# Efficient synthesis of benzene-fused 6/7-membered amides via intramolecular C-N bond formation

Xu Zhou[1,2,*], Li Ke[2], Zhai Rongliang[1,2], Liang Ting[1,2], Gui Xiaodie[2], Zhang Rongli[1]

[1]Department of Chemistry, Xuzhou Medical University, Xuzhou 221004, China

[2]Jiangsu Key Laboratory of New Drug Research and Clinical Pharmacy, Xuzhou Medical University, Xuzhou 221004, China

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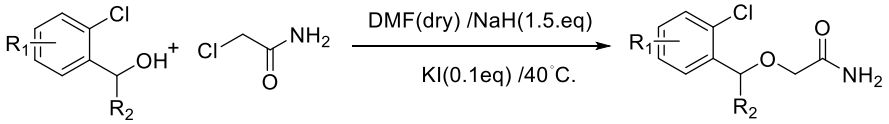
# I. General data

Commercially available reagents were used without further purification. The solvents used for experiment research were all through pretreatment on condition of anaerobic and without water. Reactions were monitored by thin layer chromatography (TLC) using Silicycle precoated silica gel plates. Flash column chromatography was performed over Silicycle silica gel (300-400 mesh). $^{1}$H NMR and $^{13}$C NMR spectra were recorded on JMTC-400/54/SS 400 MHz spectrometers using residue solvent peaks as internal standards ($CHCl_3$, $^{1}$H: 7.26 ppm; 13C:77.00 ppm). Infrared spectra were recorded with a PerkinElmer Spectrum Two FT-IR spectrometer and are reported in reciprocal centimeter ($cm^{-1}$). Mass spectra were recorded with MicroTof-II using electron spray ionization (MeOH as solvent) or Waters GCT Premier time-of-flight mass spectrometer with a field ionization (FI) ion source.

# II. Synthesis and Characterization of Substrates

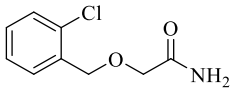
## 1. Synthesis of 2-(2-chlorophenoxy)acetamide Derivatives




$R_2$=H, $CH_3$ **1a-1j**

NaH (7.5 mmol, 0.3 g) was added to Schlenk tube. The mixture was stirred and anhydrous DMF (2 mL) was added under argon. 2-Chlorobenzyl alcohol (4.5 mmol, 0.634 g) was dissolved in dry DMF (2 mL) which was slowly added to the Schlenk tube under ice-cooling and stirred for 1.5 h. Chloroacetamide (0.3 mmol, 0.1 equiv.) was dissolved in dry DMF (1.5 mL) and was slowly dropped into the reaction flask at room temperature and stirred for another 5 h. After the reaction was finished, water was added to destroy the excess NaH and the solution was extracted by ethyl acetate (50 mL X 3). The organic phases were combined and dried by sodium sulfate and was then concentrated. The residue was purified by flash chromatography on silica gel (eluent: hexanes/ethyl acetate 5/1) to afford the desired product. The yield was 35% -60%.

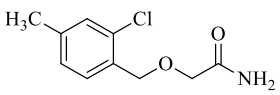
**2-((2-chlorobenzyl)oxy)acetylchloride 1a**




**1a**

56% yield, m.p.92-93 °C; $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 4.06 (s, 2H), 4.69 (s, 2H), 5.66 (s, 1H), 6.59 (s, 1H), 7.27-7.30 (m, 2H), 7.39-7.43 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 69.7, 70.8, 127.0, 129.5, 129.7, 133.5, 134.4, 172.1; IR $\nu$ ($cm^{-1}$): 3373.4, 3151.4, 1653.5, 1455.1, 1105.6; HRMS calcd for $C_9H_{10}ClNO_2$ $(M+Na)^+$ 222.0289, found 222.0285.

**2-((2-chloro-4-methylbenzyl)oxy)acetylchloride (1b)**

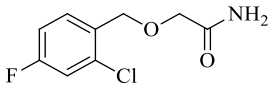



**1b**

60% yield, m.p.109-110 °C; $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 2.33 (s, 3H), 4.02 (s, 2H), 4.63 (s, 2H), 6.03 (s, 1H), 6.60

(s, 1H), 7.08 (d, *J* = 7.2 Hz, 1H), 7.21 (s, 1H), 7.25 (d, *J* = 8.4 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): *δ* ppm 20.9, 69.4, 70.7, 127.7, 129.8, 130.1, 131.2, 133.4, 140.0, 172.5; IR *v* ($cm^{-1}$): 3460.8, 3172.0, 2911.7, 1700.6, 1582.1; HRMS calcd for $C_{10}H_{12}ClNO_2$ $(M+Na)^+$ 236.0454, found 236.0453.

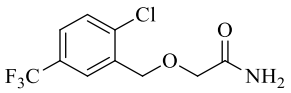
**2-((2-chloro-4-fluorobenzyl)oxy)acetamide (1c)**



**1c**

45% yield, m.p.151~152 °C; $^1$H NMR (400 MHz, $CDCl_3$): *δ* ppm 4.11 (s, 2H), 4.69 (s, 2H), 6.58 (s, 2H), 7.03 (dt, $J^1$ = 8.4 Hz, $J^2$ = 2.4 Hz, 1H), 7.14 (dd , $J^1$ = 8.4 Hz, $J^2$ = 2.4 Hz, 1H), 7.37-7.40 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): *δ* ppm 69.5, 70.2, 114.2 (d, *J* = 21.1 Hz), 117.1 (d, *J* = 24.0 Hz), 130.5 (d, *J* = 3.8 Hz), 130.9 (d, *J* = 8.6 Hz), 134.4 (d, *J* = 10.5 Hz), 162.4 (d, *J* = 249.2 Hz), 172.8; $^{19}$F NMR: *δ ppm:* -111.3; IR *v* ($cm^{-1}$): 3376.9, 3182.7, 1655.9, 1122.9, 810.8; HRMS calcd for $C_9H_9ClFNO_2$ $(M+Na)^+$ 240.0204, found 240.0228.

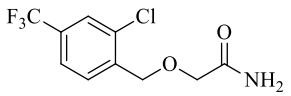
**2-((2-chloro-5-(trifluoromethyl)benzyl)oxy)acetamide (1d)**



**1d**

48% yield; $^1$H NMR (400 MHz, $CDCl_3$): *δ* ppm 4.10 (s, 2H), 4.72 (s, 2H), 6.11 (s, 1H), 6.54 (s, 1H), 7.51-7.56 (m, 2H), 7.71 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): *δ* ppm 70.0, 70.1, 123.6 (q, *J* = 271.2 Hz), 125.9 (q, *J* = 3.8 Hz), 126.1 (q, *J* = 3.9 Hz), 129.5 (q, *J* = 32.6 Hz), 130.1, 135.7, 136.7, 171.8; $^{19}$F NMR: *δ* ppm -62.4; IR *v* ($cm^{-1}$): 3459.1, 3151.4, 1699.0, 1253.5, 810.9; HRMS calcd for $C_{10}H_9ClF_3NO_2$ $(M+Na)^+$ 290.0172, found 290.0168.

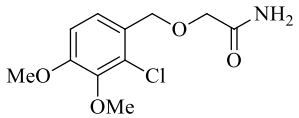
**2-((2-chloro-4-trifluoromethyl)benzyl)oxy)acetamide (1e)**



**1e**

35% yield, m.p.105~106 °C; $^1$H NMR (400 MHz, $CDCl_3$): *δ* ppm 4.19 (s, 2H), 4.73 (s, 2H), 6.02 (s, 2H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): *δ* ppm 67.9, 69.8, 123.2 (q, *J* = 271.2 Hz), 123.8 (q, *J* = 2.8 Hz), 126.3 (q, *J* = 3.8 Hz), 129.0, 131.4 (q, *J* = 33.5 Hz), 133.0, 138.8, 174.5; $^{19}$F NMR: *δ ppm* -62.7; IR *v* ($cm^{-1}$): 3459.1, 3151.4, 1699.0, 1253.5, 810.9; HRMS calcd for $C_{10}H_9ClF_3NO_2$ $(M+Na)^+$ 290.0172, found 290.0174.

**2-((2-chloro-3,4-dimethoxybenzyl)oxy)acetamide (1f)**

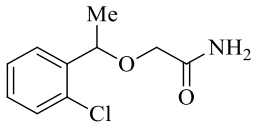


**1f**

56% yield, m.p.126~127 °C; $^1$H NMR (400 MHz, $CDCl_3$): *δ* ppm 3.87 (s, 3H), 3.89 (s, 3H), 4.02 (s, 2H), 4.62 (s, 2H), 5.58 (s, 1H), 6.58 (s, 1H), 6.83 (d, *J* = 8.0 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): *δ* ppm 56.1, 60.7, 69.4, 71.0, 110.2, 125.2, 127.2, 128.5, 145.7, 153.9, 172.2; IR *v* ($cm^{-1}$): 3355.5, 3172.8, 2905.3, 1651.9, 1583.8; HRMS

calcd for $C_{10}H_{14}ClNO_4$ $(M+Na)^+$ 282.0518, found 282.0518.

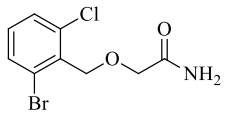
**2-(1-(2-chlorophenyl)ethoxy)acetamide (1g)**




**1g**

50% yield, m.p. 141~142 °C; $^1$H NMR (400 MHz, $CDCl_3$) : $\delta$ ppm 1.48 (d, $J$ = 6.4 Hz, 3H), 3.85 (s, 2H), 4.95 (q, $J$ = 6.4 Hz, 1H), 6.42 (s, 1H), 6.63 (s, 1H), 7.22 (t, $J$ = 7.6 Hz, 1H), 7.27-7.35 (m, 2H), 7.43 (dd, $J^1$ = 7.6 Hz, $J^2$ = 1.2 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 22.2, 68.0, 75.1, 126.4, 127.4, 128.8, 129.6, 132.4, 139.6, 172.7; IR $v$ ($cm^{-1}$): 3340.2,3161.5, 1651.1, 1455.9, 1422.1; HRMS calcd for $C_{10}H_{12}ClNO_2$ $(M + Na)^+$ 236.0454, found 236.0446.

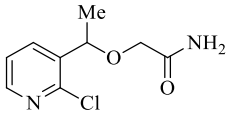
**2-((2-bromo-6-chlorobenzyl)oxy)acetamide (1h)**




**1h**

49% yield, m.p.151~160 °C; $^1$H NMR (400 MHz ,$CDCl_3$): $\delta$ ppm 4.08 (s, 2H), 4.90 (s, 2H), 5.49 (s, 1H), 6.59 (s, 1H), 7.16 (t, $J$ = 8.4 Hz, 1H), 7.39 (dd, $J^1$ = 8.0 Hz, $J^2$ = 1.2 Hz, 1H), 7.53 (dd , $J^1$ = 8.4 Hz, $J^2$ = 0.8 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 69.5, 70.2, 126.8, 129.2, 130.9, 131.9, 133.5, 136.6, 172.0; IR $v$ ($cm^{-1}$)：3371.9, 3184.1, 1634.2, 1576.4, 1342.8; HRMS calcd for $C_9H_9BrClNO_4$ $(M+Na)^+$ 301.9382, found 301.9374.

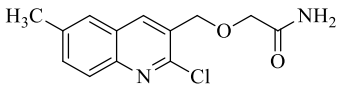
**2-(1-(2-chloropyridin-3-yl)ethoxy)acetamid (1i)**




**1i**

40% yield, m.p.139~140 °C; $^1$H NMR (400 MHz ,$CDCl_3$): $\delta$ ppm 1.51 (d, $J$ = 6.4 Hz, 3H), 3.88 (d, J = 5.6 Hz, 2H), 4.90 (q, $J$ = 6.4 Hz, 1H), 5.93 (s, 1H), 6.57 (s, 1H), 7.30 (dd, $J^1$ = 7.6 Hz, $J^2$ = 4.8 Hz, 1H), 7.78 (dd, $J^1$= 7.6 Hz, $J^2$ = 2.0 Hz, H), 8.35 (dd, $J^1$ = 7.8 Hz, $J^2$ = 2.0 Hz, H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 22.0, 68.2, 75.0, 123.2, 135.5, 136.4, 148.9, 149.4, 171.8; IR $v$ ($cm^{-1}$) 3478.0, 3193.0, 2926.9, 1658.2, 1580.2; HRMS calcd for $C_9H_{11}ClN_2O_2$ $(M+Na)^+$ 237.0407, found 237.0398.

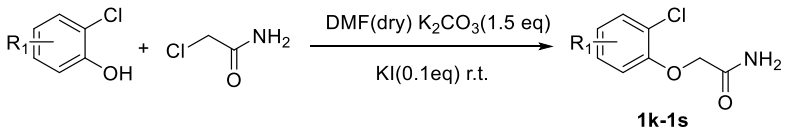
**2-((2-chloro-7-methylquinolin-3-yl)methoxy)acetamide (1j)**




**1j**

42% yield, m.p.171~172 °C; $^1$H NMR (400 MHz ,$CDCl_3$): $\delta$ ppm 2.55 (s, 3H), 4.16 (s, 2H), 4.81 (s, 2H), 5.63 (s, 1H), 6.59 (s, 1H), 7.59 (dd, $J^1$ = 10.4 Hz, $J^2$ = 2.0 Hz, 2H), 7.92 (d, $J$ = 8.4 Hz, 1H), 8.10 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 21.6, 70.1, 70.5, 126.4, 127.1, 128.0, 128.5, 133.0, 136.9, 137.6, 145.9, 148.5, 171.6; IR $v$ ($cm^{-1}$): 3473.9, 1717.7, 1329.9, 1119.8; HRMS calcd for $C_{13}H_{13}ClNO_2$ $(M+Na)^+$ 287.0563, found 287.0573.

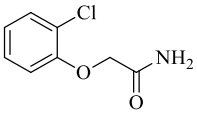
## 2. Synthesis of 2-((2-chlorobenzyl)oxy)acetyl chloride Derivatives




**1k-1s**

2-Chlorophenol (5 mmol), $K_2CO_3$ (7.5 mmol, 1.5 equiv.), chloroacetamide (5 mmol, 1.0 equiv.), KI (0.5 mmol, 0.1 equiv.) was added to a flask. The mixture was stirred at room temperature for 4 h to 5 h. After the reaction was finished, the mixture was added with water and extracted with ethyl acetate. The product was purified by column chromatography (ethyl acetate : petroleum ether = 1 : 4). The product was white flaky crystals with 80% -95% yields.

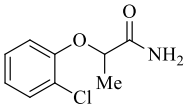
**2-(2-chlorophenoxy)acetamide (1k)**




**1k**

95% yield, m.p. 152-152.5 °C; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 4.54 (s, 2H), 6.02 (s, H), 6.84 (s, H), 6.91 (dd, $J^1$ = 8.0 Hz, $J^2$ = 1.6 Hz, 1H), 6.99 (dt, $J^1$ = 8.0 Hz, $J^2$ = 1.6 Hz, 1H), 7.28-7.24 (m, 1H), 7.40 (dd, $J^1$ = 8.0 Hz, $J^2$ = 1.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 67.6, 113.7, 122.8(0), 122.8(4), 128.1, 130.4, 152.6, 170.3; IR $\nu$ ($cm^{-1}$): 3458.6, 3143.6, 1638.1, 1580.9; HRMS calcd for $C_8H_8ClNO_2$ $(M+Na)^+$, 208.0141, found 208.0150.

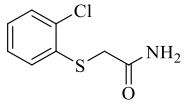
**2-(2-chlorophenoxy)propanamide (1l)**




**1l**

80% yield, m.p.142-142.5 °C; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 1.64 (d, $J$ = 6.4 Hz, 3H), 4.72 (q, $J$ = 6.4 Hz, 1H), 6.19 (s, 1H), 6.76 (s, 1H), 6.92-6.99 (m, 2H), 7.23 (dt, $J^1$ = 8.0 Hz, $J^2$ = 1.6 Hz, 1H), 7.40 (dd, $J^1$= 8.0 Hz, $J^2$= 1.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 18.3, 75.8, 114.9, 122.8, 123.5, 128.0, 130.5, 152.3, 174.4; IR $\nu$ ($cm^{-1}$): 3379.3, 3169,0, 1632.5, 1422.6, 1238.9; HRMS calcd for $C_9H_{10}ClNO_2$ $(M+Na)^+$ 222.0289, found 222.0280.

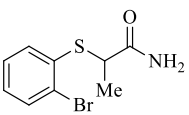
**2-((2-chlorophenyl)thio)acetamide (1m)**




**1m**

88% yield, m.p.120-120.5 °C; $^1$H NMR (400 MHz $CDCl_3$): $\delta$ ppm 3.67 (s, 2H), 5.58 (s, 1H), 6.67 (s, 1H), 7.15-7.19 (m, 1H), 7.23-7.26 (m, 2H), 7.38-7.41 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 35.8, 127.3, 127.4, 127.7, 129.9, 132.8, 133.8, 170.0; IR $\nu$ ($cm^{-1}$): 3425.6, 3178.6, 1678.5, 1634.6, 1452.8; HRMS calcd for $C_8H_8ClNOS$ $(M+Na)^+$ 223.9913, found 223.9923.

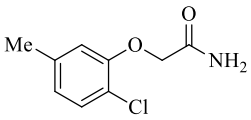
**2-((2-bromophenyl)thio)propanamide (1n)**



**1n**

86% yield, m.p.169~170 °C; $^1$H NMR (400 MHz $CDCl_3$): $\delta$ ppm 1.64 (d, $J$ = 7.2 Hz, 3H), 3.87 (q, $J$ = 7.2 Hz, 1H), 5.44 (s, 1H), 6.53 (s, 1H), 7.07-7.11 (m, 1H), 7.26-7.30 (m, 2H), 7.57 (d, $J$ = 8.4 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 18.0, 45.8, 123.9, 127.9, 128.3, 129.5, 133.2, 135.6, 174.2; IR $v$ ($cm^{-1}$): 3384.2, 3187.2, 1623.7, 1448.1, 738.2; HRMS calcd for $C_{10}H_{12}ClNO_2$ $(M+Na)^+$ 281.9564, found 281.9548.

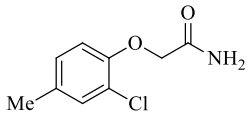
**2-(2-chloro-5-methylphenoxy)acetamide (1o)**




**1o**

93% yield, m.p.119-120 °C; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 2.29 (s, 3H), 4.50 (s, 2H), 5.96 (s, 1H), 6.79-6.81 (m, 2H), 7.02 (d, $J$ = 8.8 Hz, 1H), 7.21 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 20.3, 68.1, 113.8, 122.5, 128.5, 130.9, 132.8, 150.6, 170.5; IR $v$ ($cm^{-1}$): 3470.9, 3158.3, 2921.5, 1705.3, 1592.7; HRMS calcd for $C_9H_{10}ClNO_2$ $(M+Na)^+$ 222.0289, found 222.0292.

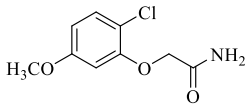
**2-(2-chloro-4-methylphenoxy)acetamide (1p)**




**1p**

95% yield, m.p. 138-139 °C; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 2.28 (s, 3H), 4.50 (s, 2H), 5.69 (s, 1H), 6.78-6.80 (m, 2H), 7.02 (dd, $J^1$ = 7.4 Hz, $J^2$ = 4.4 Hz, 1H), 7.21 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 20.3, 68.1, 113.9, 122.5, 128.4, 130.9, 132.8, 150.6, 170.7; IR $v$ ($cm^{-1}$): 3459.1, 3151.4, 1699.0, 1504.4, 1253.5; HRMS calcd for $C_9H_{10}ClNO_2$ $(M+Na)^+$ 222.0298, found 222.0287.

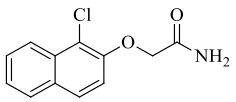
**2-(2-chloro-5-methoxyphenoxy)acetamide 1q**




**1q**

92% yield, m.p.126-126.5 °C; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 3.77 (s, 3H), 4.48 (s, 2H), 5.89 (s, 1H), 6.76-6.87 (m, 3H), 6.96-6.97 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 55.9, 68.8, 113.1, 115.3, 116.1, 123.7, 147.0, 155.0, 170.6; IR $v$ ($cm^{-1}$): 3466.9, 3145.9, 1694.9, 1273.2; HRMS calcd for $C_9H_{10}ClNO_3$ $(M + Na)^+$ 238.0247, found 238.0269.

**2-((1-chloronaphthalen-2-yl)oxy)acetamide (1r)**

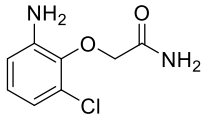



**1r**

94% yield, m.p.184-184.5 °C; $^1$H NMR (400 MHz ,$CDCl_3$): $\delta$ ppm 4.67 (s, 2H), 6.15 (s, 1H), 6.99 (s, 1H), 7.22 (d, $J$ = 8.8 Hz, 1H), 7.46 (t, $J$ = 7.6 Hz, 1H), 7.61 (t, $J$ = 7.6 Hz, 1H), 7.81 (t, $J$ = 9.6 Hz, 2H), 8.21 (d, $J$ = 8.8 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 68.7, 114.7, 123.6, 125.1, 127.8, 128.1, 128.5, 130.1, 150.3, 170.5; IR $v$ ($cm^{-1}$): 3358.0, 3173.6,

1633.7, 1276.1; HRMS calcd for $C_{12}H_{10}ClNO_2$ $(M+Na)^+$ 258.0298, found 258.0293.

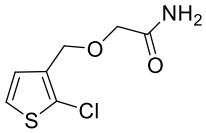
**2-(2-amino-6-chlorophenoxy)acetamide (1s)**



**1s**

72% yield, m.p. 120-120.5 °C; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 4.72 (s, 2H), 6.73 (d, $J$ = 8.8 Hz, H), 6.87 (t, $J^1$ = 8 Hz, $J^2$ = 8.2 Hz, H), 7.07 (d, $J$ = 6 Hz, H), 8.76 (s, H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 67.4, 114.3, 122.3, 122.9, 125.1, 127.2, 139.9, 165.4; IR $v$ ($cm^{-1}$): 3360.9, 3173.9, 1631.8 1108.4; HRMS calcd for $C_8H_9ClN_2O_2$ $(M+Na)^+$ 223.0250, found 223.0264.

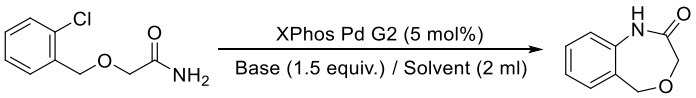
**2-((2-chlorothiophen-3-yl)methoxy)acetamide (1t)**



**1t**

51% yield, $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 7.32 (d, $J$ = 5.6 Hz, 1H), 6.94 (d, $J$ = 5.4 Hz, 1H), 6.50 (s, 1H), 5.44 (s, 1H), 4.74 (s, 2H), 4.03 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 171.8, 131.5, 127.9, 125.6, 125.1, 69.1, 65.0; IR v ($cm^{-1}$): 3362, 3178, 1633, 1111; HRMS calcd for $C_7H_8ClNO_2S$ $(M+Na)^+$ 227.9862, found 227.9872.

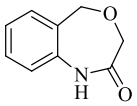
## III. General procedure for the synthesis of benzene-fused 6/7-membered amides




**1a** **2a**

2-((2-chlorobenzyl)oxy)acetyl chloride (0.25 mmol), $Cs_2CO_3$ (122.65 mg, 0.375 mmol) and Pd Xphos G2 (9.8 mg, 0.0125 mmol) were added into Schlenk tube. The mixture was stirred under argon and dry 1,4-dioxane (1 mL) was added and heated to 110℃. The reaction was determined by TLC. After the reaction finished, the mixture was purified by by column chromatography with yield of 85-99%.

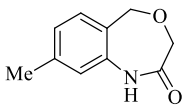
**3,5-dihydrobenzo[e][1,4]oxazepin-2(H)-one 2a [1]**



**2a**

99% yield, m.p. 156~157 °C; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 4.58 (s, 2H), 4.75 (s, 2H), 6.87 (d, $J$ = 8.0 Hz, 1H), 7.06 (t, $J$ = 7.6 Hz, 1H), 7.14 (d, $J$ = 7.2 Hz, 1H), 7.26-7.27 (m, 1H), 7.72 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 72.8, 73.5, 119.2, 123.7, 128.6, 128.7, 129.2, 135.7, 173.2; IR $v$ ($cm^{-1}$) : 3357.3, 3171.4, 1635.8, 1431.5, 1377.8; HRMS calcd for $C_9H_9NO_2$ $(M-H)^+$ 162.0555, found 162.0559.

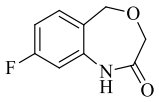
**8-methyl-3,5-dihydrobenzo[e][1,4]oxazepin-2(H)-one 2b**



**2b**

96% yield, m.p. 154~155 °C; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 2.33 (s, 3H), 4.57 (s, 2H), 4.70 (s, 2H), 6.79 (s, 1H), 6.87 (d, $J$ = 7.6 Hz, 1H), 7.02 (d, $J$ = 7.6 Hz, 1H), 8.75 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 21.0, 72.5, 73.3, 119.9, 124.5, 125.9, 128.4, 135.7, 139.3, 173.5; IR $v$ ($cm^{-1}$) : 3377.0, 3184.2, 2962.5, 1656.5, 1259.5; HRMS calcd for $C_{10}H_{11}NO_2$ $(M+Na)^+$ 200.0687, found 200.0673.

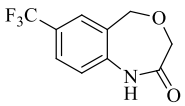
**8-fluoro-3,5-dihydrobenzo[e][1,4]oxazepin-2(H)-one 2c**



**2c**

94% yield, m.p. 166~167 °C; $^1$H NMR (400 MHz, $d^6$-DMSO): $\delta$ ppm 4.43 (s, 2H), 4.65 (s, 2H), 6.79 (dt, $J^1$ = 8.0 Hz, $J^2$ = 2.4 Hz, 1H), 6.92 (dd, $J^1$ = 10.4 Hz, $J^2$ = 2.4 Hz, 1H), 7.17 (d, $J$ = 8.4 Hz, 1H), 10.30 (s, 1H); $^{13}$C NMR (100 MHz, $d^6$-DMSO): $\delta$ ppm 71.7, 73.8, 106.2 (d, $J$ = 25.8 Hz), 109.4 (d, $J$ = 21.1 Hz), 126.0 (d, $J$ = 2.8 Hz), 130.6 (d, $J$ = 9.6 Hz), 139.1 (d, $J$ = 10.5 Hz), 162.3 (d, $J$ = 41.4 Hz), 173.4; $^{19}$F NMR: -113.9; IR $v$ ($cm^{-1}$): 3194.0, 3066.2, 1661.0, 1603.5, 1372.5; HRMS calcd for $C_9H_8FNO_2$ $(M+Na)^+$ 204.0437, found 204.0430.

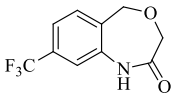
**7-(trifluoromethyl)-3,5-dihydrobenzo[e][1,4]oxazepin-2(1H)-one 2d**



**2d**

90% yield, $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 4.62 (s, 2H), 4.78 (s, 2H), 7.24-7.31 (m, 3H), 8.91 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 70.1, 70.2, 123.9 (q, $J$ = 3.9 Hz), 124.5 (q, $J$ = 267.2 Hz), 126.2 (q, $J$ = 3.9 Hz), 129.3, 131.8 (q, $J$ = 32.6 Hz), 133.5, 138.6, 171.6; $^{19}$F NMR: $\delta$ ppm -78.8; IR $v$ ($cm^{-1}$): 2979.8, 1663.7, 1334.6, 1121.5; HRMS calcd for $C_{10}H_8F_3NO_2$ (M-H) 230.0427, found 230.0425.

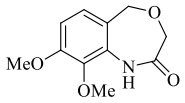
**8-(trifluoromethyl)-3,5-dihydrobenzo[e][1,4]oxazepin-2(H)-one 2e**



**2e**

92% yield, m.p. 128~129°C; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 4.56 (s, 2H), 4.77 (s, 2H), 7.09 (d, $J$ = 8.4 Hz, 1H), 7.37 (s, 1H), 7.53 (d, $J$ = 8.4 Hz , 1H) , 9.44 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 72.9, 74.0, 119.6, 123.9 (q, $J$ = 270.2 Hz), 125.7 (q, $J$ = 32.6 Hz), 125.7 (q, $J$ = 3.9 Hz), 126.4 (q, $J$ = 3.9 Hz), 129.2, 138.9, 174.5; $^{19}$F NMR: $\delta$ ppm -62.1; IR $v$ ($cm^{-1}$): 2919.9, 1658.6, 1447.8, 1084.8, 656.7; HRMS calcd for $C_{10}H_8F_3NO_2$ $(M-H)^+$ 230.0427, found 230.0429.

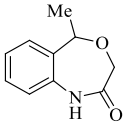
**8, 9-dimethoxy-3,5-dihydrobenzo[e][1,4]oxazepin-2(H)-one 2f**



**2f**

90% yield, m.p. 148-149 °C; $^1$H NMR (400 MHz ,$CDCl_3$): $\delta$ ppm 3.87 (s, 3H), 3.88 (s, 3H), 4.61 (s, 2H), 4.67 (s, 2H), 6.58 (d, $J$ = 8.8 Hz, 1H), 6.78 (d, $J$ = 8.8 Hz, 1H), 8.30 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 55.9, 60.8, 72.9，74.1，106.6, 121.8, 122.8, 129.5, 136.8, 152.3, 172.4; IR: $v$ ($cm^{-1}$): 3195.3, 1661.6, 1391.6, 1112.3. HRMS calcd for $C_{11}H_{13}NO_4$ $(M+Na)^+$ 246.0742, found 246.0736.

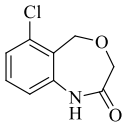
**5-methyl-3,5-dihydrobenzo[e][1,4]oxazepin-2(H)-one 2g**



**2g**

89% yield, m.p. 120~121 °C; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 1.64 (d, $J$ = 6.4 Hz, 3H), 4.54 (d, $J$ = 2.4 Hz, 2H), 4.78 (q, $J$ = 6.4 Hz, 1H), 6.99 (dd, $J^1$ = 8.4 H, $J^2$ = 0.4 Hz, 1H), 7.01 (td, $J^1$ = 7.6 Hz, $J^2$ = 0.4 Hz, 1H), 7.23-7.29 (m, 2H), 8.68 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 19.0, 71.1, 75.2, 120.0, 123.9, 125.9, 128.8, 132.7, 136.0, 173.7; IR $v$ (cm$^{-1}$): 3196.7, 3065.5, 2997.0, 2903.1, 1656.9; HRMS calcd for $C_{10}H_{11}NO_2$ $(M-H)^+$ 176.0721, found 176.0725. For corresponding chiral **R-2g**: -78° (*c* 0.08, Acetone), 83% *ee* (determined by a chiral AD-H column, $^i$PrOH/Hexane = 10/90, $t_{major}$ = 14.26 min, $t_{minor}$ = 15.40 min).

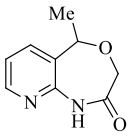
**6-chloro-3,5-dihydrobenzo[e][1,4]oxazepin-2(H)-one 2h**




**2h**

83% yield, m.p. 172~173 °C; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 4.52 (s, 2H), 4.99 (s, 2H), 6.78 (d, $J$ = 7.6 Hz, 1H), 7.11-7.19 (m, 2H), 7.70 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 69.8, 73.1, 118.2, 124.9, 126.6, 129.2, 133.7, 137.5, 173.0; IR $v$ (cm$^{-1}$): 3246.6, 2918.9, 1671.0, 1480.4, 1258.1; HRMS calcd for $C_9H_8ClNO_2$ $(M+Na)^+$ 220.0141, found 220.0143.

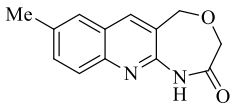
**5-methyl-3,5-dihydropyrido[2,3-e][1,4]oxazepin-2(H)-one 2i**




**2i**

89% yield, m.p. 106~106.5 °C; $^1$H NMR (400 MHz ,$CDCl_3$): $\delta$ ppm 1.64 (d, $J$ = 6.4 Hz, 3H), 4.64 (d, $J$ = 6.0 Hz, 2H), 4.73 (*q*, $J$ = 6.4 Hz, 1H), 7.04 (dd, $J^1$ = 7.6 Hz, $J^2$ = 4.8 Hz, 1H), 7.53 (d, $J$ = 7.8 Hz, 1H), 8.40 (d, $J$ = 4.8 Hz, 1H), 9.38 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 18.9, 72.2, 75.0, 118.7, 127.4, 134.7, 147.6, 149.1, 173.0; IR $v$ (cm$^{-1}$): 3180.4, 1662.7, 1634.3, 1401.8, 1315.7; HRMS calcd for $C_9H_{10}N_2O_2$ $(M+Na)^+$ 201.0640, found 201.0623.

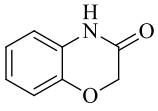
**8-methyl-3,5-dihydro-[1,4]oxazepino[5,6-b]quinolin-2(H)-one 2j**




**2j**

85% yield, m.p. 134-135 °C; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 2.51 (s, 3H), 4.69 (s, 2H), 4.85 (s, 2H), 7.51 (d, $J$ = 7.6 Hz, 2H), 7.77 (d, $J$ = 8.4 Hz, 1H), 7.80 (s, 1H), 8.47 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 21.5, 72.2, 74.3, 123.3, 125.0, 126.1, 127.2, 132.8, 135.7, 145.0, 147.6, 172.3; IR $v$ (cm$^{-1}$): 2919.9, 1658.6, 1447.8, 1084.8, 656.7; HRMS calcd for $C_{13}H_{12}N_2O_2$ $(M-H)^+$ 227.0821, found 227.0848.

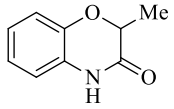
**2H-benzo[b][1,4]oxazin-3(4H)-one 2k[2-5]**




**2k**

Known compound, 99% yield; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 4.63 (s, 2H), 6.82-6.98 (m, 4H), 8.07 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 67.2, 116.0, 116.8, 122.7, 124.3, 126.0, 143.6, 165.9.

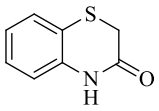
**2-methyl-2H-benzo[b][1,4]oxazin-3(4H)-one 2l[6]**



**2l**

Known compound, 97% yield; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 1.59 (d, $J$ = 6.8 Hz, 3H), 4.67 (q, $J$ = 6.8 Hz, 1H), 6.88-6.89 (m, 1H), 6.96-6.97 (m, 3H), 9.68 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 16.2, 73.2, 115.9, 117.0, 122.6, 124.1, 126.4, 143.1, 168.9.

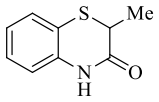
**2H-benzo[b][1,4]thiazin-3(4H)-one 2m[7-8]**



**2m**

Known compound, 99% yield; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 3.44 (s, 2H), 6.90 (d, $J$ = 8.0 Hz, 1H), 7.01 (dt, $J^1$ = 8.0 Hz, $J^2$ = 1.2 Hz, 1H), 7.17 (dt, $J^1$ = 7.6 Hz, $J^2$ = 1.2 Hz, 1H), 7.31 (d, $J$ = 7.8 Hz, 1H) , 9.11 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 29.9, 117.4, 119.9, 123.9, 127.2, 127.8, 136.3, 166.4;

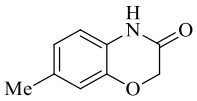
**2-methyl-2H-benzo[b][1,4]thiazin-3(4H)-one 2n[7-8]**



**2n**

Known compound, 98% yield; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 1.50 (d, $J$ = 7.2Hz, 3H), 3.56 (*q*, $J$ = 7.2 Hz, 1H), 6.89 (d, $J$ = 8.4 Hz, 1H), 7.02 (t, $J$ = 6.8 Hz, 1H), 7.18 (t, $J$ = 8.0 Hz, 1H), 7.30-7.31 (m, 1H), 8.86 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 15.4, 37.0, 116.9, 119.4, 123.8, 127.1, 128.1, 136.0, 168.9.

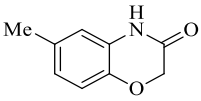
**7-methyl-2H-benzo[b][1,4]oxazin-3(4H)-one 2o[2]**



**2o**

Known compound, 95% yield; $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 2.28 (s, 3H), 4.60 (s, 2H), 6.67 (s, 1H), 6.78 (d, $J$ = 8.0 Hz, 1H), 6.87 (d, $J$ = 8.4 Hz, 1H), 9.41(s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 20.7, 67.2, 116.5, 116.7, 120.3, 124.7, 125.8, 132.5, 166.6.

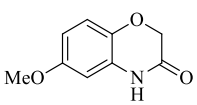
**6-methyl-2H-benzo[b][1,4]oxazin-3(4H)-one 2p[2]**



**2p**

Known compound, 95% yield, $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 2.28 (s, 3H), 4.60 (s, 2H), 6.67 (s, 1H), 6.78 (dd, $J^1$ = 8.4 Hz, $J^2$ = 1.2 Hz, 1H), 6.86 (d, $J$ = 7.6 Hz, 1H), 9.36 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 20.6, 67.2, 116.4, 116.5, 124.7, 125.7, 132.5, 141.4, 166.7.

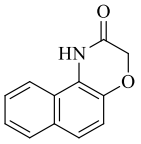
**6-methoxy-2H-benzo[b][1,4]oxazin-3(4H)-one 2q[2]**



**2q**

Known compound, 96% yield; $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ ppm 3.76 (s, 3H), 4.57 (s, 2H), 6.40 (d, $J$ = 2.4 Hz, 1H), 6.50 (dd, $J^1$ = 8.6 Hz, $J^2$ = 3.2Hz, 1H), 6.85 (d, $J$ = 8.8 Hz, 1H), 8.93 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 55.8, 67.4, 102.1, 108.8, 117.2, 126.8, 137.6, 155.3, 166.6.

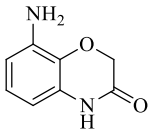
**1H-naphtho[2,1-b][1,4]oxazin-2(3H)-one 2r**



**2r**

96% yield, m.p. 207~208 $^{o}$C; $^{1}$H NMR (400 MHz ,$CDCl_3$): $\delta$ ppm 4.76 (s, 2H), 7.22 (d , $J$ = 8.2 Hz, 1H), 7.43 (td, $J^1$ = 7.8 Hz, $J^2$ = 0.8 Hz, 1H), 7.54 (d, $J$ = 9.2 Hz, 1H), 7.58 (td, $J^1$ = 7.8 Hz, $J^2$ = 1.2 Hz, 1H), 7.83 (d, $J$ = 8.4 Hz, 1H), 7.94 (d, $J$ = 8.0 Hz, 1H), 9.66 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 67.5, 117.4, 118.7, 119.0, 123.0, 124.3, 124.7, 127.0, 128.7, 130.0, 140.6, 166.0; IR $v$ ($cm^{-1}$): 3189.9, 2961.3, 2877.5, 1681.8, 1458.9; HRMS calcd for $C_{12}H_9NO_2$ $(M+Na)^+$ 222.0531, found 222.0527.

**8-amino-2H-benzo[b][1,4]oxazin-3(4H)-one 2s**[9]



**2s**

Known compound, 85% yield, $^{1}$H NMR(400 MHz , $CDCl_3$): $\delta$ ppm 4.73 (s, 2H), 6.73 (dd, $J^1$ = 8.0 Hz, $J^2$ = 1.2Hz, 1H), 6.90 (t, $J$ = 8.0 Hz, 1H), 7.06 (dd, $J^1$ = 8.0 Hz, $J^2$ = 1.2 Hz, 1H), 8.61 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ ppm 67.4, 114.3, 122.2, 122.9, 125.1, 127.1, 139.8, 165.4.

## IV. References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2. (a) C. Rajitha, P. K. Dubey, V. Sunku, F. J. Piedrafita, V. R. Veeramaneni, M.Pal, *Eur. J. Med. Chem.,* 2011, **46**, 4887; (b) C. Ramesh, B. R. Raju, V. Kavala, C. W. Kuo, C. F. Yao, Tetrahedron, 2011, **67**, 1187.
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5. D. Chen, G. Shen, W. Bao, *Org. Biomol. Chem.,* 2009, **7**, 4067.
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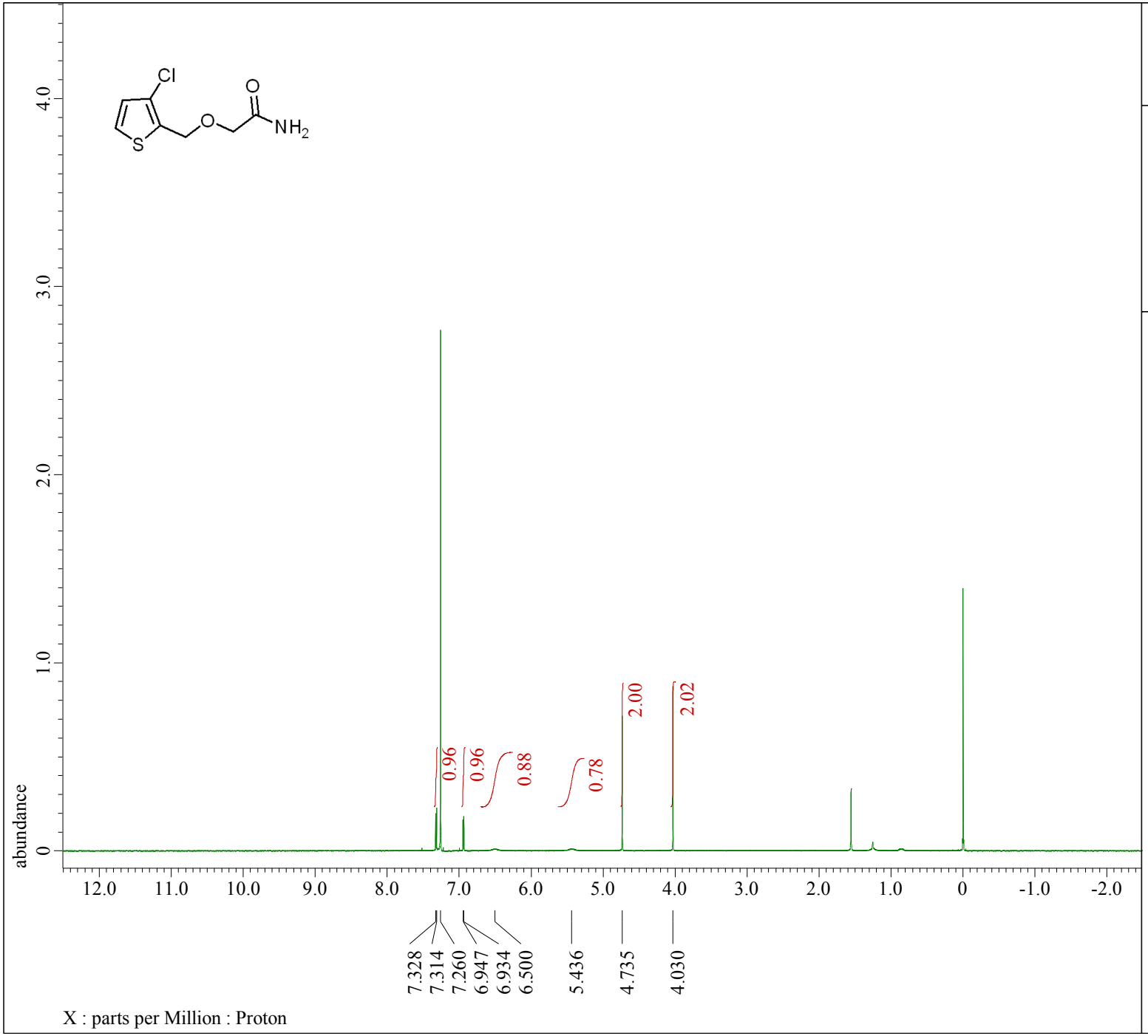
## IV. $^{1}$H and $^{13}$ C NMR spectra of the synthetic compounds




JEOL

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ppm
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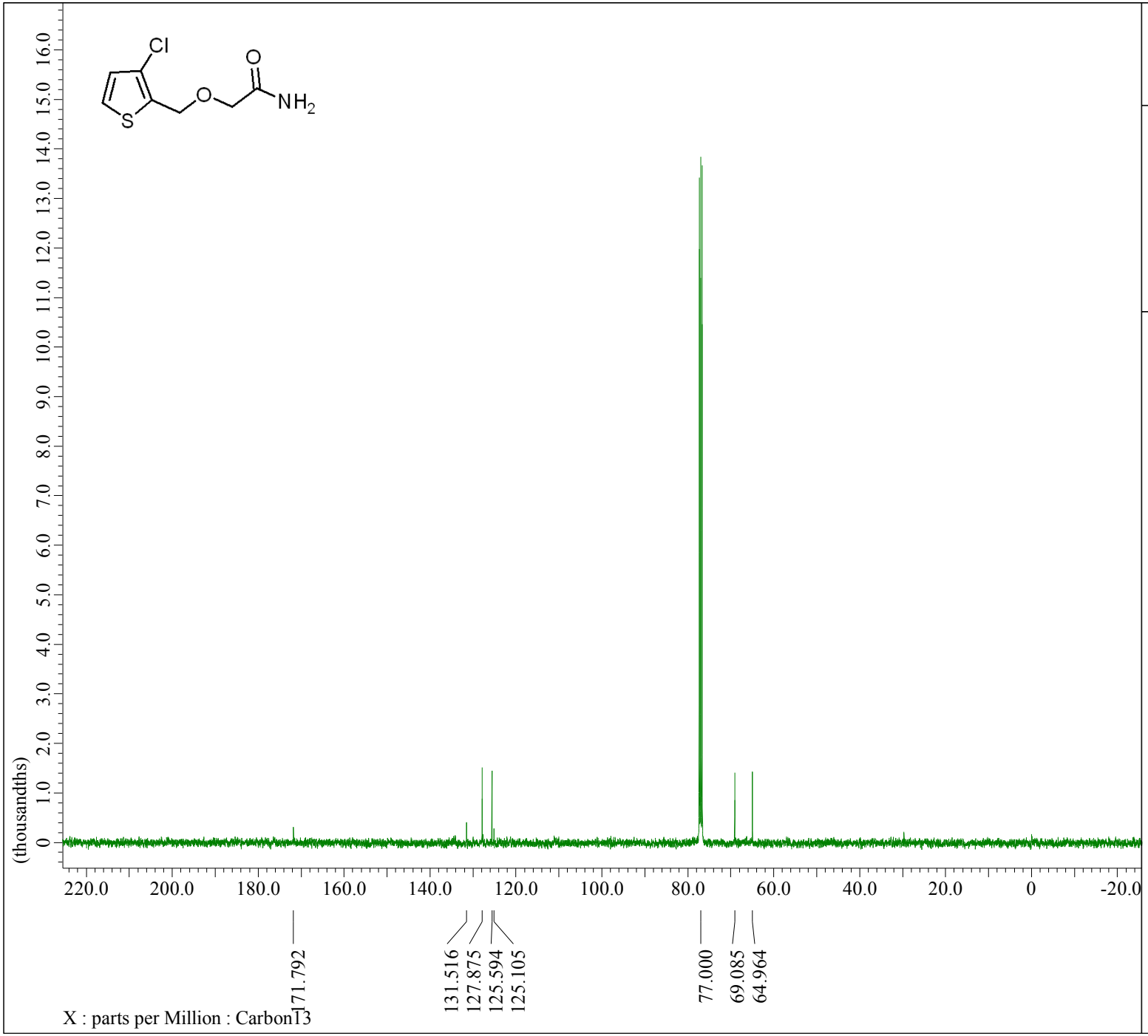


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ppm

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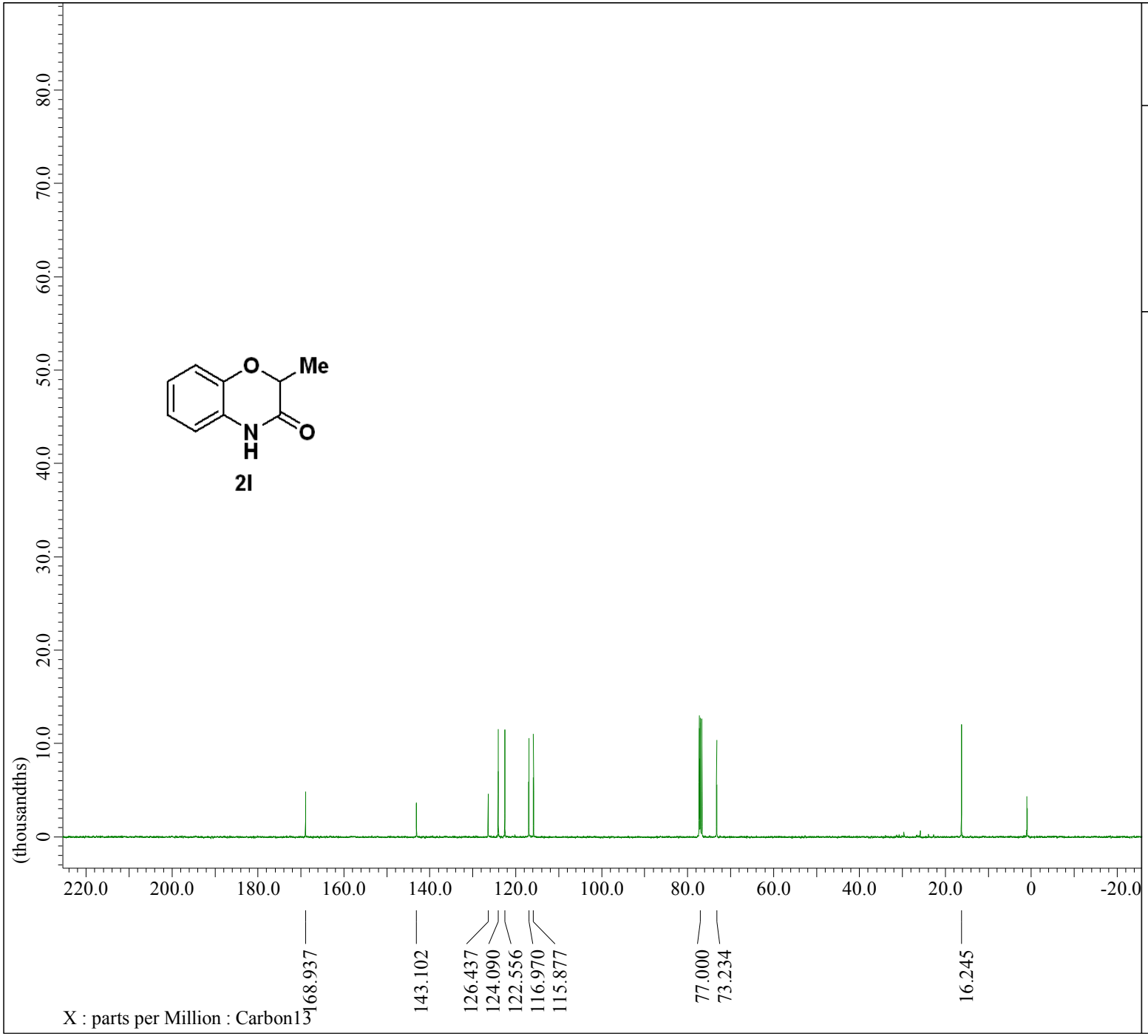


