

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*-anisaldehyde/AcOH/H₂SO₄/EtOH, or 12MoO₃·H₃PO₄/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 CHCl₃ as eluent. ¹H NMR spectra were recorded with a JEOL JMN-ECS400 (400 MHz) spectrometer referenced to the solvent peak at 7.26 ppm. ¹³C 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-BH₃ was prepared from diMeImd-CO₂ 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.

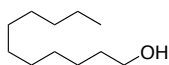
Typical Procedure for the Hydroxymethylation of alkyl iodides

1-Iodoadamantane (131 mg, 0.50 mmol), diMe-Imd-BH₃ (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%).

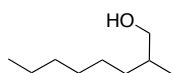
Typical Procedure for the Hydroxymethylation of aryl iodides (Table 1, entry 3)

4-Iodoanisole (116 mg, 0.50 mmol), diMe-Imd-BH₃ (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%).

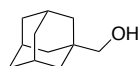
Spectroscopic Data



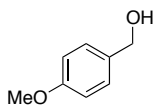
1-Undecanol (4a). ^1H NMR (CDCl_3 , 400 MHz): δ 0.88 (t, J = 5.6 Hz, 3H), 1.18-1.50 (m, 16H), 1.53-1.58 (m, 2H), 3.64 (t, J = 7.2 Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 14.27, 22.83, 25.87, 29.48, 29.58, 29.76, 32.05, 32.93, 63.23. This product is commercially available and the ^1H - and ^{13}C -NMR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



2-methyloctanol⁴ (4b). ^1H 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.

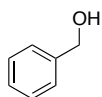


1-adamantanemethanol (4c). ^1H NMR (CDCl_3 , 400 MHz): δ 1.32 (m, 1H), 1.46-1.54 (m, 6H), 1.60-1.67 (m, 3H), 1.69-1.76 (m, 3H), 1.95-2.01 (m, 3H), 3.20 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 28.27, 34.57, 37.26, 39.13, 73.91. This product is commercially available and the ^1H - and ^{13}C -NMR spectra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

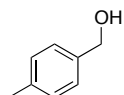


(4-methoxyphenyl)methanol (4d) ^1H NMR (CDCl_3 , 400 MHz): δ 1.53 (t, J = 6.0 Hz, 1H), 3.81 (s, 3H), 4.62 (d, J = 6.0 Hz, 2H), 6.88-6.92 (m, 2H), 7.29-7.31 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 55.42, 65.16, 114.07, 128.79, 133.22, 159.32. This product is commercially available and the ^1H - and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

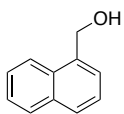
⁴ Silver, S.; Puranen, A.; Sjöholm, R.; Repo, T.; Leino, R. *Eur. J. Inorg. Chem.* **2005**, 1514.



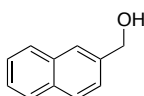
benzyl alcohol (4e) ^1H NMR (CDCl_3 , 400 MHz): δ 1.60-1.66 (m, 1H), 4.71 (d, J = 6.0 Hz, 2H), 7.26-7.38 (m, 5H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 65.16, 127.05, 127.64, 128.58, 140.91. This product is commercially available and the ^1H - and ^{13}C -NMR spectra are consistent with those of the authentic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



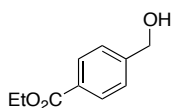
(4-methylphenyl)methyl alcohol (4f) ^1H NMR (CDCl_3 , 400 MHz): δ 1.54 (t, J = 6.0 Hz, 1H), 2.36 (s, 3H), 4.66 (d, J = 6.0 Hz, 2H), 7.18 (d, J = 7.6 Hz, 2H), 7.27 (d, J = 7.6 Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 21.25, 65.27, 127.21, 129.32, 137.44, 137.99. This product is commercially available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



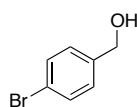
1-naphthylmethanol (4g) ^1H NMR (CDCl_3 , 400 MHz): δ 1.71 (t, J = 6.0 Hz, 1H), 5.17 (d, J = 6.0 Hz, 2H), 7.44-7.58 (m, 4H), 7.82-7.90 (m, 2H), 8.14 (d, J = 8.0 Hz, 1H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 63.64, 123.72, 125.38, 125.48, 125.95, 126.41, 128.62, 128.74, 131.27, 133.84, 136.32. This product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



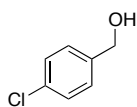
2-naphthylmethanol (4h) ^1H NMR (CDCl_3 , 400 MHz): δ 4.87 (s, 2H), 7.45-7.52 (m, 3H), 7.81-7.87 (m, 4H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 65.58, 125.29, 125.55, 126.02, 126.31, 127.84, 128.01, 128.46, 133.04, 133.46, 138.40. This product is commercially available and the ^1H - and ^{13}C -NMR spectra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



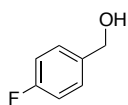
4-hydroxymethylbenzoic acid ethyl ester⁵ (4i) ¹H-NMR (CDCl₃, 400MHz) δ: 1.40 (t, *J* = 6.9 Hz, 3H), 1.76-1.82 (br, 1H), 4.35 (q, *J* = 6.9 Hz, 2H), 4.78 (d, *J* = 6.0 Hz, 2H), 7.43, (d, *J* = 8.3 Hz, 2H), 8.04 (d, *J* = 8.3 Hz, 2H); ¹³C NMR (CDCl₃, 100 MHz) δ 14.33, 61.09, 64.45, 126.44, 129.39, 129.75, 146.20, 166.76.



4-Bromophenylmethanol (4j) ¹H NMR (CDCl₃, 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); ¹³C NMR (CDCl₃, 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.

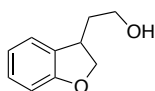


4-Chlorophenyl methanol (4k) ¹H-NMR (CDCl₃, 400MHz) δ: 1.64 (t, *J* = 6.0 Hz, 1H), 4.68 (d, *J* = 6.0 Hz, 2H), 7.29-7.35 (m, 4H); ¹³C NMR (CDCl₃, 100 MHz) δ 64.57, 128.38, 128.76, 133.42, 139.33. This product is commercially available and the ¹H- and ¹³C-NMR spectra are consistent with those of the authentic sample.

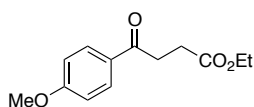


1-fluoro-4-hydroxymethylbenzene (4l) ¹H-NMR (CDCl₃, 400MHz) δ: 1.67 (t, *J* = 5.5 Hz, 1H), 4.67 (d, *J* = 5.2 Hz, 2H), 7.02-7.08 (m, 2H), 7.31-7.36 (m, 2H); ¹³C NMR (CDCl₃, 100 MHz) δ 64.71, 115.49 (d, *J*_{C-F} = 21.0 Hz), 128.88 (d, *J*_{C-F} = 7.7 Hz), 136.66 (d, *J*_{C-F} = 2.8 Hz), 162.40 (d, *J*_{C-F} = 243.5 Hz). This product is commercially available and the ¹H- and ¹³C-NMR spectra are consistent with those of the authentic sample.

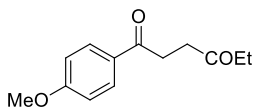
⁵ Murai, N.; Yonaga, M.; Tanaka, K. *Org. Lett.* **2012**, *14*, 1278.



2-(2,3-dihydrobenzofuran-3-yl)ethanol⁶ (4m) ¹H NMR (CDCl₃, 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); ¹³C NMR (CDCl₃, 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-butyl ethyl ester⁷ (8d) ¹H NMR (CDCl₃, 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); ¹³C NMR (CDCl₃, 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.



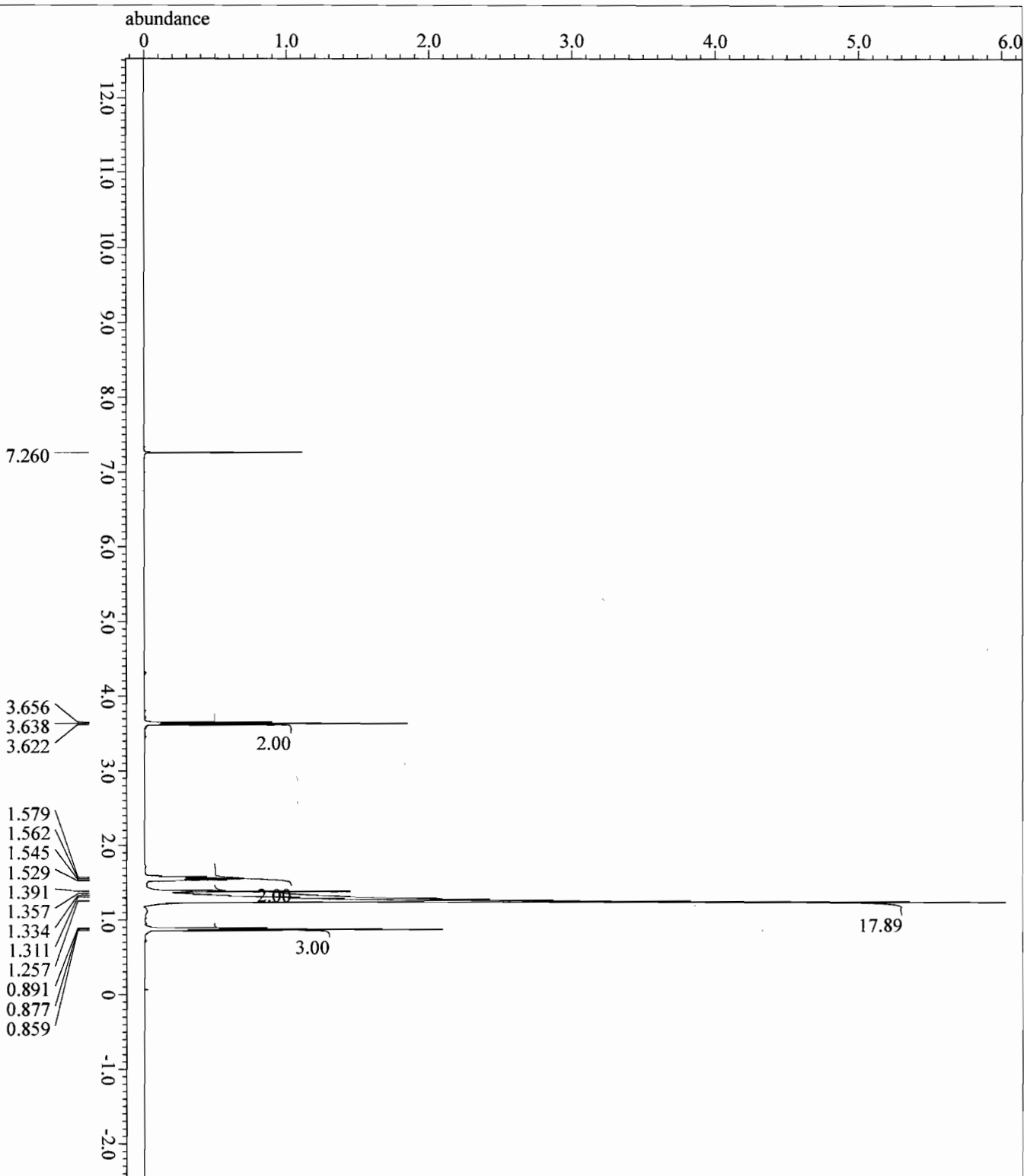
1-(4-methoxyphenyl)hexane-1,4-dione⁸ (9d) ¹H NMR (CDCl₃, 400 MHz): δ 1.10 (t, *J* = 7.2 Hz, 3H), 2.57 (q, *J* = 7.6 Hz, 2H), 2.85 (t, *J* = 6.0 Hz, 2H), 3.25 (t, *J* = 6.4 Hz, 2H), 3.87 (s, 3H), 6.92-6.95 (m, 2H), 7.96-7.98 (m, 2H); ¹³C NMR (CDCl₃, 100 MHz) δ 7.91, 32.14, 35.93, 36.16, 55.52, 113.74, 129.80, 130.37, 163.55, 197.29, 210.42.

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.

