Electronic Supplementary Information

Asymmetric synthesis of 2-arylpyrrolidines starting from γ-chloro *N*-(*tert*-butanesulfinyl)ketimines

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Experimental data

General Experimental Methods

^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were recorded with a JEOL EX 300 Eclipse NMR spectrometer. Peak assignments were obtained with the aid of DEPT, 2D-COSY and 2D-HSQC spectra. The compounds were diluted in deuterated solvents and the used solvent is indicated for each compound. Low resolution mass spectra were recorded with an Agilent 1100 Series VS (ES = 4000 V) mass spectrometer. IR spectra were recorded on a Perkin-Elmer Spectrum BX FT-IR spectrophotometer. All compounds were analysed in neat form with an ATR (Attenuated Total Reflectance) accessory. Melting points of crystalline compounds were measured with a Büchi 540 apparatus. The elemental analysis was performed with a Perkin-Elmer 2400 Elemental Analyzer. The purification of reaction mixtures by column chromatography was performed in a glass column with silica gel (Acros, particle size, 0.035-0.070 mm, pore diameter ca. 6 nm). TLC was performed on glass plates coated with silica gel 60 with F254 indicator (Merck, 0.25 mm), using UV and $KMnO_4$ as a visualizing agent.

All common reagents and solvents were obtained from commercial suppliers and used without further purification. Dichloromethane was distilled over calcium hydride, while diethyl ether and

toluene was dried over sodium benzophenone ketyl. Other solvents were used as received from the supplier.

NMR data are reported as follows: chemical shift, integration, multiplicity (s: singlet, d: doublet, t: triplet, q: quadruplet, br: broad, m: multiplet), coupling constants (*J* in Hz), allocation of the peaks.

Typical procedure for the synthesis of (R_S)-*N*-[1-aryl-4-chlorobutylidene]-*tert*-butanesulfinamides 1

As a representative example, the synthesis of (R_S)-*N*-[4-chloro-1-phenylbutylidene]-*tert*-butanesulfinamide **1a** is described here**.** Titanium(IV) ethoxide (12.49 g, 54.8 mol) and (R_S)-*tert*-butanesulfinamide (3.32 g, 27.4 mmol) were added to a solution of 4-chlorobutyrophenone (5 g, 27.4 mmol) in tetrahydrofuran (30 mL). The reaction was stirred for 48 hours at reflux temperature. After cooling, brine was added, and the resulting mixture was subsequently filtered over Celite®. The solution was extracted with EtOAc (3 x 25 mL), and the combined organic layers were dried ($MgSO_4$), filtered and evaporated under reduced pressure to afford (R_S)-**1a** (6.73 g) in 86% yield. The crude compound was purified by column chromatography (petroleum ether/EtOAc 17/3) to yield (R_S)-*N*-[4-chloro-1-phenylbutylidene]-*tert*-butanesulfinamide (R_S)-**1a** in 75% yield (5.87 g) as a brown oil. **Chromatography:** petroleum ether/EtOAc 17/3 R_f = 0.10; **Elemental analysis (%):** Found: C, 58.50; H, 7.21; N, 4.98. $C_{14}H_{20}ClNOS$ requires C, 58.83; H, 7.05; N, 4.90; **IR: ν_{max}/cm^{-1}** 2956, 1570, 1360, 1077; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.33 (9H, s, *t*Bu), 2.03-2.27 (2H, m, C<u>H</u>$_2$CH_2Cl), 3.23-3.36 and 3.40-3.52 (2H, m, C<u>H</u>$_2$-C=N), 3.64 (2H, t, *J* = 6.3 Hz, CH_2Cl), 7.40-7.51 and 7.87-7.89 (5H, m, C_6H_5); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 22.70 (CH_3, *t*Bu), 30.03 (<u>C</u>H_2-C=N), 31.62 (<u>C</u>H_2-CH_2Cl), 44.64 (CH_2Cl), 57.85 (C_q, *t*Bu), 127.40 (CH,

Ar), 128.69 (CH, Ar), 131.73 (CH, Ar), 137.47 (C_q, Ar), 178.04 (C=N); ***m/z* (ESI)** 286.2/288.3 ($[M+H]^+$, 100%); $[\alpha]_D$ = +11.9 (*c* 0.64, CH_2Cl_2).

***(S_S)*-*N*-[4-Chloro-1-phenylbutylidene]-*tert*-butanesulfinamide 1a** (63%)

$[\alpha]_D$ = -10.0 (*c* 1.00, CH_2Cl_2).

(*R_S*)-*N*-[4-Chloro-1-(4-methylphenyl)butylidene]-*tert*-butanesulfinamide 1b (68%)

Brown oil; **Chromatography:** petroleum ether/EtOAc 17/3 R_f = 0.19; **Elemental analysis (%):** Found: C, 59.94; H, 7.48; N, 4.73. $C_{15}H_{22}ClNOS$ requires C, 60.08; H, 7.40; N, 4.67; **IR:** ν_{max}/cm^{-1} 2958, 1590, 1455, 1360, 1077; δ_H **(300 MHz, $CDCl_3$, Me_4Si)** 1.32 (9H, s, *t*Bu), 2.06-2.27 (2H, m, C<u>H</u>$_2$CH_2Cl), 2.41 (3H, s, CH_3-Ar), 3.21-3.34 and 3.38-3.49 (2H, m, CH_2-C=N), 3.63-3.67 (2H, m, CH_2Cl), 7.24 (2H, d, *J* = 7.4 Hz, CH, Ar), 7.79 (2H, d, *J* = 7.4 Hz, CH, Ar); δ_C **(75 MHz, $CDCl_3$, Me_4Si)** 21.39 (CH_3, CH_3-Ar), 22.61 (CH_3, *t*Bu), 29.89 (<u>C</u>H_2-C=N), 31.67 (<u>C</u>H_2-CH_2Cl), 44.57 (CH_2Cl), 57.58 (C_q, *t*Bu), 127.38 (CH, Ar), 129.35 (CH, Ar), 134.66 (<u>C</u>$_q$-C=N, Ar), 142.27 (<u>C</u>$_q$-CH_3, Ar), 177.84 (C=N); ***m/z* (ESI)** 300.3/302.3 ($[M+H]^+$, 100%); $[\alpha]_D$ = +26.9 (*c* 1.07, CH_2Cl_2).

(*S_S*)-*N*-[4-Chloro-1-(4-methylphenyl)butylidene]-*tert*-butanesulfinamide 1b (66%)

$[\alpha]_D$ = -33.2 (*c* 1.02, CH_2Cl_2).

(*R_S*)-*N*-[4-Chloro-1-(4-chlorophenyl)butylidene]-*tert*-butanesulfinamide 1c (62%)

Orange oil; **Chromatography:** petroleum ether/EtOAc 17/3 R_f = 0.16; **Elemental analysis (%):** Found: C, 52.44; H, 6.02; N, 4.29. $C_{14}H_{19}Cl_2NOS$ requires C, 52.50; H, 5.98; N, 4.37; **IR:** ν_{max}/cm^{-1} 2959, 1585, 1456, 1360, 1077; δ_H **(300 MHz, $CDCl_3$, Me_4Si)** 1.33 (9H, s, *t*Bu), 2.03-2.27 (2H, m, C<u>H</u>$_2$CH_2Cl), 3.22-3.34 and 3.38-3.50 (2H, m, CH_2-C=N), 3.63-3.67 (2H, m,

CH_2Cl), 7.39-7.44 and 7.81-7.84 (4H, m, C_6H_4); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 22.70 (CH_3, *t*Bu), 29.80 ($\underline{C}H_2$-C=N), 31.56 ($\underline{C}H_2$-CH_2Cl), 44.57 (CH_2Cl), 57.97 (C_q, *t*Bu), 128.73 (CH, Ar), 128.91 (CH, Ar), 135.79 (C_q, Ar), 137.95 (C_q, Ar), 176.67 (C=N); ***m/z* (ESI)** 320.2/322.3/324.2 ($[M+H]^+$, 100%); **$[\alpha]_D$** = +43.4 (*c* 1.10, CH_2Cl_2).

(S_S)-*N*-[4-Chloro-1-(4-chlorophenyl)butylidene]-*tert*-butanesulfinamide 1c (73%)

$[\alpha]_D$ = -51.9 (*c* 0.99, CH_2Cl_2)

(R_S)-*N*-[4-Chloro-1-(4-methoxyphenyl)butylidene]-*tert*-butanesulfinamide 1d (63%)

Orange oil; **Chromatography:** hexane/EtOAc 17/3 R_f = 0.08; **Elemental analysis (%):** Found: C, 57.21; H, 7.13; N, 4.17. $C_{15}H_{22}ClNO_2S$ requires C, 57.04; H, 7.02; N, 4.43; **IR: ν_{max}/cm^{-1}** 2958, 1586, 1456, 1360, 1253, 1063; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.32 (9H, s, *t*Bu), 2.05-2.29 (2H, m, $C\underline{H}_2CH_2Cl$), 3.21-3.30 and 3.38-3.47 (2H, m, CH_2-C=N), 3.63-3.68 (2H, m, CH_2Cl), 3.86 (3H, s, OMe), 6.91-6.96 and 7.87-7.90 (4H, m, C_6H_4); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 22.61 (CH_3, *t*Bu), 29.91 ($\underline{C}H_2$-C=N), 31.76 ($\underline{C}H_2$-CH_2Cl), 44.77 (CH_2Cl), 55.39 (OMe), 57.44 (C_q, *t*Bu), 113.95 (CH, Ar), 129.43 (CH, Ar), 129.89 ($\underline{C}_q$-C=N, Ar), 162.59 ($\underline{C}_q$-OMe, Ar), 177.51 (C=N); ***m/z* (ESI)** 316.3/318.3 ($[M+H]^+$, 100%); **$[\alpha]_D$** = +46.2 (*c* 0.95, CH_2Cl_2).

(S_S)-*N*-[4-Chloro-1-(4-methoxyphenyl)butylidene]-*tert*-butanesulfinamide 1d (68%)

$[\alpha]_D$ = -54.6 (*c* 1.02, CH_2Cl_2).

Typical procedure for the synthesis of *N*-[1-aryl-4-chlorobutyl]-*tert*-butanesulfinamides (R_S,*R*)-2a-d and (R_S,*S*)-2a-d

As a representative example, the synthesis of *N*-[4-chloro-1-phenylbutyl]-*tert*-butanesulfinamides **(R_S,*R*)-2a** and **(R_S,*S*)-2a** is described here**.** (R_S)-*N*-[4-chloro-1-phenylbutylidene]-*tert*-

butanesulfinamide **1a** (1.45 g, 5.08 mmol) was dissolved in tetrahydrofuran (10 mL) and cooled to -78 °C. To the stirred solution was then added MeOH (0.33 g, 10.16 mmol) and $NaBH_4$ (0.38 g, 10.16 mmol). The reaction was stirred for one hour at -78 °C before quenching with $NaHCO_3$ (15 mL) and EtOAc (15 mL). The reaction mixture was filtered and the filtrate was extracted three times with EtOAc (20 mL). The combined organic layers were dried ($MgSO_4$), filtered and concentrated to furnish a mixture of *N*-[4-chloro-1-phenylbutyl]-*tert*-butanesulfinamides (R_S,R)-**2a** and (R_S,S)-**2a** in a diastereomeric ratio of 74:26. The two diastereomers were separated via column chromatography (petroleum ether/EtOAc 3/2 + 2% Et_3N) in 53% yield for (R_S,R)-**2a** (0.77 g) and 26% yield for (R_S,S)-**2a** (0.38 g). **(R_S,R)-2a**: White crystals; **Chromatography:** petroleum ether/EtOAc 3/2 + 2% Et_3N R_f = 0.16; **Melting point:** 59.2 °C - 60.2 °C; **Elemental analysis (%):** Found: C, 58.12; H, 7.87; N, 4.63. $C_{14}H_{22}ClNOS$ requires C, 58.42; H, 7.70; N, 4.87; **IR: ν_{max}/cm^{-1}** 3214, 2957, 1454, 1363, 1054; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.24 (9H, s, *t*Bu), 1.52-1.82 (2H, m, C<u>H</u>$_2$CH_2Cl), 1.85-1.97 and 2.11-2.23 (2H, m, CHC<u>H</u>$_2$), 3.40 (1H, d, J = 3.3 Hz, NH), 3.48 (2H, t, J = 6.3 Hz, CH_2Cl), 4.38 (1H, d x d x d, J = 8.5 Hz, J = 5.2 Hz, J = 3.3 Hz, C<u>H</u>NH), 7.28-7.39 (5H, m, C_6H_5); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 22.58 (CH_3, *t*Bu), 28.73 (<u>C</u>H_2-CH_2Cl), 33.88 (<u>C</u>H_2-CH), 44.63 (CH_2Cl), 55.70 (C_q, *t*Bu), 58.35 (CH-NH), 127.02 (CH, Ar), 127.93 (CH, Ar), 128.73 (CH, Ar), 141.93 (C_q, Ar); ***m/z* (ESI)** 288.3/290.3 ($[M+H]^+$, 100%); **$[\alpha]_D$** = -56.3 (*c* 0.54, CH_2Cl_2).

(R_S,S)-2a: Pale yellow (off-white) crystals; **Chromatography:** petroleum ether/EtOAc 3/1 + 2% Et_3N R_f = 0.05; **Melting point:** 81.5 °C - 82.5 °C; **Elemental analysis (%):** Found: C, 58.20; H, 8.04; N, 4.56. $C_{14}H_{22}ClNOS$ requires C, 58.42; H, 7.70; N, 4.87; **IR: ν_{max}/cm^{-1}** 3197, 2924, 1451, 1366, 1028; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.18 (9H, s, *t*Bu), 1.55-2.04 (4H, m, CHC<u>H</u>$_2$C<u>H</u>$_2$CH_2Cl), 3.44 (1H, d_{br}, J = 2.8 Hz, NH), 3.49 (2H, t x d, J = 6.6 Hz, J = 1.7 Hz,

CH_2Cl), 4.39 (1H, d x d x d, *J* = 8.3 Hz, *J* = 6.1 Hz, *J* = 3.3 Hz, C<u>H</u>NH), 7.26-7.37 (5H, m, C_6H_5); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 22.52 (CH_3, *t*Bu), 28.95 (<u>C</u>H_2-CH_2Cl), 35.86 (<u>C</u>H_2-CH), 44.55 (CH_2Cl), 55.56 (C_q, *t*Bu), 58.77 (CH-NH), 127.55 (CH, Ar), 127.84 (CH, Ar), 128.60 (CH, Ar), 141.35 (C_q, Ar); ***m/z* (ESI)** 288.3/290.3 ($[M+H]^+$, 100%); **$[\alpha]_D$** = -98.9 (*c* 0.69, CH_2Cl_2).

(*R*$_S$,*R*)-*N*-[4-Chloro-1-(4-methylphenyl)butyl]-*tert*-butanesulfinamide 2b (41%)

Orange oil; **Chromatography:** petroleum ether/EtOAc 17/3 + 2% Et_3N R_f = 0.07; **Elemental analysis (%):** Found: C, 59.61; H, 8.14; N, 4.56. $C_{15}H_{24}ClNOS$ requires C, 59.68; H, 8.01; N, 4.64; **IR: ν_{max}/cm^{-1}** 3218, 2955, 1455, 1362, 1054; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.23 (9H, s, *t*Bu), 1.52-1.67 and 1.68-1.79 (2H, m, C<u>H</u>$_2$$CH_2Cl$), 1.81-1.94 and 2.10-2.21 (2H, m, CHC<u>H</u>$_2$), 2.34 (3H, s, CH_3-Ar), 3.36 (1H, s_{br}, NH), 3.48 (2H, t, *J* = 6.6 Hz, CH_2Cl), 4.34 (1H, d x d, *J* = 8.3 Hz, *J* = 5.5 Hz, C<u>H</u>NH), 7.14-7.22 (4H, m, C_6H_4); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 21.12 (CH_3, CH_3-Ar), 22.63 (CH_3, *t*Bu), 28.84 (<u>C</u>H_2-CH_2Cl), 33.76 (<u>C</u>H_2-CH), 44.71 (CH_2Cl), 55.70 (C_q, *t*Bu), 58.17 (CH-NH), 127.02 (CH, Ar), 129.52 (CH, Ar), 137.81 (C_q, Ar), 138.88 (C_q, Ar); ***m/z* (ESI)** 302.3/304.3 ($[M+H]^+$, 100%); **$[\alpha]_D$** = -51.0 (*c* 1.11, CH_2Cl_2).

(*R*$_S$,*S*)-*N*-[4-Chloro-1-(4-methylphenyl)butyl]-*tert*-butanesulfinamide 2b (11%)

Pale yellow crystals (off-white); **Elemental analysis (%):** Found: C, 59.58; H, 8.12; N, 4.50. $C_{15}H_{24}ClNOS$ requires C, 59.68; H, 8.01; N, 4.64; **Chromatography:** petroleum ether/EtOAc 17/3 + 2% Et_3N R_f = 0.02; **Melting point:** 59.9 °C - 60.9 °C; **IR: ν_{max}/cm^{-1}** 3140, 2922, 1458, 1024; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.18 (9H, s, *t*Bu), 1.55-2.04 (4H, m, CHC<u>H</u>$_2$C<u>H</u>$_2$$CH_2Cl$), 2.35 (3H, s, CH_3-Ar), 3.39 (1H, d_{br}, *J* = 2.2 Hz, NH), 3.50 (2H, d x d x d, *J* = 6.9 Hz, *J* = 5.8 Hz, *J* = 1.1 Hz, CH_2Cl), 4.35 (1H, d x d x d, *J* = 8.3 Hz, *J* = 6.1 Hz, *J* = 2.2 Hz, C<u>H</u>NH), 7.13-7.20 (4H, m, C_6H_4); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 21.13 (CH_3, CH_3-Ar), 22.51 (CH_3, *t*Bu), 28.95

($\underline{C}H_2$-CH_2Cl), 35.85 ($\underline{C}H_2$-CH), 44.57 (CH_2Cl), 55.45 (C_q, *t*Bu), 58.43 (CH-NH), 127.44 (CH, Ar), 129.26 (CH, Ar), 137.43 (C_q, Ar), 138.22 (C_q, Ar); ***m/z* (ESI)** 302.3/304.3 ($[M+H]^+$, 100%); $[\alpha]_D$ = -91.6 (*c* 1.01, CH_2Cl_2).

(R_S,*R*)-*N*-[4-Chloro-1-(4-chlorophenyl)butyl]-*tert*-butanesulfinamide 2c (48%)

Orange oil; **Chromatography:** petroleum ether/EtOAc 1/1 + 2% Et_3N R_f = 0.27; **Elemental analysis (%):** Found: C, 51.88; H, 6.69; N, 4.53. $C_{14}H_{21}Cl_2NOS$ requires C, 52.17; H, 6.57; N, 4.35; **IR: ν_{max}/cm^{-1}** 3214, 2957, 1491, 1363, 1053; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.23 (9H, s, *t*Bu), 1.52-1.66 and 1.68-1.95 (3H, m, CHC$\underline{H}$(H)C$\underline{H}_2CH_2Cl$), 2.09-2.21 (1H, m, CHC$\underline{H}$(H)), 3.36 (1H, d, *J* = 3.9 Hz, NH), 3.49 (2H, t, *J* = 6.3 Hz, CH_2Cl), 4.35 (1H, d x d x d, *J* = 8.5 Hz, *J* = 5.2 Hz, *J* = 3.9 Hz, C$\underline{H}$NH), 7.25-7.28 and 7.32-7.36 (4H, m, C_6H_4); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 22.60 (CH_3, *t*Bu), 28.73 ($\underline{C}H_2$-CH_2Cl), 33.83 ($\underline{C}H_2$-CH), 44.57 (CH_2Cl), 55.91 (C_q, *t*Bu), 58.02 (CH-NH), 128.50 (CH, Ar), 129.03 (CH, Ar), 133.81 (C_q, Ar), 140.44 (C_q, Ar); ***m/z* (ESI)** 322.2/324.2/326.2 ($[M+H]^+$, 100%), 218.2/220.2/222.2 ($[M+H-t\text{BuS(O)}]^+$, 50%); $[\alpha]_D$ = -36.0 (*c* 1.08, CH_2Cl_2).

(R_S,*S*)-*N*-[4-Chloro-1-(4-chlorophenyl)butyl]-*tert*-butanesulfinamide 2c (17%)

Yellow crystals; **Chromatography:** petroleum ether/EtOAc 7/3 + 2% Et_3N R_f = 0.09; **Melting point:** 91.5 °C - 92.5 °C; **Elemental analysis (%):** Found: C, 52.03; H, 6.66; N, 4.29. $C_{14}H_{21}Cl_2NOS$ requires C, 52.17; H, 6.57; N, 4.35; **IR: ν_{max}/cm^{-1}** 3205, 2956, 1490, 1364, 1051; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.18 (9H, s, *t*Bu), 1.51-2.04 (4H, m, CHC$\underline{H}_2$C$\underline{H}_2CH_2Cl$), 3.43 (1H, d_{br}, *J* = 2.2 Hz, NH), 3.50 (2H, t, *J* = 6.3 Hz, CH_2Cl), 4.38 (1H, d x d x d, *J* = 8.0 Hz, *J* = 5.8 Hz, *J* = 2.2 Hz, C$\underline{H}$NH), 7.22-7.34 (4H, m, C_6H_4); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 22.51 (CH_3, *t*Bu), 28.83 ($\underline{C}H_2$-CH_2Cl), 35.76 ($\underline{C}H_2$-CH_2Cl), 44.43 (CH_2Cl), 55.62 (C_q, *t*Bu), 58.00 (CH-NH),

128.85 (CH, Ar), 128.97 (CH, Ar), 133.61 (C_q, Ar), 139.89 (C_q, Ar); ***m/z* (ESI)** 322.0/324.0/326.0 ($[M+H]^+$, 100%); $[\alpha]_D$ = -75.3 (*c* 0.97, CH_2Cl_2).

(*R*$_S$,*R*)-*N*-[4-Chloro-1-(4-methoxyphenyl)butyl]-*tert*-butanesulfinamide 2d (39%)

Viscous colorless oil; **Chromatography:** petroleum ether/EtOAc 1/1 + 2% Et_3N R_f = 0.17; **Elemental analysis (%):** Found: C, 56.61; H, 7.74; N, 4.53. $C_{15}H_{24}ClNO_2S$ requires C, 56.68; H, 7.61; N, 4.41; **IR: ν_{max}/cm^{-1}** 3218, 2955, 1513, 1362, 1052; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.23 (9H, s, *t*Bu), 1.51-1.93 (3H, m, CHC<u>H</u>(H)C<u>H</u>$_2$CH$_2$Cl), 2.10-2.21 (1H, m, CHC<u>H</u>(H)), 3.33 (1H, d, *J* = 3.3 Hz, NH), 3.48 (2H, t, *J* = 6.6 Hz, CH_2Cl), 3.81 (3H, s, OMe), 4.33 (1H, d x d x d, *J* = 8.3 Hz, *J* = 5.0 Hz, *J* = 3.3 Hz, C<u>H</u>NH), 6.87-6.91 and 7.22-7.26 (4H, m, C_6H_4); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 22.64 (CH_3, *t*Bu), 28.89 (<u>C</u>H$_2$-CH$_2$Cl), 33.77 (<u>C</u>H$_2$-CH), 44.74 (CH_2Cl), 55.29 (MeO), 55.68 (C_q, *t*Bu), 57.88 (CH-NH), 114.19 (CH, Ar), 128.28 (CH, Ar), 133.89 (<u>C</u>$_q$-CHN, Ar), 159.38 (<u>C</u>$_q$-OMe, Ar); ***m/z* (ESI)** 318.3/320.2 ($[M+H]^+$, 100%); $[\alpha]_D$ = -38.6 (*c* 1.03, CH_2Cl_2).

(*R*$_S$,*S*)-*N*-[4-Chloro-1-(4-methoxyphenyl)butyl]-*tert*-butanesulfinamide 2d (14%)

Yellow crystals; **Chromatography:** petroleum ether/EtOAc 7/3 + 2% Et_3N R_f = 0.06; **Melting point:** 77.3 °C - 78.3 °C; **Elemental analysis (%):** Found: C, 56.58; H, 7.44; N, 4.61. $C_{15}H_{24}ClNO_2S$ requires C, 56.68; H, 7.61; N, 4.41; **IR: ν_{max}/cm^{-1}** 3210, 2955, 1512, 1363, 1244, 1050; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.18 (9H, s, *t*Bu), 1.54-2.01 (4H, m, CHC<u>H</u>$_2$C<u>H</u>$_2$CH$_2$Cl), 3.37 (1H, d_{br}, *J* = 2.2 Hz, NH), 3.49 (2H, d x d x d, *J* = 6.3 Hz, *J* = 5.8 Hz, *J* = 1.1 Hz, CH_2Cl), 3.81 (3H, s, OMe), 4.34 (1H, d x d x d, *J* = 8.5 Hz, *J* = 5.8 Hz, *J* = 2.2 Hz, C<u>H</u>NH), 6.85-6.90 and 7.19-7.23 (4H, m, C_6H_4); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 22.52 (CH_3, *t*Bu), 28.98 (<u>C</u>H$_2$-CH$_2$Cl), 35.83 (<u>C</u>H$_2$-CH$_2$Cl), 44.58 (CH_2Cl), 55.19 (OMe), 55.42 (C_q, *t*Bu), 58.06 (CH-NH), 113.93 (CH,

Ar), 128.71 (CH, Ar), 133.11 ($\underline{C}_q$-CHN, Ar), 159.15 ($\underline{C}_q$-OMe, Ar); ***m/z* (ESI)** 318.3/320.2 ($[M+H]^+$, 100%); $[\alpha]_D$ = -89.2 (*c* 0.39, CH_2Cl_2).

Typical procedure for the synthesis of 2-aryl-1-(*tert*-butanesulfinyl)pyrrolidines (R_S,*R*)-3a-d

As a representative example, the synthesis of (R_S,*R*)-1-*tert*-butylsulfinyl-2-phenylpyrrolidine **3a** is described here**.** To a solution of (R_S,*R*)-*N*-[4-chloro-1-phenylbutyl]-*tert*-butanesulfinamide **2a** (0.35 g, 1.22 mmol) in a 1:1 mixture of H_2O/THF (10 mL) was added KOH (0.20 g, 3.65 mmol) and the reaction mixture was stirred for 24 hours at reflux temperature. After cooling to room temperature, a saturated solution of $NaHCO_3$ (10 mL) was added and the mixture was extracted with EtOAc (3 x 10 mL). The combined organic fractions were dried ($MgSO_4$), filtered and the solvent was removed under reduced pressure to afford (R_S,*R*)-1-*tert*-butylsulfinyl-2-phenylpyrrolidine **3a**, which was purified by recrystallisation from diethyl ether in 94% yield (0.29 g, 1.14 mmol), $[\alpha]_D$ = +124.0 (*c* 0.84, CH_2Cl_2). All ^{1}H-NMR data were in good agreement with reported data for (R_S,*R*)-1-*tert*-butylsulfinyl-2-phenylpyrrolidine **3a**, $[\alpha]_D$ = +108.8 (*c* 1.00, $CHCl_3$),[1] $[\alpha]_D$ = +141.2 (*c* 1.10, $CHCl_3$).[2]

(R_S,*R*)-1-*tert*-Butylsulfinyl-2-phenylpyrrolidine 3a (94%)

Pale yellow crystals; **Melting point:** 89.9 °C - 90.9 °C; **Elemental analysis (%):** Found: C, 66.68; H, 8.43; N, 5.77. $C_{14}H_{21}NOS$ requires C, 66.89; H, 8.42; N, 5.57; **IR:** ν_{max}**/cm^{-1}** 2924, 1448, 1057; δ_H **(300 MHz, $CDCl_3$, Me_4Si)** 1.05 (9H, s, *t*Bu), 1.71-1.94 (3H, m, CHC$\underline{H}$(H)C$\underline{H}_2$), 2.10-2.23 (1H, m, CHC$\underline{H}$(H)), 3.46-3.71 (2H, m, CH_2N), 5.08 (1H, d x d, *J* = 7.7 Hz, *J* = 2.8 Hz, CHN), 7.18-7.34 (5H, m, C_6H_5); δ_C **(75 MHz, $CDCl_3$, Me_4Si)** 23.10 (CH_3, *t*Bu), 24.18 ($\underline{C}H_2$-

[1] K. M., Brinner; J. A., Ellman, *Org. Biomol. Chem.* 2005, **3**, 2109.
[2] L. R. Reddy, M. Prashad, *Chem. Commun.*, 2010, DOI: 10.1039/b917435d.

CH_2N), 36.66 ($\underline{C}H_2$-CH), 54.98 (CH_2N), 57.47 (CHN), 57.47 (C_q, *t*Bu), 126.51 (CH, Ar), 126.56 (CH, Ar), 128.36 (CH, Ar), 144.65 (C_q, Ar); ***m/z* (ESI)** 252.2 ($[M+H]^+$, 100%); $[\alpha]_D$ = +124.0 (*c* 0.84, CH_2Cl_2).

(R_S,*R*)-1-*tert*-Butylsulfinyl-2-(4-methylphenyl)pyrrolidine 3b (85%)

Yellow crystals; **Melting point:** 116.2 °C - 117.2 °C; **Elemental analysis (%):** Found: C, 67.79; H, 8.85; N, 5.31. $C_{15}H_{23}NOS$ requires C, 67.88; H, 8.73; N, 5.28; **IR:** ν_{max}/cm^{-1} 2949, 1454, 1362, 1057; δ_H **(300 MHz, $CDCl_3$, Me_4Si)** 1.06 (9H, s, *t*Bu), 1.69-1.92 (3H, m, CHC$\underline{H}$(H)C$\underline{H}_2$), 2.07-2.19 (1H, m, CHC$\underline{H}$(H)), 2.33 (3H, s, CH_3-Ar), 3.45-3.70 (2H, m, CH_2N), 5.04 (1H, d x d, *J* = 8.3 Hz, *J* = 2.2 Hz, CHN), 7.07-7.19 (4H, m, C_6H_4); δ_C **(75 MHz, $CDCl_3$, Me_4Si)** 21.05 (CH_3, CH_3-Ar), 23.16 (CH_3, *t*Bu), 24.12 ($\underline{C}H_2$-CH_2N), 36.69 ($\underline{C}H_2$-CH), 54.68 (CH_2N), 57.45 (CHN), 57.45 (C_q, *t*Bu), 126.45 (CH, Ar), 129.05 (CH, Ar), 136.12 (C_q, Ar), 141.60 (C_q, Ar); ***m/z* (ESI)** 266.2 ($[M+H]^+$, 100%); $[\alpha]_D$ = +145.4 (*c* 0.99, CH_2Cl_2).