JEOL

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ppm
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| X_Acq_Time | = 1.03809024[s] |
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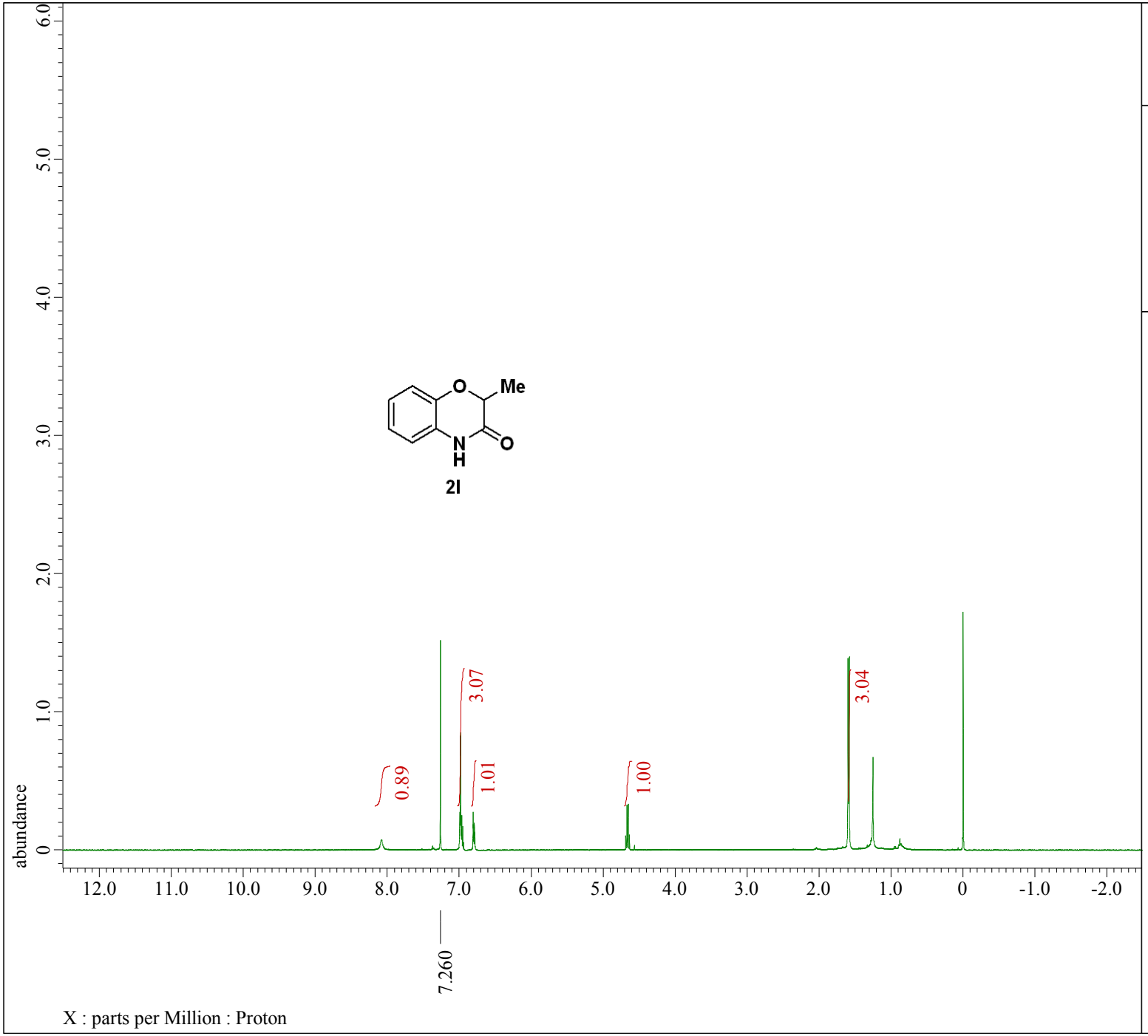


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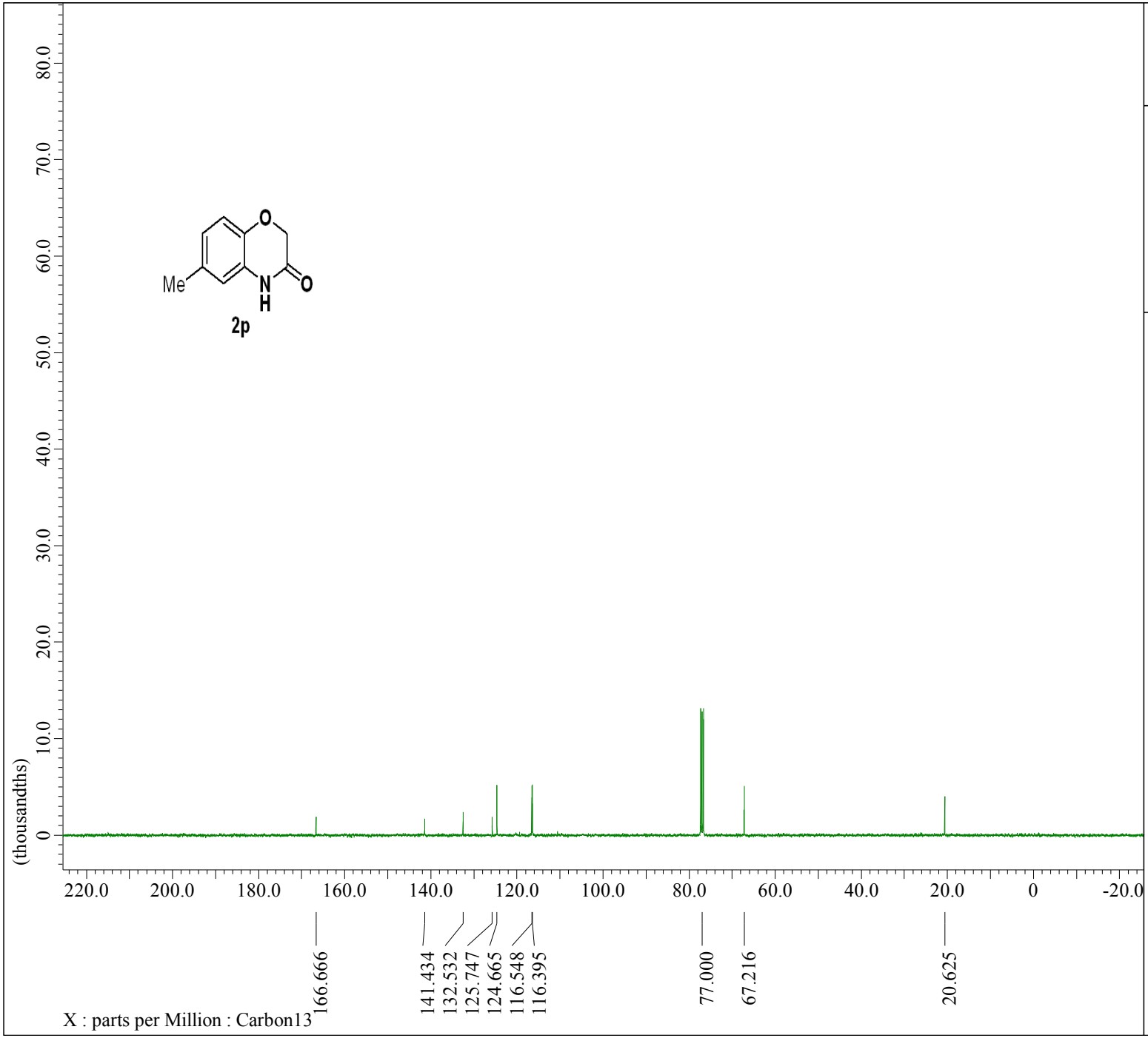


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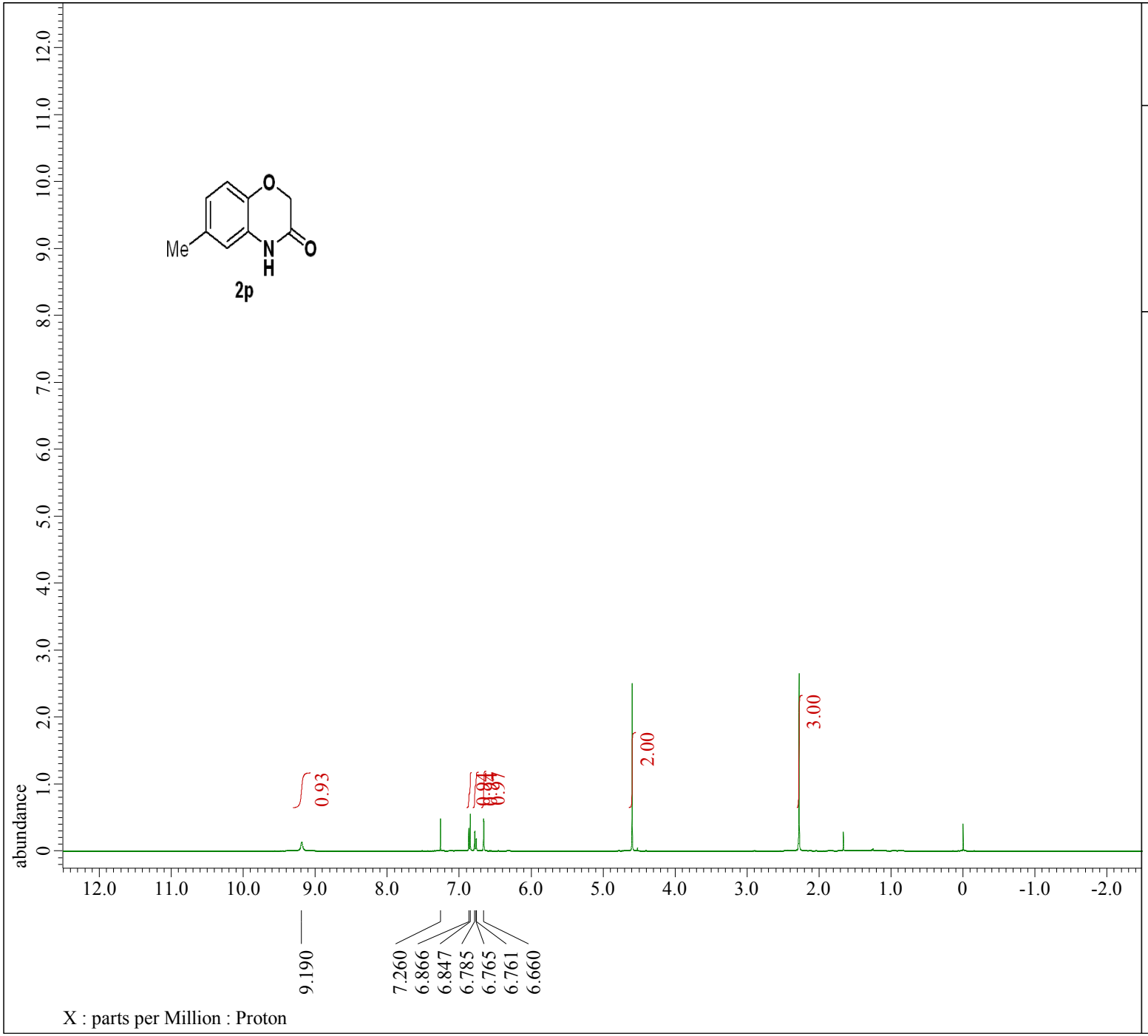


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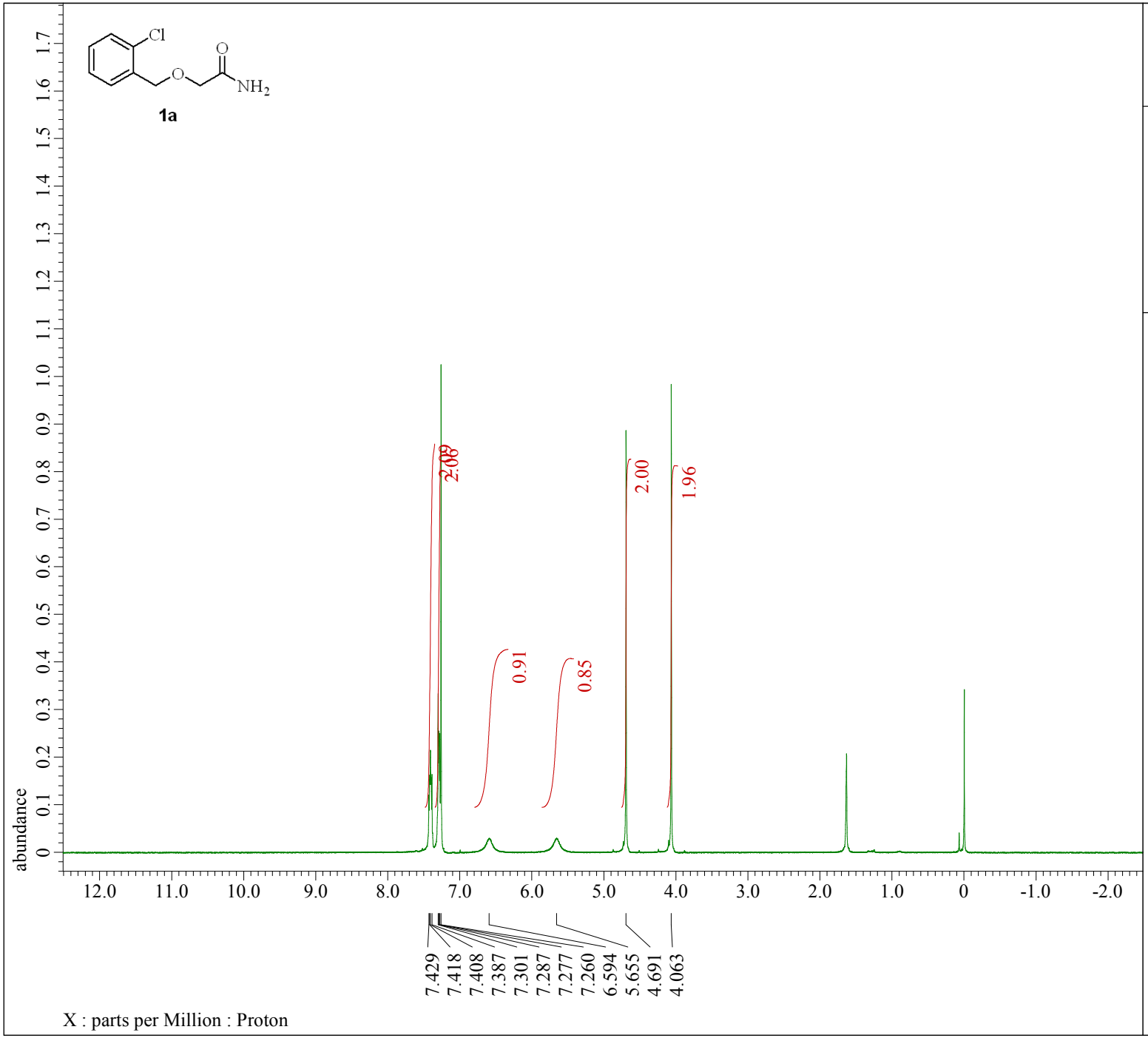


JEOL

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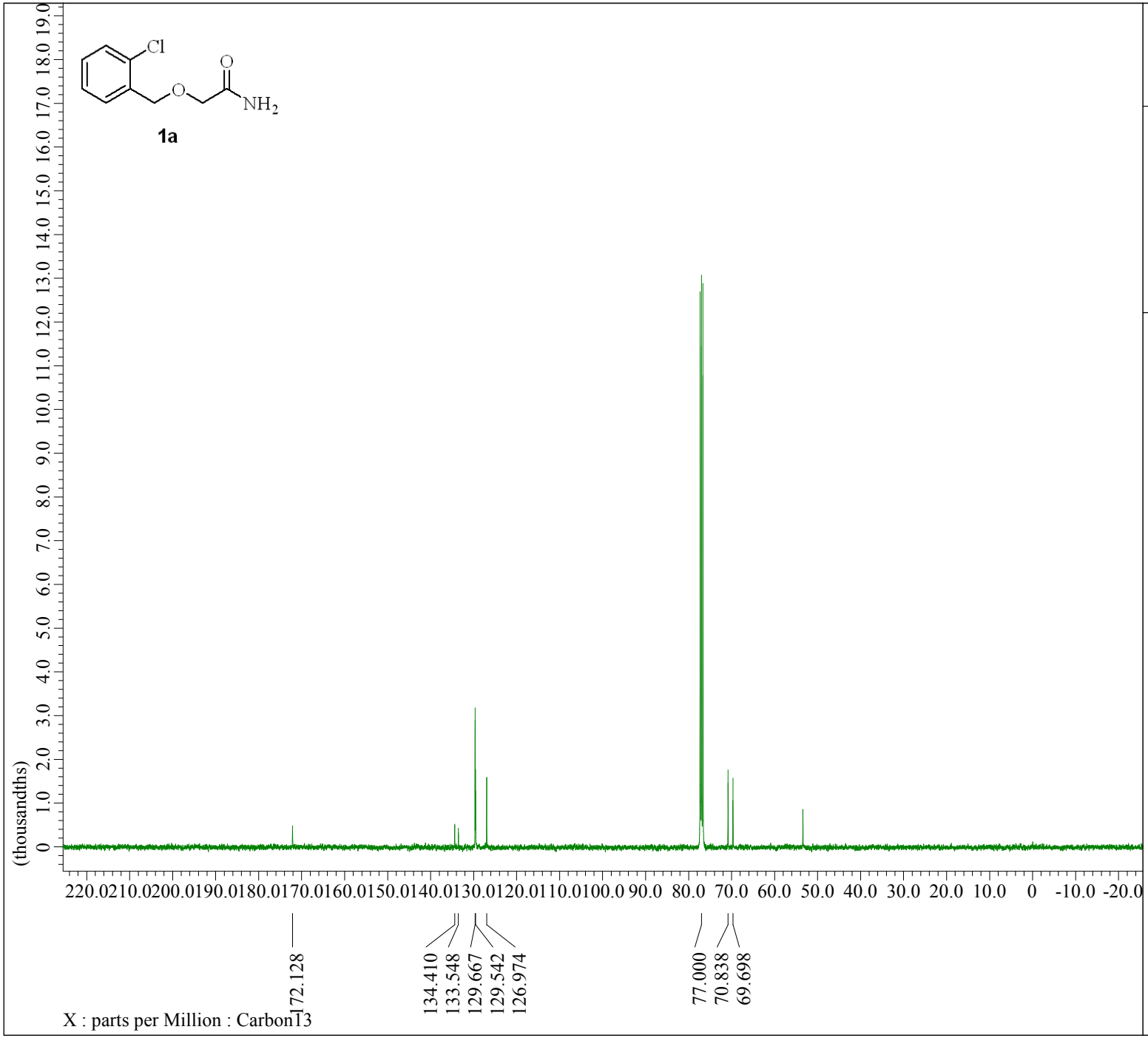
Derived from: LK-7YUANHUAN_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK-7YUANHUAN_Proton-1 |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK-7YUANHUAN |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 11-AUG-2016 10:12:23 |
| Revision_Time | = 8-AUG-2017 16:11:36 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 66 |
| Temp_Get | = 19.8[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

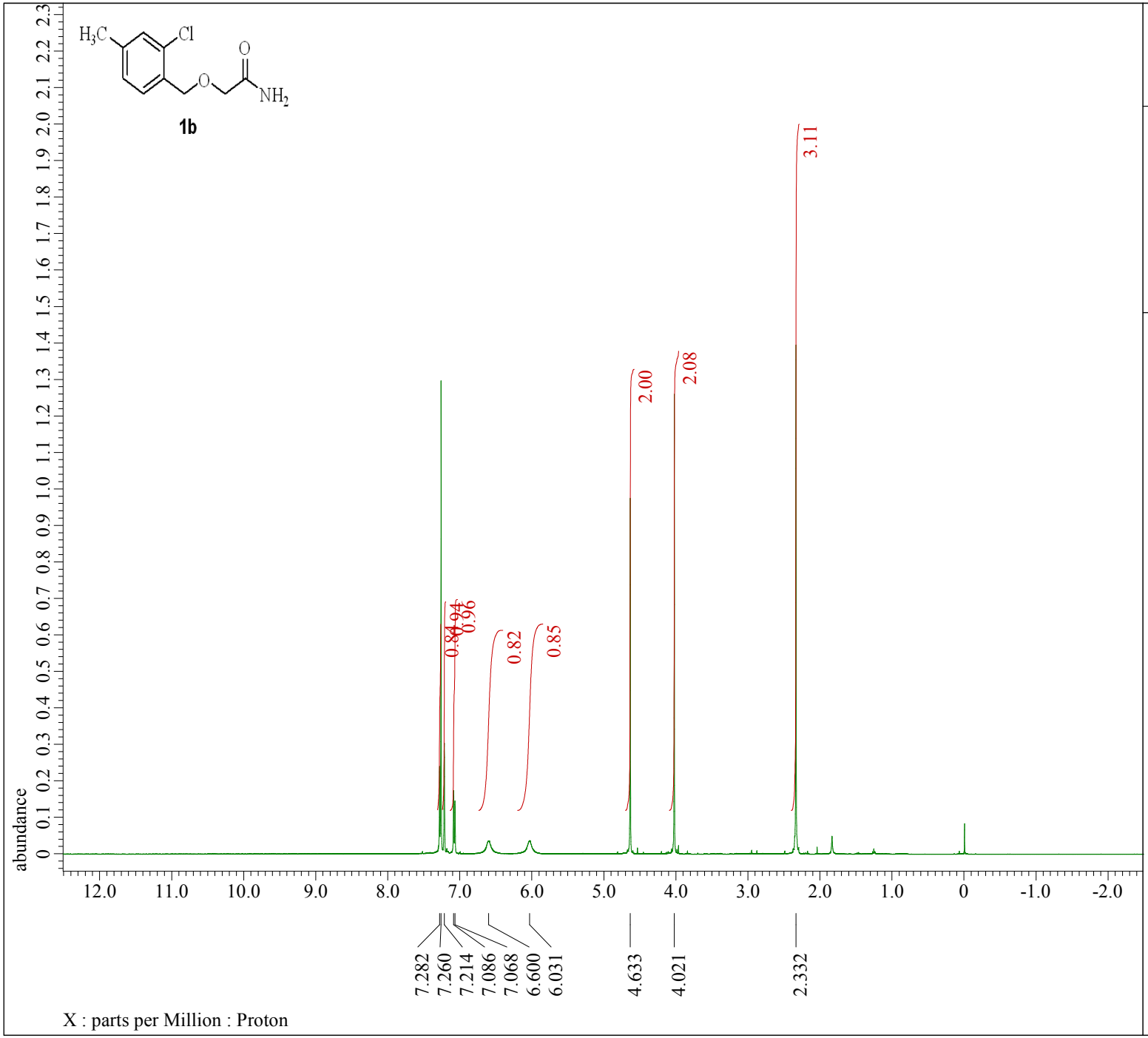



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK032117-4_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK032117-4_Carbon- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK032117-4 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 21-MAR-2017 14:15: |
| Revision_Time | = 8-AUG-2017 16:20: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 1024 |
| Total_Scans | = 1024 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 23.4[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |

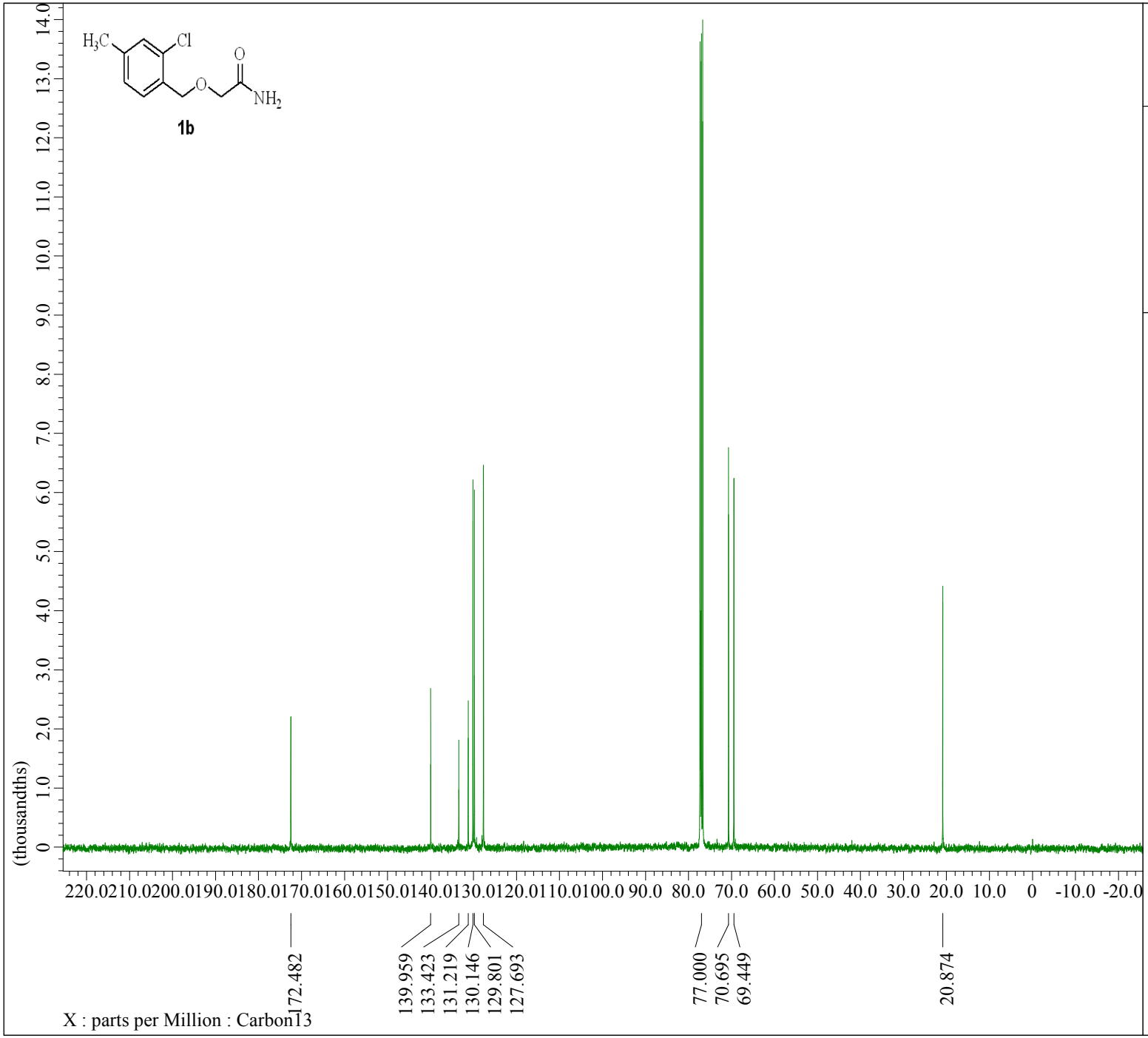



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1105-3_Proton-1-1.jdf
```

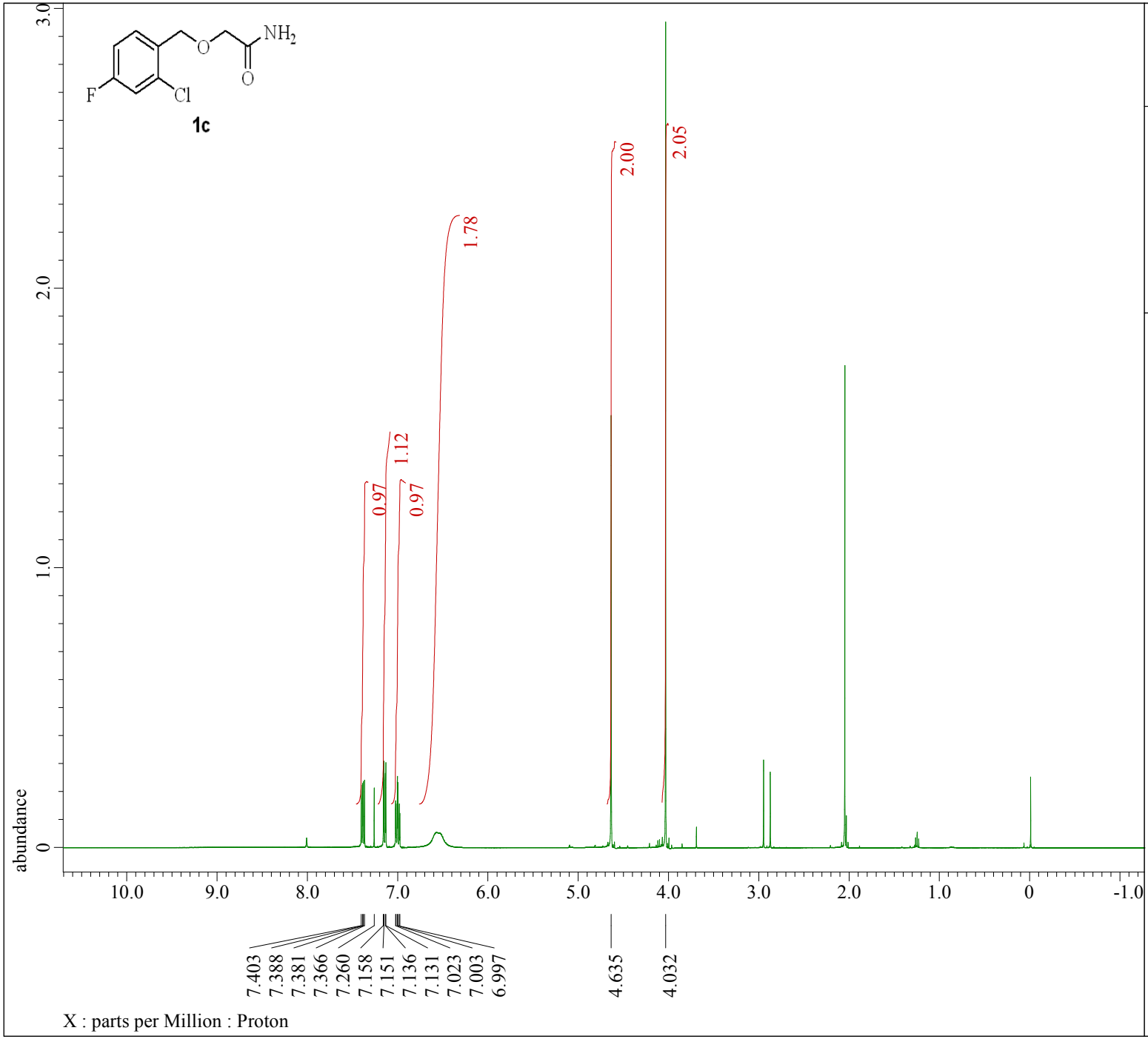
| | |
|---|---|
| Filename | = LK1105-3_Proton-1-3.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK1105-3 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 5-NOV-2016 21:23:20 |
| Revision_Time | = 8-AUG-2017 16:31:53 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 46 |
| Temp_Get | = 17.9[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1105-3_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1105-3_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK1105-3 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 6-NOV-2016 09:38: |
| Revision_Time | = 8-AUG-2017 16:29: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 1024 |
| Total_Scans | = 1024 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 18.5[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |

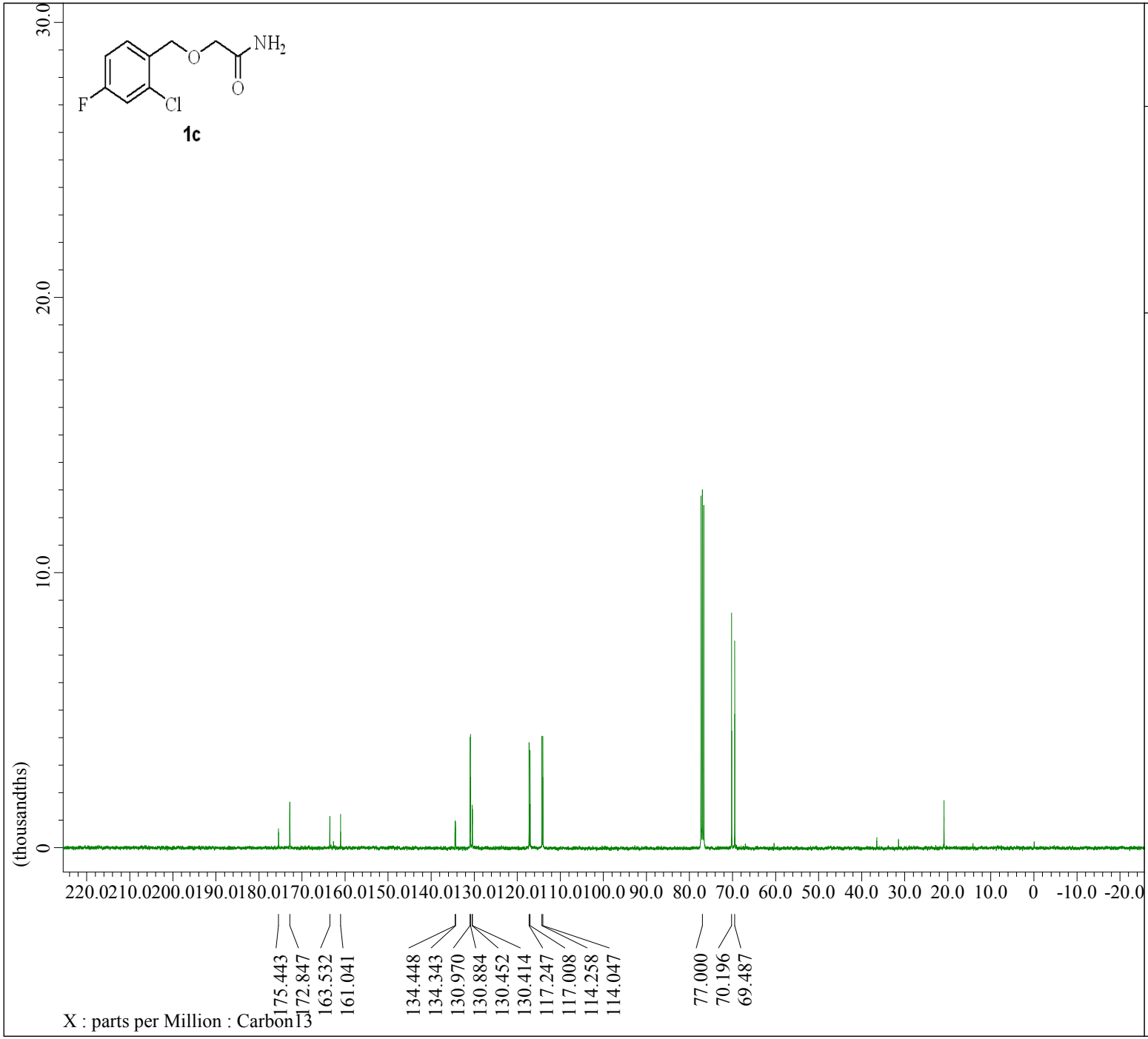



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1128-01_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1128-01_Proton-1-3. |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK1128-01 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 28-NOV-2016 16:34:02 |
| Revision_Time | = 8-AUG-2017 16:44:32 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 46 |
| Temp_Get | = 26.4[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

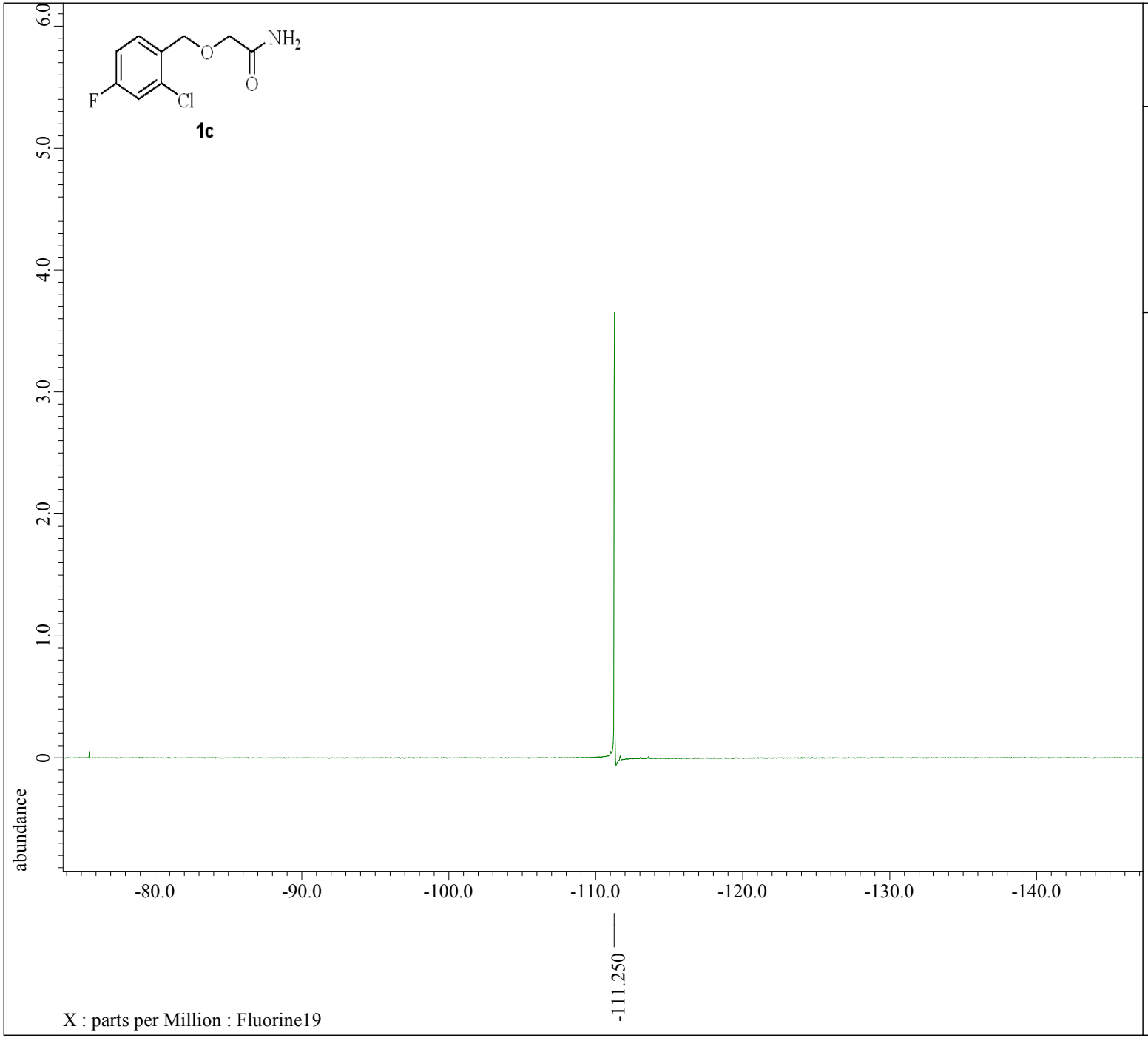



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1128-01_Carbon-1-1.jdf
```

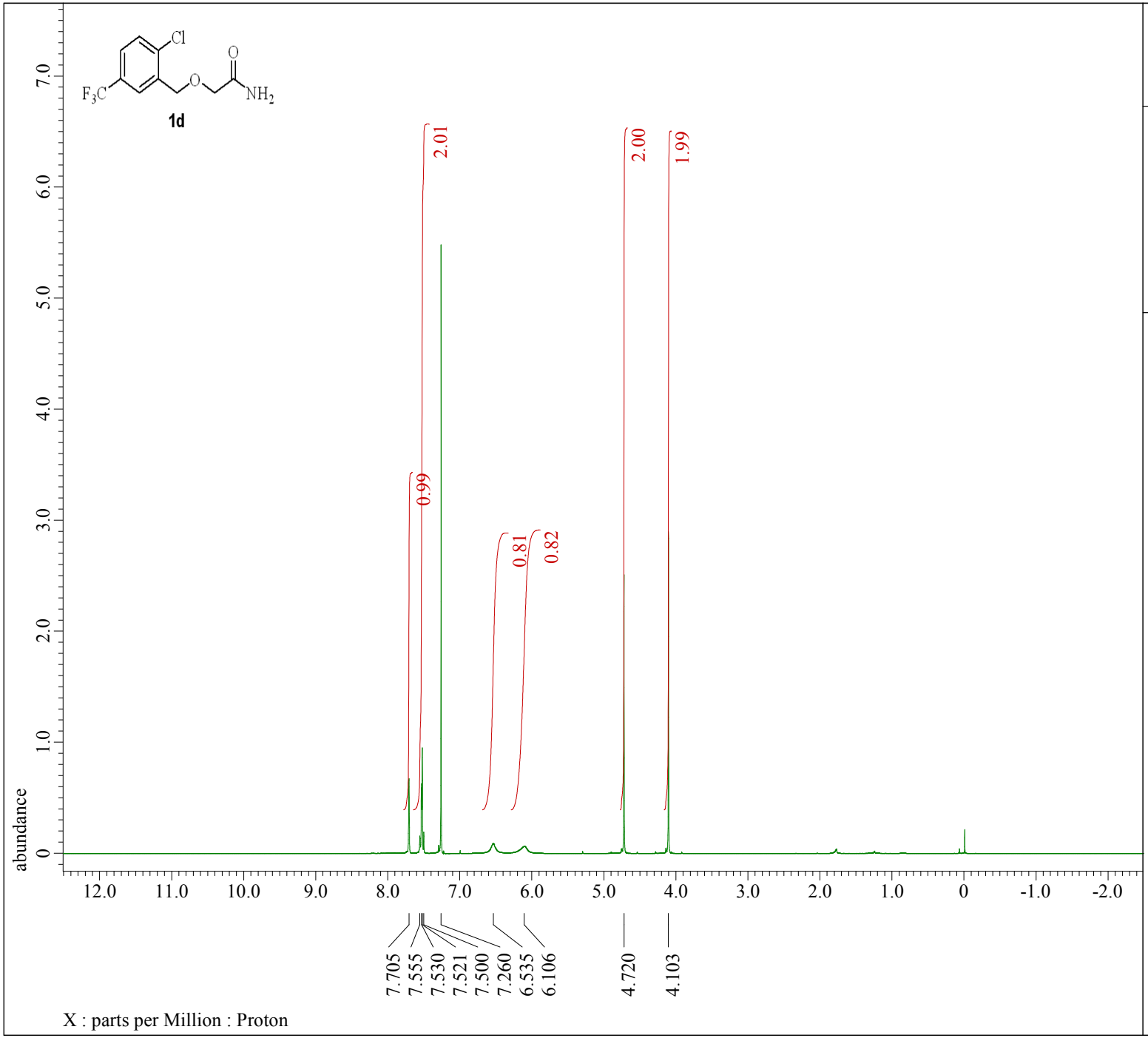
| | |
|---|---|
| Filename | = LK1128-01_Carbon-1 |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK1128-01 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 28-NOV-2016 17:29: |
| Revision_Time | = 8-AUG-2017 16:51: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 1024 |
| Total_Scans | = 1024 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 27.6[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1128-01_single_pulse-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1128-01_single_puls |
| Author | = delta |
| Experiment | = single_pulse.jxp |
| Sample_Id | = LK1128-01 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 28-NOV-2016 17:26:53 |
| Revision_Time | = 8-AUG-2017 16:59:42 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Fluorine19 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 83.88608[ms] |
| X_Domain | = 19F |
| X_Freq | = 376.17105393[MHz] |
| X_Offset | = -100[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 11.92092896[Hz] |
| X_Sweep | = 195.3125[kHz] |
| X_Sweep_Clipped | = 156.25[kHz] |
| Irr_Domain | = Fluorine19 |
| Irr_Freq | = 376.17105393[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Fluorine19 |
| Tri_Freq | = 376.17105393[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 27.2[dC] |
| X_90_Width | = 10[us] |
| X_Acq_Time | = 83.88608[ms] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.9[dB] |
| X_Pulse | = 5[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

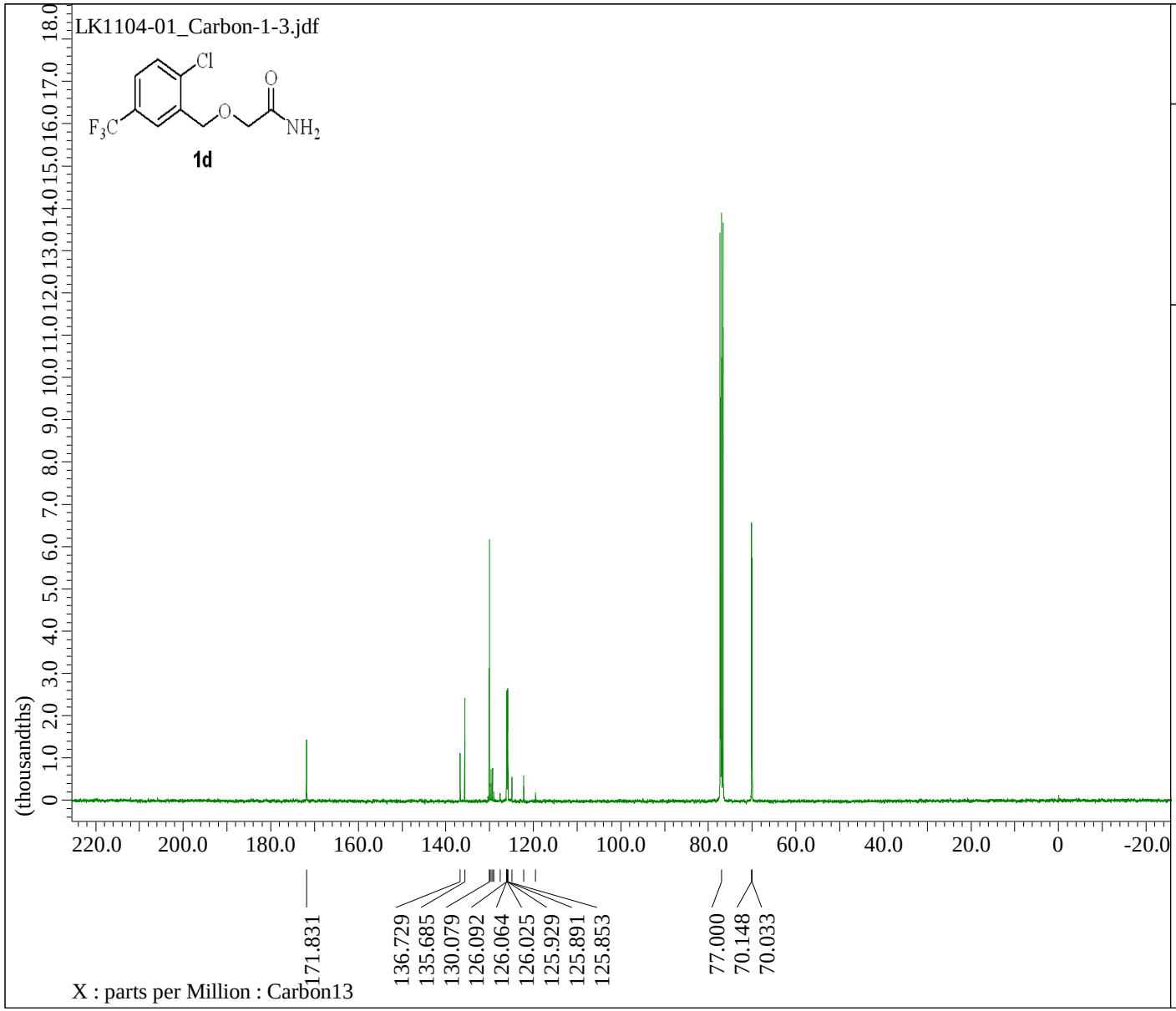



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1104-01_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1104-01_Proton-1-6. |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK1104-01 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-NOV-2016 12:18:30 |
| Revision_Time | = 8-AUG-2017 17:35:18 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 16.8[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

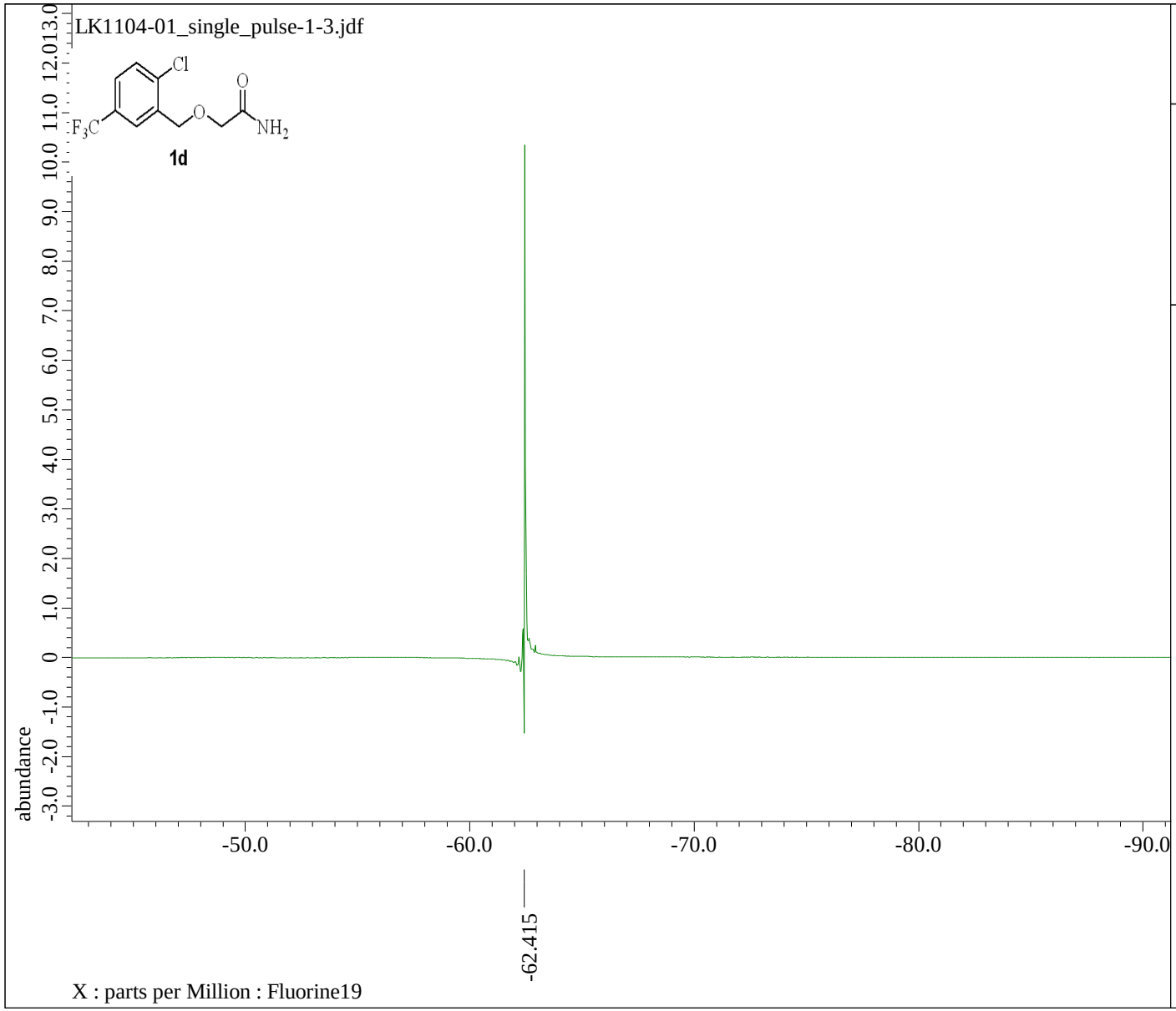



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1104-01_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1104-01_Carbo |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK1104-01 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-NOV-2016 12: |
| Revision_Time | = 8-AUG-2017 17: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 2400 |
| Total_Scans | = 2400 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 17.9[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |

