Supporting Information

Cationic palladium(II)-catalyzed dehydrative nucleophilic substitutions of benzhydryl alcohols with electron-deficient benzenethiols in water

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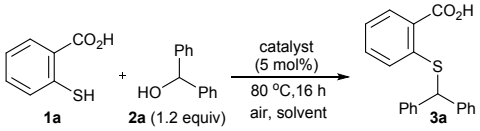
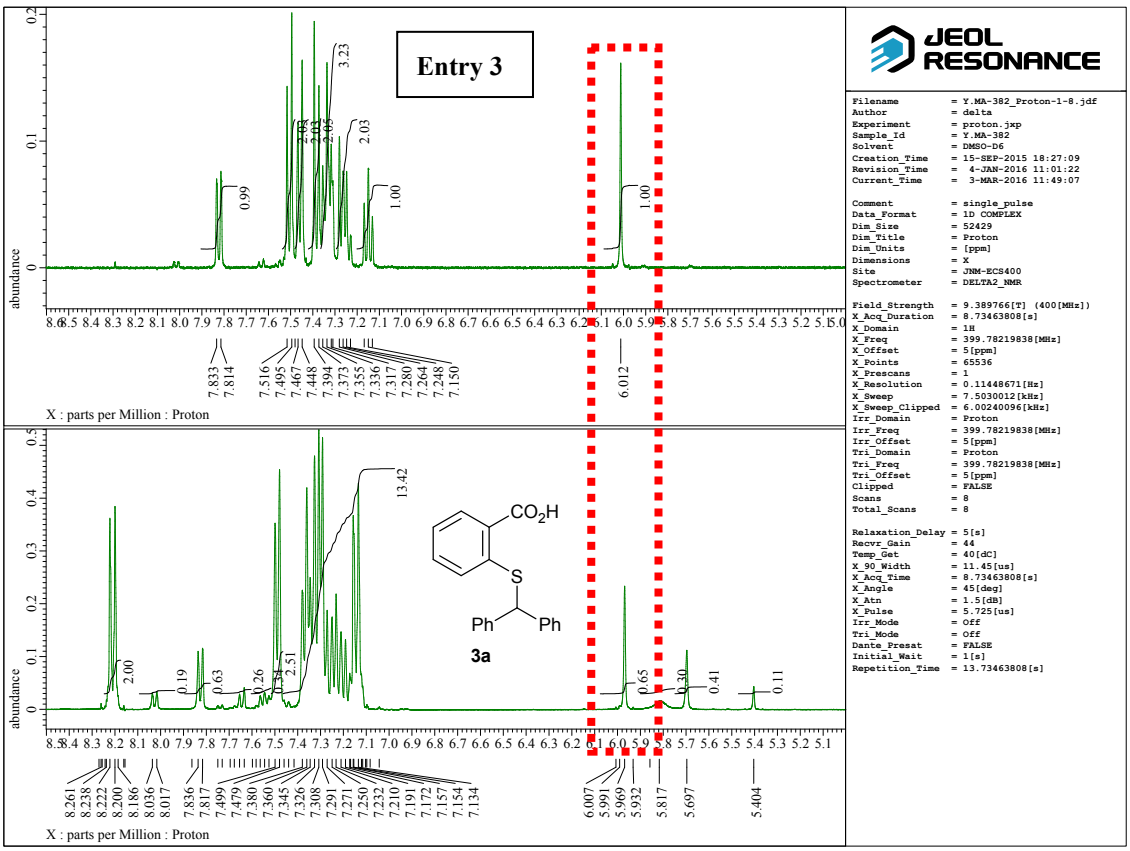
Table 1, Entry 3 (The yield was determined by ^{1}H NMR analysis of the crude product using *p*-nitroanisole as an internal standard.)



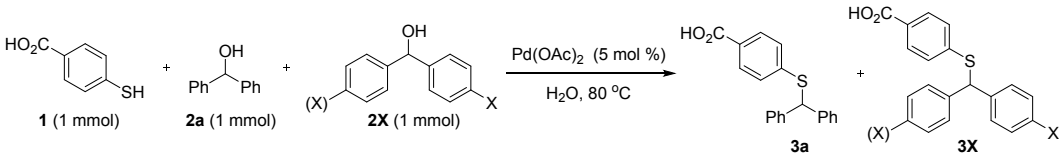
A mixture of 2-mercaptobenzoic acid **1a** (77 mg, 0.5 mmol), $PdCl_2(MeCN)_2$ (6.7 mg, 0.025 mmol), and benzhydrol **2a** (110 mg, 0.6 mmol) in H_2O (2 mL) was heated at 80 °C for 16 h in a sealed tube under air. After the reaction mixture was cooled, *p*-nitroanisole (77 mg, 0.5 mmol, internal standard) was added to the reaction mixture, which was extracted with AcOEt. The organic layer was washed with brine, and concentrated in vacuo. The residue was analyzed by ^{1}H-NMR spectroscopy.

Conversion yield was calculated by integration.

	desired **3a**	*p*-nitroanisole internal standard
Signal δ	5.97 (methin-**H**)	8.21 (Ar-**H**)
Integral value	0.63 (1H)	2.00 (2H)
Calculated ratio	65% from **1a**	77 mg (0.5 mmol)

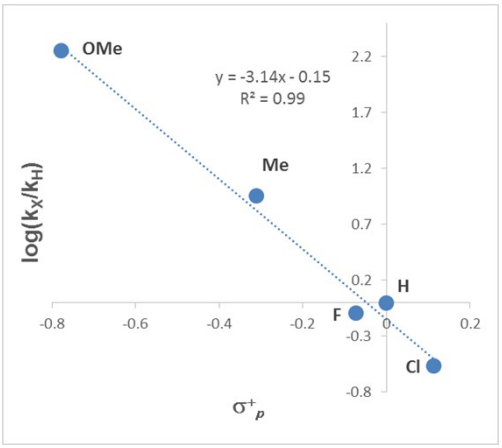


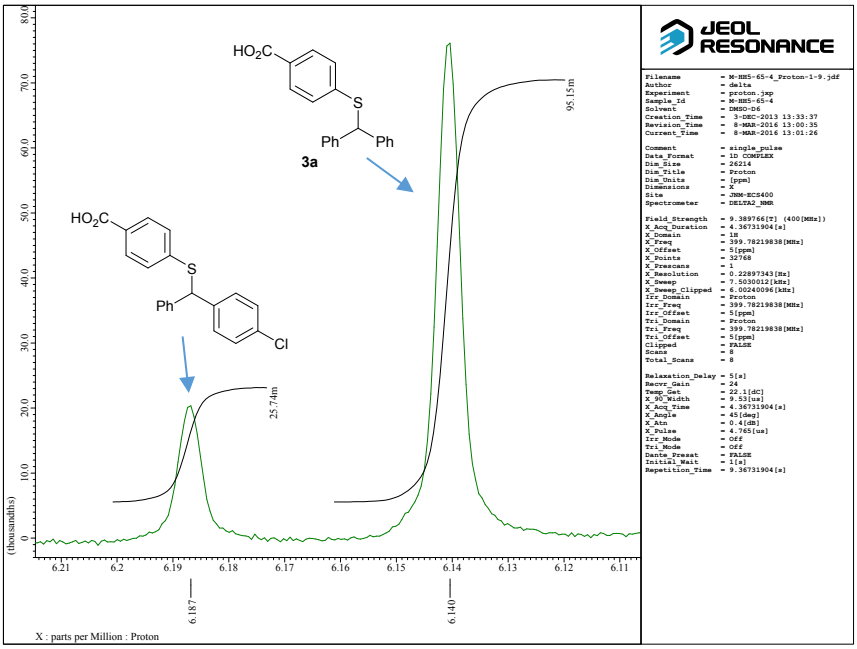
Hammett study (A)



A mixture of 4-mercaptobeozoic acid **1** (154 mg, 1 mmol), $Pd(OAc)_2$ (11 mg, 0.05 mmol), benzhydrol **2a** (184 mg, 1 mmol), and benzhydryl alcohols **2X** (1 mmol) in H_2O (4 mL) was heated at 80 °C in a sealed tube under air. After cooling, the reaction mixture was poured into water and extracted with EtOAc. The organic layer was washed with brine, dried over $MgSO_4$ and concentrated in vacuo. The residue was analyzed by ^{1}H-NMR spectroscopy.

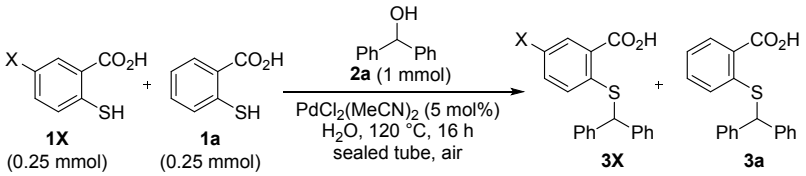
X	σ^+	$\log(k_X/k_H)$
OMe	-0.778	2.25
Me	-0.311	0.96
diF	-0.073	-0.09
H	0	0
Cl	0.114	-0.57





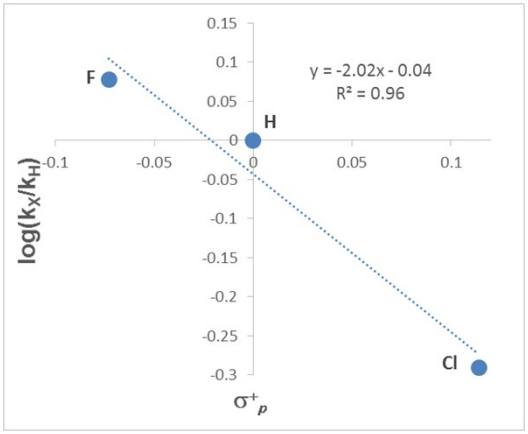
$\log(k_X/k_H) = \log(25.74/95.15) = -0.57$

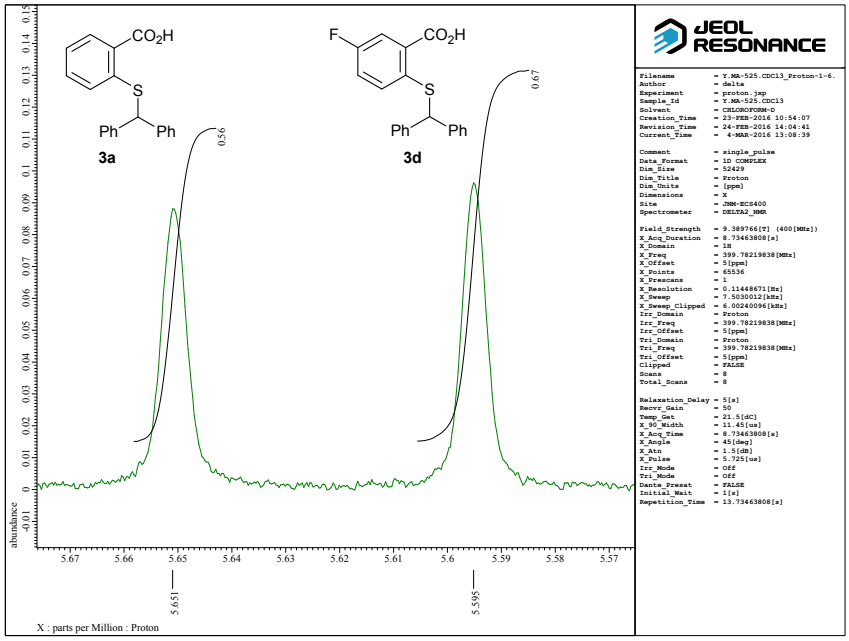
Hammett study (B)



A mixture of 5-substituted thiosalicylic acid **1X** (0.25 mmol), **1a** (34.0 mg, 0.25 mmol), $PdCl_2(MeCN)_2$ (4.1 mg, 0.016 mmol), and benzhydrol **2a** (45.9 mg, 0.25 mmol) in H_2O (1 mL) was heated at 120 °C in a sealed tube under air. After cooling, the reaction mixture was poured into water and extracted with EtOAc. The organic layer was washed with brine, dried over $MgSO_4$ and concentrated in vacuo. The residue was analyzed by ^{1}H-NMR spectroscopy.

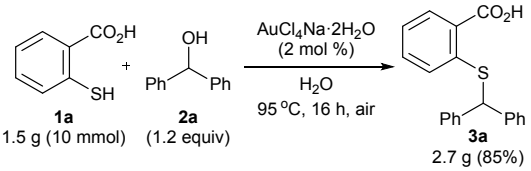
X	σ^+	$\log(k_X/k_H)$
F	-0.073	0.08
H	0	0
Cl	0.114	-0.29





$\log(k_X/k_H)$ = $\log(0.67/0.56)$ = 0.08

Scale-up experiment

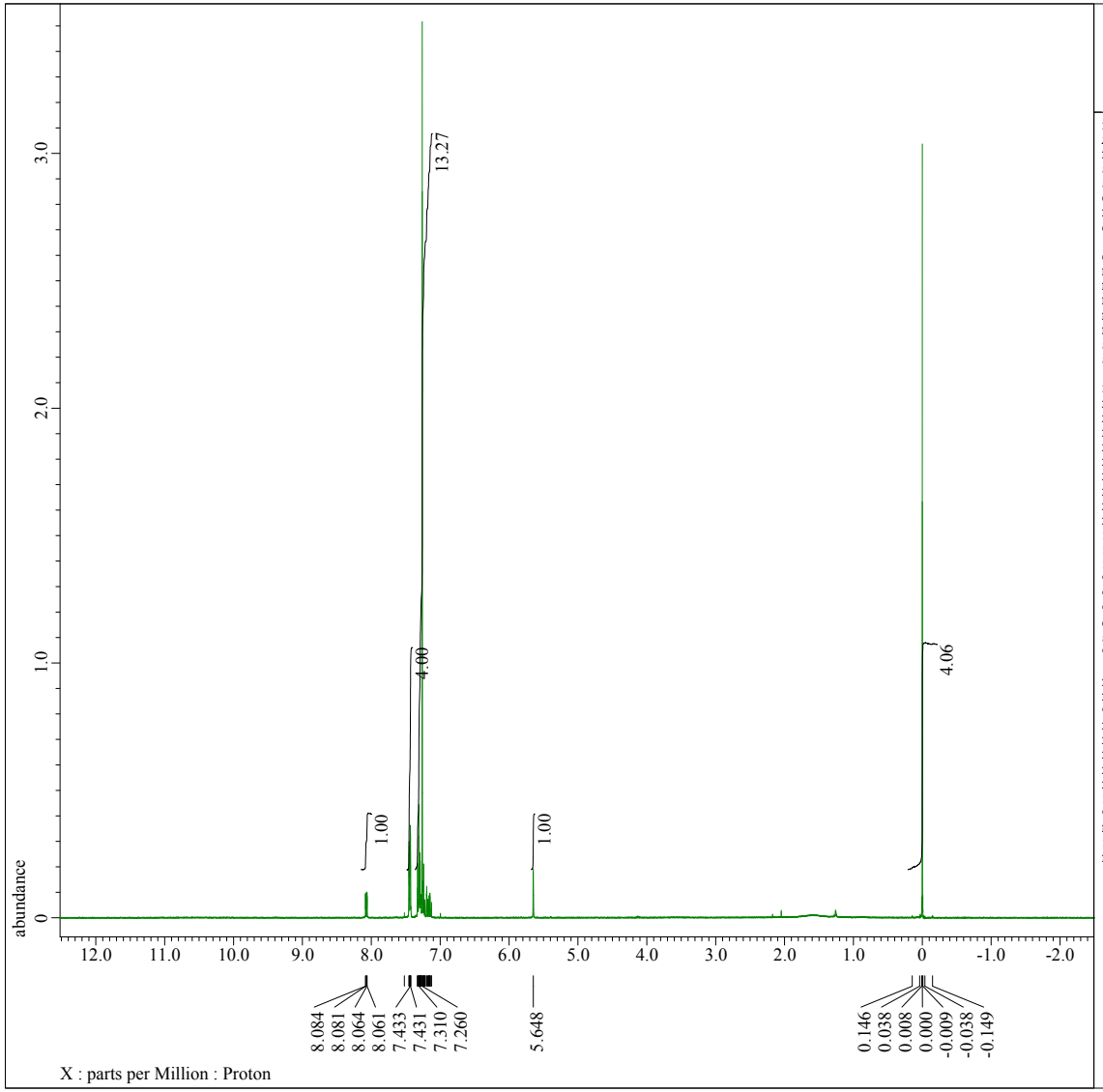


A mixture of 2-mercaptobenzoic acid **1a** (1.54 g, 10 mmol), $PdCl_2(MeCN)_2$ (129.8 mg, 0.5 mmol), and benzhydrol **2a** (2.20 g, 12 mmol) in H_2O (40 mL) was heated at 95 °C for 16 h under air. After cooling, the reaction mixture was poured into water and extracted with EtOAc. The organic layer was washed with brine, dried over $MgSO_4$ and concentrated in vacuo. The residue was recrystallized from hexane/AcOEt to give desired product **3a** (2.31 g, 72%).

5 min

30 min

16 h



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Revision_Time     =  8-MAR-2016 21:25:23
Current_Time      =  8-MAR-2016 21:25:25

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X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
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Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
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Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
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X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
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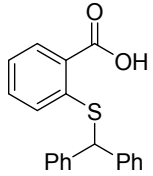
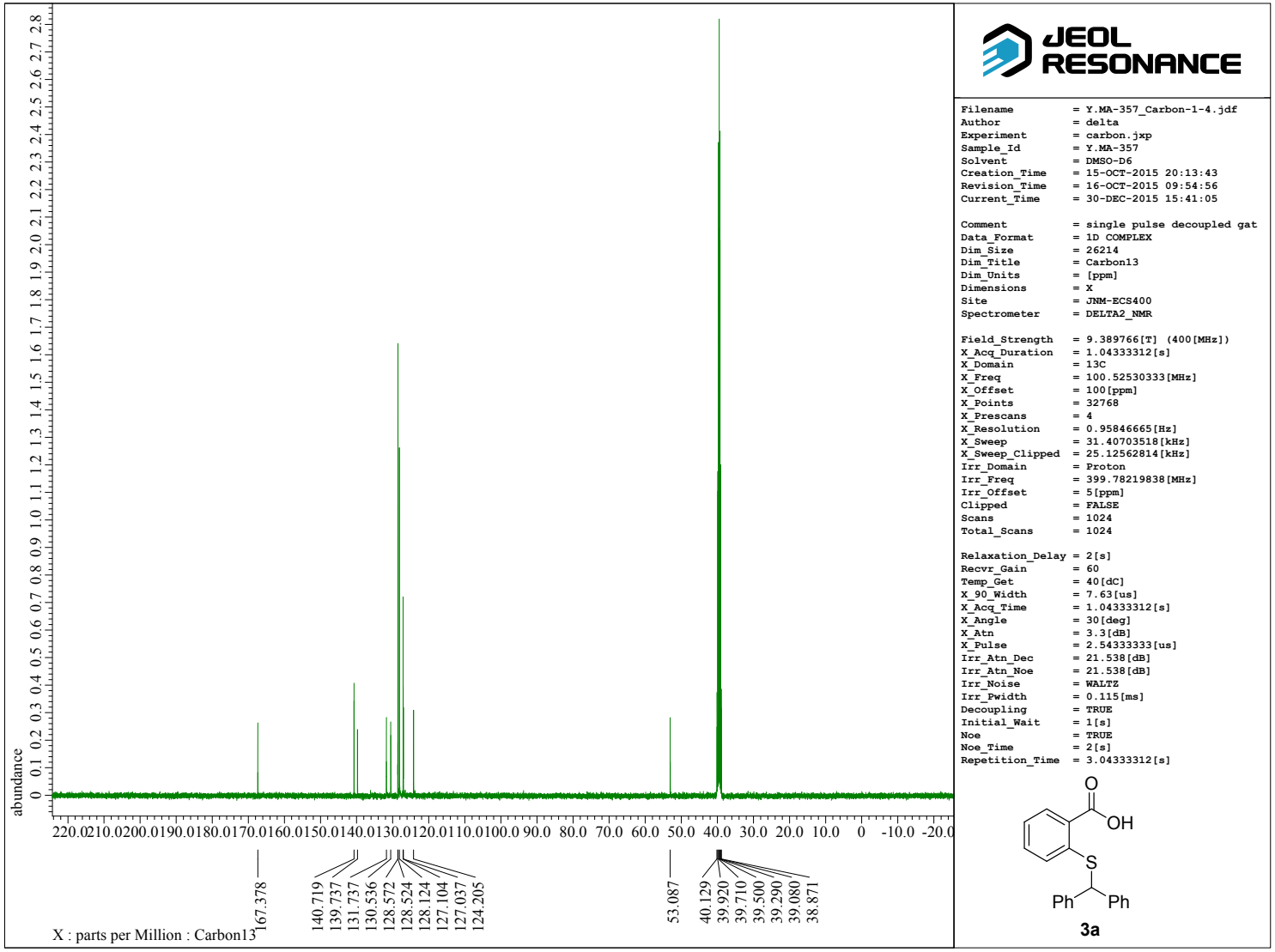


3a



JEOL RESONANCE

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Revision_Time	= 16-OCT-2015 09:54:56
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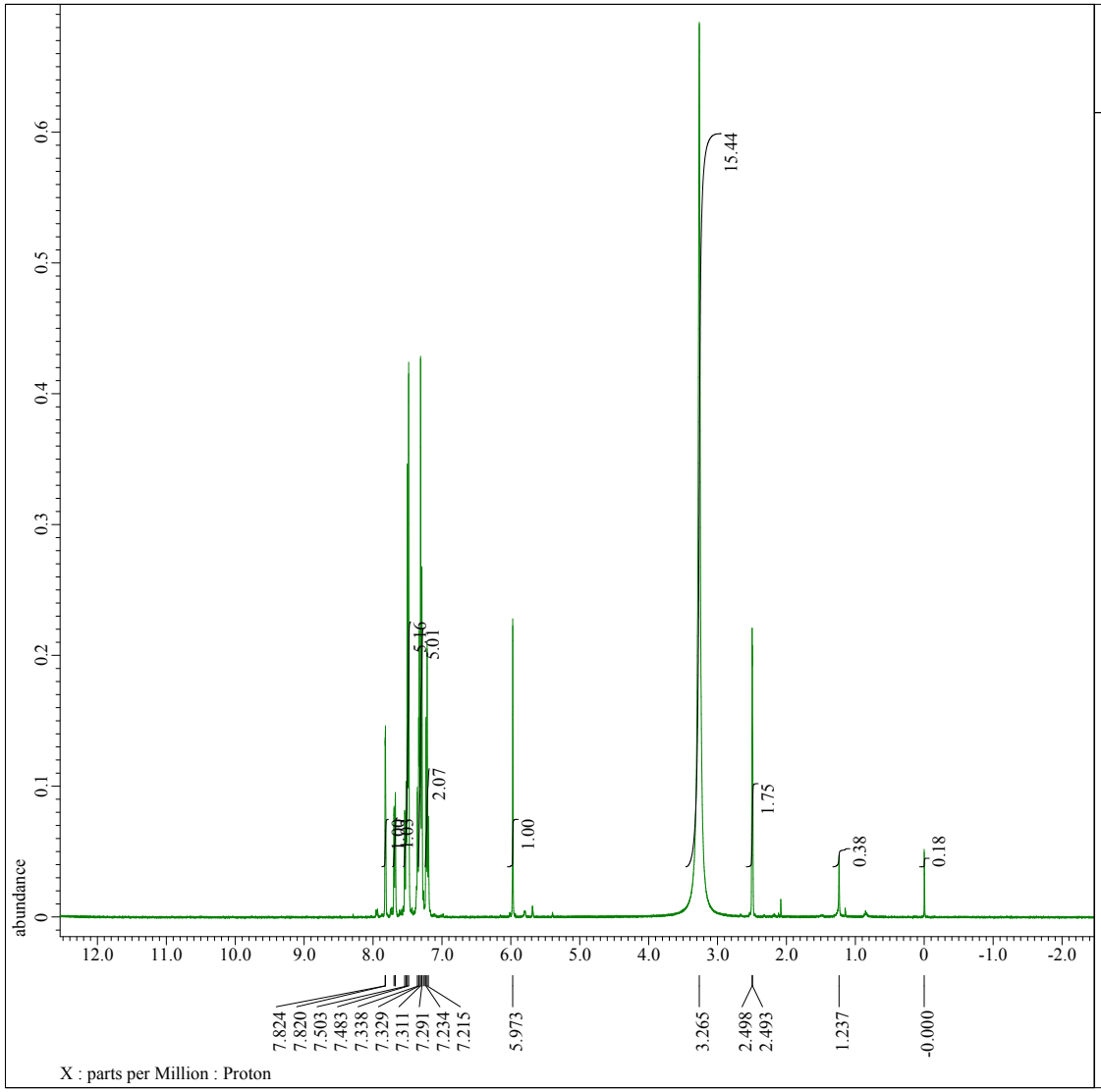
3a



JEOL RESONANCE

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Dim_Units         = [ppm]
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X_Points          = 65536
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X_Resolution      = 0.11448671[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
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Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
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Total_Scans       = 8

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Temp_Get          = 40[dC]
X_90_Width        = 11.45[us]
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X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
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Tri_Mode          = Off
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Initial_Wait      = 1[s]
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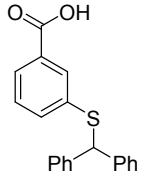

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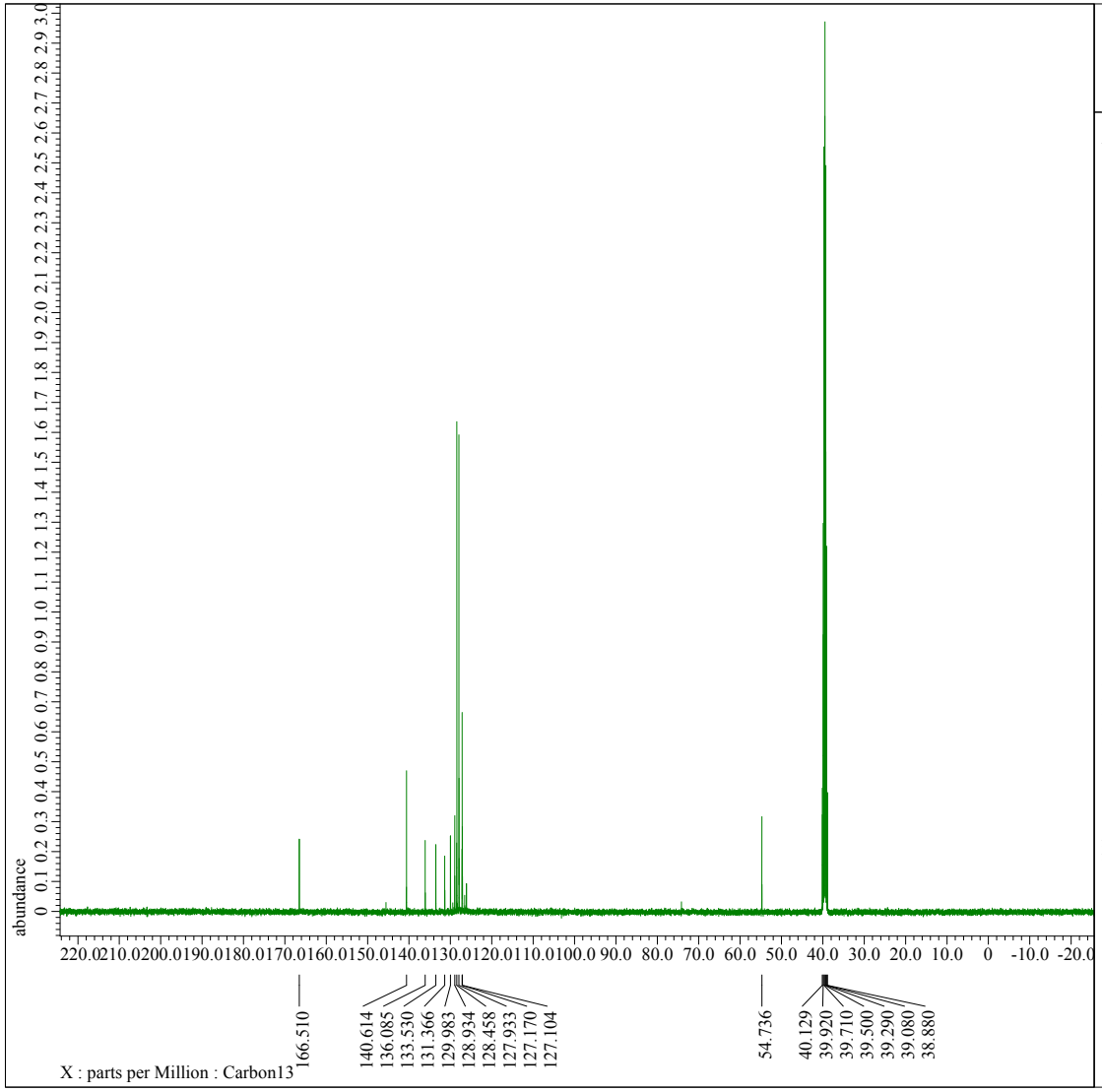

