

# AN EFFICIENT PREPARATION OF NEW SULFONYL FLUORIDES AND LITHIUM SULFONATES

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## SUPPORTING INFORMATION

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## General experimental methods

**General.** Solvents were distilled before use. Reagents were obtained commercially and used without further purification. CsF and KF were dried in an oven at 250°C overnight.  $^1\text{H}$ ,  $^{19}\text{F}$  and  $^{13}\text{C}$  NMR were recorded at room temperature in  $\text{CDCl}_3$  (unless stated otherwise cited) at 300 MHz, 282 MHz and 75 MHz respectively. Chemical shifts are given in ppm relative to residual peak of solvent ( $\delta_{\text{H}} = 7.26$  ppm for  $\text{CHCl}_3$ ,  $\delta_{\text{H}} = 2.50$  ppm for  $\text{Me}_2\text{SO}$ ,  $\delta_{\text{H}} = 2.05$  ppm for acetone,  $\delta_{\text{C}} = 77.0$  ppm for  $\text{CDCl}_3$ ,  $\delta_{\text{C}} = 39.52$  ppm for  $\text{Me}_2\text{SO}-d_6$  and  $\delta_{\text{C}} = 29.84$  ppm for acetone- $d_6$ ) and  $\text{CFCl}_3$  ( $^{19}\text{F}$ ). Coupling constants are given in Hertz. TLC analyses were carried out on silica gel deposited on aluminum plates, detection being done by UV. Silica gel chromatography was performed with silica gel (230 - 400 mesh). Mass spectrometric data (MS) were obtained by electron ionization (EI, 70 eV), chemical ionization (CI,  $\text{NH}_3$  or  $\text{CH}_4$ ), or electrospray ionization (ESI). Melting points are uncorrected and were performed in capillary tubes. HRMS or combustion of new sulfinates **7a** and **8a** is precluded by their thermal stability. As lithium sulfonates **21-27** are hygroscopic solids, their elemental analysis were not determined.

**Synthesis of 1-(Bromo-difluoro-methylsulfanyl)-benzene (1a):**<sup>1</sup> To a suspension of sodium hydride (6 g, 150 mmol) in anhydrous DMF (100 mL), was slowly added thiophenol (10.2 mL, 100 mmol) at 0°C over a period of 30 min. The reaction mixture was cooled to -50°C for 15 min before bromodifluoromethane (27 mL, 300 mmol) was added. The resulting reaction mixture was maintained at -50°C for 3 h and stirred 1 h from -50°C to room temperature. The resulting flask was cooled in an ice-water bath and excess sodium hydride was quenched by dropwise addition of water (100 mL). The aqueous phase was extracted with Et<sub>2</sub>O (3 x 100 mL), the combined organic layers washed with water (3 x 100 mL), brine (100 mL), and dried over MgSO<sub>4</sub>. Filtration and solvent evaporation left a crude product that was purified by distillation. **1a** was obtained as a colorless liquid (14.3 g, 60%). B.p. 97°C / 34 mmHg; *R*<sub>f</sub>=0.7 (Pentane); <sup>1</sup>H NMR: δ = 7.66 (d, 2H, <sup>3</sup>*J*<sub>H-H</sub> = 7.4 Hz), 7.52 (m, 1H), 7.43 (m, 2H); <sup>13</sup>C NMR: δ = 136.5, 131.2, 129.6, 127.3 (t, <sup>3</sup>*J*<sub>F-C</sub> = 1.1 Hz), 119.4 (t, <sup>1</sup>*J*<sub>F-C</sub> = 336.0 Hz); <sup>19</sup>F NMR: δ = -22.53 (s, 2F).

**1-(2-Bromo-1,1,2,2-tetrafluoro-ethylsulfanyl)-4-fluoro-benzene (2b):** colorless liquid (83% yield); b.p 85-90°C/30mmHg; *R*<sub>f</sub>=0.8 (Pentane); <sup>1</sup>H NMR: δ = 7.65 (m, 2H), 7.12 (m, 2H); <sup>13</sup>C NMR: δ = 164.8 (d, <sup>1</sup>*J*<sub>F-C</sub> = 252.5 Hz), 139.7 (d, <sup>3</sup>*J*<sub>F-C</sub> = 9.3 Hz), 122.1 (ttd, <sup>1</sup>*J*<sub>F-C</sub> = 290.9 Hz, <sup>2</sup>*J*<sub>F-C</sub> = 34.3 Hz, <sup>6</sup>*J*<sub>F-C</sub> = 1.5 Hz), 118.9 (m), 116.9 (d, <sup>2</sup>*J*<sub>F-C</sub> = 22.0 Hz) 116.8 (tt, <sup>1</sup>*J*<sub>F-C</sub> = 313.4 Hz, <sup>2</sup>*J*<sub>F-C</sub> = 40.4 Hz); <sup>19</sup>F NMR: δ = -62.71 (t, 2F, <sup>3</sup>*J*<sub>F-F</sub> = 8.0 Hz), -108.88 (t, 2F, <sup>3</sup>*J*<sub>F-F</sub> = 8.0 Hz) -108.88 (m, 1F). Anal. Calcd for C<sub>8</sub>H<sub>4</sub>BrF<sub>5</sub>S: C, 31.29; H, 1.31. Found C, 31.64; H, 1.58.

**1-Bromo-4-(2-Bromo-1,1,2,2-tetrafluoro-ethylsulfanyl)-benzene (2c):** colorless liquid (90% yield); *R*<sub>f</sub>=0.8 (Pentane); <sup>1</sup>H NMR: δ = 7.57-7.49 (m, 4H); <sup>13</sup>C NMR: δ = 138.7, 132.8, 126.4, 122.6 (t, <sup>3</sup>*J*<sub>F-C</sub> = 2.7 Hz), 121.9 (tt, <sup>1</sup>*J*<sub>F-C</sub> = 291.2 Hz, <sup>2</sup>*J*<sub>F-C</sub> = 34.2 Hz), 116.69 (tt, <sup>1</sup>*J*<sub>F-C</sub> = 312.9 Hz, <sup>2</sup>*J*<sub>F-C</sub> = 40.2 Hz); <sup>19</sup>F NMR: δ = -62.75 (t, 2F, <sup>3</sup>*J*<sub>F-F</sub> = 8.0 Hz), -85.59 (t, 2F, <sup>3</sup>*J*<sub>F-F</sub> = 8.0 Hz). Anal. Calcd for C<sub>8</sub>H<sub>4</sub>Br<sub>2</sub>F<sub>4</sub>S: C, 26.11; H, 1.10. Found C, 26.38; H, 1.38.

**2-(2-Bromo-1,1,2,2-tetrafluoro-ethylsulfanyl)-pyridine (3a):** yellow liquid (85% yield); *R*<sub>f</sub>=0.2 (Pentane/CH<sub>2</sub>Cl<sub>2</sub> 1:1); <sup>1</sup>H NMR: δ = 8.66 (m, 1H), 7.77-7.66 (m, 2H), 7.36 (ddd, 1H, <sup>3</sup>*J*<sub>H-H</sub> = 7.3 Hz, <sup>3</sup>*J*<sub>H-H</sub> = 4.8 Hz, <sup>4</sup>*J*<sub>H-H</sub> = 1.3 Hz); <sup>13</sup>C NMR: δ = 150.8, 148.0, 137.6, 130.9,

<sup>1</sup> a) Prakash, G. K. S.; Hu, J.; Olah, G. A. *J. Org. Chem.* **2003**, 68, 4457-4463. b) Reutrakul, V.; Thongpaisanwong, T.; Tuchinda, P.; Kuhakarn, C.; Pohmakotr, M. *J. Org. Chem.* **2004**, 69, 6913-6915.

124.5, 123.1 (tt,  $^1J_{\text{F-C}} = 292.3$  Hz,  $^2J_{\text{F-C}} = 34.3$  Hz), 116.8 (tt,  $^1J_{\text{F-C}} = 313.0$  Hz,  $^2J_{\text{F-C}} = 39.7$  Hz);  $^{19}\text{F}$  NMR:  $\delta = -63.12$  (t, 2F,  $^3J_{\text{F-F}} = 8.0$  Hz),  $-84.55$  (t, 2F,  $^3J_{\text{F-F}} = 8.0$  Hz). Anal. Calcd for  $\text{C}_7\text{H}_4\text{BrF}_4\text{NS}$ : C, 28.98; H, 1.39. Found C, 29.12; H, 1.56.

**[Difluoro-(4-fluoro-phenylsulfanyl)-methyl]-trimethyl-silane (4b):** yellow liquid (95% yield);  $R_f = 0.6$  (Pentane);  $^1\text{H}$  NMR:  $\delta = 7.56$  (m, 2H), 7.06 (m, 2H), 0.26 (s, 9H);  $^{13}\text{C}$  NMR:  $\delta = 169.9$  (d,  $^1J_{\text{F-C}} = 249.7$  Hz), 138.8 (d,  $^3J_{\text{F-C}} = 8.8$  Hz), 133.9 (td,  $^1J_{\text{F-C}} = 300.5$  Hz,  $^6J_{\text{F-C}} = 1.1$  Hz), 121.5 (td,  $^3J_{\text{F-C}} = 4.4$  Hz,  $^4J_{\text{F-C}} = 3.3$  Hz), 116.1 (d,  $^2J_{\text{F-C}} = 21.9$  Hz),  $-4.1$  (t,  $^3J_{\text{F-C}} = 1.4$  Hz);  $^{19}\text{F}$  NMR:  $\delta = -88.41$  (s, 2F),  $-112.06$  (m, 1F). Anal. Calcd for  $\text{C}_{10}\text{H}_{13}\text{F}_3\text{SSi}$ : C, 47.97; H, 5.23. Found C, 48.12; H, 5.49.

**Trimethyl-(1,1,2,2-tetrafluoro-2-phenylsulfanyl-ethyl)-silane (5a):** yellow liquid (90% yield);  $R_f = 0.7$  (Pentane);  $^1\text{H}$  NMR:  $\delta = 7.65$  (m, 2H), 7.48-7.36 (m, 3H), 0.27 (m, 9H);  $^{13}\text{C}$  NMR:  $\delta = 137.3$ , 130.3, 129.2, 127.5 (tt,  $^1J_{\text{F-C}} = 281.8$  Hz,  $^2J_{\text{F-C}} = 32.5$  Hz), 124.6 (m), 123.0 (tt,  $^1J_{\text{F-C}} = 273.2$  Hz,  $^2J_{\text{F-C}} = 45.3$  Hz),  $-4.0$  (m);  $^{19}\text{F}$  NMR:  $\delta = -82.88$  (t, 2F,  $^3J_{\text{F-F}} = 4.6$  Hz),  $-122.56$  (t, 2F,  $^3J_{\text{F-F}} = 4.6$  Hz). Anal. Calcd for  $\text{C}_{11}\text{H}_{14}\text{F}_4\text{SSi}$ : C, 46.79; H, 5.00. Found C, 47.01; H, 5.28.

**Trimethyl-[1,1,2,2-tetrafluoro-2-(4-fluoro-phenyl-sulfanyl)-ethyl]-silane (5b):** yellow liquid (88% yield);  $R_f = 0.6$  (Pentane);  $^1\text{H}$  NMR:  $\delta = 7.64$  (m, 2H), 7.09 (m, 2H), 0.27 (s, 9H);  $^{13}\text{C}$  NMR:  $\delta = 164.4$  (d,  $^1J_{\text{F-C}} = 251.4$  Hz), 139.5 (d,  $^3J_{\text{F-C}} = 8.8$  Hz), 127.1 (ttd,  $^1J_{\text{F-C}} = 281.2$  Hz,  $^2J_{\text{F-C}} = 32.9$  Hz,  $^6J_{\text{F-C}} = 1.4$  Hz), 122.8 (tt,  $^1J_{\text{F-C}} = 272.2$  Hz,  $^2J_{\text{F-C}} = 45.3$  Hz), 119.9 (m), 116.5 (d,  $^2J_{\text{F-C}} = 22.0$  Hz)  $-4.0$  (m);  $^{19}\text{F}$  NMR:  $\delta = -83.29$  (t, 2F,  $^3J_{\text{F-F}} = 4.6$  Hz),  $-110.55$  (m, 1F),  $-122.52$  (t, 2F,  $^3J_{\text{F-F}} = 4.6$  Hz). Anal. Calcd for  $\text{C}_{11}\text{H}_{13}\text{F}_5\text{SSi}$ : C, 43.99; H, 4.36. Found C, 44.22; H, 4.48.

**2-(1,1,2,2-Tetrafluoro-2-trimethylsilanyl-ethylsulfanyl)-pyridine (6a):** yellow liquid (76% yield);  $R_f = 0.5$  (Pentane/ $\text{CH}_2\text{Cl}_2$  1:2);  $^1\text{H}$  NMR:  $\delta = 8.68$  (ddd, 1H,  $^3J_{\text{H-H}} = 4.8$  Hz,  $^4J_{\text{H-H}} = 1.6$  Hz,  $^5J_{\text{H-H}} = 1.1$  Hz), 7.71-7.63 (m, 2H), 7.26 (ddd, 1H,  $^3J_{\text{H-H}} = 6.5$  Hz,  $^3J_{\text{H-H}} = 4.8$  Hz,  $^4J_{\text{H-H}} = 2.2$  Hz), 0.28 (s, 9H);  $^{13}\text{C}$  NMR:  $\delta = 150.5$ , 149.8, 137.3, 130.2, 127.8 (tt,  $^1J_{\text{F-C}} = 283.4$  Hz,  $^2J_{\text{F-C}} = 32.4$  Hz), 123.6, 122.5 (tt,  $^1J_{\text{F-C}} = 273.0$  Hz,  $^2J_{\text{F-C}} = 44.7$  Hz),  $-4.1$  (m);  $^{19}\text{F}$  NMR:  $\delta = -82.15$  (t, 2F,  $^3J_{\text{F-F}} = 4.6$  Hz),  $-122.48$  (t, 2F,  $^3J_{\text{F-F}} = 4.6$  Hz). Anal. Calcd for  $\text{C}_{10}\text{H}_{13}\text{F}_4\text{NSSi}$ : C, 42.39; H, 4.62. Found C, 42.54; H, 4.76.

**Synthesis of (2,2-Difluoro-1-phenyl-vinyloxy)-trimethyl-silane (9):**<sup>2</sup> Into a mixture of Mg turnings (0.2 g, 8.3 mmol) and TMSCl (2 mL, 16 mmol) in anhydrous THF (10 mL) at 0°C, was slowly added PhCOCF<sub>3</sub> (0.56 mL, 4 mmol). The reaction mixture was stirred at 0°C for 4 h. After removal of the solvent and excess TMSCl under vacuum, pentane was added. Solids were filtrated and the resulting filtrate was concentrated to give 0.92 g of crude **9** as a colorless liquid. The product is pure enough to be used for the next step. *R<sub>f</sub>*=0.7 (Petroleum ether/CH<sub>2</sub>Cl<sub>2</sub> 7:3); <sup>1</sup>H NMR: δ = 7.62 (m, 2H), 7.48 (m, 2H), 7.38 (m, 1H), 0.22 (s, 9H); <sup>19</sup>F NMR: δ = -100.29 (d, 1F, <sup>2</sup>*J*<sub>F-F</sub> = 67.7 Hz), -112.06 (d, 1F, <sup>2</sup>*J*<sub>F-F</sub> = 67.7 Hz).

**1,1,2,2-Tetrafluoro-2-(4-fluorophenylsulfanyl)-ethane-sulfonyl fluoride (13b):** yellow liquid (A: 67% yield, B: 64% yield); *R<sub>f</sub>*=0.7 (Pentane); <sup>1</sup>H NMR: δ = 7.66 (m, 2H), 7.14 (m, 2H); <sup>13</sup>C NMR: δ = 165.4 (d, <sup>1</sup>*J*<sub>F-C</sub> = 253.6 Hz), 140.0 (d, <sup>3</sup>*J*<sub>F-C</sub> = 9.3 Hz), 117.6 (m), 117.4 (d, <sup>2</sup>*J*<sub>F-C</sub> = 22.0 Hz), 121.8 (m), 116.1 (ttd, <sup>1</sup>*J*<sub>F-C</sub> = 300.6 Hz, <sup>2</sup>*J*<sub>F-C</sub> = 40.3 Hz, <sup>2</sup>*J*<sub>F-C</sub> = 33.8 Hz); <sup>19</sup>F NMR: δ = 46.01 (m, 1F), -86.99 (m, 2F), -105.70 (m, 2F), -107.67 (m, 1F); MS (EI): *m/z* = 127.3, 177.3, 310.2 (M<sup>+</sup>); HRMS: calcd for C<sub>8</sub>H<sub>4</sub>F<sub>6</sub>O<sub>2</sub>S<sub>2</sub>: 309.9557; found: 309.9559.

**1,1,2,2-Tetrafluoro-2-(4-trimethylsilanylphenylsulfanyl)-ethanesulfonyl fluoride (13c):** colorless liquid (A: 48% yield, B: 77% yield); *R<sub>f</sub>*=0.7 (Pentane); <sup>1</sup>H NMR: δ = 7.64-7.56 (m, 4H), 0.29 (s, 9H); <sup>13</sup>C NMR: δ = 145.4, 136.5, 134.6, 122.4 (t, <sup>3</sup>*J*<sub>F-C</sub> = 3.0 Hz), 121.9 (ttd, <sup>1</sup>*J*<sub>F-C</sub> = 291.0 Hz, <sup>2</sup>*J*<sub>F-C</sub> = 30.8 Hz, <sup>3</sup>*J*<sub>F-C</sub> = 1.1 Hz), 116.0 (ttd, <sup>1</sup>*J*<sub>F-C</sub> = 300.5 Hz, <sup>2</sup>*J*<sub>F-C</sub> = 40.8 Hz, <sup>2</sup>*J*<sub>F-C</sub> = 32.6 Hz), -1.2; <sup>19</sup>F NMR: δ = 46.01 (m, 1F), -86.40 (m, 2F), -105.54 (m, 2F); MS (EI): *m/z* = 265, 349, 364 (M<sup>+</sup>); HRMS: calcd for C<sub>11</sub>H<sub>13</sub>F<sub>5</sub>O<sub>2</sub>S<sub>2</sub>Si: 364.0046; found: 364.0045.

**2-(4-Bromo-phenylsulfanyl)-1,1,2,2-tetrafluoro-ethane-sulfonyl fluoride (13d):** colorless liquid (B: 62% yield); *R<sub>f</sub>* = 0.7 (Pentane); <sup>1</sup>H NMR: δ = 7.64-7.51 (m, 4H); <sup>13</sup>C NMR: δ = 138.8, 133.2, 127.1, 121.5 (ttd, <sup>1</sup>*J*<sub>F-C</sub> = 291.6 Hz, <sup>2</sup>*J*<sub>F-C</sub> = 30.8 Hz, <sup>3</sup>*J*<sub>F-C</sub> = 1.0 Hz), 121.1 (m), 115.8 (ttd, <sup>1</sup>*J*<sub>F-C</sub> = 300.6 Hz, <sup>2</sup>*J*<sub>F-C</sub> = 40.4 Hz, <sup>2</sup>*J*<sub>F-C</sub> = 32.9 Hz); <sup>19</sup>F NMR: δ = 46.06 (m, 1F), -86.59 (m, 2F), -105.72 (m, 2F); MS (EI): *m/z* = 187, 189, 237, 239, 370 (M<sup>+</sup>), 372; HRMS: calcd for C<sub>8</sub>H<sub>4</sub>BrF<sub>5</sub>O<sub>2</sub>S<sub>2</sub>: 369.8756; found: 369.8757.

**1,1,2,2-Tetrafluoro-2-(pyridin-2-ylsulfanyl)-ethane-sulfonyl fluoride (14a):** yellow liquid (A: 70% yield, B: 72% yield); *R<sub>f</sub>*=0.3 (Pentane); <sup>1</sup>H NMR: δ = 8.68 (ddd, 1H, <sup>3</sup>*J*<sub>H-H</sub> = 4.8 Hz, <sup>4</sup>*J*<sub>H-H</sub> = 1.9 Hz, <sup>5</sup>*J*<sub>H-H</sub> = 0.9 Hz), 7.78 (ddd, 1H, <sup>3</sup>*J*<sub>H-H</sub> = <sup>3</sup>*J*<sub>H-H</sub> = 7.5 Hz, <sup>4</sup>*J*<sub>H-H</sub> = 1.9 Hz), 7.72 (m,

<sup>2</sup> a) Amii, H.; Kobayashi, T.; Hatamoto, Y.; Uneyama, K. *Chem. Commun.* **1999**, 1323-1324.  
b) Prakash, G. K. S.; Hu, J.; Simon, J.; Bellew, D. R.; Olah, G. A. J. *Fluorine. Chem.* **2004**, 125, 595-601.

1H), 7.41 (ddd, 1H,  $^3J_{\text{H-H}} = 7.5$  Hz,  $^3J_{\text{H-H}} = 4.8$  Hz,  $^4J_{\text{H-H}} = 1.2$  Hz);  $^{13}\text{C}$  NMR:  $\delta = 151.2$ , 146.5 (m), 138.0, 131.5, 125.1, 126.7-114.7 (m, 2C);  $^{19}\text{F}$  NMR:  $\delta = 46.34$  (m, 1F), -85.23 (m, 2F), -105.74 (m, 2F); MS (EI):  $m/z = 293.4$  ( $\text{M}^+$ ); HRMS: calcd for  $\text{C}_7\text{H}_4\text{F}_5\text{NO}_2\text{S}_2$ : 292.9604; found: 292.9608.

**1,1-Difluoro-2-oxo-2-phenyl-ethanesulfonyl fluoride (15):** colorless liquid (A: 45% yield, B: 67% yield);  $R_f = 0.6$  (Petroleum ether/ $\text{CH}_2\text{Cl}_2$  9:1);  $^1\text{H}$  NMR:  $\delta = 8.10$  (m, 2H), 7.79 (m, 1H), 7.60 (m, 2H);  $^{13}\text{C}$  NMR:  $\delta = 181.1$  (td,  $^2J_{\text{F-C}} = 23.9$  Hz,  $^3J_{\text{F-C}} = 1.7$  Hz), 136.8, 130.5 (t,  $^4J_{\text{F-C}} = 2.7$  Hz), 129.8 (td,  $^3J_{\text{F-C}} = ^4J_{\text{F-C}} = 2.6$  Hz), 116.6 (td,  $^1J_{\text{F-C}} = 309.3$  Hz,  $^2J_{\text{F-C}} = 28.0$  Hz);  $^{19}\text{F}$  NMR:  $\delta = 41.61$  (t, 1F,  $^3J_{\text{F-F}} = 2.3$  Hz), -95.98 (d, 2F,  $^3J_{\text{F-F}} = 2.3$  Hz); MS (EI):  $m/z = 77.3$ , 105.3, 238.3 ( $\text{M}^+$ ); HRMS: calcd for  $\text{C}_8\text{H}_5\text{F}_3\text{O}_3\text{S}$ : 237.9912; found: 237.9913.

**Difluoro-phenylsulfanyl-methanesulfonyl fluoride (16a):** colorless liquid (B: 57% yield);  $R_f = 0.6$  (Pentane);  $^1\text{H}$  NMR:  $\delta = 7.71$  (d, 2H,  $^3J_{\text{H-H}} = 7.5$  Hz), 7.56 (t, 1H,  $^3J_{\text{H-H}} = 7.5$  Hz), 7.46 (dd, 2H,  $^3J_{\text{H-H}} = ^3J_{\text{H-H}} = 7.5$  Hz);  $^{13}\text{C}$  NMR:  $\delta = 137.5$  (t,  $^4J_{\text{F-C}} = 1.1$  Hz), 132.1, 130.0, 126.6 (td,  $^1J_{\text{F-C}} = 323.3$  Hz,  $^2J_{\text{F-C}} = 32.9$  Hz), 121.8 (t,  $^3J_{\text{F-C}} = 3.0$  Hz);  $^{19}\text{F}$  NMR:  $\delta = 35.06$  (t, 1F,  $^3J_{\text{F-F}} = 4.6$  Hz), -76.08 (d, 2F,  $^3J_{\text{F-F}} = 4.6$  Hz); MS (EI):  $m/z = 77$ , 109, 159, 242 ( $\text{M}^+$ ); HRMS: calcd for  $\text{C}_7\text{H}_5\text{F}_3\text{O}_2\text{S}_2$ : 241.9683; found: 241.9686.

**Difluoro-(4-fluoro-phenylsulfanyl)-methanesulfonyl fluoride (16b):** colorless liquid (B: 32% yield);  $R_f = 0.7$  (Pentane);  $^1\text{H}$  NMR:  $\delta = 7.70$  (m, 2H), 7.16 (m, 2H);  $^{13}\text{C}$  NMR:  $\delta = 165.3$  (d,  $^1J_{\text{F-C}} = 254.7$  Hz), 139.9 (d,  $^3J_{\text{F-C}} = 9.3$  Hz), 126.7 (tdd,  $^1J_{\text{F-C}} = 323.4$  Hz,  $^2J_{\text{F-C}} = 32.3$  Hz,  $^6J_{\text{F-C}} = 2.4$  Hz), 117.4 (d,  $^2J_{\text{F-C}} = 22.5$  Hz), 117.1 (m);  $^{19}\text{F}$  NMR:  $\delta = 35.2$  (t, 1F,  $^3J_{\text{F-F}} = 4.6$  Hz), -76.80 (d, 2F,  $^3J_{\text{F-F}} = 4.6$  Hz), -106.74 (m, 1F); MS (EI):  $m/z = 177$ , 260 ( $\text{M}^+$ ); HRMS: calcd for  $\text{C}_7\text{H}_4\text{F}_4\text{O}_2\text{S}_2$ : 259.9589; found: 259.9591.

**Benzenesulfinyl-difluoro-methanesulfonyl fluoride (19a):** colorless liquid (34% yield);  $R_f = 0.45$  (Pentane/ $\text{CH}_2\text{Cl}_2$  1:1);  $^1\text{H}$  NMR:  $\delta = 7.86$  (d, 2H,  $^3J_{\text{H-H}} = 7.3$  Hz), 7.77-7.63 (m, 3H);  $^{13}\text{C}$  NMR:  $\delta = 134.7$ , 134.1 (dd,  $^3J_{\text{F-C}} = ^3J_{\text{F-C}} = 2.5$  Hz), 129.9, 126.6 (dd,  $^4J_{\text{F-C}} = ^4J_{\text{F-C}} = 1.1$  Hz), 123.7 (ddd,  $^1J_{\text{F-C}} = 348.9$  Hz,  $^1J_{\text{F-C}} = 340.7$  Hz,  $^2J_{\text{F-C}} = 24.8$  Hz);  $^{19}\text{F}$  NMR:  $\delta = 49.78$  (dd, 1F,  $^3J_{\text{F-F}} = ^3J_{\text{F-F}} = 5.1$  Hz), -99.61 (dd, 1F,  $^1J_{\text{F-F}} = 215.7$  Hz,  $^3J_{\text{F-F}} = 5.1$  Hz), -105.45 (dd, 1F,  $^1J_{\text{F-F}} = 215.7$  Hz,  $^3J_{\text{F-F}} = 5.1$  Hz); MS (EI):  $m/z = 125$ , 258 ( $\text{M}^+$ ); HRMS: calcd for  $\text{C}_7\text{H}_5\text{F}_3\text{O}_3\text{S}_2$ : 257.9632; found: 257.9630.

**Benzenesulfonyl-difluoro-methanesulfonyl fluoride (20a):** colorless liquid (75% yield);  $R_f = 0.7$  (Pentane);  $^1\text{H}$  NMR:  $\delta = 8.09$  (d, 2H,  $^3J_{\text{H-H}} = 7.6$  Hz), 7.90 (t, 1H,  $^3J_{\text{H-H}} = 7.6$  Hz), 7.70 (dd, 2H,  $^3J_{\text{H-H}} = ^3J_{\text{H-H}} = 7.6$  Hz);  $^{13}\text{C}$  NMR:  $\delta = 137.7$ , 131.6, 131.0, 130.2, 118.8 (td,  $^1J_{\text{F-C}} = 336.3$  Hz,  $^2J_{\text{F-C}} = 30.0$  Hz);  $^{19}\text{F}$  NMR:  $\delta = 49.28$  (t, 1F,  $^3J_{\text{F-F}} = 5.7$  Hz), -99.40 (d, 2F,  $^3J_{\text{F-F}} =$



5.7 Hz); MS (EI):  $m/z$  = 77, 141, 274 ( $M^+$ ); HRMS: calcd for  $C_7H_5F_3O_4S_2$ : 273.9581; found: 273.9580.

**Lithium 2-benzenesulfinyl-1,1,2,2-tetrafluoro-ethanesulfonate (22):** white solid (0.15 g, 71% yield); m.p. 200°C;  $^1H$  NMR (acetone- $d_6$ ):  $\delta$  = 7.87 (d, 2H,  $^3J_{H-H}$  = 7.2 Hz), 7.70-7.61 (m, 3H), 4.2 (br s,  $H_2O$  linked);  $^{13}C$  NMR (acetone- $d_6$ ):  $\delta$  = 137.6 (dd,  $^3J_{F-C}$  =  $^3J_{F-C}$  = 2.5 Hz), 133.9, 130.0, 127.7 (d,  $^4J_{F-C}$  = 1.6 Hz), 119.2 (dddd,  $^1J_{F-C}$  = 310.5 Hz,  $^1J_{F-C}$  = 309.6 Hz,  $^2J_{F-C}$  =  $^2J_{F-C}$  = 30.5 Hz), 115.2 (dddd,  $^1J_{F-C}$  =  $^1J_{F-C}$  = 289.5 Hz,  $^2J_{F-C}$  =  $^2J_{F-C}$  = 27.8 Hz);  $^{19}F$  NMR (acetone- $d_6$ ):  $\delta$  = -113.47 (ddd, 1F,  $^2J_{F-F}$  = 265.8 Hz,  $^3J_{F-F}$  =  $^3J_{F-F}$  = 4.7 Hz), -113.51 (ddd, 1F,  $^2J_{F-F}$  = 233.7 Hz,  $^3J_{F-F}$  =  $^3J_{F-F}$  = 4.7 Hz), -114.49 (ddd, 1F,  $^2J_{F-F}$  = 265.8 Hz,  $^3J_{F-F}$  =  $^3J_{F-F}$  = 4.7 Hz), -120.80 (ddd, 1F,  $^2J_{F-F}$  = 233.7 Hz,  $^3J_{F-F}$  =  $^3J_{F-F}$  = 4.7 Hz); MS (ESI-MeOH):  $m/z$  = 304.9 ( $M^-$ ), 305.9, 306.9, 616.8.

**Lithium 2-benzenesulfonyl-1,1,2,2-tetrafluoro-ethanesulfonate (23):** white solid (0.19 g, 92% yield); m.p. 75-80°C;  $^1H$  NMR (acetone- $d_6$ ):  $\delta$  = 8.05 (d, 2H,  $^3J_{H-H}$  = 7.5 Hz), 7.94 (m, 1H), 7.79 (m, 2H), 3.01 (br s,  $H_2O$  linked);  $^{13}C$  NMR (acetone- $d_6$ ):  $\delta$  = 137.1, 134.2, 131.4, 130.6, 116.4 (tt,  $^1J_{F-C}$  = 279.9 Hz,  $^2J_{F-C}$  = 37.1 Hz,  $^3J_{F-C}$  = 35.0 Hz), 115.4 (tt,  $^1J_{F-C}$  = 287.8 Hz,  $^2J_{F-C}$  = 33.9 Hz);  $^{19}F$  NMR (acetone- $d_6$ ):  $\delta$  = -110.65 (m, 2F), -113.48 (m, 2F); MS (ESI-MeOH):  $m/z$  = 321 ( $M^-$ ), 322, 323.

**Lithium difluoro-phenylsulfanyl-methanesulfonate (24):** White solid (1.29 g, 83% yield); m.p. 175-182°C;  $^1H$  NMR (acetone- $d_6$ ):  $\delta$  = 7.63 (m, 2H), 7.49-7.39 (m, 3H), 2.88 (br s,  $H_2O$  linked);  $^{13}C$  NMR (acetone- $d_6$ ):  $\delta$  = 137.0, 130.5, 129.8, 128.2 (t,  $^1J_{F-C}$  = 315.3 Hz), 127.3 (t,  $^3J_{F-C}$  = 1.9 Hz);  $^{19}F$  NMR (acetone- $d_6$ ):  $\delta$  = -79.08 (s, 2F); MS (ESI-MeOH):  $m/z$  = 239.0 ( $M^-$ ), 240.0, 241.0, 484.9.

**Lithium benzenesulfinyl-difluoro-methanesulfonate (25):** White solid (0.16 g, 51% yield); m.p. 215-220°C;  $^1H$  NMR (acetone- $d_6$ ):  $\delta$  = 7.83 (d, 2H,  $^3J_{H-H}$  = 7.7 Hz), 7.72-7.62 (m, 3H);  $^{13}C$  NMR (acetone- $d_6$ ):  $\delta$  = 136.3 (dd,  $^3J_{F-C}$  =  $^3J_{F-C}$  = 3.0 Hz), 133.9, 130.0, 127.5 (m), 122.6 (dd,  $^1J_{F-C}$  = 341.9 Hz,  $^1J_{F-C}$  = 329.9 Hz);  $^{19}F$  NMR (acetone- $d_6$ ):  $\delta$  = -105.90 (d, 1F,  $^1J_{F-F}$  = 205.9 Hz), -113.87 (d, 1F,  $^1J_{F-F}$  = 205.9 Hz); MS (ESI-MeOH):  $m/z$  = 130.0, 131.1, 255.0 ( $M^-$ ), 256.0, 256.9.

**Lithium benzenesulfonyl-difluoro-methanesulfonate (26):** White solid (0.20 g, 72% yield); m.p. 225°C;  $^1H$  NMR (acetone- $d_6$ ):  $\delta$  = 8.02 (m, 2H), 7.83 (m, 1H), 7.63 (m, 2H), 3.20 (br s,  $H_2O$  linked);  $^{13}C$  NMR (acetone- $d_6$ ):  $\delta$  = 136.1, 135.2, 131.5 (t,  $^4J_{F-C}$  = 1.1 Hz), 129.9, 119.9 (t,  $^1J_{F-C}$  = 324.7 Hz);  $^{19}F$  NMR (acetone- $d_6$ ):  $\delta$  = -104.76 (s, 2F); MS (ESI-MeOH):  $m/z$  = 130.0, 271.0 ( $M^-$ ), 272.0, 273.0.

**Lithium 1,1-difluoro-2-oxo-2-phenyl-ethanesulfonate (27):** White solid (0.94 g, 77% yield); m.p. 118-122°C;  $^1\text{H}$  NMR (acetone- $\text{d}_6$ ):  $\delta$  = 8.25 (m, 2H), 7.67 (m, 1H), 7.51 (m, 2H), 4.06 (br s,  $\text{H}_2\text{O}$  linked);  $^{13}\text{C}$  NMR (acetone- $\text{d}_6$ ):  $\delta$  = 188.8 (t,  $^2J_{\text{F-C}} = 25.3$  Hz), 134.8, 133.8 (m), 131.5 (t,  $^4J_{\text{F-C}} = 3.0$  Hz), 129.0, 117.3 (t,  $^1J_{\text{F-C}} = 287.0$  Hz);  $^{19}\text{F}$  NMR (acetone- $\text{d}_6$ ):  $\delta$  = -104.36 (s, 2F); MS (ESI-MeOH):  $m/z$  = 235.1 ( $\text{M}^+$ ), 267.0.

