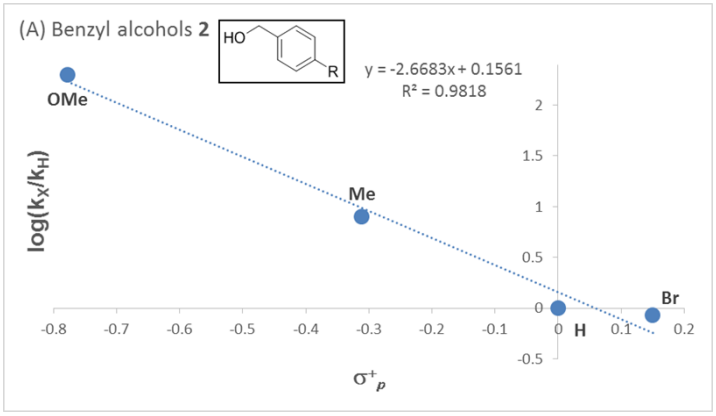
Supporting Information

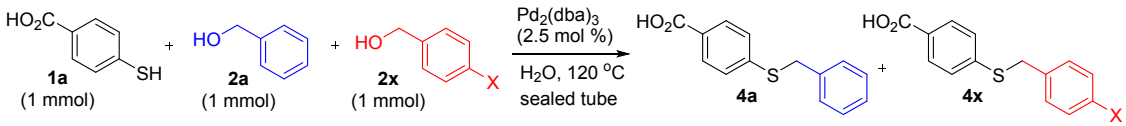
Mercaptobenzoic acid-palladium(0) complexes as active catalysts for *S*-benzylation with benzylic alcohols *via* (η^3-benzyl)palladium(II) cation in water.

Hidemasa Hikawa* and Isao Azumaya*

Faculty of Pharmaceutical Sciences, Toho University, Funabashi, Chiba 274-8510, Japan
hidemasa.hikawa@phar.toho-u.ac.jp and isao.azumaya@phar.toho-u.ac.jp

Hammett studies





A mixture of mercaptobenzoic acids **1a** (154 mg, 1 mmol), $Pd_2(dba)_3$ (23 mg, 0.025 mmol), benzyl alcohol **2a** (108 mg, 1 mmol), and benzylic alcohols **2x** (1 mmol) in H_2O (4 mL) was heated at 120 °C in sealed tube. 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.

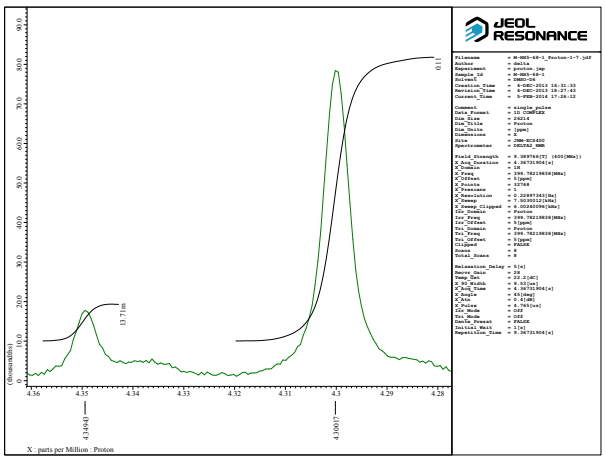
Table S1. Benzylic alcohols **2x**

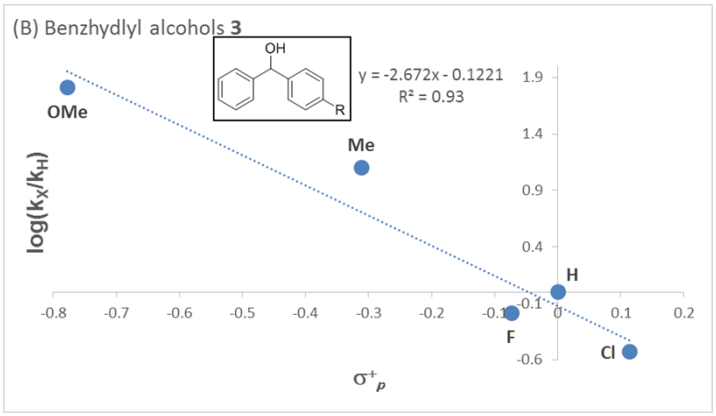
	X=OMe **4b**	Me **4c**	Br **4g**
Time	1 h	45 min	16 h
k_X/k_H [a]	1.40 / 0.007	0.11 / 0.014	0.23 / 0.27
log k_X/k_H	2.30	0.90	-0.07
σ^+	-0.778	-0.311	0.15

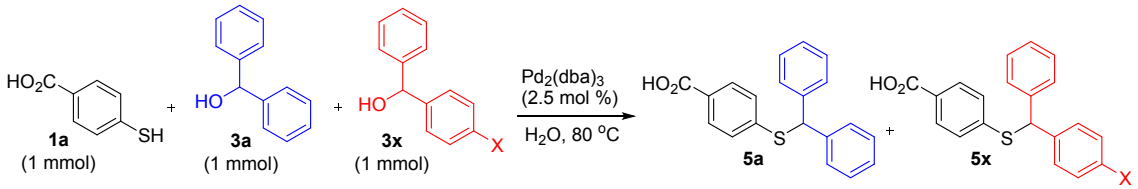
[a] Integral values which were determined by ^{1}H NMR analysis of the crude product using *p*-nitroanisole as an internal standard.

Table S1.

0.014H **(4a)**	***0.11H*** **(4c)**
X=H	X=Me
methylene H	methylene H
δ: 4.35 ppm	δ: 4.30 ppm







A mixture of mercaptobenzoic acids **1a** (154 mg, 1 mmol), $Pd_2(dba)_3$ (23 mg, 0.025 mmol), benzhydrol **3a** (184 mg, 1 mmol), and benzhydryl alcohols **3x** (1 mmol) in H_2O (4 mL) was heated at 80 °C. 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.

Table S2. Benzhydryl alcohols **3x**

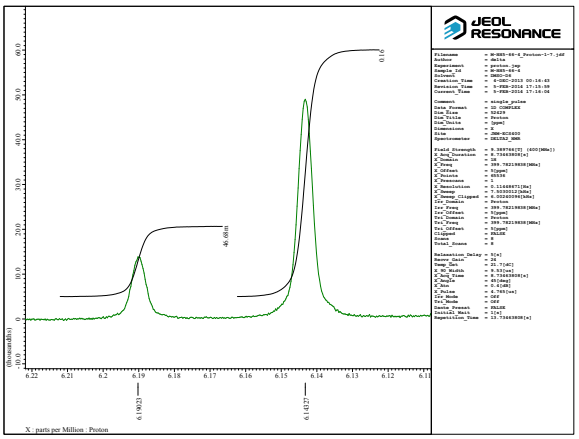
	X=OMe **5c**	Me **5d**	F **5g** [b]	Cl **5e**
Time	1 h	1 h	2 h	3 h
k_X/k_H [a]	0.77 / 0.012	0.094 / 0.0075	0.052 / 0.081	0.047 / 0.16
log k_X/k_H	1.81	1.10	-0.19	-0.53
σ^+	-0.778	-0.311	-0.073	0.114

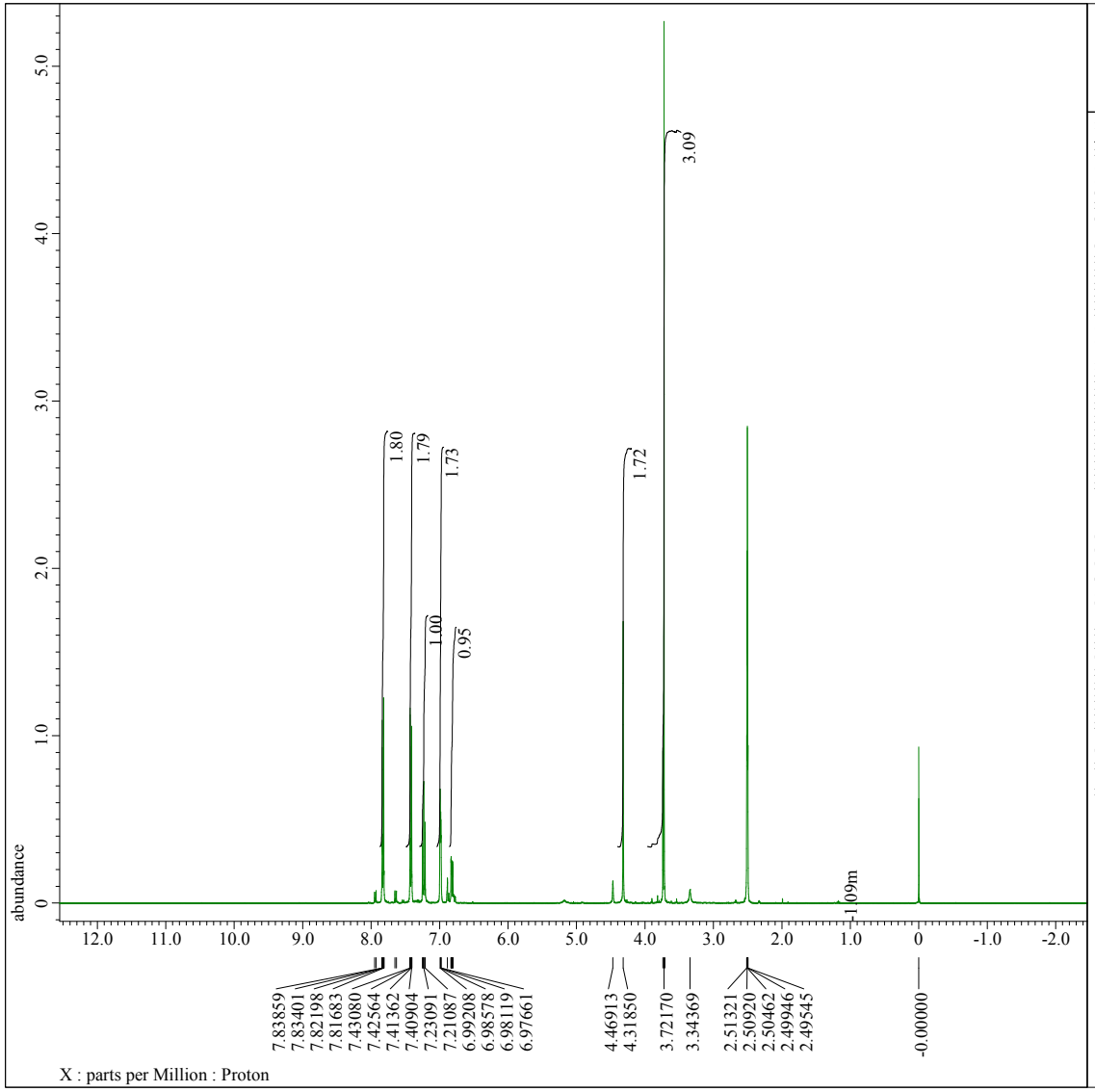
[a] Integral values which were determined by ^{1}H NMR analysis of the crude product using *p*-nitroanisole as an internal standard.

