

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.

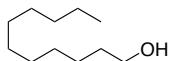
Typical Procedure for the Hydroxymethylation of alkyl iodides

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%).

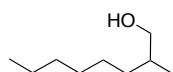
Typical Procedure for the Hydroxymethylation of aryl iodides (Table 1, entry 3)

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



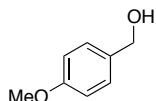
1-Undecanol (4a). ^1H NMR (CDCl_3 , 400 MHz): δ 0.88 (t, J = 5.6 Hz, 3H), 1.18-1.50 (m, 16H), 1.53-1.58 (m, 2H), 3.64 (t, J = 7.2 Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 14.27, 22.83, 25.87, 29.48, 29.58, 29.76, 32.05, 32.93, 63.23. This product is commercially available and the ^1H - and ^{13}C -NMR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

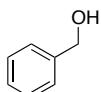


1-adamantanemethanol (4c). ^1H NMR (CDCl_3 , 400 MHz): δ 1.32 (m, 1H), 1.46-1.54 (m, 6H), 1.60-1.67 (m, 3H), 1.69-1.76 (m, 3H), 1.95-2.01 (m, 3H), 3.20 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 28.27, 34.57, 37.26, 39.13, 73.91. This product is commercially available and the ^1H - and ^{13}C -NMR spectra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

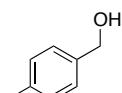


(4-methoxyphenyl)methanol (4d) ^1H NMR (CDCl_3 , 400 MHz): δ 1.53 (t, J = 6.0 Hz, 1H), 3.81 (s, 3H), 4.62 (d, J = 6.0 Hz, 2H), 6.88-6.92 (m, 2H), 7.29-7.31 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 55.42, 65.16, 114.07, 128.79, 133.22, 159.32. This product is commercially available and the ^1H - and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

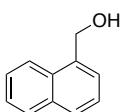
⁴ Silver, S.; Puranen, A.; Sjöholm, R.; Repo, T.; Leino, R. *Eur. J. Inorg. Chem.* **2005**, 1514.



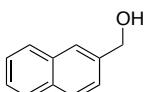
benzyl alcohol (4e) ^1H NMR (CDCl_3 , 400 MHz): δ 1.60-1.66 (m, 1H), 4.71 (d, J = 6.0 Hz, 2H), 7.26-7.38 (m, 5H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 65.16, 127.05, 127.64, 128.58, 140.91. This product is commercially available and the ^1H - and ^{13}C -NMR spectra are consistent with those of the authentic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



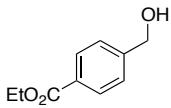
(4-methylphenyl)methyl alcohol (4f) ^1H NMR (CDCl_3 , 400 MHz): δ 1.54 (t, J = 6.0 Hz, 1H), 2.36 (s, 3H), 4.66 (d, J = 6.0 Hz, 2H), 7.18 (d, J = 7.6 Hz, 2H), 7.27 (d, J = 7.6 Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 21.25, 65.27, 127.21, 129.32, 137.44, 137.99. This product is commercially available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



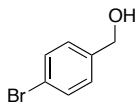
1-naphthylmethanol (4g) ^1H NMR (CDCl_3 , 400 MHz): δ 1.71 (t, J = 6.0 Hz, 1H), 5.17 (d, J = 6.0 Hz, 2H), 7.44-7.58 (m, 4H), 7.82-7.90 (m, 2H), 8.14 (d, J = 8.0 Hz, 1H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 63.64, 123.72, 125.38, 125.48, 125.95, 126.41, 128.62, 128.74, 131.27, 133.84, 136.32. This product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



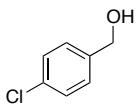
2-naphthylmethanol (4h) ^1H NMR (CDCl_3 , 400 MHz): δ 4.87 (s, 2H), 7.45-7.52 (m, 3H), 7.81-7.87 (m, 4H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 65.58, 125.29, 125.55, 126.02, 126.31, 127.84, 128.01, 128.46, 133.04, 133.46, 138.40. This product is commercially available and the ^1H - and ^{13}C -NMR spectra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



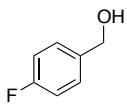
4-hydroxymethylbenzoic acid ethyl ester⁵ (4i) ¹H-NMR (CDCl₃, 400MHz) δ: 1.40 (t, J = 6.9 Hz, 3H), 1.76-1.82 (br, 1H), 4.35 (q, J = 6.9 Hz, 2H), 4.78 (d, J = 6.0 Hz, 2H), 7.43, (d, J = 8.3 Hz, 2H), 8.04 (d, J = 8.3 Hz, 2H); ¹³C NMR (CDCl₃, 100 MHz) δ 14.33, 61.09, 64.45, 126.44, 129.39, 129.75, 146.20,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

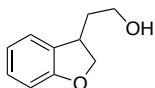


4-Chlorophenyl methanol (4k) ¹H-NMR (CDCl₃, 400MHz) δ: 1.64 (t, J = 6.0 Hz, 1H), 4.68 (d, J = 6.0 Hz, 2H), 7.29-7.35 (m, 4H); ¹³C NMR (CDCl₃, 100 MHz) δ 64.57, 128.38, 128.76, 133.42, 139.33. This product is commercially available and the 1H- and 13C-NMR spectra are consistent with those of the authentic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

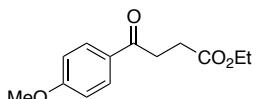


1-fluoro-4-hydroxymethylbenzene (4l) ¹H-NMR (CDCl₃, 400MHz) δ: 1.67 (t, J = 5.5 Hz, 1H), 4.67 (d, J = 5.2 Hz, 2H), 7.02-7.08 (m, 2H), 7.31-7.36 (m, 2H); ¹³C NMR (CDCl₃, 100 MHz) δ 64.71, 115.49 (d, J_{C-F} = 21.0 Hz), 128.88 (d, J_{C-F} = 7.7 Hz), 136.66 (d, J_{C-F} = 2.8 Hz), 162.40 (d, J_{C-F} = 243.5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

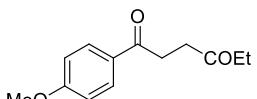
⁵ Murai, N.; Yonaga, M.; Tanaka, K. *Org. Lett.* **2012**, *14*, 1278.



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-butyric acid 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.

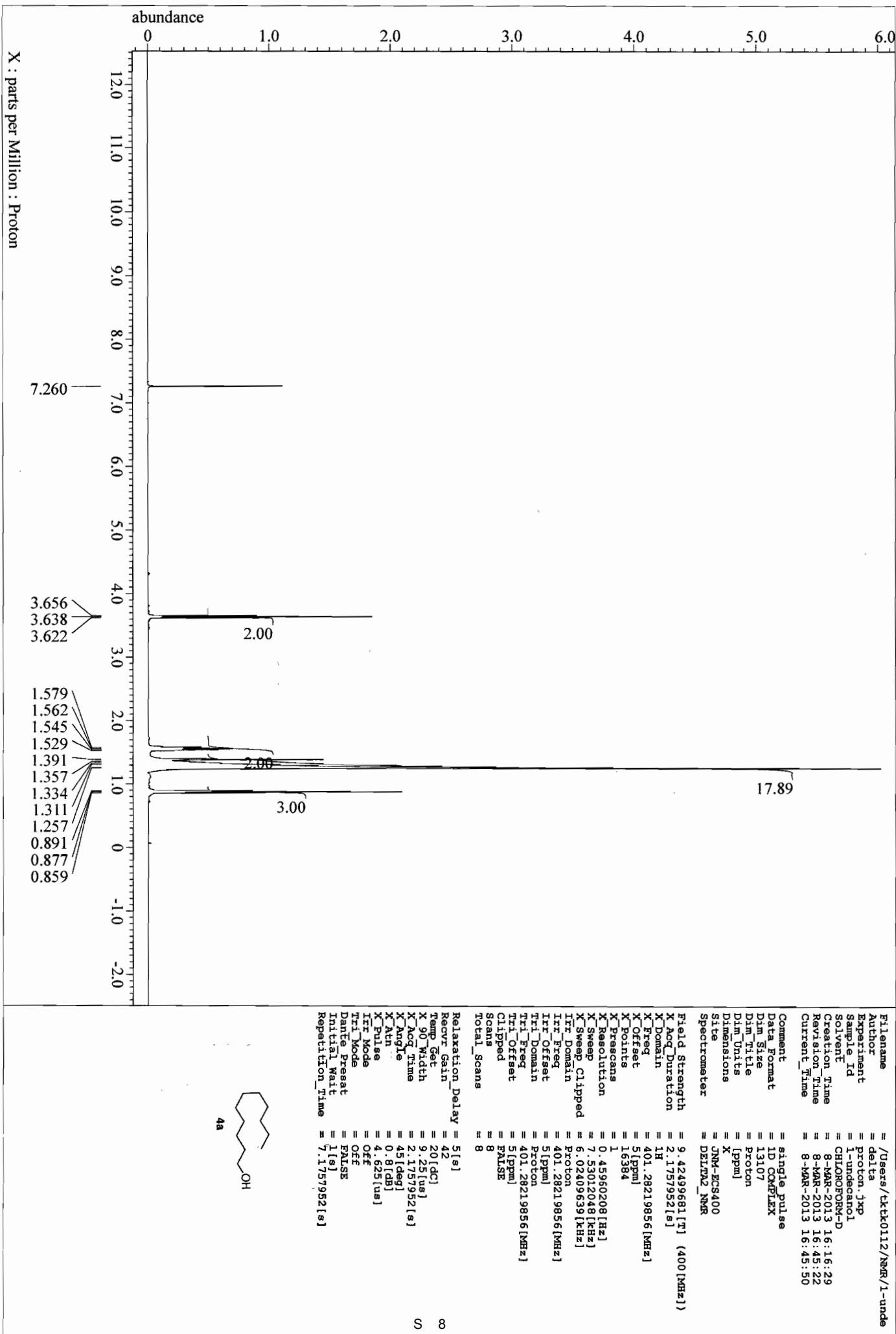


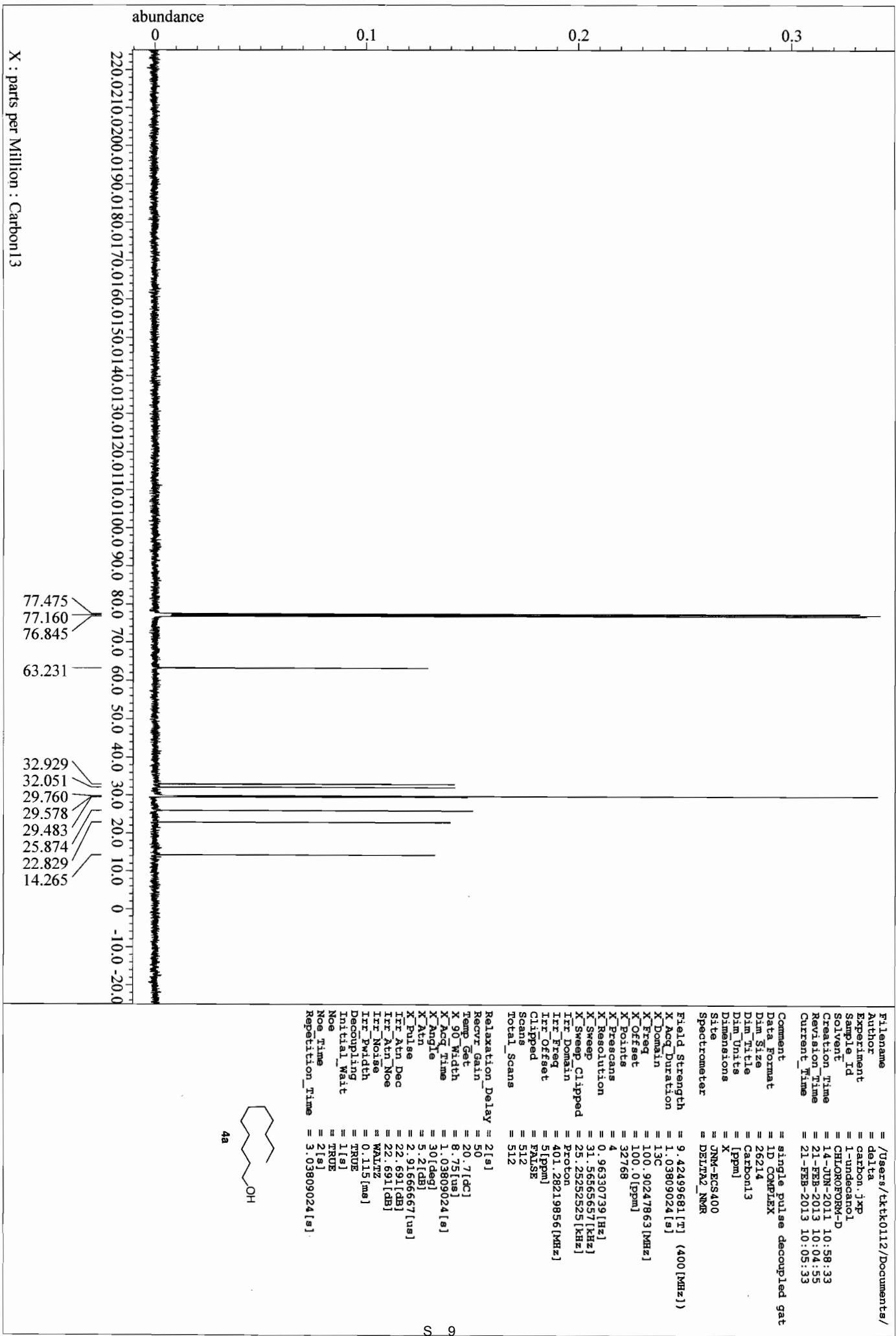
1-(4-methoxyphenyl)hexane-1,4-dione⁸ (9d) ¹H NMR (CDCl₃, 400 MHz): δ 1.10 (t, *J* = 7.2 Hz, 3H), 2.57 (q, *J* = 7.6 Hz, 2H), 2.85 (t, *J* = 6.0 Hz, 2H), 3.25 (t, *J* = 6.4 Hz, 2H), 3.87 (s, 3H), 6.92-6.95 (m, 2H), 7.96-7.98 (m, 2H); ¹³C NMR (CDCl₃, 100 MHz) δ 7.91, 32.14, 35.93, 36.16, 55.52, 113.74,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

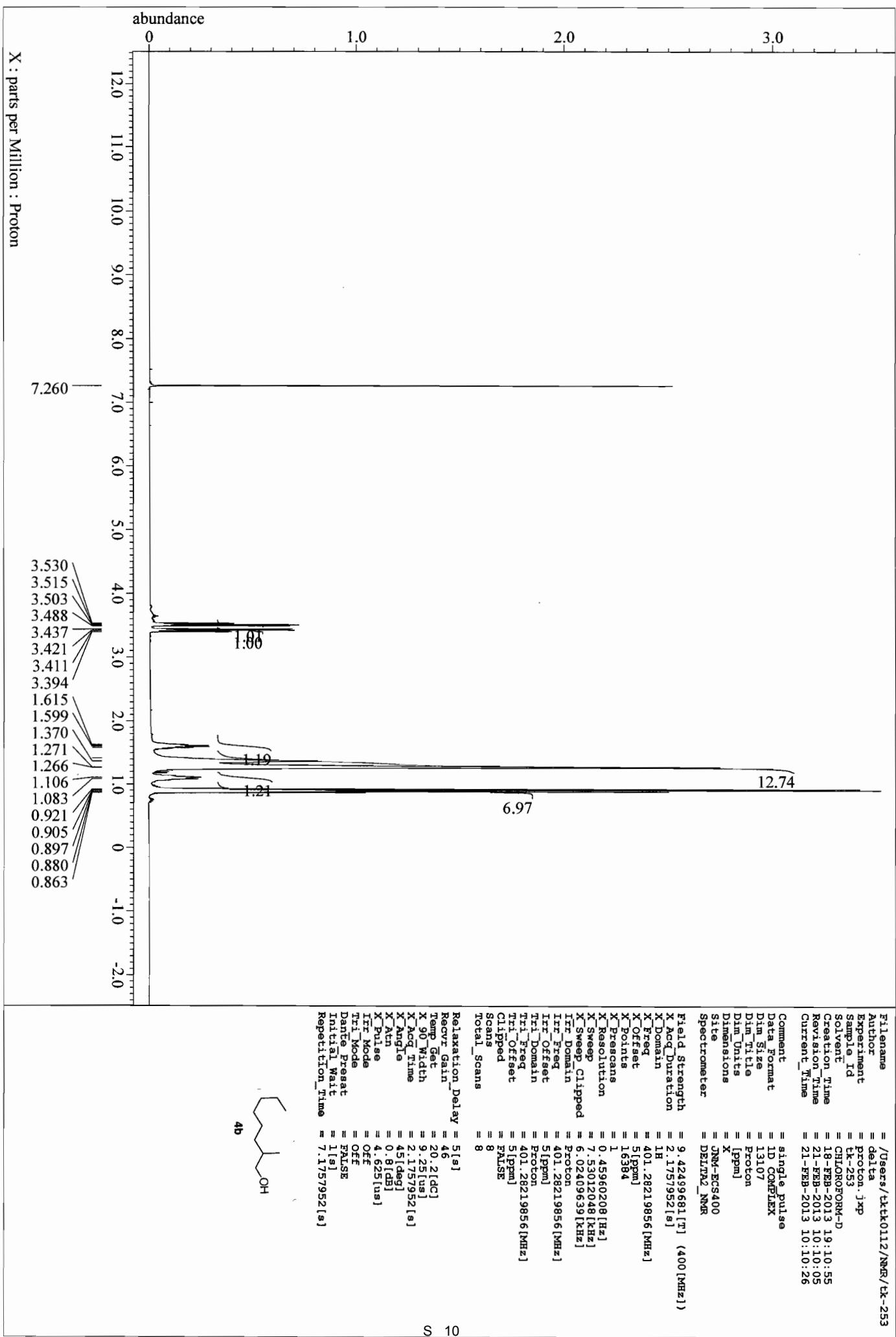
⁷ Le Bras, G.; Provot, O.; Peyrat, J.; Alami, M.; Brion, J. *Tetrahedron Lett.* **2006**, *47*, 5497.