JEOL RESONANCE

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Spectrometer      = DELTA2_NMR

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X_Sweep_Clipped   = 25.12562814[kHz]
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X_Pulse           = 2.54333333[us]
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Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
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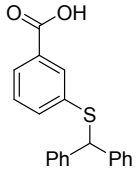

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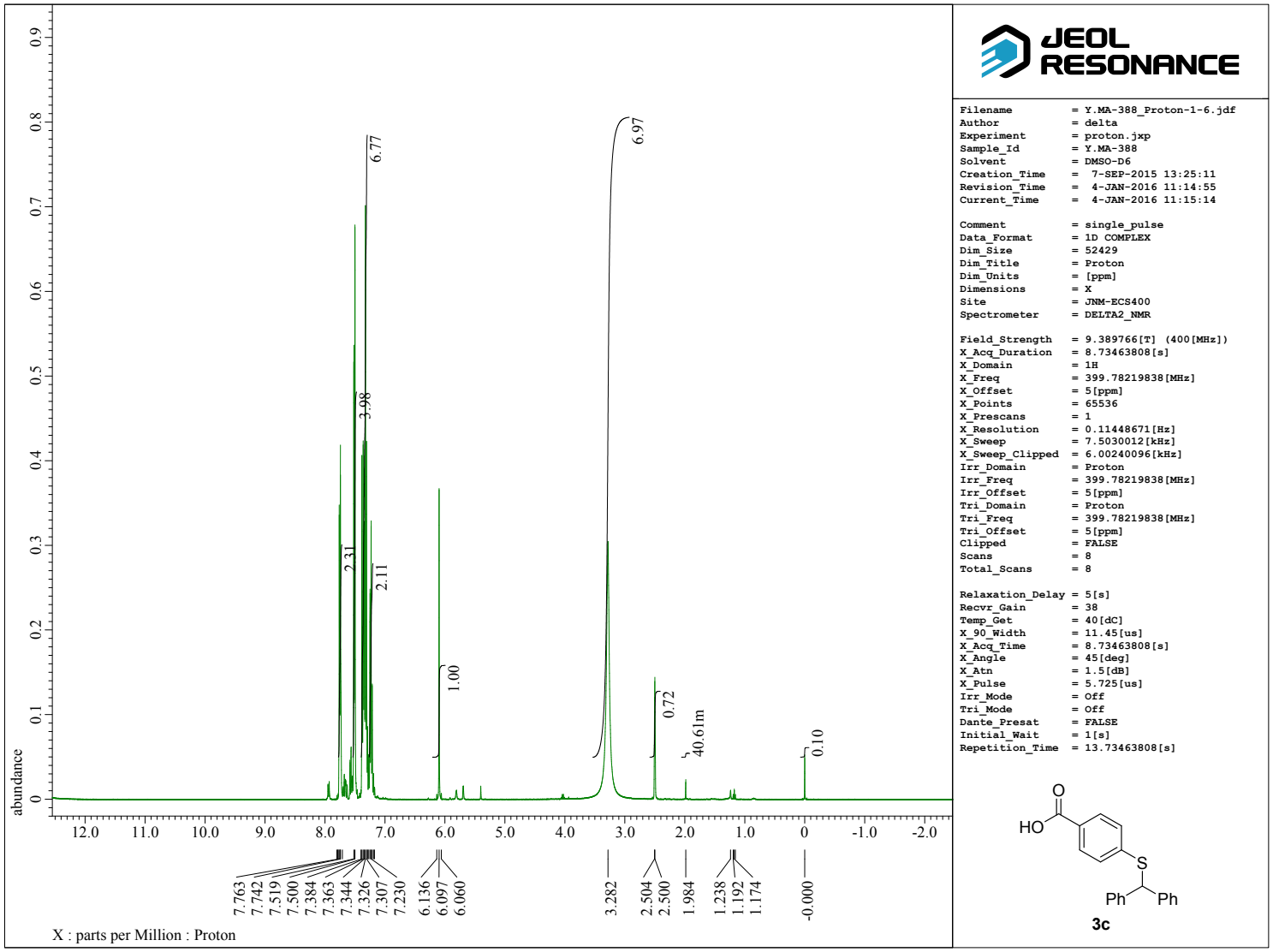

JEOL RESONANCE

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X_Resolution      = 0.11448671[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
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Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
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X_Atn             = 1.5[dB]
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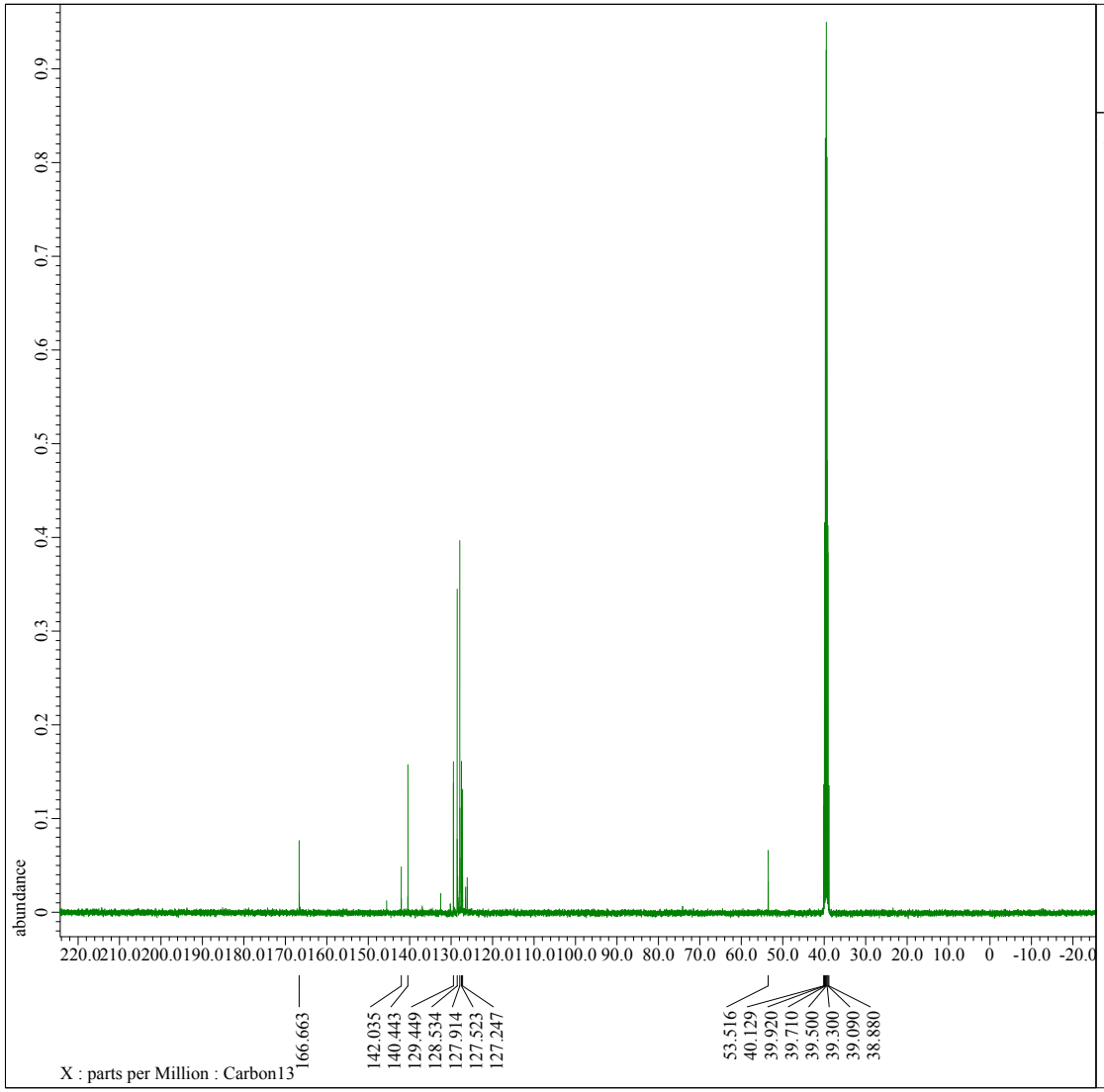
3c



JEOL RESONANCE

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X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
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Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
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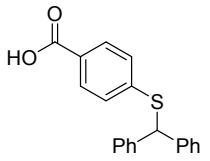

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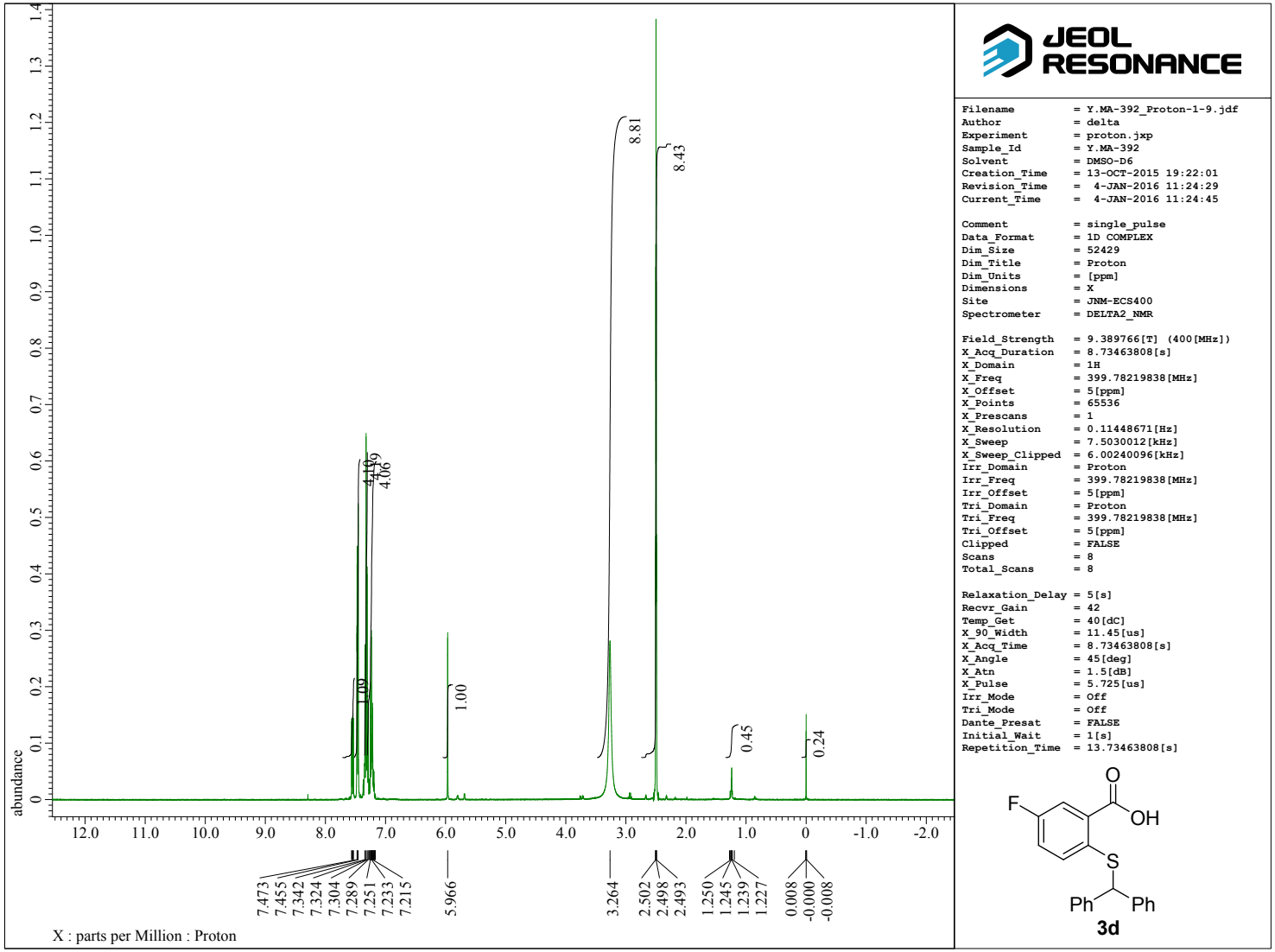

JEOL RESONANCE

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Spectrometer      = DELTA2_NMR

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X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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
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Temp_Get          = 40[dC]
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X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
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Tri_Mode          = Off
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Initial_Wait      = 1[s]
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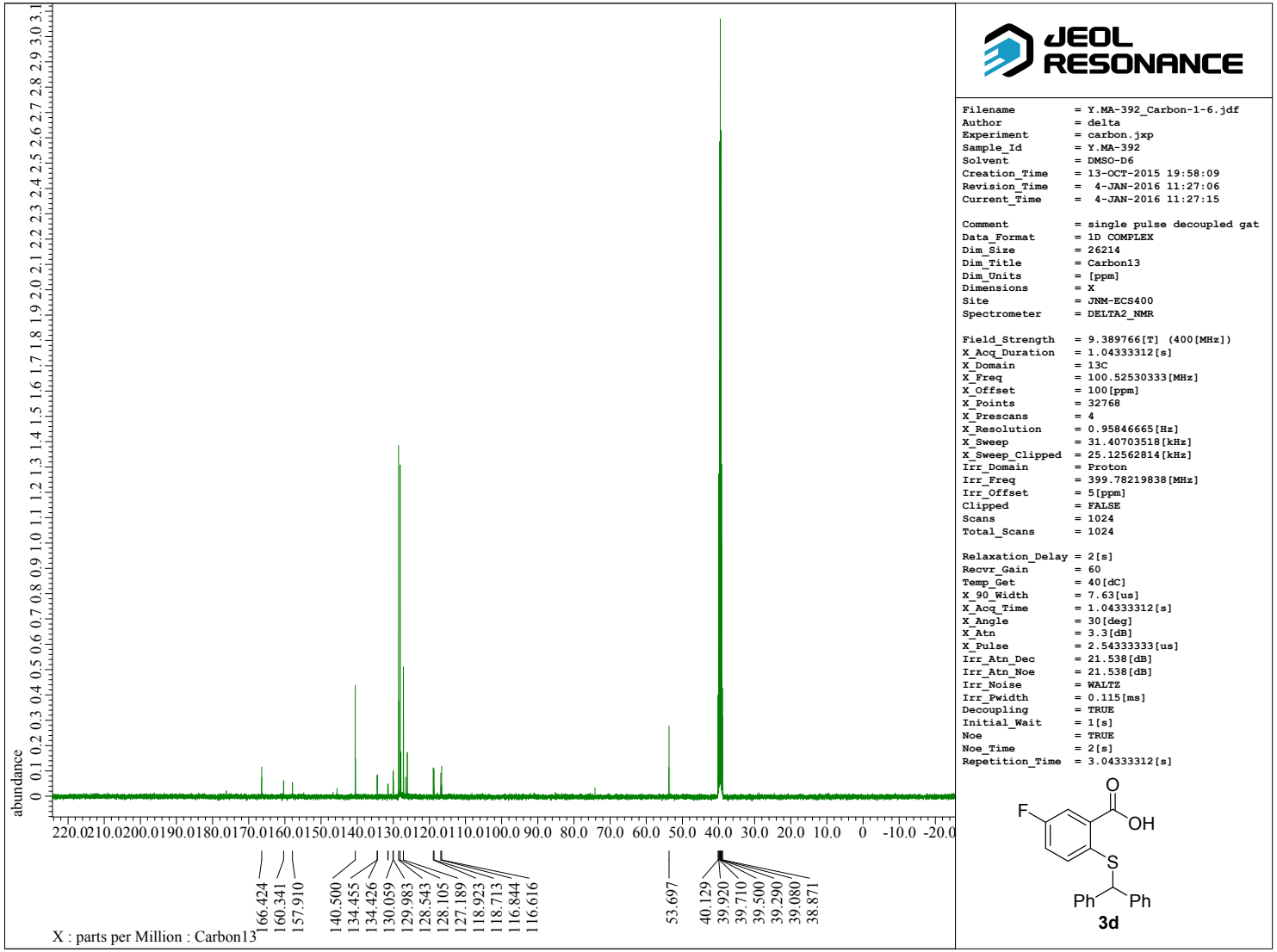
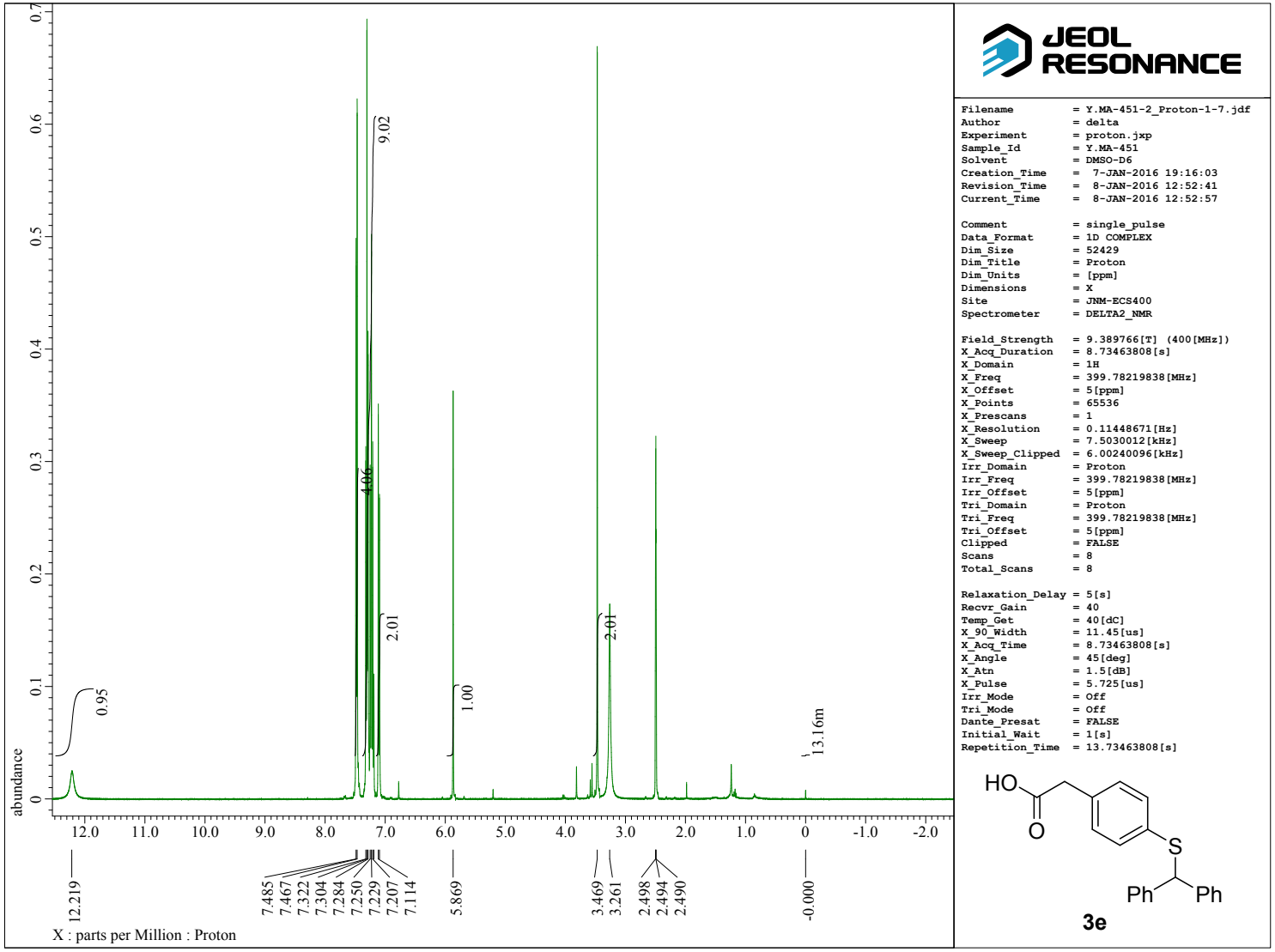
3d



JEOL RESONANCE

```
Filename          = Y.MA-392_Carbon-1-6.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-392
Solvent           = DMSO-D6
Creation_Time     = 13-OCT-2015 19:58:09
Revision_Time     =  4-JAN-2016 11:27:06
Current_Time      =  4-JAN-2016 11:27:15

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 40[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

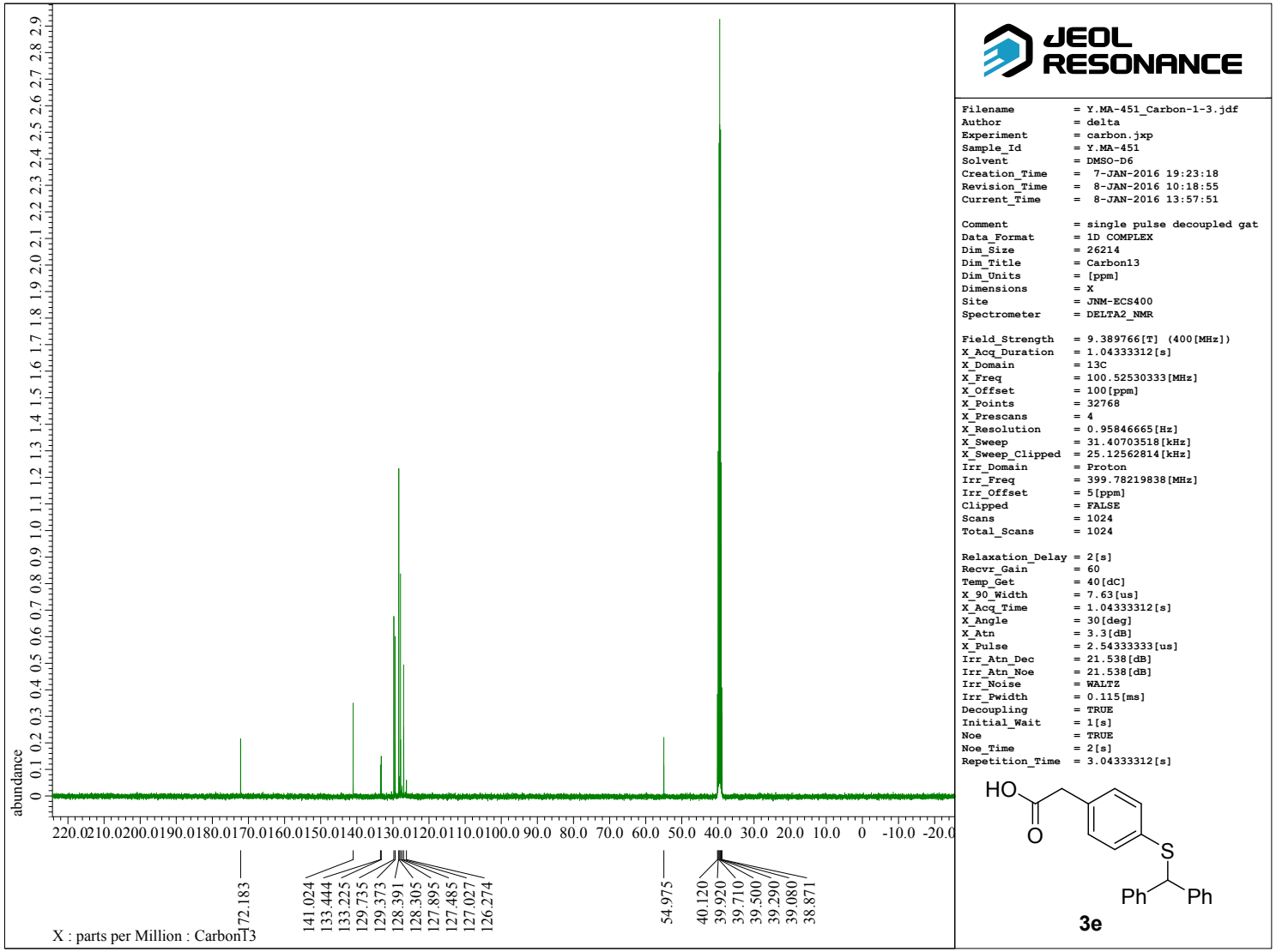

3d



JEOL RESONANCE

Filename	= Y.MA-451-2_Proton-1-7.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= Y.MA-451
Solvent	= DMSO-D6
Creation_Time	= 7-JAN-2016 19:16:03
Revision_Time	= 8-JAN-2016 12:52:41
Current_Time	= 8-JAN-2016 12:52:57
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 8.73463808[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 65536
X_Prescans	= 1
X_Resolution	= 0.11448671[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	= 40
Temp_Get	= 40[dC]
X_90_Width	= 11.45[us]
X_Acq_Time	= 8.73463808[s]
X_Angle	= 45[deg]
X_Atn	= 1.5[dB]
X_Pulse	= 5.725[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 13.73463808[s]

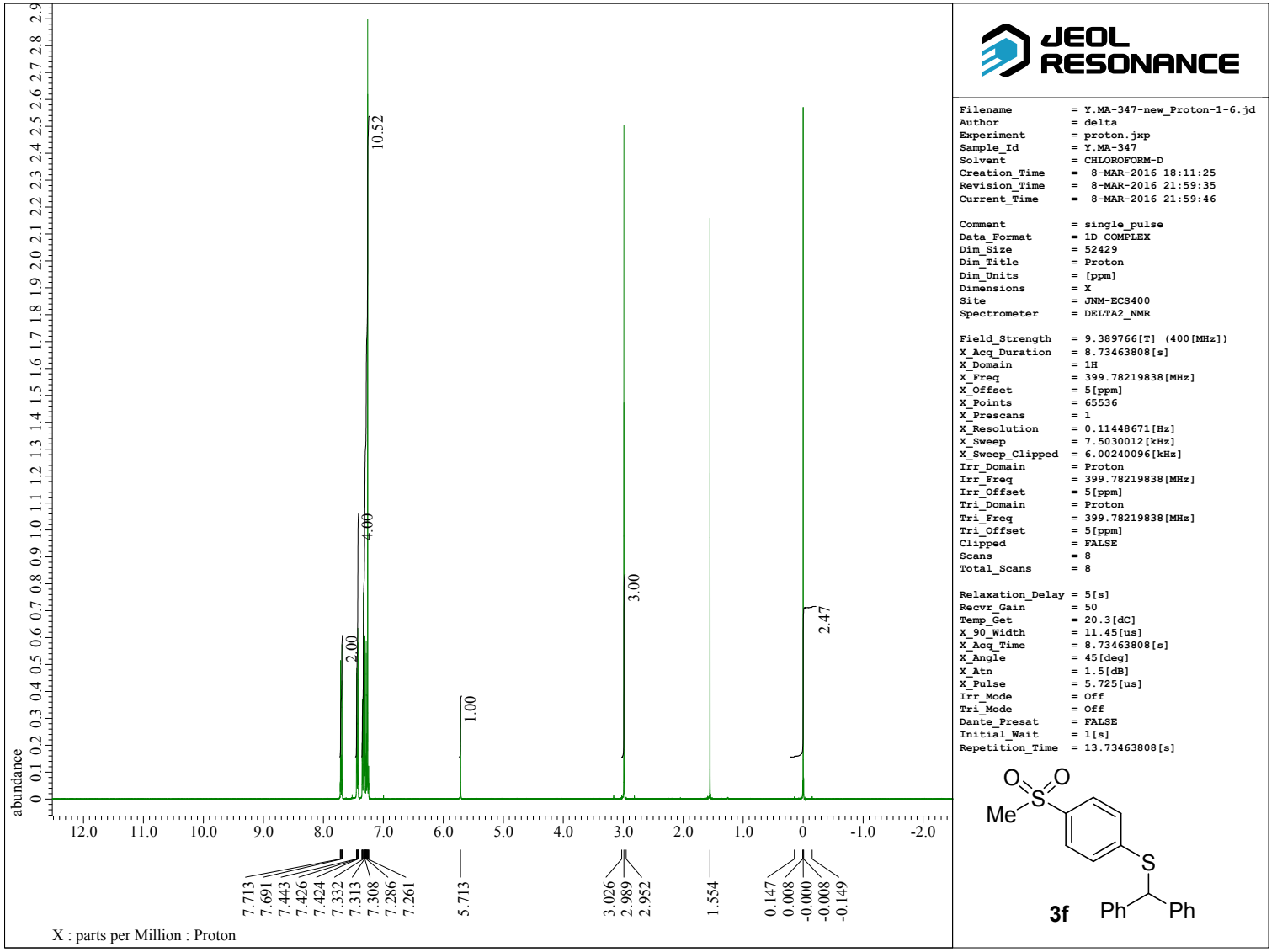
3e



JEOL RESONANCE

