Supporting Information

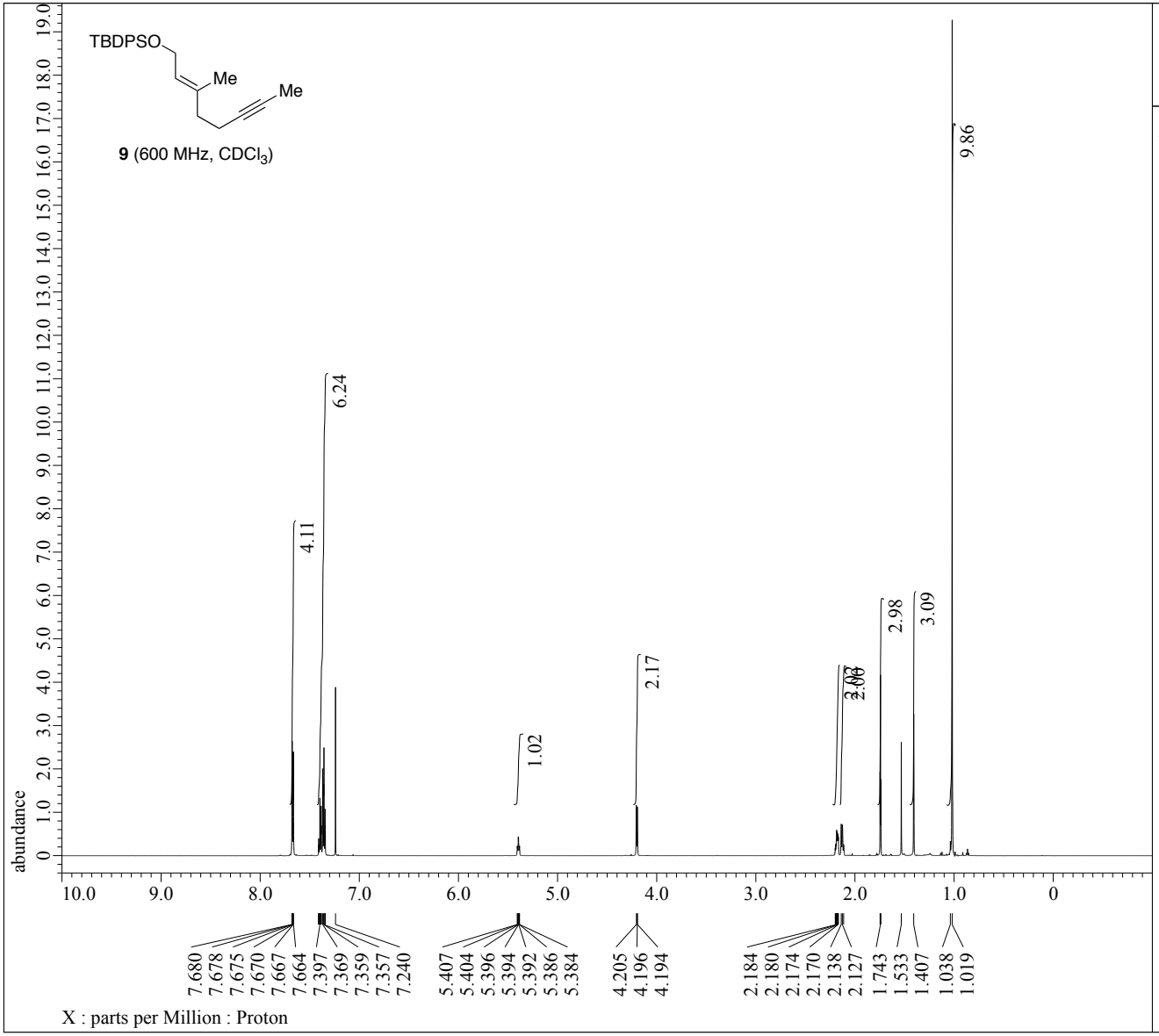
Complete Stereochemical Assignment of Campechic Acids A and B

Ruri Isaka,[†] Linkai Yu,[‡] Makoto Sasaki,[†] Yasuhiro Igarashi,[‡] and Haruhiko Fuwa*[,†]

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

[‡]Biotechnology Research Center and Department of Biotechnology, Toyama Prefectural University, 5180 Kurokawa, Imizu, Toyama 939-0398, Japan

*Corresponding author: hfuwa@m.tohoku.ac.jp

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Filename          = RI-II-035_proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-035
Solvent           = CHLOROFORM-D
Creation_Time     =  6-FEB-2015 10:14:28
Revision_Time     = 13-JAN-2016 22:13:38
Current_Time      = 13-JAN-2016 22:14:19

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        = 40
Temp_Get          = 20.1[dC]
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]
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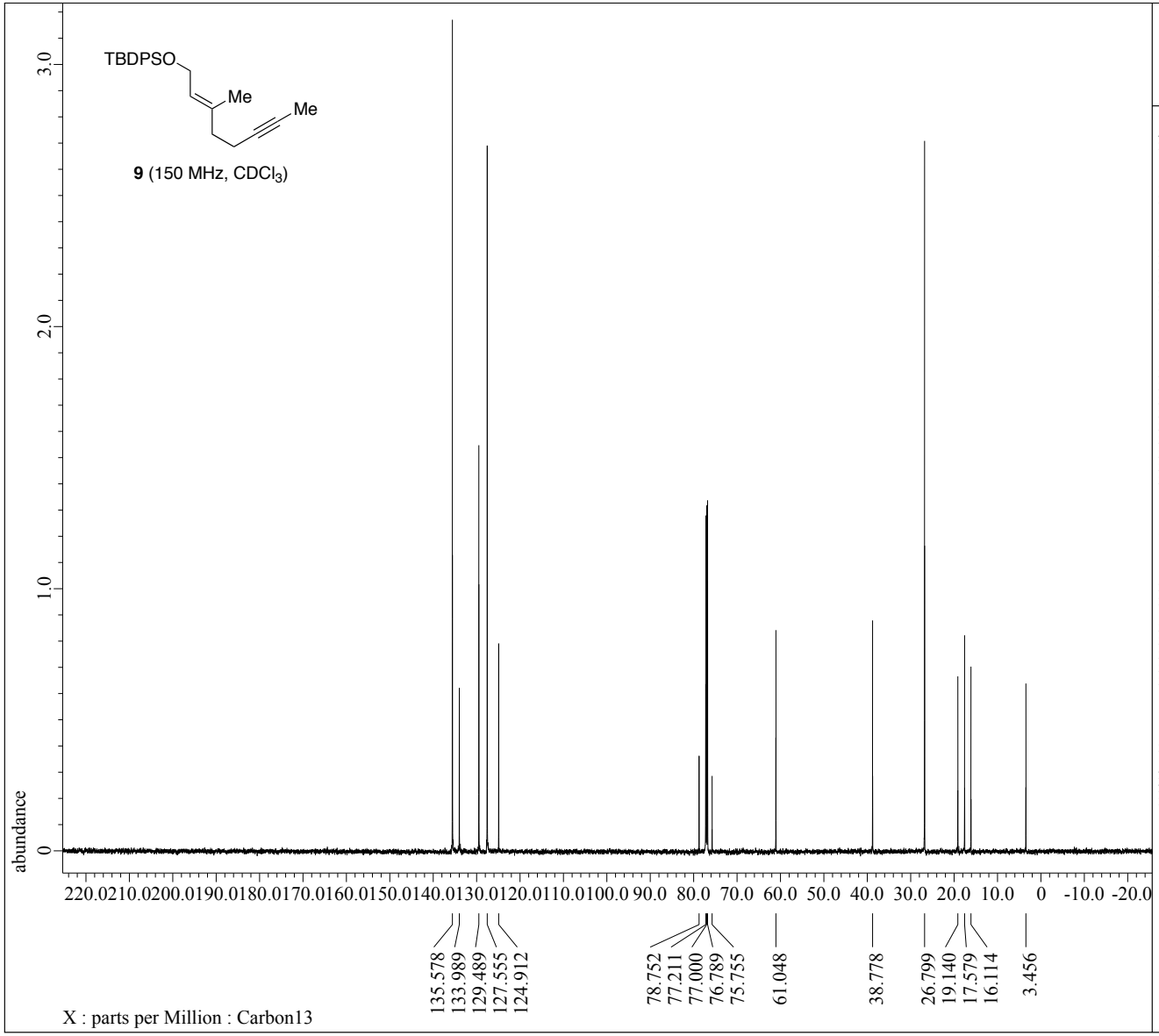

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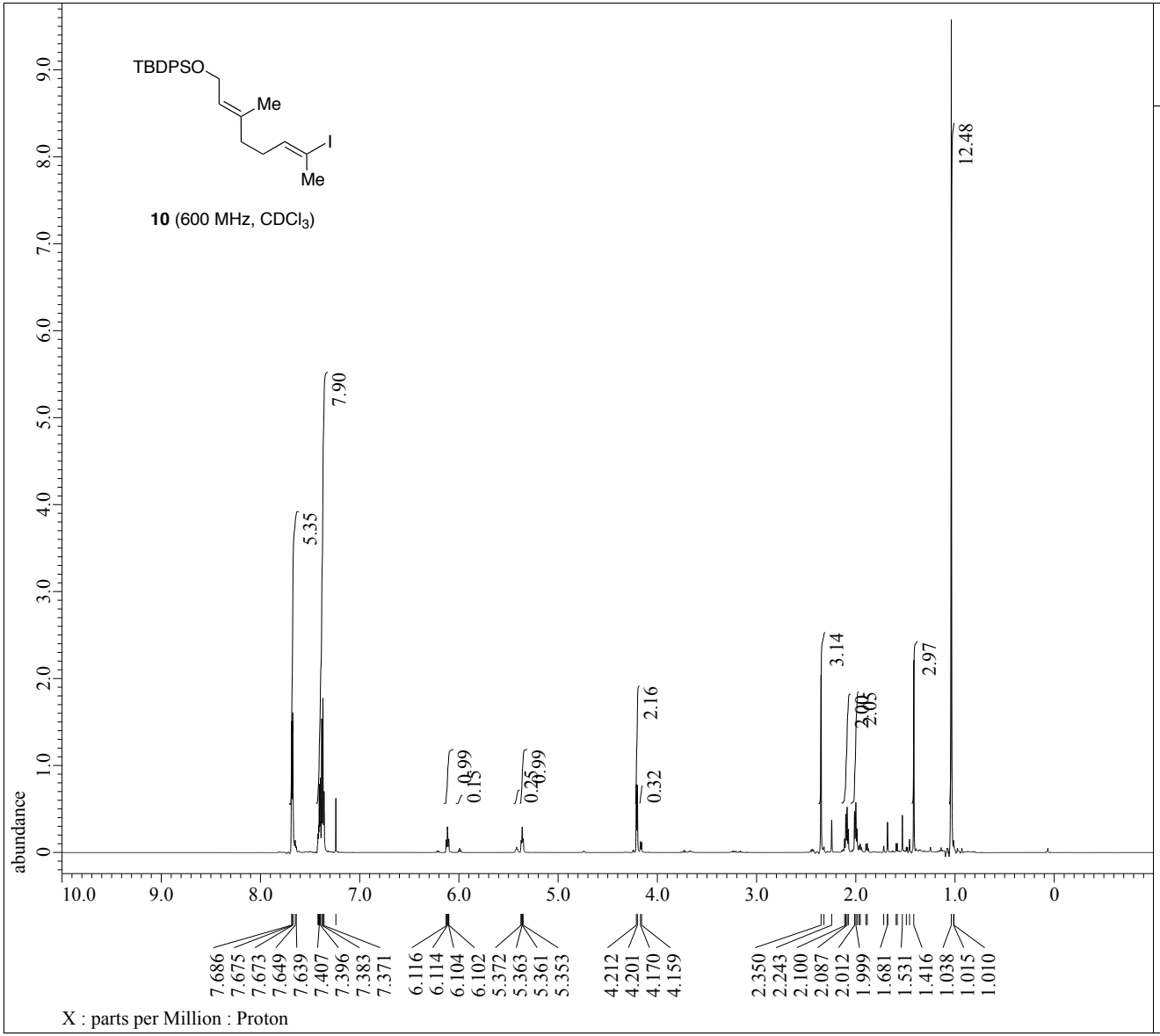
Filename          = RI-II-102_Carbon-3-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-102
Solvent           = CHLOROFORM-D
Creation_Time     =  1-JUL-2015 11:52:35
Revision_Time     = 13-JAN-2016 22:15:24
Current_Time      = 13-JAN-2016 22:15:43

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 256
Total_Scans       = 256

Relaxation_Delay  = 2[s]
Recvr_Gain        = 54
Temp_Get          = 22[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_Noe       = 24.452[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]
```



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```
Filename          = RI-III-026_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-III-026
Solvent           = Chloroform-D
Creation_Time     = 19-NOV-2015 16:01:39
Revision_Time     = 13-JAN-2016 22:20:20
Current_Time      = 13-JAN-2016 22:21:02

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        = 28
Temp_Get          = 22.2[dC]
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]
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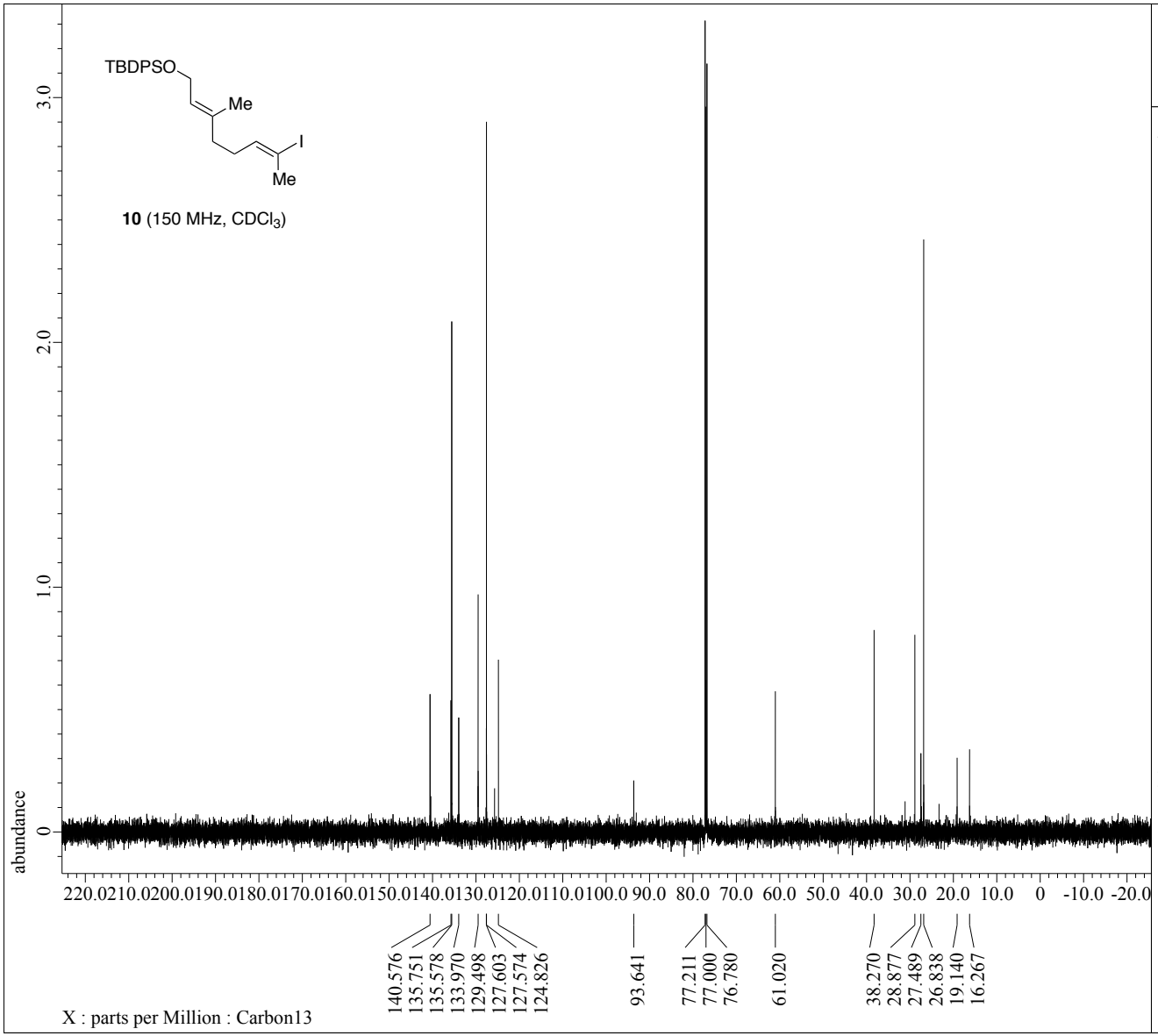


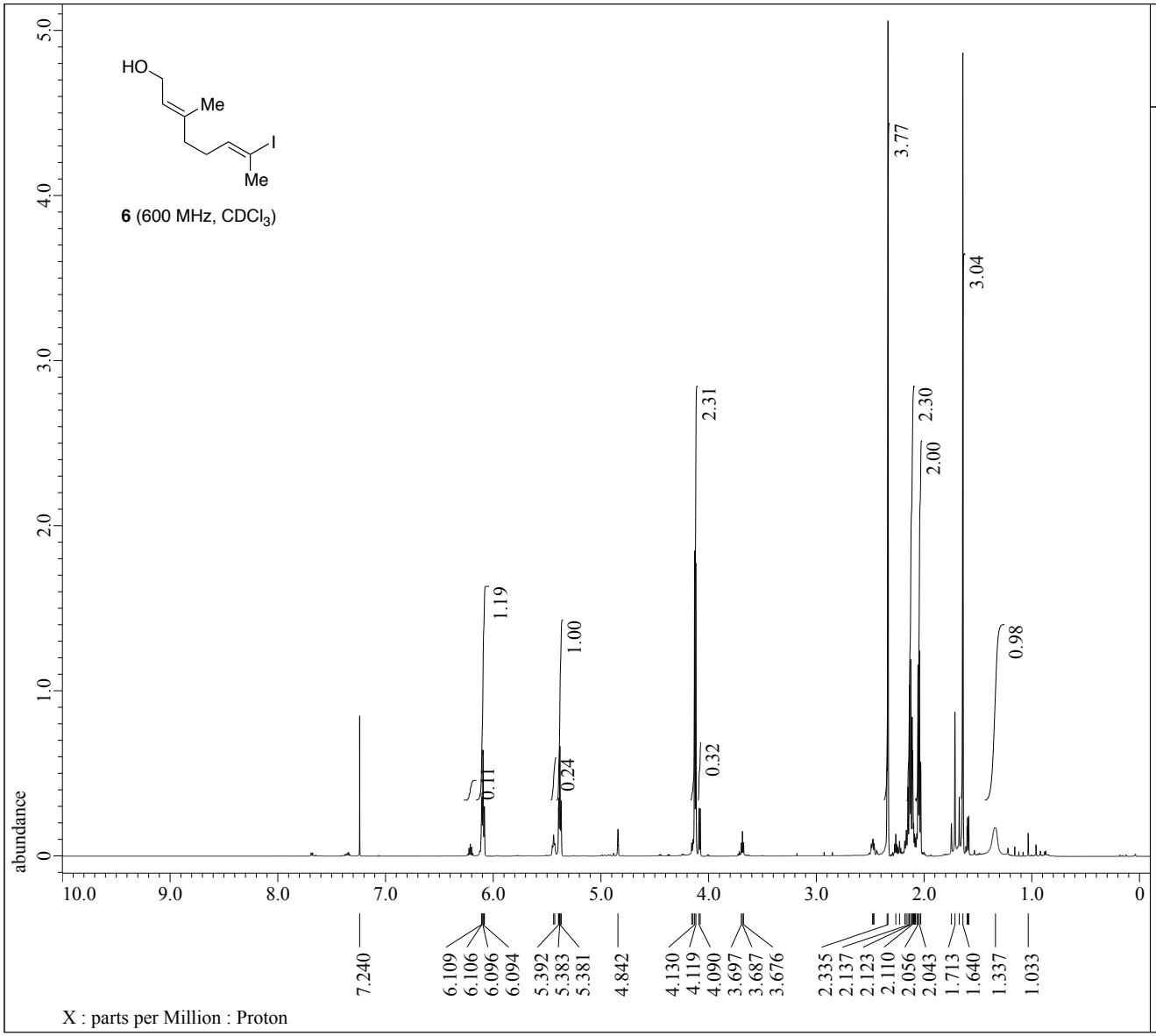
JEOL Solutions for Innovation

```
Filename          = RI-III-026_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-III-026
Solvent           = CHLOROFORM-D
Creation_Time     = 19-NOV-2015 18:59:28
Revision_Time     = 13-JAN-2016 22:22:14
Current_Time      = 13-JAN-2016 22:22:29

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 80
Total_Scans       = 80

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 21.9[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_Noe       = 24.452[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]
```



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```
Filename          = RI-III-027_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-III-027
Solvent           = CHLOROFORM-D
Creation_Time     = 20-NOV-2015 15:06:35
Revision_Time     = 13-JAN-2016 22:27:14
Current_Time      = 13-JAN-2016 22:27:40

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        = 26
Temp_Get          = 21.9[dC]
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]
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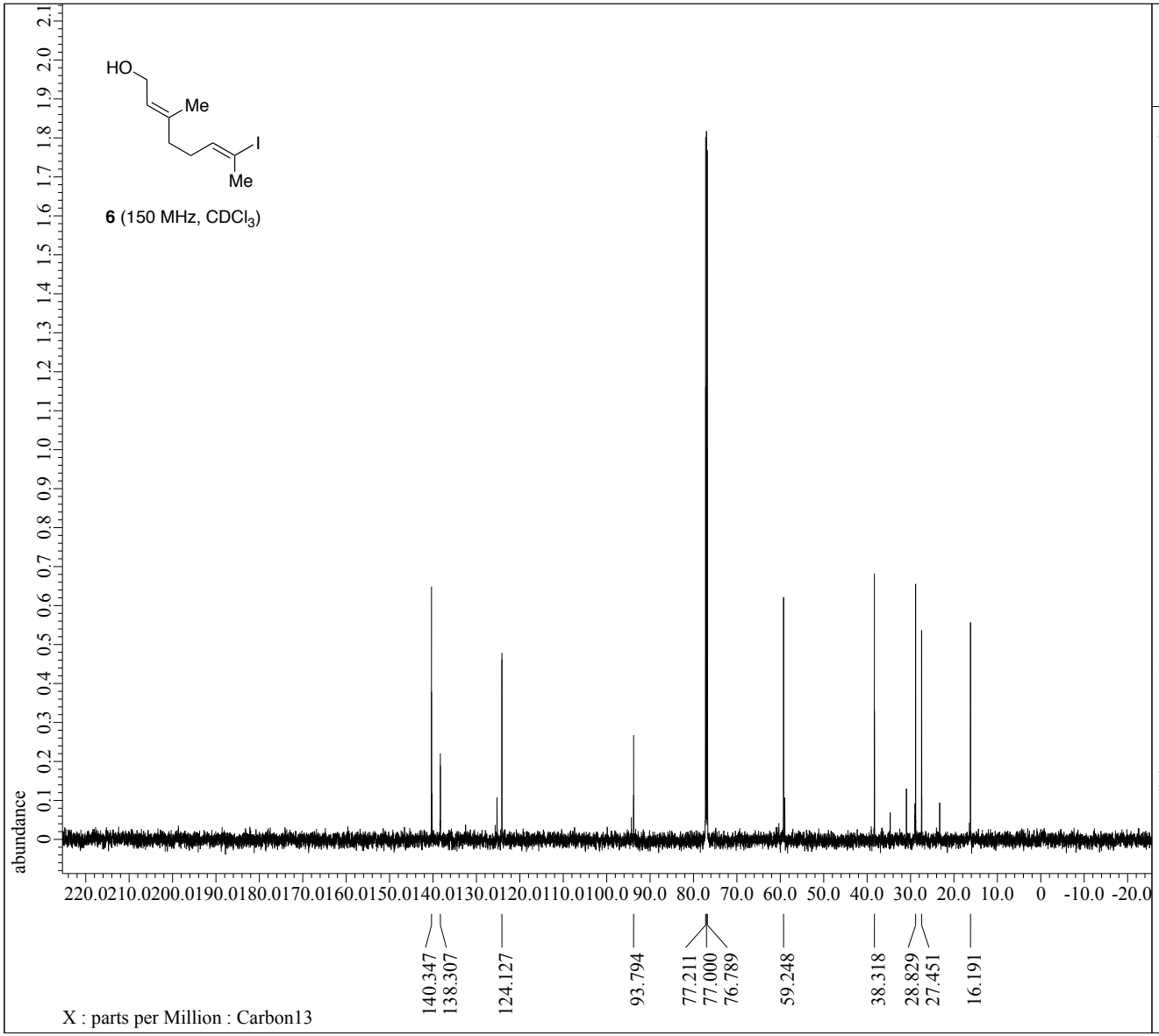


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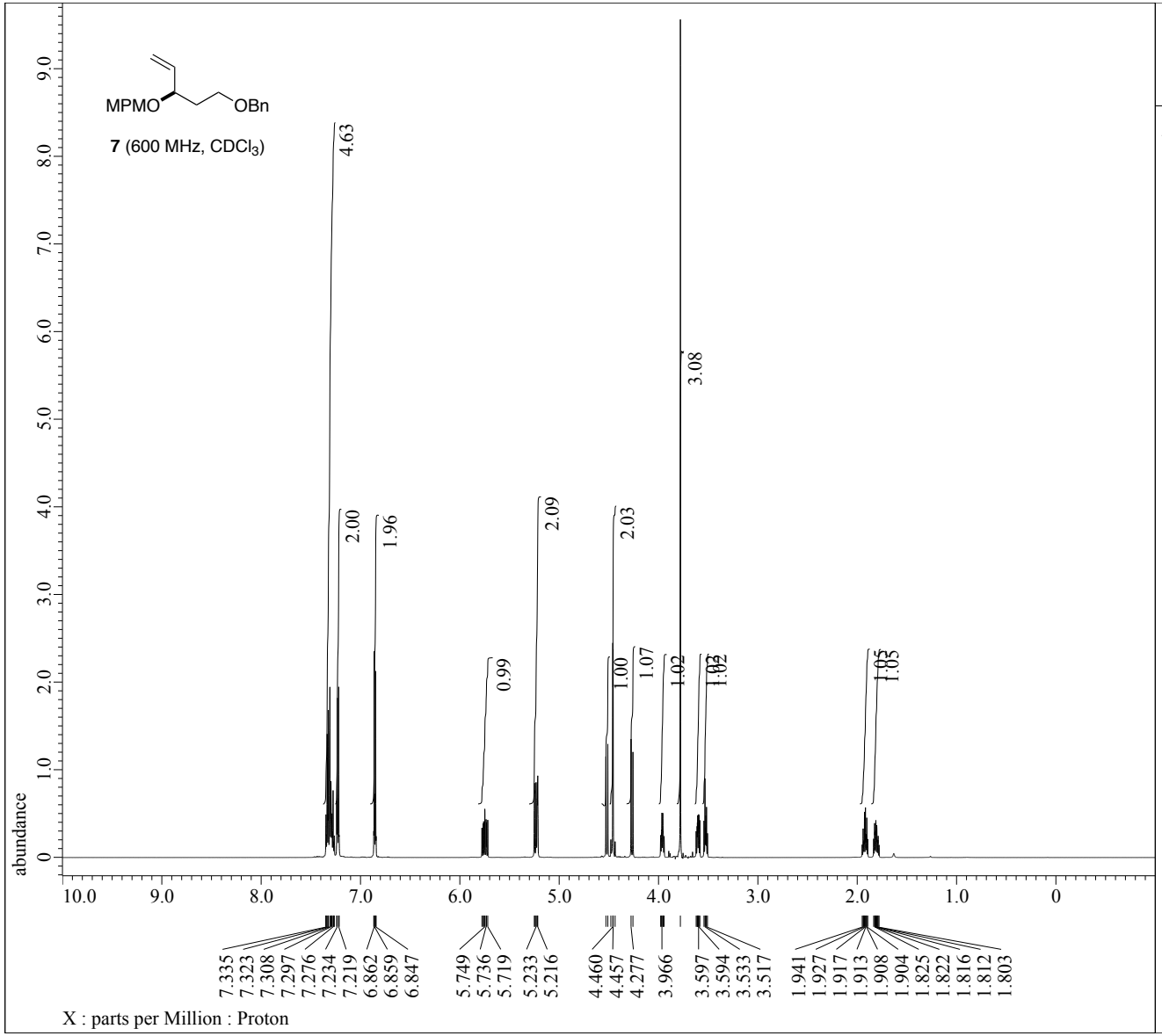
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-III-027
Solvent           = CHLOROFORM-D
Creation_Time     = 20-NOV-2015 15:10:24
Revision_Time     = 13-JAN-2016 22:29:16
Current_Time      = 13-JAN-2016 22:29:48

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 80
Total_Scans       = 80

Relaxation_Delay  = 2[s]
Recvr_Gain        = 54
Temp_Get          = 22[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_Noe       = 24.452[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]
```