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.

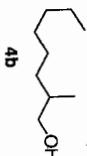
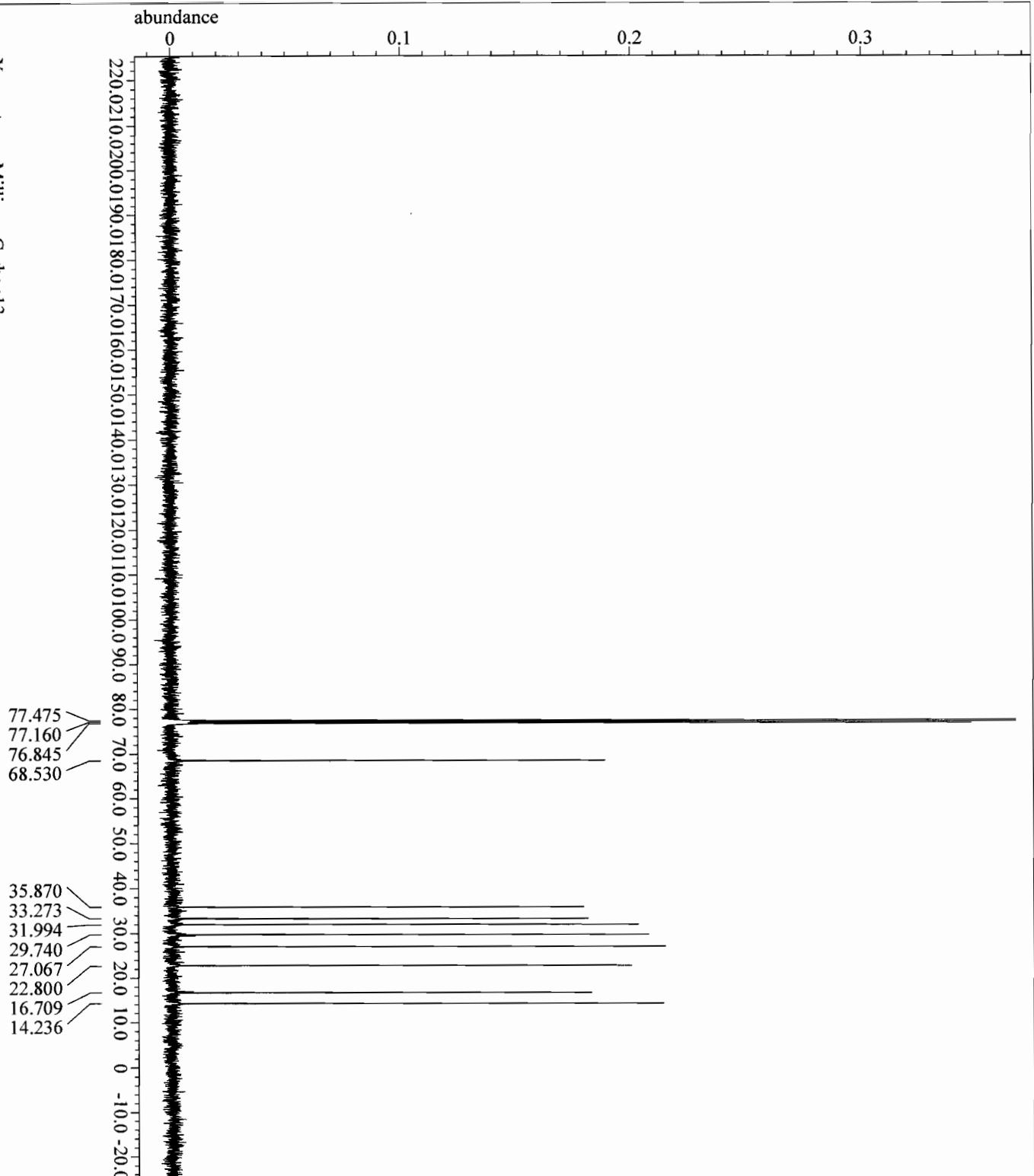




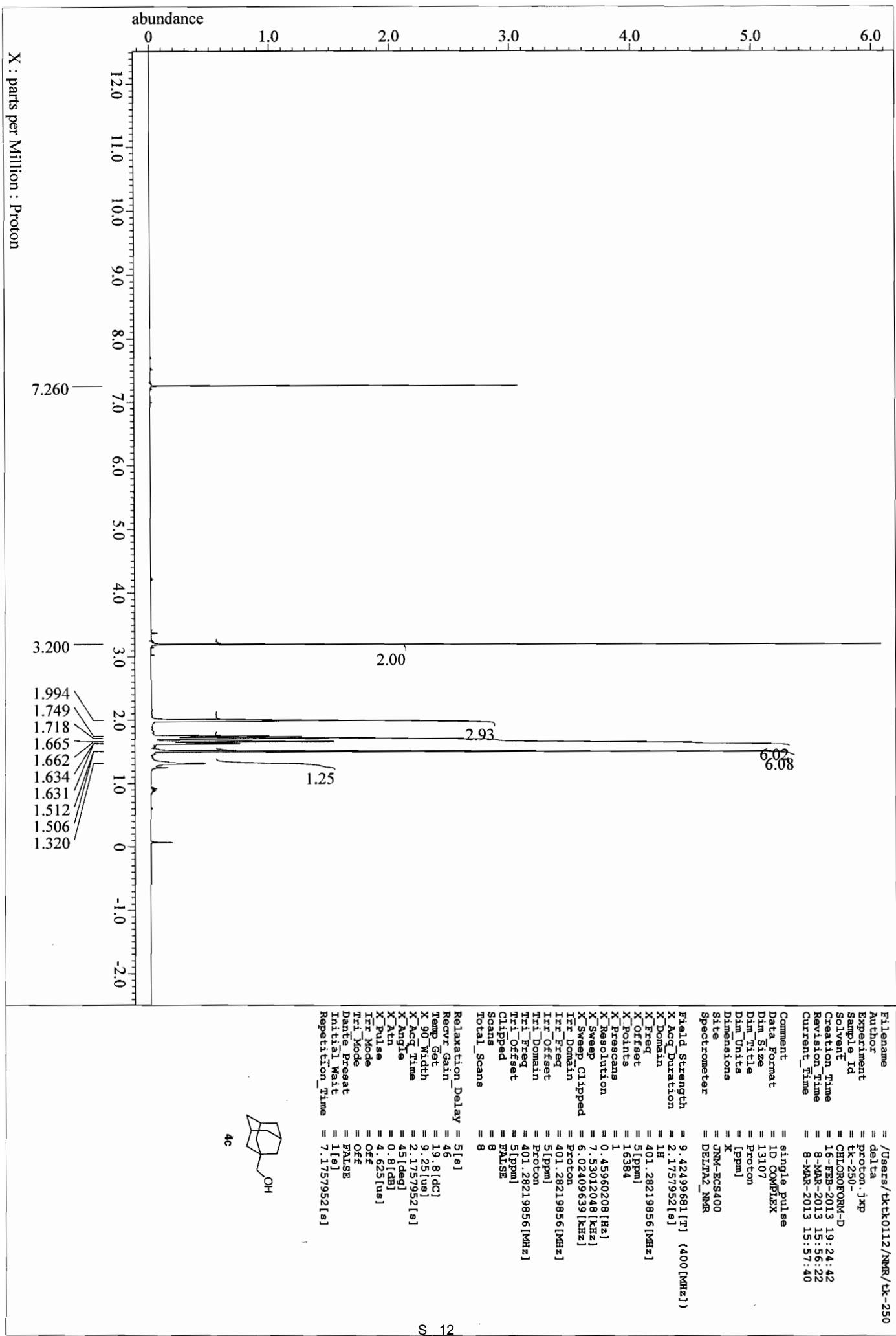
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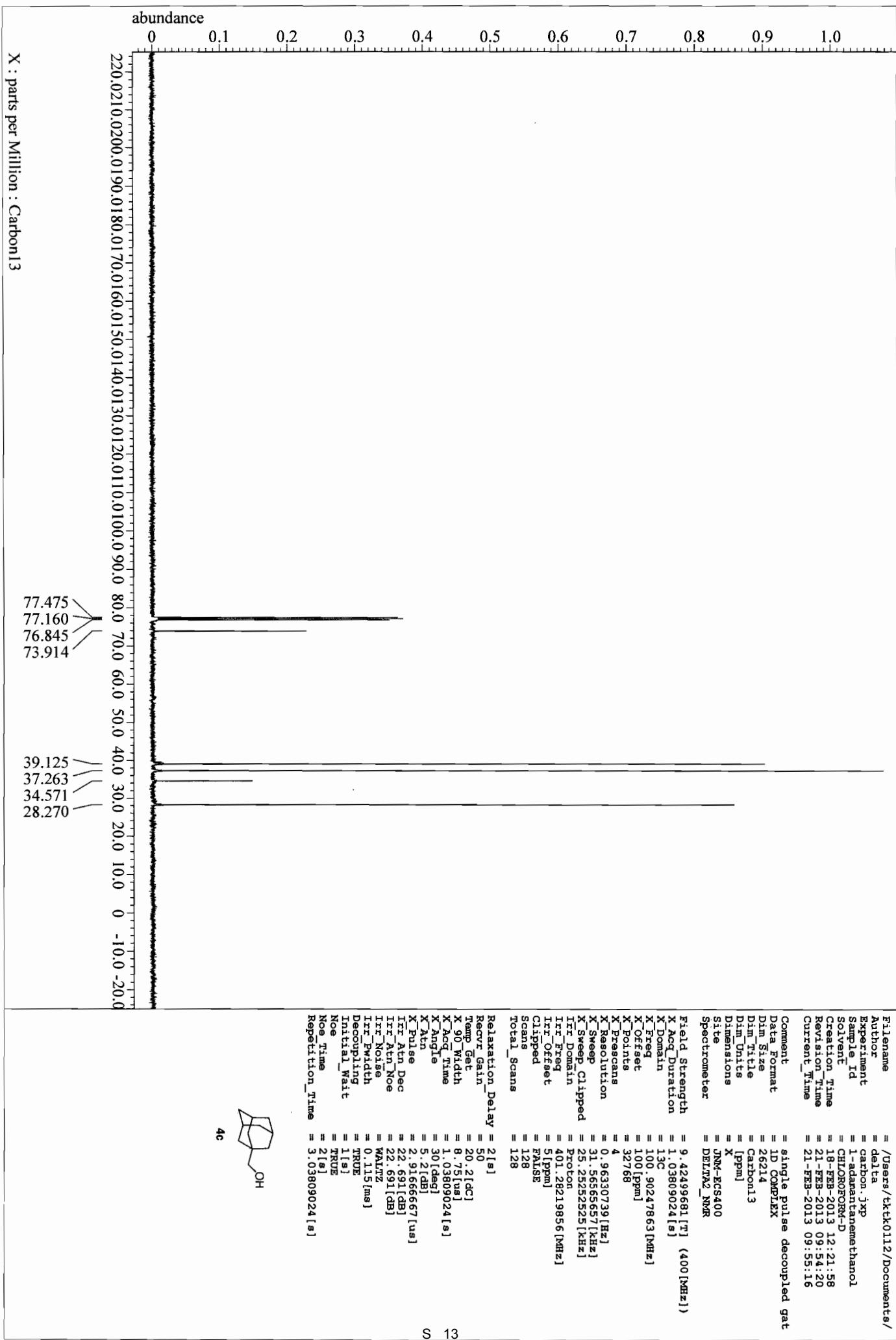
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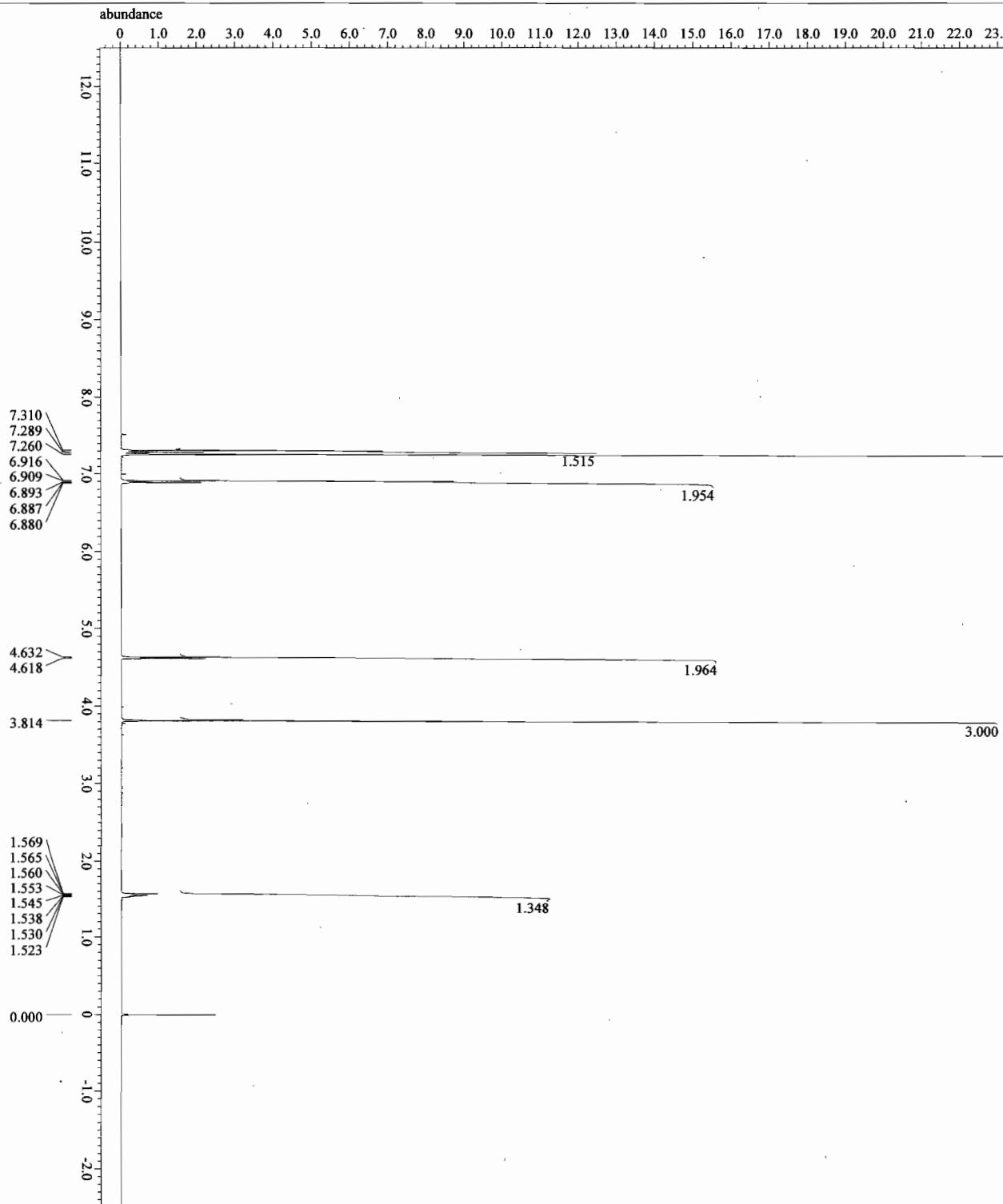
4b



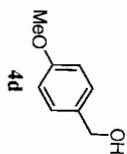
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X : parts per Million : Carbon13