```
Filename          = Y.MA-451_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-451
Solvent           = DMSO-D6
Creation_Time     =  7-JAN-2016 19:23:18
Revision_Time     =  8-JAN-2016 10:18:55
Current_Time      =  8-JAN-2016 13:57:51

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 40[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

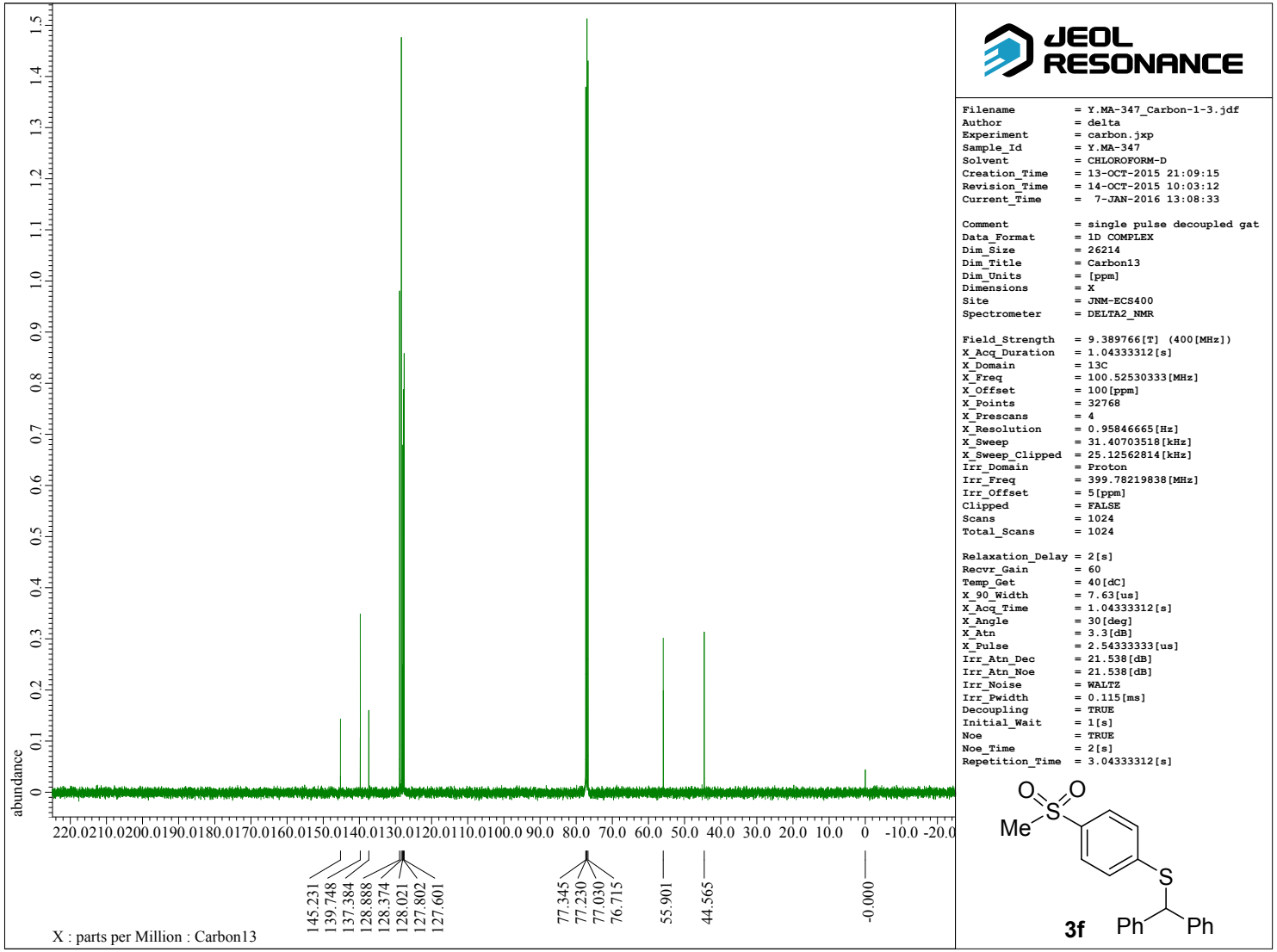

3e



JEOL RESONANCE

```
Filename          = Y.MA-347-new_Proton-1-6.jd
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-347
Solvent           = CHLOROFORM-D
Creation_Time     =  8-MAR-2016 18:11:25
Revision_Time     =  8-MAR-2016 21:59:35
Current_Time      =  8-MAR-2016 21:59:46

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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        = 50
Temp_Get          = 20.3[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```

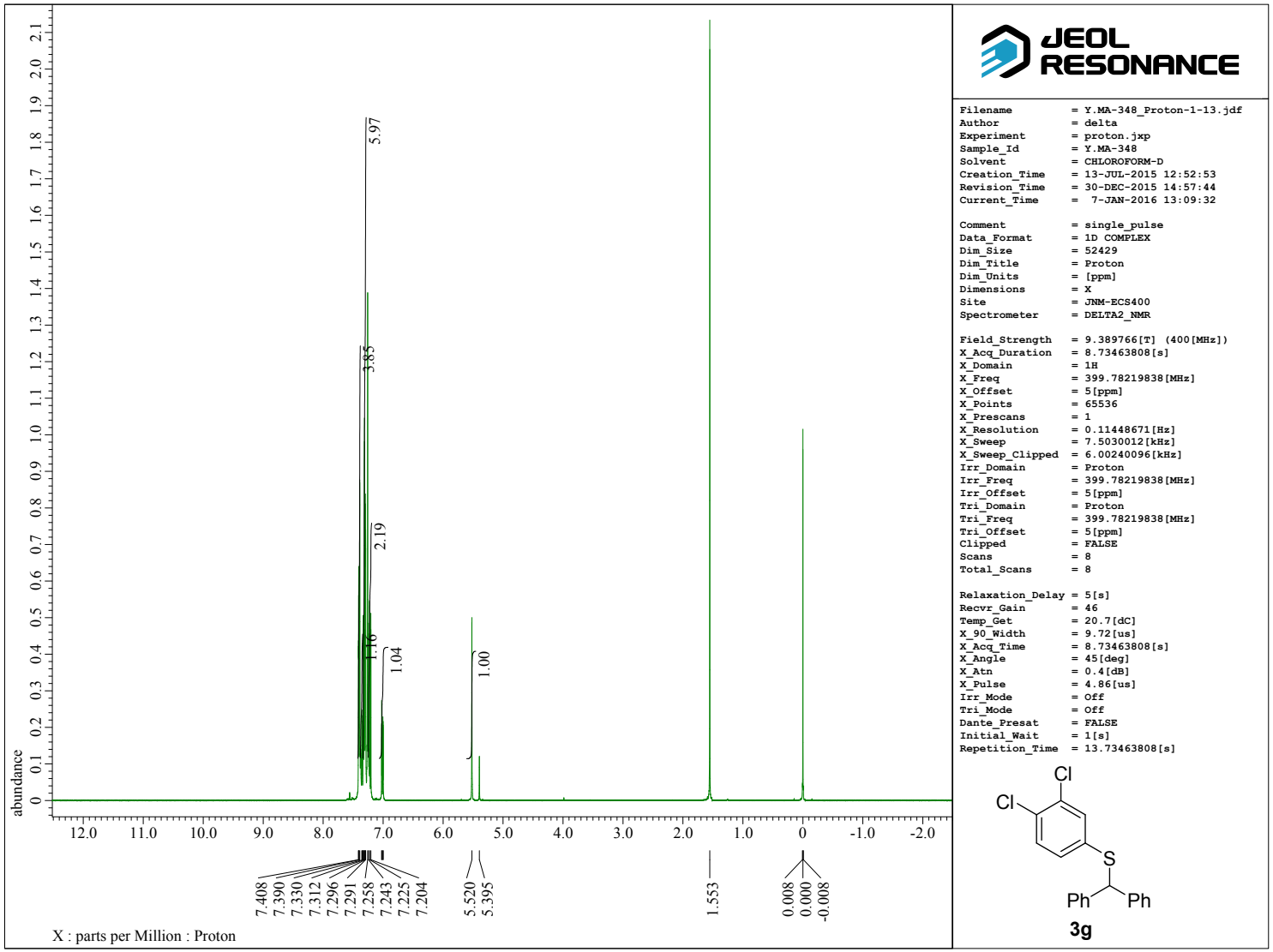

3f



JEOL RESONANCE

```
Filename          = Y.MA-347_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-347
Solvent           = CHLOROFORM-D
Creation_Time     = 13-OCT-2015 21:09:15
Revision_Time     = 14-OCT-2015 10:03:12
Current_Time      =  7-JAN-2016 13:08:33

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 40[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

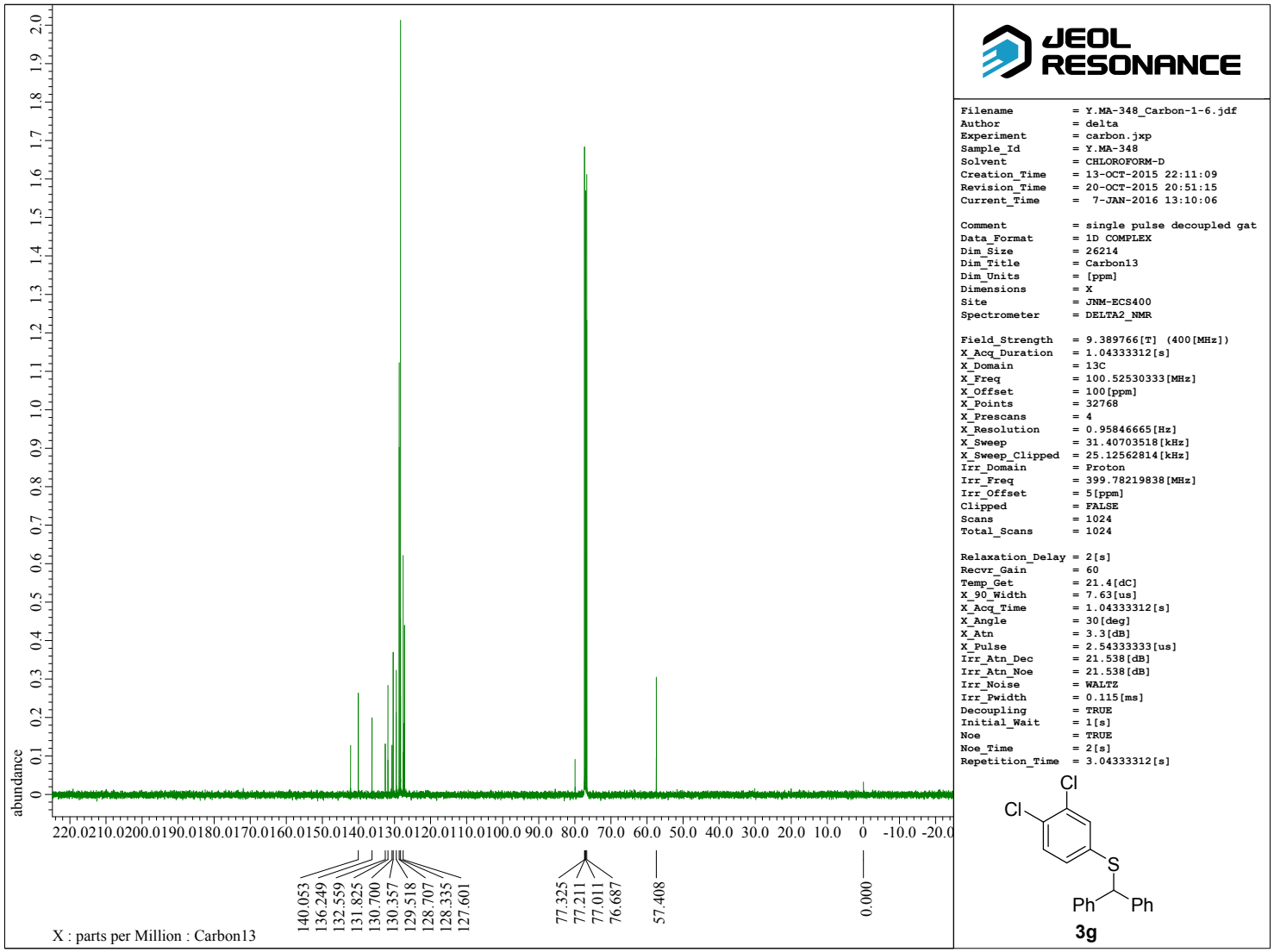

3f

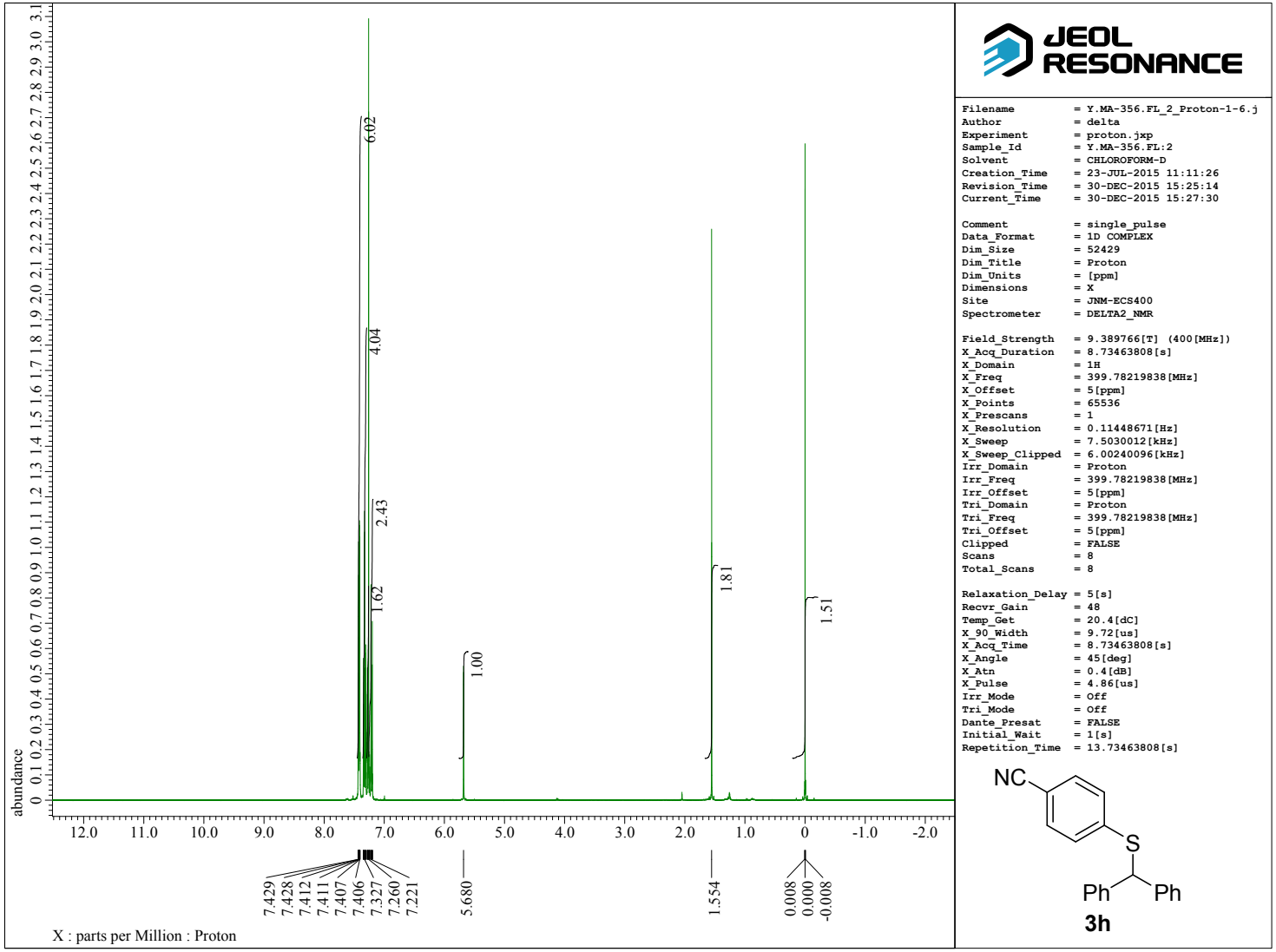


JEOL RESONANCE

```
Filename          = Y.MA-348_Proton-1-13.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-348
Solvent           = CHLOROFORM-D
Creation_Time     = 13-JUL-2015 12:52:53
Revision_Time     = 30-DEC-2015 14:57:44
Current_Time      =  7-JAN-2016 13:09:32

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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        = 46
Temp_Get          = 20.7[dC]
X_90_Width        = 9.72[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 0.4[dB]
X_Pulse           = 4.86[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```


3g

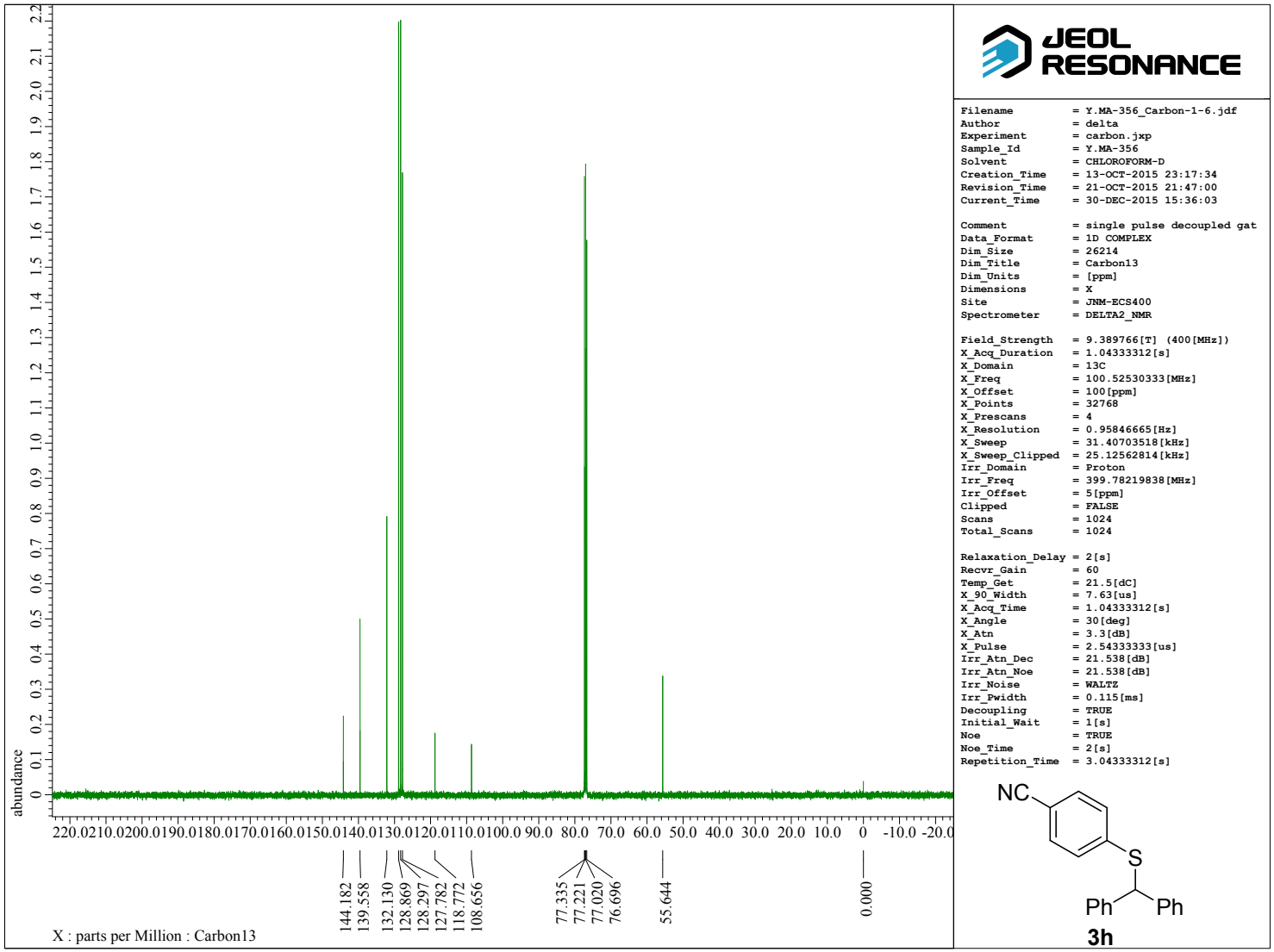

abundance
X : parts per Million : Carbon13
140.053
136.249
132.559
131.825
130.700
130.357
129.518
128.707
128.335
127.601
77.325
77.211
77.011
76.687
57.408
0.000
Filename = Y.MA-348_Carbon-1-6.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = Y.MA-348
Solvent = CHLOROFORM-D
Creation_Time = 13-OCT-2015 22:11:09
Revision_Time = 20-OCT-2015 20:51:15
Current_Time = 7-JAN-2016 13:10:06
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
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 = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.4[dC]
X_90_Width = 7.63[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 3.3[dB]
X_Pulse = 2.54333333[us]
Irr_Atn_Dec = 21.538[dB]
Irr_Atn_Noe = 21.538[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
Cl
Cl
S
Ph
Ph
3g

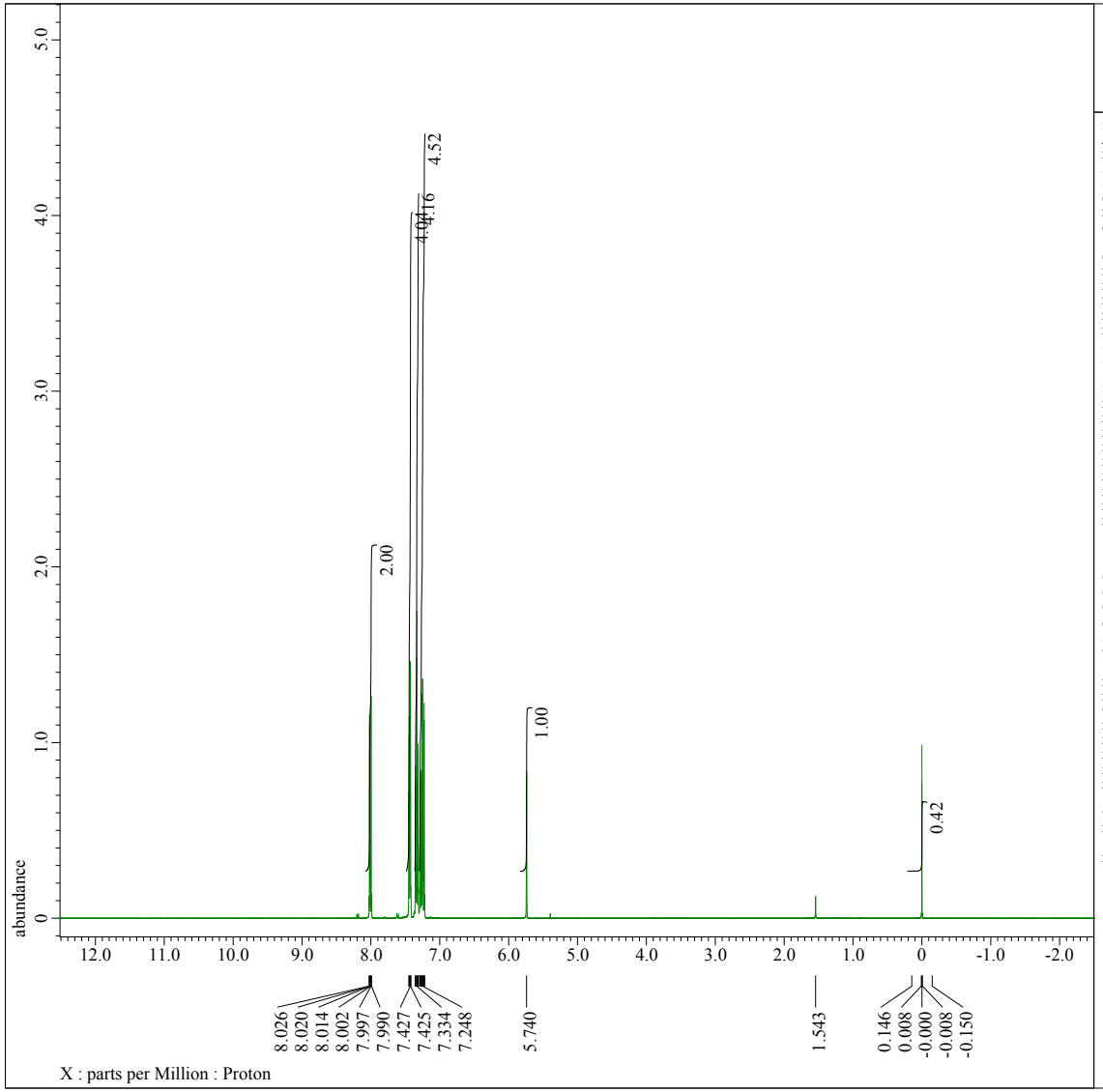


JEOL RESONANCE

Filename	= Y.MA-356.FL_2_Proton-1-6.j
Author	= delta
Experiment	= proton.jxp
Sample_Id	= Y.MA-356.FL:2
Solvent	= CHLOROFORM-D
Creation_Time	= 23-JUL-2015 11:11:26
Revision_Time	= 30-DEC-2015 15:25:14
Current_Time	= 30-DEC-2015 15:27:30
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 8.73463808[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 65536
X_Prescans	= 1
X_Resolution	= 0.11448671[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	= 48
Temp_Get	= 20.4[dC]
X_90_Width	= 9.72[us]
X_Acq_Time	= 8.73463808[s]
X_Angle	= 45[deg]
X_Atn	= 0.4[dB]
X_Pulse	= 4.86[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 13.73463808[s]

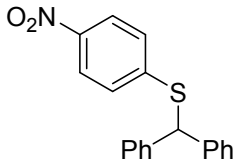
3h


abundance
X : parts per Million : Carbon13
144.182
139.558
132.130
128.869
128.297
127.782
118.772
108.656
77.335
77.221
77.020
76.696
55.644
0.000
JEOL RESONANCE
Filename = Y.MA-356_Carbon-1-6.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = Y.MA-356
Solvent = CHLOROFORM-D
Creation_Time = 13-OCT-2015 23:17:34
Revision_Time = 21-OCT-2015 21:47:00
Current_Time = 30-DEC-2015 15:36:03
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
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 = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.5[dC]
X_90_Width = 7.63[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 3.3[dB]
X_Pulse = 2.54333333[us]
Irr_Atn_Dec = 21.538[dB]
Irr_Atn_Noe = 21.538[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
NC
S
Ph
Ph
3h

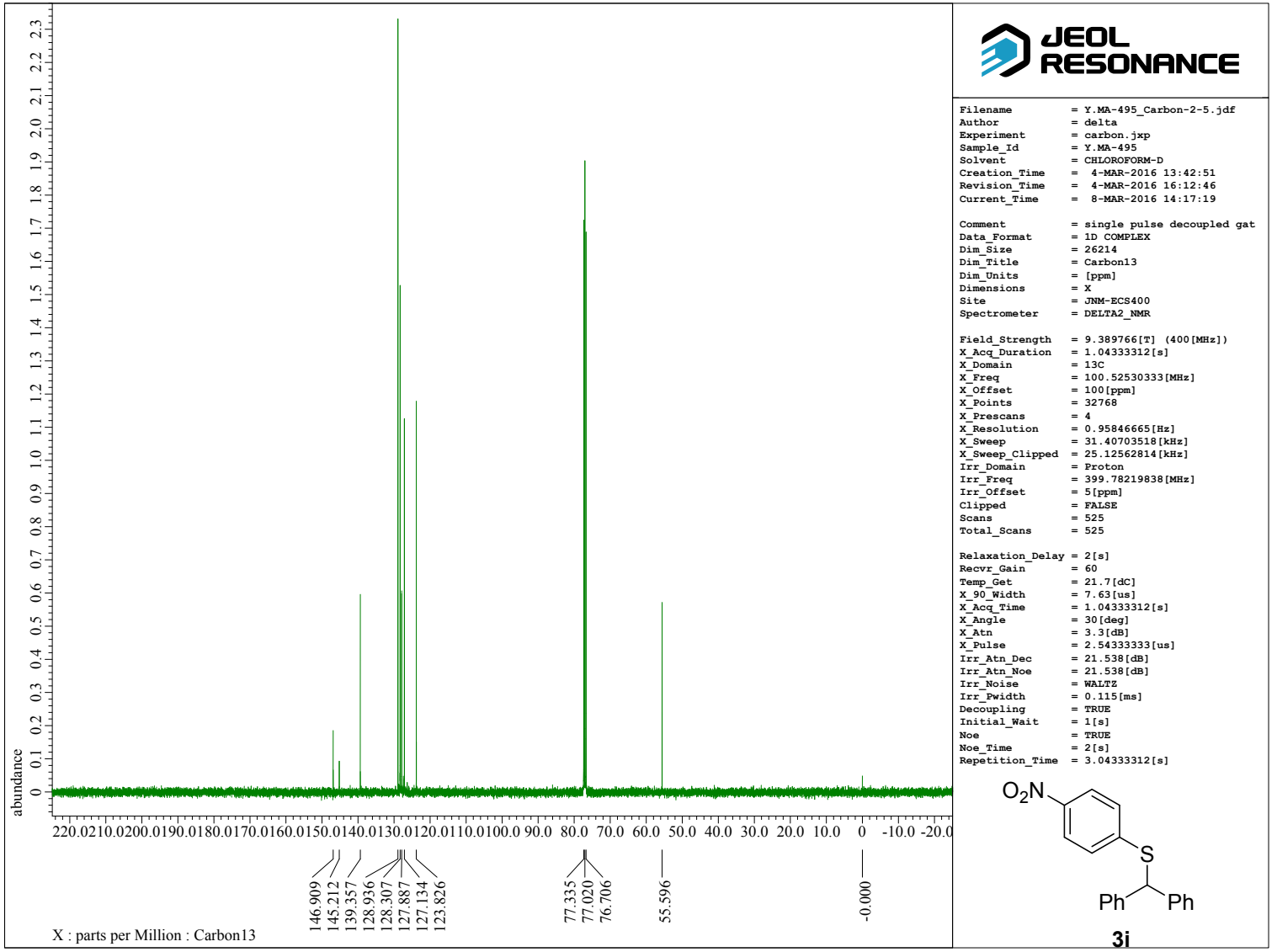


JEOL RESONANCE

