Supporting Information

Efficient Hydroxymethylation Reactions of Iodoarenes Using CO and 1,3-Dimethylimidazol-2-ylidene Borane

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General Techniques. Thin layer chromatography (TLC) was performed on Merck precoated plates (silica gel 60 F254, Art 5715, 0.25 mm) and were visualized by fluorescence quenching under UV light or by staining with *p*-anisaldeyde/AcOH/H_2SO_4/EtOH, or $12MoO_3 \cdot H_3PO_4$/EtOH. The products were purified by flash chromatography on silica gel (Kanto Chem. Co. Silica Gel 60N (spherical, neutral, 40-50 mm)) and, if necessary, were further purified by recycling preparative HPLC (Japan Analytical Industry Co. Ltd., LC-918) equipped with GPC columns (JAIGEL-1H + JAIGEL-2H columns) using $CHCl_3$ as eluent. ^{1}H NMR spectra were recorded with a JEOL JMN-ECS400 (400 MHz) spectrometer referenced to the solvent peak at 7.26 ppm. ^{13}C NMR spectra were recorded with a JEOL JMN-ECS400 (100 MHz) spectrometer and referenced to the solvent peak at 77.16 ppm. Splitting patterns are indicated as follows: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. diMeImd-BH_3 was prepared from diMeImd-CO_2 according to the literature methods.[1] 2-Iodooctane (**3b**) was prepared from 2-octanol.[2] 2-(allyloxy)iodobenzene (**3m**) was prepared from 2-iodophenol.[3] Other reagents were commercially available and used without further purification.

[1] Bissinger, P.; Braunschweig, H.; Kupfer, T.; Radacki, K. *Organometallics* **2010**, *29*, 3987.
[2] Olah, G. A.; Narang, S. C.; Gupta, B. G. B.; Malhotra, R. *J. Org. Chem.* **1979**, *44*, 1247.
[3] Dahlén, A.; Petersson, A.; Hilmersson, G. R. *Org. Biomol. Chem.* **2003**, *1*, 2423.

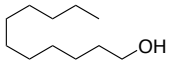
Typical Procedure for the Hydroxymethylation of alkyl iodides

1-Iodoadamantane (131 mg, 0.50 mmol), diMe-Imd-BH_3 (63 mg, 0.58 mmol), and benzene (1 mL) were placed in a Pyrex 20 mL two-necked round-bottomed flask and the mixture was irradiated by black light (15 W) with stirring for 6 h under atmosphere of CO balloon. The reaction mixture was concentrated and the residue was purified by flash chromatography on silica gel (hexane/ether = 5, 2) to give **3d** (63.5 mg, 0.38 mmol, 76%).

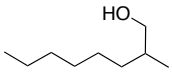
Typical Procedure for the Hydroxymethylation of aryl iodides (Table 1, entry 3)

4-Iodoanisole (116 mg, 0.50 mmol), diMe-Imd-BH_3 (84 mg, 0.76 mmol), AIBN (16 mg, 0.097 mmol), and MeCN (X mL) were placed in a 30 mL stainless steel autoclave. The autoclave was closed, purged three times with CO, pressured with 80 atm of CO, and then heated at 80 °C for 4 h. Excess CO was discharged at room temperature. The reaction mixture was concentrated and the residue was purified by flash chromatography on silica gel (hexane/ether =10, 5, 2) to give **4d** (53 mg, 0.39 mmol, 78%).

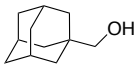
Spectroscopic Data



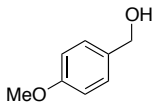
1-Undecanol (**4a**). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.88 (t, *J* = 5.6 Hz, 3H), 1.18-1.50 (m, 16H), 1.53-1.58 (m, 2H), 3.64 (t, *J* = 7.2 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 14.27, 22.83, 25.87, 29.48, 29.58, 29.76, 32.05, 32.93, 63.23. This product is commercially available and the ^{1}H- and ^{13}C-NMR spectra are consistent with those of the authentic sample.



2-methyloctanol[4] (**4b**). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.86-0.92 (m, 6H), 1.06-1.13 (m,1H) 1.19-1.49 (m, 10H), 1.55-1.65 (m, 1H), 3.42 (dd, *J* = 6.4, 10.6 Hz, 1H), 3.51 (dd, *J* = 6.0, 10.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 14.24, 16.71, 22.80, 27.07, 29.74, 31.99, 33.27, 35.87, 68.53.



1-adamantanemethanol (**4c**). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.32 (m, 1H), 1.46-1.54 (m, 6H), 1.60-1.67 (m, 3H), 1.69-1.76 (m, 3H), 1.95-2.01 (m, 3H), 3.20 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 28.27, 34.57, 37.26, 39.13, 73.91. This product is commercially available and the ^{1}H- and ^{13}C-NMR spectra are consistent with those of the authentic sample.



(4-methoxyphenyl)methanol (**4d**) ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.53 (t, *J* = 6.0 Hz, 1H), 3.81 (s, 3H), 4.62 (d, *J* = 6.0 Hz, 2H), 6.88-6.92 (m, 2H), 7.29-7.31 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 55.42, 65.16, 114.07, 128.79, 133.22, 159.32. This product is commercially available and the 1H- and 13C-NMR spectra are consistent with those of the authentic sample.

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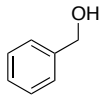
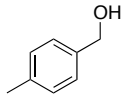
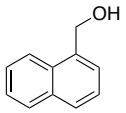
[4] Silver, S.; Puranen, A.; Sjöholm, R.; Repo, T.; Leino, R. *Eur. J. Inorg. Chem.* **2005,** 1514.



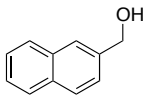
benzyl alcohol (**4e**) ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.60-1.66 (m, 1H), 4.71 (d, *J* = 6.0 Hz, 2H), 7.26-7.38 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 65.16, 127.05, 127.64, 128.58, 140.91. This product is commercially available and the 1H- and 13C-NMR spectra are consistent with those of the authentic sample.



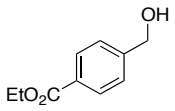
(4-methylphenyl)methyl alcohol (**4f**) ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.54 (t, *J* = 6.0 Hz, 1H), 2.36 (s, 3H), 4.66 (d, *J* = 6.0 Hz, 2H), 7.18 (d, *J* = 7.6 Hz, 2H), 7.27 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 21.25, 65.27, 127.21, 129.32, 137.44, 137.99. This product is commercially available and the 1H- and 13C-NMR spectra are consistent with those of the authentic sample.



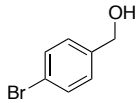
1-naphthylenemethanol (**4g**) ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.71 (t, *J* = 6.0 Hz, 1H), 5.17 (d, *J* = 6.0 Hz, 2H), 7.44-7.58 (m, 4H), 7.82-7.90 (m, 2 H), 8.14 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 63.64, 123.72, 125.38, 125.48, 125.95, 126.41, 128.62, 128.74, 131.27, 133.84, 136.32. This product is commercially available and the 1H- and 13C-NMR spectra are consistent with those of the authentic sample.



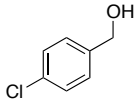
2-naphthylenemethanol (**4h**) ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.87 (s, 2 H), 7.45-7.52 (m, 3H), 7.81-7.87 (m, 4 H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 65.58, 125.29, 125.55, 126.02, 126.31, 127.84, 128.01, 128.46, 133.04, 133.46, 138.40. This product is commercially available and the 1H- and 13C-NMR spectra are consistent with those of the authentic sample.



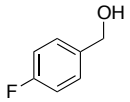
4-hydroxymethylbenzoic acid ethyl ester[5] (**4i**) ^{1}H-NMR ($CDCl_3$, 400MHz) δ: 1.40 (t, *J* = 6.9 Hz, 3H), 1.76-1.82 (br, 1H), 4.35 (q, *J* = 6.9 Hz, 2H), 4.78 (d, *J* = 6.0 Hz, 2H), 7.43, (d, *J* = 8.3 Hz, 2H), 8.04 (d, *J* = 8.3 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 14.33, 61.09, 64.45, 126.44, 129.39, 129.75, 146.20, 166.76.



4-Bromophenylmethanol (**4j**) ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.64 (t, *J* = 6.0 Hz, 1H), 4.66 (d, *J* = 5.9 Hz, 2H), 7.20-7.25 (m, 2H), 7.48-7.50 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 64.52, 121.49, 128.67, 131.67, 139.80. This product is commercially available and the 1H- and 13C-NMR spectra are consistent with those of the authentic sample.

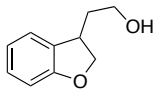


4-Chlorophenyl methanol (**4k**) ^{1}H-NMR ($CDCl_3$, 400MHz) δ: 1.64 (t, *J* = 6.0 Hz, 1H), 4.68 (d, *J* = 6.0 Hz, 2H), 7.29-7.35 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 64.57, 128.38, 128.76, 133.42, 139.33. This product is commercially available and the 1H- and 13C-NMR spectra are consistent with those of the authentic sample.

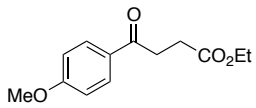


1-fluoro-4-hydroxymethylbenzene (**4l**) ^{1}H-NMR ($CDCl_3$, 400MHz) δ: 1.67 (t, *J* = 5.5 Hz, 1H), 4.67 (d, *J* = 5.2 Hz, 2H), 7.02-7.08 (m, 2H), 7.31-7.36 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 64.71, 115.49 (d, $J_{C\text{-}F}$ = 21.0 Hz), 128.88 (d, $J_{C\text{-}F}$ = 7.7 Hz), 136.66 (d, $J_{C\text{-}F}$ = 2.8 Hz), 162.40 (d, $J_{C\text{-}F}$ = 243.5 Hz). This product is commercially available and the 1H- and 13C-NMR spectra are consistent with those of the authentic sample.

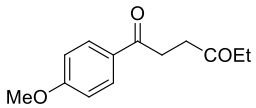
[5] Murai, N.; Yonaga, M.; Tanaka, K. *Org. Lett.* **2012**, *14*, 1278.



2-(2,3-dihydrobenzofuran-3-yl)ethanol[6] (**4m**) ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.33 (t, *J* = 5.2 Hz, 1H), 1.80-1.90 (m, 1H), 2.02-2.10 (m, 1H), 3.56-3.65 (m, 1H), 3.78 (q, *J* = 6.4 Hz, 2H), 4.28 (dd, *J* = 9.2, 6.8 Hz, 1H), 4.68 (t, *J* = 8.8 Hz, 1H), 6.89 (d, *J* = 8.4 Hz, 1H), 6.88 (t, *J* = 7.2 Hz, 1H), 7.14 (t, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 37.54, 39.15, 60.90, 77.08, 109.72, 120.57, 124.44, 128.38, 130.58, 159.87.



4-(4-methoxyphenyl)-4-oxo-butyric acid ethyl ester[7] (**8d**) ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.27 (t, *J* = 6.8 Hz, 3H), 2.74 (t, *J* = 6.4 Hz, 2H), 3.27 (t, *J* = 6.8 Hz, 2H), 3.87 (s, 3H), 4.16 (q, *J* = 8 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 7.97 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 14.24, 28.40, 33.03, 55.49, 60.63, 113.75, 129.71, 130.32, 163.57, 173.09, 196.68.



1-(4-methoxyphenyl)hexane-1,4-dione[8] (**9d**) ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.10 (t, *J* = 7.2 Hz, 3H), 2.57 (q, *J* = 7.6 Hz, 2H), 2.85 (t, *J* = 6.0 Hz, 2H), 3.25 (t, *J* = 6.4 Hz, 2H), 3.87 (s, 3H), 6.92-6.95 (m, 2H), 7.96-7.98 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 7.91, 32.14, 35.93, 36.16, 55.52, 113.74, 129.80, 130.37, 163.55, 197.29, 210.42.

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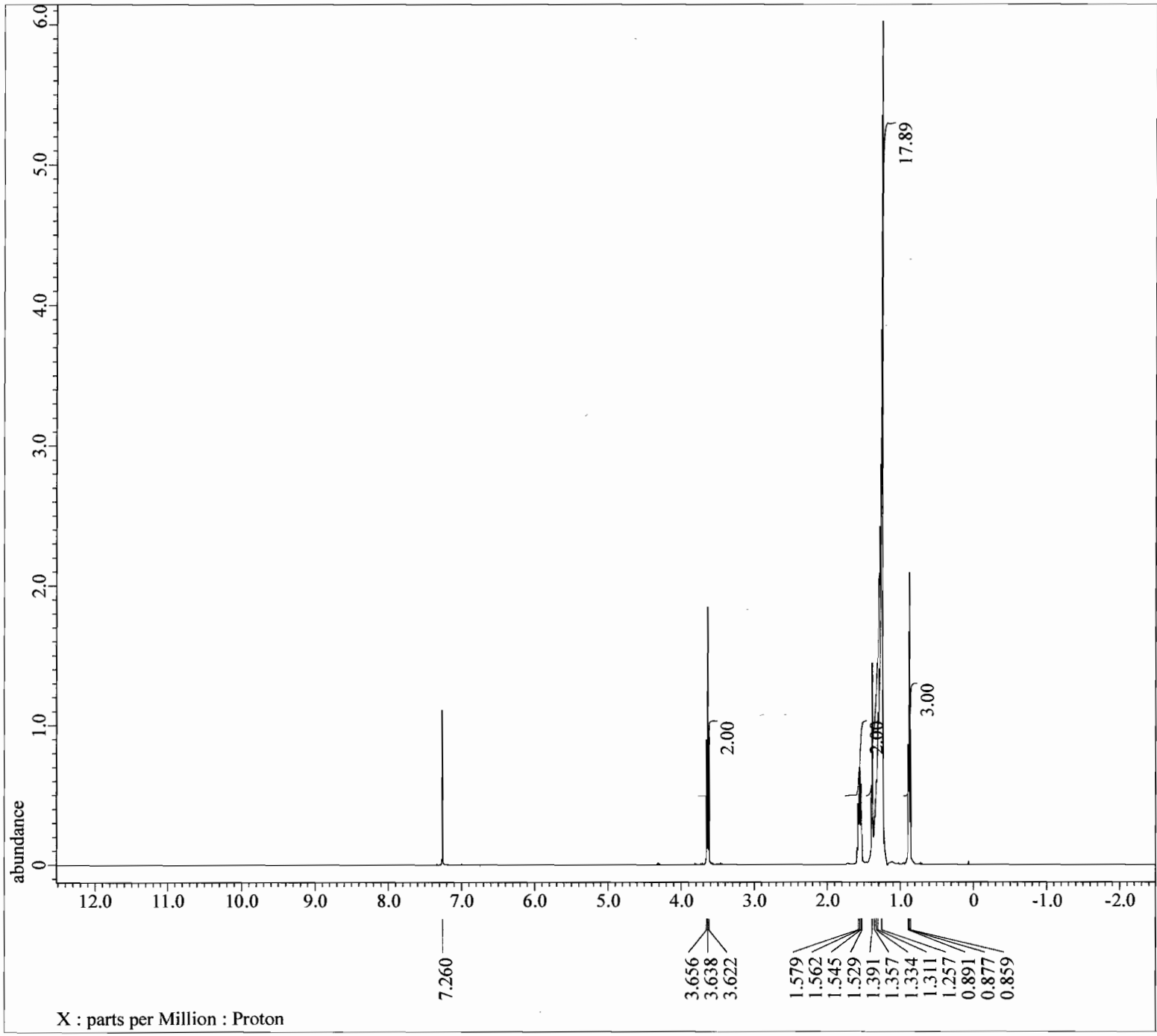
[6] Helliwell, P. A.; Bailey, V. A.; Chevet, C.; Clarke, D. B.; Lloyd, A.; Macarthur, R.; Routledge, A. *Reactive and Functional Polymers* **2010**, *70*, 110.
[7] Le Bras, G.; Provot, O.; Peyrat, J.; Alami, M.; Brion, J. Tetrahedron Lett. **2006**, *47*, 5497.
[8] Shen, Z.-L.; Goh, K. K. K.; Cheong, H.-L.; Wong, C. H. A.; Lai, Y.-C.; Yang, Y.-S.; Loh, T.-P. *J. Am. Chem. Soc.*, **2010**, *132*, 15852.