PhSCF<sub>3</sub>Br 1a

PROTON

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7.6510  
7.5437  
7.5280  
7.5192  
7.5111  
7.4991  
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1.5414

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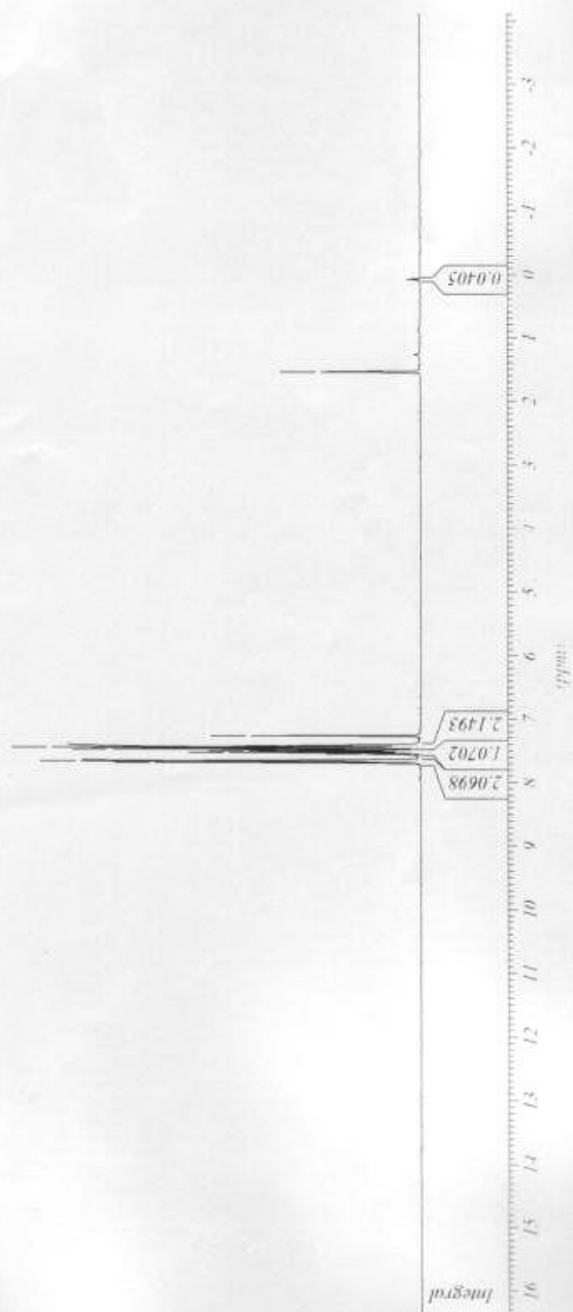
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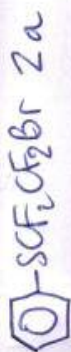
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PROTON

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7.5042  
7.4960  
7.4841  
7.4797  
7.4747  
7.4458  
7.4414  
7.4257  
7.4213  
7.4031  
7.3975  
7.3931  
7.2600

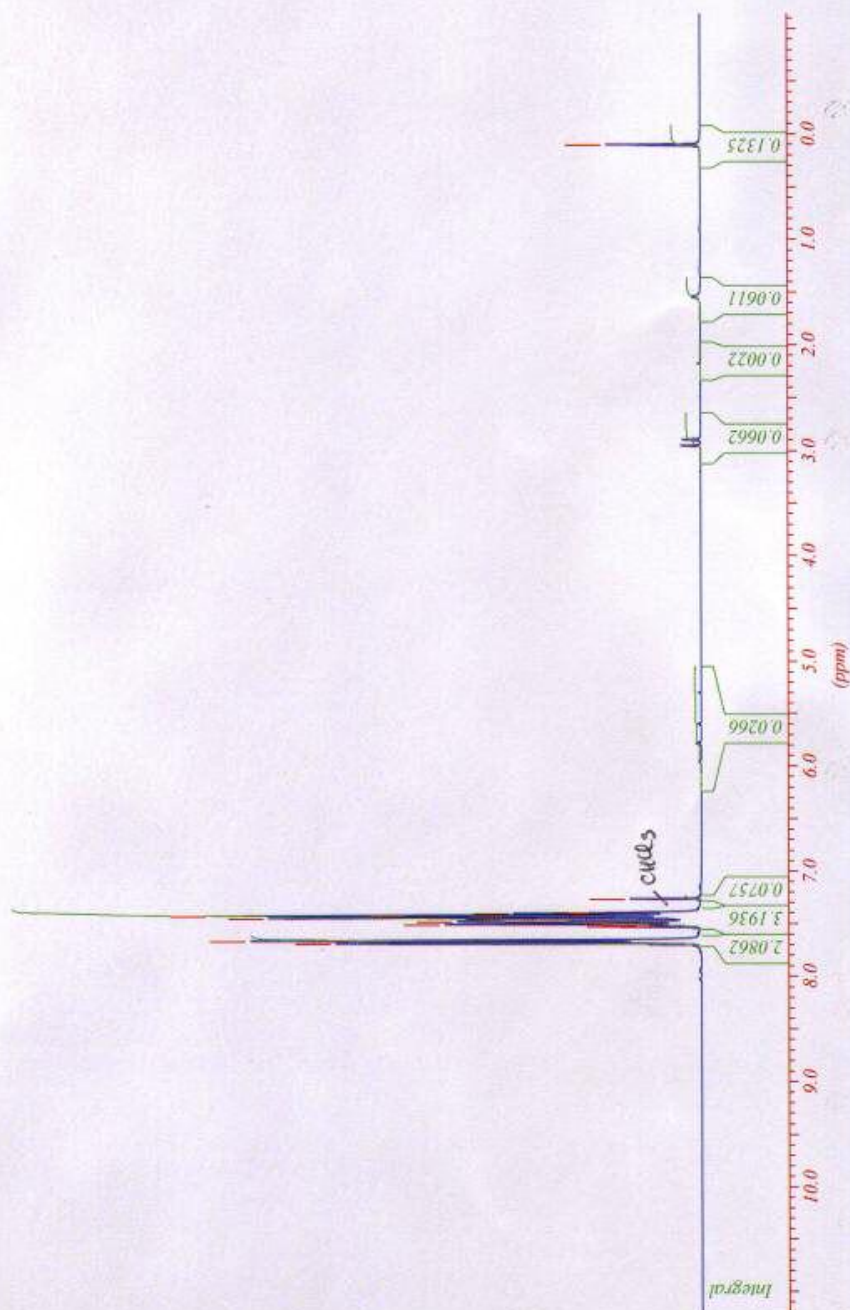
0.1015

\*\*\* Current Data Parameters \*\*\*  
NAME : ral-1  
EXPNO : 2  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*  
DATE\_1 : 05-58-11  
DATE\_d : Feb 20 2006  
DS : 0  
EXP : 8  
NS : off  
NUCLEUS : <sup>1</sup>H  
O1 : 1853.43 Hz  
O2 : 0.00 Hz  
RG : 228.1000061  
RO : 20 Hz  
SFO1 : 300.1318534 MHz  
SOLVENT : CDCl3  
SW : 20.5671 ppm  
SW\_h : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*  
GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300060 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*  
SR : 6.41 Hz  
ppm\_cm : 0.55  
Hz\_cm : 165.29  
YVal\_cm : 39669840.00  
NUCLEUS : <sup>1</sup>H  
SOLVENT : off ?



PROTON



7.6711  
7.6705  
7.6699  
7.6692  
7.6523  
7.6517  
7.6410  
7.6404  
7.6397  
7.2625  
7.2619  
7.2613  
7.2606  
7.2600  
7.1169  
7.1163  
7.1156

1.5439  
1.5433

\*\*\* Current Data Parameters \*\*\*

NAME :  $\beta$ 423d2  
EXPNO : 1  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 00-22-33  
DATE\_2 : Feb 06 2006  
DS : 0  
EXP : 8  
NUCLEUS : off  
P1 : 1853.43 Hz  
RG : 0.00 Hz  
RO : 456.1000061  
SFO : 20 Hz  
SOLVENT : C13  
SW : 20.5671 ppm  
TD : 6172.840 Hz  
TE : 32768  
300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.00000000  
LB : 0.30 Hz  
SF : 300.1300060 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 6.41 Hz  
ppm : 0.92  
Hz : 275.08  
X1 : 3436056.400  
X2 : off  
SOLVENT :



C13CPOC1K13 n sercof 2



166.5016  
166.4943  
163.1488

139.7224  
139.5988

122.1217  
118.9507  
118.9216  
118.9143  
118.8634  
118.8271  
117.0306  
117.0233  
116.8270  
116.7324

77.1600

\*\*\*Current Data Parameters\*\*\*  
NAME : p423d2  
EXPNO : 101  
PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*

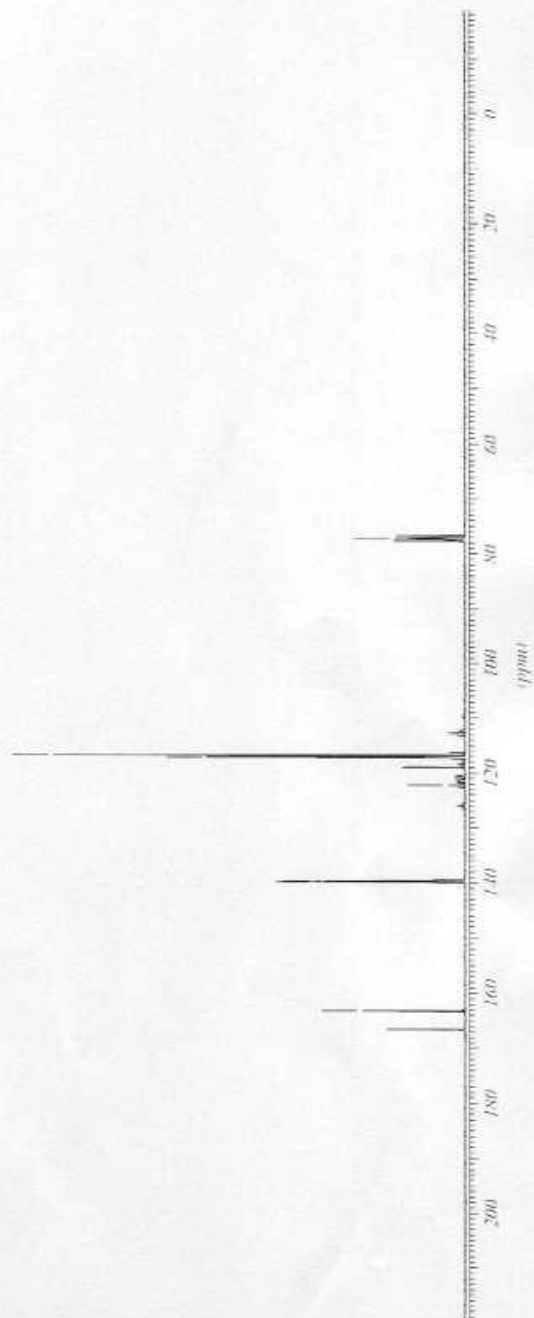
DATE\_1 : 17-09-10  
DATE\_2 : Feb 22 2006  
DS : 4  
EXP : (13C)PD  
NS : 2500  
NUCLEUS : off  
Q1 : 7576.30 Hz  
Q2 : 1200.52 Hz  
RG : 4096.000000  
RO : 20 Hz  
SFO1 : 75.4752953 MHz  
SOLVENT : C13C13  
SU : 238.2980 ppm  
SW\_h : 17985.612 Hz  
TD : 65536  
TE : 300.0 K

\*\*\*Processing Parameters\*\*\*

GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4677350 MHz

\*\*\*1D NMR Plot Parameters\*\*\*

SR : 16.01 Hz  
ppm\_cm : 10.62  
Hz\_cm : 801.50  
Y1\_of\_cm : 720331.81  
NUCLEUS : off  
SOLVENT : 9





\*\*\* Current Data Parameters \*\*\*

NAME : f423d2  
EXPNO : 2  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 00.24.21  
DATE\_2 : Feb 06 2006  
DS : 2  
EXP : PS done  
NS : 8  
NUCLEUS : off

O1 : -20615.33 Hz  
O2 : 0.00 Hz  
RG : 645.0999756  
RO : 20 Hz

SFO1 : 282.3838635 MHz

SOLVENT : CDCl3

SW : 266.2616 ppm  
SW\_h : 75187.970 Hz

TD : 131072

TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.000000  
LB : 0.30 Hz  
SF : 282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
ppm\_cm : 11.86  
Hz\_cm : 3350.62  
YVal\_cm : 69885608.00

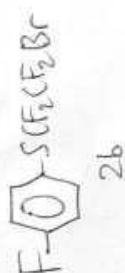
NUCLEUS : off

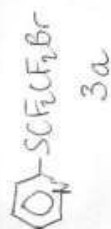
NOISE : 0

-108.8315  
-108.8518  
-108.8600  
-108.8681  
-108.8803  
-108.8965  
-108.9087  
-108.9290

-85.9920  
-86.0204  
-86.0489

-62.6852  
-62.7137  
-62.7421





PROTON

8.6697  
 8.6672  
 8.6641  
 8.6609  
 8.6554  
 8.6509  
 8.6478  
 7.7715  
 7.7452  
 7.7389  
 7.7207  
 7.7144  
 7.6912  
 7.6855  
 7.3818  
 7.3774  
 7.3654  
 7.3611  
 7.3573  
 7.3529  
 7.3416  
 7.3372  
 7.2600

\*\*\* Current Data Parameters \*\*\*  
 NAME : jh385/j  
 EXPNO : 3  
 PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_ : 08-13-14  
 DATE\_A : Dec 12 2005  
 DS : 0  
 AS : 8  
 NUC1ES : off  
 O1 : 1853.43 Hz  
 O2 : 0.00 Hz  
 RG : 512.0000000  
 RO : 20 Hz  
 SFO1 : 300.1318534 MHz  
 SOLVENT : C1813  
 SU : 20.5671 ppm  
 SW\_h : 6172.840 Hz  
 TD : 32768  
 TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
 LB : 0.30 Hz  
 SF : 300.1300060 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

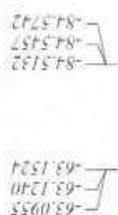
SR : 6.22 Hz  
 ppm cm : 0.92  
 Hz cm : 275.08  
 Y1 cal cm : 14416896.00  
 NUC1ES : off  
 SOLVENT :







3a



\*\*\* Current Data Parameters \*\*\*

NAME	:	f385f1
EXPNO	:	1
PROCNO	:	1

\*\*\* Acquisition Parameters \*\*\*

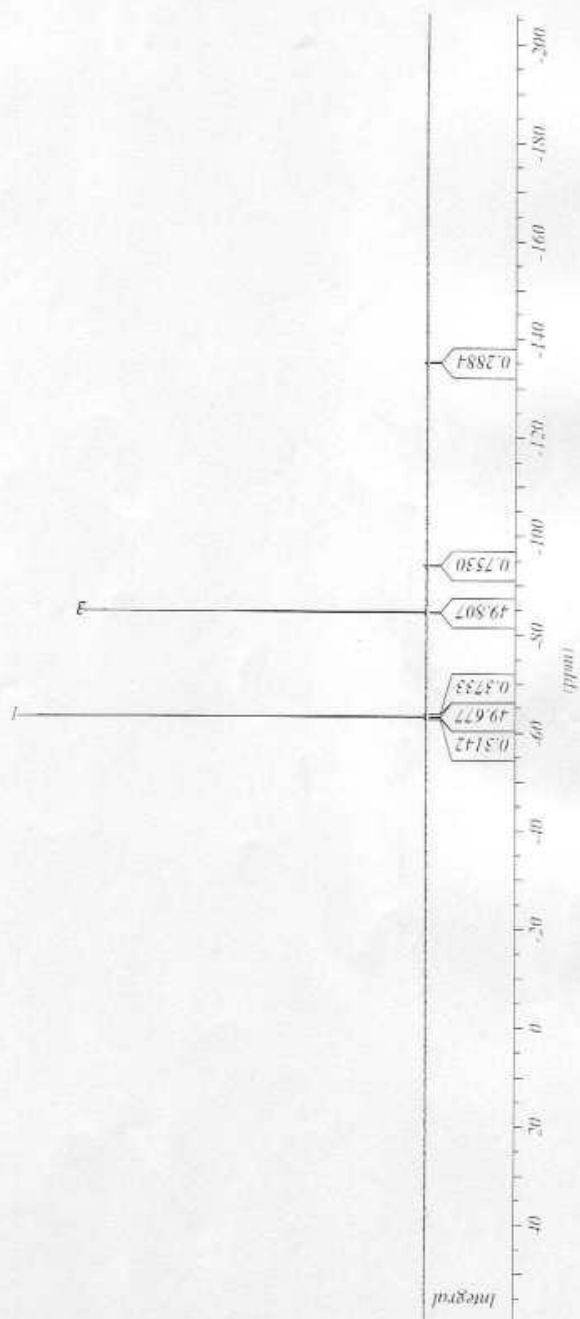
DATE_1	:	08/30/02
DATE_2	:	Dec 12 2005
DS	:	2
AS	:	8
NUCLEUS	:	off
Q1	:	-20615.53 Hz
Q2	:	0.00 Hz
RG	:	1290.1999512
RO	:	20 Hz
SFO1	:	282.3838655 MHz
SOLVENT	:	CDC13
SI	:	266.2616 ppm
SB_H	:	73187.970 Hz
TD	:	131072
TE	:	300.0 K

\*\*\* Processing Parameters \*\*\*

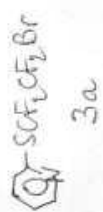
GB	:	0.0000000
LB	:	0.30 Hz
SF	:	282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR	:	0.00 Hz
ppm_cm	:	11.86
Hz_cm	:	3350.62
Wd_cm	:	33996.25200
NUCLEUS	:	off
SOLVENT	:	?



C130 PDC130131 user of 2



\*\*\* Current Data Parameters \*\*\*

NAME : 038517  
 EXPNO : 101  
 PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

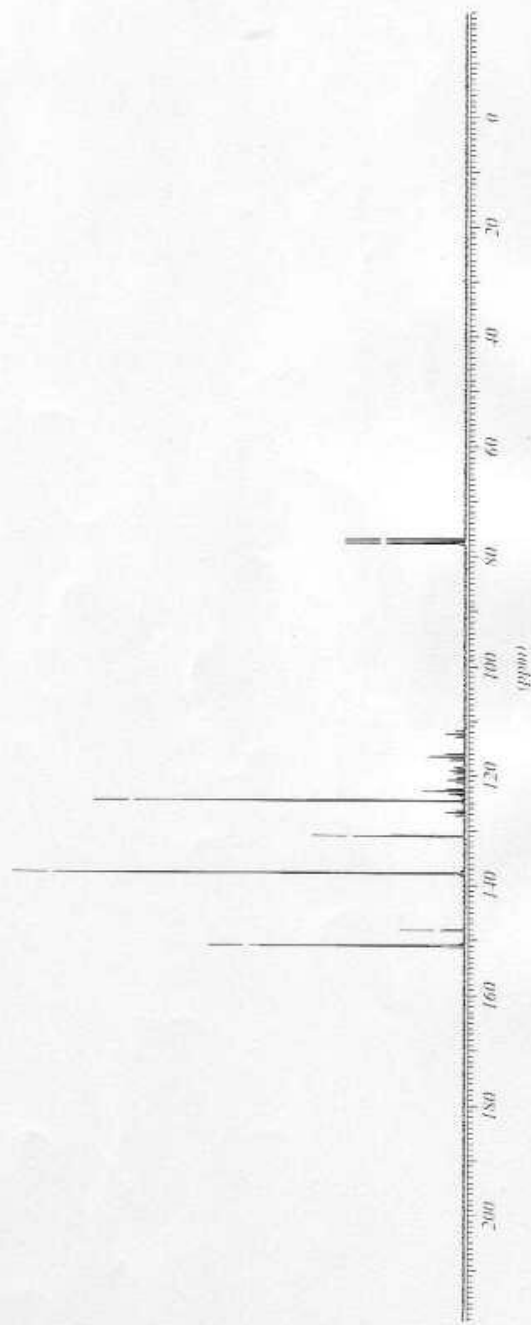
DATE\_1 : 16.06.06  
 DATE\_2 : Dec 14 2005  
 DS : 4  
 NS : 2000  
 NUCLEUS : off  
 Q1 : 7576.30 Hz  
 Q2 : 1200.52 Hz  
 RG : 7298.2001953  
 RO : 20 Hz  
 SFO1 : 75.4752953 MHz  
 SOLVENT : CDCl3  
 ST : 258.2980 ppm  
 SW\_h : 17985.612 Hz  
 TD : 65536  
 TE : 300.0 K

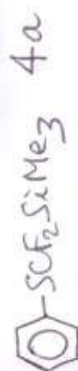
\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
 LB : 1.00 Hz  
 SF : 75.4677370 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 18.35 Hz  
 ppm\_cm : 10.62  
 Hz\_cm : 801.50  
 WId\_cm : 815695.56  
 NUCLEUS : off  
 SOLVENT : p





PROTON CDCl3 in acetof 2



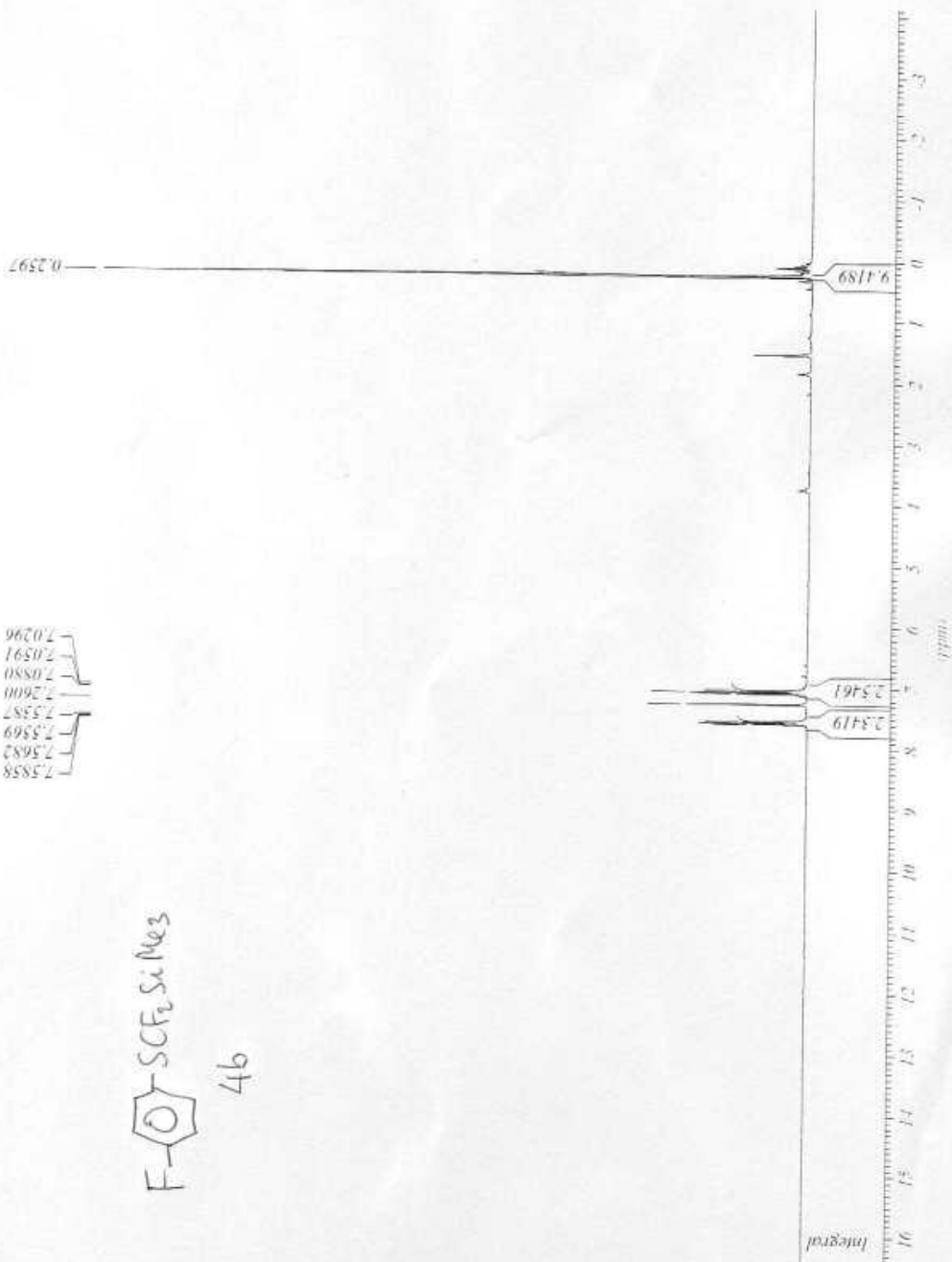
0.2487

\*\*\* Current Data Parameters \*\*\*  
 NAME : j154  
 EXPNO : 100  
 PROCNO : 1  
 \*\*\* Acquisition Parameters \*\*\*  
 DATE\_1 : 10-20-33  
 DATE\_2 : Nov 24 2004  
 DS : 0  
 EXP : PROTON  
 NS : 8  
 NUCLEUS : off  
 O1 : 1853.43 Hz  
 O2 : 0.00 Hz  
 RG : 32.0000000  
 RO : 20 Hz  
 SFO1 : 300.1318534 MHz  
 SOLVENT : CDCl3  
 SW : 20.5671 ppm  
 SW\_H : 6172.840 Hz  
 TD : 32768  
 TE : 300.0 K  
 \*\*\* Processing Parameters \*\*\*  
 GB : 0.0000000  
 LB : 0.30 Hz  
 SF : 300.1300260 MHz  
 \*\*\* 1D NMR Plot Parameters \*\*\*  
 SR : 25.70 Hz  
 ppm\_cm : 0.51  
 Hz\_cm : 132.64  
 YVal\_cm : 47998.42  
 NUCLEUS : off  
 COINTEGR : 9



PROTON

7.5858  
7.5682  
7.569  
7.5387  
7.2600  
7.0880  
7.0591  
7.0296



\*\*\*Current Data Parameters\*\*\*

NAME : J451  
EXPNO : 2  
PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*

DATE\_1 : 07-28-24  
DATE\_2 : Mar-08-2006  
DS : 0  
EXP :  
AS : 8  
NUCLEI : 1  
OL : off  
O1 : 185.343 Hz  
O2 : 0.00 Hz  
RG : \$12.0000000  
RO : 20 Hz  
SFO1 : 300.1318534 MHz  
SOLVENT : CDCl3  
SW : 20.5671 ppm  
SW\_H : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

\*\*\*Processing Parameters\*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300060 MHz

\*\*\*1D NMR Plot Parameters\*\*\*

SR : 6.41 Hz  
ppm\_cm : 0.92  
Hz\_cm : 275.08  
Y1d\_cm : 11230603.00  
NUCLEI : off  
SOLVENT :

419.30

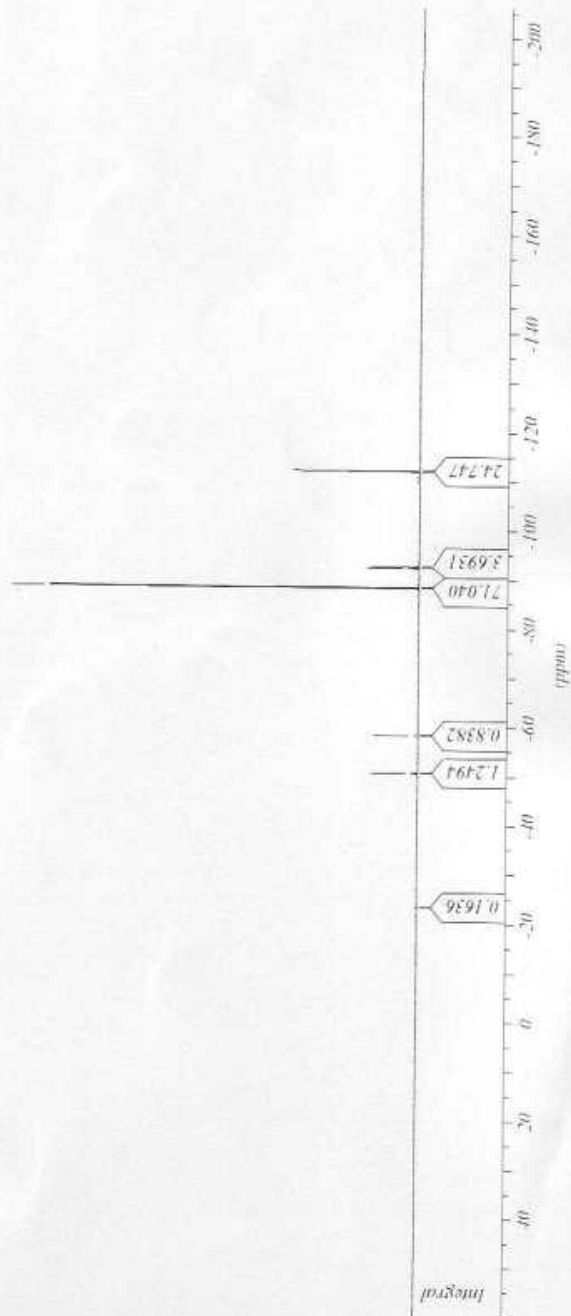


\*\*\*Current Data Parameters\*\*\*  
 NAME : 0451  
 EXPNO : 1  
 PROCNO : 1

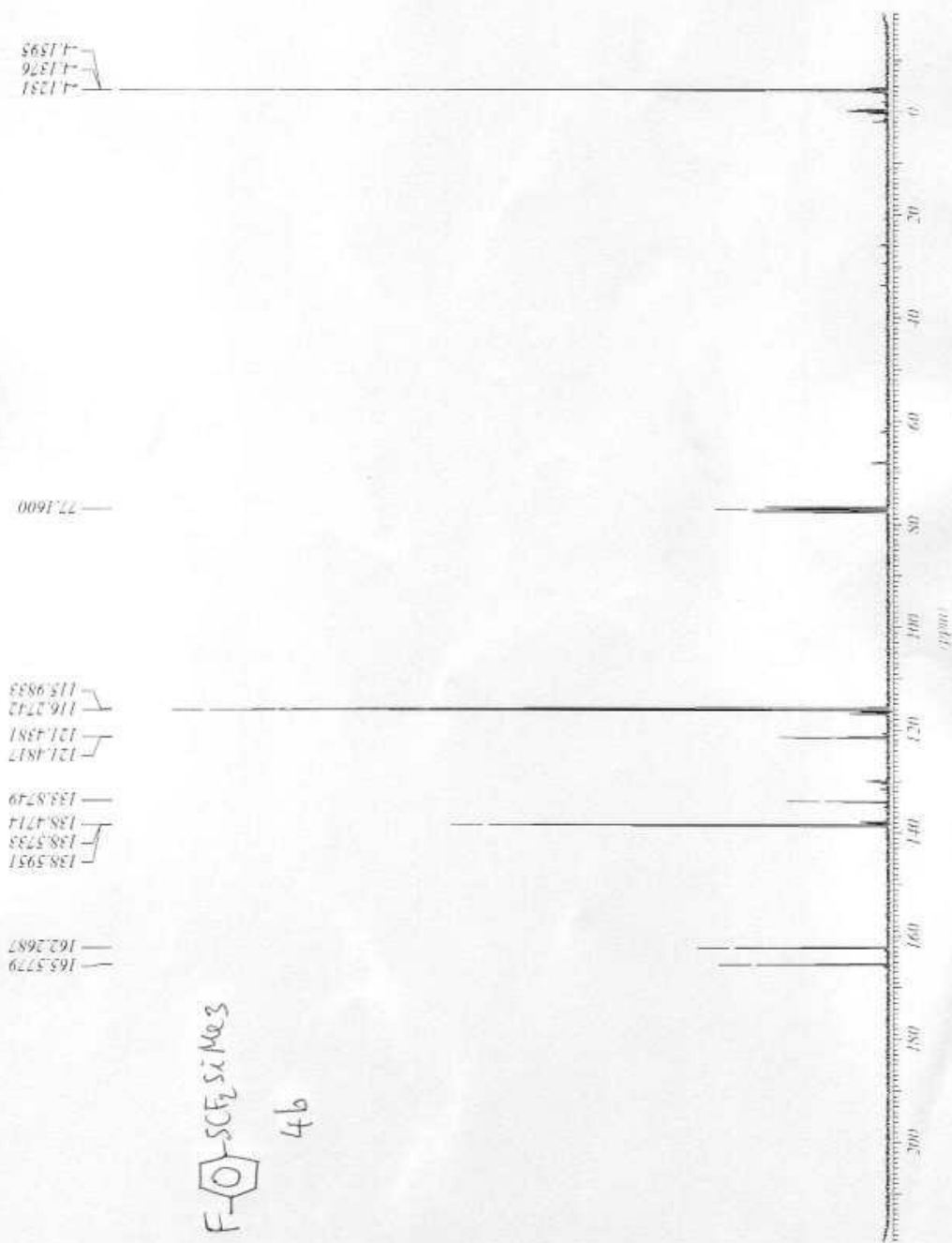
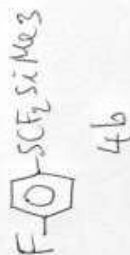
\*\*\*Acquisition Parameters\*\*\*  
 DATE\_1 : 07-26-16  
 DATE\_2 : Mon 08 2006  
 DS : 2  
 EXP : PS-1000  
 NS : 8  
 NTITLE : off  
 O1 : -20615.53 Hz  
 O2 : 0.00 Hz  
 RG : 574.7000122  
 RO : 20 Hz  
 SECT : 282.388655 MHz  
 SOLVENT : CDCl3  
 SU : 266.2616 ppm  
 SW\_H : 75187.970 Hz  
 TD : 131072  
 TE : 300.0 K

\*\*\*Processing Parameters\*\*\*  
 GB : 0.0000000  
 LB : 0.30 Hz  
 SF : 282.4044840 MHz

\*\*\*1D NMR Plot Parameters\*\*\*  
 SR : 0.00 Hz  
 ppm cm : 11.86  
 Hz cm : 3350.62  
 Y1d cm : 55156604.00  
 XTITLE : off  
 SOLVENT : ?



CTSC PD C100 13 u servof 2



\*\*\*Current Data Parameters \*\*\*

NAME : H451  
 EXPNO : 101  
 PROCNO : 1

\*\*\*Acquisition Parameters \*\*\*

DATE\_1 : 15-05-11  
 DATE\_2 : Mar 14 2006  
 DS : 4  
 EMP : C13C101  
 NS : 1800  
 NUCLES : off  
 O1 : 7576.30 Hz  
 O2 : 1200.52 Hz  
 RG : 812.7000122  
 RO : 20 Hz  
 SFO1 : 75.4752953 MHz  
 SOLVENT : CDCl3  
 SU : 238.2980 ppm  
 SW\_h : 17985.612 Hz  
 TD : 65536  
 TE : 300.0 K

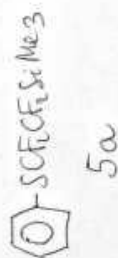
\*\*\*Processing Parameters \*\*\*

GB : 0.0000000  
 LB : 1.00 Hz  
 SF : 75.4677390 MHz

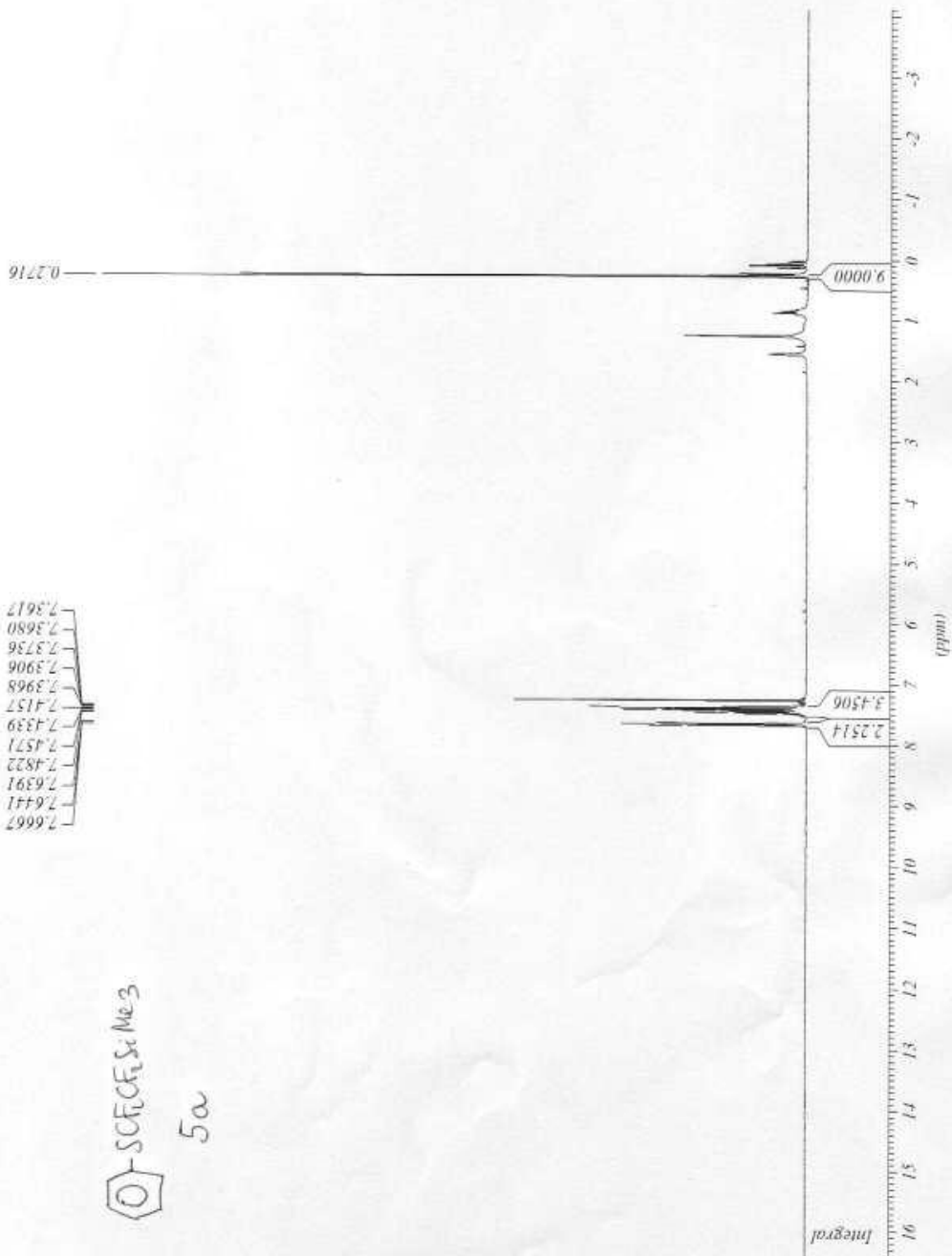
\*\*\*ID NMR Plot Parameters \*\*\*

SR : 20.40 Hz  
 ppm\_cm : 10.62  
 Hz\_cm : 801.50  
 Y1\_of\_cm : 58301.04  
 NUCLES : off  
 SOLVENT : ?

