Regioselective C-H Azidation of Anilines and Application to Synthesis of Key Intermediate for Pharmaceutical

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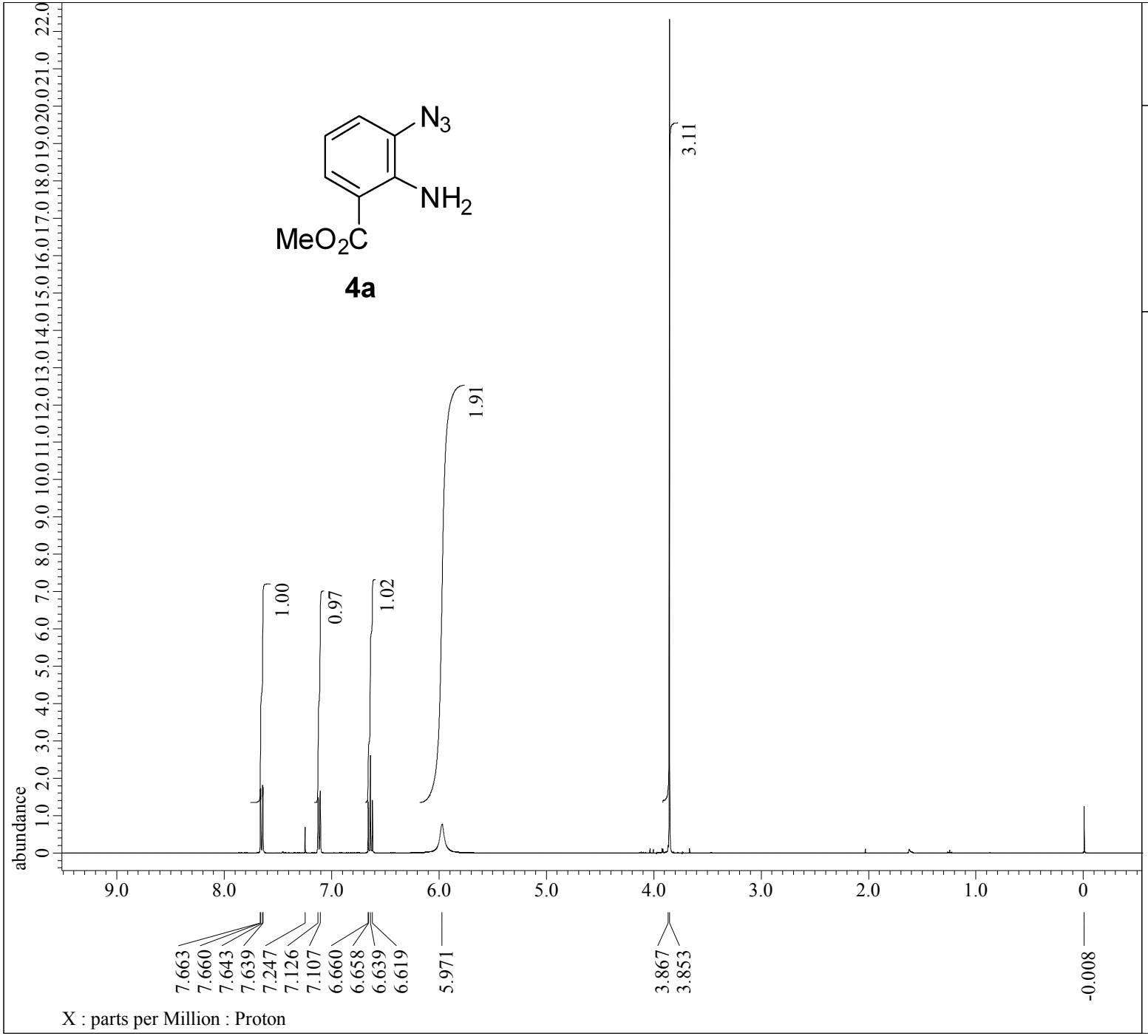
Supporting Information

Content:

NMR spectra for compounds **4a**, **4b**, **4c**, **4d**, **4e**, **4f**, **4g**, **4h**, **4i**, **4j**, **4k**, **11**, **2** S2



JEOL RESONANCE

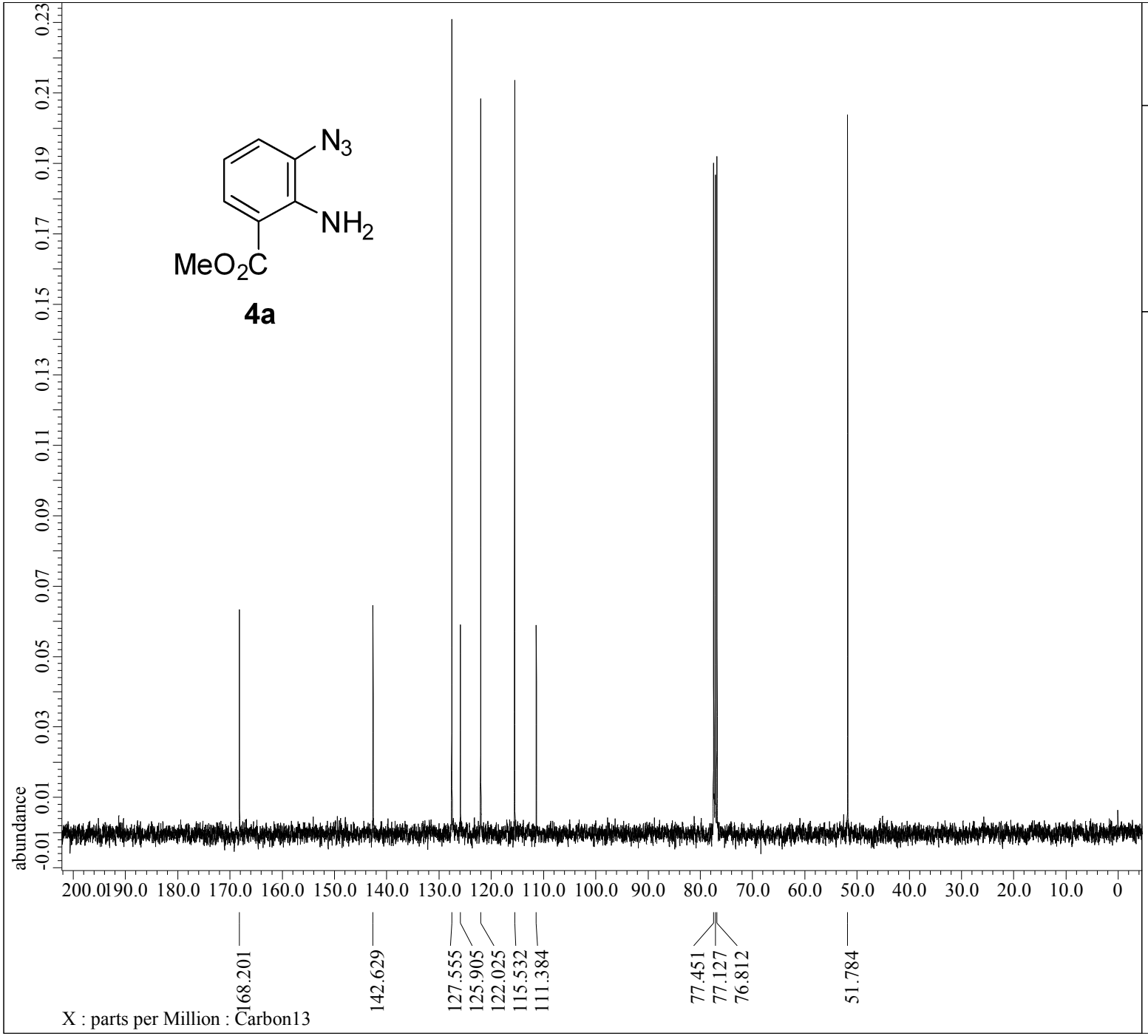
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = ytakahashi180810-2-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AAM
Solvent           = CHLOROFORM-D
Creation_Time     = 10-AUG-2018 17:29:03
Revision_Time     = 10-AUG-2018 16:57:42
Current_Time      = 25-DEC-2020 17:36:18

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 24
Temp_Get          = 24.2[dC]
X_90_Width        = 7.018[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.5[dB]
X_Pulse           = 3.509[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

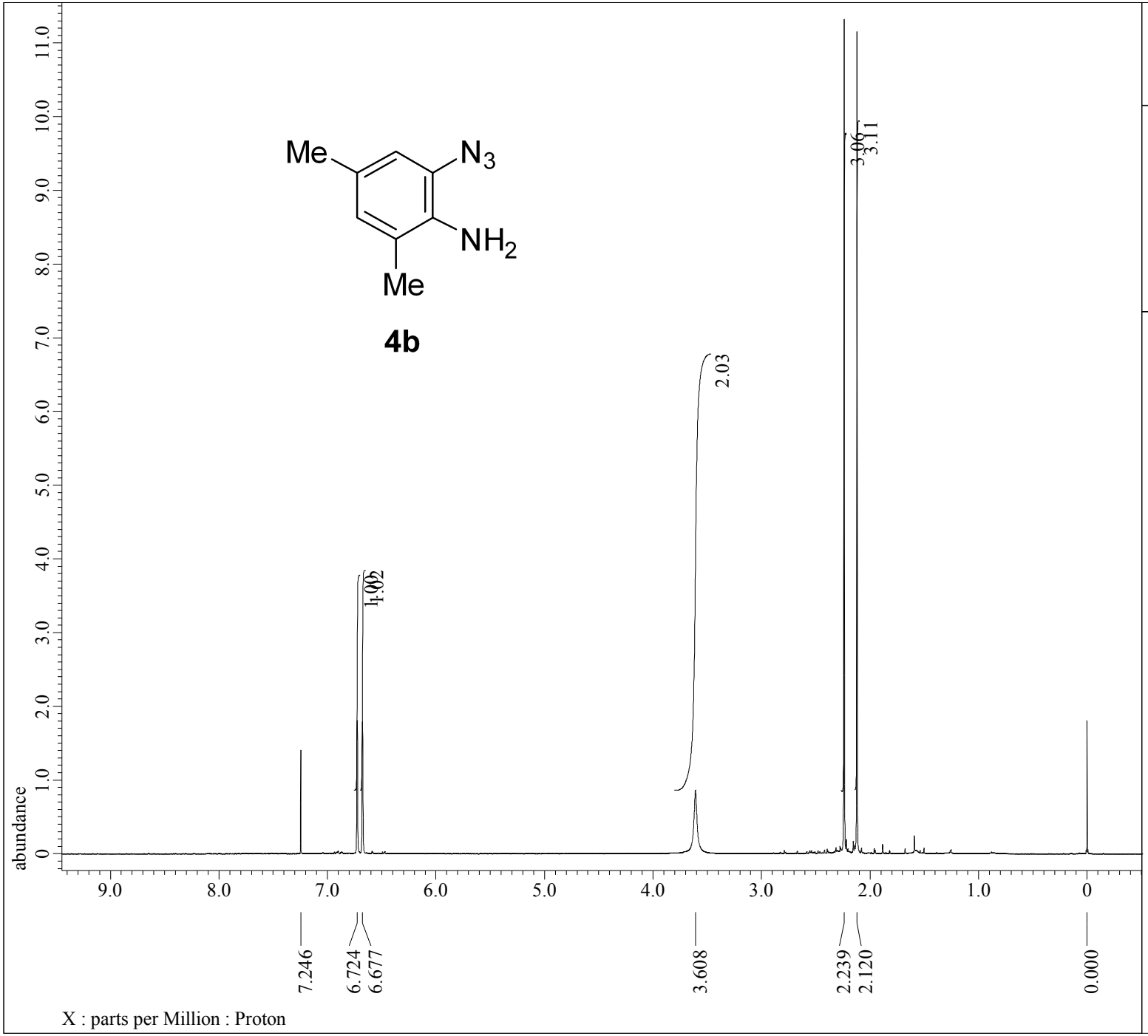
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = ytakahashi180810-3-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AAM
Solvent           = CHLOROFORM-D
Creation_Time     = 10-AUG-2018 17:33:19
Revision_Time     = 10-AUG-2018 17:36:54
Current_Time      =  5-JAN-2021 11:16:59

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 128
Total_Scans       = 128

Relaxation_Delay  = 2[s]
Recvr_Gain        = 44
Temp_Get          = 24.1[dC]
X_90_Width        = 11.329[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.77633333[us]
Irr_Atn_Dec       = 27.79[dB]
Irr_Atn_Noe       = 27.79[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



