SUPPORTING INFORMATION APPENDIX

A Combination of Directing Groups and Chiral Anion Phase-Transfer Catalysis for Enantioselective Fluorination of Alkenes

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CONTENTS

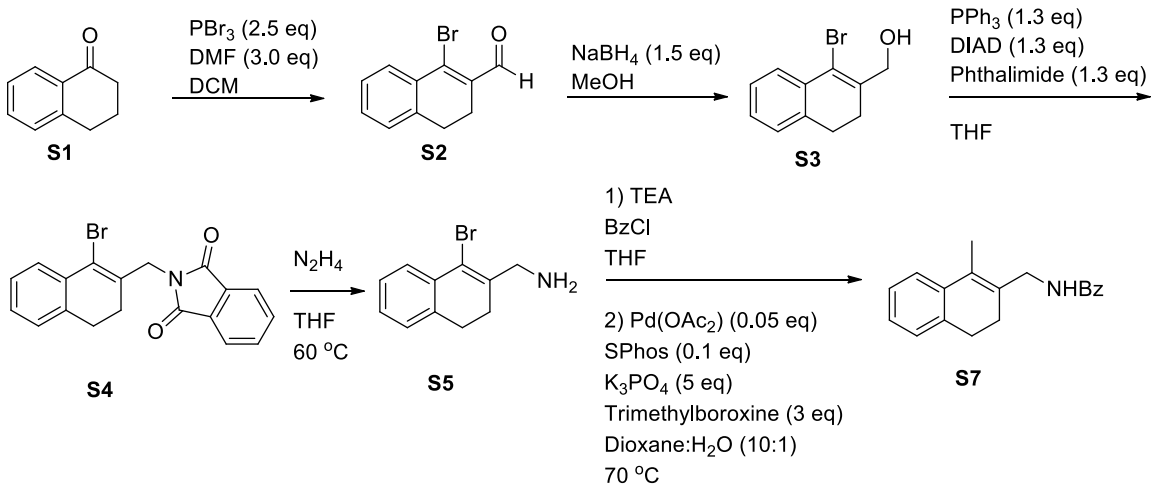
(NMR and HPLC spectra follow)

Supporting Information

General Information. Unless otherwise noted, reagents were obtained from commercial sources and used without further purification. All reactions were carried out under N_2 using Schlenk line techniques, unless otherwise stated. Dry and degassed THF, dichloromethane, diethyl ether, toluene, triethylamine, and dimethylformamide were obtained by passage through activated alumina columns under argon. All other dried solvents were obtained by storage over 3Å or 4Å molecular sieves overnight. TLC analysis of reaction mixtures was performed on Merck silica gel 60 F254 TLC plates and visualized by UV. Flash chromatography was carried out with ICN SiliTech 32-63 D 60 Å silica gel. Standard aqueous workup refers to extraction with the indicated solvent, followed by drying of the combined organic layers with magnesium sulfate, gravity filtration, and removal of solvent by rotary evaporation. ^{1}H and ^{13}C NMR spectra were recorded with Bruker AV-300, AVQ-400, AVB-400, AV-500, DRX-500, and AV-600 spectrometers and were referenced to ^{1}H (residual) and ^{13}C signals of the deuterated solvents, respectively.[1] Mass spectral and microanalytical data were obtained via the Micro-Mass/Analytical Facility operated by the College of Chemistry, University of California, Berkeley. X-Ray crystallographic analysis was carried out by Dr. Antonio DiPasquale at the College of Chemistry X-Ray Crystallographic Facility (CHEXRAY, University of California, Berkeley).

[1] According to values listed in Fulmer, G. R.; Miller, A. J. M.; Sherden, N. H.; Gottlieb, H. E.; Nudelman, A.; Stoltz, B. M.; Bercaw, J. E.; Goldberg, K. I. *Organometallics*, 2010, 29 (9), pp 2176–2179.

Representative synthesis of substrates



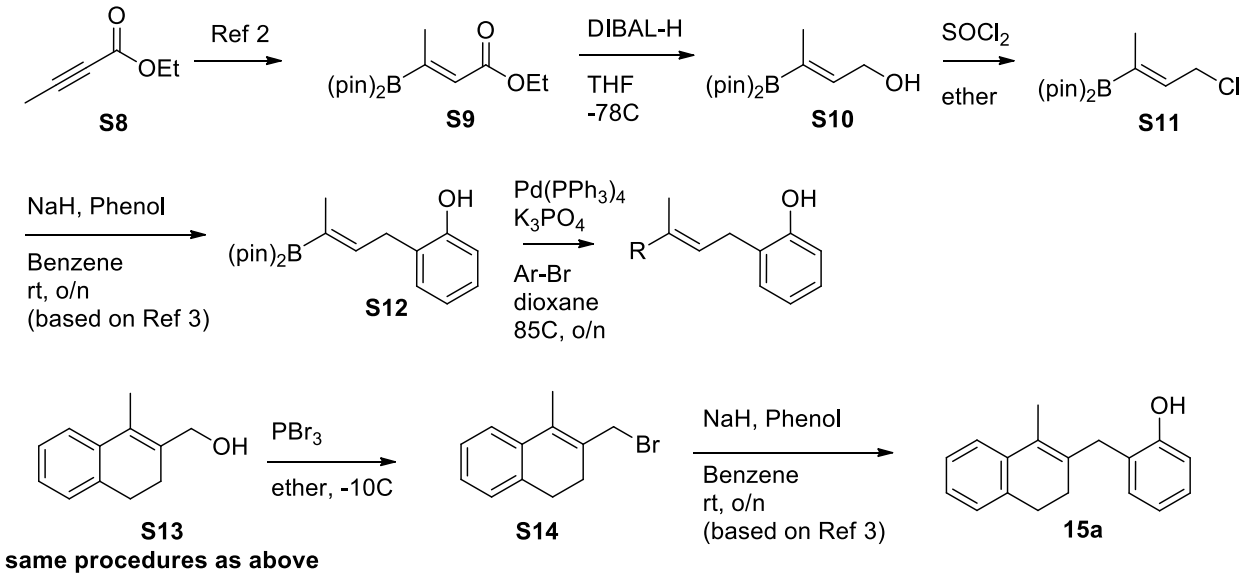
PBr_3 (8 mL, 2.5 equiv.) was added to DMF (7.8mL, 3.0 equiv.) in DCM (150 mL) at 0 °C then warmed to room temperature for 1.5 h. Starting material tetralone (5 g, 33.7mmol) was added as a solution in DCM (15 mL), then the mixture was refluxed. The reaction was quenched with water at 0 °C followed by 20 min of stirring and extraction with DCM. The organic phase was washed with brine and dried with magnesium sulfate. $NaBH_4$ (0.19 g, 1 equiv.) was added to **S2** (4.94 mmol) in MeOH (30 mL) at 0 °C and stirred for one hour. The reaction was warmed up to room temperature and stirred another hour before evaporation of the solvent. The crude mixture was partitioned between methylene chloride and water, and the organic layer separated, dried with magnesium sulfate, and chromatographed (EtOAc: Hex; 3:1) to provide white solid **S3** (88% yield).

S3 was combined with PPh_3 (1.3 equiv) and phthalimide (1.3 equiv) in THF and cooled to 0 °C, followed by slow addition (over 30 min.) of DIAD (1.3 equiv). The reaction was warmed up to room temperature and stirred another 2 h, followed by direct silica-gel chromatography (EtOAc: Hex, 4:1) to provide solid **S4** (57%).

Hydrazine hydrate (7 equiv) was added to **S4** in THF and heated to 60 °C for 16 h. The reaction mixture was diluted with methylene chloride and filtered with Celite. The organic layer was washed with water, then brine, and dried with magnesium sulfate to provide amine **S5** (95%).

Triethylamine and benzoyl chloride were added to **S5** in THF at 0 °C, and warmed up to room temperature immediately. The reaction was stirred for 8 h followed by filtration with Celite. The filtrate was partitioned between ethyl acetate and water, and the organic layer was separated, washed with brine, and dried with magnesium sulfate. Silica gel chromatography (EtOAc: Hex, 4:1) provided **S6** (85%).

$Pd(OAc)_2$ (0.05 equiv), SPhos (0.1 equiv), K_3PO_4 (5 equiv), and trimethylboroxine (3 equiv) were added to **S6** in dioxane:H_2O (10:1, 0.2 M) at room temperature, then heated to 70 °C for 18 h. The reaction mixture was filtered with Celite, followed by extraction with ethyl acetate. The organic layer was washed with ammonium chloride (sat. aq.), followed by water, then brine, and then dried with magnesium sulfate. Chromatography (EtOAc: Hex, 4:1) provided **S7** (80%).



S9 was prepared from **S8** by a precedented method.[2] Dropwise DIBAL-H addition to a THF solution of **S9** at -78°C followed by stirring for 2 h, the reaction was warmed up to 0 °C and quenched with sodium sulfate decahydrate. Vigorous stirring followed by filtration with Celite provided **S10** as an oil. Purification was done with silica gel column chromatography (0-30% EtOAc in Hexanes); fractions visualized by iodine stain.
Thionyl chloride was added dropwise to **S10** in ether at 0 °C and the reaction was stirred for 3 h. The reaction was quenched with sodium bicarbonate (saturated aqueous solution) and extracted with ether. The organic layer was washed with brine, dried with magnesium sulfate and used without further purification.
Phenol and sodium hydride were combined at 0 °C in benzene as a slurry. After 15 minutes of stirring, allylic chloride **S11** was added as a solution in benzene. The reaction stirred at rt for 18 h followed by evaporation of solvent, followed by aqueous workup as described in the literature.[3] **S12** was subjected to $Pd(PPh_3)_4$, K_3PO_4, and ArBr in dioxane under nitrogen at 85°C for 18 h, followed by filtration with Celite. Silica gel column chromatography (0-25% EtOAC in Hexanes) provided substrates.

$SOCl_2$ was added as a solution in DCM to **S13** (which was prepared with procedures described on the previous page) in diethyl ether at 0 °C. The reaction was quenched after 3 h at room temperature, with sodium bicarbonate (saturated aqueous solution), then extracted with ether. The organic layer was washed with brine, dried with magnesium sulfate, concentrated and used without further purification.
Substrate **15a** were prepared following the procedure used with intermediate **S11**.[3]

2. Ji-Eon Lee , Jisook Kwon and Jaesook Yun, *Chem. Commun.*, **2008**, 733-734.
3. Raissa M. Trend , Yeeman K. Ramtohul , and Brian M. Stoltz. *J. Am. Chem. Soc.*, **2005**, *127* (50), 17778–17788.

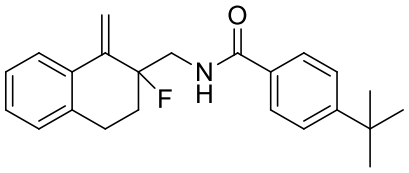
General procedure for phase transfer fluorination reactions. A one dram vial was charged with substrate (0.05-0.10 mmol), toluene (0.03 M in substrate), and a 1/2''× 1/8'' magnetic stirbar. Phosphoric acid catalyst (0.10 eq), Selectfluor (1.35 eq), and sodium carbonate (1.45 eq) were added under air, and the reaction mixture was stirred vigorously for 18 h. The reaction mixture was then directly subjected to column chromatography to afford the fluorinated product. For the one-pot dihalogenation reaction, bromination reagent (1.35 eq) and sodium carbonate (1.45 eq) were added to the reaction vial after fluorination for 18 h. The reaction mixture was stirred for an additional 18 h, and the desired dihalogenation product was isolated by column chromatography.

Characterization data of substrates and products – proton, carbon, fluorine NMR where applicable; HRMS or elemental analysis.

1a

^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.73 (d, J = 8.5 Hz, 2H), 7.47 (d, J = 8.5 Hz, 2H), 7.34-7.14 (m, 4H), 6.06 (s, 1H), 4.35 (d, J = 5 Hz, 2H), 2.77 (t, J = 7.5 Hz, 2H), 2.37-2.34 (m, 2H), 2.18 (s, 3H), 1.35 (s, 9H).^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.7, 155.0, 136.4, 135.8, 131.9, 131.7, 129.2, 127.2, 126.9, 126.7, 126.5, 125.5, 123.3, 42.2, 35.0, 31.2, 28.5, 26.9, 14.3.
HRMS (ESI) Calcd. [M+H] $C_{23}H_{28}ON$: 334.2165; found: 334.2170.

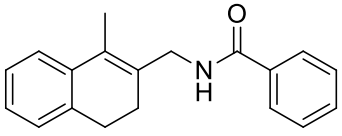
1b



^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.75 (d, J = 8.5 Hz, 2H), 7.63 (d, J = 7 Hz, 1H), 7.49 (d, J = 8.5 Hz, 2H), 7.28-7.21 (m, 2H), 7.16-7.15 (m, 1H), 6.47 (s, 1H), 5.75 (s,1H), 5.50 (s, 1H), 4.24-4.13 (m, 1H), 3.48-3.42 (m, 1H), 3.16-3.12 (m, 1H), 2.99-2.94 (m, 1H), 2.26-2.14 (m, 2H), 1.36 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.3, 155.2, 143.9 (d, J_{C-F} = 16.1 Hz), 134.9, 132.5, 131.3, 128.9, 128.4, 128.0, 126.8, 126.5, 125.6, 125.1, 124.8, 108.9 (d, J_{C-F} = 12.1 Hz), 96.5 (d, J_{C-F} = 180 Hz), 44.7 (d, J_{C-F} = 24.1 Hz), 34.9, 31.1, 30.3 (d, J_{C-F} = 21.1 Hz), 26.9 (d, J_{C-F} = 11.1 Hz). ^{19}F-NMR (376.4 MHz) δ (ppm) –161.0 - –161.2 (m).
HRMS (ESI) Calcd. for [M+H] $C_{23}H_{27}ONF$: 352.2071; found: 352.2074.
HPLC (ChiralPak IC column) 92:08 (hexane:*i*PrOH) 1mL/min; T_{major} (22.172 min), T_{minor} (25.260 min)

Catalysts **2-4** are either commercially available or previously reported.

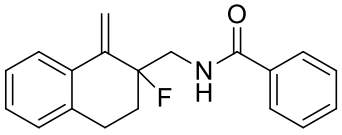
5a



^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.79 (d, *J* = 7.0 Hz, 2H), 7.54-7.44 (m, 3H), 7.34-7.32 (m, 1H), 7.26-7.19 (m, 1H), 7.18-7.14 (m, 2H), 6.10 (brs, 1H), 4.36 (d, *J* = 5.5 Hz, 2H), 2.78 (t, *J* = 7.5 Hz, 2H), 2.37 (t, *J* = 7 Hz, 2H), 2.18 (s, 3H). ^{13}C NMR (125 MHz,

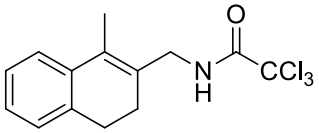
$CDCl_3$) δ (ppm) 167.7, 136.3, 135.8, 134.6, 131.6, 131.5, 129.5, 128.7, 127.2, 126.9, 126.8, 126.5, 123.3, 42.4, 28.5, 27.0, 14.3.
HRMS (ESI) Calcd. for [M+H]$C_{19}H_{20}ON$ 278.1539, found: 278.1547.

5b



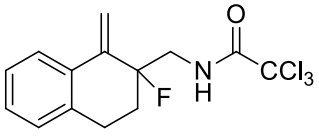
^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.81 (d, J = 7.5 Hz, 2H), 7.63 (d, J = 7.5 Hz, 1H), 7.56-7.53 (m, 1H), 7.49-7.46 (m, 2H), 7.26-7.21 (m,2H), 7.16-7.15 (m, 1H), 6.49 (brs, 1H), 5.75 (s, 1H), 5.51 (s, 1H), 4.23-4.13 (m, 1H), 3.50-3.43 (m, 1H), 3.19-3.12 (m, 1H), 2.99-2.96 (m, 1H), 2.27-2.12 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.5, 143.9 (d, J_{C-F} = 16.3 Hz), 134.9, 134.3, 132.5, 131.7, 129.0, 128.7, 128.5, 128.1, 127.1 (d, J_{C-F} = 19.0 Hz), 126.6, 124.9, 109.0 (d, J_{C-F} = 11.3 Hz), 97.2, 95.8, 44.8 (d, J_{C-F} = 25.0 Hz), 30.4 (d, J_{C-F} = 21.3 Hz), 27.0 (d, J_{C-F} = 11.3 Hz).^{19}F-NMR (376.5 MHz) δ (ppm) –150.03 - -150.06 (m).
HRMS (ESI) Calcd. for [M+H] $C_{19}H_{20}ON$ 296.1445; found: 296.1452.
HPLC (ChiralPak IC column) 92:08(hexane:*i*PrOH) 1mL/min; T_{major} (18.224 min), T_{minor} (19.572 min)

6a



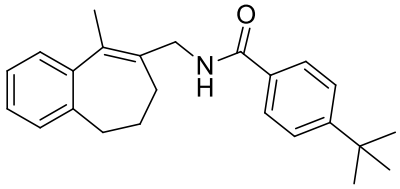
^{1}H-NMR (500MHz, $CDCl_3$) δ (ppm) 7.34-7.24 (m, 2H), 7.21-7.15 (m, 2H), 6.67 (brs, 1H), 4.27 (d, J = 5.5 Hz, 2H), 2.79 (t, J = 7.5 Hz, 2H), 2.32 (t, J = 7.5 Hz, 2H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.1, 136.0, 135.7, 130.6, 129.7, 127.3, 127.1, 126.6, 123.5, 92.7, 43.8, 28.4, 26.8, 14.3.
Elemental analysis (CHN) est: 52.77% C, 4.43% H, 4.4% N; found: 52.49% C, 4.53% H, 4.51% N.

6b



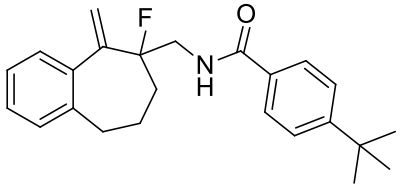
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.64 (d, J = 7.6 Hz, 1H), 7.30-7.24 (m, 2H), 7.19-7.17 (m, 1H), 7.03 (brs, 1H), 5.78 (d, J = 3.2 Hz, 1H), 5.52 (s, 1H), 4.01-3.89 (m, 1H), 3.56-3.47 (m, 1H), 3.10-3.02 (m, 2H), 2.28-2.16 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.2, 143.1 (d, J_{C-F} = 16.1 Hz), 134.5, 132.2 (d, J_{C-F} = 4.0 Hz), 128.9, 128.6, 126.8, 125.0 (d, J_{C-F} = 2.0 Hz), 109.6 (J_{C-F} = 16.1 Hz), 95.8 (d, J_{C-F} = 182 Hz), 92.5, 46.1 (d, J_{C-F} = 24.1 Hz), 30.4 (d, J_{C-F} = 21.1 Hz), 26.9 (d, J_{C-F} = 10.1 Hz). ^{19}F-NMR (376.5 MHz) δ (ppm) – 150.59 (m). Elemental analysis (CHN) est: 49.95% C, 3.89% H, 4.16% N; found: 48.96% C, 4.11% H, 3.81% N.
HPLC (ChiralPak IC column) 98:02 (hexane/*i*PrOH) 1mL/min; T_{major} (9.50 min), T_{minor} (10.90 min).

7a



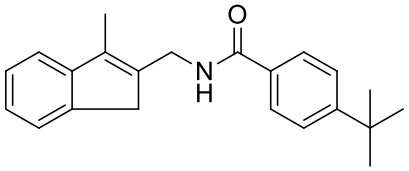
^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.73 (d, J = 8.2 Hz, 2H), 7.46 (d, J = 8.2 Hz, 2H), 7.28-7.24 (m, 2H, overlaps $CDCl_3$) 7.17 (d, J = 2.4 Hz, 2H), 6.11 (s, 1H), 4.33 (d, J = 5.3 Hz, 2H), 2.55 (t, J = 7.1 Hz, 2H), 2.17 (s, 3H), 2.13 – 2.02 (m, 2H), 1.93 – 1.86 (m, 2H), 1.34 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167, 155.0, 143.2, 140.0, 133.5, 132.6, 131.8, 128.5, 126.7, 126.7, 126.5, 126.1, 125.6, 42.2, 35.0, 34.6, 32.1, 31.2, 28.6, 18.3.
HRMS (ESI) Calcd. for [M+H] C24H30ON: 348.2322; found: 348.2330.

7b



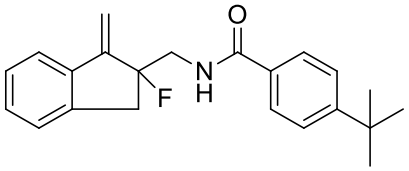
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.93 (d, J = 8.0 Hz, 2H), 7.70 (d, J = 8.0 Hz, 2H), 7.22-7.09 (m, 4H), 6.29 (brs, 1H), 5.64 (s, 1H), 5.22-5.21 (m, 1H), 3.81-3.70 (m, 1H), 3.58-3.45 (m, 1H), 2.82-2.76 (m, 2H), 2.22-1.63 (overlapping multiplets, 4H), 1.35 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.1, 155.1, 151.3 (d, $J_{C\text{-}F}$ = 19.5 Hz), 151.2, 139.5, 138.8 (d, $J_{C\text{-}F}$ = 5.1 Hz), 131.6, 129.3, 128.9, 128.3, 128.0, 126.8, 126.7, 125.6, 125.3, 114.7 (d, $J_{C\text{-}F}$ = 12.1 Hz), 98.2 (d, $J_{C\text{-}F}$ = 178 Hz), 97.30, 45.0 (d, $J_{C\text{-}F}$ = 20.4 Hz), 38.6 (d, $J_{C\text{-}F}$ = 23.6 Hz), 34.96, 31.19, 23.5 (d, $J_{C\text{-}F}$ = 11.2 Hz).
^{19}F-NMR (376.5 MHz) δ (ppm) -147.2 (broad multiplet), -149.2 (m), -151.36-151.42 (m)
HRMS (ESI) Calcd. for [M+H] $C_{24}H_{29}ONF$: 366.2228; found: 366.2229.
HPLC (ChiralPak IB column) 95:05 (hexane: *i*PrOH) 1mL/min; T_{major} (9.540 min), T_{minor} (8.808 min).

8a



^{1}H-NMR (300 MHz, $CDCl_3$) δ (ppm) 7.72-7.69 (m, 2H), 7.45-7.38 (m, 3H), 7.31-7.30 (m, 2H), 7.20-7.18 (m, 1H), 4.51 (d, J = 5.4 Hz, 2H), 3.42 (s, 2H), 2.17 (s, 3H),1.32 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.3, 155.0, 146.4, 142.5, 137.3, 136.2, 131.5, 126.7, 126.3, 125.5, 124.8, 123.4, 118.9, 39.6, 37.5, 34.9, 31.1, 10.4.
HRMS (ESI) Calcd. For $C_{22}H_{26}ON$: 320.201; found: 320.2015.

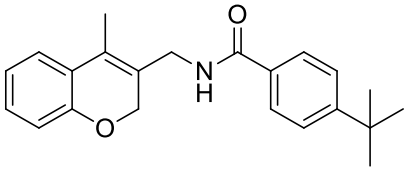
8b



^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.71 (d, J = 8.0 Hz, 2H), 7.53-7.46 (m, 3H), 7.27-7.24 (3H), 6.48 (brs, 1H), 5.78 (d, J = 4.0 Hz, 1H), 5.44 (s, 1H), 4.16-

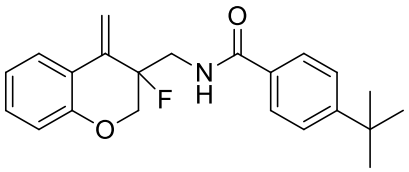
4.04 (m, 1H), 3.79-3.72 (m, 1H), 3.42-3.21 (m, 2H), 1.35 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.6, 155.3, 149.1 (d, J_{C-F} = 17.1 Hz), 140.7 (d, J_{C-F} = 3.0 Hz), 137.9 (d, J_{C-F} = 3.0 Hz), 131.3, 129.7, 127.4, 126.9, 125.6, 125.5, 121.1, 107.6 (d, J_{C-F} = 6.0 Hz), 101.7 (d, J_{C-F} = 182 Hz), 45.9 (d, J_{C-F} = 28.2 Hz), 40.7 (d, J_{C-F} = 14.1 Hz), 35.0, 31.2. ^{19}F-NMR (376.4 MHz) δ (ppm) –144.78 - –144.81 (m).
HRMS (ESI) Calcd. for $C_{22}H_{25}ONF$: 338.1915; found: 352.1923.
HPLC (ChiralPak IC column) (90:10 hexane:*i*PrOH) 1mL/min; T_{major} (22.436 min), T_{minor} (20.620 min).

9a



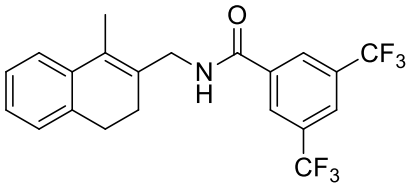
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.72 (d, 8.4Hz, 2H), 7.45 (d, 8.4Hz, 2H), 7.27-7.13 (m, 2H), 6.97-6.93 (m, 1H), 6.83 (d, 7.6Hz, 1H), 6.18 (s, 1H), 4.71 (s, 2H), 4.25 (d, 5.6Hz, 2H), 2.11 (s, 3H), 1.33 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.8, 155.2, 153.8, 131.2, 128.9, 127.4, 126.9, 125.6, 125.4, 124.7, 123.9, 121.4, 115.8, 67.0, 38.7, 35.0, 31.2, 12.9.
HRMS (ESI) Calcd. for [M+H] $C_{22}H_{26}O_2N$: 336.1958; found: 336.1963.

9b



^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.75 (d, J = 8.4 Hz, 2H), 7.62-7.60 (m, 1H), 7.50 (d, J = 8.4 Hz, 2H), 7.30-7.25 (m, 1H), 7.04-6.96 (m, 2H), 6.43 (brs, 1H), 5.811 (s, 1H), 5.50 (s, 1H), 4.37-4.33 (m, 1H), 4.24-4.12 (m, 2H), 3.82-3.72 (m, 1H), 1.38 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.4, 155.3, 152.9, 138.5 (d, J_{C-F} = 17.1 Hz), 131.2, 130.2, 126.9, 125.6, 124.7, 122.0, 119.3, 117.6, 107.3 (d, J_{C-F} = 10.1 Hz), 90.8 (d, J_{C-F} = 183 Hz), 68.0 (d, J_{C-F} = 30.2 Hz), 43.3 (d, J_{C-F} = 24.1 Hz), 35.0, 31.2. ^{19}F-NMR (376.4 MHz) δ (ppm) –166.28 - –166.40 (m).
HRMS (ESI) Calcd. for [M+H] $C_{22}H_{25}O_2NF$: 354.1864; found: 354.1874.
HPLC (ChiralPak IC column) 90:10 (hexane/*i*PrOH) 1mL/min; T_{major} (28.140 min), T_{minor} (31.536 min)

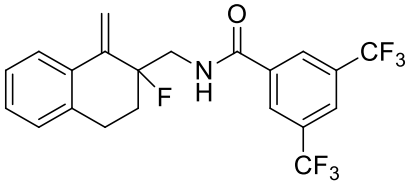
10a



^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 8.24 (s, 2H), 8.032 (s, 1H), 7.66 -7.64 (m, 1H), 7.25-7.20 (m, 1H), 7.13-7.11 (m, 1H), 6.51 (brs, 1H), 4.56-4.55 (m, 2H), 2.86 (t, J = 8.0 Hz, 2H), 2.57 (ts, J = 8.0 Hz, 2H), 1.57 (s, 3H).
^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 164.8, 136.5, 136.0, 135.7, 132.7, 132.4, 132.1, 131.8,

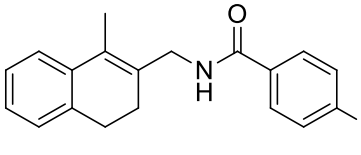
130.5, 130.2, 127.3, 127.0, 126.6, 125.1, 125.1, 125.0, 125.0, 124.0, 123.4, 121.8, 42.8, 28.4, 27.1, 14.4. HRMS (ESI) Calcd. For $C_{21}H_{18}ONF_6$: 414.1287, found: 414.1303.

10b



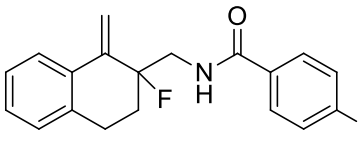
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 8.23 (s, 2H), 8.04 (s, 1H), 7.63-7.61 (m, 1H), 7.26-7.15 (m, 4H), 6.58 (brs, 1H), 5.76 (s, 1H), 5.50 (s, 1H), 4.21 -4.08 (m, 1H), 3.59-3.51 (m, 1H), 3.13-2.89 (m, 2H), 2.23-2.21 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 164.6, 143.6 (d, $J_{C\text{-}F}$ = 16.3 Hz), 136.3, 134.6, 132.5, 132.3 (d, $J_{C\text{-}F}$ = 17.6 Hz), 129.0, 128.6, 127.4, 126.7, 125.3, 124.9, 109.2 (d, $J_{C\text{-}F}$ = 12.5 Hz), 96.7 (d, $J_{C\text{-}F}$ = 179.8 Hz), 45.1 (d, $J_{C\text{-}F}$ = 23.9 Hz), 30.5 (d, $J_{C\text{-}F}$ = 21.4 Hz), 26.9 (d, $J_{C\text{-}F}$ = 11.3 Hz). ^{19}F-NMR (376.5 MHz) δ (ppm) –62.1 (s), -150.0 (m).
HRMS (ESI) Calcd. for [M+H] $C_{21}H_{17}ONF_7$: 432.119; found: 432.121.
HPLC (ChiralPak IB column) 99:01 (hexane/*i*PrOH) 1mL/min; T_{major} (21.40 min), T_{minor} (24.99min).

11a



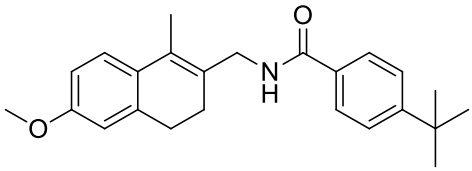
^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 8.33-8.29 (m, 2H), 8.00-7.94 (m, 2H), 7.34-7.28 (m, 1H), 7.26-7.14 (m, 3H), 6.23 (brs, 1H), 4.38-4.37 (m, 2H), 2.87 (t, *J* = 8.0 Hz, 2H), 2.38-2.35 (m, 2H), 2.19 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 165.7, 149.6, 140.1, 136.1, 135.7, 130.7, 130.0, 128.2, 127.3, 127.0, 126.6, 123.8, 123.4; 42.7, 28.4, 27.1, 14.3.
HRMS (ESI) Calcd. for [M+H] $C_{19}H_{19}O_3N_2$: 323.139; found: 323.1402.

11b



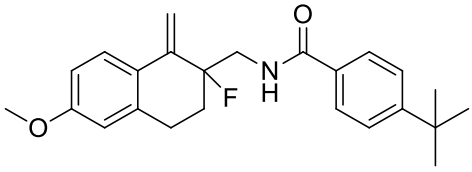
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 8.32 (d, *J* = 8.8 Hz, 2H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.62-7.60 (m, 1H), 7.25-7.15 (m, 4H), 6.50 (brs, 1H), 5.74 (m, 1H), 5.49 (s, 1H), 4.19-4.07 (m, 1H), 3.58-3.48 (m, 1H), 3.19-2.97 (m, 2H), 2.23-2.16 (m, 2H).
^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 165.5, 149.7, 143.6 (d, $J_{C\text{-}F}$ = 16.3 Hz), 139.8, 134.6, 132.3 (d, $J_{C\text{-}F}$ = 16.3 Hz), 128.97-128.61, 128.2, 126.7, 124.9, 124.0, 109.2 (d, $J_{C\text{-}F}$ = 11.3 Hz), 96.2 (d, $J_{C\text{-}F}$ = 181.0 Hz), 45.0 (d, $J_{C\text{-}F}$ = 23.9 Hz), 30.6 (d, $J_{C\text{-}F}$ = 21.4 Hz), 27.0 (d, $J_{C\text{-}F}$ = 10.1 Hz). ^{19}F-NMR (376.5 MHz) δ (ppm) –150.31 (m).
HRMS (ESI) Calcd. for [M+H] $C_{19}H_{18}O_3N_2F$: 341.1296; found: 341.1307.
HPLC (ChiralPak IA column) 90:10 (hexane/*i*PrOH) 1mL/min; T_{major} (15.868 min), T_{minor} (18.700 min).

12a



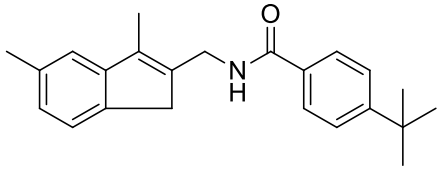
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.74 (d, *J* = 8 Hz, 2H), 7.44-7.42 (m, 2H), 7.27 -7.21 (m, 1H), 6.75-6.70 (m, 2H), 6.33 (brs, 1H), 4.41-4.29 (m, 2H), 3.93 (s, 3H), 2.74-2.7 (t, *J* = 8 Hz, 2H), 2.33-2.31 (m, 2H), 2.12 (s, 3H), 1.33 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.6, 158.3, 154.8, 137.6, 131.7, 129.4, 129.3, 128.8, 126.8, 125.4, 124.5, 113.3, 111.0, 55.2, 42.2, 34.9, 31.1, 28.9, 26.8, 14.2.
HRMS (ESI) Calcd. For $C_{24}H_{30}O_2N$: 364.227, found: 364.228.

12b



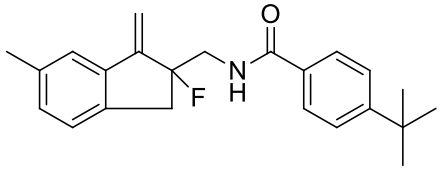
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.77 (d, *J* = 8.4 Hz, 2H), 7.58 (d, *J* = 8.8 Hz, 1H), 7.52-7.50 (m, 2H), 6.83-6.81 (m, 1H), 6.67 (s, 1H), 6.48-6.47 (m, 1H), 5.63-5.62 (m, 1H), 5.40 (s, 1H), 4.27-4.14 (m, 1H), 3.84 (s, 3H), 3.50-3.41 (m, 1H), 3.21-3.14 (m, 1H), 2.96-2.92 (m,1H), 2.27-2.13 (m, 2H), 1.39 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.4, 159.7, 155.3, 143.5, 136.4, 131.4, 126.8, 126.3, 125.6, 125.4, 113.6, 112.7, 106.7 (d, $J_{C\text{-}F}$ = 12.5 Hz), 55.3, 44.7 (d, $J_{C\text{-}F}$ = 23.9 Hz), 35.0, 31.2, 30.2 (d, $J_{C\text{-}F}$ = 21.4 Hz), 27.3 (d, $J_{C\text{-}F}$ = 11.3 Hz). ^{19}F-NMR (376.5 MHz) δ (ppm) – 150.3 (m).
HRMS (ESI) Calcd. for [M+H] $C_{24}H_{29}O_2NF$: 383.2177; found: 382.2187.
HPLC (ChiralPak IC column) 96:04 (hexane/*i*PrOH) 1mL/min; T_{major} (60.28 min), T_{minor} (64.92 min).

13a



^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.72 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.27 (s, 1H), 7.13 (s, 1H), 7.02-7.01 (m, 1H), 6.26 (brs, 1H), 4.51 (d, *J* = 5.6 Hz, 2H), 3.38 (s, 2H), 2.42 (s, 3H), 2.15 (s, 3H), 1.33 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.3, 155.0, 146.6, 139.5, 137.5, 136.2, 135.9, 131.5, 126.7, 125.6, 125.5, 123.1, 119.7, 39.18, 37.6, 34.9, 31.1, 21.5, 10.4.
HRMS (ESI) Calcd. For $C_{23}H_{28}ON$: 334.2165, found: 334.2176.

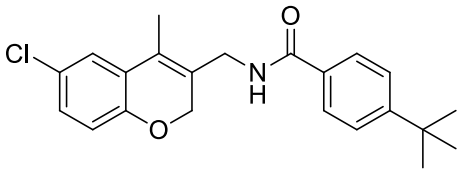
13b



^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.72 (d, *J* = 8.0 Hz, 2H),

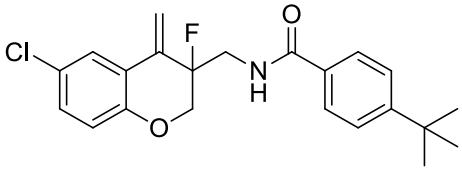
7.47 (J = 8.0 Hz, 2H), 7.33 (s, 1H), 7.11 (s, 2H), 5.75 (d, J = 4 Hz, 1H), 5.40 (d, J = 4 Hz, 1H), 4.14-4.02 (m, 1H), 3.77-3.7- (m, 1H), 3.36-3.16 (m, 2H), 2.37 (s, 3H), 1.35 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.5, 155.2, 149.1 (d, J_{C-F} = 17.1 Hz), 137.8 (d, J_{C-F} = 13.9 Hz), 137.1, 131.3, 130.7, 126.8, 125.6, 125.1, 121.5, 107.2 (d, J_{C-F} = 5.5 Hz), 102.9, 45.9 (d, J_{C-F} = 27.8 Hz), 40.3 (d, J_{C-F} = 23.7 Hz), 34.9, 31.1, 21.3. ^{19}F-NMR (376.5 MHz) δ (ppm) -144.83 - -145.01(m).
HRMS (ESI) Calcd. for [M+H] $C_{23}H_{27}ONF$:352.2071; found: 352.2084.
HPLC (ChiralPak IC column) 96:04 (hexane/*i*PrOH) 1mL/min; T_{major} (33.86 min), T_{minor} (37.06 min).

14a



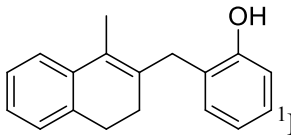
^{1}H-NMR (300 MHz, $CDCl_3$) δ (ppm) 7.70 (d, J = 6.0 Hz, 2H), 7.43 (d, J = 8.1 Hz), 7.14 (s, 1H), 7.08-7.05 (m, 1H), 6.75-6.72 (m, 1H), 6.21 (brs, 1H), 4.68 (s, 2H), 4.23 (d, J = 5.7 Hz), 2H), 2.06 (s, 3H), 1.32 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 168.0, 155.6, 152.6, 131.3, 128.7, 127.1, 127.0, 126.8, 126.5, 126.4, 125.9, 124.1, 117.3, 67.4, 38.9, 35.2, 31.4, 13.1.
HRMS (ESI) Calcd. For [M+H]$C_{22}H_{24}O_2NCl$: 370.1587; found: 370.1580.

14b



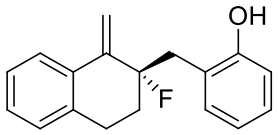
^{1}H-NMR (300 MHz, $CDCl_3$) δ (ppm) 7.71 (d, J = 9Hz, 2H), 7.51-7.44 (m, 3H), 7.18-7.14 (m, 1H), 6.38 (brs, 1H), 5.75 (s, 1H), 5.48 (s, 1H), 4.31-25 (m, 1H), 4.19-4.03 (m, 2H), 3.77-3.64 (m, 1H), 1.33 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.38, 155.45, 151.53, 137.5 (d, J_{C-F} = 17.4 Hz), 131.1, 130.1, 127.1 (d, J_{C-F} = 30.1 Hz), 125.6, 124.3, 120.8, 119.1, 108.7 (d, J_{C-F} = 9.6 Hz), 91.0 (d, J_{C-F} = 183.3Hz), 68.0 (d, J_{C-F} = 31.1 Hz), 43.1 (d, J_{C-F} = 23.3 Hz), 35.0, 31.2. ^{19}F-NMR (376.5 MHz) δ (ppm) –166.27 - –166.39 (m).
HRMS (ESI) Calcd. for [M+H] $C_{22}H_{24}O_2NClF$: 388.1493; found: 388.1488.
HPLC (ChiralPak IC column) 90:10 (hexane/*i*PrOH) 1mL/min; T_{major} (20.832 min), T_{minor} (23.336 min).

15a



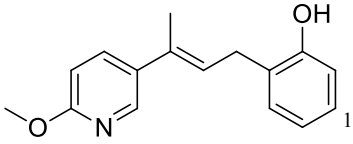
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.41-7.40 (m, 1H), 7.32-7.29 (m, 1H), 7.27-7.15 (m, 4H), 6.95-6.93 (m, 1H), 6.88-6.83 (m, 1H), 5.31 (s, 1H), 3.73 (s, 2H), 2.81 (t, J = 7.6 Hz, 2H), 2.26-2.23 (t and s overlap, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 154.4, 136.7, 135.8, 133.8, 130.2, 127.9, 127.6, 127.2, 126.5, 126.3, 125.6, 123.1, 120.9, 116.0, 115.5, 34.4, 28.6, 28.1, 14.5.
HRMS (ESI) Calcd. for [M] $C_{18}H_{18}O$: 250.1352; found: 250.1351.

15b



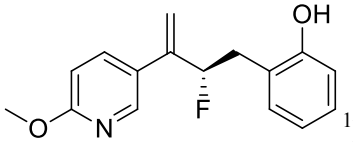
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.63-7.61 (m, 1H), 7.29-7.13 (m, 4H), 6.97-6.94 (m, 2H), 6.87-6.84 (m, 1H), 5.93 (d, J = 21 Hz, 1H), 5.62 (d, J = 4.0 Hz, 1H), 5.35 (s, 1H), 3.23-2.99 (m, 4H), 2.22-2.11 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.0, 144.9, 144.8, 134.5, 133.1, 133.1, 132.6, 128.8, 128.77, 128.3, 125.13, 125.11, 121.9, 120.6, 117.0, 108.9 (d, $J_{C\text{-}F}$ = 12.6 Hz), 100.2, 98.9 (d, $J_{C\text{-}F}$ = 176.0 Hz), 38.9 (d, $J_{C\text{-}F}$ = 23.9 Hz), 32.1 (d, $J_{C\text{-}F}$ = 22.6 Hz), 27.0 (d, $J_{C\text{-}F}$ = 11.3 Hz). ^{19}F-NMR (376.5 MHz) δ (ppm) –137.1 - –137.3 (m).
HRMS (ESI) Calcd. for [M] $C_{18}H_{16}OF$: 267.1191; found: 267.1192.
HPLC (ChiralPak IC column) 98:02 (hexane/*i*PrOH) 1mL/min; T_{major} (7.72 min), T_{minor} (8.80 min).

16a



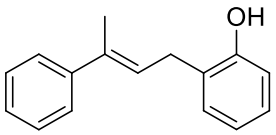
^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 8.22 (s, 1H), 7.66 (d, J = 2.5 Hz, 1H), 7.19-7.11 (m, 2H), 6.90-6.81 (m, 2H), 6.71 (d, J = 8.5 Hz, 1H), 5.93 (t, J = 3.5 Hz, 1H), 5.60 (s, 1H), 3.93 (s, 3H), 3.57 (d, J = 7.5 Hz, 2H), 2.13 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 163.1, 153.9, 143.6, 135.3, 133.0, 132.2, 130.0, 127.5, 126.7, 125.4, 120.8, 115.4, 110.1, 53.5, 29.6, 15.7.
HRMS (ESI) Calcd. for [M+H] $C_{16}H_{18}O_2N$: 256.1332; found: 256.1325.

16b



^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 8.26 (s, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.14-7.04 (m, 2H), 6.87-6.75 (m, 3H), 5.79 (s, 1H), 5.73-5.58 (m, 1H), 5.40 (s, 2H), 3.96 (s, 3H), 3.16-2.84 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 163.8, 154.1, 144.8, 143.6 (d, $J_{C\text{-}F}$ = 18.1 Hz), 137.4, 131.7, 128.3, 127.2, 123.2, 120.7, 115.6, 114.7 (d, $J_{C\text{-}F}$ = 10.1 Hz), 110.6, 94.1 (d, $J_{C\text{-}F}$ = 174.0 Hz), 53.6, 36.3 (d, $J_{C\text{-}F}$ = 23.1 Hz).
^{19}F-NMR (376.5 MHz) δ (ppm) –174.3 - –174.6 (m).
HRMS (ESI) Calcd. for [M+H] $C_{16}H_{17}O_2NF$: 274.1230; found: 274.1238.
HPLC (ChiralPak IC) 98:02 (hexane/*i*PrOH) 1mL/min; T_{major} (9.228 min), T_{minor} (10.452 min)

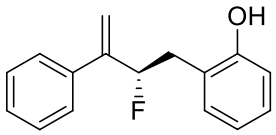
17a



^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.43-7.10 (m, 7H), 6.90 (t, J = 9.8 Hz, 1H), 6.80 (d, J = 10.4 Hz, 1H), 5.96(t, J = 8.4 Hz, 1H), 3.57 (d, J = 9.6 Hz, 2H), 2.19 (s, 3H);
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 154.0, 143.4, 136.9, 130.1, 128.3, 127.6, 127.0, 126.8, 125.8, 125.5, 121.0, 115.6, 29.9, 16.1.

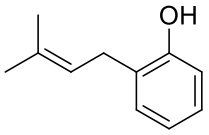
HRMS (EI) Calcd. for [M] $C_{16}H_{16}O$: 224.1201; found: 224.1204.

17b



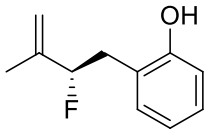
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.45-7.35 (m, 5H), 7.15 (t, J = 7.8 Hz, 1H), 7.03 (d, J = 7.2 Hz, 1H), 6.89-6.82 (m, 2H), 5.77-5.66 (m, 1H), 5.44 (d, J = 12 Hz, 2H), 5.21 (d, J = 8 Hz, 1H), 3.15-2.93 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 154.1, 146.6 (d, $J_{C\text{-}F}$ = 17.1 Hz), 138.2, 131.7, 128.5, 128.3, 128.1, 126.8, 123.4, 120.8, 115.9, 114.6 (d, $J_{C\text{-}F}$ = 11.1 Hz), 94.7 (d, $J_{C\text{-}F}$ = 173.0 Hz), 36.3 (d, $J_{C\text{-}F}$ = 23.1 Hz), 29.7. ^{19}F-NMR (376.5 MHz) δ (ppm) –173.9 - –174.2 (m).
HRMS (EI) Calcd. for [M] $C_{16}H_{15}OF$: 242.1107; found: 242.1110.
HPLC (ChiralPak IC) 94:06 (hexane/*i*PrOH) 1mL/min; T_{major} (4.384 min), T_{minor} (4.612 min).

18a



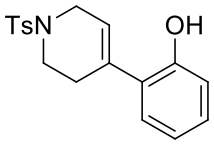
^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.15-7.12 (m, 2H), 6.84-6.82 (m, 1H), 6.76 (d, J = 8 Hz, 1H), 5.37-5.34 (m, 1H), 5.16 (s, 1H), 3.39 (d, J = 7 Hz, 2H), 1.81-1.80 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 154.2, 134.5, 130.1, 127.6, 127.3, 122.1, 120.9, 115.8, 29.6, 25.9, 17.9.
HRMS (EI) Calcd. for [M] $C_{11}H_{14}O$: 162.1045; found: 162.1048.

18b



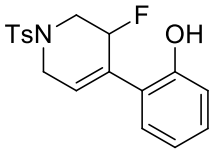
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.17-7.13 (m, 2H), 6.91-6.82 (m, 2H), 5.32 (d, J = 8.4 Hz, 1H), 5.2 (m, 1H), 4.99 (d, J = 21.6 Hz, 2H), 3.09-2.96 (m, 2H), 2.19 (s, 1H), 1.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 154.1, 142.7 (d, $J_{C\text{-}F}$ = 17.1 Hz), 131.5, 128.3, 123.6, 120.9, 116.0, 113.1 (d, $J_{C\text{-}F}$ = 10.1 Hz), 96.6 (d, $J_{C\text{-}F}$ = 170.0 Hz), 35.5 (d, $J_{C\text{-}F}$ = 23.1 Hz), 17.5 (d, $J_{C\text{-}F}$ = 3.0 Hz). ^{19}F-NMR (376.5 MHz) δ (ppm) –173.2 - –173.5 (m).
HRMS (EI) Calcd. for [M] $C_{11}H_{13}OF$: 180.0950; found: 180.0949.
HPLC (ChiralPak IC) 99:01 (hexane/*i*PrOH) 1mL/min; T_{major} (19.892 min), T_{minor} (24.844 min).

19a



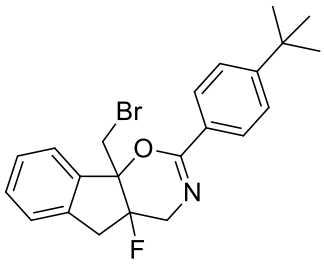
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.77 (d, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.19 (t, *J* = 6.4 Hz, 1H), 7.04-7.02 (m, 1H), 6.93-6.89 (m, 2H), 5.83 (s, 1H), 5.19 (s, 1H), 3.82-3.81 (m, 2H), 3.40 (t, *J* = 5.6 Hz, 2H), 2.58 (s, 2H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 152.2, 143.9, 134.0, 133.1, 129.8, 128.9, 128.3, 127.8, 122.5, 121.1, 120.6, 115.8, 115.5, 45.0, 43.2, 29.4, 21.6.
HRMS (ESI) Calcd. for [M-1] $C_{18}H_{18}O_3NS$: 328.1013; found: 328.1009.

19b



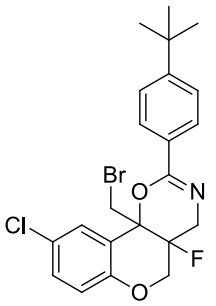
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.77 (d, J = 8.0 Hz, 2H), 7.40 (d, J = 8.4 Hz, 2H), 7.26-7.21 (m, 1H), 7.11-7.09 (m, 1H), 6.95-6.88 (m, 2H), 6.15-6.14 (m, 1H), 5.46-5.34 (m/brs overlap, 2H), 4.16-4.08 (m, 1H), 3.99-3.92 (m, 1H), 3.66-3.53 (m, 1H), 3.31-3.21 (m, 1H), 2.49 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 153.1, 144.2, 133.2, 132.6 (d, $J_{C\text{-}F}$ = 16.1 Hz), 129.9, 129.8, 129.7, 129.6, 129.56, 127.8, 125.0, 120.8, 116.1, 85.4 (d, $J_{C\text{-}F}$ = 172.0 Hz), 65.9, 47.5 (d, $J_{C\text{-}F}$ = 25.2 Hz), 44.9, 21.6.
^{19}F-NMR (376.5 MHz) δ (ppm) –168.97 (m)
HRMS (ESI) Calcd. for [M-1] $C_{18}H_{17}O_3NSF$: 346.0919; found: 346.0913.
HPLC (ChiralPak IA) 80:20 (hexane/*i*PrOH) 1mL/min; T_{major} (12.38 min), T_{minor} (14.87 min).

20



^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02 (d, J = 8.4 Hz, 2H), 7.63 (d, J = 8.0 Hz, 1H), 7.47-7.45 (m, 2H), 7.41-7.32 (m, 2H), 7.29 (s, 1H), 4.12 (t, J = 16 Hz, 1H), 4.00-3.83 (m, 2H), 3.60-3.46 (m, 2H), 3.28-3.22 (m, 1H), 1.34 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 156.4, 154.5, 141.1, 137.1, 137.06, 130.3, 129.7, 127.6, 127.3, 125.5, 125.4, 125.2, 94.49, 85.1 (d, $J_{C\text{-}F}$ = 20.1 Hz), 49.8 (d, $J_{C\text{-}F}$ = 26.2 Hz), 40.8 (d, $J_{C\text{-}F}$ = 24.1 Hz), 35.19, 35.0 (d, $J_{C\text{-}F}$ = 11.0 Hz), 31.1 (d, $J_{C\text{-}F}$ = 19.1 Hz). ^{19}F-NMR (376.5 MHz) δ (ppm) –168.45 - -168.53 (m).
HRMS (ESI) Calcd. for [M+H] $C_{22}H_{24}ONFBr$: 416.1013; found: 416.1020.
HPLC (ChiralPak IB column) 99:01 (hexane/*i*PrOH) 1mL/min; T_{major} (11.26 min), T_{minor} (9.252 min).

21

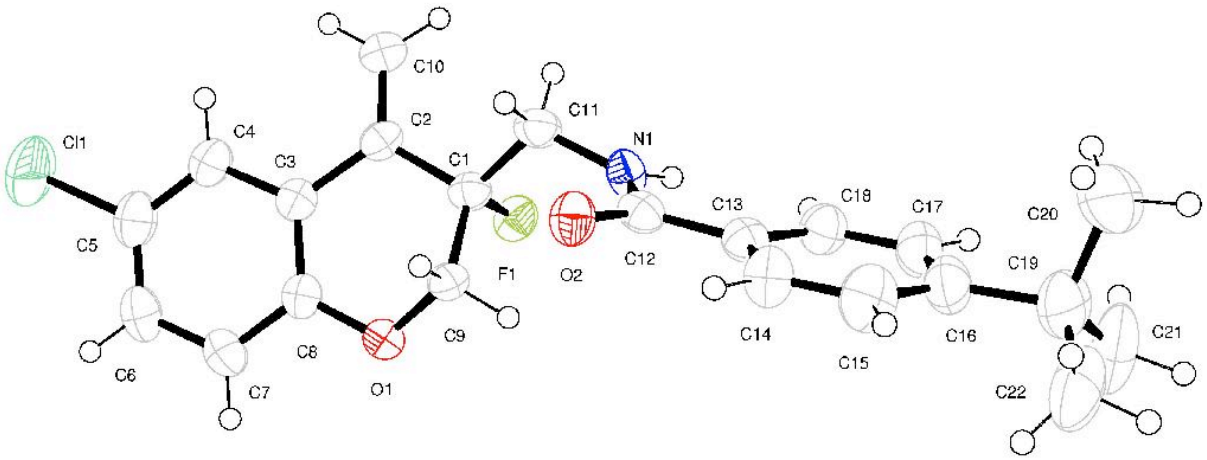


^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02(d, J = 8.0 Hz, 2H), 7.53-7.48 (m, 3H), 7.26-7.25 (m, 1H), 6.84 (d, J = 8.8 Hz, 1H), 4.63-4.58 (m, 1H), 4.27-4.25 (m, 1H), 4.21-4.10 (m, 1H), 3.95-3.70 (m, 3H), 1.36 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 154.9, 153.0, 150.5, 131.2, 129.5, 127.5, 127.2, 126.7, 125.5, 123.4, 118.5, 85.1 (d, $J_{C\text{-}F}$ = 187.1 Hz),

66.4 (d, $J_{C\text{-}F}$ = 33.2 Hz), 48.7 (d, $J_{C\text{-}F}$ = 25.6 Hz), 36.0, 35.9, 35.1, 31.3. ^{19}F-NMR (376.5 MHz) δ (ppm) –175.20- -175.33 (m).
HRMS (ESI) Calcd. for [M+H] $C_{22}H_{24}O_2NFBrCl$: 466.0575; found: 466.0579.
HPLC (ChiralPak IC column) 98:02 (hexane/*i*PrOH) 1mL/min; T_{major} (6.28 min), T_{minor} (5.66 min).

X-ray crystallography data

14b



A colorless plate 0.10 x 0.06 x 0.03 mm in size was mounted on a Cryoloop with Paratone oil.

Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 10 seconds per frame using a scan width of 1.0°. Data collection was 98.3% complete to 67.00° in θ. A total of 22020 reflections were collected covering the indices, -8<=*h*<=9, -14<=*k*<=14, -23<=*l*<=23. 6821 reflections were found to be symmetry independent, with an R_{int} of 0.0431. Indexing and unit cell refinement indicated a primitive, monoclinic lattice. The space group was found to be P2(1) (No. 4). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SIR-2008) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-97). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-97. Absolute stereochemistry was unambiguously determined to be *R* at C1 and C23, respectively.

Table 1. Crystal data and structure refinement for toste52.

