

Supporting Information

Ruthenium Hydride/Nitrogen Tridentate Ligand-Catalyzed α -Alkylation of Acetamides with Primary Alcohols.

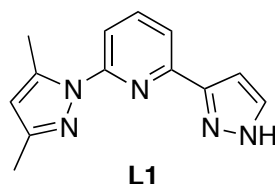
Takashi Kuwahara, Takahide Fukuyama, and Ilhyong Ryu*

*Department of Chemistry, Graduate School of Science, Osaka Prefecture University
Sakai, Osaka 599-8531, Japan
ryu@c.s.osakafu-u.ac.jp*

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General Information. ^1H NMR spectra are recorded with a JEOL ECS-400 (400 MHz) spectrometers in CDCl_3 and referenced at 0.0 ppm for TMS in CDCl_3 . ^{13}C NMR spectra were recorded with JEOL ECS-400 (100 MHz) spectrometers in CDCl_3 and are referenced at 77.16 ppm for CDCl_3 . Chemical shifts are reported in parts per million (δ). Splitting patterns are indicated as follows: br, broad; brs, broad singlet; s, singlet; d, doublet; t, triplet; q, quartet; quint, quintet; sext, sextet; m, multiplet. Infrared spectra were obtained on a JASCO FT/IR-4100 spectrometer; absorptions were reported in reciprocal centimeters. Both conventional and high resolution mass spectra were recorded with a JEOL MS-700 spectrometer. Melting point was measured by BÜCHI Melting Point B-540. The products were purified by flash column chromatography on silica gel (Kanto Chem. Co. Silica Gel 60N (spherical, neutral, 40-50 μm)) and/or preparative HPLC (Japan Analytical Industry Co., Ltd., LC-908) with GPC columns using CHCl_3 as an eluent. $\text{RuHCl}(\text{CO})(\text{PPh}_3)_3$ was purchased from Wako Pure Chemical Industries, Ltd. Other reagents were commercially available and used without further purification. **L1** was prepared with procedure according to the procedure.¹



Typical Procedure for the Ruthenium Hydride-Catalyzed α -Alkylation of Acetamides with Primary Alcohols:

<Method A>

Table 2, entry 2.

$\text{RuHCl}(\text{CO})(\text{PPh}_3)_3$ (14.6 mg, 0.015 mmol), *p*-*tert* butyl benzylalcohol (**2b**, 84.2 mg, 0.51 mmol), KO^tBu (70.3 mg, 0.63 mmol), 2,2'-bipyridine (8.1 mg, 0.052 mmol) and *N,N*-dimethylacetamide (DMA; **1a**) (2 mL) were placed in a screw capped test tube. The test tube was purged with nitrogen and sealed. The mixture was stirred at 140 °C for 18 h. When the reaction was finished, the reaction mixture was cooled to room temperature and then quenched with water (5 mL). Organic layer was extracted with Et_2O (10 mL) three times, washed by brine (30 mL), and then dried over MgSO_4 . After concentration under reduced pressure, the residue was purified by flash chromatography on silica gel (eluent: Et_2O) to give the corresponding amide **3b** (73.2 mg, 61%).

<Method B>

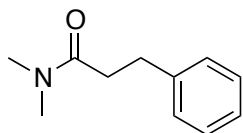
Table 2, entry 1

$\text{RuHCl}(\text{CO})(\text{PPh}_3)_3$ (14.6 mg, 0.015 mmol), benzylalcohol (**2a**, 54.7 mg, 0.51 mmol), KO^tBu (73.1 mg, 0.65 mmol), **L1** (8.3 mg, 0.034 mmol) and *N,N*-dimethylacetamide (DMA; **1a**) (2 mL) were placed in a screw capped test tube. The test tube was purged with nitrogen and sealed. The mixture was stirred at 140 °C for 18 h. When the reaction was finished, the reaction mixture was cooled to room temperature and then quenched with water (5 mL). Organic layer was extracted with Et_2O (10 mL) three times, washed by brine (30 mL), and then dried over MgSO_4 . After concentration under reduced pressure, the residue was purified by flash chromatography on silica

(1) Jin, W.; Wang, L.; Yu, Z. *Organometallics* **2012**, *31*, 5664.

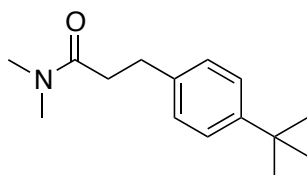
gel (eluent: Et₂O) to give the corresponding amide **3a** (66.4 mg, 74%).

N,N-Dimethyl-3-phenylpropanamide (**3a**)²



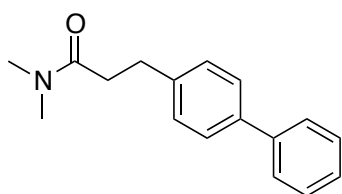
Yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 2.60-2.64 (m, 2H), 2.93-2.99 (m, 8H), 7.18-7.31 (m, 5H); ¹³C NMR (100 MHz, CDCl₃) δ 31.50, 35.47, 35.57, 37.29, 126.22 (2×CH), 128.57 (2×CH), 141.64, 172.32.

3-(4-(*tert*-Butyl)phenyl)-*N,N*-dimethylpropanamide (**3b**)



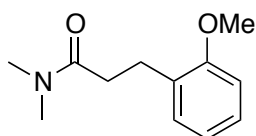
Brown solid; m.p. 68-69 °C; ¹H NMR (400 MHz, CDCl₃) δ 1.31 (s, 9H), 2.59-2.63 (m, 2H), 2.92-2.96 (m, 8H), 7.16 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 30.91, 31.53 (3×CH₃), 34.51, 35.49, 35.57, 37.29, 125.49 (2×CH), 128.20 (2×CH), 138.54, 149.05, 172.48; IR (KBr) 1639 cm⁻¹; EIMS *m/z* (relative intensity) 233 (M⁺, 89), 219 (14), 218 (86), 161 (15), 160 (22), 147 (17), 146 (18), 145 (100), 132 (14), 131 (31), 117 (38), 115 (16), 105 (12), 91 (23), 72 (25); HRMS (EI) *m/z* calcd for C₁₅H₂₃NO: 233.1780, found: 233.1786

3-([1,1'-Biphenyl]-4-yl)-*N,N*-dimethylpropanamide (**3c**)



White solid; m.p. 72-73 °C; ¹H NMR (400 MHz, CDCl₃) δ 2.64-2.68 (m, 2H), 2.96 (s, 3H), 2.97 (s, 3H), 3.00-3.04 (m, 2H), 7.29-7.35 (m, 3H), 7.41-7.45 (m, 2H), 7.52-7.61 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 31.09, 35.39, 35.60, 37.32, 127.12 (2×CH), 127.22, 127.34 (2×CH), 128.88 (2×CH), 129.01 (2×CH), 139.22, 140.78, 141.12, 172.27; IR (neat) 1636 cm⁻¹; EIMS *m/z* (relative intensity) 253 (M⁺, 7), 180 (11), 119 (35), 117 (61), 115 (59), 72 (13), 70 (19), 65 (34), 63 (100); HRMS (EI) *m/z* calcd for C₁₇H₁₉NO: 253.1467, found: 253.1460.

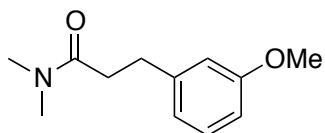
3-(2-Methoxyphenyl)-*N,N*-dimethylpropanamide (**3d**)²



Yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 2.57-2.61 (m, 2H), 2.92-2.96 (m, 8H), 3.83 (s, 3H), 6.84-6.90 (m, 2H), 7.17-7.22 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 26.82, 33.87, 35.51, 37.30, 55.33, 110.31, 120.66, 127.60, 129.80, 130.33, 157.61, 173.01.

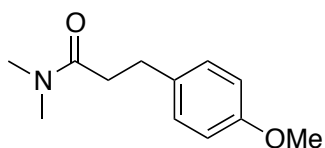
(2) Molander, G. A.; Jean-Gérald, L. *J. Org. Chem.* **2009**, *74*, 5446.

3-(3-Methoxyphenyl)-*N,N*-dimethylpropanamide (3e)



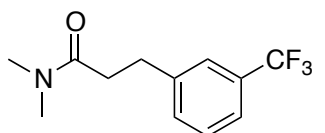
Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 2.61-2.63 (m, 2H), 2.93-2.97 (m, 8H), 3.80 (s, 3H), 6.74-6.83 (m, 3H), 7.19-7.23 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 31.56, 35.39, 35.60, 37.33, 55.32, 111.51, 114.32, 120.92, 129.60, 143.29, 159.82, 172.31; IR (neat) 1651 cm^{-1} ; EIMS m/z (relative intensity) 207 (M^+ , 27), 206 (100), 135 (12), 134 (13), 72 (13); HRMS (EI) m/z calcd for $\text{C}_{12}\text{H}_{17}\text{NO}$: 207.1259, found: 207.1256.

3-(4-Methoxyphenyl)-*N,N*-dimethylpropanamide (3f)²



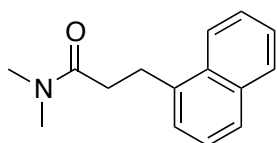
Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 2.58-2.60 (m, 2H), 2.89-2.95 (m, 8H), 3.79 (s, 3H), 6.83 (d, $J = 8.3$ Hz, 2H), 7.14 (d, $J = 8.3$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 30.63, 35.57, 35.71, 37.32, 55.40, 113.99 (2 \times CH), 129.49 (2 \times CH), 133.67, 158.08, 172.44.

N,N-Dimethyl-3-(3-(trifluoromethyl)phenyl)propanamide (3g)



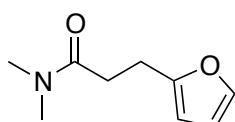
Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 2.61-2.65 (m, 2H), 2.95 (brs, 6H), 3.02-3.06 (m, 2H), 7.40-7.47 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 31.14, 34.94, 35.57, 37.24, 123.09 (d, $J_{\text{C-F}} = 3.8$ Hz), 124.30 (q, $J_{\text{C-F}} = 271.7$ Hz), 125.18 (d, $J_{\text{C-F}} = 3.9$ Hz), 128.99, 130.80 (q, $J_{\text{C-F}} = 31.8$ Hz), 132.16, 142.55, 171.67; IR (neat) 1652 cm^{-1} ; EIMS m/z (relative intensity) 245 (M^+ , 100), 226 (13), 173 (35), 172 (26), 159 (54), 153 (25), 151 (18), 133 (33), 127 (15), 119 (17), 117 (31), 115 (30), 109 (17), 103 (12), 86 (14), 73 (12), 72 (34), 65 (12), 63 (38); HRMS (EI) m/z calcd for $\text{C}_{12}\text{H}_{14}\text{F}_3\text{NO}$: 245.1027, found: 245.1206.

N,N-Dimethyl-3-(naphthalen-1-yl)propanamide (3h)



Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 2.72-2.76 (m, 2H), 2.86 (s, 3H), 2.97 (s, 3H), 3.43-3.47 (m, 2H), 7.34-7.42 (m, 2H), 7.47-7.54 (m, 2H), 7.73 (d, $J = 7.8$ Hz, 1H), 7.87 (d, $J = 7.8$ Hz, 1H), 8.06 (d, $J = 8.3$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 28.62, 34.67, 35.57, 37.23, 123.71, 125.68, 125.75, 126.15, 126.29, 127.04, 128.97, 131.81, 133.97, 137.73, 172.40; IR (neat) 1651 cm^{-1} ; EIMS m/z (relative intensity) 227 (M^+ , 91), 226 (14), 181 (13), 175 (14), 155 (46), 154 (100), 153 (73), 152 (42), 151 (12), 142 (12), 141 (79), 139 (18), 128 (23), 127 (18), 115 (39), 72 (28); HRMS (EI) m/z calcd for $\text{C}_{15}\text{H}_{17}\text{NO}$: 227.1310, found: 227.1308.

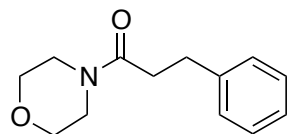
3-(Furan-2-yl)-*N,N*-dimethylpropanamide (3i)



Brown solid; m.p. 43-44 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 2.64-2.68 (m, 2H), 2.96-3.01 (m, 8H), 6.03 (d, $J = 3.7$ Hz, 1H), 6.29 (d, $J = 1.8$ Hz, 1H), 7.30 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 23.81, 31.91, 35.55, 37.19, 105.33, 110.36, 141.11, 155.13, 171.78; IR (neat) 1654 cm^{-1} ; EIMS m/z (relative intensity) 167 (M^+ , 100), 95 (13), 94 (25), 81 (26), 72 (26);

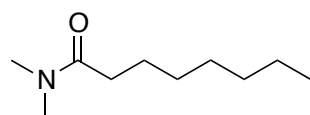
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1-Morpholino-3-phenylpropan-1-one (3j)



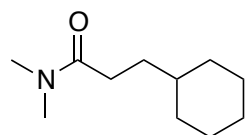
Yellow oil; 1H NMR (400 MHz, $CDCl_3$) δ 2.60-2.64 (m, 2H), 2.96-3.00 (m, 2H), 3.35-3.37 (m, 2H), 3.50-3.52 (m, 2H), 3.58-3.65 (m, 4H) 7.21-7.31 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.60, 34.95, 42.06, 46.09, 66.59, 66.98, 126.41, 128.59 (2 \times CH), 128.68 (2 \times CH), 141.18, 171.00; IR (neat) 1644 cm^{-1} ; EIMS m/z (relative intensity) 219 (98), 133 (15), 128 (31), 105 (83), 104 (45), 103 (18), 91 (100), 88 (11), 87 (33), 86 (28), 79 (12), 78 (15), 77 (27), 65 (12), 63 (28), 57 (28), 56 (16), 51 (10); HRMS (EI) m/z calcd for $C_{13}H_{17}NO_2$: 219.1259, found: 219.1267.

N,N-Dimethyloctanamide (3k)



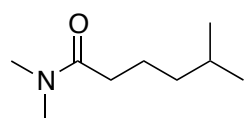
Yellow oil; 1H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, J = 6.8 Hz, 3H), 1.28-1.32 (m, 8H), 1.61-1.65 (m, 2H), 2.29-2.32 (m, 2H), 2.94 (s, 3H), 3.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.22, 22.75, 25.32, 29.25, 29.61, 31.85, 33.56, 35.47, 37.43, 173.41; IR (neat) 1659 cm^{-1} ; EIMS m/z (relative intensity) 171 (M^+ , 10), 100 (25), 87 (100), 85 (41), 83 (62), 72 (32), 57 (11); HRMS (EI) m/z calcd for $C_{10}H_{21}NO$: 171.1623, found: 171.1630.

3-Cyclohexyl-*N,N*-dimethylpropanamide (3l)



Yellow oil; 1H NMR (400 MHz, $CDCl_3$) δ 0.86-0.95 (m, 2H), 1.12-1.28 (m, 4H), 1.50-1.57 (m, 2H), 1.60-1.74 (m, 5H), 2.30-2.34 (m, 2H), 2.94 (s, 3H), 3.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.41, 26.71 (2 \times CH₂), 31.07, 32.73, 33.28 (2 \times CH₂), 35.52, 37.44, 37.60, 173.70; IR (neat) 1652 cm^{-1} ; EIMS m/z (relative intensity) 183 (M^+ , 8), 100 (36), 68 (100), 25 (36), 55 (17); HRMS (EI) m/z calcd for $C_{11}H_{21}NO$: 183.1623, found: 183.1623.

