

**Supplementary information for**

Ln(OTf)<sub>3</sub>-Catalyzed Highly Regioselective Alcoholysis of 2,3-Epoxy Alcohols

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<sup>1</sup> H-NMR, <sup>13</sup> C-NMR spectra of the catalyst screening	S2
<sup>1</sup> H-NMR, <sup>13</sup> C-NMR spectra of the application to synthesis	S7



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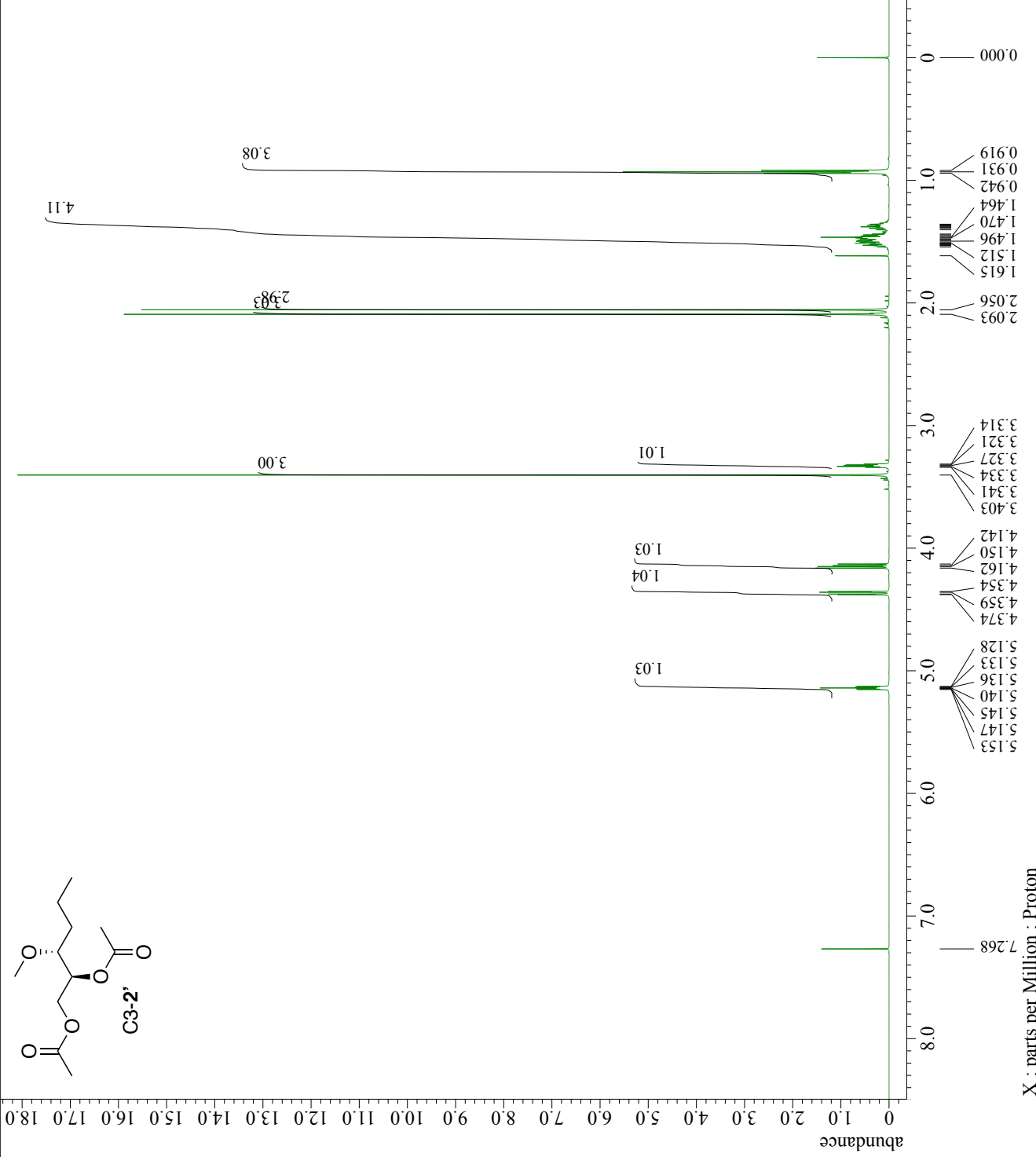
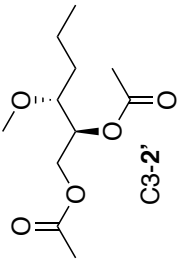
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Author = delta
Experiment = proton_jxp
Sample_id = DN-methanalysis
Solvent = CHLOROFORM-D
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Revision_Time = 25-JAN-2017 10:53:10

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Spectrometer = DELTA2_NMR

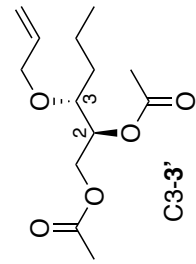
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X_Prescans = 1
X_Resolution = 0.6836375 [Hz]
X_Sweep = 11.20071685 [kHz]
X_Sweep_Clippped = 8.96057348 [kHz]
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Irr_Freq = 597.17144293 [MHz]
Irr_Offset = 5 [ppm]
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Tri_Freq = 597.17144293 [MHz]
Tri_Offset = 5 [ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16

Relaxation_Delay = 5 [s]
Recvr_Gain = 34
Temp_Get = 24.1 [dC]
X_90_Width = 7.15 [us]
X_Acq_Time = 1.46276352 [s]
X_Angle = 45 [deg]
X_Atn = 2.8 [dB]
X_Pulse = 3.575 [us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Preset = FALSE
Initial_Wait = 1 [s]
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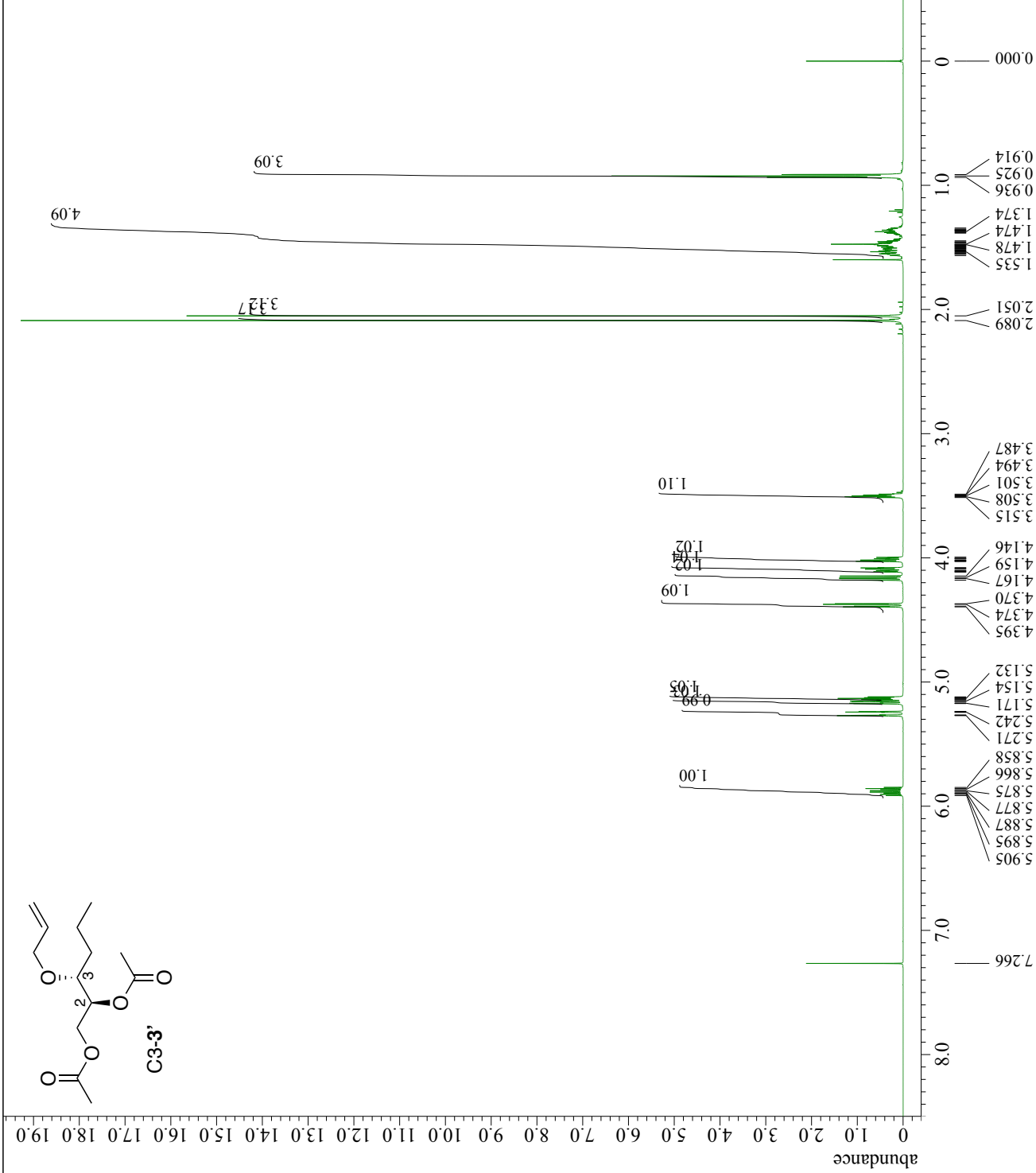
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X : parts per Million : Proton



C3-3'



X : parts per Million : Proton



Filename = DN-0299-Allyl\_proton-1-an  
 Author = delta  
 Experiment = proton.jxp  
 Sample\_Id = DN-0299-Allyl  
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 Revision\_Time = 25-JAN-2017 11:27:31  
 Comment = single\_pulse  
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 Dim\_Title = Proton  
 Dim\_Units = [ppm]  
 Dimensions = X  
 Site = JNM-ECA600  
 Spectrometer = DELTA2\_NMR  
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 X\_Acq\_Duration = 1.46276352[s]  
 X\_Domain = 1H  
 X\_Freq = 597.17144293[MHz]  
 X\_Offset = 5[ppm]  
 X\_Points = 16384  
 X\_prescans = 1  
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 X\_Sweep = 11.20071685[kHz]  
 X\_Sweep\_Clippped = 8.96057348[kHz]  
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 Irr\_Freq = 597.17144293[MHz]  
 Irr\_Offset = 5[ppm]  
 Tri\_Domain = Proton  
 Tri\_Freq = 597.17144293[MHz]  
 Tri\_Offset = 5[ppm]  
 Clipped = FALSE  
 Scans = 16  
 Total\_Scans = 16  
 Relaxation\_Delay = 5[s]  
 Recvr\_Gain = 36  
 Temp\_Get = 24.2[dC]  
 X\_90\_Width = 7.15[us]  
 X\_Acq\_Time = 1.46276352[s]  
 X\_Angle = 45[deg]  
 X\_Atn = 2.8[dB]  
 X\_Pulse = 3.575[us]  
 Irr\_Mode = Off  
 Tri\_Mode = Off  
 Dante\_Preset = FALSE  
 Initial\_Wait = 1[s]  
 Repetition\_Time = 6.46276352[s]



```

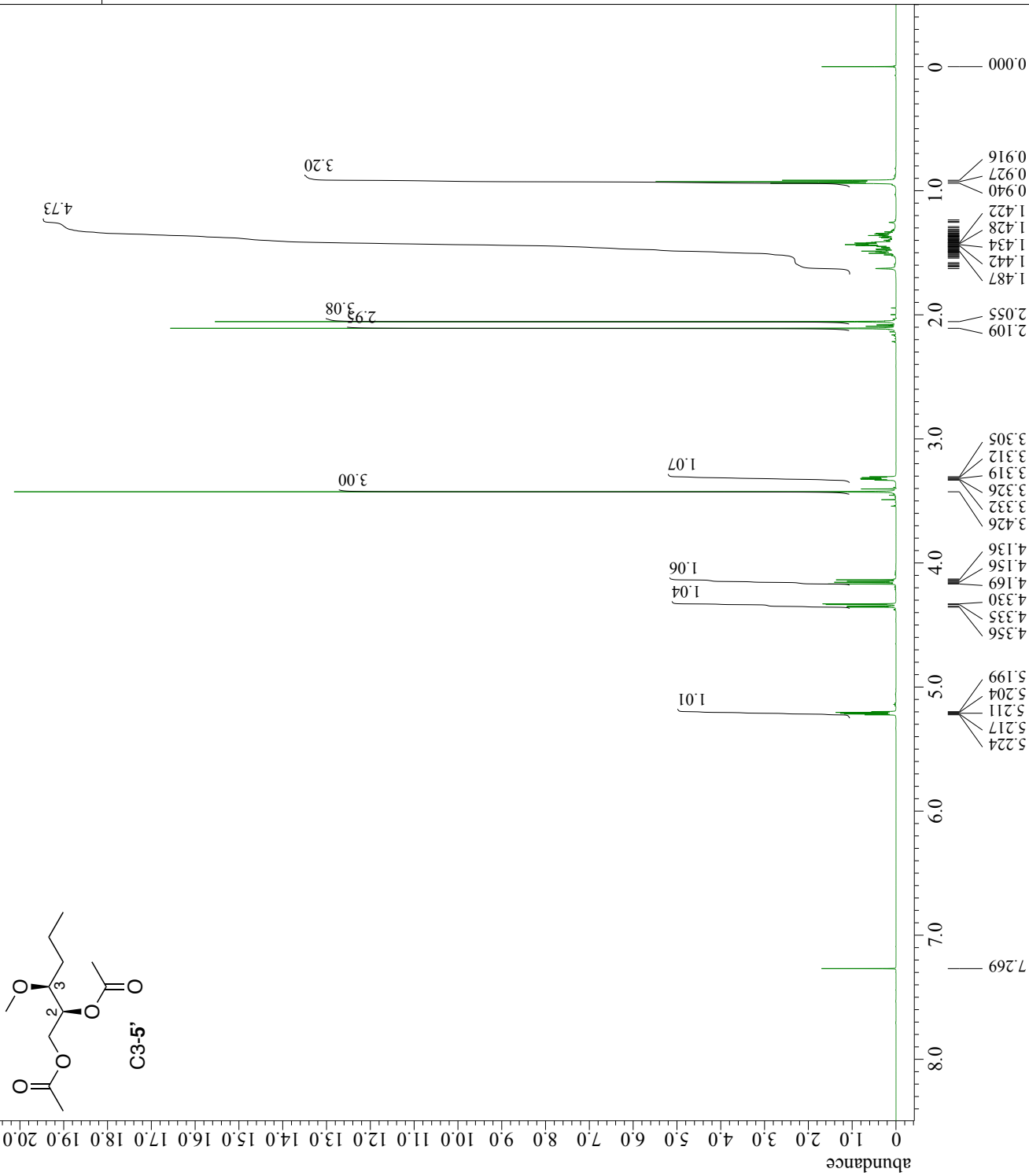
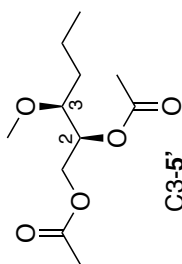
Filename = DN-0440-cis-Me-major_anal
Author = delta
Experiment = proton.jpg
Sample_Id = DN-0440-cis-Me-major
Solvent = CHLOROFORM-D
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Revision_Time = 6-NOV-2018 10:28:40

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Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR

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X_Freq = 597.17144293 [MHz]
X_Offset = 5 [ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.6836375 [Hz]
X_Sweep = 11.20071685 [kHz]
X_Sweep_Clippped = 8.96057348 [kHz]
Irr_Domain = Proton
Irr_Freq = 597.17144293 [MHz]
Irr_Offset = 5 [ppm]
Tri_Domain = Proton
Tri_Freq = 597.17144293 [MHz]
Tri_Offset = 5 [ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16

Relaxation_Delay = 5 [s]
Recvr_Gain = 34
Temp_Get = 24.1 [dC]
X_90_Width = 7.15 [us]
X_Acq_Time = 1.46276352 [s]
X_Angle = 45 [deg]
X_Atn = 2.8 [dB]
X_Pulse = 3.575 [us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1 [s]
Repetition_Time = 6.46276352 [s]

```

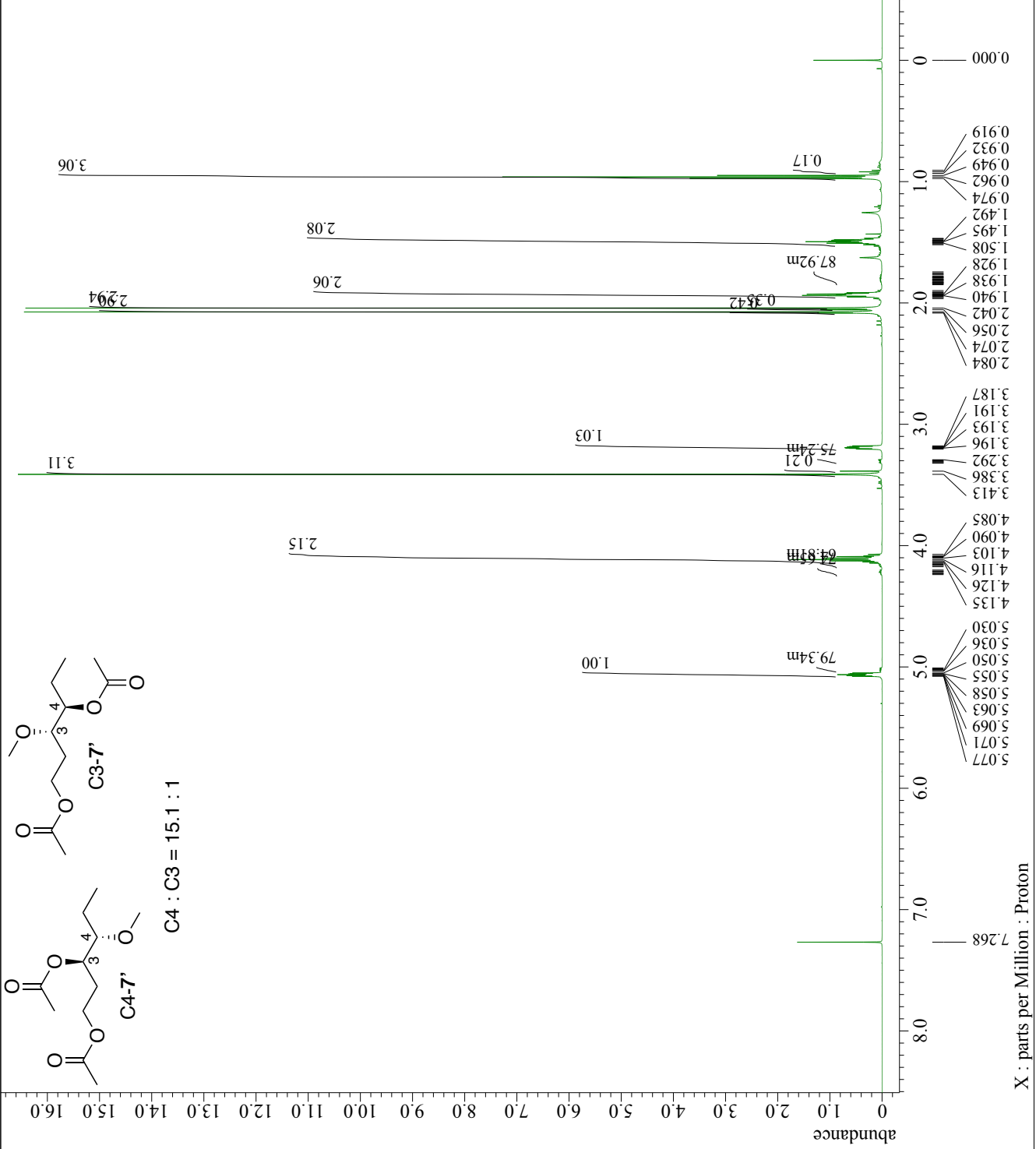




Filename = DN-0277-34Met-fast5\_proto  
 Author = delta  
 Experiment = proton.jxp  
 Sample Id = DN-0277-34Met-fast5  
 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 26-JAN-2017 10:22:01  
 Revision\_Time = 26-JAN-2017 13:52:33

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 Site = JNM-ECA600  
 Spectrometer = DELTA2\_NMR