[b] 4,4'-Difluorobenzhydrol was used.

Table S2. (Cl **5e**)

0.047H (**5e**)	***0.16H*** (**5a**)
X=Cl	X=H
methin H	methin H
δ: 6.19 ppm	δ: 6.14 ppm





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X_Atn             = 0.4[dB]
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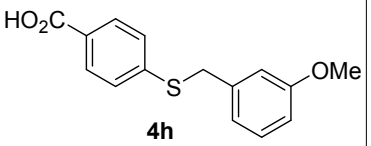

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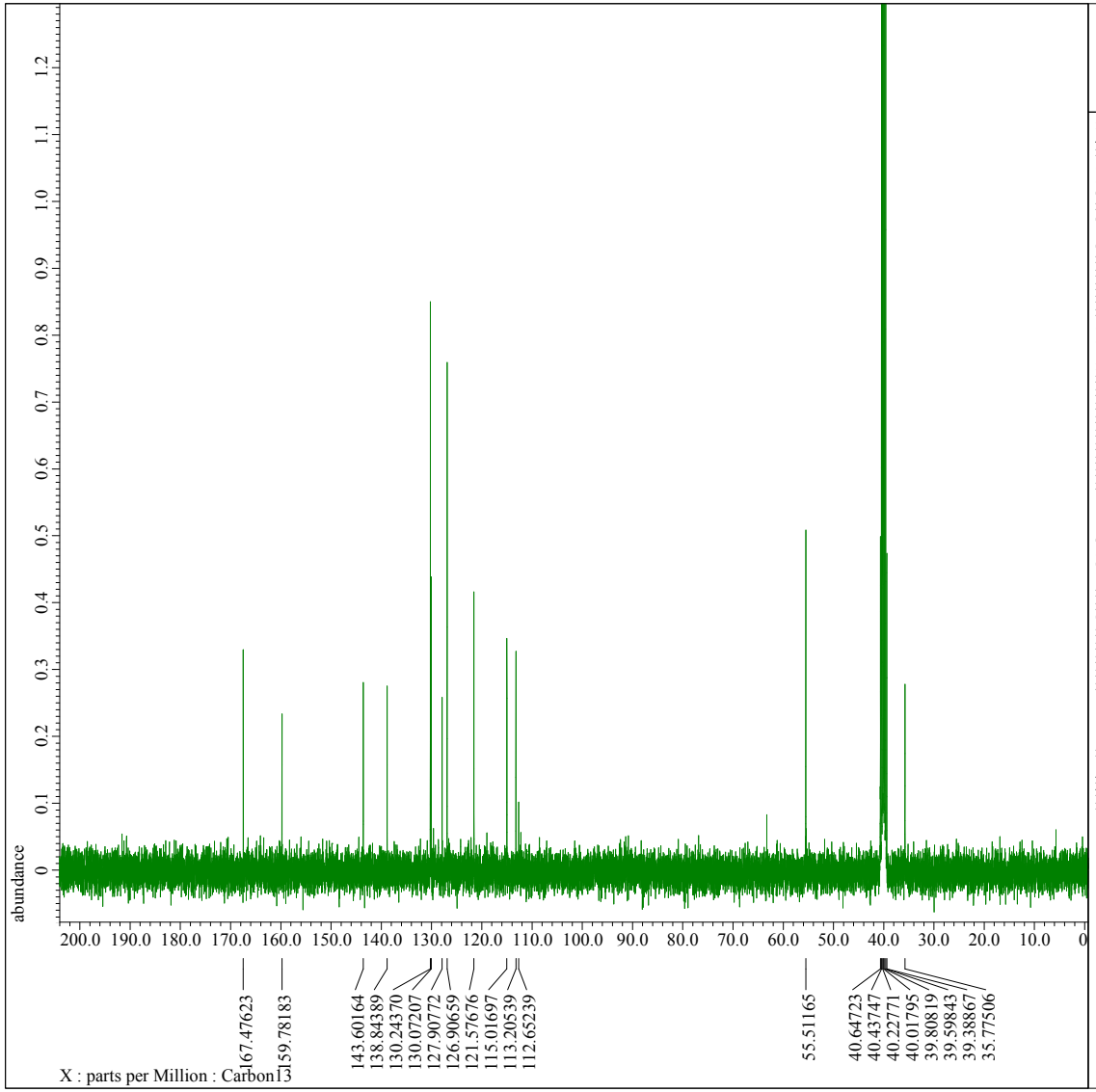

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Dimensions        = X
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Spectrometer      = DELTA2_NMR

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X_Sweep_Clipped   = 25.12562814[kHz]
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Irr_Freq          = 399.78219838[MHz]
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Temp_Get          = 20[dC]
X_90_Width        = 8[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.1[dB]
X_Pulse           = 2.66666667[us]
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Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
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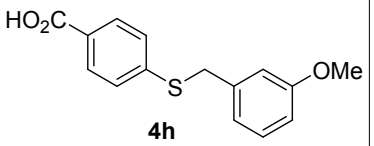

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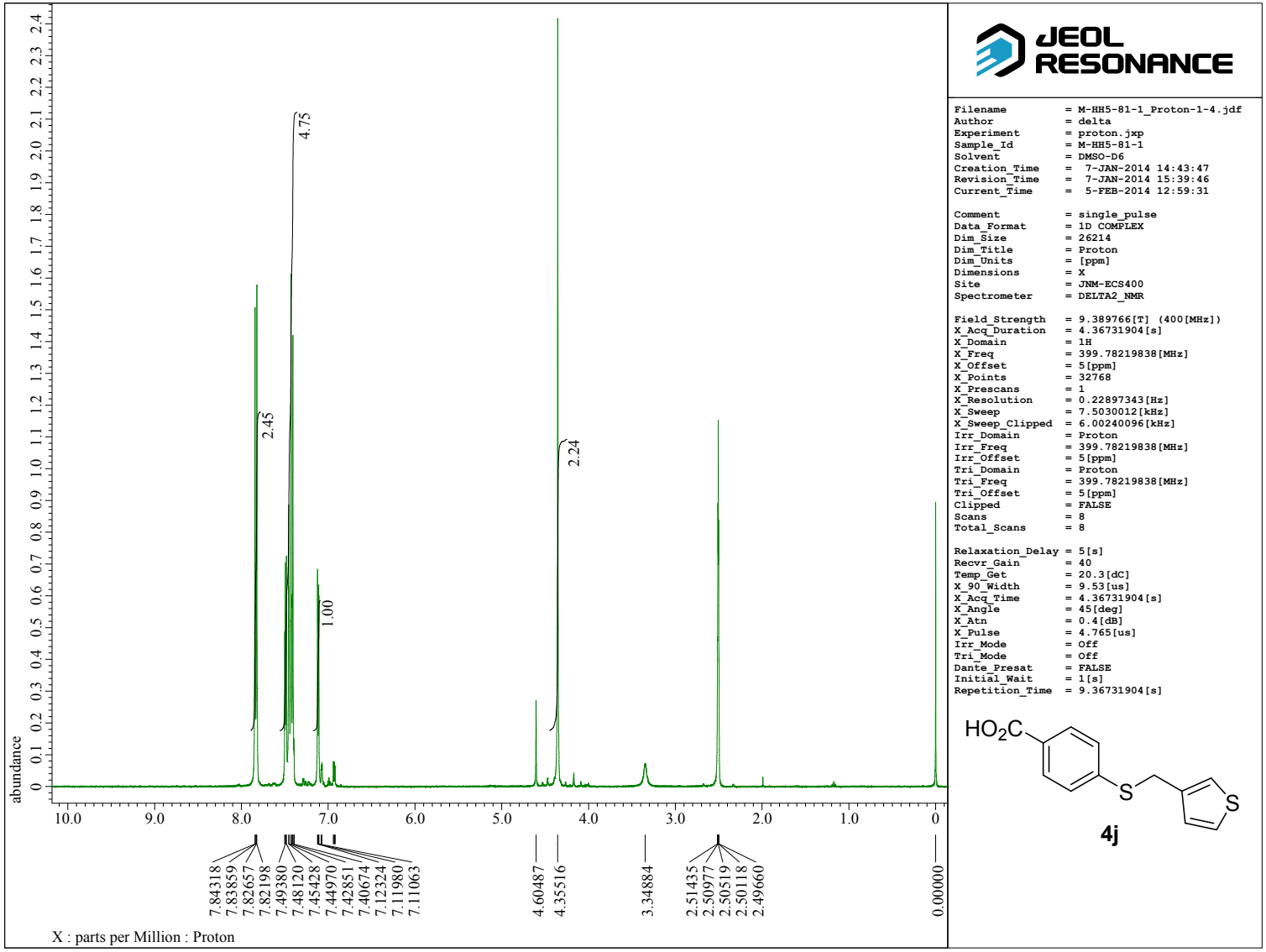