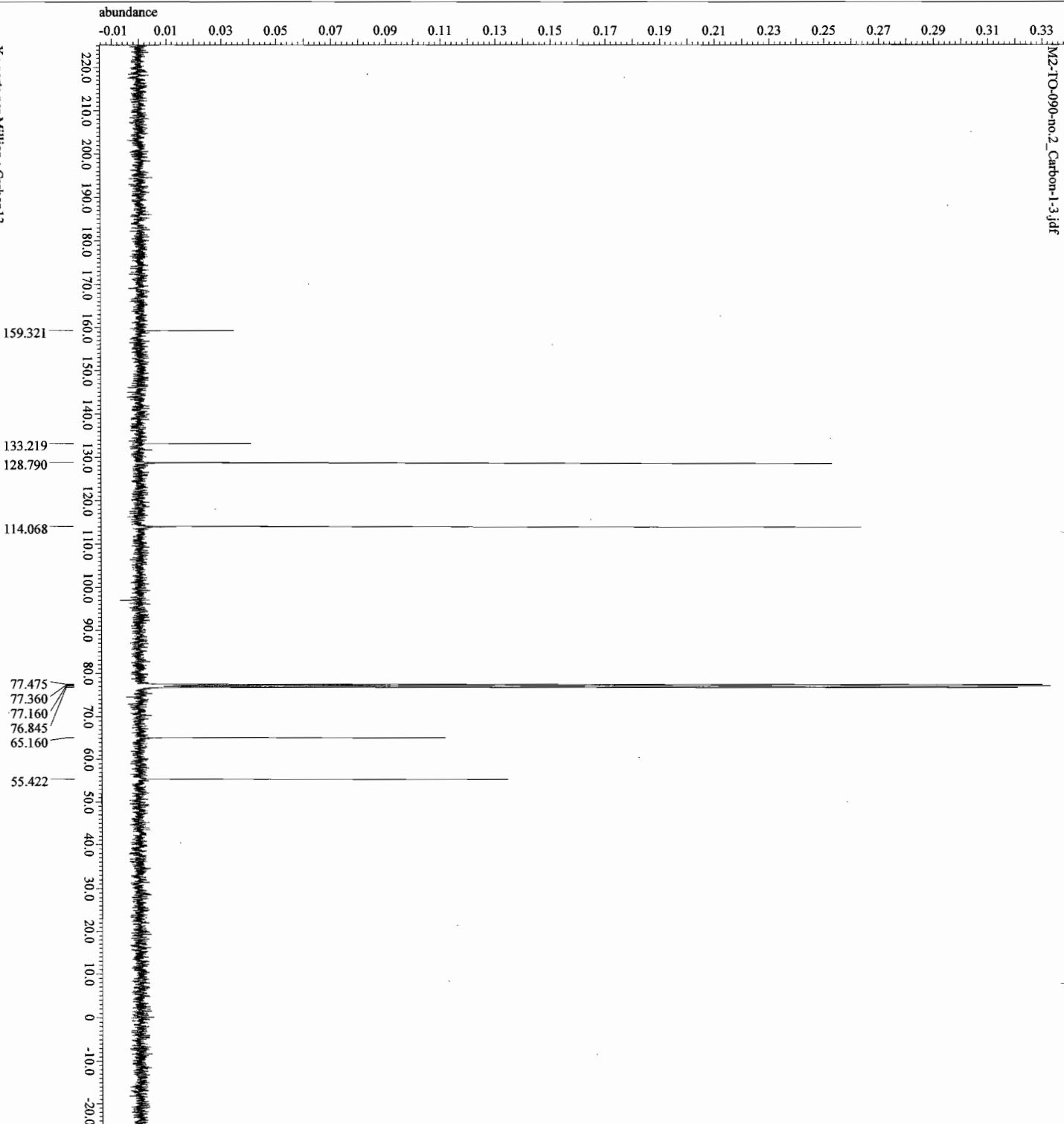
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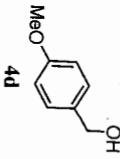
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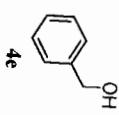
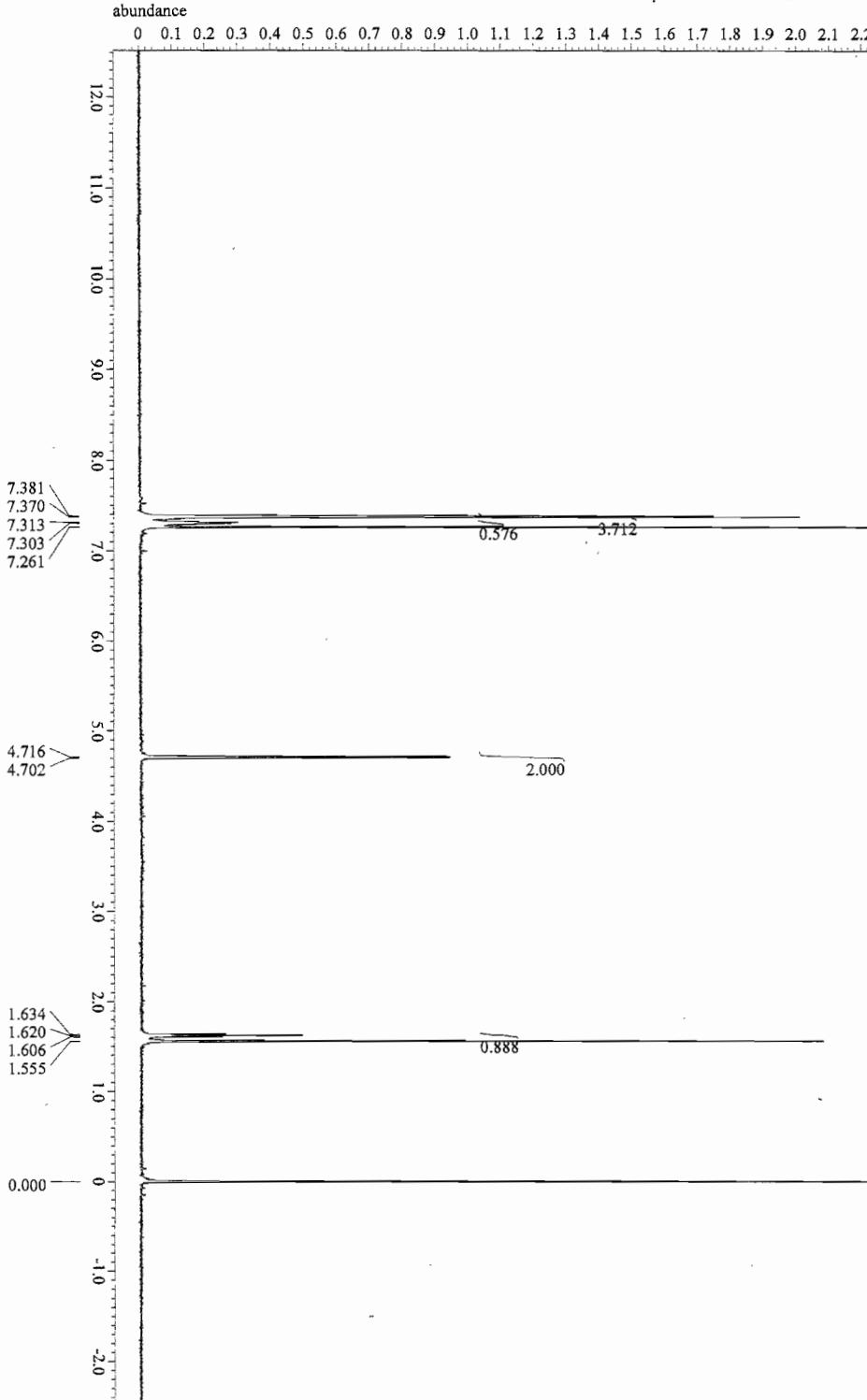
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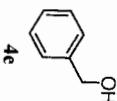
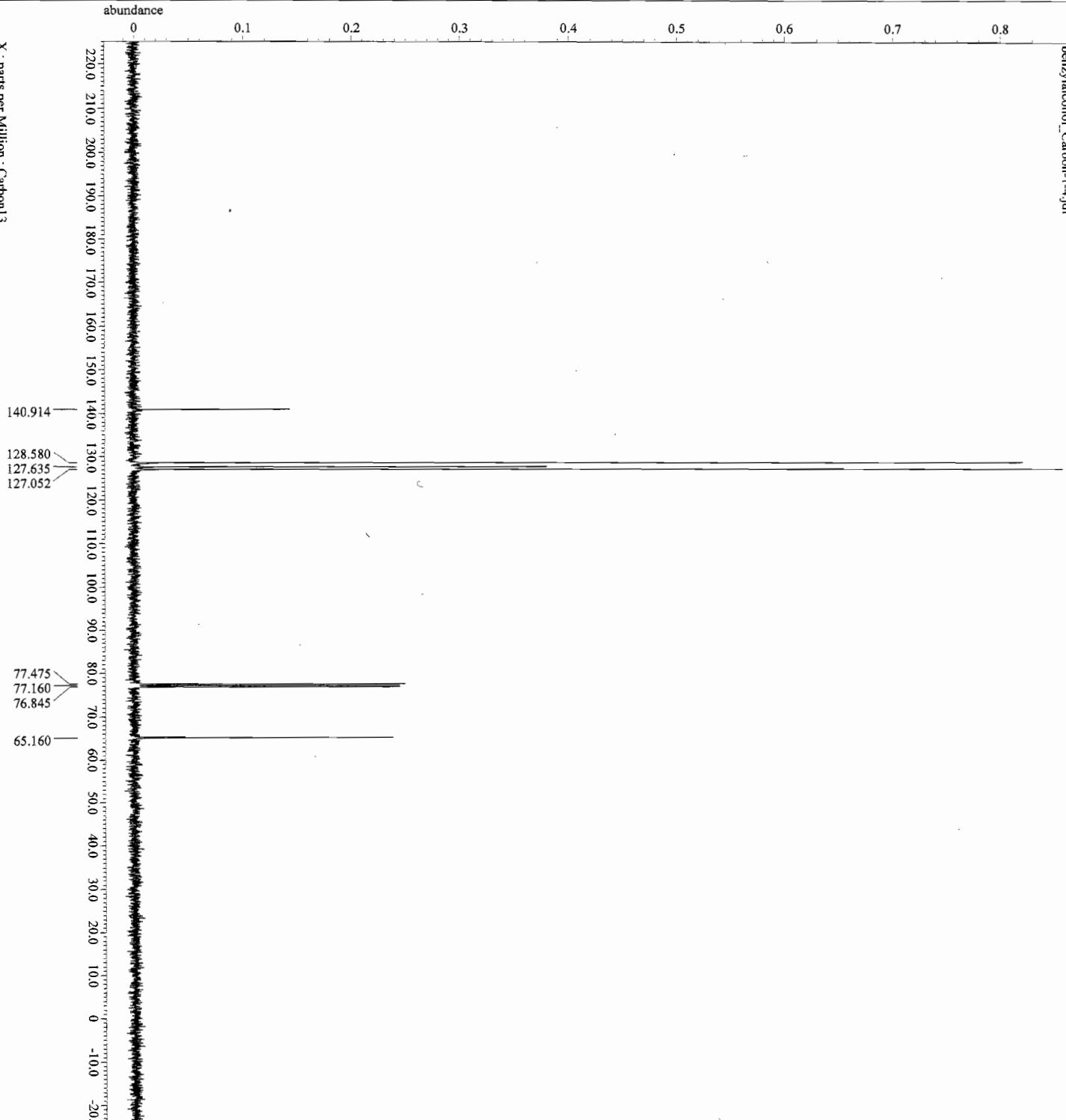
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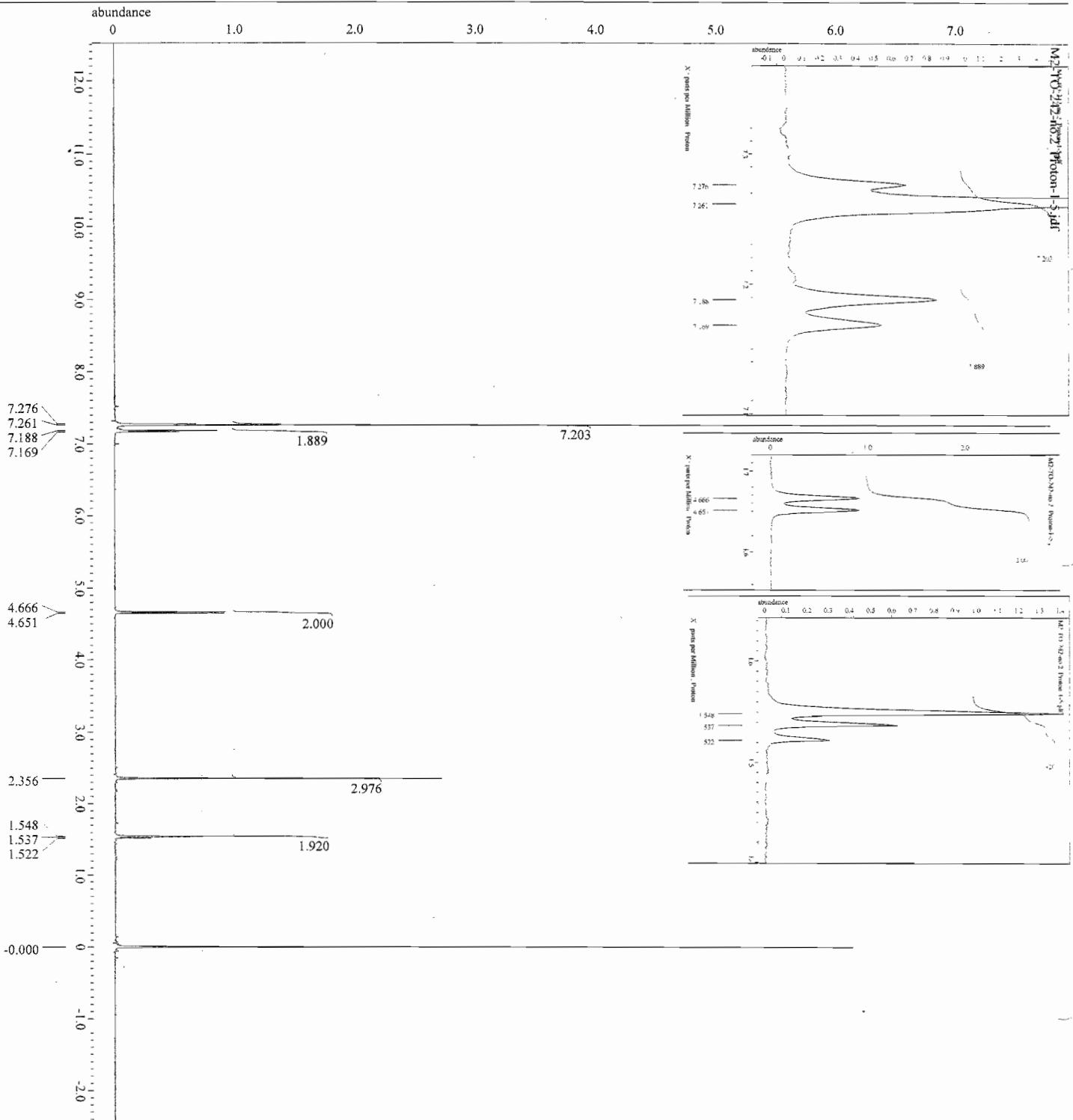