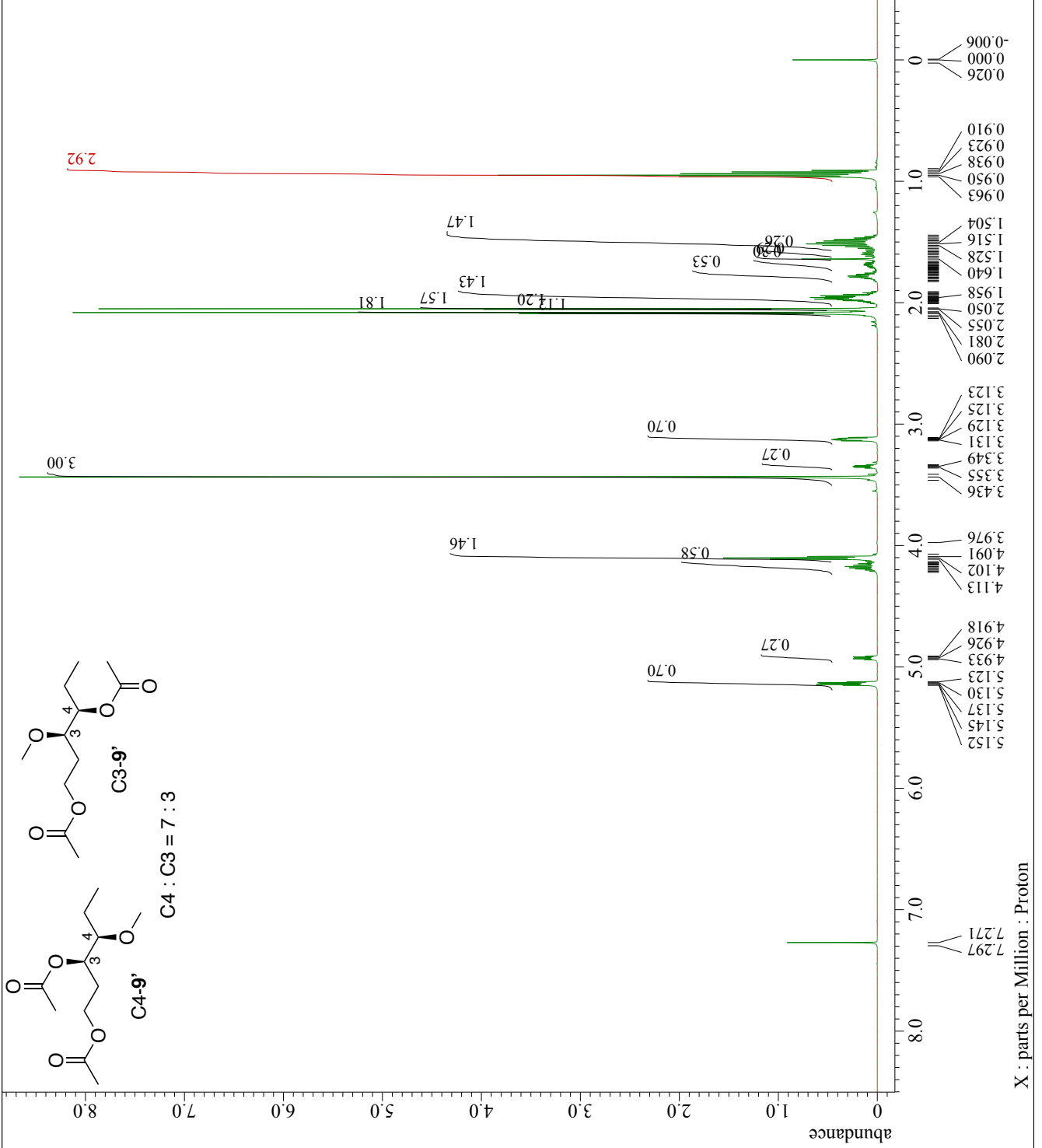
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 X\_Freq = 597.17144293 [MHz]  
 X\_Offset = 5 [ppm]  
 X\_Points = 16384  
 X\_Prescans = 1  
 X\_Resolution = 0.6836375 [Hz]  
 X\_Sweep = 11.20071685 [kHz]  
 X\_Sweep\_Clippped = 8.96057348 [kHz]  
 Irr\_Domain = Proton  
 Irr\_Freq = 597.17144293 [MHz]  
 Irr\_Offset = 5 [ppm]  
 Tri\_Domain = Proton  
 Tri\_Freq = 597.17144293 [MHz]  
 Tri\_Offset = 5 [ppm]  
 Clipped = FALSE  
 Scans = 16  
 Total\_Scans = 16  
 Relaxation\_Delay = 5 [s]  
 Recvr\_Gain = 36  
 Temp\_Get = 24.3 [dC]  
 X\_90\_Width = 7.15 [us]  
 X\_Acq\_Time = 1.46276352 [s]  
 X\_Angle = 45 [deg]  
 X\_Atn = 2.8 [dB]  
 X\_Pulse = 3.575 [us]  
 Irr\_Mode = Off  
 Tri\_Mode = Off  
 Dante\_Preset = FALSE  
 Initial\_Wait = 1 [s]  
 Repetition\_Time = 6.46276352 [s]



X : parts per Million : Proton



Filename = DN-0681-0690-cis34epo-me-  
Author = delta  
Experiment = proton.jkp  
Sample Id = DN-0681-0690-cis34epo-me-  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 31-OCT-2017 10:16:52  
Revision\_Time = 28-FEB-2019 22:31:36  
Comment = single pulse  
Data\_Format = 1D\_REAL  
Dim\_Size = 13107  
X\_Domain = Proton  
Dim\_Title = Proton  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECA600  
Spectrometer = DELTA2\_NMR  
Field\_Strength = 14.02588743[T] (600 [MHz])  
X\_Acq\_Duration = 1.46276352[s]  
X\_Domain = 1H  
X\_Freq = 597.17144293 [MHz]  
X\_Offset = 5 [ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.6836375 [Hz]  
X\_Sweep = 11.20071685 [kHz]  
X\_Sweep\_Clippped = 8.96057348 [kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 597.17144293 [MHz]  
Irr\_Offset = 5 [ppm]  
Tri\_Domain = Proton  
Tri\_Freq = 597.17144293 [MHz]  
Tri\_Offset = 5 [ppm]  
Clipped = FALSE  
Scans = 16  
Total\_Scans = 16  
Relaxation\_Delay = 5 [s]  
Recvr\_Gain = 34  
Temp\_Get = 24.3 [dC]  
X\_90\_Width = 7.15 [us]  
X\_Acq\_Time = 1.46276352 [s]  
X\_Angle = 45 [deg]  
X\_Atn = 2.8 [dB]  
X\_Pulse = 3.575 [us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Preset = FALSE  
Initial\_Wait = 1 [s]  
Repetition\_Time = 6.46276352 [s]





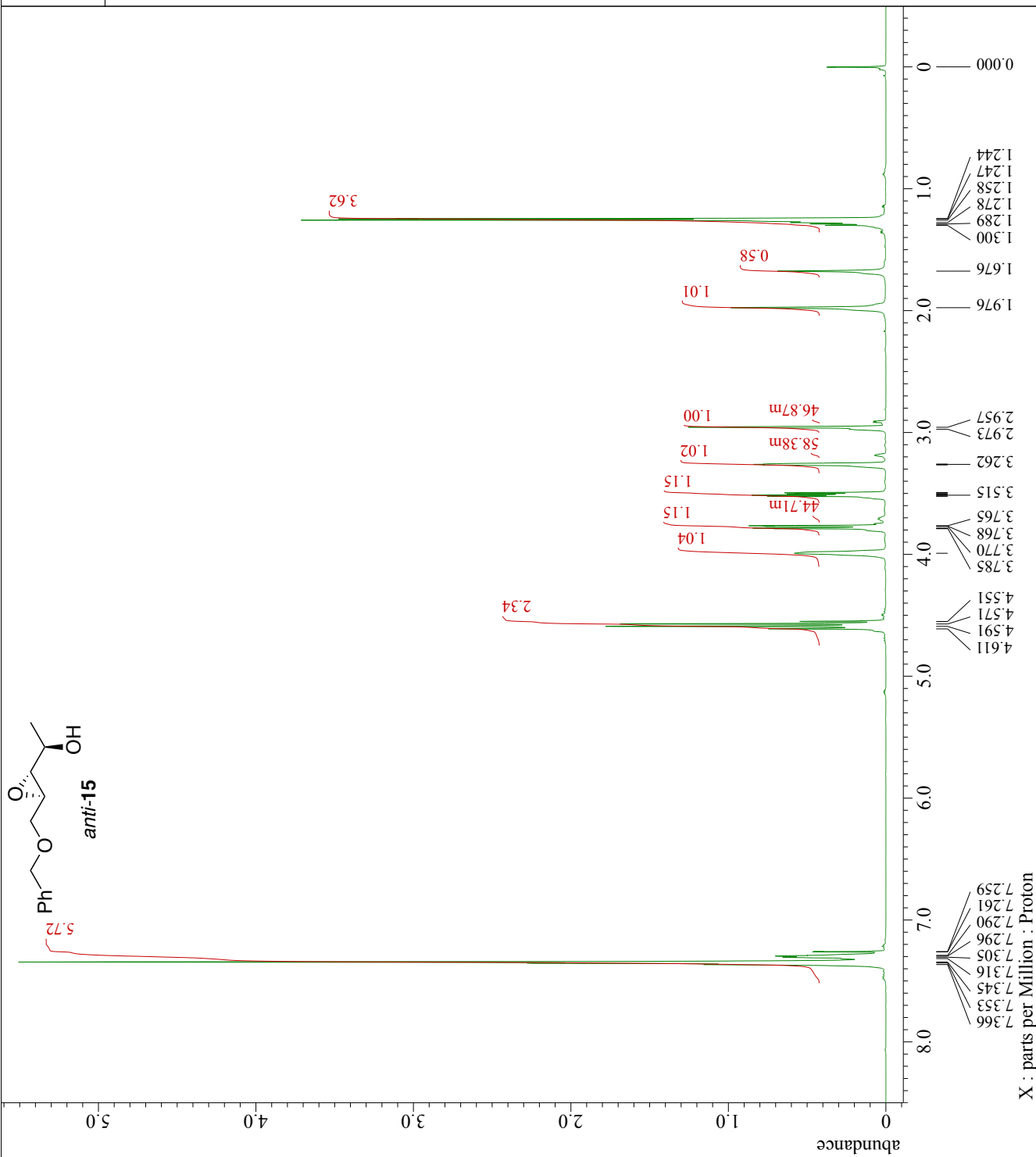
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Filename = DN-1070-epodownanti-ptlc
Author = delta
Experiment = proton.jxp
Sample_Id = DN-1070-epodownanti-ptlc
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-OCT-2018 19:33:50
Revision_Time = 25-OCT-2018 09:39:57

Comment = single_pulse
Date_Format = ID REAL
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.02588743[T] (600 [MHz])
X_Acq_Duration = 1.46276352[s]
X_Domain = 1H
X_Freq = 597.17144293 [MHz]
X_Offset = 5 [ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.6836375 [Hz]
X_Sweep = 11.20071685 [kHz]
X_Sweep_Clippped = 8.96057348 [kHz]
Irr_Domain = Proton
Irr_Freq = 597.17144293 [MHz]
Irr_Offset = 5 [ppm]
Tri_Domain = Proton
Tri_Freq = 597.17144293 [MHz]
Tri_Offset = 5 [ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16

