

Supplementary data

New Eunicellin-type Diterpenes from the Panamanian Octocoral *Briareum asbestinum*

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Figure S24. Asbestinin 28, HR-ESITOFMS spectrum

Table S1. Viability of THP-1 human macrophages treated with different concentrations of diterpenes.

Figure S1. Briarellin T, ¹H NMR spectrum

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 Revision_Time = 31-JUL-2015 07:40:50

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 Dim_Title = 1H
 Dim_Units = [ppm]
 Dimensions = X
 Site = Eclipse+ 400
 Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 2.7312128[s]
 X_Domain = 1H
 X_Freq = 399.78219838[MHz]
 X_Offset = 5[ppm]
 X_Points = 16384
 X_Prescans = 0
 X_Resolution = 0.36613771[Hz]
 X_Sweep = 5.99880024[kHz]
 Clipped = FALSE
 Scans = 32
 Total_Scans = 32

Relaxation_Delay = 4[s]
 Recvr_Gain = 16
 Temp_Get = 21.9[dC]
 X_90_Width = 9.81[us]
 X_Acq_Time = 2.7312128[s]
 X_Angle = 45[deg]
 X_Pulse = 4.905[us]
 Initial_Wait = 1[s]
 Unblank_Time = 2[us]

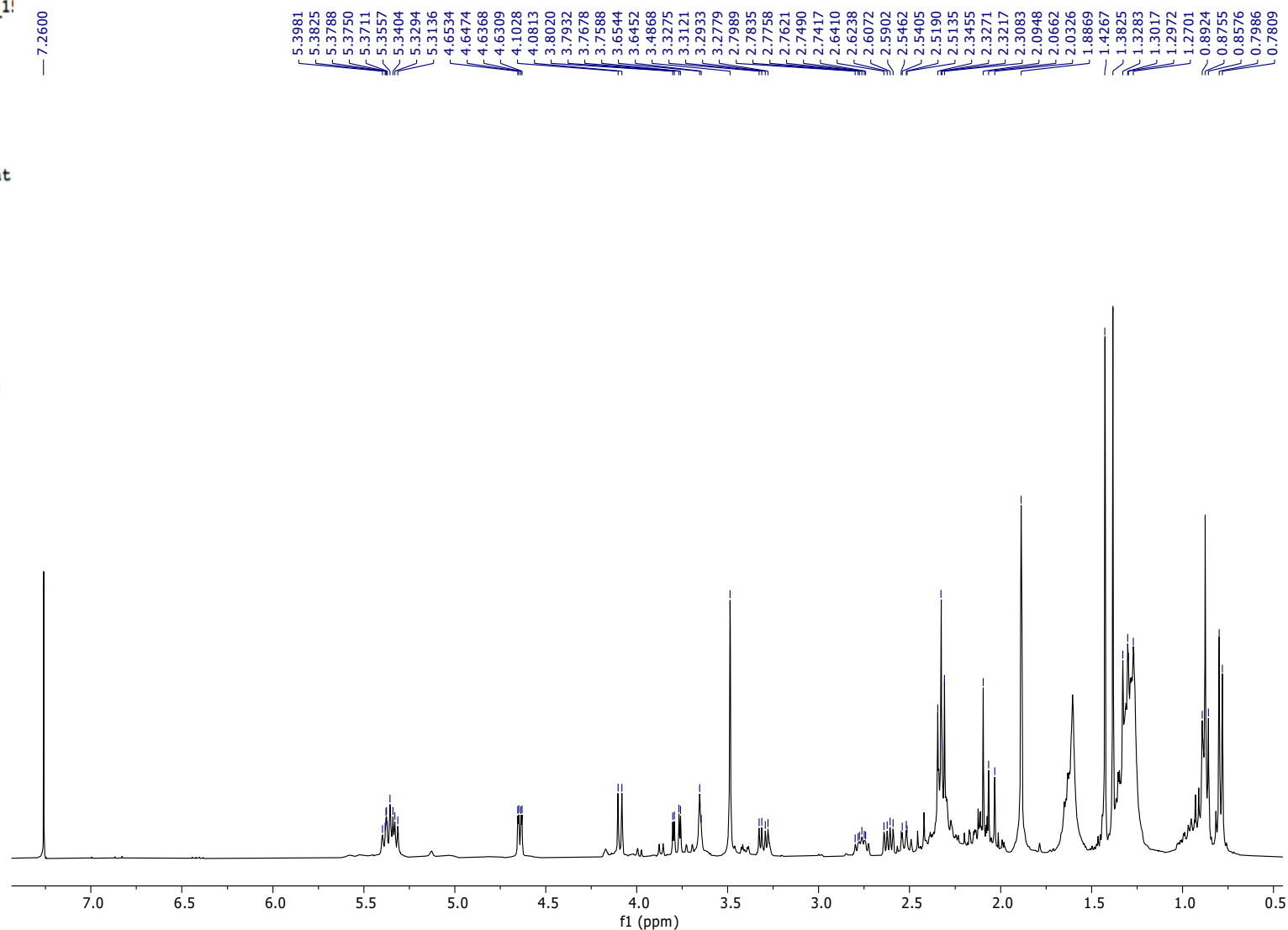


Figure S1. Briarellin T, ¹H NMR spectrum (expanded)

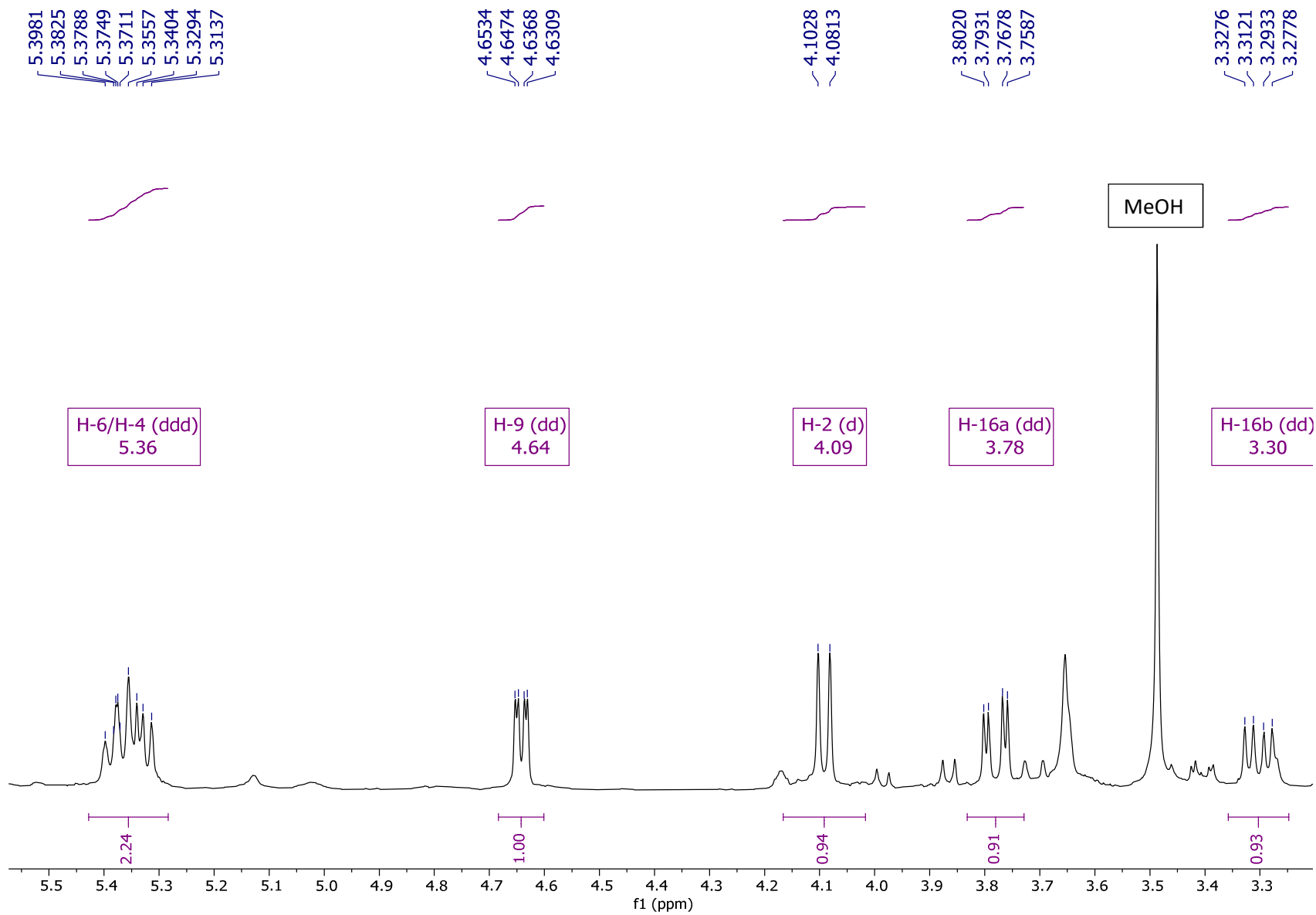


Figure S1. Briarellin T, ¹H NMR spectrum (expanded)

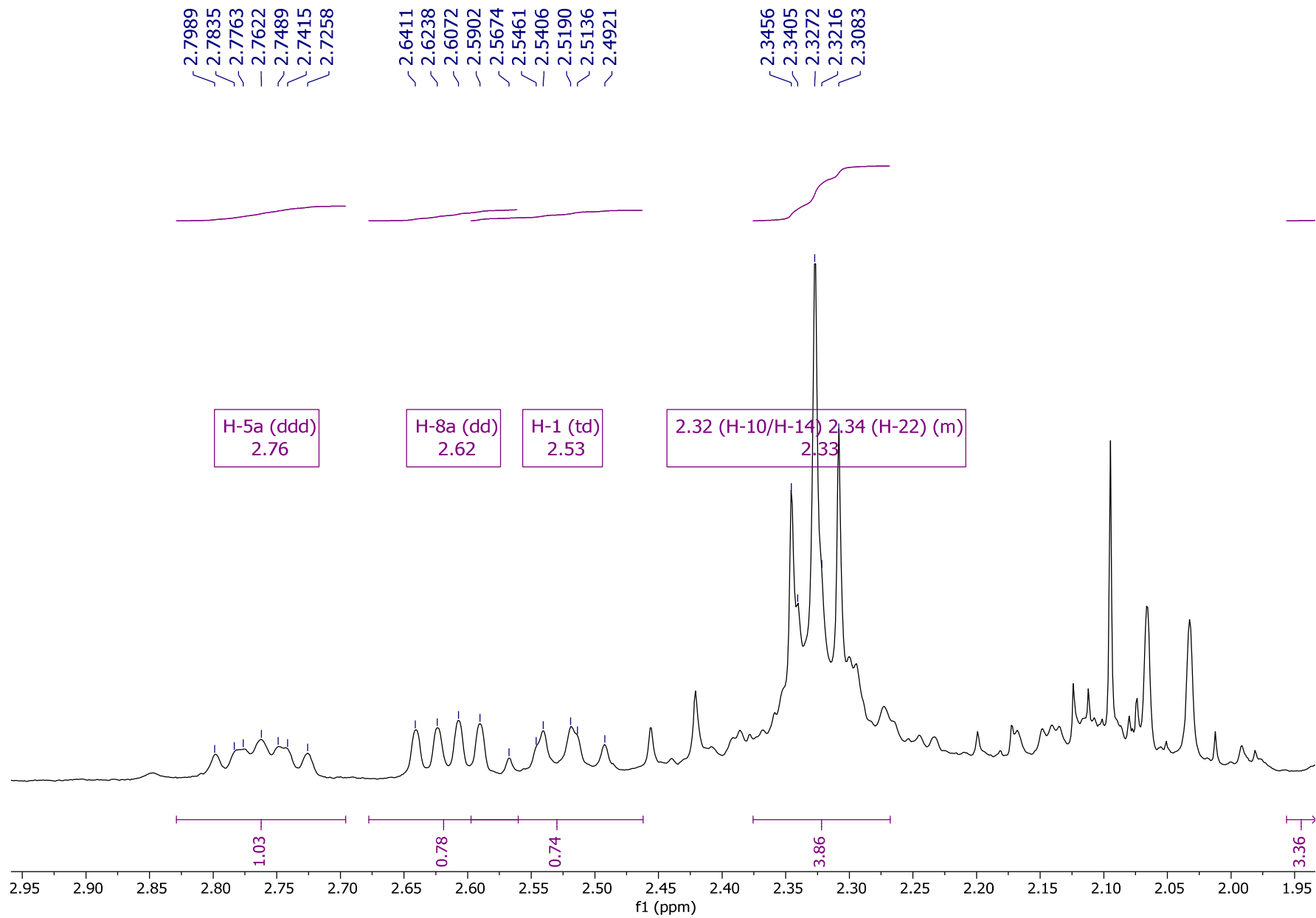


Figure S1. Briarellin T, ¹H NMR spectrum (expanded)

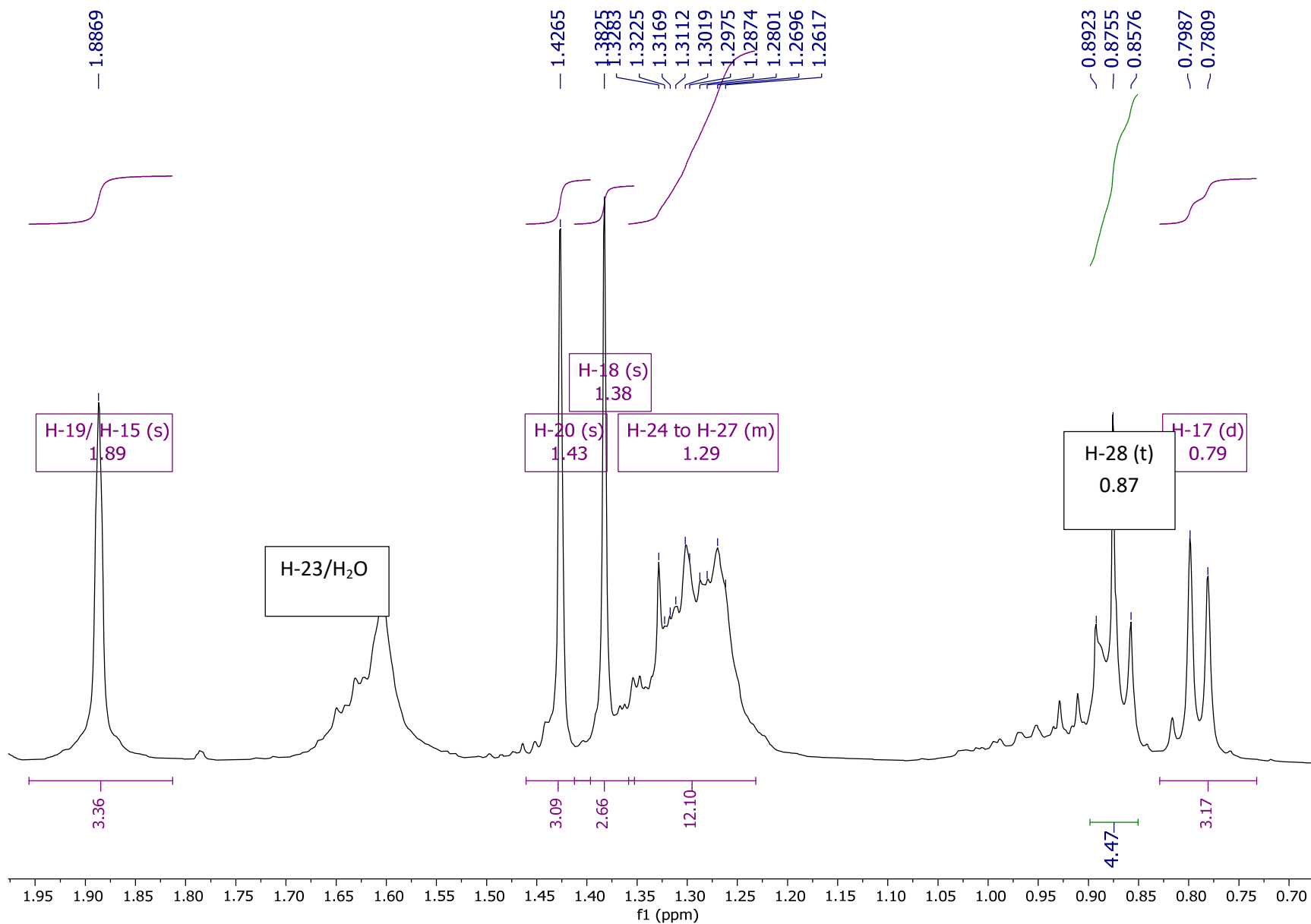


Figure S2. Briarellin T, ¹³C NMR spectrum

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 Author = DELTA — 173.50
 Experiment = single_pulse_dec
 Sample_Id = I3_062_003
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 27-JUL-2015 18:34:35
 Revision_Time = 14-JAN-2020 18:03:09

Comment = Single Pulse with Broad
 Data_Format = 1D COMPLEX
 Dim_Size = 32768
 X_Domain = 13C
 Dim_Title = 13C
 Dim_Units = [ppm]
 Dimensions = X
 Site = Eclipse+ 400
 Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 1.3008896[s]
 X_Domain = 13C
 X_Freq = 100.52530333[MHz]
 X_Offset = 100[ppm]
 X_Points = 32768
 X_Prescans = 4
 X_Resolution = 0.76870474[Hz]
 X_Sweep = 25.18891688[kHz]
 Irr_Domain = 1H
 Irr_Freq = 399.78219838[MHz]
 Irr_Offset = 5[ppm]
 Clipped = TRUE
 Scans = 15000
 Total_Scans = 15000

Relaxation_Delay = 1[s]
 Recvr_Gain = 26
 Temp_Get = 23.1[dC]
 X_90_Width = 10[us]
 X_Acq_Time = 1.3008896[s]
 X_Angle = 30[deg]
 X_Pulse = 3.33333333[us]
 Initial_Wait = 1[s]
 Unblank_Time = 2[us]

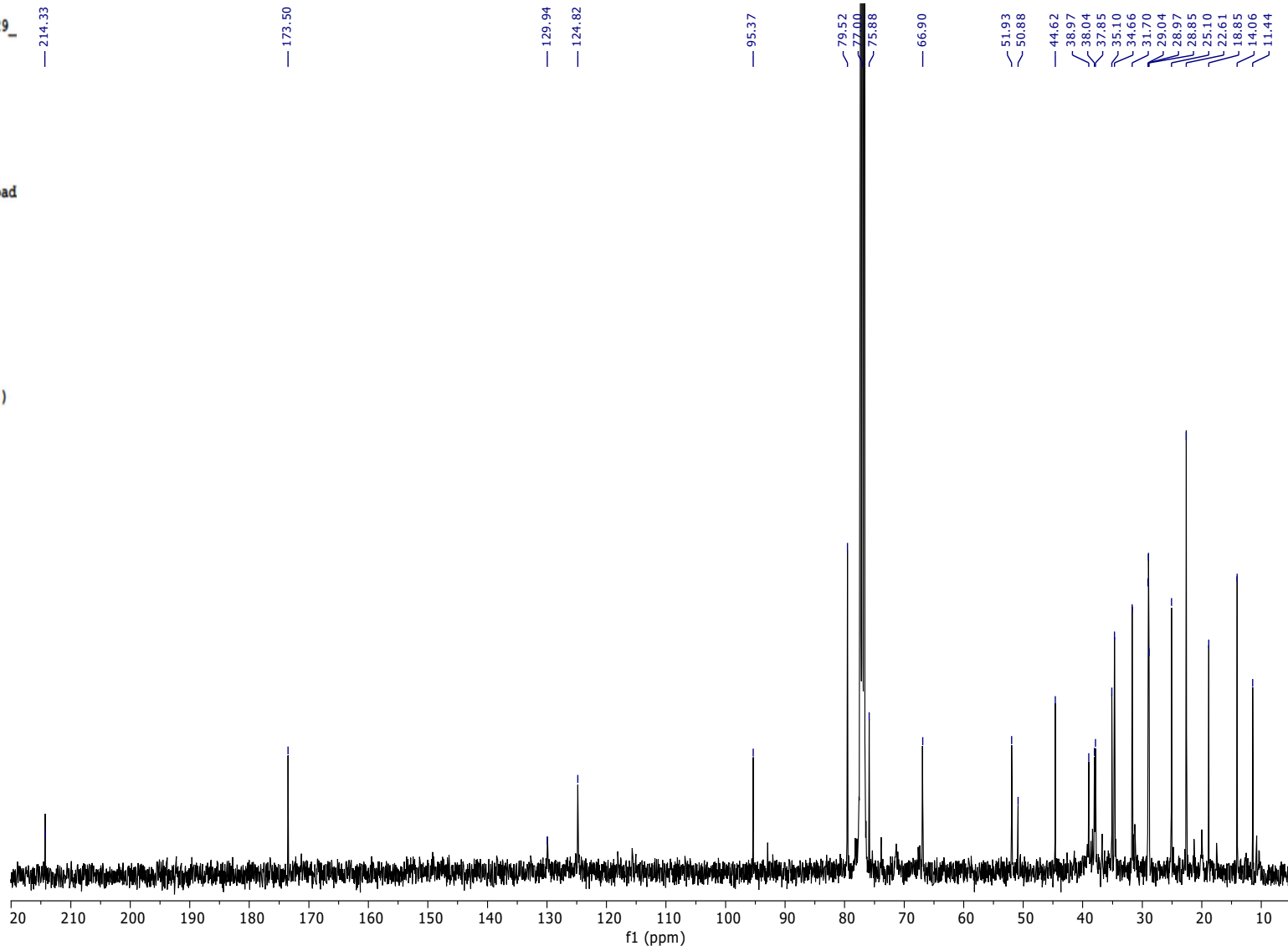


Figure S3. Briarellin T, DEPT-135 spectrum

```

Filename      = JF1_65_11 en CDC13 29 I3_062_003
Author        = DELTA
Experiment    = dept_dec.exp
Sample_Id     = I3_062_003
Solvent       = CHLOROFORM-D
Actual_Start_Time = 28-JUL-2015 04:10:36
Revision_Time = 14-JAN-2020 21:09:17

Comment       = DEPT with decoupling
Data_Format   = 1D COMPLEX
Dim_Size      = 32768
X_Domain      = 13C
Dim_Title     = 13C
Dim_Units     = [ppm]
Dimensions    = X
Site          = Eclipse+ 400
Spectrometer  = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.3008896[s]
X_Domain       = 13C
X_Freq        = 100.52530333[MHz]
X_Offset      = 100[ppm]
X_Points      = 32768
X_Prescans    = 4
X_Resolution  = 0.76870474[Hz]
X_Sweep       = 25.18891688[kHz]
Irr_Domain    = 1H
Irr_Freq      = 399.78219838[MHz]
Irr_Offset    = 5[ppm]
Clipped       = FALSE
Scans         = 3937
Total_Scans   = 3937

Relaxation_Delay = 2[s]
Recvr_Gain      = 26
Temp_Get        = 21.9[dC]
X_Acq_Time     = 1.3008896[s]
X_Pulse        = 10[us]
Irr_Pulse      = 44.5[us]
Initial_Wait    = 1[s]
J_Constant     = 140[Hz]
Selection_Angle = 135[deg]
Selection_Pulse = 66.75[us]
Unblank_Time   = 2[us]
    
```