```
Filename          = Y.MA-495_Proton-1-10.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-495
Solvent           = CHLOROFORM-D
Creation_Time     =  2-FEB-2016 16:15:27
Revision_Time     =  4-MAR-2016 16:15:02
Current_Time      =  8-MAR-2016 14:15:31

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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        = 42
Temp_Get          = 20.8[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```



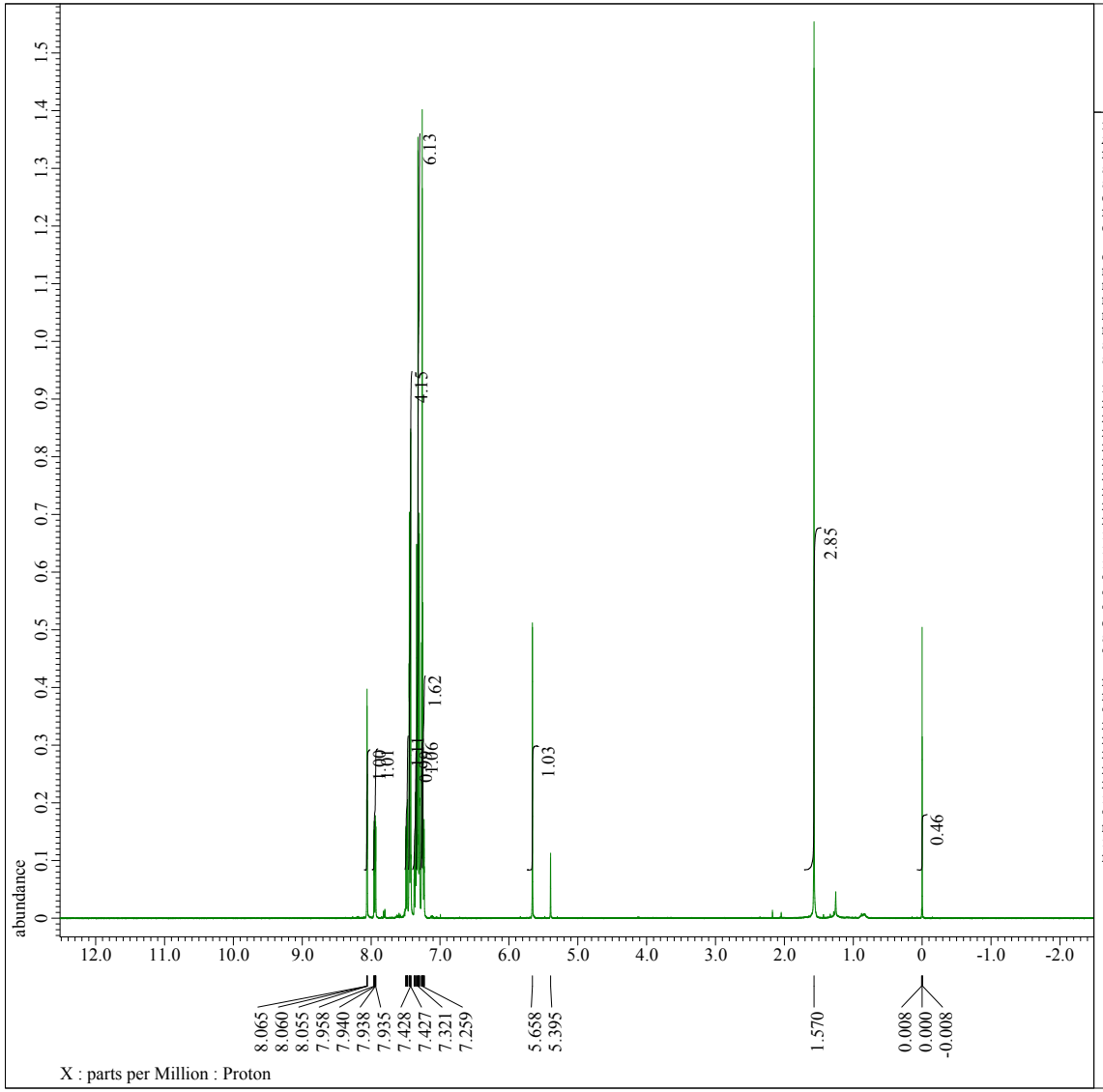
3i



JEOL RESONANCE

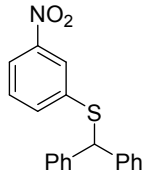
```
Filename          = Y.MA-495_Carbon-2-5.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-495
Solvent           = CHLOROFORM-D
Creation_Time     =  4-MAR-2016 13:42:51
Revision_Time     =  4-MAR-2016 16:12:46
Current_Time      =  8-MAR-2016 14:17:19

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 525
Total_Scans       = 525

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.7[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```


3i

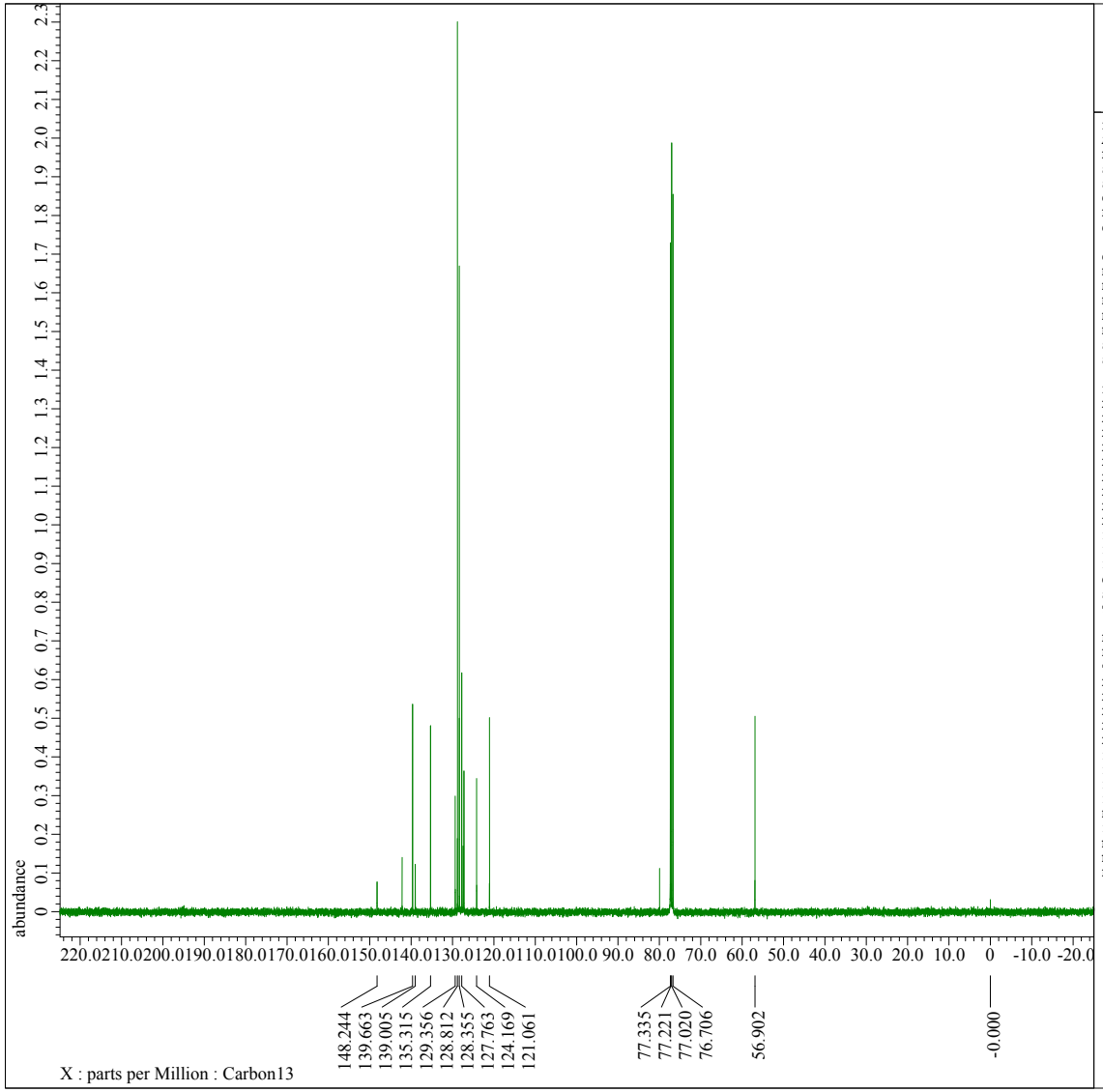


JEOL RESONANCE

```
Filename          = Y.MA-360.FL.1_Proton-1-10.
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-360.FL.1
Solvent           = CHLOROFORM-D
Creation_Time     = 22-JUL-2015 12:25:41
Revision_Time     =  8-MAR-2016 14:13:22
Current_Time      =  8-MAR-2016 14:13:23

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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          = 20.4[dC]
X_90_Width        = 9.72[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 0.4[dB]
X_Pulse           = 4.86[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```

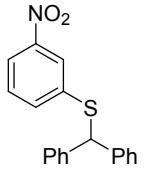


3j

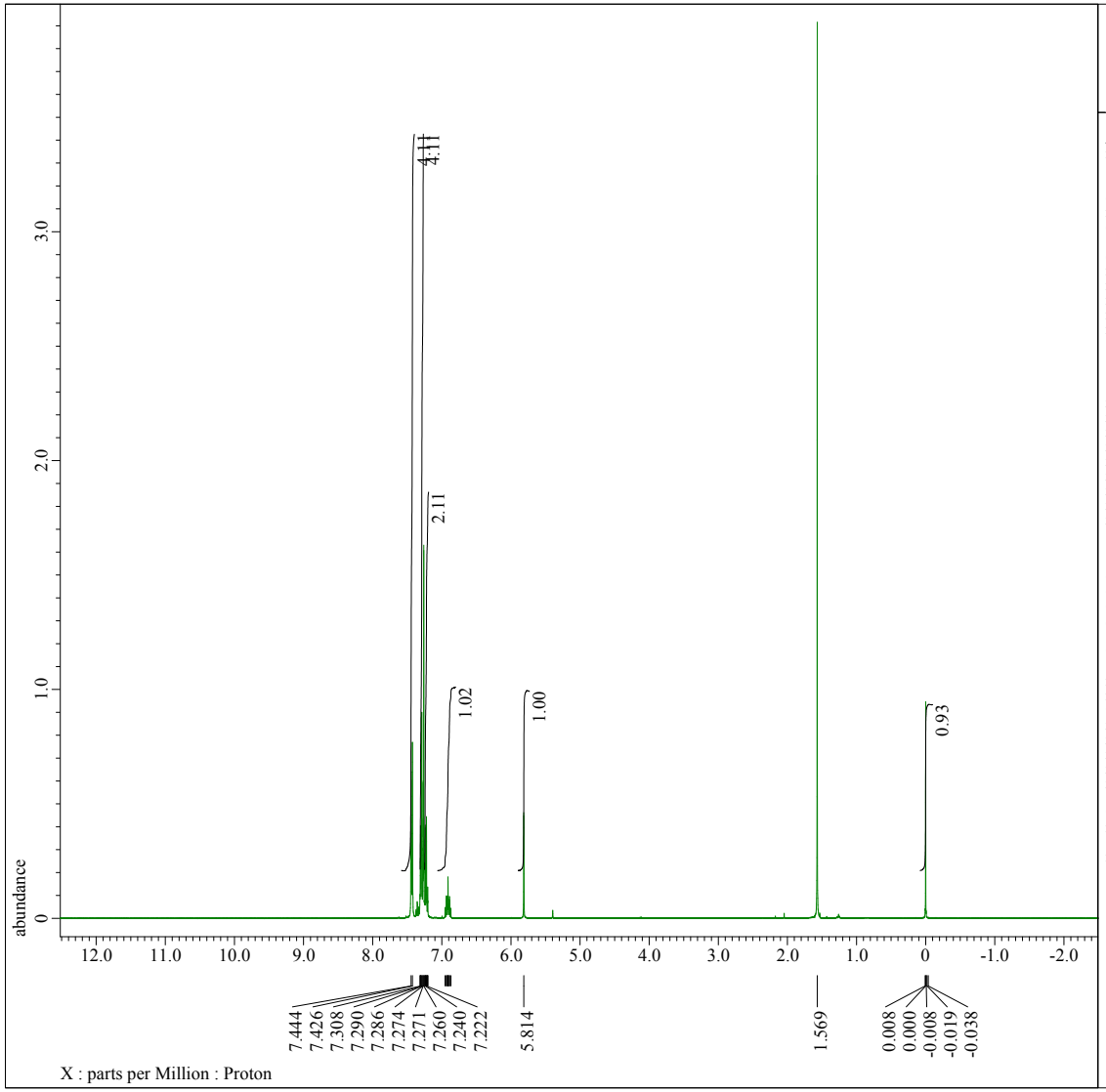


JEOL RESONANCE

```
Filename          = Y.MA-360_Carbon-1-5.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-360
Solvent           = CHLOROFORM-D
Creation_Time     =  4-MAR-2016 12:41:09
Revision_Time     =  4-MAR-2016 16:09:37
Current_Time      =  8-MAR-2016 14:14:38

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.6[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

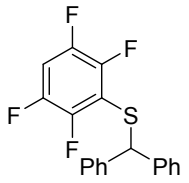


3j

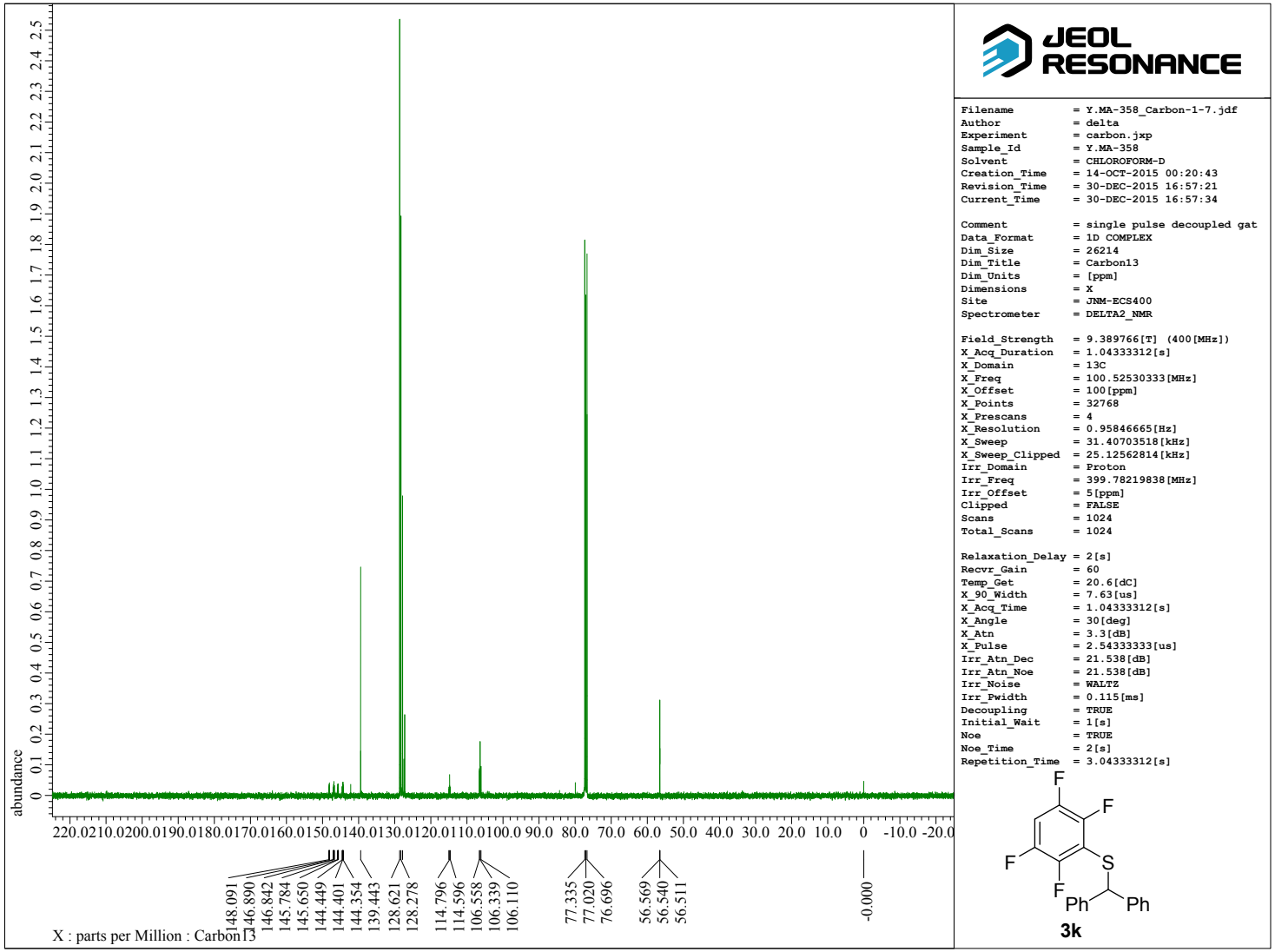


JEOL RESONANCE

```
Filename          = Y.MA-358.karamugo_Proton-1
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-358.karamugo
Solvent           = CHLOROFORM-D
Creation_Time     = 17-JUL-2015 08:51:25
Revision_Time     = 30-DEC-2015 15:42:53
Current_Time      = 30-DEC-2015 15:43:01

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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        = 48
Temp_Get          = 20.6[dC]
X_90_Width        = 9.72[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 0.4[dB]
X_Pulse           = 4.86[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```



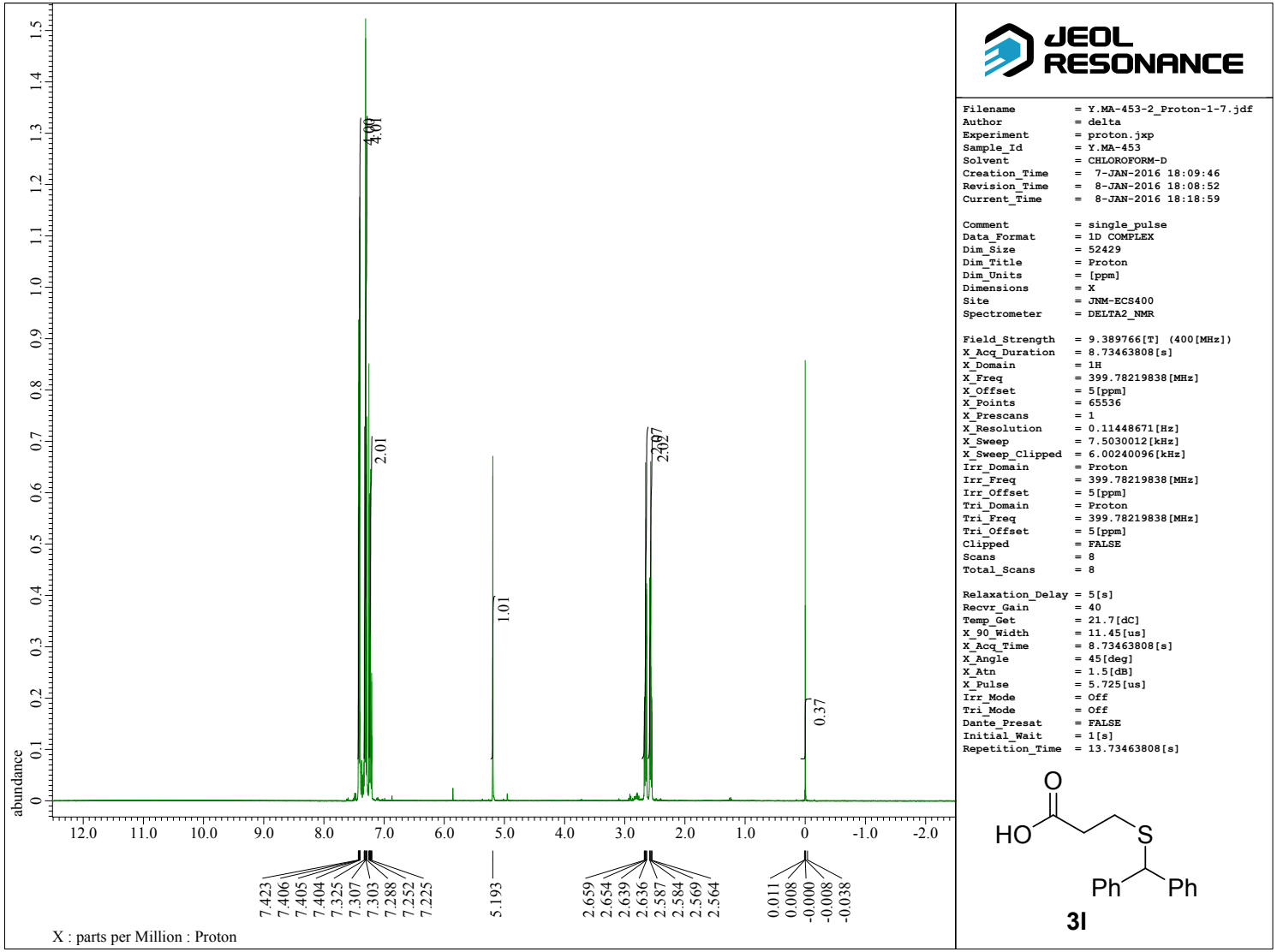
3k



JEOL RESONANCE

Filename	= Y.MA-358_Carbon-1-7.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= Y.MA-358
Solvent	= CHLOROFORM-D
Creation_Time	= 14-OCT-2015 00:20:43
Revision_Time	= 30-DEC-2015 16:57:21
Current_Time	= 30-DEC-2015 16:57:34
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
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	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20.6[dC]
X_90_Width	= 7.63[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 3.3[dB]
X_Pulse	= 2.54333333[us]
Irr_Atn_Dec	= 21.538[dB]
Irr_Atn_Noe	= 21.538[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]