(R_S,*R*)-1-*tert*-Butylsulfinyl-2-(4-chlorophenyl)pyrrolidine 3c (91%)

White crystals; **Melting point:** 108.8 °C - 109.8 °C; **Elemental analysis (%):** Found: C, 58.61; H, 7.32; N, 4.97. $C_{14}H_{20}ClNOS$ requires C, 58.83; H, 7.05; N, 4.90; **IR:** ν_{max}/cm^{-1} 2962, 1489, 1364, 1057; δ_H **(300 MHz, $CDCl_3$, Me_4Si)** 1.05 (9H, s, *t*Bu), 1.67-1.99 (3H, m, CHC$\underline{H}$(H)C$\underline{H}_2$), 2.10-2.21 (1H, m, CHC$\underline{H}$(H)), 3.51-3.68 (2H, m, CH_2N), 5.04 (1H, d x d, *J* = 7.7 Hz, *J* = 2.2 Hz, CHN), 7.17-7.30 (4H, m, C_6H_4); δ_C **(75 MHz, $CDCl_3$, Me_4Si)** 23.07 (CH_3, *t*Bu), 24.17 ($\underline{C}H_2$-CH_2N), 36.57 ($\underline{C}H_2$-CH), 54.93 (CH_2N), 56.87 (CHN), 57.50 (C_q, *t*Bu), 127.92 (CH, Ar), 128.56 (CH, Ar), 132.30 (C_q, Ar), 143.26 (C_q, Ar); ***m/z* (ESI)** 286.2/288.3 ($[M+H]^+$, 100%); $[\alpha]_D$ = +161.3 (*c* 0.73, CH_2Cl_2).

(R_S,*R*)-1-*tert*-Butylsulfinyl-2-(4-methoxyphenyl)pyrrolidine 3d (87%)

All ^{1}H-NMR data were in good agreement with reported data for (R_S,*R*)-1-*tert*-butylsulfinyl-2-phenylpyrrolidine **3a**, $[\alpha]_D$ = +139.98 (*c* 1.13, MeOH).[2]

Yellow crystals; **Melting point:** 89.6 °C - 90.6 °C; **Elemental analysis (%):** Found: C, 64.15; H, 8.23; N, 4.71. $C_{15}H_{23}NO_2S$ requires C, 64.02; H, 8.24; N, 4.98; **IR:** ν_{max}**/cm^{-1}** 2862, 1607, 1509, 1357, 1054; δ_H **(300 MHz, $CDCl_3$, Me_4Si)** 1.06 (9H, s, *t*Bu), 1.68-1.94 (3H, m, CHC<u>H</u>(H)C<u>H</u>$_2$), 2.07-2.18 (1H, m, CHC<u>H</u>(H)), 3.47-3.56 and 3.63-3.70 (2H, m, CH_2N), 3.80 (3H, s, OMe), 5.00 (1H, d x d, *J* = 8.0 Hz, *J* = 2.5 Hz, CHN), 6.83-6.87 and 7.14-7.18 (4H, m, C_6H_4); δ_C **(75 MHz, $CDCl_3$, Me_4Si)** 23.16 (CH_3, *t*Bu), 24.14 (<u>C</u>H$_2$-CH_2N), 36.66 (<u>C</u>H$_2$-CH), 54.34 (CH_2N), 55.21 (MeO), 57.35 (CHN), 57.44 (C_q, *t*Bu), 113.70 (CH, Ar), 127.64 (CH, Ar), 136.66 (<u>C</u>$_q$-CHN, Ar), 158.25 (<u>C</u>$_q$-OMe, Ar); ***m/z*** **(ESI)** 282.3 ([M+H]$^+$, 100%), 176.2 ((M+H$^+$)-*t*BuS(O), 10%); $[\alpha]_D$ = +148.0 (*c* 1.02, CH_2Cl_2).

Typical procedure for the synthesis of 2-aryl-1-(*tert*-butanesulfinyl)pyrrolidines (R_S,*S*)-3a-d and (S_S,*R*)-3a-d

As a representative example, the synthesis of (S_S,*R*)-1-(*tert*-butanesulfinyl)-2-phenylpyrrolidine **3a** is described here**.** To a solution of (S_S)-*N*-[4-chloro-1-phenylbutylidene]-*tert*-butanesulfinamide **1a** (1.53 g, 5.36 mmol) in tetrahydrofuran (20 mL) at -78 °C was added $LiBEt_3H$ (5.90 mL, 1 M solution in THF, 5.90 mmol). The reaction was stirred at -78 °C for one hour, subsequently allowed to warm up to room temperature and stirred for 20 hours. The reaction was quenched by adding a saturated solution of $NaHCO_3$ (15 mL) and filtered. The mixture was extracted with EtOAc (3 x 20 mL) and the combined organic fractions were dried ($MgSO_4$), filtered and the solvent was removed under reduced pressure to afford (S_S,*R*)-1-(*tert*-

butanesulfinyl)-2-phenylpyrrolidine **3a** (1.31 g) in 97% yield. Purification by means of column chromatography (petroleum ether/EtOAc 4/1) yielded (S_S,R)-**3a** (1.10 g) in 82% as a yellow viscous oil. $[\alpha]_D$ = +122.2 (*c* 1.02, CH_2Cl_2). All spectroscopic data were in good agreement with reported data for (S_S,R)-**3a**, $[\alpha]_D$ = +93.6 (*c* 0.99, $CHCl_3$).[1]

(R_S,S)-1-*tert*-Butylsulfinyl-2-phenylpyrrolidine 3a (91%)

Yellow viscous oil; **Chromatography:** petroleum ether/EtOAc 3/1 + 2% Et_3N R_f = 0.10; **Elemental analysis (%):** Found: C, 66.74; H, 8.53; N, 5.51. $C_{14}H_{21}NOS$ requires C, 66.89; H, 8.42; N, 5.57; **IR: ν_{max}/cm^{-1}** 3464, 2961, 1454, 1362, 1059; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.09 (9H, s, *t*Bu), 1.72-2.01 (3H, m, CHC<u>H</u>(H)C<u>H</u>$_2$), 2.18-2.29 (1H, m, CHC<u>H</u>(H)), 2.93-3.01 (1H, m, C<u>H</u>(H)N), 3.86-3.93 (1H, m, C<u>H</u>(H)N), 4.63 (1H, d x d, *J* = 7.7 Hz, *J* = 7.2 Hz, CHN), 7.19-7.35 (5H, m, C_6H_5); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 23.74 (CH_3, *t*Bu), 26.31 (<u>C</u>H$_2$-CH_2N), 35.93 (<u>C</u>H$_2$-CH), 42.03 (CH_2N), 57.06 (C_q, *t*Bu), 69.26 (CHN), 127.15 (CH, Ar), 128.22 (CH, Ar), 143.17 (C_q, Ar); ***m/z* (ESI)** 252.2 ([M+H]$^+$, 100%); $[\alpha]_D$ = -135.4 (*c* 0.60, CH_2Cl_2).

(R_S,S)-1-*tert*-Butylsulfinyl-2-(4-methylphenyl)pyrrolidine 3b (87%)

White crystals; **Chromatography:** petroleum ether/EtOAc 3/1 + 2% Et_3N, R_f = 0.14; **Melting point:** 68.1 °C - 69.1 °C; **Elemental analysis (%):** Found: C, 67.73; H, 8.82; N, 5.33. $C_{15}H_{23}NOS$ requires C, 67.88; H, 8.73; N, 5.28; **IR: ν_{max}/cm^{-1}** 2968, 1455, 1364, 1056; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.10 (9H, s, *t*Bu), 1.17-2.03 (3H, m, CHC<u>H</u>(H)C<u>H</u>$_2$), 2.17-2.25 (1H, m, CHC<u>H</u>(H)), 2.33 (3H, s, Me), 2.97 (1H, d x d x d, *J* = 10.5 Hz, *J* = 8.3 Hz, *J* = 6.6 Hz, C<u>H</u>(H)N), 3.88 (1H, d x d x d, *J* = 10.5 Hz, *J* = 8.3 Hz, *J* = 3.9 Hz, C<u>H</u>(H)N), 4.60 (1H, d x d, *J* = 7.7 Hz, *J* = 6.6 Hz, CHN), 7.12 and 7.18 (2 x 2H, 2 x d, *J* = 8.3 Hz, C_6H_4); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 21.07 (CH_3, CH_3-Ar), 23.82 (CH_3, *t*Bu), 26.31 (<u>C</u>H$_2$-CH_2N), 36.02 (<u>C</u>H$_2$-CH), 42.00 (CH_2N),

57.09 (C_q, *t*Bu), 69.00 (CHN), 127.12 (CH, Ar), 128.95 (CH, Ar), 136.74 (C_q, Ar), 140.13 (C_q, Ar); ***m/z* (ESI)** 266.2 ($[M+H]^+$, 100%), 160.5 (M-(*t*BuS(O))+H^+, 60%); $[\alpha]_D$ = -129.0 (*c* 0.48, CH_2Cl_2).

(S_S,*R*)-1-*tert*-Butylsulfinyl-2-(4-methylphenyl)pyrrolidine 3b (86%)

$[\alpha]_D$ = +141.4 (*c* 1.01, CH_2Cl_2).

(R_S,*S*)-1-*tert*-Butylsulfinyl-2-(4-chlorophenyl)pyrrolidine 3c (92%)

Yellow crystals; **Chromatography:** petroleum ether/EtOAc 7/3 + 2% Et_3N R_f = 0.12; **Melting point:** 74.3 °C - 75.3 °C; **Elemental analysis (%):** Found: C, 59.02; H, 6.84; N, 5.03. $C_{14}H_{20}ClNOS$ requires C, 58.83; H, 7.05; N, 4.90; **IR:** ν_{max}/cm^{-1} 2923, 1490, 1361, 1060; δ_H **(300 MHz, $CDCl_3$, Me_4Si)** 1.10 (9H, s, *t*Bu), 1.71-2.05 (3H, m, CHC<u>H</u>(H)C<u>H</u>$_2$), 2.20-2.29 (1H, m, CHC<u>H</u>(H)), 2.97 (1H, d x d x d, *J* = 10.2 Hz, *J* = 8.3 Hz, *J* = 6.6 Hz, C<u>H</u>(H)N), 3.89 (1H, d x d x d, *J* = 10.5 Hz, *J* = 8.3 Hz, *J* = 4.4 Hz, C<u>H</u>(H)N), 4.60 (1H, d x d, *J* = 8.3 Hz, *J* = 6.6 Hz, CHN), 7.21-7.31 (4H, m, C_6H_4); δ_C **(75 MHz, $CDCl_3$, Me_4Si)** 23.82 (CH_3, *t*Bu), 26.34 (<u>C</u>H_2-CH_2N), 36.02 (<u>C</u>H_2-CH), 42.11 (CH_2N), 57.22 (C_q, *t*Bu), 68.63 (CHN), 128.48 (CH, Ar), 128.62 (CH, Ar), 132.89 (C_q, Ar), 141.83 (C_q, Ar); ***m/z* (ESI)** 286.2/288.3 ($[M+H]^+$, 100%); $[\alpha]_D$ = -134.3 (*c* 1.05, CH_2Cl_2).

(S_S,*R*)-1-*tert*-Butylsulfinyl-2-(4-chlorophenyl)pyrrolidine 3c (91%)

$[\alpha]_D$ = +110.6 (*c* 1.00, CH_2Cl_2).

(R_S,*S*)-1-*tert*-Butylsulfinyl-2-(4-methoxyphenyl)pyrrolidine 3d (85%)

Yellow crystals; **Chromatography:** petroleum ether/EtOAc 7/3 + 2% Et_3N R_f = 0.12; **Melting point:** 61.2 °C - 62.2 °C; **Elemental analysis (%):** Found: C, 64.09; H, 8.32; N, 4.69.

$C_{15}H_{23}NO_2S$ requires C, 64.02; H, 8.24; N, 4.98; **IR: ν_{max}/cm^{-1}** 2963, 1509, 1364, 1244, 1053; **δ_H (300 MHz, $CDCl_3$, Me_4Si)** 1.09 (9H, s, *t*Bu), 1.17-2.05 and 2.17-2.27 (4H, m, CHC$\underline{H}_2$C$\underline{H}_2$), 2.96 (1H, d x d x d, *J* = 9.9 Hz, *J* = 8.3 Hz, *J* = 6.6 Hz, C$\underline{H}$(H)N), 3.80 (3H, s, OMe), 3.87 (1H, d x d x d, *J* = 10.5 Hz, *J* = 8.3 Hz, *J* = 3.9 Hz, C$\underline{H}$(H)N), 4.58 (1H, d x d, *J* = 8.3 Hz, *J* = 6.6 Hz, CHN), 6.83-6.88 and 7.19-7.29 (2 x 2H, 2 x m, C_6H_4); **δ_C (75 MHz, $CDCl_3$, Me_4Si)** 23.83 (CH_3, *t*Bu), 26.32 ($\underline{C}H_2$-CH_2N), 35.93 ($\underline{C}H_2$-CH), 41.93 (CH_2N), 55.21 (OMe), 57.09 (C_q, *t*Bu), 68.65 (CHN), 113.63 (CH, Ar), 128.40 (CH, Ar), 135.11 ($\underline{C}_q$-CHN, Ar), 158.79 ($\underline{C}_q$-OMe, Ar); ***m/z* (ESI)** 282.3 ($[M+H]^+$, 65%), 176.2 ($[M-t\text{BuS(O)}+H]^+$, 100%); **$[\alpha]_D$** = -123.9 (*c* 1.05, CH_2Cl_2).

(*S*$_S$,*R*)-1-*tert*-Butylsulfinyl-2-(4-methoxyphenyl)pyrrolidine 3d (85%)

$[\alpha]_D$ = +131.2 (*c* 1.01, CH_2Cl_2).

Typical procedure for the synthesis of 2-arylpyrrolidine hydrochlorides (*S*)-4a-d and (*R*)-4a-d

As a representative example, the synthesis of (*S*)-2-(4-methoxyphenyl)pyrrolidine hydrochloride **4d** is described here**.** To a solution of (*R*$_S$,*S*)-1-(*tert*-butanesulfinyl)-2-(4-methoxyphenyl)pyrrolidine **3d** (0.17 g, 0.60 mmol) in dioxane (10 mL) was added dropwise a freshly prepared saturated solution of dioxane/HCl (1.5 mL, ~4 M solution, 6.05 mmol) under stirring. The mixture was allowed to stir for one hour at room temperature and then concentrated in vacuo. (*S*)-2-(4-Methoxyphenyl)pyrrolidine hydrochloride **4d** was obtained after precipitation in diethyl ether in 91% yield as white crystals. **Melting point:** 158.5 °C - 159.5 °C; **Elemental analysis (%):** Found: C, 61.54; H, 7.89; N, 6.26. $C_{11}H_{16}ClNO$ requires: C, 61.82; H, 7.55; N, 6.55; **IR: ν_{max}/cm^{-1}** 2851, 1514, 1250; **δ_H (300 MHz, D_2O)** 2.07-2.29 and 2.35-2.48 (4H, m, CHC$\underline{H}_2$C$\underline{H}_2$), 3.35-3.49 (2H, m, CH_2N), 3.82 (3H, s, OMe), 4.61 (1H, d x d, *J* = 9.4 Hz, *J* = 7.2

Hz, CHN), 7.00-7.06 and 7.39-7.44 (2 x 2H, 2 x m, C_6H_4); **δ_C (75 MHz, D_2O, MeCN)** 24.10 ($\underline{C}H_2$-CH_2N), 30.57 ($\underline{C}H_2$-CH), 45.76 (CH_2N), 56.02 (OMe), 63.46 (CHN), 115.20 (CH, Ar), 127.36 (C_q, Ar), 129.75 (CH, Ar), 160.21 (C_q, Ar); ***m/z* (ESI)** 178.2 ($[M\text{-}HCl+H]^+$, 100%); **$[\alpha]_D$** = +9.8 (*c* 1.05, EtOH).

(*R*)-2-(4-Methoxyphenyl)pyrrolidine hydrochloride 4d (99%)

$[\alpha]_D$ = -12.4 (*c* 1.01, MeOH). All spectroscopic data were in good agreement with reported data for (*R*)-2-(4-methoxyphenyl)pyrrolidine hydrochloride **4d**, **$[\alpha]_D$** = -14.3 (c 0.98, MeOH).[3]

(*S*)-2-Phenylpyrrolidine hydrochloride 4a (84%)

$[\alpha]_D$ = +12.8 (*c* 1.00, MeOH).

(*R*)-2-Phenylpyrrolidine hydrochloride 4a (88%)

$[\alpha]_D$ = -9.3 (*c* 1.01, MeOH). All spectroscopic data were in good agreement with reported data for (*R*)-**4a**, **$[\alpha]_D$** = -9.1 (c 1.00, MeOH).[1]

(*S*)-2-(4-Methylphenyl)pyrrolidine hydrochloride 4b (81%)

Viscous orange oil; **Elemental analysis (%):** Found: C, 66.63; H, 8.21; N, 7.15. $C_{11}H_{16}ClN$ requires: C, 66.83; H, 8.16; N, 7.08; **IR: ν_{max}/cm^{-1}** 3396, 2918, 1454, 1022; **δ_H (300 MHz, D_2O)** 2.10-2.28 and 2.38-2.47 (4H, m, CHC$\underline{H}_2$C$\underline{H}_2$), 2.34 (3H, s, Me), 3.41-3.47 (2H, m, CH_2N), 4.62 (1H, d x d, *J* = 9.4 Hz, *J* = 7.2 Hz, CHN), 7.30-7.38 (2 x 2H, 2 x m, C_6H_4); **δ_C (75 MHz, D_2O, MeCN)** 20.83 (CH_3, CH_3-Ar), 24.08 ($\underline{C}H_2$-CH_2N), 30.68 ($\underline{C}H_2$-CH), 45.87 (CH_2N), 63.67

[3] (a) K. Higashiyama, I. Hiroaki, H. Takahashi, *Tetrahedron,* 1994, **50**, 1083. (b) M. Yus, T. Soler, F. Foubelo, *J. Org. Chem.,* 2001, **66**, 6207.

(CHN), 128.07 (CH, Ar), 130.39 (CH, Ar), 132.00 (C_q, Ar), 140.59 (C_q, Ar); ***m/z* (ESI)** 162.2 ($[M\text{-}HCl+H]^+$, 100%); $[\alpha]_D$ = +12.9 (*c* 0.65, MeOH).

(*R*)-2-(4-Methylphenyl)pyrrolidine hydrochloride 4b (99%)

$[\alpha]_D$ = -11.8 (*c* 0.78, MeOH).

(*S*)-2-(4-Chlorophenyl)pyrrolidine hydrochloride 4c (87%)

Viscous orange oil; **Elemental analysis (%):** Found: C, 54.93; H, 6.17; N, 6.33. $C_{10}H_{13}Cl_2N$ requires: C, 55.06; H, 6.01; N, 6.42; **IR:** ν_{max}/cm^{-1} 2910, 1496, 1014; δ_H **(300 MHz, D_2O)** 2.12-2.32 and 2.43-2.54 (4H, m, $CHC\underline{H}_2C\underline{H}_2$), 3.42-3.51 (2H, m, CH_2N), 4.68 (1H, d x d, *J* = 8.8 Hz, *J* = 7.2 Hz, CHN), 7.43-7.53 (2 x 2H, 2 x m, C_6H_4); δ_C **(75 MHz, D_2O, MeCN)** 24.07 ($\underline{C}H_2$-CH_2N), 30.65 ($\underline{C}H_2$-CH), 46.01 (CH_2N), 63.15 (CHN), 129.71 (CH, Ar), 129.83 (CH, Ar), 133.69 (C_q, Ar), 135.39 (C_q, Ar); ***m/z* (ESI)** 182.3/184.2 ($[M\text{-}HCl+H]^+$, 100%); $[\alpha]_D$ = +7.7 (*c* 0.98, MeOH).

(*R*)-2-(4-Chlorophenyl)pyrrolidine hydrochloride 4c (99%)

$[\alpha]_D$ = -8.6 (*c* 1.00, MeOH).

Typical procedure for the synthesis of 2-arylpyrrolidines (*S*)-5a-d and (*R*)-5a-d

As a representative example, the synthesis of (*S*)-2-(4-methoxyphenyl)pyrrolidine **5d** is described here**.** To a suspension of (*S*)-2-(4-methoxyphenyl)pyrrolidine hydrochloride **4d** (0.050 g, 0.23 mmol) in diethyl ether (5 mL) was added a saturated solution of sodium bicarbonate (5 mL) and the resulting mixture was stirred for ten minutes at room temperature. Subsequently the mixture

was extracted three times with diethyl ether (3 x 5 mL) and the combined organic fractions were dried ($MgSO_4$), filtered and the solvent was removed under reduced pressure to afford (*S*)-2-(4-methoxyphenyl)pyrrolidine **5d** (0.04 g, 0.23 mmol) as a yellow liquid in quantitative yield without further purification. All spectroscopic data were in good agreement with reported data for racemic 2-(4-methoxyphenyl)pyrrolidine **5d**,[3b] (*S*)-**5d**: $[\alpha]_D$ = -25.6 (*c* 0.89, MeOH).

(*R*)-2-(4-Methoxyphenyl)pyrrolidine 5d (99%)

$[\alpha]_D$ = +23.4 (*c* 0.75, MeOH).

(*R*)-2-Phenylpyrrolidine 5a (99%)

$[\alpha]_D$ = +29.7 (*c* 0.32, MeOH). All spectroscopic data were in good agreement with reported data for (*R*)-**5a**, $[\alpha]_D$ = +24.3 (c 0.30, MeOH) for an enantiomeric excess of 75%,[4] and $[\alpha]_D$ = +64.2 (c 1.02, CH_2Cl_2).[2]

(*S*)-2-Phenylpyrrolidine 5a (99%)

$[\alpha]_D$ = -27.9 (*c* 0.38, MeOH). All spectroscopic data were in good agreement with reported data for (*S*)-**5a**, $[\alpha]_D$ = -22 (c 0.30, MeOH),[4,5] and $[\alpha]_D$ = -64.4 (c 1.02, CH_2Cl_2).[2]

(*S*)-2-(4-Methylphenyl)pyrrolidine 5b (99%)[6]

$[\alpha]_D$ = -37.1 (*c* 0.38, MeOH).

[4] B. E. Maryanoff, D. F. McComsey, *J. Heterocycl. Chem.,* 1985, **22**, 911.
[5] (a) F. Morlacchi, V. Losacco, V. Tortorella, *Gazz. Chim. Ital.,* 1975, **105**, 349. (b) F. Morlacchi, V. Losacco, *J. Heterocycl. Chem.,* 1976, **13**, 165. (c) A. I. Meyers, L. E. Burgess, *J. Org. Chem.,* 1991, **56**, 2294. (d) L. E. Burgess, A. I. Meyers, *J. Org. Chem.,* 1992, **57**, 1656.
[6] (a) T. Severin, H. Poehlmann, *Chem. Ber.,* 1977, **110**, 491. (b) N. Viswanathan, A. R. Sidhaye, *Tetrahedron Lett.,* 1979, **52**, 5025.

(*R*)-2-(4-Methylphenyl)pyrrolidine 5b (99%)

$[\alpha]_D$ = +35.3 (*c* 0.20, MeOH).

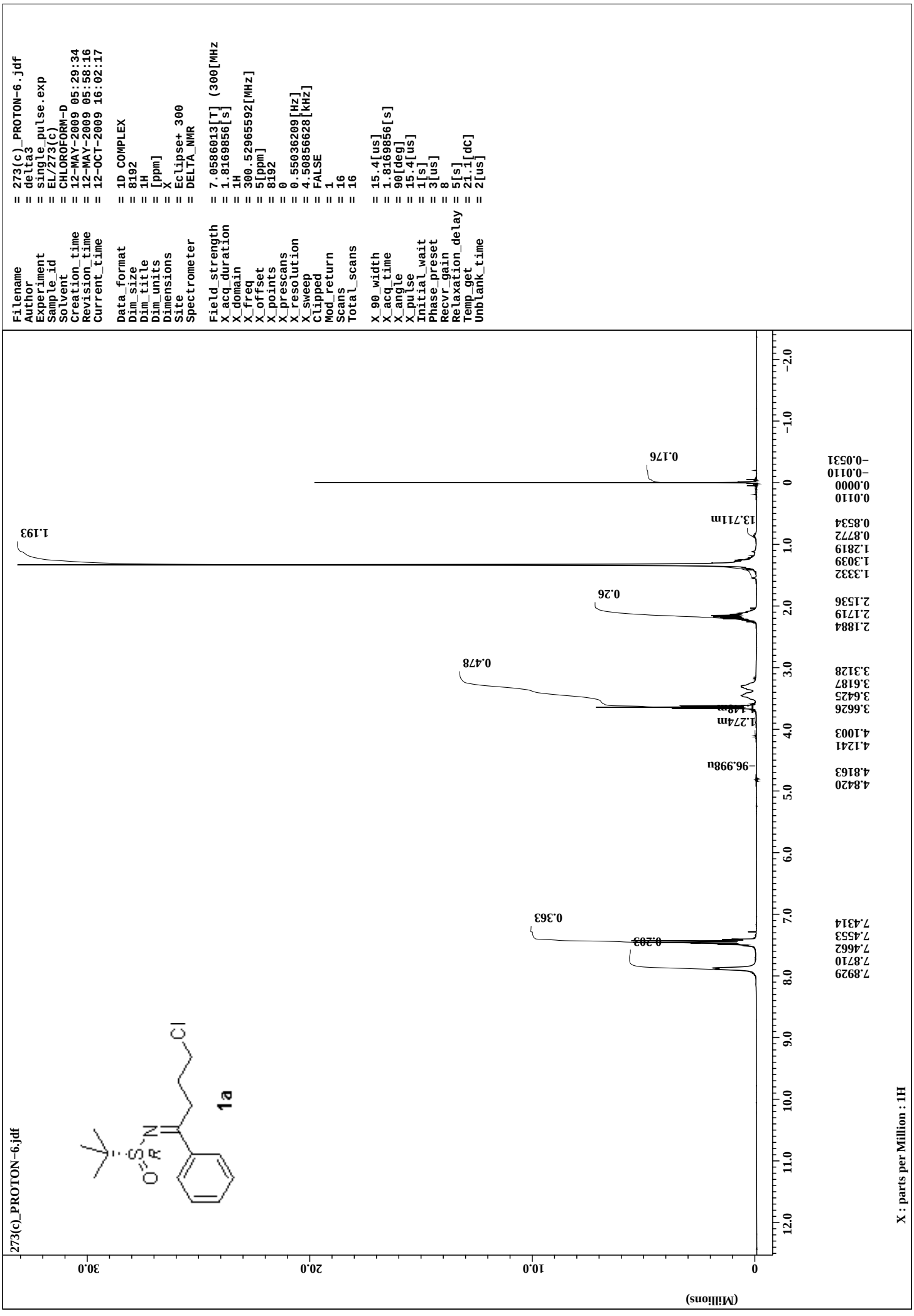
(*R*)-2-(4-Chlorophenyl)pyrrolidine 5c (99%)

$[\alpha]_D$ = +53.2 (*c* 0.99, MeOH). All spectroscopic data were in good agreement with reported data for racemic 2-(4-chlorophenyl)pyrrolidine **5c**.[7]

***(S)*-2-(4-Chlorophenyl)pyrrolidine 5c** (99%)

$[\alpha]_D$ = -48.2 (*c* 0.24, MeOH).