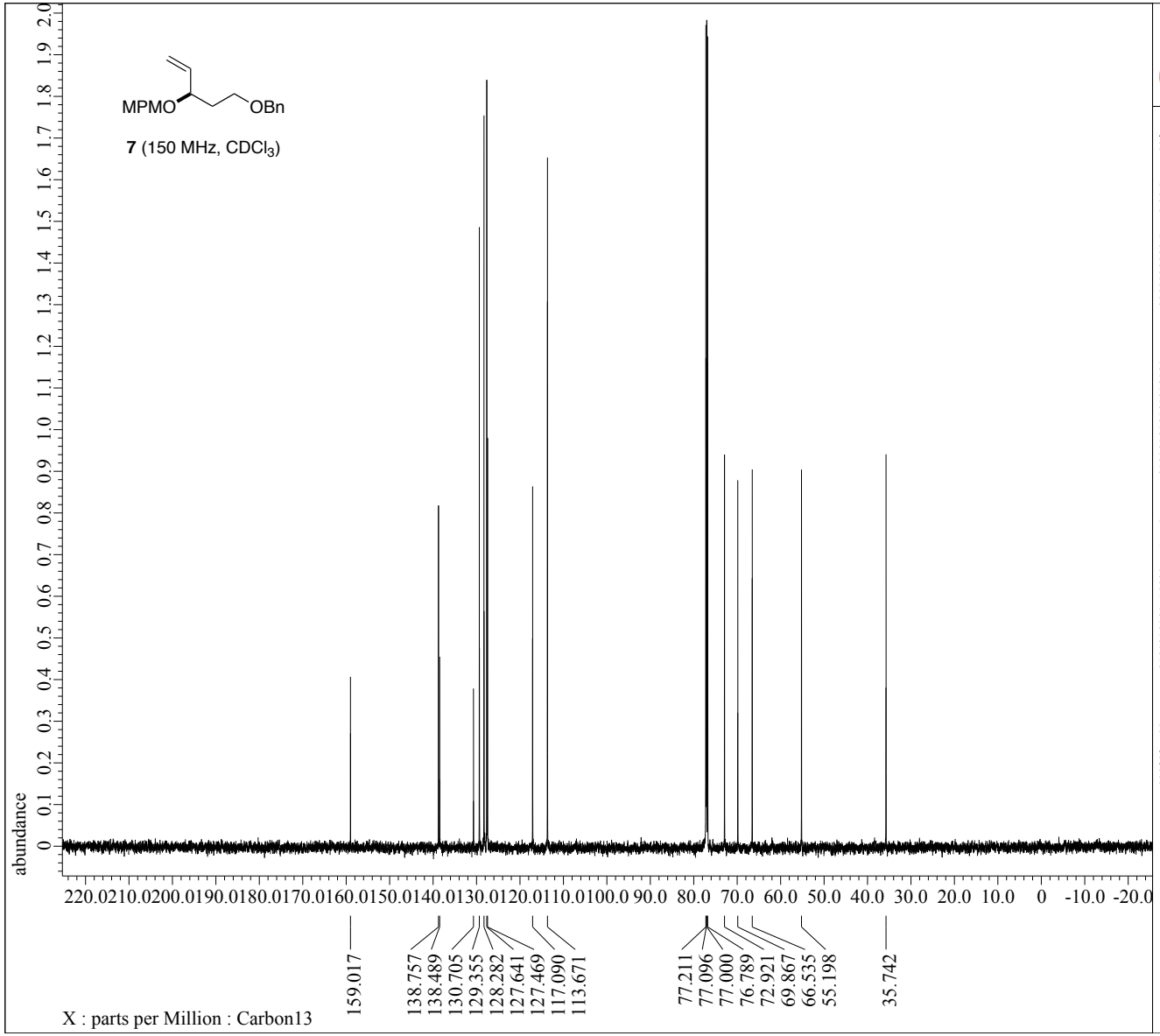



```
Filename          = /Users/HaruhikoFuwa/Deskto
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-104a
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2016 13:44:02
Revision_Time     = 19-JAN-2016 11:03:48
Current_Time      = 19-JAN-2016 11:04:24

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        = 22
Temp_Get          = 20.2[dC]
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]
```

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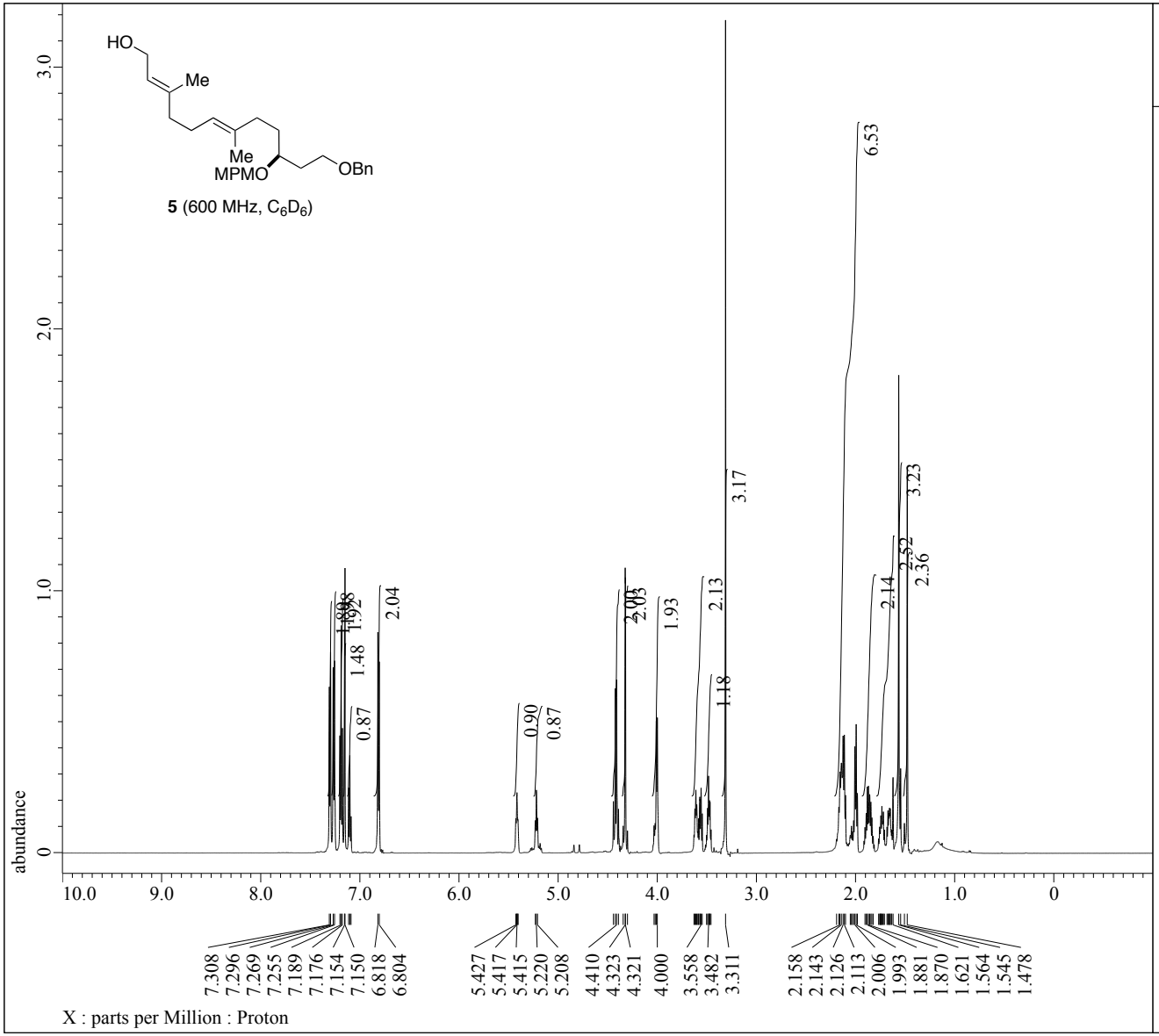
Filename          = /Users/HaruhikoFuwa/Deskto
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-104a
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2016 13:47:47
Revision_Time     = 19-JAN-2016 11:05:11
Current_Time      = 19-JAN-2016 11:05:24

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 180
Total_Scans       = 180

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 20.5[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_Noe       = 24.452[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]
```



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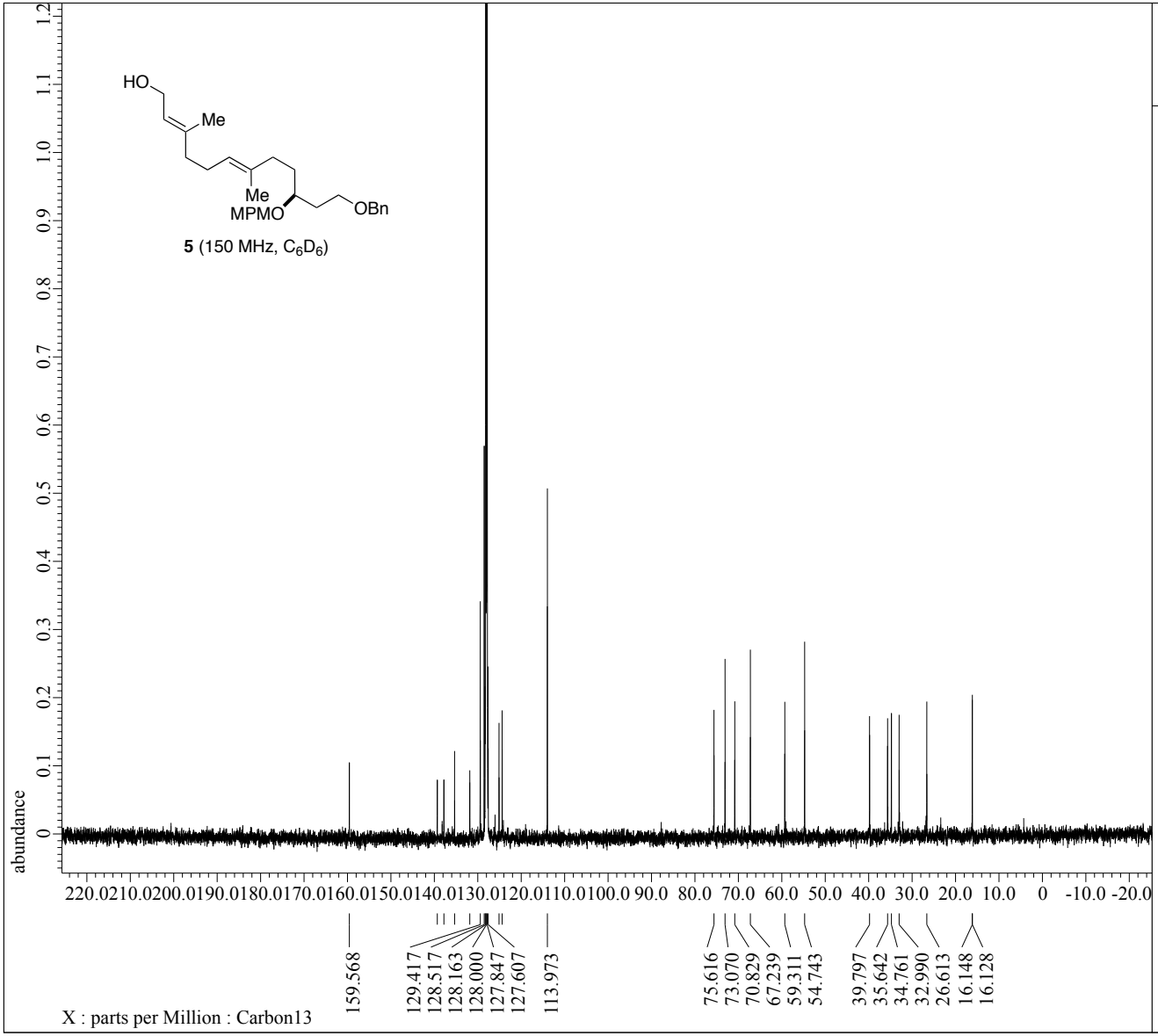
```
Filename          = RI-III-029_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-III-029
Solvent           = BENZENE-D6
Creation_Time     = 21-NOV-2015 13:28:56
Revision_Time     = 13-JAN-2016 22:34:10
Current_Time      = 13-JAN-2016 22:34:51

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        = 22
Temp_Get          = 21.8[dC]
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]
```

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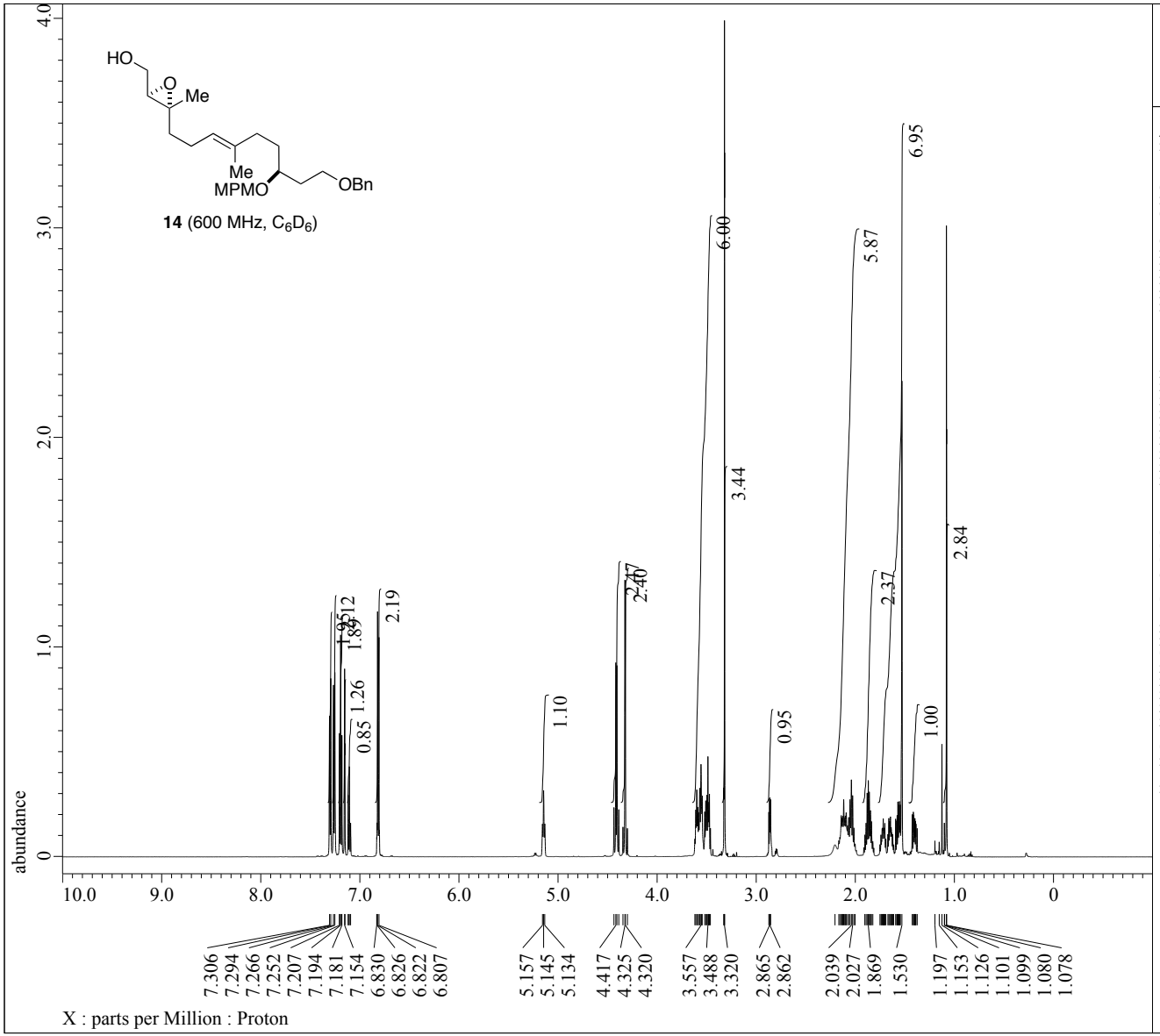
Filename          = RI-III-029_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-III-029
Solvent           = BENZENE-D6
Creation_Time     = 21-NOV-2015 13:32:19
Revision_Time     = 13-JAN-2016 22:35:48
Current_Time      = 13-JAN-2016 22:36:01

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 80
Total_Scans       = 80

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 21.8[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_Noe       = 24.452[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]
```



JEOL Solutions for Innovation

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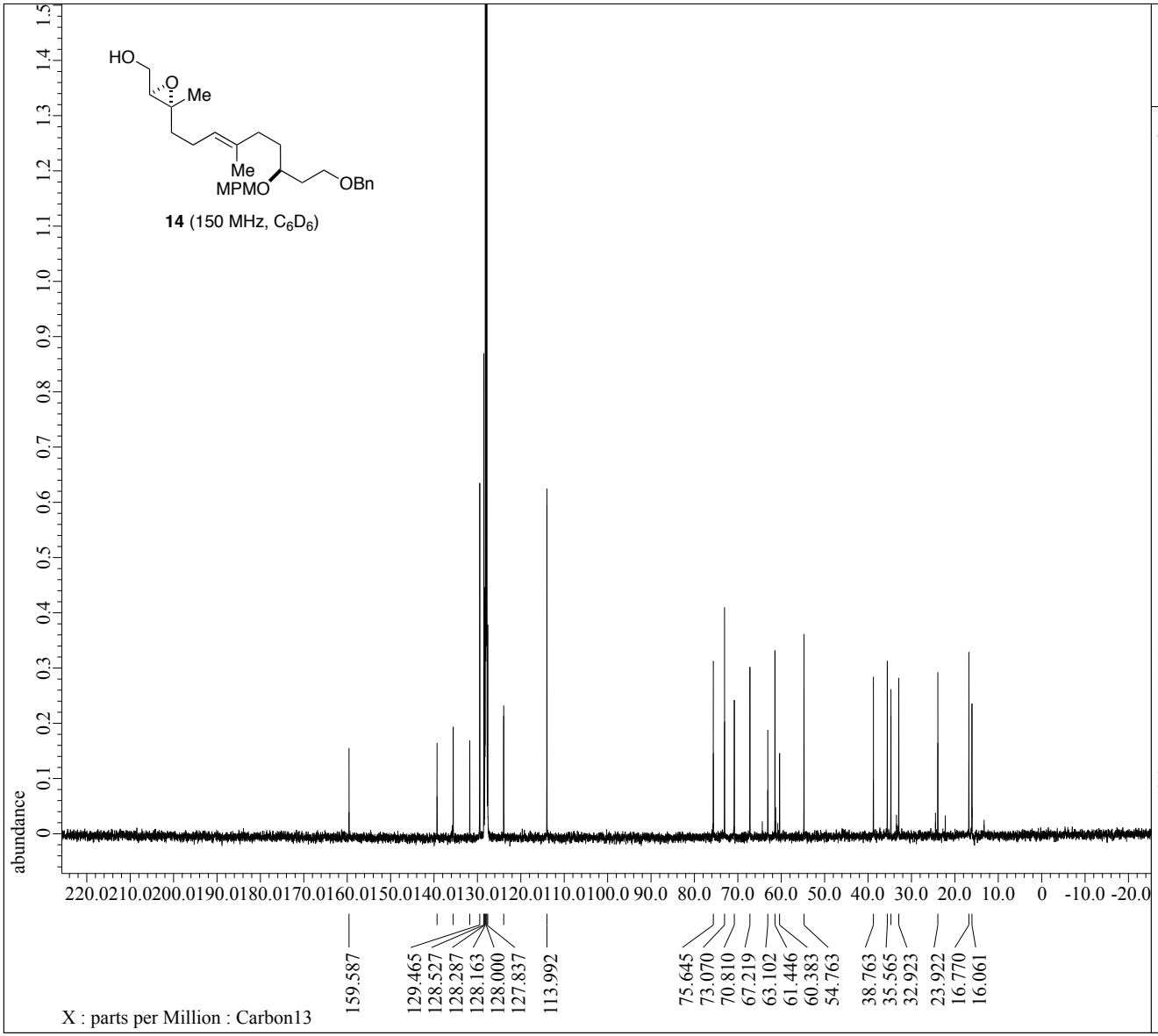
Filename          = RI-II-128_proton-3-5.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-128
Solvent           = BENZENE-D6
Creation_Time     =  7-JUL-2015 14:44:42
Revision_Time     = 13-JAN-2016 22:40:51
Current_Time      = 13-JAN-2016 22:41:20

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        = 20
Temp_Get          = 21.8[dC]
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]
```



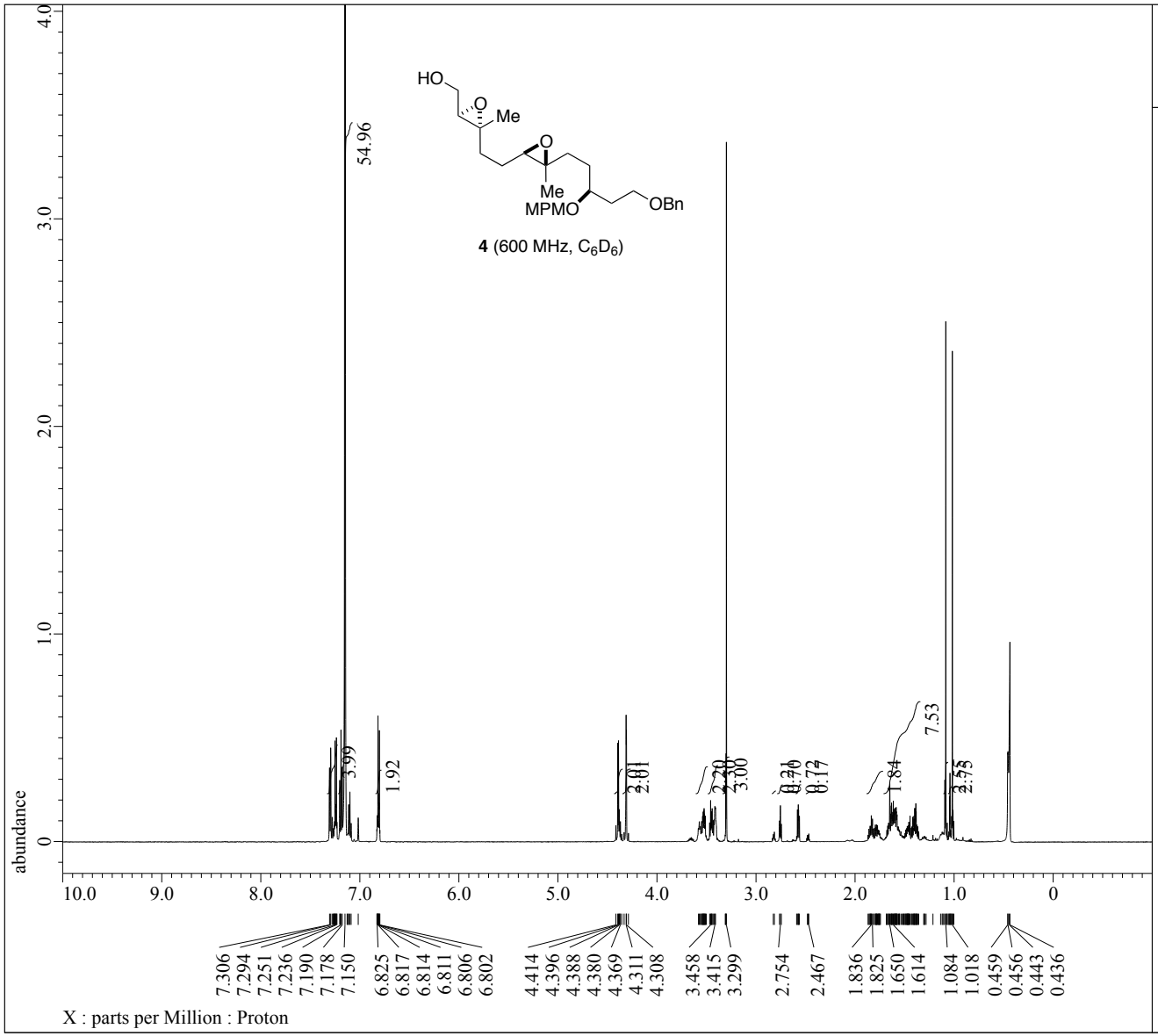
JEOL Solutions for Innovation

```
Filename          = RI-II-128_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-128
Solvent           = BENZENE-D6
Creation_Time     =  7-JUL-2015 14:48:10
Revision_Time     = 13-JAN-2016 22:42:22
Current_Time      = 13-JAN-2016 22:42:34

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 172
Total_Scans       = 172

Relaxation_Delay  = 2[s]
Recvr_Gain        = 52
Temp_Get          = 22[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_Noe       = 24.452[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]
```



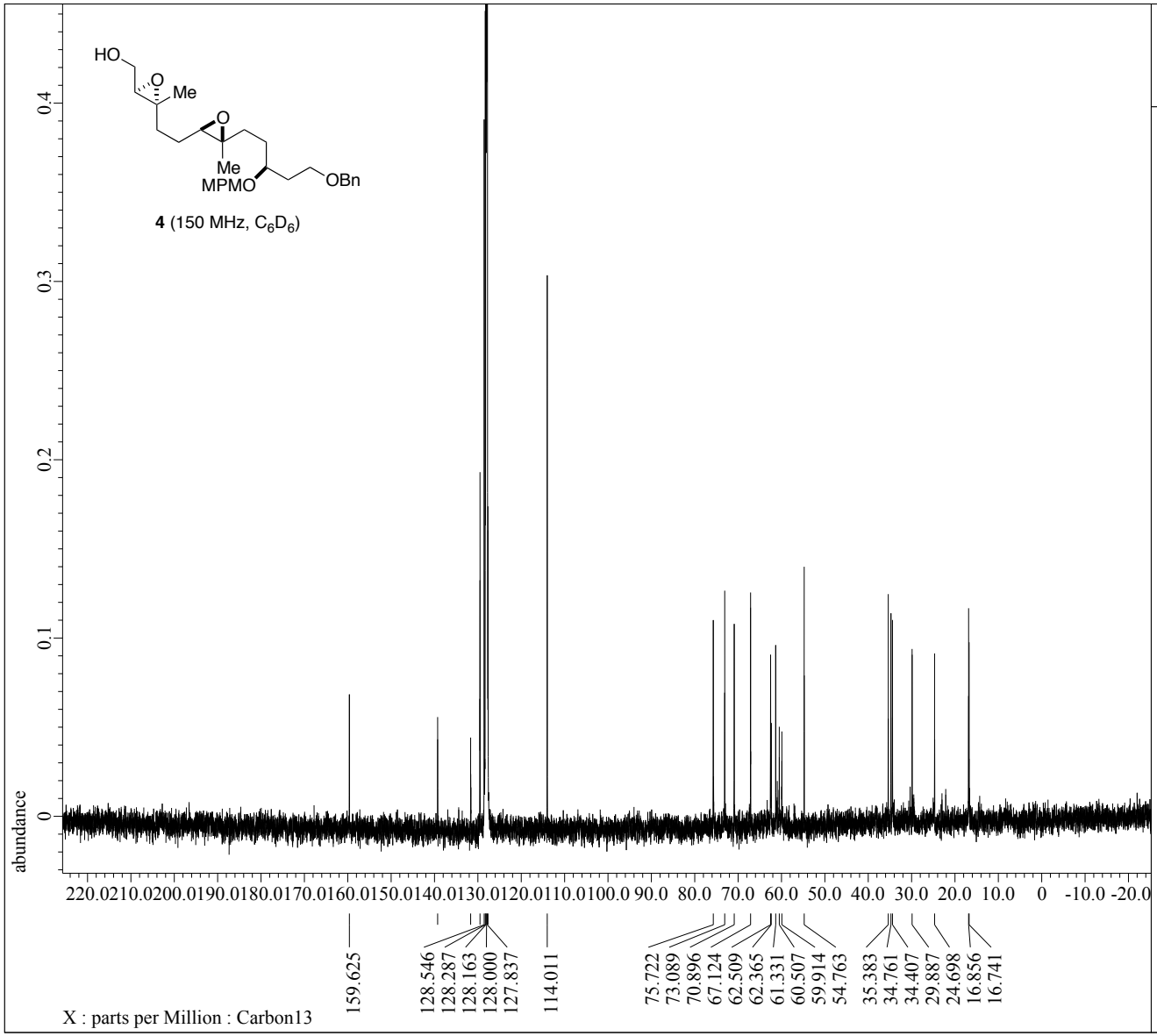
JEOL
Solutions for Innovation