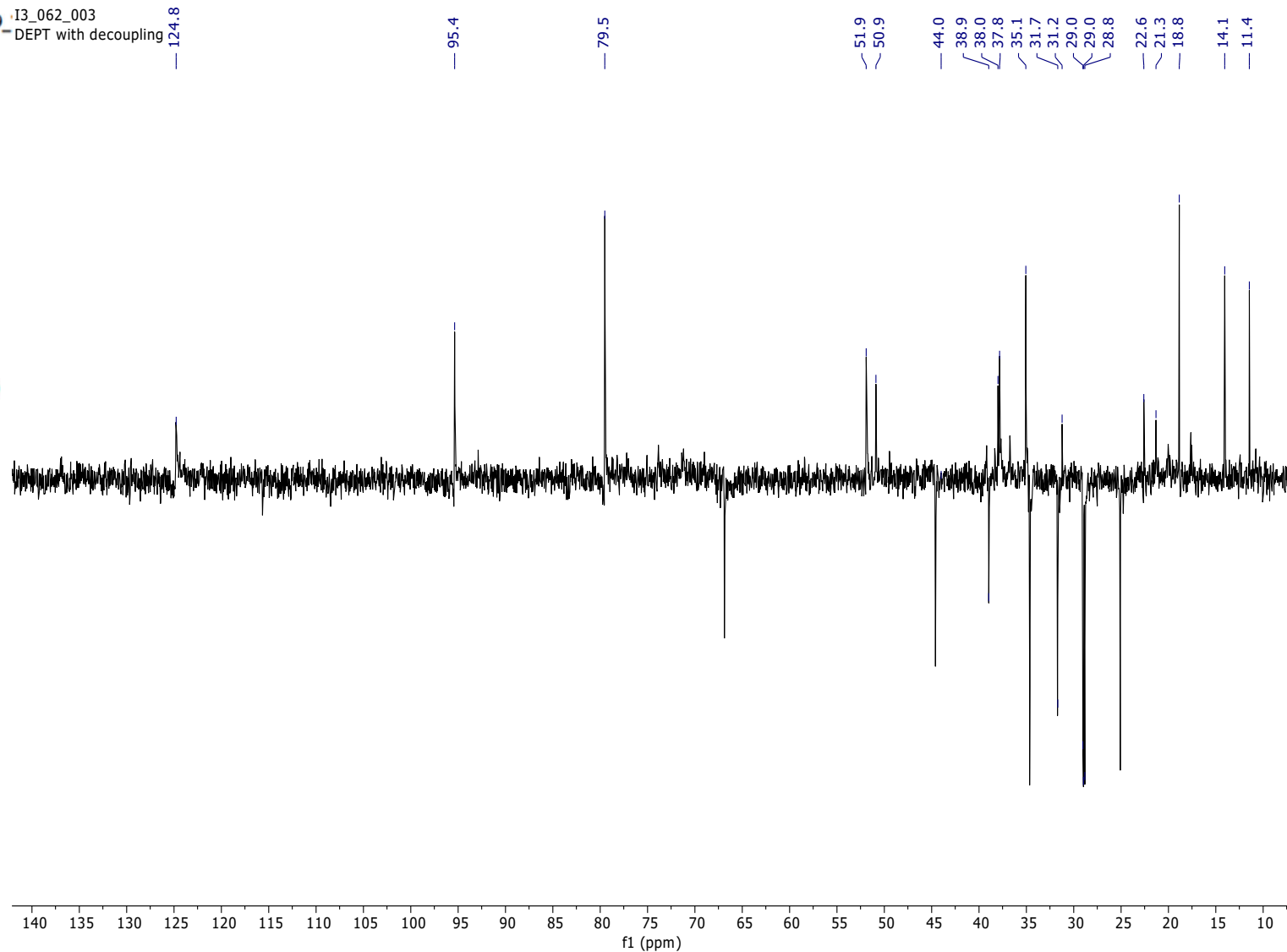


Figure S4. Briarellin T, COSY spectrum

Filename = JF1_65_11_CDC13_30_7_1
Author = DELTA
Experiment = dqf_cosy.exp
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Solvent = CHLOROFORM-D
Actual_Start_Time = 29-JUL-2015 05:54:39
Revision_Time = 23-OCT-2018 12:47:02

Comment = absolute value DQF COSY
Data_Format = 2D REAL REAL
Dim_Size = 512, 1024
X_Domain = 1H
Y_Domain = 1H
Dim_Title = 1H 1H
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Site = Eclipse+ 400
Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.1133568[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 4.68335[ppm]
X_Points = 512
X_Prescans = 4
X_Resolution = 8.8217028[Hz]
X_Sweep = 4.51671183[kHz]
Y_Domain = 1H
Y_Freq = 399.78219838[MHz]
Y_Offset = 4.68335[ppm]
Y_Points = 256
Y_Prescans = 0
Y_Resolution = 17.6434056[Hz]
Y_Sweep = 4.51671183[kHz]
Clipped = FALSE
Scans = 16
Total_Scans = 4096

Relaxation_Delay = 1.5[s]
Recvr_Gain = 15
Temp_Get = 21.6[dC]
X_Acq_Time = 0.1133568[s]
X_Pulse = 9.81[us]
Y_Acq_Time = 56.6784[ms]
Initial_Wait = 1[s]
T1 = 1[us]
Unblank_Time = 2[us]

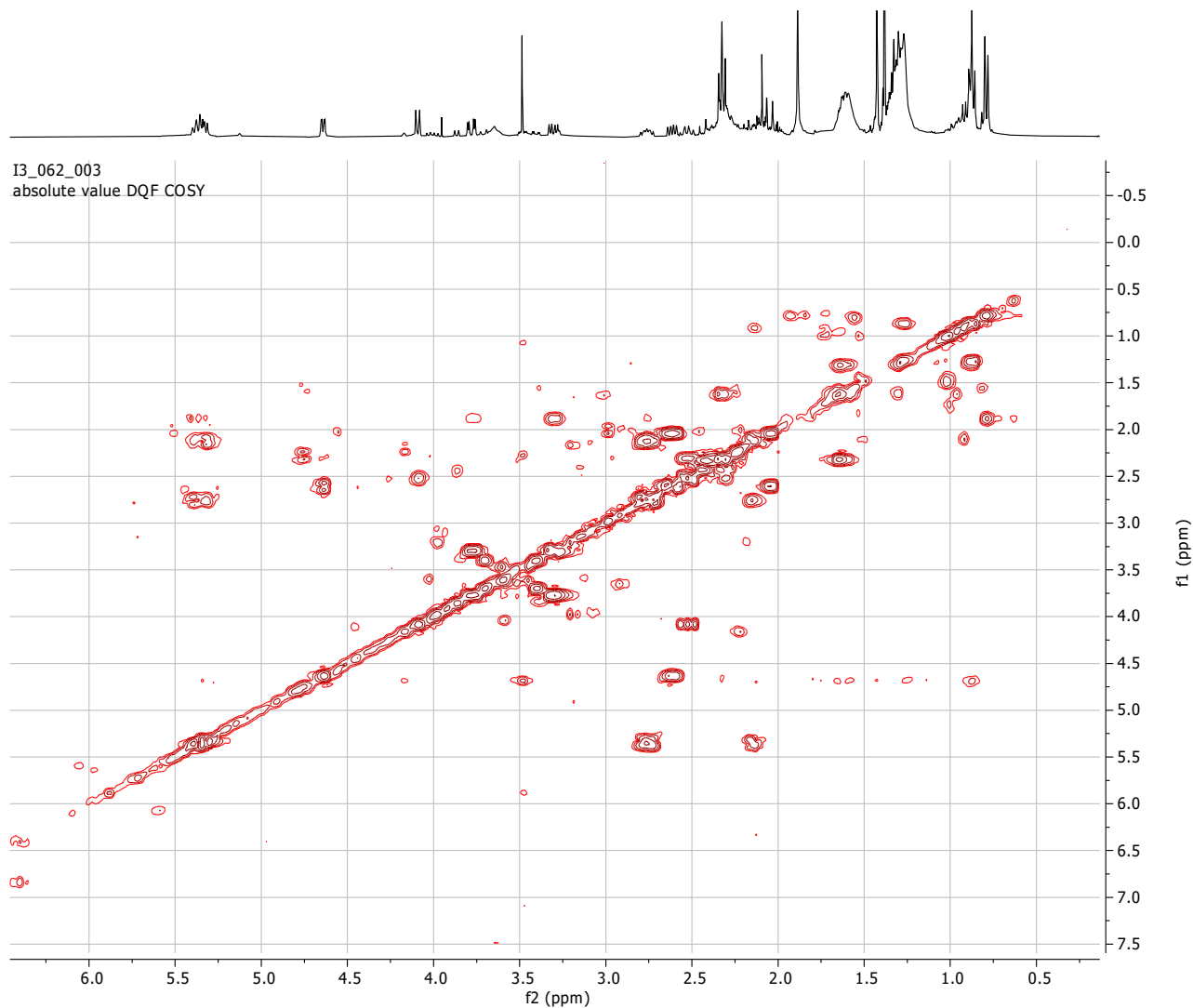


Figure S5. Briarellin T, HSQC spectrum

Filename = JF1_65_11_CDC13_29_7_1!
 Author = DELTA
 Experiment = multiplicity_hsq
 Sample_Id = I3_062_003
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 28-JUL-2015 10:56:48
 Revision_Time = 14-JAN-2020 21:23:24

Comment = Multiplicity HSQC
 Data_Format = 2D COMPLEX COMPLEX
 Dim_Size = 2048, 324
 X_Domain = 13C
 Y_Domain = 13C
 Dim_Title = 13C 13C
 Dim_Units = [ppm] [ppm]
 Dimensions = X Y
 Site = Eclipse+ 400
 Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 66.9696[ms]
 X_Domain = 13C
 X_Freq = 100.52530333[MHz]
 X_Offset = 68.30581[ppm]
 X_Points = 1024
 X_Prescans = 4
 X_Resolution = 14.93214832[Hz]
 X_Sweep = 15.29051988[kHz]
 Y_Domain = 13C
 Y_Freq = 100.52530333[MHz]
 Y_Offset = 100[ppm]
 Y_Points = 162
 Y_Prescans = 0
 Y_Resolution = 155.87978551[Hz]
 Y_Sweep = 25.25252525[kHz]
 Clipped = FALSE
 Scans = 16
 Total_Scans = 2579

Relaxation_Delay = 2[s]
 Recvr_Gain = 27
 Temp_Get = 22.1[dC]
 X_Acq_Time = 66.9696[ms]
 X_Pulse = 10[us]
 Y_Acq_Time = 10.1376[ms]
 Y_Pulse = 10[us]
 Enhance_Temp = 12
 Enhancement = 1/6J
 Grad_1 = 1[ms]
 Grad_1_Amp = 4[pnt]
 Grad_1_Value = 4[pnt*ms]
 Grad_2 = 1[ms]
 Grad_2_Amp = -1[pnt]
 Grad_2_Value = -1[pnt*ms]
 Grad_3 = 1[ms]
 Grad_3_Amp = 1[pnt]
 Grad_Recover = 0.1[ms]
 Grad_Selection = 13C = 4:1
 Grad_Shape = square
 Grad_Type = 0
 Initial_Wait = 1[s]
 J_Constant = 140[Hz]
 T1 = 1[us]
 Tau = 0.5952381[ms]

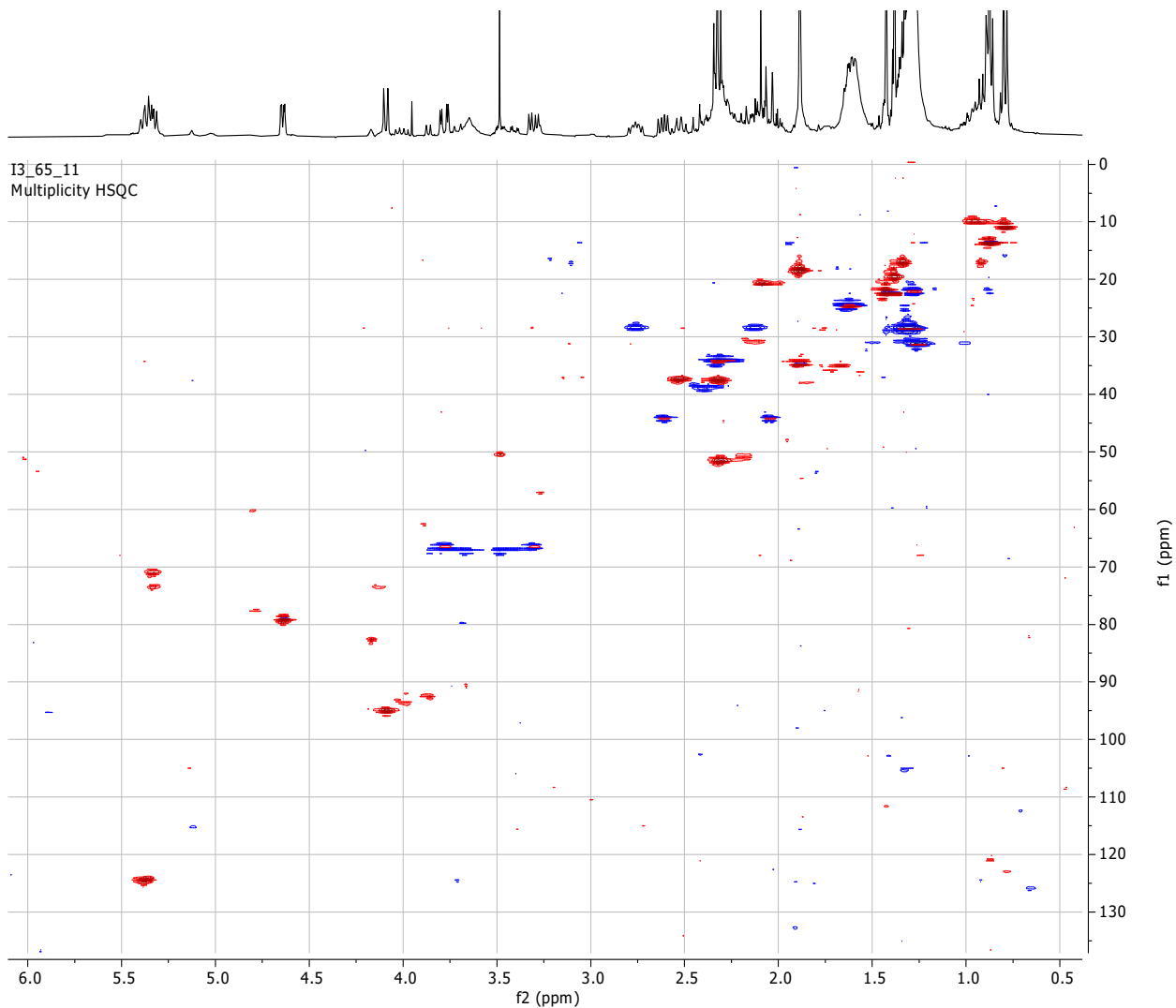


Figure S6. Briarellin T, HMBC spectrum

Filename = JF1_65_11_CDCl3_30_7_1!
Author = DELTA
Experiment = hmhc_pfg_s.exp
Sample_Id = I3_062_003
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-JUL-2015 00:40:13
Revision_Time = 31-JUL-2015 07:55:57

Comment = gradient enhanced HMBC
Data_Format = 2D REAL REAL
Dim_Size = 1024, 512
X_Domain = 1H
Y_Domain = 13C
Dim_Title = 1H 13C
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Site = Eclipse+ 400
Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.2267136[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 4.68335[ppm]
X_Points = 1024
X_Prescans = 4
X_Resolution = 4.4108514[Hz]
X_Sweep = 4.51671183[kHz]
Y_Domain = 13C
Y_Freq = 100.52530333[MHz]
Y_Offset = 100[ppm]
Y_Points = 256
Y_Prescans = 0
Y_Resolution = 98.64267677[Hz]
Y_Sweep = 25.25252525[kHz]
Clipped = FALSE
Scans = 32
Total_Scans = 8192

Relaxation_Delay = 2[s]
Recvr_Gain = 30
Temp_Get = 21.3[dC]
X_Acq_Time = 0.2267136[s]
X_Pulse = 9.81[us]
Y_Acq_Time = 10.1376[ms]
Y_Pulse = 12[us]
Grad_1 = 1[ms]
Grad_1_Amp = 10[pnt]
Grad_1_Value = 10[pnt*ms]
Grad_2 = 1[ms]
Grad_2_Amp = 10[pnt]
Grad_2_Value = 10[pnt*ms]
Grad_3 = 1[ms]
Grad_3_Amp = 5[pnt]
Grad_3_Value = 5[pnt*ms]
Grad_Recover = 0.2[ms]
Grad_Selection = 13C = 2:2:1
Grad_Shape = square
Grad_Type = 0
Initial_Wait = 1[s]
J_Constant = 140[Hz]
Long_Range_J = 8[Hz]
T1 = 1[us]
Unblank_Time = 2[us]