X-ray ID	toste52	
Sample/notebook ID	JW-08-41	
Empirical formula	C22 H23 Cl F N O2	
Formula weight	387.86	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 8.4882(3) Å	α= 90°.
	b = 11.8855(5) Å	β= 96.216(3)°.
	c = 19.4286(8) Å	γ = 90°.
Volume	1948.56(13) $Å^3$	
Z	4	
Density (calculated)	1.322 Mg/m^3	
Absorption coefficient	1.953 mm^{-1}	
F(000)	816	
Crystal size	0.10 x 0.06 x 0.03 mm^3	
Crystal color/habit	colorless plate	
Theta range for data collection	4.37 to 67.86°.	
Index ranges	-8<=h<=9, -14<=k<=14, -23<=l<=23	
Reflections collected	22020	
Independent reflections	6821 [R(int) = 0.0431]	
Completeness to theta = 67.00°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9437 and 0.8287	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6821 / 1 / 493	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0730, wR2 = 0.1882	
R indices (all data)	R1 = 0.0832, wR2 = 0.2001	
Absolute structure parameter	-0.01(3)	
Largest diff. peak and hole	0.798 and -0.438 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for toste52. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4214(5)	4439(3)	4535(2)	37(1)
C(2)	4829(5)	4120(4)	3852(2)	38(1)
C(3)	4754(5)	5039(4)	3328(2)	39(1)
C(4)	5340(6)	4891(5)	2687(3)	51(1)
C(5)	5186(7)	5740(6)	2204(3)	62(1)
C(6)	4413(7)	6725(5)	2311(3)	56(1)
C(7)	3870(6)	6904(4)	2953(2)	47(1)
C(8)	4050(5)	6071(4)	3456(2)	40(1)
C(9)	4262(5)	5694(3)	4652(2)	35(1)
C(10)	5316(6)	3090(4)	3738(3)	50(1)
C(11)	5087(6)	3825(4)	5147(2)	43(1)
C(12)	5296(5)	4865(3)	6234(2)	37(1)
C(13)	4874(5)	4903(4)	6955(2)	40(1)
C(14)	5710(6)	5647(5)	7422(3)	51(1)
C(15)	5458(7)	5665(6)	8101(3)	63(1)
C(16)	4361(6)	4971(5)	8368(3)	57(1)
C(17)	3520(6)	4244(5)	7900(3)	54(1)
C(18)	3750(6)	4219(4)	7214(3)	48(1)
C(19)	4109(9)	4941(7)	9146(3)	80(2)
C(20)	5199(19)	4005(11)	9475(4)	166(6)
C(21)	2355(11)	4761(9)	9229(4)	102(3)
C(22)	4550(10)	6092(8)	9482(3)	91(2)
C(23)	-804(5)	6703(3)	4348(2)	38(1)
C(24)	-615(5)	6248(4)	3630(2)	39(1)
C(25)	-157(5)	7111(4)	3131(2)	43(1)
C(26)	-32(6)	6841(5)	2436(3)	52(1)
C(27)	451(7)	7658(6)	1998(3)	62(1)
C(28)	776(7)	8751(5)	2218(3)	60(1)
C(29)	658(6)	9025(4)	2896(3)	54(1)
C(30)	180(5)	8219(4)	3351(3)	45(1)
C(31)	247(5)	7702(3)	4524(2)	41(1)

C(32)	-856(6)	5180(4)	3472(2)	49(1)
C(33)	-581(5)	5820(3)	4927(2)	38(1)
C(34)	586(5)	6545(3)	6039(2)	38(1)
C(35)	264(5)	7014(3)	6729(2)	38(1)
C(36)	-1125(5)	7571(4)	6829(2)	40(1)
C(37)	-1360(5)	7994(4)	7466(3)	45(1)
C(38)	-229(6)	7874(4)	8035(3)	51(1)
C(39)	1176(6)	7332(4)	7931(2)	49(1)
C(40)	1433(5)	6907(4)	7288(2)	43(1)
C(41)	-506(7)	8293(6)	8763(3)	65(2)
C(42)	-837(15)	7315(12)	9203(4)	141(5)
C(43)	-2152(13)	8927(12)	8735(5)	134(5)
C(44)	778(11)	8987(12)	9071(5)	131(4)
N(1)	4551(4)	4093(3)	5807(2)	41(1)
N(2)	-712(4)	6278(3)	5599(2)	39(1)
O(1)	3480(3)	6295(2)	4071(2)	38(1)
O(2)	6346(3)	5460(3)	6043(2)	45(1)
O(3)	39(4)	8557(2)	4013(2)	48(1)
O(4)	1930(3)	6439(3)	5883(2)	44(1)
F(1)	2601(3)	4115(2)	4492(1)	44(1)
F(2)	-2405(3)	7101(2)	4316(1)	46(1)
Cl(1)	5951(3)	5539(2)	1412(1)	94(1)
Cl(2)	678(3)	7284(2)	1137(1)	92(1)

Table 3. Bond lengths [Å] and angles [°] for toste52.

C(1)-F(1)	1.416(5)	C(16)-C(17)	1.394(8)
C(1)-C(9)	1.509(5)	C(16)-C(19)	1.550(8)
C(1)-C(11)	1.519(6)	C(17)-C(18)	1.368(7)
C(1)-C(2)	1.526(6)	C(17)-H(17)	0.9500
C(2)-C(10)	1.318(6)	C(18)-H(18)	0.9500
C(2)-C(3)	1.490(6)	C(19)-C(21)	1.529(11)
C(3)-C(8)	1.399(6)	C(19)-C(20)	1.541(11)
C(3)-C(4)	1.400(6)	C(19)-C(22)	1.545(12)
C(4)-C(5)	1.374(8)	C(20)-H(20A)	0.9800
C(4)-H(4)	0.9500	C(20)-H(20B)	0.9800
C(5)-C(6)	1.369(8)	C(20)-H(20C)	0.9800
C(5)-Cl(1)	1.751(5)	C(21)-H(21A)	0.9800
C(6)-C(7)	1.394(7)	C(21)-H(21B)	0.9800
C(6)-H(6)	0.9500	C(21)-H(21C)	0.9800
C(7)-C(8)	1.388(6)	C(22)-H(22A)	0.9800
C(7)-H(7)	0.9500	C(22)-H(22B)	0.9800
C(8)-O(1)	1.364(5)	C(22)-H(22C)	0.9800
C(9)-O(1)	1.435(5)	C(23)-F(2)	1.434(5)
C(9)-H(9A)	0.9900	C(23)-C(31)	1.502(6)
C(9)-H(9B)	0.9900	C(23)-C(24)	1.521(6)
C(10)-H(10A)	0.9500	C(23)-C(33)	1.535(6)
C(10)-H(10B)	0.9500	C(24)-C(32)	1.317(7)
C(11)-N(1)	1.441(6)	C(24)-C(25)	1.492(6)
C(11)-H(11A)	0.9900	C(25)-C(26)	1.403(7)
C(11)-H(11B)	0.9900	C(25)-C(30)	1.404(7)
C(12)-O(2)	1.226(5)	C(26)-C(27)	1.383(8)
C(12)-N(1)	1.347(6)	C(26)-H(26)	0.9500
C(12)-C(13)	1.485(6)	C(27)-C(28)	1.385(9)
C(13)-C(18)	1.389(7)	C(27)-Cl(2)	1.763(6)
C(13)-C(14)	1.403(7)	C(28)-C(29)	1.370(8)
C(14)-C(15)	1.358(8)	C(28)-H(28)	0.9500
C(14)-H(14)	0.9500	C(29)-C(30)	1.394(7)
C(15)-C(16)	1.387(8)	C(29)-H(29)	0.9500
C(15)-H(15)	0.9500	C(30)-O(3)	1.364(6)

C(31)-O(3)	1.419(5)	C(38)-C(41)	1.541(7)
C(31)-H(31A)	0.9900	C(39)-C(40)	1.388(7)
C(31)-H(31B)	0.9900	C(39)-H(39)	0.9500
C(32)-H(32A)	0.9500	C(40)-H(40)	0.9500
C(32)-H(32B)	0.9500	C(41)-C(44)	1.444(11)
C(33)-N(2)	1.429(6)	C(41)-C(42)	1.487(13)
C(33)-H(33A)	0.9900	C(41)-C(43)	1.583(11)
C(33)-H(33B)	0.9900	C(42)-H(42A)	0.9800
C(34)-O(4)	1.218(5)	C(42)-H(42B)	0.9800
C(34)-N(2)	1.358(6)	C(42)-H(42C)	0.9800
C(34)-C(35)	1.504(6)	C(43)-H(43A)	0.9800
C(35)-C(36)	1.384(6)	C(43)-H(43B)	0.9800
C(35)-C(40)	1.395(6)	C(43)-H(43C)	0.9800
C(36)-C(37)	1.370(7)	C(44)-H(44A)	0.9800
C(36)-H(36)	0.9500	C(44)-H(44B)	0.9800
C(37)-C(38)	1.391(7)	C(44)-H(44C)	0.9800
C(37)-H(37)	0.9500	N(1)-H(1)	0.8800
C(38)-C(39)	1.390(7)	N(2)-H(2)	0.8800

F(1)-C(1)-C(9)	106.7(3)	C(4)-C(5)-Cl(1)	118.9(5)
F(1)-C(1)-C(11)	107.6(3)	C(5)-C(6)-C(7)	118.5(5)
C(9)-C(1)-C(11)	110.7(3)	C(5)-C(6)-H(6)	120.8
F(1)-C(1)-C(2)	107.5(3)	C(7)-C(6)-H(6)	120.8
C(9)-C(1)-C(2)	111.8(4)	C(8)-C(7)-C(6)	119.9(5)
C(11)-C(1)-C(2)	112.2(3)	C(8)-C(7)-H(7)	120.0
C(10)-C(2)-C(3)	123.9(4)	C(6)-C(7)-H(7)	120.0
C(10)-C(2)-C(1)	121.3(4)	O(1)-C(8)-C(7)	117.1(4)
C(3)-C(2)-C(1)	114.8(4)	O(1)-C(8)-C(3)	121.8(4)
C(8)-C(3)-C(4)	117.9(4)	C(7)-C(8)-C(3)	121.2(4)
C(8)-C(3)-C(2)	120.6(4)	O(1)-C(9)-C(1)	111.8(3)
C(4)-C(3)-C(2)	121.5(4)	O(1)-C(9)-H(9A)	109.3
C(5)-C(4)-C(3)	119.9(5)	C(1)-C(9)-H(9A)	109.3
C(5)-C(4)-H(4)	120.1	O(1)-C(9)-H(9B)	109.3
C(3)-C(4)-H(4)	120.1	C(1)-C(9)-H(9B)	109.3
C(6)-C(5)-C(4)	122.4(5)	H(9A)-C(9)-H(9B)	107.9
C(6)-C(5)-Cl(1)	118.6(4)	C(2)-C(10)-H(10A)	120.0

C(2)-C(10)-H(10B)	120.0	C(19)-C(20)-H(20B)	109.5
H(10A)-C(10)-H(10B)	120.0	H(20A)-C(20)-H(20B)	109.5
N(1)-C(11)-C(1)	114.6(4)	C(19)-C(20)-H(20C)	109.5
N(1)-C(11)-H(11A)	108.6	H(20A)-C(20)-H(20C)	109.5
C(1)-C(11)-H(11A)	108.6	H(20B)-C(20)-H(20C)	109.5
N(1)-C(11)-H(11B)	108.6	C(19)-C(21)-H(21A)	109.5
C(1)-C(11)-H(11B)	108.6	C(19)-C(21)-H(21B)	109.5
H(11A)-C(11)-H(11B)	107.6	H(21A)-C(21)-H(21B)	109.5
O(2)-C(12)-N(1)	120.9(4)	C(19)-C(21)-H(21C)	109.5
O(2)-C(12)-C(13)	121.7(4)	H(21A)-C(21)-H(21C)	109.5
N(1)-C(12)-C(13)	117.2(4)	H(21B)-C(21)-H(21C)	109.5
C(18)-C(13)-C(14)	117.0(4)	C(19)-C(22)-H(22A)	109.5
C(18)-C(13)-C(12)	124.7(4)	C(19)-C(22)-H(22B)	109.5
C(14)-C(13)-C(12)	118.2(4)	H(22A)-C(22)-H(22B)	109.5
C(15)-C(14)-C(13)	121.1(5)	C(19)-C(22)-H(22C)	109.5
C(15)-C(14)-H(14)	119.5	H(22A)-C(22)-H(22C)	109.5
C(13)-C(14)-H(14)	119.5	H(22B)-C(22)-H(22C)	109.5
C(14)-C(15)-C(16)	122.4(5)	F(2)-C(23)-C(31)	106.6(3)
C(14)-C(15)-H(15)	118.8	F(2)-C(23)-C(24)	105.7(3)
C(16)-C(15)-H(15)	118.8	C(31)-C(23)-C(24)	111.8(4)
C(15)-C(16)-C(17)	116.2(5)	F(2)-C(23)-C(33)	107.3(3)
C(15)-C(16)-C(19)	123.2(6)	C(31)-C(23)-C(33)	110.5(4)
C(17)-C(16)-C(19)	120.5(5)	C(24)-C(23)-C(33)	114.4(3)
C(18)-C(17)-C(16)	122.1(5)	C(32)-C(24)-C(25)	123.8(4)
C(18)-C(17)-H(17)	118.9	C(32)-C(24)-C(23)	121.8(4)
C(16)-C(17)-H(17)	118.9	C(25)-C(24)-C(23)	114.4(4)
C(17)-C(18)-C(13)	121.1(5)	C(26)-C(25)-C(30)	118.3(4)
C(17)-C(18)-H(18)	119.5	C(26)-C(25)-C(24)	121.3(4)
C(13)-C(18)-H(18)	119.5	C(30)-C(25)-C(24)	120.3(4)
C(21)-C(19)-C(20)	113.8(9)	C(27)-C(26)-C(25)	119.3(5)
C(21)-C(19)-C(22)	105.9(7)	C(27)-C(26)-H(26)	120.4
C(20)-C(19)-C(22)	110.9(7)	C(25)-C(26)-H(26)	120.4
C(21)-C(19)-C(16)	110.2(5)	C(26)-C(27)-C(28)	122.1(5)
C(20)-C(19)-C(16)	106.3(6)	C(26)-C(27)-Cl(2)	118.4(5)
C(22)-C(19)-C(16)	109.8(6)	C(28)-C(27)-Cl(2)	119.4(4)
C(19)-C(20)-H(20A)	109.5	C(29)-C(28)-C(27)	119.1(5)

C(29)-C(28)-H(28)	120.5	C(39)-C(38)-C(41)	120.2(5)
C(27)-C(28)-H(28)	120.5	C(37)-C(38)-C(41)	122.4(5)
C(28)-C(29)-C(30)	120.2(5)	C(40)-C(39)-C(38)	121.4(4)
C(28)-C(29)-H(29)	119.9	C(40)-C(39)-H(39)	119.3
C(30)-C(29)-H(29)	119.9	C(38)-C(39)-H(39)	119.3
O(3)-C(30)-C(29)	117.2(4)	C(39)-C(40)-C(35)	120.0(4)
O(3)-C(30)-C(25)	121.9(4)	C(39)-C(40)-H(40)	120.0
C(29)-C(30)-C(25)	120.9(5)	C(35)-C(40)-H(40)	120.0
O(3)-C(31)-C(23)	112.4(4)	C(44)-C(41)-C(42)	112.9(8)
O(3)-C(31)-H(31A)	109.1	C(44)-C(41)-C(38)	112.4(6)
C(23)-C(31)-H(31A)	109.1	C(42)-C(41)-C(38)	109.4(6)
O(3)-C(31)-H(31B)	109.1	C(44)-C(41)-C(43)	111.5(8)
C(23)-C(31)-H(31B)	109.1	C(42)-C(41)-C(43)	99.8(8)
H(31A)-C(31)-H(31B)	107.9	C(38)-C(41)-C(43)	110.2(5)
C(24)-C(32)-H(32A)	120.0	C(41)-C(42)-H(42A)	109.5
C(24)-C(32)-H(32B)	120.0	C(41)-C(42)-H(42B)	109.5
H(32A)-C(32)-H(32B)	120.0	H(42A)-C(42)-H(42B)	109.5
N(2)-C(33)-C(23)	113.1(3)	C(41)-C(42)-H(42C)	109.5
N(2)-C(33)-H(33A)	109.0	H(42A)-C(42)-H(42C)	109.5
C(23)-C(33)-H(33A)	109.0	H(42B)-C(42)-H(42C)	109.5
N(2)-C(33)-H(33B)	109.0	C(41)-C(43)-H(43A)	109.5
C(23)-C(33)-H(33B)	109.0	C(41)-C(43)-H(43B)	109.5
H(33A)-C(33)-H(33B)	107.8	H(43A)-C(43)-H(43B)	109.5
O(4)-C(34)-N(2)	122.5(4)	C(41)-C(43)-H(43C)	109.5
O(4)-C(34)-C(35)	121.7(4)	H(43A)-C(43)-H(43C)	109.5
N(2)-C(34)-C(35)	115.8(4)	H(43B)-C(43)-H(43C)	109.5
C(36)-C(35)-C(40)	118.7(4)	C(41)-C(44)-H(44A)	109.5
C(36)-C(35)-C(34)	122.8(4)	C(41)-C(44)-H(44B)	109.5
C(40)-C(35)-C(34)	118.5(4)	H(44A)-C(44)-H(44B)	109.5
C(37)-C(36)-C(35)	120.8(4)	C(41)-C(44)-H(44C)	109.5
C(37)-C(36)-H(36)	119.6	H(44A)-C(44)-H(44C)	109.5
C(35)-C(36)-H(36)	119.6	H(44B)-C(44)-H(44C)	109.5
C(36)-C(37)-C(38)	121.7(4)	C(12)-N(1)-C(11)	121.7(4)
C(36)-C(37)-H(37)	119.2	C(12)-N(1)-H(1)	119.1
C(38)-C(37)-H(37)	119.2	C(11)-N(1)-H(1)	119.1
C(39)-C(38)-C(37)	117.4(4)	C(34)-N(2)-C(33)	121.8(3)

C(34)-N(2)-H(2)	119.1
C(33)-N(2)-H(2)	119.1
C(8)-O(1)-C(9)	114.5(3)
C(30)-O(3)-C(31)	115.6(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for toste52. The anisotropic 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}
C(1)	36(2)	32(2)	42(2)	-3(2)	4(2)	0(2)
C(2)	31(2)	42(2)	40(2)	-4(2)	5(2)	3(2)
C(3)	38(2)	42(2)	37(2)	-1(2)	5(2)	0(2)
C(4)	60(3)	56(3)	40(2)	-2(2)	14(2)	6(2)
C(5)	78(4)	75(4)	33(2)	2(2)	14(2)	3(3)
C(6)	67(3)	63(3)	39(2)	11(2)	7(2)	-6(2)
C(7)	51(3)	46(2)	44(2)	9(2)	2(2)	0(2)
C(8)	41(2)	45(2)	35(2)	0(2)	6(2)	-2(2)
C(9)	31(2)	36(2)	40(2)	1(2)	7(2)	5(2)
C(10)	56(3)	44(2)	53(3)	-2(2)	14(2)	11(2)
C(11)	51(2)	33(2)	46(2)	-2(2)	5(2)	6(2)
C(12)	29(2)	37(2)	44(2)	5(2)	-2(2)	1(2)
C(13)	32(2)	43(2)	42(2)	2(2)	0(2)	4(2)
C(14)	48(3)	61(3)	44(2)	-2(2)	4(2)	-13(2)
C(15)	60(3)	80(4)	45(3)	-10(3)	-8(2)	-9(3)
C(16)	56(3)	72(3)	44(3)	13(2)	9(2)	8(2)
C(17)	52(3)	61(3)	48(3)	6(2)	12(2)	-2(2)
C(18)	48(3)	50(3)	48(3)	-1(2)	8(2)	-3(2)
C(19)	98(5)	103(5)	36(3)	3(3)	-3(3)	21(4)
C(20)	286(16)	170(10)	42(4)	25(5)	12(6)	136(11)
C(21)	126(7)	131(7)	54(4)	-3(4)	40(4)	-34(6)
C(22)	93(5)	138(7)	41(3)	-9(4)	10(3)	1(5)
C(23)	34(2)	38(2)	43(2)	-2(2)	10(2)	3(2)
C(24)	38(2)	40(2)	41(2)	0(2)	6(2)	6(2)
C(25)	38(2)	47(2)	43(2)	2(2)	2(2)	6(2)
C(26)	56(3)	57(3)	41(2)	-1(2)	1(2)	-9(2)
C(27)	62(3)	84(4)	40(3)	9(3)	1(2)	-9(3)
C(28)	62(3)	65(3)	52(3)	21(2)	1(2)	-5(2)
C(29)	59(3)	47(2)	55(3)	9(2)	5(2)	8(2)
C(30)	43(2)	44(2)	48(3)	0(2)	3(2)	6(2)
C(31)	47(2)	34(2)	42(2)	-4(2)	9(2)	-1(2)

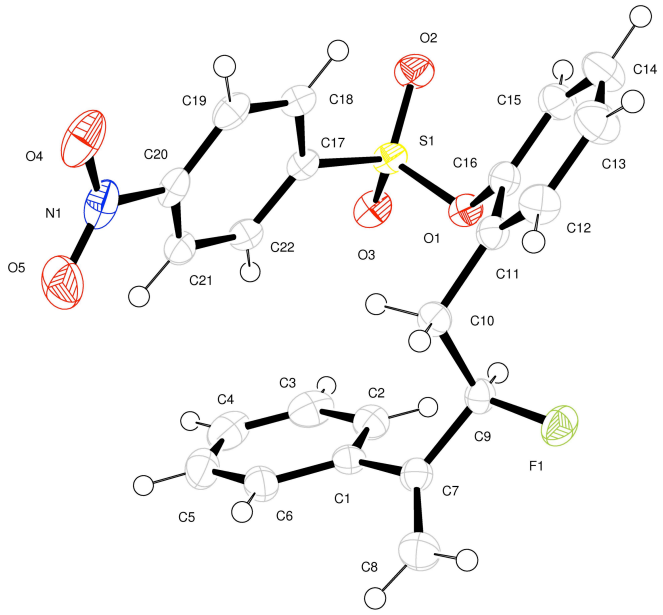
C(32)	58(3)	49(3)	39(2)	-6(2)	11(2)	1(2)
C(33)	35(2)	39(2)	42(2)	-4(2)	10(2)	-1(2)
C(34)	36(2)	33(2)	46(2)	5(2)	11(2)	0(2)
C(35)	41(2)	36(2)	39(2)	1(2)	9(2)	-7(2)
C(36)	36(2)	39(2)	45(2)	0(2)	7(2)	-4(2)
C(37)	38(2)	48(2)	51(3)	-3(2)	13(2)	-2(2)
C(38)	64(3)	48(2)	44(3)	3(2)	19(2)	-1(2)
C(39)	53(3)	59(3)	35(2)	3(2)	5(2)	4(2)
C(40)	37(2)	46(2)	46(2)	2(2)	5(2)	0(2)
C(41)	75(4)	85(4)	35(3)	-5(2)	12(2)	11(3)
C(42)	187(10)	194(12)	49(4)	-25(6)	45(5)	-94(9)
C(43)	121(7)	212(13)	68(5)	-45(7)	2(5)	60(8)
C(44)	99(6)	200(12)	97(6)	-83(7)	22(5)	-26(7)
N(1)	48(2)	39(2)	36(2)	6(2)	6(1)	-7(2)
N(2)	33(2)	41(2)	43(2)	-1(2)	11(1)	-1(1)
O(1)	41(2)	35(1)	40(2)	3(1)	7(1)	2(1)
O(2)	36(2)	54(2)	44(2)	2(1)	6(1)	-8(1)
O(3)	63(2)	31(1)	54(2)	2(1)	19(2)	0(1)
O(4)	33(2)	52(2)	46(2)	-8(1)	6(1)	-2(1)
F(1)	41(1)	43(1)	48(1)	-7(1)	11(1)	-7(1)
F(2)	42(1)	44(1)	53(2)	0(1)	10(1)	7(1)
Cl(1)	120(1)	122(2)	47(1)	4(1)	35(1)	10(1)
Cl(2)	122(2)	117(2)	38(1)	2(1)	12(1)	-22(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for toste52.

	x	y	z	U(eq)
H(4)	5842	4205	2586	61
H(6)	4251	7273	1954	67
H(7)	3376	7597	3047	57
H(9A)	3743	5874	5071	42
H(9B)	5379	5944	4733	42
H(10A)	5644	2898	3301	60
H(10B)	5337	2539	4093	60
H(11A)	4969	3005	5069	52
H(11B)	6229	4007	5168	52
H(14)	6464	6145	7261	61
H(15)	6056	6173	8404	75
H(17)	2762	3750	8063	64
H(18)	3130	3725	6910	58
H(20A)	5012	3310	9207	250
H(20B)	4972	3876	9952	250
H(20C)	6308	4233	9473	250
H(21A)	2057	3986	9103	152
H(21B)	1712	5283	8926	152
H(21C)	2173	4899	9711	152
H(22A)	4014	6182	9901	136
H(22B)	4217	6695	9154	136
H(22C)	5700	6131	9605	136
H(26)	-276	6103	2268	62
H(28)	1077	9303	1904	72
H(29)	902	9767	3055	64
H(31A)	13	8015	4974	49
H(31B)	1367	7454	4575	49
H(32A)	-739	4920	3018	58
H(32B)	-1146	4669	3813	58
H(33A)	-1388	5222	4831	46

H(33B)	475	5468	4925	46
H(36)	-1925	7660	6451	48
H(37)	-2319	8379	7520	54
H(39)	1978	7251	8309	59
H(40)	2406	6543	7227	52
H(42A)	-756	7550	9689	211
H(42B)	-65	6718	9148	211
H(42C)	-1909	7034	9062	211
H(43A)	-2414	9058	9208	202
H(43B)	-2980	8465	8484	202
H(43C)	-2081	9649	8498	202
H(44A)	415	9431	9448	197
H(44B)	1125	9494	8719	197
H(44C)	1665	8507	9253	197
H(1)	3716	3743	5934	49
H(2)	-1660	6391	5730	46

17b (nosyl-derivative)



A colorless rod 0.060 x 0.040 x 0.040 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 5 seconds per frame using a scan width of 1.0°. Data collection was 100.0% complete to 67.000° in θ. A total of 43179 reflections were collected covering the indices, -8<=*h*<=8, -16<=*k*<=16, -26<=*l*<=26. 3685 reflections were found to be symmetry independent, with an R_{int} of 0.0226. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be P 21 21 21 (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SIR-2011) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2012). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using

the appropriate HFIX command in SHELXL-2012. Absolute stereochemistry was unambiguously determined to be *R* at C9.

Table 1. Crystal data and structure refinement for toste72.

X-ray ID	toste72	
Sample/notebook ID	JW-10-NS	
Empirical formula	C22 H18 F N O5 S	
Formula weight	427.43	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 6.8101(4) Å	α= 90°.
	b = 13.2958(8) Å	β= 90°.
	c = 22.2494(14) Å	γ = 90°.
Volume	2014.6(2) $Å^3$	
Z	4	
Density (calculated)	1.409 Mg/m^3	
Absorption coefficient	1.817 mm^{-1}	
F(000)	888	
Crystal size	0.060 x 0.040 x 0.040 mm^3	
Crystal color/habit	colorless rod	
Theta range for data collection	3.873 to 68.334°.	
Index ranges	-8<=h<=8, -16<=k<=16, -26<=l<=26	
Reflections collected	43179	
Independent reflections	3685 [R(int) = 0.0226]	
Completeness to theta = 67.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.841	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3685 / 0 / 271	
Goodness-of-fit on F^2	1.065	
Final R indices [I>2sigma(I)]	R1 = 0.0209, wR2 = 0.0555	
R indices (all data)	R1 = 0.0211, wR2 = 0.0557	
Absolute structure parameter	-0.002(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.178 and -0.217 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for toste72. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5215(3)	12126(1)	1663(1)	26(1)
C(2)	7181(3)	11910(1)	1538(1)	32(1)
C(3)	8374(3)	11480(2)	1974(1)	41(1)
C(4)	7629(4)	11262(2)	2537(1)	47(1)
C(5)	5687(4)	11489(2)	2669(1)	45(1)
C(6)	4491(3)	11913(1)	2238(1)	35(1)
C(7)	3880(3)	12562(1)	1204(1)	26(1)
C(8)	2574(4)	13271(2)	1330(1)	40(1)
C(9)	4009(2)	12090(1)	588(1)	24(1)
C(10)	2945(2)	11083(1)	574(1)	25(1)
C(11)	3181(3)	10524(1)	-11(1)	26(1)
C(12)	1647(3)	10472(1)	-420(1)	33(1)
C(13)	1859(3)	9973(2)	-964(1)	41(1)
C(14)	3613(3)	9505(2)	-1105(1)	42(1)
C(15)	5178(3)	9548(2)	-710(1)	34(1)
C(16)	4936(3)	10053(1)	-170(1)	27(1)
C(17)	5427(2)	8871(1)	1041(1)	24(1)
C(18)	3986(3)	8253(1)	795(1)	26(1)
C(19)	2288(3)	8086(1)	1122(1)	28(1)
C(20)	2111(2)	8537(1)	1679(1)	27(1)
C(21)	3567(3)	9120(1)	1935(1)	28(1)
C(22)	5266(3)	9288(1)	1610(1)	26(1)
N(1)	245(2)	8409(1)	2005(1)	36(1)
O(1)	6555(2)	10168(1)	228(1)	27(1)
O(2)	7819(2)	8428(1)	168(1)	36(1)
O(3)	8948(2)	9643(1)	936(1)	33(1)
O(4)	-903(2)	7769(1)	1825(1)	45(1)
O(5)	-55(3)	8961(1)	2434(1)	51(1)
F(1)	3122(2)	12724(1)	160(1)	34(1)
S(1)	7421(1)	9220(1)	582(1)	26(1)

Table 3. Bond lengths [Å] and angles [°] for toste72.

C(1)-C(2)	1.397(3)	C(12)-H(12)	0.9500
C(1)-C(6)	1.401(2)	C(13)-C(14)	1.383(3)
C(1)-C(7)	1.484(2)	C(13)-H(13)	0.9500
C(2)-C(3)	1.388(3)	C(14)-C(15)	1.381(3)
C(2)-H(2)	0.9500	C(14)-H(14)	0.9500
C(3)-C(4)	1.383(3)	C(15)-C(16)	1.388(2)
C(3)-H(3)	0.9500	C(15)-H(15)	0.9500
C(4)-C(5)	1.388(4)	C(16)-O(1)	1.422(2)
C(4)-H(4)	0.9500	C(17)-C(22)	1.387(2)
C(5)-C(6)	1.377(3)	C(17)-C(18)	1.391(2)
C(5)-H(5)	0.9500	C(17)-S(1)	1.7613(17)
C(6)-H(6)	0.9500	C(18)-C(19)	1.383(3)
C(7)-C(8)	1.326(3)	C(18)-H(18)	0.9500
C(7)-C(9)	1.512(2)	C(19)-C(20)	1.383(3)
C(8)-H(8A)	0.9500	C(19)-H(19)	0.9500
C(8)-H(8B)	0.9500	C(20)-C(21)	1.381(3)
C(9)-F(1)	1.4080(19)	C(20)-N(1)	1.474(2)
C(9)-C(10)	1.523(2)	C(21)-C(22)	1.383(3)
C(9)-H(9)	1.0000	C(21)-H(21)	0.9500
C(10)-C(11)	1.507(2)	C(22)-H(22)	0.9500
C(10)-H(10A)	0.9900	N(1)-O(5)	1.221(2)
C(10)-H(10B)	0.9900	N(1)-O(4)	1.224(2)
C(11)-C(12)	1.387(3)	O(1)-S(1)	1.6002(12)
C(11)-C(16)	1.395(3)	O(2)-S(1)	1.4237(13)
C(12)-C(13)	1.389(3)	O(3)-S(1)	1.4214(14)

C(2)-C(1)-C(6)	118.51(18)	C(2)-C(3)-H(3)	119.8
C(2)-C(1)-C(7)	122.03(16)	C(3)-C(4)-C(5)	119.7(2)
C(6)-C(1)-C(7)	119.45(17)	C(3)-C(4)-H(4)	120.2
C(3)-C(2)-C(1)	120.44(19)	C(5)-C(4)-H(4)	120.2
C(3)-C(2)-H(2)	119.8	C(6)-C(5)-C(4)	120.4(2)
C(1)-C(2)-H(2)	119.8	C(6)-C(5)-H(5)	119.8
C(4)-C(3)-C(2)	120.3(2)	C(4)-C(5)-H(5)	119.8
C(4)-C(3)-H(3)	119.8	C(5)-C(6)-C(1)	120.7(2)

C(5)-C(6)-H(6)	119.7	C(15)-C(16)-O(1)	119.96(16)
C(1)-C(6)-H(6)	119.7	C(11)-C(16)-O(1)	117.27(14)
C(8)-C(7)-C(1)	122.97(17)	C(22)-C(17)-C(18)	122.60(16)
C(8)-C(7)-C(9)	121.68(17)	C(22)-C(17)-S(1)	119.03(13)
C(1)-C(7)-C(9)	115.22(14)	C(18)-C(17)-S(1)	118.13(13)
C(7)-C(8)-H(8A)	120.0	C(19)-C(18)-C(17)	118.58(16)
C(7)-C(8)-H(8B)	120.0	C(19)-C(18)-H(18)	120.7
H(8A)-C(8)-H(8B)	120.0	C(17)-C(18)-H(18)	120.7
F(1)-C(9)-C(7)	109.85(13)	C(20)-C(19)-C(18)	118.27(16)
F(1)-C(9)-C(10)	108.04(13)	C(20)-C(19)-H(19)	120.9
C(7)-C(9)-C(10)	110.80(14)	C(18)-C(19)-H(19)	120.9
F(1)-C(9)-H(9)	109.4	C(21)-C(20)-C(19)	123.46(16)
C(7)-C(9)-H(9)	109.4	C(21)-C(20)-N(1)	118.69(16)
C(10)-C(9)-H(9)	109.4	C(19)-C(20)-N(1)	117.83(16)
C(11)-C(10)-C(9)	113.52(14)	C(20)-C(21)-C(22)	118.35(16)
C(11)-C(10)-H(10A)	108.9	C(20)-C(21)-H(21)	120.8
C(9)-C(10)-H(10A)	108.9	C(22)-C(21)-H(21)	120.8
C(11)-C(10)-H(10B)	108.9	C(21)-C(22)-C(17)	118.64(16)
C(9)-C(10)-H(10B)	108.9	C(21)-C(22)-H(22)	120.7
H(10A)-C(10)-H(10B)	107.7	C(17)-C(22)-H(22)	120.7
C(12)-C(11)-C(16)	117.14(16)	O(5)-N(1)-O(4)	124.62(17)
C(12)-C(11)-C(10)	120.75(16)	O(5)-N(1)-C(20)	117.37(17)
C(16)-C(11)-C(10)	122.10(16)	O(4)-N(1)-C(20)	118.00(17)
C(11)-C(12)-C(13)	121.20(18)	C(16)-O(1)-S(1)	120.46(11)
C(11)-C(12)-H(12)	119.4	O(3)-S(1)-O(2)	120.81(8)
C(13)-C(12)-H(12)	119.4	O(3)-S(1)-O(1)	103.36(7)
C(14)-C(13)-C(12)	120.12(19)	O(2)-S(1)-O(1)	109.54(7)
C(14)-C(13)-H(13)	119.9	O(3)-S(1)-C(17)	110.26(8)
C(12)-C(13)-H(13)	119.9	O(2)-S(1)-C(17)	109.08(8)
C(15)-C(14)-C(13)	120.30(17)	O(1)-S(1)-C(17)	102.05(7)
C(15)-C(14)-H(14)	119.8		
C(13)-C(14)-H(14)	119.8		
C(14)-C(15)-C(16)	118.60(18)		
C(14)-C(15)-H(15)	120.7		
C(16)-C(15)-H(15)	120.7		
C(15)-C(16)-C(11)	122.61(17)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for toste72. The anisotropic 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}
C(1)	32(1)	21(1)	26(1)	-4(1)	-1(1)	-5(1)
C(2)	31(1)	32(1)	33(1)	-2(1)	-6(1)	-4(1)
C(3)	37(1)	35(1)	52(1)	-6(1)	-19(1)	-3(1)
C(4)	68(2)	33(1)	42(1)	1(1)	-32(1)	-9(1)
C(5)	70(2)	37(1)	27(1)	1(1)	-9(1)	-19(1)
C(6)	46(1)	31(1)	28(1)	-4(1)	2(1)	-12(1)
C(7)	26(1)	25(1)	28(1)	1(1)	4(1)	-2(1)
C(8)	43(1)	38(1)	38(1)	-1(1)	6(1)	10(1)
C(9)	22(1)	27(1)	24(1)	4(1)	-1(1)	2(1)
C(10)	21(1)	27(1)	27(1)	0(1)	4(1)	1(1)
C(11)	27(1)	24(1)	27(1)	1(1)	5(1)	-2(1)
C(12)	30(1)	34(1)	35(1)	-1(1)	-1(1)	2(1)
C(13)	43(1)	47(1)	34(1)	-7(1)	-8(1)	0(1)
C(14)	52(1)	45(1)	29(1)	-10(1)	4(1)	0(1)
C(15)	36(1)	34(1)	33(1)	-3(1)	12(1)	1(1)
C(16)	28(1)	27(1)	27(1)	2(1)	3(1)	-3(1)
C(17)	19(1)	20(1)	32(1)	2(1)	2(1)	1(1)
C(18)	27(1)	21(1)	32(1)	0(1)	-1(1)	0(1)
C(19)	23(1)	23(1)	39(1)	6(1)	-5(1)	-3(1)
C(20)	23(1)	23(1)	36(1)	11(1)	3(1)	1(1)
C(21)	32(1)	24(1)	28(1)	3(1)	3(1)	2(1)
C(22)	26(1)	22(1)	31(1)	0(1)	-2(1)	-2(1)
N(1)	29(1)	35(1)	44(1)	17(1)	7(1)	3(1)
O(1)	23(1)	25(1)	32(1)	0(1)	5(1)	0(1)
O(2)	33(1)	31(1)	44(1)	-4(1)	11(1)	6(1)
O(3)	20(1)	32(1)	46(1)	4(1)	2(1)	-1(1)
O(4)	27(1)	42(1)	66(1)	21(1)	3(1)	-6(1)
O(5)	45(1)	58(1)	49(1)	6(1)	22(1)	2(1)
F(1)	38(1)	29(1)	34(1)	6(1)	-11(1)	1(1)
S(1)	20(1)	24(1)	35(1)	0(1)	5(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for toste72.

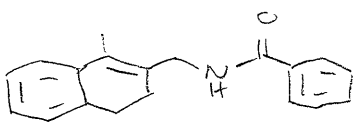
	x	y	z	U(eq)
H(2)	7705	12059	1152	38
H(3)	9708	11334	1884	50
H(4)	8443	10958	2833	57
H(5)	5179	11352	3058	54
H(6)	3162	12062	2333	42
H(8A)	2462	13522	1728	48
H(8B)	1750	13527	1021	48
H(9)	5420	11986	479	29
H(10A)	3450	10657	905	30
H(10B)	1529	11199	648	30
H(12)	429	10782	-325	40
H(13)	797	9954	-1241	50
H(14)	3743	9153	-1474	50
H(15)	6394	9238	-808	41
H(18)	4165	7953	412	32
H(19)	1270	7672	967	34
H(21)	3405	9397	2326	33
H(22)	6301	9681	1773	32

JW_07-159ph AV-500 new TBI(HXP) probe
1D 1H starting parameters

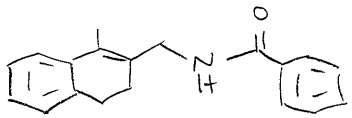
7.801 7.787 7.540 7.525 7.511 7.473 7.457 7.443 7.338 7.323 7.279 7.258 7.245 7.228 7.192 7.177 7.163 7.153 7.140 7.068 6.101 5.319

4.363 4.352 4.269 4.146 4.132 2.869 2.798 2.783 2.767 2.744 2.384 2.370 2.355 2.309 2.184 2.066 1.609 1.292 1.278 1.264 0.991 0.978 0.914 0.901 0.887 0.874 0.866 0.859 0.853

NAME	JW-07-159-Ph
EXPNO	1
PROCNO	1
Date_	20111116
Time	13.42
INSTRUM	AV-500
PROBHD	5 mm TBI 1H/31
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	322.5
DW	48.400 usec
DE	6.00 usec
TE	292.4 K
D1	0.10000000 sec
TD0	2
======== CHANNEL f1 ========	
NUC1	1H
P1	7.30 usec
PL1	0.00 dB
PL1W	12.55943203 W
SFO1	500.2330889 MHz
SI	65536
SF	500.2300165 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00

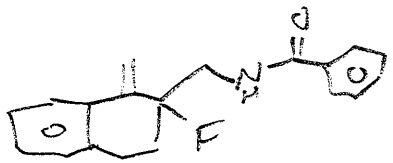


DRX-500 5mm TBIC probe 13C starting parameters. Rev 1/11/
With CPD proton decoupling. Use ns*td0 scans

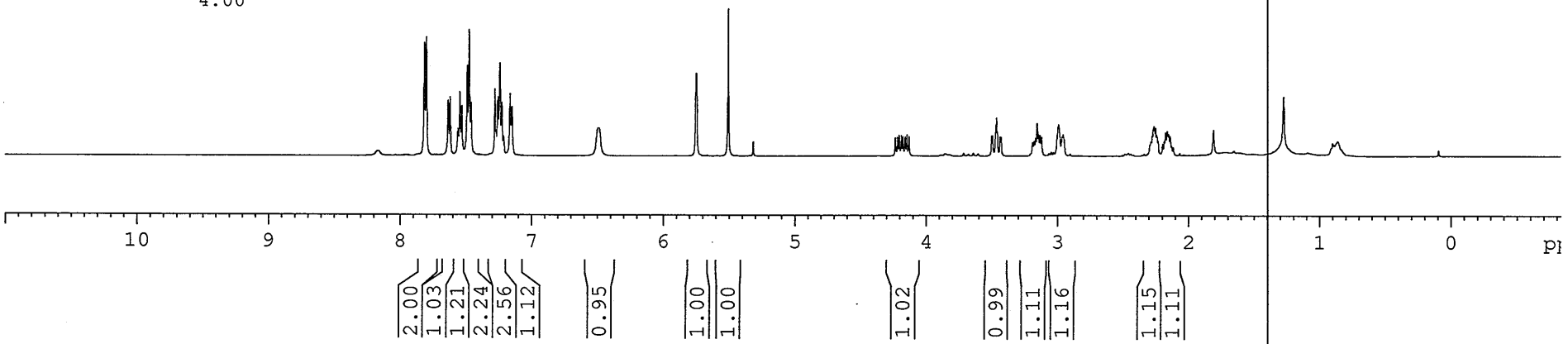


NAME	AD-JW-7-158C
EXPNO	1
PROCNO	1
Date_	20120210
Time	10.45
INSTRUM	DRX-500
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	154
DS	0
SWH	41322.312 Hz
FIDRES	0.630528 Hz
AQ	0.7930356 sec
RG	8192
DW	12.100 usec
DE	6.00 usec
TE	293.6 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	10000
======== CHANNEL f1 ========	
NUC1	13C
P1	10.75 usec
PL1	0.00 dB
SFO1	125.7175545 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-5.00 dB
PL12	7.04 dB

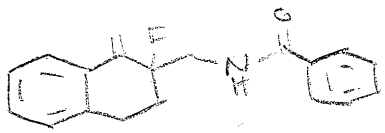
JW-0879 AV-500 new TBI(HXP) probe
1D 1H starting parameters



NAME	JW-08-79-protonchec	
EXPNO	1	
PROCNO	1	
Date_	20120518	
Time	11.08	
INSTRUM	AV-500	
PROBHD	5 mm TBI 1H/31	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	0	
SWH	10330.578	Hz
FIDRES	0.157632	Hz
AQ	3.1720407	sec
RG	128	
DW	48.400	usec
DE	6.00	usec
TE	292.8	K
D1	0.10000000	sec
TD0	4	
======== CHANNEL f1 ========		
NUC1	1H	
P1	7.30	usec
PL1	0.00	dB
PL1W	12.55943203	W
SFO1	500.2330889	MHz
SI	65536	
SF	500.2300165	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	4.00	



DRX-500 5mm TBIC probe 13C starting parameters. Rev 1/11/
With CPD proton decoupling. Use ns*td0 scans

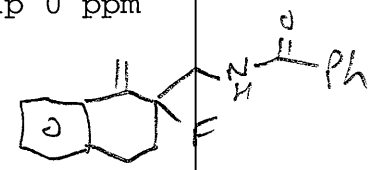


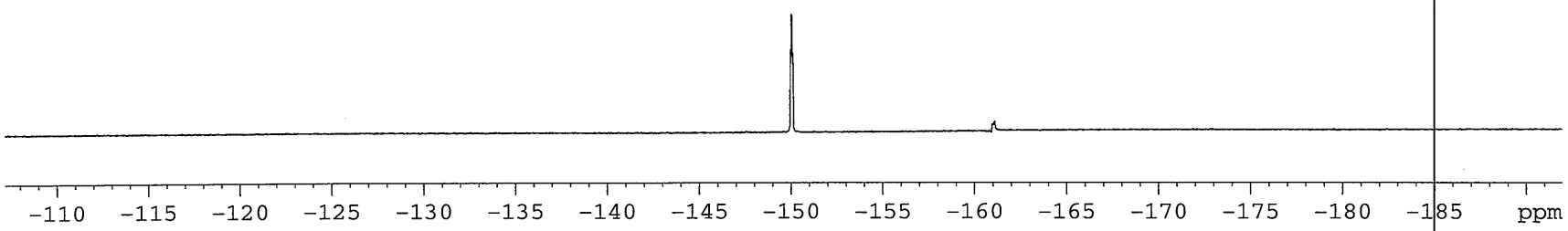
NAME	AD-JW-7-79
EXPNO	1
PROCNO	1
Date_	20120210
Time	10.13
INSTRUM	DRX-500
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	568
DS	0
SWH	41322.312 Hz
FIDRES	0.630528 Hz
AQ	0.7930356 sec
RG	3649.1
DW	12.100 usec
DE	6.00 usec
TE	293.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	10000
========	CHANNEL f1 ========
NUC1	13C
P1	10.75 usec
PL1	0.00 dB
SFO1	125.7175545 MHz
========	CHANNEL f2 ========
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-5.00 dB
PL12	7.04 dB

9check AVQ-400 QNP Probe 19F starting parameters. (revised P1, 2/12
chemical shifts relative to CFCl3 at 0 ppm (082103 HvH)
sw 239.28 ppm; o1p 0 ppm

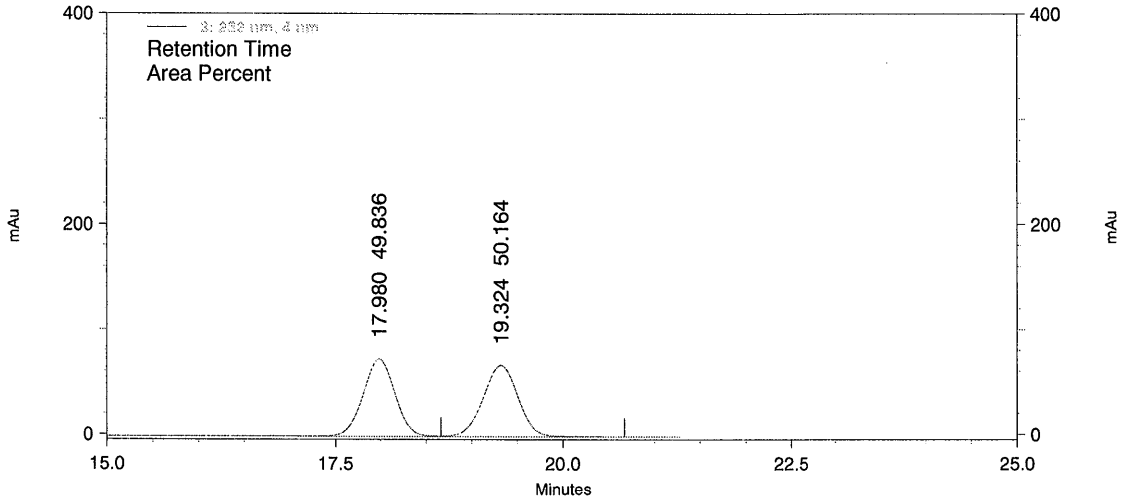
NAME	JW-08-79fCheck
EXPNO	1
PROCNO	1
Date_	20120518
Time	11.16
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	32
DS	0
SWH	90090.094 Hz
FIDRES	0.687333 Hz
AQ	0.7275051 sec
RG	1024
DW	5.550 usec
DE	6.00 usec
TE	292.6 K
D1	1.00000000 sec
TD0	4
======== CHANNEL f1 ========	
NUC1	19F
P1	16.00 usec
PL1	-3.00 dB
PL1W	20.04748917 W
SFO1	376.4607042 MHz
SI	65536
SF	376.4980736 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	14.00

-150.03
-150.06



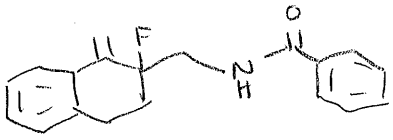


JW-08-79rac / 07-162

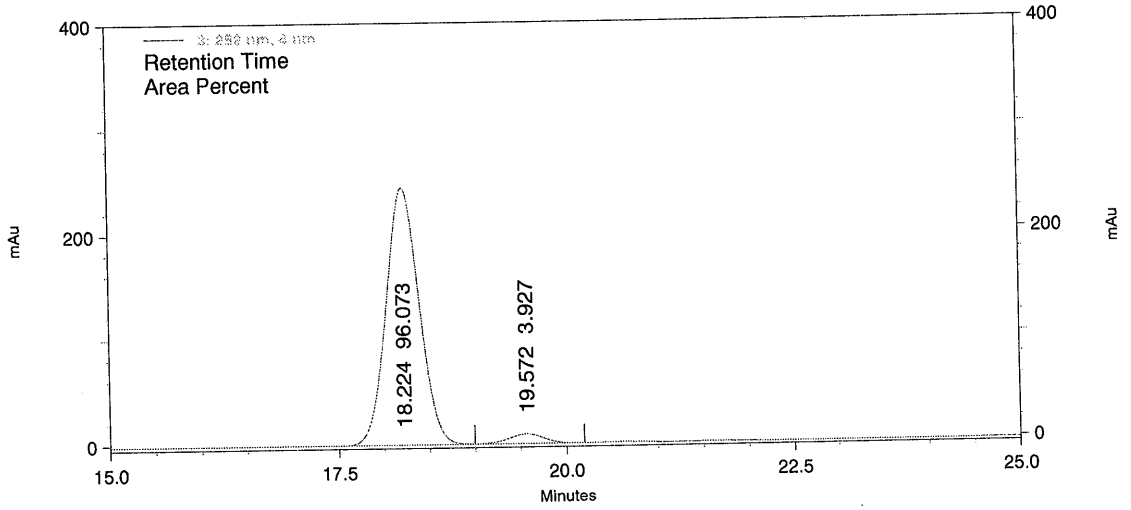


3: 252 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	17.980	49.836	287
2	19.324	50.164	204



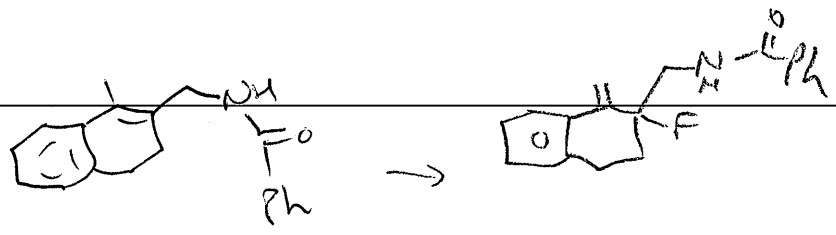
JW-08-79



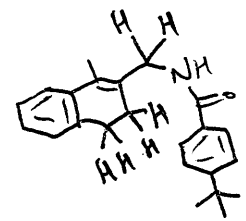
3: 252 nm, 4 nm

Results

Pk #	Retention Time	Area Percent	Lambda Max
1	18.224	96.073	482
2	19.572	3.927	205



JW-07-ymw substrate suzuki AV-500 new TBI(HXP) probe
1D 1H starting parameters



NAME	JW-07-ymwSuzuki
EXPNO	1
PROCNO	1
Date_	20111023
Time	9.56
INSTRUM	AV-500
PROBHD	5 mm TBI 1H/31
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	574.7
DW	48.400 use
DE	6.00 use
TE	292.3 K
D1	0.10000000 sec
TD0	2

======= CHANNEL f1 =======	
NUC1	1H
P1	7.30 use
PL1	0.00 dB
PL1W	12.55943203 W
SFO1	500.2330889 MHz
SI	65536
SF	500.2300165 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00

7.739 7.722 7.477 7.460 7.335 7.320 7.278 7.258 7.244 7.229 7.189 7.175 7.160 7.151 7.136 7.067 6.059

4.354 4.344

2.786 2.771 2.754 2.372 2.357 2.341 2.179 2.065 1.586 1.472 1.347 1.220 0.900

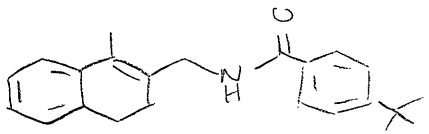
10 9 8 7 6 5 4 3 2 1 0 ppm

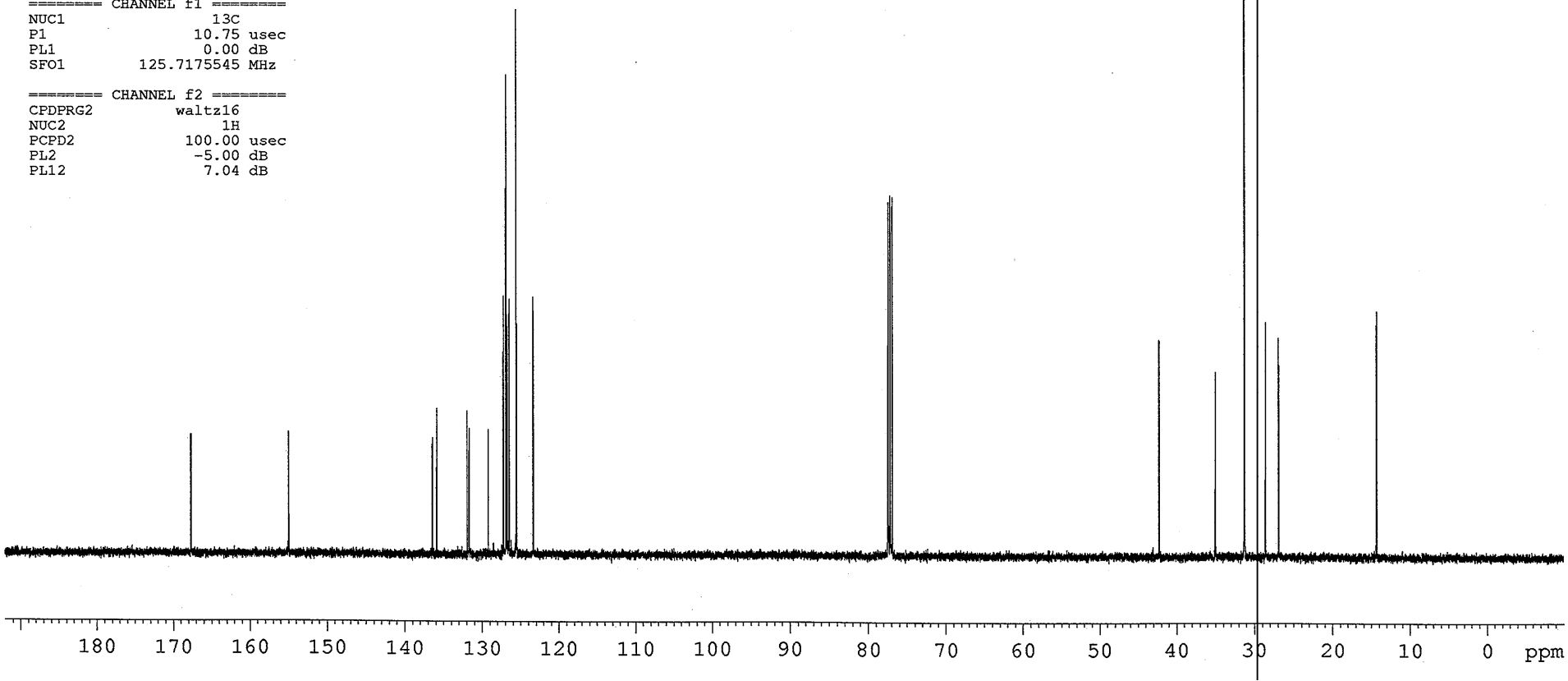
2.08 2.39 6.18 1.61 1.03 1.95 2.00 2.16 2.68 3.82 8.81

DRX-500 5mm TBIC probe 13C starting parameters. Rev 1/11/
With CPD proton decoupling. Use ns*td0 scans

167.66
154.96
136.40
135.82
131.91
131.67
129.19
127.22
126.87
126.72
126.48
125.53
123.30
77.39
77.13
76.88
42.22
34.95
31.22
28.53
26.85
14.27

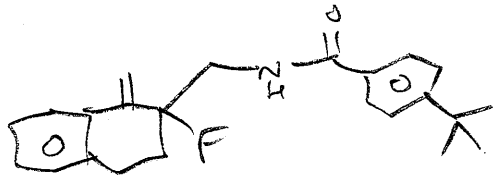
NAME	AD-JW-77-SM
EXPNO	1
PROCNO	1
Date_	20120209
Time	16.44
INSTRUM	DRX-500
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	176
DS	0
SWH	41322.312 Hz
FIDRES	0.630528 Hz
AQ	0.7930356 sec
RG	3251
DW	12.100 usec
DE	6.00 usec
TE	292.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	10000
======== CHANNEL f1 ========	
NUC1	13C
P1	10.75 usec
PL1	0.00 dB
SFO1	125.7175545 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-5.00 dB
PL12	7.04 dB



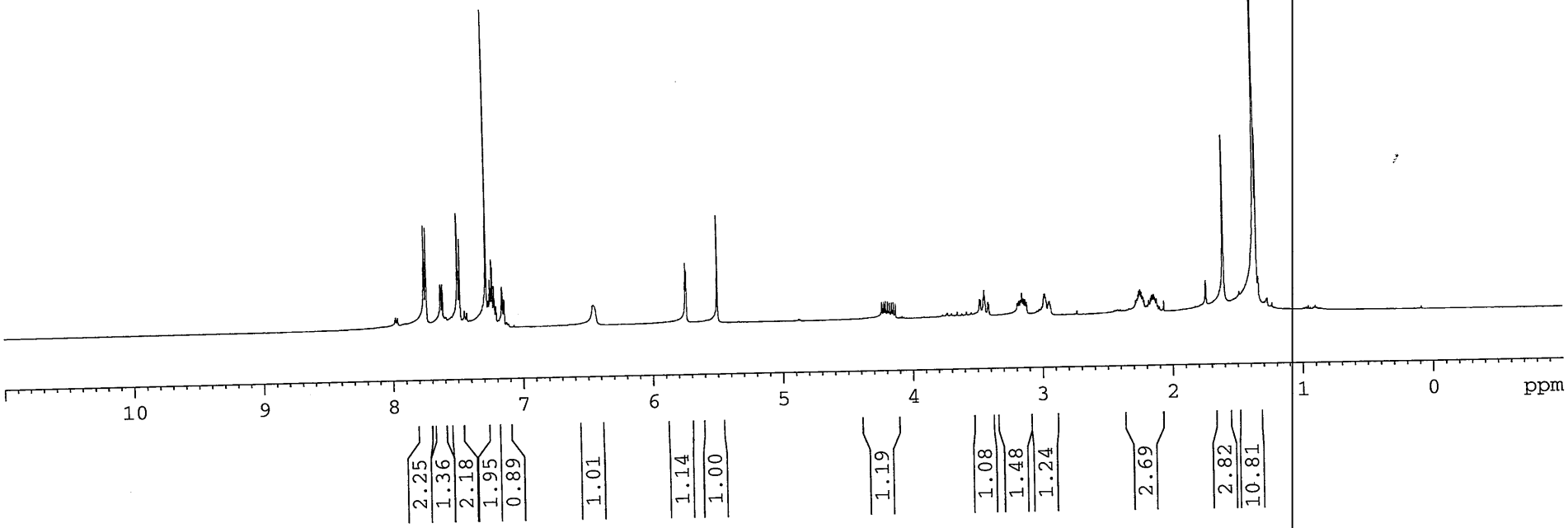


JW-08-16A AV-500 new TBI(HXP) probe
1D 1H starting parameters

7.980 7.963 7.757 7.740 7.631 7.617 7.498 7.482 7.448 7.431 7.278 7.263 7.252 7.249 7.238 7.234 7.221 7.207 7.159 7.144 6.455 5.745 5.738 5.500 4.237 4.221 4.208 4.191 4.178 4.162 4.149 4.133 3.482 3.475 3.452 3.446 3.439 3.417 3.410 3.190 3.178 3.155 3.144 3.132 3.121 2.978 2.944 2.255 2.249 2.244 2.237 2.229 2.179 2.167 2.157 2.145 2.136 2.123 2.066 1.743 1.605 1.484 1.360 1.351 1.338 1.335 1.270