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X_Prescans        = 1
X_Resolution      = 0.22897343[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 40
Temp_Get          = 20.3[dC]
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X_Angle           = 45[deg]
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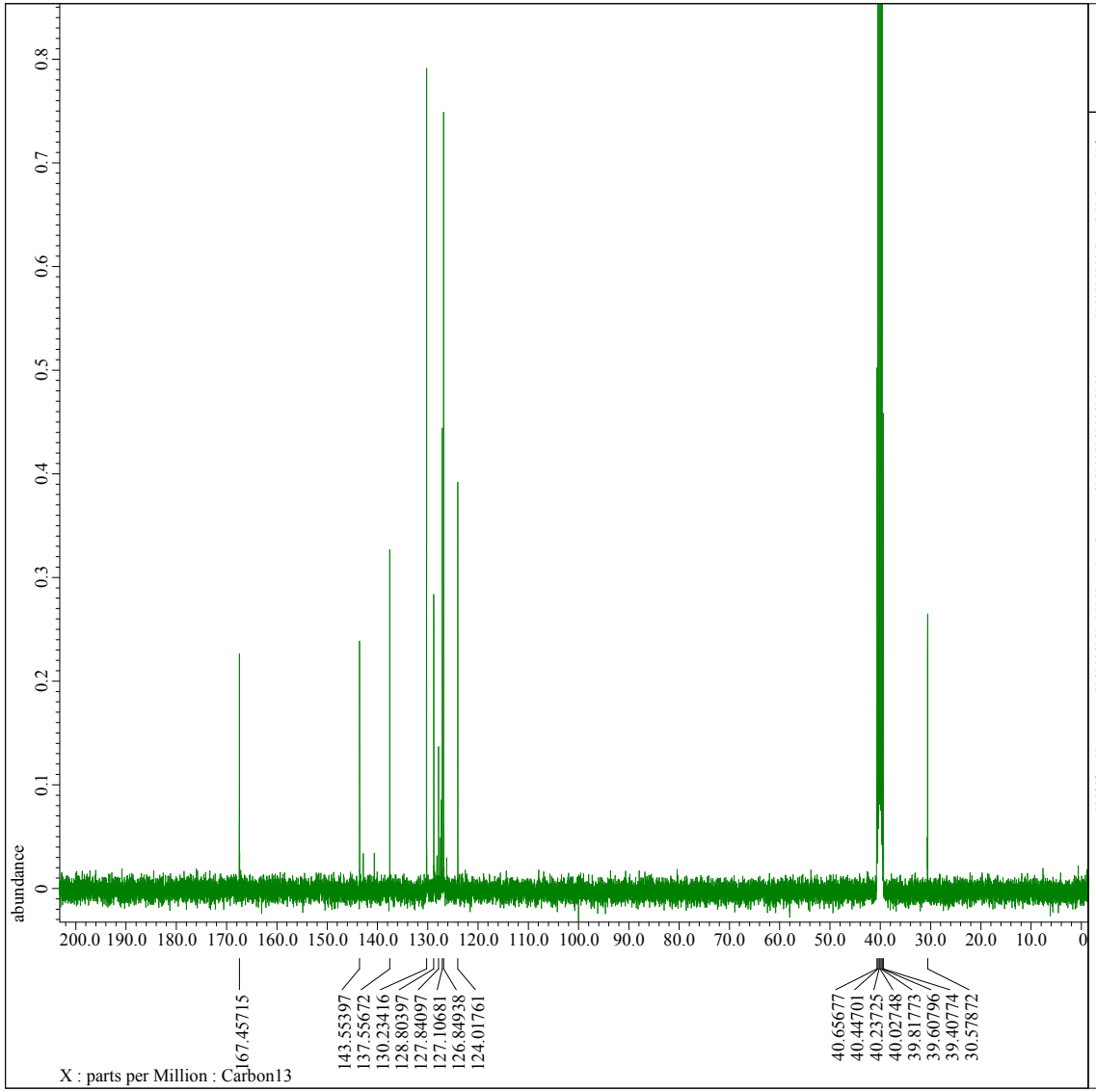
4j



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Irr_Atn_Noe       = 21.763[dB]
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Irr_Pwidth        = 0.115[ms]
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Initial_Wait      = 1[s]
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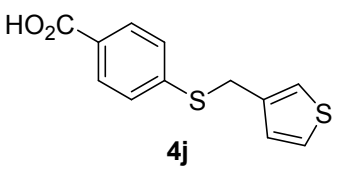

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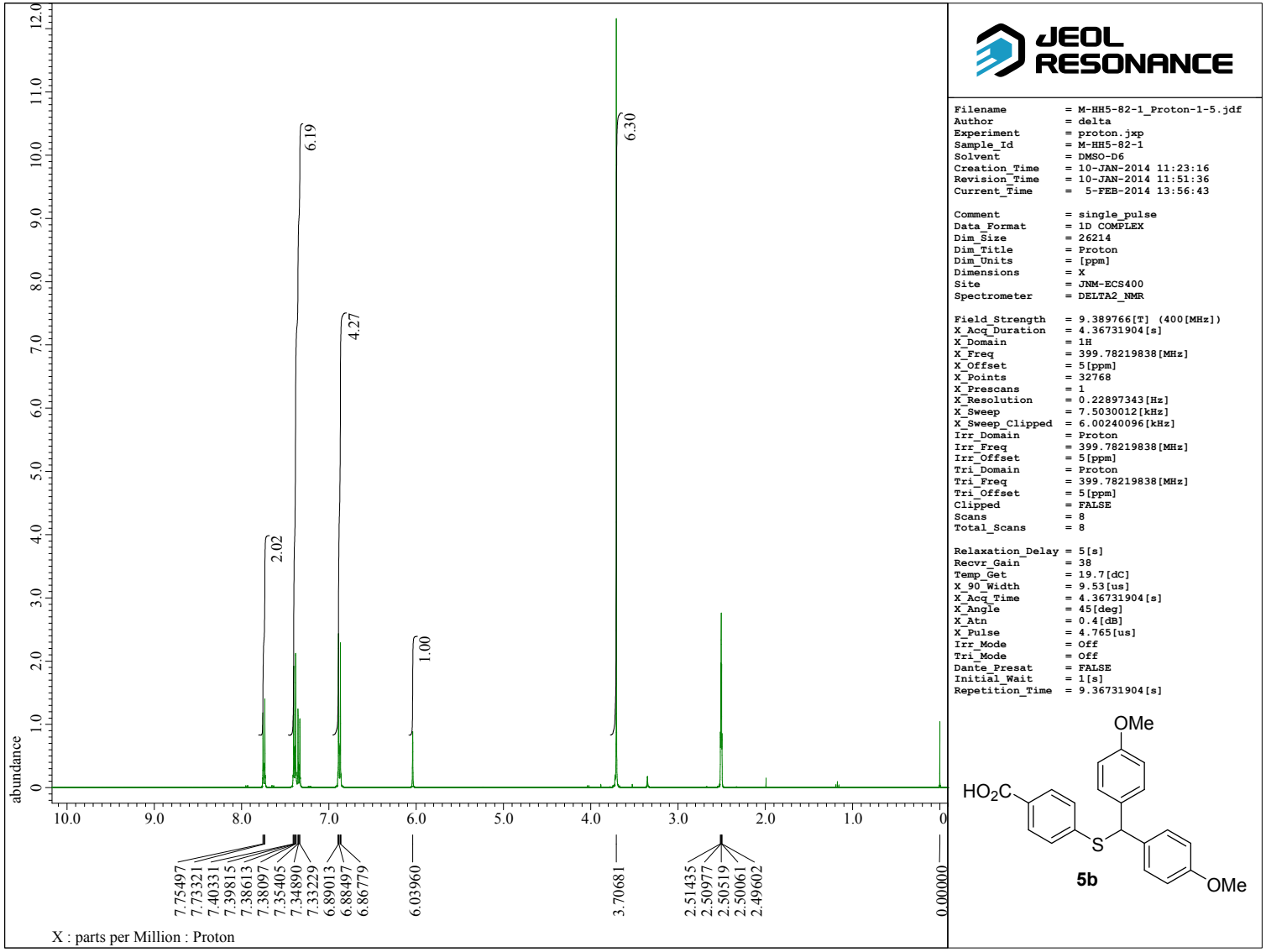

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X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
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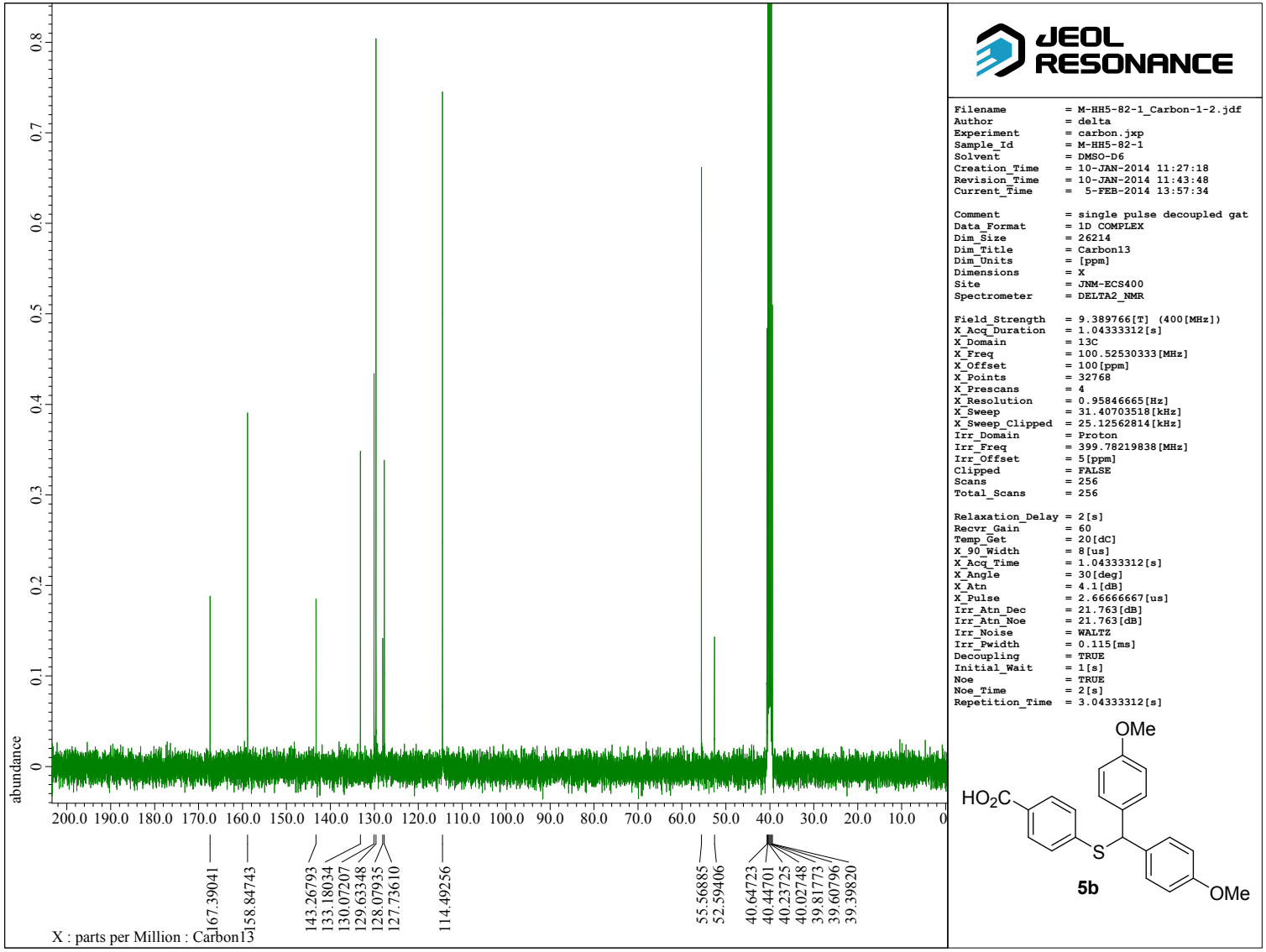
5b