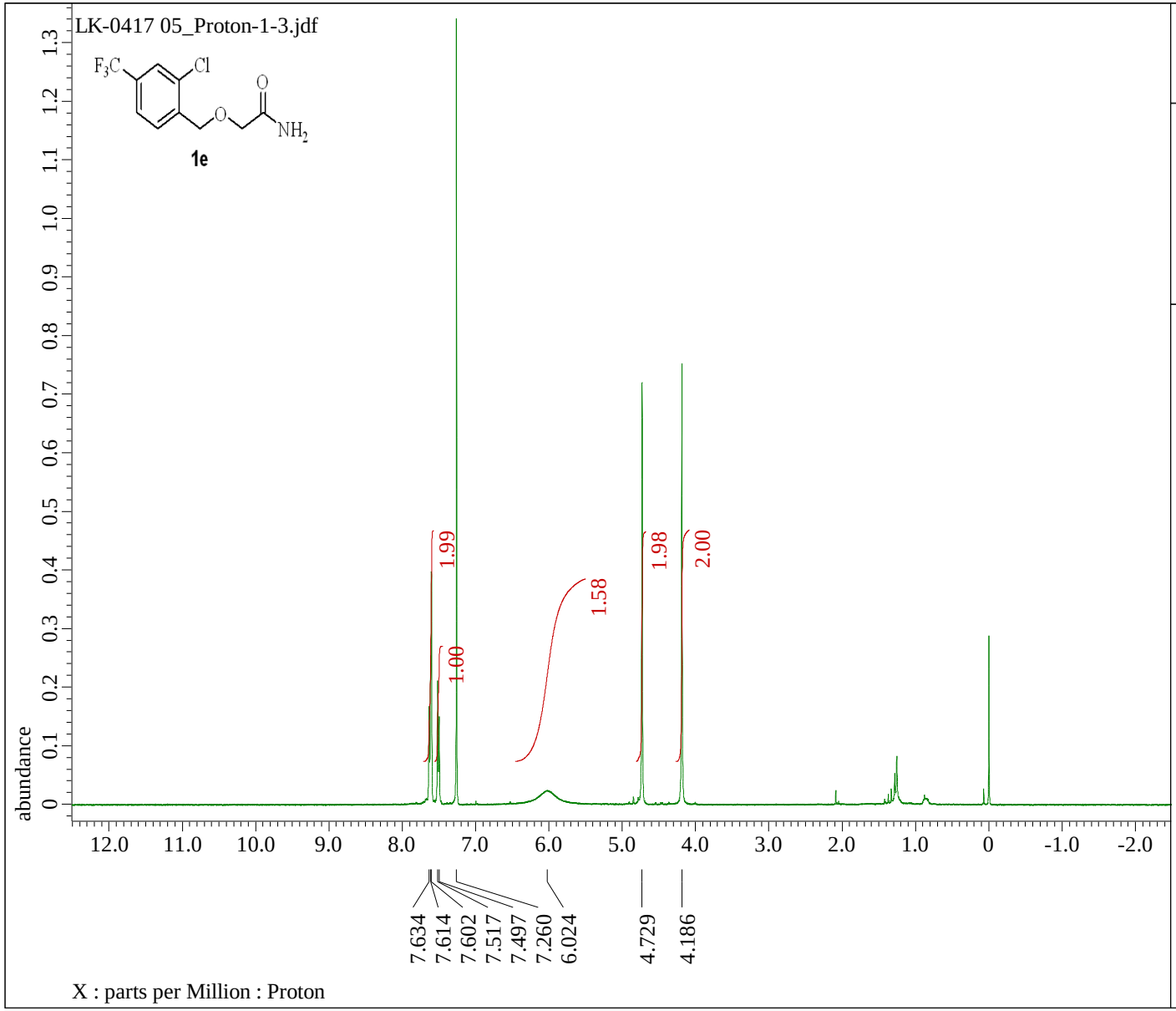



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1104-01_single_pulse-1-1.j
```

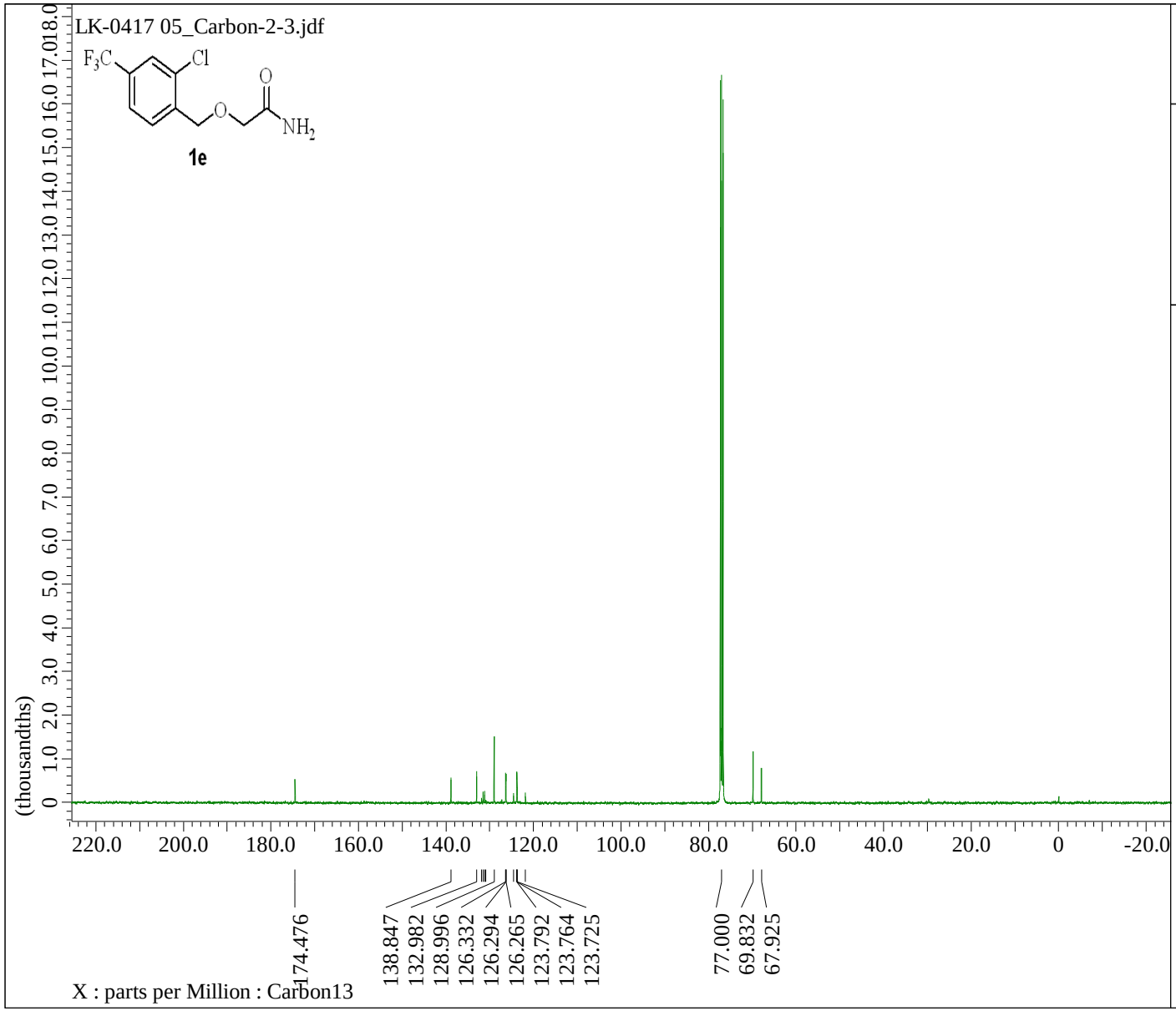
| | |
|---|---|
| Filename | = LK1104-01_single_p |
| Author | = delta |
| Experiment | = single_pulse.jxp |
| Sample_Id | = LK1104-01 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-NOV-2016 12:32: |
| Revision_Time | = 10-AUG-2017 16:09: |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Fluorine19 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 83.88608[ms] |
| X_Domain | = 19F |
| X_Freq | = 376.17105393[MHz] |
| X_Offset | = -100[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 11.92092896[Hz] |
| X_Sweep | = 195.3125[kHz] |
| X_Sweep_Clipped | = 156.25[kHz] |
| Irr_Domain | = Fluorine19 |
| Irr_Freq | = 376.17105393[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Fluorine19 |
| Tri_Freq | = 376.17105393[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 17[dC] |
| X_90_Width | = 10[us] |
| X_Acq_Time | = 83.88608[ms] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK-0417 05_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK-0417 05_Proton- |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK-0417 05 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 17-APR-2017 11:43: |
| Revision_Time | = 9-AUG-2017 11:20: |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 66 |
| Temp_Get | = 21.8[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |

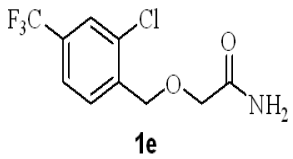



```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK-0417 05_Carbon-2-1.jdf
```

| | |
|---|---|
| Filename | = LK-0417 05_Carb |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK-0417 05 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 17-APR-2017 12: |
| Revision_Time | = 9-AUG-2017 11: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 4800 |
| Total_Scans | = 4800 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21.9[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |

LK-0417 05_single_pulse-1-3.jdf




1e

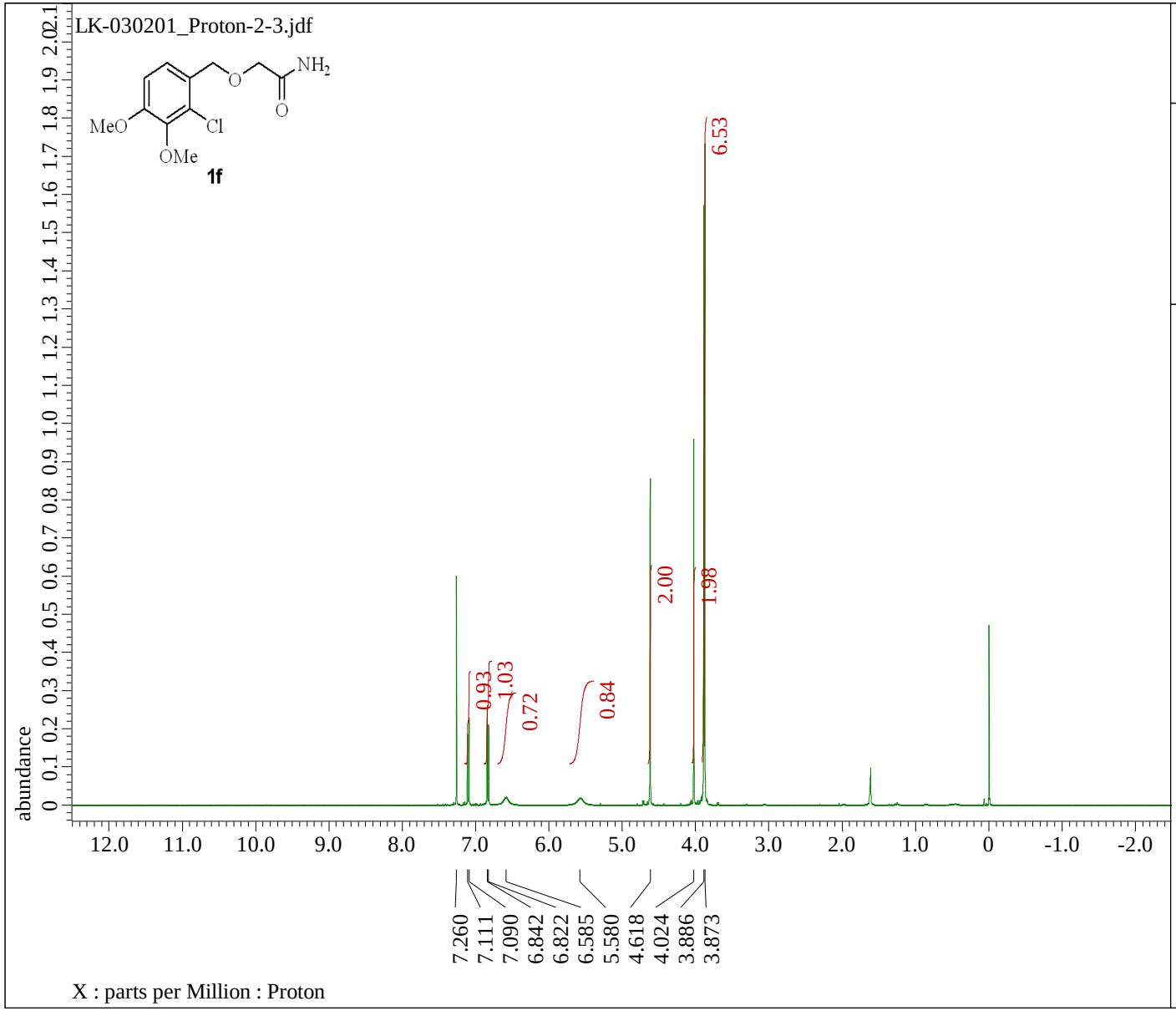



X : parts per Million : Fluorine19

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK-0417 05_single_pulse-1-1.
```

| | |
|---|---|
| Filename | = LK-0417 05_single_ |
| Author | = delta |
| Experiment | = single_pulse.jxp |
| Sample_Id | = LK-0417 05 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 17-APR-2017 11:44: |
| Revision_Time | = 9-AUG-2017 11:18: |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Fluorine19 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 83.88608[ms] |
| X_Domain | = 19F |
| X_Freq | = 376.17105393[MHz] |
| X_Offset | = -100[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 11.92092896[Hz] |
| X_Sweep | = 195.3125[kHz] |
| X_Sweep_Clipped | = 156.25[kHz] |
| Irr_Domain | = Fluorine19 |
| Irr_Freq | = 376.17105393[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Fluorine19 |
| Tri_Freq | = 376.17105393[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21.8[dC] |
| X_90_Width | = 10[us] |
| X_Acq_Time | = 83.88608[ms] |




JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

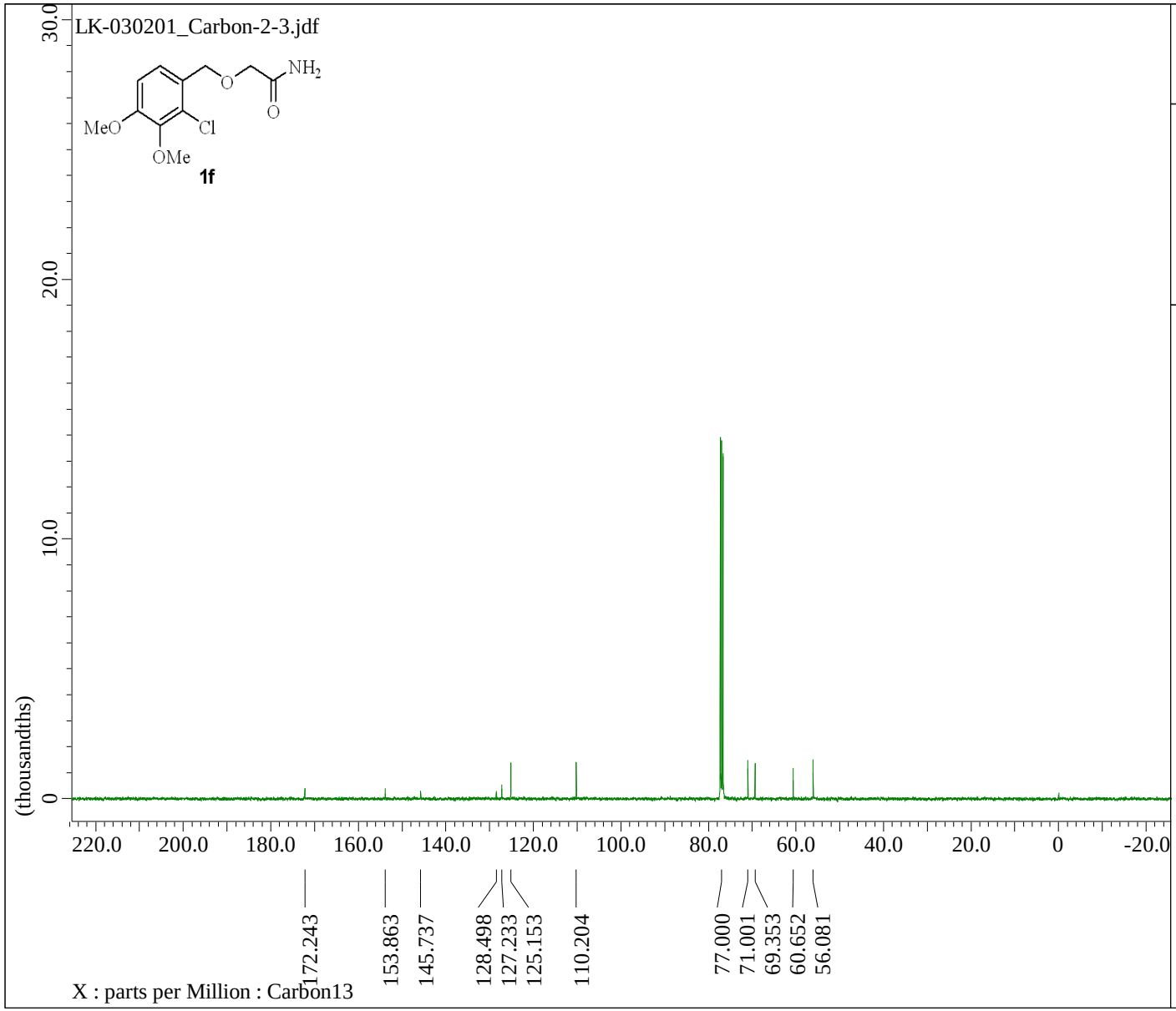
Derived from: LK-030201_Proton-2-1.jdf
```

```
Filename              = LK-030201_Proton-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = LK-030201
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 23-MAR-2017 17:43:
Revision_Time         = 10-AUG-2017 14:45:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 20.2[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```

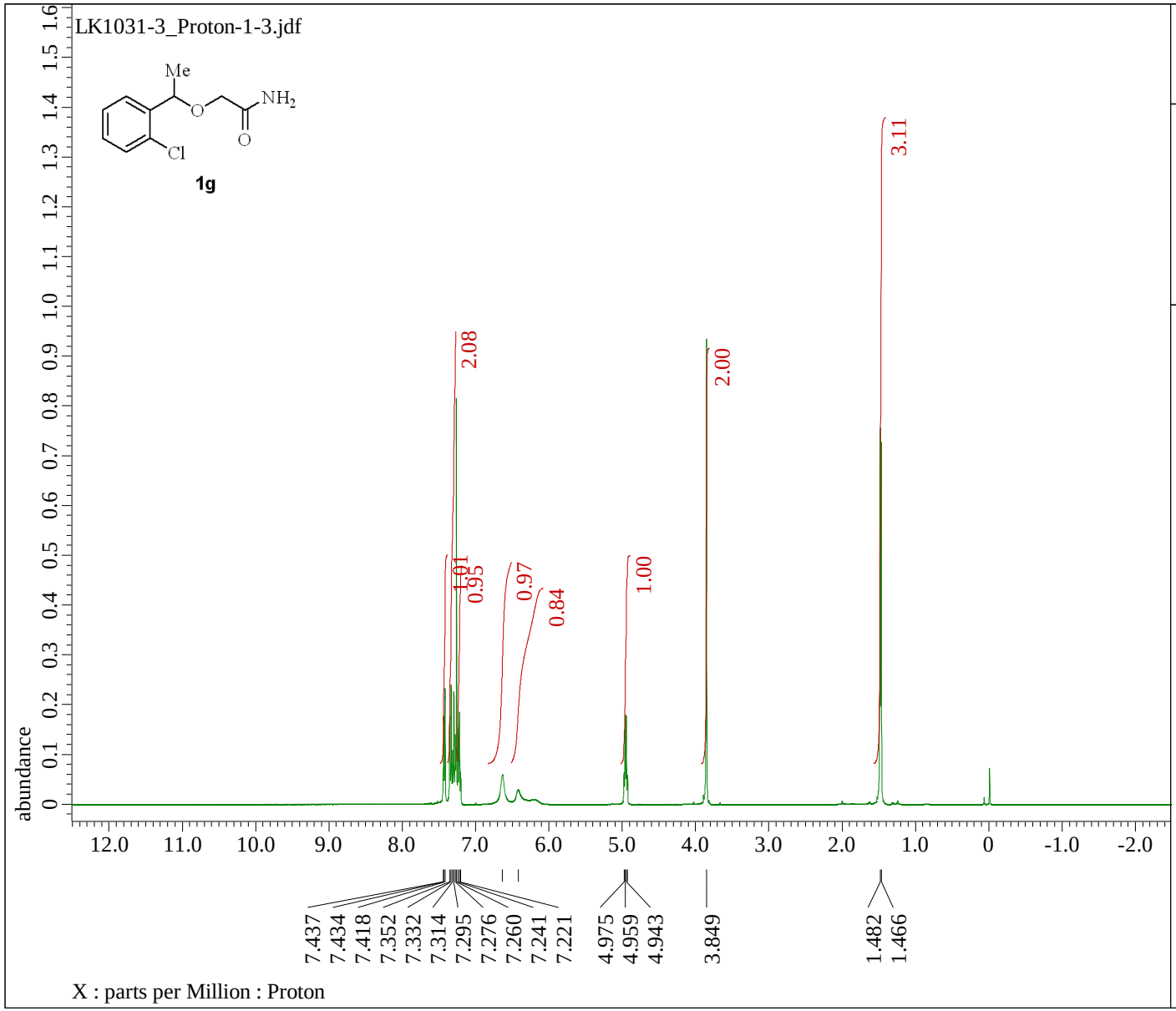



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK-030201_Carbon-2-1.jdf
```

| | |
|---|---|
| Filename | = LK-030201_Carbo |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK-030201 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 23-MAR-2017 17: |
| Revision_Time | = 10-AUG-2017 14: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 1024 |
| Total_Scans | = 1024 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 18.7[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |



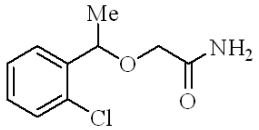

JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

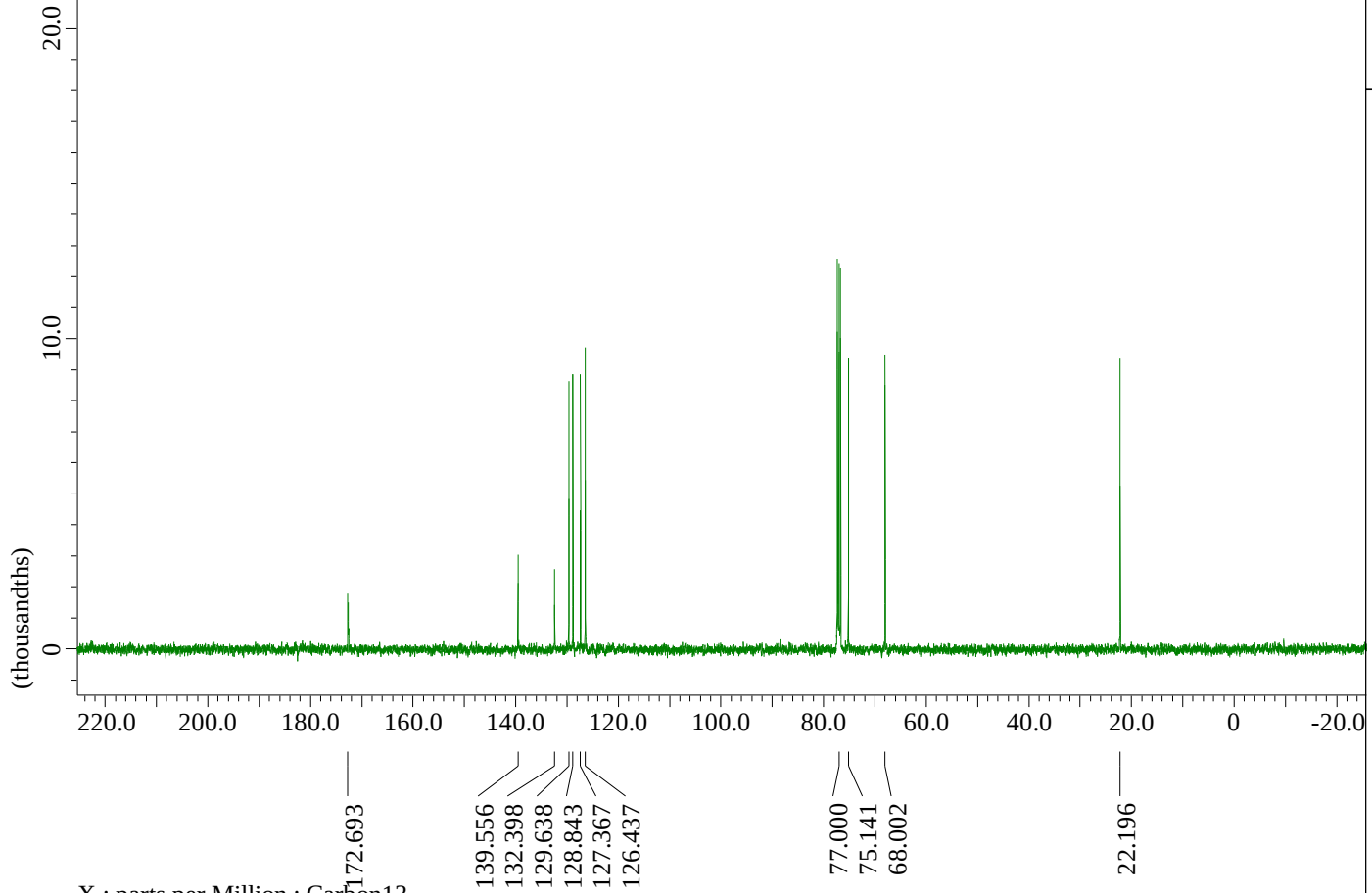
Derived from: LK1031-3_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1031-3_Proton-1- |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK1031-3 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 31-OCT-2016 16:31: |
| Revision_Time | = 10-AUG-2017 16:19: |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 46 |
| Temp_Get | = 14[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |

LK1031-3_Carbon-1-3.jdf




**1g**

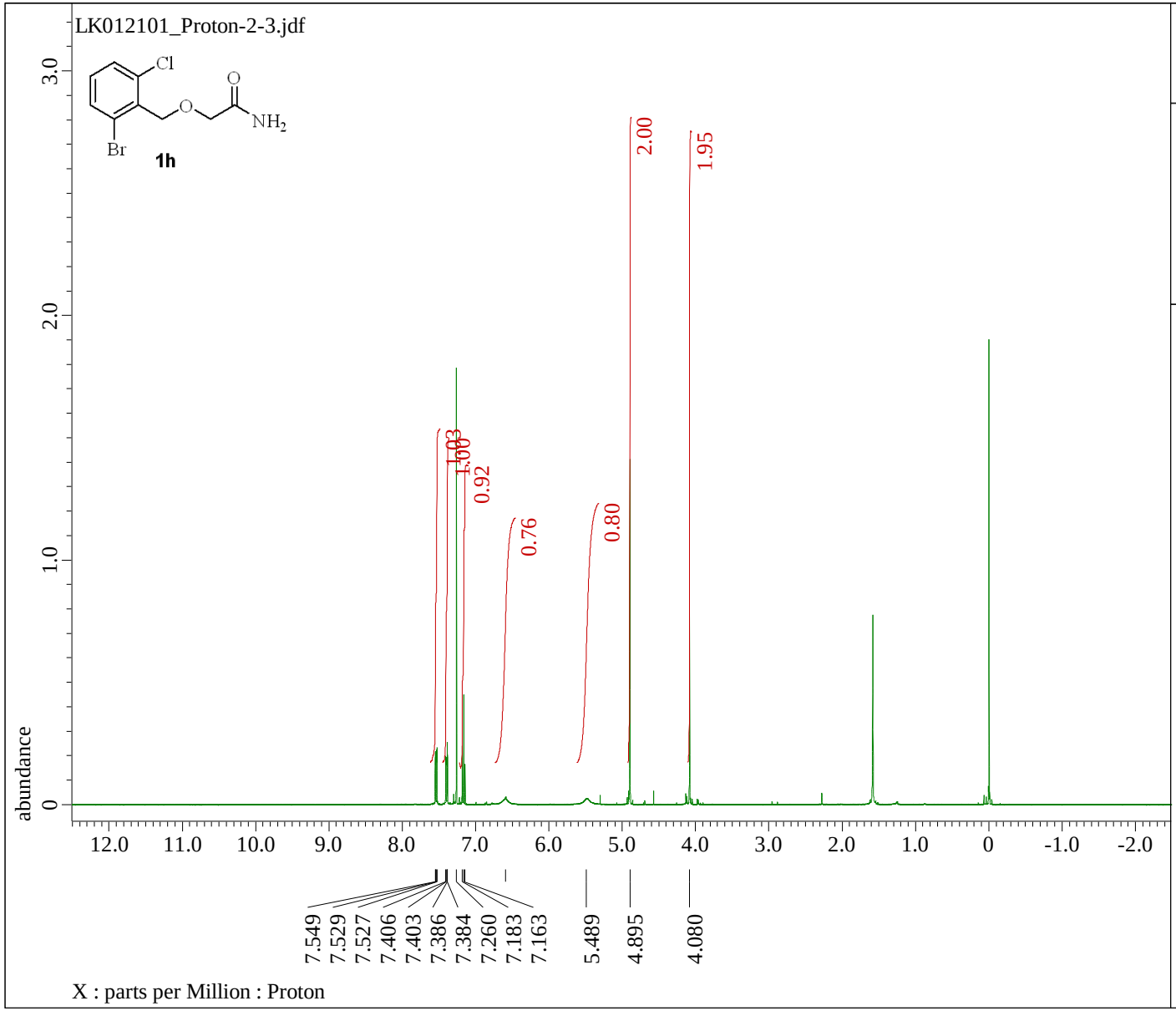



X : parts per Million : Carbon13

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1031-3_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1031-3_Carbon |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK1031-3 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 31-OCT-2016 17: |
| Revision_Time | = 10-AUG-2017 16: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 144 |
| Total_Scans | = 144 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 15.8[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |




JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

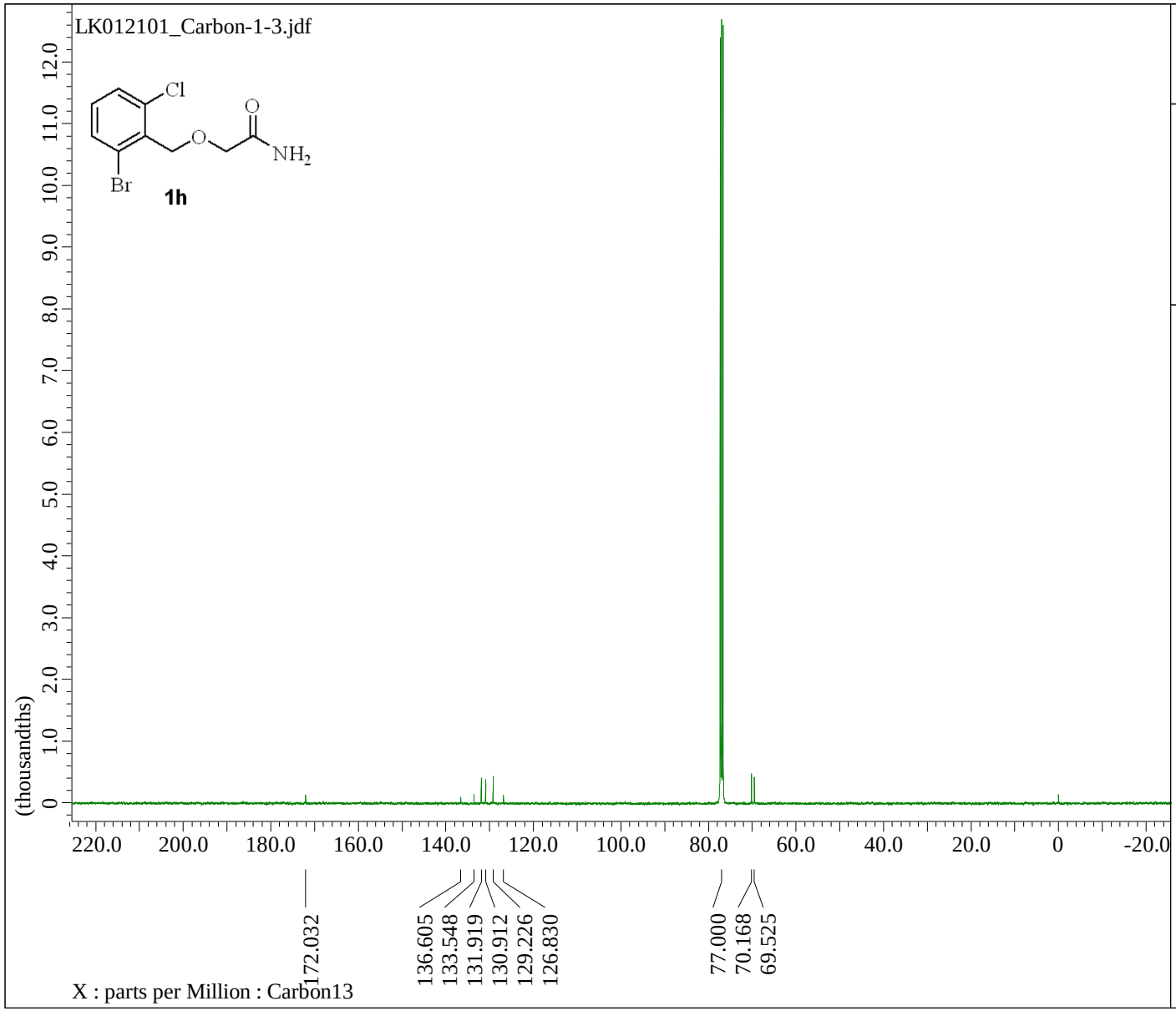
Derived from: LK012101_Proton-2-1.jdf
```

```
Filename                = LK012101_Proton-2-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = LK012101
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 22-JAN-2017 17:39:
Revision_Time           = 10-AUG-2017 16:29:

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 2.18628096[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45739775[Hz]
X_Sweep                 = 7.4940048[kHz]
X_Sweep_Clipped         = 5.99520384[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 66
Temp_Get                = 18.5[dC]
X_90_Width              = 9.5[us]
X_Acq_Time              = 2.18628096[s]
```

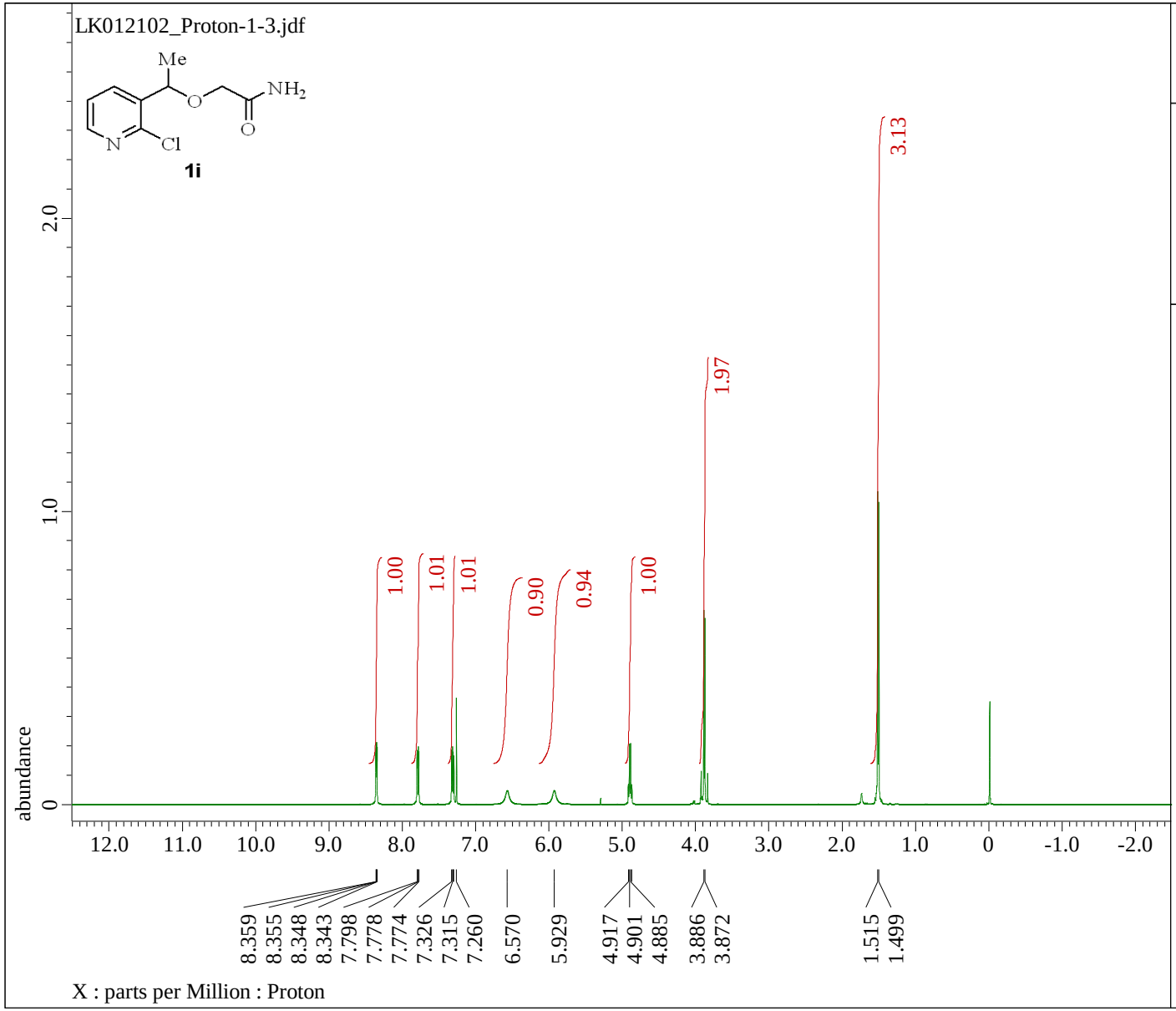



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK012101_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK012101_Carbon |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK012101 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 22-JAN-2017 17: |
| Revision_Time | = 10-AUG-2017 16: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 10000 |
| Total_Scans | = 10000 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 13.9[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |




JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

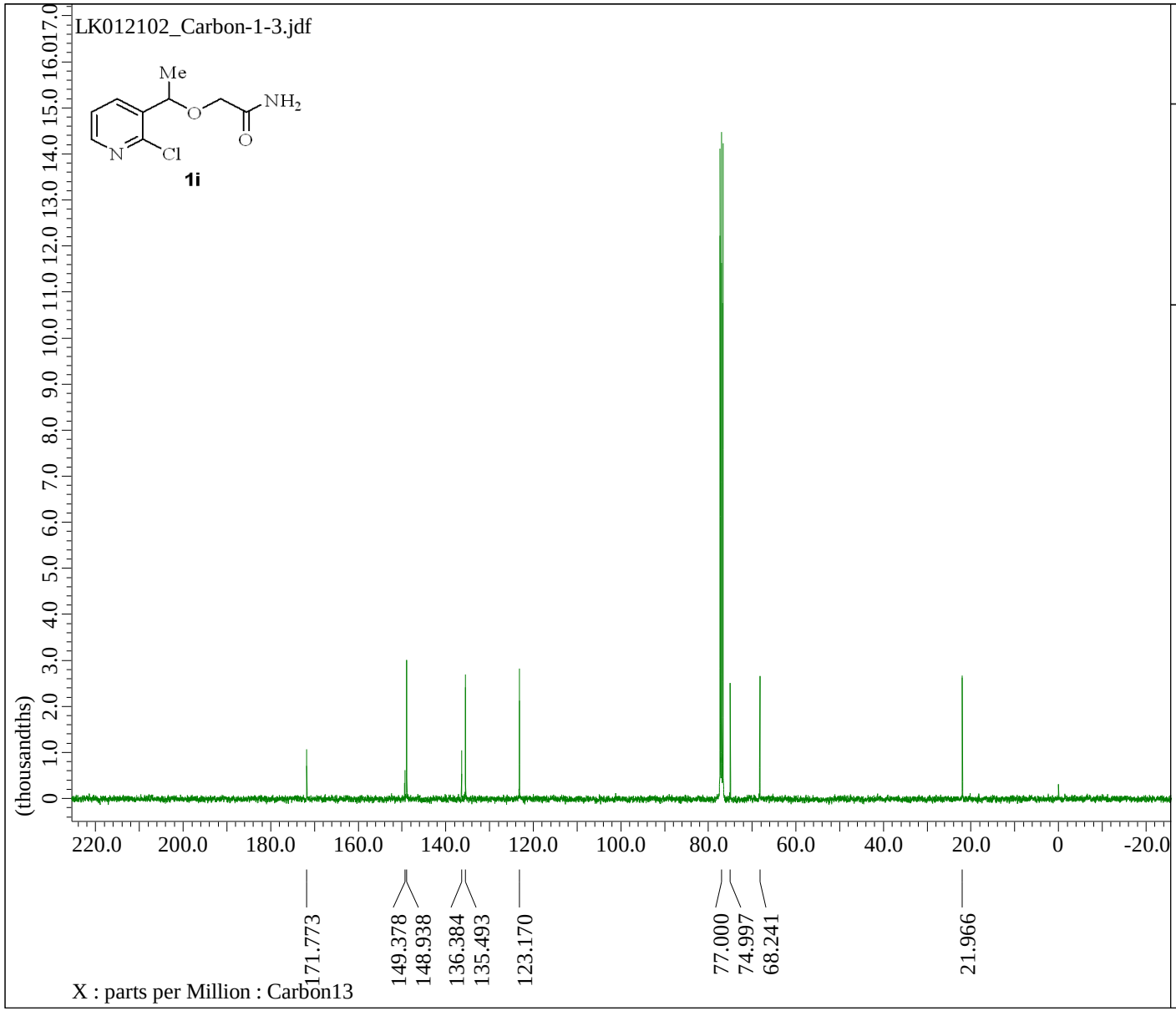
Derived from: LK012102_Proton-1-1.jdf
```

```
Filename              = LK012102_Proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = LK012102
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 22-JAN-2017 14:50:
Revision_Time         = 10-AUG-2017 16:42:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 13.8[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```

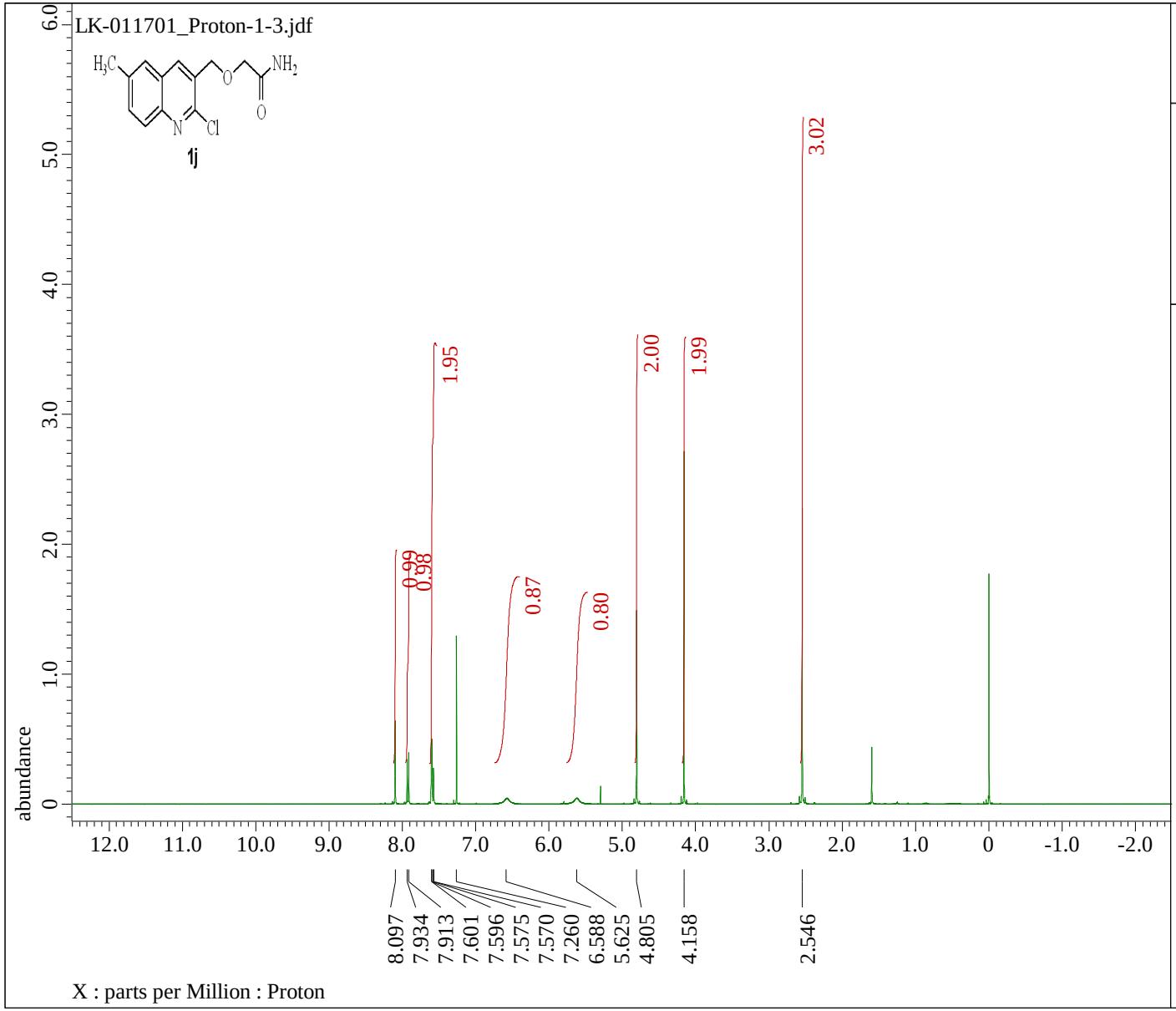



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK012102_Carbon-1-1.jdf
```

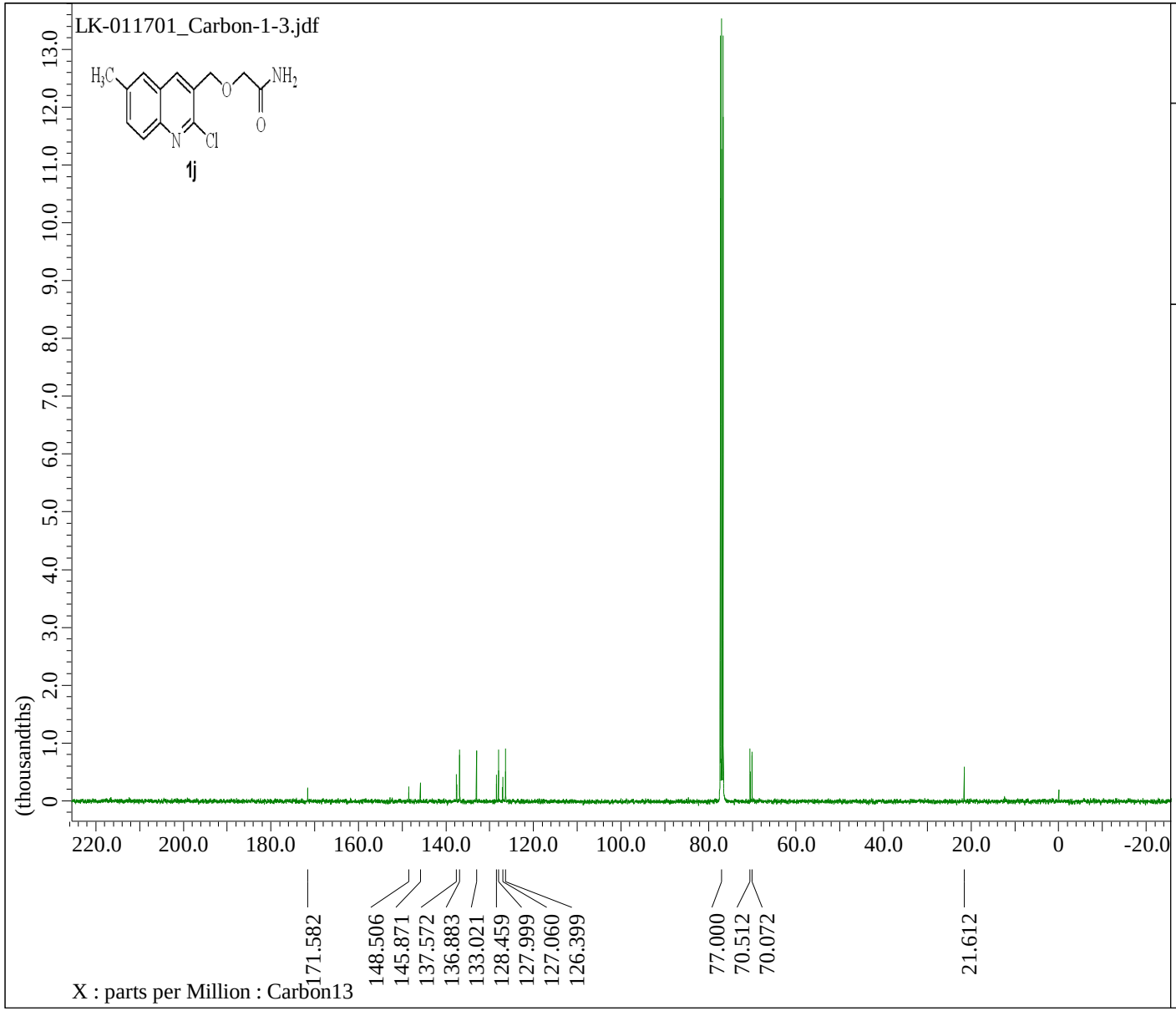
| | |
|---|---|
| Filename | = LK012102_Carbon |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK012102 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 22-JAN-2017 15: |
| Revision_Time | = 10-AUG-2017 16: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 805 |
| Total_Scans | = 805 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 15.4[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK-011701_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK-011701_Proton-1 |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK-011701 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 17-JAN-2017 17:48: |
| Revision_Time | = 10-AUG-2017 17:01: |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 66 |
| Temp_Get | = 24.1[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |





```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

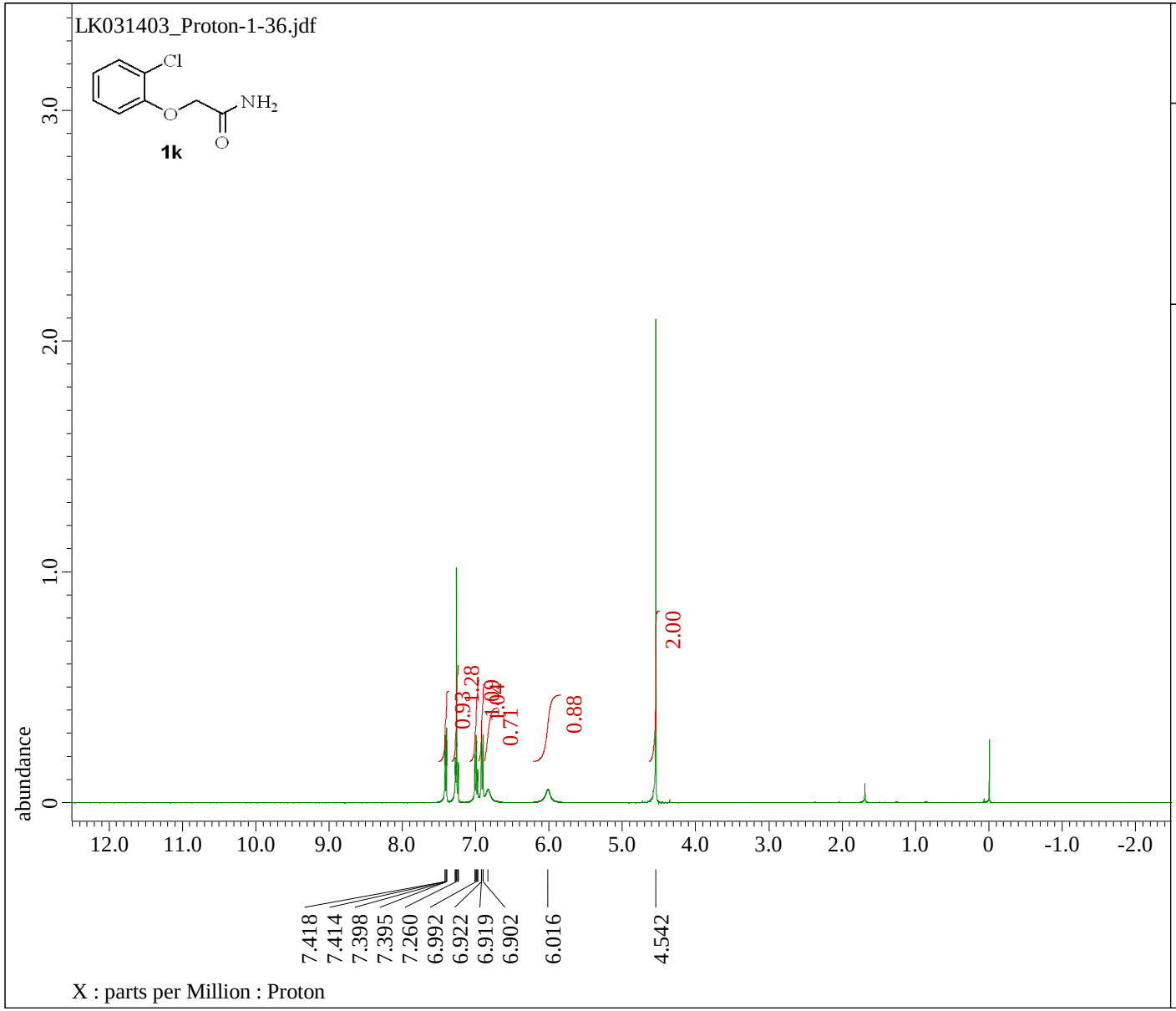
Derived from: LK-011701_Carbon-1-1.jdf

Filename                = LK-011701_Carbo
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = LK-011701
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 17-JAN-2017 21:
Revision_Time           = 10-AUG-2017 17:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 2400
Total_Scans             = 2400