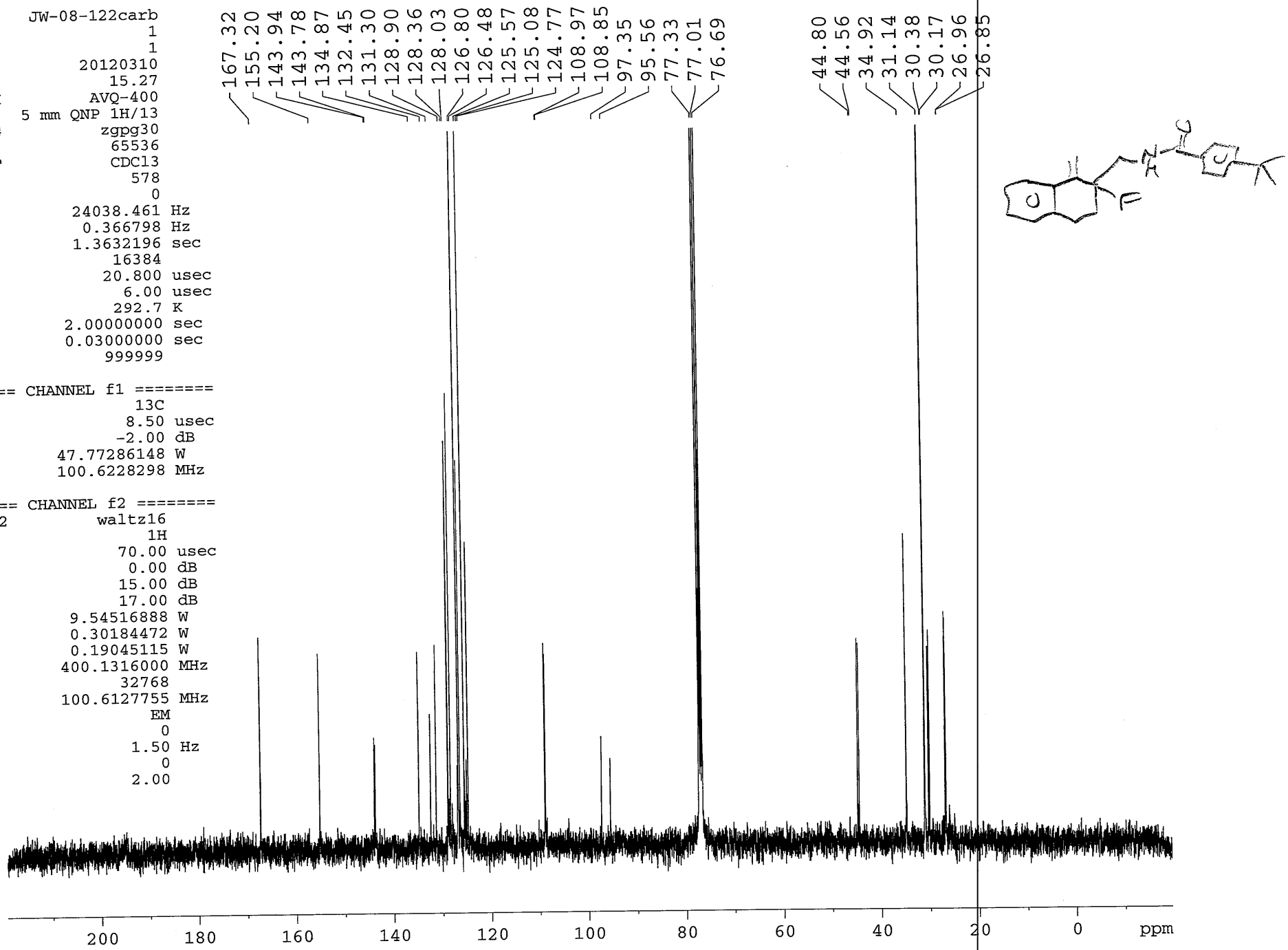


NAME	JW-08-16A
EXPNO	1
PROCNO	1
Date_	20120106
Time	13.51
INSTRUM	AV-500
PROBHD	5 mm TBI 1H/31
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	24
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	256
DW	48.400 use
DE	6.00 use
TE	292.3 K
D1	0.10000000 sec
TD0	3
======== CHANNEL f1 =======	
NUC1	1H
P1	7.30 use
PL1	0.00 dB
PL1W	12.55943203 W
SFO1	500.2330889 MHz
SI	65536
SF	500.2300165 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00

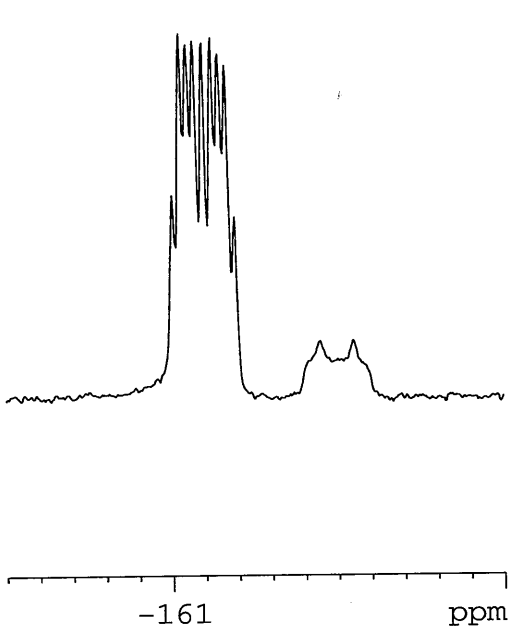


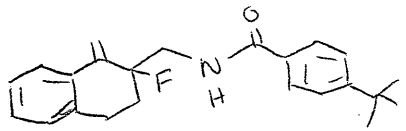
122 AVQ-400 QNP Carbon Starting parameters 7/16/03 r

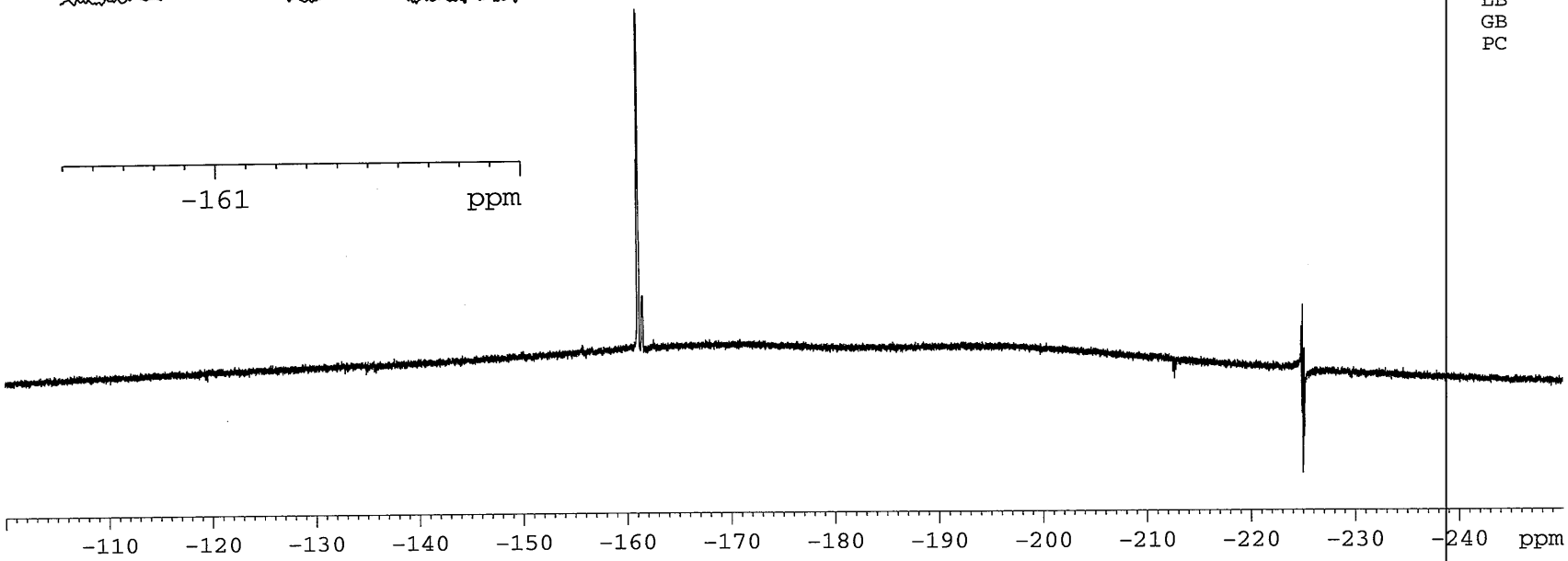
NAME	JW-08-122carb
EXPNO	1
PROCNO	1
Date_	20120310
Time	15.27
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	578
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3632196 sec
RG	16384
DW	20.800 usec
DE	6.00 usec
TE	292.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	999999
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	17.00 dB
PL2W	9.54516888 W
PL12W	0.30184472 W
PL13W	0.19045115 W
SFO2	400.1316000 MHz
SI	32768
SF	100.6127755 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	2.00



AVQ-400 QNP Probe 19F starting parameters. (revised P
chemical shifts relative to CFCl3 at 0 ppm (082103 Hv

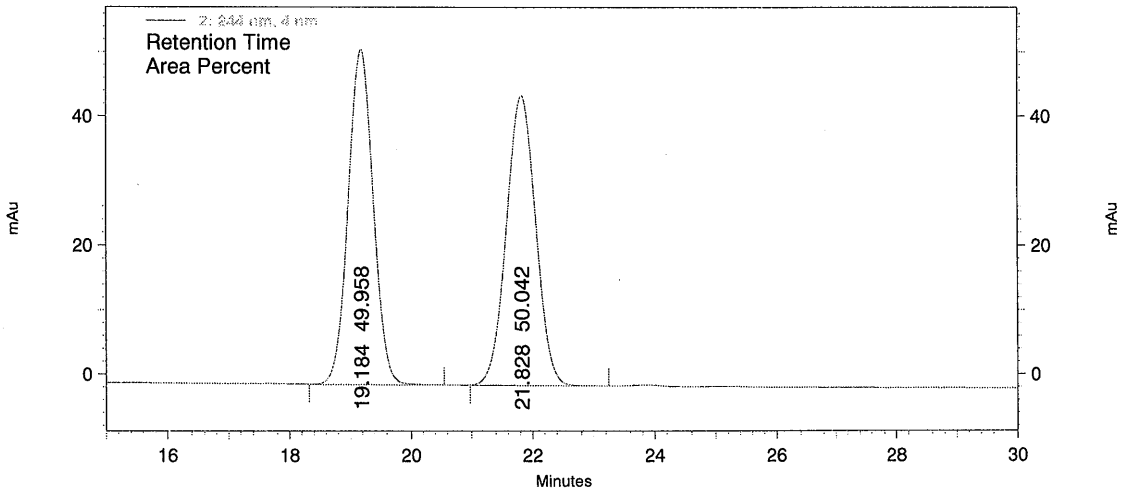






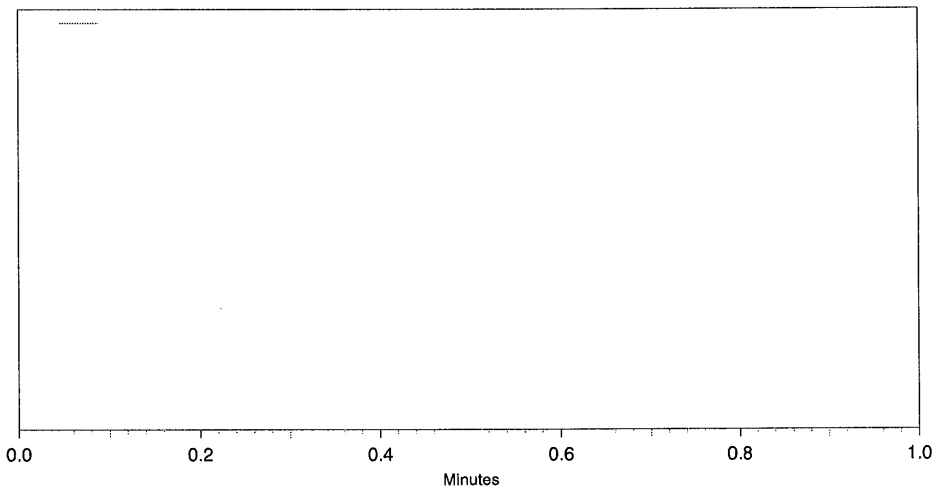
NAME	JW-07-117RacF
EXPNO	
PROCNO	
Date_	2011102
Time	7.5
INSTRUM	AVQ-4C
PROBHD	5 mm QNP 1H/1
PULPROG	zgflq
TD	13107
SOLVENT	CDCl
NS	2
DS	
SWH	90090.09
FIDRES	0.68733
AQ	0.727505
RG	25
DW	5.55
DE	6.C
TE	292.
D1	1.000000C
TD0	
======== CHANNEL f1 ==	
NUC1	19
P1	16.C
PL1	-3.C
PL1W	20.0474891
SFO1	376.441879
SI	6553
SF	376.498073
WDW	E
SSB	
LB	2.C
GB	
PC	4.C

JW-07-119rac_IC9208_30min

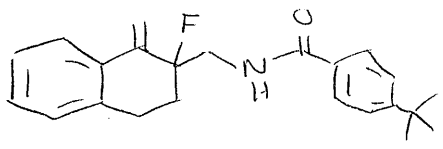


2: 244 nm, 4 nm
Results

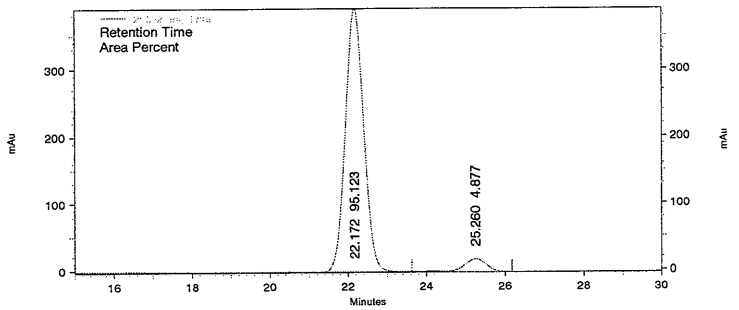
Pk #	Retention Time	Area Percent	Lambda Max
1	19.184	49.958	205
2	21.828	50.042	205

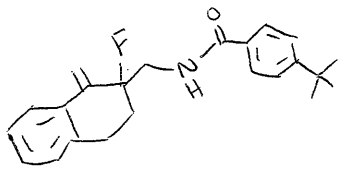


Pk #	Retention Time	Area Percent	Lambda Max



JW-08-16a

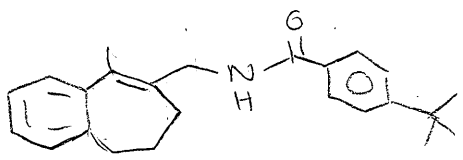




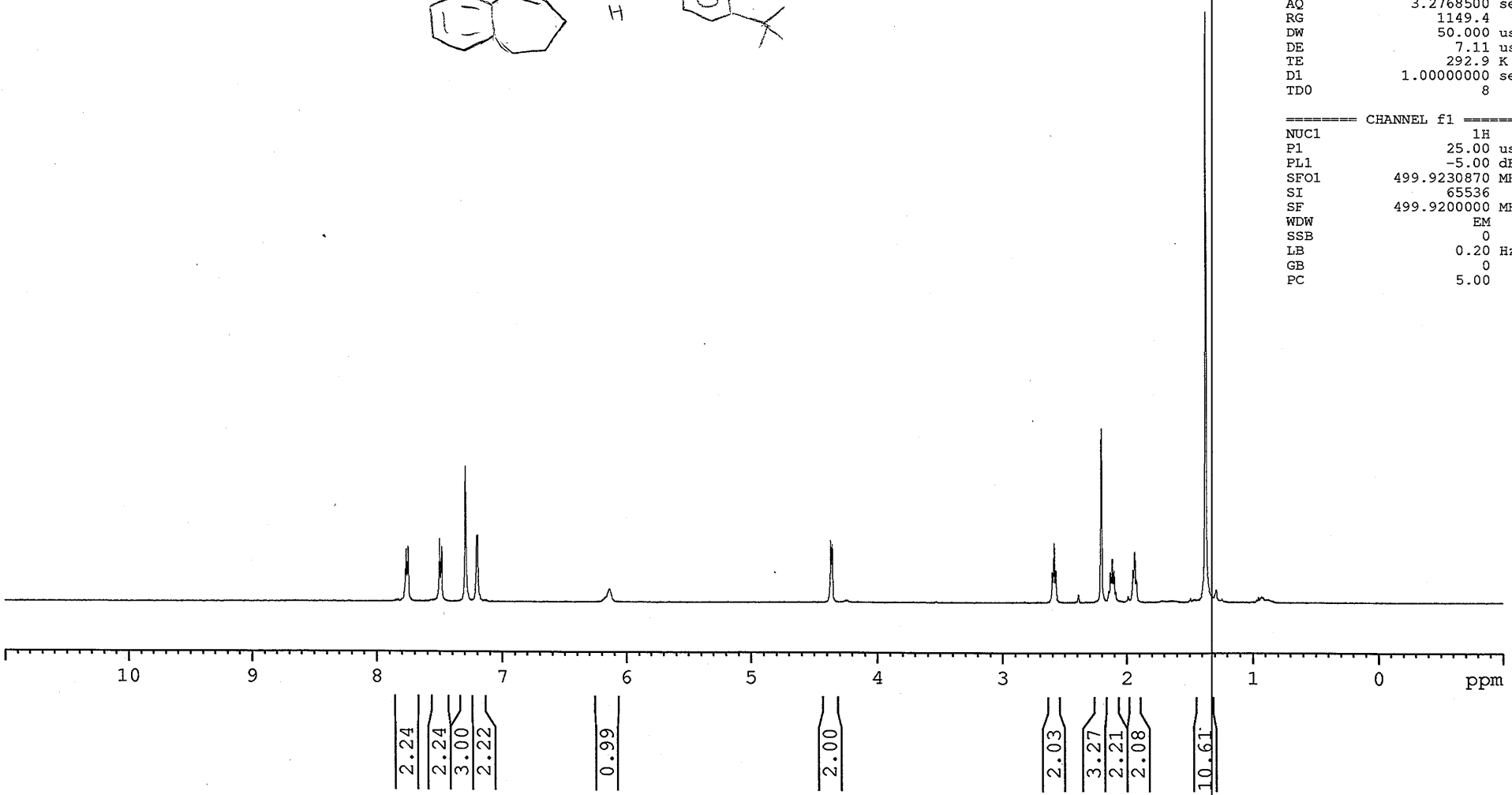
2: 252 nm, 4 nm
Results

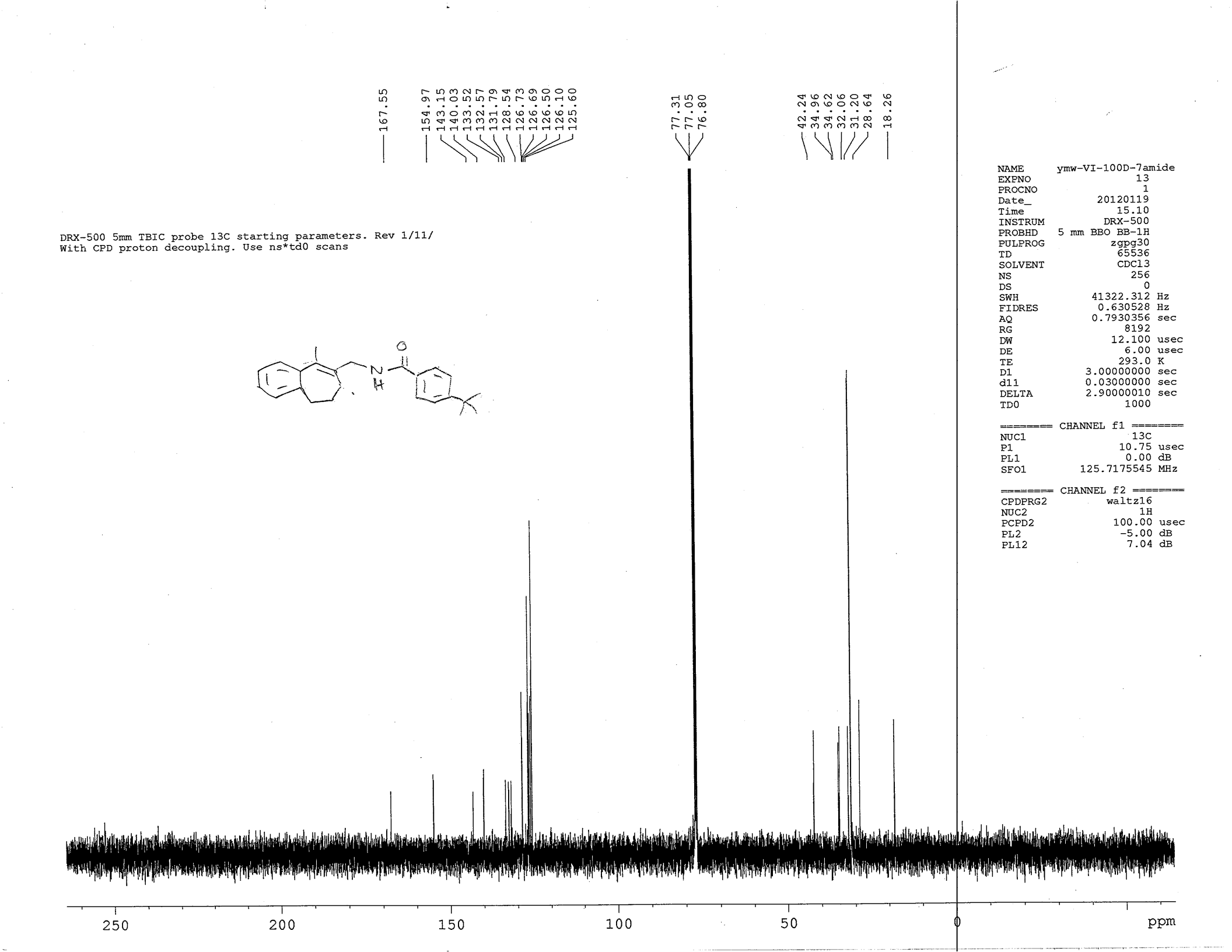
Pk #	Retention Time	Area Percent	Lambda Max
1	22.172	95.123	191
2	25.260	4.877	205

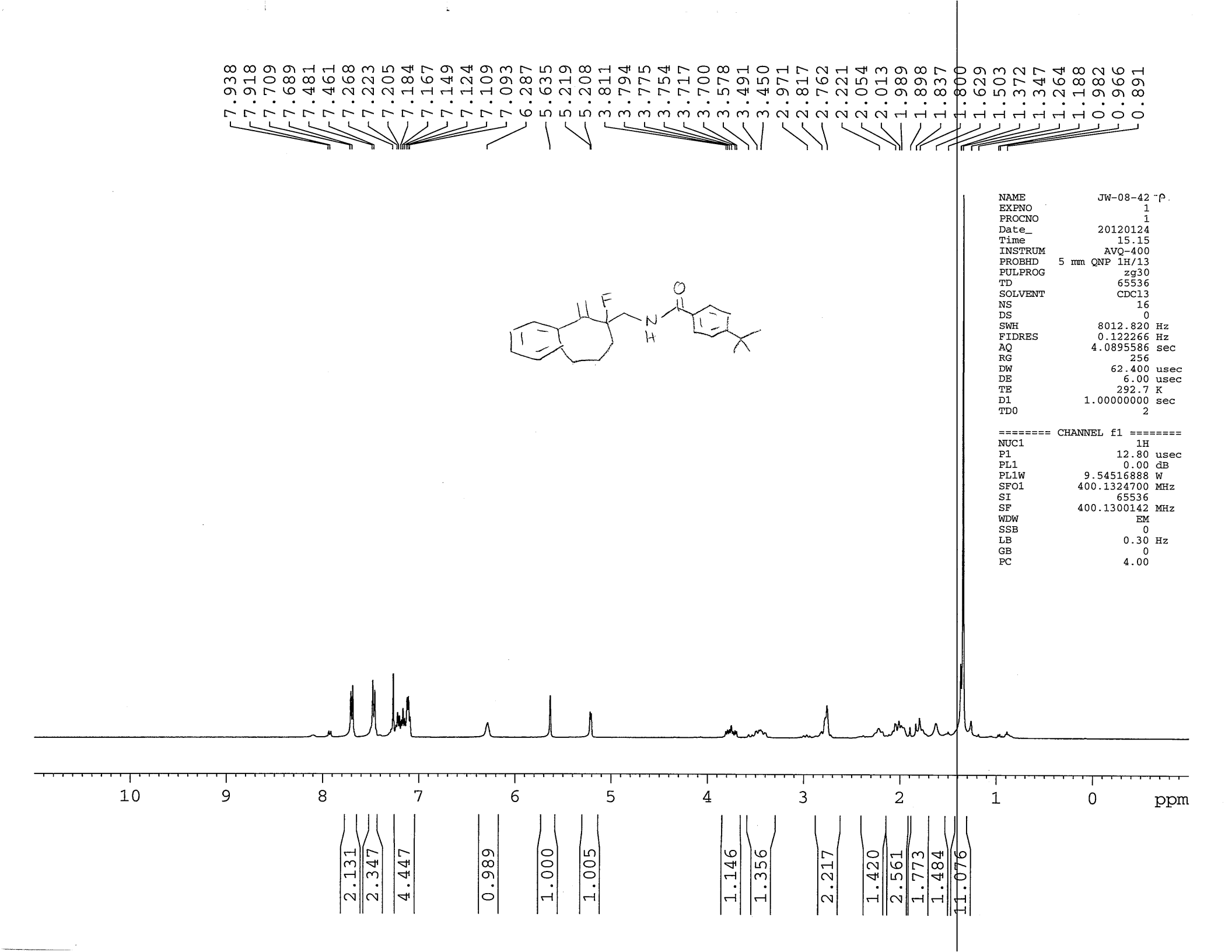
1H starting parameters (zg30)
DRX-500 TBIC
011112 CCC



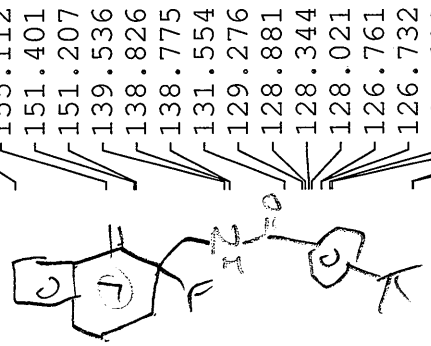
NAME	ymw-VI-100D-7amide
EXPNO	1
PROCNO	1
Date_	20120119
Time	15.08
INSTRUM	DRX-500
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	1149.4
DW	50.000 use
DE	7.11 use
TE	292.9 K
D1	1.00000000 sec
TD0	8
========	CHANNEL f1 =======
NUC1	1H
P1	25.00 use
PL1	-5.00 dB
SFO1	499.9230870 MHz
SI	65536
SF	499.9200000 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	5.00




167.55
154.97
143.15
140.03
133.52
132.57
131.79
128.54
126.73
126.69
126.50
126.10
125.60
77.31
77.05
76.80
42.24
34.96
34.62
32.06
31.20
28.64
18.26
DRX-500 5mm TBIC probe 13C starting parameters. Rev 1/11/
With CPD proton decoupling. Use ns*td0 scans
NAME ymw-VI-100D-7amide
EXPNO 13
PROCNO 1
Date_ 20120119
Time 15.10
INSTRUM DRX-500
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 41322.312 Hz
FIDRES 0.630528 Hz
AQ 0.7930356 sec
RG 8192
DW 12.100 usec
DE 6.00 usec
TE 293.0 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 2.90000010 sec
TD0 1000
======== CHANNEL f1 ========
NUC1 13C
P1 10.75 usec
PL1 0.00 dB
SFO1 125.7175545 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -5.00 dB
PL12 7.04 dB
250
200
150
100
50
0
ppm


7.938
7.918
7.709
7.689
7.481
7.461
7.268
7.223
7.205
7.184
7.167
7.149
7.124
7.109
7.093
6.287
5.635
5.219
5.208
3.811
3.794
3.775
3.754
3.717
3.700
3.578
3.491
3.450
2.971
2.817
2.762
2.221
2.054
2.013
1.989
1.898
1.837
1.800
1.629
1.503
1.372
1.347
1.264
1.188
0.982
0.966
0.891
F
O
N
H
NAME JW-08-42-P
EXPNO 1
PROCNO 1
Date_ 20120124
Time 15.15
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 256
DW 62.400 usec
DE 6.00 usec
TE 292.7 K
D1 1.00000000 sec
TD0 2
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.131
2.347
4.447
0.989
1.000
1.005
1.146
1.356
2.217
1.420
2.561
1.773
1.484
11.076

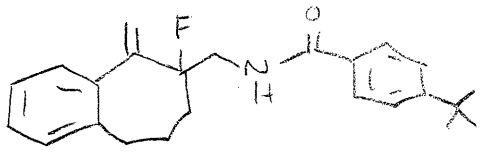
JW-08-124 AVB-400 ZBO Carbon Starting paramters 6/11/03 RN



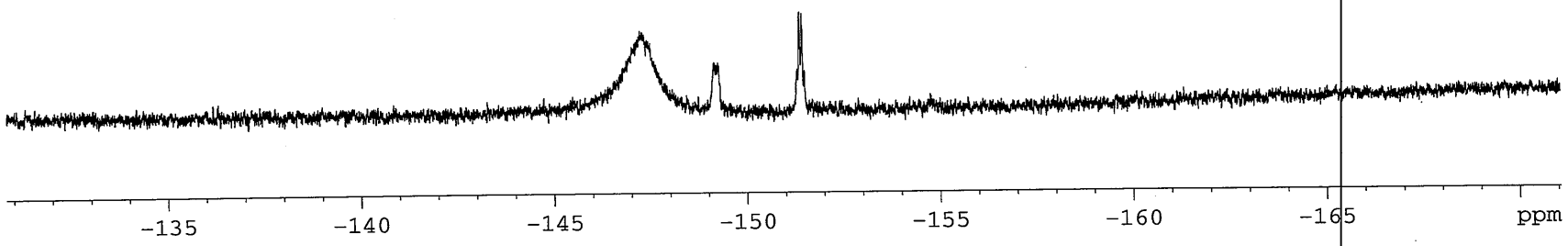
NAME	JW-08-124
EXPNO	1
PROCNO	1
Date_	20120310
Time	16.39
INSTRUM	AVB-400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1601
DS	0
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	16384
DW	20.850 usec
DE	6.00 usec
TE	297.6 K
D1	1.50000000 sec
D11	0.03000000 sec
TD0	10000
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	-3.00 dB
PL12	16.00 dB
PL13	16.00 dB
PL2W	23.05461311 W
PL12W	0.29024038 W
PL13W	0.29024038 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	1.60

JW-08-42 AVQ-400 QNP Probe 19F starting parameters. (
chemical shifts relative to CFCl3 at 0 ppm (082103 Hv

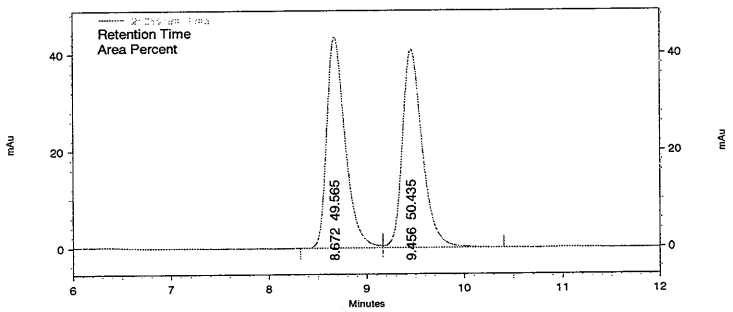
-147.23
-149.15
-151.36
-151.42



NAME	JW-08-42
EXPNO	
PROCNO	
Date_	2012012
Time	15.1
INSTRUM	AVQ-40
PROBHD	5 mm QNP 1H/1
PULPROG	zgflq
TD	13107
SOLVENT	CDCl
NS	3
DS	
SWH	90090.09
FIDRES	0.68733
AQ	0.727505
RG	5160.
DW	5.55
DE	6.0
TE	292.
D1	1.000000(
TD0	
======== CHANNEL f1 ==	
NUC1	19
P1	16.0
PL1	-3.0
PL1W	20.0474891
SFO1	376.460704
SI	6553
SF	376.498073
WDW	E
SSB	
LB	2.0
GB	
PC	4.0



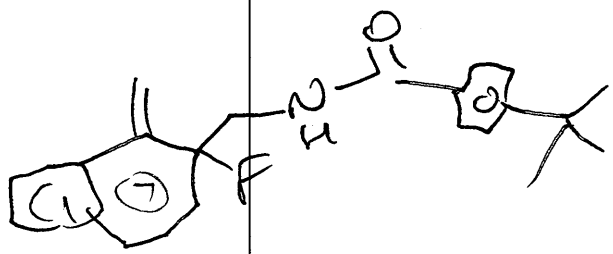
JW-08-42-rac (ad)



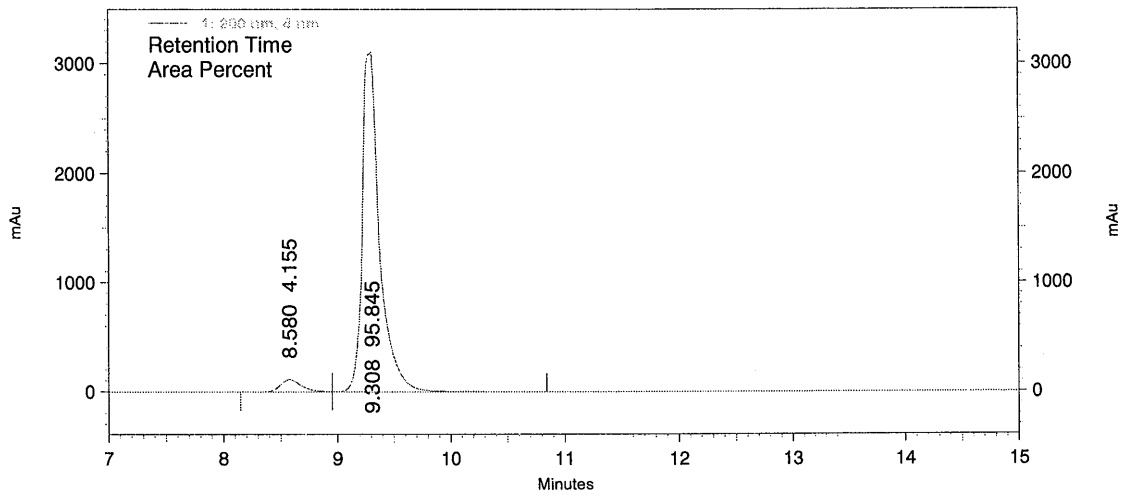
2: 255 nm, 4 nm

Results

Pk #	Retention Time	Area Percent	Lambda Max
1	8.672	49.565	205
2	9.456	50.435	205



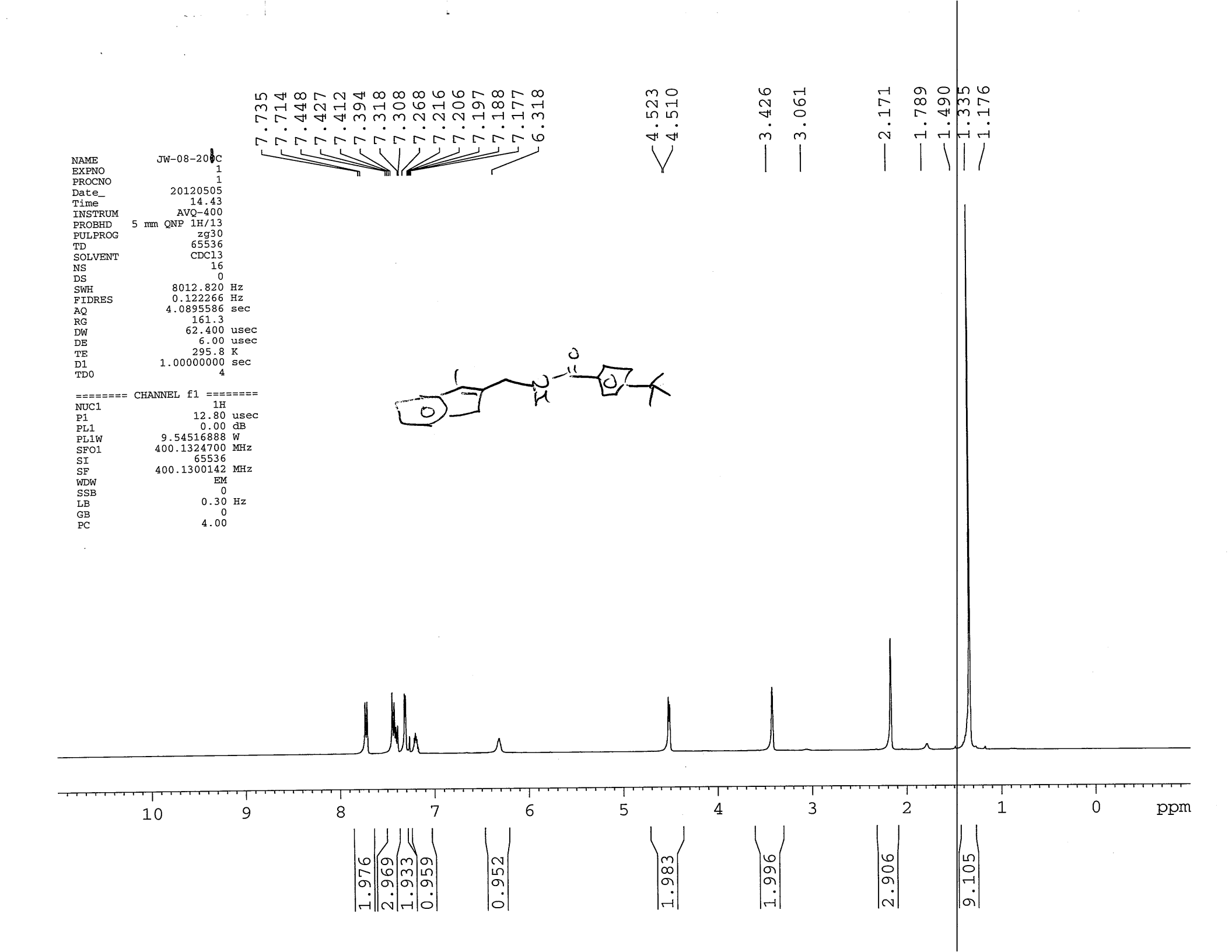
JW-08-124 IB9505_15

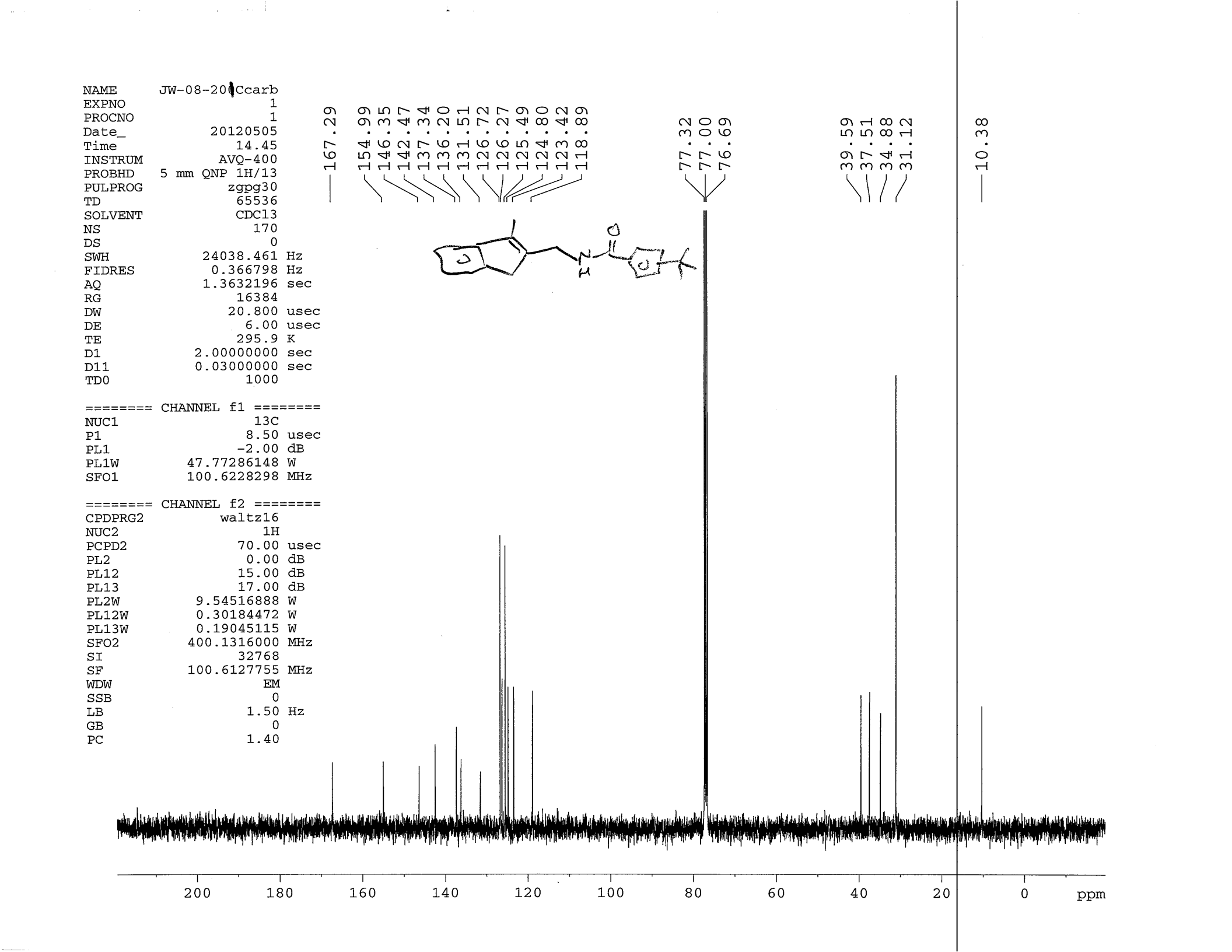


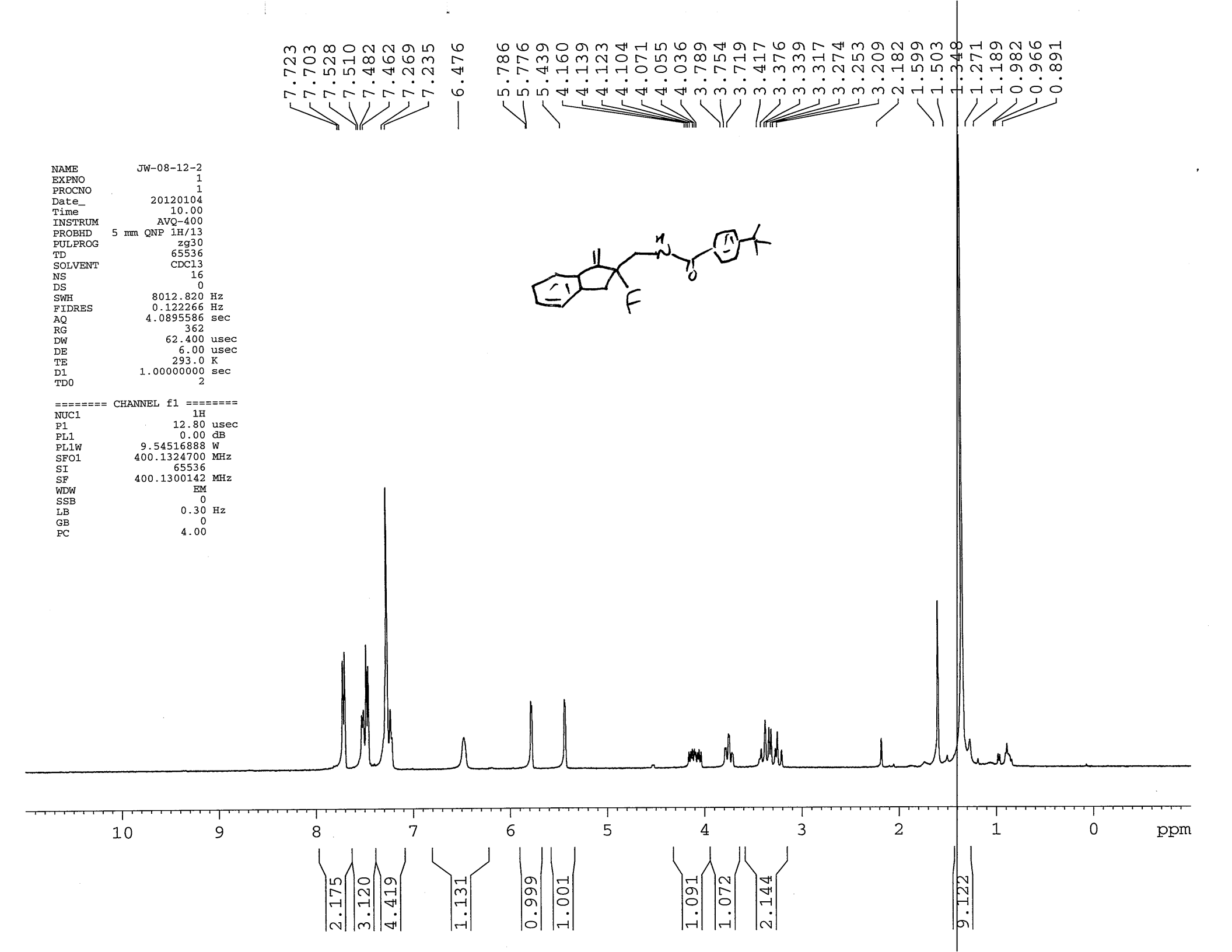
1: 200 nm, 4 nm

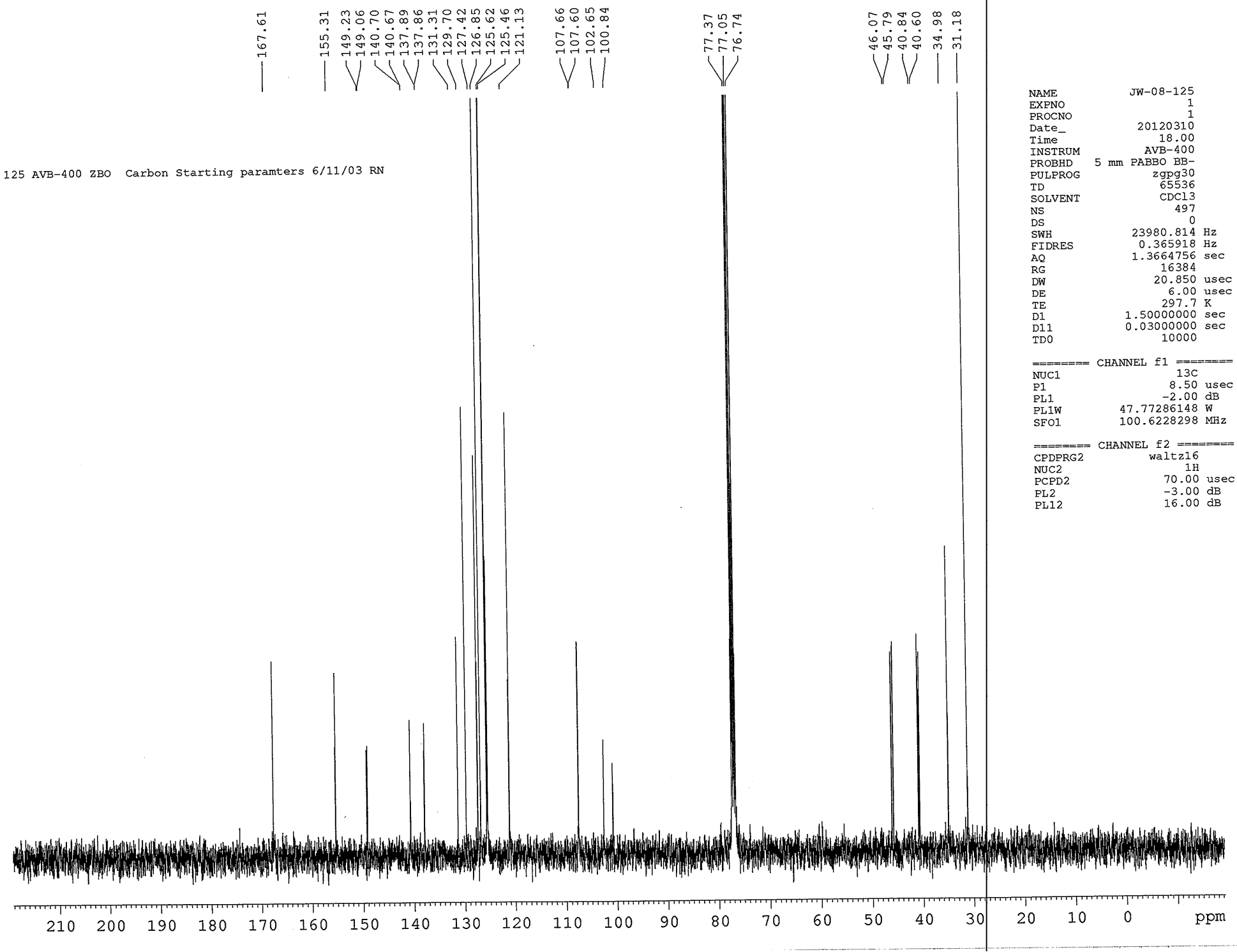
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	8.580	4.155	205
2	9.308	95.845	202


7.735
7.714
7.448
7.427
7.412
7.394
7.318
7.308
7.268
7.216
7.206
7.197
7.188
7.177
6.318
4.523
4.510
3.426
3.061
2.171
1.789
1.490
1.335
1.176
NAME JW-08-20C
EXPNO 1
PROCNO 1
Date_ 20120505
Time 14.43
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 161.3
DW 62.400 usec
DE 6.00 usec
TE 295.8 K
D1 1.00000000 sec
TD0 4
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
O
H
O
10
9
8
7
6
5
4
3
2
1
0
ppm
1.976
2.969
1.933
0.959
0.952
1.983
1.996
2.906
9.105


NAME JW-08-20Ccarb
EXPNO 1
PROCNO 1
Date_ 20120505
Time 14.45
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 170
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 16384
DW 20.800 usec
DE 6.00 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1000
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 17.00 dB
PL2W 9.54516888 W
PL12W 0.30184472 W
PL13W 0.19045115 W
SFO2 400.1316000 MHz
SI 32768
SF 100.6127755 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40
167.29
154.99
146.35
142.47
137.34
136.20
131.51
126.72
126.27
125.49
124.80
123.42
118.89
77.32
77.00
76.69
39.59
37.51
34.88
31.12
10.38
200
180
160
140
120
100
80
60
40
20
0
ppm

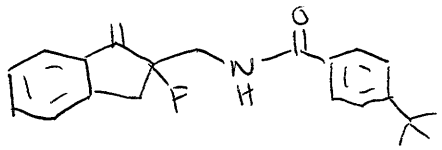

7.723
7.703
7.528
7.510
7.482
7.462
7.269
7.235
6.476
5.786
5.776
5.439
4.160
4.139
4.123
4.104
4.071
4.055
4.036
3.789
3.754
3.719
3.417
3.376
3.339
3.317
3.274
3.253
3.209
2.182
1.599
1.503
1.348
1.271
1.189
0.982
0.966
0.891
NAME JW-08-12-2
EXPNO 1
PROCNO 1
Date_ 20120104
Time 10.00
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 362
DW 62.400 usec
DE 6.00 usec
TE 293.0 K
D1 1.00000000 sec
TD0 2
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
F
H
N
O
10
9
8
7
6
5
4
3
2
1
0
ppm
2.175
3.120
4.419
1.131
0.999
1.001
1.091
1.072
2.144
9.122

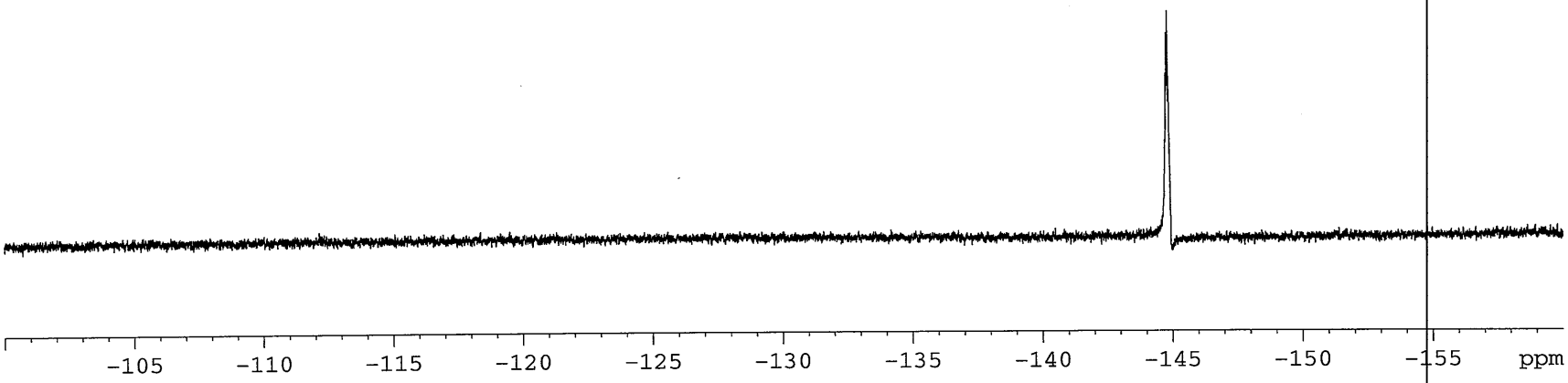

167.61
155.31
149.23
149.06
140.70
140.67
137.89
137.86
131.31
129.70
127.42
126.85
125.62
125.46
121.13
107.66
107.60
102.65
100.84
77.37
77.05
76.74
46.07
45.79
40.84
40.60
34.98
31.18
125 AVB-400 ZBO Carbon Starting paramters 6/11/03 RN
NAME JW-08-125
EXPNO 1
PROCNO 1
Date_ 20120310
Time 18.00
INSTRUM AVB-400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 497
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 297.7 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 10000
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.00 dB
PL12 16.00 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

400 QNP Probe 19F starting parameters. (revised
ical shifts relative to CFCl3 at 0 ppm (082103

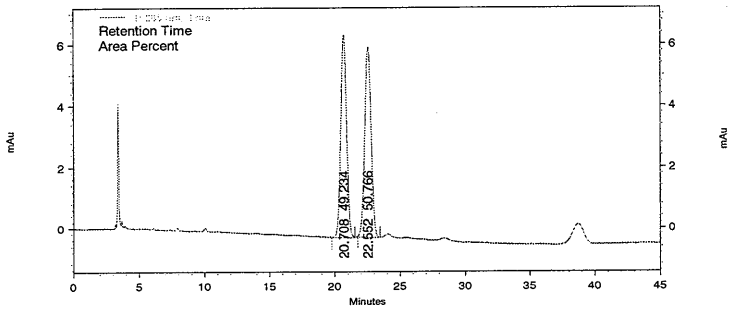
-144.78
-144.81

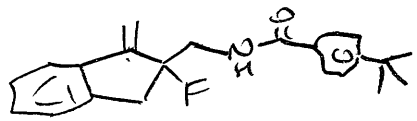
NAME	JW-08-12-2F
EXPNO	1
PROCNO	1
Date_	20120104
Time	10.03
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	8
DS	0
SWH	90090.094 Hz
FIDRES	0.687333 Hz
AQ	0.7275051 sec
RG	4096
DW	5.550 usec
DE	6.00 usec
TE	292.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	16.00 usec
PL1	-3.00 dB
PL1W	20.04748917 W
SFO1	376.4607042 MHz
SI	65536
SF	376.4980736 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	4.00





JW-08-31



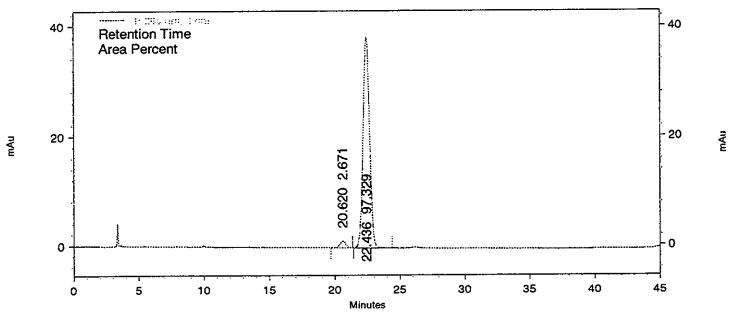


1: 285 nm, 4 nm

Results

Pk #	Retention Time	Area Percent	Lambda Max
1	20.708	49.234	205
2	22.552	50.766	205

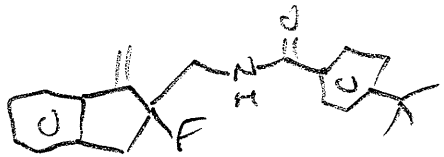
JW-08-31



1: 285 nm, 4 nm

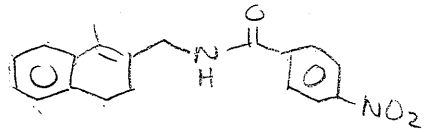
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	20.620	2.671	205
2	22.436	97.329	204