[7] C. J. Rogers, T. J. Dickerson, A. P. Brogan, K. D. Janda, *J. Org. Chem.,* 2005, **70**, 3705.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X_pulse = 15.4[us]
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Phase_preset = 3[us]
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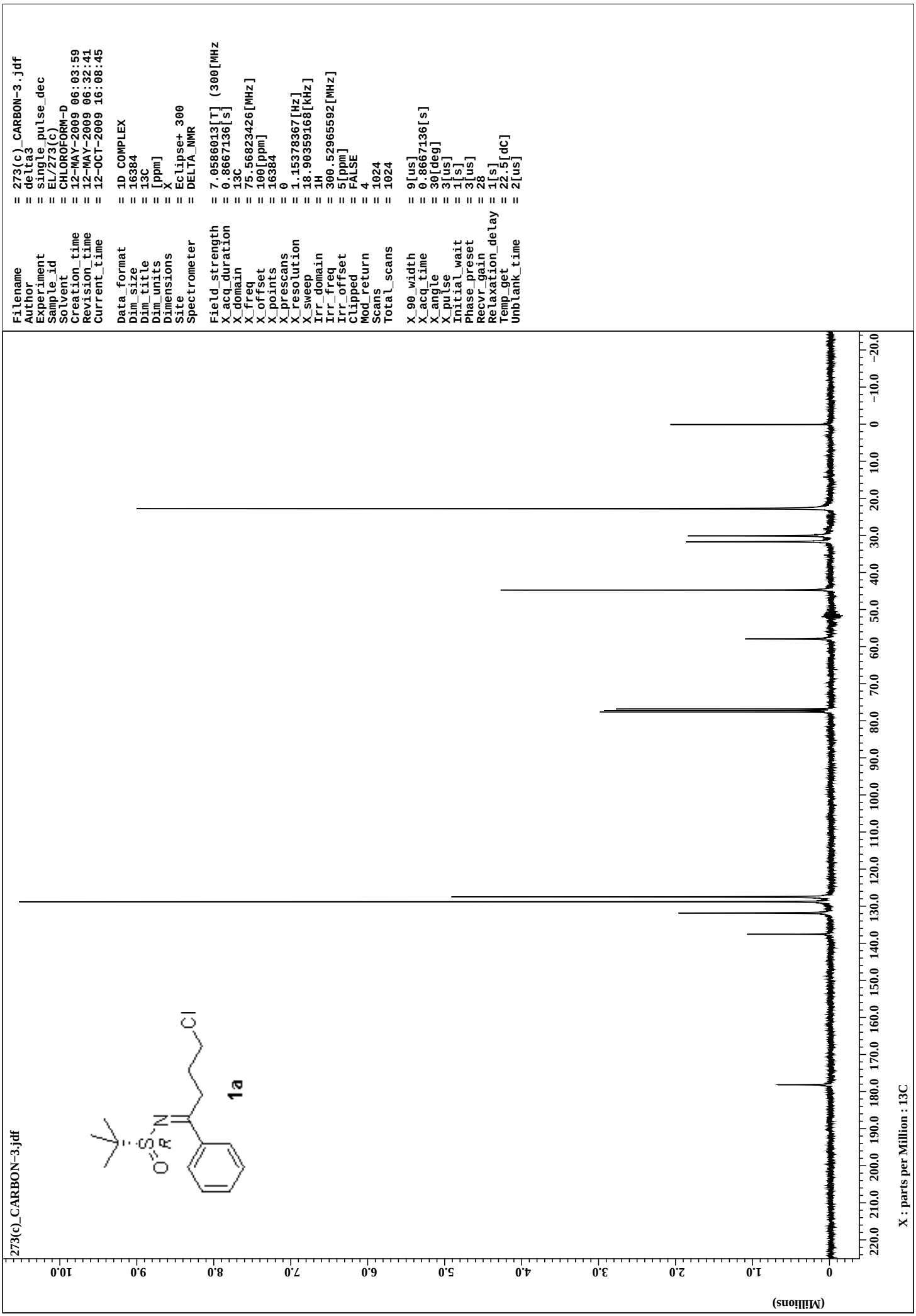
Relaxation_delay = 5[s]
Temp_get = 21.1[dC]
Unblank_time = 2[us]
273(c)_PROTON-6.jdf
1a
(Millions)
X : parts per Million : 1H
1.193
13.711m
0.176
0.26
0.478
0.363
0.203
1.274m
96.998u
7.8929
7.8710
7.4662
7.4553
7.4314
4.8420
4.8163
4.1241
4.1003
3.6626
3.6425
3.6187
3.3128
2.1884
2.1719
2.1536
1.3332
1.3039
1.2819
0.8772
0.8534
0.0110
0.0000
-0.0110
-0.0531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X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 1024
Total_scans = 1024
X_90_width = 9[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
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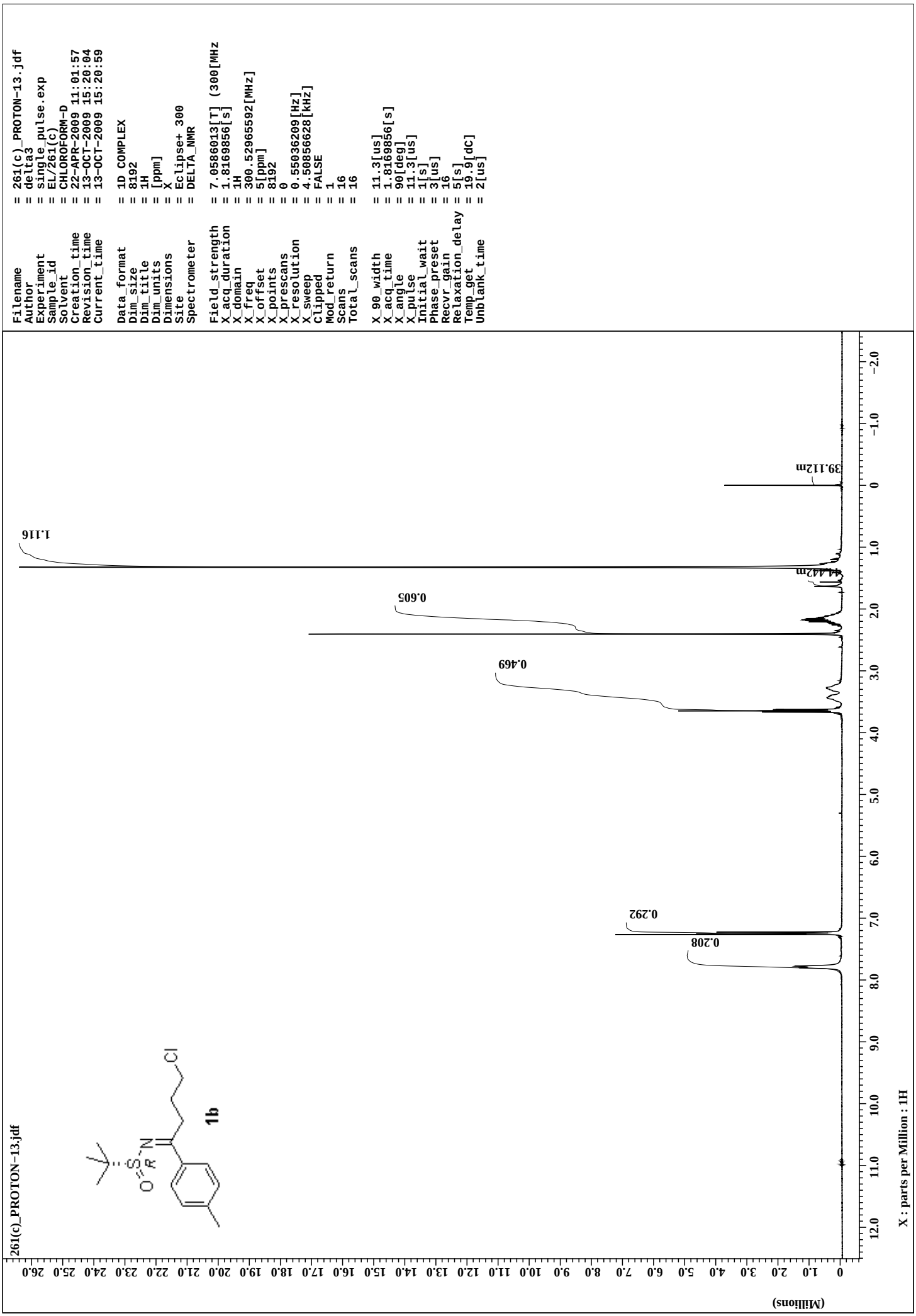
273(c)_CARBON-3.jdf
1a
(Millions)
X : parts per Million : 13C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X_pulse = 11.3[us]
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Phase_preset = 3[us]
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Relaxation_delay = 5[s]
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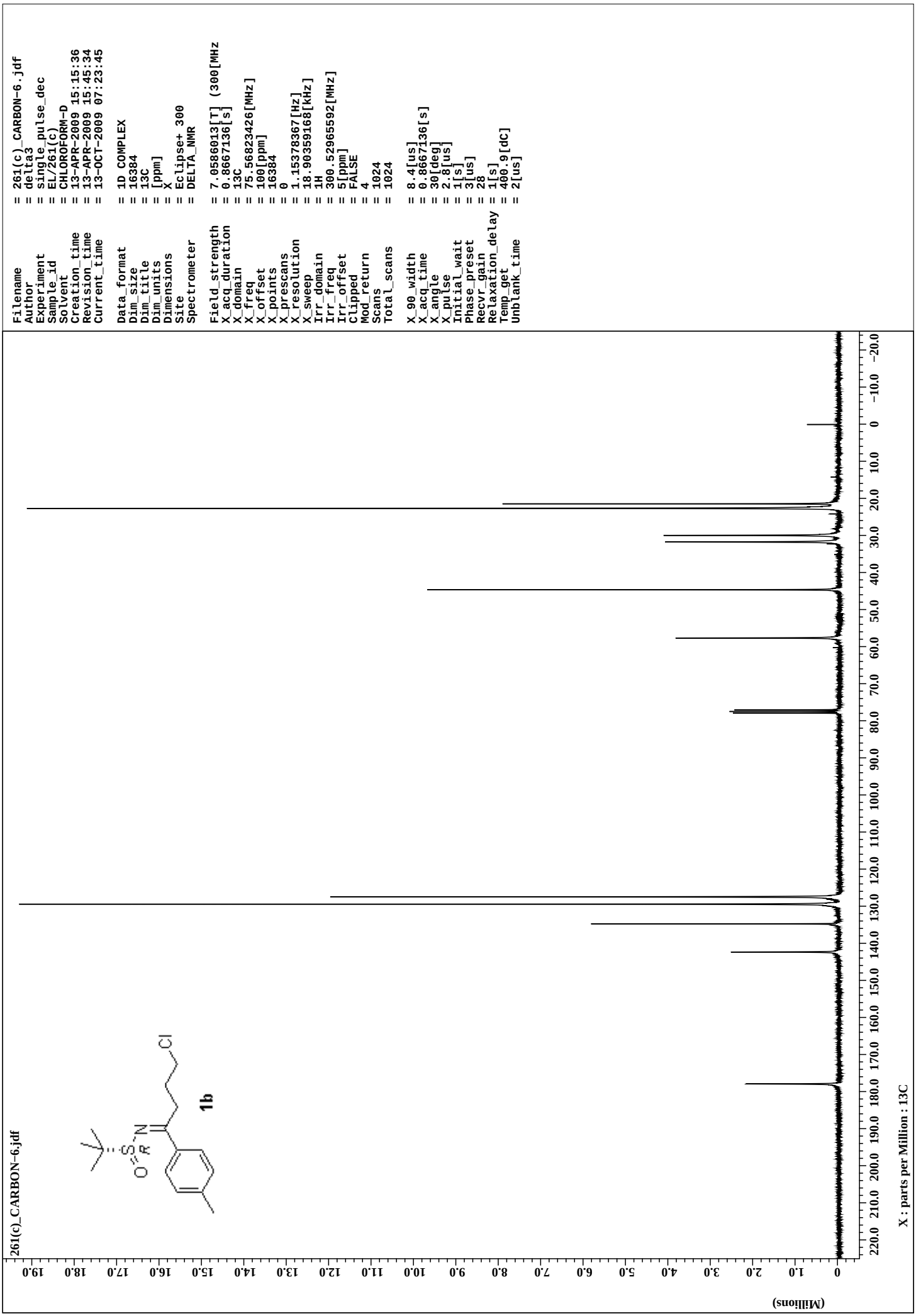
Unblank_time = 2[us]
261(c)_PROTON-13.jdf
1b
1.116
0.605
0.469
0.292
0.208
39.112m
4.442m
(Millions)
X : parts per Million : 1H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Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
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X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
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Irr_freq = 300.52965592[MHz]
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Mod_return = 4
Scans = 1024
Total_scans = 1024
X_90_width = 8.4[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 2.8[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
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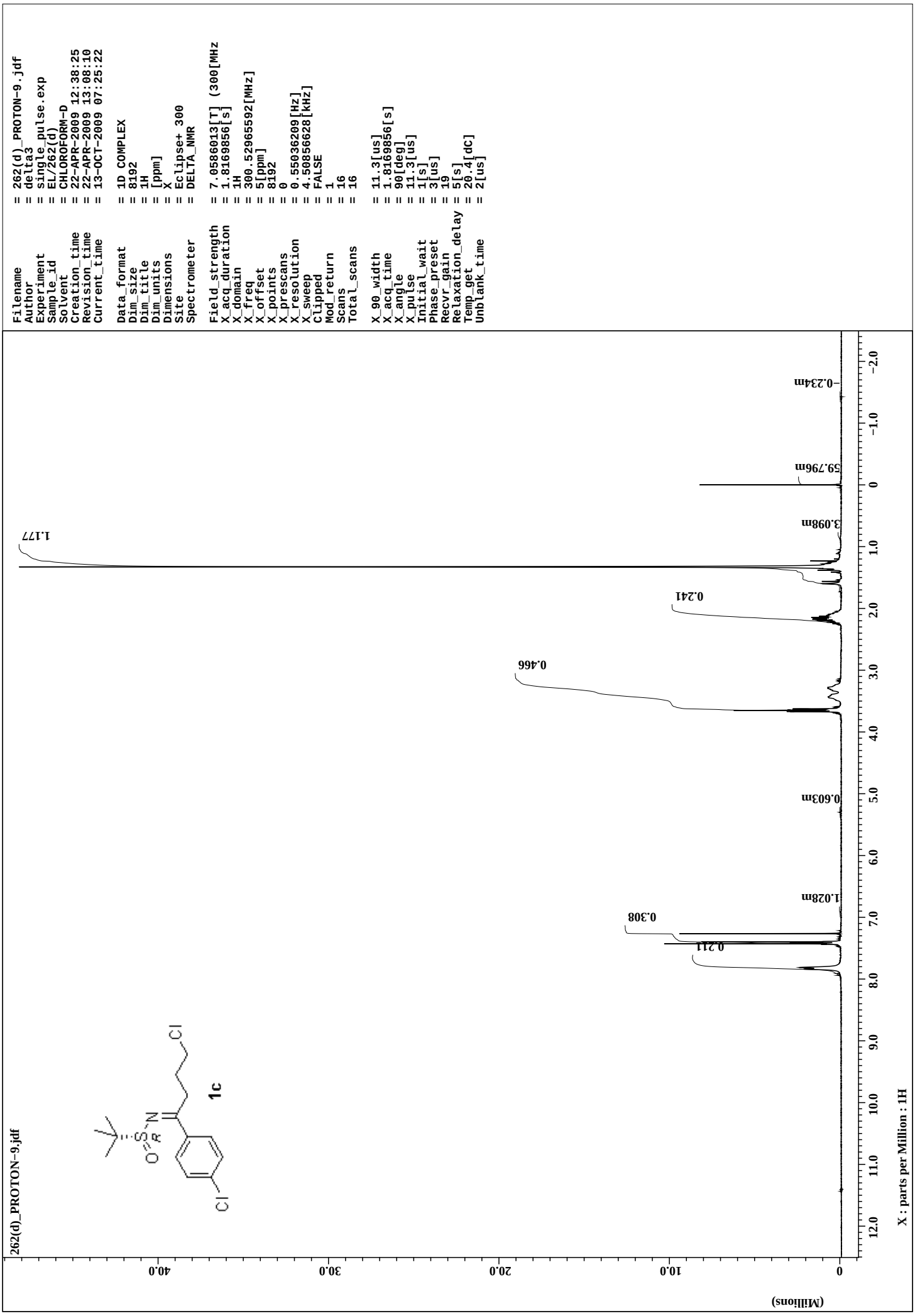
261(c)_CARBON-6.jdf
1b
(Millions)
X : parts per Million : 13C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X_sweep = 4.50856628[kHz]
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Mod_return = 1
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Total_scans = 16
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Phase_preset = 3[us]
Recvr_gain = 19
Relaxation_delay = 5[s]
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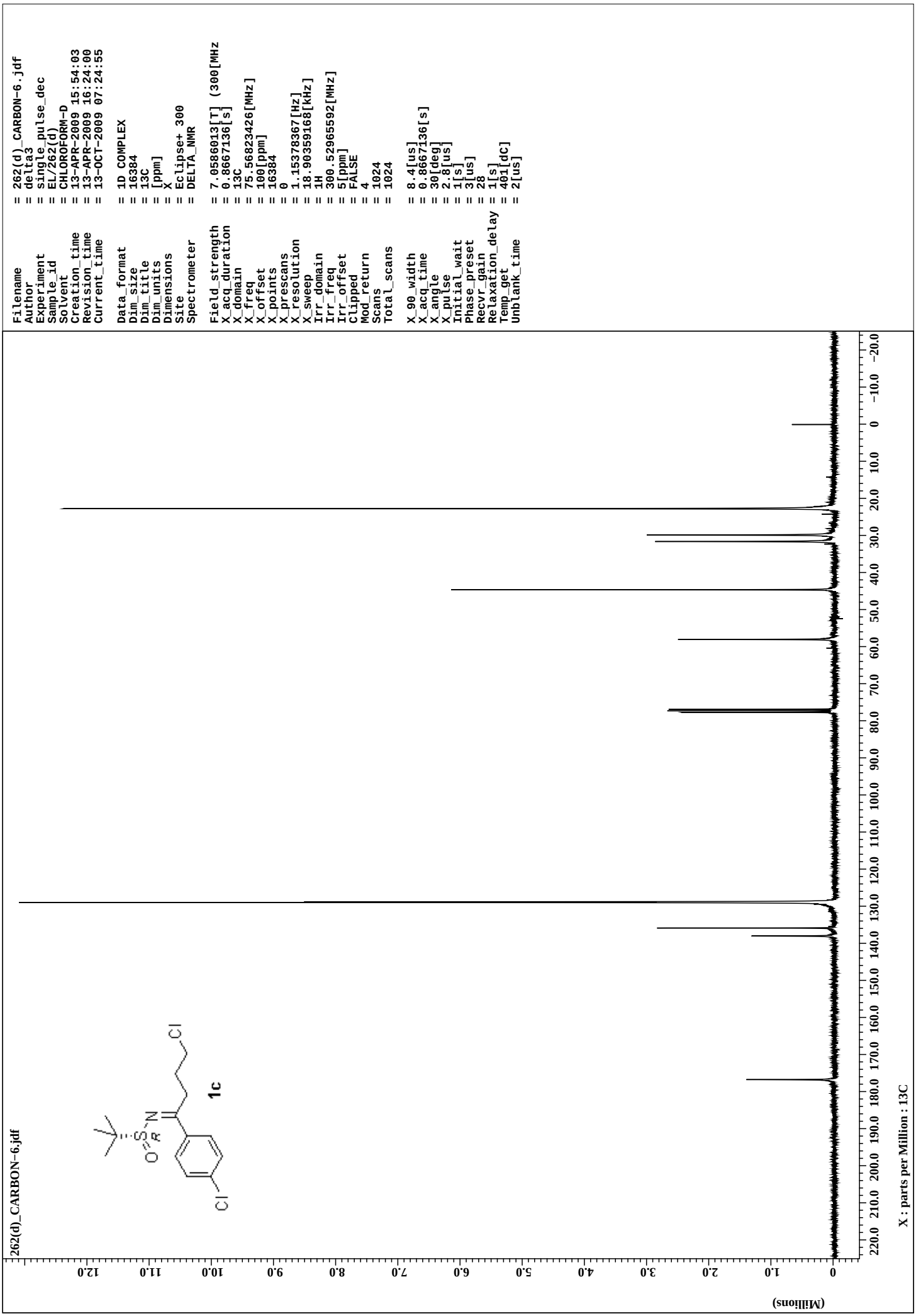
Unblank_time = 2[us]
262(d)_PROTON-9.jdf
1c
1.177
3.098m
59.796m
0.234m
0.241
0.466
0.603m
1.028m
0.308
0.211
(Millions)
X : parts per Million : 1H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X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
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Mod_return = 4
Scans = 1024
Total_scans = 1024
X_90_width = 8.4[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 2.8[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
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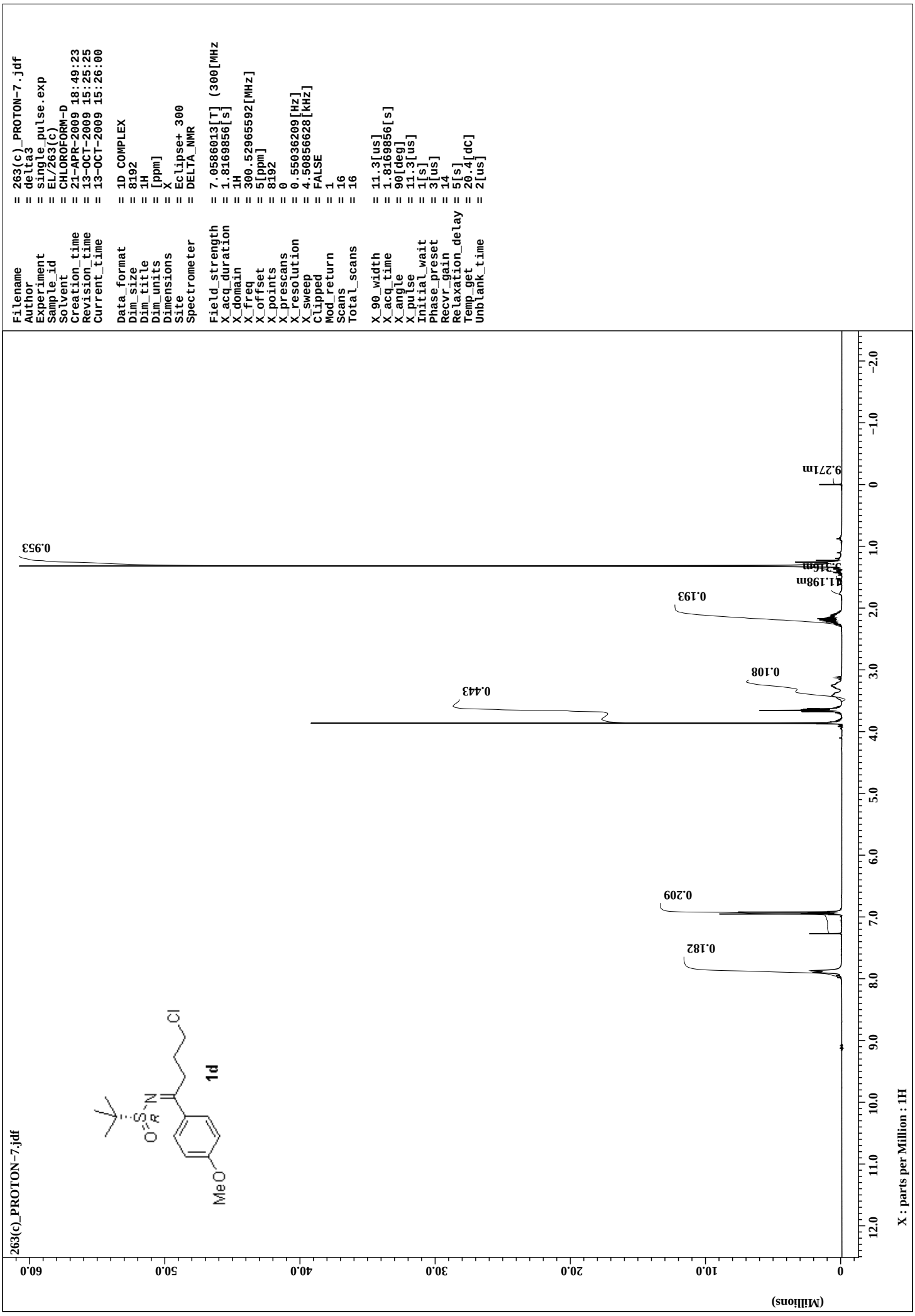
262(d)_CARBON-6.jdf
1c
(Millions)
X : parts per Million : 13C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X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
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X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11.3[us]
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X_angle = 90[deg]
X_pulse = 11.3[us]
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Recvr_gain = 14
Relaxation_delay = 5[s]
Temp_get = 20.4[dC]
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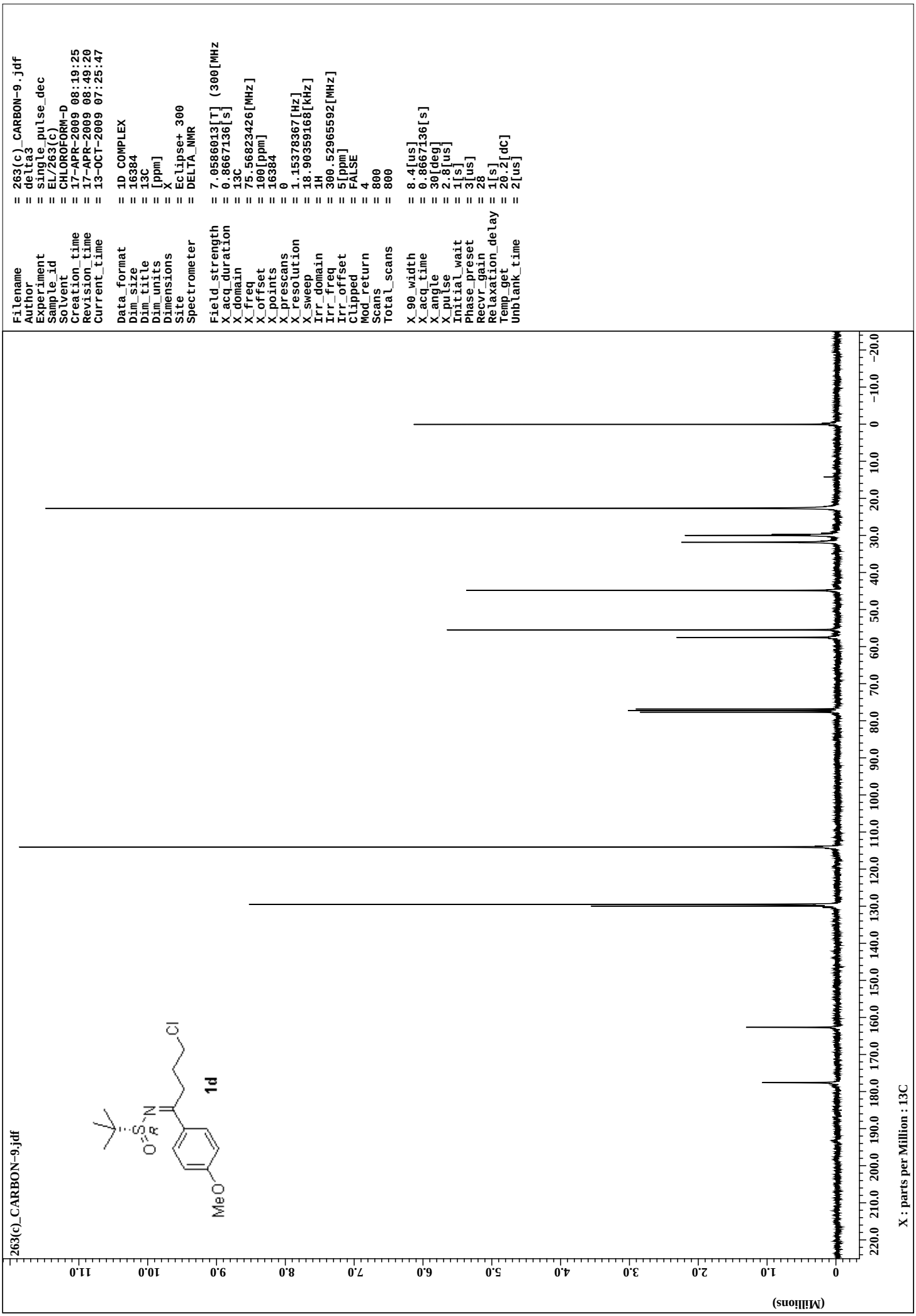
263(c)_PROTON-7.jdf
1d
MeO
Cl
0.953
9.271m
3.316m
1.198m
0.193
0.108
0.443
0.209
0.182
(Millions)
X : parts per Million : 1H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X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 800
Total_scans = 800
X_90_width = 8.4[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 2.8[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 20.2[dC]
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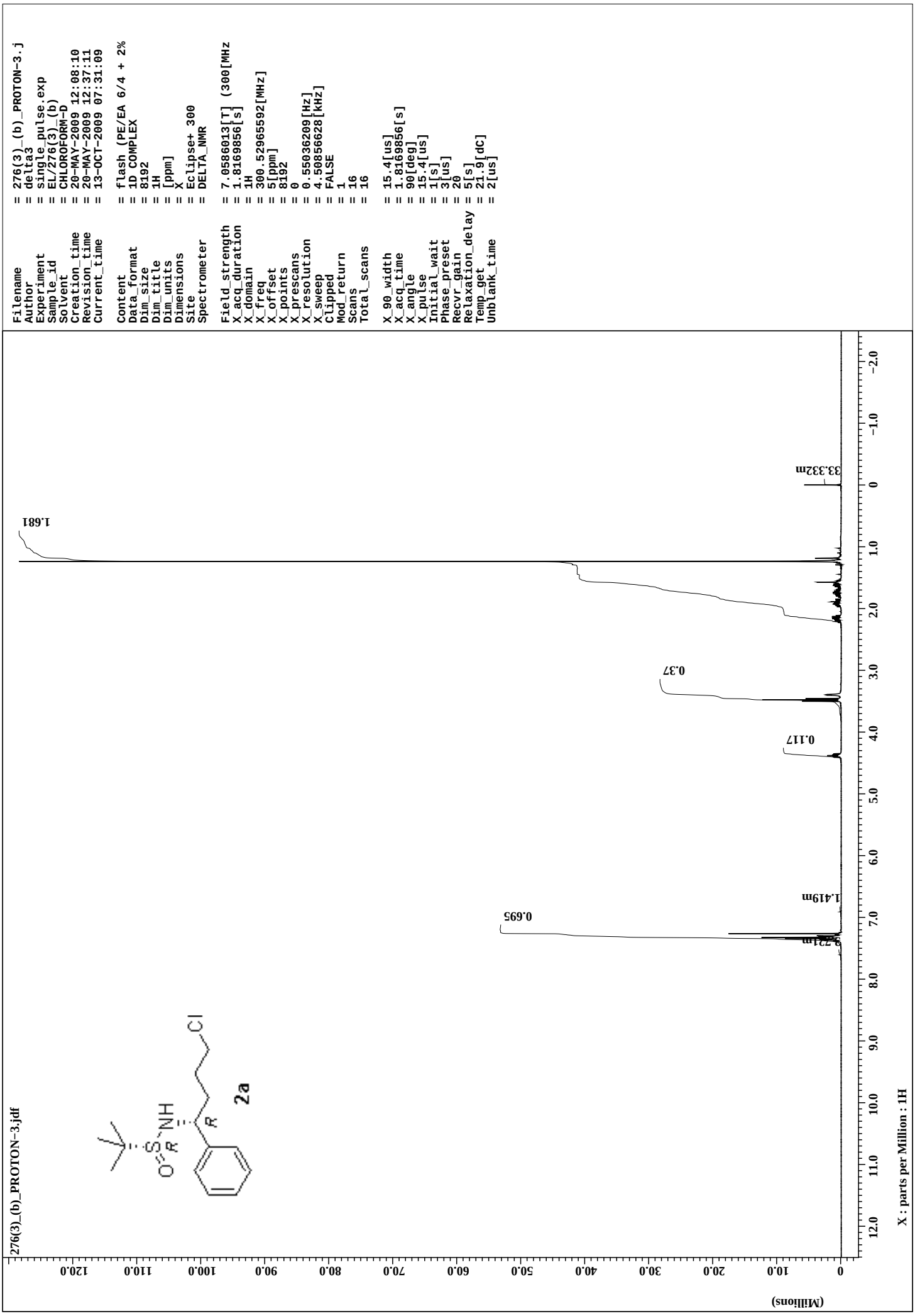
263(c)_CARBON-9.jdf
1d
MeO
Cl
(Millions)
X : parts per Million : 13C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Clipped = FALSE
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Total_scans = 16
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X_angle = 90[deg]
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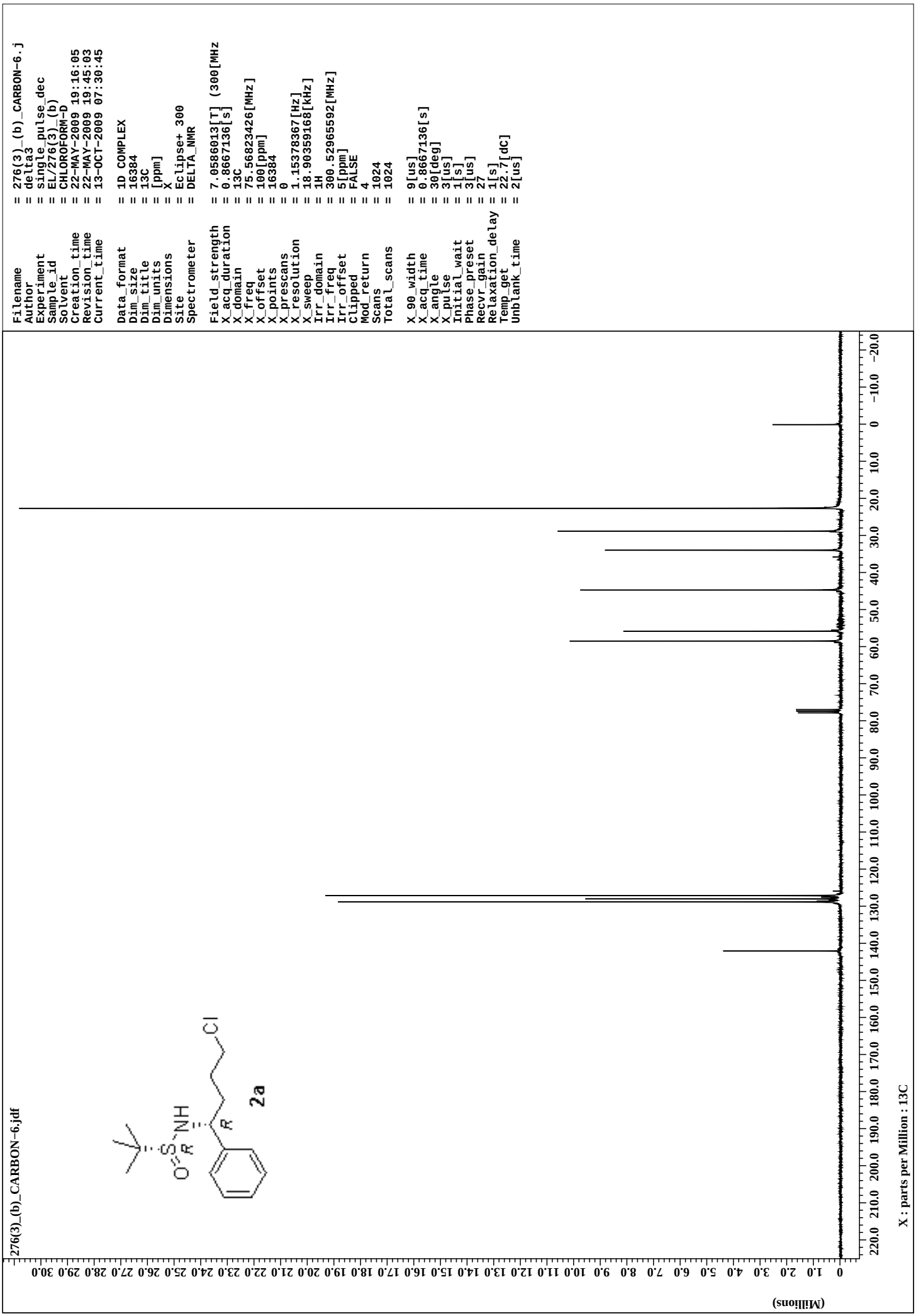
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 20
Relaxation_delay = 5[s]
Temp_get = 21.9[dC]
Unblank_time = 2[us]
276(3)_(b)_PROTON-3.jdf
1.681
0.37
0.117
0.695
1.419m
7.221m
33.332m
2a
(Millions)
X : parts per Million : 1H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X_sweep = 18.90359168[kHz]
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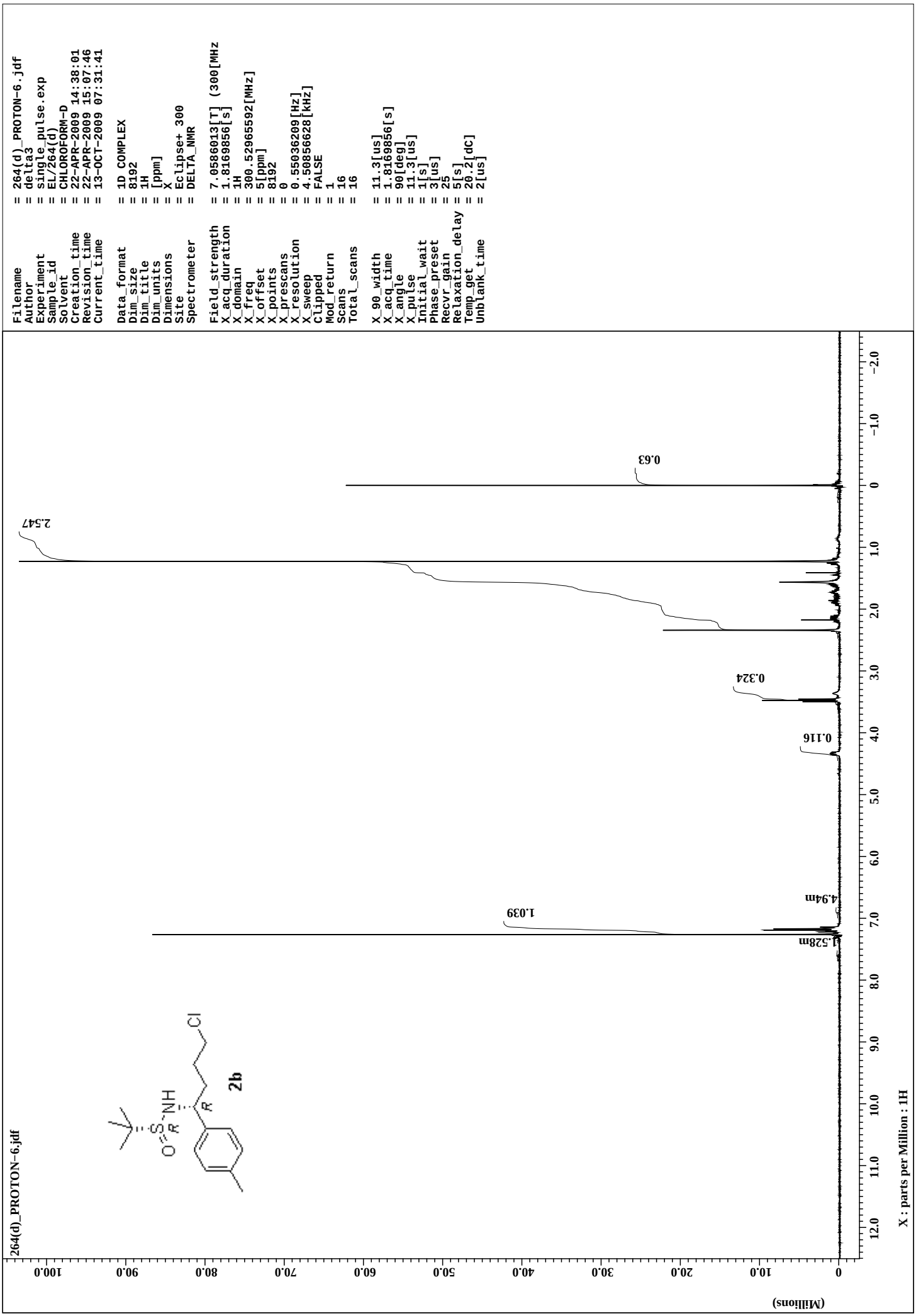
O
S
R
NH
R
Cl
2a
(Millions)
X : parts per Million : 13C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X_freq = 300.52965592[MHz]
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X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11.3[us]
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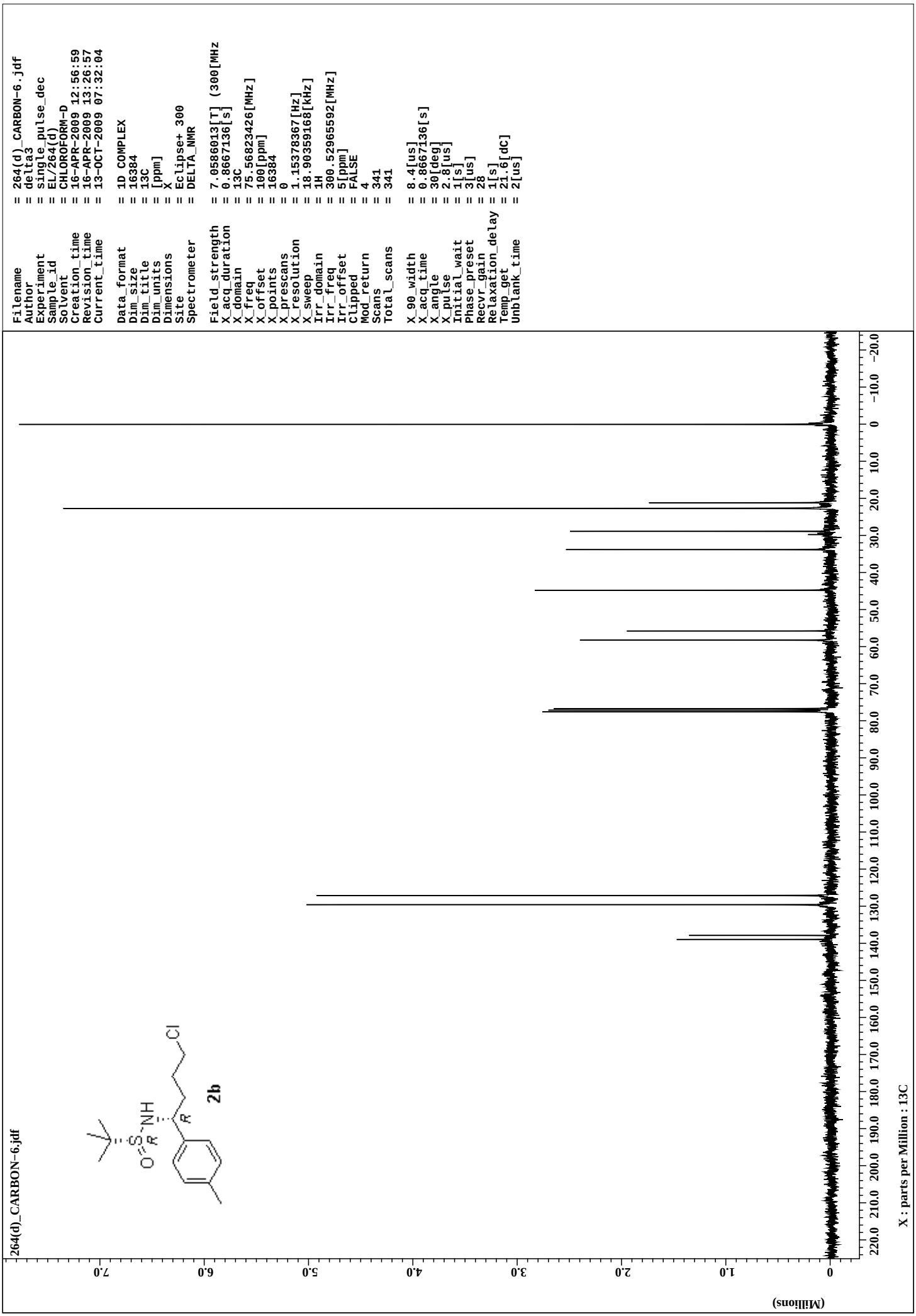
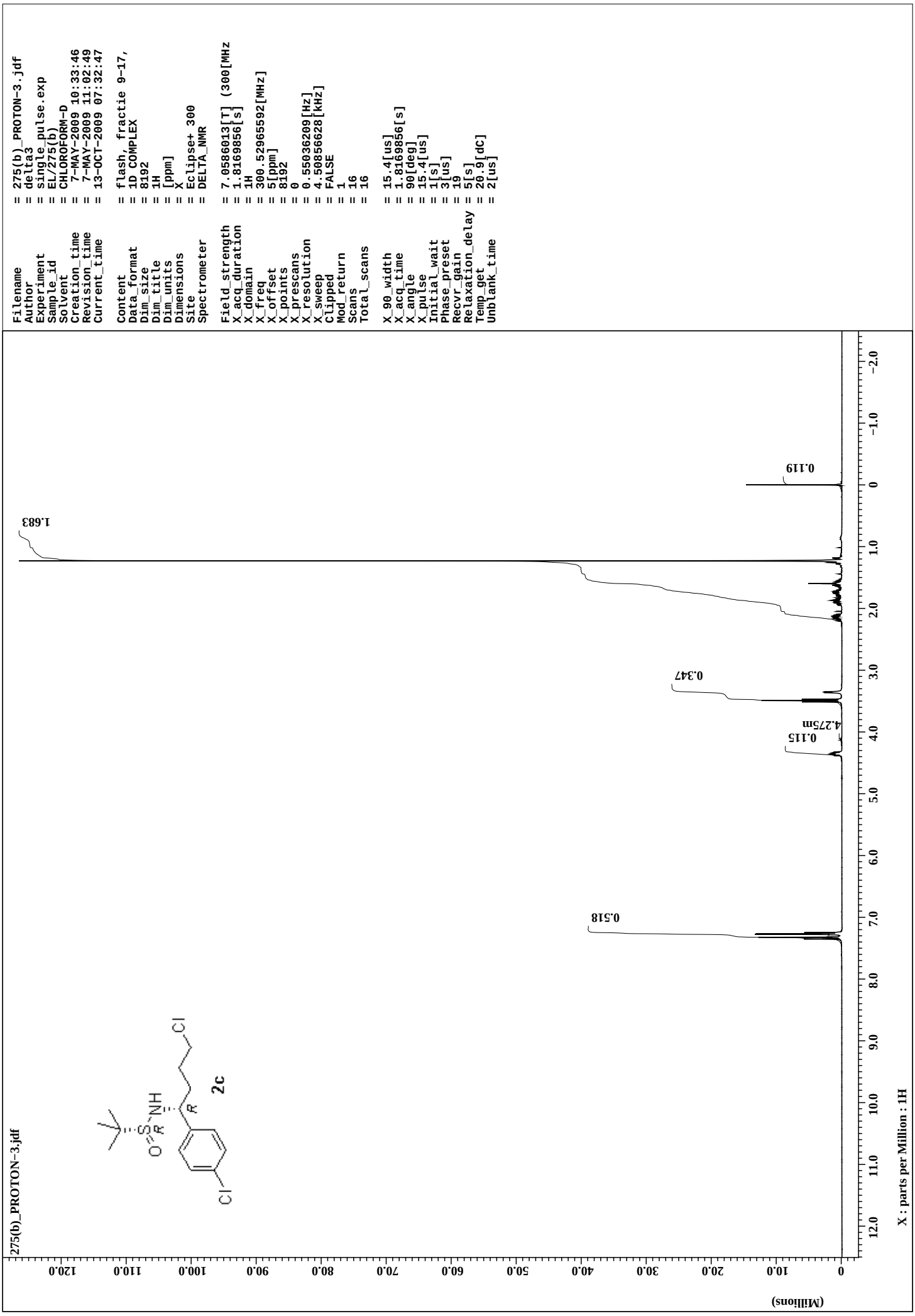
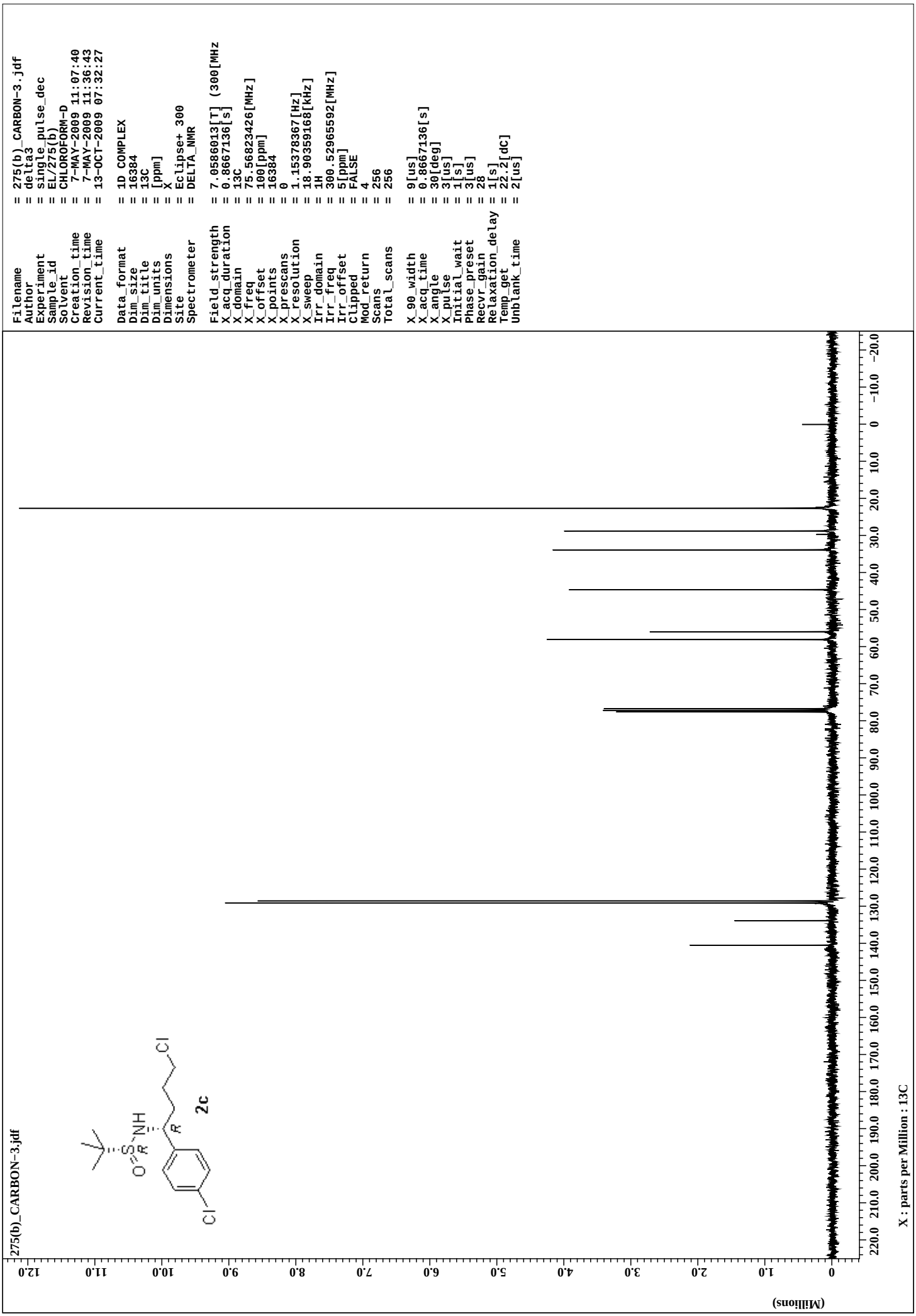
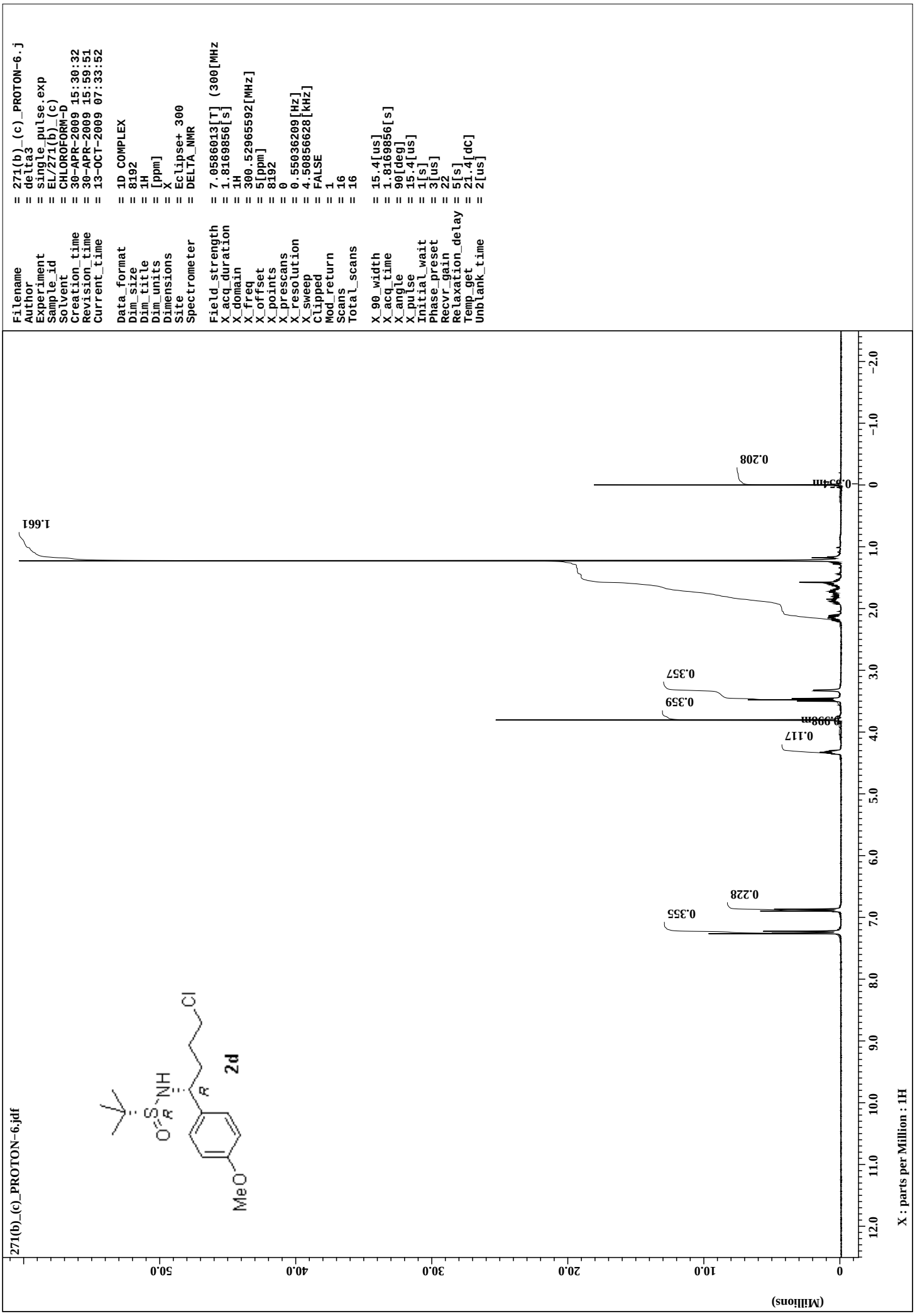
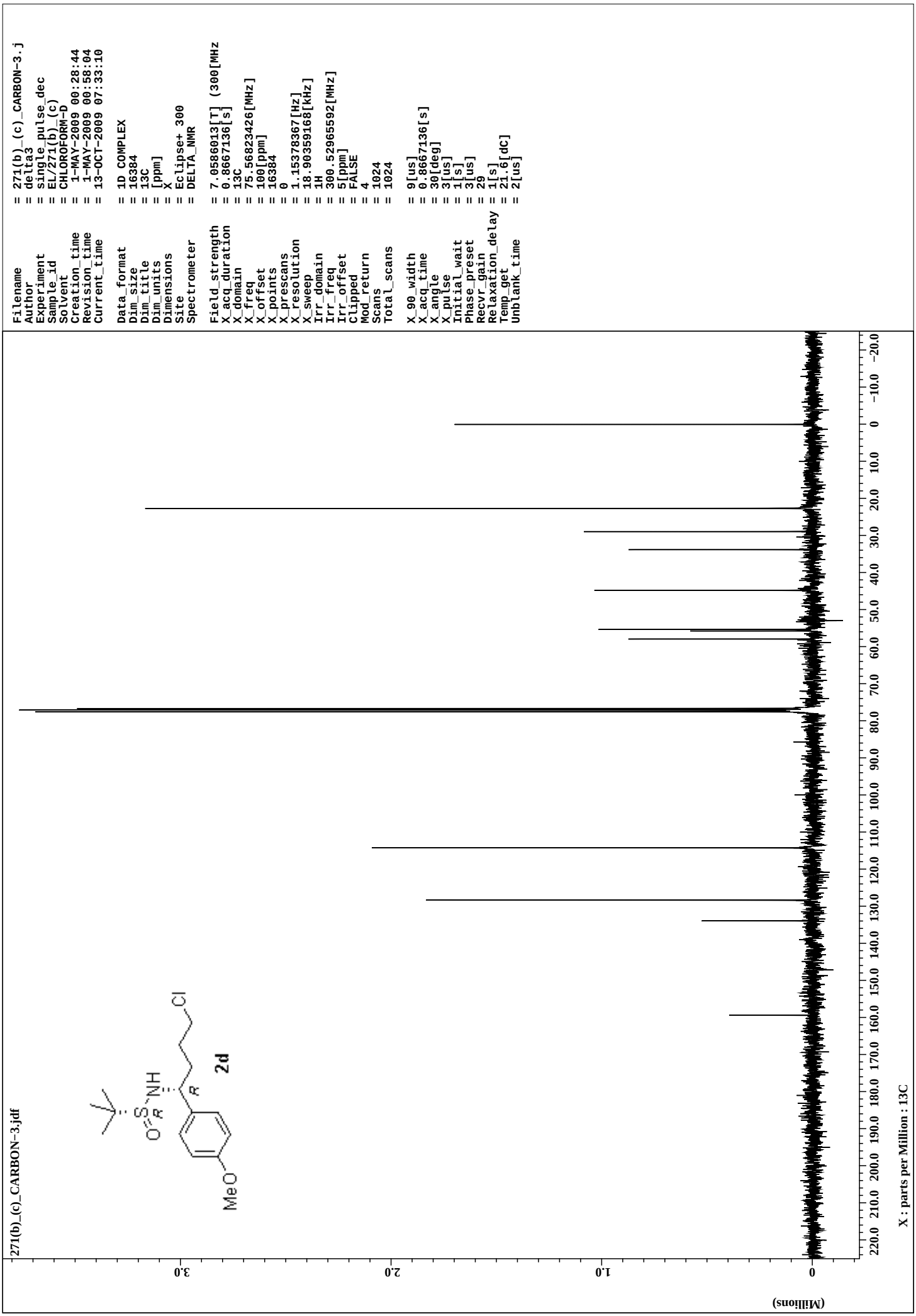
2b
2.547
0.63
0.324
0.116
1.039
4.94m
1.528m
(Millions)
X : parts per Million : 1H