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X_Sweep_Clipped   = 25.12562814[kHz]
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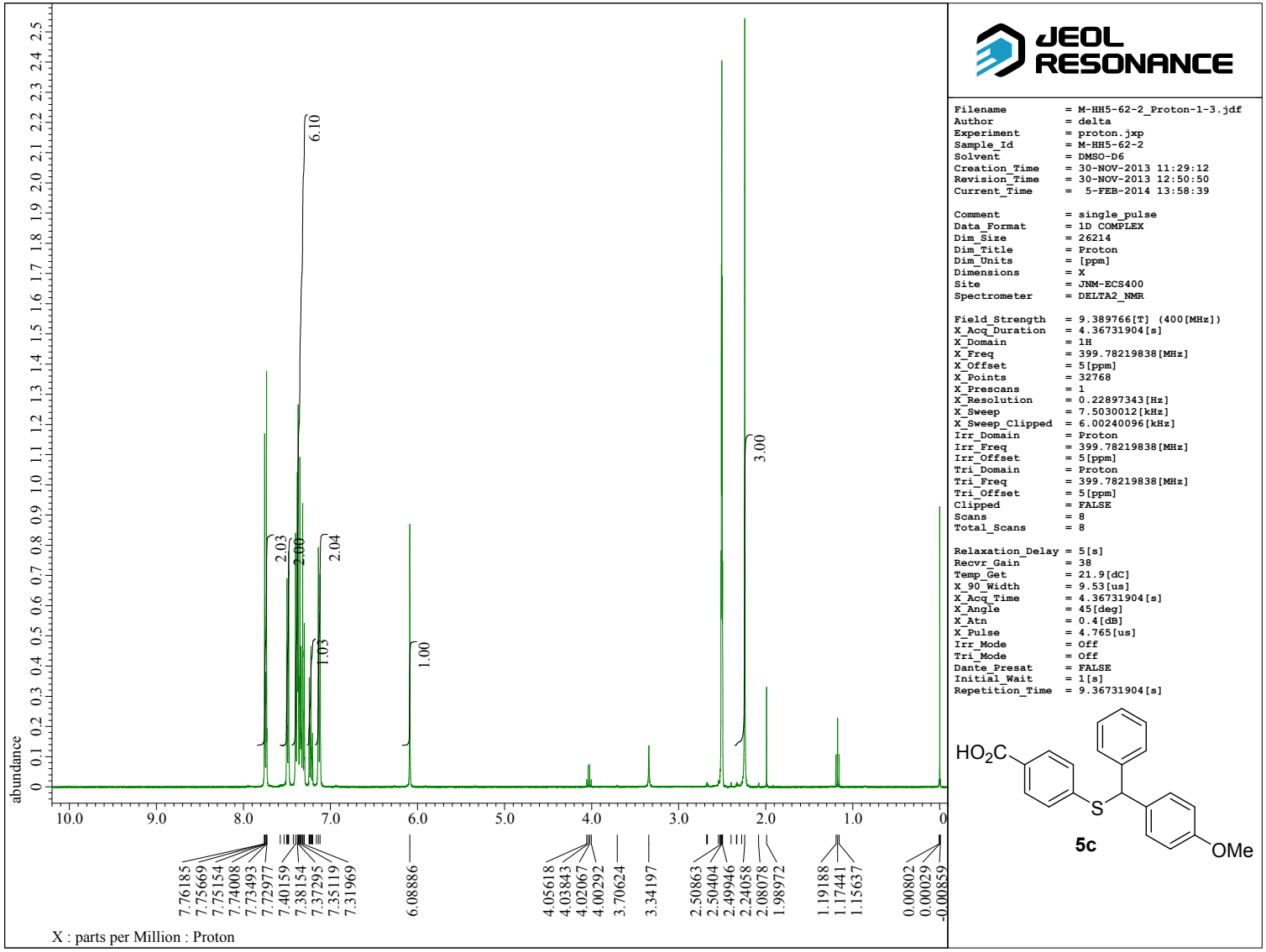
5b



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X_Sweep	= 7.5030012[kHz]
X_Sweep_Clipped	= 6.00240096[kHz]
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Tri_Freq	= 399.78219838[MHz]
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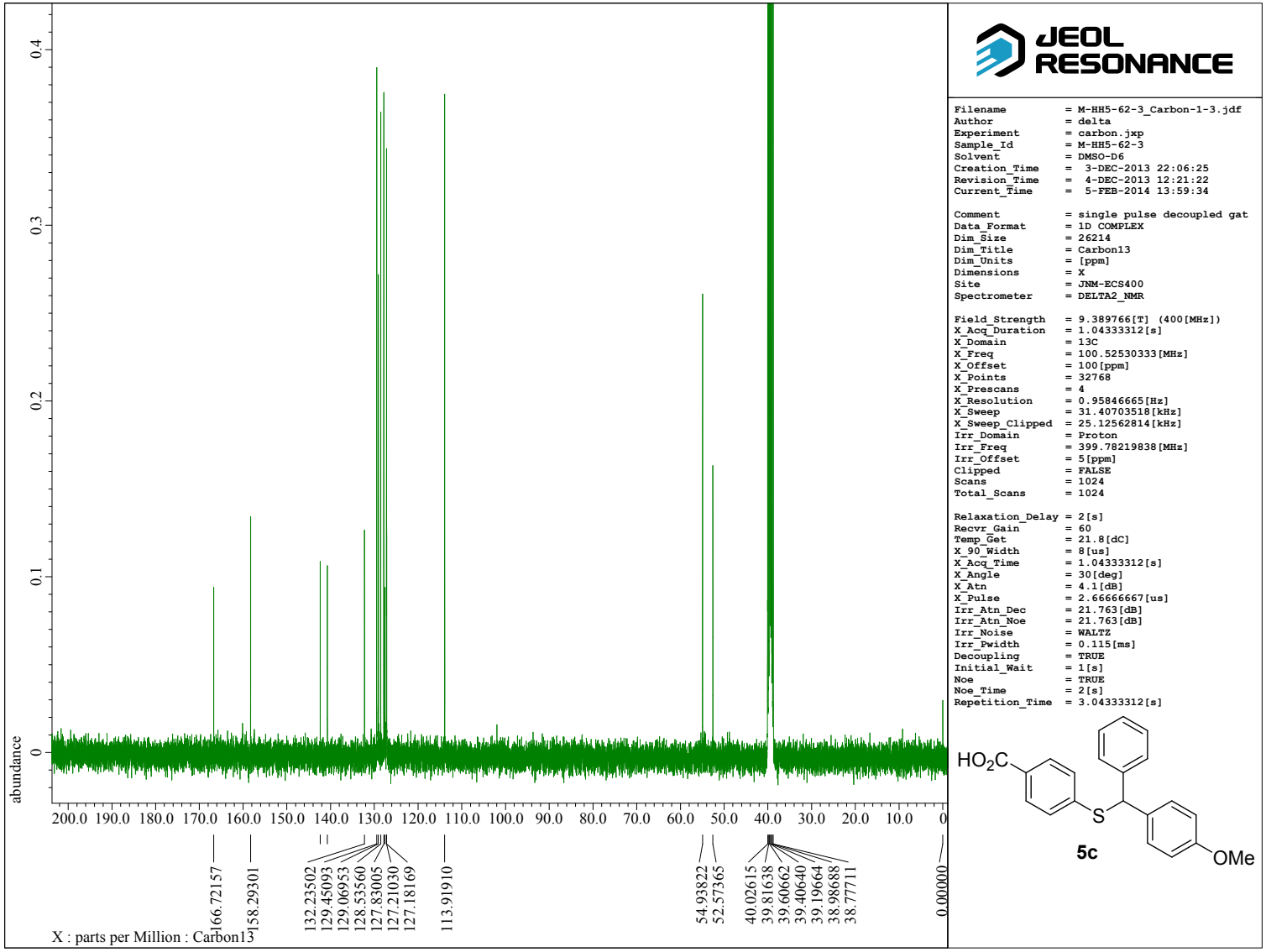
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0.3
0.2
0.1
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
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158.29301
132.23502
129.45093
129.06953
128.53560
127.83005
127.21030
127.18169
113.91910
54.93822
52.57365
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X : parts per Million : Carbon13
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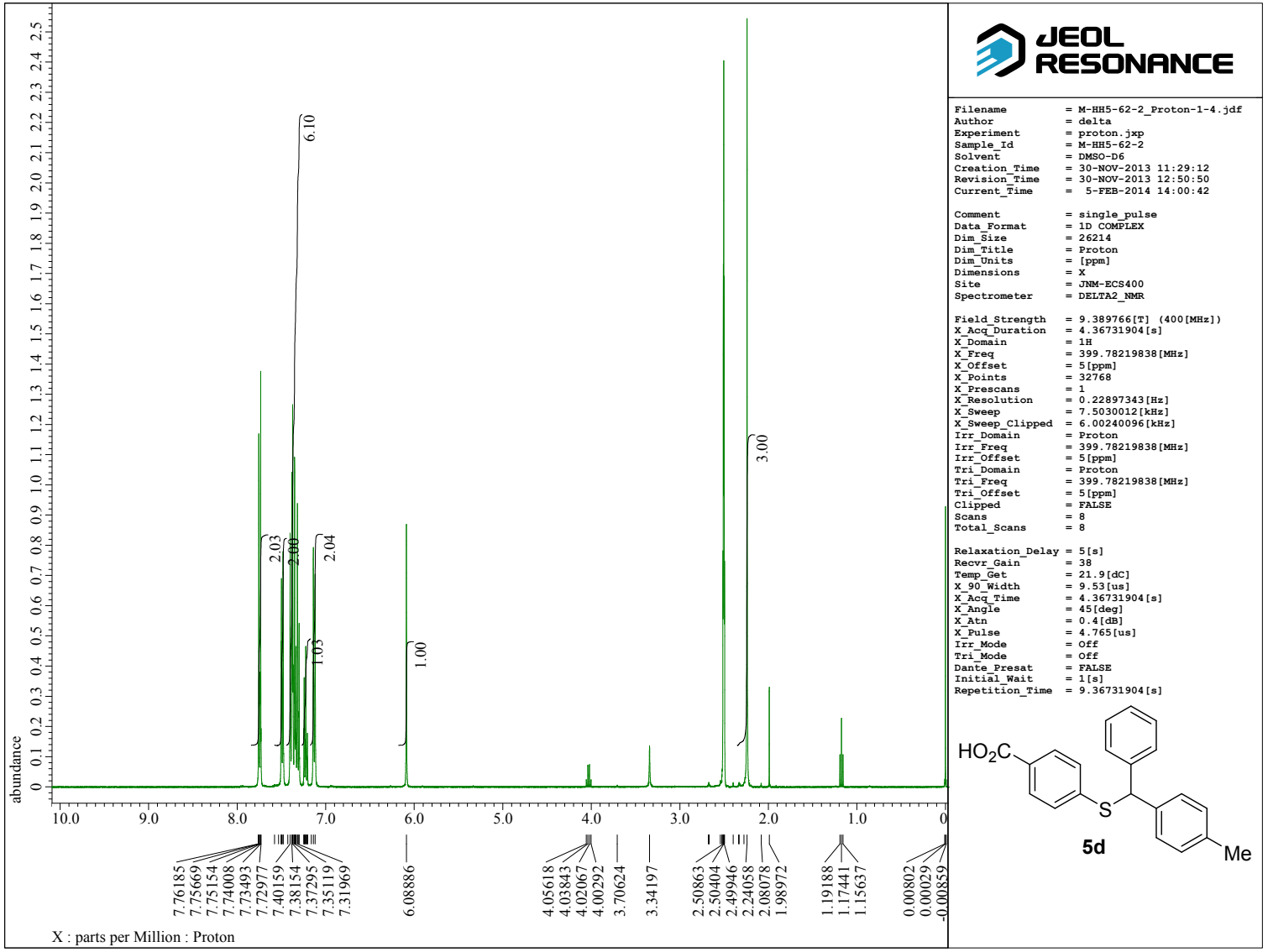
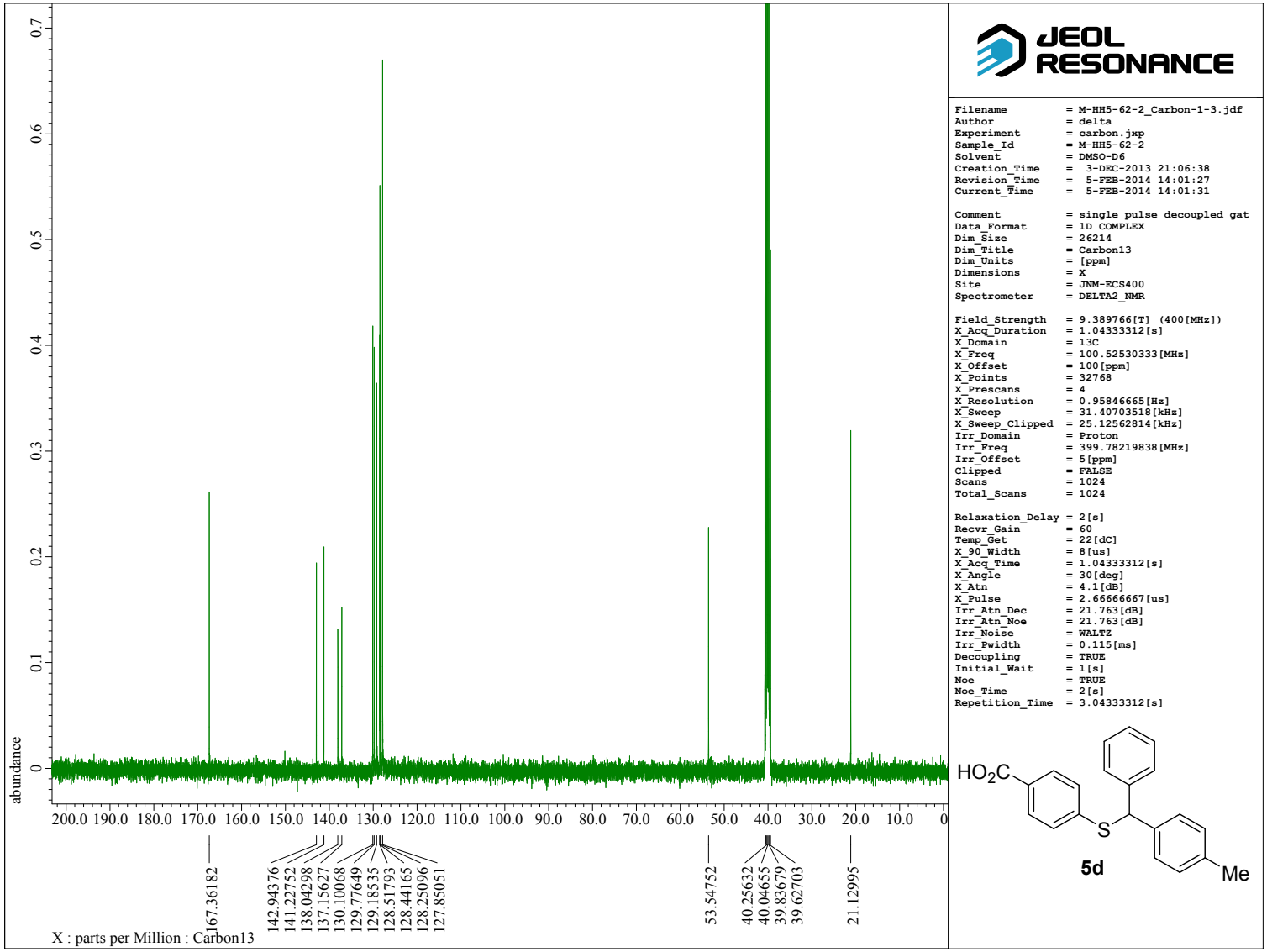
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.8[dC]
X_90_Width = 8[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 2.66666667[us]
Irr_Atn_Dec = 21.763[dB]
Irr_Atn_Noe = 21.763[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]
HO2C
S
OMe
5c