JEOL RESONANCE

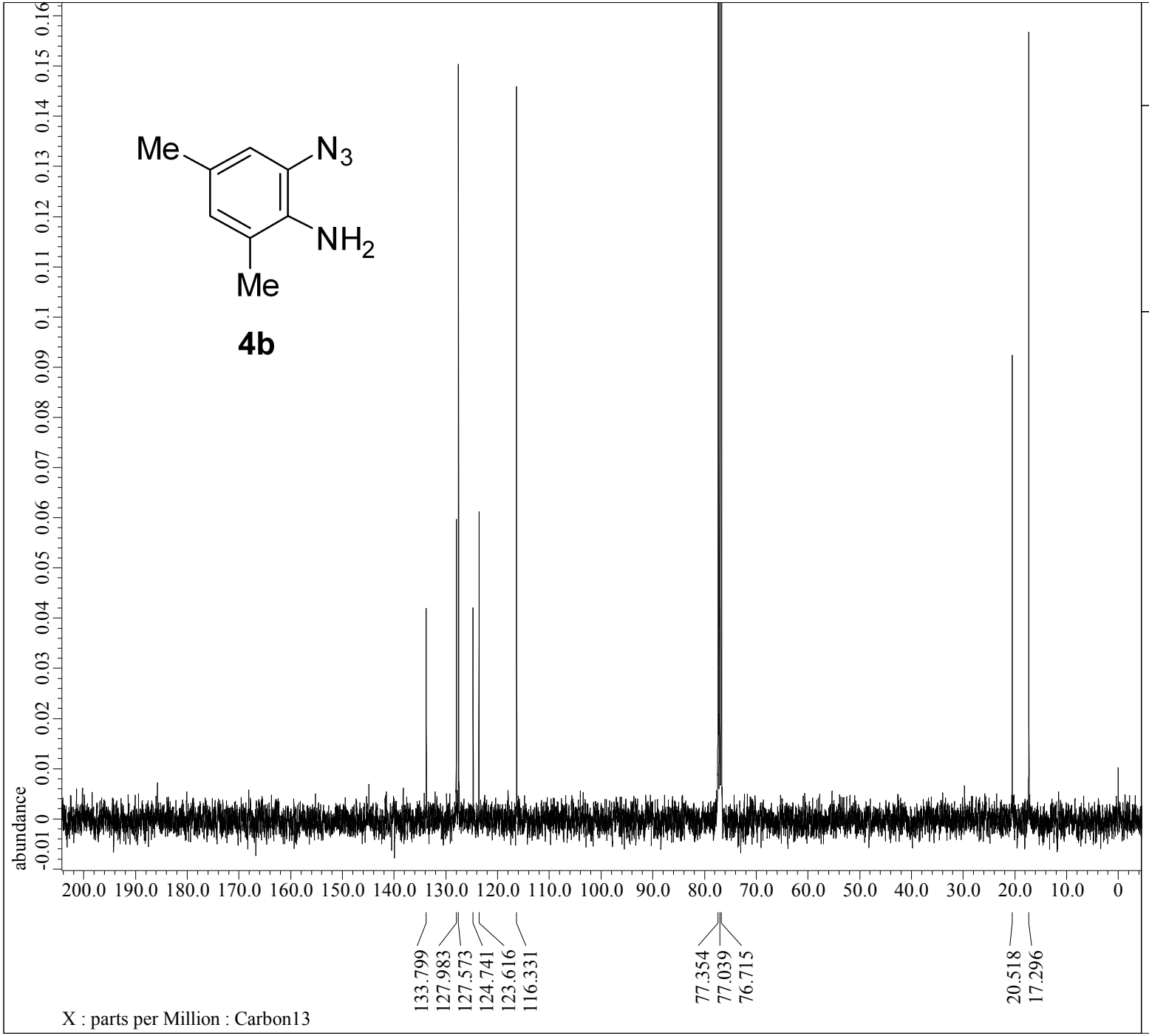
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.00007[ppm], 2.5[ppm] )
reference( 2.5[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190116-1-7.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 2-アジド-4,6-ジメチルアニリン
Solvent           = CHLOROFORM-D
Creation_Time     = 16-JAN-2019 17:07:38
Revision_Time     = 16-JAN-2019 16:48:05
Current_Time      = 25-DEC-2020 17:39:59

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 28
Temp_Get          = 25.1[dC]
X_90_Width        = 7.018[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.5[dB]
X_Pulse           = 3.509[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

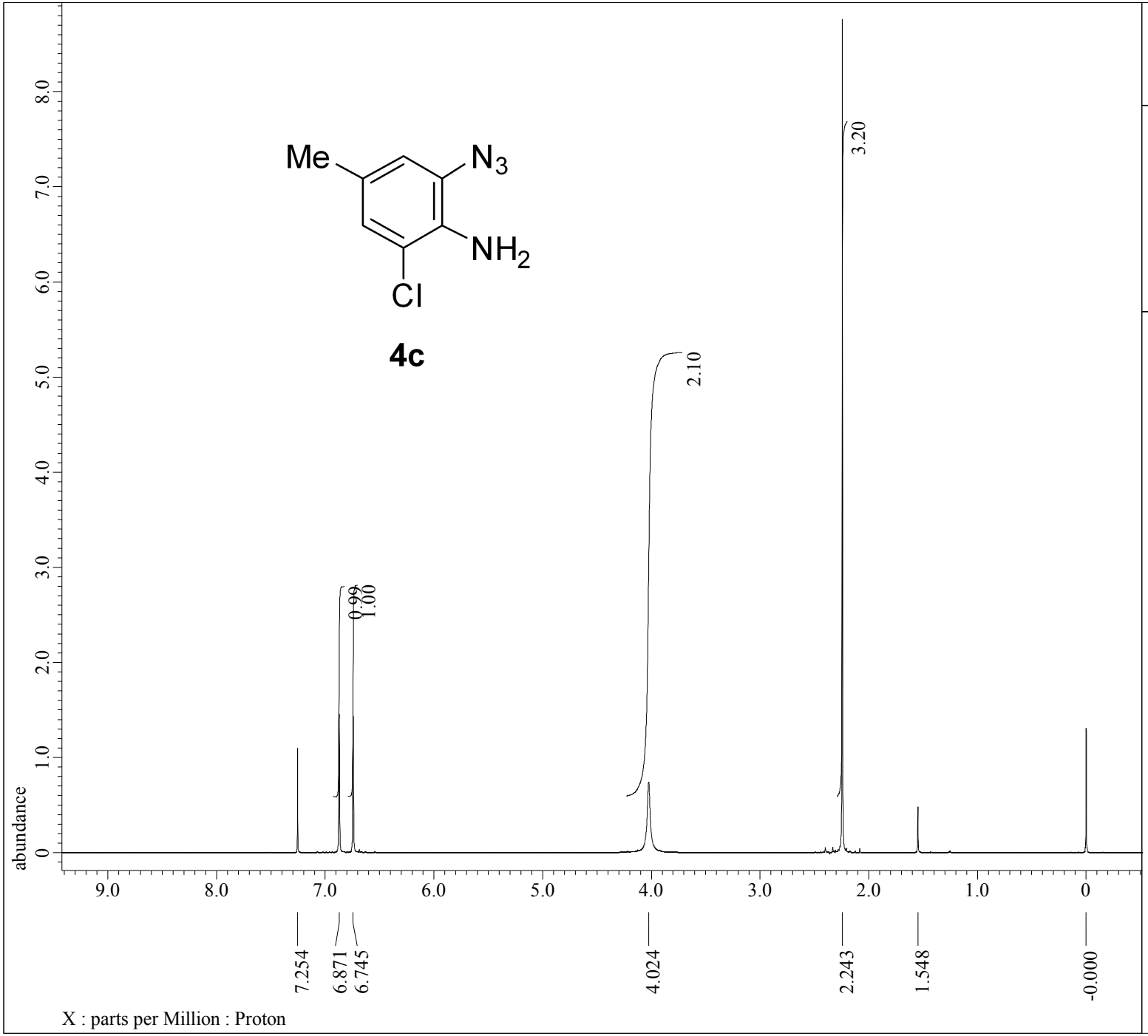
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 0.07759[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190116-2-4.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 2-アジド-4,6-ジメチルアニリン
Solvent           = CHLOROFORM-D
Creation_Time     = 16-JAN-2019 17:11:35
Revision_Time     = 16-JAN-2019 16:49:05
Current_Time      =  5-JAN-2021 11:20:09

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 200
Total_Scans       = 200

Relaxation_Delay  = 2[s]
Recvr_Gain        = 48
Temp_Get          = 25[dC]
X_90_Width        = 11.329[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.77633333[us]
Irr_Atn_Dec       = 27.79[dB]
Irr_Atn_Noe       = 27.79[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



JEOL RESONANCE

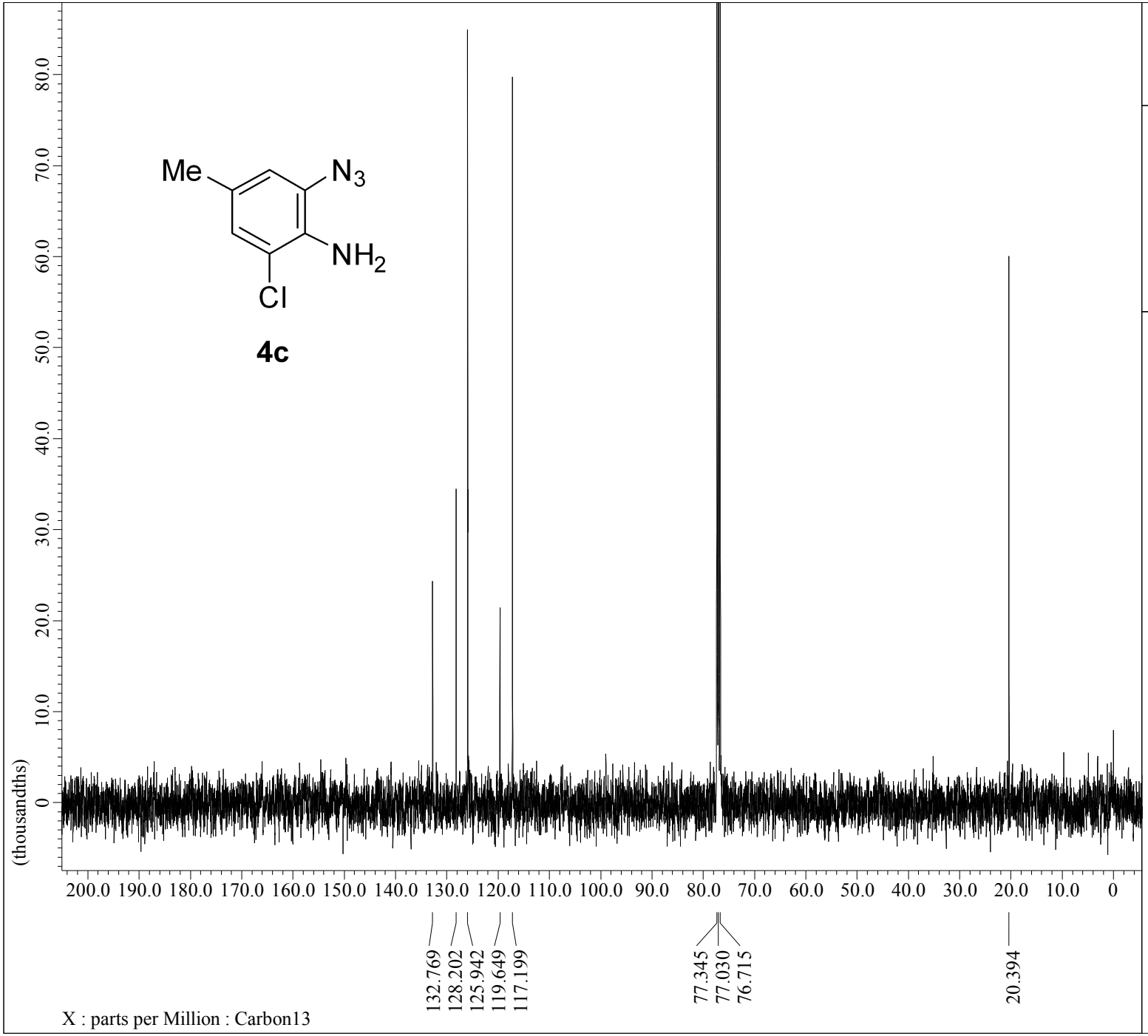
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.00809[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190118-1-6.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 2-アジド-4-メチル-6-クロロアニリン
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2019 17:45:11
Revision_Time     = 18-JAN-2019 17:25:27
Current_Time      = 25-DEC-2020 17:42:16

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 24.7[dC]
X_90_Width        = 7.018[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.5[dB]
X_Pulse           = 3.509[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

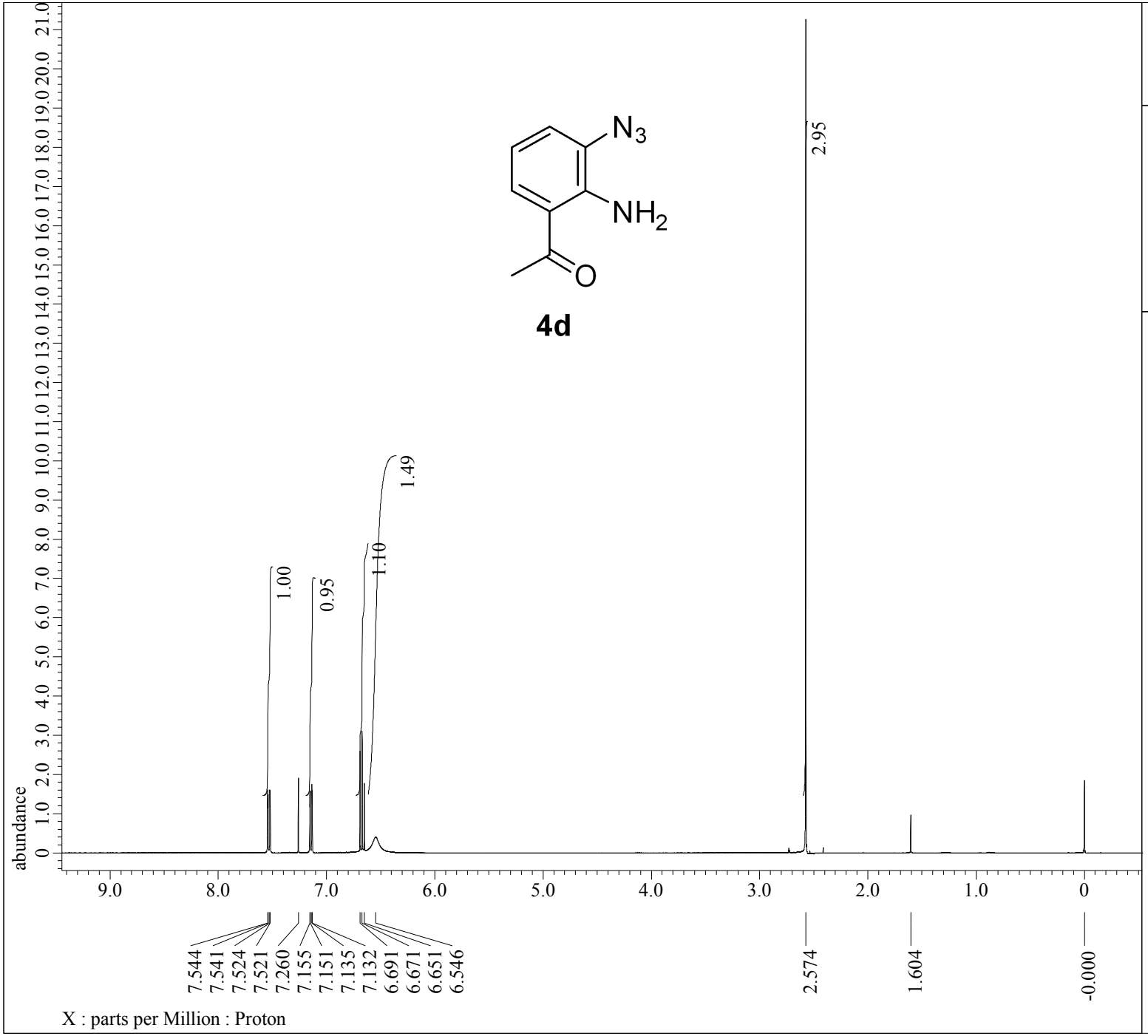
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 0.06806[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190118-2-4.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 2-アジド-4-メチル-6-クロロアニリン
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2019 17:49:07
Revision_Time     = 18-JAN-2019 17:24:25
Current_Time      =  5-JAN-2021 11:24:09

