

**STUDIES TOWARD THE TOTAL SYNTHESIS OF AMPHIDINOLIDE N:
STEREOCONTROLLED SYNTHESIS OF THE C13–C29 SEGMENT**

Makoto Sasaki*, Yuki Kawashima, and Haruhiko Fuwa

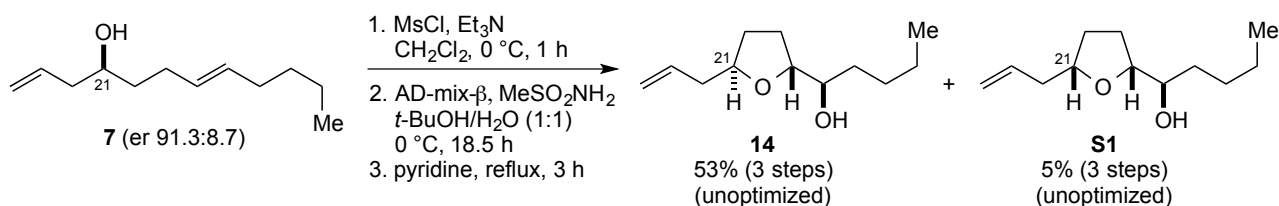
Graduate School of Life Sciences, Tohoku University, 2-1-1 Katahira, Aoba-ku
Sendai 980-8577, Japan

e-mail: masasaki@m.tohoku.ac.jp

Supporting Information for

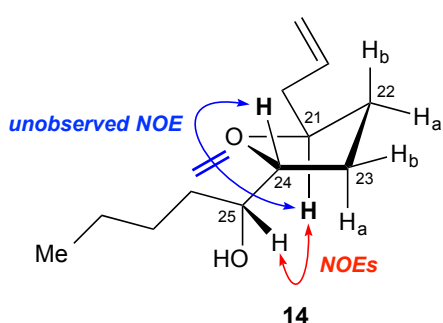
Proofs for the stereochemical assignment of compound 14	S2
Experimental procedure for triol 15	S3
¹ H and ¹³ C NMR spectra for all new compounds	S4–S53

Proofs for stereochemical assignment for compound **14**

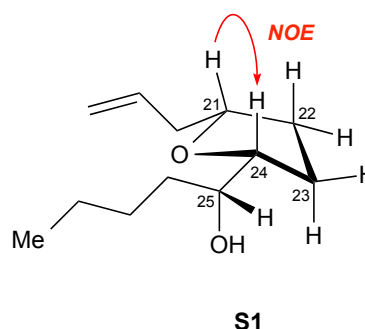


Homoallylic alcohol **7** with a low enantiomer ratio of 91.3:8.7, which was obtained in Keck asymmetric allylation, could be converted to a mixture of the desired **14** and its C21 diastereomer **S1** in a three-step sequence including mesylation, Sharpless asymmetric dihydroxylation using AD-mix-β, and base-treatment. Compound **S1** was readily separable by flash column chromatography on silica gel and subjected to NOE experiment.

Data for compound **S1**: $[\alpha]_D^{26} -3.3$ (*c* 0.70, CHCl₃); IR (film) 3444, 3076, 2932, 2857, 1642, 1260, 1083, 1042 cm⁻¹; ¹H NMR (600 MHz, CDCl₃) δ 5.82 (dddd, *J* = 17.0, 10.1, 6.9, 6.9 Hz, 1H), 5.06 (ddd, *J* = 17.0, 3.2, 1.4 Hz, 1H), 5.02 (ddd, *J* = 10.1, 3.2, 1.4 Hz, 1H), 3.56 (m, 1H), 3.36 (dddd, *J* = 10.6, 6.9, 6.9, 4.1 Hz, 1H), 3.29 (ddd, *J* = 6.9, 6.9, 6.9 Hz, 1H), 2.31 (dddd, *J* = 12.8, 6.9, 6.9, 1.4, 1.4 Hz, 1H), 2.15 (dddd, *J* = 12.8, 6.9, 6.9, 1.4, 1.4 Hz, 1H), 1.94 (dddd, *J* = 13.7, 3.2, 3.2, 3.2 Hz, 1H), 1.87 (m, 1H), 1.67–1.45 (m, 4H), 1.39–1.28 (m, 5H), 0.88 (t, *J* = 7.3 Hz, 3H), (one proton missing due to H/D exchange); ¹³C NMR (150 MHz, CDCl₃) δ 134.8, 116.6, 80.1, 77.7, 66.1, 40.6, 31.4, 30.8, 27.7, 25.4, 22.6, 13.9; HRMS (ESI) calcd for C₁₂H₂₂O₂Na [(M + Na)⁺] 221.1512, found 221.1522.

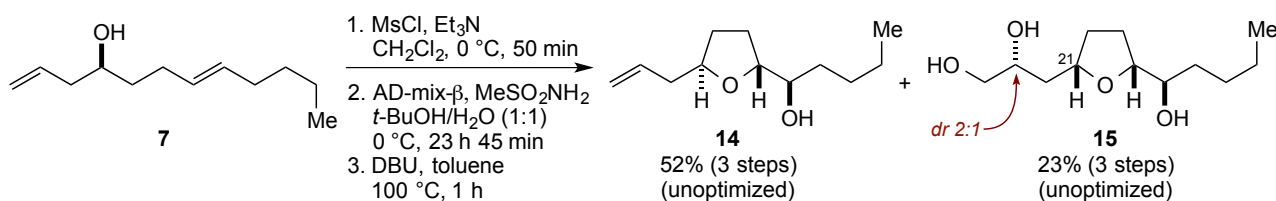


The absence of NOE between H-21 and H-24 and the observation of NOE between H-21 and H-25 suggests a 2,5-*trans* configuration.



The observation of NOE between H-21 and H-24 suggests 2,5-*cis* configuration.

Experimental procedure for triol **15**



To a solution of homoallylic alcohol **7** (189.7 mg, 1.041 mmol) in CH₂Cl₂ (10 mL) at 0 °C were added Et₃N (280 μL, 2.00 mmol) and MsCl (120 μL, 1.55 mmol), and the resultant solution was stirred at 0 °C for 50 min. The reaction mixture was diluted with EtOAc and washed successively with 1 M aqueous HCl solution, saturated aqueous NaHCO₃ solution, and brine. The organic layer was dried over Na₂SO₄, filtered, and concentrated under reduced pressure to give crude mesylate (255.1 mg), which was used in the next reaction without further purification.

To a solution of the above mesylate in *t*-BuOH/H₂O (1:1, v/v, 10 mL) at 0 °C were added MeSO₂NH₂ (95.5 mg, 1.00 mmol) and AD-mix-β (1.40 g), and the resultant mixture was vigorously stirred at 0 °C for 23 h 45 min. The reaction was quenched with solid Na₂SO₃. The resultant mixture was stirred at room temperature for 1 h and then extracted with EtOAc. The organic layer was washed with 3 M aqueous NaOH solution and brine, dried over Na₂SO₄, filtered, and concentrated under reduced pressure to give crude product (260.4 mg), which was used in the next reaction without further purification.

To a solution of the above material in toluene (10 mL) was added DBU (220 μL, 1.47 mmol), and the resultant solution was stirred at 100 °C for 1 h. The reaction mixture was cooled to room temperature and concentrated under reduced pressure. Purification of the residue by column chromatography (silica gel, 10% EtOAc/hexane then acetone) gave tetrahydrofuran **14** (106.8 mg, 52% for the three steps) as a colorless oil and triol **15** (54.8 mg, 23% for the three steps) as an approximately 2:1 mixture of diastereomers (estimated by 600 MHz ¹H NMR analysis) and white solids. Recrystallization of **15** twice from CHCl₃/hexanes afforded a crystal suitable for X-ray crystallographic analysis. Data for **15**: mp 119.5–120.6 °C; [α]_D²³ +4.2 (*c* 0.10, CHCl₃); ¹H NMR (600 MHz, CDCl₃) δ 4.02 (m, 1H), 3.92 (m, 1H), 3.89 (ddd, *J* = 8.3, 6.0, 6.0 Hz, 1H), 3.62 (dd, *J* = 11.4, 3.7 Hz, 1H), 3.48 (dd, *J* = 11.4, 5.5 Hz, 1H), 2.12 (m, 1H), 1.96 (m, 1H), 1.75–1.44 (m, 6H), 1.42–1.39 (m, 2H), 1.37–1.26 (m, 3H), 0.88 (t, *J* = 7.4 Hz, 3H), (three protons missing due to H/D exchange); ¹³C NMR (150 MHz, CDCl₃) δ 82.5, 79.3, 73.6, 71.7, 66.6, 38.5, 33.5, 33.1, 27.8 (2C), 22.7, 14.0; HRMS (ESI) calcd for C₁₂H₂₄O₄Na [(M + Na)⁺] 255.1567, found 255.1585.

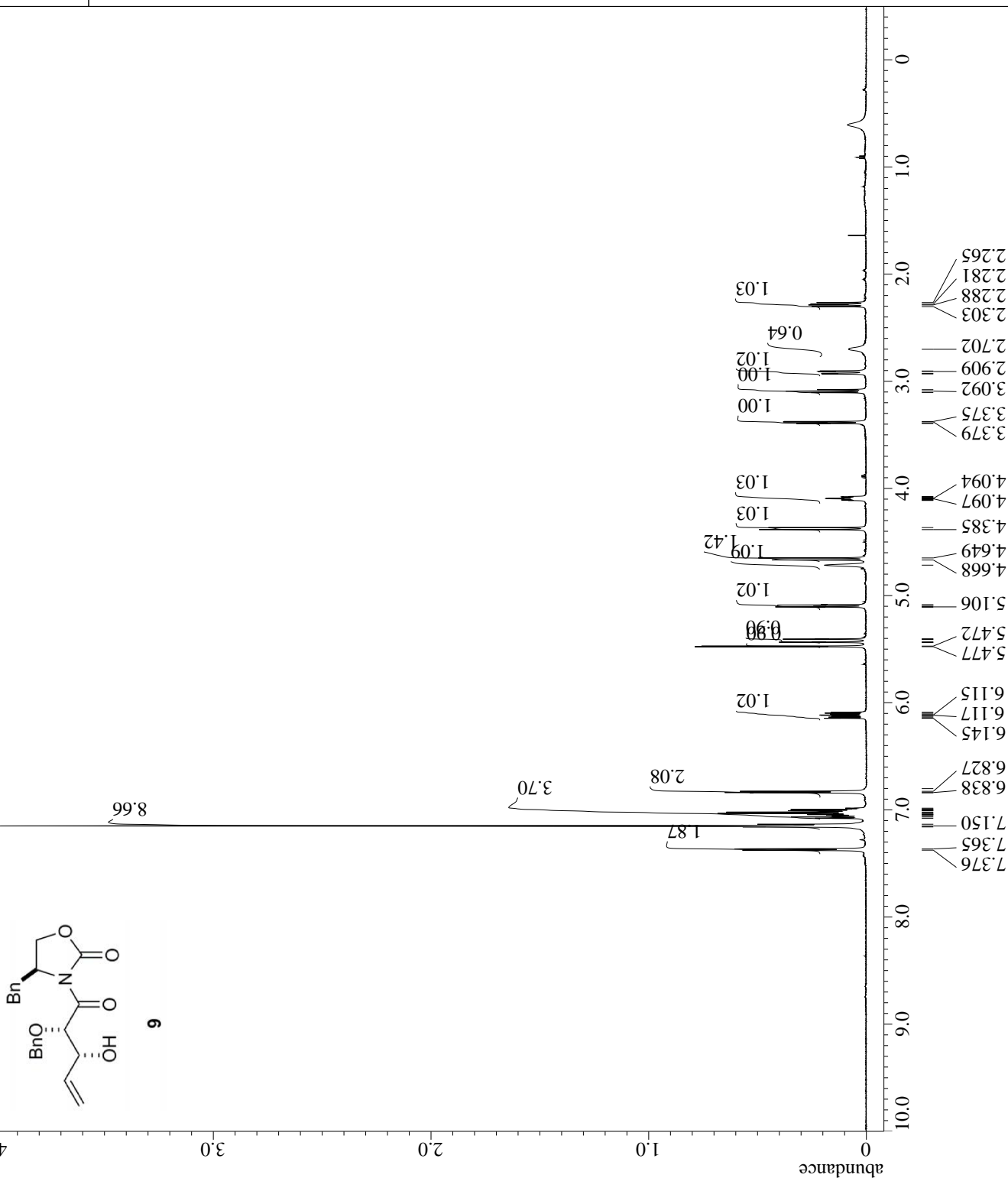
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = Proton.jxp
Sample_Id = YK-II-195
Solvent = BENZENE-D6
Creation_Time = 3-OCT-2013 10:12:38
Revision_Time = 24-JUN-2014 00:23:36
Current_Time = 24-JUN-2014 00:24:14

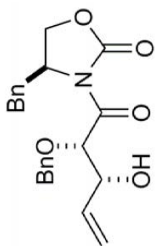
Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 40
Temp_Get = 21.4[degC]
X_90_Width = 14.3[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Pulse = 4[us]
Irr_Mode = 7.15[us]
Tri_Mode = OFF
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```



X : parts per Million : Proton



9

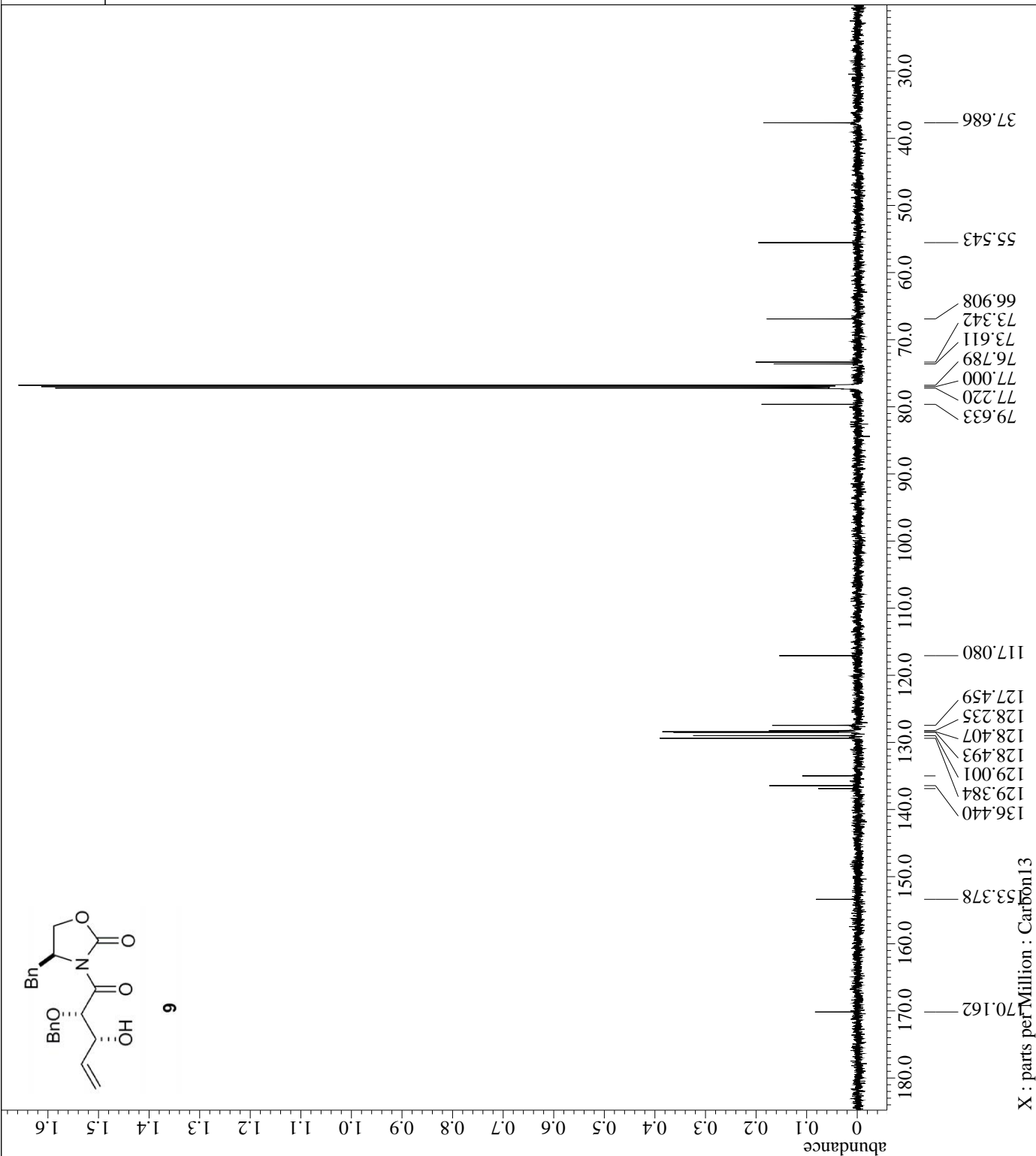
```

Filename = /Users/skk_macbookpro/Desktop
Author = delta
Experiment = carbon_jxp
Sample_Id = YK-II-195
Solvent = CHLOROFORM-D
Creation_Time = 3-OCT-2013 22:14:21
Revision_Time = 24-JUN-2014 00:27:16
Current_Time = 24-JUN-2014 00:30:37

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

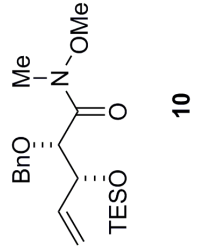
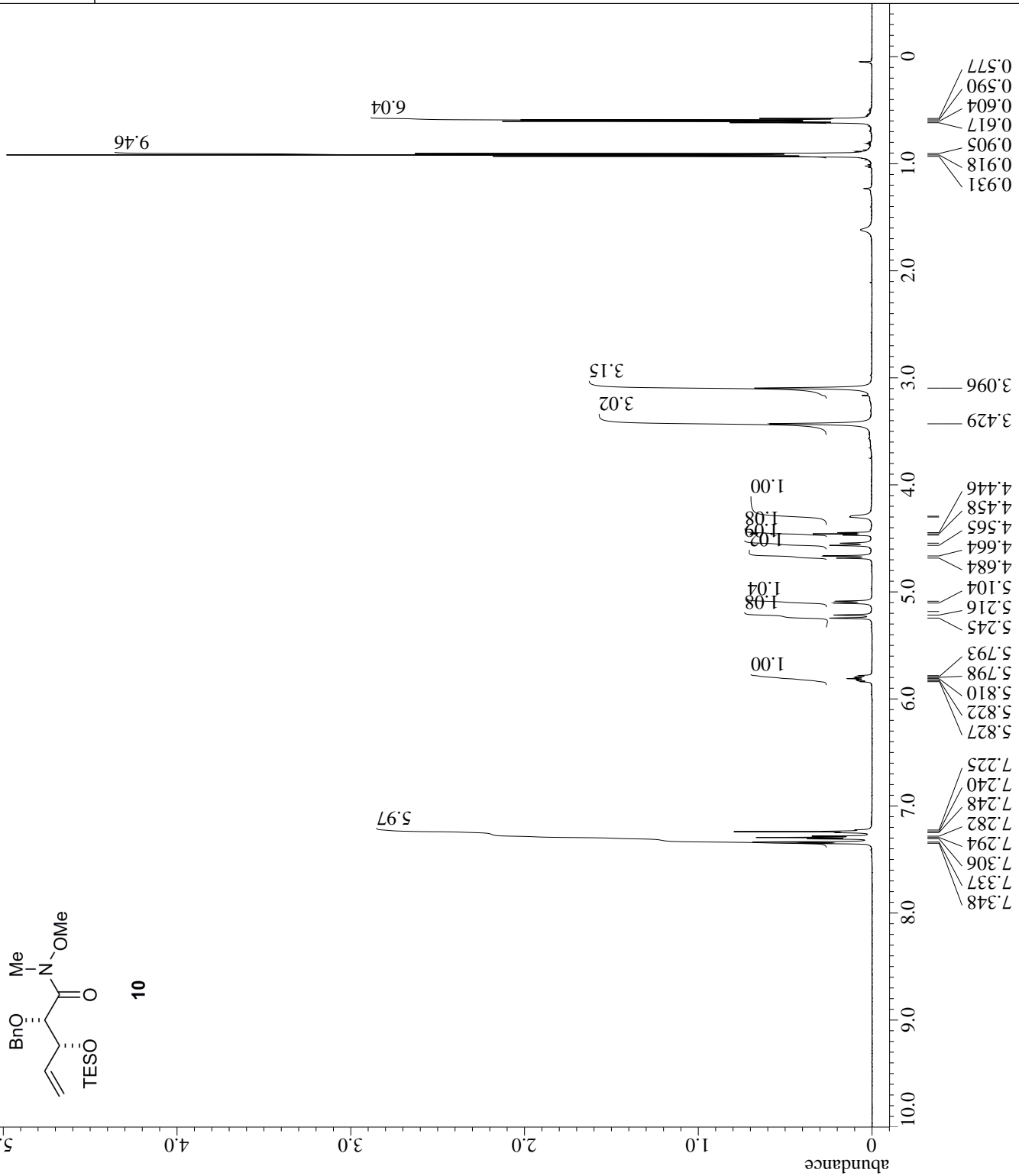
Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 0.69206016[s]
X Domain = 13C
X Freq = 150.91343039[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 1.44496109[Hz]
X Sweep = 47.34848485[kHz]
X Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 348
Total_Scans = 348

Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.6[dc]
X_90_Width = 10[us]
X Acq_Time = 0.69206016[s]
X Angle = 30[deg]
X Atn = 8[db]
X Pulse = 3.33333333[us]
Irr_Atn_Dec = 18.24[db]
Irr_Atn_Noise = 18.24[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```





Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = Proton.jxp
Sample_id = YK-III-018
Solvent = CHLOROFORM-D
Creation_Time = 18-OCT-2013 22:41:39
Revision_Time = 24-JUN-2014 00:38:35
Current_Time = 24-JUN-2014 00:39:03
Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 2.18103808[s]
X Domain = 1H
X Freq = 600.1723046[MHz]
X Offset = 5[ppm]
X Points = 32768
X Prescans = 1
X Resolution = 0.45849727[Hz]
X Sweep = 15.02403846[kHz]
X Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 2[s]
Recvr_Gain = 38
Temp_Get = 21.2[degC]
X 90_Width = 14.3[us]
X Acq_Time = 2.18103808[s]
X Angle = 45[deg]
X Actn = 4[dB]
X Pulse = 7.15[us]
Irr_Mode = OFF
Tri_Mode = OFF
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]



X : parts per Million : Proton

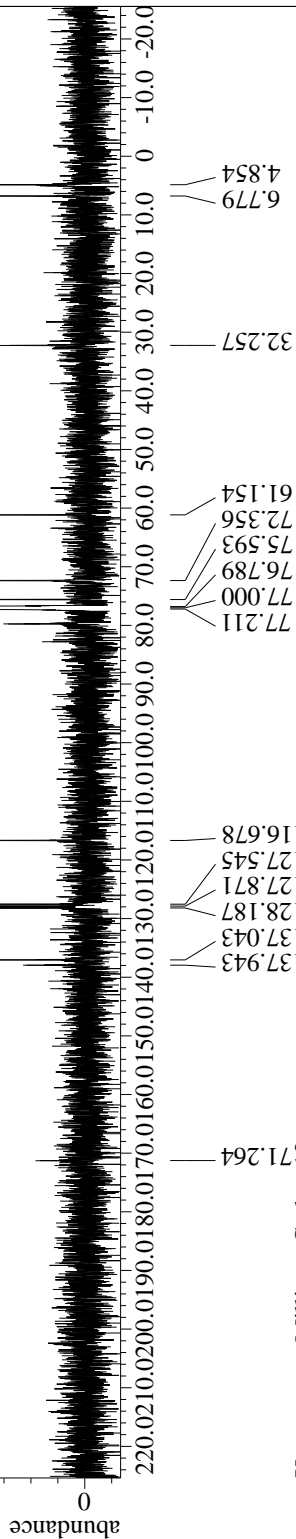
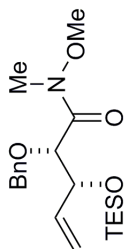
```

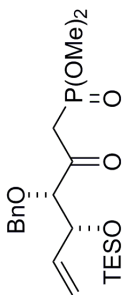
Filename = /Users/skk_macbookpro/Desktop
Author = delta
Experiment = carbon_jxp
Sample_Id = YK-III-018
Solvent = CHLOROFORM-D
Creation_Time = 18-OCT-2013 22:49:52
Revision_Time = 24-JUN-2014 00:47:00
Current_Time = 24-JUN-2014 00:47:54

