
Supporting Information

Novel Synthesis of (Z)-Difluoroacrylates *via* Highly Stereoselective Addition-elimination Reaction

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Experimental section

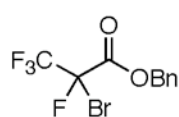
1. General Method.

All reactions were carried out in an oven-dried glassware under an atmosphere of argon, and all the reagents and anhydrous solvents were commercially available. The reagents were used without further purification or, if necessary, purified by distillation on appropriate drying agents. The isomeric mixtures of β -bromostyrene were employed in the reaction. Melting points were recorded on a Shimadzu MM-2 type instrument at atmospheric pressure. ^1H and ^{13}C NMR spectra were measured with a Bruker DRX-500 spectrometer operating at 500.13 MHz and 125.75 MHz, respectively. CDCl_3 was used as solvent in all NMR measurements and chemical shifts were recorded in ppm relative to internal tetramethylsilane. ^{19}F NMR spectra were measured for CDCl_3 solutions with a JEOL JNM-EX90A spectrometer operating at 84.10 MHz. All ^{19}F chemical shifts were reported in ppm relative to trichlorofluoromethane (CFCl_3) as an internal standard. IR spectra were determined with a Shimadzu FT-IR 8200 PC spectrophotometer. High resolution mass spectra were taken with a JEOL JMS-700 MS spectrometer. Elemental analyses were conducted with a Yanaco CHN CORDER MT-5 instrument. Column chromatography was carried out on silica gel (Wako gel C-200) and TLC analysis was performed on silica gel TLC plates (Merck, Silica gel 60 F₂₅₄).

2. Preparation of benzyl 2-bromo-2,3,3,3-tetrafluoropropanoate

A 50 mL-three necked round bottomed flask equipped with a magnetic stirrer bar, a thermometer, a rubber septum and an inlet tube for argon was charged with a solution of benzyl alcohol (3.244g, 30 mmol) and Et_3N (2.277 g, 22 mmol) in diethyl ether (26 mL). To this solution was slowly added 3.487 g (14 mmol) of 2-bromo-2,3,3,3-tetrafluoropropanoyl chloride in Et_2O (4 mL) *via* a syringe at 0 °C. After being stirred for 15 min. at 0 °C and then stirred for 20 h at room temperature. The reaction mixture was poured into ice-cooled water (50 mL), followed by extraction with ether (30 mL \times 5). The organic layers were dried over anhydrous sodium sulfate, filtered and concentrated with a rotary evaporator. Column chromatography of the residue using hexane/benzene (2:1) yielded pure product, benzyl 2-bromo-2,3,3,3-tetrafluoropropanoate (4.233g, 94%).

2.1. Benzyl 2-bromo-2,3,3,3-tetrafluoropropanoate

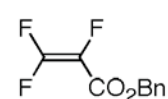


^1H NMR (CDCl_3) δ = 5.16 (s, 2H), 7.20 (s, 5H); ^{13}C NMR (CDCl_3) δ = 69.7, 88.8 (dq, J = 57.5, 272.3 Hz), 119.6 (dq, J = 29.5, 284.0 Hz), 128.3, 128.7, 129.0, 133.5, 160.5 (d, J = 26.5 Hz); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -77.99 (d, J = 8.8 Hz, 3F), -135.16 (q, J = 8.8 Hz, 1F); IR (neat) 3040 (w), 1774 (vs), 1501 (w), 1457 (w), 1304 (m), 1265 (m), 1192 (m), 1134 (s), 1018 (s), 976 (w), 918 (s) cm^{-1} ; HRMS (FAB) calcd for (M^+) $\text{C}_{10}\text{H}_7\text{F}_4\text{BrO}_2$: 313.9566, found 313.9573. Anal. Calcd for $\text{C}_{10}\text{H}_7\text{F}_4\text{BrO}_2$: C, 38.12; H, 2.24. Found: C, 38.02; H, 2.28.

3. Preparation of benzyl 2,3,3-trifluoroacrylate (1)

A 50 mL-three necked round bottomed flask equipped with a magnetic stirrer bar, a thermometer, a rubber septum and an inlet tube for argon was charged with a suspended solution of Zn dust (0.420 g, 11 mmol) in diethyl ether (16 mL). To this suspended solution was slowly added diethylaluminum chloride in hexane (0.95 mL, 1.0 mmol) and benzyl 2-bromo-2,3,3,3-tetrafluoropropanoate (3.139 g, 10 mmol) in Et_2O . After being stirred for 30 min. at room temperature, the reaction mixture was poured into an ice-cooled saturated aqueous ammonium chloride (50 mL). The resultant mixture was extracted with ether (30 mL \times 5) and the organic layers were dried over anhydrous sodium sulfate, filtered and concentrated with a rotary evaporator under reduced pressure. Column chromatography of the residue using hexane/benzene (5:1) gave pure product, benzyl 2,3,3-trifluoroacrylate.

3.1. Benzyl 2,3,3-trifluoroacrylate (1)



^1H NMR (CDCl_3) δ = 5.29 (s, 2H), 7.32~7.38 (m, 5H); ^{13}C NMR (CDCl_3) δ = 67.5, 121.6 (ddd, J = 19.2, 38.5, 238.6 Hz), 128.3, 128.6, 128.6, 134.5, 158.0 (dt, J = 41.5, 300.9 Hz), 158.7 (ddd, J = 7.7, 7.7, 26.5 Hz); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -83.95 (dd, J = 19.8, 35.2 Hz, 1F), -95.28 (dd, J = 19.8, 112.2 Hz, 1F), -184.04 (dd, J = 35.2, 112.2 Hz, 1F); IR (neat) 1747 (vs), 1396 (s), 1350 (vs), 1319 (s), 1200 (vs), 1088 (vs) cm^{-1} ; HRMS (EI) calcd for (M^+) $\text{C}_{10}\text{H}_7\text{F}_3\text{O}_2$: 216.0398, found 216.0374. Anal. Calcd for $\text{C}_{10}\text{H}_7\text{F}_3\text{O}_2$: C, 55.56; H, 3.26. Found: C, 55.68; H, 3.34.

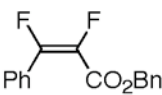
4. Typical procedure for reaction of **1** with phenylmagnesium bromide (**3a**) in the presence of a catalytic amount of CuBr

A 50 mL-three necked round bottomed flask equipped with a magnetic stirrer bar, a thermometer, a rubber septum and an inlet tube for argon was charged with a suspended solution of cuprous bromide (0.018 g, 0.125 mmol) in THF (0.5 mL). To this suspended solution was slowly dropwise added a solution of phenylmagnesium bromide (**a**, 1.5mmol) in THF at -78 °C. To the resulting solution was slowly added 0.108 g (0.50 mmol) of **1** in THF (1.5 mL) *via* a syringe at -78 °C. After being stirred for 1 h at -78 °C, the reaction mixture was poured into ice-cooled water (50 mL), followed by extraction with ether (30 mL × 5). The organic layers were dried over anhydrous sodium sulfate, filtered and concentrated with a rotary evaporator. Column chromatography of the residue using hexane/benzene (2:1) yielded pure product, benzyl 2,3-difluoro-3-phenylacrylate (**2a**). The stereoisomers of all compounds except for **2e**, **2j**, **2m**, and **2n** could not be separated by silica gel column chromatography.

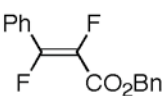
4.1. Benzyl 2,3-difluoro-3-phenylacrylate (**2a**)

M.P. 60~61 °C; IR (KBr) 3040 (w), 1736 (vs), 1666 (vs), 1447 (s), 1393 (s), 1277 (vs), 1165 (s), 1084 (vs), 1026 (s), 968 (vs), 945 (s) cm⁻¹; HRMS (EI) calcd for (M+) C₁₆H₁₂F₂O₂: 274.0805, found 274.0801. Anal. Calcd for C₁₆H₁₂F₂O₂: C, 70.07; H, 4.41. Found: C, 69.67; H, 4.27.

Z isomer

 ¹H NMR (CDCl₃) δ= 5.17 (s, 2H), 7.17-7.32 (m, 5H), 7.36~7.53 (m, 5H); ¹³C NMR (CDCl₃) δ= 67.2, 128.0, 128.5, 129.3 (dd, *J* = 3.3, 3.3 Hz), 314.1, 134.5, 135.1, 137.2 (dd, *J* = 21.9, 254.5 Hz), 156.3 (dd, *J* = 16.4, 267.1 Hz), 160.2 (dd, *J* = 8.0, 29.4 Hz); ¹⁹F NMR (CDCl₃, CFCl₃) δ= -99.88 (d, *J* = 6.6 Hz, 1F), -148.73 (d, *J* = 6.6 Hz, 1F).

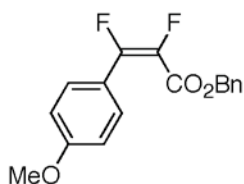
E isomer

 ¹H NMR (CDCl₃) δ= 5.15 (s, 2H), 7.15~7.32 (m, 5H), 7.34~7.51 (m, 5H); ¹³C NMR (CDCl₃) δ= 67.2, 128.0, 128.5, 129.3 (dd, *J* = 3.3, 3.3 Hz), 314.1, 134.5, 135.1, 137.2 (dd, *J* = 21.9, 254.5 Hz), 156.3 (dd, *J* = 16.4, 267.1 Hz), 160.2 (dd, *J* = 8.0, 29.4 Hz); ¹⁹F NMR (CDCl₃, CFCl₃) δ= -133.85 (d, *J* = 127.6 Hz, 1F), -162.16 (d, *J* = 127.6 Hz, 1F).

4.2. Benzyl 2,3-difluoro-3-(4-methoxyphenyl)acrylate (**2b**)

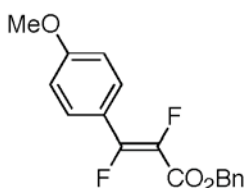
M.P. 47~49 °C; IR (KBr) 3506 (w), 1720 (vs), 1605 (vs), 1512 (s), 1462 (m), 1389 (s), 1258 (vs), 1180 (vs), 1088 (vs), 988 (m) cm^{-1} ; HRMS (EI) calcd for (M+) $\text{C}_{17}\text{H}_{14}\text{F}_2\text{O}_3$: 304.0911, found 304.0909. Anal. Calcd for $\text{C}_{17}\text{H}_{14}\text{F}_2\text{O}_3$: C, 67.10; H, 4.64. Found: C, 67.37; H, 4.57.

Z isomer



^1H NMR (CDCl_3) δ = 3.79 (s, 3H), 5.17 (s, 2H), 6.83~7.47 (m, 9H); ^{13}C NMR (CDCl_3) δ = 55.2, 67.1, 113.4, 128.3, 128.4, 128.4, 130.9, 131.0, 134.6, 136.7 (dd, J = 23.0, 253.1 Hz), 156.5 (dd, J = 16.5, 266.5 Hz), 160.4 (dd, J = 8.4, 29.0 Hz), 161.8; ^{19}F NMR (CDCl_3 , CFCl_3) δ = -99.04 (d, J = 7.7 Hz, 1F), -150.075 (d, J = 7.7 Hz, 1F).

E isomer

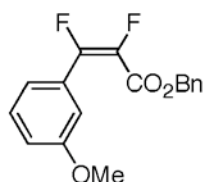


^1H NMR (CDCl_3) δ = 3.79 (s, 3H), 5.17 (s, 2H), 6.83~7.47 (m, 9H); ^{13}C NMR (CDCl_3) δ = 55.2, 67.1, 113.4, 128.3, 128.4, 128.4, 130.9, 131.0, 134.6, 136.7 (dd, J = 23.0, 253.1 Hz), 156.5 (dd, J = 16.5, 266.5 Hz), 160.4 (dd, J = 8.4, 29.0 Hz), 161.8; ^{19}F NMR (CDCl_3 , CFCl_3) δ = -133.49 (d, J = 126.5 Hz, 1F), -164.69 (d, J = 126.5 Hz, 1F).

4.3. Benzyl 2,3-difluoro-3-(3-methoxyphenyl)acrylate (**2c**)

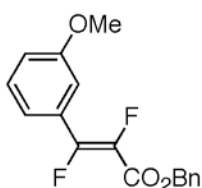
IR (KBr) 3067 (m), 2961 (m), 1732 (vs), 1686 (s), 1581 (s), 1492 (s), 1383 (s), 1294 (vs), 1165 (vs), 1095 (vs) cm^{-1} ; HRMS (FAB) calcd for (M+) $\text{C}_{17}\text{H}_{14}\text{F}_2\text{O}_3$: 304.0911, found 304.0919.

Z isomer



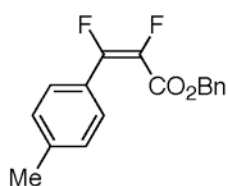
^1H NMR (CDCl_3) δ = 3.77 (s, 3H), 5.18 (s, 2H), 7.00~7.47 (m, 9H); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -99.86 (d, J = 8.5 Hz, 1F), -148.39 (d, J = 8.5 Hz, 1F).

E isomer



$^1\text{H NMR}$ (CDCl_3) δ = 3.84 (s, 3H), 5.38 (s, 2H), 7.00~7.47 (m, 9H); $^{19}\text{F NMR}$ (CDCl_3 , CFCl_3) δ = -133.32 (d, J = 127.1 Hz, 1F), -161.29 (d, J = 127.1 Hz, 1F).

4.4. Benzyl (Z)-2,3-difluoro-3-(4-methylphenyl)acrylate (**2e**)

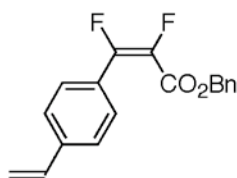


M.P. 58~59 °C; $^1\text{H NMR}$ (CDCl_3) δ = 2.38 (s, 3H), 5.17 (s, 2H), 7.16~7.20 (m, 4H), 7.30~7.42 (m, 5H); $^{13}\text{C NMR}$ (CDCl_3) δ = 21.5, 67.2, 125.0, 158.2, 128.3, 128.43, 128.5, 128.8, 129.2 (dd, J = 3.3, 3.3 Hz), 134.6, 137.0 (dd, J = 22.9, 254.3 Hz), 156.6 (dd, J = 16.3, 267.0 Hz), 160.4 (dd, J = 8.3, 29.0 Hz); $^{19}\text{F NMR}$ (CDCl_3 , CFCl_3) δ = -99.41 (d, J = 6.6 Hz, 1F), -149.46 (d, J = 6.6 Hz, 1F); IR (neat) 2920 (w), 1724 (vs), 1682 (s), 1497 (w), 1327 (s), 1281 (s), 1169 (vs), 1092 (vs), 984 (s) cm^{-1} ; HRMS (EI) calcd for (M+) $\text{C}_{17}\text{H}_{14}\text{F}_2\text{O}_2$: 288.0962, found 288.0943. Anal. Calcd for $\text{C}_{17}\text{H}_{14}\text{F}_2\text{O}_2$: C, 70.83; H, 4.89. Found: C, 71.14; H, 4.93.

4.5. Benzyl 2,3-difluoro-3-(4-vinylphenyl)acrylate (**2f**)

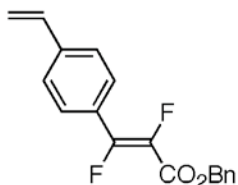
M.P. 54~55 °C; IR (KBr) 2372 (w), 1736 (vs), 1666 (s), 1454 (m), 1393 (m), 1277 (m), 1180 (m), 1084 (vs) cm^{-1} ; HRMS (FAB) calcd for (M+) $\text{C}_{18}\text{H}_{14}\text{F}_2\text{O}_2$: 300.0962, found 300.0964.

Z isomer



$^1\text{H NMR}$ (CDCl_3) δ = 5.18 (s, 2H), 5.36 (d, J = 8.5 Hz, 1H), 5.82 (d, J = 17.7 Hz, 1H), 6.71 (dd, J = 10.8 Hz, 17.7 Hz, 1H), 7.17~7.49 (m, 9H); $^{13}\text{C NMR}$ (CDCl_3) δ = 67.3, 116.1, 125.8, 128.3, 128.5, 129.6 (dd, J = 3.2, 3.2 Hz), 134.5, 135.7, 135.9, 137.2 (dd, J = 23.3, 255.0 Hz), 140.3, 140.4, 156.2 (dd, J = 16.9, 266.5 Hz), 160.2 (dd, J = 8.4, 29.1 Hz); $^{19}\text{F NMR}$ (CDCl_3 , CFCl_3) δ = -100.84 (d, J = 4.4 Hz, 1F), -148.45 (d, J = 4.4 Hz, 1F).

E isomer

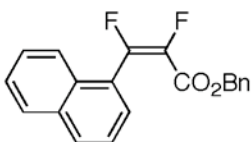


^1H NMR (CDCl_3) δ = 5.18 (s, 2H), 5.38 (d, J = 8.0 Hz, 1H), 5.86 (d, J = 17.9 Hz, 1H), 6.71 (dd, J = 10.8 Hz, 17.9 Hz, 1H), 7.17~7.49 (m, 9H); ^{13}C NMR (CDCl_3) δ = 67.2, 116.5, 126.4, 128.3, 128.5, 129.6 (dd, J = 3.2, 3.2 Hz), 134.5, 135.7, 135.9, 137.2 (dd, J = 23.3, 255.0 Hz), 140.3, 140.4, 156.2 (dd, J = 16.9, 266.5 Hz), 160.2 (dd, J = 8.4, 29.1 Hz); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -134.51 (d, J = 125.4 Hz, 1F), -161.85 (d, J = 125.4 Hz, 1F).

4.6. Benzyl 2,3-difluoro-3-(1-naphthyl)acrylate (**2h**)

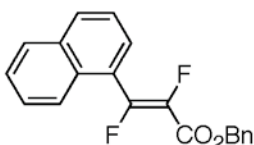
M.P. 36~38 °C; IR (KBr) 3063 (w), 2959 (w), 1732 (vs), 1686 (m), 1385 (m), 1319 (s), 1288 (m), 1169 (s), 1123 (s), 1042 (s) cm^{-1} ; HRMS (FAB) calcd for (M^+) $\text{C}_{20}\text{H}_{14}\text{F}_2\text{O}_2$: 324.0962, found 324.0965. Anal. Calcd for $\text{C}_{20}\text{H}_{14}\text{F}_2\text{O}_2$: C, 74.07; H, 4.35. Found: C, 73.97; H, 4.48.

Z isomer



^1H NMR (CDCl_3) δ = 4.94 (s, 2H), 6.76 (m, 2H), 7.11~7.22 (m, 3H), 7.39~7.42 (m, 1H), 7.51~7.55 (m, 3H), 7.86~7.93 (m, 3H); ^{13}C NMR (CDCl_3) δ = 67.2, 124.3, 124.7, 126.5, 127.4, 127.8, 128.2, 128.3, 128.5, 129.5, 131.2, 131.61, 131.64, 133.3, 134.1, 138.5 (dd, J = 21.6, 254.5 Hz), 155.0 (dd, J = 15.9, 271.3 Hz), 160.0 (dd, J = 8.4, 30.2 Hz); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -94.87 (d, J = 11.0 Hz, 1F), -147.01 (d, J = 11.0 Hz, 1F).

E isomer

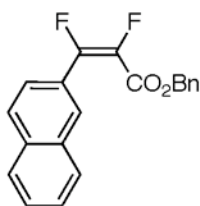


^1H NMR (CDCl_3) δ = 5.43 (s, 2H), 7.35~7.42 (m, 5H), 7.48~7.57 (m, 5H), 7.96~7.99 (m, 2H); ^{13}C NMR (CDCl_3) δ = 67.2, 124.4, 124.7, 126.5, 127.4, 127.8, 128.2, 128.3, 128.5, 129.5, 131.2, 131.61, 131.64, 133.3, 134.1, 138.5 (dd, J = 21.6, 254.5 Hz), 155.0 (dd, J = 15.9, 271.3 Hz), 160.0 (dd, J = 8.4, 30.2 Hz); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -114.56 (d, J = 137.6 Hz, 1F), -160.00 (d, J = 137.6 Hz, 1F).

4.7. Benzyl 2,3-difluoro-3-(2-naphthyl)acrylate (**2i**)

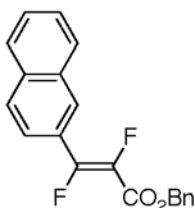
M.P. 79~80 °C; IR (KBr) 3063 (w), 1736 (s), 1678 (m), 1501 (w), 1454 (w), 1323 (m), 1231 (w), 1153 (w), 1080 (vs) cm^{-1} ; HRMS (FAB) calcd for (M⁺) $\text{C}_{20}\text{H}_{14}\text{F}_2\text{O}_2$: 324.0962, found 324.0959. Anal. Calcd for $\text{C}_{20}\text{H}_{14}\text{F}_2\text{O}_2$: C, 74.07; H, 4.35. Found: C, 73.82; H, 4.58.

Z isomer



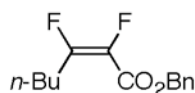
^1H NMR (CDCl_3) δ = 5.13 (s, 2H), 7.05-7.23 (m, 5H), 7.47-7.55 (m, 3H), 7.75-7.82 (m, 3H), 8.02 (s, 1H); ^{13}C NMR (CDCl_3) δ = 67.26, 125.21, 125.35, 125.37, 126.69, 127.69, 127.79, 127.84, 128.19, 128.37, 128.71, 130.18, 132.22, 134.27, 134.38, 137.41 (dd, J = 22.2 Hz, 254.6 Hz), 156.44 (dd, J = 16.6 Hz, 267.3 Hz), 160.24 (dd, J = 8.1 Hz, 29.4 Hz); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -99.67 (d, J = 7.8 Hz, 1F), -147.96 (d, J = 7.8 Hz, 1F).