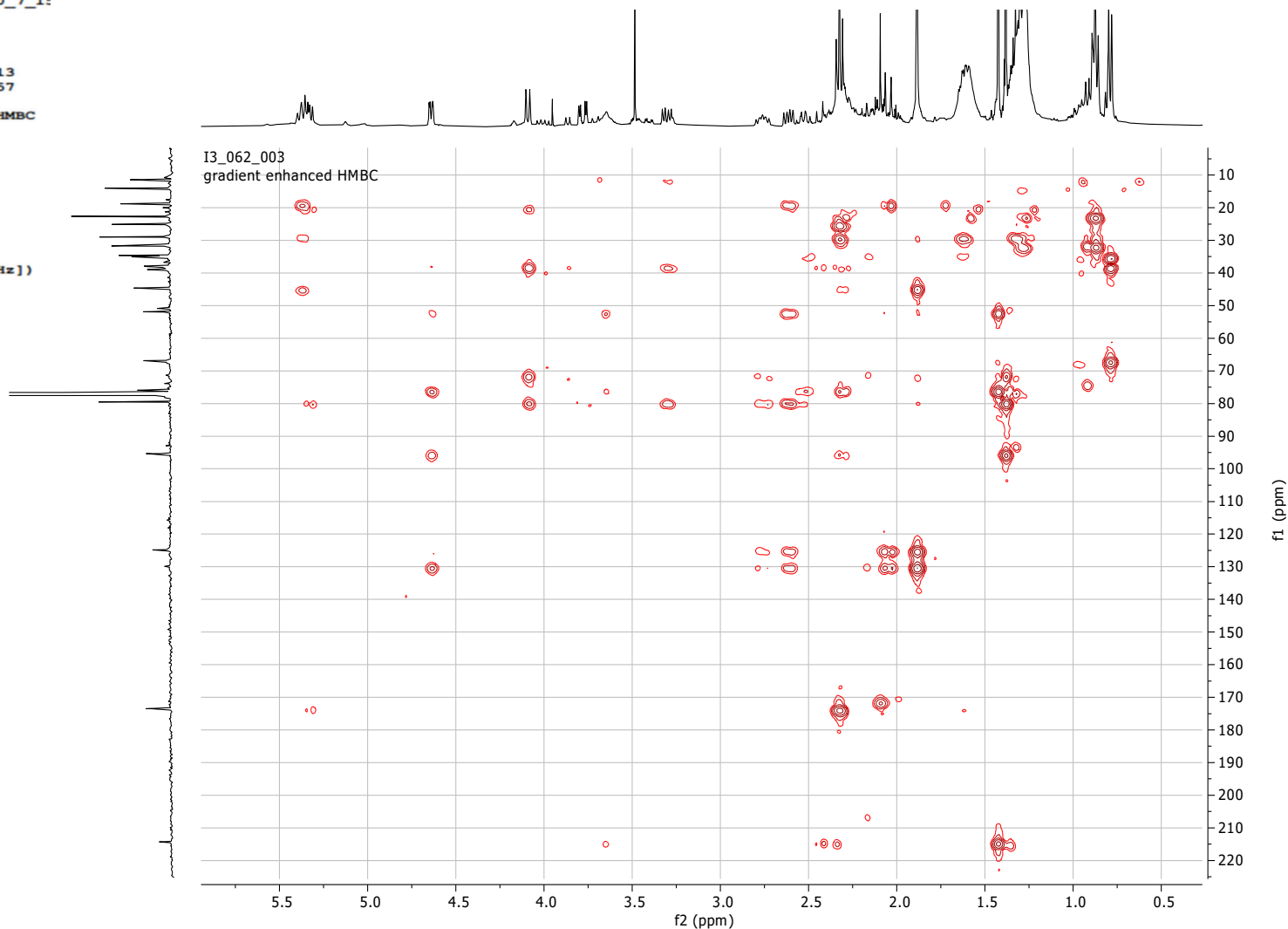


Figure S7. Briarellin T, NOE spectra

Irradiation of H-17

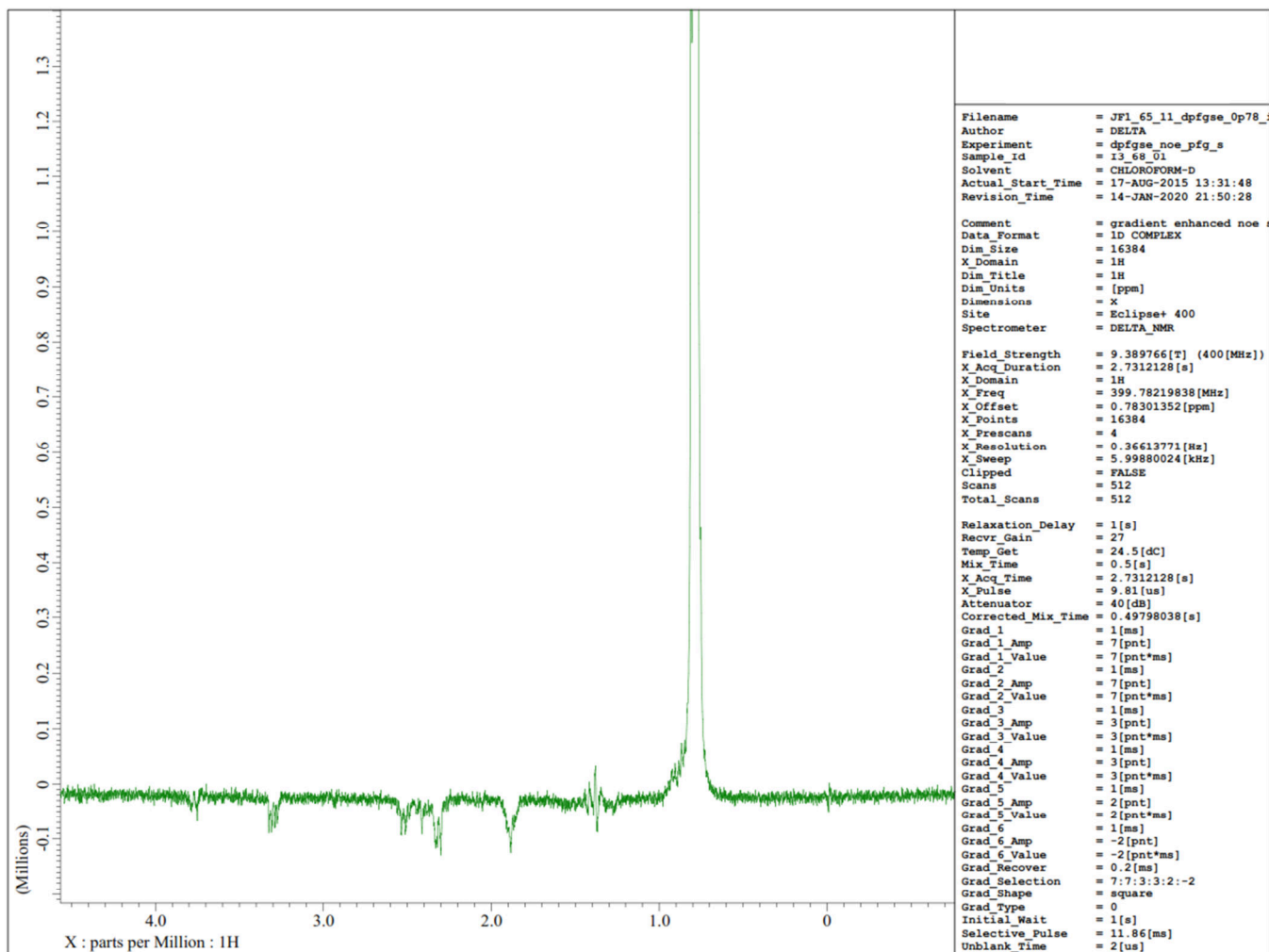


Figure S7. Briarellin T, NOE spectra

Irradiation of H-18

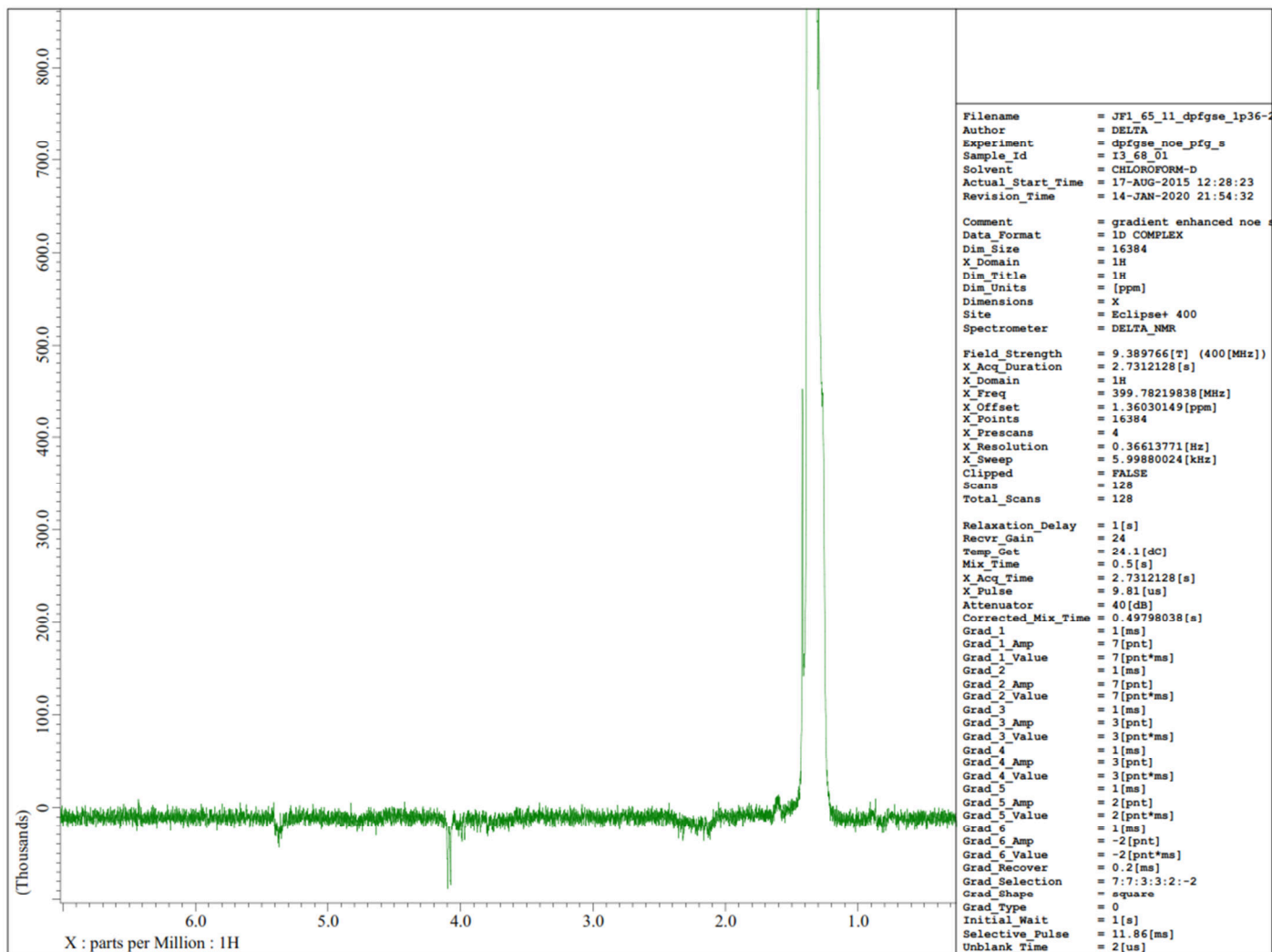


Figure S7. Briarellin T, NOE spectra

Irradiation of H-20

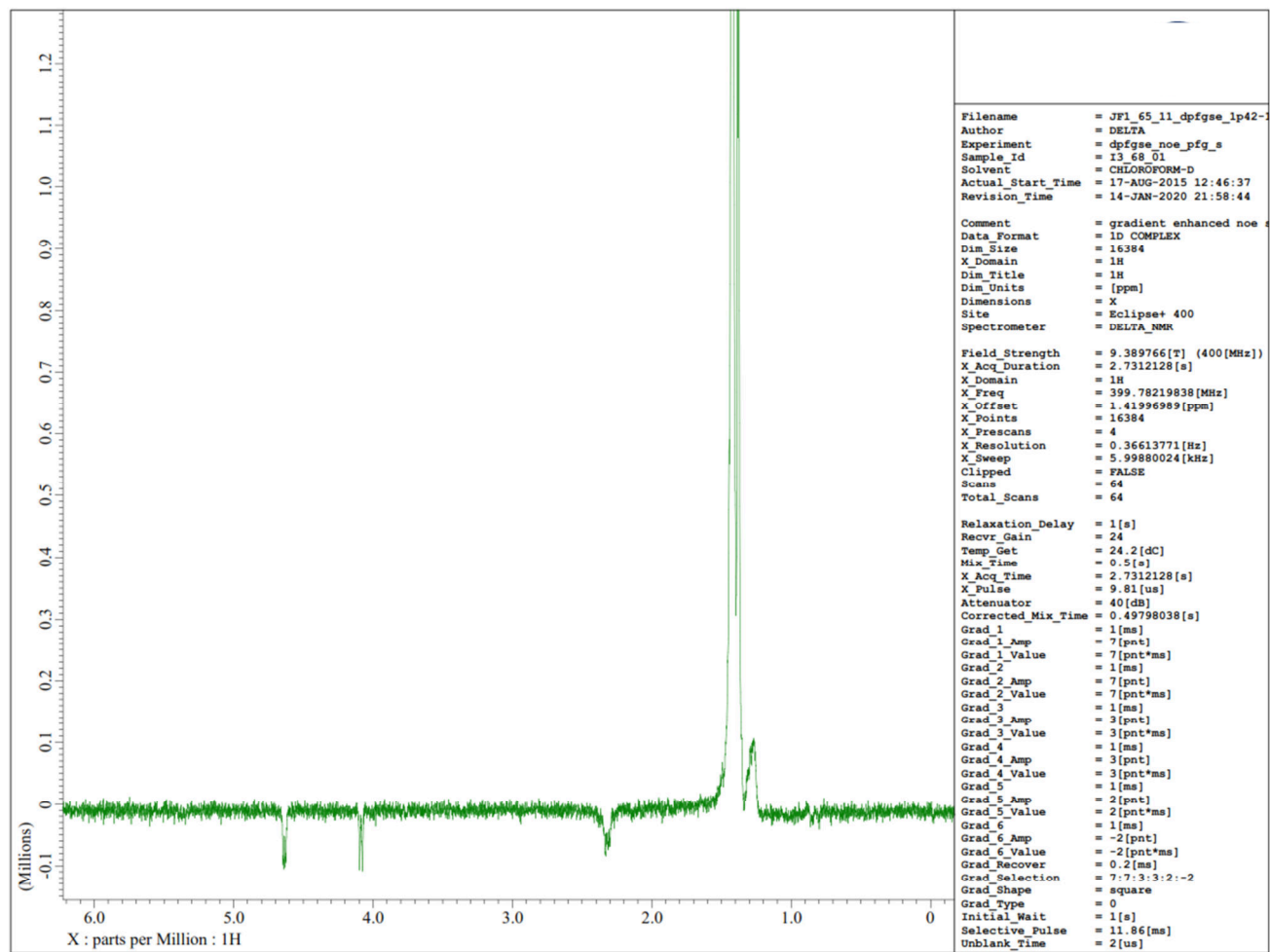


Figure S8. Briarellin T, HR-ESITOFMS spectrum

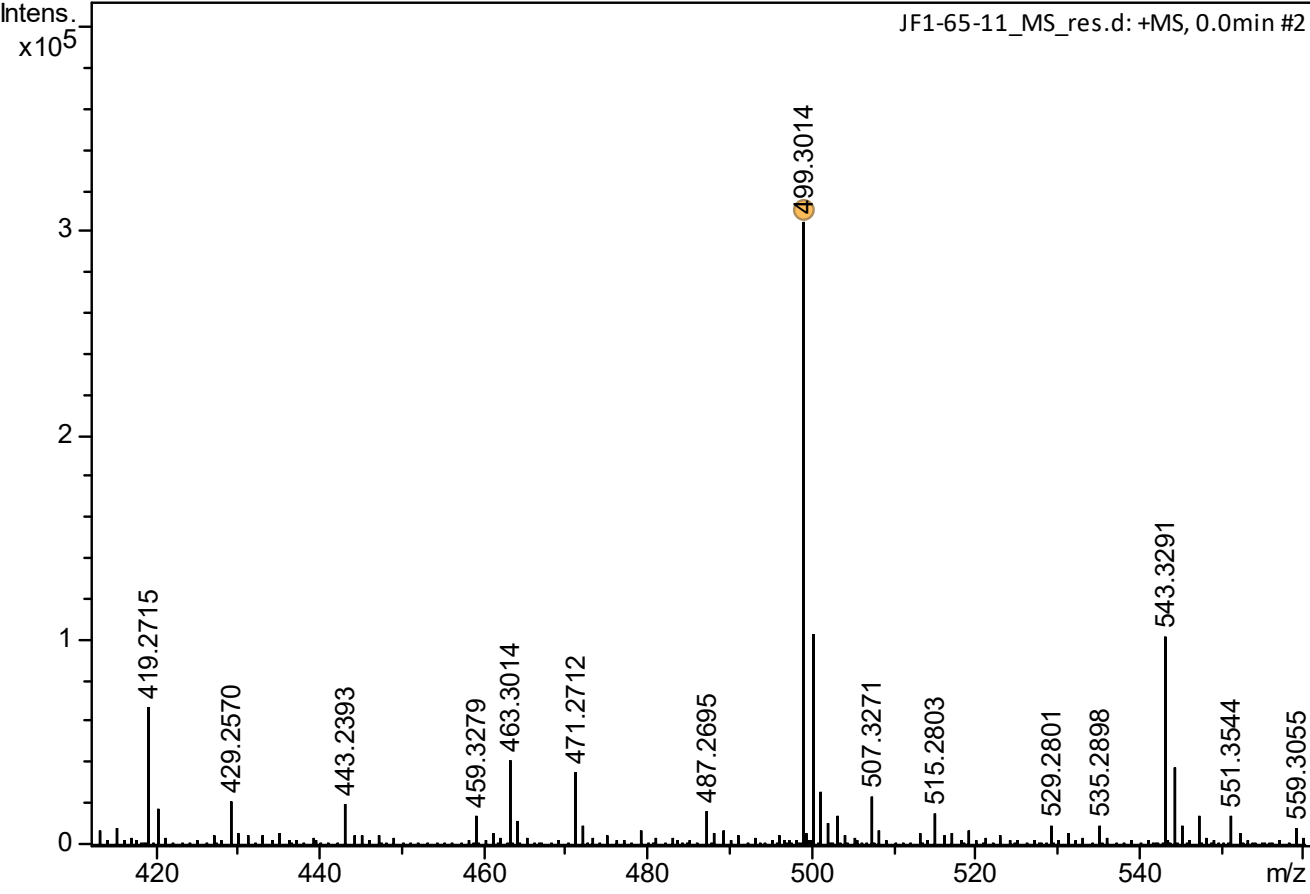


Figure S9. Asbestinin 27, ¹H NMR spectrum

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Author = DELTA
Experiment = single_pulse.exp
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Solvent = CHLOROFORM-D
Actual_Start_Time = 17-AUG-2015 15:51:50
Revision_Time = 19-AUG-2015 15:41:04

Comment = Single Pulse Experiment
Data_Format = 1D COMPLEX
Dim_Size = 16384
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = Eclipse+ 400
Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.7312128[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 0
X_Resolution = 0.36613771[Hz]
X_Sweep = 5.99880024[kHz]
Clipped = FALSE
Scans = 16
Total_Scans = 16

Relaxation_Delay = 4[s]
Recvr_Gain = 17
Temp_Get = 25[dC]
X_90_Width = 9.81[us]
X_Acq_Time = 2.7312128[s]
X_Angle = 45[deg]
X_Pulse = 4.905[us]
Initial_Wait = 1[s]
Unblank_Time = 2[us]

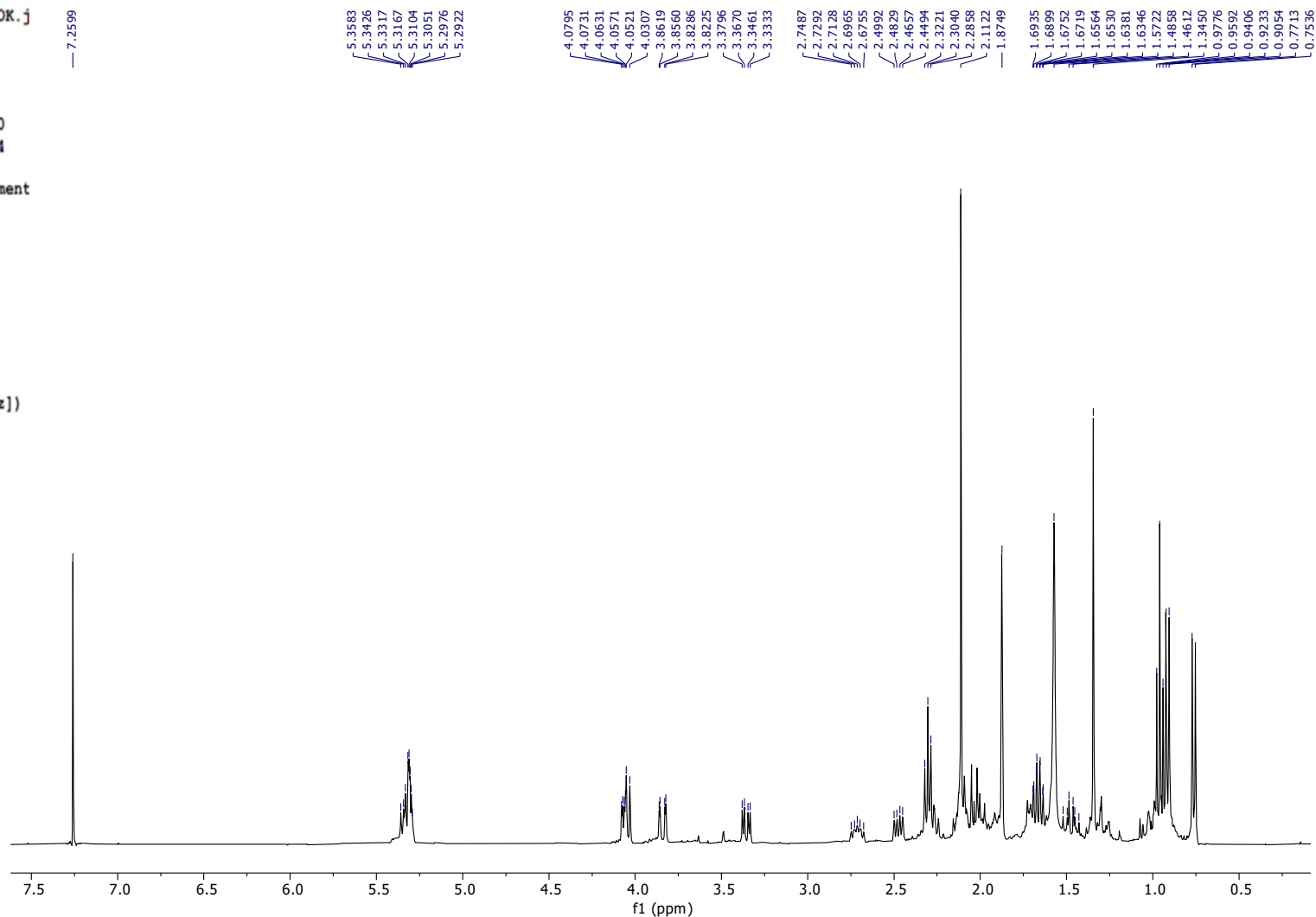


Figure S9. Asbestinin 27, ¹H NMR spectrum (expanded)

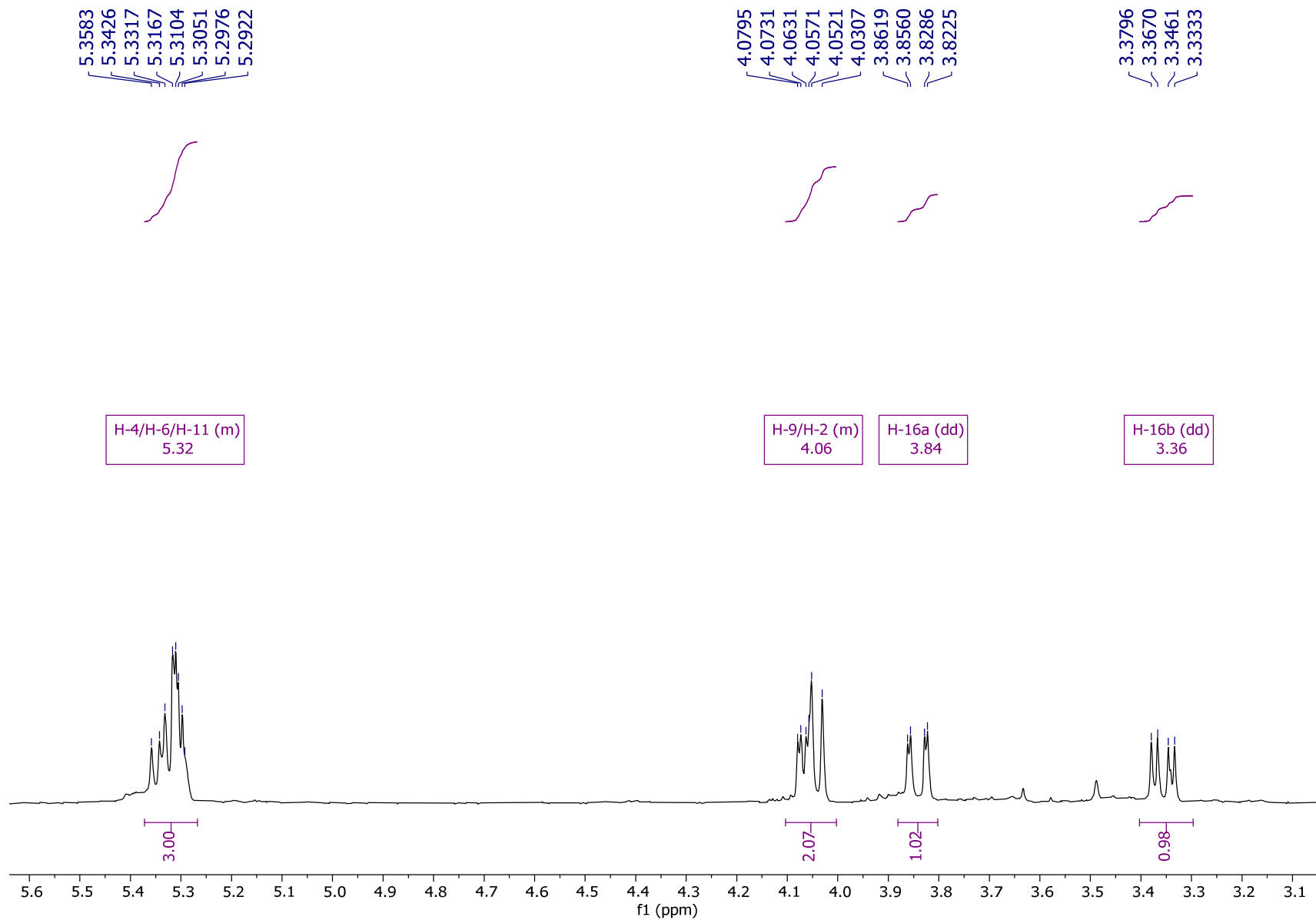


Figure S9. Asbestinin 27, ¹H NMR spectrum (expanded)

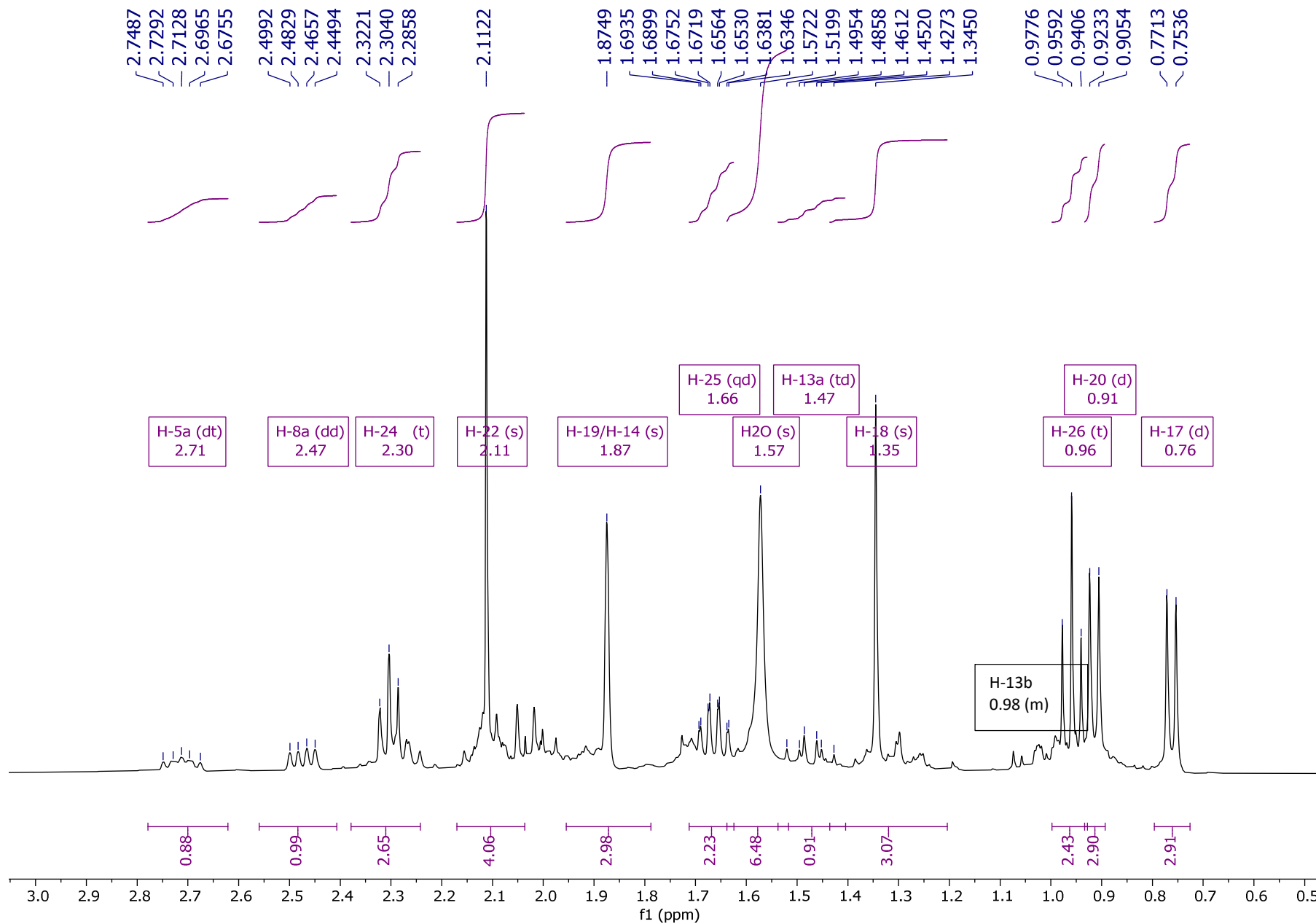


Figure S10. Asbestinin 27, ¹³C NMR spectrum

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Author = DELTA
Experiment = single_pulse_dec
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Solvent = CHLOROFORM-D
Actual_Start_Time = 5-AUG-2015 16:50:00
Revision_Time = 8-AUG-2015 03:05:23

Comment = Single Pulse with Broad
Data_Format = 1D COMPLEX
Dim_Size = 32768
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = Eclipse+ 400
Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.3008896[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.76870474[Hz]
X_Sweep = 25.18891688[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 16384
Total_Scans = 16384

Relaxation_Delay = 1[s]
Recvr_Gain = 27
Temp_Get = 26.8[dC]
X_90_Width = 10[us]
X_Acq_Time = 1.3008896[s]
X_Angle = 30[deg]
X_Pulse = 3.33333333[us]
Initial_Wait = 1[s]
Unblank_Time = 2[us]