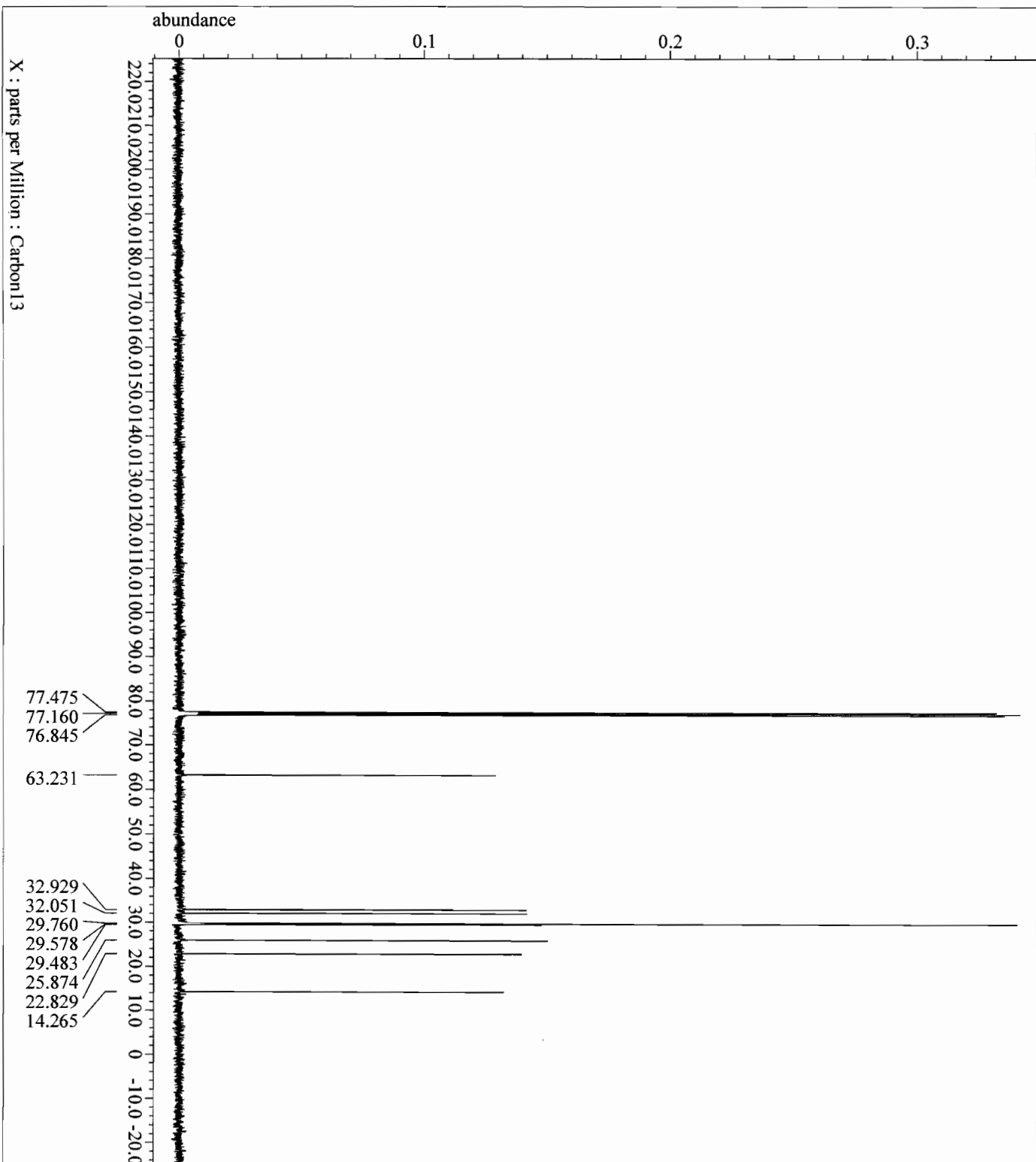
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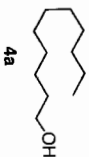
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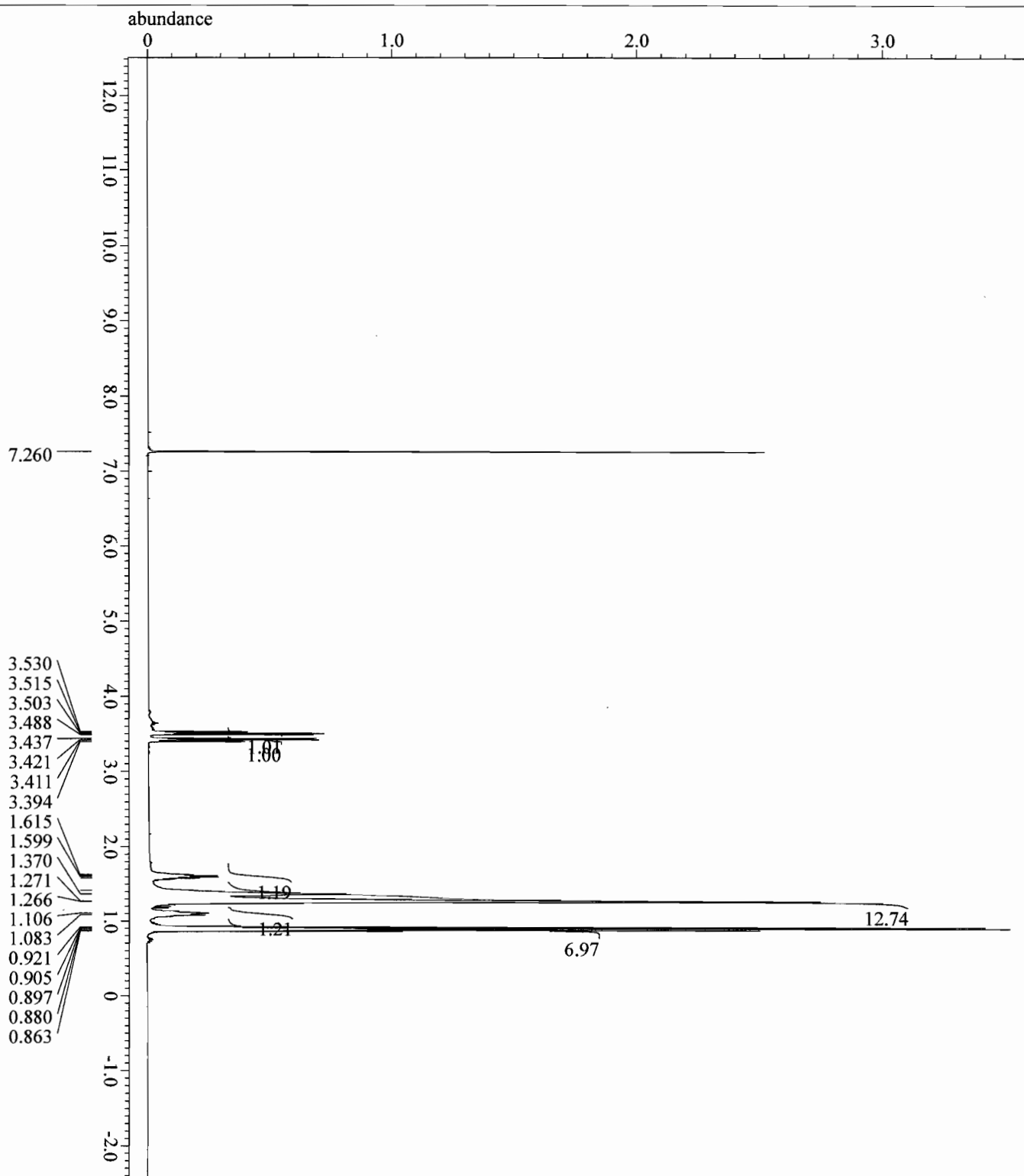


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4a

X : parts per Million : Proton

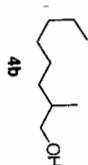


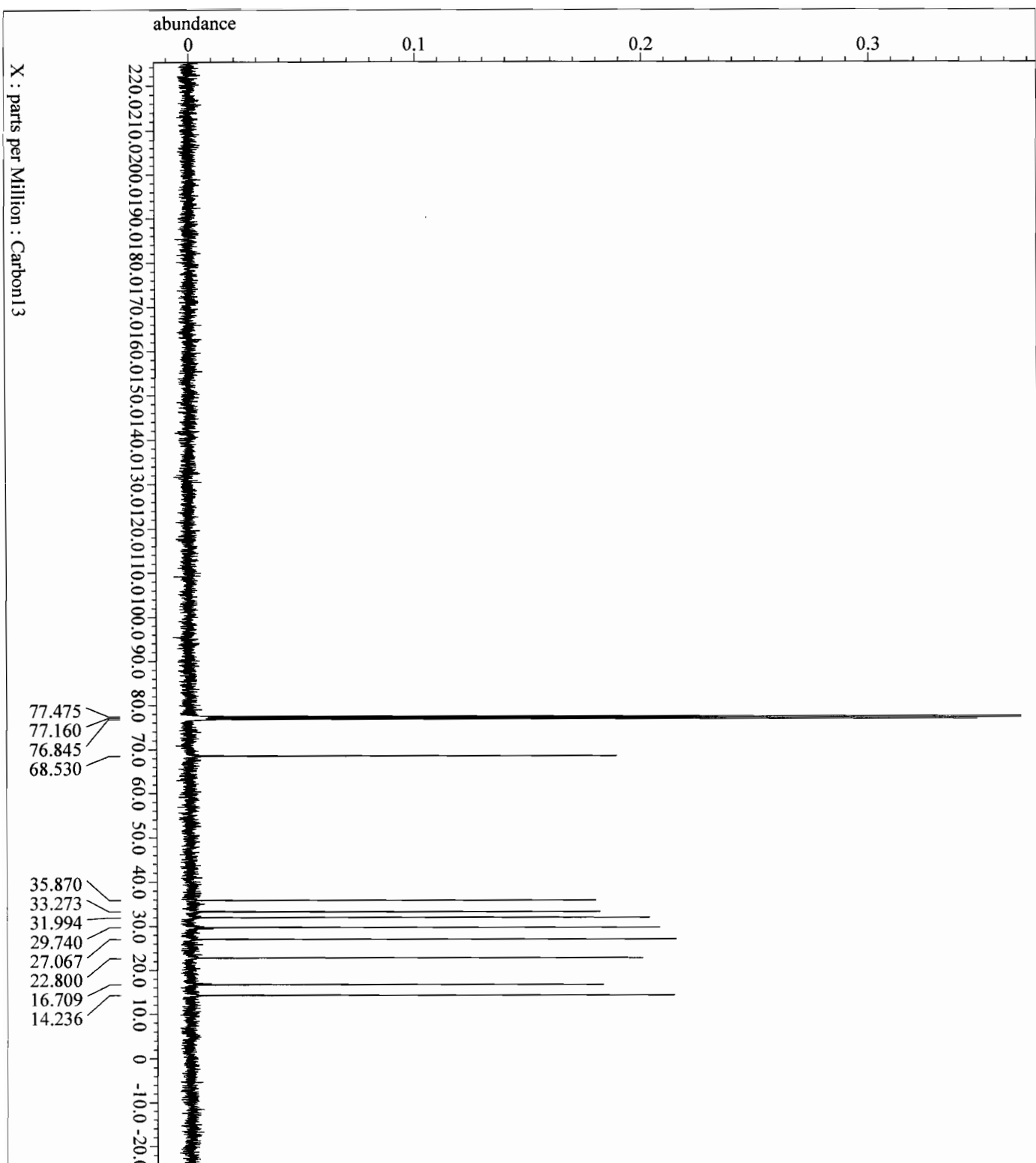
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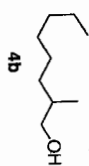
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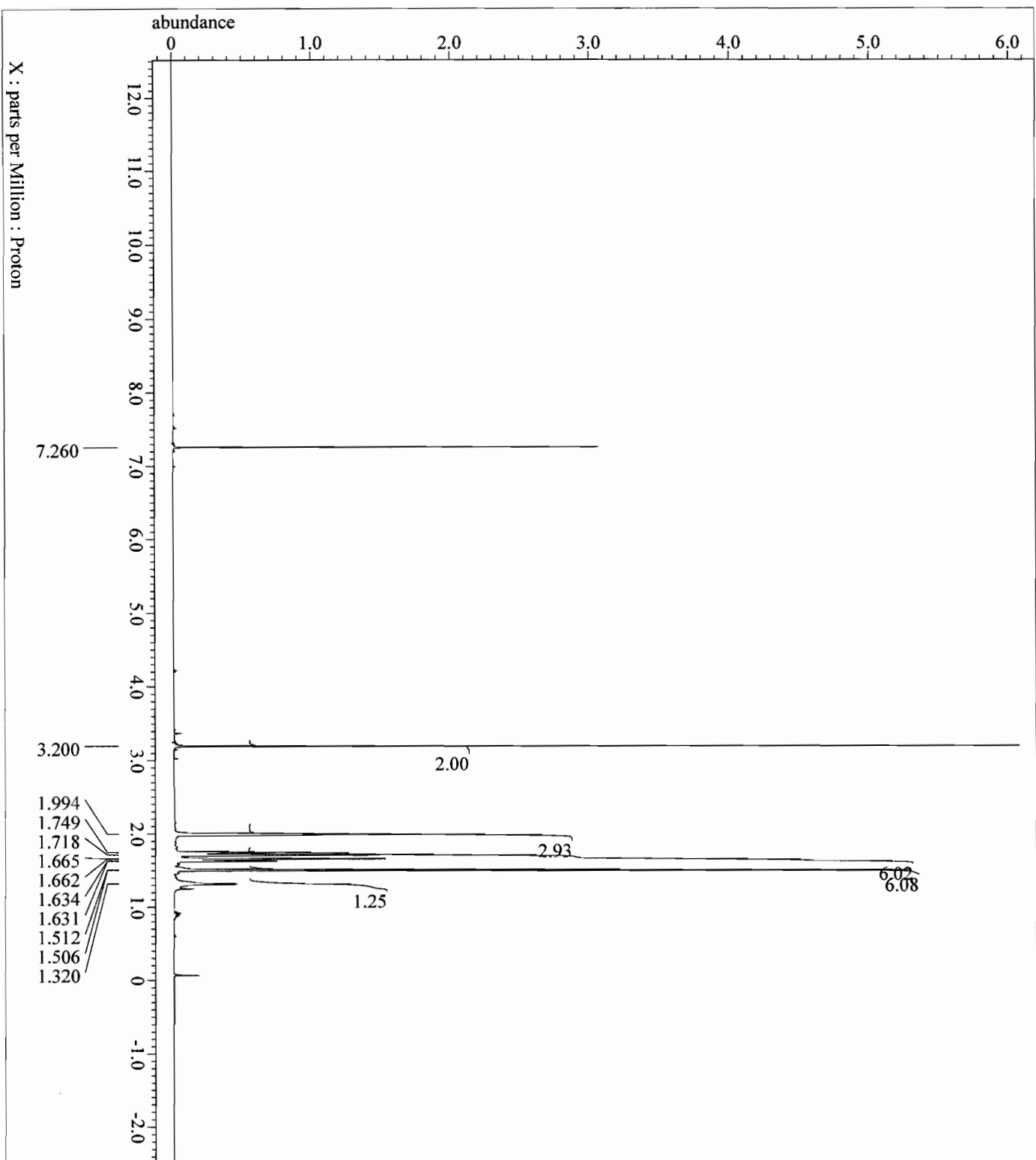
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Repetition_Time = 3.03809024 [s]

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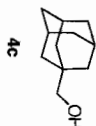


