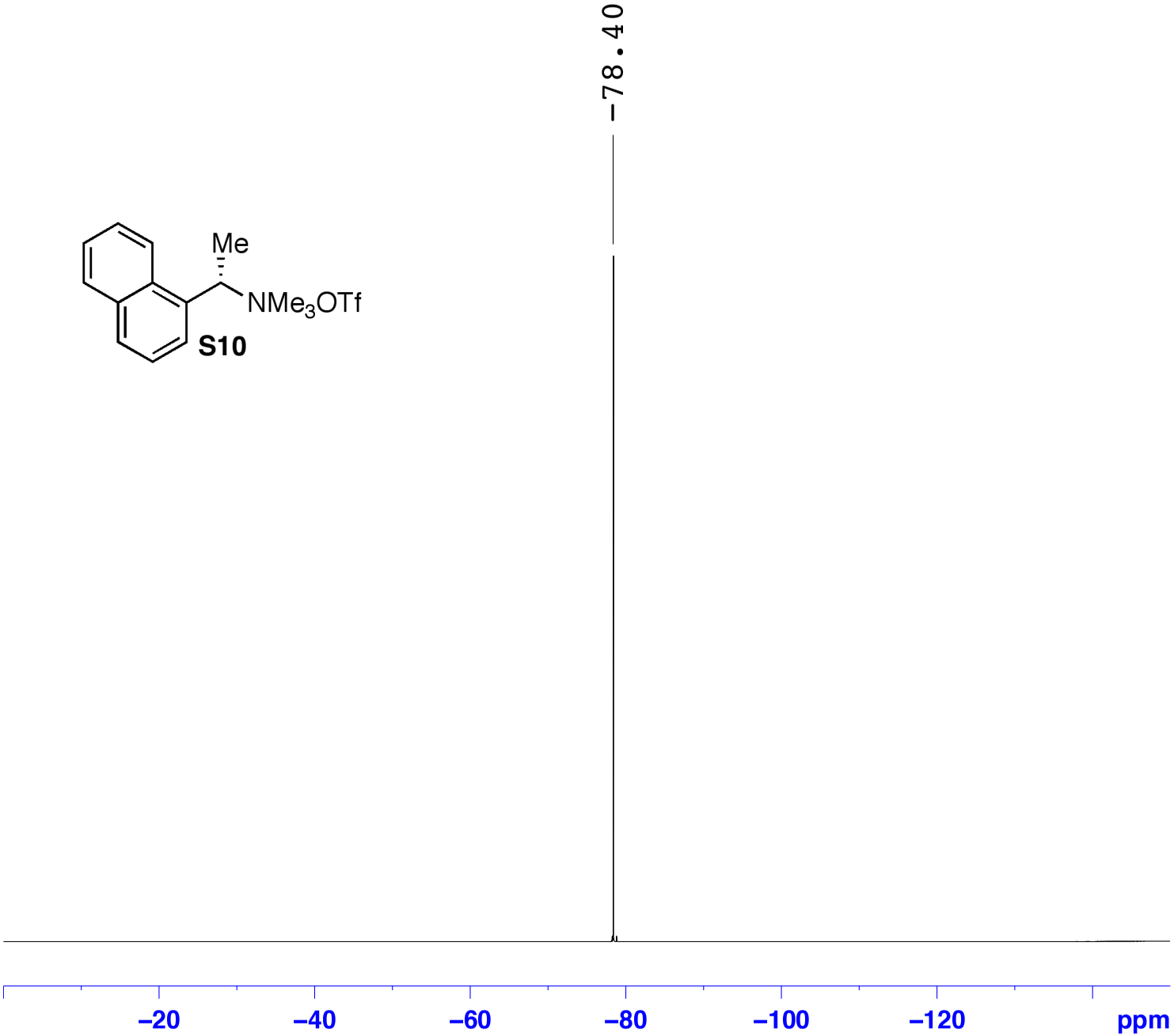
Current Data Parameters
NAME DMM3-CNSI-SALT-14C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120805
Time 8.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg55
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 2050
DW 14.400 usec
DE 19.34 usec
TE 300.2 K
D1 1.10000002 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 150.9656784 MHz
NUC1 13C
P1 10.63 usec

F2 - Processing parameters
SI 32768
SF 150.9505840 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound **S10** 19FNMR



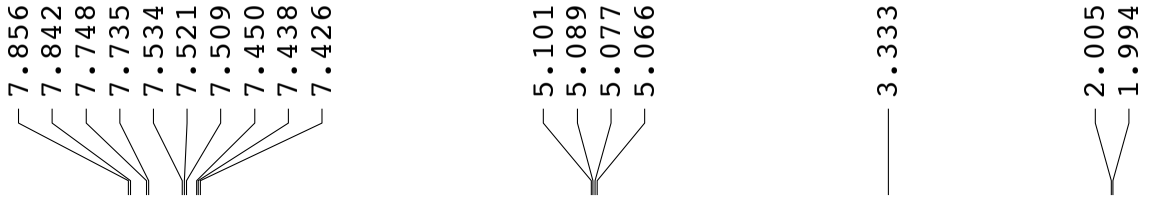

```
Current Data Parameters
NAME      DMM3-CNSI-SALT14
EXPNO                    3
PROCNO                   1

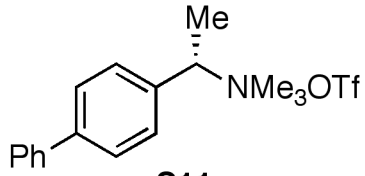
F2 - Acquisition Parameters
Date_           20120803
Time              19.09
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG        zgfhigqn
TD               131072
SOLVENT            CDCl3
NS                    16
DS                     4
SWH           133928.578 Hz
FIDRES          1.021794 Hz
AQ             0.4893855 sec
RG                   362
DW                 3.733 usec
DE                 8.00 usec
TE                300.2 K
D1           3.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        564.8086803 MHz
NUC1                19F
P1                11.62 usec

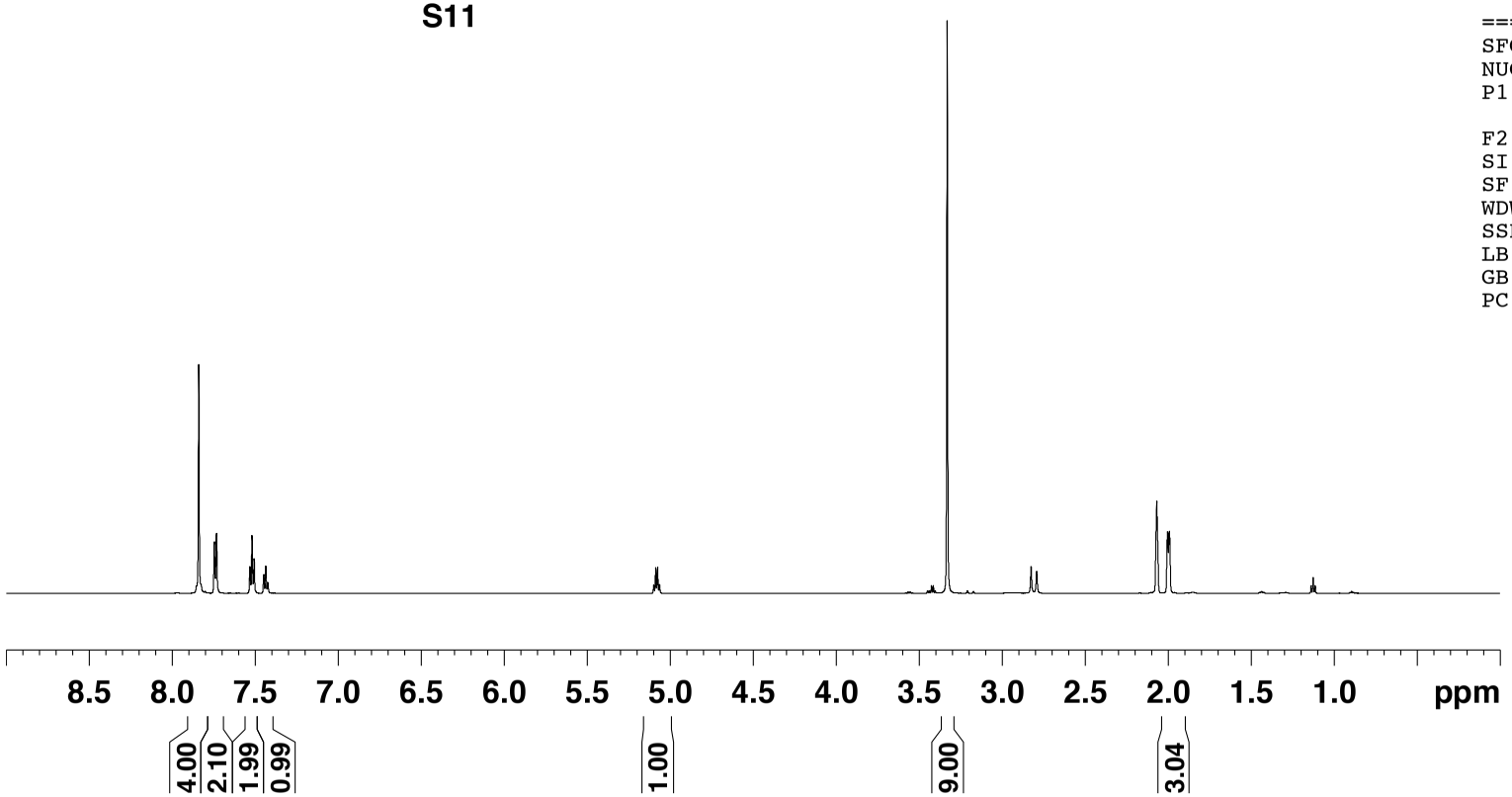
F2 - Processing parameters
SI                 65536
SF          564.8651670 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

Compound **S11** 1HNMR





S11



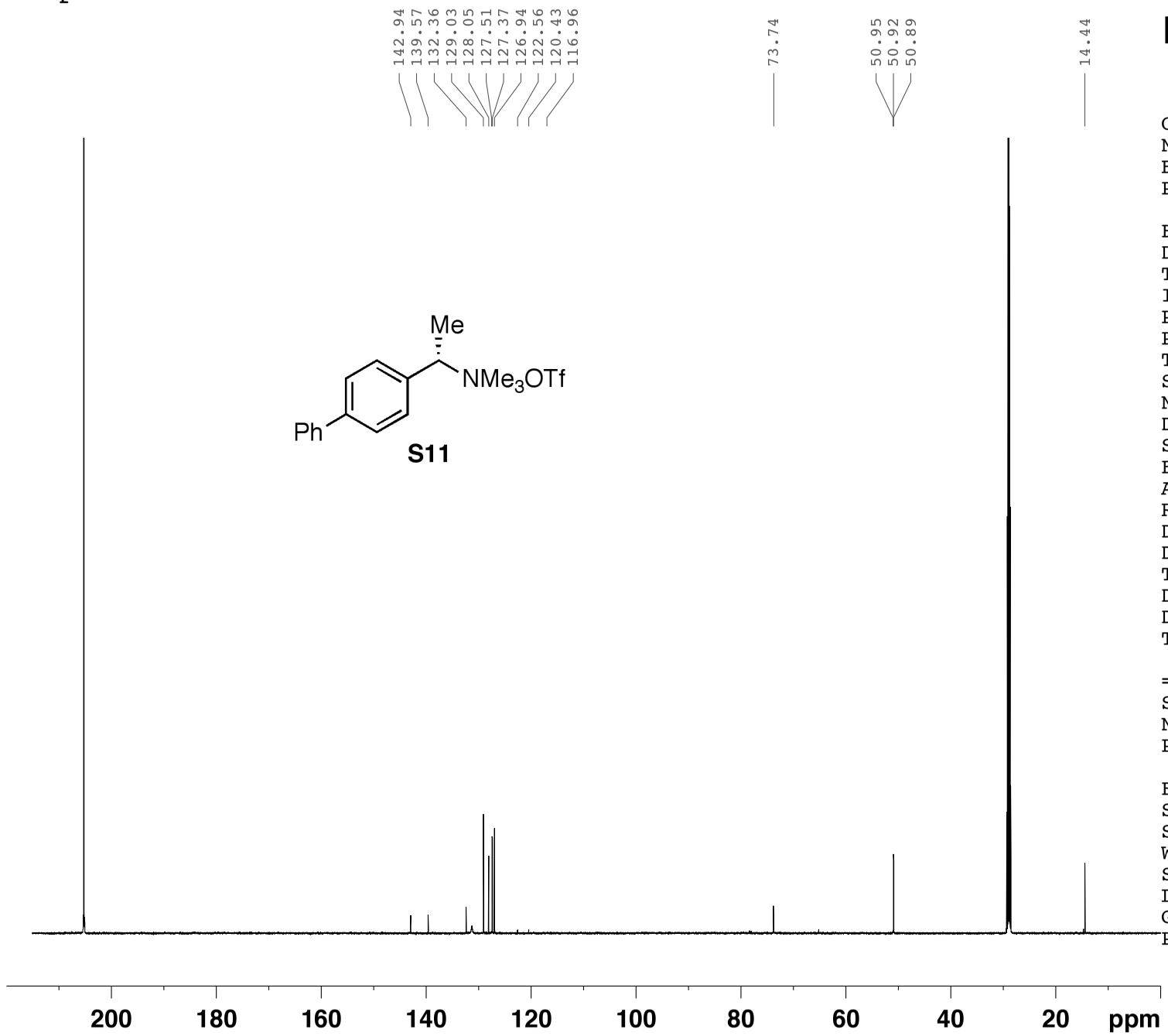

```
Current Data Parameters
NAME      DMM3-CNSI-SALT15-C2
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20120807
Time                 11.00
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT            Acetone
NS                       8
DS                       2
SWH               8403.361 Hz
FIDRES            0.128225 Hz
AQ                3.8994420 sec
RG                     161
DW                  59.500 usec
DE                  17.39 usec
TE                  300.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           600.3233018 MHz
NUC1                    1H
P1                   10.77 usec

F2 - Processing parameters
SI                     65536
SF             600.3200000 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

Compound **S11** 13CNMR




```
Current Data Parameters
NAME      DMM3-CNSI-SALT15-C2
EXPNO                      3
PROCNO                     1

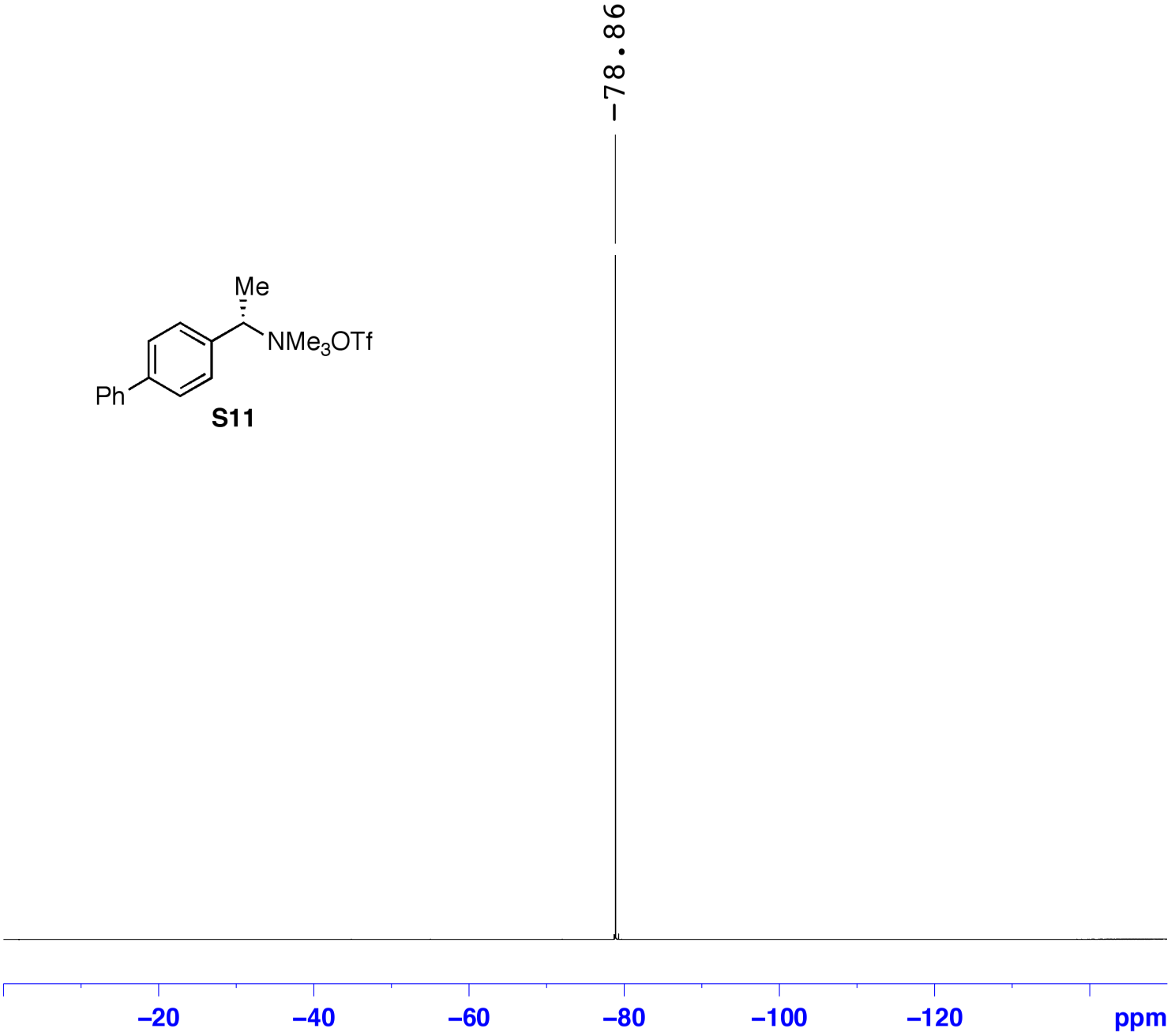
F2 - Acquisition Parameters
Date_              20120808
Time                  20.30
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg55
TD                    65536
SOLVENT             Acetone
NS                     2048
DS                        4
SWH              34722.223 Hz
FIDRES            0.529819 Hz
AQ                0.9437684 sec
RG                     2050
DW                   14.400 usec
DE                   19.34 usec
TE                   300.2 K
D1               1.10000002 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           150.9656784 MHz
NUC1                    13C
P1                   10.63 usec

F2 - Processing parameters
SI                    32768
SF             150.9505840 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

Compound **S11** 19FNMR

S11



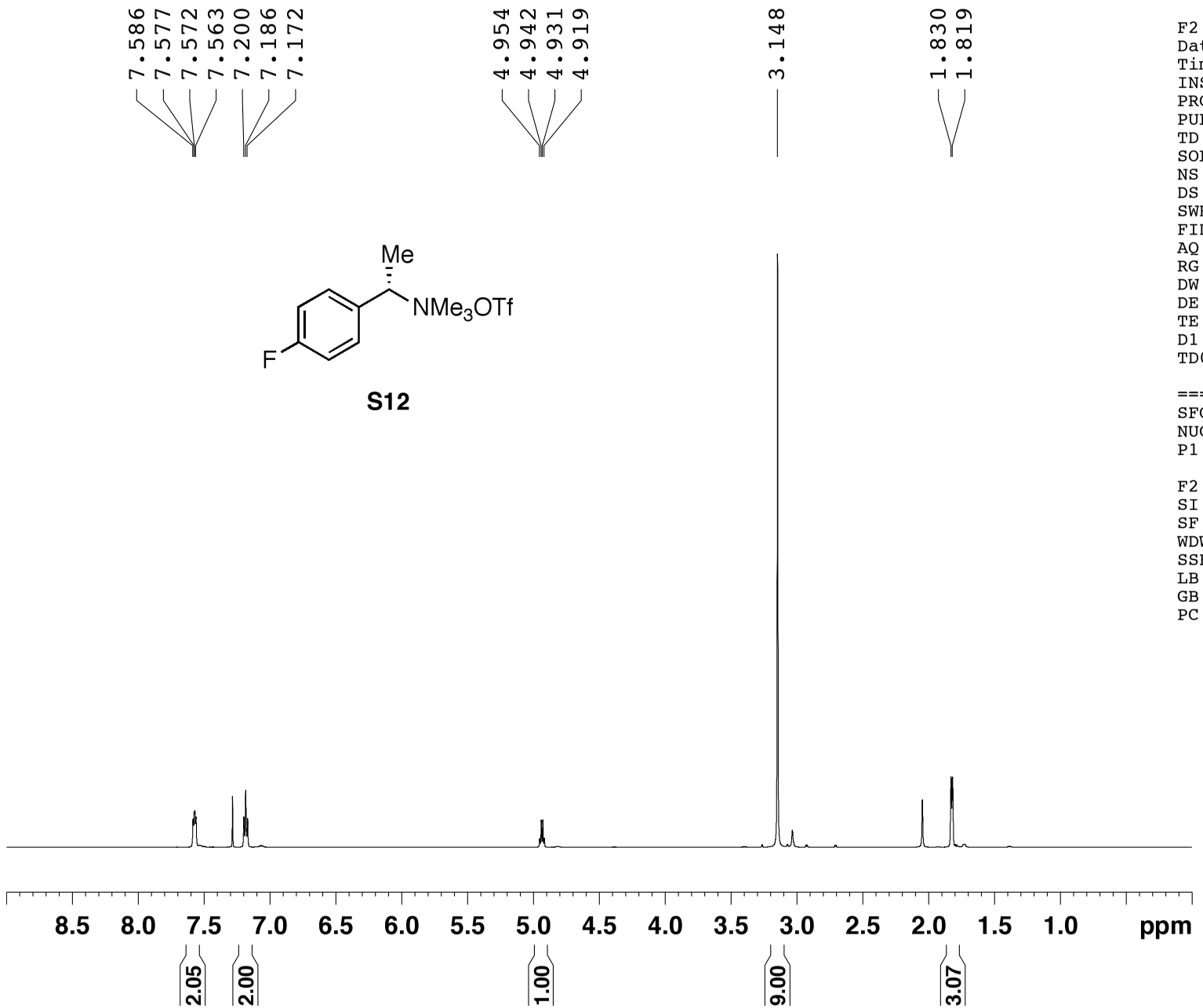

```
Current Data Parameters
NAME      DMM3-CNSI-SALT15-C2
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_            20120807
Time                11.02
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgfhigqn
TD                 131072
SOLVENT           Acetone
NS                      16
DS                       4
SWH             133928.578 Hz
FIDRES            1.021794 Hz
AQ               0.4893855 sec
RG                     456
DW                   3.733 usec
DE                    8.00 usec
TE                   300.2 K
D1              3.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          564.8086803 MHz
NUC1                   19F
P1                   11.62 usec