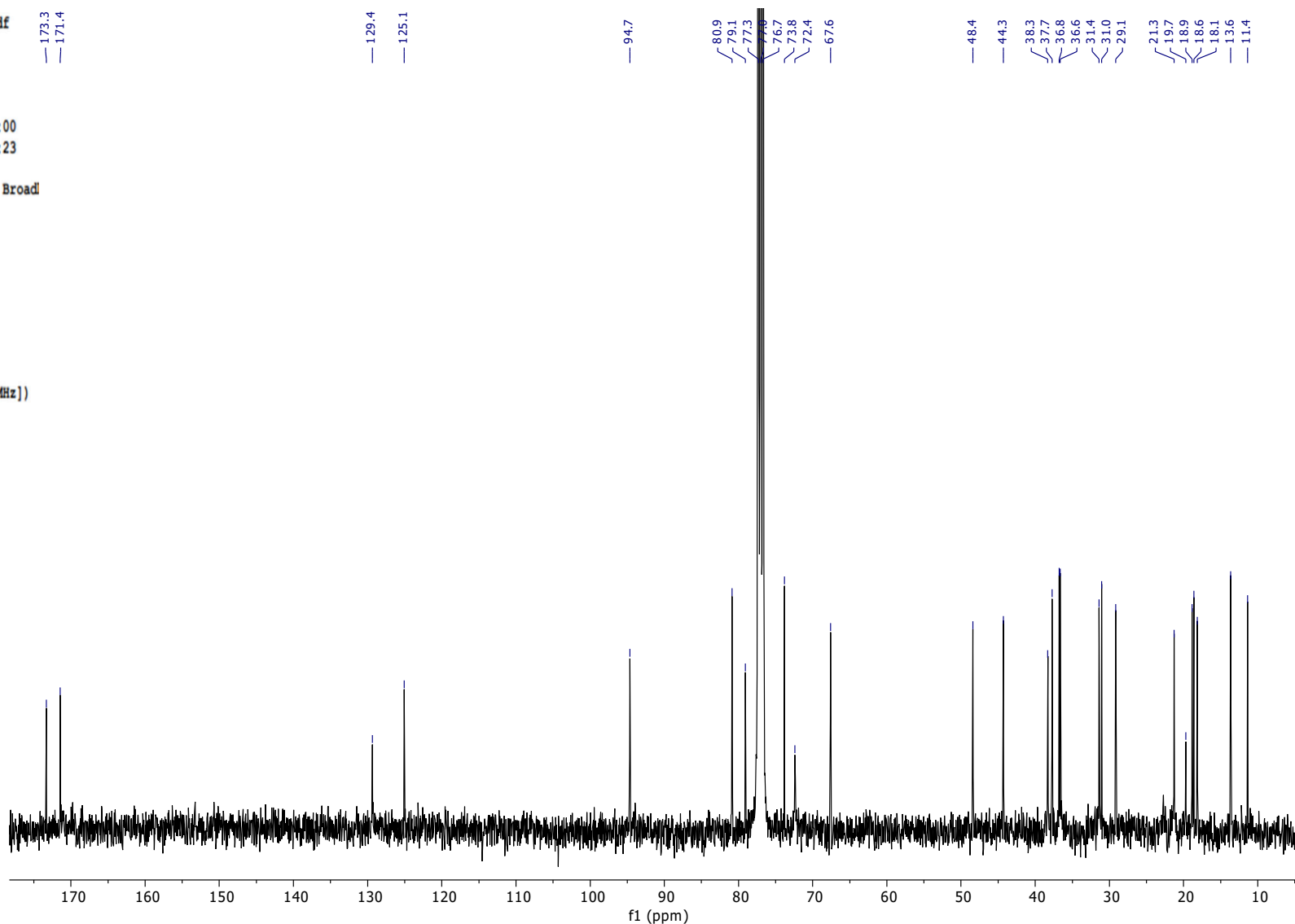


Figure S11. Asbestinin 27, DEPT-135 spectrum

Filename = JF1_65_05_dept135-2.jdf
 Author = DELTA
 Experiment = dept_dec.exp
 Sample_Id = I3_68_02
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 17-AUG-2015 15:56:24
 Revision_Time = 14-JAN-2020 22:39:27

Comment = DEPT with decoupling
 Data_Format = 1D COMPLEX
 Dim_Size = 32768
 X_Domain = 13C
 Dim_Title = 13C
 Dim_Units = [ppm]
 Dimensions = X
 Site = Eclipse+ 400
 Spectrometer = DELTA_NMR

Field Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 1.3008896[s]
 X_Domain = 13C
 X_Freq = 100.52530333[MHz]
 X_Offset = 100[ppm]
 X_Points = 32768
 X_Prescans = 4
 X_Resolution = 0.76870474[Hz]
 X_Sweep = 25.18891688[kHz]
 Irr_Domain = 1H
 Irr_Freq = 399.78219838[MHz]
 Irr_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 1024
 Total_Scans = 1024

Relaxation_Delay = 2[s]
 Recvr_Gain = 27
 Temp_Get = 25.7[dC]
 X_Acq_Time = 1.3008896[s]
 X_Pulse = 10[us]
 Irr_Pulse = 44.5[us]
 Initial_Wait = 1[s]
 J_Constant = 140[Hz]
 Selection_Angle = 135[deg]
 Selection_Pulse = 66.75[us]
 Unblank_Time = 2[us]

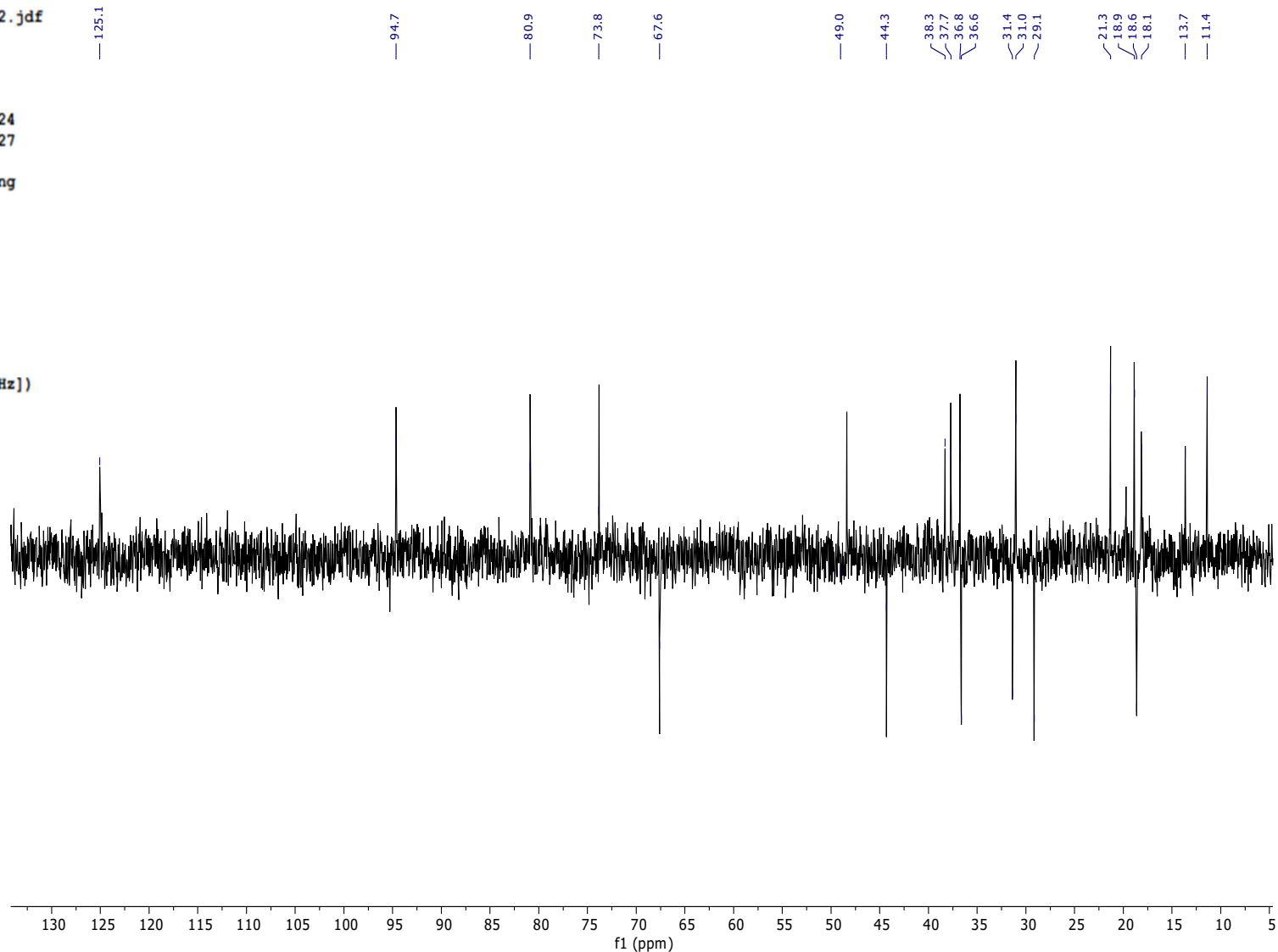


Figure S12. Asbestinin 27, COSY spectrum

```

Filename      = JF1_65_05_cosy-2.jdf
Author       = DELTA
Experiment   = cosy_pfg_s.exp
Sample Id    = I3_68_02
Solvent      = CHLOROFORM-D
Actual_Start_Time = 18-AUG-2015 04:45:39
Revision_Time  = 14-JAN-2020 22:44:12

Comment      = gradient absolute value
Data_Format  = 2D REAL REAL
Dim_Size     = 1024, 1024
X_Domain     = 1H
Y_Domain     = 1H
Dim_Title    = 1H 1H
Dim_Units    = [ppm] [ppm]
Dimensions   = X Y
Site         = Eclipse+ 400
Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.2900992[s]
X_Domain       = 1H
X_Freq         = 399.78219838[MHz]
X_Offset       = 3.62959[ppm]
X_Points       = 1024
X_Prescans    = 4
X_Resolution  = 3.44709672[Hz]
X_Sweep       = 3.52982704[kHz]
Y_Domain       = 1H
Y_Freq         = 399.78219838[MHz]
Y_Offset       = 3.62959[ppm]
Y_Points       = 256
Y_Prescans    = 0
Y_Resolution  = 13.78838687[Hz]
Y_Sweep       = 3.52982704[kHz]
Clipped       = FALSE
Scans         = 8
Total_Scans   = 2048

Relaxation_Delay = 1[s]
Recvr_Gain       = 18
Temp_Get         = 23.6[dC]
X_90_Width      = 9.81[us]
X_Acq_Time      = 0.2900992[s]
X_Pulse         = 9.81[us]
Y_Acq_Time      = 72.5248[ms]
Grad_1          = 1[ms]
Grad_1_Amp      = 5[pnt]
Grad_1_Value    = 5[pnt*ms]
Grad_2          = 1[ms]
Grad_2_Amp      = 5[pnt]
Grad_2_Value    = 5[pnt*ms]
Grad_Recover    = 1[ms]
Grad_Selection  = 1:1
Grad_Shape      = square
Grad_Type       = 0
Initial_Wait    = 0.1[s]
Pulse_1         = 9.81[us]
Pulse_2         = 9.81[us]
Pulse_Angle_1  = 90[deg]
Pulse_Angle_2  = 90[deg]
T1              = 1[us]
Unblank_Time    = 2[us]
    
```

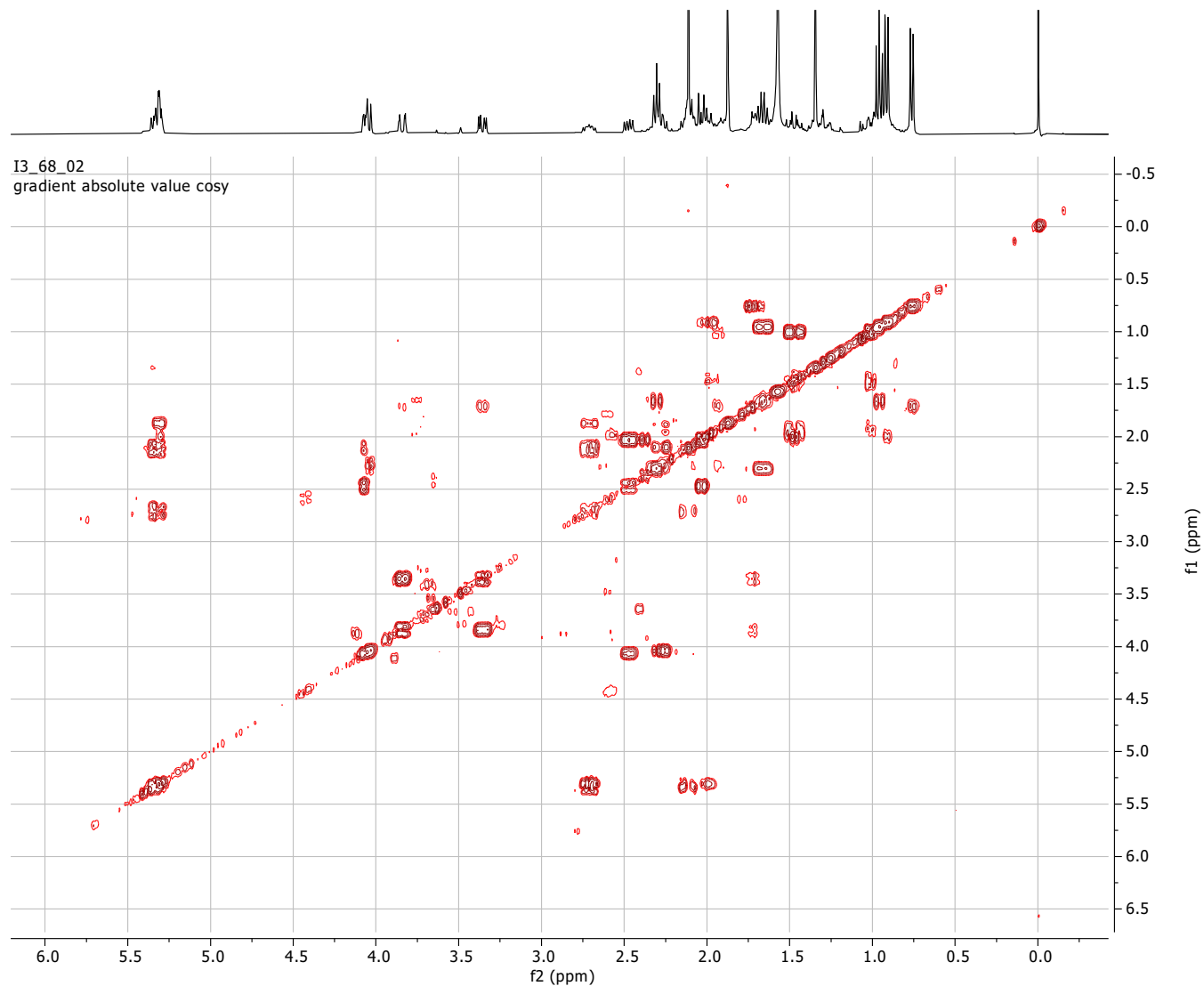


Figure S13. Asbestinin 27, HSQC spectrum

Filename = JF1_65_05_hsqc-2.jdf
 Author = DELTA
 Experiment = multiplicity_hsq
 Sample_Id = I3_68_02
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 17-AUG-2015 17:02:39
 Revision_Time = 14-JAN-2020 22:50:48

Comment = Multiplicity HSQC
 Data_Format = 2D COMPLEX COMPLEX
 Dim_Size = 2048, 512
 X_Domain = 1H
 Y_Domain = 13C
 Dim_Title = 1H 13C
 Dim_Units = [ppm] [ppm]
 Dimensions = X Y
 Site = Eclipse+ 400
 Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 0.2900992[s]
 X_Domain = 1H
 X_Freq = 399.78219838[MHz]
 X_Offset = 3.62959[ppm]
 X_Points = 1024
 X_Prescans = 4
 X_Resolution = 3.44709672[Hz]
 X_Sweep = 3.52982704[kHz]
 Y_Domain = 13C
 Y_Freq = 100.52530333[MHz]
 Y_Offset = 100[ppm]
 Y_Points = 256
 Y_Prescans = 0
 Y_Resolution = 98.64267677[Hz]
 Y_Sweep = 25.25252525[kHz]
 Clipped = FALSE
 Scans = 16
 Total_Scans = 4096

Relaxation_Delay = 2[s]
 Recvr_Gain = 30
 Temp_Get = 24.7[dC]
 X_Acq_Time = 0.2900992[s]
 X_Pulse = 9.81[us]
 Y_Acq_Time = 10.1376[ms]
 Y_Pulse = 12[us]
 Enhance_Temp = 12
 Enhancement = 1/6J
 Grad_1 = 1[ms]
 Grad_1_Amp = 4[pnt]
 Grad_1_Value = 4[pnt*ms]
 Grad_2 = 1[ms]
 Grad_2_Amp = -1[pnt]
 Grad_2_Value = -1[pnt*ms]
 Grad_3 = 1[ms]
 Grad_3_Amp = 1[pnt]
 Grad_Recover = 0.1[ms]
 Grad_Selection = 13C = 4:1
 Grad_Shape = square
 Grad_Type = 0
 Initial_Wait = 1[s]
 J_Constant = 140[Hz]
 T1 = 1[us]
 Tau = 0.5952381[ms]

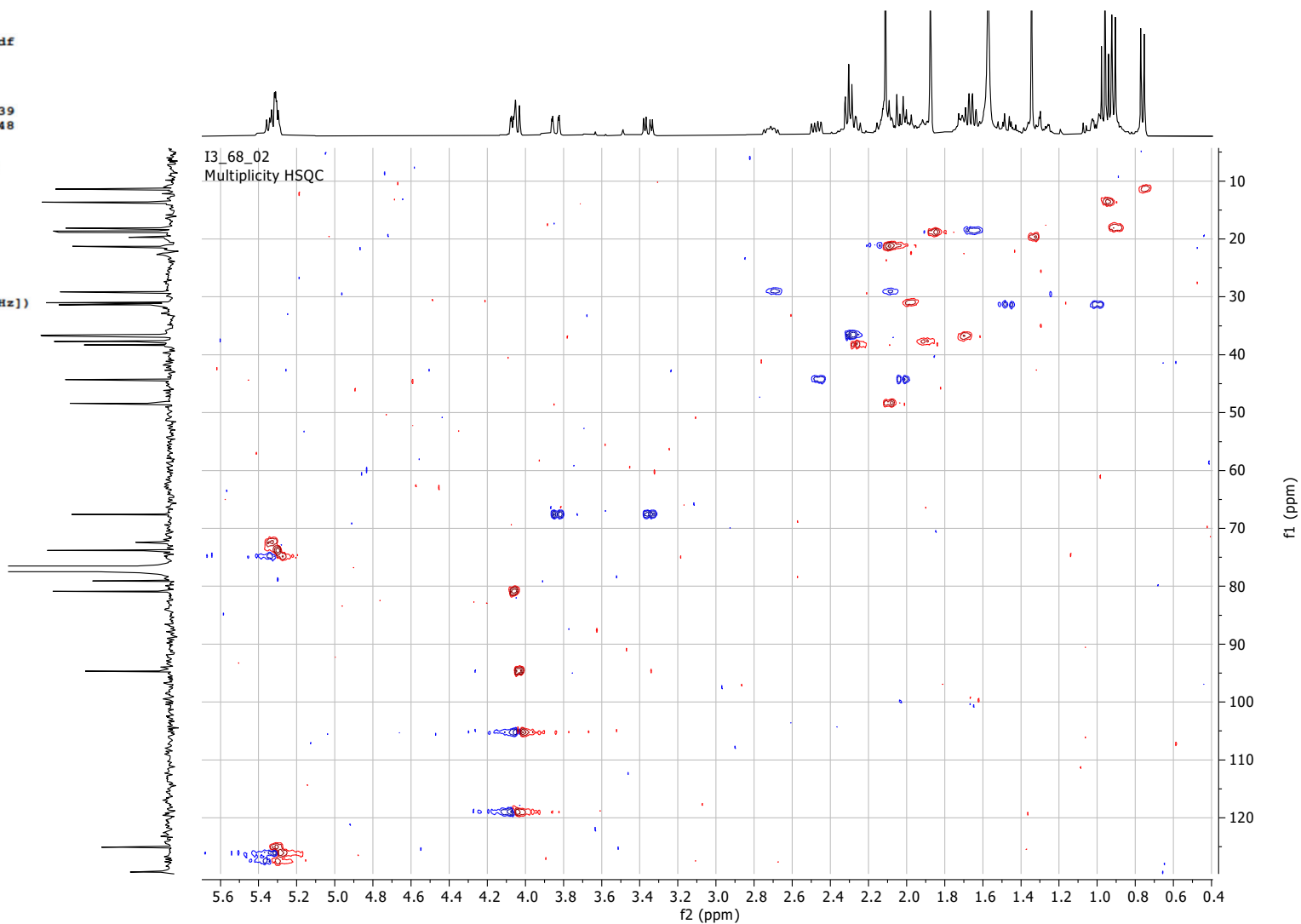


Figure S14. Asbestinin 27, HMBC spectrum

Filename = JF1_65_05_hmbcOKOKOK-2.
Author = DELTA
Experiment = hmbc_pfg_s.exp
Sample_Id = I3_68_02
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-AUG-2015 22:19:20
Revision_Time = 5-JUL-2019 17:15:31

Comment = gradient enhanced HMBC
Data_Format = 2D REAL REAL
Dim_Size = 1024, 512
X_Domain = 1H
Y_Domain = 13C
Dim_Title = 1H 13C
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Site = Eclipse+ 400
Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.2900992[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 3.62959[ppm]
X_Points = 1024
X_Prescans = 4
X_Resolution = 3.44709672[Hz]
X_Sweep = 3.52982704[kHz]
Y_Domain = 13C
Y_Freq = 100.52530333[MHz]
Y_Offset = 100[ppm]
Y_Points = 256
Y_Prescans = 0
Y_Resolution = 98.64267677[Hz]
Y_Sweep = 25.25252525[kHz]
Clipped = FALSE
Scans = 32
Total_Scans = 8192

Relaxation_Delay = 2[s]
Recvr_Gain = 30
Temp_Get = 23.9[dc]
X_Acq_Time = 0.2900992[s]
X_Pulse = 9.81[us]
Y_Acq_Time = 10.1376[ms]
Y_Pulse = 12[us]
Grad_1 = 1[ms]
Grad_1_Amp = 10[pnt]
Grad_1_Value = 10[pnt*ms]
Grad_2 = 1[ms]
Grad_2_Amp = 10[pnt]
Grad_2_Value = 10[pnt*ms]
Grad_3 = 1[ms]
Grad_3_Amp = 5[pnt]
Grad_3_Value = 5[pnt*ms]
Grad_Recover = 0.2[ms]
Grad_Selection = 13C = 2:2:1
Grad_Shape = square
Grad_Type = 0
Initial_Wait = 1[s]
J_Constant = 140[Hz]
Long_Range_J = 8[Hz]
T1 = 1[us]
Unblank_Time = 2[us]