```
Filename          = RI-II-147_proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-147
Solvent           = BENZENE-D6
Creation_Time     = 10-JUL-2015 18:18:17
Revision_Time     = 13-JAN-2016 22:48:17
Current_Time      = 13-JAN-2016 22:49:10

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_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        = 42
Temp_Get          = 22.3[dC]
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]
```



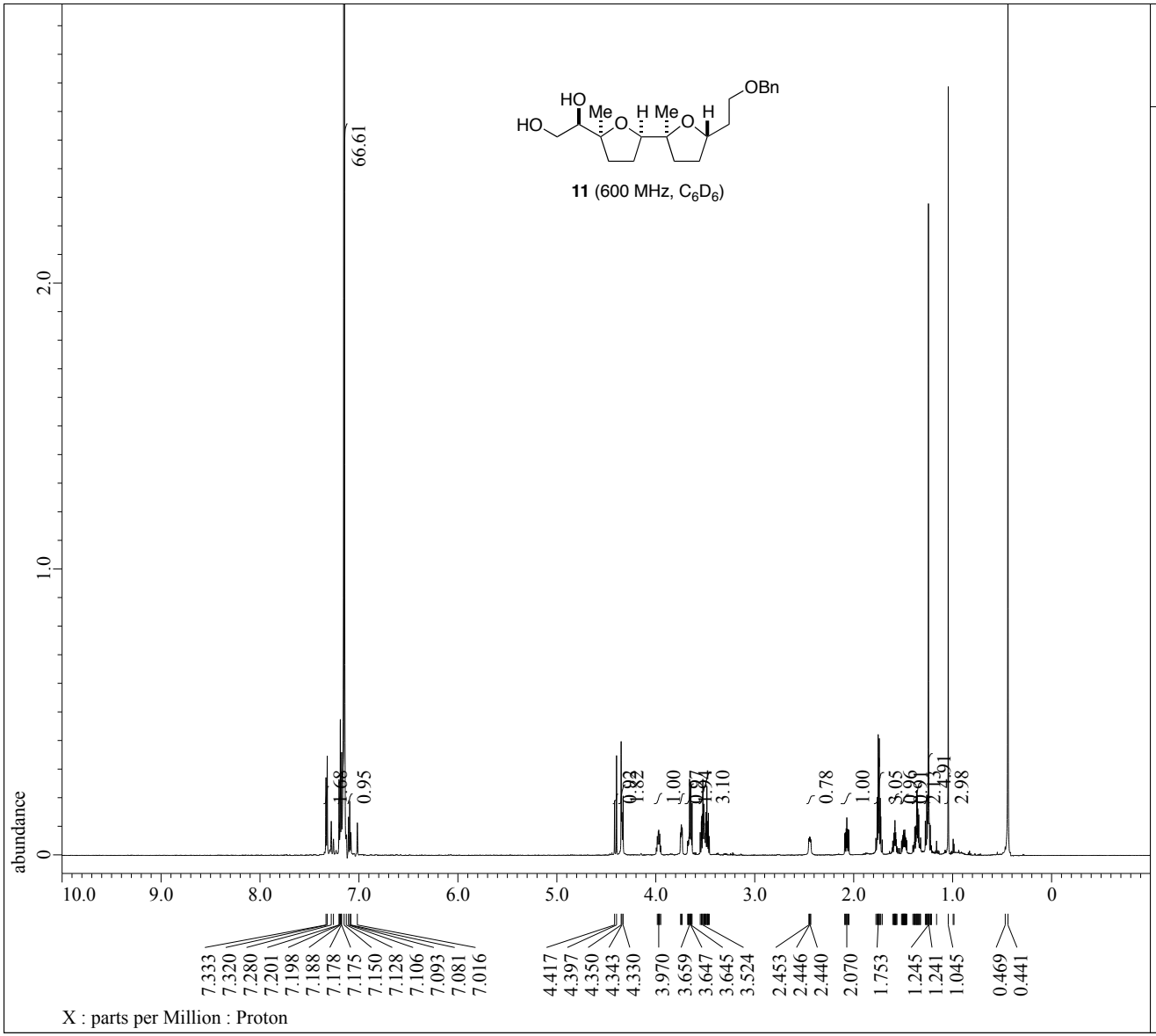
JEOL Solutions for Innovation

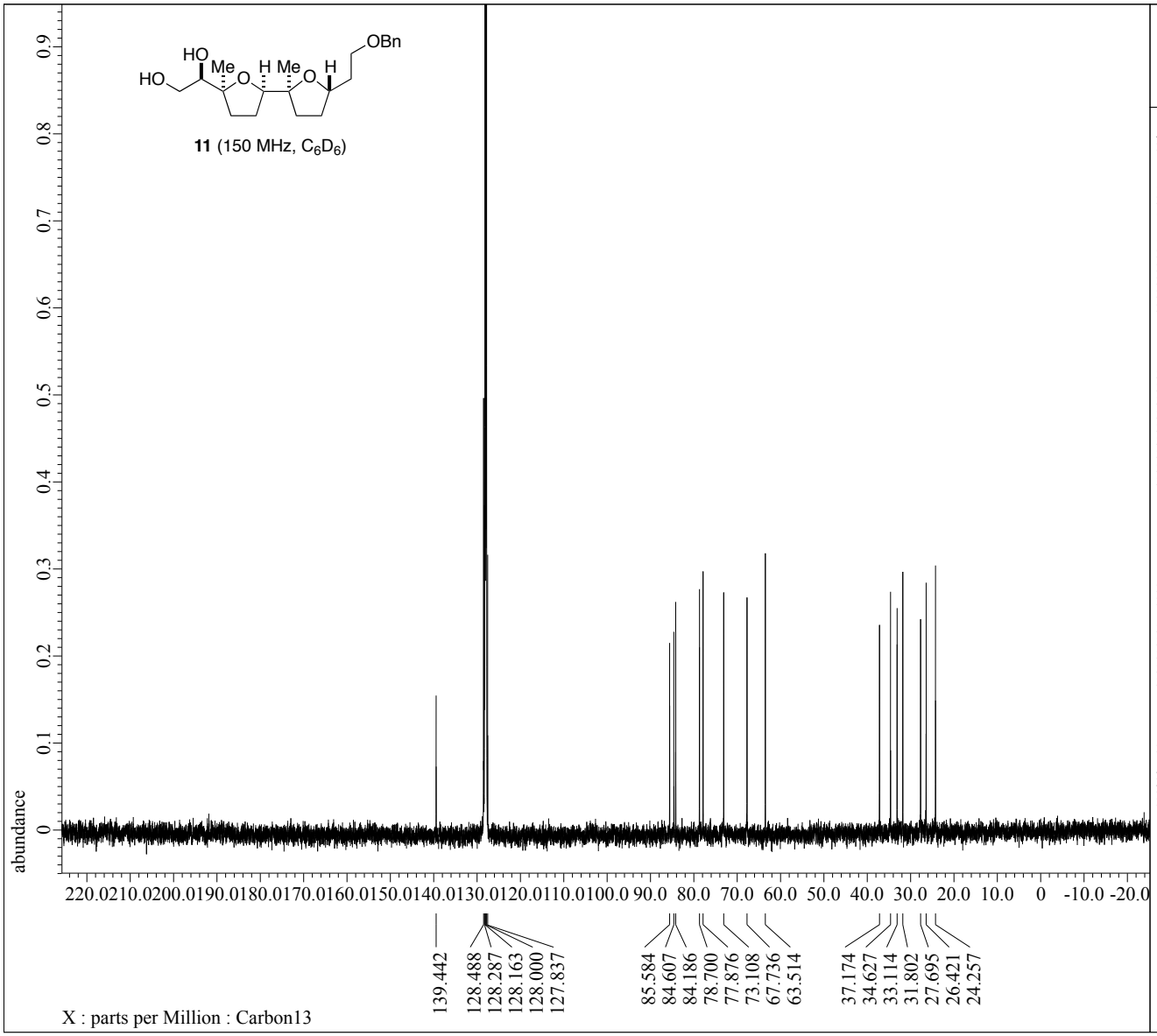
```
Filename          = RI-II-146_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-146
Solvent           = BENZENE-D6
Creation_Time     =  9-JUL-2015 18:46:54
Revision_Time     = 13-JAN-2016 22:50:11
Current_Time      = 13-JAN-2016 22:50:23

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 256
Total_Scans       = 256

Relaxation_Delay  = 2[s]
Recvr_Gain        = 52
Temp_Get          = 22.2[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_Noe       = 24.452[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]
```


HO
HO
Me
O
H
Me
O
H
OBn
11 (600 MHz, C6D6)
66.61
1.68
0.95
4.42
4.41
4.40
4.39
4.38
4.37
4.36
4.35
4.34
4.33
4.32
4.31
4.30
1.82
1.00
3.97
3.96
3.95
3.94
3.93
3.92
3.91
3.90
3.89
3.88
3.87
3.86
3.85
3.84
3.83
3.82
3.81
3.80
3.79
3.78
3.77
3.76
3.75
3.74
3.73
3.72
3.71
3.70
3.69
3.68
3.67
3.66
3.65
3.64
3.63
3.62
3.61
3.60
3.59
3.58



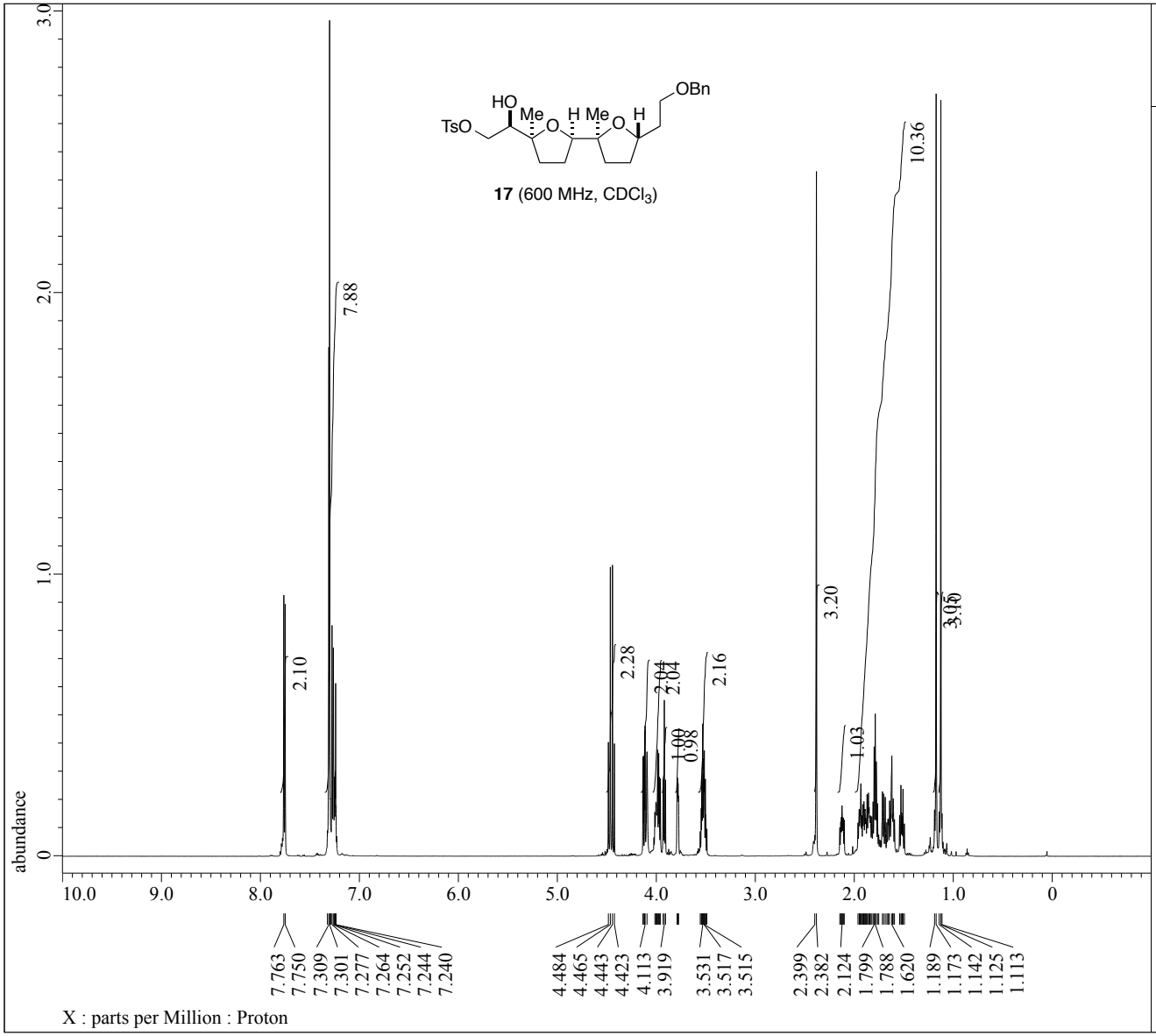
JEOL
Solutions for Innovation

```
Filename          = RI-II-151_Carbon-1-4.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-151
Solvent           = BENZENE-D6
Creation_Time     = 15-JUL-2015 13:14:31
Revision_Time     = 13-JAN-2016 22:55:49
Current_Time      = 13-JAN-2016 22:56:03

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.8[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_Noe       = 24.452[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]
```



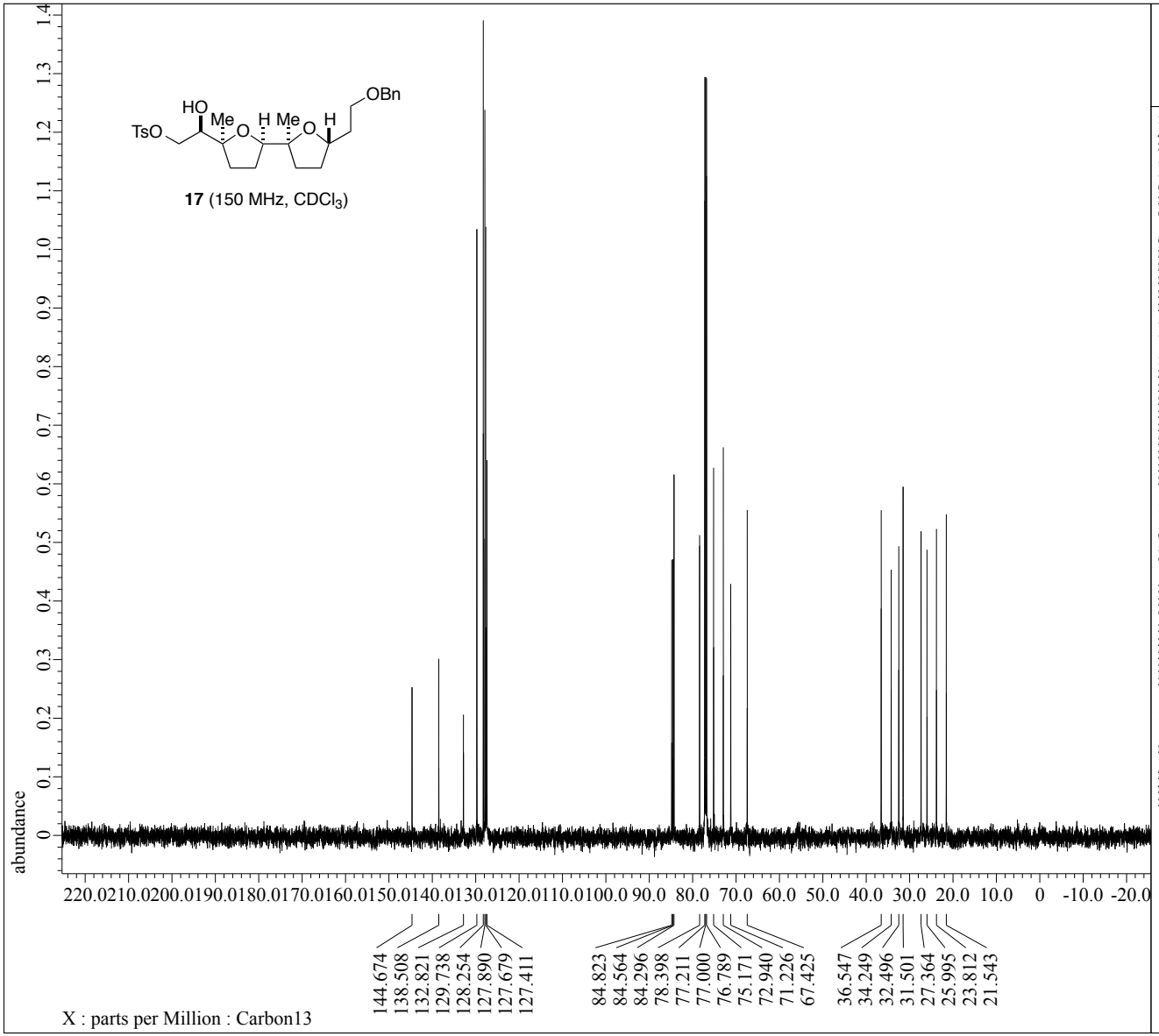
JEOL
Solutions for Innovation

```
Filename          = RI-II-150_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-150
Solvent           = CHLOROFORM-D
Creation_Time     = 14-JUL-2015 22:46:35
Revision_Time     = 13-JAN-2016 23:33:31
Current_Time      = 13-JAN-2016 23:34:11

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        = 20
Temp_Get          = 22.7[dC]
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]
```



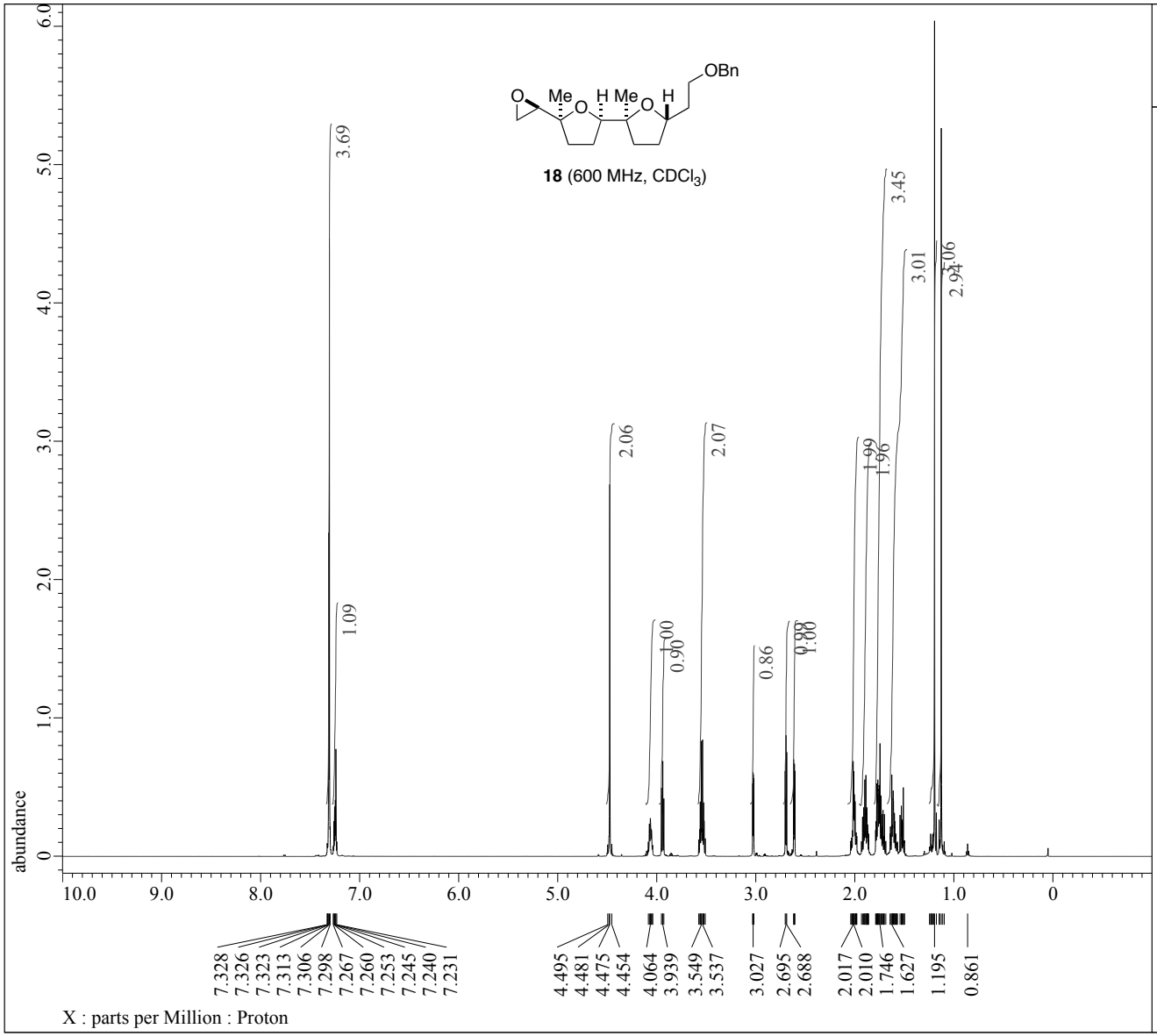
JEOL Solutions for Innovation

```
Filename          = RI-II-150_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-150
Solvent           = CHLOROFORM-D
Creation_Time     = 14-JUL-2015 22:50:15
Revision_Time     = 13-JAN-2016 23:35:26
Current_Time      = 13-JAN-2016 23:35:41

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_Clipped   = 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          = 22.8[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_Noe       = 24.452[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]
```



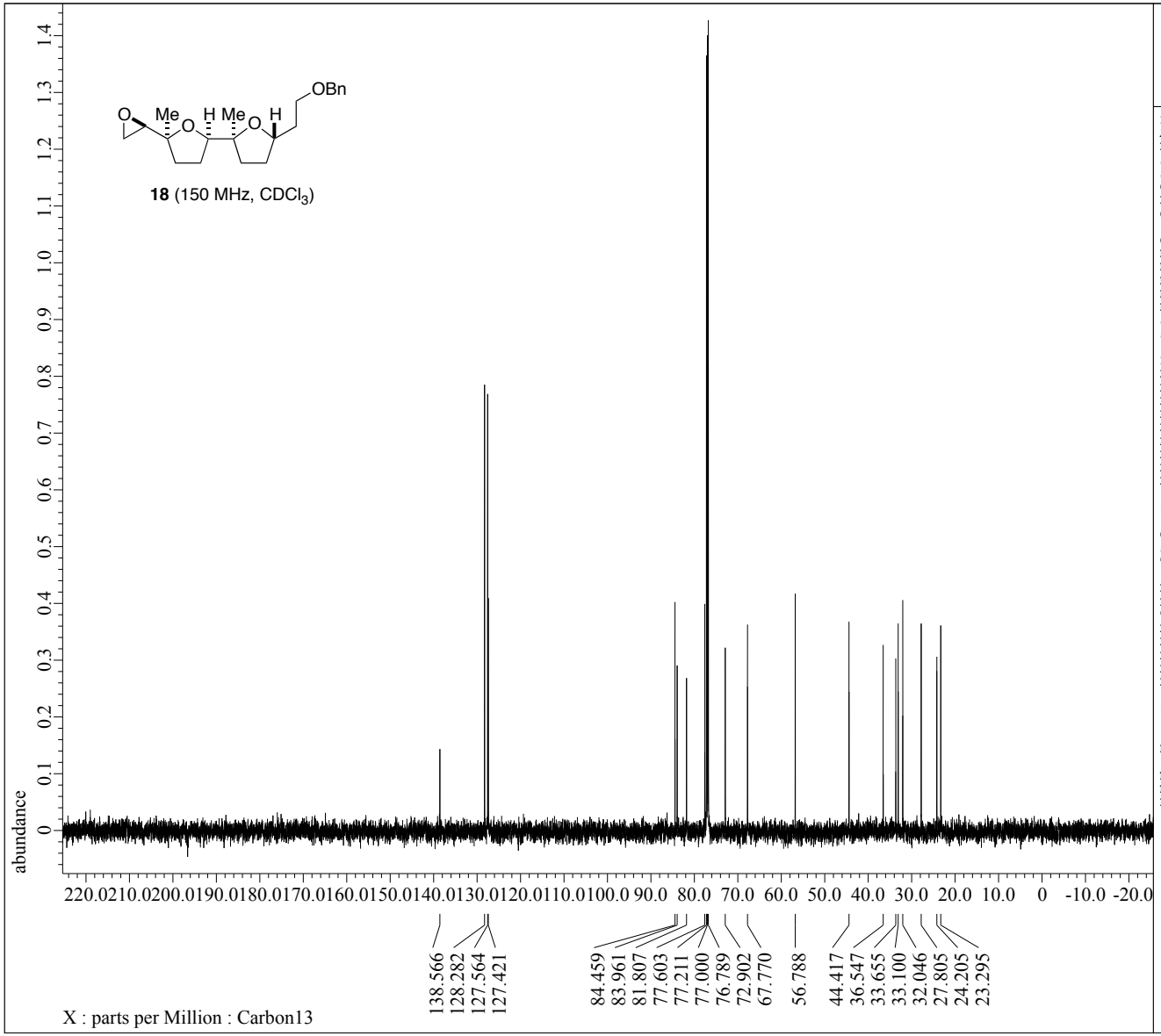
JEOL Solutions for Innovation

```
Filename          = RI-II-152_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-152
Solvent           = CHLOROFORM-D
Creation_Time     = 15-JUL-2015 19:54:17
Revision_Time     = 13-JAN-2016 23:37:47
Current_Time      = 13-JAN-2016 23:38:13