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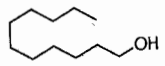
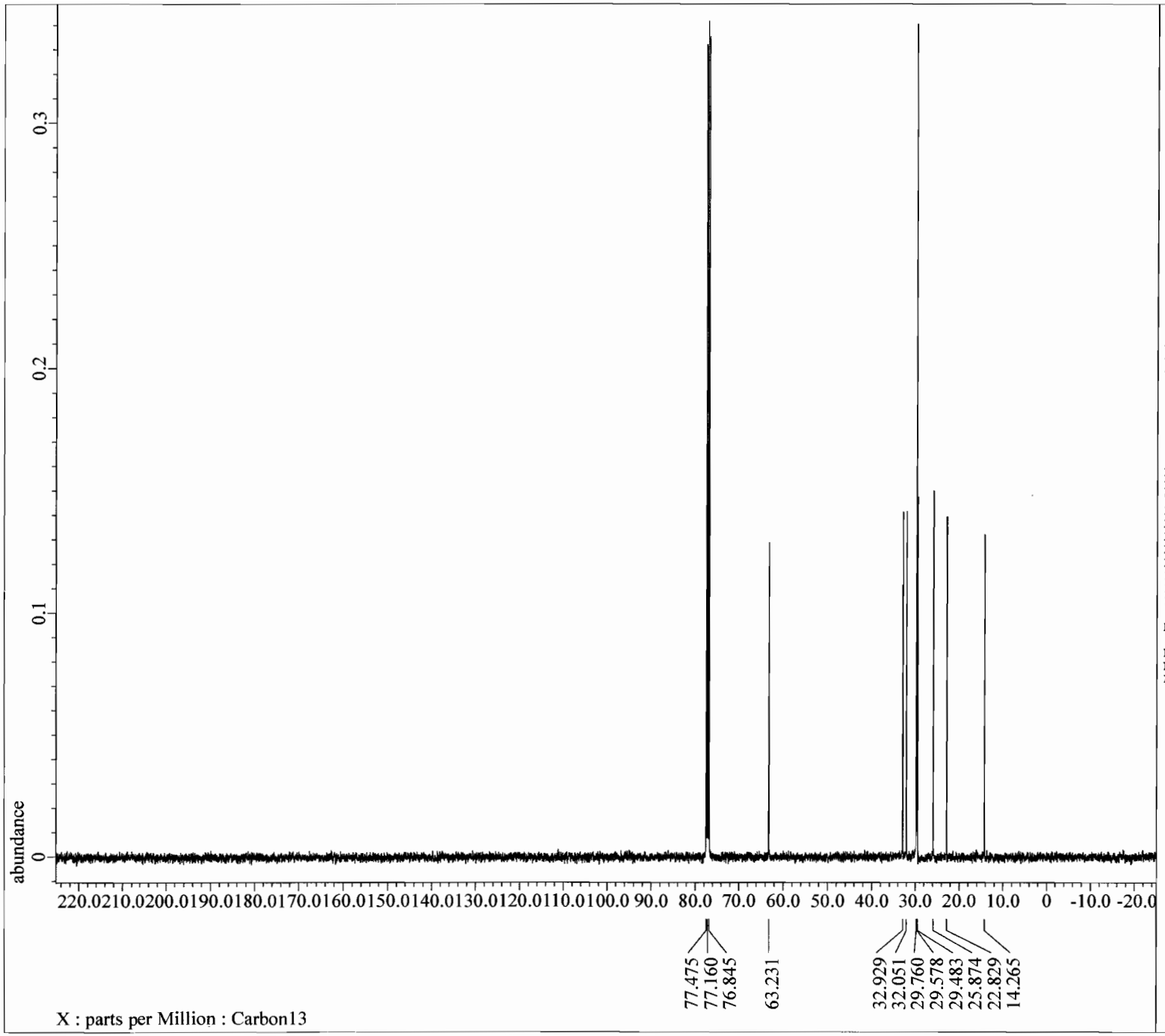


4a

S 8

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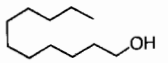
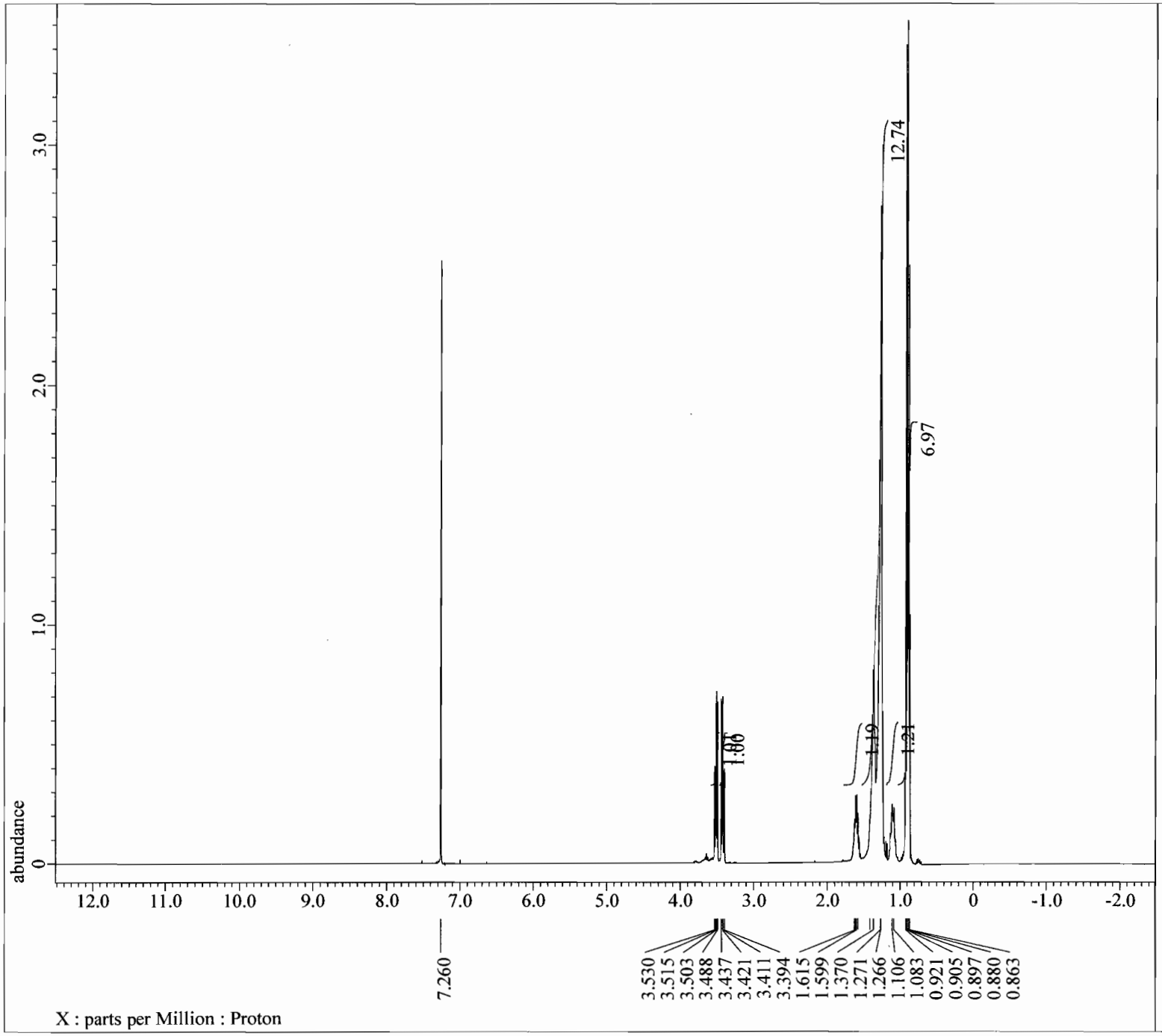


4a

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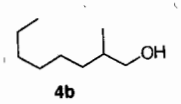
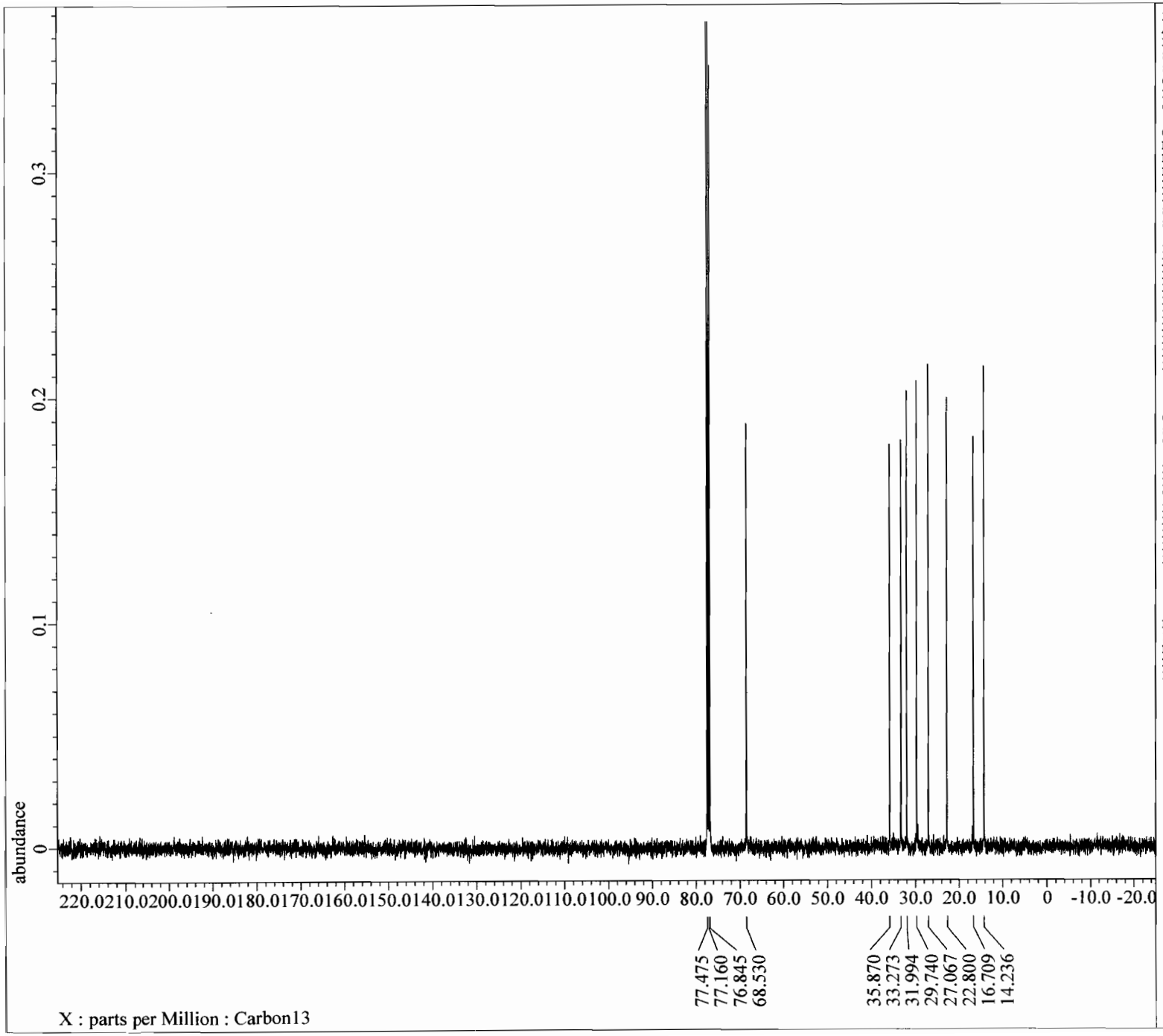
X_Prescans        = 1
X_Resolution      = 0.45960208[Hz]
X_Sweep           = 7.53012048[kHz]
X_Sweep_Clipped   = 6.02409639[kHz]
Irr_Domain        = Proton
Irr_Freq          = 401.28219856[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 401.28219856[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 46
Temp_Get          = 20.2[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]
```



4b

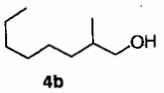



```
Filename          = /Users/tktk0112/NMR/2-hydr
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 2-hydroxymethyl-octane 1
Solvent           = CHLOROFORM-D
Creation_Time     = 18-FEB-2013 12:11:39
Revision_Time     = 21-FEB-2013 10:06:55
Current_Time      = 21-FEB-2013 10:07:23

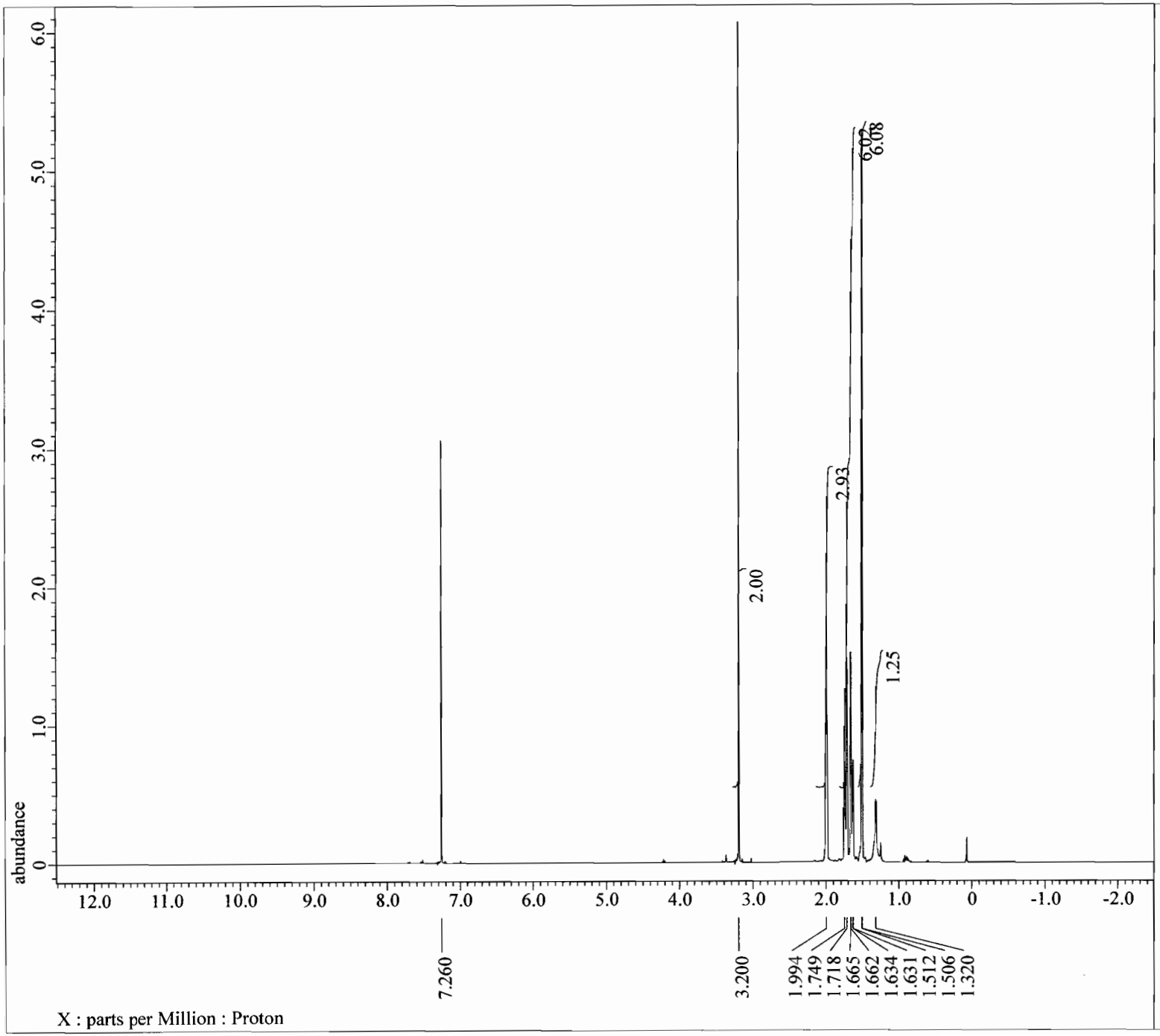
Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.42499681[T] (400[MHz])
X_Acq_Duration    = 1.03809024[s]
X_Domain          = 13C
X_Freq            = 100.90247863[MHz]
X_Offset          = 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          = 401.28219856[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 128
Total_Scans       = 128

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 19.9[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_Noe       = 22.691[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.03809024[s]
```



4b

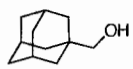



```
Filename          = /Users/tktk0112/NMR/tk-250
Author            = delta
Experiment        = proton.jxp
Sample_Id         = tk-250-
Solvent           = CHLOROFORM-D
Creation_Time     = 16-FEB-2013 19:24:42
Revision_Time     =  8-MAR-2013 15:56:22
Current_Time      =  8-MAR-2013 15:57:40

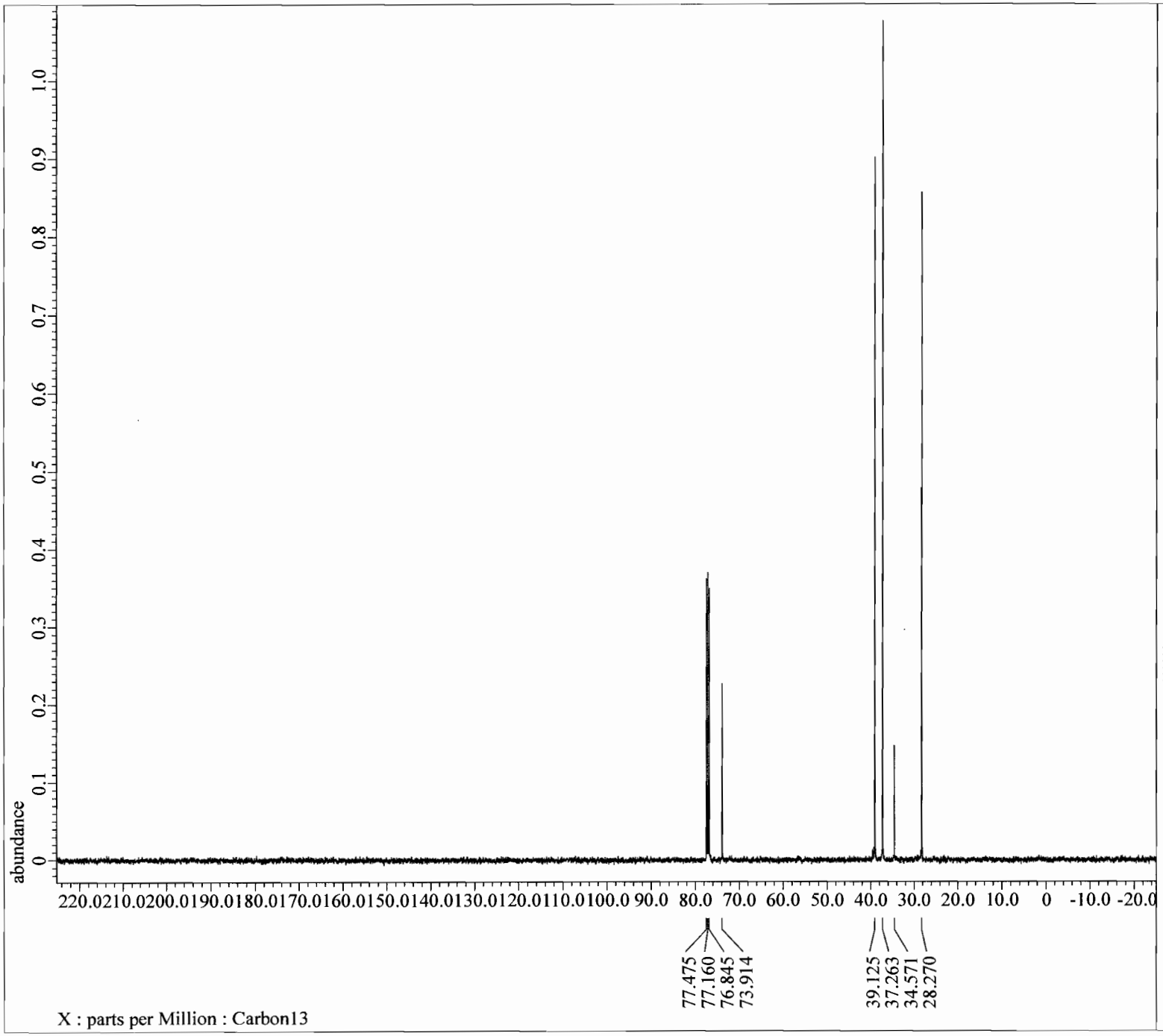
Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