F2 - Processing parameters
SI                    65536
SF            564.8651670 MHz
WDW                      EM
SSB                       0
LB                     2.00 Hz
GB                        0
PC                     1.00
```

Compound **S12** 1HNMR



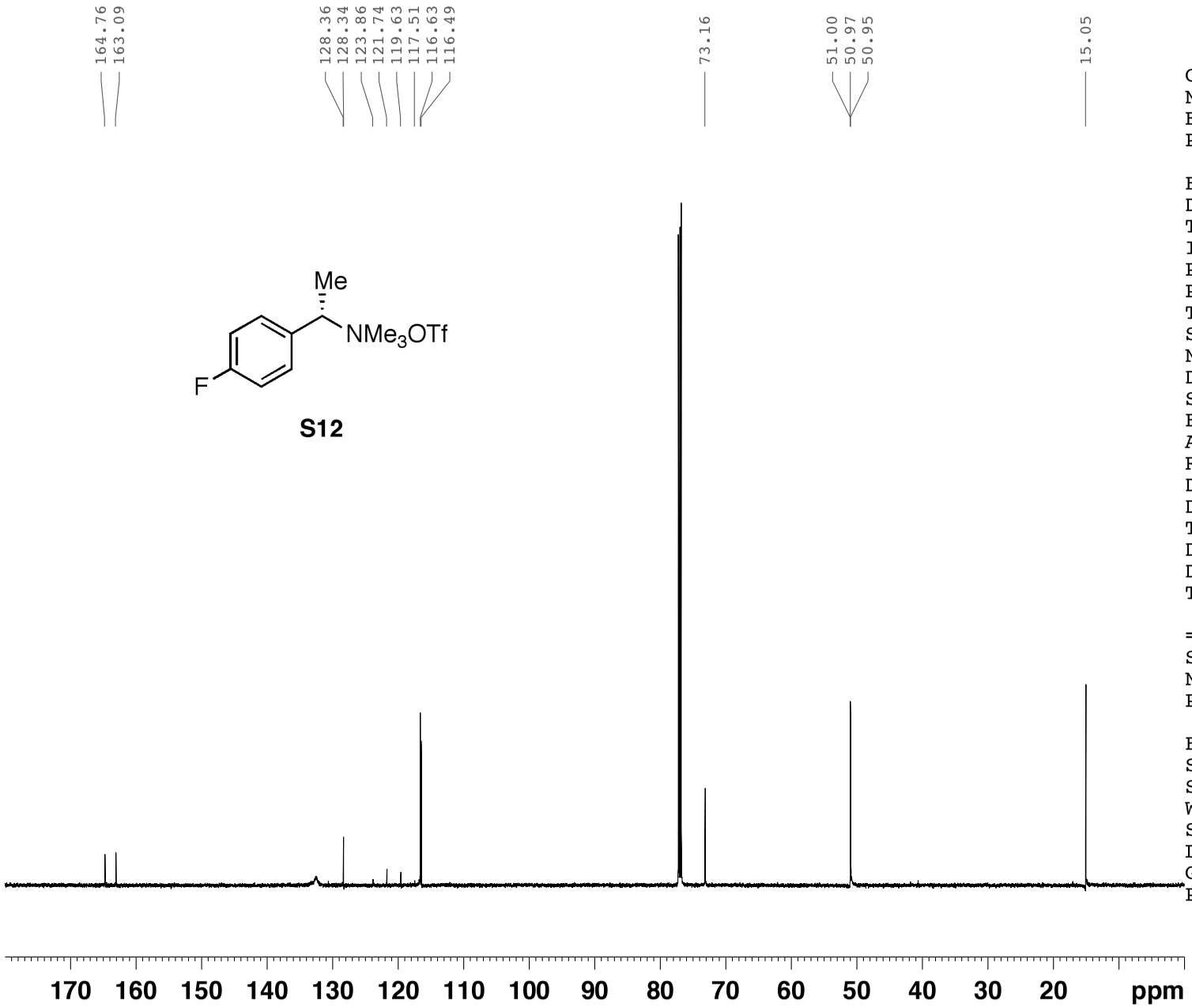

```
Current Data Parameters
NAME      DMM3-CNSI-SALT16
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120803
Time                19.29
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8403.361 Hz
FIDRES           0.128225 Hz
AQ               3.8994420 sec
RG                    161
DW                 59.500 usec
DE                 17.39 usec
TE                 300.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          600.3233018 MHz
NUC1                    1H
P1                  10.77 usec

F2 - Processing parameters
SI                    65536
SF            600.3200000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

Compound **S12** 13CNMR



S171

Current Data Parameters
NAME DMM3-CNSI-SALT-16C
EXPNO 1
PROCNO 1

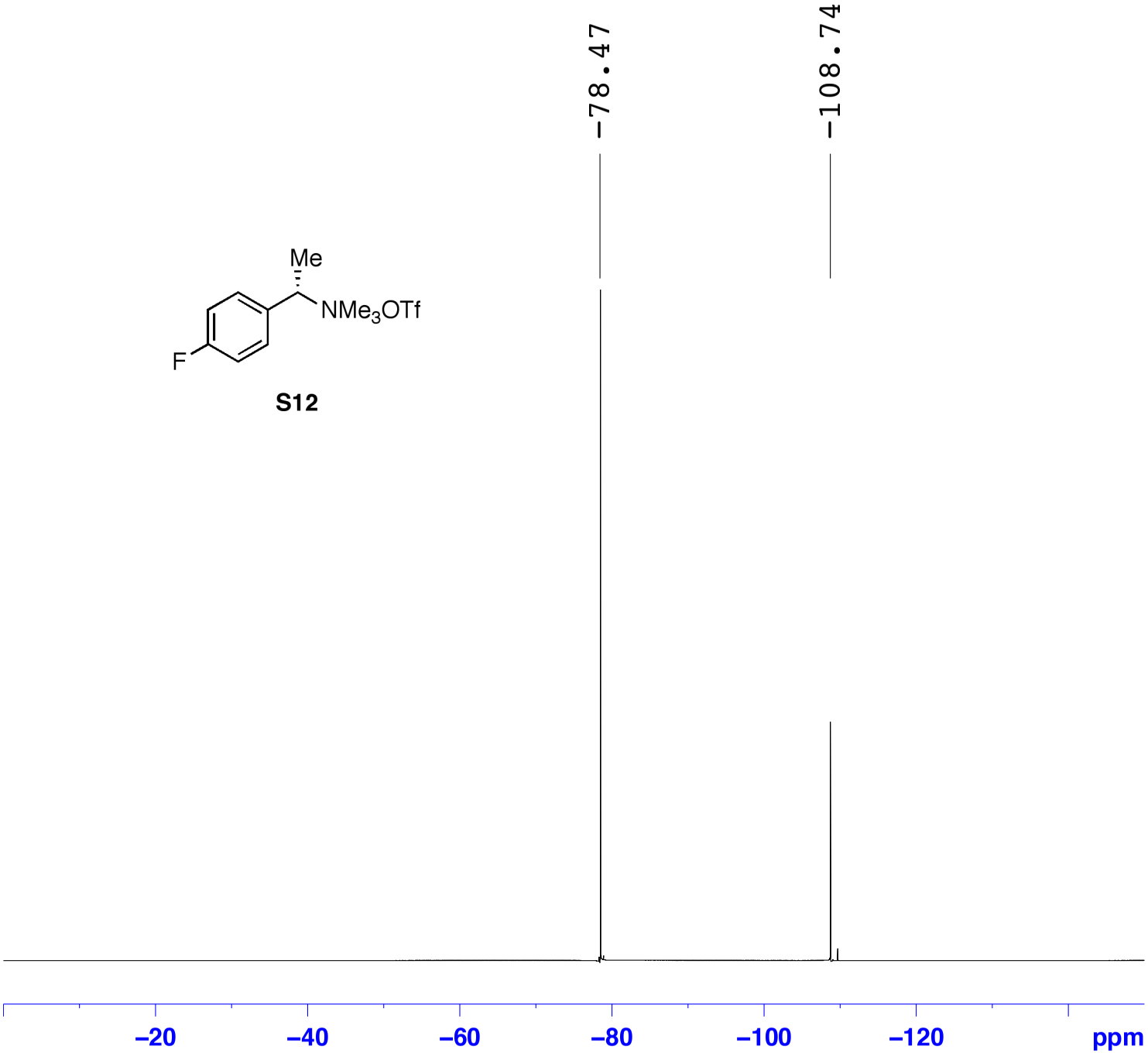
F2 - Acquisition Parameters
Date_ 20120805
Time 9.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg55
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 2050
DW 14.400 usec
DE 19.34 usec
TE 300.2 K
D1 1.10000002 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 150.9656784 MHz
NUC1 13C
P1 10.63 usec

F2 - Processing parameters
SI 32768
SF 150.9505840 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound **S12** 19FNMR

S12



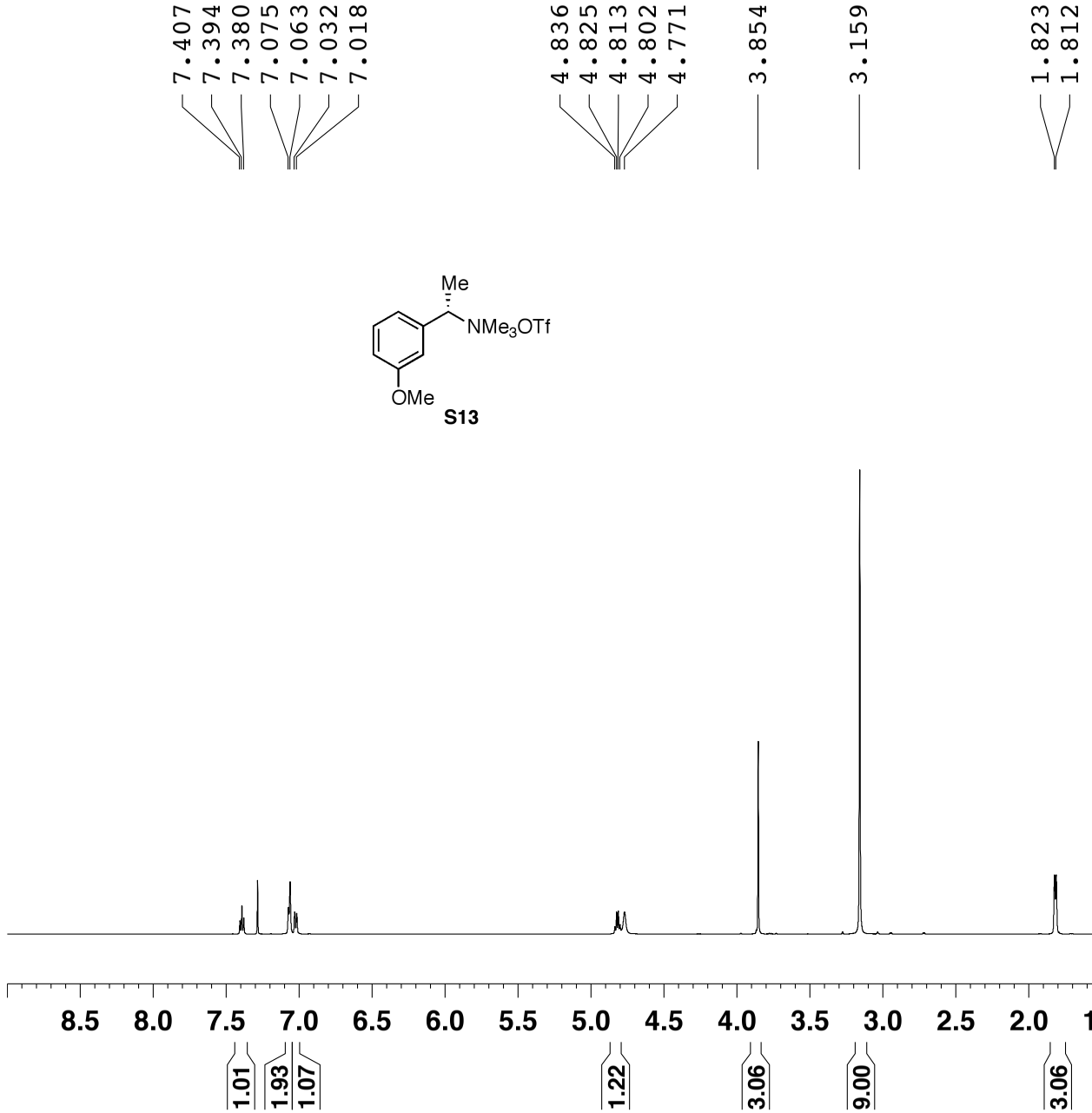

```
Current Data Parameters
NAME      DMM3-CNSI-SALT16
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120803
Time                 19.42
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                      16
DS                       4
SWH             133928.578 Hz
FIDRES            1.021794 Hz
AQ                0.4893855 sec
RG                     362
DW                   3.733 usec
DE                    8.00 usec
TE                   300.2 K
D1              3.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          564.8086803 MHz
NUC1                   19F
P1                   11.62 usec

F2 - Processing parameters
SI                   65536
SF            564.8651670 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.00
```

Comound **S13** 1HNMR



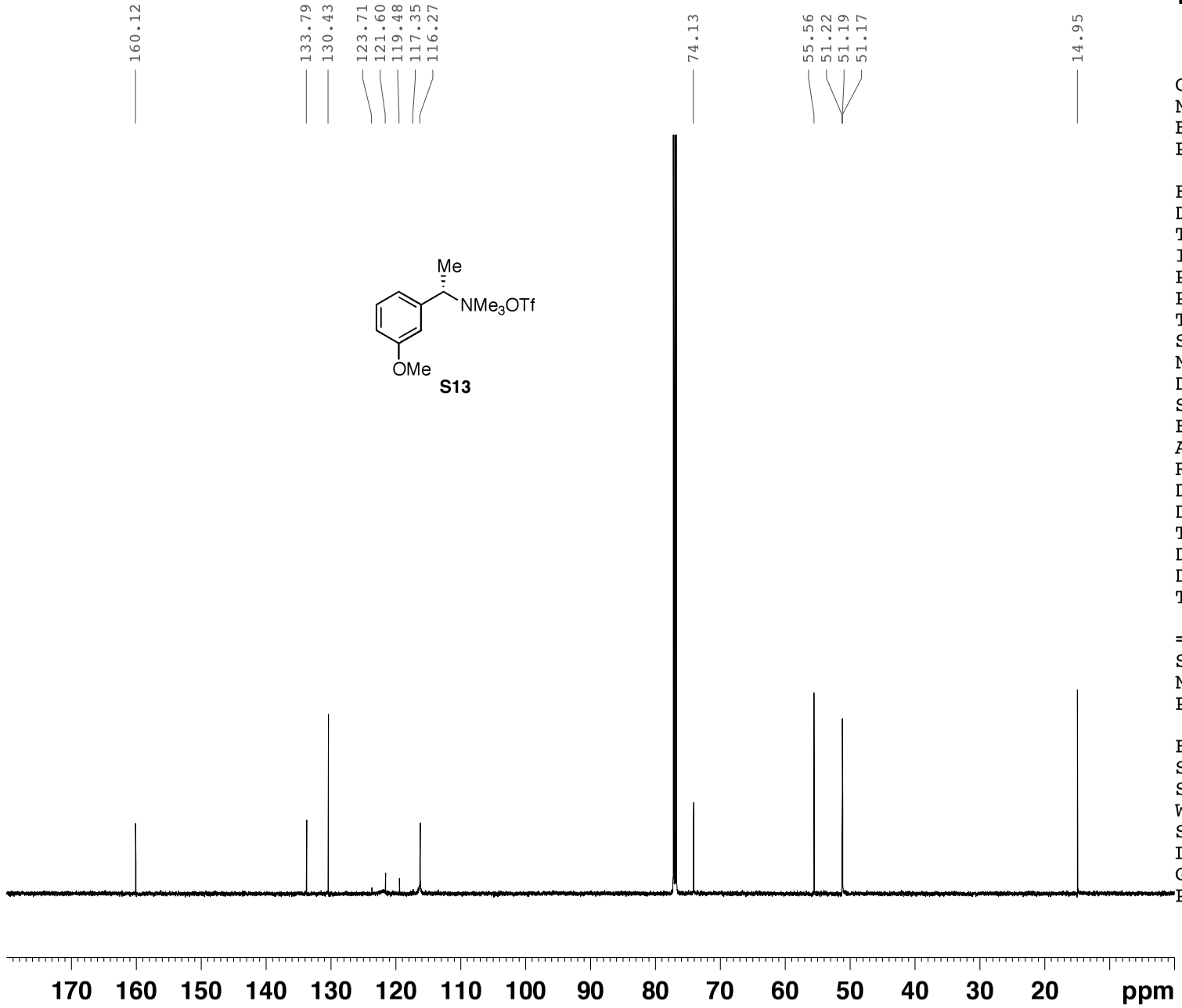

```
Current Data Parameters
NAME      DMM3-CNSI-SALT17
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120803
Time                 19.45
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8403.361 Hz
FIDRES            0.128225 Hz
AQ                3.8994420 sec
RG                     161
DW                  59.500 usec
DE                  17.39 usec
TE                  300.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          600.3233018 MHz
NUC1                    1H
P1                  10.77 usec

F2 - Processing parameters
SI                   65536
SF            600.3200000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

Compound **S13** 13CNMR



Current Data Parameters

NAME	DMM3-CNSI-SALT-17C
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120805
Time	10.57
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg55
TD	65536
SOLVENT	CDCl3
NS	2048
DS	4
SWH	34722.223 Hz
FIDRES	0.529819 Hz
AQ	0.9437684 sec
RG	2050
DW	14.400 usec
DE	19.34 usec
TE	300.2 K
D1	1.10000002 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========

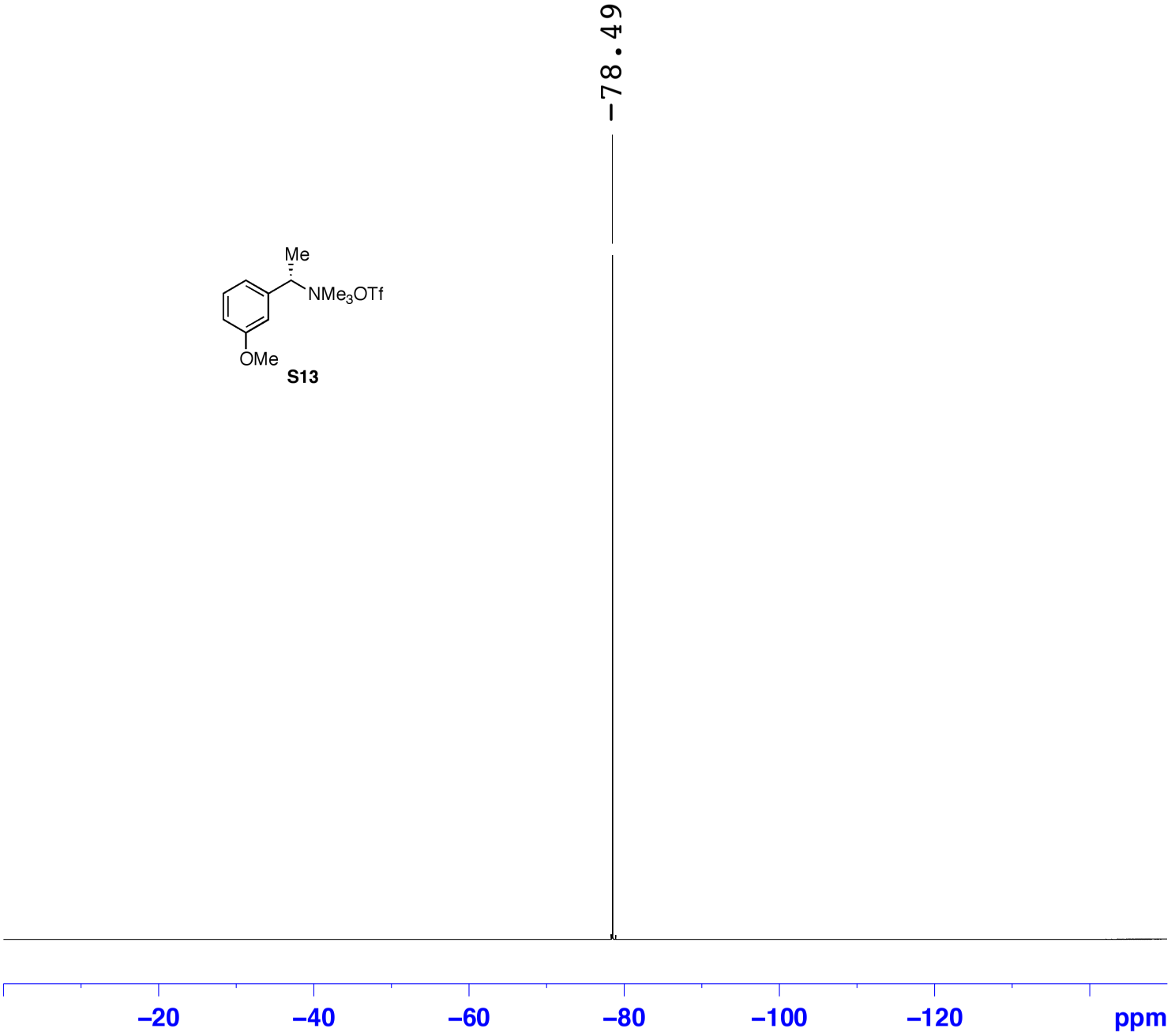
SFO1	150.9656784 MHz
NUC1	13C
P1	10.63 usec

F2 - Processing parameters

SI	32768
SF	150.9505840 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Compound **S13** 19FNMR

S13



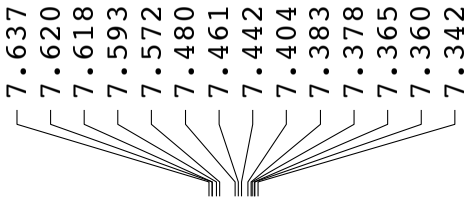

```
Current Data Parameters
NAME      DMM3-CNSI-SALT17
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120803
Time                 19.58
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                      16
DS                       4
SWH             133928.578 Hz
FIDRES            1.021794 Hz
AQ                0.4893855 sec
RG                     362
DW                   3.733 usec
DE                   8.00 usec
TE                  300.2 K
D1             3.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0                      1

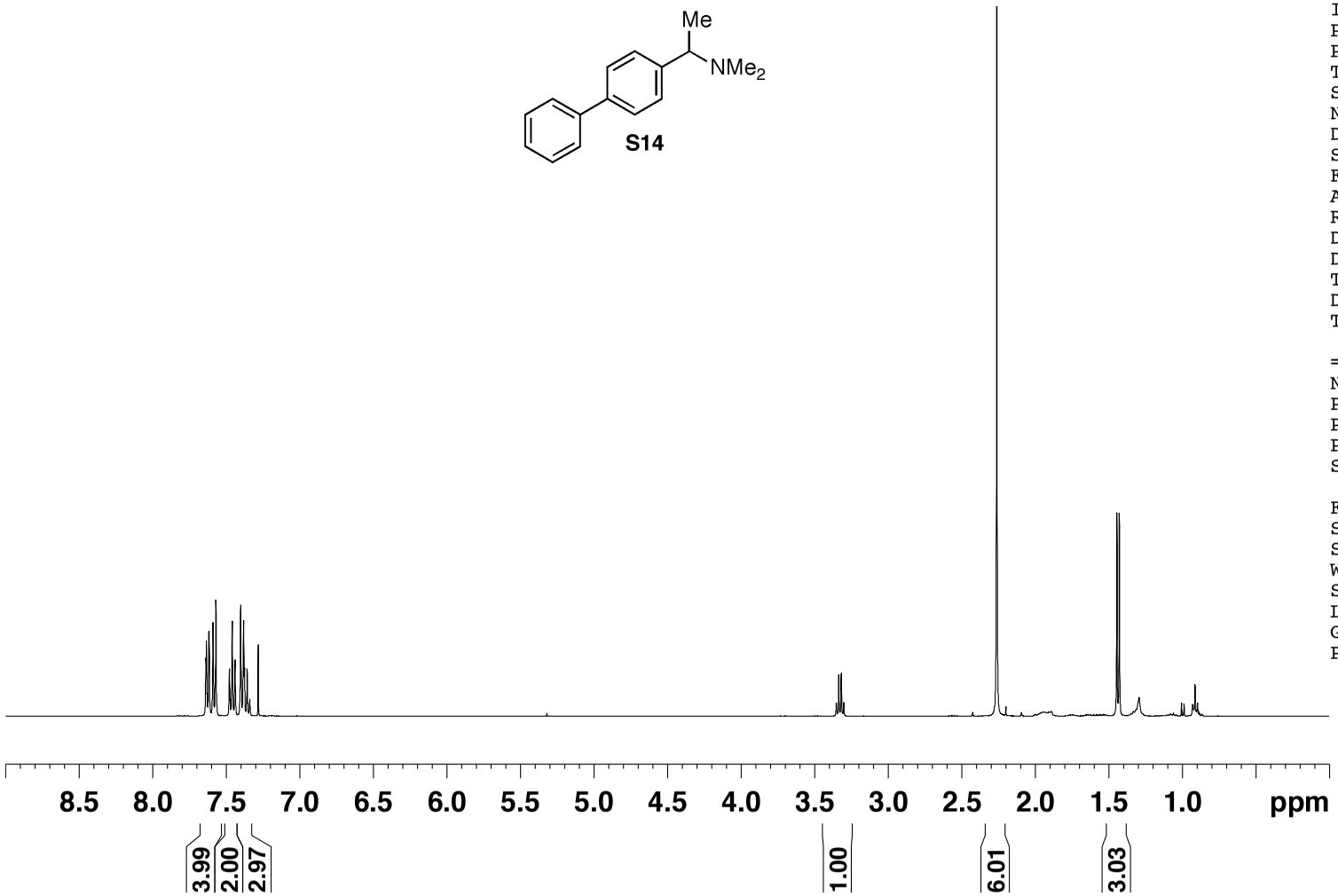
======== CHANNEL f1 ========
SFO1          564.8086803 MHz
NUC1                   19F
P1                   11.62 usec