PROTON



7.6667  
 7.6441  
 7.6391  
 7.4822  
 7.4571  
 7.4339  
 7.4157  
 7.3968  
 7.3906  
 7.3736  
 7.3680  
 7.3617



\*\*\*Current Data Parameters\*\*\*

NAME : f178  
 EXPNO : 1  
 PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*

DATE\_1 : 02-55:37  
 DATE\_2 : Jan 26 2005  
 DS : 0  
 AS : 8  
 NUCLEUS : off  
 OF : 1853.43 Hz  
 O2 : 0.00 Hz  
 RG : 256.0000000  
 RO : 20 Hz  
 SFO1 : 300.1318534 MHz  
 SOLVENT : CDCl3  
 SU : 20.5671 ppm  
 SW\_H : 6172.840 Hz  
 TD : 32768  
 TE : 300.0 K

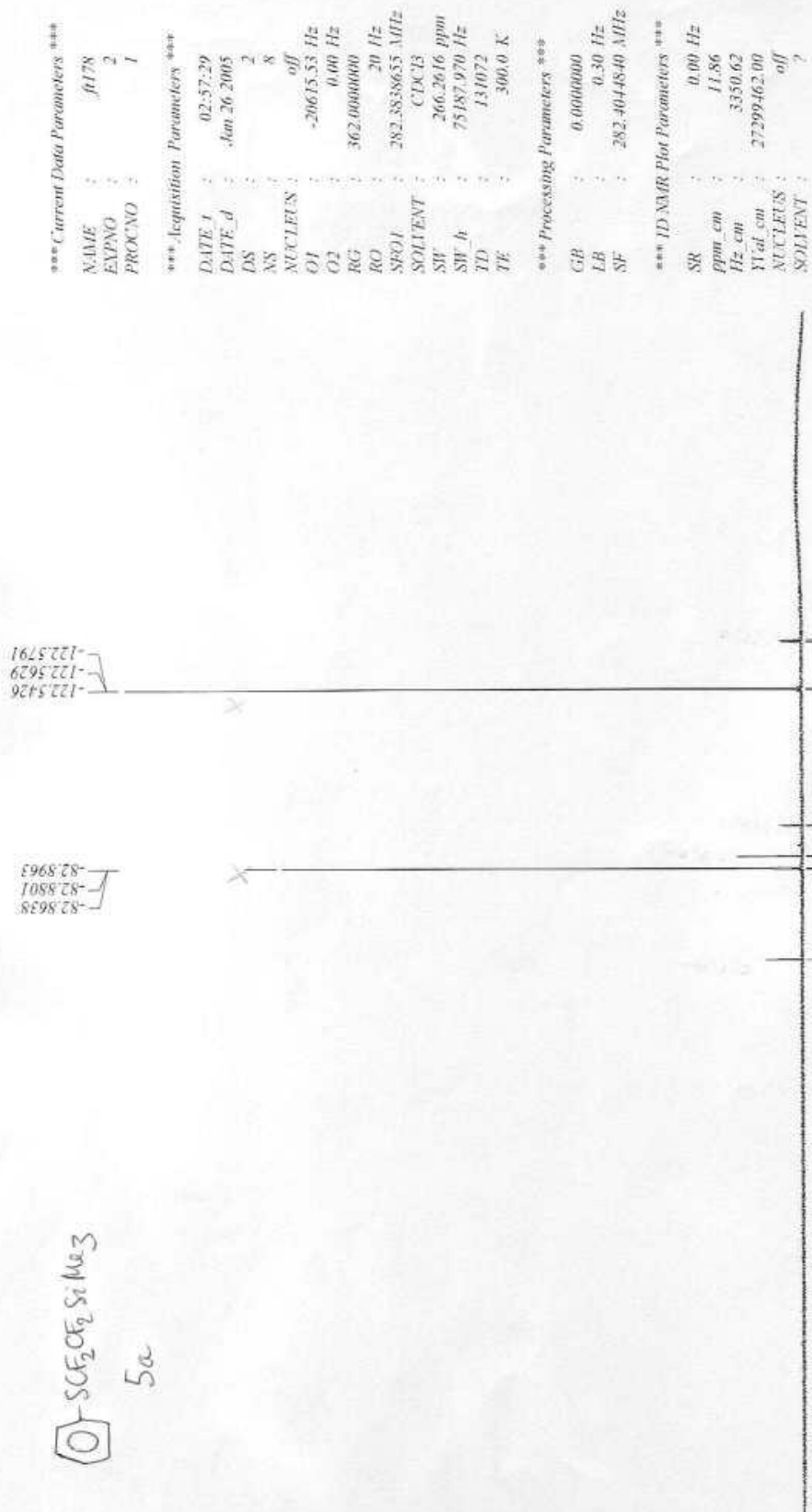
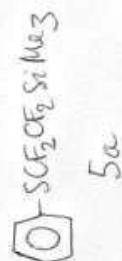
\*\*\*Processing Parameters\*\*\*

GB : 0.0000000  
 LB : 0.30 Hz  
 SF : 300.1300060 MHz

\*\*\*1D NMR Plot Parameters\*\*\*

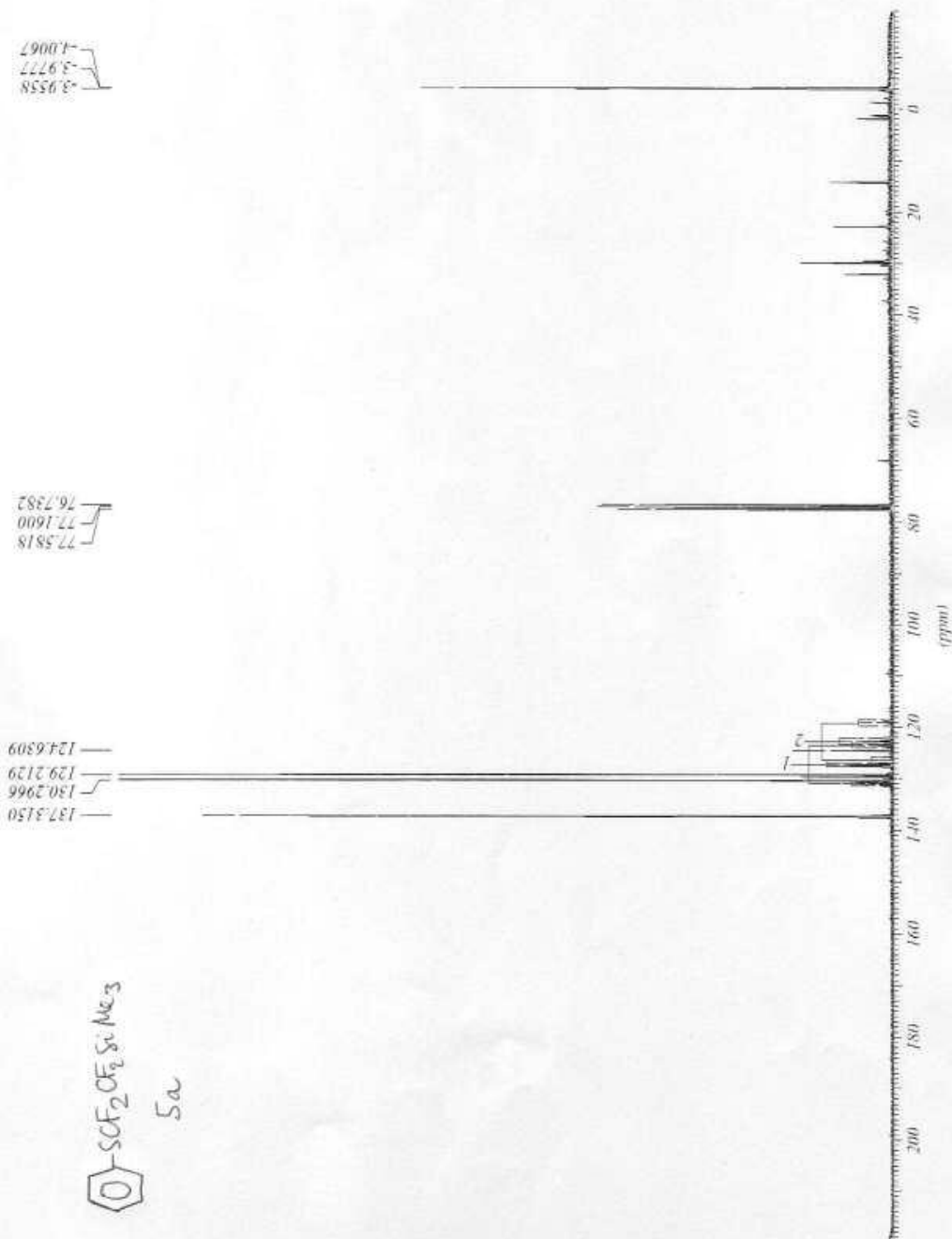
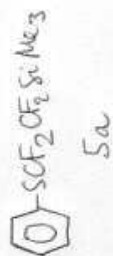
SR : 6.41 Hz  
 ppm cm : 0.92  
 Hz cm : 275.08  
 IT al cm : 15334935.00  
 NUCLEUS : off  
 SOLVENT : ?

F19\_30





<sup>13</sup>C NMR (CDCl<sub>3</sub>) δ



\*\*\* Current Data Parameters \*\*\*

NAME : f178  
 EXPNO : 101  
 PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 18-5-137  
 DATE\_2 : Jan 27 2005  
 DS : 4  
 NS : 4000  
 NUCLEUS : off  
 O1 : 7576.30 Hz  
 O2 : 1200.52 Hz  
 RG : 1824.5999736  
 RO : 20 Hz  
 SFO1 : 75.4752953 MHz  
 SOLVENT : CDCl<sub>3</sub>  
 SW : 238.2980 ppm  
 SW\_H : 17985.612 Hz  
 TD : 65536  
 TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
 LB : 1.00 Hz  
 SF : 75.4677400 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

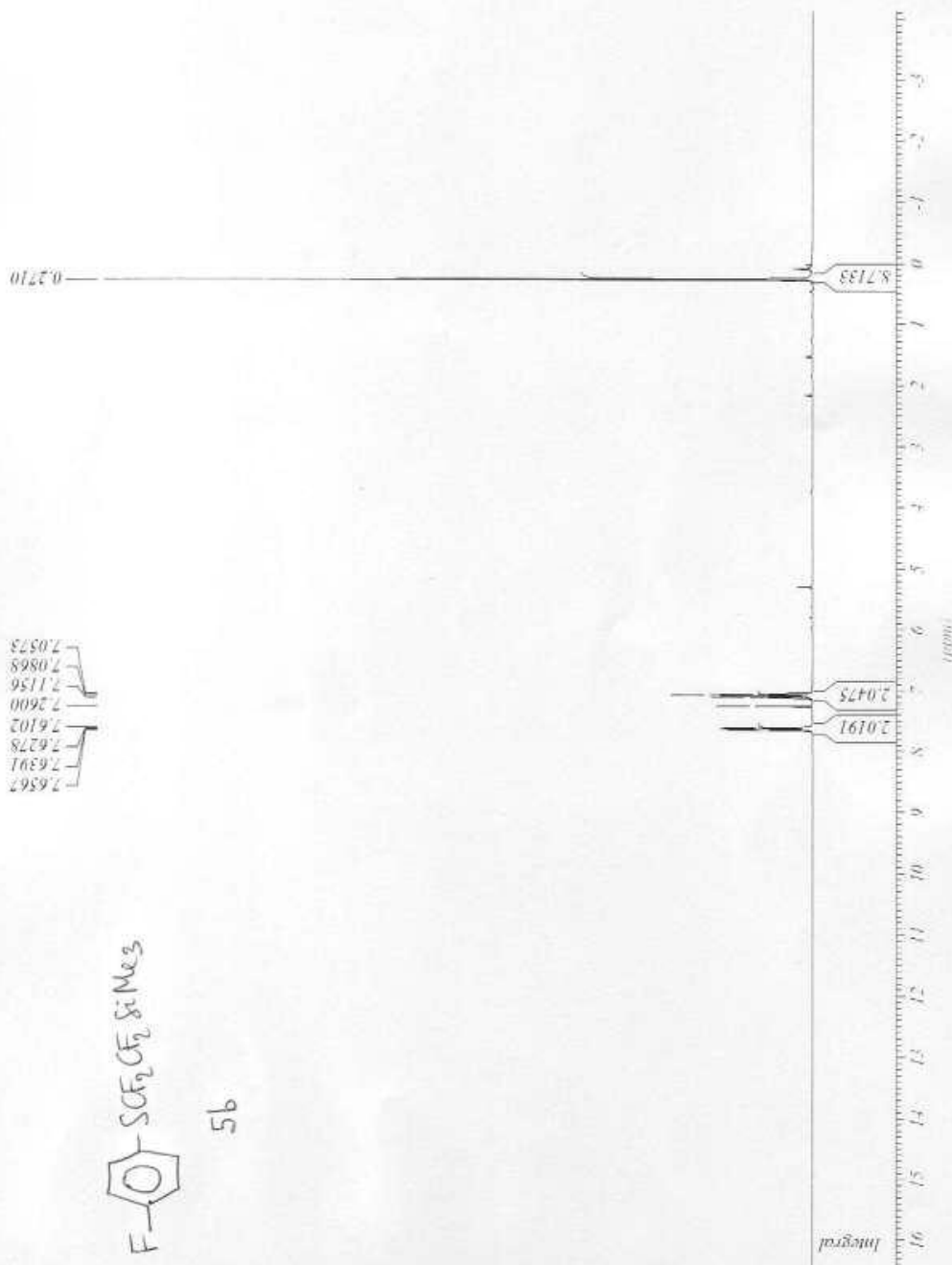
SR : 21.50 Hz  
 ppm\_cm : 10.62  
 Hz\_cm : 801.50  
 Y1d\_cm : 13.4867.23  
 NUCLEUS : off  
 SOLVENT : ?

PROTON



5b

7.6567  
7.6391  
7.6278  
7.6102  
7.2600  
7.1156  
7.0868  
7.0573



\*\*\*Current Data Parameters\*\*\*  
NAME : J428  
EXPNO : 1  
PROCNO : 1  
\*\*\*Acquisition Parameters\*\*\*  
DATE\_ : 00.16.18  
DATE : Feb 14 2006  
IN : 0  
EXP :  
AS : 8  
NUCLEI : off  
P1 : 1853.43 Hz  
P2 : 0.00 Hz  
RG : 228.0000061  
RO : 20 Hz  
SFO1 : 300.1318534 MHz  
SOLVENT : CDCl3  
SU : 20.5671 ppm  
SV : 6172.840 Hz  
TD : 32768  
TE : 300.0 K  
\*\*\*Processing Parameters\*\*\*  
GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300060 MHz  
\*\*\*1D NMR Plot Parameters\*\*\*  
SR : 6.41 Hz  
ppm : 0.92  
Hz : 275.08  
Wid : 252163.08 Hz  
NUCLEI : off  
SOLVENT :

F19\_30



56

122.5515  
122.5182  
122.5020  
110.5906  
110.5863  
110.5703  
110.5419  
110.5215  
110.4931  
83.2782  
83.2945  
83.3107

\*\*\* Current Data Parameters \*\*\*  
NAME : f428  
EXPNO : 2  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 00.18.07  
DATE\_2 : Feb 14 2006  
DS : 2  
EXP : PS done  
AS : 8  
NUCLEUS : off  
Q1 : -20015.53 Hz  
Q2 : 0.00 Hz  
RG : 512.0000000  
RO : 20 Hz  
SFO1 : 282.3838655 MHz  
SOLVENT : CDCl3  
SU : 266.2616 ppm  
SW : 75187.970 Hz  
TD : 131072  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
ppm : 11.86  
Hz : 3350.62  
YVal : 82652936.00  
NUCLEUS : off  
SOLVENT :



13C T1D1 1D 13 H NUC1013

166.0725  
162.7415  
139.5769  
139.5697  
139.5624  
139.4533  
139.4460  
127.1037  
122.7545  
119.9833  
119.9689  
119.9616  
119.9471  
119.9326  
119.9180  
119.9035  
119.8889  
119.8671  
116.6306  
116.3397

77.1600

3.9849  
4.0067  
4.0140  
4.0286  
4.0358  
4.0649  
4.0867

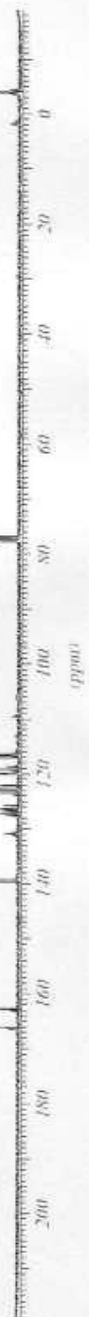


\*\*\* Current Data Parameters \*\*\*  
NAME : f428  
EXPNO : 2  
PROCNO : 1

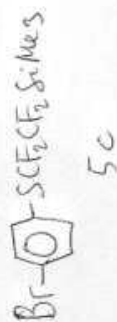
\*\*\* Acquisition Parameters \*\*\*  
DATE\_1 : 20-11-15  
DATE\_2 : Feb 22 2006  
DS : 4  
EXP : (13C70)  
AS : 2500  
NUCLEUS : off  
O1 : 7576.30 Hz  
O2 : 1200.52 Hz  
RG : 2580.300488  
R0 : 20 Hz  
SFO1 : 75.4753953 MHz  
SOLVENT : CDCl3  
SW : 238.2980 ppm  
SW\_H : 17985.612 Hz  
TD : 65536  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*  
GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4677360 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*  
SR : 17.11 Hz  
ppm\_cm : 10.62  
Hz\_cm : 801.50  
NUC1 : 13C  
SOLVENT : off



PROTON



7.3161  
7.3123  
7.2600

0.2653

\*\*\* Current Data Parameters \*\*\*

NAME : j042611  
EXPNO : 2  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 09.16.10  
DATE\_2 : Feb 15 2006  
IN : 0  
EXP : 8  
NS : 8  
NUCLEUS : off  
O1 : 1853.43 Hz  
O2 : 0.00 Hz  
RG : 456.1000061  
RO : 20 Hz  
SF : 300.1318534 MHz  
SOLVENT : CDCl3  
SH : 20.5671 ppm  
SH\_h : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

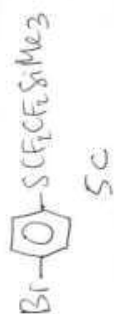
GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300070 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 6.60 Hz  
ppm cm : 0.92  
Hz cm : 275.08  
YI cm : 26957906.00  
NUCLEUS : off  
SOLVENT :



F19.40



-82.7948  
 -82.8110  
 -82.8313

-122.3841  
 -122.4004  
 -122.4207

\*\*\* Current Data Parameters \*\*\*

NAME : j426f1  
 EXPNO : 1  
 PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 23.49.23  
 DATE\_d : Feb 14 2006  
 DS : 2  
 EXP : PS done  
 NS : 8  
 NUCLEUS : off  
 O1 : -20615.53 Hz  
 O2 : 0.00 Hz  
 RG : 512.000000  
 RO : 20 Hz  
 SFO1 : 282.3838655 MHz  
 SOLVENT : CDCl3  
 SW : 266.2616 ppm  
 SW\_h : 75187.970 Hz  
 TD : 131072  
 TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

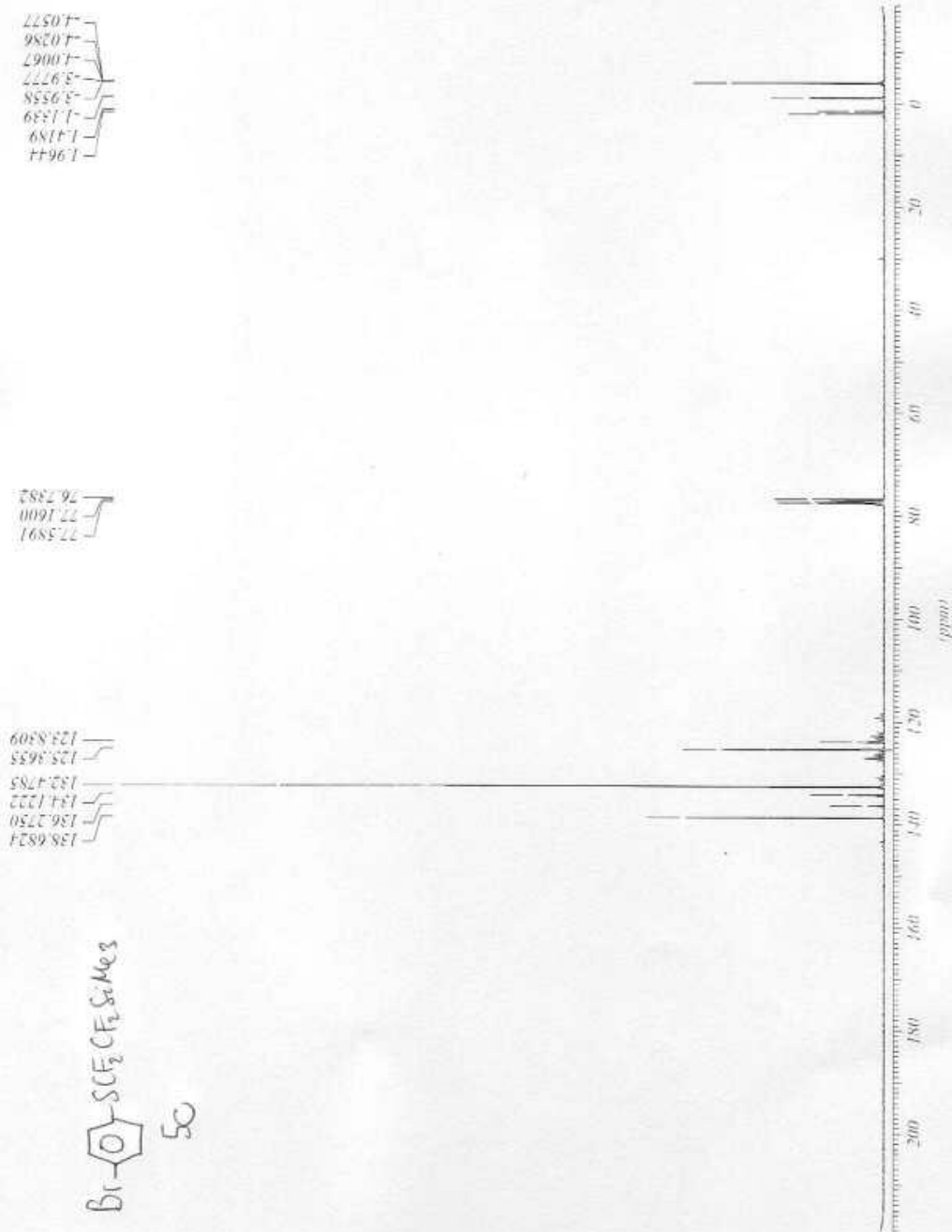
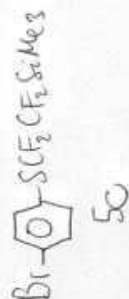
GB : 0.0000000  
 LB : 0.30 Hz  
 SF : 282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
 ppm\_cm : 11.86  
 Hz\_cm : 3350.62  
 YVal\_cm : 38868220.00  
 NUCLEUS : off  
 SOLVENT : ?



<sup>13</sup>C NMR (CDCl<sub>3</sub>) δ



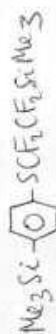
\*\*\*Current Data Parameters\*\*\*  
NAME : J41261T  
EXPNO : 101  
PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*  
DATE\_1 : 16-10-26  
DATE\_2 : Feb 23 2006  
INSTRUM : spect  
PROBHD : 5mm  
PULPROG : zgpg30  
F2 - 125.7630 MHz  
F1 - 125.7630 MHz  
RG : 645.0999756  
RO : 20 Hz  
SFO : 125.7630311 MHz  
SOLVENT : CDCl<sub>3</sub>  
NUC1 : 13C  
NUC2 : 1H  
TD : 65536  
TE : 300.2 K

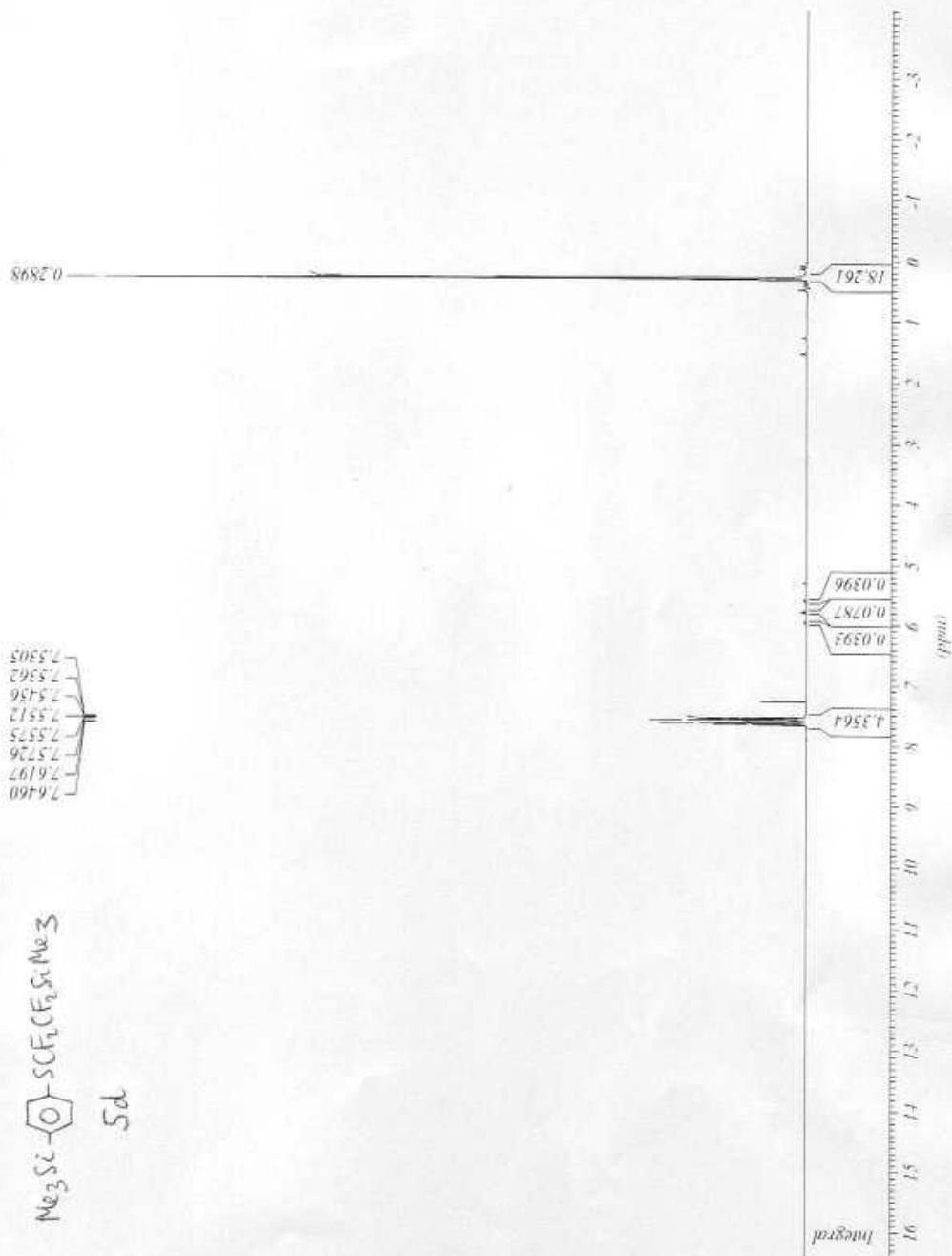
\*\*\*Processing Parameters\*\*\*  
GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4677390 MHz

\*\*\*1D NMR Plot Parameters\*\*\*  
SR : 19.86 Hz  
PPM : 10.62  
HZ : 801.50  
YF : 100036.82  
NUC1 : 13C  
SOLVENT : off

PROTON



5d



\*\*\*Current Data Parameters\*\*\*  
 NAME : j389H  
 EXPNO : 2  
 PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*  
 DATE\_1 : 07-09-15  
 DATE\_2 : Dec 20 2005  
 DS : 0  
 AS : 8  
 NUC1 : 1H  
 P1 : 1853.43 Hz  
 O1 : 0.00 Hz  
 O2 : 128.0000000  
 RG : 300.1318534 MHz  
 RO : 20 Hz  
 SFO1 : 300.1318534 MHz  
 SOLVENT : CHCl3  
 SH : 20.5671 ppm  
 SW\_H : 6172.840 Hz  
 TD : 32768  
 TE : 300.0 K

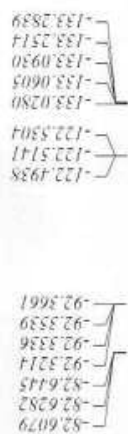
\*\*\*Processing Parameters\*\*\*  
 GB : 0.0000000  
 LB : 0.30 Hz  
 SF : 300.1300060 MHz

\*\*\*1D NMR Plot Parameters\*\*\*  
 SR : 6.41 Hz  
 ppm : 0.92  
 Hz : 275.08  
 Y1 : 10885316.00  
 NUC1 : 1H  
 SOLVENT : CHCl3





5d



CH<sub>2</sub> of 5d

CH of 5d

CH<sub>2</sub> of 5d

CH of 5d



\*\*\* Current Data Parameters \*\*\*

NAME : f389f1  
EXPNO : 1  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 07-07-11  
DATE\_2 : Dec 20 2005  
DS : 2  
NS : 8  
NUCLEUS : off  
P1 : -20615.53 Hz  
P2 : 0.00 Hz  
RG : 1149.4000244  
RO : 20 Hz  
SFO1 : 282.583655 MHz  
SFO2 : 101.626126 MHz  
SFO3 : 266.2616 MHz  
SFO4 : 75187.970 Hz  
TD : 131022  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
ppm\_cm : 11.86  
Hz\_cm : 3350.62  
Wid\_cm : 29590832.00  
NUCLEUS : off  
SOLVENT : 2

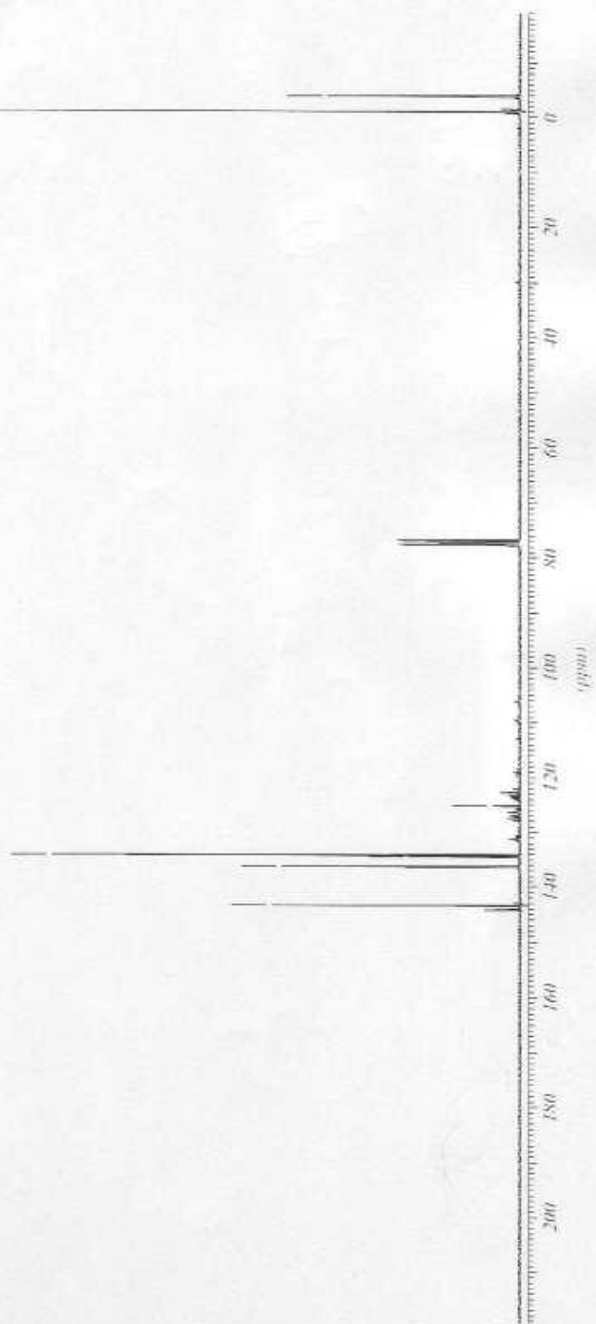
C13C PD C1X 13 u.s. ref 3



143.3153  
 136.2823  
 134.1204  
 134.1295  
 125.1255

1.1194  
 3.8904  
 3.9195  
 3.9413  
 3.9631  
 3.9922

\*\*\*Current Data Parameters \*\*\*  
 NAME :   
 EXPNO : 101  
 PROCNO : 1  
 \*\*\*Acquisition Parameters \*\*\*  
 DATE\_1 : 21.24.30  
 DATE\_2 : Dec 20 2005  
 DS : 4  
 NS : 3000  
 NUC1ES : off  
 OL : 7576.30 Hz  
 O2 : 1200.52 Hz  
 RG : 4597.6000977  
 RO : 20 Hz  
 SFO1 : 75.4752953 MHz  
 SOL1ENT : C1X13  
 SW : 238.2980 ppm  
 SIU\_h : 17985.612 Hz  
 TD : 65536  
 TE : 300.0 K  
 \*\*\*Processing Parameters \*\*\*  
 GB : 0.0000000  
 LB : 1.00 Hz  
 SF : 75.4677390 MHz  
 \*\*\*ID NMR Plot Parameters \*\*\*  
 SR : 19.86 Hz  
 ppm\_cm : 10.62  
 Hz\_cm : 801.50  
 IT\_d\_cm : 647109.63  
 NUCLES : off  
 SOLVENT : ?