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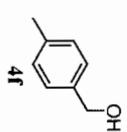
File name = \Users\dealta\Documents\JED
Author = da18
Sample ID = carbon-13D
Sample Name = benzylalcohol
Sweep Frequency = 8-1400-2013 19:51:40
Sweep Time = 8-1400-2013 20:02:07
Current Time = 8-1400-2013 20:03:21
Comment = single pulse decoupled qat
Data Format = 1D COMPLEX
Data Size = 26214
Data Tilt = 0
Dimensions = [ppm]
X = X
Site = JNM-ECX400
Spectrometer = DEUTRO_NMR
Field Strength = 9.42499861[Hz]
X Axis Duration = 1.03809924[s]
X Domain = 13C
X Freq = 100.90247763[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 0.96330739[Hz]
X Sweep = 5.56565657[Hz]
X Sweep Clipped = 25.25525525[Hz]
Irr. Domain = Proton
Irr. Freq = 401.28219556[MHz]
Irr. Offset = 5[ppm]
Clipped = FALSE
Scans = 64
Total Scans =
Relaxation Delay = 2[s]
Recur. Gain =
Temp. Get = 20.1 [deg]
X 90 Width = 6.75[us]
X Acq. Time = 1.03809924[s]
X Angle = 30[deg]
X Att. = 5.2[db]
X Pulse = 2.93658567[us]
Irr. Att. Dec = 22.691[us]
Irr. Att. Rec = 22.691[us]
Irr. Noise = 0.115[ms]
Irr. Width = 700
Decoupling = 1.01
Initial Wait =
None =
Noe_Time = 2[us]
Repulsion_Time = 3.03809924[s]

```

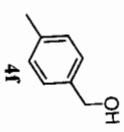
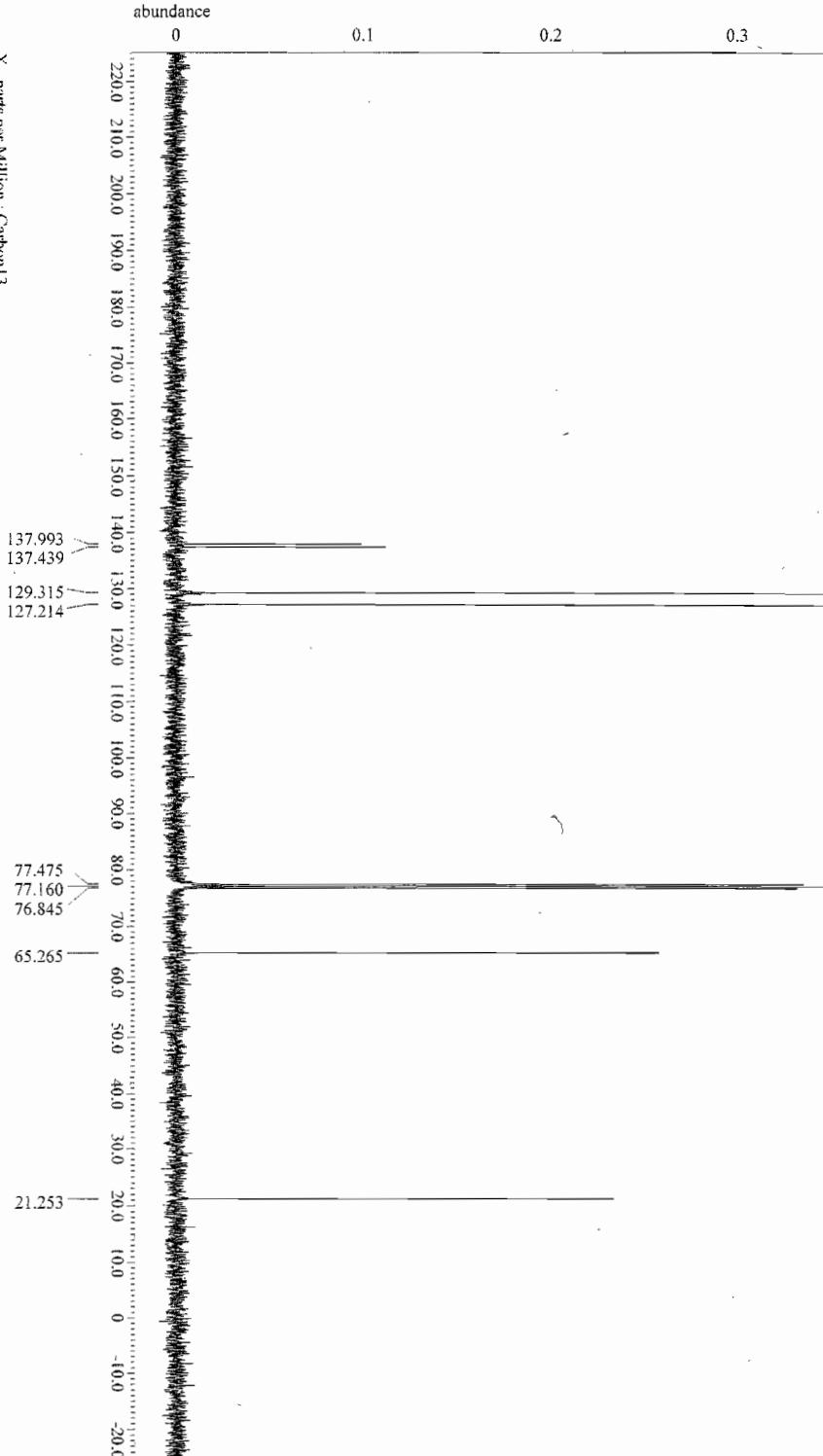


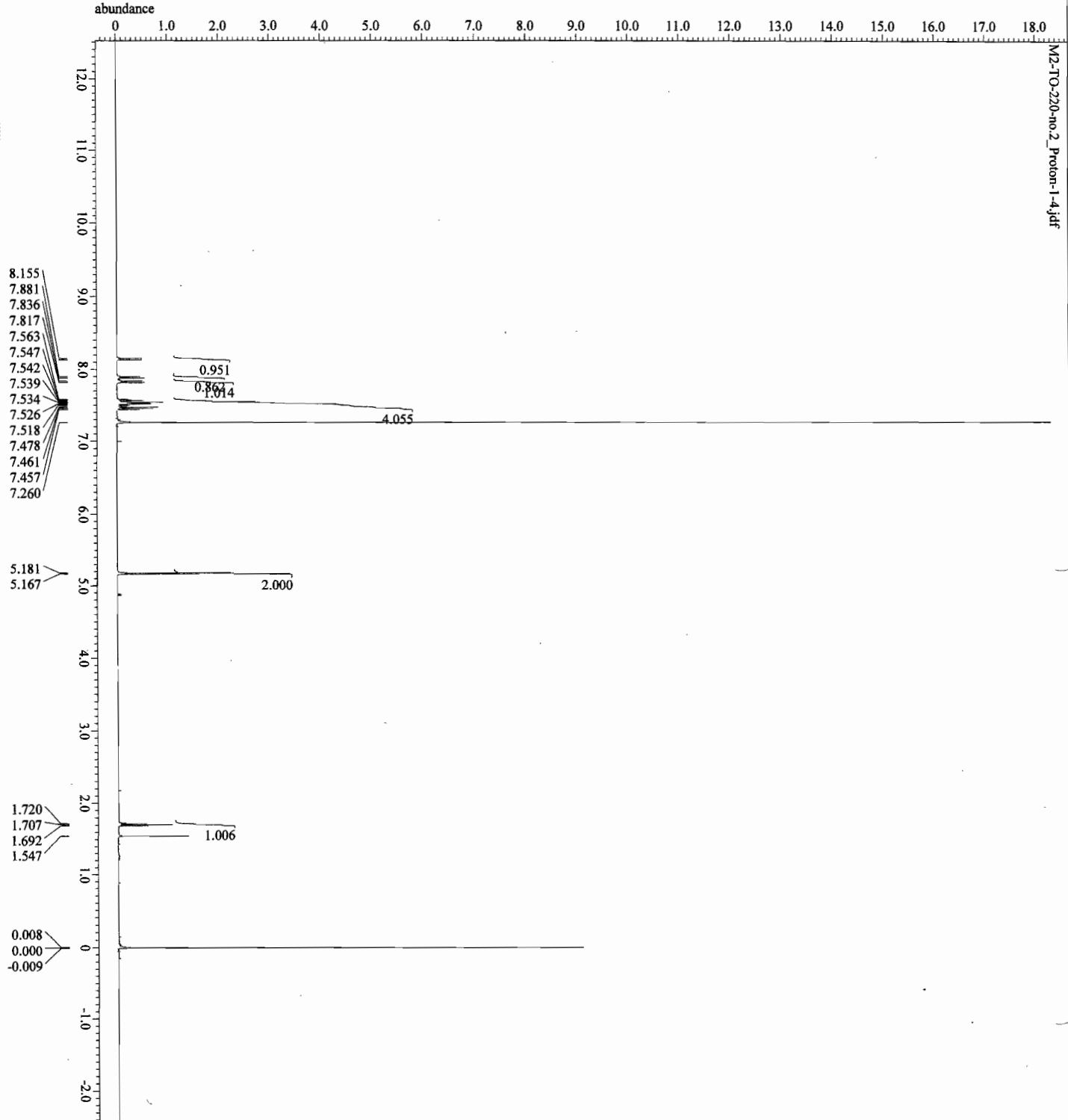


File Name = \Users\delta\Documents\J\B0
 Author = delta
 Experiment = M2-TO-M2-002
 Sample ID = M2-TO-M2-002
 Solvent = CHLOROFORM-D
 Creation Time = 21-FEB-2013 01:54:38
 Current Time = 21-FEB-2013 04:34:53
 Comment =
 Data Format = single pulse
 Dim Size = 1D
 Dim Title = proton
 Dim Units = {ppm}
 Dimensions = X
 Site = JNM-ECIS400
 Spectrometer = DELTA II NMR
 Field Strength = 9.42499681[T] (400[Hz])
 X_Acq_Duration = 2.1757952[ss]
 X_Domain = 1H
 X_Freq = #01-28219856[MHz]
 X_Offset = 51[ppm]
 X_Points = 16384
 X_Precs = 1
 X_Resolution = 0.43965208[Hz]
 X_Sweep = 7.53012081[Hz]
 X_Sweep_Clip = 6.02409659[Hz]
 Xr_Domain = Proton
 Xr_Freq = #01-28219856[MHz]
 Xr_Offset = 51[ppm]
 Xr_Domain = Proton
 Xr_Freq = #01-28219856[MHz]
 Xr_Offset = 51[ppm]
 Clipped = FALSE
 Stays = 8
 Total_Stays = 8
 Relaxation_Delay = 5[ss]
 Recv_Gain = 56
 Recv_Gain = 0.8[ad]
 Recv_Set = 9.25[us]
 X_90deg = 2.1757952[ss]
 X_Acq_Time = 4.11[ss]
 X_Am = 0.8[ad]
 X_Pow = 1.625[us]
 IR_Fade = OFF
 Data_Presat = 10[ss]
 Trig_Wait = 11[ss]
 Repetition_Time = 7.1757952[ss]



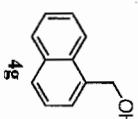
File name = \Users\dat1ta\Documents\J\JEOL
 Author = delta
 Experiment = carbon_13P
 Sample ID = M2-PO-242-no.2C
 Solvent = CHLOROFORM-D
 Creation Time = 21-FEB-2013 04:07:36
 Current Time = 21-FEB-2013 04:36:46
 Comment =
 Data Format = single pulse decoupled 9at
 Dim Size = 1D COMPLEX
 Dim Title = Carbon13
 Dim Units = [ppm]
 Dimensions = X
 Site = JMM-EC540
 Spectrometer = DEUTA2_NMR
 Field Strength = 9.42499681(r) (400[MHz])
 X_Acq_Duration = 1.03809024[e]
 X_Domain = 1.3C
 X_Freq = 100.9024763[MHz]
 X_Offset = 100[ppm]
 X_Points = 32768
 X_ProcScan = 4
 X_Resolution = 0.96330739[us]
 X_Sweep = 31.9656657[KHz]
 X_Sweep_Clipped = 25.2553525[KHz]
 Irr_Domain = Proton
 Irr_Freq = 401.20219556[MHz]
 Irr_Offset = 51ppm
 Clipped = F1ASB
 Scans = 64
 Total_Scans =
 Relaxation_Delay = 2.0s
 Recover_Gain = 50
 Temp_Get = 19.9[deg]
 X_90_Width = 6.75[us]
 X_Acq_Time = 1.03809024[3]
 X_ProcTime = 0.10691
 X_Atn = 5.21[deg]
 X_ProcAvg = 2.916651[us]
 Irr_Atn_Dsc = 1.9811[us]
 Irr_Atn_Neg = 22.6391[us]
 Irr_Bandwidth = 0.0772[us]
 Irr_Bw0 = 0.115[us]
 Decoupling = 1.0s
 Decoupling_Wait = 0.001s
 Noe_Time = 2.0s
 Repetition_Time = 3.03809024[us]



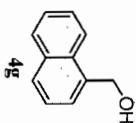
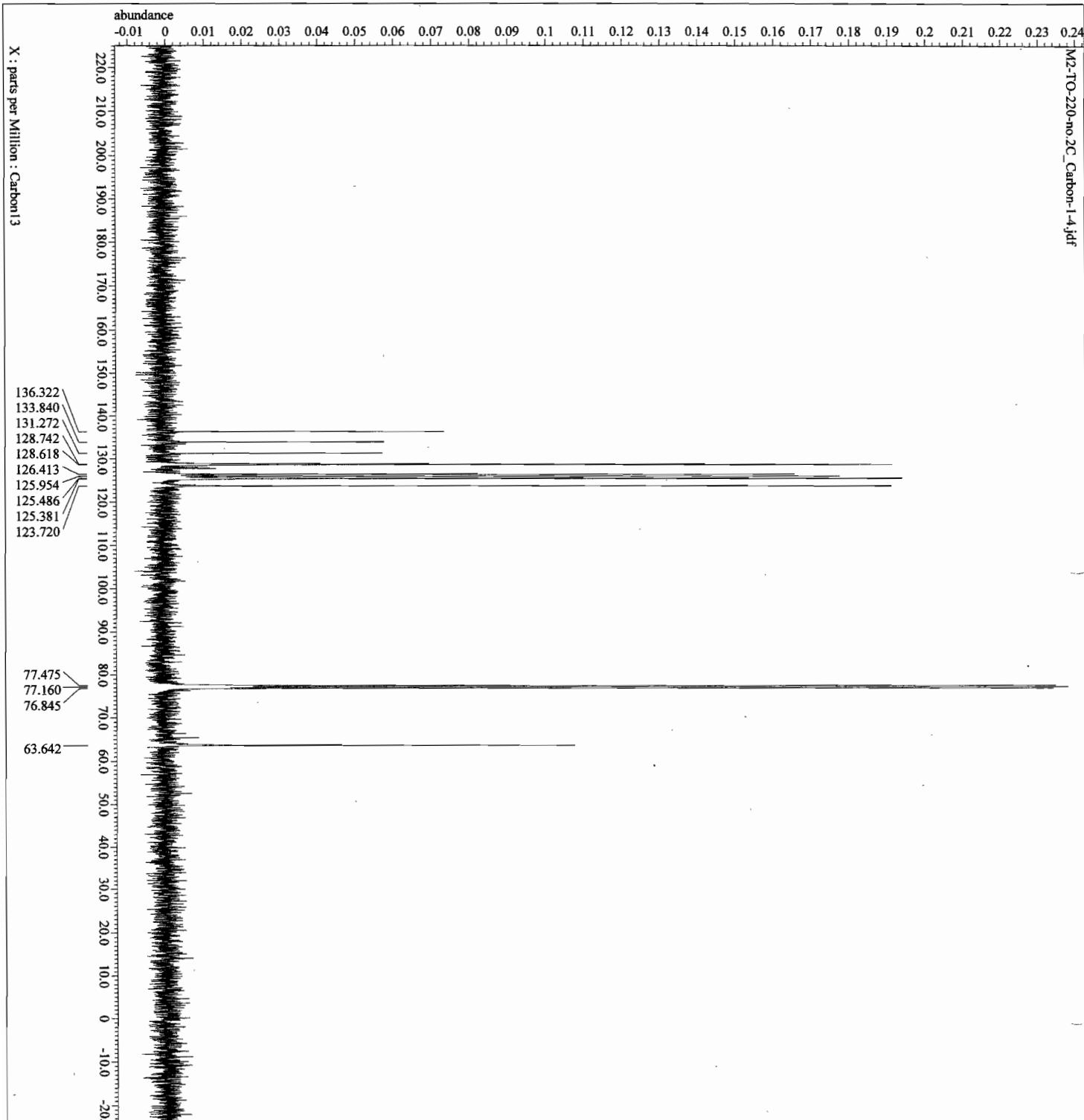


File Name = \User\deltaelta\Documents\JRD
 Author = delta
 Experiment = proton.jdp
 Sample_Id = M2-TO-220-no.2
 Solvent = CHLOROFORM-D
 Creation_Time = 30-JAN-2013 22:25:15
 Revision_Time = 31-JAN-2013 14:07:40
 Current_Time = 31-JAN-2013 14:07:51
 Comment =
 Data_Format = 1D COMPLEX
 Dim_Size = 13107
 Dim_Title = Proton
 Dim_Units = [PPM]
 Dimensions = X
 Site = DBN-REG400
 Spectrometer = DELTA2_NMR
 Field_Strength = 9.42449811771 (400 MHz)
 X_Acq_Duration = 2.1757932 [s]
 X_Domain = 1H
 X_Freq = 401.20219855 [MHz]
 X_Offset = 51ppm
 X_Points = 16384
 X_Pressures = 1
 X_Resolution = 0.459602081 [Hz]
 X_Sweep = 7.350120481 [kHz]
 X_Sweep_Clipped = 6.02409339 [kHz]
 IRR_Domain = Proton
 IRR_Freq = 401.20219855 [MHz]
 IRR_Offset = 51ppm
 T1_Domain = Proton
 T1_Freq = 401.20219855 [MHz]
 T1_Offset = 5 [ppm]
 T1_Signed = FALSE
 Scan = 9
 Total_Scans = 8

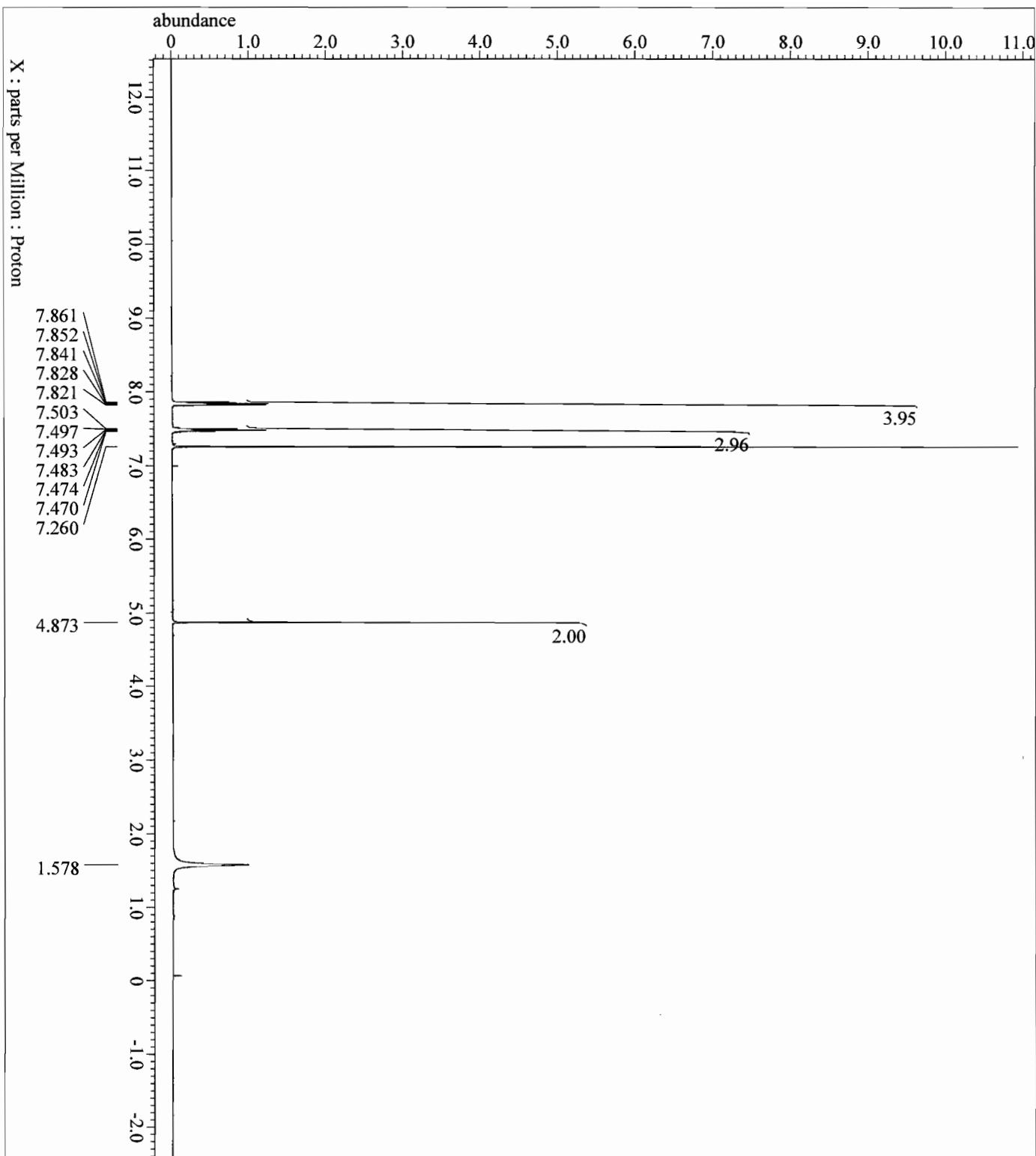
Relaxation_Delay = 5 [s]
 Recv_Gain = 54
 Temp_Cat = 20 [mJ]
 X_90_Width = 9.25 [us]
 X_Acq_Time = 2.1757932 [s]
 X_Angle = 45 [deg]
 X_Atn = 0.81 [dB]
 X_Pulse = 4.625 [us]
 IRR_Mode = off
 T1L_Mode = off
 Dancer_Press = FALSE
 Initial_Matt = 1 [s]
 Repetition_Time = 7.1757932 [s]



JEOL
RESONANCE



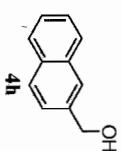
JEOL
RESONANCE

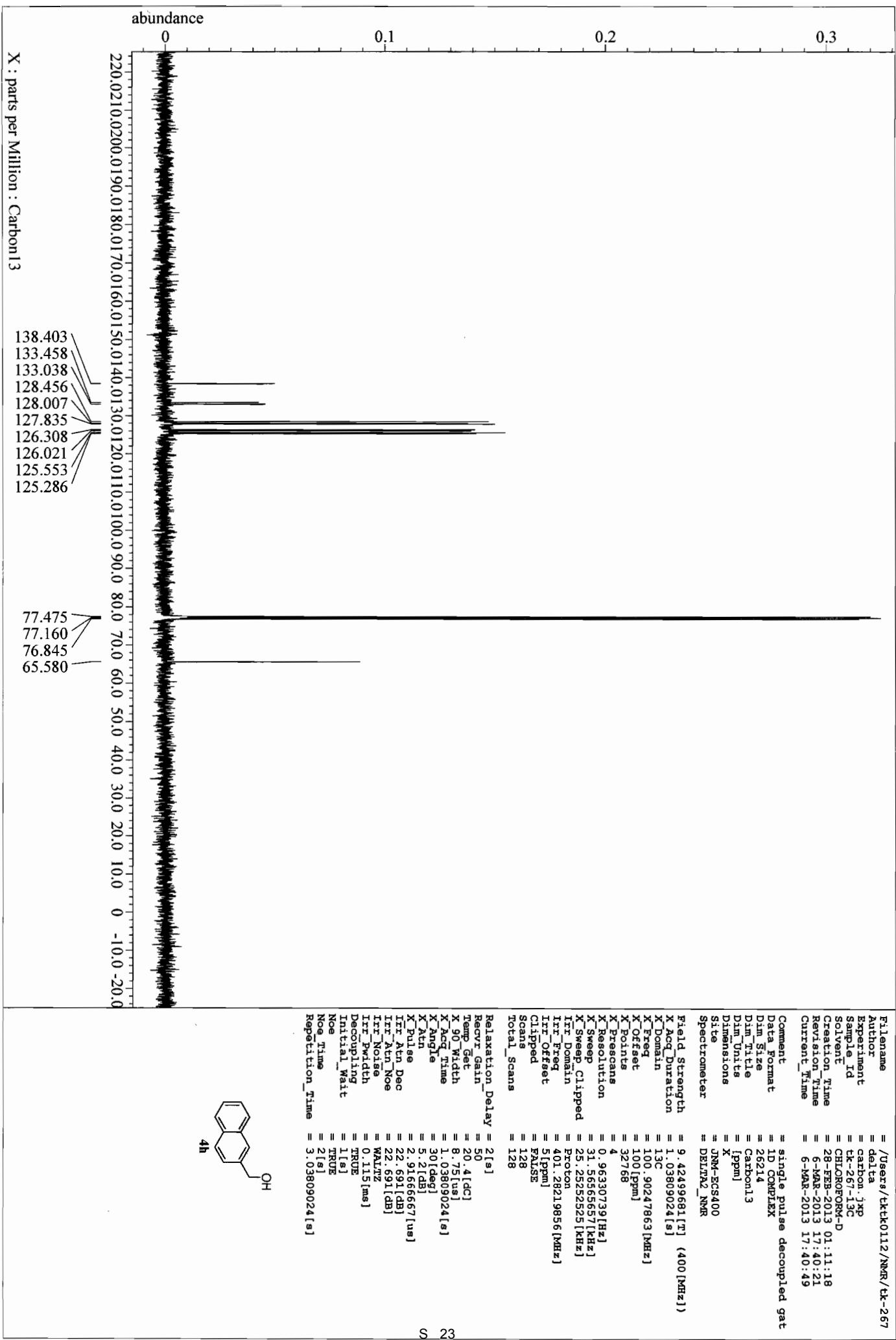


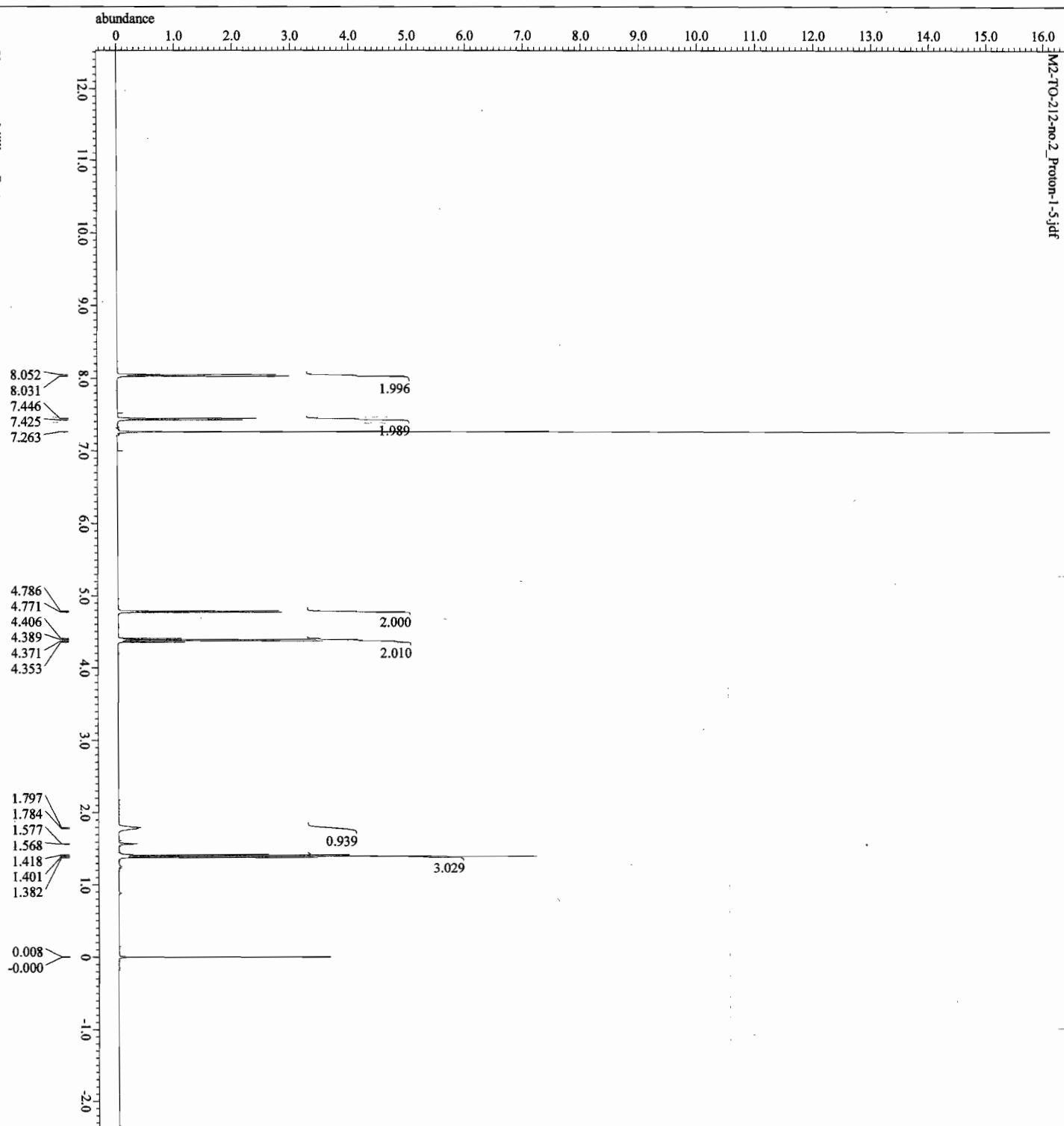
```