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           = 7.53012048[kHz]
X_Sweep_Clipped   = 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             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 46
Temp_Get          = 19.8[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]
```



4c

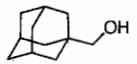



```
Filename          = /Users/tktk0112/Documents/
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 1-adamantanemethanol
Solvent           = CHLOROFORM-D
Creation_Time     = 18-FEB-2013 12:21:58
Revision_Time     = 21-FEB-2013 09:54:20
Current_Time      = 21-FEB-2013 09:55:16

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

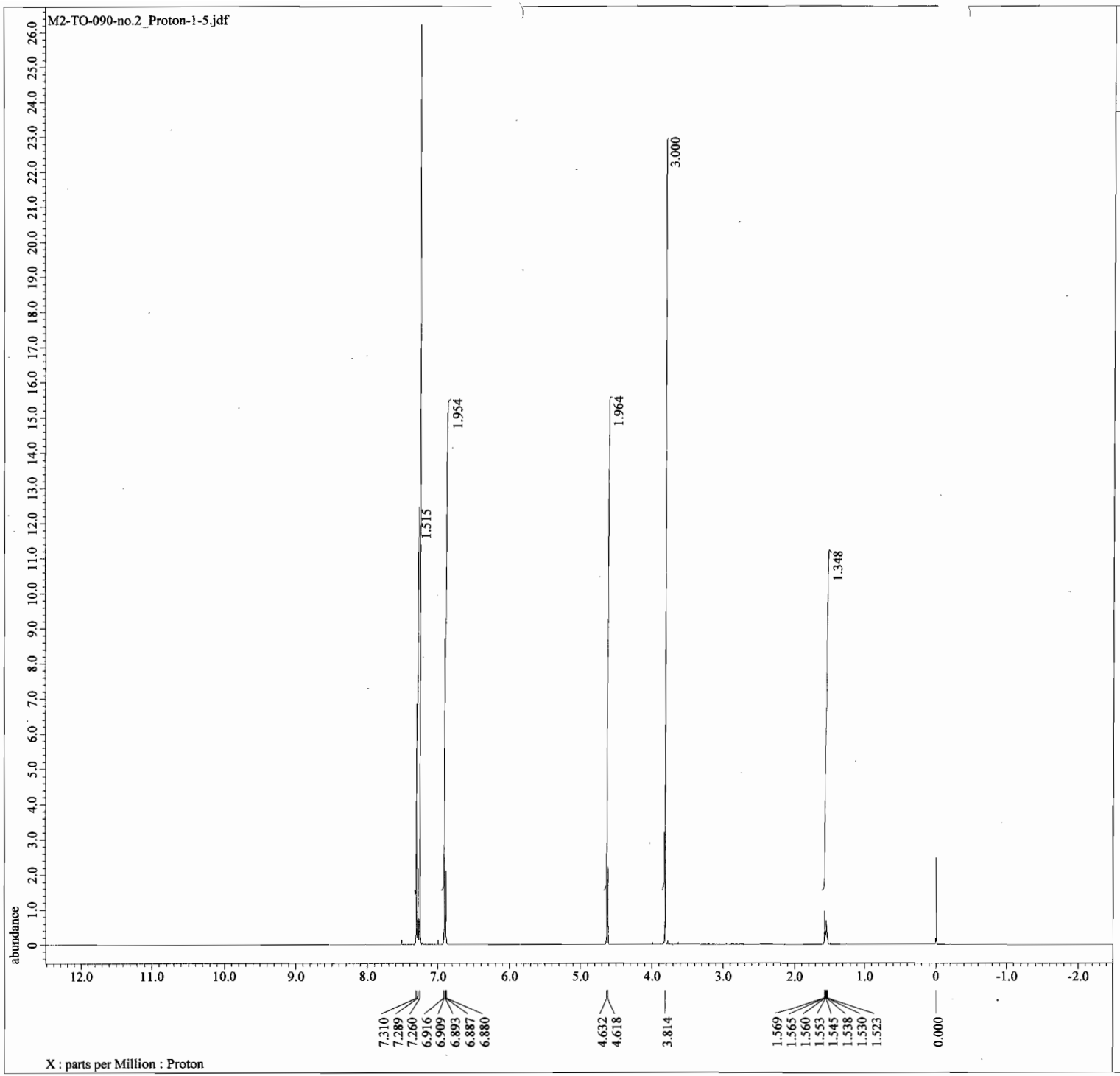
Field_Strength    = 9.42499681[T] (400[MHz])
X_Acq_Duration    = 1.03809024[s]
X_Domain          = 13C
X_Freq            = 100.90247863[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.96330739[Hz]
X_Sweep           = 31.56565657[kHz]
X_Sweep_Clipped   = 25.25252525[kHz]
Irr_Domain        = Proton
Irr_Freq          = 401.28219856[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 128
Total_Scans       = 128

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 20.2[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_Noe       = 22.691[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.03809024[s]
```



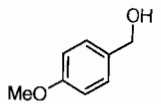
4c

S 13



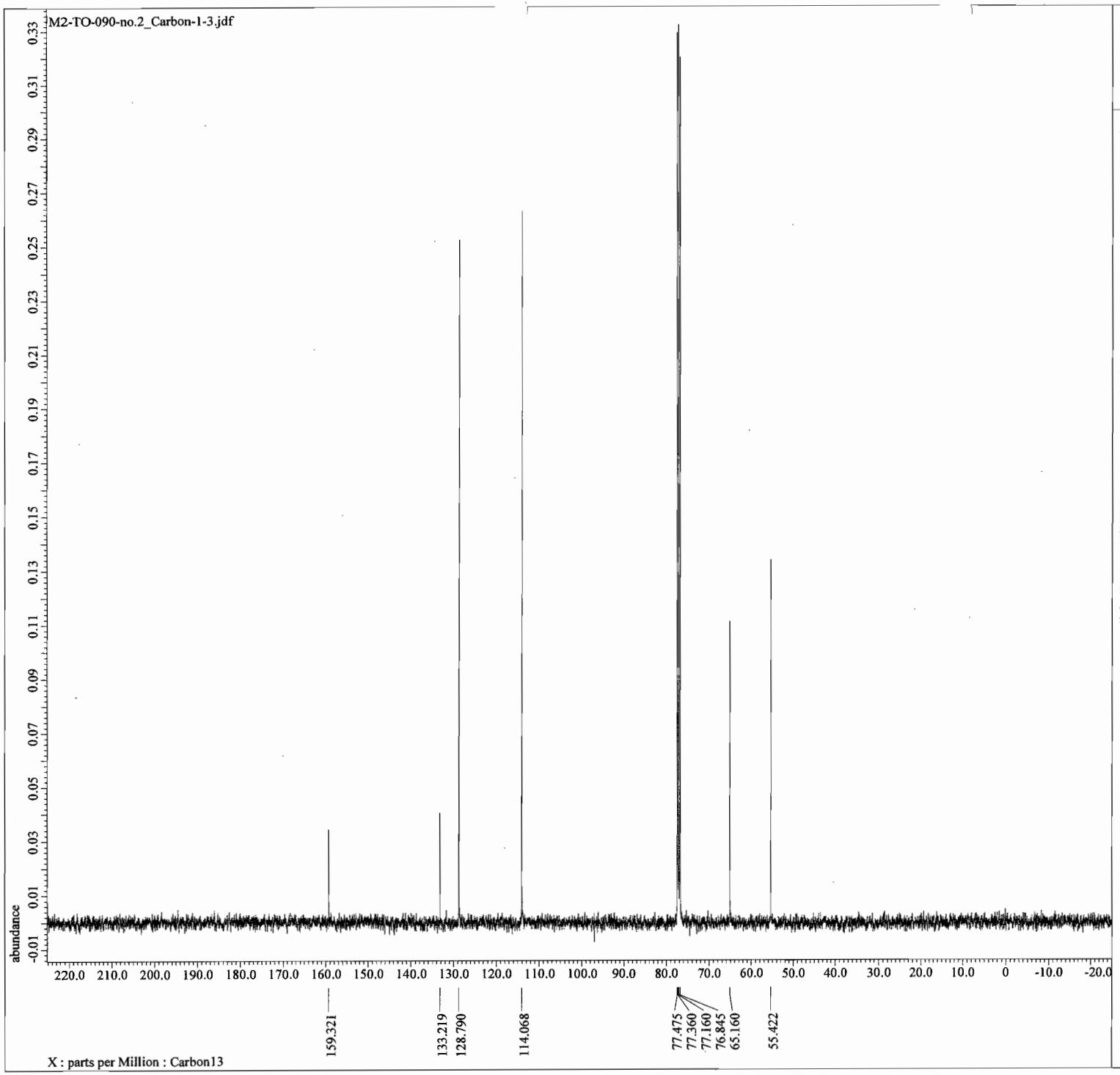
JEOL RESONANCE

Filename	= C:\Users\delta\Documents\J
Author	= delta
Experiment	= proton.jxp
Sample_Id	= M2-TO-090-no.2
Solvent	= CHLOROFORM-D
Creation_Time	= 3-OCT-2012 17:57:24
Revision_Time	= 3-OCT-2012 18:54:50
Current_Time	= 3-OCT-2012 18:54:56
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
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	= 7.53012048[kHz]
X_Sweep_Clipped	= 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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 48
Temp_Get	= 21.2[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]



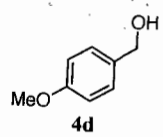
4d

S 14

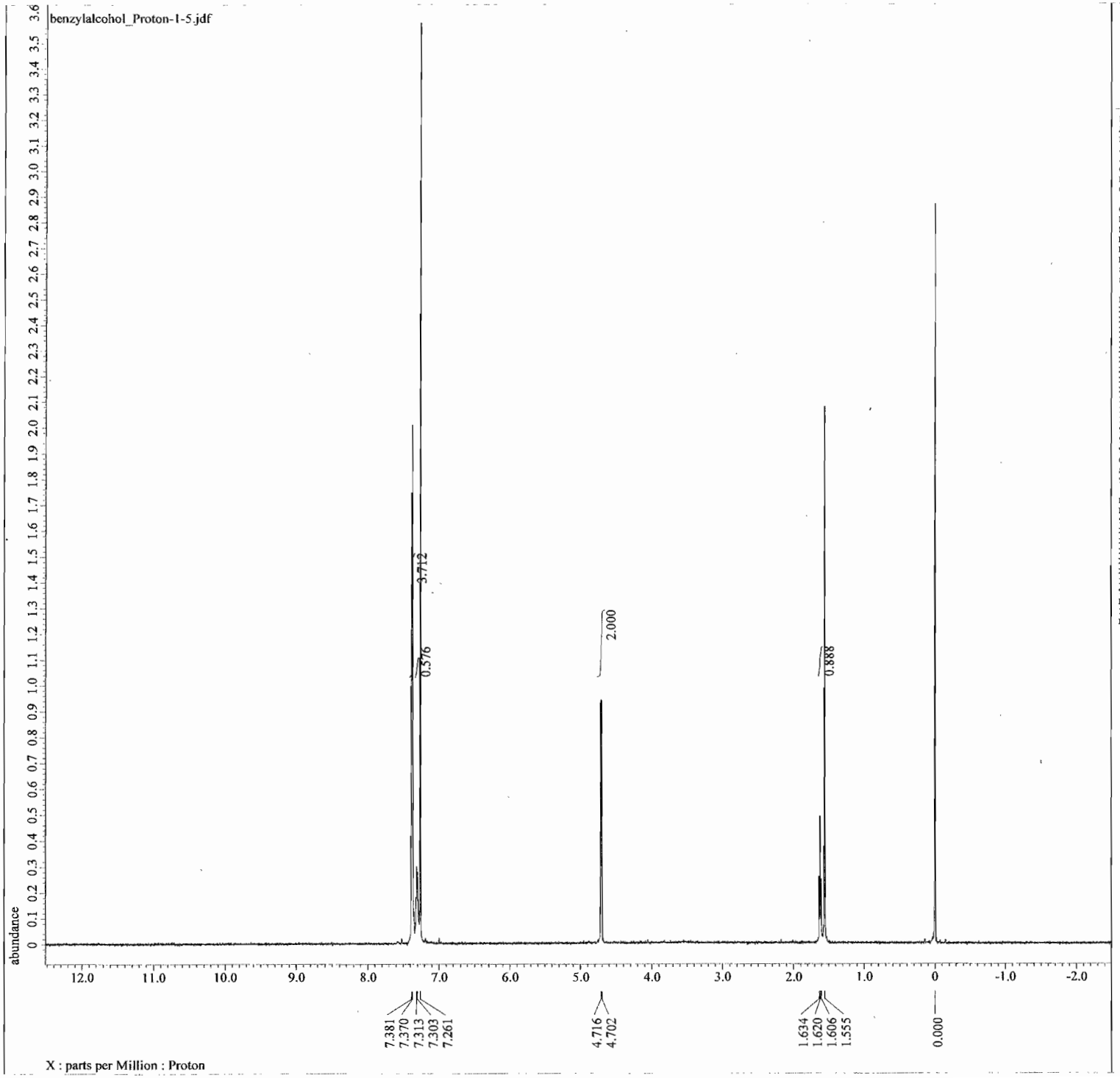


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= M2-TO-090-no.2
Solvent	= CHLOROFORM-D
Creation_Time	= 3-OCT-2012 20:57:32
Revision_Time	= 3-OCT-2012 21:18:48
Current_Time	= 3-OCT-2012 21:19:38
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 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	= 401.28219856[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.6[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_Noe	= 22.691[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.03809024[s]

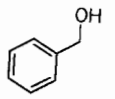


4d

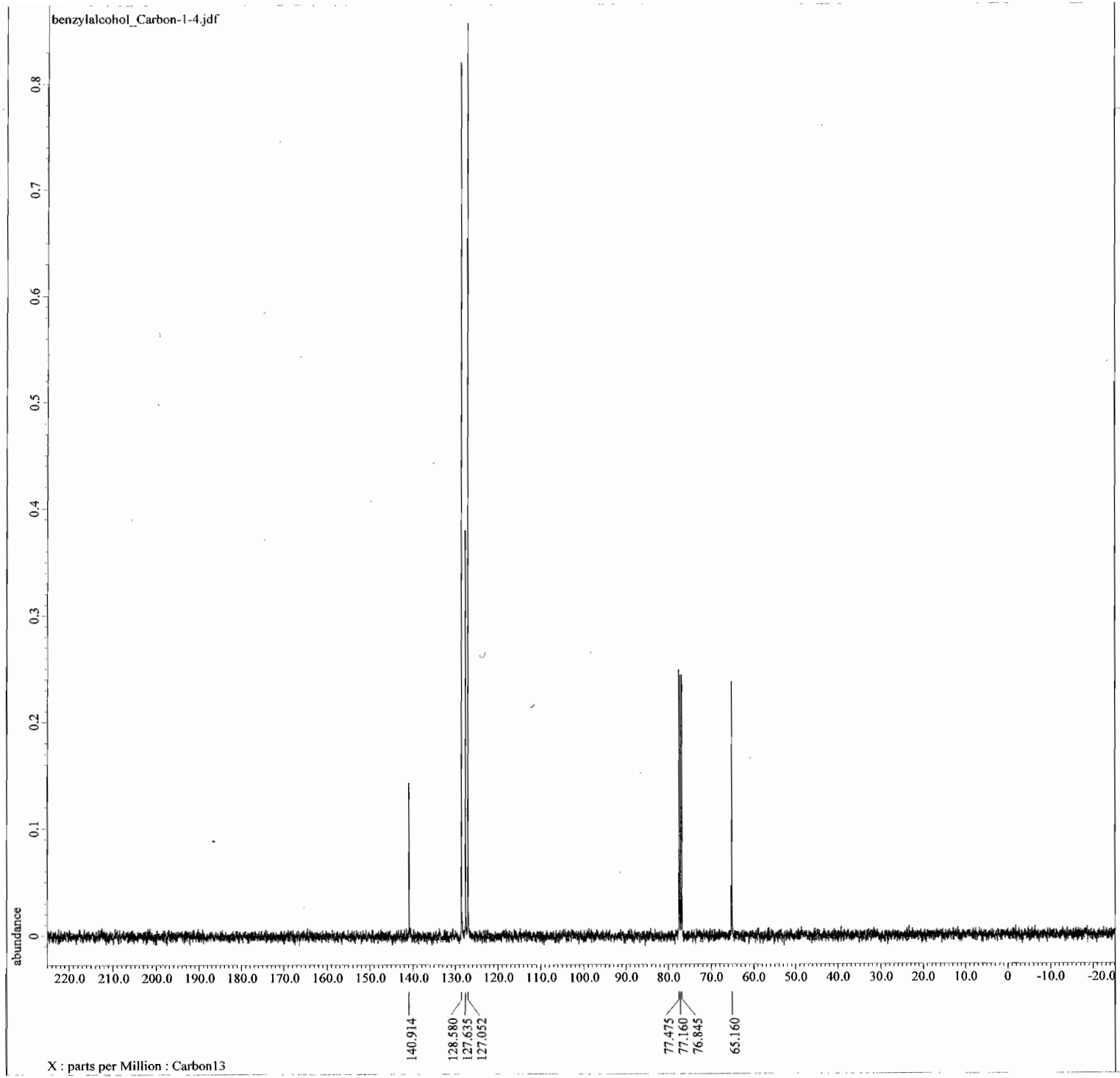


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= benzylalcohol
Solvent	= CHLOROFORM-D
Creation_Time	= 8-MAR-2013 17:03:05
Revision_Time	= 8-MAR-2013 20:05:04
Current_Time	= 8-MAR-2013 20:05:10
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
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	= 7.53012048[kHz]
X_Sweep_Clipped	= 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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 54
Temp_Get	= 20.1[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]



4e



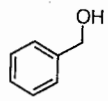
JEOL RESONANCE