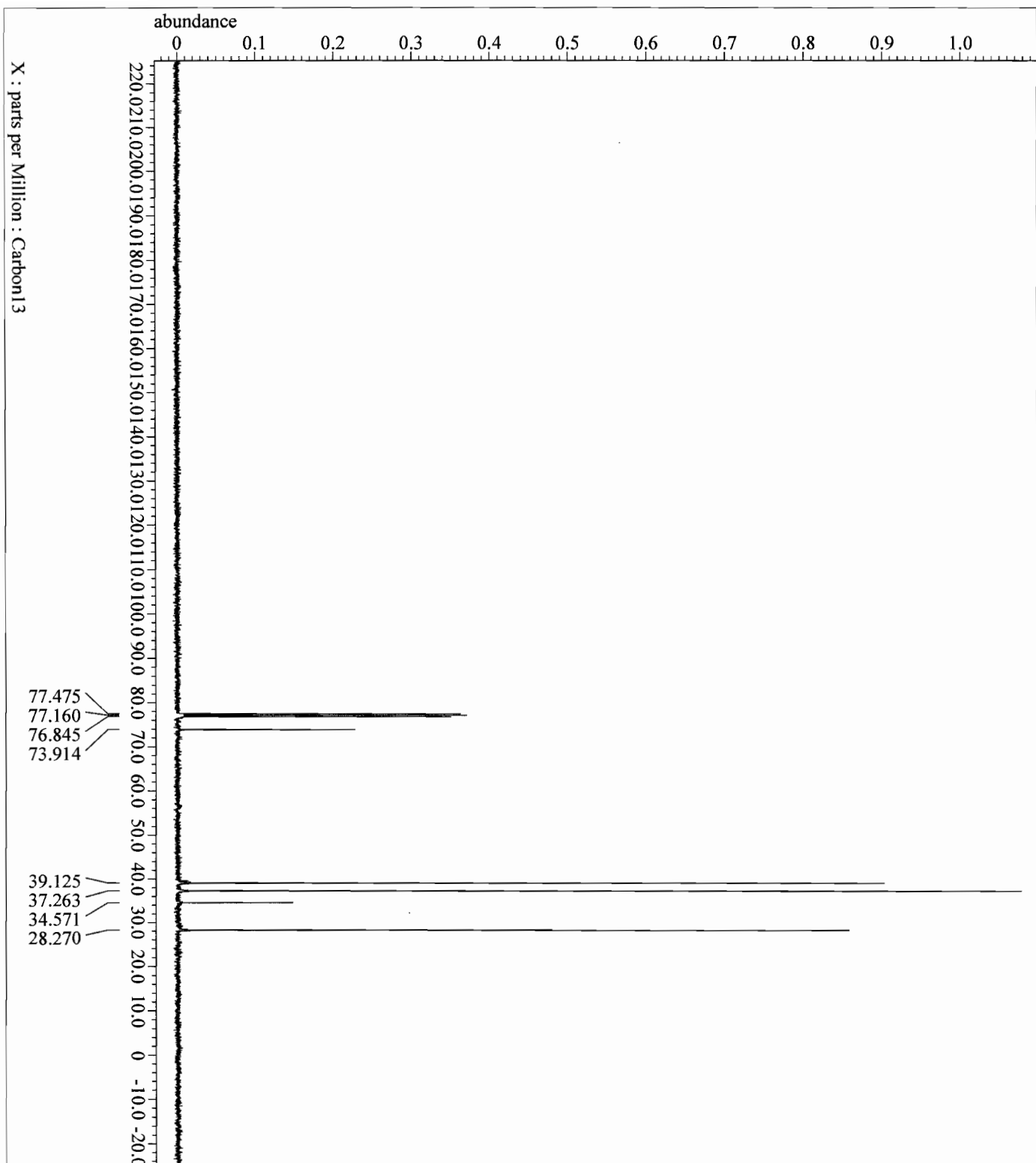
Filename = /Users/cktk0112/NMR/tk-250
 Author = delta
 Experiment = proton_jxp
 Sample Id = tk-250-
 Solvent = CHLOROFORM-D
 Creation Time = 16-FEB-2013 19:24:42
 Revision Time = 8-MAR-2013 15:56:22
 Current Time = 8-MAR-2013 15:57:40

Comment = single pulse
 Data Format = ID COMPLEX
 Dim Size = 13107
 Dim Title = Proton
 Dim Units = [ppm]
 Dimensions = X
 Site = JNM-EC5400
 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 = 51 [ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.45960208 [Hz]
 X_Sweep = 7.53012048 [kHz]
 X_Sweep_Clippped = 6.02409639 [kHz]
 Irr_Domain = Proton
 Irr_Freq = 401.28219856 [MHz]
 Irr_Offset = 51 [ppm]
 Irr_Domain = Proton
 Tri_Freq = 401.28219856 [MHz]
 Tri_Offset = 51 [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_Preset = FALSE
 Initial_Wait = 1 [s]
 Repetition_Time = 7.1757952 [s]



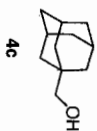


Filename = /Users/cktk0112/Documents/
 Author = delta
 Experiment = carbon-jyp
 Sample_Id = 1-
 Solvent = CHLOROFORM-D
 Creation_Time = 18-FEB-2013 12:21:58
 Revision_Time = 21-FEB-2013 09:54:20
 Current_Time = 21-FEB-2013 09:55:16

Comment = single pulse decoupled gat
 Data Format = ID COMPLEX
 Dim Size = 26214
 Dim Title = Carbon13
 Dim Units = [ppm]
 Dimensions = X
 Site = JNM-ECX400
 Spectrometer = DELTA2 NMR

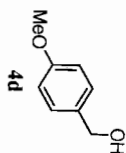
Field Strength = 9.4249681 [T] (400 [MHz])
 X_Acq Duration = 1.03809024 [s]
 X_Domain = 13C
 X_Freq = 100.90247863 [MHz]
 X_Offset = 100 [ppm]
 X_Points = 32768
 X_Frescans = 4
 X_Resolution = 0.96330739 [Hz]
 X_Sweep = 31.56565657 [kHz]
 X_Sweep_C1ipped = 25.25252525 [kHz]
 Irr_Domain = Proton
 Irr_Freq = 401.28219856 [MHz]
 Irr_Offset = 5 [ppm]
 Clipped = FALSE
 Scans = 128
 Total_Scans = 128

Relaxation_Delay = 2 [s]
 Recv Gain = 50
 Temp_Gat = 20.21 [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 = VAI12
 Irr_Width = 0.115 [ms]
 Decoupling = TRUE
 Initial_Wait = 1 [s]
 Noe = TRUE
 Noe Time = 2 [s]
 Repetition_Time = 3.03809024 [s]





S 14

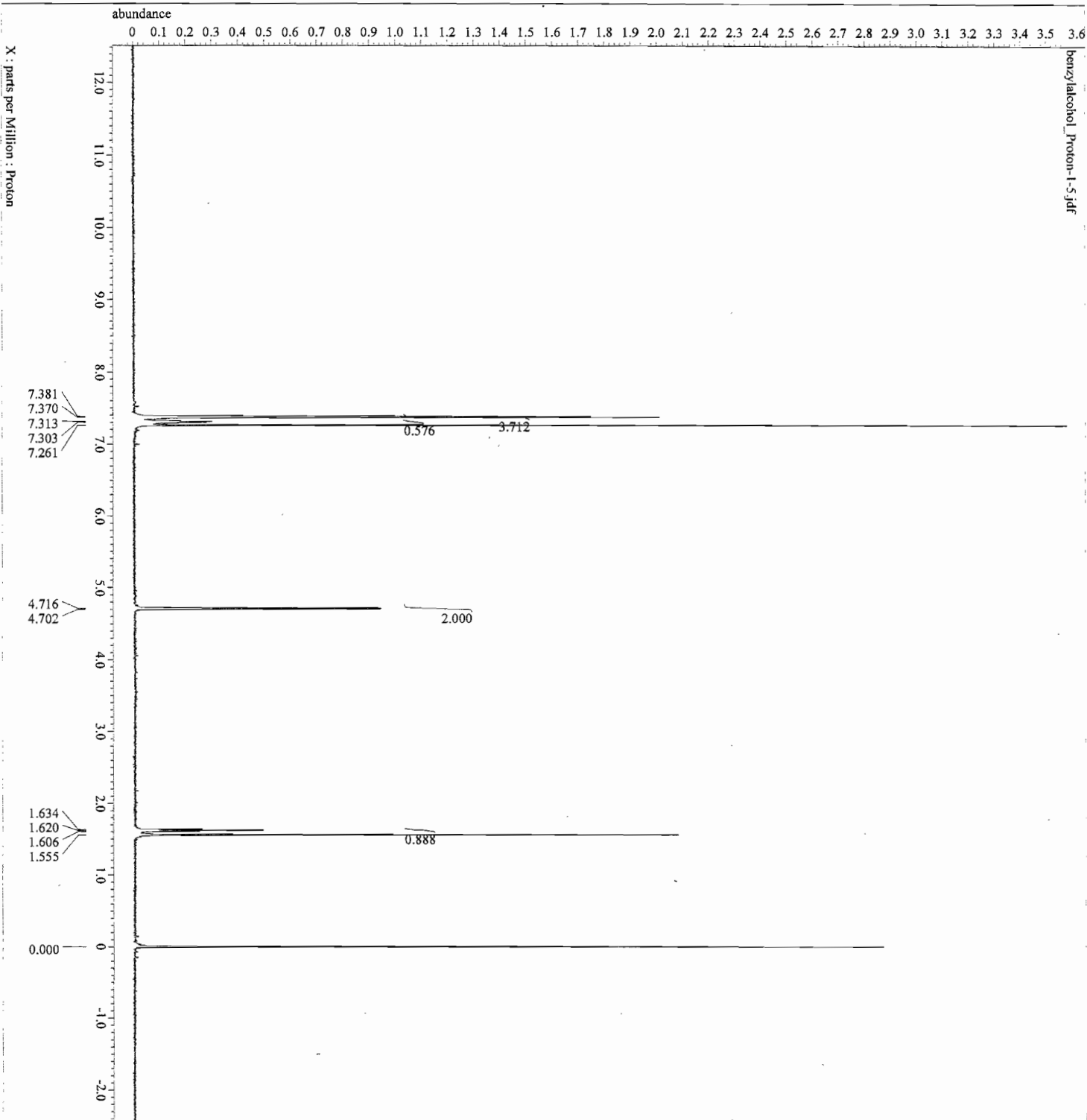
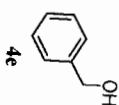


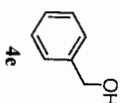
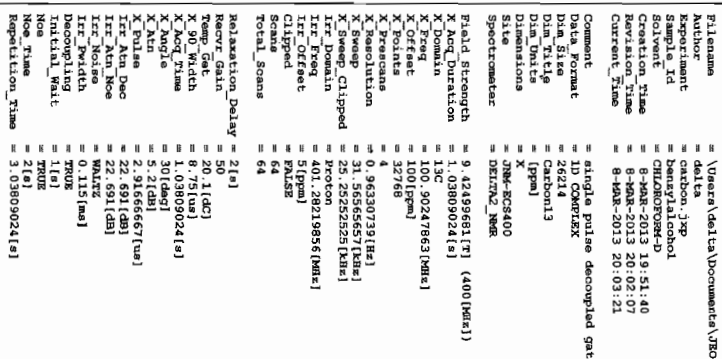


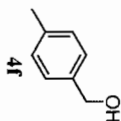
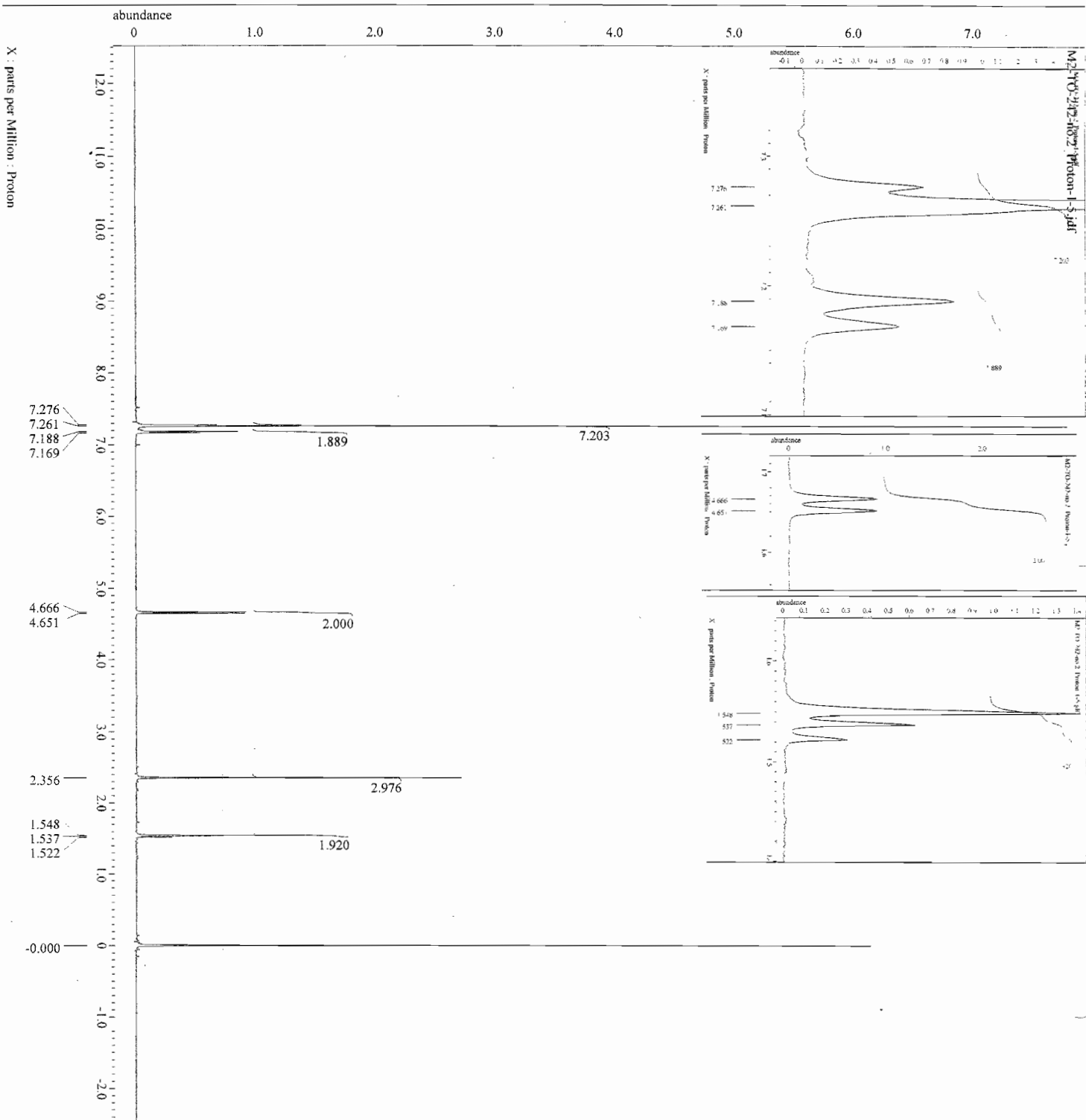
Repetition_Time = 3.03809024 [s]