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        = 24
Temp_Get          = 22.9[dC]
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]
```



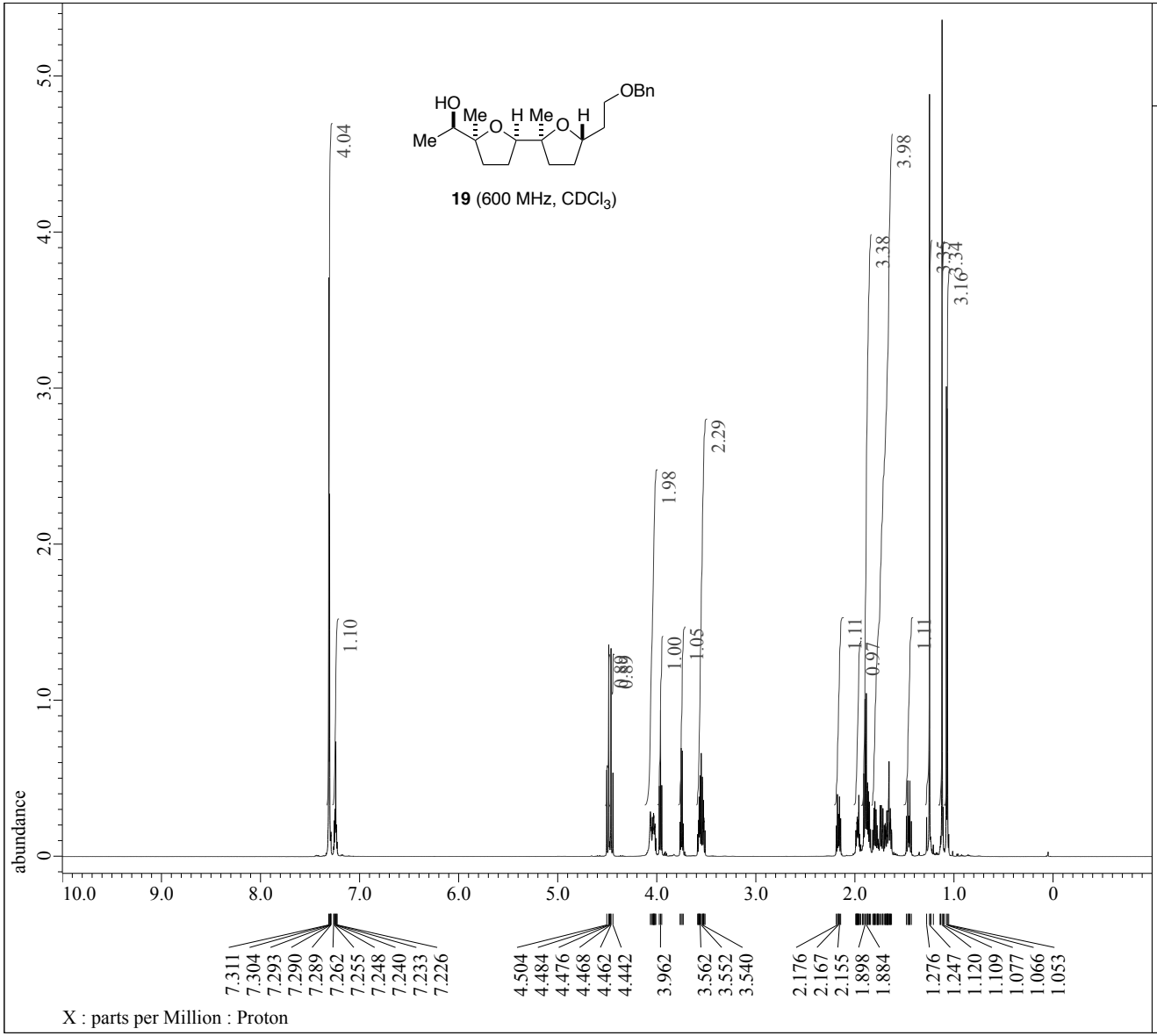
JEOL Solutions for Innovation

```
Filename          = RI-II-152_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-152
Solvent           = CHLOROFORM-D
Creation_Time     = 15-JUL-2015 19:57:55
Revision_Time     = 13-JAN-2016 23:38:44
Current_Time      = 13-JAN-2016 23:38:56

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 2[s]
Recvr_Gain        = 54
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_Noe       = 24.452[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]
```

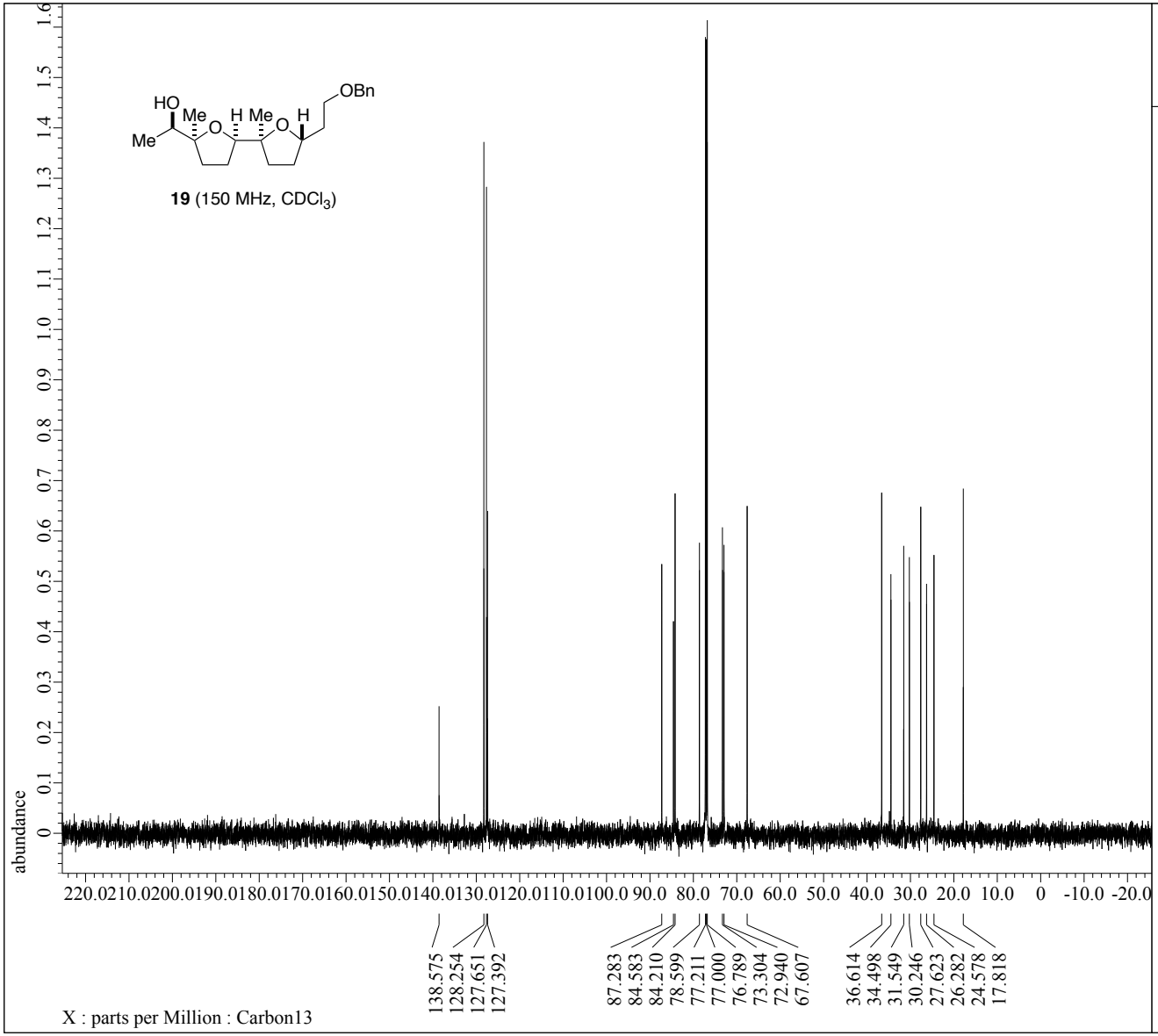



```
Filename          = RI-II-153_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-153
Solvent           = CHLOROFORM-D
Creation_Time     = 16-JUL-2015 15:26:04
Revision_Time     = 13-JAN-2016 23:41:07
Current_Time      = 13-JAN-2016 23:41:33

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_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        = 22
Temp_Get          = 22.6[dC]
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]
```



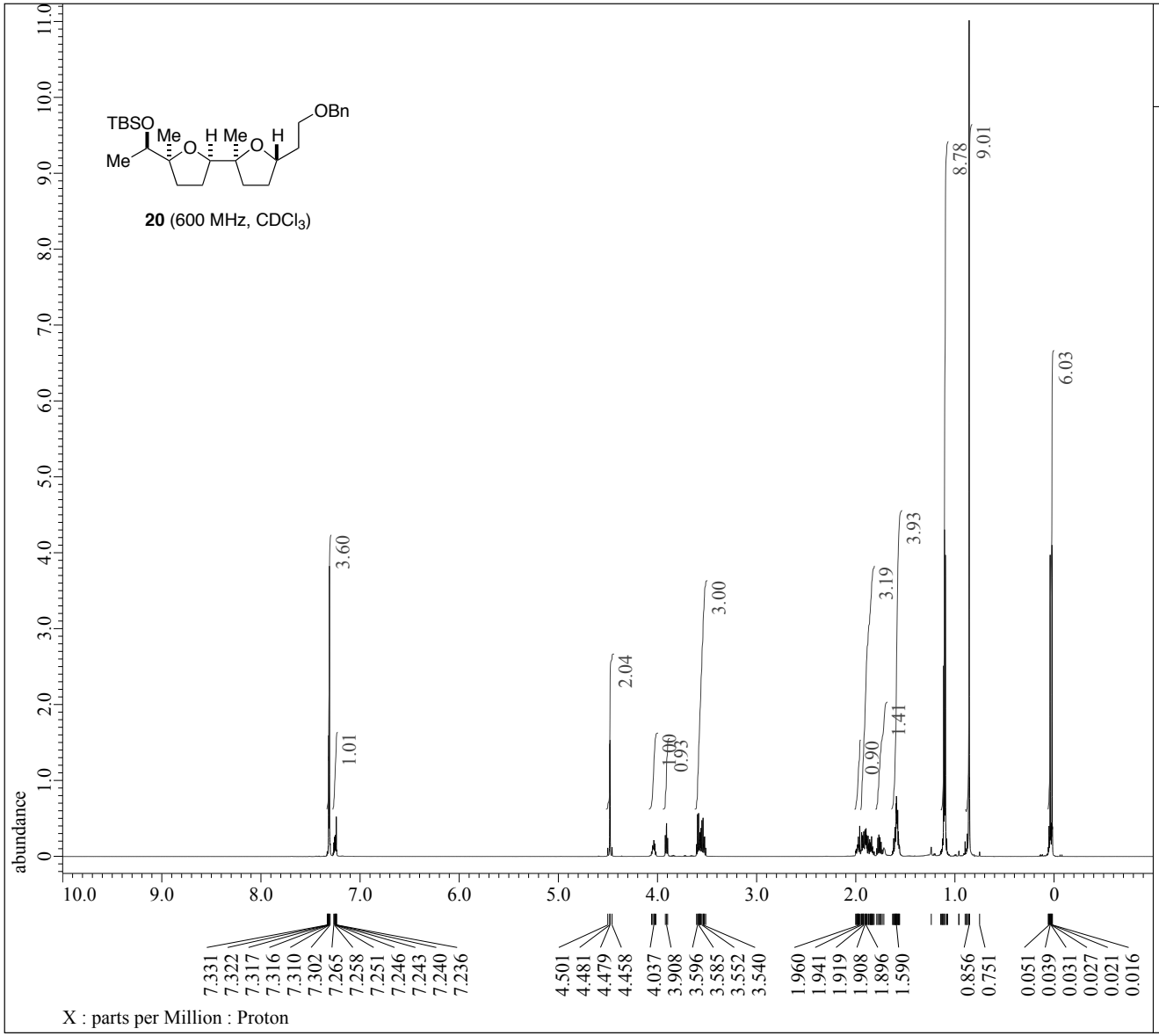
JEOL Solutions for Innovation

```
Filename          = RI-II-153_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-153
Solvent           = CHLOROFORM-D
Creation_Time     = 16-JUL-2015 15:29:45
Revision_Time     = 13-JAN-2016 23:42:02
Current_Time      = 13-JAN-2016 23:42:17

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 68
Total_Scans       = 68

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 22.8[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_Noe       = 24.452[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]
```



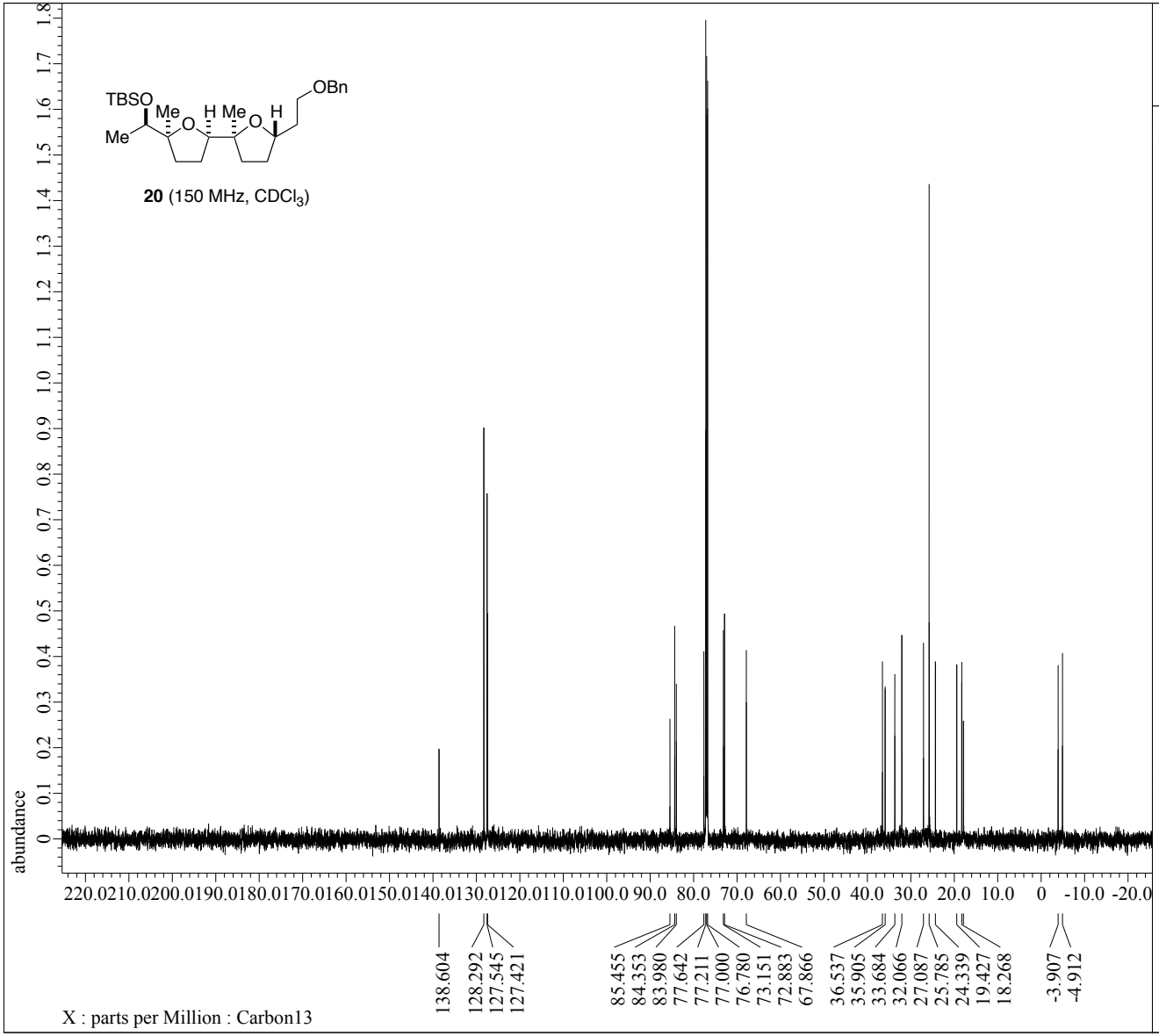
JEOL Solutions for Innovation

```
Filename          = RI-II-162_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-162
Solvent           = CHLOROFORM-D
Creation_Time     = 28-JUL-2015 17:17:30
Revision_Time     = 13-JAN-2016 23:44:34
Current_Time      = 13-JAN-2016 23:45:01

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_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        = 22
Temp_Get          = 22.9[dC]
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]
```



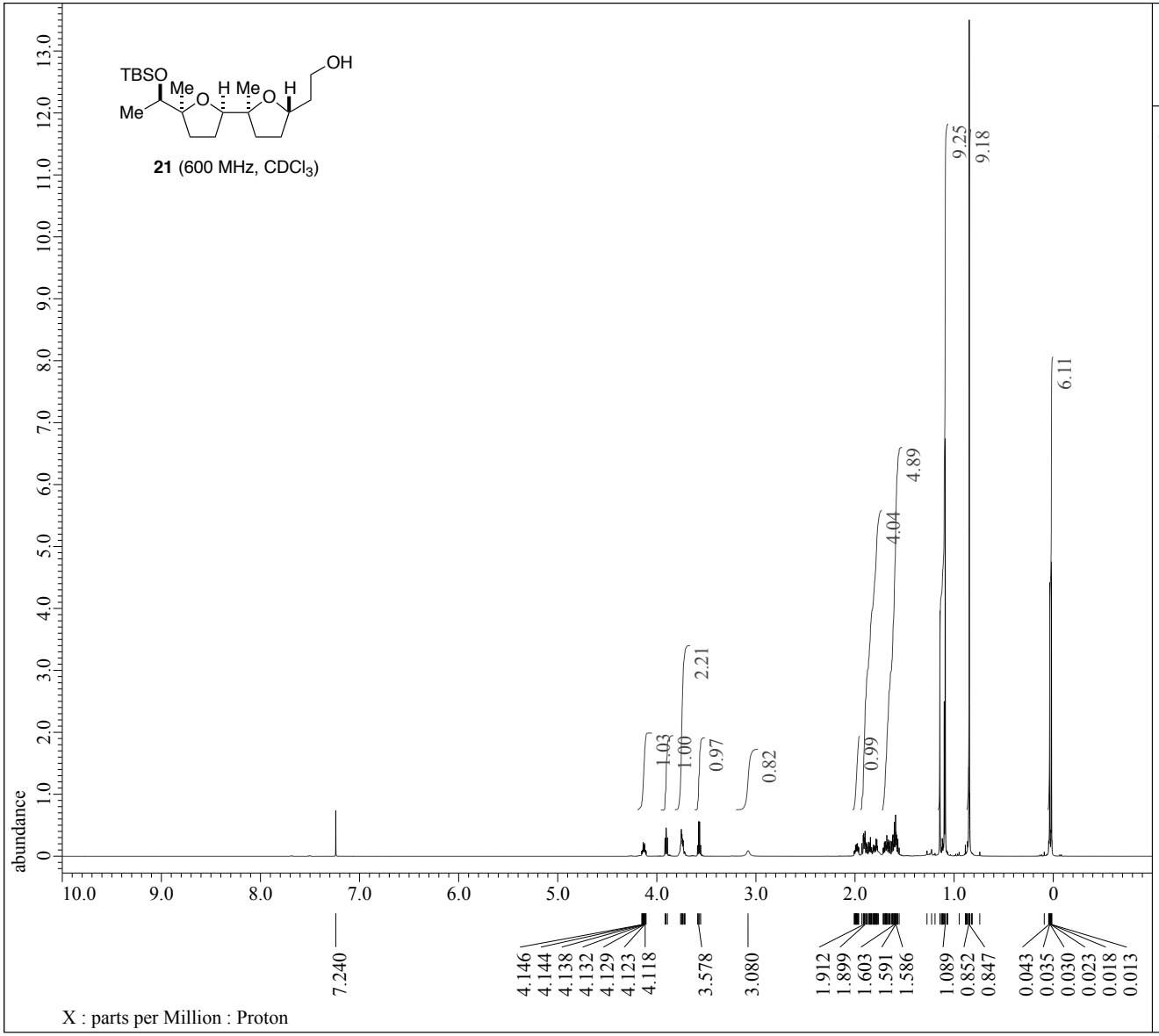
JEOL Solutions for Innovation

```
Filename          = RI-II-162_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-162
Solvent           = CHLOROFORM-D
Creation_Time     = 28-JUL-2015 17:24:49
Revision_Time     = 13-JAN-2016 23:45:25
Current_Time      = 13-JAN-2016 23:45:35

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 92
Total_Scans       = 92

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 23.1[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_Noe       = 24.452[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]
```



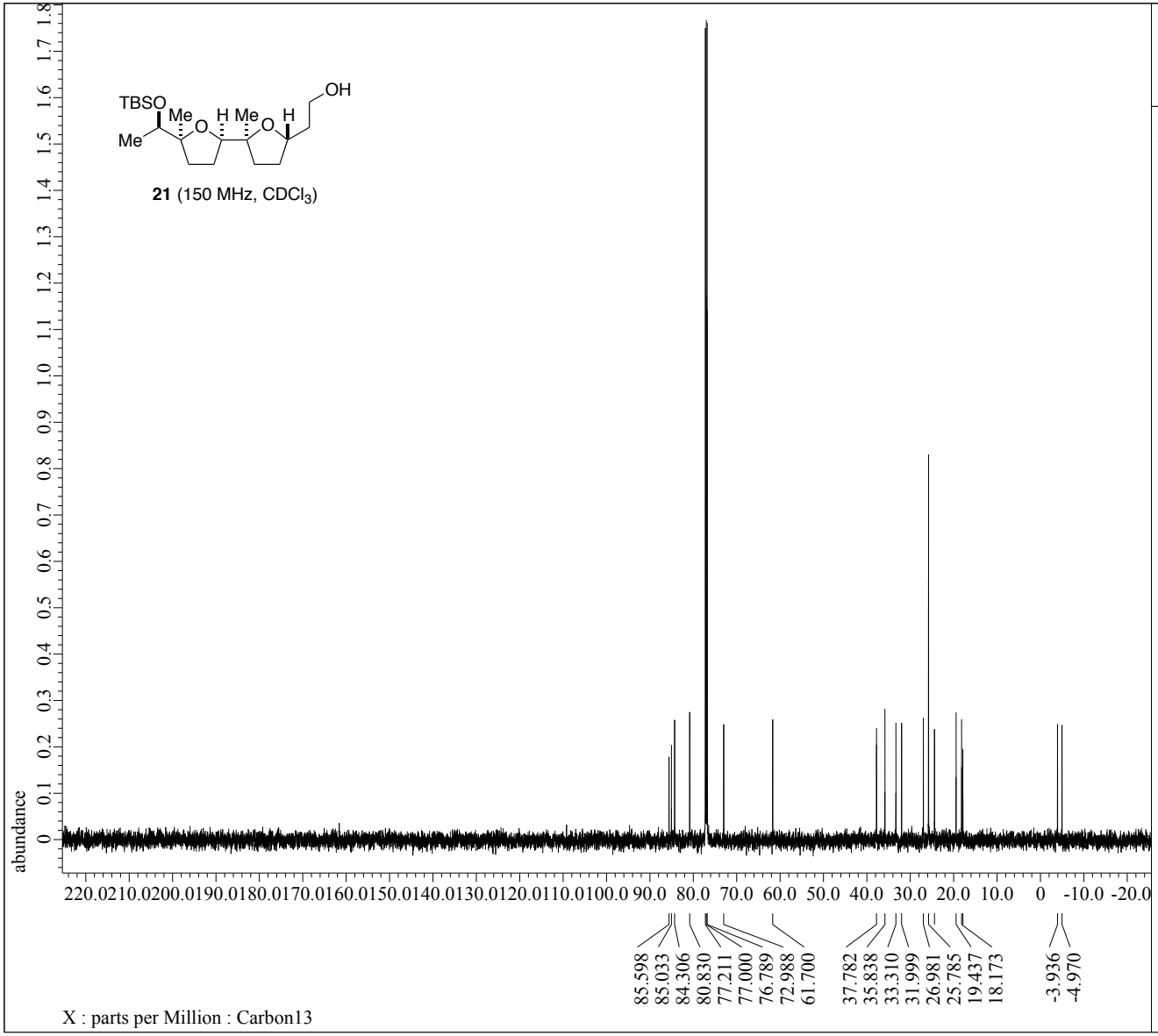
JEOL Solutions for Innovation

```
Filename          = RI-II-163_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-163
Solvent           = CHLOROFORM-D
Creation_Time     = 29-JUL-2015 17:45:48
Revision_Time     = 13-JAN-2016 23:48:44
Current_Time      = 13-JAN-2016 23:49:13

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        = 26
Temp_Get          = 23[dC]
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]
```



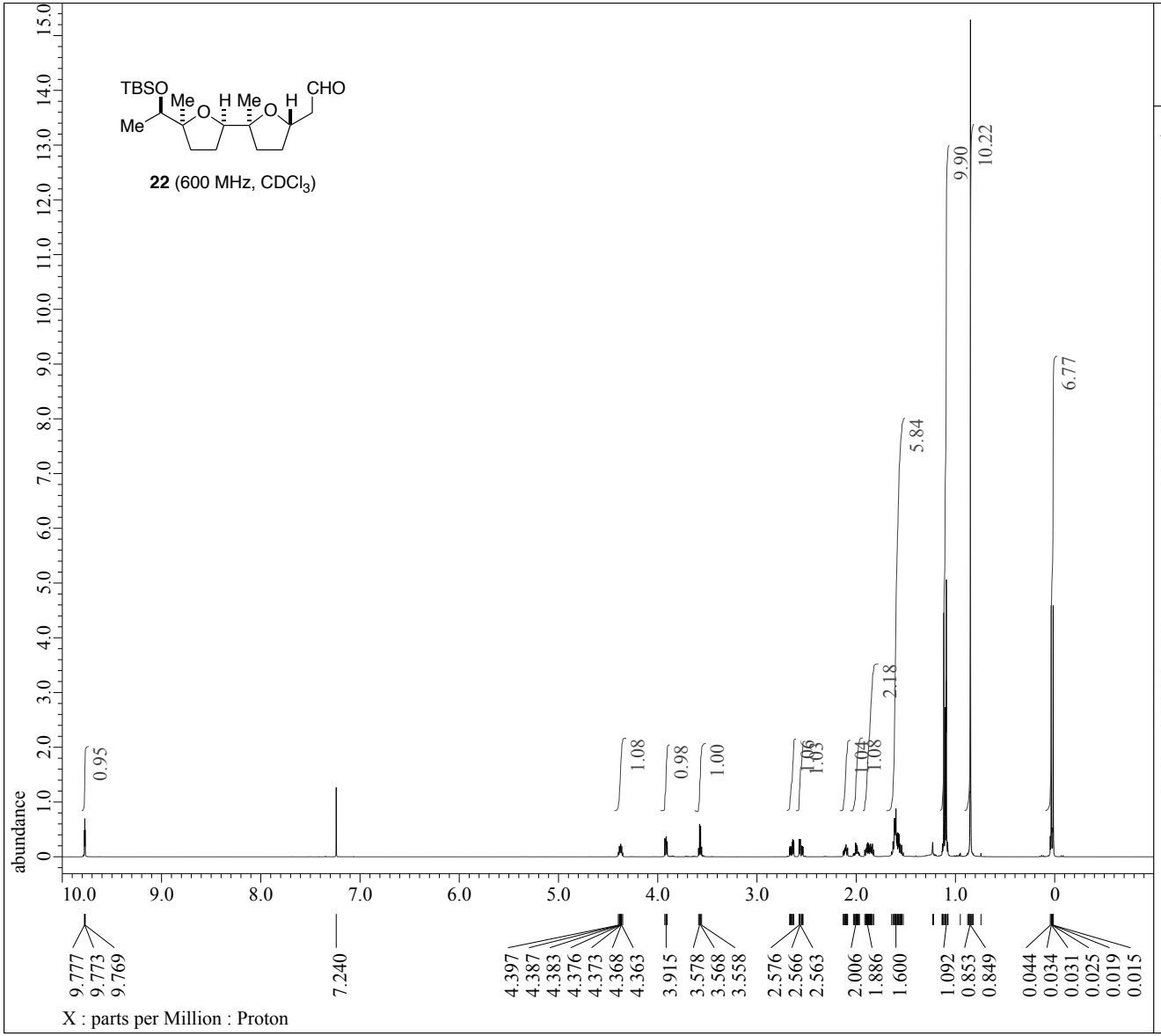
JEOL Solutions for Innovation

```
Filename          = RI-II-163_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-163
Solvent           = CHLOROFORM-D
Creation_Time     = 29-JUL-2015 17:49:20
Revision_Time     = 13-JAN-2016 23:49:42
Current_Time      = 13-JAN-2016 23:49:51