Relaxation_Delay = 5[s]
Recvr Gain = 36
Temp Get = 24.4 [dC]
X_90_Width = 7.15 [us]
X_Acq_Time = 1.46276352 [s]
X_Angle = 45 [deg]
X_Atn = 2.8 [dB]
X_Pulse = 3.575 [us]
Irr_Mode = Off
Dante_Presat = FALSE
Initial Wait = 1[s]
Repetition_Time = 6.46276352 [s]
  
```



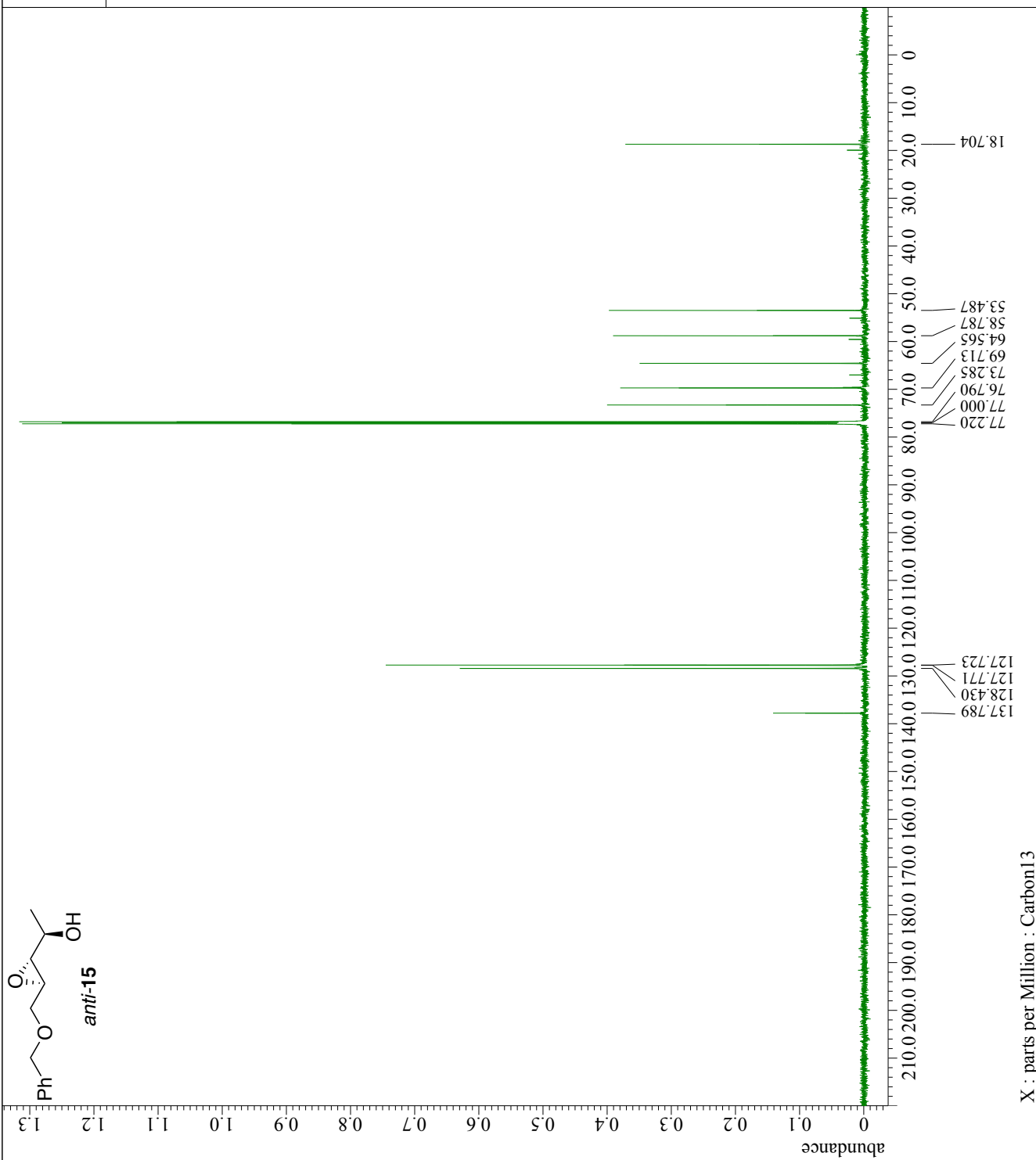


Filename = DN-1070-epodownanti-ptlc-  
Author = delta  
Experiment = carbon\_jxp  
Sample\_Id = DN-1070-epodownanti-ptlc  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 19-OCT-2018 19:38:14  
Revision\_Time = 25-OCT-2018 09:45:06

Comment = single pulse decoupled ga  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
X\_Domain = Carbon  
Dim\_Title = Carbon13  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECA600  
Spectrometer = DELTA2\_NMR

Field Strength = 14.02588743[T] (600[MHz])  
X\_Acq\_Duration = 0.69730304[s]  
X\_Domain = 13C  
X\_Freq = 150.1588632[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 1.43409672[Hz]  
X\_Sweep = 46.9924812[kHz]  
X\_Sweep\_Clipped = 37.59398496[kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 597.17144293[MHz]  
Irr\_Offset = 5[ppm]  
Clipped = TRUE  
Scans = 1024  
Total\_Scans = 1024

Relaxation\_Delay = 2[s]  
Recvr Gain = 58  
Temp\_Get = 24.5[dc]  
X\_90\_Width = 11.6[us]  
X\_Acq\_Time = 0.69730304[s]  
X\_Angle = 30[deg]  
X\_Atn = 8[db]  
X\_Pulse = 3.86666667[us]  
Irr\_Atn\_Dec = 23.33[db]  
Irr\_Atn\_Noise = 23.33[db]  
Irr\_Noise = WALTZ  
Irr\_Fwidth = 76[us]  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE  
Noe\_Time = 2[s]  
Repetition\_Time = 2.69730304[s]



X : parts per Million : Carbon13



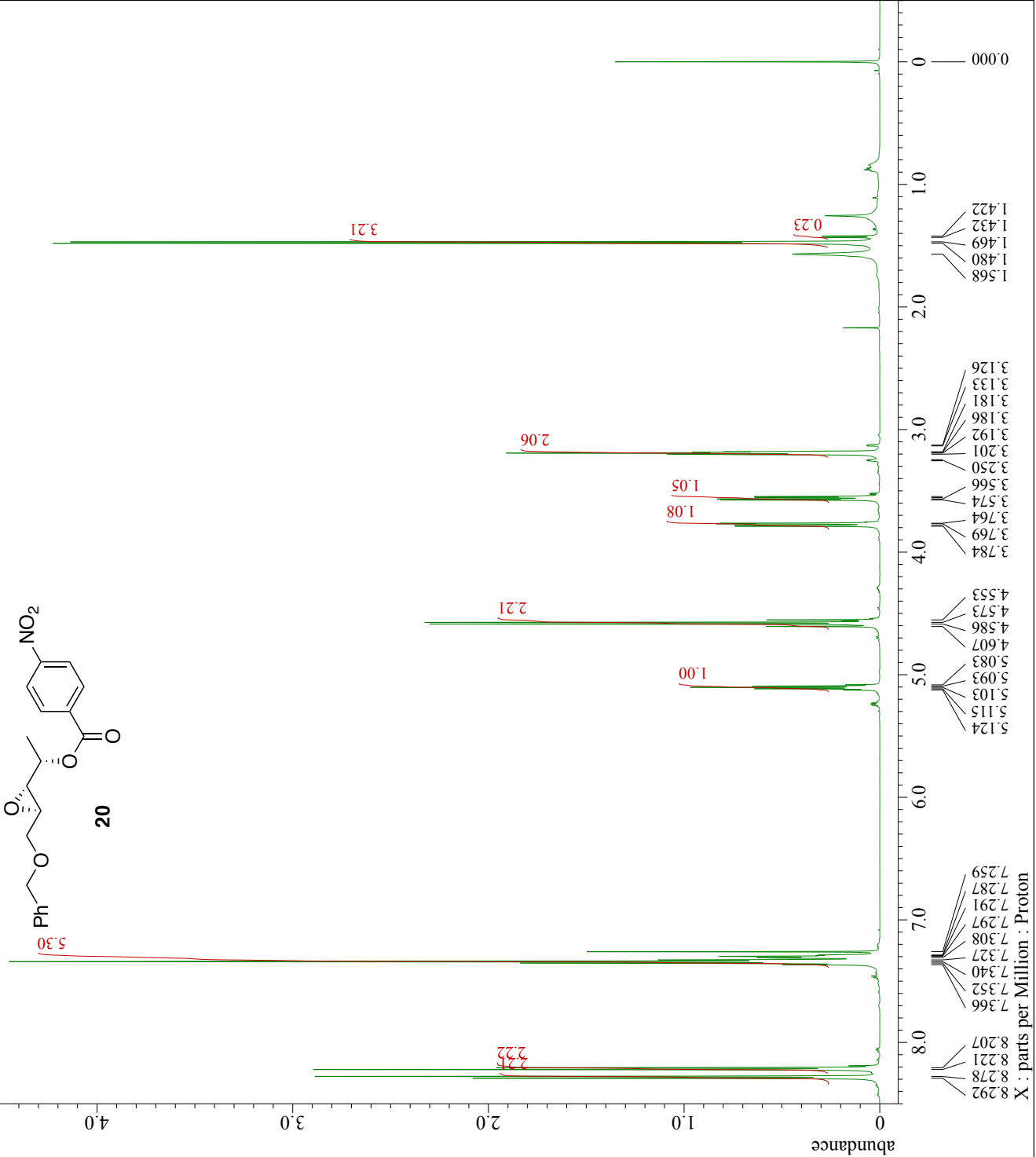


Filename = DN-1072-epo-MITSUNOBU-GPC  
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 Experiment = proton\_jxp  
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 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 2-NOV-2018 17:47:13  
 Revision\_Time = 2-NOV-2018 18:29:36

Comment = single\_pulse  
 Data\_Format = ID REAL  
 Dim\_Size = 13107  
 X\_Domain = Proton  
 Dim\_Title = Proton  
 Dim\_Units = [ppm]  
 Dimensions = X  
 Site = JNM-ECA600  
 Spectrometer = DELTA2\_NMR

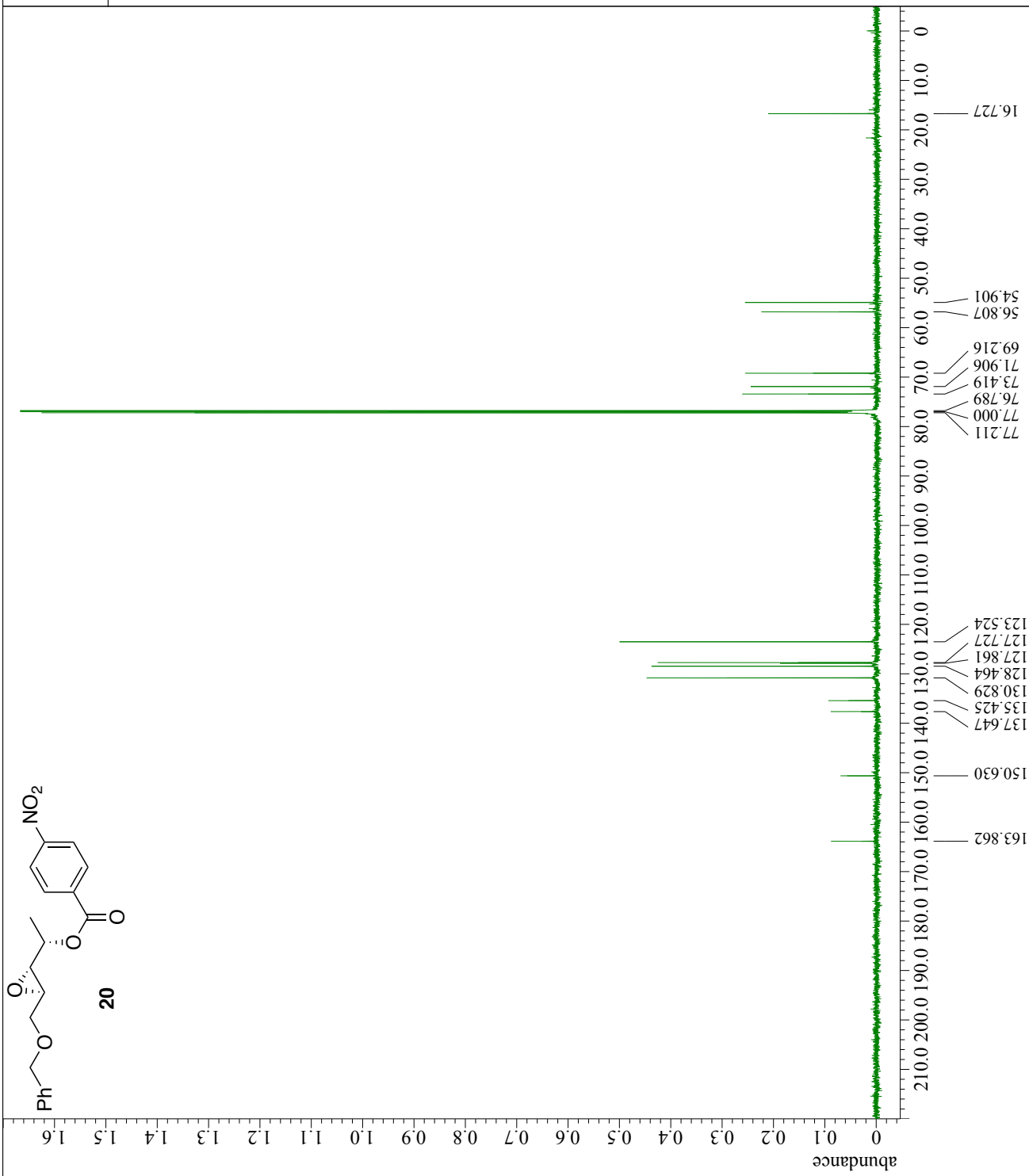
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 X\_Acq\_Duration = 1.46276352[s]  
 X\_Domain = 1H  
 X\_Freq = 597.17144293[MHz]  
 X\_Offset = 5[ppm]  
 X\_Points = 16384  
 X\_Prescans = 1  
 X\_Resolution = 0.6836375[Hz]  
 X\_Sweep = 11.20071685[kHz]  
 X\_Sweep\_Clippped = 8.96057348[kHz]  
 Irr\_Domain = Proton  
 Irr\_Freq = 597.17144293[MHz]  
 Irr\_Offset = 5[ppm]  
 Tri\_Domain = Proton  
 Tri\_Freq = 597.17144293[MHz]  
 Tri\_Offset = 5[ppm]  
 Clipped = FALSE  
 Scans = 16  
 Total\_Scans = 16

Relaxation\_Delay = 5[s]  
 Recvr Gain = 42  
 Temp\_Get = 24.1[deg]  
 X\_90\_Width = 7.15[us]  
 X\_Acq\_Time = 1.46276352[s]  
 X\_Angle = 45[deg]  
 X\_Atn = 2.8[dB]  
 X\_Pulse = 3.575[us]  
 Irr\_Mode = Off  
 Tri\_Mode = Off  
 Dante\_Presat = FALSE  
 Initial\_Wait = 1[s]  
 Repetition\_Time = 6.46276352[s]





Filename = DN-1072-epo-MITSUNOBU-pt1  
Author = gosei  
Experiment = single\_pulse\_dec  
Sample\_Id = dn  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 24-OCT-2018 00:56:46  
Revision\_Time = 25-OCT-2018 10:10:00  
Comment = single pulse decoupled ga  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
X\_Domain = 13C  
Dim\_Title = 13C  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECA600  
Spectrometer = JNM-ECA600  
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]  
Irr\_Domain = 1H  
Irr\_Freq = 600.1723046 [MHz]  
Irr\_Offset = 5 [ppm]  
Clipped = TRUE  
Scans = 1024  
Total\_Scans = 1024  
Relaxation\_Delay = 2 [s]  
Recvr Gain = 58  
Temp\_Get = 26.1 [dC]  
X\_90\_Width = 14.8 [us]  
X\_Acq\_Time = 0.69206016 [s]  
X\_Angle = 30 [deg]  
X\_Atn = 7.5 [dB]  
X\_Pulse = 4.93333333 [us]  
Irr\_Atn\_Dec = 17.094 [dB]  
Irr\_Atn\_Noise = 17.094 [dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1 [s]  
Noe\_Time = TRUE  
Repetition\_Time = 2 [s]



X : parts per Million : 13C



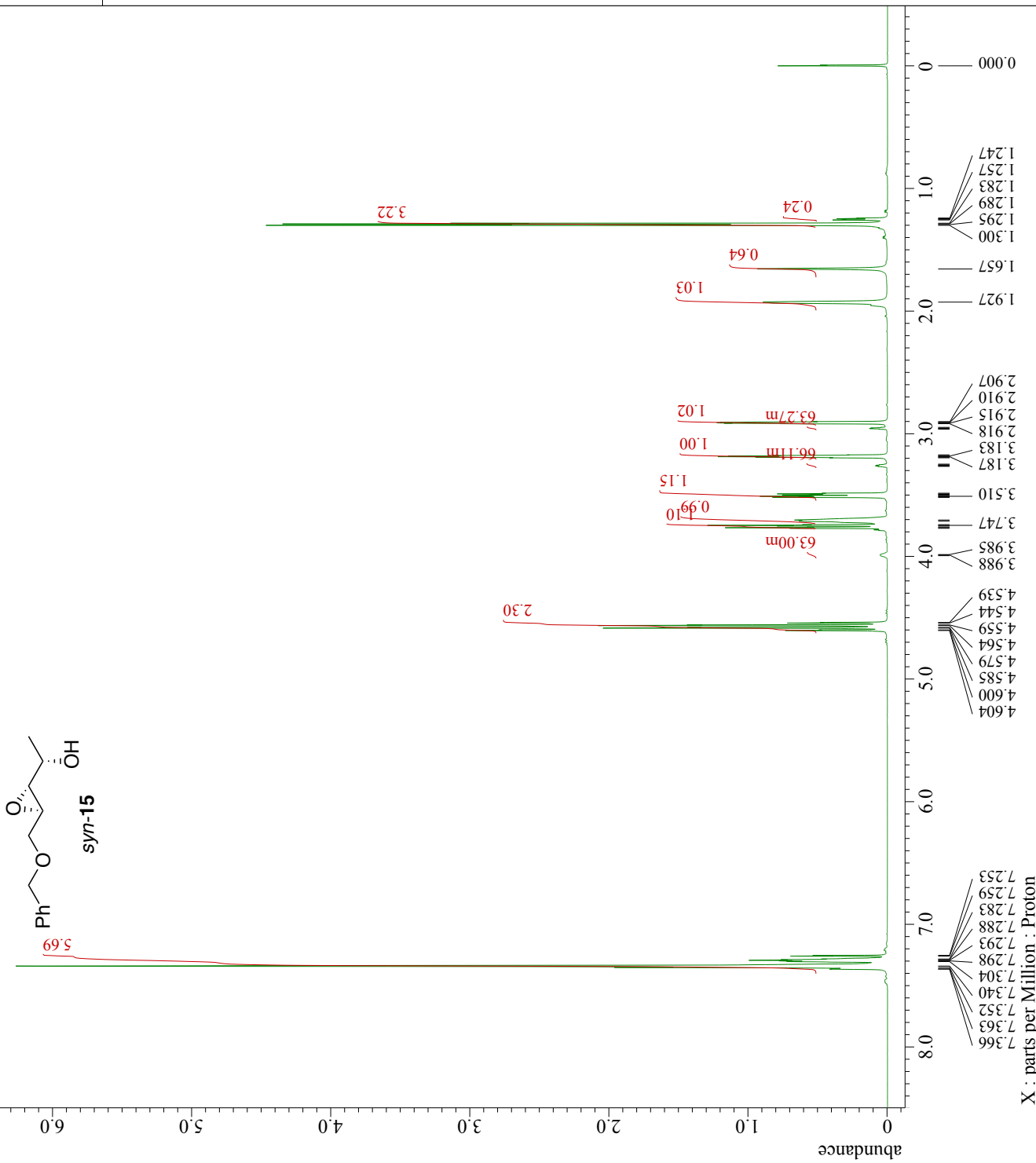
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Filename = DN-1073-epodownsyn-ptlc-a
Author = delta
Experiment = proton.jxp
Sample Id = DN-1073-epodownsyn-ptlc
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-OCT-2018 00:36:05
Revision_Time = 27-OCT-2018 00:23:54

Comment = single pulse
Data Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim Title = Proton
Dim Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR

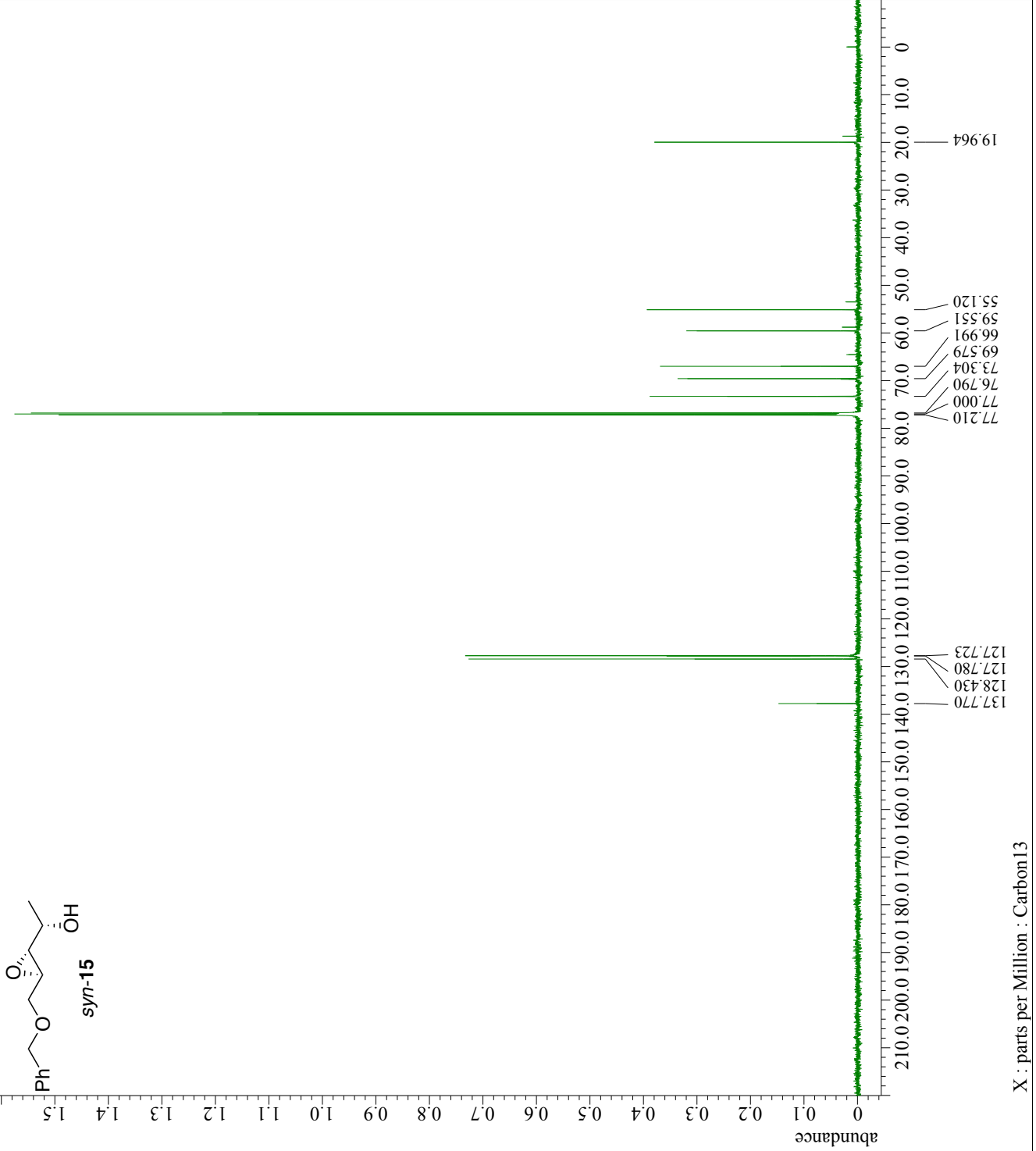
Field_Strength = 14.02588743 [T] (600 [MHz])
X_Acq_Duration = 1.46276352 [s]
X_Domain = 1H
X_Freq = 597.17144293 [MHz]
X_Offset = 5 [ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.6836375 [Hz]
X_Sweep = 11.20071685 [kHz]
X_Sweep_Clippped = 8.96057348 [kHz]
Irr_Domain = proton
Irr_Freq = 597.17144293 [MHz]
Irr_Offset = 5 [ppm]
Tri_Domain = Proton
Tri_Freq = 597.17144293 [MHz]
Tri_Offset = 5 [ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16

Relaxation_Delay = 5 [s]
Recvr_Gain = 38
Temp_Get = 24.2 [dC]
X_90_Width = 7.15 [us]
X_Acq_Time = 1.46276352 [s]
X_Angle = 45 [deg]
X_Atn = 2.8 [dB]
X_Pulse = 3.575 [us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1 [s]
Repetition_Time = 6.46276352 [s]
  
```





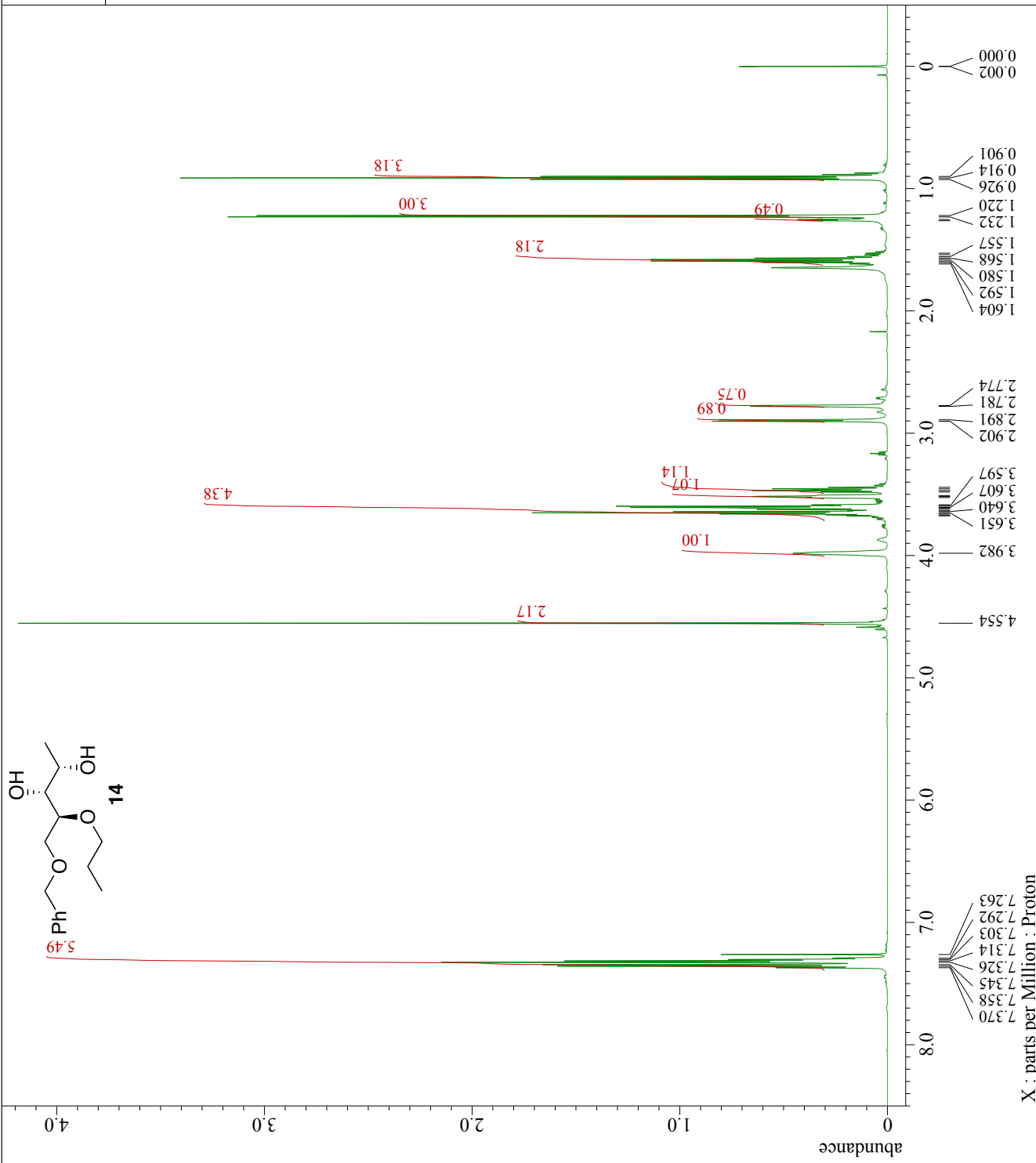
Filename = DN-1073-epodownsyn-ptlc\_c  
Author = delta  
Experiment = carbon.jpg  
Sample\_Id = DN-1073-epodownsyn-ptlc  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 20-OCT-2018 00:40:31  
Revision\_Time = 25-OCT-2018 09:54:13  
Comment = single pulse decoupled ga  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
X\_Domain = Carbon  
Dim\_Title = Carbon13  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECA600  
Spectrometer = DELTA2\_NMR  
Field\_Strength = 14.02588743[T] (600[MHz])  
X\_Acq\_Duration = 0.69730304[s]  
X\_Domain = 13C  
X\_Freq = 150.1588632[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 1.43409672[Hz]  
X\_Sweep = 46.9924812[kHz]  
X\_Sweep\_Clippped = 37.59398496[kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 597.17144293[MHz]  
Irr\_Offset = 5[ppm]  
Clipped = TRUE  
Scans = 1024  
Total\_Scans = 1024  
Relaxation\_Delay = 2[s]  
Recvr\_Gain = 58  
Temp\_Get = 24.4[dc]  
X\_90\_Width = 11.6[us]  
X\_Acq\_Time = 0.69730304[s]  
X\_Angle = 30[deg]  
X\_Atn = 8[db]  
X\_Pulse = 3.86666667[us]  
Irr\_Atn\_Dec = 23.33[db]  
Irr\_Atn\_Noie = 23.33[db]  
Irr\_Noie = WALTZ  
Irr\_Pwidth = 76[us]  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE  
Noe\_Time = 2[s]  
Repetition\_Time = 2.69730304[s]