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 200
Total_Scans       = 200

Relaxation_Delay  = 2[s]
Recvr_Gain        = 46
Temp_Get          = 24.7[dC]
X_90_Width        = 11.329[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.77633333[us]
Irr_Atn_Dec       = 27.79[dB]
Irr_Atn_Noe       = 27.79[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



JEOL RESONANCE

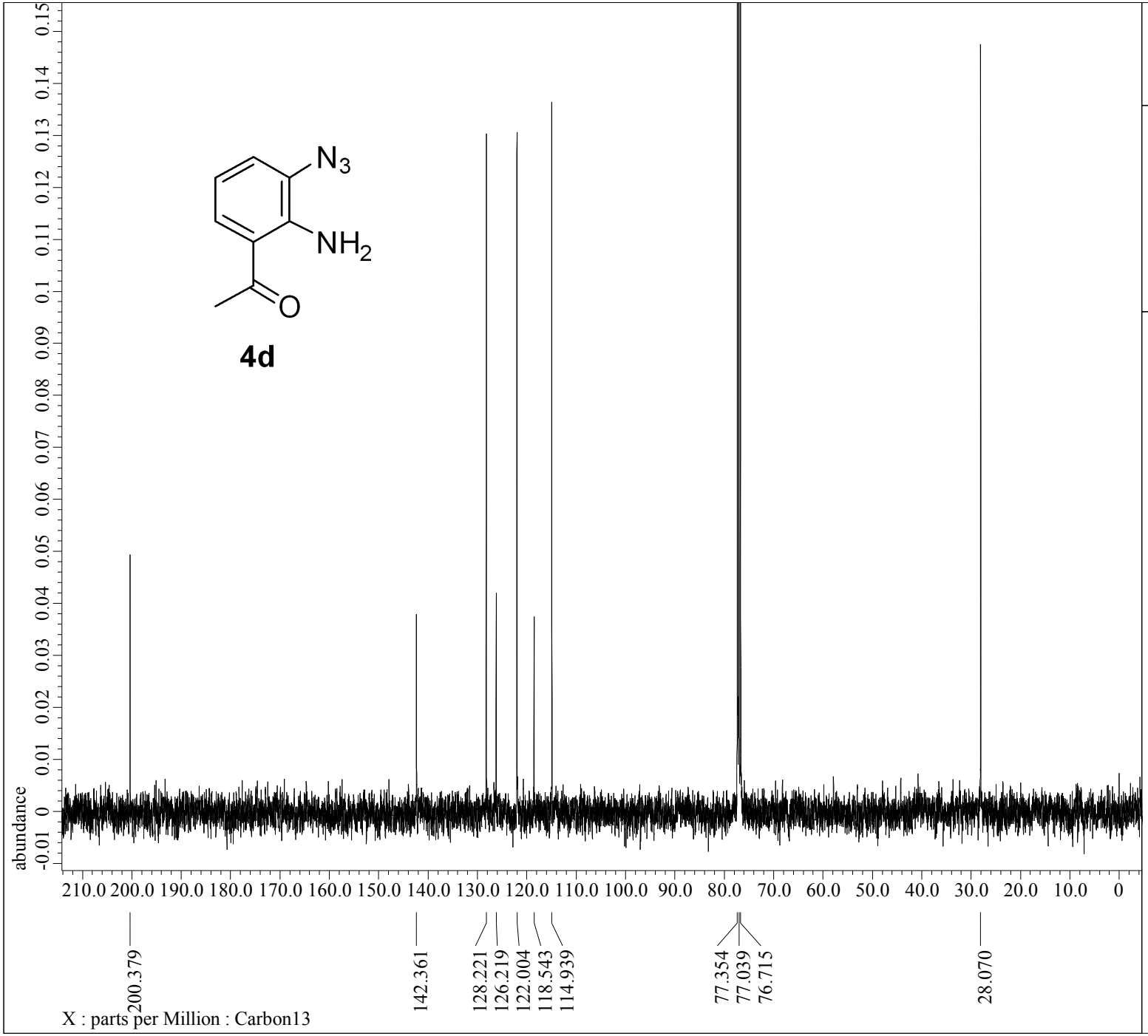
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.01381[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190116-3-6.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 2-アミノ-3-アジドアセトフェノン
Solvent           = CHLOROFORM-D
Creation_Time     = 16-JAN-2019 17:32:33
Revision_Time     = 16-JAN-2019 16:54:26
Current_Time      = 25-DEC-2020 17:40:49

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 25[dC]
X_90_Width        = 7.018[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.5[dB]
X_Pulse           = 3.509[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

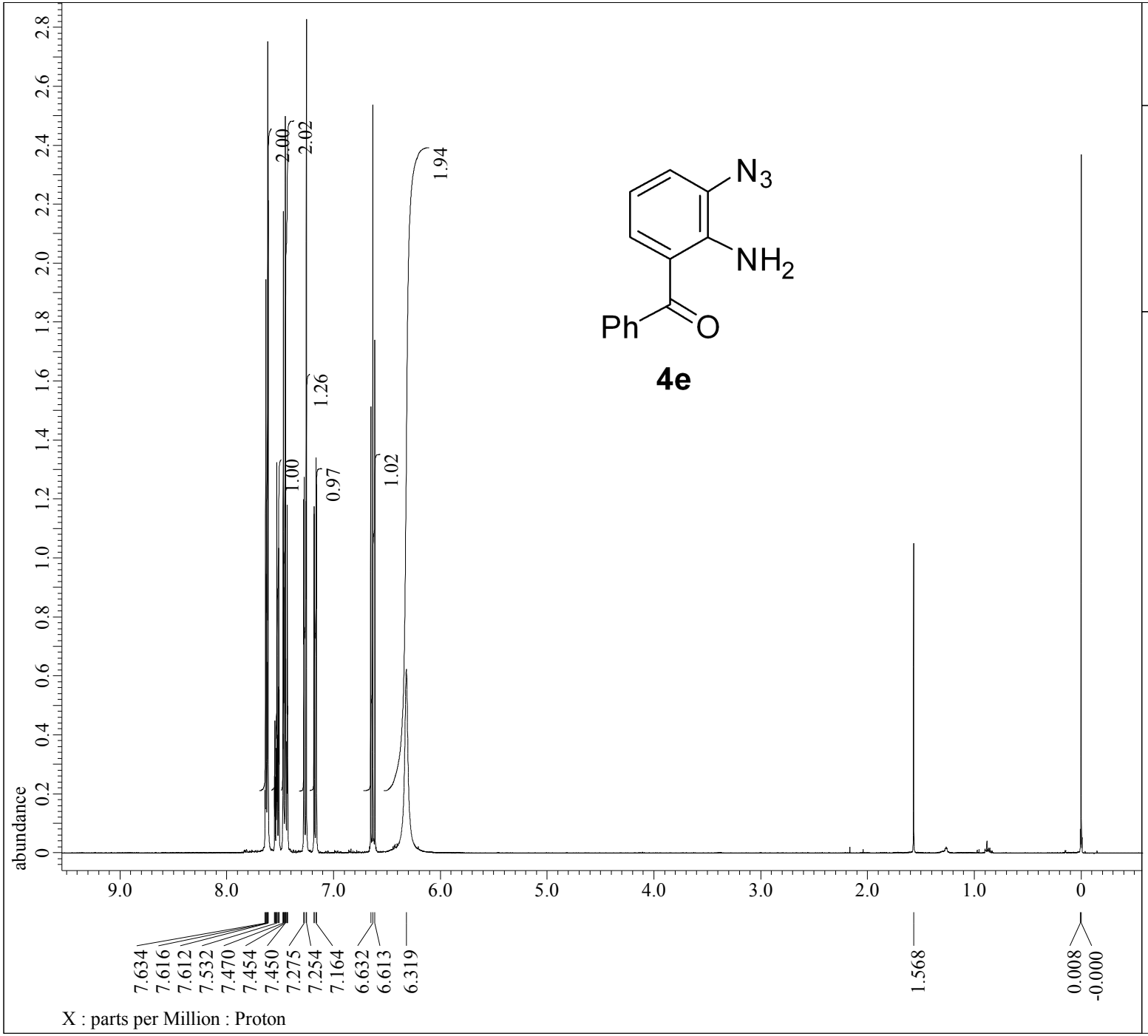
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 0.06806[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190116-4-4.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 2-アミノ-3-アジドアセトフェノン
Solvent           = CHLOROFORM-D
Creation_Time     = 16-JAN-2019 17:36:24
Revision_Time     = 16-JAN-2019 17:12:08
Current_Time      =  5-JAN-2021 11:21:41

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 200
Total_Scans       = 200

Relaxation_Delay  = 2[s]
Recvr_Gain        = 48
Temp_Get          = 25[dC]
X_90_Width        = 11.329[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.77633333[us]
Irr_Atn_Dec       = 27.79[dB]
Irr_Atn_Noe       = 27.79[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



JEOL RESONANCE

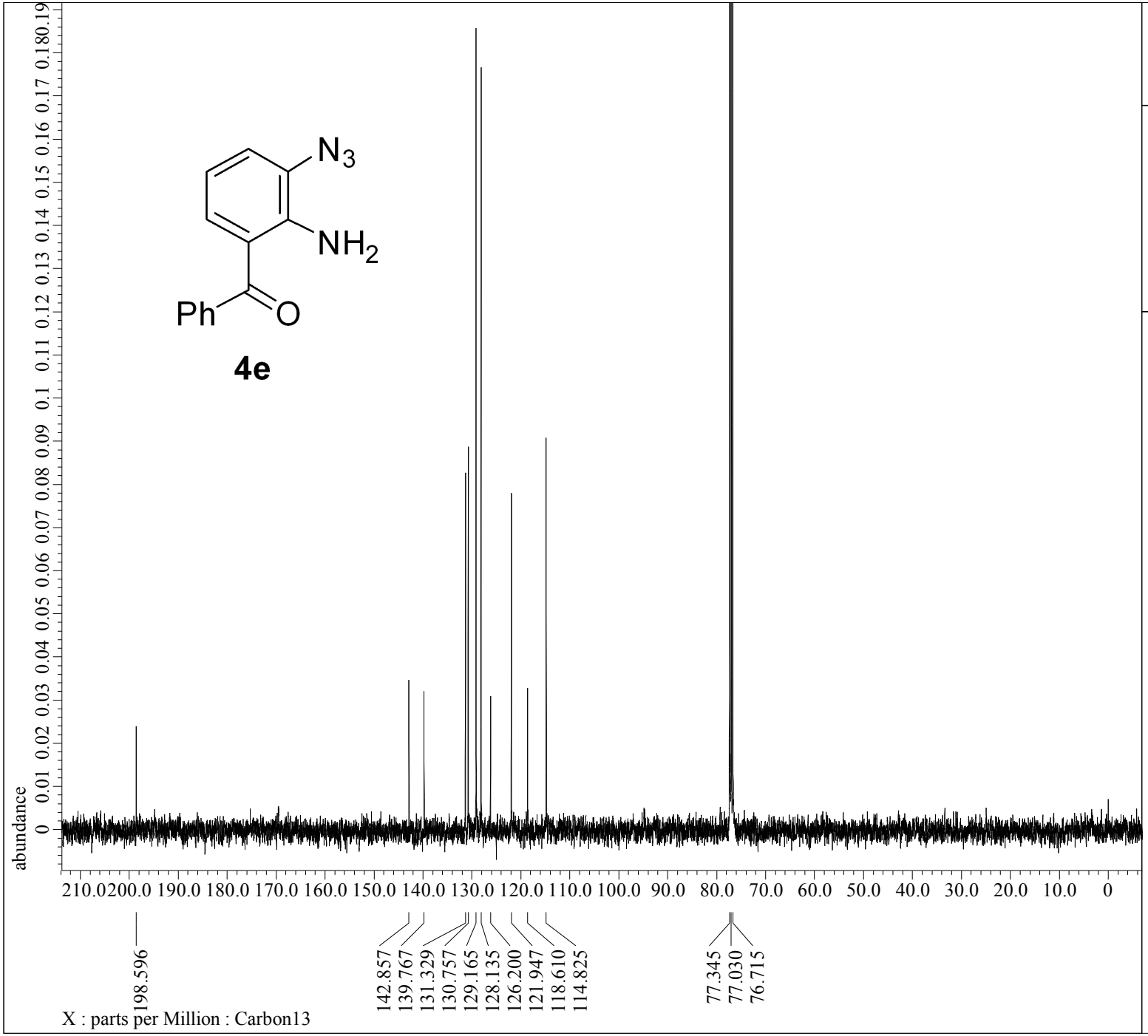
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.00809[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190118-3-6.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 2-アミノ-3-アジド-ベンゾフェノン
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2019 18:10:14
Revision_Time     = 18-JAN-2019 17:58:55
Current_Time      = 25-DEC-2020 17:43:28