```
Filename          = \Users\delta\Documents\JEO
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = benzylalcohol
Solvent           = CHLOROFORM-D
Creation_Time     =  8-MAR-2013 19:51:40
Revision_Time     =  8-MAR-2013 20:02:07
Current_Time      =  8-MAR-2013 20:03:21

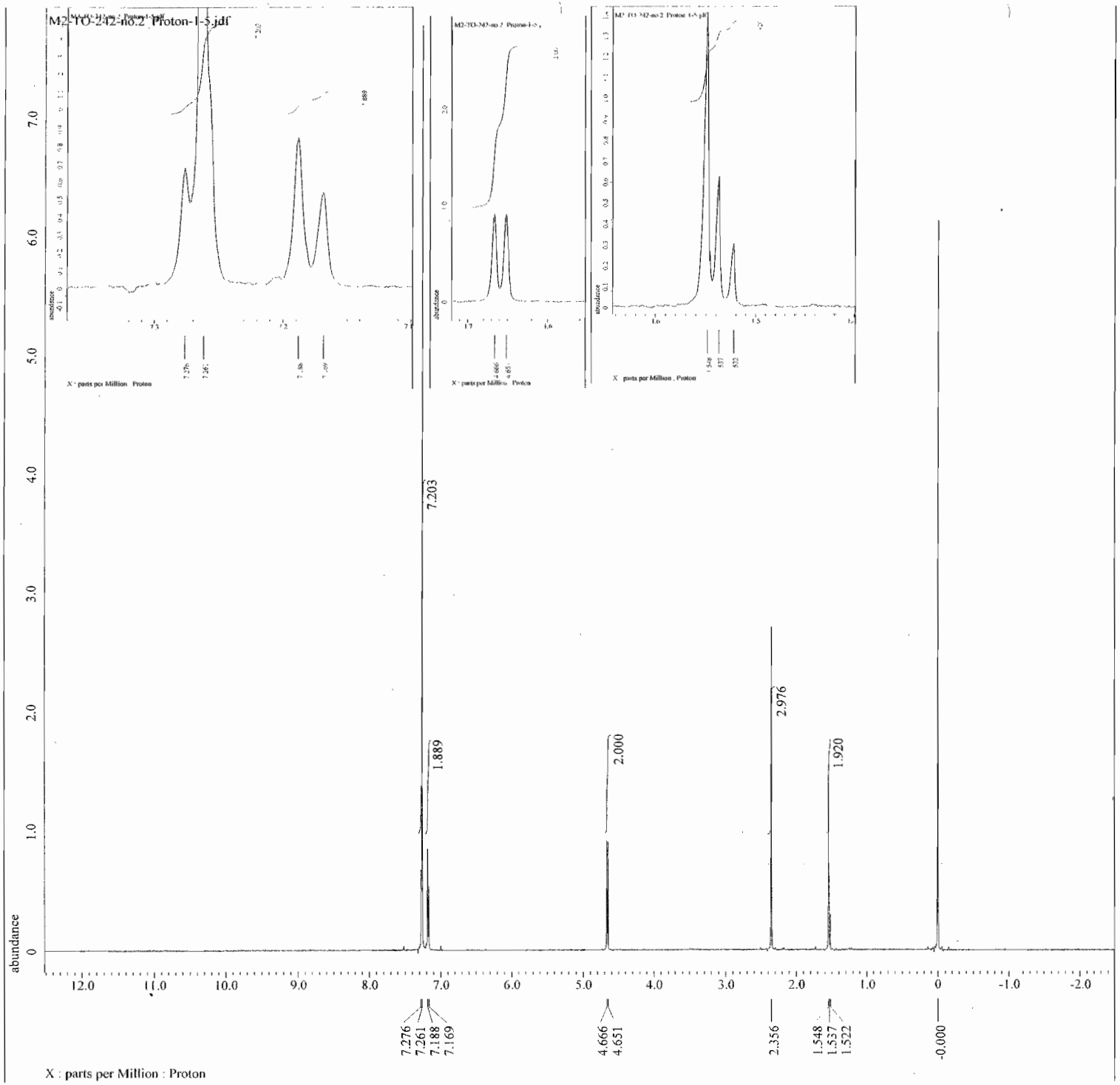
Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.42499681[T]  (400[MHz])
X_Acq_Duration    = 1.03809024[s]
X_Domain          = 13C
X_Freq            = 100.90247863[MHz]
X_Offset          = 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          = 401.28219856[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay = 2[s]
Recvr_Gain        = 50
Temp_Get          = 20.1[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       = 22.69[dB]
Irr_Atn_Noe       = 22.69[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.03809024[s]
```

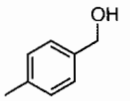


4e

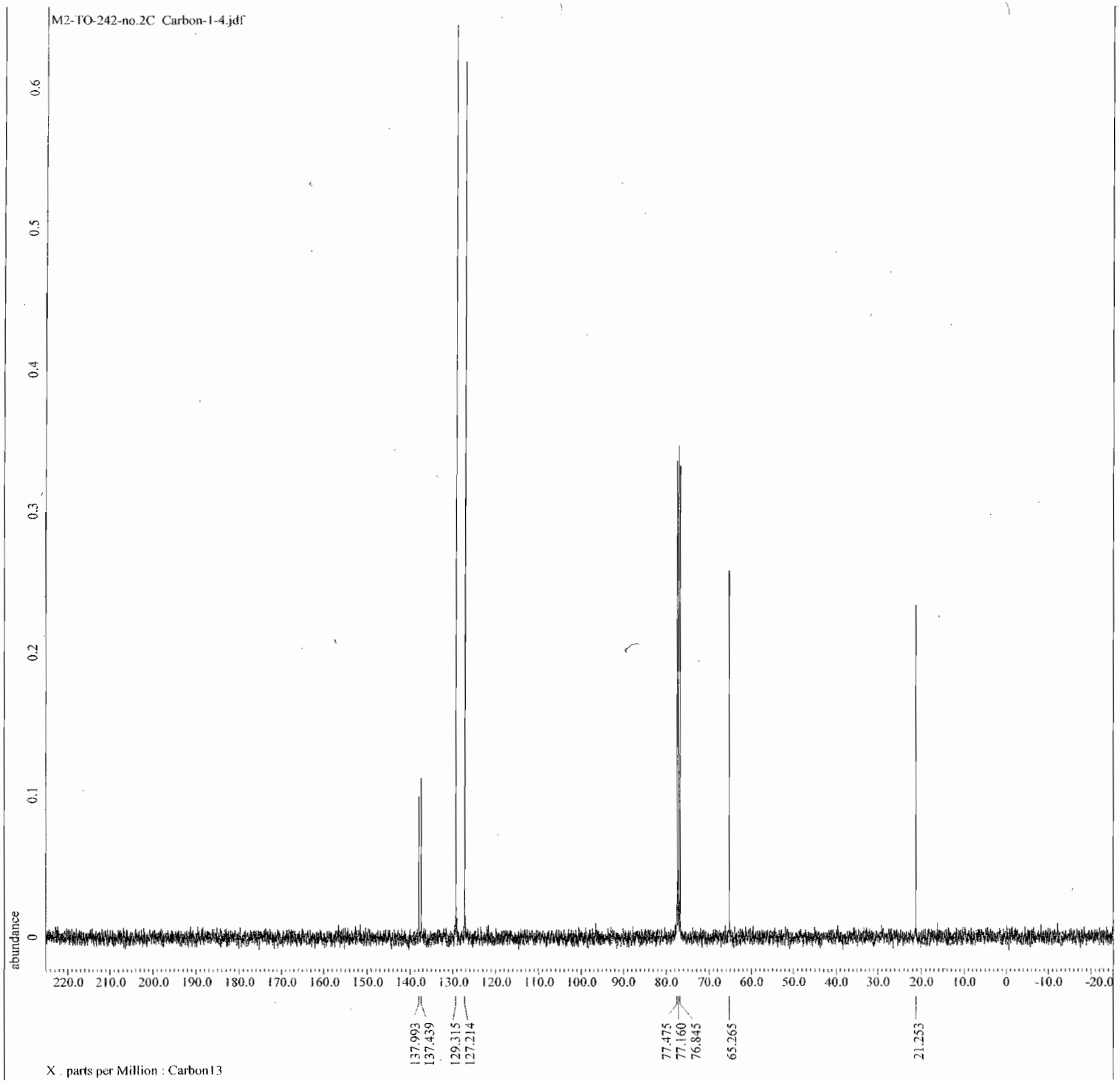


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= M2-TO-242-no.2
Solvent	= CHLOROFORM-D
Creation_Time	= 21-FEB-2013 03:54:38
Revision_Time	= 21-FEB-2013 04:34:53
Current_Time	= 21-FEB-2013 04:35:35
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
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	= 7.53012048[kHz]
X_Sweep_Clipped	= 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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.8[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]



4f



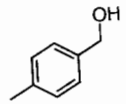
JEOL RESONANCE

```
Filename          = \Users\delta\Documents\JEO
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M2-TO-242-no.2C
Solvent           = CHLOROFORM-D
Creation_Time     = 21-FEB-2013 04:07:38
Revision_Time     = 21-FEB-2013 04:36:46
Current_Time      = 21-FEB-2013 04:37:11

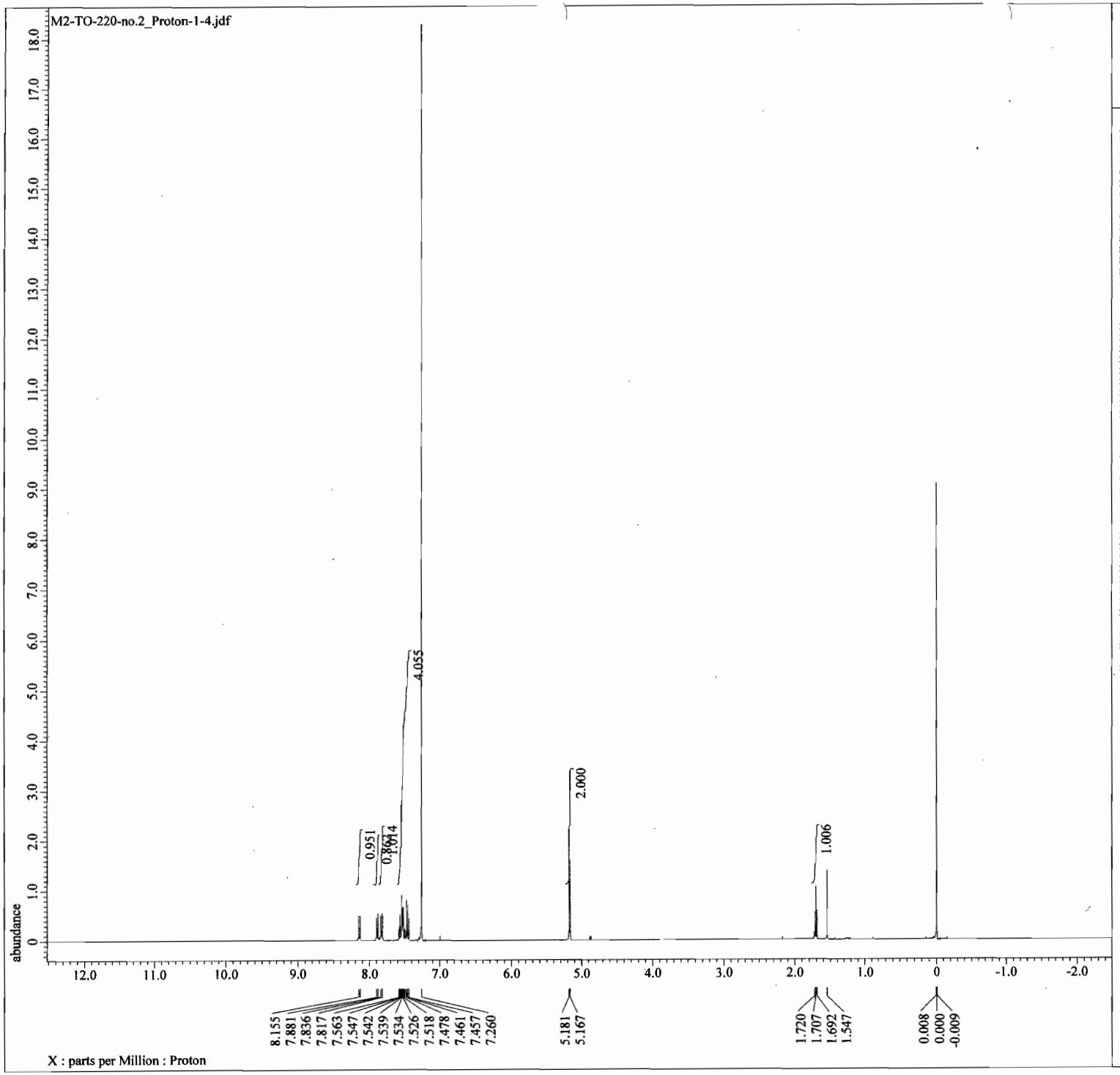
Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.42499681[T] (400[MHz])
X_Acq_Duration    = 1.03809024[s]
X_Domain          = 13C
X_Freq            = 100.90247863[MHz]
X_Offset          = 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          = 401.28219856[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 19.9[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       = 22.69[dB]
Irr_Atn_Noe       = 22.69[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.03809024[s]
```

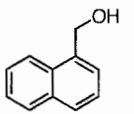


4f

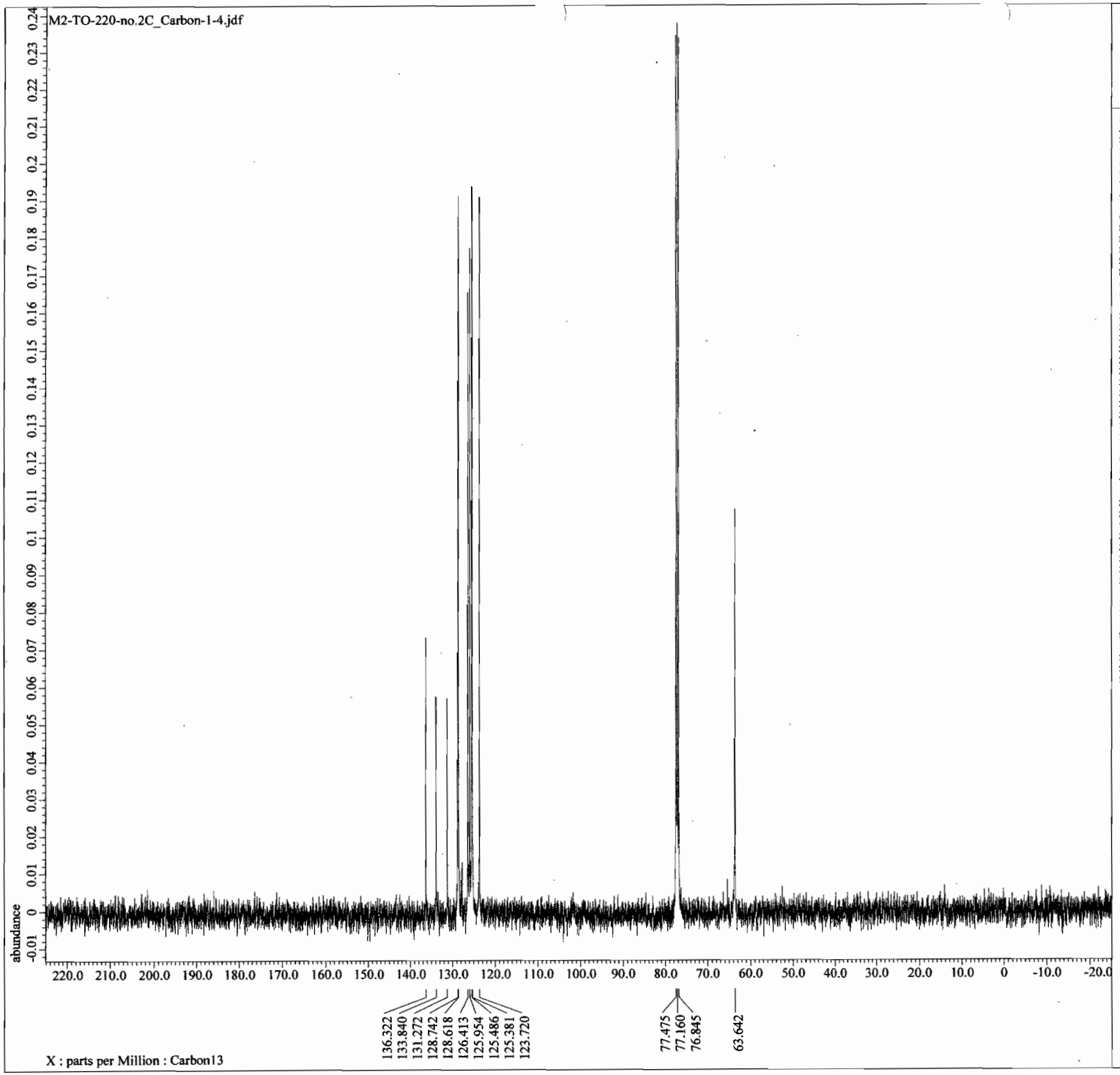


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= M2-TO-220-no.2
Solvent	= CHLOROFORM-D
Creation_Time	= 30-JAN-2013 22:25:15
Revision_Time	= 31-JAN-2013 14:07:40
Current_Time	= 31-JAN-2013 14:07:51
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
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	= 7.53012048[kHz]
X_Sweep_Clipped	= 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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 54
Temp_Get	= 20[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]

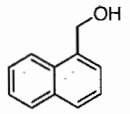


4g

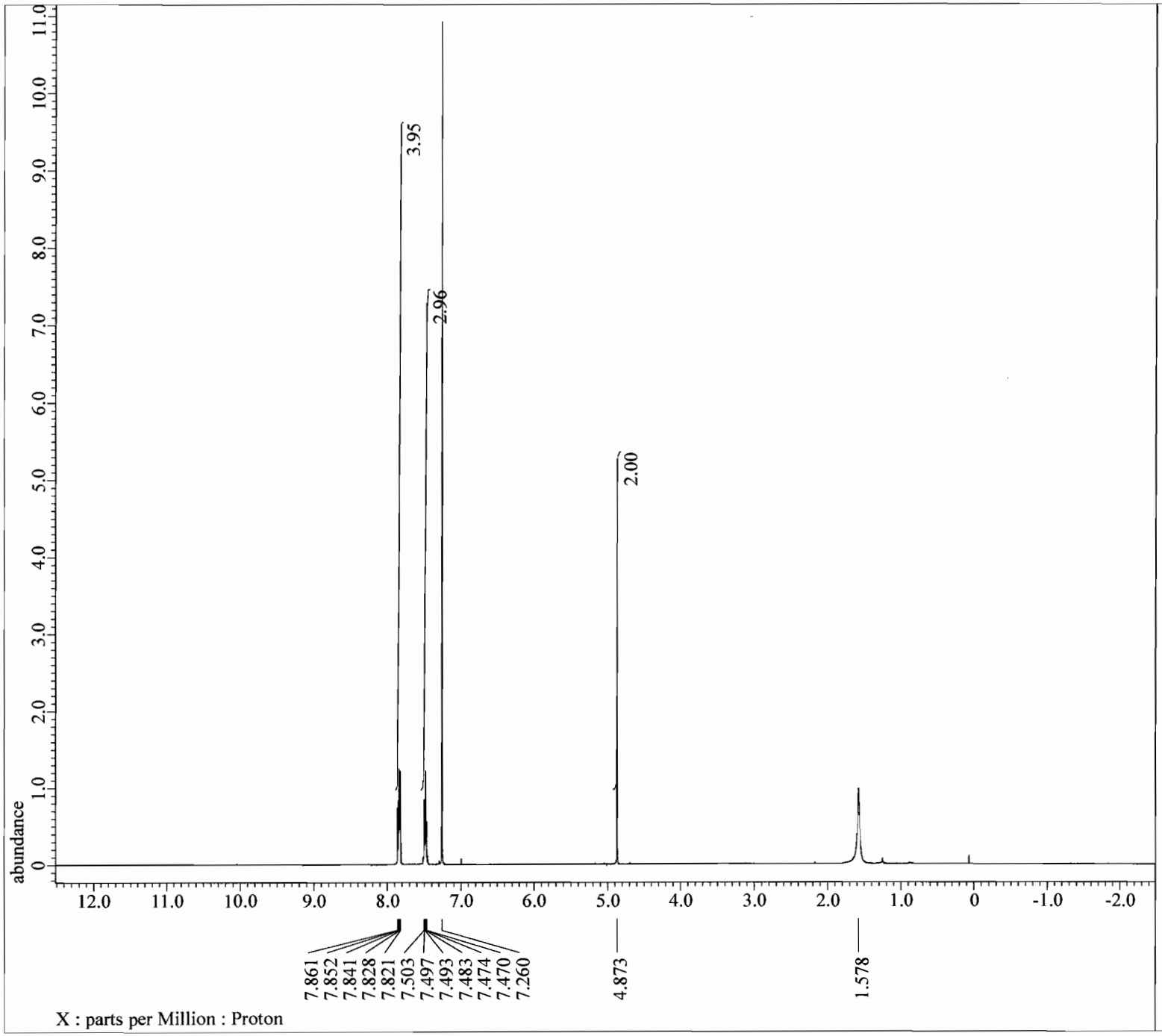


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= M2-TO-220-no.2C
Solvent	= CHLOROFORM-D
Creation_Time	= 30-JAN-2013 22:31:28
Revision_Time	= 31-JAN-2013 14:10:25
Current_Time	= 31-JAN-2013 14:11:21
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 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	= 401.28219856[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20[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_Noe	= 22.691[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.03809024[s]



4g

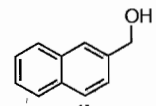