X : parts per Million : Carbon13

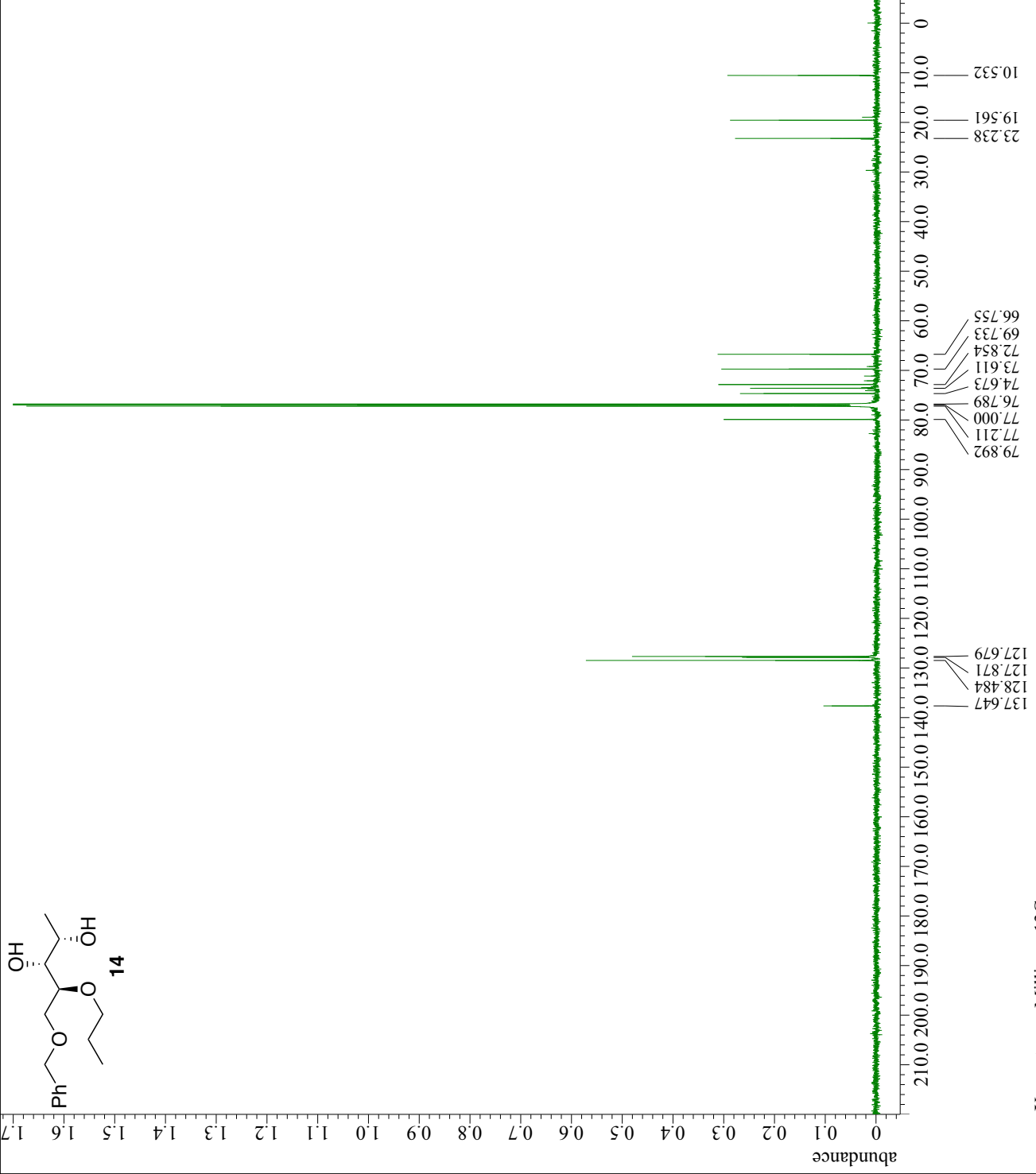


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Author = delta  
Experiment = proton.jxp  
Sample\_Id = DN-1077-syn-epoopen-5per-  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 2-NOV-2018 17:58:58  
Revision\_Time = 2-NOV-2018 19:02:48  
Comment = single\_pulse  
Data\_Format = 1D REAL  
Dim\_Size = 13107  
X\_Domain = Proton  
Dim\_Title = Proton  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECA600  
Spectrometer = DELTA2\_NMR  
Field\_Strength = 14.02588743[T] (600[MHz])  
X\_Acq\_Duration = 1.46276352[s]  
X\_Domain = 1H  
X\_Freq = 597.17144293[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.6836375[Hz]  
X\_Sweep = 11.20071685[kHz]  
X\_Sweep\_Clippped = 8.96057348[kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 597.17144293[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = Proton  
Tri\_Freq = 597.17144293[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 16  
Total\_Scans = 16  
Relaxation\_Delay = 5[s]  
Recvr\_Gain = 36  
Temp\_Get = 24.1[dC]  
X\_90\_Width = 7.15[us]  
X\_Acq\_Time = 1.46276352[s]  
X\_Angle = 45[deg]  
X\_Atn = 2.8[dB]  
X\_Pulse = 3.575[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Preset = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 6.46276352[s]





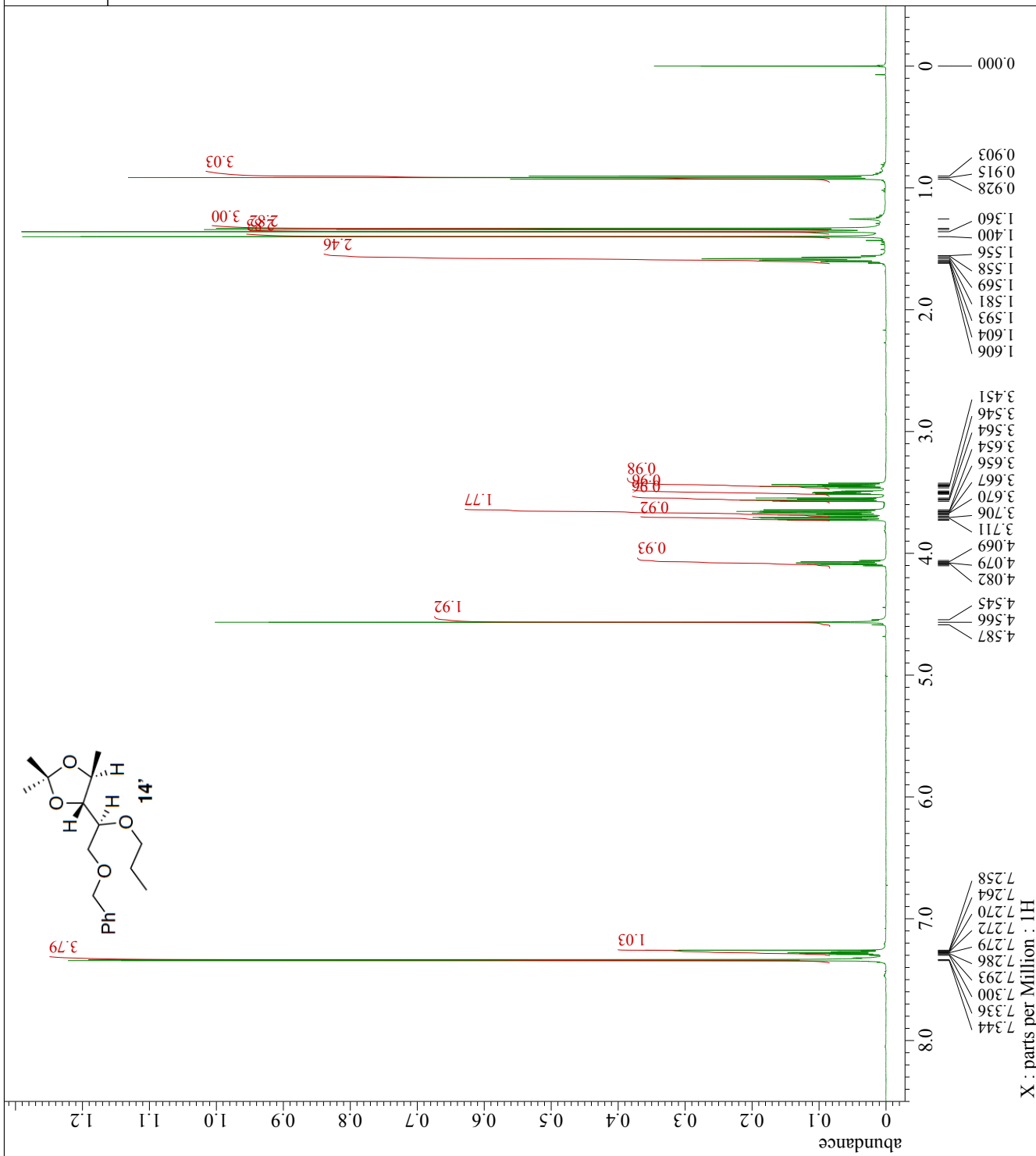
Filename = DN-1077-alcoholysis-propan  
Author = gesei  
Experiment = single\_pulse\_dec  
Sample\_Id = dn  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 23-OCT-2018 20:34:12  
Revision\_Time = 25-OCT-2018 10:16:17  
Comment = single pulse decoupled ga  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
X\_Domain = 13C  
Dim\_Title = 13C  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECA600  
Spectrometer = JNM-ECA600  
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\_Frescans = 4  
X\_Resolution = 1.44496109 [Hz]  
X\_Sweep = 47.34848485 [kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 600.1723046 [MHz]  
Irr\_Offset = 5 [ppm]  
Clipped = FALSE  
Scans = 1024  
Total\_Scans = 1024  
Relaxation\_Delay = 2 [s]  
Recvr\_Gain = 58  
Temp\_Get = 26.2 [dC]  
X\_90\_Width = 14.8 [us]  
X\_Acq\_Time = 0.69206016 [s]  
X\_Angle = 30 [deg]  
X\_Atn = 7.5 [dB]  
X\_Pulse = 4.93333333 [us]  
Irr\_Atn\_Dec = 17.094 [dB]  
Irr\_Atn\_Noise = 17.094 [dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1 [s]  
Noe = TRUE  
Noe\_Time = 2 [s]  
Repetition\_Time = 2.69206016 [s]

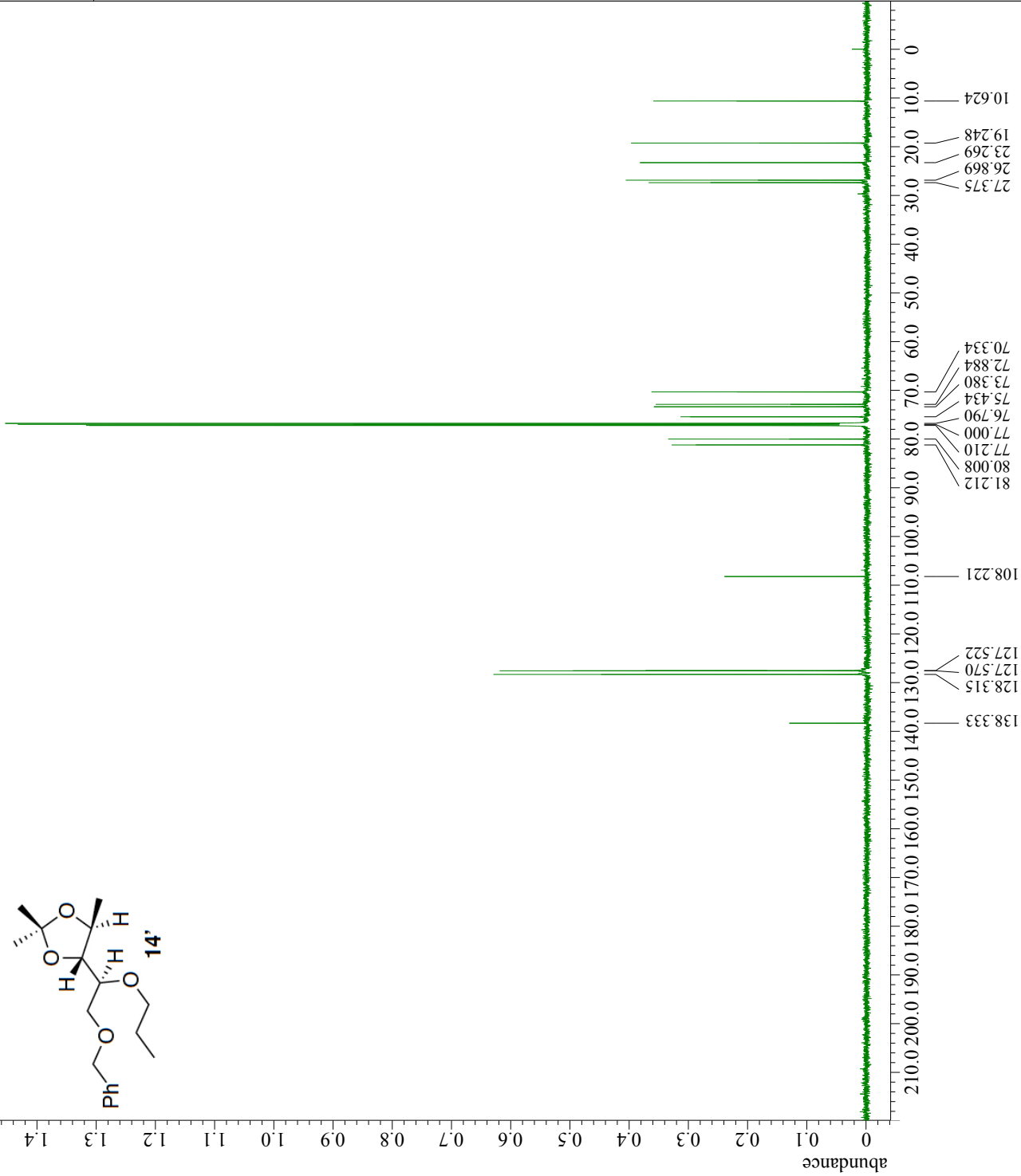
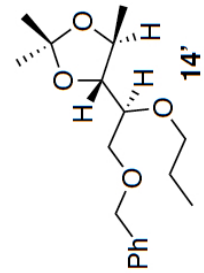


X : parts per Million : 13C



Filename = DN-1038-ptlc-an\_proton-2.  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = km  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 14-OCT-2018 21:25:12  
Revision\_Time = 25-OCT-2018 01:11:37  
Comment = a-NON  
Data\_Format = 1D REAL  
Dim\_Size = 52428  
X\_Domain = 1H  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECA 600SL  
Spectrometer = JNM-ECA600  
Field\_Strength = 13.95540559[T] (590[MHz])  
X\_Acq\_Duration = 5.88251136[s]  
X\_Domain = 1H  
X\_Freq = 594.17058168[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 65536  
X\_Prescans = 1  
X\_Resolution = 0.16999542[Hz]  
X\_Sweep = 11.14081996[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 594.17058168[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 594.17058168[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8  
Relaxation\_Delay = 5[s]  
Recvr\_Gain = 38  
Temp\_Get = 25.4[dc]  
X\_90\_Width = 14[us]  
X\_Acq\_Time = 5.88251136[s]  
X\_Angle = 45[deg]  
X\_Atn = 2.5[db]  
X\_Pulse = 7[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Preset = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 10.88251136[s]





X : parts per Million : Carbon13

Filename = DN-1038-acetal4noe-pt1c-a  
 Author = delta  
 Experiment = carbon.jxp  
 Sample\_Id = DN-1038-acetal4noe-pt1c  
 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 19-OCT-2018 17:24:57  
 Revision\_Time = 25-OCT-2018 09:49:36  
 Comment = single pulse decoupled ga  
 Data\_Format = 1D COMPLEX  
 Dim\_Size = 26214  
 X\_Domain = Carbon  
 Dim\_Title = Carbon13  
 Dim\_Units = [ppm]  
 Dimensions = X  
 Site = JNM-ECA600  
 Spectrometer = DELTA2\_NMR  
 Field\_Strength = 14.02588743 [T] (600 [MHz])  
 X\_Acq\_Duration = 0.69730304 [s]  
 X\_Domain = 13C  
 X\_Freq = 150.1588632 [MHz]  
 X\_Offset = 100 [ppm]  
 X\_Points = 32768  
 X\_Prescans = 4  
 X\_Resolution = 1.43409672 [Hz]  
 X\_Sweep = 46.9924812 [kHz]  
 X\_Sweep\_Clipped = 37.59398496 [kHz]  
 Irr\_Domain = Proton  
 Irr\_Freq = 597.17144293 [MHz]  
 Irr\_Offset = 5 [ppm]  
 Clipped = TRUE  
 Scans = 1024  
 Total\_Scans = 1024  
 Relaxation\_Delay = 2 [s]  
 Recvr\_Gain = 58  
 Temp\_Get = 24.6 [dC]  
 X\_90\_Width = 11.6 [us]  
 X\_Acq\_Time = 0.69730304 [s]  
 X\_Angle = 30 [deg]  
 X\_Atn = 8 [dB]  
 X\_Pulse = 3.86666667 [us]  
 Irr\_Atn\_Dec = 23.33 [dB]  
 Irr\_Atn\_Noise = 23.33 [dB]  
 Irr\_Noise = WALTZ  
 Irr\_Pwidth = 76 [us]  
 Decoupling = TRUE  
 Initial\_Wait = 1 [s]  
 Noe\_Time = TRUE  
 Noe\_Time = 2 [s]  
 Repetition\_Time = 2.69730304 [s]