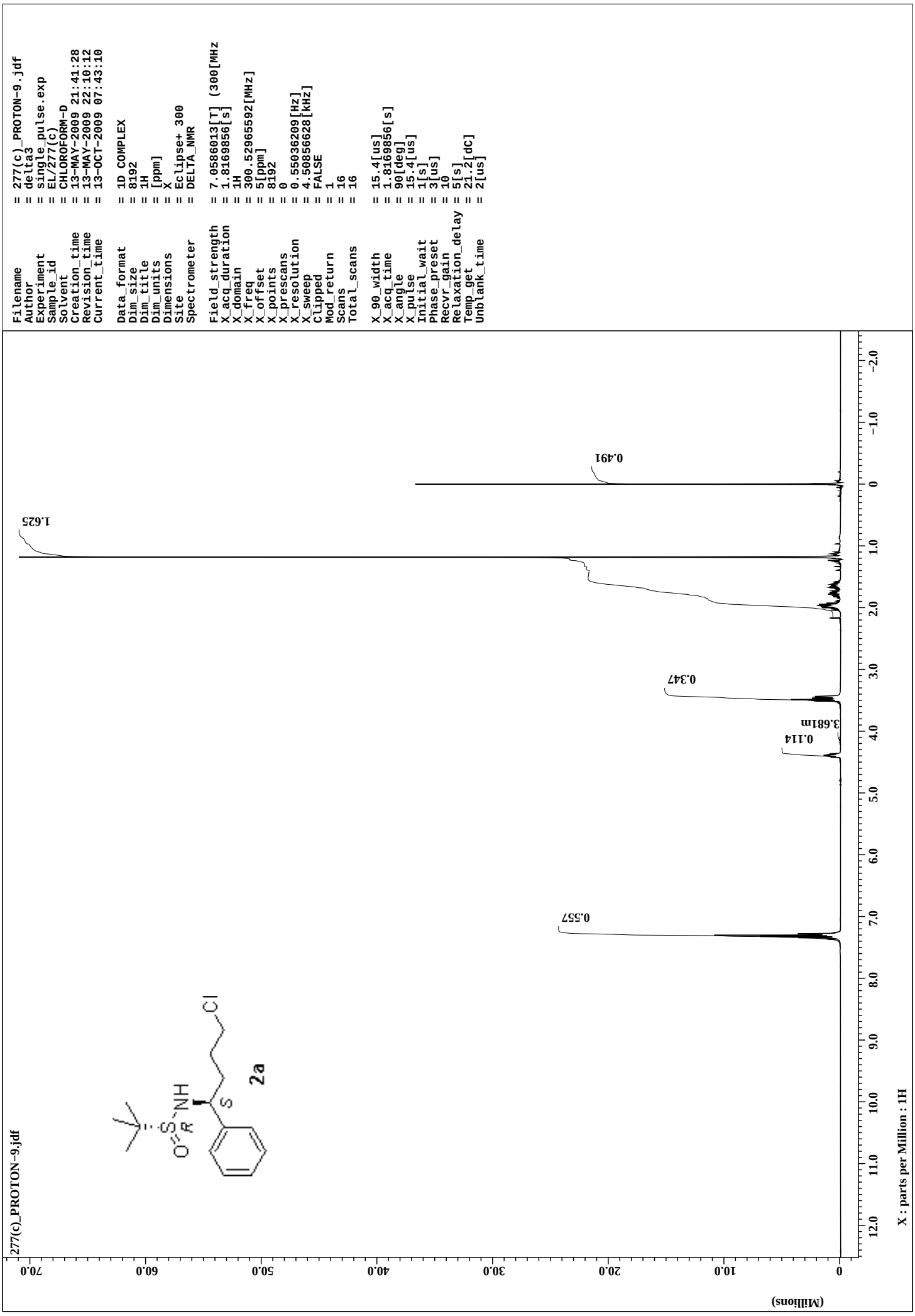

264(d)_CARBON-6.jdf
Filename = 264(d)_CARBON-6.jdf
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/264(d)
Solvent = CHLOROFORM-D
Creation_time = 16-APR-2009 12:56:59
Revision_time = 16-APR-2009 13:26:57
Current_time = 13-OCT-2009 07:32:04
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 341
Total_scans = 341
X_90_width = 8.4[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 2.8[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 21.6[dC]
Unblank_time = 2[us]
2b
Cl
NH
O
S
R
R
(Millions)
X : parts per Million : 13C