E isomer



^1H NMR (CDCl_3) δ = 5.40 (s, 2H), 7.34-7.42 (m, 3H), 7.46-7.47 (m, 2H), 7.50-7.59 (m, 2H), 7.79-7.91 (m, 4H), 8.29 (s, 1H); ^{13}C NMR (CDCl_3) δ = 67.26, 125.21, 125.35, 125.37, 126.69, 127.69, 127.79, 127.84, 128.19, 128.37, 128.71, 130.18, 132.22, 134.27, 134.38, 137.41 (dd, J = 22.2 Hz, 254.6 Hz), 156.44 (dd, J = 16.6 Hz, 267.3 Hz), 160.24 (dd, J = 8.1 Hz, 29.4 Hz); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -133.51 (d, J = 127.7 Hz, 1F), -161.98 (d, J = 127.7 Hz, 1F).

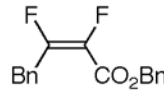
4.8. Benzyl (Z)-3-butyl-2,3-difluoroacrylate (**2j**)



^1H NMR (CDCl_3) δ = 0.89 (t, J = 7.3 Hz, 3H), 1.30-1.38 (m, 2H), 1.54~1.60 (m, 2H), 2.74 (ddt, J = 3.0 Hz, 8.0 Hz, 27.0 Hz, 2H), 5.26 (s, 2H), 7.32~7.39 (m, 5H); ^{13}C NMR (CDCl_3) δ = 13.6, 22.0, 27.9 (d, J = 2.7 Hz), 27.7 (dd, J = 2.0, 20.5 Hz), 67.1, 128.4, 128.5, 128.6, 134.9, 136.8 (dd, J = 19.2, 251.5 Hz), 160.4 (dd, J = 11.6, 272.4 Hz), 160.9 (dd, J = 10.1, 27.5 Hz); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -106.17 (dt, J = 4.4 Hz, 27.0 Hz, 1F), -155.07 (d, J =

4.4 Hz, 1F); IR (neat) 3036 (w), 2874 (w), 1732 (s), 1686 (m), 1501 (w), 1431 (w), 1312 (s), 1157 (m), 1022 (m) cm^{-1} ; HRMS (EI) calcd for (M+) $\text{C}_{14}\text{H}_{16}\text{F}_2\text{O}_2$: 254.1118, found 254.1112. Anal. Calcd for $\text{C}_{14}\text{H}_{16}\text{F}_2\text{O}_2$: C, 66.13; H, 6.34. Found: C, 66.52; H, 6.44.

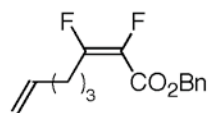
4.9. Benzyl (Z)-3-benzyl-2,3-difluoroacrylate (**2k**)

 ^1H NMR (CDCl_3) δ = 4.01 (dd, J = 2.8 Hz, 26.9 Hz, 2H), 5.24 (s, 2H), 7.16-7.33 (m, 10H); ^{13}C NMR (CDCl_3) δ = 34.59 (d, J = 20.6 Hz), 67.42, 127.35, 128.47, 128.69, 128.74, 128.83, 134.40, 134.42, 134.74, 136.92 (dd, J = 18.9 Hz, 254.7 Hz), 157.95 (dd, J = 13.0 Hz, 272.6 Hz), 160.90 (dd, J = 9.5 Hz, 27.7 Hz); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -105.70 (dt, J = 2.0 Hz, 26.9 Hz, 1F), -153.65 (d, J = 2.0 Hz, 1F); IR (neat) 3067 (w), 3032 (w), 1732 (vs), 1690 (vs), 1605 (w), 1497 (m), 1454 (m), 1420 (w), 1385 (s), 1312 (vs), 1258 (w), 1181 (vs), 1146 (vs), 1076 (s), 1030 (vs), 799 (w), 764 (s), 706 (vs) cm^{-1} ; HRMS (EI) calcd for (M+) $\text{C}_{17}\text{H}_{14}\text{F}_2\text{O}_2$: 288.0962, found 288.0961. Anal. Calcd for $\text{C}_{17}\text{H}_{14}\text{F}_2\text{O}_2$: C, 70.83; H, 4.89. Found: C, 70.91; H, 5.07.

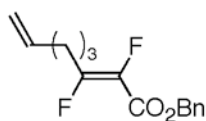
4.10. Benzyl 2,3-difluoro-3-(4-pentenyl)acrylate (**2l**)

IR (neat) 3069 (vs), 2939 (vs), 1685 (vs), 1609 (m), 1499 (vs), 1383 (vs), 1147 (vs), 1028 (vs) cm^{-1} ; HRMS (EI) calcd for (M+) $\text{C}_{15}\text{H}_{16}\text{F}_2\text{O}_2$: 266.1118, found 266.1111.

Z isomer

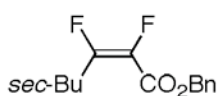
 ^1H NMR (CDCl_3) δ =1.72 (tt, J = 7.5, 7.5 Hz, 2H), 2.09 (dt, J = 7.5, 7.5 Hz, 2H), 2.77 (dtd, J = 25.4, 7.5, 2.4 Hz, 2H), 4.99 (dd, J = 11.3, 1.6 Hz, 1H), 5.02 (dd, J = 17.1, 1.6 Hz, 1H), 5.28 (s, 2H), 5.76 (dt, J = 11.3, 7.5 Hz, 1H), 7.33~7.45 (m, 5H); ^{13}C NMR (CDCl_3) δ = 15.20, 25.08, 27.93 (d, J = 20.3 Hz), 32.82, 65.78, 67.16, 115.43, 128.62, 129.37, 134.84, 136.85 (dd, J = 252.0, 19.1Hz), 137.31, 160.03 (dd, J = 272.2, 12.6 Hz), 160.86 (dd, J = 27.5, 9.5 Hz); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -106.49 (t, J = 25.4 Hz, 1F), -154.54 (s, 1F).

E isomer



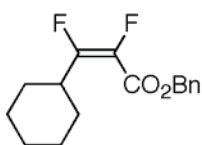
$^1\text{H NMR}$ (CDCl_3) δ =1.70-1.80 (m, 2H), 2.15 (dt, J = 6.1, 6.1 Hz, 2H), 2.52 (ddt, J = 22.5, 6.1, 6.1 Hz, 2H), 5.00-5.10 (m, 2H), 5.31 (s, 2H), 5.72~5.85 (m, 1H), 7.33~7.45 (m, 5H); $^{19}\text{F NMR}$ (CDCl_3 , CFCl_3) δ = -124.06 (dt, J = 129.9, 22.5 Hz, 1F), -167.08 (d, J = 129.9 Hz, 1F).

4.11. Benzyl (*Z*)-3-*sec*-butyl-2,3-difluoroacrylate (**2m**)



$^1\text{H NMR}$ (CDCl_3) δ = 0.82 (t, J = 7.5 Hz, 3H), 1.09 (d, J = 3.5 Hz, 3H), 1.46 (dq, J = 7.5 Hz, 42.5 Hz, 2H), 3.35 (dtq, J = 3.5 Hz, 30.8 Hz, 42.5 Hz, 1H), 5.21 (d, J = 7.5 Hz, 2H), 7.26~7.32 (m, 5H); $^{13}\text{C NMR}$ (CDCl_3) δ = 11.6, 16.6, 26.2, 34.1 (d, J = 19.8 Hz), 67.1, 128.3, 128.6, 128.7, 134.9, 136.8 (dd, J = 19.2, 251.5 Hz), 160.1 (dd, J = 11.6, 272.4 Hz), 161.3 (dd, J = 10.1, 27.5 Hz); $^{19}\text{F NMR}$ (CDCl_3 , CFCl_3) δ = -121.14 (d, J = 30.8 Hz, 1F), -155.41 (s, 1F); IR (neat) 2970 (m), 2936 (w), 1732 (vs), 1682 (m), 1308 (vs), 1130 (m), 1022 (m) cm^{-1} ; HRMS (FAB) calcd for (M^+) $\text{C}_{14}\text{H}_{16}\text{F}_2\text{O}_2$: 254.1118, found 254.1120. Anal. Calcd for $\text{C}_{14}\text{H}_{16}\text{F}_2\text{O}_2$: C, 66.13; H, 6.34. Found: C, 65.95; H, 6.70.

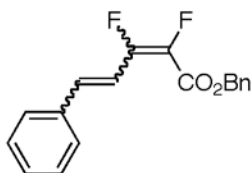
4.12. Benzyl (*Z*)-3-cyclohexyl-2,3-difluoroacrylate (**2n**)



M.P. 60~62 °C; $^1\text{H NMR}$ (CDCl_3) δ = 1.13~1.31 (m, 4H), 1.46~1.54 (m, 2H), 1.67~1.80 (m, 4H), 3.33 (dtt, J = 12.0 Hz, 12.0 Hz, 32.7 Hz, 1H), 5.27 (s, 2H), 7.34~7.39 (m, 5H); $^{13}\text{C NMR}$ (CDCl_3) δ = 25.4, 25.6, 28.5 (d, J = 1.7 Hz), 37.0 (dd, J = 1.6, 19.3 Hz), 67.1, 128.3, 128.5, 128.6, 134.9, 136.9 (dd, J = 19.6 Hz, 257.3 Hz), 161.0 (dd, J = 10.0, 27.7 Hz), 163.3 (dd, J = 10.7, 275.5 Hz); $^{19}\text{F NMR}$ (CDCl_3 , CFCl_3) δ = -117.31 (d, J = 32.7 Hz, 1F), -156.80 (s, 1F); IR (neat) 2932 (vs), 2855 (m), 1728 (vs), 1674 (vs), 1454 (s), 1327 (vs), 1258 (m), 1126 (vs), 1018 (vs) cm^{-1} ; HRMS (EI) calcd for (M^+) $\text{C}_{16}\text{H}_{18}\text{F}_2\text{O}_2$: 280.1275, found 280.1273. Anal. Calcd for $\text{C}_{16}\text{H}_{18}\text{F}_2\text{O}_2$: C, 68.56; H, 6.47. Found: C, 68.69; H, 6.24.

4.13. Benzyl 2,3-difluoro-3-(2-phenylethenyl)acrylate (**2o**)

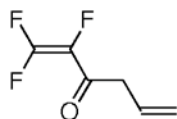
The products were obtained as an inseparable isomeric mixtures.



^1H NMR (CDCl_3) δ =5.34 (s, 3H), 5.35 (s, 3H), 5.37 (s, 3H), 6.65~6.75 (m, 4H), 6.80~7.00 (m, 4H), 7.15~7.65 (m, 40H); ^{19}F NMR (CDCl_3 , CFCl_3) δ =-113.33 (dd, J = 14.2, 14.2 Hz, 1F), -125.70 (dd, J = 25.3, 25.3 Hz, 1F), -140.07 (dd, J = 119.9, 25.3 Hz, 1F), -147.26 (s, 1F), -149.94 (s, 1F), -162.68 (d, J = 119.9 Hz, 1F); IR (neat) 3029 (w), 2359 (w), 1723 (vs), 1639 (s), 1496 (m), 1384 (s), 1319 (vs), 1165 (vs), 1075 (vs) cm^{-1} ; HRMS (FAB) calcd for ($\text{M}+\text{Na}$) $\text{C}_{18}\text{H}_{14}\text{F}_2\text{O}_2\text{Na}$: 323.0860, found 323.0863.

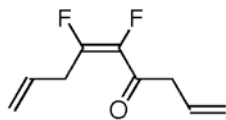
4.14. 1,1,2-Trifluorohexa-1,5-diene-3-one (**4p**) and 5,6-Difluoronona-1,5-diene-4-one (**5p**)

Products **4p** and **5p** could not be separated by a silica gel column chromatography as a sole product. Therefore, the chemical shifts of **4p** and **5p** are determined based on the ^1H and ^{19}F NMR analyses of the mixture (**4p** and **5p**).



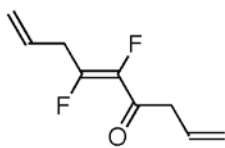
^1H NMR (CDCl_3) δ = 2.37 (dd, J = 8.3 Hz, 13.7 Hz, 1H), 2.55 (dd, J = 6.8 Hz, 13.7 Hz, 1H), 5.13-5.25 (m, 2H), 5.76-5.87 (m, 1H); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -101.11 (dd, J = 33.1 Hz, 83.6 Hz, 1F), -116.36 (dd, J = 83.6 Hz, 112.2 Hz, 1F), -178.044 (dd, J = 33.1 Hz, 112.2 Hz, 1F)

Z isomer



^1H NMR (CDCl_3) δ = 2.26 (dd, J = 8.5 Hz, 13.5 Hz, 1H), 2.37 (dd, J = 8.0 Hz, 13.5 Hz, 1H), 2.54 (dd, J = 6.5 Hz, 14.0 Hz, 1H), 2.57~2.62 (m, 1H), 3.22~3.28 (m, 1H), 5.09~5.24 (m, 2H), 5.75~5.85 (m, 1H); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -130.03 (t, J = 25.3 Hz, 1F), -143.27 (s, 1F).

E isomer

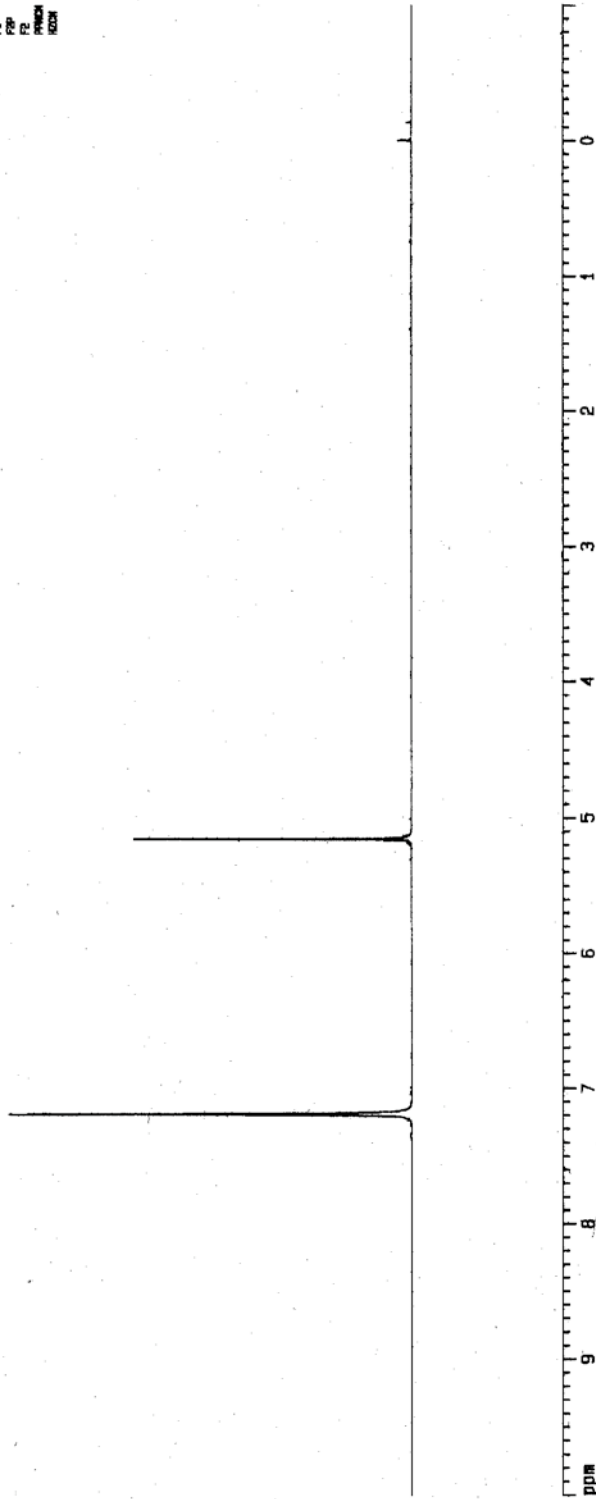
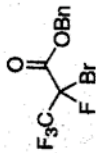


^1H NMR (CDCl_3) δ = 2.26 (dd, J = 8.5 Hz, 13.5 Hz, 1H), 2.37 (dd, J = 8.0 Hz, 13.5 Hz, 1H), 2.54 (dd, J = 6.5 Hz, 14.0 Hz, 1H), 2.57-2.62 (m, 1H), 3.06~3.13 (m, 1H), 5.09~5.24 (m, 2H), 5.75~5.85 (m, 1H); ^{19}F NMR (CDCl_3 , CFCl_3) δ = -15.056 (dt, J = 23.1 Hz, 127.6 Hz, 1F), -158.55 (d, J = 127.6 Hz, 1F).

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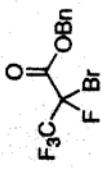


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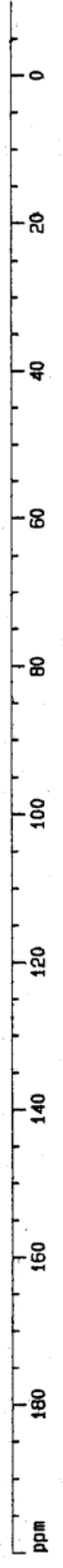
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ppm

515




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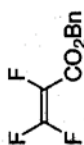
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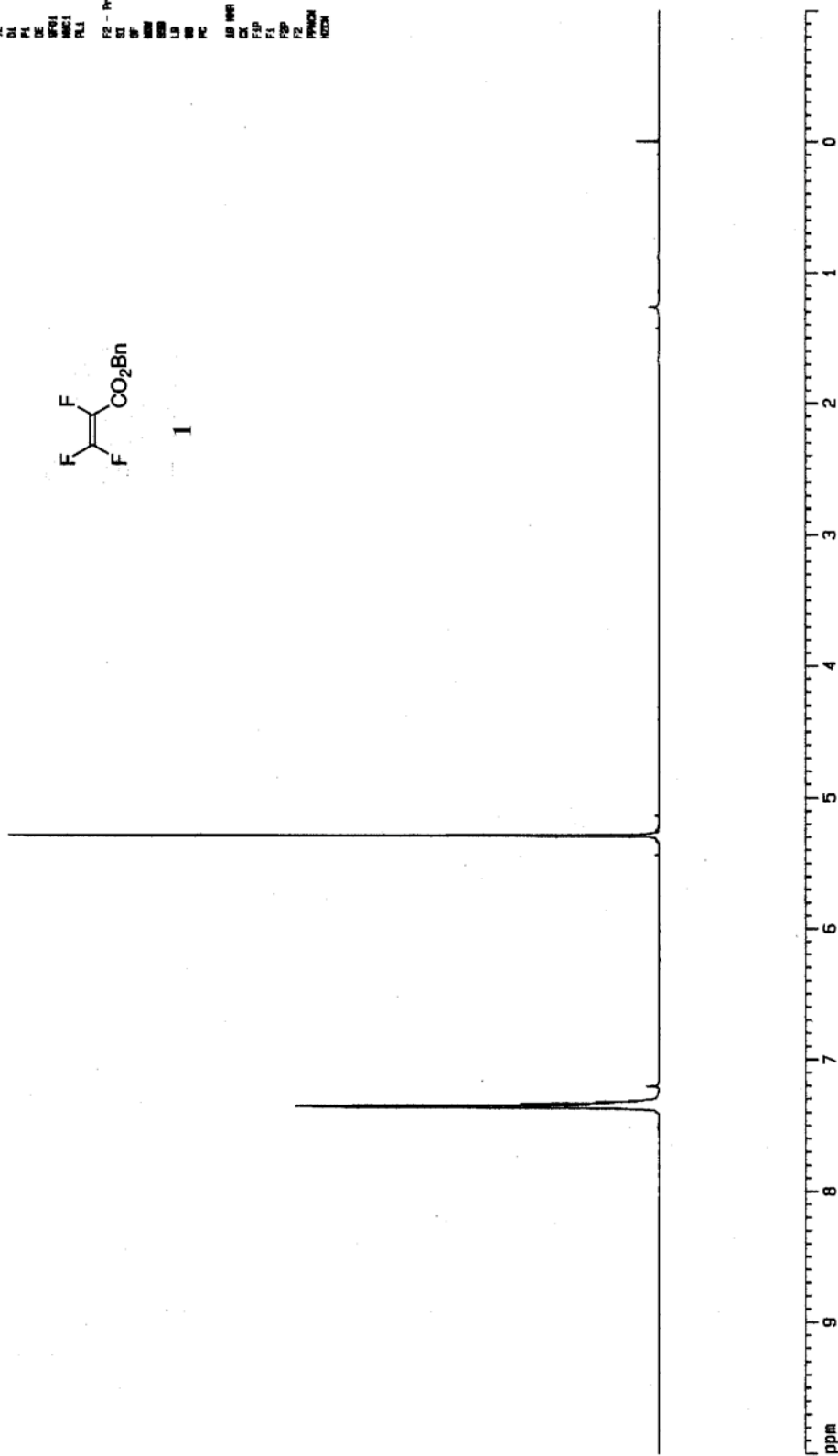
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1