Filename = /Users/tkttk0112/NMR/tk-269
Author = delta
Experiment = proton.jmp
Sample_Id = tk-269-15-14
Solvent_T = CHLOROFORM-D
Creation_Time = 4-MAR-2013 23:37:02
Revision_Time = 6-MAR-2013 17:33:24
Current_Time = 6-MAR-2013 17:33:25
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_Accq_Duration = 2.1757952[s]
X_Domain = IH
X_Freq = 401.28219856[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Pressans =
X_Resolution = 0.45960208[Hz]
X_Sweep = 7.53012008[kHz]
X_Sweep_Clipped = 6.02409639[kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856[MHz]
Irr_Offset = 5[ppm]
Irr_Domain =
Tri_Freq = proton
Tri_Offset = 401.28219856[MHz]
Clipped =
Scans = 5[ppm]
Total_Scans = 8
Relaxation_Delay = 5[s]
Recv_Gain = 58
Temp_Ggt = 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
Dant_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.1757952[s]

```







JEOL
RESONANCE

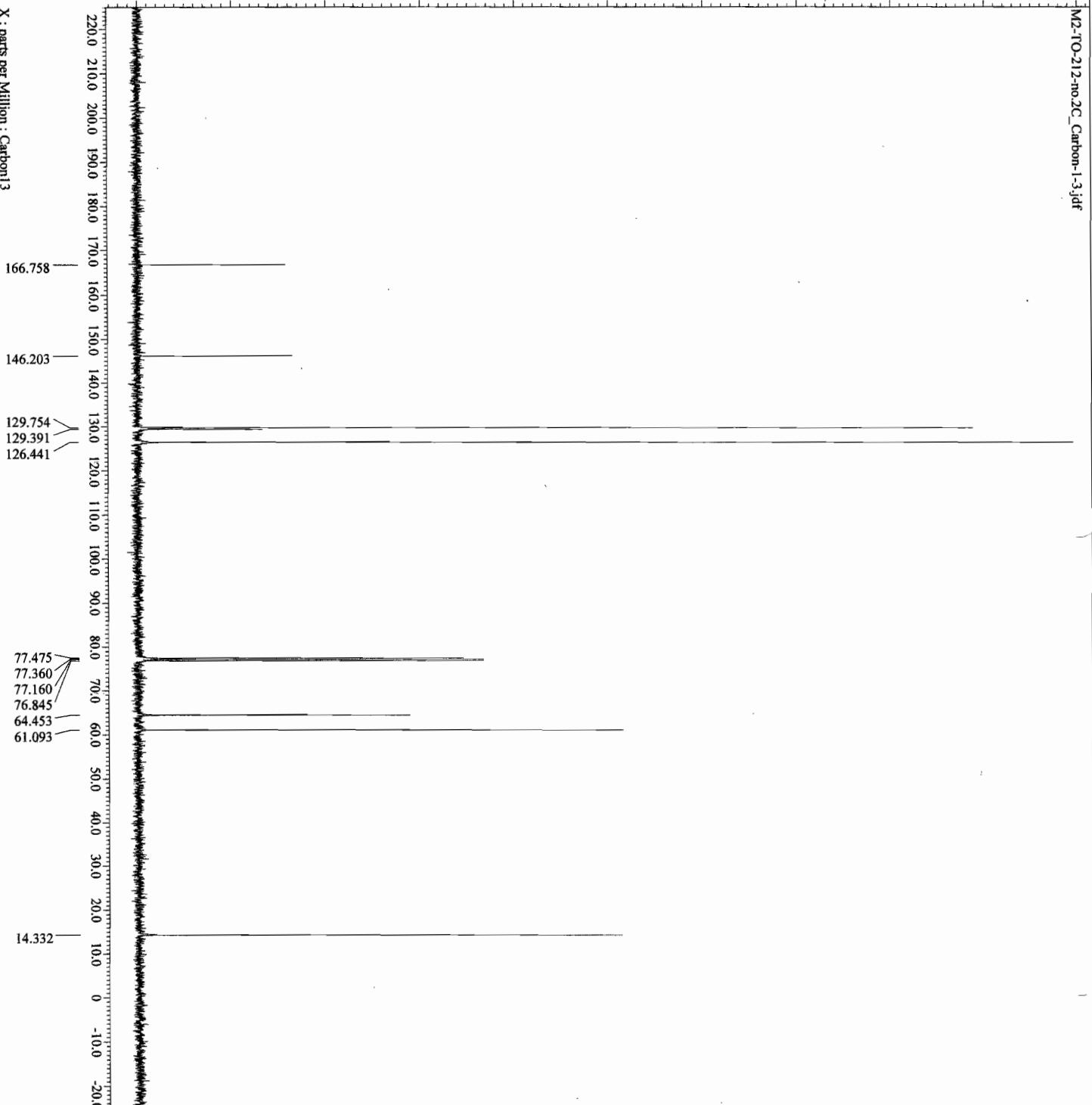
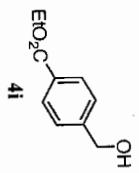
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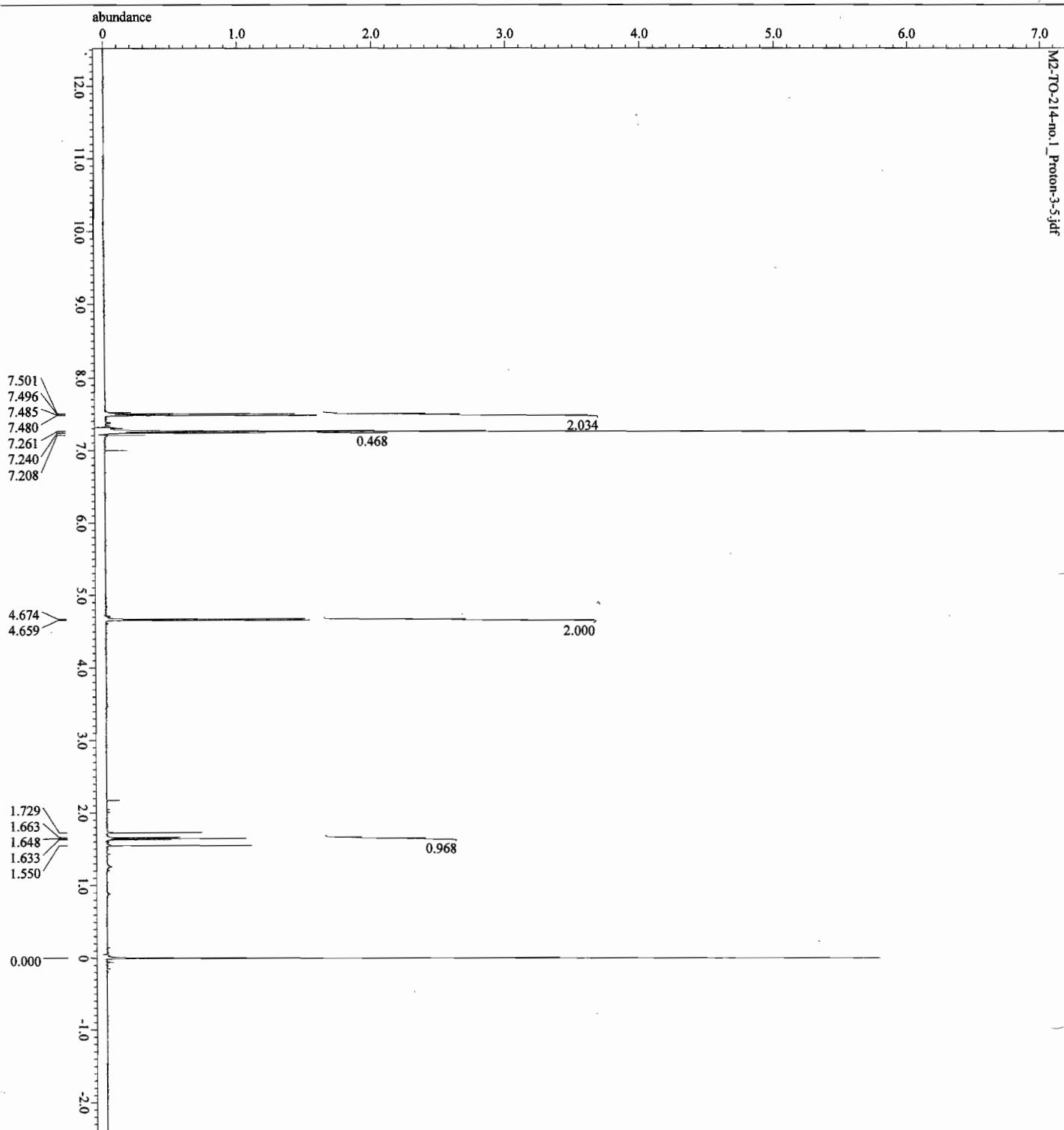
File name = \Users\deltaica\Documents\J\BO
Author = proton
Experiment = proton.jdp
Sample_Id = M2-TO-212-no_2
Solvant = CHLOROFORM-D
Creation Time = 21-7-2013 19:55:50
Revision Time = 21-7-2013 21:00:35
Current Time = 21-7-2013 21:03:47
Comment = single pulse
Data Format = 1D COMPLEX
Data Size = 13107
Dim_Fitie = Proton
Dim_Orts = [1ppm]
Dimensions = X
Bits = 32b-PE8400
Spectrometer = DRX202 NMR
Field Strength = 9.42496811[T] (400 [MHz])
X_Acc_Duration = 2.1757952 [s]
X_Domain = 1K
X_Prog = 401.28219856 [MHz]
X_Offset = 5 [ppm]
X_Points = 16384
X_Pressure = 1
X_Prov = 0.45960208 [Hz]
X_Saturation = 7.55012048 [kHz]
X_Sweep_Clipped = 6.02409659 [kHz]
Irr_Domain = Proton
Irr_Freq = 401.28219856 [MHz]
Irr_Offset = 5 [ppm]
Irr_Domain = Proton
Irr_Freq = 401.28219856 [MHz]
Irr_Offset = 5 [ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5 [s]
Reinv_Gain = 50
Temp_Gain = 20.4161
X_90_Width = 9.22 [us]
X_Acc_Time = 2.1757952 [s]
X_Angle = 45 [deg]
X_Atn = 0.8 [deg]
X_Pulse = 4.625 [us]
Irr_Mode = off
Tril_Mode = off
Dwca_Preset = PULSE
Initial_Watt = 1 [a]
Initial_Watt = 1 [a]
Repetition_Time = 7.1757952 [s]