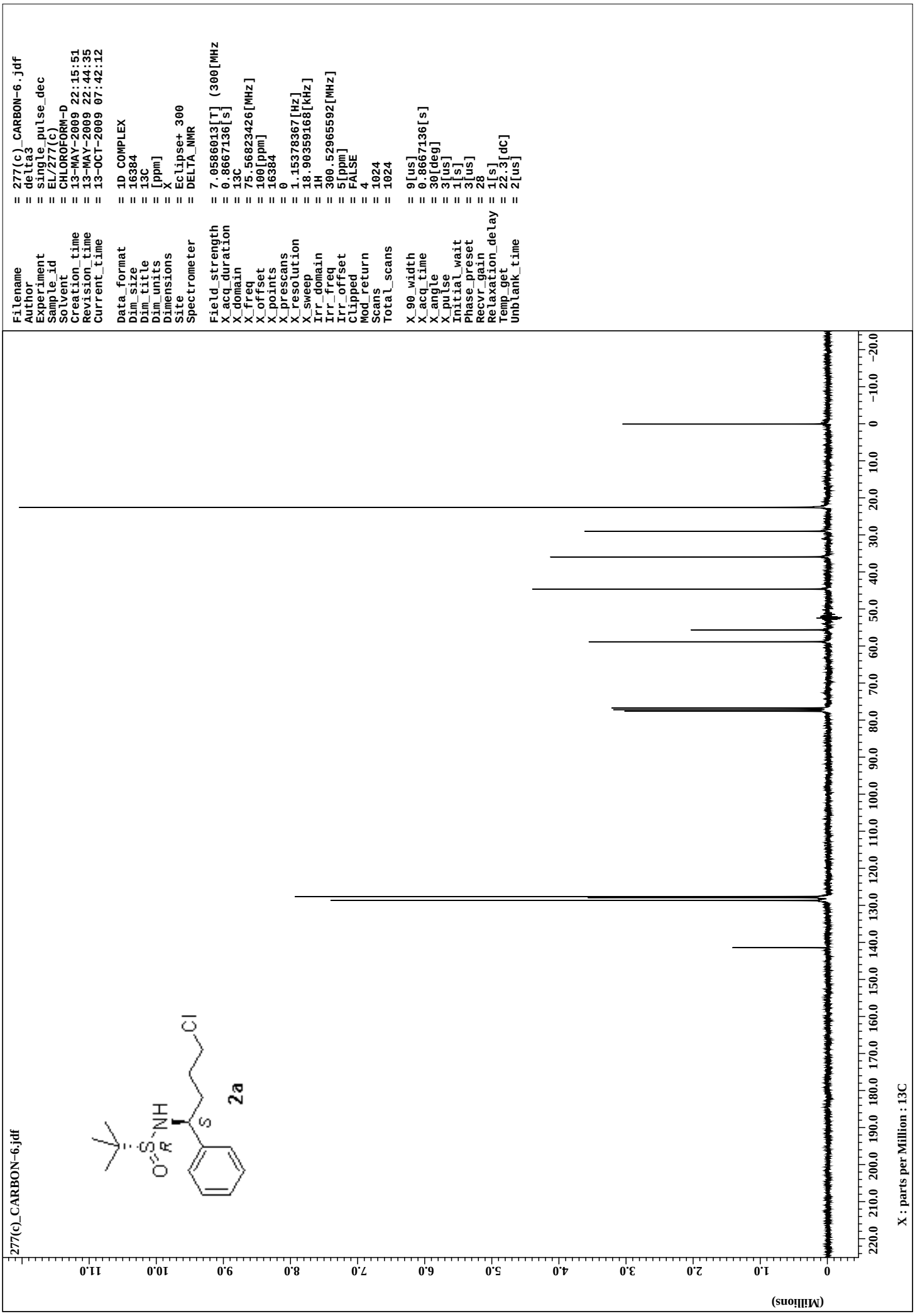

Filename = 275(b)_PROTON-3.jdf
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/275(b)
Solvent = CHLOROFORM-D
Creation_time = 7-MAY-2009 10:33:46
Revision_time = 7-MAY-2009 11:02:49
Current_time = 13-OCT-2009 07:32:47
Content = flash, fractie 9-17,
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 15.4[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 15.4[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 19
Relaxation_delay = 5[s]
Temp_get = 20.9[dC]
Unblank_time = 2[us]
275(b)_PROTON-3.jdf
1.683
0.119
0.347
4.275m
0.115
0.518
2c
(Millions)
X : parts per Million : 1H

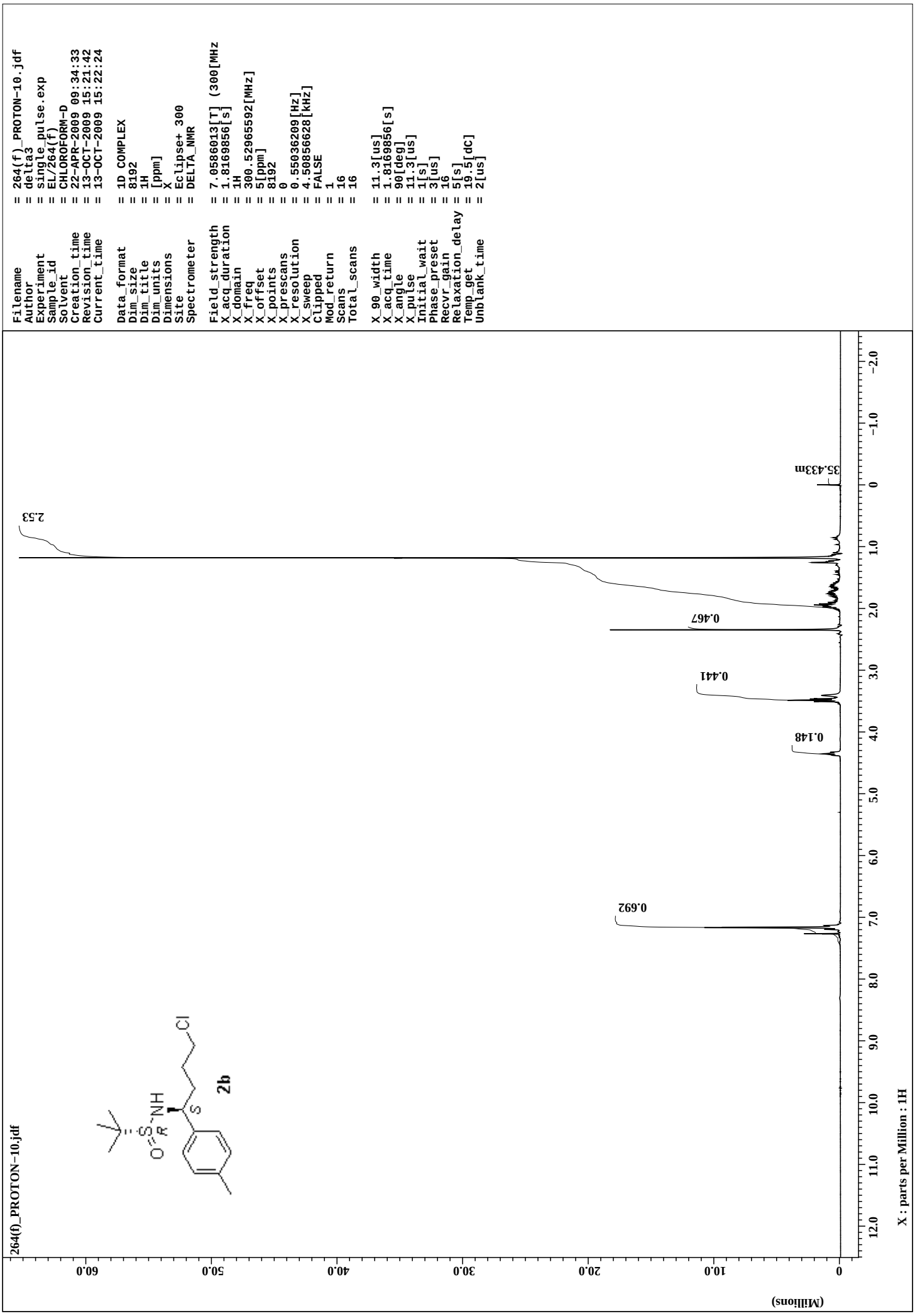

Filename = 275(b)_CARBON-3.jdf
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/275(b)
Solvent = CHLOROFORM-D
Creation_time = 7-MAY-2009 11:07:40
Revision_time = 7-MAY-2009 11:36:43
Current_time = 13-OCT-2009 07:32:27
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 22.2[dC]
Unblank_time = 2[us]
275(b)_CARBON-3.jdf
2c
(Millions)
X : parts per Million : 13C

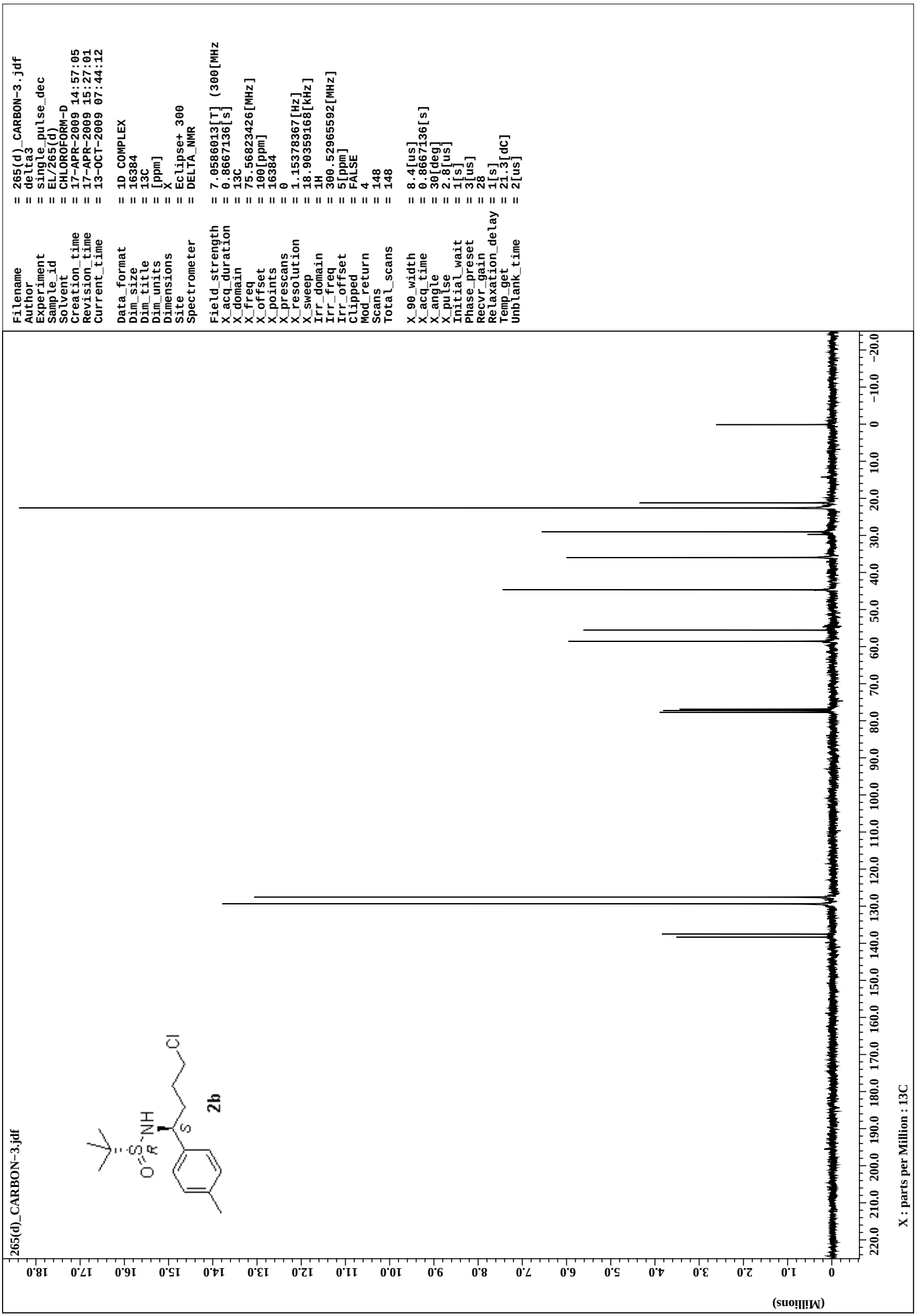

Filename = 271(b)_(c)_PROTON-6.j
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/271(b)_(c)
Solvent = CHLOROFORM-D
Creation_time = 30-APR-2009 15:30:32
Revision_time = 30-APR-2009 15:59:51
Current_time = 13-OCT-2009 07:33:52
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 15.4[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 15.4[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 22
Relaxation_delay = 5[s]
Temp_get = 21.4[dC]
Unblank_time = 2[us]
271(b)_(c)_PROTON-6.jdf
1.661
0.208
0.357
0.359
0.117
0.355
0.228
2d
MeO
Cl
(Millions)
X : parts per Million : 1H

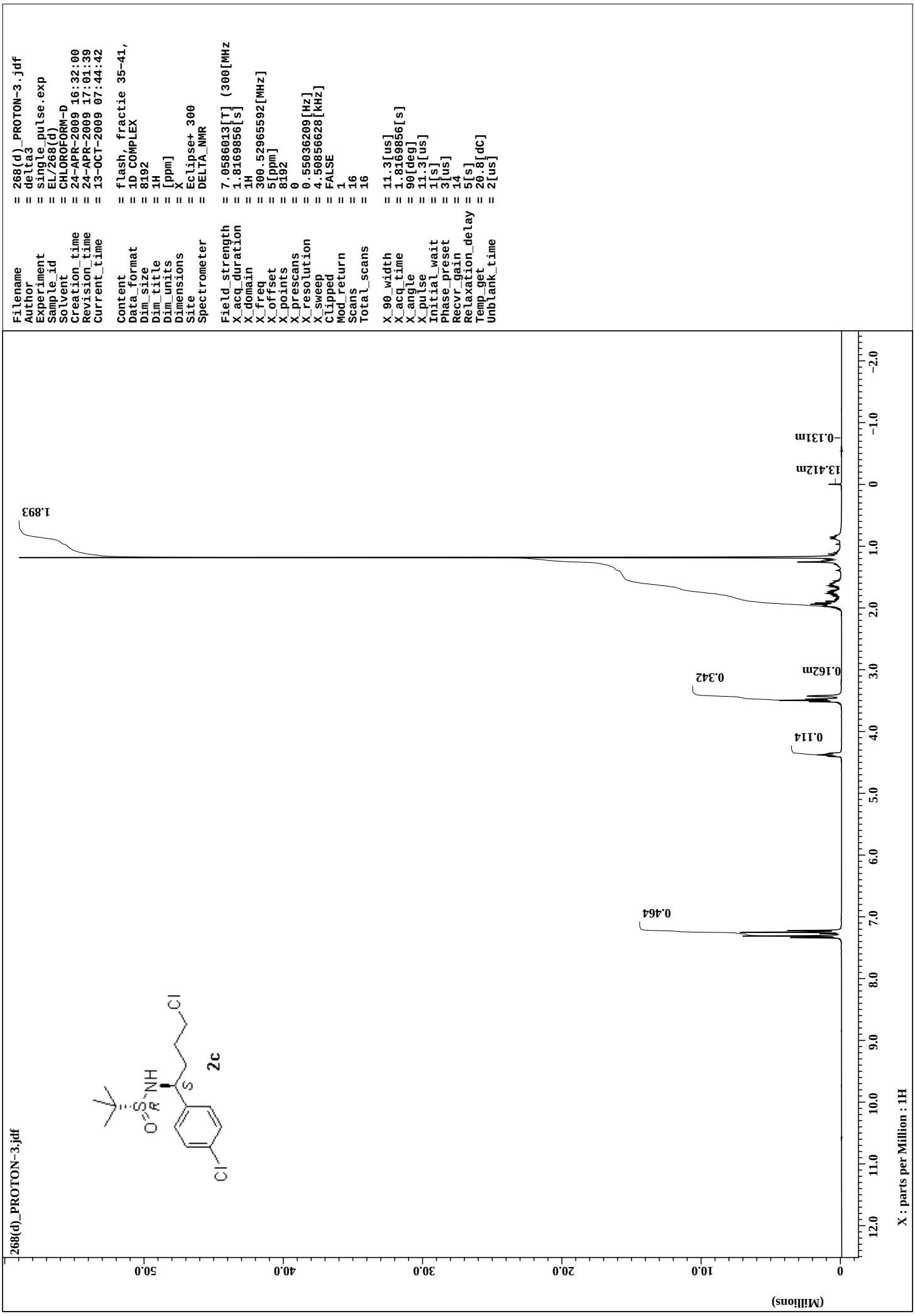

271(b)_(c)_CARBON-3.jdf
Filename = 271(b)_(c)_CARBON-3.j
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/271(b)_(c)
Solvent = CHLOROFORM-D
Creation_time = 1-MAY-2009 00:28:44
Revision_time = 1-MAY-2009 00:58:04
Current_time = 13-OCT-2009 07:33:10
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 1024
Total_scans = 1024
X_90_width = 9[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 29
Relaxation_delay = 1[s]
Temp_get = 21.6[dC]
Unblank_time = 2[us]
2d
MeO
O
S
NH
R
Cl
(Millions)
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : 13C

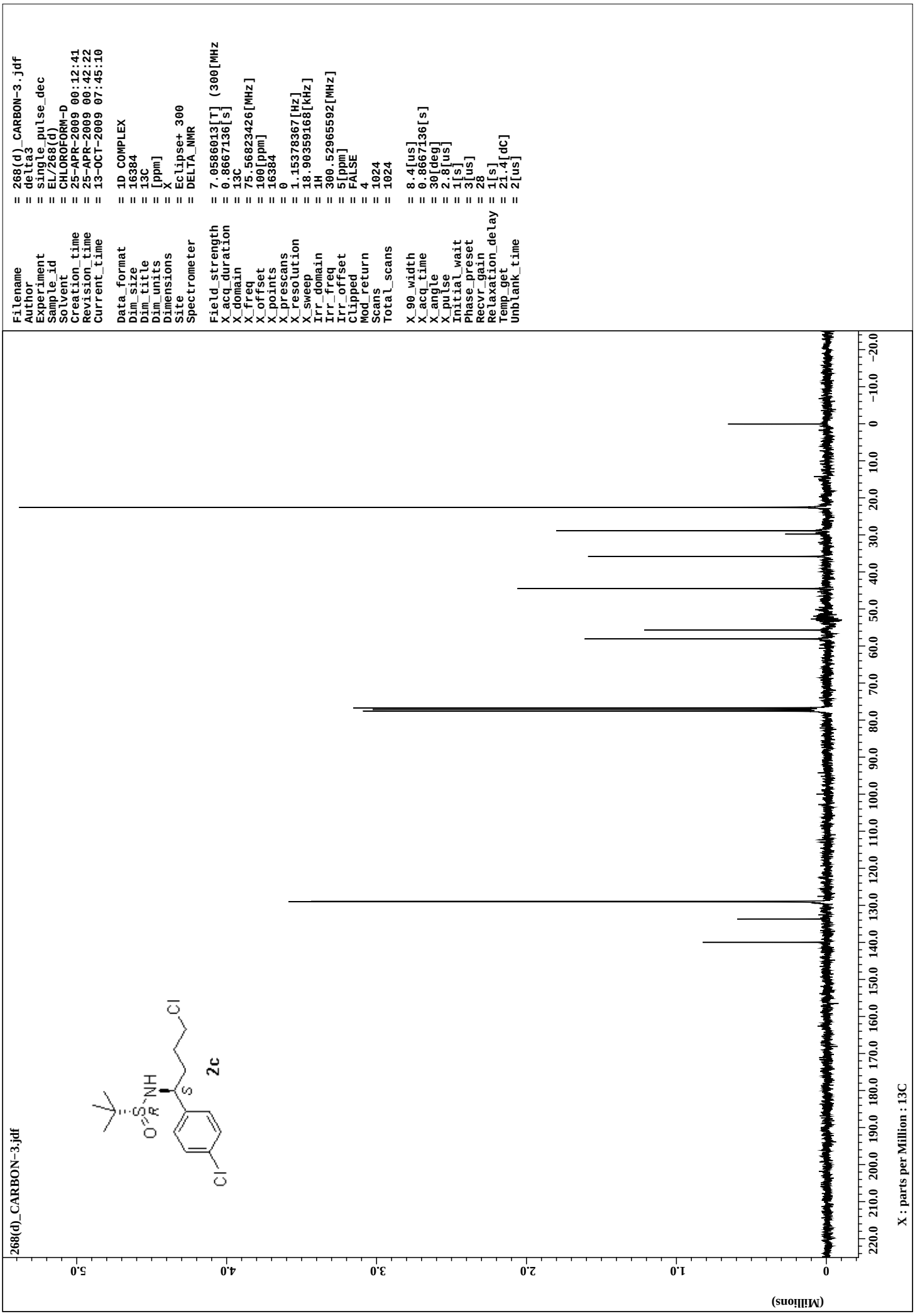

Filename = 277(c)_PROTON-9.jdf
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/277(c)
Solvent = CHLOROFORM-D
Creation_time = 13-MAY-2009 21:41:28
Revision_time = 13-MAY-2009 22:10:12
Current_time = 13-OCT-2009 07:43:10
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 15.4[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 15.4[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 10
Relaxation_delay = 5[s]
Temp_get = 21.2[dC]
Unblank_time = 2[us]
277(c)_PROTON-9.jdf
1.625
0.491
0.347
3.681m
0.114
0.557
2a
(Millions)
X : parts per Million : 1H

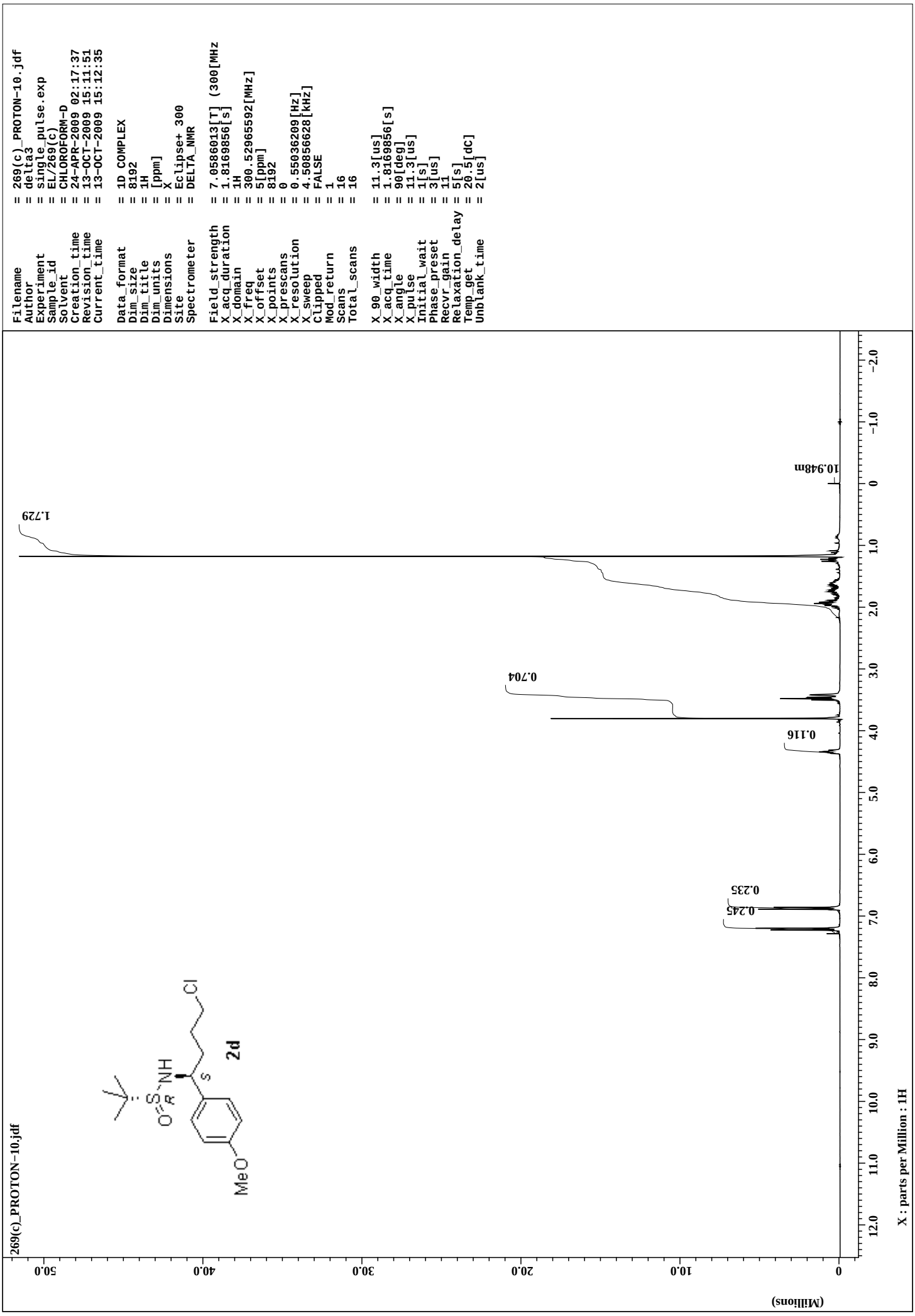

Filename = 277(c)_CARBON-6.jdf
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/277(c)
Solvent = CHLOROFORM-D
Creation_time = 13-MAY-2009 22:15:51
Revision_time = 13-MAY-2009 22:44:35
Current_time = 13-OCT-2009 07:42:12
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 1024
Total_scans = 1024
X_90_width = 9[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 22.3[dC]
Unblank_time = 2[us]
277(c)_CARBON-6.jdf
2a
(Millions)
X : parts per Million : 13C

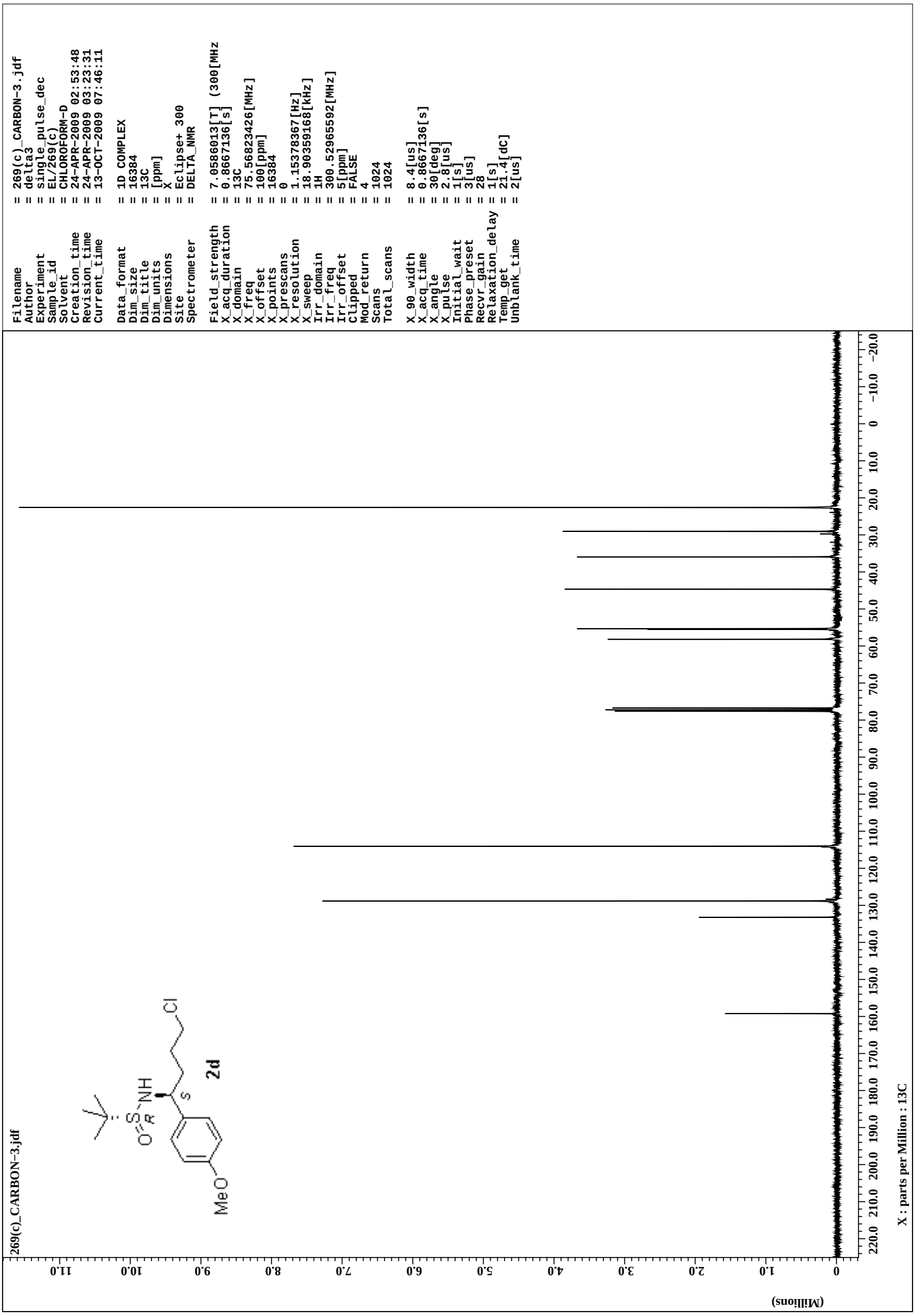

Filename = 264(f)_PROTON-10.jdf
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/264(f)
Solvent = CHLOROFORM-D
Creation_time = 22-APR-2009 09:34:33
Revision_time = 13-OCT-2009 15:21:42
Current_time = 13-OCT-2009 15:22:24
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11.3[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 11.3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 16
Relaxation_delay = 5[s]
Temp_get = 19.5[dC]
Unblank_time = 2[us]
264(f)_PROTON-10.jdf
2b
2.53
35.433m
0.467
0.441
0.148
0.692
(Millions)
X : parts per Million : 1H