8.6204  
8.6239  
8.6274  
8.6095  
7.7144  
7.7082  
7.6881  
7.6818  
7.6655  
7.6611  
7.6397  
7.3052  
7.1977  
7.2889  
7.2813  
7.2763  
7.2675  
7.2600

CN1C=CC=C(C1)SC(F)(F)F 6a

NAME	?	0.387-2
EXTNO	?	1
PROCNO	?	1

DATE	12	23:55:17
DATE_d	2	Dec 13 2005
OS	7	0

01	1853.43 H
02	0.00 H
RG	128.0000000

SW	20.5671	pl
SW/h	6.172840	FI
FI	32768	

Processing Parameters	
GB	0.0000000
LB	0.30 HB

333 MHz <sup>1</sup> H NMR Flou Parameters	
SR	0.41 Hz
ppm cm	0.97

*Bo* NUCLEUS





6a

122.4654  
122.4816  
122.4979

82.1366  
82.1529  
82.1691

\*\*\*Current Data Parameters\*\*\*  
NAME : f387-2  
EXPNO : 2  
PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*

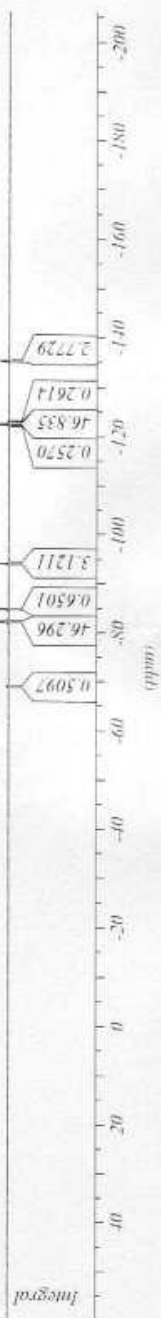
DATE\_1 : 23-57-16  
DATE\_2 : Dec 13 2005  
DS : 2  
SS : 8  
NUCLEUS : off  
O1 : -20615.53 Hz  
O2 : 0.00 Hz  
RG : 1024.000000  
RO : 20 Hz  
SFOF : 282.3838655 MHz  
SOLVENT : CDCl3  
SW : 266.2616 ppm  
SW\_H : 75187.970 Hz  
TD : 131072  
TE : 300.0 K

\*\*\*Processing Parameters\*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 282.4044840 MHz

\*\*\*1D NMR Plot Parameters\*\*\*

SR : 0.00 Hz  
ppm\_cm : 11.86  
Hz\_cm : 3350.62  
V1\_d\_cm : 68024616.00  
NUCLEUS : off  
SOLVENT :

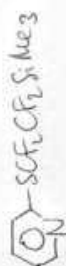




4.0649  
4.0867  
4.1158  
4.1376  
4.1667

77.1600

150.5446  
150.5083  
149.7882  
149.7664  
149.7446  
137.6132  
137.2714  
131.5257  
130.1584  
128.1656  
127.7728  
123.6345  
123.5181  
122.4708  
121.8817  
118.8561

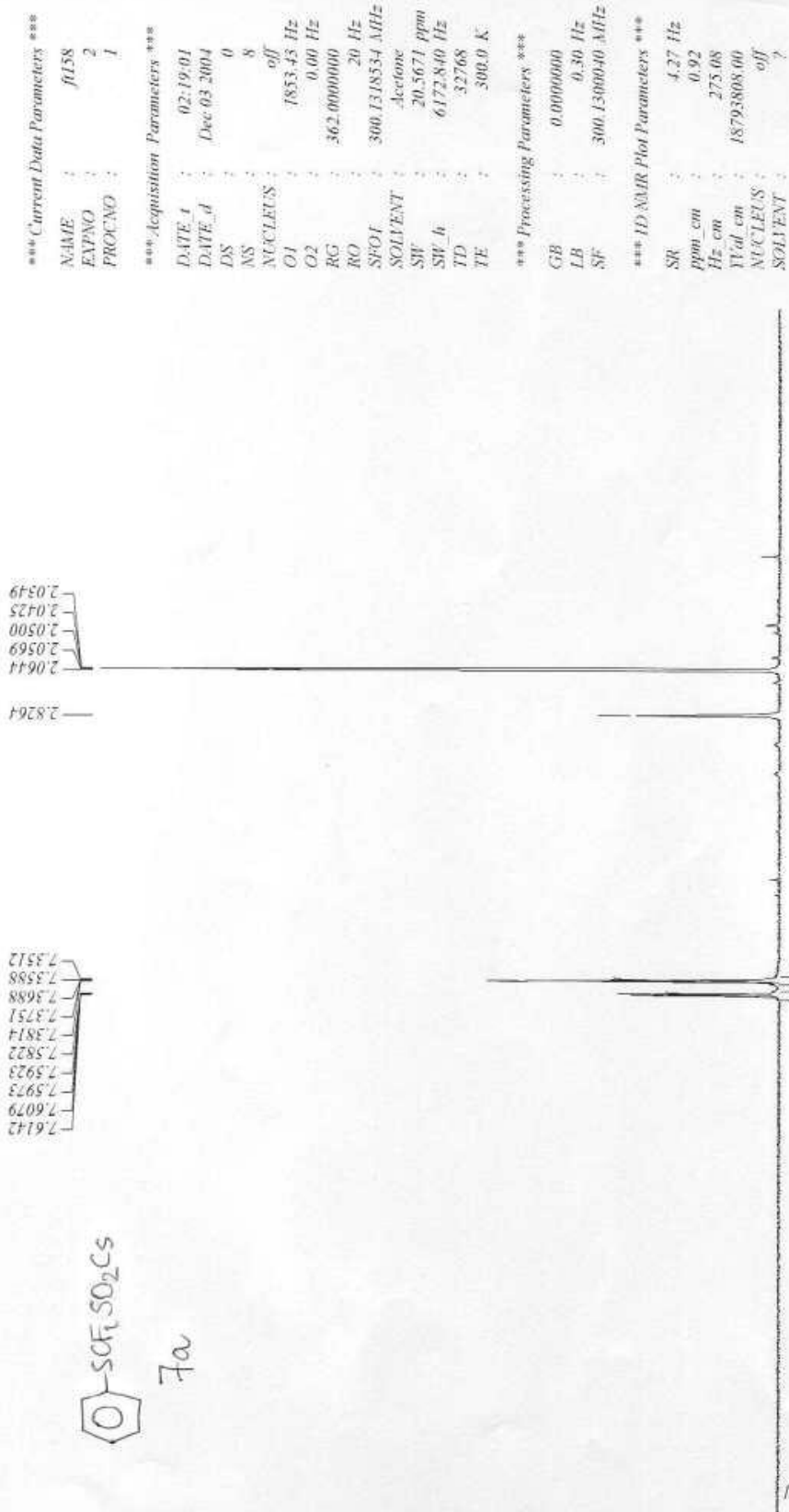


6a

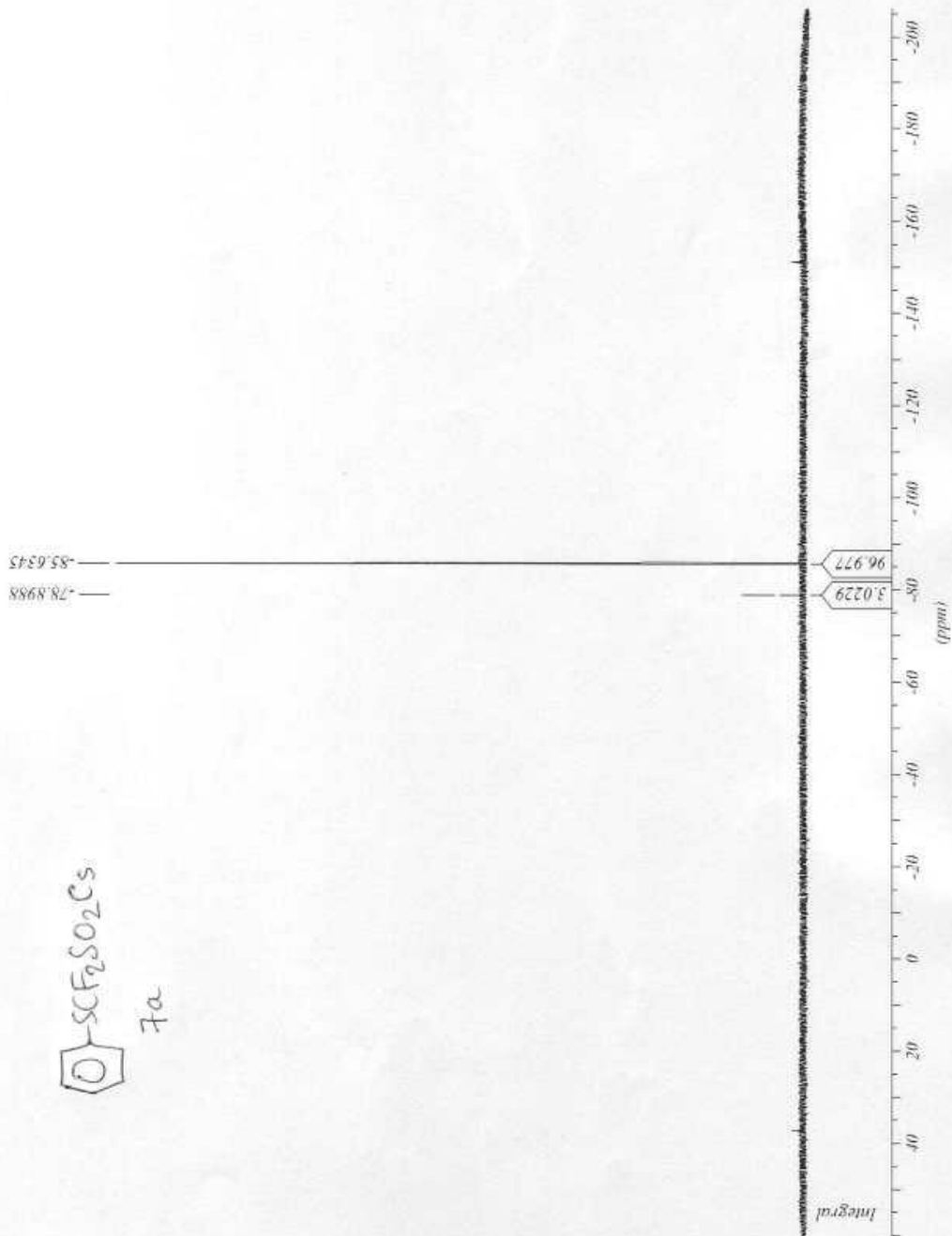
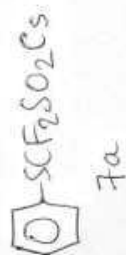
\*\*\* Current Data Parameters \*\*\*  
NAME : j417  
EXPNO : 101  
PROCNO : 1  
\*\*\* Acquisition Parameters \*\*\*  
DATE\_1 : 20.03.28  
DATE\_2 : Feb 07 2006  
DS : 4  
EXP : C13CPD  
NS : 4000  
NUCLEUS : off  
O1 : 7576.30 Hz  
O2 : 1200.52 Hz  
RG : 812.7000122  
RO : 20 Hz  
SFO1 : 75.4752953 MHz  
SOLVENT : CDCl3  
SW : 238.2980 ppm  
SW\_H : 17985.612 Hz  
TD : 65536  
TE : 300.0 K  
\*\*\* Processing Parameters \*\*\*  
GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4677440 MHz  
\*\*\* 1D NMR Plot Parameters \*\*\*  
SR : 24.79 Hz  
ppm\_cm : 10.62  
Hz\_cm : 801.50  
YVal\_cm : 152380.41  
NUCLEUS : off



PROTON



F19\_30



\*\*\* Current Data Parameters \*\*\*

NAME : f158  
EXPNO : 1  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 02.17.30  
DATE\_d : Dec 03 2004  
DS : 2  
NS : 8  
NUCLEUS : off  
O1 : -20615.53 Hz  
O2 : 0.00 Hz  
RG : 1290.1999512  
RO : 20 Hz  
SFO1 : 282.3838655 MHz  
SOLVENT : Acetone  
SW : 266.2616 ppm  
SW\_h : 75187.970 Hz  
TD : 131072  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 282.4044840 MHz

\*\*\* ID NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
ppm\_cm : 11.86  
Hz\_cm : 3350.62  
Y1\_d\_cm : 31618912.00  
NUCLEUS : off  
SOLVENT : Acetone



7a

141.1505  
136.7207  
135.6587  
132.2982  
129.0541  
128.9449  
127.8029  
127.7739  
127.7520

206.6662

30.7332

Identifier	Chem. Shift [ppm]	J [Hz]	Multiplicity	Connections
1	127.7763	1.9211	3	J(1,0)
2	18.3687	333.9418	3	J(2,0)

## \*\*\* Current Data Parameters \*\*\*

NAME : fl158

EXPNO : 101

PROCNO : 1

## \*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 11-12-06

DATE\_2 : Dec 16 2004

DS : 4

AS : 3072

NUCLEUS : off

O1 : 7576.30 Hz

O2 : 1200.52 Hz

RG : 4096.0000000

RO : 20 Hz

SFO1 : 75.475953 MHz

SOLVENT : DMSO

SF : 238.2980 ppm

SW\_h : 17985.612 Hz

TD : 65536

TE : 296.2 K

## \*\*\* Processing Parameters \*\*\*

GB : 0.0000000

LB : 1.00 Hz

SF : 75.4587880 MHz

## \*\*\* 1D NMR Plot Parameters \*\*\*

SR : 62.09 Hz

ppm\_cm : 16.62

Hz\_cm : 801.50

Y1\_cm : 198513.92

NUCLEUS : off

SOLVENT : 2







\*\*\* Current Data Parameters \*\*\*

NAME : j6257  
EXPNO : 100  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 18-52-47  
DATE\_2 : May 26 2005  
DS : 0  
EXP : PROTON  
NS : 8  
NUCLEUS : off

O1 : 1853.43 Hz  
O2 : 0.00 Hz  
RG : 203.1999969  
RO : 20 Hz  
SF01 : 300.1316534 MHz  
SOLVENT : DMSO  
SW : 20.3671 ppm  
SW\_h : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300000 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : -0.00 Hz  
ppm\_cm : 0.92  
Hz\_cm : 275.08  
Y1val\_cm : 6315.96  
NUCLEUS : off

4.1374  
2.5074

7.6203  
7.5977  
7.5192  
7.4966  
7.4841  
7.4602



8a

PROTON DMSO-d6 300K 311



F19\_30



8a

-127.2551  
-127.2795  
-127.2998

-85.2120  
-85.2323  
-85.2567

\*\*\* Current Data Parameters \*\*\*  
NAME : f1257  
EXPNO : 2  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*  
DATE\_1 : 03-02-38  
DATE\_2 : May 20 2005  
DS : 2  
NS : 8  
NUCLEUS : off  
O1 : -20615.53 Hz  
O2 : 0.00 Hz  
RG : 512.0000000  
RO : 20 Hz  
SFO1 : 282.3838655 MHz  
SOLVENT : DMSO  
SW : 266.2616 ppm  
SW\_H : 75187.970 Hz  
TD : 131072  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*  
GB : 0.0000000  
LB : 0.30 Hz  
SF : 282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*  
SR : 0.00 Hz  
ppm\_cm : 11.86  
Hz\_cm : 3350.62  
Fid\_cm : 57739740.00  
NUCLEUS : off  
SOLVENT : ?



F19\_30



8a

-127.2551  
-127.2795  
-127.2998

-85.2120  
-85.2323  
-85.2567

\*\*\* Current Data Parameters \*\*\*  
NAME : f1257  
EXPNO : 2  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*  
DATE\_1 : 03-02-38  
DATE\_2 : May 20 2005  
DS : 2  
NS : 8  
NUCLEUS : off  
O1 : -20615.53 Hz  
O2 : 0.00 Hz  
RG : 512.0000000  
RO : 20 Hz  
SFO1 : 282.3838655 MHz  
SOLVENT : DMSO  
SW : 266.2616 ppm  
SW\_H : 75187.970 Hz  
TD : 131072  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*  
GB : 0.0000000  
LB : 0.30 Hz  
SF : 282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*  
SR : 0.00 Hz  
ppm\_cm : 11.86  
Hz\_cm : 3350.62  
Fid\_cm : 57739740.00  
NUCLEUS : off  
SOLVENT : 2





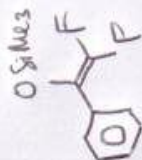
\*\*\* Current Data Parameters \*\*\*  
NAME : j652-1  
EXPNO : 2  
PROCNO : 1  
\*\*\* Acquisition Parameters \*\*\*  
DATE\_1 : 07:58:10  
DATE\_2 : May 04 2004  
DS : 0  
EXP :  
NS : 8  
NUCLEUS : off  
O1 : 1833.43 Hz  
O2 : 0.00 Hz  
RG : 128.000000  
RO : 20 Hz  
SFO1 : 300.1318534 MHz  
SOLVENT : CDCl3  
SW : 20.5671 ppm  
SW\_H : 6172.840 Hz  
TD : 32768  
TE : 300.0 K  
\*\*\* Processing Parameters \*\*\*  
GB : 0.000000  
LB : 0.30 Hz  
SF : 300.1300000 MHz  
\*\*\* 1D NMR Plot Parameters \*\*\*  
SR : -0.00 Hz  
ppm\_cm : 0.49  
Hz\_cm : 148.56  
YVal\_cm : 126206792.00  
NUCLEUS : off  
SOLVENT :



0.2214  
0.2183

2.9850  
2.9229  
2.9210

7.4132  
7.3956  
7.3899  
7.3742  
7.3699  
7.3316  
7.3272  
7.3234  
7.3109  
7.3033  
7.2952  
7.2801  
7.2217  
6.3217  
6.1434



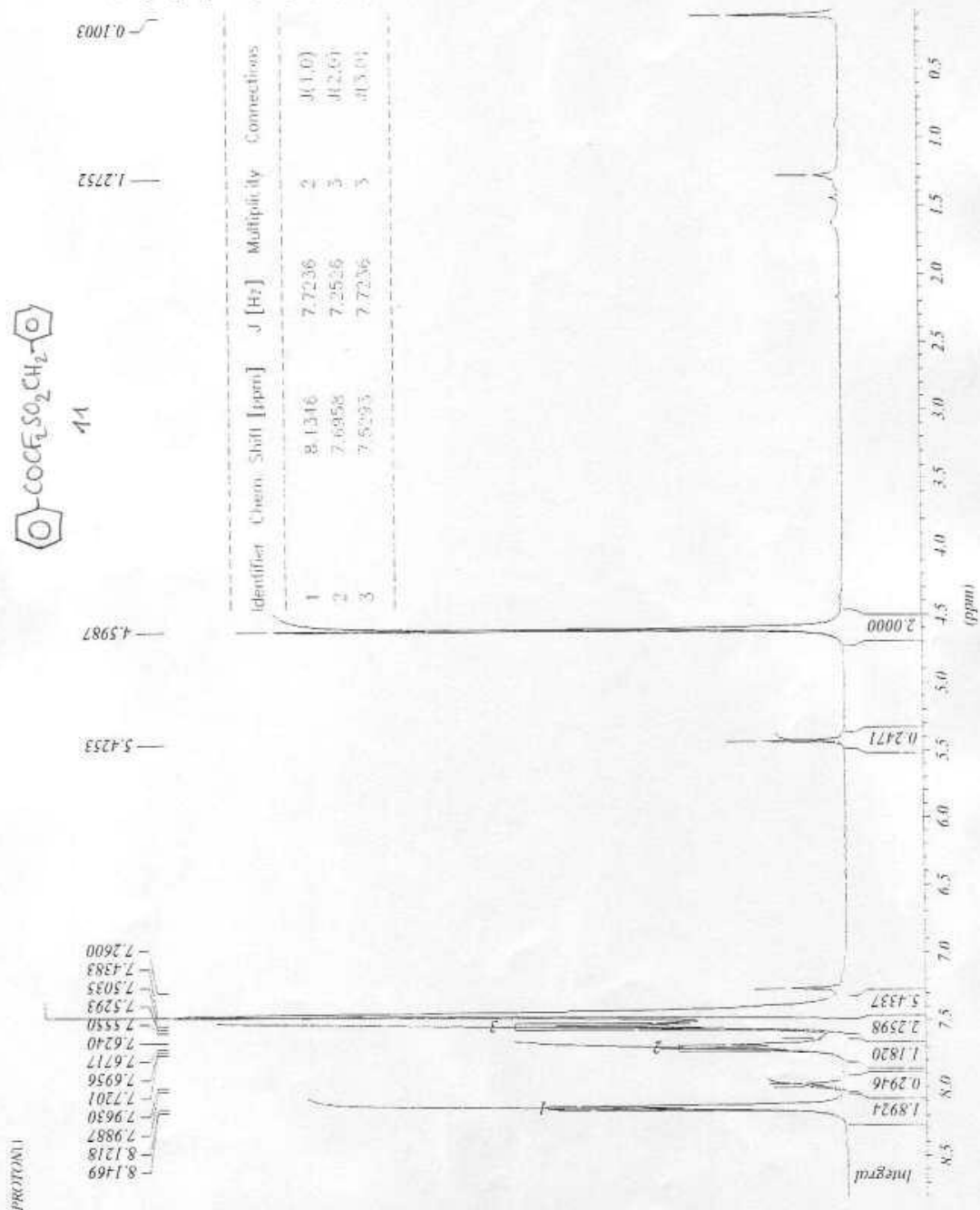
g

7.3  
1.1878  
7.4  
2.2444  
7.5  
2.3950





\*\*\* Current Data Parameters \*\*\*  
NAME : f69-2  
EXPNO : 1  
PROCNO : 1  
\*\*\* Acquisition Parameters \*\*\*  
DATE\_1 : 07:56:44  
DATE\_2 : May 28 2004  
DS : 0  
NS : 8  
NUCLEUS : off  
O1 : 1853.43 Hz  
O2 : 0.00 Hz  
RG : 128.000000  
RO : 20 Hz  
SFO1 : 300.1318534 MHz  
SOLVENT : CDCl3  
SW : 20.5671 ppm  
SW\_H : 6172.840 Hz  
TD : 32768  
TE : 300.0 K  
\*\*\* Processing Parameters \*\*\*  
GB : 0.000000  
LB : 0.30 Hz  
SF : 300.1300060 MHz  
\*\*\* 1D NMR Plot Parameters \*\*\*  
SR : 6.03 Hz  
ppm\_cm : 0.39  
Hz\_cm : 117.15  
YVal\_cm : 20928072.00  
NUCLEUS : off  
SOLVENT :



F19\_30



11

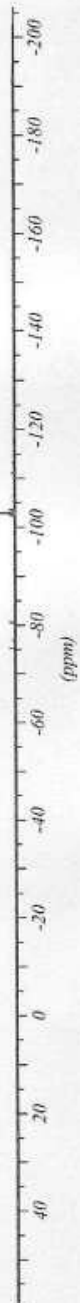
-103.0302

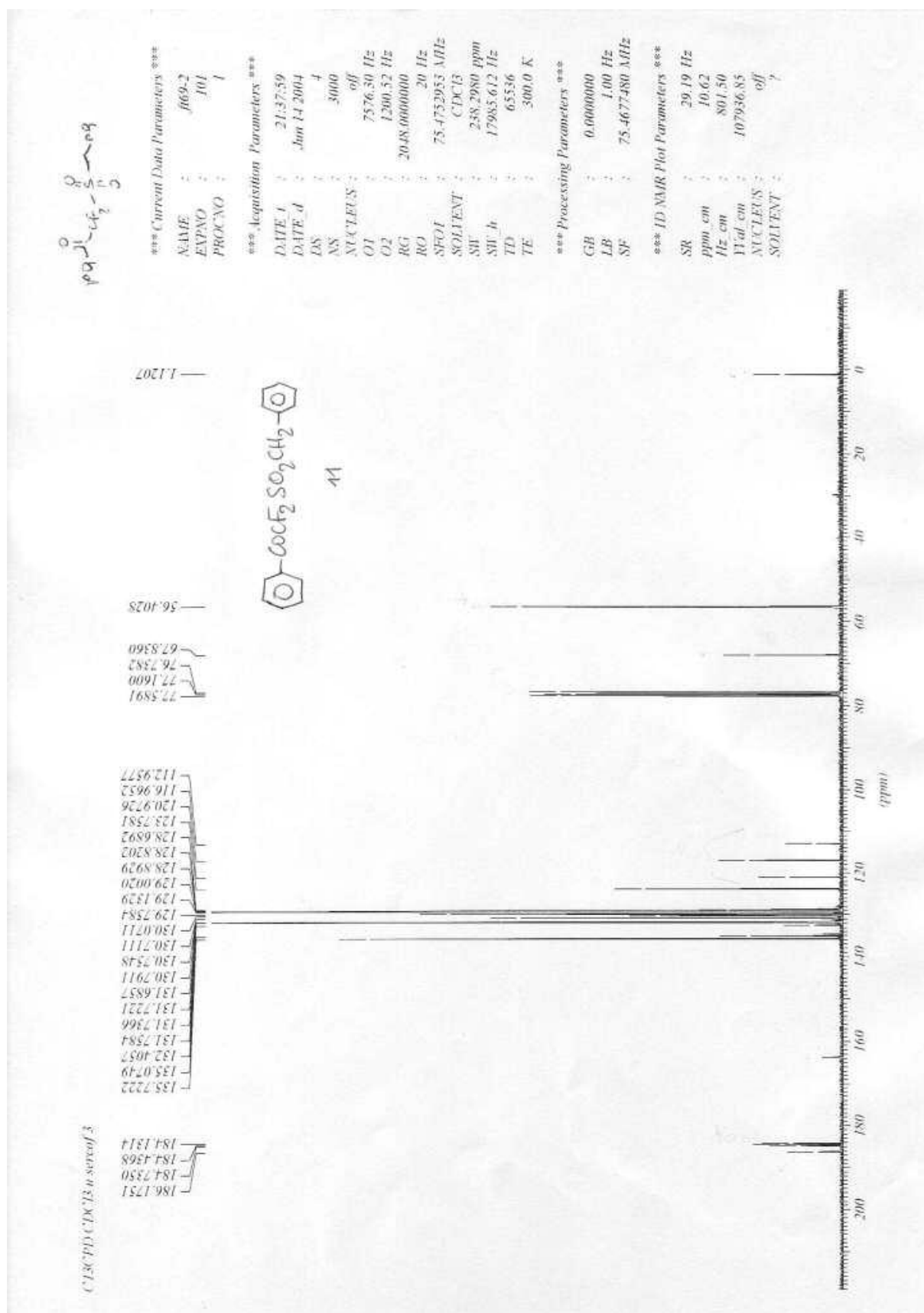
\*\*\* Current Data Parameters \*\*\*  
 NAME : f69-2  
 EXPNO : 2  
 PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*  
 DATE\_1 : 07-58:26  
 DATE\_2 : May 28 2004  
 DS : 2  
 EXP : PS done  
 NS : 8  
 NUCLEUS : off  
 O1 : -20615.53 Hz  
 O2 : 0.00 Hz  
 RG : 574.7000122  
 RO : 20 Hz  
 SFO1 : 282.3838655 MHz  
 SOLVENT : CDCl3  
 SW : 266.2616 ppm  
 SW\_h : 75187.970 Hz  
 TD : 131072  
 TE : 300.0 K

\*\*\* Processing Parameters \*\*\*  
 GB : 0.0000000  
 LB : 0.30 Hz  
 SF : 282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*  
 SR : 0.00 Hz  
 ppm\_cm : 11.86  
 Hz\_cm : 3350.62  
 YVal\_cm : 31979594.00  
 NUCLEUS : off  
 SOLVENT : ?







\*\*\* Current Data Parameters \*\*\*

NAME : f1833d1  
EXPNO : 1  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 09-07-31  
DATE\_2 : Feb 14 2005  
DS : 0  
AS : 8  
NUCLEUS : off

Q1 : 1833.43 Hz

Q2 : 0.00 Hz

RG : 406.3999939

RO : 20 Hz

SFO1 : 300.1318334 MHz

SOLVENT : CDCl3

SU : 20.5671 ppm

SU\_b : 6172.840 Hz

TD : 32768

TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000

LB : 0.30 Hz

SF : 300.1300070 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 6.00 Hz

ppm/cm : 0.92

Hz/cm : 275.08

Y1/ol cm : 43004356.00

NUCLEUS : off

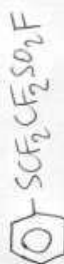
SOLVENT :

1.5415

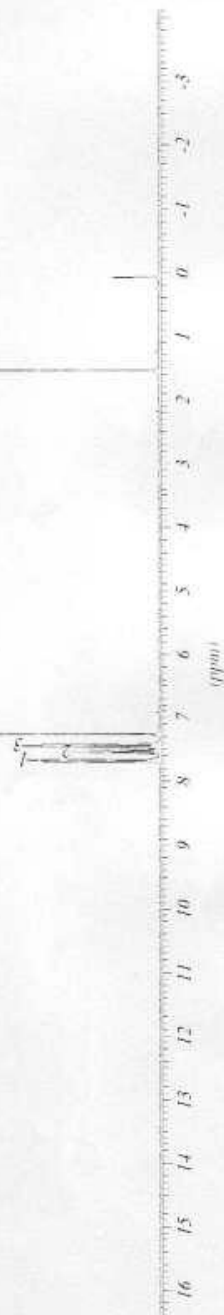
7.6874  
7.6623  
7.5381  
7.4433  
7.2600

Identifier Chem. Shift [ppm] J [Hz] Multiplicity Connections

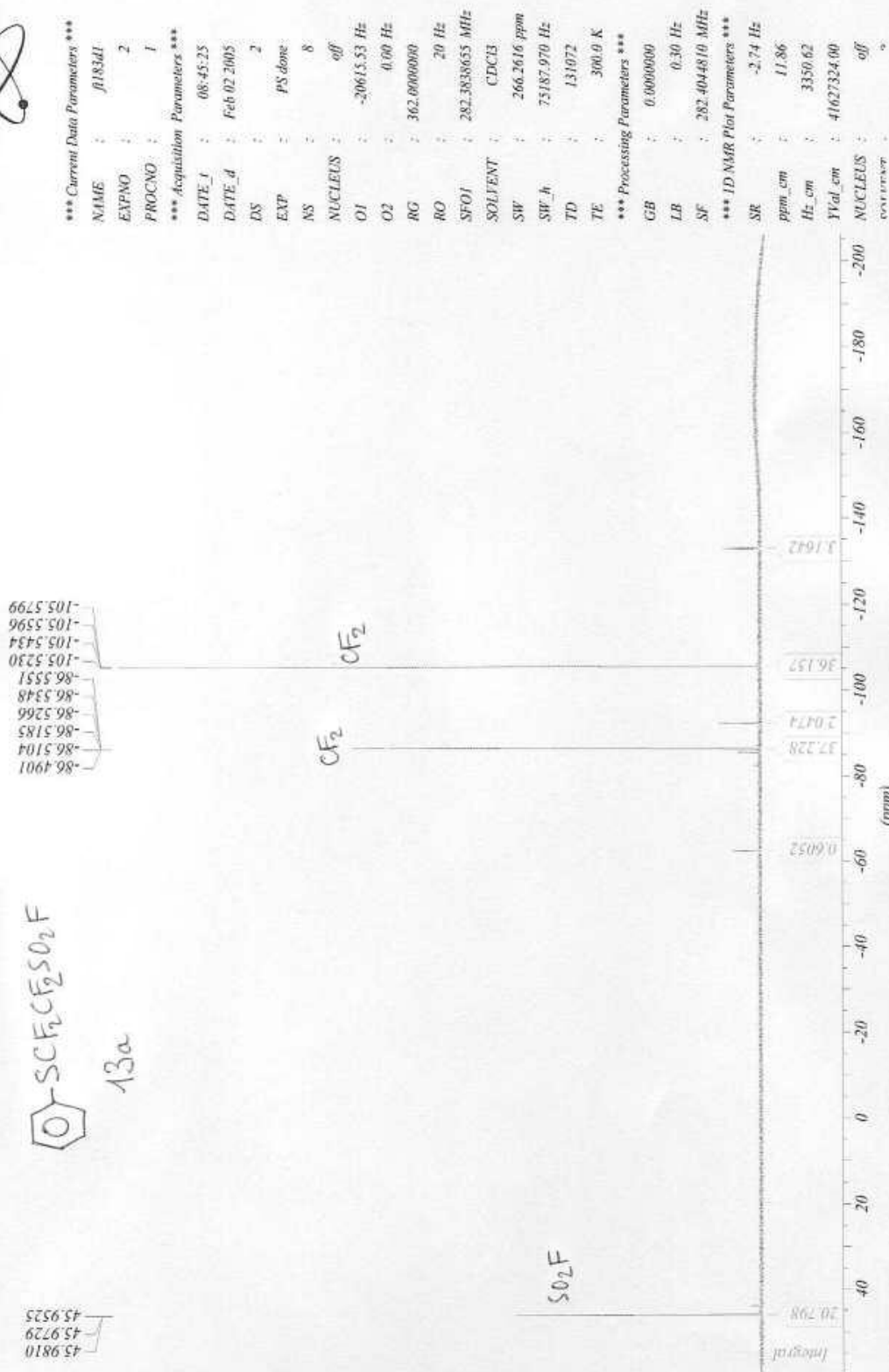
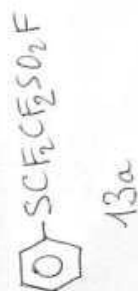
1	7.6749	7.5352	2	d(1,0)
2	7.5381	7.1584	3	d(2,0)
3	7.4435	7.4410	3	d(3,0)



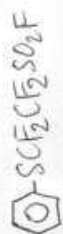
13a







C13C PDC1X13 n 800012



13a

137.5832  
131.6785  
129.8020  
125.6128  
122.0926  
121.7581  
117.9034  
116.1215  
115.6924  
112.1432

77.1600

\*\*\* Current Data Parameters \*\*\*  
NAME : f183.d  
EXPNO : 101  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 21-01-57  
DATE\_2 : Feb 14 2005  
DS : 4  
AS : 3500  
NUCLEUS : off  
O1 : 7576.30 Hz  
O2 : 1290.52 Hz  
RG : 2580.3000488  
RO : 20 Hz  
SF01 : 75.4752953 MHz  
SOLVENT : C13C13  
SW\_h : 238.2980 ppm  
SW\_w : 17985.612 Hz  
TD : 65536  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4677380 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 18.76 Hz  
ppm\_cm : 10.62  
Hz\_cm : 801.50  
Y1\_of\_cm : 104807.91  
NUCLEUS : off  
SOLVENT :





\*\*\* Current Data Parameters \*\*\*

NAME : f441d  
EXPNO : 1  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 07.10.35  
DATE\_2 : Mar 06 2006  
DS : 0  
EXP :  
NS : 8

\*\*\* Processing Parameters \*\*\*

NUCLEUS : off  
O1 : 1853.43 Hz  
O2 : 0.00 Hz  
RG : 574.7000122  
RO : 20 Hz

\*\*\* 1D NMR Plot Parameters \*\*\*

SFO1 : 300.1318534 MHz  
SOLVENT : CDCl3  
SW : 20.5671 ppm  
SW\_h : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300000 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 6.41 Hz  
ppm\_cm : 0.39  
Hz\_cm : 117.54  
YVal\_cm : 20173622.00

\*\*\* Processing Parameters \*\*\*

NUCLEUS : off  
CONVLEV : ?



13b

7.6925  
7.6749  
7.6686  
7.6630  
7.6460  
7.2600  
7.1753  
7.1527  
7.1476  
7.1458  
7.1401  
7.1175

Integral

2.0214  
2.0000

(ppm)

F19\_30

45.9916  
45.9835  
45.9672



13b

105.6749  
105.6953  
105.7115  
105.7278  
107.6290  
107.6453  
107.6575  
107.6737  
107.6859  
107.6940  
107.7022  
107.7225

86.9629  
86.9832  
86.9914  
86.9995  
87.0076  
87.0279

\*\*\* Current Data Parameters \*\*\*  
NAME : f141d  
EXPNO : 2  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

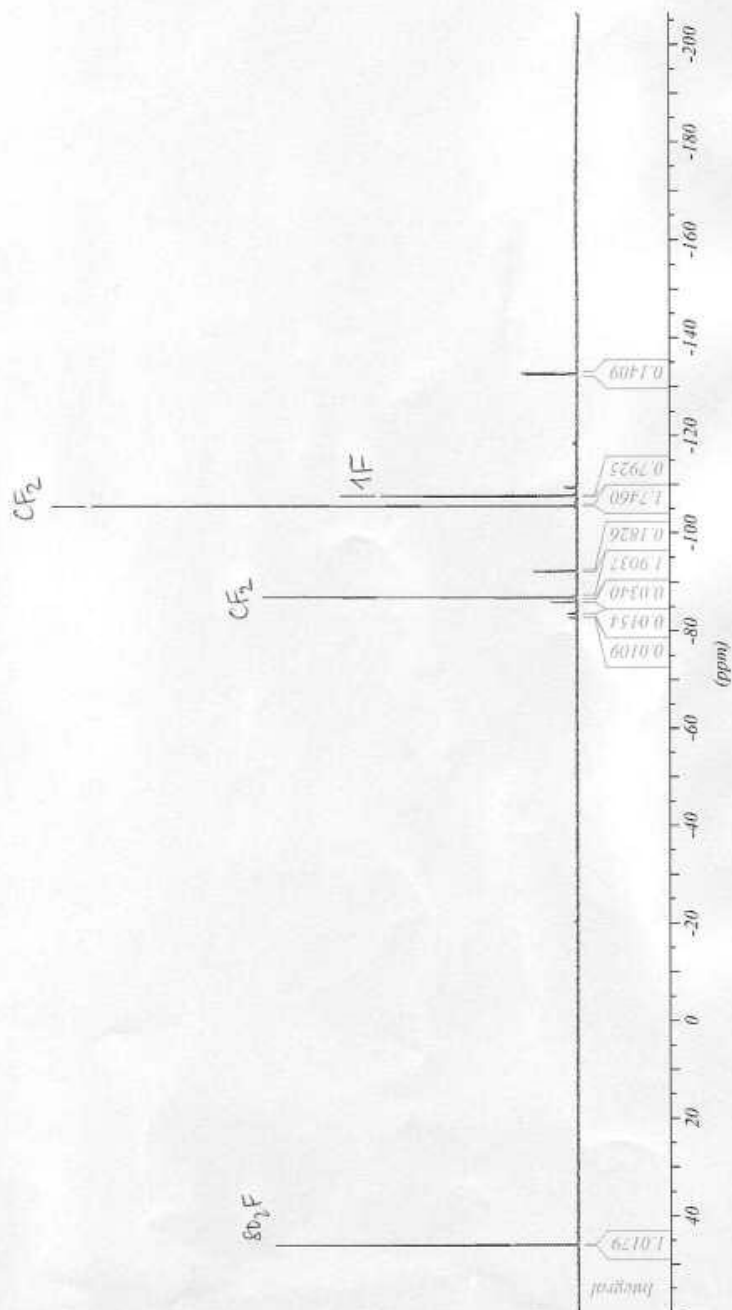
DATE\_1 : 07:12:28  
DATE\_d : Mar 06 2006  
DS : 2  
EXP : PS done  
NS : 8  
NUCLEUS : off  
O1 : -20615.53 Hz  
O2 : 0.00 Hz  
RG : 645.0999756  
RO : 20 Hz  
SF01 : 282.3838655 MHz  
SOLVENT : CDCl3  
SW : 266.2616 ppm  
SW\_h : 75187.970 Hz  
TD : 131072  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
ppm\_cm : 11.88  
Hz\_cm : 3355.58  
YVal\_cm : 46056456.00  
NUCLEUS : off  
SOLVENT : ?