JEOL RESONANCE

Filename	= M-HH5-62-2_Proton-1-4.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= M-HH5-62-2
Solvent	= DMSO-D6
Creation_Time	= 30-NOV-2013 11:29:12
Revision_Time	= 30-NOV-2013 12:50:50
Current_Time	= 5-FEB-2014 14:00:42
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 4.36731904[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.22897343[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	= 21.9[dC]
X_90_Width	= 9.53[us]
X_Acq_Time	= 4.36731904[s]
X_Angle	= 45[deg]
X_Atn	= 0.4[dB]
X_Pulse	= 4.765[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 9.36731904[s]

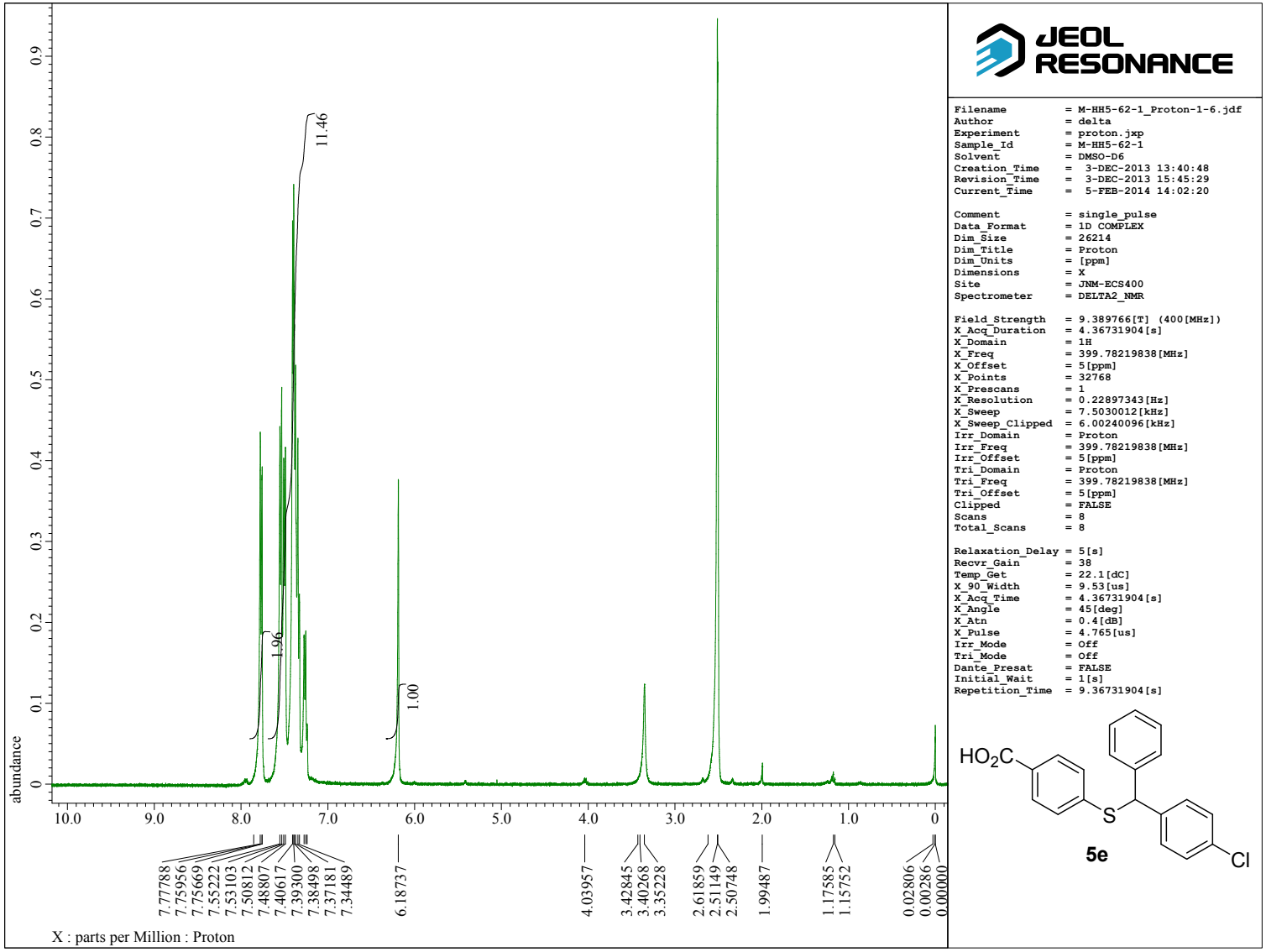
5d



JEOL RESONANCE

```
Filename          = M-HH5-62-2_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH5-62-2
Solvent           = DMSO-D6
Creation_Time     =  3-DEC-2013 21:06:38
Revision_Time     =  5-FEB-2014 14:01:27
Current_Time      =  5-FEB-2014 14:01:31

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          = 22[dC]
X_90_Width        = 8[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.1[dB]
X_Pulse           = 2.66666667[us]
Irr_Atn_Dec       = 21.763[dB]
Irr_Atn_Noe       = 21.763[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]
```