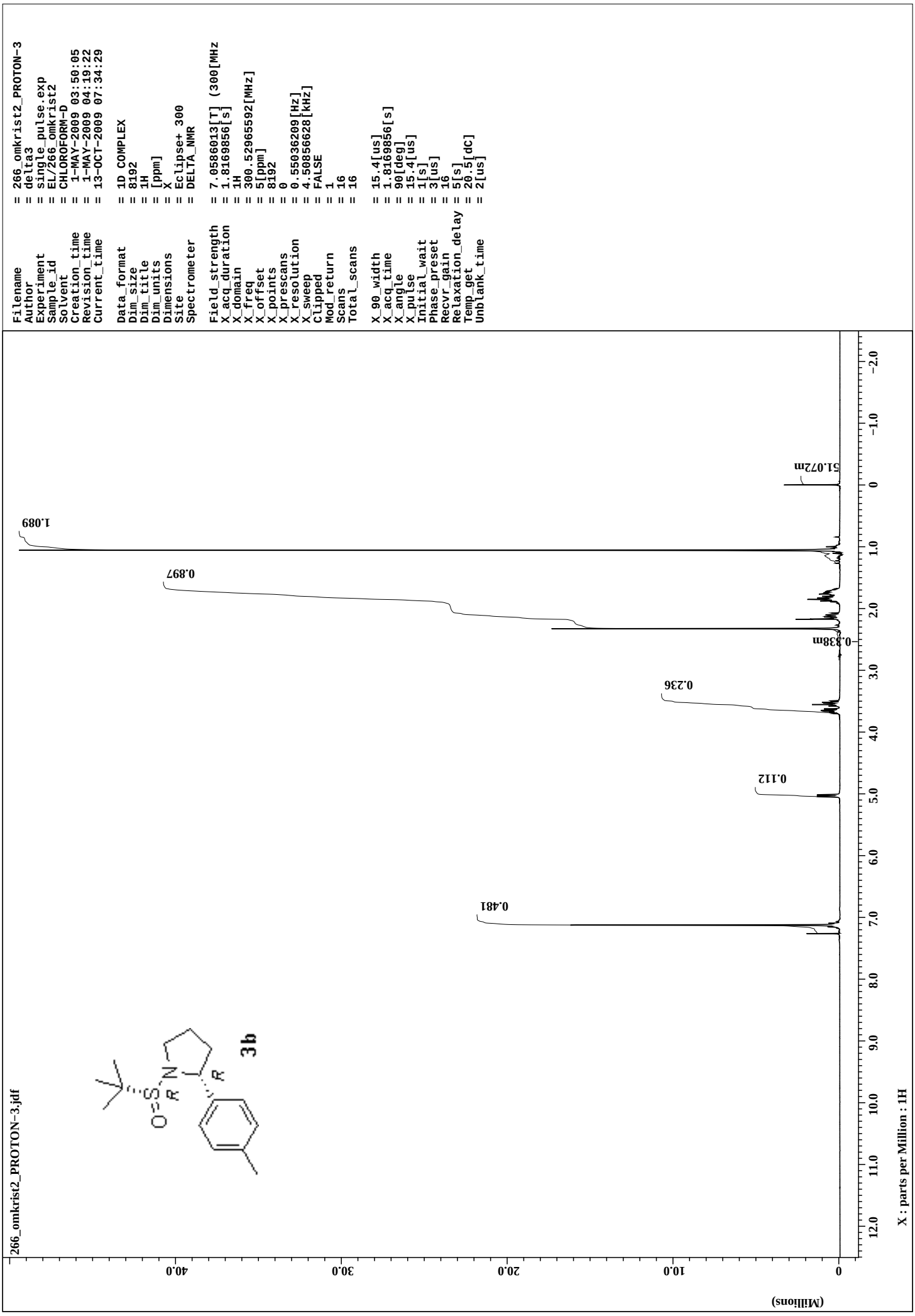

265(d)_CARBON-3.jdf
Filename = 265(d)_CARBON-3.jdf
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/265(d)
Solvent = CHLOROFORM-D
Creation_time = 17-APR-2009 14:57:05
Revision_time = 17-APR-2009 15:27:01
Current_time = 13-OCT-2009 07:44:12
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 148
Total_scans = 148
X_90_width = 8.4[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 2.8[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 21.3[dC]
Unblank_time = 2[us]
2b
(Millions)
X : parts per Million : 13C

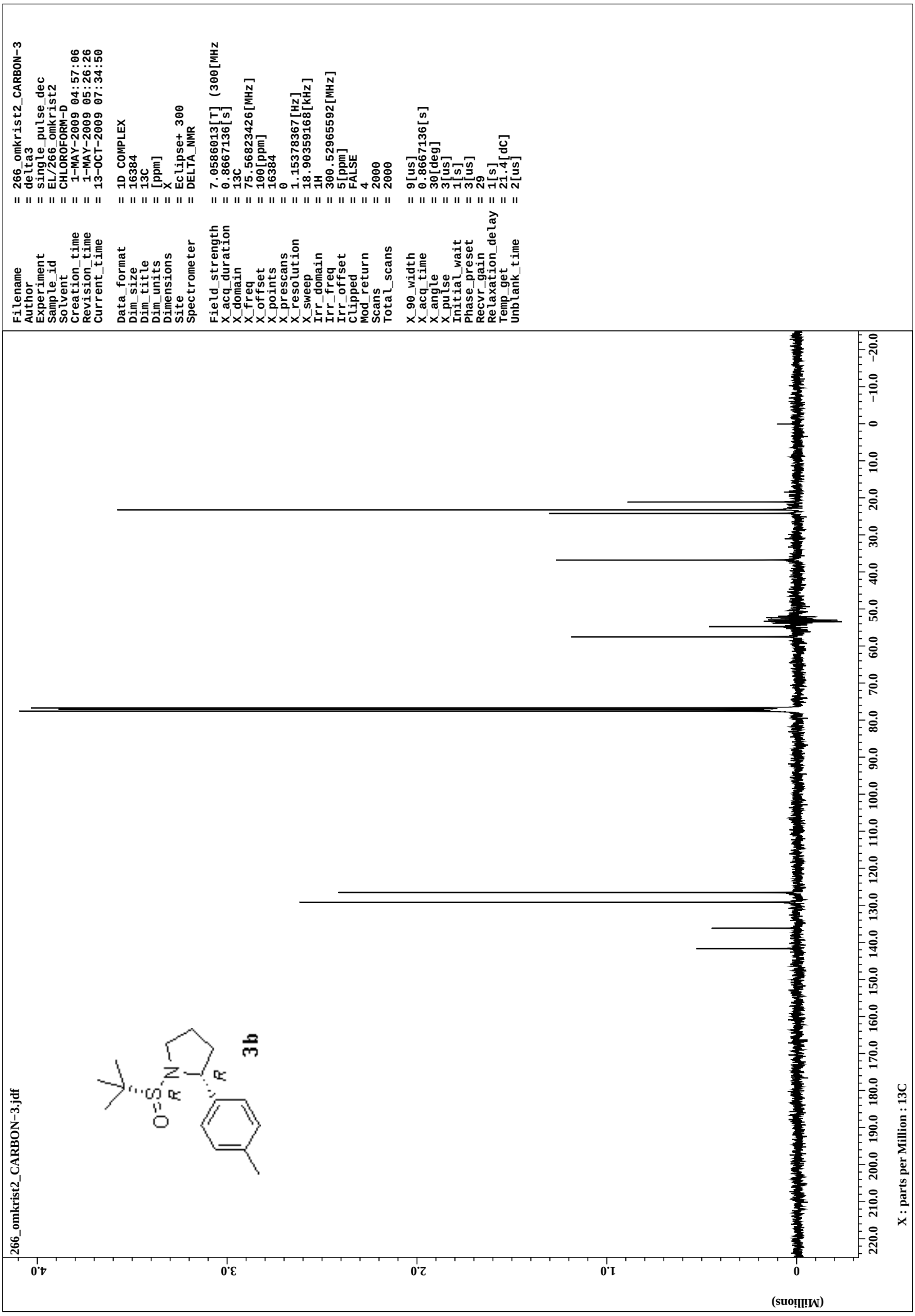

Filename = 268(d)_PROTON-3.jdf
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/268(d)
Solvent = CHLOROFORM-D
Creation_time = 24-APR-2009 16:32:00
Revision_time = 24-APR-2009 17:01:39
Current_time = 13-OCT-2009 07:44:42
Content = flash, fractie 35-41,
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11.3[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 11.3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 14
Relaxation_delay = 5[s]
Temp_get = 20.8[dC]
Unblank_time = 2[us]
268(d)_PROTON-3.jdf
1.893
13.412m
0.131m
0.464
0.342
0.162m
0.114
2c
(Millions)
X : parts per Million : 1H

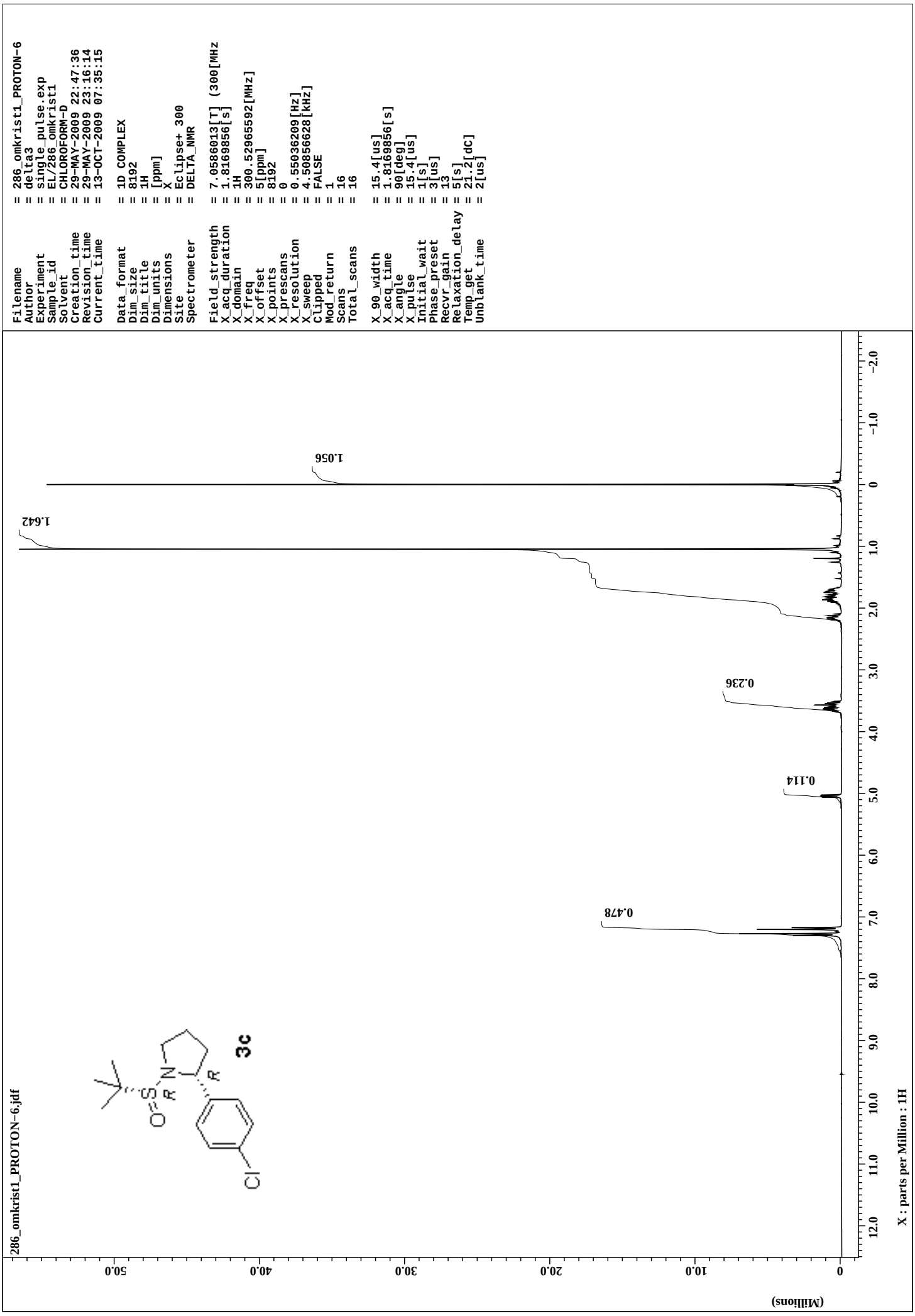

Filename = 268(d)_CARBON-3.jdf
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/268(d)
Solvent = CHLOROFORM-D
Creation_time = 25-APR-2009 00:12:41
Revision_time = 25-APR-2009 00:42:22
Current_time = 13-OCT-2009 07:45:10
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 1024
Total_scans = 1024
X_90_width = 8.4[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 2.8[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 21.4[dC]
Unblank_time = 2[us]
268(d)_CARBON-3.jdf
2c
(Millions)
X : parts per Million : 13C

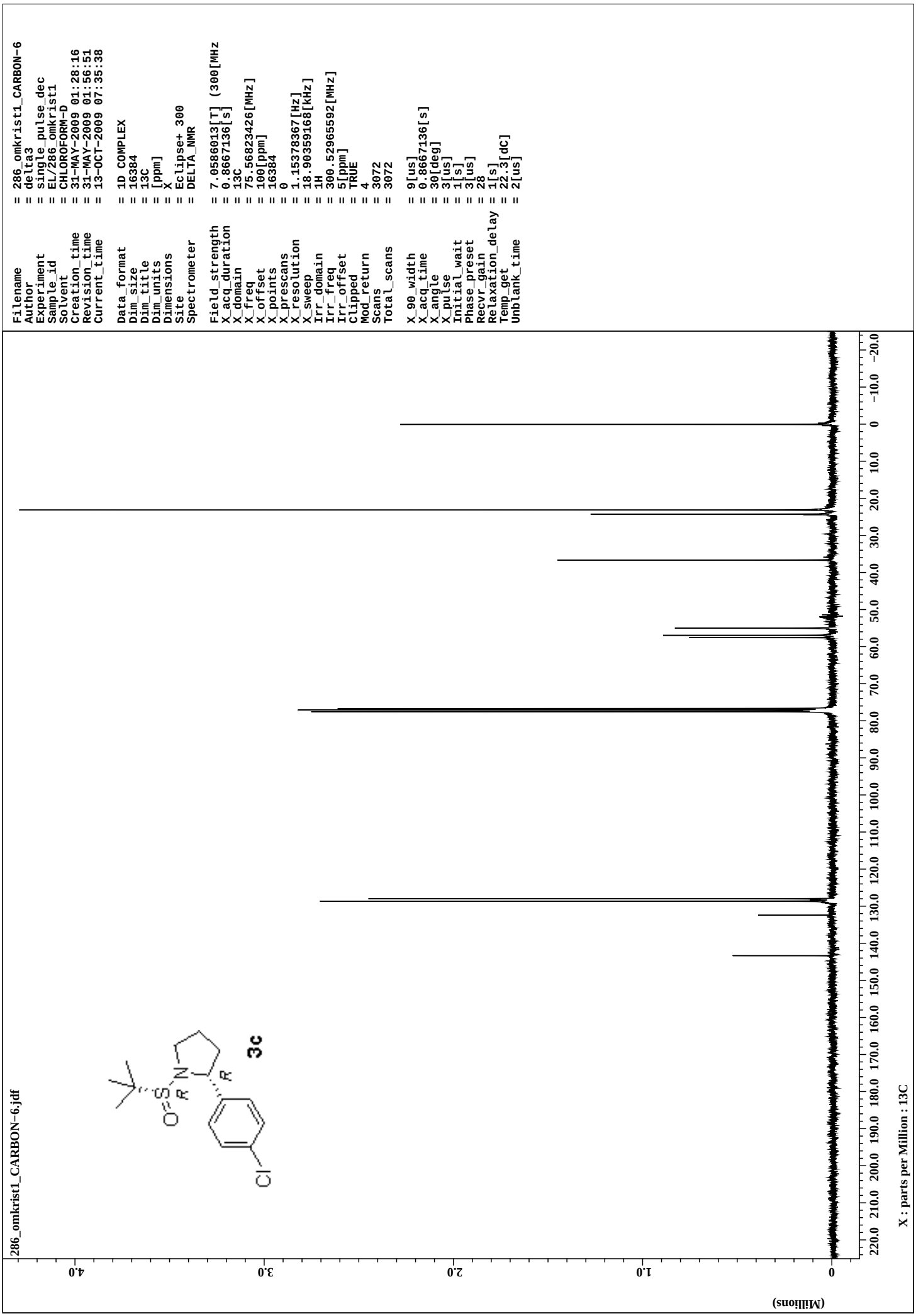

Filename = 269(c)_PROTON-10.jdf
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/269(c)
Solvent = CHLOROFORM-D
Creation_time = 24-APR-2009 02:17:37
Revision_time = 13-OCT-2009 15:11:51
Current_time = 13-OCT-2009 15:12:35
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11.3[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 11.3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 11
Relaxation_delay = 5[s]
Temp_get = 20.5[dC]
Unblank_time = 2[us]
269(c)_PROTON-10.jdf
1.729
0.704
0.116
0.245
0.235
10.948m
2d
MeO
(Millions)
X : parts per Million : 1H

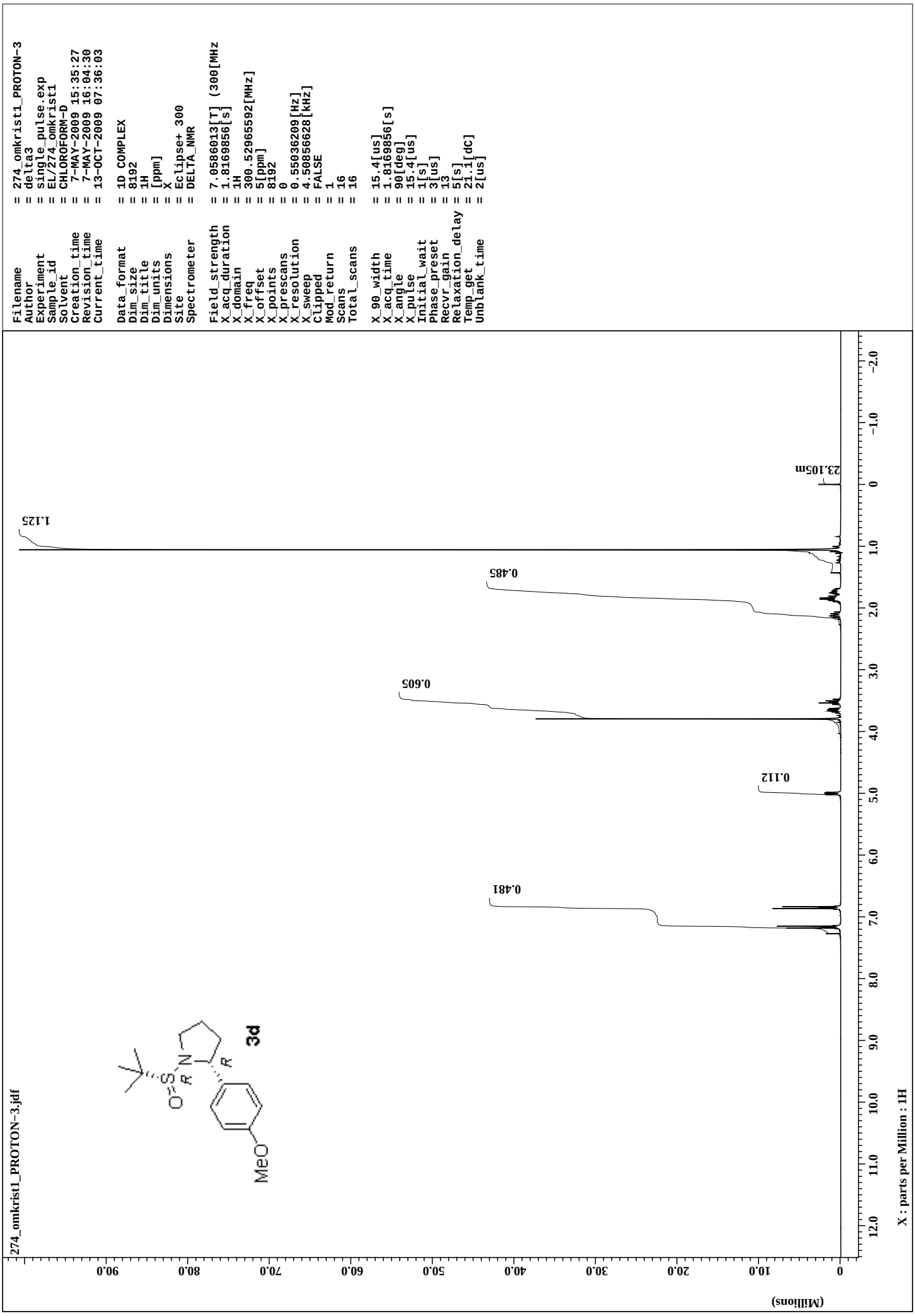

Filename = 269(c)_CARBON-3.jdf
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/269(c)
Solvent = CHLOROFORM-D
Creation_time = 24-APR-2009 02:53:48
Revision_time = 24-APR-2009 03:23:31
Current_time = 13-OCT-2009 07:46:11
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 1024
Total_scans = 1024
X_90_width = 8.4[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 2.8[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 21.4[dC]
Unblank_time = 2[us]
269(c)_CARBON-3.jdf
2d
MeO
O=S
NH
Cl
(Millions)
X : parts per Million : 13C

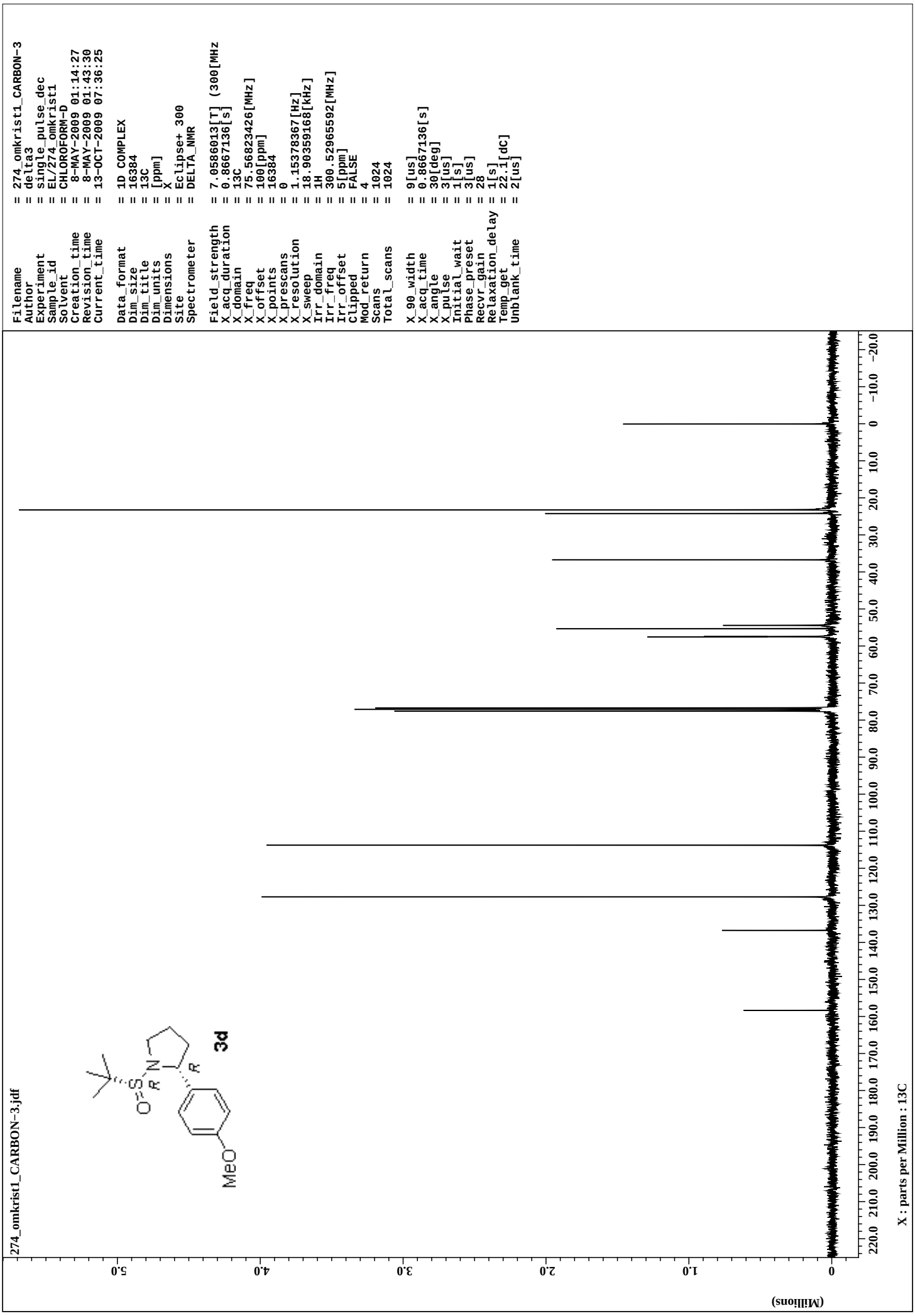

Filename = 266_omkrist2_PROTON-3
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/266_omkrist2
Solvent = CHLOROFORM-D
Creation_time = 1-MAY-2009 03:50:05
Revision_time = 1-MAY-2009 04:19:22
Current_time = 13-OCT-2009 07:34:29
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 15.4[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 15.4[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 16
Relaxation_delay = 5[s]
Temp_get = 20.5[dC]
Unblank_time = 2[us]
1.089
0.897
0.338m
0.236
0.112
0.481
51.072m
266_omkrist2_PROTON-3.jdf
3b
(Millions)
X : parts per Million : 1H

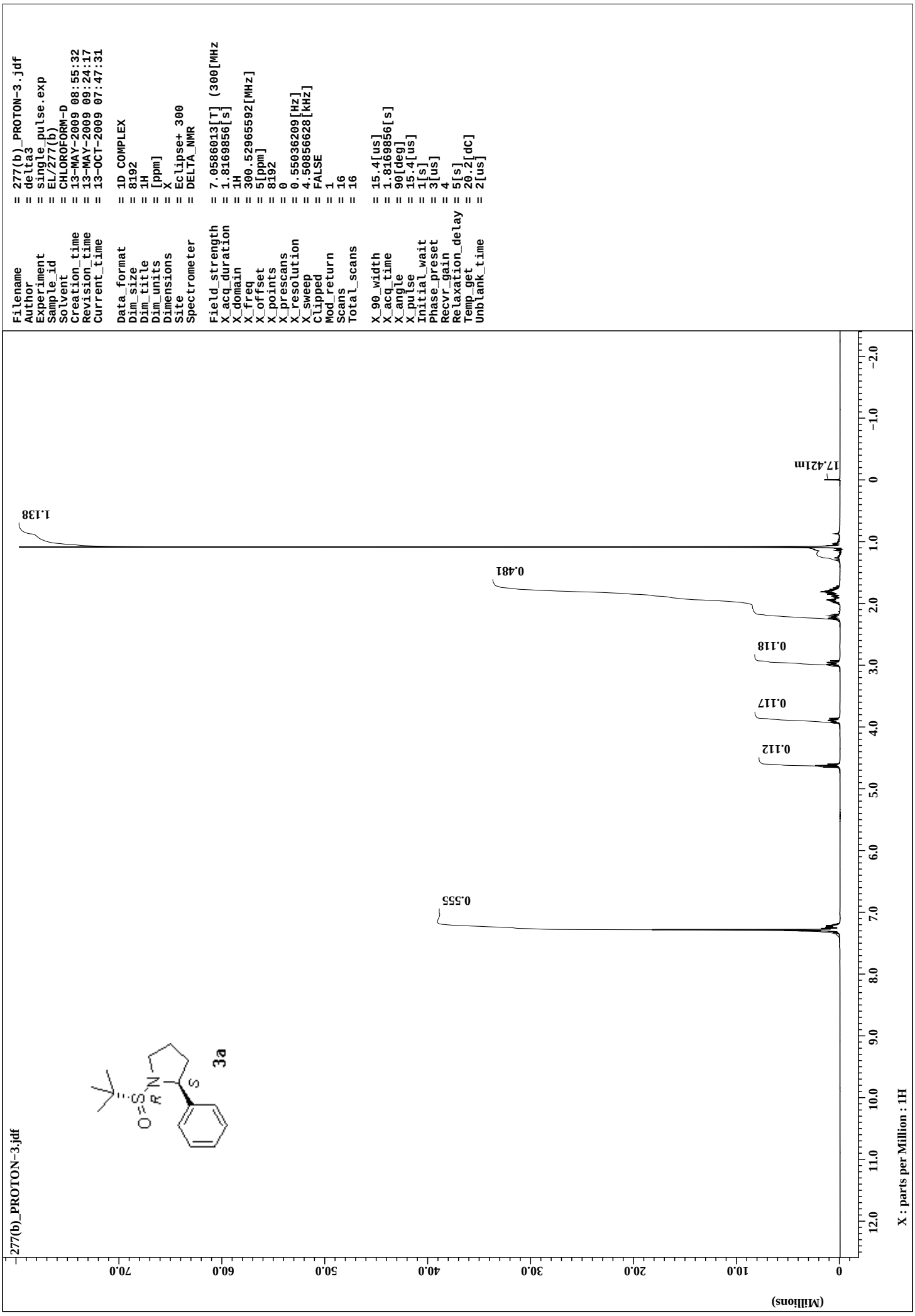

Filename = 266_omkrist2_CARBON-3
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/266_omkrist2
Solvent = CHLOROFORM-D
Creation_time = 1-MAY-2009 04:57:06
Revision_time = 1-MAY-2009 05:26:26
Current_time = 13-OCT-2009 07:34:50
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 2000
Total_scans = 2000
X_90_width = 9[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 29
Relaxation_delay = 1[s]
Temp_get = 21.4[dC]
Unblank_time = 2[us]
266_omkrist2_CARBON-3.jdf
3b
(Millions)
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : 13C