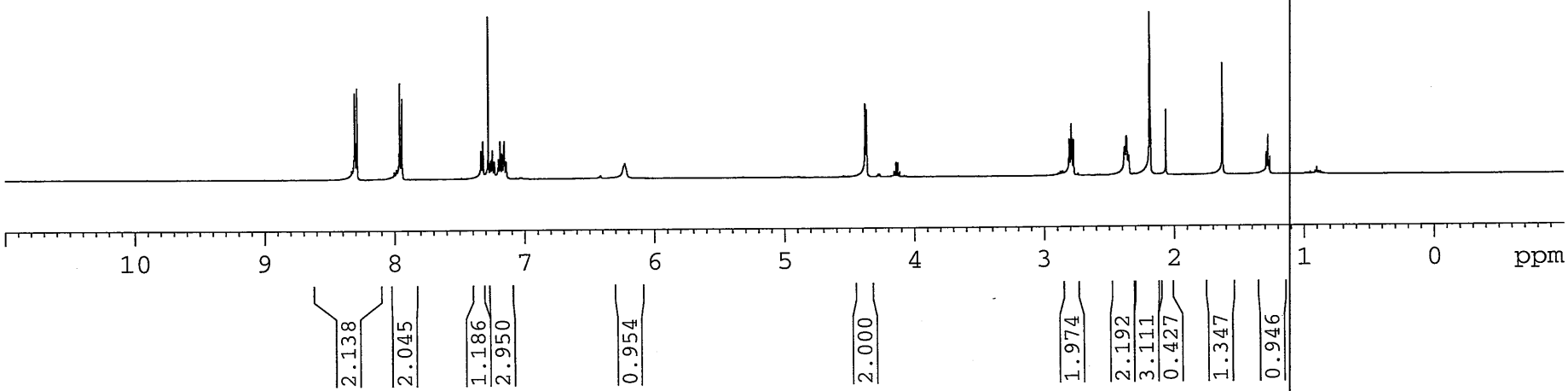


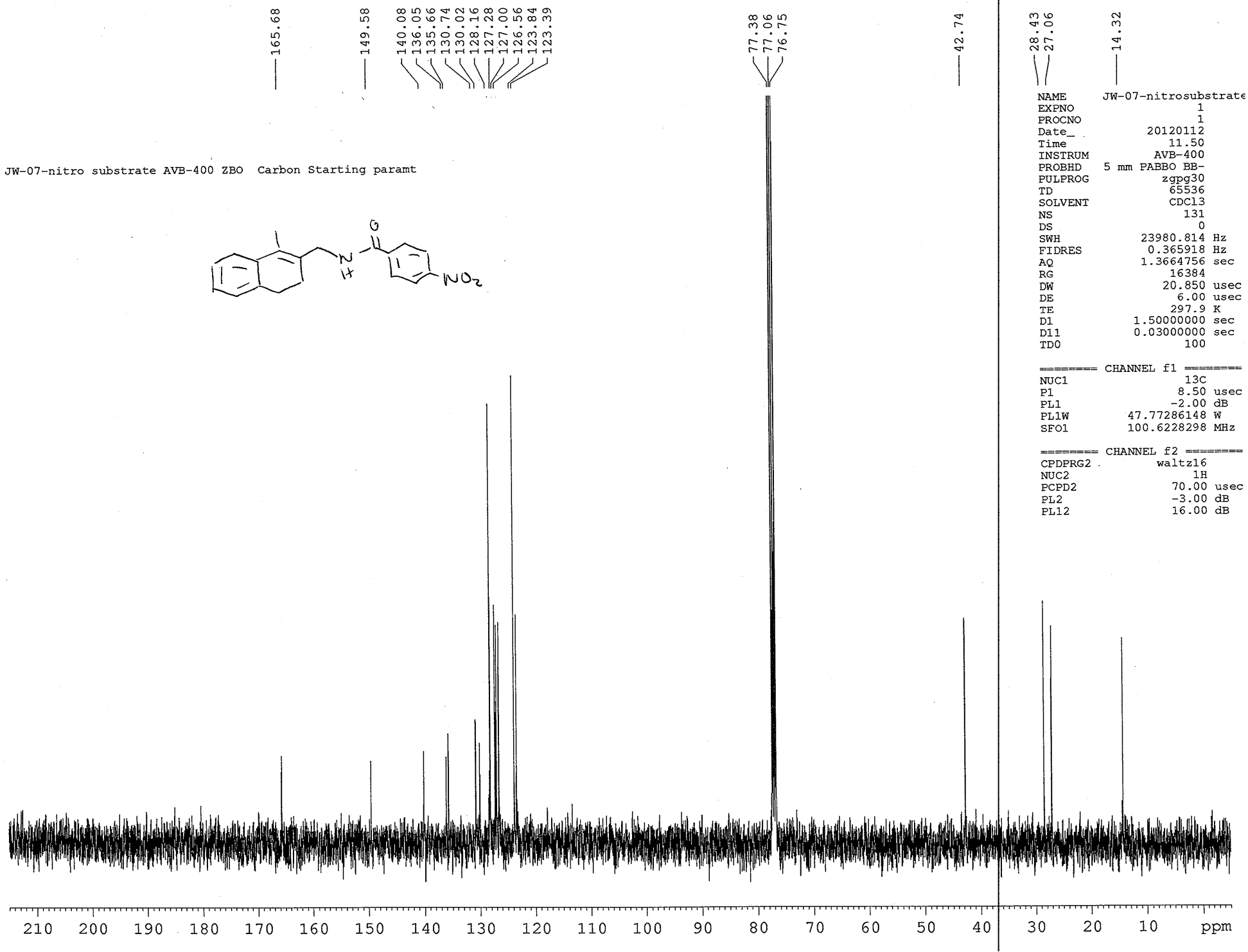
JW_07-159NO2 AV-500 new TBI(HXP) probe
1D 1H starting parameters

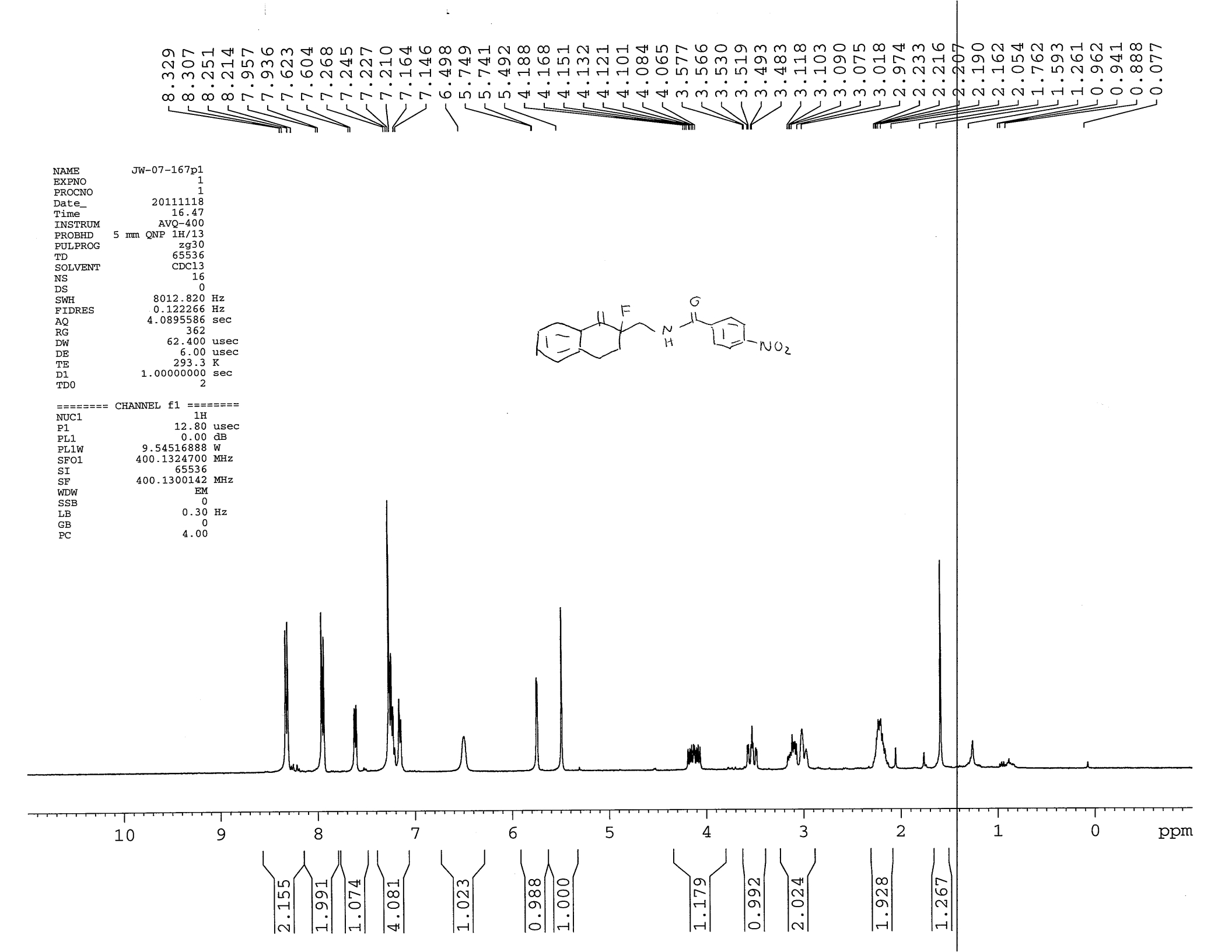
8.331 8.312 8.307 8.303 8.293 8.289 8.285 8.003 7.986 7.965 7.961 7.957 7.947 7.943 7.938 7.336 7.321 7.279 7.264 7.261 7.249 7.247 7.234 7.231 7.204 7.201 7.189 7.186 7.174 7.172 7.158 7.144 6.415 6.228 4.378 4.367 4.279 4.267 4.156 4.142 4.127 4.113 2.890 2.874 2.858 2.806 2.790 2.774 2.378 2.365 2.350 2.187 2.184 2.062 1.625 1.289 1.285 1.275 1.260 0.951 0.913 0.899 0.885 0.873



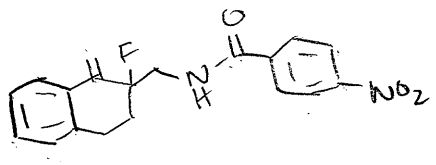
NAME	UW-07-159-NO2
EXPNO	1
PROCNO	1
Date_	20111116
Time	13.45
INSTRUM	AV-500
PROBHD	5 mm TBI 1H/31
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	181
DW	48.400 usec
DE	6.00 usec
TE	292.4 K
D1	0.10000000 sec
TD0	2
======== CHANNEL f1 ========	
NUC1	1H
P1	7.30 usec
PL1	0.00 dB
PL1W	12.55943203 W
SFO1	500.2330889 MHz
SI	65536
SF	500.2300165 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00




165.68
149.58
140.08
136.05
135.66
130.74
130.02
128.16
127.28
127.00
126.56
123.84
123.39
77.38
77.06
76.75
42.74
28.43
27.06
14.32
JW-07-nitro substrate AVB-400 ZBO Carbon Starting paramt
NAME JW-07-nitrosubstrate
EXPNO 1
PROCNO 1
Date_ 20120112
Time 11.50
INSTRUM AVB-400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 131
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 297.9 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 100
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.00 dB
PL12 16.00 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.329
8.307
8.251
8.214
7.957
7.936
7.623
7.604
7.268
7.245
7.227
7.210
7.164
7.146
6.498
5.749
5.741
5.492
4.188
4.168
4.151
4.132
4.121
4.101
4.084
4.065
3.577
3.566
3.530
3.519
3.493
3.483
3.118
3.103
3.090
3.075
3.018
2.974
2.233
2.216
2.207
2.190
2.162
2.054
1.762
1.593
1.261
0.962
0.941
0.888
0.077
NAME JW-07-167p1
EXPNO 1
PROCNO 1
Date_ 20111118
Time 16.47
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 362
DW 62.400 usec
DE 6.00 usec
TE 293.3 K
D1 1.00000000 sec
TD0 2
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
F
O
N
H
NO2
10
9
8
7
6
5
4
3
2
1
0
ppm
2.155
1.991
1.074
4.081
1.023
0.988
1.000
1.179
0.992
2.024
1.928
1.267

DRX-500 5mm TBIC probe 13C starting parameters. Rev 1/11/12 CGC
With CPD proton decoupling. Use ns*td0 scans



Current Data Parameters

NAME	AD-II-nitro_product3
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120203
Time	9.54
INSTRUM	DRX-500
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1256
DS	0
SWH	41322.312 Hz
FIDRES	0.630528 Hz
AQ	0.7930356 sec
RG	2298.8
DW	12.100 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	10000

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

NUC1	13C
P1	10.75 usec
PL1	0.00 dB
SFO1	125.7175545 MHz

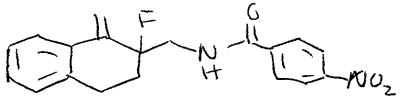
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-5.00 dB
PL12	7.04 dB
PL13	22.00 dB
SFO2	499.9221551 MHz

F2 - Processing parameters

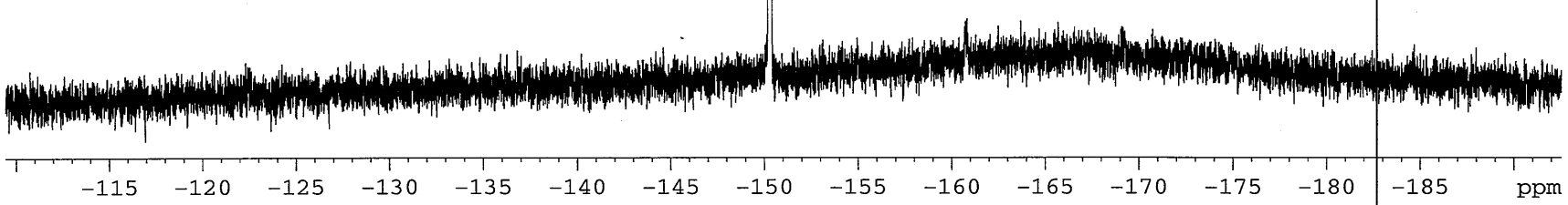
SI	131072
SF	125.7049840 MHz
WDW	EM
SSB	0
LB	0.75 Hz
GB	0
PC	2.00

00 QNP Probe 19F starting parameters. (revised
ical shifts relative to CFC13 at 0 ppm (082103

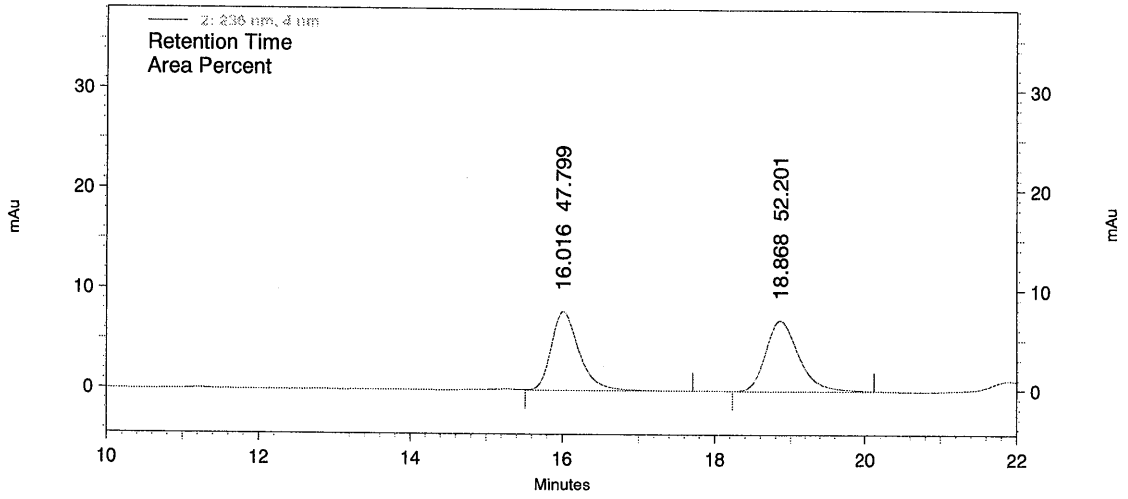


-150.31

NAME	JW-07-167p1-F
EXPNO	1
PROCNO	1
Date_	20111118
Time	16.49
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgflqn
TD	131072
SOLVENT	CDC13
NS	32
DS	0
SWH	90090.094 Hz
FIDRES	0.687333 Hz
AQ	0.7275051 sec
RG	5792.6
DW	5.550 usec
DE	6.00 usec
TE	293.3 K
D1	1.00000000 sec
TD0	4
======== CHANNEL f1 ========	
NUC1	19F
P1	16.00 usec
PL1	-3.00 dB
PL1W	20.04748917 W
SFO1	376.4607042 MHz
SI	65536
SF	376.4980736 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	4.00

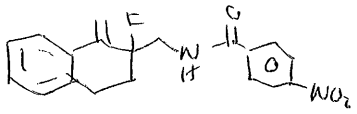


JW-08-35p

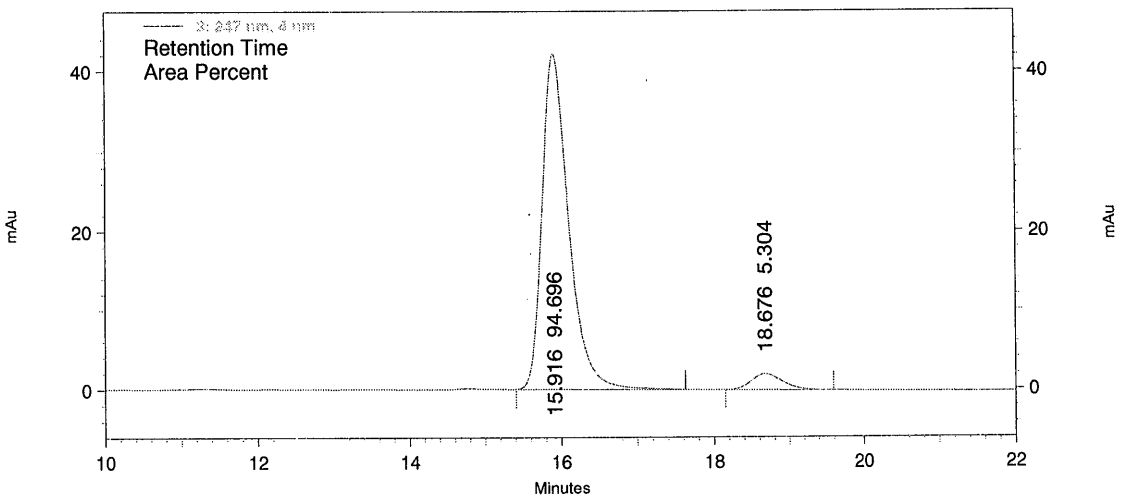


2: 236 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	16.016	47.799	208
2	18.868	52.201	208

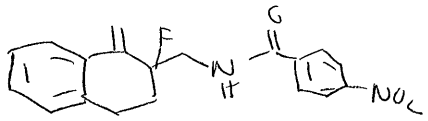


JW-08-35p

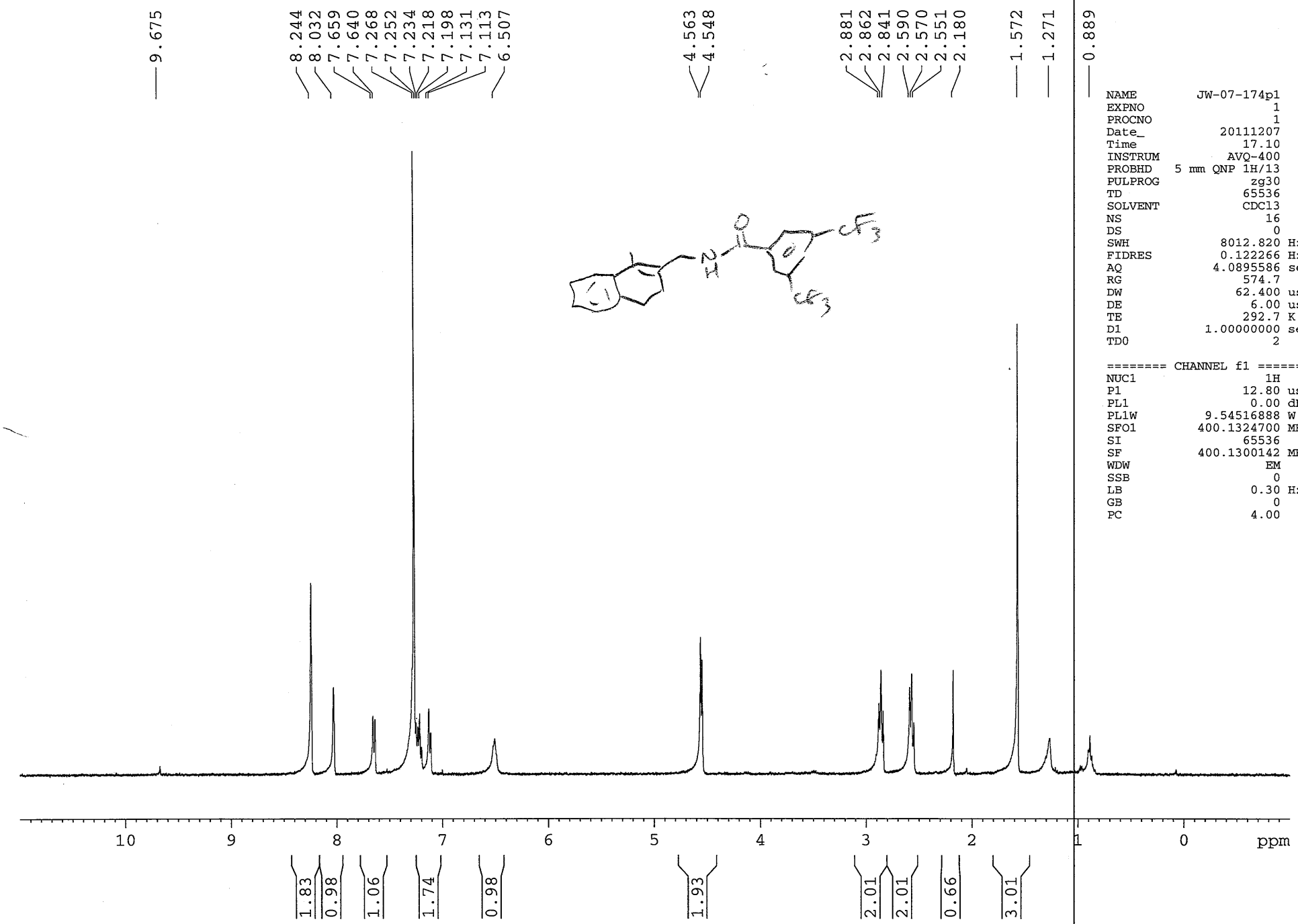


3: 247 nm, 4 nm
Results

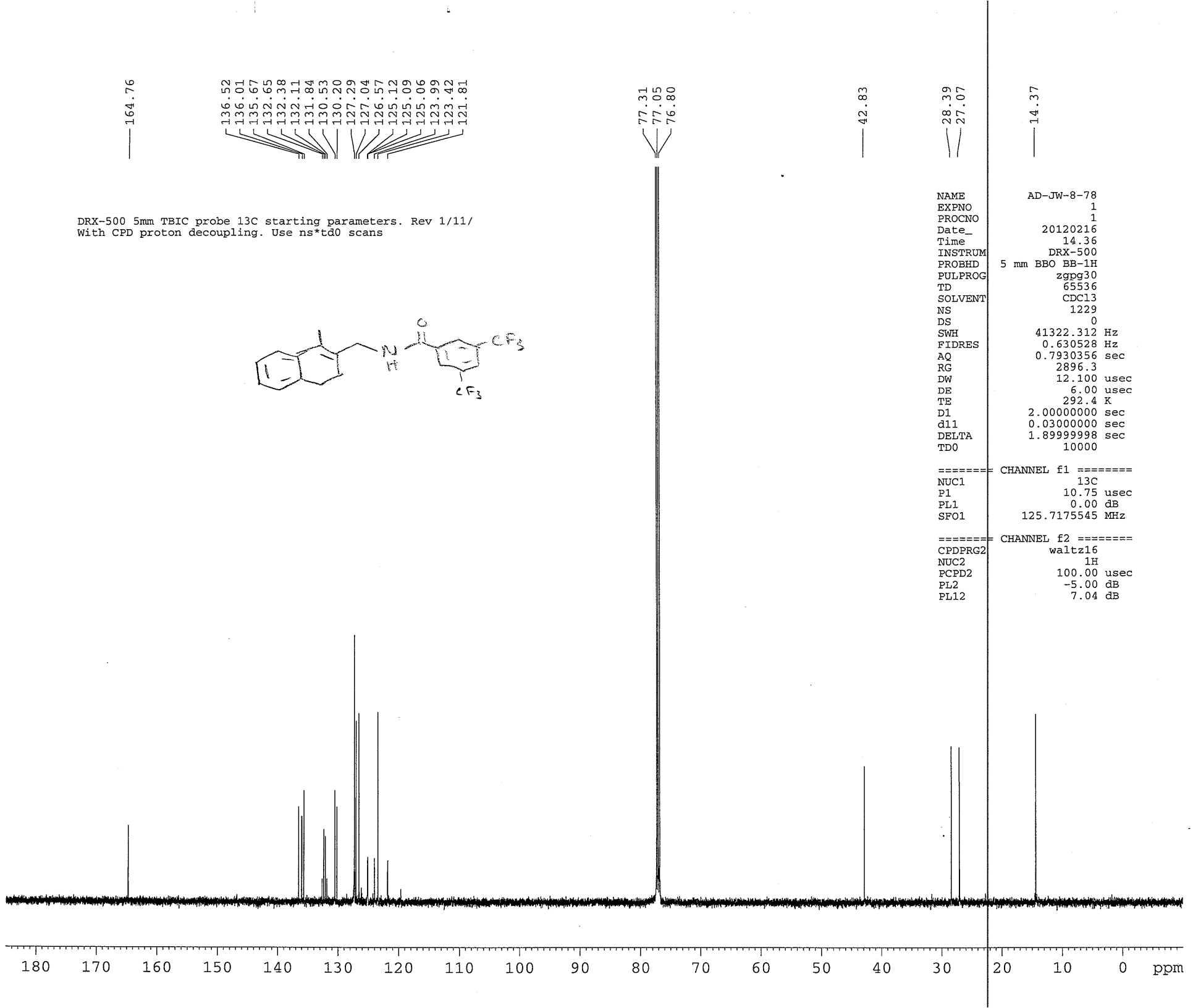
Pk #	Retention Time	Area Percent	Lambda Max
1	15.916	94.696	208
2	18.676	5.304	206



JW-07-174p1 AVQ-400 QNP Proton starting parameters. 7/16/03. Revised



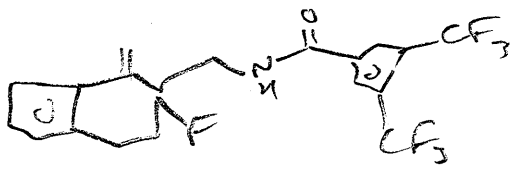
NAME	JW-07-174p1
EXPNO	1
PROCNO	1
Date_	20111207
Time	17.10
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0895586 sec
RG	574.7
DW	62.400 use
DE	6.00 use
TE	292.7 K
D1	1.00000000 sec
TD0	2
======== CHANNEL f1 =======	
NUC1	1H
P1	12.80 use
PL1	0.00 dB
PL1W	9.54516888 W
SFO1	400.1324700 MHz
SI	65536
SF	400.1300142 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00


164.76
136.52
136.01
135.67
132.65
132.38
132.11
131.84
130.53
130.20
127.29
127.04
126.57
125.12
125.09
125.06
123.99
123.42
121.81
77.31
77.05
76.80
42.83
28.39
27.07
14.37
DRX-500 5mm TBIC probe 13C starting parameters. Rev 1/11/
With CPD proton decoupling. Use ns*td0 scans
NAME AD-JW-8-78
EXPNO 1
PROCNO 1
Date_ 20120216
Time 14.36
INSTRUM DRX-500
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1229
DS 0
SWH 41322.312 Hz
FIDRES 0.630528 Hz
AQ 0.7930356 sec
RG 2896.3
DW 12.100 usec
DE 6.00 usec
TE 292.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 10000
======== CHANNEL f1 ========
NUC1 13C
P1 10.75 usec
PL1 0.00 dB
SFO1 125.7175545 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -5.00 dB
PL12 7.04 dB
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

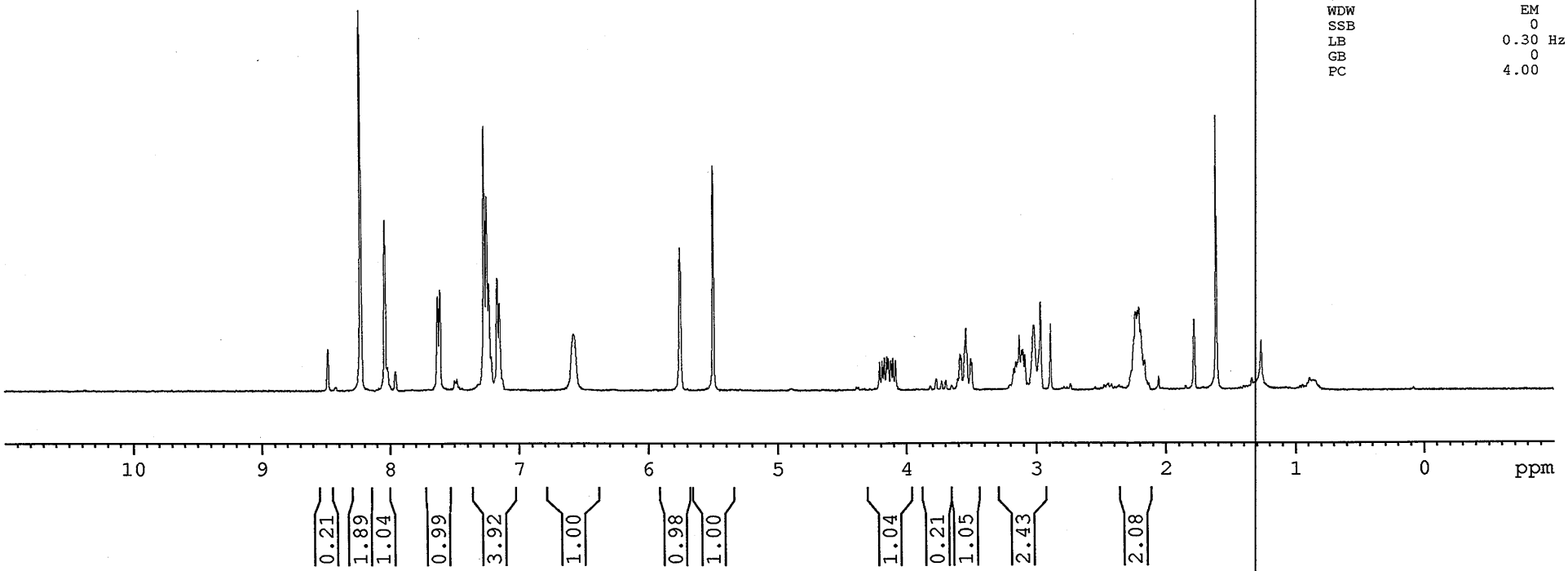
AVQ-400 QNP Proton starting parameters. 7/16/03. Revised 7/22/03 RN

8.485 8.228 8.039 7.957 7.629 7.611 7.481 7.267 7.248 7.231 7.167 7.149 6.580

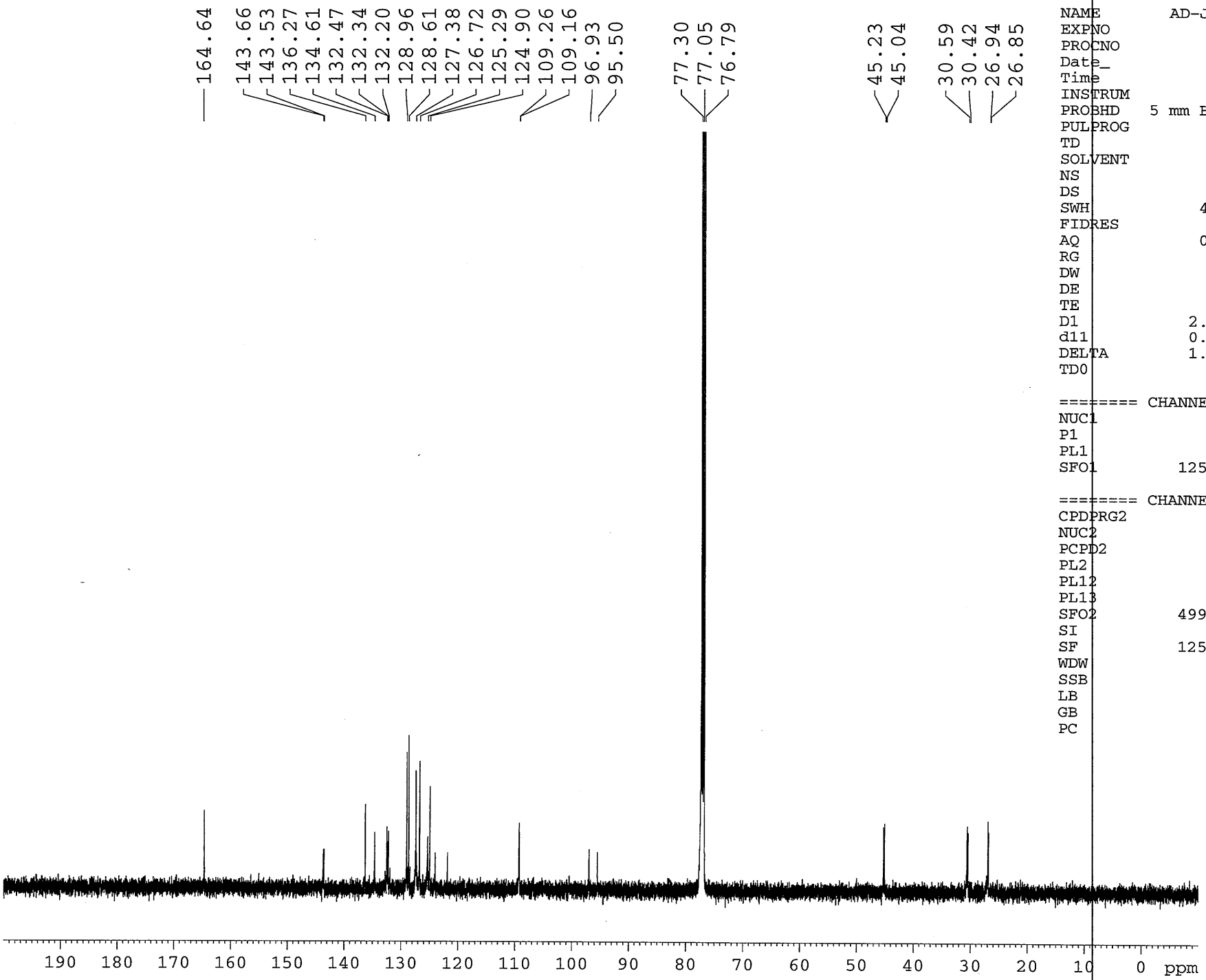
5.755 5.497 4.208 4.188 4.172 4.152 4.140 4.119 4.103 4.083 3.771 3.730 3.696 3.587 3.541 3.505 3.131 3.103 3.088 3.019 2.966 2.889 2.737 2.232 2.219 2.205 2.163 2.054 1.781 1.608 1.264 0.888



NAME	JW-08-80
EXPNO	1
PROCNO	1
Date_	20120209
Time	18.19
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	322.5
DW	62.400 use
DE	6.00 use
TE	292.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.80 use
PL1	0.00 dB
PL1W	9.54516888 W
SFO1	400.1324700 MHz
SI	65536
SF	400.1300142 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00

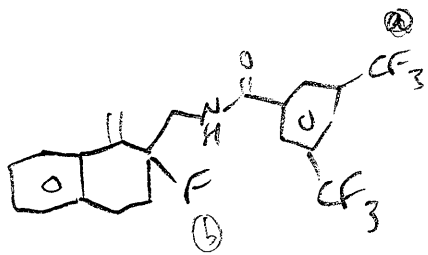


DRX-500 5mm TBIC probe 13C starting parameters. Rev 1
With CPD proton decoupling. Use ns*td0 scans



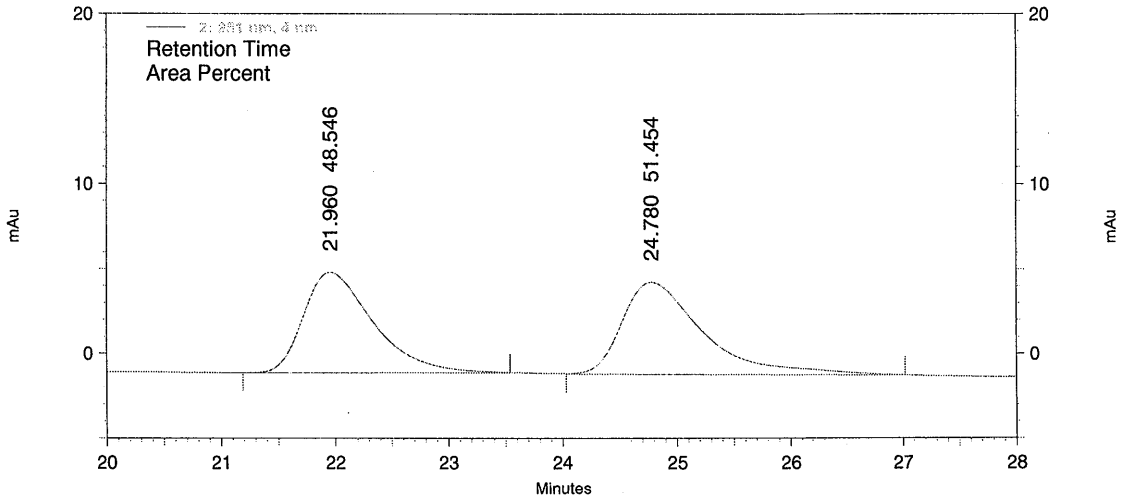
NAME	AD-JW-80-CF3
EXPNO	1
PROCNO	1
Date_	20120210
Time	14.05
INSTRUM	DRX-500
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1099
DS	0
SWH	41322.312 Hz
FIDRES	0.630528 Hz
AQ	0.7930477 sec
RG	8192
DW	12.100 use
DE	6.00 use
TE	293.4 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	10000
======== CHANNEL f1 =======	
NUC1	13C
P1	10.75 use
PL1	0.00 dB
SFO1	125.7175545 MHz
======== CHANNEL f2 =======	
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 use
PL2	-5.00 dB
PL12	7.04 dB
PL13	22.00 dB
SFO2	499.9221551 MHz
SI	131072
SF	125.7049840 MHz
WDW	EM
SSB	0
LB	0.75 Hz
GB	0
PC	2.40

198-p1 AVQ-400 QNP Probe 19F starting parameters. (revise chemical shifts relative to CFCl3 at 0 ppm (082103 HvH)
sw 239.28 ppm; o1p 0 ppm



NAME	JW-07-198-p1F
EXPNO	1
PROCNO	1
Date_	20111208
Time	11.35
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	0
SWH	90090.094 Hz
FIDRES	0.687333 Hz
AQ	0.7274996 sec
RG	3251
DW	5.550 usec
DE	6.00 usec
TE	292.5 K
D1	1.00000000 sec
TD0	2
======== CHANNEL f1 ========	
NUC1	19F
P1	16.00 usec
PL1	-3.00 dB
PL1W	20.04748917 W
SFO1	376.4607042 MHz
SI	65536
SF	376.4980736 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	4.00

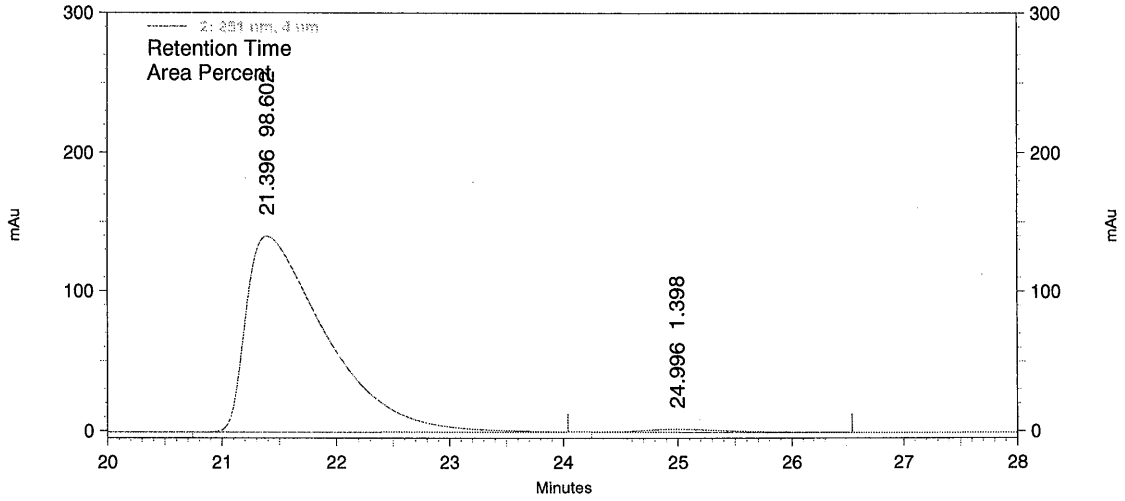
JW-08-80rac



2: 251 nm, 4 nm
Results

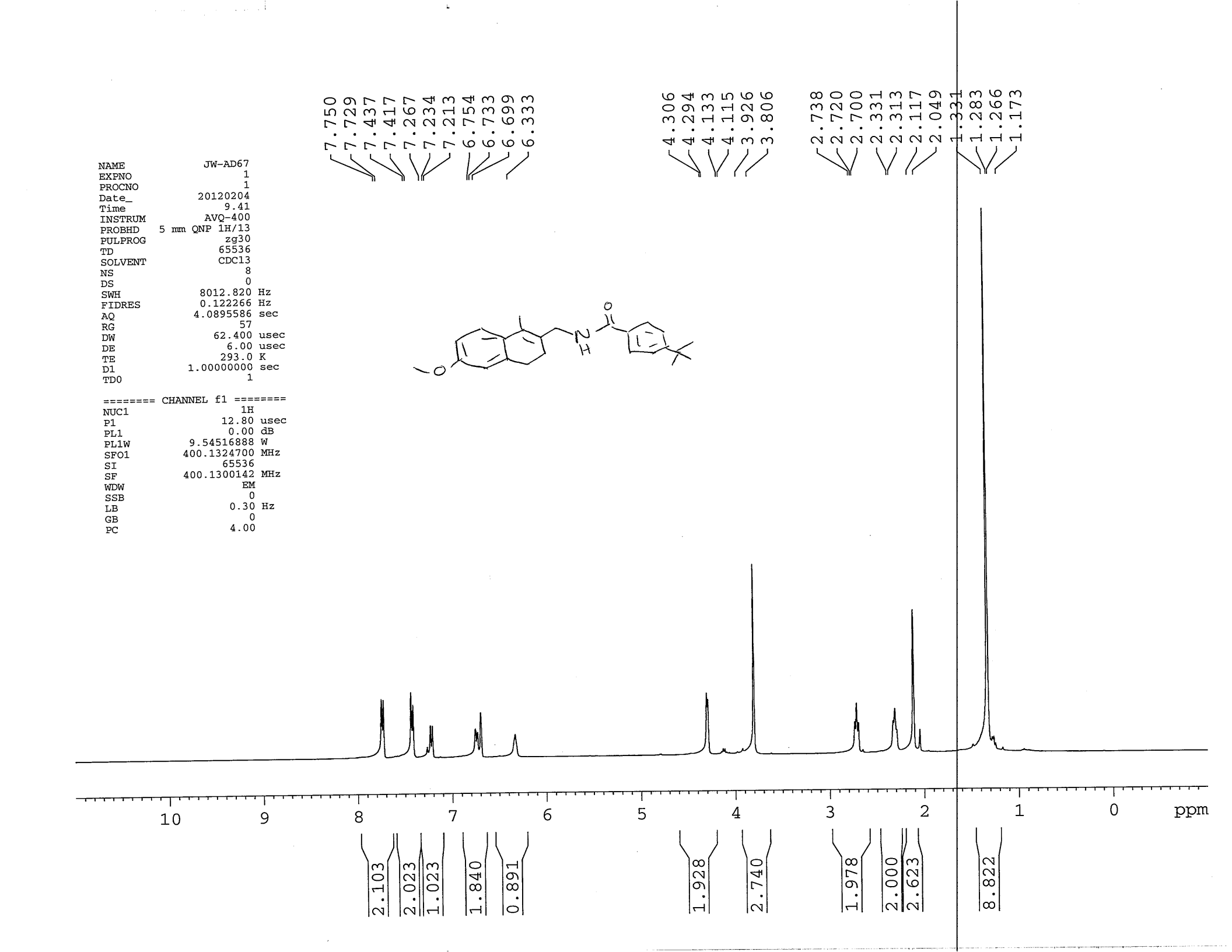
Pk #	Retention Time	Area Percent	Lambda Max
1	21.960	48.546	213
2	24.780	51.454	213

JW-08-80rep-IB9901-30min



2: 251 nm, 4 nm
Results

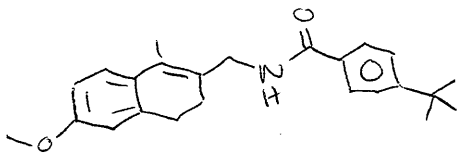
Pk #	Retention Time	Area Percent	Lambda Max
1	21.396	98.602	209
2	24.996	1.398	214

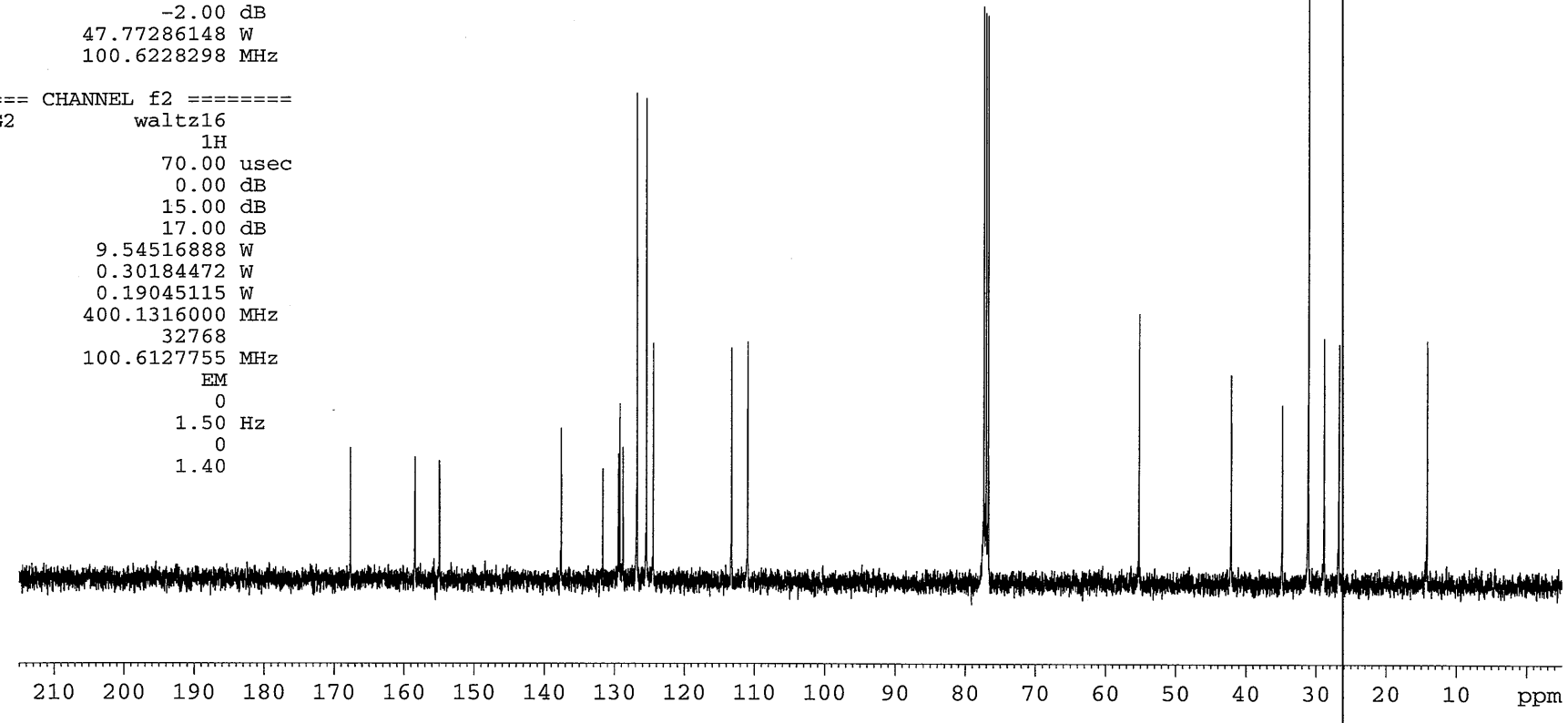

7.750
7.729
7.437
7.417
7.267
7.234
7.213
6.754
6.733
6.699
6.333
4.306
4.294
4.133
4.115
3.926
3.806
2.738
2.720
2.700
2.331
2.313
2.117
2.049
1.331
1.283
1.266
1.173
NAME JW-AD67
EXPNO 1
PROCNO 1
Date_ 20120204
Time 9.41
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 57
DW 62.400 usec
DE 6.00 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
O
N
H
O
10
9
8
7
6
5
4
3
2
1
0
ppm
2.103
2.023
1.023
1.840
0.891
1.928
2.740
1.978
2.000
2.623
8.822

JW-AD 67 AVQ-400 QNP Carbon Starting parameters 7/16

NAME	JW-AD67C
EXPNO	1
PROCNO	1
Date_	20120204
Time	9.42
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	73
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3632196 sec
RG	16384
DW	20.800 usec
DE	6.00 usec
TE	293.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	100000
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	17.00 dB
PL2W	9.54516888 W
PL12W	0.30184472 W
PL13W	0.19045115 W
SFO2	400.1316000 MHz
SI	32768
SF	100.6127755 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	1.40

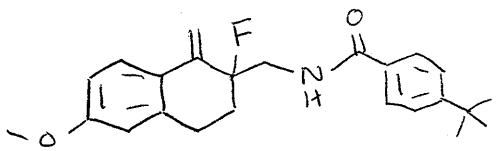
167.56 158.34 154.84 137.60 131.66 129.44 129.25 128.80 126.79 125.44 124.46 113.26 110.95 77.39 77.07 76.75 55.20 42.15 34.87 31.14 28.92 26.79 14.22



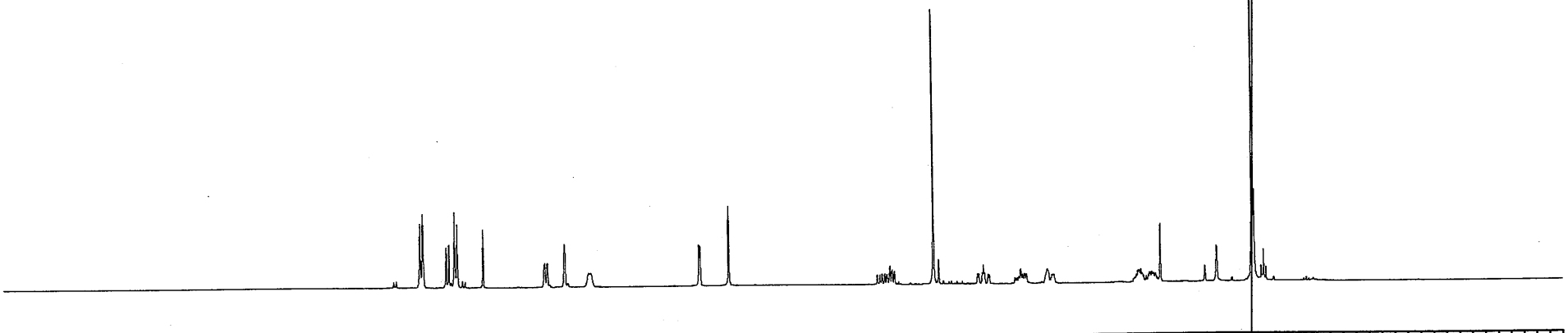


JW-08-76-1 AVB-400 ZBO Proton starting parameters. 6/11/03 RN

7.986 7.965 7.784 7.763 7.587 7.565 7.522 7.502 7.463 7.442 7.303 6.832 6.826 6.810 6.804 6.672 6.481 6.469 5.629 5.622 5.403 4.272 4.251 4.235 4.214 4.198 4.175 4.157 4.140 3.841 3.800 3.501 3.492 3.456 3.448 3.420 3.411 3.212 3.197 3.182 3.168 3.153 3.139 3.124 2.962 2.919 2.272 2.263 2.256 2.249 2.240 2.231 2.217 2.196 2.181 2.168 2.153 2.142 2.126 2.088 1.748 1.658 1.386 1.374 1.320 1.303 1.285

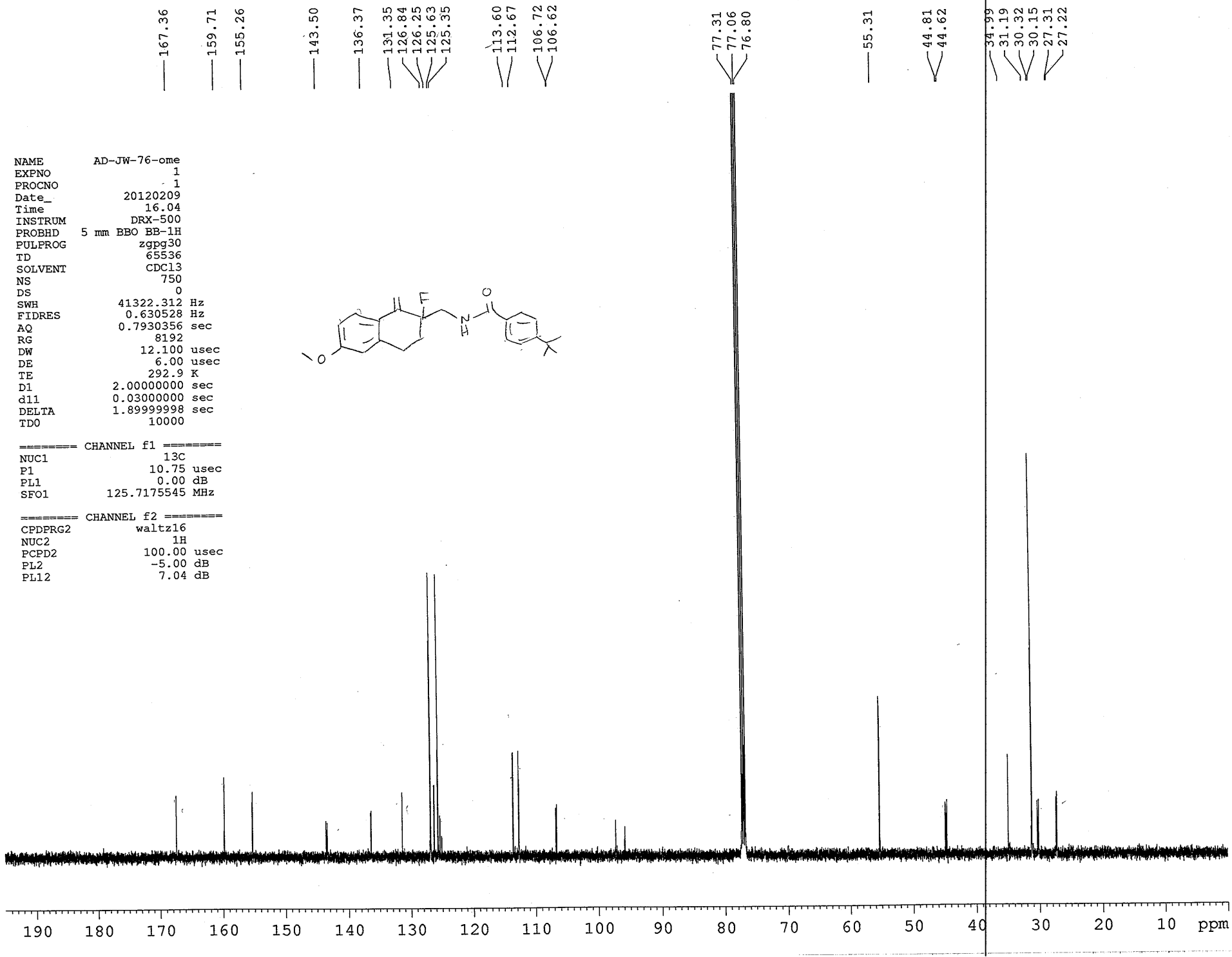


NAME	JW-08-76-1
EXPNO	1
PROCNO	1
Date_	20120208
Time	10.27
INSTRUM	AVB-400
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	0
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	181
DW	60.400 use
DE	6.00 use
TE	297.5 K
D1	1.00000000 sec
TD0	4
======== CHANNEL f1 =======	
NUC1	1H
P1	8.20 use
PL1	-3.00 dB
PL1W	23.05461311 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00



1.99 1.04 2.02 1.04 0.99 0.96 0.97 1.00 1.32 2.96 1.01 1.07 1.08 2.07 0.63 0.27 0.69 9.35

DRX-500 5mm TBIC probe 13C starting parameters. Rev 1/11/
With CPD proton decoupling. Use ns*td0 scans



NAME	AD-JW-76-ome
EXPNO	1
PROCNO	1
Date_	20120209
Time	16.04
INSTRUM	DRX-500
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	750
DS	0
SWH	41322.312 Hz
FIDRES	0.630528 Hz
AQ	0.7930356 sec
RG	8192
DW	12.100 usec
DE	6.00 usec
TE	292.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	10000