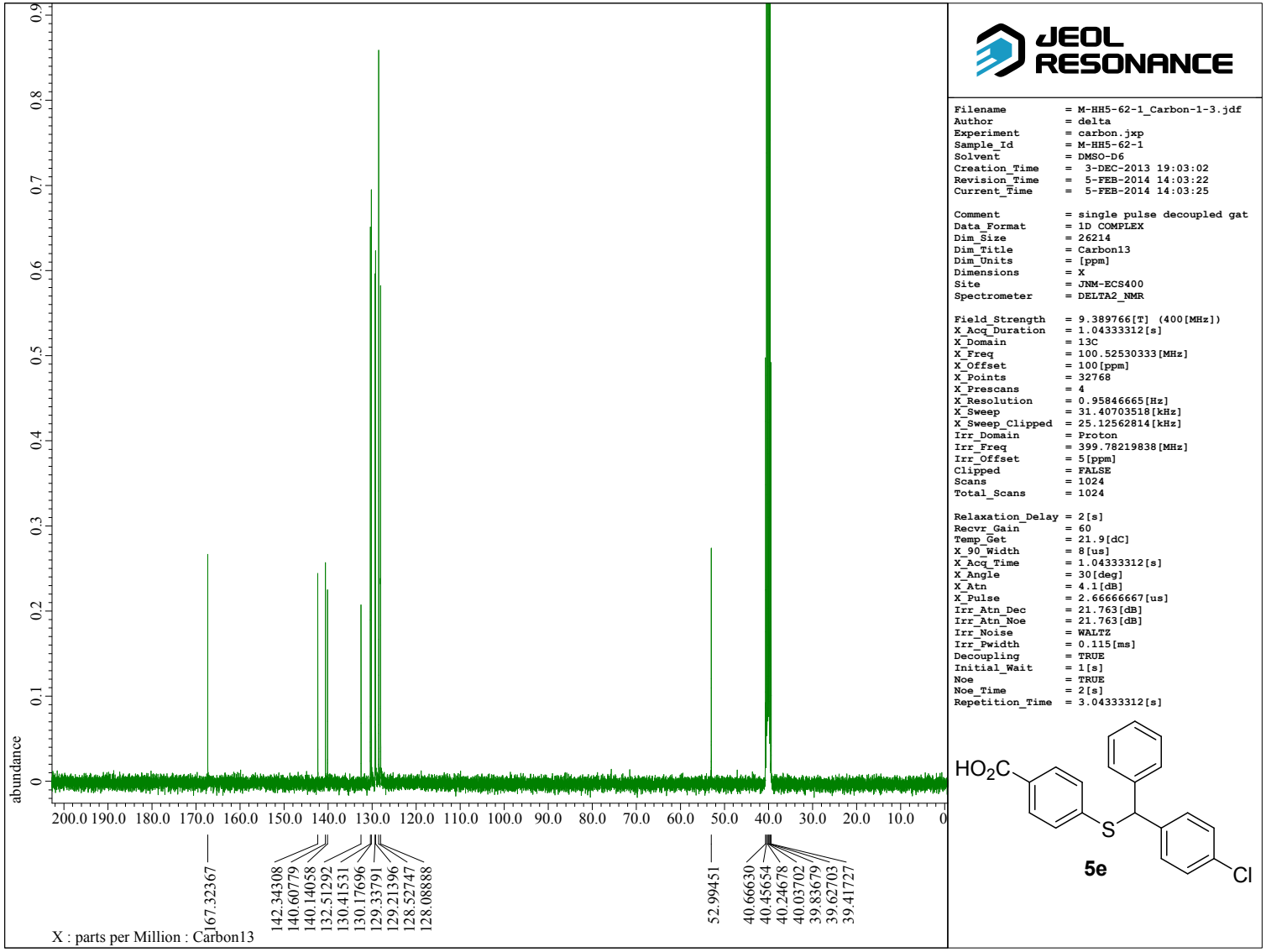

5d



JEOL RESONANCE

```
Filename          = M-HH5-62-1_Proton-1-6.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH5-62-1
Solvent           = DMSO-D6
Creation_Time     =  3-DEC-2013 13:40:48
Revision_Time     =  3-DEC-2013 15:45:29
Current_Time      =  5-FEB-2014 14:02:20

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 4.36731904[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 32768
X_Prescans        = 1
X_Resolution      = 0.22897343[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          = 22.1[dC]
X_90_Width        = 9.53[us]
X_Acq_Time        = 4.36731904[s]
X_Angle           = 45[deg]
X_Atn             = 0.4[dB]
X_Pulse           = 4.765[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 9.36731904[s]
```

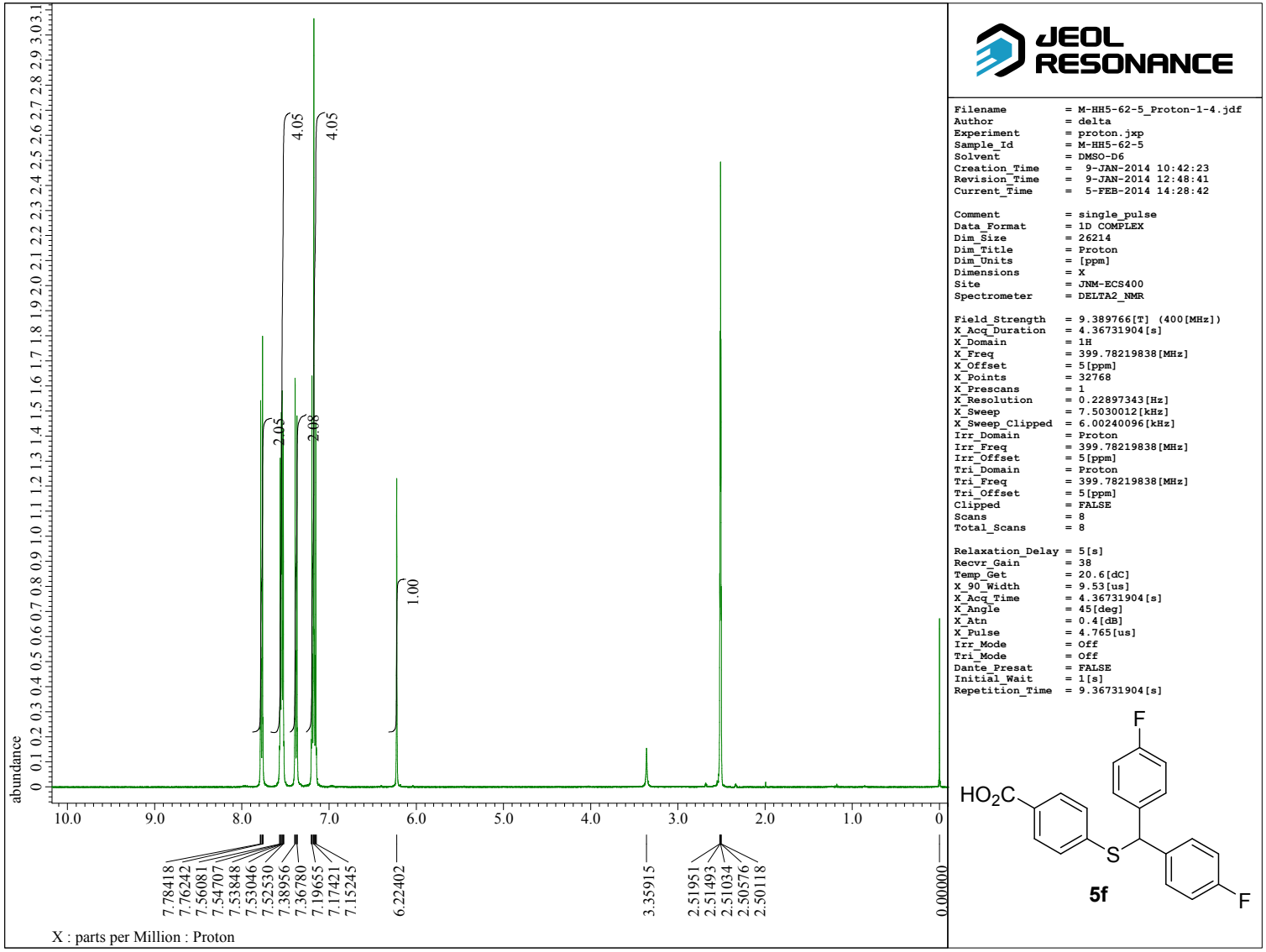

5e



JEOL RESONANCE

```
Filename          = M-HH5-62-1_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH5-62-1
Solvent           = DMSO-D6
Creation_Time     =  3-DEC-2013 19:03:02
Revision_Time     =  5-FEB-2014 14:03:22
Current_Time      =  5-FEB-2014 14:03:25

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        = 8[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.1[dB]
X_Pulse           = 2.66666667[us]
Irr_Atn_Dec       = 21.763[dB]
Irr_Atn_Noe       = 21.763[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]
```