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 24.7[dC]
X_90_Width        = 7.018[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.5[dB]
X_Pulse           = 3.509[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

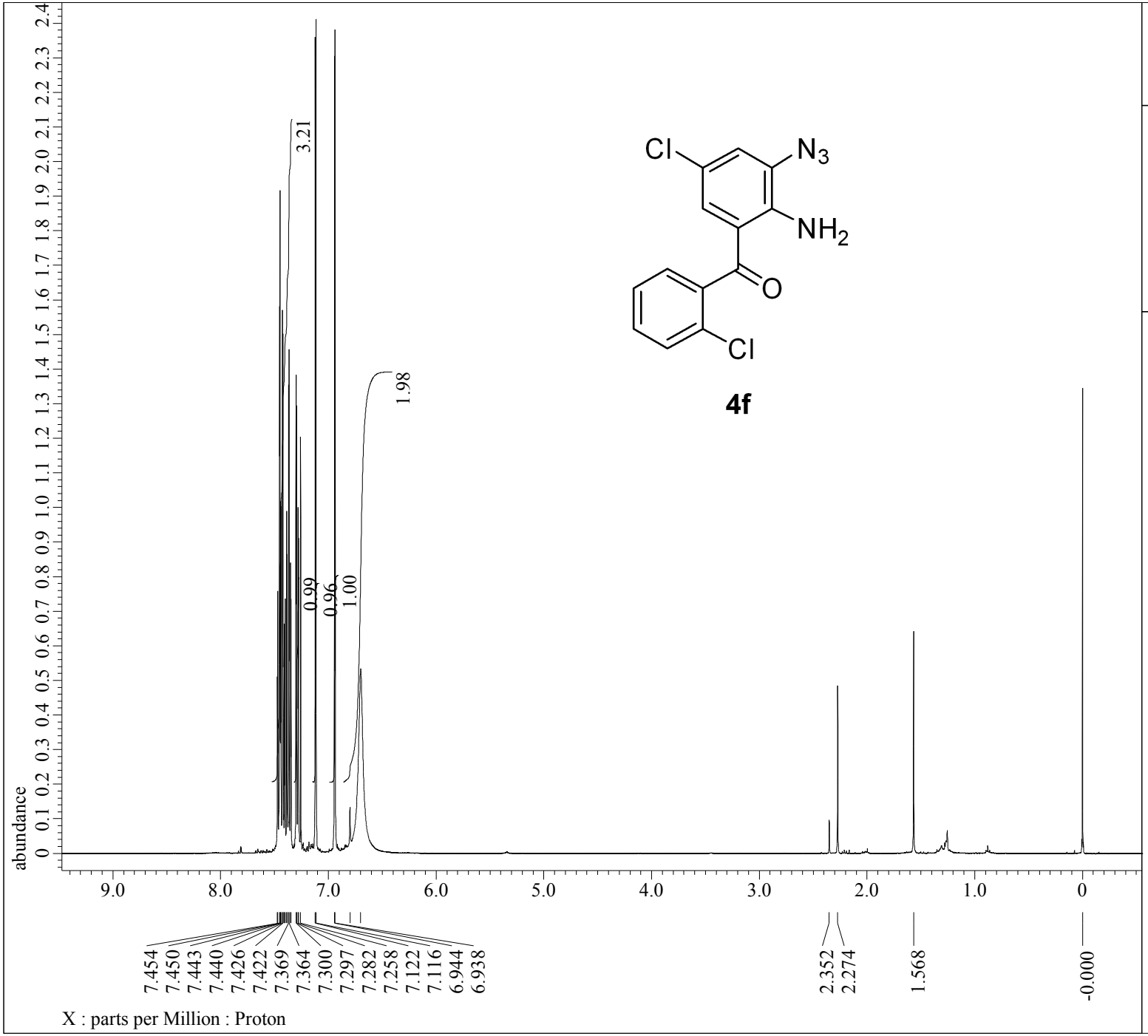
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 0.07759[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190118-4-4.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 2-アミノ-3-アジド-ベンゾフェノン
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2019 18:14:21
Revision_Time     = 18-JAN-2019 17:57:40
Current_Time      =  5-JAN-2021 11:25:45

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 200
Total_Scans       = 200

Relaxation_Delay  = 2[s]
Recvr_Gain        = 46
Temp_Get          = 24.7[dC]
X_90_Width        = 11.329[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.77633333[us]
Irr_Atn_Dec       = 27.79[dB]
Irr_Atn_Noe       = 27.79[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



JEOL RESONANCE

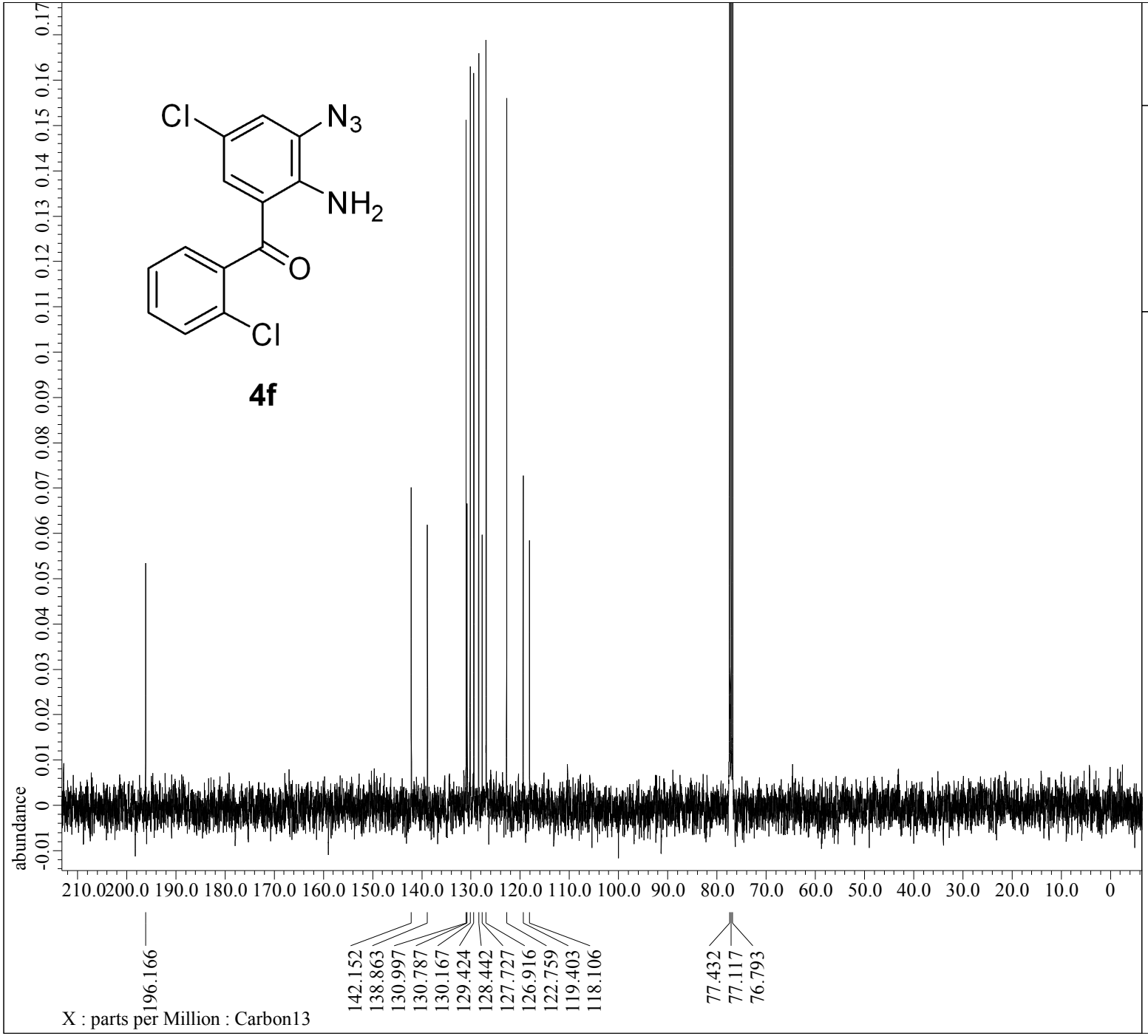
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.01038[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190308-1-6.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 2-アミノ-3-アジド-2',5-クロロベンゾフ
Solvent           = CHLOROFORM-D
Creation_Time     =  8-MAR-2019 15:50:07
Revision_Time     =  8-MAR-2019 15:27:39
Current_Time      = 25-DEC-2020 17:47:10

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 24[dC]
X_90_Width        = 7.166[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.5[dB]
X_Pulse           = 3.583[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

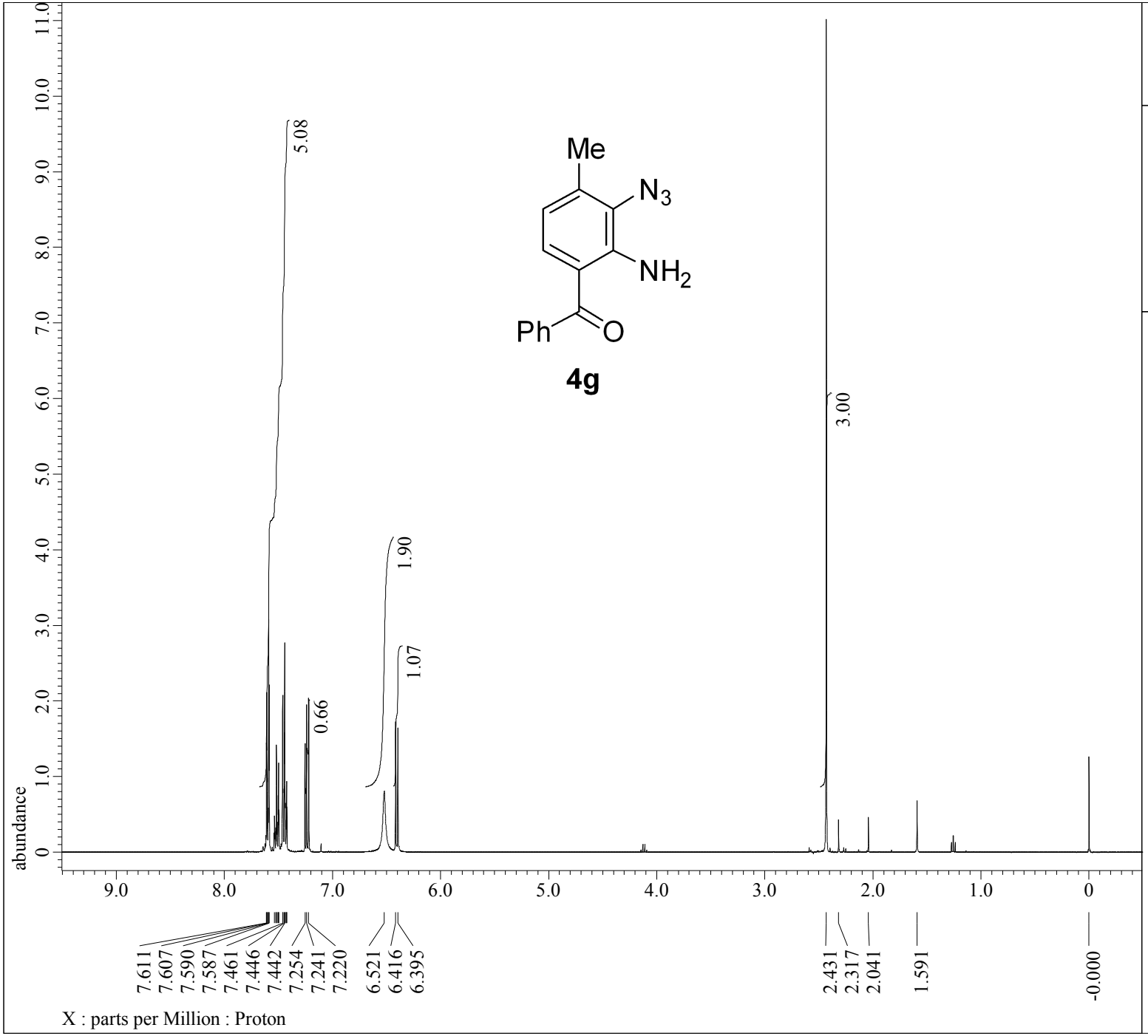
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = ytakahashi190308-2-5.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 2-アミノ-3-アジド-2',5-クロロベンゾフ
Solvent           = CHLOROFORM-D
Creation_Time     =  8-MAR-2019 15:54:07
Revision_Time     =  5-JAN-2021 11:31:32
Current_Time      =  5-JAN-2021 11:31:56

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 150
Total_Scans       = 150

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 24[dC]
X_90_Width        = 11.736[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.912[us]
Irr_Atn_Dec       = 27.608[dB]
Irr_Atn_Noe       = 27.608[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