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

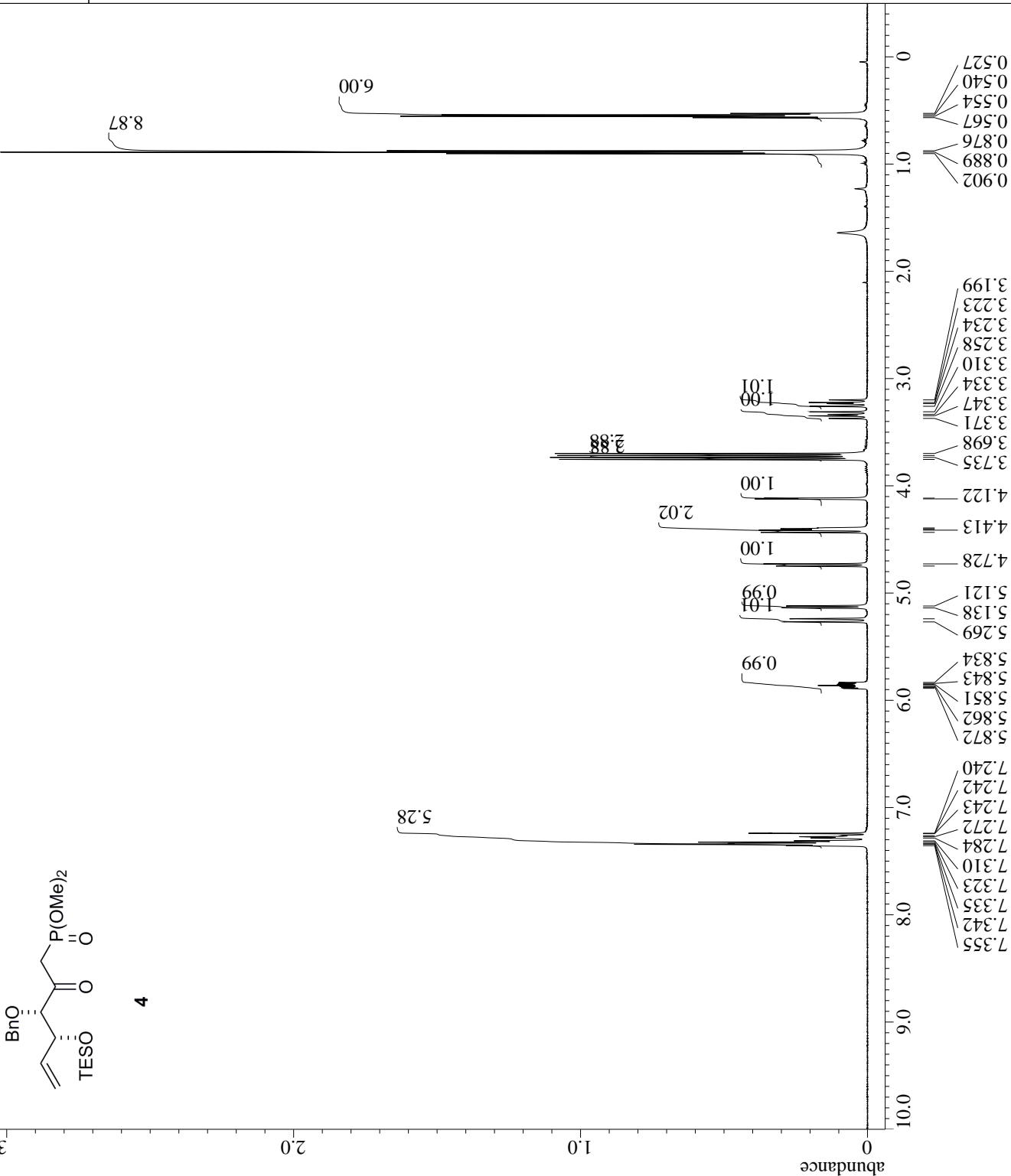
Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 0.69206016[s]
X Domain = 13C
X Freq = 150.91343039[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 1.44496109[Hz]
X Sweep = 47.34848485[kHz]
X Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 268
Total_Scans = 268

Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 22.4[dc]
X_90_Width = 10[us]
X Acq_Time = 0.69206016[s]
X Angle = 30[deg]
X Atn = 8[db]
X Pulse = 3.33333333[us]
Irr_Atn_Dec = 18.24[db]
Irr_Atn_Noise = 18.24[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```





4



X : parts per Million : Proton



```

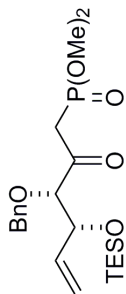
Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = proton_jxp
Sample_Id = YK-III-019
Solvent = CHLOROFORM-D
Creation_Time = 19-OCT-2013 13:57:34
Revision_Time = 23-JUN-2014 23:03:04
Current_Time = 23-JUN-2014 23:36:44

Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

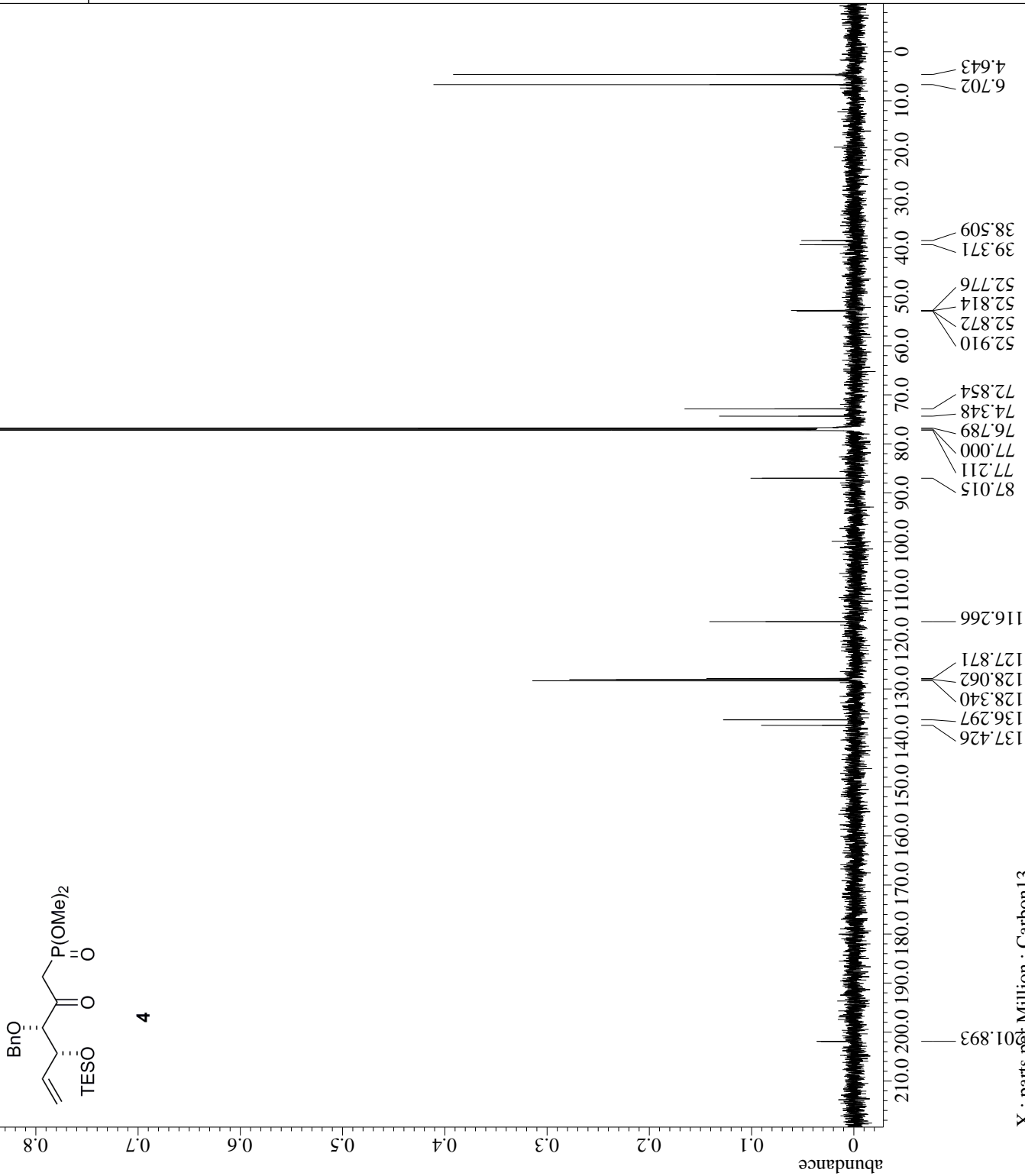
Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Phase = 32768
X_Points = 1
X_Prescans = 0.45849727[Hz]
X_Resolution = 15.02403846[kHz]
X_Sweep = 12.01923077[kHz]
X_Sweep_Clippped = Proton
Irr_Domain = 600.1723046[MHz]
Irr_Freq = 5[ppm]
Irr_Offset = Proton
Tri_Domain = 600.1723046[MHz]
Tri_Freq = 5[ppm]
Tri_Offset = FALSE
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 38
Temp_Get = 21.1[degC]
X_90_Width = 14.3[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Pulse = 7.15[us]
Irr_Mode = OFF
Tri_Mode = OFF
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]

```



4



X : parts per Million : Carbon13



```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon.jxp
Sample_Id = YK-III-019
Solvent = CHLOROFORM-D
Creation_Time = 19-OCT-2013 14:00:17
Revision_Time = 23-JUN-2014 23:37:46
Current_Time = 23-JUN-2014 23:38:42

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = 13C
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 224
Total_Scans = 224

Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 22.3[dc]
X_90_Width = 10[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 8[db]
X_Pulse = 3.33333333[us]
Irr_Atn_Dec = 18.24[db]
Irr_Atn_Noise = 18.24[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]

```

```

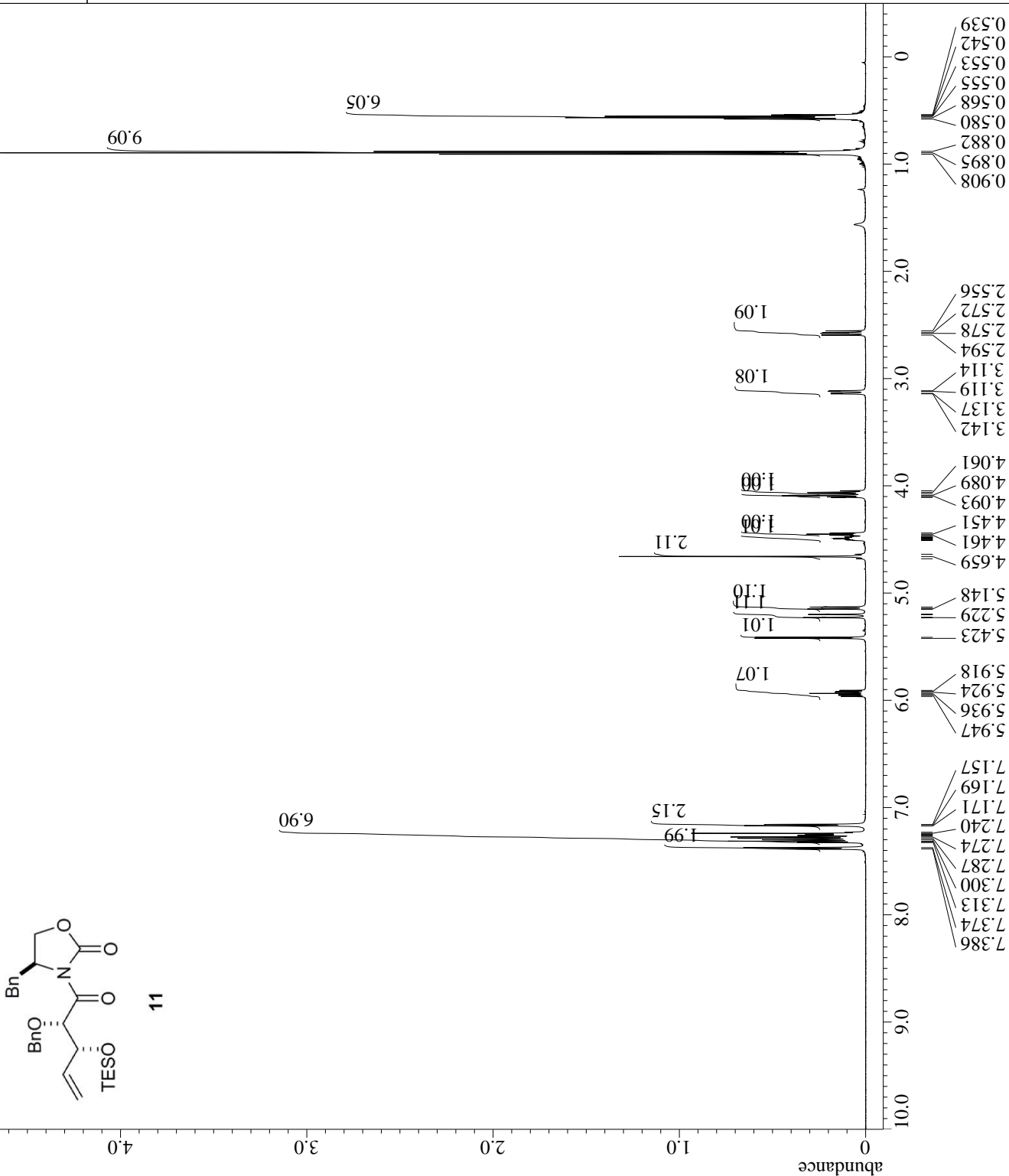
Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = Proton.jpg
Sample_Id = YK-II-197
Solvent = CHLOROFORM-D
Creation_Time = 4-OCT-2013 22:35:41
Revision_Time = 24-JUN-2014 01:16:49
Current_Time = 24-JUN-2014 01:17:21

Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Phases = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 36
Temp_Get = 21.3[degC]
X_90_Width = 14.3[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Pulse = 4[dB]
X_Pulse_Prog = 7.15[us]
Irr_Mode = OFF
Tri_Mode = OFF
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]

```



X : parts per Million : Proton

```

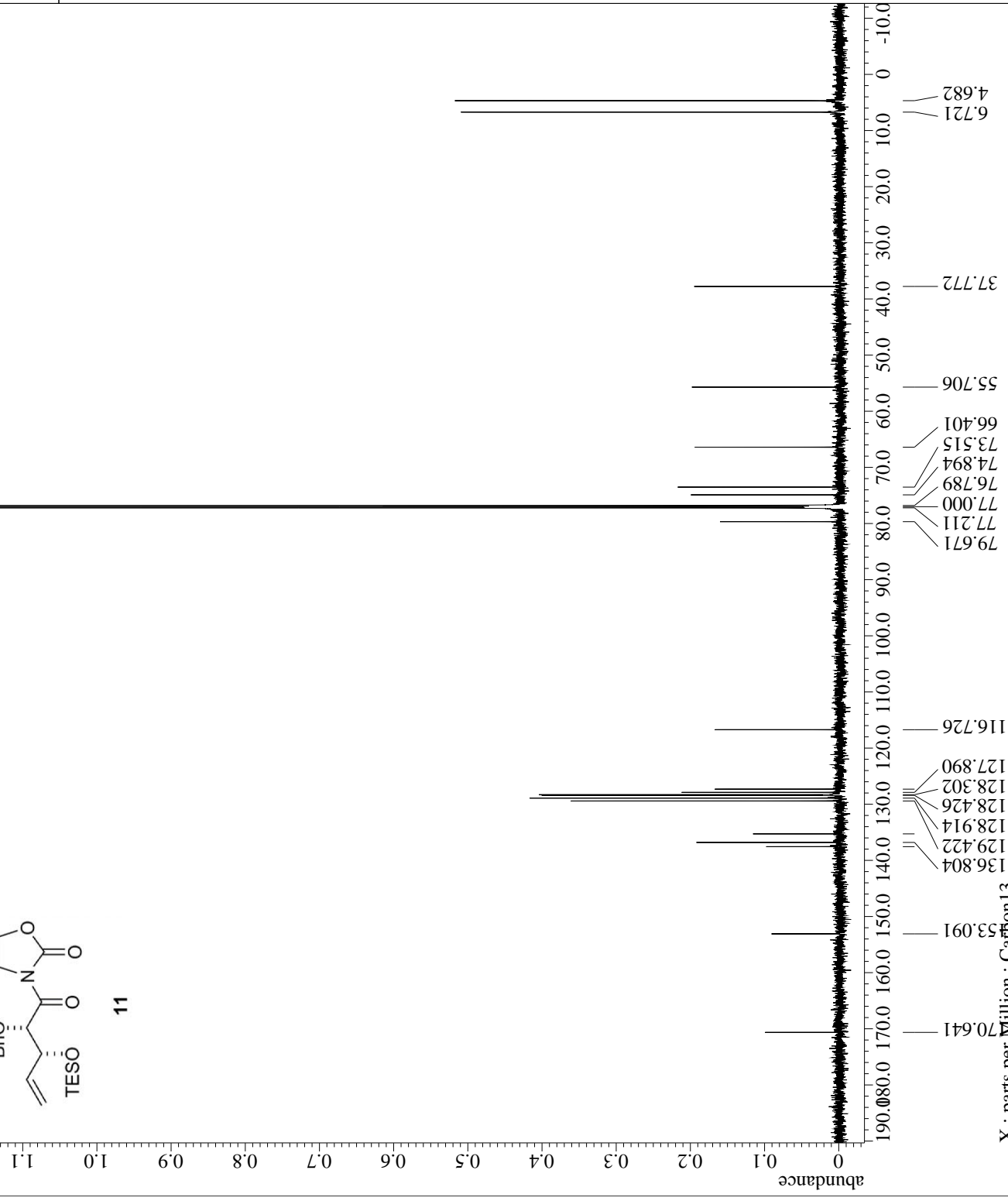
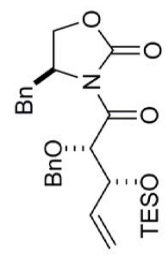
Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon.jxp
Sample_Id = YK-II-197
Solvent = CHLOROFORM-D
Creation_Time = 4-OCT-2013 22:38:43
Revision_Time = 24-JUN-2014 01:18:02
Current_Time = 24-JUN-2014 01:18:42

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 0.69206016[s]
X Domain = 13C
X Freq = 150.91343039[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 1.44496109[Hz]
X Sweep = 47.34848485[kHz]
X Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 580
Total_Scans = 580

Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.7[dc]
X_90_Width = 10[us]
X Acq_Time = 0.69206016[s]
X Angle = 30[deg]
X Atn = 8[db]
X Pulse = 3.33333333[us]
Irr_Atn_Dec = 18.24[db]
Irr_Atn_Noise = 18.24[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]

```



```

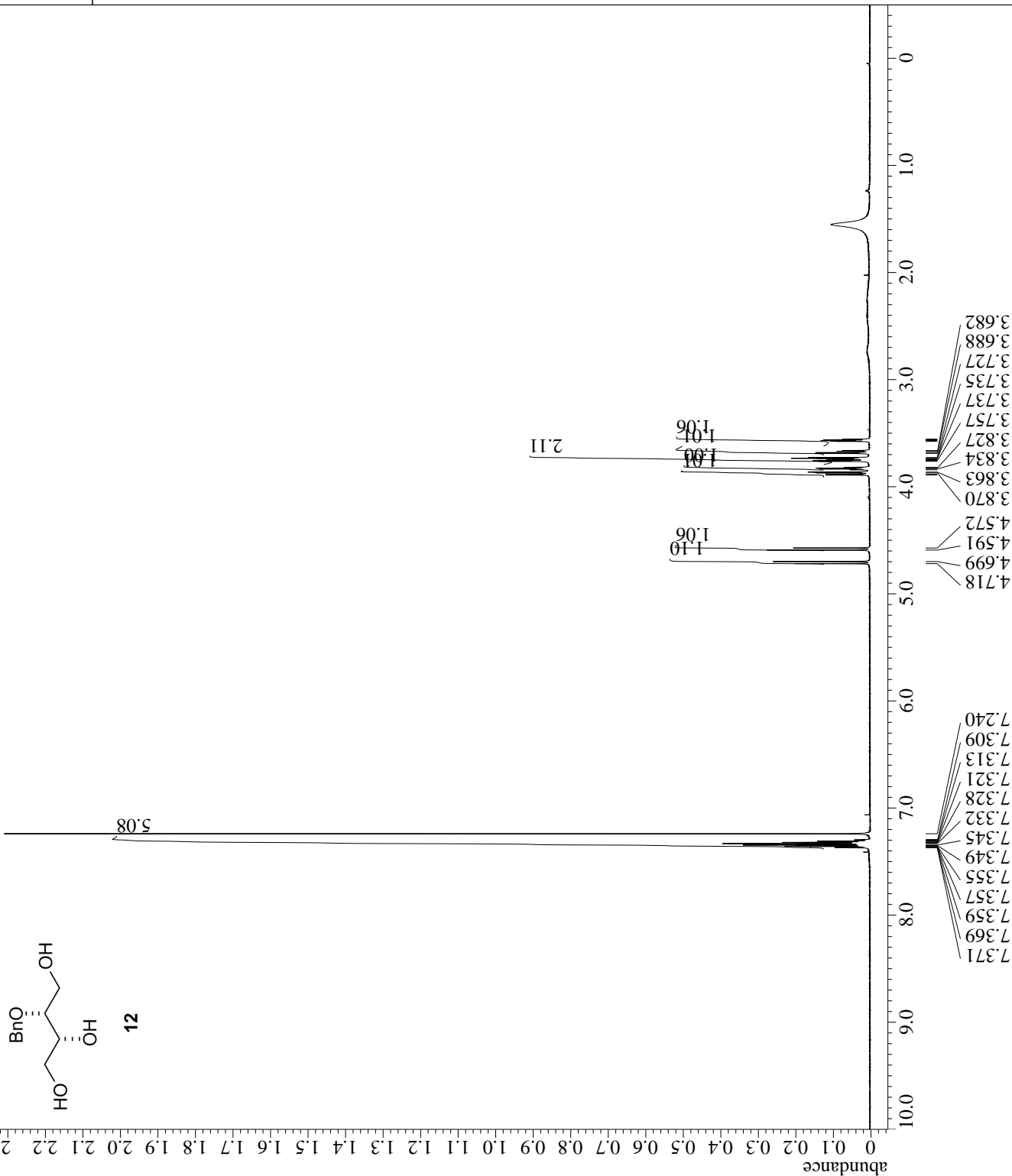
Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = Proton.jxp
Sample_Id = YK-II-174b
Solvent = CHLOROFORM-D
Creation_Time = 6-SEP-2013 12:11:35
Revision_Time = 24-JUN-2014 14:12:28
Current_Time = 24-JUN-2014 14:13:10

Comment = single pulse
Data_Format = 1D_COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32

Relaxation_Delay = 2[s]
Recvr_Gain = 44
Temp_Get = 22.1[degC]
X_90_Width = 14.3[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Acn = 4[deg]
X_Pulse = 7.15[us]
Irr_Mode = OFF
Tri_Mode = OFF
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]

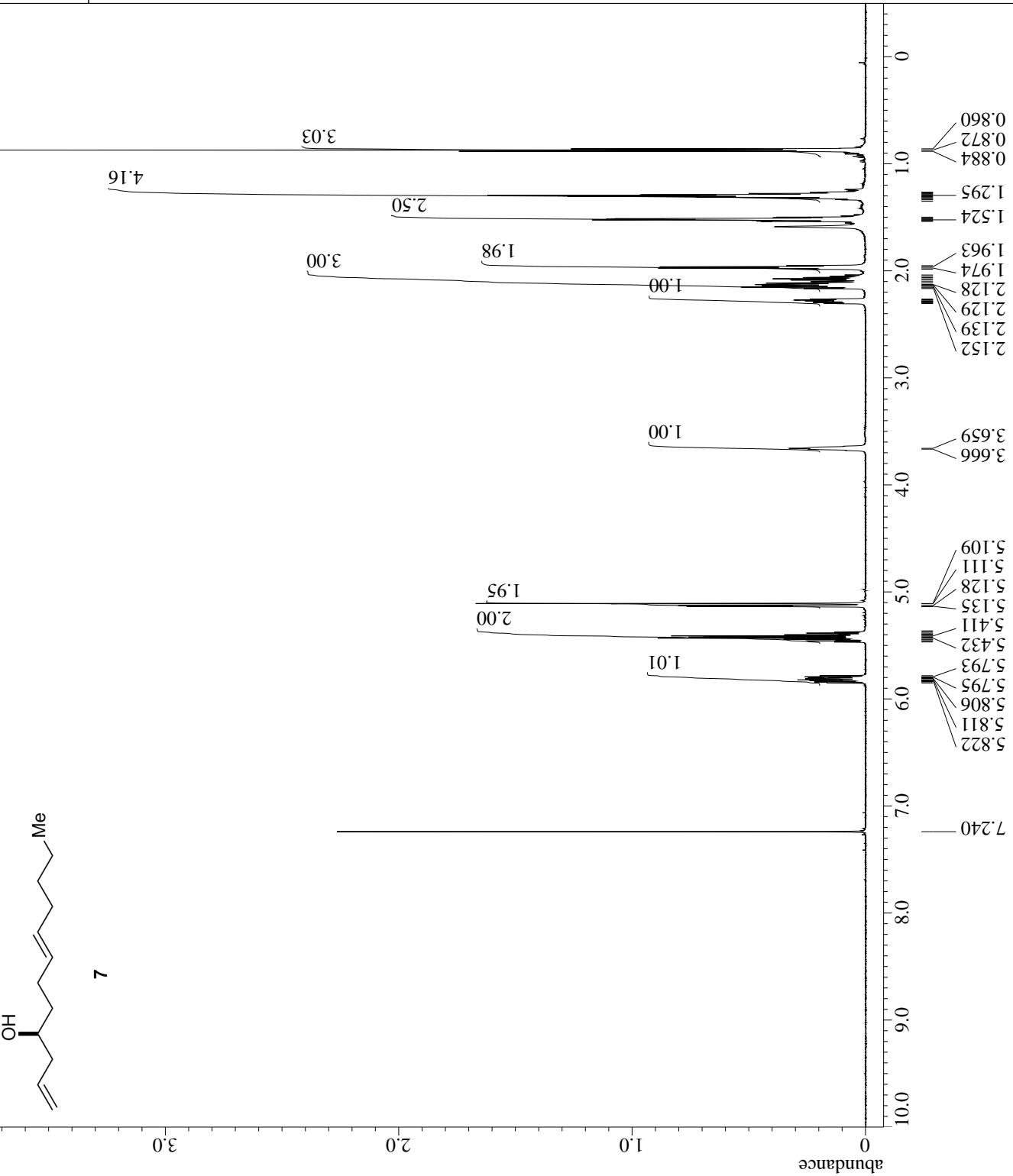
```