F2 - Processing parameters
SI                   65536
SF            564.8651670 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.00
```

Compound, S-14, 1HNMR



S14



BRUKER

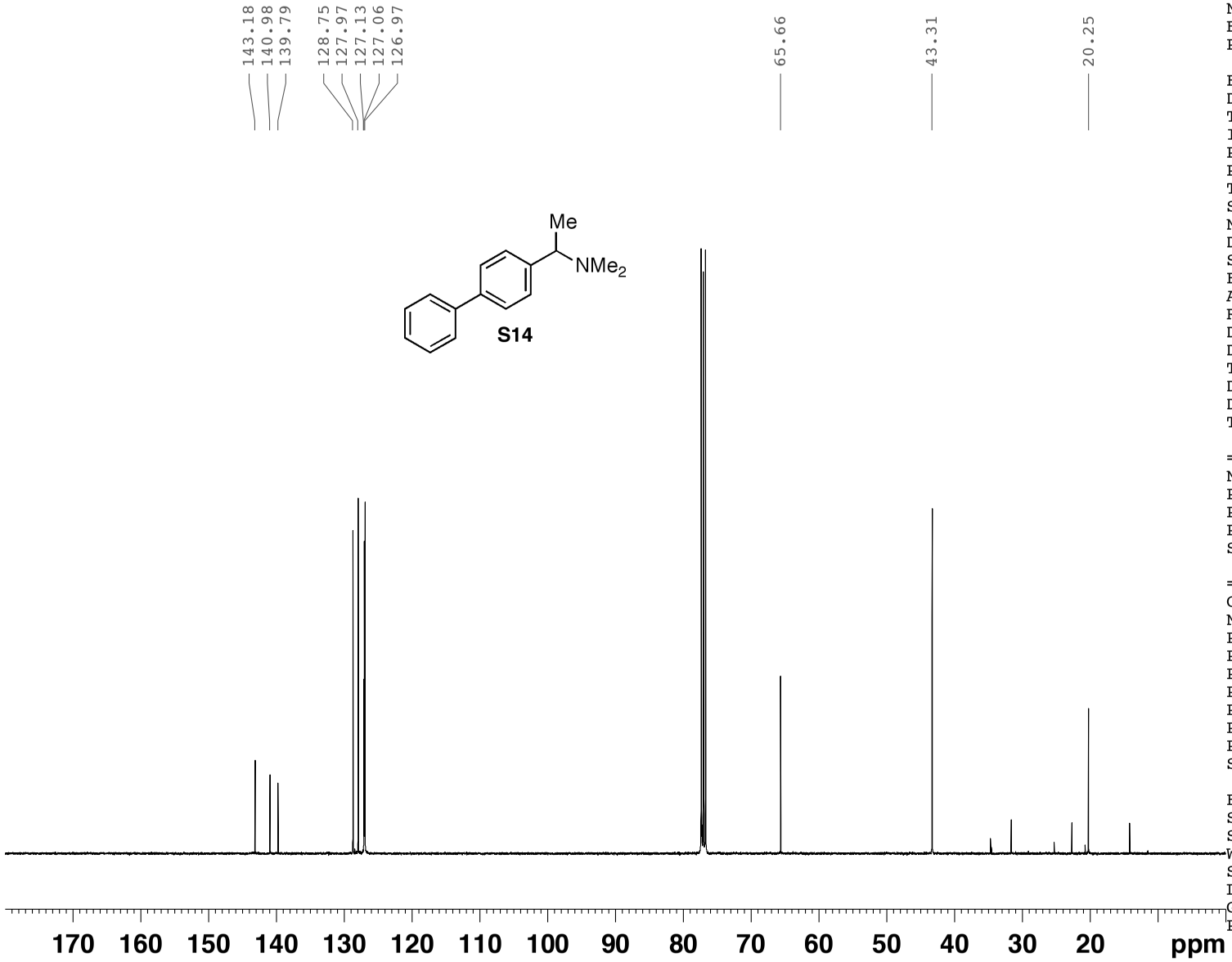

```
Current Data Parameters
NAME                  PM-4-12
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20120628
Time                    13.19
INSTRUM                 spect
PROBHD    5 mm CPQNP 1H/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8278.146 Hz
FIDRES               0.126314 Hz
AQ                   3.9584243 sec
RG                       10.1
DW                     60.400 usec
DE                      6.00 usec
TE                     298.2 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     15.00 usec
PL1                     4.90 dB
PL1W              3.30822015 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                      32768
SF              400.1300000 MHz
WDW                        EM
SSB                         0
LB                     0.30 Hz
GB                          0
PC                      1.00
```

Compound S-14, 13CNMR



Current Data Parameters
NAME PM-4-12
EXPNO 2
PROCNO 1

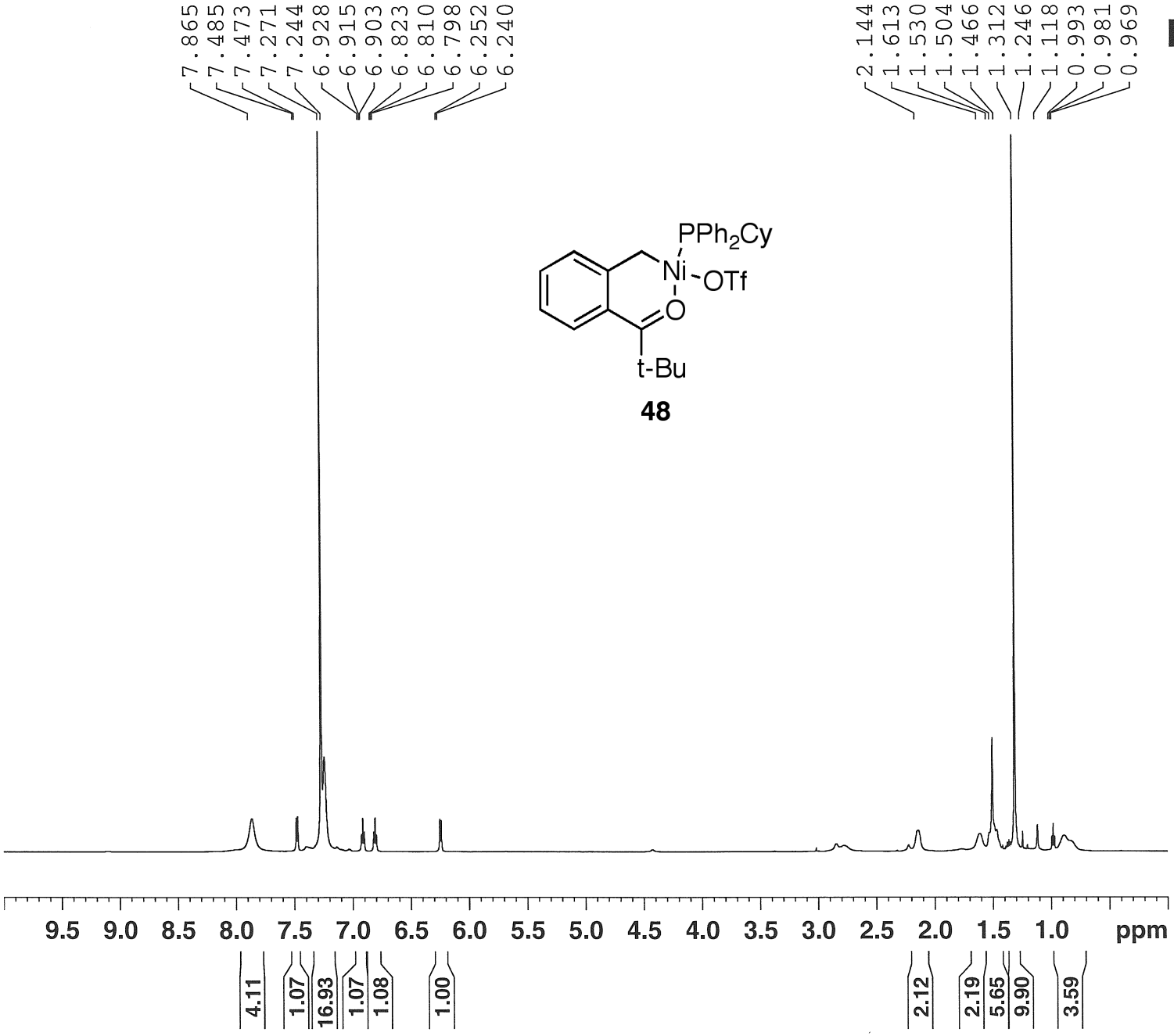
F2 - Acquisition Parameters
Date_ 20120628
Time 22.36
INSTRUM spect
PROBHD 5 mm CPQNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 512
DW 20.850 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PL1 0.55 dB
PL1W 35.18820572 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 4.90 dB
PL12 20.46 dB
PL13 21.00 dB
PL2W 3.30822015 W
PL12W 0.09195905 W
PL13W 0.08120718 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound **48**, 1H NMR

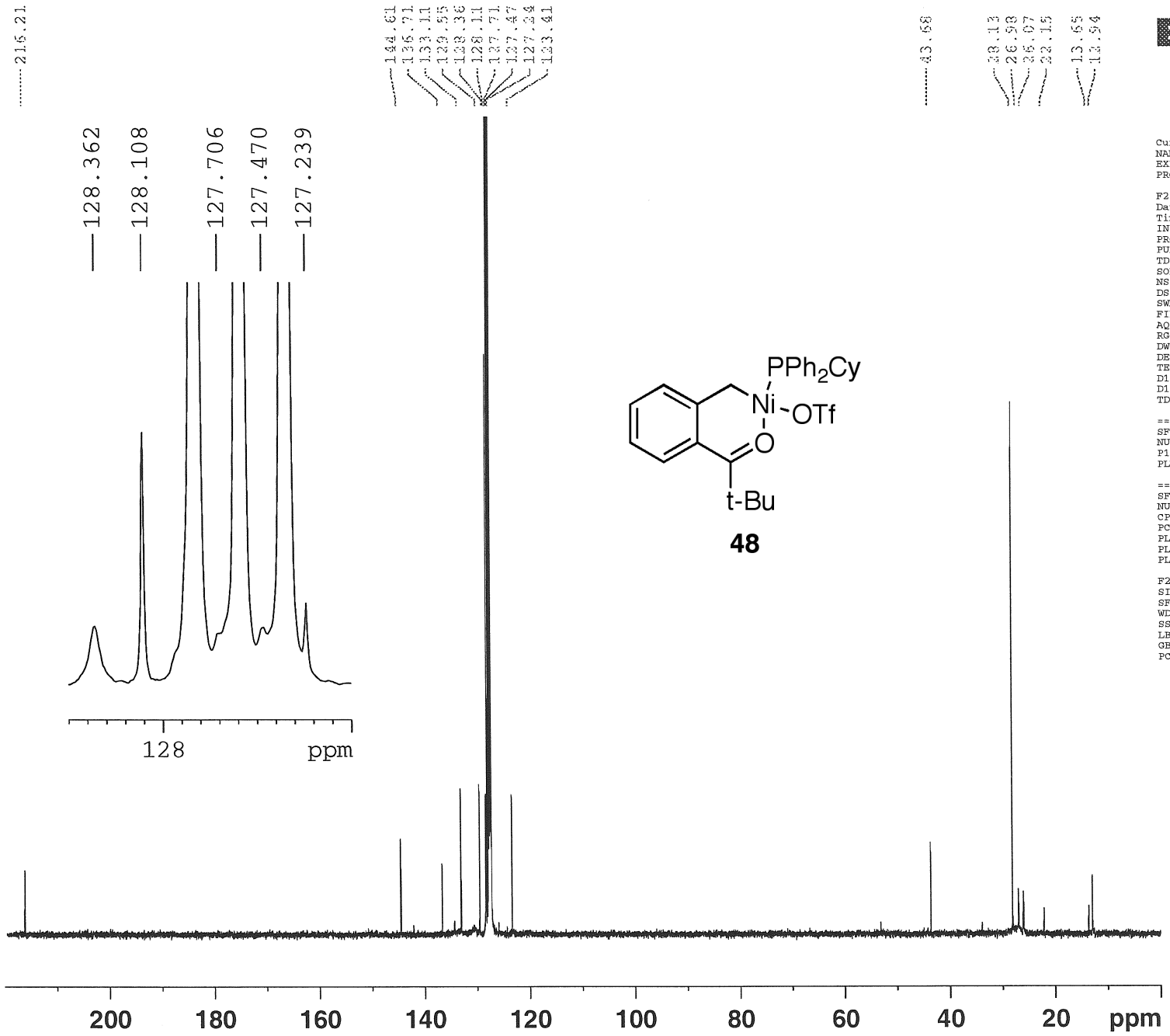


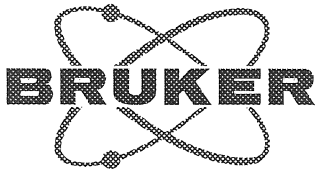
BRUKER

S178

NAME	first
EXPNO	1
PROCNO	1
Date_	20120831
Time	10.36
INSTRUM	spect
PROBHD	5 mm PATXI 1H/
PULPROG	zg30
TD	65536
SOLVENT	C6D6
NS	16
DS	2
SWH	12376.237 Hz
FIDRES	0.188846 Hz
AQ	2.6477449 sec
RG	35.9
DW	40.400 use
DE	6.50 use
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
NUC1	1H
P1	9.90 use
PL1	0.00 dB
PL1W	14.97084332 W
SFO1	600.1337060 MHz
SI	32768
SF	600.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

Compound **48**, 13C NMR





S179

```
Current Data Parameters
NAME      DMM3-PM-Nickel complex benzyl amine derivative-c
EXPNO                 1
PROCNO                1

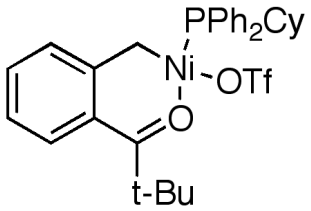
F2 - Acquisition Parameters
Date_          20120829
Time              19.22
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT            C6D6
NS                  999
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                  203
DW               20.800 usec
DE               22.82 usec
TE               333.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6278593 MHz
NUC1               13C
P1               10.00 usec
PLW1        43.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        10.00000000 W
PLW12        0.27042001 W
PLW13        0.21904001 W

F2 - Processing parameters
SI                32768
SF          100.6177980 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

Compound **48**, 19F NMR



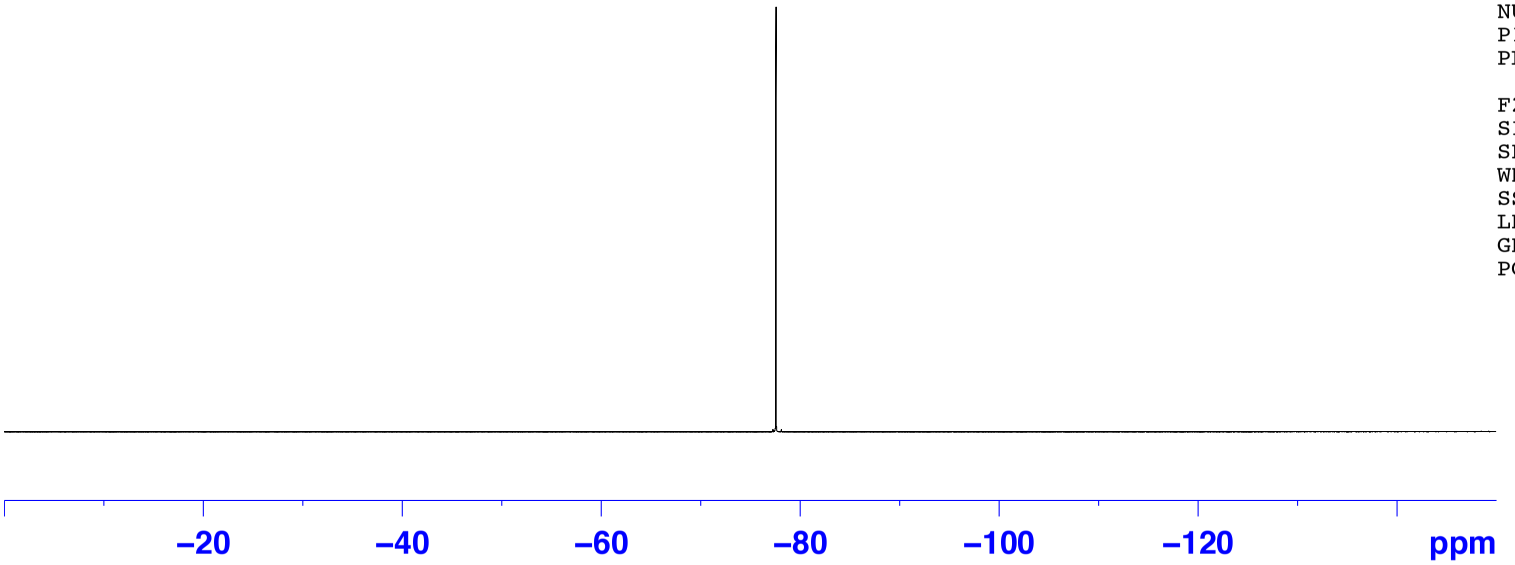
48


```
Current Data Parameters
NAME        PM-3-279-1-F
EXPNO                  3
PROCNO                 1

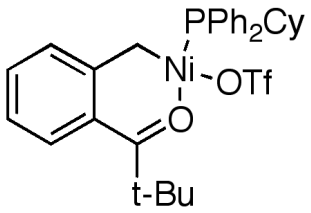
F2 - Acquisition Parameters
Date_           20120609
Time              17.04
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD               131072
SOLVENT            C6D6
NS                   16
DS                    4
SWH           89285.711 Hz
FIDRES         0.681196 Hz
AQ            0.7340032 sec
RG                  203
DW                5.600 usec
DE               10.00 usec
TE                300.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        376.4795333 MHz
NUC1               19F
P1               15.00 usec
PLW1        13.50000000 W

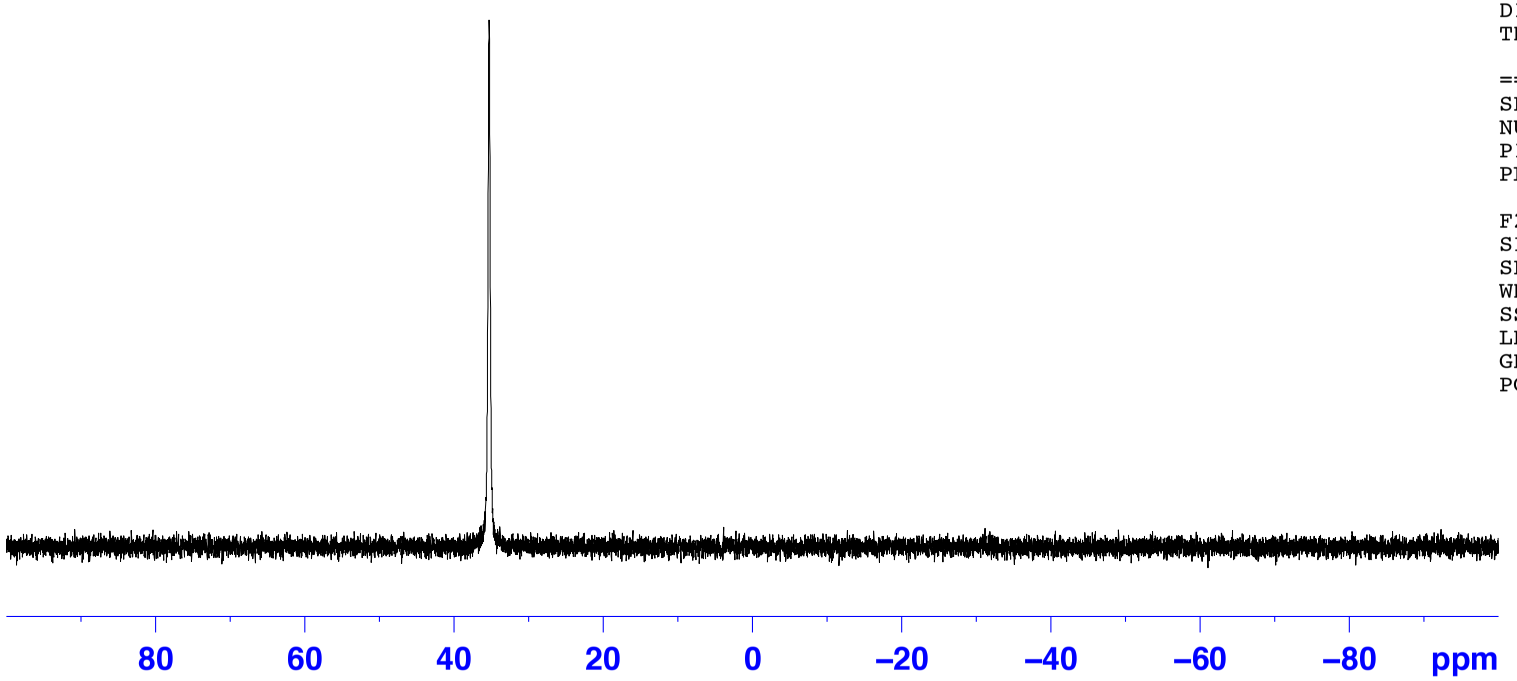
F2 - Processing parameters
SI                65536
SF          376.5171850 MHz
WDW                EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.00
```