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 20.7[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```




JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

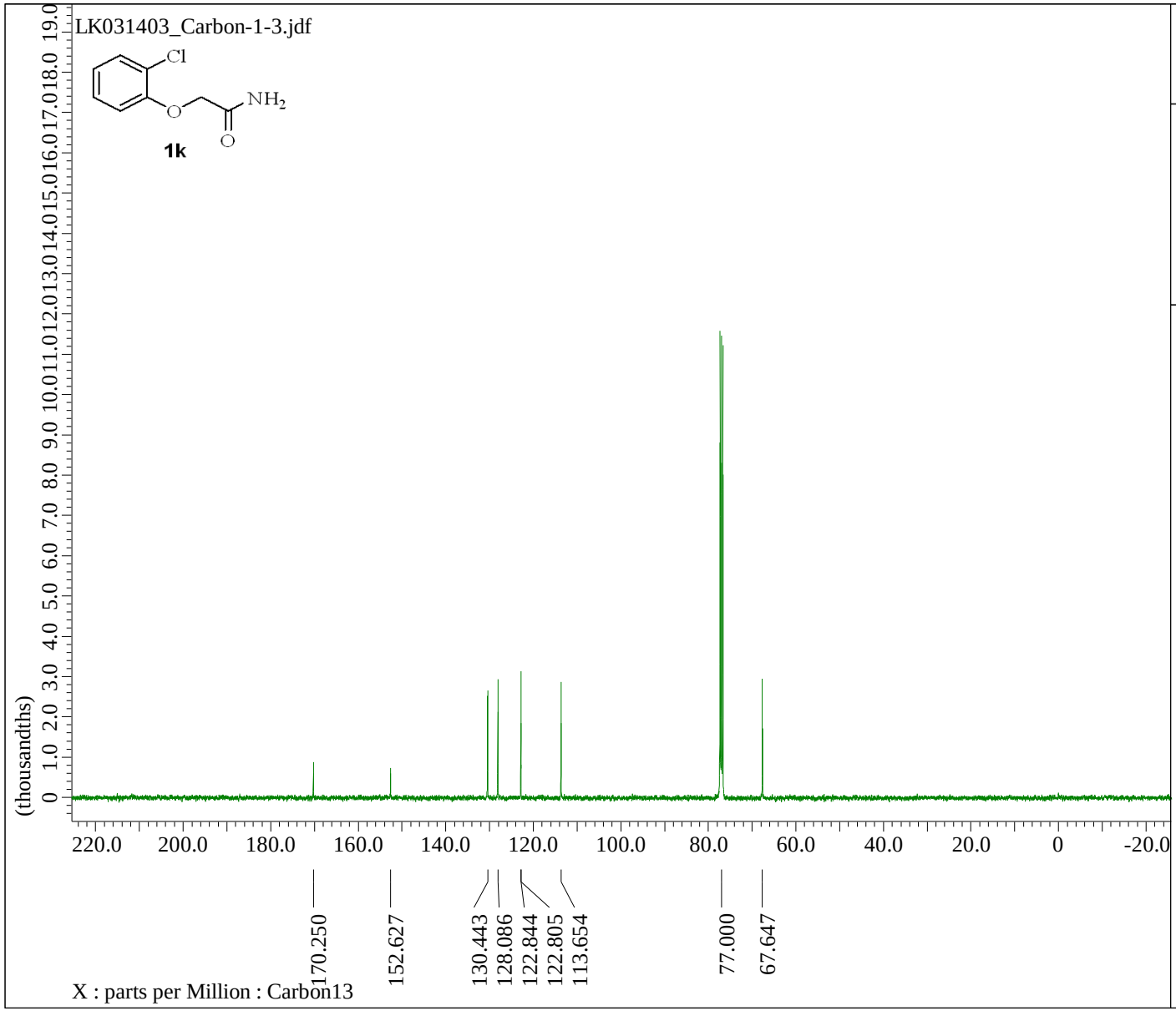
Derived from: LK031403_Proton-1-1.jdf
```

```
Filename                = LK031403_Proton-1-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = LK031403
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 14-MAR-2017 15:53:
Revision_Time           = 10-AUG-2017 17:14:

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 2.18628096[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45739775[Hz]
X_Sweep                 = 7.4940048[kHz]
X_Sweep_Clipped         = 5.99520384[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 15.1[dC]
X_90_Width              = 9.5[us]
X_Acq_Time              = 2.18628096[s]
```

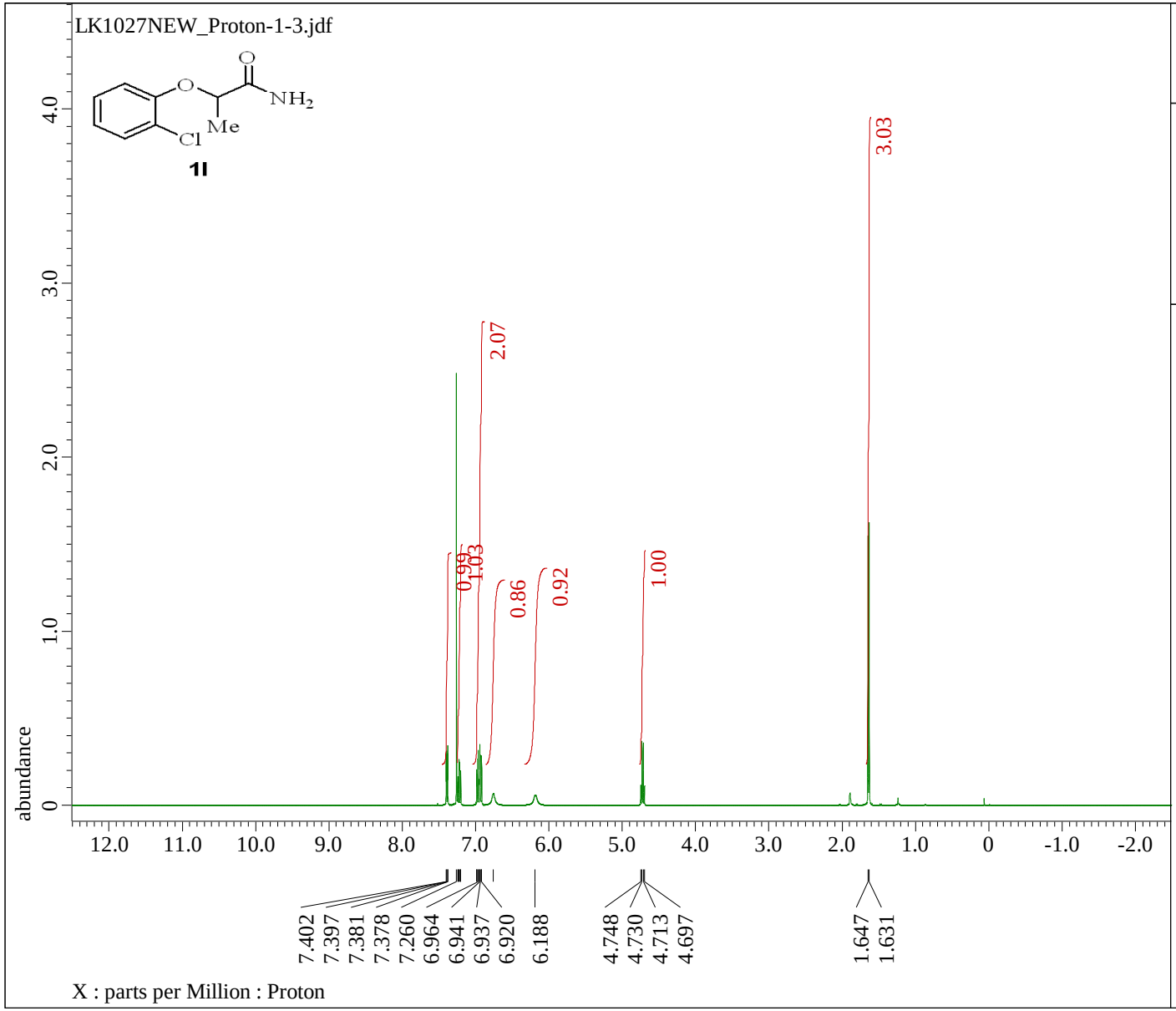



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK031403_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK031403_Carbon |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK031403 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-MAR-2017 18: |
| Revision_Time | = 10-AUG-2017 17: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 1024 |
| Total_Scans | = 1024 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 15.5[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |

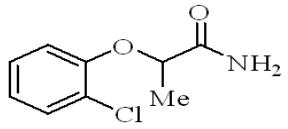



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1027NEW_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1027NEW_Proton-1 |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK1027NEW |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 31-OCT-2016 16:25: |
| Revision_Time | = 10-AUG-2017 17:54: |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 46 |
| Temp_Get | = 14.1[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |

LK1027NEW_Carbon-1-3.jdf



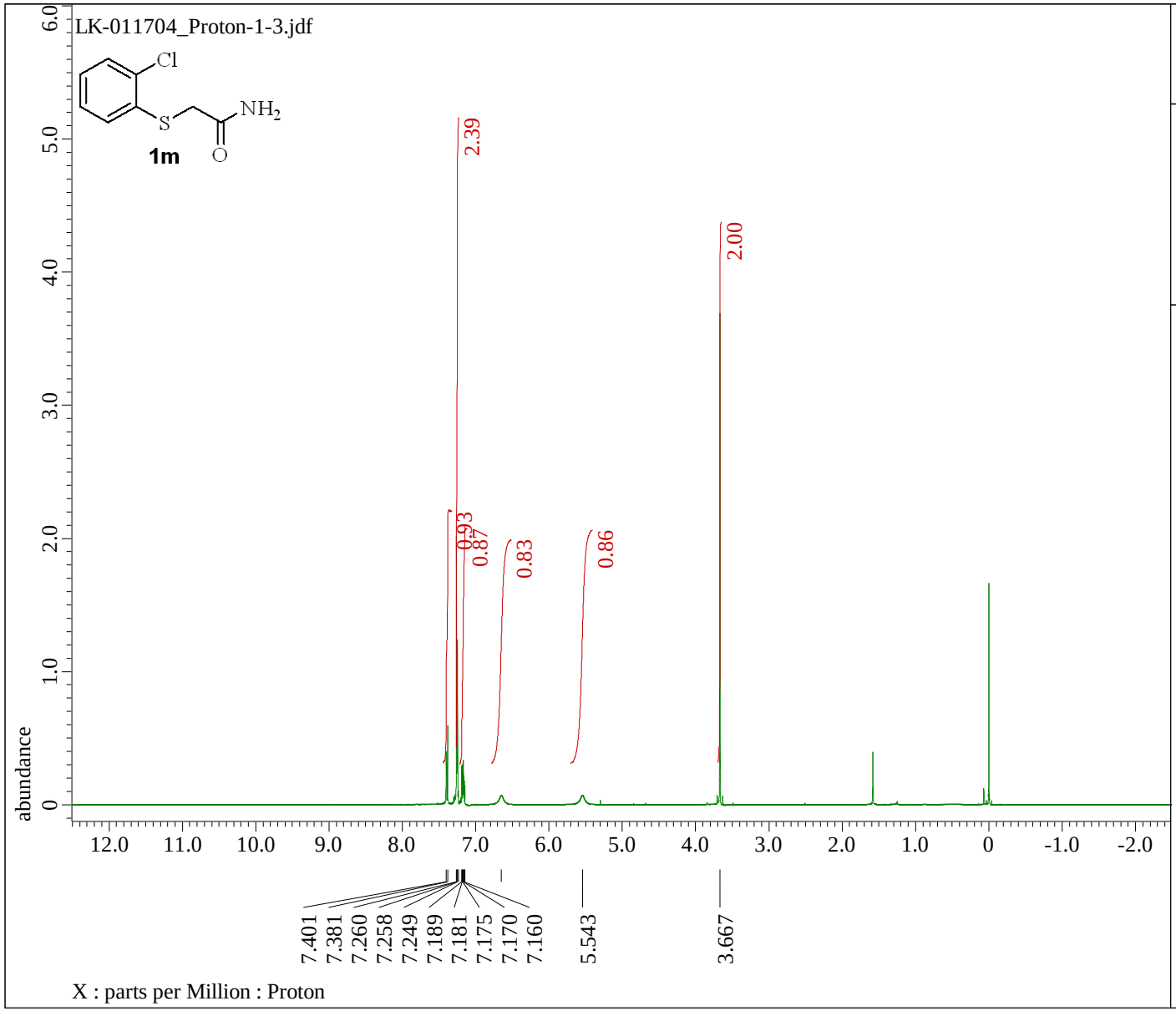

**1l**




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1027NEW_Carbon-1-1.jdf
```

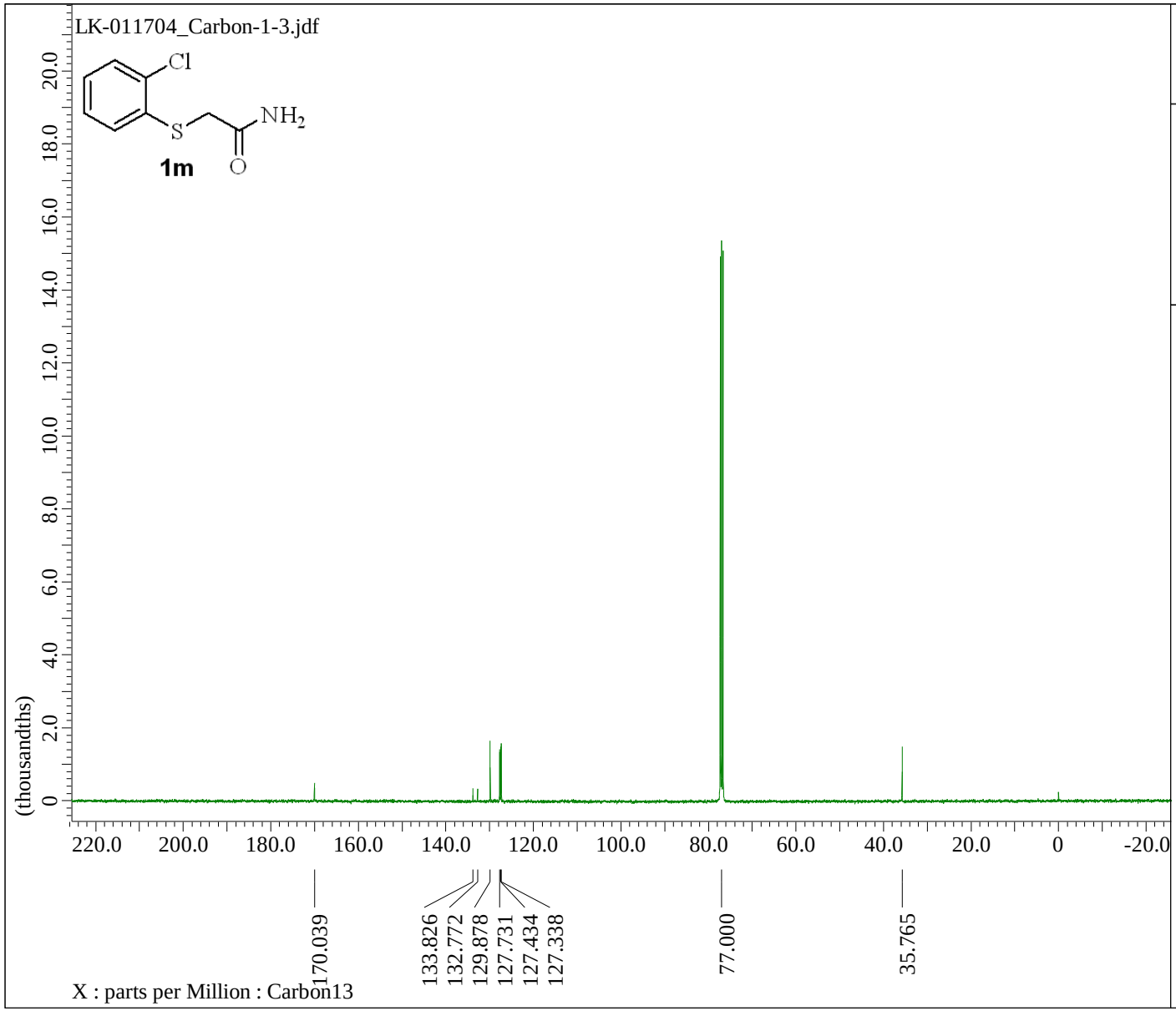
| | |
|---|---|
| Filename | = LK1027NEW_Carbo |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK1027NEW |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 31-OCT-2016 16: |
| Revision_Time | = 10-AUG-2017 17: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 302 |
| Total_Scans | = 302 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 14.4[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK-011704_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK-011704_Proton-1 |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK-011704 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 17-JAN-2017 18:02: |
| Revision_Time | = 10-AUG-2017 15:29: |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 66 |
| Temp_Get | = 23.8[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |




JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

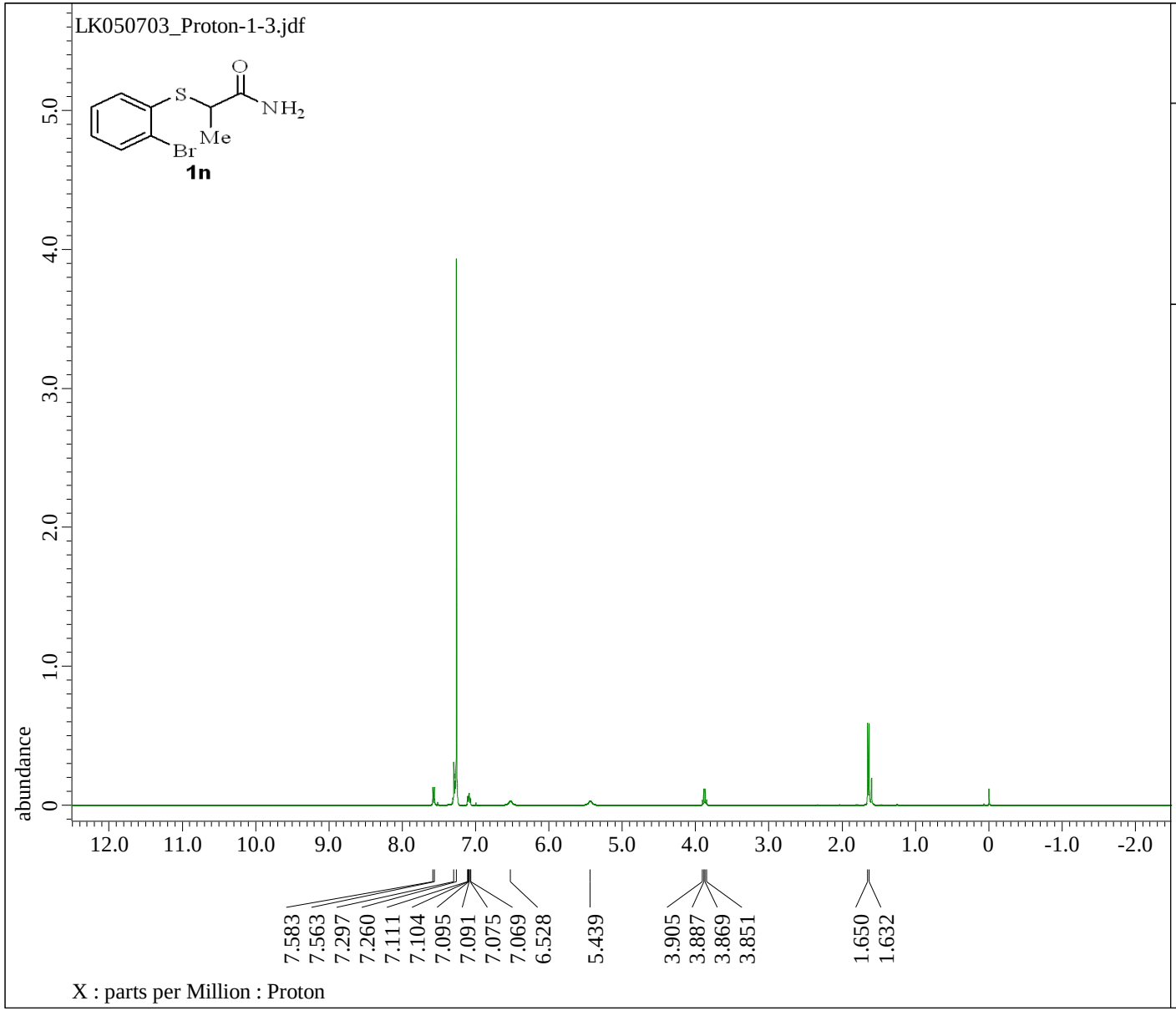
Derived from: LK-011704_Carbon-1-1.jdf
```

```
Filename                = LK-011704_Carbo
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = LK-011704
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 18-JAN-2017 04:
Revision_Time           = 10-AUG-2017 15:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = TRUE
Scans                   = 2400
Total_Scans             = 2400

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 17[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

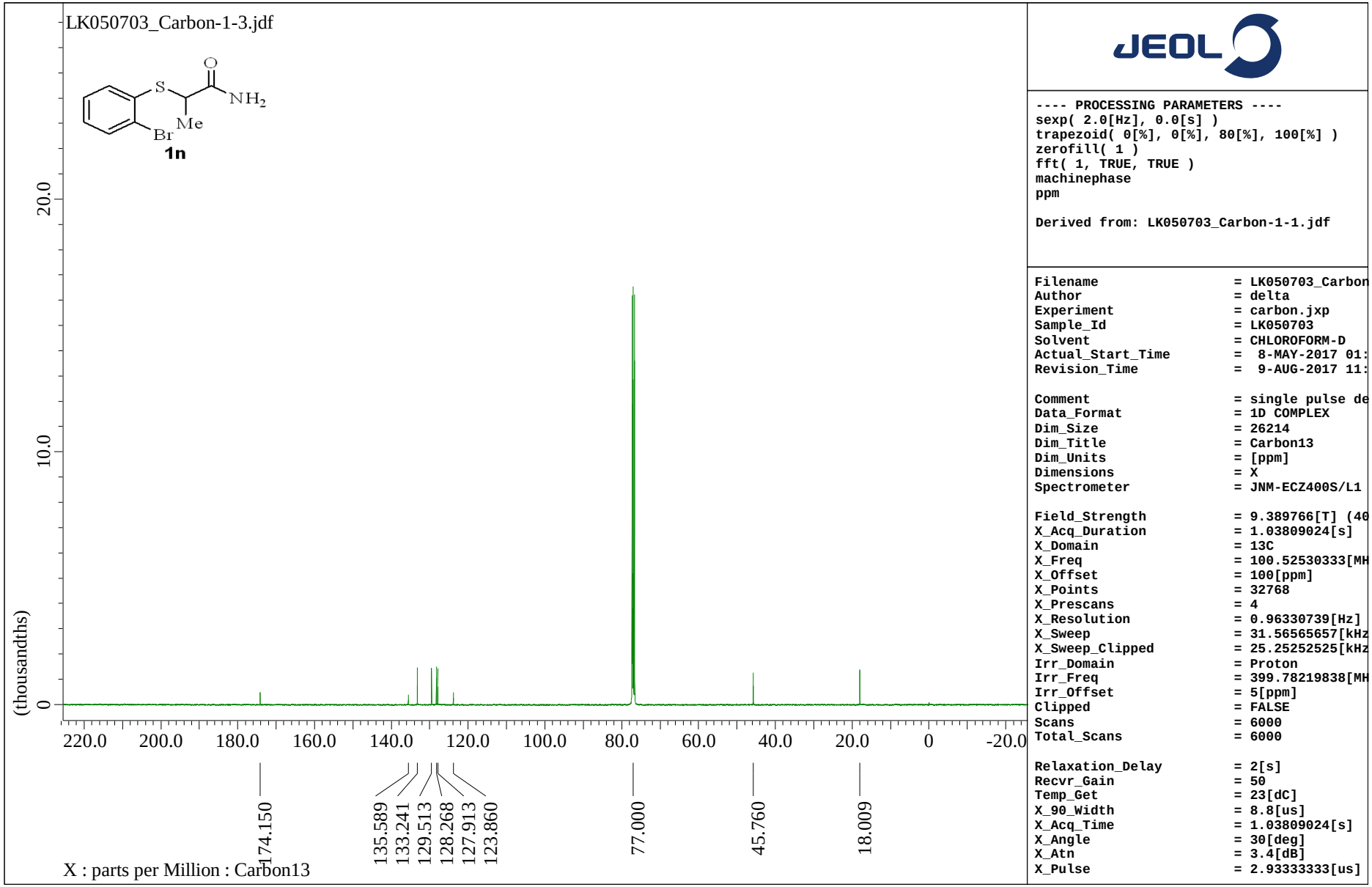
Derived from: LK050703_Proton-1-1.jdf
```

```
Filename              = LK050703_Proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = LK050703
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  7-MAY-2017 17:29:
Revision_Time         =  9-AUG-2017 11:45:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.2[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```

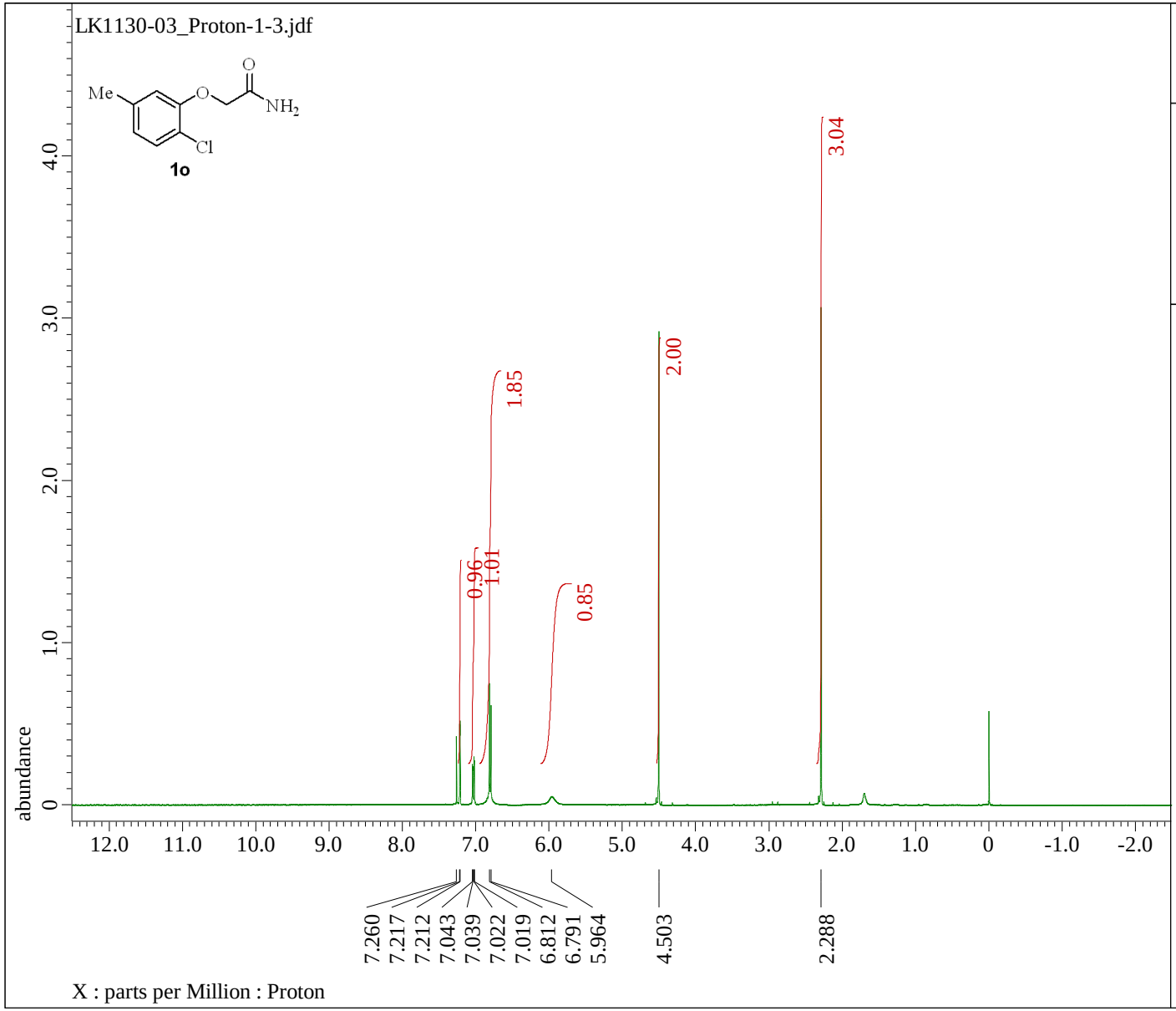



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK050703_Carbon-1-1.jdf
```

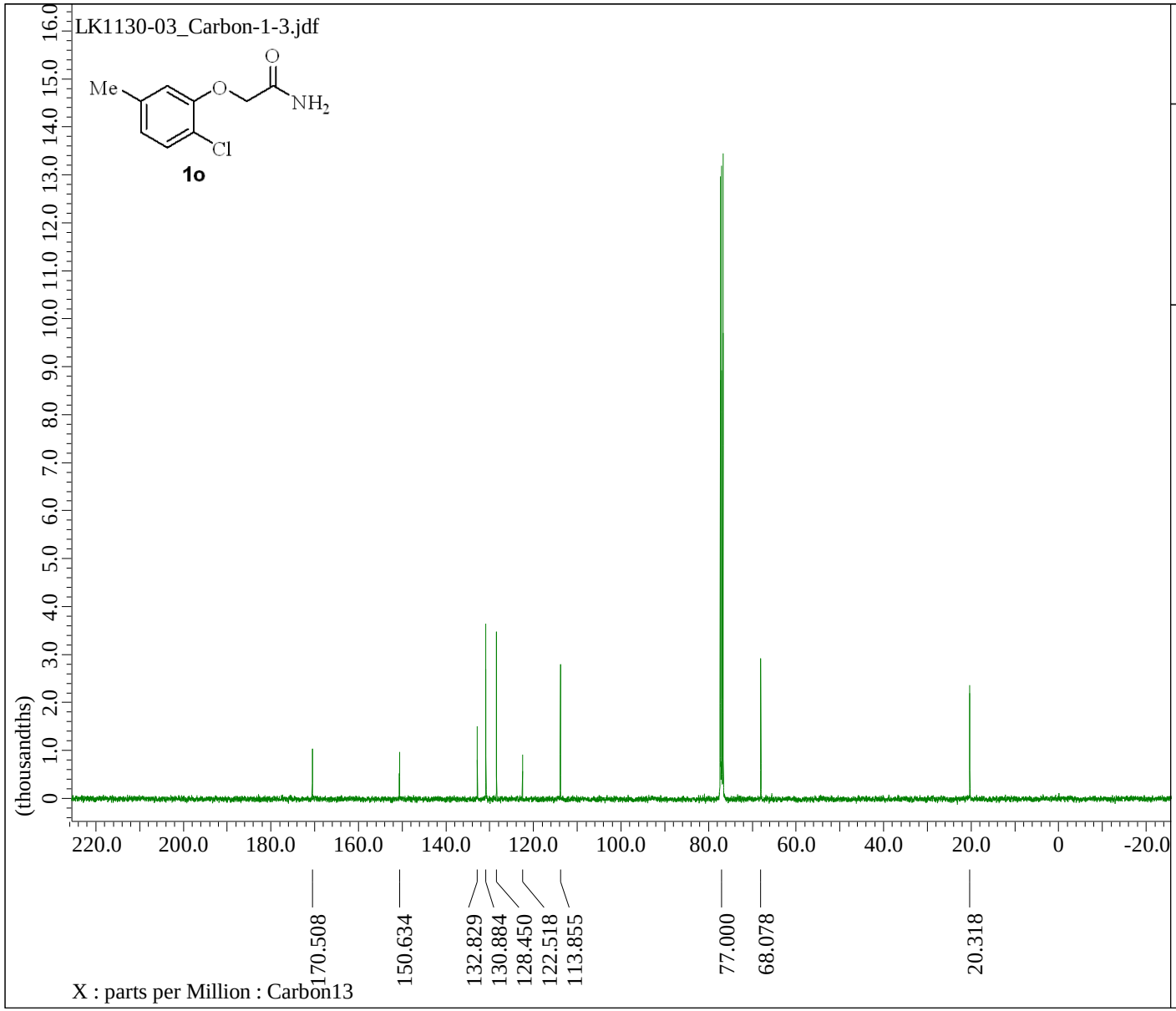
| | |
|---|---|
| Filename | = LK050703_Carbon |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK050703 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 8-MAY-2017 01: |
| Revision_Time | = 9-AUG-2017 11: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 6000 |
| Total_Scans | = 6000 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 23[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1130-03_Proton-1-1.jdf
```

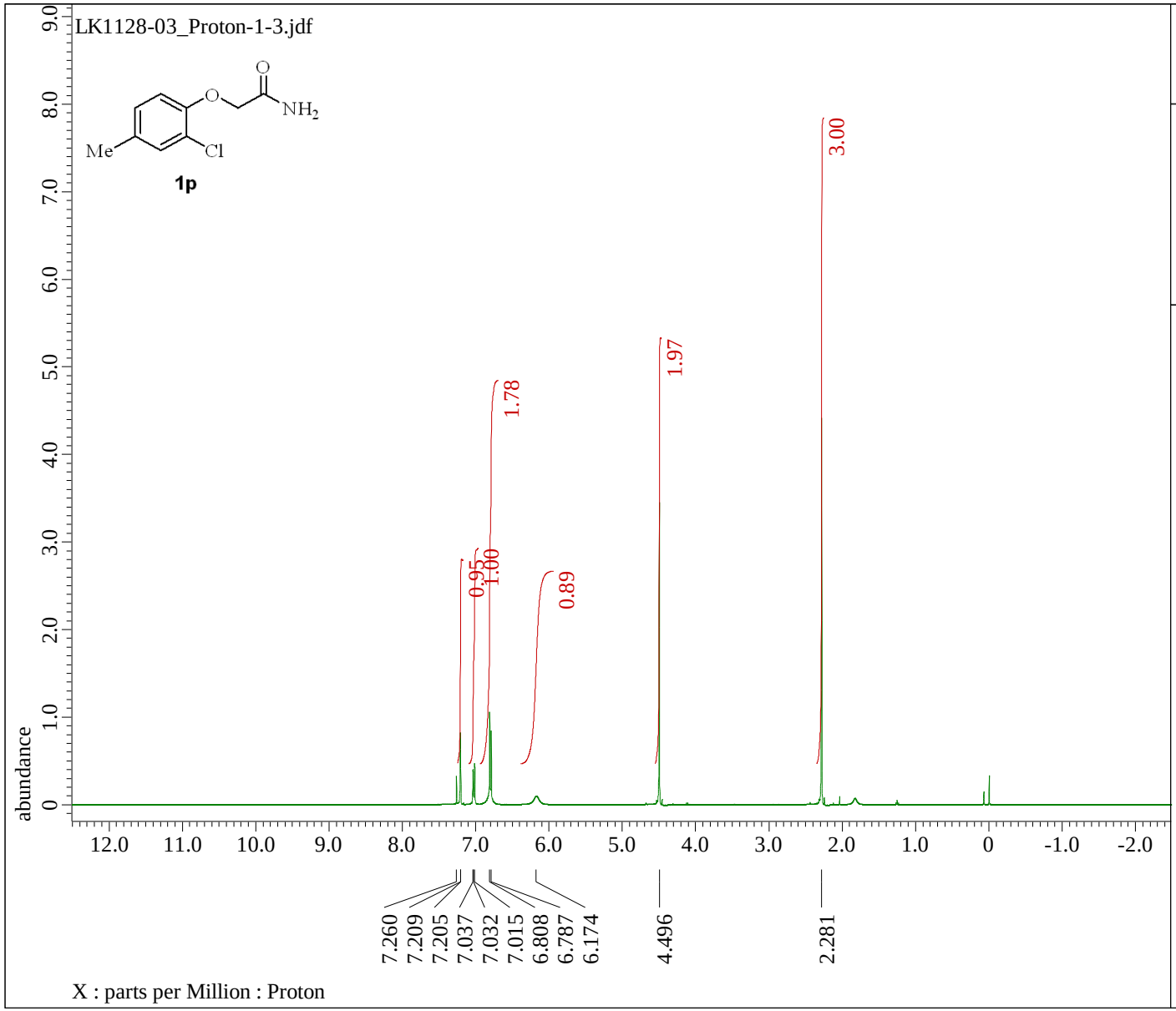
| | |
|---|---|
| Filename | = LK1130-03_Proton-1 |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK1130-03 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 30-NOV-2016 18:02: |
| Revision_Time | = 10-AUG-2017 15:10: |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 25.2[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1130-03_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1130-03_Carbo |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK1130-03 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 30-NOV-2016 19: |
| Revision_Time | = 10-AUG-2017 15: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 1024 |
| Total_Scans | = 1024 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 24.4[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |



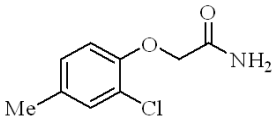

JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

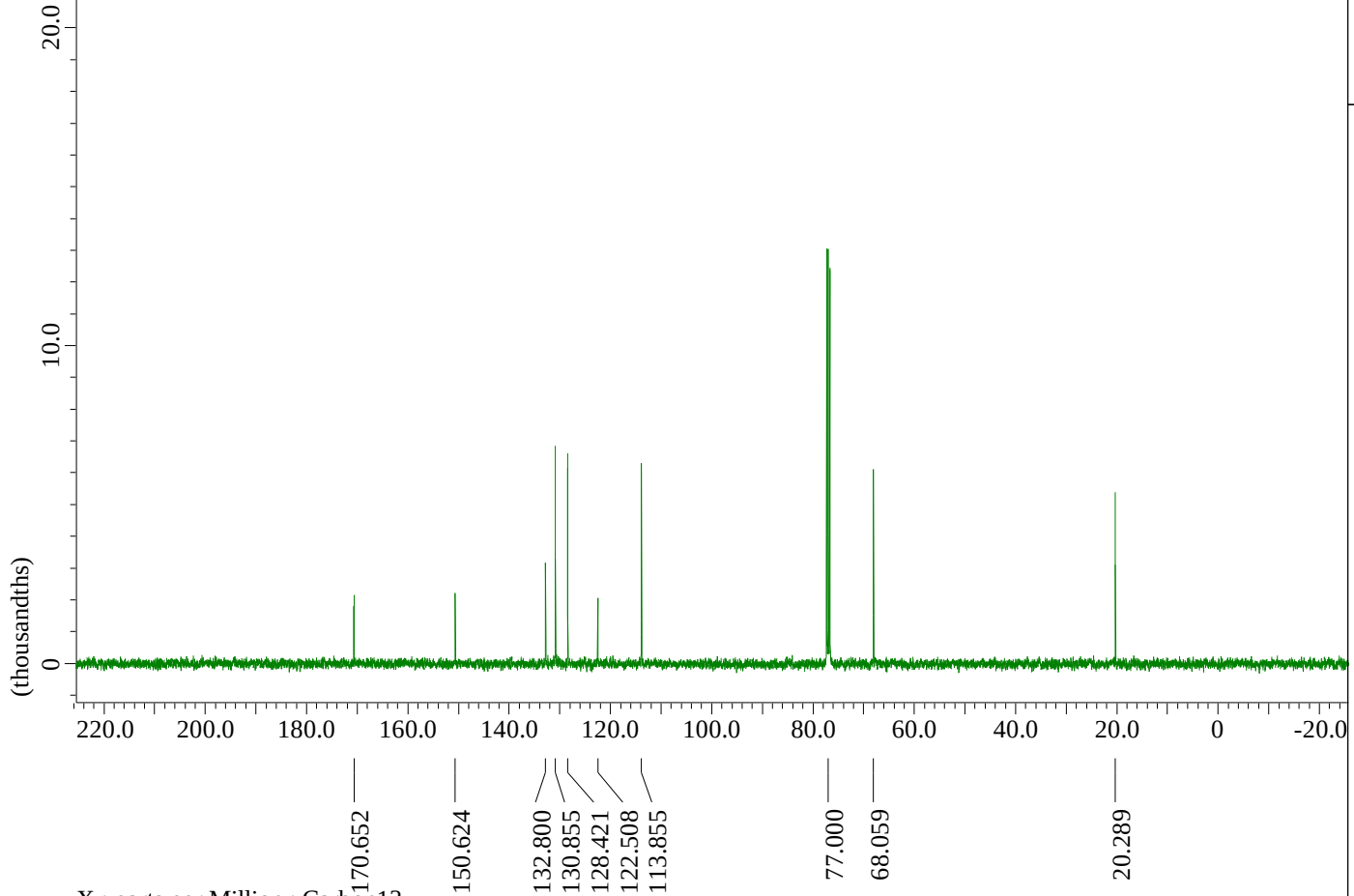
Derived from: LK1128-03_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1128-03_Proton-1 |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK1128-03 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 28-NOV-2016 16:42: |
| Revision_Time | = 10-AUG-2017 17:42: |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 27[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |

LK1128-03_Carbon-1-3.jdf




**1p**

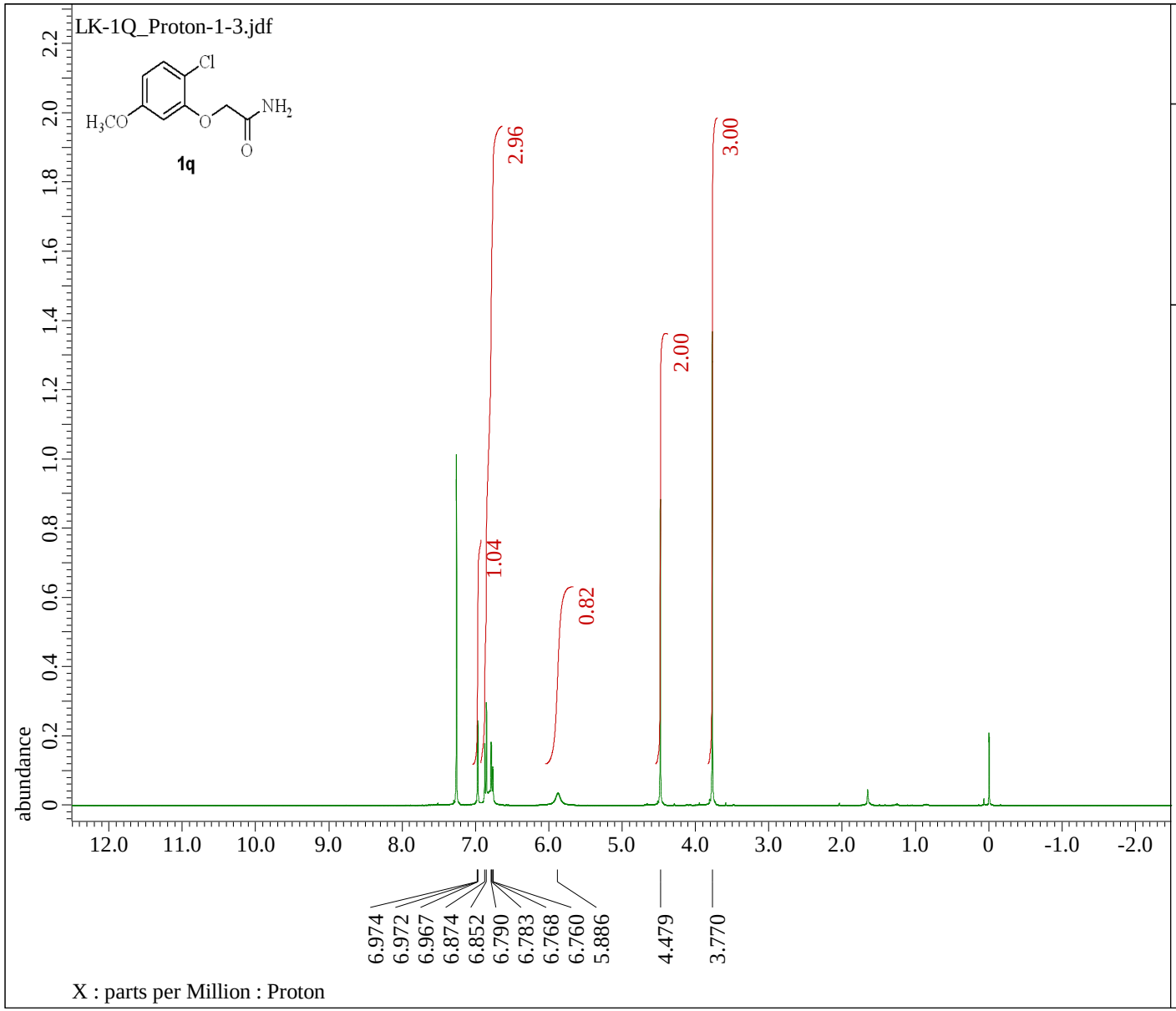



X : parts per Million : Carbon13

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1128-03_Carbon-1-1.jdf
```

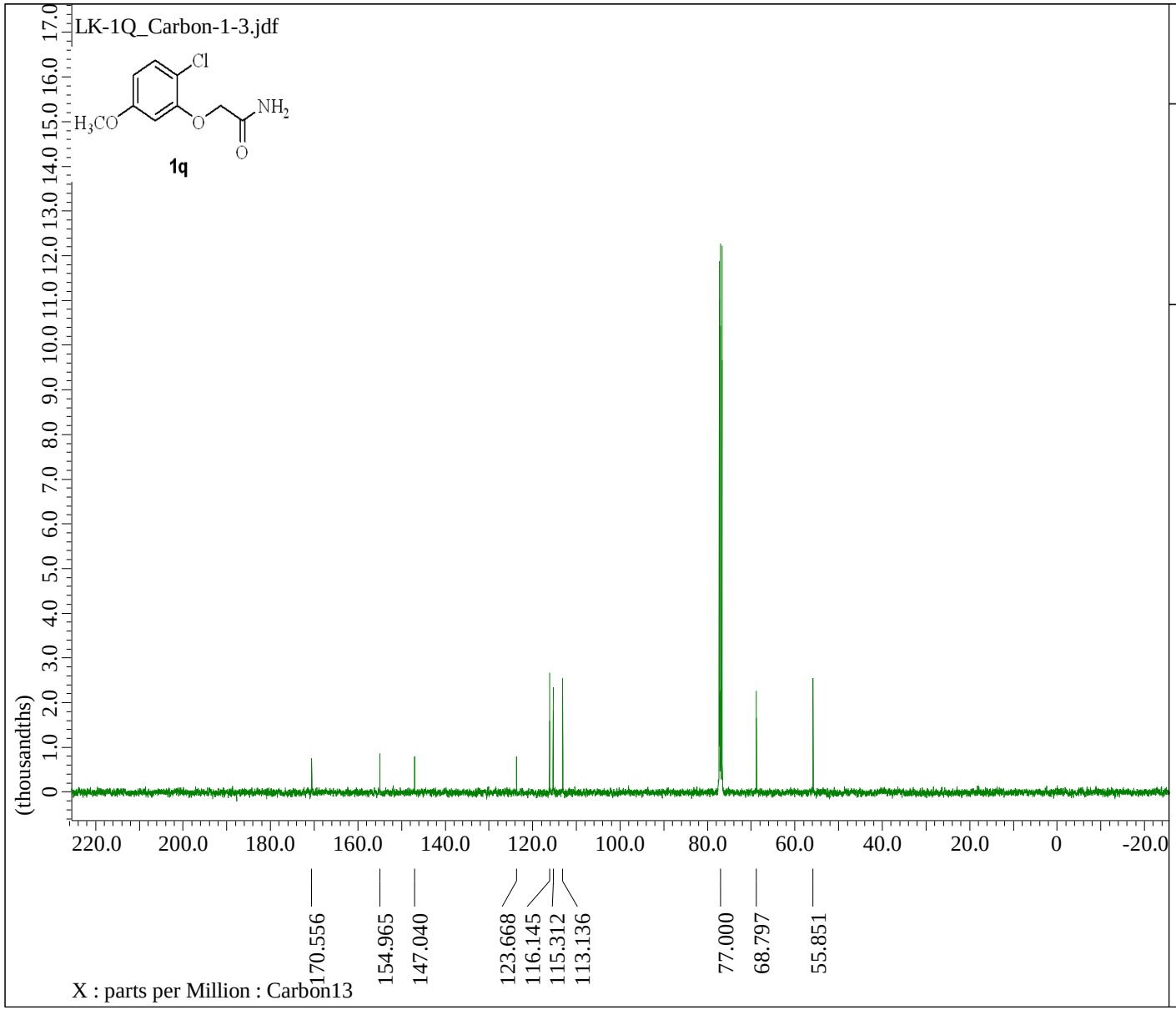
| | |
|---|---|
| Filename | = LK1128-03_Carbo |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK1128-03 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 28-NOV-2016 18: |
| Revision_Time | = 10-AUG-2017 17: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = TRUE |
| Scans | = 128 |
| Total_Scans | = 128 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 27.3[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK-1Q_Proton-1-1.jdf
```