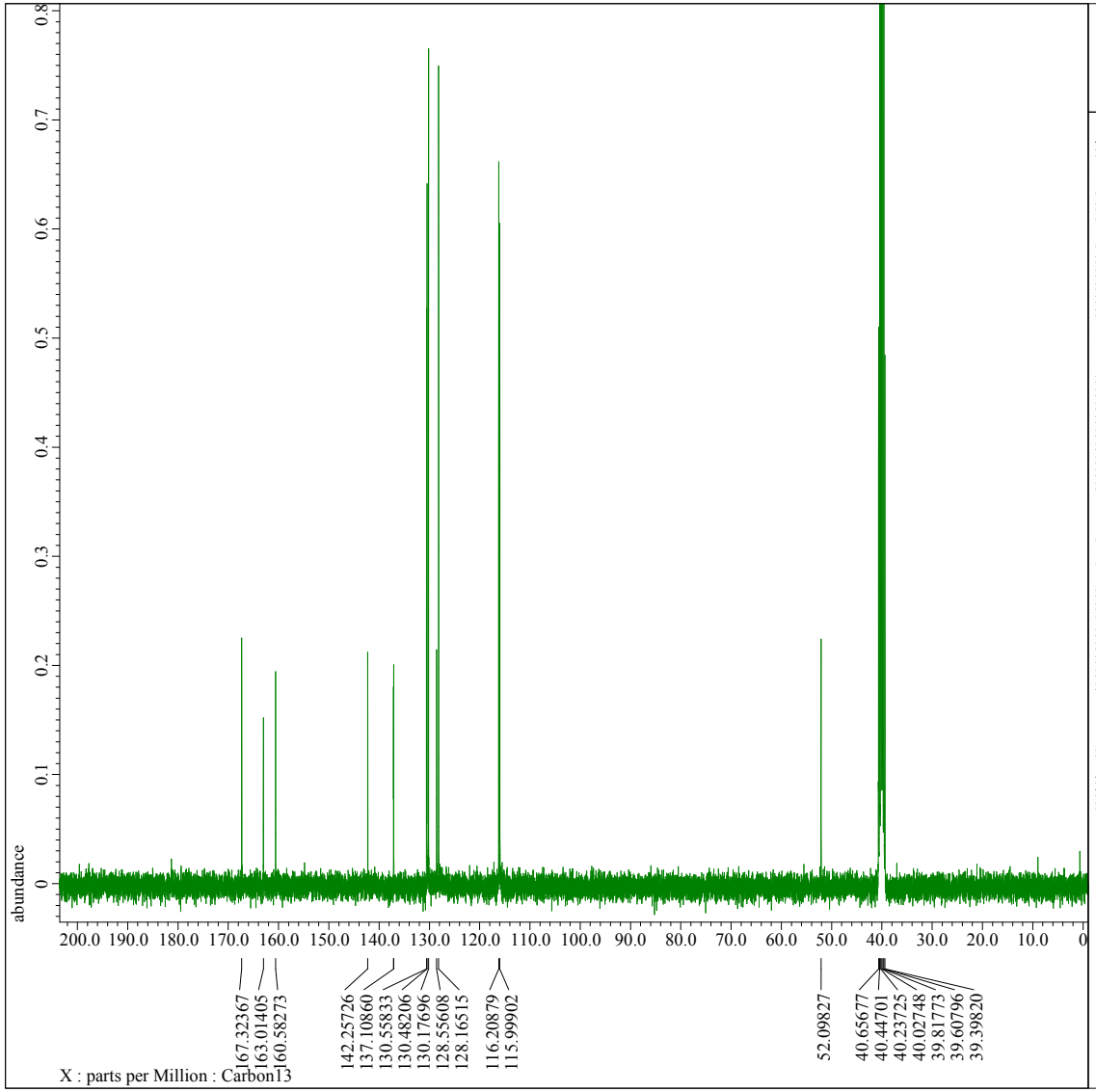

5e



JEOL RESONANCE

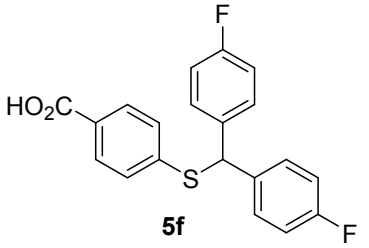
```
Filename          = M-HH5-62-5_Proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH5-62-5
Solvent           = DMSO-D6
Creation_Time     =  9-JAN-2014 10:42:23
Revision_Time     =  9-JAN-2014 12:48:41
Current_Time      =  5-FEB-2014 14:28:42

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 4.36731904[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 32768
X_Prescans        = 1
X_Resolution      = 0.22897343[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          = 20.6[dC]
X_90_Width        = 9.53[us]
X_Acq_Time        = 4.36731904[s]
X_Angle           = 45[deg]
X_Atn             = 0.4[dB]
X_Pulse           = 4.765[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 9.36731904[s]
```


5f

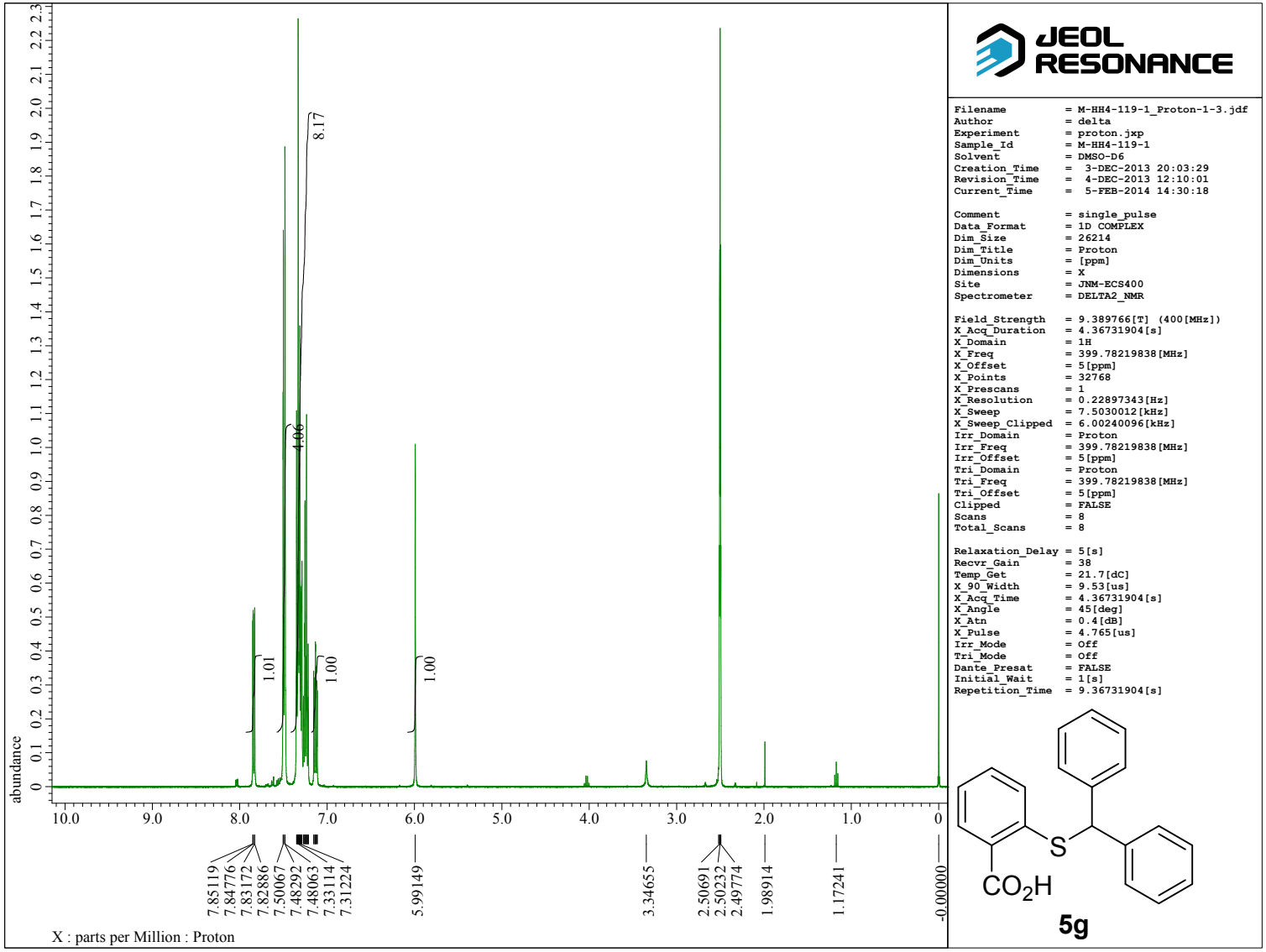


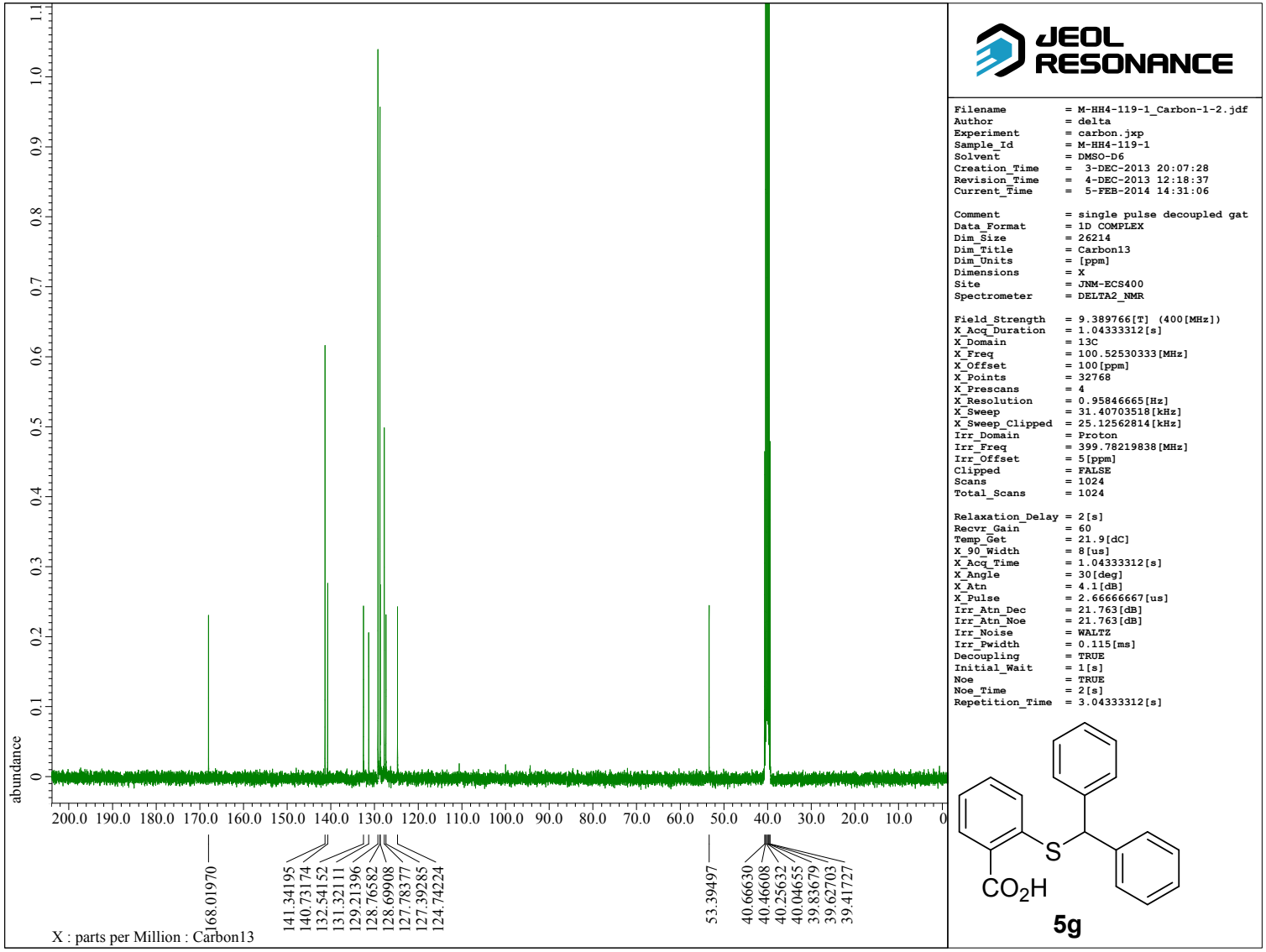
JEOL RESONANCE

```
Filename          = M-HH5-62-5_Carbon-1-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH5-62-5
Solvent           = DMSO-D6
Creation_Time     =  9-JAN-2014 13:47:34
Revision_Time     =  9-JAN-2014 17:49:19
Current_Time      =  5-FEB-2014 14:29:26

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             = 512
Total_Scans       = 512

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 20.8[dC]
X_90_Width        = 8[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.1[dB]
X_Pulse           = 2.66666667[us]
Irr_Atn_Dec       = 21.763[dB]
Irr_Atn_Noe       = 21.763[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]
```