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 92
Total_Scans       = 92

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 23.1[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_Noe       = 24.452[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]
```



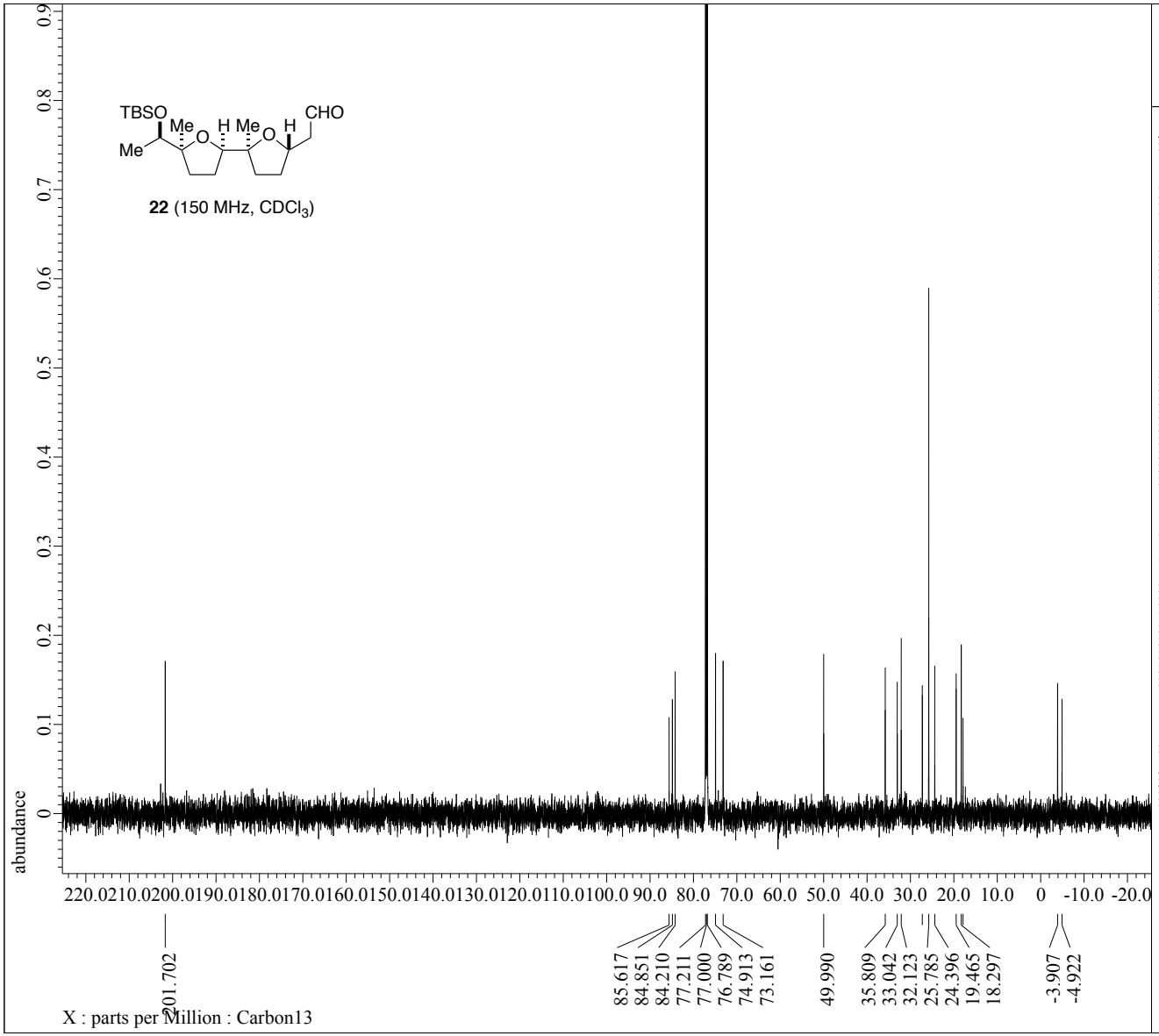
JEOL
Solutions for Innovation

```
Filename          = RI-II-169_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-169
Solvent           = CHLOROFORM-D
Creation_Time     = 20-AUG-2015 13:43:38
Revision_Time     = 13-JAN-2016 23:51:42
Current_Time      = 13-JAN-2016 23:52:08

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        = 30
Temp_Get          = 22.7[dC]
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]
```



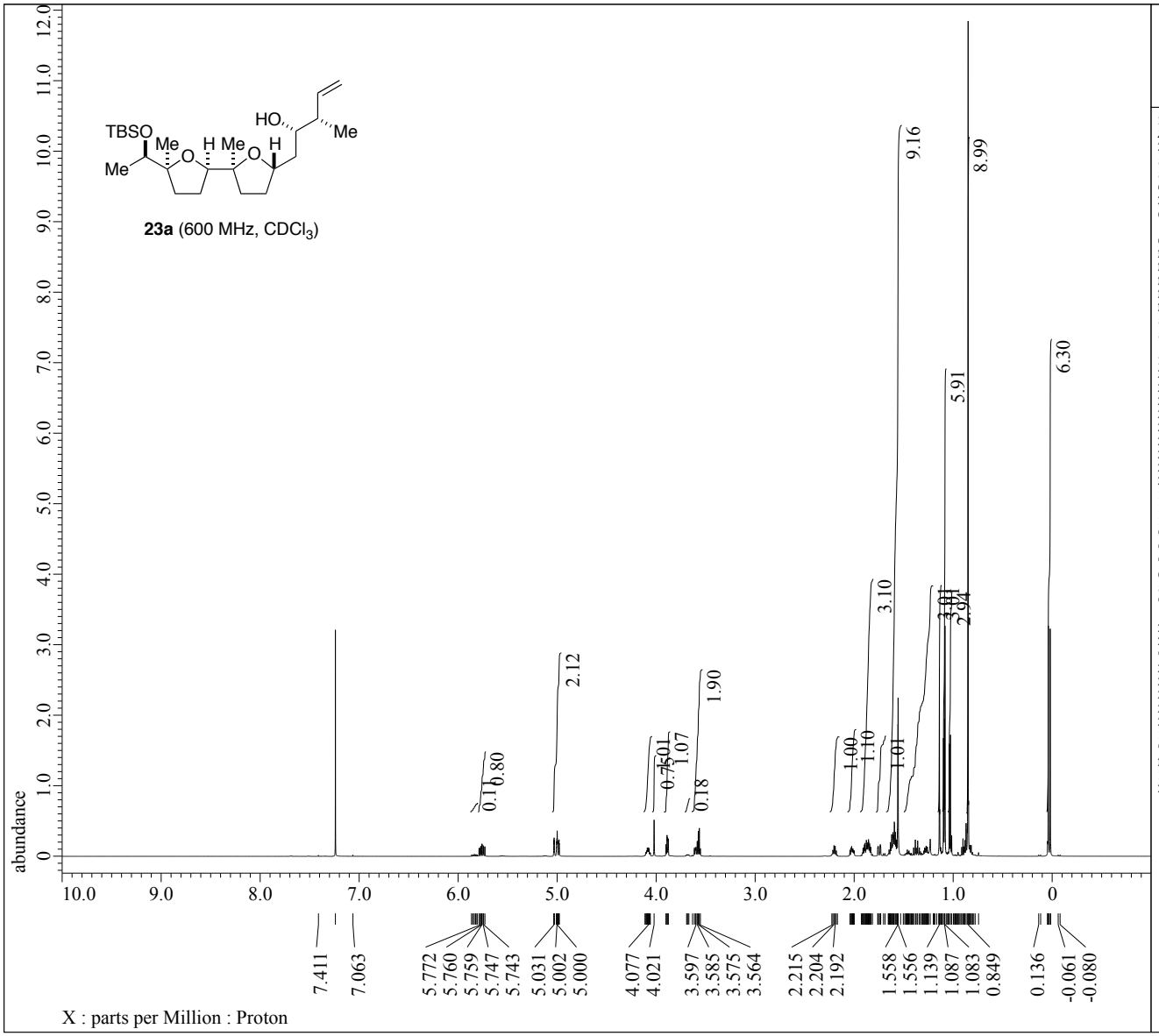
JEOL
Solutions for Innovation

```
Filename          = RI-II-169_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-169
Solvent           = CHLOROFORM-D
Creation_Time     = 20-AUG-2015 13:47:12
Revision_Time     = 13-JAN-2016 23:52:49
Current_Time      = 13-JAN-2016 23:52:58

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 124
Total_Scans       = 124

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 22.9[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_Noe       = 24.452[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]
```



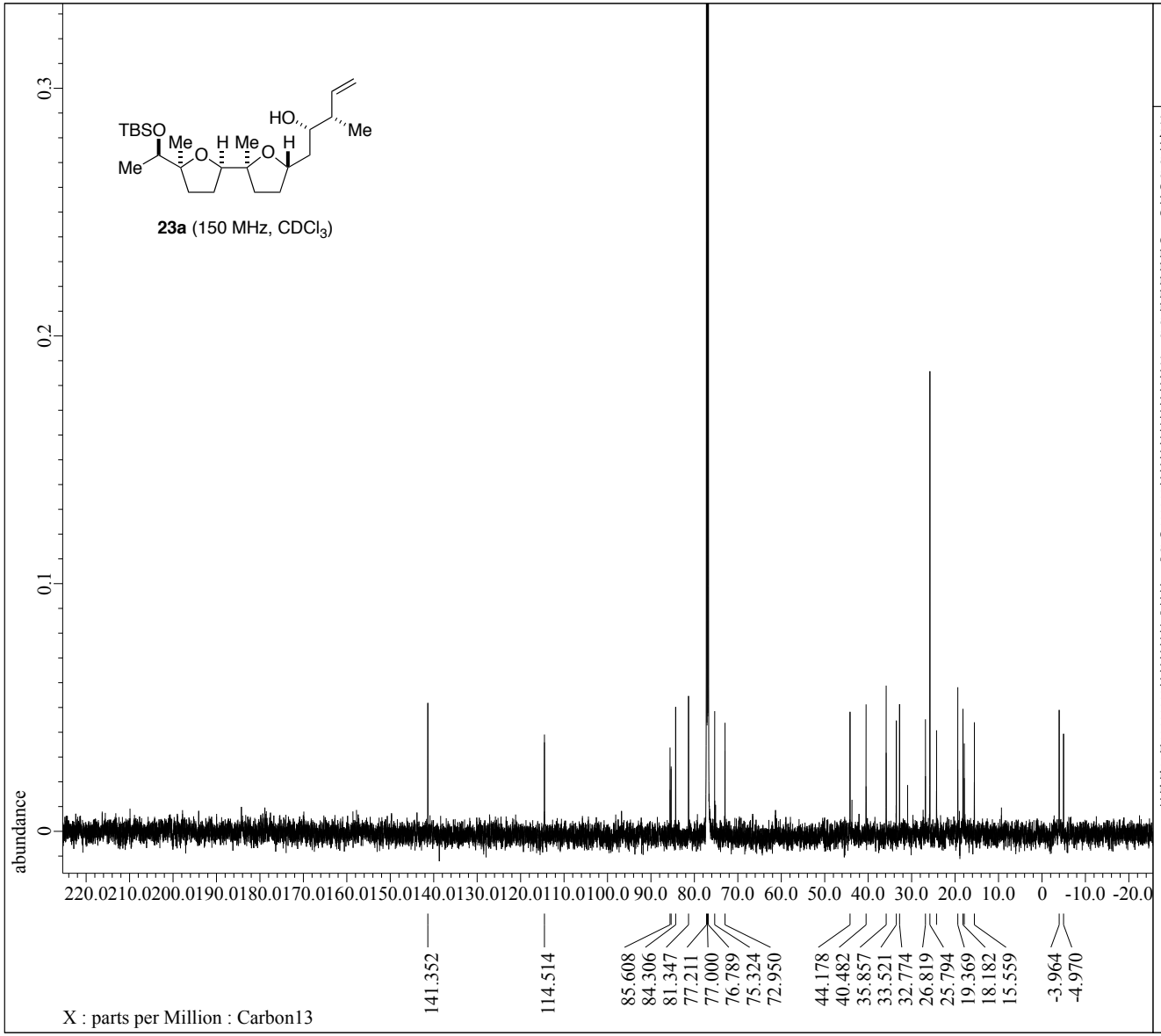
JEOL Solutions for Innovation

```
Filename          = RI-II-160A_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-160A
Solvent           = CHLOROFORM-D
Creation_Time     = 20-AUG-2015 21:46:53
Revision_Time     = 14-JAN-2016 19:57:51
Current_Time      = 14-JAN-2016 19:58:26

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        = 38
Temp_Get          = 22.7[dC]
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]
```



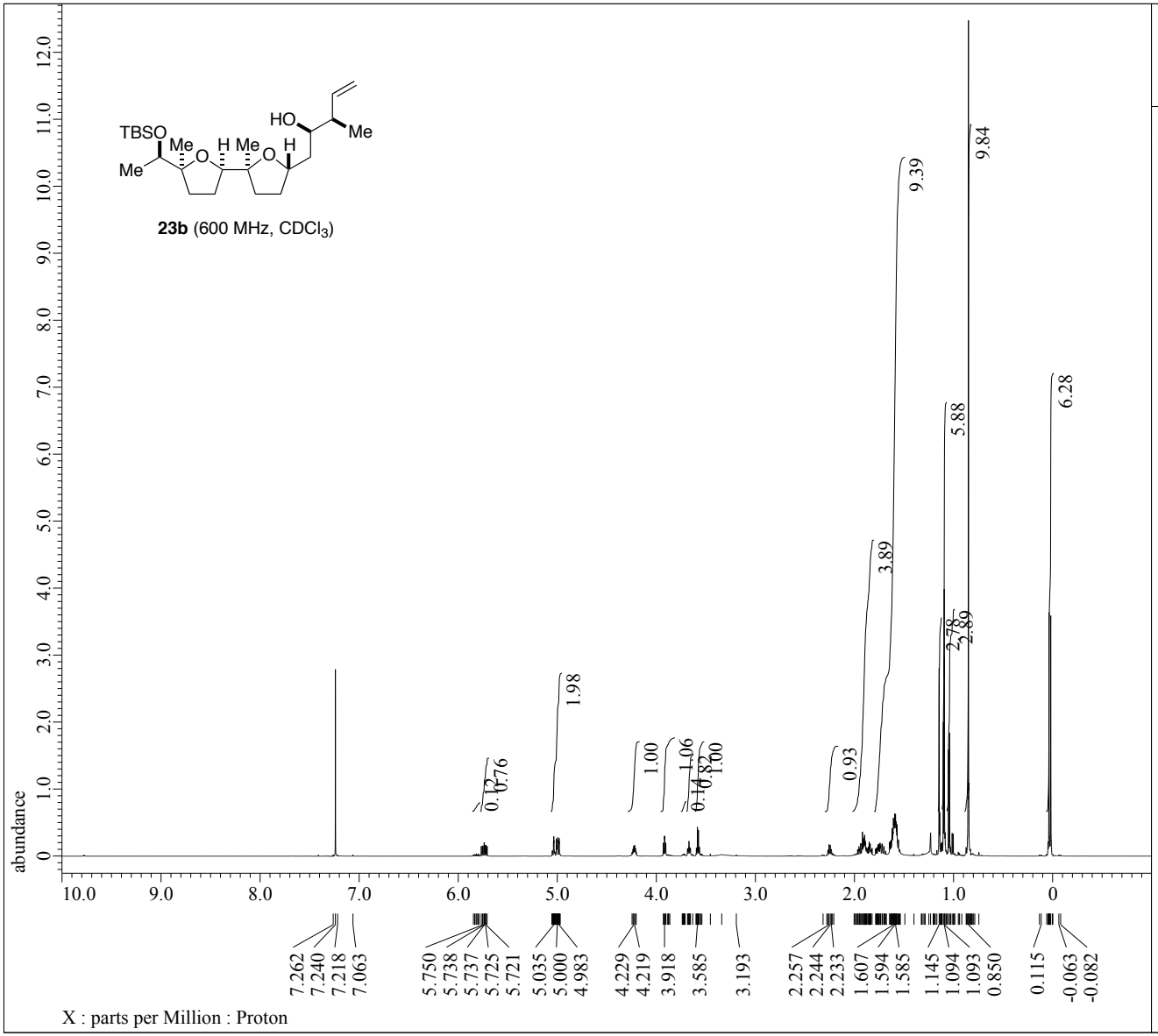
JEOL
Solutions for Innovation

```
Filename          = RI-II-160A_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-160A
Solvent           = CHLOROFORM-D
Creation_Time     =  3-SEP-2015 09:19:44
Revision_Time     = 14-JAN-2016 19:59:05
Current_Time      = 14-JAN-2016 19:59:20

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 1276
Total_Scans       = 1276

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_Noe       = 24.452[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]
```



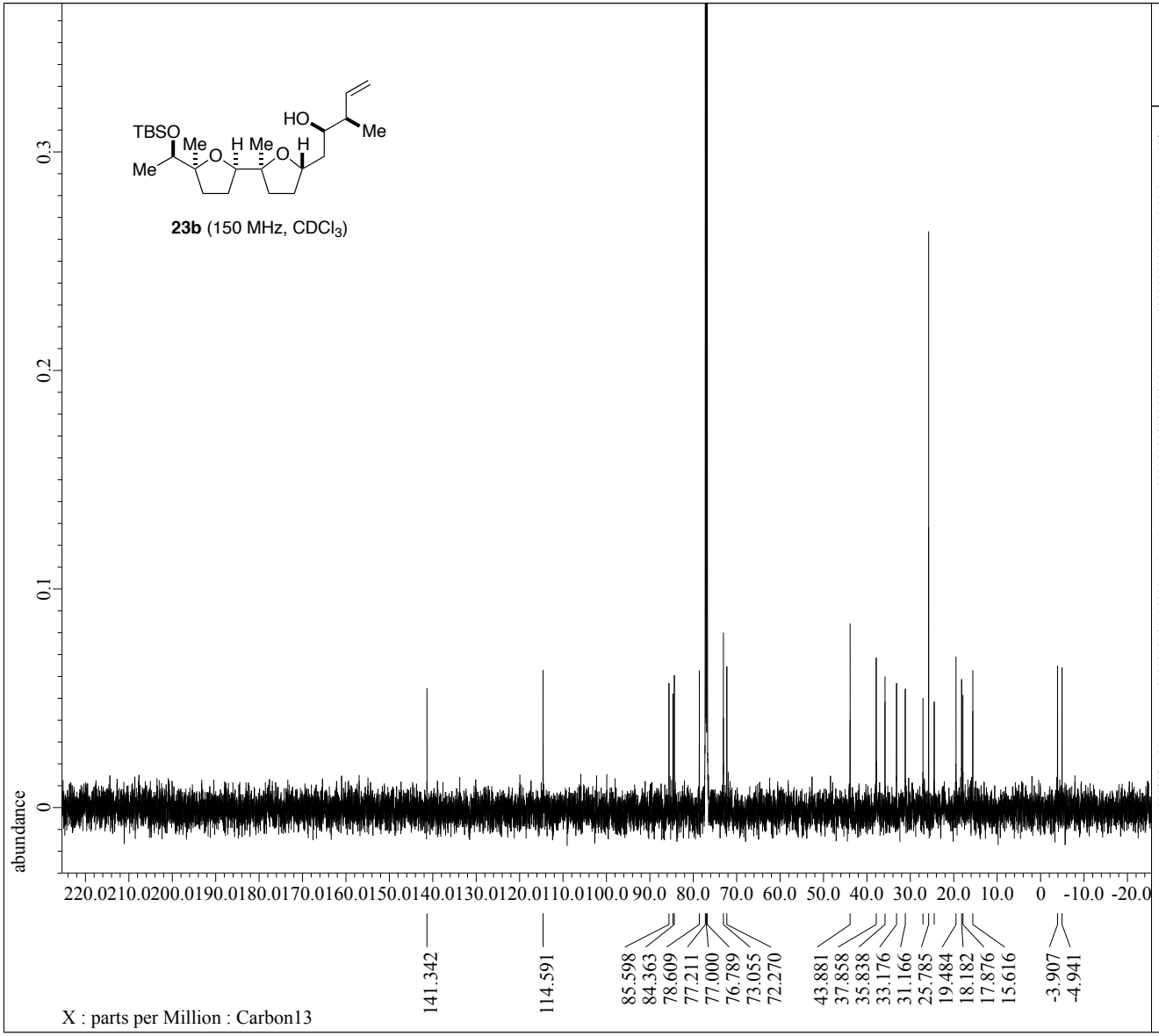
JEOL Solutions for Innovation

```
Filename          = RI-II-170c_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-170c
Solvent           = CHLOROFORM-D
Creation_Time     = 21-AUG-2015 16:47:04
Revision_Time     = 14-JAN-2016 20:03:18
Current_Time      = 14-JAN-2016 20:03:42

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        = 38
Temp_Get          = 22.7[dC]
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]
```



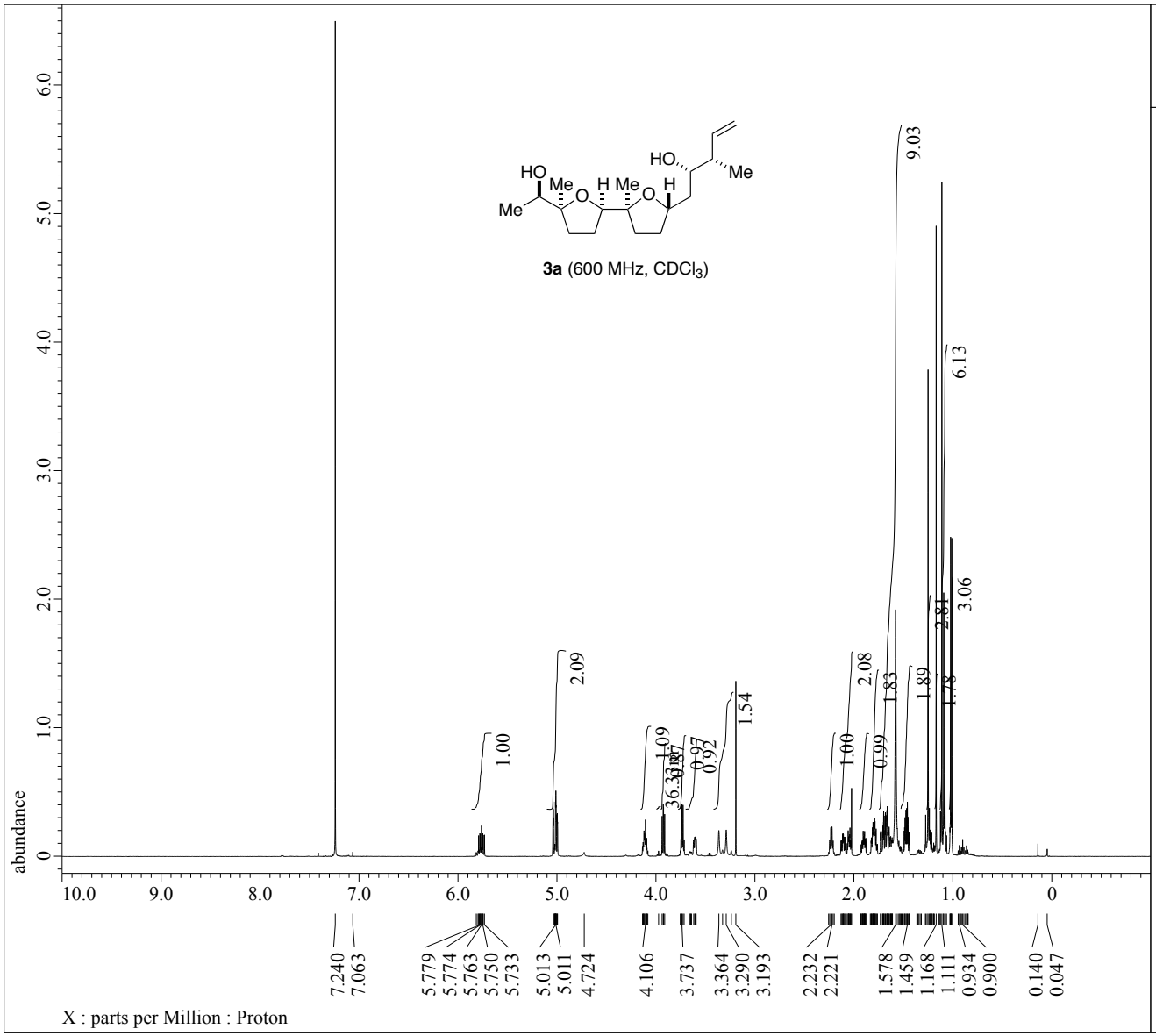
JEOL Solutions for Innovation

```
Filename          = RI-II-167B_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-167B
Solvent           = CHLOROFORM-D
Creation_Time     = 27-AUG-2015 17:24:40
Revision_Time     = 14-JAN-2016 20:04:24
Current_Time      = 14-JAN-2016 20:04:35

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 376
Total_Scans       = 376