Filename = \\trear\\data\\Documents\\JNO
 Author = delta
 Experiment = proton_jnp
 Sample_id = benzylalcohol
 Solvent = CDCl3/CDCl3
 Creation_Time = 8-04-2013 17:03:05
 Acquisition_Time = 8-04-2013 17:03:10
 Current_Time = 8-04-2013 20:05:10
 Comment = single pulse
 Data_Format = 1D CPMAS
 Dia_Size = 13107
 Dia_Tile = Proton
 Dia_Unit = ppm
 Dia_Units = ppm
 Site = JNM-EC5400
 Spectrometer = DELTA2 400
 Field_Strength = 9.424968117 (400 MHz)
 X_Acq_Duration = 2.17579521s
 X_Domain = 401.28219856 [MHz]
 X_Freq = 51 [ppm]
 X_Offset = 16384
 X_Points = 1
 X_Prescans = 0.45960208 [Hz]
 X_Resolution = 7.53012048 [Hz]
 X_Sweep_Clippped = 6.03409839 [Hz]
 X_Sweep_Duration = 401.28219856 [MHz]
 X_Freq = 51 [ppm]
 X_Offset = 401.28219856 [MHz]
 X_Domain = 401.28219856 [MHz]
 X_Freq = 51 [ppm]
 X_Offset = FALSE
 X_Points = 8
 Total_Scans = 8
 Relaxation_Delay = 5 [s]
 Recv_Gain = 54
 Temp_Get = 20.1 [C]
 X_90_Width = 9.23 [us]
 X_Acq_Time = 2.17579521s
 X_Acq_Time = 451 [us]
 X_Acq = 0.8 [dB]
 X_Pulse = 4.625 [us]
 X_Mode = OFF
 X_Pulse = OFF
 X_Pulse = FALSE
 X_Pulse = 1 [us]
 X_Pulse = 1.17579521s
 X_Pulse = 1.17579521s







Filename	="/Users/dalila/Documents/301b"
Author	="dalila"
Experiment	="precon_jazp"
Sample ID	="precon_jazp-2"
Sample Name	="precon_jazp-2"
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"
Dir Path	="/Users/dalila/301b"
Dir Name	="31307"
Data Title	="precon"
Data Units	="ppm"
Dimensions	="X"
Size	="10M-RC3400"
Spectrometer	="HPLC_NMR"
Field Strength	="9.422966611THz (400MHz)"
X Acq Duration	="2.1757952[s]"
X Domain	="1H"
X Freq	="401.28219856[MHz]"
X Offset	="5.1ppm"
X Offset2	="1.45360208[Hz]"
X Pulse	="1"
X Resolution	="7.55012048[kHz]"
X Sweep	="6.02409091[kHz]"
X Swap	="0"
X Temp_Clipped	="precon"
1st Domain	="401.28219856[MHz]"
1st Freq	="401.28219856[MHz]"
1st Domain	="1H"
1st Freq	="401.28219856[MHz]"
1st Offset	="5.1ppm"
Clipped	="FALSE"
Total Scans	="8"
Relaxation Delay	="5[s]"
Precr Gain	="18[dB]"
Temp_Gate	="9.25[us]"
X 90 Width	="2.1757952[s]"
X Angle	="15.0[deg]"
X Delay	="4.625[us]"
X Delay2	="OFF"
1st Mode	="OFF"
Dante Present	="FALSE"
Initial_Mat	="1.1[s]"
Deposition Time	="7.1157952[s]"

```

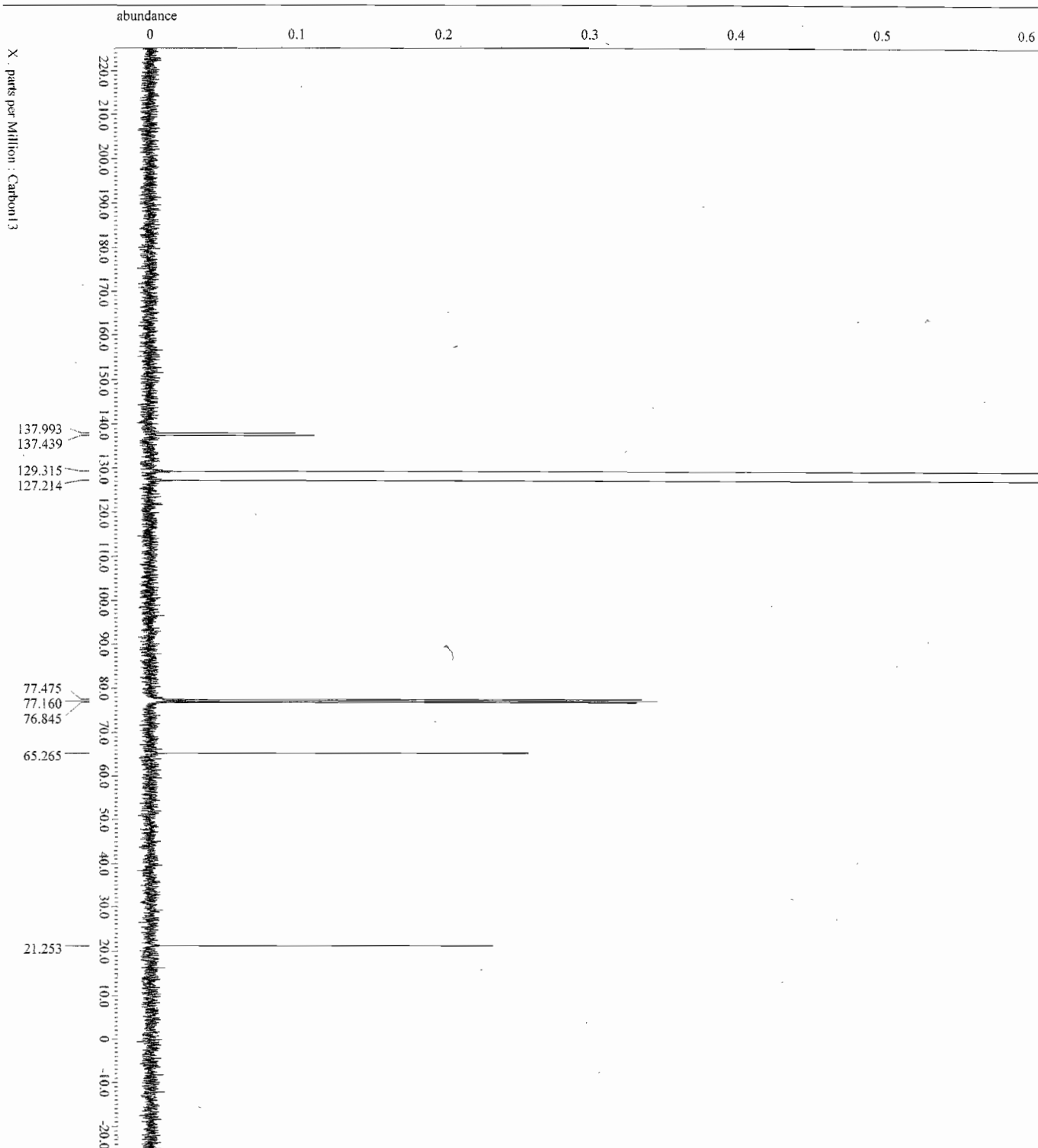
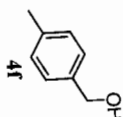
File Name      = V:\data\data\Documents\JBO
Author         = delta
Experiment     = carbon_13p
Sample Id      = M2-10-242-no.2C
Solvent        = CHLOROFORM-D
Creation Time   = 21-Feb-2013 04:07:38
Revision Time  = 21-Feb-2013 04:14:15
Current Time   = 21-Feb-2013 04:37:11

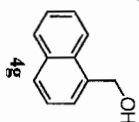
Comment       = single pulse decoupled gqt
Data Format    = 1D COMPLEX
Data Size     = 26214
Data Title    = Carbon13
Date_Units    = [ppm]
Dimensions    = 2
Site          = JNM-ECS400
Spectrometer  = DELTA2 NMR

F1d4_Strength = 9.4249661[T] (400[Mhz])
X_Acq_Duration = 1.03809024[s]
X_Domain       = 100.90247663[Mhz]
X_Freq         = 100.62598
X_Offset       = 100.62598
X_Points       = 32768
X_Frescan     = 4
X_Resolution   = 0.96330739[Hz]
X_Sweep         = 31.56565697[KHz]
X_Sweep_Clip    = 29.25525253[KHz]
X_Freq_Min     = 100.62598
X_Freq_Max     = 401.28219856[Mhz]
X_Freq_Offset  = 51[ppm]
X_Freq_Clip    = FALSE
Scans          = 64
Total_Scans    = 64

Relaxation_Delay = 3[s]
Purge_Gas       = 50
Temp_Gas        = 19.9[degC]
X_90_Width      = 8.75[us]
X_Acq_Time      = 1.03809024[s]
X_Angle         = 30[deg]
X_Axis          = 5.21[deg]
X_Pulse         = 2.34[us]
X_P1_Ap0 Dec   = 22.691[deg]
X_P1_Ap0 Dec   = 22.691[deg]
X_P1_Ap0 Dec   = VALTZ
X_P1_Ap0 Dec   = 0.115[us]
X_P1_Ap0 Dec   = YNUC
Decoupling      = 1[s]
X_P1_Ap0 Dec   = 21[us]
X_P1_Ap0 Dec   = 21[us]
Repetition_Time = 3.03809024[s]

```





S 20

abundance

-0.01 0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17 0.18 0.19 0.2 0.21 0.22 0.23 0.24

220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0

X : parts per Million : Carbon13

136.322
133.840
131.272
128.742
128.618
126.413
125.954
125.486
125.381
123.72077.475
77.160
76.845

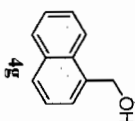
63.642

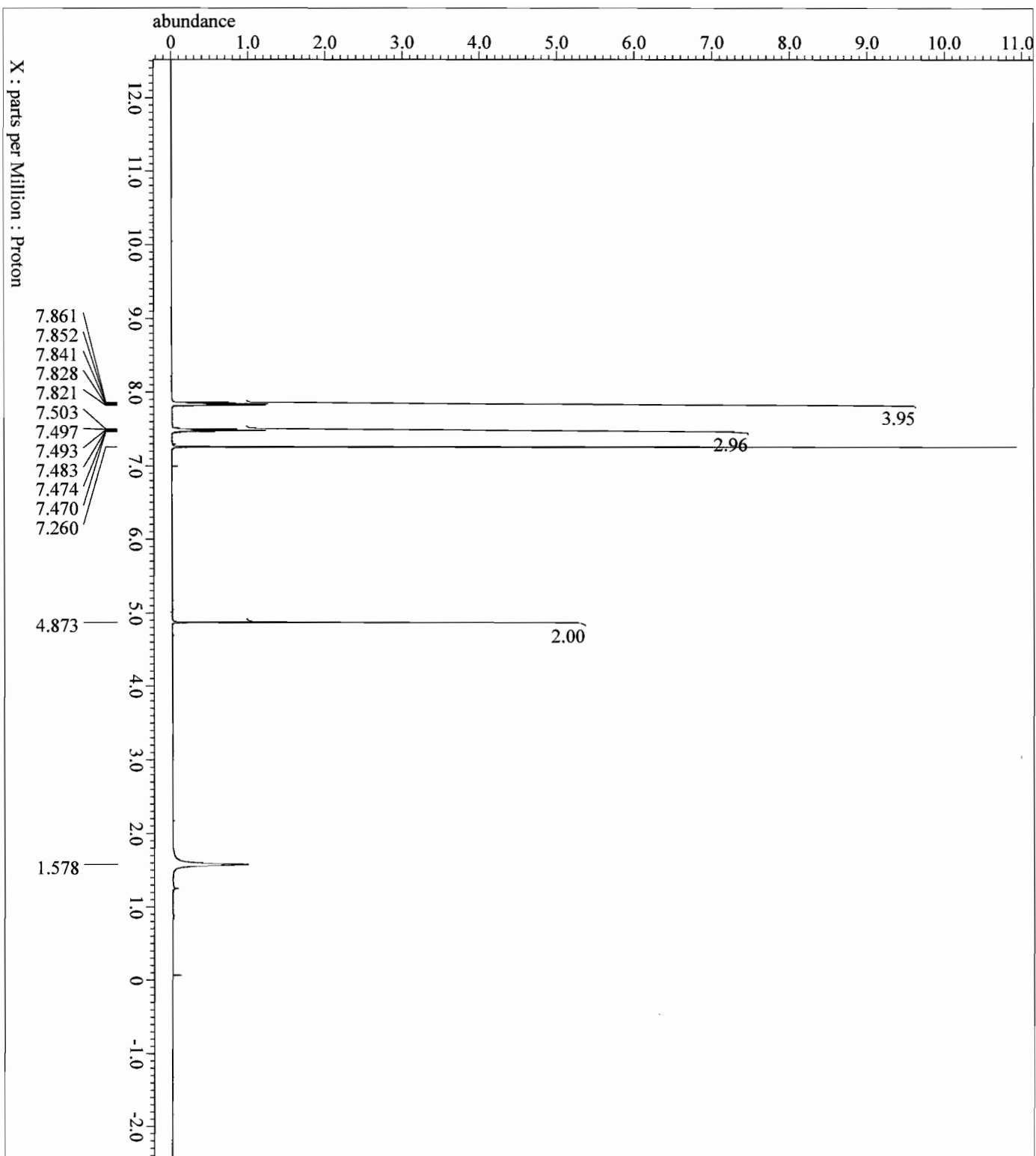


```

=====
Experiment      = carbon_jmp
Sample_id       = M2-TO-220-no.2C
Solvent         = CDCl3
Acquisition     = 31-JAN-2013 22:31:28
Current_time    = 31-JAN-2013 14:10:25
Current_time    = 31-JAN-2013 14:11:21
=====
Data Format      = single pulse decoupled gbt
Data Size       = 1D COMETEX
Data Title      = 26214
Data File       = Carbon13
Data Units      = [ppm]
Dimensions      = X
Site            = JNM-SC3400
Spectrometer    = DELTA2_NMR
=====
Field Strength  = 9.4249661[T] (400 MHz)
X_Acq Duration  = 1.03809024[s]
X_Domain        = 13C
X_Freq          = 100.6024763[MHz]
X_Offset        = 100.0[ppm]
X_Pulses        = 32768
X_Pulse_Program = 4
X_Resolution    = 0.9630739[Hz]
X_Sweep_Clip    = 31.5656567[Hz]
X_Sweep         = 25.2525252[MHz]
X_Domain        = Proton
X_Freq          = 401.2821985[MHz]
X_Offset        = 5[ppm]
X_Pulse_Program = PULPRO
X_Pulses        = 128
X_Scans         = 128
Total_Scans     = 128
=====
Relaxation_Delay = 2[s]
=====
Recycle_Delay   = 50
Temp_Det       = 20[deg]
X_P0_Width     = 8.75[us]
X_Acq_Time      = 1.03809024[s]
X_Angle         = 30[deg]
X_P1           = 3.21[us]
X_P2           = 2.2846667[us]
X_P3           = 22.691[us]
X_P4           = 22.691[us]
X_P5           = 22.691[us]
X_P6           = 22.691[us]
X_P7           = 22.691[us]
X_P8           = 22.691[us]
X_P9           = 22.691[us]
X_P10          = 22.691[us]
X_P11          = 22.691[us]
X_P12          = 22.691[us]
X_P13          = 22.691[us]
X_P14          = 22.691[us]
X_P15          = 22.691[us]
X_P16          = 22.691[us]
X_P17          = 22.691[us]
X_P18          = 22.691[us]
X_P19          = 22.691[us]
X_P20          = 22.691[us]
X_P21          = 22.691[us]
X_P22          = 22.691[us]
X_P23          = 22.691[us]
X_P24          = 22.691[us]
X_P25          = 22.691[us]
X_P26          = 22.691[us]
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X_P35          = 22.691[us]
X_P36          = 22.691[us]
X_P37          = 22.691[us]
X_P38          = 22.691[us]
X_P39          = 22.691[us]
X_P40          = 22.691[us]
X_P41          = 22.691[us]
X_P42          = 22.691[us]
X_P43          = 22.691[us]
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X_P48          = 22.691[us]
X_P49          = 22.691[us]
X_P50          = 22.691[us]
X_P51          = 22.691[us]
X_P52          = 22.691[us]
X_P53          = 22.691[us]
X_P54          = 22.691[us]
X_P55          = 22.691[us]
X_P56          = 22.691[us]
X_P57          = 22.691[us]
X_P58          = 22.691[us]
X_P59          = 22.691[us]
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X_P61          = 22.691[us]
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X_P63          = 22.691[us]
X_P64          = 22.691[us]
X_P65          = 22.691[us]
X_P66          = 22.691[us]
X_P67          = 22.691[us]
X_P68          = 22.691[us]
X_P69          = 22.691[us]
X_P70          = 22.691[us]
X_P71          = 22.691[us]
X_P72          = 22.691[us]
X_P73          = 22.691[us]
X_P74          = 22.691[us]
X_P75          = 22.691[us]
X_P76          = 22.691[us]
X_P77          = 22.691[us]
X_P78          = 22.691[us]
X_P79          = 22.691[us]
X_P80          = 22.691[us]
X_P81          = 22.691[us]
X_P82          = 22.691[us]
X_P83          = 22.691[us]
X_P84          = 22.691[us]
X_P85          = 22.691[us]
X_P86          = 22.691[us]
X_P87          = 22.691[us]
X_P88          = 22.691[us]
X_P89          = 22.691[us]
X_P90          = 22.691[us]
X_P91          = 22.691[us]
X_P92          = 22.691[us]
X_P93          = 22.691[us]
X_P94          = 22.691[us]
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X_P96          = 22.691[us]
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X_P114         = 22.691[us]
X_P115         = 22.691[us]
X_P116         = 22.691[us]
X_P117         = 22.691[us]
X_P118         = 22.691[us]
X_P119         = 22.691[us]
X_P120         = 22.691[us]
X_P121         = 22.691[us]
X_P122         = 22.691[us]
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X_P125         = 22.691[us]
X_P126         = 22.691[us]
X_P127         = 22.691[us]
X_P128         = 22.691[us]
=====
Repetition_Time = 3.03809024[s]
=====