Compound **48**, 31P NMR



48



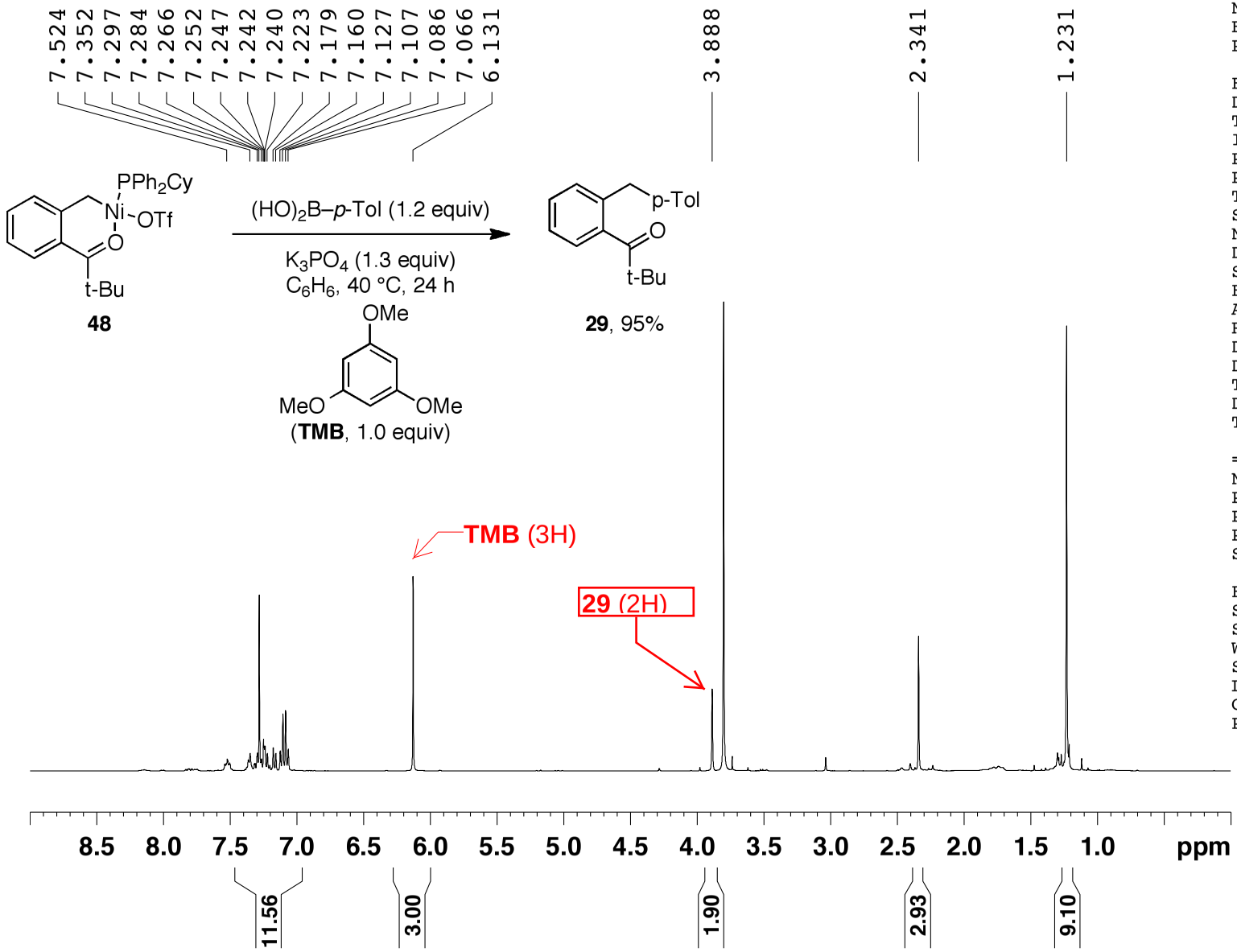

```
Current Data Parameters
NAME        PM-3-279-1-P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120609
Time              16.51
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT            C6D6
NS                   32
DS                    4
SWH           64102.562 Hz
FIDRES         0.978127 Hz
AQ            0.5111808 sec
RG                  203
DW                7.800 usec
DE                6.50 usec
TE                300.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        161.9755899 MHz
NUC1               31P
P1                8.00 usec
PLW1        35.00000000 W

F2 - Processing parameters
SI                32768
SF          161.9836890 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Compound 29, 1HNMR with internal standard-1



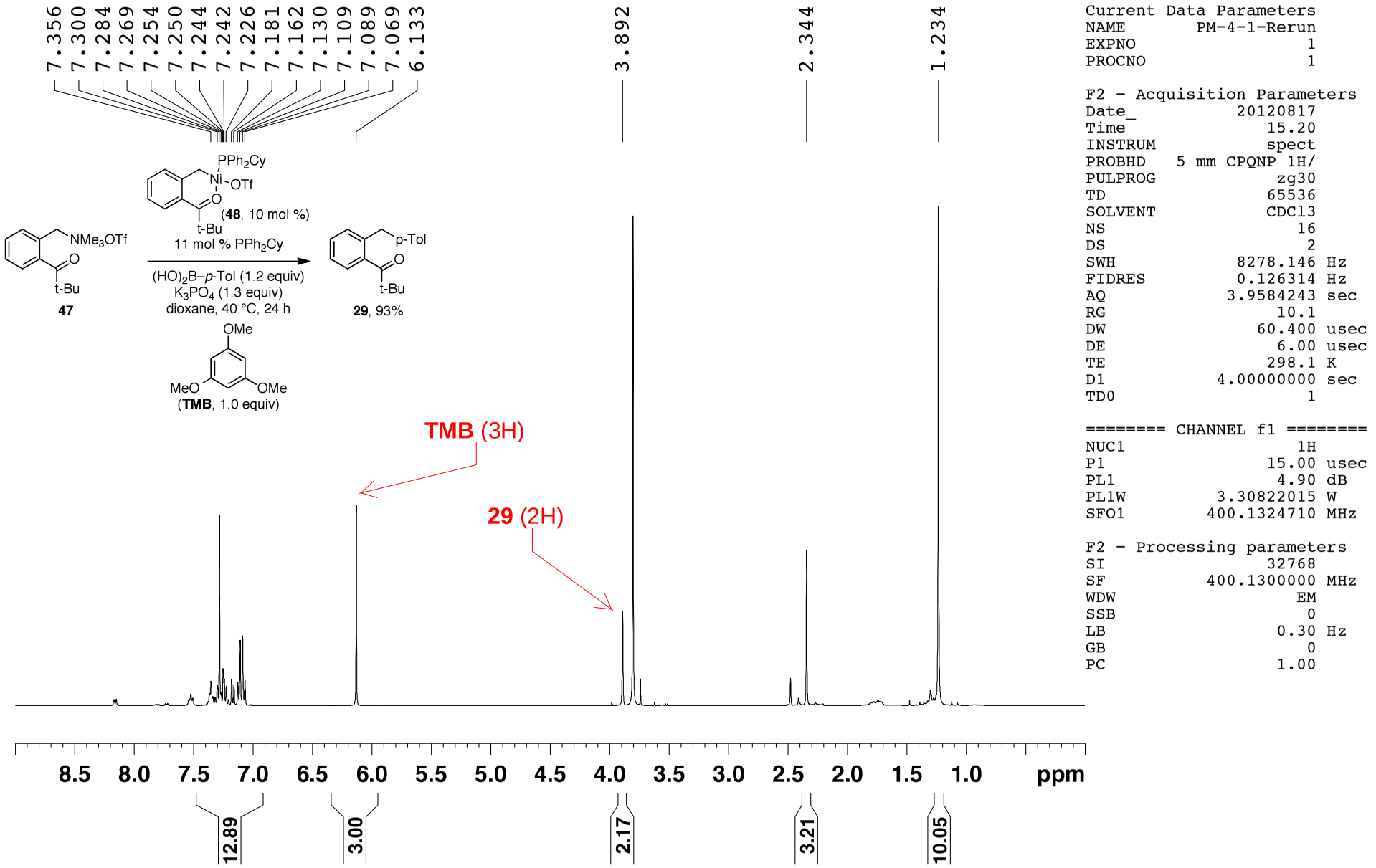

```
Current Data Parameters
NAME        PM-4-2-Rerun
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20120817
Time               15.27
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG                    9
DW               60.400 usec
DE                6.00 usec
TE                298.2 K
D1            4.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W          3.30822015 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                32768
SF           400.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