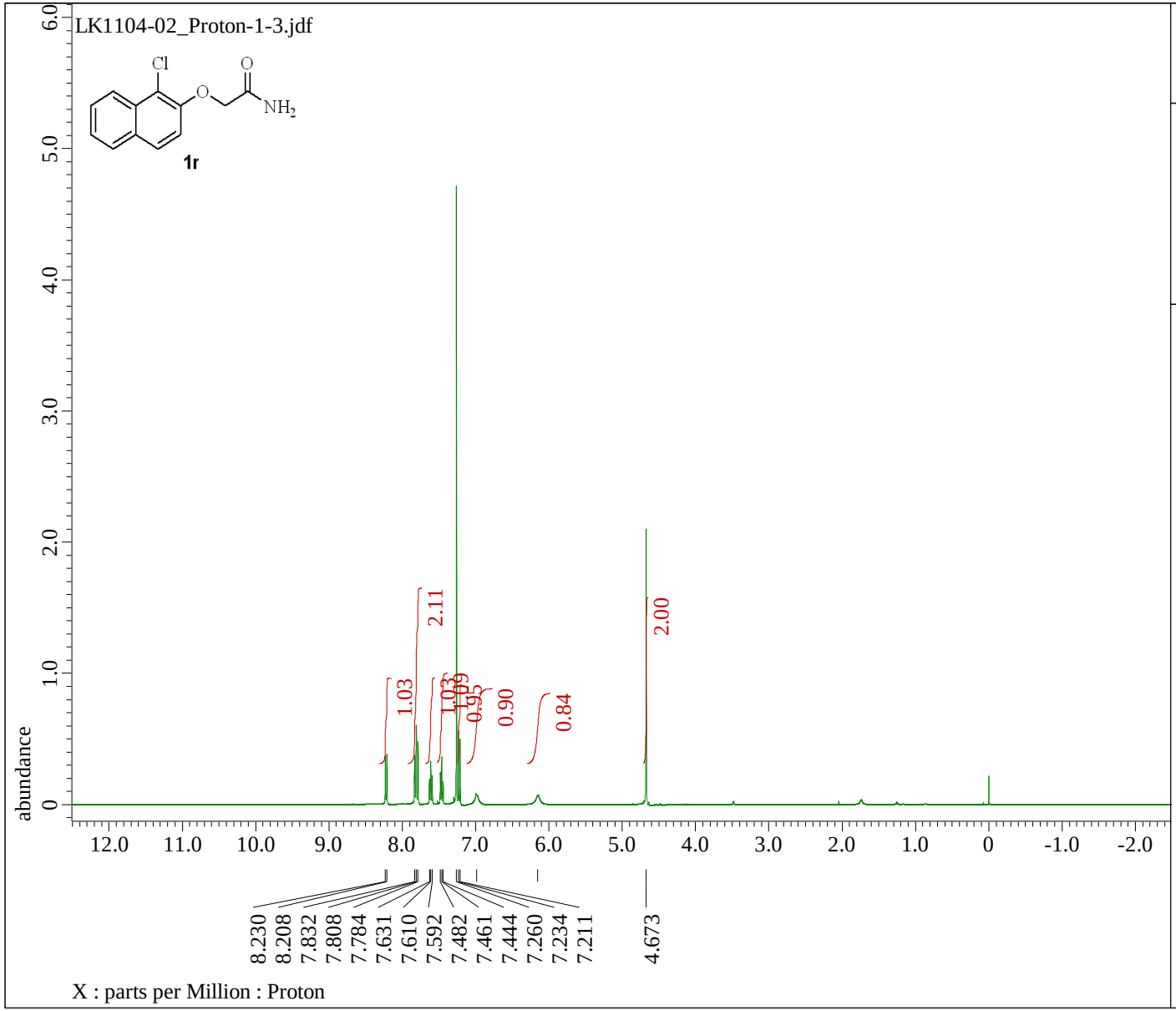
| | |
|---|---|
| Filename | = LK-1Q_Proton-1-3.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK-1Q |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 11-AUG-2017 11:26: |
| Revision_Time | = 11-AUG-2017 12:32: |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 20.2[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK-1Q_Carbon-1-1.jdf
```

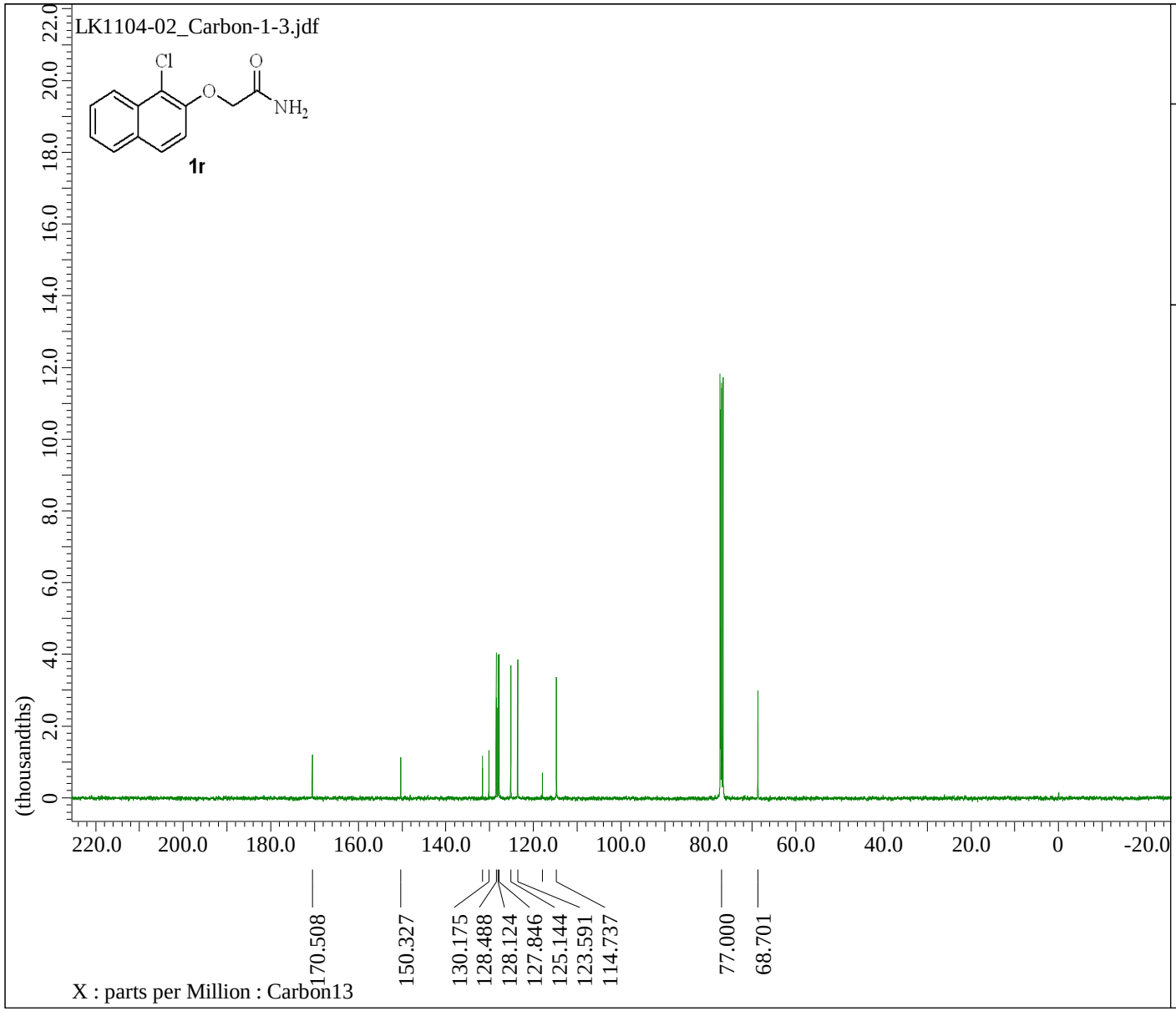
| | |
|---|---|
| Filename | = LK-1Q_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK-1Q |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 11-AUG-2017 12: |
| Revision_Time | = 11-AUG-2017 12: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 468 |
| Total_Scans | = 468 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.4[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1104-02_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1104-02_Proton-1 |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK1104-02 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-NOV-2016 12:22: |
| Revision_Time | = 10-AUG-2017 15:18: |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 16.9[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |

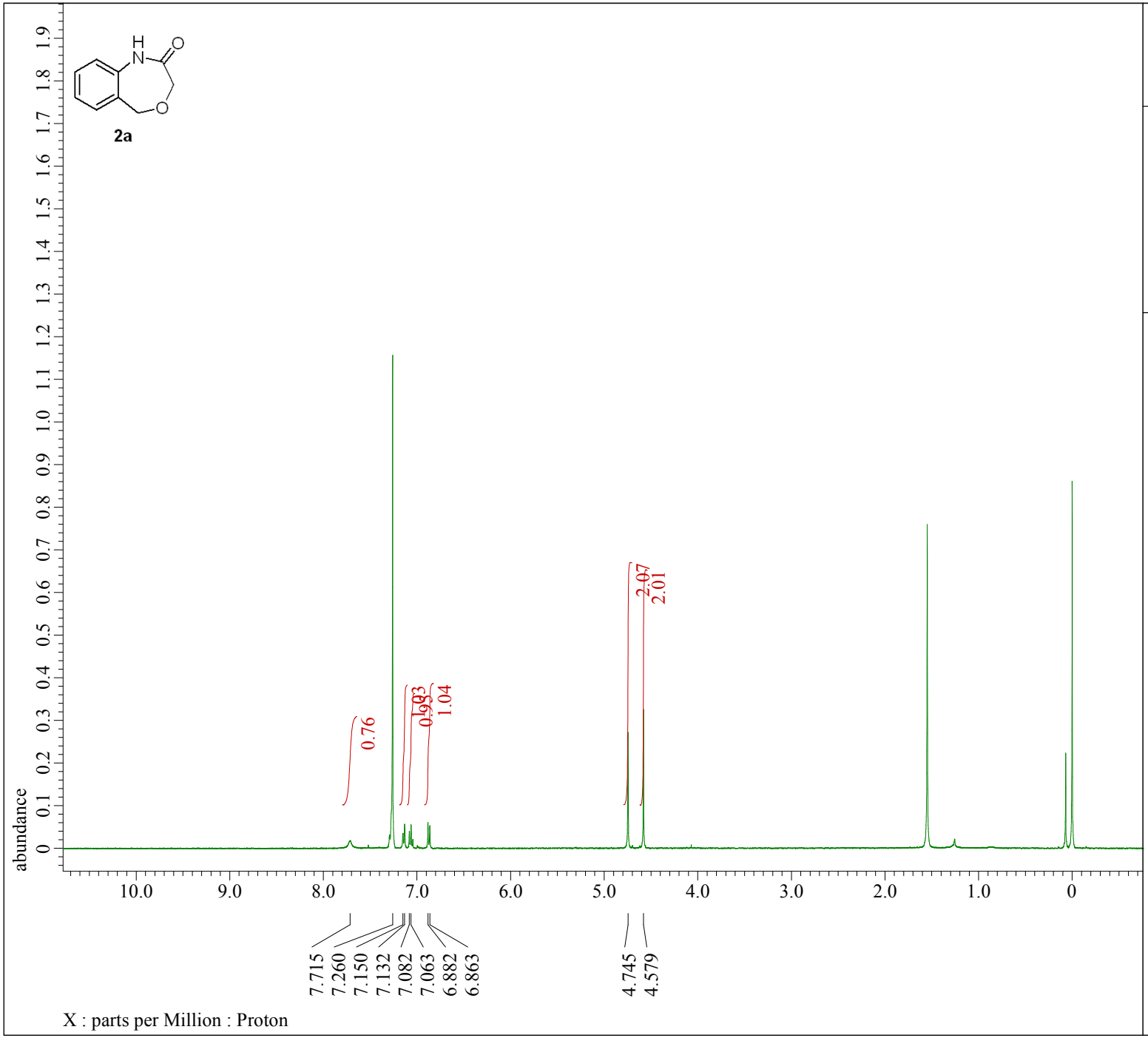



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1104-02_Carbon-1-1.jdf
```

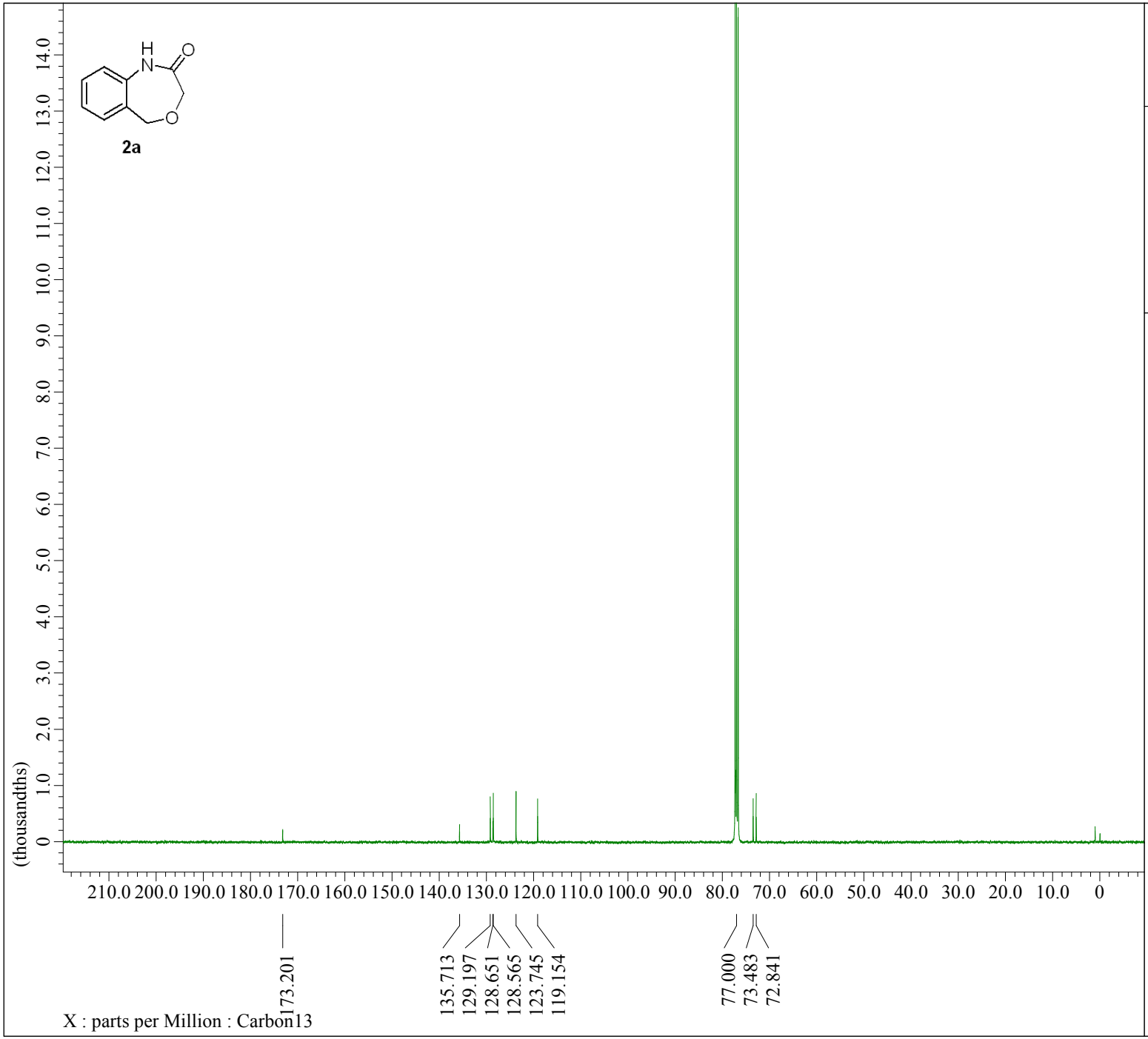
| | |
|---|---|
| Filename | = LK1104-02_Carbo |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK1104-02 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-NOV-2016 15: |
| Revision_Time | = 10-AUG-2017 15: |
| Comment | = single pulse de |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (40 |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MH |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz |
| X_Sweep_Clipped | = 25.25252525[kHz |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MH |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 1201 |
| Total_Scans | = 1201 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 23.1[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

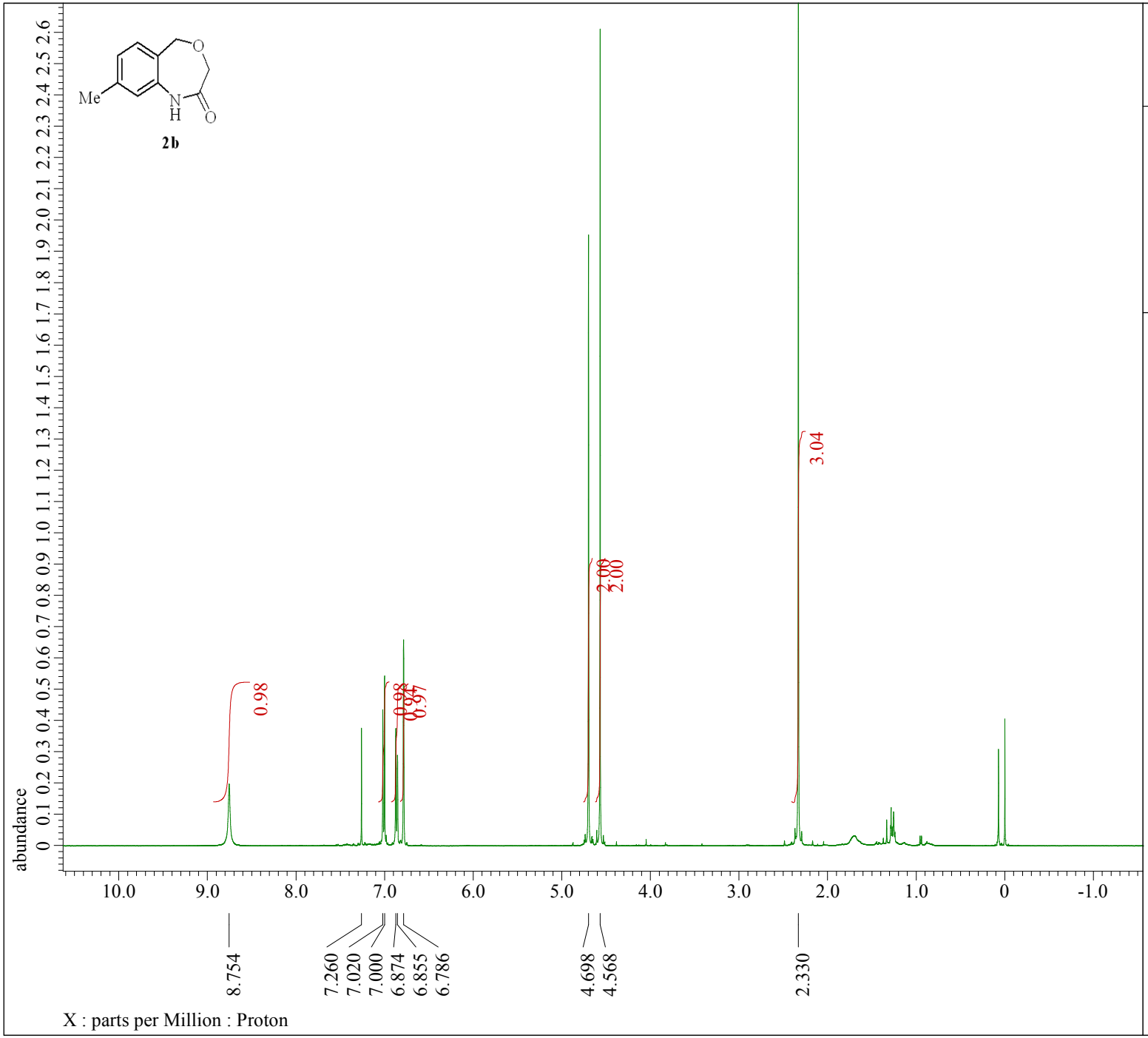
Derived from: LK031407_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK031407_Proton-1-3.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK031407 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 21-MAR-2017 17:33:48 |
| Revision_Time | = 4-AUG-2017 16:54:55 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 66 |
| Temp_Get | = 23.9[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

| | |
|---|---|
| Filename | = LK031407_Carbon-2- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK031407 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-MAR-2017 23:39: |
| Revision_Time | = 4-AUG-2017 17:00: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 10240 |
| Total_Scans | = 10240 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 11.7[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |

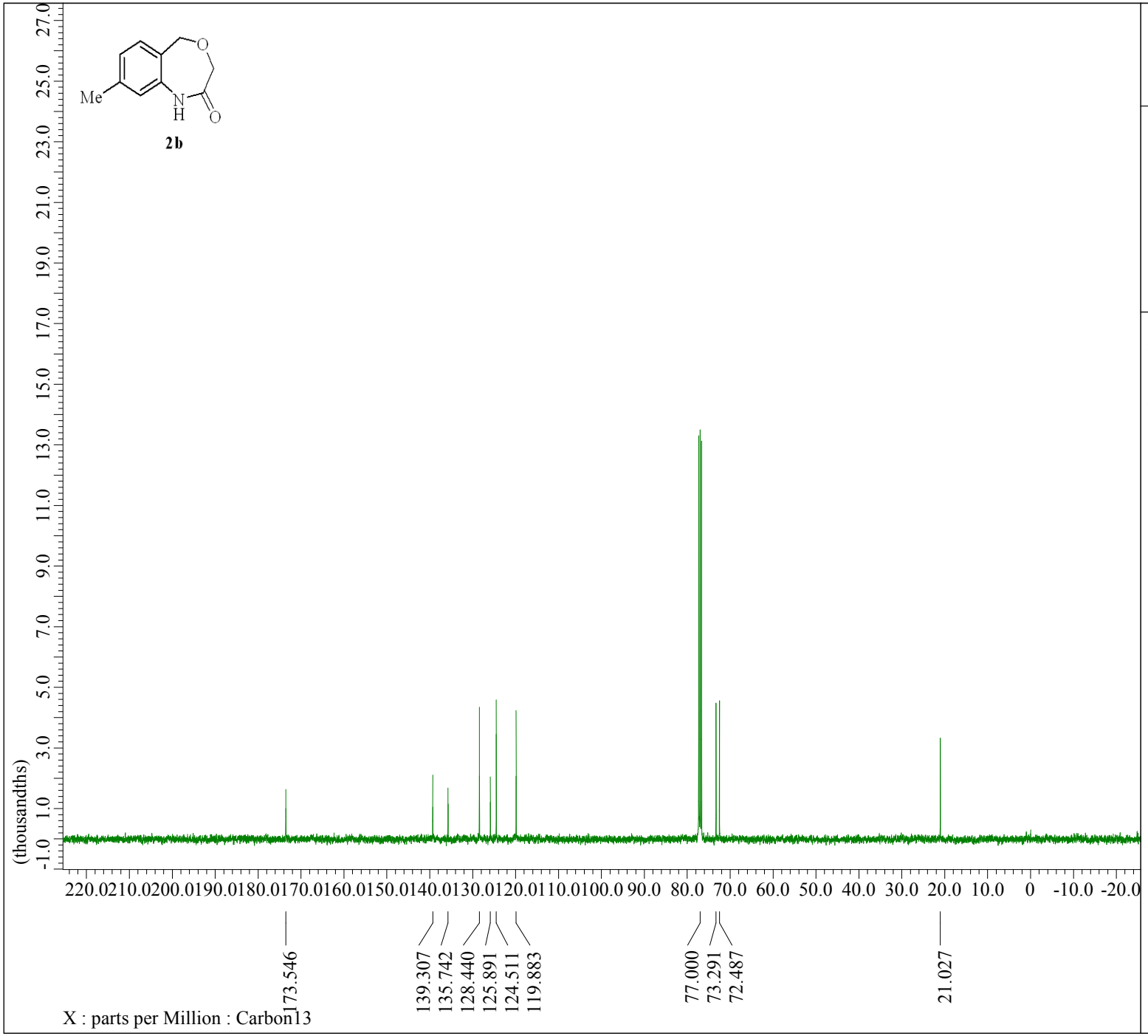



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK120905_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK120905_Proton-1-3.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK120905 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-DEC-2016 11:57:03 |
| Revision_Time | = 4-AUG-2017 17:14:25 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 21.2[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

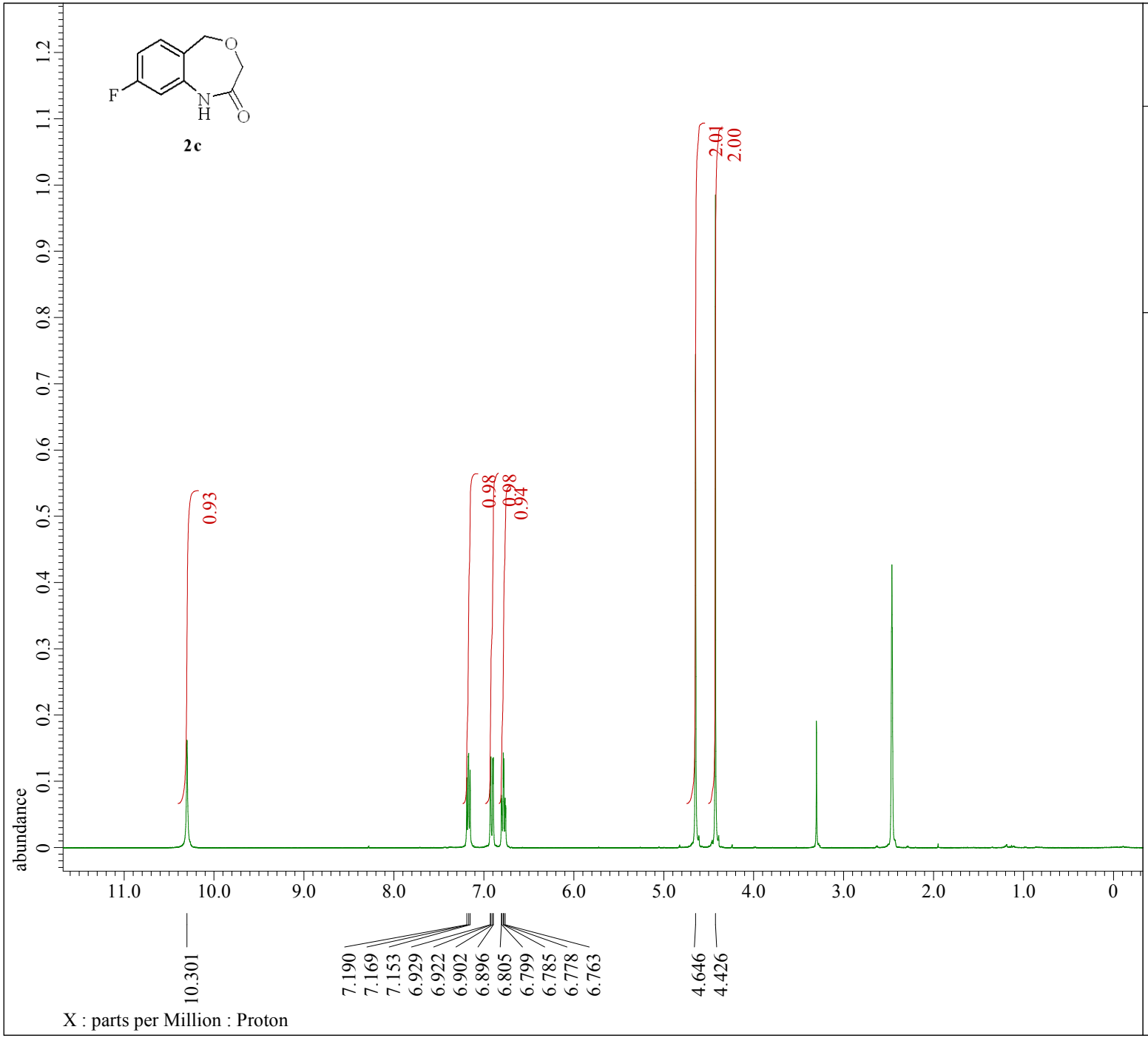



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK120905_Carbon-1-1.jdf
```

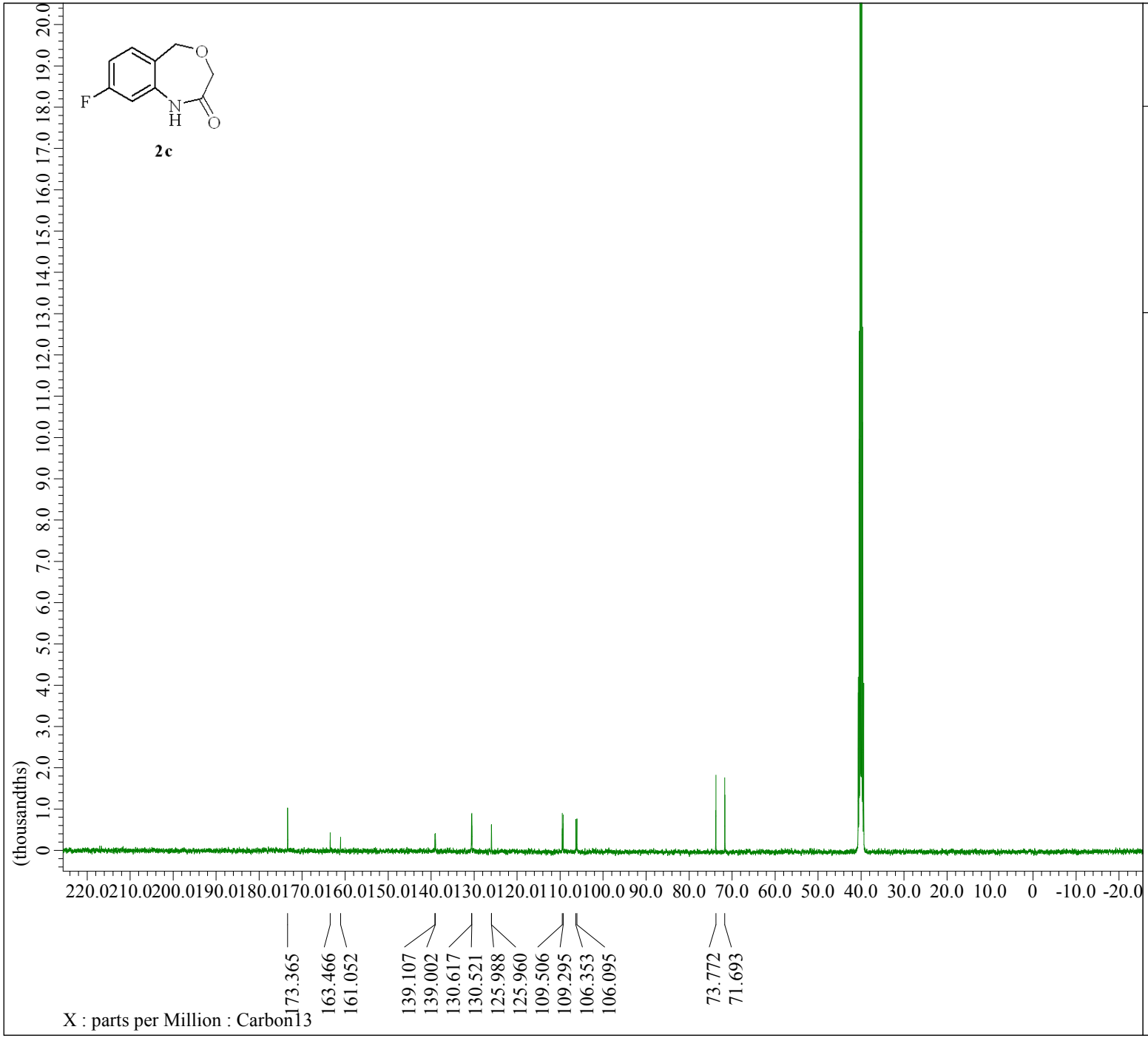
| | |
|---|---|
| Filename | = LK120905_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK120905 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-DEC-2016 14:25: |
| Revision_Time | = 4-AUG-2017 17:12: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 240 |
| Total_Scans | = 240 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21.7[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1206-3_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1206-3_Proton-1-3.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK1206-3 |
| Solvent | = DMSO-D6 |
| Actual_Start_Time | = 6-DEC-2016 11:33:51 |
| Revision_Time | = 4-AUG-2017 17:21:11 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 18.8[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

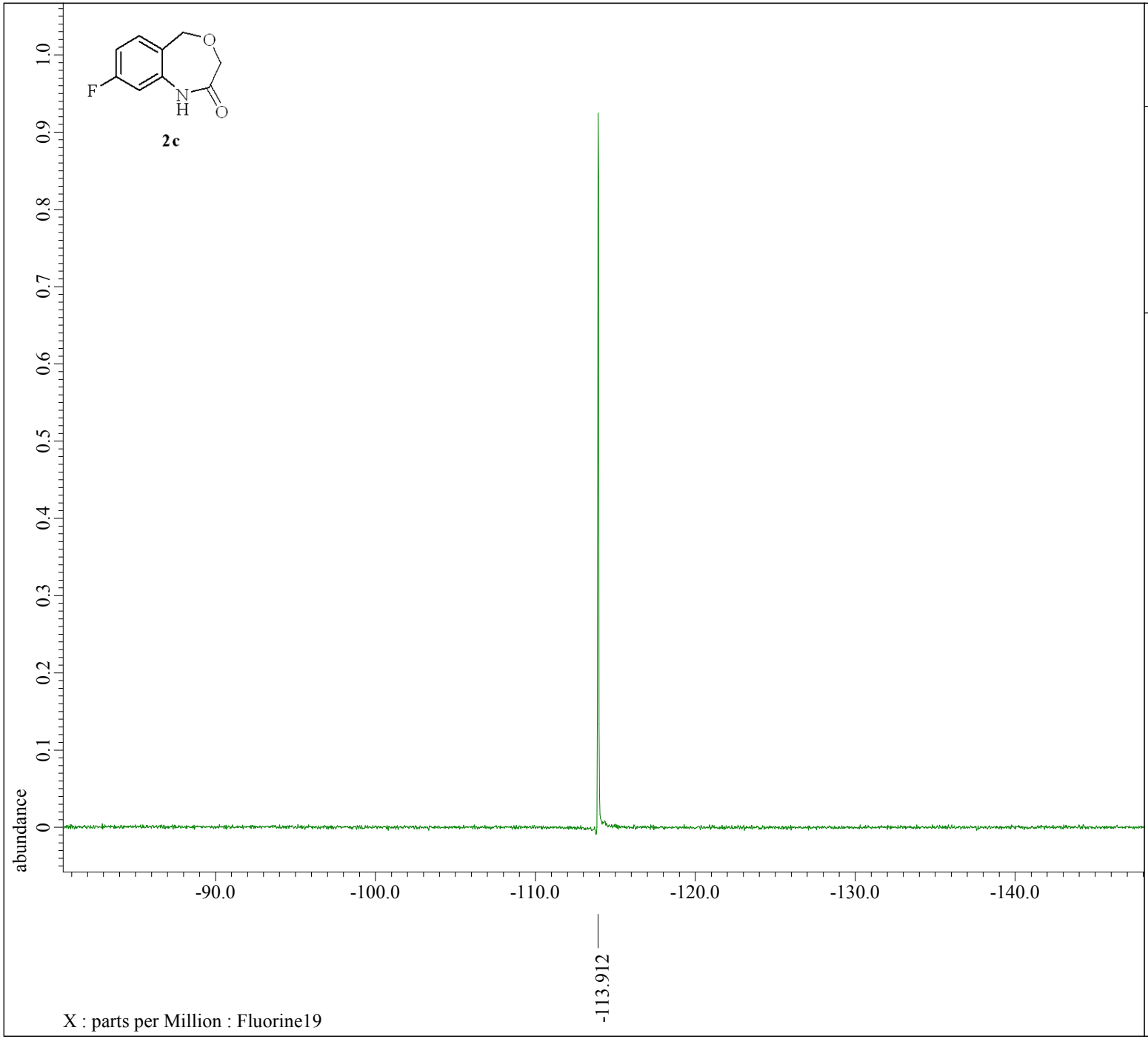



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1206-3_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK1206-3_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK1206-3 |
| Solvent | = DMSO-D6 |
| Actual_Start_Time | = 6-DEC-2016 12:41: |
| Revision_Time | = 4-AUG-2017 17:56: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 1024 |
| Total_Scans | = 1024 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 19.2[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |

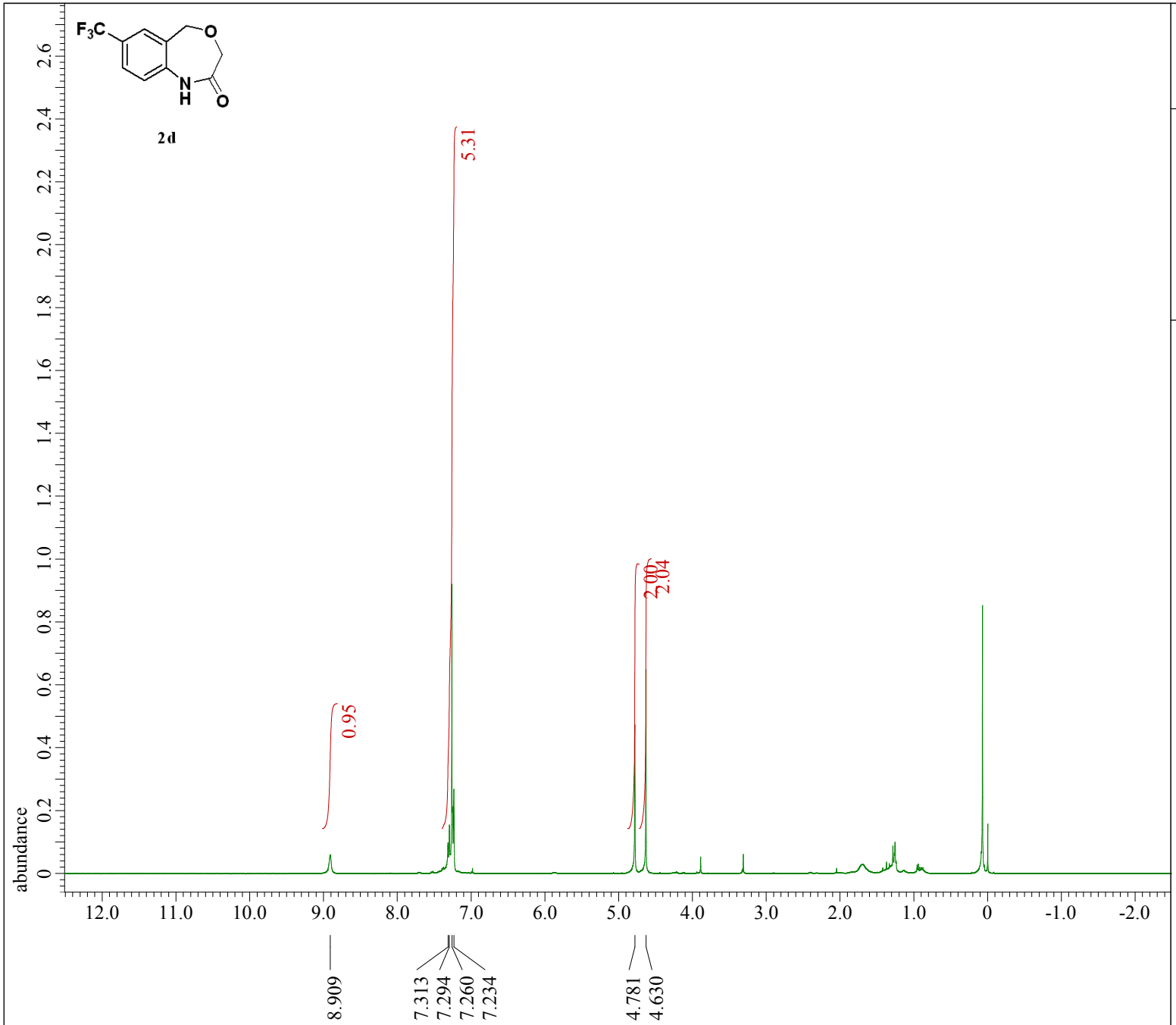



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1206-3_single_pulse-1-1.jdf
```

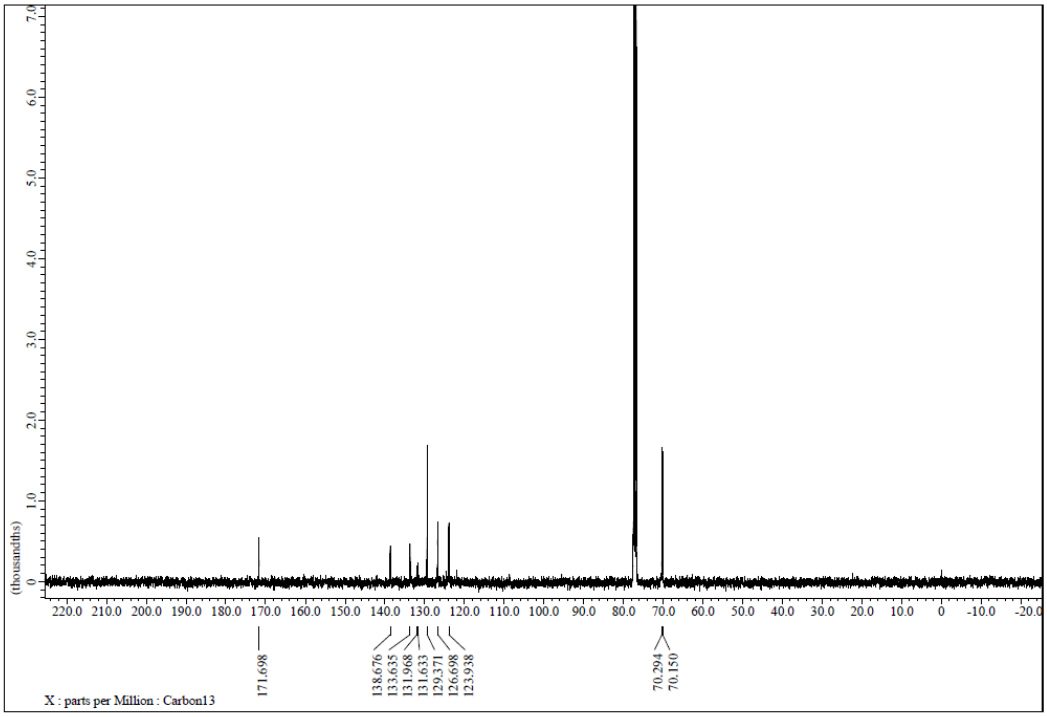
| | |
|---|---|
| Filename | = LK1206-3_single_pulse |
| Author | = delta |
| Experiment | = single_pulse.jxp |
| Sample_Id | = LK1206-3 |
| Solvent | = DMSO-D6 |
| Actual_Start_Time | = 6-DEC-2016 11:35:47 |
| Revision_Time | = 4-AUG-2017 17:47:44 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Fluorine19 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 83.88608[ms] |
| X_Domain | = 19F |
| X_Freq | = 376.17105393[MHz] |
| X_Offset | = -100[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 11.92092896[Hz] |
| X_Sweep | = 195.3125[kHz] |
| X_Sweep_Clipped | = 156.25[kHz] |
| Irr_Domain | = Fluorine19 |
| Irr_Freq | = 376.17105393[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Fluorine19 |
| Tri_Freq | = 376.17105393[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 18.8[dC] |
| X_90_Width | = 10[us] |
| X_Acq_Time | = 83.88608[ms] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.9[dB] |
| X_Pulse | = 5[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

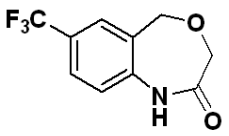



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

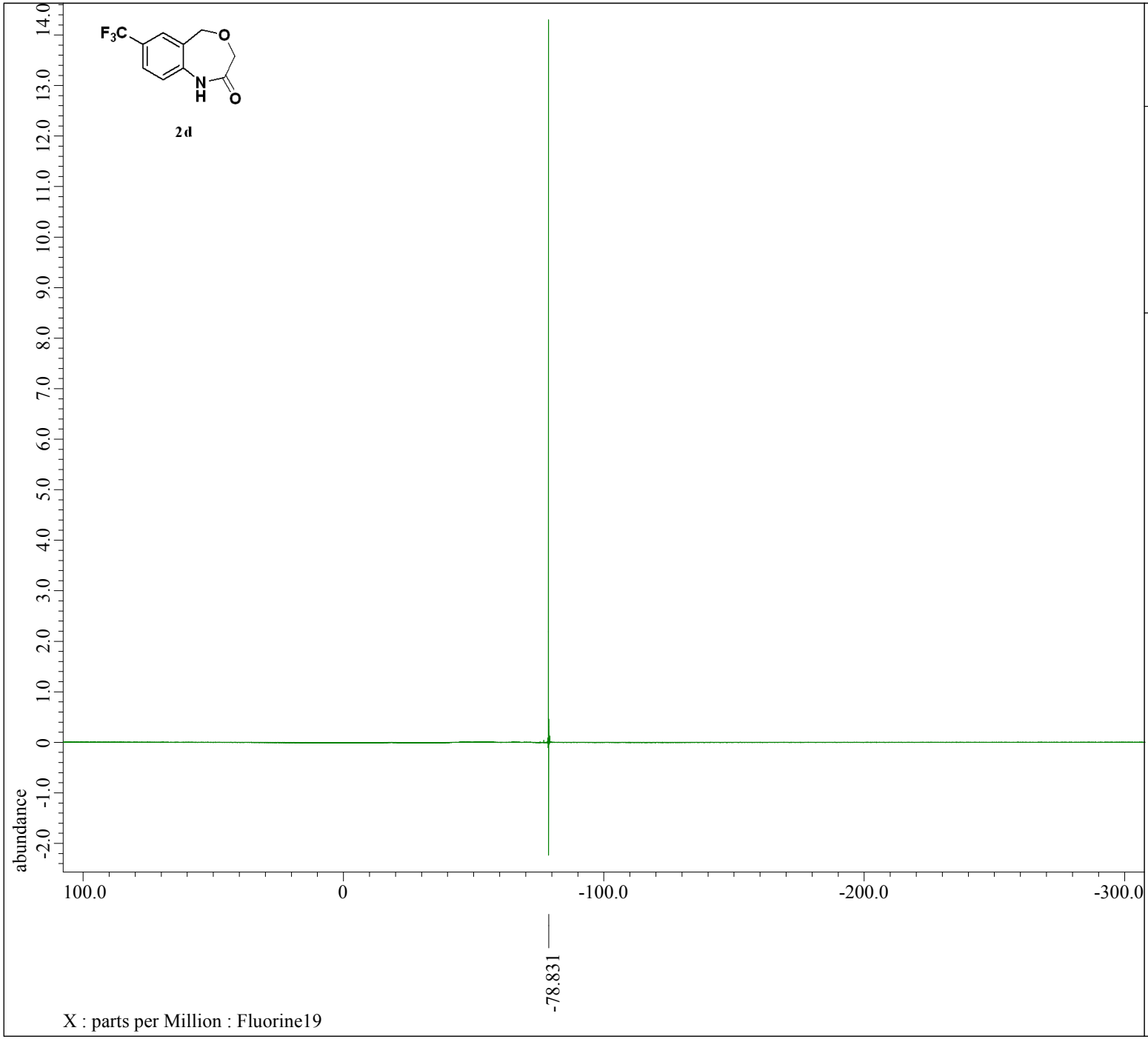
Derived from: LK0420-01_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK0420-01_Proton-1-3. |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK0420-01 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 20-APR-2017 15:00:45 |
| Revision_Time | = 4-AUG-2017 18:36:12 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 20.6[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |


(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
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
171.698
138.676
133.635
131.968
131.633
129.371
126.698
123.938
70.294
70.150
X : parts per Million : Carbon13