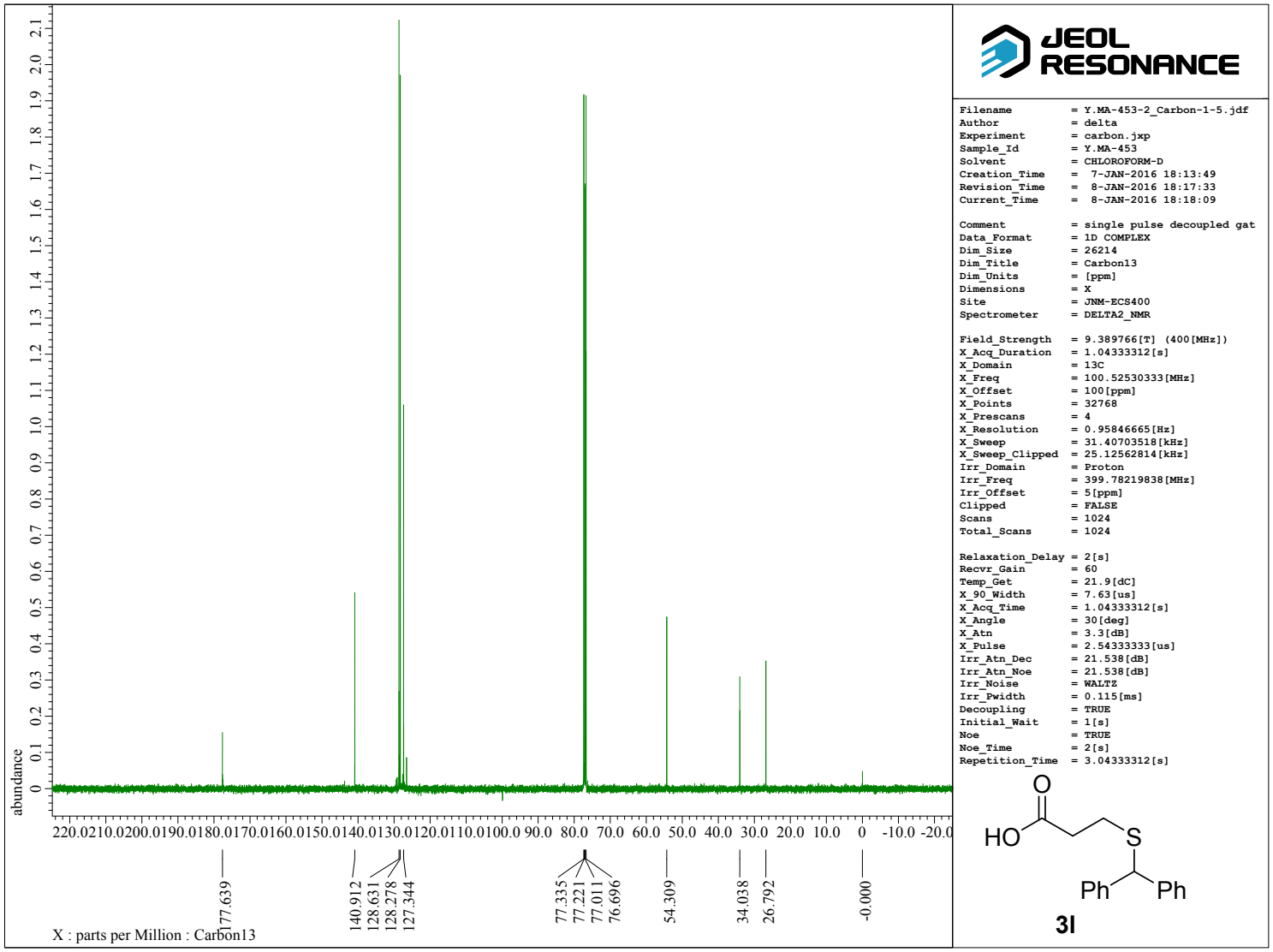
3k



JEOL RESONANCE

```
Filename          = Y.MA-453-2_Proton-1-7.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-453
Solvent           = CHLOROFORM-D
Creation_Time     =  7-JAN-2016 18:09:46
Revision_Time     =  8-JAN-2016 18:08:52
Current_Time      =  8-JAN-2016 18:18:59

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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        = 40
Temp_Get          = 21.7[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```

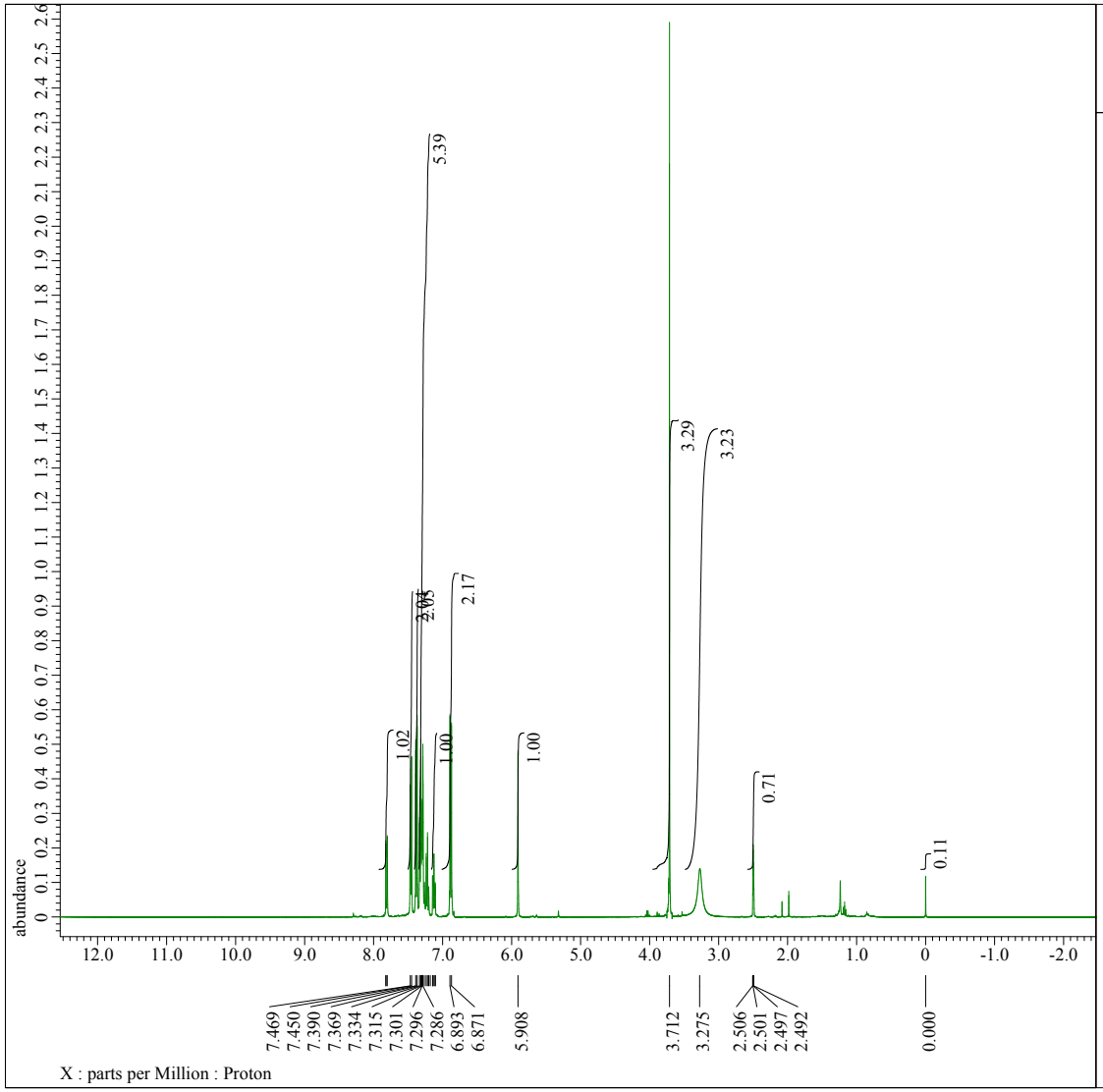

3l



JEOL RESONANCE

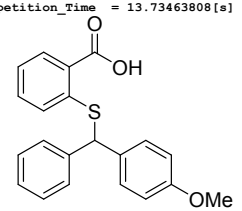
```
Filename          = Y.MA-453-2_Carbon-1-5.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-453
Solvent           = CHLOROFORM-D
Creation_Time     =  7-JAN-2016 18:13:49
Revision_Time     =  8-JAN-2016 18:17:33
Current_Time      =  8-JAN-2016 18:18:09

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.9[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```


3l

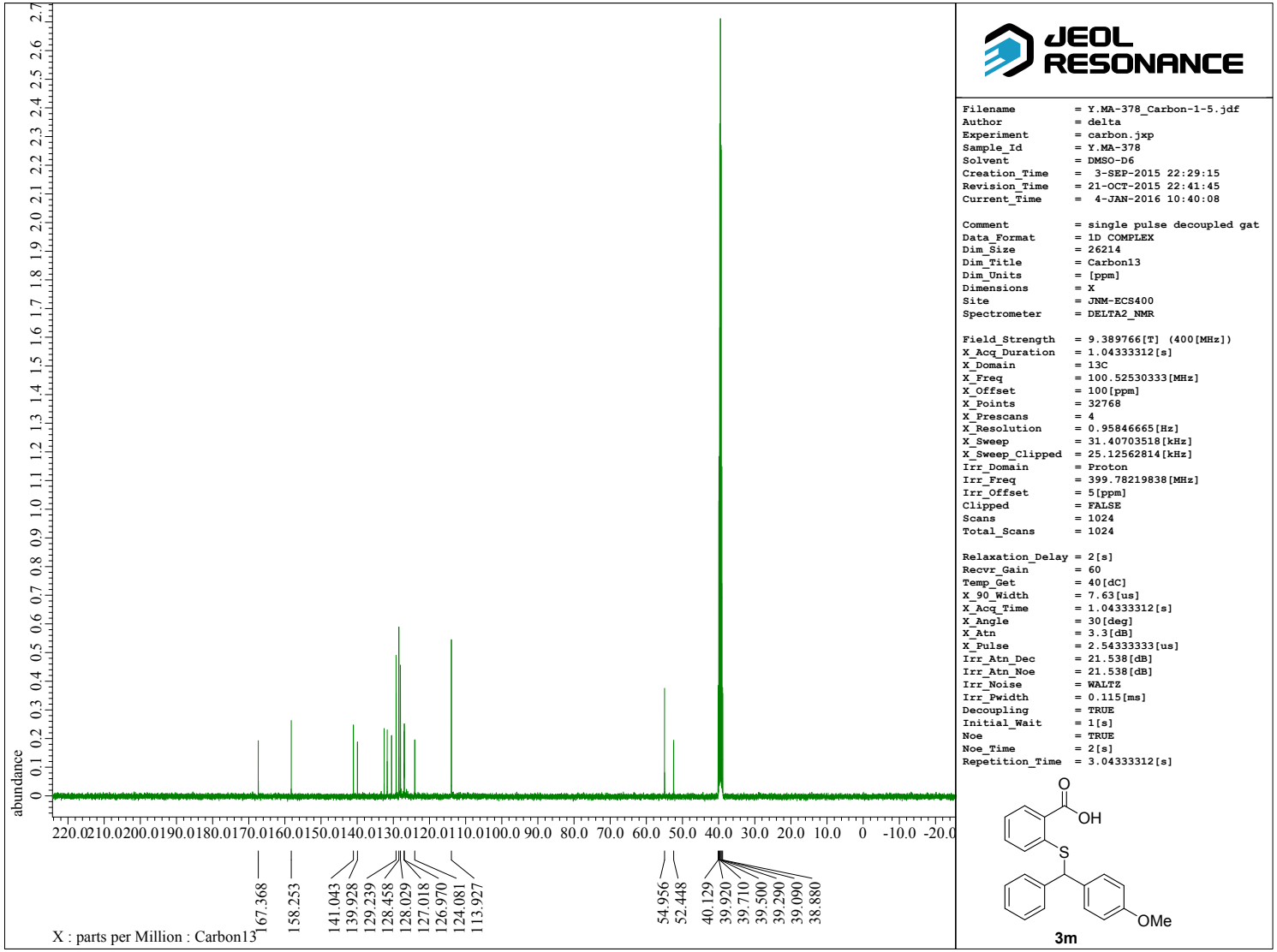


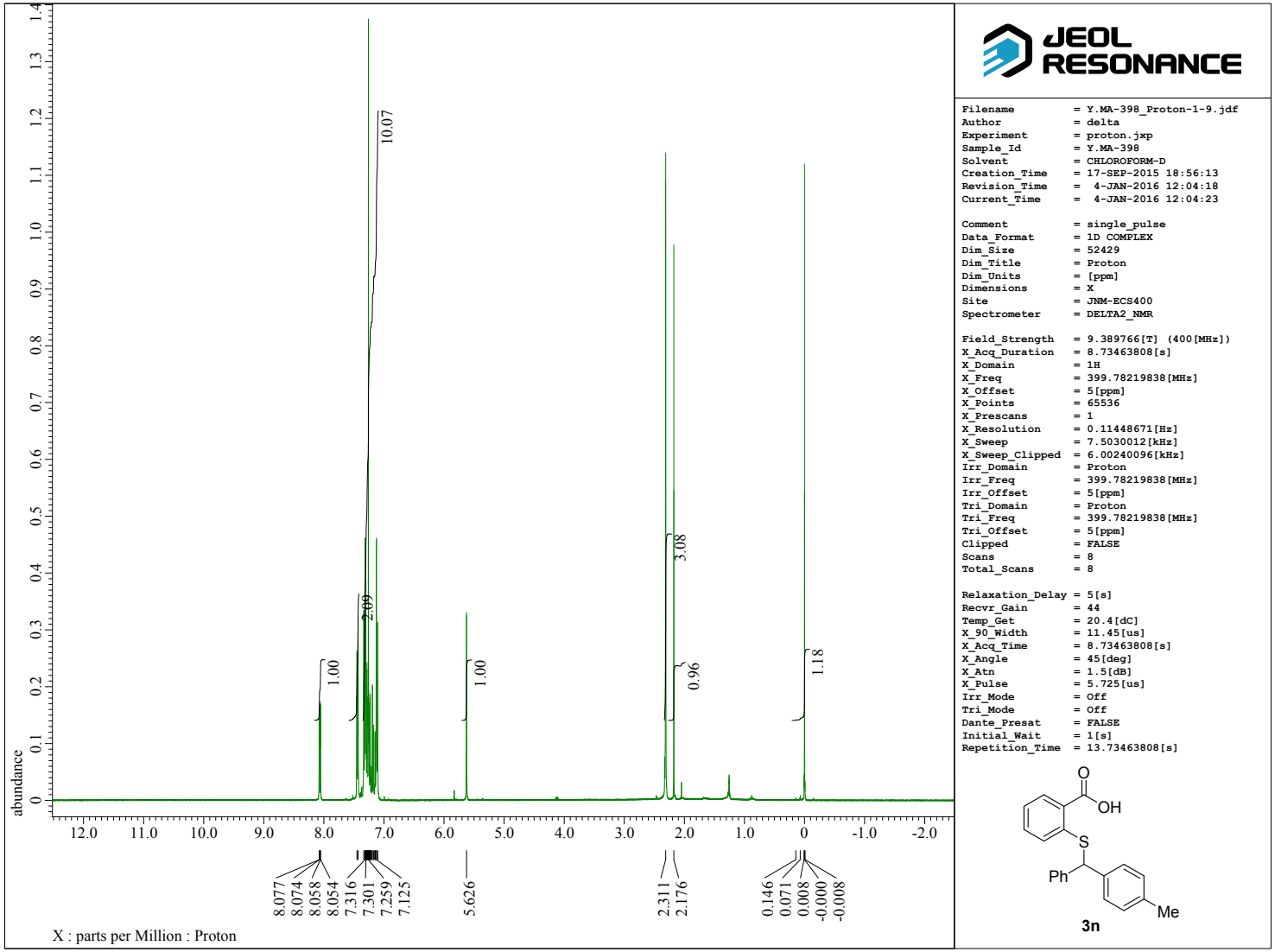
JEOL RESONANCE

```
Filename          = Y.MA-378_Proton-2-7.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-378
Solvent           = DMSO-D6
Creation_Time     =  3-SEP-2015 22:21:44
Revision_Time     =  4-JAN-2016 10:32:26
Current_Time      =  4-JAN-2016 10:32:41

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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        = 40
Temp_Get          = 40[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```



3m

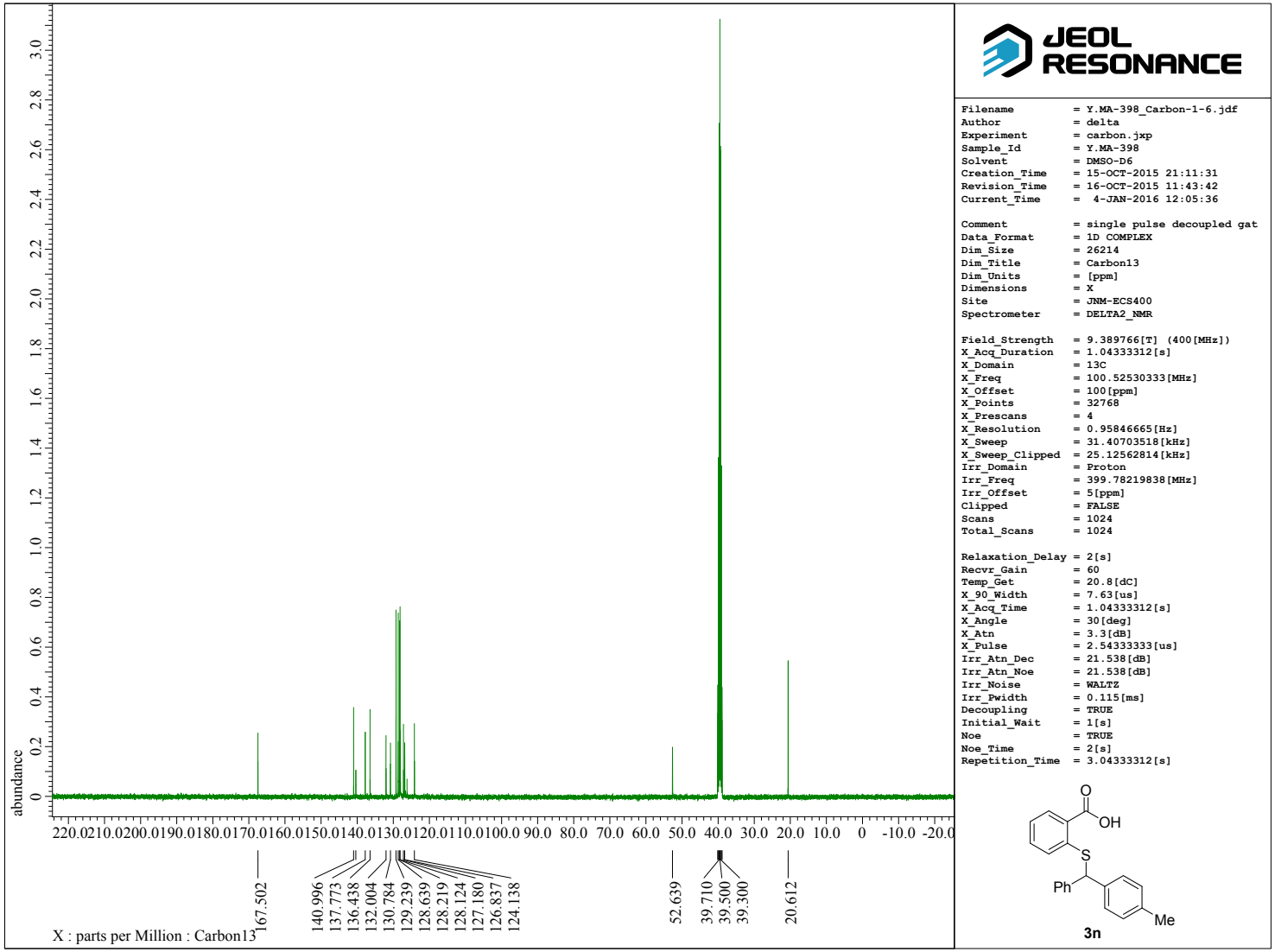

abundance
X : parts per Million : Carbon13
167.368
158.253
141.043
139.928
129.239
128.458
128.029
127.018
126.970
124.081
113.927
54.956
52.448
40.129
39.920
39.710
39.500
39.290
39.090
38.880
JEOL RESONANCE
Filename = Y.MA-378_Carbon-1-5.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = Y.MA-378
Solvent = DMSO-D6
Creation_Time = 3-SEP-2015 22:29:15
Revision_Time = 21-OCT-2015 22:41:45
Current_Time = 4-JAN-2016 10:40:08
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
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 = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 40[dC]
X_90_Width = 7.63[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 3.3[dB]
X_Pulse = 2.54333333[us]
Irr_Atn_Dec = 21.538[dB]
Irr_Atn_Noe = 21.538[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
O
OH
S
OMe
3m



JEOL RESONANCE

```
Filename          = Y.MA-398_Proton-1-9.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-398
Solvent           = CHLOROFORM-D
Creation_Time     = 17-SEP-2015 18:56:13
Revision_Time     =  4-JAN-2016 12:04:18
Current_Time      =  4-JAN-2016 12:04:23

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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          = 20.4[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```

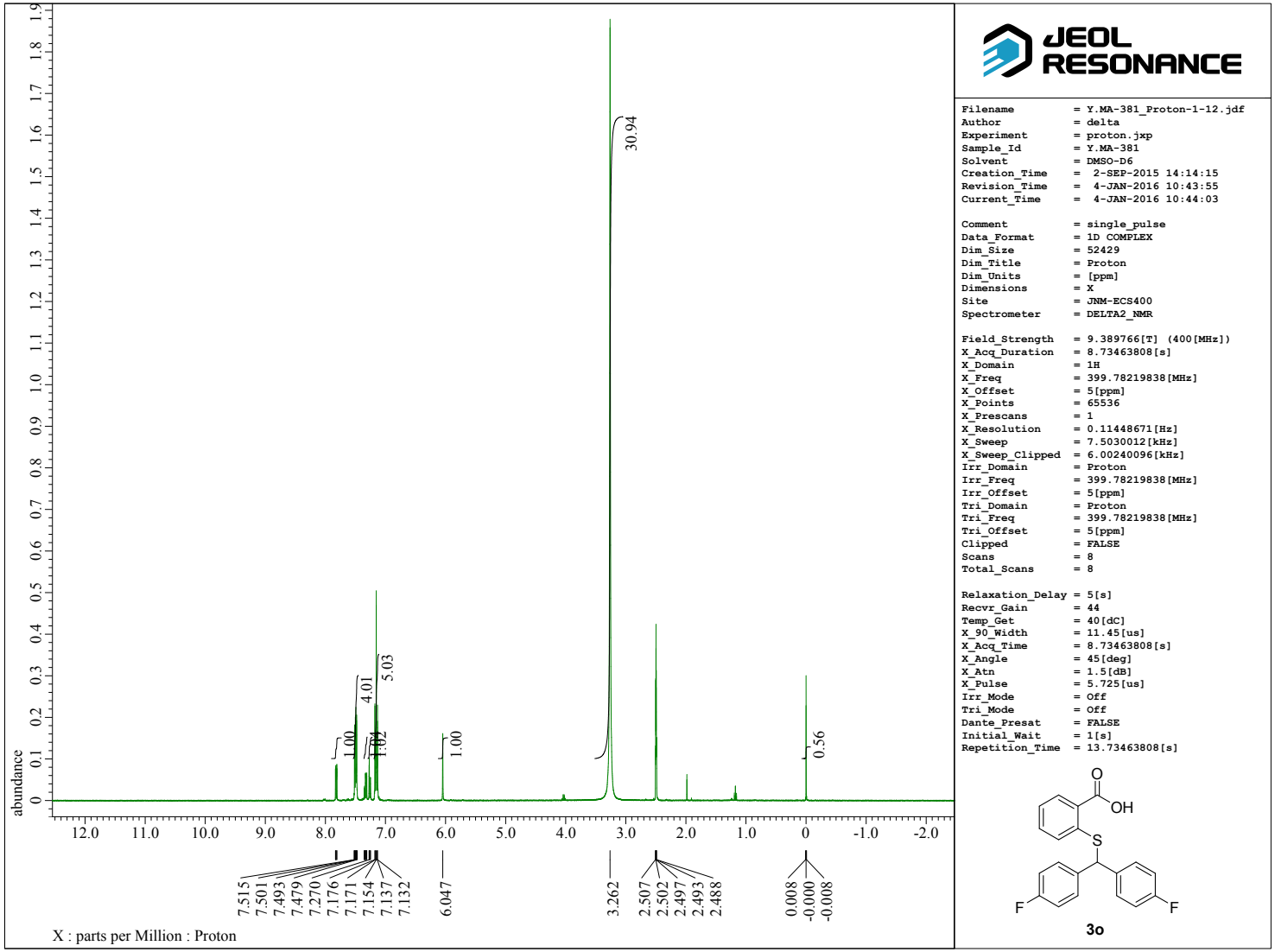

3n



JEOL RESONANCE

```
Filename          = Y.MA-398_Carbon-1-6.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-398
Solvent           = DMSO-D6
Creation_Time     = 15-OCT-2015 21:11:31
Revision_Time     = 16-OCT-2015 11:43:42
Current_Time      =  4-JAN-2016 12:05:36

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 20.8[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

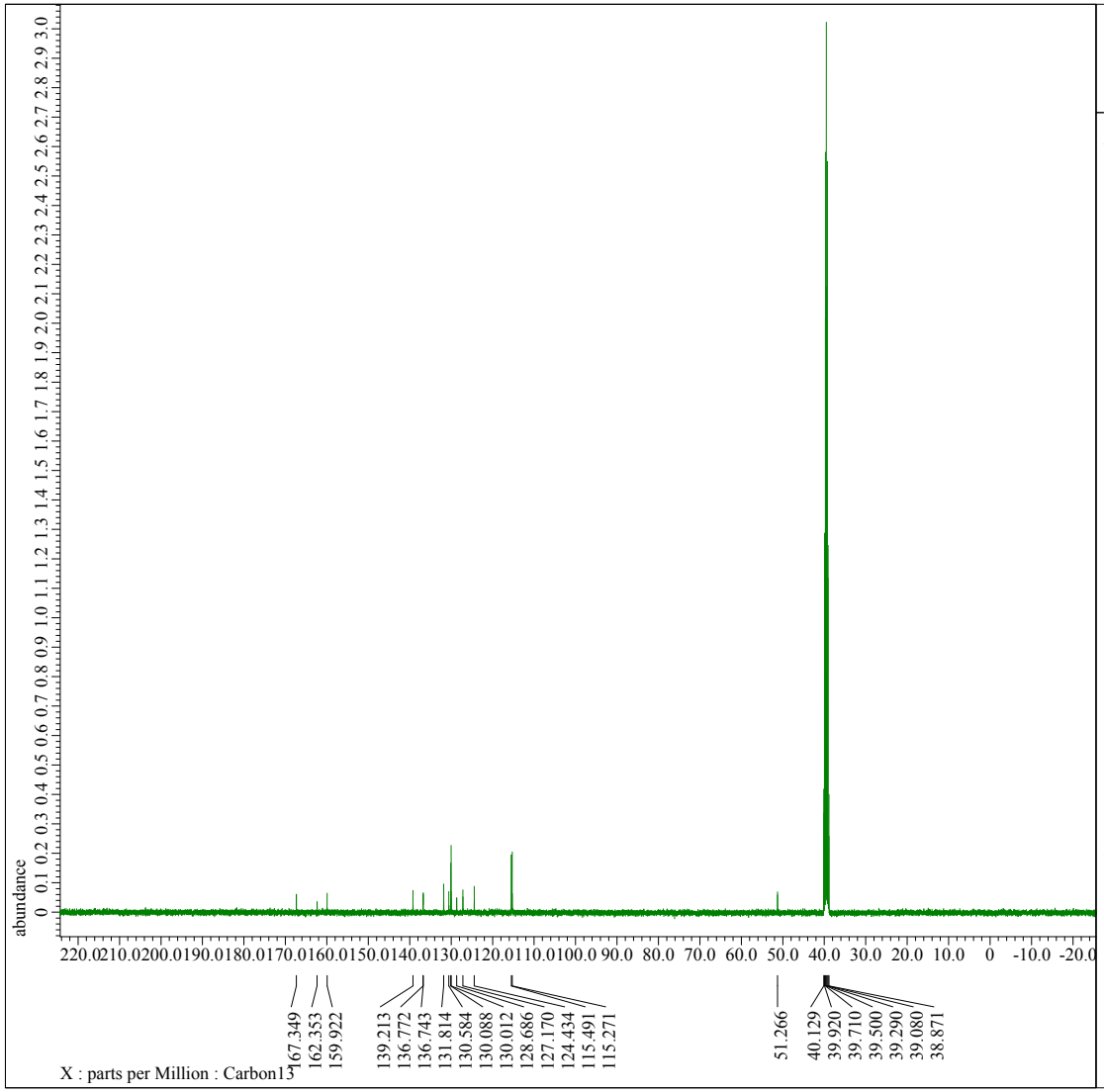

3n



JEOL RESONANCE

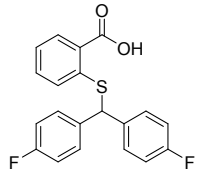
```
Filename          = Y.MA-381_Proton-1-12.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-381
Solvent           = DMSO-D6
Creation_Time     =  2-SEP-2015 14:14:15
Revision_Time     =  4-JAN-2016 10:43:55
Current_Time      =  4-JAN-2016 10:44:03

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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          = 40[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```