X : parts per Million : Proton



7



X : parts per Million : Proton



```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = Proton.jxp
Sample_Id = YK-II-70b
Solvent = CHLOROFORM-D
Creation_Time = 24-MAY-2013 15:42:44
Revision_Time = 23-JUN-2014 23:58:49
Current_Time = 23-JUN-2014 23:59:03

Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Phases = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clip = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 42
Temp_Get = 21.3[degC]
X_90_Width = 11.6[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Pulse = 3[db]
Irr_Mode = 5.8[us]
Irr_Mode = OFF
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```

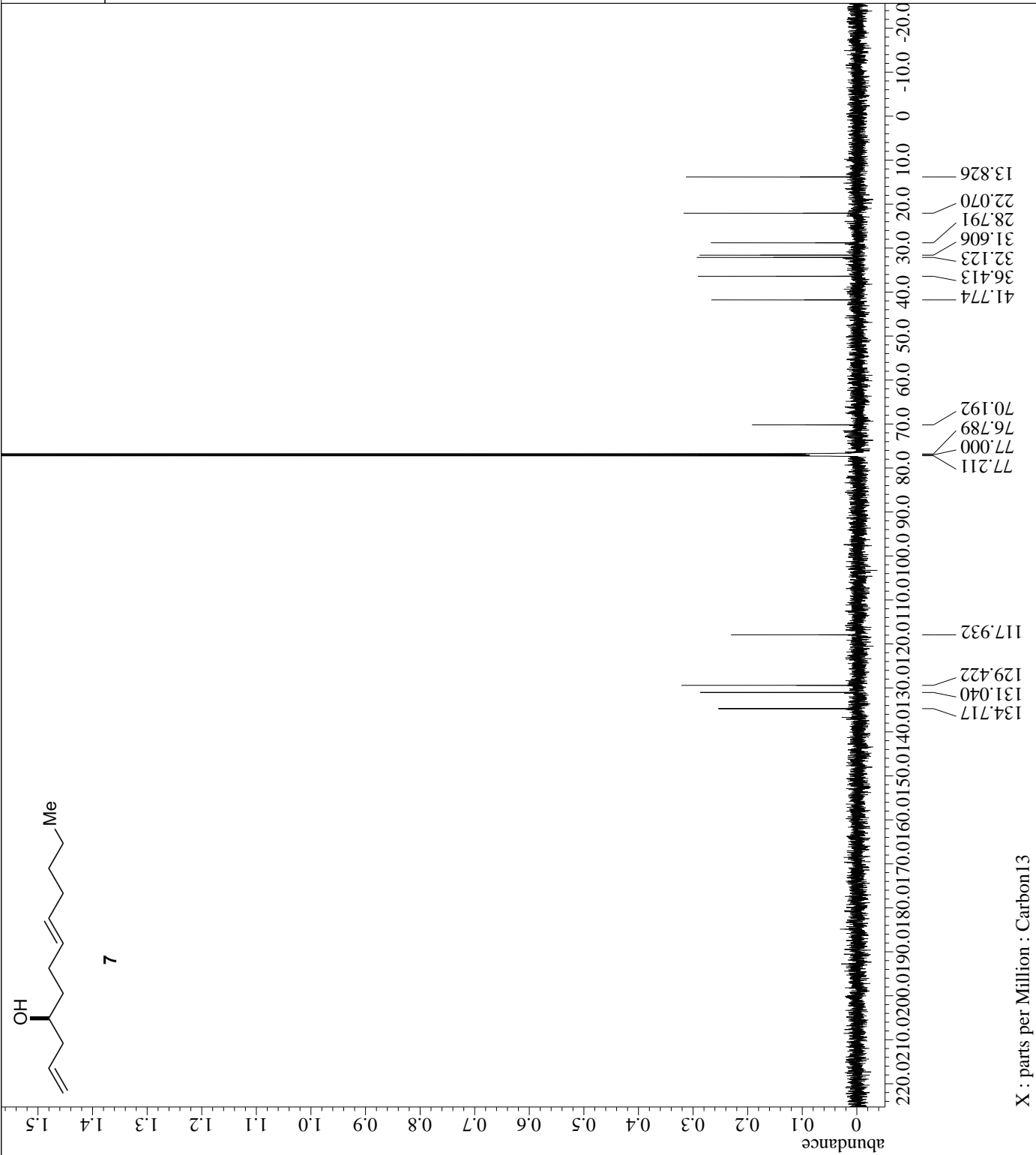
```

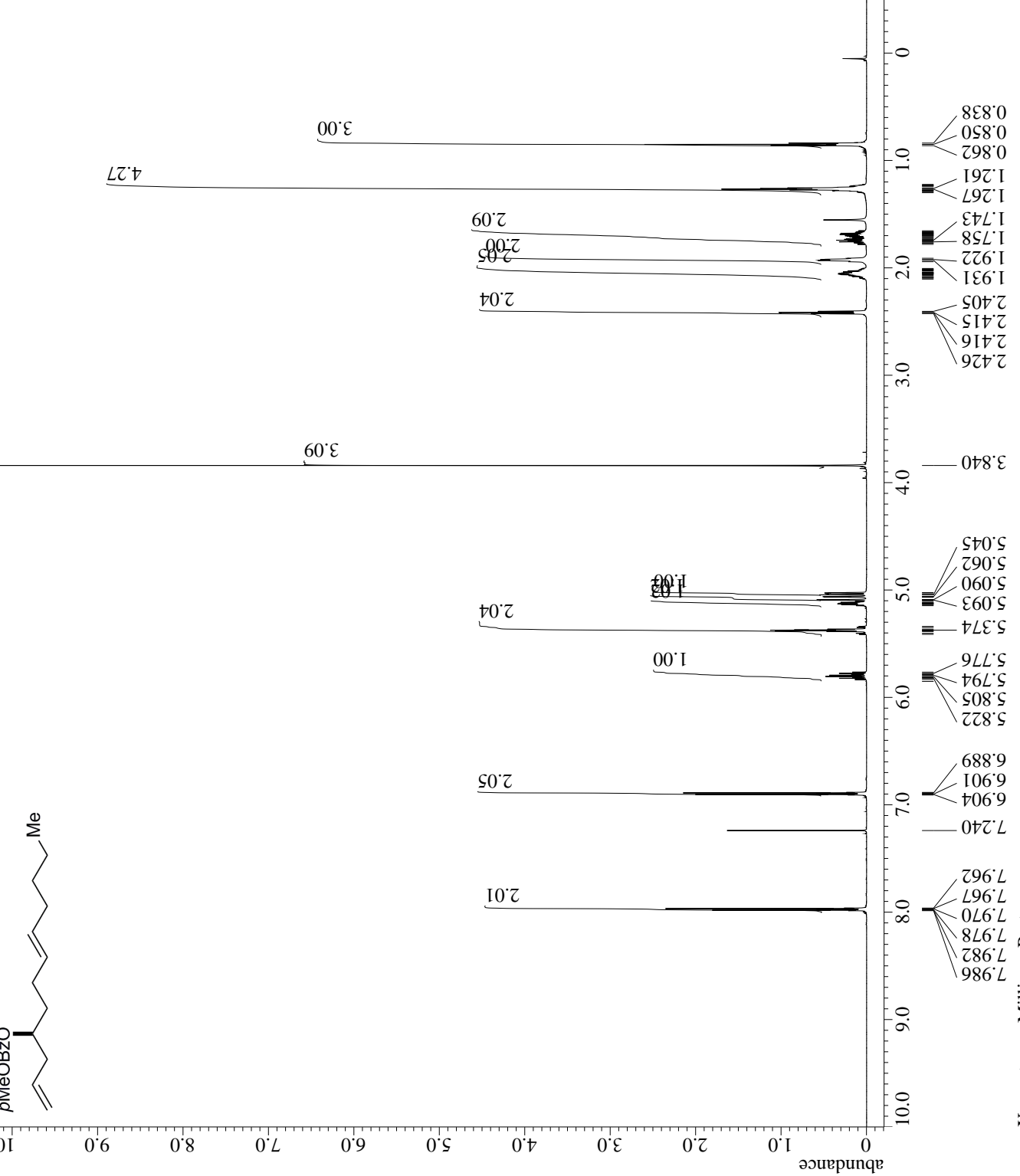
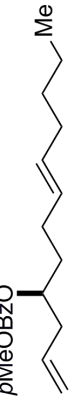
Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon.jxp
Sample_Id = YK-II-70b
Solvent = CHLOROFORM-D
Creation_Time = 24-JUN-2014 09:02:40
Revision_Time = 24-JUN-2014 14:05:33
Current_Time = 24-JUN-2014 14:06:35

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 0.69206016[s]
X Domain = 13C
X Freq = 150.91343039[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 1.44496109[Hz]
X Sweep = 47.34848485[kHz]
X Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 128
Total_Scans = 128

Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.3[dc]
X_90_Width = 10.5[us]
X Acq_Time = 0.69206016[s]
X Angle = 30[deg]
X Atn = 7.4[db]
X Pulse = 3.5[us]
Irr_Atn_Dec = 24.452[db]
Irr_Atn_Noise = 24.452[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```





X : parts per Million : Proton



```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = Proton.jmp
Sample_Id = YK-II-74
Solvent = CHLOROFORM-D
Creation_Time = 25-MAY-2013 15:23:31
Revision_Time = 24-JUN-2014 00:08:32
Current_Time = 24-JUN-2014 00:08:46

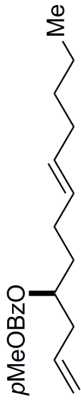
Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 38
Temp_Get = 21.2[degC]
X_90_Width = 11.6[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Pulse = 3[dB]
X_Acn = 5.8[us]
Irr_Mode = OFF
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```



Filename = /Users/skk_macbookpro/Desktop
Author = delta
Experiment = carbon.jxp
Sample_Id = YK-II-74
Solvent = CHLOROFORM-D
Creation_Time = 24-JUN-2014 12:17:25
Revision_Time = 24-JUN-2014 14:07:38
Current_Time = 24-JUN-2014 14:08:11
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 0.69206016[s]
X Domain = 13C
X Freq = 150.91343039[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 1.44496109[Hz]
X Sweep = 47.34848485[kHz]
X Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.5[dc]
X_90_Width = 10.5[us]
X Acq_Time = 0.69206016[s]
X Angle = 30[deg]
X Atn = 7.4[db]
X Pulse = 3.5[us]
Irr_Atn_Dec = 24.452[db]
Irr_Atn_Noise = 24.452[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]



0.7

0.6

0.5

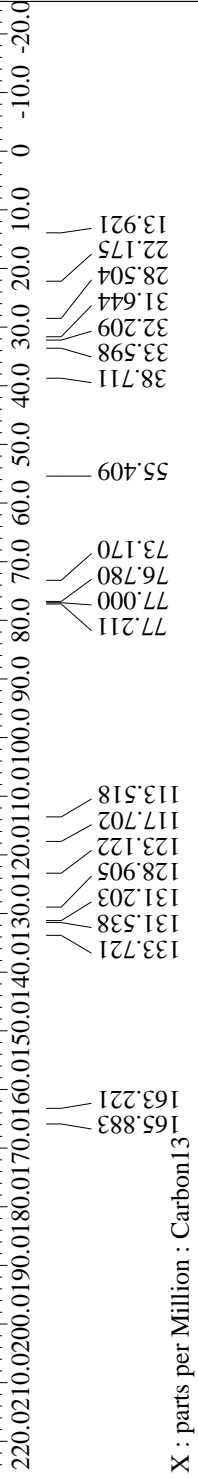
0.4

0.3

0.2

0.1

abundance



X : parts per Million : Carbon13

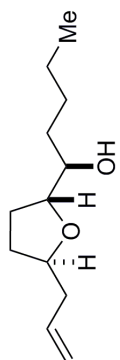
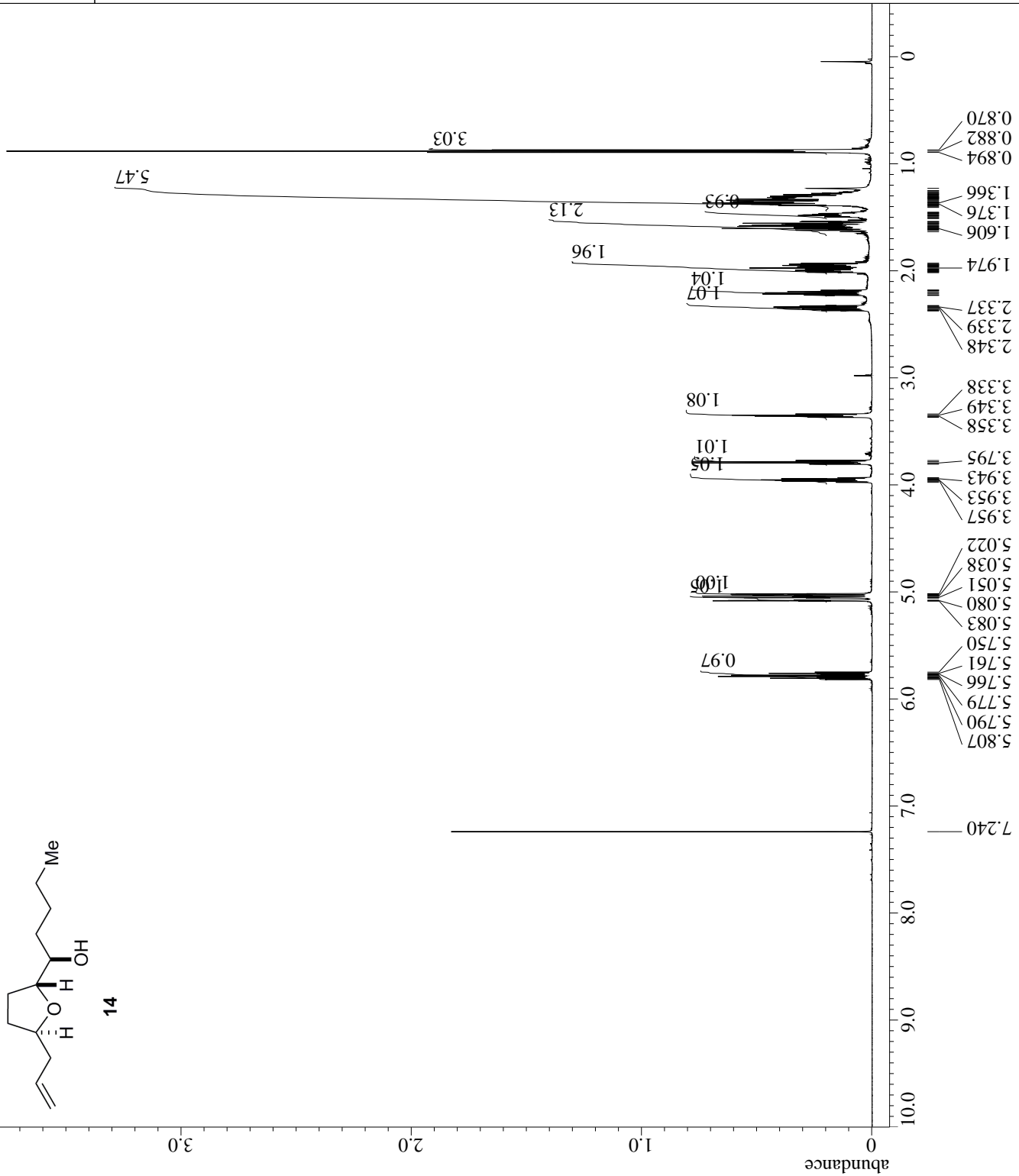
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = proton_jmp
Sample_Id = YK-II-95a
Solvent = CHLOROFORM-D
Creation_Time = 24-JUN-2014 15:37:47
Revision_Time = 24-JUN-2014 16:01:19
Current_Time = 24-JUN-2014 16:03:07

Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 32
Temp_Get = 22.5[degC]
X_90_Width = 7.215[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Atn = 4[dB]
X_Pulse = 3.6075[us]
Irr_Mode = OFF
Tri_Mode = OFF
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```



X : parts per Million : Proton

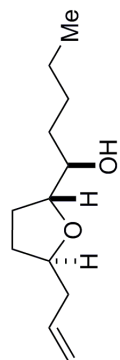
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon_jmp
Sample_Id = YK-II-95a
Solvent = CHLOROFORM-D
Creation_Time = 24-JUN-2014 15:41:17
Revision_Time = 24-JUN-2014 16:03:48
Current_Time = 24-JUN-2014 16:04:22

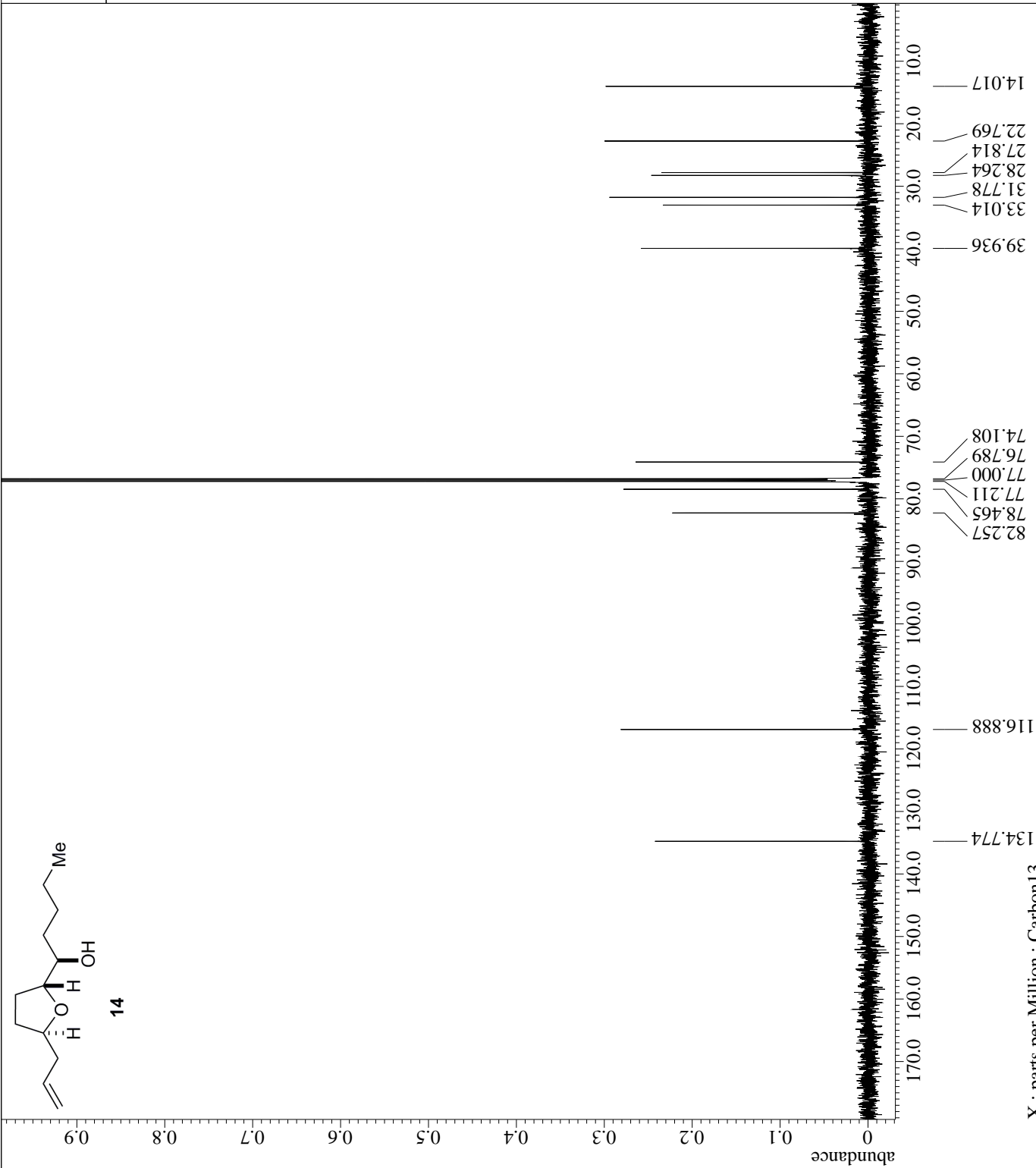
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = 13C
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 260
Total_Scans = 260

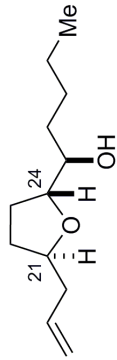
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 23[dc]
X_90_Width = 10.5[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 7.4[db]
X_Pulse = 3.5[us]
Irr_Atn_Dec = 24.452[db]
Irr_Atn_Noise = 24.452[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```



14



Differential NOE experiment (CDCl₃)



14

19-H

21-H (irr)

25-H

20-H

22-H

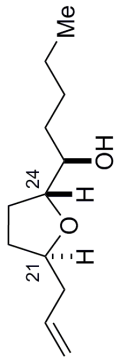
23-H

(thousands)

6.0 6.9 5.8 5.7 5.6 5.5 5.4 5.3 5.2 5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1

X : parts per Million : Proton

Differential NOE experiment (CDCl₃)



14

23-H

24-H (irr)

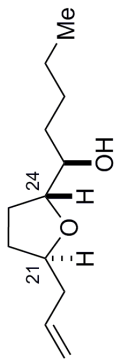
22-H

(thousands)

5.9 5.8 5.7 5.6 5.5 5.4 5.3 5.2 5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2

X : parts per Million : Proton

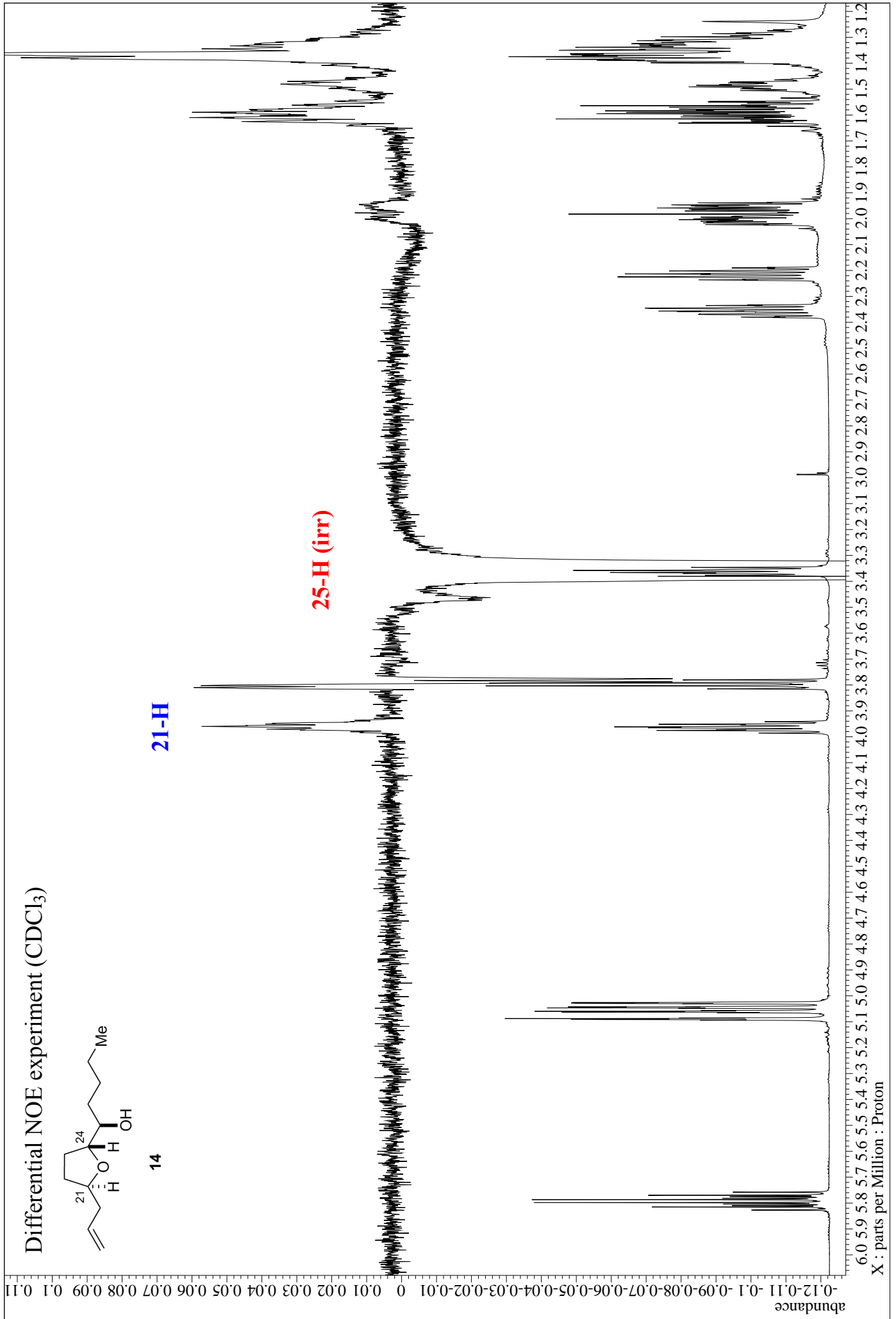
Differential NOE experiment (CDCl₃)



14

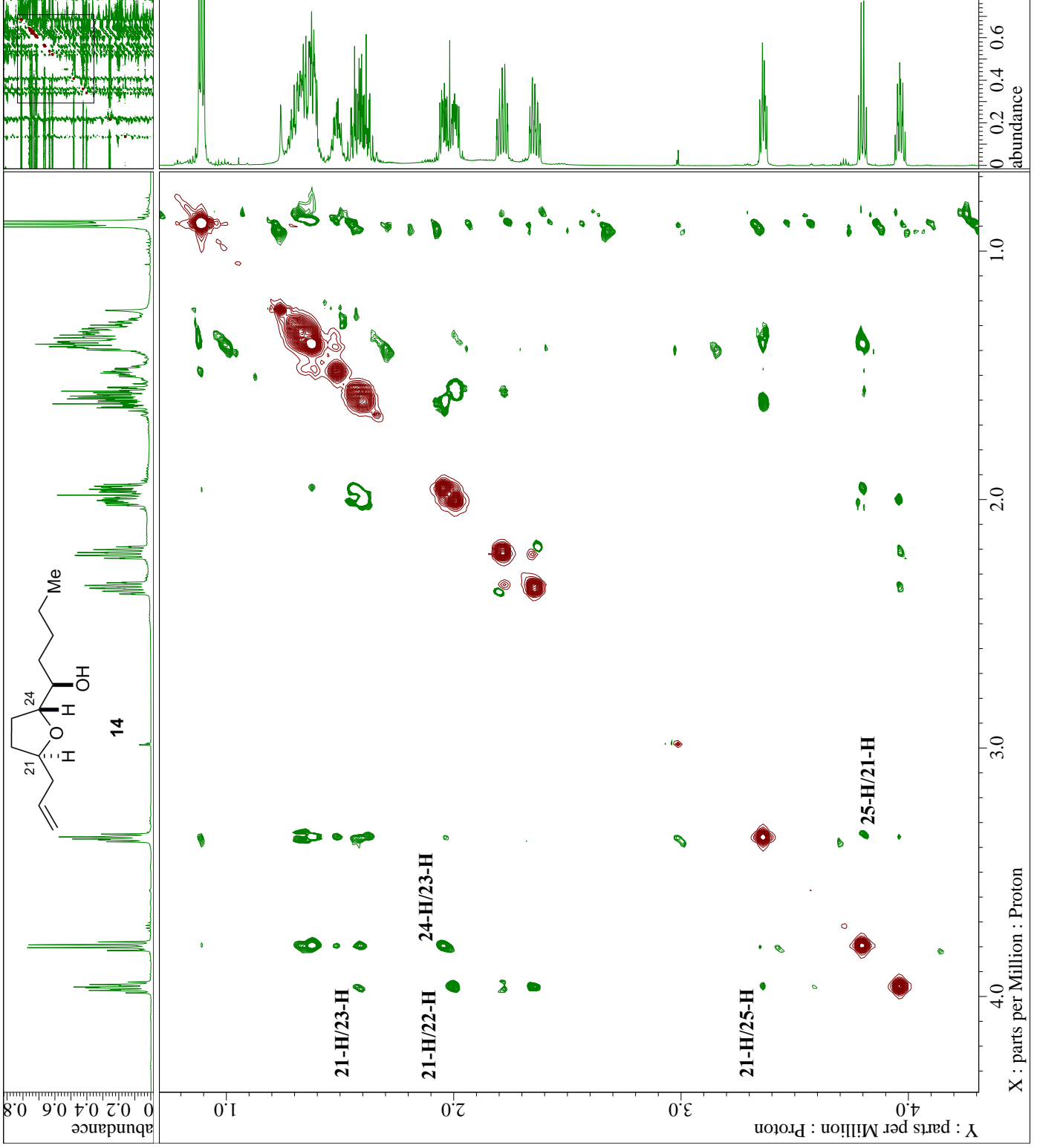
21-H

25-H (irr)



X : parts per Million : Proton

NOESY spectrum (CDCl₃)