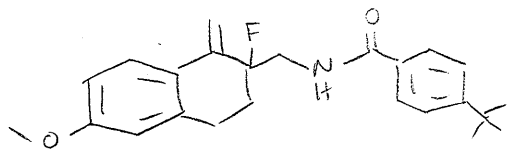
======== CHANNEL f1 ========

NUC1	13C
P1	10.75 usec
PL1	0.00 dB
SFO1	125.7175545 MHz

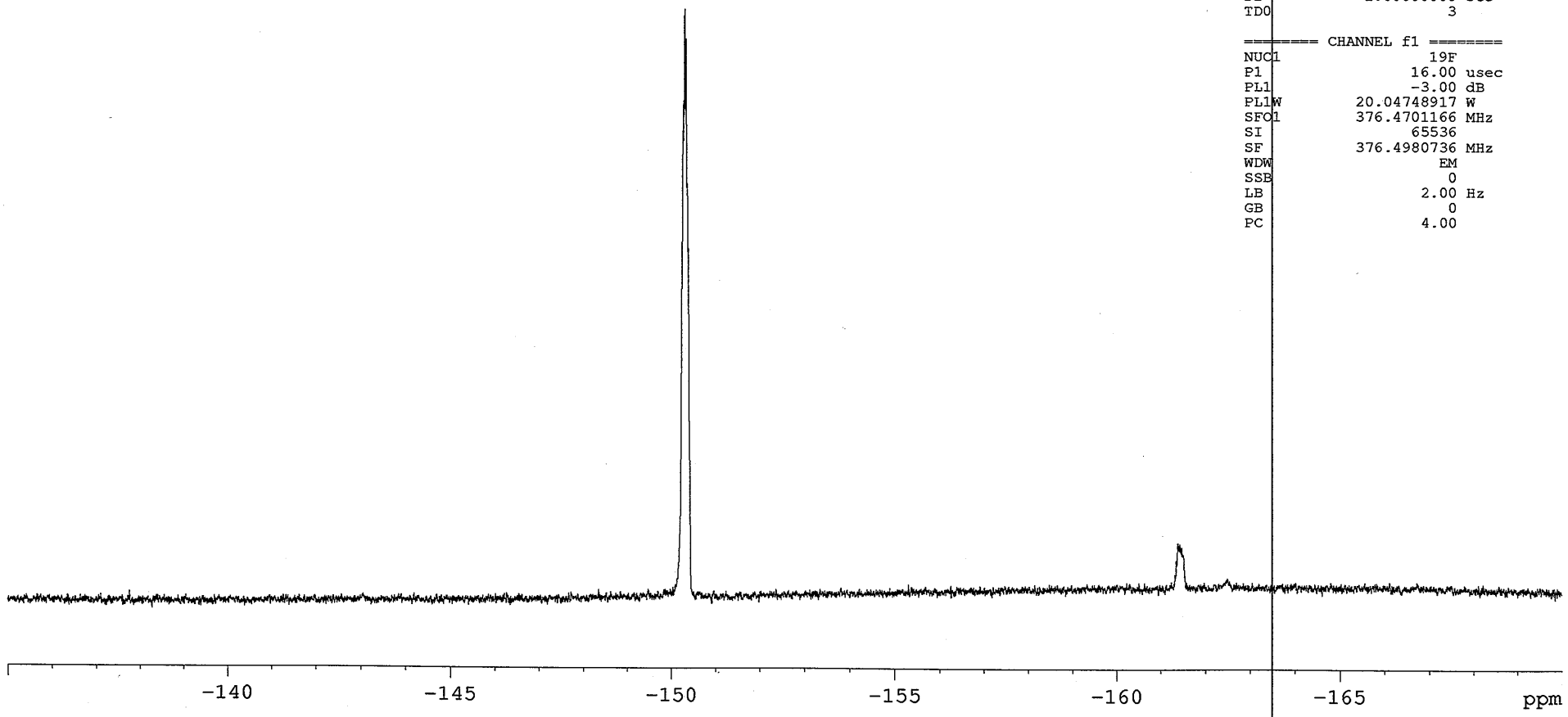
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-5.00 dB
PL12	7.04 dB

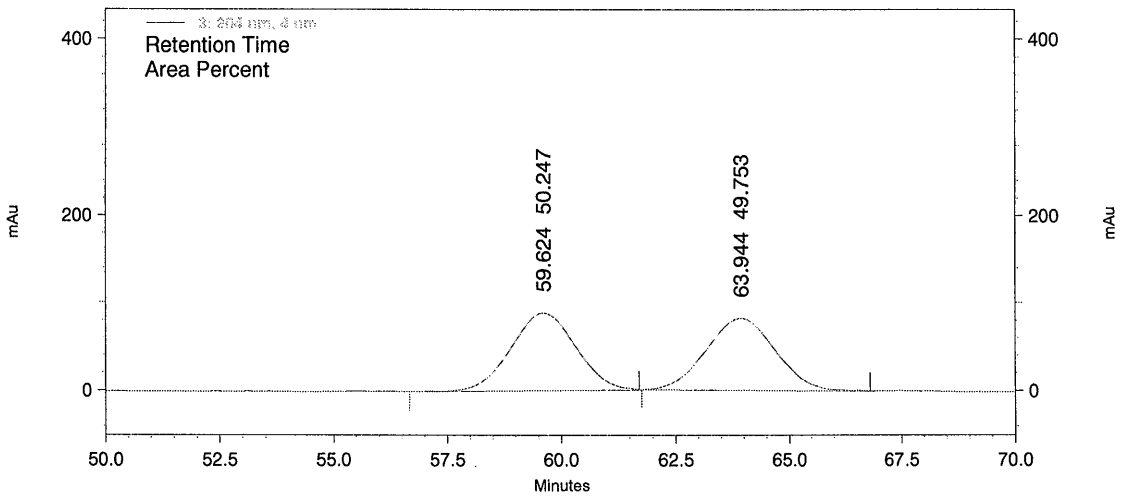
AVQ-400 QNP Probe 19F starting parameters. (revised P1, 2
chemical shifts relative to CFCl3 at 0 ppm (082103 HvH)
sw 239.28 ppm; o1p 0 ppm



NAME	AD-JW-76-ome-F
EXPNO	1
PROCNO	1
Date_	20120209
Time	16.48
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	24
DS	0
SWH	90090.094 Hz
FIDRES	0.687333 Hz
AQ	0.7274996 sec
RG	4597.6
DW	5.550 usec
DE	6.00 usec
TE	292.8 K
D1	1.00000000 sec
TD0	3
======== CHANNEL f1 ========	
NUC1	19F
P1	16.00 usec
PL1	-3.00 dB
PL1W	20.04748917 W
SFO1	376.4701166 MHz
SI	65536
SF	376.4980736 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	4.00

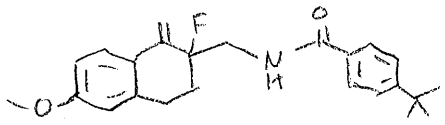


AD-2-68rac-ic9604-70min

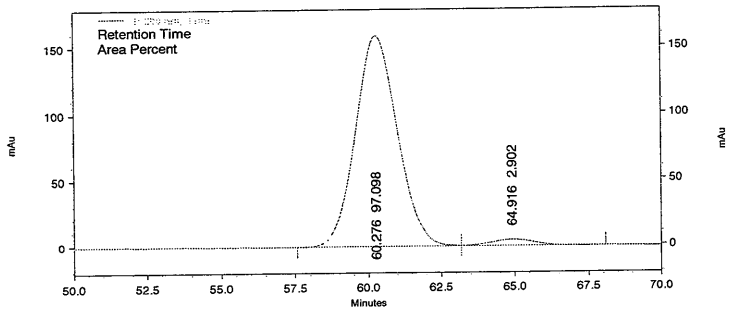


3: 204 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	59.624	50.247	204
2	63.944	49.753	204



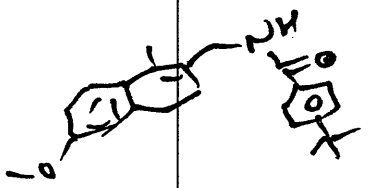
JW-08-76

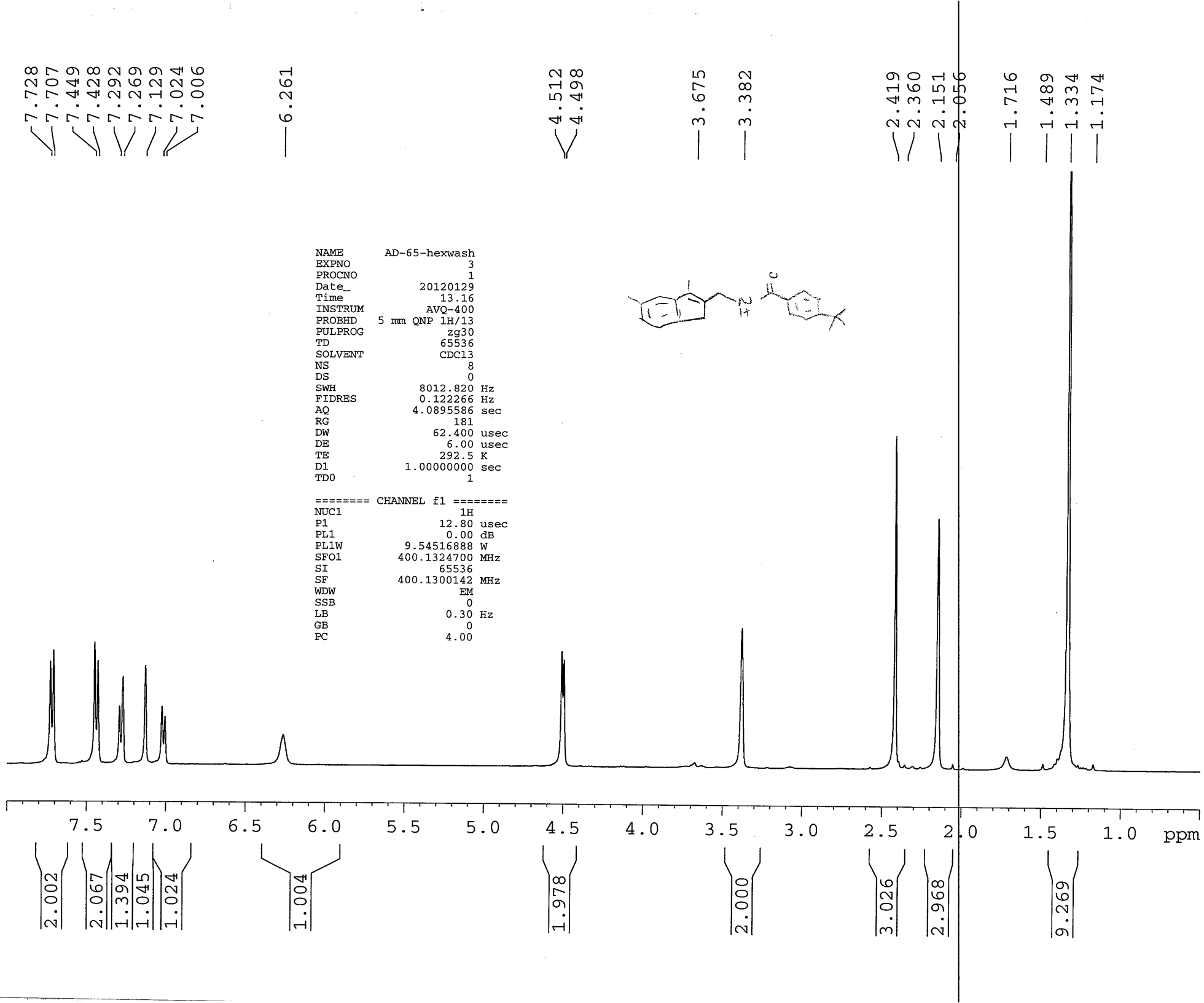


1: 208 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	60.276	97.098	203
2	64.916	2.902	204

IC9604-70




7.728
7.707
7.449
7.428
7.292
7.269
7.129
7.024
7.006
6.261
4.512
4.498
3.675
3.382
2.419
2.360
2.151
2.056
1.716
1.489
1.334
1.174
NAME AD-65-hexwash
EXPNO 3
PROCNO 1
Date_ 20120129
Time 13.16
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 181
DW 62.400 usec
DE 6.00 usec
TE 292.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.002
2.067
1.394
1.045
1.024
1.004
1.978
2.000
3.026
2.968
9.269

NAME	AD-65-hexwash-C
EXPNO	3
PROCNO	1
Date_	20120129
Time	13.20
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	329
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3632196 sec
RG	16384
DW	20.800 usec
DE	6.00 usec
TE	292.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1000

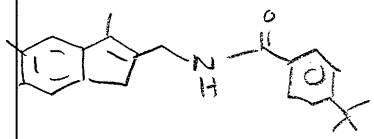
======== CHANNEL f1 ========

NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz

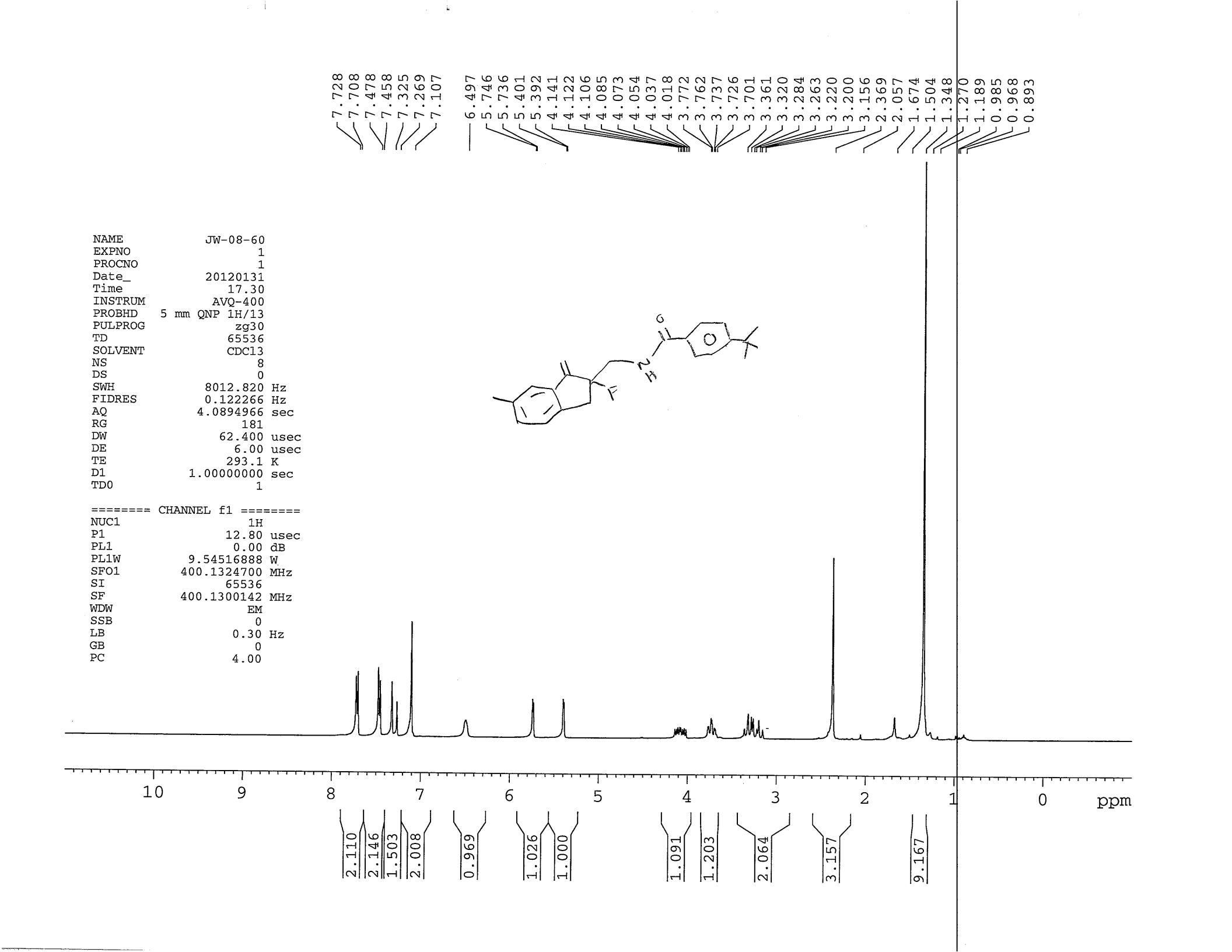
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	17.00 dB
PL2W	9.54516888 W
PL12W	0.30184472 W
PL13W	0.19045115 W
SFO2	400.1316000 MHz
SI	32768
SF	100.6127755 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	1.40

167.26
154.96
146.56
139.50
137.48
136.17
135.87
131.52
126.70
125.59
125.50
123.11
119.68
77.33
77.21
77.01
76.69
39.18
37.55
34.89
31.13
21.53
10.40



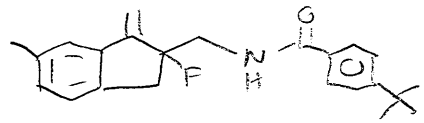
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

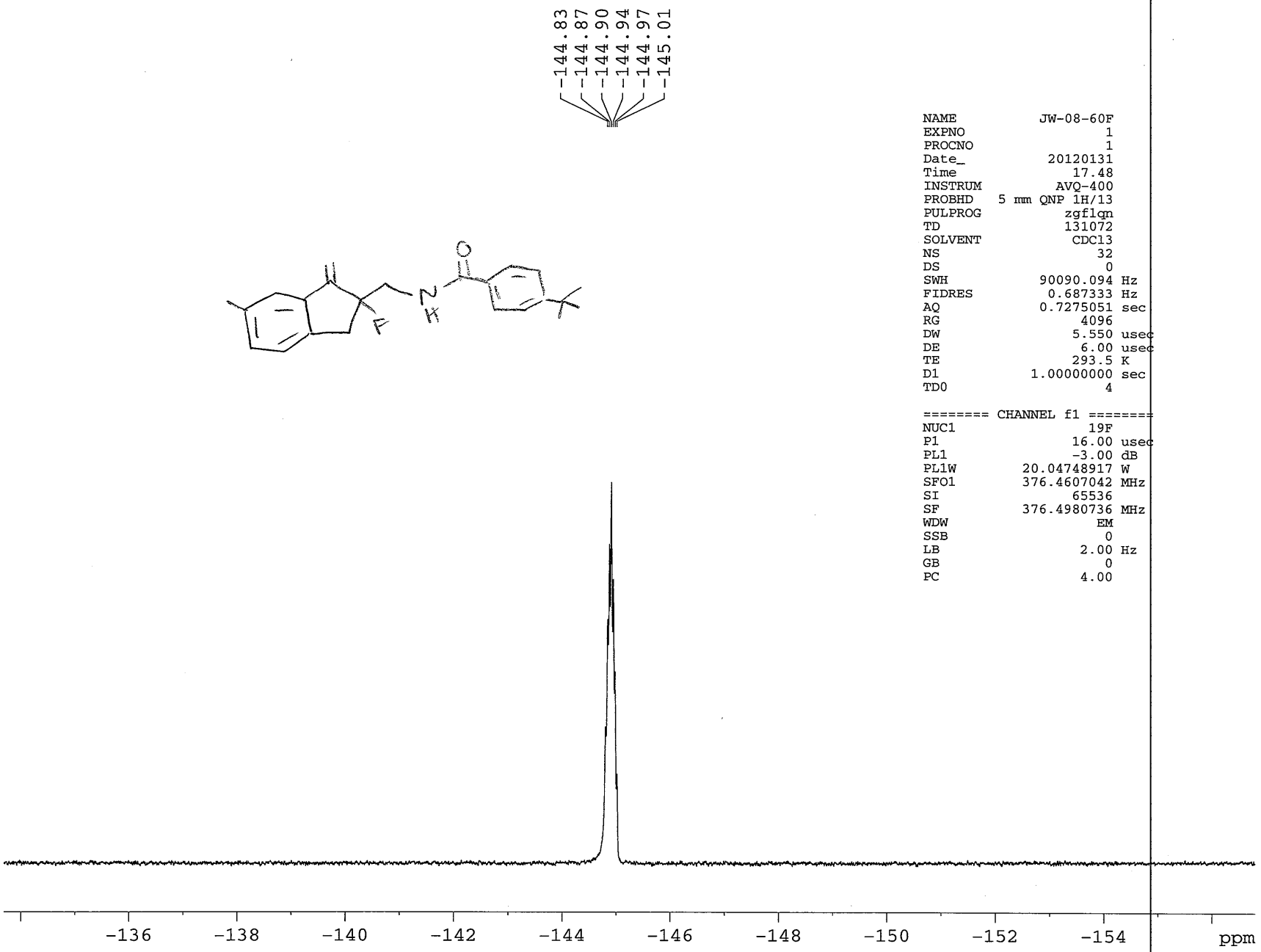

7.728
7.708
7.478
7.458
7.325
7.269
7.107
6.497
5.746
5.736
5.401
5.392
4.141
4.122
4.106
4.085
4.073
4.054
4.037
4.018
3.772
3.762
3.737
3.726
3.701
3.361
3.320
3.284
3.263
3.220
3.200
3.156
2.369
2.057
1.674
1.504
1.348
1.270
1.189
0.985
0.968
0.893
NAME JW-08-60
EXPNO 1
PROCNO 1
Date_ 20120131
Time 17.30
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 181
DW 62.400 usec
DE 6.00 usec
TE 293.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
O
N
H
F
10
9
8
7
6
5
4
3
2
1
0
ppm
2.110
2.146
1.503
2.008
0.969
1.026
1.000
1.091
1.203
2.064
3.157
9.167

AVQ-400 QNP Carbon Starting parameters 7/16/03 revised 7/22/03 RN

NAME	JW-08-60carb
EXPNO	1
PROCNO	1
Date_	20120131
Time	17.31
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	297
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	16384
DW	20.800 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	100000
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	17.00 dB
PL2W	9.54516888 W
PL12W	0.30184472 W
PL13W	0.19045115 W
SFO2	400.1316000 MHz
SI	32768
SF	100.6127755 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	1.40

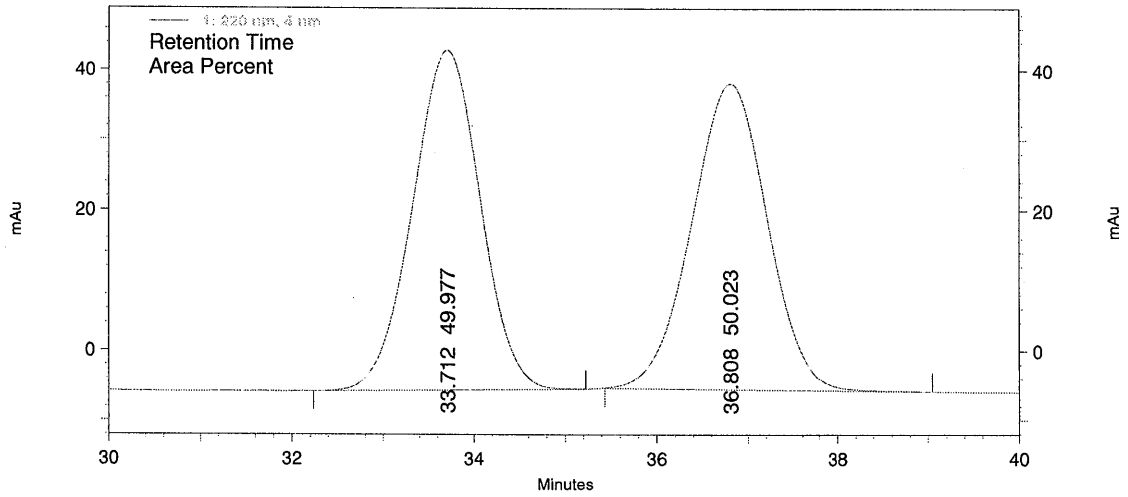
167.532
155.226
149.188
149.018
137.834
137.695
137.063
131.257
130.714
126.792
125.562
125.125
121.454
107.194
107.139
102.905
77.318
77.000
76.683
46.031
45.755
40.424
40.188
34.920
31.126
21.336





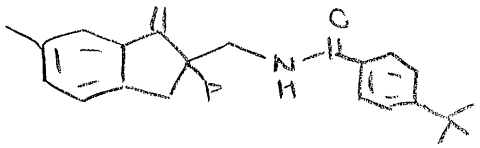
NAME	JW-08-60F
EXPNO	1
PROCNO	1
Date_	20120131
Time	17.48
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	32
DS	0
SWH	90090.094 Hz
FIDRES	0.687333 Hz
AQ	0.7275051 sec
RG	4096
DW	5.550 usec
DE	6.00 usec
TE	293.5 K
D1	1.00000000 sec
TD0	4
======== CHANNEL f1 ========	
NUC1	19F
P1	16.00 usec
PL1	-3.00 dB
PL1W	20.04748917 W
SFO1	376.4607042 MHz
SI	65536
SF	376.4980736 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	4.00

JW-08-60rac/ADII-66

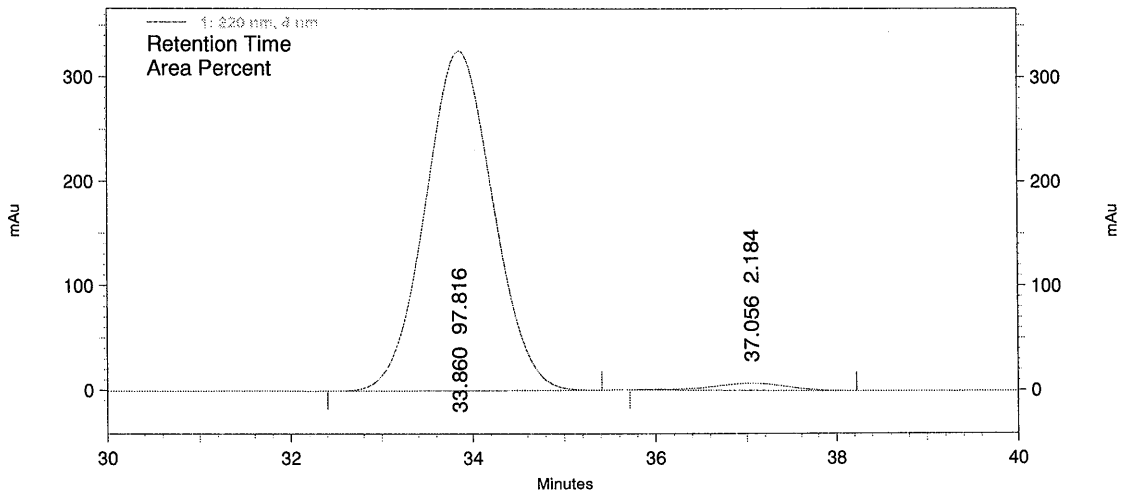


1: 220 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	33.712	49.977	204
2	36.808	50.023	204

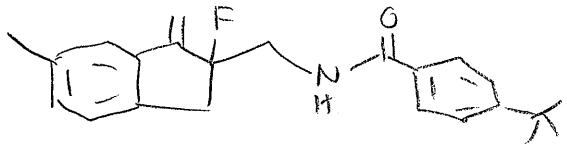


JW-08-60

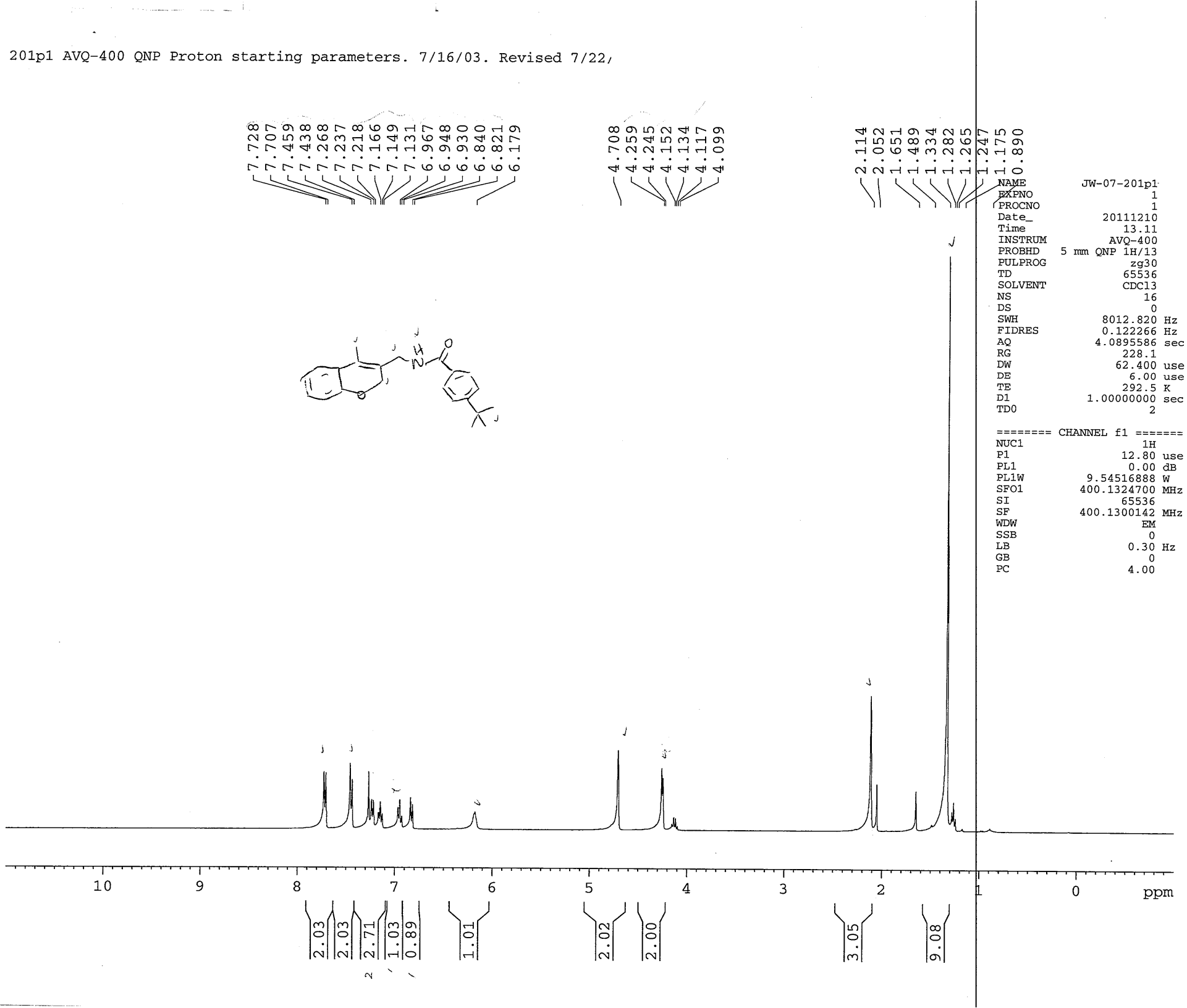


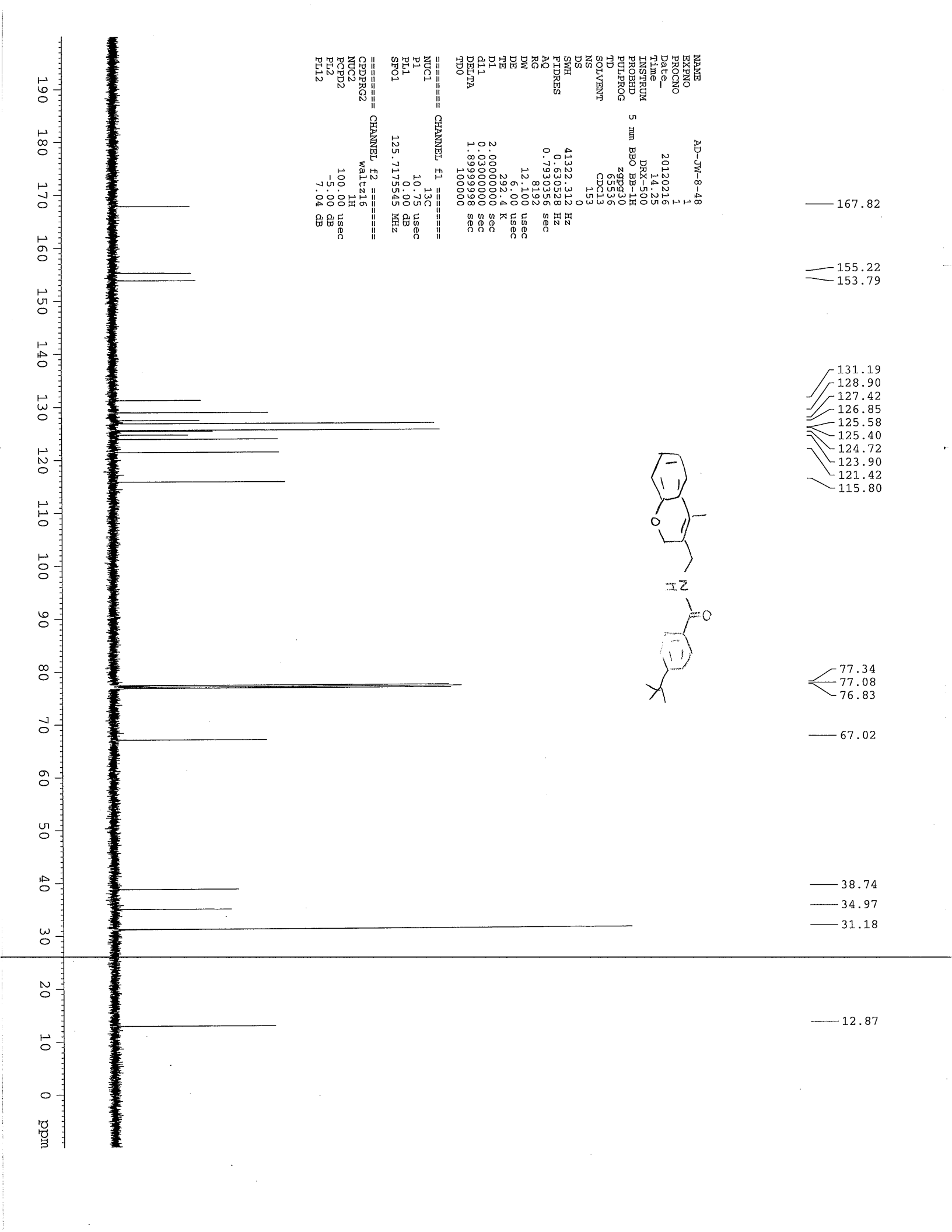
1: 220 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	33.860	97.816	202
2	37.056	2.184	204



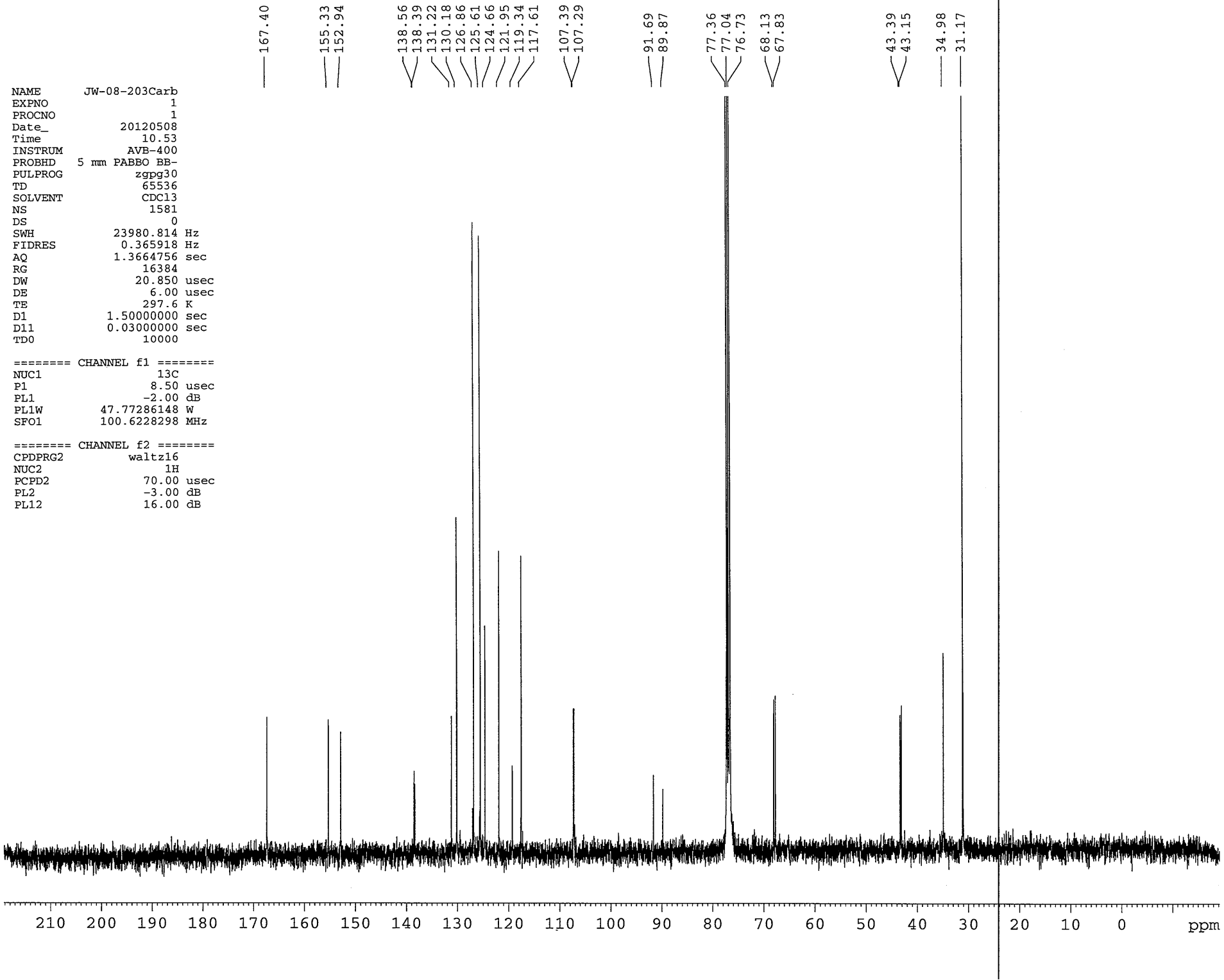
201p1 AVQ-400 QNP Proton starting parameters. 7/16/03. Revised 7/22/




NAME AD-JW-8-48
EXPNO 1
PROCNO 1
Date_ 20120216
Time_ 14.25
INSTRUM DRX-500
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 153
DS 0
SWH 41322.312 Hz
FIDRES 0.630528 Hz
AQ 0.7930356 sec
RG 8192
DW 12.100 usec
DE 6.00 usec
TE 292.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 100000
========== CHANNEL f1 ========
NUC1 13C
P1 10.75 usec
PL1 0.00 dB
SFO1 125.7175545 MHz
========== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -5.00 dB
PL12 7.04 dB
167.82
155.22
153.79
131.19
128.90
127.42
126.85
125.58
125.40
124.72
123.90
121.42
115.80
77.34
77.08
76.83
67.02
38.74
34.97
31.18
12.87
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

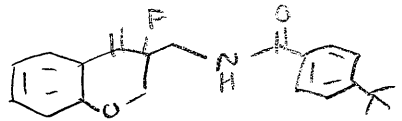
JW-08-203 AVB-400 ZBO Proton starting parameters. 6/11/03 RN
7.763
7.742
7.622
7.604
7.509
7.488
7.303
7.291
7.270
7.252
7.043
7.025
7.007
6.975
6.955
6.907
6.886
6.431
5.811
5.750
5.652
5.495
5.370
4.371
4.356
4.344
4.329
4.240
4.222
4.203
4.184
4.178
4.155
4.142
4.127
4.116
3.949
3.922
3.818
3.806
3.781
3.768
3.756
3.731
3.719
2.159
2.087
1.692
1.537
1.381
1.302
1.222
1.002
0.980
0.928
2.054
1.069
2.152
1.542
2.128
0.997
0.964
0.950
1.021
2.081
1.079
9.900
ppm

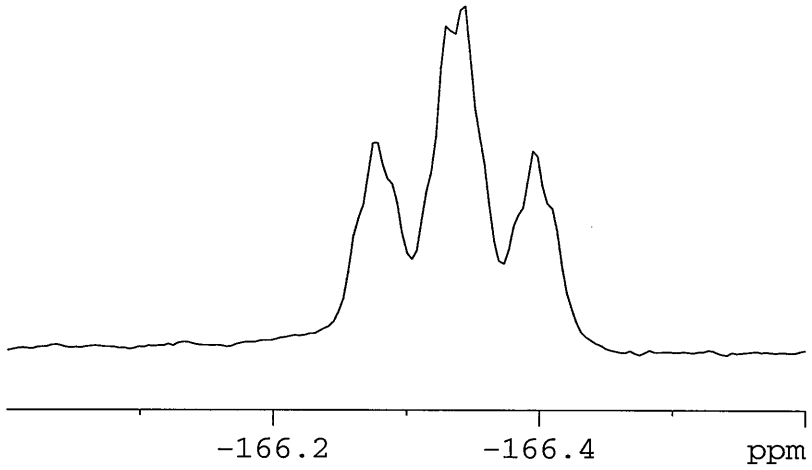
JW-08-203 AVB-400 ZBO Carbon Starting paramters 6/11/03 RN



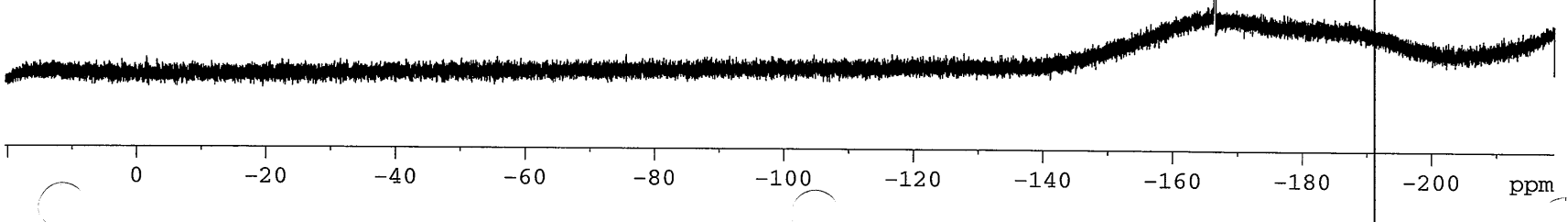
NAME	JW-08-203Carb
EXPNO	1
PROCNO	1
Date_	20120508
Time	10.53
INSTRUM	AVB-400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1581
DS	0
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	16384
DW	20.850 usec
DE	6.00 usec
TE	297.6 K
D1	1.50000000 sec
D11	0.03000000 sec
TD0	10000
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	-3.00 dB
PL12	16.00 dB

204p2 AVQ-400 QNP Probe 19F starting parameters. (rev
chemical shifts relative to CFCl3 at 0 ppm (082103 Hv



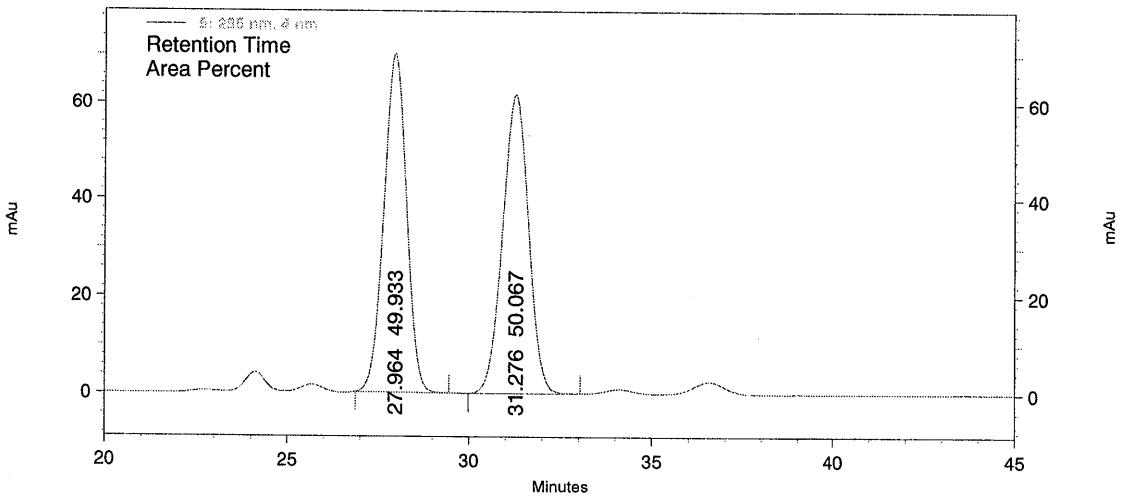


-166.28
-166.34
-166.40



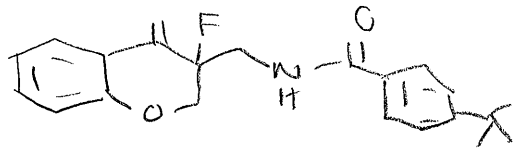
NAME	JW-07-204p2
EXPNO	
PROCNO	
Date_	2011121
Time	10.3
INSTRUM	AVQ-4C
PROBHD	5 mm QNP 1H/1
PULPROG	zgflq
TD	13107
SOLVENT	CDCl
NS	2
DS	
SWH	90090.09
FIDRES	0.68733
AQ	0.727505
RG	1149.
DW	5.55
DE	6.C
TE	292.
D1	1.000000C
TD0	
======== CHANNEL f1 ==	
NUC1	19
P1	16.C
PL1	-3.C
PL1W	20.0474891
SFO1	376.460704
SI	6553
SF	376.498073
WDW	E
SSB	
LB	2.C
GB	
PC	4.C

JW-08-59rac/07-204rac

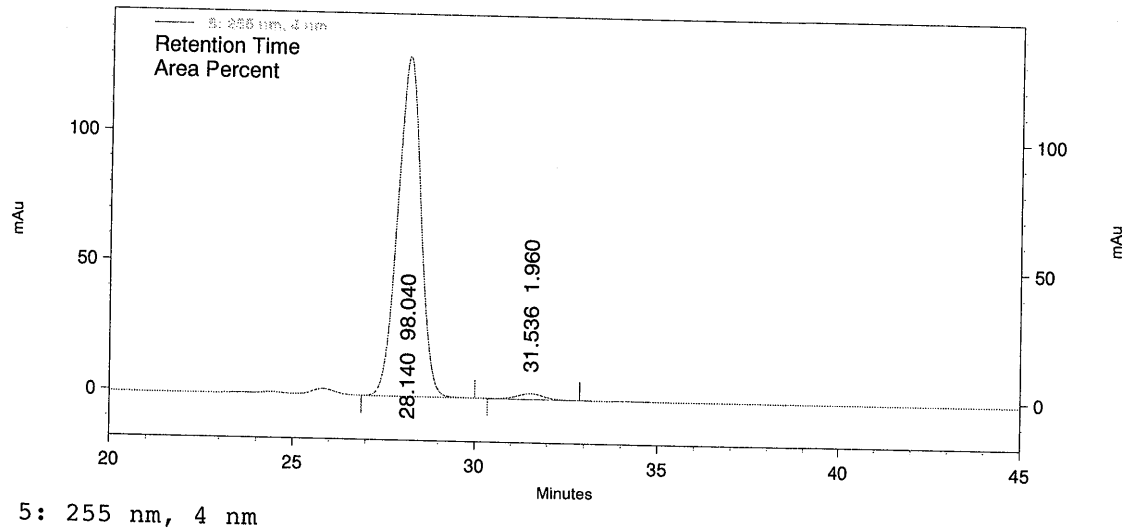


5: 255 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	27.964	49.933	204
2	31.276	50.067	204

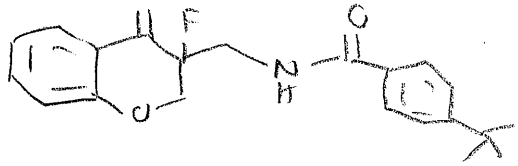


JW-08-59

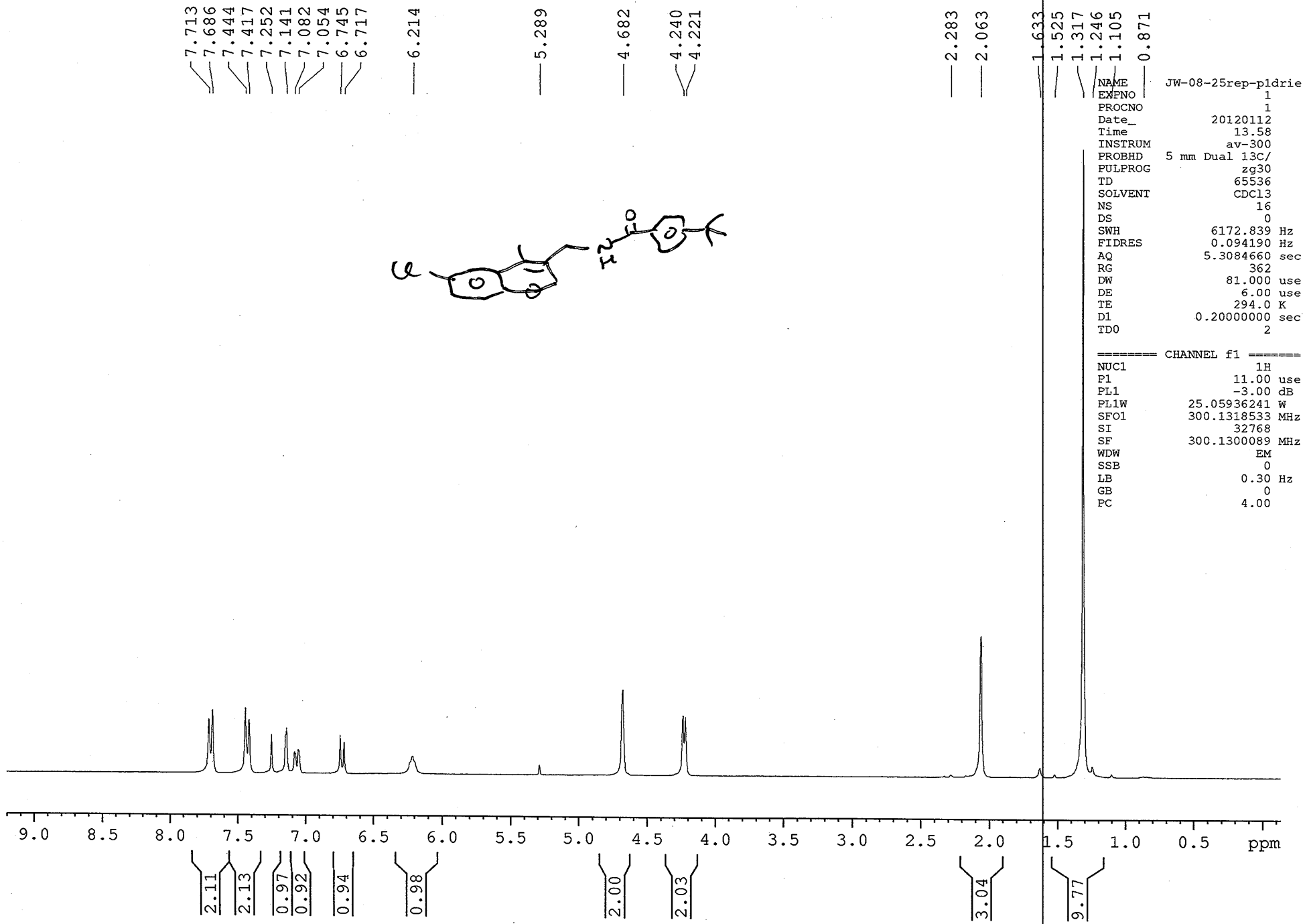


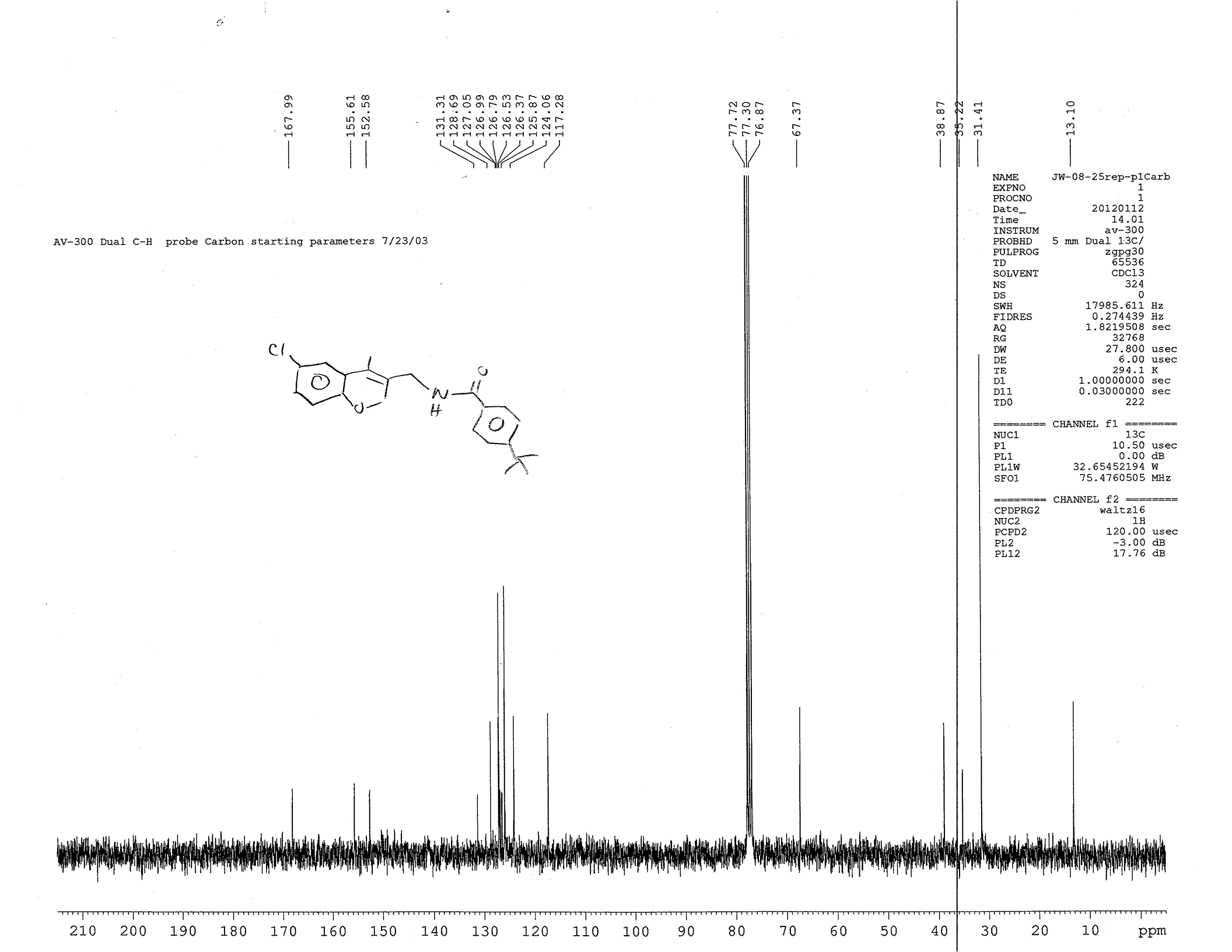
5: 255 nm, 4 nm
Results

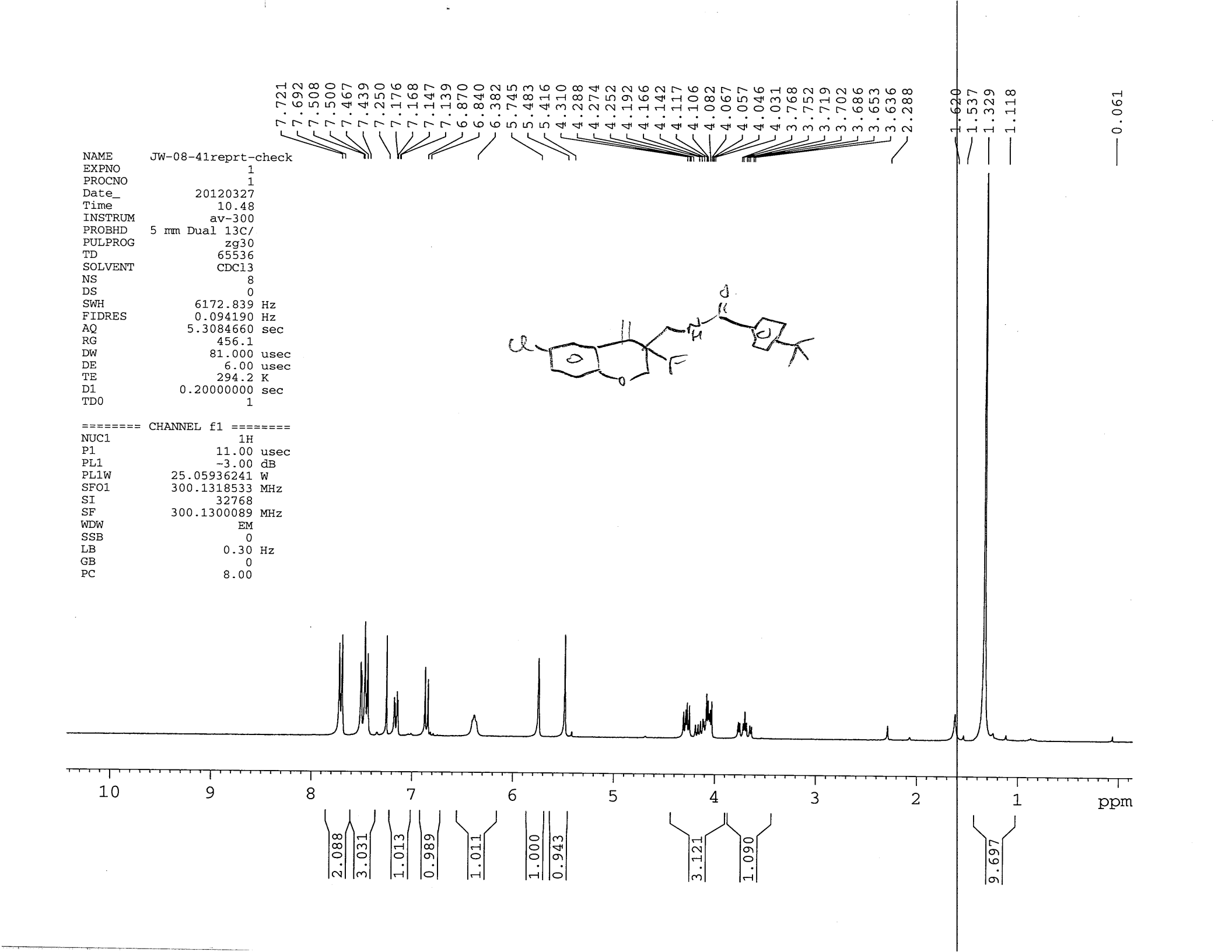
Pk #	Retention Time	Area Percent	Lambda Max
1	28.140	98.040	204
2	31.536	1.960	205