N,N-Dimethyl-5-methylhexanamide (3m)

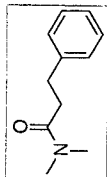


Yellow oil; 1H NMR (400 MHz, $CDCl_3$) δ 0.80-0.95 (m, 5H), 1.19-1.24 (m, 2H), 1.53-1.67 (m, 4H), 2.27-2.31 (m, 2H), 2.94 (s, 3H), 3.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.69 (2 \times CH₃), 23.19, 28.06, 33.79, 35.48, 37.43, 38.91, 173.39; IR (neat) 1651 cm^{-1} ; EIMS m/z (relative intensity) 157 (M^+ , 16), 114 (19), 100 (17), 87 (100), 72 (44), 63 (16); HRMS (EI) m/z calcd for $C_9H_{19}NO$: 157.1467, found: 157.1460.



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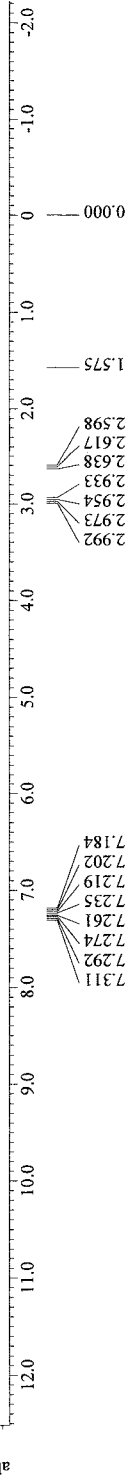
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8.036

2.000

6.857

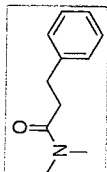


X: parts per Million - Proton



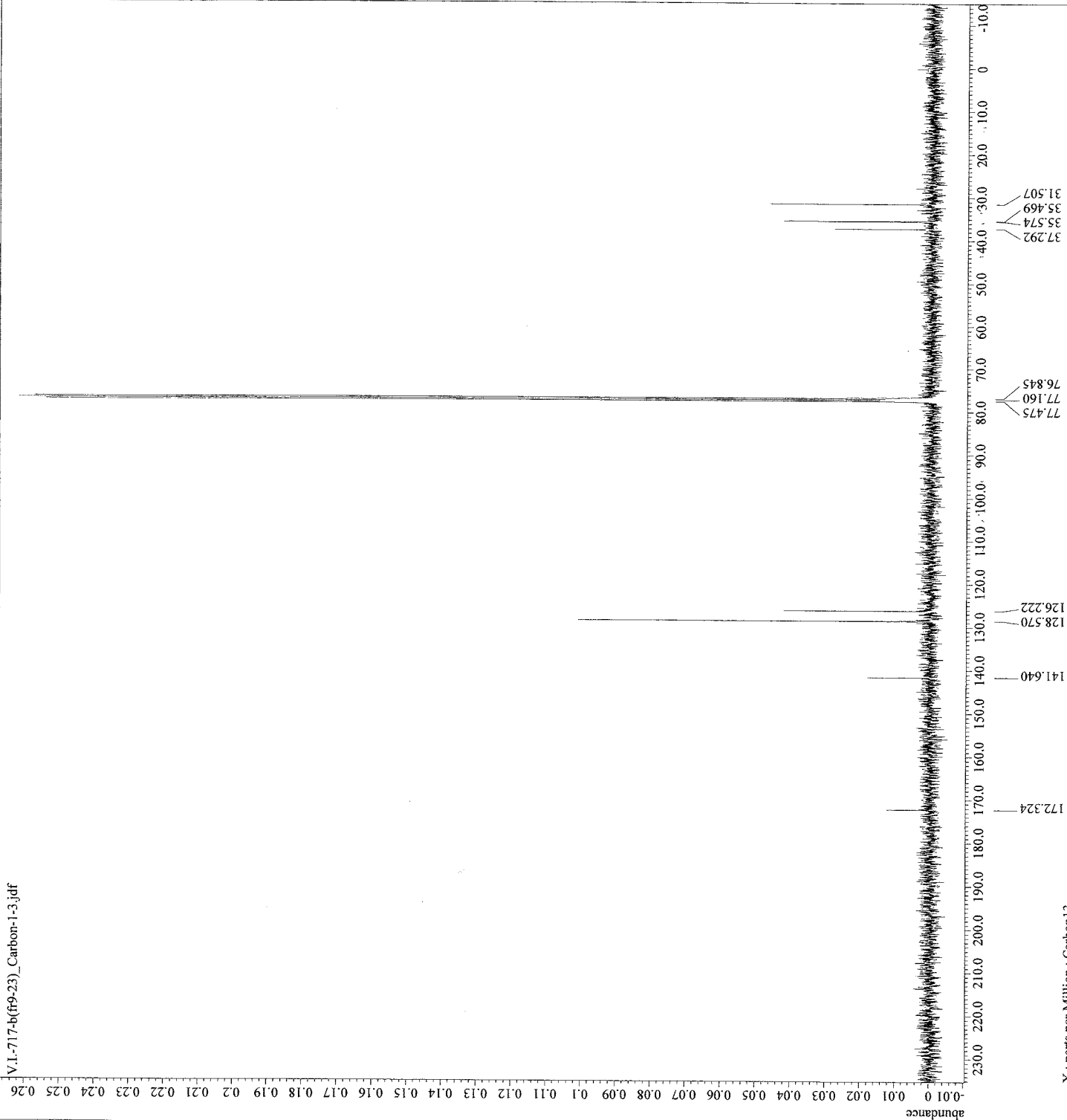
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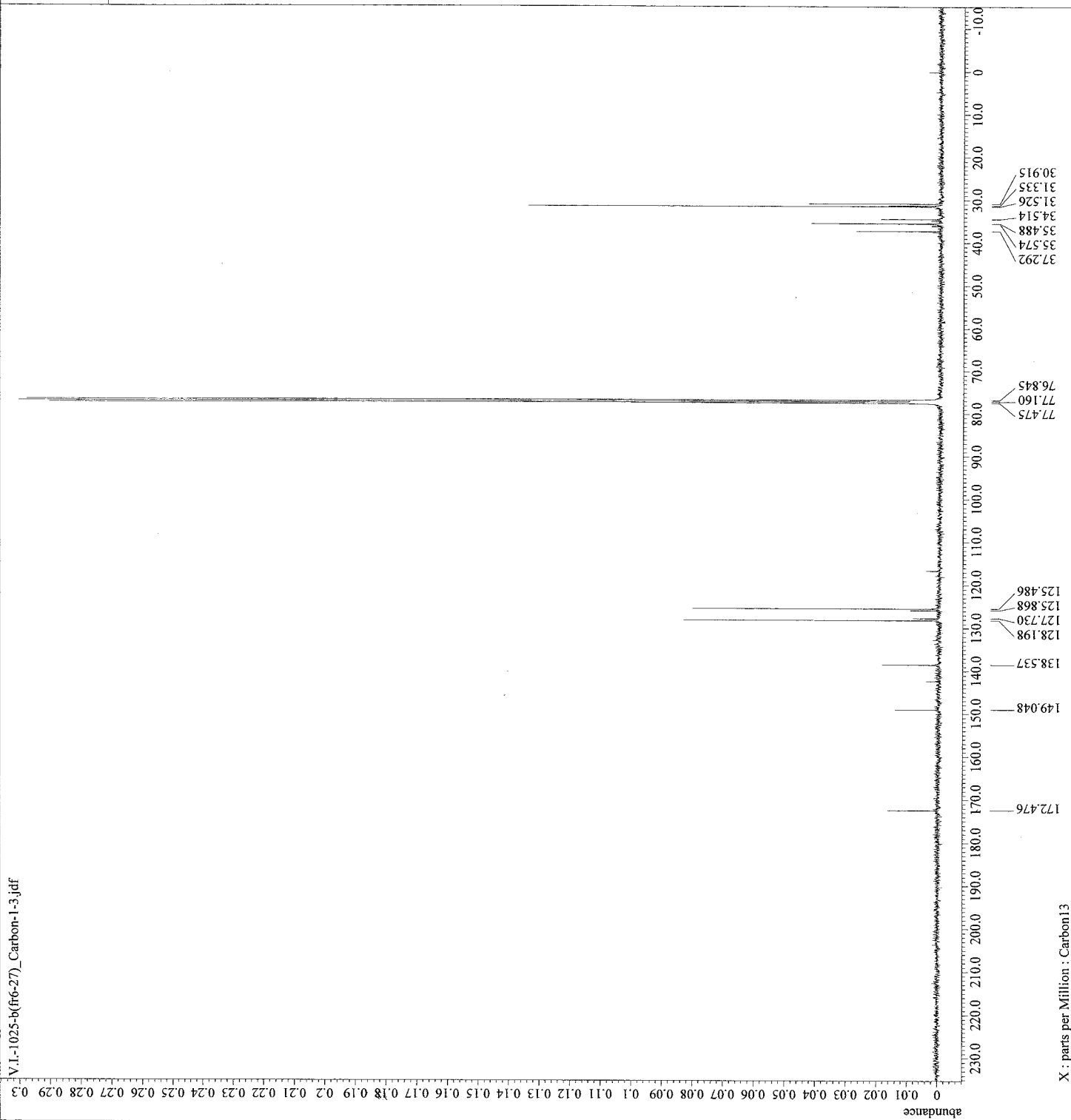
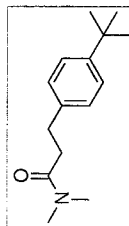
X: parts per Million : Carbon13

V.I.-717-b(f9-23)_Carbon-1-1.jdf



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Relaxation_Delay = 2[s]
Recycle_Delay = 5[s]
Temp_Gst = 21.5[ac]
X_90_Width = 8.75[us]
X_AcqTime = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 5.2[db]
X_Pulse_Dec = 23.966667[us]
Irr_Atn_Nee = 22.691[db]
Irr_Noise = WALNZ
Irr_Width = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe_Time = 2[s]
Repetition_Time = 3.03809024[s]
    
```



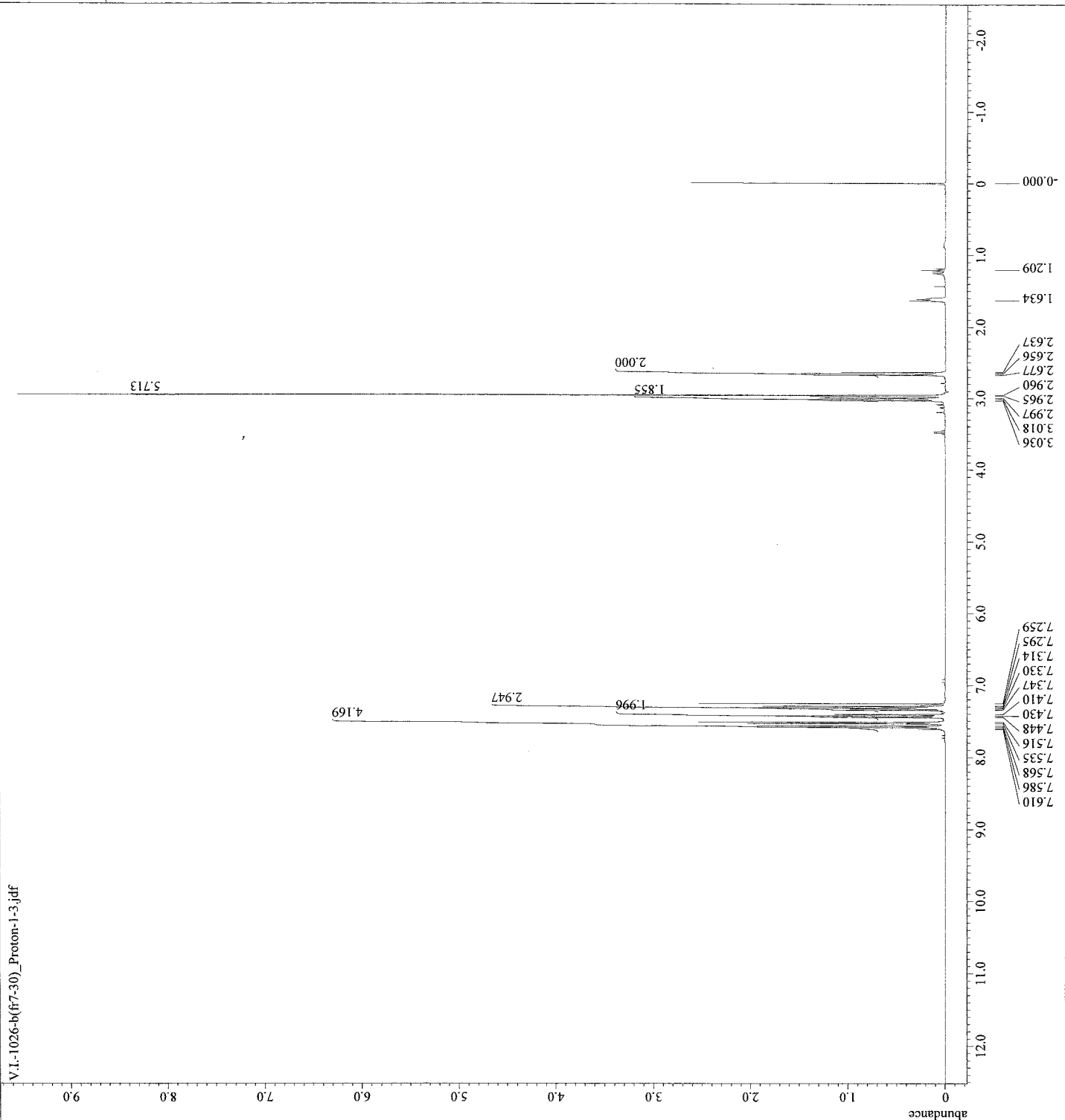
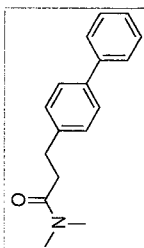
X : parts per Million : Carbon13

V.I.-1025-b(f6-27)_Carbon-1-3.jdf



```

Filename = \\Users\delta\Documents\JBO
Author = delta
Experiment = proton_3xp
Sample_Id = V.I.-1026-b(ff7-30)
Solvent = CHLOROFORM-D
Acquisition_Time = 27-SEP-2012 09:58:31
Reason_Time = 27-SEP-2012 09:58:31
Current_Time = 27-SEP-2012 09:58:43
Comment = single_pulse
Data_Format = 1D_COMPLEX
Dim_Size = 13107
Dim_Units = Proton
Dim_Values = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.4249661[T] (400[MHz])
Freq = 21.757952[Hz]
X_Freq = 401.28219856[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Frescans = 1
X_Resolution = 0.45960208[Hz]
X_Sweep = 1.570436[MHz]
X_Sweep_Clippped = 6.0240659[MHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 401.28219856[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
NUC1 = 13C
X_90_Sch = 9.25[us]
X_Acq_Time = 2.1757952[s]
X_Angle = 45[deg]
X_Attn = 0.8[db]
X_Pulse = 4.625[us]
Irr_Mode = Off
Irr_Pulse = 4.625[us]
Irr_Press = FALSE
Data_Press = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.1757952[s]
    