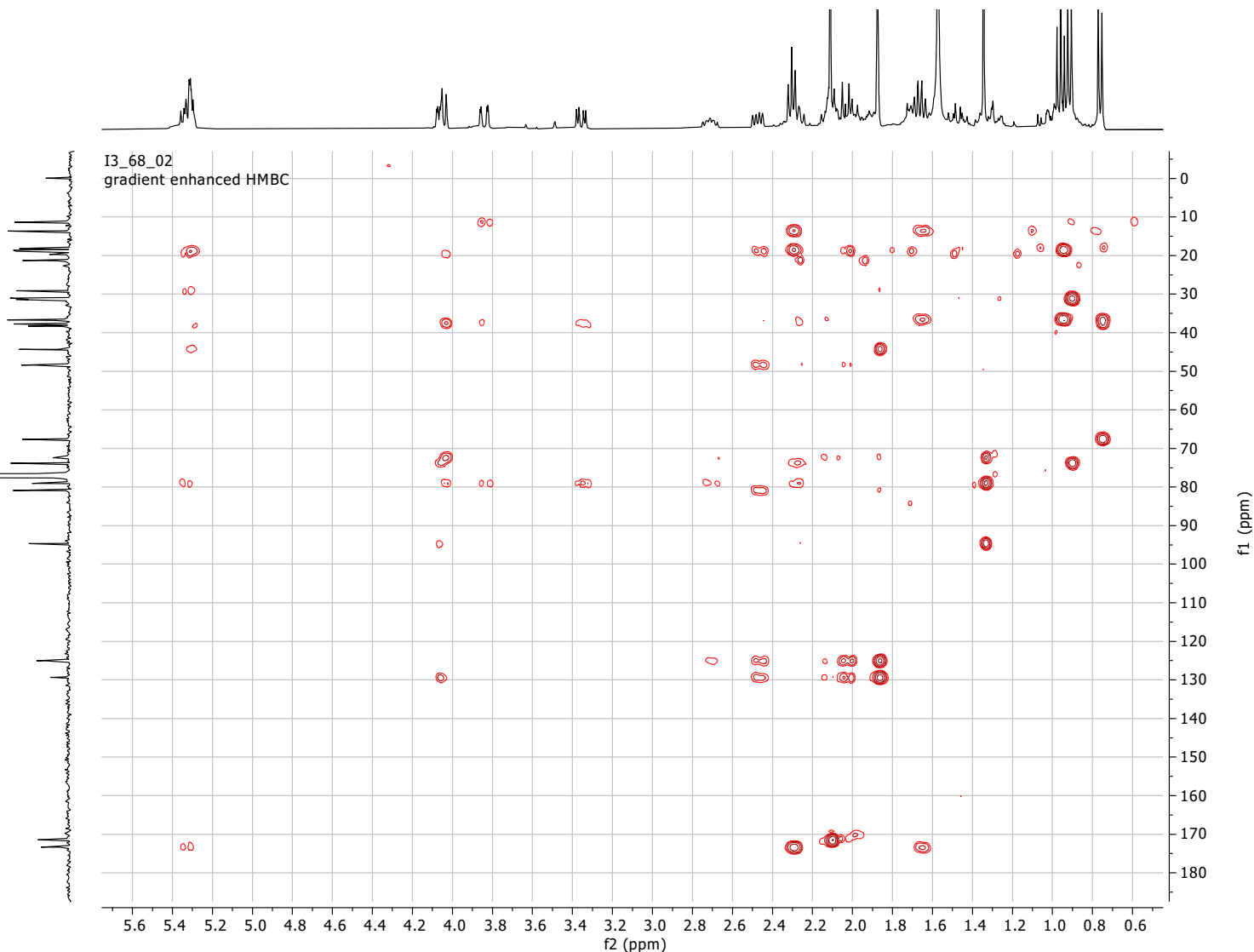


Figure S15. Asbestinin 27, NOE spectra

Irradiation of H-17

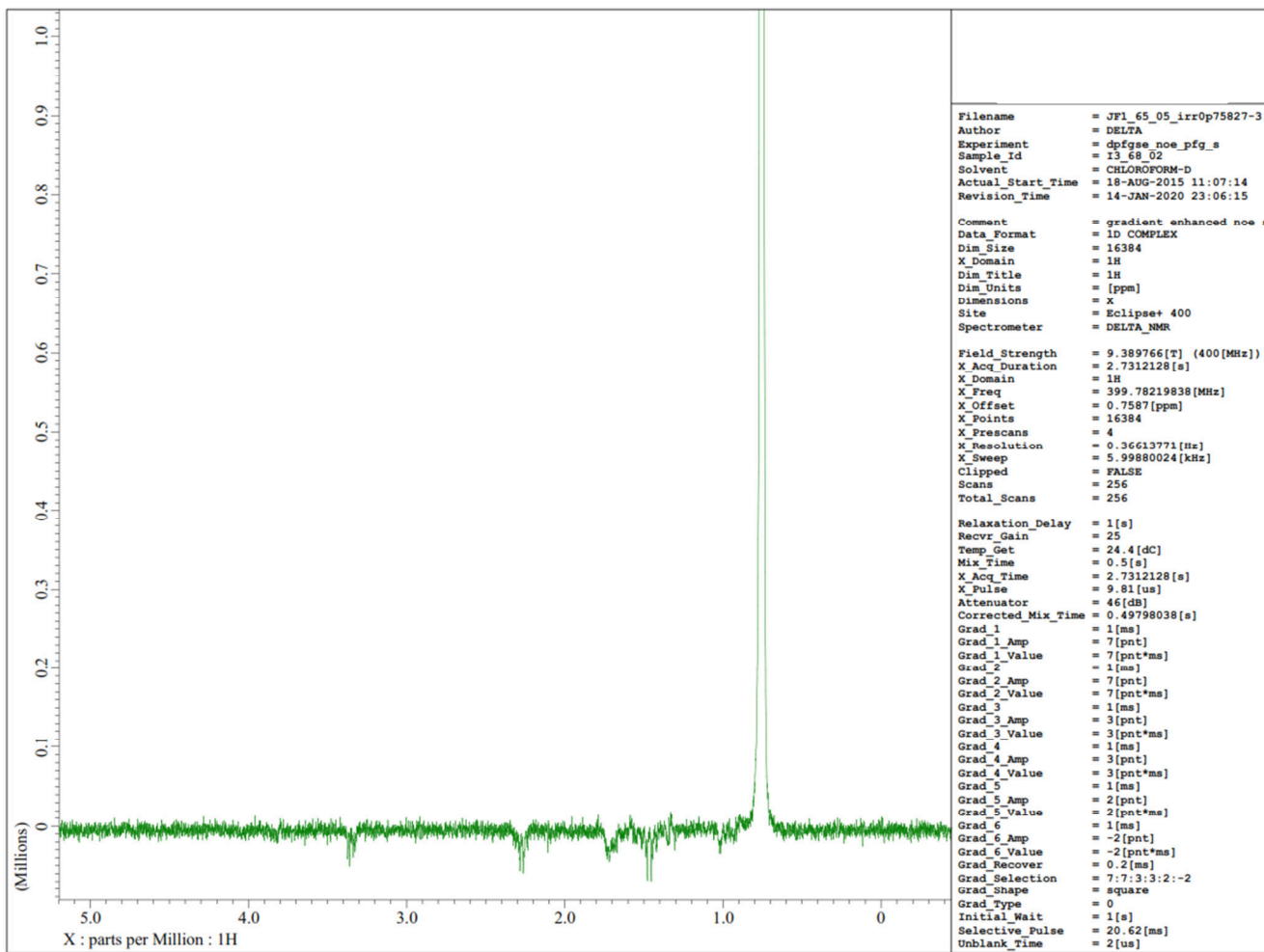


Figure S15. Asbestinin 27, NOE spectra

Irradiation of H-2

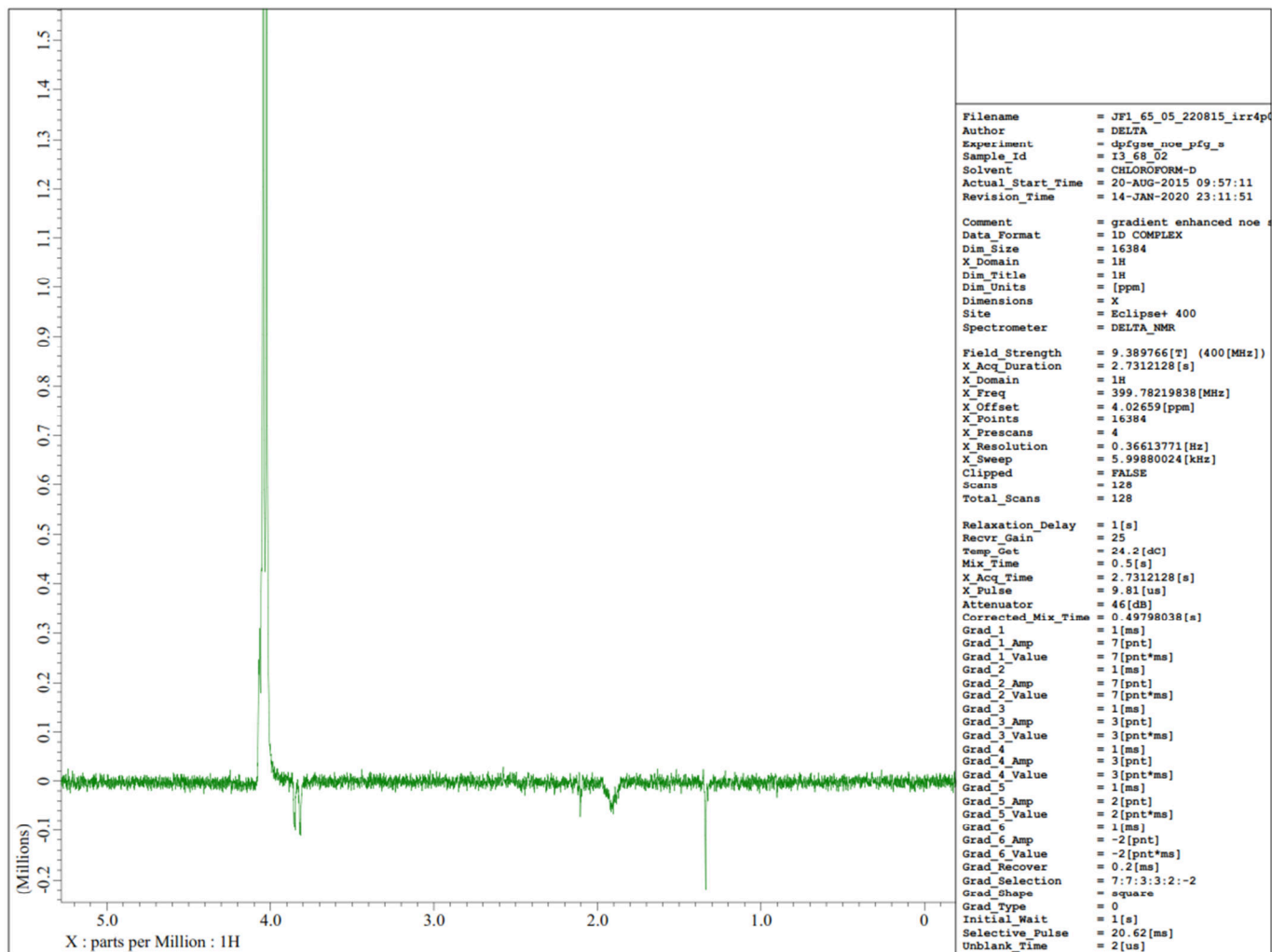


Figure S15. Asbestinin 27, NOE spectra

Irradiation of H-18

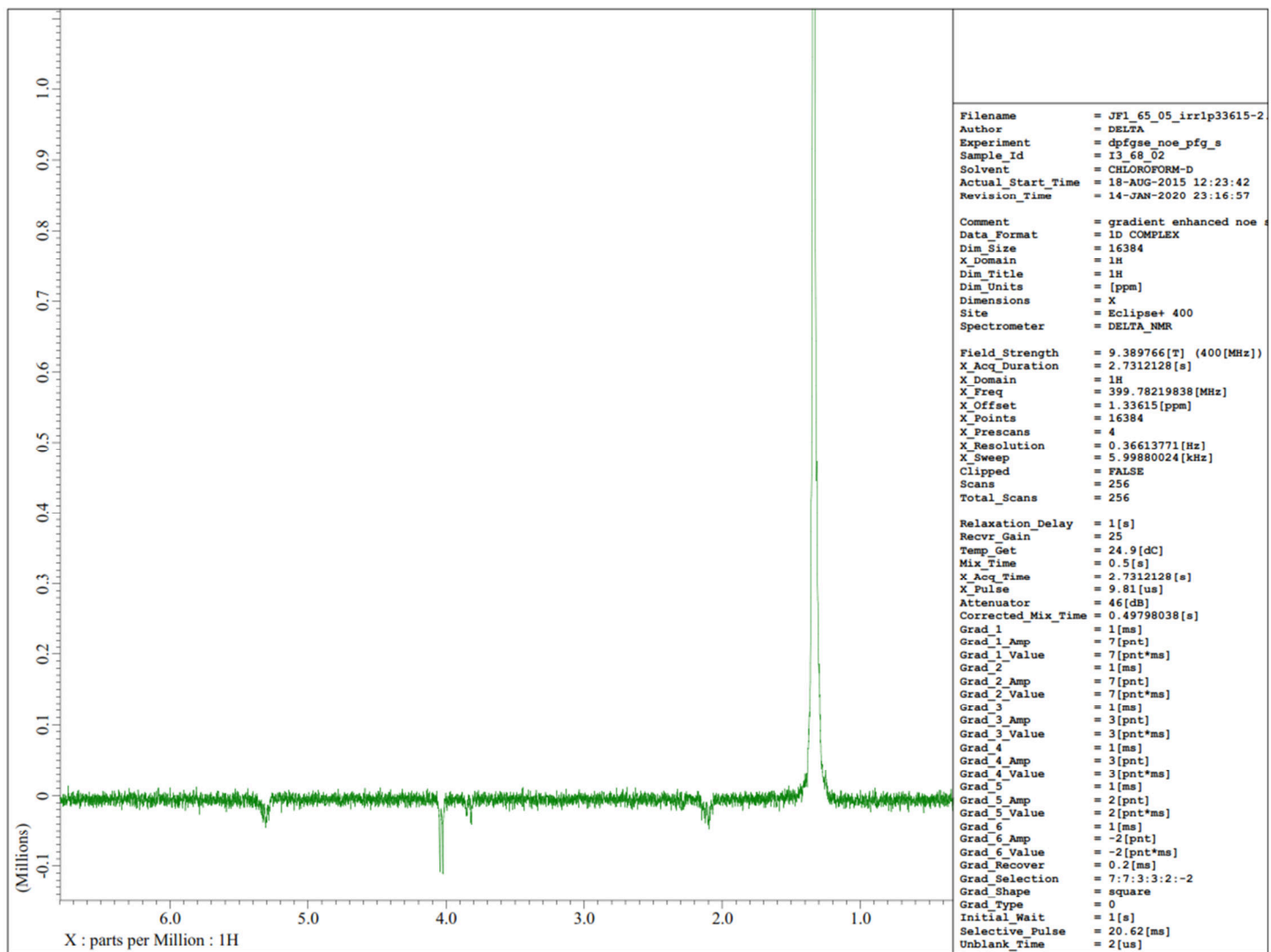


Figure S15. Asbestinin 27, NOE spectra

Irradiation of H-10

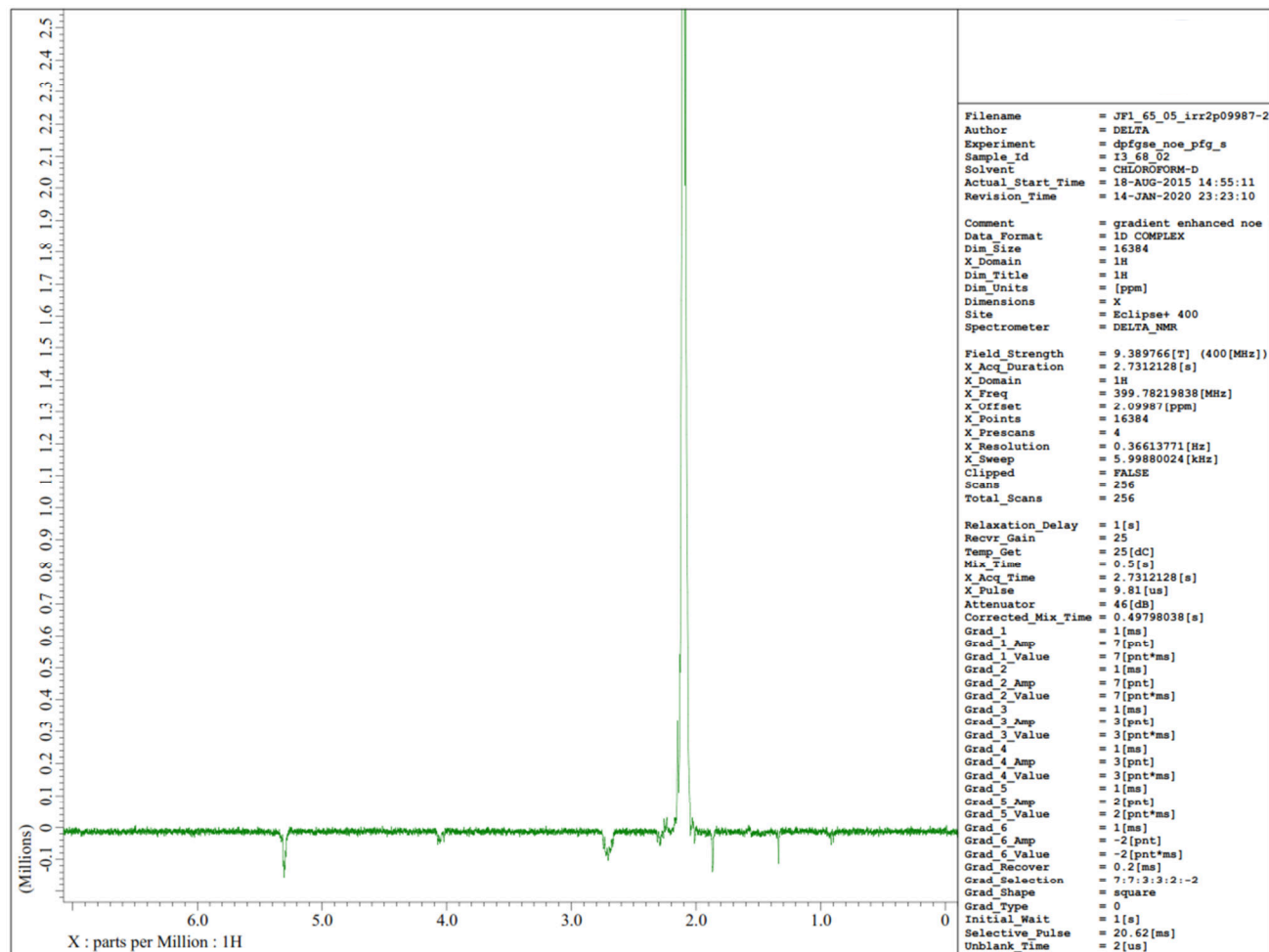


Figure S15. Asbestinin 27, NOE spectra

Irradiation of H-1

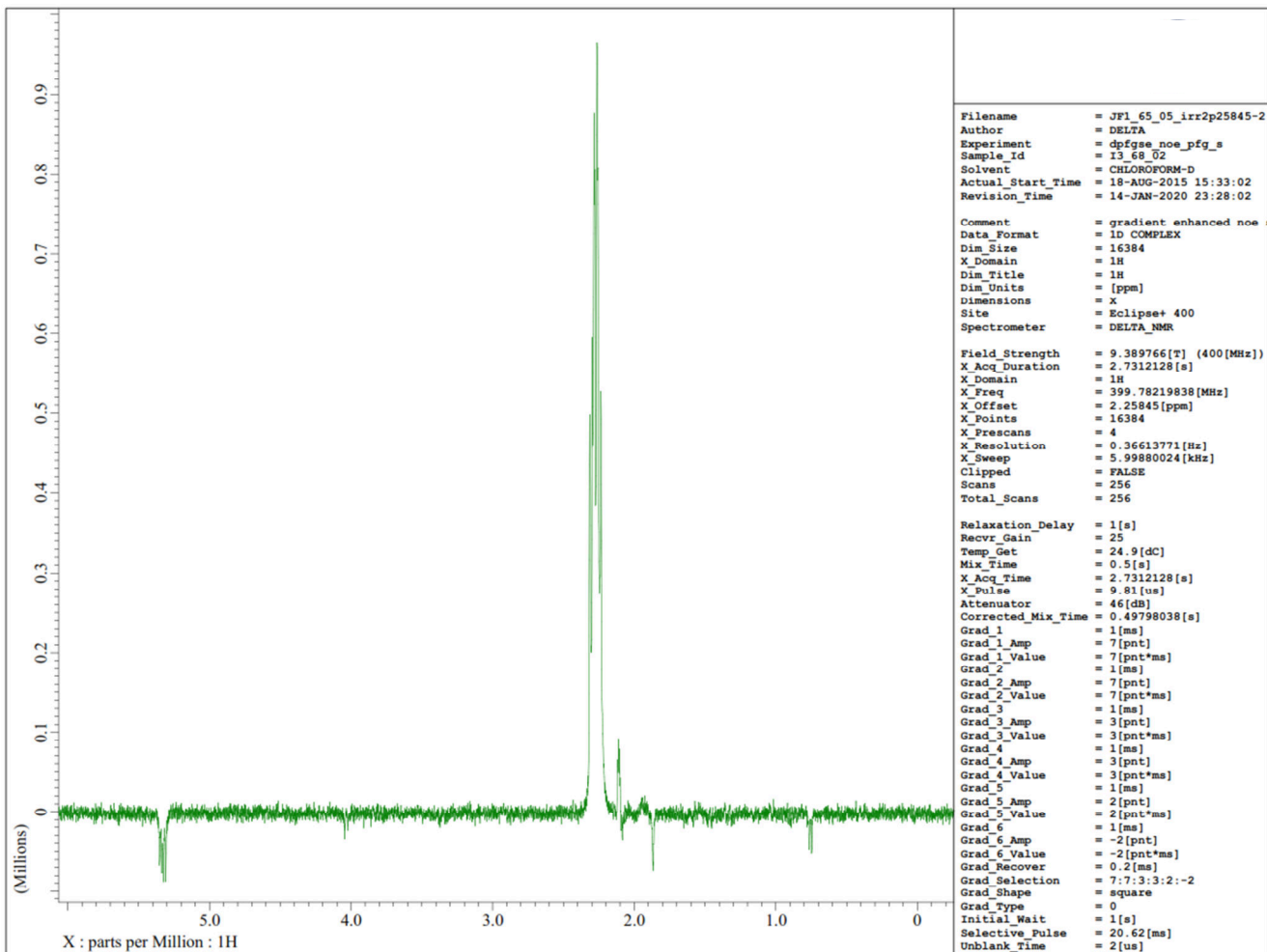


Figure S15. Asbestinin 27, NOE spectra

Irradiation of H-12

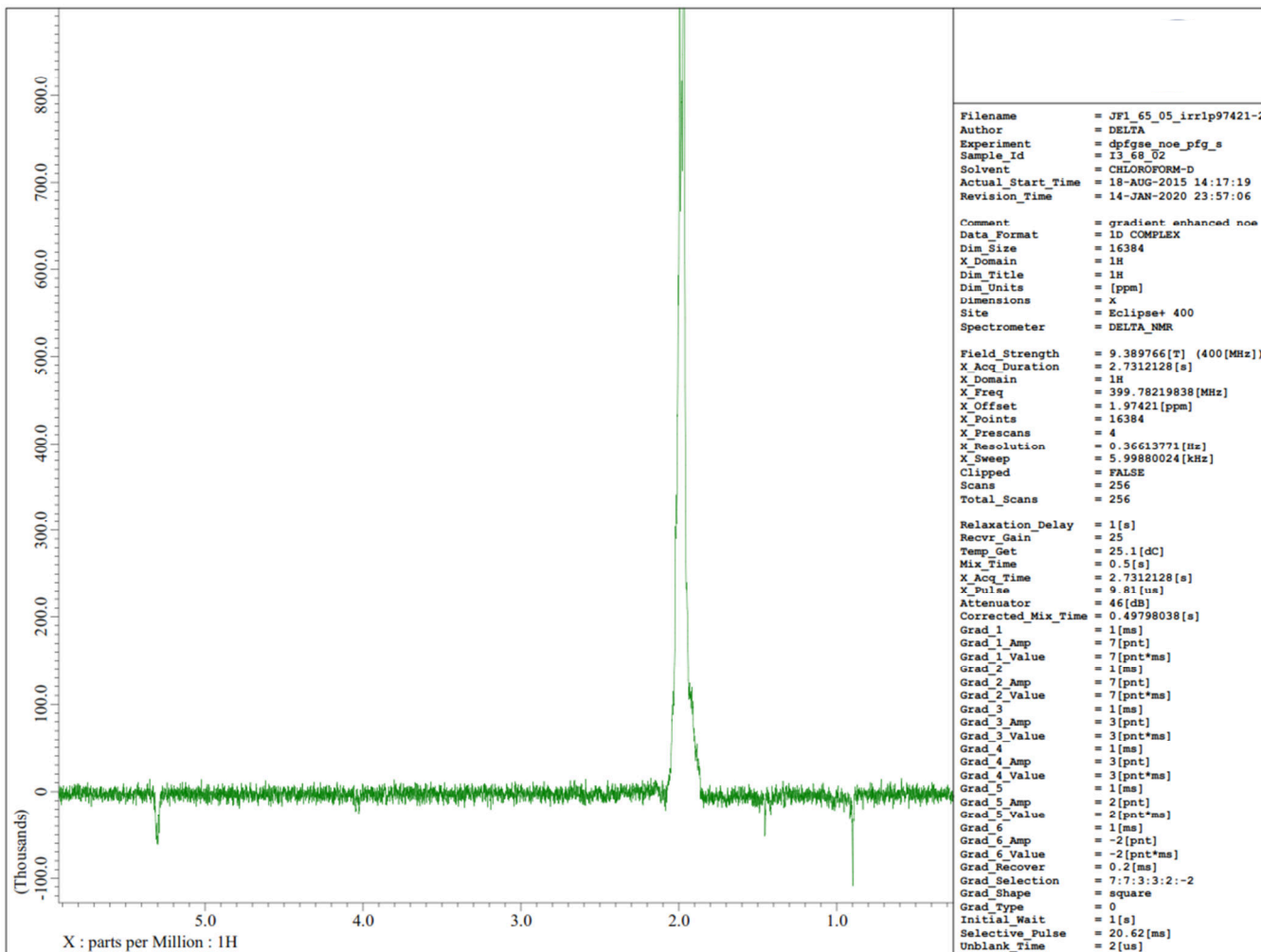


Figure S16. Asbestinin 27, HR-ESITOFMS spectra

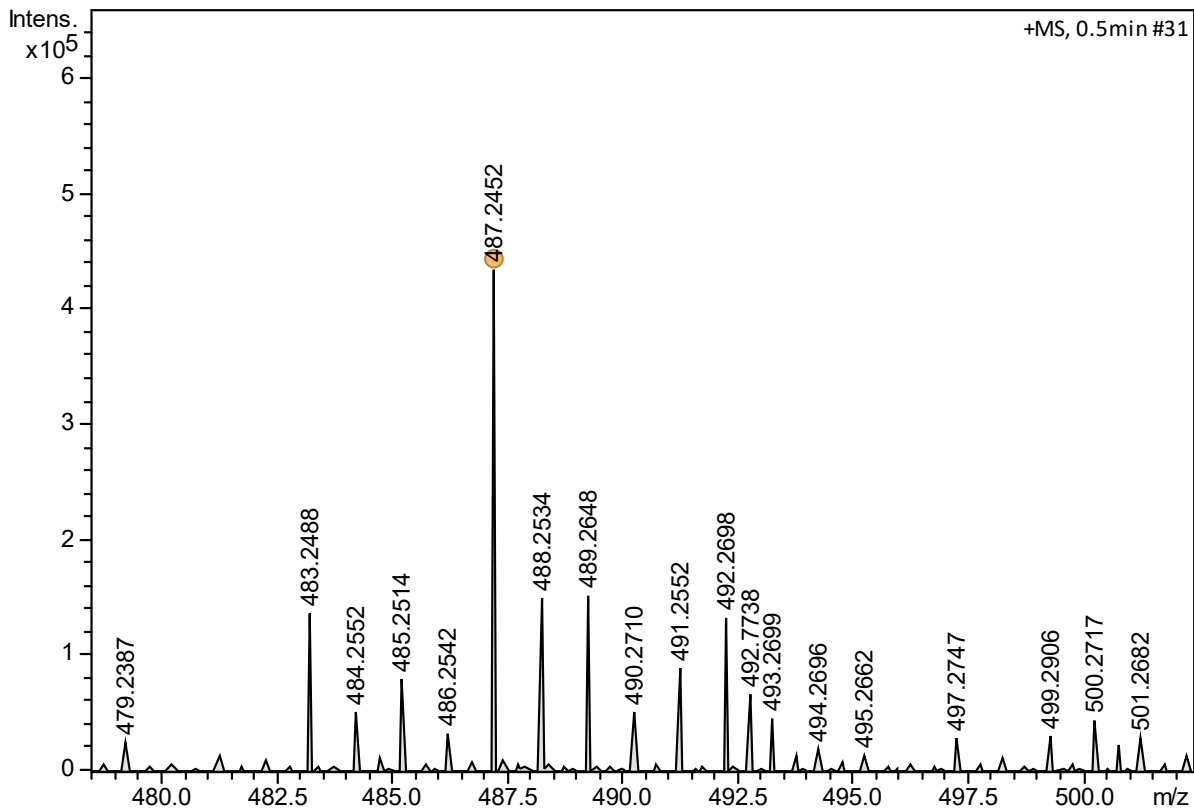


Figure S17. Asbestinin 28, ¹H NMR spectrum

```

Filename      = JF1_65_09-4.jdf
Author       = DELTA
Experiment    = single_pulse.exp
Sample_Id    = I3_62_05
Solvent      = CHLOROFORM-D
Actual_Start_Time = 3-AUG-2015 18:05:47
Revision_Time  = 22-AUG-2015 07:42:29

Comment      = Single Pulse Experiment,
Data_Format  = 1D COMPLEX
Dim_Size     = 16384
X_Domain     = 1H
Dim_Title    = 1H
Dim_Units    = [ppm]
Dimensions   = X
Site         = Eclipse+ 400
Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.048[s]
X_Domain      = 1H
X_Freq       = 399.78219838[MHz]
X_Offset     = 7[ppm]
X_Points     = 16384
X_Prescans   = 0
X_Resolution = 0.48828125[Hz]
X_Sweep      = 8[kHz]
Clipped      = FALSE
Scans        = 8
Total_Scans  = 8

Relaxation_Delay = 4[s]
Recvr_Gain      = 13
Temp_Get       = 24.7[dC]
X_90_Width    = 9.81[us]