F3C
O
N
H
O

**2d**

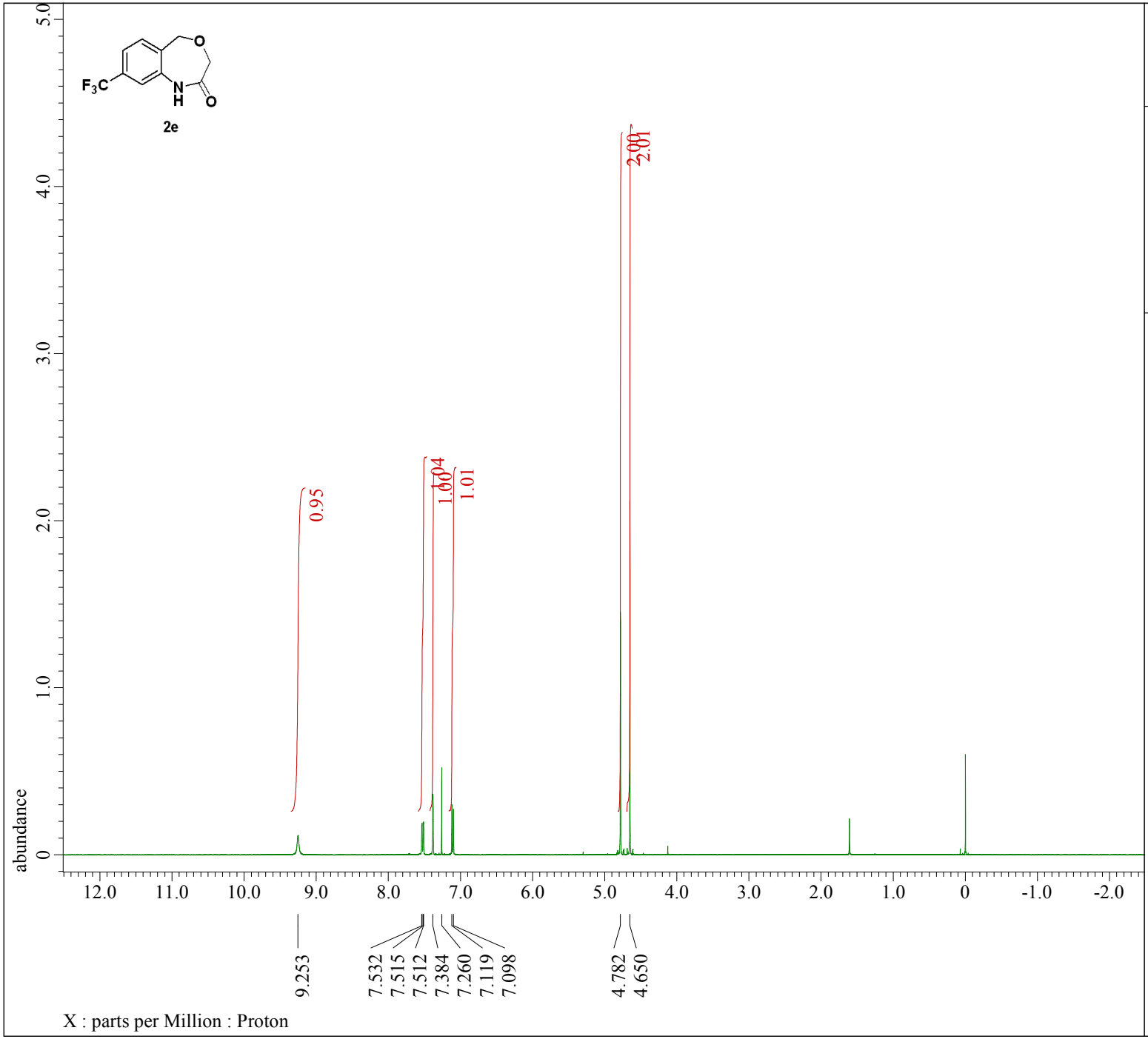



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

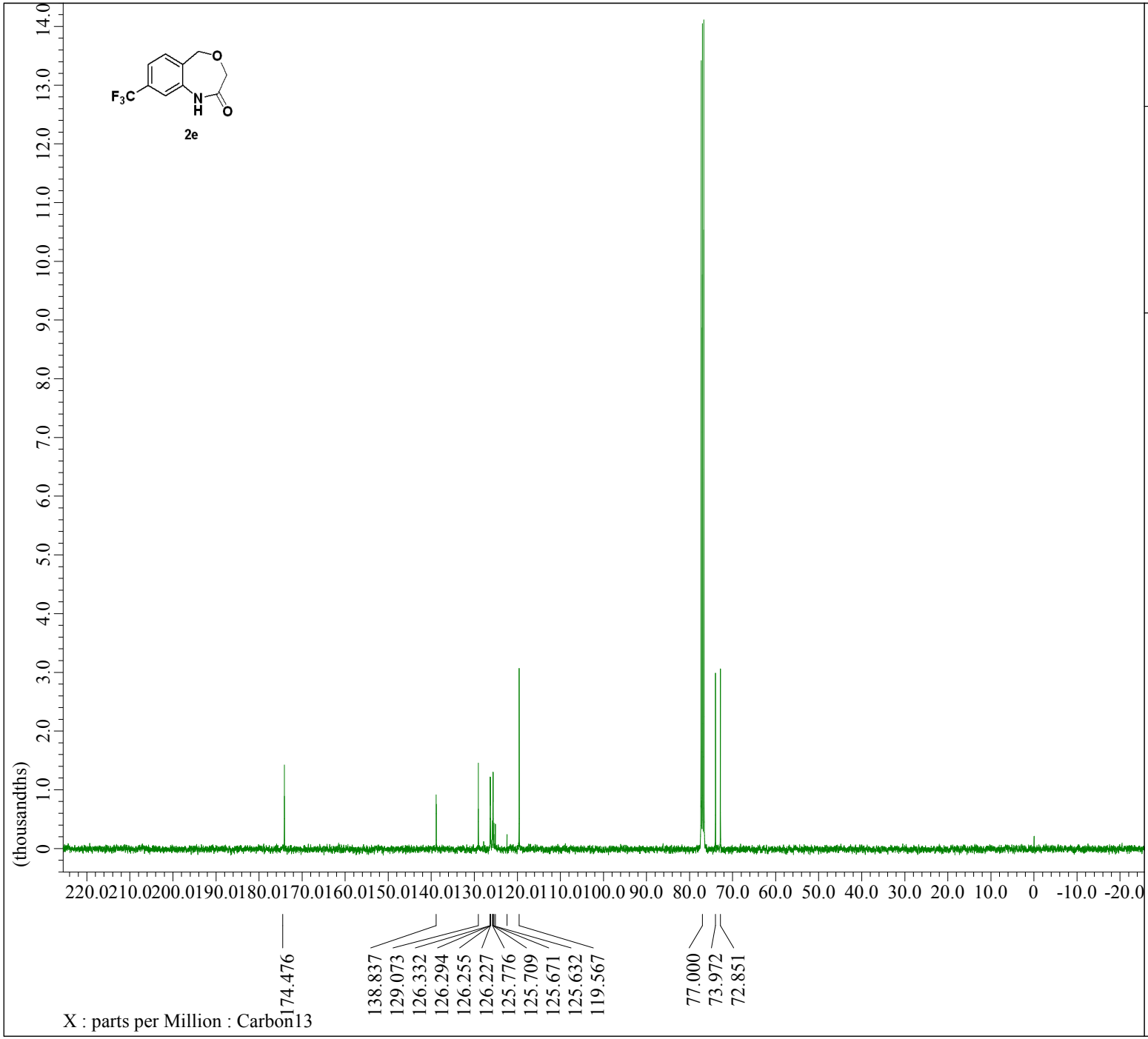
Derived from: LK0420-01_single_pulse-1-1.jdf
```

| | |
|---|---|
| Filename | = LK0420-01_single_puls |
| Author | = delta |
| Experiment | = single_pulse.jxp |
| Sample_Id | = LK0420-01 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 21-APR-2017 14:01:02 |
| Revision_Time | = 4-AUG-2017 18:43:58 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Fluorine19 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 83.88608[ms] |
| X_Domain | = 19F |
| X_Freq | = 376.17105393[MHz] |
| X_Offset | = -100[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 11.92092896[Hz] |
| X_Sweep | = 195.3125[kHz] |
| X_Sweep_Clipped | = 156.25[kHz] |
| Irr_Domain | = Fluorine19 |
| Irr_Freq | = 376.17105393[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Fluorine19 |
| Tri_Freq | = 376.17105393[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20.1[dC] |
| X_90_Width | = 10[us] |
| X_Acq_Time | = 83.88608[ms] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.9[dB] |
| X_Pulse | = 5[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

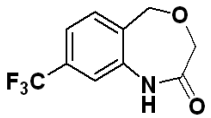
| | |
|---|---|
| Filename | = LK121402_Proton-1-4.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK121402 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-DEC-2016 12:05:31 |
| Revision_Time | = 4-AUG-2017 18:48:52 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 21.1[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK121402_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK121402_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK121402 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-DEC-2016 16:31: |
| Revision_Time | = 4-AUG-2017 18:53: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 1024 |
| Total_Scans | = 1024 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21.9[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |



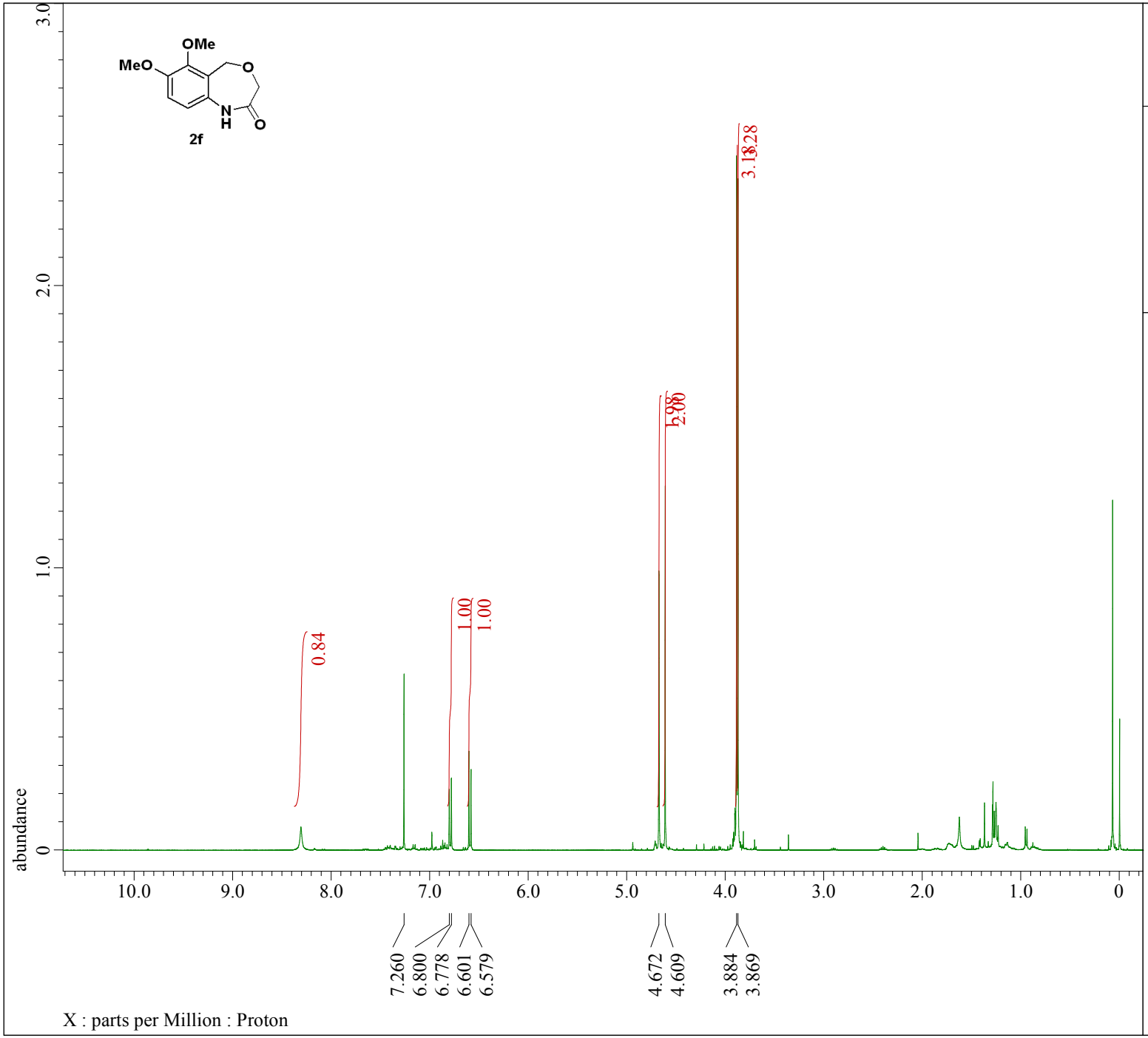

2e




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1206-4_single_pulse-1-1.jdf
```

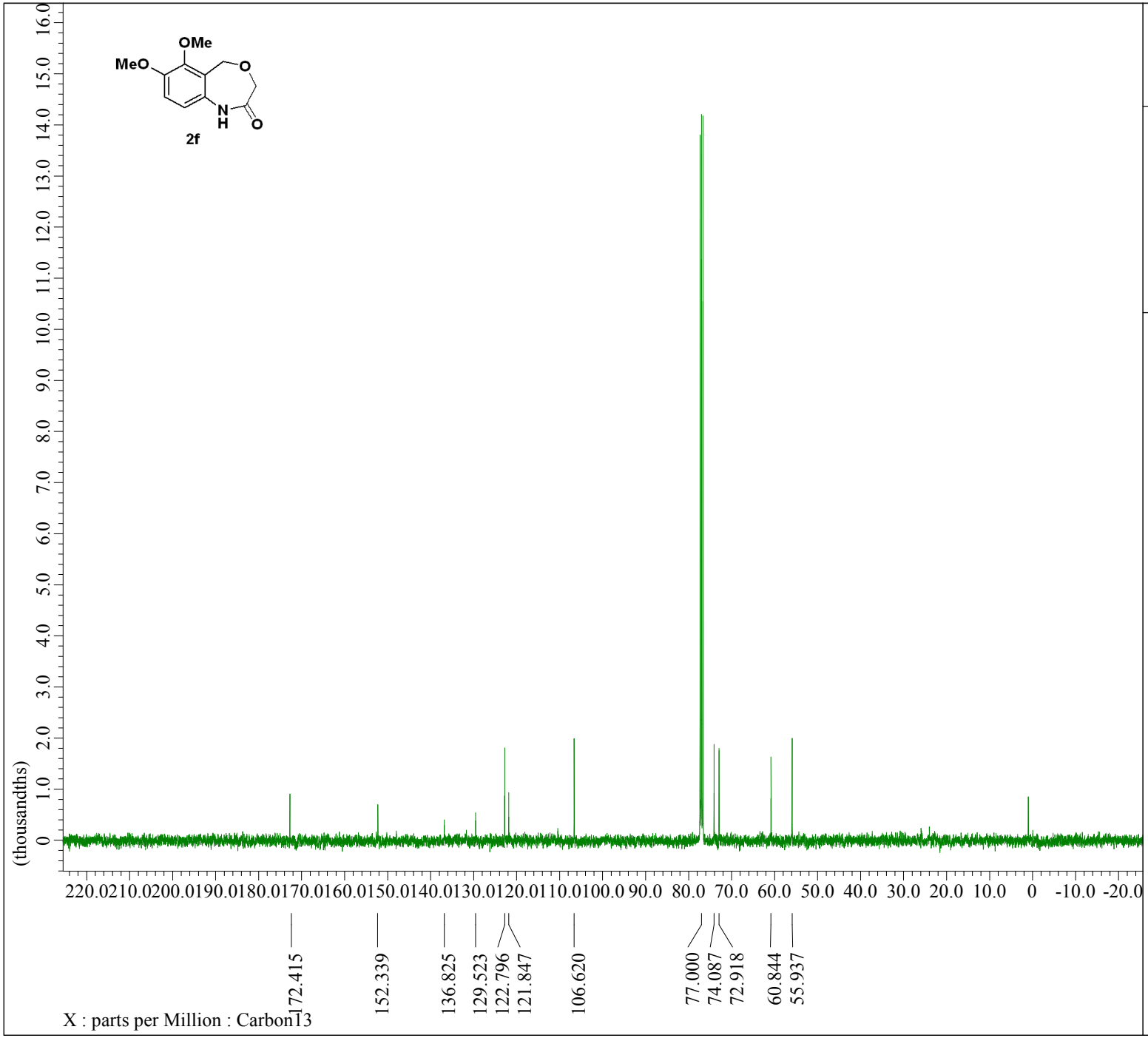
| | |
|---|---|
| Filename | = LK1206-4_single_pulse |
| Author | = delta |
| Experiment | = single_pulse.jxp |
| Sample_Id | = LK1206-4 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 6-DEC-2016 11:42:25 |
| Revision_Time | = 4-AUG-2017 18:54:57 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Fluorine19 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 83.88608[ms] |
| X_Domain | = 19F |
| X_Freq | = 376.17105393[MHz] |
| X_Offset | = -100[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 11.92092896[Hz] |
| X_Sweep | = 195.3125[kHz] |
| X_Sweep_Clipped | = 156.25[kHz] |
| Irr_Domain | = Fluorine19 |
| Irr_Freq | = 376.17105393[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Fluorine19 |
| Tri_Freq | = 376.17105393[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 18.8[dC] |
| X_90_Width | = 10[us] |
| X_Acq_Time | = 83.88608[ms] |
| X_Angle | = 45[deg] |
| X_Atn | = 0.9[dB] |
| X_Pulse | = 5[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK032117-1_Proton-1-1.jdf
```

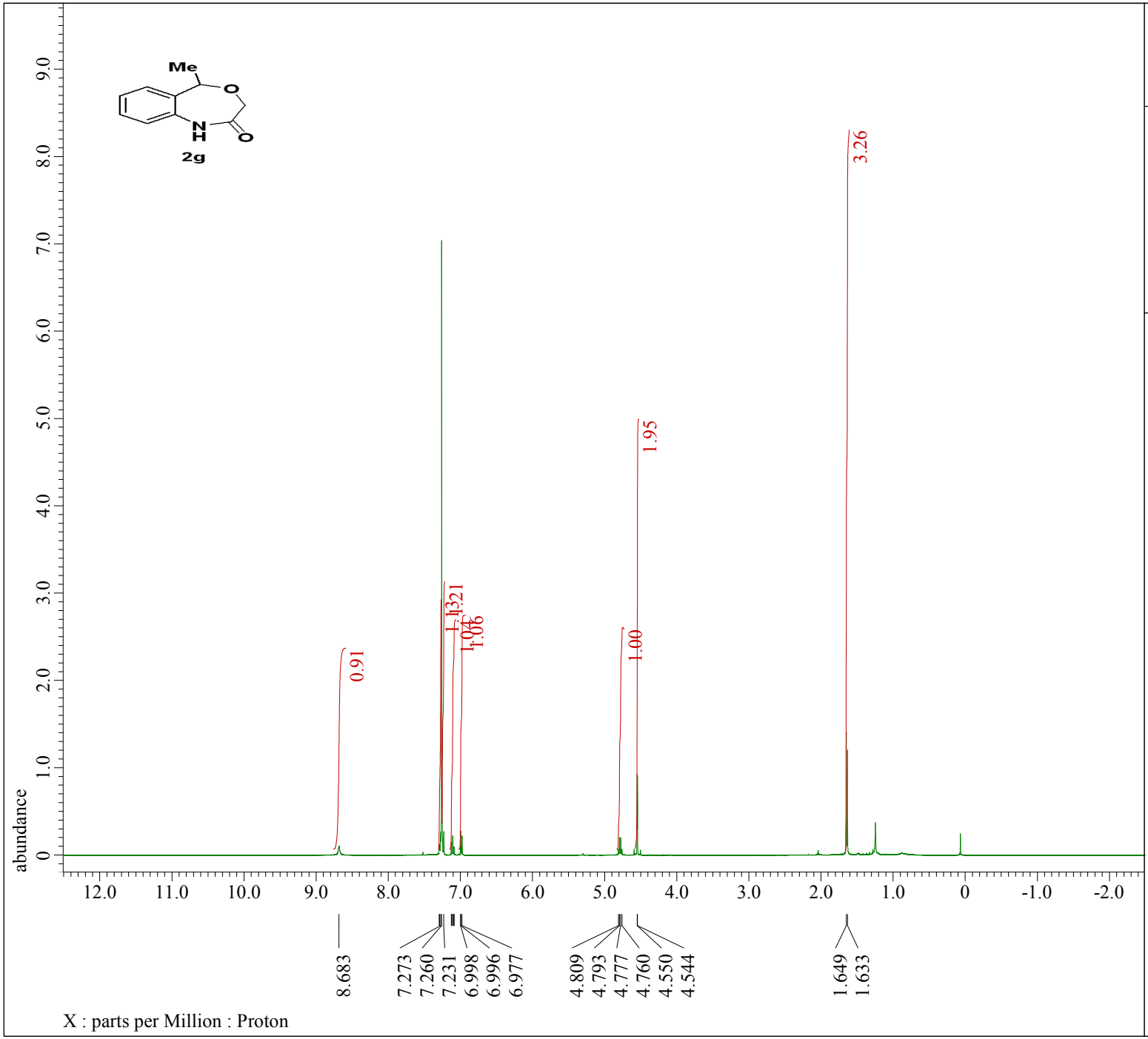
| | |
|---|---|
| Filename | = LK032117-1_Proton-1-3 |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK032117-1 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 21-MAR-2017 10:14:14 |
| Revision_Time | = 4-AUG-2017 18:58:24 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 21.3[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK032117-1_Carbon-1-1.jdf
```

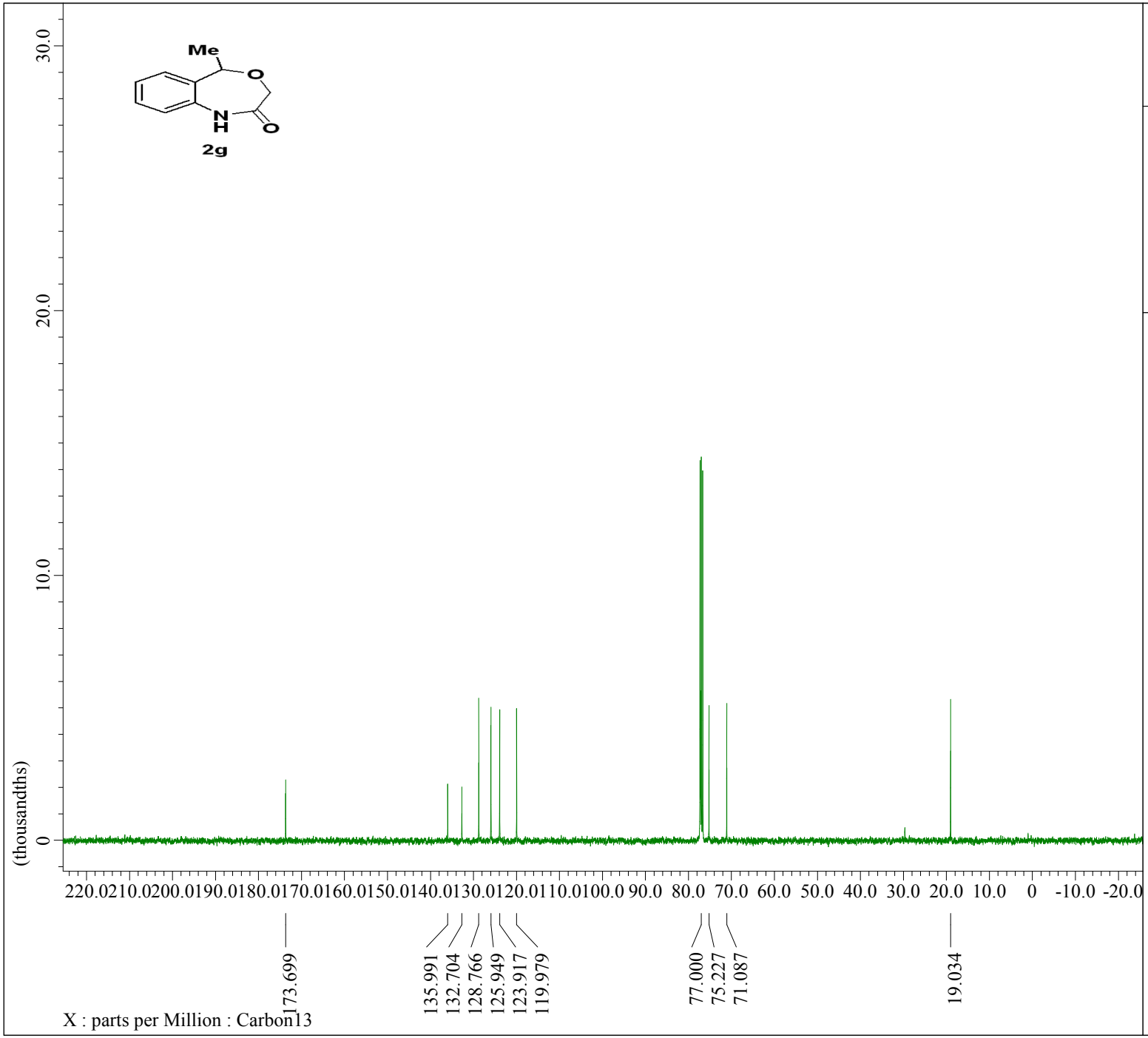
| | |
|---|---|
| Filename | = LK032117-1_Carbon- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK032117-1 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 21-MAR-2017 10:35: |
| Revision_Time | = 4-AUG-2017 19:01: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 263 |
| Total_Scans | = 263 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21.7[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |




JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

| | |
|---|---|
| Filename | = LK1031-1_Proton-1-5.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK1031-1 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 31-OCT-2016 14:48:09 |
| Revision_Time | = 4-AUG-2017 22:28:58 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 14.2[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

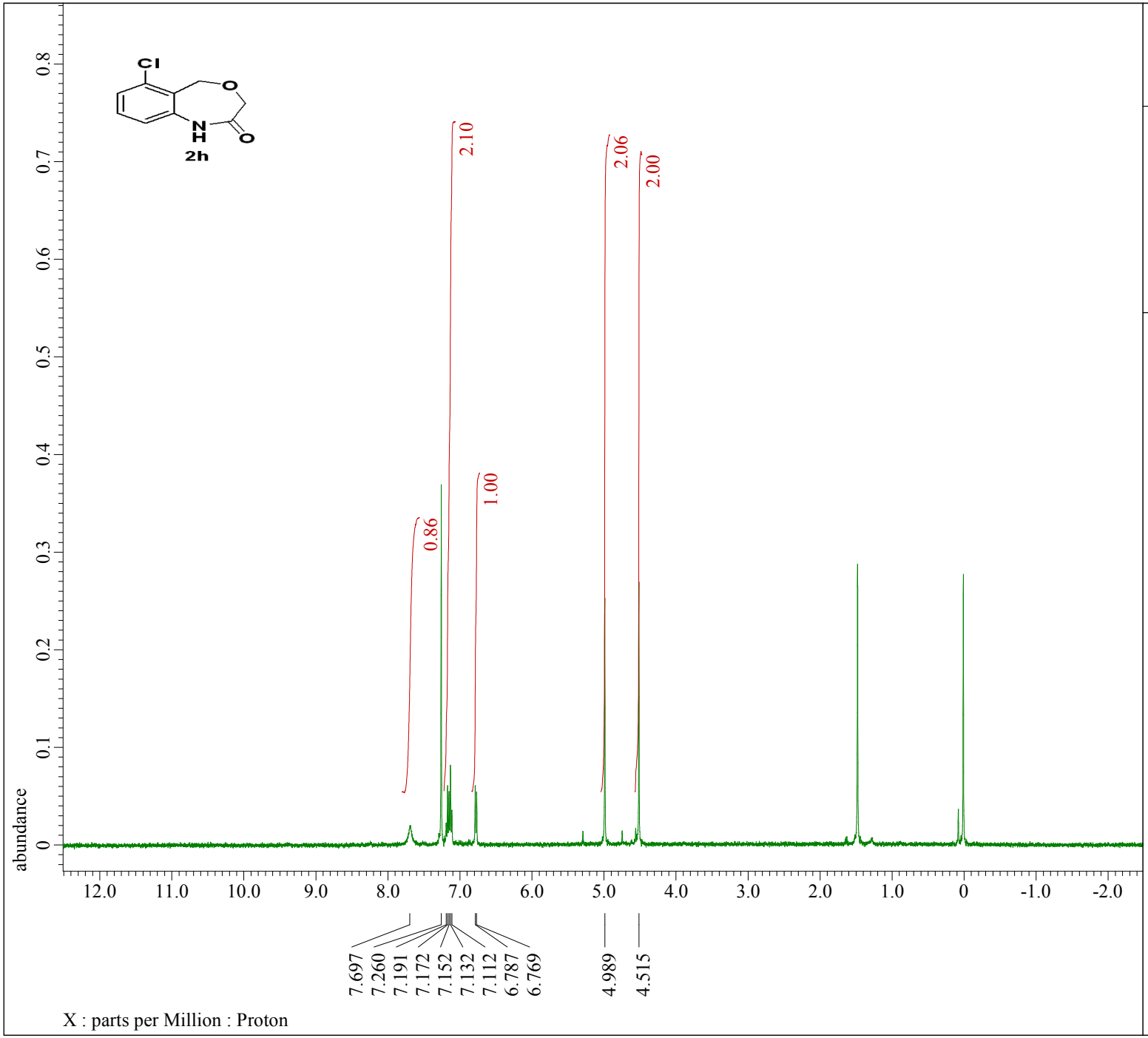



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1031-1_Carbon-1-1.jdf
```

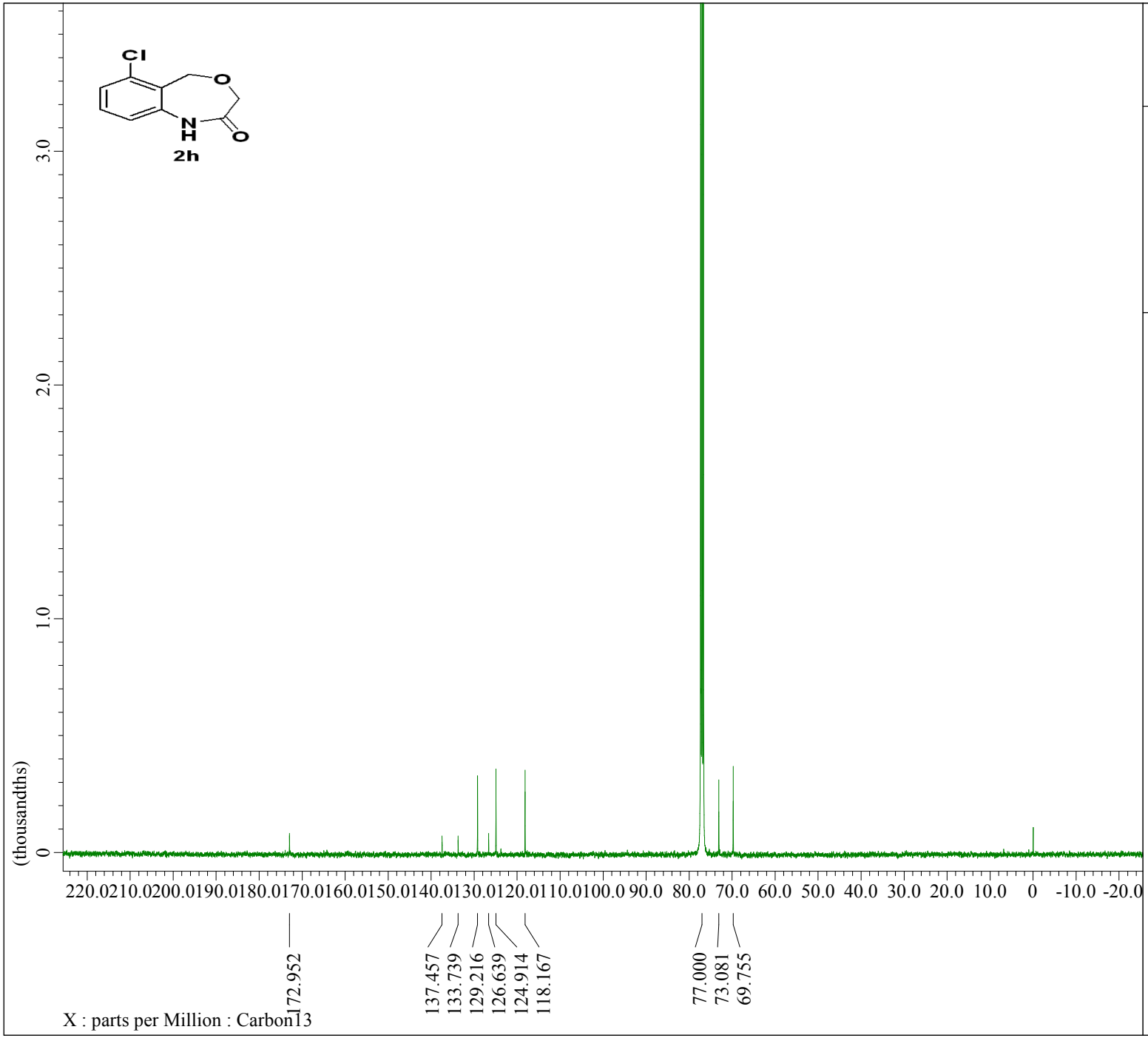
| | |
|---|---|
| Filename | = LK1031-1_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK1031-1 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 31-OCT-2016 15:25: |
| Revision_Time | = 4-AUG-2017 22:35: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 295 |
| Total_Scans | = 295 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 14.5[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |




JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

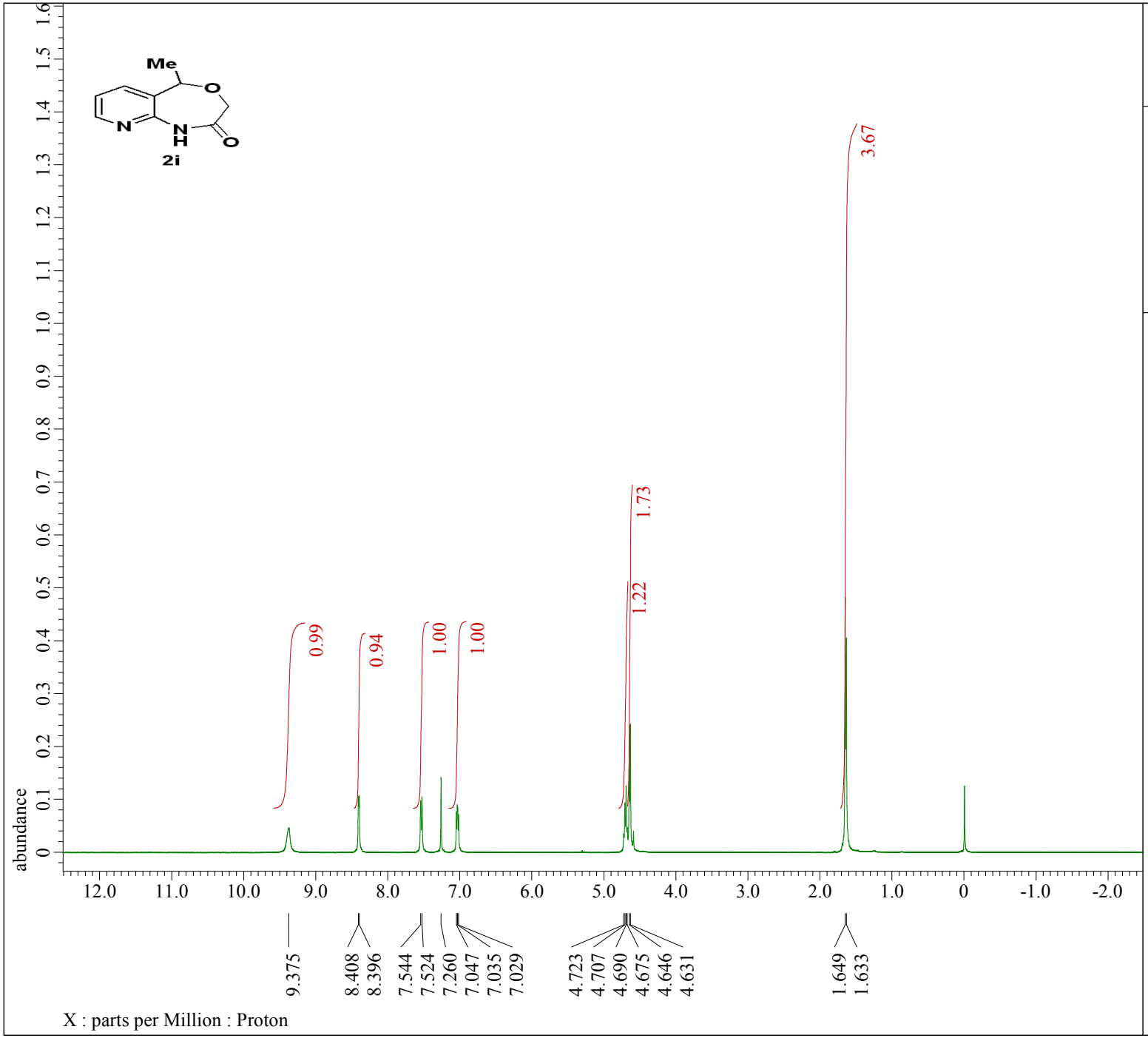
| | |
|---|---|
| Filename | = LK012401_Proton-1-4.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK012401 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 24-JAN-2017 10:37:28 |
| Revision_Time | = 4-AUG-2017 22:44:47 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 66 |
| Temp_Get | = 55[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK012401_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK012401_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK012401 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 24-JAN-2017 10:50: |
| Revision_Time | = 4-AUG-2017 22:41: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = TRUE |
| Scans | = 36000 |
| Total_Scans | = 36000 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 55[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |




JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

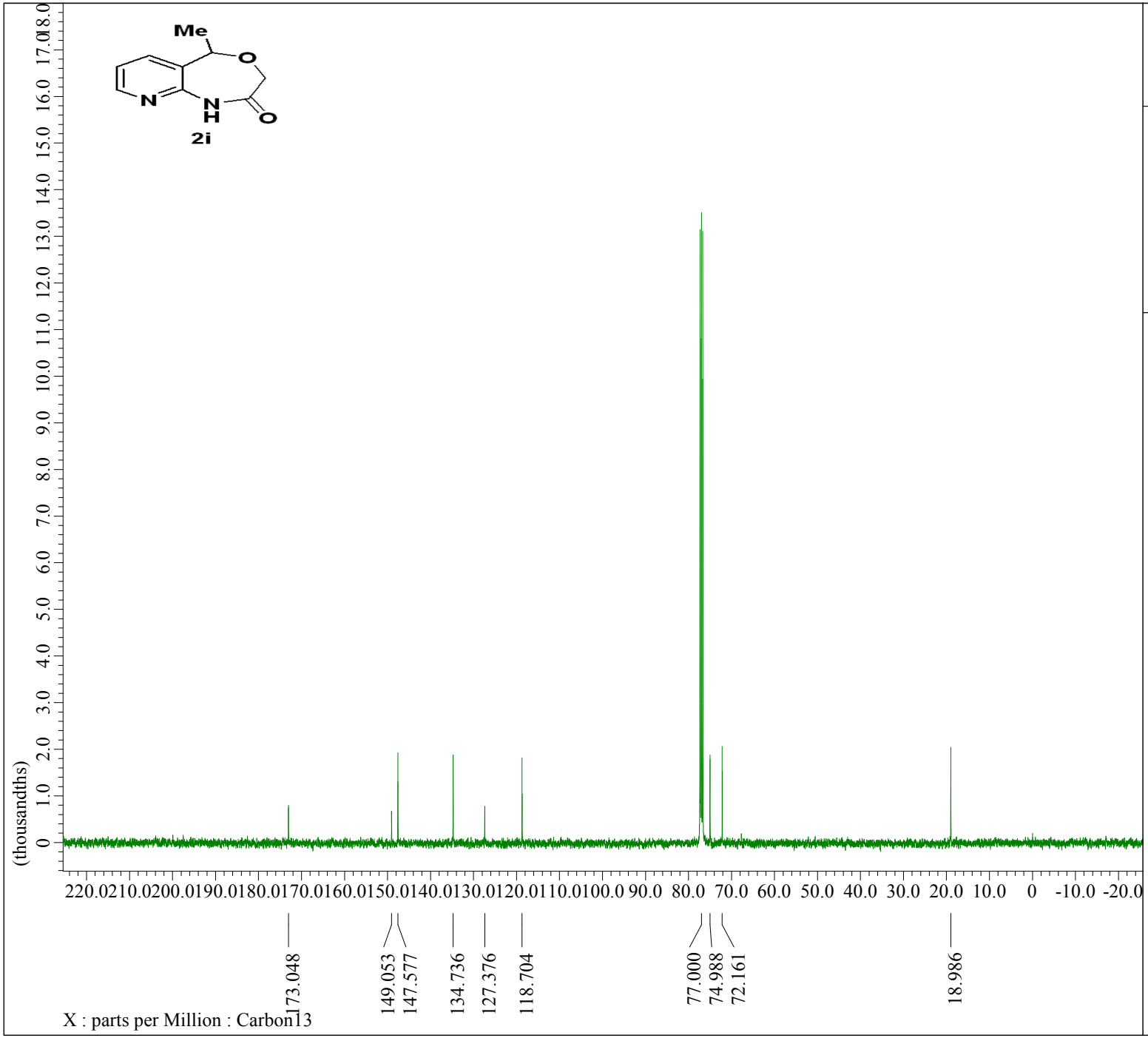
Derived from: LK012302_Proton-1-1.jdf
```

```
Filename              = LK012302_Proton-1-3.j
Author                = delta
Experiment            = proton.jxp
Sample_Id             = LK012302
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 23-JAN-2017 11:24:43
Revision_Time         =  4-AUG-2017 22:51:53

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[MHz]
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

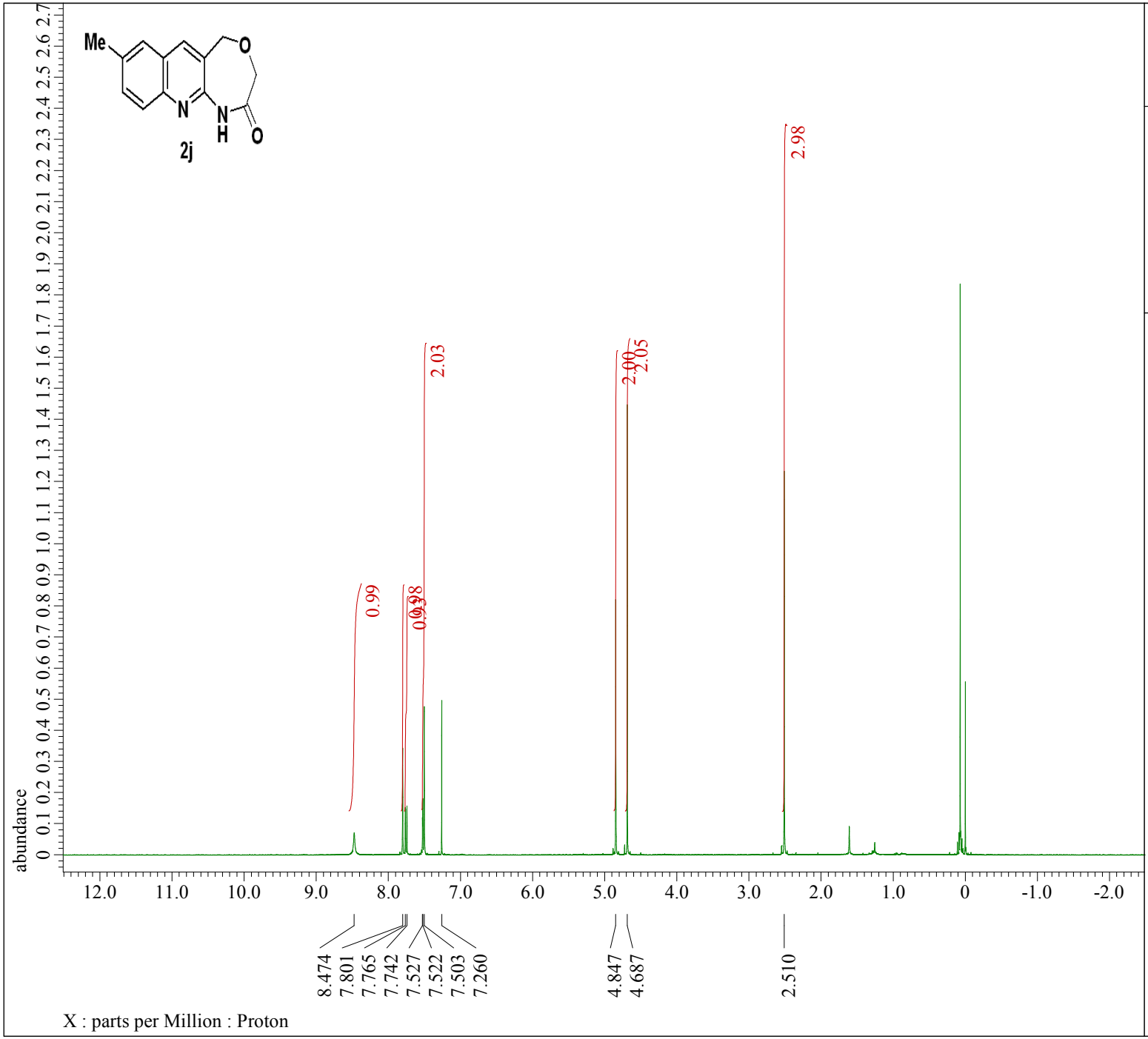
Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 13[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
X_Angle               = 45[deg]
X_Atn                 = 2[dB]
X_Pulse               = 4.75[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
Dante_Presat          = FALSE
```




JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

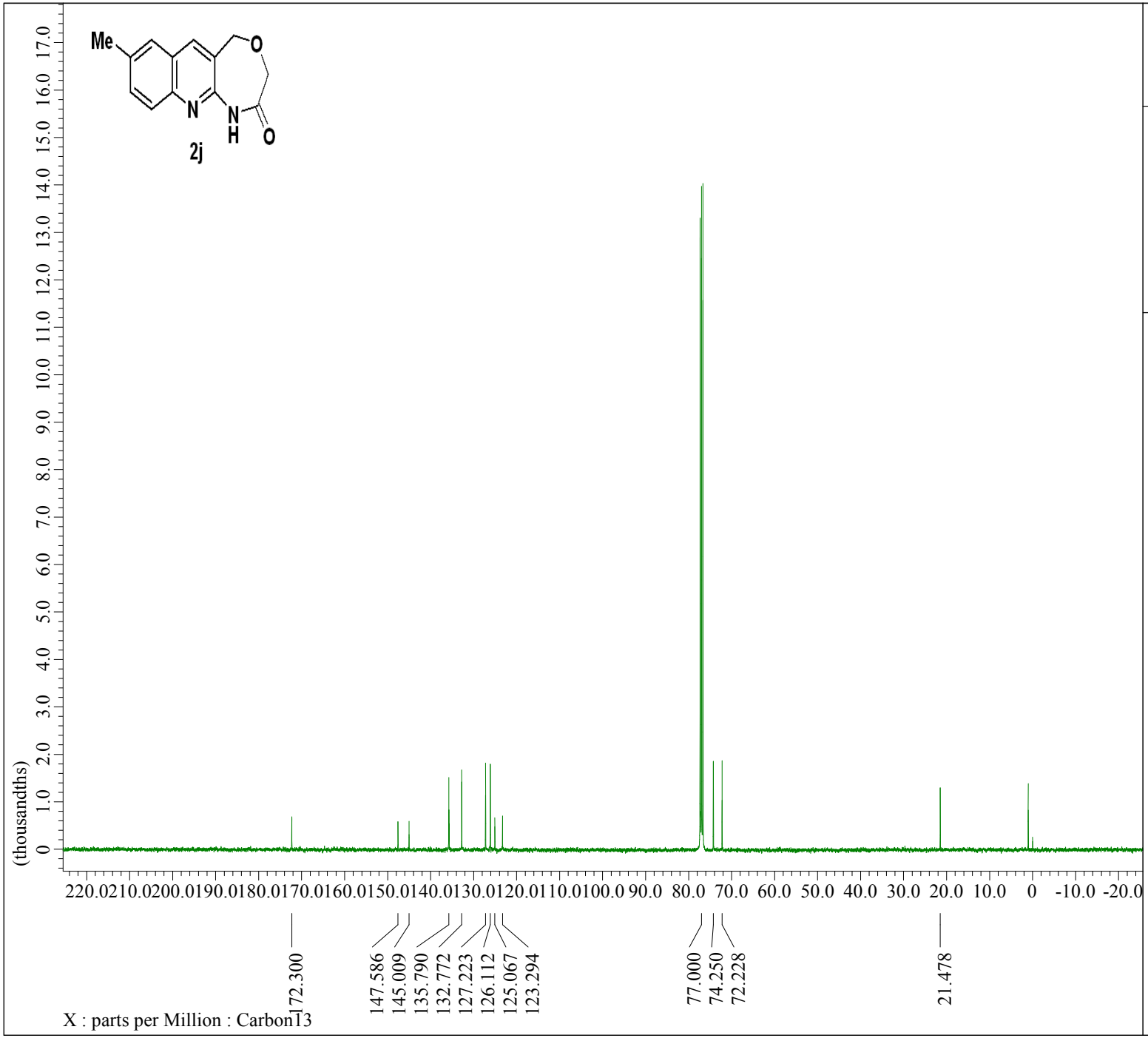
| | |
|---|---|
| Filename | = LK012302_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK012302 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 23-JAN-2017 11:30: |
| Revision_Time | = 4-AUG-2017 22:57: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 531 |
| Total_Scans | = 531 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 13.1[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK-011702_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK-011702_Proton-1-3. |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK-011702 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 17-JAN-2017 17:53:21 |
| Revision_Time | = 4-AUG-2017 23:08:13 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 24.1[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

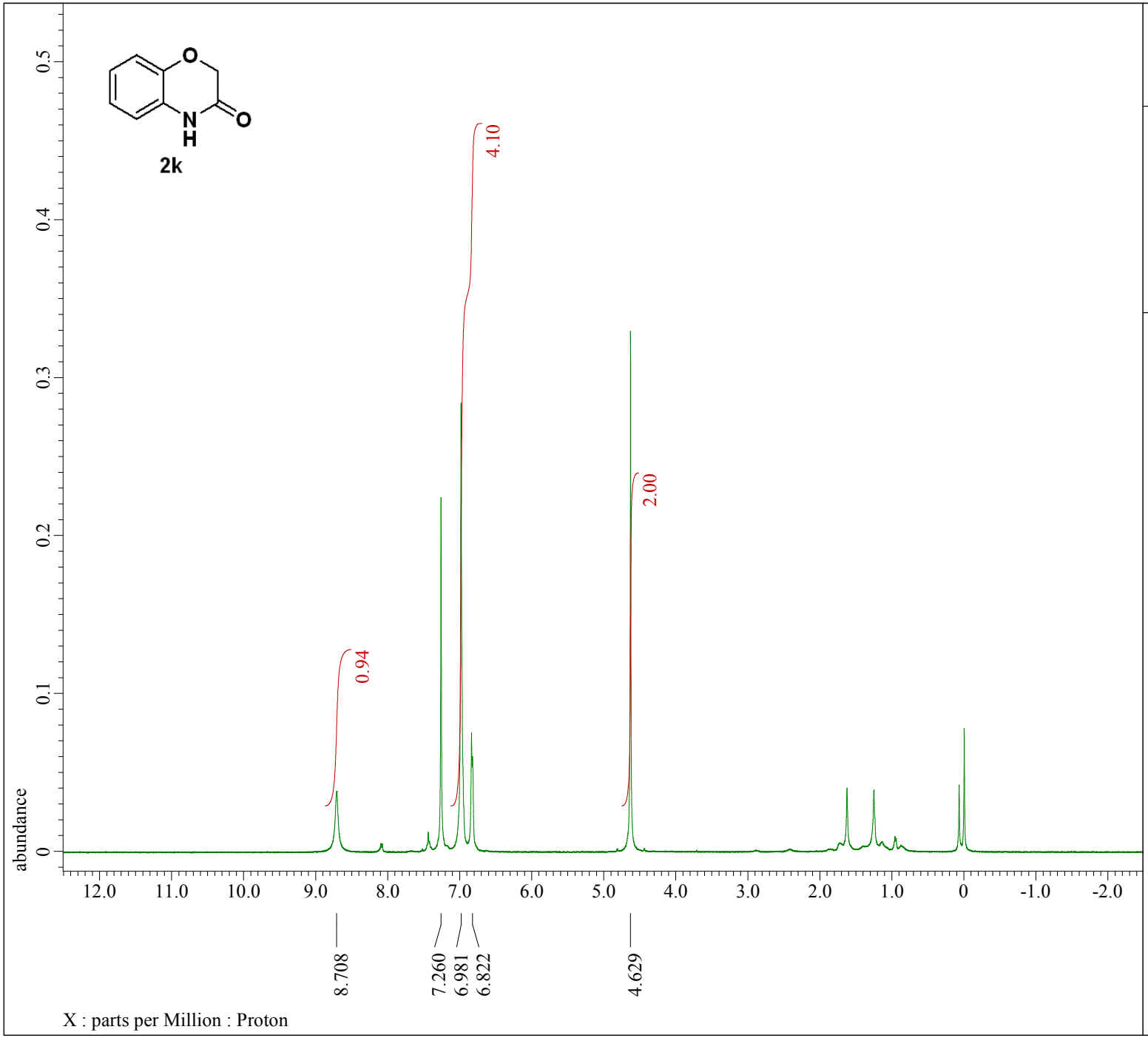



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK-011702_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK-011702_Carbon-1 |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK-011702 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 17-JAN-2017 23:54: |
| Revision_Time | = 4-AUG-2017 23:03: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 2400 |
| Total_Scans | = 2400 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 18.9[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |

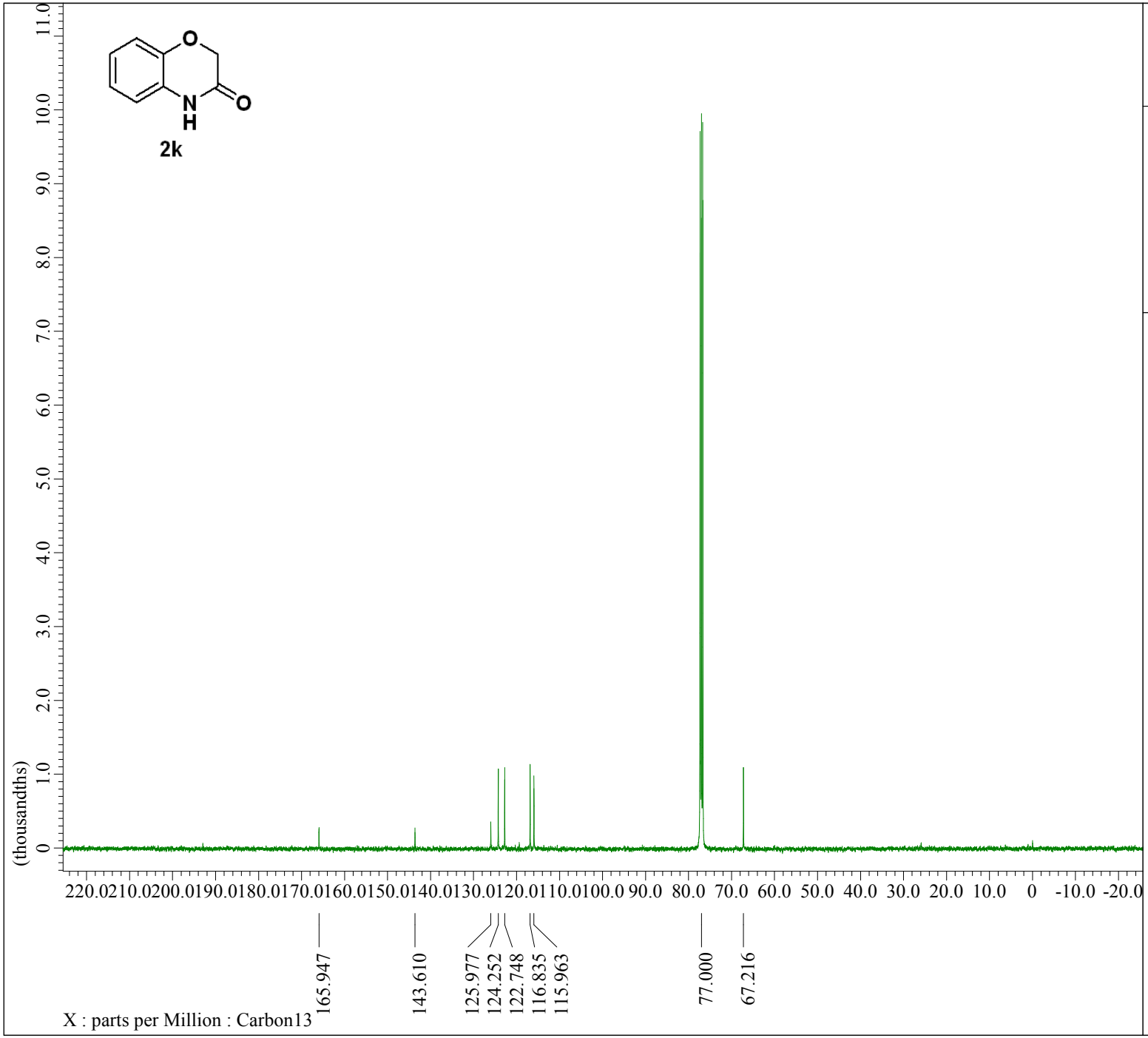



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK031404_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK031404_Proton-1-3.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK031404 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-MAR-2017 15:57:53 |
| Revision_Time | = 4-AUG-2017 23:19:24 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 15.2[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