```
Filename          = /Users/tktk0112/NMR/tk-269
Author            = delta
Experiment        = proton.jxp
Sample_Id         = tk-269-13-14
Solvent           = CHLOROFORM-D
Creation_Time     =  4-MAR-2013 23:37:02
Revision_Time     =  6-MAR-2013 17:32:45
Current_Time      =  6-MAR-2013 17:33:28

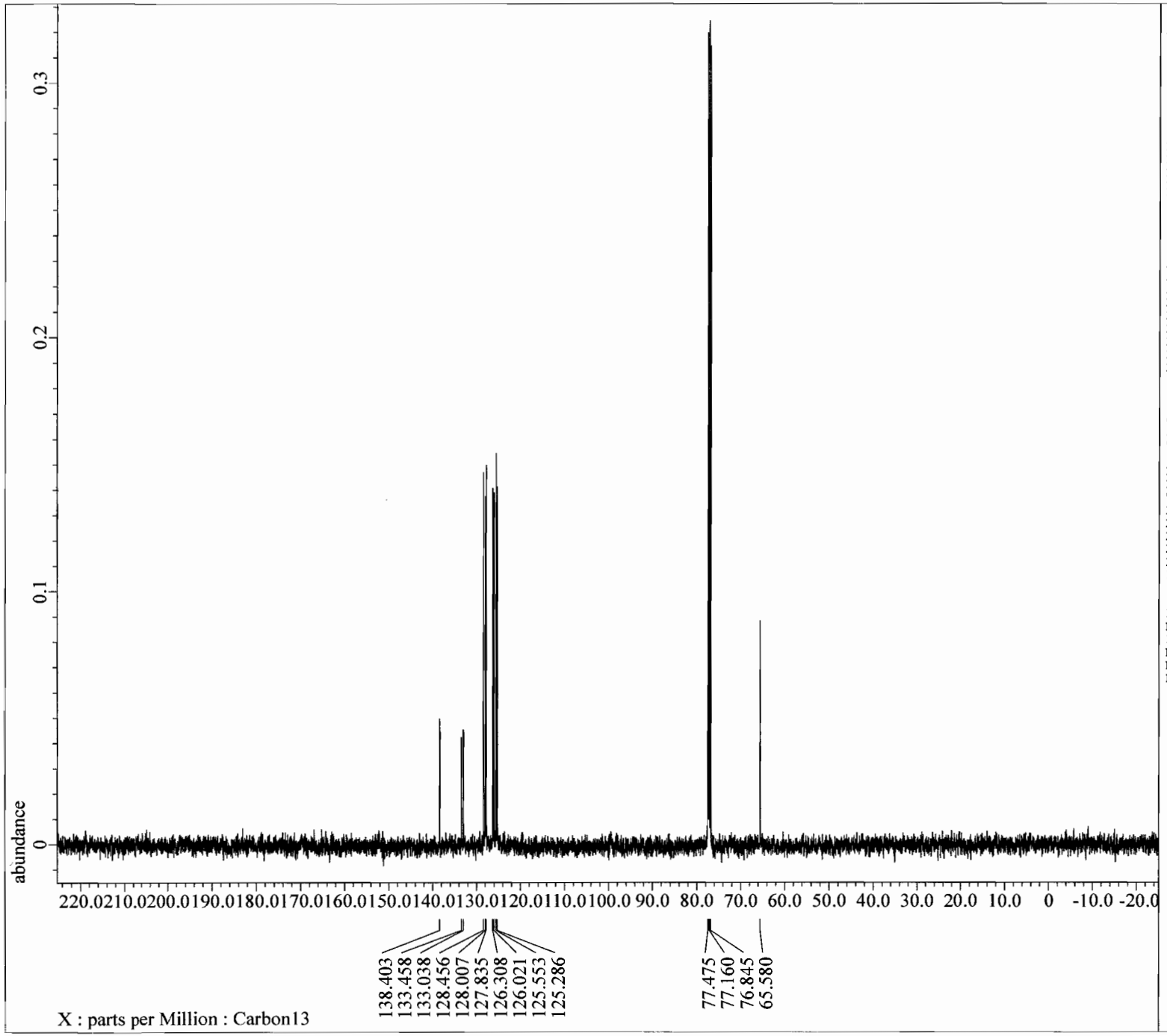
Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

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           = 7.53012048[kHz]
X_Sweep_Clipped   = 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             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 58
Temp_Get          = 19.6[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]
```



4h

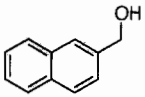



```
Filename          = /Users/tktk0112/NMR/tk-267
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = tk-267-13C
Solvent           = CHLOROFORM-D
Creation_Time     = 28-FEB-2013 01:11:18
Revision_Time     =  6-MAR-2013 17:40:21
Current_Time      =  6-MAR-2013 17:40:49

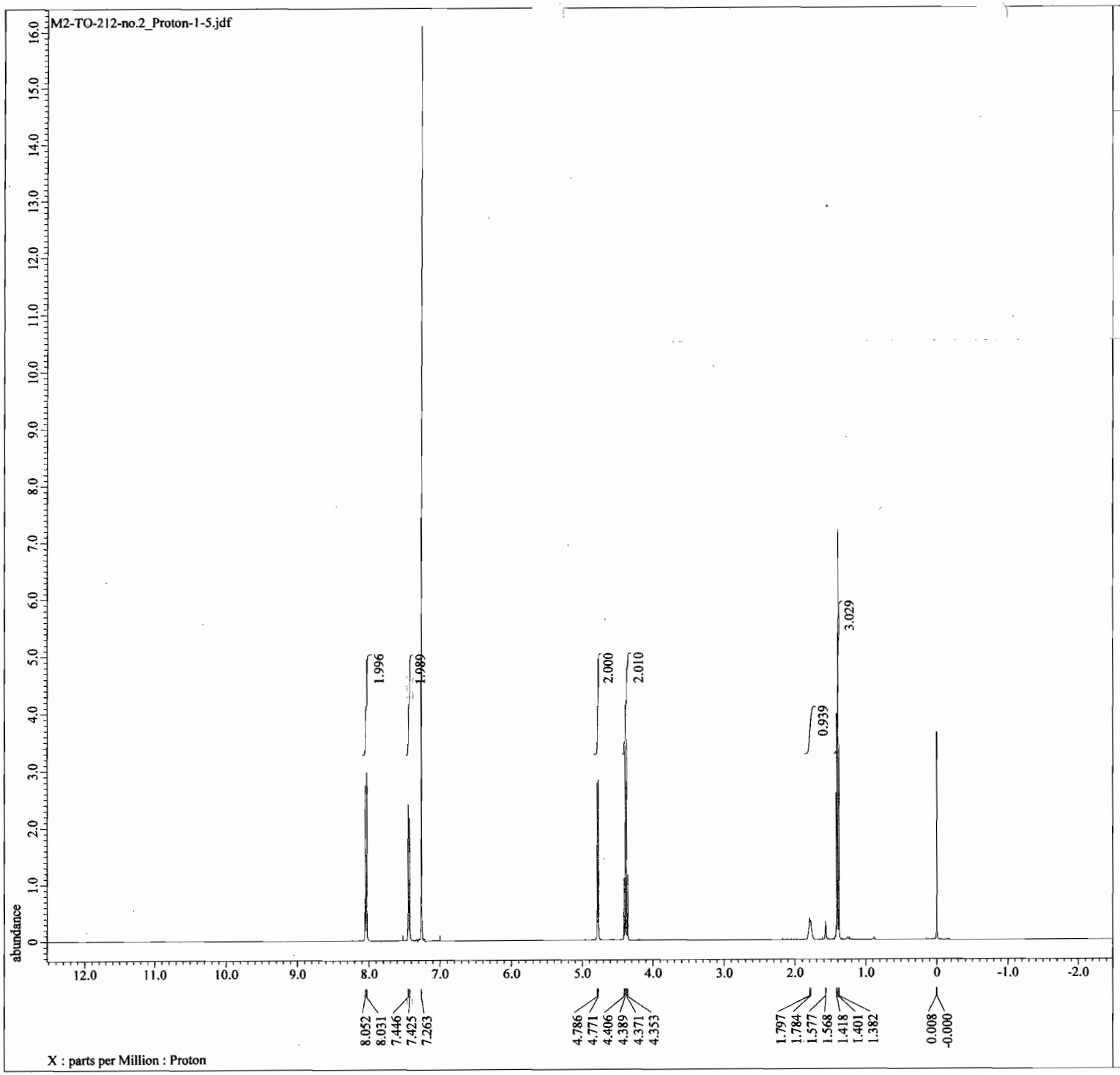
Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.42499681[T] (400[MHz])
X_Acq_Duration    = 1.03809024[s]
X_Domain          = 13C
X_Freq            = 100.90247863[MHz]
X_Offset          = 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          = 401.28219856[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 128
Total_Scans       = 128