```



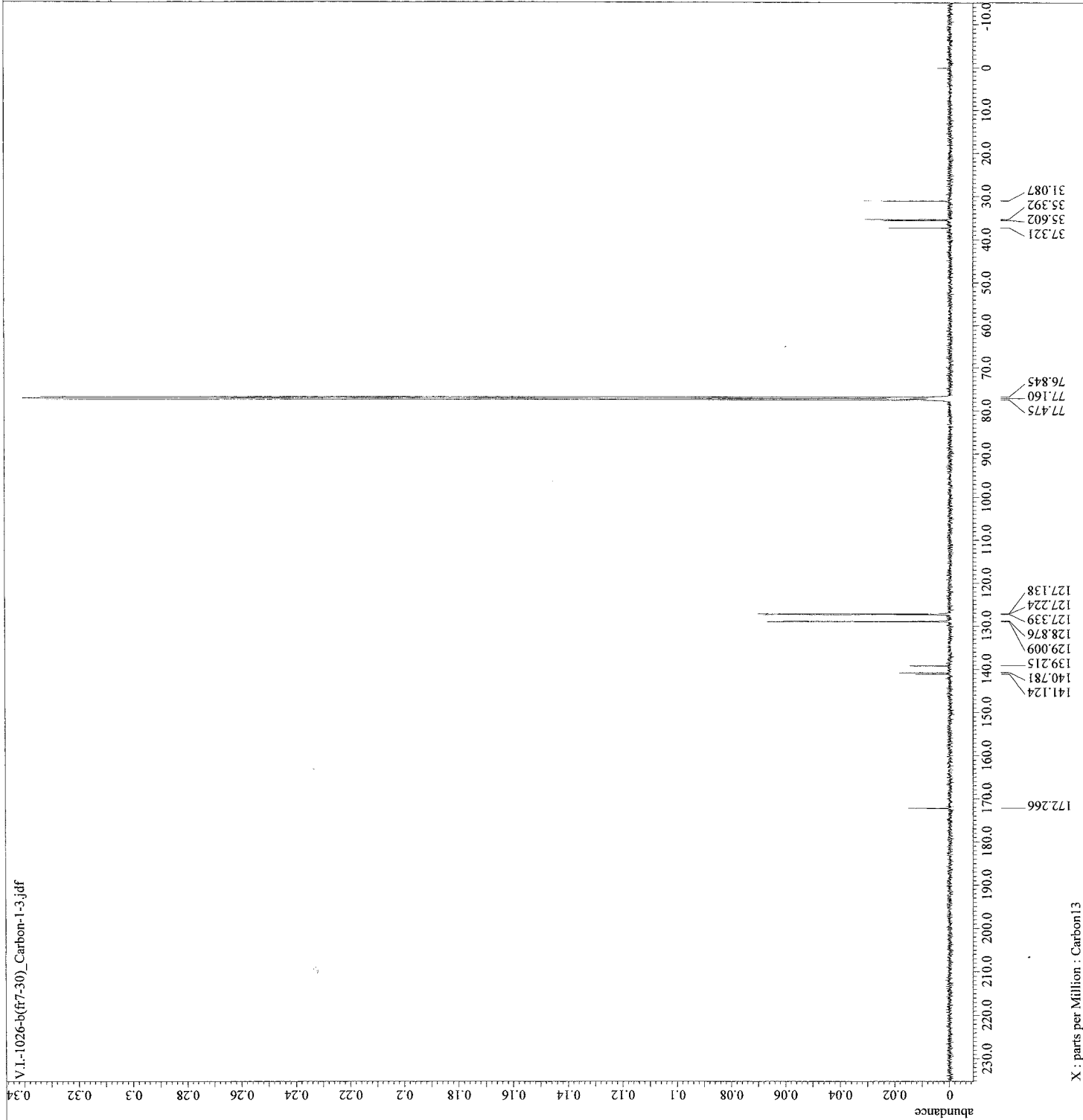
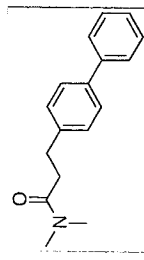
V.I.-1026-b(ff7-30)_Proton-1-3.jdf

X: parts per Million : Proton



```

Filename = \Users\delta\Documents\JEO
Author = delta
Experiment = carbon.jxp
Sample_Id = V.I.-1026-b(fr7-30)
Solvent = CHLOROFORM-d
Acquisition_Time = 27-SEP-2012 08:09:08
Revelation_Time = 27-SEP-2012 10:03:20
Current_Time = 27-SEP-2012 10:04:08
Comment = single pulse decoupled gat
Data_Format = ID COMPLEX
Dat_Size = 28214
F1 = 125.761
Dim_Units = ppm
Dimensions = X
Site = JNM-ECX400
Spectrometer = DELTA2_NMR
Field_Strength = 9.42496681[T] (400[MHz])
X_Duration = 1.03809024[s]
X_Freq = 100.90247863[MHz]
X_Offset = 110[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.6310798[Hz]
X_Sweep = 31.5585657[Hz]
X_Sweep_Clipped = 25.25252525[MHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recovery_Delay = 50
Recovery_Gain = 21.2[ac]
Temp_Get = 8.75[us]
X_90_Width = 1.03809024[s]
X_Acq_Time = 3[s]
X_Pulses = 5.2[db]
X_Pulse = 2.91666667[us]
Irr_Atn_Dec = 22.691[db]
Irr_Atn_Noise = 22.691[db]
Irr_Noise = WALTZ
Irr_Width = 0.115[ms]
Recycling_Delay = 1[s]
Initial_Heat = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.03809024[s]
    
```

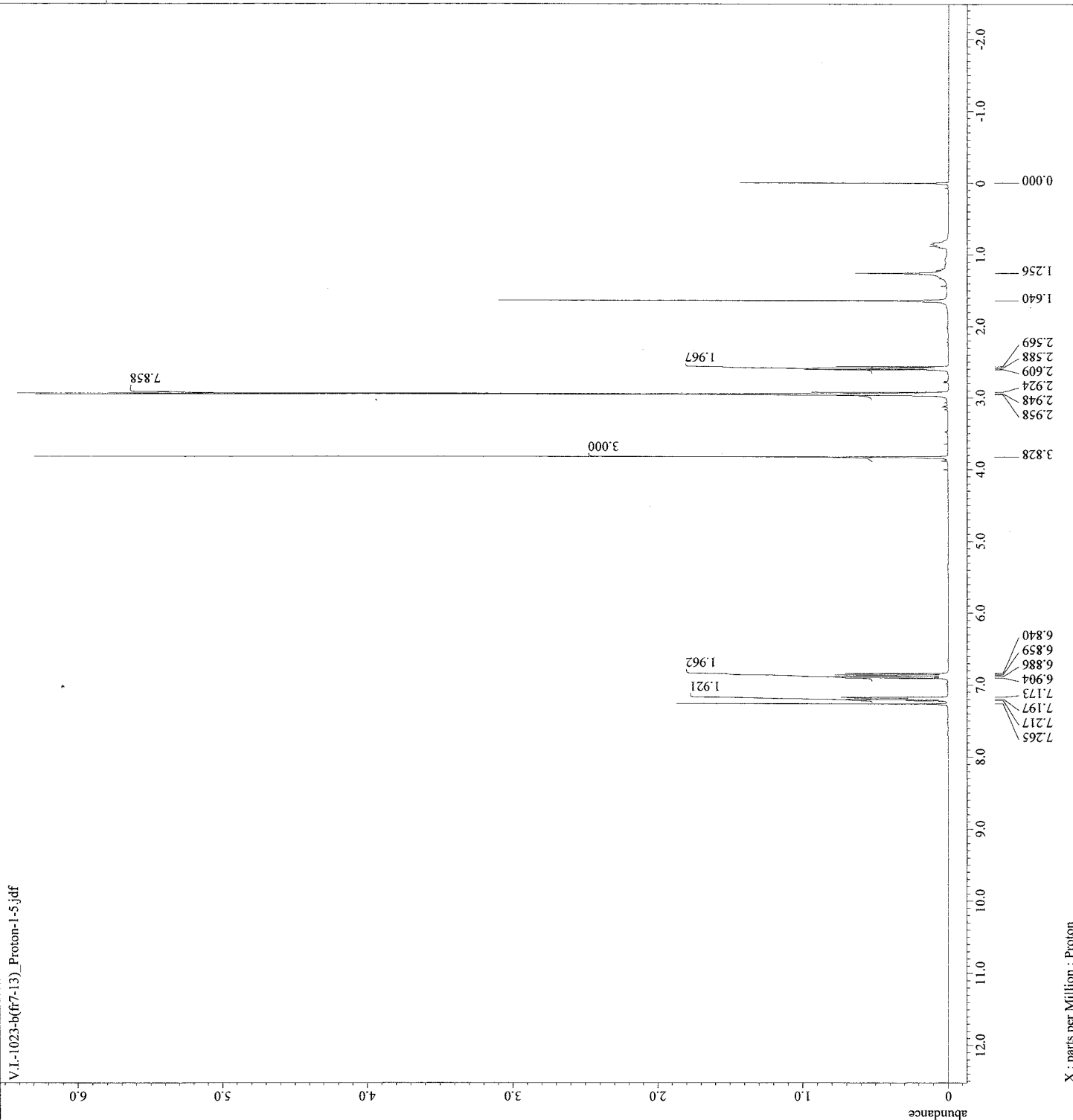
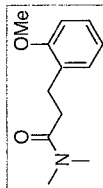


X : parts per Million : Carbon13



```

Filename = \\Users\delta\Documents\JEO
Author = delta
Experiment = proton_jmp
Sample_Id = V.I.-1023-b(fr7-13)
ConvTime = 20:36:34
Current_Time = 24-SEP-2012 21:05:04
Revision_Time = 24-SEP-2012 21:05:04
Current_Time = 24-SEP-2012 21:05:18
Comment = single_pulse
Date_Format = DD_COMPLEX
Dim_Units = ppm
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA_XMR
Field_Strength = 9.4249681 [T] (400 [MHz])
X_Acq_Duration = 2.1757952 [s]
X_Domain = 1H
X_Freq = 401.28219856 [MHz]
X_Offset = 5 [ppm]
X_Points = 16384
X_Prescans = 6
X_Resolution = 0.4594008 [Hz]
X_Sweep = 7.53012048 [kHz]
X_Sweep_Clippped = 6.02409639 [kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856 [MHz]
Irr_Offset = 5 [ppm]
Tri_Domain = Proton
Tri_Freq = 401.28219856 [MHz]
Tri_Offset = 5 [ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5 [s]
AcqGain = 16
RG = 26 [dc]
X_90_Width = 9.25 [us]
X_Acq_Time = 2.1757952 [s]
X_Angle = 45 [deg]
X_Atn = 0.8 [dB]
X_Pulse = 4.625 [us]
Irr_Mode = Off
Tri_Mode = Off
DANTE_Presat = FALSE
Initial_Wait = 1 [s]
Repetition_Time = 7.1757952 [s]
    
```



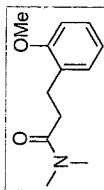
V.I.-1023-b(fr7-13)_Proton-1-5.jdf

X : parts per Million : Proton

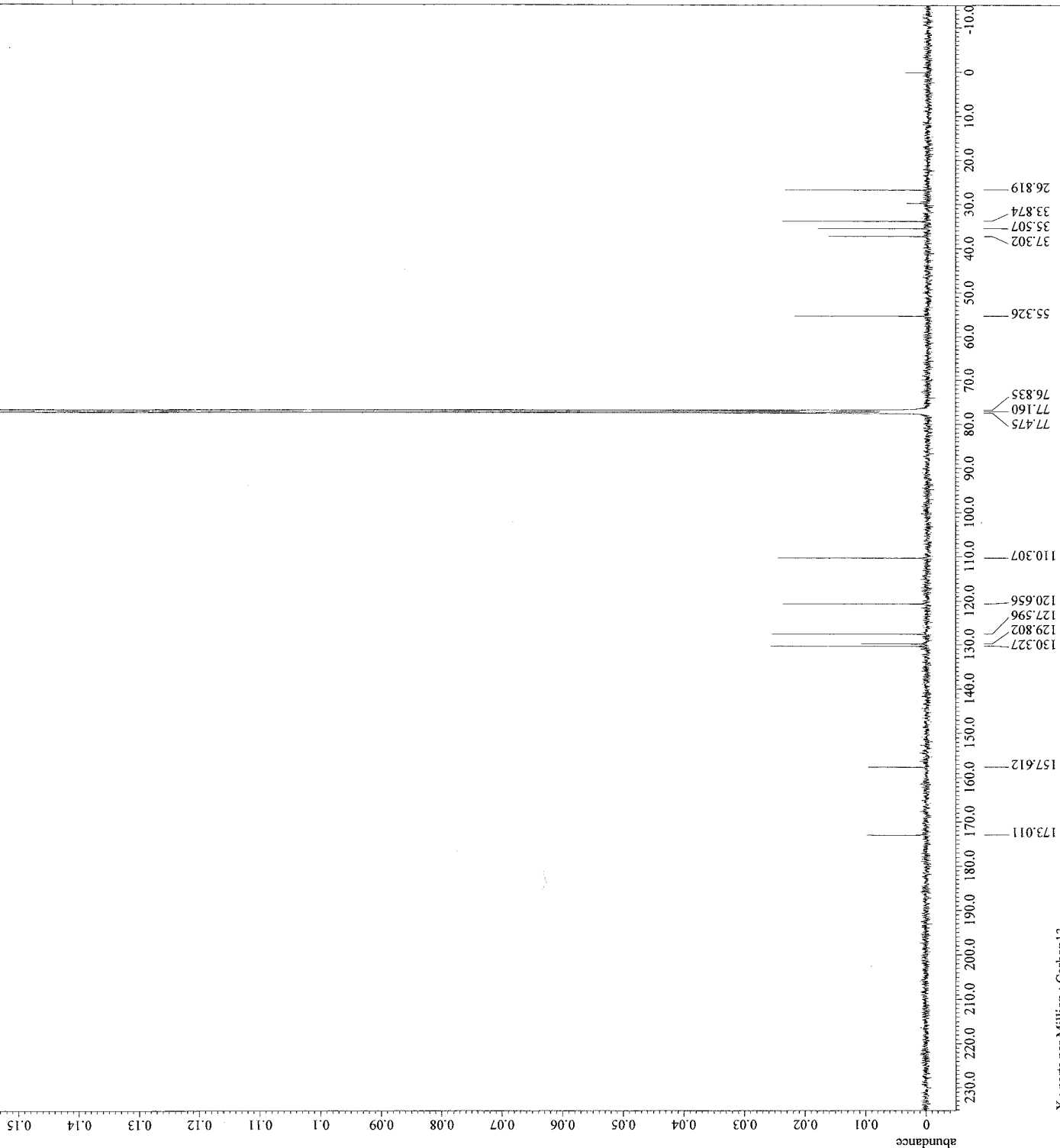


```

Filename = \Users\delta\Documents\JRCO
Author = delta
Experiment = carbon.jxp
Sample_Id = V.I.-1023-b(fr7-13)
Solvent = CHLOROFORM-D
Acquisition_Time = 25-SEP-2012 09:03:44
Revelation_Time = 25-SEP-2012 11:34:37
Current_Time = 25-SEP-2012 11:35:33
Comment = single pulse decoupled gat
Data_Format = ID COMPLEX
Dm_Size = 68214
Dm_Units = Carbon13
Dm_Inits = [ppm]
Dimensions = X
Site = JNM-RCS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.4498681 [T] (400 [MHz])
X_Coupling = 1.03809024 [s]
X_Domain = 13c
X_Freq = 100.90247863 [MHz]
X_Offset = 110 [ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.9630738 [Hz]
X_Sweep = 1.865 [Hz]
X_Sweep_Clippped = 25.25252525 [kHz]
IR_Domain = Proton
IR_Freq = 401.28219856 [MHz]
IR_Offset = 5 [ppm]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2 [s]
Recvr_Gain = 50
Temp_Get = 21.5 [dc]
X_90_Width = 8.75 [us]
X_Acq_Time = 3.03809024 [s]
X_Angle = 1 [us]
X_Pulse = 5 [dB]
X_Pulse_Program = 2.91666667 [us]
IR_Atn_Dec = 22.691 [dB]
IR_Atn_Noise = 22.691 [dB]
IR_Noise = WALZ
IR_Width = 0.115 [ms]
Decoupling = 1 [s]
Isolator_Heat = TRUE
Noe_Time = 2 [s]
Repetition_Time = 3.03809024 [s]
    