Compound 29, 1HNMR, with Internal Standard-2



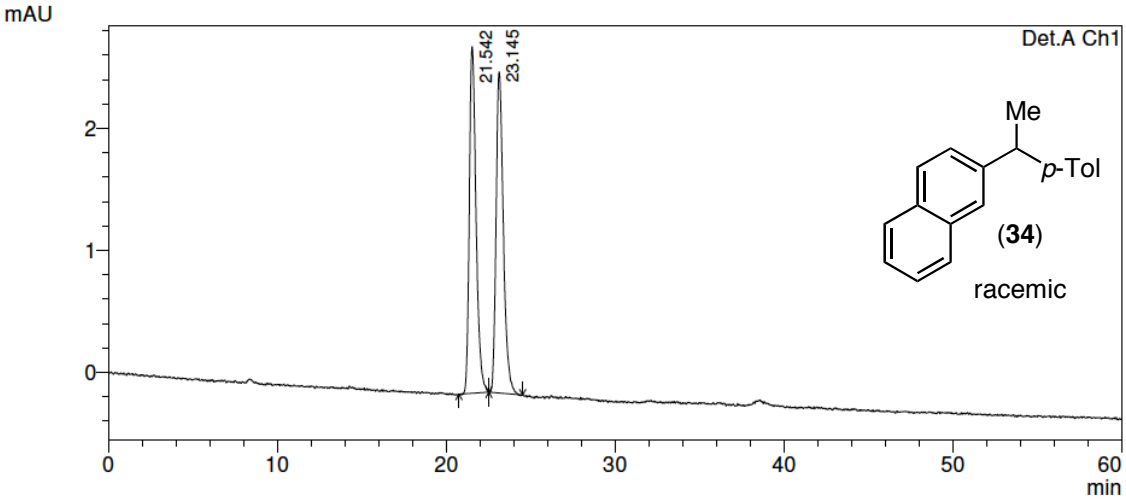

```
Current Data Parameters
NAME        PM-4-1-Rerun
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20120817
Time               15.20
INSTRUM            spect
PROBHD   5 mm CPQNP 1H/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                 10.1
DW                60.400 usec
DE                 6.00 usec
TE                298.1 K
D1             4.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                4.90 dB
PL1W          3.30822015 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                32768
SF           400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

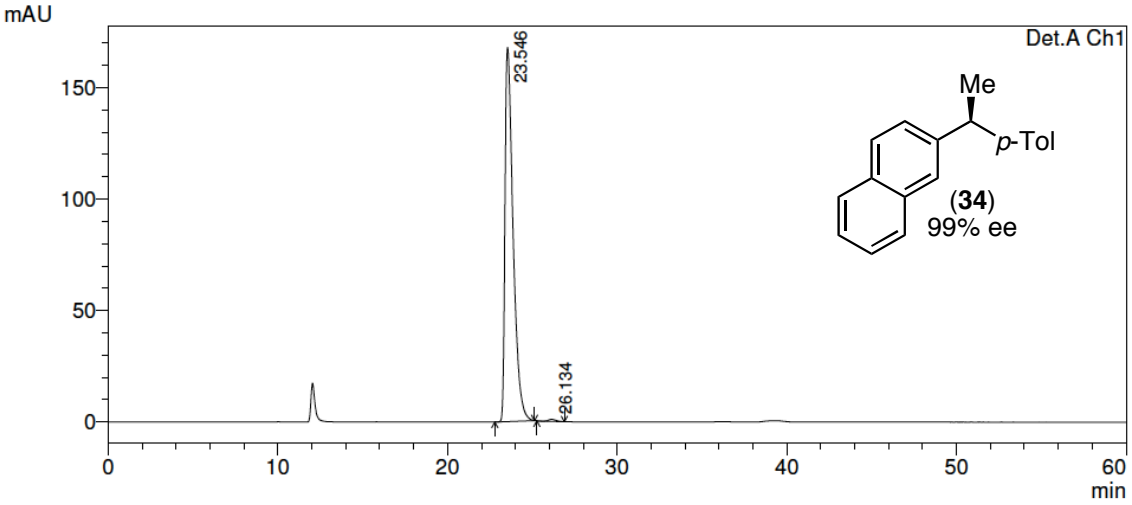
Compound 34, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.542	78839	2843	50.033	51.898
2	23.145	78735	2635	49.967	48.102
Total		157574	5478	100.000	100.000

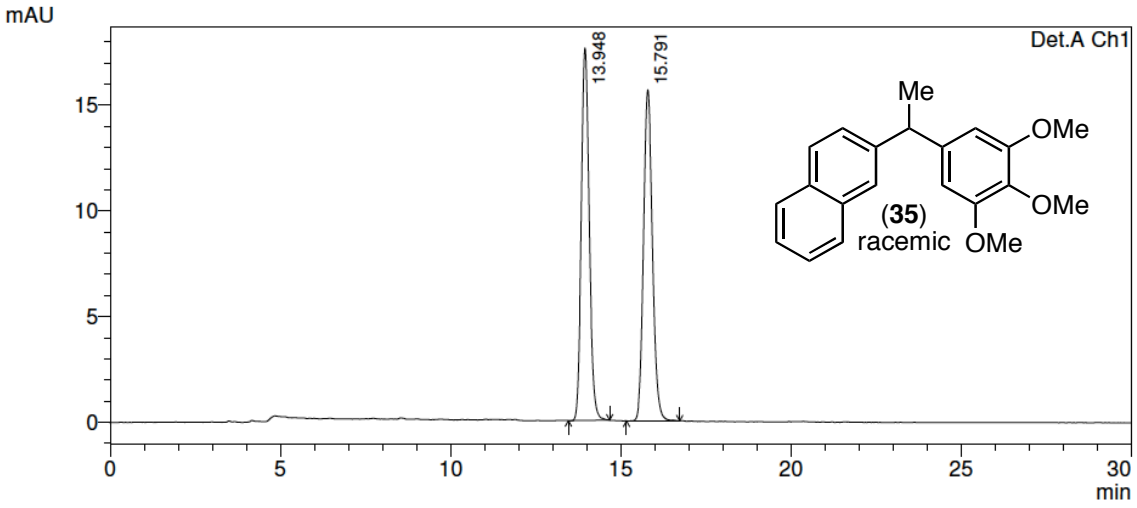
Compound 34, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.546	5566610	167841	99.555	99.426
2	26.134	24902	968	0.445	0.574
Total		5591512	168810	100.000	100.000

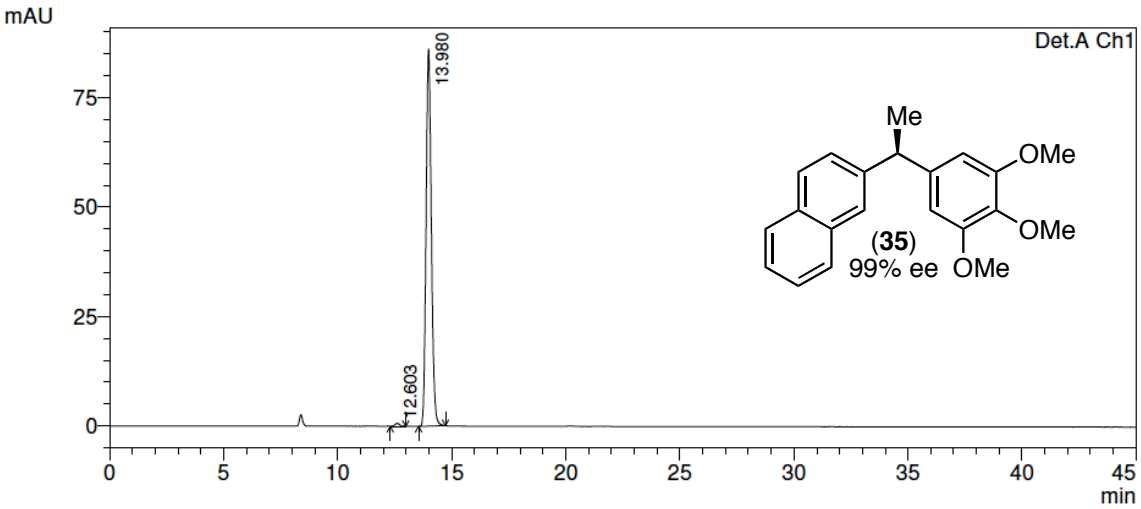
Compound 35, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.948	285216	17625	49.867	52.956
2	15.791	286735	15657	50.133	47.044
Total		571950	33282	100.000	100.000

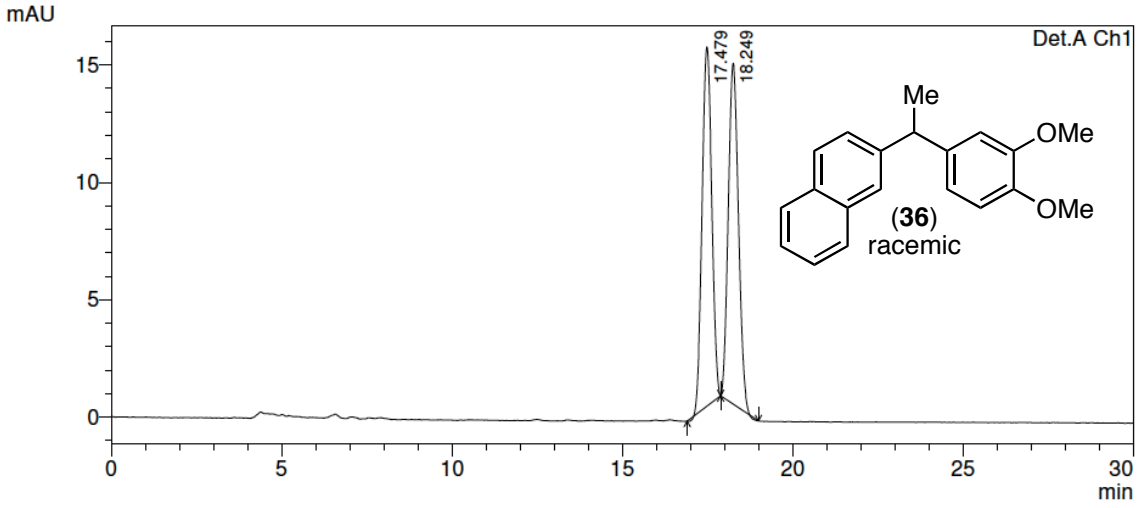
Compound 35, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.603	9624	673	0.691	0.776
2	13.980	1383627	86096	99.309	99.224
Total		1393251	86769	100.000	100.000

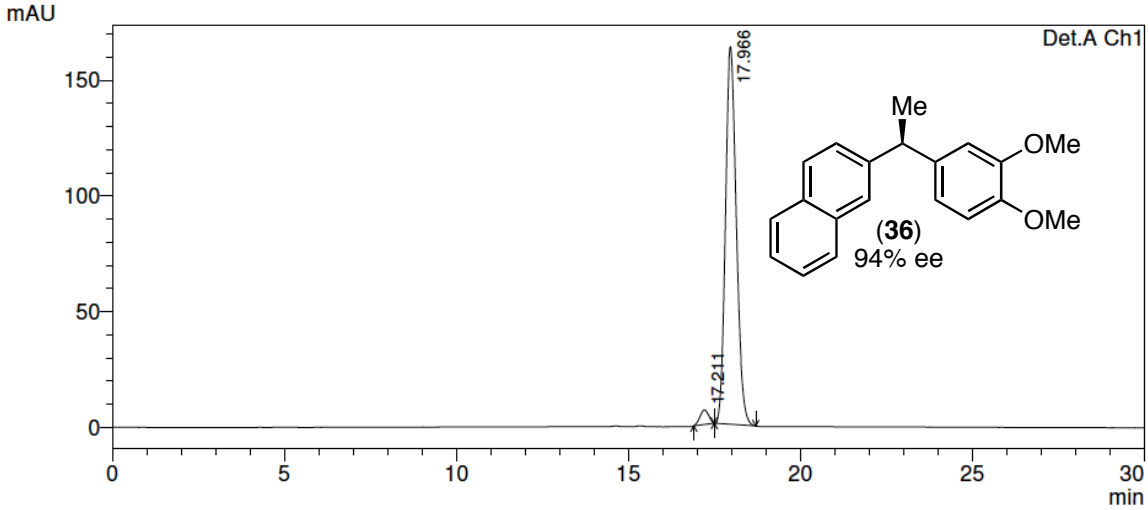
Compound 36, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.479	302437	15327	50.083	51.327
2	18.249	301434	14534	49.917	48.673
Total		603871	29861	100.000	100.000

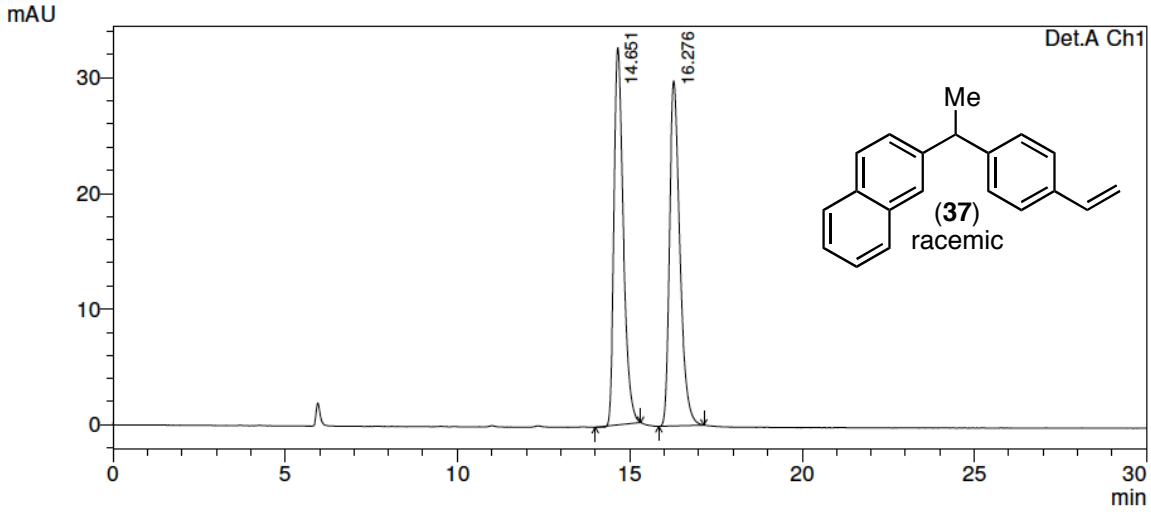
Compound 36, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.211	109447	6268	2.965	3.698
2	17.966	3582462	163249	97.035	96.302
Total		3691909	169517	100.000	100.000

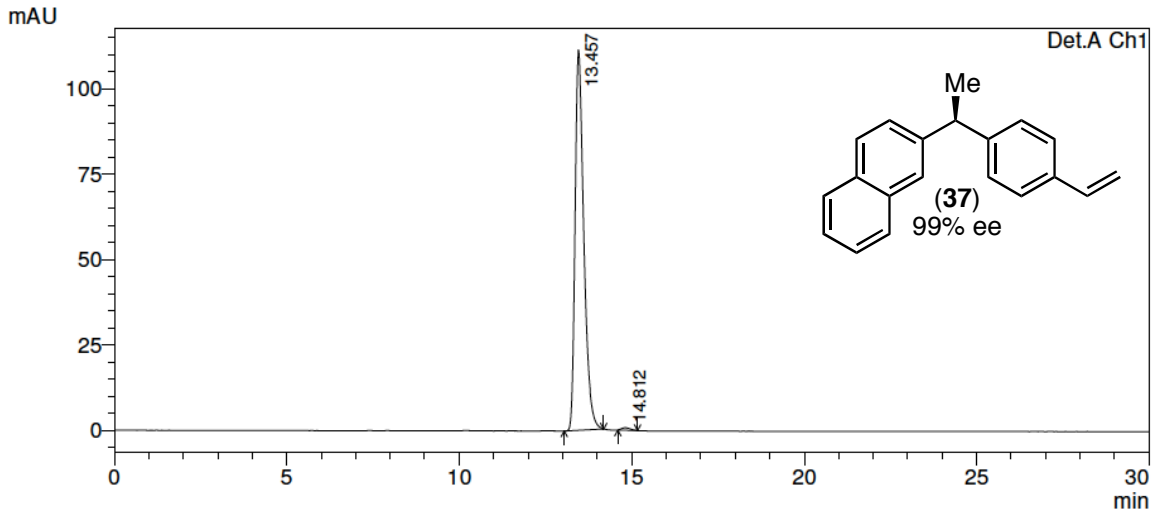
Compound 37, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.651	613434	32600	49.600	52.224
2	16.276	623336	29824	50.400	47.776
Total		1236770	62424	100.000	100.000

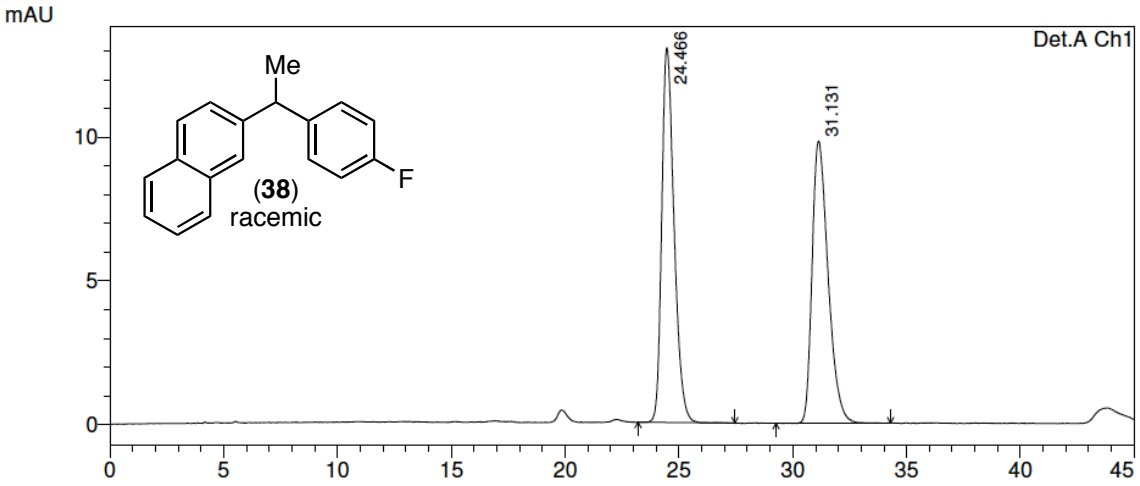
Compound 37, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.457	1974070	111453	99.363	99.316
2	14.812	12651	768	0.637	0.684
Total		1986720	112220	100.000	100.000

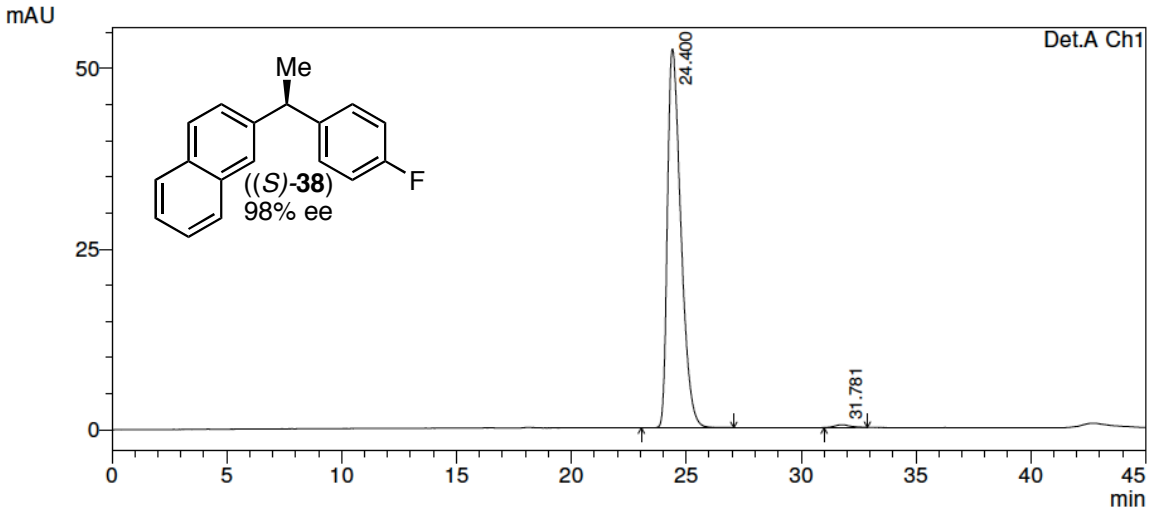
Compound 38, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.466	492703	13047	50.652	57.061
2	31.131	480018	9818	49.348	42.939
Total		972721	22865	100.000	100.000

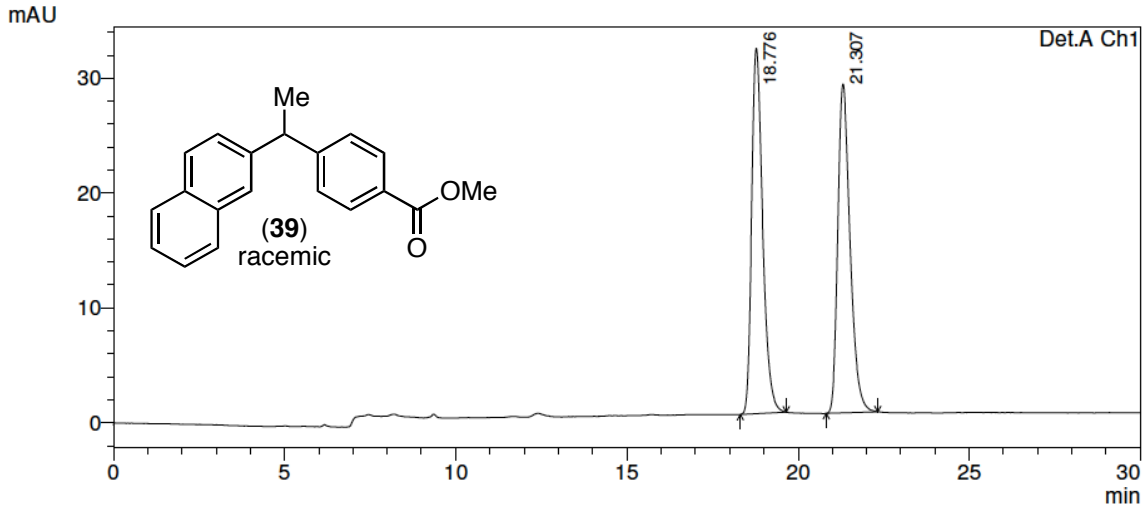
Compound (*S*)-38, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.400	2134769	52398	99.141	99.241
2	31.781	18499	401	0.859	0.759
Total		2153267	52798	100.000	100.000

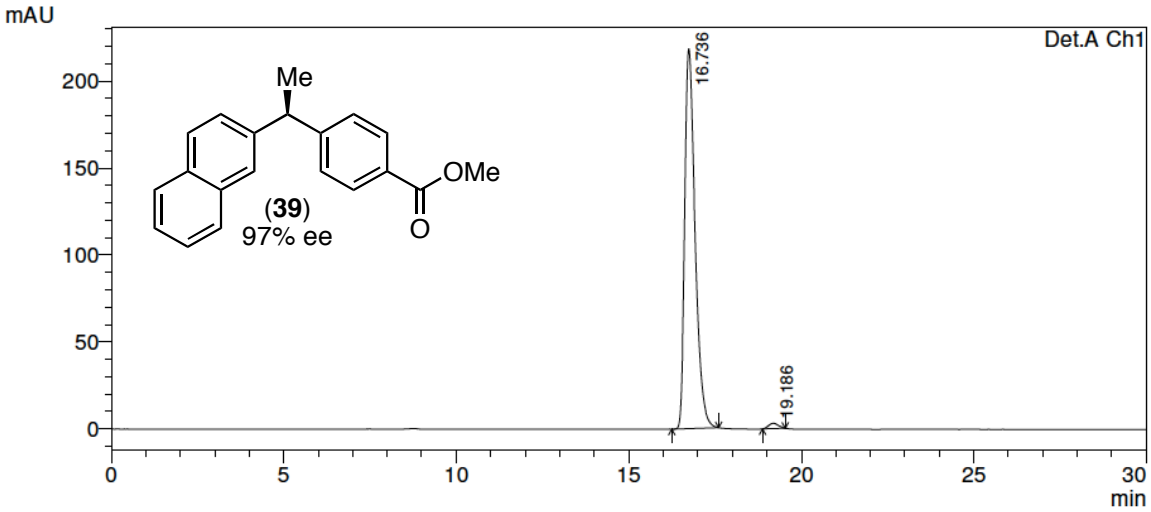
Compound 39, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.776	710130	31808	49.943	52.627
2	21.307	711755	28632	50.057	47.373
Total		1421885	60439	100.000	100.000

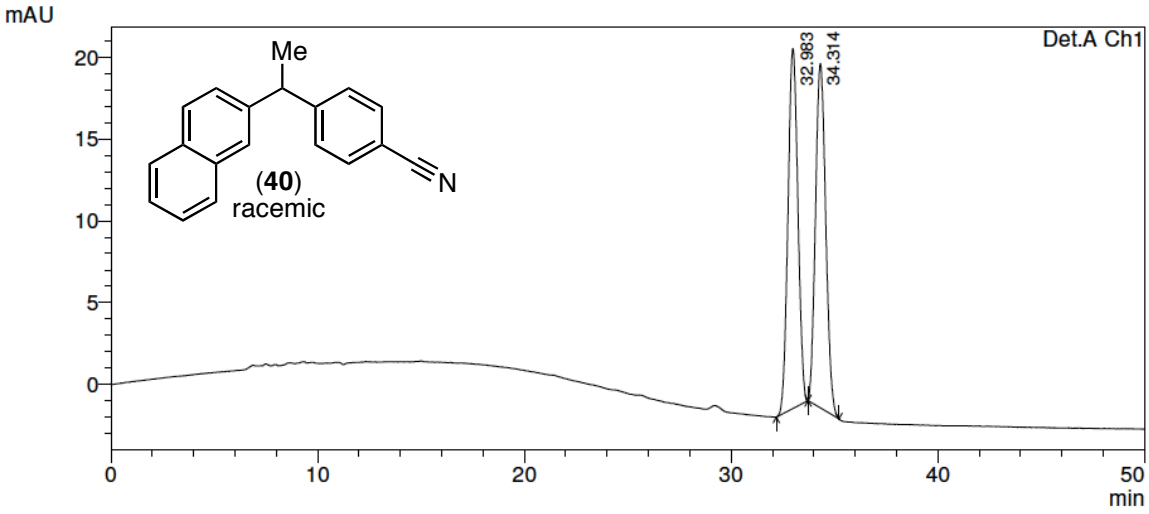
Compound 39, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.736	4554335	218340	98.733	98.654
2	19.186	58440	2979	1.267	1.346
Total		4612775	221319	100.000	100.000

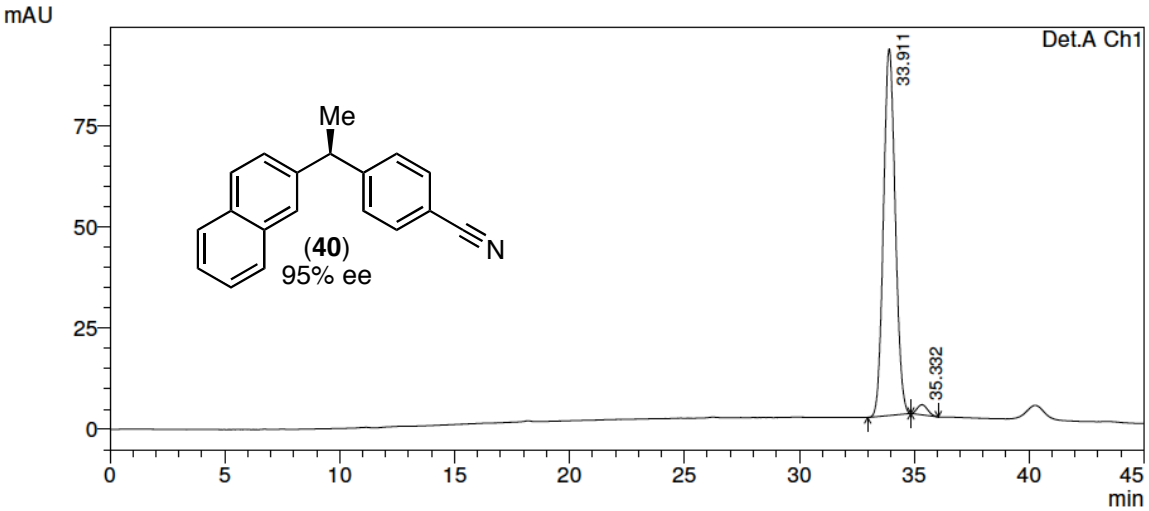
Compound 40, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	32.983	730166	22010	50.195	51.100
2	34.314	724491	21062	49.805	48.900
Total		1454656	43072	100.000	100.000

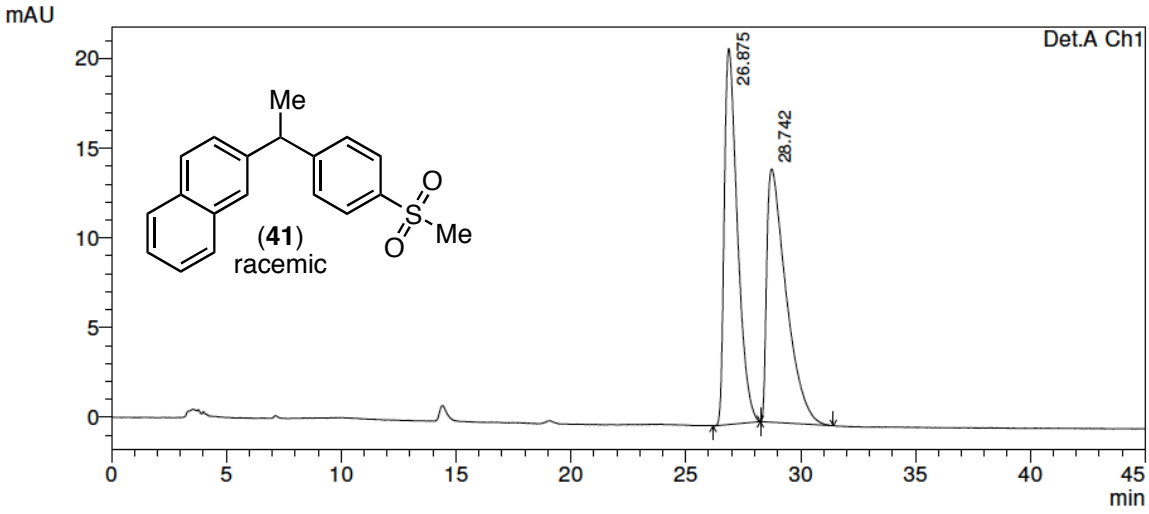
Compound 40, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	33.911	3237525	90626	97.585	97.294
2	35.332	80119	2521	2.415	2.706
Total		3317644	93147	100.000	100.000

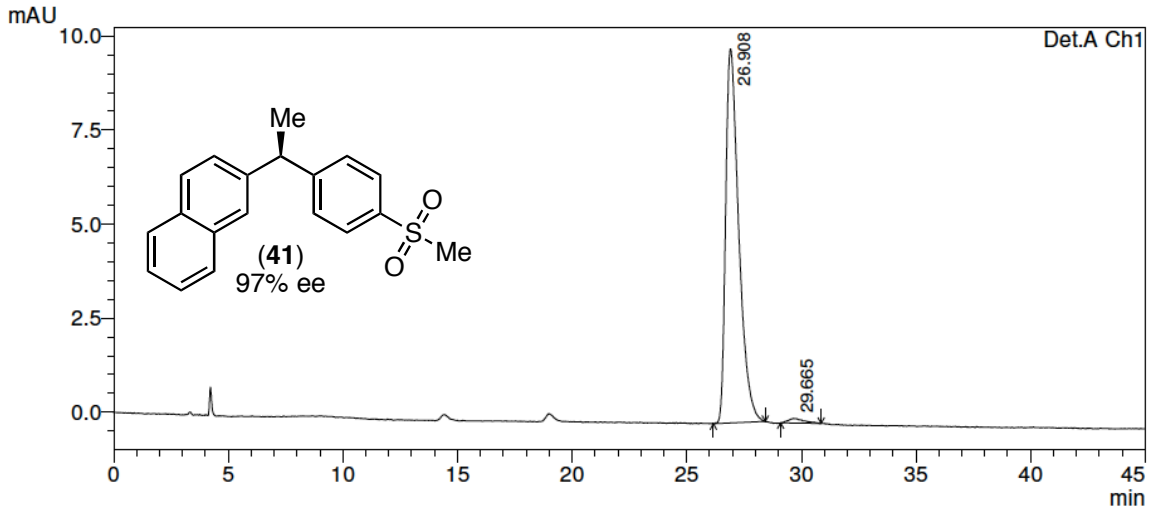
Compound 41, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.875	834248	20960	50.169	59.752
2	28.742	828620	14118	49.831	40.248
Total		1662868	35078	100.000	100.000

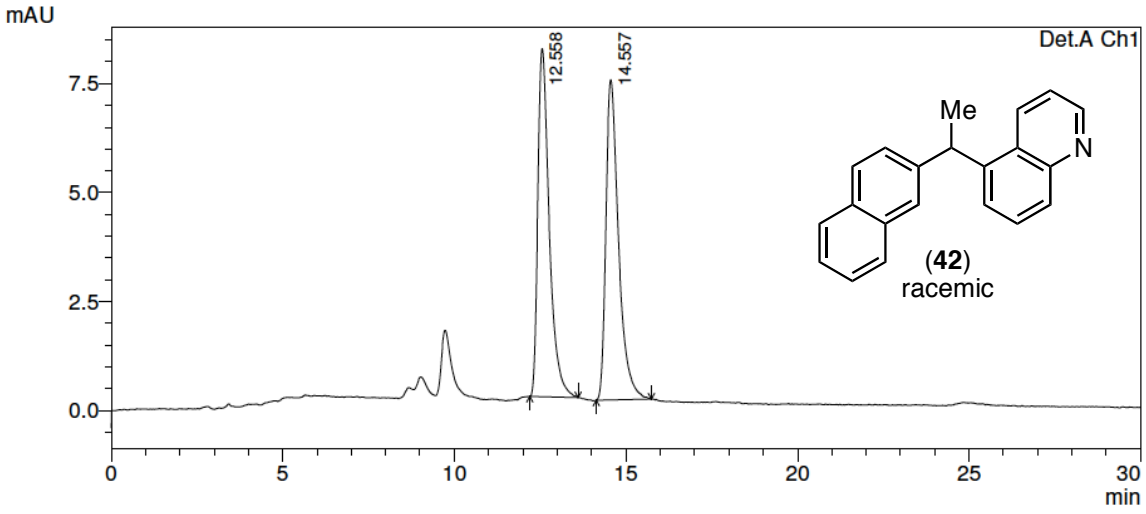
Compound 41, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.908	394994	9940	98.526	98.737
2	29.665	5908	127	1.474	1.263
Total		400903	10067	100.000	100.000

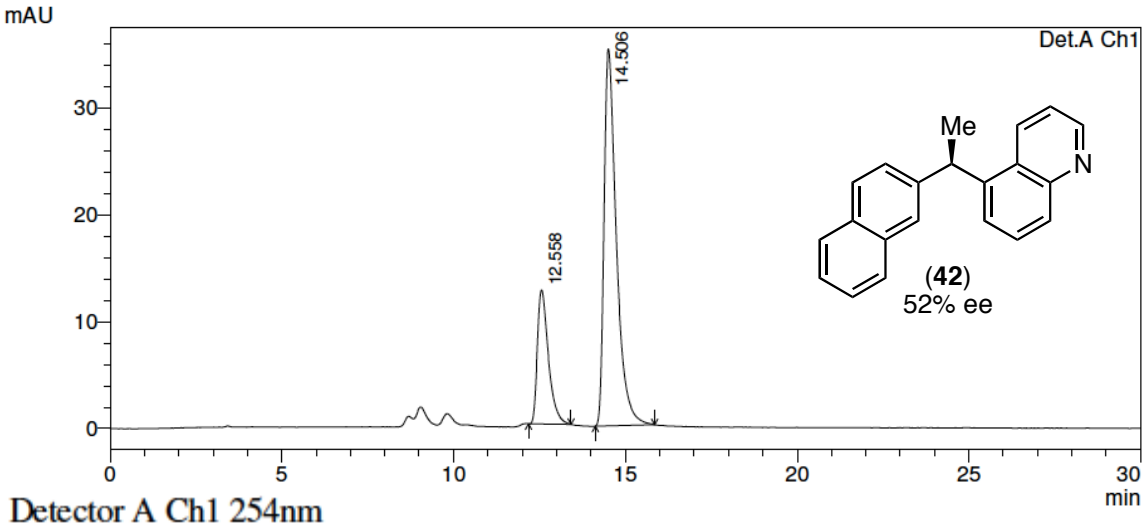
Compound 42, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.558	184602	7985	49.489	52.083
2	14.557	188417	7346	50.511	47.917
Total		373020	15331	100.000	100.000

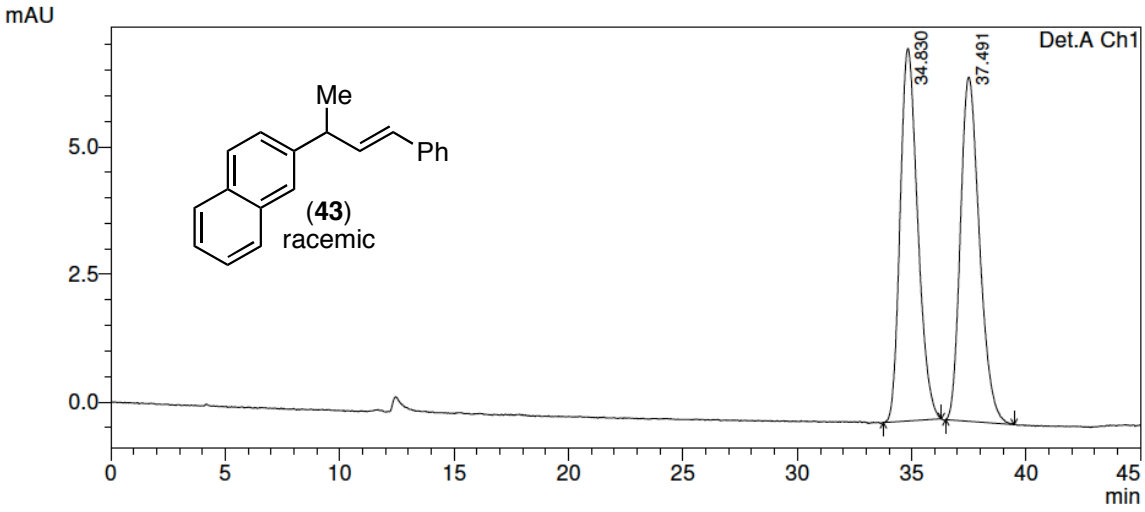
Compound 42, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.558	279764	12542	24.105	26.230
2	14.506	880842	35272	75.895	73.770
Total		1160606	47814	100.000	100.000

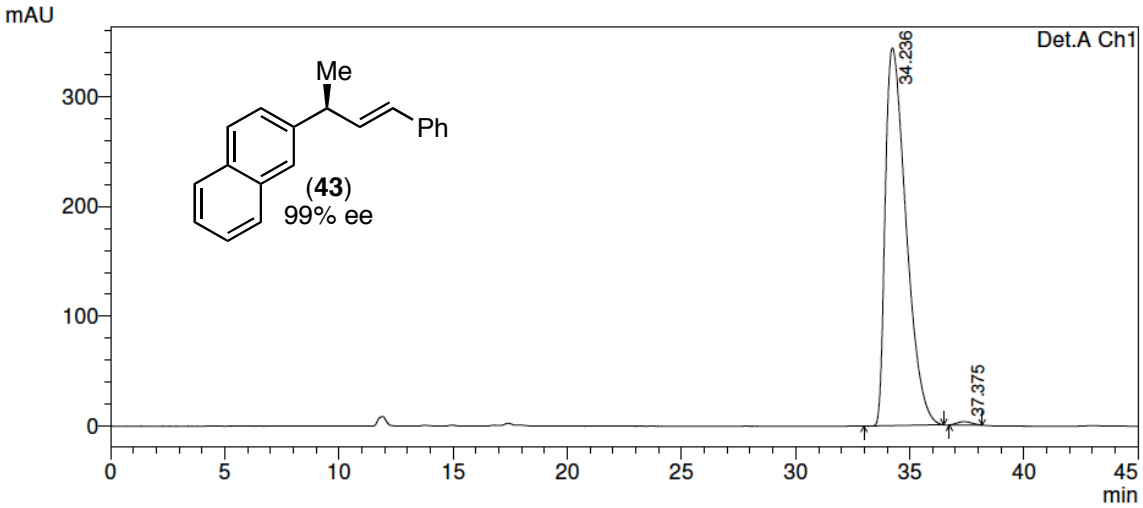
Compound 43, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	34.830	389304	7298	49.955	51.983
2	37.491	390003	6741	50.045	48.017
Total		779307	14038	100.000	100.000

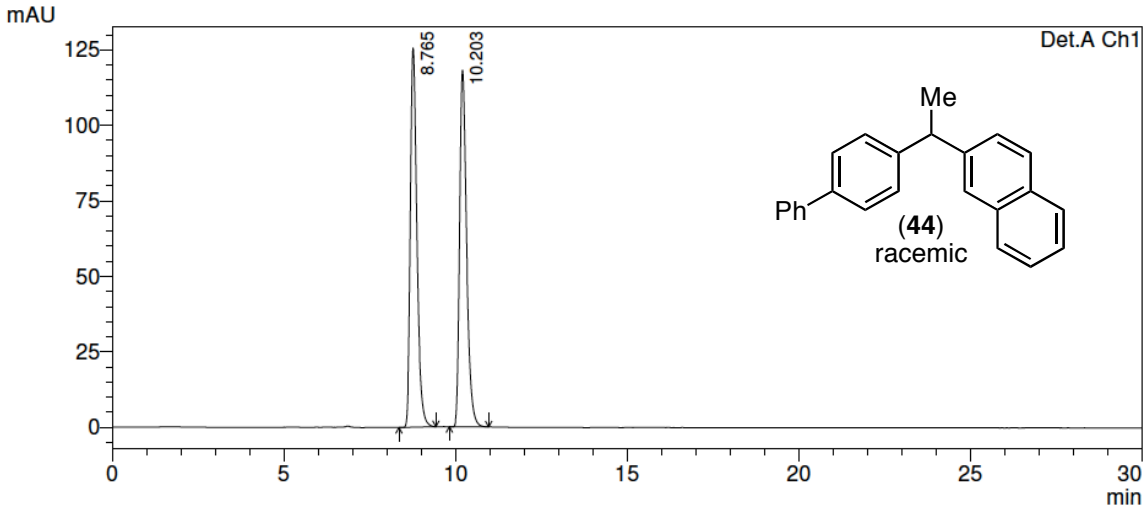
Compound 43, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	34.236	21826981	343641	99.373	99.144
2	37.375	137641	2967	0.627	0.856
Total		21964622	346608	100.000	100.000

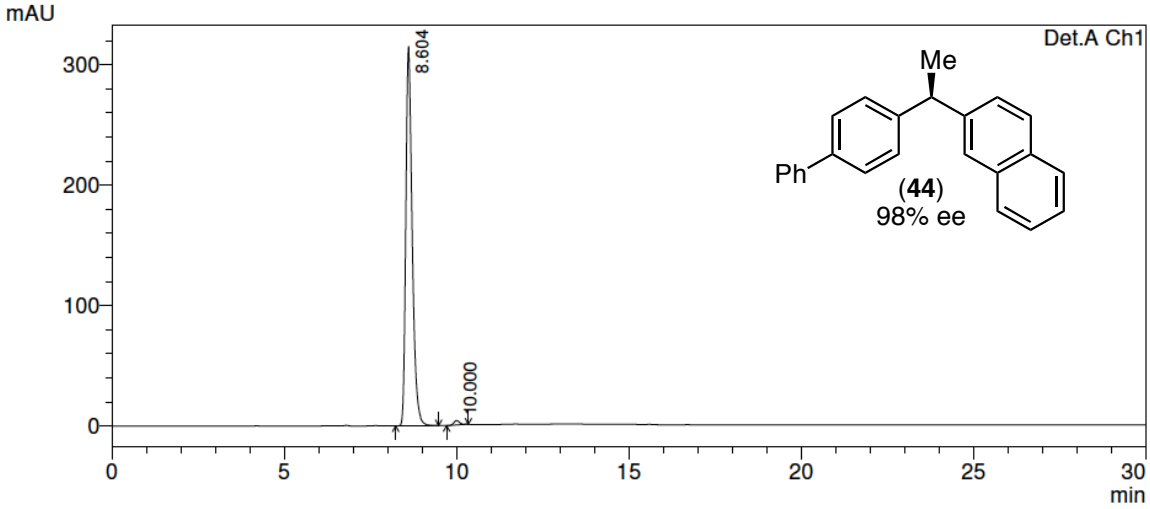
Compound 44, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.765	1662393	125567	49.963	51.518
2	10.203	1664847	118166	50.037	48.482
Total		3327239	243733	100.000	100.000

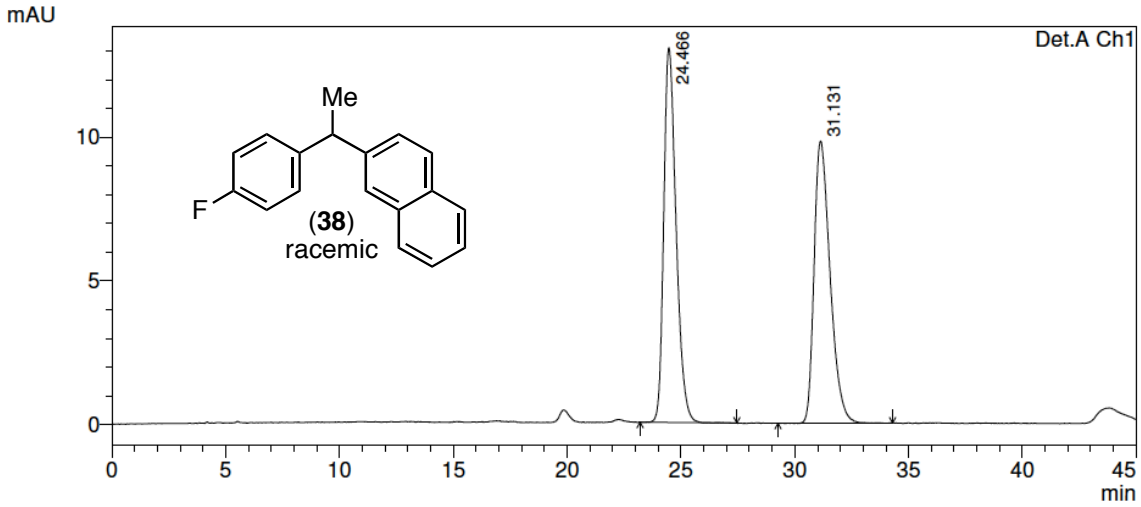
Compound 44, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.604	4111465	314829	98.933	98.839
2	10.000	44336	3697	1.067	1.161
Total		4155800	318526	100.000	100.000

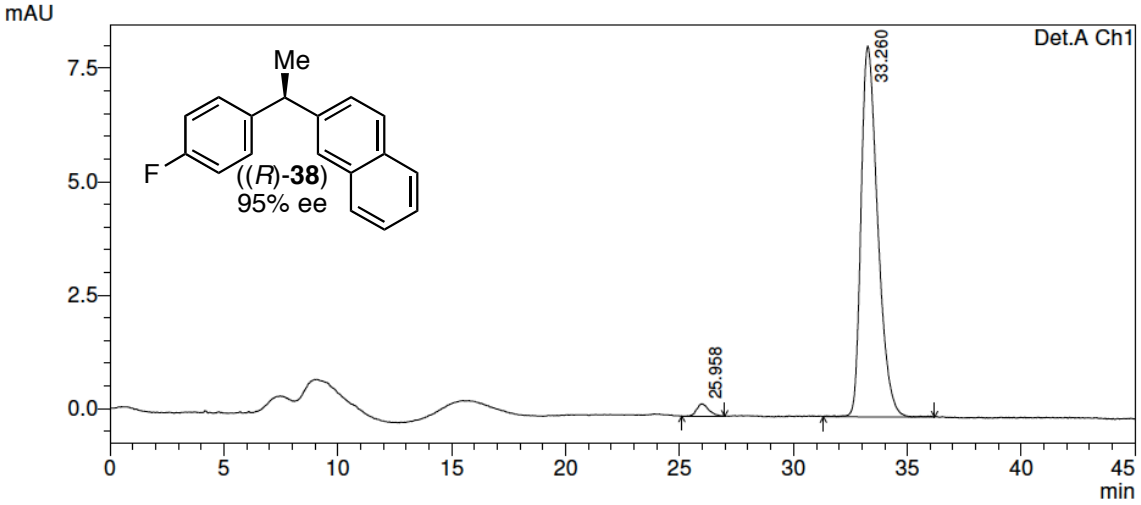
Compound 38, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.466	492703	13047	50.652	57.061
2	31.131	480018	9818	49.348	42.939
Total		972721	22865	100.000	100.000

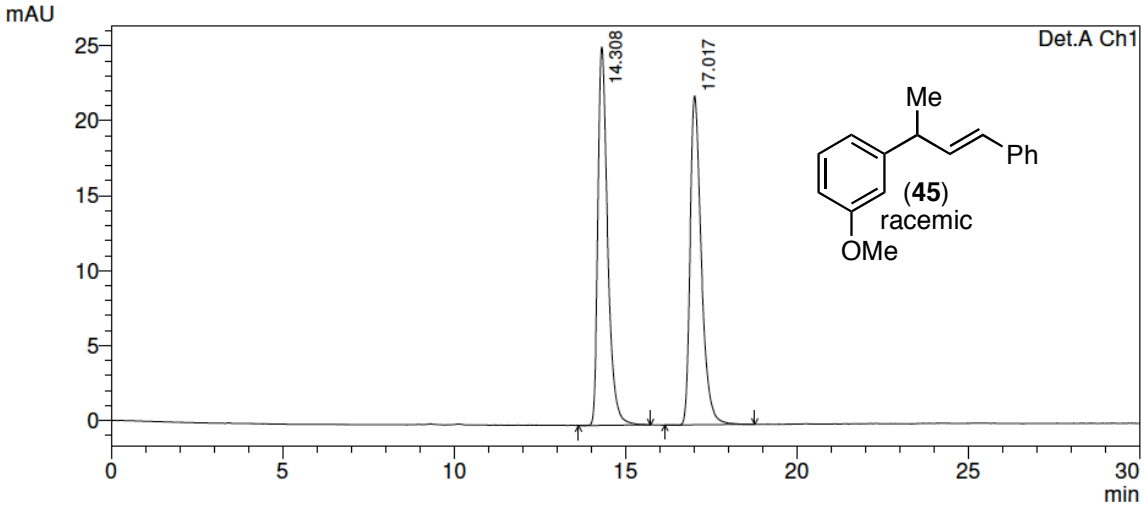
Compound (*R*)-38, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	25.958	10035	269	2.358	3.194
2	33.260	415574	8167	97.642	96.806
Total		425609	8436	100.000	100.000

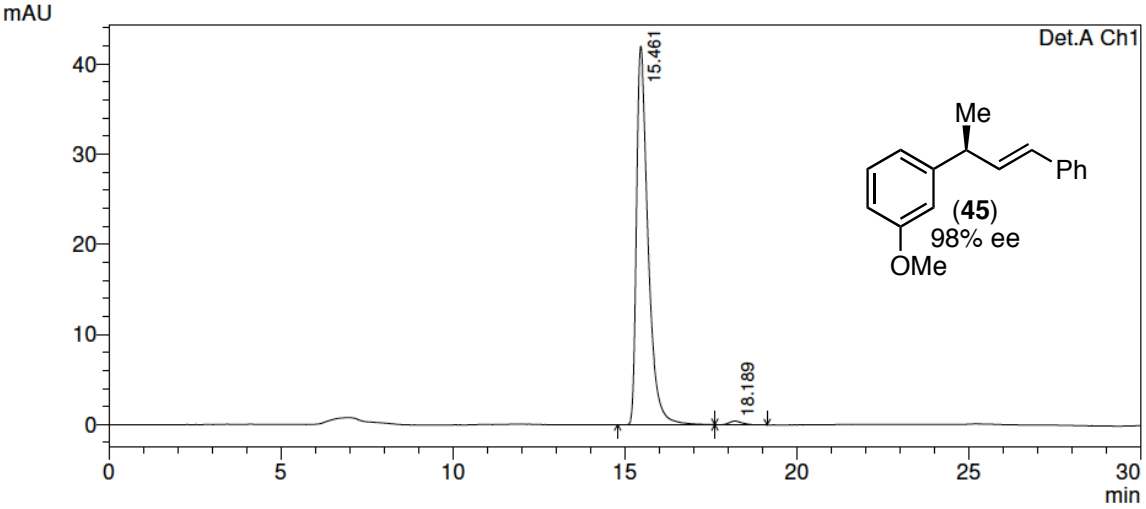
Compound 45, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.308	499610	25230	50.047	53.498
2	17.017	498666	21930	49.953	46.502
Total		998275	47160	100.000	100.000

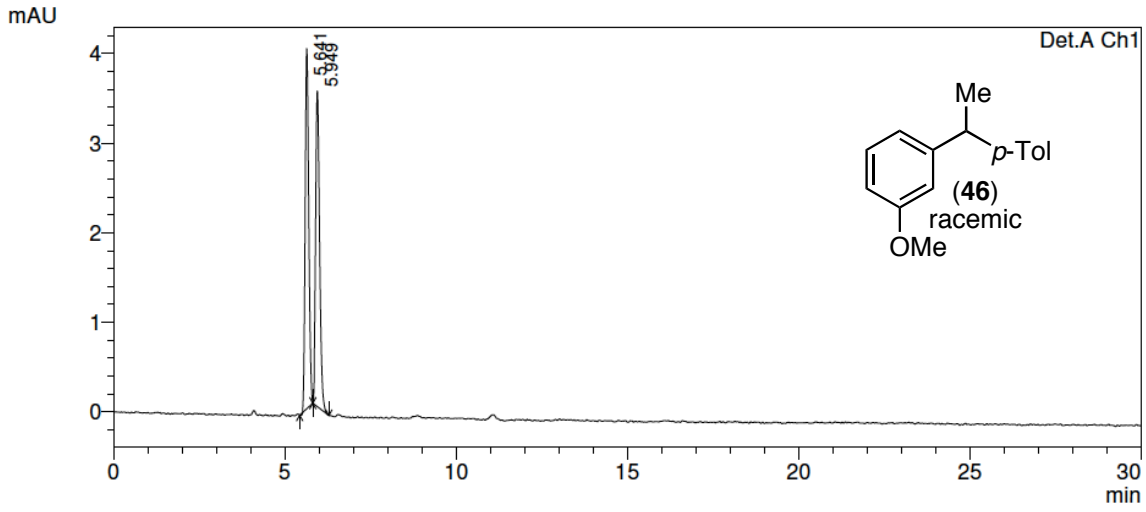
Compound 45, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.461	976356	41973	98.985	99.093
2	18.189	10007	384	1.015	0.907
Total		986363	42357	100.000	100.000

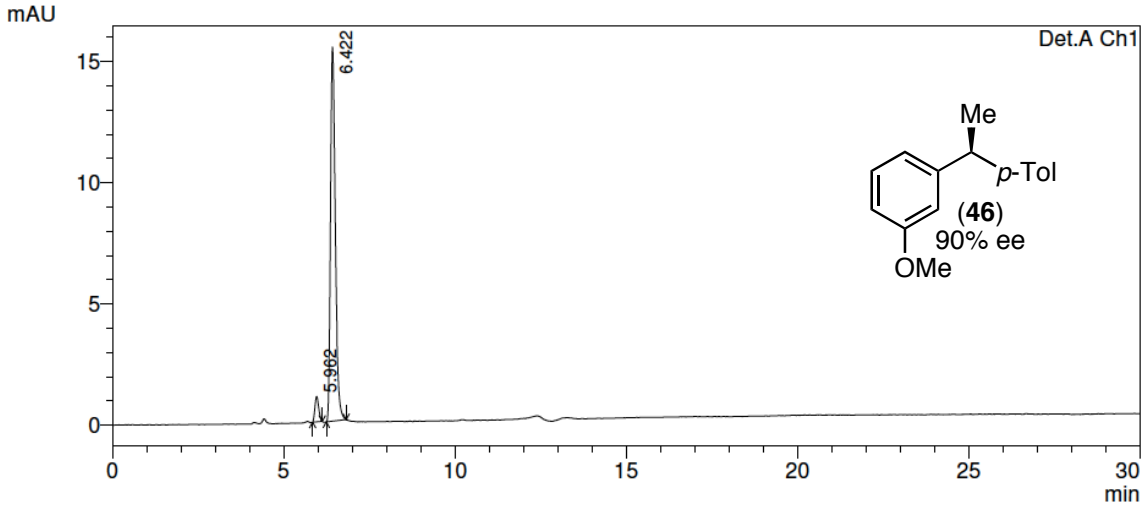
Compound 46, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.641	28336	4020	50.186	53.282
2	5.949	28127	3525	49.814	46.718
Total		56463	7545	100.000	100.000

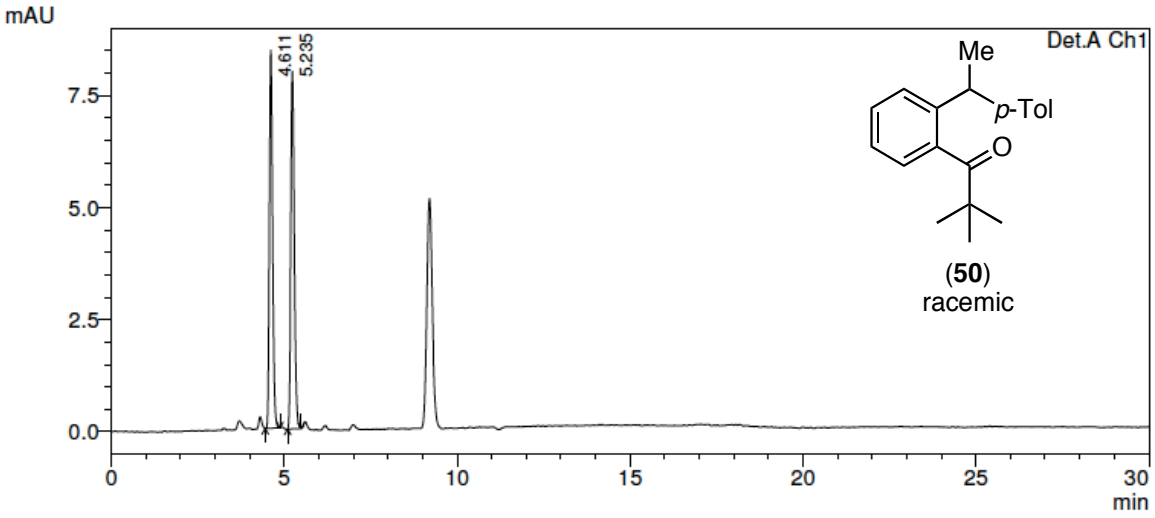
Compound 46, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.962	7825	1055	4.985	6.402
2	6.422	149147	15426	95.015	93.598
Total		156972	16481	100.000	100.000

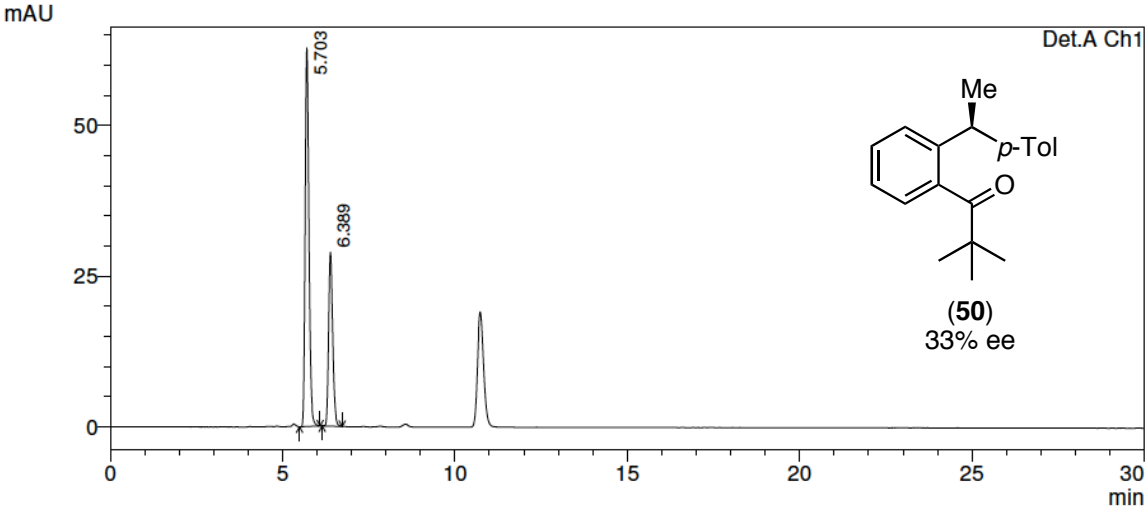
Compound 50, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.611	53325	8434	48.734	51.409
2	5.235	56095	7972	51.266	48.591
Total		109420	16407	100.000	100.000

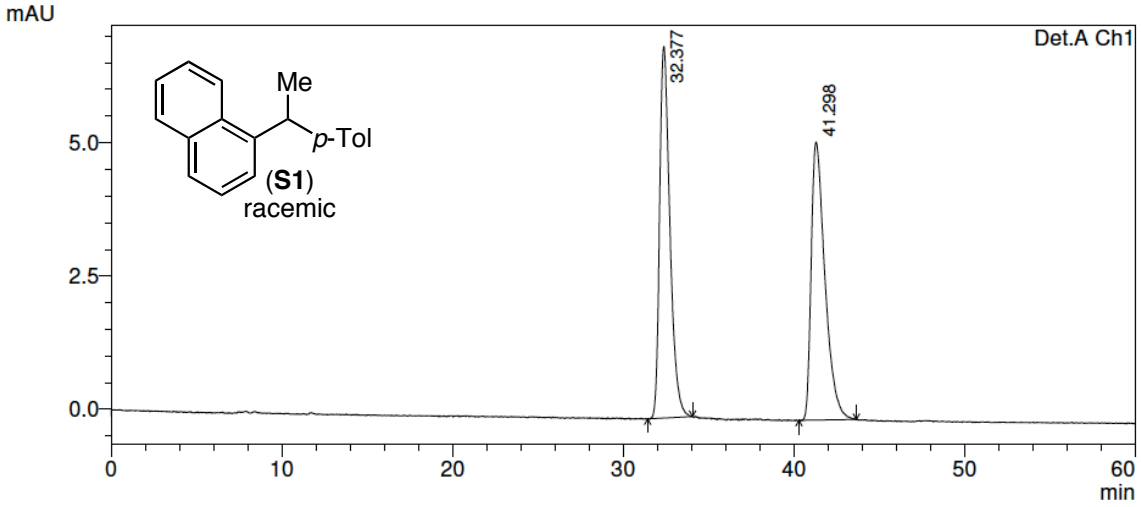
Compound 50, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.703	469993	62856	66.765	68.521
2	6.389	233958	28876	33.235	31.479
Total		703952	91732	100.000	100.000

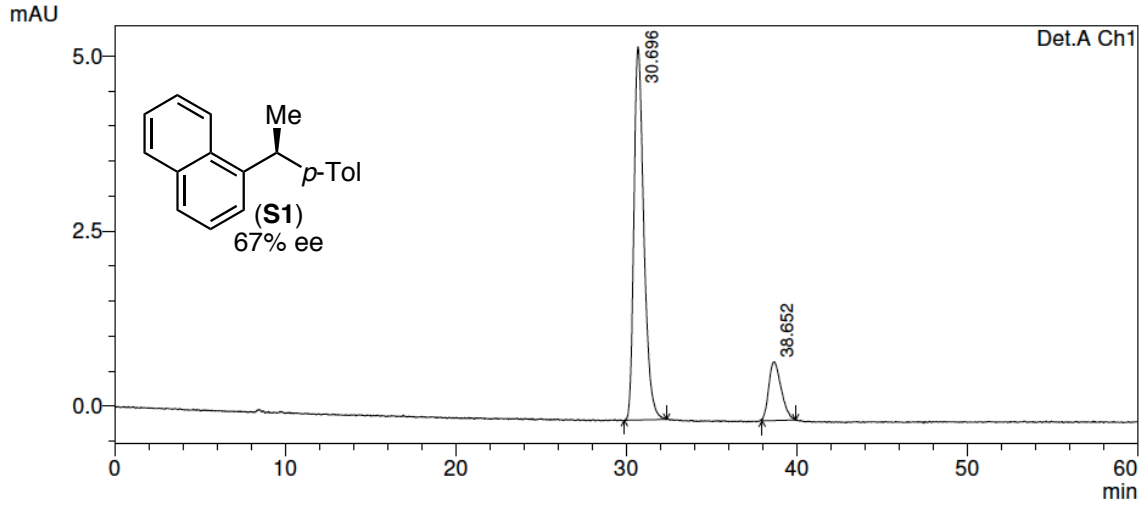
Compound S1, racemic



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	32.377	291855	6966	49.978	57.194
2	41.298	292111	5214	50.022	42.806
Total		583967	12180	100.000	100.000

Compound S1, enantioenriched



Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	30.696	215910	5328	83.499	86.431
2	38.652	42669	837	16.501	13.569
Total		258579	6165	100.000	100.000

Crystal Structure Report for 48 & (*R*)-38

The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. Data were corrected for absorption effects using numerical methods based on indexed crystal faces.

No symmetry higher than triclinic was observed for **48** and solution in the centrosymmetric space group option yielded chemically reasonable and computationally stable results of refinement. The systematic absences in the diffraction data were consistent with $P2_1$ and $P2_1/m$ for (*R*)-**38**. The resolved chirality of the target compound for (*R*)-**38** is consistent with the noncentrosymmetric space group option and refinement in $P2_1$ yielded a nil absolute structure parameter indicating the true hand of the data has been determined. Two symmetry unique but chemically identical molecules of the target molecule are observed in the asymmetric unit for (*R*)-**38**. All nonhydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were treated as idealized contributions. The structures were solved and refined using the Bruker SHELXTL Software Package (Sheldrick, G.M. 2008. Acta Cryst. A64, 112-122). CIFs are deposited with the CSD under depositary numbers 899359 (**48**) & 899360 ((*R*)-**38**).