JEOL RESONANCE

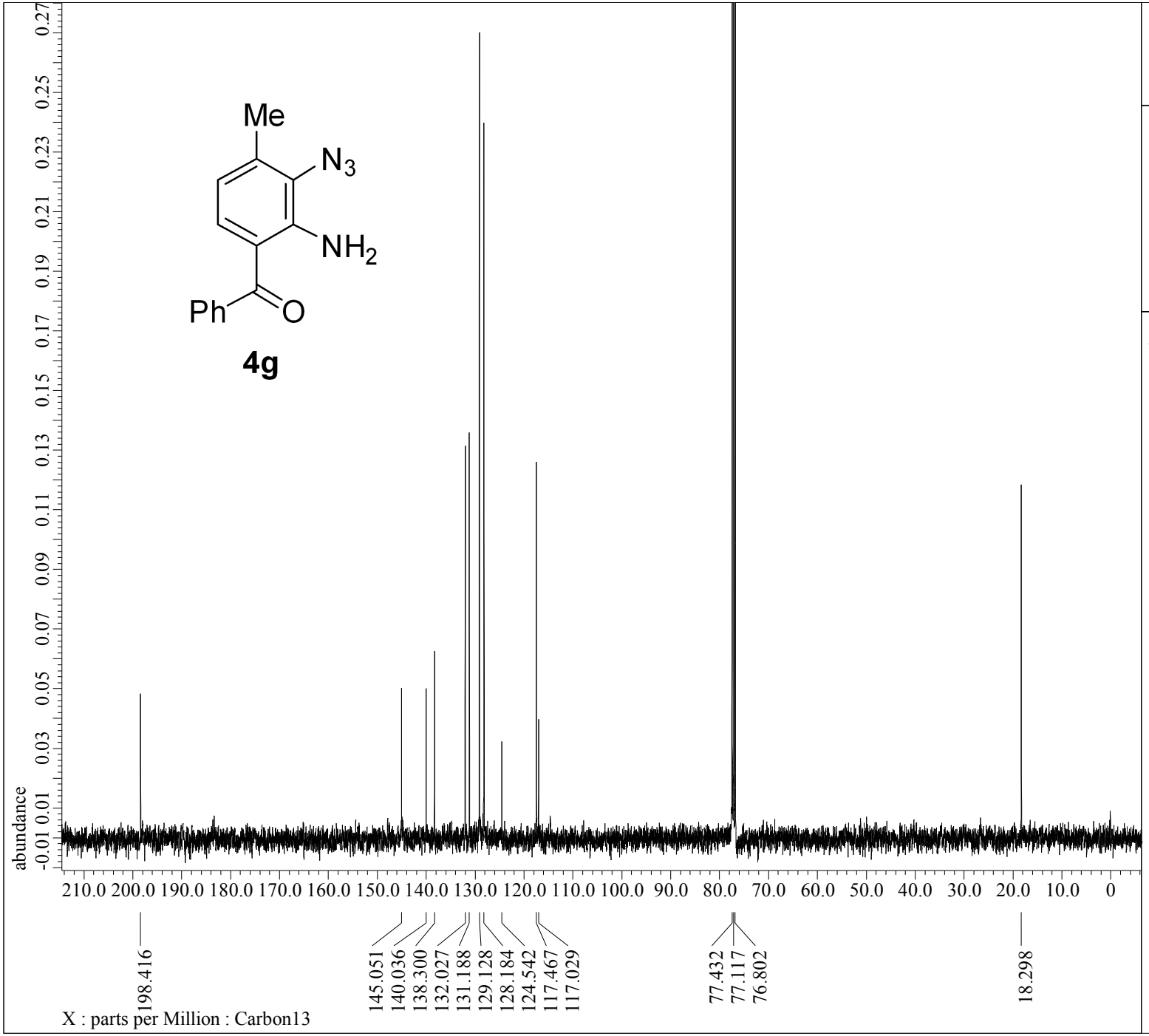
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.00809[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190322-3-6.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 2-アミノ-3-アジド-4-メチルベンゾフェノン
Solvent           = CHLOROFORM-D
Creation_Time     = 22-MAR-2019 18:02:47
Revision_Time     = 22-MAR-2019 17:37:59
Current_Time      = 25-DEC-2020 17:47:39

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 23.6[dC]
X_90_Width        = 7.166[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.5[dB]
X_Pulse           = 3.583[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

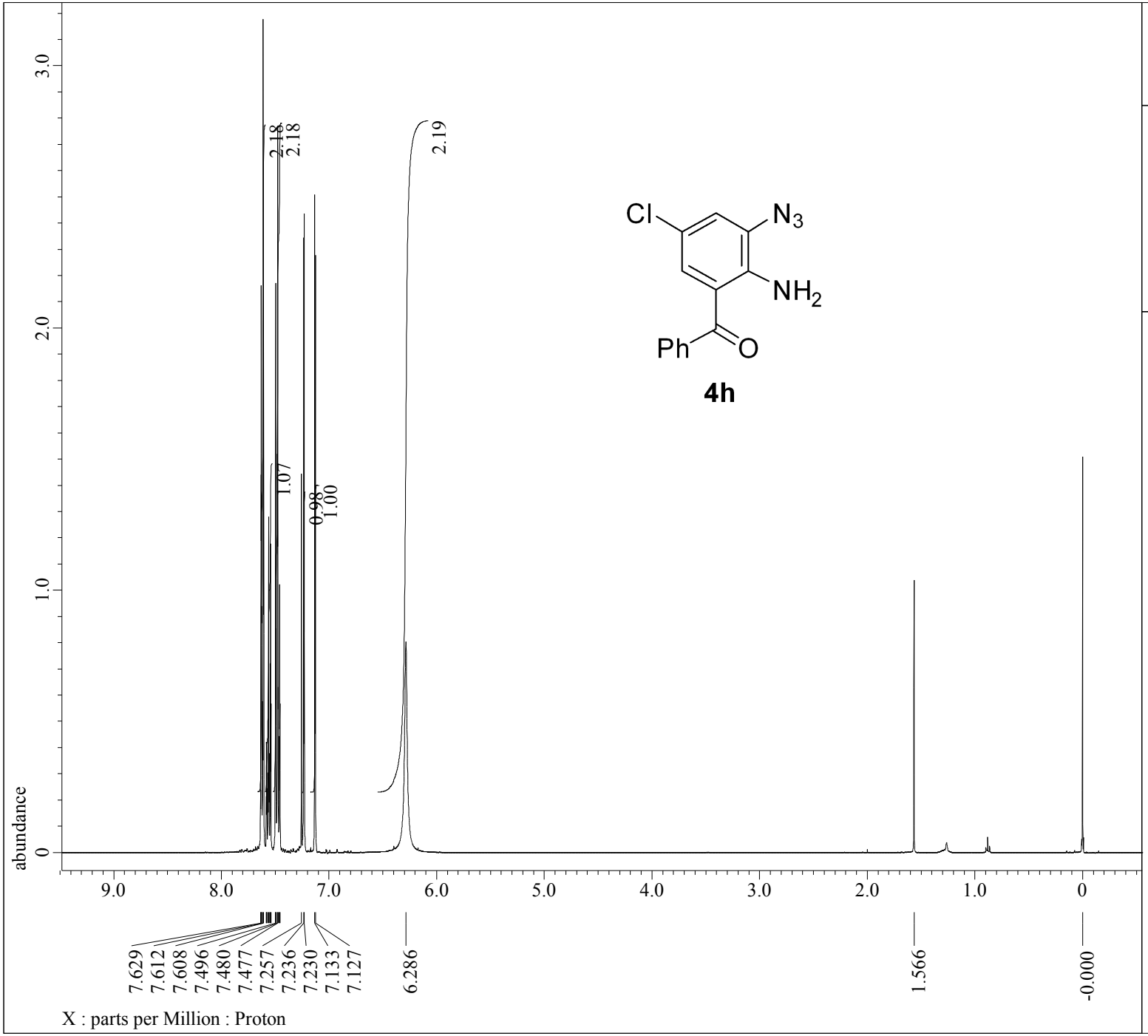
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = ytakahashi190322-4-5.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 2-アミノ-3-アジド-4-メチルベンゾフェノン
Solvent           = CHLOROFORM-D
Creation_Time     = 22-MAR-2019 18:07:23
Revision_Time     =  5-JAN-2021 11:32:39
Current_Time      =  5-JAN-2021 11:32:59

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 150
Total_Scans       = 150

Relaxation_Delay  = 2[s]
Recvr_Gain        = 48
Temp_Get          = 23.6[dC]
X_90_Width        = 11.736[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.912[us]
Irr_Atn_Dec       = 27.608[dB]
Irr_Atn_Noe       = 27.608[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



4h

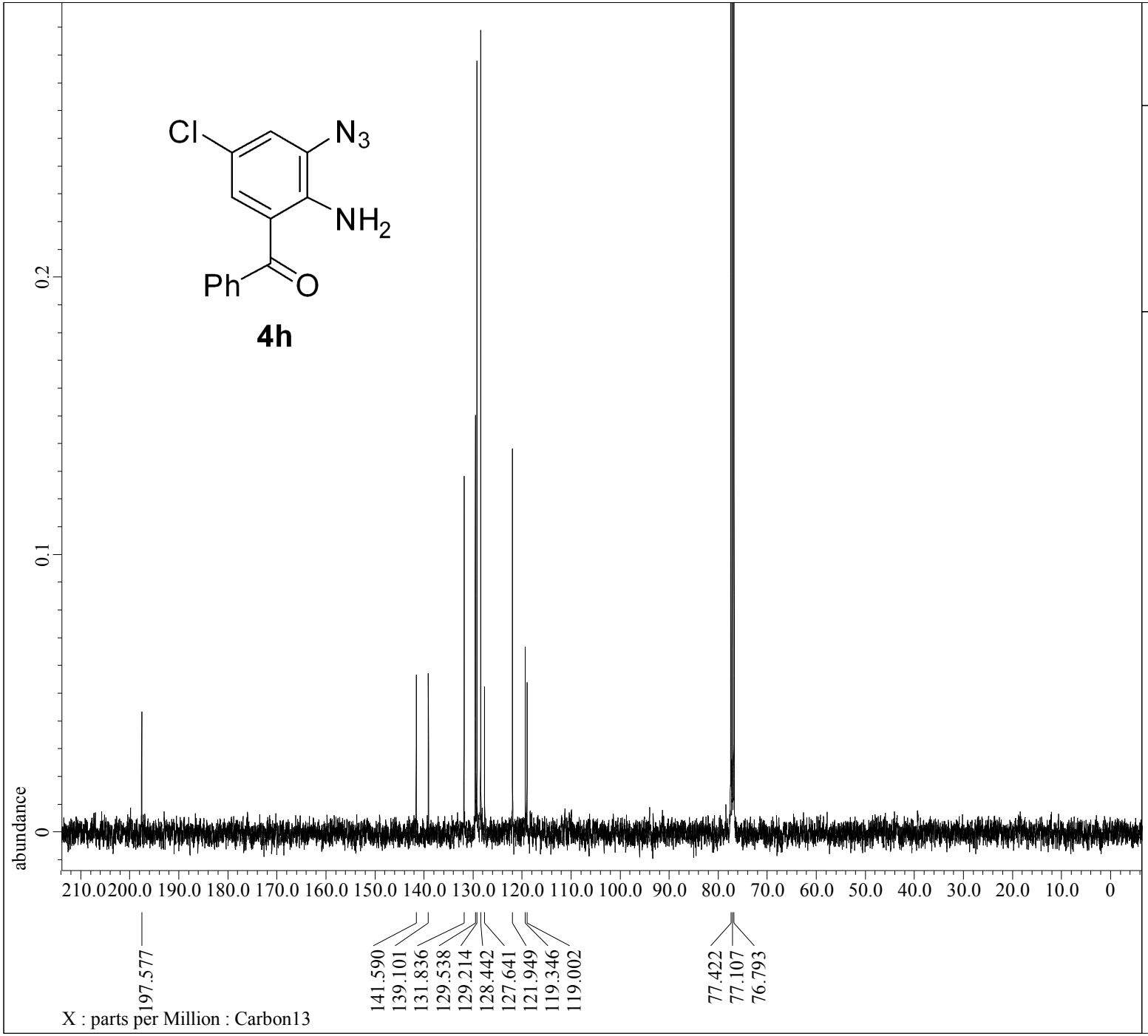
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.01038[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190306-3-6.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 2-アミノ-3-アジド-5-クロロベンゾフェノン
Solvent           = CHLOROFORM-D
Creation_Time     =  6-MAR-2019 12:26:02
Revision_Time     =  6-MAR-2019 12:08:20
Current_Time      = 25-DEC-2020 17:46:05

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 24.6[dC]
X_90_Width        = 7.166[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.5[dB]
X_Pulse           = 3.583[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