```



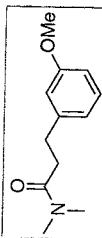
V.I.-1023-b(fr7-13)_Carbon-1-3.jdf



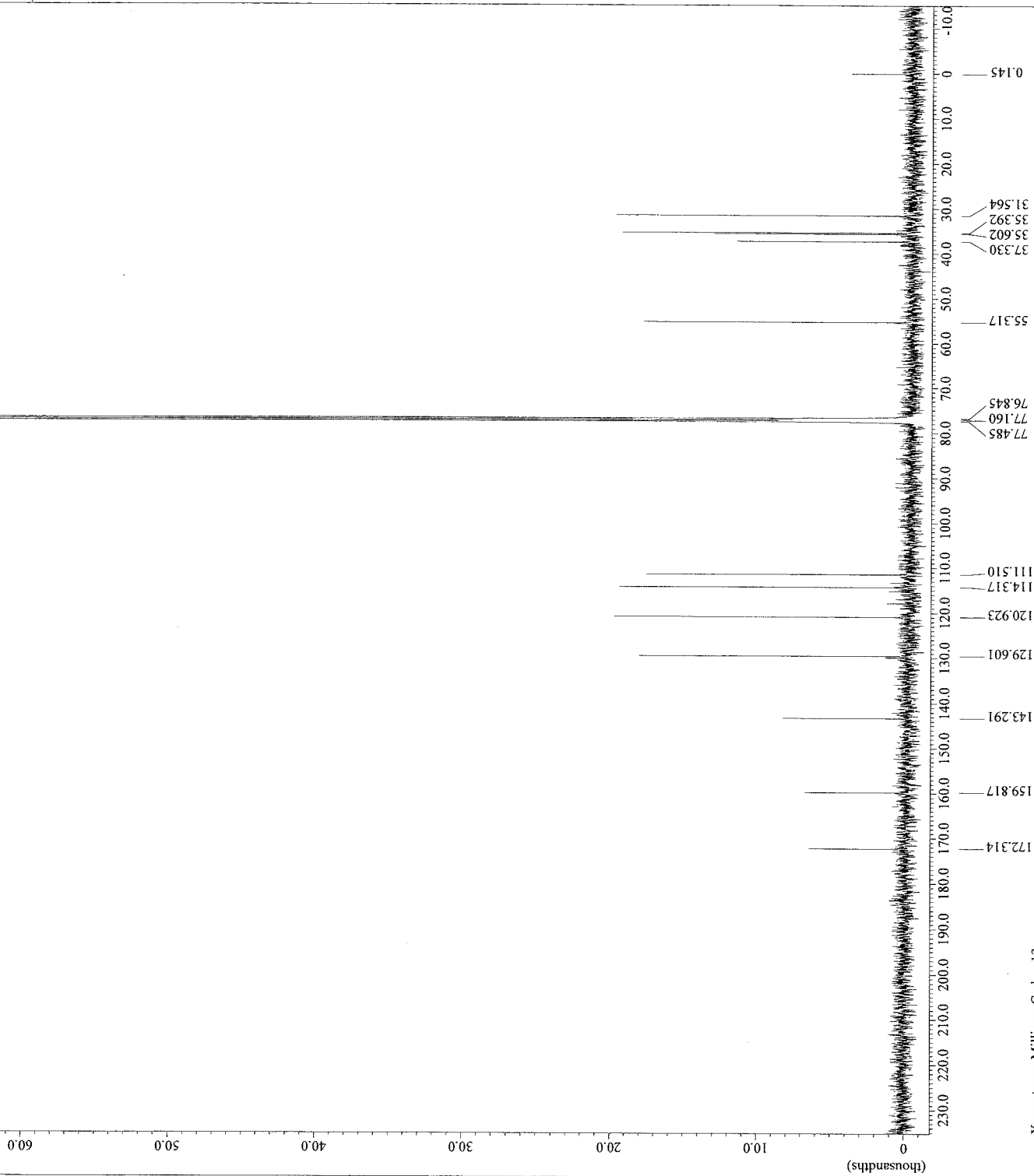
X : parts per Million : Carbon13



Filename = \Users\deltaelta\Documents\JBO
Author = delta
Experiment = CHLORFORM-D
Sample_Id = V.L.1024-b(f13-30)
Solvent = CHLORFORM-D
Creation_Time = 25-SEP-2012 06:35:04
Revision_Time = 25-SEP-2012 11:35:52
Current_Time = 25-SEP-2012 11:37:06
Comment = single pulse decoupled gat
ID = COPE2BK
Date_Format = 26214
Date_Size = Carbon13
Dim_Title = [ppm]
Dimensions = X
Site = JNM-EC5400
Spectrometer = DELTA2_NMR
Field_Strength = 9.4249681 [T] (400 [MHz])
X_Acq_Duration = 1.03809024 [s]
X_Domain = 13C
X_Freq = 100.90247863 [MHz]
X_Offset = 110 [ppm]
X_Pulses = 32768
X_Pulses_Programs = 4
X_Resolution = 0.96330739 [Hz]
X_Sweep = 31.56565657 [kHz]
X_Sweep_Clip = 25.25252525 [kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856 [MHz]
Irr_Offset = 1 [ppm]
Irr_Pulses = 4096
Irr_Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2 [s]
Recov_Gain = 50
X1_Offset = 1 [dC]
X1_Pulses = 675 [us]
X1_Scans = 1.03809024 [s]
X1_Acq_Time = 30 [deg]
X1_Angle = 5.2 [dB]
X1_Atn = 2.91666667 [us]
X1_Pulse_Programs = 22.691 [dB]
Irr_Atn_Dec = 22.691 [dB]
Irr_Atn_Res = 22.691 [dB]
Irr_Atn_Min = 22.691 [dB]
Irr_Width = 0.115 [ms]
Decoupling = TRUE
Initial_Wait = 1 [s]
Noe = TRUE
Noe_Time = 2 [s]
Repetition_Time = 3.03809024 [s]



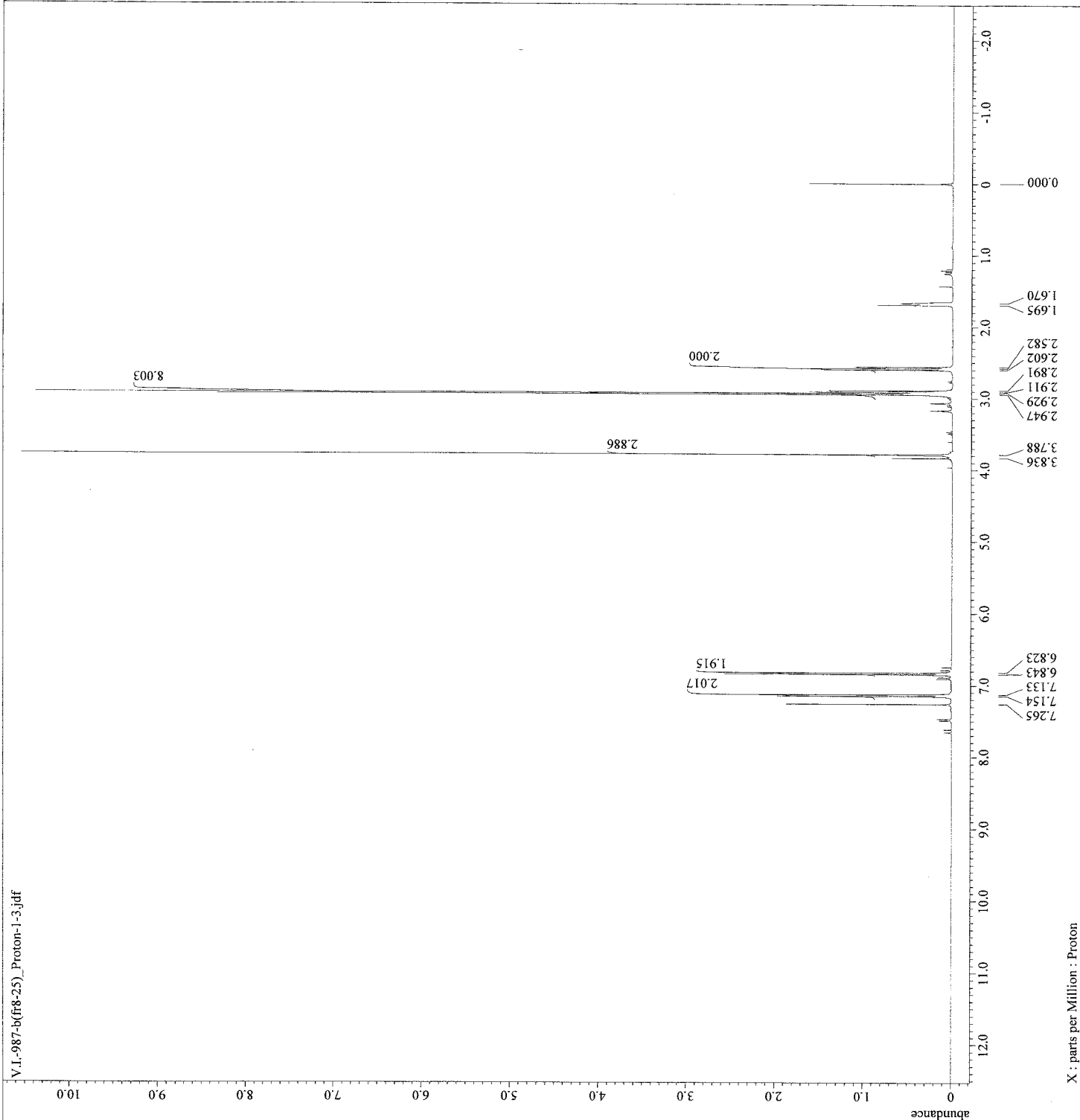
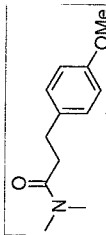
V.L.1024-b(f13-30)_Carbon-1-3.jdf





```

File Name = \Users\delta\Documents\JEO
Author = delta
Experiment = proton.jxp
Sample Id = V.I.-987-b(fr8-25)
Solvent = CHLOROFORM-D
Creation Time = 7-SEP-2012 22:18:07
Revision Time = 7-SEP-2012 22:13:51
Current Time = 7-SEP-2012 22:16:05
Comment = single pulse
Data Format = 1D COMPLEX
Dir Size = 13107
Dir Title =
Dir Units = Proton
Dimensions = X(ppm)
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field Strength = 9.42499681[T] (400[MHz])
X_AcqDuration = 2.1757952[s]
X_F1_Freq = 401.28219856[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45960208[Hz]
X_Sweep Clipped = 7.53012048[MHz]
X_Time Domain = 6.02409659[MHz]
X_F2_Domain = 6.02409659[MHz]
X_Ir_Freq = 401.28219856[MHz]
X_Ir_Offset = 5[ppm]
X_Tri_Domain = Proton
X_Tri_Freq = 401.28219856[MHz]
X_Tri_Offset = 5[ppm]
X_Shaped Pulse = FIDSE
Total Scans = 16
Relaxation Delay = 5[s]
Recvr Gain = 44
Temp_Get = 21.7[dc]
X_30_Acch = 2.25[us]
X_Cycle Time = 4.45[sec]
X_Angle = 45[deg]
X_Atn = 0.8[db]
X_Pulse = 4.625[us]
X_Mode = Off
Tri Mode = Off
Pulse_Program = FIDSE
Data_Recv = 1
Repetition Time = 7.1757952[s]
    
```



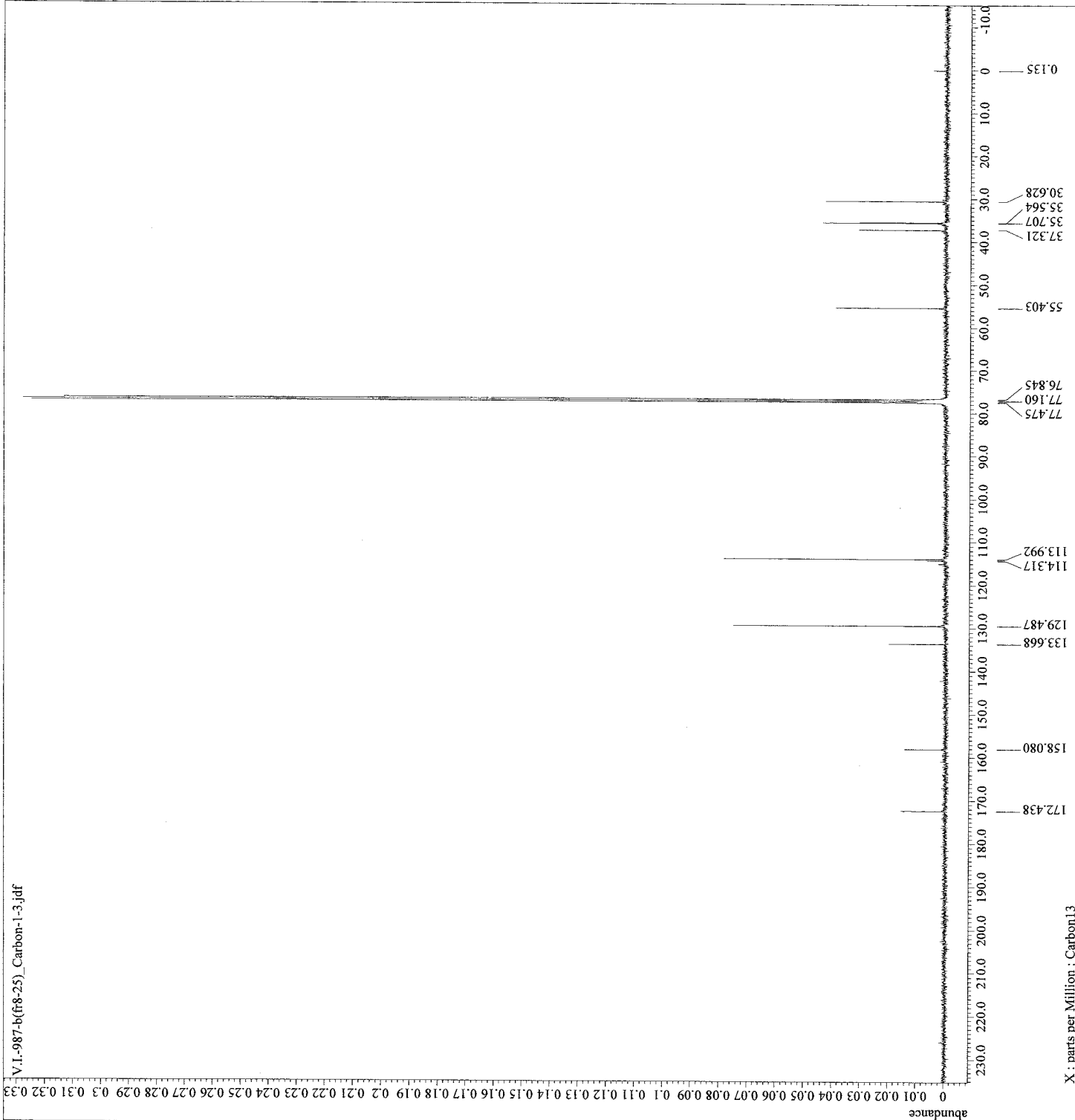
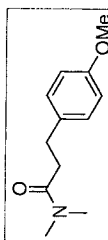
X: parts per Million : Proton

V.I.-987-b(fr8-25)_Proton-1-3.jdf