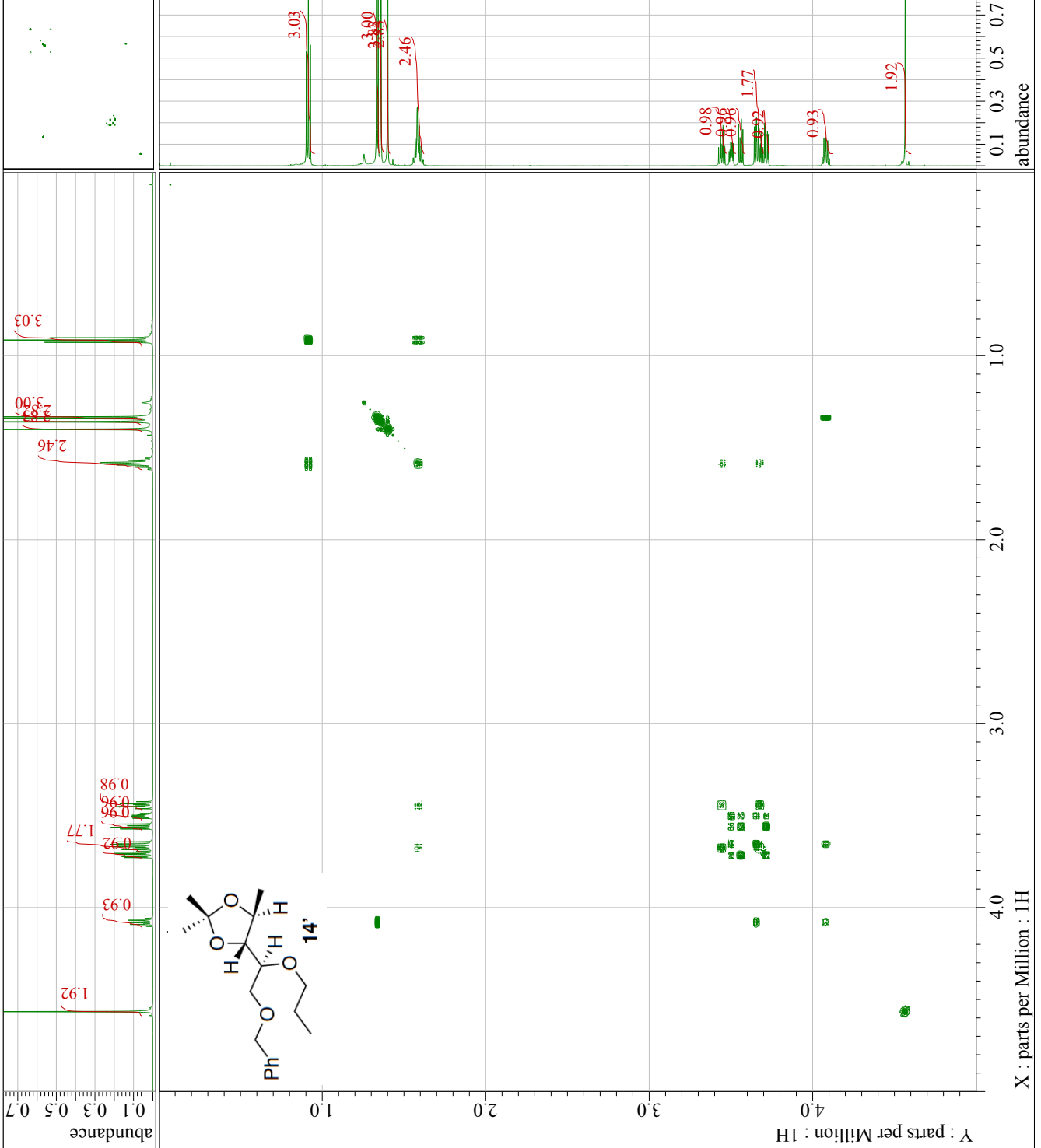






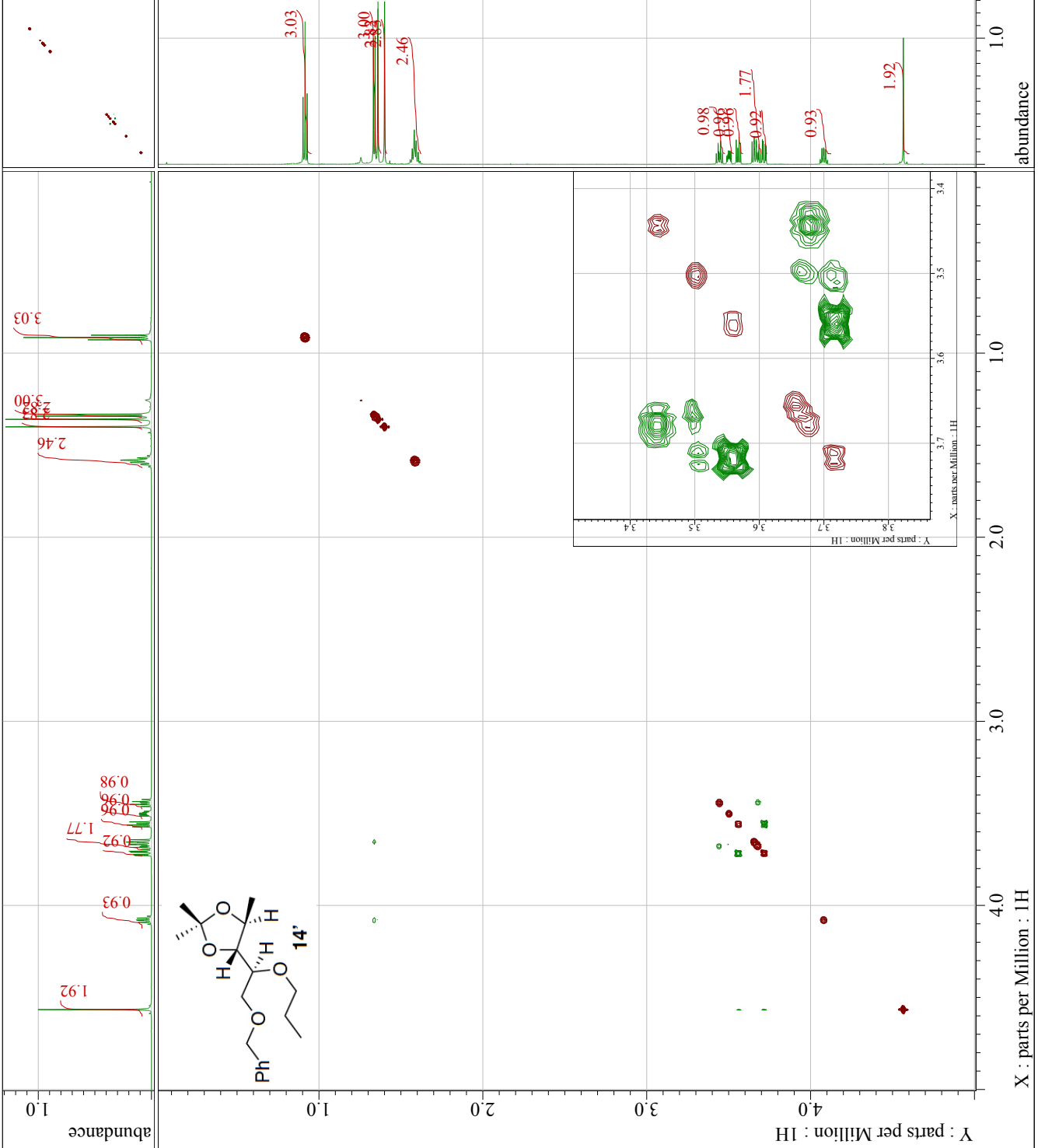
```

Filename = DN-1038-ptlc_cosy-2.jdf
Author = delta
Experiment = cosy.ex2
Sample_Id = km
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-OCT-2018 21:27:42
Revision_Time = 6-NOV-2018 09:43:35
Comment = absolute value COSY
Data_Format = 2D REAL REAL
Dim_Size = 1024, 1024
X_Domain = 1H
Y_Domain = 1H
Dim_Title = 1H 1H
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Site = ECA 600SL
Spectrometer = JNM-ECA600
Field_Strength = 13.95540559 [T] (590 [MHz])
X_Acq_Duration = 0.3446784 [s]
X_Domain = 1H
X_Freq = 594.17058168 [MHz]
X_Offset = 2.5 [ppm]
X_Points = 1280
X_Prescans = 4
X_Resolution = 2.9012552 [Hz]
X_Sweep = 3.71360665 [kHz]
Y_Domain = 1H
Y_Freq = 594.17058168 [MHz]
Y_Offset = 2.5 [ppm]
Y_Points = 256
Y_Prescans = 0
Y_Resolution = 11.605208 [Hz]
Y_Sweep = 2.97088532 [kHz]
Irr_Domain = 1H
Irr_Freq = 594.17058168 [MHz]
Irr_Offset = 5 [ppm]
Tri_Domain = 1H
Tri_Freq = 594.17058168 [MHz]
Tri_Offset = 5 [ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 1024
Relaxation_Delay = 1.5 [s]
Recvr_Gain = 34
Temp_Get = 25.4 [dC]
X_90_Width = 14 [us]
X_Acq_Time = 0.3446784 [s]
X_Attn = 2.5 [dB]
X_Pulse = 14 [us]
Y_Acq_Time = 86.1696 [ms]
Y_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Delta = 0 [ms]
Initial_Wait = 1 [s]
Pulse_1 = 14 [us]
Pulse_2 = 14 [us]
Pulse_Angle_1 = 90 [deg]
  
```



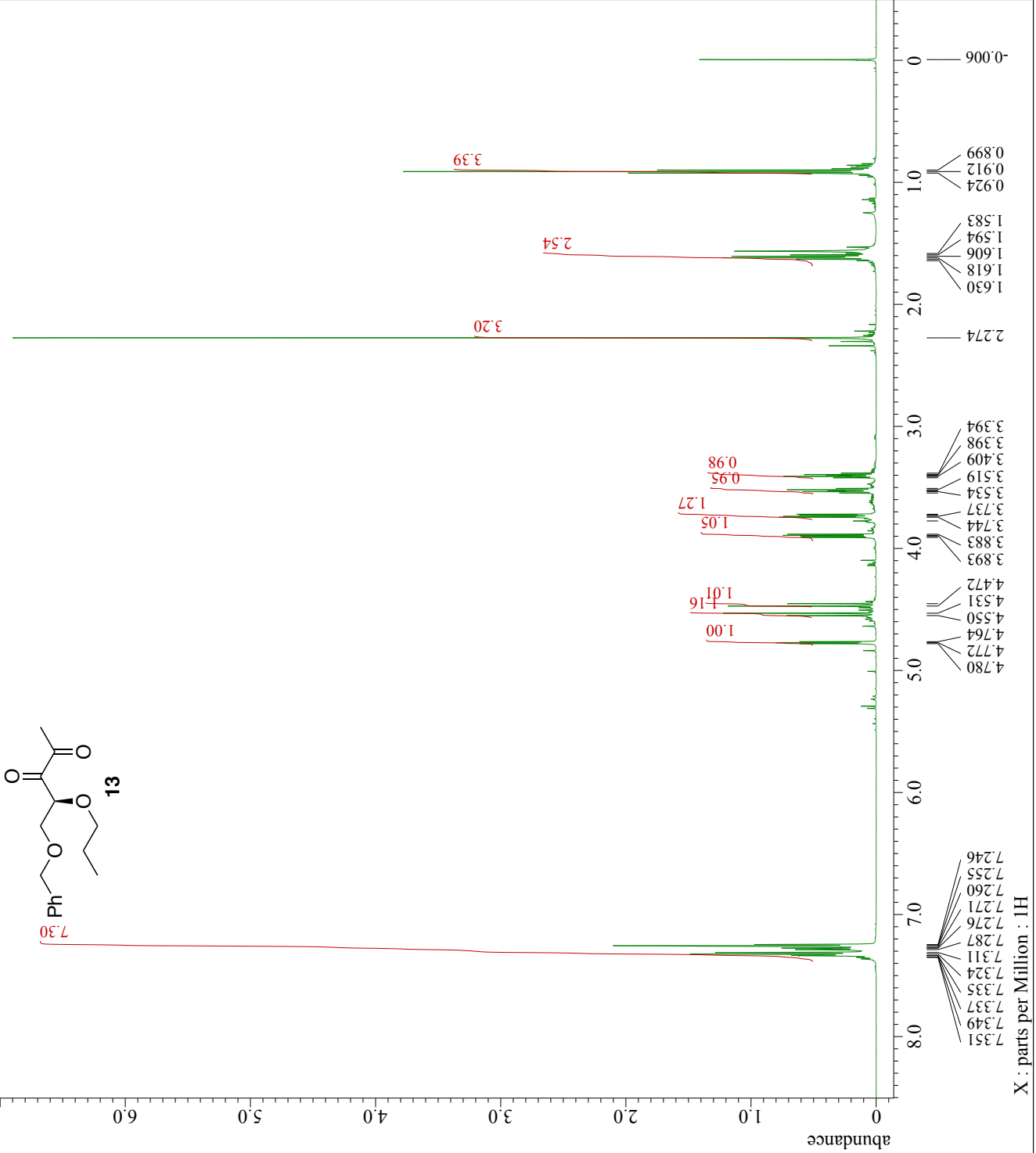


Filename = DN-1038-ptlc\_noesy-2.jdf  
Author = delta  
Experiment = noesy\_phase.ex2  
Sample Id = km  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 14-OCT-2018 22:55:57  
Revision\_Time = 6-NOV-2018 09:58:45  
Comment = phase sensitive noesy  
Data Format = 2D COMPLEX COMPLEX  
Dim\_Size = 819, 512  
X\_Domain = 1H  
Y\_Domain = 1H  
Dim Title = 1H 1H  
Dim Units = [ppm] [ppm]  
Dimensions = X Y  
Site = ECA 600SL  
Spectrometer = JNM-ECA600  
Field\_Strength = 13.95540559[T] (590[MHz])  
X\_Acq\_Duration = 0.2756608[s]  
X\_Domain = 1H  
X\_Freq = 594.17058168 [MHz]  
X\_Offset = 2.5 [ppm]  
X\_Points = 1024  
X\_Frescans = 4  
X\_Resolution = 3.62764673 [Hz]  
Y\_Sweep = 3.71471025 [kHz]  
Y\_Domain = 1H  
Y\_Freq = 594.17058168 [MHz]  
Y\_Offset = 2.5 [ppm]  
Y\_Points = 256  
Y\_Frescans = 0  
Y\_Resolution = 11.6050208 [Hz]  
Y\_Sweep = 2.97088532 [kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 594.17058168 [MHz]  
Irr\_Offset = 5 [ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 594.17058168 [MHz]  
Tri\_Offset = 5 [ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 2048  
Relaxation\_Delay = 1.5 [s]  
Recvr Gain = 34  
Temp\_Get = 25.4 [C]  
Mix\_Time = 1.4 [s]  
X\_Acq\_Time = 0.2756608 [s]  
X\_Attn = 2.5 [dB]  
X\_Pulse = 14 [us]  
Y\_Acq\_Time = 86.1696 [ms]  
Y\_P0\_Correction = 0  
Y\_P1\_Correction = 180  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Preset = FALSE  
Initial\_Wait = 1 [s]  
Repetition\_Time = 1.7756608 [s]  
Scramble = 1 [ms]





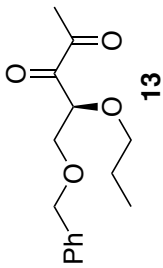
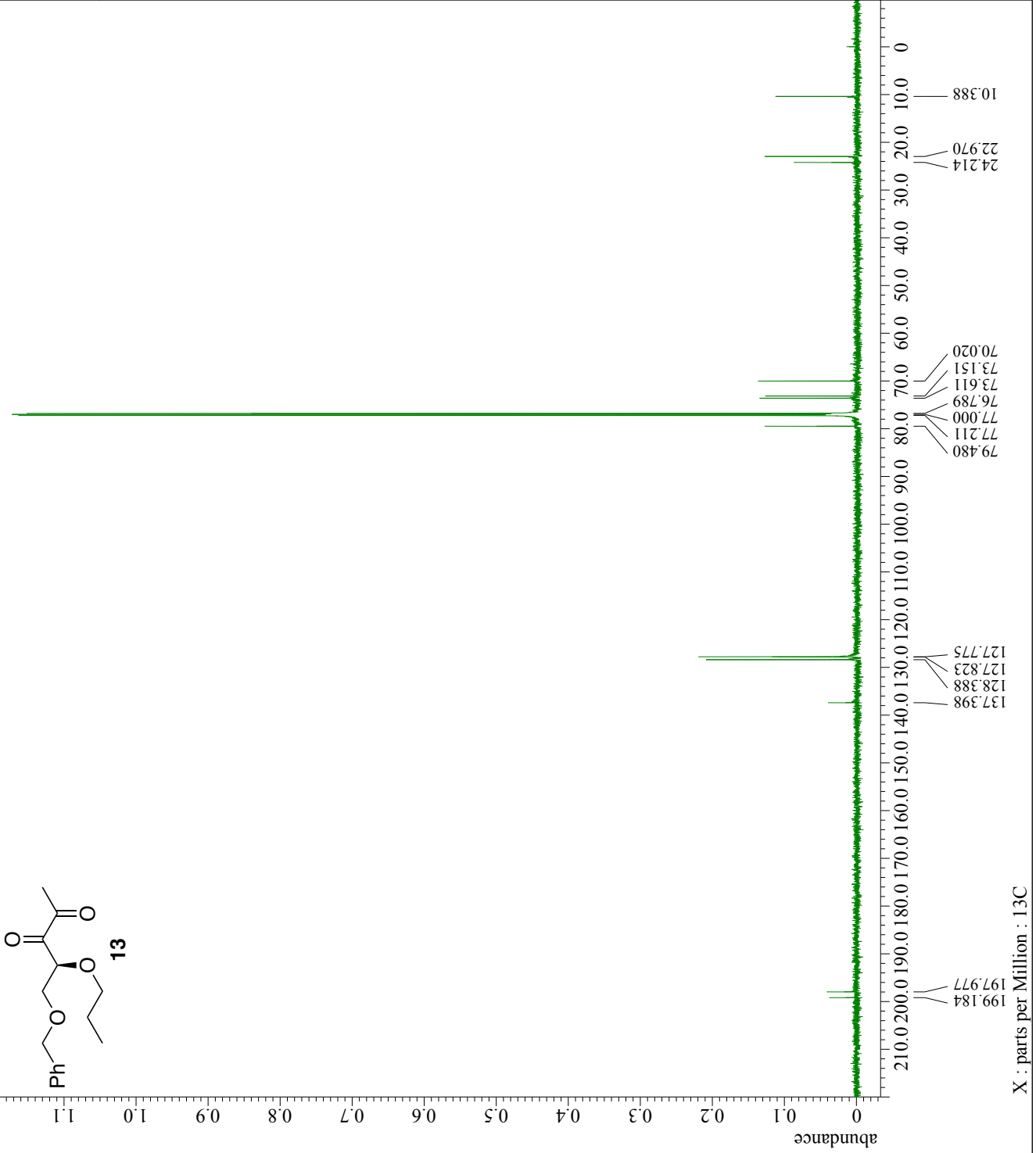
Filename = DN-1081-AZADOX-diketone-p  
Author = Gosei  
Experiment = single\_pulse.ex2  
Sample\_id = dn  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 24-OCT-2018 02:52:49  
Revision\_Time = 26-OCT-2018 21:30:39  
Comment = single\_pulse  
Data\_Format = 1D REAL  
Dim\_Size = 13107  
X\_Domain = 1H  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECA600  
Spectrometer = JNM-ECA600  
Field\_Strength = 14.09636928[T] (600[MHz])  
X\_Acq\_Duration = 1.4548992[s]  
X\_Domain = 1H  
X\_Freq = 600.1723046[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.68733284[Hz]  
X\_Sweep = 11.26126126[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 600.1723046[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 600.1723046[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 16  
Total\_Scans = 16  
Relaxation\_Delay = 5[s]  
Recvr\_Gain = 40  
Temp\_Get = 24.9[dc]  
X\_90\_Width = 15.1[us]  
X\_Acq\_Time = 1.4548992[s]  
X\_Angle = 45[deg]  
X\_Atn = 3[db]  
X\_Pulse = 7.55[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 6.4548992[s]