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_Noe       = 24.452[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]
```

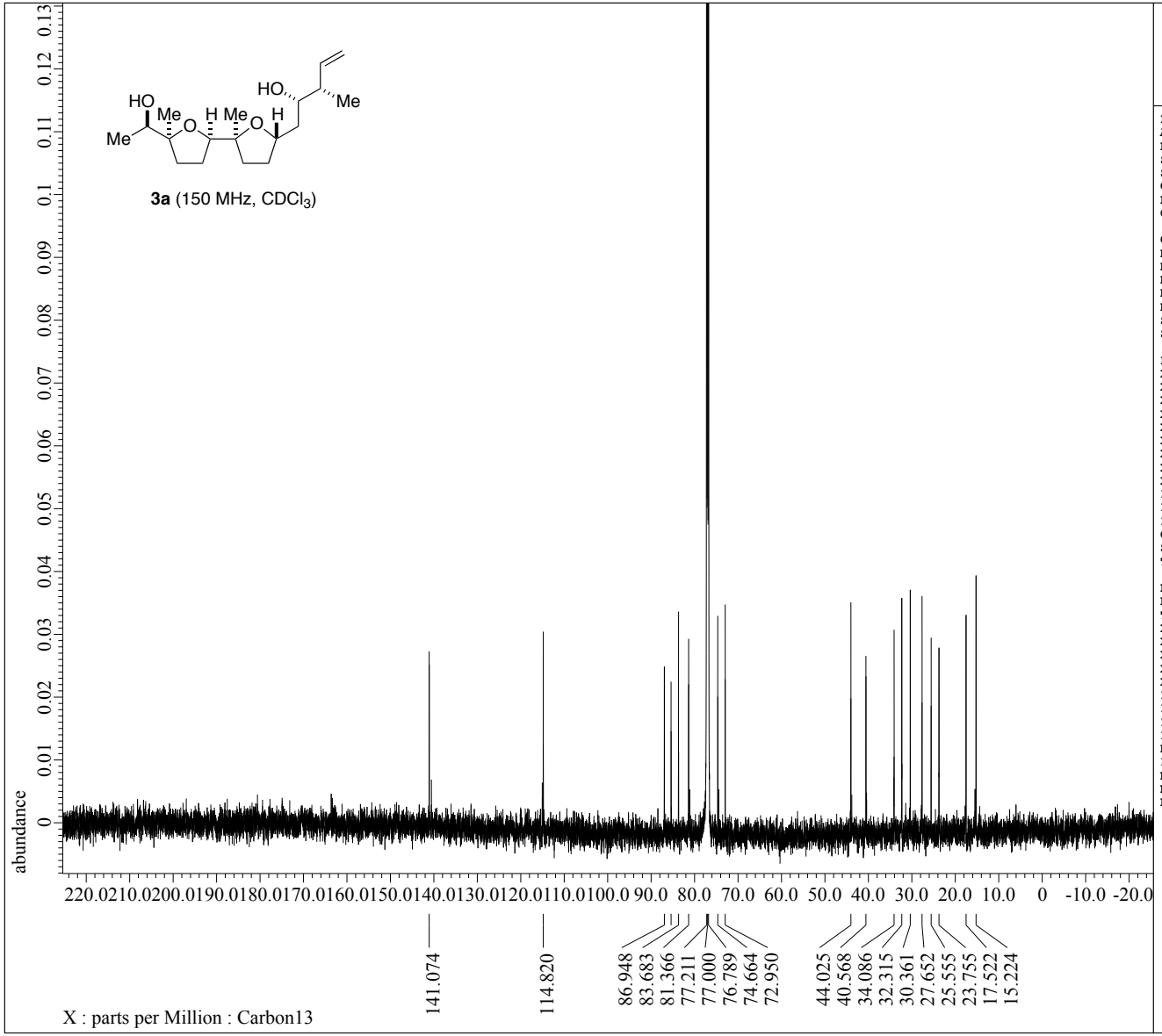


Filename = RI-II-177_proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = RI-II-177
Solvent = CHLOROFORM-D
Creation_Time = 2-SEP-2015 16:14:49
Revision_Time = 14-JAN-2016 20:50:12
Current_Time = 14-JAN-2016 20:50:57

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 = 44
Temp_Get = 22.8[dC]
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]

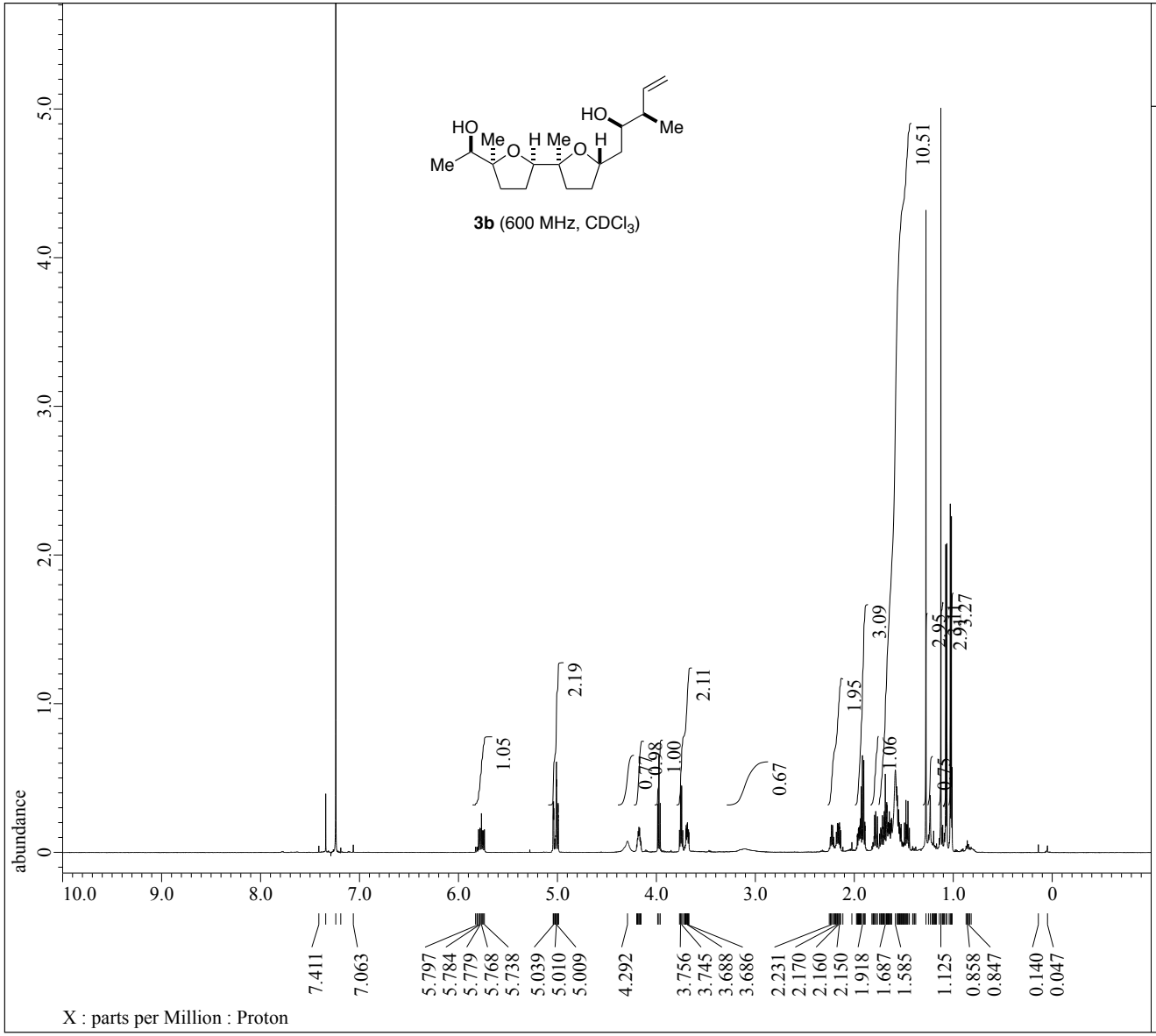



```
Filename          = RI-II-177_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-177
Solvent           = CHLOROFORM-D
Creation_Time     =  3-SEP-2015 04:43:36
Revision_Time     = 14-JAN-2016 20:51:38
Current_Time      = 14-JAN-2016 20:51:51

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 5880
Total_Scans       = 5880

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
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_Noe       = 24.452[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]
```



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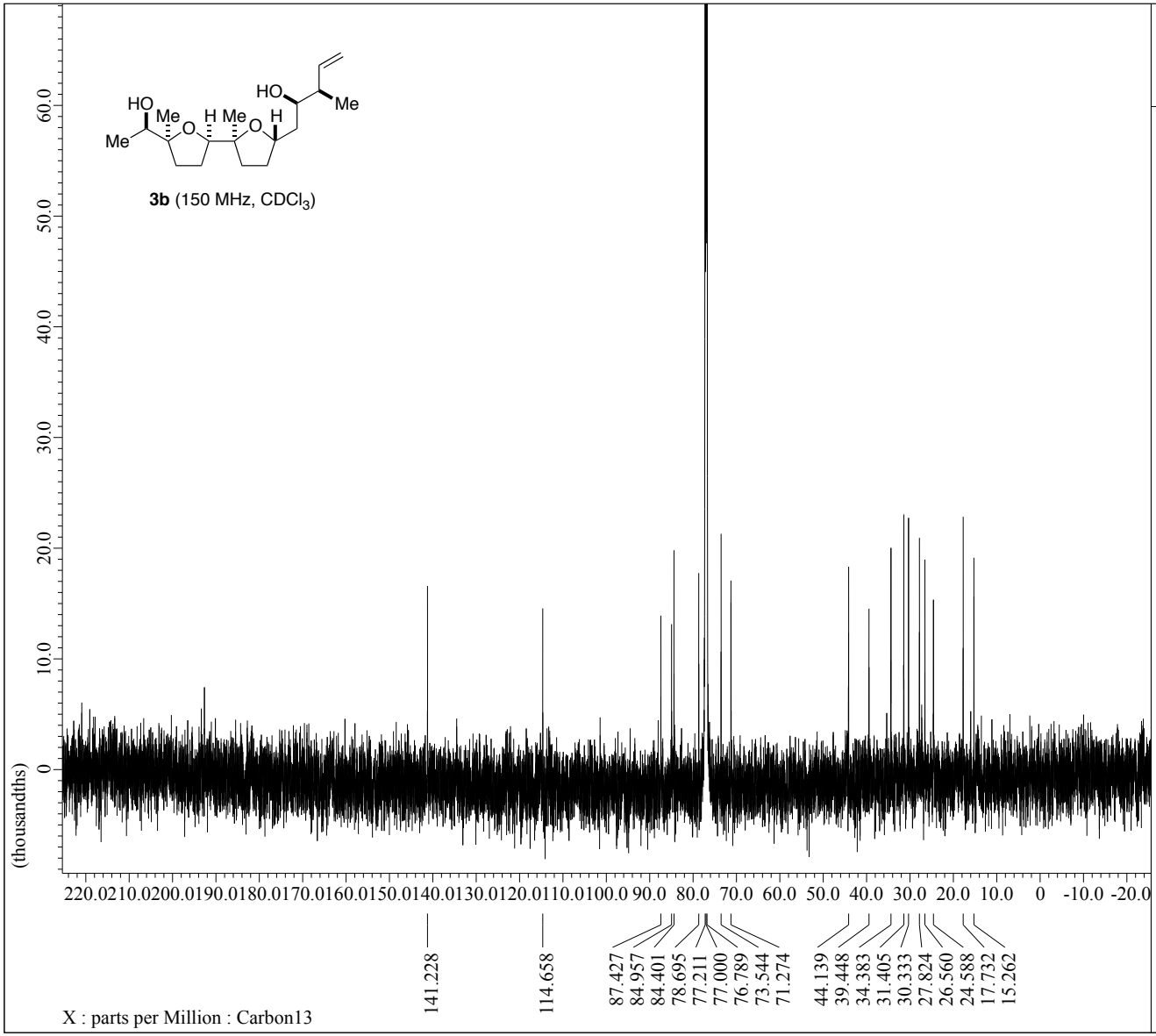
```
Filename          = RI-II-174_proton-2-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-174
Solvent           = CHLOROFORM-D
Creation_Time     = 20-OCT-2015 23:14:22
Revision_Time     = 14-JAN-2016 20:55:20
Current_Time      = 14-JAN-2016 20:55:49

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        = 46
Temp_Get          = 22.1[dC]
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]
```



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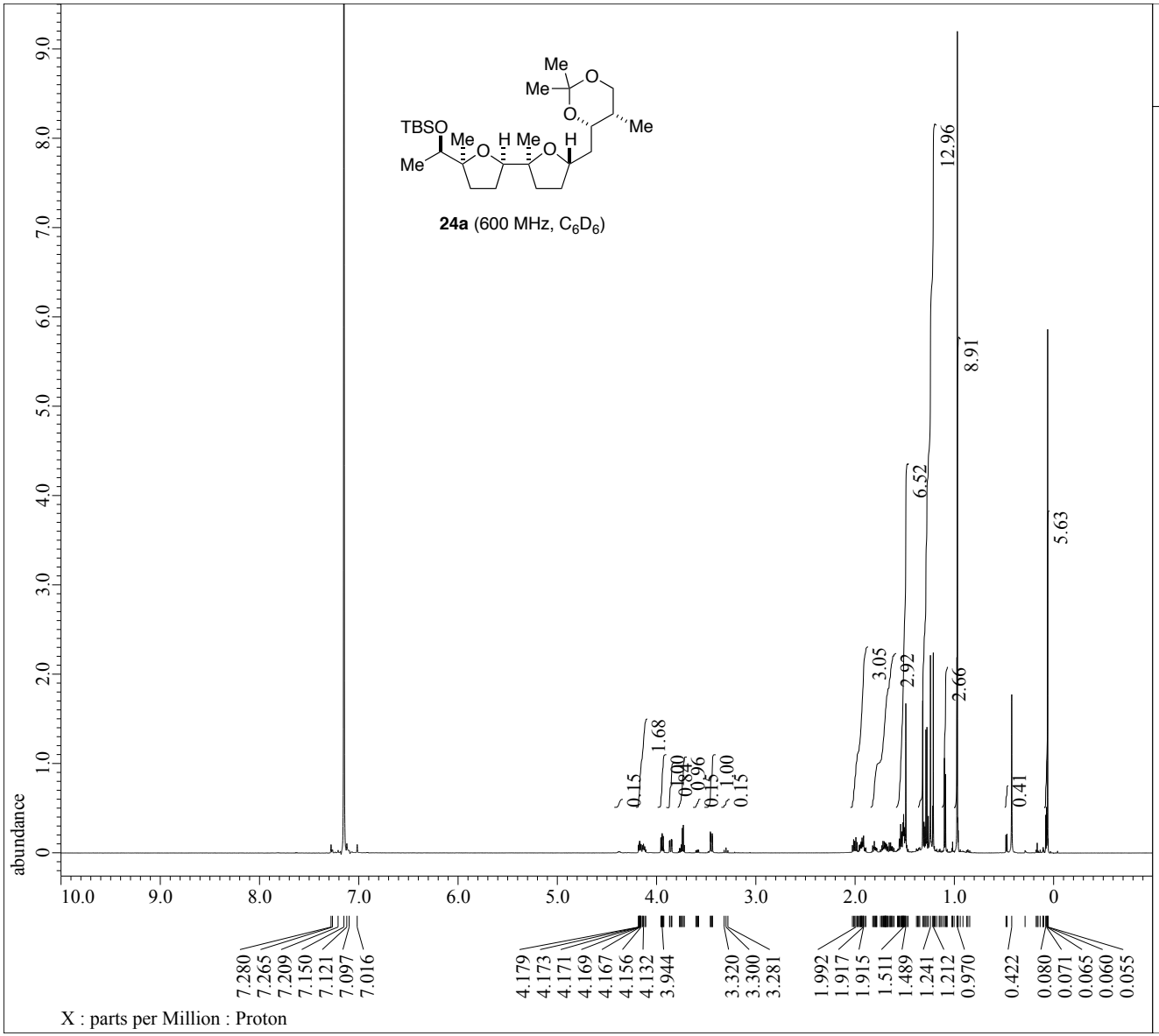
```
Filename          = RI-II-174_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-174
Solvent           = CHLOROFORM-D
Creation_Time     = 21-OCT-2015 00:15:19
Revision_Time     = 14-JAN-2016 20:56:30
Current_Time      = 14-JAN-2016 20:56:45

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 2650
Total_Scans       = 2650

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 22[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_Noe       = 24.452[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]
```

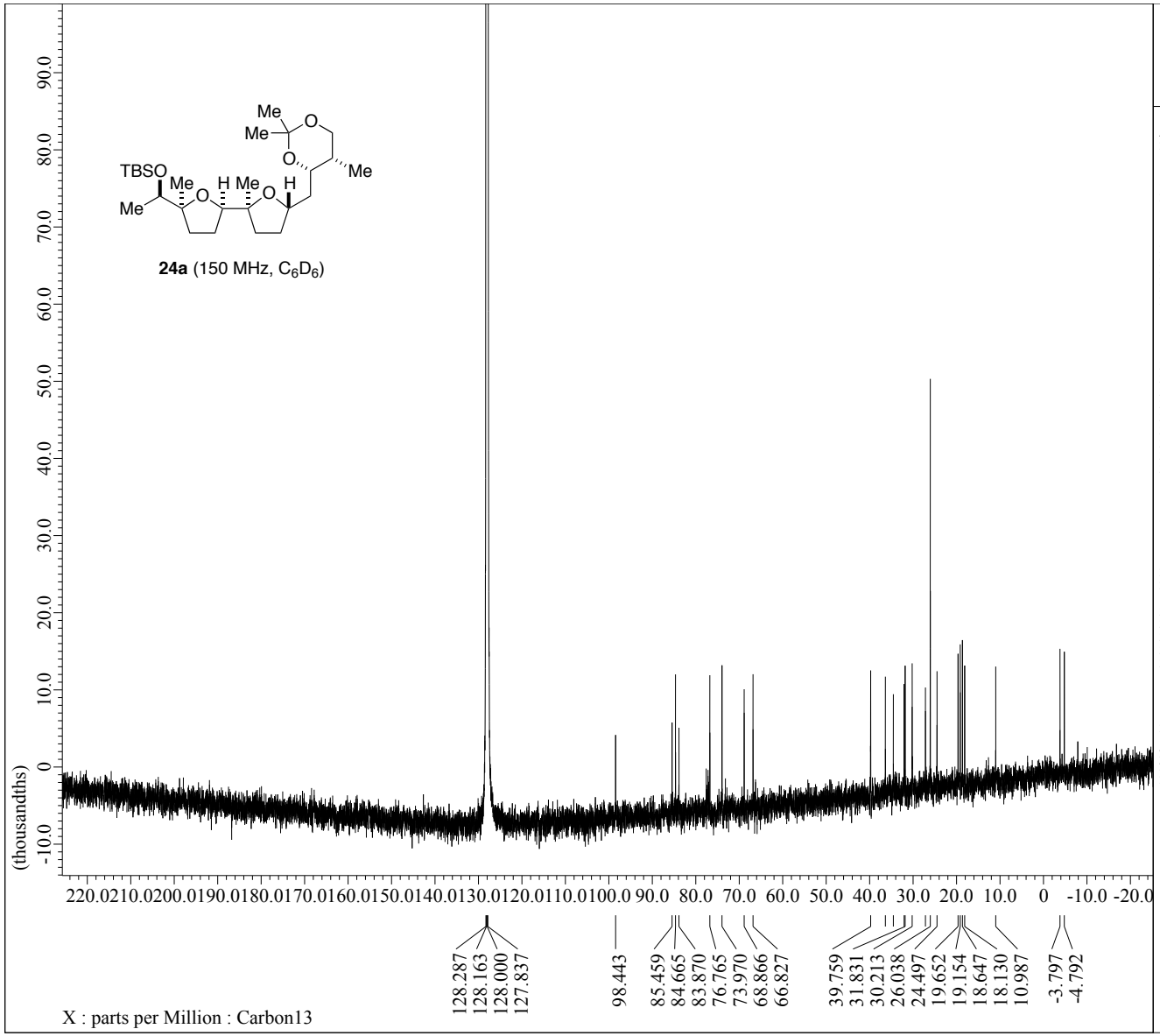



```
Filename          = /Users/HaruhikoFuwa/Docume
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-181-benzene
Solvent           = BENZENE-D6
Creation_Time     =  8-SEP-2015 15:15:01
Revision_Time     = 21-JAN-2016 09:45:22
Current_Time      = 21-JAN-2016 09:46:14

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_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        = 40
Temp_Get          = 22.4[dC]
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]
```

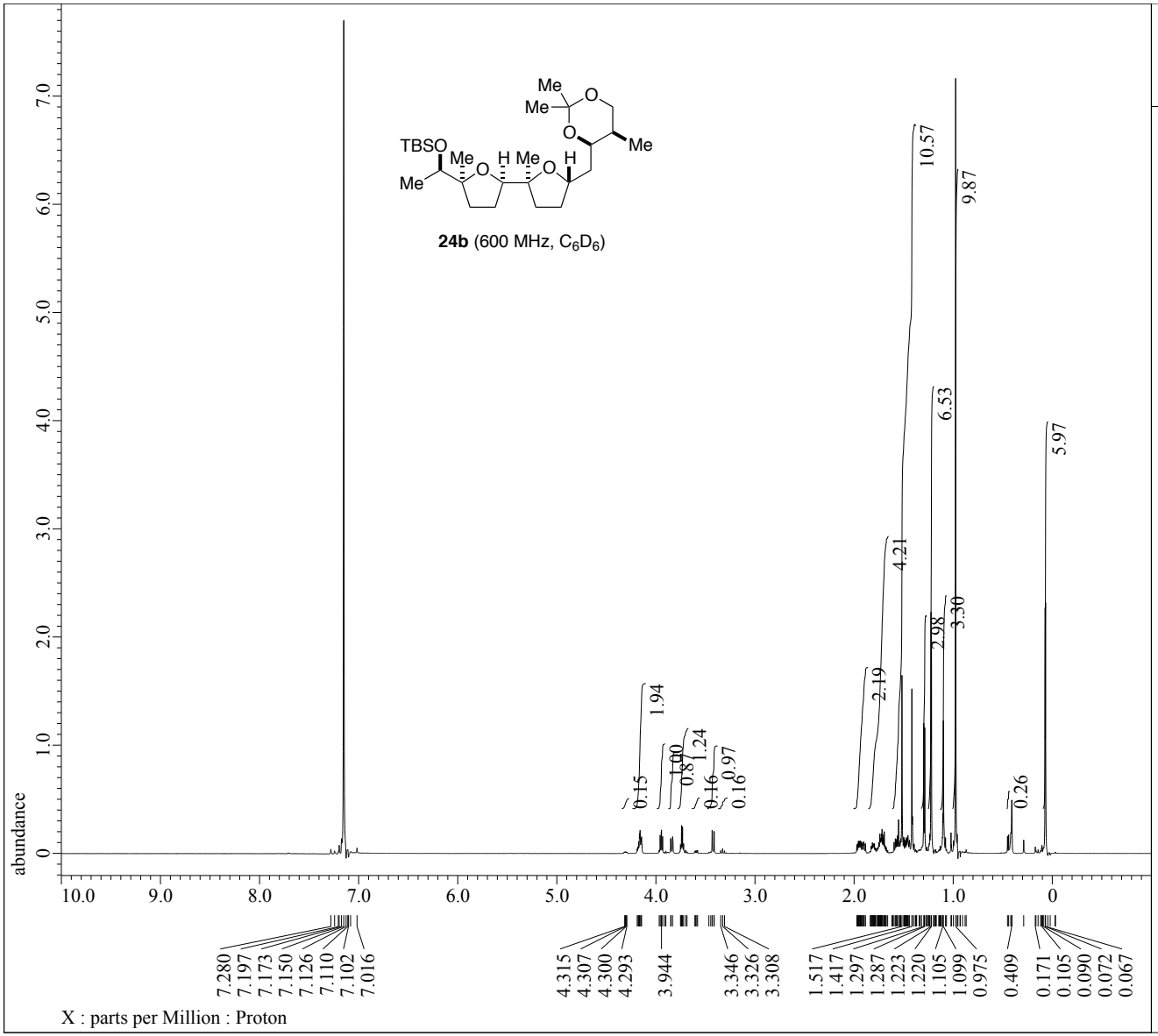



```
Filename          = /Users/HaruhikoFuwa/Docume
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-181
Solvent           = BENZENE-D6
Creation_Time     = 10-SEP-2015 06:31:44
Revision_Time     = 21-JAN-2016 09:48:12
Current_Time      = 21-JAN-2016 09:48:30

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 3832
Total_Scans       = 3832

Relaxation_Delay  = 2[s]
Recvr_Gain        = 52
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_Noe       = 24.452[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]
```

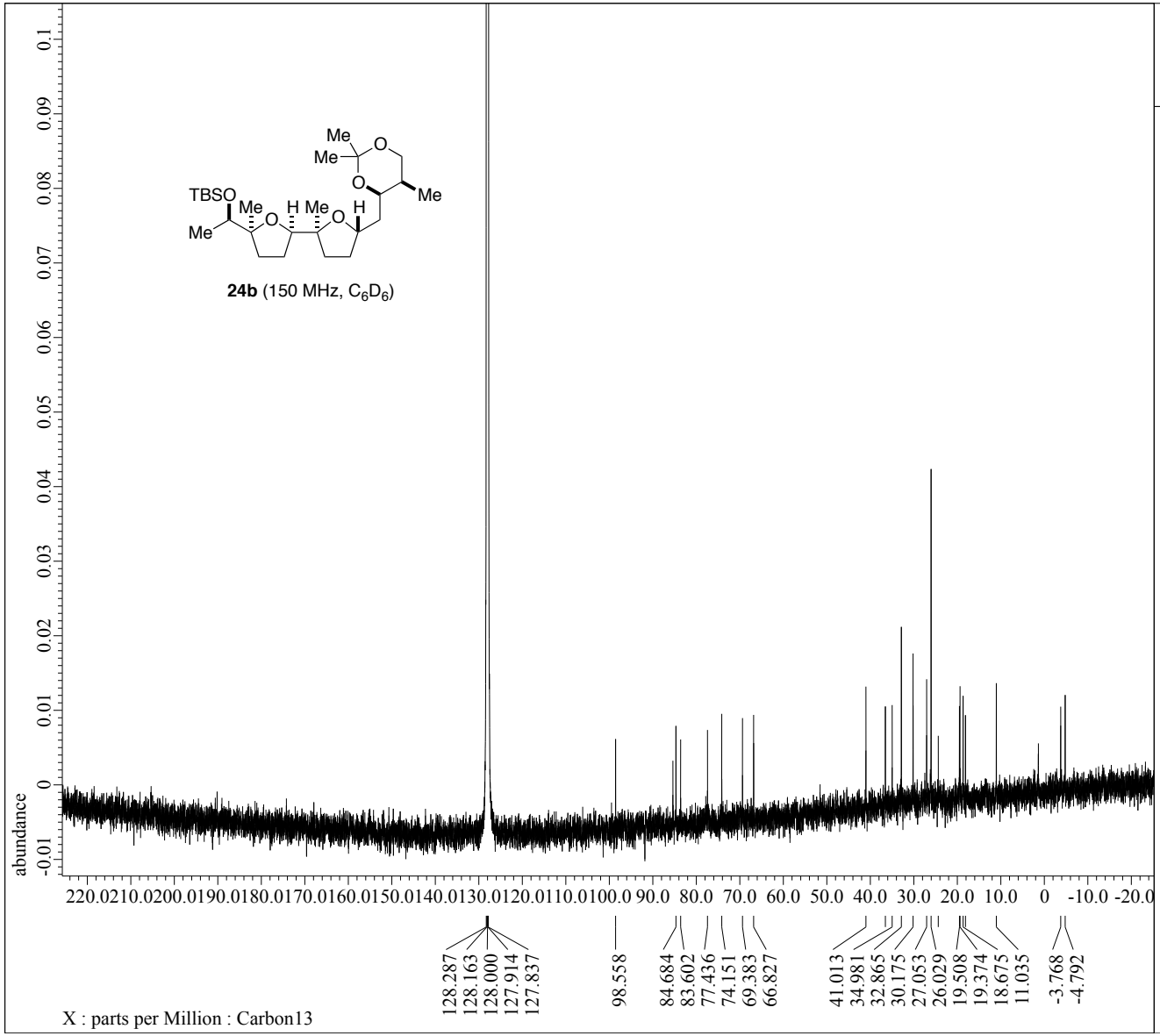



```
Filename          = /Users/HaruhikoFuwa/Docume
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-III-024
Solvent           = BENZENE-D6
Creation_Time     = 12-NOV-2015 15:43:17
Revision_Time     = 21-JAN-2016 09:56:42
Current_Time      = 21-JAN-2016 09:57:20