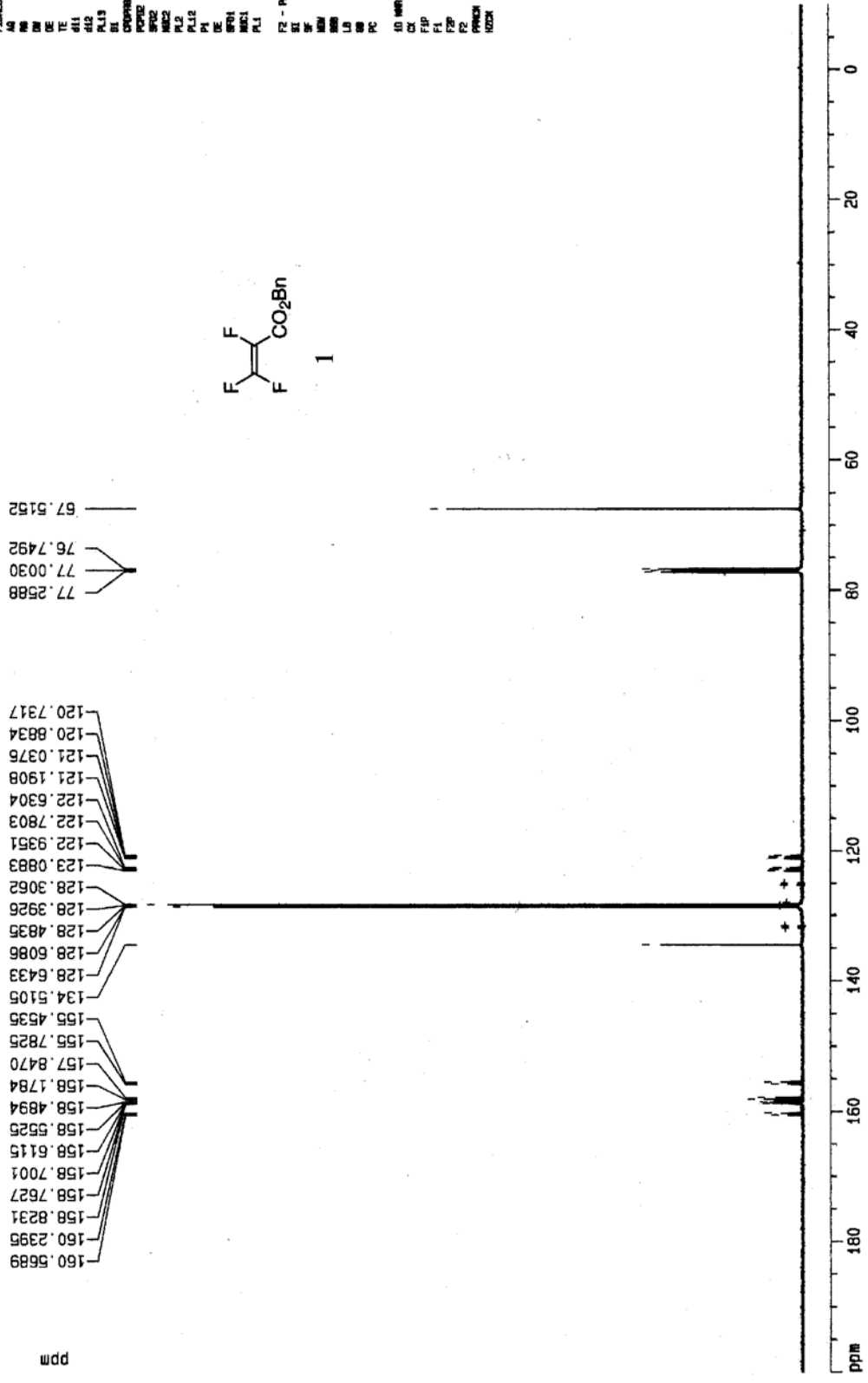
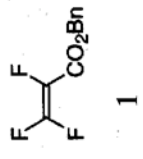
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 GB: 0
 PC: 1.40

10 MHz plot parameters
 CX: 25.00 cm
 FAP: 200.000 MHz
 F1: 28351.00 Hz
 F2: -10.000 MHz
 F3: -1257.00 Hz
 PPRCH: 8.00000 MHz
 NUC2: 100MHz

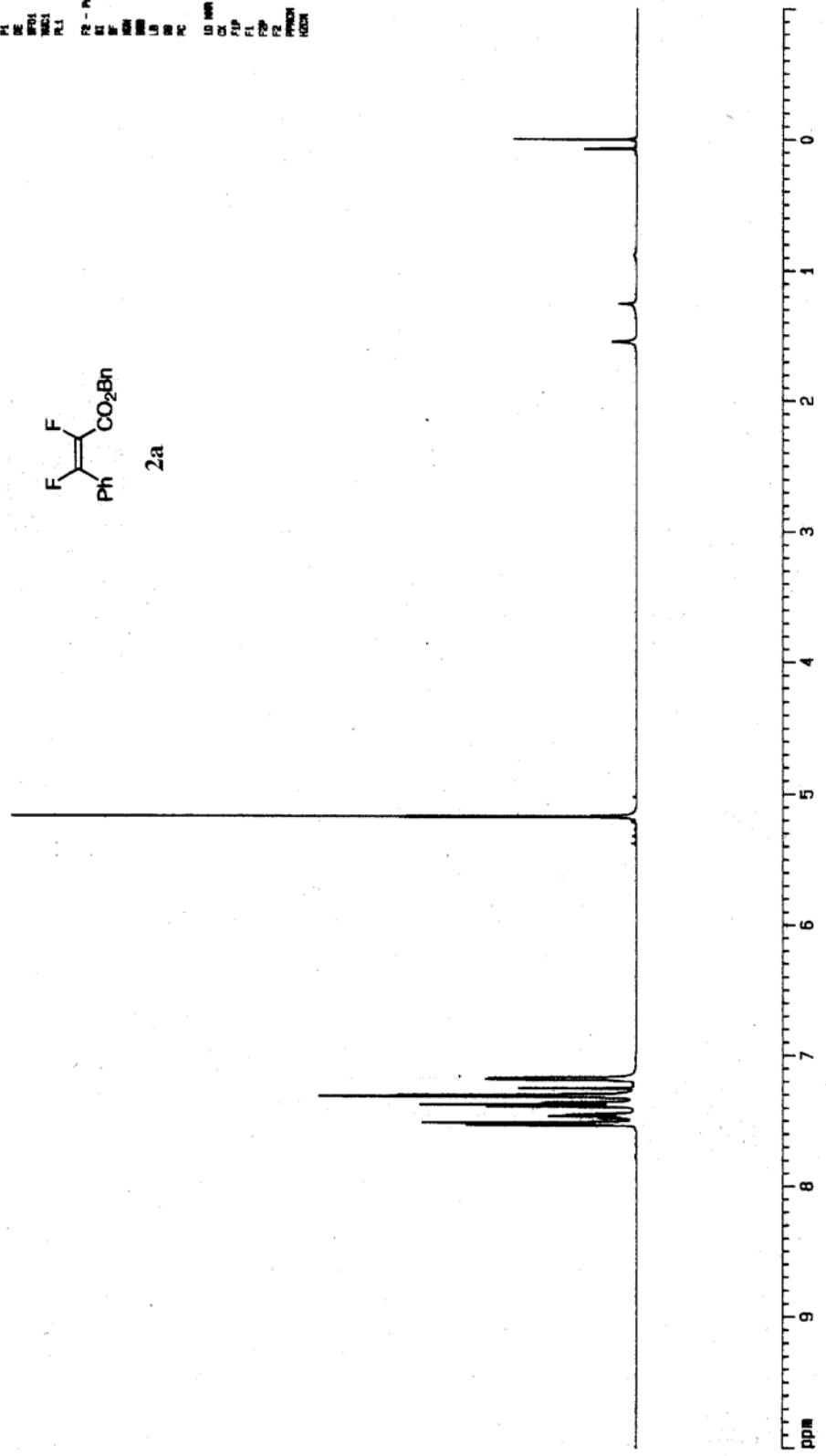
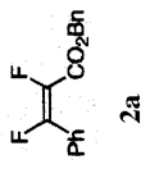


Current Data Parameters
 NAME: Name-4-5
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_ : 000000
 Time : 0.48
 JMODNAM : 0702000
 PROCPRG : 0 am NoLine
 PULPROG : zgpg
 TO : 32740
 SOLVENT : CDCl3
 NS : 16
 DS : 2
 SWH : 10200.870 Hz
 F2 - 100.62604 Hz
 AQ : 1.1888212 sec
 RG : 409.1
 GB : 0.000000 sec
 PC : 0.000000 sec
 VC : 0.000000 sec
 DI : 0.000000 sec
 DE : 0.000000 sec
 DF : 0.000000 sec
 WFO1 : 000.1320000 MHz
 WFO2 :
 PL1 : -0.00 dB

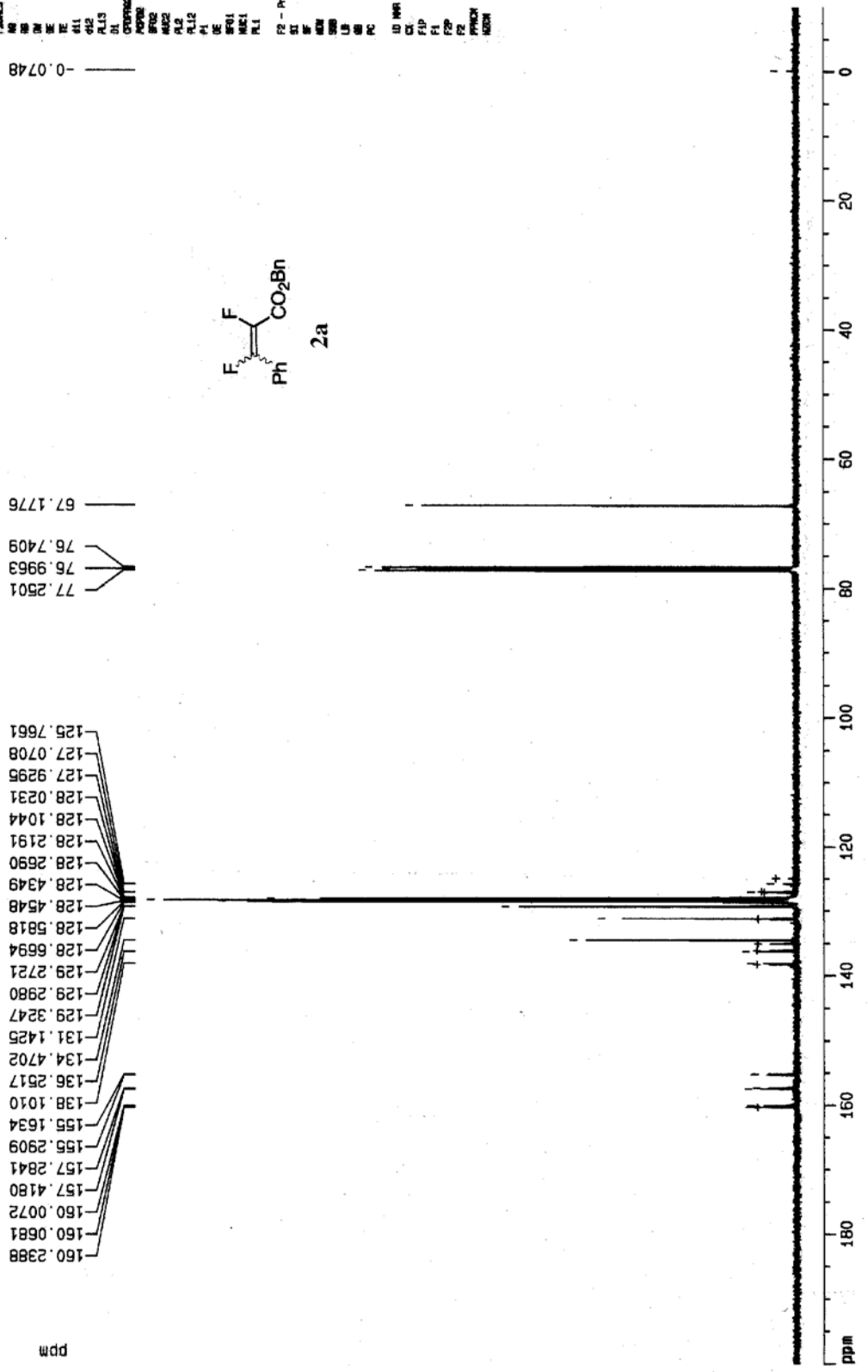
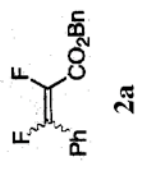
F2 - Processing parameters
 SI : 65536
 SF : 000.13200170 MHz
 HF : 0
 LB : 0.100 Hz
 GB : 0
 PC : 1.00

1D NMR plot parameters
 CX : 20.00 cm
 ZF1 : 50.000 MHz
 F1 : 0001.300 Hz
 F2 : -1.000 MHz
 F2 : -000.10 Hz
 FWHM : 0.44000 MHz
 GCEN : 200.00724 Hz



Current Data Parameters
 NAME: Name-2-18
 EXNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 000000
 Time: 00.00
 INSTRUM: EXFLN00
 PROCNO: 5
 PULPROG: zgpg30
 IN: 1000000000
 SOLVENT: CDCl3
 NS: 1000
 DS: 4
 SWH: 30000.000 Hz
 FREQ0: 0.00000000 Hz
 FREQ1: 0.00000000 Hz
 MR: 22000.000 Hz
 INJ: 10.00000000 um
 DE: 6.00000000 um
 TE: 300.2 K
 SI: 0.00000000 mm
 PR: 0.00000000 mm
 PI: 0.00000000 mm
 PL1: 50.00000000 dB
 PL2: 50.00000000 dB
 PL3: 50.00000000 dB
 PL4: 50.00000000 dB
 PL5: 50.00000000 dB
 PL6: 50.00000000 dB
 PL7: 50.00000000 dB
 PL8: 50.00000000 dB
 PL9: 50.00000000 dB
 PL10: 50.00000000 dB
 PL11: 50.00000000 dB
 PL12: 50.00000000 dB
 PL13: 50.00000000 dB
 PL14: 50.00000000 dB
 PL15: 50.00000000 dB
 PL16: 50.00000000 dB
 PL17: 50.00000000 dB
 PL18: 50.00000000 dB
 PL19: 50.00000000 dB
 PL20: 50.00000000 dB
 PL21: 50.00000000 dB
 PL22: 50.00000000 dB
 PL23: 50.00000000 dB
 PL24: 50.00000000 dB
 PL25: 50.00000000 dB
 PL26: 50.00000000 dB
 PL27: 50.00000000 dB
 PL28: 50.00000000 dB
 PL29: 50.00000000 dB
 PL30: 50.00000000 dB
 PL31: 50.00000000 dB
 PL32: 50.00000000 dB
 PL33: 50.00000000 dB
 PL34: 50.00000000 dB
 PL35: 50.00000000 dB
 PL36: 50.00000000 dB
 PL37: 50.00000000 dB
 PL38: 50.00000000 dB
 PL39: 50.00000000 dB
 PL40: 50.00000000 dB
 PL41: 50.00000000 dB
 PL42: 50.00000000 dB
 PL43: 50.00000000 dB
 PL44: 50.00000000 dB
 PL45: 50.00000000 dB
 PL46: 50.00000000 dB
 PL47: 50.00000000 dB
 PL48: 50.00000000 dB
 PL49: 50.00000000 dB
 PL50: 50.00000000 dB
 PL51: 50.00000000 dB
 PL52: 50.00000000 dB
 PL53: 50.00000000 dB
 PL54: 50.00000000 dB
 PL55: 50.00000000 dB
 PL56: 50.00000000 dB
 PL57: 50.00000000 dB
 PL58: 50.00000000 dB
 PL59: 50.00000000 dB
 PL60: 50.00000000 dB
 PL61: 50.00000000 dB
 PL62: 50.00000000 dB
 PL63: 50.00000000 dB
 PL64: 50.00000000 dB
 PL65: 50.00000000 dB
 PL66: 50.00000000 dB
 PL67: 50.00000000 dB
 PL68: 50.00000000 dB
 PL69: 50.00000000 dB
 PL70: 50.00000000 dB
 PL71: 50.00000000 dB
 PL72: 50.00000000 dB
 PL73: 50.00000000 dB
 PL74: 50.00000000 dB
 PL75: 50.00000000 dB
 PL76: 50.00000000 dB
 PL77: 50.00000000 dB
 PL78: 50.00000000 dB
 PL79: 50.00000000 dB
 PL80: 50.00000000 dB
 PL81: 50.00000000 dB
 PL82: 50.00000000 dB
 PL83: 50.00000000 dB
 PL84: 50.00000000 dB
 PL85: 50.00000000 dB
 PL86: 50.00000000 dB
 PL87: 50.00000000 dB
 PL88: 50.00000000 dB
 PL89: 50.00000000 dB
 PL90: 50.00000000 dB
 PL91: 50.00000000 dB
 PL92: 50.00000000 dB
 PL93: 50.00000000 dB
 PL94: 50.00000000 dB
 PL95: 50.00000000 dB
 PL96: 50.00000000 dB
 PL97: 50.00000000 dB
 PL98: 50.00000000 dB
 PL99: 50.00000000 dB
 PL100: 50.00000000 dB

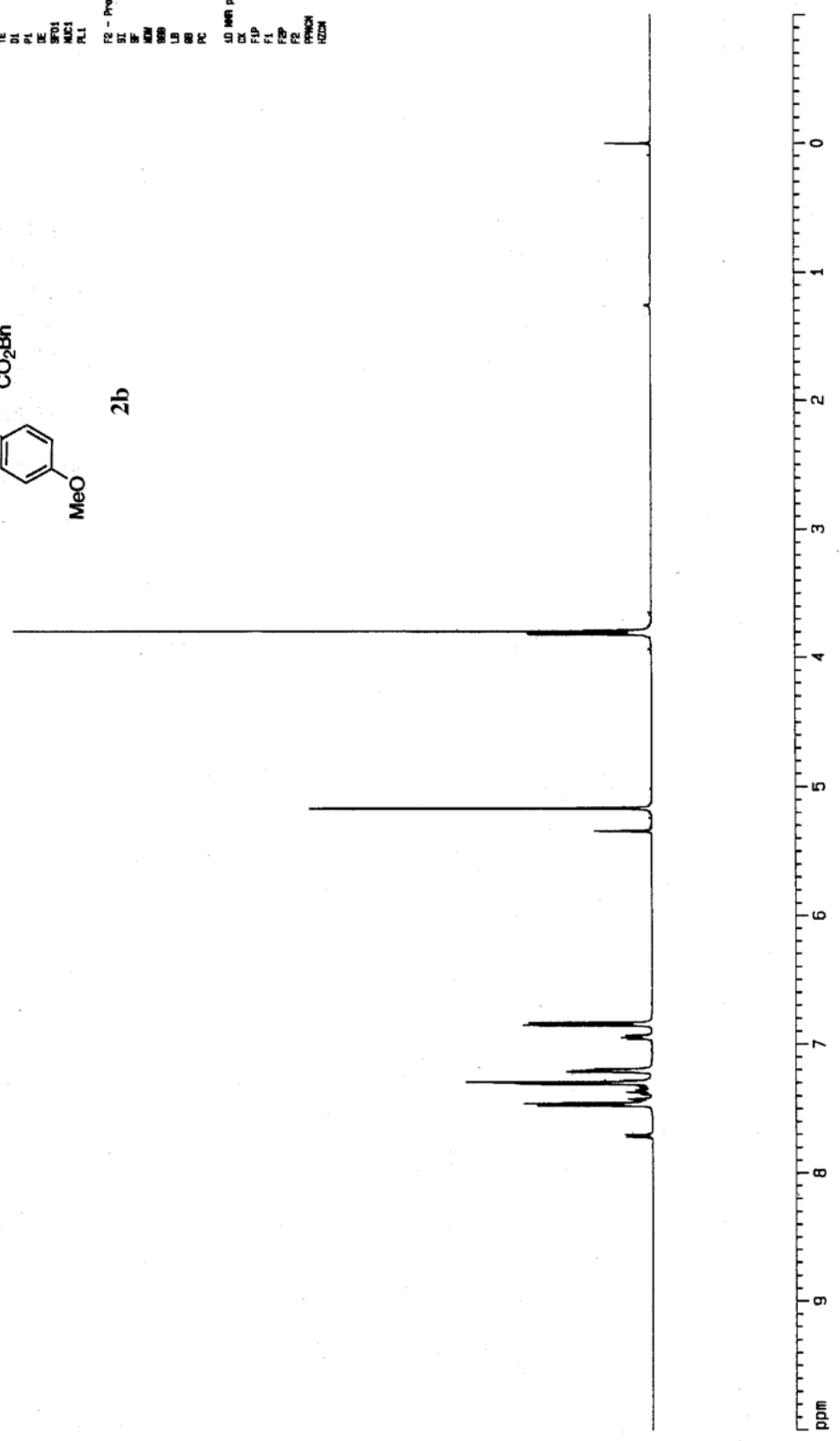
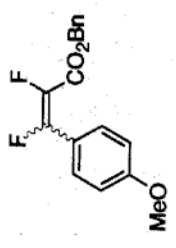


Current Data Parameters
 NAME Name-4-28
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 200000
 Time 16.28
 INSTRUM DR0050
 PROBRD 5 mm NUC1H
 PULPROG zgpg30
 TO 32700
 SOLVENT CDCl3
 DS 0
 SWH 10330.576 Hz
 FIDRES 0.310264 Hz
 AQ 1.1856212 sec
 RG 64
 IN 40,400 use
 DE 6.00 use
 TE 300.0 K
 DL 1.0000000 sec
 FL 9.30 use
 DE 6.00 use
 SFO1 500.1300880 MHz
 NUC1 1H
 P11 -6.00 dB

F2 - Processing parameters
 SI 32768
 SF 500.1300881 MHz
 MM 30
 EN 0
 LB 0.30 Hz
 GB 0
 PC 1.00

LJ MMR plot parameters
 CX 25.00 cm
 FLP 10.000 ppb
 FI 5001.30 Hz
 FZ -1.000 ppb
 PZ -500.13 Hz
 PRACH 0.40000 ppb
 RDCN 250.00725 Hz