```

JEOL
RESONANCE

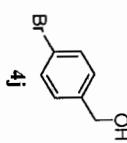
File name = \Users\deltaeta\Documents\JTO
 Author = delta
 Experiment = carbon_13p
 Sample Id = M2-TO-212-no.2C
 Solvent = CHLOROFORM-D
 Creation Time = 21-JAN-2013 20:00:23
 Revision Time = 21-JAN-2013 21:02:13
 Current Time = 21-JAN-2013 21:06:35
 Comment = single pulse decoupled get
 Data Format = 1D COMPLEX
 Dm Size = 26214
 Dm Title = Carbon-13
 Dm Units = [ppm]
 Dimensions = X
 Site = JNM-EC6400
 Spectrometer = DEUTZEL_NMR
 Field Strength = 9.42499681 [T] (400.00001)
 Acq. Duration = 1.03000024 [s]
 X_Domain = 13C
 X_Pfreq = 100.000000 [MHz]
 X_Offset = 100.000000 [ppm]
 X_Points = 32768
 X_Prescans = 4
 X_Resolution = 0.065330739 [Hz]
 X_Sweep = 31.56565657 [Hz]
 X_Sweep_Clipset = 25.223252525 [Hz]
 Xr_Domain = Proton
 Irc_Freq = 401.38219856 [MHz]
 Irc_Offset = 5 [ppm]
 Irc_Clipset = FALSE
 Scans = 64
 Total_Scans = 64
 Relaxation_Delay = 2 [s]
 Rovtr_Gain = 50
 Rovtr_Gain = 20.61 [dB]
 X_90_Width = 8.75 [us]
 X_Acq_Time = 1.03600024 [s]
 X_Angle = 30 [deg]
 X_Amt = 5.2 [dB]
 X_Pulse = 2.91666667 [us]
 Irc_Atn_Dec = 22.631 [dB]
 Irc_Atn_Nose = 22.631 [dB]
 Irc_Noise = 0.113 [mV]
 Irc_Pw1ch = TRUE
 Decoupling = TRUE
 Initial_Wait = 1 [s]
 Nco = TRUE
 Nco_Time = 2 [s]
 Repetition_Time = 3.03809024 [s]





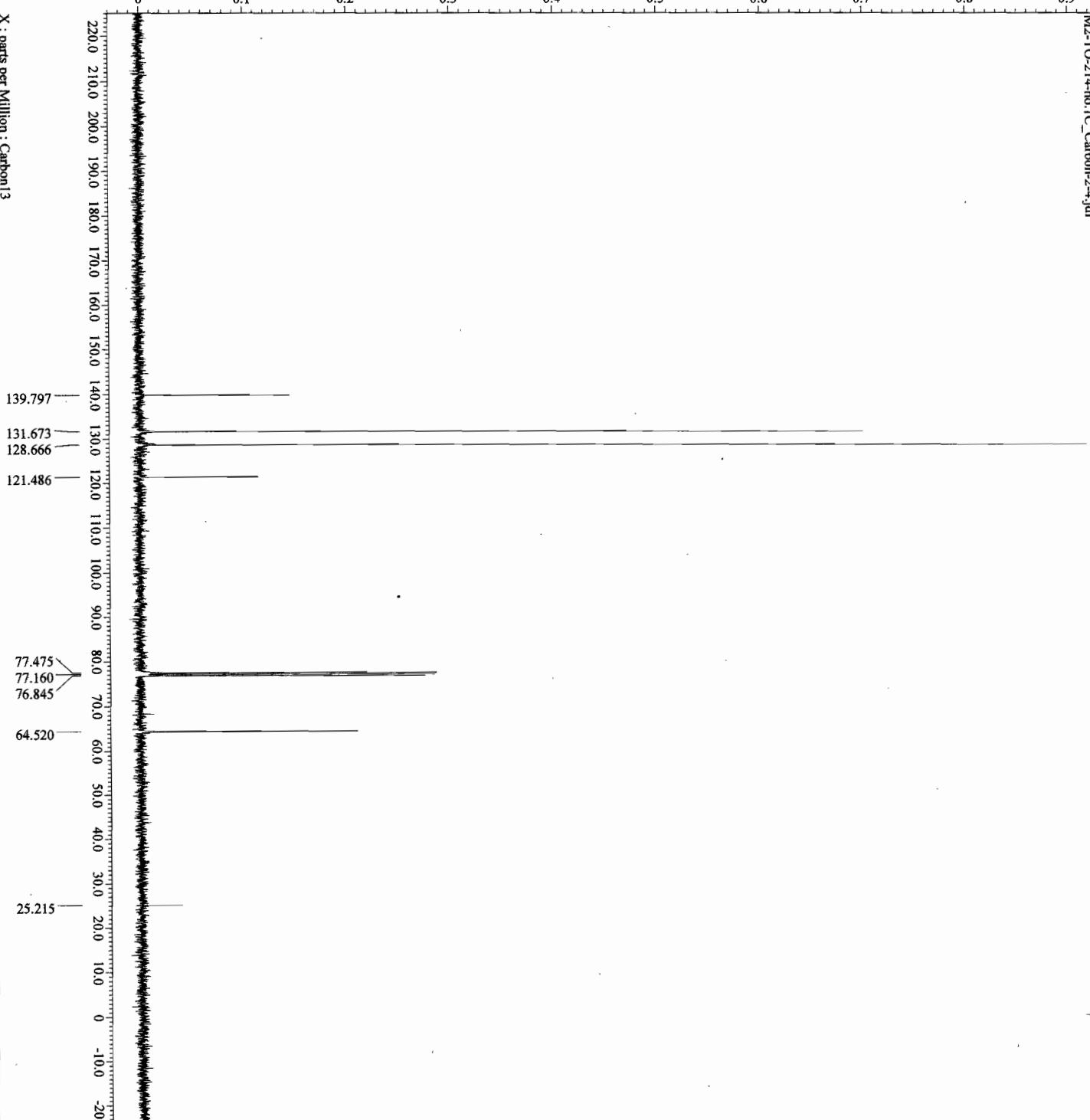
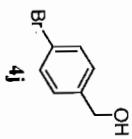
JEOL
RESONANCE

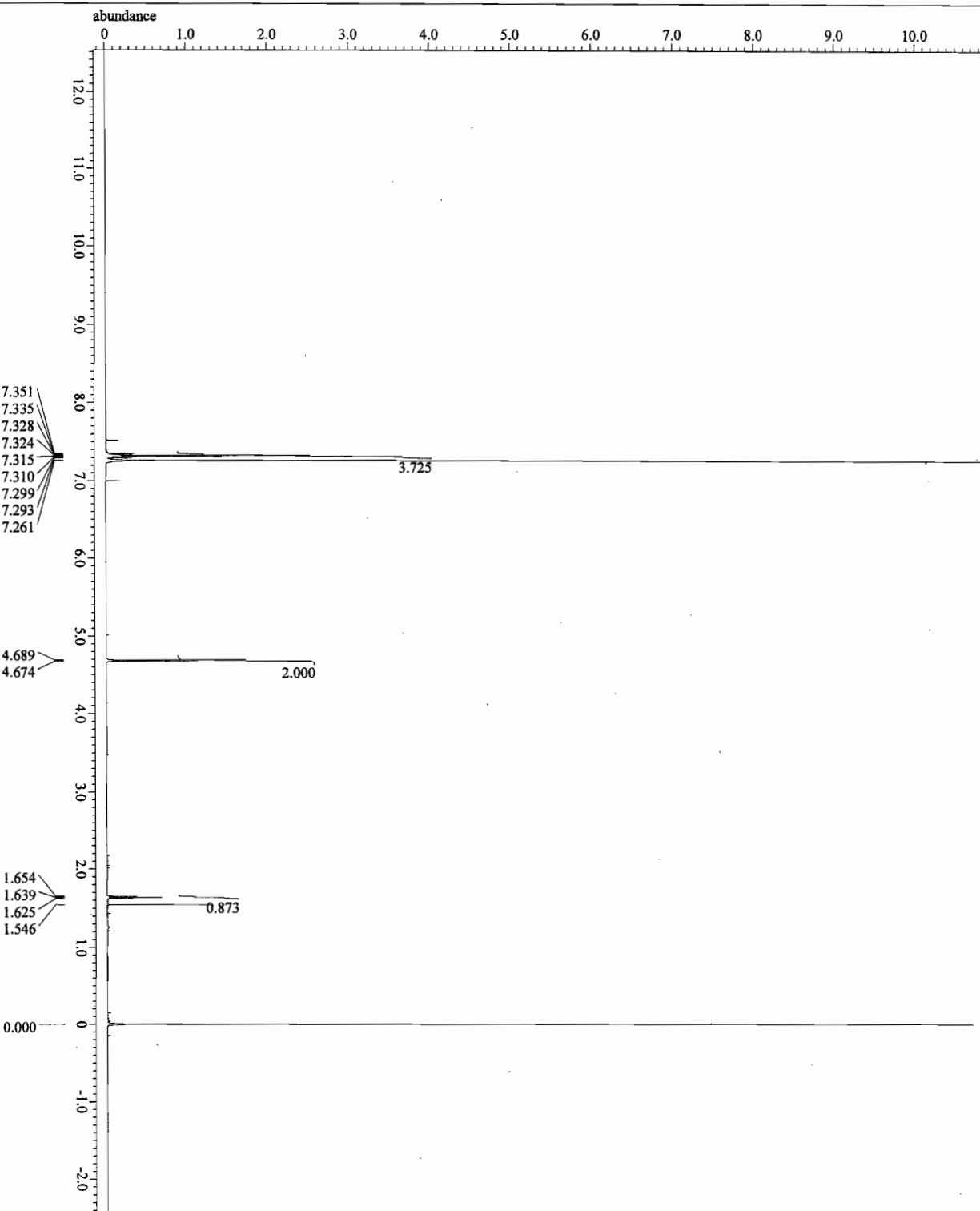
File Name = 'Users\dat\Documents\J00
Author = dat.ca
Experiment = proton.jdp
Sample Id = M2-T0-214-no.1
Solvent = CHLOROFORM-D
Creation Time = 22-JAN-2013 19:23:43
Revision Time = 22-JAN-2013 21:25:03
Current Time = 22-JAN-2013 21:25:20
Comment =
Data Format = 1D COMPLEX
Dim_Size = 13107
Dim_Ratio = Proton
Dim_Units = [ppm]
Dimensions = X
S1ts = JMR-SCS400
Spectrometer = DELTA2_NMR
Field Strength = 9.42499881 [T] (400 [MHz])
X_Acq_Duration = 2.17579521 [s]
X_Domain = 1H
X_Freq = 401.28219856 [MHz]
X_Offset = 5 [ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45960208 [Hz]
X_Sweep = 7.532048 [Hz]
X_Sweep_Clipped = 6.02409353 [Hz]
IRr_Domain = Proton
IRr_Freq = 401.28219855 [MHz]
IRr_Offset = 5 [ppm]
IRr_Domain = Proton
Tr1_Freq = 401.28219855 [MHz]
Tr1_Offset = 5 [ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5 [s]
Recv_Gain = 54
Temp_Gain = 10.9 [dB]
X_90_Width = 9.25 [deg]
X_Acq_Time = 2.17579521 [s]
X_Angle = 45 [deg]
X_Atn = 0.8 [dB]
X_Pulse = 4.625 [us]
IRr_Mode = OFF
Tr1_Mode = OFF
Dwts_Preset = PULSE
Initial_Wait = 1 [s]
Repetition_Time = 7.17579521 [s]



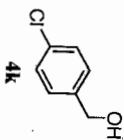
JEOL
RESONANCE

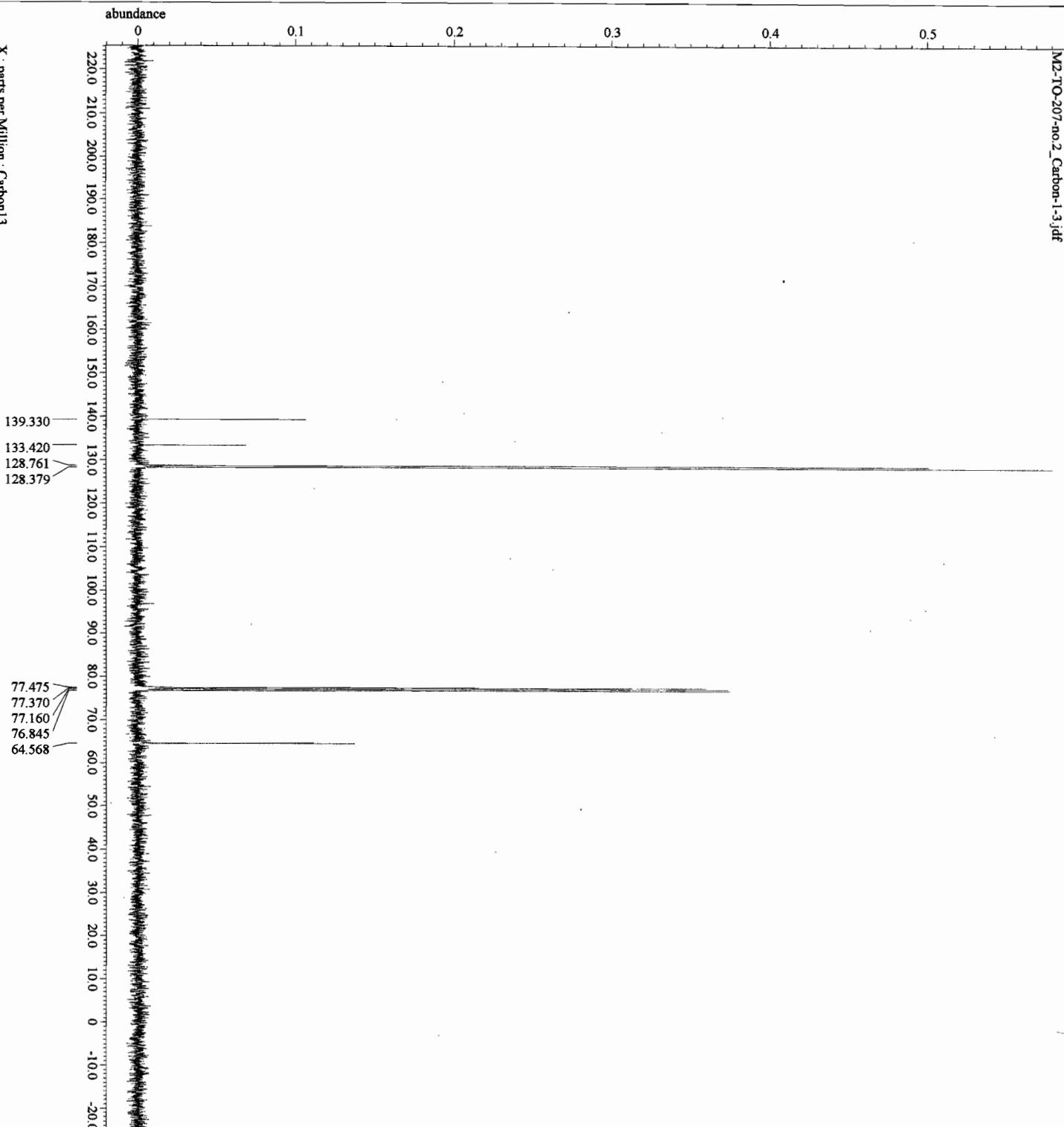
Filenamme = \Users\deltaetta\Documents\JMD
 Author = delta
 Experiment = carbon_1H
 Sample_ID = M2-TO-214-no.1C
 Solvent = CDCl3
 Creation_Time = 22-JAN-2013 19:33:24
 Revision_Time = 22-JAN-2013 21:23:04
 Current_Time = 22-JAN-2013 21:23:38
 Comment = single pulse decoupled gat
 Data_Format = 1D COMPLEX
 Dim_Size = 26214
 Dim_Title = Carbon13
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECX8400
 Spectrometer = DEUTRU2_NMR
 Field_Strength = 9.42999681 [T] (400.0MHz)
 X_Acq_Duration = 1.03809028 [s]
 X_Domain = 13C
 X_Freq = 100.00247653 [MHz]
 X_Offset = 100 [ppm]
 X_Points = 32768
 X_Precision = 4
 X_Resolution = 0.96330739 [Hz]
 X_Sweep = 31.56565657 [Hz]
 X_Sweep_Clipped = 25.23255255 [Hz]
 ITC_Domain = proton
 ITC_Freq = 401.36219615 [MHz]
 ITC_Offset = 5 [ppm]
 ITC_Scale = 1024
 Scans = 64
 Total_Scans = 64
 Relaxation_Delay = 2 [s]
 Rovor_Gain = 50
 Temp_Gain = 20.6 [dc]
 X_90_Watch = 8.75 [us]
 X_Acq_Time = 1.03809024 [s]
 X_Angle = 30 [deg]
 X_Apple = 5.2 [deg]
 X_Pulse = 2.91666667 [us]
 ITC_Alt_Dec = 22.691 [deg]
 ITC_Alt_Ice = 22.691 [deg]
 ITC_Noise = WALKER
 ITC_Pwdch = 0.115 [nm]
 Decoupling = F2DM
 Initial_Wait = 1 [s]
 Note = TRUE
 Note_Time = 2 [s]
 Repetition_Time = 3.03809024 [s]





File name = \Users\deltaelta\Documents\J30
 Author = delta
 Experiment = proton-1D
 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 = simple pulse
 Data Format = 1D_CPMAS
 Data File = 13107
 Dim_Slice = Proton
 Dim_Slice = [ppm]
 Dimensions = X
 Bits = 32K-256400
 Spectrometer = DELTA2_NMR
 Field Strength = 9.4249988171 [T] (400 [MHz])
 X_Acc_Duration = 2.1757952 [s]
 X_Domain = 1H
 X_Freq = 401.282195156 [MHz]
 X_Offset = 5 [ppm]
 X_Points = 15384
 X_Program = 1
 X_Program = 0.459602081 [Hz]
 X_Sweep = 7.350120481 [kHz]
 X_Sweep_Clipped = 6.024095379 [kHz]
 IRR_Domain = Proton
 IRR_Freq = 401.28219556 [MHz]
 IRR_Offset = 5 [ppm]
 IRR_Domain = Proton
 IRR_Freq = 401.28219556 [MHz]
 IRR_Offset = 5 [ppm]
 Clipped = FALSE
 Slices = 8
 Total_Slices = 8
 Relaxation_Pulse = 5 [s]
 Reserve_Gain = 34
 Temp_Gain = 20 [dB]
 X_90_Width = 9.25 [us]
 X_Acc_Time = 2.1757952 [s]
 X_Angle = 45 [deg]
 X_Atn = 0.8 [dB]
 X_Pulse = 4.625 [us]
 IRR_Mode = off
 IRR_Offset = off
 Danto_Preset = PMSA
 Initial_Phase = 1 [o]
 Repetition_Time = 7.1757952 [s]