```

Filename = \\Users\delta\Documents\JEO
Author = delta
Experiment = carbon_jkp
Sample_Id = V.I.-987-b(fr8-25)
Solvent = CHLOROFORM-D
Revision_Time = 8-SEP-2012 13:35:04
Current_Time = 8-SEP-2012 13:35:54
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_1_Size = 2624
Dim_2_Size = 65536
Dim_Units = ppm
Dimensions = X
Site = JNM-EC5400
Spectrometer = DELTA2_NMR
Field_Strength = 400.1363631 [T] (400.1363631 MHz)
X_Domain = 13C
X_Freq = 100.6251250024 [s]
X_Offset = 100.90247863 [MHz]
X_Points = 110 [ppm]
X_Rescans = 32768
X_Resolution = 4
X_Sweep = 9.6330798 [Hz]
X_Sweep_Clip = 25.25252525 [MHz]
X_Sweep_Clipped = Proton
Irr_Domain = Proton
Irr_Freq = 401.28219856 [MHz]
Irr_Offset = 5 [ppm]
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2 [s]
Recvr_Gain = 50
Temp_Get = 22.1 [dC]
X_90_Width = 8.75 [us]
X_Acq_Time = 3.03809024 [s]
X_Cycle = 30 [deg]
X_Pn = 5 [2 dB]
X_Pulse = 2.91666667 [us]
Irr_Atn_Dec = 22.691 [dB]
Irr_Atn_Noise = 22.691 [dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115 [ms]
Spectral_Width = 114
Initial_Wat = 1 [s]
Noe_Time = TRUE
Repetition_Time = 3.03809024 [s]
    
```



X: parts per Million : Carbon13

V.I.-987-b(fr8-25)_Carbon-1-3.jdf



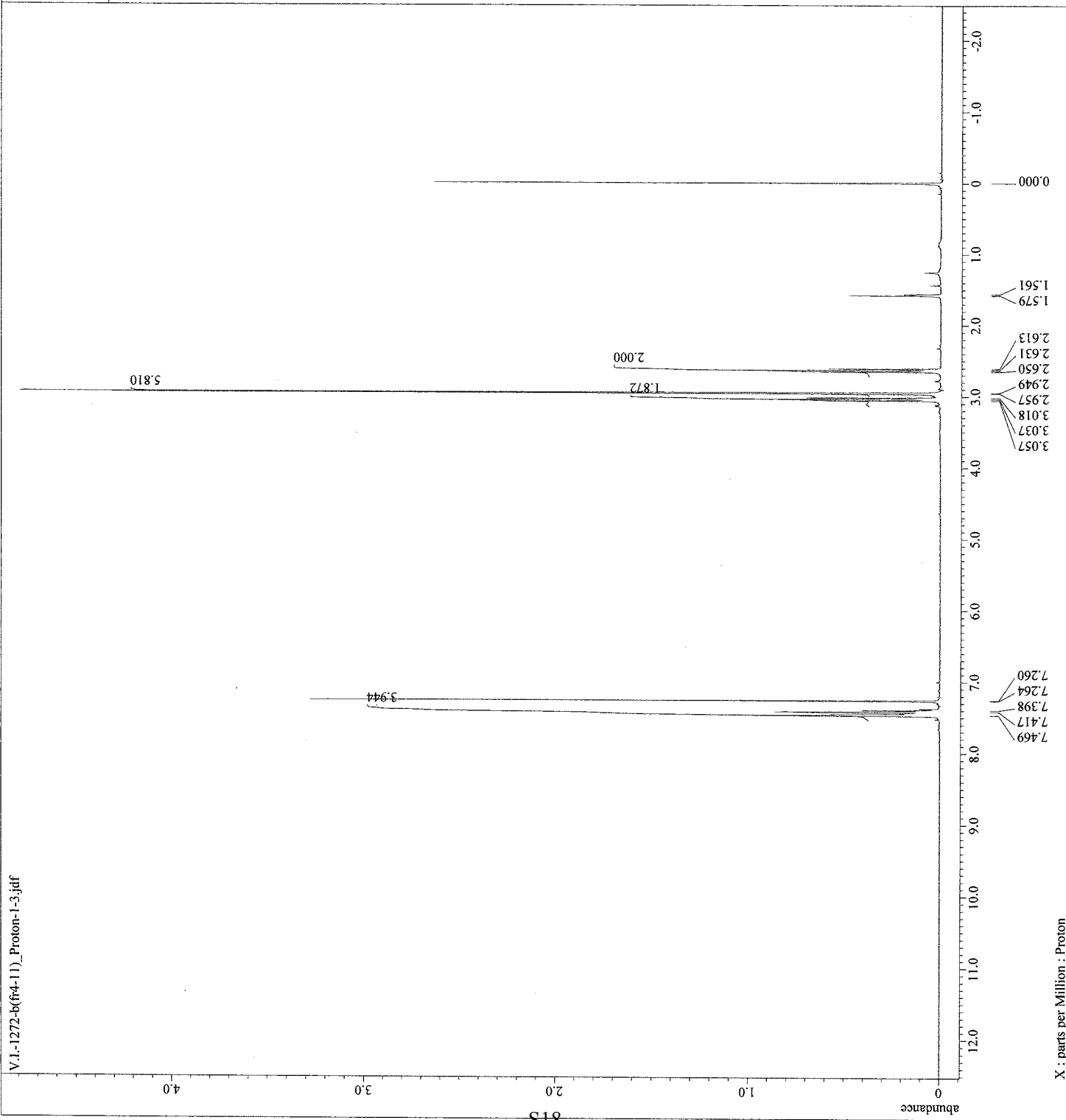
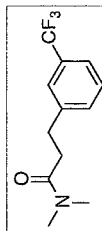
```

Filename = \\Users\delta\Documents\JEO
Author = delta
Experiment = proton.jpg
Sample_Id = V.I.-1272-b(fr4-11)
Solvent = CHLOROFORM-D
Creation_Time = 20-JAN-2013 21:40:41
Revision_Time = 20-JAN-2013 21:41:37
Current_Time = 20-JAN-2013 21:42:03

Comment = single_pulse
Data_Fomat = 15
Data_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECX400
Spectrometer = DELTA2_NMR

Field_Strength = 9.4249681[T] (400[Mhz])
X_Acq_Duration = 2.1757952[s]
X_Domain = 1H
X_Freq = 401.28219856[Mhz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.4566208[Hz]
X_Sweep_Clippped = 7.5302048[Mhz]
X_Sweep_Domain = 6.02409639[Mhz]
X_Sweep_Offset = 401.28219856[Mhz]
X_Sweep_Width = 5[ppm]
T1_Domain = Proton
T1_Offset = 5[ppm]
T1_Freq = 401.28219856[Mhz]
T1_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16

Relaxation_Delay = 5[s]
Recvr_Gain = 52
Temp_Get = 19.8[degC]
X_90_Width = 9.25[us]
X_Acq_Time = 2.1757952[s]
X_Angle = 45[deg]
X_Azn = 0.8[deg]
X_Pulse = 4.625[us]
X_Mode = CF
X_Prog = CF
Pulse_Program = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.1757952[s]
    
```



X : parts per Million : Proton

V.I.-1272-b(fr4-11)_Proton-1-3.jdf



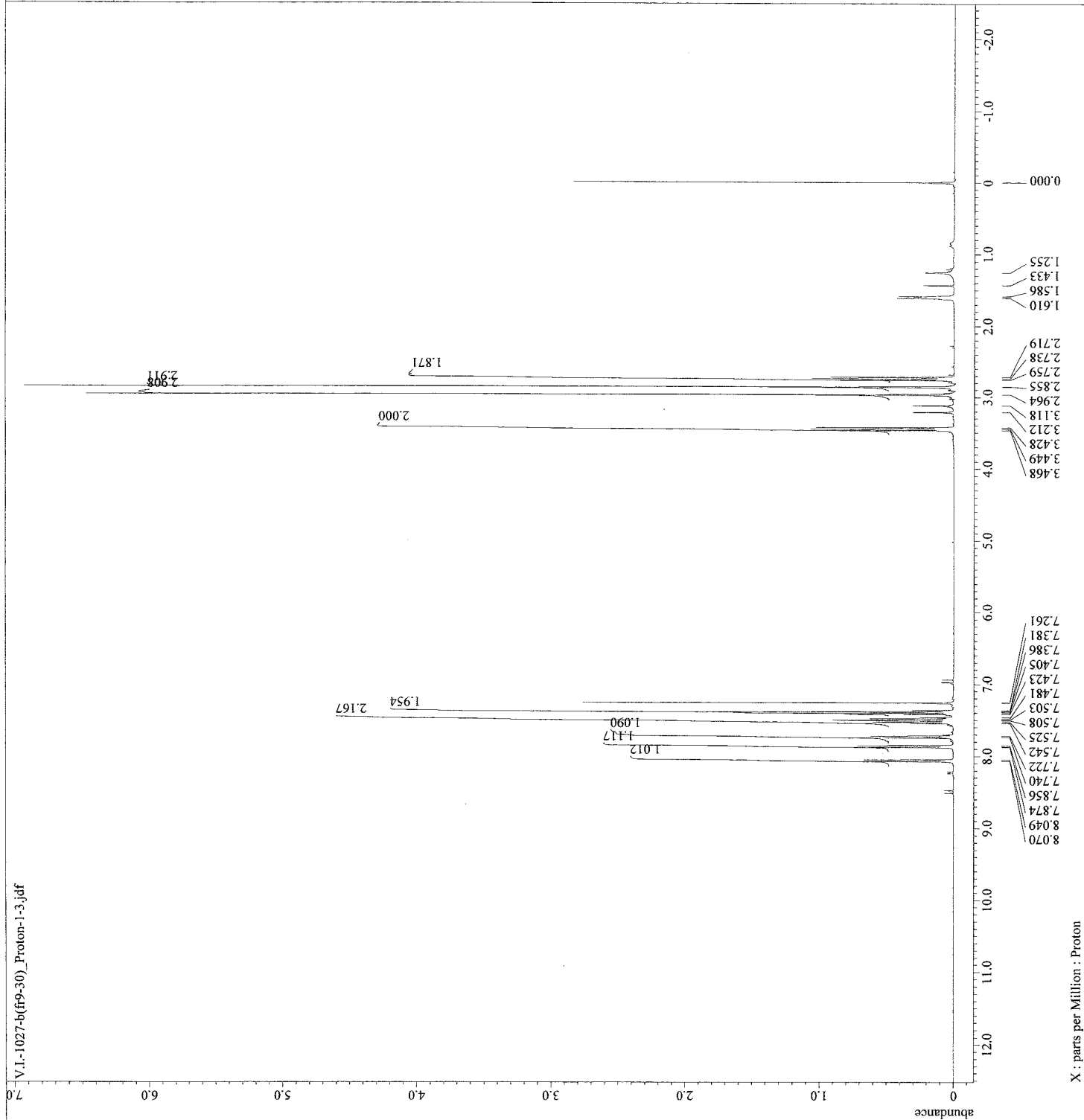
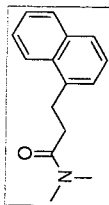
```

Filename = \Users\delta\Documents\VEO
Author = delta
Experiment = prcton.jpg
Sample_Id = V.1-1027-b(ff9-30)
Solvent = CHLOROFORM-D
Acquisition_Time = 27-SEP-2012 04:11:57
Relaxation_Time = 27-SEP-2012 10:00:00
Current_Time = 27-SEP-2012 10:00:17

Comment = single_pulse
Data_Format = ID COMPLEX
Data_Size = 83107
Dimensions = 1D
Site = JNM-ECS400
Spectrometer = DELTA2_NMR

Field_Strength = 9.42498681[T] (400[MHz])
Acquisition = 2.1757952[s]
X_Domain = 1H
X_Freq = 401.28219856[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Frescans = 1
X_Resolution = 0.45566208[Hz]
X_Sweep_Rate = 0.00000000[Hz]
X_Sweep_Clippped = 6.02409639[MHz]
IRF_Domain = Proton
IRF_Freq = 401.28219856[MHz]
IRF_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 401.28219856[MHz]
Sweep_Offset = 5[ppm]
Clipped = RMSSE
Scans = 16
Total_Scans = 16

Relaxation_Delay = 5[s]
Recov_Gain = 48
Temp = 4[degC]
X_90_Width = 9.25[us]
X_Acq_Time = 2.1757952[s]
X_Angle = 45[deg]
X_Atn = 0.8[db]
X_Pulse = 4.625[us]
IRF_Mode = Cirf
IRF_Pulse = 4.625[us]
IRF_Offset = RMSSE
Initial_Wait = 1[s]
Repetition_Time = 7.1757952[s]
    
```



V.1-1027-b(ff9-30)_Proton-1-3.jdf



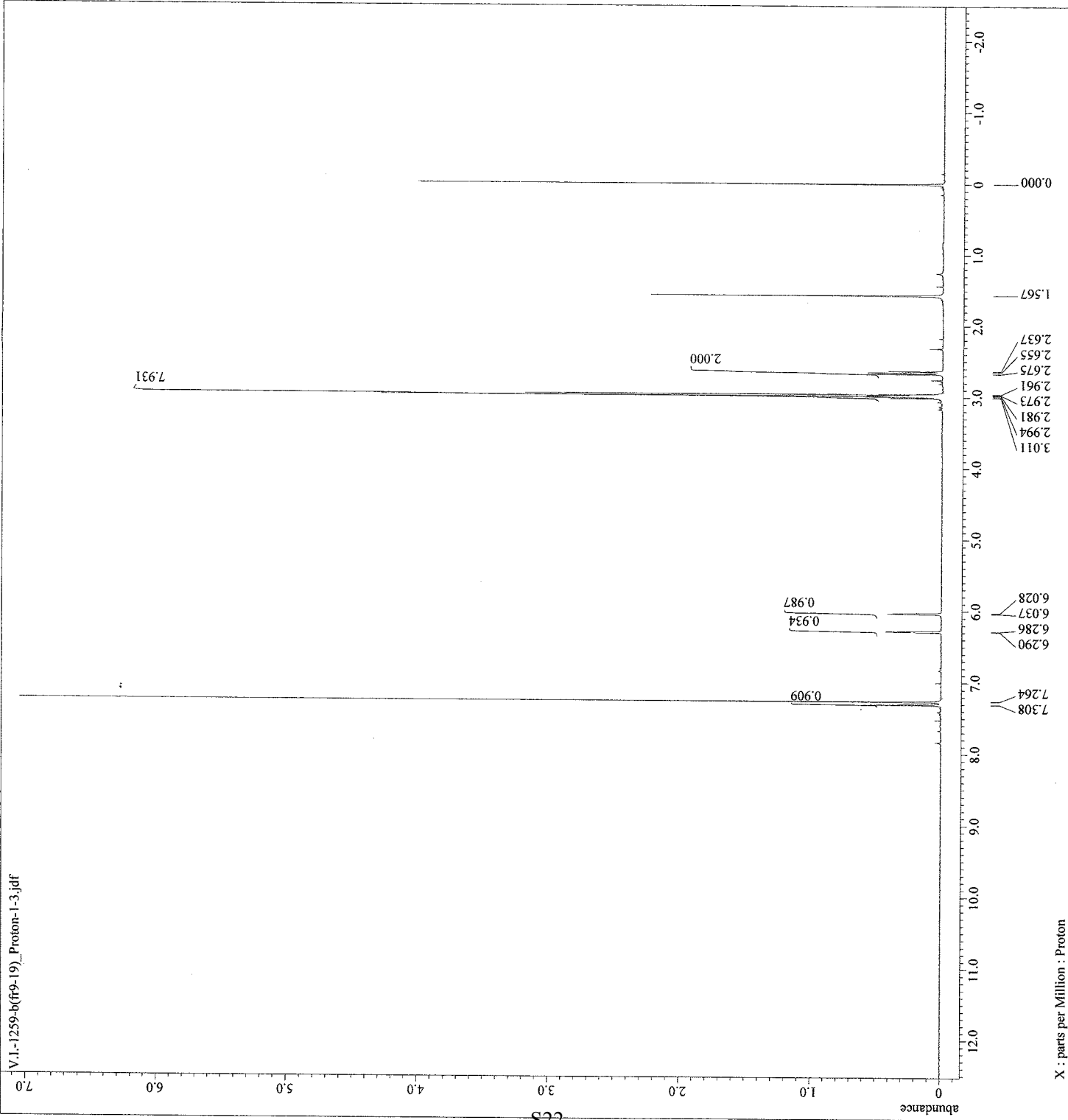
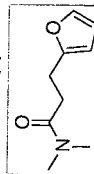
```