```

= /Volumes/YUHKI_USB/kawashi
= delta
= noesy.jxp
= YK-II-95a
= CHLOROFORM-D
= 26-JUN-2014 05:25:11
= 27-JUN-2014 15:53:15
= 27-JUN-2014 15:59:19

= phase sensitive noesy
= 2D COMPLEX COMPLEX
= 819, 512
= Proton Proton
= [ppm] [ppm]
= X Y
= ECA600
= DELTA2_NMR

Spectrometer
= 14.09636928[G] (600[MHz])
Field Strength
X Acq_Duration = 0.19202048[s]
X Domain = 1H
X Freq = 600.1723046[MHz]
X Offset = 3.58316[ppm]
X Points = 1024
X Prescans = 4
X Resolution = 5.20777784[Hz]
X Sweep = 5.33276451[kHz]
X Sweep_Clippped = 4.2662116[kHz]
Y Domain = 1H
Y Freq = 600.1723046[MHz]
Y Offset = 3.58316[ppm]
Y Points = 256
Y Prescans = 0
Y Resolution = 16.65920334[Hz]
Y Sweep = 4.26475606[kHz]

Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 12
Total_Scans = 3072

Relaxation_Delay = 1.5[s]
Recvr_Gain = 30
Temp_Get = 22.5[degC]
Mix_Time = 0.5[s]
X Acq_Time = 0.19202048[s]
X Atn = 4[dB]
X Pulse = 7.215[us]
Y Acq_Time = 60.02688[ms]
Y PI_Correction = 180.0
Irr_Mode = Off
Tri_Mode = Off
Adiabatic_Pulse = 50[ms]
Bl_Atn = 43.80211242[dB]
Band_Width = 30[kHz]
Chirp_Atn = 31.19788758[dB]
Chirp_Pulse = 50[ms]
Chirp_Shape = CHIRP
Chirp_Smooth = 10[%]
Dante_Preset = FALSE
Grad_Spoil = 1[ms]
Grad_Spoil_Amp = 6[mr/m]
Hard_Zqg_Amp = 24[mr/m]
Hard_Square_Atn = 75[dB]
Initial_Wait = 1[s]
    
```

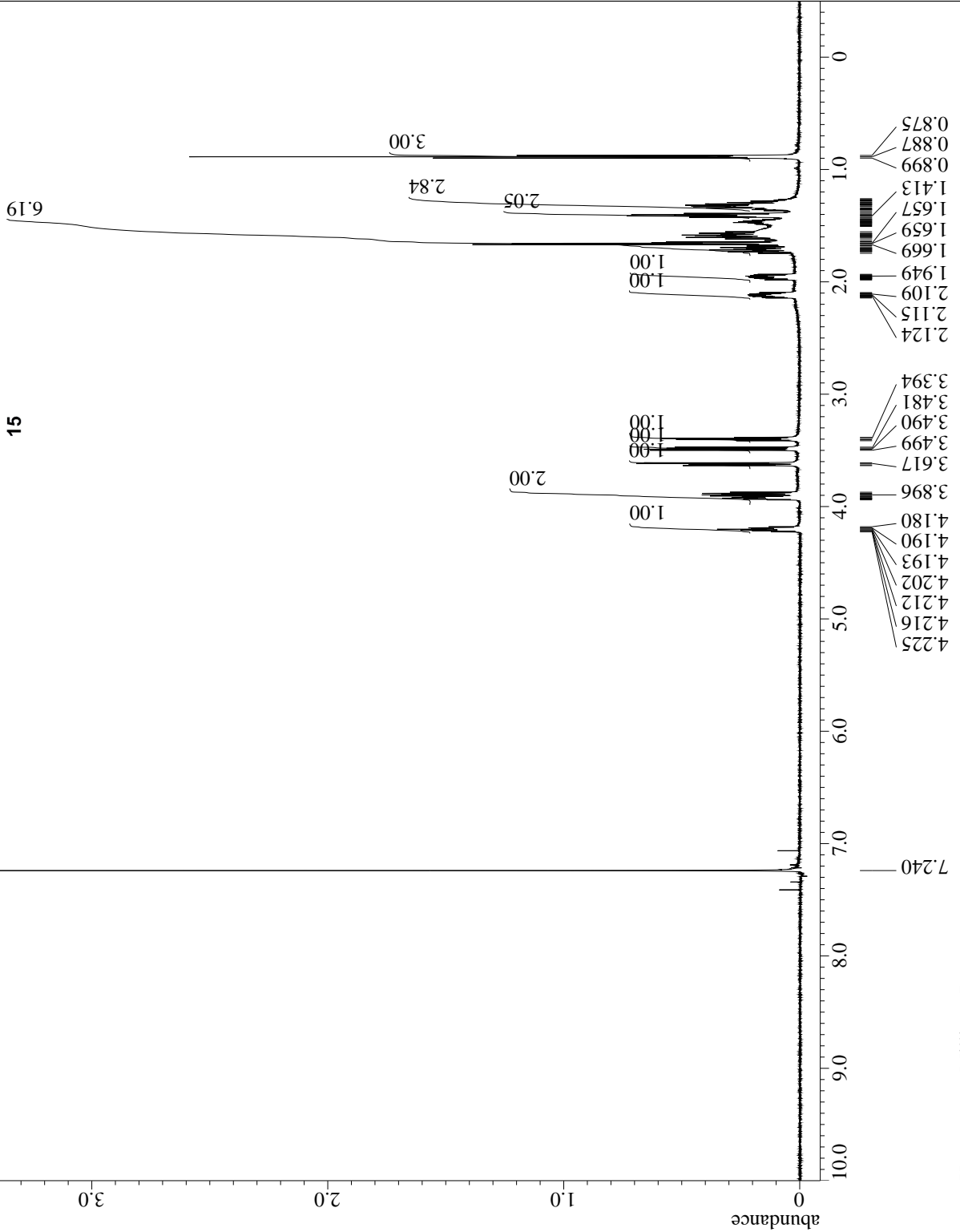
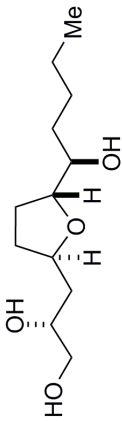
```

Filename = /Volumes/YUHKI_USB/YK-IV-0
Author = delta
Experiment = Proton.jpg
Sample_Id = YK-IV-007b
Solvent = CHLOROFORM-D
Creation_Time = 28-JUN-2014 10:27:33
Revision_Time = 7-JUL-2014 20:47:26
Current_Time = 7-JUL-2014 20:48:29

Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.5[degC]
X_90_Width = 7.215[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Atn = 4[dB]
X_Pulse = 3.6075[us]
Irr_Mode = OFF
Tri_Mode = OFF
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```



X : parts per Million : Proton

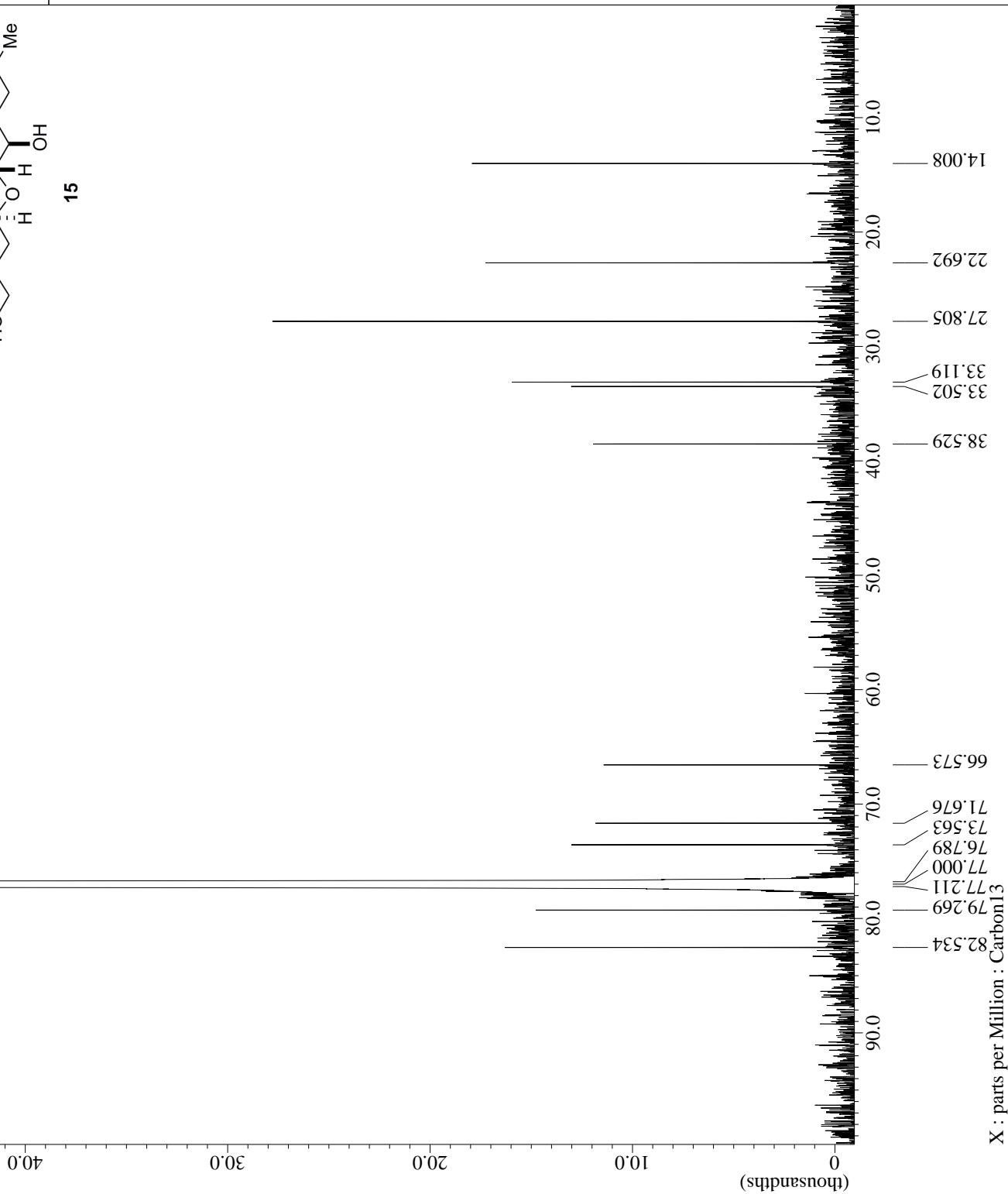
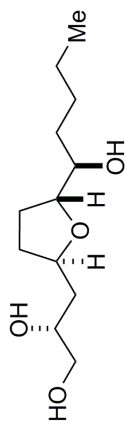
```

Filename = /Volumes/YUHKI_USB/YK-IV-0
Author = delta
Experiment = carbon.jxp
Sample_Id = YK-IV-007
Solvent = CHLOROFORM-D
Creation_Time = 6-JUL-2014 21:57:52
Revision_Time = 7-JUL-2014 20:49:14
Current_Time = 7-JUL-2014 20:49:48

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 0.69206016[s]
X Domain = 13C
X Freq = 150.91343039[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 1.44496109[Hz]
X Sweep = 47.34848485[kHz]
X Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 14784
Total_Scans = 14784

Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.6[dc]
X_90_Width = 10.5[us]
X Acq_Time = 0.69206016[s]
X Angle = 30[deg]
X Atn = 7.4[db]
X Pulse = 3.5[us]
Irr_Atn_Dec = 24.452[db]
Irr_Atn_Noise = 24.452[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```



X : parts per Million : Carbon13

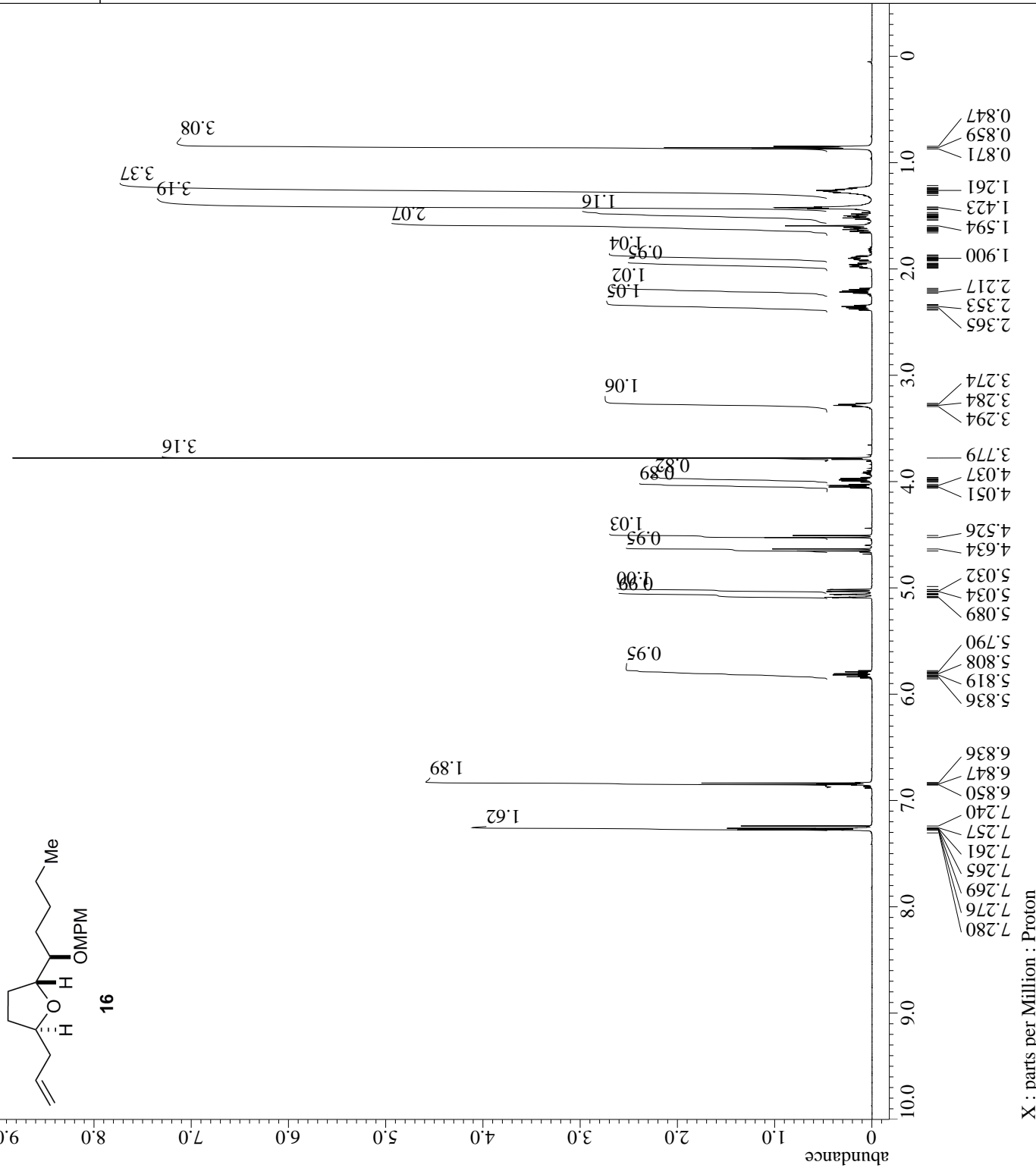
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = proton_jxp
Sample_Id = YK-II-123a
Solvent = CHLOROFORM-D
Creation_Time = 1-JUL-2013 11:56:55
Revision_Time = 24-JUN-2014 16:14:05
Current_Time = 24-JUN-2014 16:14:33

Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 38
Temp_Get = 21.3[degC]
X_90_Width = 11.6[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 5.8[us]
Irr_Mode = OFF
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```





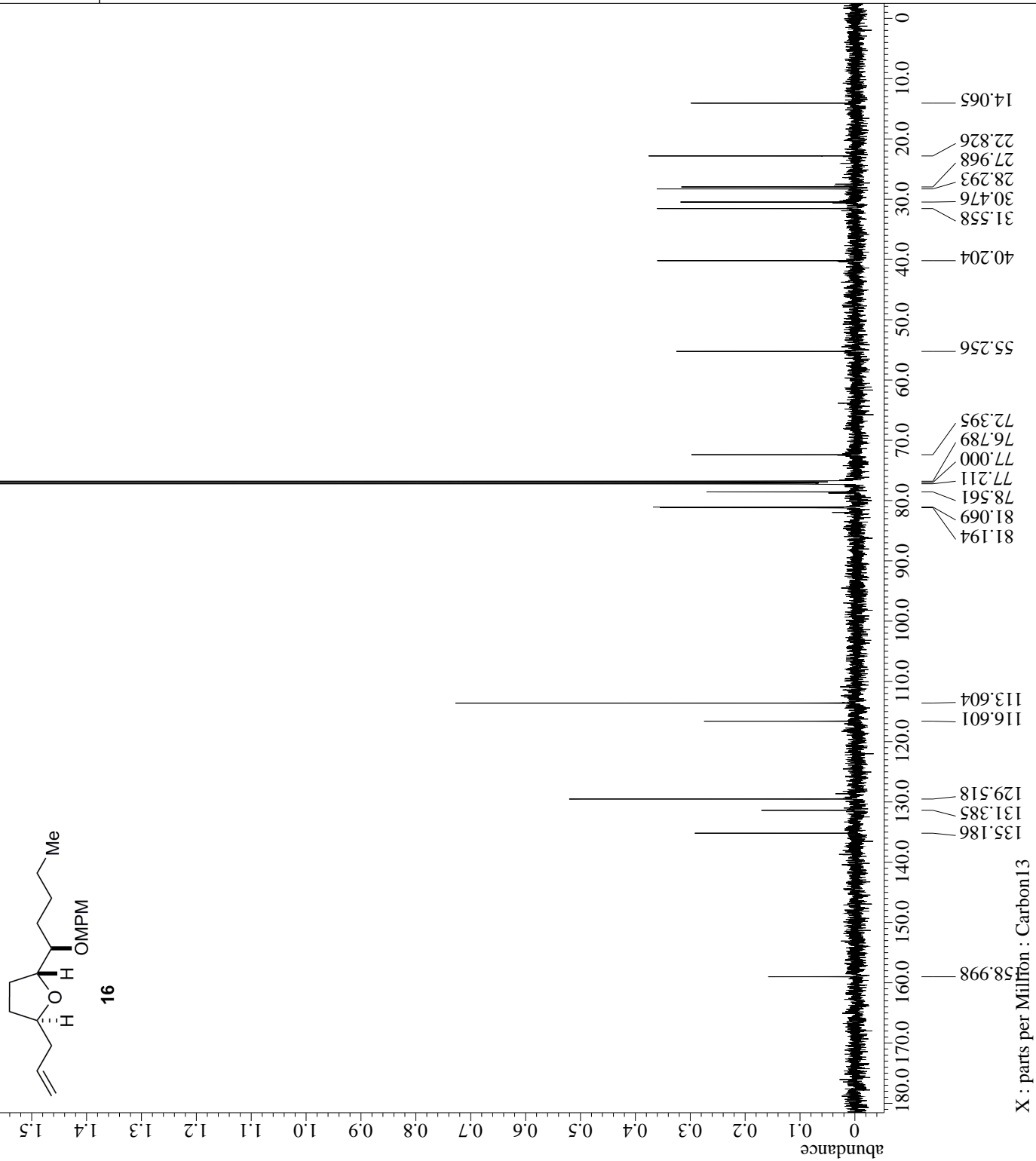
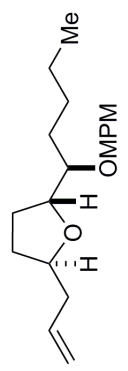
Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon.jxp
Sample_id = YK-II-123a
Solvent = CHLOROFORM-D
Creation_Time = 1-JUL-2013 18:42:48
Revision_Time = 24-JUN-2014 16:06:35
Current_Time = 24-JUN-2014 16:08:37

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 0.69206016[s]
X Domain = 13C
X Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clippped = 37.87878788[kHz]

Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 116.0
Total_Scans = 116.0

Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.1[dc]
X_90_Width = 9.25[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 8[db]
X_Pulse = 3.08333333[us]
Irr_Atn_Dec = 19.327[db]
Irr_Atn_Noise = 19.327[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]



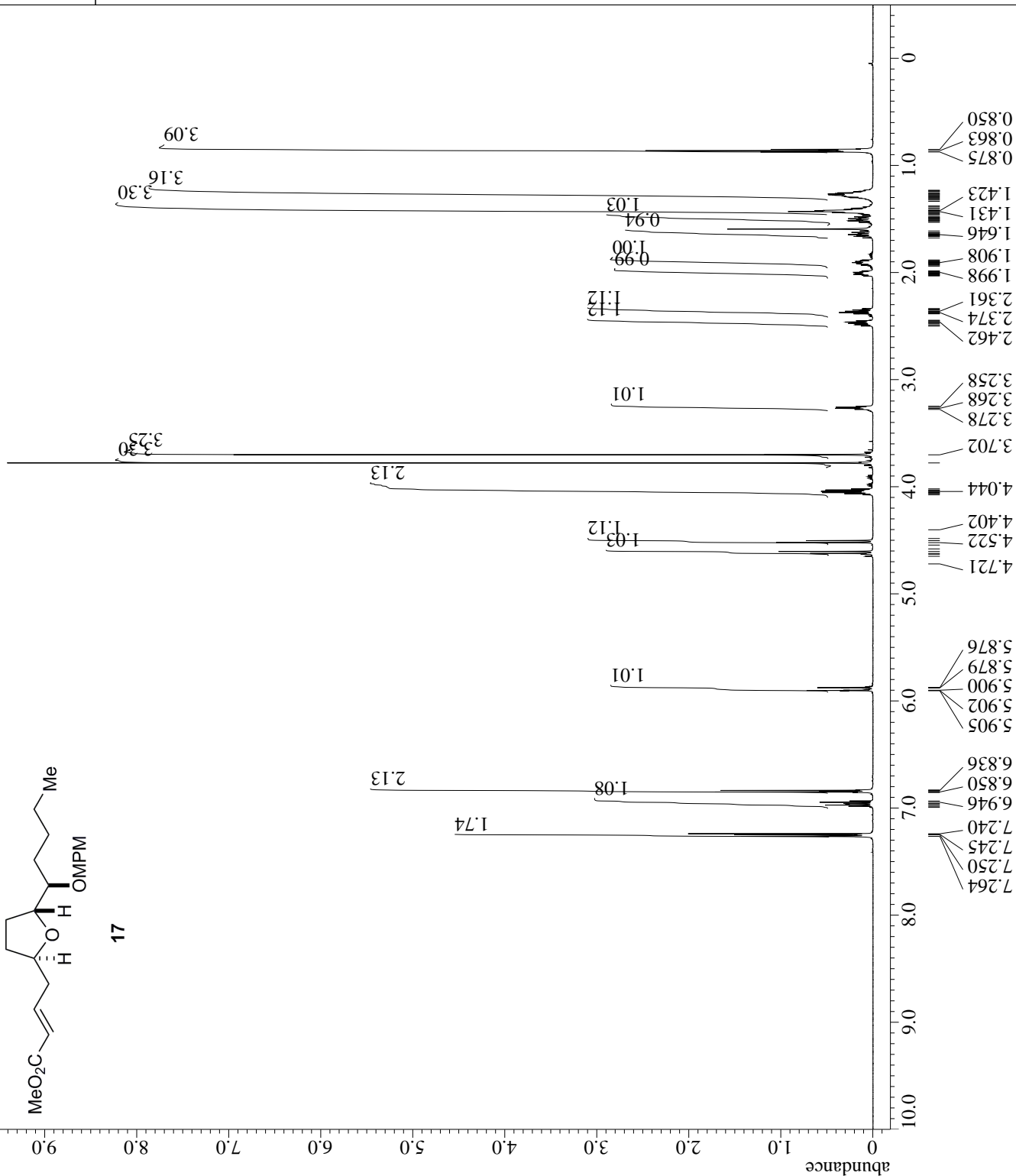
```