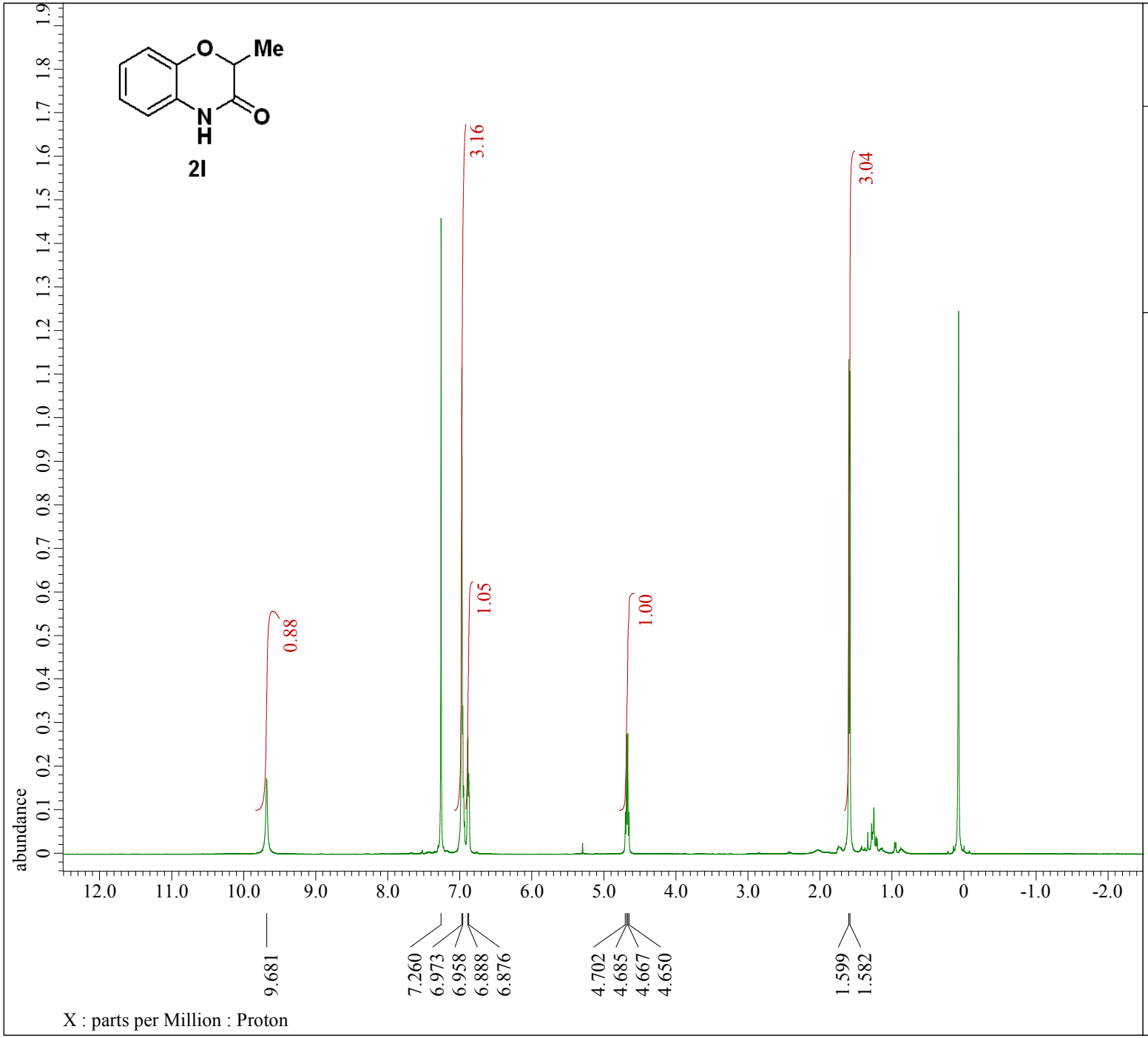



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK031404_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK031404_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK031404 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-MAR-2017 19:30: |
| Revision_Time | = 4-AUG-2017 23:20: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 4800 |
| Total_Scans | = 4800 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 13.2[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |

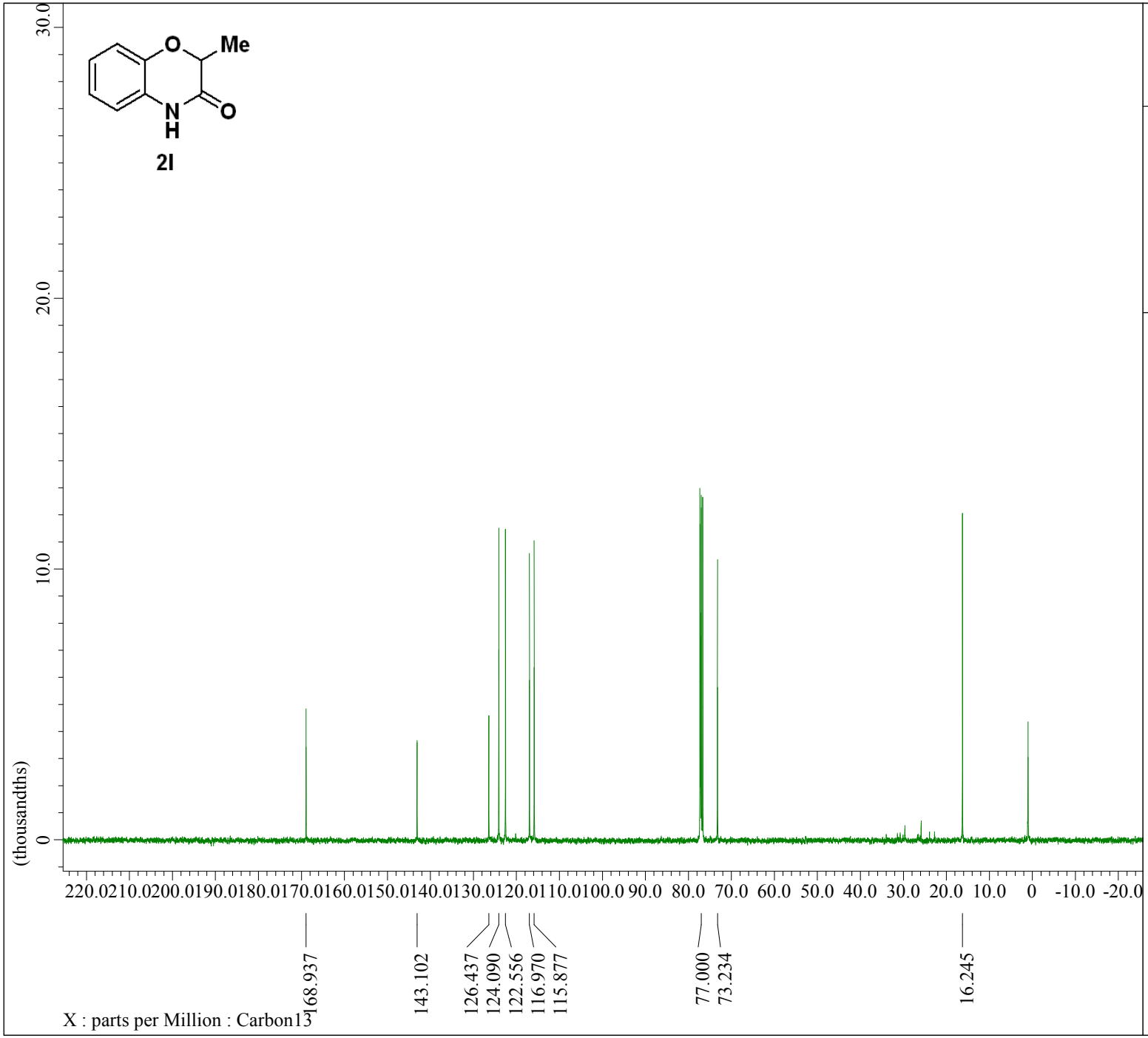



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK-1027-PRODUCT_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK-1027-PRODUCT_Proto |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK-1027-PRODUCT |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 1-NOV-2016 14:43:21 |
| Revision_Time | = 4-AUG-2017 23:28:06 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 46 |
| Temp_Get | = 14.3[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

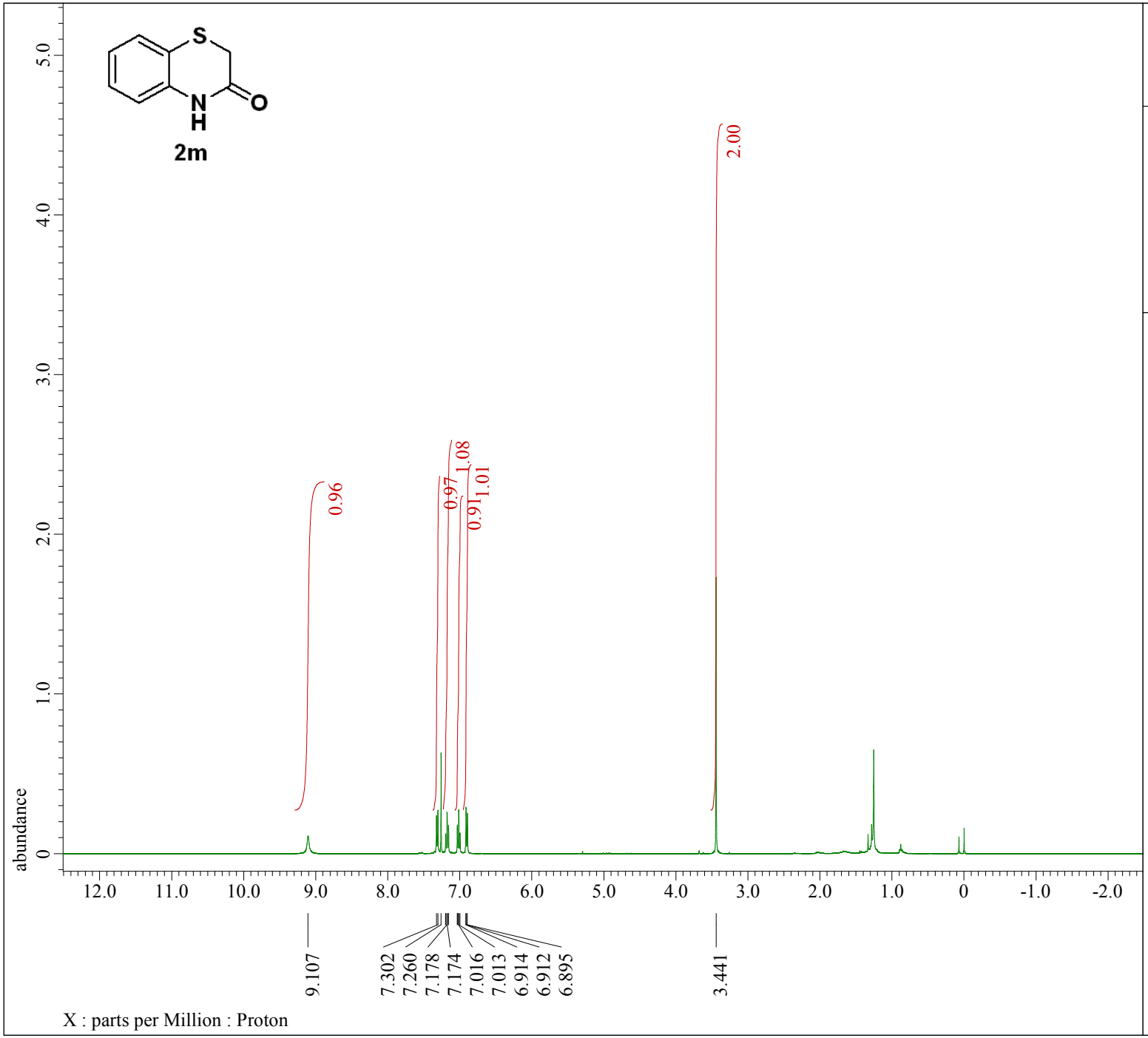



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK-1027-PRODUCT_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK-1027-PRODUCT_Ca |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK-1027-PRODUCT |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 1-NOV-2016 14:51: |
| Revision_Time | = 4-AUG-2017 23:23: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 406.0 |
| Total_Scans | = 406.0 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 14.8[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |

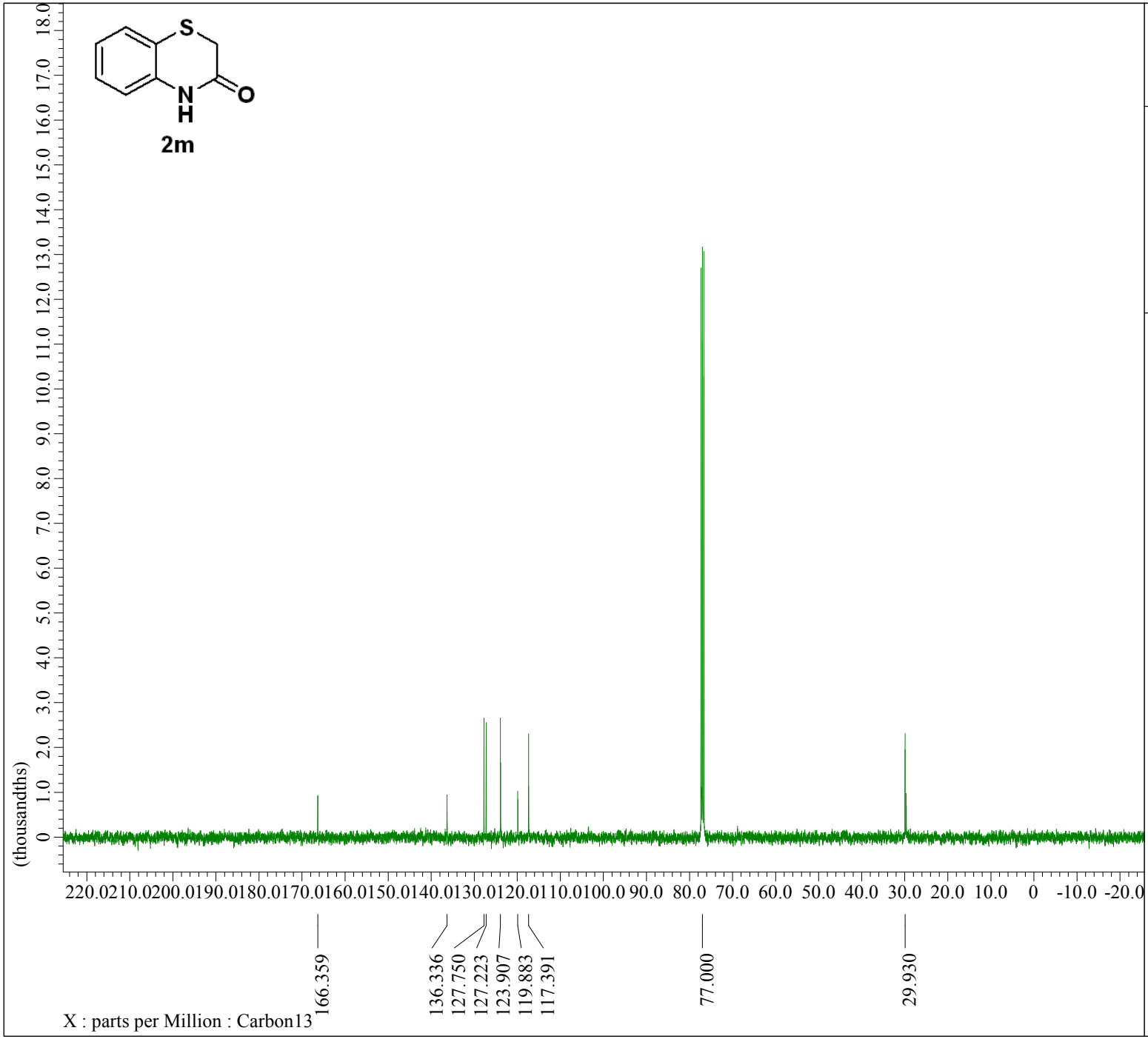



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK0224-1_Proton-1-1.jdf
```

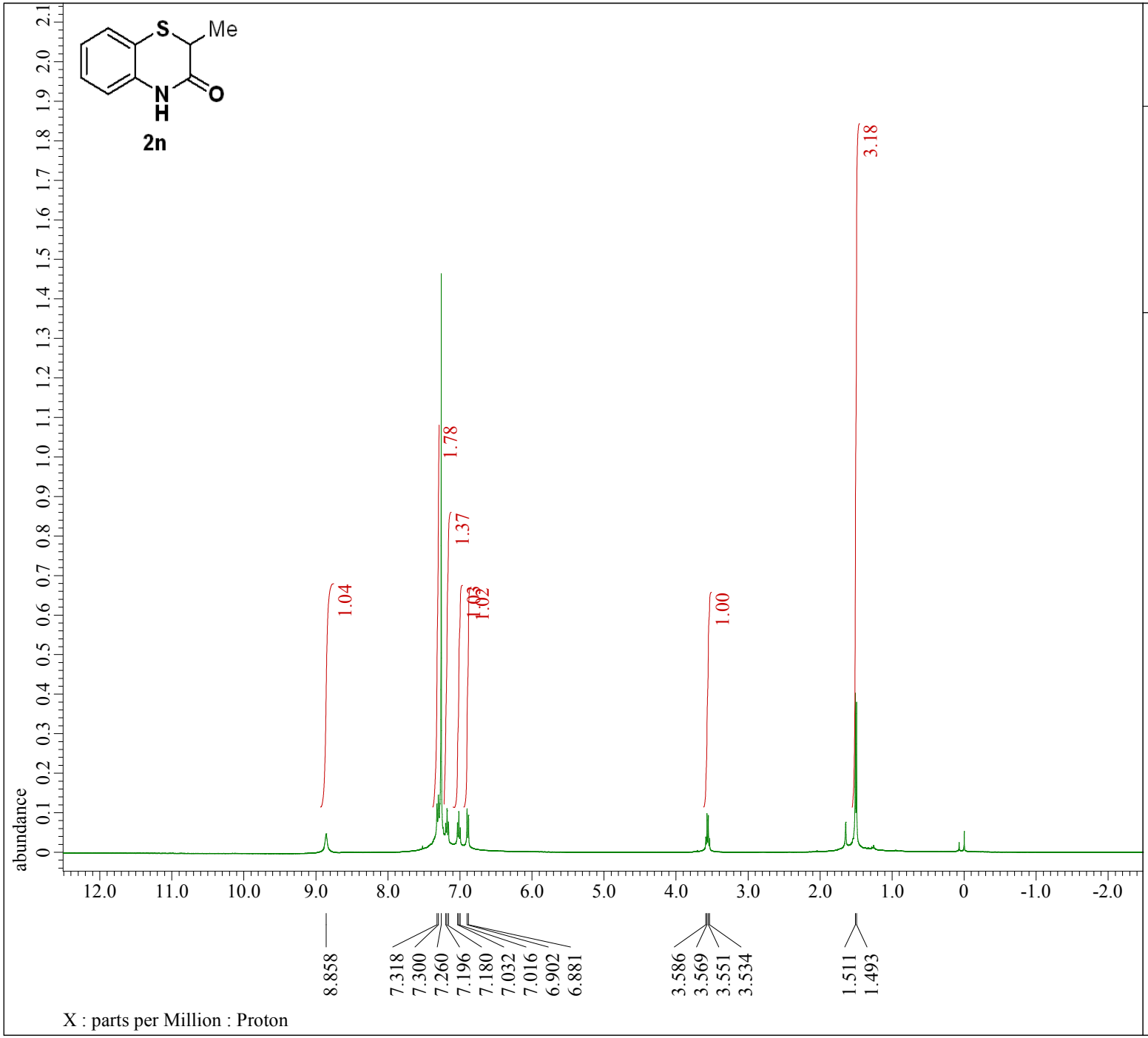
| | |
|---|---|
| Filename | = LK0224-1_Proton-1-3.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK0224-1 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 24-FEB-2017 17:15:06 |
| Revision_Time | = 4-AUG-2017 23:34:00 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 22[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK0224-1_Carbon-1-1.jdf
```

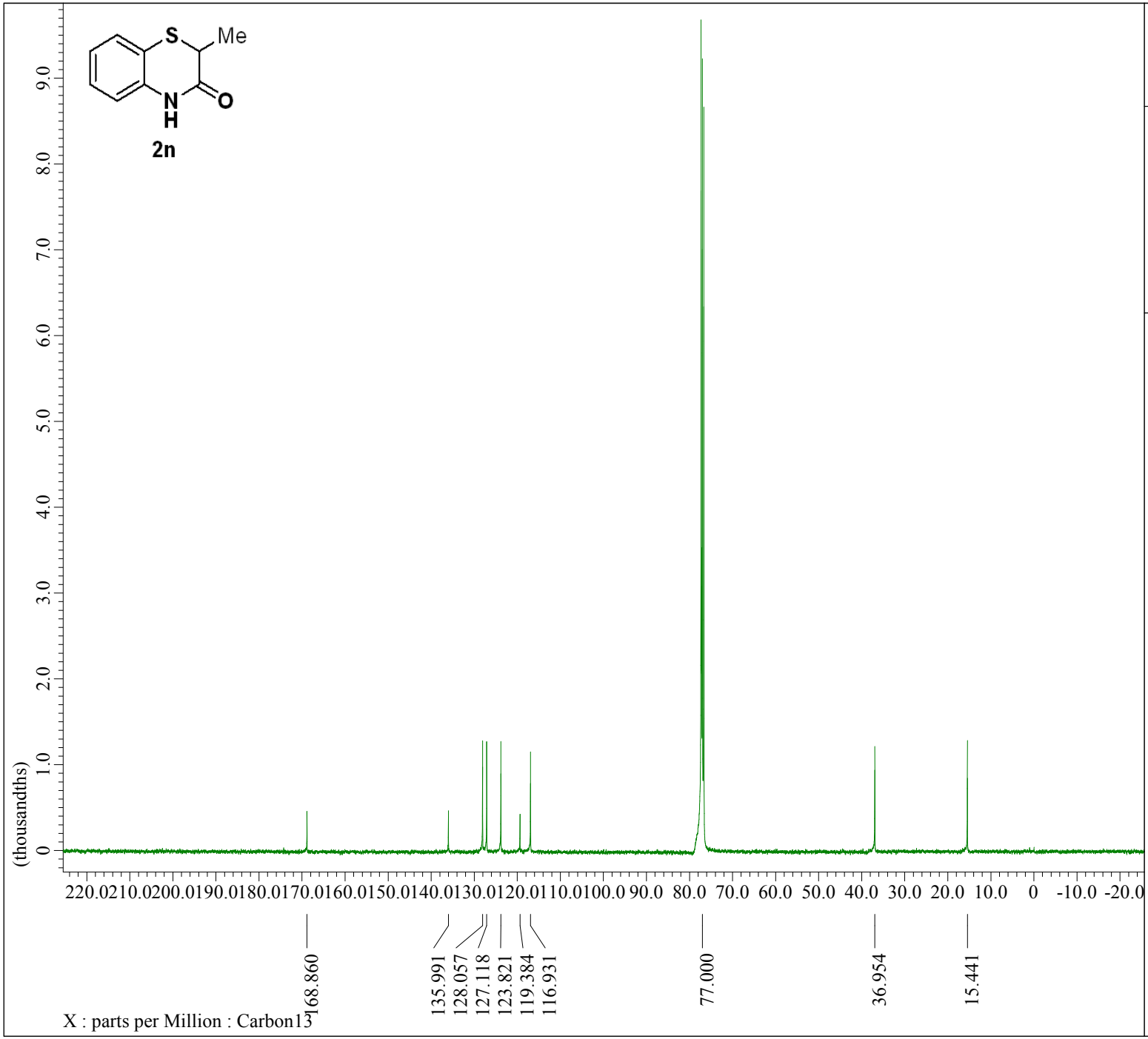
| | |
|---|---|
| Filename | = LK0224-1_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK0224-1 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 24-FEB-2017 17:25: |
| Revision_Time | = 4-AUG-2017 23:38: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 183 |
| Total_Scans | = 183 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21.9[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK050702_Proton-1-1.jdf
```

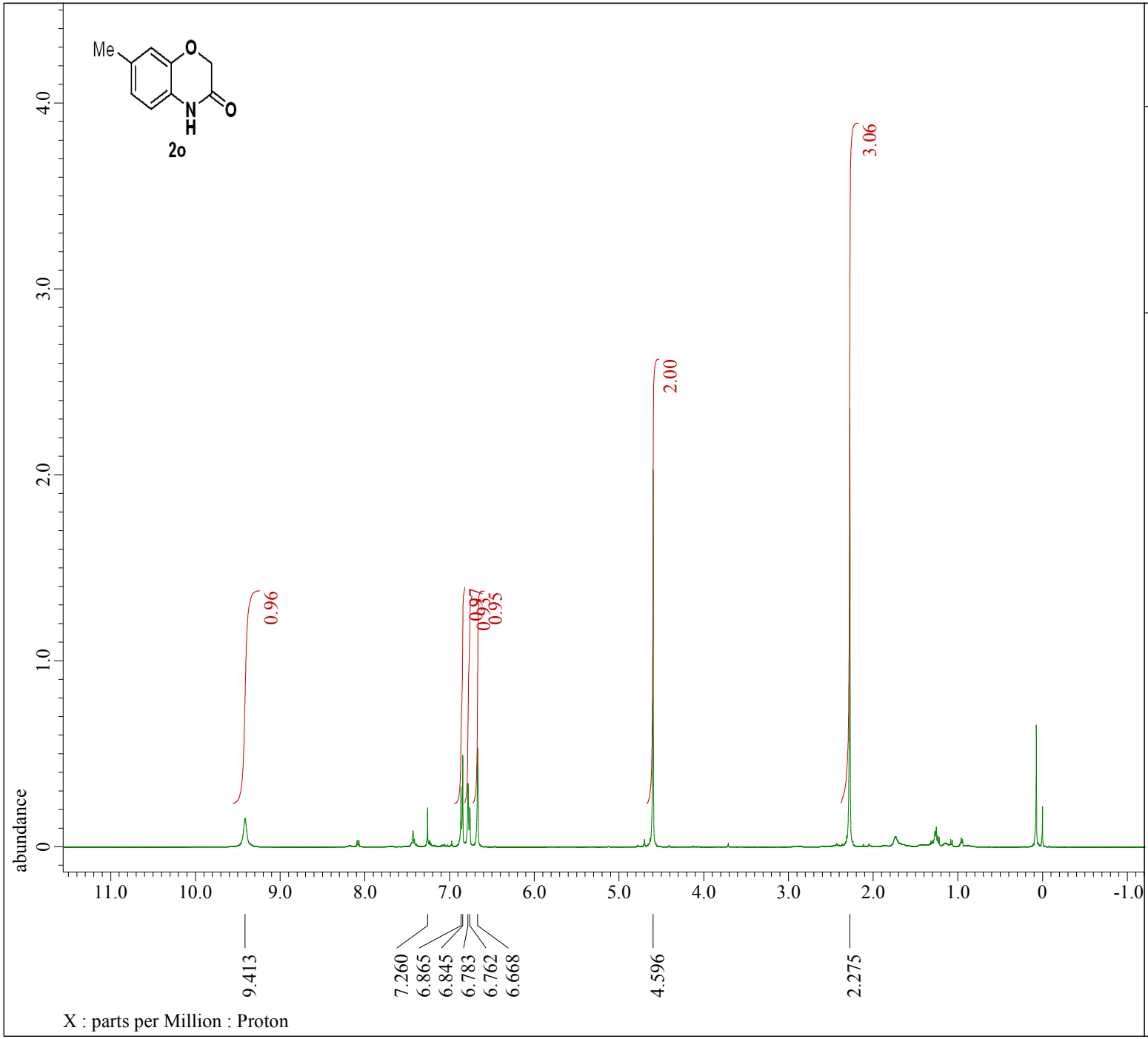
| | |
|---|---|
| Filename | = LK050702_Proton-1-4.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK050702 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 7-MAY-2017 17:24:59 |
| Revision_Time | = 5-AUG-2017 01:12:25 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 22.2[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK050702_Carbon-1-1.jdf
```

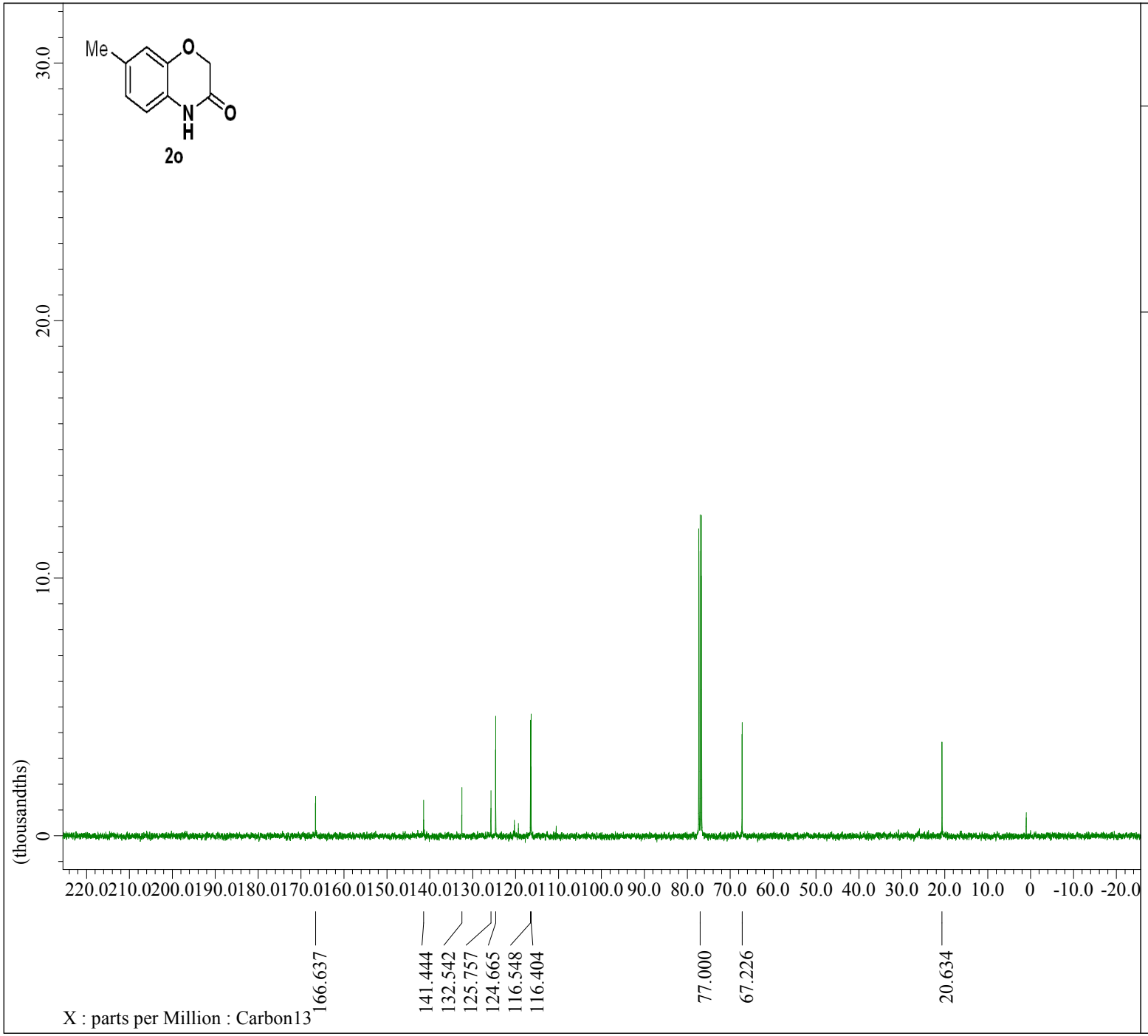
| | |
|---|---|
| Filename | = LK050702_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK050702 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 7-MAY-2017 18:25: |
| Revision_Time | = 5-AUG-2017 01:17: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8000 |
| Total_Scans | = 8000 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 23[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK120904_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK120904_Proton-1-3.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK120904 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-DEC-2016 11:52:16 |
| Revision_Time | = 4-AUG-2017 23:45:21 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 21.1[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

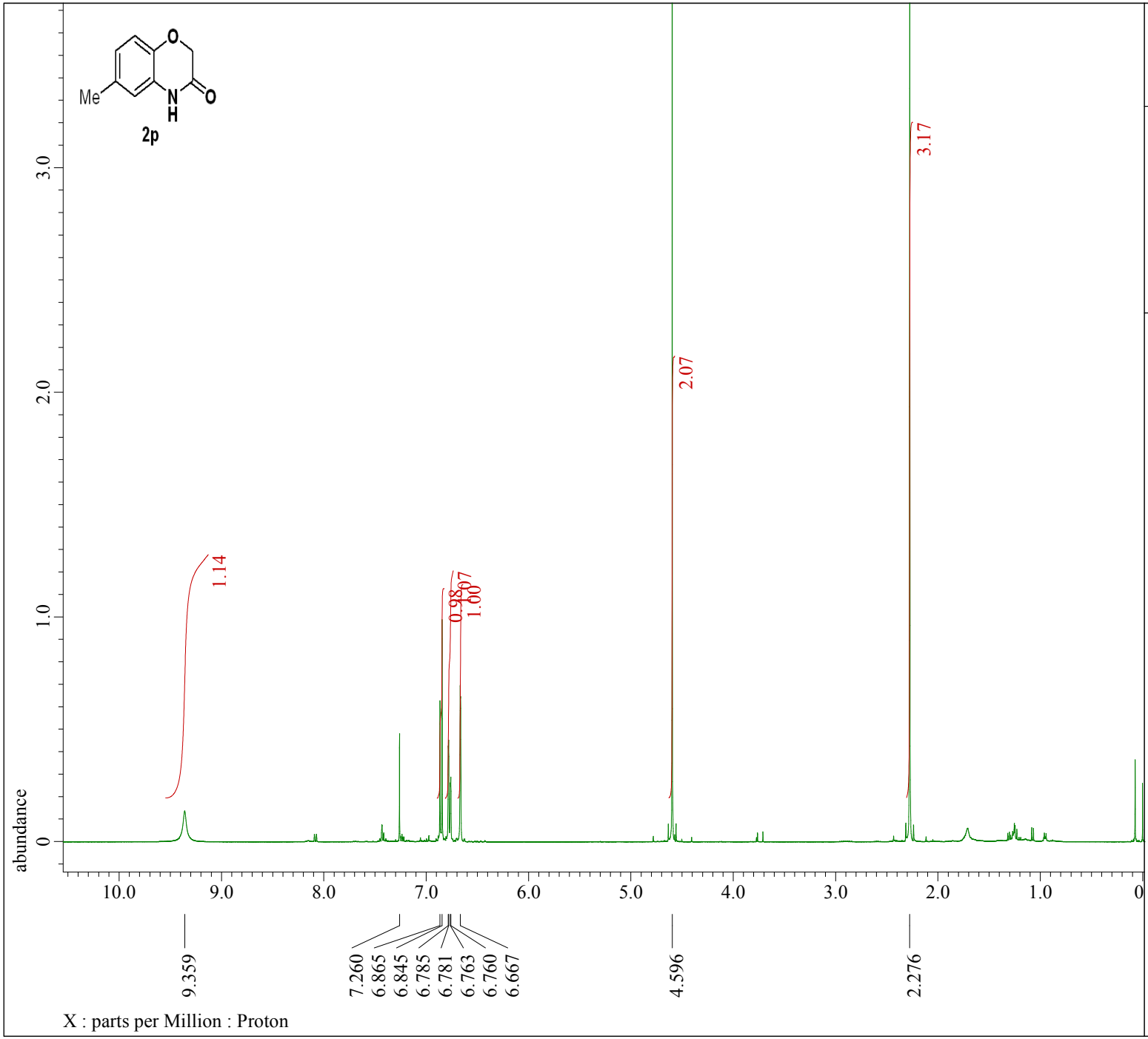



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK120904_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK120904_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK120904 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-DEC-2016 14:07: |
| Revision_Time | = 4-AUG-2017 23:42: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 248 |
| Total_Scans | = 248 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21.5[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |

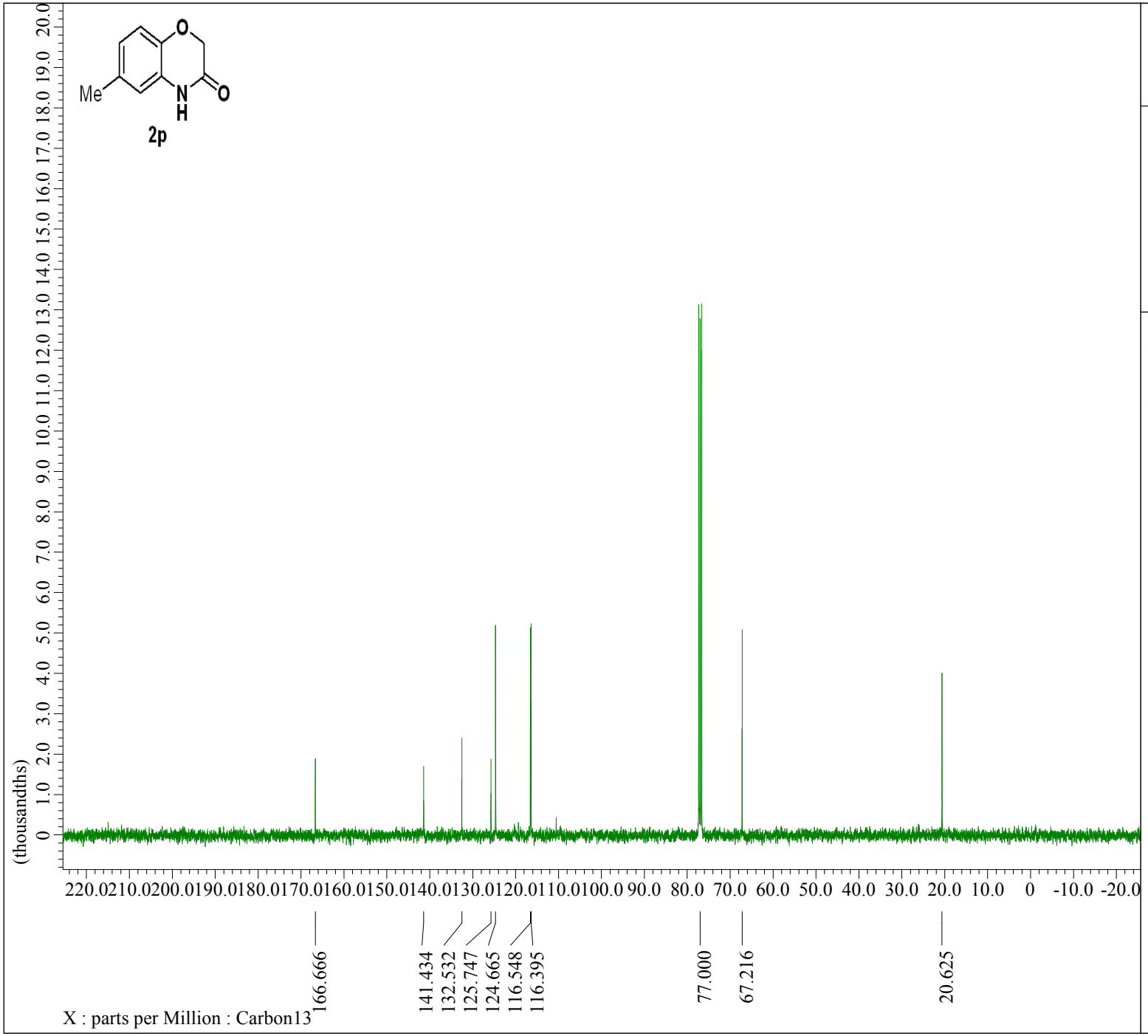



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK120903_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK120903_Proton-1-3.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK120903 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-DEC-2016 11:48:44 |
| Revision_Time | = 4-AUG-2017 23:51:59 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 21.1[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |

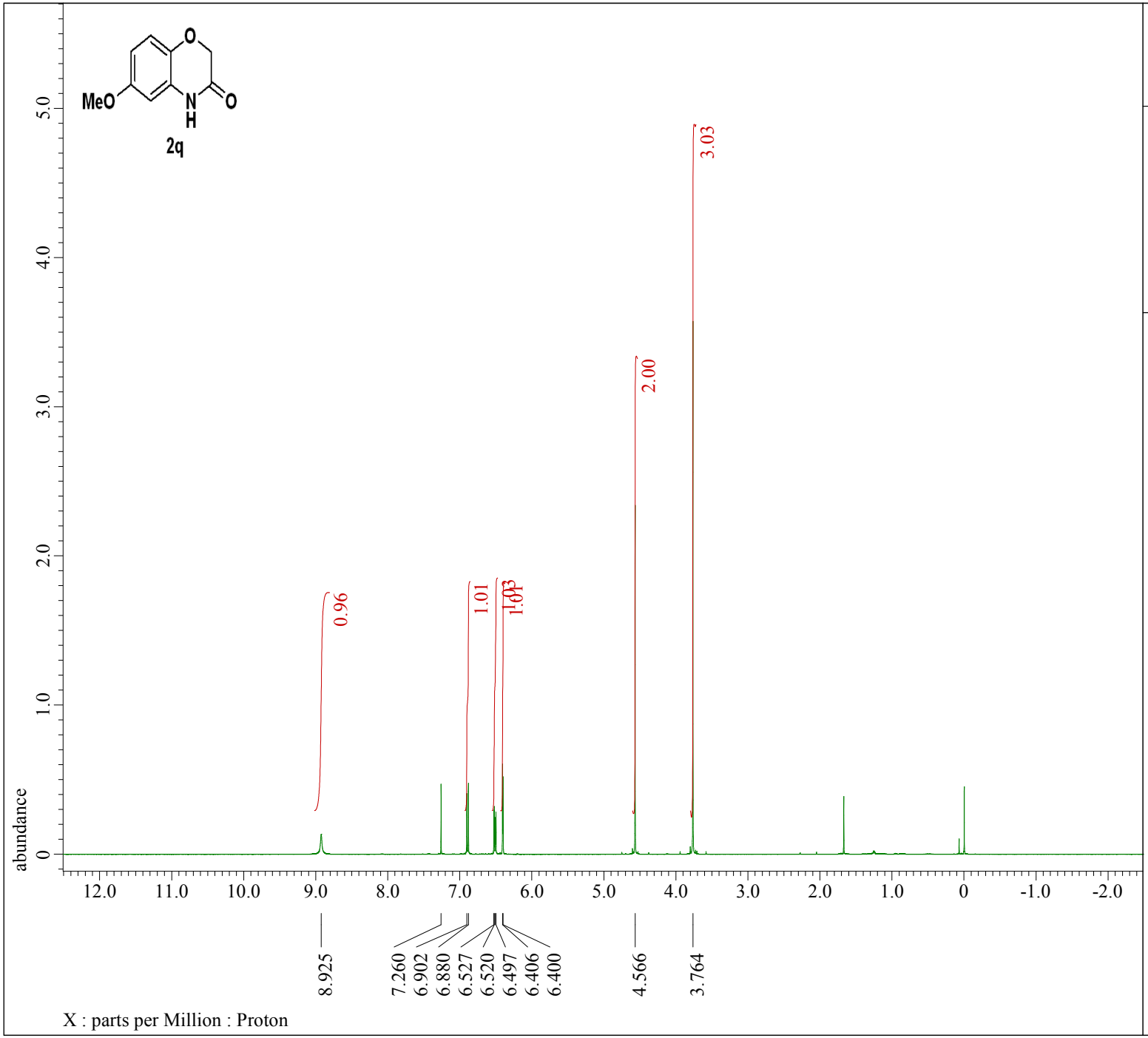



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

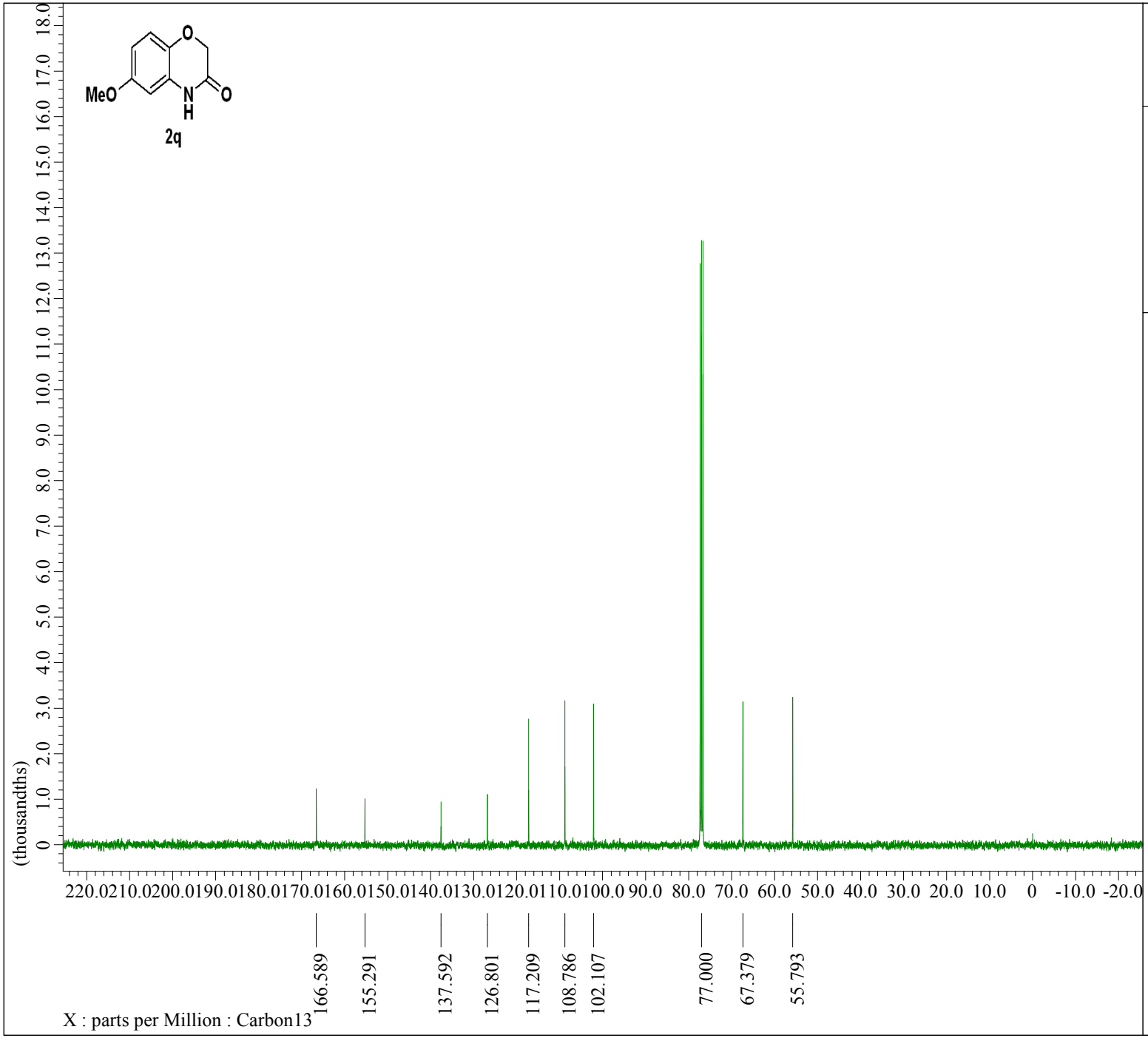
Derived from: LK120903_Carbon-1-1.jdf
```

| | |
|---|---|
| Filename | = LK120903_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK120903 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 14-DEC-2016 13:53: |
| Revision_Time | = 4-AUG-2017 23:54: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 161 |
| Total_Scans | = 161 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 21.3[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

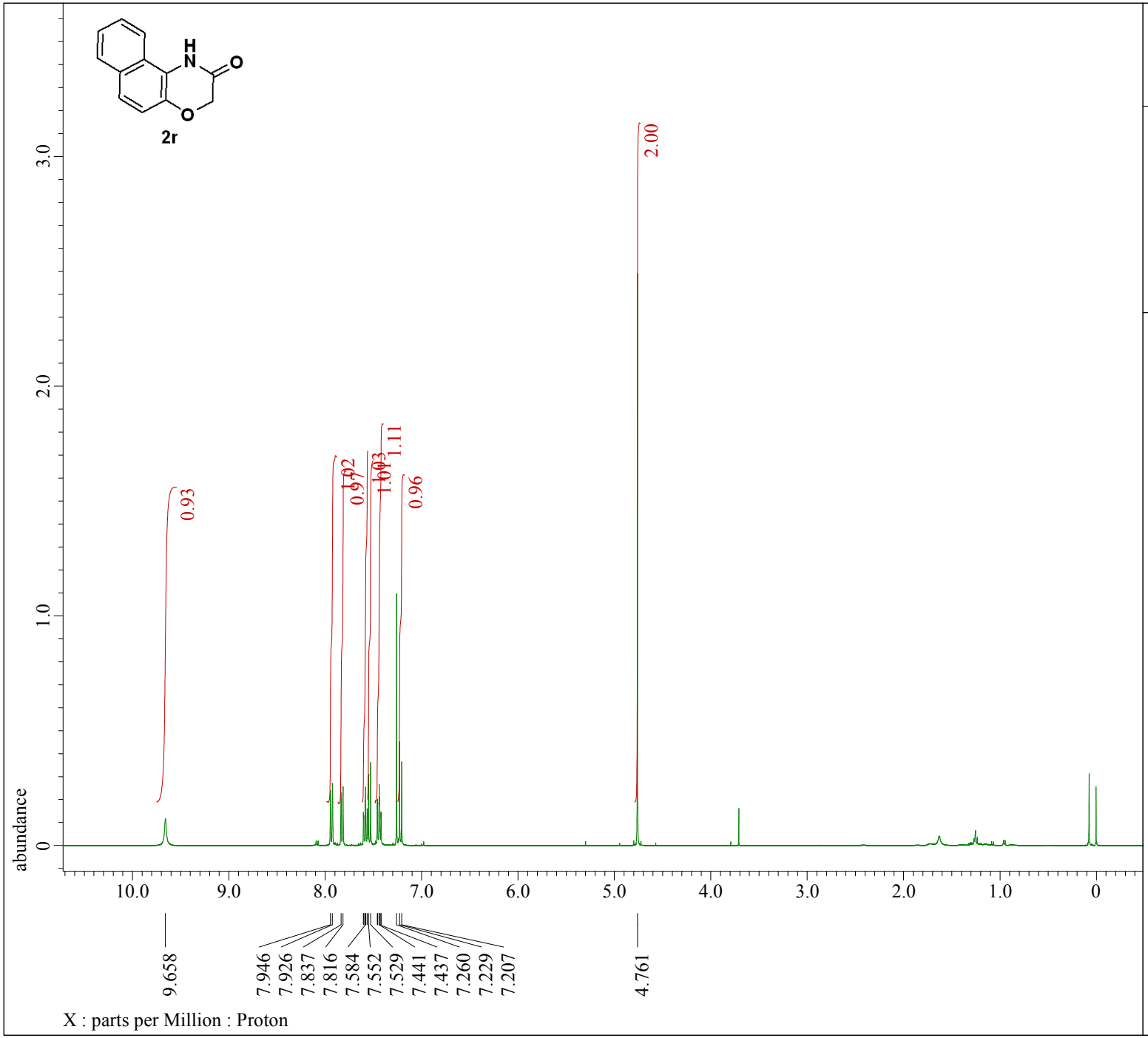
| | |
|---|---|
| Filename | = LK1206-5_Proton-1-3.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK1206-5 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 6-DEC-2016 12:08:28 |
| Revision_Time | = 5-AUG-2017 00:03:47 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 18.6[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK1206-5_Carbon-1-1.jdf
```