Filename = \\Users\delta\Documents\JEO
Author = delta
Experiment = proton_jkp
Sample_Id = V.I.-1259-b(fr9-19)
Solvent = CHLOROFORM-D
Creation_Time = 18-JAN-2013 22:20:49
Revision_Time = 18-JAN-2013 22:52:10
Current_Time = 18-JAN-2013 22:52:35

Comment = single_pulse
Data_Format = 1D_COMPLEX
Dir_Scale = 133.67
Dim_Units = ppm
Dimensions = X
Site = JMS-EGS400
Spectrometer = DELTA2_NMR

Field_Strength = 9.4249681[T] (400 [MHz])
X_Acq_Duration = 2.1757952[s]
X_Domain = 1H
X_Freq = 401.28219856 [MHz]
X_Offset = 5 [ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45960208 [Hz]
X_Sweep = 7.53012048 [MHz]
X_Sweep_Clippped = 6.02409639 [MHz]
Xf1_Domain = Proton
Xf1_Freq = 401.28219856 [MHz]
Xf1_Offset = 5 [ppm]
Xf1_Points = 16384
Xf1_Prescans = 1
Xf1_Resolution = 0.45960208 [Hz]
Xf1_Sweep = 7.53012048 [MHz]
Xf1_Sweep_Clippped = 6.02409639 [MHz]
Xf2_Domain = Proton
Xf2_Freq = 401.28219856 [MHz]
Xf2_Offset = 5 [ppm]
Xf2_Points = 16384
Xf2_Prescans = 1
Xf2_Resolution = 0.45960208 [Hz]
Xf2_Sweep = 7.53012048 [MHz]
Xf2_Sweep_Clippped = 6.02409639 [MHz]
Total_Scans = 16

Relaxation_Delay = 5[s]
Recvr_Gain = 54
Temp_Get = 19.5 [dC]
X_90_Width = 9.25 [us]
X_Acq_Time = 2.1757952 [s]
X_Angle = 45 [deg]
X_Atn = 0.8 [dB]
X_Pulse = 4.625 [us]
Xf1_Mode = OFF
Xf2_Mode = OFF
Xf1_Offset = FALSE
Xf2_Offset = FALSE
Xf1_Wait = 1 [s]
Xf2_Wait = 1 [s]
Repetition_Time = 7.1757952 [s]
    
```



V.I.-1259-b(fr9-19)_Proton-1-3.jif

X : parts per Million : Proton



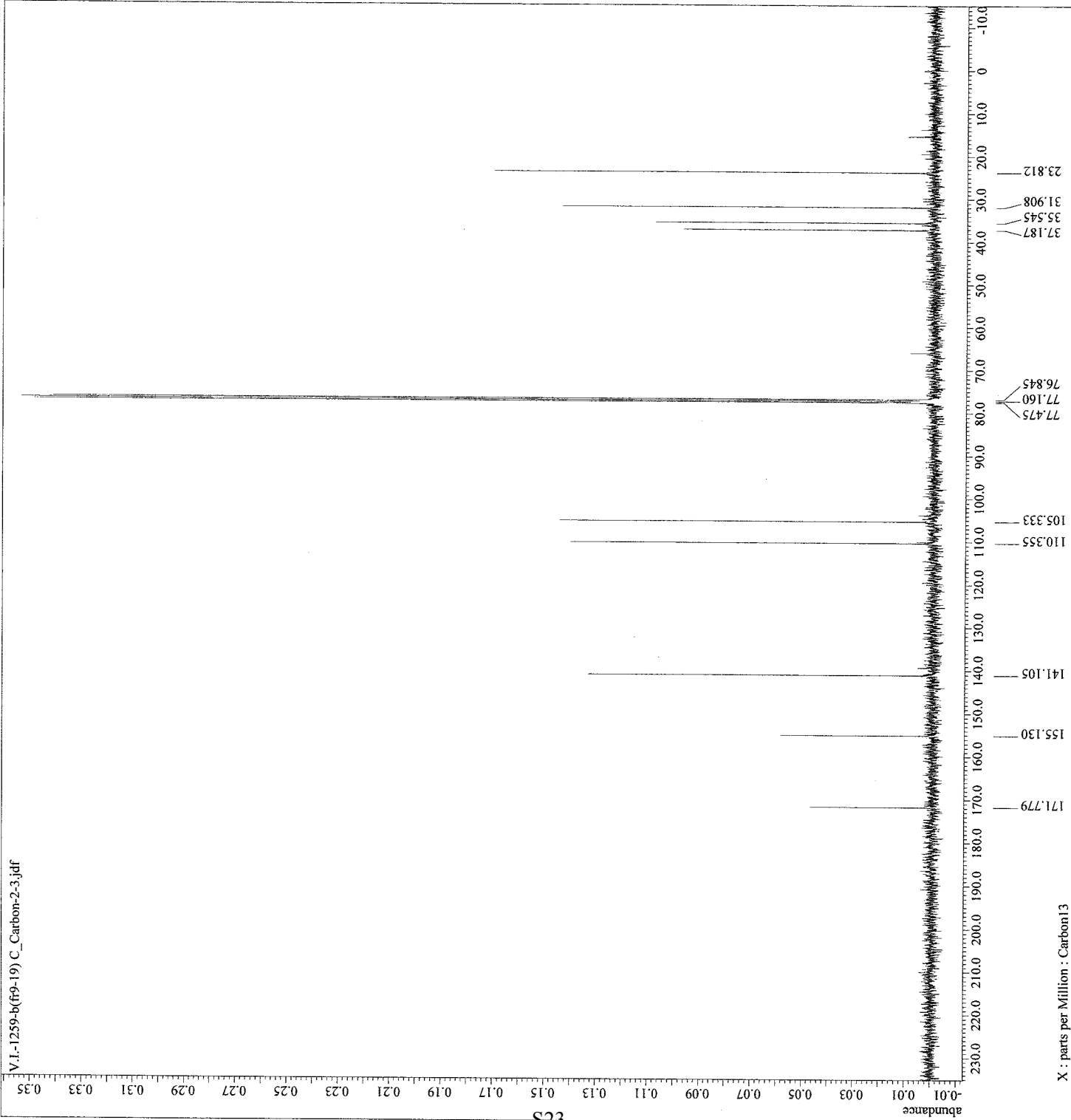
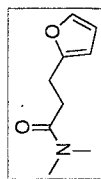
```

File Name      = \Users\delta\Documents\J20
Author         = delta
Experiment     = carbon_jmp
Sample_Id      = V.I.-1259-b(fr-19) C
Solvent        = CHLOROFORM-D
Creation_Time  = 19-JAN-2013 18:33:17
Revision_Time  = 19-JAN-2013 19:05:01
Current_Time   = 19-JAN-2013 19:05:43

Comment       = single pulse decoupled gat
Data Format    = ID COMPLEX
D1m_S1s       = 20214
D1m_S1s2      = Carbon13
D1m_In1s      = X
Dimensions    = X
Site          = JNM-ECS400
Spectrometer  = DELTA2_NMR

Field Strength = 9.42499681[T] (400[MHz])
X_Acq_Duration = 1.03809024[s]
X_Domain       = 13C
X_Freq         = 100.90247863[MHz]
X_Offset       = 110[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       = 401.28219895[MHz]
Irr_Offset     = 4[ppm]
Clipped        = FALSE
Scans          = 256
Total_Scans    = 256

Relaxation_Delay = 2[s]
Recvr_Gain      = 50
Temp_Get        = 19.8[degC]
X_90_Width     = 8.75[us]
X_Acq_Time      = 1.03809024[s]
X_Angle         = 30[deg]
X_Atn          = 5.2[dB]
X_Pulse        = 2.91666667[us]
Irr_Atn_Dec    = 22.691[dB]
Irr_Atn_Noise = 22.691[dB]
Irr_Noise      = WALTZ
Irr_Fwidth     = 0.115[ms]
Decoupling     = PROE
Initial_Wait   = 1[s]
NS              = 32768
No Time        = 2[0]
Repetition_Time = 3.03809024[s]
    
```



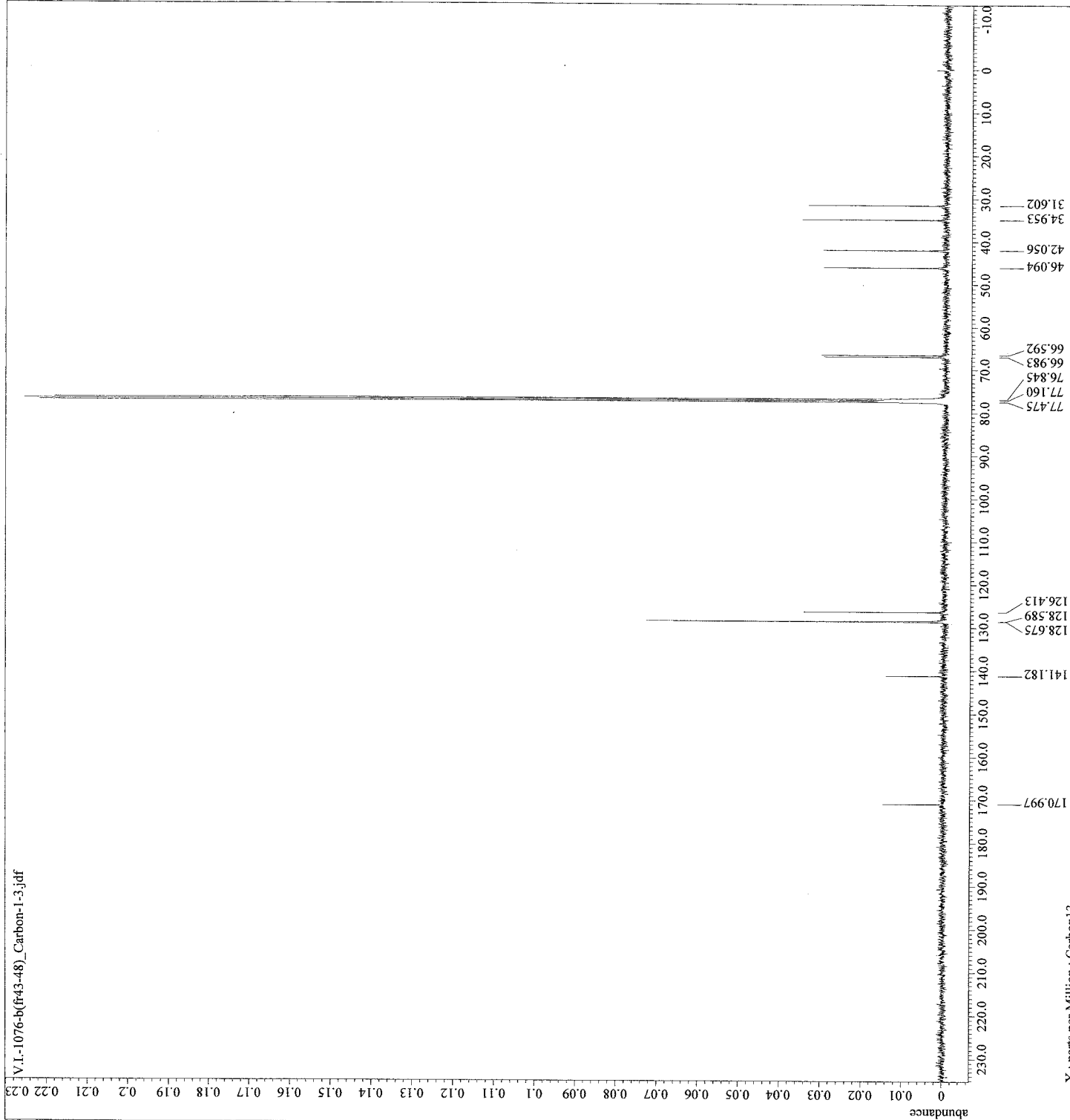
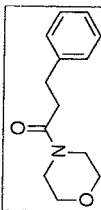
V.I.-1259-b(fr-19) C_Carbon-2-3.jdf

X : parts per Million : Carbon13



```

Filename = C:\Users\delta\Documents\J
Author = delta
Experiment = carbon.kxp
Sample_Id = V.I.-1076-b(fr43-48)
Solvent = CHLOROFORM-D
Creation_Time = 19-OCT-2012 08:05:08
Current_Time = 19-OCT-2012 13:10:36
Current_Time = 19-OCT-2012 13:11:39
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title =
Dimensions =
Site = JNM-ECX400
Spectrometer = DELTA2_NMR
Field_Strength = 9.42499681[T] (400[MHz])
X_Acq_Duration = 1.03809024[s]
X_Cycle = 100
X_Freq = 100.90247863[MHz]
X_Offset = 110[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330738[Hz]
X_Sweep_Clippped = 31.58585657[KHz]
X_Sweep_Time = 55.23252525[s]
X_T1 = 1.03809024[s]
X_T1_Rho = 401.28219856[MHz]
Irr_Freq = 5[ppm]
Irr_Offset = FALSE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recur_Gain = 50
Temp_Get = 21.6[degC]
X_90_Width = 8.75[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Pulse = 2.81666667[us]
X_P1 = 2.81666667[us]
Irr_Atn_Dec = 22.691[dB]
Irr_Atn_Noise = WALTZ
Irr_Noise = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 2[s]
Noe_Time = 2[s]
Repetition_Time = 3.03809024[s]
    