X : parts per Million : 1H

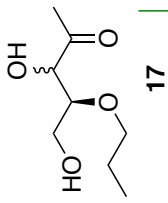
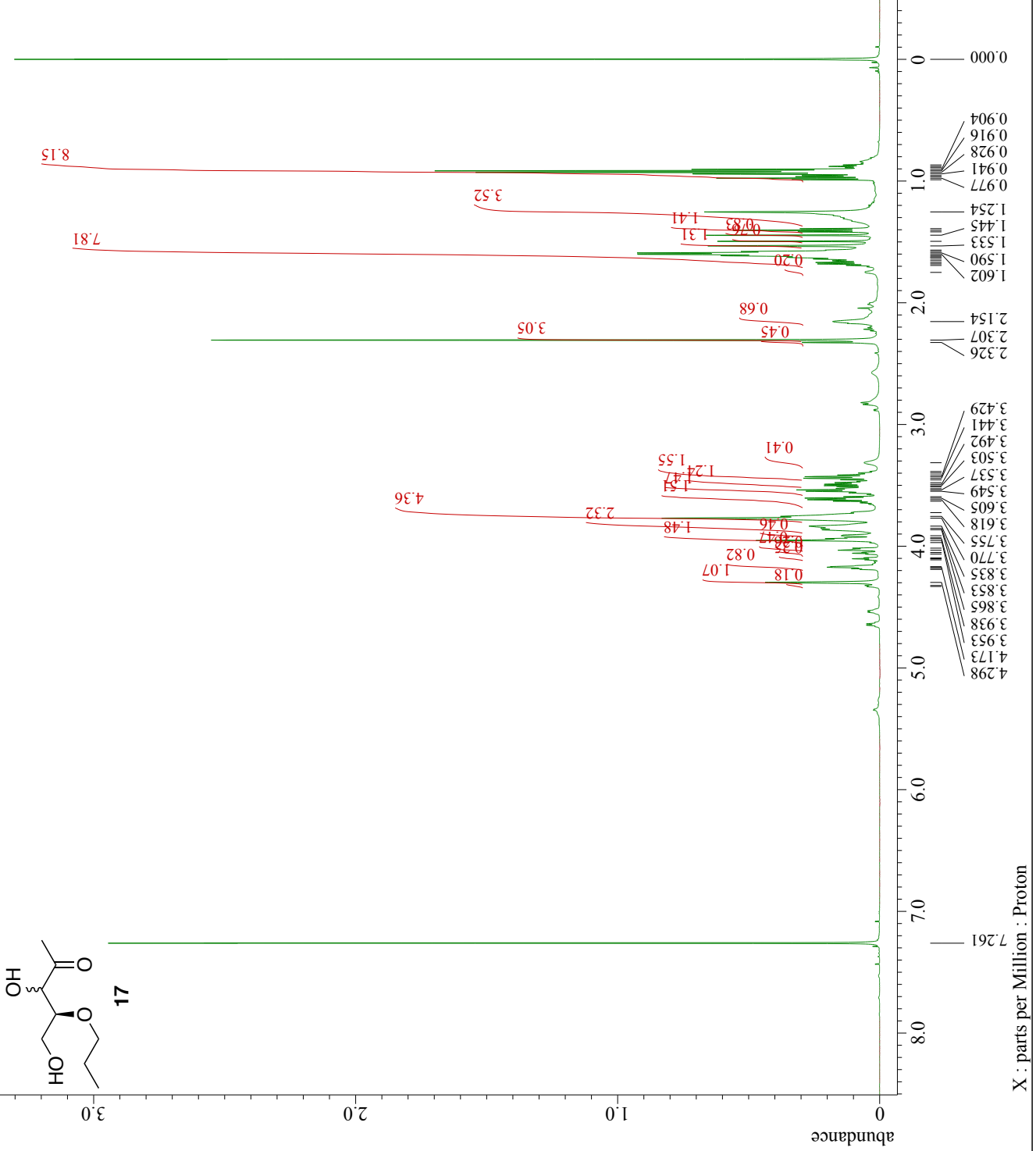


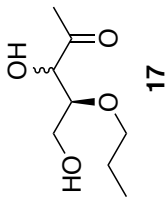
Filename = DN-1081-AZADOX-diketone-p  
Author = gosei  
Experiment = single\_pulse\_dec  
Sample\_Id = dn  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 24-OCT-2018 02:57:58  
Revision\_Time = 25-OCT-2018 10:03:16  
Comment = single pulse decoupled ga  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
X\_Domain = 13C  
Dim\_Title = 13C  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECA600  
Spectrometer = JNM-ECA600  
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]  
Irr\_Domain = 1H  
Irr\_Freq = 600.1723046[MHz]  
Irr\_Offset = 5 [ppm]  
Clipped = FALSE  
Scans = 1024  
Total\_Scans = 1024  
Relaxation\_Delay = 2 [s]  
Recvr\_Gain = 56  
Temp\_Get = 26.3 [dC]  
X\_90\_Width = 14.8 [us]  
X\_Acq\_Time = 0.69206016[s]  
X\_Angle = 30 [deg]  
X\_Atn = 7.5 [dB]  
X\_Pulse = 4.93333333 [us]  
Irr\_Atn\_Dec = 17.094 [dB]  
Irr\_Atn\_Noise = 17.094 [dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1 [s]  
Noe = TRUE  
Noe\_Time = 2 [s]  
Repetition\_Time = 2.69206016 [s]





Filename = DN-1219-PdCdeBn-AD-Diketo  
Author = delta  
Experiment = proton.jxp  
Sample Id = DN-1211-PdCdeBn-AD-Diketo  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 20-FEB-2019 00:13:39  
Revision\_Time = 27-FEB-2019 14:10:05  
Comment = single pulse  
Data Format = 1D REAL  
Dim\_Size = 13107  
X\_Domain = Proton  
Dim\_Title = Proton  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECA600  
Spectrometer = DELTA2\_NMR  
Field Strength = 14.02588743[T] (600 [MHz])  
X\_Acq\_Duration = 1.46276352 [s]  
X\_Domain = 1H  
X\_Freq = 597.17144293 [MHz]  
X\_Offset = 5 [ppm]  
X Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.6836375 [Hz]  
X\_Sweep = 11.20071685 [kHz]  
X\_Sweep Clipped = 8.96057348 [kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 597.17144293 [MHz]  
Irr\_Offset = 5 [ppm]  
Tri\_Domain = Proton  
Tri\_Freq = 597.17144293 [MHz]  
Tri\_Offset = 5 [ppm]  
Clipped = FALSE  
Scans = 128  
Total\_Scans = 128  
Relaxation\_Delay = 5 [s]  
Recvr\_Gain = 50  
Temp\_Get = 24.2 [dc]  
X\_90\_Width = 7.15 [us]  
X\_Acq\_Time = 1.46276352 [s]  
X\_Angle = 45 [deg]  
X\_Actn = 2.8 [dB]  
X\_Pulse = 3.575 [us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Preset = FALSE  
Initial\_Wait = 1 [s]  
Repetition\_Time = 6.46276352 [s]





```

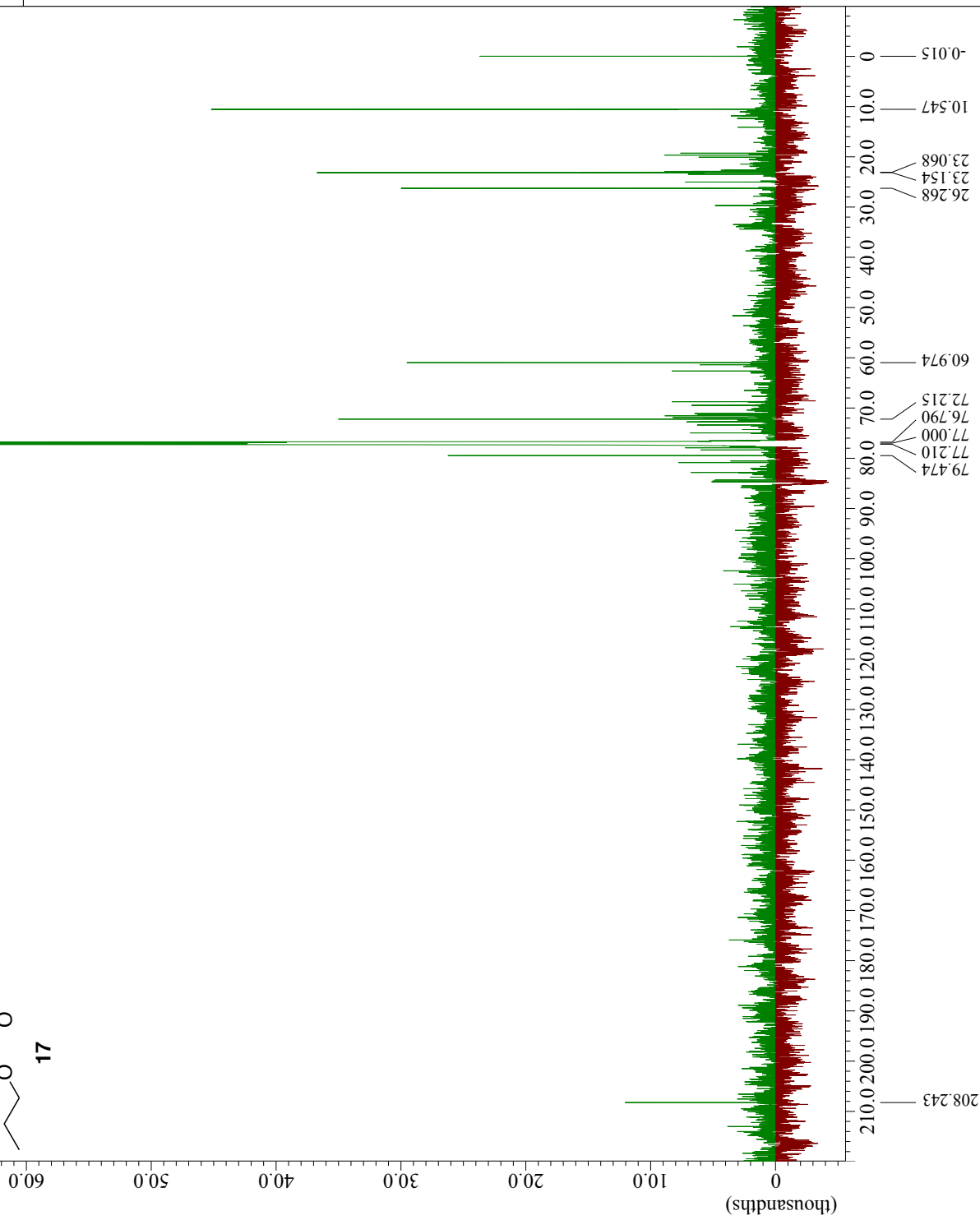
Filename = DN-1219-PdCdeBn-AD-Diketo
Author = delta
Experiment = carbon.jxp
Sample Id = DN-1211-PdCdeBn-AD-Diketo
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-FEB-2019 00:49:52
Revision_Time = 27-FEB-2019 12:29:02

Comment = single pulse decoupled ga
Data_Format = 1D REAL
Dim_Size = 26214
X_Domain = Carbon
Dim Title = Carbon13
Dim Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR

Field_Strength = 14.02588743[T] (600[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 150.1588632[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clippped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 597.17144293[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 10000
Total_Scans = 10000

Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 24[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 8[db]
X_Pulse = 3.86666667[us]
Irr_Atn_Dec = 23.33[db]
Irr_Atn_Noise = 23.33[db]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe Time = 2[s]
Repetition_Time = 2.69730304[s]

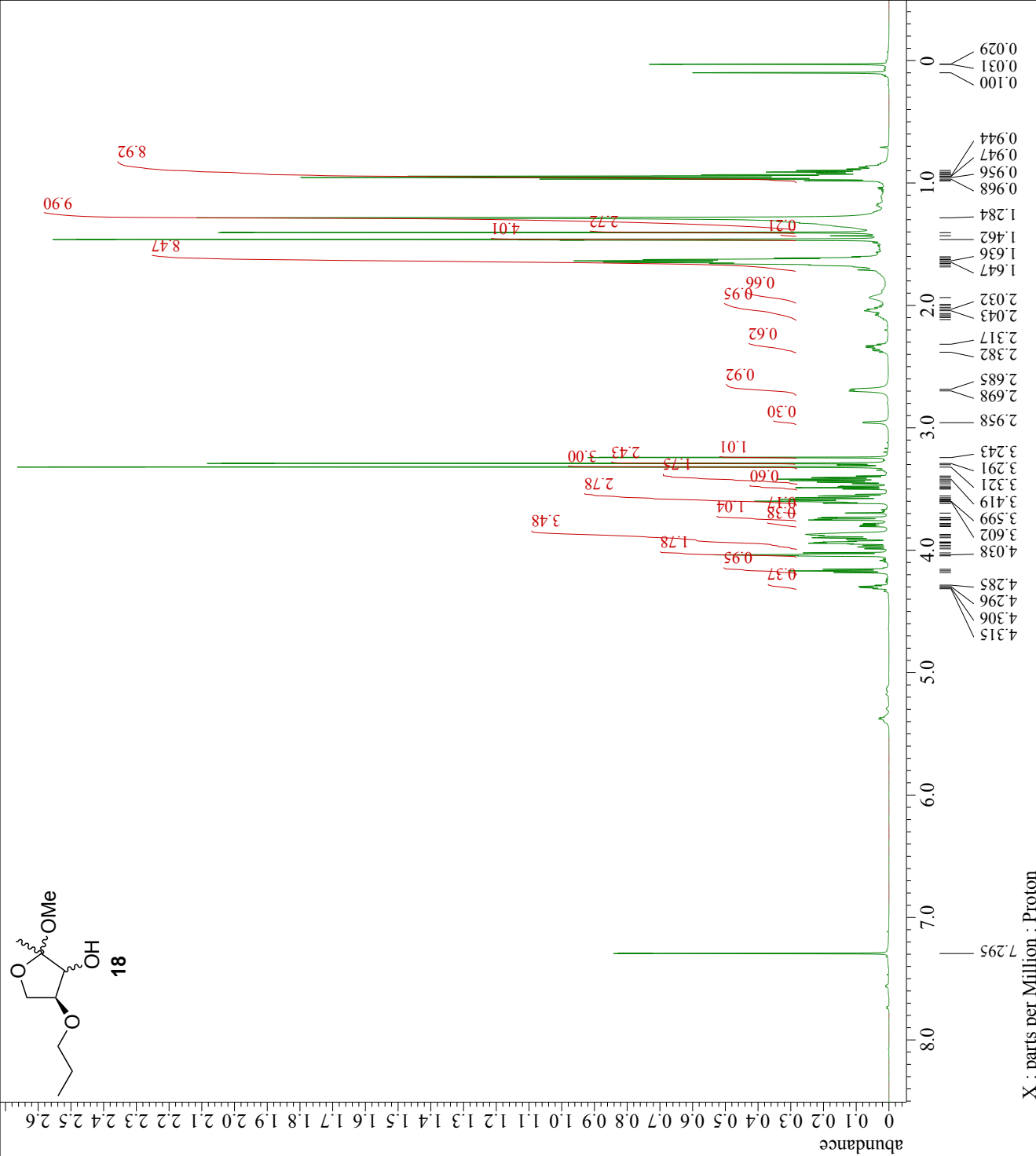
```



X : parts per Million : Carbon13



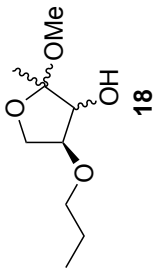
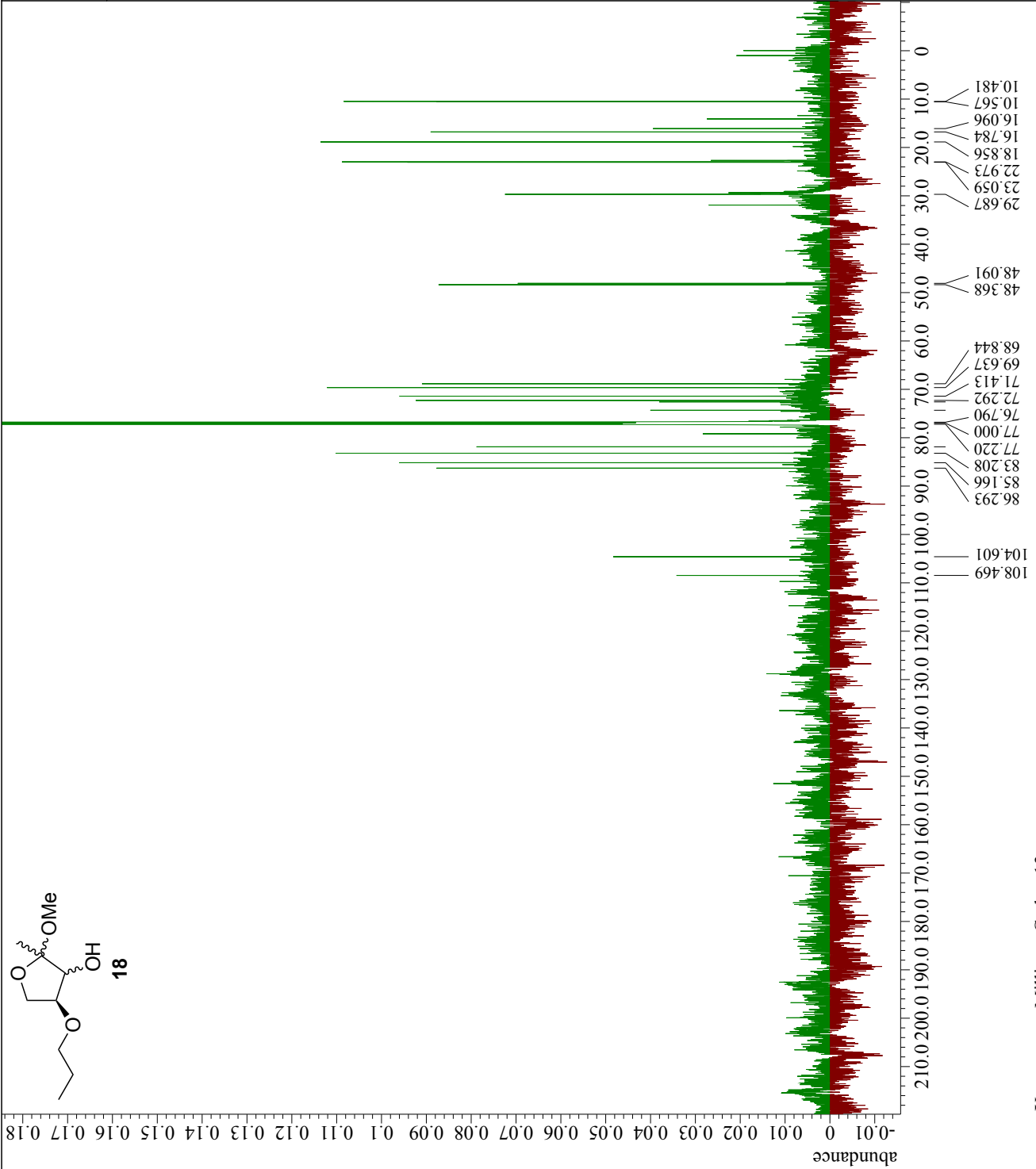
Filename = DN-1223-Meac-clm\_proton-a  
Author = delta  
Experiment = proton.jxp  
Sample Id = DN-1220-MeAC-clm  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 21-FEB-2019 23:11:43  
Revision\_Time = 27-FEB-2019 12:03:08  
Comment = single\_pulse  
Data\_Format = 1D\_REAL  
Dim\_Size = 13107  
X\_Domain = Proton  
Dim\_Title = Proton  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECA600  
Spectrometer = DELTA2\_NMR  
Field\_Strength = 14.02588743 [T] (600 [MHz])  
X\_Acq\_Duration = 1.46276352 [s]  
X\_Domain = 1H  
X\_Freq = 597.17144293 [MHz]  
X\_Offset = 5 [ppm]  
X\_Points = 16384  
X\_Frescans = 1  
X\_Resolution = 0.6836375 [Hz]  
X\_Sweep = 11.20071685 [kHz]  
X\_Sweep\_Clippped = 8.96057348 [kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 597.17144293 [MHz]  
Irr\_Offset = 5 [ppm]  
Tri\_Domain = Proton  
Tri\_Freq = 597.17144293 [MHz]  
Tri\_Offset = 5 [ppm]  
Clipped = FALSE  
Scans = 128  
Total\_Scans = 128  
Relaxation\_Delay = 5 [s]  
Recvr\_Gain = 40  
Temp\_Get = 24.1 [dC]  
X\_90\_Width = 7.15 [us]  
X\_Acq\_Time = 1.46276352 [s]  
X\_Angle = 45 [deg]  
X\_Atn = 2.8 [dB]  
X\_Pulse = 3.575 [us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1 [s]  
Repetition\_Time = 6.46276352 [s]