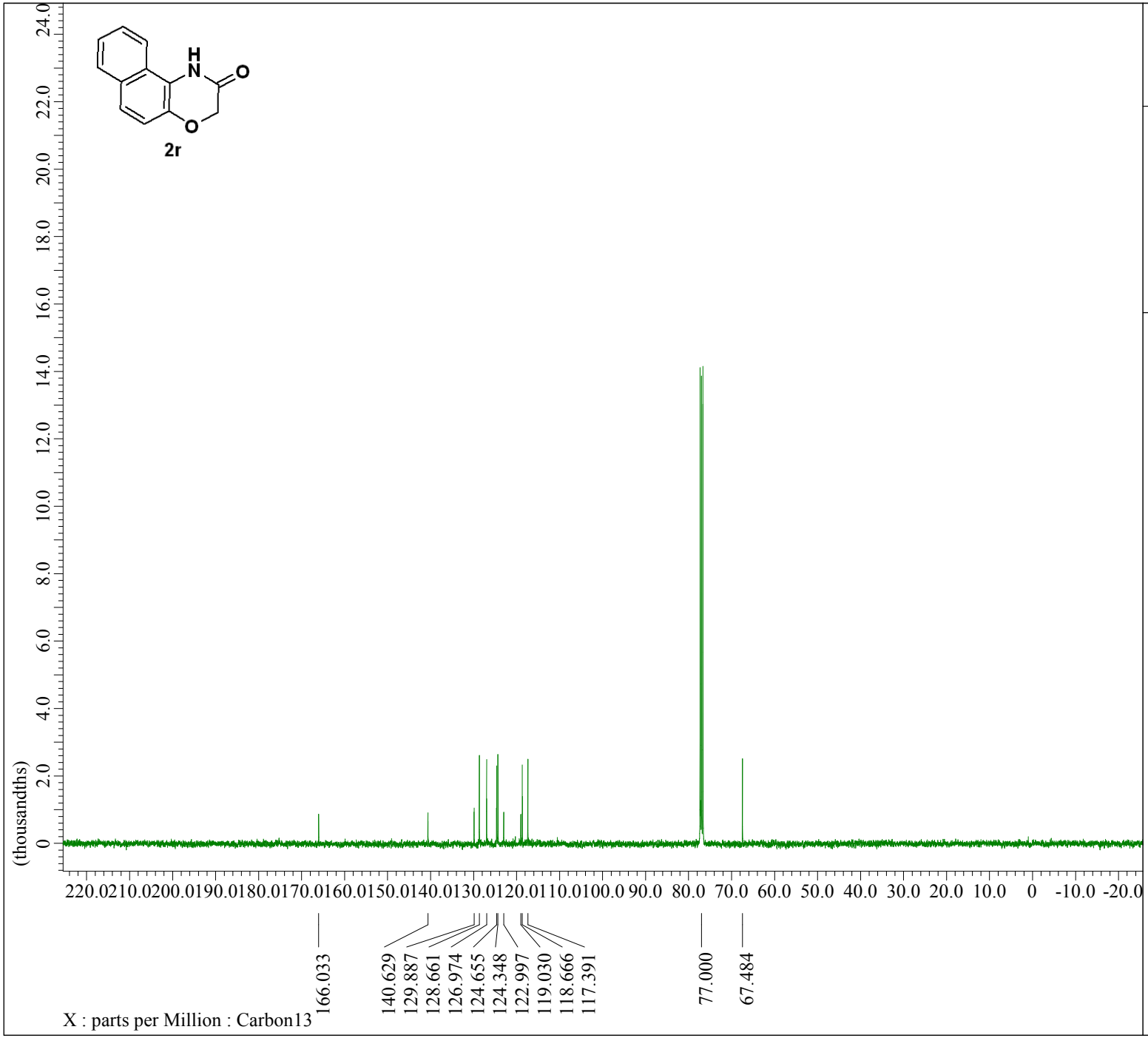
| | |
|---|---|
| Filename | = LK1206-5_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK1206-5 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 6-DEC-2016 15:26: |
| Revision_Time | = 4-AUG-2017 23:58: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = TRUE |
| Scans | = 502.0 |
| Total_Scans | = 502.0 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 20[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK0224-4_Proton-1-1.jdf
```

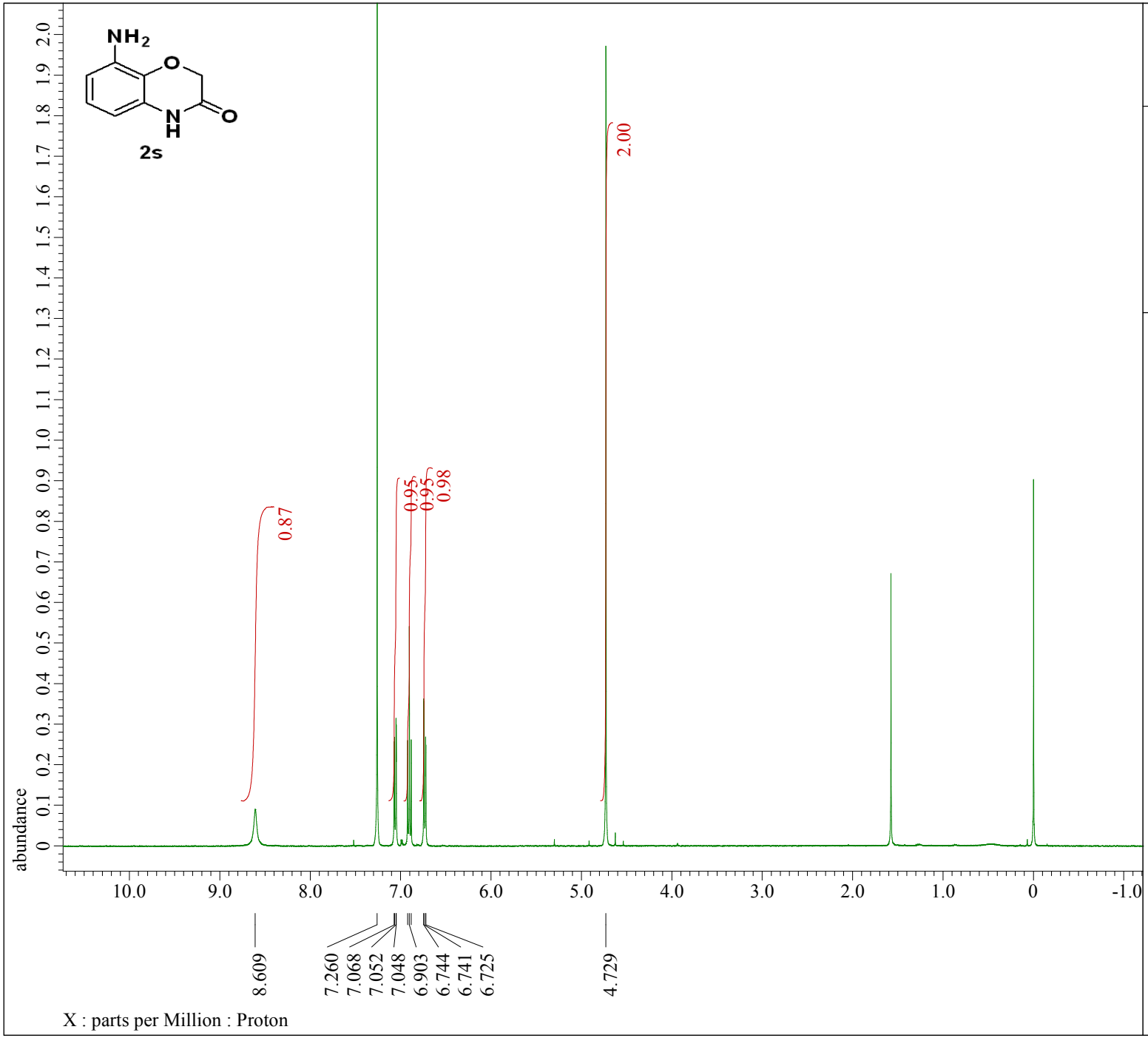
| | |
|---|---|
| Filename | = LK0224-4_Proton-1-3.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK0224-4 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 24-FEB-2017 18:07:08 |
| Revision_Time | = 5-AUG-2017 00:15:37 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 20.9[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |




---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK0224-4_Carbon-1-1.jdf

| | |
|---|---|
| Filename | = LK0224-4_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK0224-4 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 24-FEB-2017 18:10: |
| Revision_Time | = 5-AUG-2017 00:25: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 417 |
| Total_Scans | = 417 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 19.7[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |

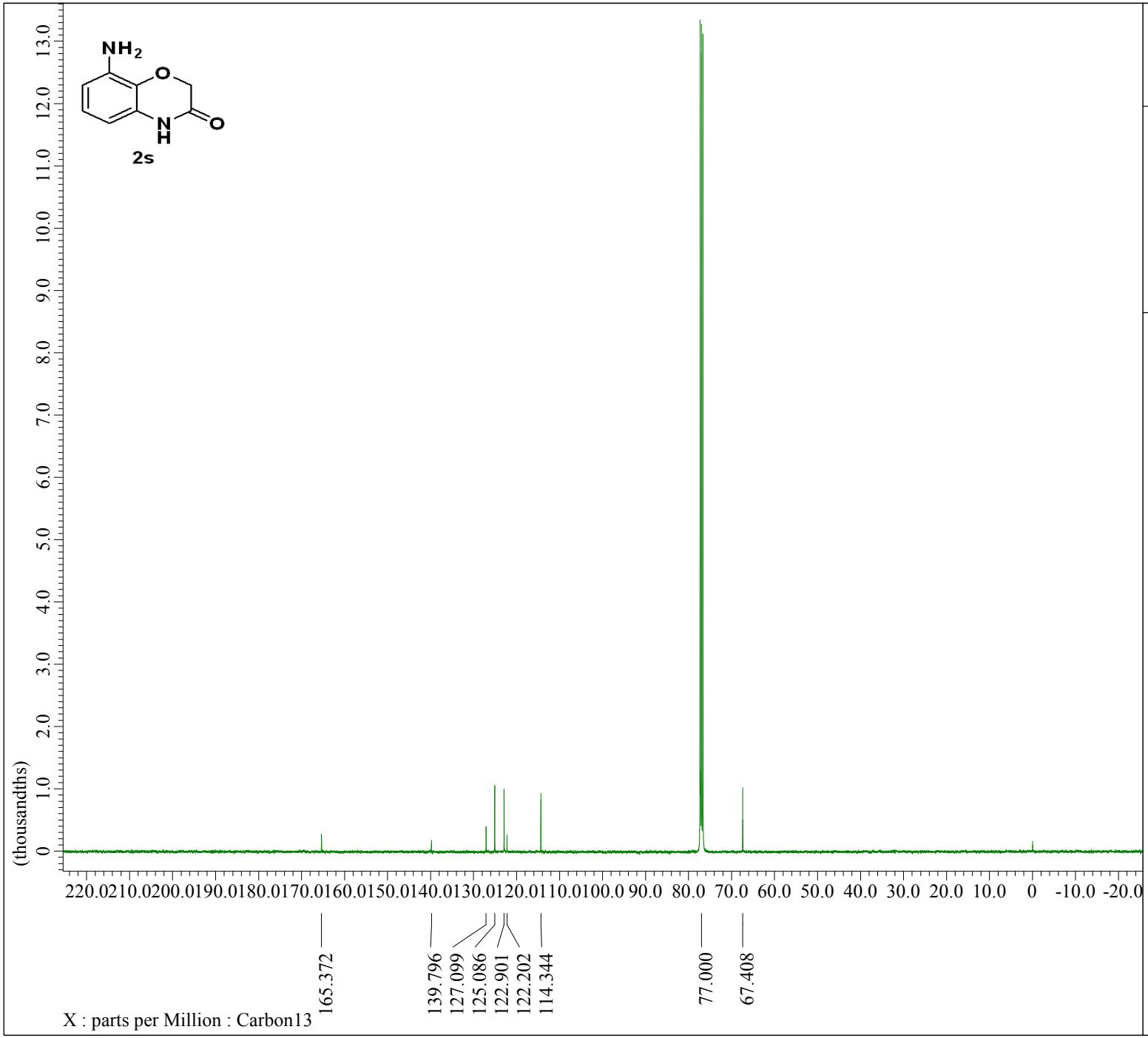



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK0224-3_Proton-1-1.jdf
```

| | |
|---|---|
| Filename | = LK0224-3_Proton-1-3.j |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = LK0224-3 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 24-FEB-2017 17:45:29 |
| Revision_Time | = 5-AUG-2017 00:31:21 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[MHz] |
| X_Acq_Duration | = 2.18628096[s] |
| X_Domain | = 1H |
| X_Freq | = 399.78219838[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.45739775[Hz] |
| X_Sweep | = 7.4940048[kHz] |
| X_Sweep_Clipped | = 5.99520384[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.78219838[MHz] |
| Tri_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 8 |
| Total_Scans | = 8 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 66 |
| Temp_Get | = 22.1[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 2.18628096[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 2[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: LK0224-3_Carbon-1-1.jdf
```

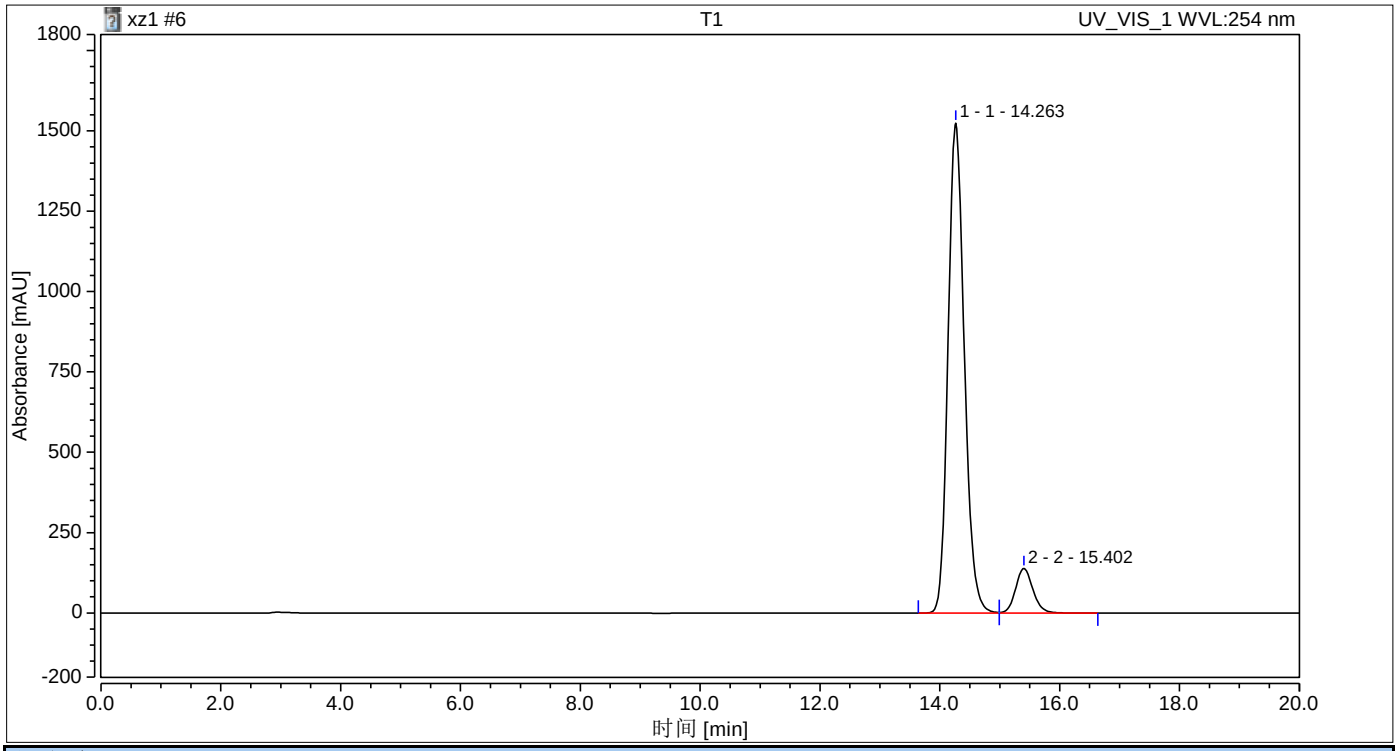
| | |
|---|---|
| Filename | = LK0224-3_Carbon-1- |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = LK0224-3 |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 24-FEB-2017 23:57: |
| Revision_Time | = 5-AUG-2017 00:29: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.389766[T] (400[M |
| X_Acq_Duration | = 1.03809024[s] |
| X_Domain | = 13C |
| X_Freq | = 100.52530333[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 0.96330739[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.78219838[MHz] |
| Irr_Offset | = 5[ppm] |
| Clipped | = FALSE |
| Scans | = 10240 |
| Total_Scans | = 10240 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 50 |
| Temp_Get | = 14[dC] |
| X_90_Width | = 8.8[us] |
| X_Acq_Time | = 1.03809024[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 3.4[dB] |
| X_Pulse | = 2.93333333[us] |
| Irr_Atn_Dec | = 23.66[dB] |
| Irr_Atn_Dec_Calc | = 23.66[dB] |
| Irr_Atn_Dec_Default_Calc | = 23.66[dB] |
| Irr_Atn_Noe | = 23.66[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96303566[ppm] |
| Irr_Dec_Freq | = 399.78219838[MHz] |

# 色谱图和结果

## 进样信息

| | | | |
|---|---|---|---|
| *进样名称:* | **T1** | *运行时间 (min):* | **20.00** |
| *瓶号:* | **RA2** | *进样量:* | **10.00** |
| *进样类型:* | **未知** | *通道:* | **UV_VIS_1** |
| *校准级别:* | | *波长:* | **254.0** |
| *仪器方法:* | **xz1** | *带宽:* | **n.a.** |
| *处理方法:* | **xz1** | *稀释因子:* | **1.0000** |
| *进样日期/时间:* | **2017/10/14 16:39** | *样品重量:* | **1.0000** |

## 色谱图




## 积分结果

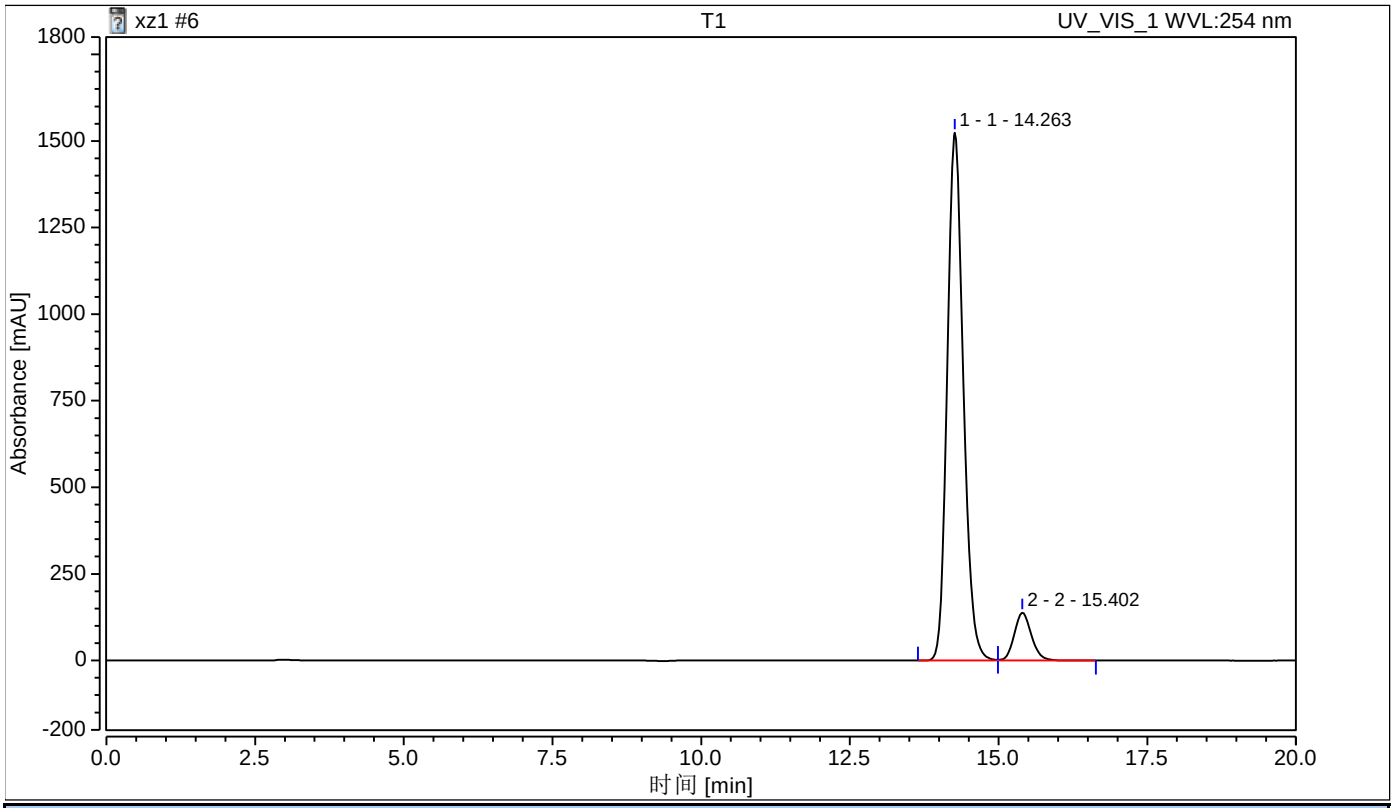
| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 14.263 | 478.044 | 1524.272 | 91.15 | 91.65 | n.a. |
| 2 | 2 | 15.402 | 46.435 | 138.783 | 8.85 | 8.35 | n.a. |
| **总和:** | | | **524.479** | **1663.054** | **100.00** | **100.00** | |

# 色谱图和 SST 结果

## 进样信息

| | | | |
|---|---|---|---|
| *进样名称:* | **T1** | *运行时间 (min):* | **20.00** |
| *瓶号:* | **RA2** | *进样量:* | **10.00** |
| *进样类型:* | **未知** | *通道:* | **UV_VIS_1** |
| *校准级别:* | | *波长:* | **254.0** |
| *仪器方法:* | **xz1** | *带宽:* | **n.a.** |
| *处理方法:* | **xz1** | *稀释因子:* | **1.0000** |
| *进样日期/时间:* | **2017/10/14 16:39** | *样品重量:* | **1.0000** |

## 色谱图




## SST 结果

| 序号 | 名称 | 进样条件 | 峰 | 测试结果 | 进样 |
|---|---|---|---|---|---|

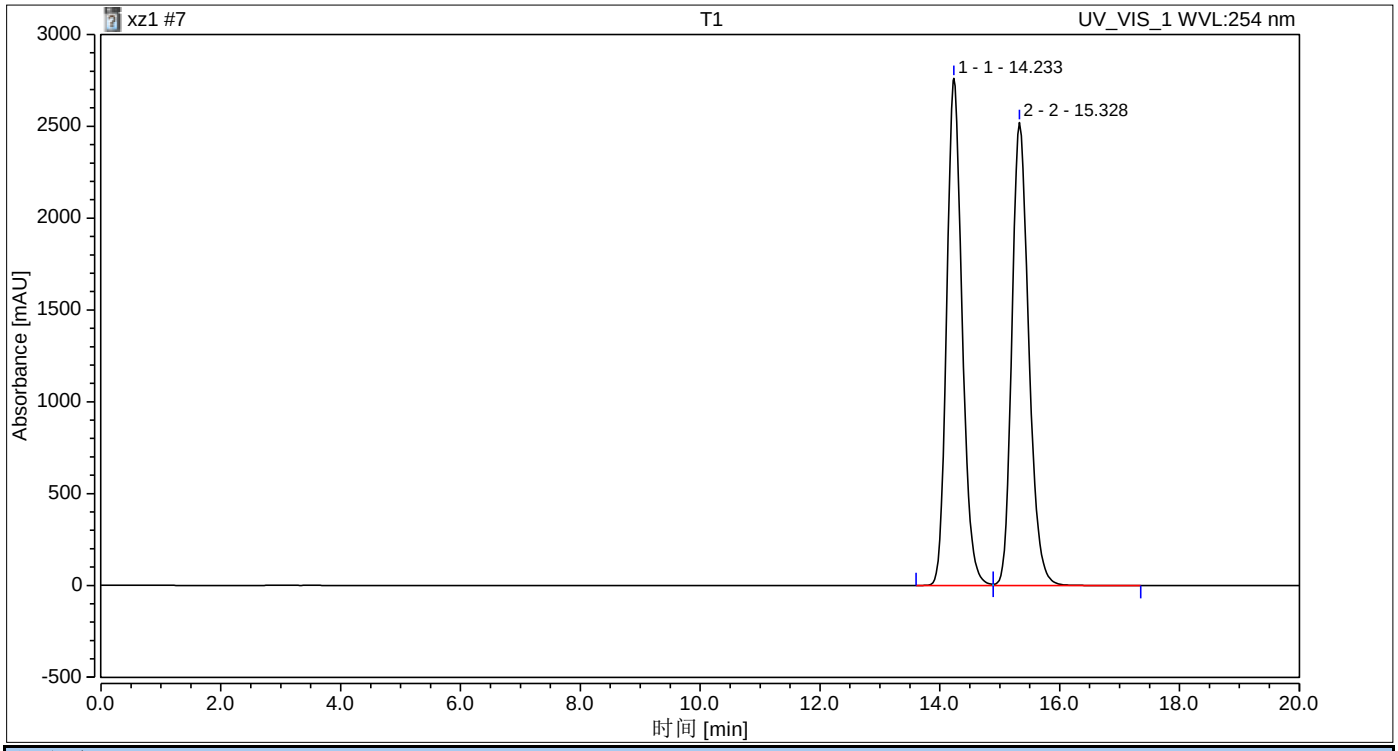
**已执行的测试用例数目:** **n.a.** **总结果:** **通过**

# 色谱图和结果

## 进样信息

| | | | |
|---|---|---|---|
| *进样名称:* | **T1** | *运行时间 (min):* | **20.00** |
| *瓶号:* | **RA1** | *进样量:* | **10.00** |
| *进样类型:* | **未知** | *通道:* | **UV_VIS_1** |
| *校准级别:* | | *波长:* | **254.0** |
| *仪器方法:* | **xz1** | *带宽:* | **n.a.** |
| *处理方法:* | **xz1** | *稀释因子:* | **1.0000** |
| *进样日期/时间:* | **2017/10/14 17:03** | *样品重量:* | **1.0000** |

## 色谱图




## 积分结果

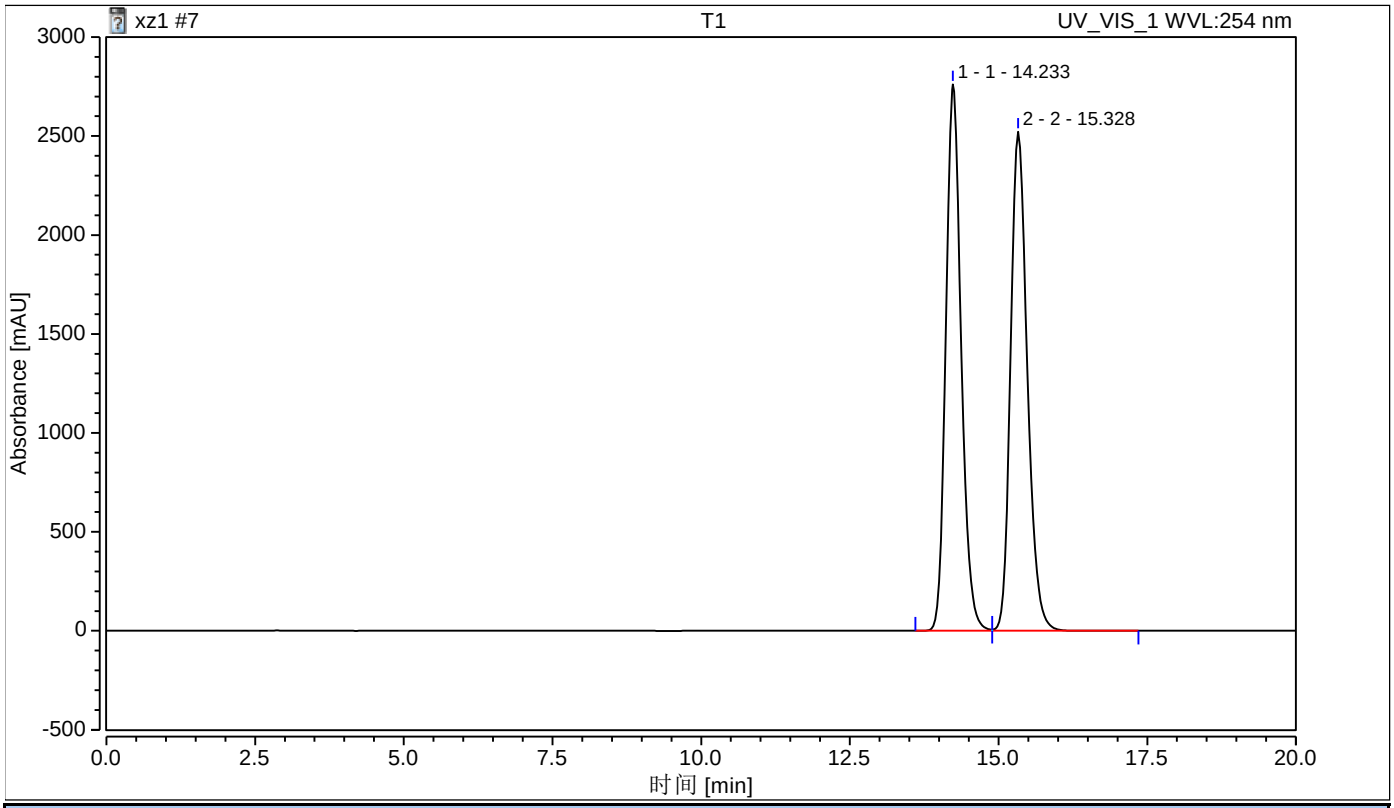
| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 14.233 | 822.481 | 2760.764 | 50.02 | 52.27 | n.a. |
| 2 | 2 | 15.328 | 821.960 | 2521.193 | 49.98 | 47.73 | n.a. |
| **总和:** | | | **1644.441** | **5281.957** | **100.00** | **100.00** | |

# 色谱图和 SST 结果

## 进样信息

| | | | |
|---|---|---|---|
| *进样名称:* | **T1** | *运行时间 (min):* | **20.00** |
| *瓶号:* | **RA1** | *进样量:* | **10.00** |
| *进样类型:* | **未知** | *通道:* | **UV_VIS_1** |
| *校准级别:* | | *波长:* | **254.0** |
| *仪器方法:* | **xz1** | *带宽:* | **n.a.** |
| *处理方法:* | **xz1** | *稀释因子:* | **1.0000** |
| *进样日期/时间:* | **2017/10/14 17:03** | *样品重量:* | **1.0000** |

## 色谱图




## SST 结果

| 序号 | 名称 | 进样条件 | 峰 | 测试结果 | 进样 |
|---|---|---|---|---|---|

**已执行的测试用例数目:** **n.a.** **总结果:** **通过**

# 总结

## 序列信息

| | | | |
|---|---|---|---|
| *名称:* | **xz1** | *创建日期:* | **2017/10/14 14:40:11** |
| *目录:* | **xz1** | *创建者:* | **Administrator** |
| *数据仓:* | **Data** | *更新日期:* | **2017/10/14 17:23:15** |
| *进样数:* | **7** | *更新者:* | **Administrator** |

**按组分** **1**

| 序号 | 进样名称 | 保留时间 min UV_VIS_1 1 | 峰面积 mAU*min UV_VIS_1 1 | 峰高 mAU UV_VIS_1 1 | 样品量 UV_VIS_1 1 | 相对峰面积 % UV_VIS_1 1 | 峰类型 UV_VIS_1 1 |
|---|---|---|---|---|---|---|---|
| 1 | T1 | n.a. | n.a. | n.a. | n.a. | n.a. | n.a. |
| 2 | T1 | n.a. | n.a. | n.a. | n.a. | n.a. | n.a. |
| 3 | T1 | n.a. | n.a. | n.a. | n.a. | n.a. | n.a. |
| 4 | T1 | n.a. | n.a. | n.a. | n.a. | n.a. | n.a. |
| 5 | T1 | n.a. | n.a. | n.a. | n.a. | n.a. | n.a. |
| 6 | T1 | 14.263 | 478.044 | 1524.272 | n.a. | 91.15 | M |
| 7 | T1 | 14.233 | 822.481 | 2760.764 | n.a. | 50.02 | M |

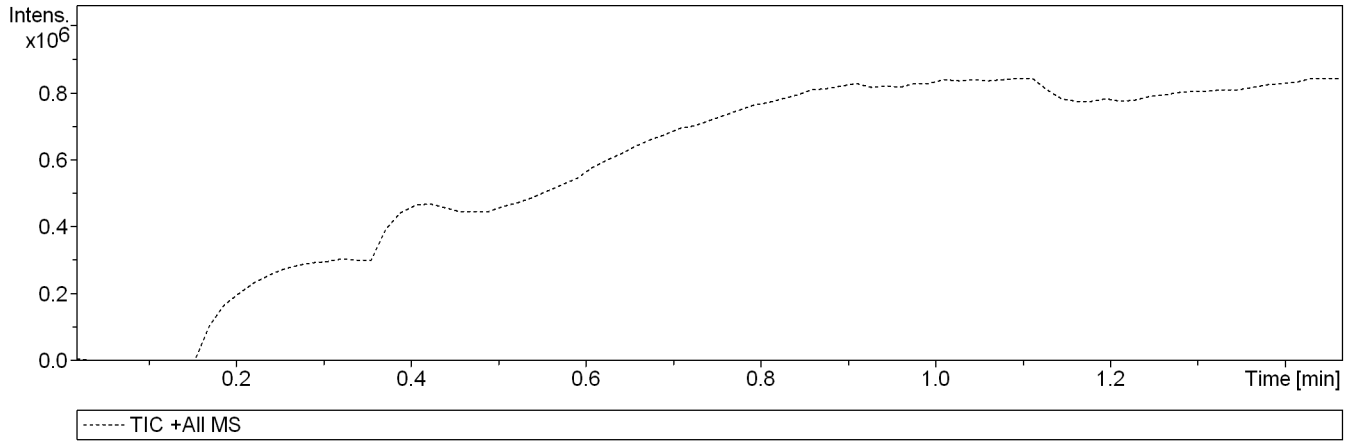
# Display Report

**Analysis Info**

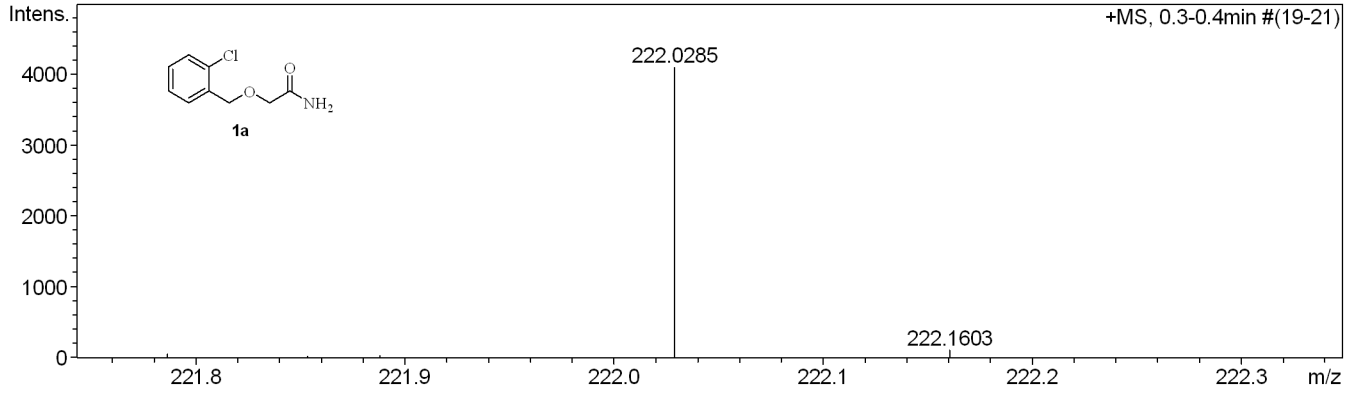
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\du\xz\201703112\21.d | Acquisition Date | 3/11/2017 8:26:26 PM |
| Method | tune_low.m | Operator | XZNU |
| Sample Name | | Instrument | micrOTOF-Q 134 |
| Comment | | | |

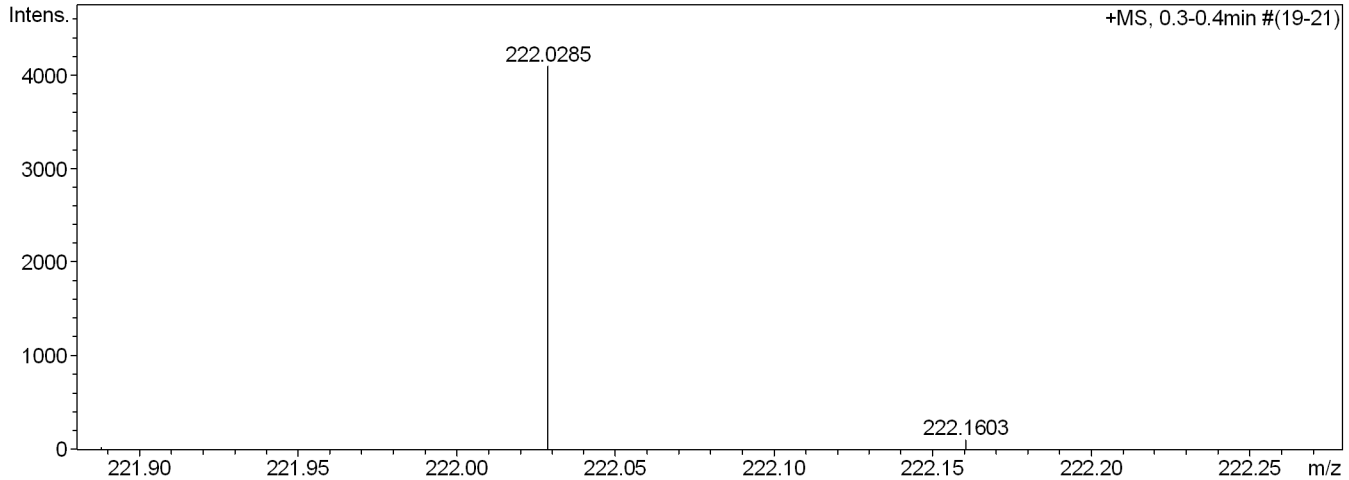
**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 4500 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Source |




TIC +All MS



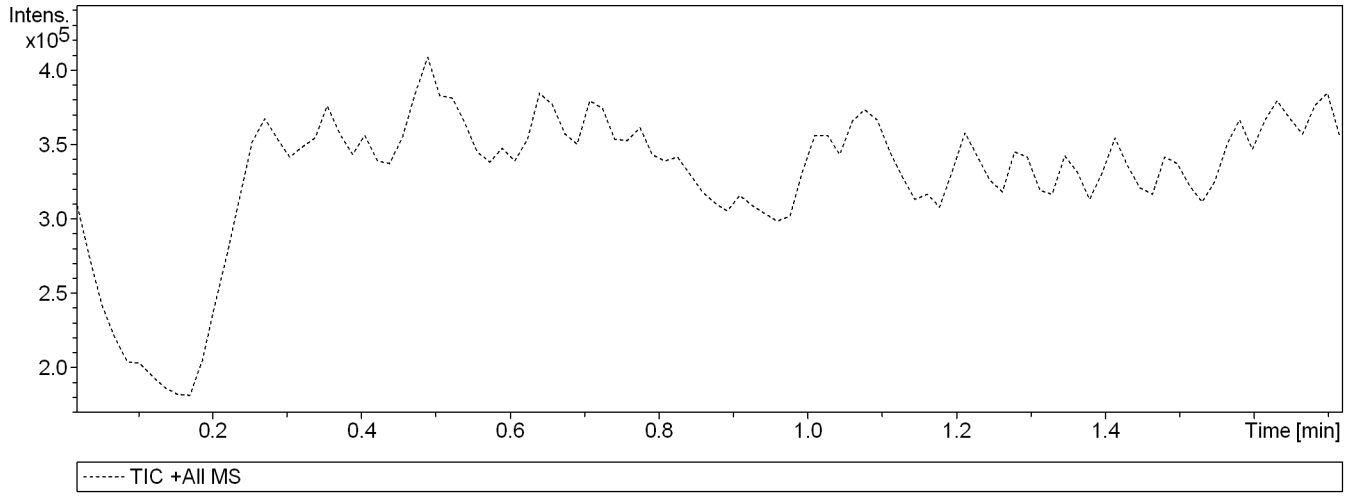
# Display Report

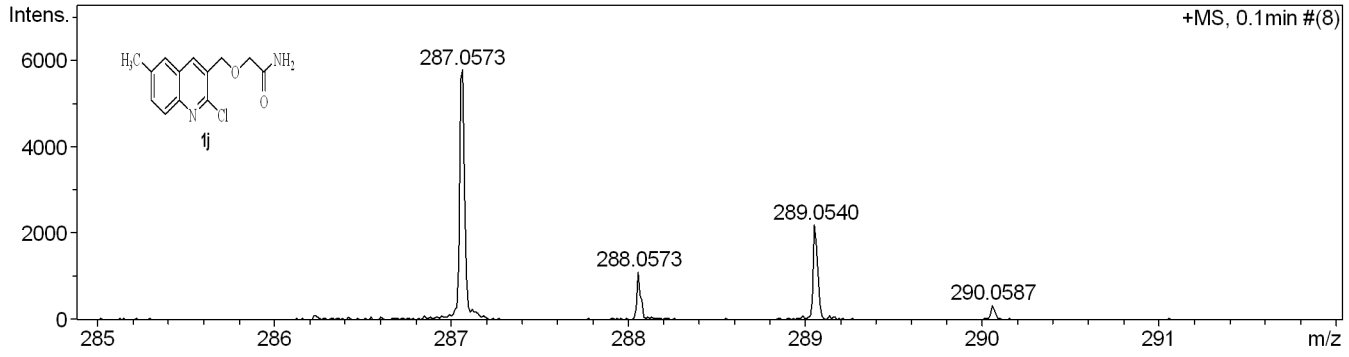
**Analysis Info**

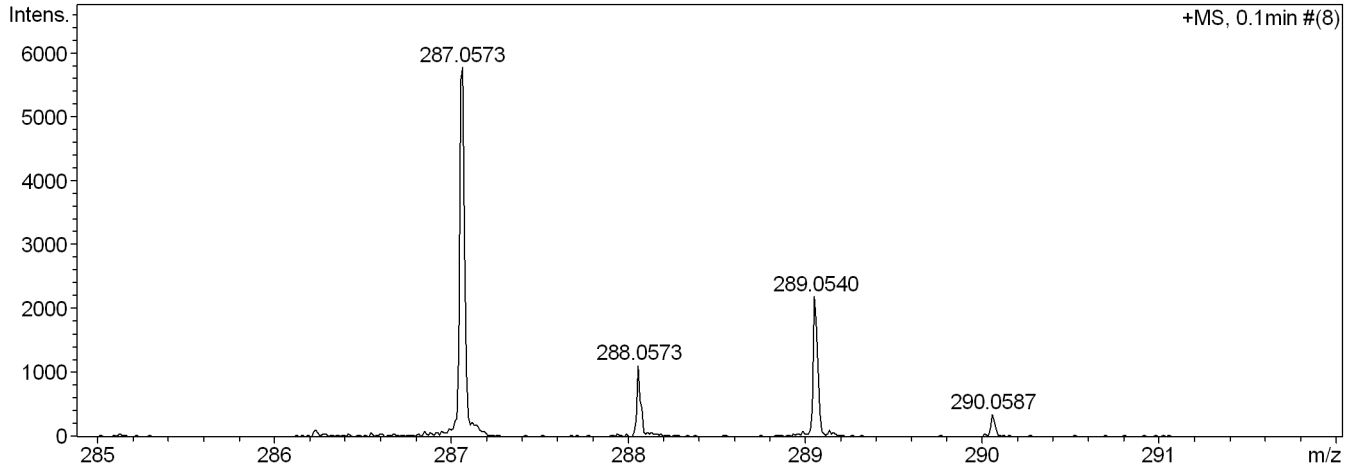
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\XZ\201710102\1j.d | Acquisition Date | 10/11/2017 9:38:11 PM |
| Method | tune_low.m | Operator | XZNU |
| Sample Name | ZX-9aa | Instrument | micrOTOF-Q 134 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 4500 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Source |



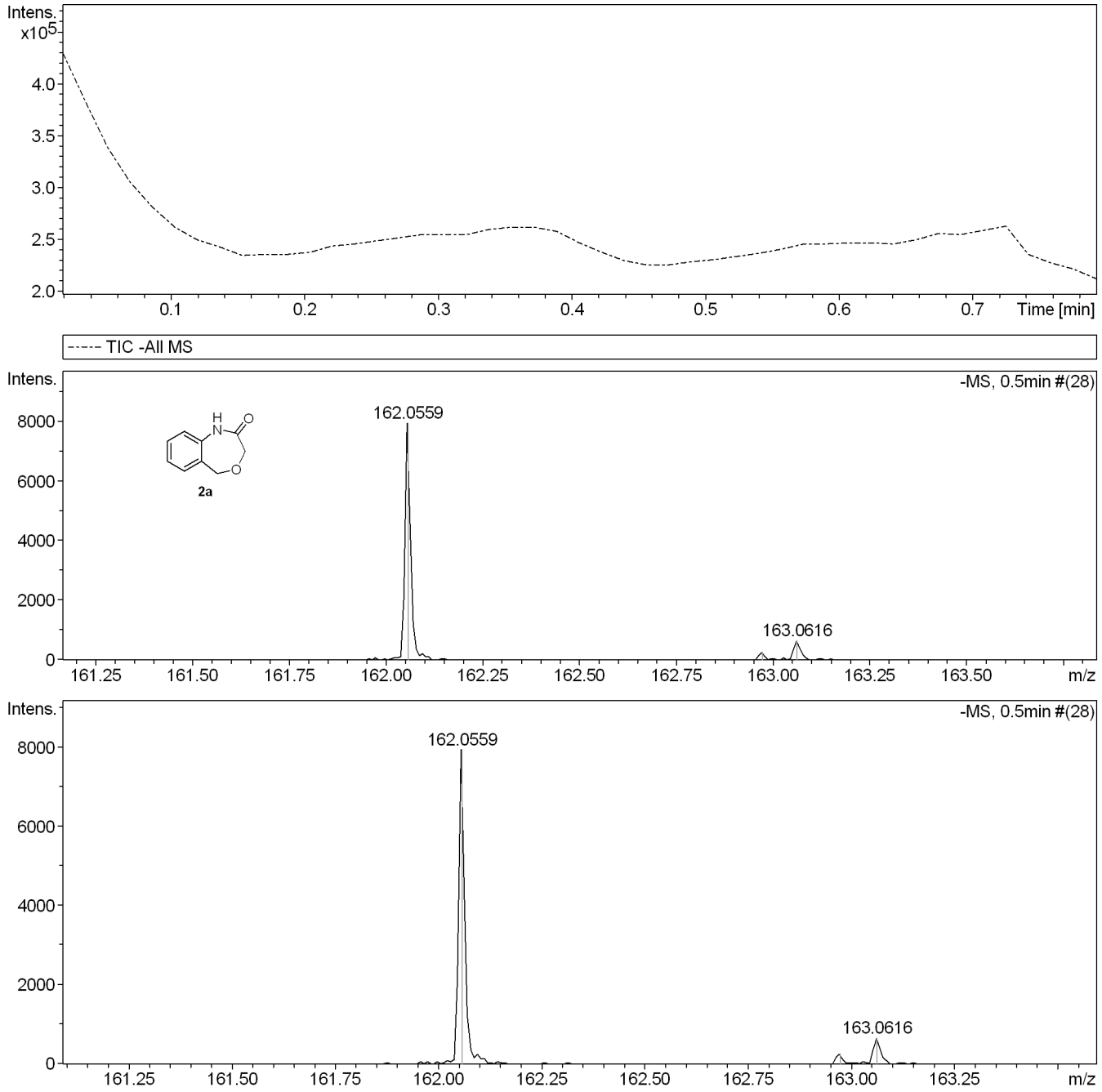
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\du\20170603XZ\10.d | Acquisition Date | 6/4/2017 9:32:49 AM |
| Method | tune_low_neg.m | Operator | XZNU |
| Sample Name | zq34b2 | Instrument | micrOTOF-Q 134 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Negative | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 3500 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Source |



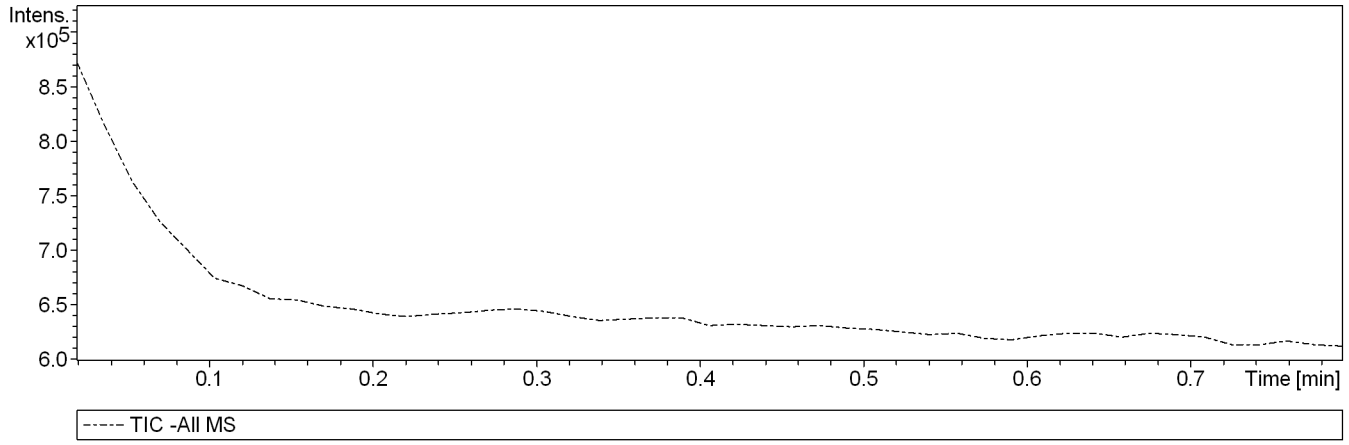
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\du\20170603XZ\8B.d | Acquisition Date | 6/4/2017 9:26:34 AM |
| Method | tune_low_neg.m | Operator | XZNU |
| Sample Name | zq34b2 | Instrument | micrOTOF-Q 134 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Negative | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 3500 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Source |

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