X_Acq_Time    = 2.048[s]
X_Angle       = 45[deg]
X_Pulse       = 4.905[us]
Initial_Wait  = 1[s]
Unblank_Time  = 2[us]
    
```

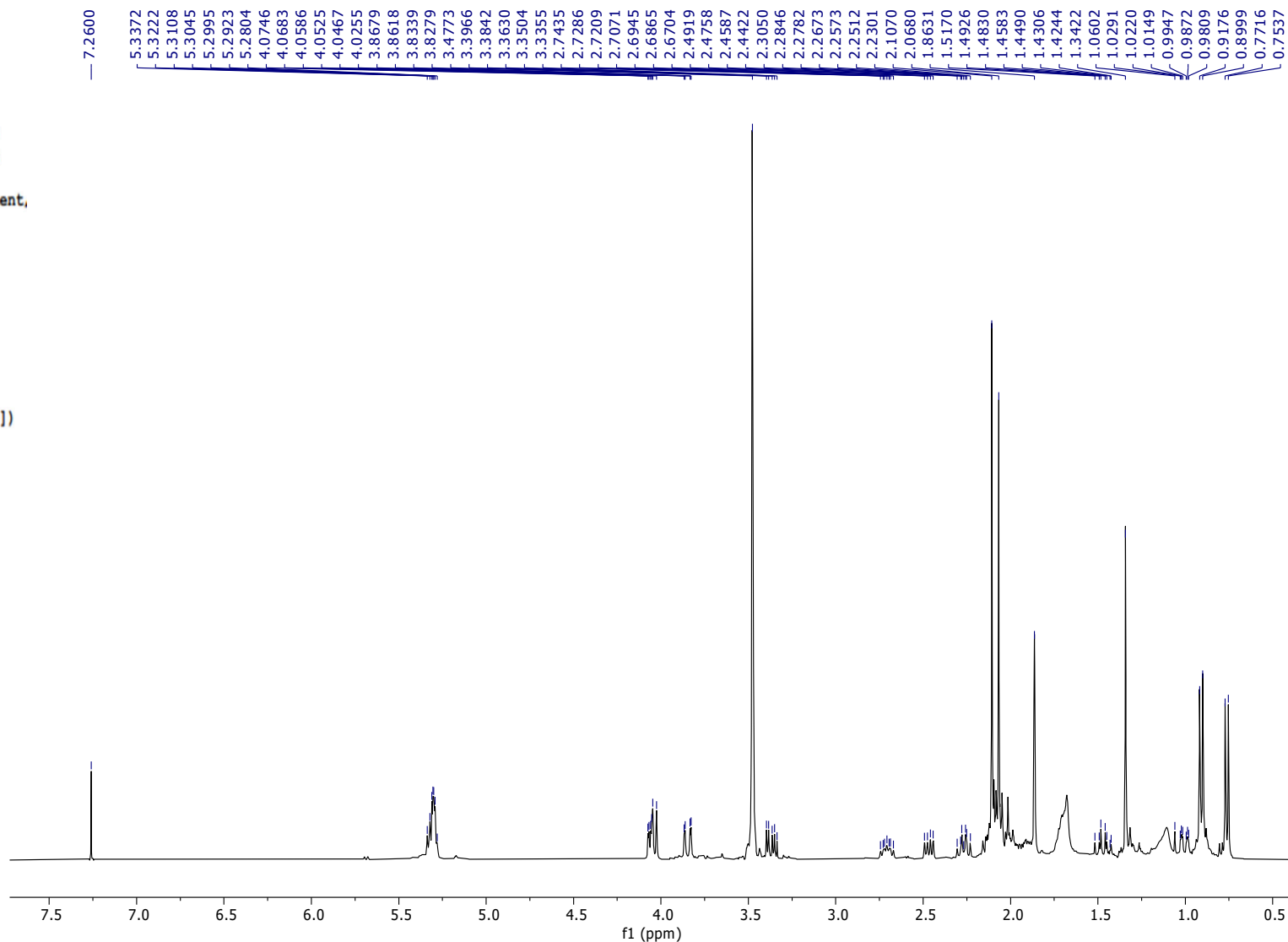


Figure S17. Asbestinin 28, ¹H NMR spectrum (expanded)

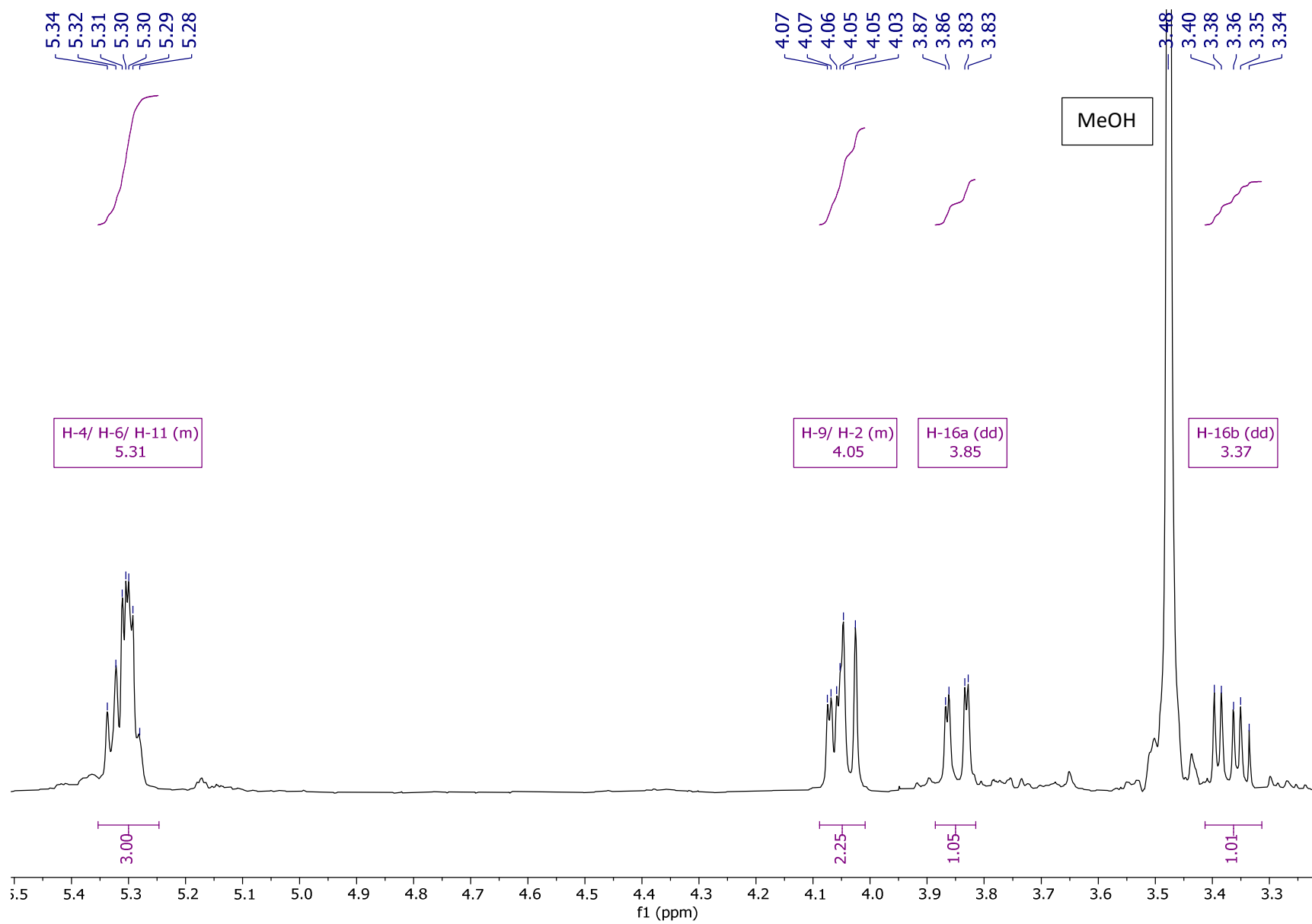


Figure S17. Asbestinin 28, ¹H NMR spectrum (expanded)

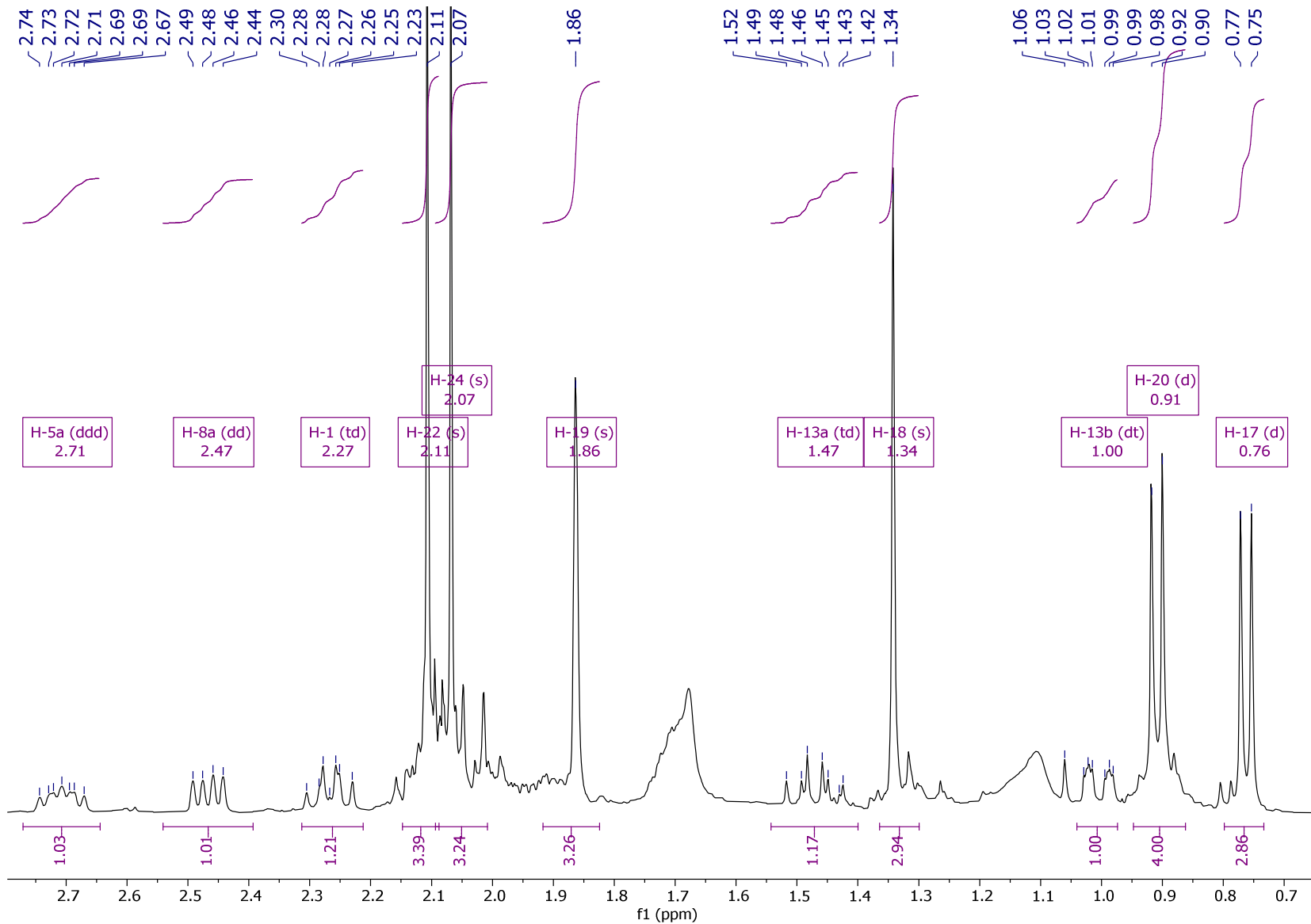


Figure S18. Asbestinin 28, ¹³C NMR spectrum

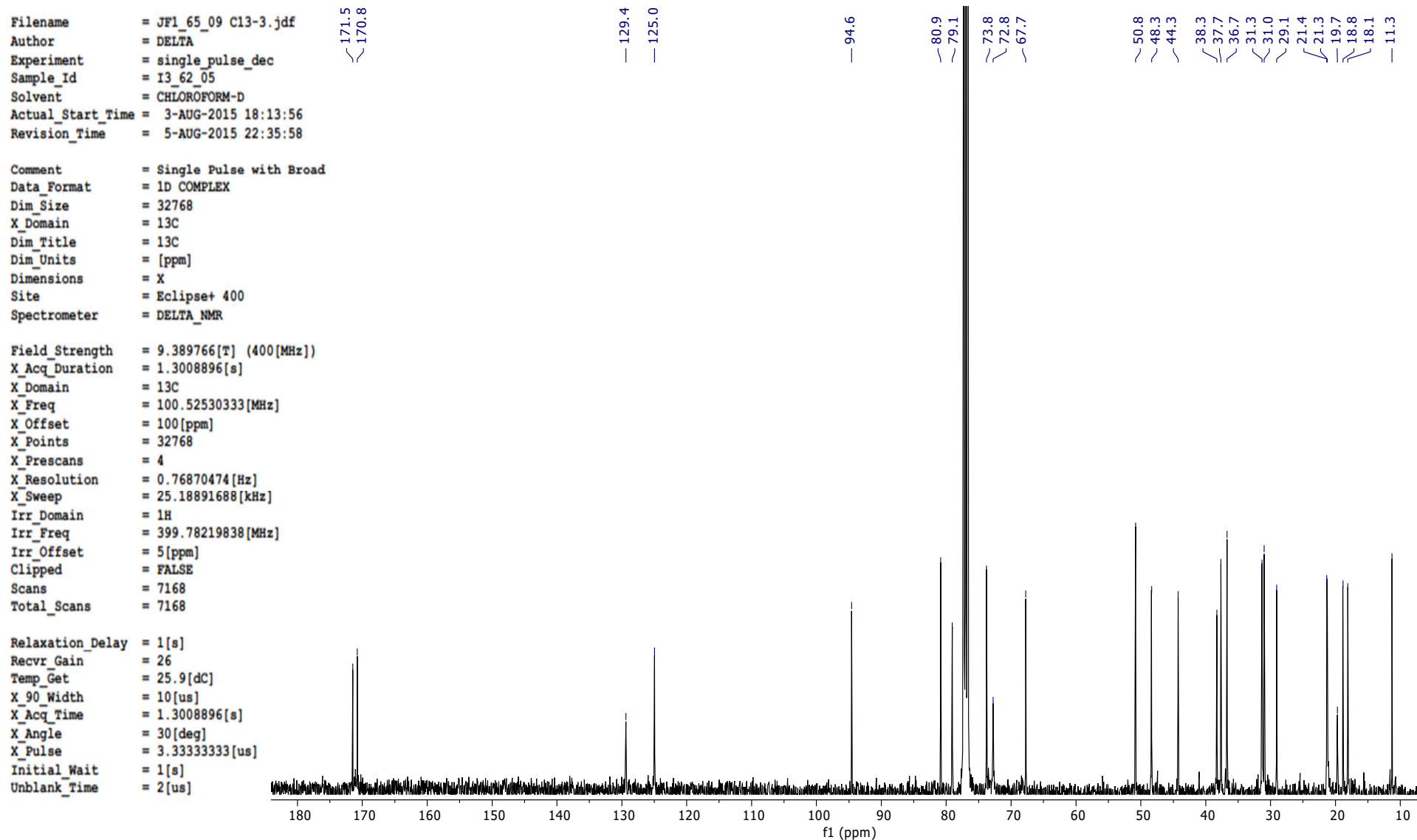


Figure S19. Asbestinin 28, DEPT-135 spectrum

Filename = JF1_65_09 dept135-2.jdf
Author = DELTA
Experiment = dept_dec.exp
Sample_Id = I3_62_05
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-AUG-2015 22:49:50
Revision_Time = 6-AUG-2015 01:26:36

Comment = DEPT with decoupling
Data_Format = 1D COMPLEX
Dim_Size = 32768
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = Eclipse+ 400
Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.3008896[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.76870474[Hz]
X_Sweep = 25.18891688[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 3072
Total_Scans = 3072

Relaxation_Delay = 2[s]
Recvr_Gain = 26
Temp_Get = 24.9[dC]
X_Acq_Time = 1.3008896[s]
X_Pulse = 10[us]
Irr_Pulse = 44.5[us]
Initial_Wait = 1[s]
J_Constant = 140[Hz]
Selection_Angle = 135[deg]
Selection_Pulse = 66.75[us]
Unblank_Time = 2[us]

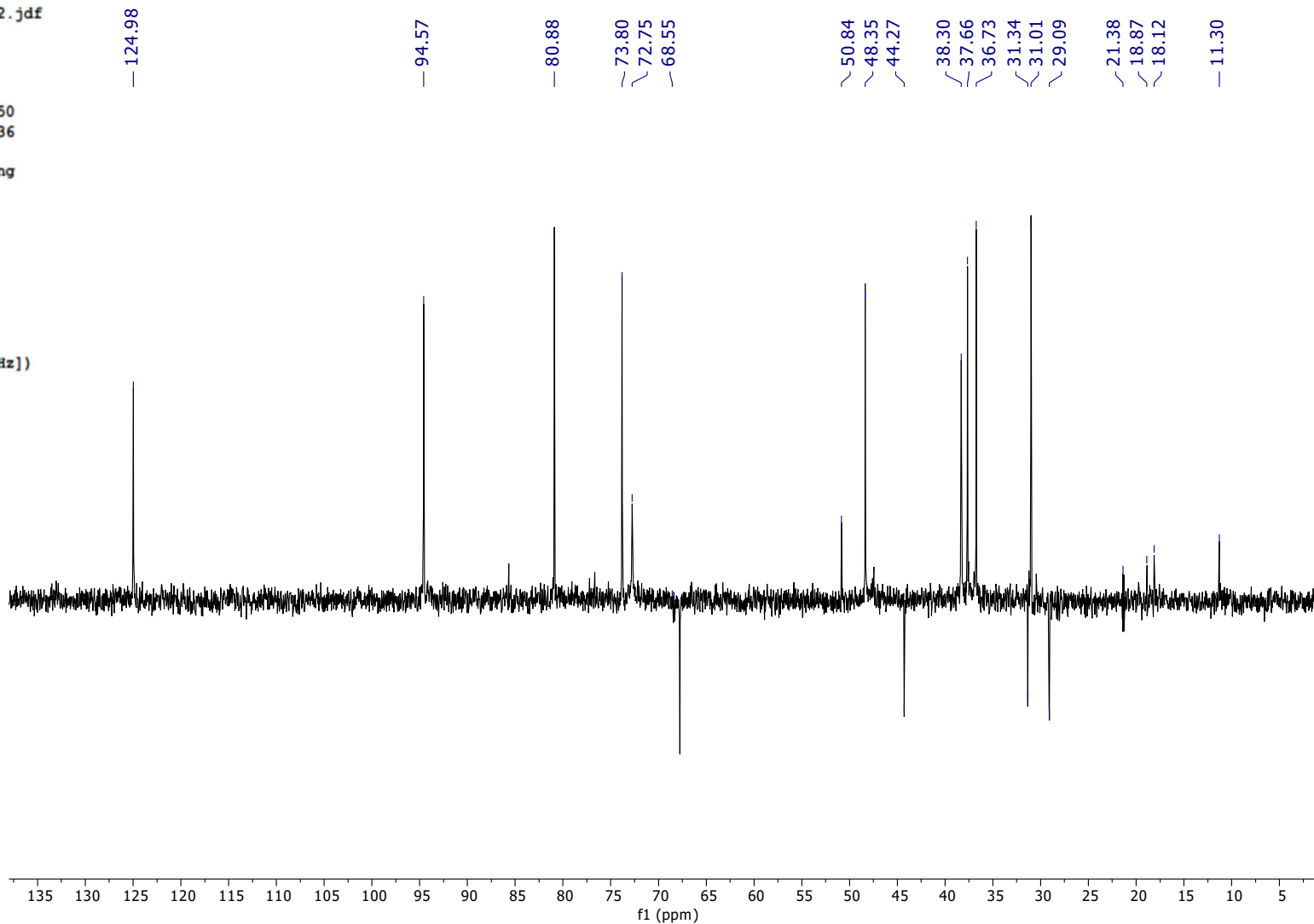


Figure S20. Asbestinin 28, COSY spectrum

Filename = JF1_65_09_pfgcosy-2.jdf
Author = DELTA
Experiment = cosy_pfg_s_exp
Sample_Id = I3_62_05
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-AUG-2015 14:37:02
Revision_Time = 6-AUG-2015 15:54:25