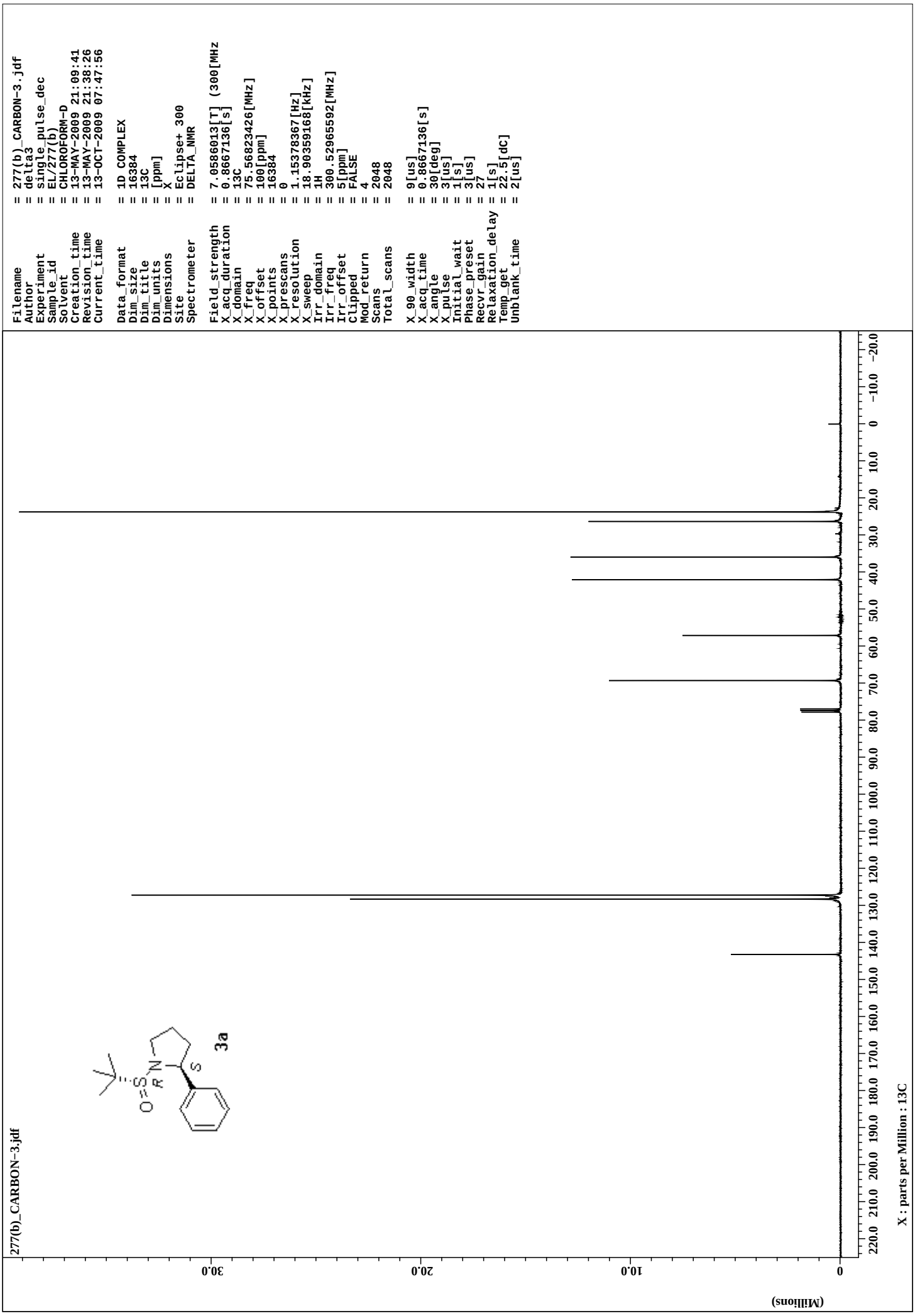

Filename = 286_omkrist1_PROTON-6
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/286_omkrist1
Solvent = CHLOROFORM-D
Creation_time = 29-MAY-2009 22:47:36
Revision_time = 29-MAY-2009 23:16:14
Current_time = 13-OCT-2009 07:35:15
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 15.4[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 15.4[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 13
Relaxation_delay = 5[s]
Temp_get = 21.2[dC]
Unblank_time = 2[us]
1.642
1.056
0.478
0.236
0.114
3c
286_omkrist1_PROTON-6.jdf
(Millions)
X : parts per Million : 1H

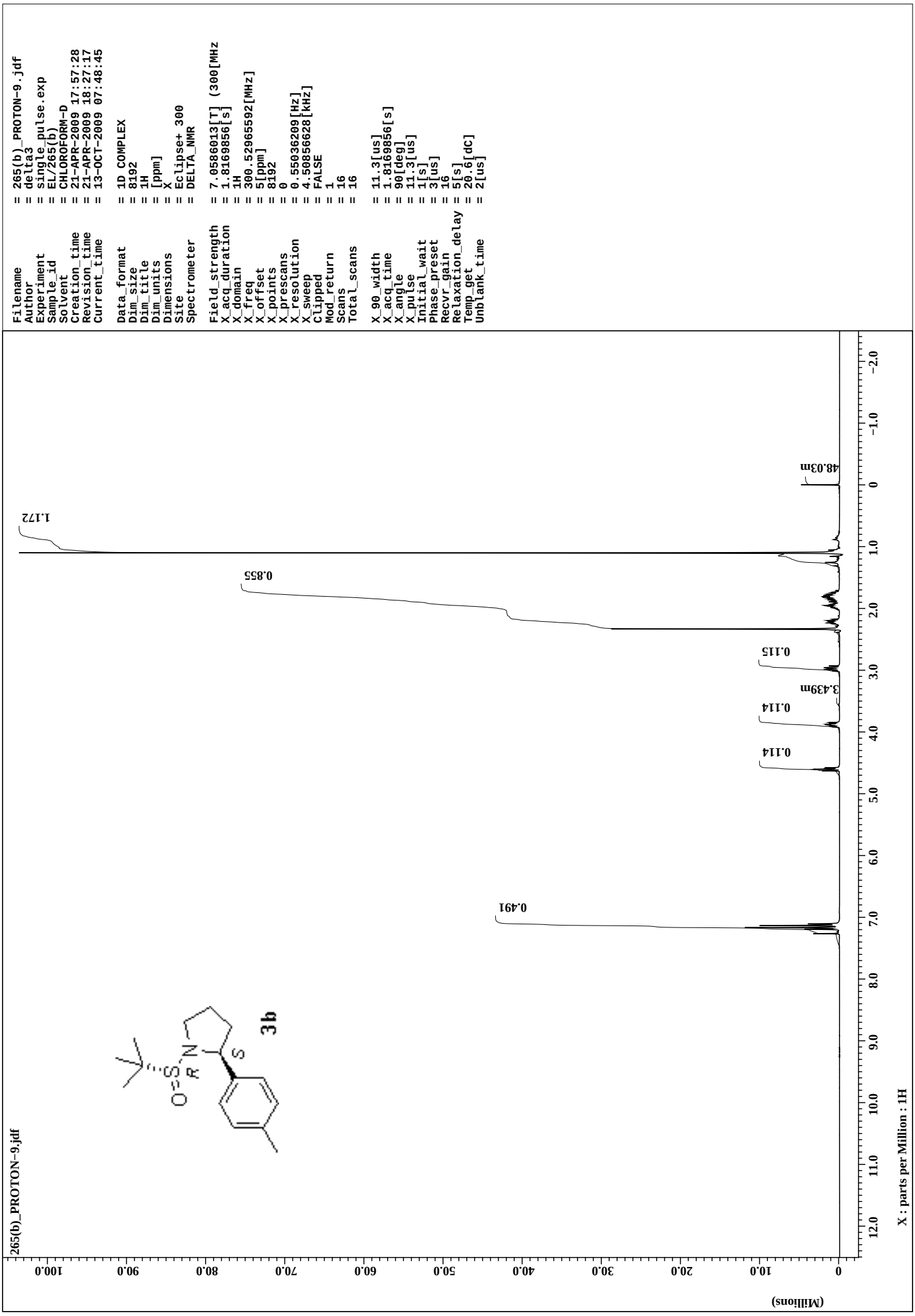

Filename = 286_omkrist1_CARBON-6
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/286_omkrist1
Solvent = CHLOROFORM-D
Creation_time = 31-MAY-2009 01:28:16
Revision_time = 31-MAY-2009 01:56:51
Current_time = 13-OCT-2009 07:35:38
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 4
Scans = 3072
Total_scans = 3072
X_90_width = 9[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 22.3[dC]
Unblank_time = 2[us]
286_omkrist1_CARBON-6.jdf
3c
(Millions)
X : parts per Million : 13C

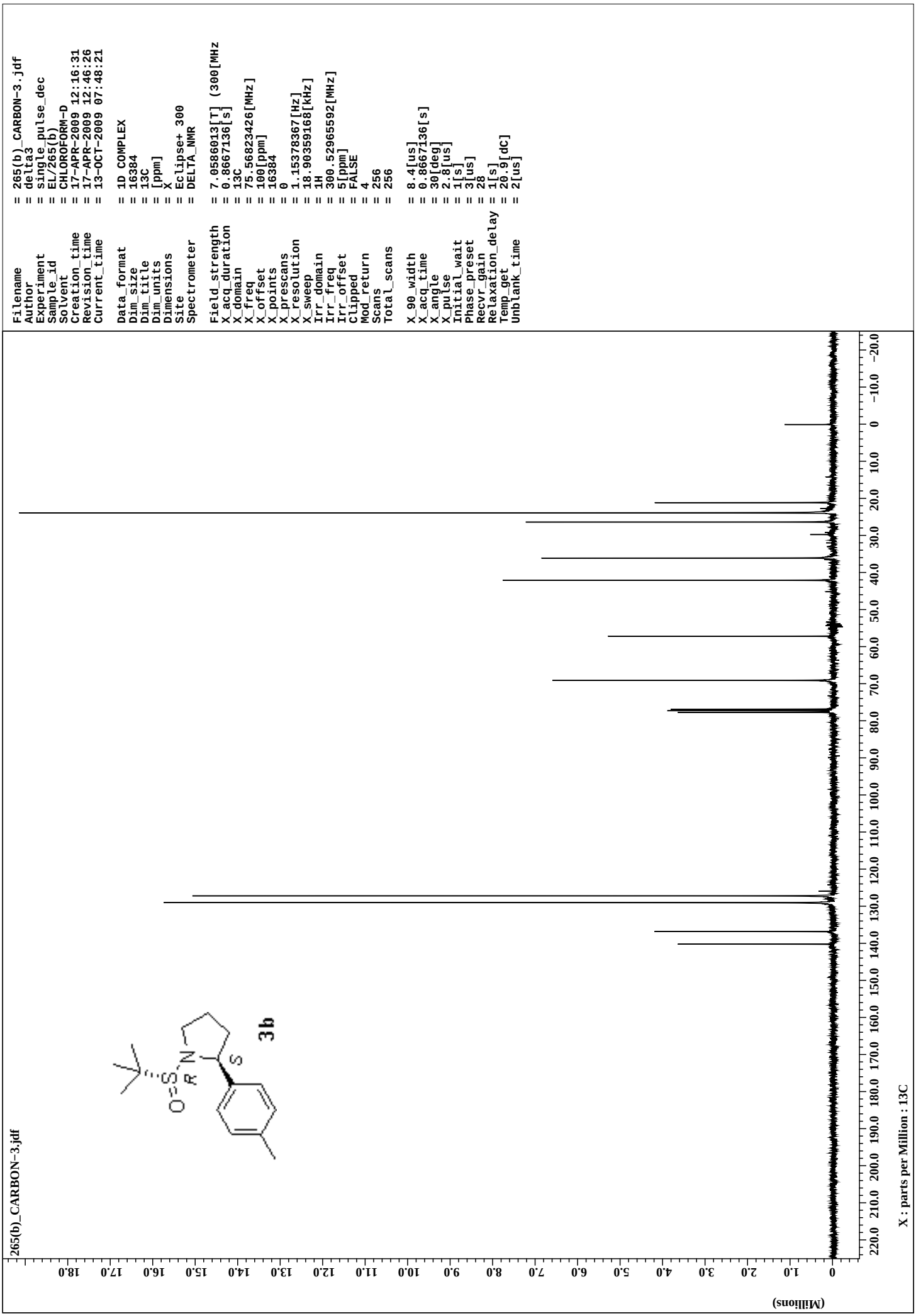

Filename = 274_omkrist1_PROTON-3
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/274_omkrist1
Solvent = CHLOROFORM-D
Creation_time = 7-MAY-2009 15:35:27
Revision_time = 7-MAY-2009 16:04:30
Current_time = 13-OCT-2009 07:36:03
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 15.4[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 15.4[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 13
Relaxation_delay = 5[s]
Temp_get = 21.1[dC]
Unblank_time = 2[us]
1.125
23.105m
0.485
0.605
0.112
0.481
(Millions)
X : parts per Million : 1H
274_omkrist1_PROTON-3.jdf
3d
MeO

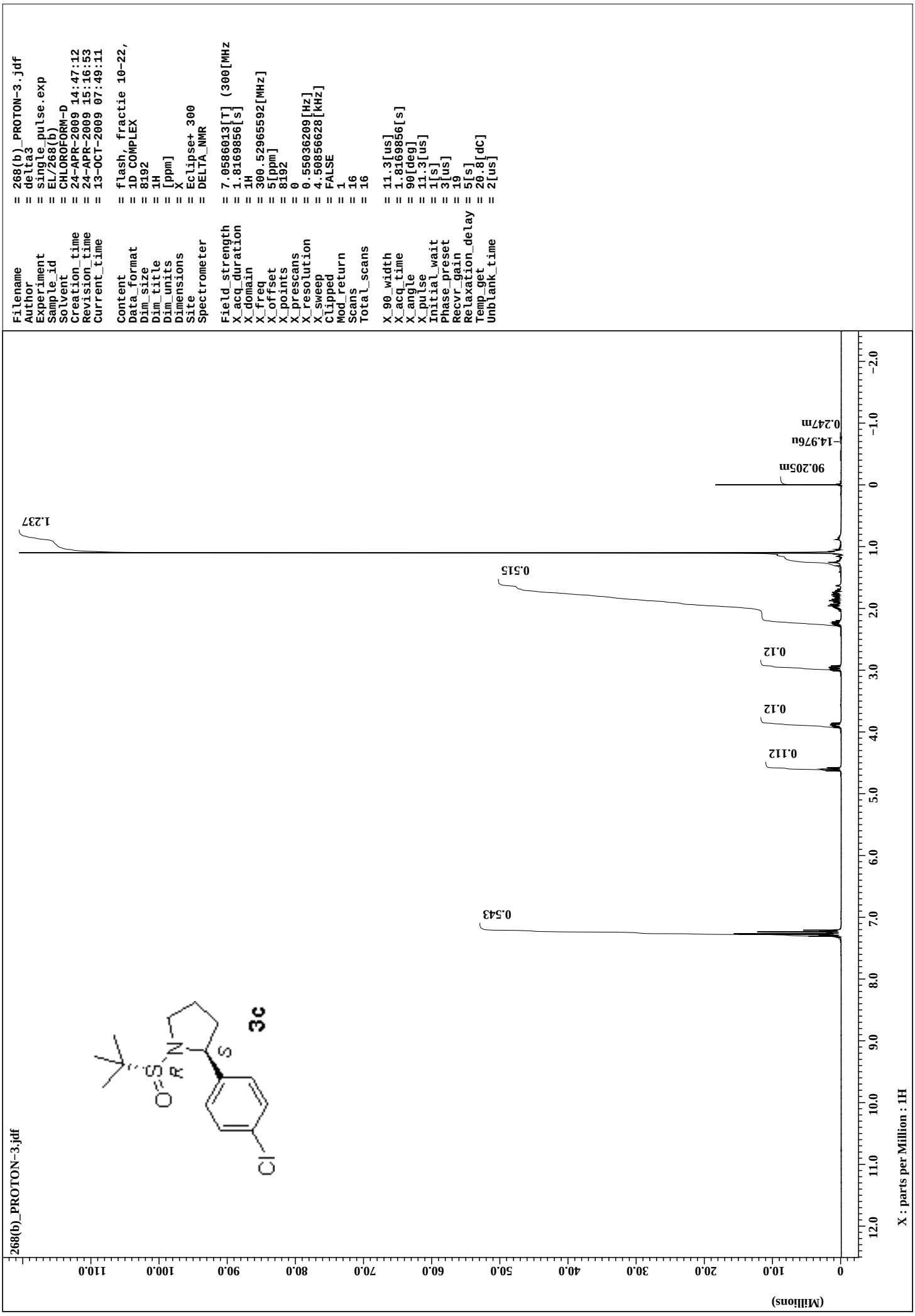

Filename = 274_omkrist1_CARBON-3
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/274_omkrist1
Solvent = CHLOROFORM-D
Creation_time = 8-MAY-2009 01:14:27
Revision_time = 8-MAY-2009 01:43:30
Current_time = 13-OCT-2009 07:36:25
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 1024
Total_scans = 1024
X_90_width = 9[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 22.1[dC]
Unblank_time = 2[us]
274_omkrist1_CARBON-3.jdf
3d
MeO
(Millions)
X : parts per Million : 13C

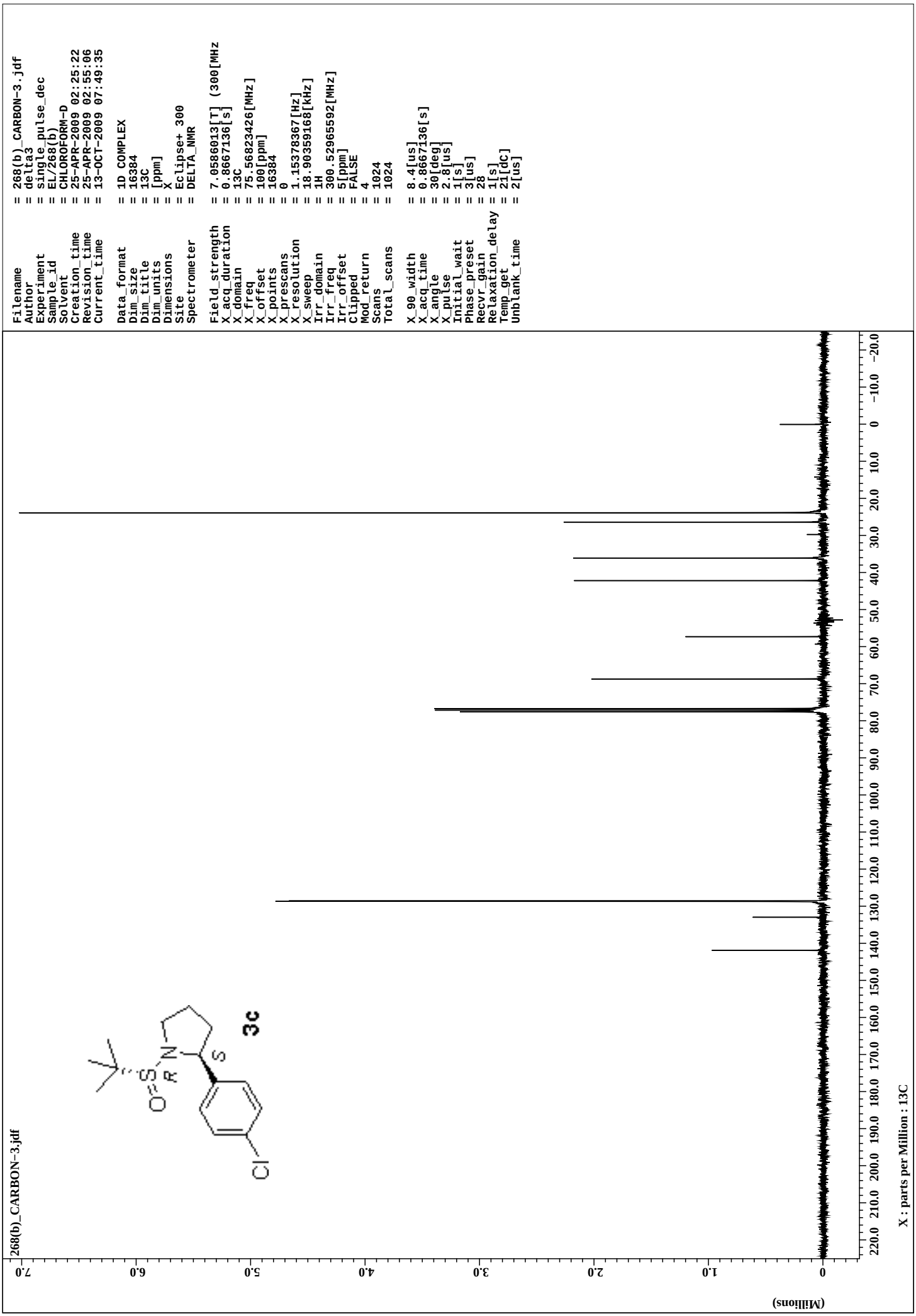

Filename = 277(b)_PROTON-3.jdf
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/277(b)
Solvent = CHLOROFORM-D
Creation_time = 13-MAY-2009 08:55:32
Revision_time = 13-MAY-2009 09:24:17
Current_time = 13-OCT-2009 07:47:31
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 15.4[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 15.4[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 4
Relaxation_delay = 5[s]
Temp_get = 20.2[dC]
Unblank_time = 2[us]
277(b)_PROTON-3.jdf
3a
1.138
17.421m
0.481
0.118
0.117
0.112
0.555
(Millions)
X : parts per Million : 1H

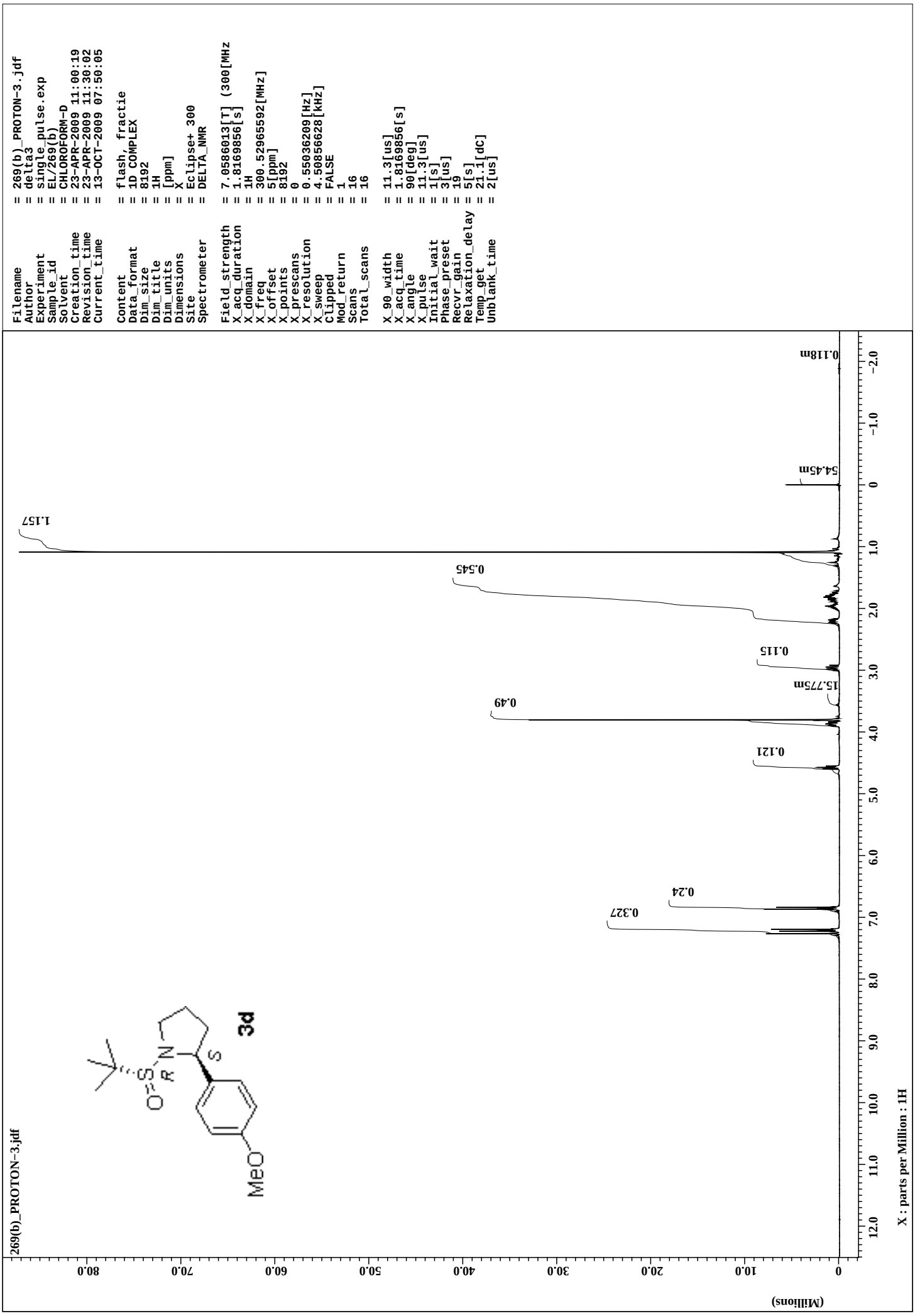

Filename = 277(b)_CARBON-3.jdf
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/277(b)
Solvent = CHLOROFORM-D
Creation_time = 13-MAY-2009 21:09:41
Revision_time = 13-MAY-2009 21:38:26
Current_time = 13-OCT-2009 07:47:56
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 2048
Total_scans = 2048
X_90_width = 9[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 27
Relaxation_delay = 1[s]
Temp_get = 22.5[dC]
Unblank_time = 2[us]
277(b)_CARBON-3.jdf
3a
(Millions)
30.0
20.0
10.0
0
X : parts per Million : 13C
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0

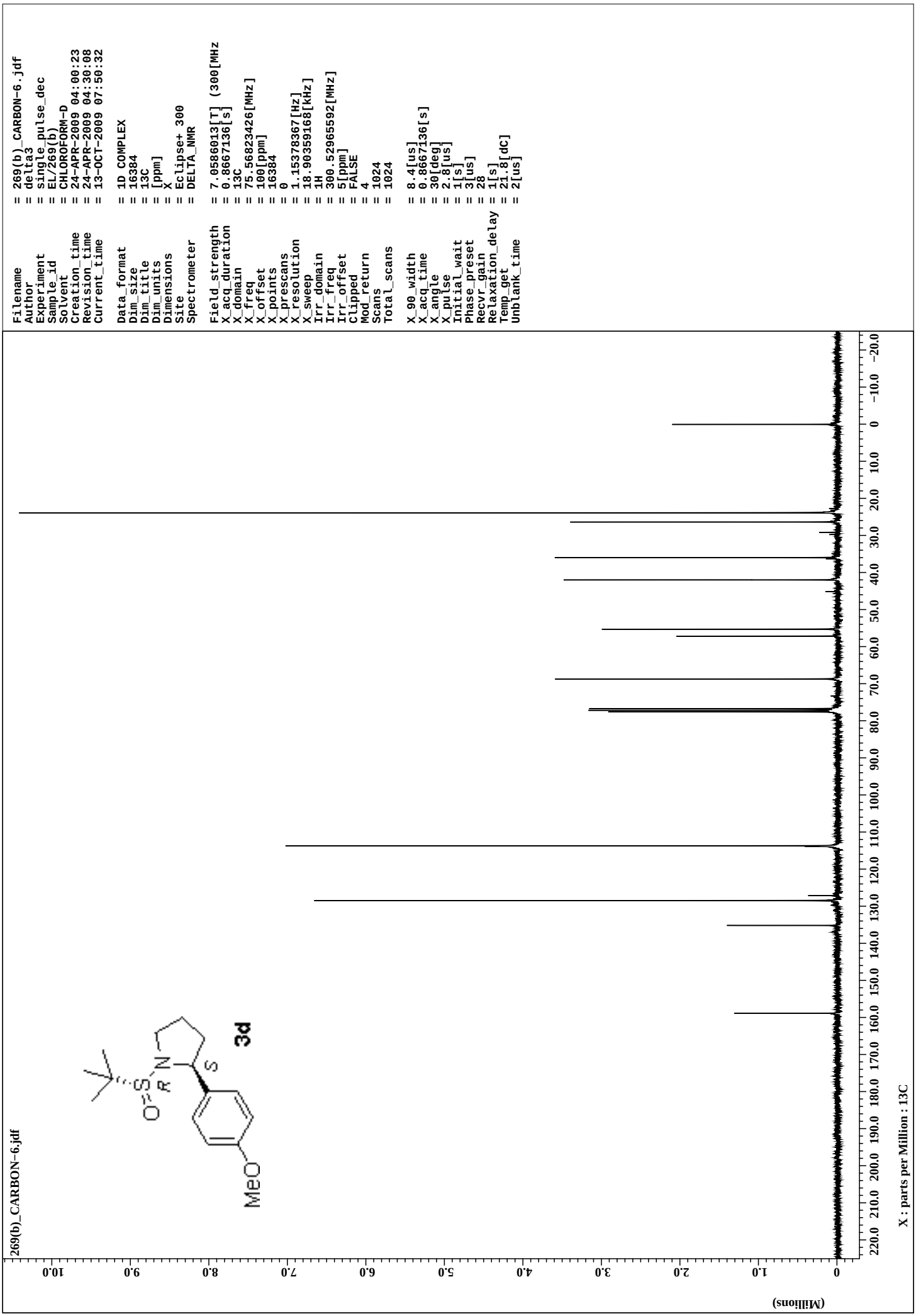

Filename = 265(b)_PROTON-9.jdf
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/265(b)
Solvent = CHLOROFORM-D
Creation_time = 21-APR-2009 17:57:28
Revision_time = 21-APR-2009 18:27:17
Current_time = 13-OCT-2009 07:48:45
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11.3[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 11.3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 16
Relaxation_delay = 5[s]
Temp_get = 20.6[dC]
Unblank_time = 2[us]
1.172
0.855
0.491
0.115
3.439m
0.114
0.114
48.03m
3b
265(b)_PROTON-9.jdf
X : parts per Million : 1H
(Millions)