/Users/skt_macbookpro/Desktop
= delta
Author = proton_jxp
Experiment = YK-II-130c
Sample_Id = CHLOROFORM-D
Solvent = CHLOROFORM-D
Creation_Time = 11-JUL-2013 14:17:35
Revision_Time = 24-JUN-2014 02:05:27
Current_Time = 24-JUN-2014 02:05:56

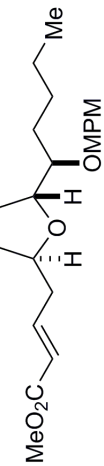
= single pulse
Comment =
Data Format = 1D COMPLEX
Dim Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field Strength = 14.09636928[T] (600[MHz])
X Acq Duration = 2.18103808[s]
X Domain = 1H
X Freq = 600.1723046[MHz]
X Offset = 5[ppm]
X Points = 32768
X Prescans = 1
X Resolution = 0.45849727[Hz]
X Sweep = 15.02403846[kHz]
X Sweep_Clippped = 12.01923077[kHz]
Irr Domain = Proton
Irr Freq = 600.1723046[MHz]
Irr Offset = 5[ppm]
Tri Domain = Proton
Tri Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr Gain = 40
Temp_Get = 21.8[degC]
X 90_Width = 11.6[us]
X Acq_Time = 2.18103808[s]
X Angle = 45[deg]
X Actn = 3[dB]
X Pulse = 5.8[us]
Irr_Mode = OFF
Tri_Mode = OFF
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```



X : parts per Million : Proton



17



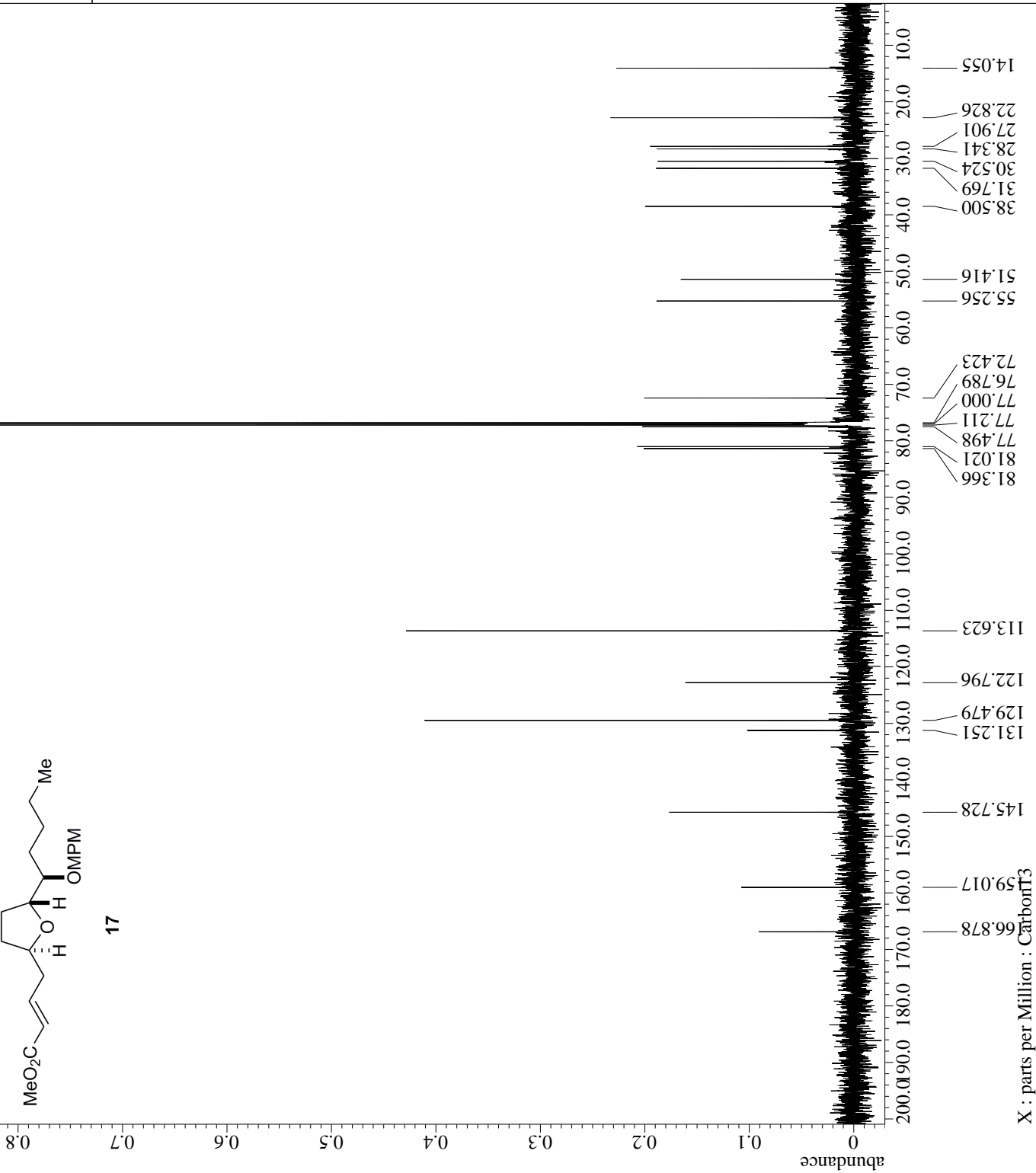
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon.jxp
Sample_Id = YK-II-130c
Solvent = CHLOROFORM-D
Creation_Time = 11-JUL-2013 18:41:21
Revision_Time = 24-JUN-2014 02:06:33
Current_Time = 24-JUN-2014 02:07:27

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = 13C
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.172304046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 96
Total_Scans = 96

Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 22.5[dc]
X_90_Width = 9.25[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 8[db]
X_Pulse = 3.08333333[us]
Irr_Atn_Dec = 19.327[db]
Irr_Atn_Noise = 19.327[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```



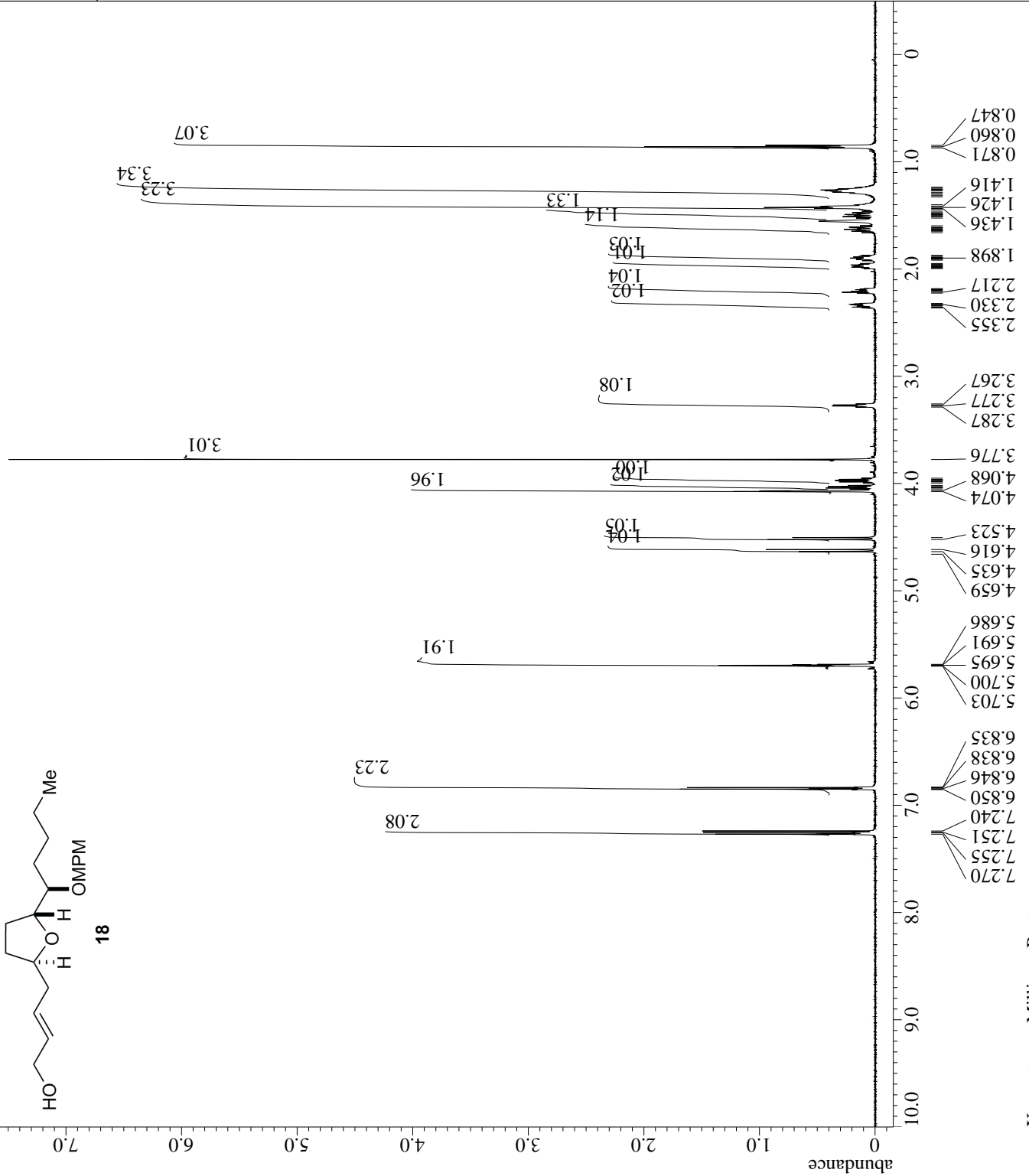
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = Proton.jxp
Sample_Id = YK-II-151
Solvent = CHLOROFORM-D
Creation_Time = 8-AUG-2013 14:22:38
Revision_Time = 24-JUN-2014 02:14:50
Current_Time = 24-JUN-2014 02:15:01

Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.2[degC]
X_90_Width = 11.6[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Acn = 3[db]
X_Pulse = 5.8[us]
Irr_Mode = OFF
Tri_Mode = OFF
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```



X : parts per Million : Proton

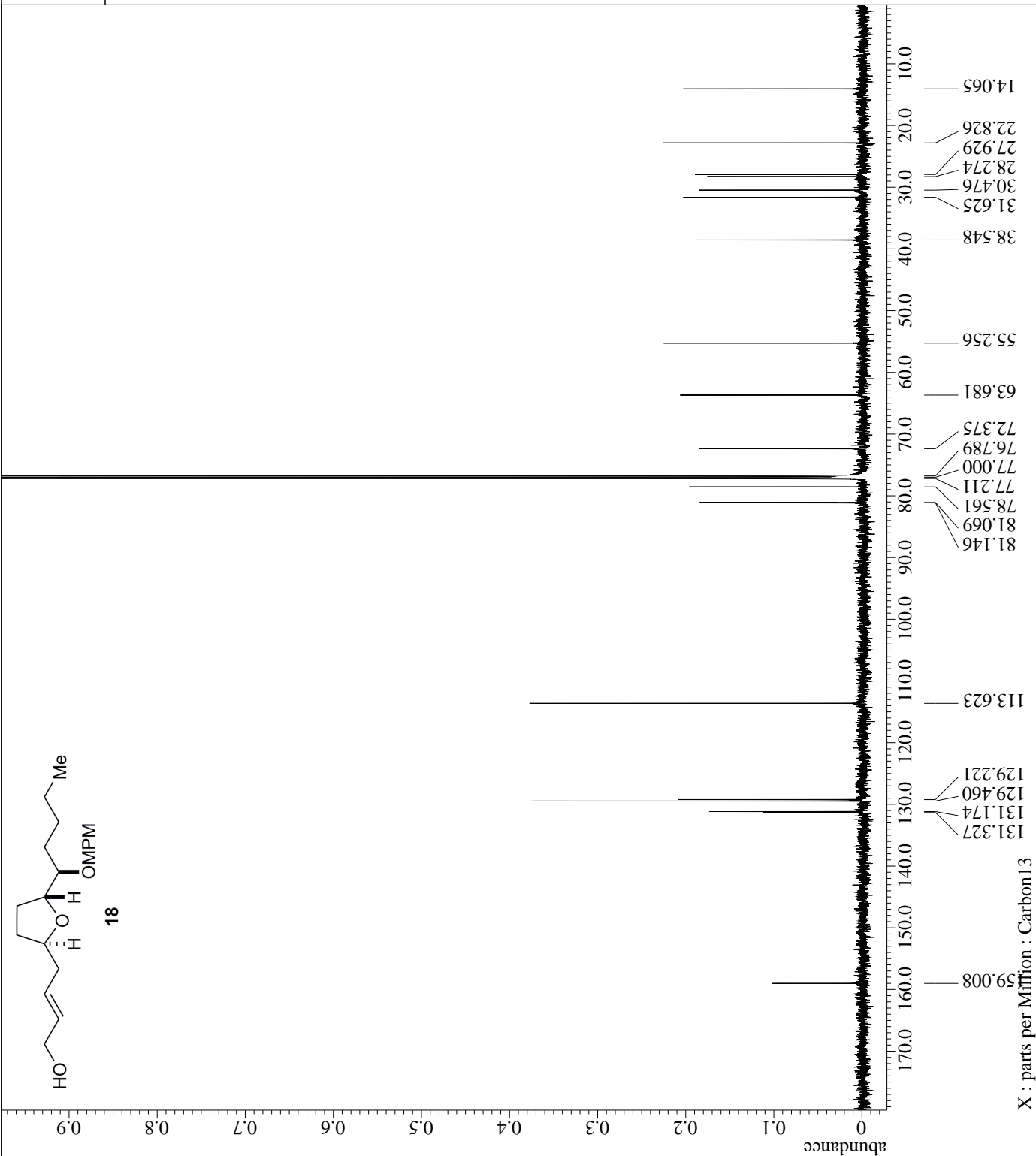
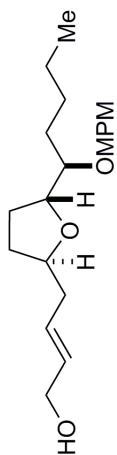
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon_jmp
Sample_Id = YK-II-151
Solvent = CHLOROFORM-D
Creation_Time = 24-JUN-2014 10:44:36
Revision_Time = 24-JUN-2014 14:14:46
Current_Time = 24-JUN-2014 14:15:13

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.0963928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = 13C
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 424
Total_Scans = 424

Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 22.4[dc]
X_90_Width = 10.5[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 7.4[db]
X_Pulse = 3.5[us]
Irr_Atn_Dec = 24.452[db]
Irr_Atn_Noise = 24.452[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```



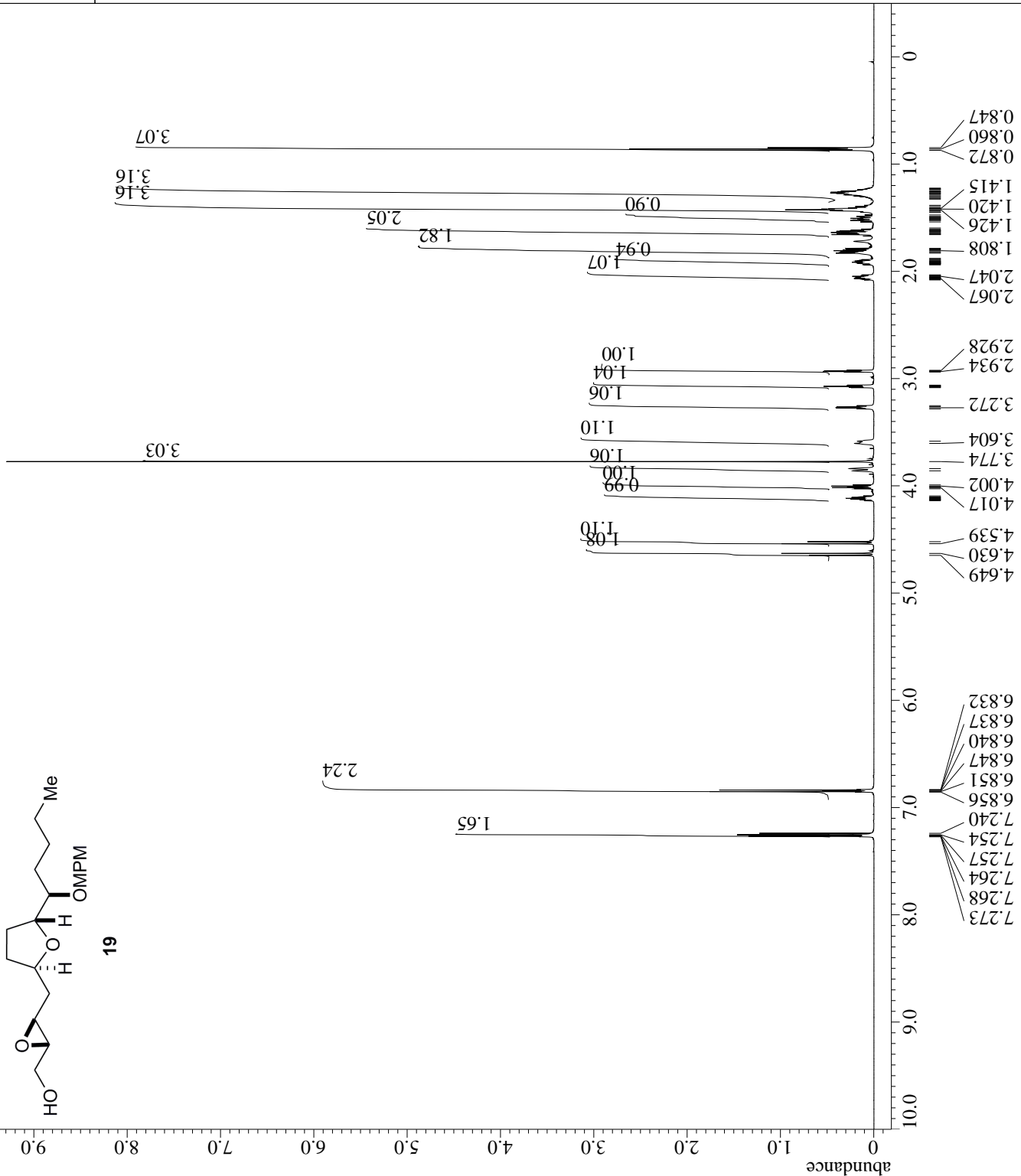
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = proton_jxp
Sample_Id = YK-II-158
Solvent = CHLOROFORM-D
Creation_Time = 22-AUG-2013 13:14:26
Revision_Time = 24-JUN-2014 02:40:47
Current_Time = 24-JUN-2014 02:41:21

Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 36
Temp_Get = 21.8[degC]
X_90_Width = 11.6[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Pulse = 3[db]
X_Acn = 5.8[us]
Irr_Mode = OFF
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```



X : parts per Million : Proton

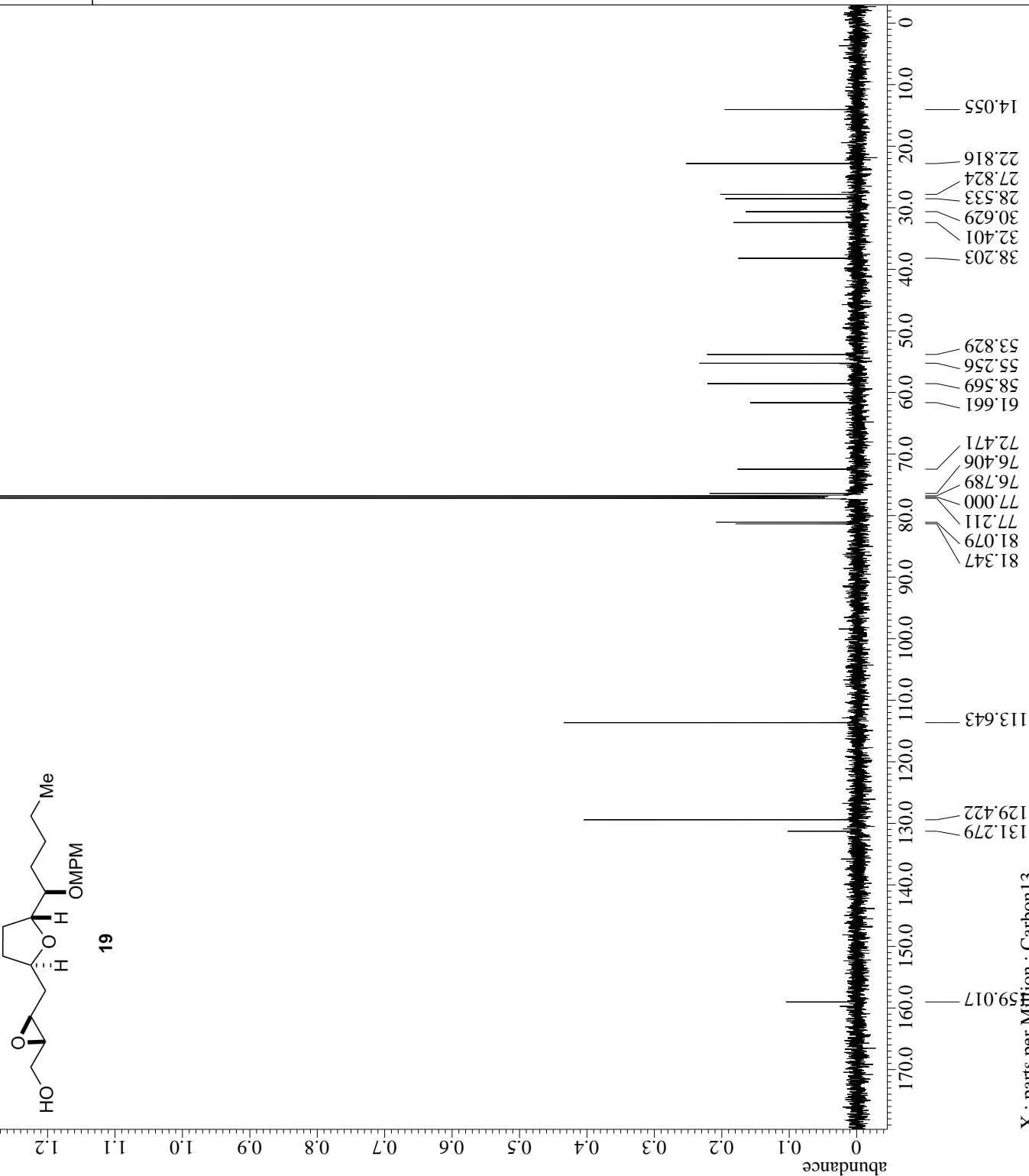
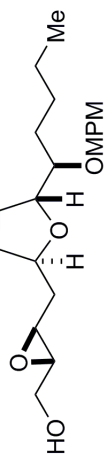
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon.jxp
Sample_Id = YK-II-158
Solvent = CHLOROFORM-D
Creation_Time = 23-JUN-2014 14:37:44
Revision_Time = 24-JUN-2014 02:45:27
Current_Time = 24-JUN-2014 02:46:06