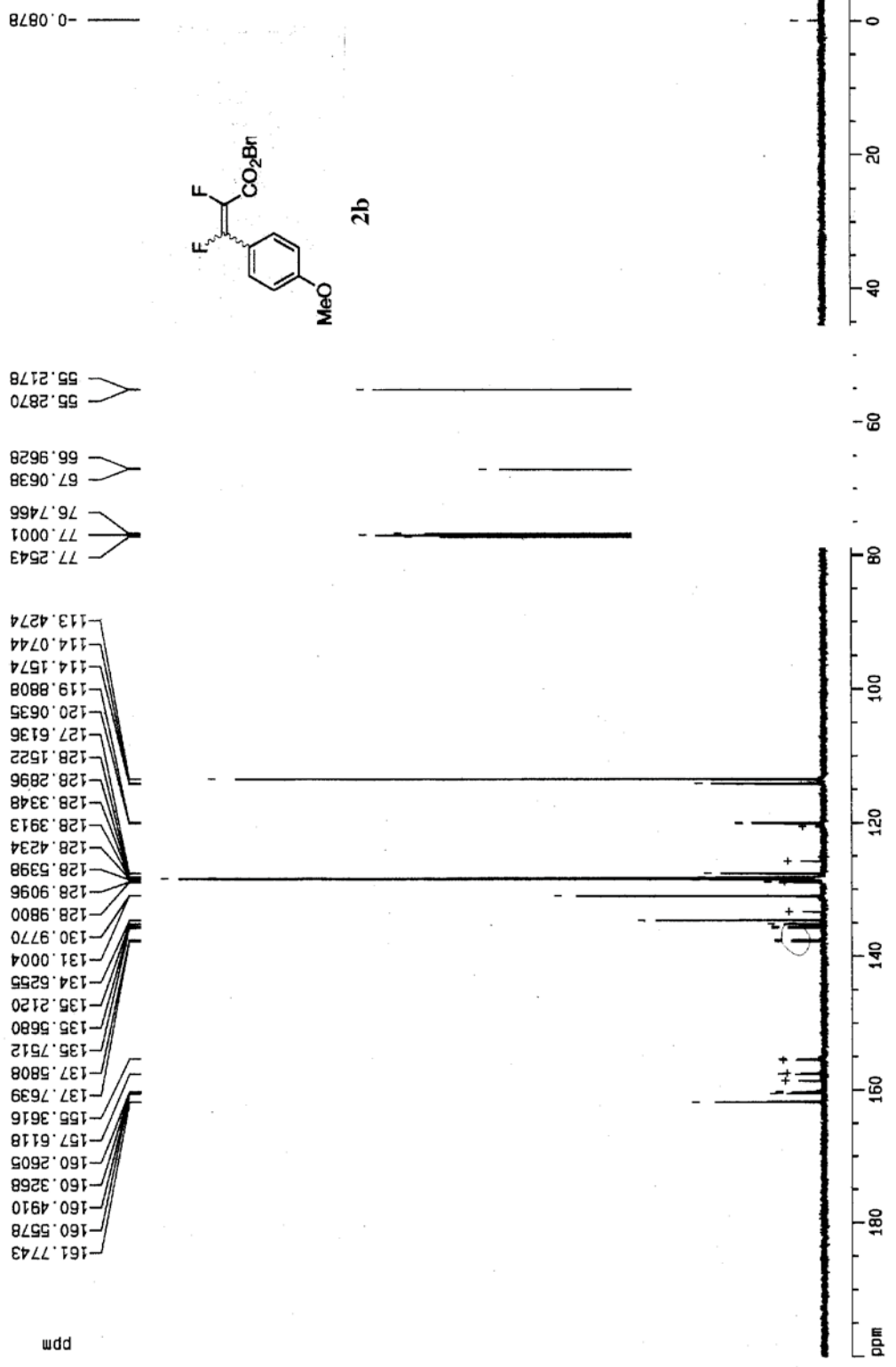


Current Data Parameters
 NAME: Name-4-2b
 EXPNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 200000
 Time: 18.41
 INSTRUM: spect
 PROCNO: 5
 PULPROG: zgpg30
 TD: 65536
 SFO: 500.135
 F2: 500.135
 SI: 2
 SF: 500.135
 AQ: 0.600007 Hz
 AS: 0.600007 Hz
 RM: 4997.5
 DM: 12.000 us
 DE: 6.00 us
 TE: 300.2 K
 FID1: 0.000000 us
 FID2: 0.000000 us
 PL13: 18.00 dB
 DI: 2.00000000 us
 CHARGE: wait218
 POP2: 100.00 us
 SFO2: 500.135000 MHz
 PL12: -5.00 dB
 PL11: 18.00 dB
 P1: 6.30 us
 DE: 6.00 us
 SF01: 128.778214 MHz
 NUC1: 13C
 PL1: -2.00 dB

F2 - Processing parameters
 SI: 32768
 SF: 128.778214 MHz
 HN: EN
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1D NMR plot parameters
 CX: 28.00 cm
 FID: 200.000 pp
 F1: 25181.58 Hz
 F2: -10.000 pp
 F3: -1287.38 Hz
 PRNCH: 8.40000 pp
 NZCN: 1068.38688 Hz



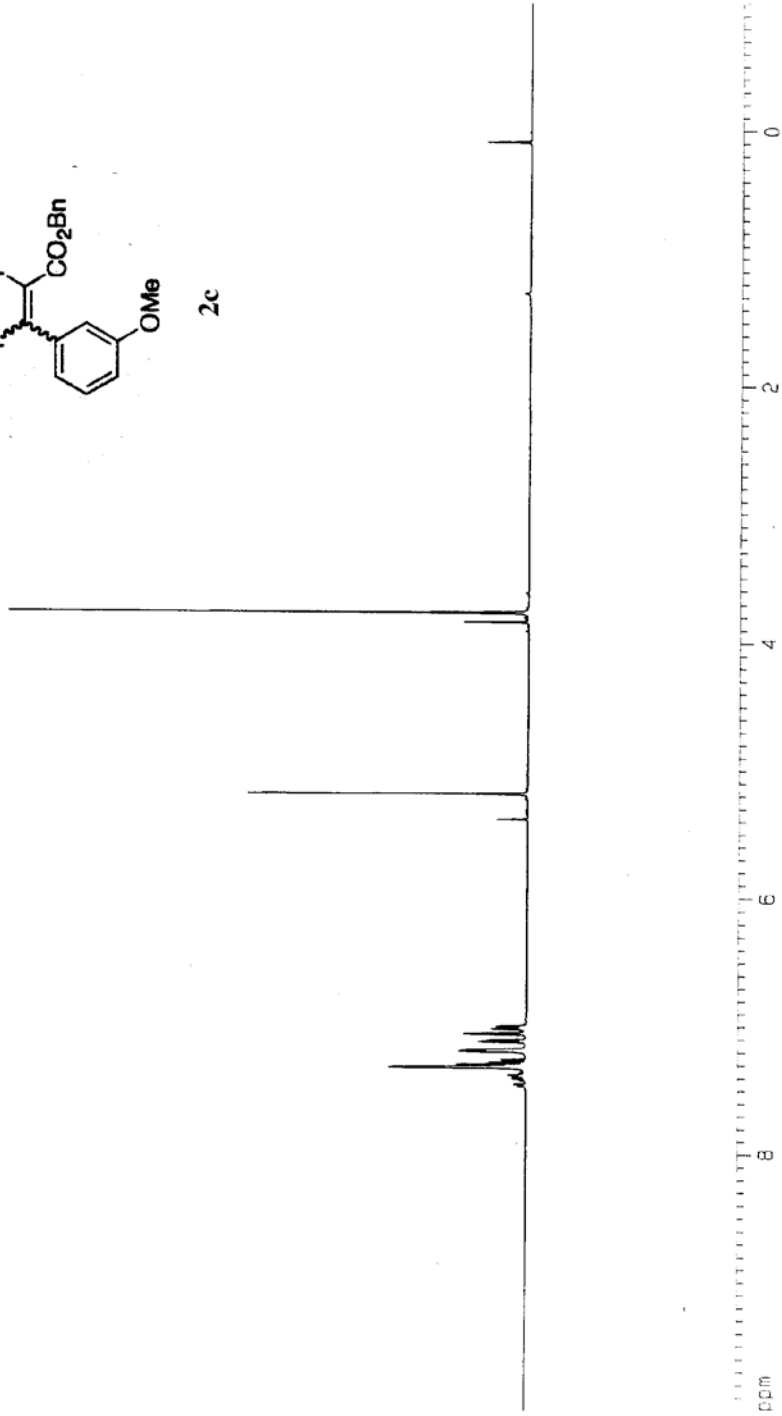
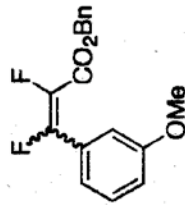
Current Data Parameters
 NAME yemada-05.11.16G
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051116
 Time 9 34
 INSTRUM drx500
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 128
 DW 48.400 USEC
 DE 6.00 USEC
 TE 296.3 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCMRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.30 USEC
 PL1 -6.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300131 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 7.43 cm
 F1P 10.000 ppm
 F1 5001.30 Hz
 F2P -1.000 ppm
 F2 -500.13 Hz
 PPMCH 0.55000 ppm/cm
 HZCM 275.07150 Hz/cm

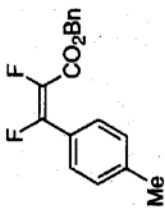


Current Data Parameters
 NAME: Name-23
 EXNO: 1
 PROCNO: 1

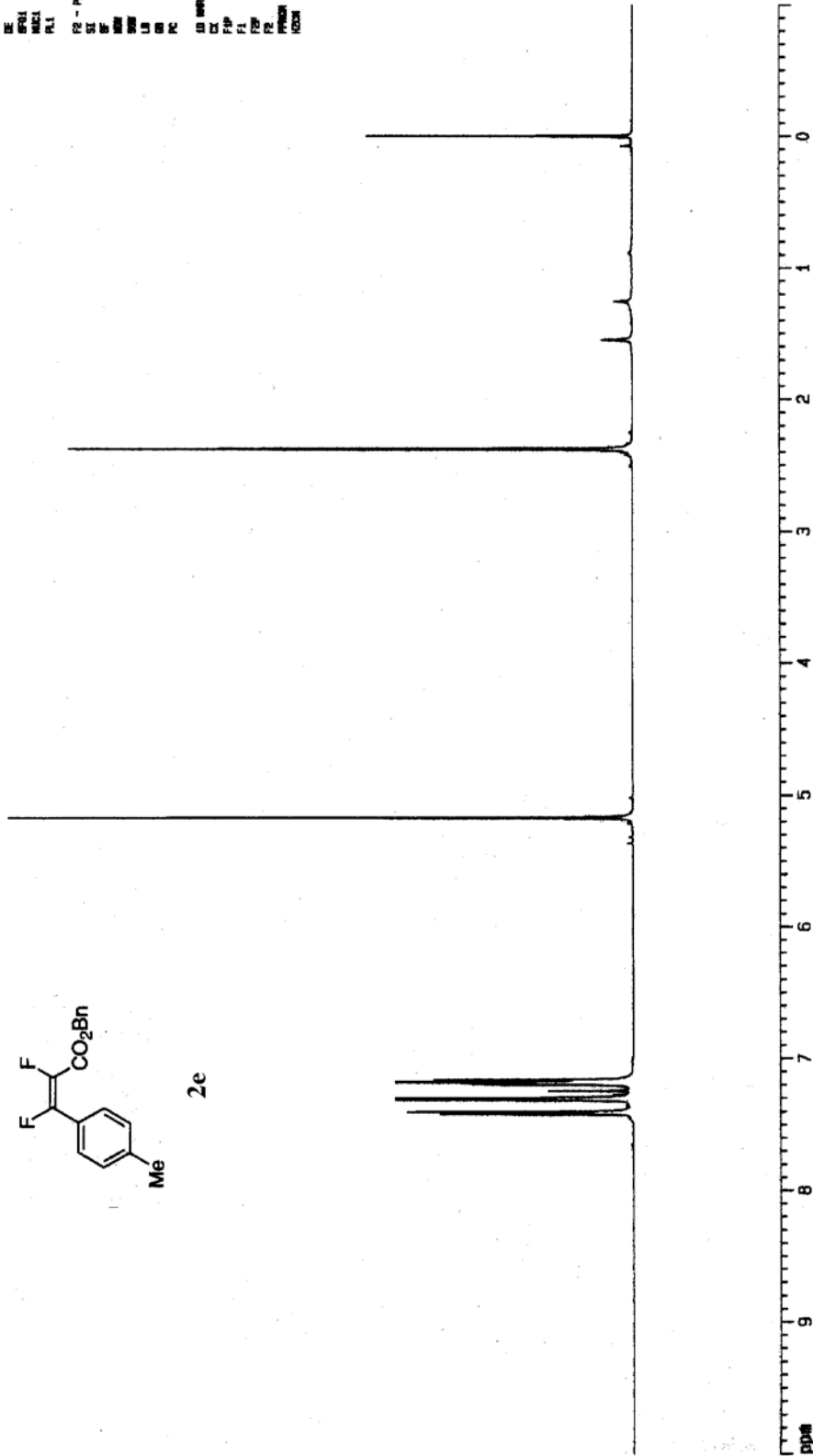
F2 - Acquisition Parameters
 Date_: 000000
 Time: 14.00
 INSTRUM: 400PQ00
 PRGMRD: 9 nm Multisim
 PULPROG: zgpg30
 TD: 32768
 SALTYP: CACD13
 DS: 0
 SWH: 10000.576 Hz
 F2RES: 0.305264 Hz
 AQ: 1.0000000000000000
 RG: 164
 DM: 400.000 MHz
 DE: 6.000 MHz
 TE: 300.2 K
 D1: 1.0000000000000000
 P1: 0.200 MHz
 DE: 0.200 MHz
 SF21: 500.132600000 MHz
 NUC1: 13C
 P11: -6.00 dB

F2 - Processing parameters
 CX: 10000
 CF: 500.132600000 MHz
 SWH: 0
 LB: 0.200 MHz
 GB: 0
 PC: 1.00

13 NMR plot parameters
 CX: 85.00 cm
 F1P: 50.000 MHz
 F1: 5001.200 Hz
 F2P: -1.000 MHz
 F2: -500.13 Hz
 PRGM: 0.40000 MHz
 NUCN: 200.10712 Hz



2e

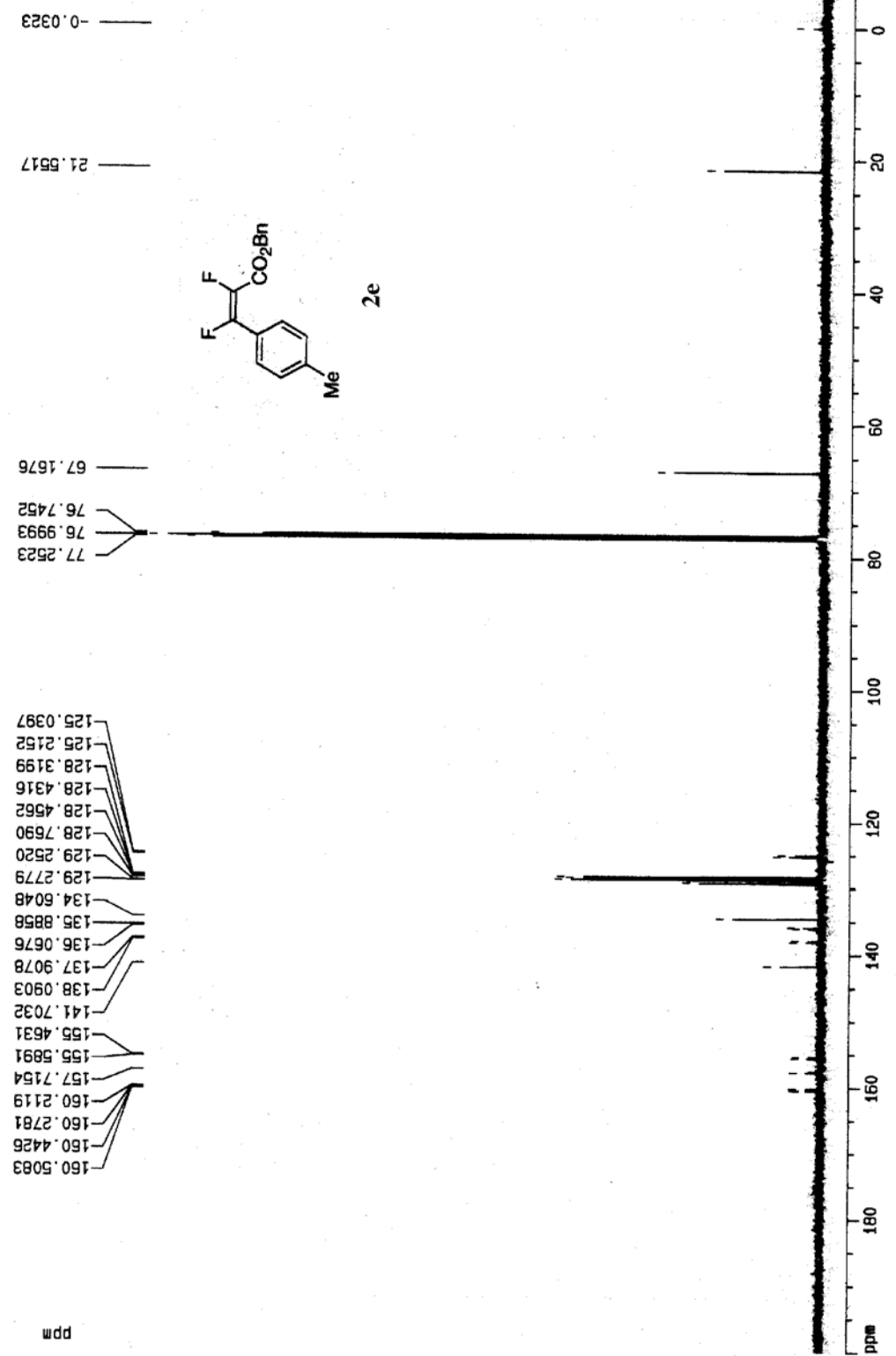


Current Data Parameters
 NAME Name-23
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 000000
 Time 15.11
 INSTRUM spect
 PULPROG zgpg30
 TO 00000
 DELTAT 0.000000
 ACQ 0.000000
 PR 0.000000
 FIDRES 0.000000
 AQ 0.000000
 SFO 300.1350000 MHz
 P1 18.00
 PL1 0.00
 PL2 0.00
 PL3 0.00
 PL4 0.00
 PL5 0.00
 PL6 0.00
 PL7 0.00
 PL8 0.00
 PL9 0.00
 PL10 0.00
 PL11 0.00
 PL12 0.00
 PL13 0.00
 PL14 0.00
 PL15 0.00
 PL16 0.00
 PL17 0.00
 PL18 0.00
 PL19 0.00
 PL20 0.00
 PL21 0.00
 PL22 0.00
 PL23 0.00
 PL24 0.00
 PL25 0.00
 PL26 0.00
 PL27 0.00
 PL28 0.00
 PL29 0.00
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 PL38 0.00
 PL39 0.00
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 PL42 0.00
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 PL47 0.00
 PL48 0.00
 PL49 0.00
 PL50 0.00
 PL51 0.00
 PL52 0.00
 PL53 0.00
 PL54 0.00
 PL55 0.00
 PL56 0.00
 PL57 0.00
 PL58 0.00
 PL59 0.00
 PL60 0.00
 PL61 0.00
 PL62 0.00
 PL63 0.00
 PL64 0.00
 PL65 0.00
 PL66 0.00
 PL67 0.00
 PL68 0.00
 PL69 0.00
 PL70 0.00
 PL71 0.00
 PL72 0.00
 PL73 0.00
 PL74 0.00
 PL75 0.00
 PL76 0.00
 PL77 0.00
 PL78 0.00
 PL79 0.00
 PL80 0.00
 PL81 0.00
 PL82 0.00
 PL83 0.00
 PL84 0.00
 PL85 0.00
 PL86 0.00
 PL87 0.00
 PL88 0.00
 PL89 0.00
 PL90 0.00
 PL91 0.00
 PL92 0.00
 PL93 0.00
 PL94 0.00
 PL95 0.00
 PL96 0.00
 PL97 0.00
 PL98 0.00
 PL99 0.00
 PL100 0.00

F2 - Processing parameters
 SI 32768
 SF 300.1350000 MHz
 EQ 0
 GE 0.00
 GR 0.00
 GU 0.00
 GV 0.00
 HW 0.00
 HY 0.00
 HZ 0.00
 IY 0.00
 IZ 0.00
 JX 0.00
 JY 0.00
 JZ 0.00
 KX 0.00
 KY 0.00
 KZ 0.00
 LX 0.00
 LY 0.00
 LZ 0.00
 MZ 0.00
 NX 0.00
 NY 0.00
 NZ 0.00
 OX 0.00
 OY 0.00
 OZ 0.00
 PX 0.00
 PY 0.00
 PZ 0.00
 QX 0.00
 QY 0.00
 QZ 0.00
 RX 0.00
 RY 0.00
 RZ 0.00
 SX 0.00
 SY 0.00
 SZ 0.00
 TX 0.00
 TY 0.00
 TZ 0.00
 VX 0.00
 VY 0.00
 VZ 0.00
 WX 0.00
 WY 0.00
 WZ 0.00
 YX 0.00
 YY 0.00
 YZ 0.00
 ZX 0.00
 ZY 0.00
 ZZ 0.00

SD NMR list parameters
 CX 20.00
 CY 20.00
 CZ 20.00
 F1 20.00
 F2 20.00
 F3 20.00
 F4 20.00
 F5 20.00
 F6 20.00
 F7 20.00
 F8 20.00
 F9 20.00
 F10 20.00
 F11 20.00
 F12 20.00
 F13 20.00
 F14 20.00
 F15 20.00
 F16 20.00
 F17 20.00
 F18 20.00
 F19 20.00
 F20 20.00
 F21 20.00
 F22 20.00
 F23 20.00
 F24 20.00
 F25 20.00
 F26 20.00
 F27 20.00
 F28 20.00
 F29 20.00
 F30 20.00
 F31 20.00
 F32 20.00
 F33 20.00
 F34 20.00
 F35 20.00
 F36 20.00
 F37 20.00
 F38 20.00
 F39 20.00
 F40 20.00
 F41 20.00
 F42 20.00
 F43 20.00
 F44 20.00
 F45 20.00
 F46 20.00
 F47 20.00
 F48 20.00
 F49 20.00
 F50 20.00
 F51 20.00
 F52 20.00
 F53 20.00
 F54 20.00
 F55 20.00
 F56 20.00
 F57 20.00
 F58 20.00
 F59 20.00
 F60 20.00
 F61 20.00
 F62 20.00
 F63 20.00
 F64 20.00
 F65 20.00
 F66 20.00
 F67 20.00
 F68 20.00
 F69 20.00
 F70 20.00
 F71 20.00
 F72 20.00
 F73 20.00
 F74 20.00
 F75 20.00
 F76 20.00
 F77 20.00
 F78 20.00
 F79 20.00
 F80 20.00
 F81 20.00
 F82 20.00
 F83 20.00
 F84 20.00
 F85 20.00
 F86 20.00
 F87 20.00
 F88 20.00
 F89 20.00
 F90 20.00
 F91 20.00
 F92 20.00
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 F96 20.00
 F97 20.00
 F98 20.00
 F99 20.00
 F100 20.00