3o

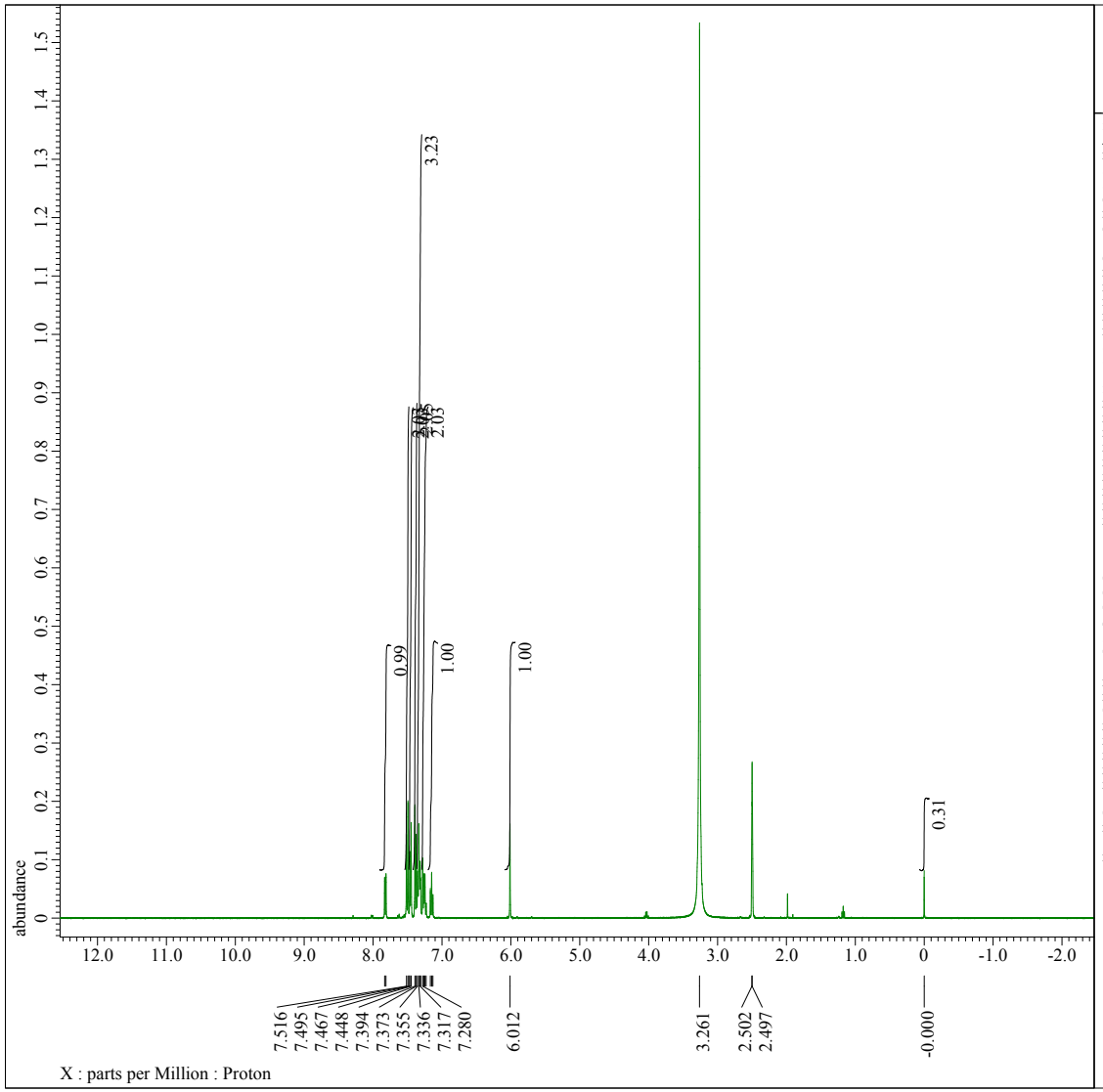


JEOL RESONANCE

```
Filename          = Y.MA-381_Carbon-1-8.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-381
Solvent           = DMSO-D6
Creation_Time     =  3-SEP-2015 23:30:32
Revision_Time     =  4-JAN-2016 10:46:19
Current_Time      =  4-JAN-2016 10:46:32

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 40[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

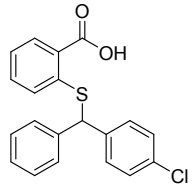


3o

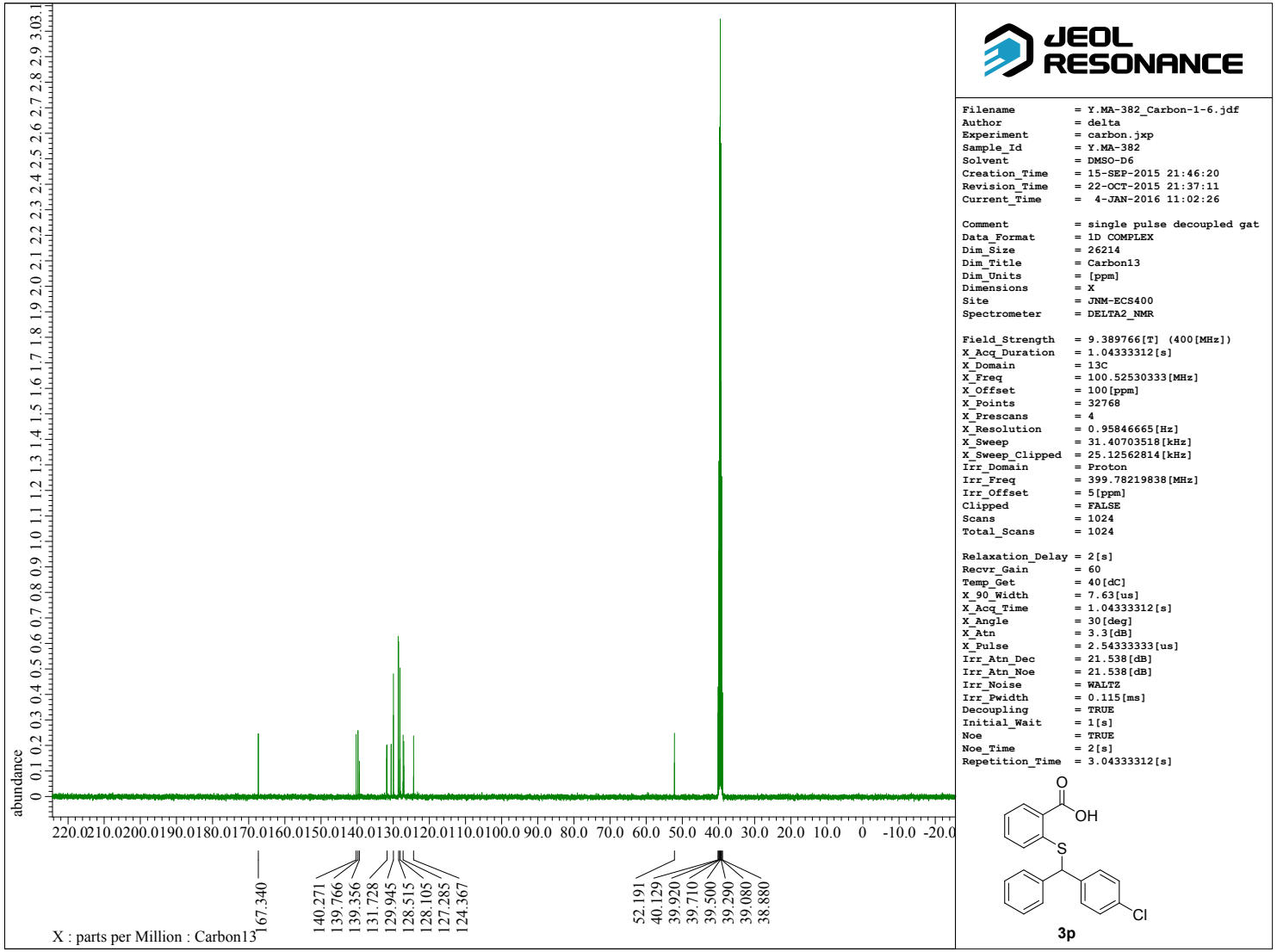


JEOL RESONANCE

```
Filename          = Y.MA-382_Proton-1-8.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-382
Solvent           = DMSO-D6
Creation_Time     = 15-SEP-2015 18:27:09
Revision_Time     =  4-JAN-2016 11:01:22
Current_Time      =  4-JAN-2016 11:01:28

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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          = 40[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```



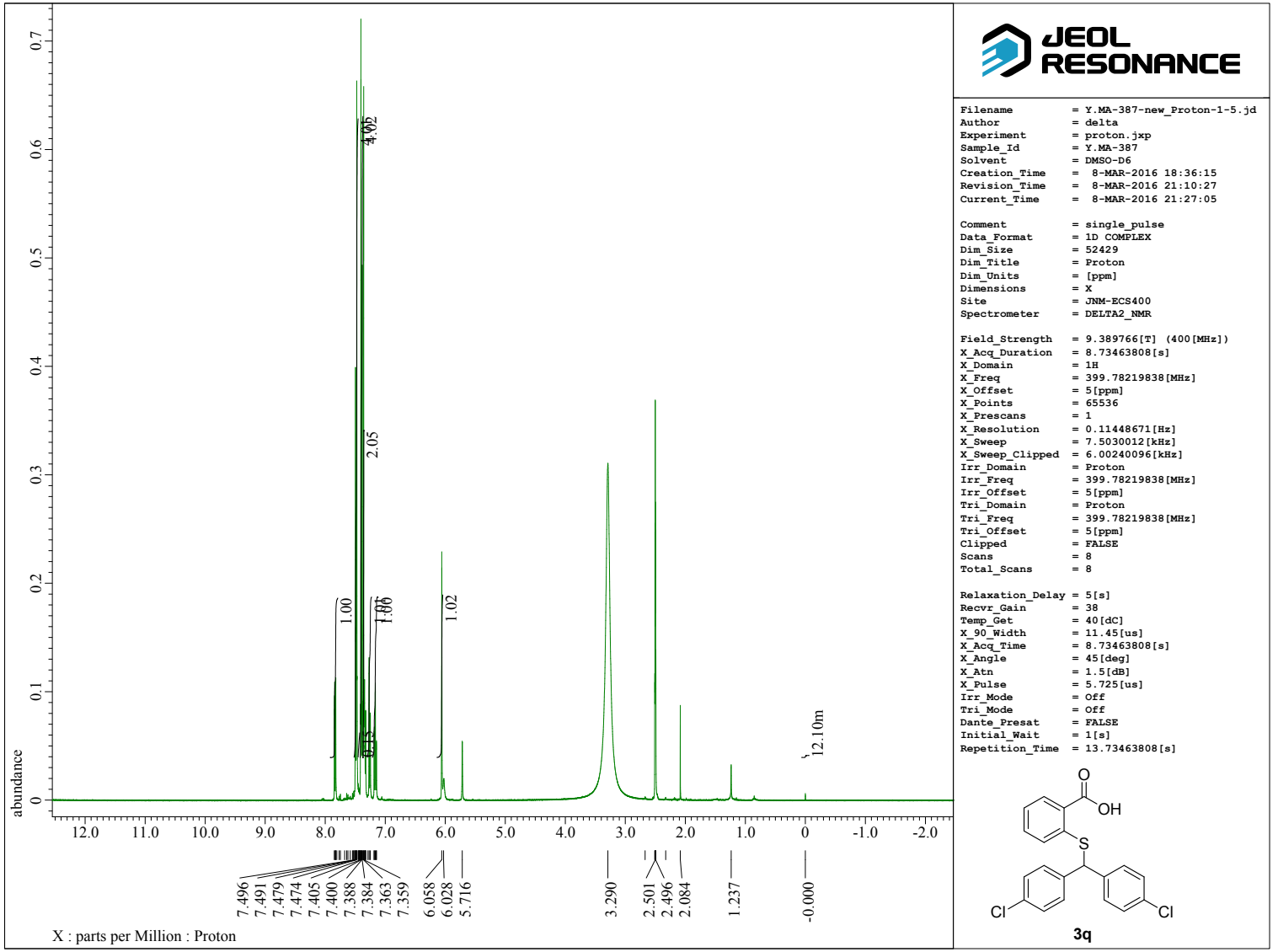
3p



JEOL RESONANCE

```
Filename          = Y.MA-382_Carbon-1-6.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-382
Solvent           = DMSO-D6
Creation_Time     = 15-SEP-2015 21:46:20
Revision_Time     = 22-OCT-2015 21:37:11
Current_Time      =  4-JAN-2016 11:02:26

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 40[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

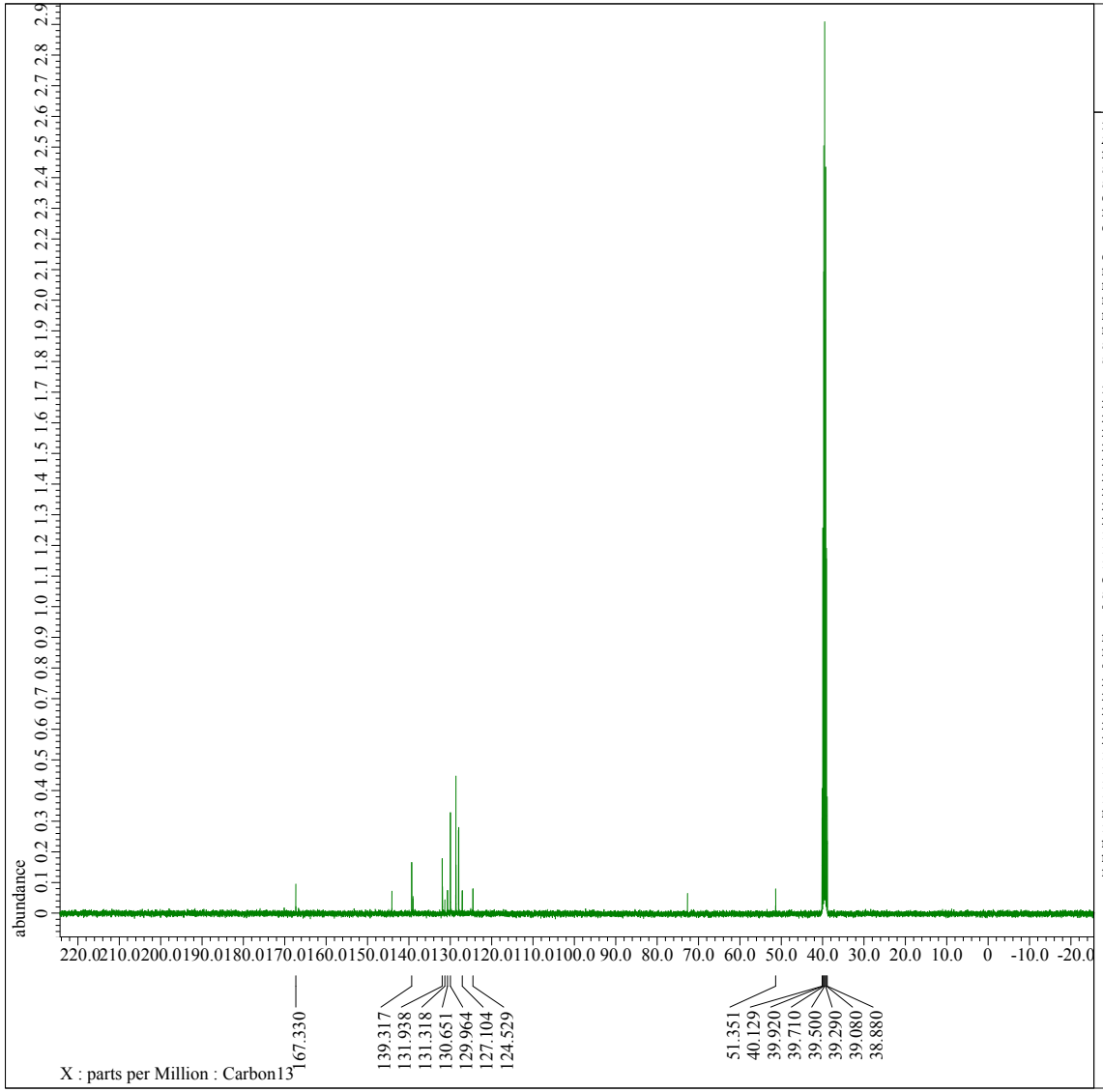

3p



JEOL RESONANCE

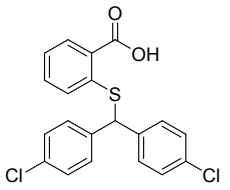
Filename	= Y.MA-387-new_Proton-1-5.jd
Author	= delta
Experiment	= proton.jxp
Sample_Id	= Y.MA-387
Solvent	= DMSO-D6
Creation_Time	= 8-MAR-2016 18:36:15
Revision_Time	= 8-MAR-2016 21:10:27
Current_Time	= 8-MAR-2016 21:27:05
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 8.73463808[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 65536
X_Prescans	= 1
X_Resolution	= 0.11448671[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	= 40[dC]
X_90_Width	= 11.45[us]
X_Acq_Time	= 8.73463808[s]
X_Angle	= 45[deg]
X_Atn	= 1.5[dB]
X_Pulse	= 5.725[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 13.73463808[s]

3q

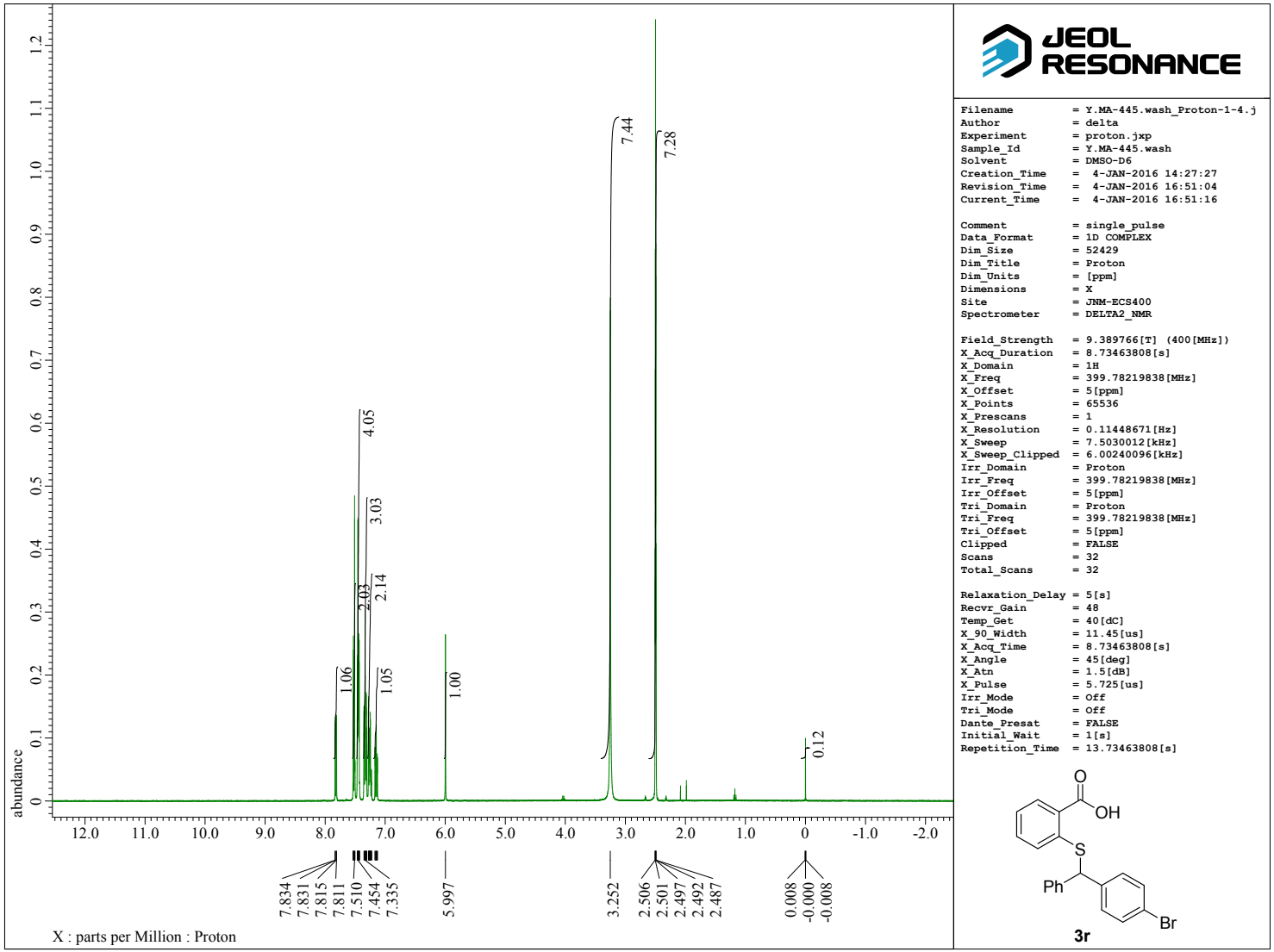


JEOL RESONANCE

```
Filename          = Y.MA-387-new_Carbon-1-5.jd
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-387
Solvent           = DMSO-D6
Creation_Time     =  8-MAR-2016 18:42:06
Revision_Time     =  8-MAR-2016 21:18:15
Current_Time      =  8-MAR-2016 21:27:21

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 40[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



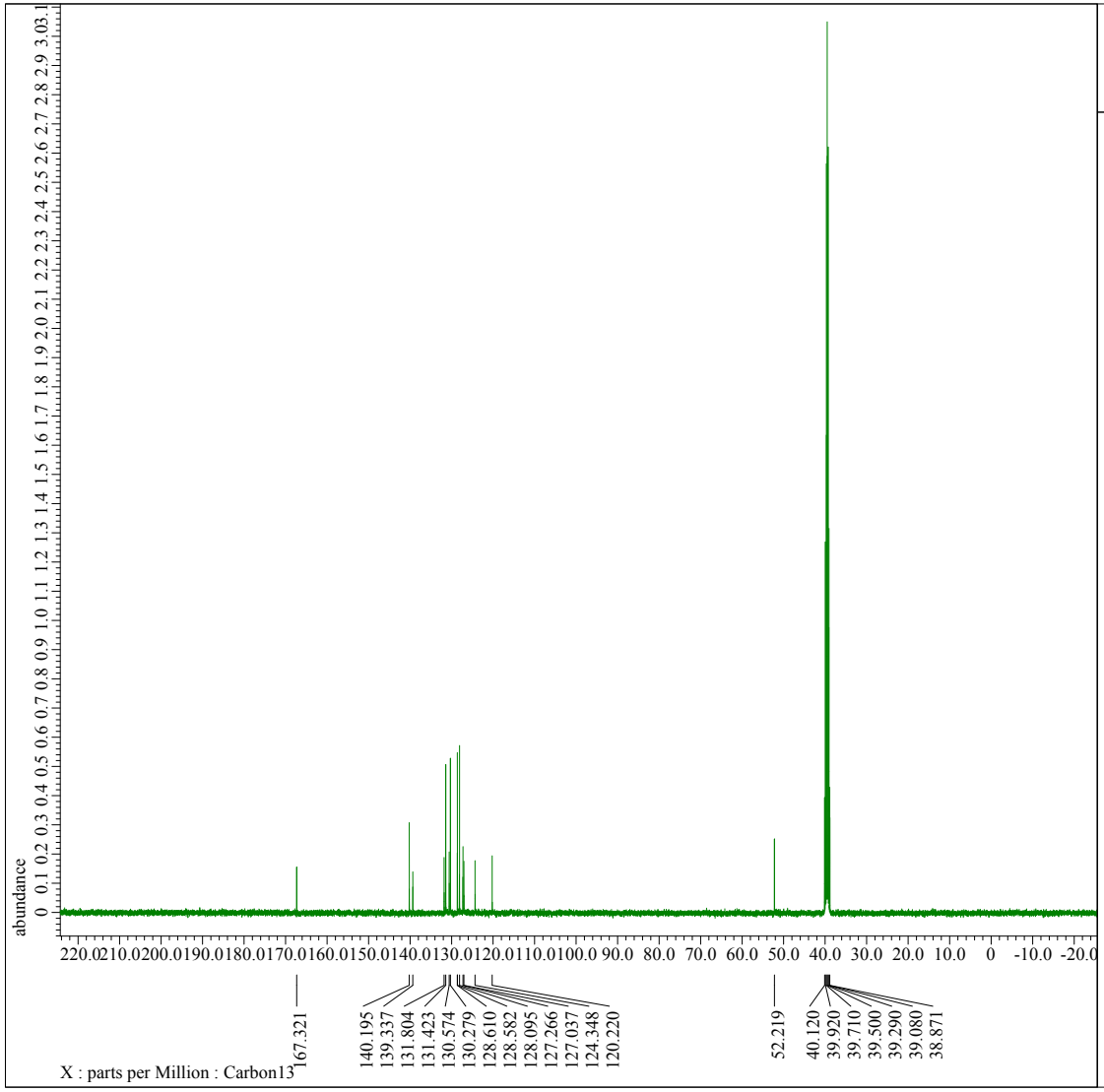
3q



JEOL RESONANCE

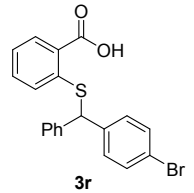
```
Filename          = Y.MA-445.wash_Proton-1-4.j
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-445.wash
Solvent           = DMSO-D6
Creation_Time     =  4-JAN-2016 14:27:27
Revision_Time     =  4-JAN-2016 16:51:04
Current_Time      =  4-JAN-2016 16:51:16

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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             = 32
Total_Scans       = 32

Relaxation_Delay = 5[s]
Recvr_Gain        = 48
Temp_Get          = 40[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```


3r

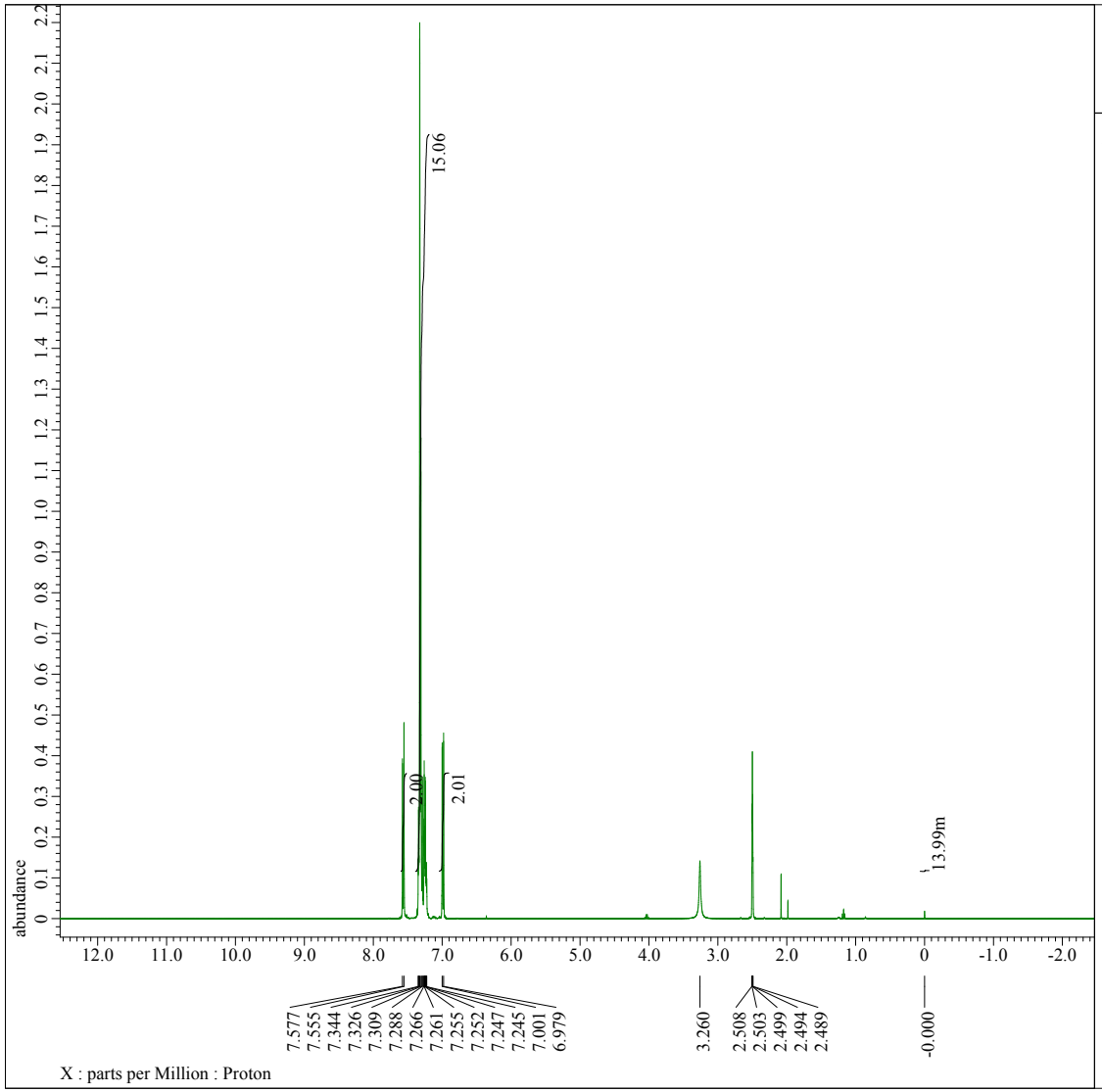


JEOL RESONANCE

Filename	= Y.MA-445.wash_Carbon-1-3.j
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= Y.MA-445.wash
Solvent	= DMSO-D6
Creation_Time	= 4-JAN-2016 14:59:21
Revision_Time	= 4-JAN-2016 17:06:20
Current_Time	= 4-JAN-2016 17:06:49
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
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	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 40[dC]
X_90_Width	= 7.63[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 3.3[dB]
X_Pulse	= 2.54333333[us]
Irr_Atn_Dec	= 21.538[dB]
Irr_Atn_Noe	= 21.538[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]

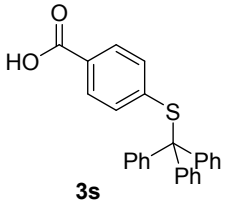


3r

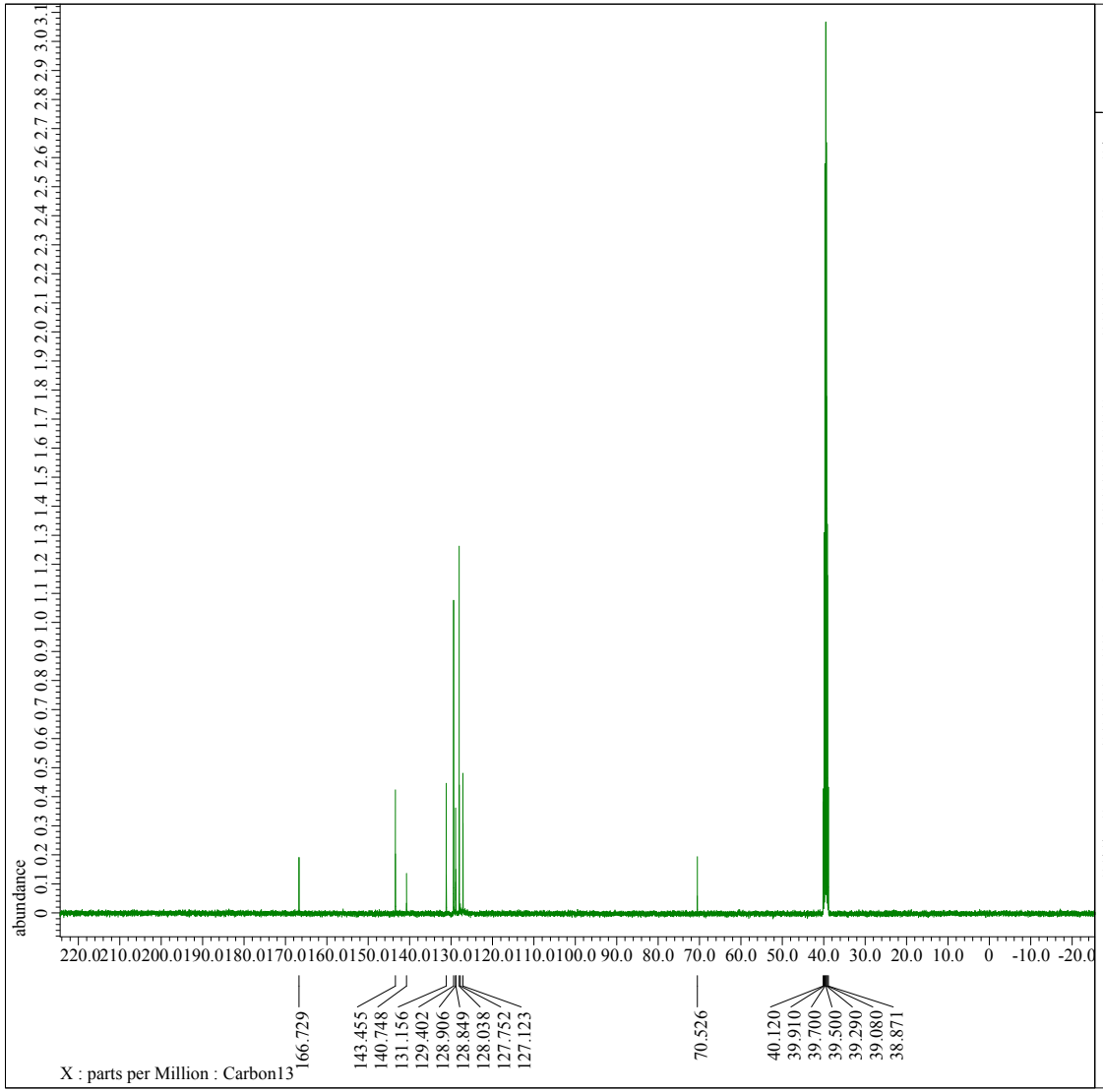


JEOL RESONANCE