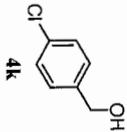


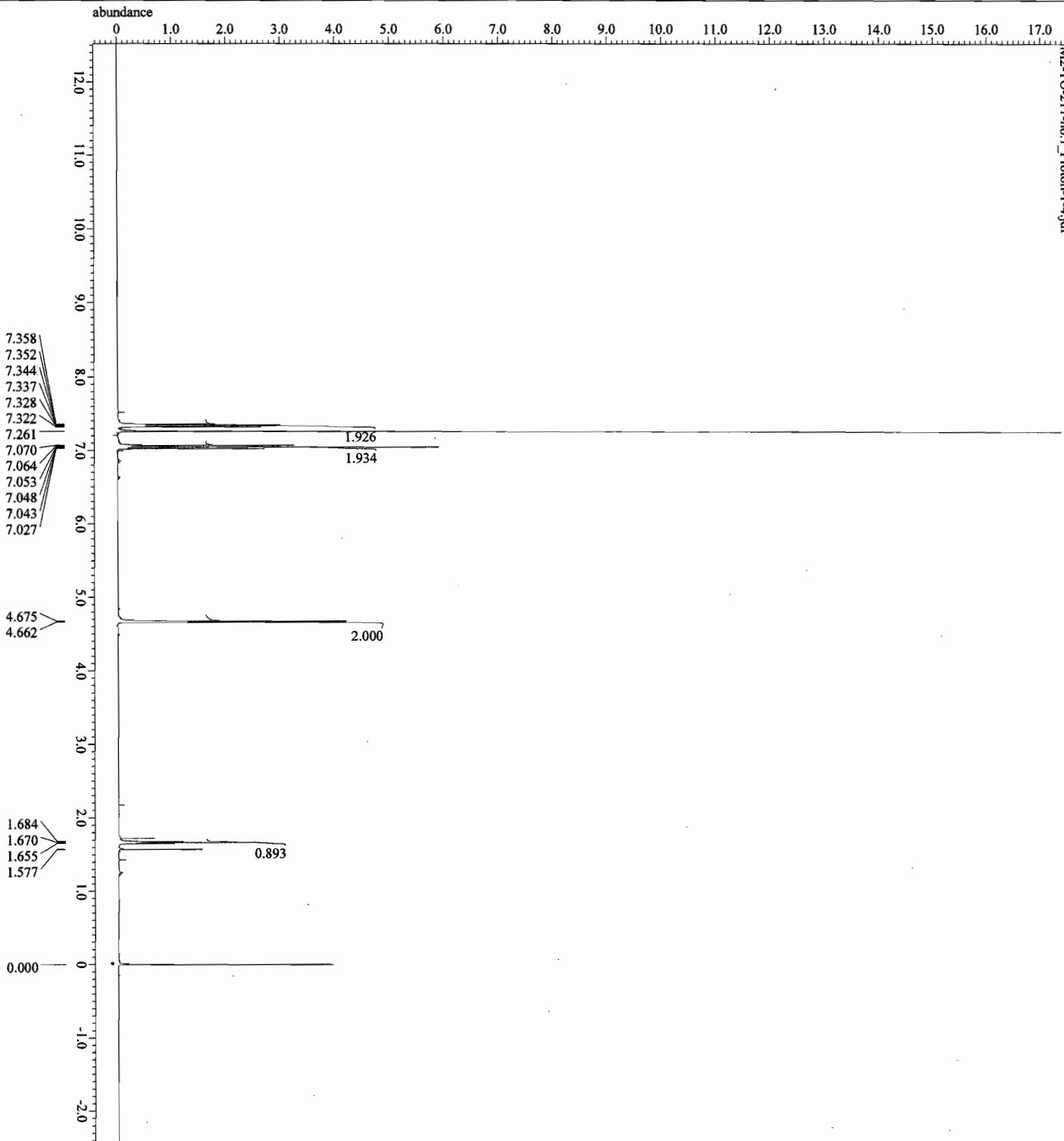
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File name = \Users\delta\Documents\J00
Author = delta
Experiment = carbon-32P
Sample_Id = M2-PO-207-no_2
Solvent = CHLOROFORM-D
Creation_Time = 18-JAN-2013 10:34:41
Revision_Time = 18-JAN-2013 10:34:51
Current_Time = 18-JAN-2013 10:35:45
Comment = single pulse decoupled gat
Data Format = 1D_COSY
Dim_1Size = 6224
Dim_2Size = 6224
Dim_3Size = 6224
Dimensions = 3
Slice = 304-4054.000
Spectrometer = DRX202_NMR
Field Strength = 9.42499481 [T]
X_Domain = 1.03809202 [s]
X_Freq = 13C
X_Offset = 100.90247963 [MHz]
X_Pow = 1.00 [ppm]
X_Bolts = 32768
X_Procvara = 4
X_Resolution = 0.96330739 [Hz]
X_Sweep = 25.25253525 [Hz]
X_Sweep_C1_Offset = 401.28219815 [MHz]
IR_Freq = 401.28219815 [MHz]
IR_Offset = 5 [ppm]
ClipPsd = FALSE
Scans = 70
Total_Scans = 70

Relaxation_Delay = 2 [s]
Recv_Gain = 50
Temp_Gat = 19.6 [dC]
X_90_Width = 6.75 [us]
X_Hqg_Time = 1.03809024 [s]
X_Ample = 30 [deg]
X_Atn = 5.2 [dB]
X_Pulse = 2.91666667 [us]
X_Pulse_Atn_Dec = 22.691 [dB]
IR_Atn_Rose = 22.691 [dB]
IR_Noise = 5000
IR_Pwth = 0.115 [ms]
Decoupling = 1 [s]
Initial_Wait = 1000
New_Time = 2 [s]
Repetition_Time = 3.03809024 [s]

```

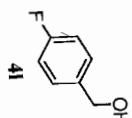


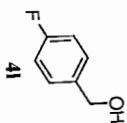
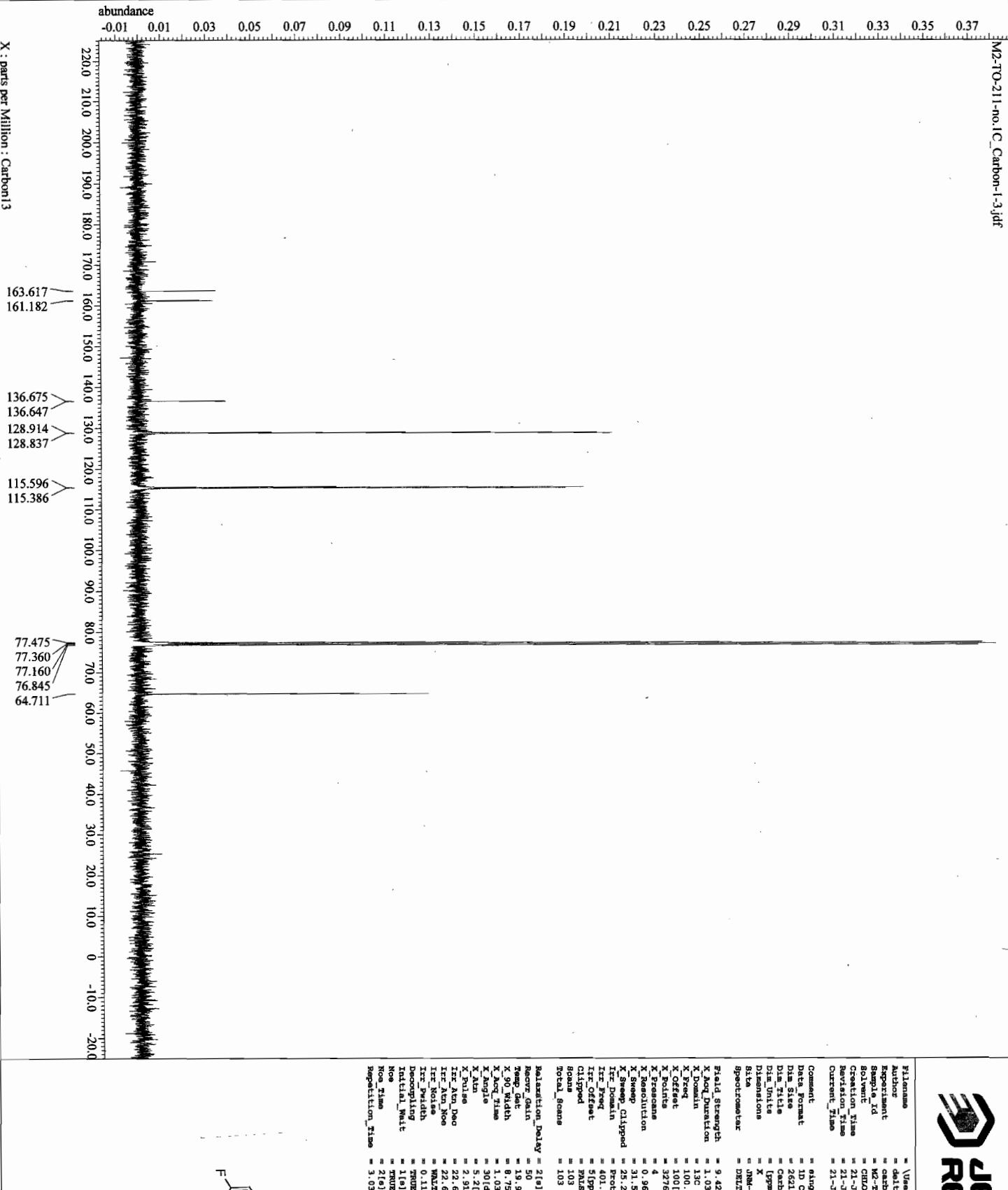


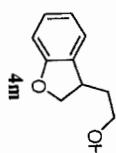
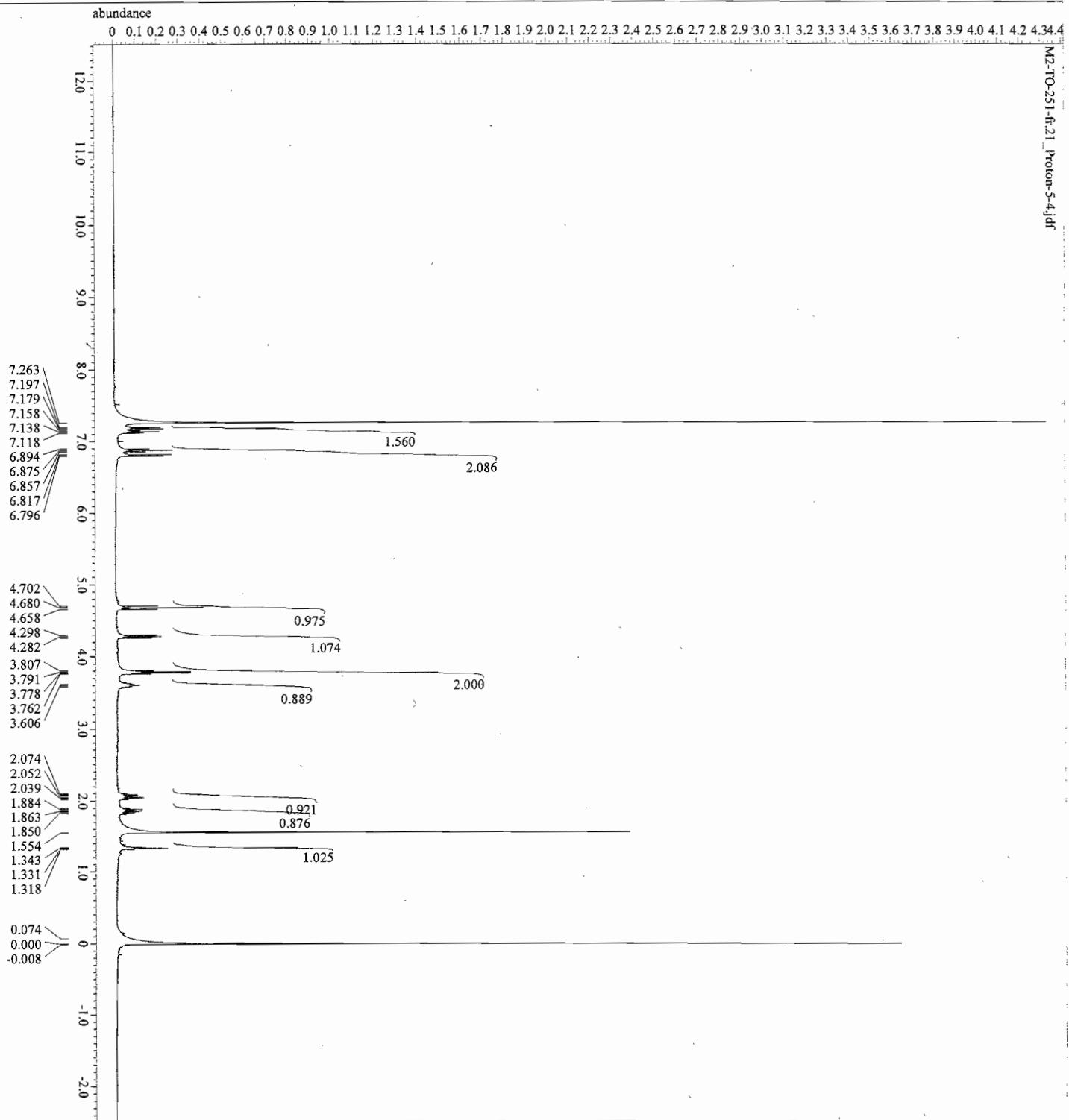
```