\*\*\* Current Data Parameters \*\*\*

NAME : f441d  
EXPNO : 101  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 14.29.58  
DATE\_2 : Mar 13 2006  
DS : 4  
EXP : C13CPD  
NS : 4000  
NUCLEUS : off  
O1 : 7576.30 Hz  
O2 : 1200.52 Hz  
RG : 1824.5999736  
RO : 20 Hz  
SF01 : 75.4752953 MHz  
SOLVENT : CDCl3  
SW : 238.2980 ppm  
SW\_h : 17985.612 Hz  
TD : 65536  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000680  
LB : 1.00 Hz  
SF : 75.4677340 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 14.92 Hz  
ppm\_cm : 10.62  
Hz\_cm : 801.50  
YVal\_cm : 145044.03  
NUCLEUS : off  
PULPROG : zgpg30

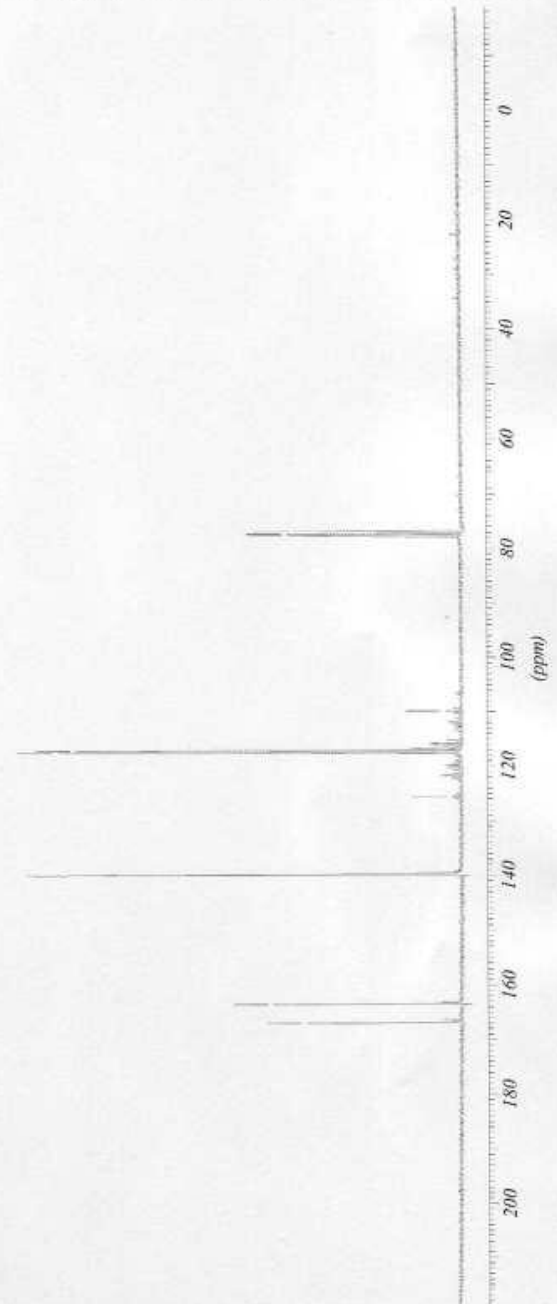
76.7382  
77.1600  
77.5818

109.7140  
117.0452  
117.3361  
117.3725  
117.4161  
117.4597  
117.4743  
125.4237  
125.4382  
125.4528  
139.7515  
139.8751

166.8289  
163.4688



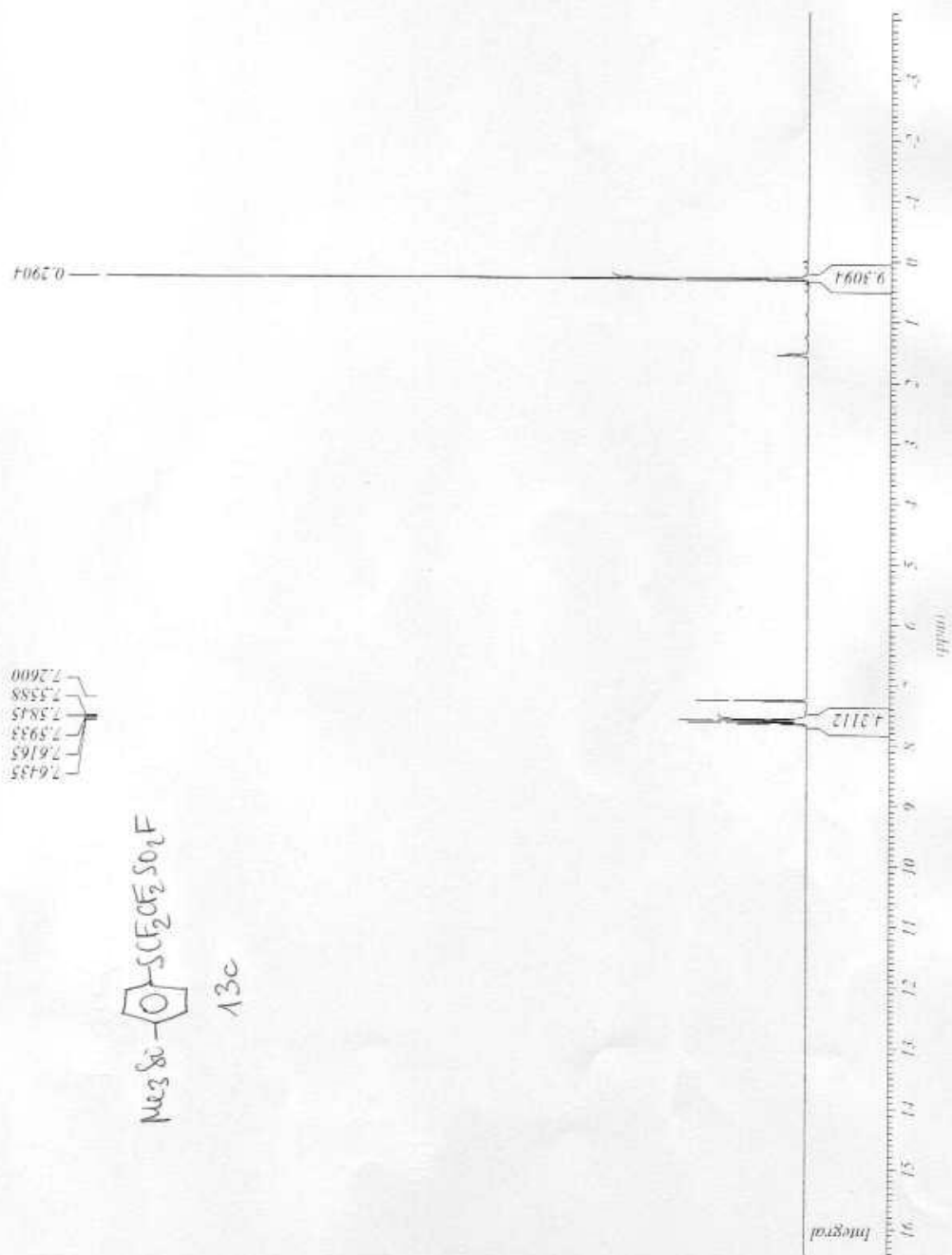
136



C13CPD/CDC13, w. solvent 1

PROTON

7.6435  
7.6165  
7.5933  
7.5815  
7.5588  
7.2600



```

***Current Data Parameters***
NAME      :  B440f2
EXPNO     :  2
PROCNO    :  1

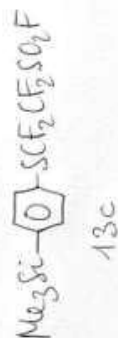
***Acquisition Parameters***
DATE_     :  08-19-11
DATE_     :  Mar 08 2006
DS        :  0
EXP       :  0
AQ        :  8
NUC1      :  13C
P1        :  1853.43 Hz
Q1        :  0.00 Hz
RG        :  512.0000000
RO        :  20 Hz
SFO1      :  300.1318531 MHz
SOLVENT   :  CDCl3
SI        :  20.5671 ppm
SU_h      :  6172.840 Hz
TD        :  32768
TE        :  300.0 K

***Processing Parameters***
GB        :  0.0000000
LB        :  0.30 Hz
SF        :  300.1300060 MHz

***1D NMR Plot Parameters***
SR        :  6.22 Hz
ppm_cm    :  0.92
Hz_cm     :  275.08
YVal_cm   :  41285720.00
NUC1      :  13C
SOLVENT   :
  
```

F19\_30

45.9916  
45.9835  
45.9672



86.3698  
86.3860  
86.3942  
86.4064  
86.4145  
86.4307  
105.5165  
105.5368  
105.5531  
105.5734

CF<sub>2</sub>

CF<sub>2</sub>

SO<sub>2</sub>F

Integral

0.9901

1.8348

1.7439

(ppm)

\*\*\* Current Data Parameters \*\*\*

NAME :  $\beta$ 4402  
 EXPNO : 1  
 PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE : 08-27-52  
 DATE\_d : Mar 08 2006  
 DS : 2  
 EXP : PS done  
 NS : 8  
 NUCLEUS : off  
 O1 : -20615.53 Hz  
 O2 : 0.00 Hz  
 RG : 362.0000000  
 RO : 20 Hz  
 SFO1 : 282.3838635 MHz  
 SOLVENT : CDCl<sub>3</sub>  
 SW : 266.2616 ppm  
 SW\_h : 75187.970 Hz  
 TD : 131072  
 TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.000000  
 LB : 0.30 Hz  
 SF : 282.4044840 MHz

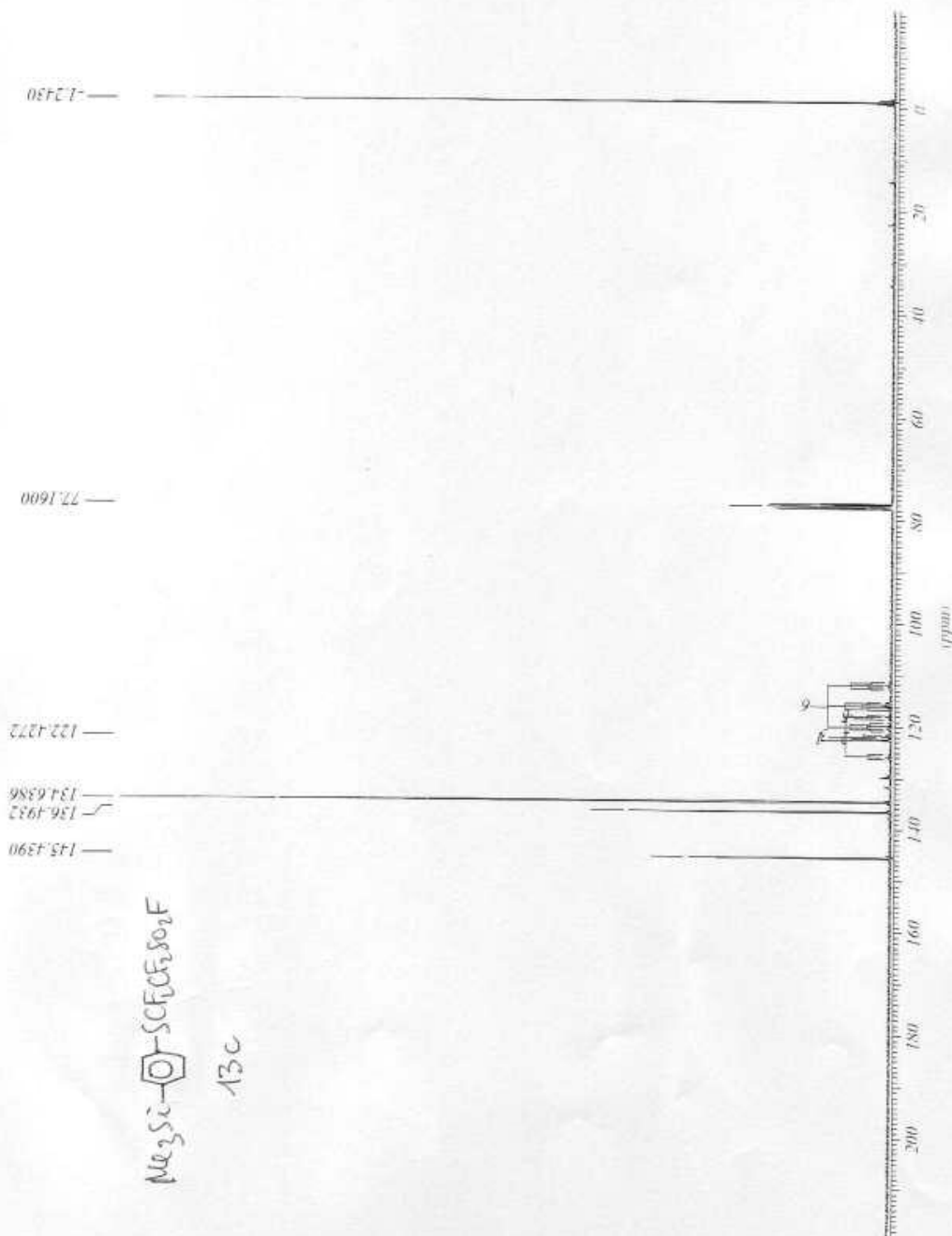
\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
 ppm\_cm : 11.86  
 Hz\_cm : 3350.62  
 YVal\_cm : 45382756.00  
 NUCLEUS : off  
 SOLVENT : ?

C136 JDC1013 a sercof 3



13C



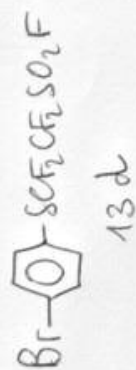
\*\*\*Current Data Parameters\*\*\*  
 NAME : f4402  
 EXPNO : 101  
 PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*  
 DATE\_1 : 21-4-02  
 DATE\_2 : Mar 13 2006  
 DS : 4  
 EXP : C13C10  
 NS : 3000  
 NTCLIN : off  
 O1 : 7576.30 Hz  
 O2 : 1200.52 Hz  
 RG : 1824.5999756  
 RO : 20 Hz  
 SPOL : 75.4752953 MHz  
 SOLVENT : C13C13  
 SW : 238.2980 ppm  
 SW\_H : 17985.612 Hz  
 TD : 65536  
 TE : 300.0 K

\*\*\*Processing Parameters\*\*\*  
 GB : 0.0000000  
 LB : 1.00 Hz  
 SF : 75.4677360 MHz

\*\*\*IDNMR Plot Parameters\*\*\*  
 SR : 17.11 Hz  
 ppm\_cm : 10.62  
 Hz\_cm : 801.50  
 Yref\_cm : 209142.14  
 NUCLES : off  
 SOLVENT :





PROTON C13 NMR of 3

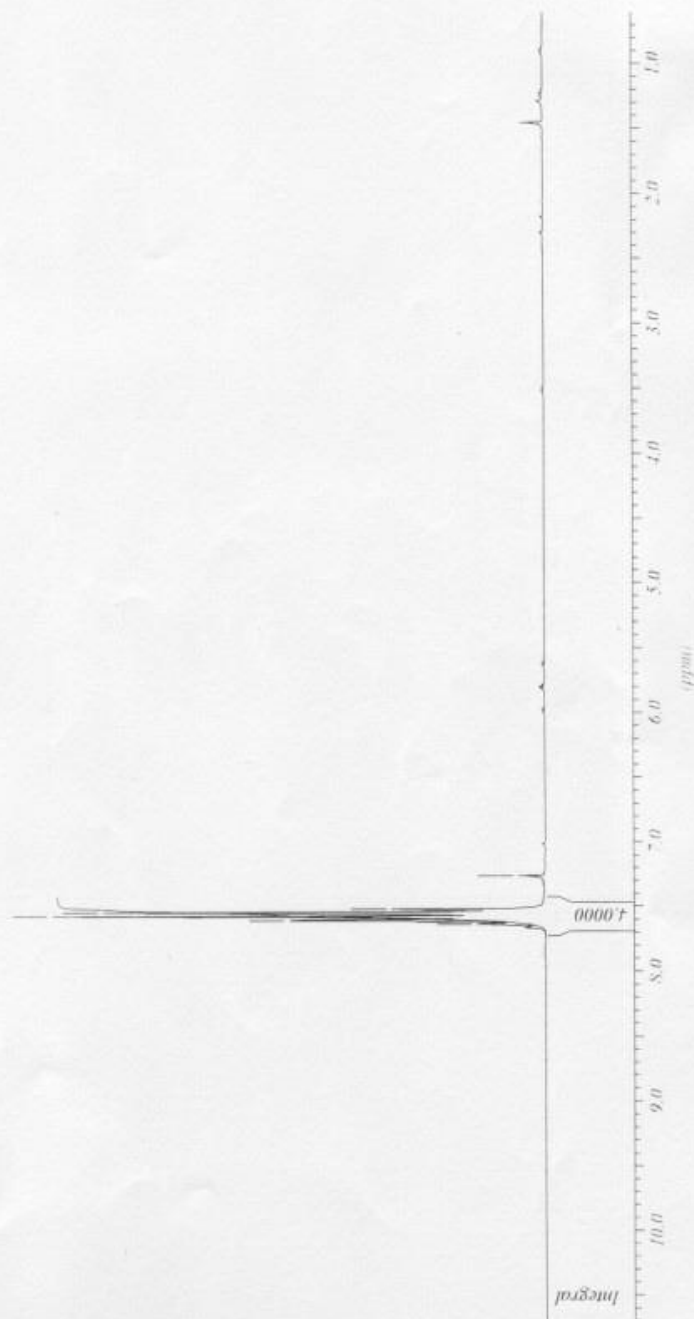
7.6335  
7.6165  
7.6065  
7.5989  
7.5814  
7.5770  
7.5701  
7.5456  
7.5173  
7.2600

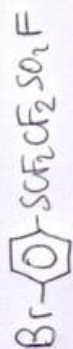
\*\*\*Current Data Parameters\*\*\*  
 NAME : f1436d2  
 EXPNO : 100  
 PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*  
 DATE\_1 : 17:36:07  
 DATE\_2 : Feb 23 2006  
 IN : 0  
 EXP : PROTON  
 AS : 8  
 ATCLETS : off  
 O1 : 1853.43 Hz  
 O2 : 0.00 Hz  
 RG : 128.000000  
 RO : 20 Hz  
 SFO1 : 300.1318534 MHz  
 SOLVENT : CDCl3  
 SU : 20.5671 ppm  
 SU\_h : 6172.840 Hz  
 TD : 32768  
 TE : 300.0 K

\*\*\*Processing Parameters\*\*\*  
 GB : 0.0000000  
 LB : 0.30 Hz  
 SF : 300.1300060 MHz

\*\*\*1D NMR Plot Parameters\*\*\*  
 SR : 5.84 Hz  
 ppm\_cm : 0.45  
 Hz\_cm : 135.09  
 F1d\_cm : 11875.35  
 ATCLETS : off  
 SOLVENT :





13d

F19\_30

46.0322  
46.0119  
45.9713

-86.5648  
-86.5810  
-86.5892  
-86.6014  
-86.6095  
-86.6257  
-105.6912  
-105.7074  
-105.7237  
-105.7440

\*\*\* Current Data Parameters \*\*\*  
NAME : f1436d2  
EXPNO : 1  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

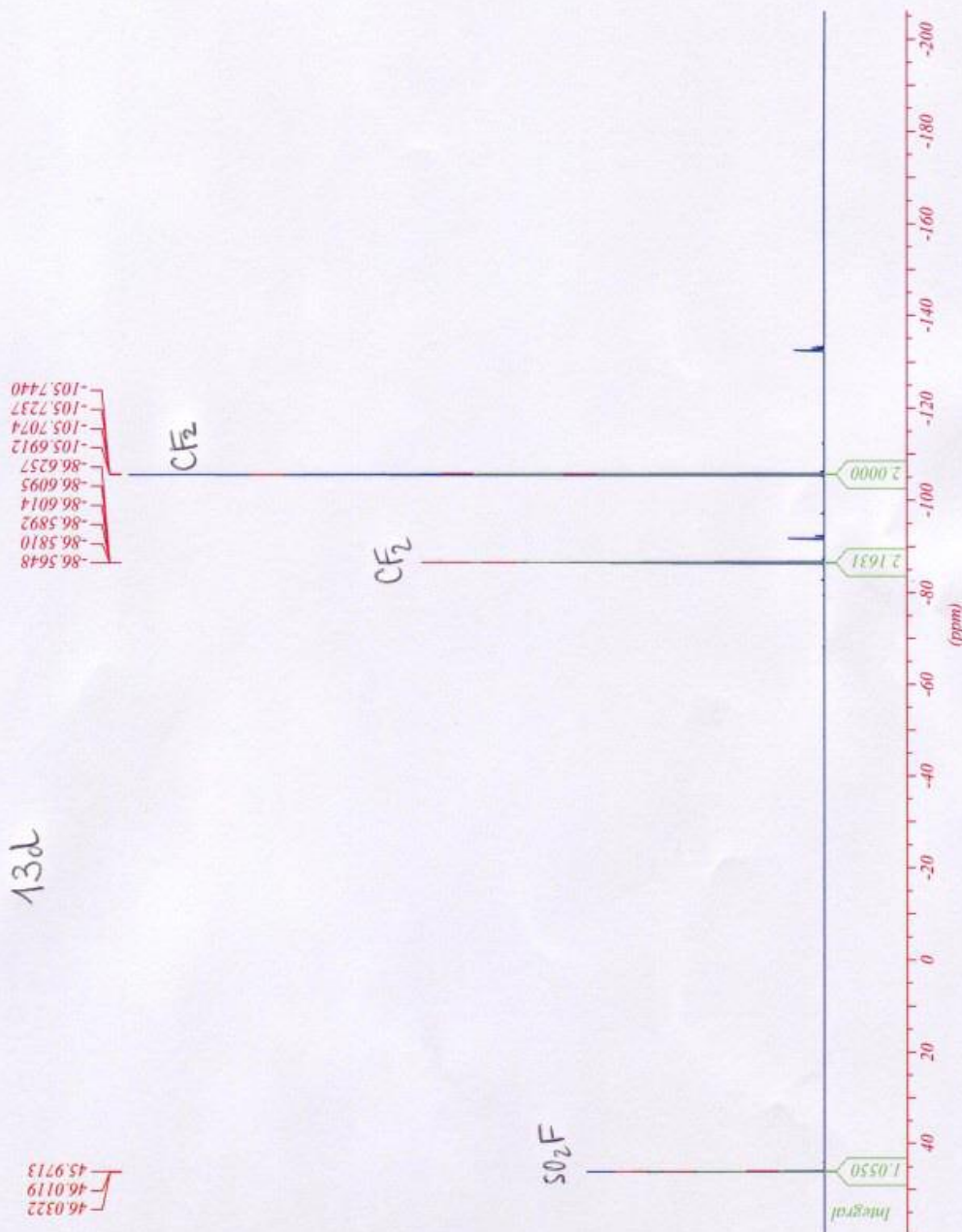
DATE\_t : 06-11-21  
DATE\_d : Feb 23 2006  
DS : 2  
EXP : PS done  
NS : 8  
NUCLEUS : off  
O1 : -20615.53 Hz  
O2 : 0.00 Hz  
RG : 362.0000000  
RO : 20 Hz  
SFO1 : 282.3838635 MHz  
SOLVENT : CDCl3  
SW : 266.2616 ppm  
SW\_h : 75187.970 Hz  
TD : 131072  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

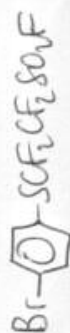
GB : 0.0000000  
LB : 0.30 Hz  
SF : 282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
ppm\_cm : 11.86  
Hz\_cm : 3350.62  
YVal\_cm : 25396936.00  
NUCLEUS : off  
SOLVENT : ?



C13C PD C13X13 u ser of 3



138.8133  
133.1549  
127.0747  
125.3073  
121.1472  
121.1253  
121.0962  
121.0817  
121.0526  
121.0381

77.5891  
77.1600  
76.7382

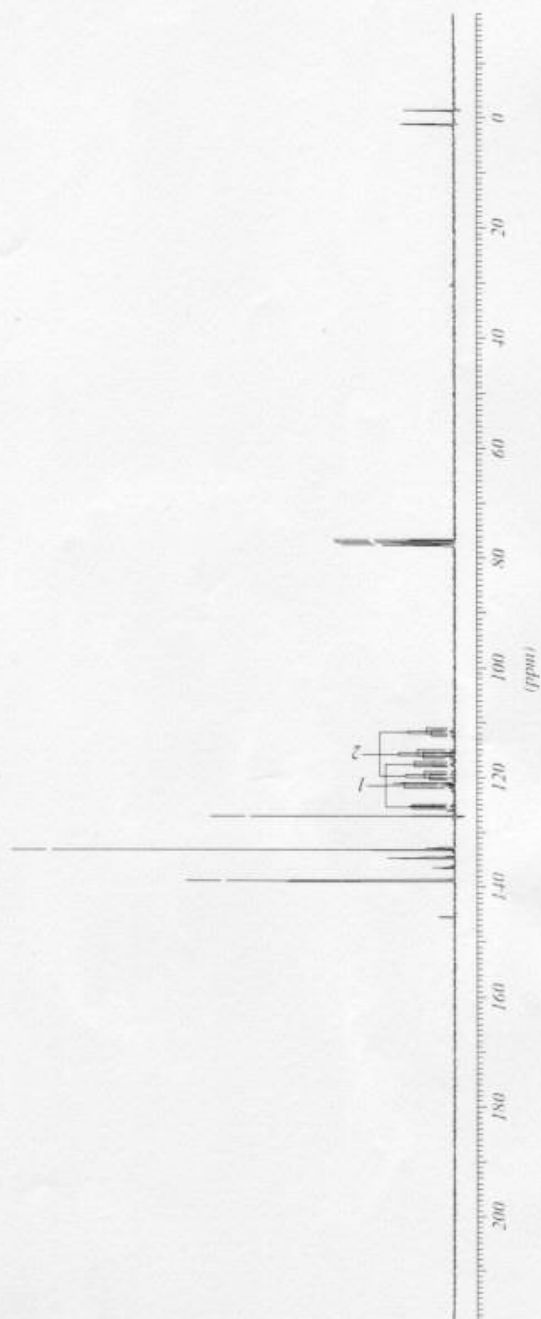
13d

\*\*\*Current Data Parameters\*\*\*  
NAME : j436d2  
EXPNO : 101  
PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*  
DATE\_1 : 2016-55  
DATE\_2 : Feb 23 2006  
DS : 4  
EXP : C13C PD  
AS : 2500  
NUCLEUS : off  
P1 : 7576.30 Hz  
P2 : 1200.52 Hz  
RG : 2048.000000  
RO : 20 Hz  
SFO1 : 75.4752953 MHz  
SOLVENT : C13D13  
SW : 238.2980 ppm  
SW\_h : 17985.612 Hz  
TD : 65536  
TE : 300.0 K

\*\*\*Processing Parameters\*\*\*  
GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4677370 MHz

\*\*\*1D NMR Plot Parameters\*\*\*  
SR : 18.21 Hz  
ppm\_cm : 10.62  
Hz\_cm : 801.50  
Y1ad\_cm : 327638.97  
NUCLEUS : off  
SOLVENT :





PROTON

8.7130  
 8.7105  
 8.7068  
 8.7043  
 8.6967  
 8.6942  
 8.6911  
 8.8274  
 7.8211  
 7.8017  
 7.7954  
 7.7766  
 7.7703  
 7.7333  
 7.7075  
 7.4527  
 7.4483  
 7.4364  
 7.4320  
 7.4276  
 7.4238  
 7.4119  
 7.4075

\*\*\* Current Data Parameters \*\*\*  
 NAME : f388  
 EXPNO : 2  
 PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE : 00:14:44  
 DATE\_d : Dec 16 2005  
 DS : 0  
 EXP : 8  
 NS : off  
 NUCLEUS :  $^{13}\text{C}$   
 O1 : 1853.43 Hz  
 O2 : 0.00 Hz  
 RG : 456.1000061  
 RO : 20 Hz  
 SFO1 : 300.1318534 MHz  
 SOLVENT : CDCl<sub>3</sub>  
 SW : 20.5671 ppm  
 SW\_h : 6172.840 Hz  
 TD : 32768  
 TE : 300.0 K

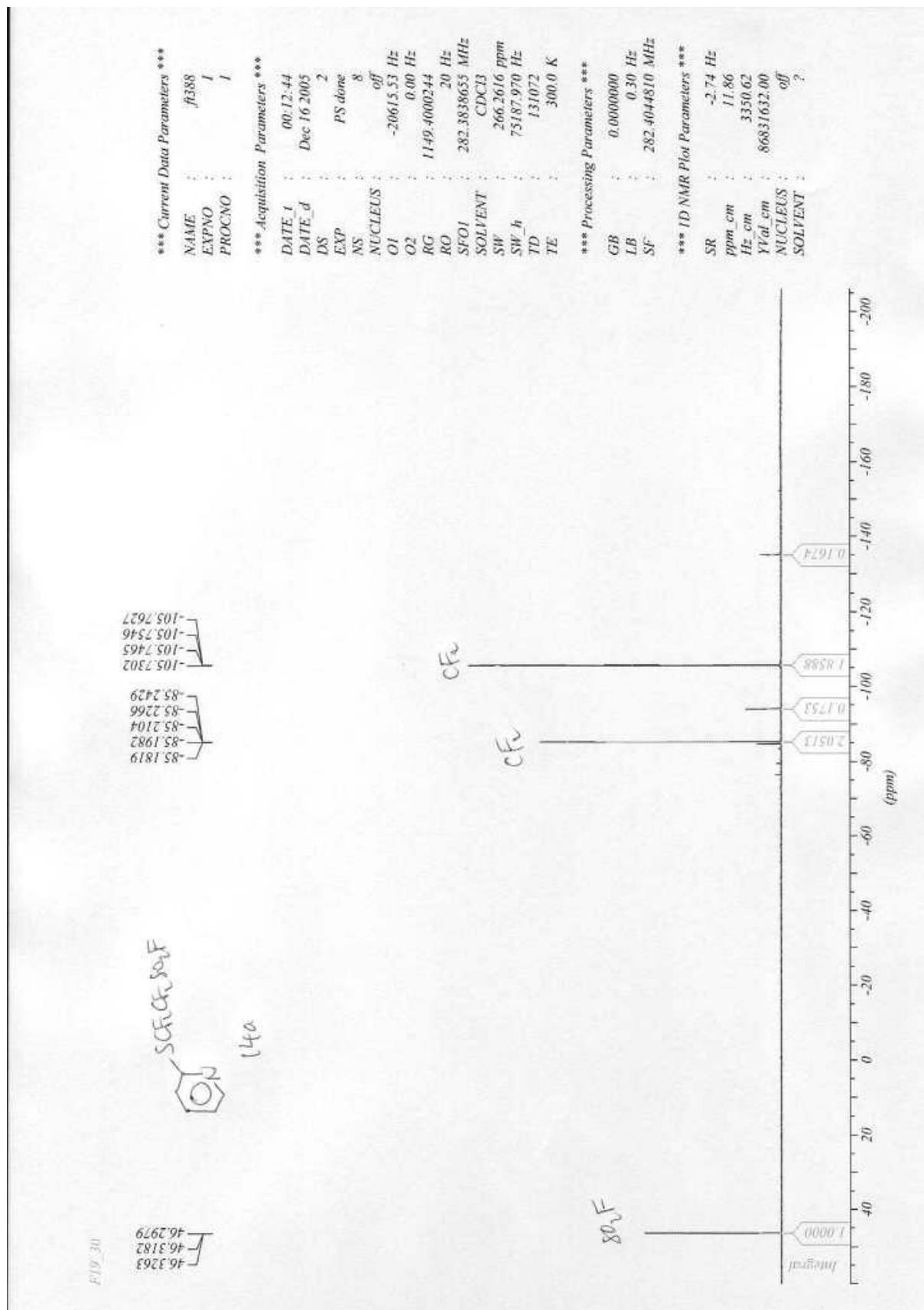
\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
 LB : 0.30 Hz  
 SF : 300.1300000 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : -0.00 Hz  
 ppm\_cm : 0.92  
 Hz\_cm : 275.08  
 YVd\_cm : 35234788.00  
 NUCLEUS : off  
 SOLVENT : ?





C13CPD.CDC/13 u.serveof 2



151.1628  
 150.4719  
 146.5663  
 146.5517  
 146.5227  
 146.5081  
 146.4790  
 146.4645  
 137.9623  
 137.5841  
 131.4675  
 131.4457  
 129.2638  
 128.0929  
 128.0492  
 126.7183  
 126.5219  
 125.1037  
 123.4745  
 122.2235  
 114.7614  
 106.6884  
 106.2302  
 105.7720

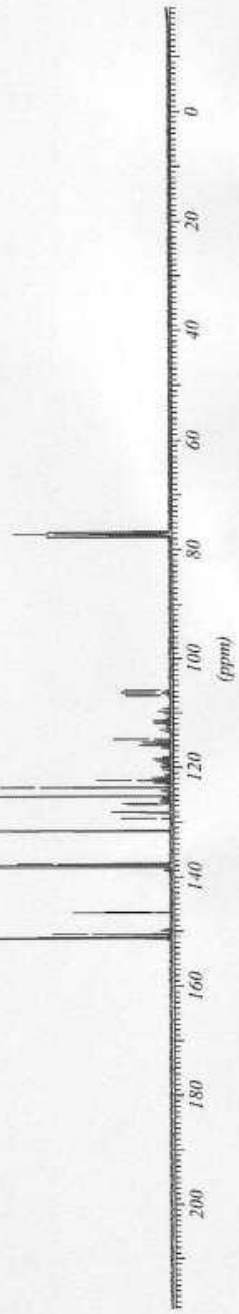
77.1600

\*\*\* Current Data Parameters \*\*\*  
 NAME : j420d  
 EXPNO : 101  
 PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*  
 DATE\_1 : 18-58-32  
 DATE\_d : Feb 09 2006  
 DS : 4  
 EXP : C13CPD  
 NS : 2500  
 NUCLEUS : off  
 O1 : 7576.30 Hz  
 O2 : 1200.52 Hz  
 RG : 1824.5999756  
 RO : 20 Hz  
 SFO1 : 75.4752953 MHz  
 SOLVENT : CDCl3  
 SW : 238.2980 ppm  
 SW\_h : 17985.612 Hz  
 TD : 65536  
 TE : 300.0 K

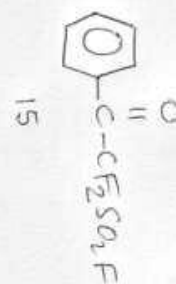
\*\*\* Processing Parameters \*\*\*  
 GB : 0.0000000  
 LB : 1.00 Hz  
 SF : 75.4677420 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*  
 SR : 23.15 Hz  
 ppm\_cm : 10.62  
 Hz\_cm : 801.50  
 YVal\_cm : 177614.80  
 NUCLEUS : off  
 SOLVENT : ?



PROTON CDCl3 400MHz

8.1130  
8.1086  
8.1055  
8.0841  
8.0810  
7.8192  
7.8149  
7.8117  
7.7897  
7.7872  
7.7816  
7.7690  
7.7653  
7.7621  
7.7577  
7.6278  
7.6266  
7.6228  
7.6197  
7.6027  
7.6002  
7.5814  
7.5782  
7.5757  
7.5745  
7.2600



\*\*\* Current Data Parameters \*\*\*  
NAME : g151  
EXPNO : 100  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*  
DATE\_1 : 18.19.25  
DATE\_2 : Nov 24 2004  
DS : 0  
EXP : PROTON  
NS : 8  
NUCLEUS : off  
O1 : 1853.43 Hz  
O2 : 0.00 Hz  
RG : 203.1999969  
RO : 20 Hz  
SF01 : 300.1318534 MHz  
SOLVENT : CDCl3  
SW : 20.5671 ppm  
SW\_h : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

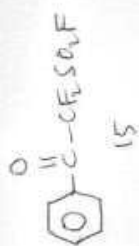
\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300070 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 6.60 Hz  
ppm\_cm : 0.92  
Hz\_cm : 275.08  
Yval\_cm : 5940.69  
NUCLEUS : off  
SOLVENT : ?

F19\_30 CDCl3 isorevof 3



41.4700  
41.4619  
41.4537

96.0264  
96.0346

CF<sub>3</sub>

SO<sub>2</sub>F

\*\*\* Current Data Parameters \*\*\*

NAME : fl51  
EXPNO : 106  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

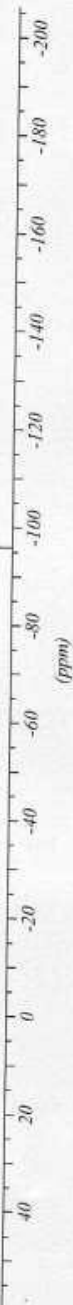
DATE\_1 : 22-36-28  
DATE\_d : Nov 24 2004  
DS : 2  
EXP : F19\_30  
AS : 8  
NUCLEUS : off  
O1 : -20615.53 Hz  
O2 : 0.00 Hz  
RG : 362.0000000  
RO : 20 Hz  
SFO1 : 282.3838655 MHz  
SOLVENT : CDCl3  
SW : 266.2616 ppm  
SW\_h : 75187.970 Hz  
TD : 131072  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0500000  
LB : 0.30 Hz  
SF : 282.4044810 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
ppm\_cm : 11.86  
Hz\_cm : 3350.62  
YVal\_cm : 13102.43  
NUCLEUS : off  
SOLVENT : ?







\*\*\* Acquisition Parameters \*\*\*

NAME : H131  
EXPNO : 101  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 21.12.27  
DATE\_2 : Nov 24 2004  
INSTR : 4  
NS : 2  
DS : 4  
SWH : 3000  
NUCLEUS : off  
Q1 : 7576.30 Hz  
Q2 : 1200.52 Hz  
RG : 1448.1999312  
RO : 20 Hz  
SFO1 : 75.4752953 MHz  
SOLVENT : CDCl3  
SH : 258.2980 ppm  
SW\_H : 17083.612 Hz  
TD : 65536  
TE : 300.0 K

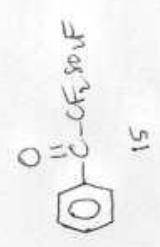
\*\*\* Processing Parameters \*\*\*

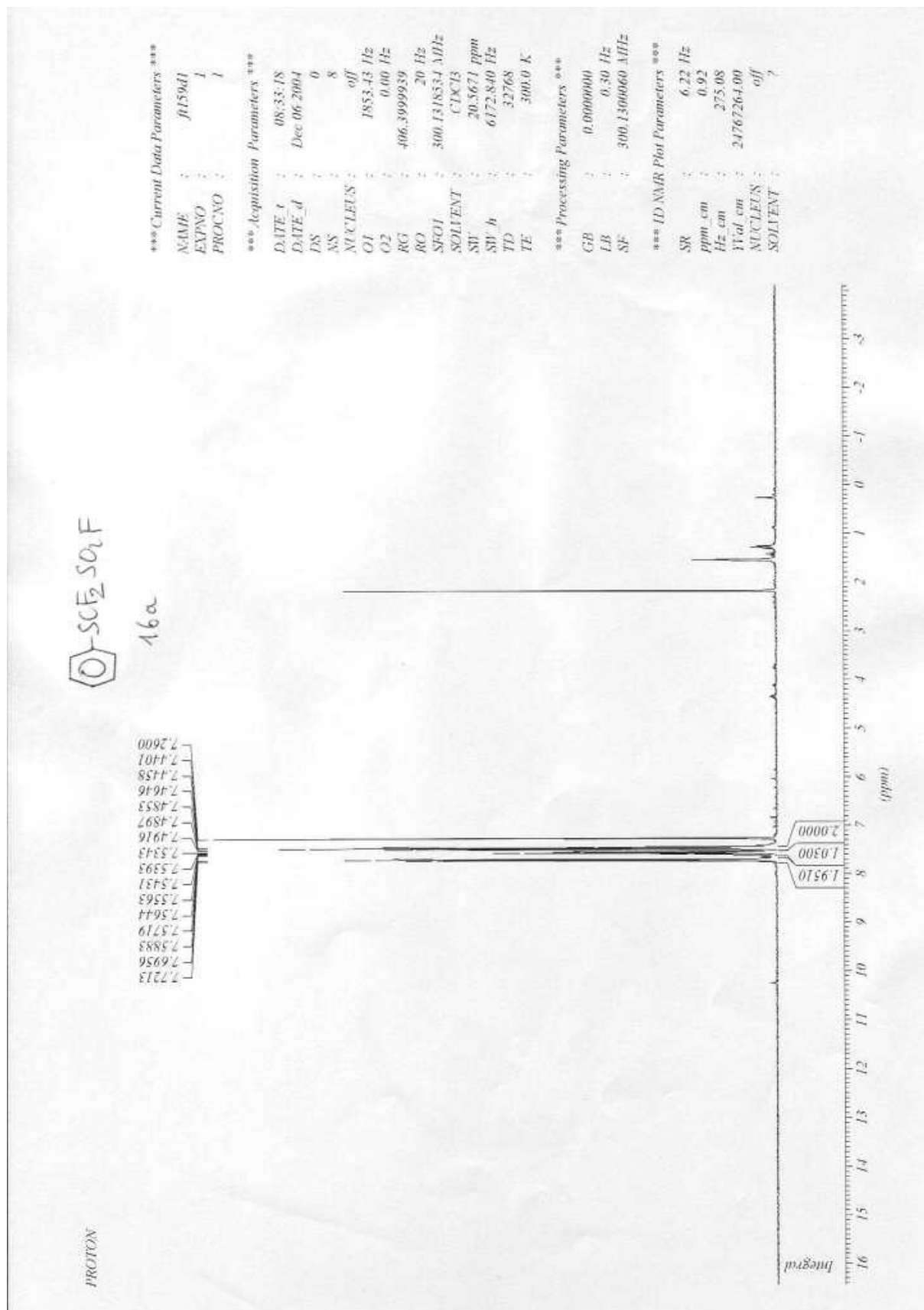
GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4677590 MHz  
\*\*\* ID NMR Plot Parameters \*\*\*  
SR : 19.86 Hz  
ppm cm : 10.62  
Hz cm : 801.50  
Y1 cm : 65920.58  
NUCLEUS : off  
SOLVENT : ?