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 20.4[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_Noe       = 22.691[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.03809024[s]
```

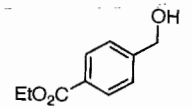


4h

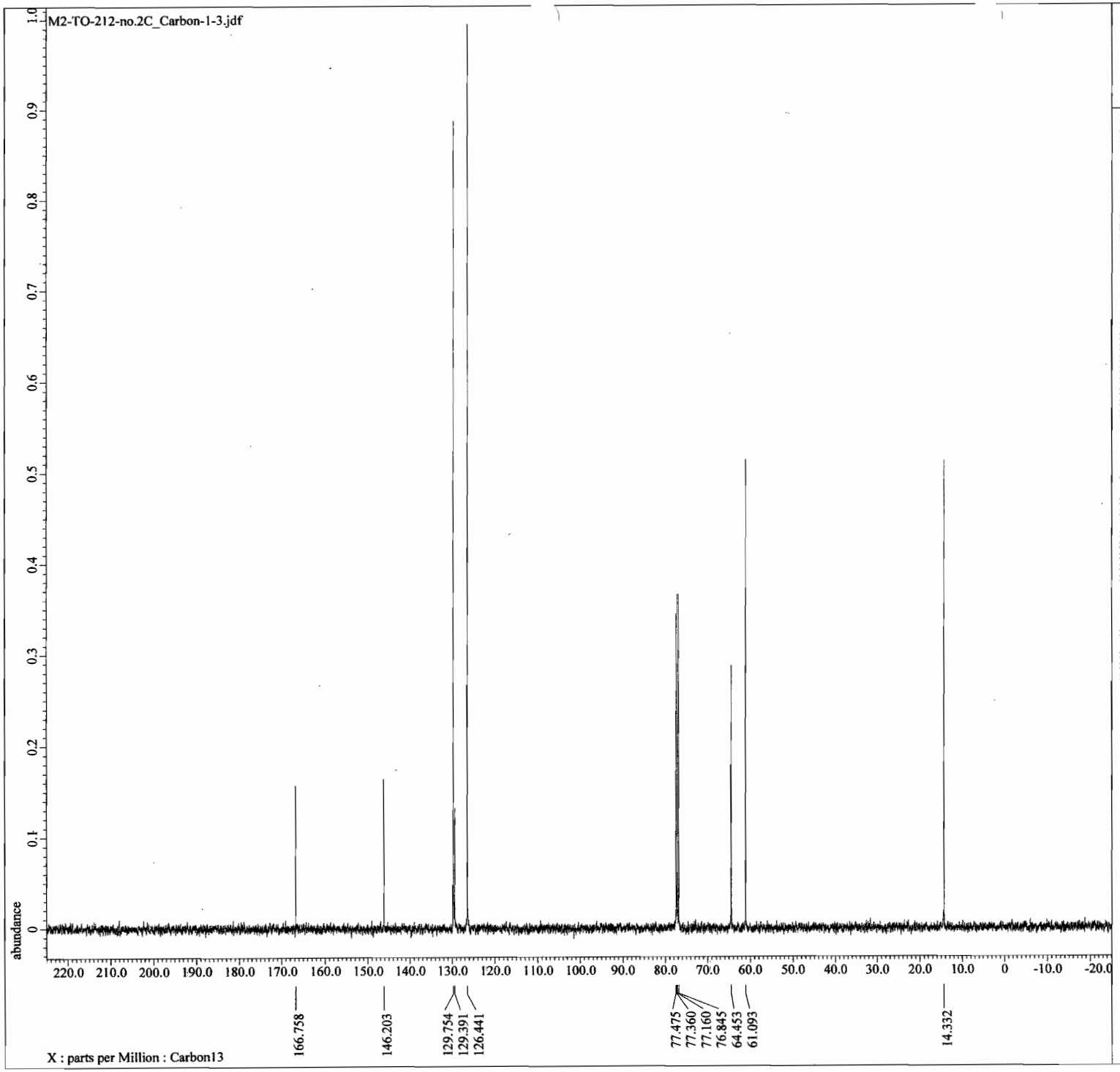


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= M2-TO-212-no.2
Solvent	= CHLOROFORM-D
Creation_Time	= 21-JAN-2013 19:55:50
Revision_Time	= 21-JAN-2013 21:00:35
Current_Time	= 21-JAN-2013 21:03:47
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
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	= 7.53012048[kHz]
X_Sweep_Clipped	= 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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 50
Temp_Get	= 20.2[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]

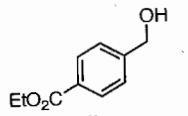


4i

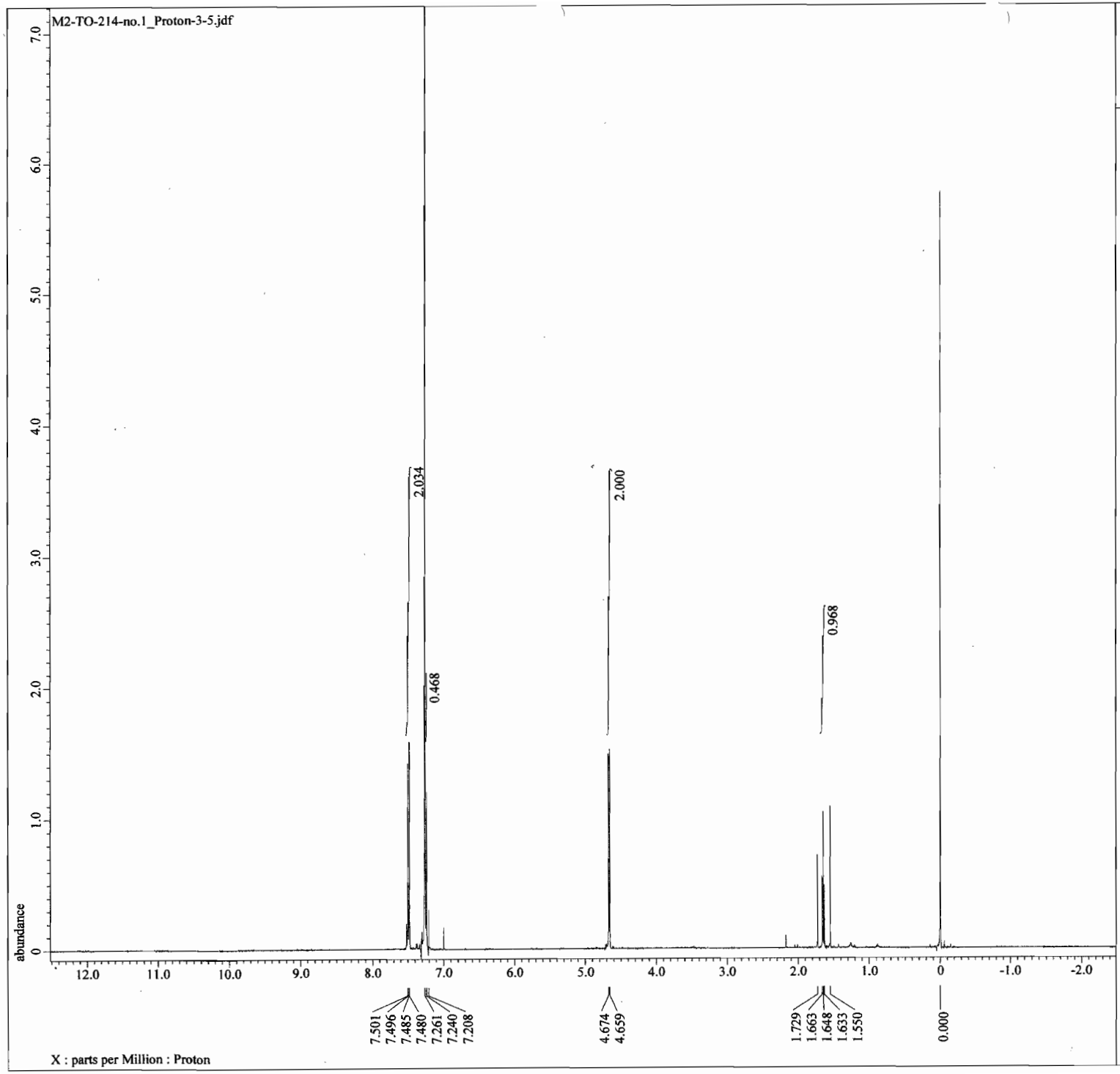


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= M2-TO-212-no.2C
Solvent	= CHLOROFORM-D
Creation_Time	= 21-JAN-2013 20:00:23
Revision_Time	= 21-JAN-2013 21:02:13
Current_Time	= 21-JAN-2013 21:06:55
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 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	= 401.28219856[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.6[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_Noe	= 22.691[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.03809024[s]

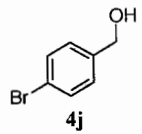


4i

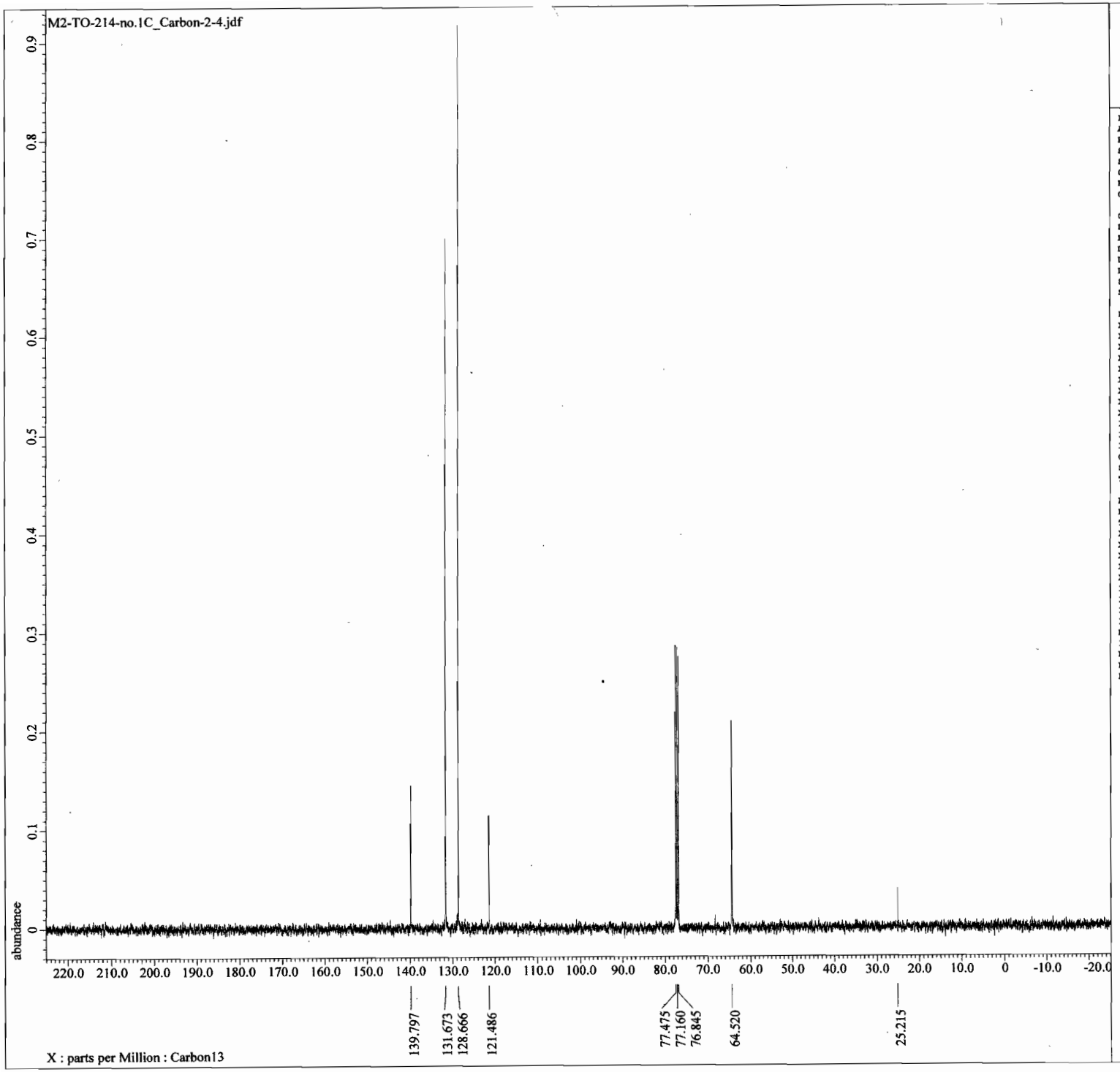


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= M2-TO-214-no.1
Solvent	= CHLOROFORM-D
Creation_Time	= 22-JAN-2013 19:23:43
Revision_Time	= 22-JAN-2013 21:25:03
Current_Time	= 22-JAN-2013 21:25:20
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-EC8400
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	= 7.53012048[kHz]
X_Sweep_Clipped	= 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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 54
Temp_Get	= 19.9[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]

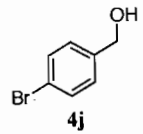


4j

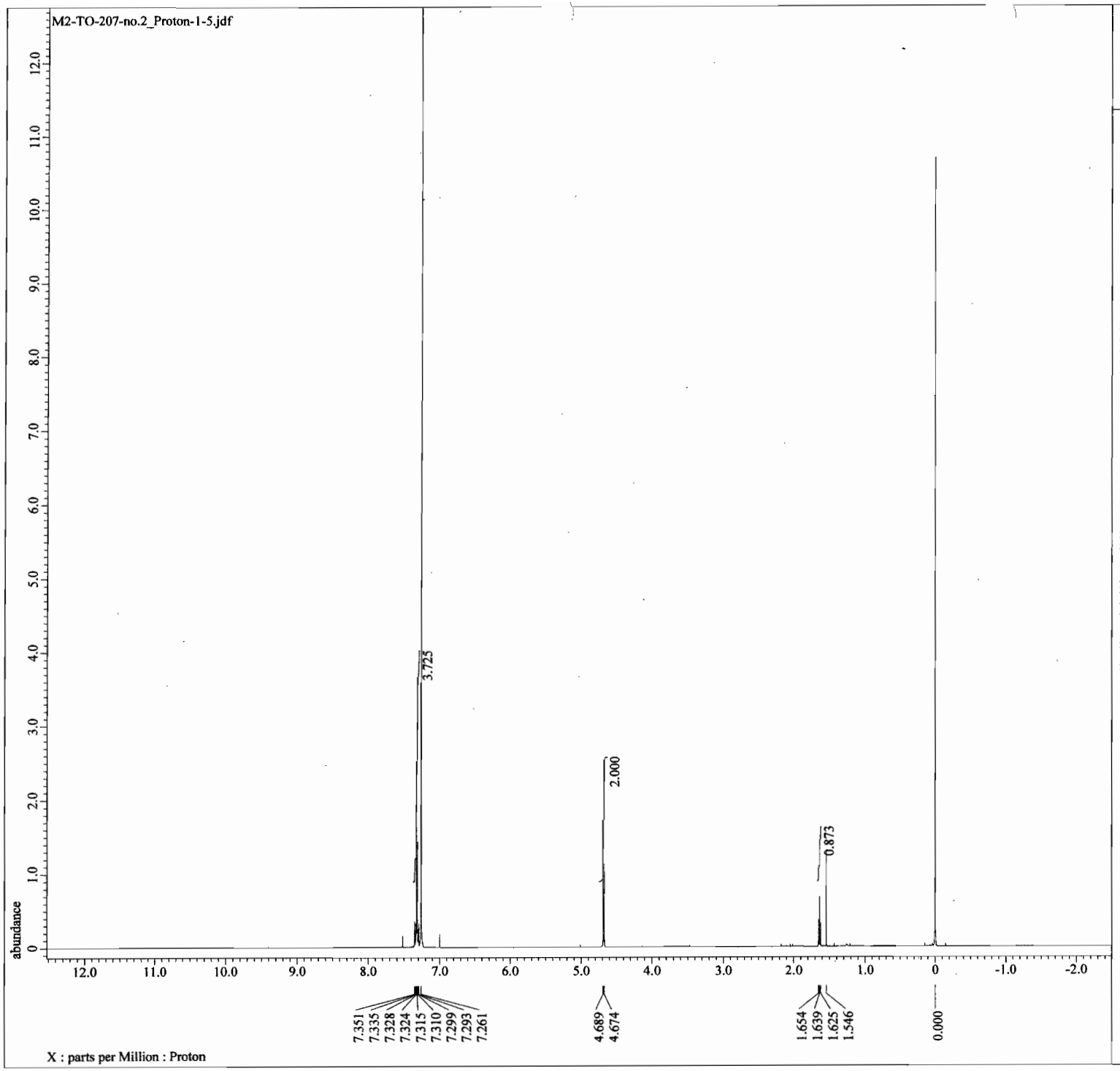


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= M2-TO-214-no.1C
Solvent	= CHLOROFORM-D
Creation_Time	= 22-JAN-2013 19:33:24
Revision_Time	= 22-JAN-2013 21:23:04
Current_Time	= 22-JAN-2013 21:23:38
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 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	= 401.28219856[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.6[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	= 22.69[dB]
Irr_Atn_Noe	= 22.69[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.03809024[s]

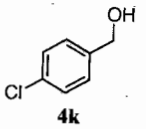


4j

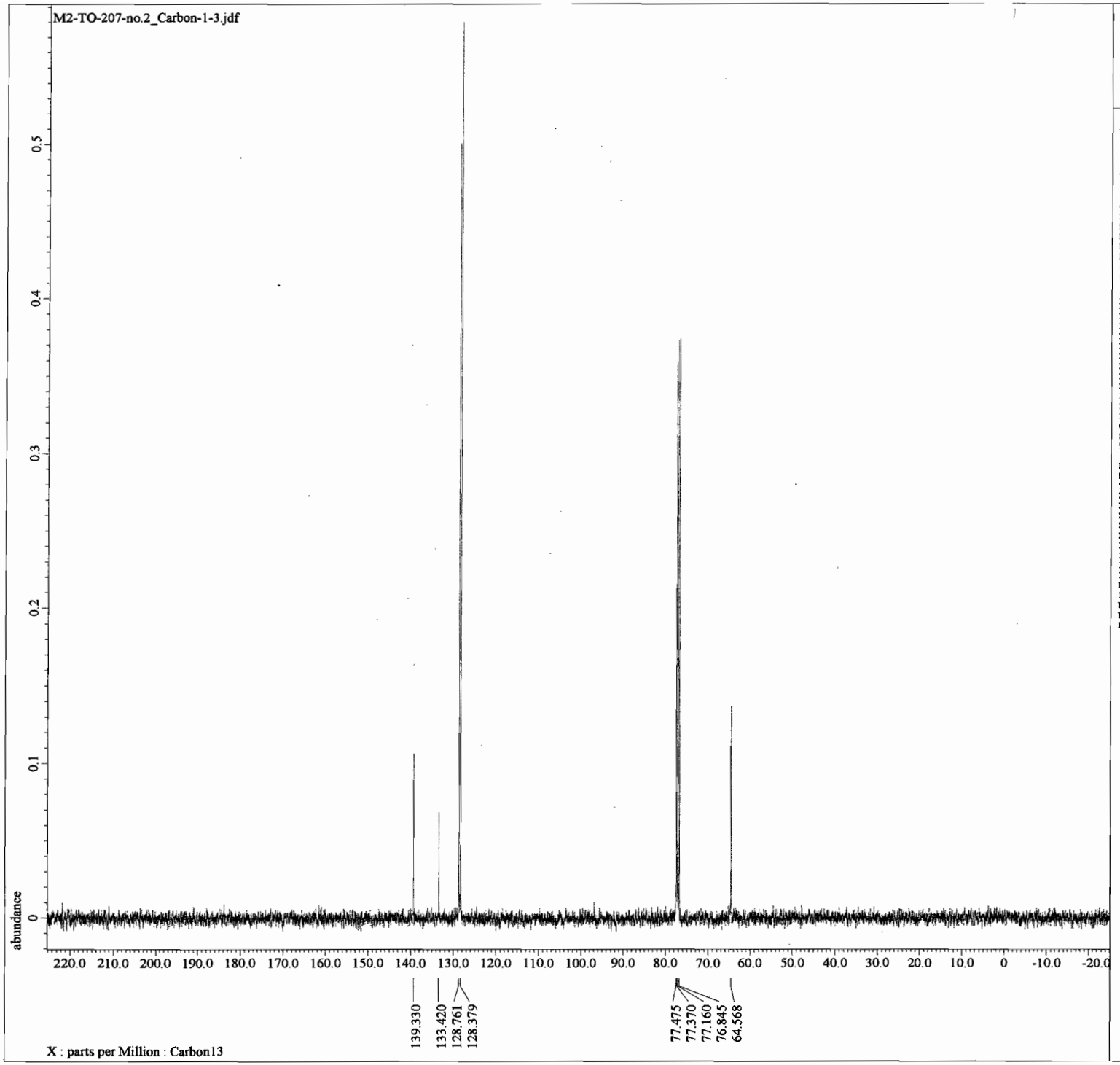


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= M2-TO-207-no.2
Solvent	= CHLOROFORM-D
Creation_Time	= 17-JAN-2013 20:15:41
Revision_Time	= 18-JAN-2013 10:38:02
Current_Time	= 18-JAN-2013 10:38:28
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
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	= 7.53012048[kHz]
X_Sweep_Clipped	= 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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 54
Temp_Get	= 20[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]

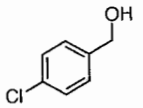


4k

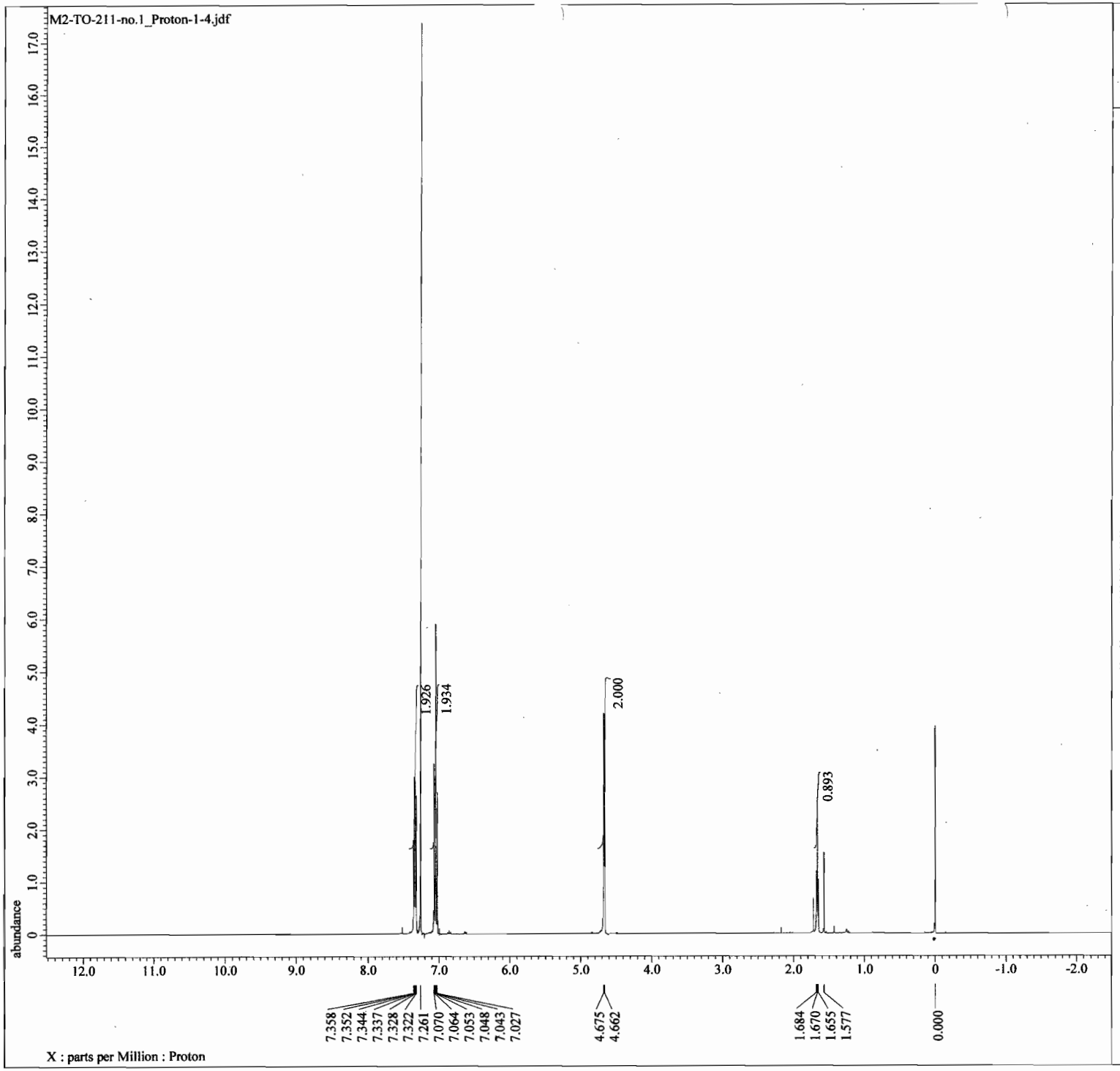


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= M2-TO-207-no.2
Solvent	= CHLOROFORM-D
Creation_Time	= 18-JAN-2013 10:34:41
Revision_Time	= 18-JAN-2013 10:34:31
Current_Time	= 18-JAN-2013 10:35:45
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 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	= 401.28219856[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 70
Total_Scans	= 70
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.6[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_Noe	= 22.691[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.03809024[s]

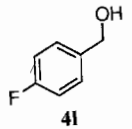


4k

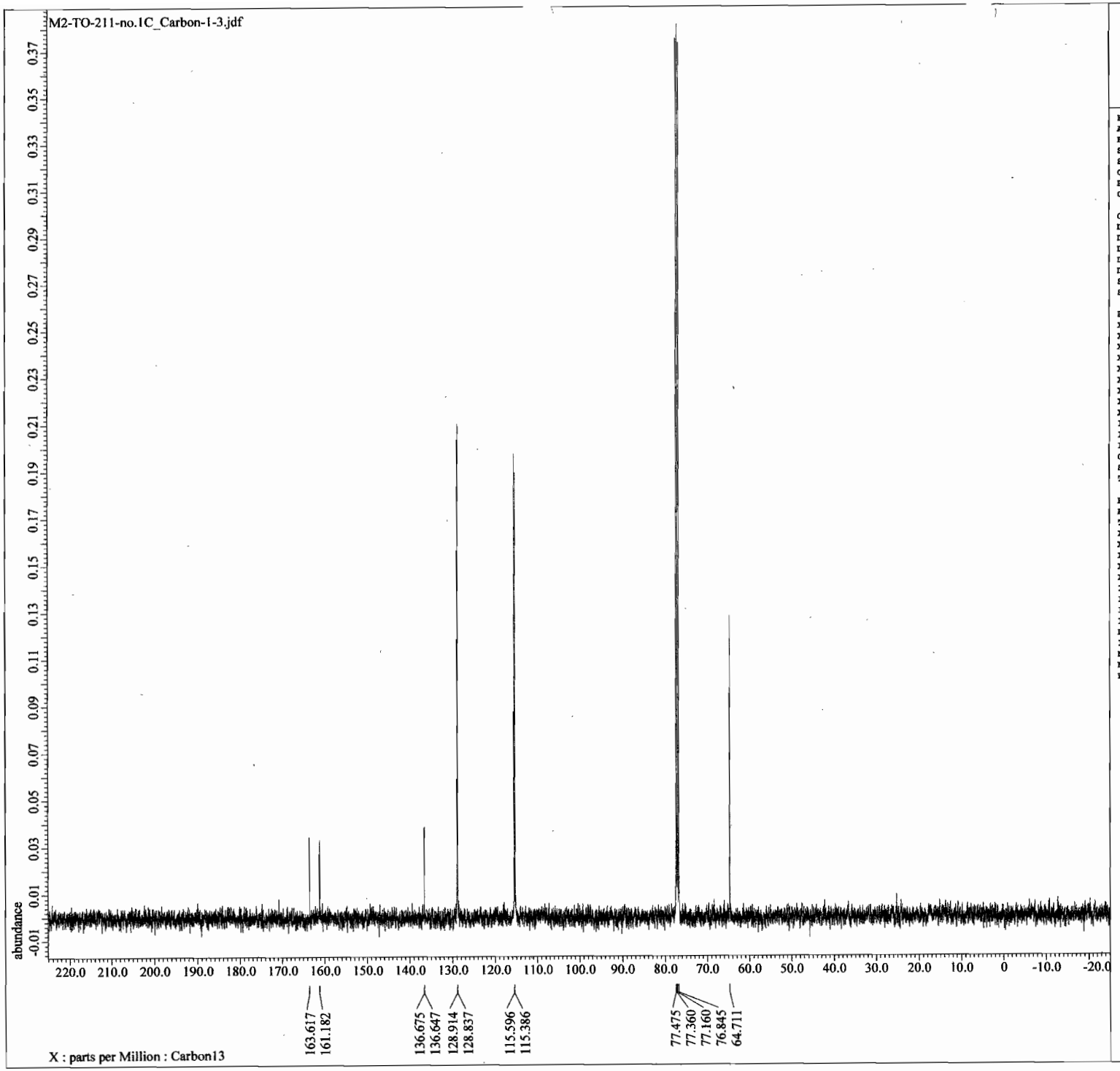


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= M2-TO-211-no.1
Solvent	= CHLOROFORM-D
Creation_Time	= 21-JAN-2013 10:50:19
Revision_Time	= 21-JAN-2013 10:46:58
Current_Time	= 21-JAN-2013 10:47:15
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
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	= 7.53012048[kHz]
X_Sweep_Clipped	= 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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 50
Temp_Get	= 19.9[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]

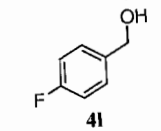


41

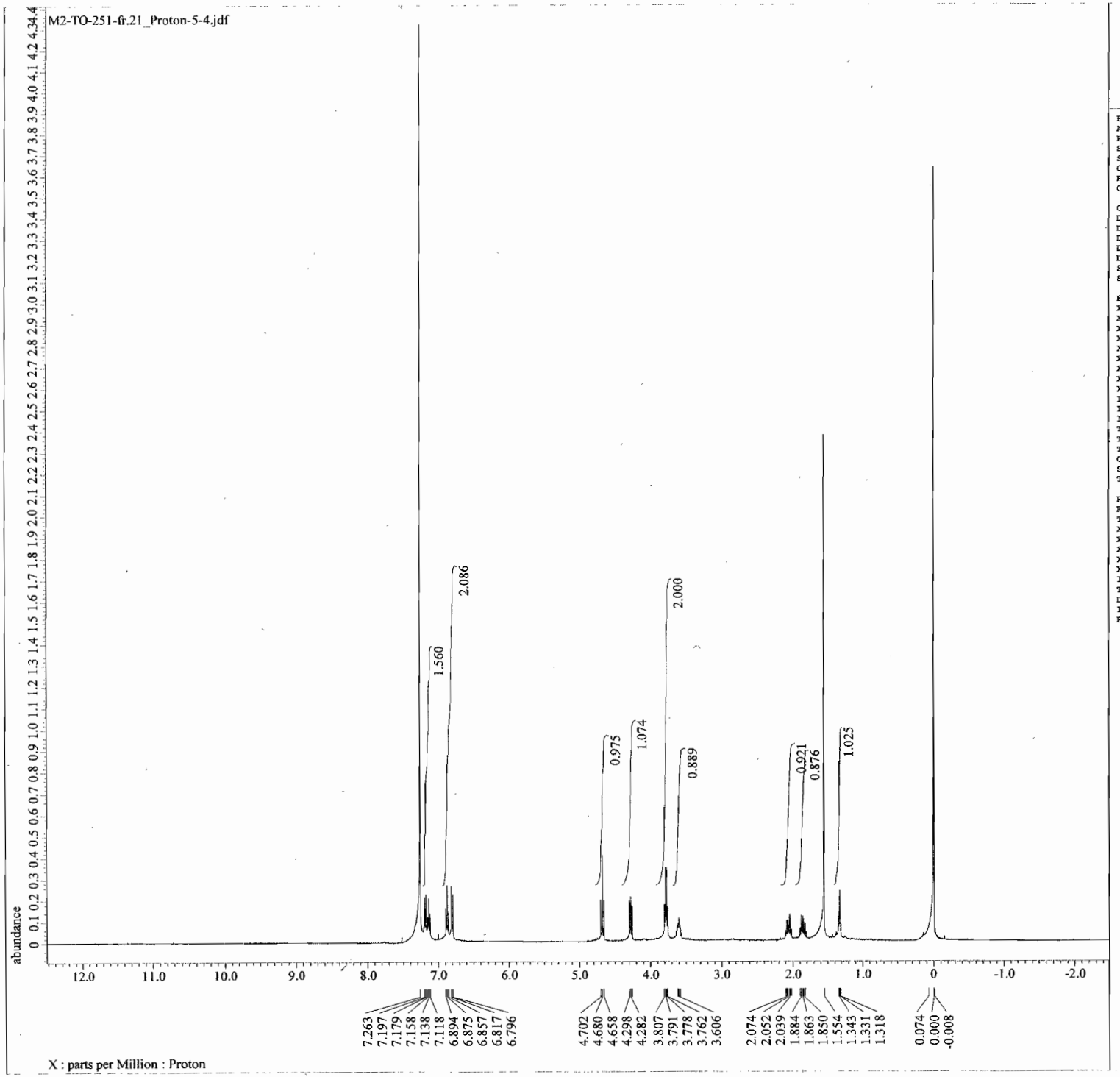


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= M2-TO-211-no.1C
Solvent	= CHLOROFORM-D
Creation_Time	= 21-JAN-2013 10:41:12
Revision_Time	= 21-JAN-2013 19:42:11
Current_Time	= 21-JAN-2013 19:43:05
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 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	= 401.28219856[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 103
Total_Scans	= 103
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.9[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_Noe	= 22.691[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.03809024[s]



41



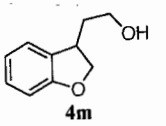
JEOL RESONANCE