X : parts per Million : Proton



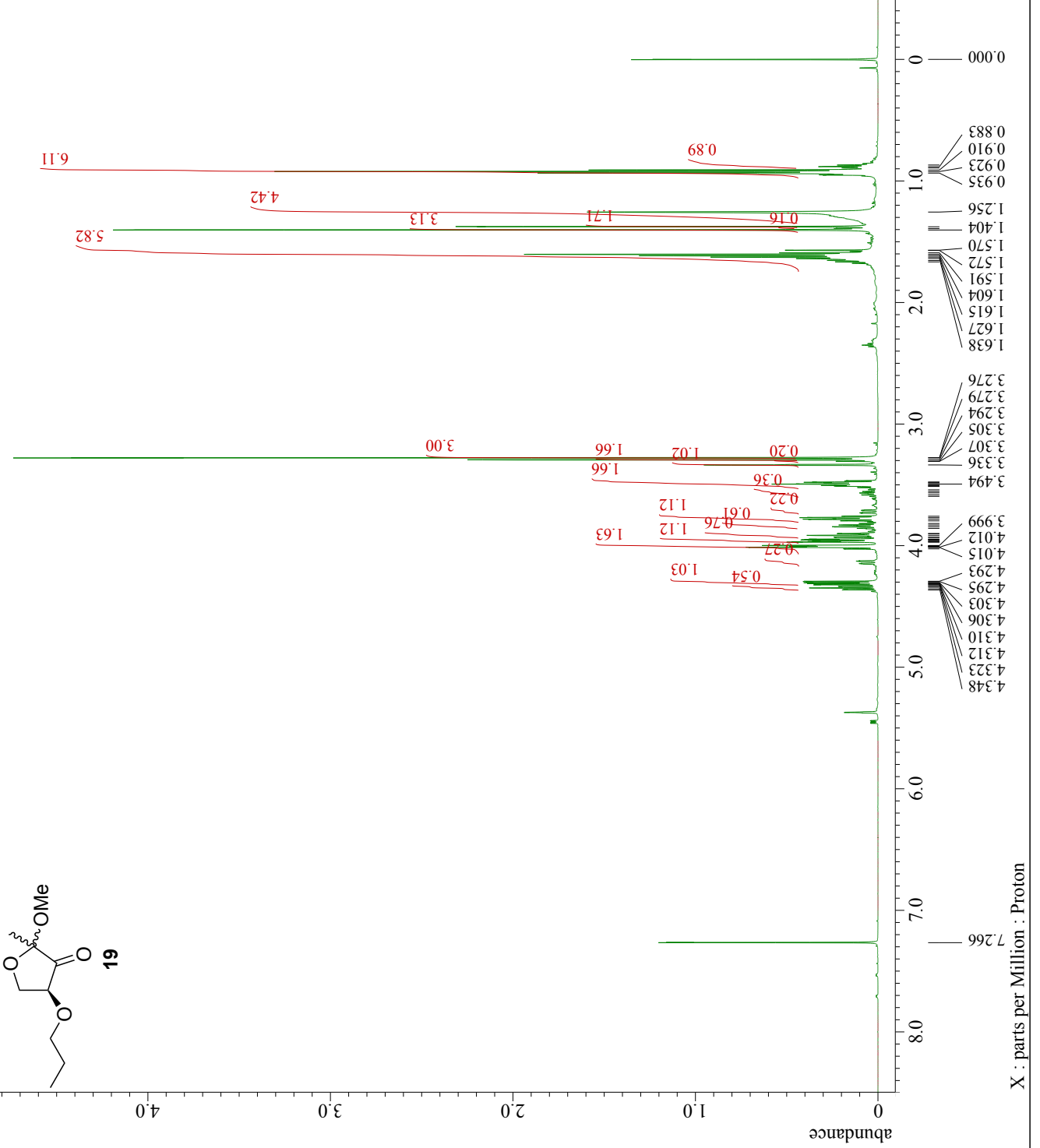
Filename = DN-1223-MeAc-clm\_carbon-a  
Author = delta  
Experiment = carbon\_jxp  
Sample\_Id = DN-1220-MeAc-clm  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 21-FEB-2019 23:29:38  
Revision\_Time = 27-FEB-2019 21:10:02  
Comment = single pulse decoupled ga  
Data\_Format = ID REAL  
Dim\_Size = 26214  
X\_Domain = Carbon  
Dim\_Title = Carbon13  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECA600  
Spectrometer = DELTA2\_NMR  
Field\_Strength = 14.02588743 [T] (600 [MHz])  
X\_Acq\_Duration = 0.69730304 [s]  
X\_Domain = 13C  
X\_Freq = 150.1588632 [MHz]  
X\_Offset = 100 [ppm]  
X\_Points = 32766  
X\_Prescans = 4  
X\_Resolution = 1.43409672 [Hz]  
X\_Sweep = 46.9924812 [kHz]  
X\_Sweep\_Clippped = 37.59398496 [kHz]  
Irr\_Domain = proton  
Irr\_Freq = 597.17144293 [MHz]  
Irr\_Offset = 5 [ppm]  
Clipped = TRUE  
Scans = 1024  
Total\_Scans = 1024  
Relaxation\_Delay = 2 [s]  
Recvr\_Gain = 58  
Temp\_Get = 24.3 [dc]  
X\_90\_Width = 11.6 [us]  
X\_Acq\_Time = 0.69730304 [s]  
X\_Angle = 30 [deg]  
X\_Atn = 8 [dB]  
X\_Pulse = 3.86666667 [us]  
Irr\_Atn\_Dec = 23.33 [dB]  
Irr\_Atn\_Noise = 23.33 [dB]  
Irr\_Noise = WALTZ  
Irr\_Width = 76 [us]  
Decoupling = TRUE  
Initial\_Wait = 1 [s]  
Noe = TRUE  
Noe\_Time = 2 [s]  
Repetition\_Time = 2.69730304 [s]







Filename = DN-1224-MeAcal-Ox-clm-2di  
Author = delta  
Experiment = proton.jxp  
Sample\_Id = DN-122x-MeAcal-Ox-clm-2di  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 23-FEB-2019 11:20:54  
Revision\_Time = 27-FEB-2019 19:47:28  
Comment = single\_pulse  
Data\_Format = 1D REAL  
Dim\_Size = 13107  
X\_Domain = Proton  
Dim\_Title = Proton  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECA600  
Spectrometer = DELTA2\_NMR  
Field\_Strength = 14.02588743[T] (600 [MHz])  
X\_Acq\_Duration = 1.46276352[s]  
X\_Domain = 1H  
X\_Freq = 597.17144293 [MHz]  
X\_Offset = 5 [ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.6836375 [Hz]  
X\_Sweep = 11.20071685 [kHz]  
X\_Sweep\_Clipped = 8.96057348 [kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 597.17144293 [MHz]  
Irr\_Offset = 5 [ppm]  
Tri\_Domain = Proton  
Tri\_Freq = 597.17144293 [MHz]  
Tri\_Offset = 5 [ppm]  
Clipped = FALSE  
Total\_Scans = 128  
Relaxation\_Delay = 5 [s]  
Recvr\_Gain = 42  
Temp\_Get = 23.9 [dc]  
X\_90\_Width = 7.15 [us]  
X\_Acq\_Time = 1.46276352 [s]  
X\_Angle = 45 [deg]  
X\_Atn = 2.8 [dB]  
X\_Pulse = 3.575 [us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Date\_Presat = FALSE  
Initial\_Wait = 1 [s]  
Repetition\_Time = 6.46276352 [s]



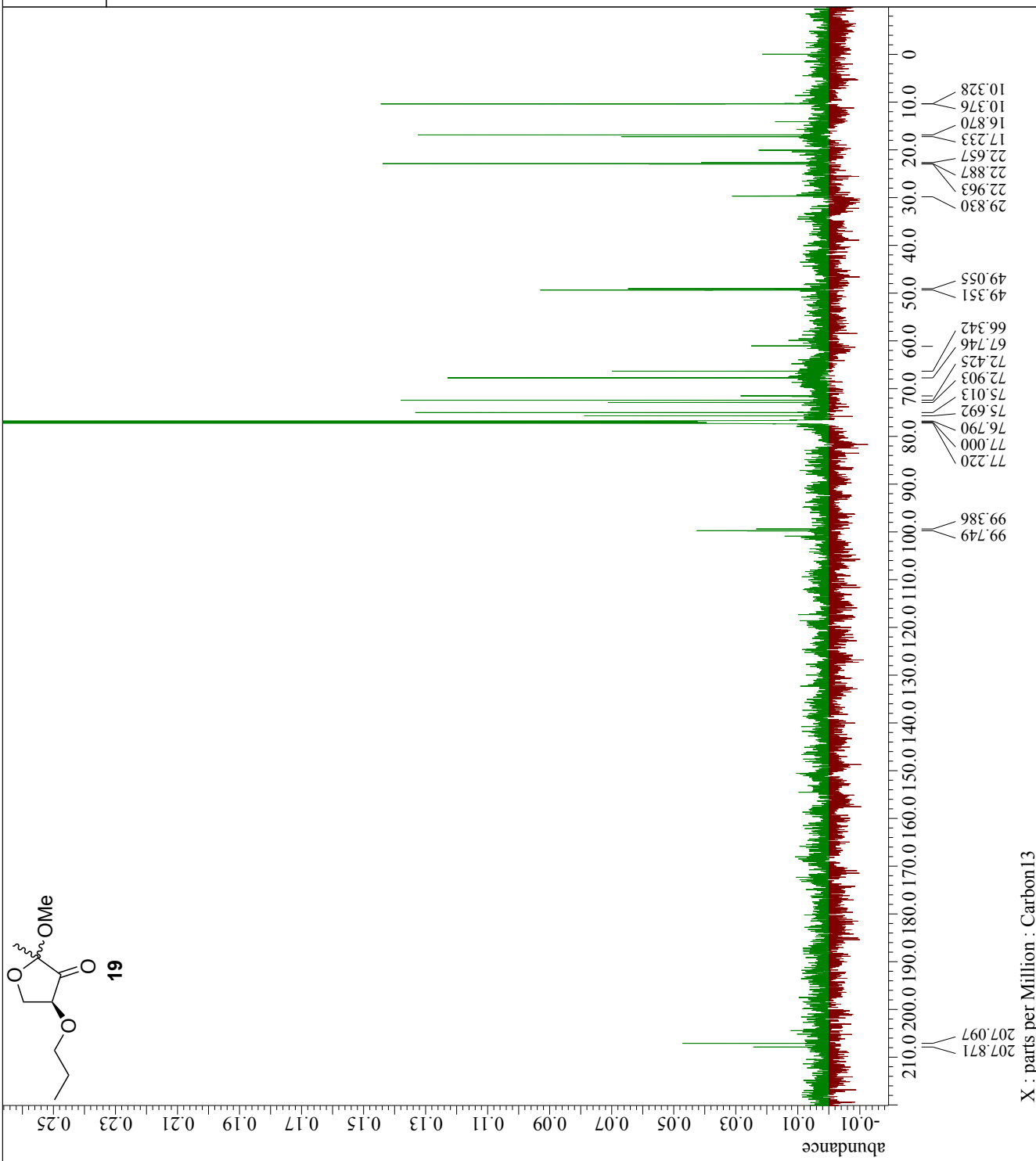
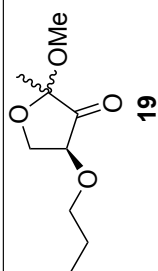


Filename = DN-1224-MeAcAl-Ox-clm-2dd  
Author = delta  
Experiment = carbon.jxp  
Sample Id = DN-122x-MeAcAl-Ox-clm-2dd  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 23-FEB-2019 11:37:28  
Revision\_Time = 27-FEB-2019 20:01:40

Comment = single pulse decoupled ga  
Data\_Format = 1D REAL  
Dim\_Size = 26214  
X\_Domain = Carbon  
Dim Title = Carbon13  
Dim Units = [ppm]  
Dimensions = X  
Site = JNM-ECA600  
Spectrometer = DELTA2\_NMR

Field\_Strength = 14.02588743 [T] (600 [MHz])  
X\_Acq\_Duration = 0.69730304 [s]  
X\_Domain = 13C  
X\_Freq = 150.1588632 [MHz]  
X\_Offset = 100 [ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 1.43409672 [Hz]  
X\_Sweep = 46.9924812 [kHz]  
X\_Sweep\_Clippped = 37.59398496 [kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 597.17144293 [MHz]  
Irr\_Offset = 5 [ppm]  
Clipped = TRUE  
Scans = 1024  
Total\_Scans = 1024

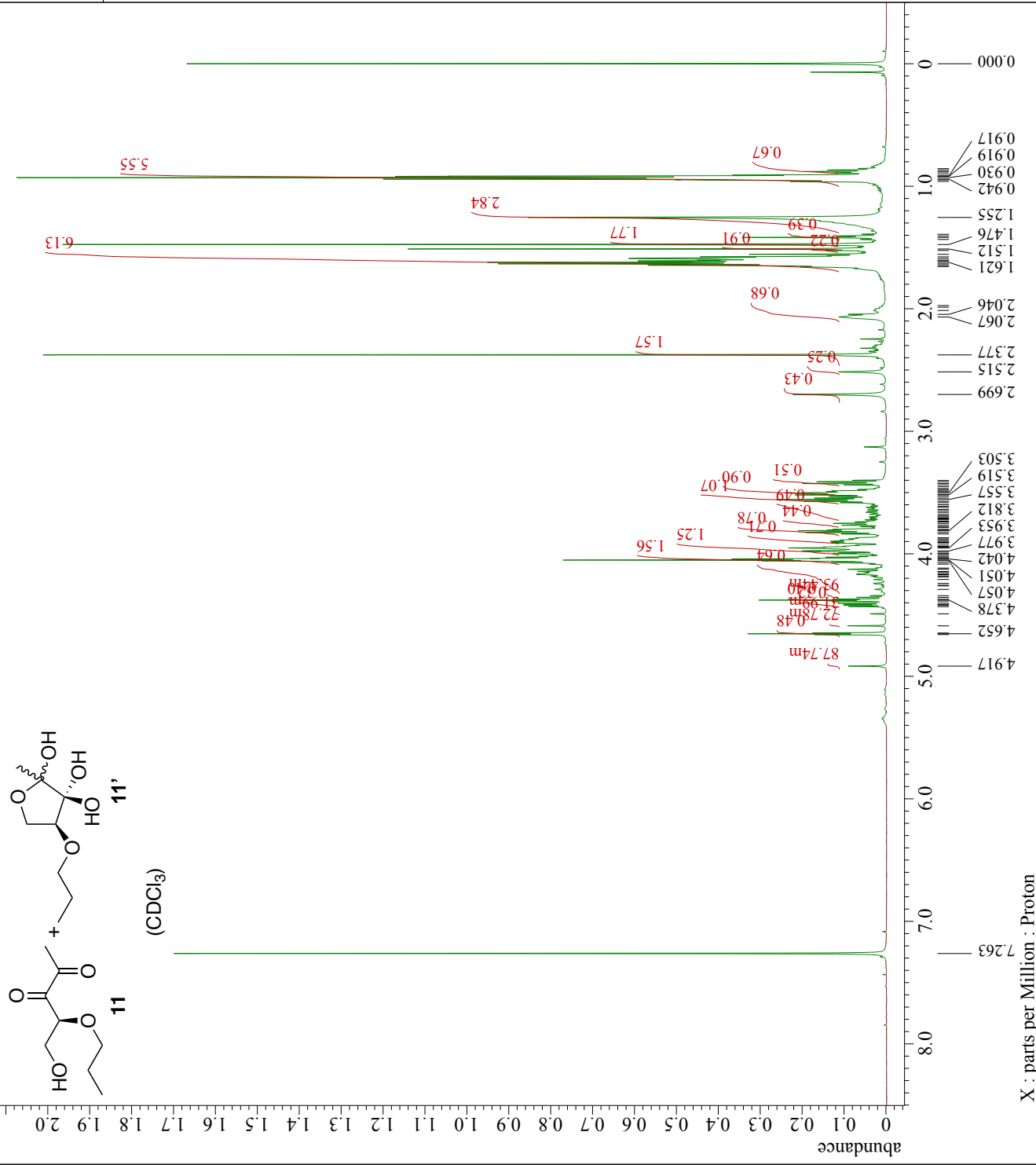
Relaxation\_Delay = 2 [s]  
Recvr Gain = 58  
Temp\_Get = 24 [dC]  
X\_90\_Width = 11.6 [us]  
X\_Acq\_Time = 0.69730304 [s]  
X\_Angle = 30 [deg]  
X\_Atn = 8 [dB]  
X\_Pulse = 3.86666667 [us]  
Irr\_Atn\_Dec = 23.33 [dB]  
Irr\_Atn\_Noie = 23.33 [dB]  
Irr\_Noise = WALTZ  
Irr\_Pwidth = 76 [us]  
Decoupling = TRUE  
Initial\_Wait = 1 [s]  
Noe = TRUE  
Noe Time = 2 [s]  
Repetition\_Time = 2.69730304 [s]



X : parts per Million : Carbon13



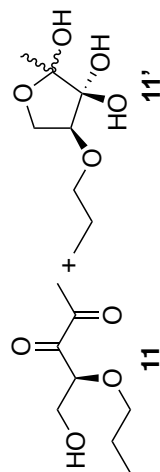
Filename = DN-1225-QSEG-Clm\_proton-a  
Author = delta  
Experiment = proton.jxp  
Sample Id = DN-1225-QSEG-Clm  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 24-FEB-2019 19:31:29  
Revision\_Time = 27-FEB-2019 21:32:44  
Comment = single\_pulse  
Data\_Format = ID COMPLEX  
Dim\_Size = 13107  
X\_Domain = Proton  
Dim Title = Proton  
Dim Units = [ppm]  
Dimensions = X  
Site = JNM-ECA600  
Spectrometer = DELTA2\_NMR  
Field Strength = 14.02588743 [T] (600 [MHz])  
X\_Acq\_Duration = 1.46276352 [s]  
X\_Domain = 1H  
X\_Freq = 597.17144293 [MHz]  
X\_Offset = 5 [ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.6836375 [Hz]  
X\_Sweep = 11.20071685 [kHz]  
X\_Sweep\_Clippped = 8.96057348 [kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 597.17144293 [MHz]  
Irr\_Offset = 5 [ppm]  
Tri\_Domain = Proton  
Tri\_Freq = 597.17144293 [MHz]  
Tri\_Offset = 5 [ppm]  
Clipped = FALSE  
Scans = 64  
Total\_Scans = 64  
Relaxation\_Delay = 5 [s]  
Recvr\_Gain = 50  
Temp\_Get = 24.1 [dc]  
X\_90\_Width = 7.15 [us]  
X\_Acq\_Time = 1.46276352 [s]  
X\_Angle = 45 [deg]  
X\_Atn = 2.8 [dB]  
X\_Pulse = 3.575 [us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1 [s]  
Repetition\_Time = 6.46276352 [s]