```

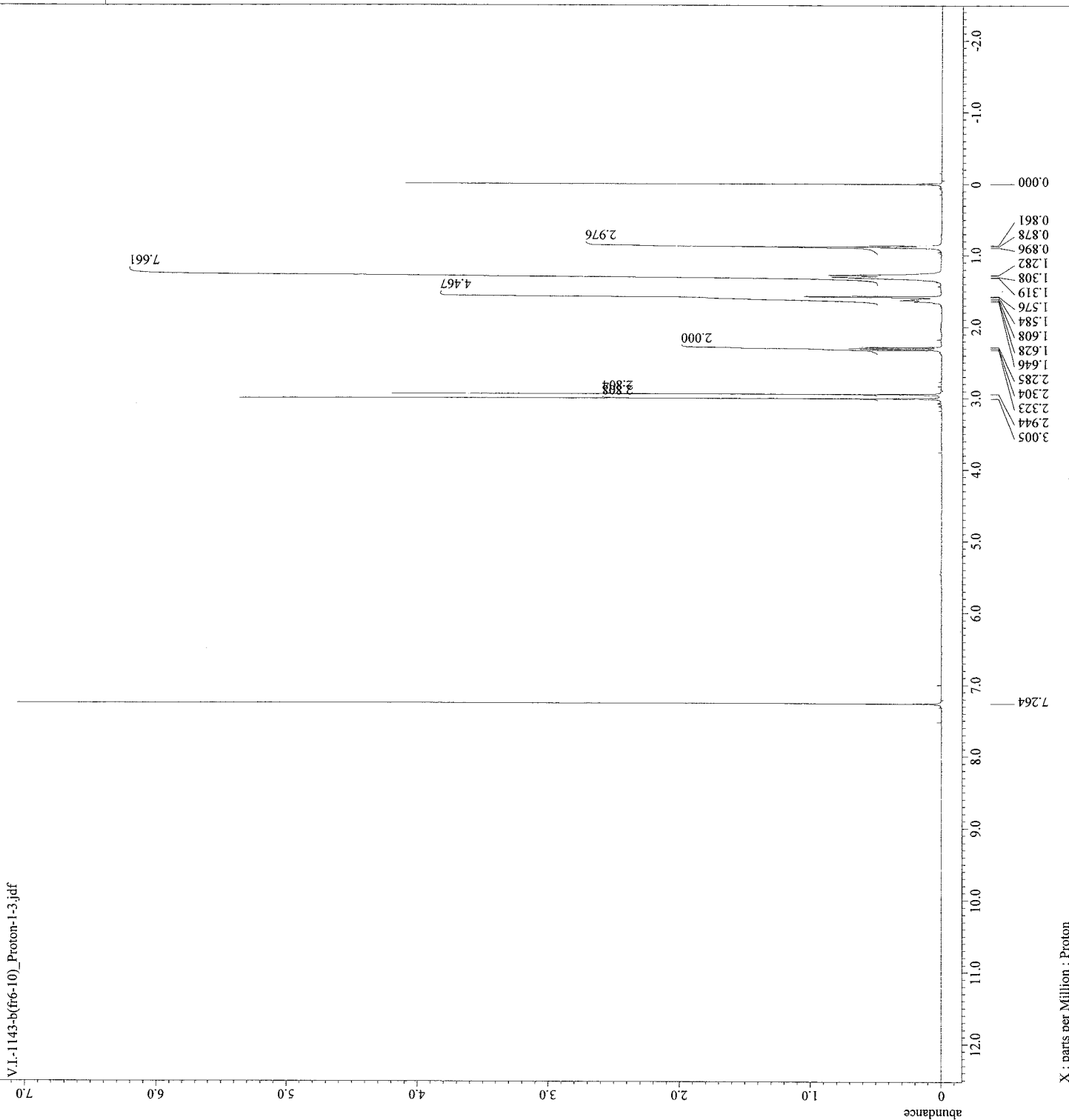


X: parts per Million : Carbon13



```

Filespec = \\users\delta\Documents\JBO
Author = delta
Experiment = proton_1xp
Sample_Id = V.I.-1143-b(fr6-10)
Solvent = CHLOROFORM-D
Creation_Time = 15-NOV-2012 01:31:24
Revision_Time = 15-NOV-2012 01:29:10
Current_Time = 15-NOV-2012 01:29:42
Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title =
Dim_Units = [ppm]
Dimensions =
Site = JNM-EC5400
Spectrometer = DELTA2_NMR
Field_Strength = 9.42499681[T] (400[Mhz])
X_Acq_Duration = 2.1757952[s]
X_Domain = 1H
X_Freq = 401.28219856[Mhz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45960208[Hz]
X_Sweep_Clippped = 7.53012048[Mhz]
X_Sweep_Domain = 6.02409639[Mhz]
X_Sweep_Offset = 45[ppm]
X_Sweep_Time = 40.20219856[Mhz]
X_T1_Offset = 5[ppm]
X_T1_Domain = Proton
X_T1_Freq = 401.28219856[Mhz]
X_T1_Offset = 5[ppm]
X_T1_Offset = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 20.5[degC]
X_90_Width = 9.25[us]
X_Cpd_Time = 41.25792[s]
X_Offset = 0.8[db]
X_Pulse = 4.625[us]
X_Mode = Off
Tri_Mode = Off
Dante_Preset = FALSE
Initial_Wat = 19
Repetition_Time = 7.1757952[s]
    
```



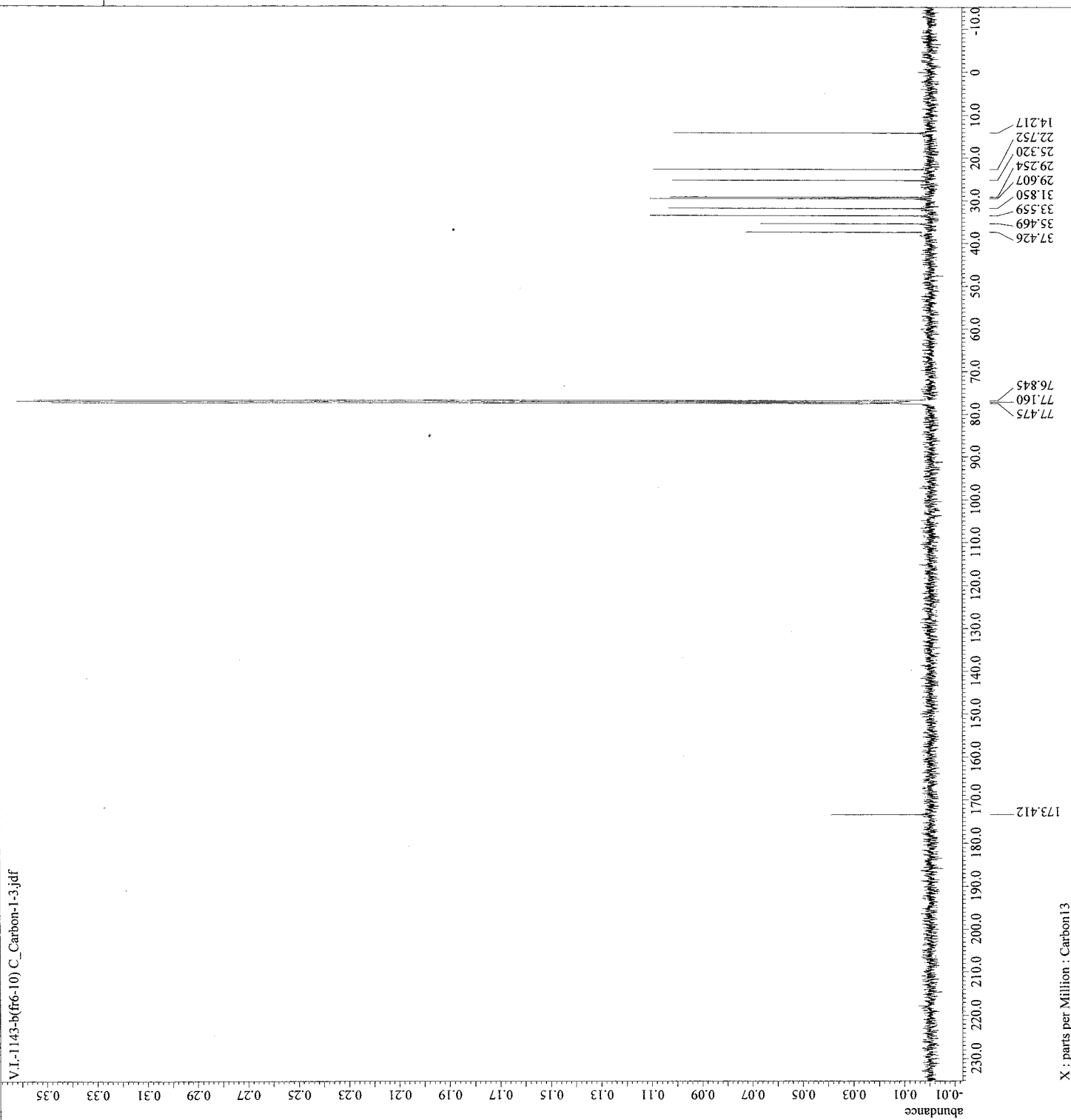
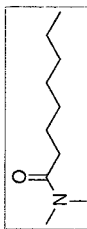
V.I.-1143-b(fr6-10)_Proton-1-3.jdf

X : paris per Million : Proton



```

Filename = C:\Users\delta\Documents\
Author = delta
Experiment = carbon_2kp
Sample_Id = V.I.-1143-b(fr6-10) C
Solvent = CDCl3
AcqDate_Time = 16-NOV-2012 00:59:04
RevsTime = 16-NOV-2012 10:25:03
Current_Time = 16-NOV-2012 10:25:40
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EGS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.450661 [T] (400 [MHz])
X_Domain = 13c
X_Freq = 100.90247863 [MHz]
X_Offset = 110 [ppm]
X_Points = 32768
X_Frescans = 4
X_Resolution = 4.9630798 [Hz]
X_Sweep = 31.665666 [Hz]
X_Sweep_Clippped = 25.25252525 [kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856 [MHz]
Irr_Offset = 5 [ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2 [s]
Recvr_Gain = 50
Temp_Get = 21 [dc]
X_90_Width = 8.75 [us]
X_Acq_Time = 3.03809024 [s]
X_Pulse_Program = zgpg30
X_Pulse = 2.91666667 [us]
Irr_Atn_Dec = 22.691 [dB]
Irr_Atn_Noise = 22.691 [dB]
Irr_Pw1th = 0.115 [ms]
Decoupling = WALTZ
T1_Rho_Exit = 1 [s]
Noe_Time = TRUZE
Repetition_Time = 2 [s]
    
```

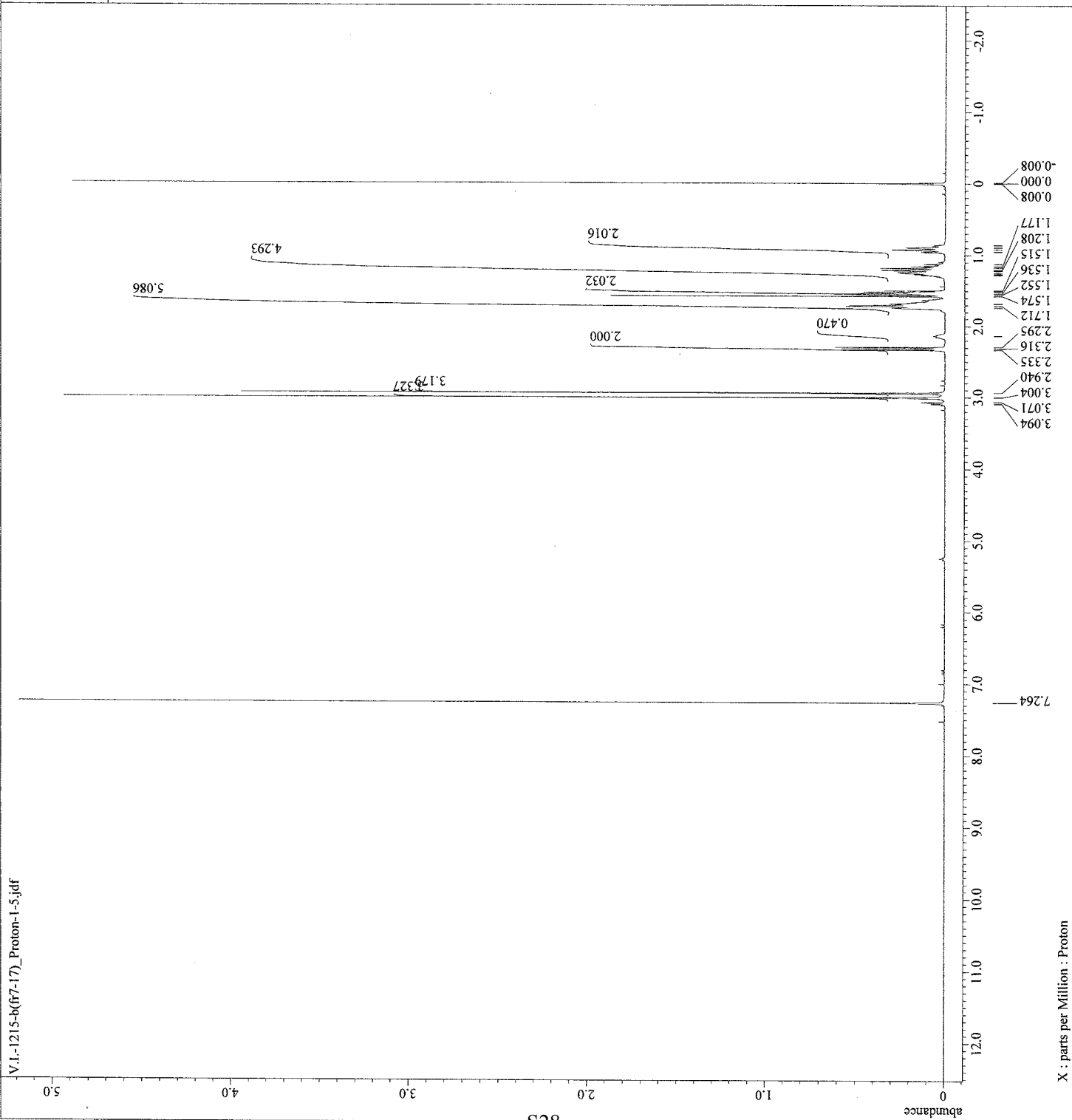
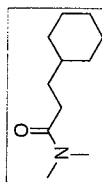


V.I.-1143-b(fr6-10) C_carbon-1-3.jdf



```

Filename = \\Users\delta\Documents\JBO
Author = delta
Experiment = proton.jpg
Sample_Id = V.I.-1215-b(fr7-17)
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2012 04:15:55
Revision_Time = 21-DEC-2012 04:22:27
Current_Time = 21-DEC-2012 04:22:50
Comment = single_pulse
Data_Format = 1D COMPLEX
Dm_Size = 13107
Dm_Title = Proton
Dm_Units = [ppm]
Dm_Extensions =
Site = 30X-PCS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.42499681 [T] (400 [MHz])
X_Acq_Duration = 2.17579521[s]
X_Domain = 1H
X_Freq = 401.28219856 [MHz]
X_Offset = 5 [ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45960208 [Hz]
X_Sweep = 7.53012048 [kHz]
X_Sweep_Clipped = 6.02409639 [kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856 [MHz]
Irr_Offset = 5 [ppm]
Irr_Domain = Proton
Irr_Prescans = 1
Irr_Resolution = 0.45960208 [Hz]
Irr_Sweep = 7.53012048 [kHz]
Irr_Sweep_Clipped = 6.02409639 [kHz]
Pulse_Program = zgpg30
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5 [s]
Recvr_Gain = 50
Temp_Get = 20.5 [dC]
X_90_Width = 9.25 [us]
X_Acq_Time = 2.17579521 [s]
X_Angle = 45 [deg]
X_Altz = 0.8 [dB]
X_Pulse = 4.625 [us]
Irr_Mode = OFF
Irr_Mode = OFF
Dmto_Preset = FPUSE
Initial_Wait = 1 [s]
Repetition_Time = 7.17579521 [s]
    