Table 1. Sample and crystal data for 48.

Identification code	43	
Chemical formula	$C_{31}H_{36}F_3NiO_4PS$	
Formula weight	651.34	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal size	0.180 x 0.210 x 0.220 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.3072(18) Å	α = 109.485(3)°
	b = 11.549(2) Å	β = 93.164(3)°
	c = 15.755(3) Å	γ = 112.720(3)°
Volume	1593.9(5) $Å^3$	

Z	2
Density (calculated)	1.357 g/cm^3
Absorption coefficient	0.775 mm^{-1}
F(000)	680

Table 2. Data collection and structure refinement for 48.

Theta range for data collection	2.01 to 27.51°	
Index ranges	-13<=h<=13, -14<=k<=14, -20<=l<=20	
Reflections collected	20891	
Independent reflections	7291 [R(int) = 0.0437]	
Coverage of independent reflections	99.6%	
Absorption correction	numerical	
Max. and min. transmission	0.8757 and 0.8450	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-97 (Sheldrick, 2008)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	7291 / 0 / 373	
Goodness-of-fit on F^2	1.051	
Δ/σ_{max}	0.001	
Final R indices	5371 data; I>2σ(I)	R1 = 0.0486, wR2 = 0.1207
	all data	R1 = 0.0693, wR2 = 0.1341
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0635P)^2+0.4840P]$	

	where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.719 and -0.697 eÅ^{-3}
R.M.S. deviation from mean	0.069 eÅ^{-3}

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 48.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Ni	0.51910(3)	0.67620(3)	0.71652(2)	0.02760(12)
P1	0.34330(7)	0.48633(7)	0.69627(5)	0.02441(16)
S1	0.76868(8)	0.60835(9)	0.79505(5)	0.0394(2)
F1	0.7961(5)	0.8411(4)	0.9091(2)	0.177(2)
F2	0.9605(4)	0.7848(3)	0.9415(2)	0.1557(18)
F3	0.9548(4)	0.8539(3)	0.8278(3)	0.1406(16)
O1	0.6697(2)	0.8504(2)	0.73278(14)	0.0382(5)
O2	0.6784(2)	0.6204(2)	0.72680(13)	0.0357(5)
O3	0.6936(3)	0.5375(4)	0.8469(2)	0.1036(13)
O4	0.8754(3)	0.5698(4)	0.7595(2)	0.0841(10)
C1	0.3867(3)	0.7513(3)	0.7028(2)	0.0354(6)
C2	0.4234(3)	0.8756(3)	0.7861(2)	0.0409(7)
C3	0.3164(4)	0.8915(4)	0.8338(3)	0.0617(10)
C4	0.3454(6)	0.0068(4)	0.9106(3)	0.0884(16)
C5	0.4811(6)	0.1118(4)	0.9420(4)	0.0975(18)
C6	0.5891(5)	0.1008(4)	0.8969(3)	0.0722(13)
C7	0.5639(4)	0.9842(3)	0.8194(2)	0.0451(8)

C8	0.6777(3)	0.9666(3)	0.7714(2)	0.0381(7)
C9	0.8055(3)	0.0832(3)	0.7616(2)	0.0465(8)
C10	0.7559(4)	0.1815(4)	0.7402(3)	0.0650(11)
C11	0.9225(4)	0.1594(4)	0.8519(3)	0.0701(12)
C12	0.8699(4)	0.0211(4)	0.6832(3)	0.0626(11)
C13	0.2180(4)	0.4492(3)	0.5238(2)	0.0434(8)
C14	0.1067(4)	0.3903(4)	0.4464(2)	0.0581(10)
C15	0.9699(4)	0.3060(4)	0.4477(3)	0.0636(11)
C16	0.9412(4)	0.2800(4)	0.5259(3)	0.0587(10)
C17	0.0517(3)	0.3368(3)	0.6023(2)	0.0432(8)
C18	0.1906(3)	0.4231(3)	0.60261(19)	0.0299(6)
C19	0.1644(3)	0.5378(3)	0.8200(2)	0.0330(6)
C20	0.1232(3)	0.5552(3)	0.9039(2)	0.0405(7)
C21	0.1932(3)	0.5351(3)	0.9713(2)	0.0406(7)
C22	0.3055(3)	0.4992(3)	0.9554(2)	0.0428(7)
C23	0.3476(3)	0.4821(3)	0.87175(19)	0.0367(7)
C24	0.2768(3)	0.5003(3)	0.80246(18)	0.0268(5)
C25	0.2772(3)	0.2116(3)	0.6717(2)	0.0393(7)
C26	0.3374(4)	0.1065(3)	0.6596(2)	0.0485(8)
C27	0.3967(5)	0.0797(4)	0.5722(3)	0.0594(10)
C28	0.5050(4)	0.2096(4)	0.5671(3)	0.0547(9)
C29	0.4450(3)	0.3148(3)	0.5803(2)	0.0390(7)
C30	0.3929(3)	0.3428(3)	0.67067(19)	0.0301(6)
C31	0.8718(7)	0.7810(6)	0.8745(4)	0.0992(19)

Table 4. Bond lengths (Å) for 48.

Ni-C1	1.915(3)	Ni-O1	1.929(2)
Ni-O2	1.9994(19)	Ni-P1	2.1434(8)
P1-C24	1.824(3)	P1-C18	1.824(3)
P1-C30	1.845(3)	S1-O3	1.400(3)
S1-O4	1.415(3)	S1-O2	1.459(2)
S1-C31	1.795(6)	F1-C31	1.266(6)
F2-C31	1.334(5)	F3-C31	1.381(7)
O1-C8	1.243(4)	C1-C2	1.482(4)
C1-H1A	0.99	C1-H1B	0.99
C2-C3	1.403(5)	C2-C7	1.421(4)
C3-C4	1.380(6)	C3-H3	0.95
C4-C5	1.373(7)	C4-H4	0.95
C5-C6	1.377(6)	C5-H5	0.95
C6-C7	1.404(5)	C6-H6	0.95
C7-C8	1.473(5)	C8-C9	1.537(4)
C9-C10	1.533(5)	C9-C12	1.533(5)
C9-C11	1.551(5)	C10-H10A	0.98
C10-H10B	0.98	C10-H10C	0.98
C11-H11A	0.98	C11-H11B	0.98
C11-H11C	0.98	C12-H12A	0.98
C12-H12B	0.98	C12-H12C	0.98
C13-C18	1.392(4)	C13-C14	1.398(5)
C13-H13	0.95	C14-C15	1.376(5)
C14-H14	0.95	C15-C16	1.383(5)
C15-H15	0.95	C16-C17	1.386(4)

C16-H16	0.95	C17-C18	1.391(4)
C17-H17	0.95	C19-C20	1.385(4)
C19-C24	1.396(4)	C19-H19	0.95
C20-C21	1.382(4)	C20-H20	0.95
C21-C22	1.381(4)	C21-H21	0.95
C22-C23	1.386(4)	C22-H22	0.95
C23-C24	1.397(4)	C23-H23	0.95
C25-C26	1.528(4)	C25-C30	1.530(4)
C25-H25A	0.99	C25-H25B	0.99
C26-C27	1.522(5)	C26-H26A	0.99
C26-H26B	0.99	C27-C28	1.517(5)
C27-H27A	0.99	C27-H27B	0.99
C28-C29	1.526(4)	C28-H28A	0.99
C28-H28B	0.99	C29-C30	1.527(4)
C29-H29A	0.99	C29-H29B	0.99
C30-H30	1.0		

Table 5. Bond angles (°) for 48.

C1-Ni-O1	86.61(11)	C1-Ni-O2	171.49(11)
O1-Ni-O2	85.32(9)	C1-Ni-P1	90.28(9)
O1-Ni-P1	176.85(6)	O2-Ni-P1	97.77(6)
C24-P1-C18	107.98(12)	C24-P1-C30	105.14(12)
C18-P1-C30	103.23(13)	C24-P1-Ni	109.15(9)
C18-P1-Ni	116.57(9)	C30-P1-Ni	113.99(9)
O3-S1-O4	114.9(2)	O3-S1-O2	114.88(16)

O4-S1-O2	112.74(14)	O3-S1-C31	106.1(3)
O4-S1-C31	102.9(3)	O2-S1-C31	103.57(18)
C8-O1-Ni	129.9(2)	S1-O2-Ni	140.27(13)
C2-C1-Ni	108.6(2)	C2-C1-H1A	110.0
Ni-C1-H1A	110.0	C2-C1-H1B	110.0
Ni-C1-H1B	110.0	H1A-C1-H1B	108.4
C3-C2-C7	117.3(3)	C3-C2-C1	120.0(3)
C7-C2-C1	122.6(3)	C4-C3-C2	121.9(4)
C4-C3-H3	119.0	C2-C3-H3	119.0
C5-C4-C3	120.5(4)	C5-C4-H4	119.8
C3-C4-H4	119.8	C4-C5-C6	119.5(4)
C4-C5-H5	120.2	C6-C5-H5	120.2
C5-C6-C7	121.5(4)	C5-C6-H6	119.3
C7-C6-H6	119.3	C6-C7-C2	119.3(3)
C6-C7-C8	123.1(3)	C2-C7-C8	117.6(3)
O1-C8-C7	119.3(3)	O1-C8-C9	116.4(3)
C7-C8-C9	124.3(3)	C10-C9-C8	110.5(3)
C10-C9-C12	110.0(3)	C8-C9-C12	108.1(3)
C10-C9-C11	110.4(3)	C8-C9-C11	109.5(3)
C12-C9-C11	108.3(3)	C9-C10-H10A	109.5
C9-C10-H10B	109.5	H10A-C10-H10B	109.5
C9-C10-H10C	109.5	H10A-C10-H10C	109.5
H10B-C10-H10C	109.5	C9-C11-H11A	109.5
C9-C11-H11B	109.5	H11A-C11-H11B	109.5
C9-C11-H11C	109.5	H11A-C11-H11C	109.5
H11B-C11-H11C	109.5	C9-C12-H12A	109.5

C9-C12-H12B	109.5	H12A-C12-H12B	109.5
C9-C12-H12C	109.5	H12A-C12-H12C	109.5
H12B-C12-H12C	109.5	C18-C13-C14	120.1(3)
C18-C13-H13	120.0	C14-C13-H13	120.0
C15-C14-C13	120.1(3)	C15-C14-H14	119.9
C13-C14-H14	119.9	C14-C15-C16	120.3(3)
C14-C15-H15	119.9	C16-C15-H15	119.9
C15-C16-C17	119.7(3)	C15-C16-H16	120.2
C17-C16-H16	120.2	C16-C17-C18	121.0(3)
C16-C17-H17	119.5	C18-C17-H17	119.5
C13-C18-C17	118.8(3)	C13-C18-P1	118.0(2)
C17-C18-P1	122.7(2)	C20-C19-C24	120.6(3)
C20-C19-H19	119.7	C24-C19-H19	119.7
C21-C20-C19	120.1(3)	C21-C20-H20	119.9
C19-C20-H20	119.9	C22-C21-C20	120.0(3)
C22-C21-H21	120.0	C20-C21-H21	120.0
C21-C22-C23	120.2(3)	C21-C22-H22	119.9
C23-C22-H22	119.9	C22-C23-C24	120.5(3)
C22-C23-H23	119.7	C24-C23-H23	119.7
C19-C24-C23	118.5(2)	C19-C24-P1	122.6(2)
C23-C24-P1	118.7(2)	C26-C25-C30	109.9(2)
C26-C25-H25A	109.7	C30-C25-H25A	109.7
C26-C25-H25B	109.7	C30-C25-H25B	109.7
H25A-C25-H25B	108.2	C27-C26-C25	111.6(3)
C27-C26-H26A	109.3	C25-C26-H26A	109.3
C27-C26-H26B	109.3	C25-C26-H26B	109.3

H26A-C26-H26B	108.0	C28-C27-C26	112.3(3)
C28-C27-H27A	109.1	C26-C27-H27A	109.1
C28-C27-H27B	109.1	C26-C27-H27B	109.1
H27A-C27-H27B	107.9	C27-C28-C29	111.9(3)
C27-C28-H28A	109.2	C29-C28-H28A	109.2
C27-C28-H28B	109.2	C29-C28-H28B	109.2
H28A-C28-H28B	107.9	C30-C29-C28	110.2(2)
C30-C29-H29A	109.6	C28-C29-H29A	109.6
C30-C29-H29B	109.6	C28-C29-H29B	109.6
H29A-C29-H29B	108.1	C29-C30-C25	110.6(2)
C29-C30-P1	111.09(19)	C25-C30-P1	115.37(19)
C29-C30-H30	106.4	C25-C30-H30	106.4
P1-C30-H30	106.4	F1-C31-F2	109.9(5)
F1-C31-F3	106.6(5)	F2-C31-F3	107.9(5)
F1-C31-S1	113.9(5)	F2-C31-S1	109.8(4)
F3-C31-S1	108.4(4)		

Table 6. Torsion angles (°) for 48.

C1-Ni-P1-C24	-78.10(13)	O1-Ni-P1-C24	-87.5(12)
O2-Ni-P1-C24	104.67(11)	C1-Ni-P1-C18	44.52(14)
O1-Ni-P1-C18	35.1(12)	O2-Ni-P1-C18	-132.71(12)
C1-Ni-P1-C30	164.69(13)	O1-Ni-P1-C30	155.3(12)
O2-Ni-P1-C30	-12.54(11)	C1-Ni-O1-C8	35.7(3)
O2-Ni-O1-C8	-147.0(3)	P1-Ni-O1-C8	45.1(14)
O3-S1-O2-Ni	50.3(3)	O4-S1-O2-Ni	-175.5(2)

C31-S1-O2-Ni	-64.9(3)	C1-Ni-O2-S1	114.5(7)
O1-Ni-O2-S1	96.1(2)	P1-Ni-O2-S1	-84.6(2)
O1-Ni-C1-C2	-56.8(2)	O2-Ni-C1-C2	-75.2(8)
P1-Ni-C1-C2	123.7(2)	Ni-C1-C2-C3	-128.7(3)
Ni-C1-C2-C7	53.4(4)	C7-C2-C3-C4	-0.8(6)
C1-C2-C3-C4	-178.7(4)	C2-C3-C4-C5	1.2(8)
C3-C4-C5-C6	-0.7(9)	C4-C5-C6-C7	-0.2(8)