136.7696  
130.4566  
130.4202  
130.3839  
129.8602  
129.8338  
129.7947  
129.7584  
129.5838  
120.8635  
120.853  
116.7613  
116.5906  
112.6668  
112.2959

181.4622  
181.4104  
181.1914  
181.1276  
180.8294  
180.8076

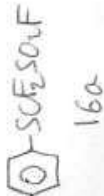
	1	2	3	4	5	6
Chemical Shift (ppm)	136.7696	130.4566	130.4202	130.3839	129.8602	129.8338
Integration	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Area	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Height	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Width	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Volume	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000





F19\_3013

195CF<sub>3</sub>SO<sub>2</sub>F



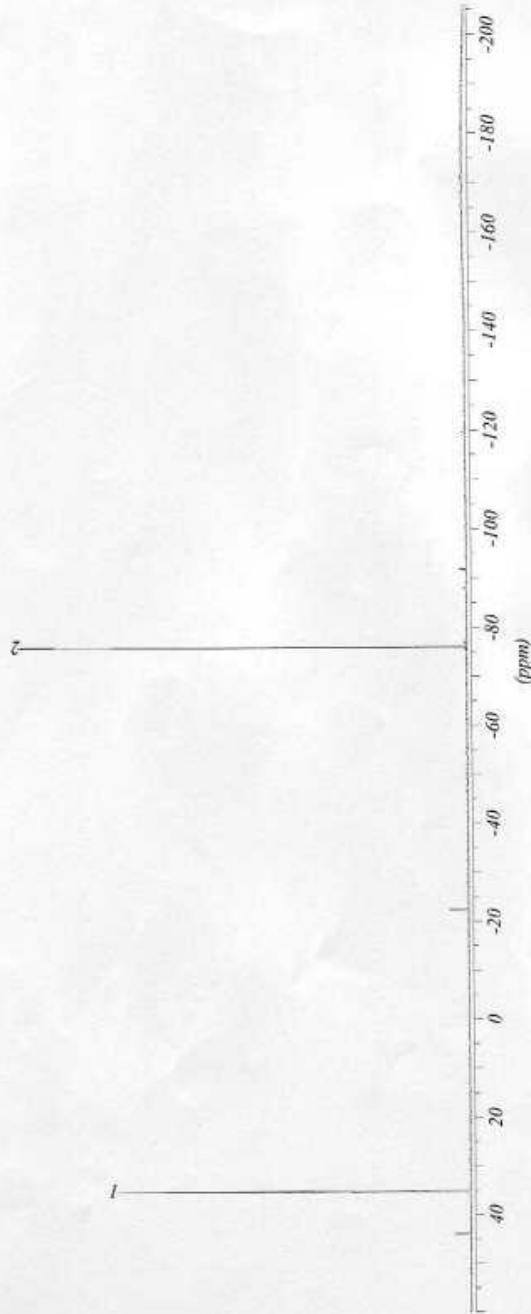
35.0756  
35.0593  
35.0431

76.0794  
76.0956

Identifier	Chem. Shift [ppm]	J [Hz]	Multiplicity	Connections
1	35.0593	4.5891	3	J(1,0)
2	-76.0875	4.5891	2	J(2,0)



\*\*\* Current Data Parameters \*\*\*  
 NAME : f159d2  
 EXPNO : 1  
 PROCNO : 1  
 \*\*\* Acquisition Parameters \*\*\*  
 DATE\_1 : 08-41-50  
 DATE\_2 : Dec 06 2004  
 DS : 2  
 NS : 8  
 NUCLEUS : off  
 O1 : -20615.53 Hz  
 O2 : 0.00 Hz  
 RG : 512.000000  
 RO : 20 Hz  
 SFO1 : 282.3838655 MHz  
 SOLVENT : CDCl<sub>3</sub>  
 SW : 266.2616 ppm  
 SW\_H : 75187.970 Hz  
 TD : 131072  
 TE : 300.0 K  
 \*\*\* Processing Parameters \*\*\*  
 GB : 0.000000  
 LB : 0.30 Hz  
 SF : 282.4044840 MHz  
 \*\*\* 1D NMR Plot Parameters \*\*\*  
 SR : 0.60 Hz  
 ppm\_cm : 11.86  
 Hz\_cm : 3350.62  
 YVal\_cm : 41312472.00  
 NUCLEUS : off  
 SOLVENT : ?





137.5259  
137.5114  
137.1294  
130.8493  
129.9475  
126.5655  
122.2817  
121.8672  
121.8308  
121.7872

Identifier	Chem. Shift [ppm]	J [Hz]	Multiplicity	Connections
1	126.8286	323.2887	3	J(1,0)
2	122.0935	3.0188	3	J(2,0)

## \*\*\* Current Data Parameters \*\*\*

NAME : R159d3

EXPNO : 101

PROCNO : 1

## \*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 22-09-00

DATE\_2 : Dec-09-2004

DS : 4

NS : 1024

NUCLEUS : off

Q1 : 7376.30 Hz

Q2 : 1200.52 Hz

RG : 1448.1990512

RO : 20 Hz

SFO1 : 75.4752953 MHz

SOLVENT : CDCl3

SW : 238.2980 ppm

SW\_H : 17985.612 Hz

TD : 65536

TE : 300.0 K

## \*\*\* Processing Parameters \*\*\*

GB : 0.0000000

LB : 1.00 Hz

SF : 75.4677390 MHz

## \*\*\* ID NMR Plot Parameters \*\*\*

SR : 19.86 Hz

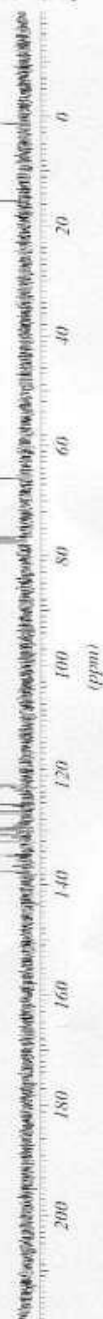
ppm cm : 10.63

Hz cm : 801.86

Y1 of cm : 17631.50

NUCLEUS : off

SOLVENT : ?





166

7.7490  
7.7320  
7.7195  
7.7025  
7.2814  
7.2123  
7.1834  
7.1552

\*\*\* Current Data Parameters \*\*\*

NAME : f453d  
EXPNO : 1  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 05:13:22  
DATE\_d : Mar 13 2006  
DS : 0

EXP : 8

NUCLEUS : <sup>1</sup>H

O1 : 1853.43 Hz

O2 : 0.00 Hz

RG : 456.1000061

RO : 20 Hz

SFO1 : 300.1318334 MHz

SOLVENT : CDCl<sub>3</sub>

SW : 20.5671 ppm

SW\_h : 6172.840 Hz

TD : 32768

TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000

LB : 0.30 Hz

SF : 300.1300000 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : -0.00 Hz

ppm\_cm : 0.62

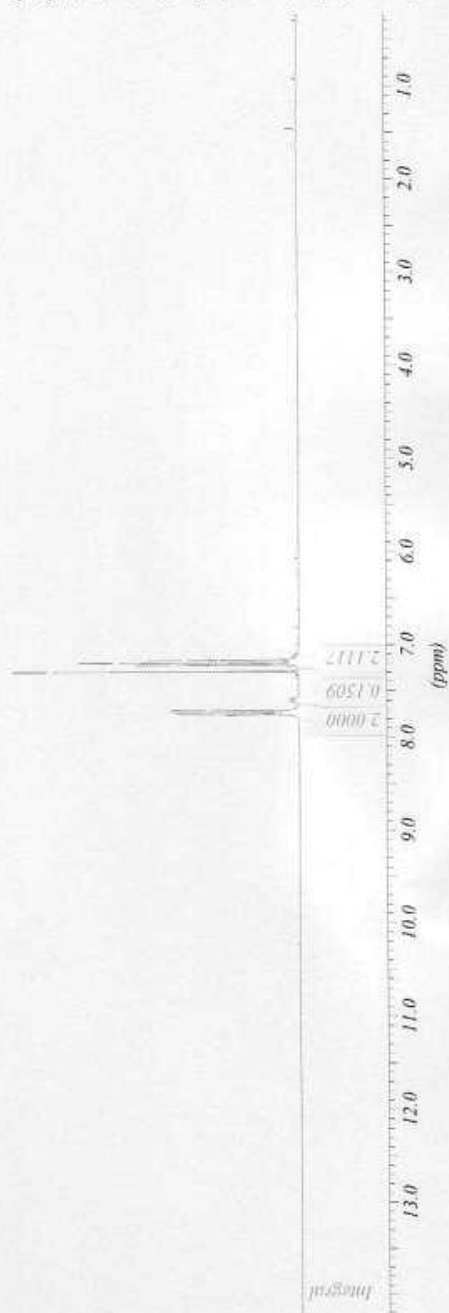
Hz\_cm : 187.33

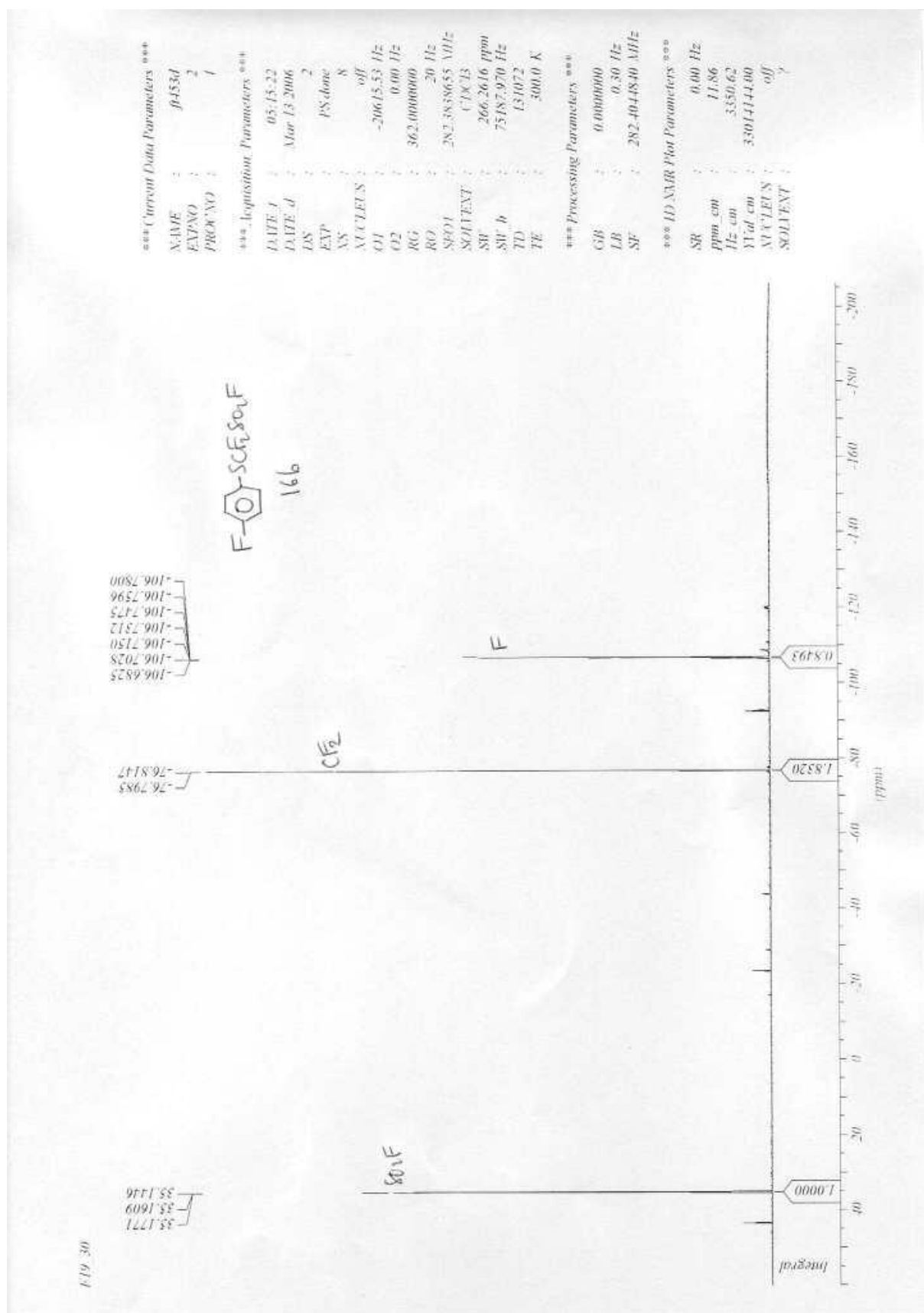
YVol\_cm : 25026782.00

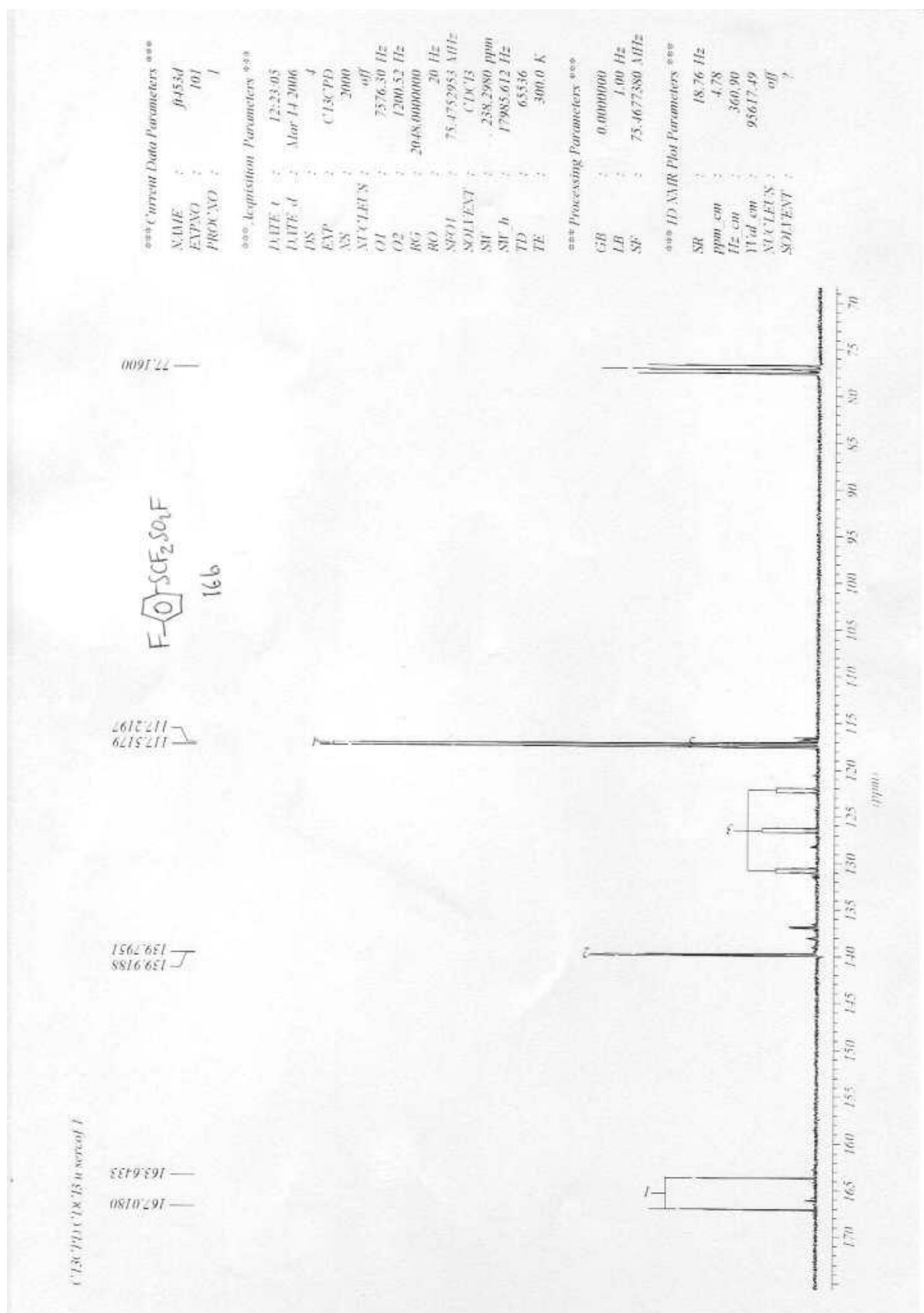
NUCLEUS : <sup>1</sup>H

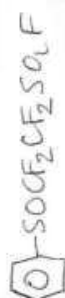
EXPNO : 1

PROTON









17a

PROTON CDCl3 u.sereof 1

7.8343  
7.8098  
7.7282  
7.7207  
7.7125  
7.7100  
7.7019  
7.6969  
7.6705  
7.6504  
7.6460  
7.6441  
7.6278  
7.6228  
7.6178  
7.2600  
7.2575  
5.2929

CH<sub>2</sub>Cl<sub>2</sub>

\*\*\* Current Data Parameters \*\*\*

NAME : jf2673  
EXPNO : 100  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

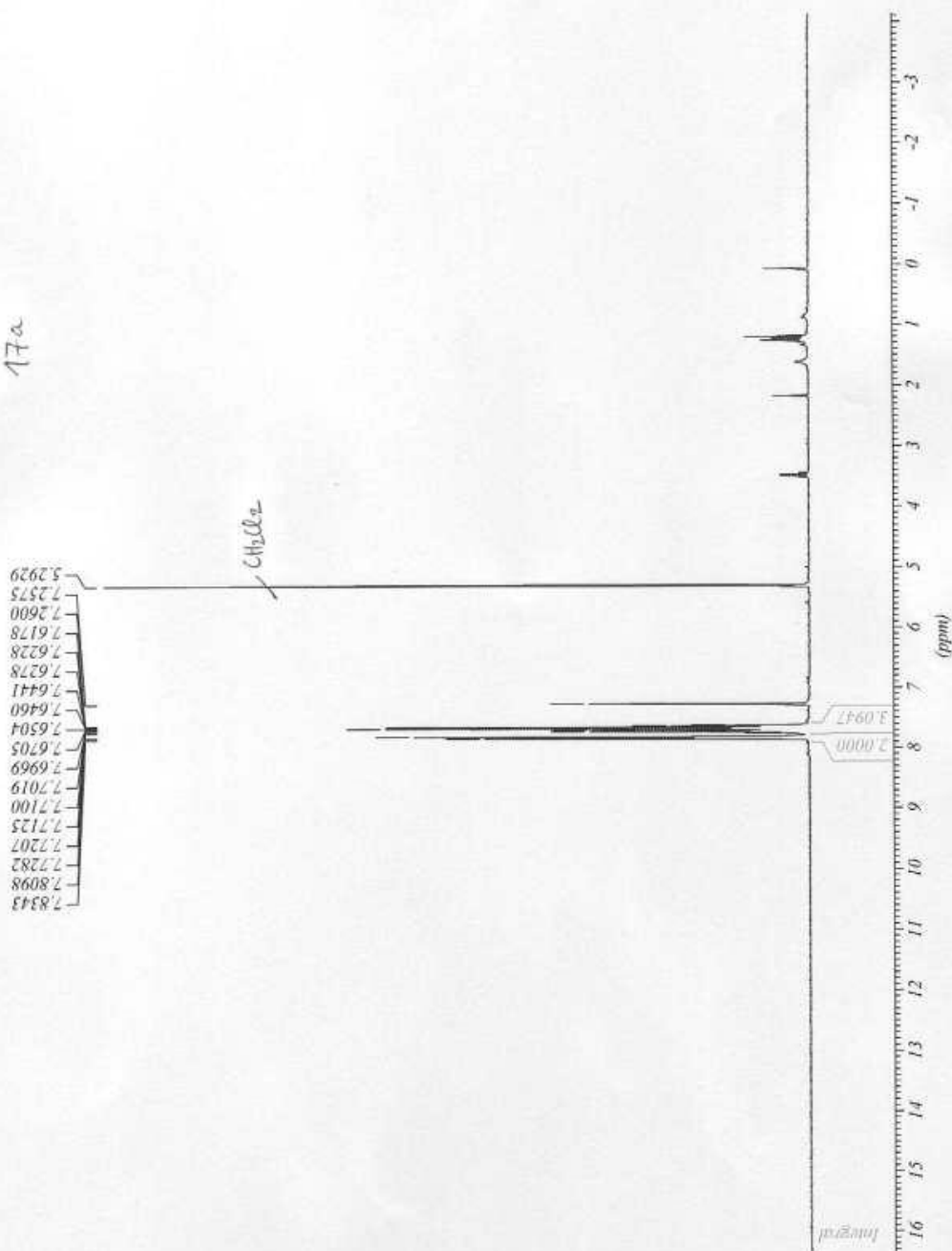
DATE\_1 : 10-23-21  
DATE\_d : Jun 07 2005  
DS : 0  
EXP : PROTON  
NS : 8  
NUCLEUS : off  
O1 : 1853.43 Hz  
O2 : 0.00 Hz  
RG : 256.0000000  
RO : 20 Hz  
SFO1 : 300.1318534 MHz  
SOLVENT : CDCl3  
SW : 20.5671 ppm  
SW\_h : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300060 MHz

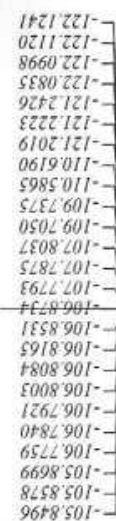
\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 6.41 Hz  
ppm\_cm : 0.92  
Hz\_cm : 275.08  
YVal\_cm : 4957.33  
NUCLEUS : off  
SOLVENT : ?





F19\_30



\*\*\* Current Data Parameters \*\*\*

NAME	β2673
EXPNO	2
PROCNO	1

\*\*\* Acquisition Parameters \*\*\*

DATE_1	08:23:36
DATE_d	May 27 2005
DS	2
NS	8
NUCLEUS	off
O1	-20613.53 Hz
O2	0.00 Hz
RG	574.7000122
RO	20 Hz
SFO1	282.3838655 MHz
SOLVENT	CDCl3
SW	266.2616 ppm
SW_h	75187.970 Hz
TD	131072
TE	300.0 K

\*\*\* Processing Parameters \*\*\*

GB	0.0000000
LB	0.30 Hz
SF	282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR	0.00 Hz
ppm_cm	11.86
Hz_cm	3350.62
YVal_cm	33206902.00
NUCLEUS	off
SOLVENT	?

SO<sub>2</sub>F

CF<sub>3</sub>

CF<sub>2</sub>

Integral

(ppm)

C13CPD(CDCl3) 4 scans of 1



17a

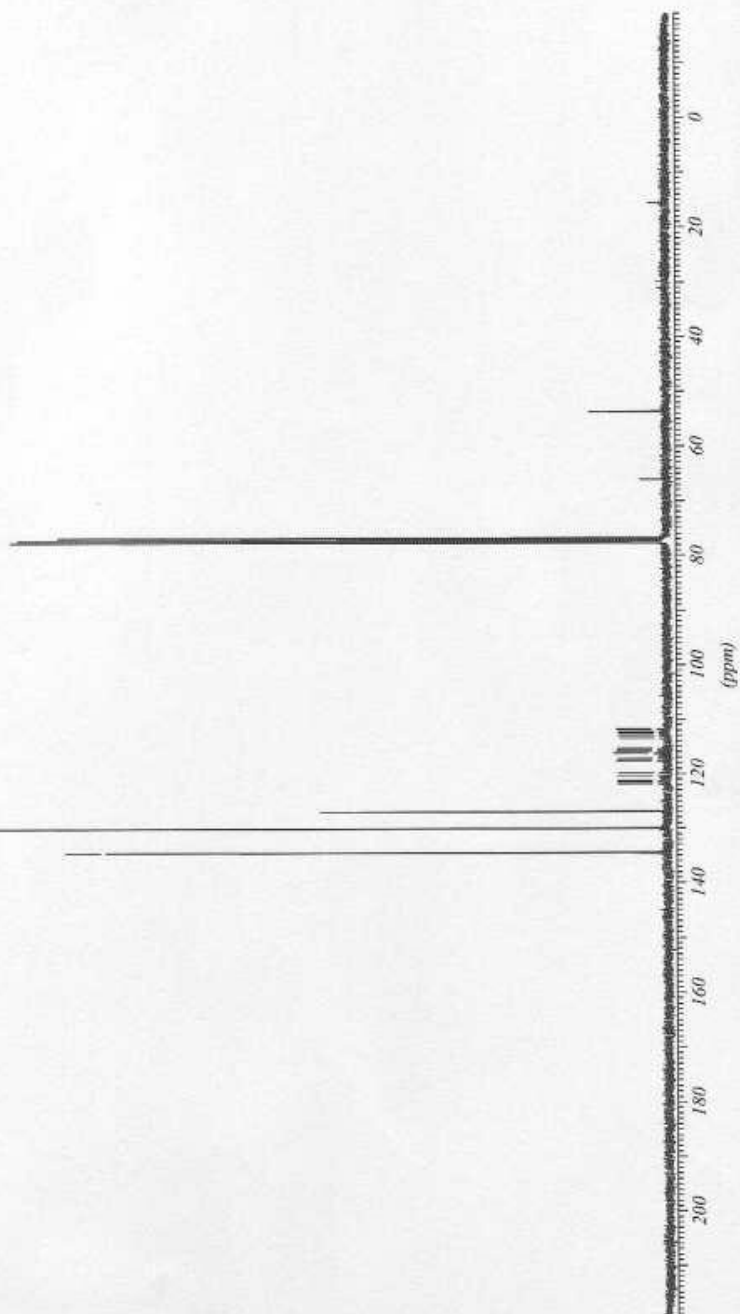
134.4058  
129.8747  
126.8419  
126.8201  
121.6999  
121.2708  
121.2490  
120.2453  
119.7653  
117.6415  
117.2124  
116.2670  
115.8160  
115.4087  
113.4232  
112.9650  
112.5432  
112.2959  
112.2813  
111.8013

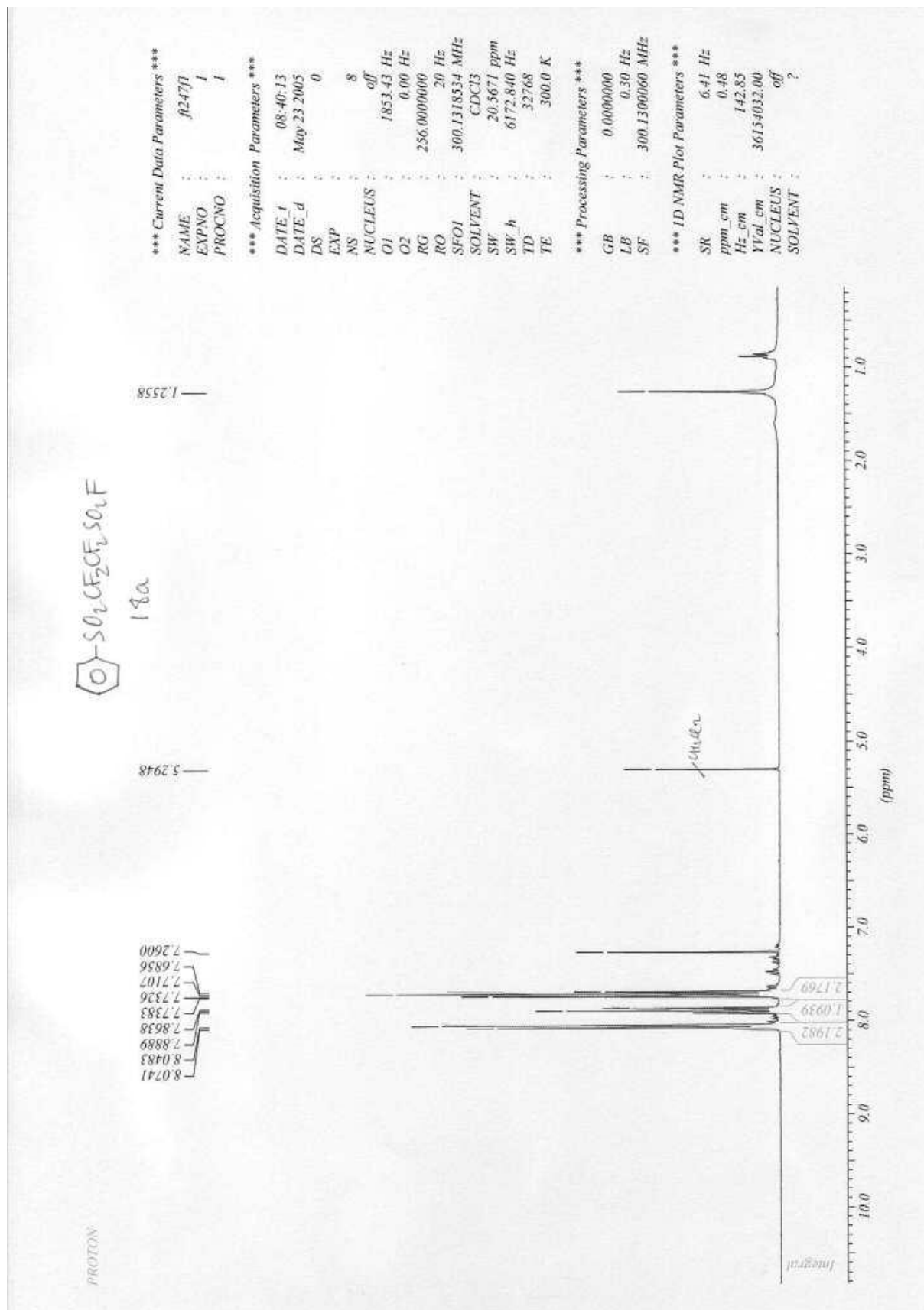
\*\*\* Current Data Parameters \*\*\*  
NAME : f2673  
EXPNO : 101  
PROCNO : 1

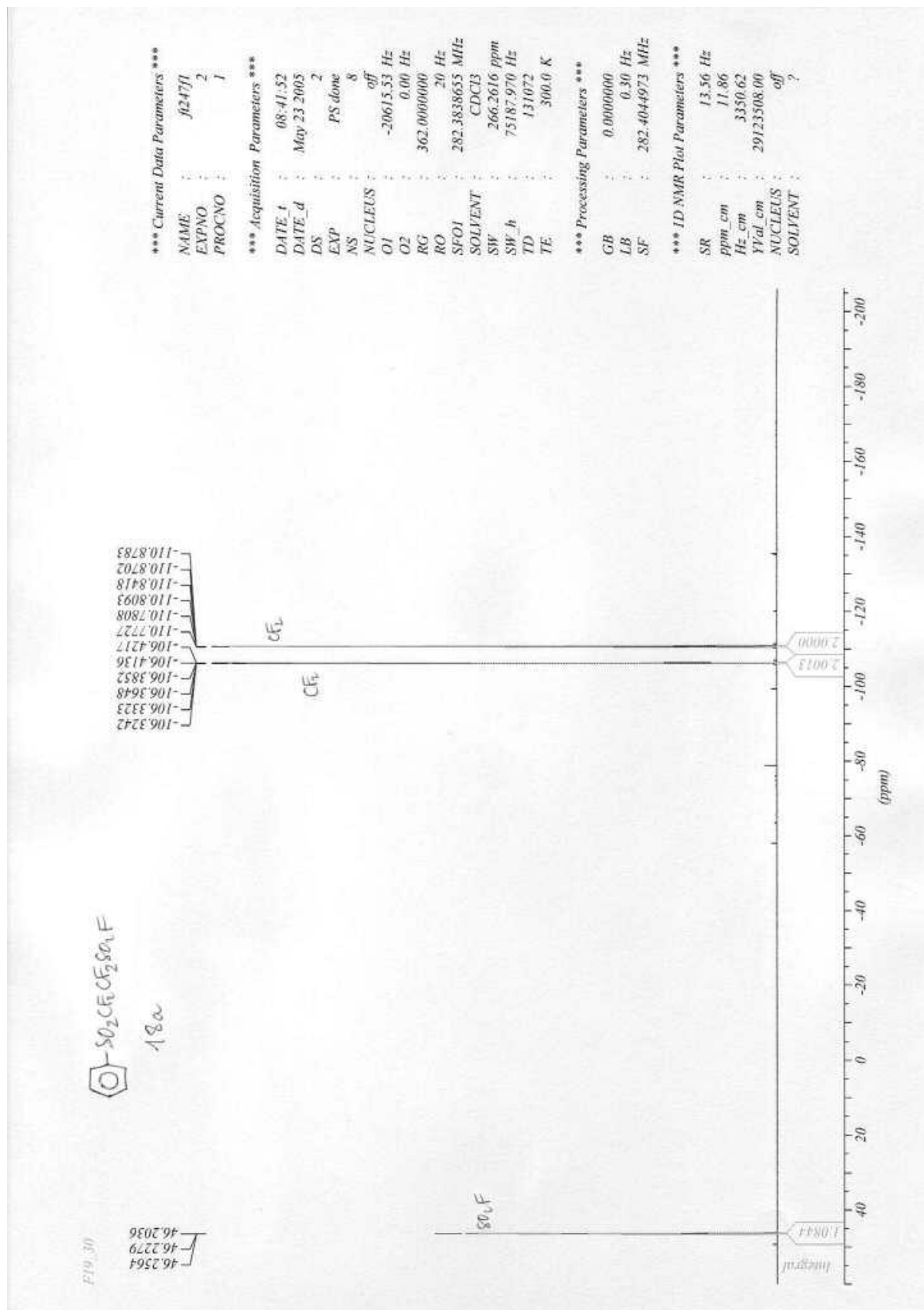
\*\*\* Acquisition Parameters \*\*\*  
DATE\_1 : 15-42:42  
DATE\_2 : Jun 07 2005  
DS : 4  
EXP : C13CPD  
NS : 5000  
NUCLEUS : off  
O1 : 7576.30 Hz  
O2 : 1200.52 Hz  
RG : 4597.6000977  
RO : 20 Hz  
SFO1 : 75.4752953 MHz  
SOLVENT : CDCl3  
SW\_h : 238.2989 ppm  
SW\_w : 17985.612 Hz  
TD : 65536  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*  
GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4677390 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*  
SR : 19.86 Hz  
ppm\_cm : 10.62  
Hz\_cm : 801.50  
Y1\_al\_cm : 194046.06  
NUCLEUS : off  
SOLVENT : ?







C13CPD CDCl3 u servcof/2



18a

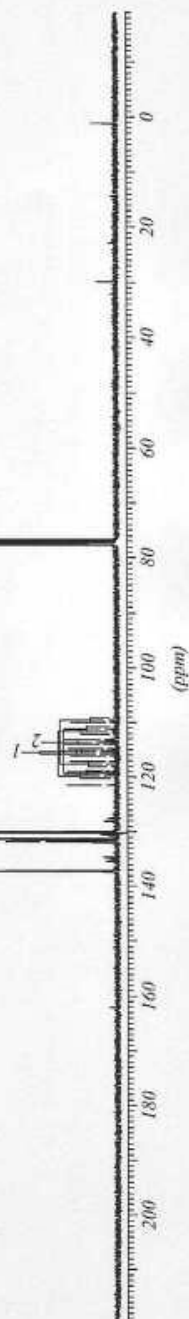


\*\*\* Current Data Parameters \*\*\*  
 NAME : j247j  
 EXPNO : 101  
 PROCNO : 1

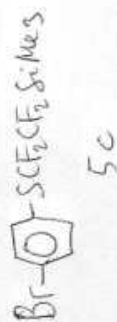
\*\*\* Acquisition Parameters \*\*\*  
 DATE\_1 : 18.36.34  
 DATE\_2 : Jun 06 2005  
 DS : 4  
 NS : 4000  
 NUCLEUS : off  
 O1 : 7576.30 Hz  
 O2 : 1200.52 Hz  
 RG : 9195.2001953  
 RO : 20 Hz  
 SFO1 : 75.4752953 MHz  
 SOLVENT : CDCl3  
 SW : 238.2980 ppm  
 SW\_H : 17985.612 Hz  
 TD : 65536  
 TE : 300.0 K

\*\*\* Processing Parameters \*\*\*  
 GB : 0.0000000  
 LB : 1.00 Hz  
 SF : 75.4677380 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*  
 SR : 19.31 Hz  
 ppm\_cm : 10.62  
 Hz\_cm : 801.50  
 YVal\_cm : 611422.25  
 NUCLEUS : off  
 SOLVENT : ?