Comment = gradient absolute value
Data_Format = 2D REAL REAL
Dim_Size = 1024, 1024
X_Domain = 1H
Y_Domain = 1H
Dim_Title = 1H 1H
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Site = Eclipse+ 400
Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.2832384[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 3.76611[ppm]
X_Points = 1024
X_Prescans = 4
X_Resolution = 3.53059472[Hz]
X_Sweep = 3.61532899[kHz]
Y_Domain = 1H
Y_Freq = 399.78219838[MHz]
Y_Offset = 3.76611[ppm]
Y_Points = 256
Y_Prescans = 0
Y_Resolution = 14.12237889[Hz]
Y_Sweep = 3.61532899[kHz]
Clipped = TRUE
Scans = 16
Total_Scans = 4096

Relaxation_Delay = 1[s]
Recvr_Gain = 22
Temp_Get = 25.8[dC]
X_90_Width = 9.81[us]
X_Acq_Time = 0.2832384[s]
X_Pulse = 9.81[us]
Y_Acq_Time = 70.8096[ms]
Grad_1 = 1[ms]
Grad_1_Amp = 5[pnt]
Grad_1_Value = 5[pnt*ms]
Grad_2 = 1[ms]
Grad_2_Amp = 5[pnt]
Grad_2_Value = 5[pnt*ms]
Grad_Recover = 1[ms]
Grad_Selection = 1:1
Grad_Shape = square
Grad_Type = 0
Initial_Wait = 0.1[s]
Pulse_1 = 9.81[us]
Pulse_2 = 9.81[us]
Pulse_Angle_1 = 90[deg]
Pulse_Angle_2 = 90[deg]
T1 = 1[us]
Unblank_Time = 2[us]

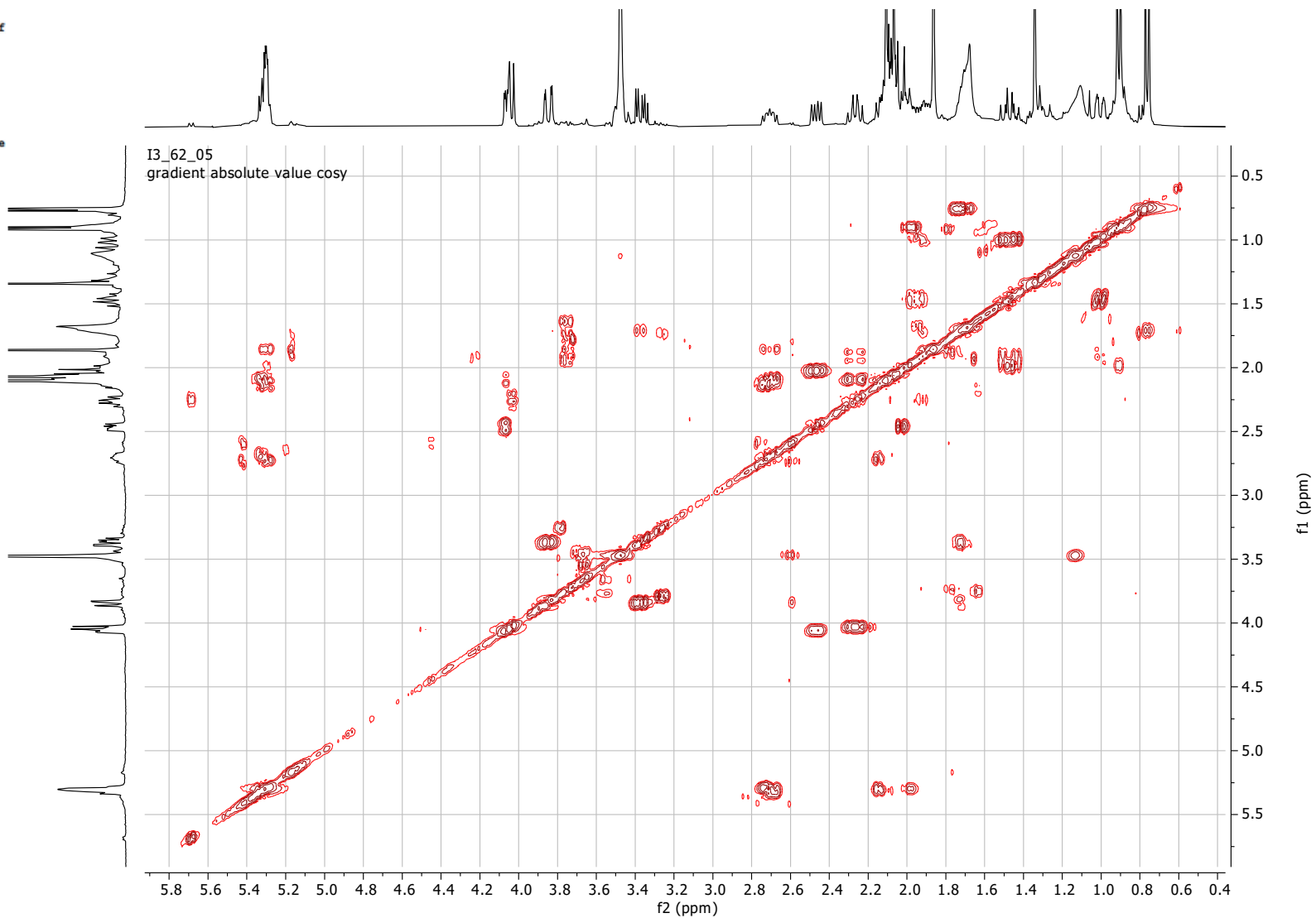


Figure S21. Asbestinin 28, HSQC spectrum

Filename = JF1_65_09 hsqc-4.jdf
Author = DELTA
Experiment = multiplicity_hsqc
Sample_Id = I3_62_05
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-AUG-2015 04:31:29
Revision_Time = 21-AUG-2015 06:18:42

Comment = Multiplicity HSQC
Data_Format = 2D COMPLEX COMPLEX
Dim_Size = 1024, 512
X_Domain = 1H
Y_Domain = 13C
Dim_Title = 1H 13C
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Site = Eclipse+ 400
Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.2832384[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 3.76611[ppm]
X_Points = 1024
X_Prescans = 4
X_Resolution = 3.53059472[Hz]
X_Sweep = 3.61532899[kHz]
Y_Domain = 13C
Y_Freq = 100.52530333[MHz]
Y_Offset = 100[ppm]
Y_Points = 256
Y_Prescans = 0
Y_Resolution = 98.64267677[Hz]
Y_Sweep = 25.25252525[kHz]
Clipped = FALSE
Scans = 8
Total_Scans = 2048

Relaxation_Delay = 2[s]
Recvr_Gain = 30
Temp_Get = 24.1[dC]
X_Acq_Time = 0.2832384[s]
X_Pulse = 9.81[us]
Y_Acq_Time = 10.1376[ms]
Y_Pulse = 12[us]
Enhance_Temp = 12
Enhancement = 1/6J
Grad_1 = 1[ms]
Grad_1_Amp = 4[pnt]
Grad_1_Value = 4[pnt*ms]
Grad_2 = 1[ms]
Grad_2_Amp = -1[pnt]
Grad_2_Value = -1[pnt*ms]
Grad_3 = 1[ms]
Grad_3_Amp = 1[pnt]
Grad_Recover = 0.1[ms]
Grad_Selection = 13C = 4:1
Grad_Shape = square
Grad_Type = 0
Initial_Wait = 1[s]
J_Constant = 140[Hz]
T1 = 1[us]
Tau = 0.5952381[ms]

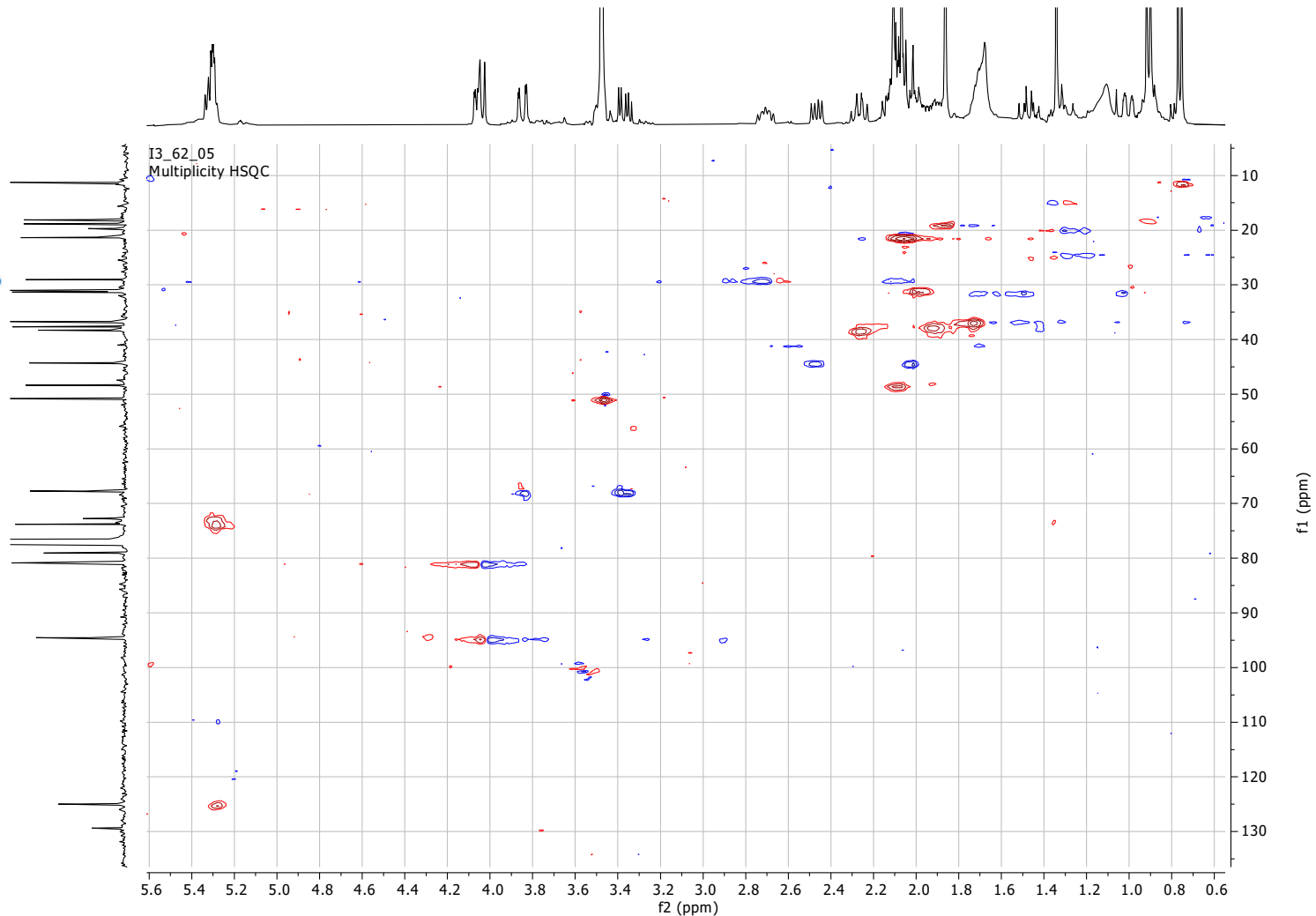


Figure S22. Asbestinin 28, HMBC spectrum

Filename = JF1_65_09_210815_hmbc-3
 Author = DELTA
 Experiment = hmbc_pfg_s.exp
 Sample_Id = I3_68_06
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 19-AUG-2015 15:04:21
 Revision_Time = 22-AUG-2015 01:38:21

Comment = gradient enhanced HMBC
 Data_Format = 2D REAL REAL
 Dim_Size = 1024, 512
 X_Domain = 1H
 Y_Domain = 13C
 Dim_Title = 1H 13C
 Dim_Units = [ppm] [ppm]
 Dimensions = X Y
 Site = Eclipse+ 400
 Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 0.2961408[s]
 X_Domain = 1H
 X_Freq = 399.78219838[MHz]
 X_Offset = 3.59946[ppm]
 X_Points = 1024
 X_Prescans = 4
 X_Resolution = 3.37677213[Hz]
 X_Sweep = 3.45781466[kHz]
 Y_Domain = 13C
 Y_Freq = 100.52530333[MHz]
 Y_Offset = 100[ppm]
 Y_Points = 256
 Y_Prescans = 0
 Y_Resolution = 98.64267677[Hz]
 Y_Sweep = 25.25252525[kHz]
 Clipped = FALSE
 Scans = 64
 Total_Scans = 16384

Relaxation_Delay = 2[s]
 Recvr_Gain = 30
 Temp_Get = 23.5[dC]
 X_Acq_Time = 0.2961408[s]
 X_Pulse = 9.81[us]
 Y_Acq_Time = 10.1376[ms]
 Y_Pulse = 12[us]
 Grad_1 = 1[ms]
 Grad_1_Amp = 10[pnt]
 Grad_1_Value = 10[pnt*ms]
 Grad_2 = 1[ms]
 Grad_2_Amp = 10[pnt]
 Grad_2_Value = 10[pnt*ms]
 Grad_3 = 1[ms]
 Grad_3_Amp = 5[pnt]
 Grad_3_Value = 5[pnt*ms]
 Grad_Recover = 0.2[ms]
 Grad_Selection = 13C = 2:2:1
 Grad_Shape = square
 Grad_Type = 0
 Initial_Wait = 1[s]
 J_Constant = 140[Hz]
 Long_Range_J = 8[Hz]
 T1 = 1[us]
 Unblank_Time = 2[us]