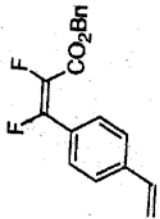


Current Data Parameters
 NAME: name-11-20
 EXPNO: 1
 PROCNO: 1

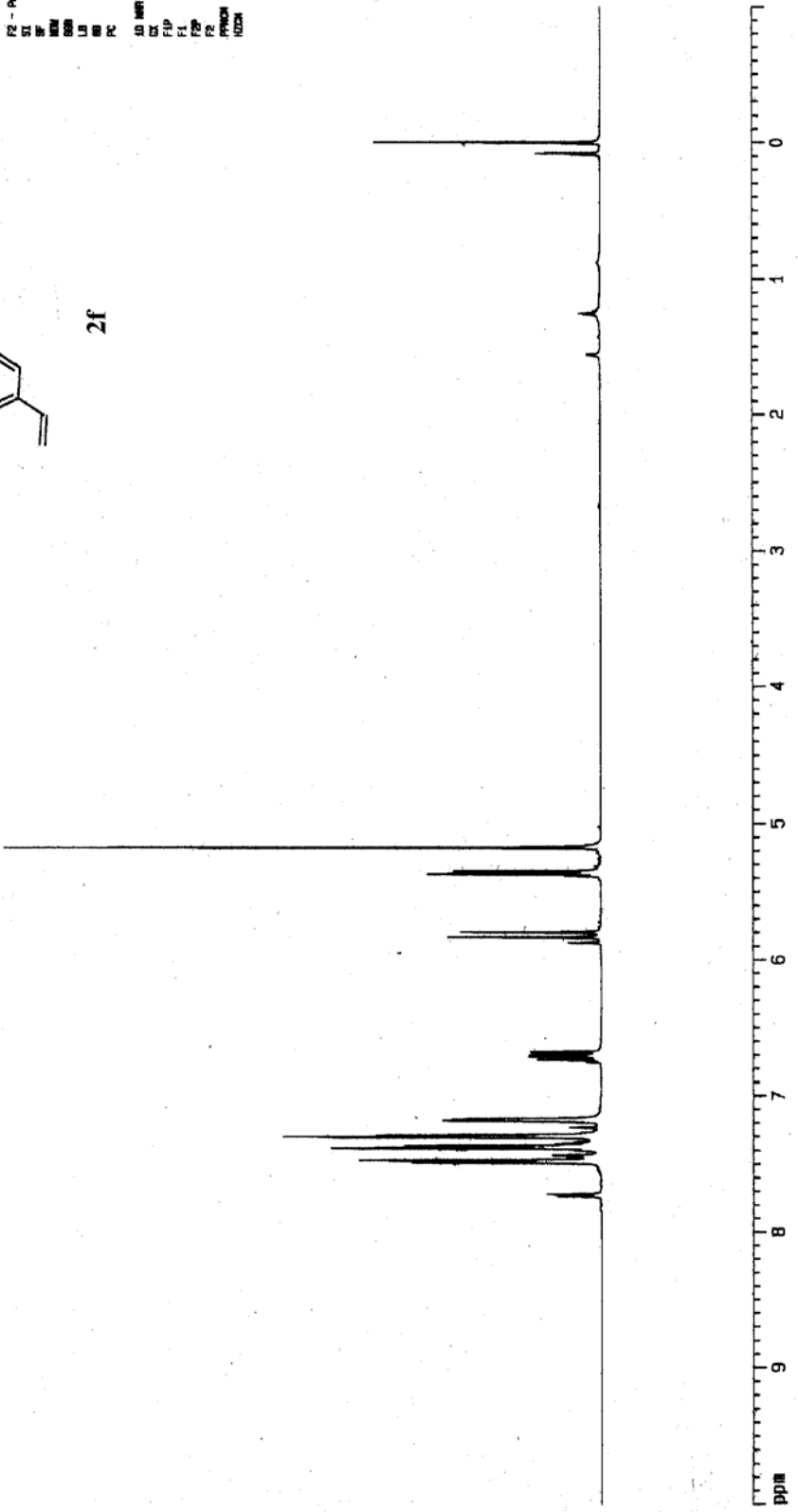
F2 - Acquisition Parameters
 Date_: 20021128
 Time: 17.22
 INSTRUM: spect
 PROBRD: 5 mm Multis
 PULPROG: zgpg30
 TO: 32760
 SALVBT: CDC13
 NS: 6
 DS: 4
 SWH: 10000.674 Hz
 FIDRES: 0.510064 Hz
 AQ: 1.3980612 sec
 RG: 203.2
 DM: 48.400 um
 DE: 6.00 um
 TE: 300.0 K
 B1: 1.0000000 um
 P1: 9.30 um
 SFO1: 500.1300000 MHz
 NUC1: 13C
 PL1: -6.00 dB

F2 - Processing parameters
 SI: 1024
 SF: 500.1300000 MHz
 DS: 4
 OS: 0
 LB: 0.20 Hz
 GB: 0
 BR: 0
 PC: 1.00

1D NMR list parameters
 CX: 25.00 cm
 FIP: 10.000 pp
 F1: 5001.30 Hz
 F2: -1.000 pp
 F3: -500.13 Hz
 PPM0: 0.44000 pp
 HZ00: 220.00725 Hz



2f



Current Data Parameters
 NAME: rsm-11-20
 EXPNO: 0
 PROCNO: 1

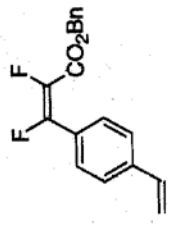
F2 - Acquisition Parameters
 Date_: 20021120
 Time: 17.39
 INSTRUM: BRUKER
 PROBRD: 5 mm NalLinn
 PULPROG: zgpg30
 TD: 65536
 SFO: 500.1360000 MHz
 AQ: 0.10000000 sec
 AS: 0.00000000 sec
 DM: 12.000000 sec
 DE: 7.000000 sec
 TE: 300.2 K
 D1: 0.05000000 sec
 d11: 0.00000000 sec
 d12: 0.00000000 sec
 PL13: 18.00 dB
 DI: 0.00000000 sec
 CHPROG: waltz16
 POPRO: 100.000000 sec
 SF2: 500.1360000 MHz
 NU2: 5H
 PL2: -8.00 dB
 PL12: 18.00 dB
 SFO1: 500.1360000 MHz
 NU1: 13C
 PL1: -2.00 dB

F2 - Processing parameters
 SI: 32768
 SF: 125.7677084 MHz
 EN: 0
 BR: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

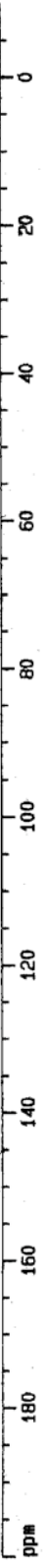
3D NMR plot parameters
 CL: 25.00 cm
 FLIP: 200.00000000
 F1: 250.13600000 MHz
 F2: -120.00000000 MHz
 F3: 6.40000000 MHz
 PROCN: 10204
 FREQ: 1005.36548 Hz

67.2671
 76.7488
 77.0023
 77.2572

116.1416
 125.7622
 128.2503
 128.3316
 128.4875
 128.6143
 129.5324
 129.5576
 134.4698
 135.8702
 140.3611



ppm

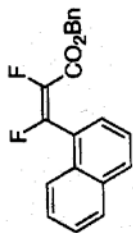


Current Date Parameters
 NAME: none-2-14
 EXPNO: 4
 PROCNO: 1

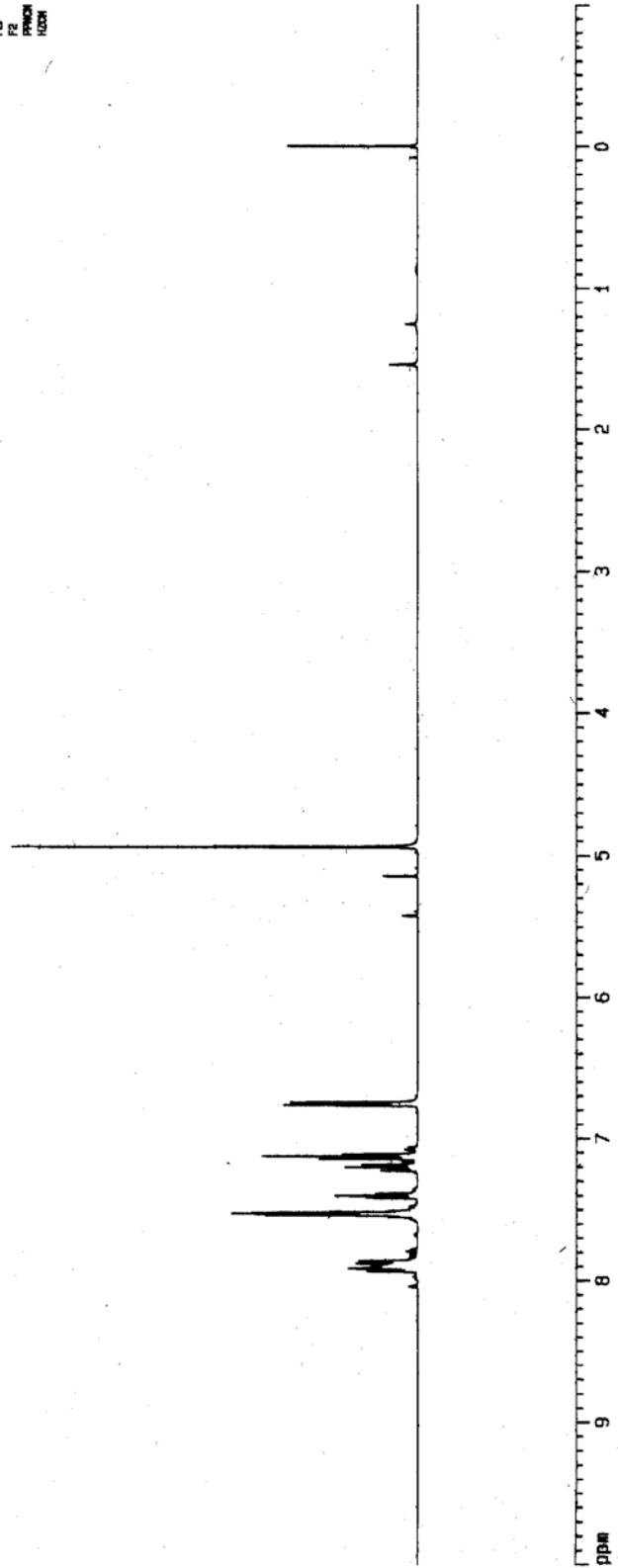
F2 - Acquisition Parameters
 Date_: 20020814
 Time: 16.30
 INSTRUM: DRIVEN
 PROBRD: 5 mm NUTLIN
 PULPROG: zgpg30
 TD: 32768
 SFO1: 500.1330682 MHz
 MISC1: 5H
 P1: 9.30 us
 PL1: -6.00 dB

F2 - Processing parameters
 SI: 1024
 SF: 500.1330682 MHz
 WF: 0
 WD: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

ID MRB plot parameters
 CX: 25.00 cm
 FIP: 10.000 pp
 F1: 5001.30 Hz
 F2: -1.000 pp
 F3: -800.13 Hz
 FWHM: 0.44000 pp
 HOOK: 250.00725 Hz



2h



Current Data Parameters
 NAME name-9-14
 EXPNO 5
 PROCNO 1

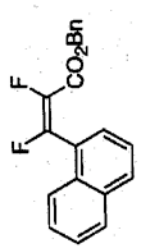
F2 - Acquisition Parameters
 Date_ 20020814
 Time 18.46
 INSTRUM spect
 PROBRW 5 mm Multinu
 PULPROG zgpg30
 TO 00000
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH32.828 Hz
 FIDRES 0.88807 Hz
 AQ 0.82800 sec
 AS 7269.2
 DM 12.000 sec
 DE 7.50 sec
 TE 300.0 K
 d11 0.0300000 sec
 d12 0.0000000 sec
 PL13 18.00 dB
 DI 0.0000000 sec
 CHPROG waltz16
 PCPDZ 100.00 sec
 PRG2 060.1520000 MHz
 RFL 1.00 Hz
 PL1 4.00 dB
 PL2 19.00 dB
 PL3 19.00 dB
 PL4 19.00 dB
 PL5 19.00 dB
 SF31 126.770514 MHz
 NS2 128
 PL1 -2.00 dB

F2 - Processing parameters
 SI 32768
 SF 126.767794 MHz
 AM 0
 EN 0
 LB 1.00 Hz
 GB 0
 PC 1.40

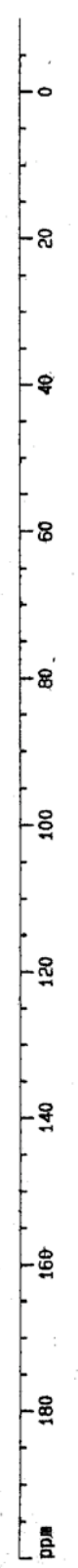
GD NMR pilot parameters
 C2 256.00 sec
 F1P 200.000 MHz
 F1 250161.58 Hz
 F2P -10.000 MHz
 F2 -1257.58 Hz
 FWHM 6.40000 MHz
 NZCN 1000.36048 Hz

67.1674
 76.7438
 76.9988
 77.2518

124.3496
 124.7429
 126.5058
 127.4035
 127.8347
 128.1897
 128.2602
 128.4922
 129.4711
 131.1682
 131.6113
 131.6380
 133.2502
 133.2646
 134.1255



ppm

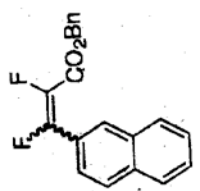


Current Data Parameters
NAME: 1
EXPNO: 1
PROCNO: 1

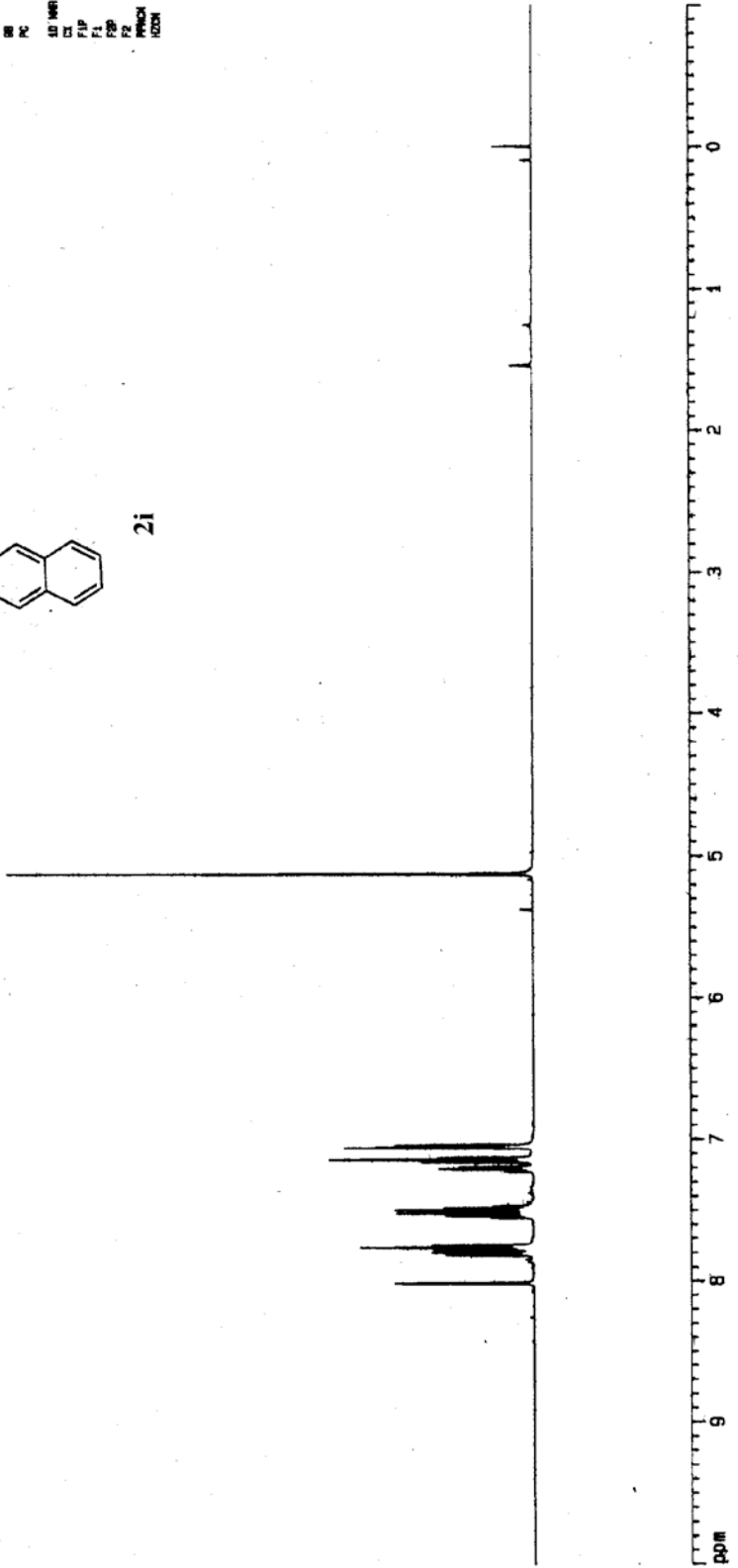
F2 - Acquisition Parameters
Date_ 20020909
Time 12.40
INSTRUM ERX000
PROBHD 5 mm NalLinu
TD 65536
SOLVENT CDCl3
NS 16
DS 2
AQ 1020.876 Hz
RG 0.318264 Hz
FIDRES 1.889812 Hz
AQ 48.400 Hz
RG 8.00 Hz
TE 300.2 K
D1 1.00000000 sec
P1 0.30 sec
SFO1 500.1300000 MHz
NUC1 1H
PUL1 zgpg30

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

40 Mhz plot parameters
SI 32768
SF 10.000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2i

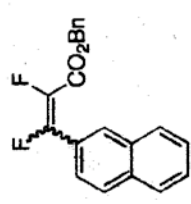


Current Data Parameters
 NAME: none-0-0
 EXPNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_ : 20020809
 Time : 13.00
 INSTRUM : DR5000
 PROBHD : 5 mm Multinu
 PULPROG : zgpg30
 TD : 65536
 SOLVENT : CDCl3
 NS : 2048
 DS : 2
 SWH : 50886.336 Hz
 FIDRES : 0.000047 Hz
 AQ : 0.00000000 sec
 RG : 9192.2
 DE : 12.000 um
 TE : 300.2 K
 D1 : 0.00000000 sec
 d12 : 0.00000000 sec
 RL1 : 50.00 dB
 D1 : 0.00000000 sec
 CHPROG : waltz16
 PCPD2 : 100.00 um
 SFO2 : 100.626090 MHz
 NUC2 : 1H
 PL2 : -0.00 dB
 PL12 : 50.00 dB
 PA : 5.70 um
 SFO1 : 125.770014 MHz
 NUC1 : 13C
 PL1 : -0.00 dB

F2 - Processing parameters
 SI : 32768
 SF : 125.770014 MHz
 MD : EN
 SSB : 0
 LB : 1.00 Hz
 GB : 0
 BR : 0
 PC : 1.40

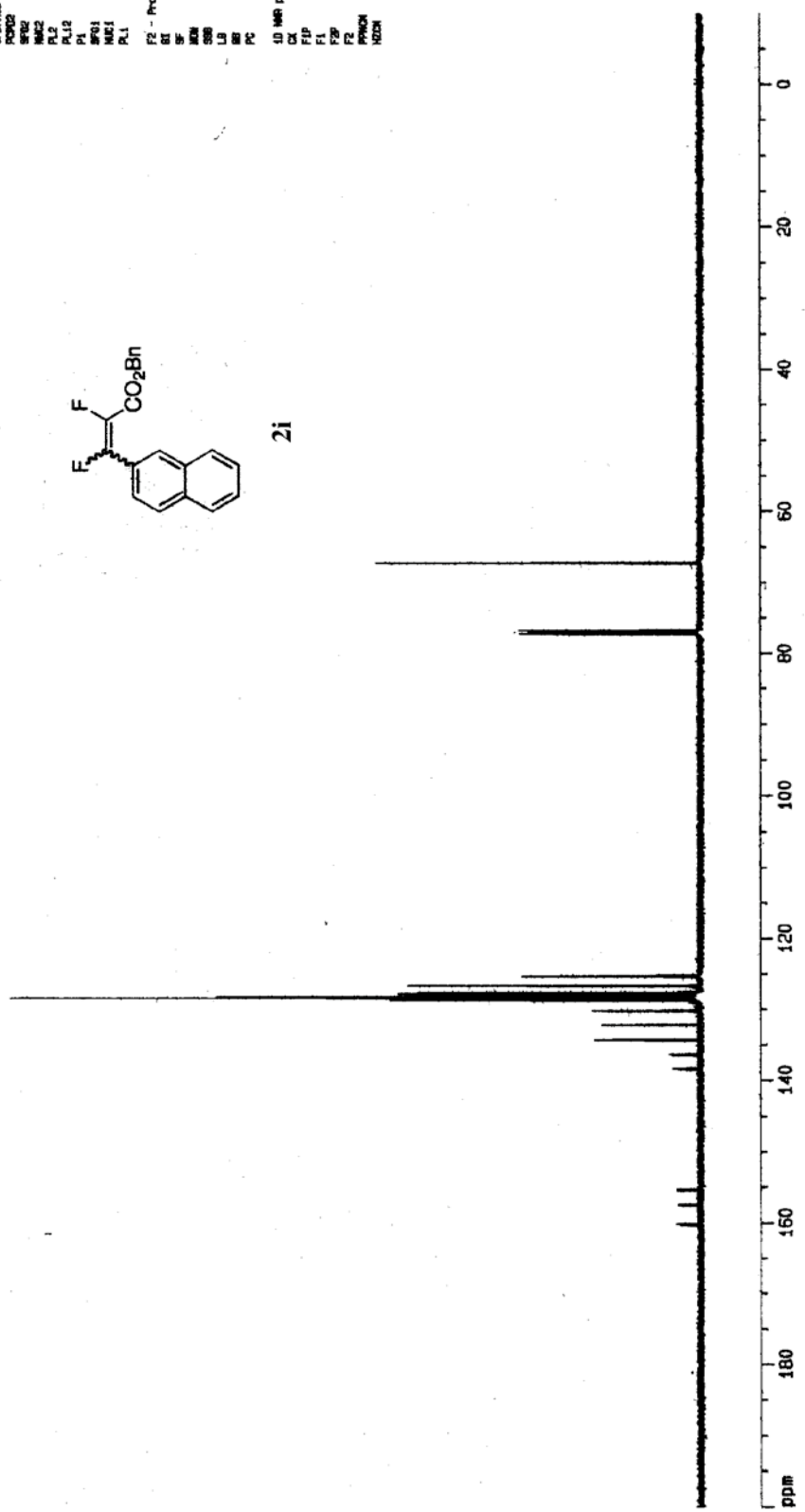
SD NMR plot parameters
 CX : 25.00 cm
 FIP : 200.000 sp
 FI : 25184.00 Hz
 FSP : -15.000 pp
 FZ : -1257.00 Hz
 SFO : 125.770014 MHz
 NUCN : 13C