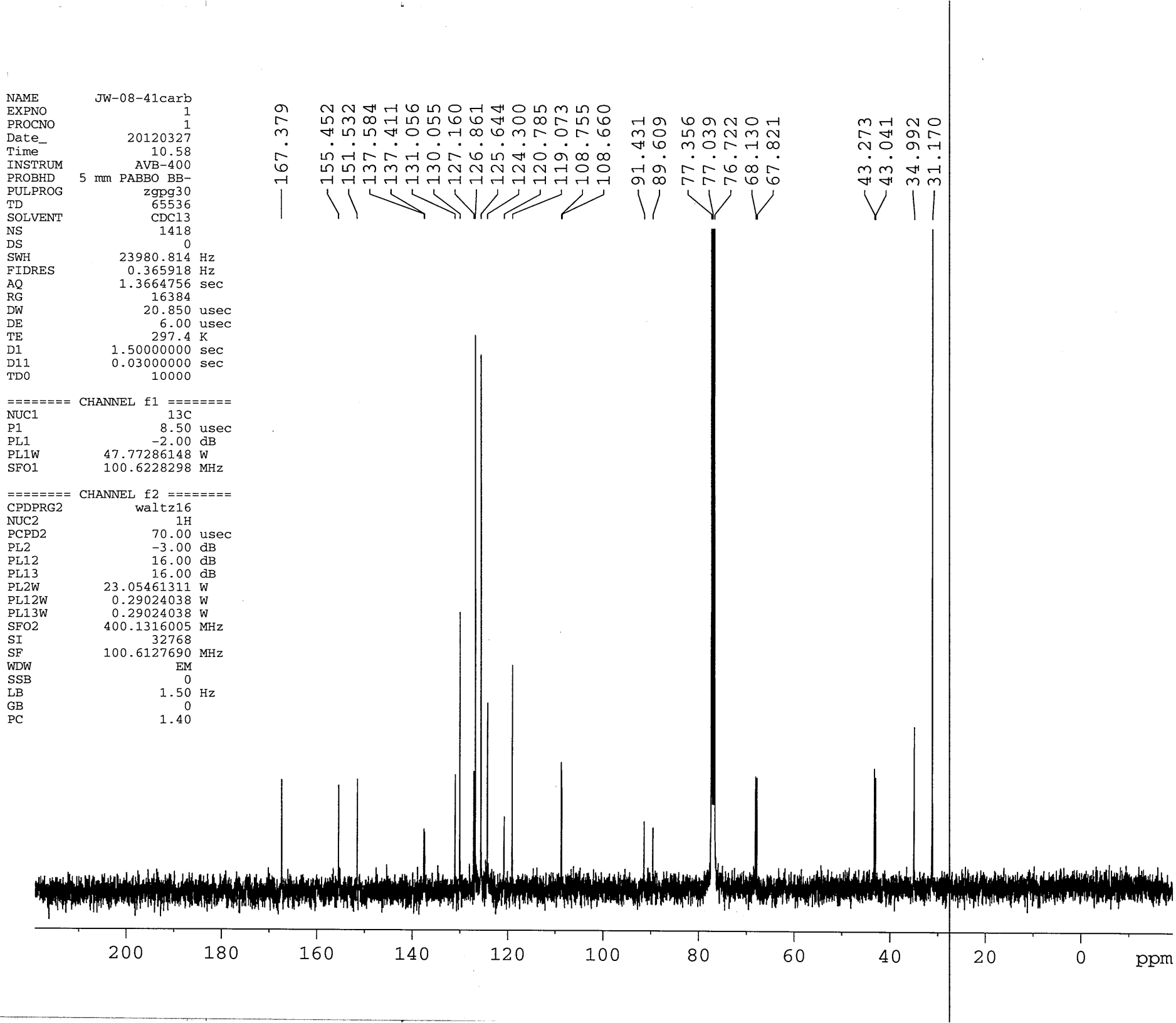


JW-08-25p1 dry AV-300 Dual C-H probe proton starting parameters 7/2

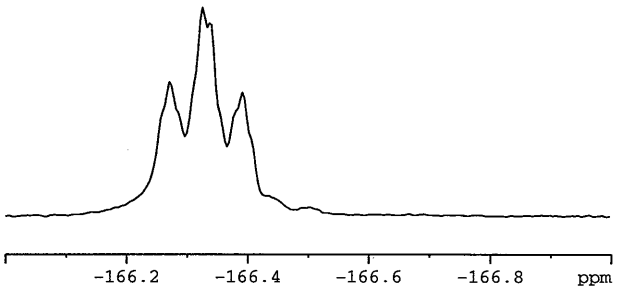



167.99
155.61
152.58
131.31
128.69
127.05
126.99
126.79
126.53
126.37
125.87
124.06
117.28
77.72
77.30
76.87
67.37
38.87
35.22
31.41
13.10
AV-300 Dual C-H probe Carbon starting parameters 7/23/03
NAME JW-08-25rep-p1Carb
EXPNO 1
PROCNO 1
Date_ 20120112
Time 14.01
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 324
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 222
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 0.00 dB
PL1W 32.65452194 W
SFO1 75.4760505 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 120.00 usec
PL2 -3.00 dB
PL12 17.76 dB
Cl
O
N
H
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.721
7.692
7.508
7.500
7.467
7.439
7.250
7.176
7.168
7.147
7.139
6.870
6.840
6.382
5.745
5.483
5.416
4.310
4.288
4.274
4.252
4.192
4.166
4.142
4.117
4.106
4.082
4.067
4.057
4.046
4.031
3.768
3.752
3.719
3.702
3.686
3.653
3.636
2.288
1.620
1.537
1.329
1.118
0.061
NAME JW-08-41reprt-check
EXPNO 1
PROCNO 1
Date_ 20120327
Time 10.48
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 456.1
DW 81.000 usec
DE 6.00 usec
TE 294.2 K
D1 0.20000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -3.00 dB
PL1W 25.05936241 W
SFO1 300.1318533 MHz
SI 32768
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 8.00
10
9
8
7
6
5
4
3
2
1
ppm
2.088
3.031
1.013
0.989
1.011
1.000
0.943
3.121
1.090
9.697

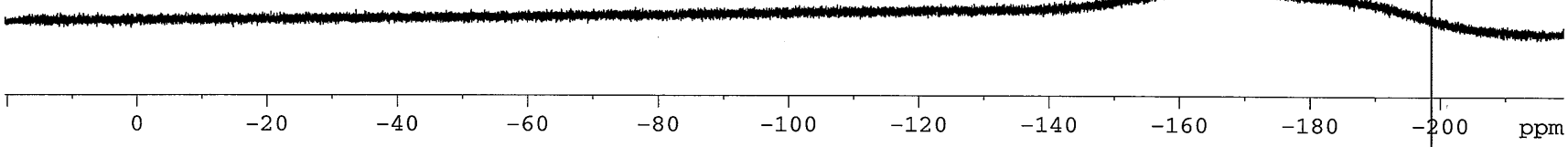

NAME JW-08-41carb
EXPNO 1
PROCNO 1
Date_ 20120327
Time 10.58
INSTRUM AVB-400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1418
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 297.4 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 10000
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.00 dB
PL12 16.00 dB
PL13 16.00 dB
PL2W 23.05461311 W
PL12W 0.29024038 W
PL13W 0.29024038 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40
167.379
155.452
151.532
137.584
137.411
131.056
130.055
127.160
126.861
125.644
124.300
120.785
119.073
108.755
108.660
91.431
89.609
77.356
77.039
76.722
68.130
67.821
43.273
43.041
34.992
31.170
200
180
160
140
120
100
80
60
40
20
0
ppm

400 QNP Probe 19F starting parameters. (revised
ical shifts relative to CFCl3 at 0 ppm (082103

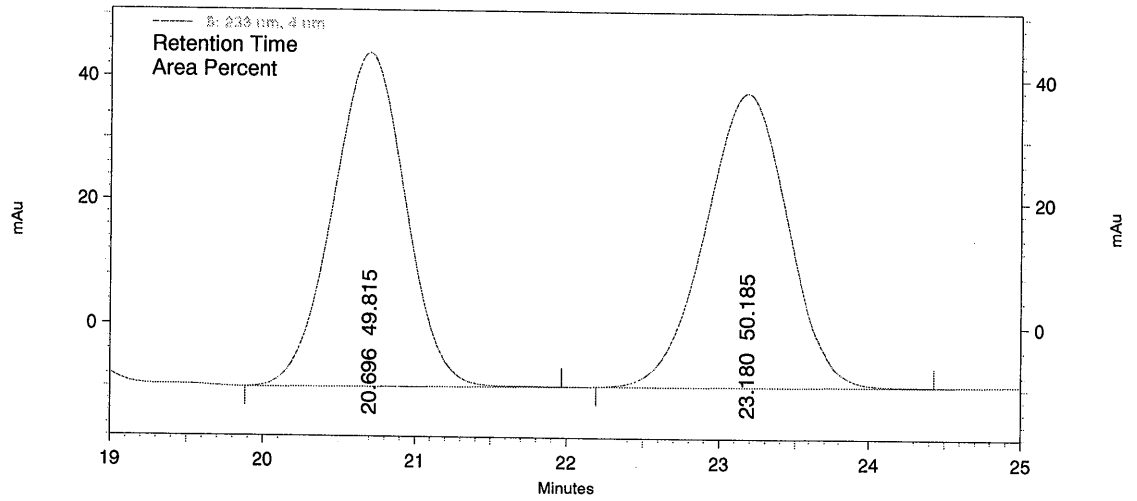


-166.27
-166.33
-166.39

NAME	JW-08-41p1-F
EXPNO	1
PROCNO	1
Date_	20120124
Time	15.11
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	32
DS	0
SWH	90090.094 Hz
FIDRES	0.687333 Hz
AQ	0.7275051 sec
RG	256
DW	5.550 usec
DE	6.00 usec
TE	292.7 K
D1	1.00000000 sec
TD0	4
======== CHANNEL f1 ========	
NUC1	19F
P1	16.00 usec
PL1	-3.00 dB
PL1W	20.04748917 W
SFO1	376.4607042 MHz
SI	65536
SF	376.4980736 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	4.00

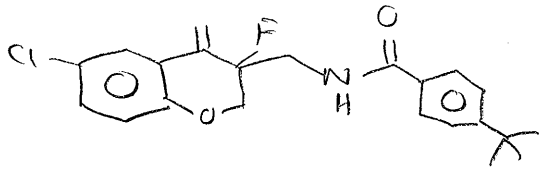


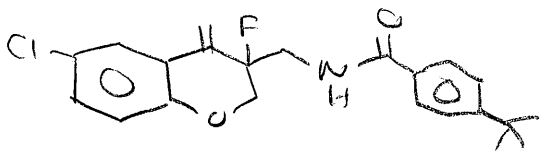
JW-08-28rac



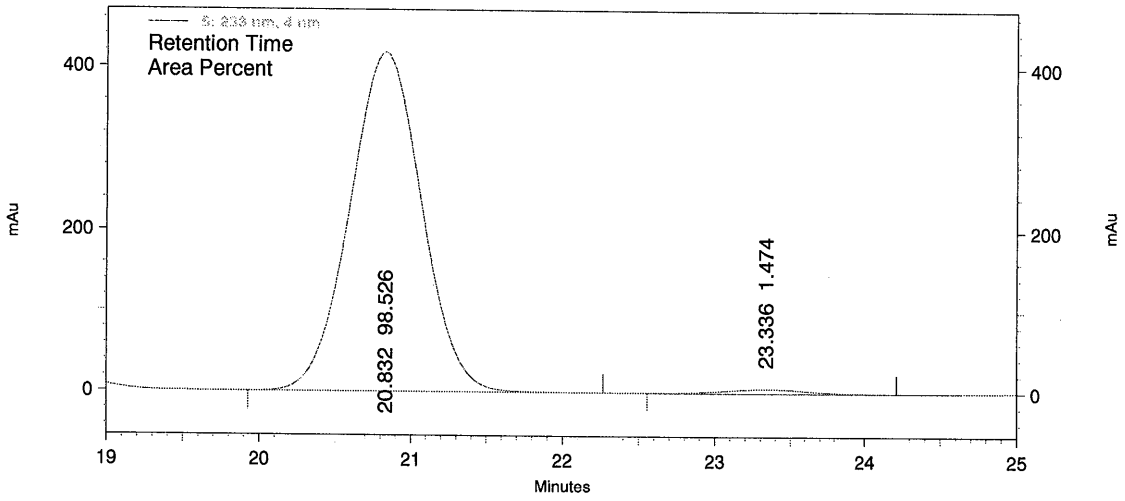
5: 233 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	20.696	49.815	202
2	23.180	50.185	202



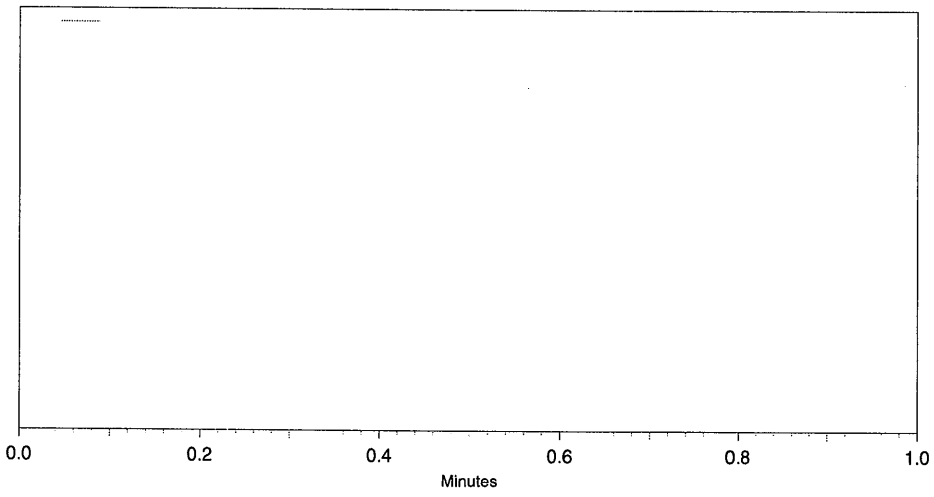


JW-08-41rt



5: 233 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	20.832	98.526	226
2	23.336	1.474	204



Pk #	Retention Time	Area Percent	Lambda Max

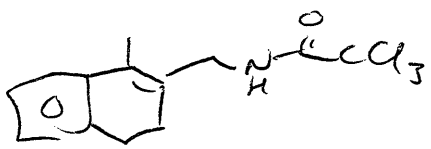
JW-08-184 AV-500 new TBI(HXP) probe
1D 1H starting parameters

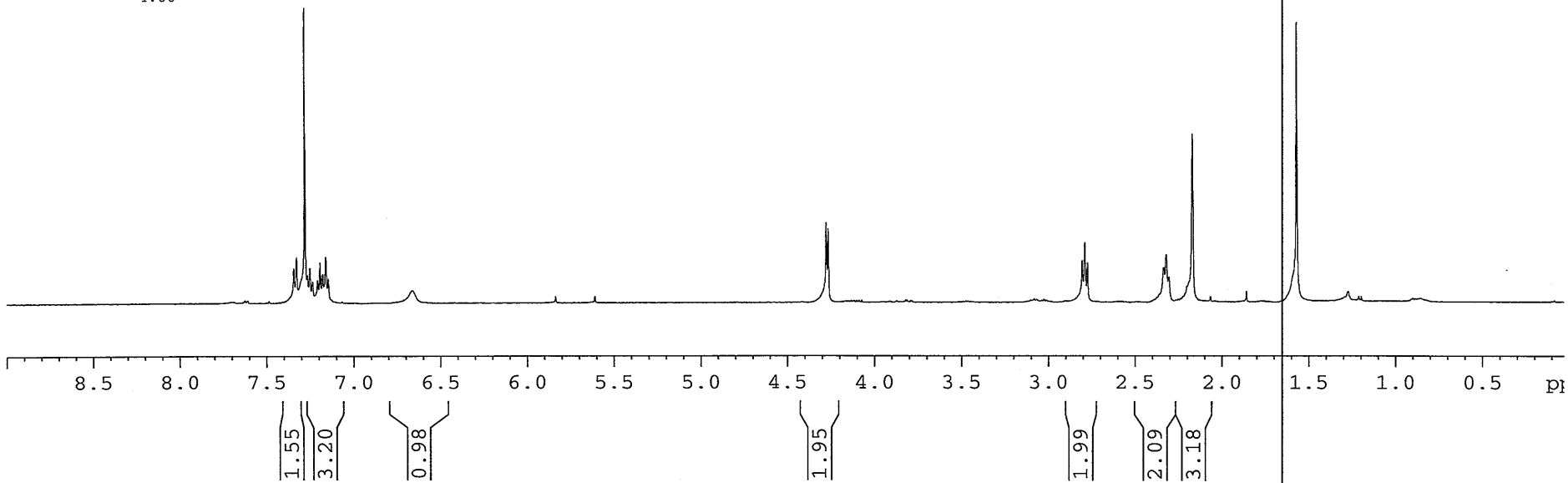
7.625 7.486 7.342 7.327 7.279 7.265 7.251 7.236 7.207 7.192 7.178 7.160 7.147 6.665 5.836 5.609 4.276 4.265 4.117 3.821 3.082 3.025 2.805 2.790 2.773 2.335 2.321 2.305 2.169 2.065 1.859 1.570 1.272 1.212 1.198 0.900

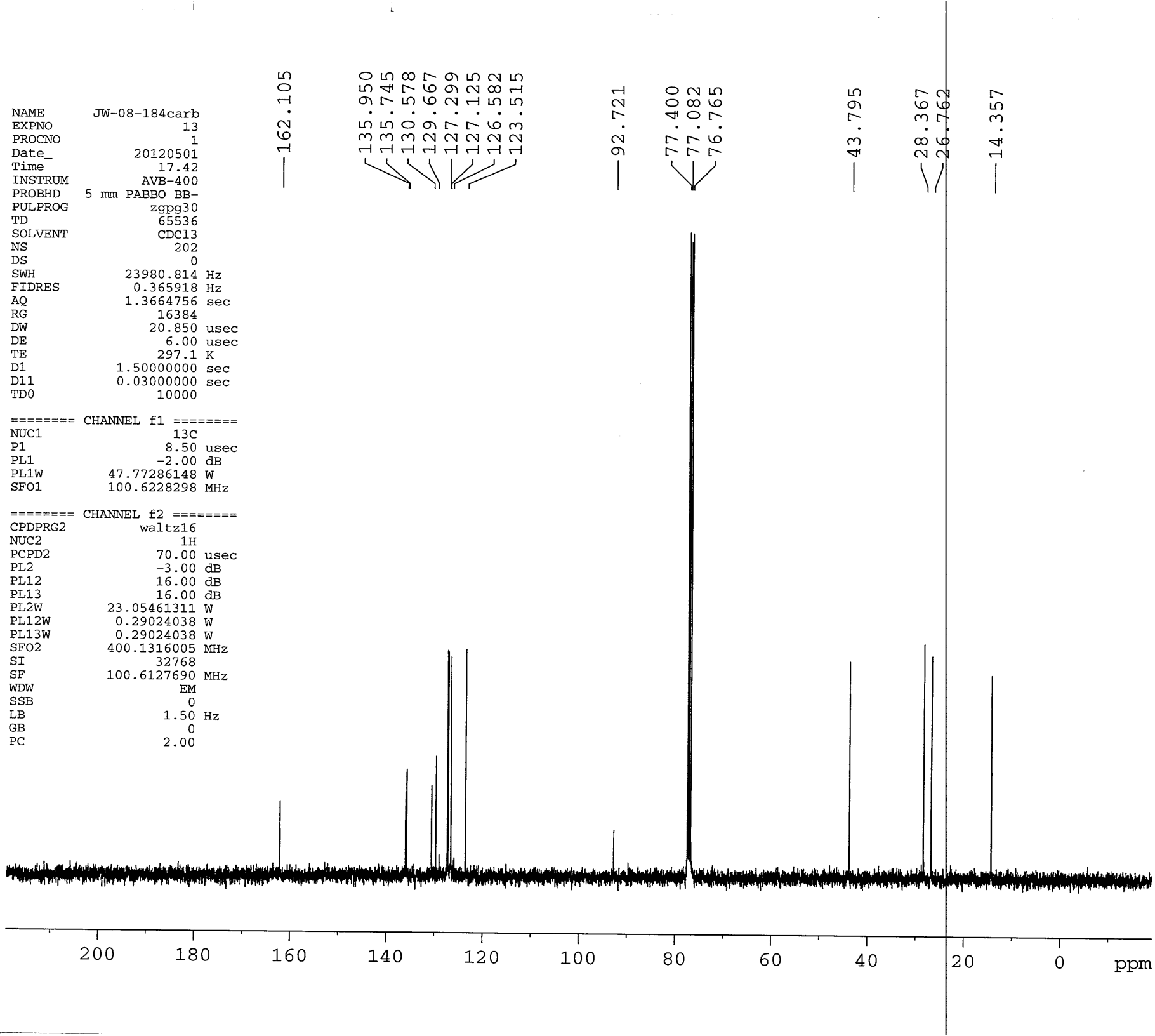
NAME	JW-08-184
EXPNO	1
PROCNO	1
Date_	20120418
Time	16.31
INSTRUM	AV-500
PROBHD	5 mm TBI 1H/31
PULPROG	zg30
TD	65536
SOLVENT	CDC13
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	574.7
DW	48.400 usec
DE	6.00 usec
TE	293.4 K
D1	0.10000000 sec
TD0	4

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

NUC1	1H
P1	7.30 usec
PL1	0.00 dB
PL1W	12.55943203 W
SFO1	500.2330889 MHz
SI	65536
SF	500.2300165 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00

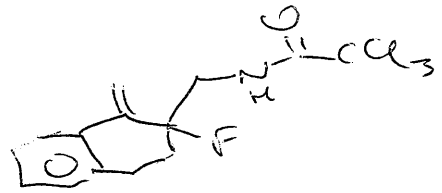


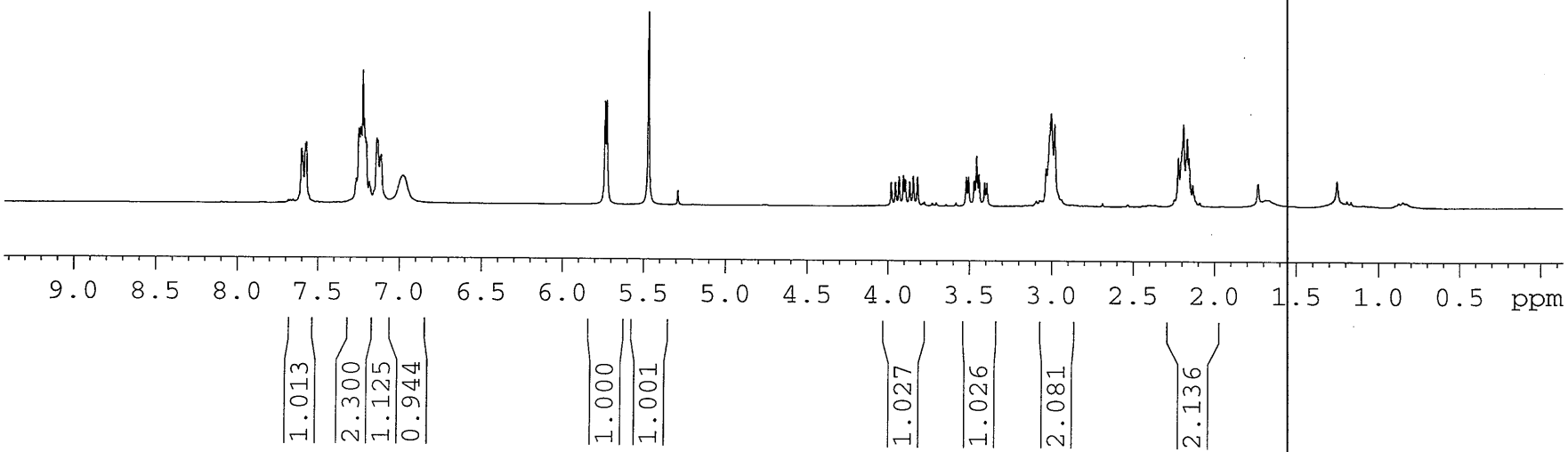



NAME JW-08-184carb
EXPNO 13
PROCNO 1
Date_ 20120501
Time 17.42
INSTRUM AVB-400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 202
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 297.1 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 10000
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.00 dB
PL12 16.00 dB
PL13 16.00 dB
PL2W 23.05461311 W
PL12W 0.29024038 W
PL13W 0.29024038 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 2.00
162.105
135.950
135.745
130.578
129.667
127.299
127.125
126.582
123.515
92.721
77.400
77.082
76.765
43.795
28.367
26.762
14.357
200
180
160
140
120
100
80
60
40
20
0
ppm

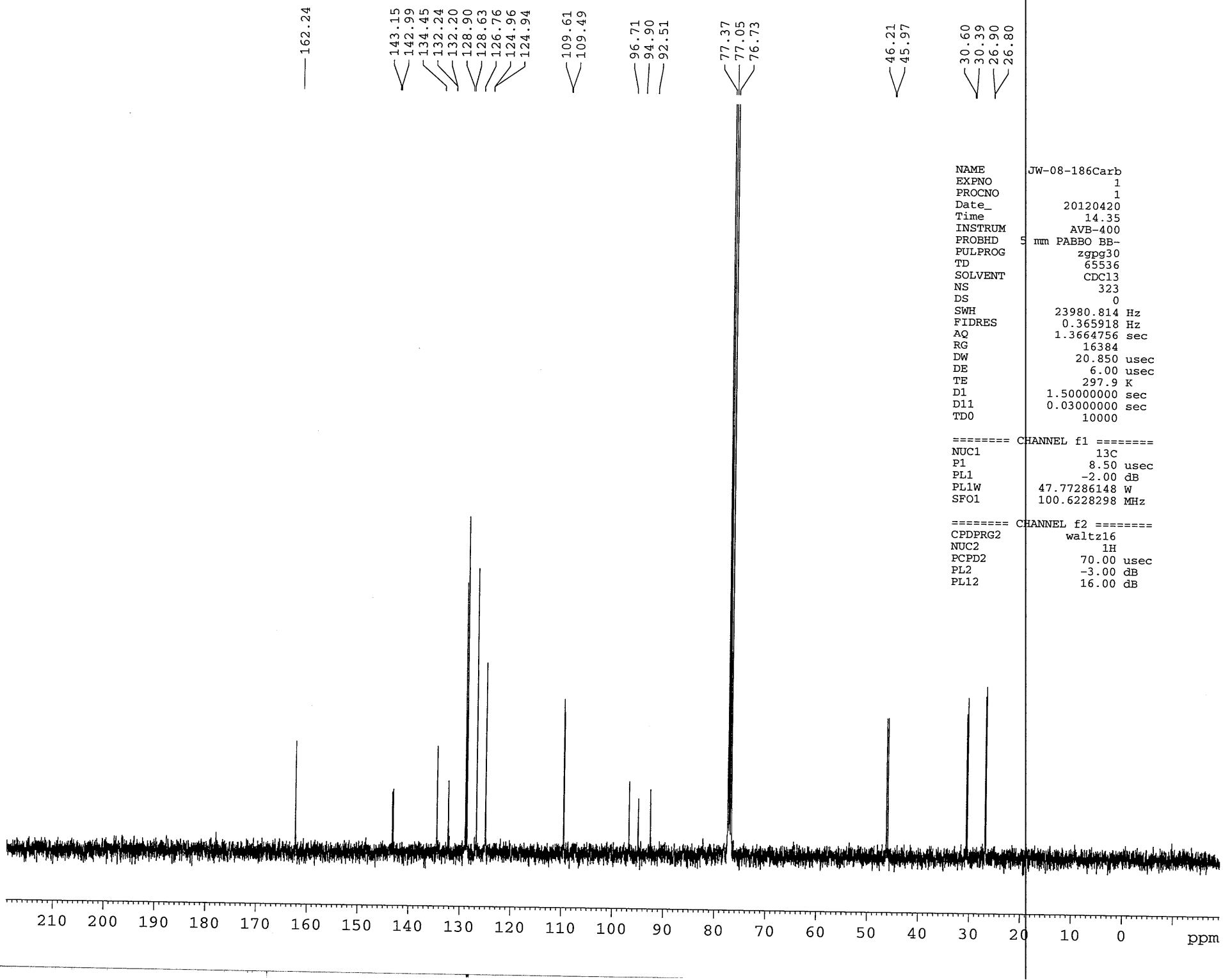
AV-300 Dual C-H probe proton starting parameters 7/23/03 RN.

7.604 7.581 7.574 7.264 7.252 7.247 7.240 7.235 7.226 7.217 7.204 7.186 7.141 7.134 7.113 6.977 5.738 5.727 5.470 5.290 3.980 3.953 3.931 3.905 3.893 3.866 3.844 3.818 3.519 3.505 3.470 3.456 3.441 3.407 3.393 3.093 3.033 3.002 2.981 2.221 2.188 2.166 2.155 2.132 1.730 1.676 1.250 1.189 1.165 0.875 0.850





186 AVB-400 ZBO Carbon Starting paramters 6/11/03 RN

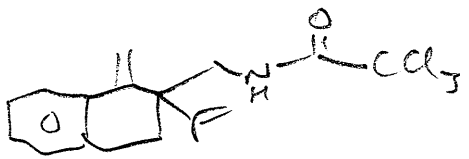


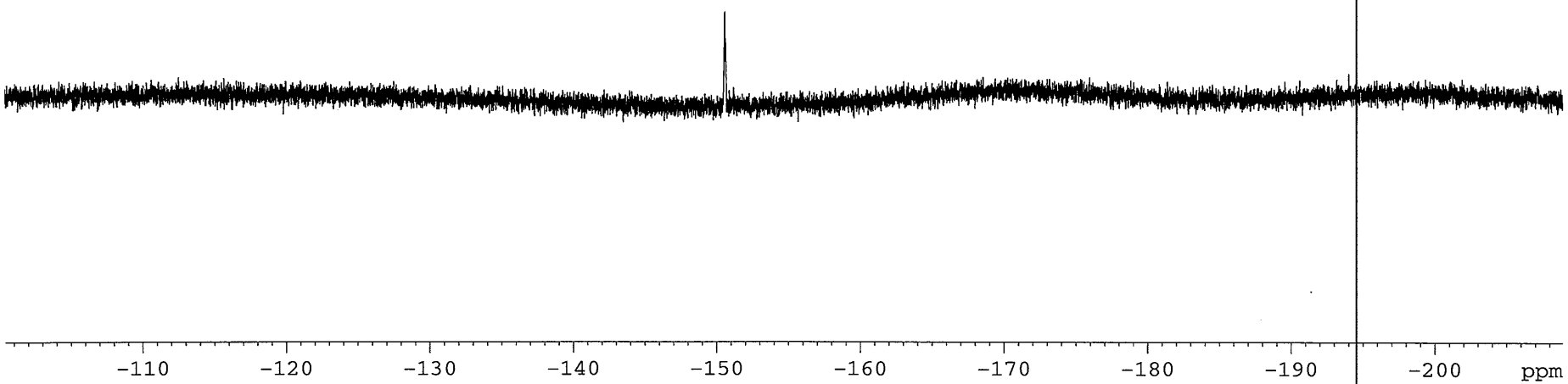
NAME	JW-08-186Carb
EXPNO	1
PROCNO	1
Date_	20120420
Time	14.35
INSTRUM	AVB-400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	323
DS	0
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	16384
DW	20.850 usec
DE	6.00 usec
TE	297.9 K
D1	1.50000000 sec
D11	0.03000000 sec
TD0	10000
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	-3.00 dB
PL12	16.00 dB

} p AVQ-400 QNP Probe 19F starting parameters. (revised P1, 2/12/04
chemical shifts relative to CFCl3 at 0 ppm (082103 HvH)
sw 239.28 ppm; o1p 0 ppm

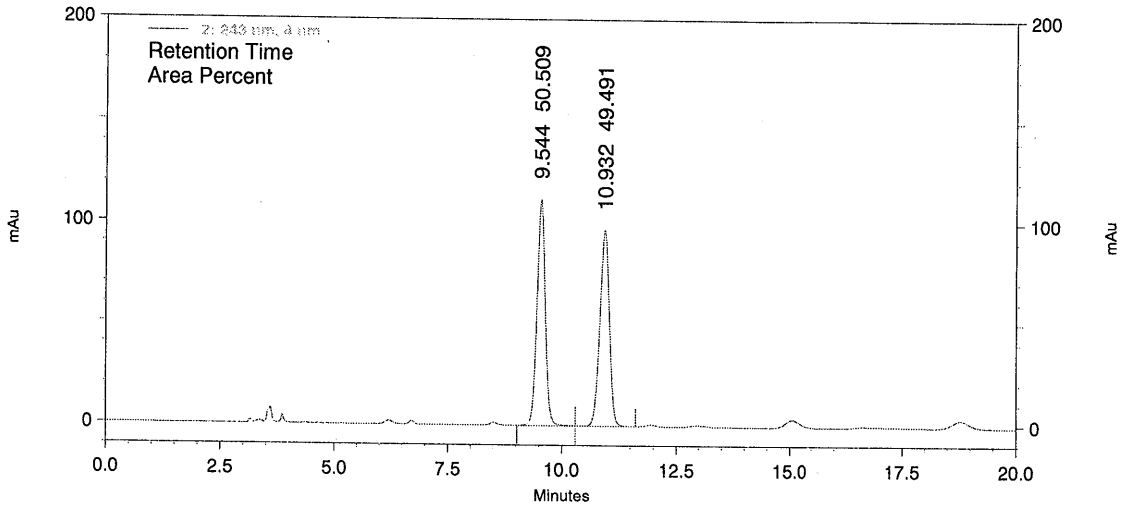
NAME	JW-ADccl3P-F
EXPNO	1
PROCNO	1
Date_	20120518
Time	11.20
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	32
DS	0
SWH	90090.094 Hz
FIDRES	0.687333 Hz
AQ	0.7275051 sec
RG	256
DW	5.550 usec
DE	6.00 usec
TE	292.6 K
D1	1.00000000 sec
TD0	4
======== CHANNEL f1 ========	
NUC1	19F
P1	16.00 usec
PL1	-3.00 dB
PL1W	20.04748917 W
SFO1	376.4607042 MHz
SI	65536
SF	376.4980736 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	4.00

-150.59





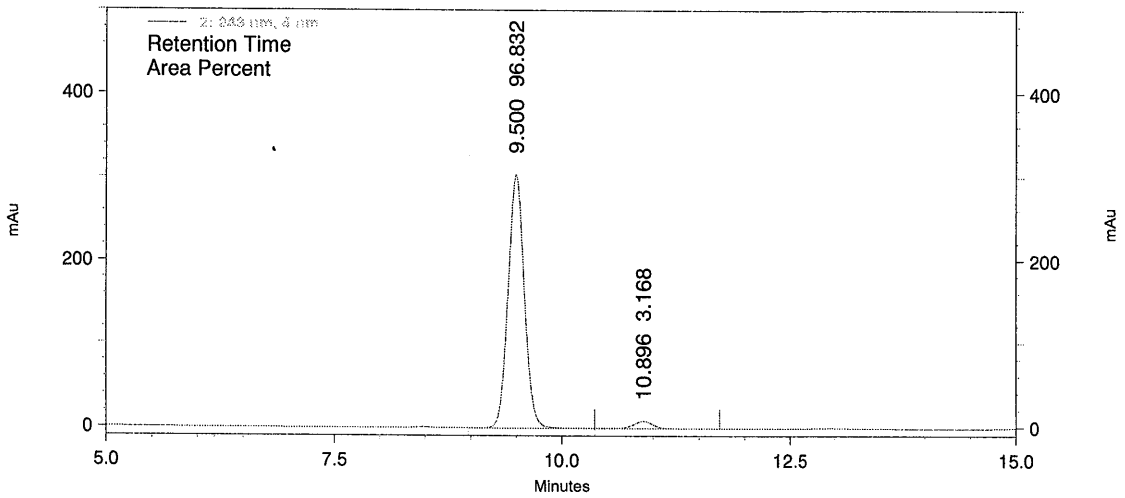
JW-08-117rac IC9802_30min



2: 243 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	9.544	50.509	209
2	10.932	49.491	209

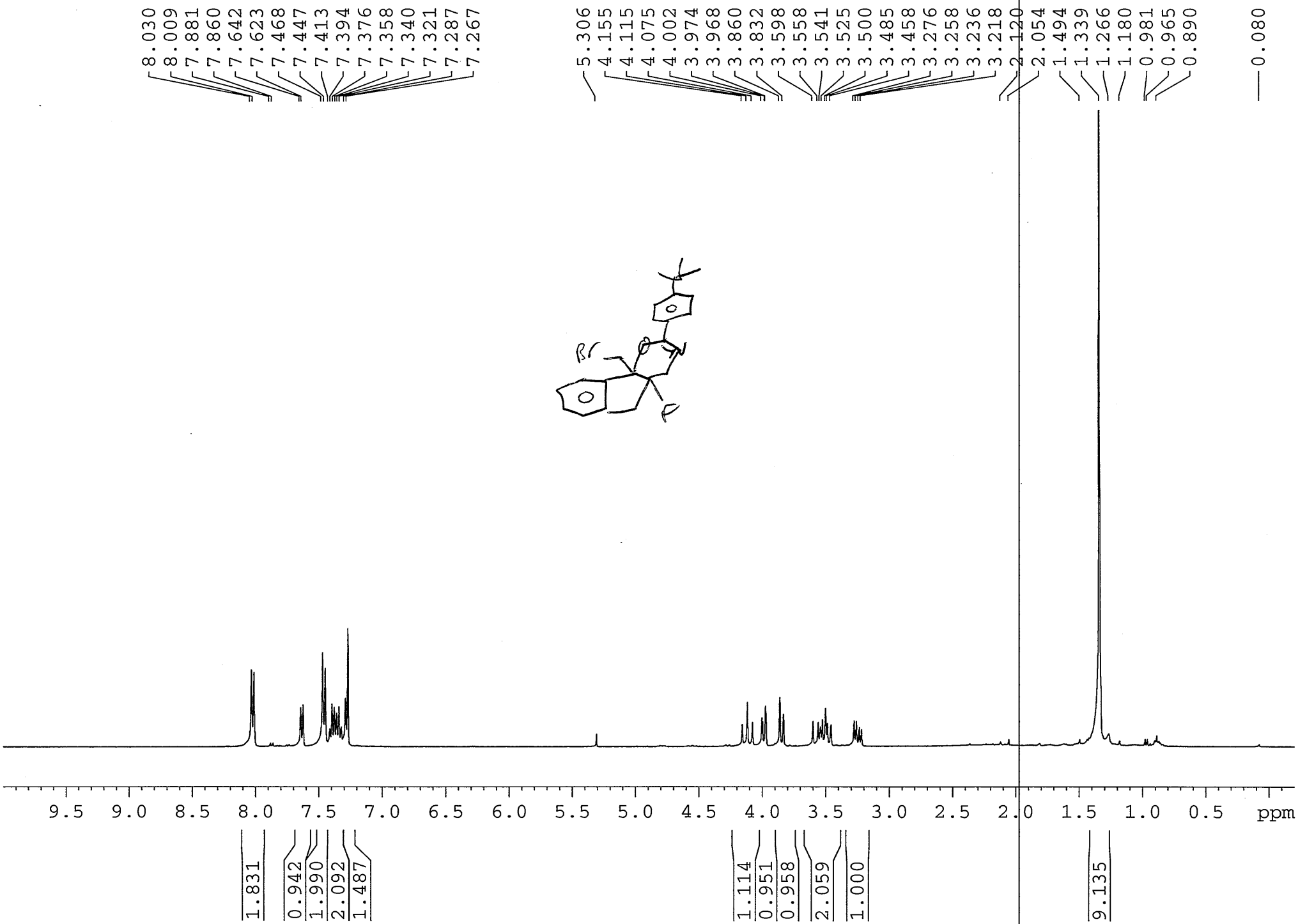
JW-08-121 IC9802_30min



2: 243 nm, 4 nm
Results

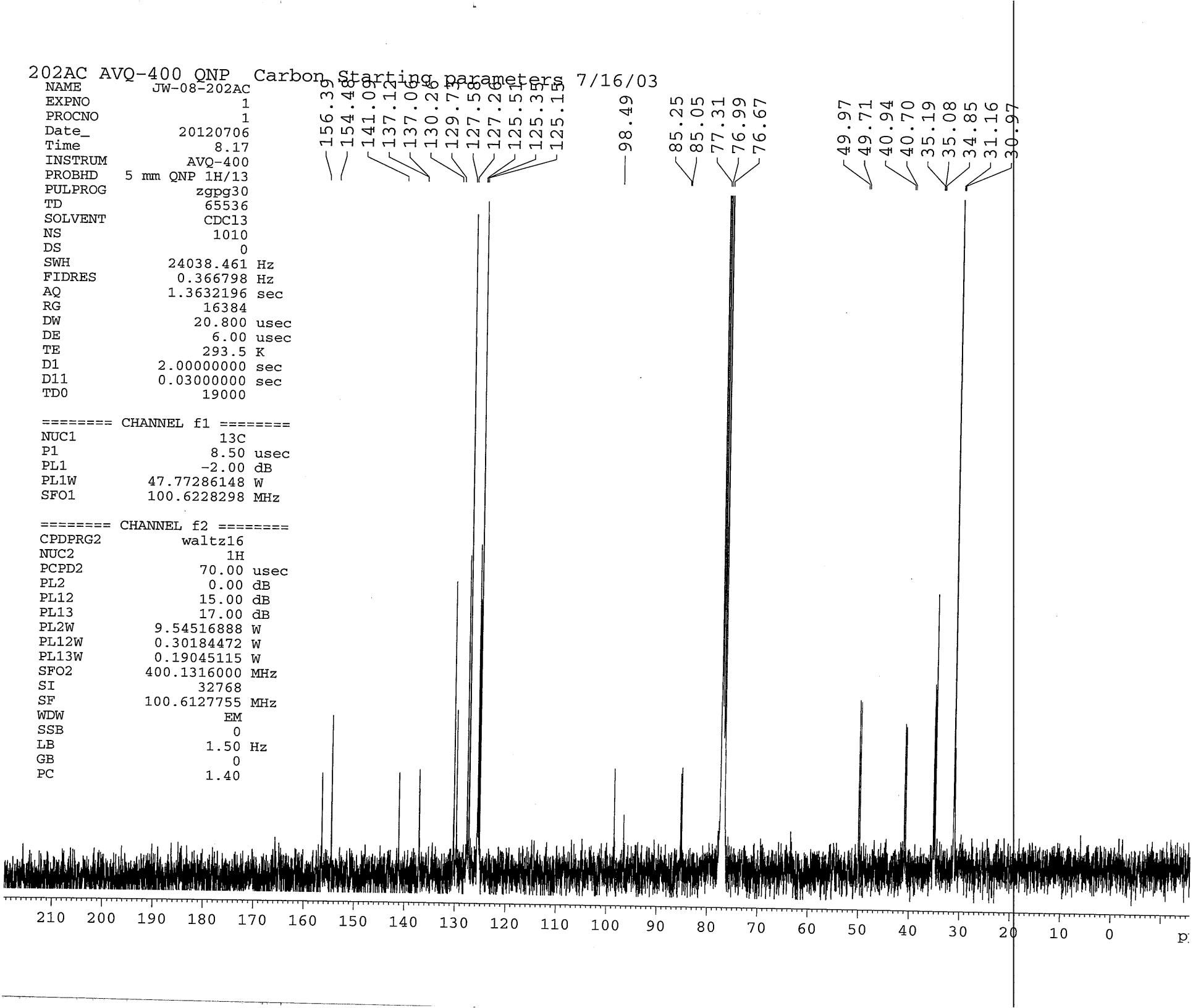
Pk #	Retention Time	Area Percent	Lambda Max
1	9.500	96.832	209
2	10.896	3.168	210

8-202A AVQ-400 QNP Proton starting parameters. 7/16/03. Revised 7/22/0



202AC AVQ-400 QNP Carbon Starting parameters 7/16/03

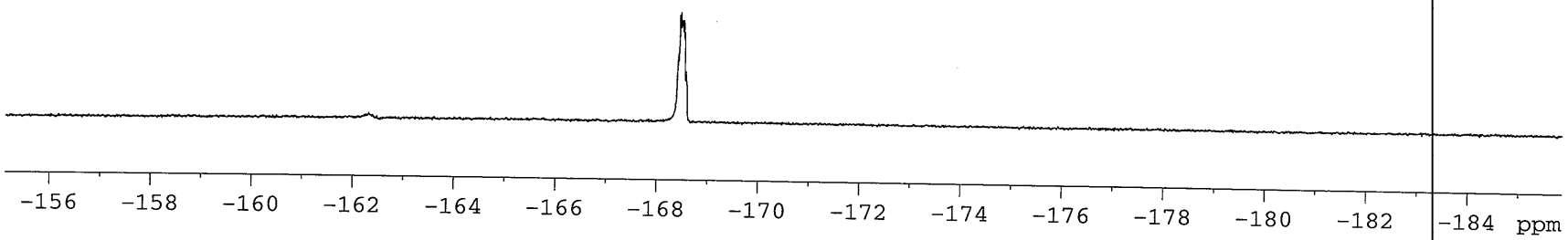
NAME	JW-08-202AC
EXPNO	1
PROCNO	1
Date_	20120706
Time	8.17
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	1010
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3632196 sec
RG	16384
DW	20.800 usec
DE	6.00 usec
TE	293.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	19000
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	17.00 dB
PL2W	9.54516888 W
PL12W	0.30184472 W
PL13W	0.19045115 W
SFO2	400.1316000 MHz
SI	32768
SF	100.6127755 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	1.40



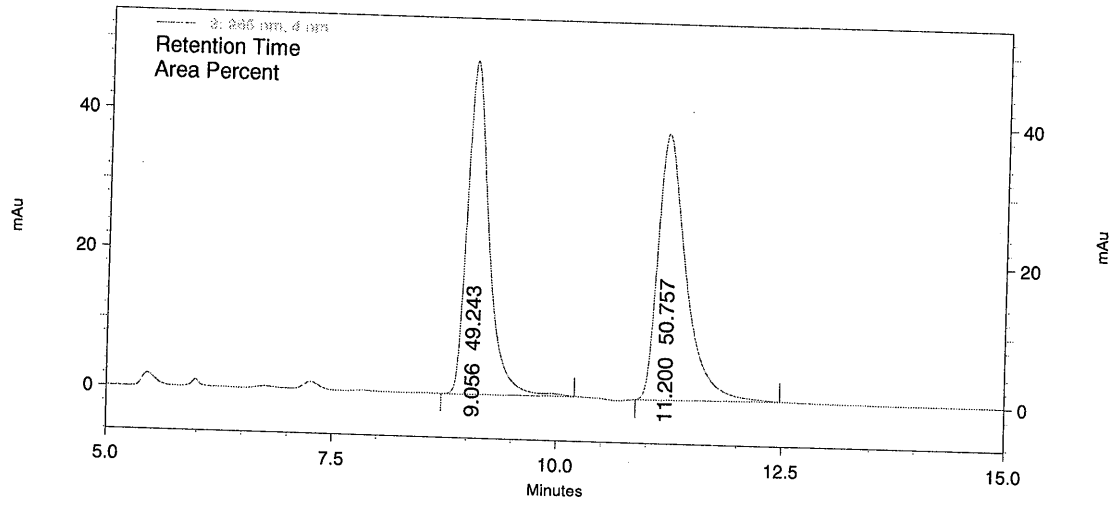
NAME	JW-08-202A-p1F
EXPNO	1
PROCNO	1
Date_	20120509
Time	15.27
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	32
DS	0
SWH	90090.094 Hz
FIDRES	0.687333 Hz
AQ	0.7275051 sec
RG	3649.1
DW	5.550 usec
DE	6.00 usec
TE	293.0 K
D1	1.00000000 sec
TD0	4
======== CHANNEL f1 ========	
NUC1	19F
P1	16.00 usec
PL1	-3.00 dB
PL1W	20.04748917 W
SFO1	376.4607042 MHz
SI	65536
SF	376.4980736 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	4.00

2A AVQ-400 QNP Probe 19F starting parameters. (revised P1, 2/12/04 F
chemical shifts relative to CFCl3 at 0 ppm (082103 HvH)
sw 239.28 ppm; o1p 0 ppm

-168.45
-168.47
-168.53

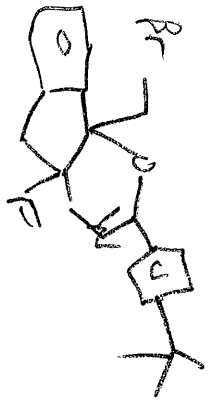


JW-08-207rac- IB9901_15

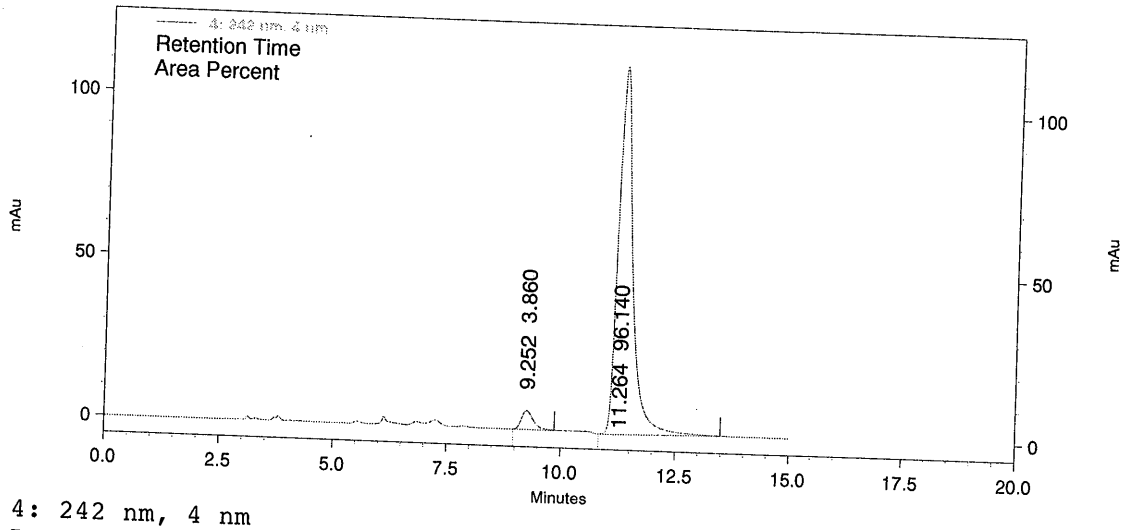


3: 265 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	9.056	49.243	203
2	11.200	50.757	203



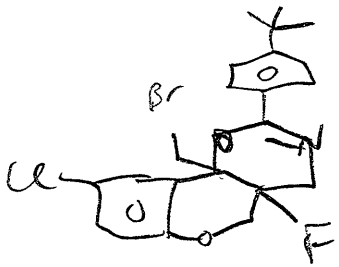
JW-08-202B IB9901



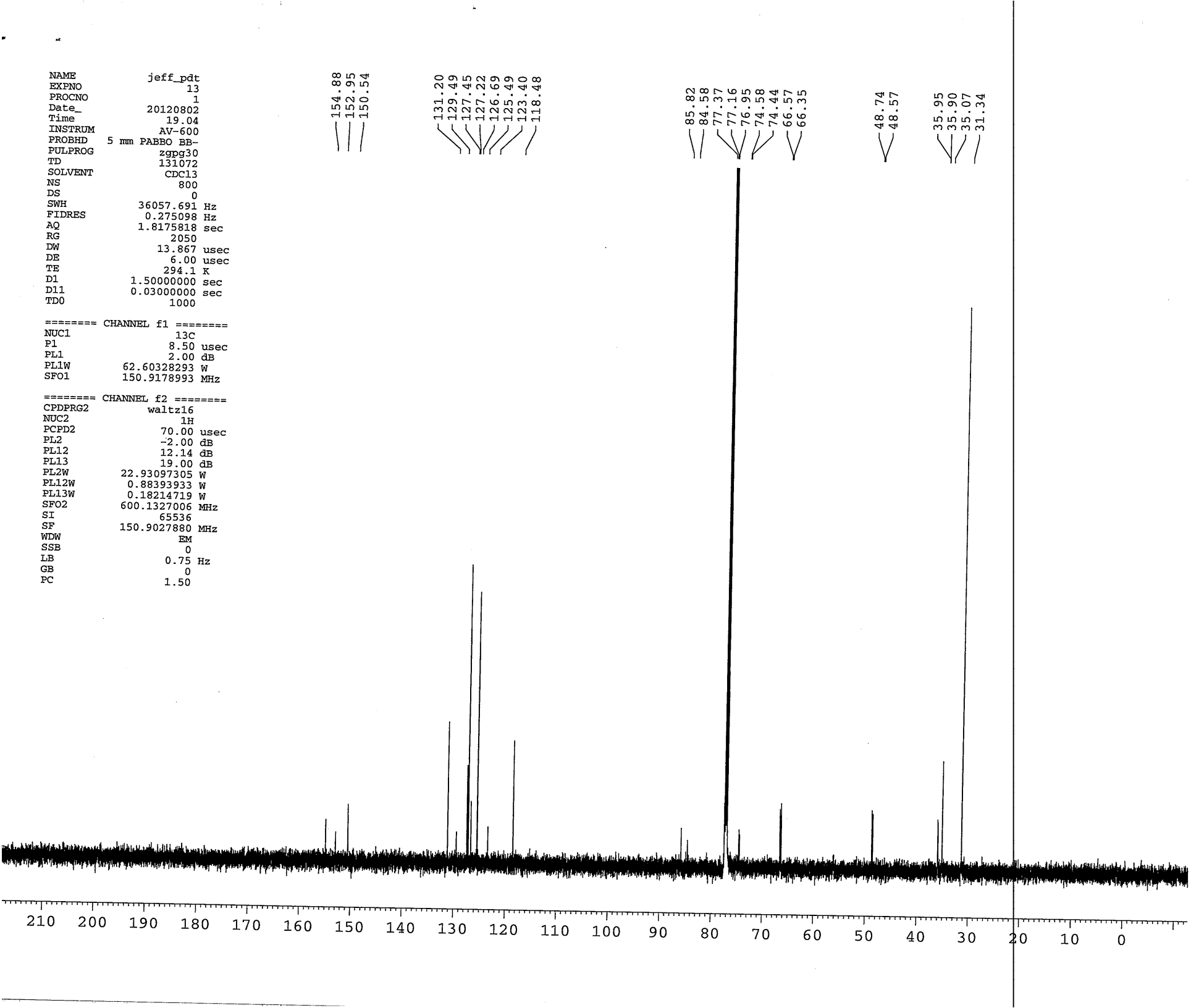
4: 242 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	9.252	3.860	209
2	11.264	96.140	203

NAME	jeff_pdt
EXPNO	1
PROCNO	1
Date_	20120802
Time	19.01
INSTRUM	AV-600
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	1
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	128
DW	41.600 usec
DE	6.00 usec
TE	294.0 K
D1	0.10000000 sec
TD0	8
======== CHANNEL f1 ========	
NUC1	1H
P1	13.75 usec
PL1	-2.00 dB
PL1W	22.93097305 W
SFO1	600.1339008 MHz
SI	65536
SF	600.1300184 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00



NAME	jeff_pdt
EXPNO	13
PROCNO	1
Date_	20120802
Time	19.04
INSTRUM	AV-600
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	131072
SOLVENT	CDCl3
NS	800
DS	0
SWH	36057.691 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	2050
DW	13.867 usec
DE	6.00 usec
TE	294.1 K
D1	1.50000000 sec
D11	0.03000000 sec
TD0	1000
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	2.00 dB
PL1W	62.60328293 W
SFO1	150.9178993 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	-2.00 dB
PL12	12.14 dB
PL13	19.00 dB
PL2W	22.93097305 W
PL12W	0.88393933 W
PL13W	0.18214719 W
SFO2	600.1327006 MHz
SI	65536
SF	150.9027880 MHz
WDW	EM
SSB	0
LB	0.75 Hz
GB	0
PC	1.50