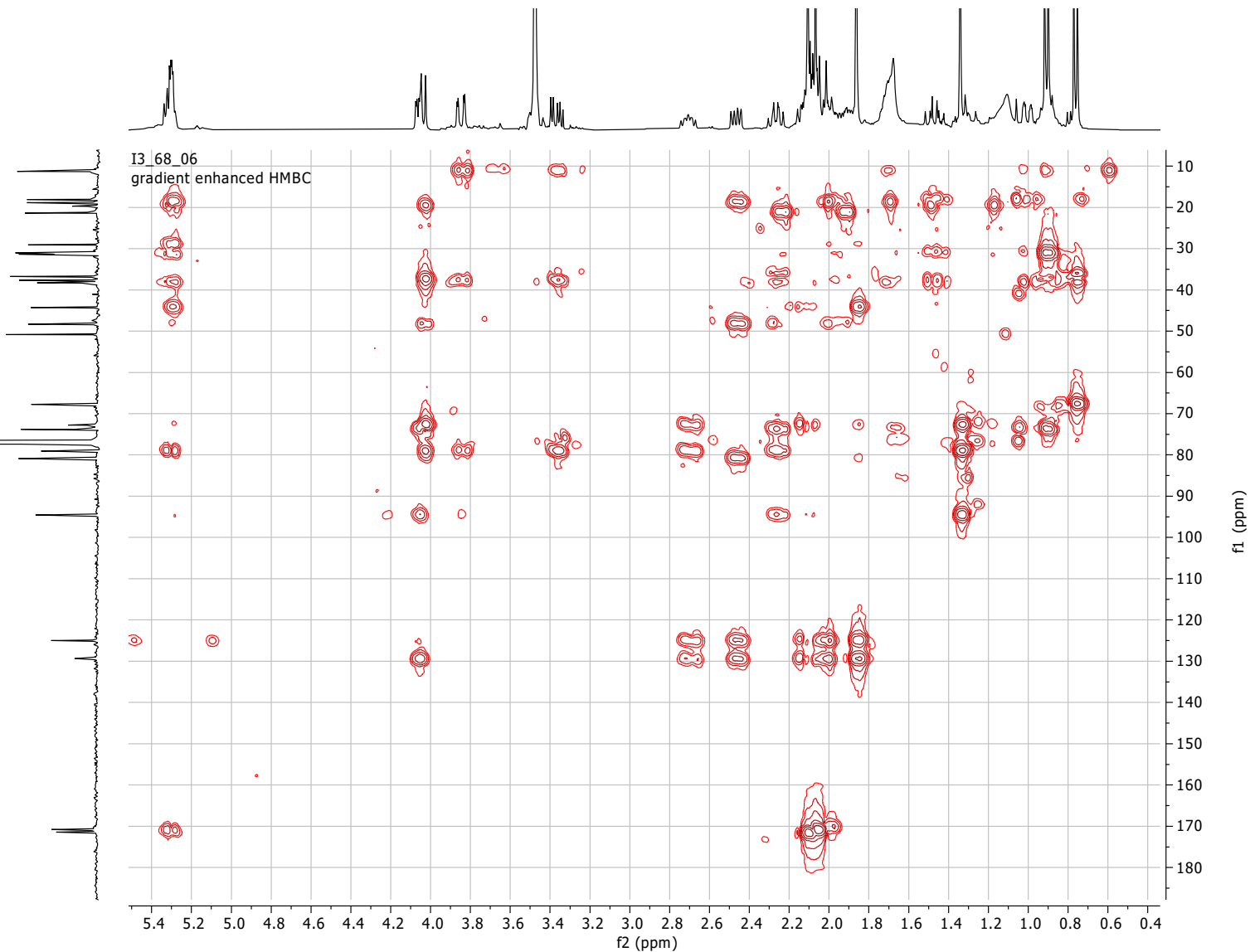


Figure S23. Asbestinin 28, NOE spectra

Irradiation of Proton H-17

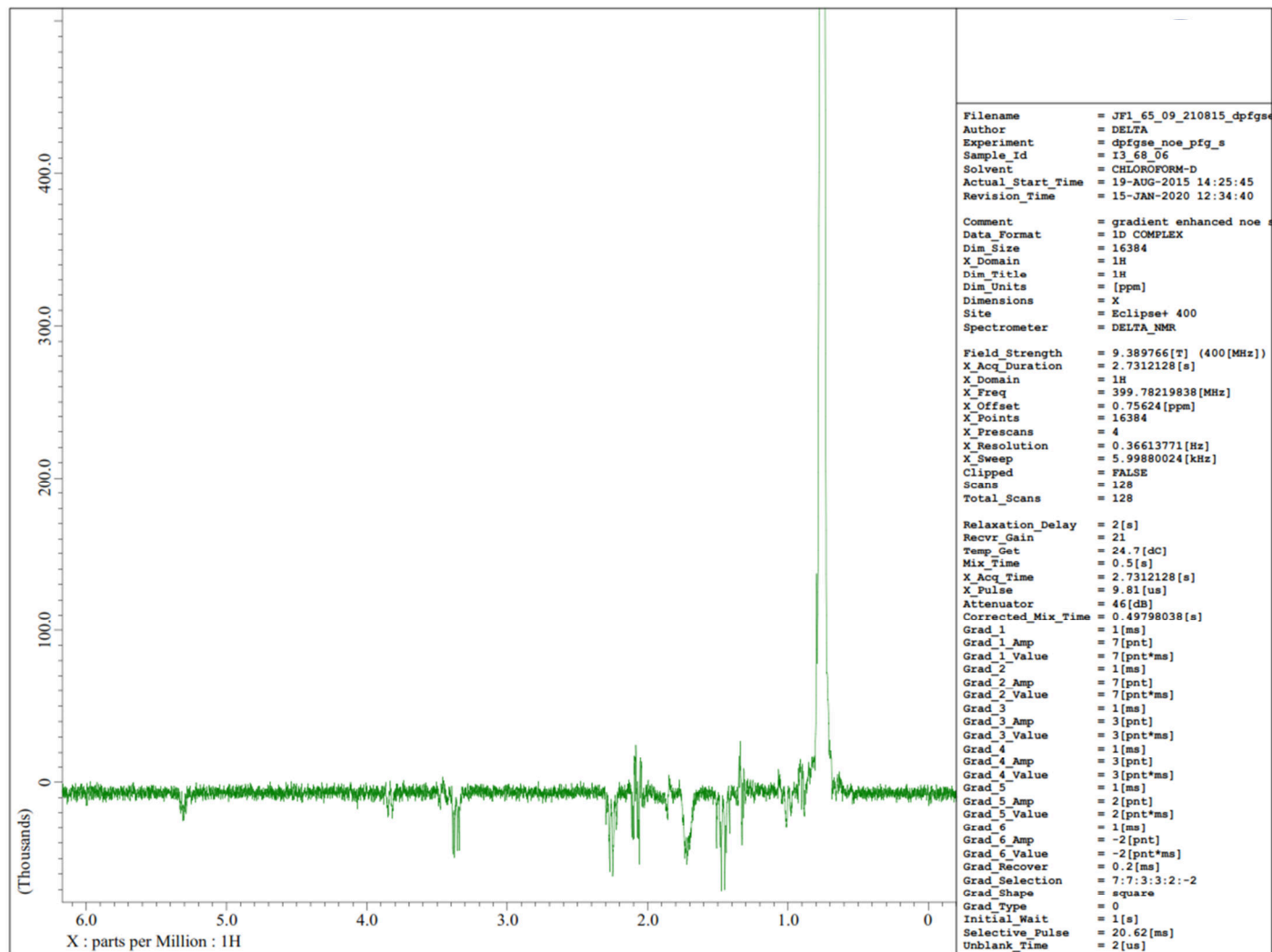


Figure S23. Asbestinin 28, NOE spectra

Irradiation of Proton H-18

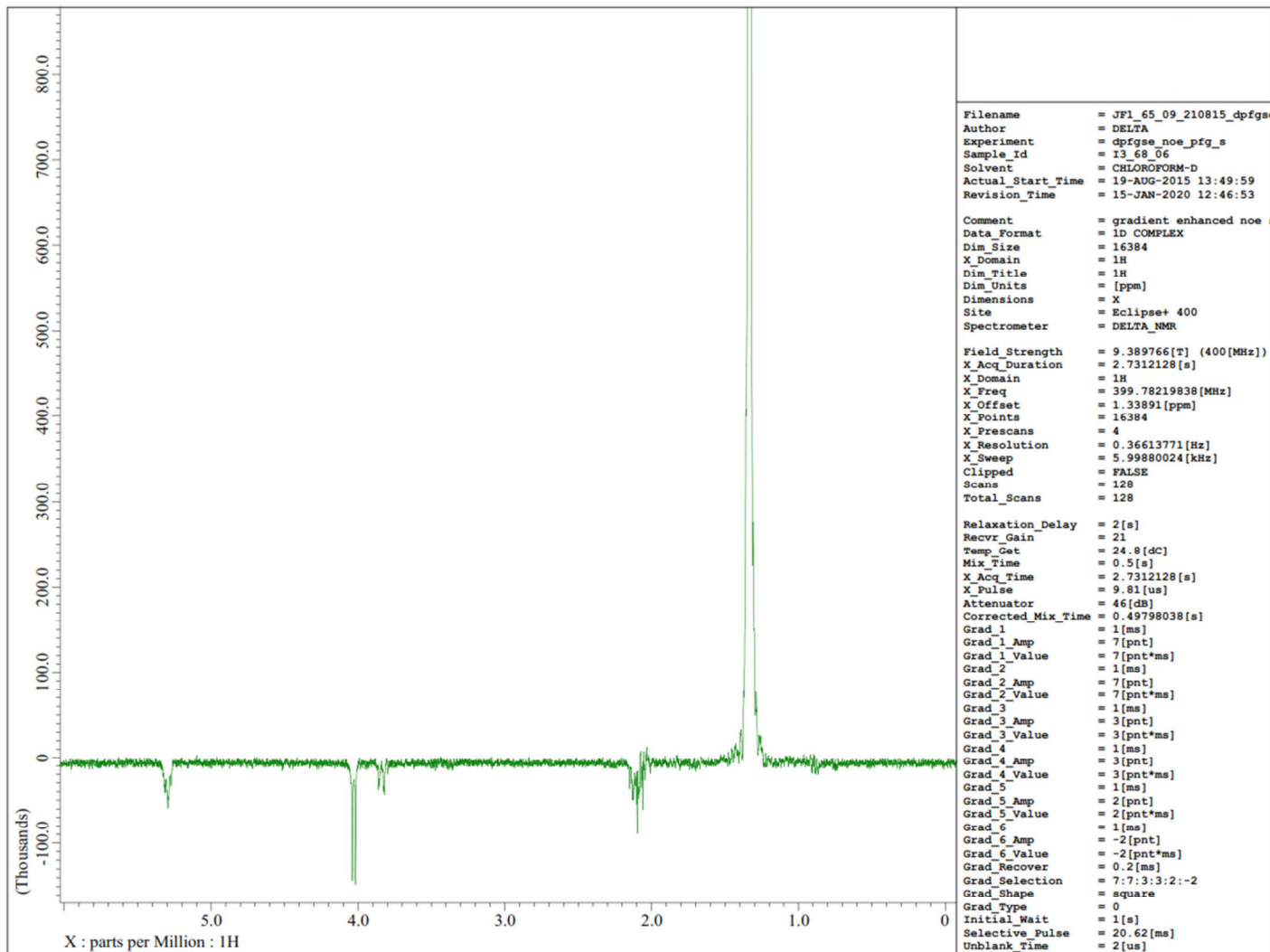


Figure S23. Asbestinin 28, NOE spectra

Irradiation of Proton H-19

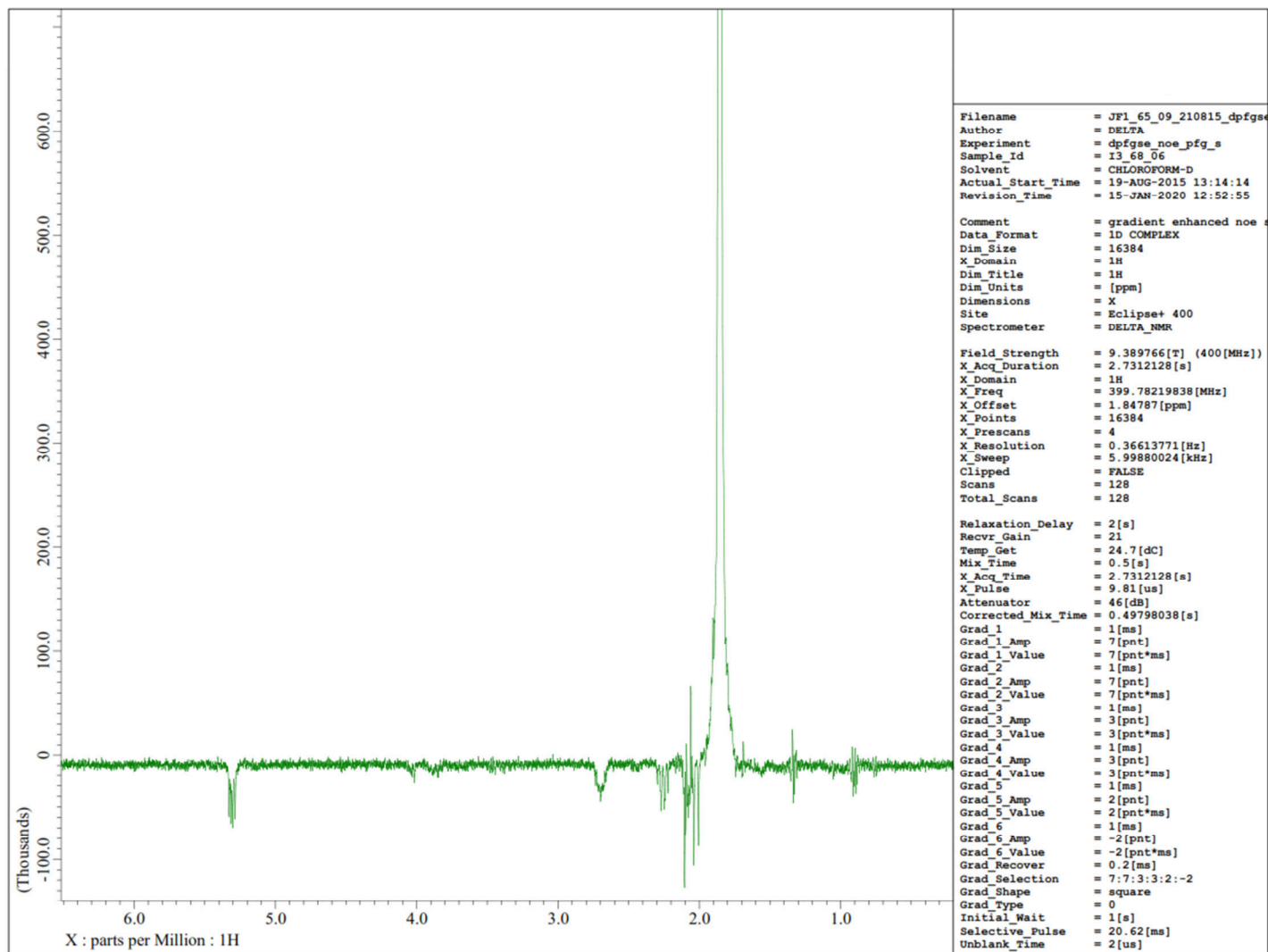


Figure S23. Asbestinin 28, NOE spectra

Irradiation of Proton H-14

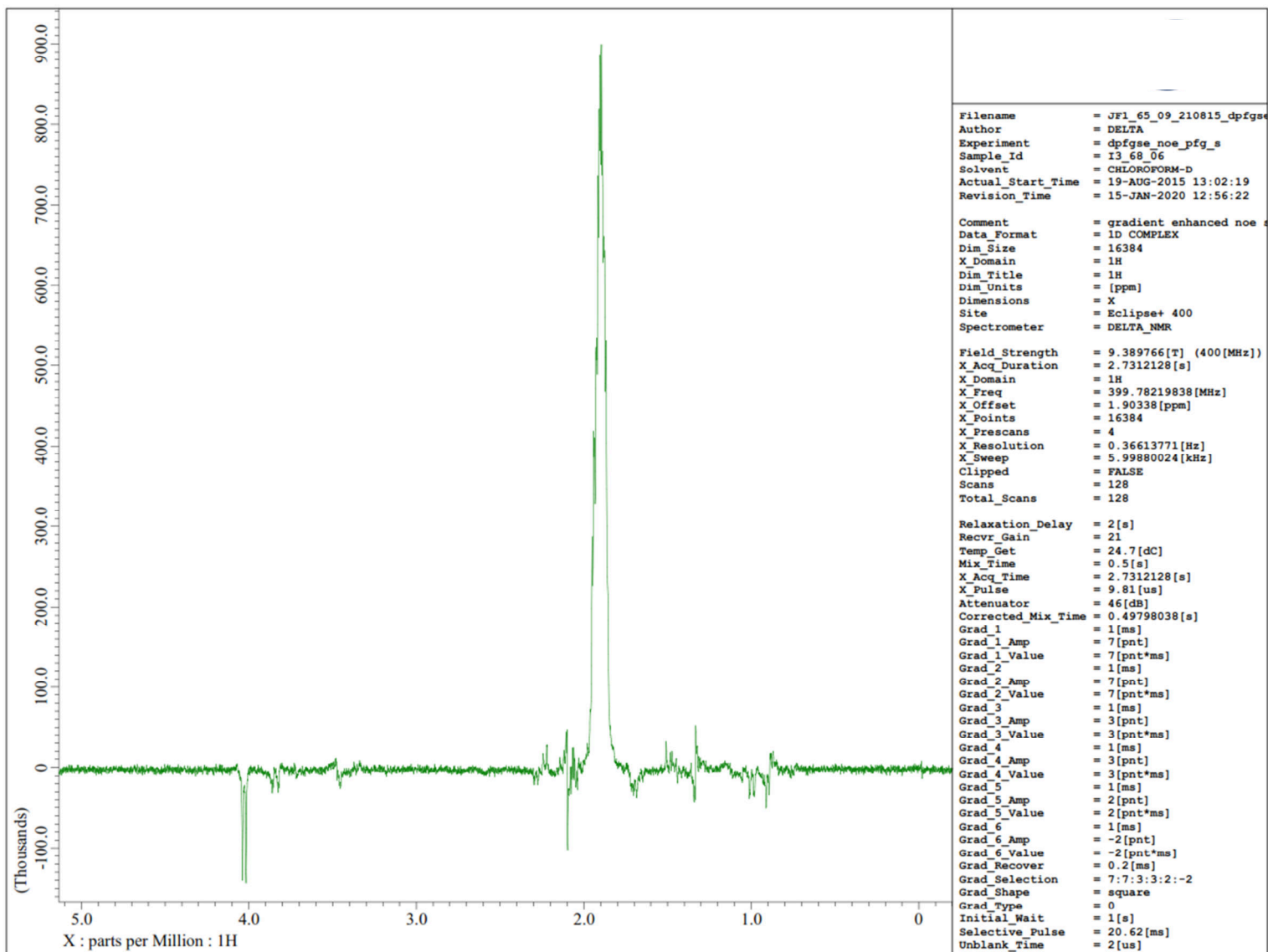


Figure S23. Asbestinin 28, NOE spectra

Irradiation of Proton H-1

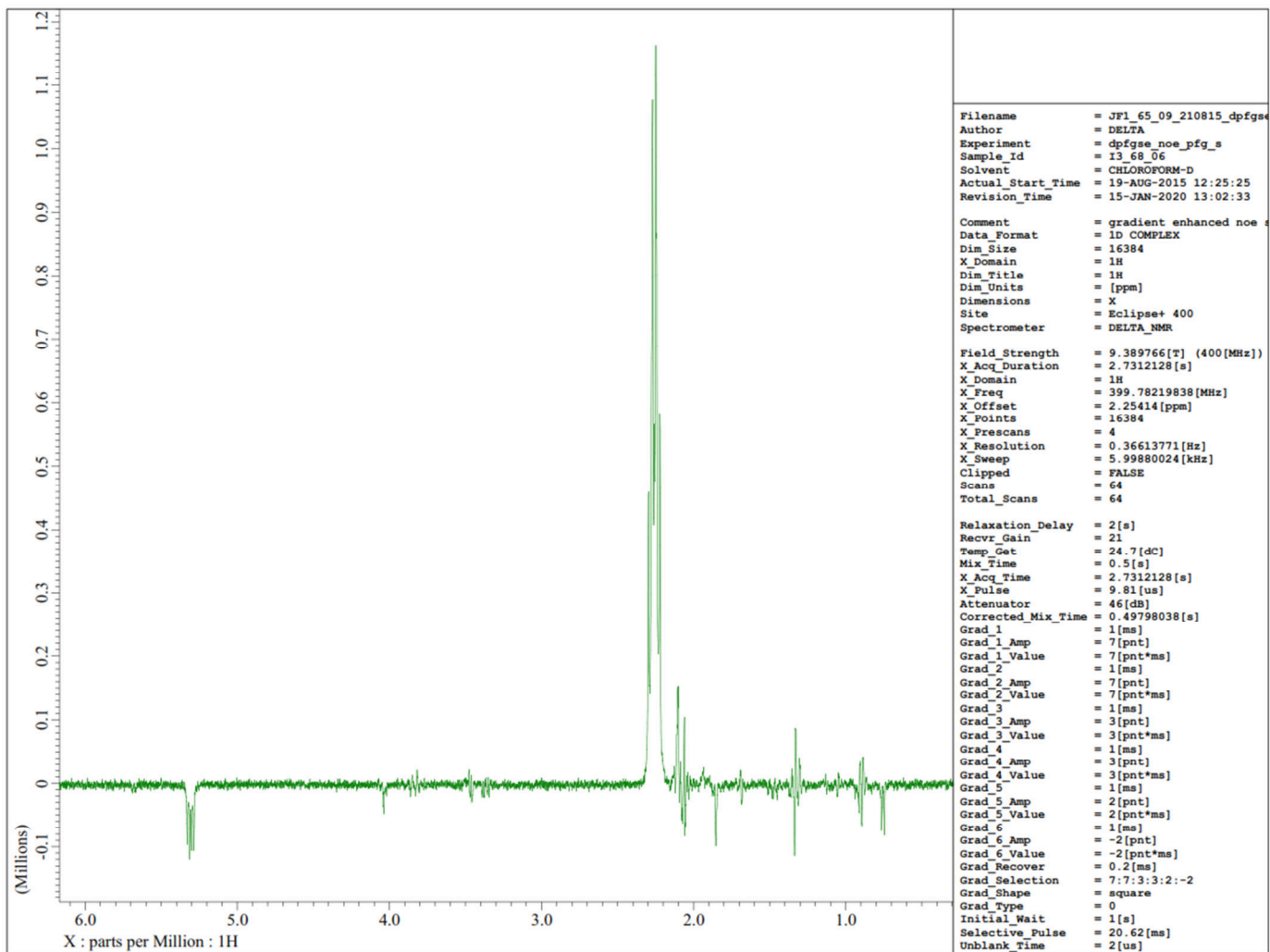


Figure S23. Asbestinin 28, NOE spectra

Irradiation of Proton H-2

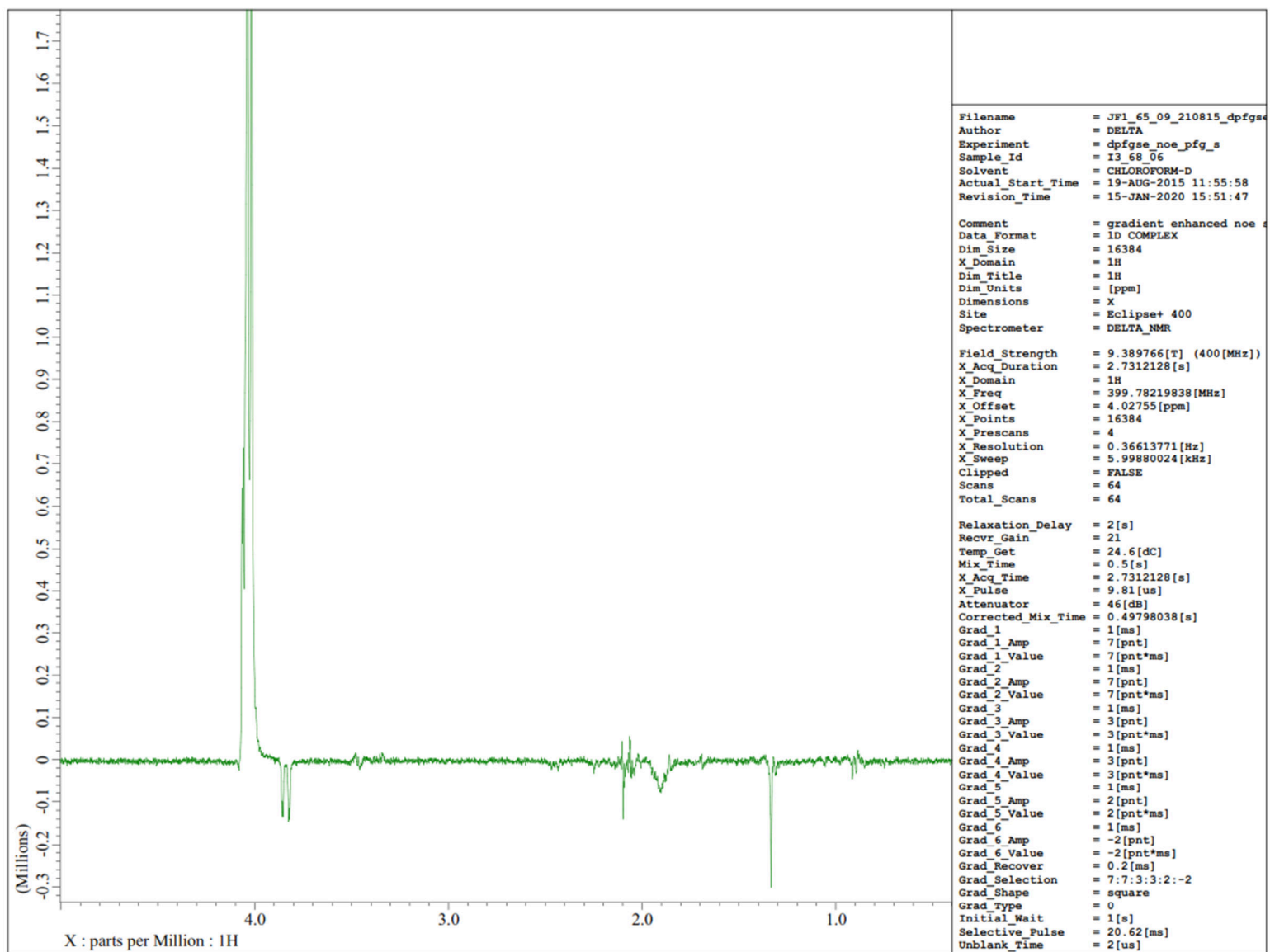


Figure S23. Asbestinin 28, NOE spectra

Irradiation of Proton H-9

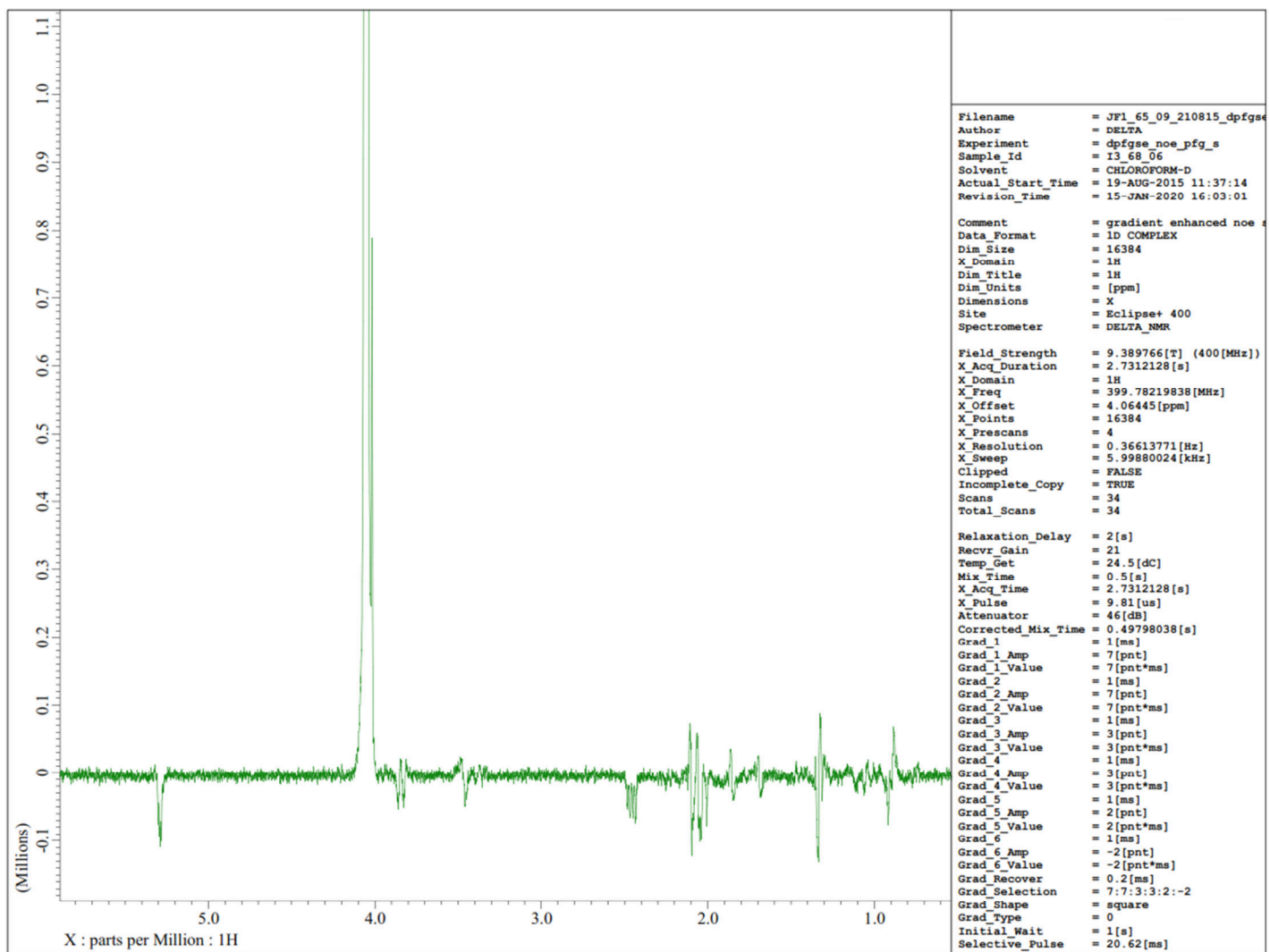


Figure S24. Asbestinin 28, HR-ESITOFMS spectrum

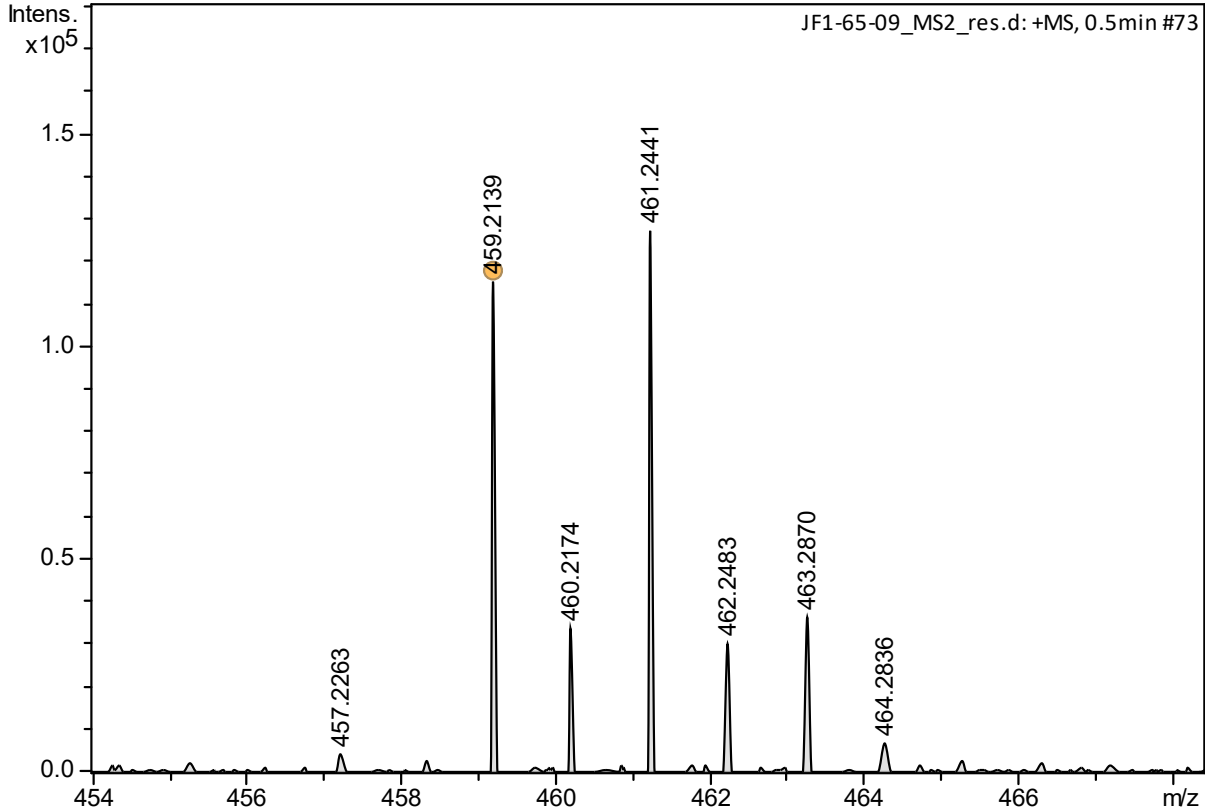


Table S1. Viability of THP-1 human macrophages treated with different concentrations of diterpenes. Values are mean \pm SEM (%) of three independent experiments in duplicate (n = 3).

	% Viability THP-1 macrophages (24 h)				
(μ M)	10	20	50	100	IC ₅₀
Briarellin T (1)	99.5 \pm 2.0	98.5 \pm 1.2	101.4 \pm 0.5	98.5 \pm 1.0	> 100
Asbestinin 27 (2)	100.5 \pm 1.3	99.5 \pm 0.9	98.6 \pm 2.1	97.4 \pm 1.1	> 100
Asbestinin 28 (3)	98.5 \pm 3.1	99.1 \pm 1.4	97.0 \pm 1.0	99.5 \pm 2.0	> 100
Asbestinin 17 (4)	102.2 \pm 1.5	100.5 \pm 0.8	98.0 \pm 2.0	99.5 \pm 1.2	> 100