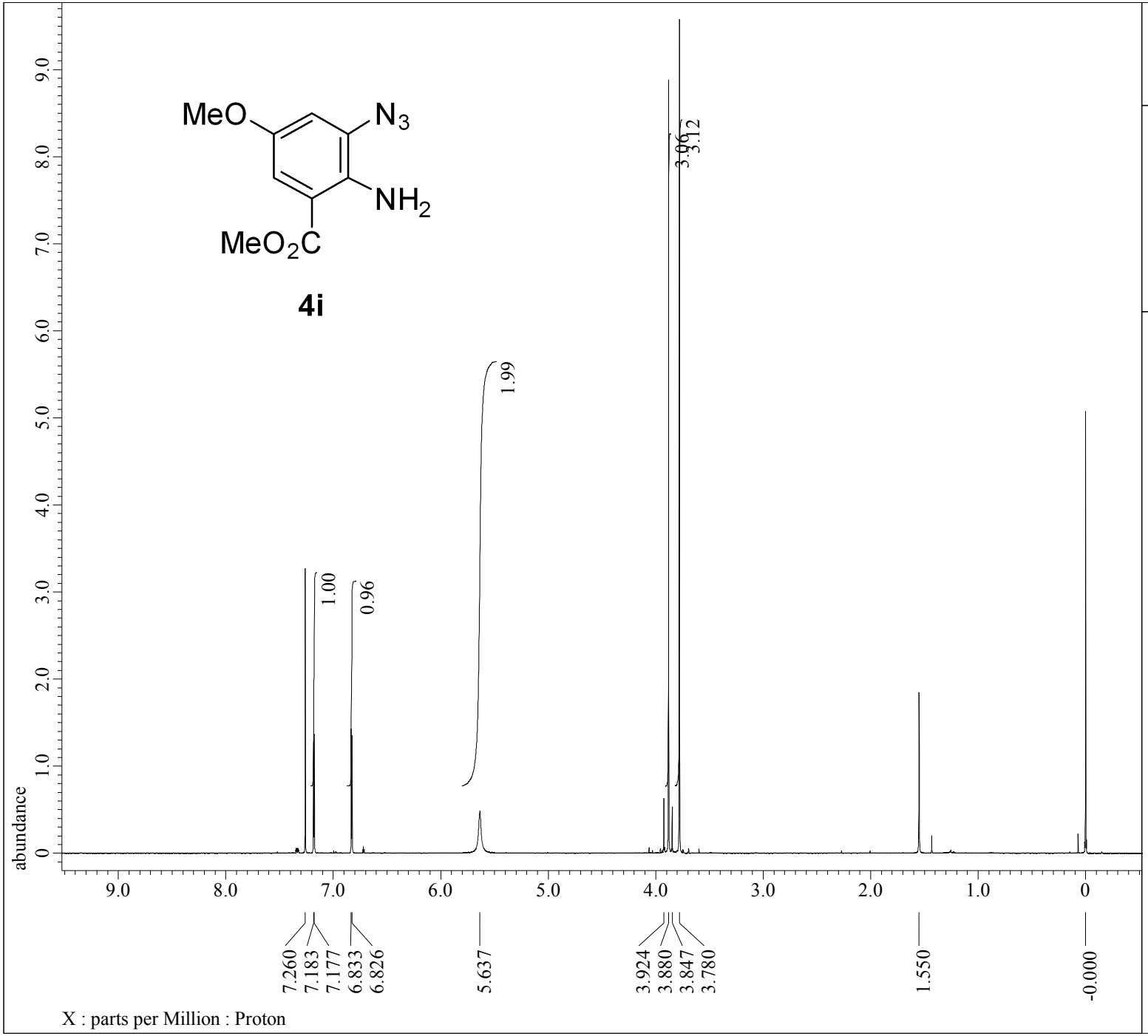
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = ytakahashi190306-4-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 2-アミノ-3-アジド-5-クロロベンゾフェノン
Solvent           = CHLOROFORM-D
Creation_Time     =  6-MAR-2019 12:29:46
Revision_Time     =  5-JAN-2021 11:29:29
Current_Time      =  5-JAN-2021 11:30:00

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 150
Total_Scans       = 150

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 24.6[dC]
X_90_Width        = 11.736[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.912[us]
Irr_Atn_Dec       = 27.608[dB]
Irr_Atn_Noe       = 27.608[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



JEOL RESONANCE

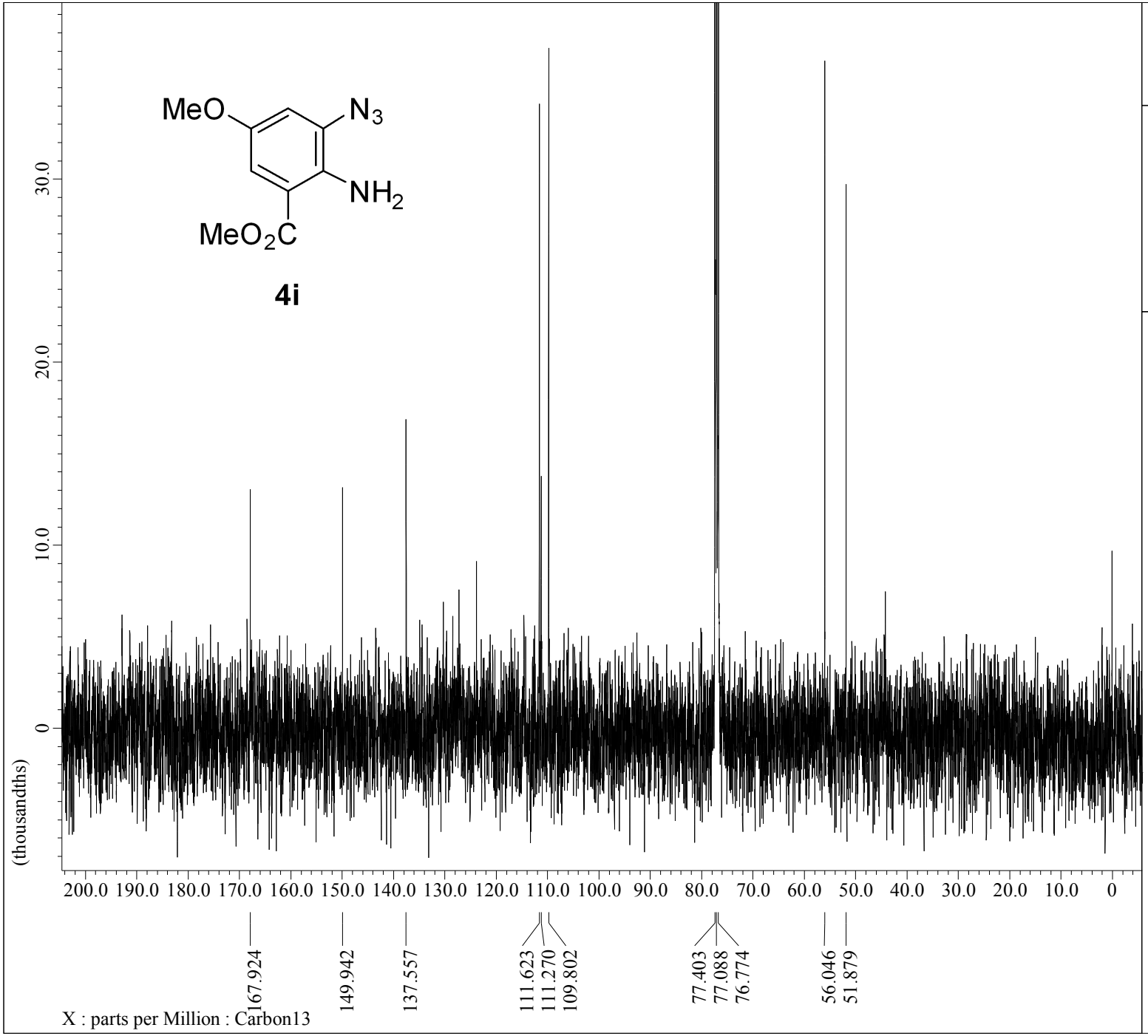
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.01381[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190306-7-6.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 2-アミノ-3-アジド-5-メトキシ安息香酸
Solvent           = CHLOROFORM-D
Creation_Time     =  6-MAR-2019 13:40:20
Revision_Time     =  6-MAR-2019 13:22:51
Current_Time      = 25-DEC-2020 17:46:39

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 38
Temp_Get          = 24.5[dC]
X_90_Width        = 7.166[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.5[dB]
X_Pulse           = 3.583[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

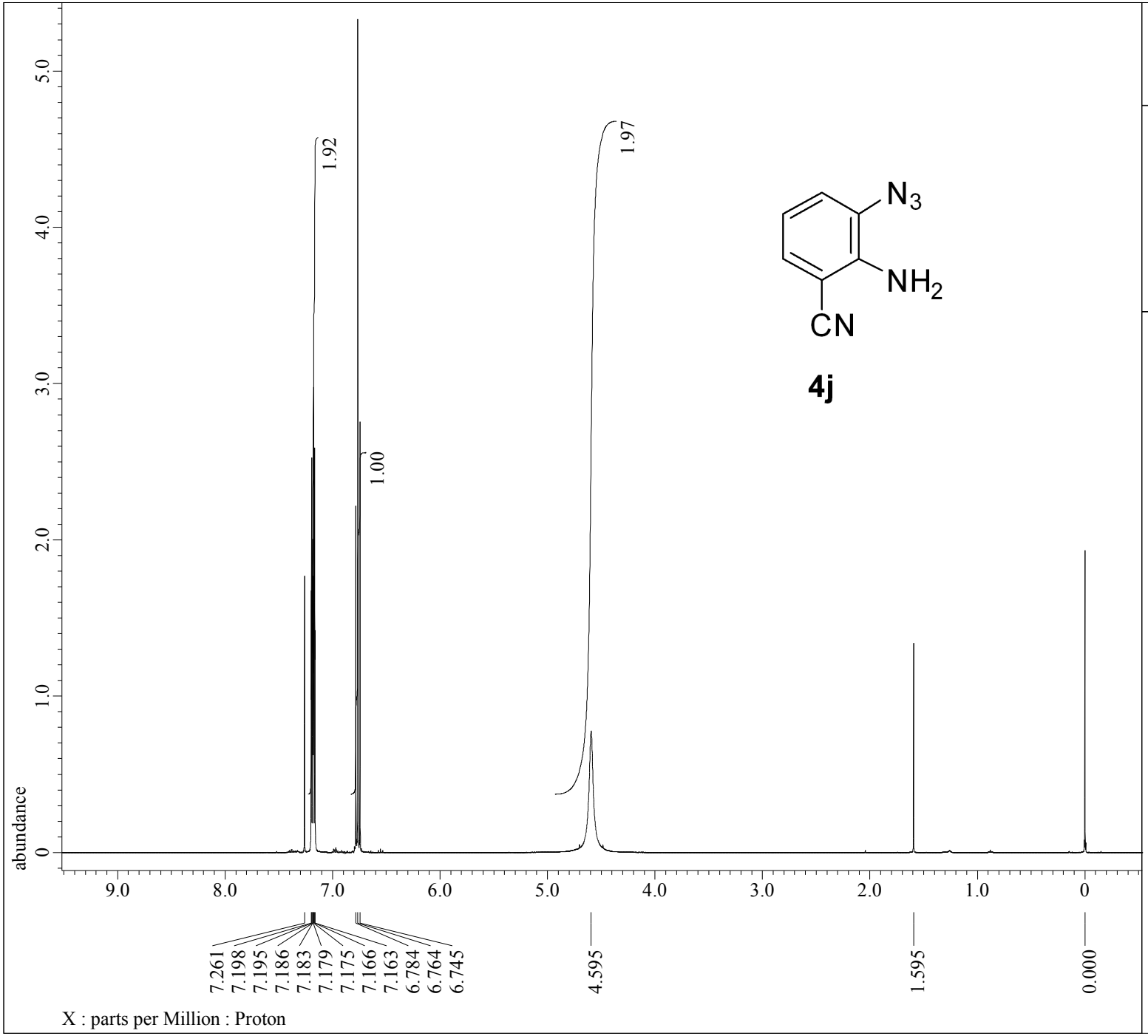
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = ytakahashi190306-8-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 2-アミノ-3-アジド-5-メトキシ安息香酸
Solvent           = CHLOROFORM-D
Creation_Time     =  6-MAR-2019 13:44:18
Revision_Time     =  5-JAN-2021 11:38:08
Current_Time      =  5-JAN-2021 11:38:48

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 300
Total_Scans       = 300

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 24.5[dC]
X_90_Width        = 11.736[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.912[us]
Irr_Atn_Dec       = 27.608[dB]
Irr_Atn_Noe       = 27.608[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



4j

JEOL RESONANCE

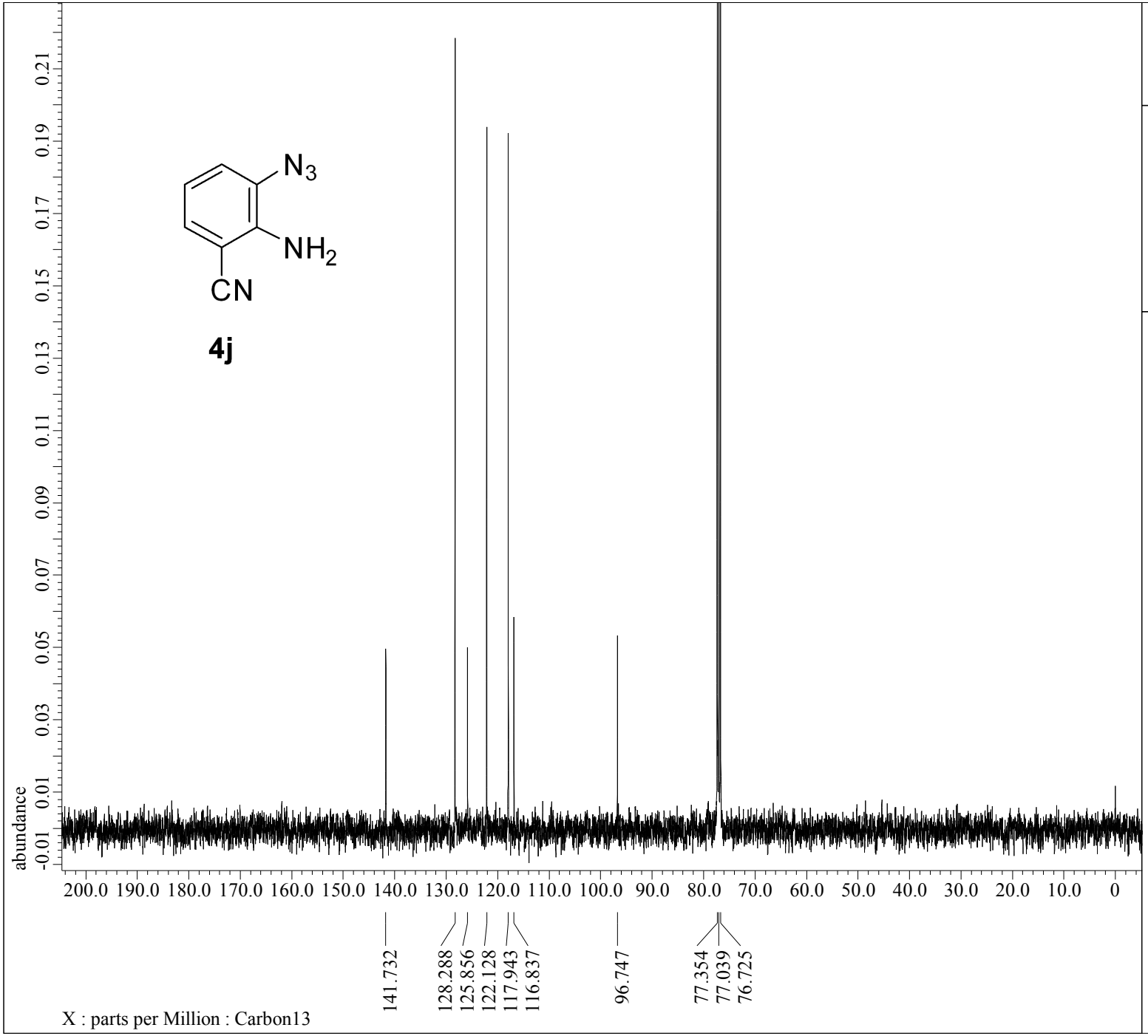
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.01496[ppm], 0[ppm] )
reference( 0.0[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190116-5-7.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 2-アミノ-3-アジドベンゾニトリル
Solvent           = CHLOROFORM-D
Creation_Time     = 16-JAN-2019 17:58:05
Revision_Time     = 16-JAN-2019 17:36:58
Current_Time      = 25-DEC-2020 17:41:26