67.2623
 76.7503
 77.0041
 77.2590

125.3513
 125.3685
 126.6909
 127.6877
 127.7914
 127.8367
 128.1920
 128.3668
 128.7105
 130.1783
 132.2216
 134.2721
 134.3807

ppm

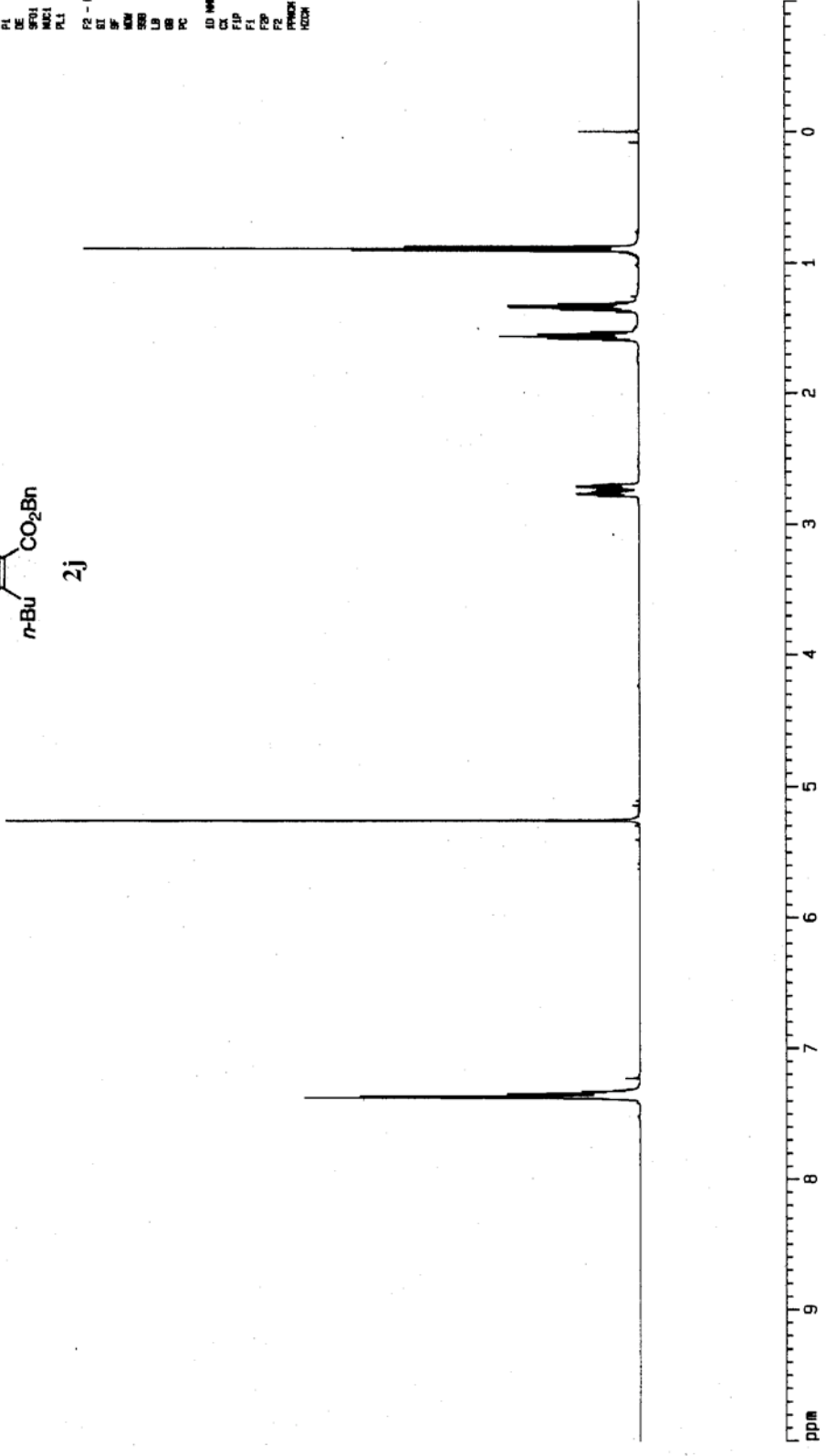
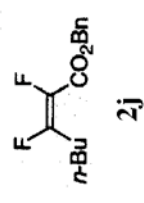


Current Data Parameters
 NAME Home-S-9
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 500000
 Time 9.17
 INSTRUM spect
 PULPROG zgpg30
 TD 65536
 SFO1 500.1350699 MHz
 F2 500.1350699 MHz
 PC 1.00

F2 - Processing parameters
 SI 32768
 SF 500.1350699 MHz
 MD 32
 LB 0.30 Hz
 GB 0
 PC 1.00

3D MR plot parameters
 CX 25.00 cm
 FIP 10.000 00
 FI 0001.30 Hz
 FQ -1.000 00
 F2 -500.13 Hz
 FREQH 0.44589 00
 FREQW 220.00722 Hz

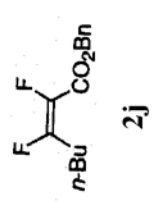
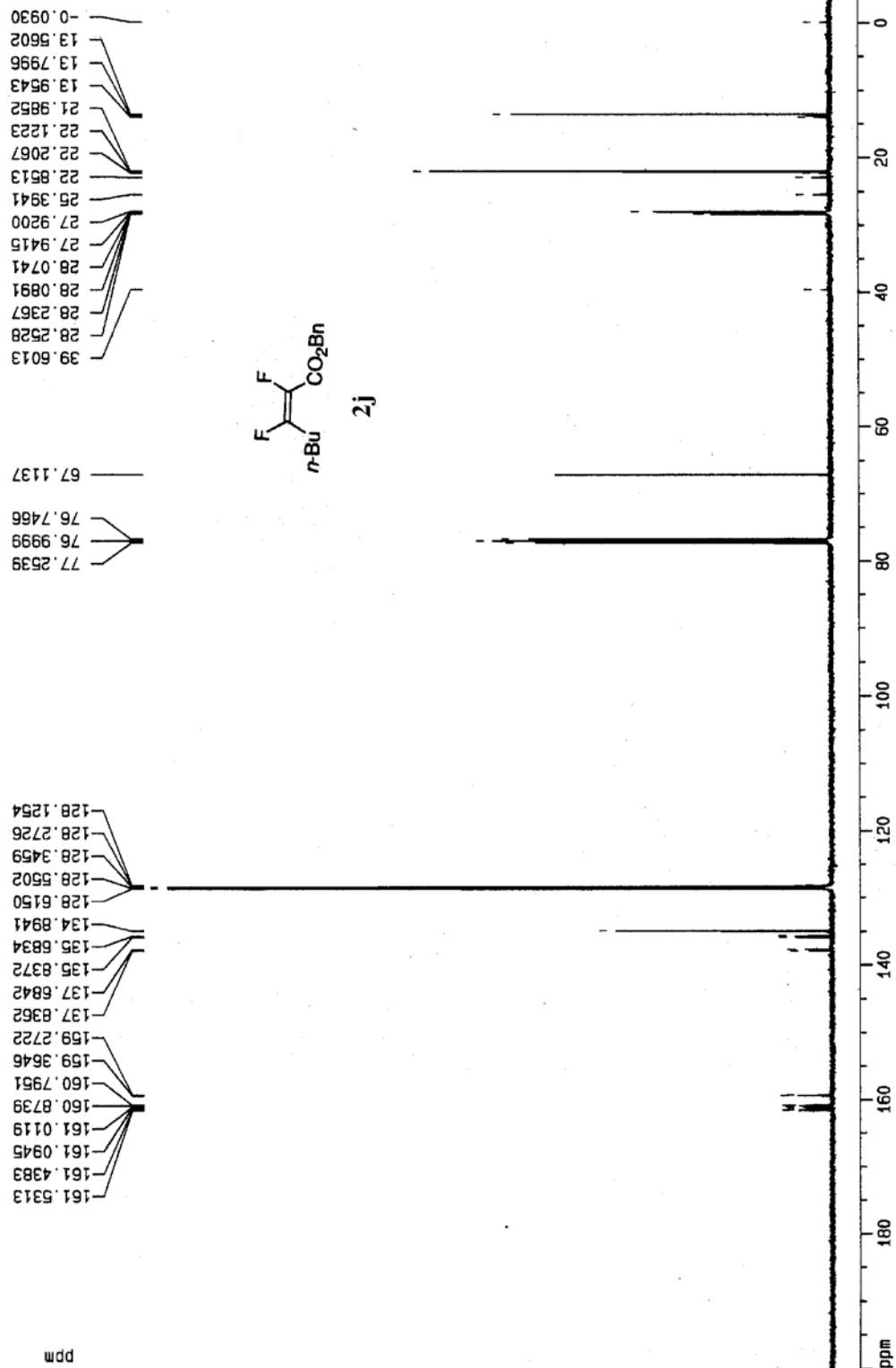


Current Data Parameters
 NAME: Name-6-a
 EXPNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 000000
 Time: 9.31
 INSTRUM: DPM0000
 PROBRD: 5 mm Multima
 PULPROG: zgpg30
 TD: 65536
 SFO: 500.130460 MHz
 AQ: 2.00000000
 SI: 32768
 SF: 500.130460 MHz
 DQ: 1.00000000
 PC: 1.40

1D NMR plot parameters
 CX: 28.0000 Hz
 FID: 200.000 Hz
 F1: 25.000 Hz
 F2: -10.000 Hz
 F3: -1507.00 Hz
 PPM0: 8.40000 Hz
 XZCN: 1.00000 Hz

F2 - Processing parameters
 SI: 32768
 SF: 500.130460 MHz
 MM: EN
 SFO: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

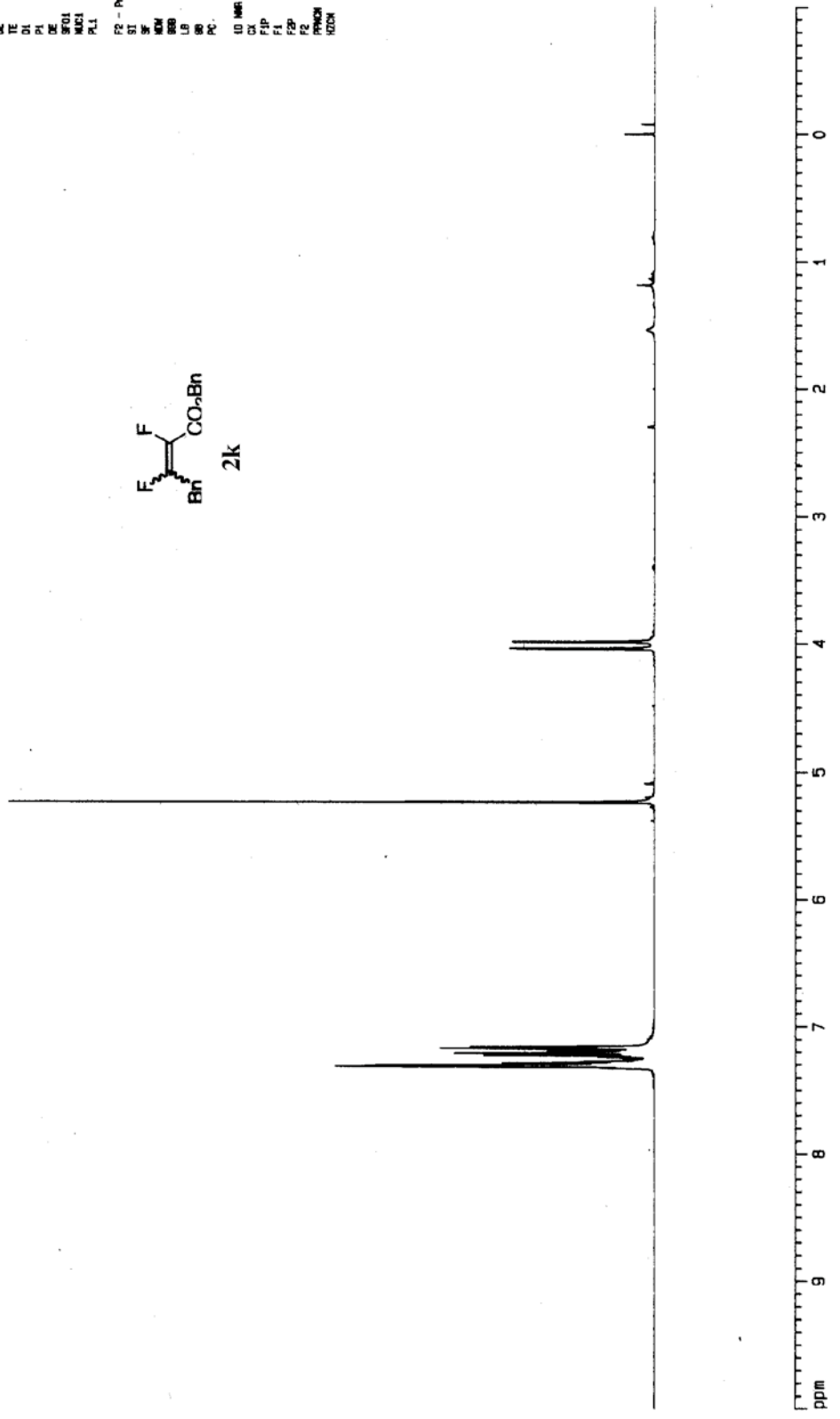
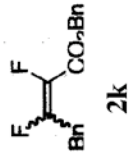


Current Data Parameters
 NAME: Name-0-9
 EXPNO: 3
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 000000
 Time: 20.06
 INSTRUM: DR0500
 PULPROG: zgpg30
 TD: 65536
 SFO: 500.136
 AQ: 1.00000000
 DE: 0.00000000
 TE: 300.2 K
 F1: 0.30 us
 F2: 0.30 us
 F3: 0.30 us
 F4: 0.30 us
 F5: 0.30 us
 F6: 0.30 us
 F7: 0.30 us
 F8: 0.30 us
 F9: 0.30 us
 F10: 0.30 us
 F11: 0.30 us
 F12: 0.30 us
 F13: 0.30 us
 F14: 0.30 us
 F15: 0.30 us
 F16: 0.30 us
 F17: 0.30 us
 F18: 0.30 us
 F19: 0.30 us
 F20: 0.30 us
 F21: 0.30 us
 F22: 0.30 us
 F23: 0.30 us
 F24: 0.30 us
 F25: 0.30 us
 F26: 0.30 us
 F27: 0.30 us
 F28: 0.30 us
 F29: 0.30 us
 F30: 0.30 us
 F31: 0.30 us
 F32: 0.30 us
 F33: 0.30 us
 F34: 0.30 us
 F35: 0.30 us
 F36: 0.30 us
 F37: 0.30 us
 F38: 0.30 us
 F39: 0.30 us
 F40: 0.30 us
 F41: 0.30 us
 F42: 0.30 us
 F43: 0.30 us
 F44: 0.30 us
 F45: 0.30 us
 F46: 0.30 us
 F47: 0.30 us
 F48: 0.30 us
 F49: 0.30 us
 F50: 0.30 us
 F51: 0.30 us
 F52: 0.30 us
 F53: 0.30 us
 F54: 0.30 us
 F55: 0.30 us
 F56: 0.30 us
 F57: 0.30 us
 F58: 0.30 us
 F59: 0.30 us
 F60: 0.30 us
 F61: 0.30 us
 F62: 0.30 us
 F63: 0.30 us
 F64: 0.30 us
 F65: 0.30 us
 F66: 0.30 us
 F67: 0.30 us
 F68: 0.30 us
 F69: 0.30 us
 F70: 0.30 us
 F71: 0.30 us
 F72: 0.30 us
 F73: 0.30 us
 F74: 0.30 us
 F75: 0.30 us
 F76: 0.30 us
 F77: 0.30 us
 F78: 0.30 us
 F79: 0.30 us
 F80: 0.30 us
 F81: 0.30 us
 F82: 0.30 us
 F83: 0.30 us
 F84: 0.30 us
 F85: 0.30 us
 F86: 0.30 us
 F87: 0.30 us
 F88: 0.30 us
 F89: 0.30 us
 F90: 0.30 us
 F91: 0.30 us
 F92: 0.30 us
 F93: 0.30 us
 F94: 0.30 us
 F95: 0.30 us
 F96: 0.30 us
 F97: 0.30 us
 F98: 0.30 us
 F99: 0.30 us
 F100: 0.30 us

F2 - Processing parameters
 SI: 16384
 SF: 500.1360330 MHz
 MD: EN
 AS: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 SI: 16384
 SF: 500.1360330 MHz
 MD: EN
 AS: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00



Current Data Parameters
 NAME: None-0-0
 EXPNO: 4
 PROCNO: 1

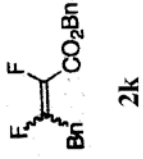
F2 - Acquisition Parameters

Date_: 000000
 Time: 21.00
 INSTRUM: DR0500
 PULPROG: zgpg30
 SOLVENT: CDCl3
 NS: 200
 DS: 2
 SWH: 50002.630 Hz
 FIDRES: 0.400007 Hz
 AQ: 0.30200336 sec
 RG: 1825.15
 INUM: 12.000 us
 DE: 6.00 us
 TE: 300.2 K
 SI: 0.000000 sec
 PL1: 0.000000 sec
 PL2: 18.00 dB
 PL3: 18.00 dB
 PL4: 18.00 dB
 PL5: 18.00 dB
 PL6: 18.00 dB
 PL7: 18.00 dB
 PL8: 18.00 dB
 PL9: 18.00 dB
 PL10: 18.00 dB
 PL11: 18.00 dB
 PL12: 18.00 dB
 PL13: 18.00 dB
 PL14: 18.00 dB
 PL15: 18.00 dB
 PL16: 18.00 dB
 PL17: 18.00 dB
 PL18: 18.00 dB
 PL19: 18.00 dB
 PL20: 18.00 dB
 PL21: 18.00 dB
 PL22: 18.00 dB
 PL23: 18.00 dB
 PL24: 18.00 dB
 PL25: 18.00 dB
 PL26: 18.00 dB
 PL27: 18.00 dB
 PL28: 18.00 dB
 PL29: 18.00 dB
 PL30: 18.00 dB
 PL31: 18.00 dB
 PL32: 18.00 dB
 PL33: 18.00 dB
 PL34: 18.00 dB
 PL35: 18.00 dB
 PL36: 18.00 dB
 PL37: 18.00 dB
 PL38: 18.00 dB
 PL39: 18.00 dB
 PL40: 18.00 dB
 PL41: 18.00 dB
 PL42: 18.00 dB
 PL43: 18.00 dB
 PL44: 18.00 dB
 PL45: 18.00 dB
 PL46: 18.00 dB
 PL47: 18.00 dB
 PL48: 18.00 dB
 PL49: 18.00 dB
 PL50: 18.00 dB
 PL51: 18.00 dB
 PL52: 18.00 dB
 PL53: 18.00 dB
 PL54: 18.00 dB
 PL55: 18.00 dB
 PL56: 18.00 dB
 PL57: 18.00 dB
 PL58: 18.00 dB
 PL59: 18.00 dB
 PL60: 18.00 dB
 PL61: 18.00 dB
 PL62: 18.00 dB
 PL63: 18.00 dB
 PL64: 18.00 dB
 PL65: 18.00 dB
 PL66: 18.00 dB
 PL67: 18.00 dB
 PL68: 18.00 dB
 PL69: 18.00 dB
 PL70: 18.00 dB
 PL71: 18.00 dB
 PL72: 18.00 dB
 PL73: 18.00 dB
 PL74: 18.00 dB
 PL75: 18.00 dB
 PL76: 18.00 dB
 PL77: 18.00 dB
 PL78: 18.00 dB
 PL79: 18.00 dB
 PL80: 18.00 dB
 PL81: 18.00 dB
 PL82: 18.00 dB
 PL83: 18.00 dB
 PL84: 18.00 dB
 PL85: 18.00 dB
 PL86: 18.00 dB
 PL87: 18.00 dB
 PL88: 18.00 dB
 PL89: 18.00 dB
 PL90: 18.00 dB
 PL91: 18.00 dB
 PL92: 18.00 dB
 PL93: 18.00 dB
 PL94: 18.00 dB
 PL95: 18.00 dB
 PL96: 18.00 dB
 PL97: 18.00 dB
 PL98: 18.00 dB
 PL99: 18.00 dB
 PL100: 18.00 dB