```



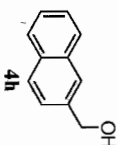


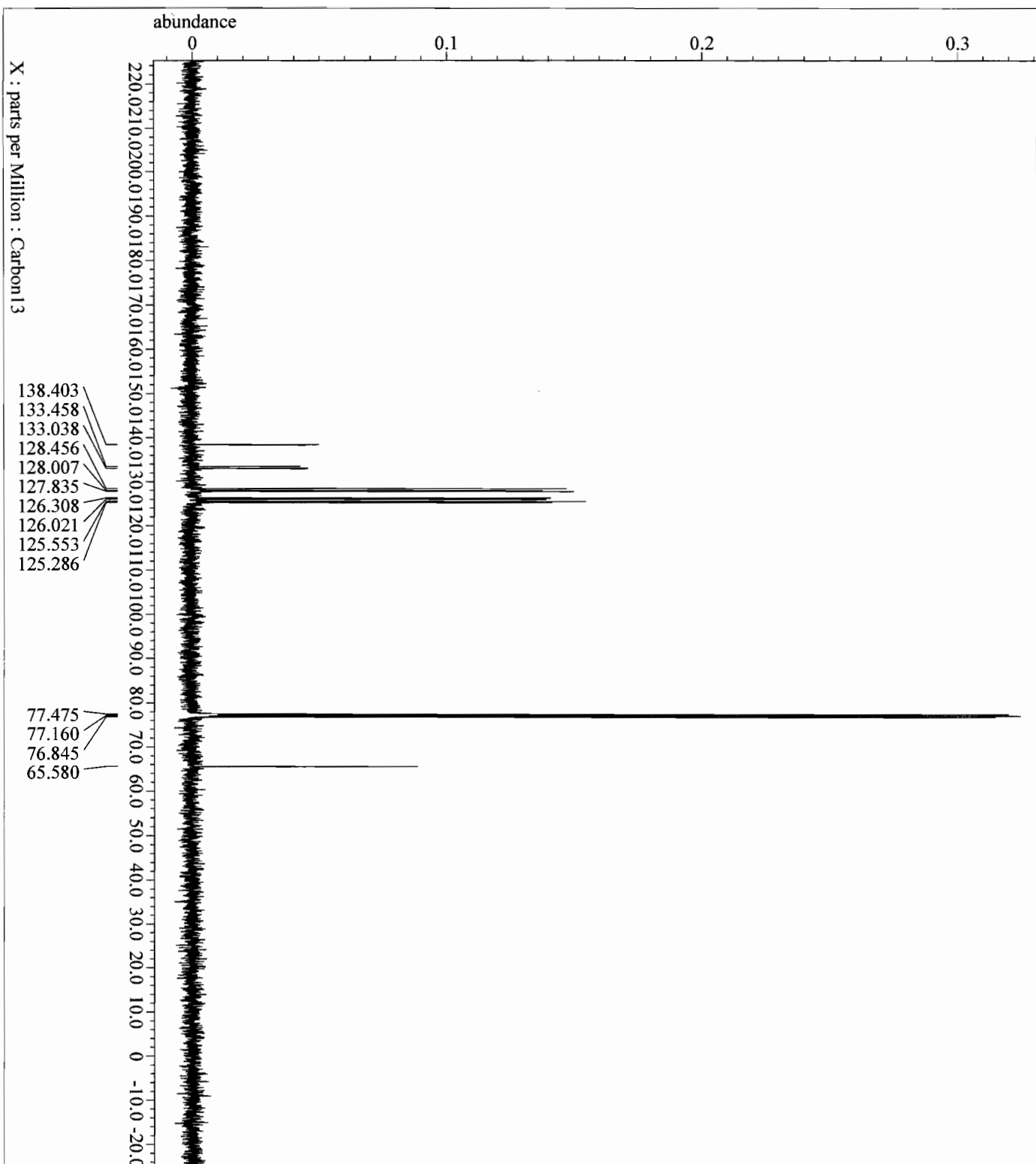
Filename = /Users/cktk0112/NMR/tk-269
 Author = delta
 Experiment = proton.jxp
 Sample_Id = tk-269-13-14
 Solvent = CHLOROFORM-D
 Creation_Time = 4-MAR-2013 23:37:02
 Revision_Time = 6-MAR-2013 17:32:45
 Current_Time = 6-MAR-2013 17:33:28

Comment = single pulse
 Data_Format = ID COMPLEX
 Dim_Size = 13107
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECX400
 Spectrometer = DELTA2_NMR

Field_Strength = 9.42496681 [T] (400 [MHz])
 X_Acq_Duration = 2.1757952 [s]
 X_Domain = 1H
 X_Freq = 401.28219856 [MHz]
 X_Offset = 51 [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 = 51 [ppm]
 Tri_Domain = Proton
 Tri_Freq = 401.28219856 [MHz]
 Tri_Offset = 51 [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_Rtn = 0.8 [dB]
 X_Pulse = 4.625 [us]
 Irr_Mode = Off
 Dante_Preset = FALSE
 Initial_Wait = 1 [s]
 Repetition_Time = 7.1757952 [s]



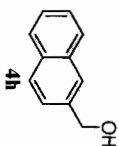


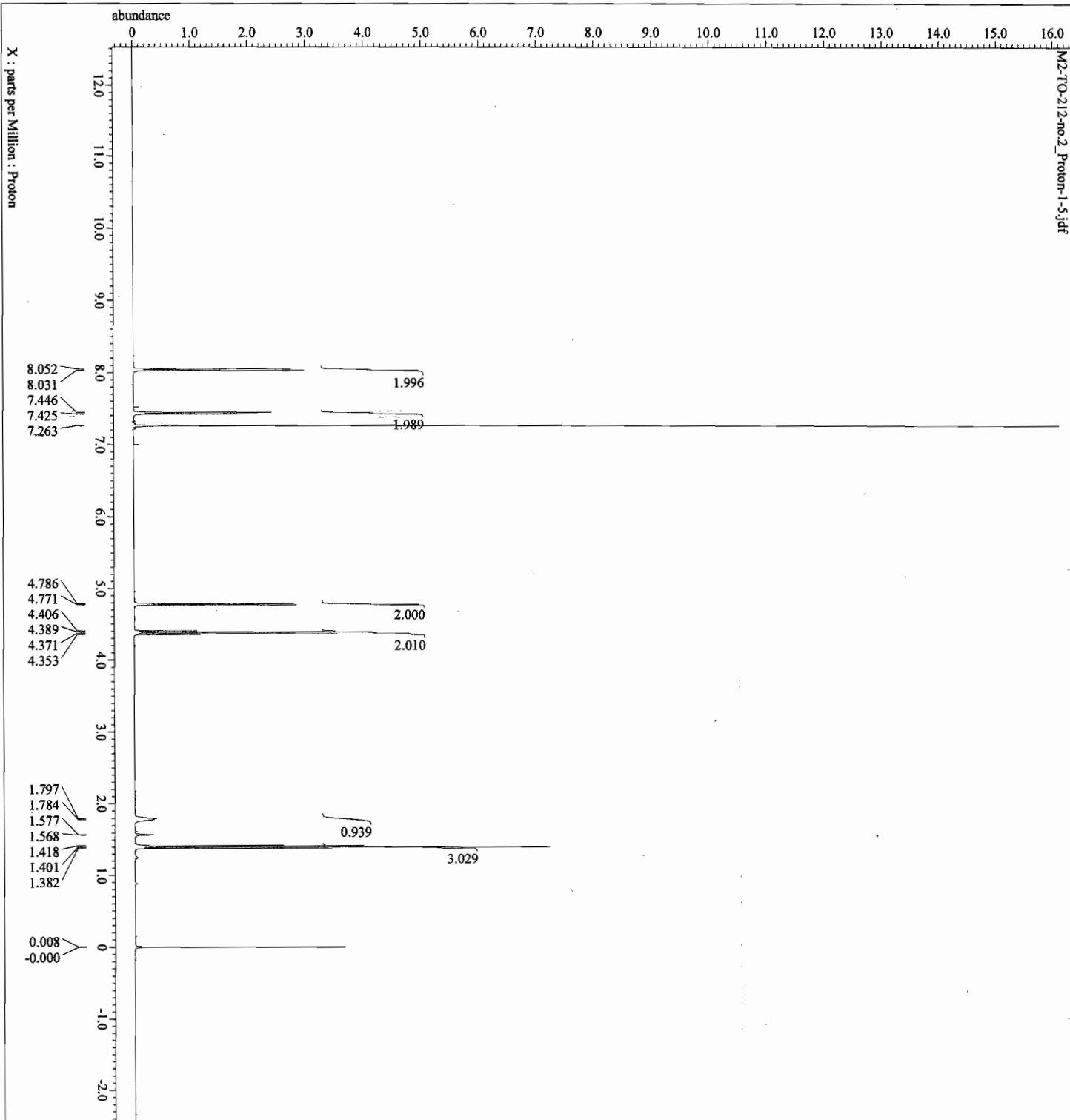
Filename = /Users/cktk0112/NMR/tk-267
 Author = delta
 Experiment = carbon_jxp
 Sample_Id = tk-267-13C
 Solvent = CHLOROFORM-D
 Creation_Time = 28-FEB-2013 01:11:18
 Revision_Time = 6-MAR-2013 17:40:21
 Current_Time = 6-MAR-2013 17:40:49

Comment = single pulse decoupled gat
 Data Format = 1D COMPLEX
 Dim Size = 26214
 Dim Title = Carbon13
 Dim Units = [ppm]
 Dimensions = X
 Site = JNM-ECX400
 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 = 100 [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 = Proton
 Irr_Freq = 401.28219856 [MHz]
 Irr_Offset = 51 [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_Aun_Dec = 22.691 [dB]
 Irr_Aun_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]