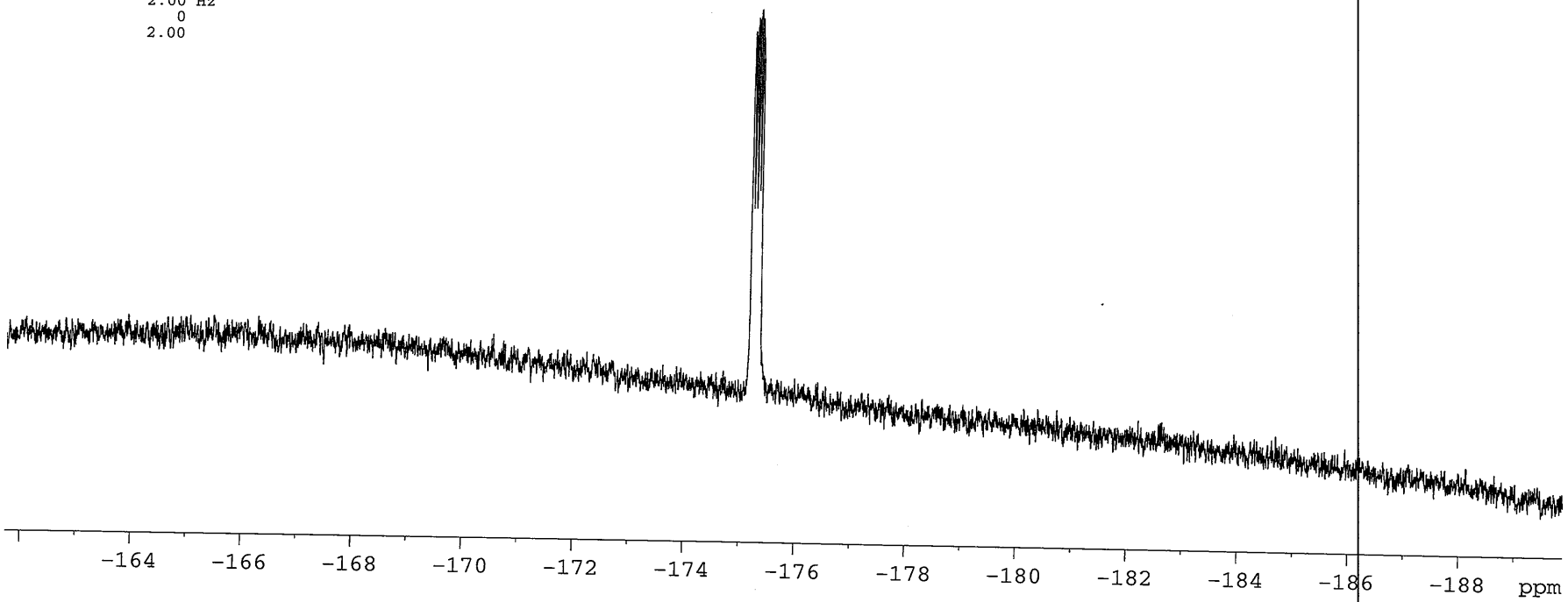
NAME	JW-08-194-bottombandF
EXPNO	1
PROCNO	1
Date_	20120430
Time	11.18
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	32
DS	0
SWH	90090.094 Hz
FIDRES	0.687333 Hz
AQ	0.7275051 sec
RG	3251
DW	5.550 usec
DE	6.00 usec
TE	293.5 K
D1	1.00000000 sec
TD0	4

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

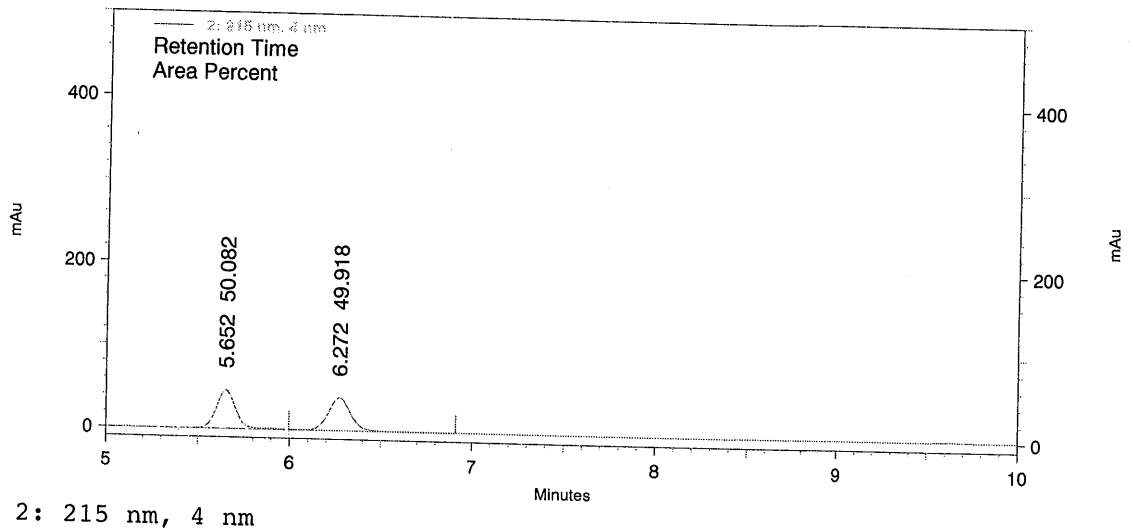
NUC1	19F
P1	16.00 usec
PL1	-3.00 dB
PL1W	20.04748917 W
SFO1	376.4607042 MHz
SI	65536
SF	376.4980736 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	2.00

ɔottomband AVQ-400 QNP Probe 19F starting parameters. (revised P1, 2
chemical shifts relative to CFCl3 at 0 ppm (082103 HvH)
sw 239.28 ppm; o1p 0 ppm

-175.20
-175.25
-175.30
-175.33

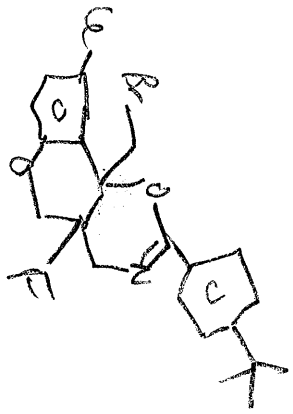


JW-08-194rac IC9802_30min

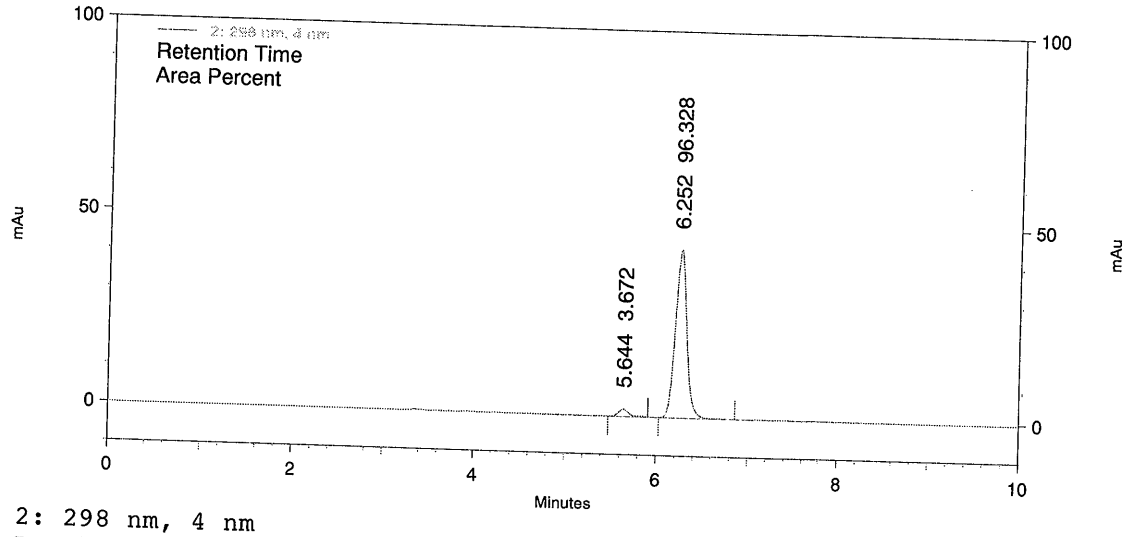


2: 215 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	5.652	50.082	204
2	6.272	49.918	204

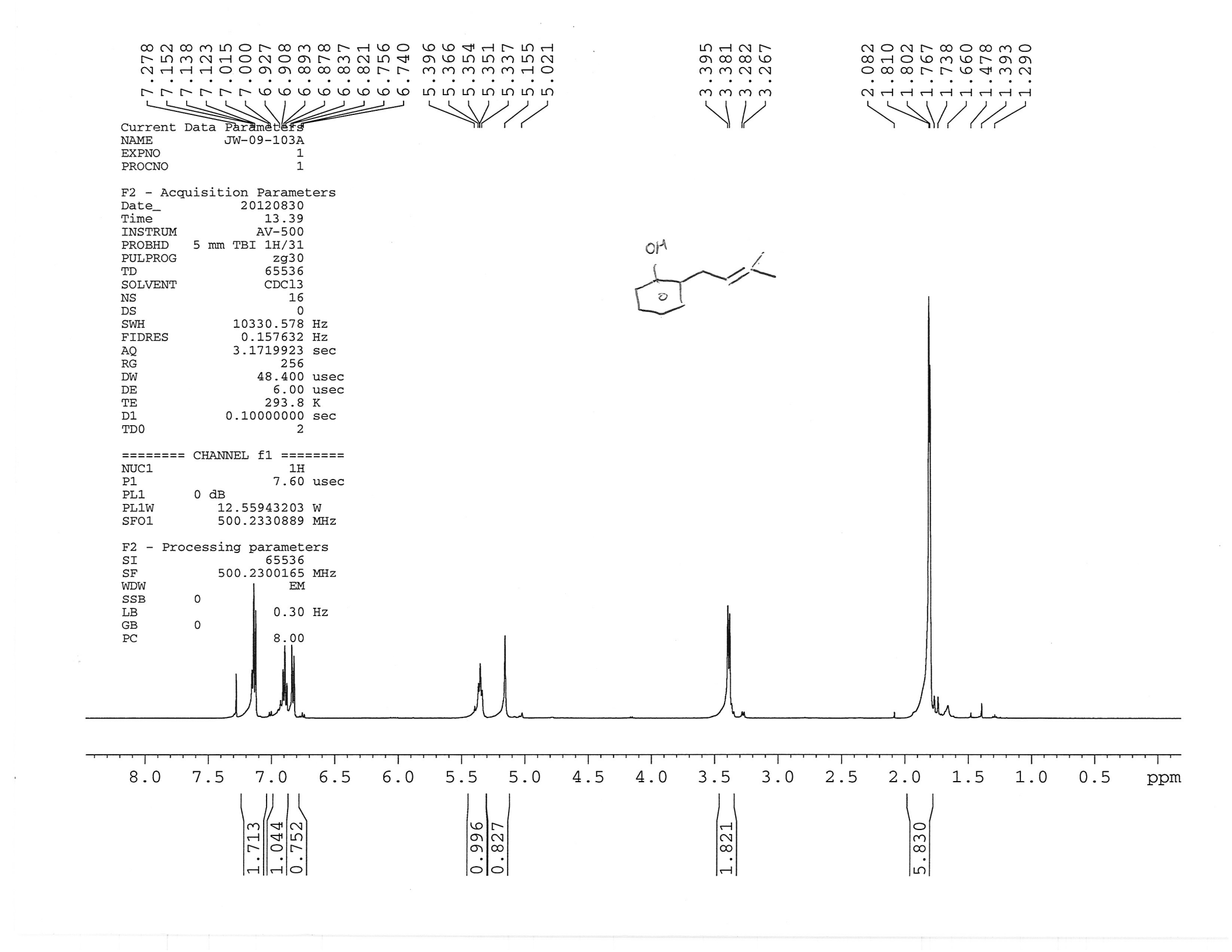


JW-09-6 IC9802_15min



2: 298 nm, 4 nm
Results

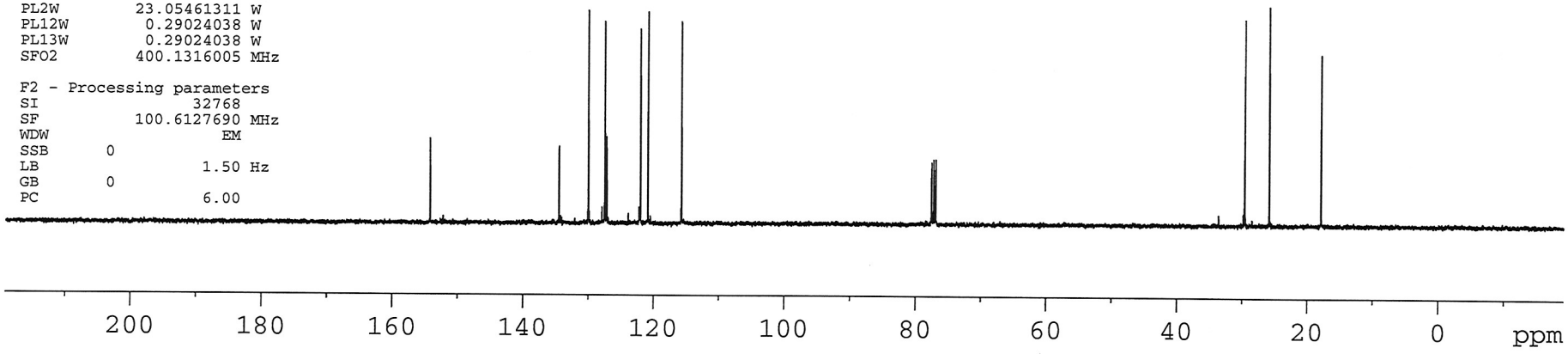
Pk #	Retention Time	Area Percent	Lambda Max
1	5.644	3.672	204
2	6.252	96.328	205

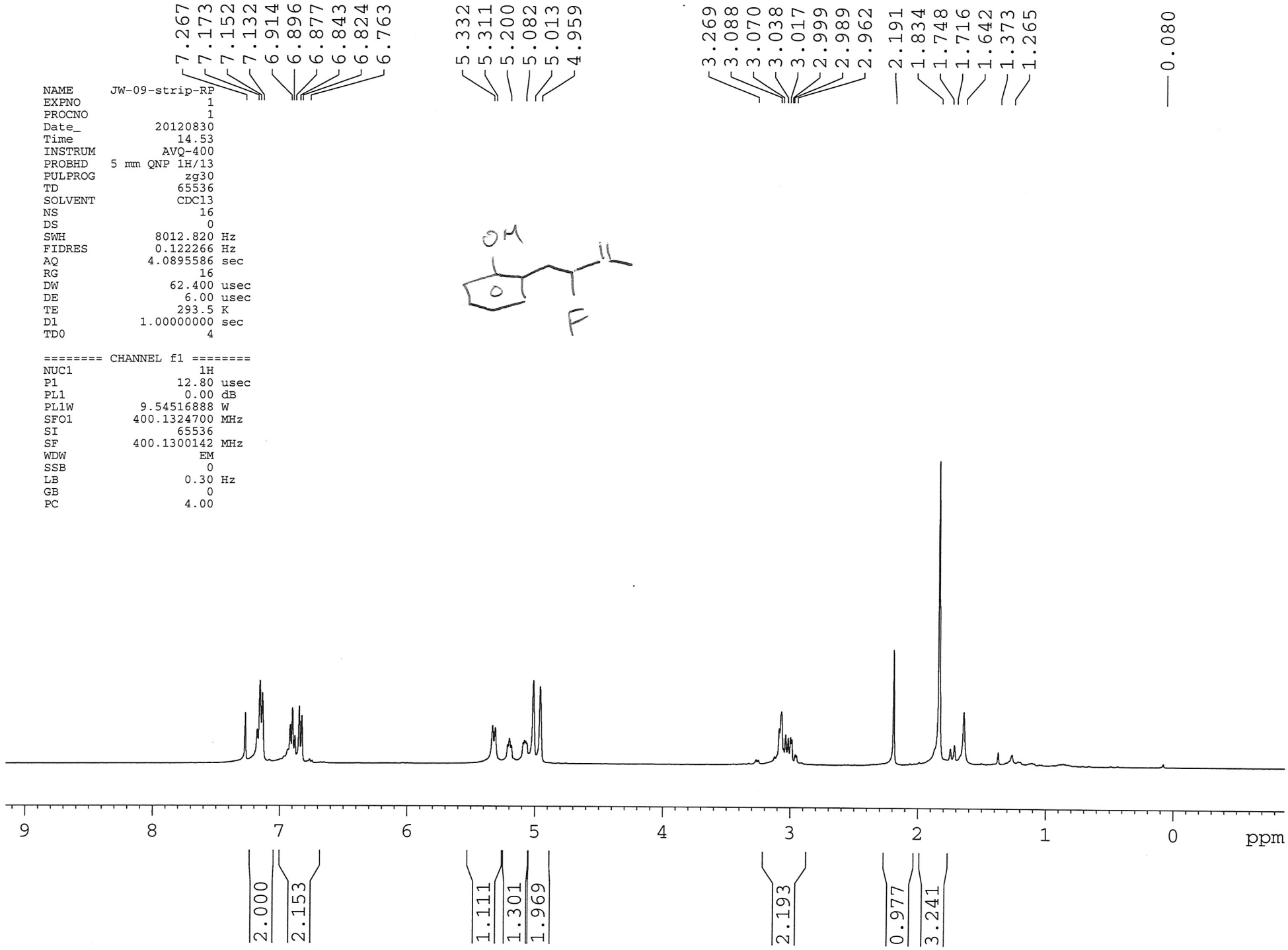

7.278
7.152
7.138
7.123
7.015
7.000
6.927
6.908
6.893
6.878
6.837
6.821
6.756
6.740
5.396
5.366
5.354
5.351
5.337
5.155
5.021
3.395
3.381
3.282
3.267
2.082
1.810
1.802
1.767
1.738
1.660
1.478
1.393
1.290
Current Data Parameters
NAME JW-09-103A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120830
Time 13.39
INSTRUM AV-500
PROBHD 5 mm TBI 1H/31
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 256
DW 48.400 usec
DE 6.00 usec
TE 293.8 K
D1 0.10000000 sec
TD0 2
======== CHANNEL f1 ========
NUC1 1H
P1 7.60 usec
PL1 0 dB
PL1W 12.55943203 W
SFO1 500.2330889 MHz
F2 - Processing parameters
SI 65536
SF 500.2300165 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 8.00
OH
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.713
1.044
0.752
0.996
0.827
1.821
5.830

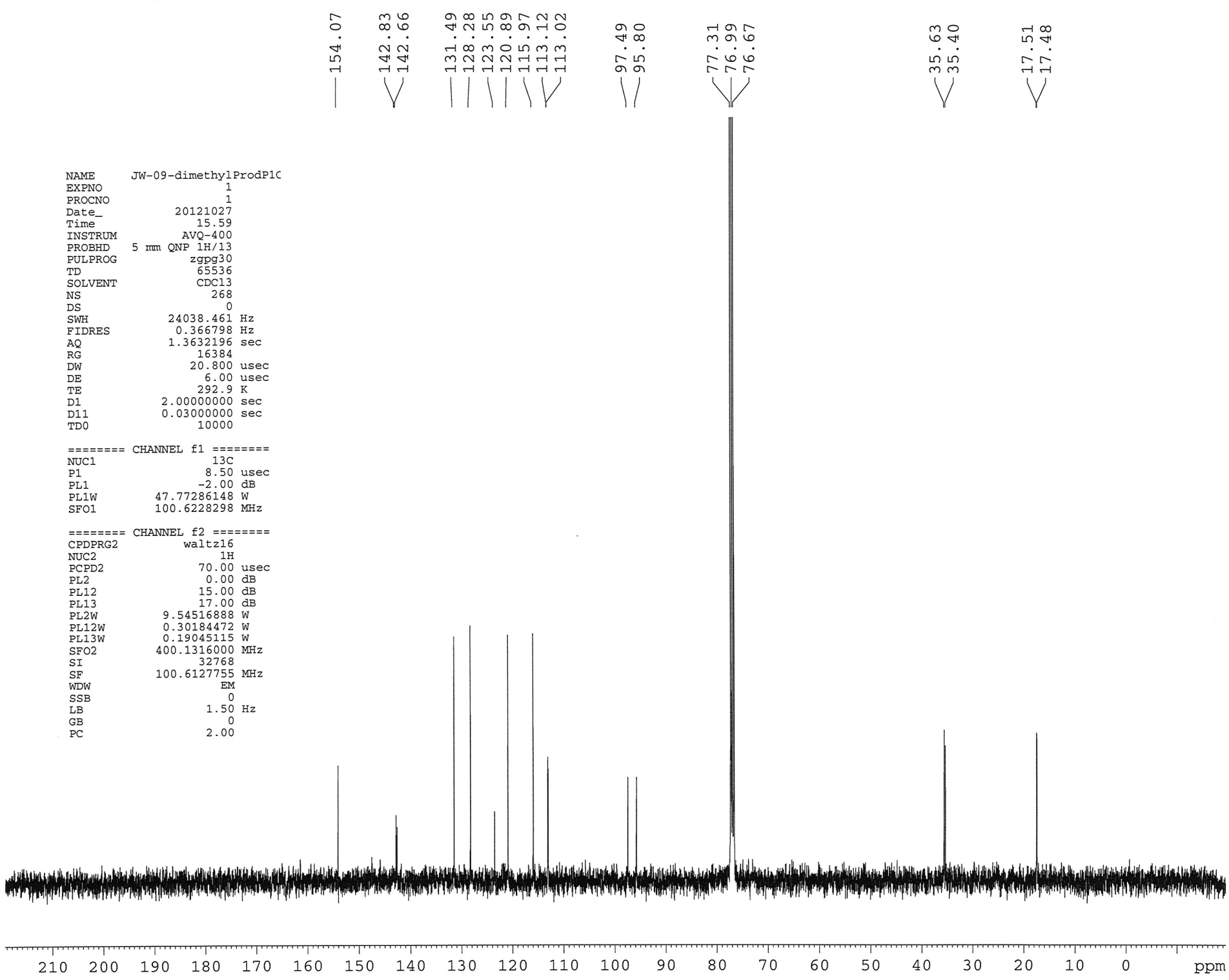
154.228
134.538
130.069
127.555
127.260
122.069
120.925
115.780
77.571
77.252
76.934
29.637
25.884
17.937

103A AVB-400 ZBO Carbon Starting paramters 6/11/03 RN

```
Current Data Parameters
NAME      JW-09-103ACarb
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20121004
Time               17.00
INSTRUM          AVB-400
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   34
DS                    0
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                16384
DW               20.850 usec
DE                6.00 usec
TE               297.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0               1000

======== CHANNEL f1 ========
NUC1                13C
P1                 8.50 usec
PL1               -2.00 dB
PL1W        47.77286148 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             70.00 usec
PL2               -3.00 dB
PL12              16.00 dB
PL13              16.00 dB
PL2W        23.05461311 W
PL12W        0.29024038 W
PL13W        0.29024038 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB       0
LB                1.50 Hz
GB        0
PC                6.00
```



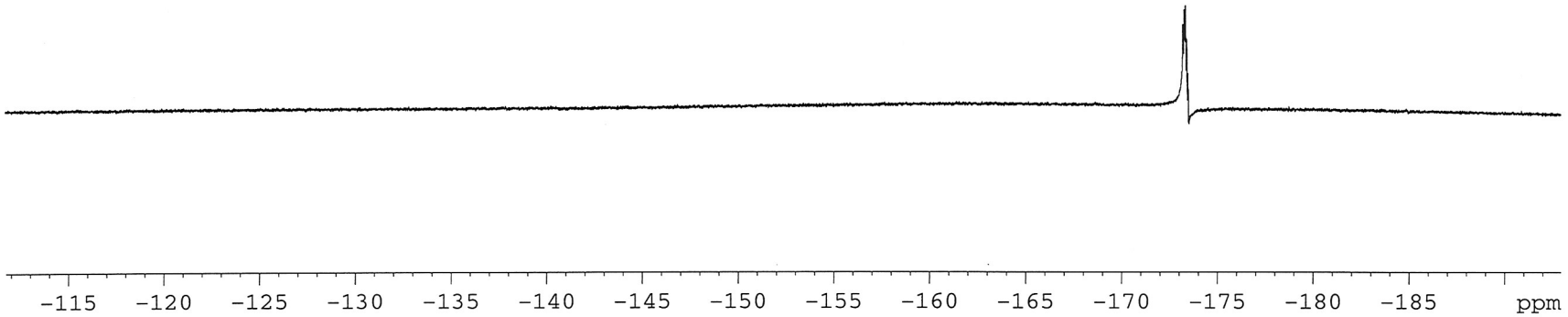

7.267
7.173
7.152
7.132
6.914
6.896
6.877
6.843
6.824
6.763
5.332
5.311
5.200
5.082
5.013
4.959
3.269
3.088
3.070
3.038
3.017
2.999
2.989
2.962
2.191
1.834
1.748
1.716
1.642
1.373
1.265
0.080
NAME JW-09-strip-RP
EXPNO 1
PROCNO 1
Date_ 20120830
Time 14.53
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 16
DW 62.400 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 4
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
OH
O
F
9
8
7
6
5
4
3
2
1
0
ppm
2.000
2.153
1.111
1.301
1.969
2.193
0.977
3.241


154.07
142.83
142.66
131.49
128.28
123.55
120.89
115.97
113.12
113.02
97.49
95.80
77.31
76.99
76.67
35.63
35.40
17.51
17.48
NAME JW-09-dimethylProdP1C
EXPNO 1
PROCNO 1
Date_ 20121027
Time 15.59
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 268
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 16384
DW 20.800 usec
DE 6.00 usec
TE 292.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10000
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 17.00 dB
PL2W 9.54516888 W
PL12W 0.30184472 W
PL13W 0.19045115 W
SFO2 400.1316000 MHz
SI 32768
SF 100.6127755 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 2.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

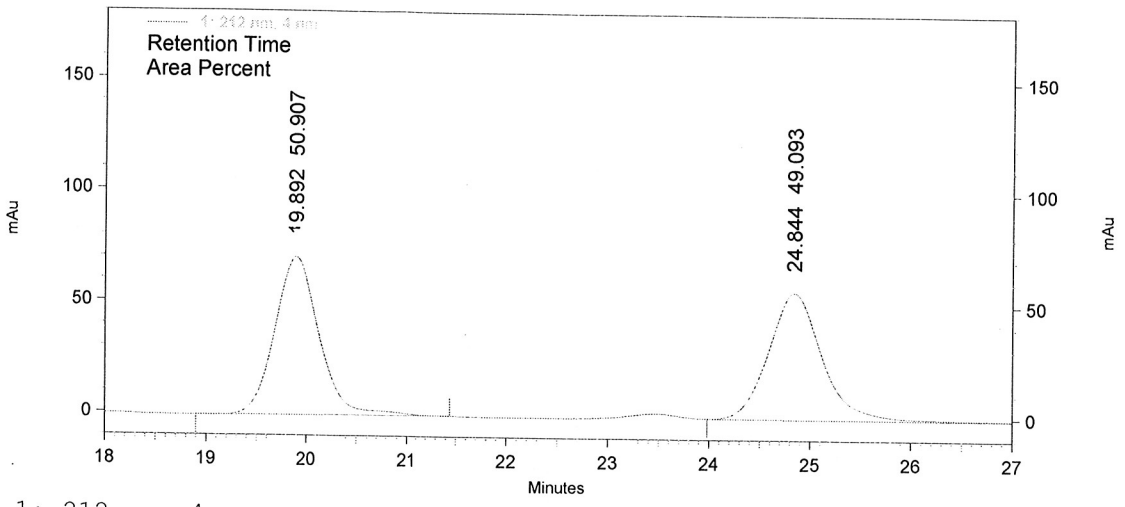
AVQ-400 QNP Probe 19F starting parameters. (revised P1, 2/12/04 RN)
chemical shifts relative to CFCl3 at 0 ppm (082103 HvH)
sw 239.28 ppm; o1p 0 ppm

NAME	JW-09-strip-RP-F-100
EXPNO	1
PROCNO	1
Date_	20120830
Time	14.57
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	0
SWH	90090.094 Hz
FIDRES	0.687333 Hz
AQ	0.7275051 sec
RG	3649.1
DW	5.550 usec
DE	6.00 usec
TE	293.4 K
D1	1.00000000 sec
TD0	2
======== CHANNEL f1 ========	
NUC1	19F
P1	16.00 usec
PL1	-3.00 dB
PL1W	20.04748917 W
SFO1	376.4607042 MHz
SI	65536
SF	376.4980736 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	4.00

-173.20
-173.28
-173.33
-173.41
-173.47



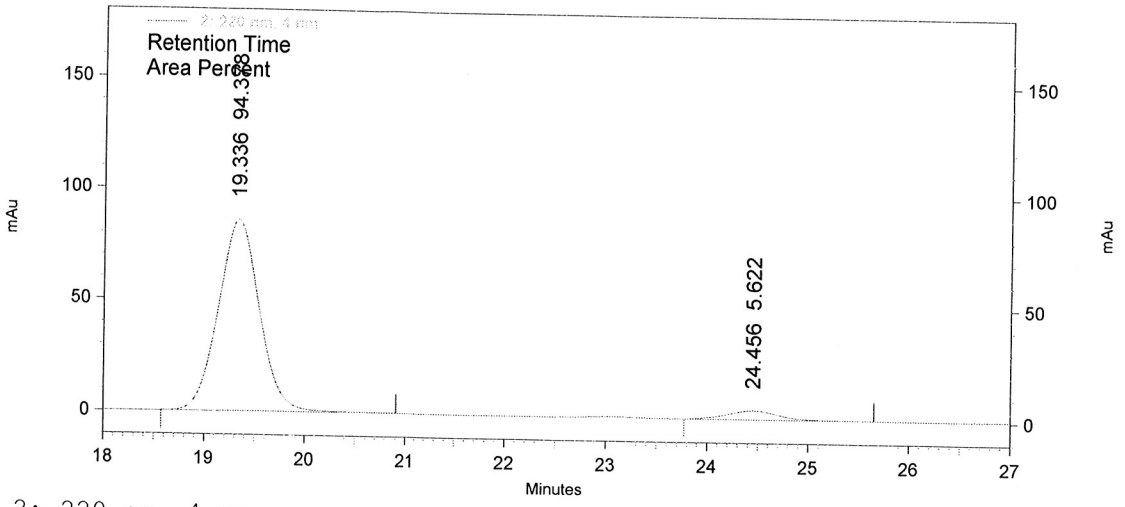
JW-09-102rac ic9901-45



1: 212 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	19.892	50.907	200
2	24.844	49.093	200

JW-09-102strip ic9901-45



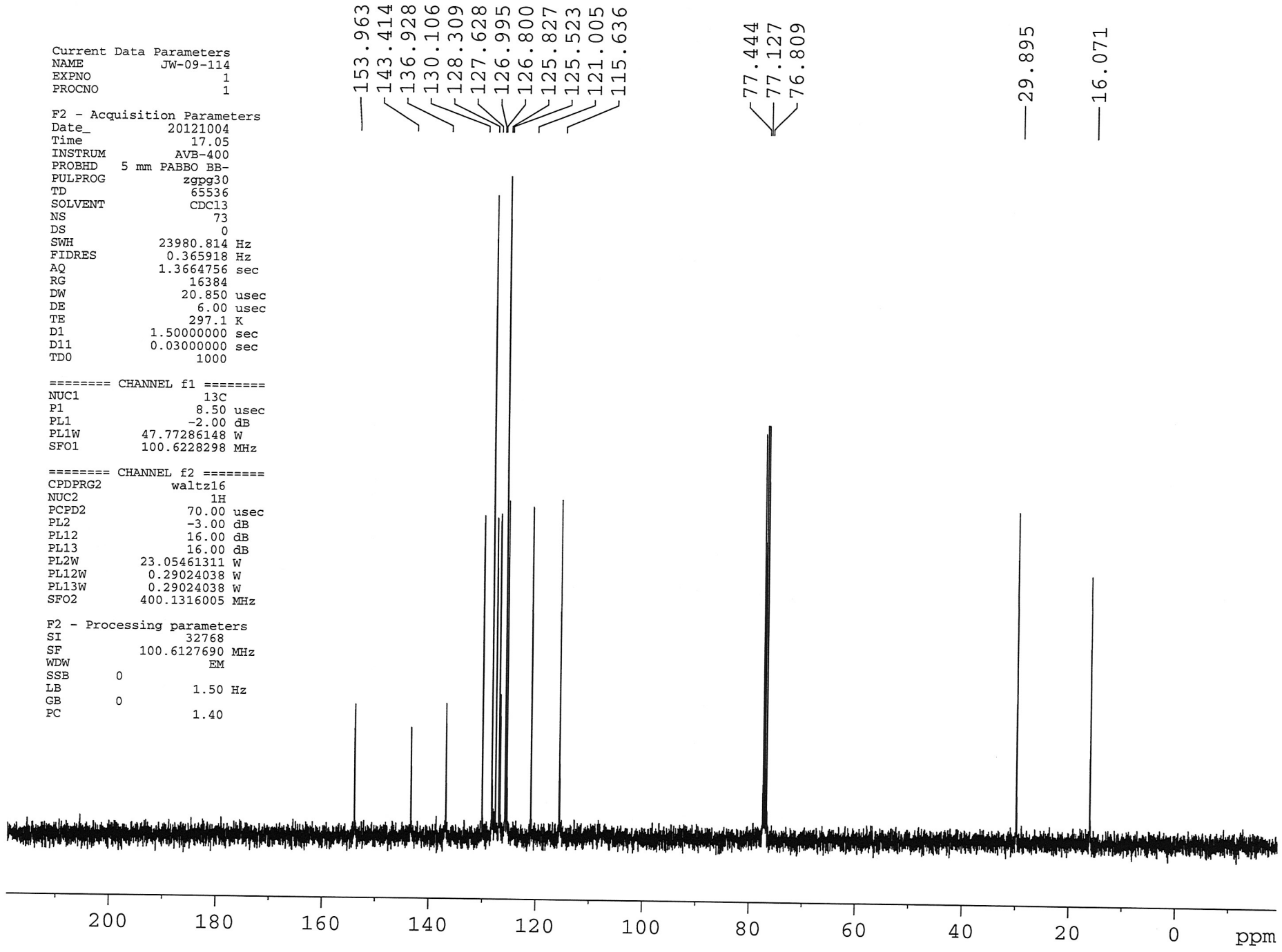
2: 220 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	19.336	94.378	200
2	24.456	5.622	217

9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
7.489
1.965
1.000
0.950
2.042
2.981

7.427
7.403
7.340
7.316
7.291
7.261
7.252
7.237
7.213
7.195
7.170
7.156
7.130
7.104
7.006
6.971
6.920
6.896
6.871
6.816
6.790
6.731
6.704
5.983
5.962
5.937
4.955
4.891
4.848
4.781
3.586
3.562
3.498
3.348
2.398
2.188
2.130
2.101
2.062
1.977
1.764
1.634
1.268

AVB-400 ZBO Carbon Starting paramters 6/11/03 RN



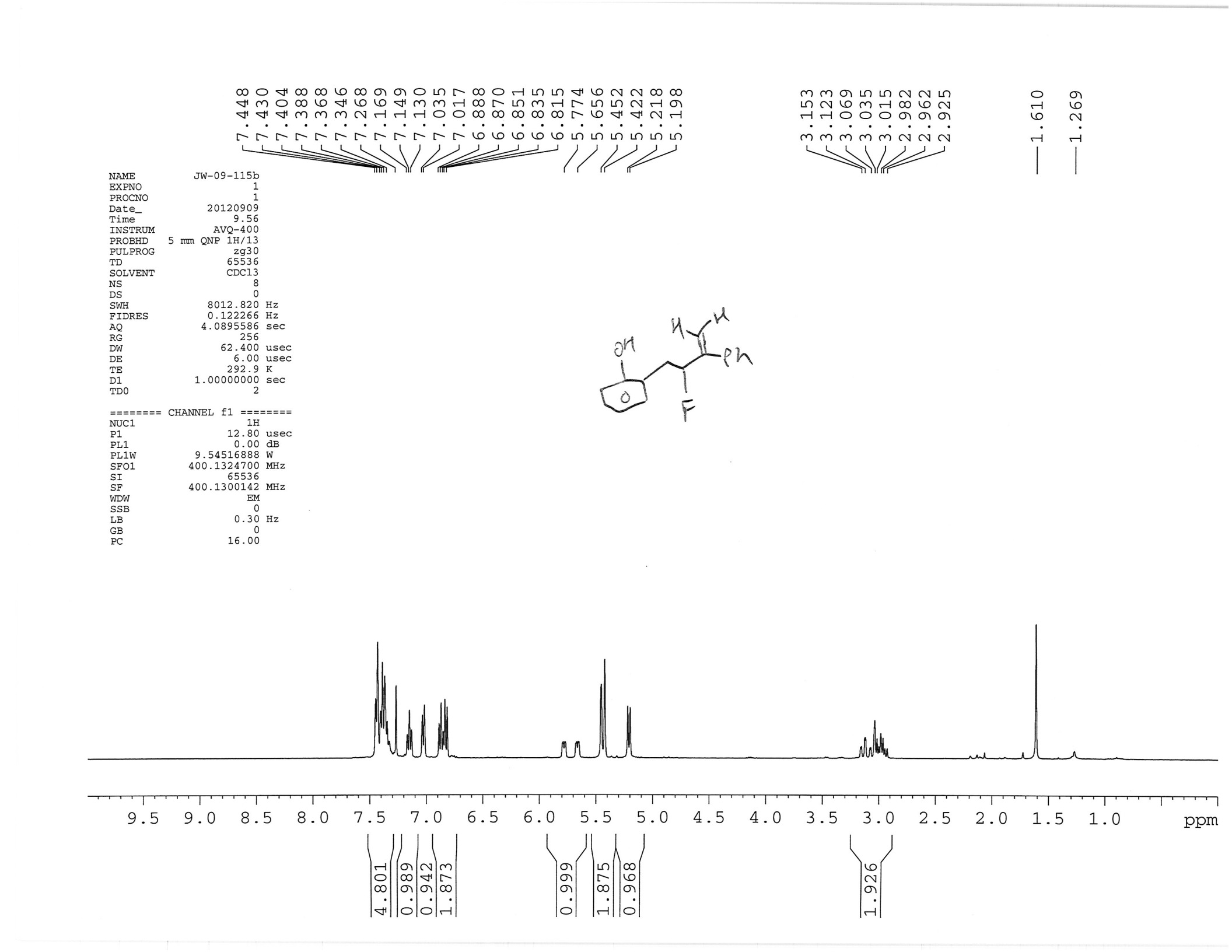
Current Data Parameters
NAME JW-09-114
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121004
Time 17.05
INSTRUM AVB-400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 73
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 297.1 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1000

======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz

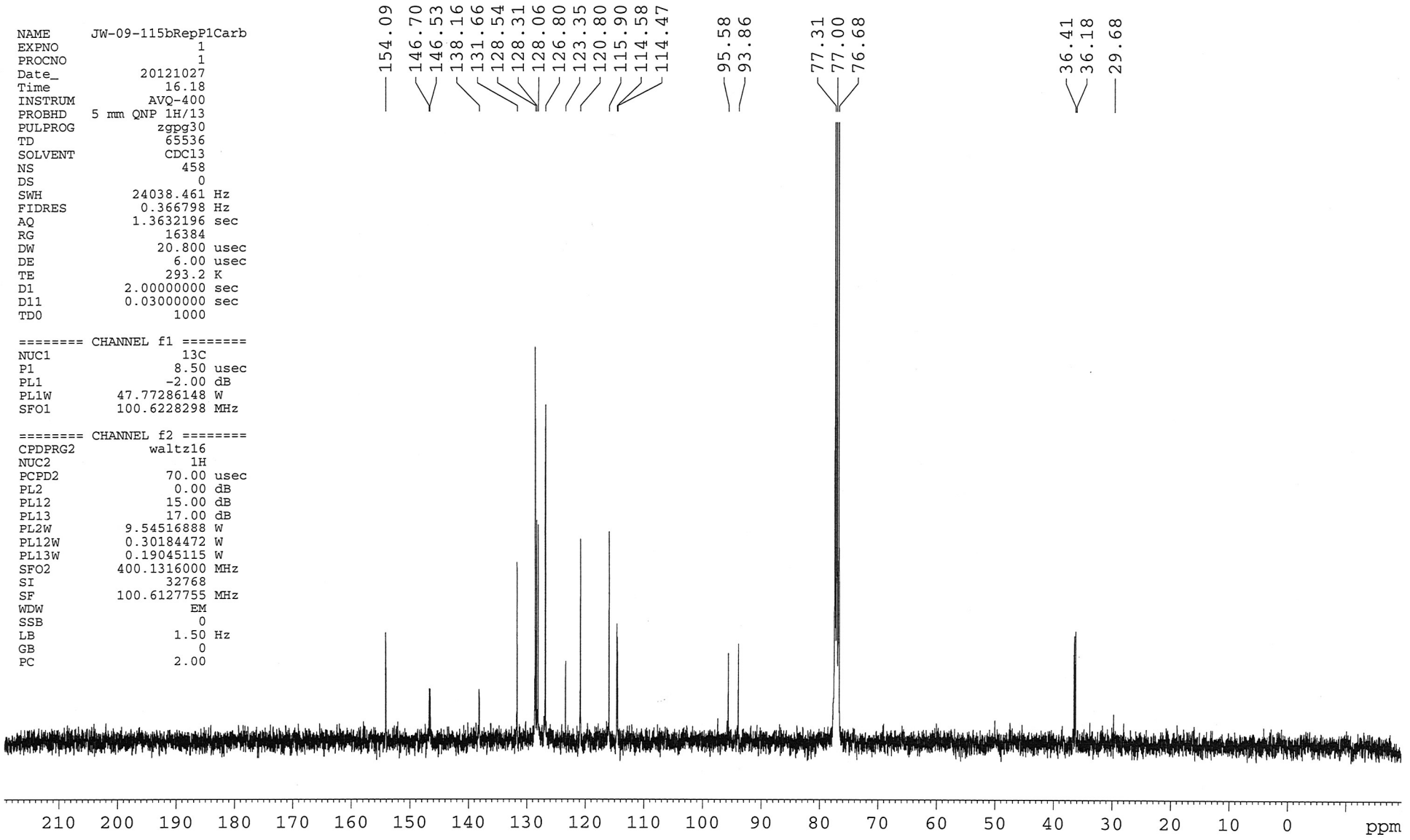
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.00 dB
PL12 16.00 dB
PL13 16.00 dB
PL2W 23.05461311 W
PL12W 0.29024038 W
PL13W 0.29024038 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40


7.448
7.430
7.404
7.388
7.368
7.346
7.268
7.169
7.149
7.130
7.035
7.017
6.888
6.870
6.851
6.835
6.815
5.774
5.656
5.452
5.422
5.218
5.198
3.153
3.123
3.069
3.035
3.015
2.982
2.962
2.925
1.610
1.269
NAME JW-09-115b
EXPNO 1
PROCNO 1
Date_ 20120909
Time 9.56
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 256
DW 62.400 usec
DE 6.00 usec
TE 292.9 K
D1 1.00000000 sec
TD0 2
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 16.00
OH
H
H
Ph
O
F
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
ppm
4.801
0.989
0.942
1.873
0.999
1.875
0.968
1.926

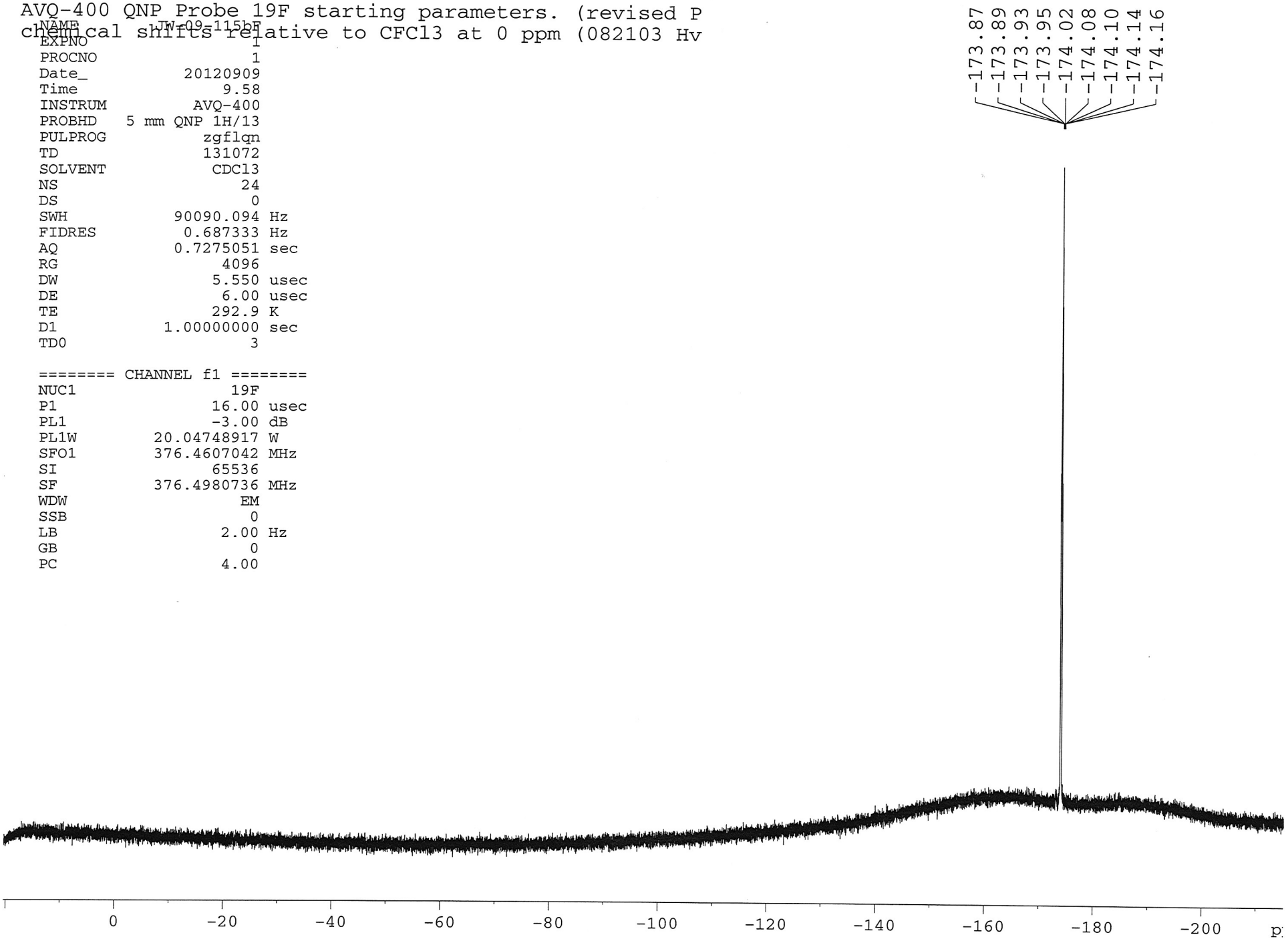
55b rep AVQ-400 QNP Carbon Starting parameters 7/16/03 revised 7/2

NAME	JW-09-115bRepP1Carb
EXPNO	1
PROCNO	1
Date_	20121027
Time	16.18
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	458
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3632196 sec
RG	16384
DW	20.800 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1000
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	17.00 dB
PL2W	9.54516888 W
PL12W	0.30184472 W
PL13W	0.19045115 W
SFO2	400.1316000 MHz
SI	32768
SF	100.6127755 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	2.00

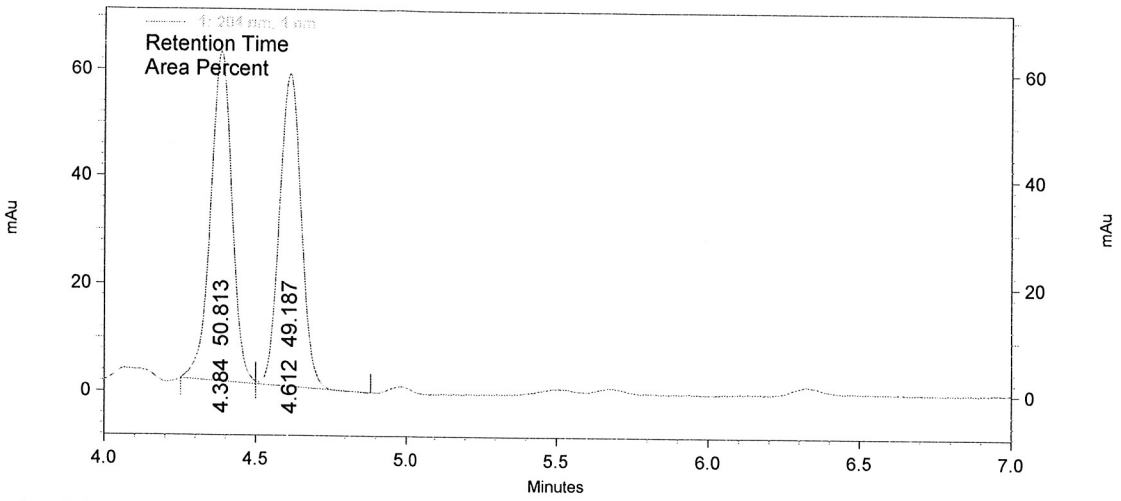


AVQ-400 QNP Probe 19F starting parameters. (revised P
chemical shifts relative to CFCl3 at 0 ppm (082103 Hv

NAME	JW-09-115bF	
EXPNO	1	
PROCNO	1	
Date_	20120909	
Time	9.58	
INSTRUM	AVQ-400	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgflqn	
TD	131072	
SOLVENT	CDCl3	
NS	24	
DS	0	
SWH	90090.094	Hz
FIDRES	0.687333	Hz
AQ	0.7275051	sec
RG	4096	
DW	5.550	usec
DE	6.00	usec
TE	292.9	K
D1	1.00000000	sec
TD0	3	
======== CHANNEL f1 ========		
NUC1	19F	
P1	16.00	usec
PL1	-3.00	dB
PL1W	20.04748917	W
SFO1	376.4607042	MHz
SI	65536	
SF	376.4980736	MHz
WDW	EM	
SSB	0	
LB	2.00	Hz
GB	0	
PC	4.00	



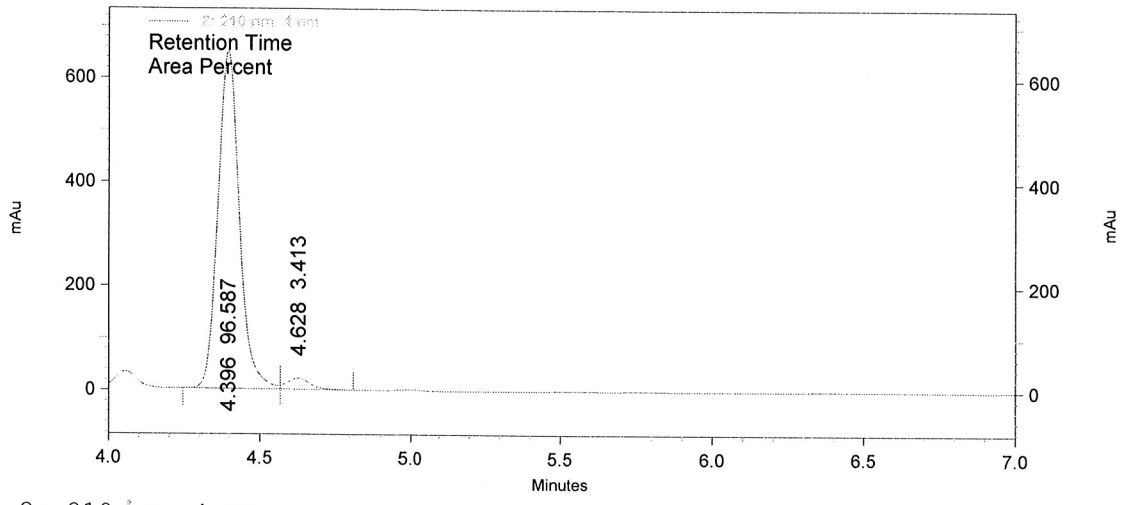
JW-09-115rac- IC9406



1: 204 nm, 4 nm
Results

Pk #	Retention Time	Area Percent	Lambda Max
1	4.384	50.813	205
2	4.612	49.187	205

JW-09-115B- IC9406

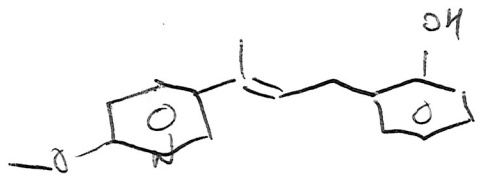


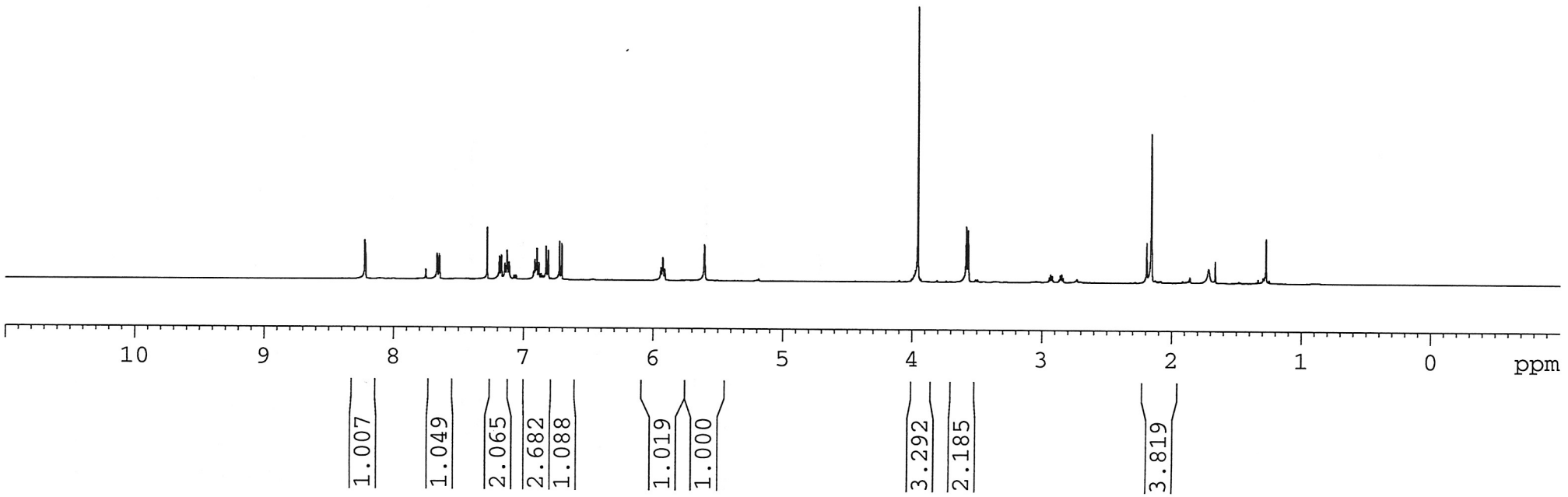
2: 210 nm, 4 nm
Results

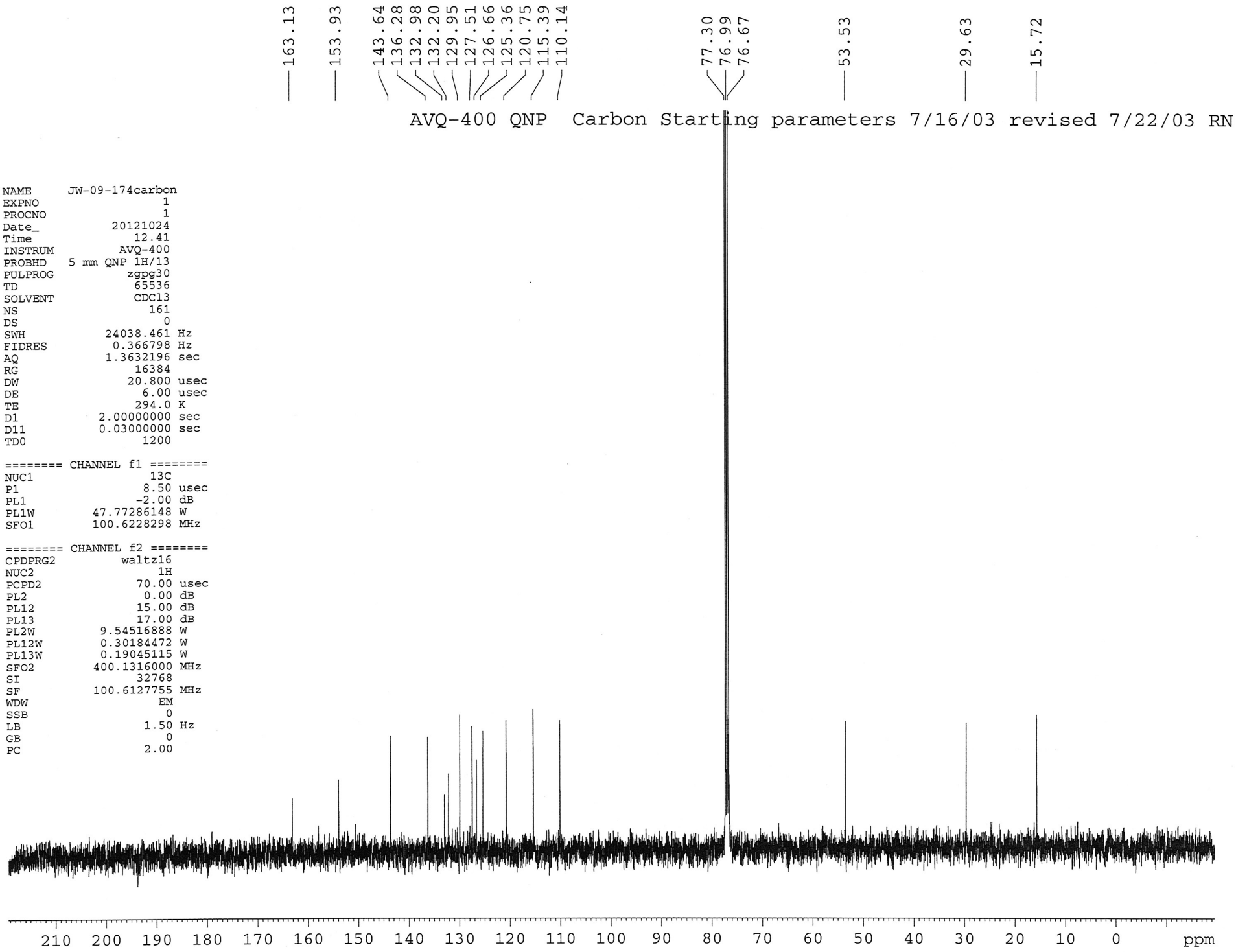
Pk #	Retention Time	Area Percent	Lambda Max
1	4.396	96.587	205
2	4.628	3.413	205