F2 - Processing parameters

SI: 32768
 SF: 125.767970 MHz
 RG: 1825.15
 IN: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40
 ID: 1000 plot parameters
 CX: 25.00 cm
 FIP: 200.000 pp
 FL: 20181.006 Hz
 FZ: -10.000 pp
 F2: -1.267.58 Hz
 PPM0: 0.40000 pp
 HZ0: 1000.38646 Hz

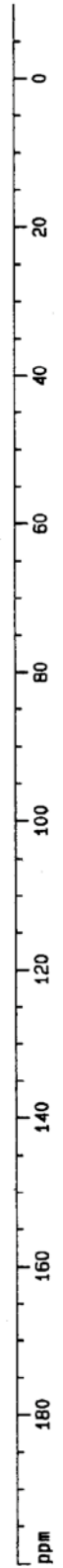
34.5076
 34.6715



67.4203
 76.7460
 76.9996
 77.2529

127.3456
 128.4717
 128.6935
 128.7413
 128.8287
 134.4042
 134.4237
 134.7355
 135.8285
 135.9807
 137.8562
 138.0046
 156.8108
 156.9127
 158.9777
 159.0818
 160.7521
 160.8273
 160.9720
 161.0477

ppm



Current Data Parameters
NAME yamada-05.11.10
EXPNO 1
PROCNO 1

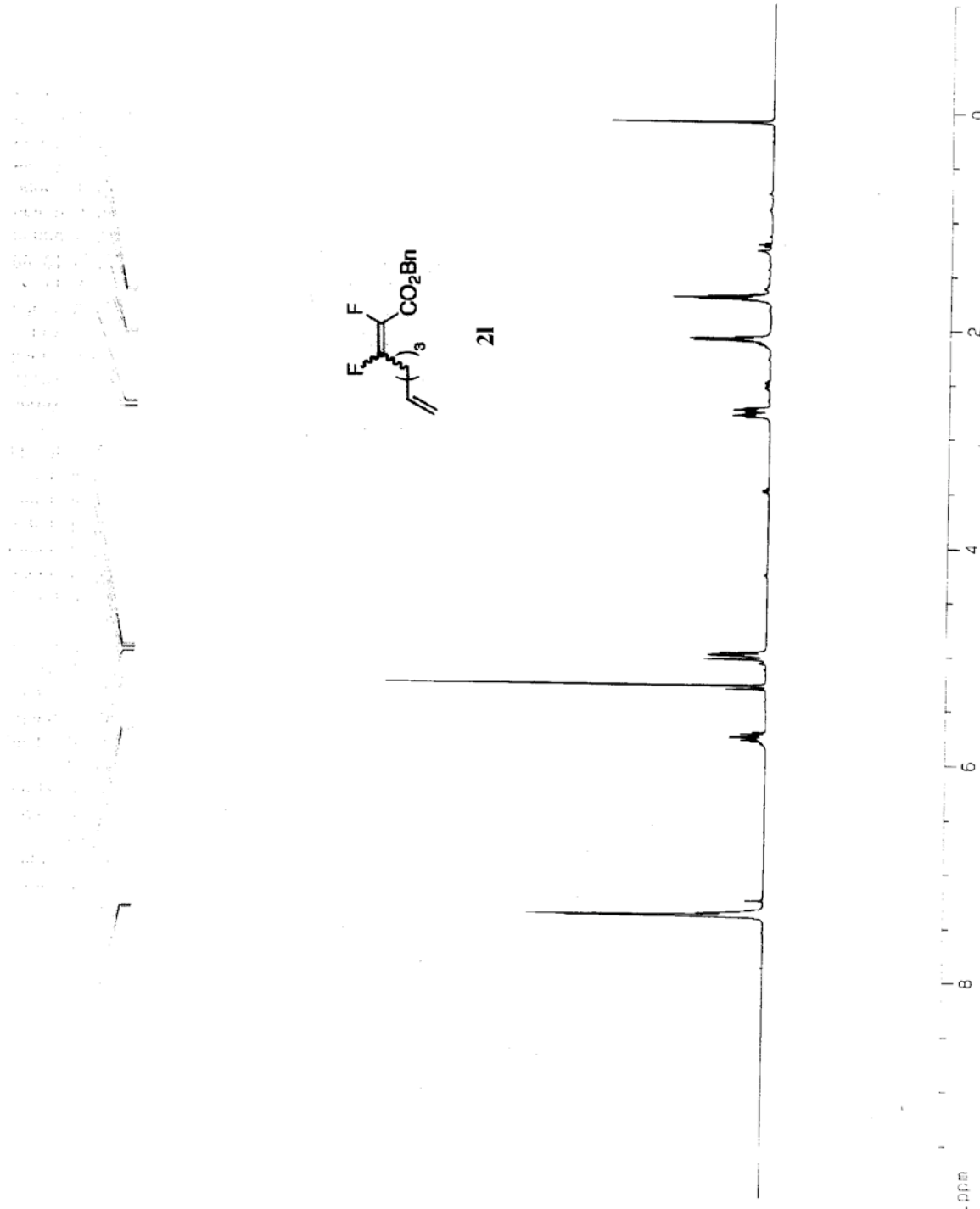
F2 - Acquisition Parameters

Date_ 20051110
Time 15.20
INSTRUM drx500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT COC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157532 Hz
AQ 3.1719923 sec
RG 57
DM 48.400 usec
JE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SF01 500.1330885 MHz

F2 - Processing parameters

SI 32768
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.33 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm



Current Data Parameters
 NAME Yamada-05.11.15
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

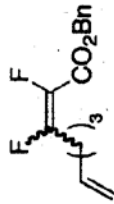
Date_ 20051115
 Time 21.33
 INSTRUM dfx500
 PROBHD 5 mm Multinuc1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 2
 SMH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912244 sec
 RG 9195.2
 DM 16.650 usec
 DE 6.00 usec
 TE 297.2 K
 D1 0.50000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWPK 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 5.70 usec
 PL1 -2.00 dB
 SF01 125.7703643 MHz

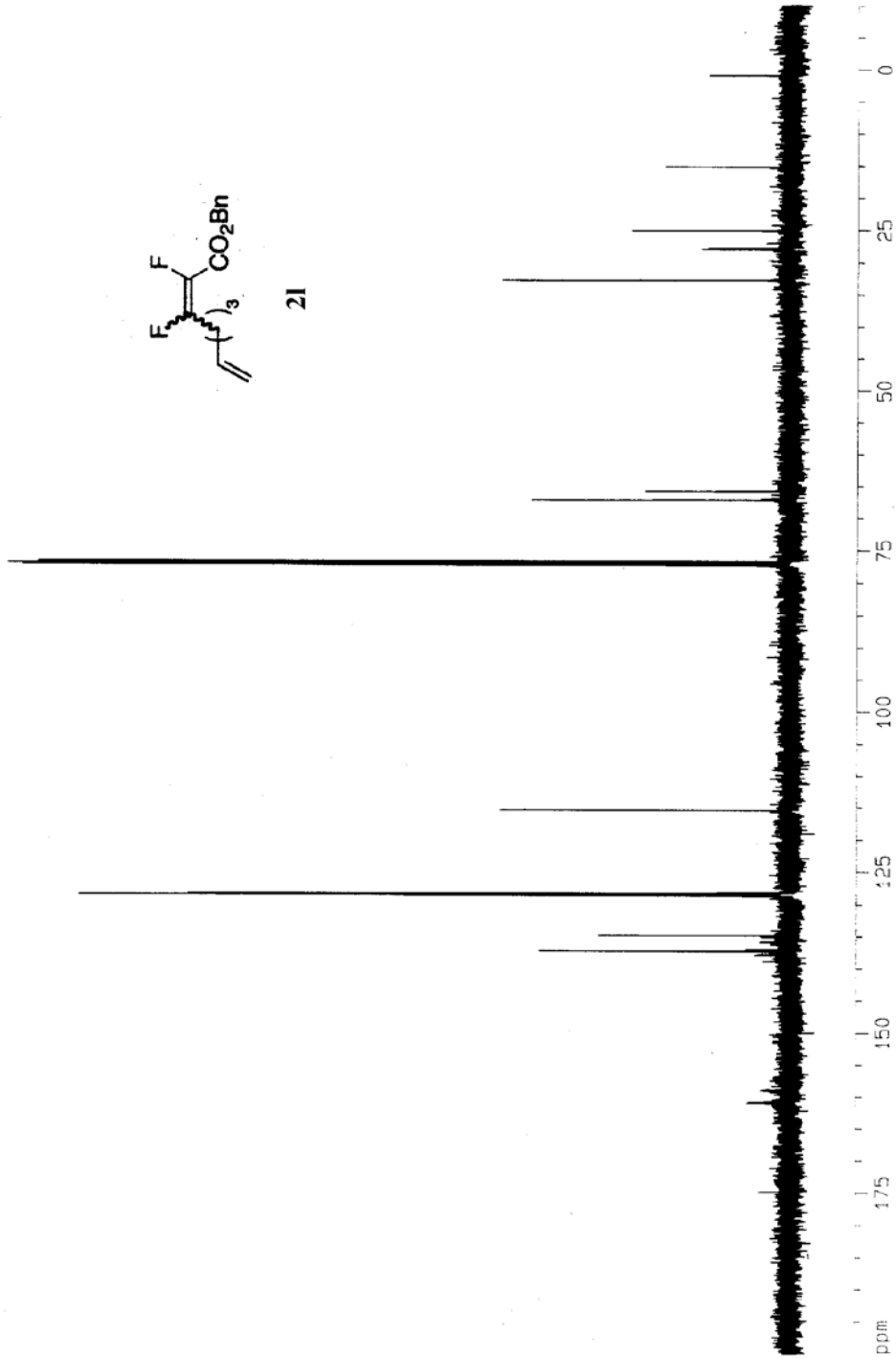
***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -6.00 dB
 PL12 13.74 dB
 PL13 13.74 dB
 SF02 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577987 MHz
 MDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 11.54 cm
 FJP 200.000 ppm
 F1 25151.56 Hz
 F2 -10.000 ppm
 PPMCM 10.50000 ppm/cm
 HZCM 1320.45679 Hz/cm



21

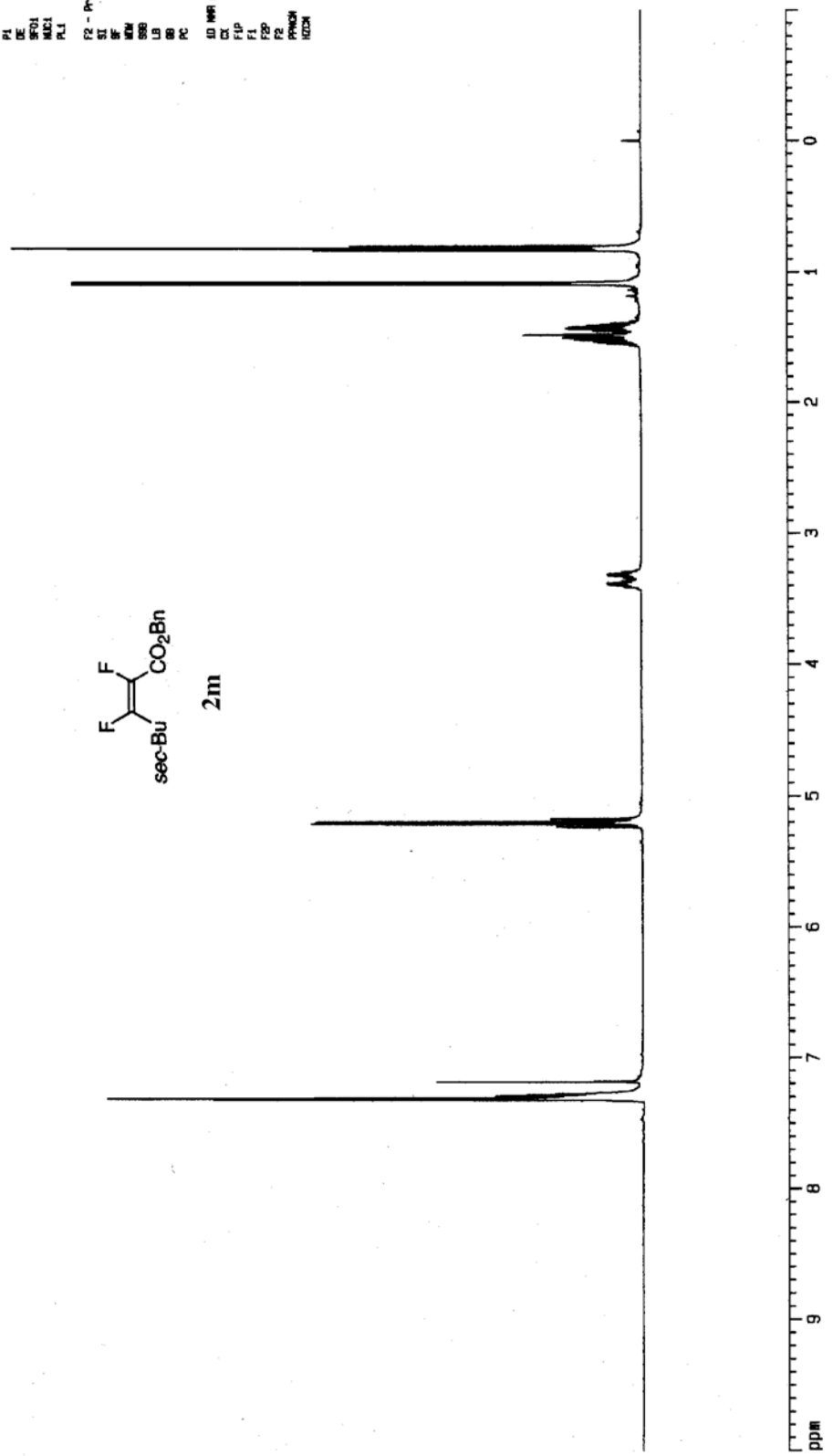
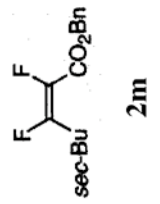


Current Data Parameters
 NAME Name-9-9
 CONNO 1
 PROONO 1

F2 - Acquisition Parameters
 Date_ 500000
 Time 20.26
 INSTRUM BRUKER
 PULPROG zgpg30
 TD 32768
 SFO1 500.1300604 MHz
 D0 1.00000000 mm
 DE 6.00 um
 TE 300.2 K
 F1 9.30 um
 DE 6.00 um
 SFO1 500.1300604 MHz
 AQC1 3H
 P1 8.00 dB

F2 - Processing parameters
 SI 32768
 SF 500.1300604 MHz
 WID 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

4D NMR plot parameters
 CX 25.00 cm
 FIP 50.000 ppb
 F1 5001.30 Hz
 F2 -1.000 ppb
 F3 -500.13 Hz
 PUNCH 0.44600 ppb
 INDCN 220.00752 Hz



Current Data Parameters
 NAME Name-9-9
 EPOCH 2
 PROCNO 1

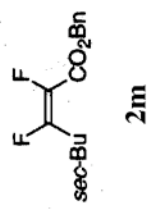
F2 - Acquisition Parameters
 Date_ 500000
 Time 20.48
 INSTRM D05000
 PRBHD 5 mm Multim
 PULPROG zgpg30
 TD 65538
 SOLVENT CDCl3
 NS 2
 DS 2
 SWH 34382.838 Hz
 FIDRES 0.469507 Hz
 AQ 0.639638 sec
 RG 4098
 DM 12.500 us
 DE 6.00 us
 TE 300.0 K
 d11 0.0300000 sec
 d12 0.0000000 sec
 PL13 16.00 dB
 D1 2.00000000 sec
 CPDPRG2 waltz16
 PCPD2 100.00 us
 SF02 500.1350048 MHz
 PL2 -4.00 dB
 PL12 18.00 dB
 PL1 8.30 us
 DE 6.00 us
 SF01 128.778214 MHz
 NU1 193
 PL1 -2.00 dB

F2 - Processing parameters
 SI 32788
 SF 128.7577934 MHz
 MM EN
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

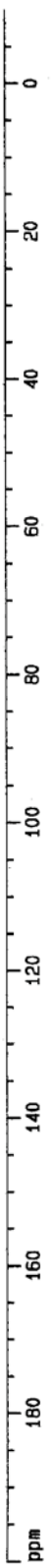
4D NMR plot parameters
 CX 25.00 cm
 FIP 200.000 Hz
 F1 20381.86 Hz
 F2P -10.000 Hz
 F2 -1267.88 Hz
 PPM0H 8.40000 Hz
 N2DM 1056.36548 Hz

11.6198
 16.6519
 26.1550
 34.0290
 34.1862
 67.1211
 76.7417
 76.9973
 77.2503

128.3161
 128.5661
 128.6550
 134.9414
 160.9210



ppm

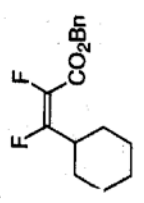


Current Data Parameters
 NAME: Name-9-28
 EXPNO: 1
 PROCNO: 1

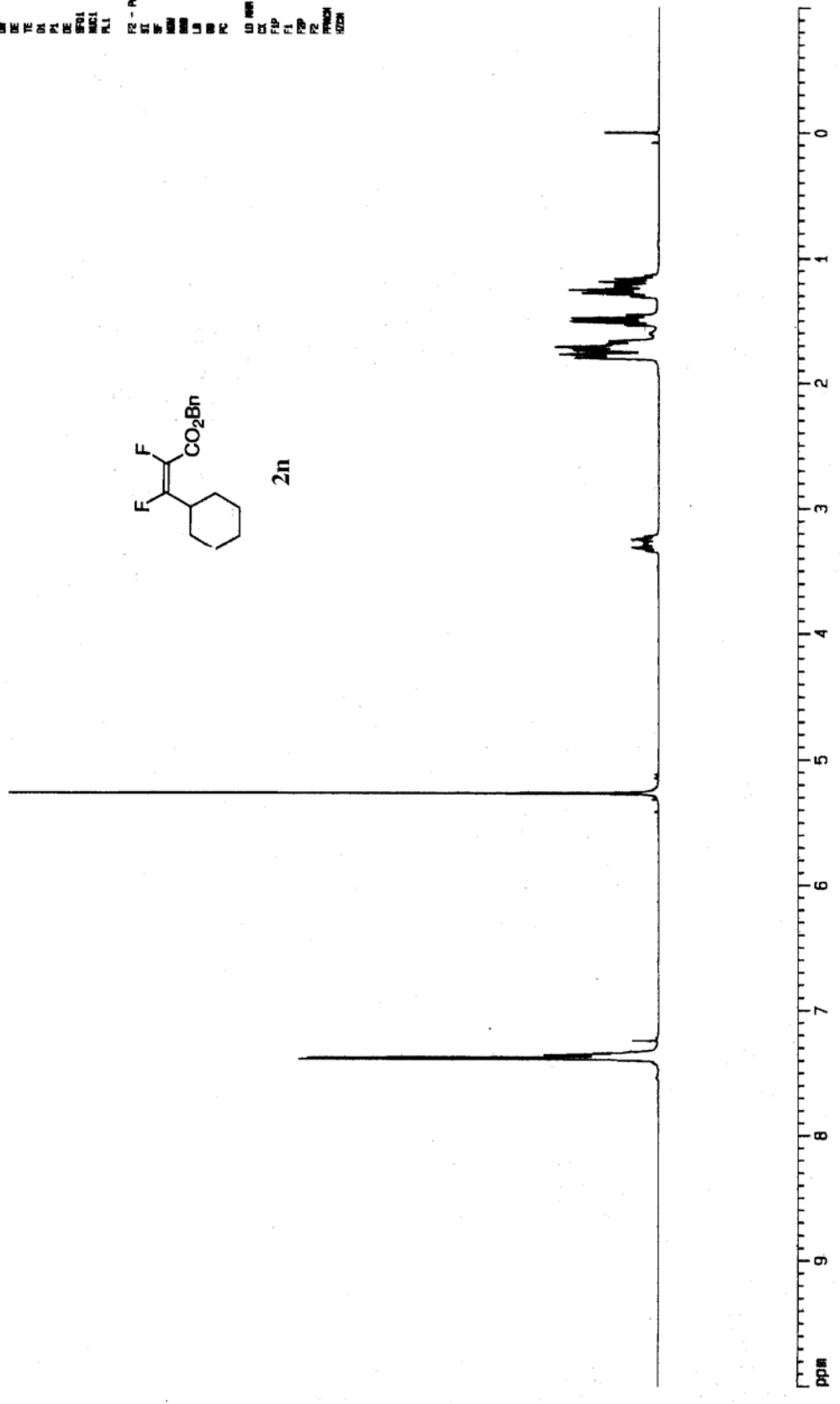
F2 - Acquisition Parameters
 Date_ :
 Time : 21.48
 JMODPRG : JMODPRG
 PROCNO : 5
 TO : 207.00
 SOLVENT : CDCl3
 NS : 16
 DS : 2
 SWH : 10000.878 Hz
 FIDRES : 0.318264 Hz
 AQ : 1.0000012 sec
 RG : 327.5
 DC : 0.00000000
 WDE : 1.00000000
 PR : 8.30 sec
 DE : 0.00 sec
 EFG1 : 000.1500000 MHz
 MC1 : 1H
 FL1 : -0.00 dB

F2 - Processing parameters
 SI : 65536
 SF : 500.1300010 MHz
 DS : 4
 SWH : 10000.878 Hz
 WDE : 1.00000000
 PR : 8.30 sec
 DE : 0.00 sec
 EFG1 : 000.1500000 MHz
 MC1 : 1H
 FL1 : -0.00 dB