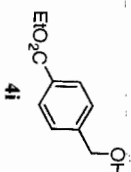




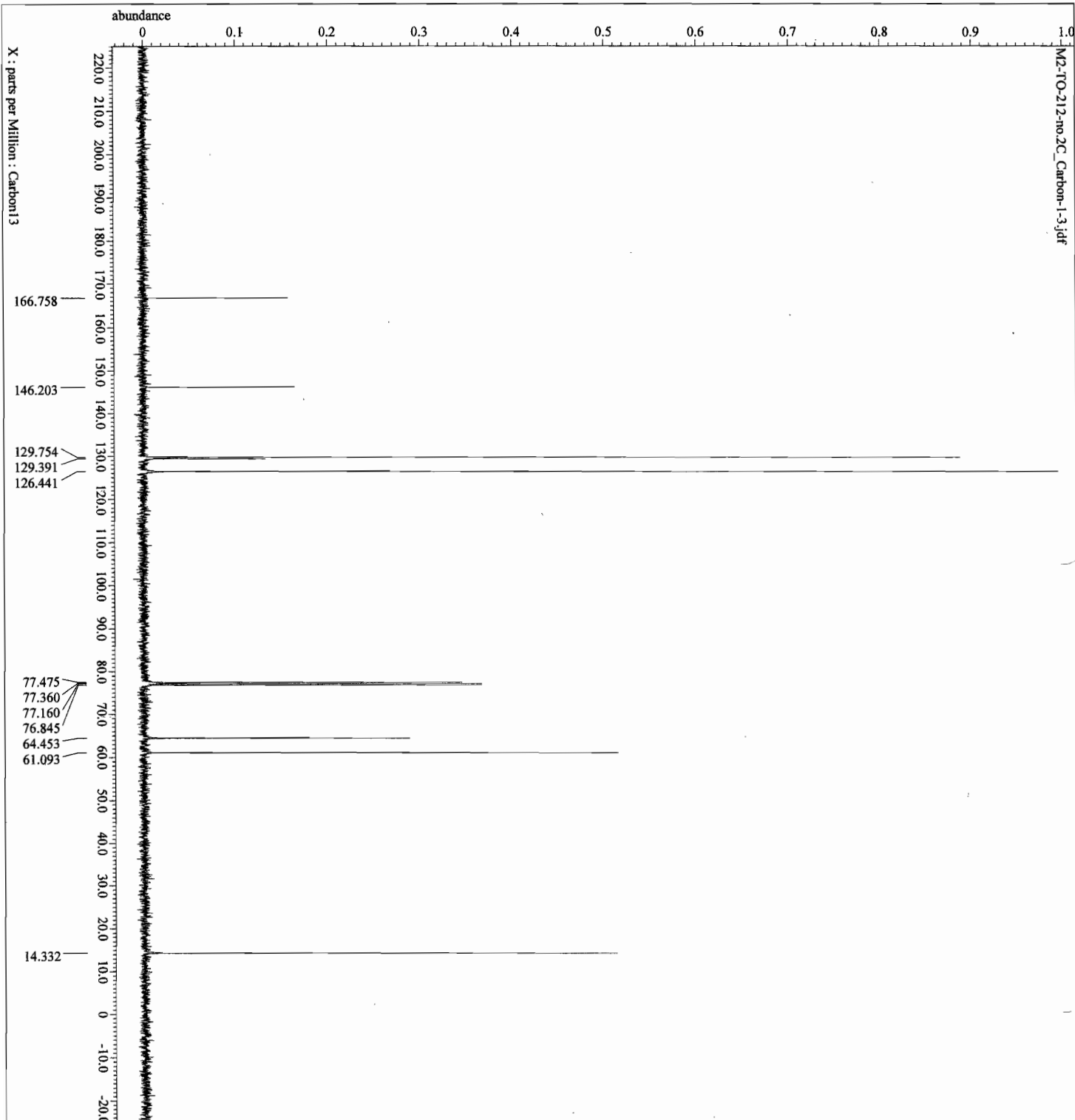
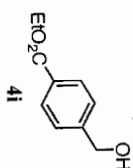
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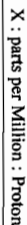
=====
File Name      = /Users/delta/Documents/4i
Author         = delta
Experiment     = proton_1p
Sample Id      = M2-TO-212-no.2
Solvent        = CDCl3
Acquisition    = 21-JUN-2013 19:55:50
F1 Frequency    = 21-JUN-2013 21:00:35
Current Time    = 21-JUN-2013 21:03:47
=====
Comment       = single pulse
Data Format    = ID CDETEX
P1m Size      = 13107
P1m Title     = Proton
P1m Units     = [ppm]
Dimensions    = X
Bits          = 16
Spectrometer  = DELTA 500
=====
Yield Strength = 9.4249681 [V] (400 [Hz])
X Acq Duration = 2.175921[s]
X Domain       = 16
X Freq         = 401.28219856 [MHz]
X Offset       = 51 [ppm]
X P1           = 13.584
X P2           = 1.0584
X Resolution    = 0.4596208 [Hz]
X Sweep Clipped = 7.53012048 [Hz]
X F2           = 6.02409639 [Hz]
X Domain       = Proton
X Freq         = 401.28219856 [MHz]
X Offset       = 51 [ppm]
X P1           = 5 [ppm]
X P2           = 401.28219856 [MHz]
X F2           = 51 [ppm]
X Offset       = FALSE
X Clipped      = FALSE
Scans          = 8
Total Scans    = 8
=====
Relaxation Delay = 5 [s]
=====
Name          = 4i
Temp (deg)    = 30.21 [deg]
X P1          = 20.25 [s]
X P2          = 2.175921[s]
X Acq         = 45 [deg]
X Aro         = 0.81 [dB]
X P1         = 4.625 [us]
X Mode        = OFF
X P1         = OFF
X P2         = FALSE
X P1         = 1 [s]
X P2         = 7.157952 [s]
=====

```



Filename = \\usera\delta\Documents\XMO
 Author = delta
 Experiment = carbon_jsp
 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 gnt
 Data Format = ID CDEPRX
 Data Size = 26214
 Data Title = Carbon13
 Data Units = (ppm)
 Dimensions = 1D
 Site = NM-EC3400
 Spectrometer = DELTA2_NMR
 Field Strength = 9.42499681[T] (400[Mhz])
 X Acq Duration = 1.03809024[s]
 X Domain = 13C
 X Freq = 100.62247863[Mhz]
 X Offset = 100.10000000[Mhz]
 X Points = 32768
 X Prescans = 4
 X Resolution = 0.96330739[HHz]
 X Sweep_Clippeak = 31.56565657[HHz]
 X Sweep_Clippeak = 25.25252525[HHz]
 X Domain = Proton
 X Freq = 401.28219856[Mhz]
 X Offset = 51ppm
 X Pulse = PULS8
 X Total_Scans = 64
 Relaxation_Delay = 2[s]
 Recv Gain = 50
 Temp_Gat = 20.6[deg]
 X 90_Rdch = 8.75[us]
 X Acq Time = 1.03809024[s]
 X Angle = 30[deg]
 X Alt = 5.2[deg]
 X Pulse = 2.91666667[us]
 X Alt_Dec = 22.691[deg]
 X Alt_Noe = 22.691[deg]
 X Noise = WALTZ
 X Pwldch = 0.115[us]
 X TROU = TROU
 Decoupling = 1[s]
 Initial_Walt = TROU
 Noe_Time = 210s
 Repetition_Time = 3.03809024[s]

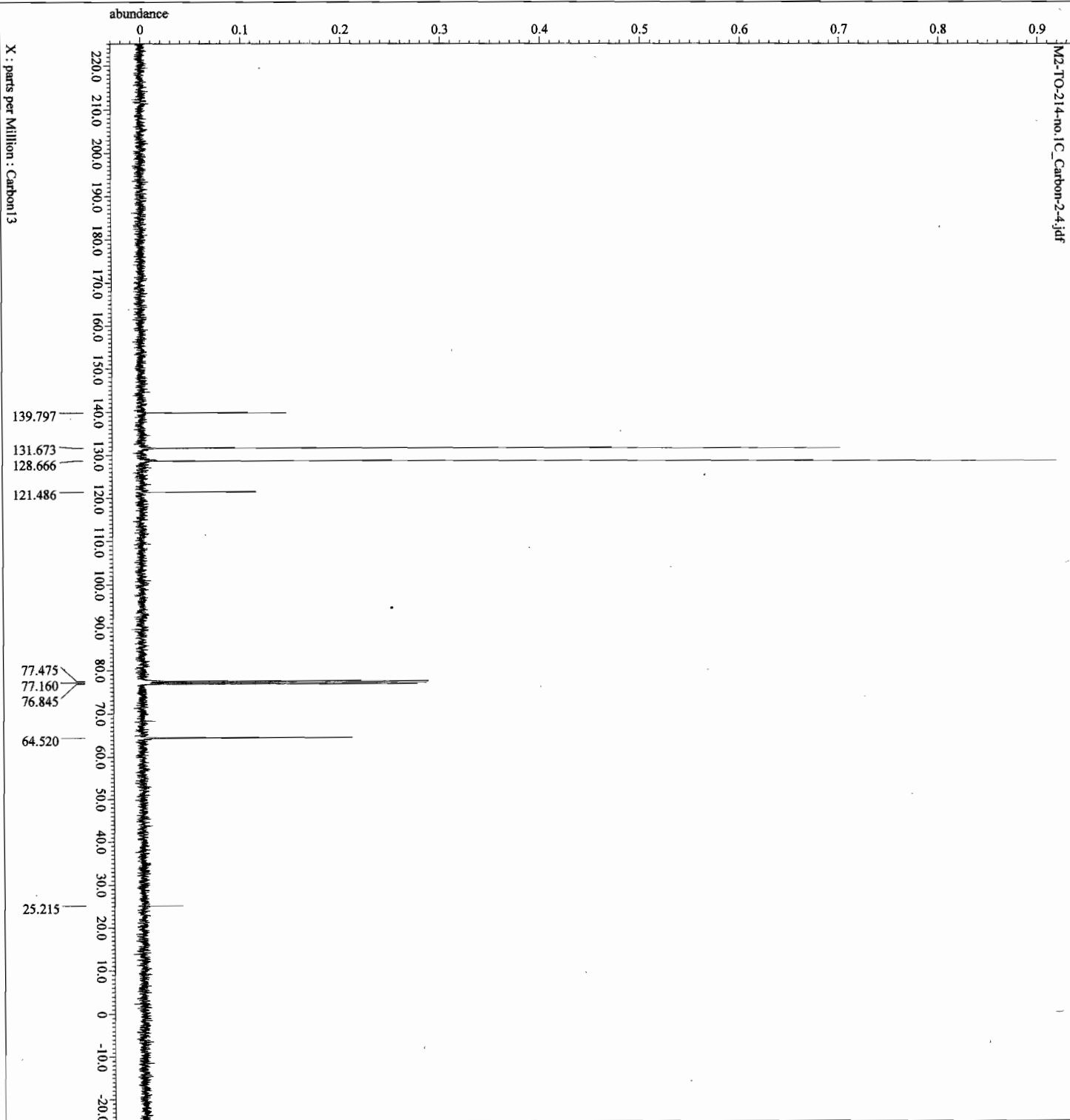
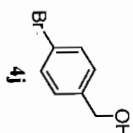




4j

Oc1ccc(Br)cc1

Filename = \\user\delta\Documents\JMO
 Author = delta
 Experiment = carbon_jsp
 Sample Id = M2-TO-214-no-1C
 Solvent = CHLOROTORM-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 gnt
 Data Format = 1D COMPRX
 Num Size = 26214
 Dir Title = carbon13
 Dir Units = ppm
 Dimensions = 1
 File Name = M2-TO-214-NO-1C
 File = M2TO214_NMR
 Spectrometer = DELTA2_NMR
 Field Strength = 9.424966171 (400MHz)
 X Acq Duration = 1.03809024[s]
 X Domain = 13C
 X Freq = 100.6247863[MHz]
 X Offset = 32768
 X Points = 4
 X Prescans = 0.96330739[Hz]
 X Resolution = 31.56565657[Hz]
 X Sweep Clipped = 29.25252525[Hz]
 X Domain = Proton
 X Freq = 401.28219856[MHz]
 X Offset = 51[ppm]
 X Phase = F2L58
 X Total Scans = 64
 Relaxation Delay = 21[s]
 Recv Gain = 50
 Temp Set = 20.6[deg]
 X 90 Width = 8.75[us]
 X Acq Time = 1.03809024[s]
 X Angle = 30[deg]
 X Alt = 5.21[deg]
 X Pulse = 2.91666667[us]
 X Alt Dec = 22.691[deg]
 X Alt Inc = 22.691[deg]
 X Noise = WALTZ
 X Phase = 0.115[us]
 Decoupling = PRRF
 Initial Wait = 1[s]
 Noe Time = 21[s]
 Repetition Time = 3.103809024[s]



```

=====
Filename      = \\usera\data\Documents\NMR
Author        = delta
Experiment    = proton_jmp
Sample_id     = M2-TO-207-no.2
Solvent       = CDCl3
Creation_Time = 18-JUN-2013 10:15:41
Acquisition_Time = 18-JUN-2013 10:38:02
Current_Time  = 18-JUN-2013 10:38:28

=====
Comment      = single pulse
Data Format   = 1D CPMAS
Pul_Prog     = zgpg30
Pul_P1       = 13107
Pul_P2       = 13107
Pul_P3       = 13107
Pul_P4       = 13107
Pul_P5       = 13107
Pul_P6       = 13107
Pul_P7       = 13107
Pul_P8       = 13107
Pul_P9       = 13107
Pul_P10      = 13107
Pul_P11      = 13107
Pul_P12      = 13107
Pul_P13      = 13107
Pul_P14      = 13107
Pul_P15      = 13107
Pul_P16      = 13107
Pul_P17      = 13107
Pul_P18      = 13107
Pul_P19      = 13107
Pul_P20      = 13107
Pul_P21      = 13107
Pul_P22      = 13107
Pul_P23      = 13107
Pul_P24      = 13107
Pul_P25      = 13107
Pul_P26      = 13107
Pul_P27      = 13107
Pul_P28      = 13107
Pul_P29      = 13107
Pul_P30      = 13107
Pul_P31      = 13107
Pul_P32      = 13107
Pul_P33      = 13107
Pul_P34      = 13107
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Pul_P36      = 13107
Pul_P37      = 13107
Pul_P38      = 13107
Pul_P39      = 13107
Pul_P40      = 13107
Pul_P41      = 13107
Pul_P42      = 13107
Pul_P43      = 13107
Pul_P44      = 13107
Pul_P45      = 13107
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Pul_P47      = 13107
Pul_P48      = 13107
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Pul_P59      = 13107
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Pul_P61      = 13107
Pul_P62      = 13107
Pul_P63      = 13107
Pul_P64      = 13107
Pul_P65      = 13107
Pul_P66      = 13107
Pul_P67      = 13107
Pul_P68      = 13107
Pul_P69      = 13107
Pul_P70      = 13107
Pul_P71      = 13107
Pul_P72      = 13107
Pul_P73      = 13107
Pul_P74      = 13107
Pul_P75      = 13107
Pul_P76      = 13107
Pul_P77      = 13107
Pul_P78      = 13107
Pul_P79      = 13107
Pul_P80      = 13107
Pul_P81      = 13107
Pul_P82      = 13107
Pul_P83      = 13107
Pul_P84      = 13107
Pul_P85      = 13107
Pul_P86      = 13107
Pul_P87      = 13107
Pul_P88      = 13107
Pul_P89      = 13107
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Pul_P94      = 13107
Pul_P95      = 13107
Pul_P96      = 13107
Pul_P97      = 13107
Pul_P98      = 13107
Pul_P99      = 13107
Pul_P100     = 13107