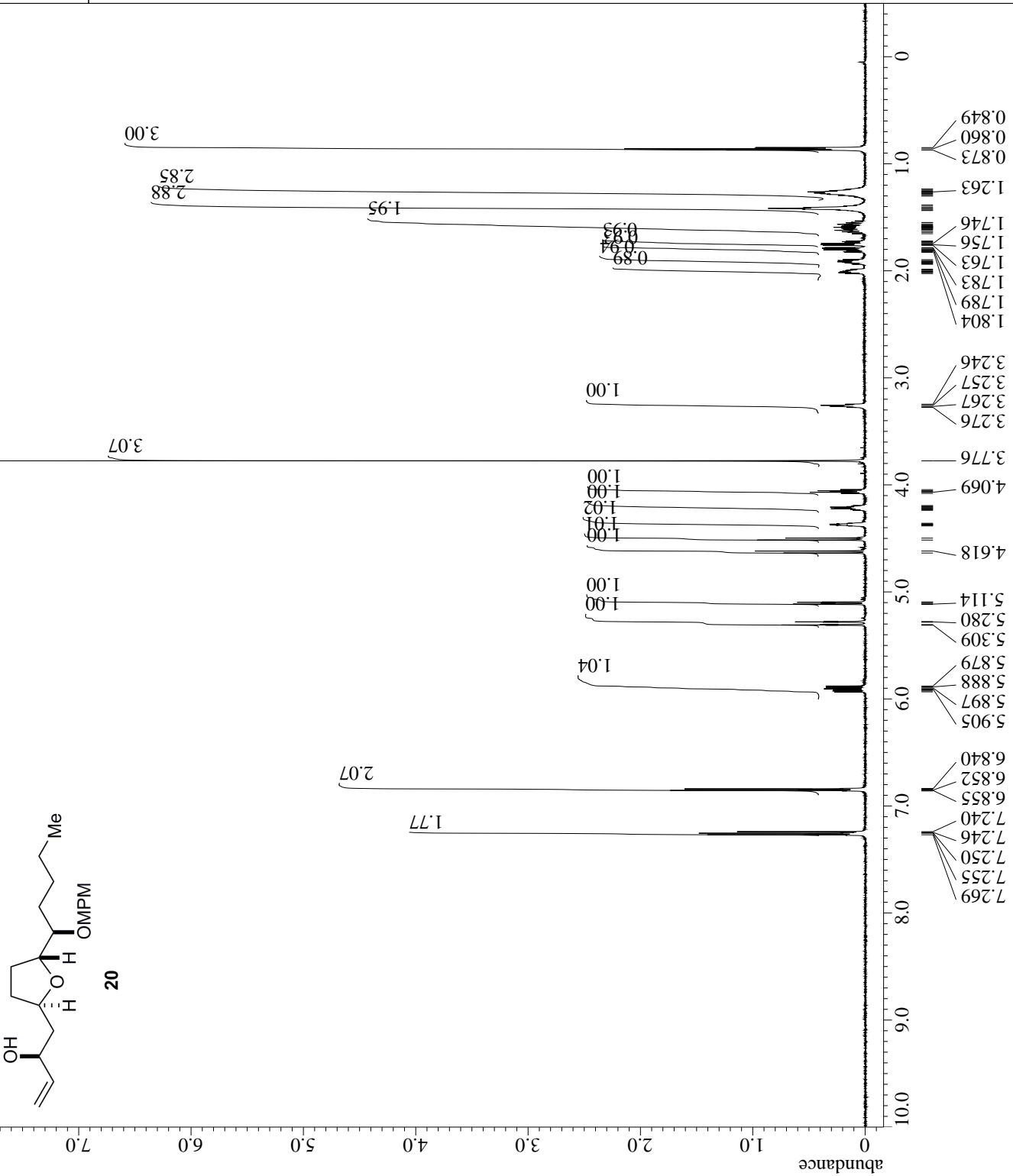
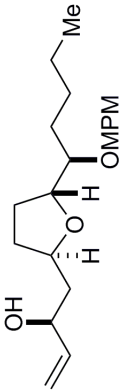
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = 13C
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 160
Total_Scans = 160

Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.5[dc]
X_90_Width = 10.5[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 7.4[db]
X_Pulse = 3.5[us]
Irr_Atn_Dec = 24.452[db]
Irr_Atn_Noise = 24.452[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```



X : parts per Million : Carbon13



Filename = /Users/skt_macbookpro/Desk
 Author = delta
 Experiment = proton_jmp
 Sample_id = YK-II-154
 Solvent = CHLOROFORM-D
 Creation_Time = 20-AUG-2013 18:15:07
 Revision_Time = 24-JUN-2014 02:51:37
 Current_Time = 24-JUN-2014 02:53:43
 Comment = single pulse
 Data_Format = 1D COMPLEX
 Dim_Size = 26214
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Site = ECA600
 Spectrometer = DELTA2_NMR
 Field_Strength = 14.09636928[T] (600[MHz])
 X_Acq_Duration = 2.18103808[s]
 X_Domain = 1H
 X_Freq = 600.1723046[MHz]
 X_Offset = 5[ppm]
 X_Points = 32768
 X_Prescans = 1
 X_Resolution = 0.45849727[Hz]
 X_Sweep = 15.02403846[kHz]
 X_Sweep_Clippped = 12.01923077[kHz]
 Irr_Domain = Proton
 Irr_Freq = 600.1723046[MHz]
 Irr_Offset = 5[ppm]
 Tri_Domain = Proton
 Tri_Freq = 600.1723046[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 8
 Total_Scans = 8
 Relaxation_Delay = 2[s]
 Recvr_Gain = 60
 Temp_Get = 21.8[deg]
 X_90_Width = 11.6[us]
 X_Acq_Time = 2.18103808[s]
 X_Angle = 45[deg]
 X_Atn = 3[db]
 X_Pulse = 5.8[us]
 Irr_Mode = OFF
 Tri_Mode = OFF
 Dante_Presat = FALSE
 Initial_Wait = 1[s]
 Repetition_Time = 4.18103808[s]



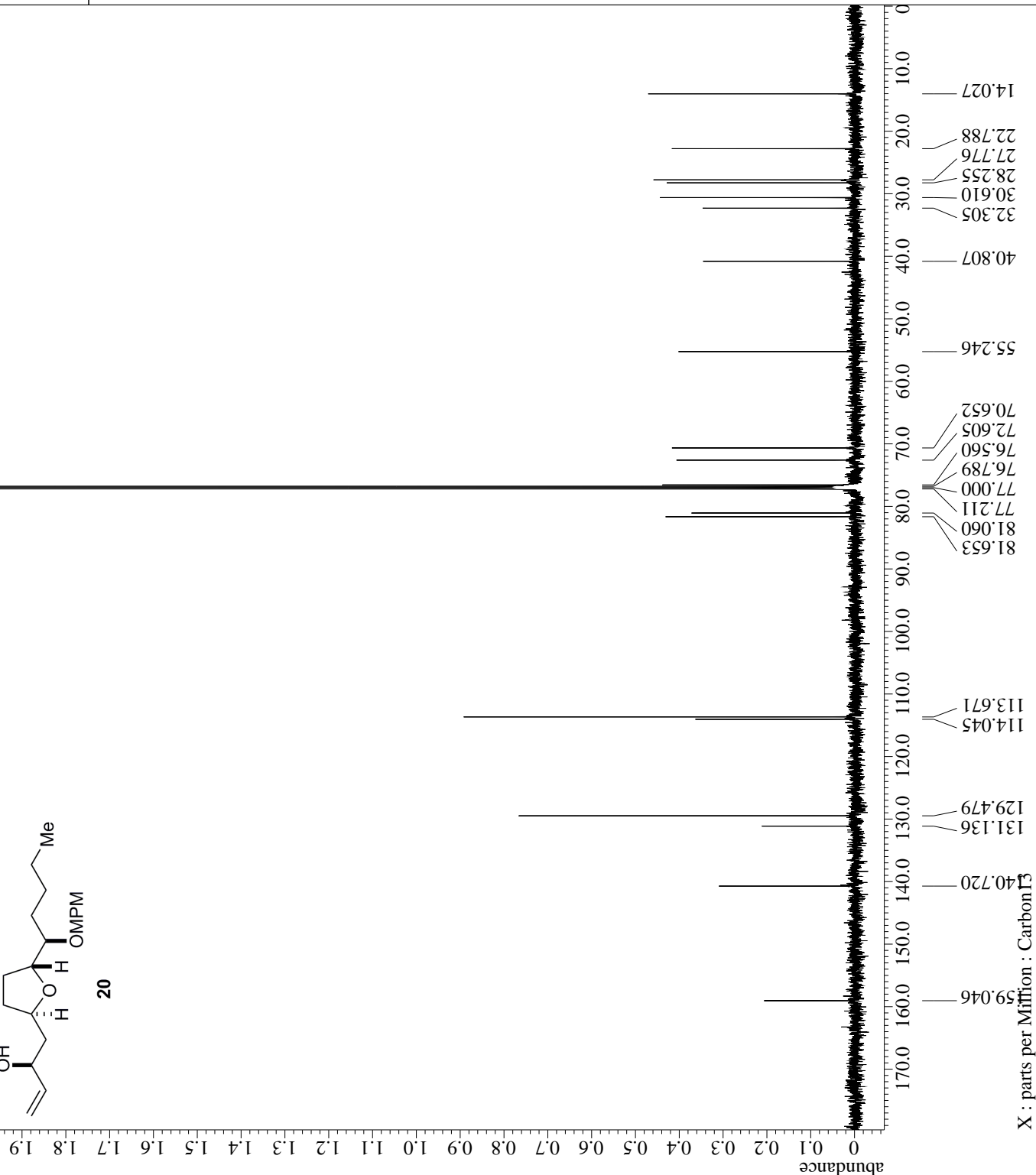
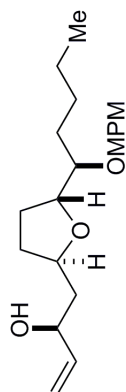
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon_jmp
Sample_Id = YK-II-154
Solvent = CHLOROFORM-D
Creation_Time = 20-AUG-2013 18:18:18
Revision_Time = 24-JUN-2014 02:54:20
Current_Time = 24-JUN-2014 02:54:54

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 0.69206016[s]
X Domain = 13C
X Freq = 150.91343039[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 1.44496109[Hz]
X Sweep = 47.34848485[kHz]
X Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 128
Total_Scans = 128

Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.4[dc]
X_90_Width = 9.25[us]
X Acq_Time = 0.69206016[s]
X Angle = 30[deg]
X Atn = 8[db]
X Pulse = 3.08333333[us]
Irr_Atn_Dec = 19.327[db]
Irr_Atn_Noise = 19.327[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```



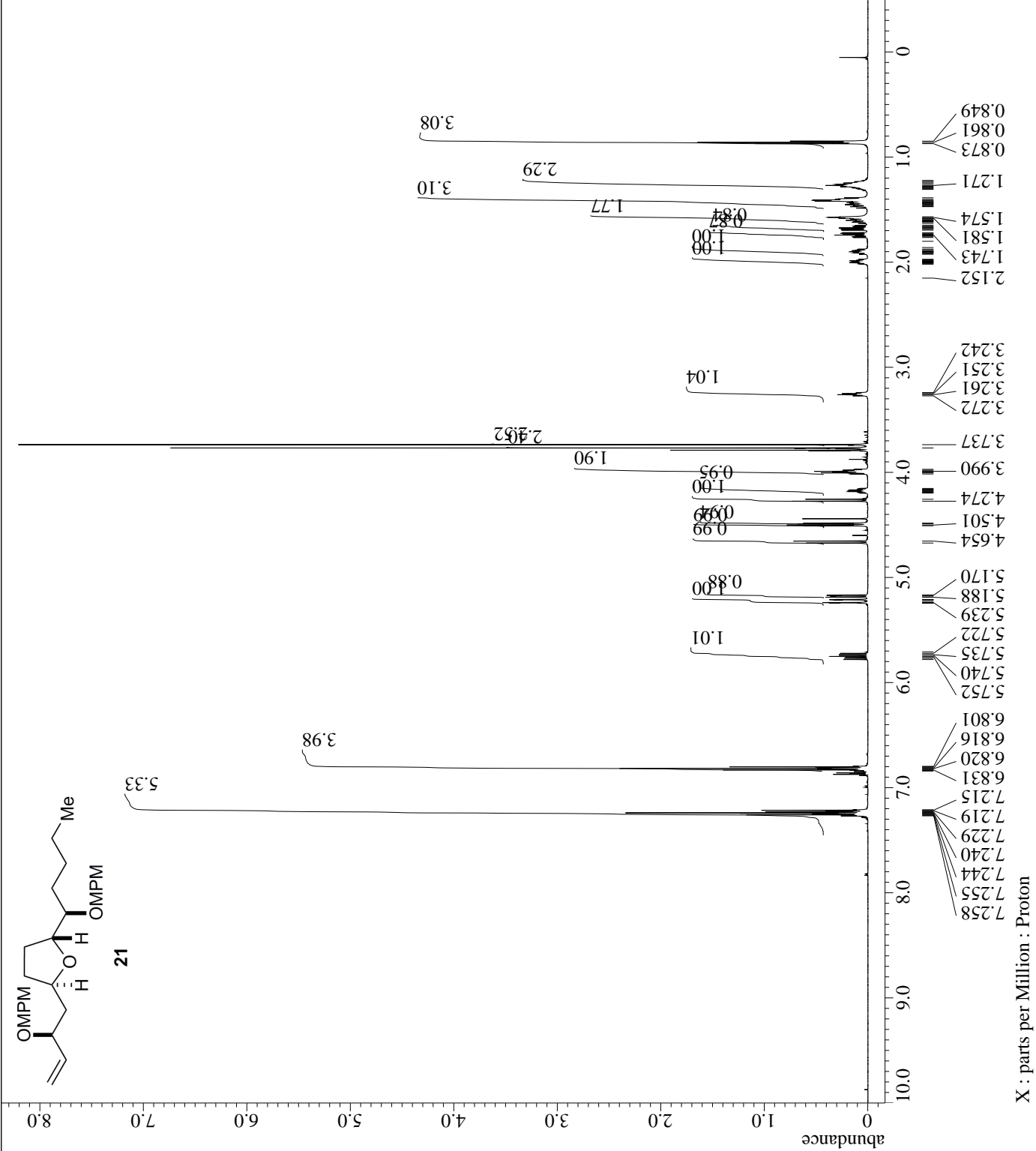
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = Proton.jxp
Sample_Id = YK-II-161
Solvent = CHLOROFORM-D
Creation_Time = 23-AUG-2013 14:56:39
Revision_Time = 24-JUN-2014 03:10:24
Current_Time = 24-JUN-2014 03:10:50

Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 40
Temp_Get = 22.2[degC]
X_90_Width = 11.6[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Acn = 3[dB]
X_Pulse = 5.8[us]
Irr_Mode = OFF
Tri_Mode = OFF
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```



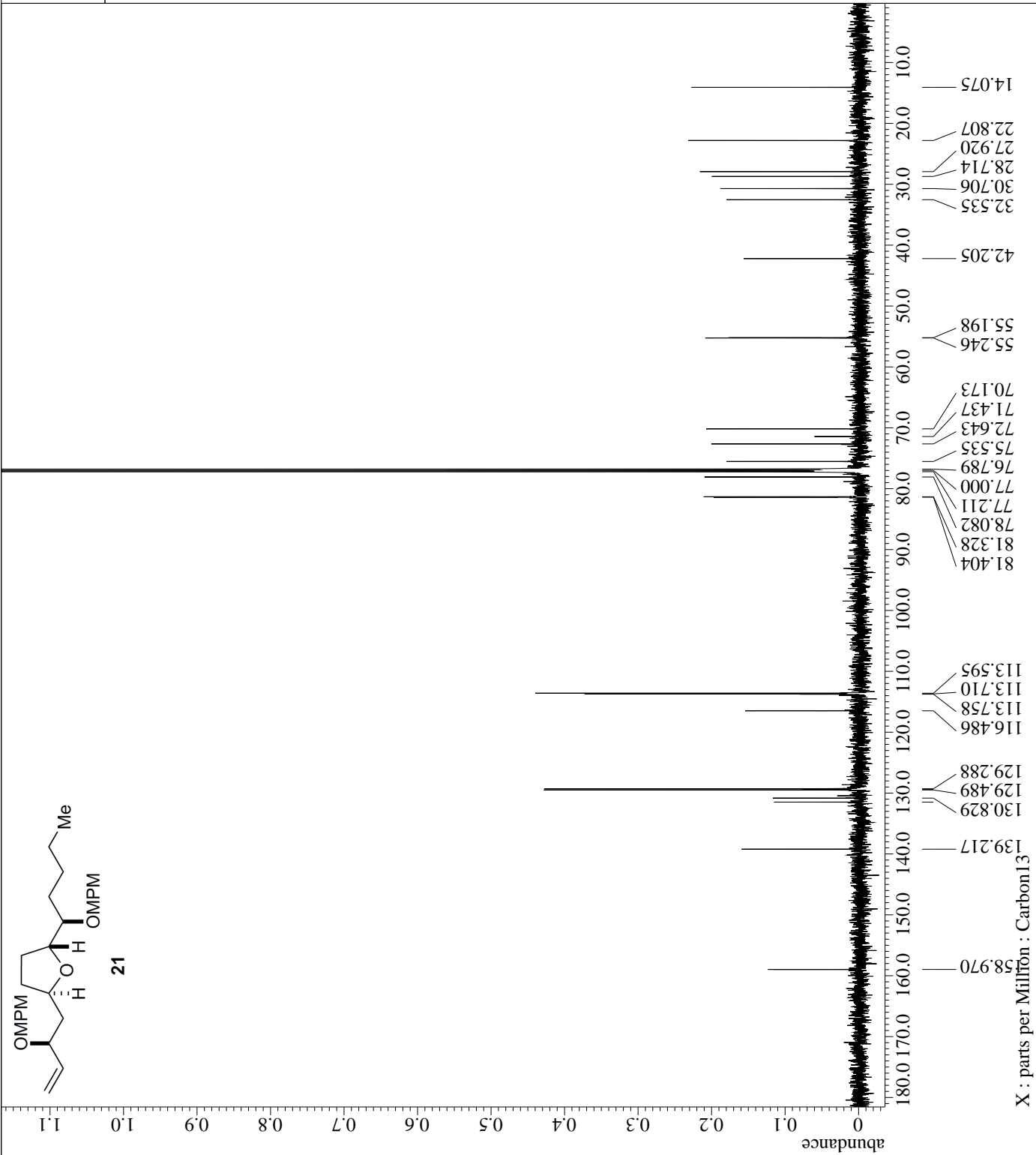
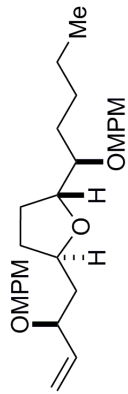
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon.jxp
Sample_Id = YK-II-161
Solvent = CHLOROFORM-D
Creation_Time = 23-AUG-2013 14:59:52
Revision_Time = 24-JUN-2014 03:11:44
Current_Time = 24-JUN-2014 03:12:13

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = 13C
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clippped = 37.87878788[kHz]
X_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 225
Total_Scans = 225

Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.5[dc]
X_90_Width = 9.25[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 8[db]
X_Pulse = 3.08333333[us]
Irr_Atn_Dec = 19.327[db]
Irr_Atn_Noise = 19.327[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```




```

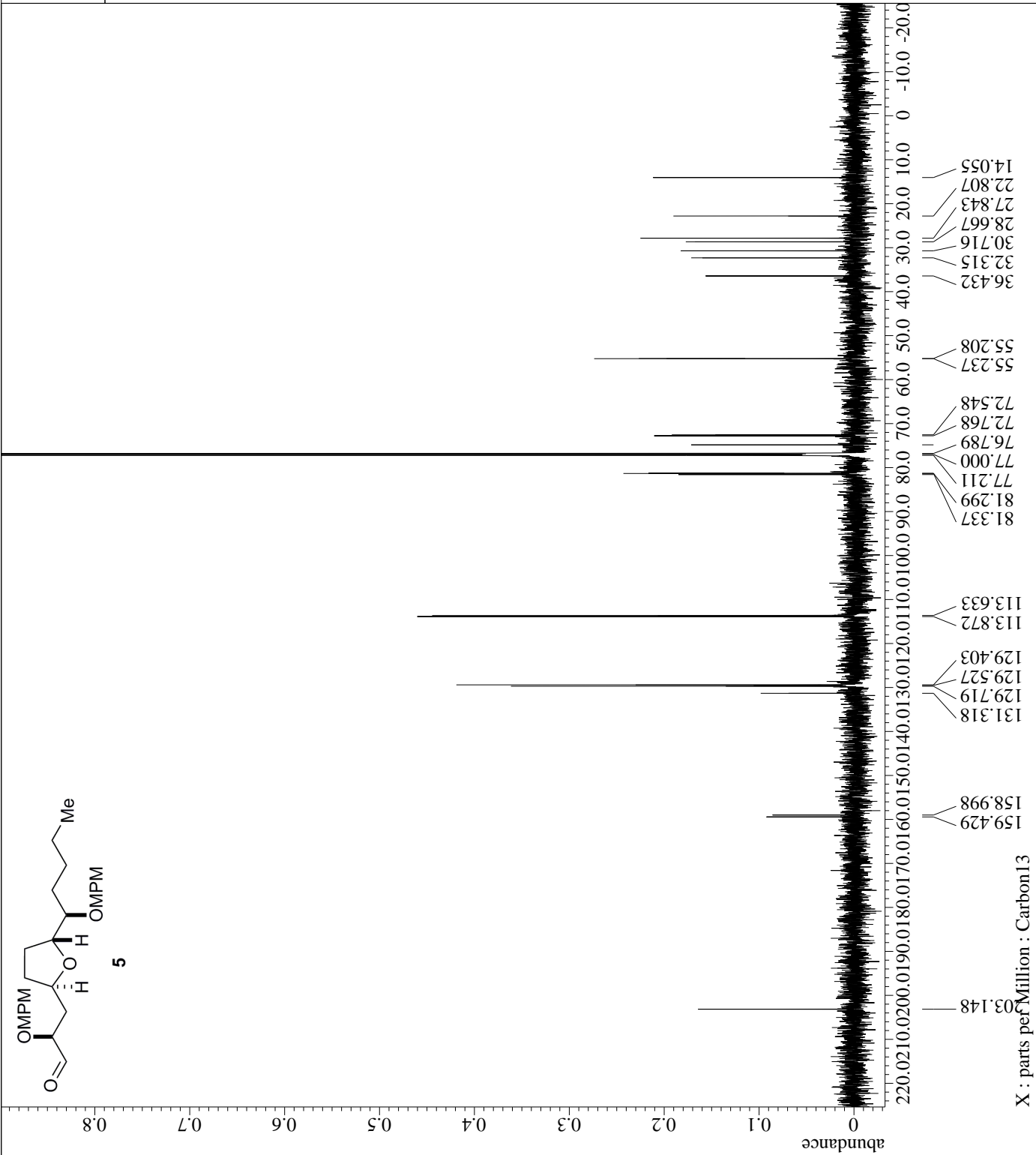
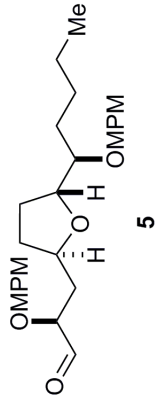
Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon_jxp
Sample_id = YK-III-021
Solvent = CHLOROFORM-D
Creation_Time = 21-OCT-2013 14:15:03
Revision_Time = 24-JUN-2014 09:46:50
Current_Time = 24-JUN-2014 09:47:19

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 0.69206016[s]
X Domain = 13C
X Freq = 150.91343039[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 1.44496109[Hz]
X Sweep = 47.34848485[kHz]
X Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 160
Total_Scans = 160

Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.3[dc]
X_90_Width = 10[us]
X Acq_Time = 0.69206016[s]
X Angle = 30[deg]
X Atn = 8[db]
X Pulse = 3.33333333[us]
Irr_Atn_Dec = 18.24[db]
Irr_Atn_Noise = 18.24[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]