LO MHz (list parameters)
 CX : 400.00 MHz
 F1P : 50.000 MHz
 F1 : 5001.30 Hz
 F2P : -1.000 MHz
 F2 : -100.15 Hz
 FREQH : 0.44000 MHz
 IZOH : 220.00720 Hz



2n



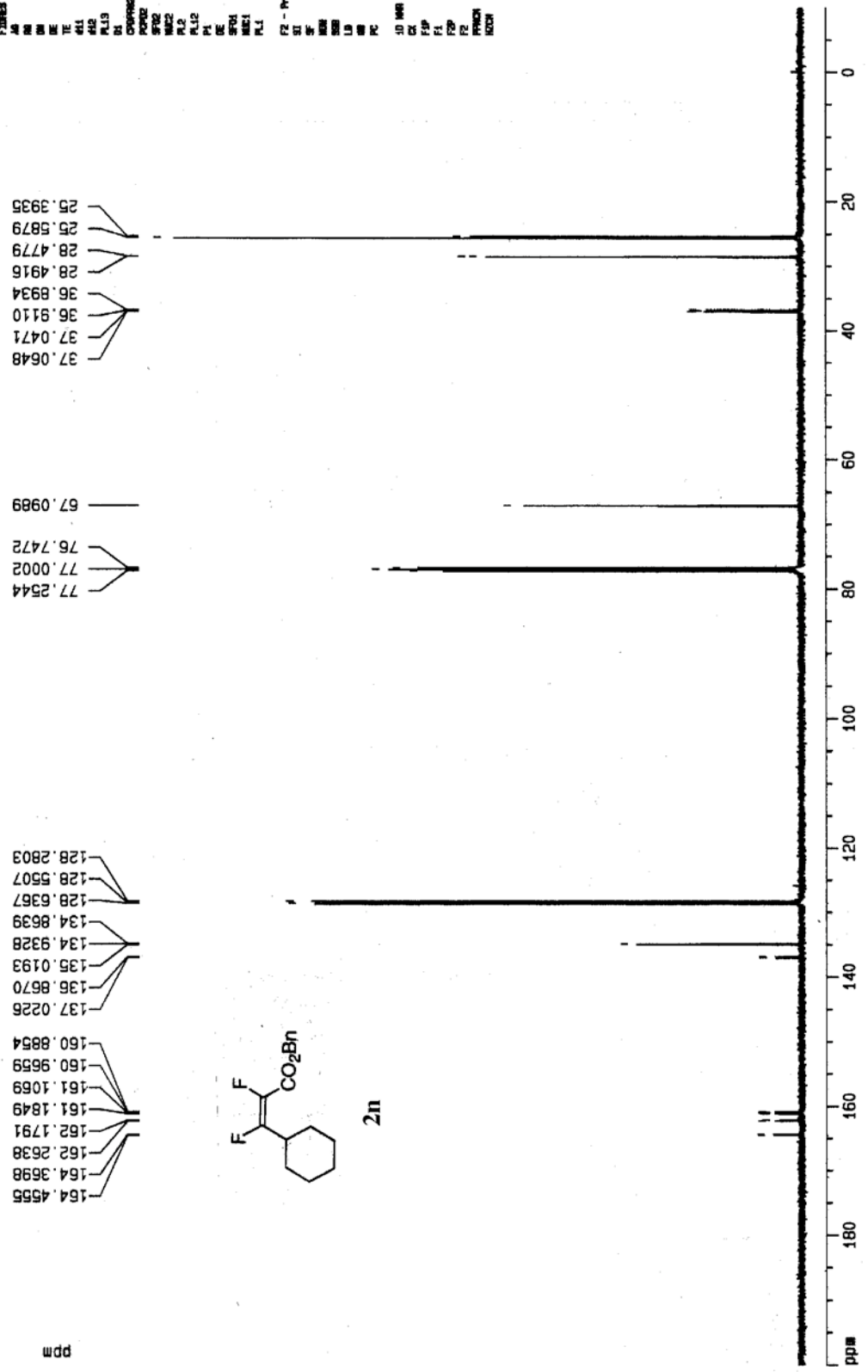
Current Data Parameters
 Name: 2
 Date: 2
 Run: 1

F2 - Acquisition Parameters
 Date: 08/08/00
 Time: 21.00
 INSTRUM: DPM000
 PULPROG: zgpg30
 TO: 000000
 SOLVENT: CDCl3
 NS: 2048
 DS: 2
 SWH: 50000.000 Hz
 FIDRES: 0.100000 Hz
 AQ: 0.160000 sec
 RG: 327.681
 GB: 12.000 cm
 SC: 8.000 cm
 TE: 300.0 K
 AT: 0.000000 sec
 AL1: 0.000000 sec
 AL2: 0.000000 sec
 AL3: 0.000000 sec
 SI: 2.000000 sec

PROBHD: 5mm QNP1H
 PULPROG: zgpg30
 F2: 500.135060 MHz
 F1: 125.761155 MHz
 NUC1: 1H
 NUC2: 13C
 PL1: -1.00 dB
 PL2: -1.00 dB
 PL3: 19.00 dB
 PL4: 19.00 dB
 PL5: 19.00 dB
 PL6: 19.00 dB
 PL7: 19.00 dB
 PL8: 19.00 dB
 PL9: 19.00 dB
 PL10: 19.00 dB
 PL11: 19.00 dB
 PL12: 19.00 dB
 PL13: 19.00 dB
 PL14: 19.00 dB
 PL15: 19.00 dB
 PL16: 19.00 dB
 PL17: 19.00 dB
 PL18: 19.00 dB
 PL19: 19.00 dB
 PL20: 19.00 dB
 PL21: 19.00 dB
 PL22: 19.00 dB
 PL23: 19.00 dB
 PL24: 19.00 dB
 PL25: 19.00 dB
 PL26: 19.00 dB
 PL27: 19.00 dB
 PL28: 19.00 dB
 PL29: 19.00 dB
 PL30: 19.00 dB
 PL31: 19.00 dB
 PL32: 19.00 dB
 PL33: 19.00 dB
 PL34: 19.00 dB
 PL35: 19.00 dB
 PL36: 19.00 dB
 PL37: 19.00 dB
 PL38: 19.00 dB
 PL39: 19.00 dB
 PL40: 19.00 dB
 PL41: 19.00 dB
 PL42: 19.00 dB
 PL43: 19.00 dB
 PL44: 19.00 dB
 PL45: 19.00 dB
 PL46: 19.00 dB
 PL47: 19.00 dB
 PL48: 19.00 dB
 PL49: 19.00 dB
 PL50: 19.00 dB
 PL51: 19.00 dB
 PL52: 19.00 dB
 PL53: 19.00 dB
 PL54: 19.00 dB
 PL55: 19.00 dB
 PL56: 19.00 dB
 PL57: 19.00 dB
 PL58: 19.00 dB
 PL59: 19.00 dB
 PL60: 19.00 dB
 PL61: 19.00 dB
 PL62: 19.00 dB
 PL63: 19.00 dB
 PL64: 19.00 dB
 PL65: 19.00 dB
 PL66: 19.00 dB
 PL67: 19.00 dB
 PL68: 19.00 dB
 PL69: 19.00 dB
 PL70: 19.00 dB
 PL71: 19.00 dB
 PL72: 19.00 dB
 PL73: 19.00 dB
 PL74: 19.00 dB
 PL75: 19.00 dB
 PL76: 19.00 dB
 PL77: 19.00 dB
 PL78: 19.00 dB
 PL79: 19.00 dB
 PL80: 19.00 dB
 PL81: 19.00 dB
 PL82: 19.00 dB
 PL83: 19.00 dB
 PL84: 19.00 dB
 PL85: 19.00 dB
 PL86: 19.00 dB
 PL87: 19.00 dB
 PL88: 19.00 dB
 PL89: 19.00 dB
 PL90: 19.00 dB
 PL91: 19.00 dB
 PL92: 19.00 dB
 PL93: 19.00 dB
 PL94: 19.00 dB
 PL95: 19.00 dB
 PL96: 19.00 dB
 PL97: 19.00 dB
 PL98: 19.00 dB
 PL99: 19.00 dB
 PL100: 19.00 dB

F2 - Processing parameters
 SI: 32768
 SF: 500.135060 MHz
 EQ: 0
 EN: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1D NMR plot parameters
 CA: 28.00 cm
 CL: 280.000 Hz
 CP: 280.000 Hz
 CZ: 280.000 Hz
 F2: -1287.000 Hz
 F3: 0.000000 Hz
 F4: 0.000000 Hz
 F5: 0.000000 Hz
 F6: 0.000000 Hz
 F7: 0.000000 Hz
 F8: 0.000000 Hz
 F9: 0.000000 Hz
 F10: 0.000000 Hz
 F11: 0.000000 Hz
 F12: 0.000000 Hz
 F13: 0.000000 Hz
 F14: 0.000000 Hz
 F15: 0.000000 Hz
 F16: 0.000000 Hz
 F17: 0.000000 Hz
 F18: 0.000000 Hz
 F19: 0.000000 Hz
 F20: 0.000000 Hz
 F21: 0.000000 Hz
 F22: 0.000000 Hz
 F23: 0.000000 Hz
 F24: 0.000000 Hz
 F25: 0.000000 Hz
 F26: 0.000000 Hz
 F27: 0.000000 Hz
 F28: 0.000000 Hz
 F29: 0.000000 Hz
 F30: 0.000000 Hz
 F31: 0.000000 Hz
 F32: 0.000000 Hz
 F33: 0.000000 Hz
 F34: 0.000000 Hz
 F35: 0.000000 Hz
 F36: 0.000000 Hz
 F37: 0.000000 Hz
 F38: 0.000000 Hz
 F39: 0.000000 Hz
 F40: 0.000000 Hz
 F41: 0.000000 Hz
 F42: 0.000000 Hz
 F43: 0.000000 Hz
 F44: 0.000000 Hz
 F45: 0.000000 Hz
 F46: 0.000000 Hz
 F47: 0.000000 Hz
 F48: 0.000000 Hz
 F49: 0.000000 Hz
 F50: 0.000000 Hz
 F51: 0.000000 Hz
 F52: 0.000000 Hz
 F53: 0.000000 Hz
 F54: 0.000000 Hz
 F55: 0.000000 Hz
 F56: 0.000000 Hz
 F57: 0.000000 Hz
 F58: 0.000000 Hz
 F59: 0.000000 Hz
 F60: 0.000000 Hz
 F61: 0.000000 Hz
 F62: 0.000000 Hz
 F63: 0.000000 Hz
 F64: 0.000000 Hz
 F65: 0.000000 Hz
 F66: 0.000000 Hz
 F67: 0.000000 Hz
 F68: 0.000000 Hz
 F69: 0.000000 Hz
 F70: 0.000000 Hz
 F71: 0.000000 Hz
 F72: 0.000000 Hz
 F73: 0.000000 Hz
 F74: 0.000000 Hz
 F75: 0.000000 Hz
 F76: 0.000000 Hz
 F77: 0.000000 Hz
 F78: 0.000000 Hz
 F79: 0.000000 Hz
 F80: 0.000000 Hz
 F81: 0.000000 Hz
 F82: 0.000000 Hz
 F83: 0.000000 Hz
 F84: 0.000000 Hz
 F85: 0.000000 Hz
 F86: 0.000000 Hz
 F87: 0.000000 Hz
 F88: 0.000000 Hz
 F89: 0.000000 Hz
 F90: 0.000000 Hz
 F91: 0.000000 Hz
 F92: 0.000000 Hz
 F93: 0.000000 Hz
 F94: 0.000000 Hz
 F95: 0.000000 Hz
 F96: 0.000000 Hz
 F97: 0.000000 Hz
 F98: 0.000000 Hz
 F99: 0.000000 Hz
 F100: 0.000000 Hz



Current Data Parameters
NAME Yamada-05.11.11
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

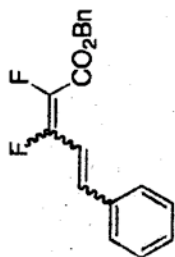
Date_ 20051111
Time 20.56
INSTRUM drx500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 128
DM 48.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRRK 0.01500000 sec

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

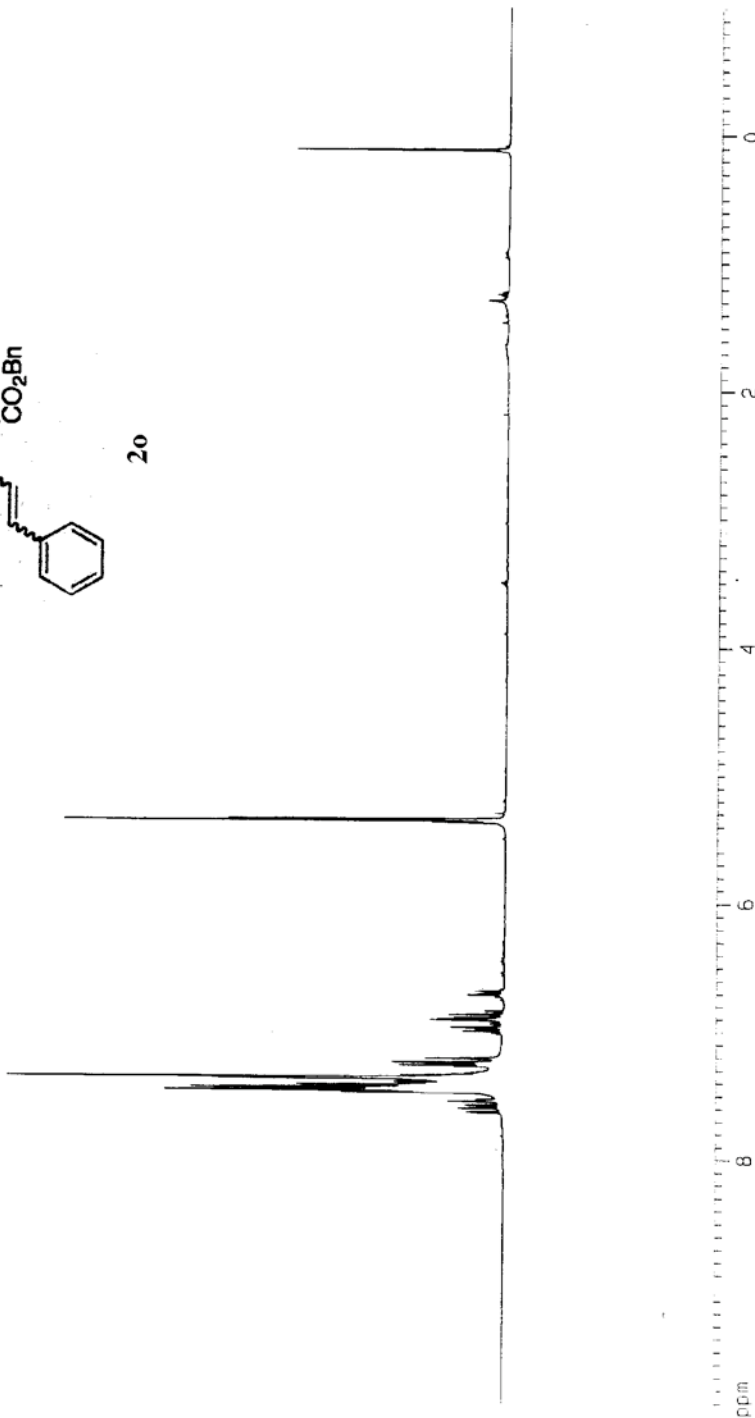
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SF01 500.1330885 MHz

F2 - Processing parameters

SI 32768
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0.30 HZ
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 7.03 cm
FIP 10.000 ppm
F1 5001.30 HZ
F2P -1.000 ppm
F2 -500.13 HZ
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm



20



Current Date Parameters
 Name: 12-1
 EXPNO: 1
 PROCNO: 1

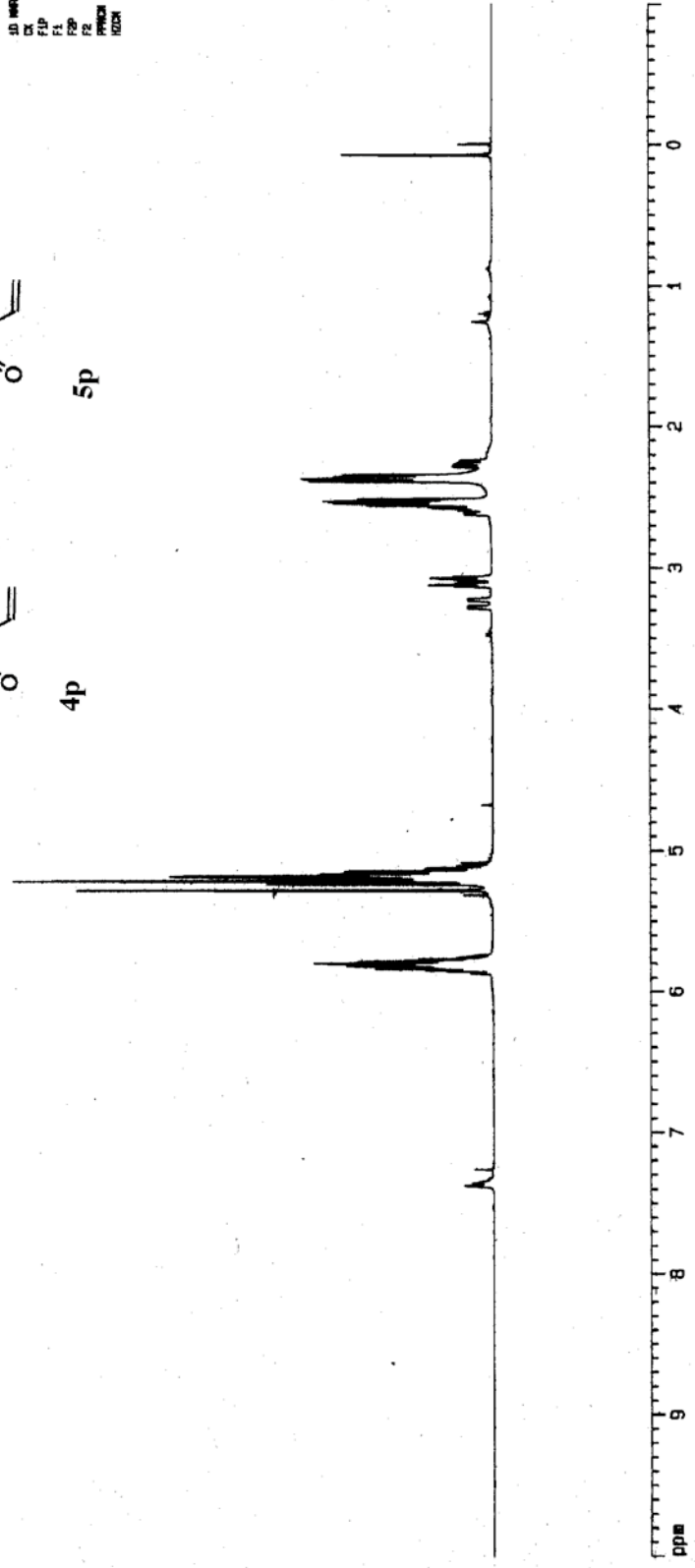
F2 - Acquisition Parameters
 Date_: 20021204
 Time: 16.30
 INSTRUM: DRG500
 PROBRD: 5 mm Multilin
 PULPROG: zgpg30
 TD: 32768
 SOLVENT: CDCl3
 NS: 16
 DS: 2
 SWH: 10230.070 Hz
 FIDRES: 0.133584 Hz
 AQRES: 1.058921 s
 DE: 40.15
 DM: 40.000 um
 DE: 6.00 um
 TE: 300.0 K
 D1: 1.00000000 s
 PL: 6.30 um
 SF01: 500.133068 MHz
 NUC1: 1H
 P1: 6.00 dB

F2 - Processing parameters
 SI: 16384
 SF: 500.133068 MHz
 NH: 64
 SH: 64
 AZ: 0
 DE: 0.30 Hz
 DM: 0
 PC: 1.00

1D NMR plot parameters
 CX: 25.00 cm
 F1P: 10.000 pp
 F1: 5001.50 Hz
 F2P: -1.000 pp
 F2: -500.13 Hz
 PRACH: 0.44000 pp
 RDCH: 220.06721 Hz



5p
4p



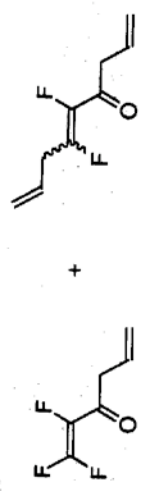
Current Data Parameters
 NAME: none-12-4
 EXPNO: 4
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20021204
 Time: 16.38
 INSTRUM: DRGDS0
 PROBRD: 5 mm NAL31ms
 PULPROG: zgpg30
 TD: 65535
 SFO: 500.135
 AQ: 4.000
 RG: 2
 SWH: 5000.000 Hz
 FIDRES: 0.000007 Hz
 AQRES: 0.020000 Hz
 AS: 4000
 DM: 12.000 us
 DE: 7.00 us
 TE: 300.2 K
 411: 0.0000000 us
 412: 0.0000000 us
 PL13: 18.00 dB
 DI: 0.0000000 us
 CHPROG: waltz16
 PCPD2: 100.00 us
 WPC2: 500.1350000 MHz
 PL2: -9.00 dB
 PL12: 18.00 dB
 PL1: 6.70 us
 SF01: 528.778214 MHz
 NS21: 13C
 PL1: -9.00 dB

F2 - Processing parameters
 SI: 32768
 SF: 128.7377948 MHz
 NH: 64
 SH: 0
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.46

LD MR plot parameters
 CX: 50.00 CH
 F1P: 200.000 PP
 F1: 25481.76 Hz
 F2P: -10.000 PP
 F2: -1207.00 Hz
 PRNCH: 0.40000 PP
 NZCN: 1000.00000 Hz

42.8241
 42.8031
 42.2534
 42.2365



132.3881
 131.5508
 120.3702
 120.1247
 119.5152

ppm