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 24.9[dC]
X_90_Width        = 7.018[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.5[dB]
X_Pulse           = 3.509[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

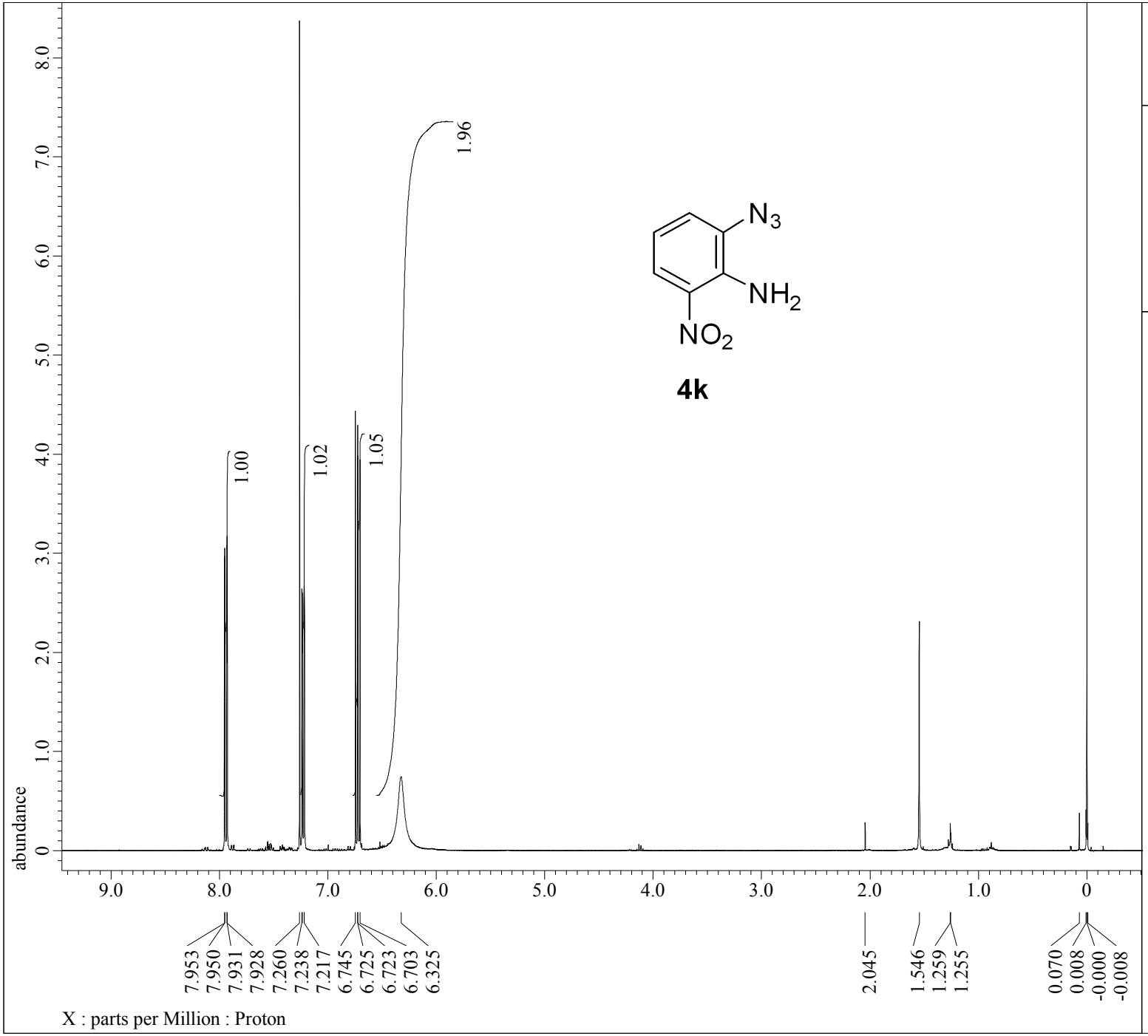
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = ytakahashi190116-6-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 2-アミノ-3-アジドベンゾニトリル
Solvent           = CHLOROFORM-D
Creation_Time     = 16-JAN-2019 18:02:25
Revision_Time     = 16-JAN-2019 17:37:39
Current_Time      =  5-JAN-2021 11:23:06

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 200
Total_Scans       = 200

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 24.9[dC]
X_90_Width        = 11.329[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.77633333[us]
Irr_Atn_Dec       = 27.79[dB]
Irr_Atn_Noe       = 27.79[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



JEOL RESONANCE

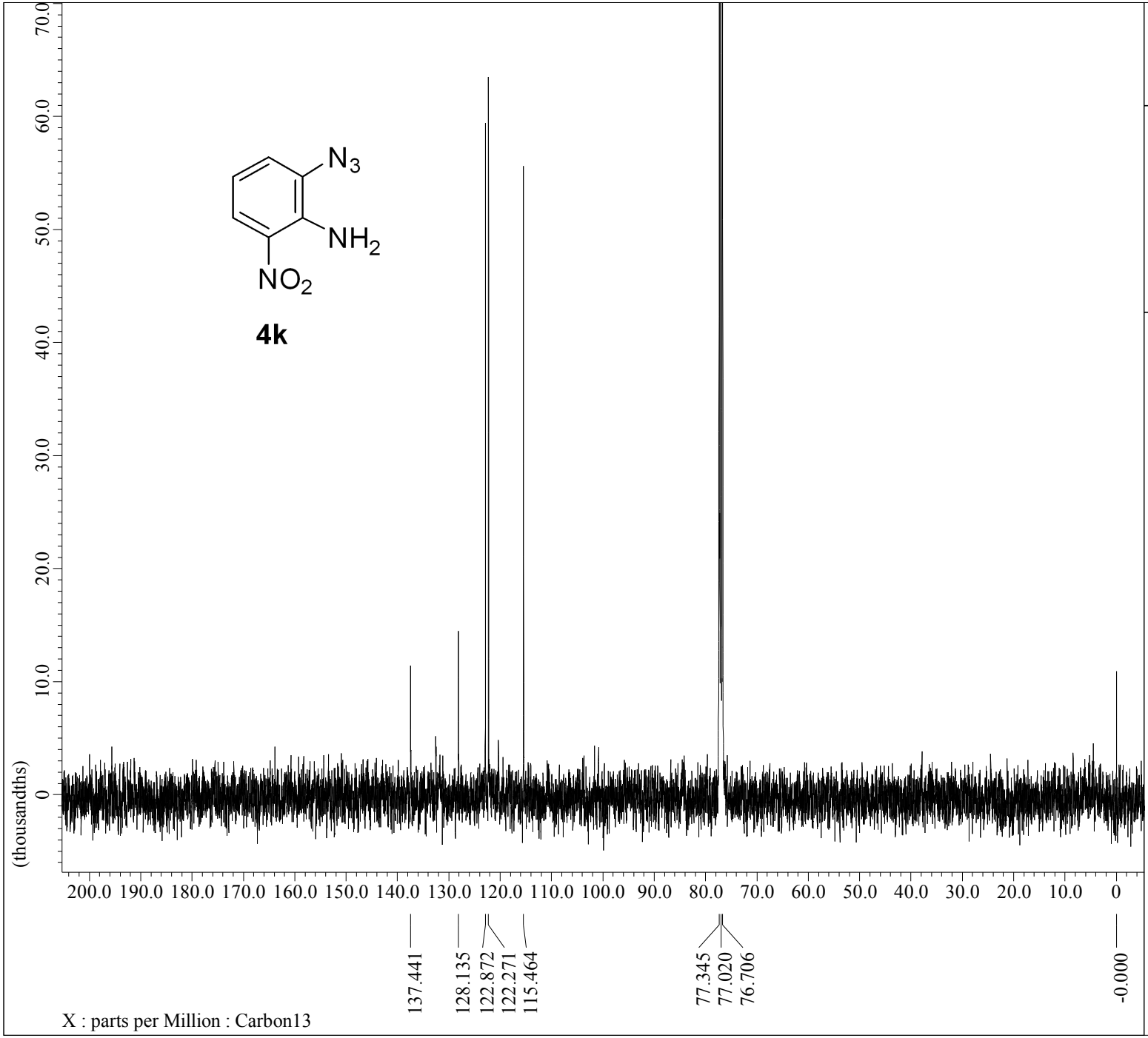
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.01381[ppm], 0[ppm] )
phase( 4, 0, 50[%] )
```

```
Filename          = ytakahashi190118-5-8.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 2-アジド-6-ニトロアニリン
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2019 18:43:29
Revision_Time     = 18-JAN-2019 18:52:35
Current_Time      = 25-DEC-2020 17:44:14

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 44
Temp_Get          = 24.7[dC]
X_90_Width        = 7.018[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3.5[dB]
X_Pulse           = 3.509[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

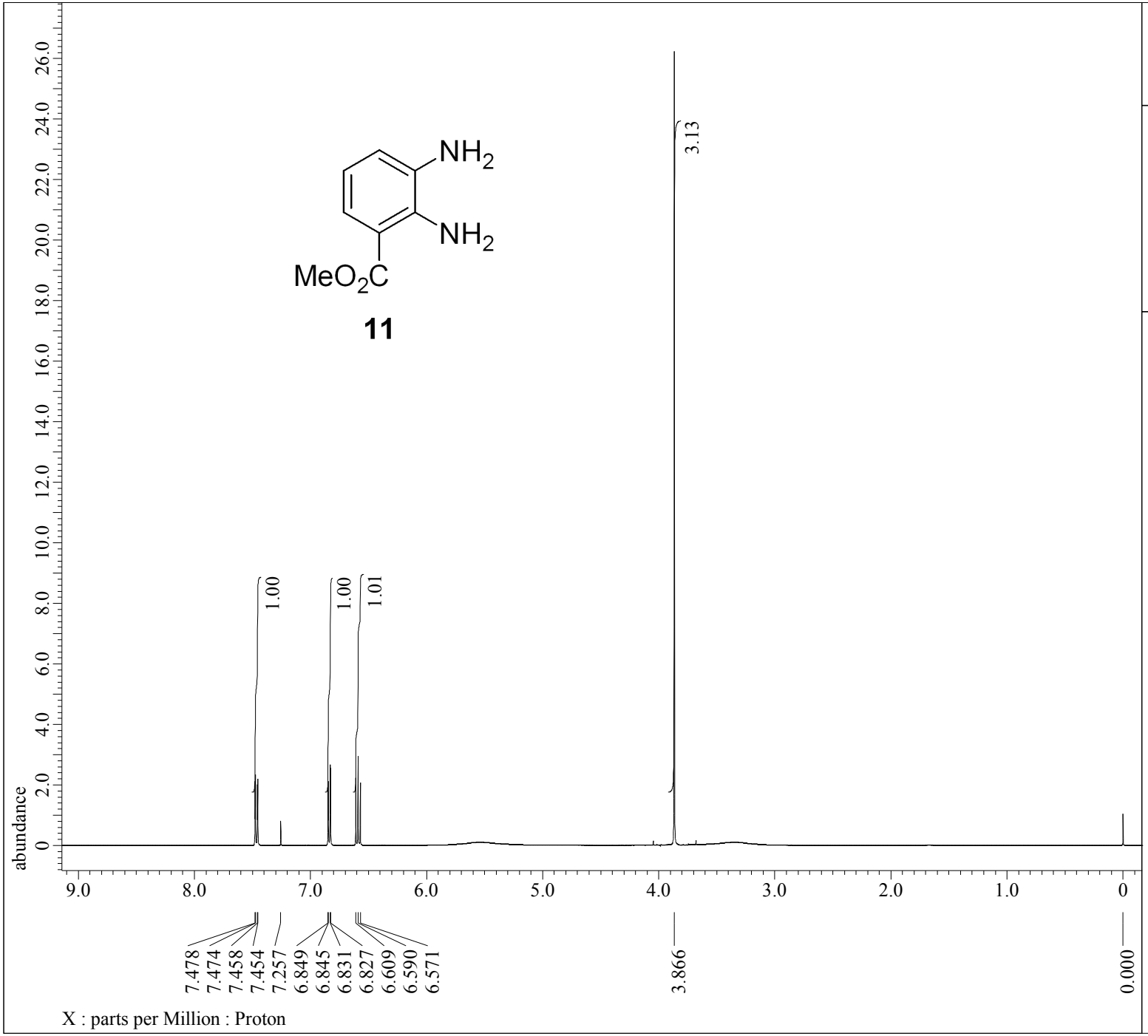
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 0.06806[ppm], 0[ppm] )
```