```



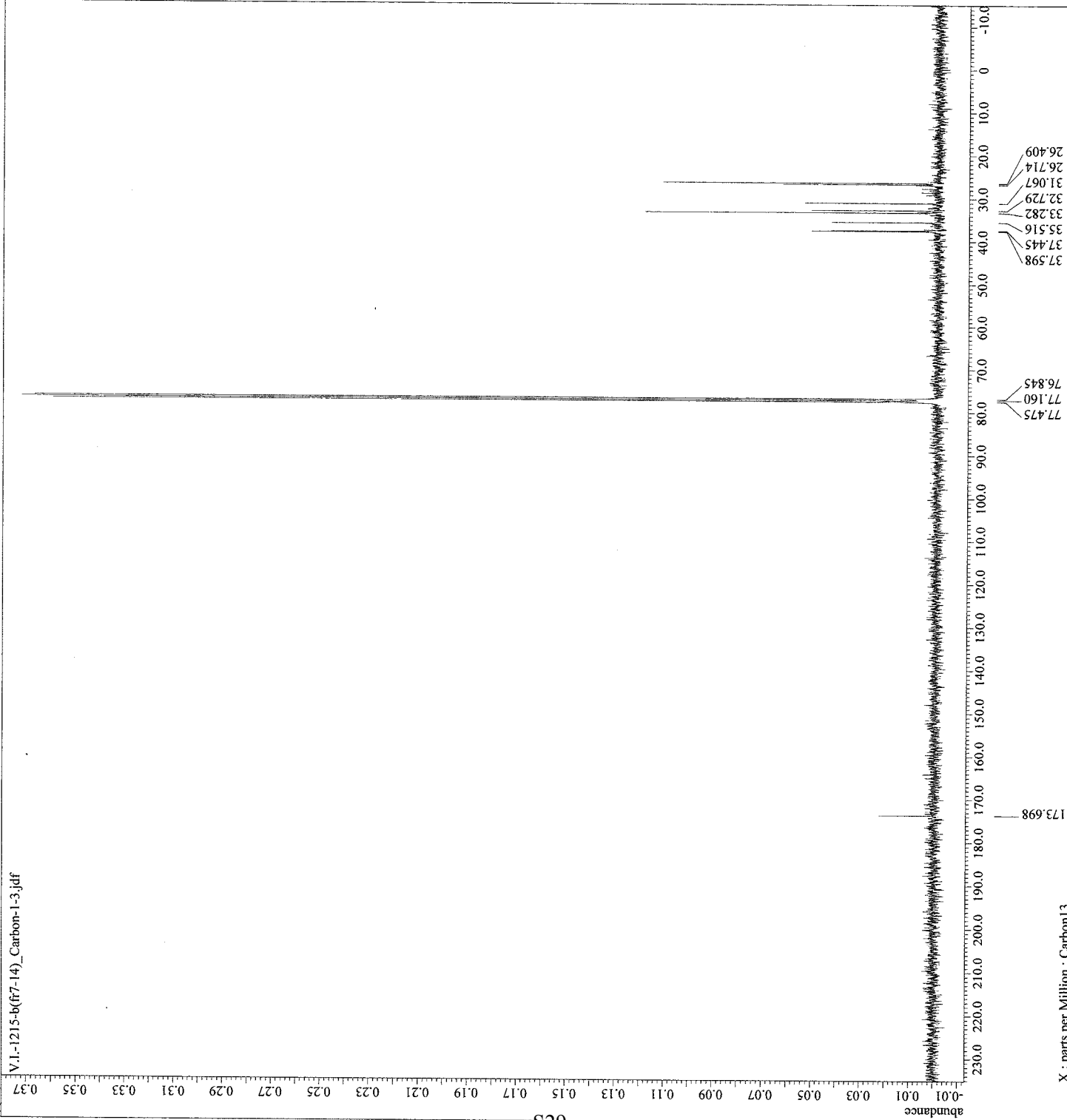
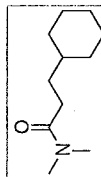
V.I.-1215-b(fr7-17)_Proton-1-5.jdf

X : parts per Million : Proton



```

Filename = C:\Users\delta\Documents\
Author = delta
Experiment = carbon_13p
Sample_Id = V.I.-1215-b(fr7-14)
Solvent = CHLOROFORM-D
Creation_Time = 22-DEC-2012 17:04:22
Revision_Time = 22-DEC-2012 22:39:54
Current_Time = 22-DEC-2012 22:40:31
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = 1
Site = JNM-ECX400
Spectrometer = DELTA2_NMR
Field_Strength = 9.42499681 [T] (400 [MHz])
X_AcqDuration = 1.03809024 [s]
X_Domain = 13C
X_Freq = 100.90247863 [MHz]
X_Offset = 110 [ppm]
X_Points = 32768
X_Prescans = 4
X_Prescans = 0.96330795 [Hz]
X_Resolution = 31.56565657 [kHz]
X_Sweep = 25.25252525 [kHz]
X_Sweep_Clippped = Proton
Irr_Domain = Proton
Irr_Freq = 401.28219855 [MHz]
Irr_Offset = 5 [ppm]
Irr_Pulse = 24dB
SOLVENT = CDCl3
Total_Scans = 256
Relaxation_Delay = 2 [s]
Recvr_Gain = 50
Temp_Get = 21.1 [dC]
X_90_Width = 8.75 [us]
X_AcqTime = 1.03809024 [s]
X_Angle = 30 [deg]
X_Atn = 5.2 [dB]
X_Pulse = 2.91666667 [us]
Irr_Atn_Dec = 22.691 [dB]
Irr_Atn_Noise = 22.691 [dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115 [ms]
Decoupling = TRAP
Initial_Wait = 1 [s]
No_Flags = 0
No_Time = 3 [s]
Repetition_Time = 3.03809024 [s]
    
```



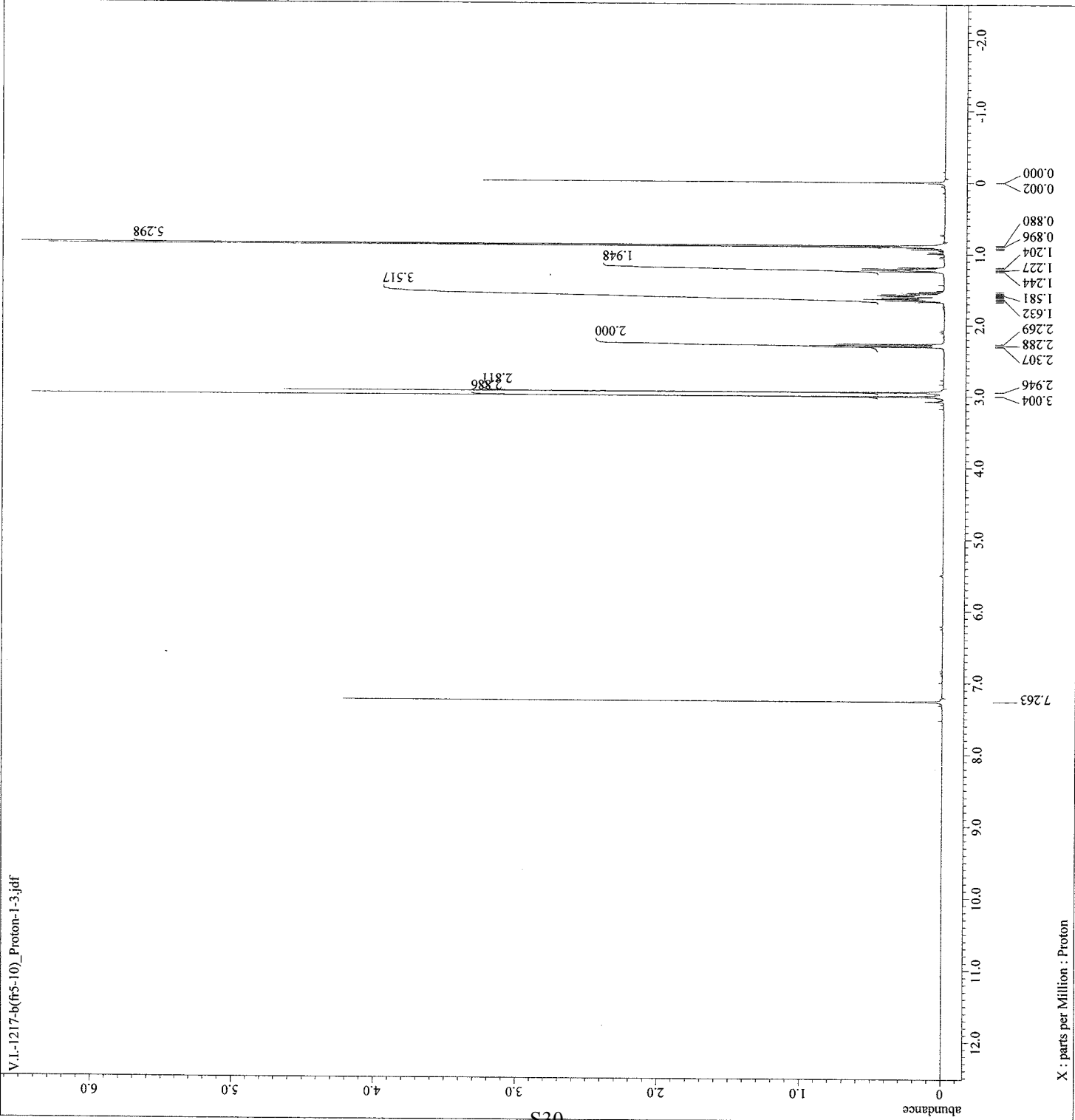
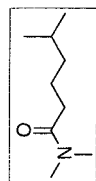
X : parts per Million : Carbon13

V.I.-1215-b(fr7-14)_Carbon-1-3.jdf



```

Filename = \\users\delta\Documents\JBO
Author = delta
Experiment = proton_1xp
Sample_Id = V.I.-1217-b(fr5-10)
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2012 04:27:48
Revision_Time = 21-DEC-2012 04:27:17
Current_Time = 21-DEC-2012 04:27:55
Comment = single_pulse
Data_Format = ID COMPLEX
Dm_Size = 13107
Dm_Title = Proton
Dm_Units = [ppm]
Substitutions =
Site = DM-FCS(400)
Spectrometer = DELTA2_NMR
Field_Strength = 9.42499681[T] (400 [MHz])
X_Acq_Duration = 2.1757952[s]
X_Domain = 1H
X_Freq = 401.28219856 [MHz]
X_Offset = 5 [ppm]
X_Points = 16384
X_Prescans = 1
X_Resolutions = 0.45960208 [Hz]
X_Sweep = 7.53012048 [kHz]
X_Sweep_Clippped = 6.02409639 [kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856 [MHz]
Irr_Offset = 5 [ppm]
Irr_Domain = Proton
Irr_Freq = 401.28219856 [MHz]
Irr_Offset = 5 [ppm]
Irr_Mode = F1SE
Clipped = FALSE
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 20.5 [dC]
X_90_Width = 9.25 [us]
X_Acq_Time = 2.1757952[s]
X_Angle = 45 [deg]
X_Atn = 0.8 [dB]
X_Pulse = 4.625 [us]
Irr_Mode = OFF
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.1757952[s]
    
```



V.I.-1217-b(fr5-10)_Proton-1-3.jdf

X : parts per Million : Proton



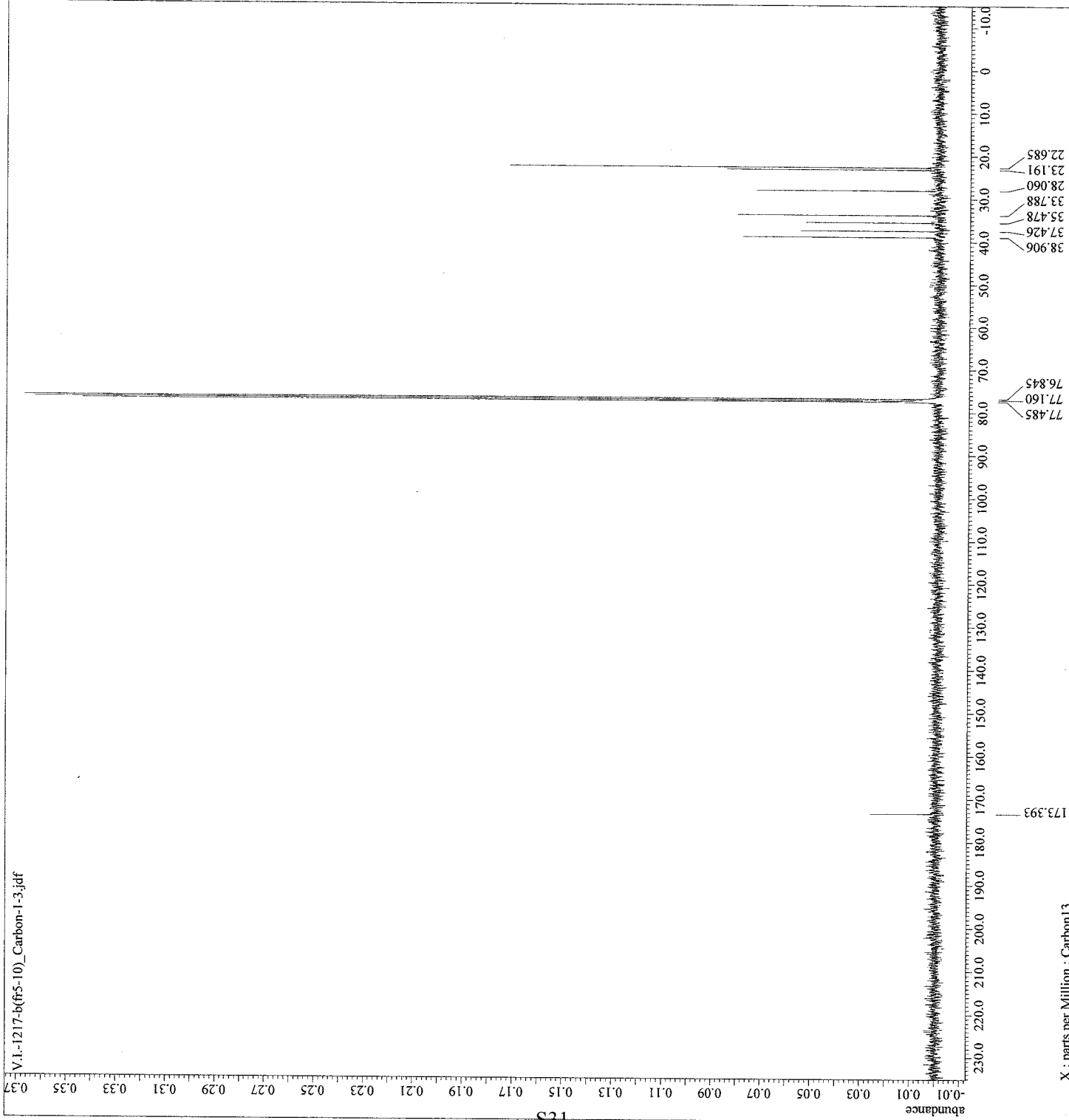
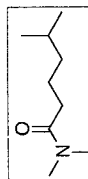
```

FileNames = Users\delta\Documents\JEO
Author = delta
Experiment = carbon_jxp
Sample_Id = V.I.-1217-b(fr5-10)
Solvent = CHLOROFORM-D
Creation_Time = 22-DEC-2012 17:38:07
Revision_Time = 22-DEC-2012 22:36:53
Current_Time = 22-DEC-2012 22:37:28

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_1 = 26214
Dim_2 = 1
Dim_Units = carbon13
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTAZ_NMR

Field_Strength = 9.4249681[T] (400[Mhz])
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.90247863[Mhz]
X_Offset = 110[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep_Clippped = 31.56565657[KHz]
X_Sweep = 25.25252525[KHz]
Irr_Domain = ZCON
Irr_Freq = 501.29219856[Mhz]
Irr_Offset = 50[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256

Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.1[dc]
X_90_Width = 8.75[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 5.2[db]
X_Pulse = 2.91666667[us]
Irr_Atn_Dec = 22.691[db]
Irr_Atn_Noise = 22.691[db]
Irr_Noise = WALTZ
Irr_Fwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noise = 1[s]
Nox_Time = 2[bl]
Repetition_Time = 3.03809024[s]
    
```



X : parts per Million : Carbon13

V.I.-1217-b(fr5-10)_Carbon-1-3.jdf