C5-C6-C7-C2	0.6(7)	C5-C6-C7-C8	-177.7(4)
C3-C2-C7-C6	-0.1(5)	C1-C2-C7-C6	177.8(3)
C3-C2-C7-C8	178.3(3)	C1-C2-C7-C8	-3.8(5)
Ni-O1-C8-C7	4.8(4)	Ni-O1-C8-C9	-172.66(18)
C6-C7-C8-O1	149.2(4)	C2-C7-C8-O1	-29.2(4)
C6-C7-C8-C9	-33.6(5)	C2-C7-C8-C9	148.1(3)
O1-C8-C9-C10	136.0(3)	C7-C8-C9-C10	-41.4(4)
O1-C8-C9-C12	15.5(4)	C7-C8-C9-C12	-161.8(3)
O1-C8-C9-C11	-102.2(4)	C7-C8-C9-C11	80.5(4)
C18-C13-C14-C15	-0.2(5)	C13-C14-C15-C16	0.6(6)
C14-C15-C16-C17	-1.5(6)	C15-C16-C17-C18	1.9(6)
C14-C13-C18-C17	0.7(5)	C14-C13-C18-P1	173.0(3)
C16-C17-C18-C13	-1.5(5)	C16-C17-C18-P1	-173.5(3)
C24-P1-C18-C13	157.3(2)	C30-P1-C18-C13	-91.6(2)
Ni-P1-C18-C13	34.1(3)	C24-P1-C18-C17	-30.6(3)
C30-P1-C18-C17	80.4(3)	Ni-P1-C18-C17	-153.9(2)
C24-C19-C20-C21	-0.2(5)	C19-C20-C21-C22	0.7(5)
C20-C21-C22-C23	-0.5(5)	C21-C22-C23-C24	-0.3(5)
C20-C19-C24-C23	-0.6(4)	C20-C19-C24-P1	-176.0(2)

C22-C23-C24-C19	0.9(4)	C22-C23-C24-P1	176.5(2)
C18-P1-C24-C19	-35.0(3)	C30-P1-C24-C19	-144.7(2)
Ni-P1-C24-C19	92.6(2)	C18-P1-C24-C23	149.6(2)
C30-P1-C24-C23	39.9(3)	Ni-P1-C24-C23	-82.8(2)
C30-C25-C26-C27	-55.8(4)	C25-C26-C27-C28	53.2(4)
C26-C27-C28-C29	-52.9(4)	C27-C28-C29-C30	55.3(4)
C28-C29-C30-C25	-58.5(3)	C28-C29-C30-P1	172.1(2)
C26-C25-C30-C29	58.8(3)	C26-C25-C30-P1	-174.1(2)
C24-P1-C30-C29	177.5(2)	C18-P1-C30-C29	64.5(2)
Ni-P1-C30-C29	-63.0(2)	C24-P1-C30-C25	50.7(2)
C18-P1-C30-C25	-62.4(2)	Ni-P1-C30-C25	170.21(18)
O3-S1-C31-F1	-65.0(5)	O4-S1-C31-F1	174.0(4)
O2-S1-C31-F1	56.3(5)	O3-S1-C31-F2	58.8(6)
O4-S1-C31-F2	-62.3(5)	O2-S1-C31-F2	-179.9(5)
O3-S1-C31-F3	176.5(3)	O4-S1-C31-F3	55.5(3)
O2-S1-C31-F3	-62.2(4)		

Table 7. Anisotropic atomic displacement parameters (Å²) for 48.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni	0.02274(18)	0.0295(2)	0.0324(2)	0.01558(16)	0.00605(14)	0.00993(15)
P1	0.0232(3)	0.0265(4)	0.0258(3)	0.0116(3)	0.0072(3)	0.0113(3)
S1	0.0342(4)	0.0506(5)	0.0399(4)	0.0233(4)	0.0067(3)	0.0199(4)
F1	0.291(5)	0.196(4)	0.0644(19)	-0.035(2)	-0.043(2)	0.207(4)
F2	0.204(4)	0.100(2)	0.110(2)	-0.0212(18)	-0.107(2)	0.084(3)

F3	0.083(2)	0.085(2)	0.213(4)	0.068(3)	-0.053(2)	-0.0028(17)
O1	0.0295(10)	0.0344(12)	0.0492(13)	0.0216(10)	0.0056(9)	0.0081(9)
O2	0.0289(10)	0.0444(12)	0.0392(11)	0.0192(10)	0.0058(9)	0.0188(9)
O3	0.0612(19)	0.163(3)	0.095(2)	0.103(3)	0.0074(17)	0.013(2)
O4	0.086(2)	0.147(3)	0.0678(18)	0.046(2)	0.0259(16)	0.093(2)
C1	0.0299(15)	0.0326(15)	0.0451(17)	0.0174(14)	0.0055(13)	0.0131(13)
C2	0.0438(18)	0.0317(16)	0.0490(19)	0.0173(14)	0.0140(15)	0.0160(14)
C3	0.060(2)	0.041(2)	0.083(3)	0.021(2)	0.034(2)	0.0209(18)
C4	0.102(4)	0.055(3)	0.097(4)	0.018(3)	0.062(3)	0.027(3)
C5	0.114(4)	0.045(2)	0.094(4)	-0.003(2)	0.058(3)	0.016(3)
C6	0.079(3)	0.038(2)	0.063(2)	0.0045(19)	0.026(2)	0.000(2)
C7	0.053(2)	0.0300(16)	0.0449(18)	0.0139(14)	0.0142(16)	0.0104(15)
C8	0.0354(16)	0.0342(17)	0.0364(16)	0.0159(14)	-0.0030(13)	0.0061(13)
C9	0.0331(16)	0.0385(18)	0.060(2)	0.0276(16)	-0.0007(15)	0.0016(14)
C10	0.052(2)	0.056(2)	0.100(3)	0.054(2)	0.017(2)	0.0155(18)
C11	0.051(2)	0.048(2)	0.085(3)	0.021(2)	-0.017(2)	0.0029(18)
C12	0.045(2)	0.059(2)	0.084(3)	0.042(2)	0.026(2)	0.0086(18)
C13	0.0465(18)	0.057(2)	0.0347(16)	0.0207(15)	0.0101(14)	0.0277(16)
C14	0.077(3)	0.069(3)	0.0315(17)	0.0151(17)	0.0027(18)	0.039(2)
C15	0.062(3)	0.065(3)	0.050(2)	0.0083(19)	-0.0194(19)	0.028(2)
C16	0.0372(18)	0.055(2)	0.064(2)	0.0171(19)	-0.0129(17)	0.0082(16)
C17	0.0328(16)	0.0455(19)	0.0422(17)	0.0189(15)	-0.0002(13)	0.0072(14)
C18	0.0278(14)	0.0292(14)	0.0308(14)	0.0100(12)	0.0027(11)	0.0121(12)
C19	0.0342(15)	0.0366(16)	0.0367(15)	0.0183(13)	0.0144(12)	0.0191(13)
C20	0.0415(17)	0.0386(17)	0.0471(18)	0.0166(15)	0.0249(15)	0.0208(14)
C21	0.0457(18)	0.0371(17)	0.0336(16)	0.0126(13)	0.0185(14)	0.0119(14)

C22	0.0425(18)	0.053(2)	0.0324(16)	0.0198(15)	0.0063(13)	0.0177(15)
C23	0.0324(15)	0.0465(18)	0.0334(15)	0.0167(14)	0.0085(12)	0.0179(14)
C24	0.0255(13)	0.0275(13)	0.0266(13)	0.0113(11)	0.0070(10)	0.0097(11)
C25	0.0420(17)	0.0325(16)	0.0462(18)	0.0166(14)	0.0130(14)	0.0169(14)
C26	0.057(2)	0.0340(17)	0.059(2)	0.0200(16)	0.0154(17)	0.0225(16)
C27	0.083(3)	0.042(2)	0.063(2)	0.0164(18)	0.022(2)	0.040(2)
C28	0.075(3)	0.056(2)	0.058(2)	0.0249(18)	0.036(2)	0.047(2)
C29	0.0506(19)	0.0386(17)	0.0385(16)	0.0160(14)	0.0198(14)	0.0273(15)
C30	0.0320(14)	0.0302(14)	0.0339(15)	0.0143(12)	0.0116(12)	0.0169(12)
C31	0.117(5)	0.095(4)	0.072(3)	0.006(3)	-0.039(3)	0.062(4)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 48.

	x/a	y/b	z/c	U(eq)
H1A	0.3932	0.7741	0.6475	0.042
H1B	0.2871	0.6842	0.6953	0.042
H3	0.2213	0.8209	0.8125	0.074
H4	0.2709	1.0136	0.9419	0.106
H5	0.5004	1.1914	0.9945	0.117
H6	0.6828	1.1738	0.9188	0.087
H10A	0.6808	1.1316	0.6837	0.097
H10B	0.8378	1.2530	0.7317	0.097
H10C	0.7174	1.2227	0.7914	0.097
H11A	0.8841	1.2021	0.9026	0.105
H11B	1.0068	1.2296	0.8441	0.105
H11C	0.9505	1.0947	0.8659	0.105

H12A	0.9085	0.9644	0.6997	0.094
H12B	0.9475	1.0941	0.6729	0.094
H12C	0.7949	0.9652	0.6268	0.094
H13	0.3124	0.5072	0.5226	0.052
H14	0.1255	0.4086	0.3927	0.07
H15	-0.1052	0.2655	0.3948	0.076
H16	-0.1537	0.2234	0.5273	0.07
H17	0.0324	0.3165	0.6552	0.052
H19	0.1157	0.5515	0.7739	0.04
H20	0.0468	0.5810	0.9151	0.049
H21	0.1641	0.5461	1.0285	0.049
H22	0.3539	0.4861	1.0020	0.051
H23	0.4253	0.4579	0.8614	0.044
H25A	0.2451	0.2311	0.7309	0.047
H25B	0.1929	0.1749	0.6213	0.047
H26A	0.4150	0.1397	0.7135	0.058
H26B	0.2603	0.0204	0.6568	0.058
H27A	0.4433	0.0185	0.5701	0.071
H27B	0.3161	0.0329	0.5179	0.071
H28A	0.5324	0.1881	0.5065	0.066
H28B	0.5929	0.2485	0.6153	0.066
H29A	0.5206	0.4002	0.5810	0.047
H29B	0.3639	0.2806	0.5282	0.047
H30	0.4771	0.3726	0.7204	0.036

Table 1. Sample and crystal data for (*R*)-38.

Identification code	39	
Chemical formula	$C_{18}H_{15}F$	
Formula weight	250.30	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal size	0.150 x 0.350 x 0.480 mm	
Crystal system	monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 5.90540(10) Å	α = 90°
	b = 16.7300(3) Å	β = 96.1650(10)°
	c = 13.3212(2) Å	γ = 90°
Volume	1308.49(4) $Å^3$	
Z	4	
Density (calculated)	1.271 g/cm^3	
Absorption coefficient	0.650 mm^{-1}	
F(000)	528	

Table 2. Data collection and structure refinement for (*R*)-38.

Theta range for data collection	3.34 to 68.54°
Index ranges	-6<=h<=6, -19<=k<=19, -14<=l<=15
Reflections collected	13728
Independent reflections	4325 [R(int) = 0.0245]
Coverage of independent reflections	94.0%
Absorption correction	numerical

Max. and min. transmission	0.9065 and 0.7460	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-97 (Sheldrick, 2008)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	4325 / 1 / 346	
Goodness-of-fit on F^2	1.051	
Δ/σ_{max}	0.001	
Final R indices	4271 data; $I>2\sigma(I)$	R1 = 0.0256, wR2 = 0.0743
	all data	R1 = 0.0259, wR2 = 0.0746
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0535P)^2+0.0621P]$ where $P=(F_o^2+2F_c^2)/3$	
Absolute structure parameter	-0.0(1)	
Extinction coefficient	0.0063(5)	
Largest diff. peak and hole	0.128 and -0.136 $eÅ^{-3}$	
R.M.S. deviation from mean	0.027 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å²) for (*R*)-38.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
F1	0.78102(16)	0.28608(5)	0.70926(7)	0.0617(2)
F2	0.25541(13)	0.02974(5)	0.77523(6)	0.0511(2)

C1	0.7711(2)	0.07812(8)	0.63582(10)	0.0406(3)
C2	0.8474(2)	0.15017(8)	0.67892(10)	0.0457(3)
C3	0.7067(2)	0.21504(8)	0.66718(10)	0.0416(3)
C4	0.4944(2)	0.21182(8)	0.61473(10)	0.0453(3)
C5	0.4221(2)	0.13964(8)	0.57175(10)	0.0414(3)
C6	0.55754(19)	0.07171(7)	0.58146(8)	0.0318(2)
C7	0.46627(19)	0.99324(7)	0.53480(8)	0.0326(2)
C8	0.3827(2)	0.00438(8)	0.42189(10)	0.0434(3)
C9	0.63220(18)	0.92413(6)	0.55010(8)	0.0301(2)
C10	0.82302(19)	0.91873(7)	0.49396(9)	0.0367(3)
C11	0.9720(2)	0.85664(7)	0.50721(10)	0.0363(3)
C12	0.94320(19)	0.79510(7)	0.57731(8)	0.0309(2)
C13	0.09678(19)	0.73014(7)	0.59358(9)	0.0364(3)
C14	0.0636(2)	0.67254(7)	0.66276(9)	0.0390(3)
C15	0.8750(2)	0.67610(8)	0.71843(9)	0.0393(3)
C16	0.72346(19)	0.73758(7)	0.70446(8)	0.0344(3)
C17	0.75329(18)	0.79895(6)	0.63399(8)	0.0285(2)
C18	0.60086(18)	0.86450(7)	0.61811(8)	0.0306(2)
C19	0.23448(19)	0.82968(7)	0.87665(9)	0.0361(3)
C20	0.16757(19)	0.89905(8)	0.82428(9)	0.0382(3)
C21	0.31925(19)	0.96132(7)	0.82591(8)	0.0358(3)
C22	0.53324(19)	0.95748(7)	0.87681(9)	0.0389(3)
C23	0.59690(19)	0.88762(7)	0.92893(9)	0.0381(3)
C24	0.44974(18)	0.82264(7)	0.93039(8)	0.0319(2)