```
Filename          = ytakahashi190118-6-4.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 2-アジド-6-ニトロアニリン
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2019 18:48:25
Revision_Time     = 18-JAN-2019 18:50:19
Current_Time      =  5-JAN-2021 11:24:54

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 700
Total_Scans       = 700

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 24.5[dC]
X_90_Width        = 11.329[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.77633333[us]
Irr_Atn_Dec       = 27.79[dB]
Irr_Atn_Noe       = 27.79[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



JEOL RESONANCE

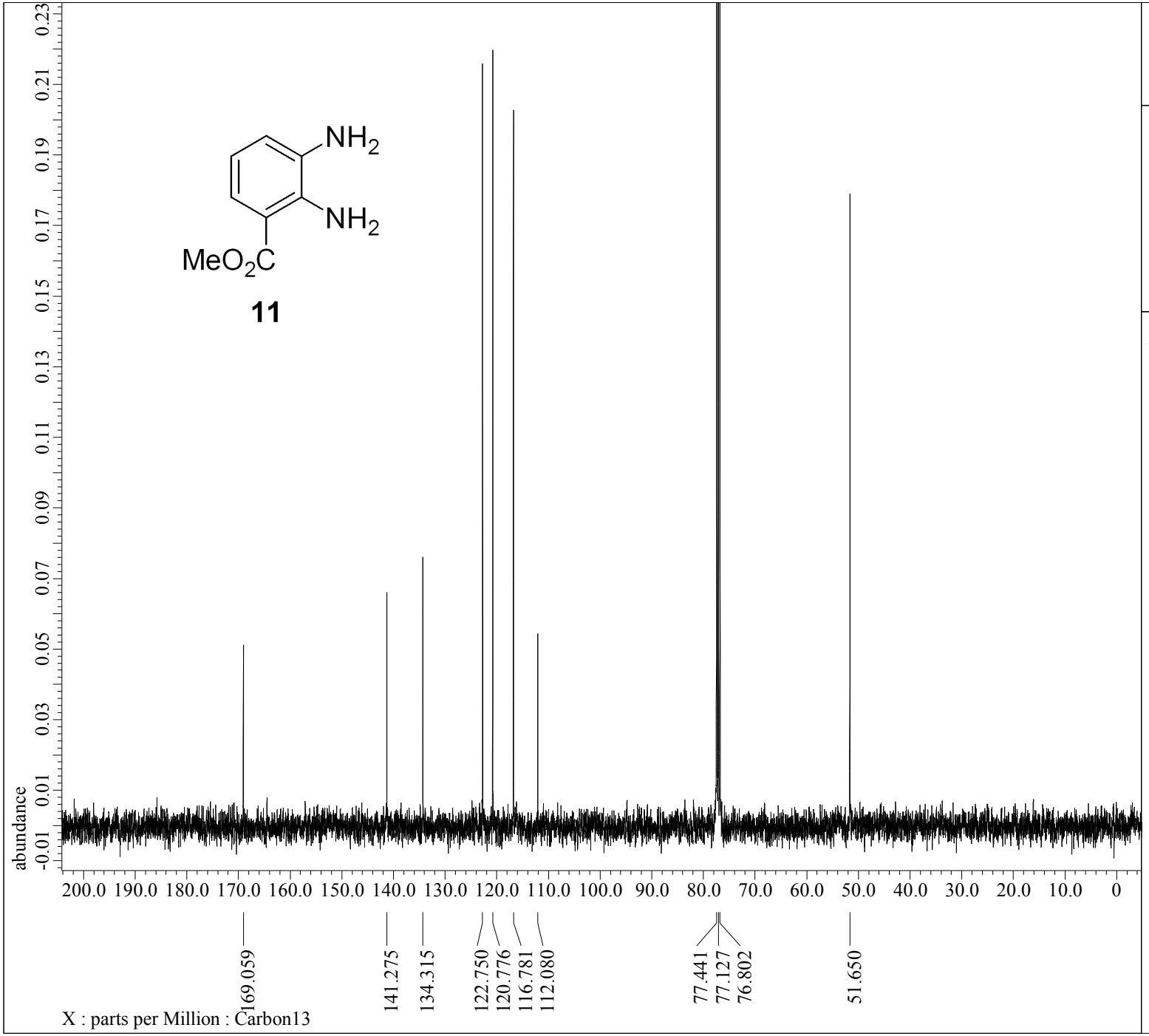
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.00923[ppm], 0[ppm] )
phase( 10, 1, 57.59194[%] )
```

```
Filename          = ytakahashi210118-1-7.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 安息香酸メチル_ジアミン体
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2021 16:06:20
Revision_Time     = 18-JAN-2021 15:13:46
Current_Time      = 18-JAN-2021 15:14:24

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 25.3[dC]
X_90_Width        = 6.8[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

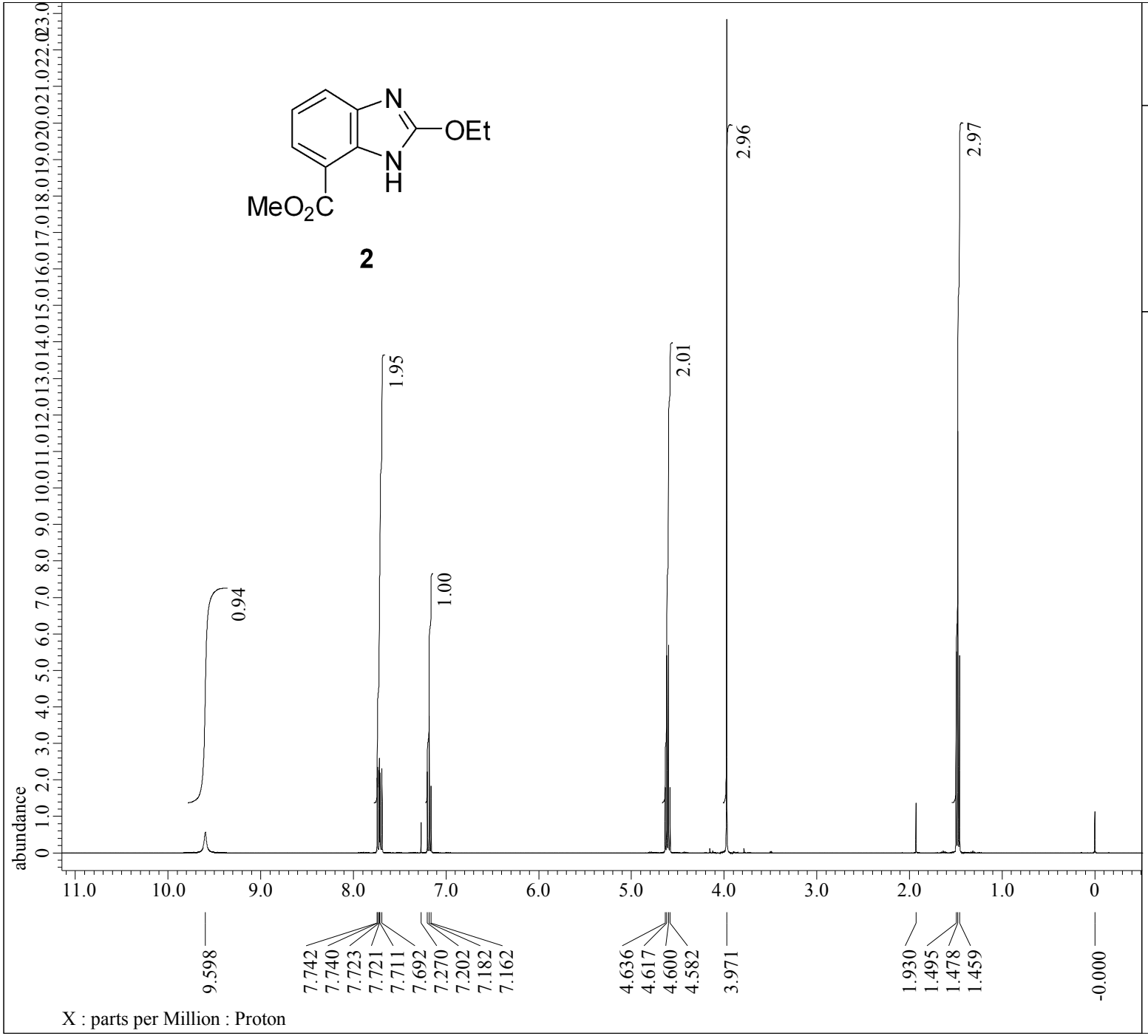
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = 安息香酸メチル_ジアミン体_Carbon-1
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 安息香酸メチル_ジアミン体
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2021 16:09:40
Revision_Time     = 19-JAN-2021 14:56:05
Current_Time      = 19-JAN-2021 14:56:10

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 200
Total_Scans       = 200

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 25.3[dC]
X_90_Width        = 11.75[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.91666667[us]
Irr_Atn_Dec       = 27.06[dB]
Irr_Atn_Noe       = 27.06[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



JEOL RESONANCE

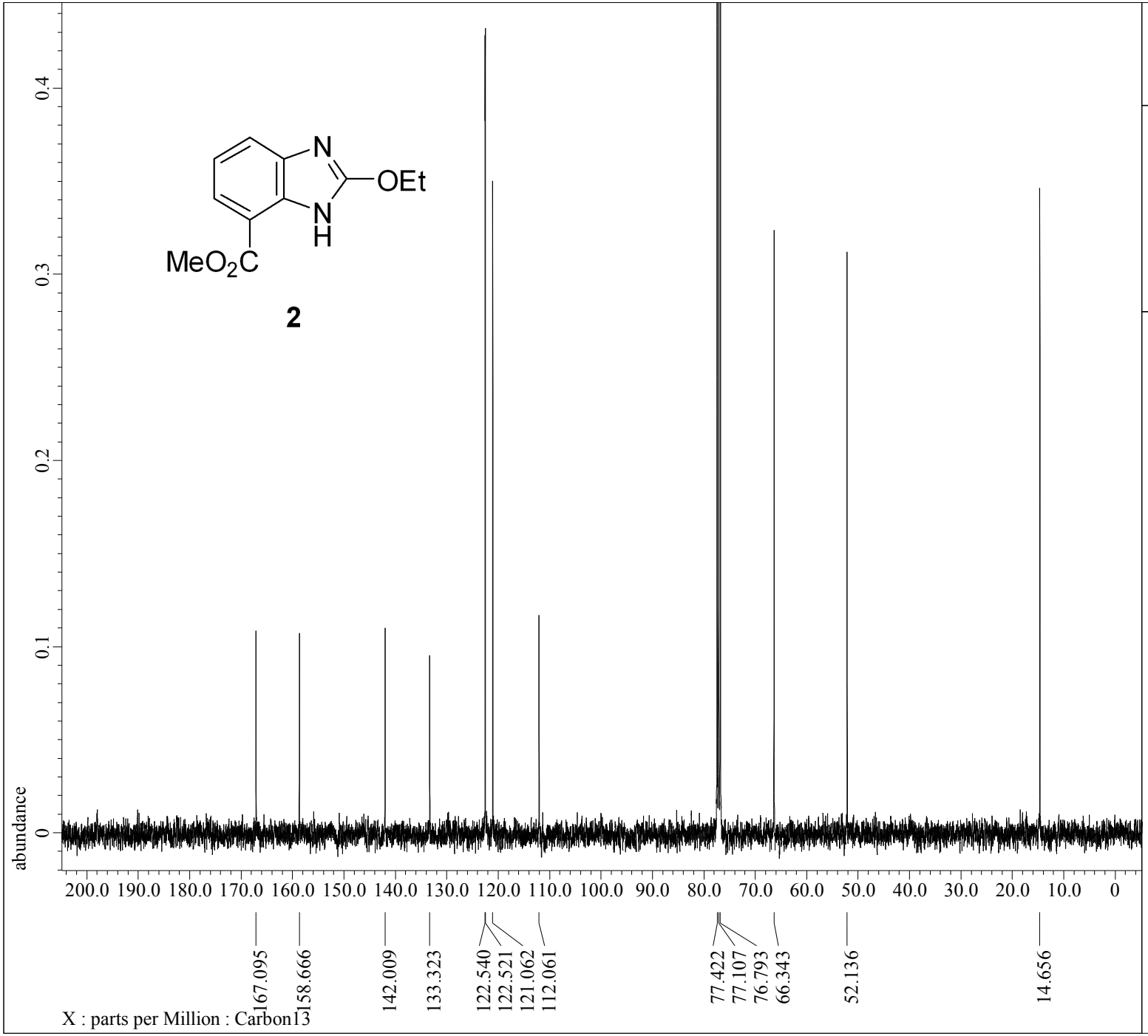
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.02298[ppm], 0[ppm] )
phase( 0, -2, 57.01969[%] )
```

```
Filename          = ytakahashi210118-2-7.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 安息香酸メチル_アミン体
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2021 16:28:42
Revision_Time     = 18-JAN-2021 15:36:39
Current_Time      = 18-JAN-2021 15:36:49

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 25.3[dC]
X_90_Width        = 6.8[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



JEOL RESONANCE

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = ytakahashi210118-3-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 安息香酸メチル_アミン体
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2021 16:31:58
Revision_Time     = 19-JAN-2021 14:56:52
Current_Time      = 19-JAN-2021 14:56:56

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA400II
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 200
Total_Scans       = 200

Relaxation_Delay  = 2[s]
Recvr_Gain        = 54
Temp_Get          = 25.3[dC]
X_90_Width        = 11.75[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 8.8[dB]
X_Pulse           = 3.91666667[us]
Irr_Atn_Dec       = 27.06[dB]
Irr_Atn_Noe       = 27.06[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```