```
Filename          = Y.MA-410-wash_Proton-1-7.j
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-410
Solvent           = DMSO-D6
Creation_Time     =  7-JAN-2016 20:24:27
Revision_Time     =  8-JAN-2016 12:47:24
Current_Time      =  8-JAN-2016 12:47:49

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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        = 40
Temp_Get          = 40[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```

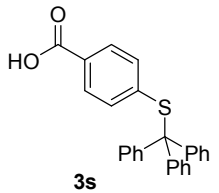


3s

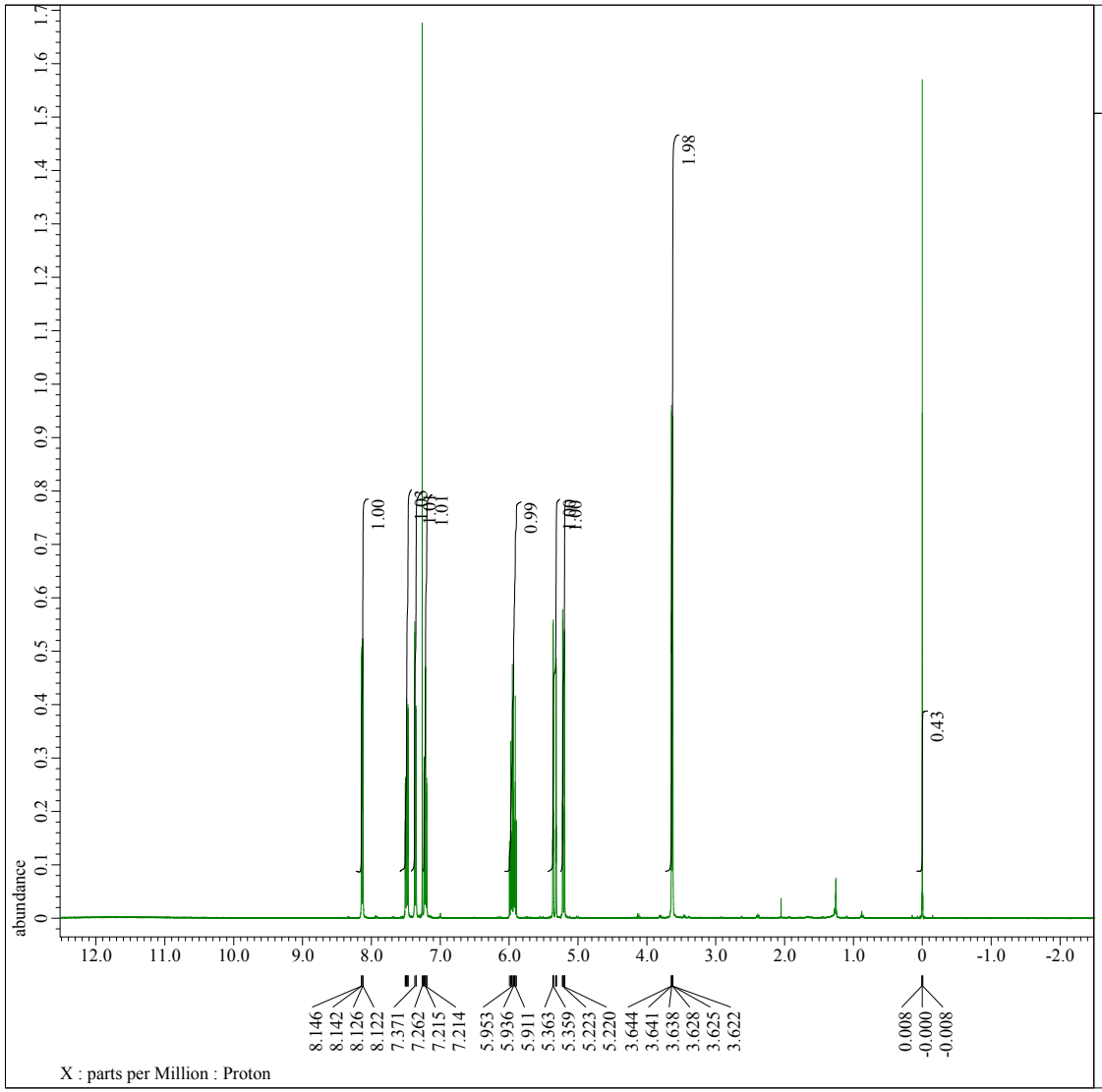


JEOL RESONANCE

```
Filename          = Y.MA-410-wash_Carbon-1-3.j
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-410
Solvent           = DMSO-D6
Creation_Time     =  7-JAN-2016 20:28:29
Revision_Time     =  8-JAN-2016 10:20:14
Current_Time      =  8-JAN-2016 12:41:07

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.8[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

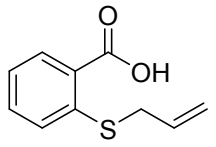


3s

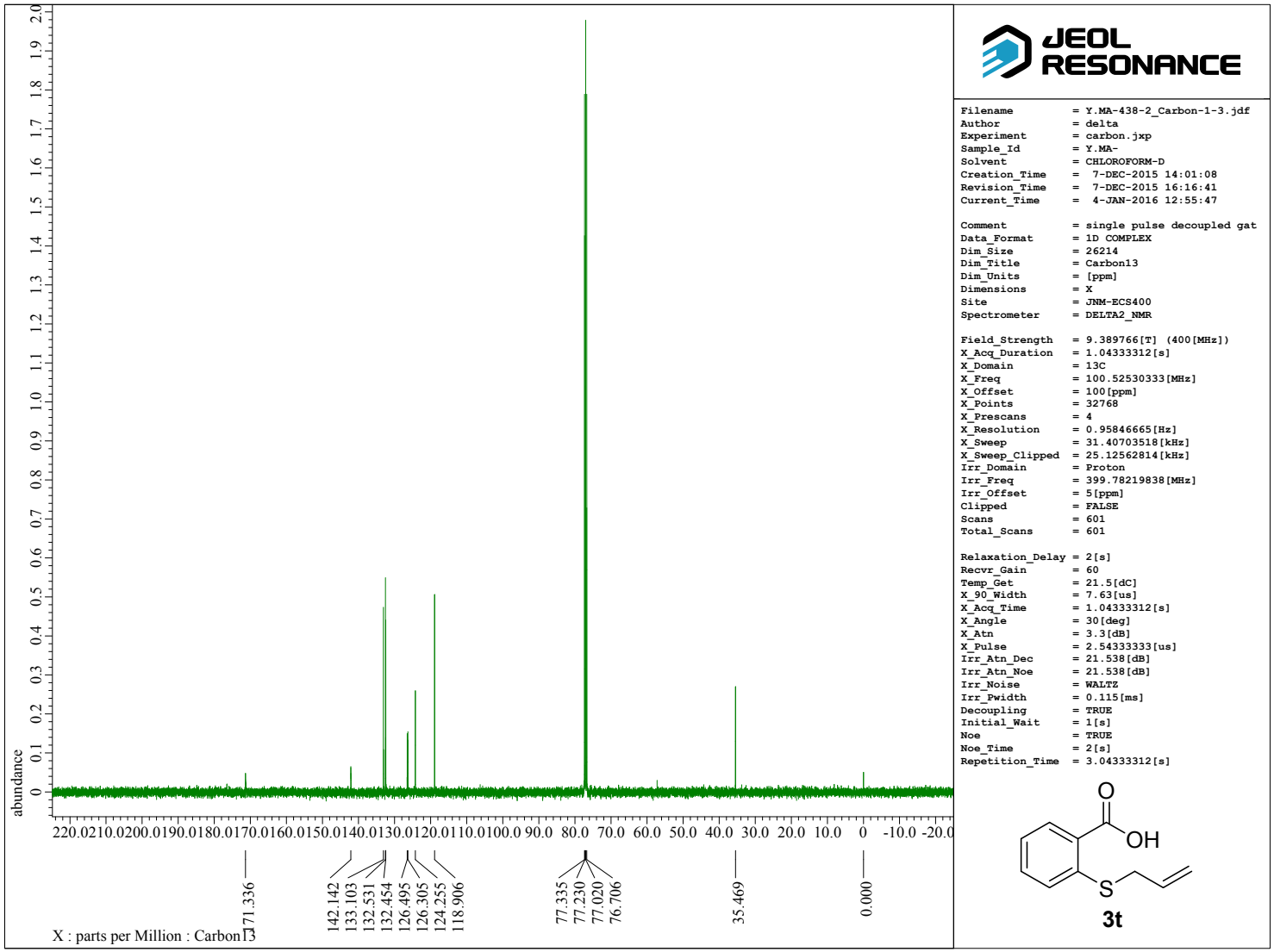


JEOL RESONANCE

```
Filename          = Y.MA-438_Proton-1-10.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-438
Solvent           = CHLOROFORM-D
Creation_Time     = 21-OCT-2015 12:55:27
Revision_Time     =  4-JAN-2016 12:46:58
Current_Time      =  4-JAN-2016 12:47:11

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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          = 20.4[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```



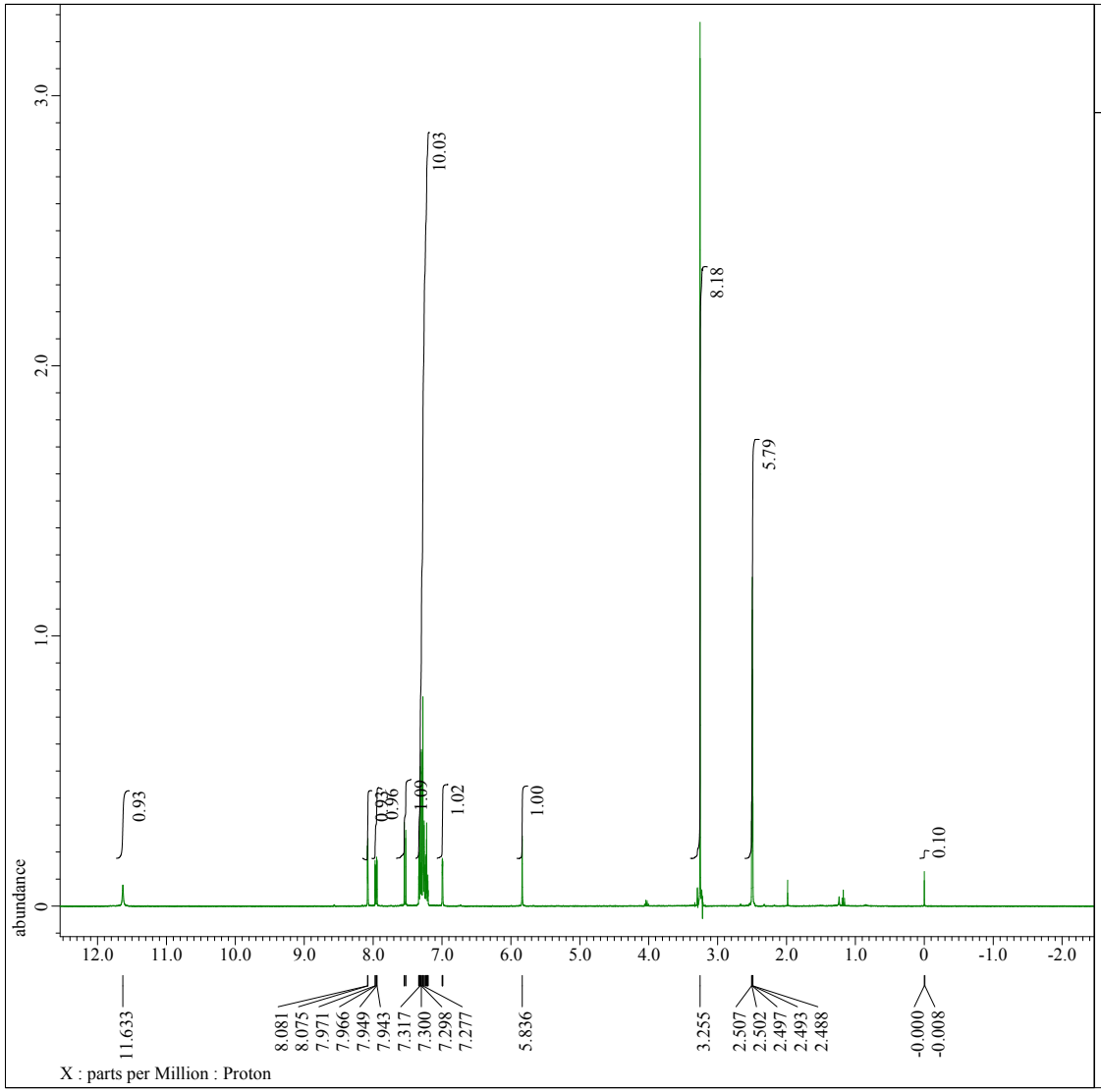
3t



JEOL RESONANCE

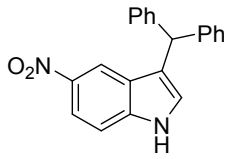
```
Filename          = Y.MA-438-2_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-
Solvent           = CHLOROFORM-D
Creation_Time     =  7-DEC-2015 14:01:08
Revision_Time     =  7-DEC-2015 16:16:41
Current_Time      =  4-JAN-2016 12:55:47

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 601
Total_Scans       = 601

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.5[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```


3t

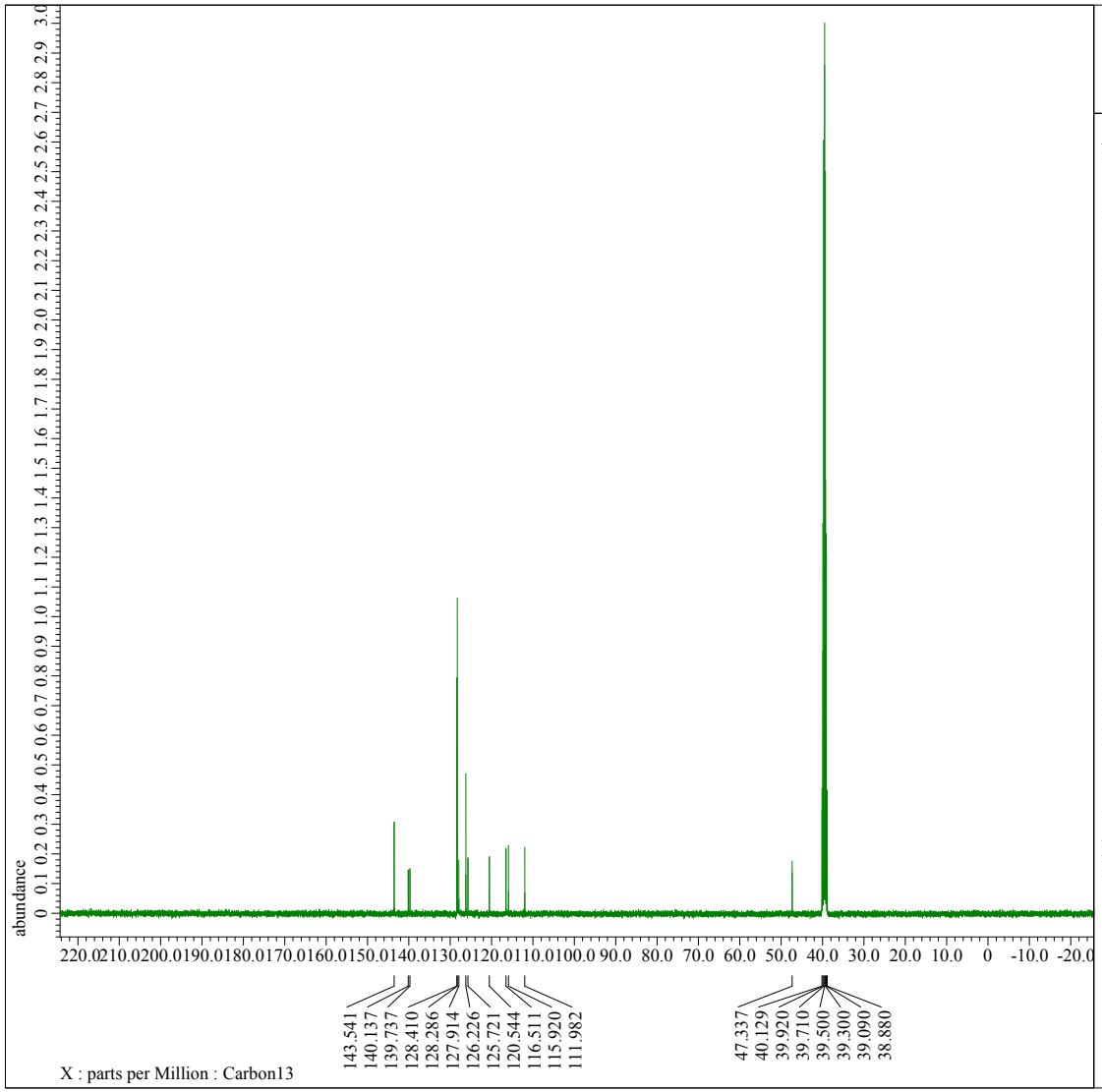


JEOL RESONANCE

```
Filename          = Y.MA-431_Proton-1-8.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-431
Solvent           = DMSO-D6
Creation_Time     = 23-OCT-2015 10:45:47
Revision_Time     = 23-OCT-2015 14:39:02
Current_Time      =  4-JAN-2016 17:20:15

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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        = 46
Temp_Get          = 40[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```

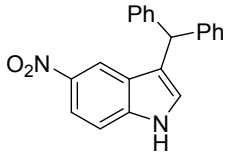


5a

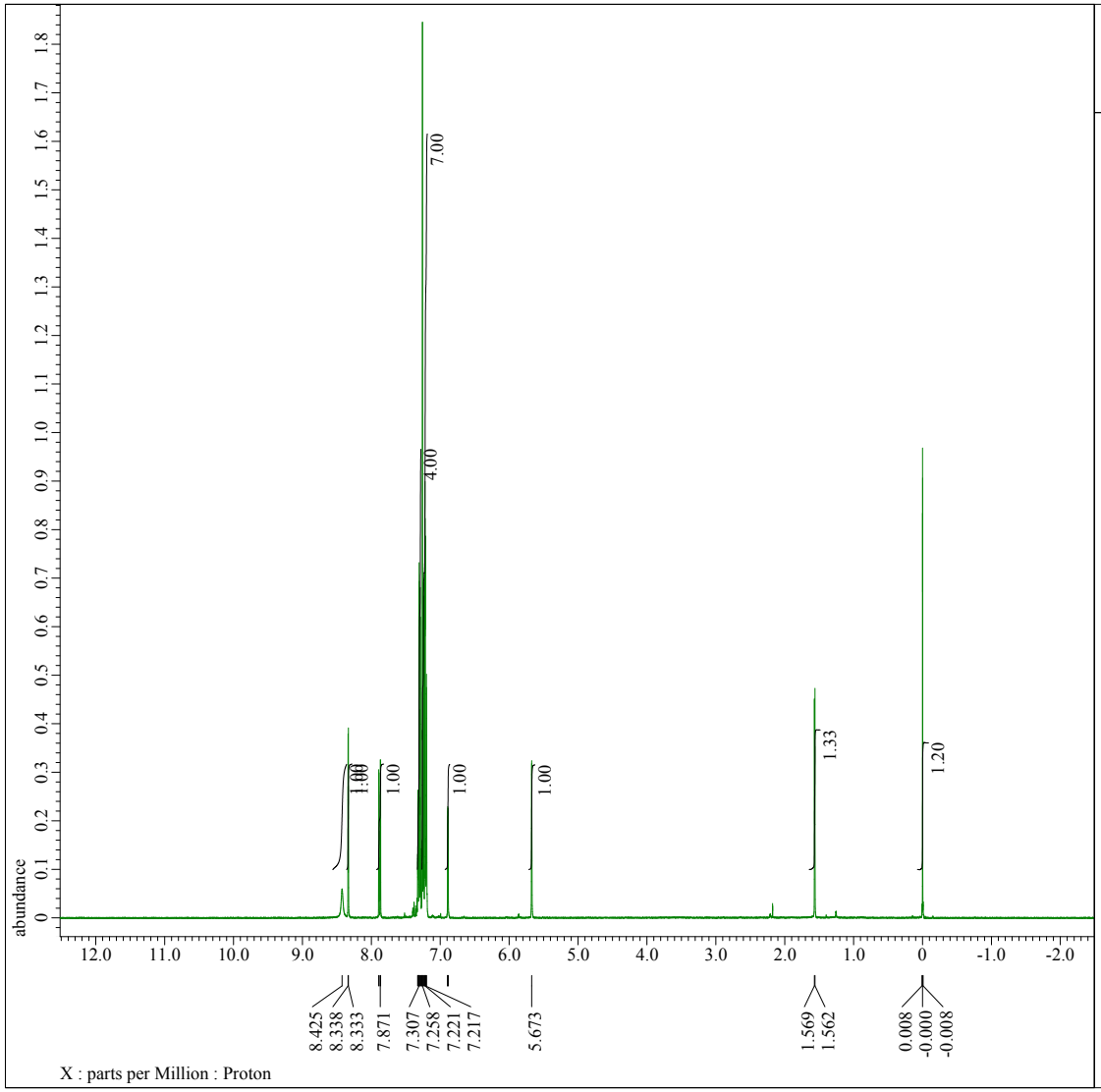


JEOL RESONANCE

```
Filename          = Y.MA-431_Carbon-1-5.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-431
Solvent           = DMSO-D6
Creation_Time     = 23-OCT-2015 11:40:14
Revision_Time     = 24-OCT-2015 15:03:41
Current_Time      =  4-JAN-2016 17:22:11

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 40[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

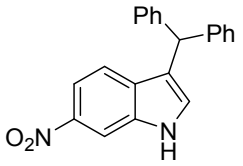


5a

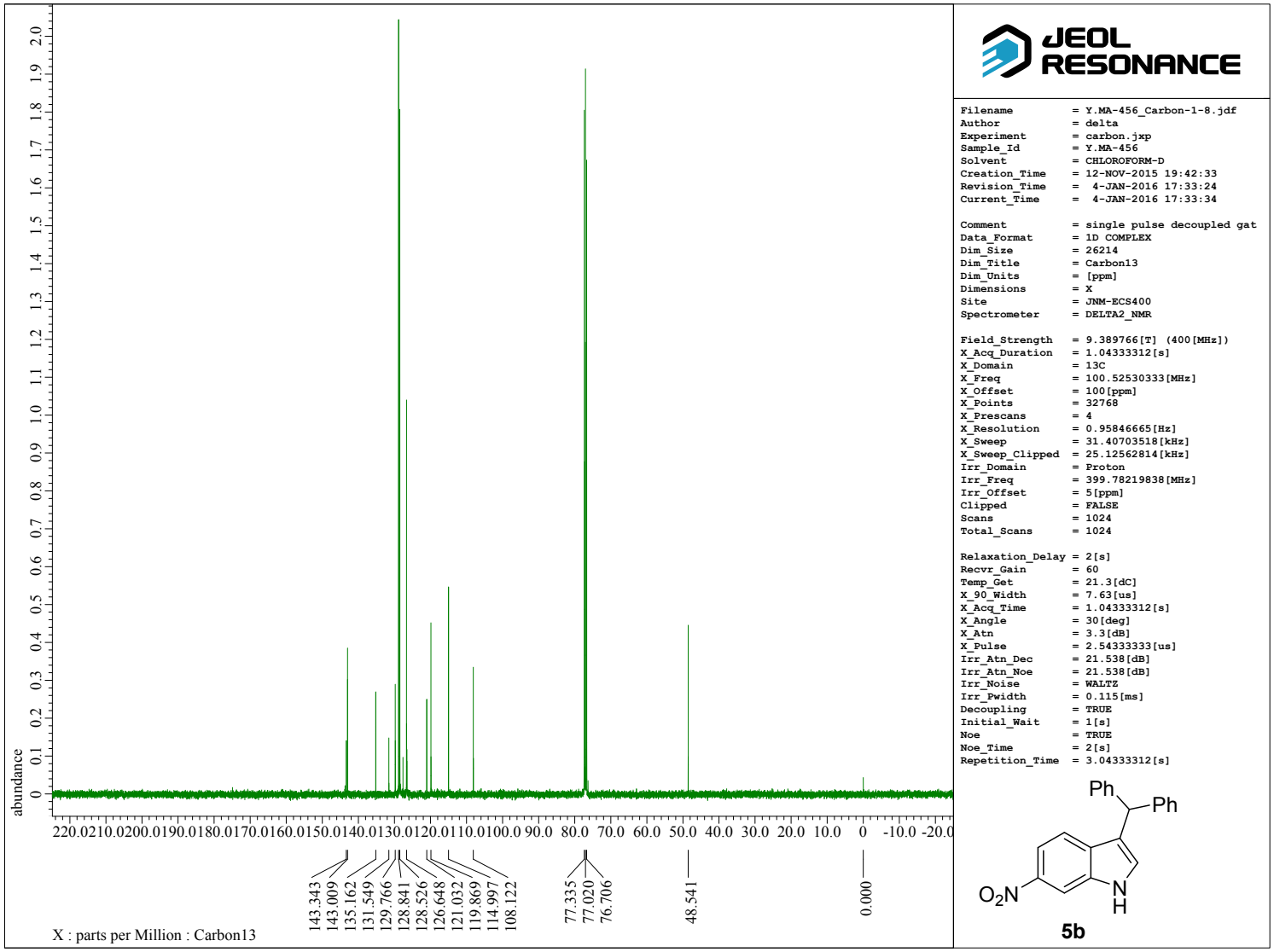


JEOL RESONANCE