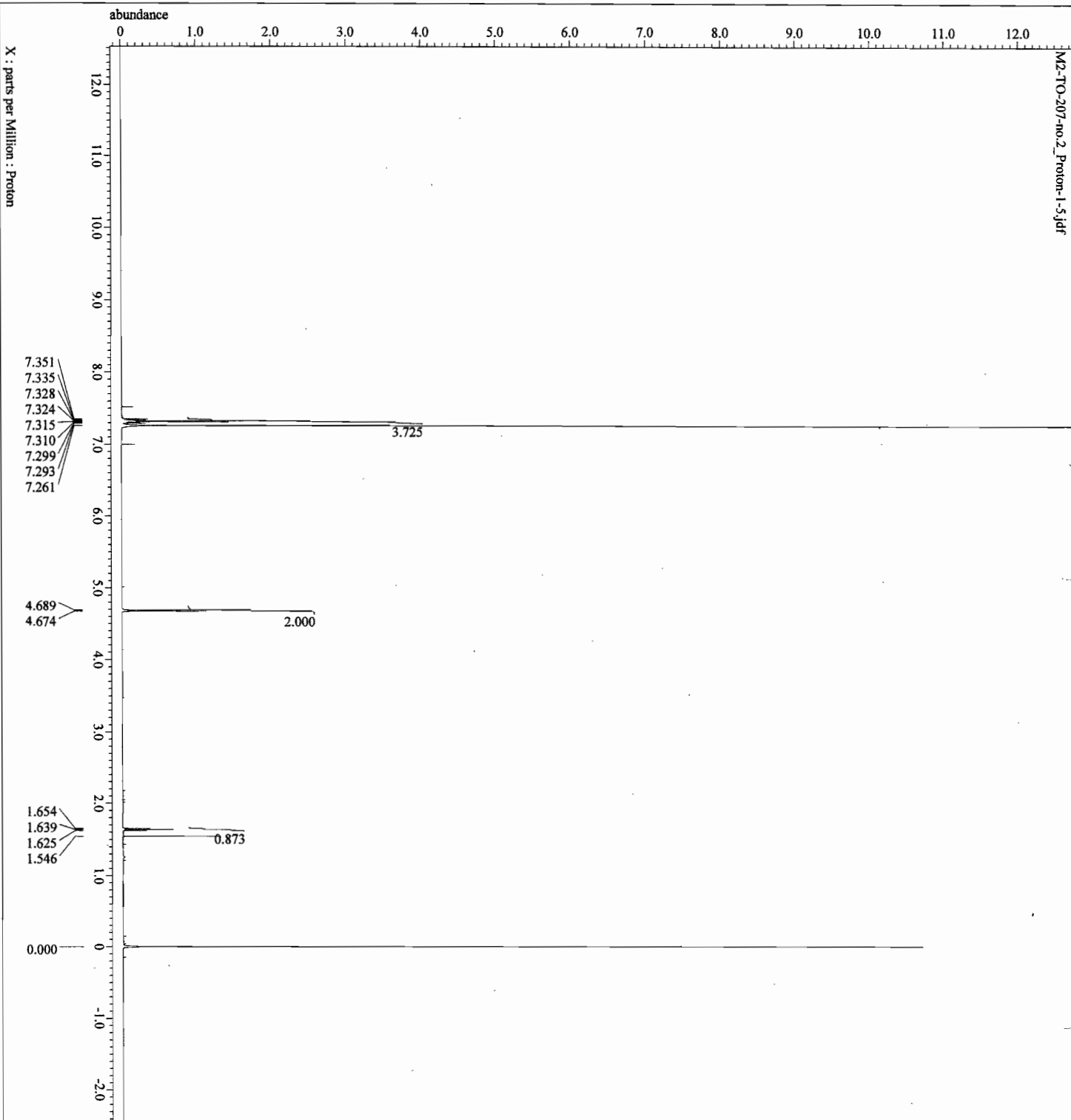
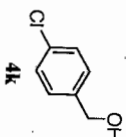
=====
Spectrum     = 1D CPMAS
Spectrum_NMR = DELTA_NMR

=====
Field Strength = 9.4249681 [T] (400 [MHz])
X_Acq_P1       = 2.175952 [s]
X_Acq_P2       = 2.175952 [s]
X_Acq_P3       = 2.175952 [s]
X_Acq_P4       = 2.175952 [s]
X_Acq_P5       = 2.175952 [s]
X_Acq_P6       = 2.175952 [s]
X_Acq_P7       = 2.175952 [s]
X_Acq_P8       = 2.175952 [s]
X_Acq_P9       = 2.175952 [s]
X_Acq_P10      = 2.175952 [s]
X_Acq_P11      = 2.175952 [s]
X_Acq_P12      = 2.175952 [s]
X_Acq_P13      = 2.175952 [s]
X_Acq_P14      = 2.175952 [s]
X_Acq_P15      = 2.175952 [s]
X_Acq_P16      = 2.175952 [s]
X_Acq_P17      = 2.175952 [s]
X_Acq_P18      = 2.175952 [s]
X_Acq_P19      = 2.175952 [s]
X_Acq_P20      = 2.175952 [s]
X_Acq_P21      = 2.175952 [s]
X_Acq_P22      = 2.175952 [s]
X_Acq_P23      = 2.175952 [s]
X_Acq_P24      = 2.175952 [s]
X_Acq_P25      = 2.175952 [s]
X_Acq_P26      = 2.175952 [s]
X_Acq_P27      = 2.175952 [s]
X_Acq_P28      = 2.175952 [s]
X_Acq_P29      = 2.175952 [s]
X_Acq_P30      = 2.175952 [s]
X_Acq_P31      = 2.175952 [s]
X_Acq_P32      = 2.175952 [s]
X_Acq_P33      = 2.175952 [s]
X_Acq_P34      = 2.175952 [s]
X_Acq_P35      = 2.175952 [s]
X_Acq_P36      = 2.175952 [s]
X_Acq_P37      = 2.175952 [s]
X_Acq_P38      = 2.175952 [s]
X_Acq_P39      = 2.175952 [s]
X_Acq_P40      = 2.175952 [s]
X_Acq_P41      = 2.175952 [s]
X_Acq_P42      = 2.175952 [s]
X_Acq_P43      = 2.175952 [s]
X_Acq_P44      = 2.175952 [s]
X_Acq_P45      = 2.175952 [s]
X_Acq_P46      = 2.175952 [s]
X_Acq_P47      = 2.175952 [s]
X_Acq_P48      = 2.175952 [s]
X_Acq_P49      = 2.175952 [s]
X_Acq_P50      = 2.175952 [s]
X_Acq_P51      = 2.175952 [s]
X_Acq_P52      = 2.175952 [s]
X_Acq_P53      = 2.175952 [s]
X_Acq_P54      = 2.175952 [s]
X_Acq_P55      = 2.175952 [s]
X_Acq_P56      = 2.175952 [s]
X_Acq_P57      = 2.175952 [s]
X_Acq_P58      = 2.175952 [s]
X_Acq_P59      = 2.175952 [s]
X_Acq_P60      = 2.175952 [s]
X_Acq_P61      = 2.175952 [s]
X_Acq_P62      = 2.175952 [s]
X_Acq_P63      = 2.175952 [s]
X_Acq_P64      = 2.175952 [s]
X_Acq_P65      = 2.175952 [s]
X_Acq_P66      = 2.175952 [s]
X_Acq_P67      = 2.175952 [s]
X_Acq_P68      = 2.175952 [s]
X_Acq_P69      = 2.175952 [s]
X_Acq_P70      = 2.175952 [s]
X_Acq_P71      = 2.175952 [s]
X_Acq_P72      = 2.175952 [s]
X_Acq_P73      = 2.175952 [s]
X_Acq_P74      = 2.175952 [s]
X_Acq_P75      = 2.175952 [s]
X_Acq_P76      = 2.175952 [s]
X_Acq_P77      = 2.175952 [s]
X_Acq_P78      = 2.175952 [s]
X_Acq_P79      = 2.175952 [s]
X_Acq_P80      = 2.175952 [s]
X_Acq_P81      = 2.175952 [s]
X_Acq_P82      = 2.175952 [s]
X_Acq_P83      = 2.175952 [s]
X_Acq_P84      = 2.175952 [s]
X_Acq_P85      = 2.175952 [s]
X_Acq_P86      = 2.175952 [s]
X_Acq_P87      = 2.175952 [s]
X_Acq_P88      = 2.175952 [s]
X_Acq_P89      = 2.175952 [s]
X_Acq_P90      = 2.175952 [s]
X_Acq_P91      = 2.175952 [s]
X_Acq_P92      = 2.175952 [s]
X_Acq_P93      = 2.175952 [s]
X_Acq_P94      = 2.175952 [s]
X_Acq_P95      = 2.175952 [s]
X_Acq_P96      = 2.175952 [s]
X_Acq_P97      = 2.175952 [s]
X_Acq_P98      = 2.175952 [s]
X_Acq_P99      = 2.175952 [s]
X_Acq_P100     = 2.175952 [s]

=====
Relaxation_Delay = 5 [s]
Sweep_Gain       = 56
Sweep_Gain2      = 20 [dB]
X_SQ_Width       = 9.25 [us]
X_Acq_Time       = 2.175952 [s]
X_Acq_Freq       = 400.146 [MHz]
X_Acq_P1         = 0.8 [us]
X_Acq_P2         = 4.625 [us]
X_Acq_P3         = 0.8 [us]
X_Acq_P4         = 0.8 [us]
X_Acq_P5         = 0.8 [us]
X_Acq_P6         = 0.8 [us]
X_Acq_P7         = 0.8 [us]
X_Acq_P8         = 0.8 [us]
X_Acq_P9         = 0.8 [us]
X_Acq_P10        = 0.8 [us]
X_Acq_P11        = 0.8 [us]
X_Acq_P12        = 0.8 [us]
X_Acq_P13        = 0.8 [us]
X_Acq_P14        = 0.8 [us]
X_Acq_P15        = 0.8 [us]
X_Acq_P16        = 0.8 [us]
X_Acq_P17        = 0.8 [us]
X_Acq_P18        = 0.8 [us]
X_Acq_P19        = 0.8 [us]
X_Acq_P20        = 0.8 [us]
X_Acq_P21        = 0.8 [us]
X_Acq_P22        = 0.8 [us]
X_Acq_P23        = 0.8 [us]
X_Acq_P24        = 0.8 [us]
X_Acq_P25        = 0.8 [us]
X_Acq_P26        = 0.8 [us]
X_Acq_P27        = 0.8 [us]
X_Acq_P28        = 0.8 [us]
X_Acq_P29        = 0.8 [us]
X_Acq_P30        = 0.8 [us]
X_Acq_P31        = 0.8 [us]
X_Acq_P32        = 0.8 [us]
X_Acq_P33        = 0.8 [us]
X_Acq_P34        = 0.8 [us]
X_Acq_P35        = 0.8 [us]
X_Acq_P36        = 0.8 [us]
X_Acq_P37        = 0.8 [us]
X_Acq_P38        = 0.8 [us]
X_Acq_P39        = 0.8 [us]
X_Acq_P40        = 0.8 [us]
X_Acq_P41        = 0.8 [us]
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X_Acq_P47        = 0.8 [us]
X_Acq_P48        = 0.8 [us]
X_Acq_P49        = 0.8 [us]
X_Acq_P50        = 0.8 [us]
X_Acq_P51        = 0.8 [us]
X_Acq_P52        = 0.8 [us]
X_Acq_P53        = 0.8 [us]
X_Acq_P54        = 0.8 [us]
X_Acq_P55        = 0.8 [us]
X_Acq_P56        = 0.8 [us]
X_Acq_P57        = 0.8 [us]
X_Acq_P58        = 0.8 [us]
X_Acq_P59        = 0.8 [us]
X_Acq_P60        = 0.8 [us]
X_Acq_P61        = 0.8 [us]
X_Acq_P62        = 0.8 [us]
X_Acq_P63        = 0.8 [us]
X_Acq_P64        = 0.8 [us]
X_Acq_P65        = 0.8 [us]
X_Acq_P66        = 0.8 [us]
X_Acq_P67        = 0.8 [us]
X_Acq_P68        = 0.8 [us]
X_Acq_P69        = 0.8 [us]
X_Acq_P70        = 0.8 [us]
X_Acq_P71        = 0.8 [us]
X_Acq_P72        = 0.8 [us]
X_Acq_P73        = 0.8 [us]
X_Acq_P74        = 0.8 [us]
X_Acq_P75        = 0.8 [us]
X_Acq_P76        = 0.8 [us]
X_Acq_P77        = 0.8 [us]
X_Acq_P78        = 0.8 [us]
X_Acq_P79        = 0.8 [us]
X_Acq_P80        = 0.8 [us]
X_Acq_P81        = 0.8 [us]
X_Acq_P82        = 0.8 [us]
X_Acq_P83        = 0.8 [us]
X_Acq_P84        = 0.8 [us]
X_Acq_P85        = 0.8 [us]
X_Acq_P86        = 0.8 [us]
X_Acq_P87        = 0.8 [us]
X_Acq_P88        = 0.8 [us]
X_Acq_P89        = 0.8 [us]
X_Acq_P90        = 0.8 [us]
X_Acq_P91        = 0.8 [us]
X_Acq_P92        = 0.8 [us]
X_Acq_P93        = 0.8 [us]
X_Acq_P94        = 0.8 [us]
X_Acq_P95        = 0.8 [us]
X_Acq_P96        = 0.8 [us]
X_Acq_P97        = 0.8 [us]
X_Acq_P98        = 0.8 [us]
X_Acq_P99        = 0.8 [us]
X_Acq_P100       = 0.8 [us]