```



X : parts per Million : Carbon13

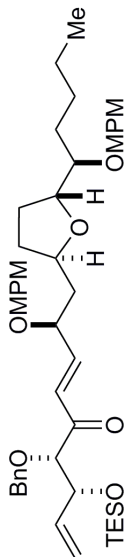
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = Proton.jpg
Sample_Id = YK-III-023
Solvent = CHLOROFORM-D
Creation_Time = 23-OCT-2013 13:19:25
Revision_Time = 24-JUN-2014 03:39:13
Current_Time = 24-JUN-2014 03:39:40

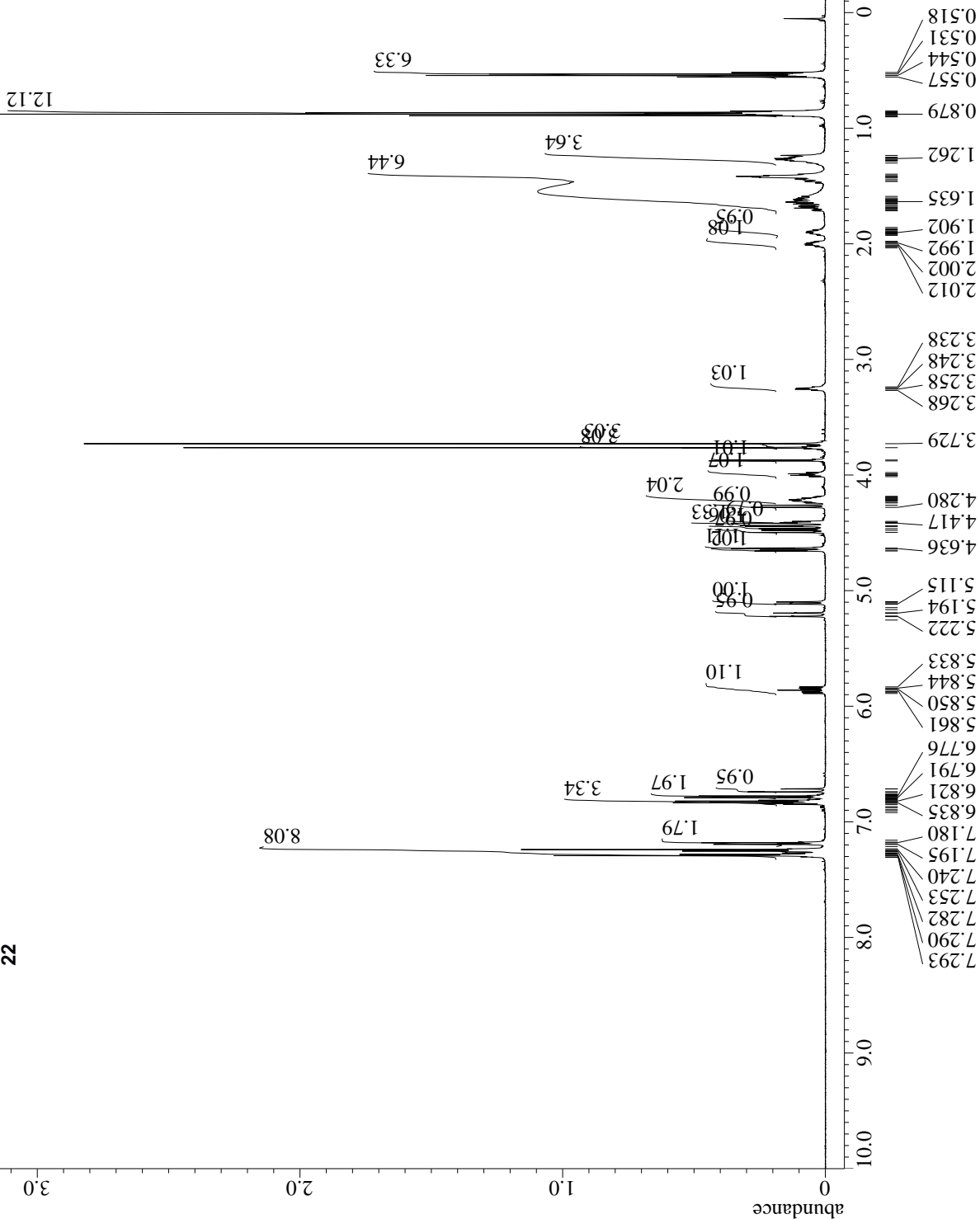
Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clipped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

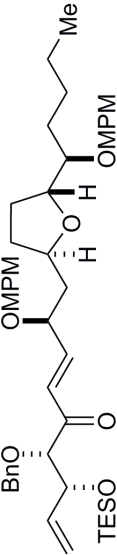
Relaxation_Delay = 2[s]
Recvr_Gain = 36
Temp_Get = 21[dc]
X_90_Width = 14.3[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Acn = 4[db]
X_Pulse = 7.15[us]
Irr_Mode = OFF
Tri_Mode = OFF
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```



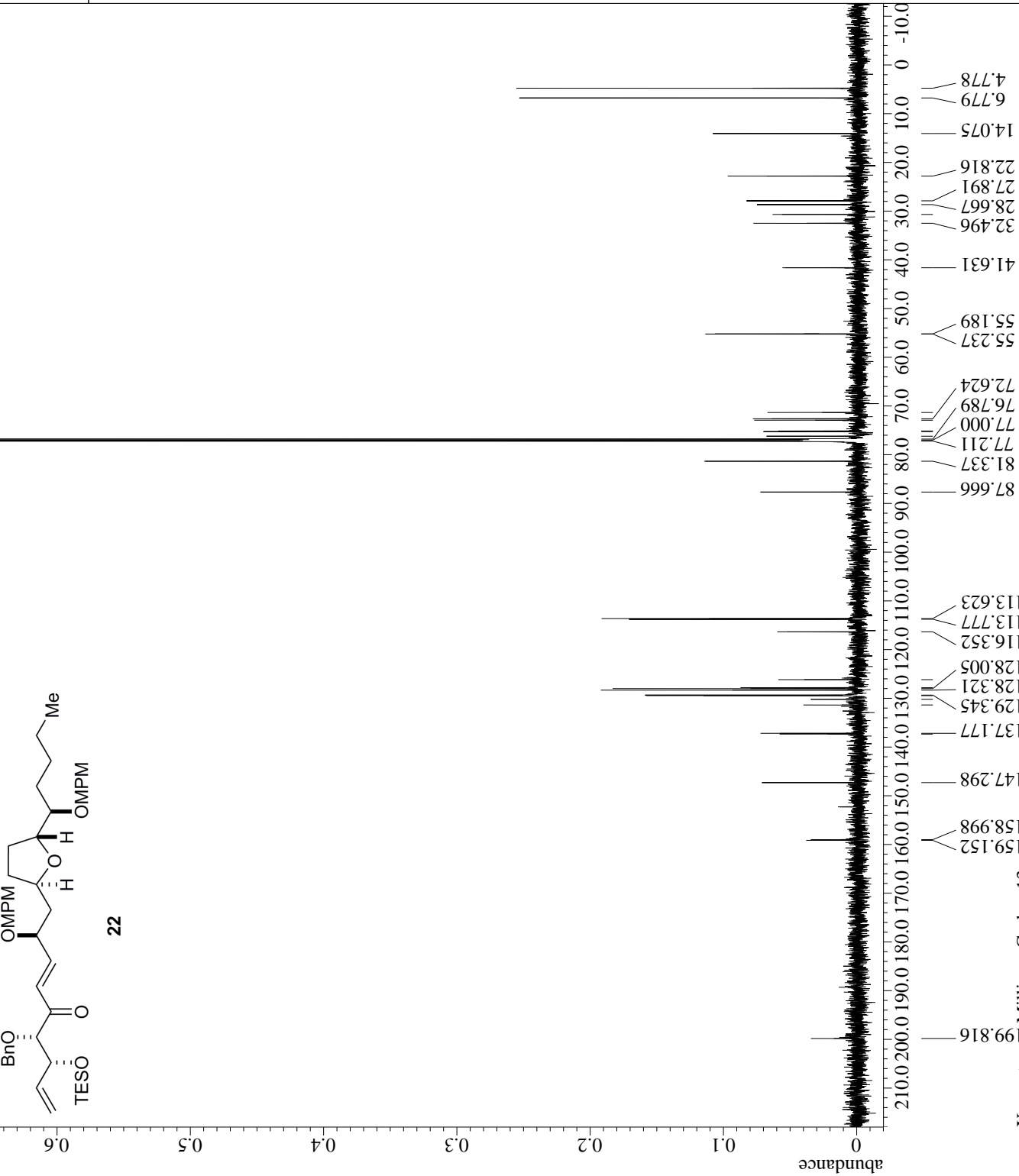
22



X : parts per Million : Proton



22



```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon_jxp
Sample_Id = YK-III-023
Solvent = CHLOROFORM-D
Creation_Time = 23-OCT-2013 13:22:10
Revision_Time = 24-JUN-2014 03:40:19
Current_Time = 24-JUN-2014 03:40:56

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 0.69206016[s]
X Domain = 13C
X Freq = 150.91343039[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 1.44496109[Hz]
X Sweep = 47.34848485[kHz]
X Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr Freq = 600.172304046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 428
Total_Scans = 428

Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 22.3[deg]
X 90_Width = 10[us]
X Acq_Time = 0.69206016[s]
X Angle = 30[deg]
X Atn = 8[db]
X Pulse = 3.33333333[us]
Irr_Atn_Dec = 18.24[db]
Irr_Atn_Noise = 18.24[db]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]

```



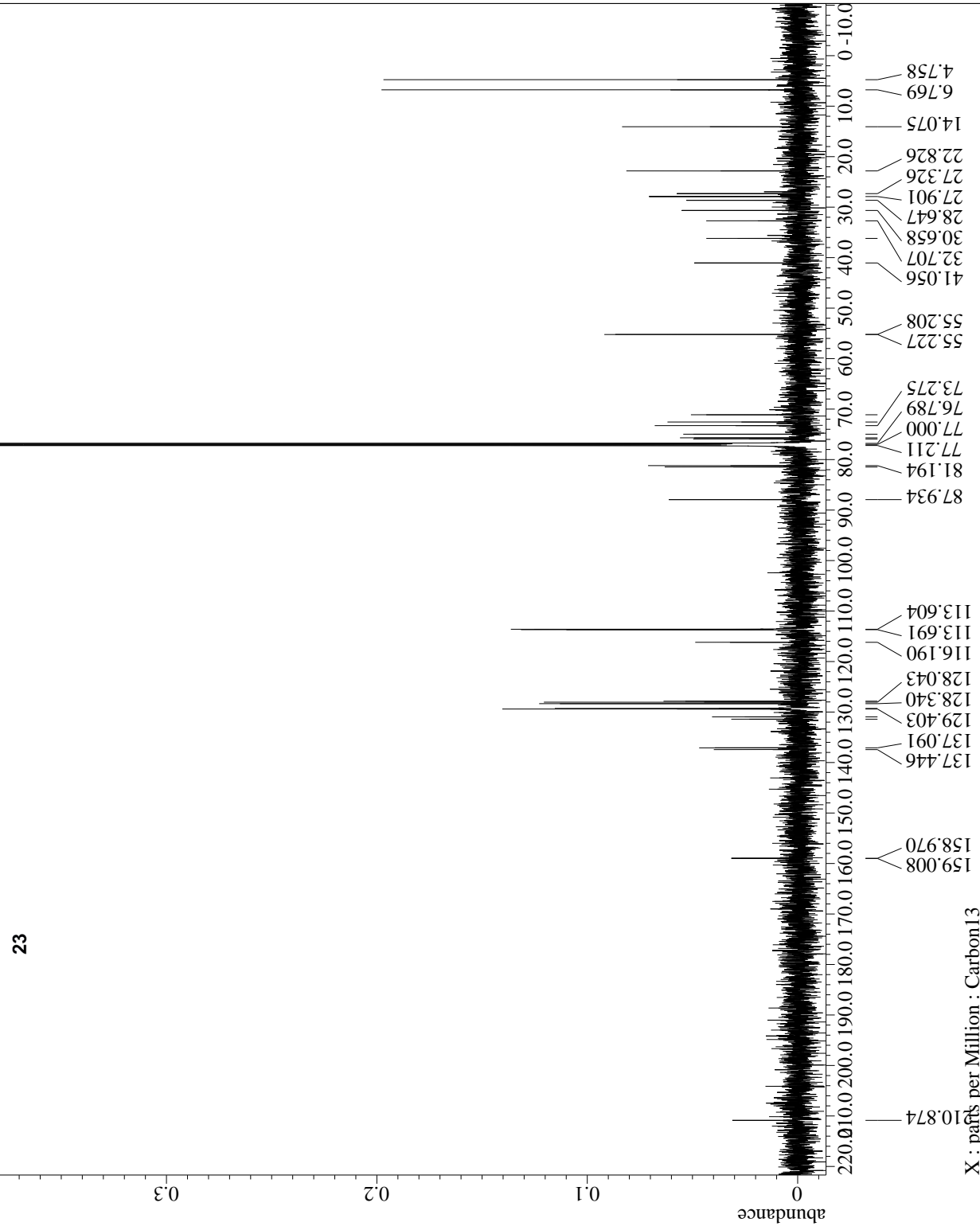
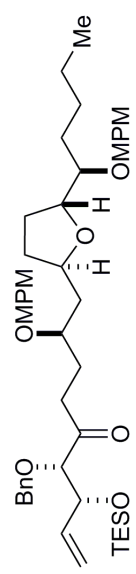

```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon_jxp
Sample_Id = YK-III-026
Solvent = CHLOROFORM-D
Creation_Time = 25-OCT-2013 15:25:49
Revision_Time = 24-JUN-2014 03:41:42
Current_Time = 24-JUN-2014 03:43:08

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

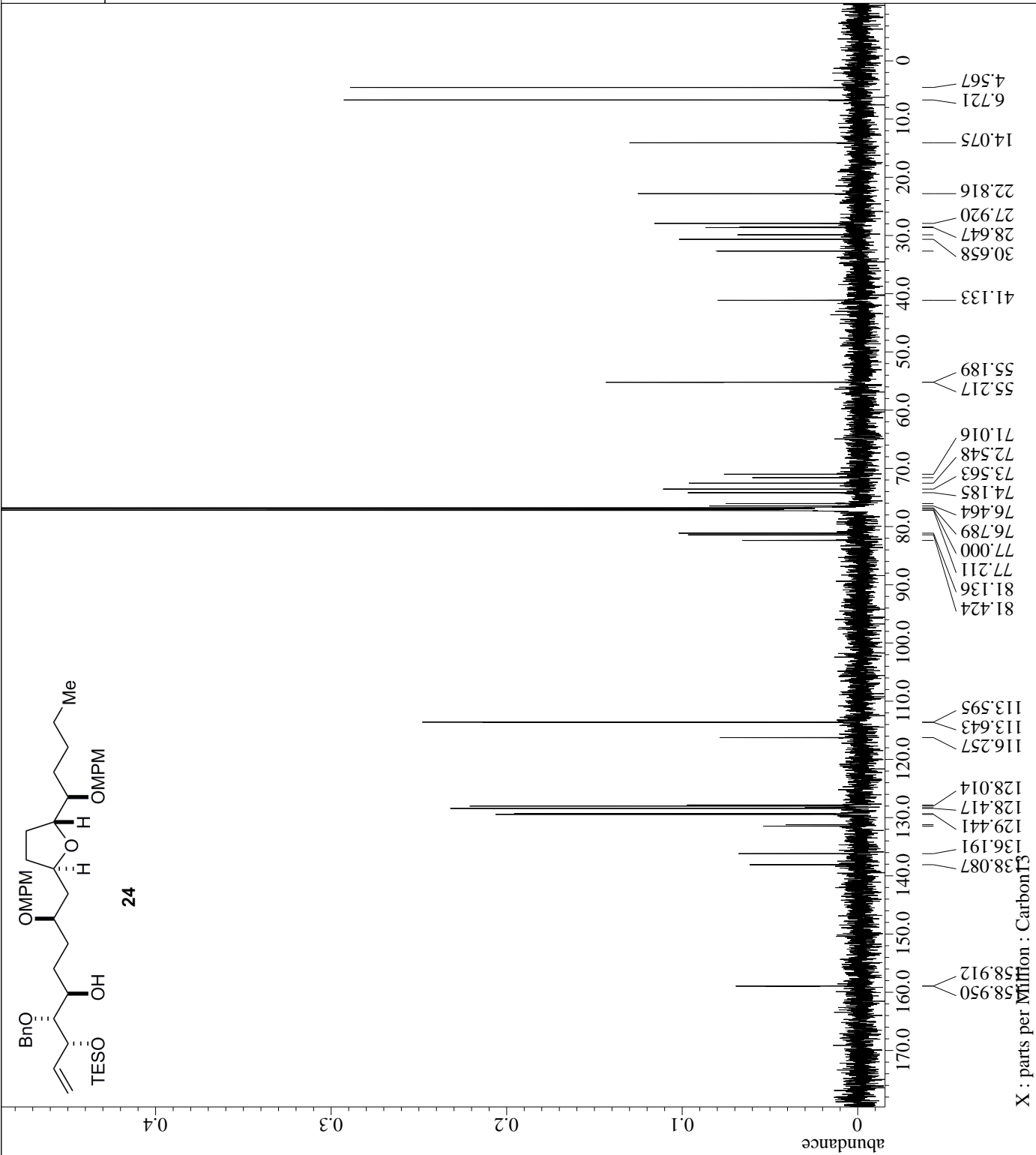
Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = 13C
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 288
Total_Scans = 288

Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 22.3[deg]
X_90_Width = 10[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 8[db]
X_Pulse = 3.33333333[us]
Irr_Atn_Dec = 18.24[db]
Irr_Atn_Noise = 18.24[db]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```





Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon_jxp
Sample_Id = YK-III-029
Solvent = CHLOROFORM-D
Creation_Time = 28-OCT-2013 15:45:40
Revision_Time = 24-JUN-2014 04:03:58
Current_Time = 24-JUN-2014 04:04:16
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 0.69206016[s]
X Domain = 13C
X Freq = 150.91343039[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 1.44496109[Hz]
X Sweep = 47.34848485[kHz]
X Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 257
Total_Scans = 257
Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 22.5[dc]
X_90_Width = 10[us]
X Acq_Time = 0.69206016[s]
X Angle = 30[deg]
X Atn = 8[db]
X Pulse = 3.33333333[us]
Irr_Atn_Dec = 18.24[db]
Irr_Atn_Noise = 18.24[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]



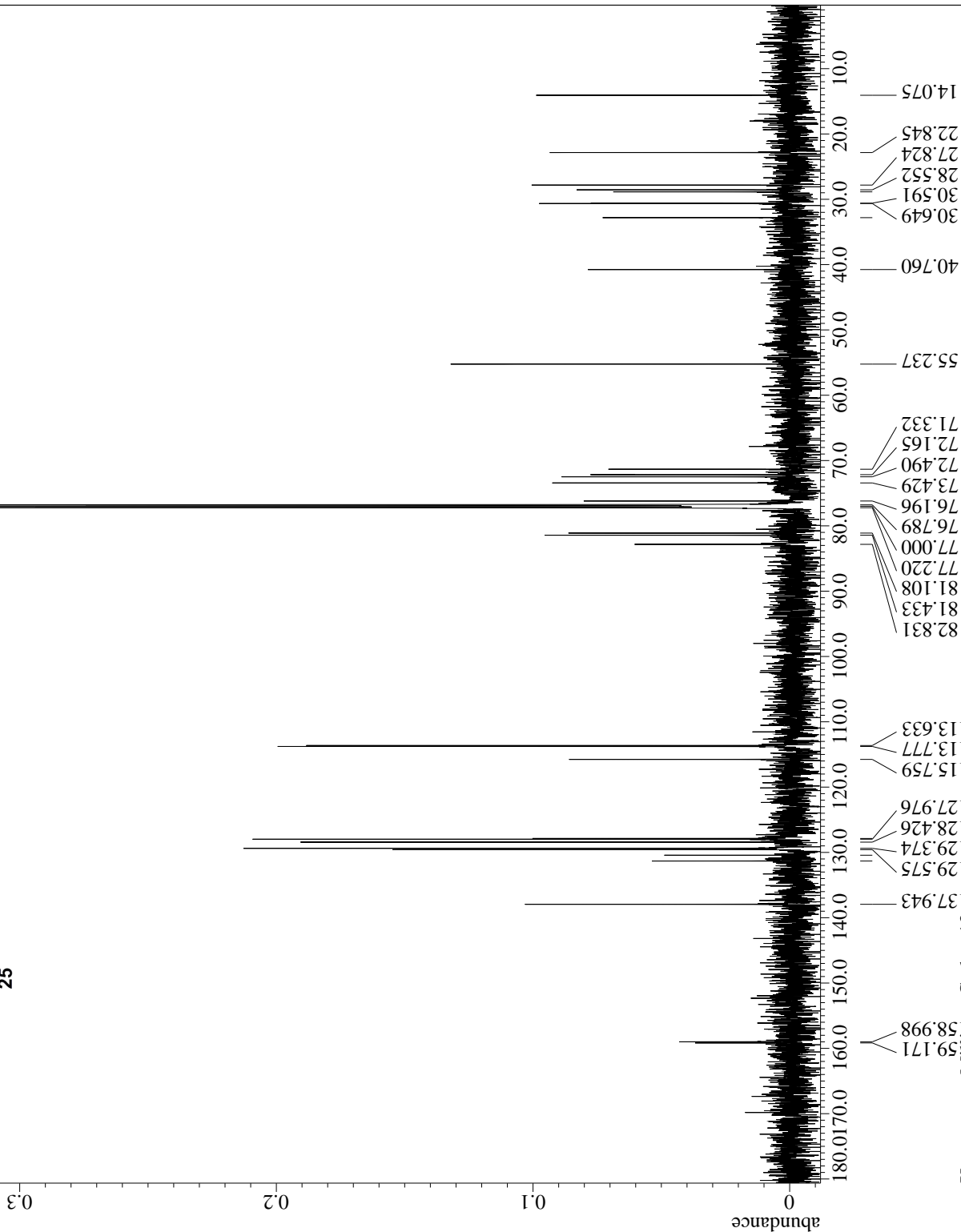
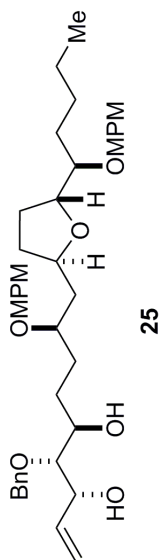

```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon_jxp
Sample_Id = YK-III-032
Solvent = CHLOROFORM-D
Creation_Time = 31-OCT-2013 10:31:50
Revision_Time = 24-JUN-2014 04:04:55
Current_Time = 24-JUN-2014 04:05:26