C25	0.53247(18)	0.74660(7)	0.98635(9)	0.0346(3)
C26	0.6088(2)	0.76320(8)	0.09843(10)	0.0451(3)

C27	0.36375(18)	0.67799(6)	0.97332(9)	0.0314(2)
C28	0.17501(19)	0.67313(7)	0.03108(9)	0.0362(3)
C29	0.02140(19)	0.61201(7)	0.01739(9)	0.0346(3)
C30	0.04250(18)	0.55201(6)	0.94417(8)	0.0301(2)
C31	0.88028(19)	0.49013(7)	0.92416(9)	0.0354(3)
C32	0.9036(2)	0.43519(7)	0.85032(10)	0.0401(3)
C33	0.0923(2)	0.43779(7)	0.79438(9)	0.0381(3)
C34	0.2538(2)	0.49587(7)	0.81319(9)	0.0339(3)
C35	0.23254(18)	0.55543(6)	0.88714(8)	0.0283(2)
C36	0.38926(18)	0.61900(7)	0.90441(8)	0.0302(2)

Table 4. Bond lengths (Å) for (*R*)-38.

F1-C3	1.3662(15)	F2-C21	1.3615(14)
C1-C6	1.3892(17)	C1-C2	1.3893(18)
C2-C3	1.3656(19)	C3-C4	1.369(2)
C4-C5	1.3844(19)	C5-C6	1.3878(17)
C6-C7	1.5258(16)	C7-C9	1.5151(15)
C7-C8	1.5431(16)	C9-C18	1.3734(16)
C9-C10	1.4206(15)	C10-C11	1.3607(17)
C11-C12	1.4126(17)	C12-C13	1.4171(16)
C12-C17	1.4191(15)	C13-C14	1.3620(18)
C14-C15	1.4041(18)	C15-C16	1.3630(17)
C16-C17	1.4148(16)	C17-C18	1.4201(15)
C19-C20	1.3895(18)	C19-C24	1.3953(16)
C20-C21	1.3726(17)	C21-C22	1.3700(17)

C22-C23	1.3904(18)	C23-C24	1.3932(16)
C24-C25	1.5280(16)	C25-C27	1.5176(15)
C25-C26	1.5379(17)	C27-C36	1.3672(16)
C27-C28	1.4231(16)	C28-C29	1.3661(17)
C29-C30	1.4145(16)	C30-C31	1.4162(16)
C30-C35	1.4223(15)	C31-C32	1.3639(18)
C32-C33	1.4062(18)	C33-C34	1.3656(17)
C34-C35	1.4161(16)	C35-C36	1.4124(15)

Table 5. Bond angles (°) for (*R*)-38.

C6-C1-C2	121.23(12)	C3-C2-C1	118.42(11)
C2-C3-F1	118.68(12)	C2-C3-C4	122.66(11)
F1-C3-C4	118.66(12)	C3-C4-C5	118.06(12)
C4-C5-C6	121.77(11)	C5-C6-C1	117.86(11)
C5-C6-C7	119.45(10)	C1-C6-C7	122.68(10)
C9-C7-C6	114.00(9)	C9-C7-C8	110.96(10)
C6-C7-C8	110.80(10)	C18-C9-C10	118.15(10)
C18-C9-C7	120.80(10)	C10-C9-C7	121.05(10)
C11-C10-C9	121.25(10)	C10-C11-C12	121.33(10)
C11-C12-C13	122.64(10)	C11-C12-C17	118.49(10)
C13-C12-C17	118.87(10)	C14-C13-C12	120.65(11)
C13-C14-C15	120.49(11)	C16-C15-C14	120.41(11)
C15-C16-C17	120.77(11)	C16-C17-C12	118.81(10)
C16-C17-C18	122.49(10)	C12-C17-C18	118.70(10)
C9-C18-C17	122.08(10)	C20-C19-C24	121.49(11)

C21-C20-C19	118.43(10)	F2-C21-C22	118.45(11)
F2-C21-C20	119.00(10)	C22-C21-C20	122.55(11)
C21-C22-C23	118.17(11)	C22-C23-C24	121.82(10)
C23-C24-C19	117.54(11)	C23-C24-C25	119.29(9)
C19-C24-C25	123.13(10)	C27-C25-C24	113.72(9)
C27-C25-C26	111.59(10)	C24-C25-C26	111.61(9)
C36-C27-C28	118.10(10)	C36-C27-C25	120.30(10)
C28-C27-C25	121.60(10)	C29-C28-C27	121.20(10)
C28-C29-C30	121.12(10)	C29-C30-C31	122.73(10)
C29-C30-C35	118.21(10)	C31-C30-C35	119.05(10)
C32-C31-C30	120.64(10)	C31-C32-C33	120.57(11)
C34-C33-C32	120.14(11)	C33-C34-C35	121.07(10)
C36-C35-C34	122.52(10)	C36-C35-C30	118.96(10)
C34-C35-C30	118.50(10)	C27-C36-C35	122.37(10)

Table 6. Torsion angles (°) for (*R*)-38.

C6-C1-C2-C3	0.3(2)	C1-C2-C3-F1	-179.89(11)
C1-C2-C3-C4	-0.1(2)	C2-C3-C4-C5	-0.4(2)
F1-C3-C4-C5	179.46(12)	C3-C4-C5-C6	0.5(2)
C4-C5-C6-C1	-0.27(19)	C4-C5-C6-C7	178.39(11)
C2-C1-C6-C5	-0.19(19)	C2-C1-C6-C7	-178.80(11)
C5-C6-C7-C9	179.44(10)	C1-C6-C7-C9	-1.97(16)
C5-C6-C7-C8	53.42(14)	C1-C6-C7-C8	-127.99(12)
C6-C7-C9-C18	105.88(11)	C8-C7-C9-C18	-128.19(11)
C6-C7-C9-C10	-74.73(13)	C8-C7-C9-C10	51.20(14)

C18-C9-C10-C11	-0.37(16)	C7-C9-C10-C11	-179.78(10)
C9-C10-C11-C12	-0.04(18)	C10-C11-C12-C13	-179.30(11)
C10-C11-C12-C17	0.32(16)	C11-C12-C13-C14	179.30(11)
C17-C12-C13-C14	-0.32(16)	C12-C13-C14-C15	0.69(17)
C13-C14-C15-C16	-0.46(18)	C14-C15-C16-C17	-0.14(18)
C15-C16-C17-C12	0.50(16)	C15-C16-C17-C18	-179.22(10)
C11-C12-C17-C16	-179.91(10)	C13-C12-C17-C16	-0.27(14)
C11-C12-C17-C18	-0.18(14)	C13-C12-C17-C18	179.46(9)
C10-C9-C18-C17	0.52(15)	C7-C9-C18-C17	179.92(9)
C16-C17-C18-C9	179.47(10)	C12-C17-C18-C9	-0.24(15)
C24-C19-C20-C21	0.30(18)	C19-C20-C21-F2	-179.73(10)
C19-C20-C21-C22	0.17(18)	F2-C21-C22-C23	179.61(10)
C20-C21-C22-C23	-0.29(18)	C21-C22-C23-C24	-0.05(18)
C22-C23-C24-C19	0.49(17)	C22-C23-C24-C25	178.11(11)
C20-C19-C24-C23	-0.61(17)	C20-C19-C24-C25	-178.14(11)
C23-C24-C25-C27	-174.34(10)	C19-C24-C25-C27	3.15(16)
C23-C24-C25-C26	58.33(14)	C19-C24-C25-C26	-124.19(12)
C24-C25-C27-C36	98.96(12)	C26-C25-C27-C36	-133.70(11)
C24-C25-C27-C28	-80.59(13)	C26-C25-C27-C28	46.75(14)
C36-C27-C28-C29	-0.90(17)	C25-C27-C28-C29	178.66(10)
C27-C28-C29-C30	-0.99(17)	C28-C29-C30-C31	-176.61(10)
C28-C29-C30-C35	2.02(16)	C29-C30-C31-C32	177.66(10)
C35-C30-C31-C32	-0.95(15)	C30-C31-C32-C33	1.61(17)
C31-C32-C33-C34	-0.40(17)	C32-C33-C34-C35	-1.48(17)
C33-C34-C35-C36	-176.22(10)	C33-C34-C35-C30	2.08(16)
C29-C30-C35-C36	-1.18(14)	C31-C30-C35-C36	177.50(9)

C29-C30-C35-C34	-179.54(9)	C31-C30-C35-C34	-0.86(14)
C28-C27-C36-C35	1.75(16)	C25-C27-C36-C35	-177.82(9)
C34-C35-C36-C27	177.58(10)	C30-C35-C36-C27	-0.71(15)

Table 7. Anisotropic atomic displacement parameters (Å^2) for (*R*)-38.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	0.0848(6)	0.0394(5)	0.0614(5)	-0.0184(4)	0.0105(4)	-0.0157(4)
F2	0.0571(5)	0.0446(4)	0.0510(4)	0.0109(4)	0.0033(3)	0.0041(3)
C1	0.0399(7)	0.0361(6)	0.0438(6)	-0.0038(5)	-0.0040(5)	0.0042(5)
C2	0.0436(7)	0.0465(7)	0.0450(7)	-0.0088(6)	-0.0045(5)	-0.0045(6)
C3	0.0576(7)	0.0322(6)	0.0367(6)	-0.0070(5)	0.0121(5)	-0.0095(5)
C4	0.0541(7)	0.0327(7)	0.0495(7)	-0.0012(5)	0.0071(6)	0.0073(6)
C5	0.0372(6)	0.0386(7)	0.0476(7)	-0.0014(5)	0.0008(5)	0.0026(5)
C6	0.0328(6)	0.0324(6)	0.0308(5)	0.0019(4)	0.0060(4)	-0.0010(4)
C7	0.0314(5)	0.0321(6)	0.0344(6)	0.0023(5)	0.0042(4)	-0.0027(4)
C8	0.0496(7)	0.0404(7)	0.0384(6)	0.0010(5)	-0.0038(5)	-0.0017(5)
C9	0.0311(5)	0.0281(6)	0.0309(5)	-0.0028(4)	0.0029(4)	-0.0039(4)
C10	0.0395(6)	0.0331(6)	0.0389(6)	0.0028(5)	0.0108(5)	-0.0059(5)
C11	0.0340(6)	0.0368(6)	0.0400(6)	-0.0025(5)	0.0128(5)	-0.0054(5)
C12	0.0302(5)	0.0324(6)	0.0302(5)	-0.0060(5)	0.0035(4)	-0.0066(4)
C13	0.0313(5)	0.0408(6)	0.0372(6)	-0.0066(5)	0.0046(4)	0.0003(5)
C14	0.0362(6)	0.0371(6)	0.0421(6)	-0.0027(5)	-0.0034(5)	0.0065(5)
C15	0.0428(7)	0.0394(7)	0.0343(6)	0.0065(5)	-0.0019(5)	-0.0017(5)
C16	0.0341(6)	0.0392(7)	0.0298(5)	0.0009(5)	0.0036(4)	-0.0030(5)

C17	0.0290(5)	0.0291(6)	0.0268(5)	-0.0049(4)	0.0000(4)	-0.0055(4)
C18	0.0300(5)	0.0320(6)	0.0302(5)	-0.0041(4)	0.0046(4)	-0.0033(4)
C19	0.0288(5)	0.0359(6)	0.0428(6)	-0.0054(5)	0.0005(5)	-0.0051(4)
C20	0.0309(6)	0.0433(7)	0.0392(6)	-0.0035(5)	-0.0014(5)	0.0012(5)
C21	0.0405(6)	0.0362(6)	0.0316(6)	-0.0006(5)	0.0078(5)	0.0025(5)
C22	0.0367(6)	0.0371(7)	0.0431(6)	-0.0025(5)	0.0056(5)	-0.0081(5)
C23	0.0282(6)	0.0430(7)	0.0425(6)	-0.0037(5)	0.0001(5)	-0.0031(5)
C24	0.0276(5)	0.0329(6)	0.0351(5)	-0.0071(5)	0.0031(4)	0.0001(4)
C25	0.0275(5)	0.0328(6)	0.0432(6)	-0.0074(5)	0.0027(4)	0.0015(4)
C26	0.0477(7)	0.0407(7)	0.0444(7)	-0.0043(5)	-0.0070(5)	-0.0001(5)
C27	0.0296(5)	0.0289(6)	0.0352(6)	-0.0008(5)	0.0009(4)	0.0035(4)
C28	0.0384(6)	0.0336(6)	0.0374(6)	-0.0070(5)	0.0074(5)	0.0067(5)
C29	0.0315(6)	0.0384(6)	0.0356(6)	0.0025(5)	0.0108(5)	0.0047(5)
C30	0.0299(5)	0.0303(6)	0.0298(5)	0.0075(4)	0.0016(4)	0.0052(4)
C31	0.0313(6)	0.0357(6)	0.0390(6)	0.0085(5)	0.0035(5)	-0.0008(5)
C32	0.0414(6)	0.0328(6)	0.0442(7)	0.0055(5)	-0.0040(5)	-0.0055(5)
C33	0.0499(7)	0.0304(6)	0.0330(6)	-0.0010(5)	-0.0006(5)	0.0009(5)
C34	0.0390(6)	0.0322(6)	0.0309(5)	0.0024(5)	0.0055(5)	0.0039(5)
C35	0.0293(5)	0.0277(6)	0.0274(5)	0.0052(4)	0.0004(4)	0.0041(4)
C36	0.0281(5)	0.0317(6)	0.0312(5)	0.0026(4)	0.0056(4)	0.0038(4)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å²) for (*R*)-38.

	x/a	y/b	z/c	U(eq)
H1A	0.8667	1.0324	0.6437	0.049
H2A	0.9940	1.1542	0.7157	0.055

H4A	0.3996	1.2578	0.6080	0.054
H5A	0.2757	1.1365	0.5346	0.05
H7A	0.3301	0.9785	0.5694	0.039
H8A	0.3383	0.9524	0.3919	0.065
H8B	0.5055	1.0273	0.3871	0.065
H8C	0.2513	1.0405	0.4150	0.065
H10A	0.8470	0.9592	0.4463	0.044
H11A	1.0980	0.8546	0.4685	0.044
H13A	1.2241	0.7267	0.5559	0.044
H14A	1.1688	0.6296	0.6734	0.047
H15A	0.8529	0.6354	0.7661	0.047
H16A	0.5963	0.7393	0.7425	0.041
H18A	0.4732	0.8672	0.6557	0.037
H19A	0.1313	0.7860	0.8759	0.043
H20A	0.0203	0.9033	0.7882	0.046
H22A	0.6353	1.0014	0.8765	0.047
H23A	0.7448	0.8841	0.9645	0.046
H25A	0.6712	0.7287	0.9557	0.041
H26A	0.6589	0.7132	1.1321	0.068
H26B	0.4810	0.7855	1.1305	0.068
H26C	0.7351	0.8015	1.1040	0.068
H28A	0.1555	0.7131	1.0800	0.043
H29A	-0.1017	0.6098	1.0577	0.042
H31A	-0.2460	0.4868	0.9625	0.042
H32A	-0.2086	0.3948	0.8366	0.048
H33A	0.1075	0.3990	0.7434	0.046

H34A	0.3824	0.4963	0.7761	0.041
H36A	0.5170	0.6208	0.8668	0.036