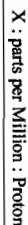
=====
Initial_Pulse   = 1 [s]
Repetition_Time = 7.175952 [s]
=====

```



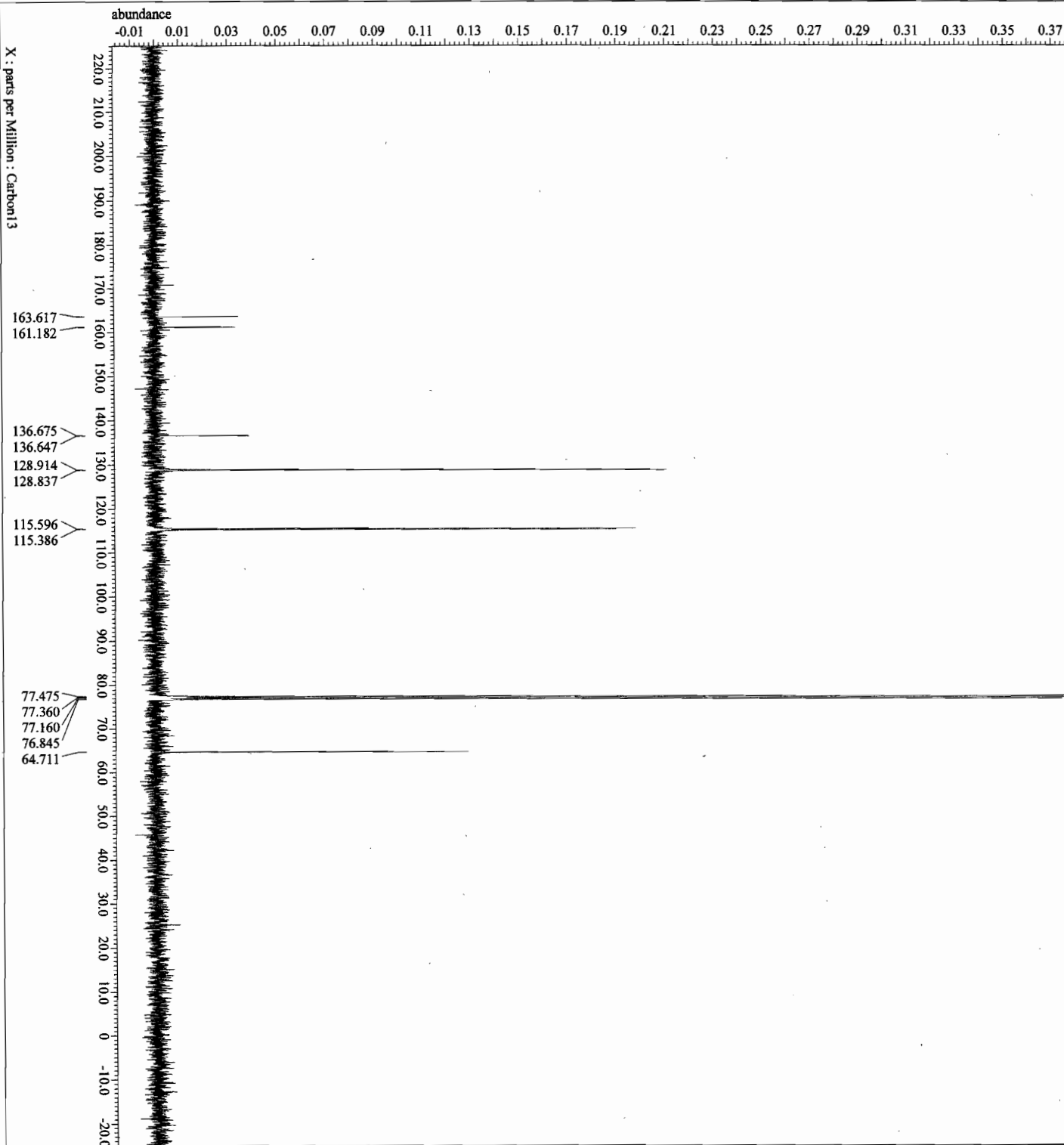
4k

OCC1=CC=C(Cl)C=C1

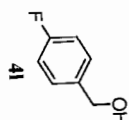


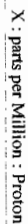
41

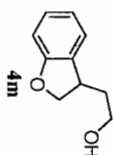
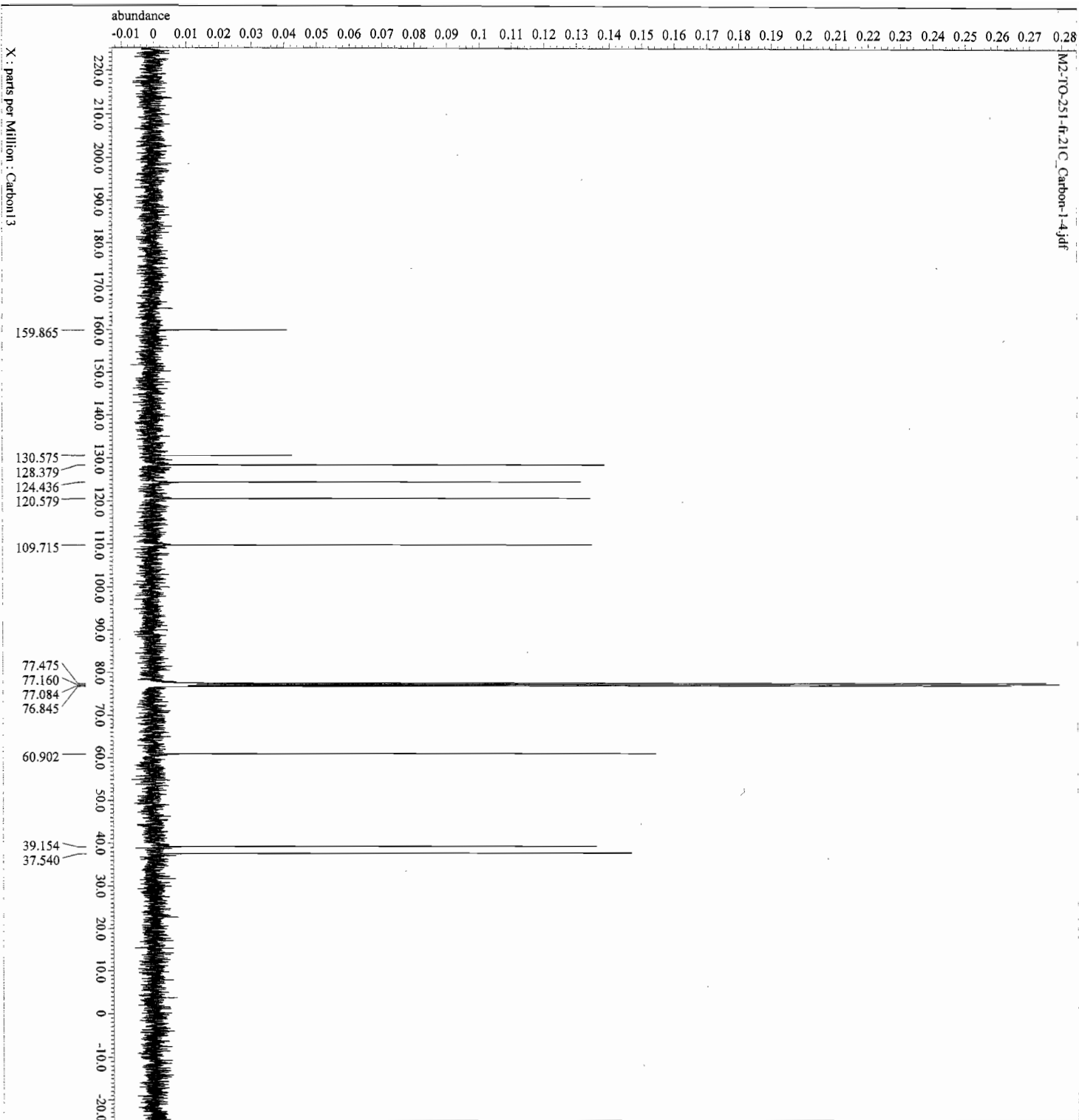
OCC1=CC=C(C=C1)F



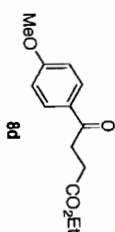
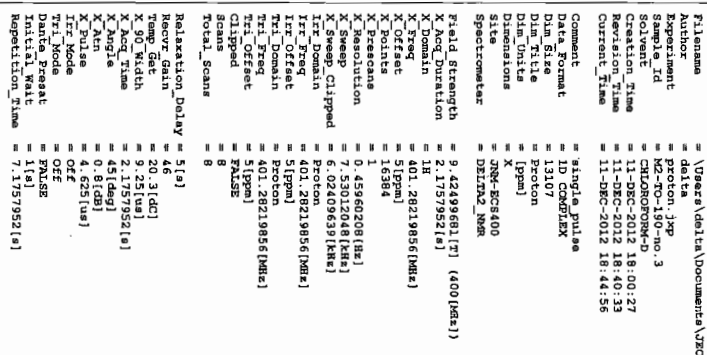
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Author	'Users\Delta\Documents\302'
Experiment	'data'
Sample_id	'cachon_jsp'
Botwell	'W-70-211-no.1C'
Swetlow_Times	'CHRONOM-ND'
Derivation	'0-0-14.12'
Current_Times	'21-NN-2013 19:42:11'
Current_Times	'21-NN-2013 19:43:05'
Comment	'single pulse decoupled gate'
Data Format	'ID COMPLEX'
Data Size	'26214'
Data Title	'Cachon3'
Data Units	'[pnm]'
Dimensions	'X'
Bitva	'MM-RC400'
Spectrometer	'DIRIG_3MR'
Field Strength	'9.4029666117' (400 [MHz])
X_Acq Duration	'1.0380902041[s]'
X_Domain	'13C'
X_Freq	'100.90247863 [MHz]'
X_Offset	'100 [ppm]'
X_Points	'32768'
X_Fresnoans	'4'
X_Resolution	'0.965300739 [Hz]'
X_Sweep	'31.56565657 [kHz]'
X_Clipppd	'25.25232523 [kHz]'
Iter_Domain	'pnm'
Iter_Freq	'51.62219586 [MHz]'
Iter_Offset	'5 [ppm]'
Clipppd	'pnm'
Gamma	'103'
Total_Scans	'103'
Relaxation_Delay	'2[s]'
Recvr_Gain	'50'
Temp_Gain	'19.9 [dC]'
90_Watch	'8.75 [us]'
X_Acq_Times	'1.0380902041[s]'
X_Angle	'30 [deg]'
X_Pulse	'2.91666667 [us]'
Iter_Acq_Dur	'22.651 [ms]'
Iter_Acq_Nos	'22.651 [dB]'
Iter_Pulse	'WALTZ'
Decoupling	'0.115 [ms]'
Initial_Walt	'1[s]'
Noise	'FMZC'
Repetition_Time	'2[s]'
Repetition_Time	'1.0380902041[s]'

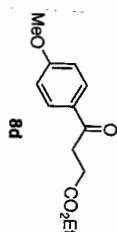
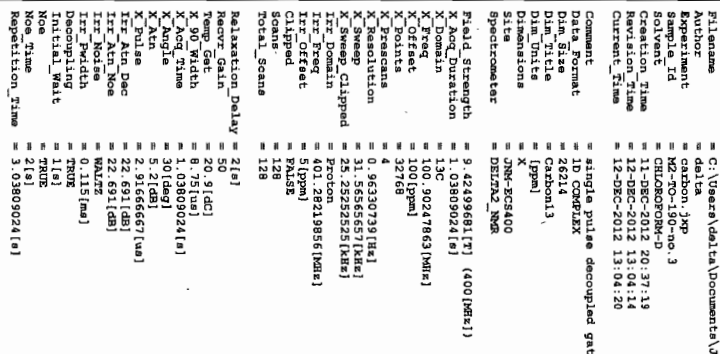


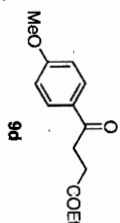
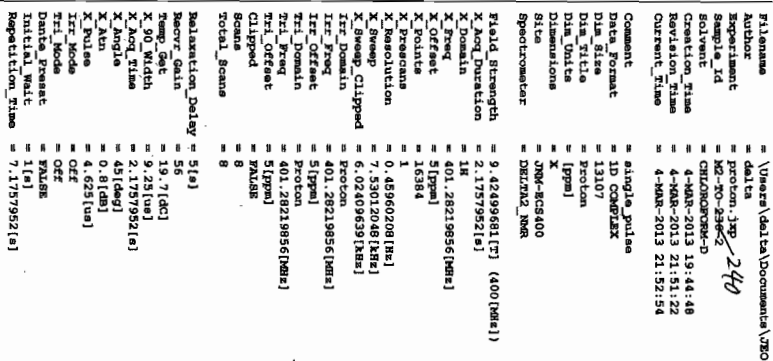
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Filename	= Users\deltaelta\Documents\J20C
Author	= delta
Sample_Id	= casbon_jsp
Solvent	= M2-NC-251-fc 21C
ChemicalName	= CHLOROACETONE
Revision_Time	= 8-NOV-2013 9:41:08
Revision_Time	= 8-NOV-2013 10:01:05
Current_Time	= 8-NOV-2013 20:01:54
Comment	= single pulses decoupled gated
Data_Format	= ID Complex
Data_Size	= 26214
Data_Title	= Casbon31
Data_Units	= (ppm)
Dimensions	= X-YM-ZC&400
Site	= DELTA2_NMR
Spectrometer	
Field Strength	= 9.42496961(T) (400(MHz))
X_AcqDuration	= 1.03860024(s)
X_ProgScan	= 100.90247863(MHz)
X_Offset	= 100(ppm)
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96350739(Hz)
X_Sweep_Clippped	= 31.5655657(Hz)
X_ProgScan	= 25.25252525(MHz)
X_AcqDuration	= 401.28213956(MHz)
X_Offset	= 51(ppm)
X_ProgScan	= FALST
Scans	= 128
Total Scans	= 128
Relaxation_Delay	= 2(s)
Temp_Sol	= 20.21(C)
X_90_RfGain	= 8.75(wu)
X_Acq Time	= 1.038609024(s)
X_Angle	= 30(deg)
X_Ain	= 5.21(dB)
X_Pulse	= 3.9166667(µs)
Trf_Ain_Dec	= 22.691(dB)
Trf_Ain_Pow	= 22.691(dB)
Trf_MixDec	= WALTZ
Trf_Pwldth	= 0.115[µs]
Decoupling	= TRUE
Initial_Wait	= 1(s)
Nuc	= 13C
Nuc	= 13C
Deposition_Time	= 3.038609024(s)







```

=====
File Name      = V:\area\data\Documents\JBO
Author         = delta
Experiment     = carbon_jrp
Sample Id      = M2-TO-240-HPLC3C
Solvent        = CHLOROFORM-D
Concentration   = 23.41:51
Current Time    = 23-FEB-2013 00:44:26
Current Date    = 23-FEB-2013 00:44:51
=====
Comment
Data Format     = single pulse decoupled gat
Data Size      = 26214
Dim Title      = Carbon13
Dim Units      = Xppm
Dimension       = 1
Site           = JNM-ECX400
Spectrometer    = DELTA2_NMR

Field Strength  = 9.4249681[T] (400[Mhz])
X_Acq_Duration  = 1.03809024[s]
X_Prog          = zgpg30
X_Freq          = 100.624763[Mhz]
X_Offset        = 100.1ppm
X_Points        = 32768
X_Prescans      = 4
X_Rescans       = 0.9630739[Mhz]
X_Resolution    = 31.3636567[Mhz]
X_Sweep_Clip    = 31.3636567[Mhz]
X_Sweep         = 401.28219856[Mhz]
X_Freq          = 401.28219856[Mhz]
X_Offset        = 51ppm
X_Prog          = FALSE
X_Points        = 64
Total_Scans     = 64
Relaxation_Delay = 2[s]
Recur_Gain      = 50
Temp_Get        = 20.2[degC]
X_90_Width      = 8.75[us]
X_Acq_Time      = 1.03809024[s]
X_Angle         = 30[deg]
X_Ain           = 3.416667[us]
X_Aout          = 3.416667[us]
X_Ain_Prog      = 22.691[us]
X_Ain_Noise     = VALTZ
X_PeakWidth     = 0.115[ms]
X_Peak          = RMUS
Decoupling       = 1[s]
Noisetime        = 2141
Repetition_Time = 3.03809024[s]
=====

```