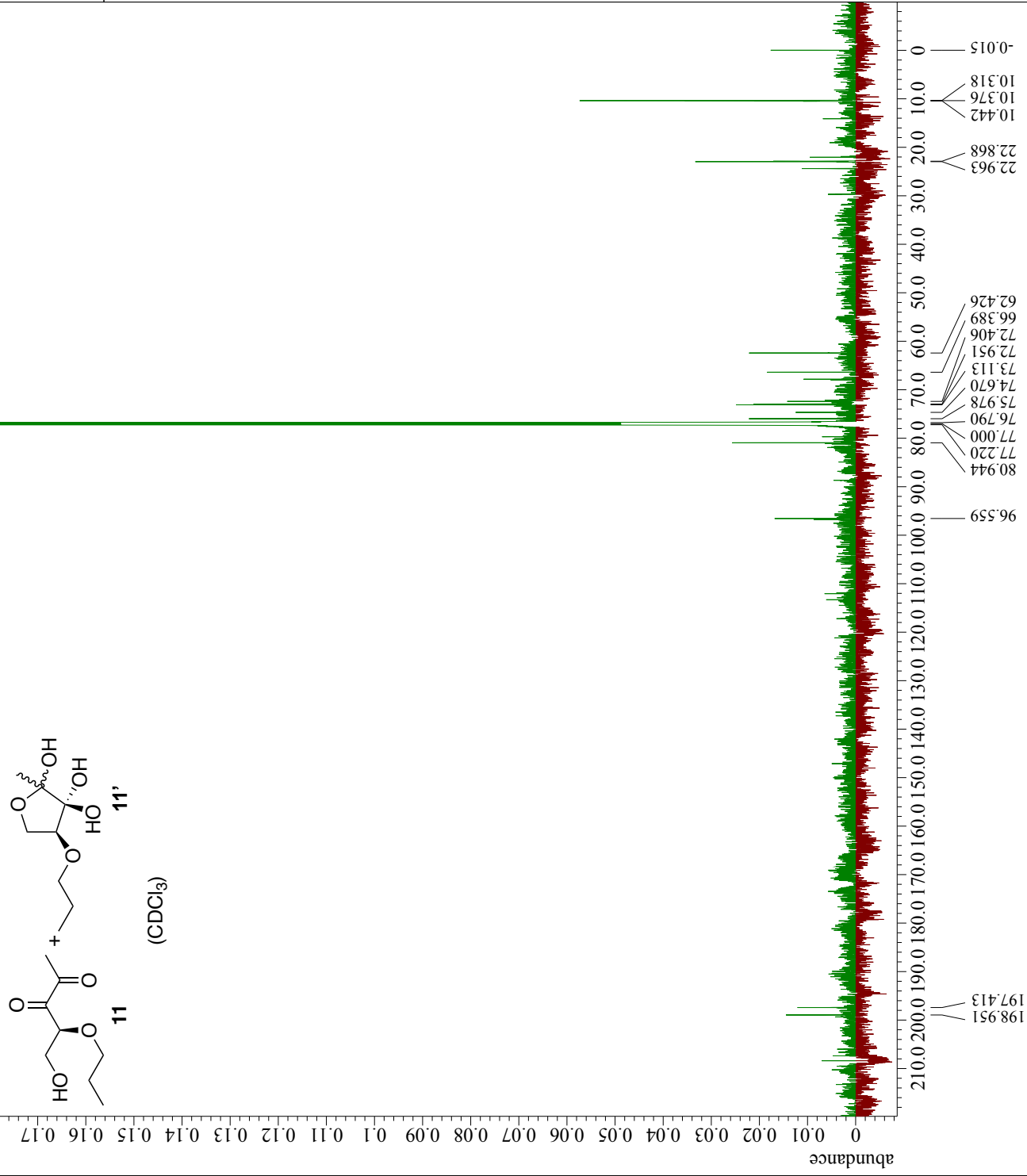
X : parts per Million : Proton



Filename = DN-1225-QSEG-Clm\_carbon\_3  
Author = delta  
Experiment = carbon\_jxp  
Sample Id = DN-1225-QSEG-Clm  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 24-FEB-2019 20:34:51  
Revision\_Time = 27-FEB-2019 16:48:52  
Comment = single pulse decoupled ga  
Data\_Format = 1D REAL  
Dim\_Size = 26214  
X\_Domain = Carbon  
Dim\_Title = Carbon13  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECA600  
Spectrometer = DELTA2\_NMR  
Field\_Strength = 14.02588743[T] (600 [MHz])  
X\_Acq\_Duration = 0[s]  
X\_Domain = 13C  
X\_Freq = 150.1588632 [MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 1.43409672 [Hz]  
X\_Sweep = 46.9924812 [kHz]  
X\_Sweep\_Clipped = 37.59398496 [kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 597.17144293 [MHz]  
Irr\_Offset = 5 [ppm]  
Clipped = TRUE  
Incomplete\_Copy = TRUE  
Scans = 3601  
Total\_Scans = 3601  
Relaxation\_Delay = 2[s]  
Recvr Gain = 58  
Temp\_Get = 24.3 [dC]  
X\_90\_Width = 11.6 [us]  
X\_Acq\_Time = 0.69730304 [s]  
X\_Angle = 30 [deg]  
X\_Atn = 8 [dB]  
X\_Pulse = 3.86666667 [us]  
Irr\_Atn\_Dec = 23.33 [dB]  
Irr\_Atn\_Noise = 23.33 [dB]  
Irr\_Noise = WALTZ  
Irr\_Width = 76 [us]  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE  
Noe\_Time = 2[s]  
Repetition\_Time = 2.69730304 [s]



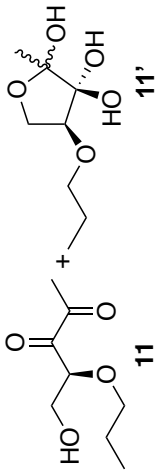
(CDCl<sub>3</sub>)



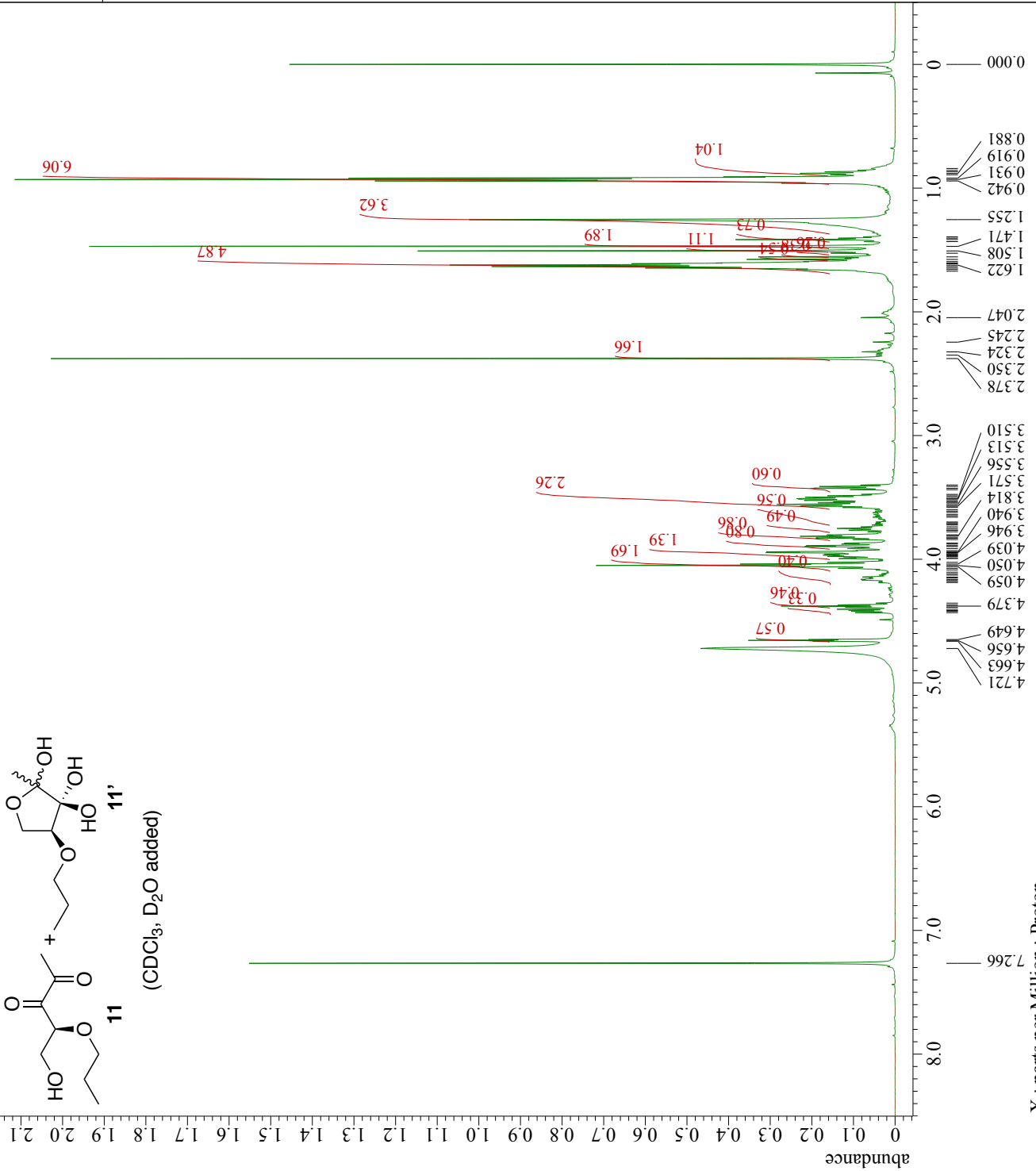
X : parts per Million : Carbon13



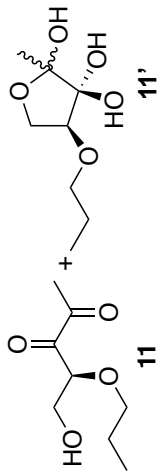
Filename = DN-1225-QSEG-Clm-addD2O\_p  
Author = del ta  
Experiment = proton.jxp  
Sample\_Id = DN-1225-QSEG-Clm-addD2O  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 24-FEB-2019 23:27:56  
Revision\_Time = 27-FEB-2019 17:41:36  
Comment = single\_pulse  
Data\_Format = ID REAL  
Dim\_Size = 13107  
X\_Domain = Proton  
Dim\_Title = Proton  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECA600  
Spectrometer = DELTA2\_NMR  
Field\_Strength = 14.02588743 [T] (600 [MHz])  
X\_Acq\_Duration = 1.46276352 [s]  
X\_Domain = 1H  
X\_Freq = 597.17144293 [MHz]  
X\_Offset = 5 [ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.6836375 [Hz]  
X\_Sweep = 11.20071685 [kHz]  
X\_Sweep\_Clippped = 8.96057348 [kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 597.17144293 [MHz]  
Irr\_Offset = 5 [ppm]  
Tri\_Domain = Proton  
Tri\_Freq = 597.17144293 [MHz]  
Tri\_Offset = 5 [ppm]  
Clipped = FALSE  
Scans = 128  
Total\_Scans = 128  
Relaxation\_Delay = 5 [s]  
Recvr\_Gain = 50  
Temp\_Get = 24.3 [dC]  
X\_90\_Width = 7.15 [us]  
X\_Acq\_Time = 1.46276352 [s]  
X\_Angle = 45 [deg]  
X\_Atn = 2.8 [dB]  
X\_Pulse = 3.575 [us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Preset = FALSE  
Initial\_Wait = 1 [s]  
Repetition\_Time = 6.46276352 [s]



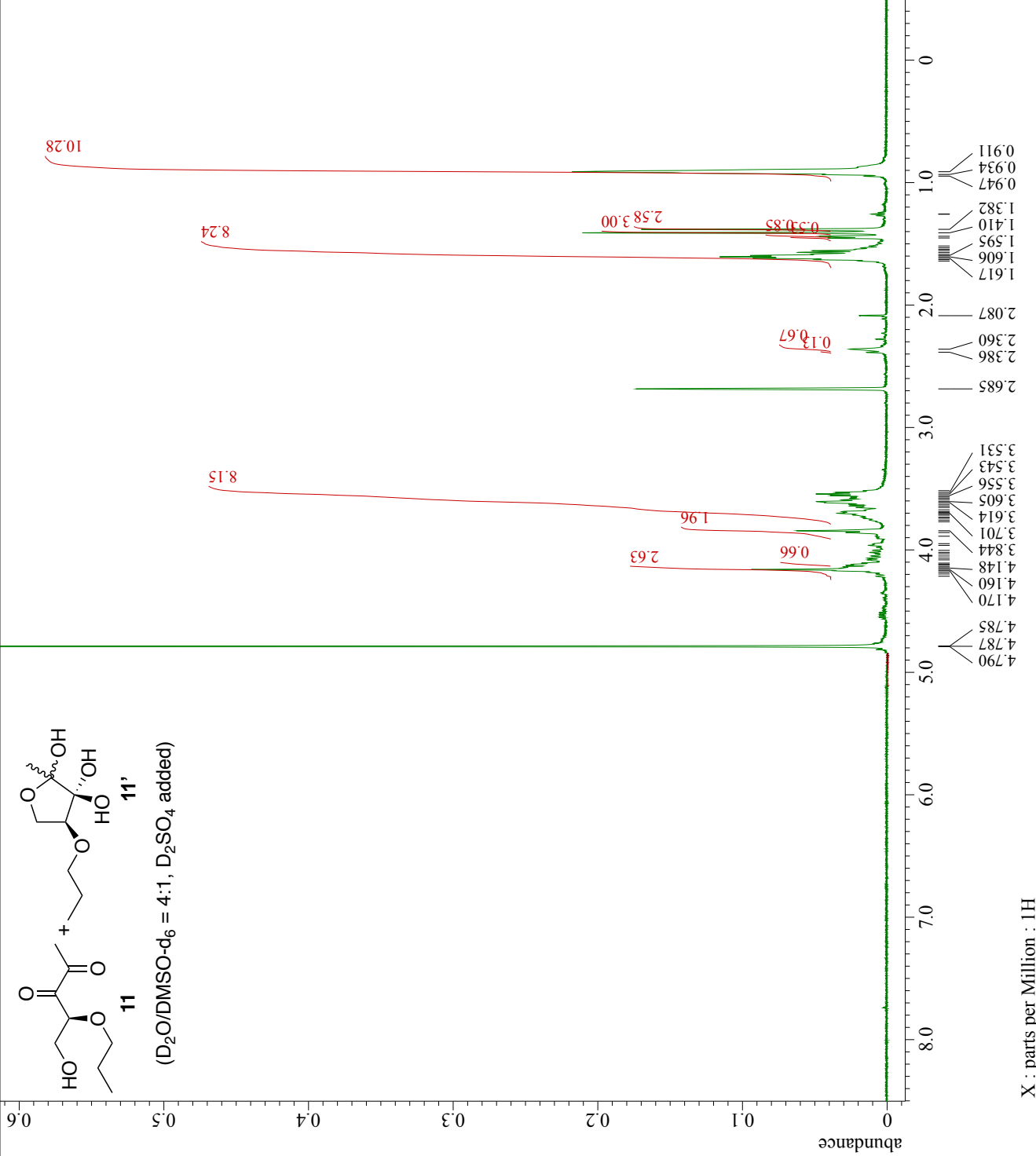
(CDCl<sub>3</sub>, D<sub>2</sub>O added)



X : parts per Million : Proton



(D<sub>2</sub>O/DMSO-d<sub>6</sub> = 4:1, D<sub>2</sub>SO<sub>4</sub> added)



```

Filename = nakamura_1H_D2O-an-1.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = km
Solvent = D2O
Actual_Start_Time = 19-FEB-2019 18:36:23
Revision_Time = 27-FEB-2019 18:36:40

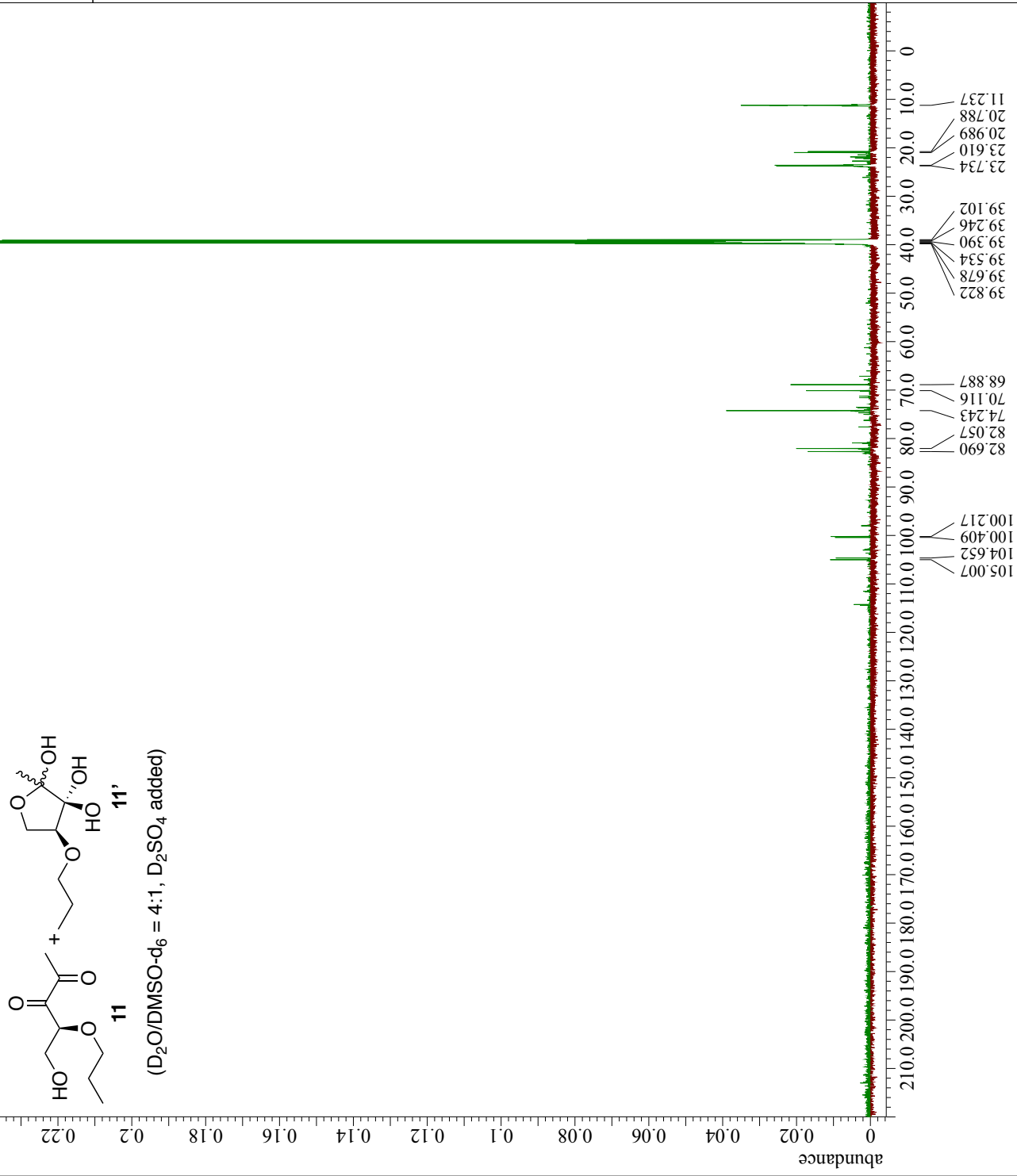
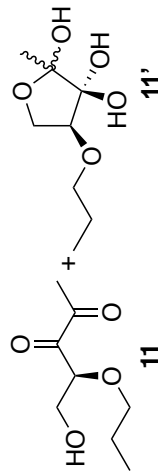
Comment = a-NON
Data_Format = 1D COMPLEX
Dim_Size = 52428
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECA 600SL
Spectrometer = JNM-ECA600

Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 5.88251136[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 0.16999542[Hz]
X_Sweep = 11.14081996[kHz]
Irr_Domain = 1H
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32

Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 25.5[dc]
X_90_Width = 14[us]
X_Acq_Time = 5.88251136[s]
X_Angle = 45[deg]
X_Atn = 2.5[db]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 10.88251136[s]

```

X : parts per Million : 1H



JEOL

Filename = nakamura\_13C\_D2O-3.jdf  
 Author = delta  
 Experiment = single\_pulse\_dec  
 Sample Id = km  
 Solvent = D2O  
 Actual\_Start\_Time = 19-FEB-2019 19:03:43  
 Revision\_Time = 28-FEB-2019 09:58:41

Comment = a-COM  
 Data\_Format = 1D COMPLEX  
 Dim\_Size = 26214  
 X\_Domain = 13C  
 Dim\_Title = 13C  
 Dim\_Units = [ppm]  
 Dimensions = X  
 Site = ECA 600SL  
 Spectrometer = JNM-ECA600

Field Strength = 13.95540559[T] (590 [MHz])  
 X\_Acq\_Duration = 0.69730304[s]  
 X\_Domain = 13C  
 X\_Freq = 149.40429612 [MHz]  
 X\_Offset = 100 [ppm]  
 X\_Points = 32768  
 X\_Prescans = 4  
 X\_Resolution = 1.43409672 [Hz]  
 X\_Sweep = 46.9924812 [kHz]  
 Irr\_Domain = 1H  
 Irr\_Freq = 594.17058168 [MHz]  
 Irr\_Offset = 5 [ppm]  
 Clipped = TRUE  
 Scans = 28881  
 Total\_Scans = 28881

Relaxation\_Delay = 2 [s]  
 Recvr\_Gain = 58  
 Temp\_Get = 26 [dC]  
 X\_90\_Width = 12 [us]  
 X\_Acq\_Time = 0.69730304 [s]  
 X\_Angle = 30 [deg]  
 X\_Atn = 8.6 [dB]  
 X\_Pulse = 4 [us]  
 Irr\_Atn\_Dec = 17.194 [dB]  
 Irr\_Atn\_Noise = 17.194 [dB]  
 Irr\_Noise = WALTZ  
 Decoupling = TRUE  
 Initial\_Wait = 1 [s]  
 Noe\_Time = TRUE  
 Repetition\_Time = 2 [s]

X : parts per Million : 13C