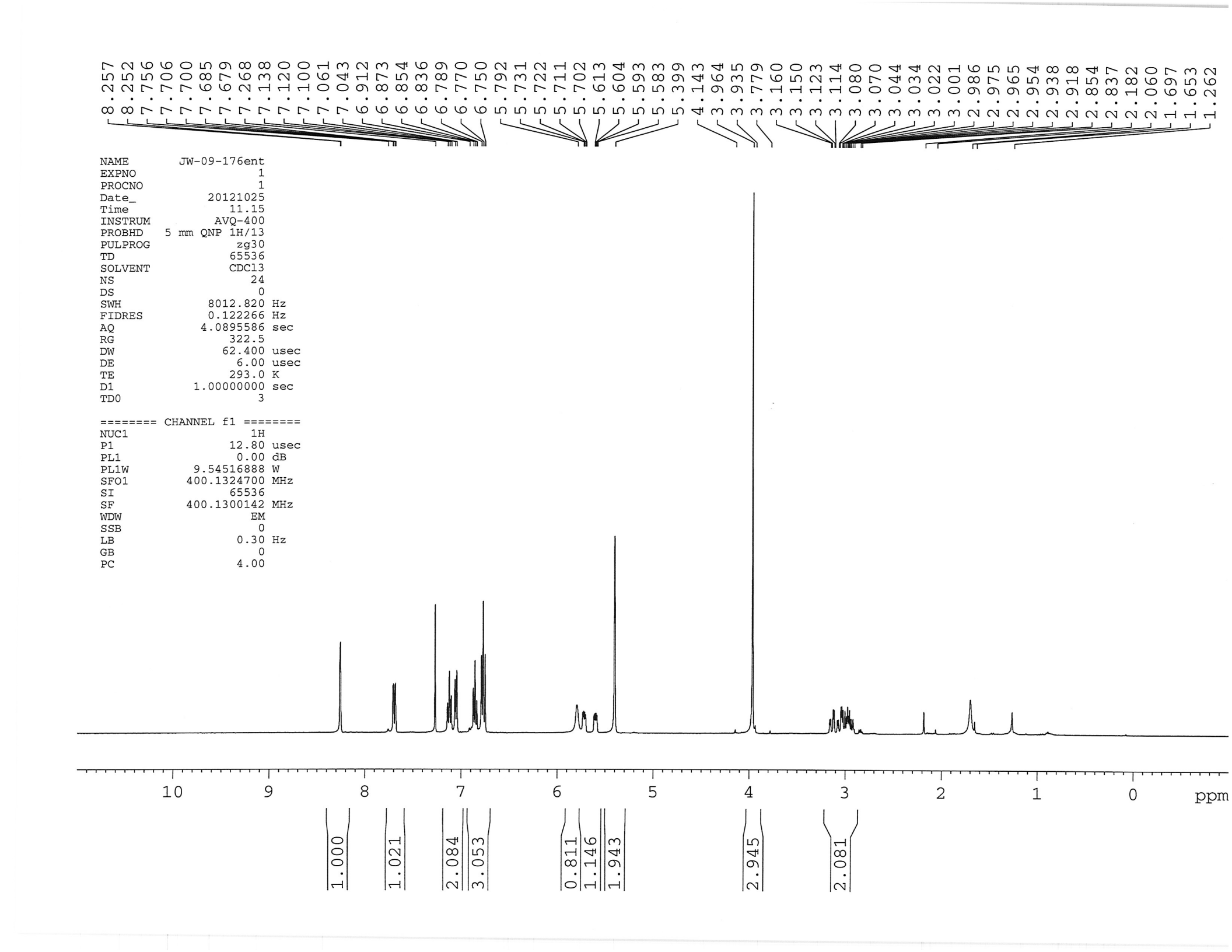
8.221 8.216 7.750 7.666 7.661 7.649 7.644 7.279 7.185 7.170 7.143 7.128 7.112 7.073 7.058 6.921 6.912 6.897 6.882 6.867 6.852 6.827 6.811 6.723 6.706 5.938 5.926 5.924 5.911 5.604 3.985 3.972 3.954 3.931 3.581 3.566 3.509 3.494 2.942 2.932 2.920 2.912 2.866 2.859 2.847 2.836 2.729 2.191 2.155 2.126 1.873 1.859 1.714 1.663 1.334 1.295 1.283 1.272 1.248

NAME	JW-09-174P1
EXPNO	1
PROCNO	1
Date_	20121024
Time	11.41
INSTRUM	AV-500
PROBHD	5 mm TBI 1H/31
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	24
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	128
DW	48.400 usec
DE	6.00 usec
TE	293.7 K
D1	0.10000000 sec
TD0	3
======== CHANNEL f1 ========	
NUC1	1H
P1	7.30 usec
PL1	0.00 dB
PL1W	12.55943203 W
SFO1	500.2330889 MHz
SI	65536
SF	500.2300165 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00



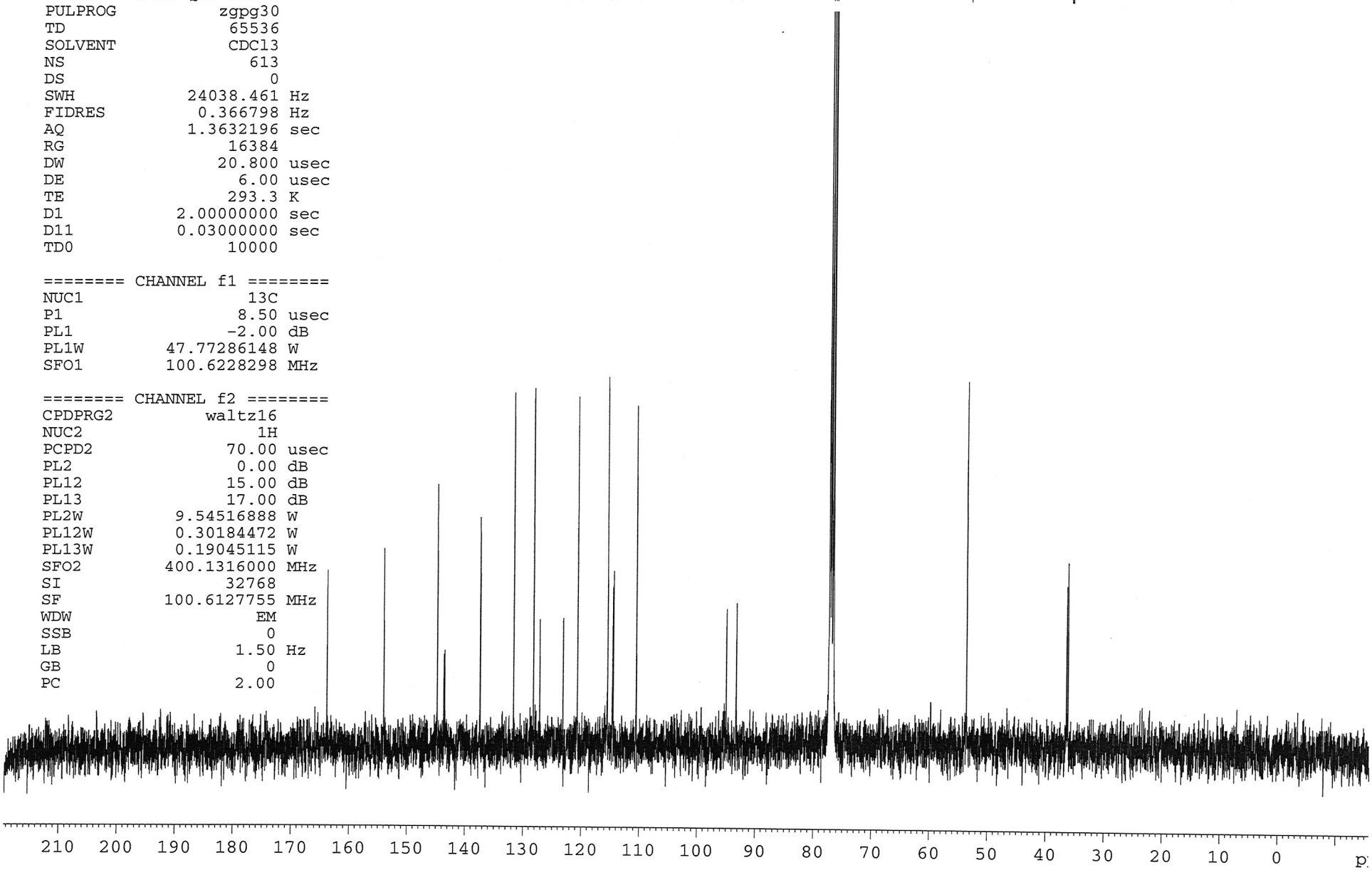



163.13
153.93
143.64
136.28
132.98
132.20
129.95
127.51
126.66
125.36
120.75
115.39
110.14
77.30
76.99
76.67
53.53
29.63
15.72
AVQ-400 QNP Carbon Starting parameters 7/16/03 revised 7/22/03 RN
NAME JW-09-174carbon
EXPNO 1
PROCNO 1
Date_ 20121024
Time 12.41
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 161
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 16384
DW 20.800 usec
DE 6.00 usec
TE 294.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1200
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 17.00 dB
PL2W 9.54516888 W
PL12W 0.30184472 W
PL13W 0.19045115 W
SFO2 400.1316000 MHz
SI 32768
SF 100.6127755 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 2.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.257
8.252
7.756
7.706
7.700
7.685
7.679
7.268
7.138
7.120
7.100
7.061
7.043
6.912
6.873
6.854
6.836
6.789
6.770
6.750
5.792
5.731
5.722
5.711
5.702
5.613
5.604
5.593
5.583
5.399
4.143
3.964
3.935
3.779
3.160
3.150
3.123
3.114
3.080
3.070
3.044
3.034
3.022
3.001
2.986
2.975
2.965
2.954
2.938
2.918
2.854
2.837
2.182
2.060
1.697
1.653
1.262
NAME JW-09-176ent
EXPNO 1
PROCNO 1
Date_ 20121025
Time 11.15
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 322.5
DW 62.400 usec
DE 6.00 usec
TE 293.0 K
D1 1.00000000 sec
TD0 3
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.021
2.084
3.053
0.811
1.146
1.943
2.945
2.081

176 AVQ-400 QNP Carbon Starting parameters 7/16/03 r

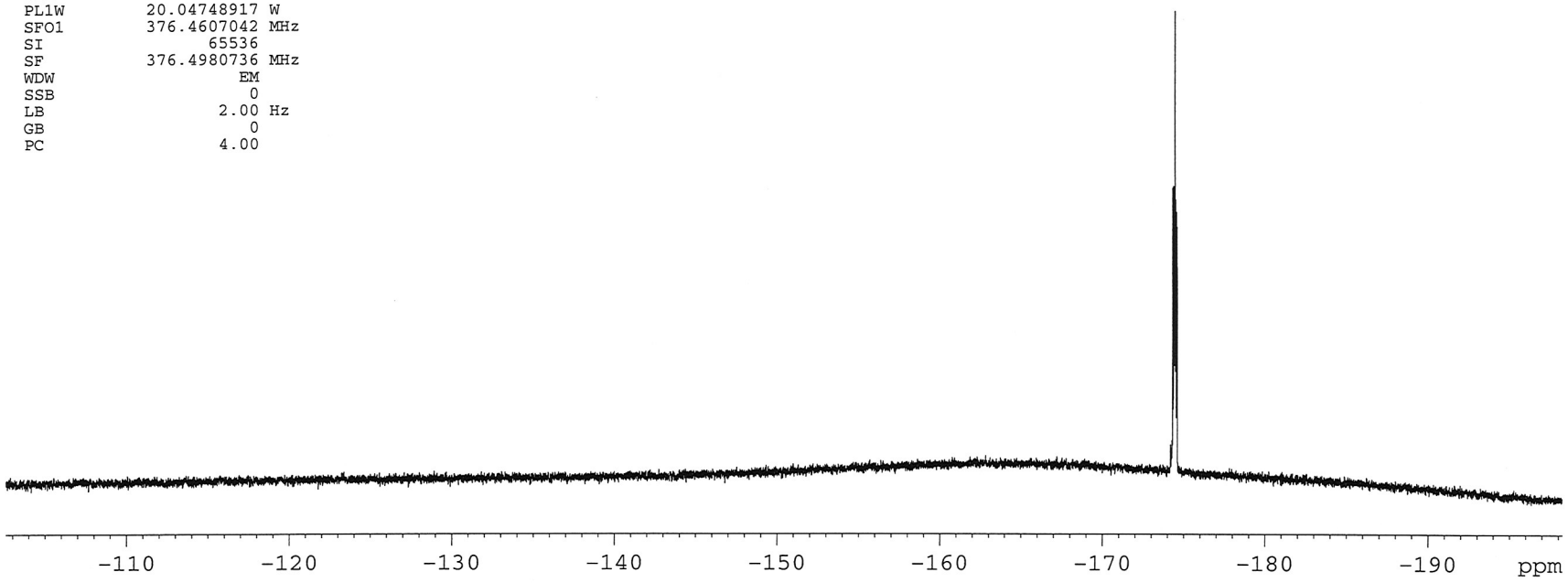
NAME	JW-09-176carb
EXPNO	1
PROCNO	1
Date_	20121025
Time	13.07
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	613
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3632196 sec
RG	16384
DW	20.800 usec
DE	6.00 usec
TE	293.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10000
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	17.00 dB
PL2W	9.54516888 W
PL12W	0.30184472 W
PL13W	0.19045115 W
SFO2	400.1316000 MHz
SI	32768
SF	100.6127755 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	2.00



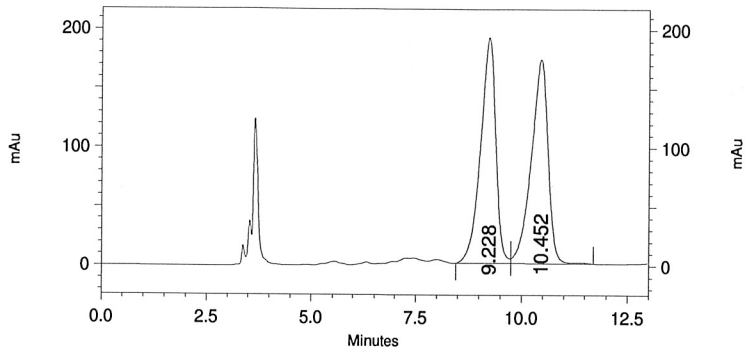
AVQ-400 QNP Probe 19F starting parameters. (revised P1, 2/12/04 RN)
chemical shifts relative to CFCl3 at 0 ppm (082103 HvH)
sw 239.28 ppm; o1p 0 ppm

NAME	JW-09-176Fent
EXPNO	1
PROCNO	1
Date_	20121025
Time	11.18
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	18
DS	0
SWH	90090.094 Hz
FIDRES	0.687333 Hz
AQ	0.7275051 sec
RG	4597.6
DW	5.550 usec
DE	6.00 usec
TE	293.0 K
D1	1.00000000 sec
TD0	3
======== CHANNEL f1 ========	
NUC1	19F
P1	16.00 usec
PL1	-3.00 dB
PL1W	20.04748917 W
SFO1	376.4607042 MHz
SI	65536
SF	376.4980736 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	4.00

-174.32
-174.37
-174.41
-174.45
-174.50
-174.53
-174.58



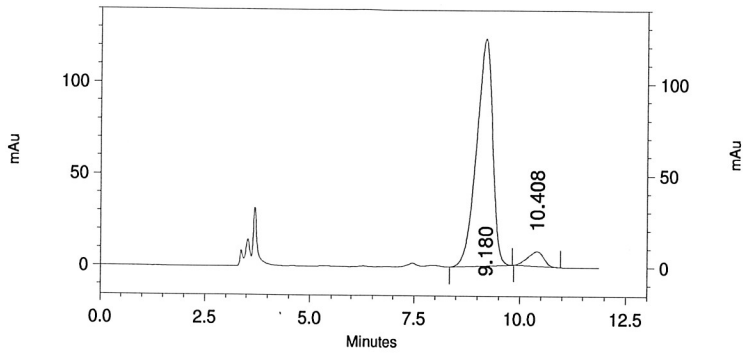
JW-09-176rac



1: 222 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
9.228	4754400	50.011	205
10.452	4752224	49.989	205

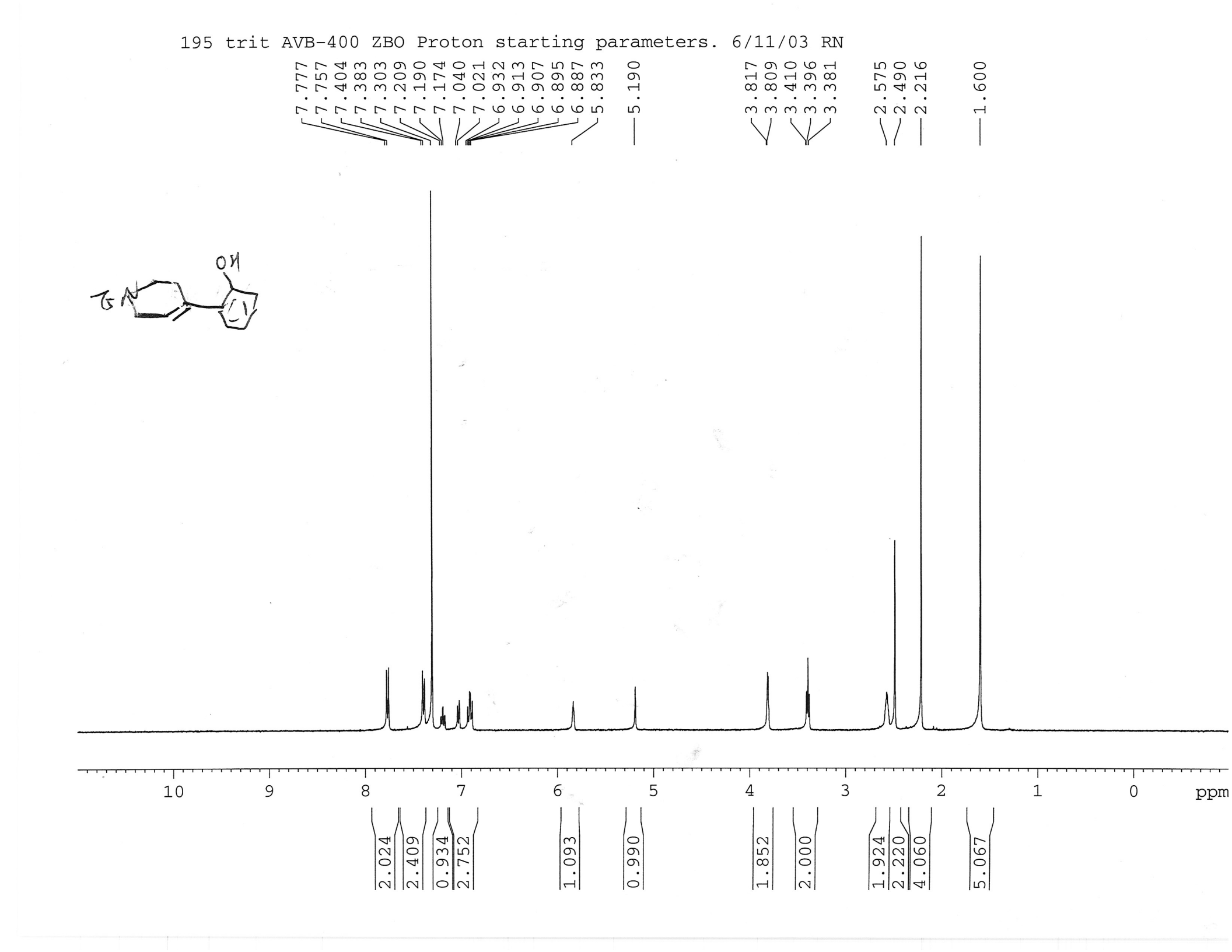
JW-09-176ent



1: 222 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
9.180	3250038	93.910	245
10.408	210767	6.090	246

195 trit AVB-400 ZBO Proton starting parameters. 6/11/03 RN



152.22
143.92
134.01
133.09
129.81
128.90
128.32
127.79
122.45
121.08
120.55
115.80
115.46

77.39
77.07
76.75

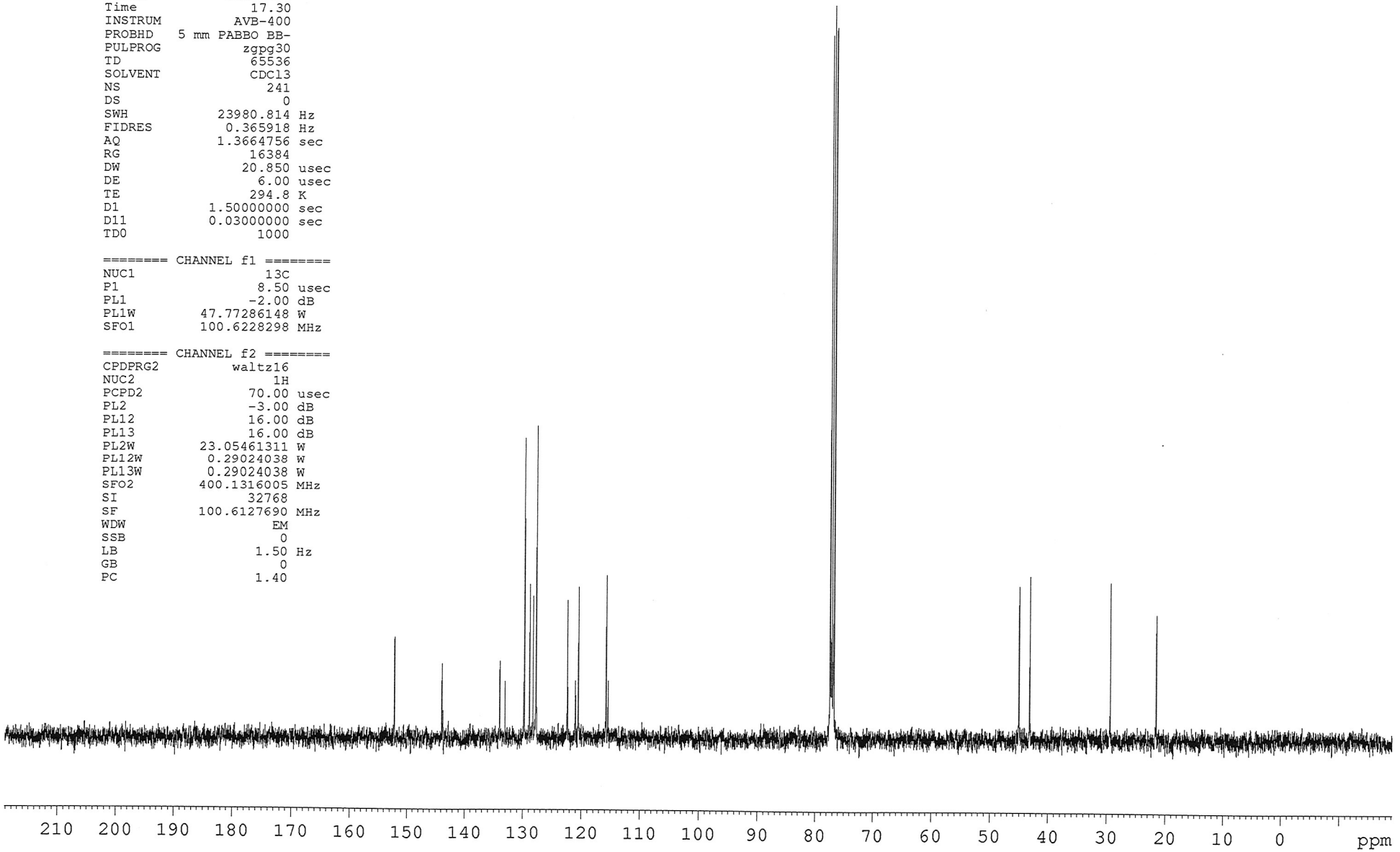
45.02
43.15

29.42

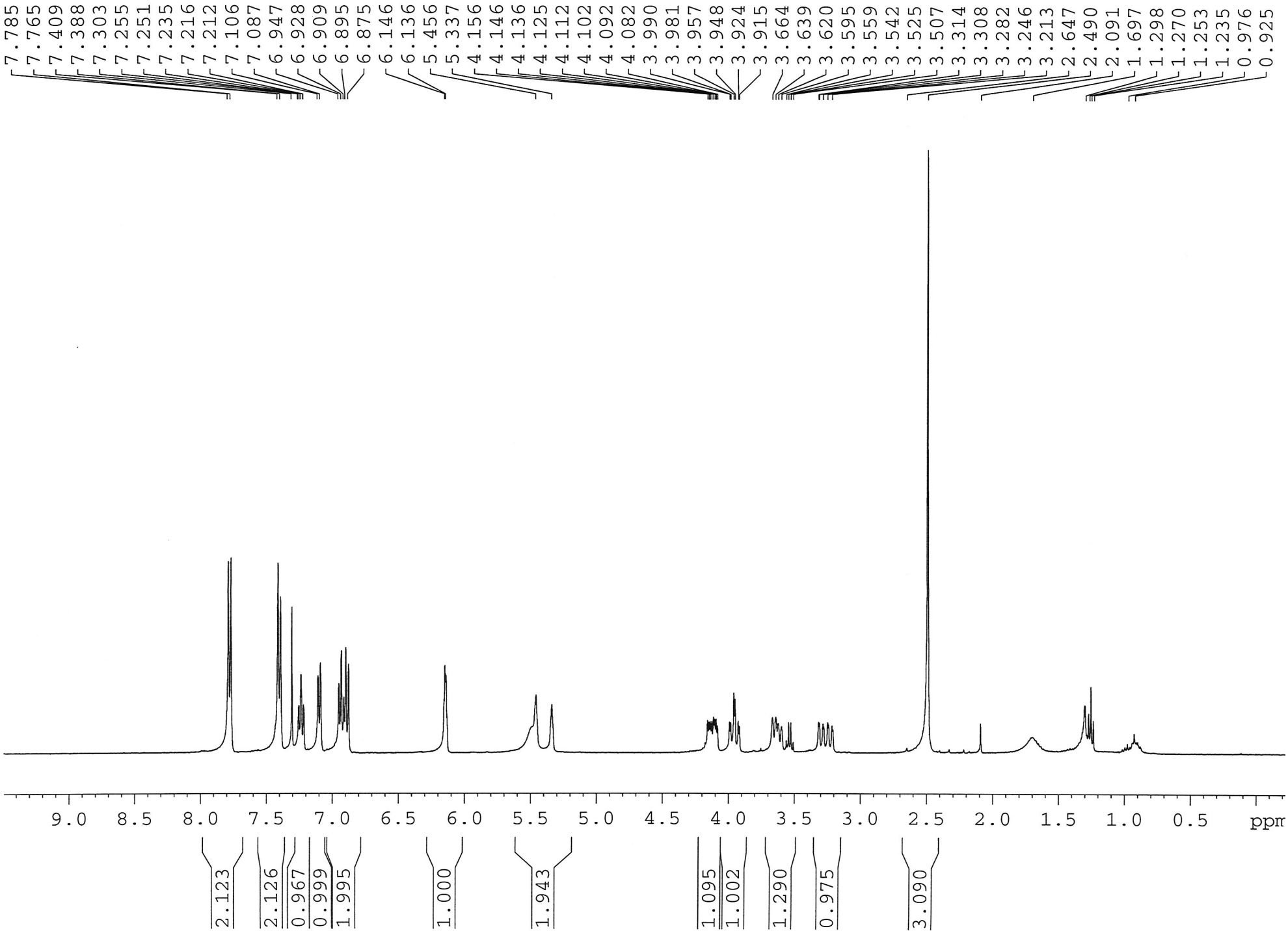
21.58

199 AVB-400 ZBO Carbon Starting paramters 6/11/03

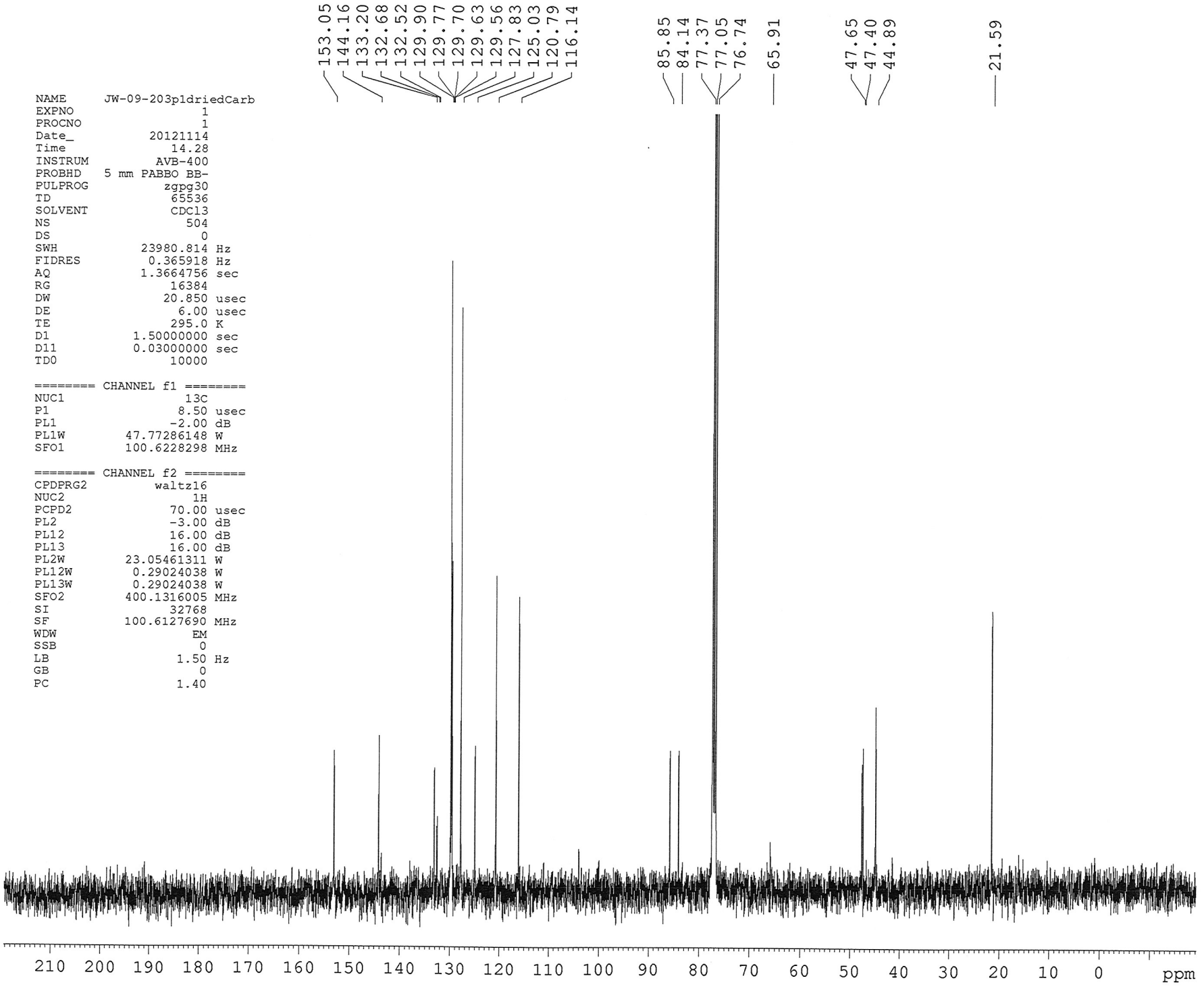
NAME	JW-09-199carb
EXPNO	1
PROCNO	1
Date_	20121114
Time	17.30
INSTRUM	AVB-400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	241
DS	0
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	16384
DW	20.850 usec
DE	6.00 usec
TE	294.8 K
D1	1.50000000 sec
D11	0.03000000 sec
TD0	1000
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	-3.00 dB
PL12	16.00 dB
PL13	16.00 dB
PL2W	23.05461311 W
PL12W	0.29024038 W
PL13W	0.29024038 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	1.40



203 AVB-400 ZBO Proton starting parameters. 6/11/03 RN



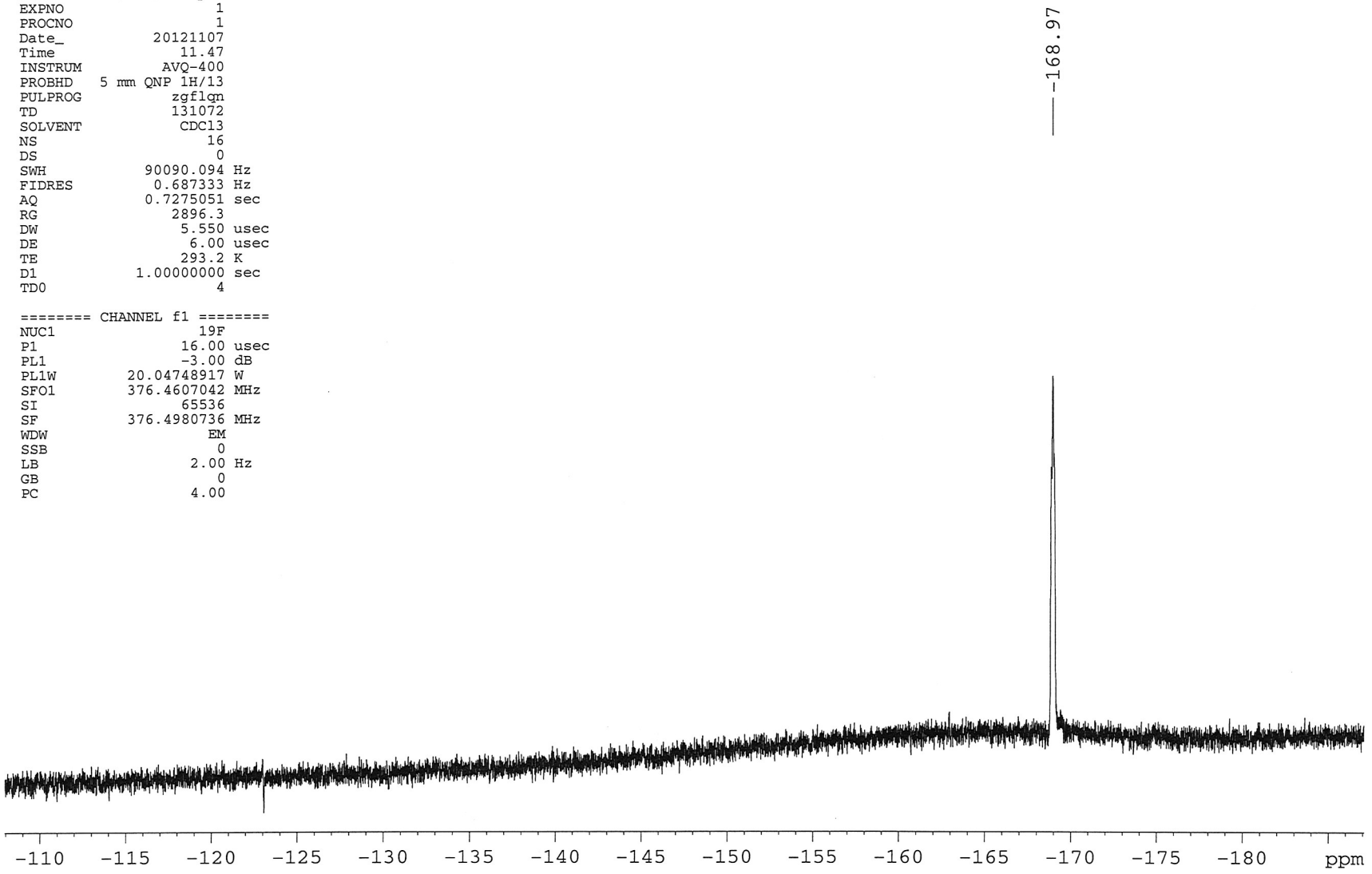
203 AVB-400 ZBO Carbon Starting paramters 6/11/03

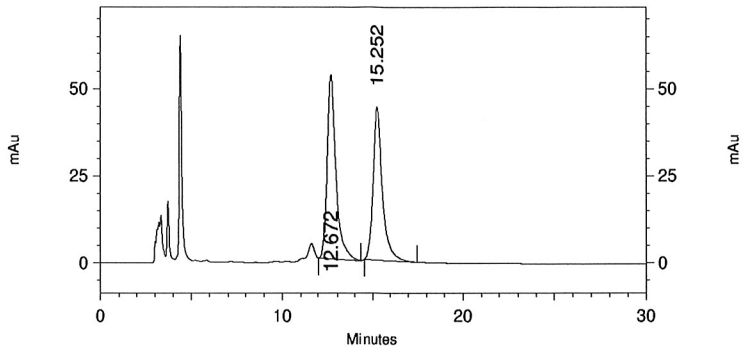


NAME	JW-09-203p1driedCarb
EXPNO	1
PROCNO	1
Date_	20121114
Time	14.28
INSTRUM	AVB-400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	504
DS	0
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	16384
DW	20.850 usec
DE	6.00 usec
TE	295.0 K
D1	1.50000000 sec
D11	0.03000000 sec
TD0	10000
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	-3.00 dB
PL12	16.00 dB
PL13	16.00 dB
PL2W	23.05461311 W
PL12W	0.29024038 W
PL13W	0.29024038 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	1.40

AVQ-400 QNP Probe 19F starting parameters. (revised P1, 2/12/04 RN)
chemical shifts relative to CFCl3 at 0 ppm (082103 HvH)
sw 239.28 ppm; o1p 0 ppm

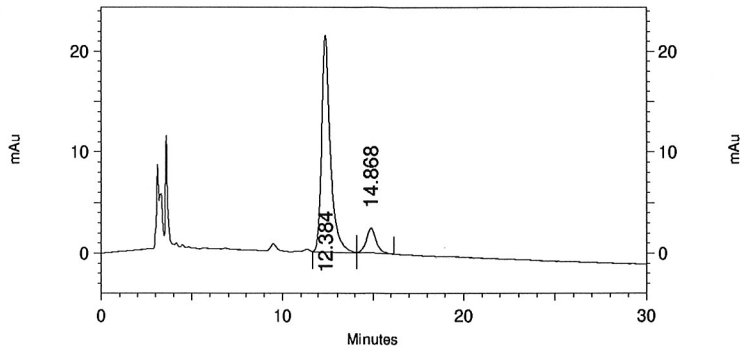
NAME	JW-09-198p1F	
EXPNO	1	
PROCNO	1	
Date_	20121107	
Time	11.47	
INSTRUM	AVQ-400	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgflqn	
TD	131072	
SOLVENT	CDCl3	
NS	16	
DS	0	
SWH	90090.094	Hz
FIDRES	0.687333	Hz
AQ	0.7275051	sec
RG	2896.3	
DW	5.550	usec
DE	6.00	usec
TE	293.2	K
D1	1.00000000	sec
TD0	4	
======== CHANNEL f1 ========		
NUC1	19F	
P1	16.00	usec
PL1	-3.00	dB
PL1W	20.04748917	W
SFO1	376.4607042	MHz
SI	65536	
SF	376.4980736	MHz
WDW	EM	
SSB	0	
LB	2.00	Hz
GB	0	
PC	4.00	





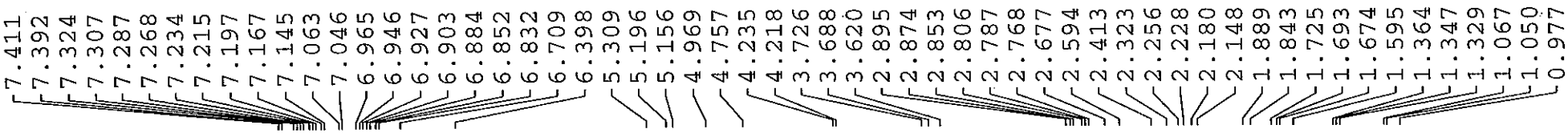
1: 223 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
12.672	1731570	50.077	208
15.252	1726247	49.923	208



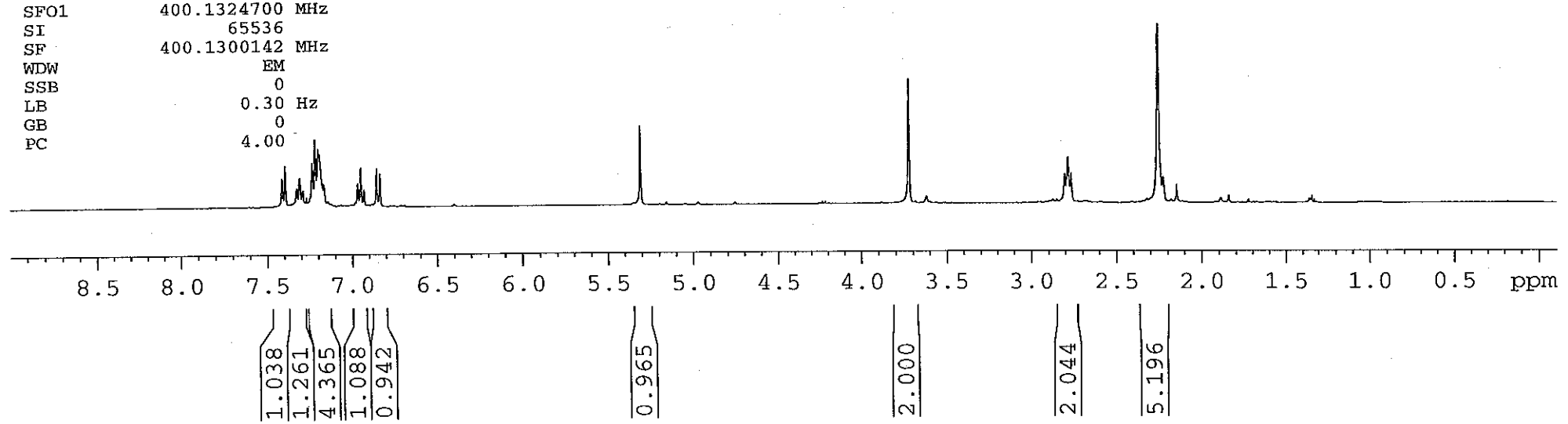
1: 223 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
12.384	685715	88.375	207
14.868	90201	11.625	206



NAME	JW-10-40-pH
EXPNO	1
PROCNO	1
Date_	20130108
Time	11.43
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0895586 sec
RG	45.3
DW	62.400 usec
DE	6.00 usec
TE	292.8 K
D1	1.00000000 sec
TD0	2

======== CHANNEL f1 ========	
NUC1	1H
P1	12.80 usec
PL1	0.00 dB
PL1W	9.54516888 W
SFO1	400.1324700 MHz
SI	65536
SF	400.1300142 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00



AVQ-400 QNP Carbon Starting parameters 7/16/03 revised 7/22/03 RN

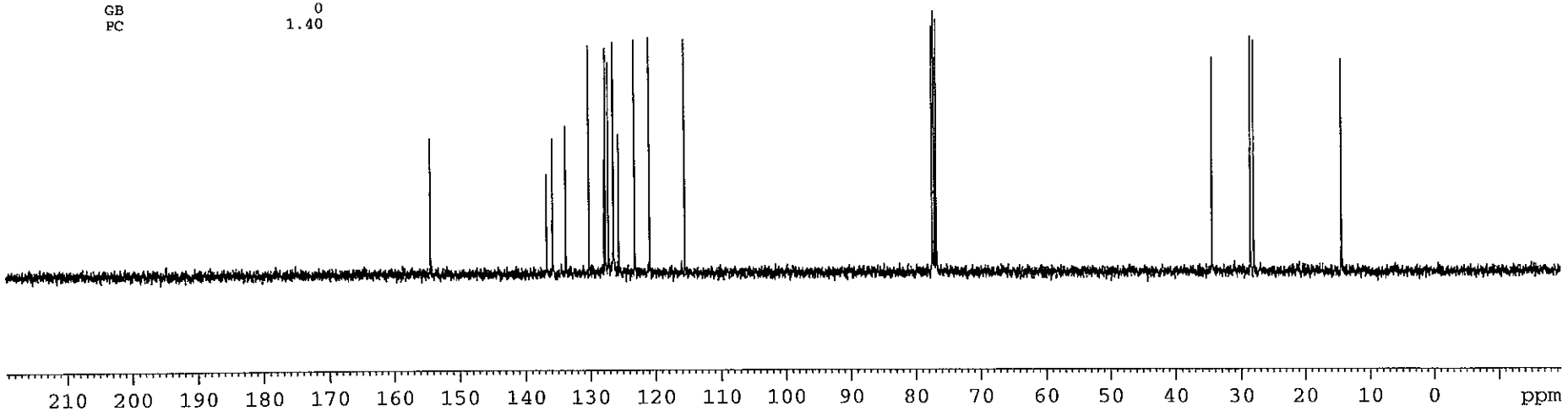
NAME	JW-10-40p1Carbon
EXPNO	1
PROCNO	1
Date_	20130108
Time	11.55
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	59
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3632196 sec
RG	16384
DW	20.800 usec
DE	6.00 usec
TE	292.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	11000
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	17.00 dB
PL2W	9.54516888 W
PL12W	0.30184472 W
PL13W	0.19045115 W
SFO2	400.1316000 MHz
SI	32768
SF	100.6127755 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	1.40

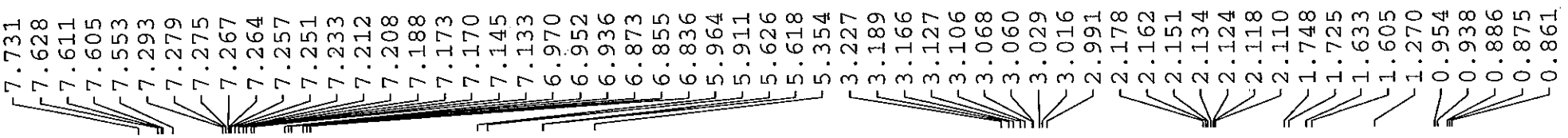
154.37 136.74 135.79 133.76 130.18 127.85 127.60 127.17 126.45 126.34 125.56 123.13 120.85 115.98 115.54

77.42 77.11 76.79

34.43 28.55 28.05

14.45

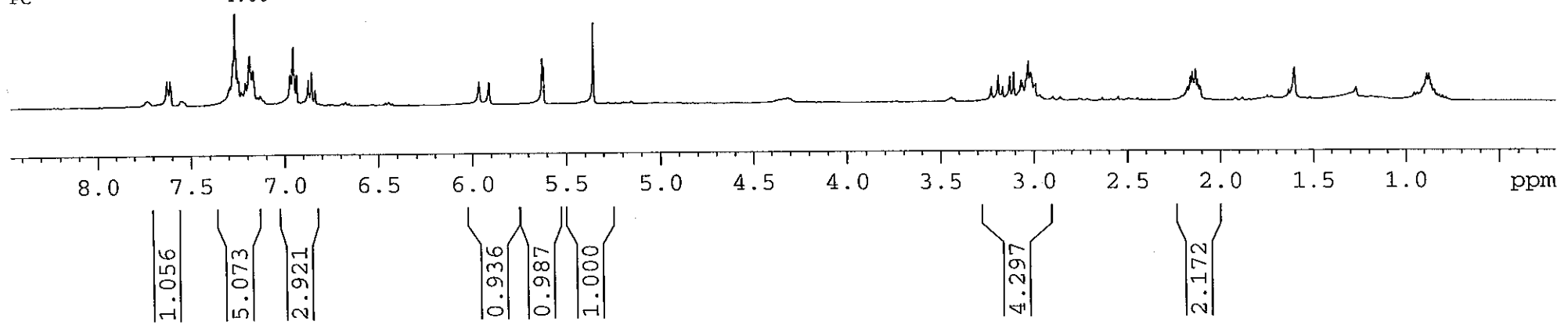




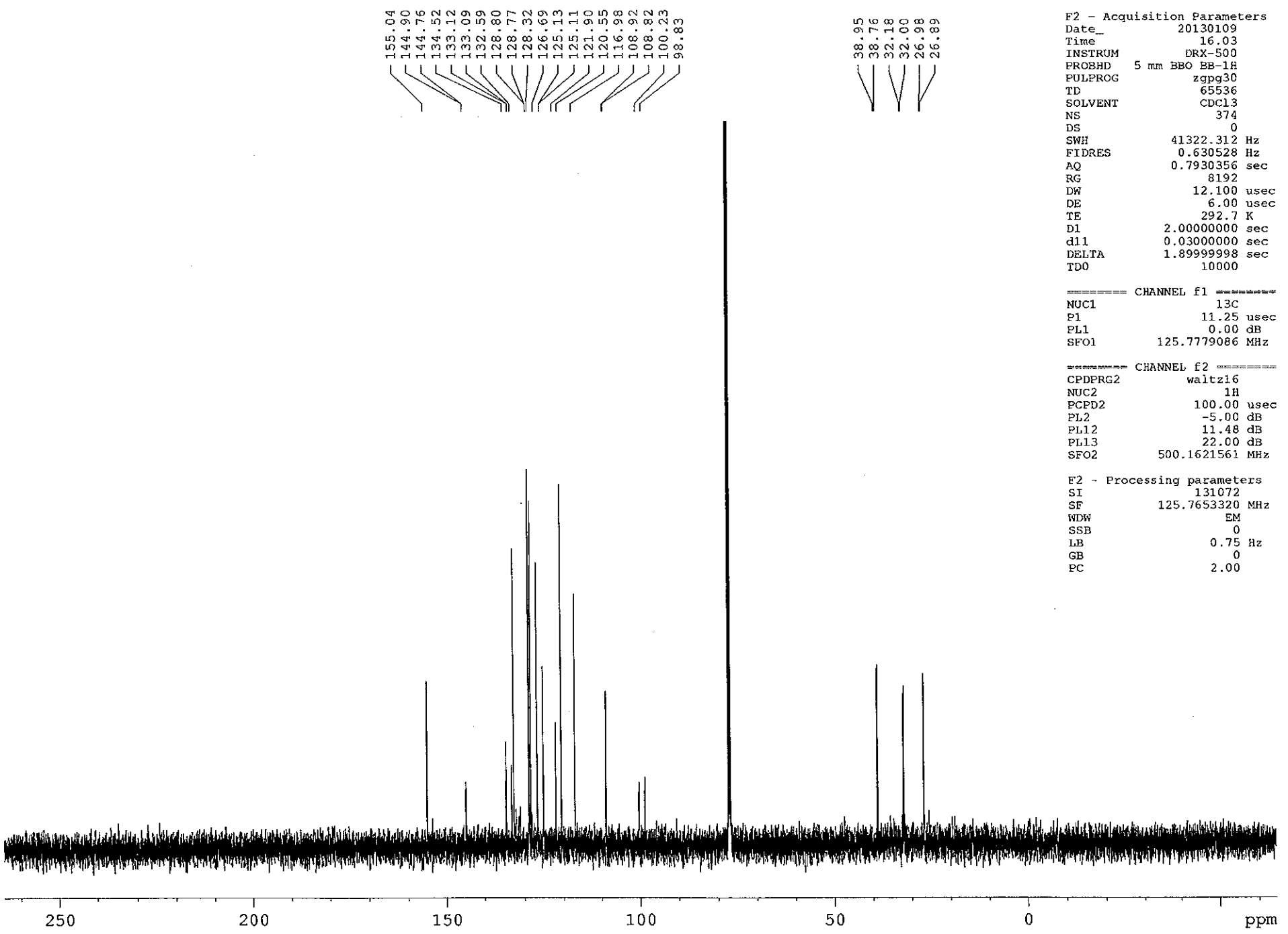
NAME	JW-10-41p1
EXPNO	1
PROCNO	1
Date_	20130109
Time	13.58
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	27
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0895586 sec
RG	228.1
DW	62.400 usec
DE	6.00 usec
TE	293.1 K
D1	1.00000000 sec
TD0	4

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

NUC1	1H
P1	12.80 usec
PL1	0.00 dB
PL1W	9.54516888 W
SFO1	400.1324700 MHz
SI	65536
SF	400.1300142 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00



DRX-500 5mm ZBO probe 13C starting parameters. Rev 6/12/12 CGC
With CPD proton decoupling. Use ns*td0 scans



Current Data Parameters

NAME	JW-10-41Carbon
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20130109
Time	16.03
INSTRUM	DRX-500
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	374
DS	0
SWH	41322.312 Hz
FIDRES	0.630528 Hz
AQ	0.7930356 sec
RG	8192
DW	12.100 usec
DE	6.00 usec
TE	292.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	10000

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

NUC1	13C
P1	11.25 usec
PL1	0.00 dB
SFO1	125.7779086 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-5.00 dB
PL12	11.48 dB
PL13	22.00 dB
SFO2	500.1621561 MHz

F2 - Processing parameters

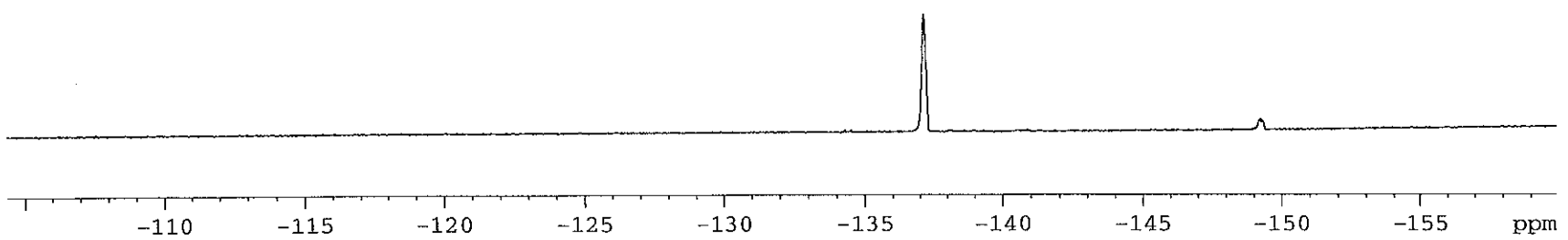
SI	131072
SF	125.7653320 MHz
WDW	EM
SSB	0
LB	0.75 Hz
GB	0
PC	2.00

AVQ-400 QNP Probe 19F starting parameters. (revised P1, 2/12/04 RN)
chemical shifts relative to CFCl3 at 0 ppm (082103 HvH)
sw 239.28 ppm; o1p 0 ppm

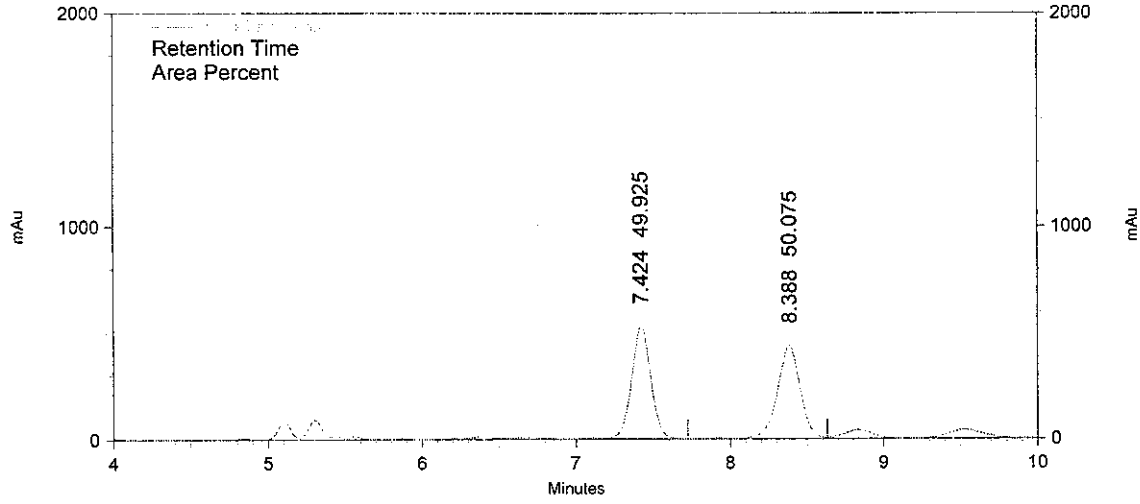
NAME	JW-10-41p1F-100	
EXPNO	1	
PROCNO	1	
Date_	20130109	
Time	13.55	
INSTRUM	AVQ-400	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgflqn	
TD	131072	
SOLVENT	CDCl3	
NS	32	
DS	0	
SWH	90090.094	Hz
FIDRES	0.687333	Hz
AQ	0.7275051	sec
RG	3251	
DW	5.550	usec
DE	6.00	usec
TE	293.1	K
D1	1.00000000	sec
TD0	4	
======== CHANNEL f1 ========		
NUC1	19F	
P1	16.00	usec
PL1	-3.00	dB
PL1W	20.04748917	W
SFO1	376.4607042	MHz
SI	65536	
SF	376.4980736	MHz
WDW	EM	
SSB	0	
LB	2.00	Hz
GB	0	
PC	4.00	

-137.12
-137.15
-137.18
-137.21
-137.26

-149.25



JW-10-41rac

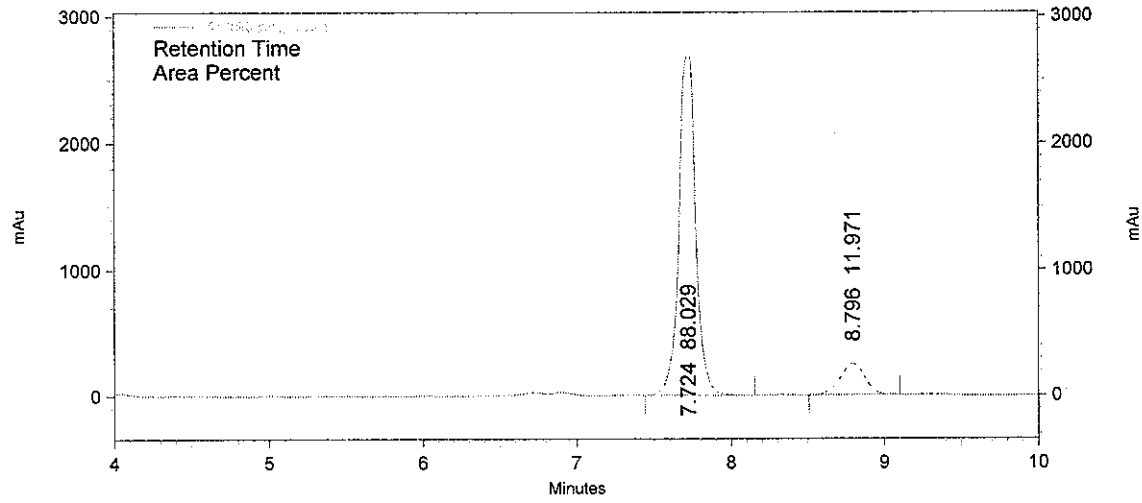


1: 190 nm, 4 nm

Results

Pk #	Retention Time	Area Percent	Lambda Max
1	7.424	49.925	203
2	8.388	50.075	203

JW-10-41



1: 190 nm, 4 nm

Results

Pk #	Retention Time	Area Percent	Lambda Max
1	7.724	88.029	247
2	8.796	11.971	203