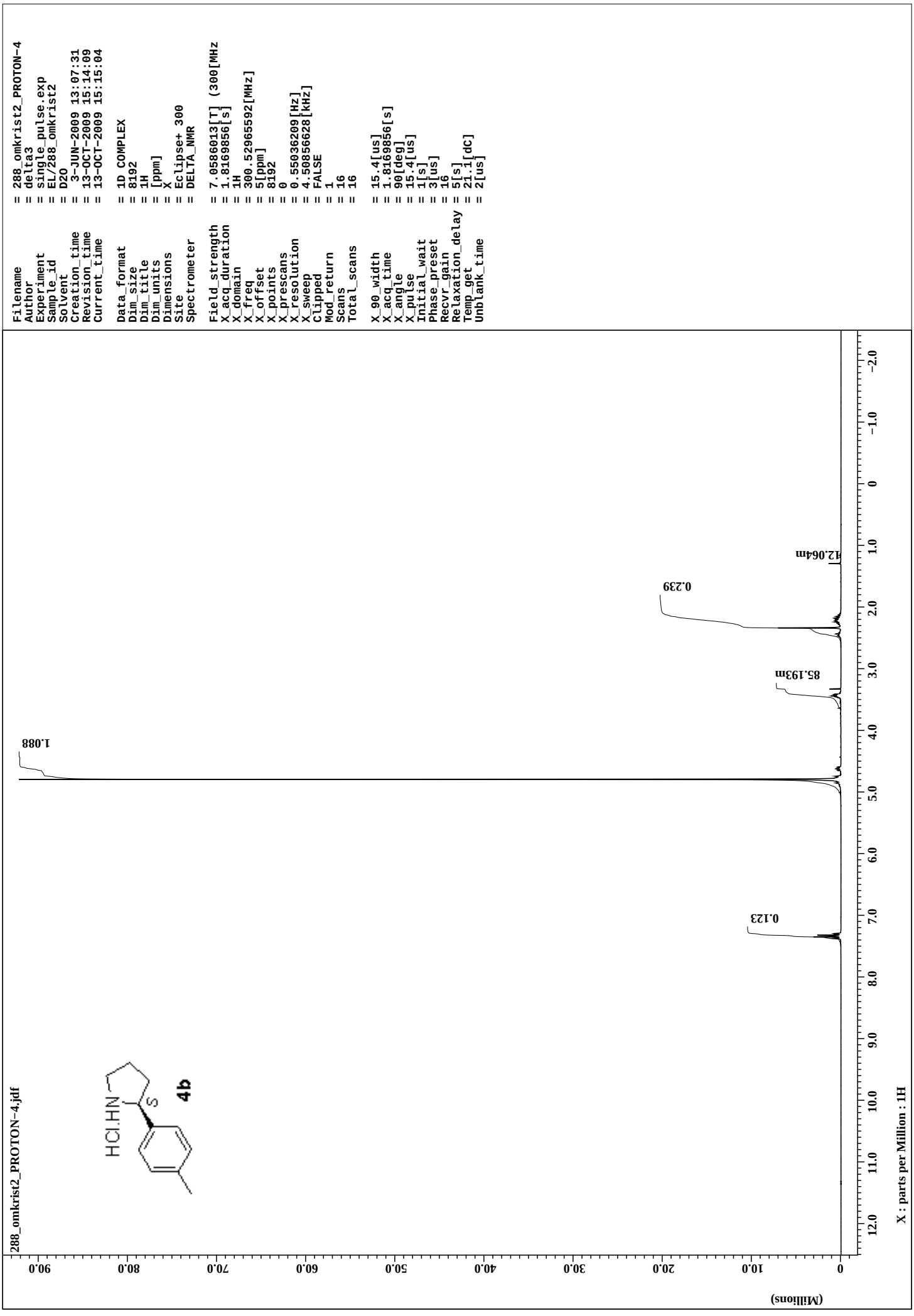

Filename = 265(b)_CARBON-3.jdf
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/265(b)
Solvent = CHLOROFORM-D
Creation_time = 17-APR-2009 12:16:31
Revision_time = 17-APR-2009 12:46:26
Current_time = 13-OCT-2009 07:48:21
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 256
Total_scans = 256
X_90_width = 8.4[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 2.8[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 20.9[dC]
Unblank_time = 2[us]
265(b)_CARBON-3.jdf
3b
(Millions)
X : parts per Million : 13C

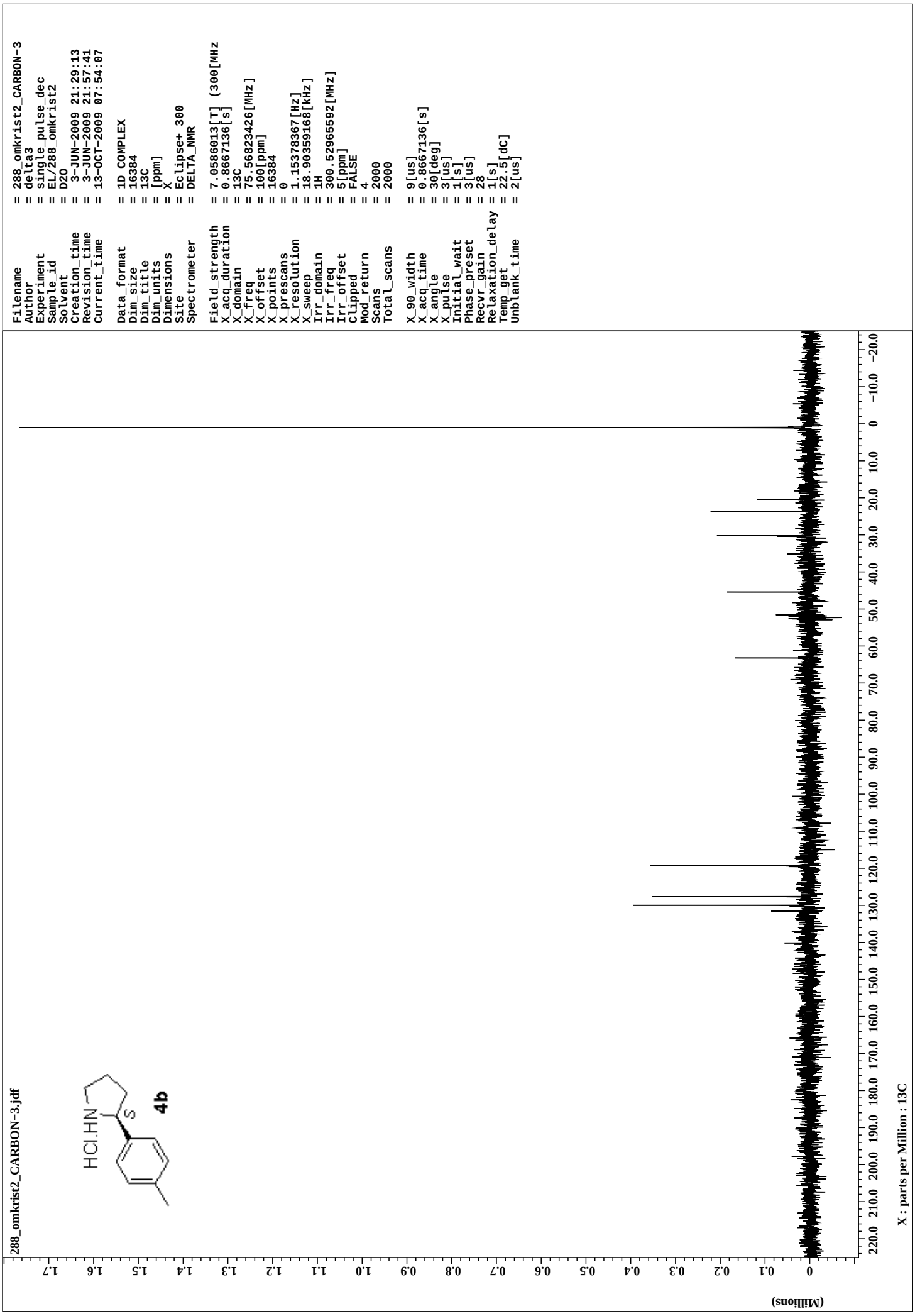

Filename = 268(b)_PROTON-3.jdf
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/268(b)
Solvent = CHLOROFORM-D
Creation_time = 24-APR-2009 14:47:12
Revision_time = 24-APR-2009 15:16:53
Current_time = 13-OCT-2009 07:49:11
Content = flash, fractie 10-22,
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11.3[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 11.3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 19
Relaxation_delay = 5[s]
Temp_get = 20.8[dC]
Unblank_time = 2[us]
268(b)_PROTON-3.jdf
3c
1.237
0.515
0.543
0.12
0.12
0.112
90.205m
14.976u
0.247m
(Millions)
X : parts per Million : 1H

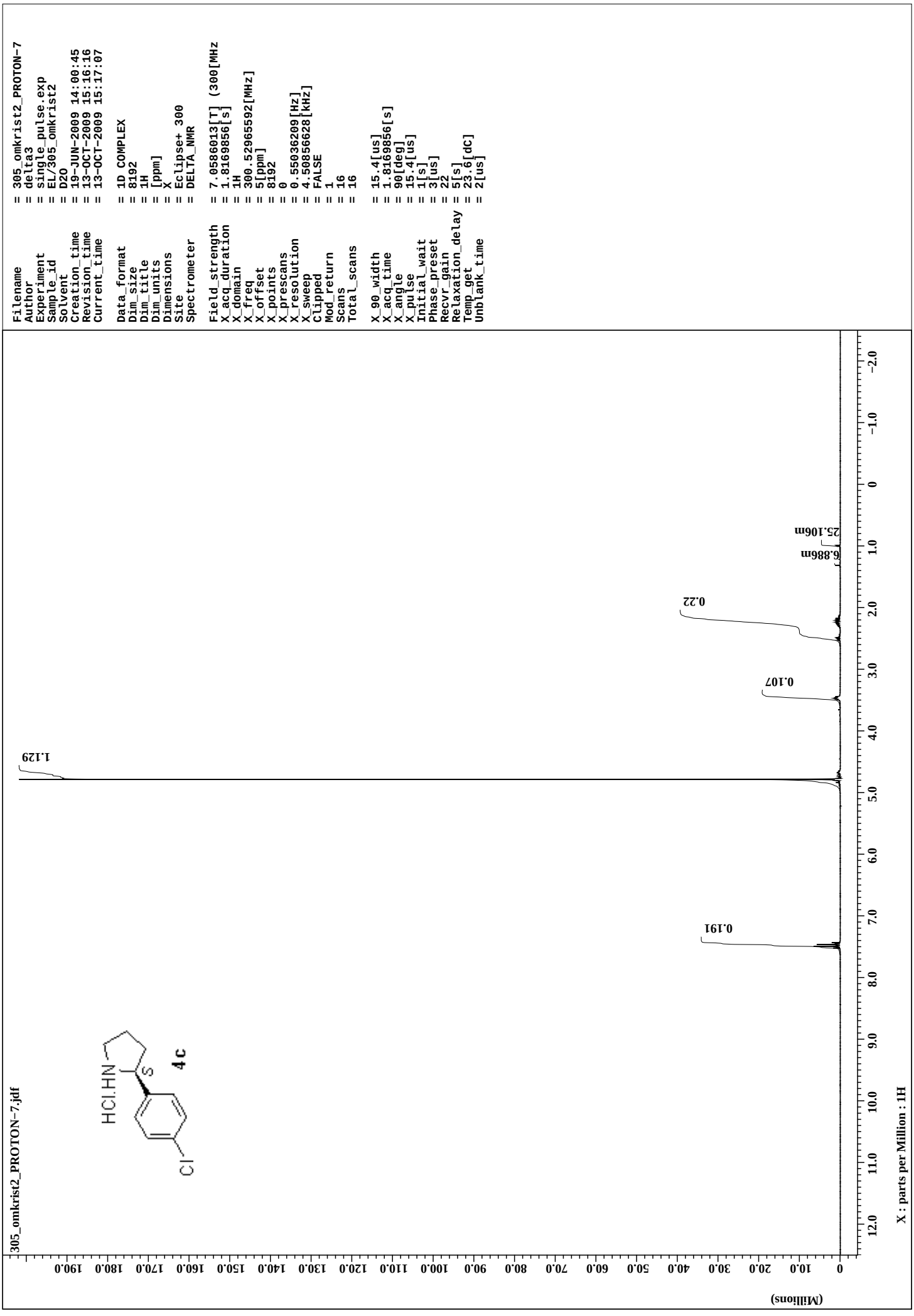

Filename = 268(b)_CARBON-3.jdf
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/268(b)
Solvent = CHLOROFORM-D
Creation_time = 25-APR-2009 02:25:22
Revision_time = 25-APR-2009 02:55:06
Current_time = 13-OCT-2009 07:49:35
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 1024
Total_scans = 1024
X_90_width = 8.4[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 2.8[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 21[dC]
Unblank_time = 2[us]
268(b)_CARBON-3.jdf
3c
(Millions)
X : parts per Million : 13C

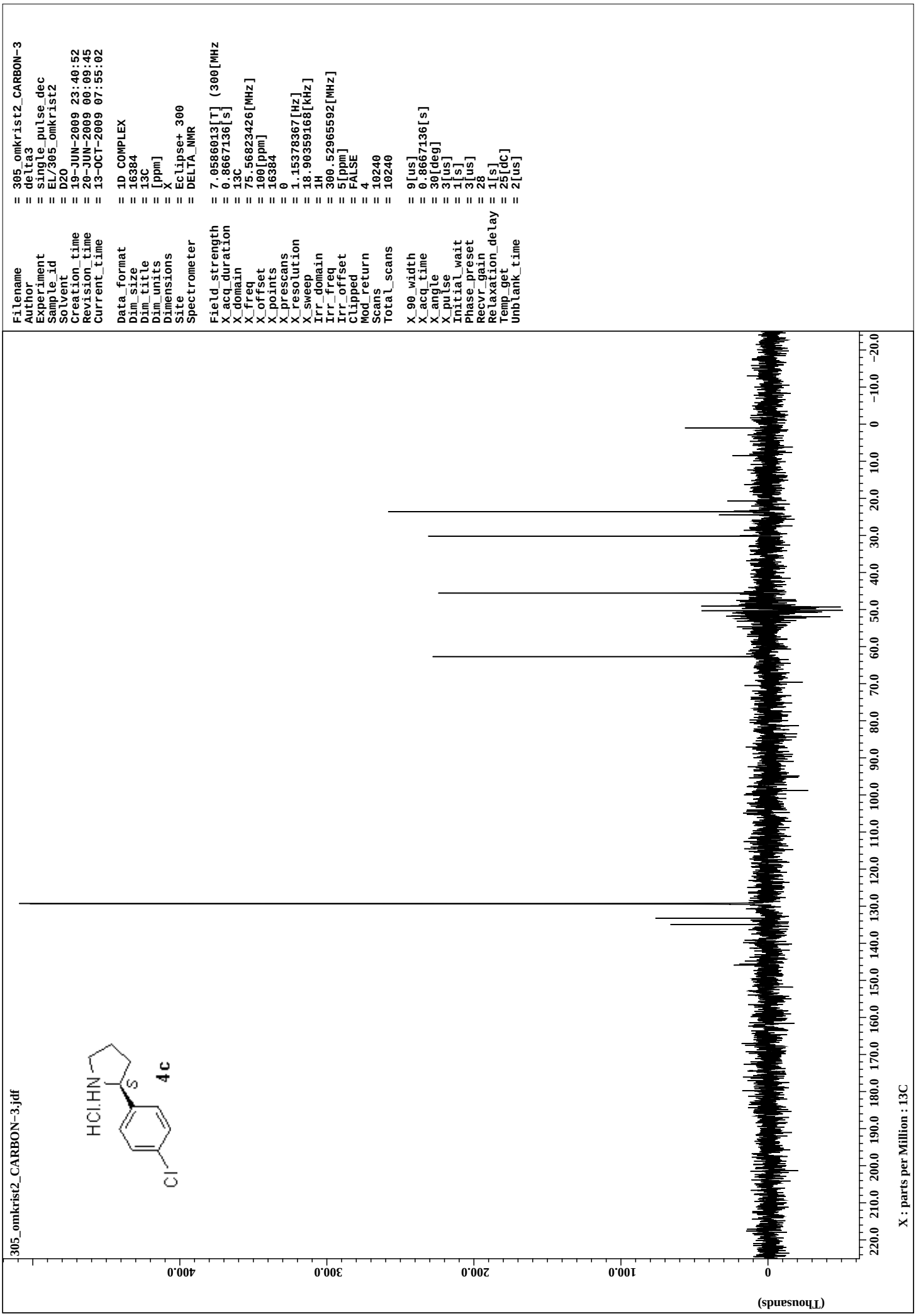

Filename = 269(b)_PROTON-3.jdf
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/269(b)
Solvent = CHLOROFORM-D
Creation_time = 23-APR-2009 11:00:19
Revision_time = 23-APR-2009 11:30:02
Current_time = 13-OCT-2009 07:50:05
Content = flash, fractie
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11.3[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 11.3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 19
Relaxation_delay = 5[s]
Temp_get = 21.1[dC]
Unblank_time = 2[us]
269(b)_PROTON-3.jdf
3d
MeO
1.157
0.545
0.49
0.327
0.24
0.121
0.115
15.775m
54.45m
0.118m
(Millions)
X : parts per Million : 1H

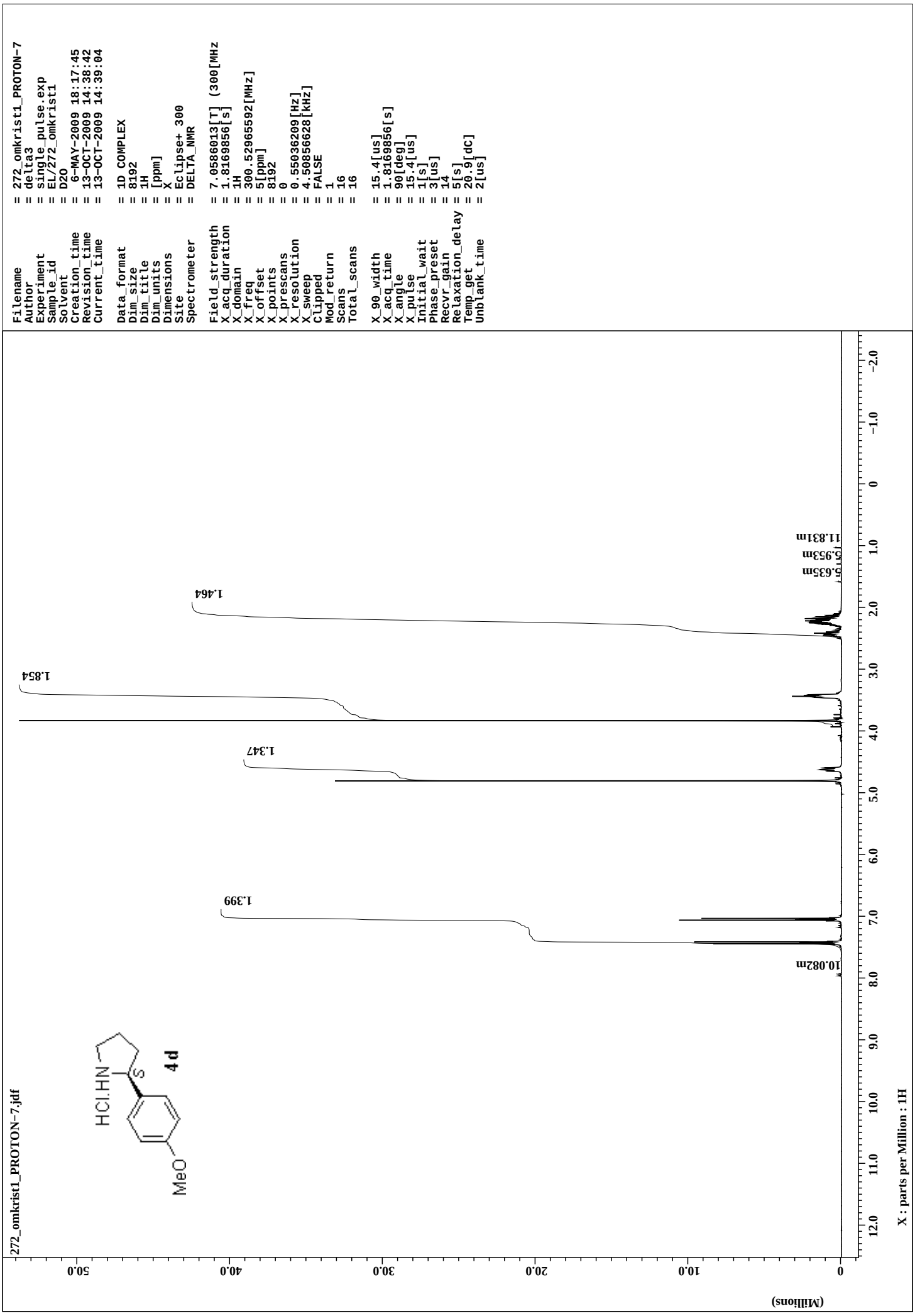

Filename = 269(b)_CARBON-6.jdf
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/269(b)
Solvent = CHLOROFORM-D
Creation_time = 24-APR-2009 04:00:23
Revision_time = 24-APR-2009 04:30:08
Current_time = 13-OCT-2009 07:50:32
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 1024
Total_scans = 1024
X_90_width = 8.4[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 2.8[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 21.8[dC]
Unblank_time = 2[us]
269(b)_CARBON-6.jdf
3d
MeO
(Millions)
X : parts per Million : 13C

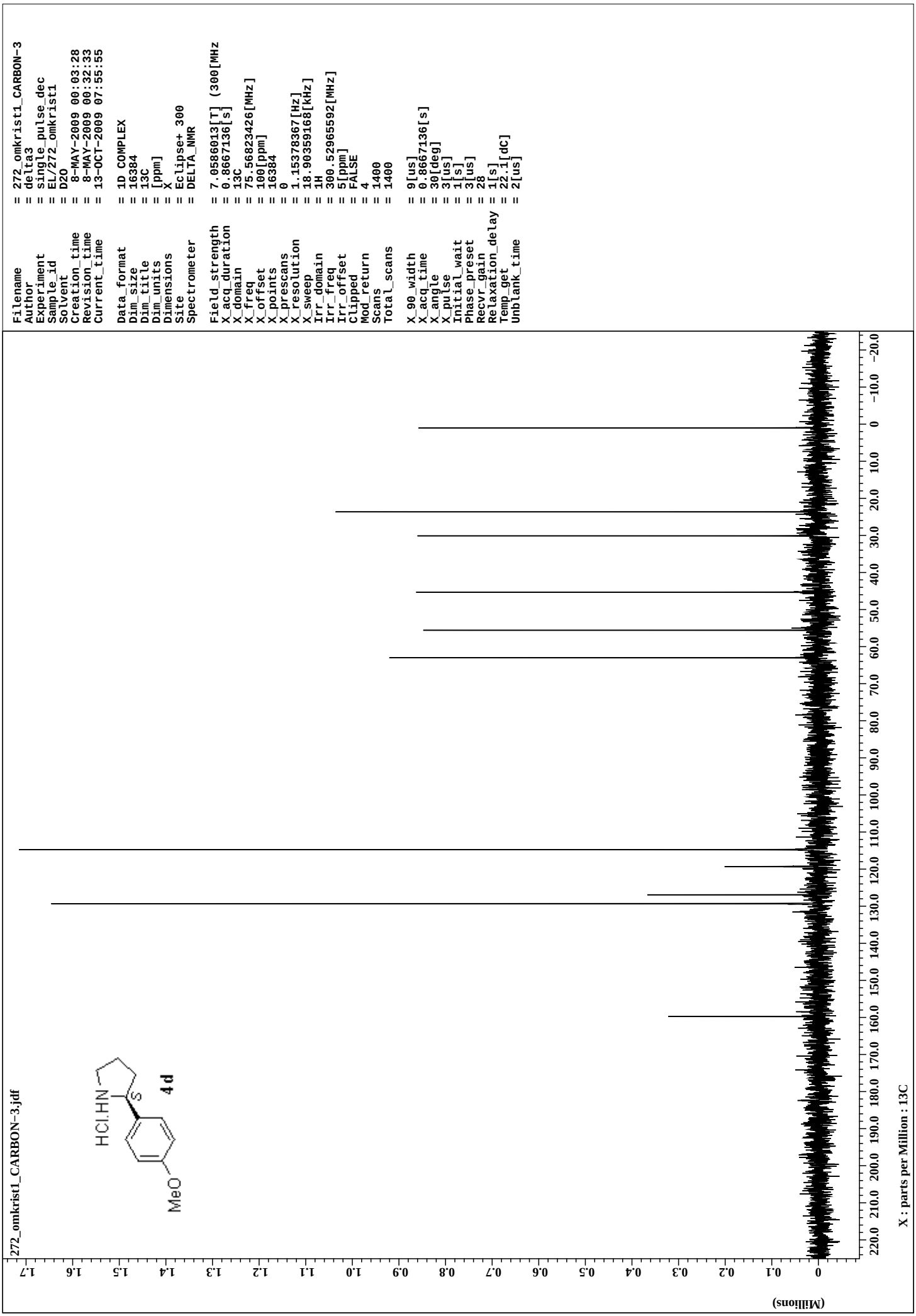

Filename = 288_omkrist2_PROTON-4
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/288_omkrist2
Solvent = D2O
Creation_time = 3-JUN-2009 13:07:31
Revision_time = 13-OCT-2009 15:14:09
Current_time = 13-OCT-2009 15:15:04
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 15.4[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 15.4[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 16
Relaxation_delay = 5[s]
Temp_get = 21.1[dC]
Unblank_time = 2[us]
288_omkrist2_PROTON-4.jdf
HCl.HN
S
4b
1.088
0.123
85.193m
0.239
12.064m
(Millions)
X : parts per Million : 1H


288_omkrist2_CARBON-3.jdf
HCl.HN
S
4b
Filename = 288_omkrist2_CARBON-3
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/288_omkrist2
Solvent = D2O
Creation_time = 3-JUN-2009 21:29:13
Revision_time = 3-JUN-2009 21:57:41
Current_time = 13-OCT-2009 07:54:07
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 2000
Total_scans = 2000
X_90_width = 9[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 22.5[dC]
Unblank_time = 2[us]
(Millions)
X : parts per Million : 13C


Filename = 305_omkrist2_PROTON-7
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/305_omkrist2
Solvent = D2O
Creation_time = 19-JUN-2009 14:00:45
Revision_time = 13-OCT-2009 15:16:16
Current_time = 13-OCT-2009 15:17:07
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 15.4[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 15.4[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 22
Relaxation_delay = 5[s]
Temp_get = 23.6[dC]
Unblank_time = 2[us]
305_omkrist2_PROTON-7.jdf
HCl.HN
S
Cl
4c
1.129
0.191
0.107
0.22
6.886m
25.106m
(Millions)
X : parts per Million : 1H


Filename = 305_omkrist2_CARBON-3
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/305_omkrist2
Solvent = D2O
Creation_time = 19-JUN-2009 23:40:52
Revision_time = 20-JUN-2009 00:09:45
Current_time = 13-OCT-2009 07:55:02
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 10240
Total_scans = 10240
X_90_width = 9[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 25[dC]
Unblank_time = 2[us]
305_omkrist2_CARBON-3.jdf
HCl.HN
S
Cl
4c
(Thousands)
400.0
300.0
200.0
100.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : 13C


Filename = 272_omkrist1_PROTON-7
Author = delta3
Experiment = single_pulse.exp
Sample_id = EL/272_omkrist1
Solvent = D2O
Creation_time = 6-MAY-2009 18:17:45
Revision_time = 13-OCT-2009 14:38:42
Current_time = 13-OCT-2009 14:39:04
Data_format = 1D COMPLEX
Dim_size = 8192
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 1.8169856[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 8192
X_prescans = 0
X_resolution = 0.55036209[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 15.4[us]
X_acq_time = 1.8169856[s]
X_angle = 90[deg]
X_pulse = 15.4[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 14
Relaxation_delay = 5[s]
Temp_get = 20.9[dC]
Unblank_time = 2[us]
272_omkrist1_PROTON-7.jdf
HCl.HN
S
MeO
4 d
1.854
1.464
1.347
1.399
10.082m
6.635m
6.353m
3.953m
1.831m
(Millions)
X : parts per Million : 1H


Filename = 272_omkrist1_CARBON-3
Author = delta3
Experiment = single_pulse_dec
Sample_id = EL/272_omkrist1
Solvent = D2O
Creation_time = 8-MAY-2009 00:03:28
Revision_time = 8-MAY-2009 00:32:33
Current_time = 13-OCT-2009 07:55:55
Data_format = 1D COMPLEX
Dim_size = 16384
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR
Field_strength = 7.0586013[T] (300[MHz
X_acq_duration = 0.8667136[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 1.15378367[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 4
Scans = 1400
Total_scans = 1400
X_90_width = 9[us]
X_acq_time = 0.8667136[s]
X_angle = 30[deg]
X_pulse = 3[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 28
Relaxation_delay = 1[s]
Temp_get = 22.1[dC]
Unblank_time = 2[us]
272_omkrist1_CARBON-3.jdf
HCl.HN
S
MeO
4 d
(Millions)
X : parts per Million : 13C