PROTON



7.3161  
7.3123  
7.2600

0.2653

\*\*\* Current Data Parameters \*\*\*

NAME : j042611  
EXPNO : 2  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 09.16.10  
DATE\_2 : Feb 15 2006  
IN : 0  
EXP : 8  
NS : 8  
NUCLEUS : off  
O1 : 1853.43 Hz  
O2 : 0.00 Hz  
RG : 456.1000061  
RO : 20 Hz  
SF : 300.1318534 MHz  
SOLVENT : CDCl3  
SH : 20.5671 ppm  
SI : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300070 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 6.60 Hz  
ppm : 0.92  
Hz : 275.08  
Y : 26957906.00  
NUCLEUS : off  
SOLVENT :



F19.40



-82.7948  
 -82.8110  
 -82.8313

-122.3841  
 -122.4004  
 -122.4207

\*\*\* Current Data Parameters \*\*\*

NAME : j426f1  
 EXPNO : 1  
 PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

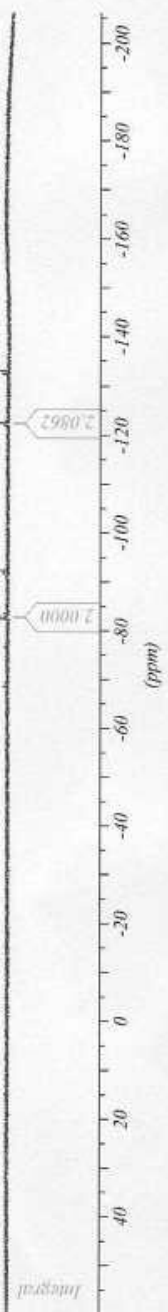
DATE\_1 : 23.49.23  
 DATE\_d : Feb 14 2006  
 DS : 2  
 EXP : PS done  
 NS : 8  
 NUCLEUS : off  
 O1 : -20615.53 Hz  
 O2 : 0.00 Hz  
 RG : 512.000000  
 RO : 20 Hz  
 SFO1 : 282.3838655 MHz  
 SOLVENT : CDCl3  
 SW : 266.2616 ppm  
 SW\_h : 75187.970 Hz  
 TD : 131072  
 TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

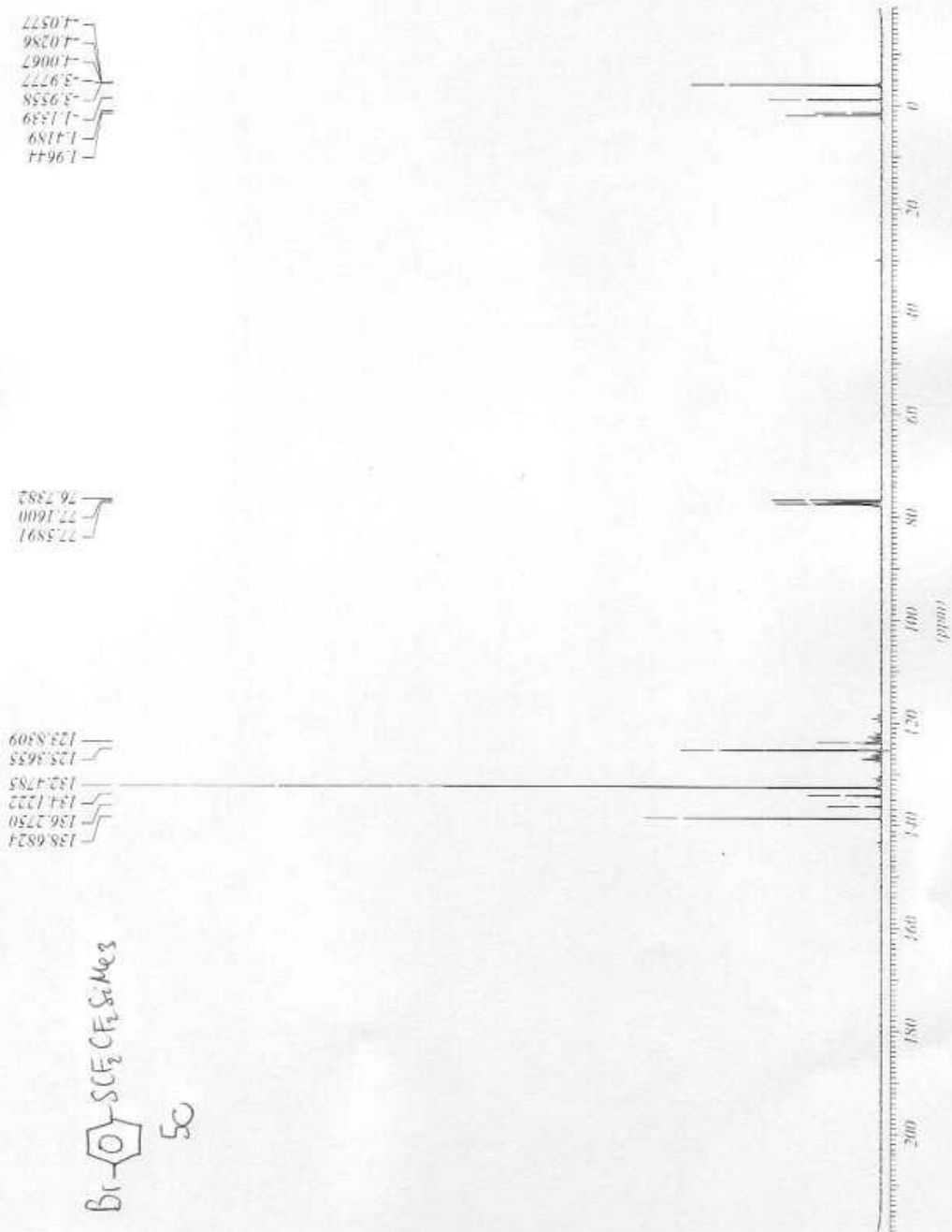
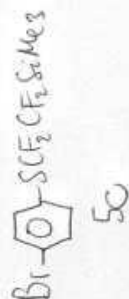
GB : 0.0000000  
 LB : 0.30 Hz  
 SF : 282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
 ppm\_cm : 11.86  
 Hz\_cm : 3350.62  
 YVal\_cm : 38868220.00  
 NUCLEUS : off  
 SOLVENT : ?



<sup>13</sup>C NMR (CDCl<sub>3</sub>) 125 MHz



\*\*\*Current Data Parameters\*\*\*  
NAME : J41261T  
EXPNO : 101  
PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*  
DATE\_1 : 16-10-26  
DATE\_2 : Feb 23 2006  
INSTRUM : spect  
PROBHD : 5mm  
PULPROG : zgpg30  
F2 - 125.7630 MHz  
F1 - 125.7630 MHz  
RG : 645.0999756  
RO : 20 Hz  
SFO : 125.7630311 MHz  
SOLVENT : CDCl<sub>3</sub>  
NUC1 : 13C  
NUC2 : 1H  
TD : 65536  
TE : 300.0 K

\*\*\*Processing Parameters\*\*\*  
GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4677390 MHz

\*\*\*1D NMR Plot Parameters\*\*\*  
SR : 19.86 Hz  
ppm : 10.62  
Hz : 801.50  
Y1 : 100036.82  
X1 : off  
SOLVENT : CDCl<sub>3</sub>





19a

PROTON

7.8400  
7.8161  
7.7345  
7.7301  
7.7201  
7.7100  
7.7019  
7.6906  
7.6862  
7.6812  
7.6554  
7.6422  
7.6353  
7.6297  
7.6121  
7.6065  
7.6014

\*\*\* Current Data Parameters \*\*\*  
NAME f335g3  
EXPNO 1  
PROCNO 1

\*\*\* Acquisition Parameters \*\*\*

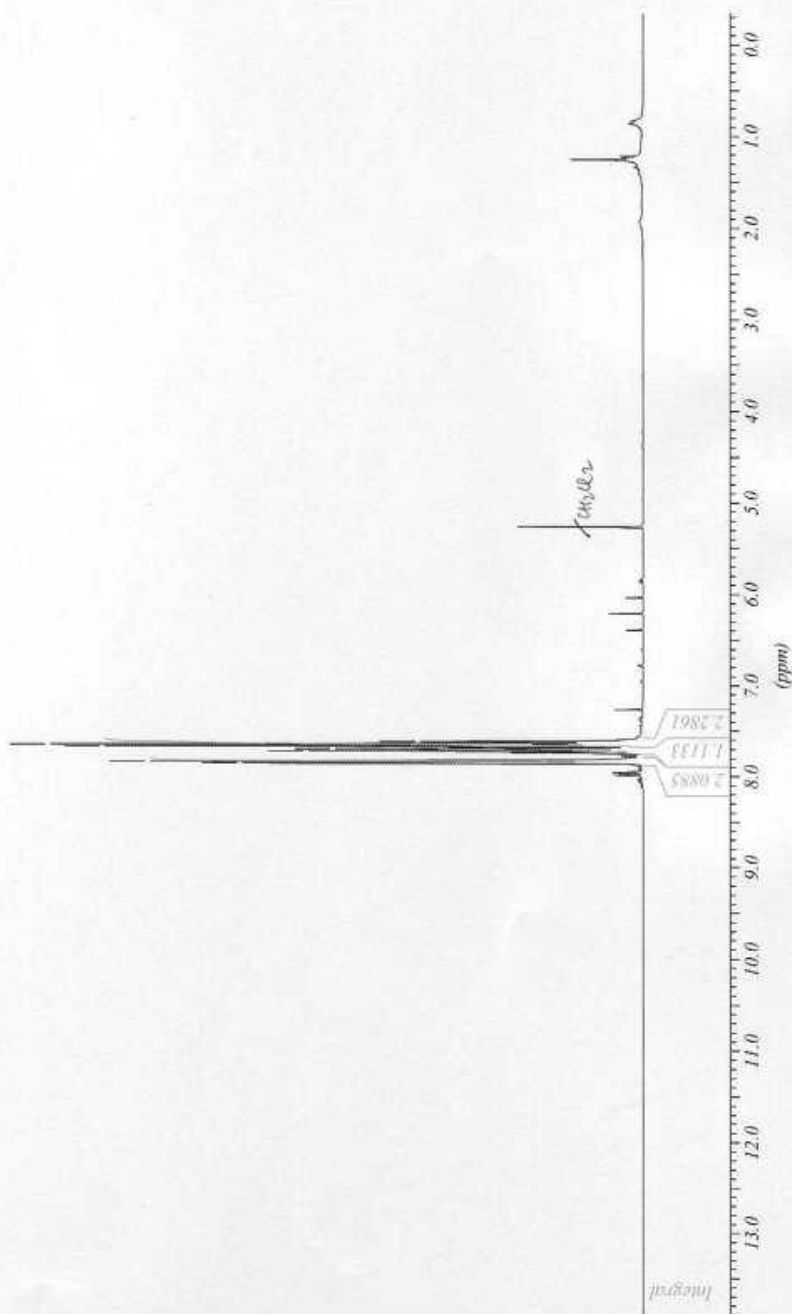
DATE\_1 05-58-04  
DATE\_d Oct 28 2005  
DS 0  
EXP  
NS 8  
NUCLEUS off  
O1 1853.43 Hz  
O2 0.00 Hz  
RG 71.8000031  
RO 20 Hz  
SFO1 300.1318534 MHz  
SOLVENT CDCl3  
SW\_h 20.5671 ppm  
SW\_h 6172.840 Hz  
TD 32768  
TE 300.0 K

\*\*\* Processing Parameters \*\*\*

GB 0.0000000  
LB 0.30 Hz  
SF 300.1300060 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR 6.22 Hz  
ppm\_cm 0.64  
Hz\_cm 190.60  
YVal\_cm 36093196.00  
NUCLEUS off  
SOLVENT 2





\*\*\* Current Data Parameters \*\*\*

NAME : j356j3  
EXPNO : 2  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 06.00.00  
DATE\_2 : Oct 28 2005  
DS : 2  
EXP : PS dome  
NS : 8  
NUCLEUS : off

O1 : -20615.53 Hz  
O2 : 0.00 Hz  
RG : 203.1999969  
RO : 20 Hz  
SFO1 : 282.3838655 MHz

SOLVENT : CDCl3  
SW : 266.2616 ppm  
SW\_h : 75187.970 Hz  
TD : 131072  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 282.4045112 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 27.48 Hz  
ppm\_cm : 11.86  
Hz\_cm : 3350.62  
YVal\_cm : 36561908.00  
NUCLEUS : off

-106.2151  
-106.1988  
-105.4513  
-105.4351  
-99.9628  
-99.9425  
-99.1991  
-99.1788



SO<sub>2</sub>F

CF<sub>2</sub>

F19 30'

49.5790  
49.5587  
49.5424

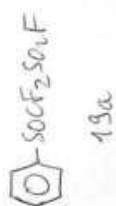
33.453

14.049  
17.399  
0.5259  
17.484  
13.267  
0.5495  
3.2715

(ppm)

134.6676  
134.1294  
134.0931  
134.0640  
129.9111  
128.2856  
128.1510  
126.6310  
126.6164  
126.6019  
123.9691  
123.8600  
123.6418  
123.5527  
119.3434  
119.0161

77.1600



\*\*\*Current Data Parameters\*\*\*  
 NAME : B3503  
 EXPNO : 101  
 PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*  
 DATE\_1 : 18-07-38  
 DATE\_2 : Nov 02 2005  
 DS : 4  
 AS : 3000  
 NTCLFS : off  
 O1 : 7576.30 Hz  
 O2 : 1290.52 Hz  
 RG : 5160.6000977  
 RO : 20 Hz  
 SFO1 : 75.4752955 MHz  
 SOLVENT : CDCl3  
 SU : 238.3980 ppm  
 ST\_H : 17985.612 Hz  
 TD : 65536  
 TE : 300.0 K

\*\*\*Processing Parameters\*\*\*  
 GB : 0.0000000  
 LB : 1.00 Hz  
 SF : 75.4677470 MHz

\*\*\*1D NMR Plot Parameters\*\*\*  
 SR : 27.54 Hz  
 ppm\_cm : 10.62  
 Hz\_cm : 801.69  
 T1\_rho\_cm : 2359960.00  
 NTCLFS : off  
 SOLVENT :



PROTON



20a

8.1023  
8.0772  
7.9372  
7.9121  
7.8870  
7.7540  
7.7270  
7.7006

\*\*\* Current Data Parameters \*\*\*

NAME : f268f1  
EXPNO : 1  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

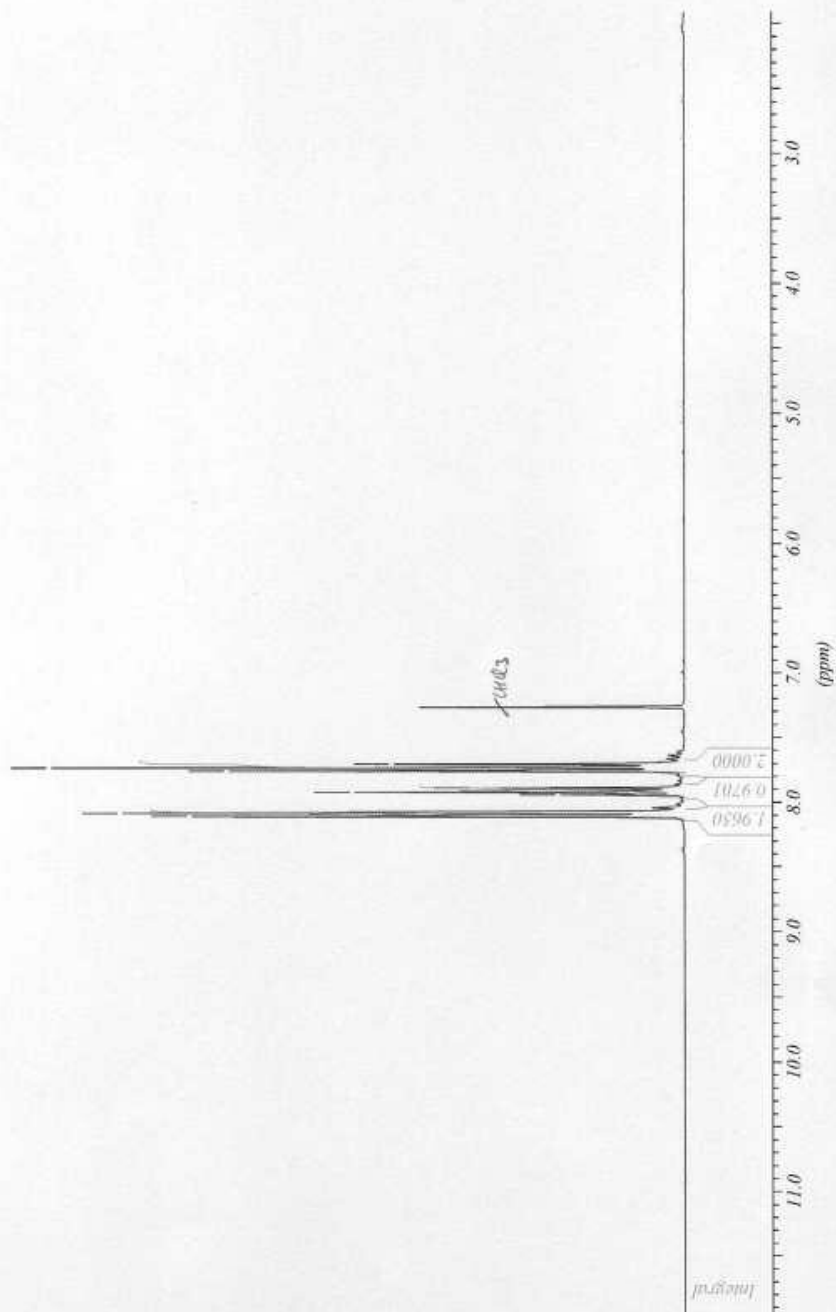
DATE\_1 : 08:54:15  
DATE\_d : Jun 14 2005  
DS : 0  
EXP :  
NS : 8  
NUCLEUS : off  
O1 : 1853.43 Hz  
O2 : 0.00 Hz  
RG : 256.0000000  
RO : 20 Hz  
SFO1 : 300.1318534 MHz  
SOLVENT : CDCl3  
SW\_h : 20.5671 ppm  
SW\_w : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

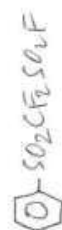
\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300060 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 6.41 Hz  
ppm\_cm : 0.45  
Hz\_cm : 134.28  
Y1\_val\_cm : 45125148.00  
NUCLEUS : off  
SOLVENT : ?





2.0a

99.3821  
99.4024

CF<sub>3</sub>

SO<sub>2</sub>F

64.497

7.4991

33.004

(ppm)

\*\*\* Current Data Parameters \*\*\*

NAME : jz268f1  
EXPNO : 2  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 08.56.04  
DATE\_2 : Jun 14 2005  
DS : 2  
EXP : PS done  
NS : 8  
NUCLEUS : off  
O1 : -20615.33 Hz  
O2 : 0.00 Hz  
RG : 724.6999756  
RO : 20 Hz  
SFO1 : 282.3838655 MHz  
SOLVENT : CDCl3  
SW : 266.2616 ppm  
SW\_H : 75187.970 Hz  
TD : 131072  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 282.3044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
ppm\_cm : 11.86  
Hz\_cm : 3350.62  
YVal\_cm : 3164334.00  
NUCLEUS : off  
CONVLEV : 9

F719\_301

49.3025  
49.2822  
49.2660

C13CPD CDCB h30rc0f 1



137.6641  
131.5839  
130.9875  
130.2384  
123.3727  
122.9654  
118.9143  
118.5070  
114.4560  
114.0487

77.5891  
77.1600  
76.7382

\*\*\* Current Data Parameters \*\*\*

NAME : f268f  
EXPNO : 101  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

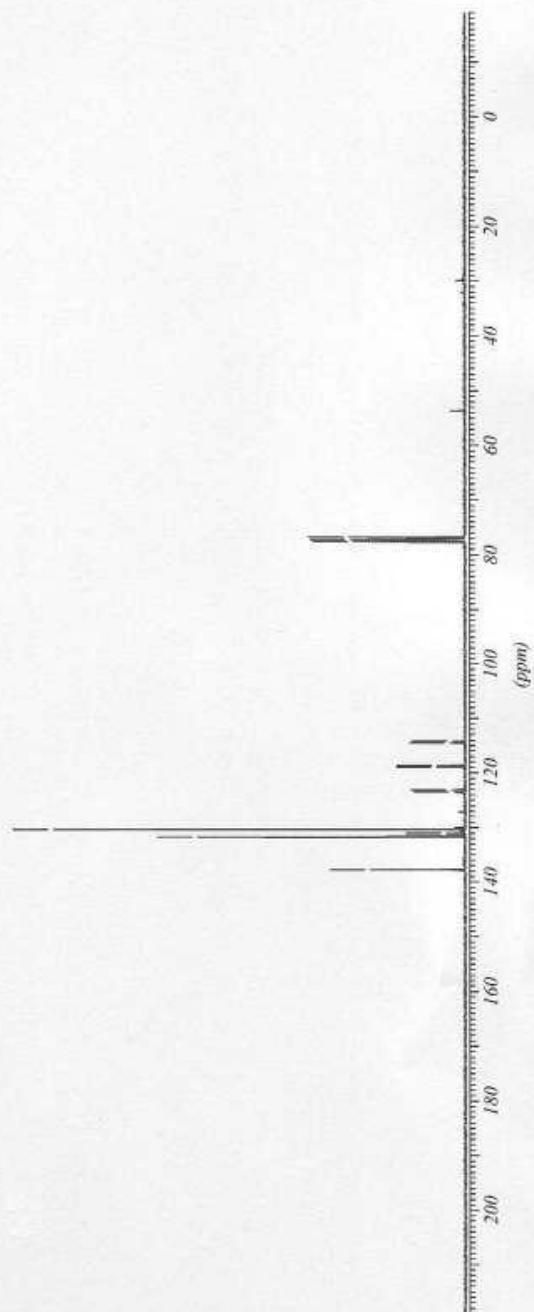
DATE\_1 : 13:26:00  
DATE\_d : Jun 20 2005  
DS : 4  
EXP : C13CPD  
NS : 3000  
NUCLEUS : off  
O1 : 7576.30 Hz  
O2 : 1200.52 Hz  
RG : 4096.000000  
RO : 20 Hz  
SFO1 : 75.4732953 MHz  
SOLVENT : CDCl3  
SW : 238.2980 ppm  
SW\_h : 17985.612 Hz  
TD : 65536  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4677390 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 20.40 Hz  
ppm\_cm : 10.62  
Hz\_cm : 801.50  
YIol\_cm : 540225.50  
NUCLEUS : off  
SOLVENT : ?



PROTON

7.6776  
7.6738  
7.6519  
7.6462  
7.5602  
7.5307  
7.5213  
7.5132  
7.5075  
7.5019  
7.4925  
7.4874  
7.4736  
7.4686  
7.4611  
7.4517  
7.4460  
7.4391

3.1390  
3.1158

— 2.0500



21

\*\*\* Current Data Parameters \*\*\*  
NAME : f211  
EXPNO : 1  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

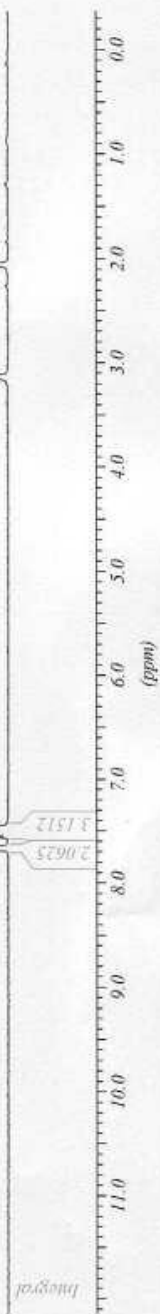
DATE\_1 : 00:14:42  
DATE\_d : Mar 11 2005  
DS : 0  
EXP :  
NS : 8  
NUCLEUS : <sup>1</sup>H  
O1 : 1853.43 Hz  
O2 : 0.00 Hz  
RG : 512.000000  
RO : 20 Hz  
SFO1 : 300.1318534 MHz  
SOLVENT : Acetone  
SW\_h : 20.5671 ppm  
SW\_v : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300040 MHz

\*\*\* ID NMR Plot Parameters \*\*\*

SR : 4.08 Hz  
ppm\_cm : 0.56  
Hz\_cm : 167.33  
YVal\_cm : 60524532.00  
NUCLEUS : <sup>1</sup>H  
SOLVENT : ?



F19\_300

$\text{p}(\text{SCF}_2\text{C}_6\text{SO}_3^-) \text{ Li}^+$

21



\*\*\* Current Data Parameters \*\*\*

NAME : p211  
EXPNO : 2  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 00.16.31  
DATE\_2 : Mar 11 2005  
DS : 2  
AS : 8  
NUCLEI : off

O1 : -20615.53 Hz  
O2 : 0.00 Hz

RG : 1149.4000244  
RO : 20 Hz

SFO1 : 282.3838655 MHz

SOLVENT : acetone

SW : 266.2616 ppm  
SW\_H : 75187.970 Hz

TD : 131072  
TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz

SF : 282.4044840 MHz

\*\*\* 1D NMR Parameters \*\*\*

SR : 0.00 Hz

ppm cm : 11.86

Hz cm : 3350.62

31 ad cm : 88794132.00

NUCLEI : off

SOLVENT :

-113.7960  
-113.8203  
-113.8447

-85.4658  
-85.4842  
-85.5085

Identifer Chem, Shift [ppm] J [Hz] Multiplicity Coupling

1	-85.4655	6.5100	5	d(1.0)
2	-113.8203	0.3857	5	d(2.0)







\*\*\* Current Data Parameters \*\*\*

NAME : j211  
EXPNO : 101  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 16.10.52  
DATE\_2 : Mar 23 2005  
DS : 4  
EXP : C13CPD  
AS : 5500

\*\*\* Processing Parameters \*\*\*

NUCLEUS : off  
O1 : 7576.30 Hz  
O2 : 1200.52 Hz  
RG : 1625.5000000  
RO : 20 Hz

SFO1 : 75.4752953 MHz

SOLVENT : Acetone

SW : 238.2980 ppm

SW\_H : 17985.612 Hz

TD : 65536

TE : 300.0 K

\*\*\* Processing Parameters \*\*\*

GB : 0.0000000

LB : 1.00 Hz

SF : 75.4676980 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : -29.40 Hz

ppm\_cm : 10.62

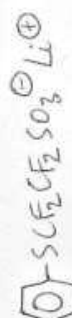
Hz\_cm : 801.50

YVal\_cm : 309684.34

NUCLEUS : off

SOLVENT :

137.7715  
131.2549  
130.0694  
128.6075  
128.1784  
125.7056  
125.6765  
125.6401  
125.2037  
124.7746  
124.3455  
121.3636  
120.9345  
120.5054  
119.7053  
119.2762  
118.8544  
115.8870  
115.4579  
115.0361  
112.0687  
111.6396  
111.2177



21

206.9524

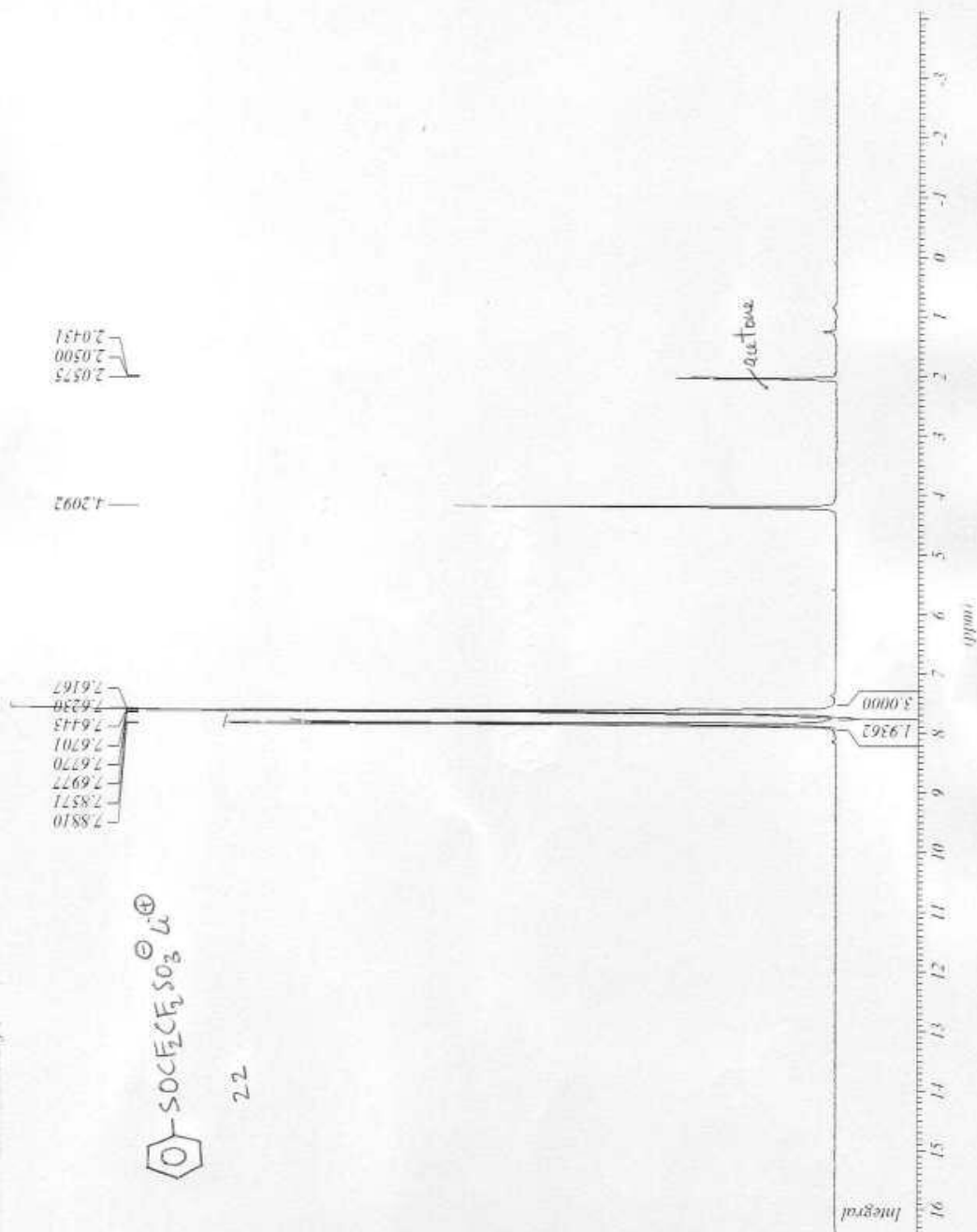
C13CPD Acetone is added 11



PROTON, Acetone d6, ref 1

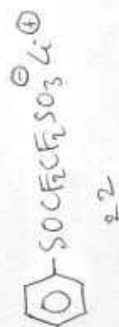


22



\*\*\* Current Data Parameters \*\*\*  
 NAME : f320  
 EXPNO : 100  
 PROCNO : 1  
 \*\*\* Acquisition Parameters \*\*\*  
 DATE\_1 : 10-12-50  
 DATE\_2 : Oct 13 2005  
 DS : 0  
 AS : 8  
 NUCLEUS : off  
 Q1 : 1853.43 Hz  
 Q2 : 0.00 Hz  
 RG : 181.000000  
 RO : 20 Hz  
 SFO1 : 300.1318534 MHz  
 SOLVENT : Acetone  
 SW : 20.5671 ppm  
 SW\_H : 6172.840 Hz  
 TD : 32768  
 TE : 300.0 K  
 \*\*\* Processing Parameters \*\*\*  
 GB : 0.000000  
 LB : 0.30 Hz  
 SF : 300.1300050 MHz  
 \*\*\* 1D NMR Plot Parameters \*\*\*  
 SR : 5.21 Hz  
 ppm\_cm : 0.92  
 Hz\_cm : 275.08  
 Yval\_cm : 4564.97  
 NUCLEUS : off  
 SOLVENT :

F19\_30 Acetone n sercof 1



-121.9834  
 -112.9997  
 -113.0139  
 -113.0688  
 -113.0891  
 -113.1053  
 -113.9056  
 -113.9260  
 -113.9381  
 -113.9544  
 -114.0031  
 -114.0235  
 -114.0438  
 -114.9456  
 -114.9700  
 -114.9822  
 -120.3813  
 -120.3935  
 -120.4098  
 -121.1979  
 -121.2141  
 -121.2304

\*\*\* Current Data Parameters \*\*\*

NAME : f320  
 EXPNO : 105  
 PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

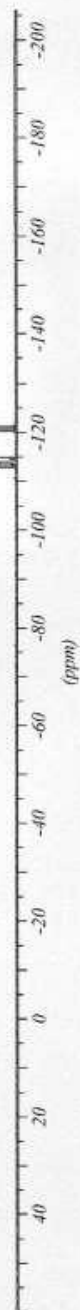
DATE\_1 : 15:18:06  
 DATE\_d : Oct 13 2005  
 DS : 2  
 EXP : F19\_30  
 NS : 8  
 NUCLEUS : off  
 O1 : -20615.53 Hz  
 O2 : 0.00 Hz  
 RG : 362.000000  
 RO : 20 Hz  
 SFO1 : 282.3838655 MHz  
 SOLVENT : Acetone  
 SW : 266.2616 ppm  
 SW\_h : 75187.970 Hz  
 TD : 131072  
 TE : 300.0 K

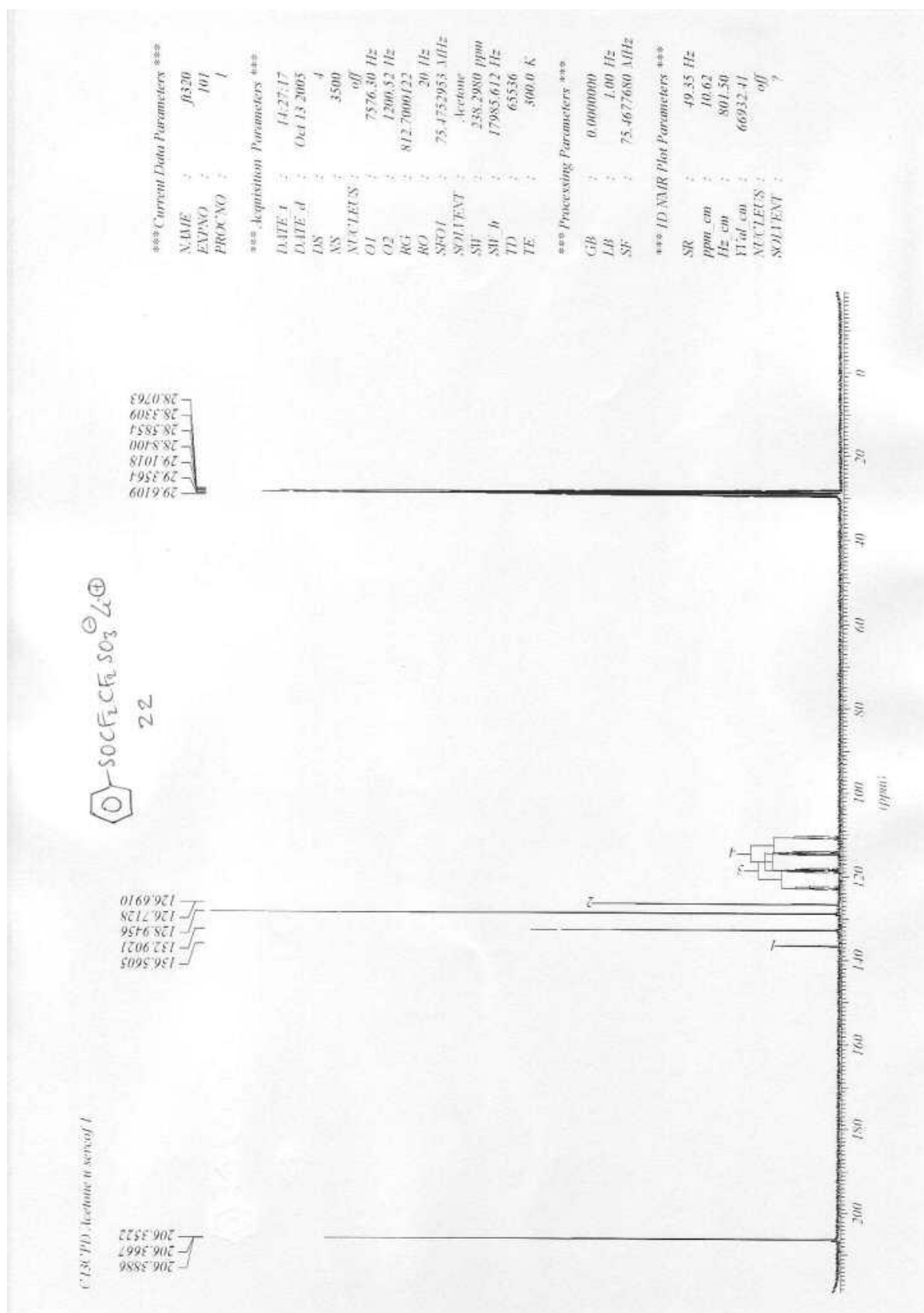
\*\*\* Processing Parameters \*\*\*

GB : 0.0500000  
 LB : 0.30 Hz  
 SF : 282.4044810 MHz

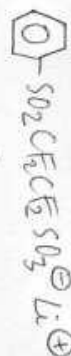
\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
 ppm\_cm : 11.86  
 Hz\_cm : 3350.62  
 Y1val\_cm : 5201.09  
 NUCLEUS : off  
 SOLVENT : ?





PROTON



23

8.0592  
8.0341  
7.9657  
7.9475  
7.9406  
7.9343  
7.9199  
7.9155  
7.9117  
7.8188  
7.8138  
7.7925  
7.7730  
7.7674

3.0279  
2.9959  
2.0864  
2.0644  
2.0575  
2.0500  
2.0431  
2.0356



\*\*\* Current Data Parameters \*\*\*  
NAME : B348  
EXPNO : 3  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 00:31:41  
DATE\_2 : Oct 18 2005  
DS : 0  
NS : 8  
NUC1ETS : off  
QT : 1853.43 Hz  
Q2 : 0.00 Hz  
RG : 456.1000061  
RG2 : 20 Hz  
SFO1 : 300.1318534 MHz  
SOLVENT : acetone  
SF : 29.5671 ppm  
SF\_H : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

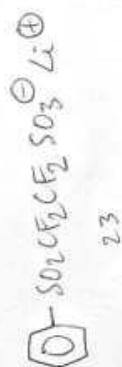
\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300040 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 4.08 Hz  
ppm\_cm : 0.92  
Hz\_cm : 275.08  
F1d\_cm : 30961156.00  
NUC1ETS : off  
SOLVENT : ?