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        = 40
Temp_Get          = 22.1[dC]
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]
```

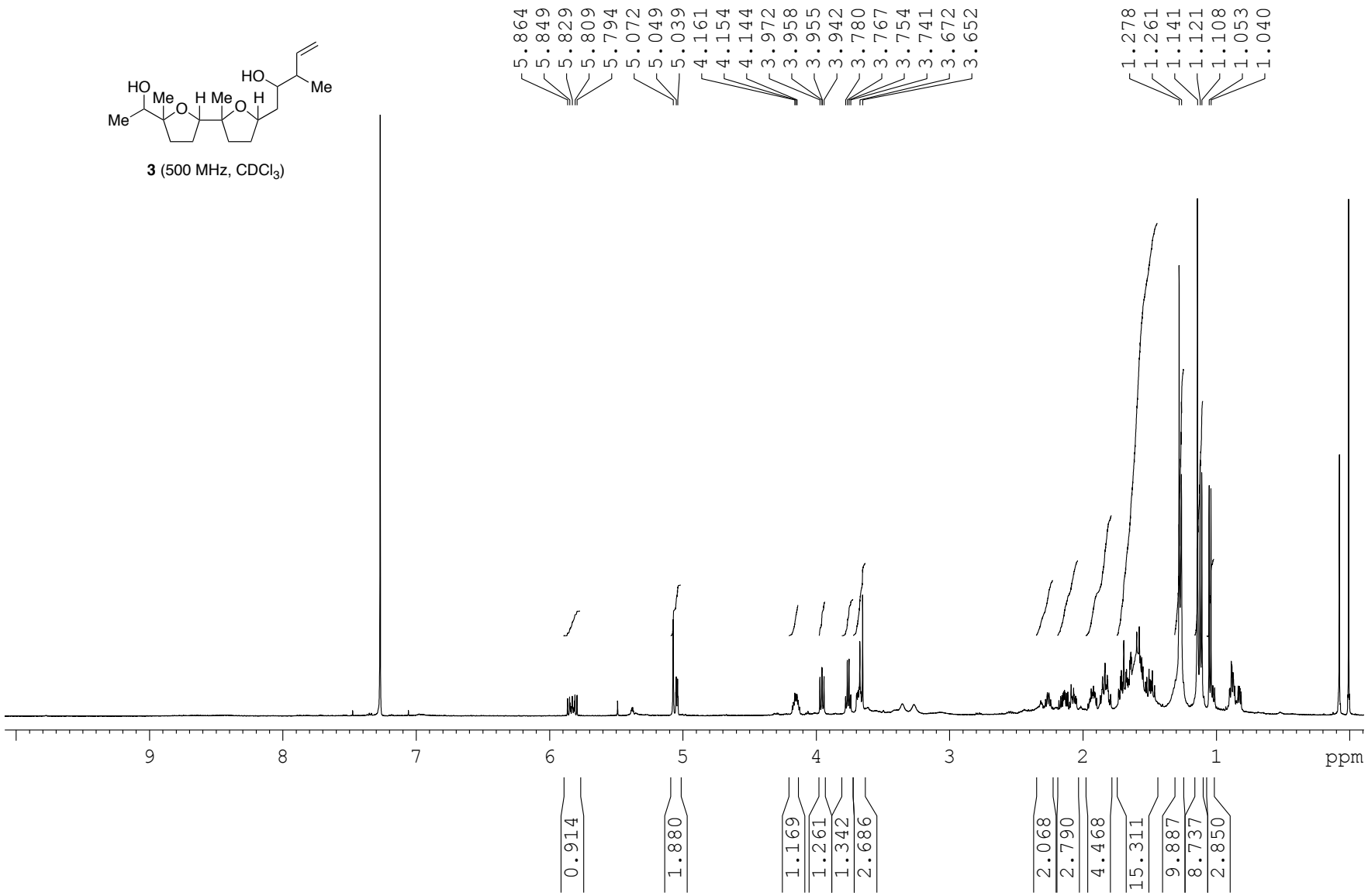


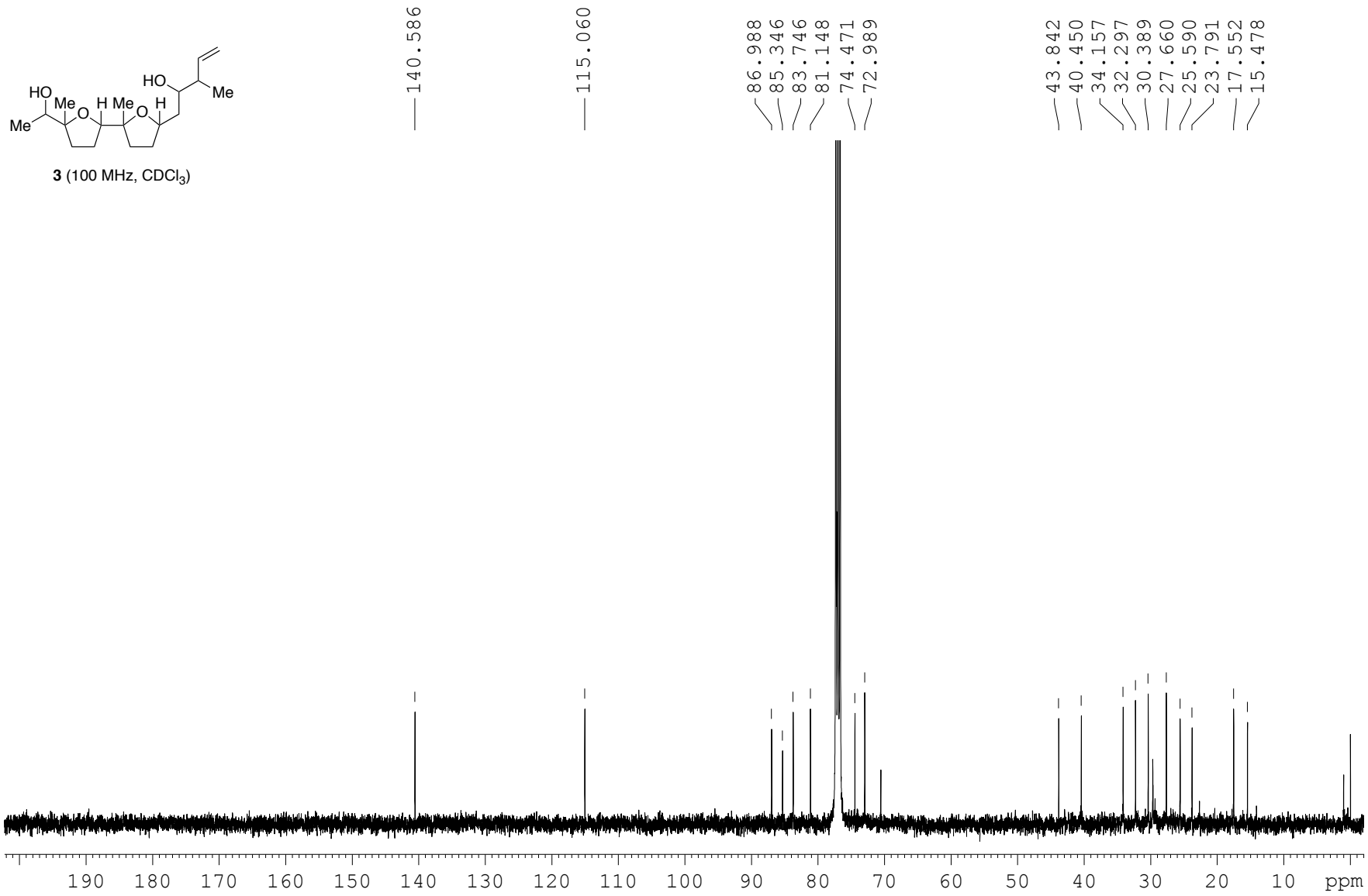

```
Filename          = /Users/HaruhikoFuwa/Docume
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-III-024
Solvent           = BENZENE-D6
Creation_Time     =  9-NOV-2015 23:21:12
Revision_Time     = 21-JAN-2016 09:58:06
Current_Time      = 21-JAN-2016 09:58:26

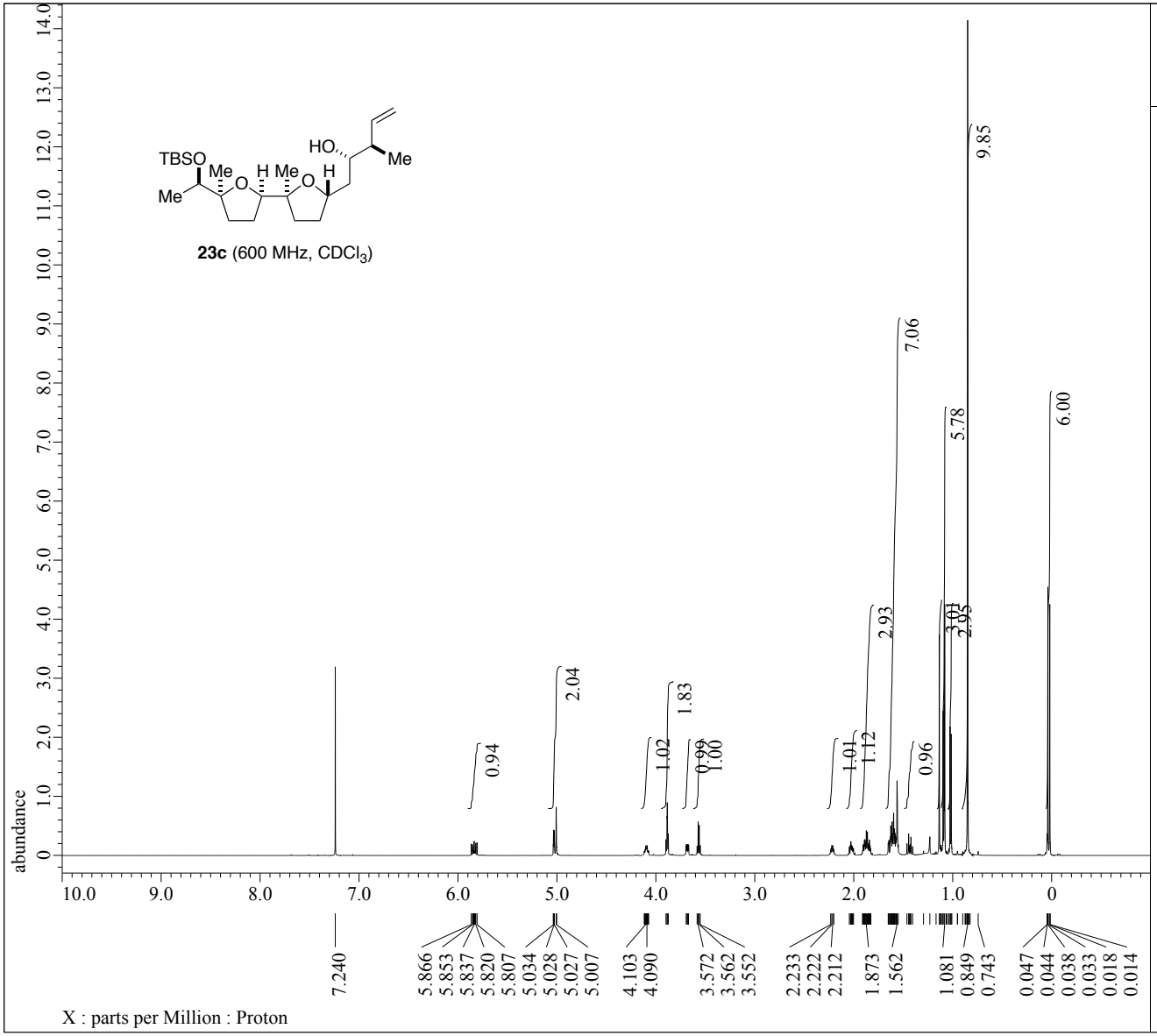
Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA600
Spectrometer      = DELTA2_NMR

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 2560
Total_Scans       = 2560

Relaxation_Delay = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.1[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_Noe       = 24.452[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]
```


HO
Me
Me
O
H
Me
O
H
HO
Me
3 (500 MHz, CDCl3)
5.864
5.849
5.829
5.809
5.794
5.072
5.049
5.039
4.161
4.154
4.144
3.972
3.958
3.955
3.942
3.780
3.767
3.754
3.741
3.672
3.652
1.278
1.261
1.141
1.121
1.108
1.053
1.040
9
8
7
6
5
4
3
2
1
ppm
0.914
1.880
1.169
1.261
1.342
2.686
2.068
2.790
4.468
15.311
9.887
8.737
2.850


HO
Me
H Me
O
O
H
HO
Me
Me
3 (100 MHz, CDCl3)
140.586
115.060
86.988
85.346
83.746
81.148
74.471
72.989
43.842
40.450
34.157
32.297
30.389
27.660
25.590
23.791
17.552
15.478
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



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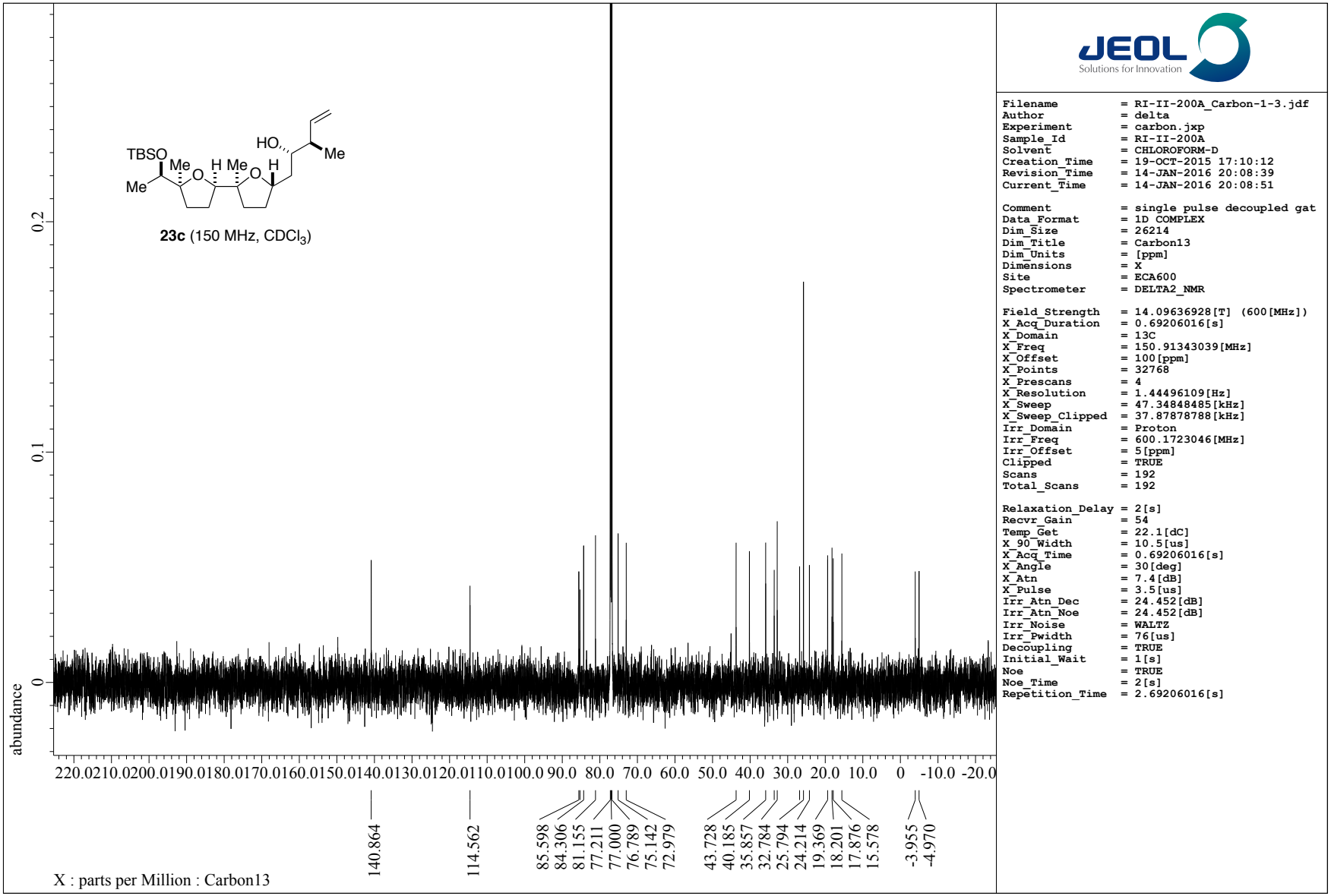
```
Filename          = RI-II-200A_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-200A
Solvent           = CHLOROFORM-D
Creation_Time     = 19-OCT-2015 14:33:06
Revision_Time     = 14-JAN-2016 20:07:38
Current_Time      = 14-JAN-2016 20:07:59

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        = 38
Temp_Get          = 22.1[dC]
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]
```


TBSO
Me
Me
H
Me
O
O
H
HO
Me
23c (150 MHz, CDCl3)
abundance
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
140.864
114.562
85.598
84.306
81.155
77.211
77.000
76.789
75.142
72.979
43.728
40.185
35.857
32.784
25.794
24.214
19.369
18.201
17.876
15.578
-3.955
-4.970
X : parts per Million : Carbon13
JEOL
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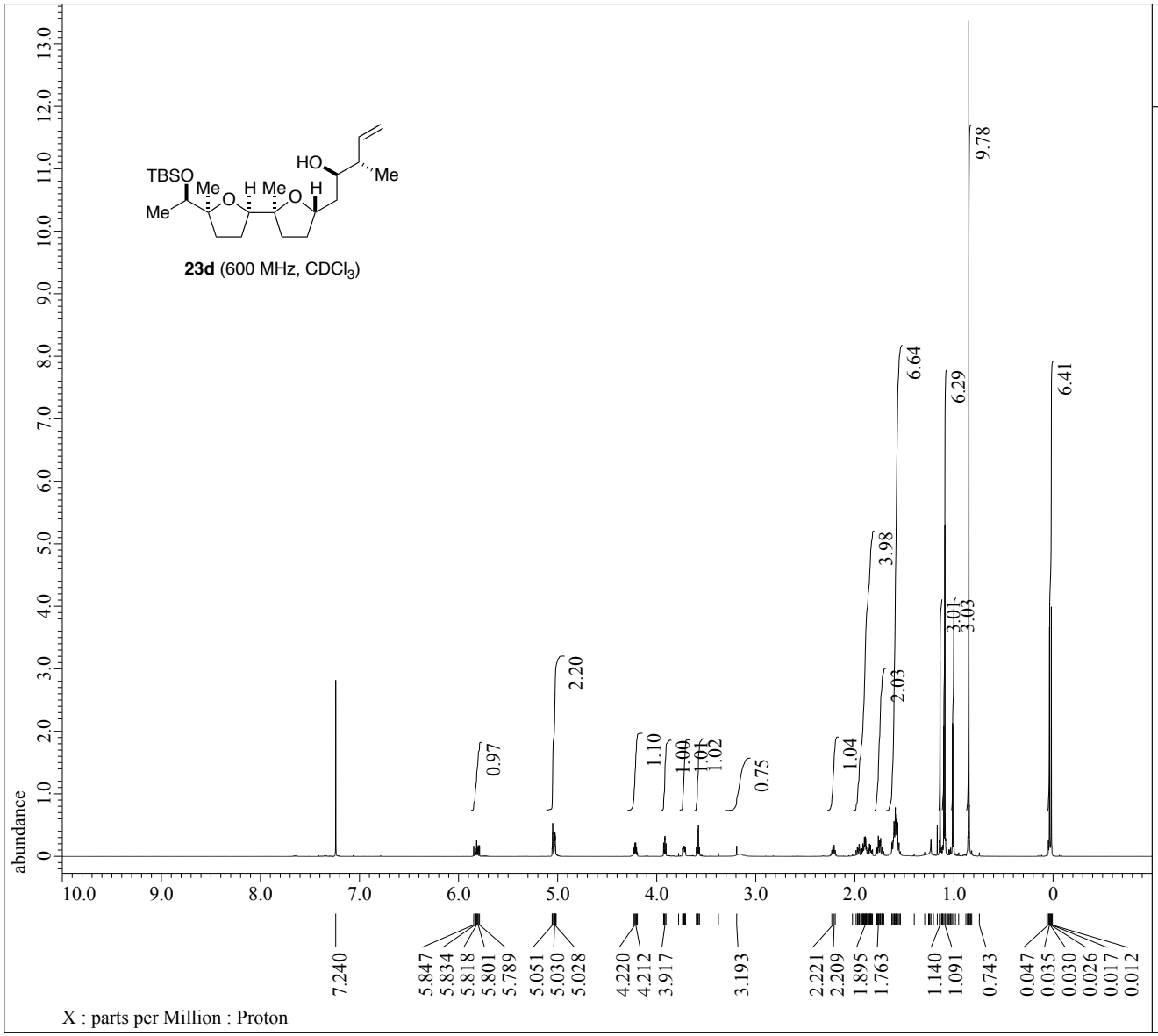
Filename = RI-II-200A_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = RI-II-200A
Solvent = CHLOROFORM-D
Creation_Time = 19-OCT-2015 17:10:12
Revision_Time = 14-JAN-2016 20:08:39
Current_Time = 14-JAN-2016 20:08:51
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 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_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 192
Total_Scans = 192
Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 22.1[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_Noe = 24.452[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]



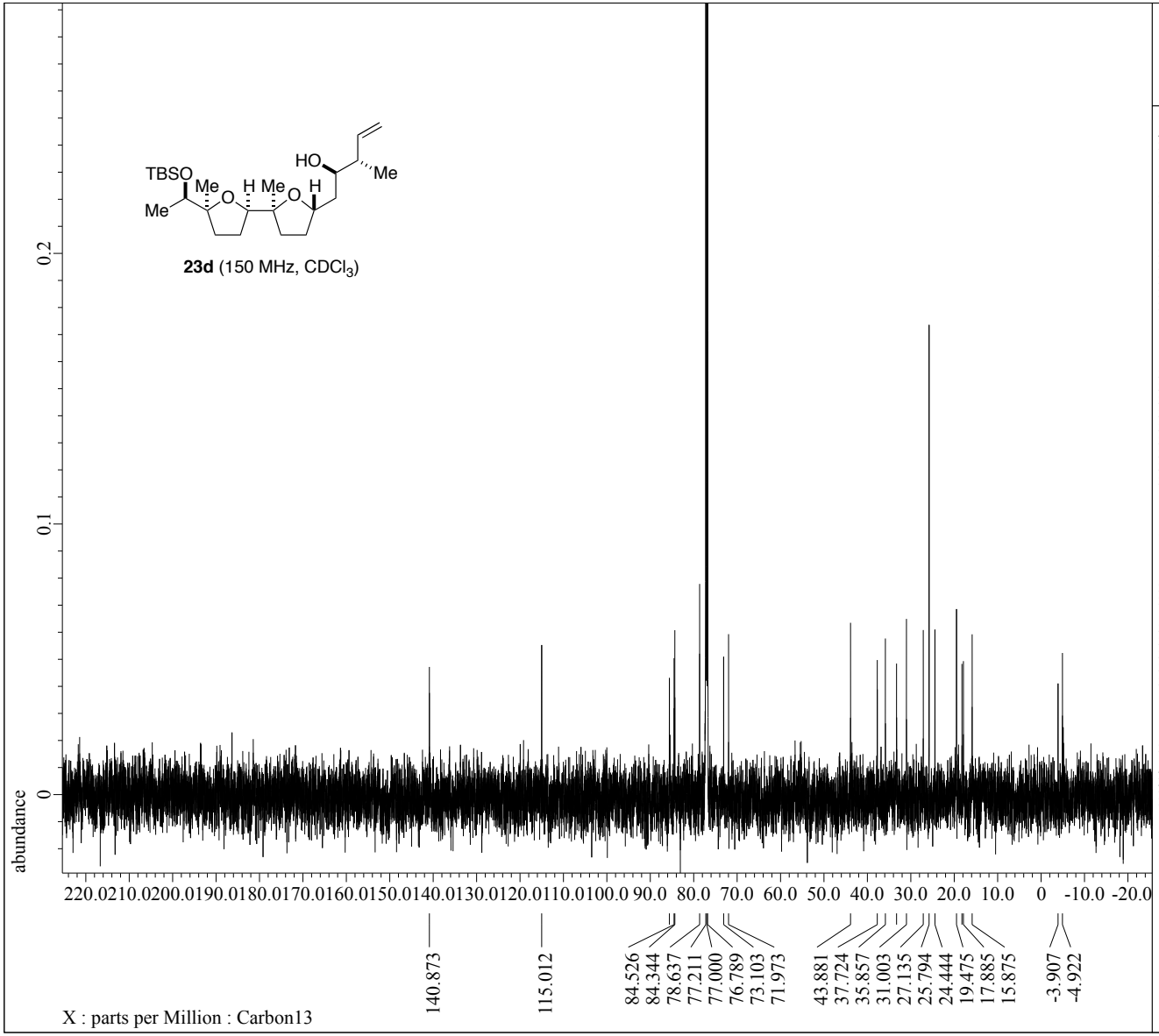
JEOL Solutions for Innovation

```
Filename          = RI-II-200B_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-II-200B
Solvent           = CHLOROFORM-D
Creation_Time     = 19-OCT-2015 14:45:35
Revision_Time     = 14-JAN-2016 20:11:22
Current_Time      = 14-JAN-2016 20:11:45

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        = 38
Temp_Get          = 22.1[dC]
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]
```



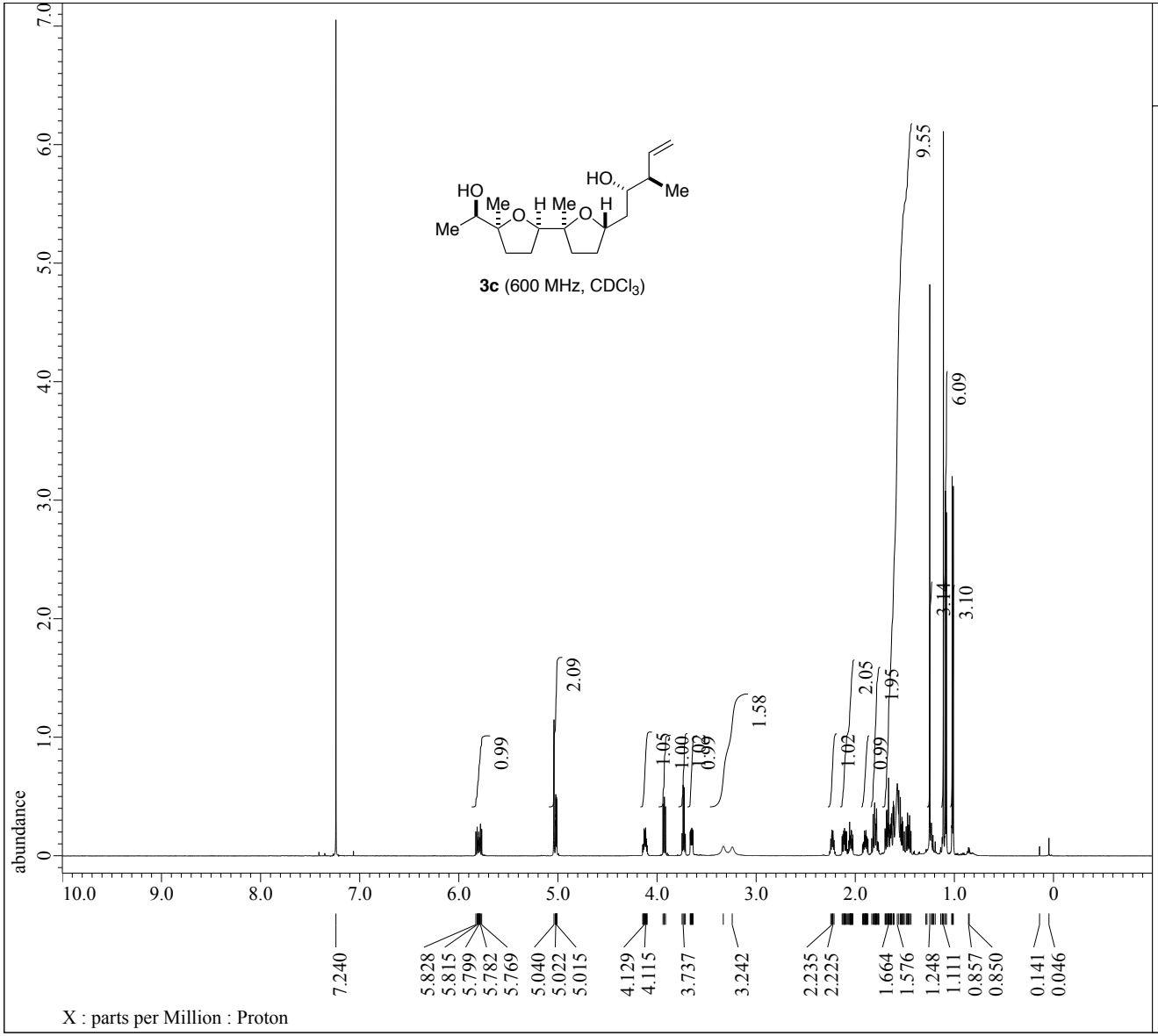
JEOL
Solutions for Innovation

```
Filename          = RI-II-200B_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-II-200B
Solvent           = CHLOROFORM-D
Creation_Time     = 19-OCT-2015 17:29:38
Revision_Time     = 14-JAN-2016 20:12:26
Current_Time      = 14-JAN-2016 20:12:36

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 216
Total_Scans       = 216