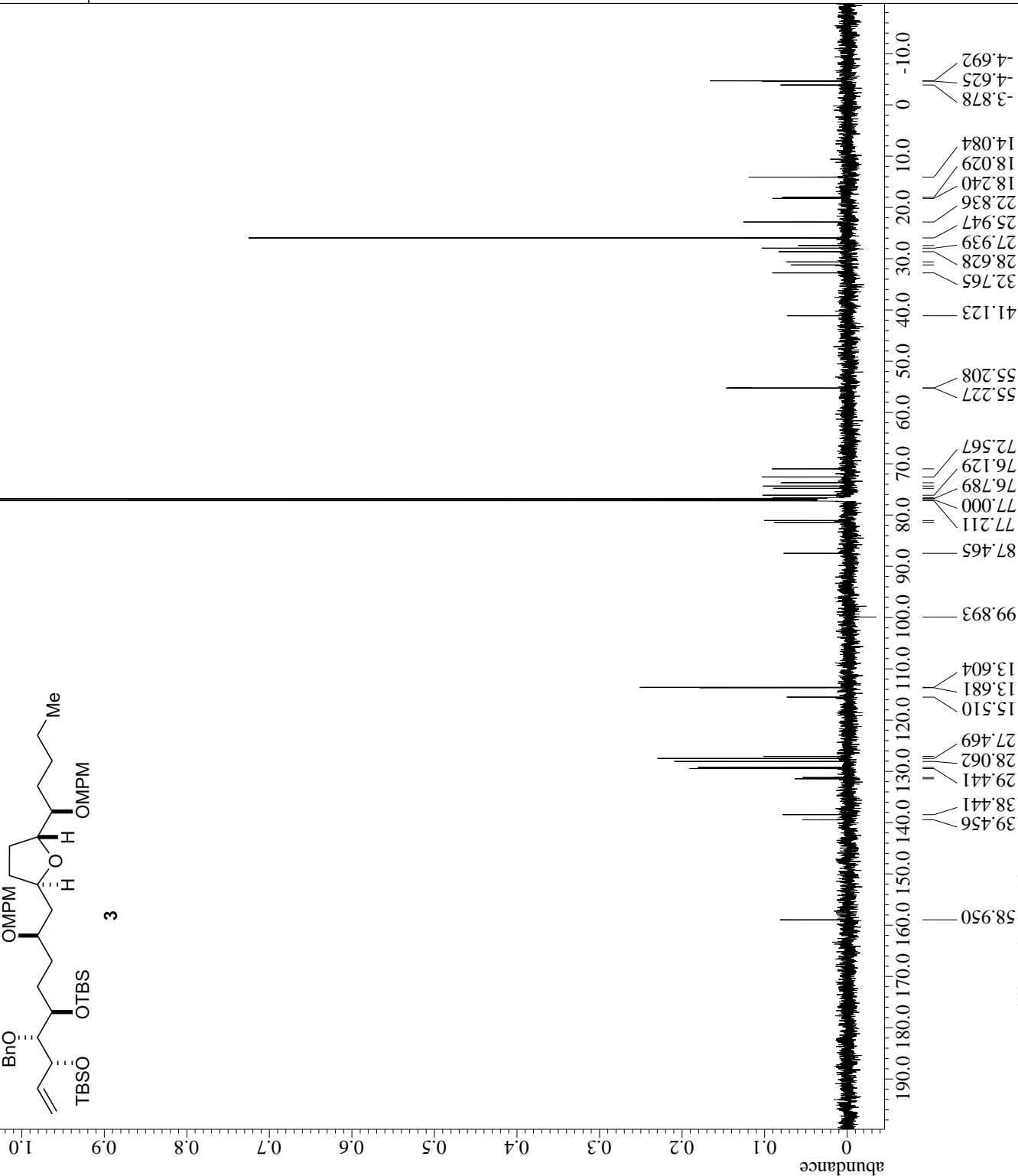
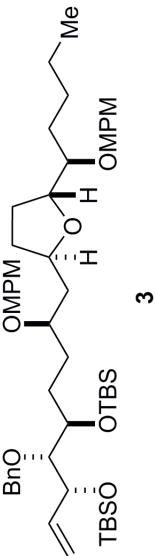
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = 13C
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 272
Total_Scans = 272

Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 22.4[dc]
X_90_Width = 10[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 8[db]
X_Pulse = 3.33333333[us]
Irr_Atn_Dec = 18.24[db]
Irr_Atn_Noise = 18.24[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```



X : parts per Million : Carbon13



Filename = /Users/skt_macbookpro/Desktop
 Author = delta
 Experiment = carbon_jxp
 Sample_Id = YK-III-033
 Solvent = CHLOROFORM-D
 Creation_Time = 31-OCT-2013 19:08:58
 Revision_Time = 23-JUN-2014 22:41:28
 Current_Time = 23-JUN-2014 22:44:43
 Comment = single pulse decoupled gat
 Data_Format = 1D COMPLEX
 Dim_Size = 26214
 Dim_Title = Carbon13
 Dim_Units = [ppm]
 Dimensions = X
 Site = ECA600
 Spectrometer = DELTA2_NMR
 Field_Strength = 14.09636928[T] (600[MHz])
 X Acq_Duration = 0.69206016[s]
 X Domain = 13C
 X Freq = 150.91343039[MHz]
 X Offset = 100[ppm]
 X Points = 32768
 X Prescans = 4
 X Resolution = 1.44496109[Hz]
 X Sweep = 47.34848485[kHz]
 X Sweep_Clippped = 37.87878788[kHz]
 Irr_Domain = Proton
 Irr_Freq = 600.1723046[MHz]
 Irr_Offset = 5[ppm]
 Clipped = TRUE
 Scans = 200
 Total_Scans = 200
 Relaxation_Delay = 2[s]
 Recvr_Gain = 54
 Temp_Get = 22.4[dc]
 X_90_Width = 10[us]
 X Acq_Time = 0.69206016[s]
 X Angle = 30[deg]
 X Atn = 8[db]
 X Pulse = 3.33333333[us]
 Irr_Atn_Dec = 18.24[db]
 Irr_Atn_Noise = 18.24[db]
 Irr_Noise = WALTZ
 Irr_Width = 76[us]
 Decoupling = TRUE
 Initial_Wait = 1[s]
 Noe = TRUE
 Noe_Time = 2[s]
 Repetition_Time = 2.69206016[s]

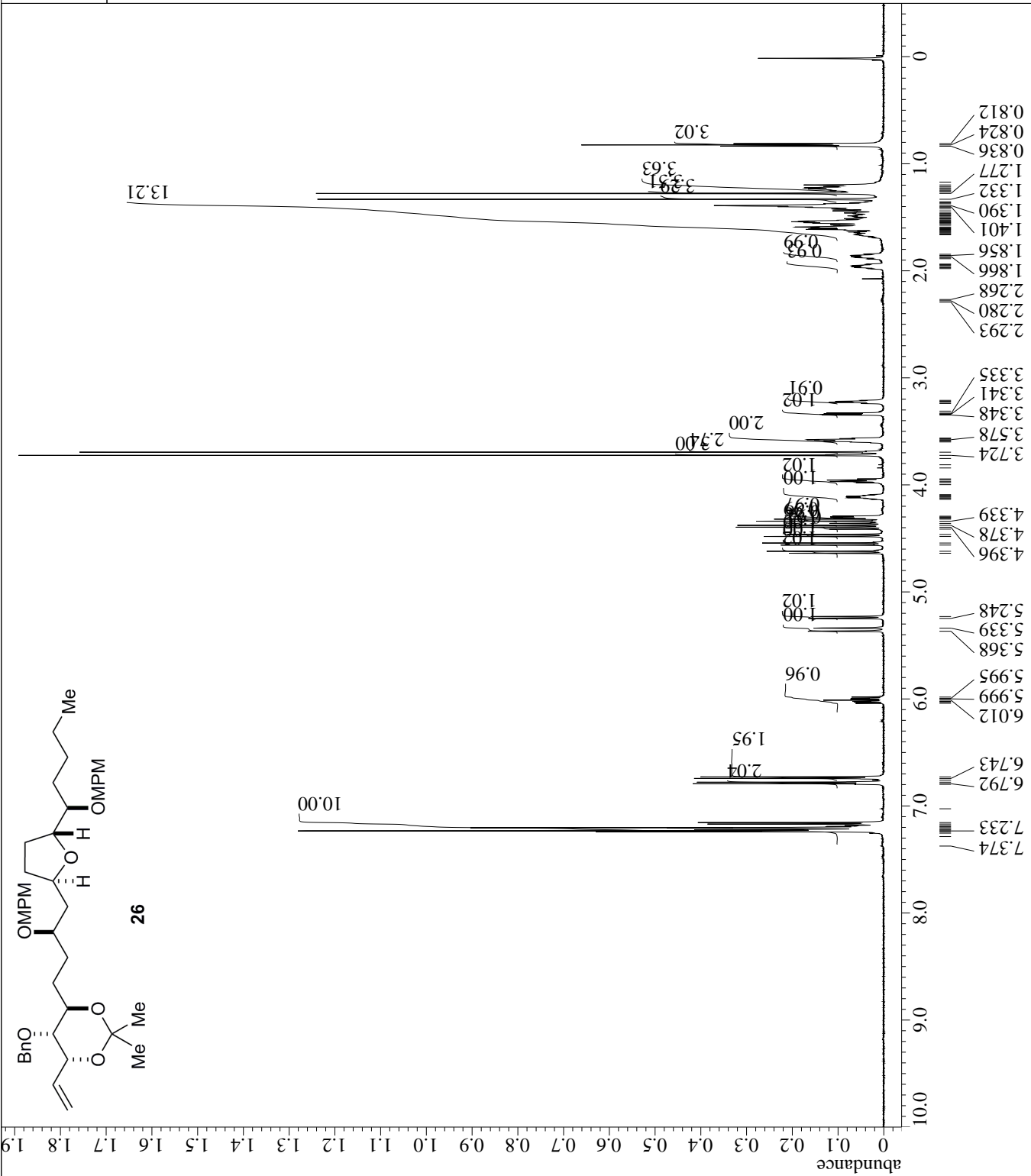
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = Proton_jmp
Sample_Id = YK-III-045
Solvent = CHLOROFORM-D
Creation_Time = 12-NOV-2013 17:10:46
Revision_Time = 24-JUN-2014 04:12:58
Current_Time = 24-JUN-2014 04:14:10

Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 38
Temp_Get = 21.1[degC]
X_90_Width = 14.3[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Acn = 4[deg]
X_Pulse = 7.15[us]
Irr_Mode = OFF
Tri_Mode = OFF
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```



X : parts per Million : Proton

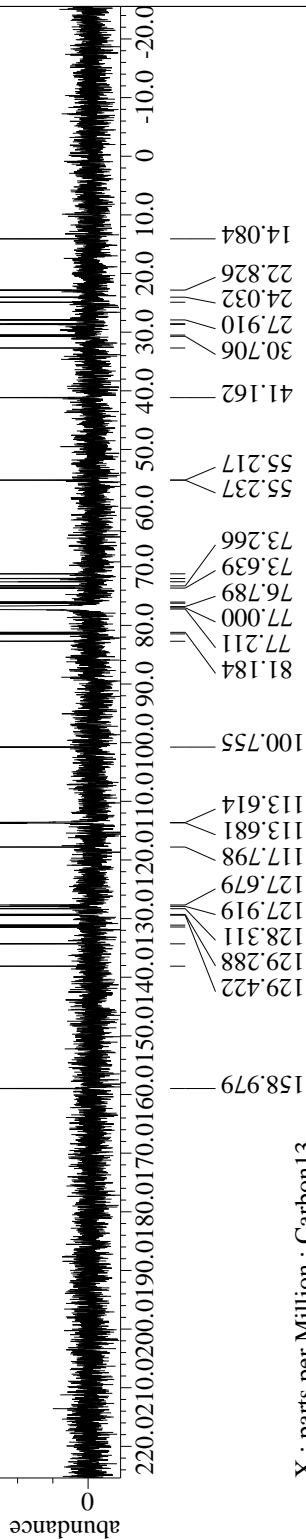
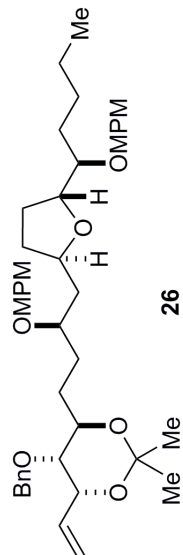
```

Filename = /Users/skt_macbookpro/Desktop
Author = delta
Experiment = carbon_jxp
Sample_Id = YK-III-045
Solvent = CHLOROFORM-D
Creation_Time = 12-NOV-2013 17:21:43
Revision_Time = 24-JUN-2014 04:07:13
Current_Time = 24-JUN-2014 04:07:38

Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X Acq_Duration = 0.69206016[s]
X Domain = 13C
X Freq = 150.91343039[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 1.44496109[Hz]
X Sweep = 47.34848485[kHz]
X Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 800
Total_Scans = 800

Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 22.1[dc]
X_90_Width = 10[us]
X Acq_Time = 0.69206016[s]
X Angle = 30[deg]
X Atn = 8[db]
X Pulse = 3.33333333[us]
Irr_Atn_Dec = 18.24[db]
Irr_Atn_Noise = 18.24[db]
Irr_Noise = WALTZ
Irr_Width = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```



X : parts per Million : Carbon13

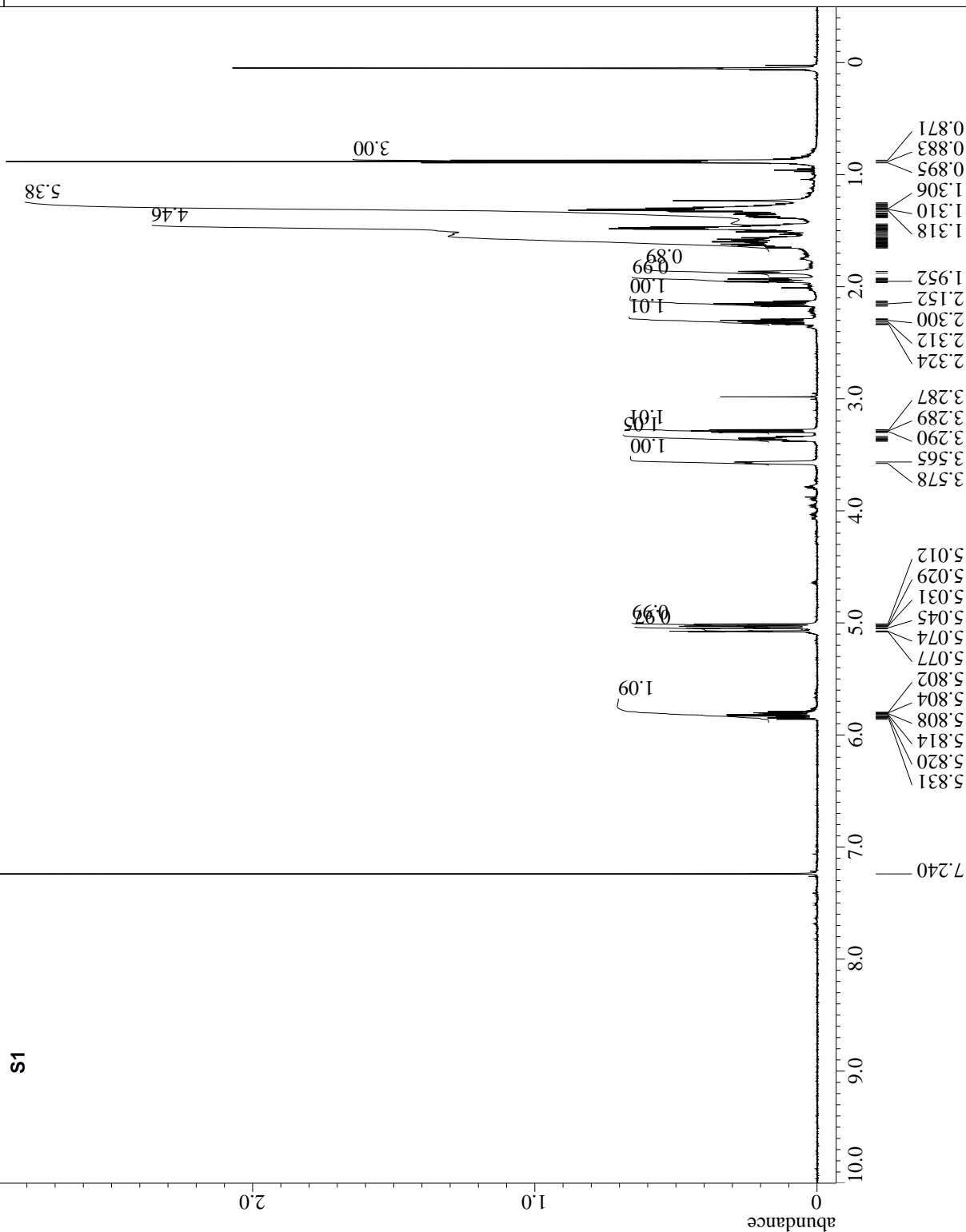
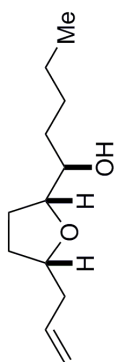
```

Filename = /Volumes/YUHKI_USB/kawashi
Author = delta
Experiment = Proton_jxp
Sample_Id = YK-II-117b
Solvent = CHLOROFORM-D
Creation_Time = 25-JUN-2013 20:50:33
Revision_Time = 25-JUN-2014 22:43:29
Current_Time = 25-JUN-2014 22:43:44

Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Phases = 32768
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 15.02403846[kHz]
X_Sweep_Clippped = 12.01923077[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 2[s]
Recvr_Gain = 44
Temp_Get = 21.6[degC]
X_90_Width = 11.6[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Acn = 3[db]
X_Pulse = 5.8[us]
Irr_Mode = OFF
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.18103808[s]
  
```



X : parts per Million : Proton

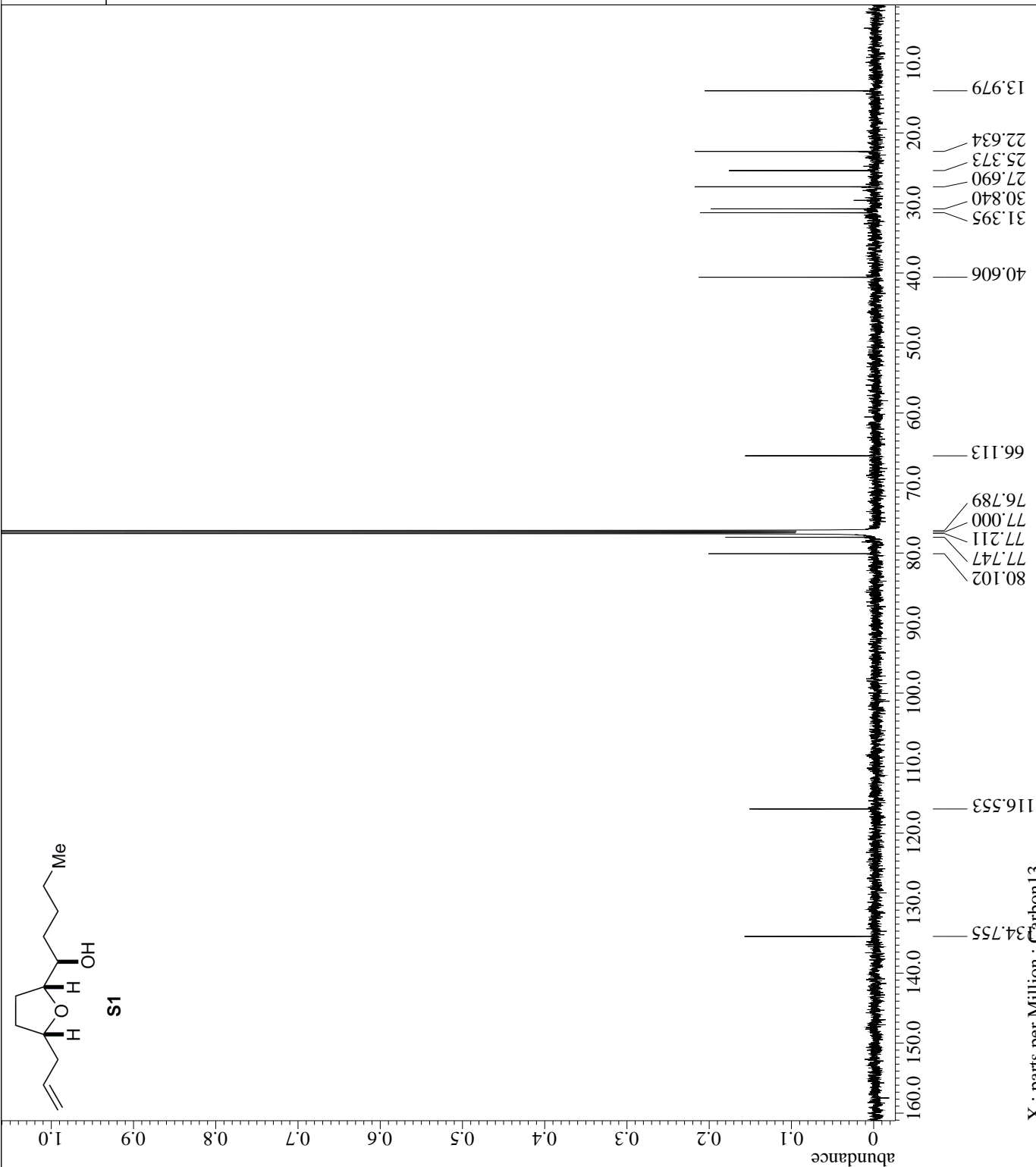
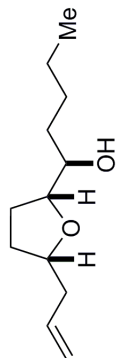
```

Filename = /Volumes/YUHKI_USB/kawashi
Author = delta
Experiment = carbon_jxp
Sample_Id = YK-II-117b
Solvent = CHLOROFORM-D
Creation_Time = 26-JUN-2013 21:12:10
Revision_Time = 25-JUN-2014 22:44:48
Current_Time = 25-JUN-2014 22:45:37

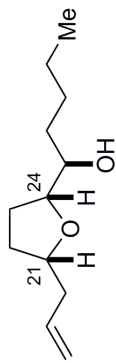
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = 13C
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clippped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.17230406[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 528
Total_Scans = 528

Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.3[dc]
X_90_Width = 9.25[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 8[db]
X_Pulse = 3.08333333[us]
Irr_Atn_Dec = 19.327[db]
Irr_Atn_Noise = 19.327[db]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69206016[s]
  
```



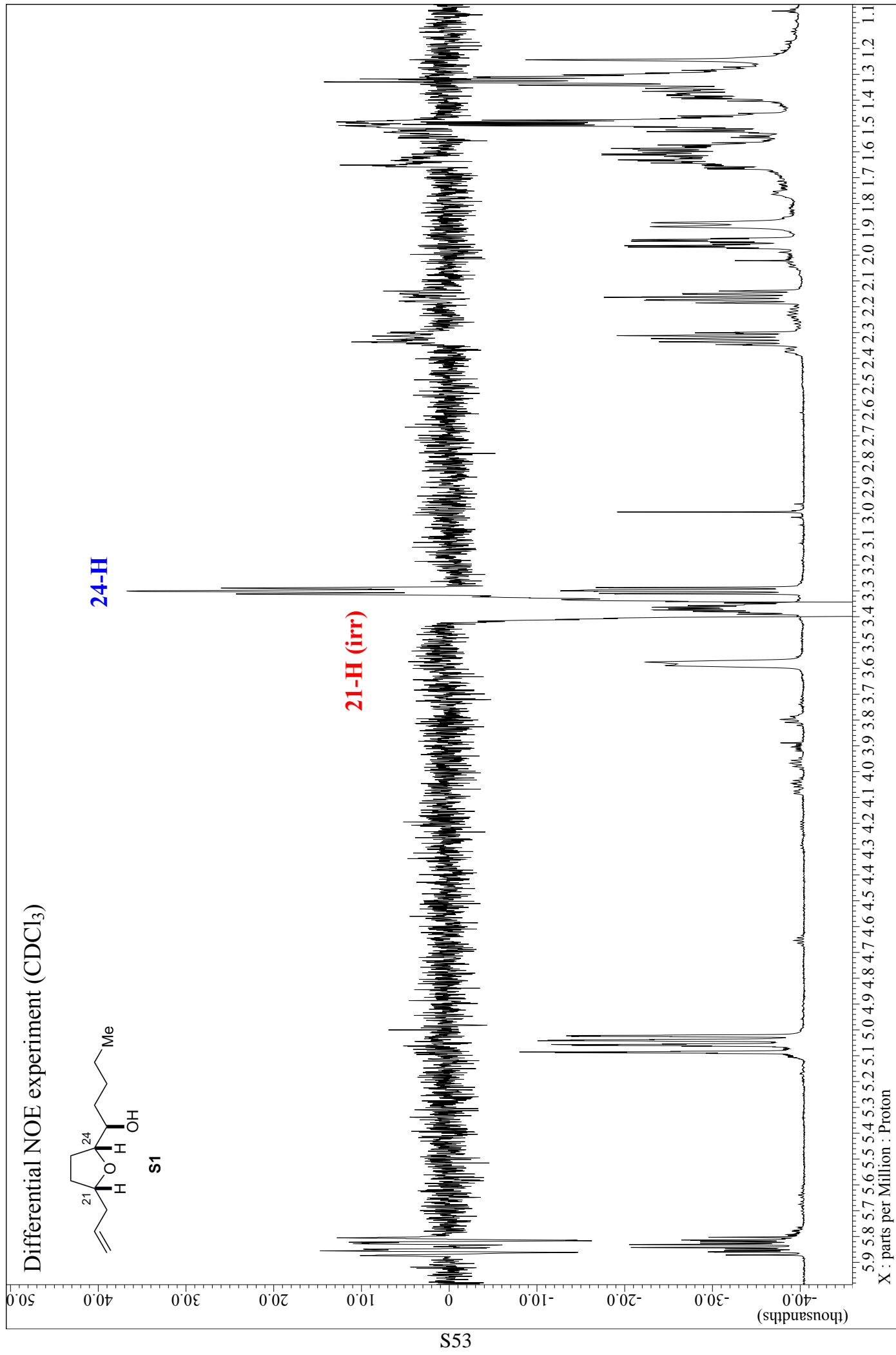
Differential NOE experiment (CDCl₃)



S1

24-H

21-H (irr)



5.9 5.8 5.7 5.6 5.5 5.4 5.3 5.2 5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1

X : parts per Million : Proton