F19 30 Acetone d6 servof 2



-110.5784  
-110.6312  
-110.6475  
-110.6556  
-110.6637  
-110.6759  
-110.7287  
-113.3978  
-113.4506  
-113.4709  
-113.4791  
-113.4953  
-113.5481

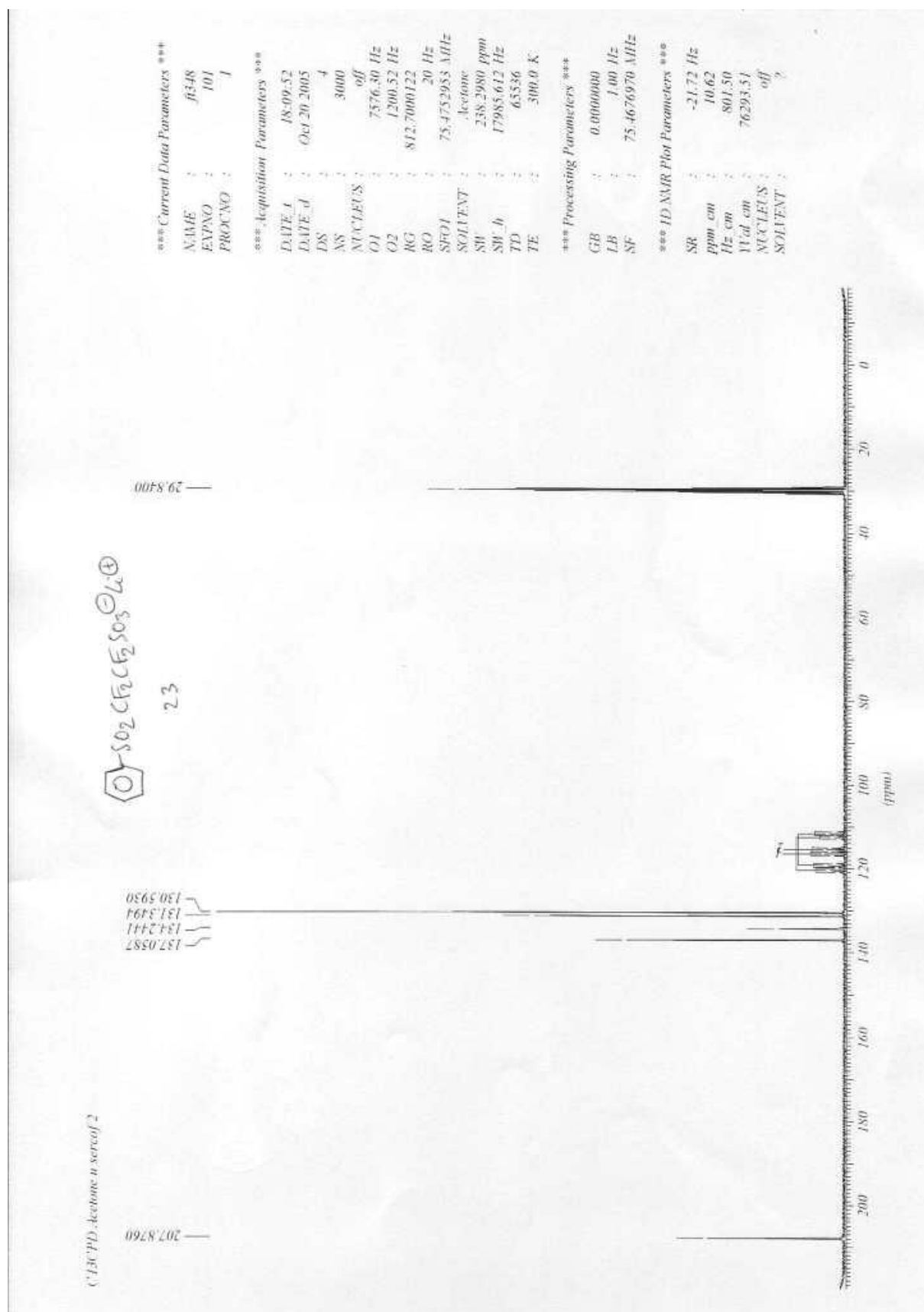
```
***Current Data Parameters ***
NAME      : j348
EXPNO     : 105
PROCNO    : 1

***Acquisition Parameters ***
DATE_     : 19-00-49
DATE_d    : Oct 20 2005
DS        : 2
AS        : 8
NUCLEUS   : off
O1        : -20615.53 Hz
O2        : 0.00 Hz
RG        : 287.3999939
RO        : 20 Hz
SFO1      : 282.3638655 MHz
SOLVENT   : Acetone
SW        : 266.2616 ppm
SW_h      : 75187.970 Hz
TD        : 131072
TE        : 300.0 K

***Processing Parameters ***
GB        : 0.0500000
LB        : 0.30 Hz
SF        : 282.4044810 MHz

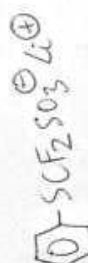
***1D NMR Plot Parameters ***
SR        : 0.00 Hz
ppm_cm    : 11.86
Hz_cm     : 3350.62
Yval_cm   : 12256.76
NUCLEUS   : off
SOLVENT   : ?
```





PROTON128

7.6406  
7.6349  
7.6153  
7.6086  
7.4485  
7.4422  
7.4353  
7.4171



24

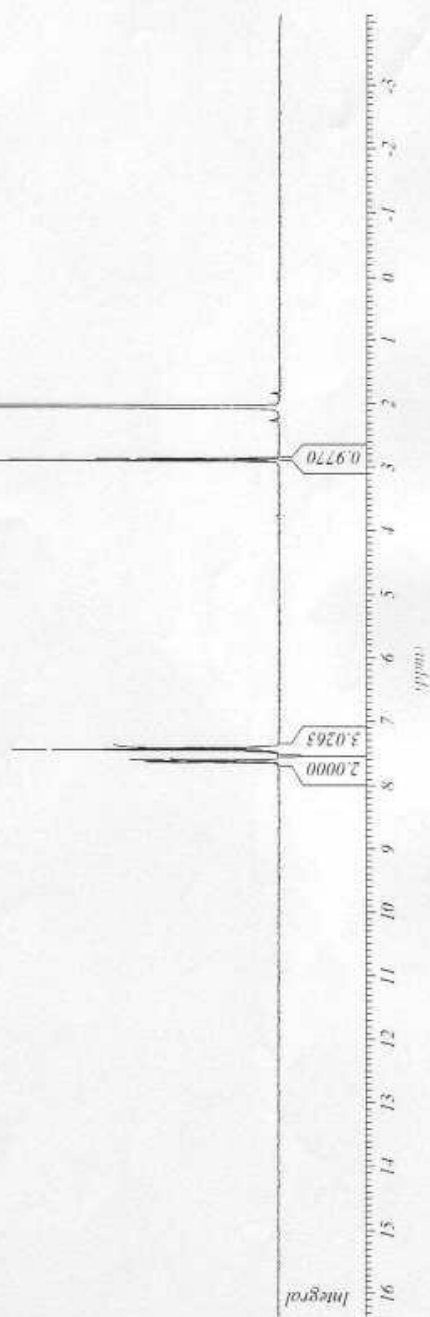
2.9030  
2.8716  
2.0575  
2.0500  
2.0431  
2.0356

\*\*\* Current Data Parameters \*\*\*  
NAME : p197  
EXPNO : 2  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*  
DATE\_1 : 08-19-37  
DATE\_2 : Feb 24 2005  
DS : 0  
AS : 56  
NUCLEUS : off  
O1 : 1853.43 Hz  
O2 : 0.00 Hz  
RG : 574.7000122  
RO : 20 Hz  
SFO1 : 300.1318534 MHz  
SOLVENT : Acetone  
SW\_h : 20.5671 ppm  
SW : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

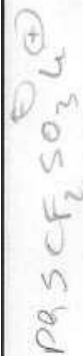
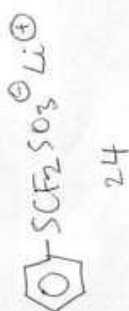
\*\*\* Processing Parameters \*\*\*  
GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300040 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*  
SR : 4.08 Hz  
ppm\_cm : 0.92  
Hz\_cm : 275.08  
Y1\_sol\_cm : 20006132.00  
NUCLEUS : off  
SOLVENT : ?





F19\_30



-79.0775

```

***Current Data Parameters ***
NAME : f197
EXPNO : 1
PROCNO : 1

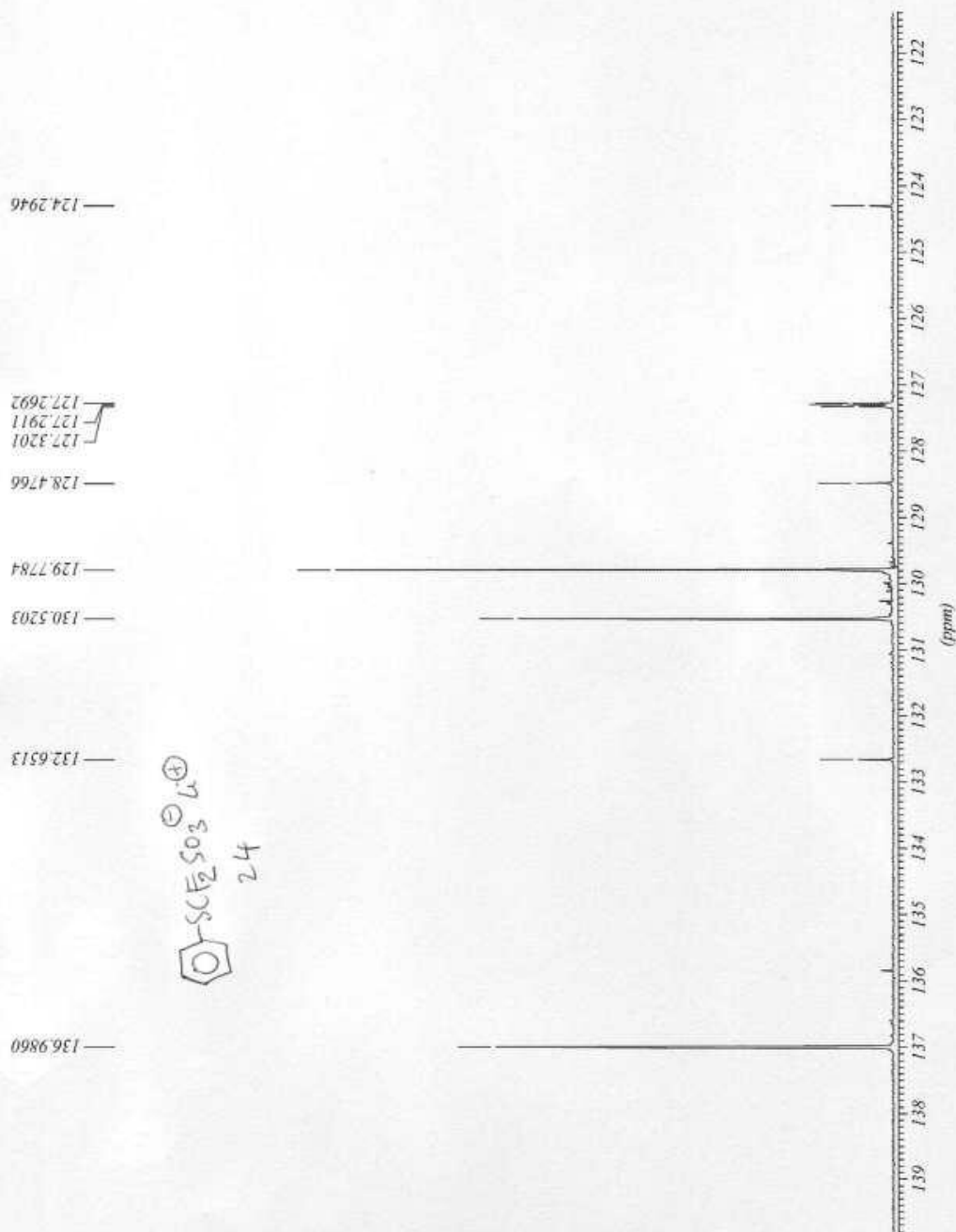
*** Acquisition Parameters ***
DATE_1 : 06.53.53
DATE_2 : Feb 24 2005
DS : 2
SS : 8
NUCLEUS : off
O1 : -20615.53 Hz
O2 : 0.00 Hz
RG : 1149.4000244
RO : 20 Hz
SFO1 : 282.3838655 MHz
SOLVENT : Acetone
SI : 266.2616 ppm
SW_h : 75187.970 Hz
TD : 131072
TE : 300.0 K

*** Processing Parameters ***
GB : 0.0000000
LB : 0.30 Hz
SF : 283.4044840 MHz

*** 1D NMR Plot Parameters ***
SR : 0.00 Hz
ppm cm : 11.86
Hz cm : 3350.62
Y1d cm : 2236.3636.00
NUCLEUS : off
SOLVENT :
  
```



C13CPD Acetone d6 ref 3



\*\*\* Current Data Parameters \*\*\*

NAME : fl97  
EXPNO : 101  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 21:10:16  
DATE\_d : Mar 16 2005  
DS : 4  
EXP : C13CPD  
NS : 3000  
NUCLEUS : off  
O1 : 7576.30 Hz  
O2 : 1200.52 Hz  
RG : 1625.5000000  
RO : 20 Hz  
SFO1 : 75.4752953 MHz  
SOLVENT : Acetone  
SW : 238.2980 ppm  
SW\_h : 17985.612 Hz  
TD : 65536  
TE : 300.0 K

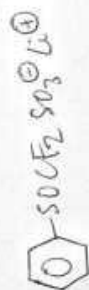
\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4676990 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : -20.07 Hz  
ppm\_cm : 0.82  
Hz\_cm : 62.10  
Y1d\_cm : 196348.30  
NUCLEUS : off  
SOLVENT : ?

PROTON, acetone-d6, 25



25

2.0575  
2.0500  
2.0431

7.8634  
7.8377  
7.7253  
7.7197  
7.7015  
7.6996  
7.6902  
7.6782  
7.6726  
7.6481  
7.6268

\*\*\*Current Data Parameters\*\*\*

NAME :  $\beta$ 362  
EXPNO : 100  
PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*

DATE\_1 : 14-01-06  
DATE\_2 : Nov 17 2005  
INSTR : 0  
PULPROG : zgpg30  
F2 - F1 : 1853.43 Hz  
F2 - F1 : 0.00 Hz  
RG : 128.0000000  
RO : 20 Hz  
SFO : 300.1318534 MHz  
SOLVENT : acetone  
SH : 20.5671 ppm  
SF : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

\*\*\*Processing Parameters\*\*\*

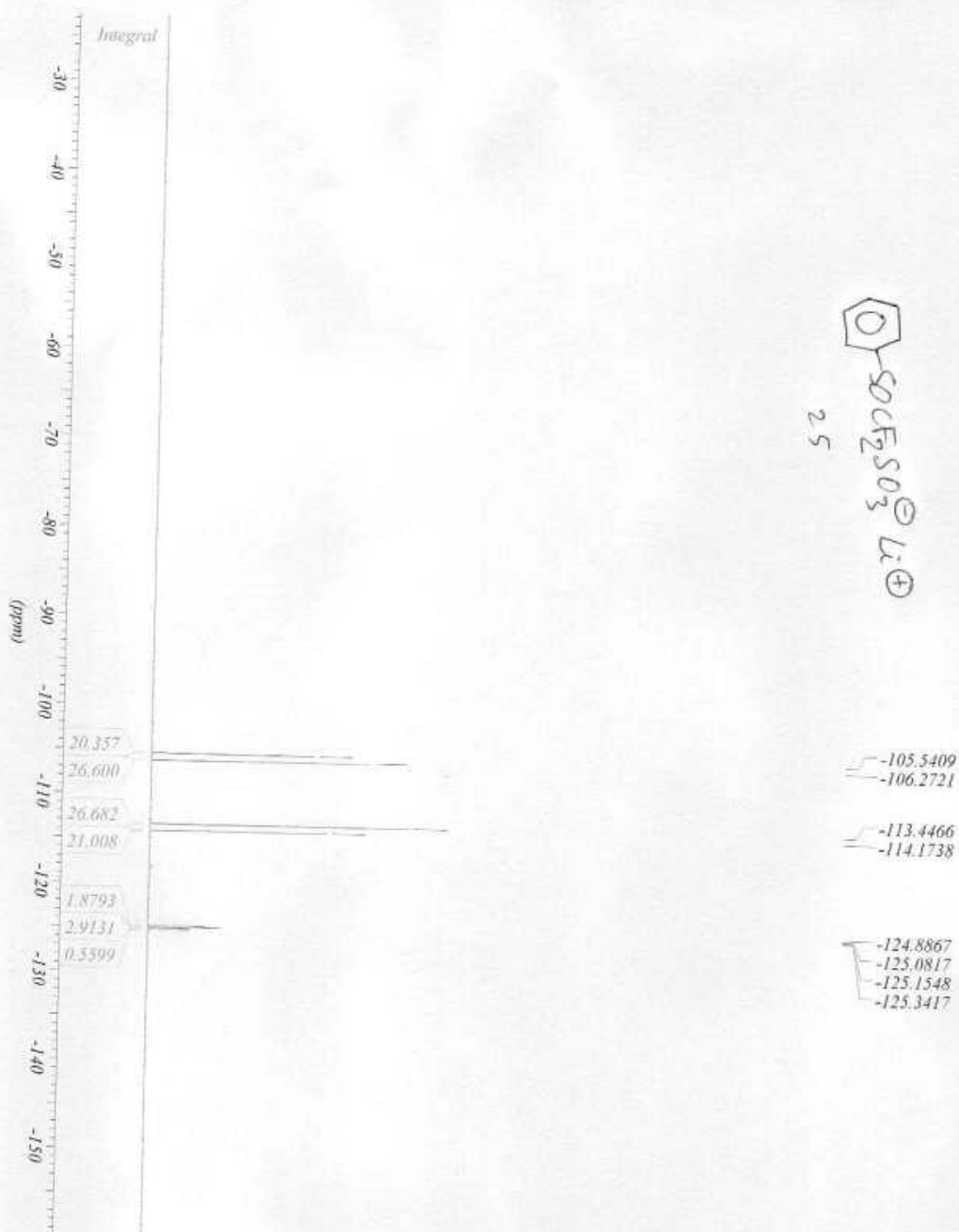
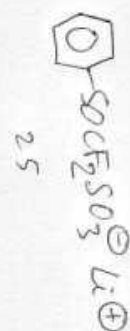
GB : 0.0000000  
LB : 0.30 Hz  
SP : 300.1300040 MHz

\*\*\*1D NMR Plot Parameters\*\*\*

SR : 4.08 Hz  
ppm/cm : 0.92  
Hz/cm : 275.08  
FID/cm : 5094.46  
NUCLEUS : off  
SOLVENT : acetone



F19 301



\*\*\*Current Data Parameters\*\*\*

NAME : j362  
EXPNO : 3  
PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*

DATE\_1 : 00-38-15  
DATE\_2 : Nov 07 2005  
DS : 2  
EXP : PS done  
NS : 8

NUCLEUS : <sup>13</sup>C  
O1 : -20615.53 Hz  
O2 : 0.00 Hz

RG : 574.7000122  
RO : 20 Hz  
SFO1 : 282.3836035 MHz

SOLVENT : Acetone  
SW : 266.2616 ppm  
SW\_H : 75187.970 Hz

TD : 131072  
TE : 300.0 K

\*\*\*Processing Parameters\*\*\*  
GB : 0.0000000  
LB : 0.30 Hz  
SF : 282.4044840 MHz

\*\*\*1D NMR Plot Parameters\*\*\*  
SR : 0.00 Hz  
ppm\_cm : 6.13  
Hz\_cm : 1730.02

Yref\_cm : 12101796.00  
NUCLEUS : <sup>13</sup>C  
CONVLEV : 9



25

118.4616

122.9927  
122.8327

127.5165  
127.5020  
127.3688

129.9894

130.7385

133.8513

136.6296  
136.6078  
136.5860  
136.5714

C13CPID\_Acetone d6 (ref) 2

\*\*\*Current Data Parameters\*\*\*

NAME : J36.2  
EXPNO : 101  
PROCNO : 1

\*\*\*Acquisition Parameters\*\*\*

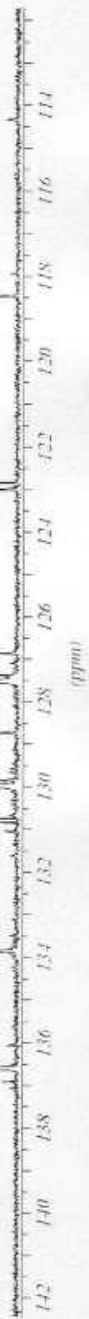
DATE\_1 : 17:25:19  
DATE\_2 : Nov 17 2005  
IN : 4  
AS : 3100  
NUCLEUS : off  
P1 : 7576.30 Hz  
P2 : 1290.52 Hz  
RG : 1290.1999512  
RO : 20 Hz  
SFO1 : 75.4752953 MHz  
SOLVENT : Acetone  
SW : 238.2980 ppm  
SW\_H : 17985.612 Hz  
TD : 65536  
TE : 300.0 K

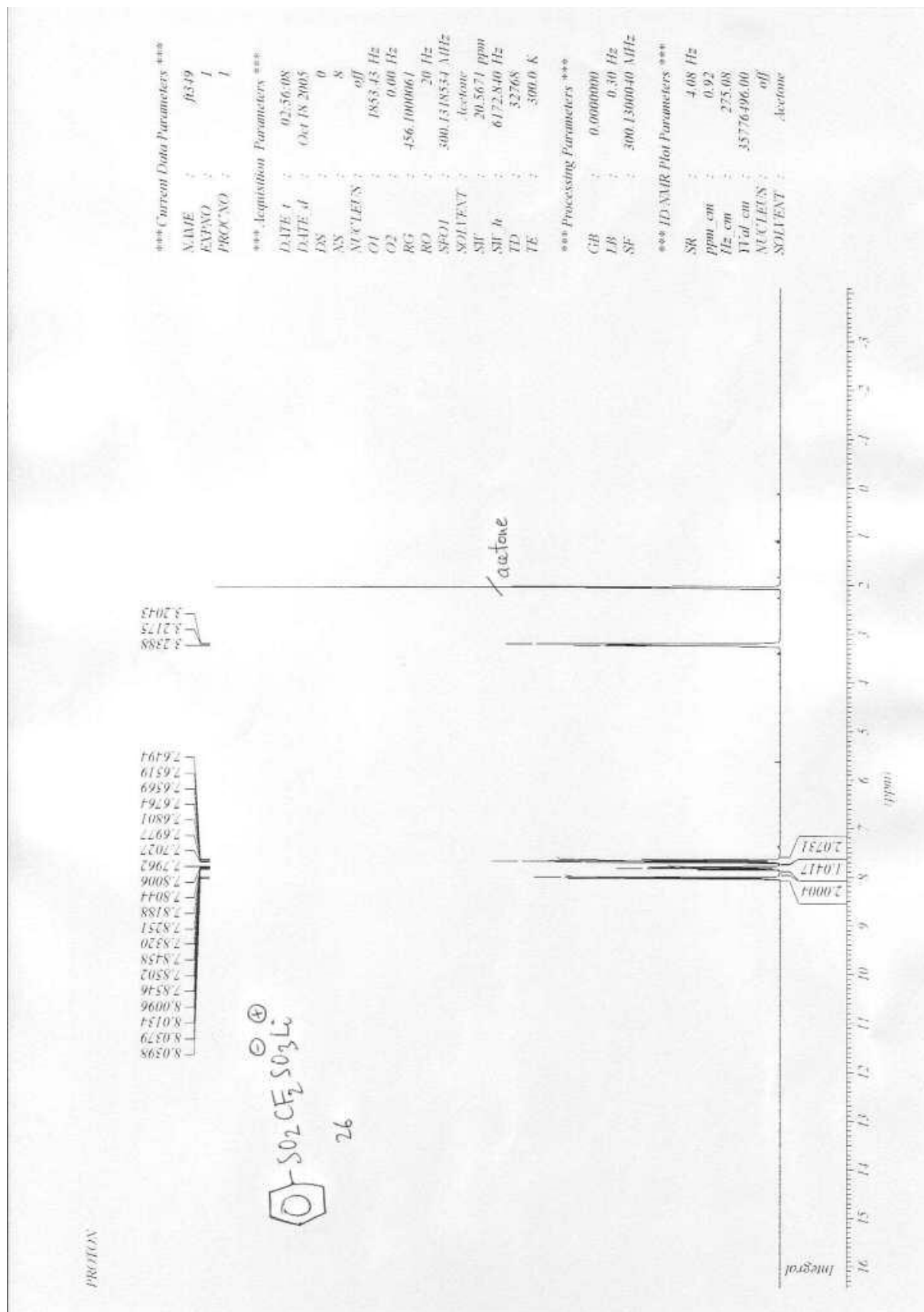
\*\*\*Processing Parameters\*\*\*

GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4676930 MHz

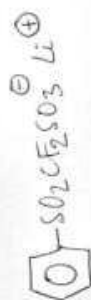
\*\*\*1D NMR Plot Parameters\*\*\*

SR : -25.56 Hz  
ppm : 1.37  
Hz : 103.46  
Total : 50943.98  
NUCLEUS : off  
SOLVENT :





F19\_30



26

104.7649

\*\*\* Current Data Parameters \*\*\*  
 NAME : f349  
 EXPNO : 2  
 PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

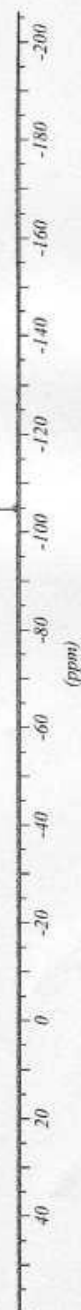
DATE\_1 : 02:57:59  
 DATE\_2 : Oct 18 2005  
 DS : 2  
 EXP : PS done  
 NS : 8  
 NUCLEUS : off  
 O1 : -20615.53 Hz  
 O2 : 0.00 Hz  
 RG : 643.0999736  
 RO : 20 Hz  
 SF01 : 282.3838655 MHz  
 SOLVENT : Acetone  
 SW : 266.2616 ppm  
 SW\_h : 75187.970 Hz  
 TD : 131072  
 TE : 300.0 K

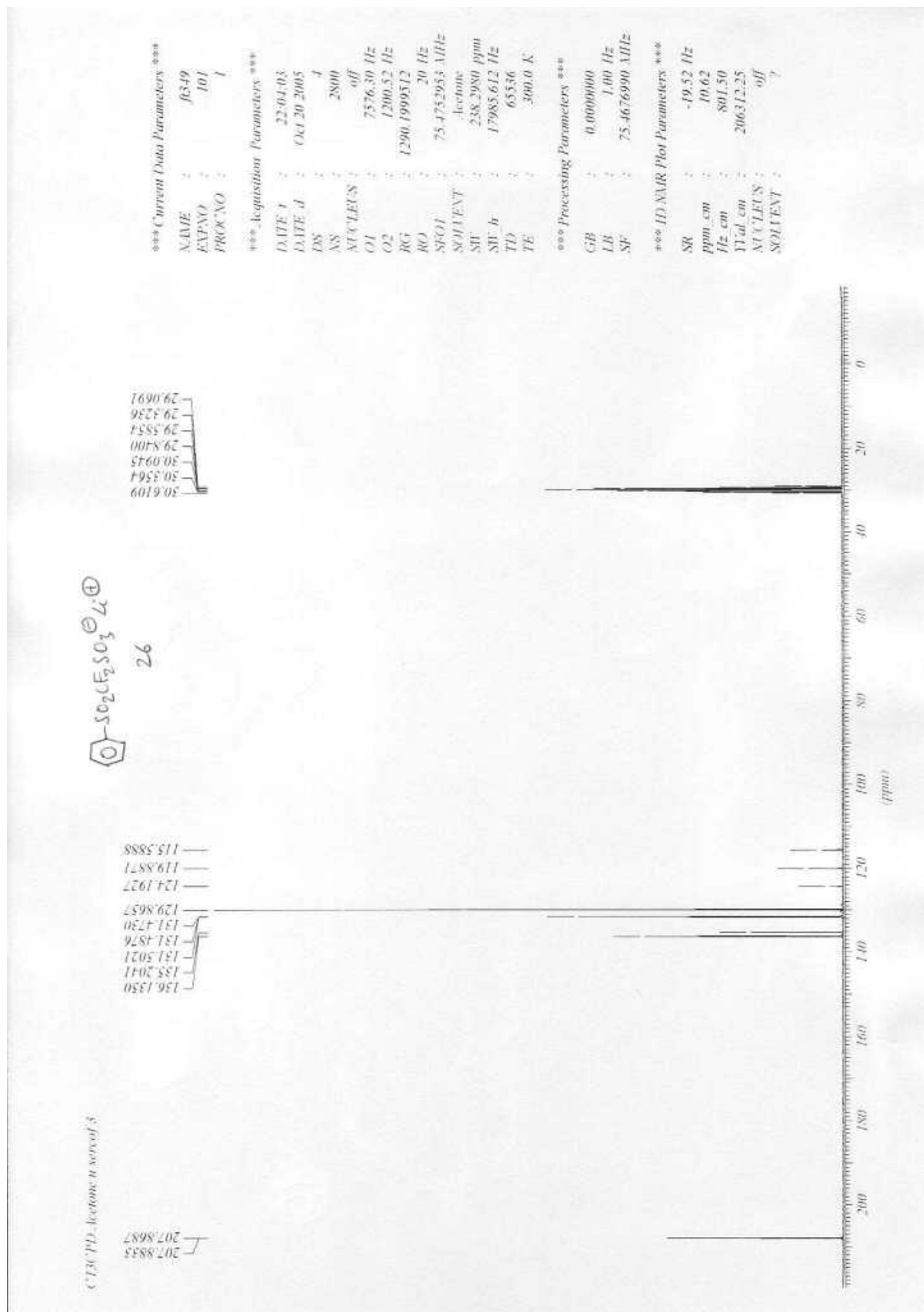
\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
 LB : 0.30 Hz  
 SF : 282.4044840 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 0.00 Hz  
 ppm\_cm : 11.86  
 Hz\_cm : 3350.62  
 YVal\_cm : 28309930.00  
 NUCLEUS : off  
 SOLVENT : ?







PROTON



27

8.2846  
8.2601  
8.2563  
7.6469  
7.6261  
7.6218  
7.5238  
7.5182  
7.4981  
7.4724

2.8804  
2.8490

\*\*\* Current Data Parameters \*\*\*  
NAME : f133s2  
EXPNO : 8  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

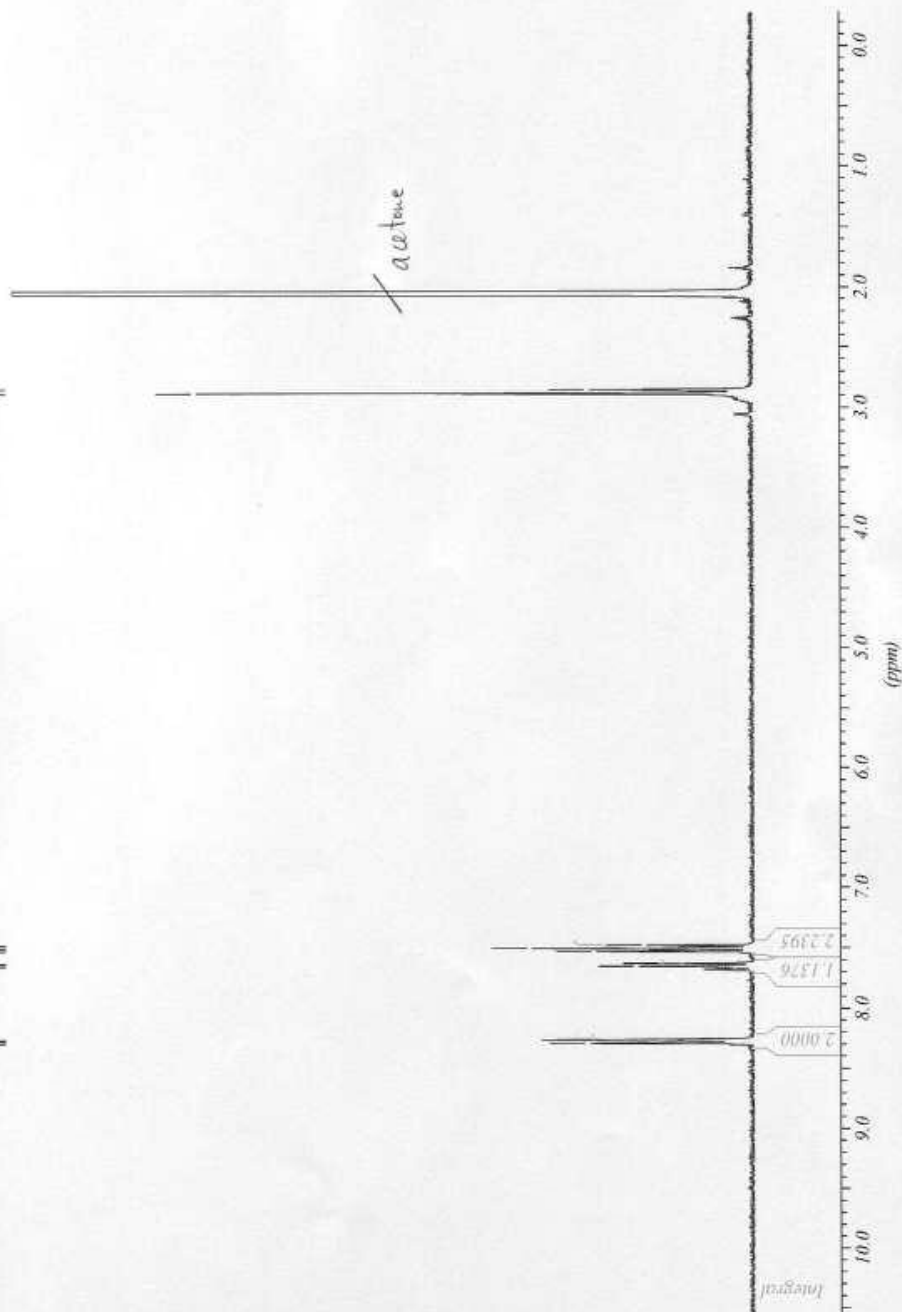
DATE\_1 : 02-07-06  
DATE\_d : Oct 21 2004  
DS : 0  
EXP :  
NS : 8  
NUCLEUS : off  
O1 : 1853.43 Hz  
O2 : 0.00 Hz  
RG : 456.1000061  
RO : 20 Hz  
SFO1 : 300.1318534 MHz  
SOLVENT : Acetone  
SW\_h : 20.5671 ppm  
SW\_k : 6172.840 Hz  
TD : 32768  
TE : 300.0 K

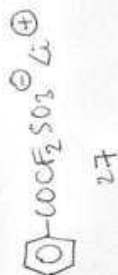
\*\*\* Processing Parameters \*\*\*

GB : 0.0000000  
LB : 0.30 Hz  
SF : 300.1300040 MHz

\*\*\* 1D NMR Plot Parameters \*\*\*

SR : 4.27 Hz  
ppm\_cm : 0.48  
Hz\_cm : 144.89  
YVol\_cm : 5788325.50  
NUCLEUS : off  
SOLVENT : ?





104.3587



\*\*\* Current Data Parameters \*\*\*  
NAME : J13352  
EXPNO : 6  
PROCNO : 1  
\*\*\* Acquisition Parameters \*\*\*  
DATE\_1 : 09.26.30  
DATE\_2 : Oct 20 2004  
DS : 2  
AS : 8  
NUCLEUS : off  
Q1 : -20615.53 Hz  
Q2 : 0.00 Hz  
RG : 1625.5000000  
RO : 20 Hz  
SFO1 : 282.3838655 MHz  
SOLVENT : Acetone  
SF : 266.2616 ppm  
SW\_H : 75187.970 Hz  
TD : 131072  
TE : 300.0 K  
\*\*\* Processing Parameters \*\*\*  
GB : 0.0000000  
LB : 0.30 Hz  
SF : 282.4044840 MHz  
\*\*\* ID NMR Parameters \*\*\*  
SR : 0.00 Hz  
ppm\_cm : 11.86  
Hz\_cm : 3350.62  
Y1\_of\_cm : 51606680.00  
NUCLEUS : off  
SOLVENT :





27

(C1H3PT) Acetone d6 served T0

29.6109  
29.5491  
29.0945  
28.8400  
28.5854  
28.3236  
28.0690

133.7821  
132.8221  
132.8076  
130.5529  
130.5093  
130.4729  
127.9928  
120.1307  
116.3269  
112.5232

206.2794  
206.2649  
188.0824  
187.7478  
187.4133

Identif	Chem. Shift [ppm]	$\delta$ [ppm]	Multiplicity	Integrations
1	187.7478	25.2484	3	J(1,0)
2	132.8148	1.0978	3	J(2,0)
3	130.5112	3.0188	3	J(3,0)
4	116.3269	297.0528	3	J(4,0)

\*\*\* Current Data Parameters \*\*\*

NAME : 013382  
EXPNO : 101  
PROCNO : 1

\*\*\* Acquisition Parameters \*\*\*

DATE\_1 : 14.08.19  
DATE\_2 : Nov 08 2004  
DS : 4  
AS : 4500

\*\*\* Processing Parameters \*\*\*

NUCLEUS : off  
P1 : 7576.30 Hz  
P2 : 1200.52 Hz  
RG : 1250.1999312  
RO : 20 Hz  
SFO1 : 75.4752953 MHz  
SOLVENT : Acetone  
ST : 238.2980 ppm  
SW\_h : 17985.612 Hz  
TD : 65536  
TE : 300.0 K

\*\*\* ID NMR Plot Parameters \*\*\*

GB : 0.0000000  
LB : 1.00 Hz  
SF : 75.4677670 MHz  
SR : 48.26 Hz  
ppm\_cm : 10.62  
Hz\_cm : 801.50  
Y1\_cm : 359.16.07  
Y2\_cm : off  
X1\_cm : 0  
X2\_cm : 0