```
Filename          = \Users\delta\Documents\JEO
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M2-TO-251-fr.21
Solvent           = CHLOROFORM-D
Creation_Time     =  8-MAR-2013 21:26:23
Revision_Time     =  8-MAR-2013 21:26:07
Current_Time      =  8-MAR-2013 21:27:12

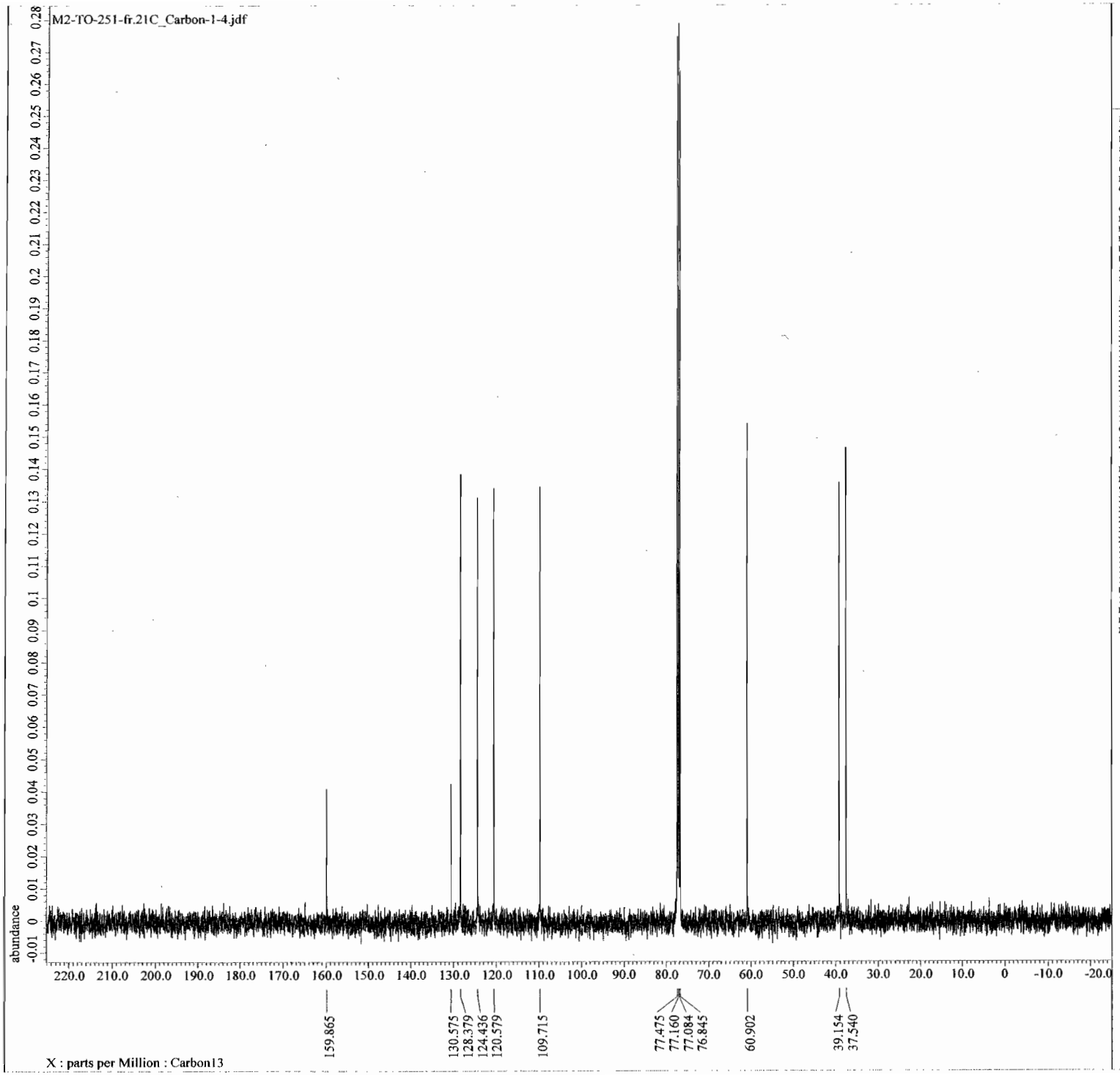
Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-EC8400
Spectrometer      = DELTA2_NMR

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           = 7.53012048[kHz]
X_Sweep_Clipped   = 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             = 32
Total_Scans       = 32