```
Filename          = Y.MA-456_Proton-1-10.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-454
Solvent           = CHLOROFORM-D
Creation_Time     = 11-NOV-2015 22:13:25
Revision_Time     = 16-NOV-2015 15:08:30
Current_Time      =  4-JAN-2016 17:31:31

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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        = 46
Temp_Get          = 20.8[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```



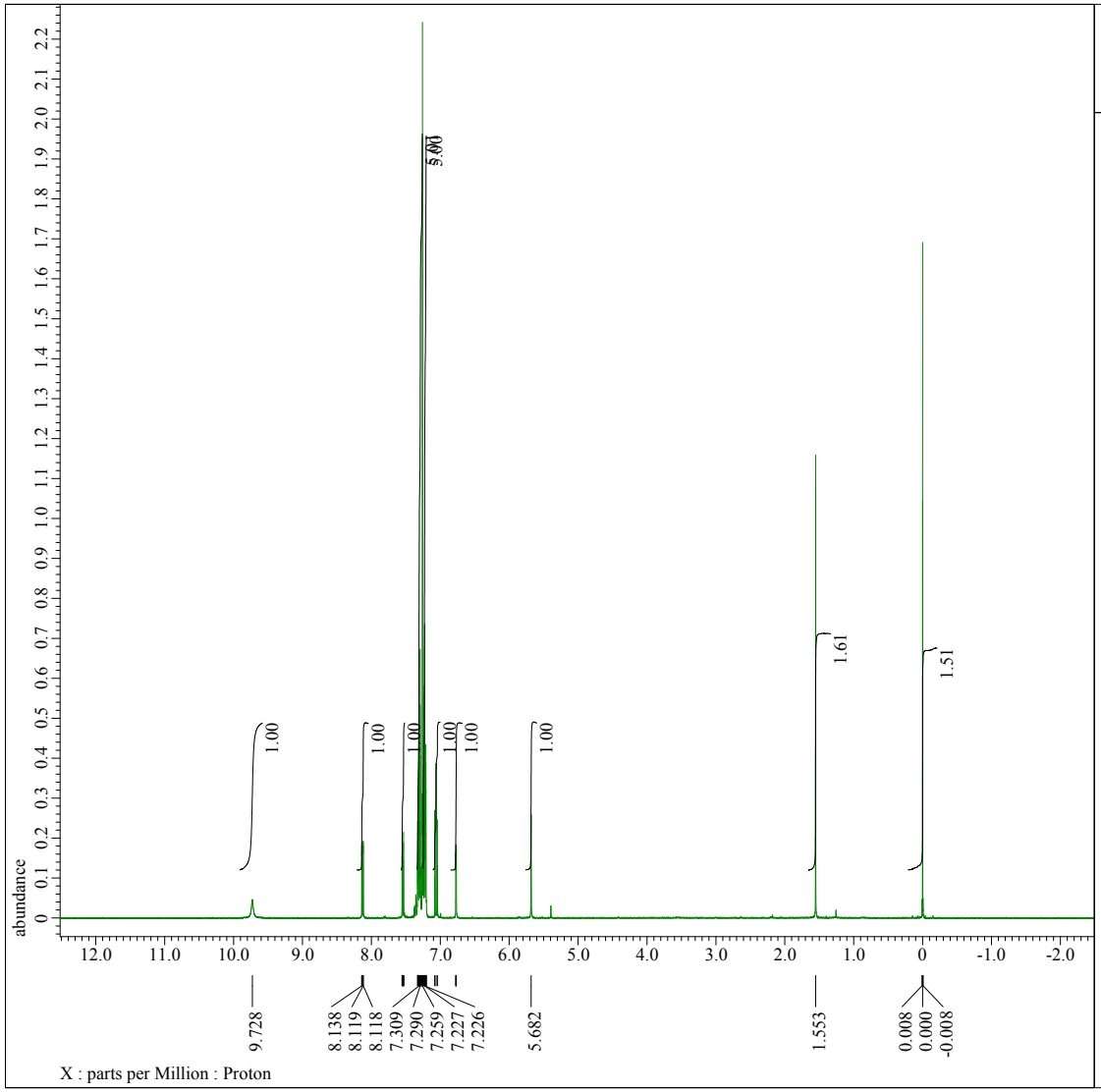
5b



JEOL RESONANCE

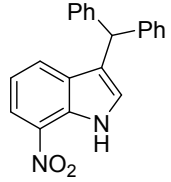
```
Filename          = Y.MA-456_Carbon-1-8.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-456
Solvent           = CHLOROFORM-D
Creation_Time     = 12-NOV-2015 19:42:33
Revision_Time     =  4-JAN-2016 17:33:24
Current_Time      =  4-JAN-2016 17:33:34

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.3[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time  = 3.04333312[s]
```


5b

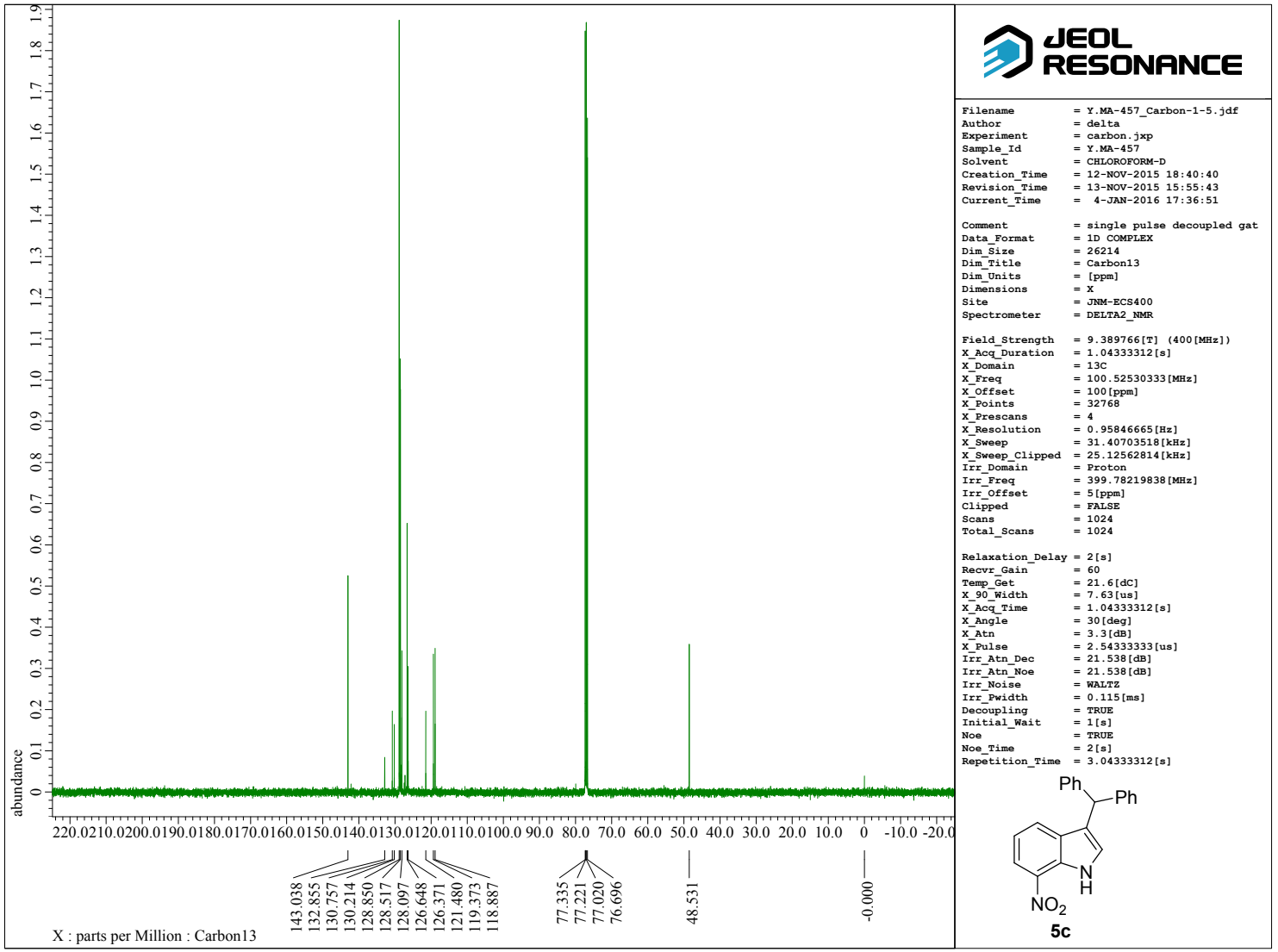


JEOL RESONANCE

```
Filename          = Y.MA-457_Proton-2-8.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-457
Solvent           = CHLOROFORM-D
Creation_Time     = 12-NOV-2015 17:51:03
Revision_Time     =  4-JAN-2016 17:35:30
Current_Time      =  4-JAN-2016 17:35:43

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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        = 46
Temp_Get          = 20.3[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```



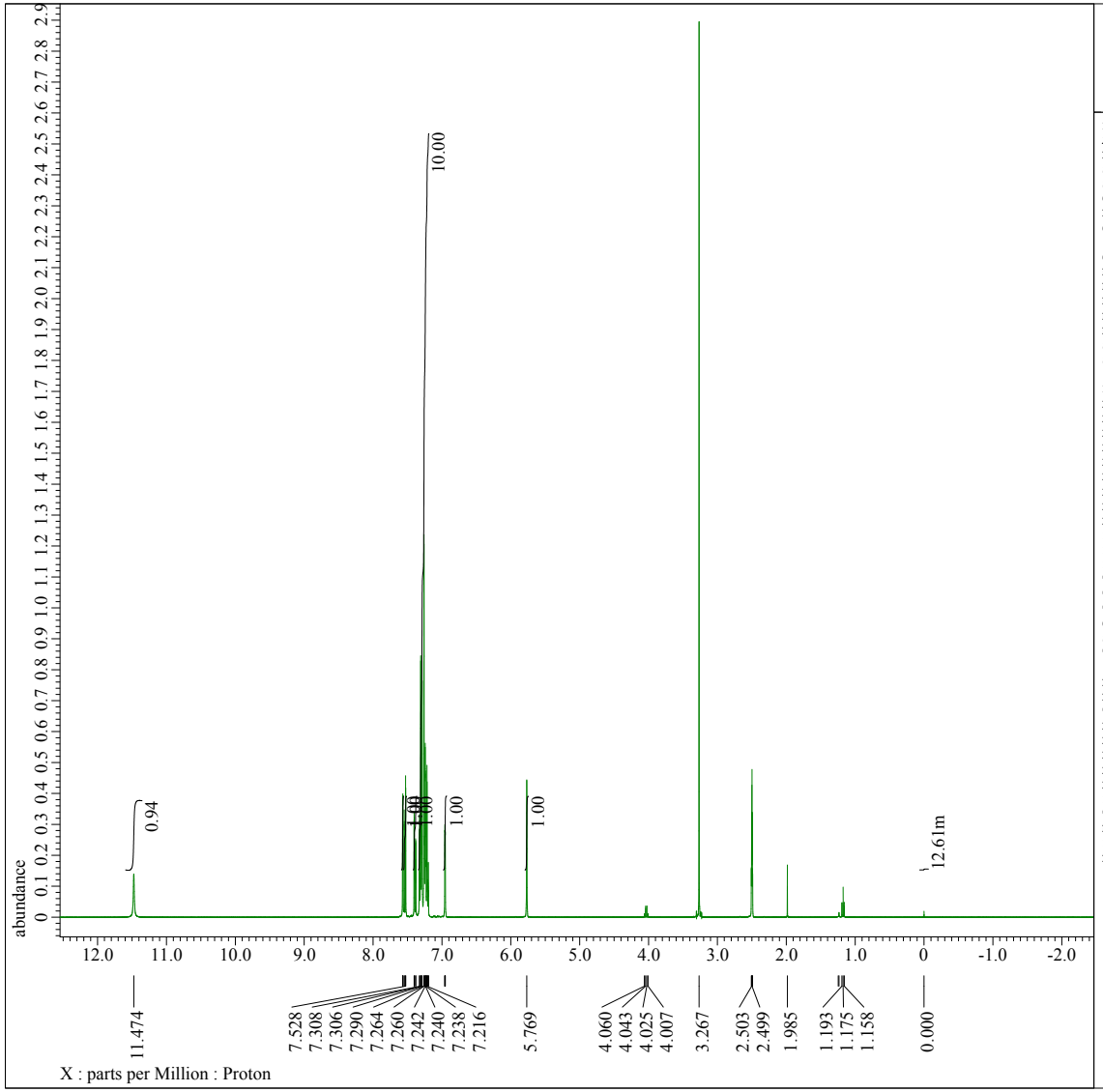
5c



JEOL RESONANCE

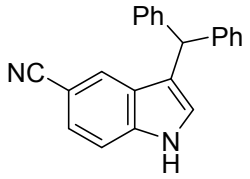
```
Filename          = Y.MA-457_Carbon-1-5.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-457
Solvent           = CHLOROFORM-D
Creation_Time     = 12-NOV-2015 18:40:40
Revision_Time     = 13-NOV-2015 15:55:43
Current_Time      =  4-JAN-2016 17:36:51

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.6[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```


5c

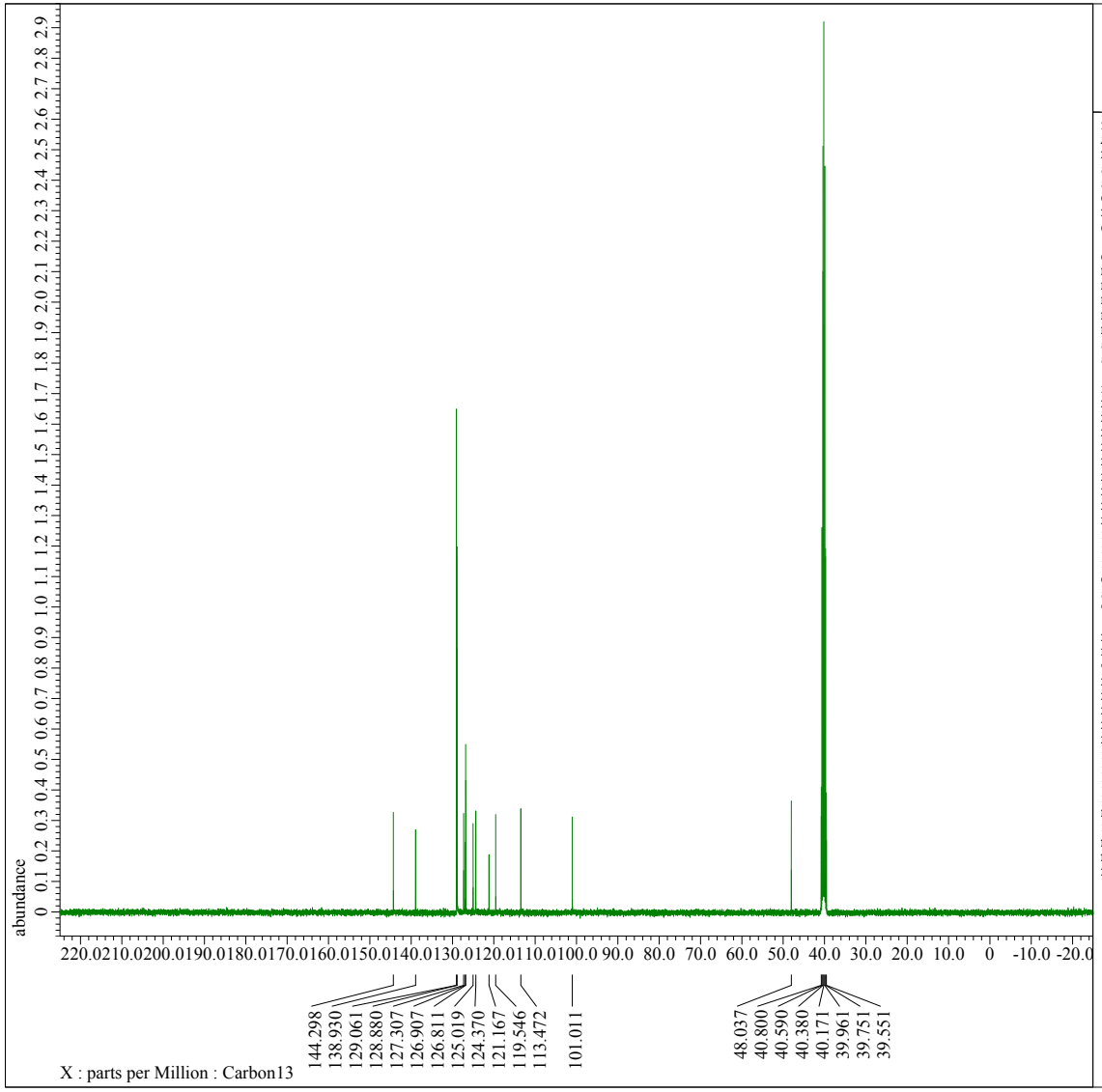


JEOL RESONANCE

```
Filename          = Y.MA-513_Proton-1-7.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-513
Solvent           = DMSO-D6
Creation_Time     =  4-MAR-2016 15:17:14
Revision_Time     =  4-MAR-2016 16:35:49
Current_Time      =  8-MAR-2016 14:04:46

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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        = 40
Temp_Get          = 40[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```

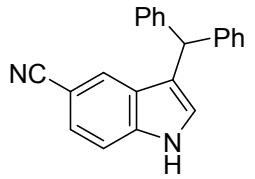


5d

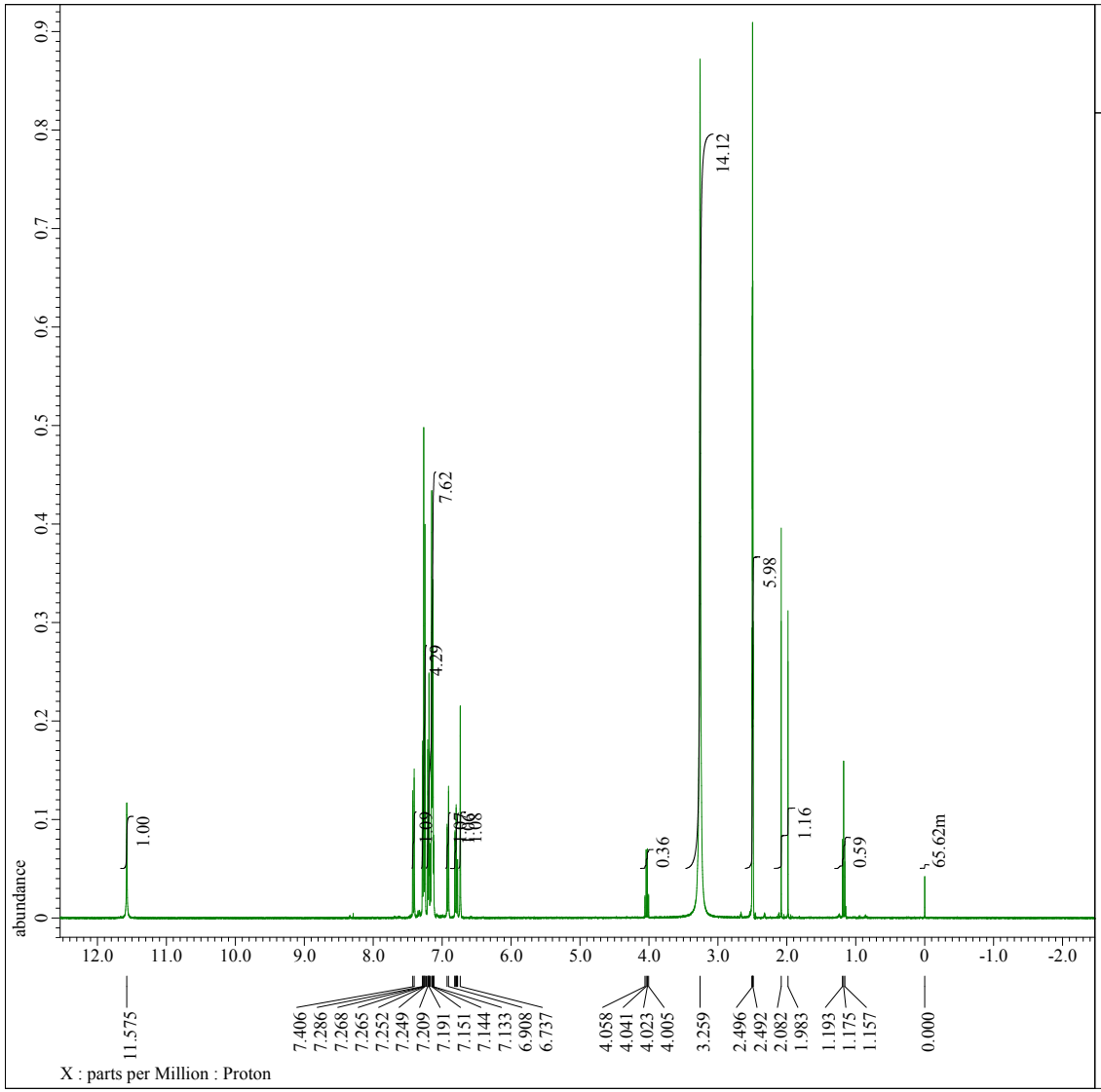


JEOL RESONANCE

```
Filename          = Y.MA-513_Carbon-1-5.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-513
Solvent           = DMSO-D6
Creation_Time     =  4-MAR-2016 14:19:30
Revision_Time     =  4-MAR-2016 15:33:13
Current_Time      =  8-MAR-2016 14:09:35

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 40[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

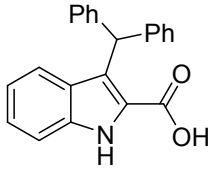


5d

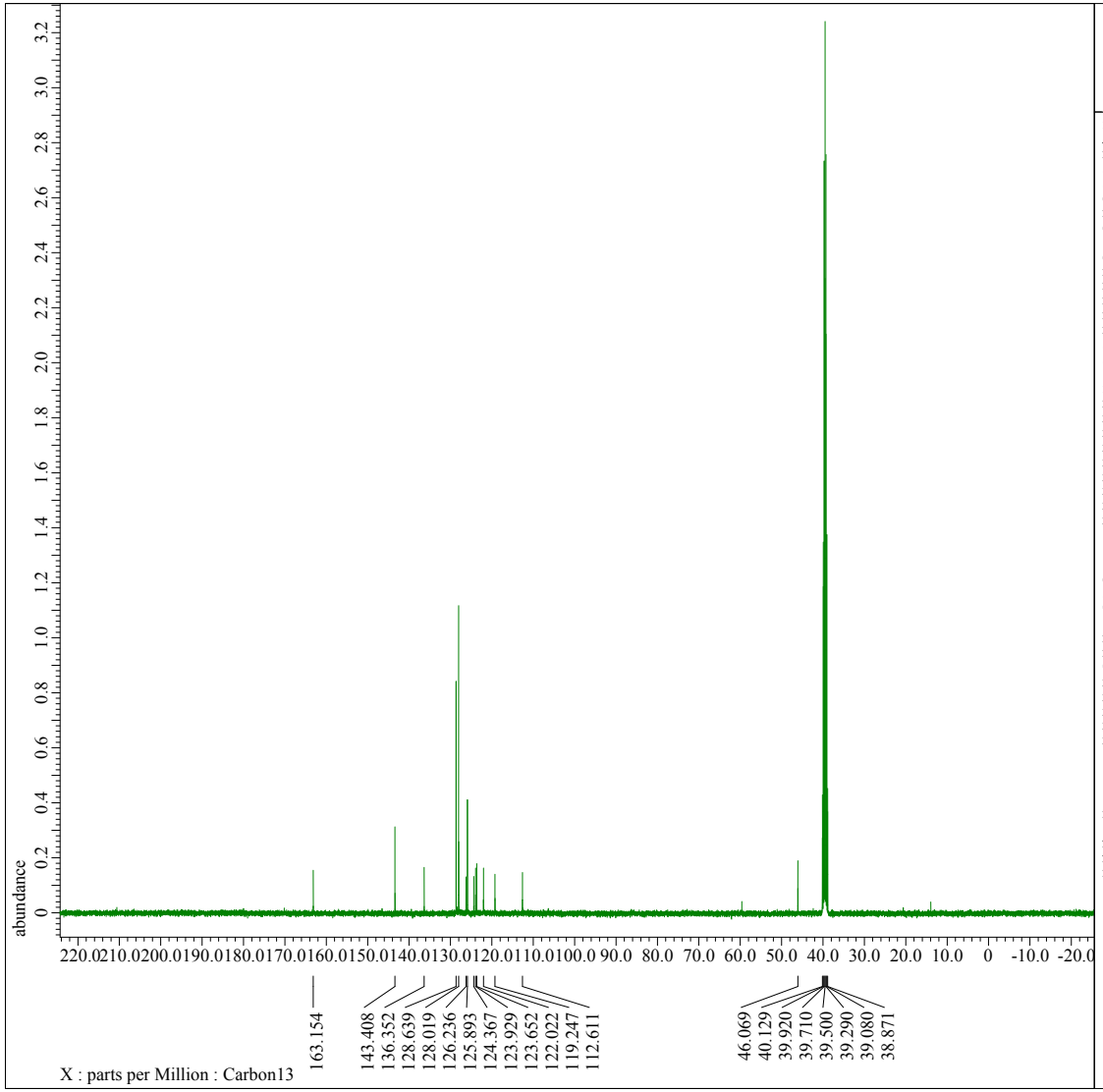


JEOL RESONANCE

```
Filename          = Y.MA-463_Proton-1-6.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = Y.MA-463
Solvent           = DMSO-D6
Creation_Time     = 20-NOV-2015 12:16:24
Revision_Time     =  4-JAN-2016 17:39:31
Current_Time      =  4-JAN-2016 17:39:56

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 8.73463808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 65536
X_Prescans        = 1
X_Resolution      = 0.11448671[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          = 40[dC]
X_90_Width        = 11.45[us]
X_Acq_Time        = 8.73463808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.725[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 13.73463808[s]
```

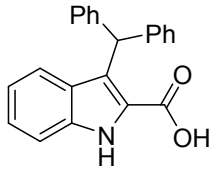


5e



JEOL RESONANCE

```
Filename          = Y.MA-463_Carbon-1-5.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = Y.MA-463
Solvent           = DMSO-D6
Creation_Time     = 20-NOV-2015 19:46:29
Revision_Time     = 20-NOV-2015 21:14:46
Current_Time      =  4-JAN-2016 17:41:05

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
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             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 40[dC]
X_90_Width        = 7.63[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 2.54333333[us]
Irr_Atn_Dec       = 21.538[dB]
Irr_Atn_Noe       = 21.538[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



5e