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
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_Noe       = 24.452[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]
```



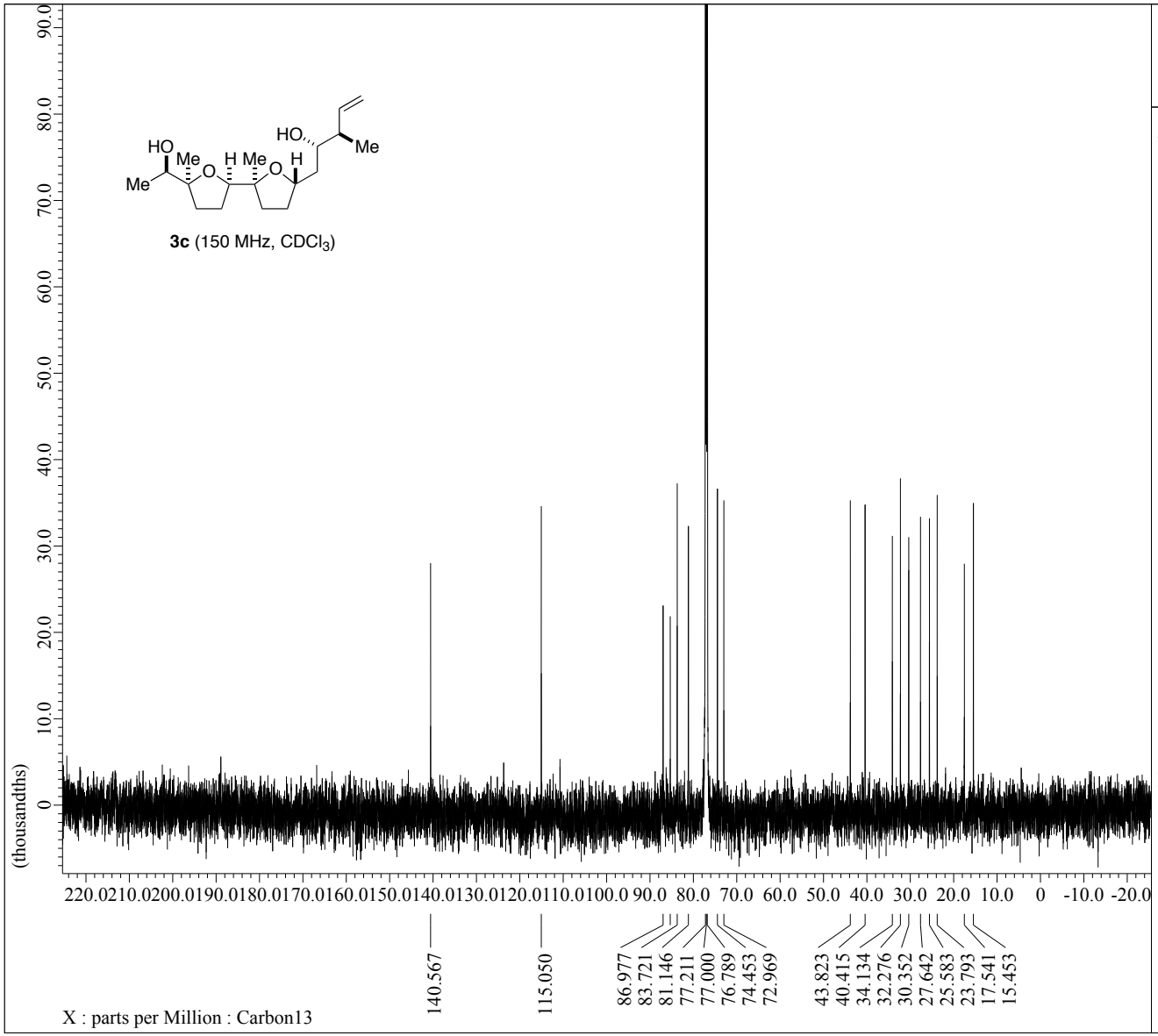
JEOL Solutions for Innovation

```
Filename          = RI-III-009_proton-2-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-III-009
Solvent           = CHLOROFORM-D
Creation_Time     = 27-OCT-2015 23:12:38
Revision_Time     = 14-JAN-2016 21:00:05
Current_Time      = 14-JAN-2016 21:00:25

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        = 44
Temp_Get          = 22[dC]
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]
```



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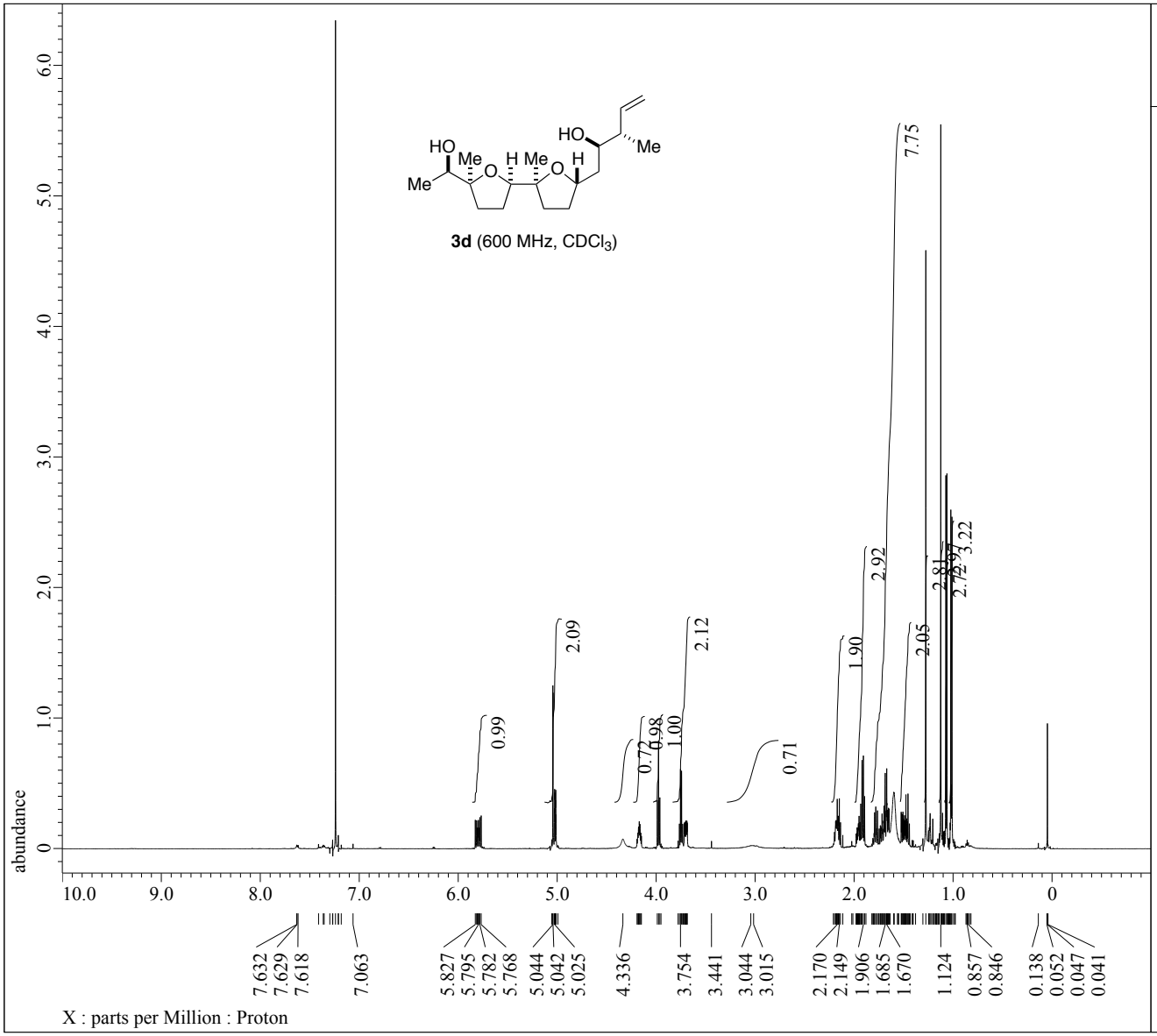
```
Filename          = RI-III-009_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-III-009
Solvent           = CHLOROFORM-D
Creation_Time     = 27-OCT-2015 23:16:15
Revision_Time     = 14-JAN-2016 21:01:00
Current_Time      = 14-JAN-2016 21:01:15

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 2650
Total_Scans       = 2650

Relaxation_Delay = 2[s]
Recvr_Gain        = 54
Temp_Get          = 22[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_Noe       = 24.452[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]
```

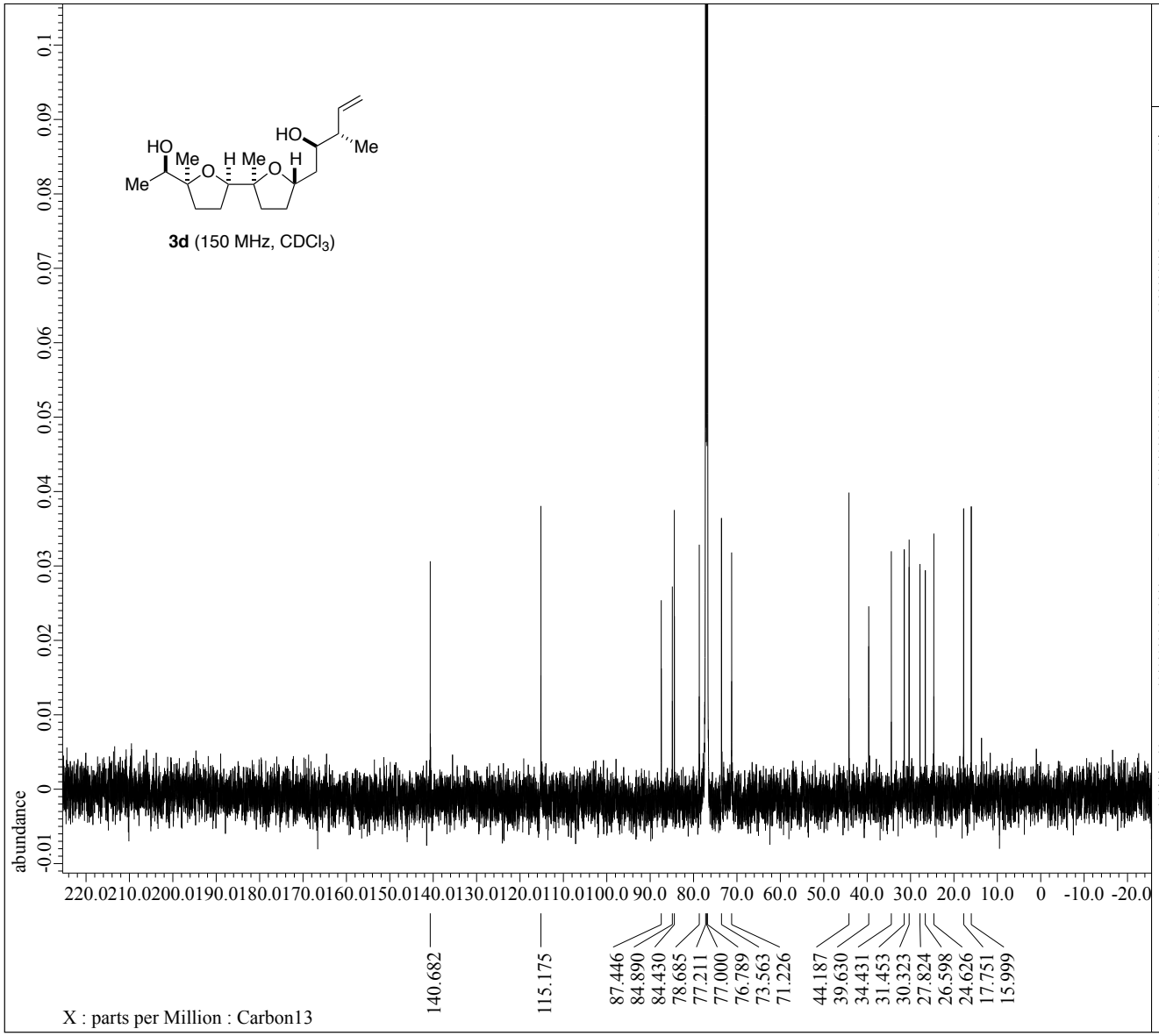



```
Filename          = RI-III-011_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-III-011
Solvent           = CHLOROFORM-D
Creation_Time     = 28-OCT-2015 15:37:42
Revision_Time     = 14-JAN-2016 21:03:39
Current_Time      = 14-JAN-2016 21:04:04

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        = 44
Temp_Get          = 22.1[dC]
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]
```



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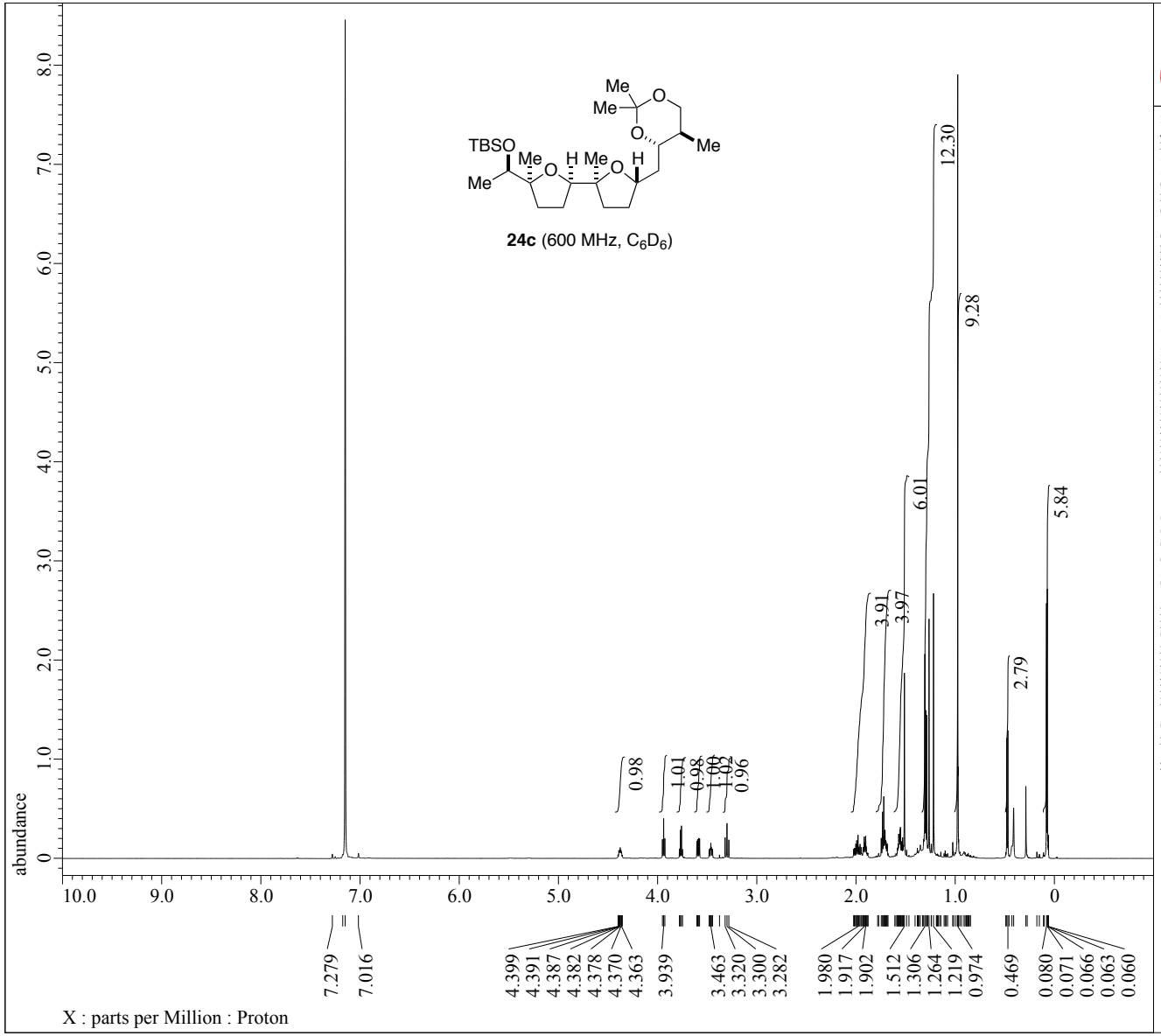
```
Filename          = RI-III-011_Carbon-1-4.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-III-011
Solvent           = CHLOROFORM-D
Creation_Time     = 30-OCT-2015 23:12:34
Revision_Time     = 14-JAN-2016 21:04:59
Current_Time      = 14-JAN-2016 21:05:11

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 2600
Total_Scans       = 2600

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 21.9[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_Noe       = 24.452[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]
```

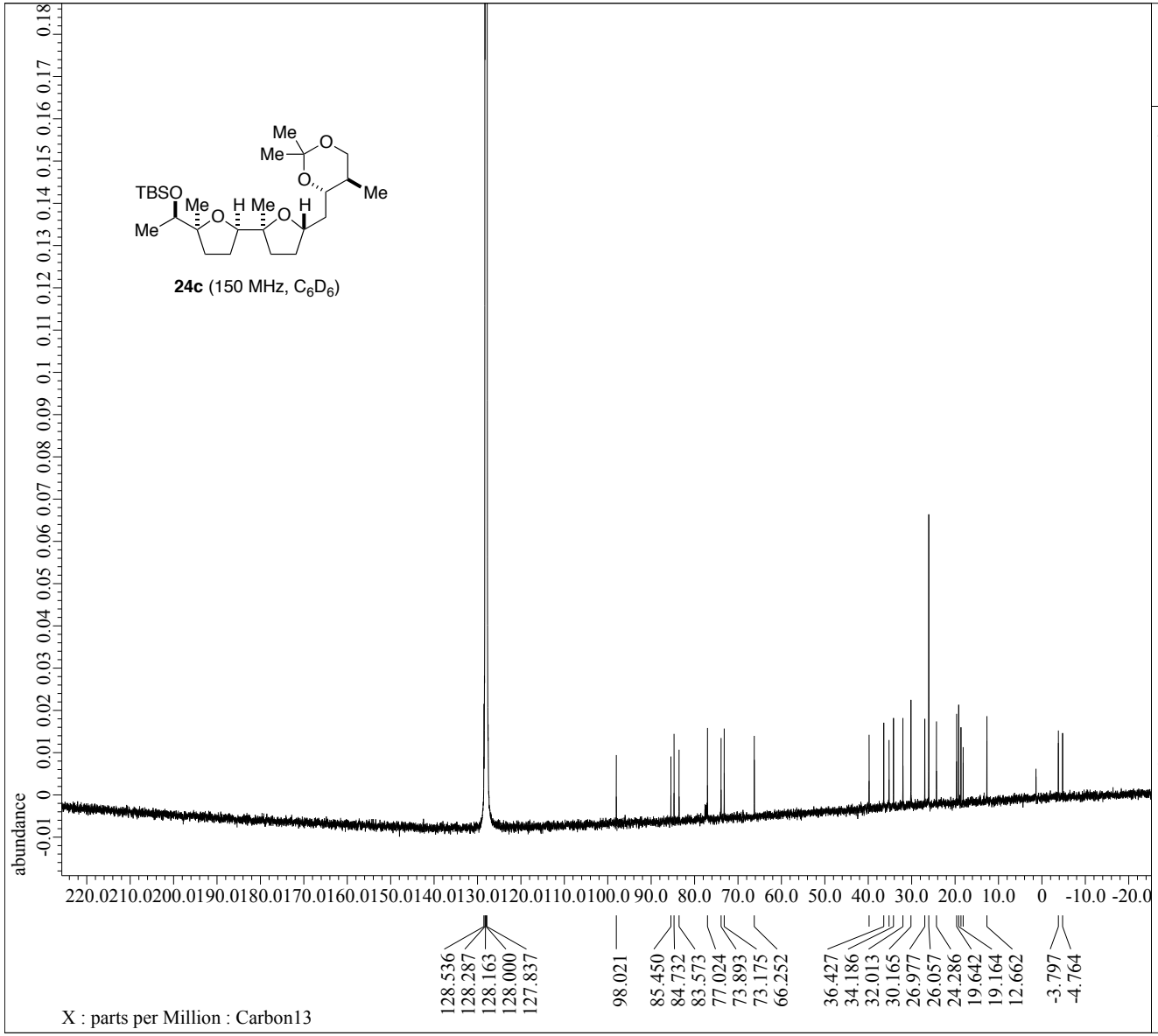



```
Filename          = /Users/HaruhikoFuwa/Docume
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-III-003
Solvent           = BENZENE-D6
Creation_Time     = 31-OCT-2015 09:42:24
Revision_Time     = 21-JAN-2016 10:04:10
Current_Time      = 21-JAN-2016 10:04:34

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        = 40
Temp_Get          = 21.7[dC]
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]
```

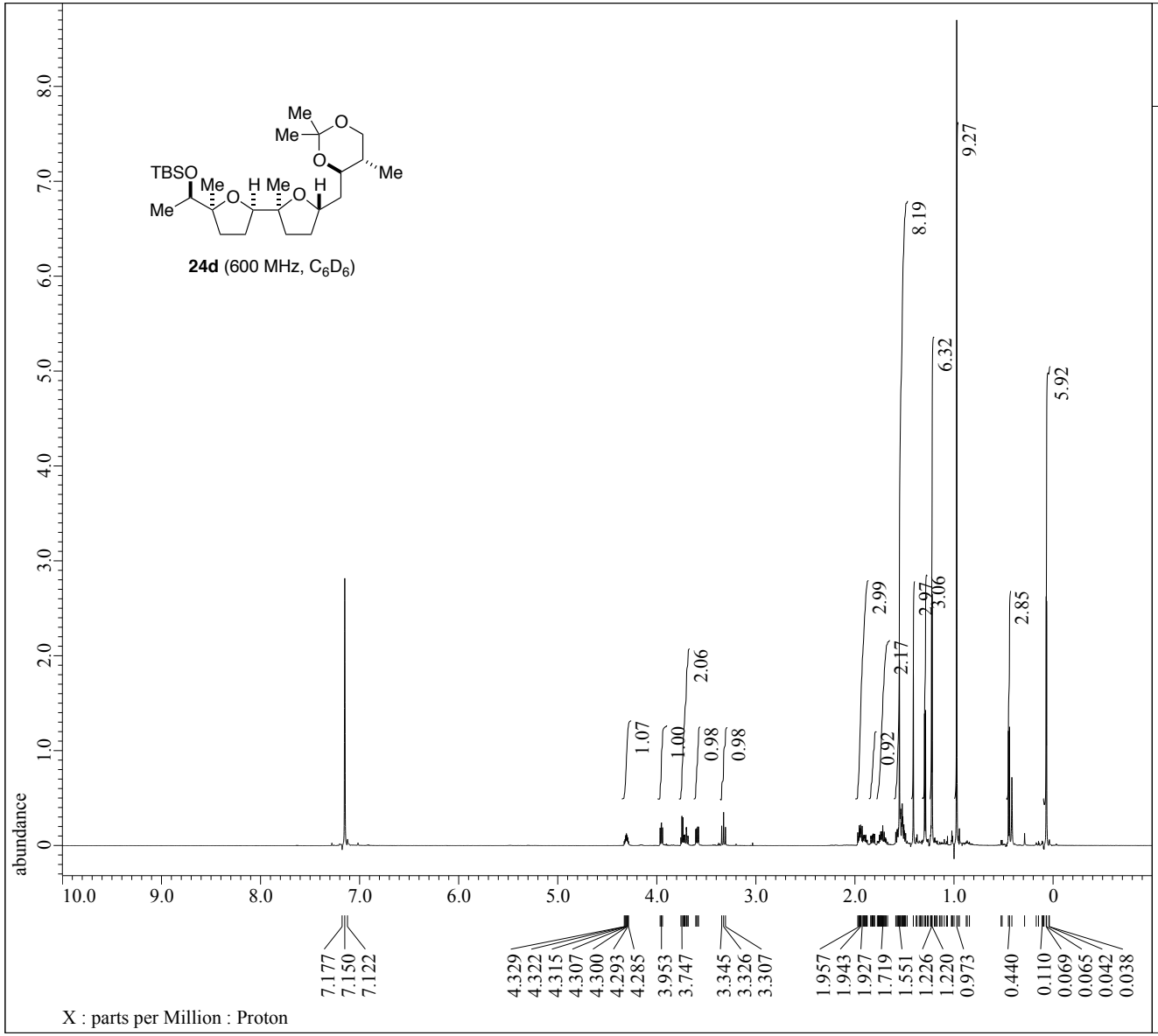



```
Filename          = /Users/HaruhikoFuwa/Docume
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-III-003
Solvent           = BENZENE-D6
Creation_Time     = 26-OCT-2015 00:40:59
Revision_Time     = 21-JAN-2016 10:05:38
Current_Time      = 21-JAN-2016 10:05:53

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 11612
Total_Scans       = 11612

Relaxation_Delay  = 2[s]
Recvr_Gain        = 52
Temp_Get          = 21.9[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_Noe       = 24.452[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]
```

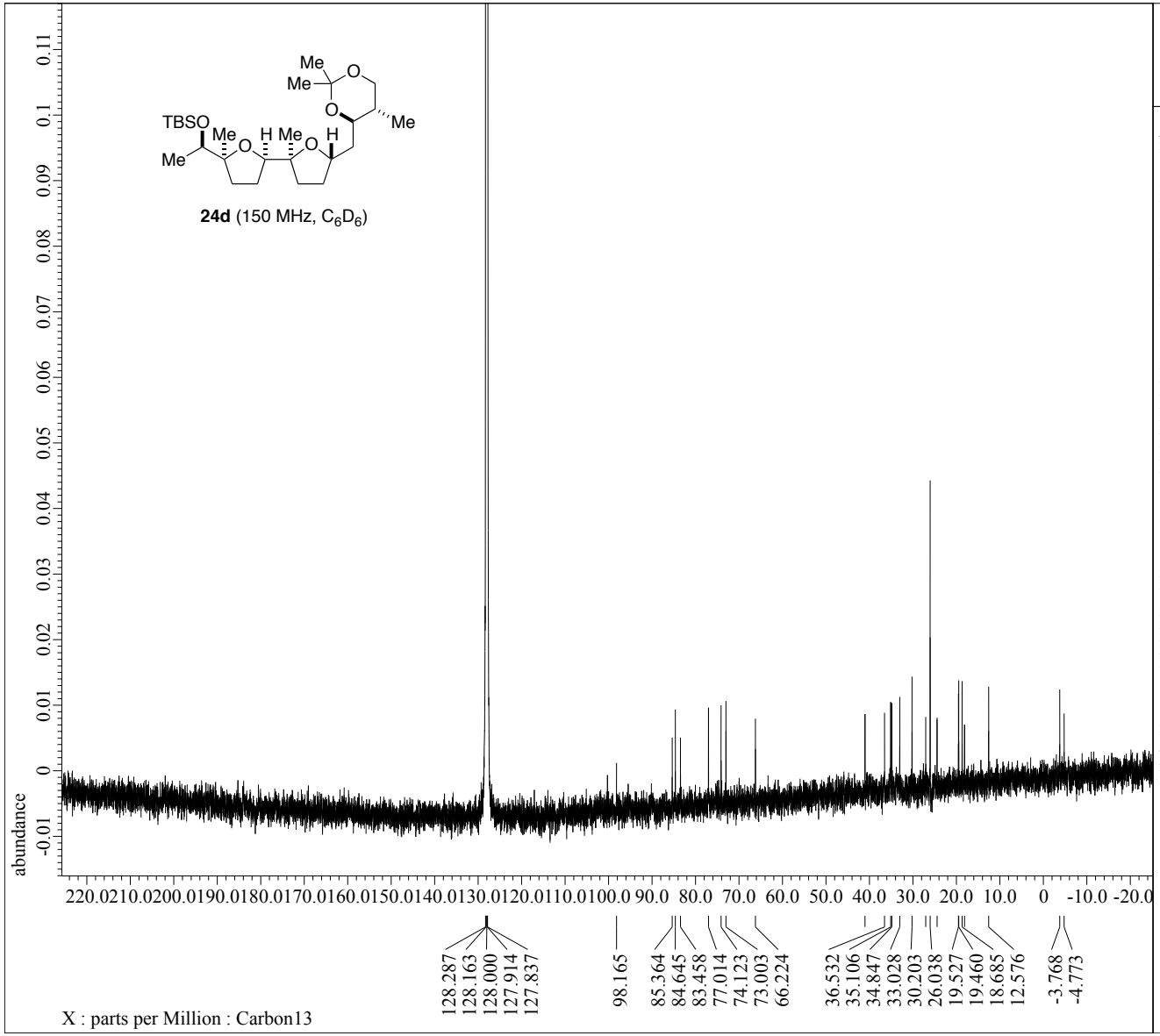



```
Filename          = /Users/HaruhikoFuwa/Docume
Author            = delta
Experiment        = proton.jxp
Sample_Id         = RI-III-021
Solvent           = BENZENE-D6
Creation_Time     = 18-NOV-2015 17:19:33
Revision_Time     = 21-JAN-2016 10:11:53
Current_Time      = 21-JAN-2016 10:12:14

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_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        = 42
Temp_Get          = 21.9[dC]
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]
```




```
Filename          = /Users/HaruhikoFuwa/Docume
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = RI-III-021
Solvent           = BENZENE-D6
Creation_Time     = 18-NOV-2015 00:21:08
Revision_Time     = 21-JAN-2016 10:20:53
Current_Time      = 21-JAN-2016 10:21:21

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_Clipped   = 37.87878788[kHz]
Irr_Domain        = Proton
Irr_Freq          = 600.1723046[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 2600
Total_Scans       = 2600

Relaxation_Delay  = 2[s]
Recvr_Gain        = 52
Temp_Get          = 22[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_Noe       = 24.452[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]
```