Relaxation_Delay = 5[s]
Recvr_Gain        = 56
Temp_Get          = 20.3[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]
```

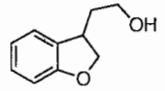


4m

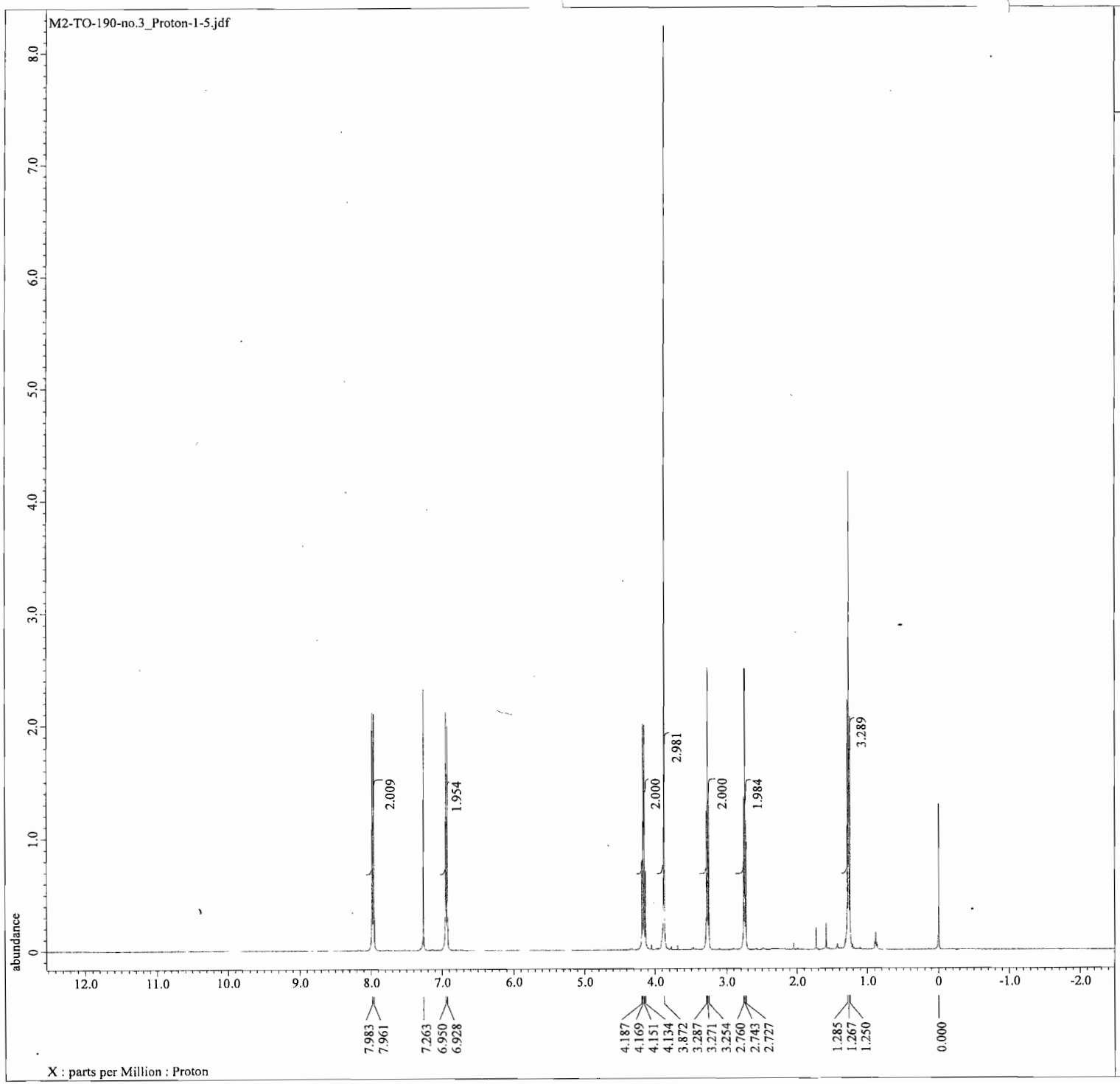


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= M2-TO-251-fr.21C
Solvent	= CHLOROFORM-D
Creation_Time	= 8-MAR-2013 19:41:08
Revision_Time	= 8-MAR-2013 20:01:05
Current_Time	= 8-MAR-2013 20:01:54
Comment	= single pulse decouplad gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 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	= 401.28219856[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.2[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_Noe	= 22.691[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.03809024[s]

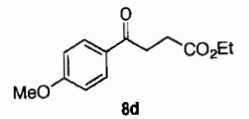


4m

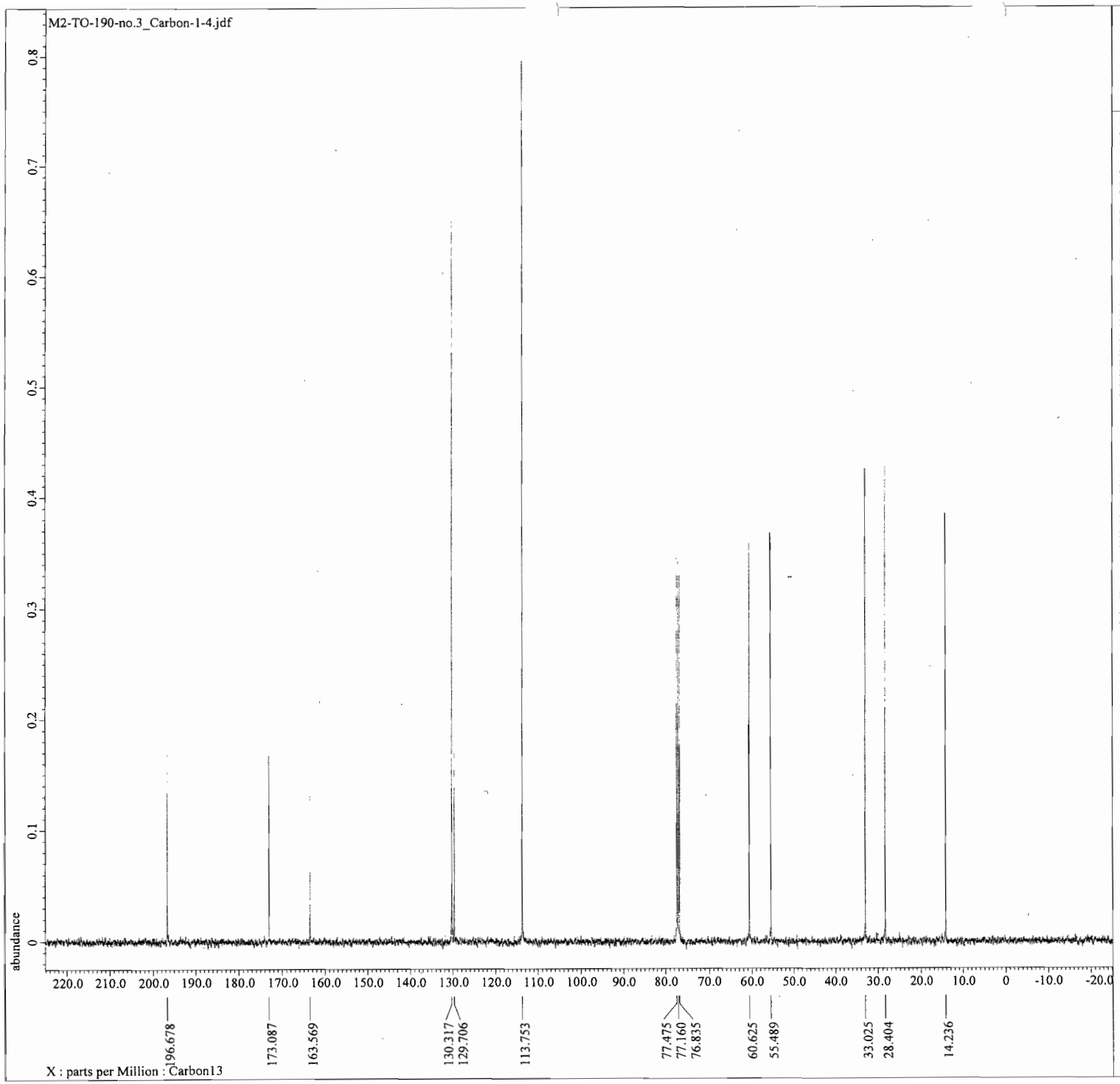


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= M2-TO-190-no.3
Solvent	= CHLOROFORM-D
Creation_Time	= 11-DEC-2012 18:00:27
Revision_Time	= 11-DEC-2012 18:40:33
Current_Time	= 11-DEC-2012 18:44:56
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
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	= 7.53012048[kHz]
X_Sweep_Clipped	= 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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 20.3[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]

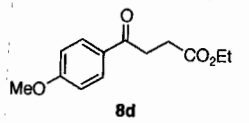


8d

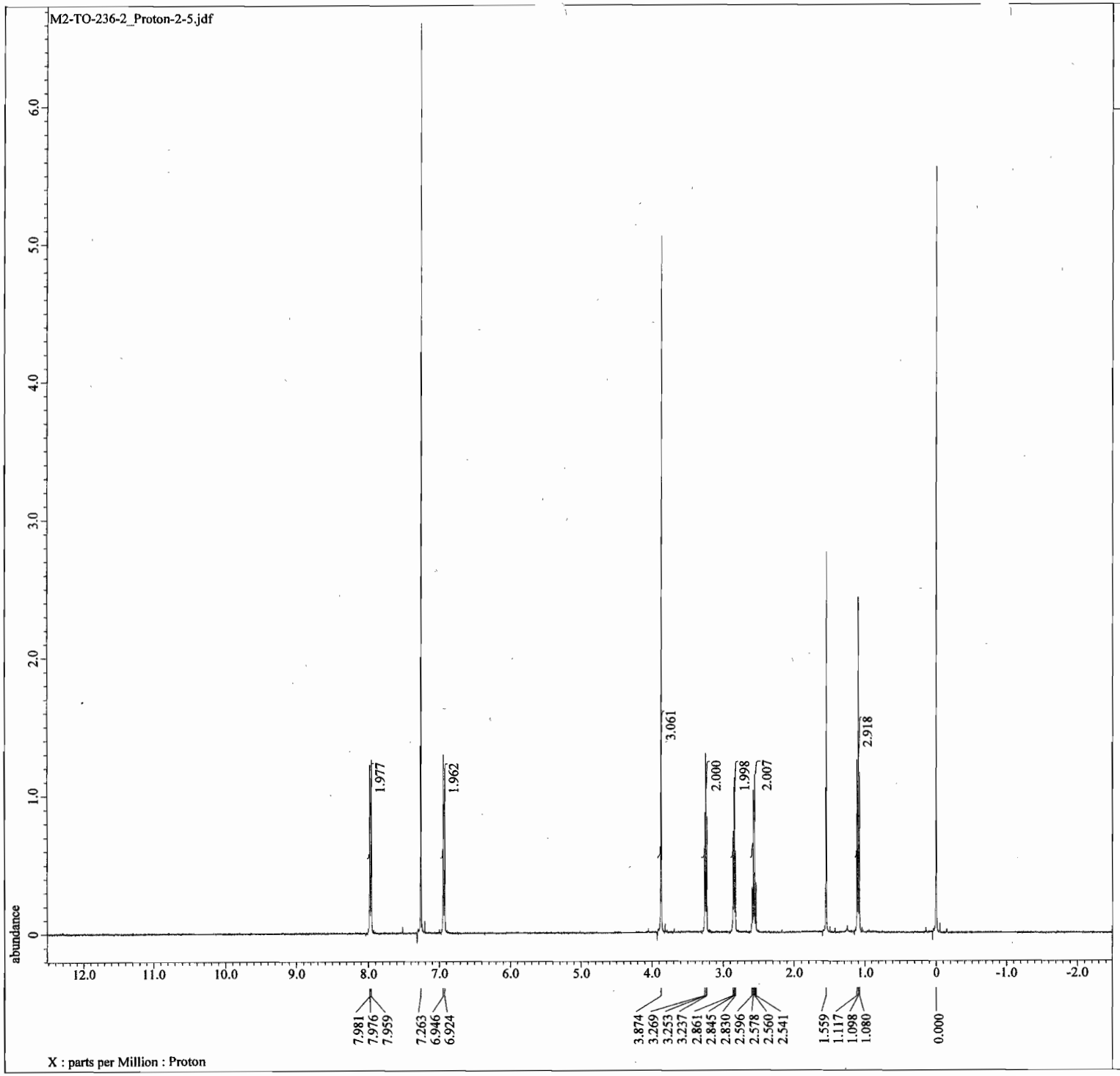


JEOL RESONANCE

Filename	= C:\Users\delta\Documents\J
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= M2-TO-190-no.3
Solvent	= CHLOROFORM-D
Creation_Time	= 11-DEC-2012 20:37:19
Revision_Time	= 12-DEC-2012 13:04:14
Current_Time	= 12-DEC-2012 13:04:20
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 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	= 401.28219856[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.9[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_Noe	= 22.691[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.03809024[s]

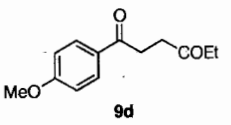


8d

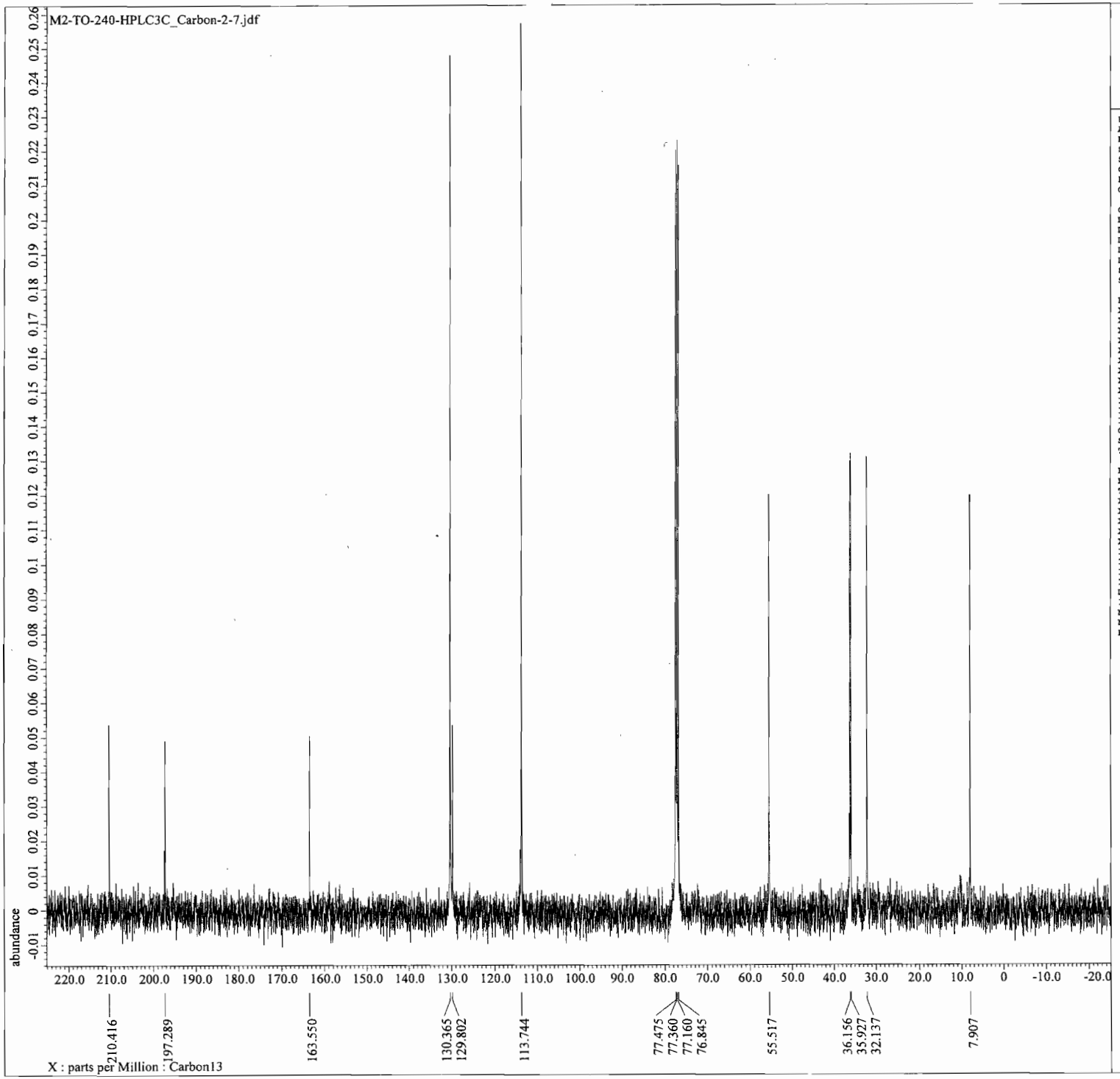


JEOL RESONANCE

Filename	= \Users\delta\Documents\JEO
Author	= delta
Experiment	= proton.jxp 240
Sample_Id	= M2-TO-~~236~~-2
Solvent	= CHLOROFORM-D
Creation_Time	= 4-MAR-2013 19:44:48
Revision_Time	= 4-MAR-2013 21:51:22
Current_Time	= 4-MAR-2013 21:52:54
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
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	= 7.53012048[kHz]
X_Sweep_Clipped	= 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	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.7[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]



9d



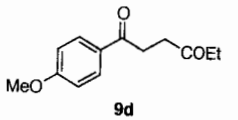
JEOL RESONANCE

```
Filename          = \Users\delta\Documents\JEO
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M2-TO-240-HPLC3C
Solvent           = CHLOROFORM-D
Creation_Time     = 22-FEB-2013 23:51:51
Revision_Time     = 23-FEB-2013 00:44:26
Current_Time      = 23-FEB-2013 00:44:51

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
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          = 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          = 401.28219856[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 20.2[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_Noe       = 22.691[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.03809024[s]
```



9d