Filepath           = \Users\data\Documents\JEOL
Author            = dalia
Experiment        = proton-1D
Sample_ID         = M2-TO-211-no.1
Solvent           = CHLOROFORM-D
Creation_Time    = 21-DM-2013 10:50:19
Revision_Time    = 21-DM-2013 10:46:56
Current_Time     = 21-DM-2013 10:47:15
Comment          = single pulse
Data_Format      = 1D COMPLEX
Data_Size         = 13107
Data_Fitfile    = Proton
Data_Imtta       = [ppm]
Dimensions       = X
Size              = 304-65440
Spectrumator     = DELTA2_NMR
Spectrumator     = 9.4249961171 (400[MHz])
Field_Strength   = 2.17579521(s)
X_Hor_Buraction = 1M
X_Domain         = 401.28219356[MHz]
X_Freq            = 51[ppm]
X_Offset          = 16384
X_Points          = 1
X_Prescans        = 0.45960208[Hz]
X_Resolution      = 7.53012048[Hz]
X_Sweep            = 6.02409631[Hz]
X_Sweep_clipped  = Proton
IRX_Domain        = 401.28219356[MHz]
IRX_Freq           = 51[ppm]
IRX_Offset         = 401.28219356[MHz]
IRX_Points         = 1
IRX_Prescans      = 0.45960208[Hz]
IRX_Resolution    = 51[ppm]
TRI_Offset         = 51[ppm]
TRI_Pfreq          = 51[ppm]
TRI_Scans          = 8
Total_Scans        = 8
Relaxation_Delay = 51(s)
Relax_Gain         = 50
Temp_Got           = 19.91[°C]
Temp_Offset        = 0.25[°C]
X_Hock_Time       = 2.17579521(s)
X_Angle            = 45 [deg]
X_Atn              = 0.81[deg]
X_Pulse             = 4.655[us]
TRI_Mode           = OFF
Dante_Presat      = FALSE
Initial_Wait      = 1(s)
Repetition_Time   = 7.17579521(s)

```







File name = \Users\delta1\Documents\JED
 Author = delta
 Experiment = proton.jdp
 Sample Id = M2-TO-251-f.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 = JMR-EC2400
 Spectrometer = DEUTRON_NMR
 Field Strength = 9.424996611["] (400 [MHz])
 X-MSD-Direction = 1H
 X-Domain = 401.28219856 [MHz]
 X-Freq = 51ppm
 X-Offset = 1684
 X-Points = 1
 X-Progress = 1
 X-Resolution = 7.53012081 [Hz]
 X-Sweep = 6.02409529 [Hz]
 X-Step = 0.0001 [Hz]
 X-Width = 401.28219856 [MHz]
 X1-Offset = Proton
 X1-Domain = 401.28219856 [MHz]
 X1-Freq = 51 [ppm]
 X1-Offset = 51 [ppm]
 X1-Pulse = 10 [us]
 X1-Scans = 32
 Total Scans = 32
 Relaxation Delay = 5 [s]
 Receiver Gain = 56
 Temp (deg) = 20.3 [deg]
 X90 Width = 9.25 [us]
 X90 Time = 2.1757952 [s]
 X-Angle = 45 [deg]
 X-Arin = 0.8 [dB]
 X-Pulse = 4.625 [us]
 X1-Pulse = Off
 TR Mode = Off
 Dancr Preest = FALSE
 Initial Preest = 1 [s]
 Repetition time = 7.1757952 [s]

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```

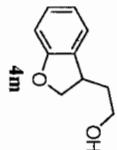
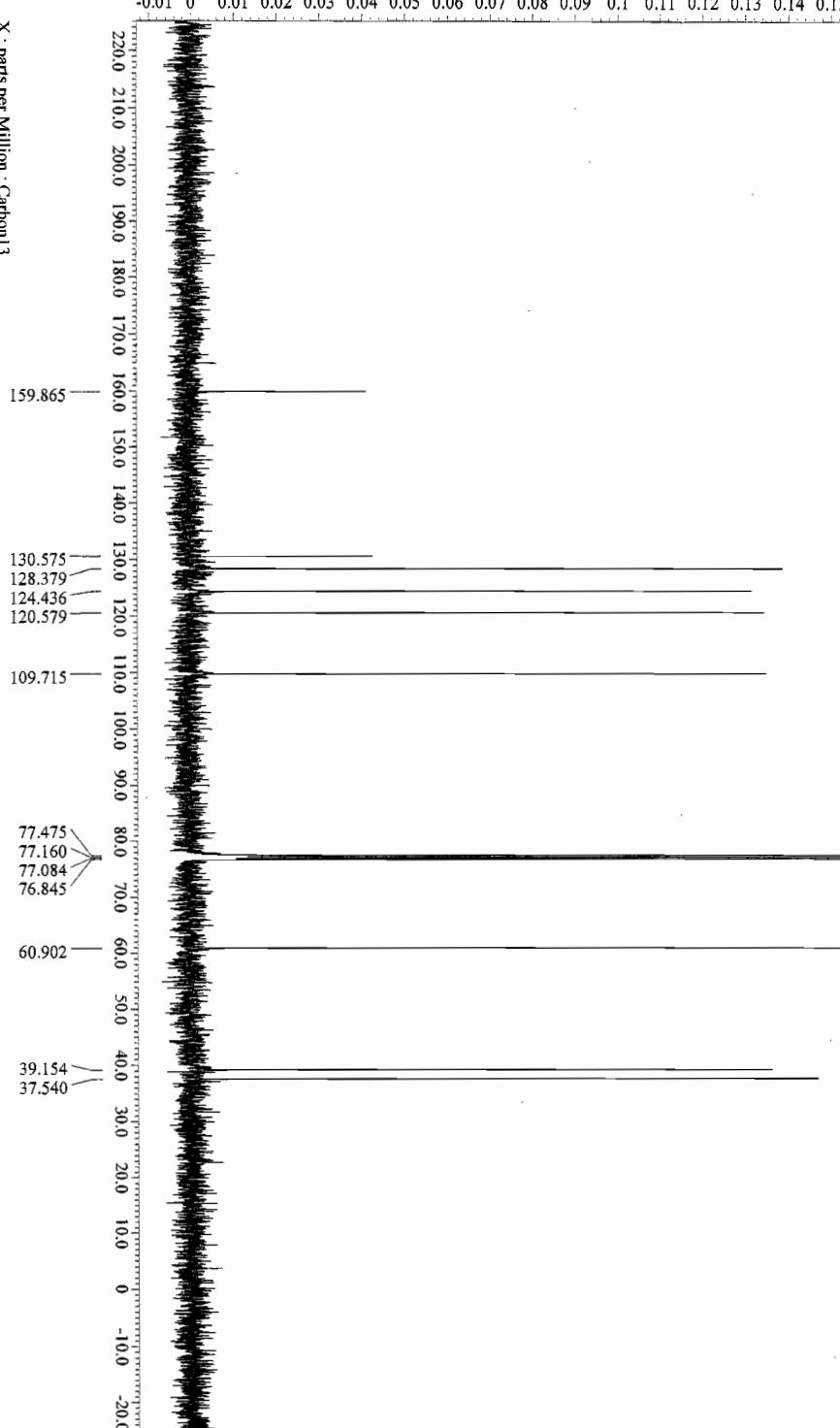
File Name          = 'U:\eara\data\Documents\JBO
Number           = data
Sample Id        = 00000000000000000000000000000000
Sweep Id         = X2-TO-21C-fr.21C
Sweep Type       = CH2-TO-FID
Creation Time    = 8-MAR-2013 19:41:08
Revision Time    = 8-MAR-2013 20:01:05
Current Time     = 8-MAR-2013 20:01:54

Comment          = simple pulse decoupled 90°
Data Format      = 1D COMPLEX
Data Size        = 26214
Data Title       = Carbon13
Data Units       = [ppm]
Dimensions       = X
Site             = JNM-WS400
Spectrometer     = DEUTZER_NMR

Field Strength   = 9.42499881 [T] (400 [MHz])
X_Acc_Duration  = 1.03809024 [s]
X_Domain        = 13C
X_Proc          = 100.9024763 [MHz]
X_Offset        = 100 [ppm]
X_Points         = 32768
X_Prescans      = 4
X_Resolution    = 0.96330739 [Hz]
X_Sweep          = 31.5656567 [Hz]
X_Sweep_Clipped = 25.2525525 [Hz]
Irr_Domain      = Proton
Irr_Freq         = 401.20229856 [MHz]
Irr_Offset       = 5 [ppm]
Clipped          = FALSE
Scans            = 128
Total Scans     = 128

Relaxation Delay = 21 [s]
Recover_Gain    = 50
Temp_Gain       = 20.2 [oC]
X_90_Width      = 8.75 [us]
X_Nch_Time      = 1.03809024 [s]
X_Angle          = 30 [deg]
X_Atn            = 5.21 [deg]
X_Pulse          = 2.93666657 [us]
Irr_Atn_Dec     = 22.691 [deg]
Irr_Atn_Noe     = 22.691 [deg]
Irr_Noise        = NOIZE
Irr_Pw1d         = 0.115 [ms]
Decoupling       = TROK
Initial_Wait    = 1.0
Noise            = TROK
Now_Time         = 2.01
Repetition_Time  = 3.03809024 [s]

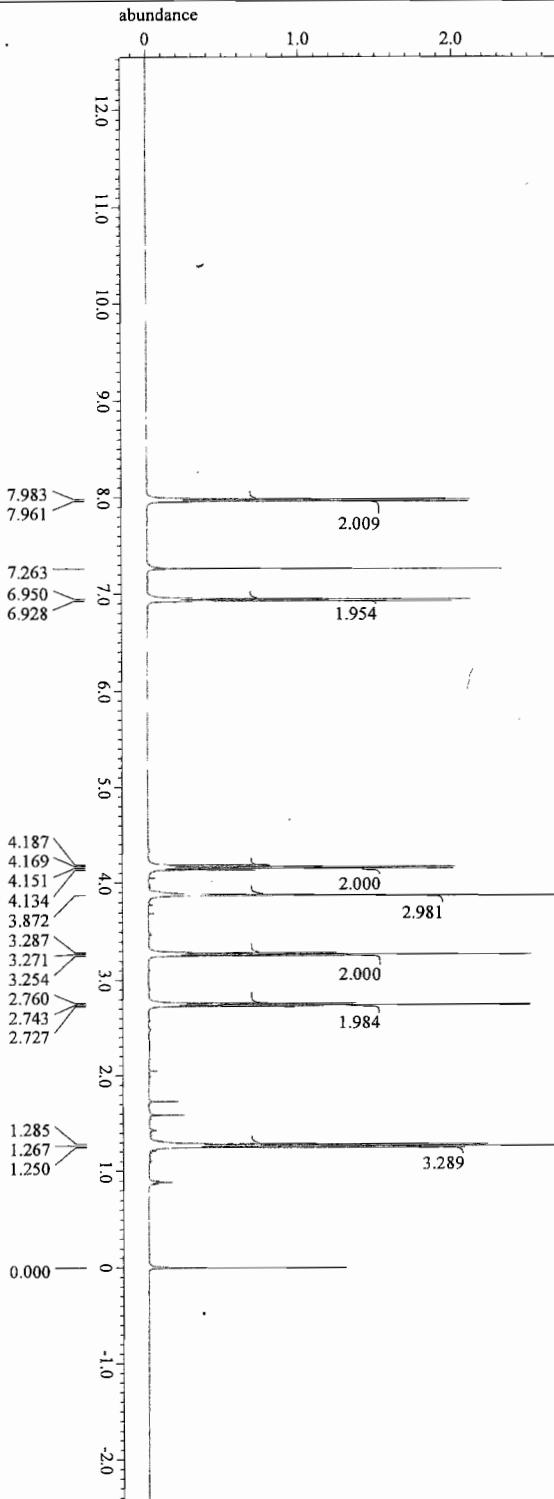
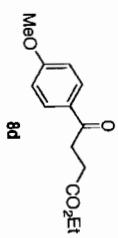
```

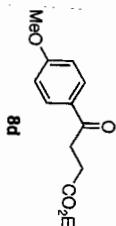
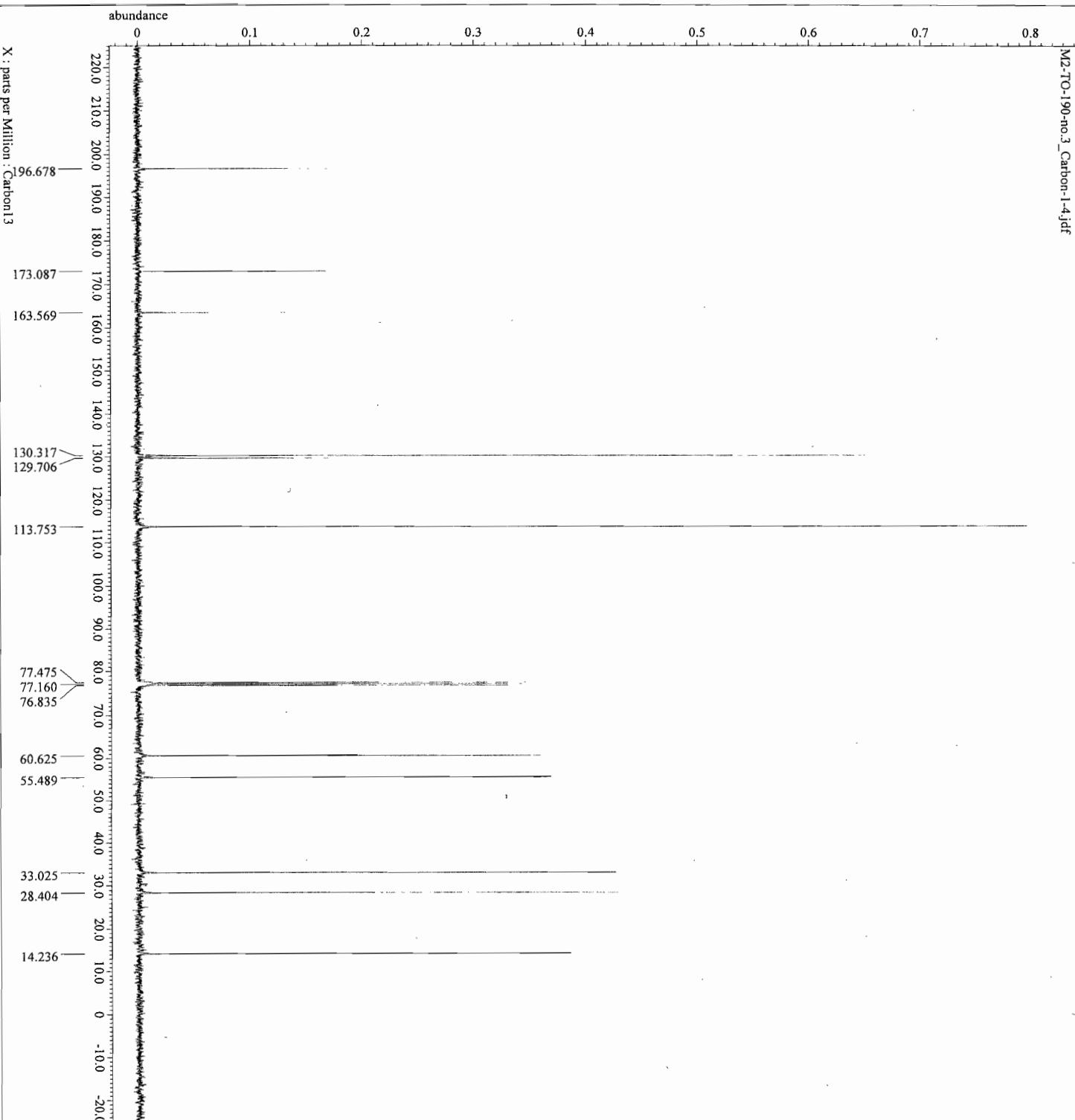


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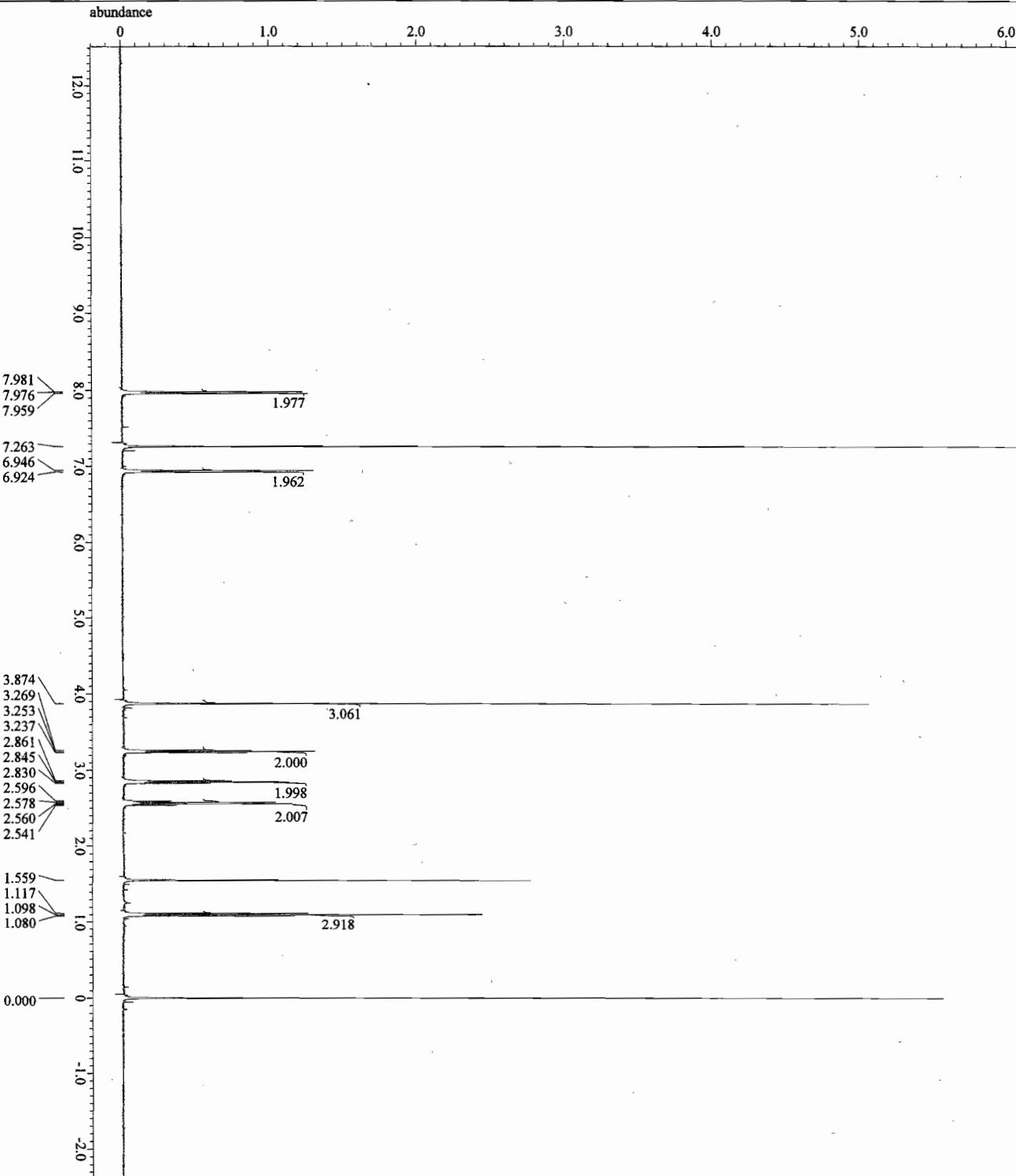
Filepath = \Users\deltaeta\Documents\JRD
Author = delta
Experiment = proton-19P
Sample_Id = M2-TO-190-no.3
Solvent = CHLOROPHEN-D
Revision_Time = 11-DEC-2012 18:00:27
Current_Time = 11-DEC-2012 18:40:33
Comment = single pulse
Data_Format = ID COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECX400
Spectrometer = DELTA2_NMR
Field_Strength = 9.4249968171 (400 [MHz])
X_Acc_Duration = 2.175992 [s]
X_Domain = H
X_Freq = 01.28229856 [MHz]
X_Offset = 5 [ppm]
X_Points = 16384
X_Precision = 1
X_Resolution = 0.45980208 [Hz]
X_Sweep = 7.53020481 [kHz]
X_Sweep_Cliped = 6.02409539 [kHz]
Irr_Domain = Proton
Irr_Freq = 01.28229856 [MHz]
Irr_Offset = 5 [ppm]
Irr_Domain = Proton
Irr_Freq = 01.28229856 [MHz]
Irr_Offset = 5 [ppm]
Irr_Offset = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5 [s]
Recover_Gain = 16
Tuning_Gate = 20.3 [Hz]
X_0_Offset = 9.35 [ppm]
X_Acc_Time = 2.175992 [s]
X_Amplitude = 4.5 [deg]
X_BW = 0.8 [Hz]
X_Pulse = 4.625 [us]
Irr_Slope = OFF
Irr_Sign = OFF
Doxic_Preset = PR18
Initial_Wait = 1 [s]
Repetition_Time = 7.175952 [s]

```





JEOL
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```

File name = \Users\deltaelta\Documents\J20
Author = delta
Experiment = proton-2-5
Sample_Id = M2-TO-236-2
Solvant = 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 = simple pulse
Data Format = 1D COMPLEX
Dim_1[1] = 13107
Dim_2[1] = Proton
Dim_3[1] = [ppm]
Dimensions = X
Site = 204-82940
Spectrometer = DMX202_NMR
Field Strength = 9.4249968177 (400 (MHz))
X_Hor_Duration = 2.1757952 [s]
X_Domain = 1K
X_Freq = 401.28219556 [MHz]
X_Offset = 51ppm
X_Polnts = 15364
X_Precision = 1
X_Protection = 0.489602091 [Hz]
X_Sweep = 7.550120468 [kHz]
X_Sweep_Clipped = 6.02409639 [kHz]
Xr_Domain = Proton
Irr_Freq = 401.28219556 [MHz]
Irr_Offset = 51ppm
Tri_Domain = Proton
Tri_Freq = 401.28219556 [MHz]
Tri_Offset = 51ppm
Clipped = 51ppm
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5 [s]
Reverb_Gain = 56
Reverb_Gain = 19.7 [deg]
Temp_Get = 9.22 [deg]
X_90_Width = 9.22 [deg]
X_Acc_Time = 2.1757952 [s]
X_Angle = 45 [deg]
X_Atn = 0.8 [deg]
X_Pulse = 4.625 [us]
Irr_Mode = off
Tri_Mode = off
Dante_Preset = FALSE
Initial_Wait = 1 [s]
Repetition_Time = 7.1757952 [s]

```