5f

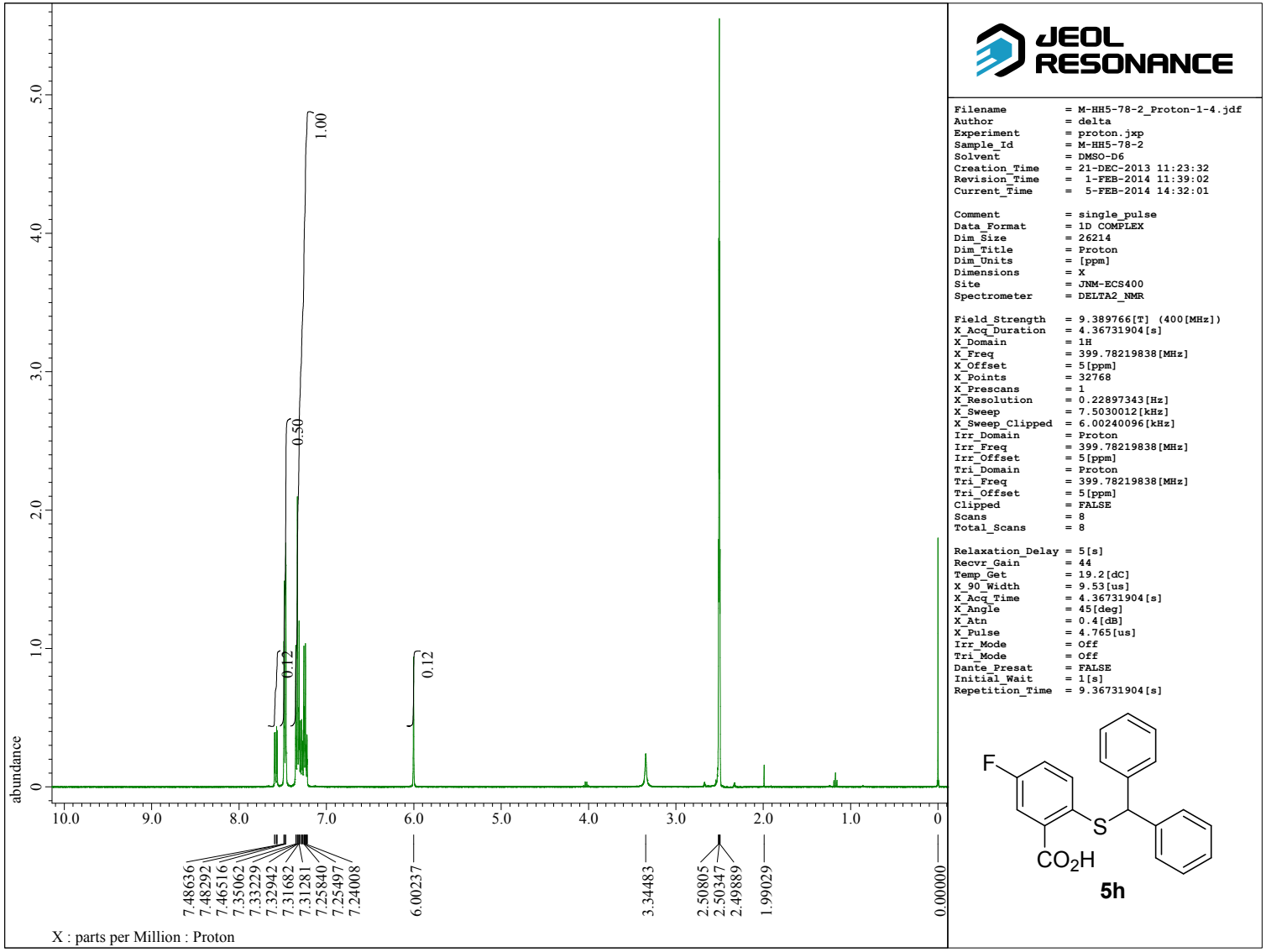

abundance
8.17
4.86
1.01
1.00
1.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.85119
7.84776
7.83172
7.82886
7.50067
7.48292
7.48063
7.33114
7.31224
5.99149
3.34655
2.50691
2.50232
2.49774
1.98914
1.17241
-0.00000
X : parts per Million : Proton
JEOL RESONANCE
Filename = M-HH4-119-1_Proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = M-HH4-119-1
Solvent = DMSO-D6
Creation_Time = 3-DEC-2013 20:03:29
Revision_Time = 4-DEC-2013 12:10:01
Current_Time = 5-FEB-2014 14:30:18
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 21.7[dC]
X_90_Width = 9.53[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.4[dB]
X_Pulse = 4.765[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]
S
CO2H
5g



JEOL RESONANCE

```
Filename          = M-HH4-119-1_Carbon-1-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH4-119-1
Solvent           = DMSO-D6
Creation_Time     =  3-DEC-2013 20:07:28
Revision_Time     =  4-DEC-2013 12:18:37
Current_Time      =  5-FEB-2014 14:31:06

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          = 21.9[dC]
X_90_Width        = 8[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.1[dB]
X_Pulse           = 2.66666667[us]
Irr_Atn_Dec       = 21.763[dB]
Irr_Atn_Noe       = 21.763[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]
```

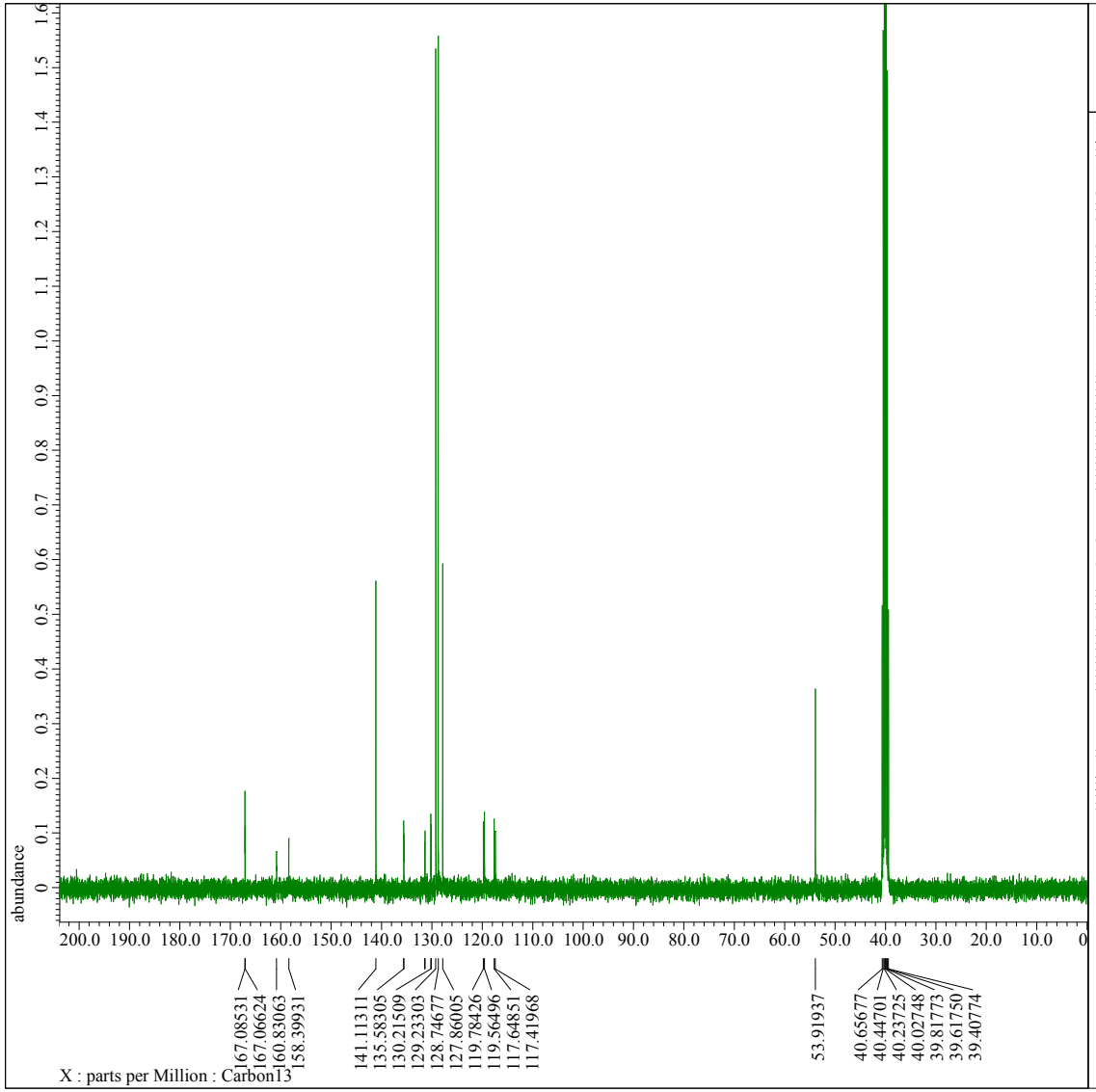

5g



JEOL RESONANCE

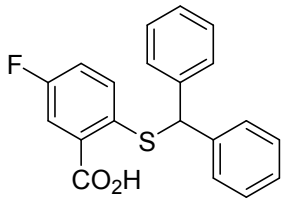
```
Filename          = M-HH5-78-2_Proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH5-78-2
Solvent           = DMSO-D6
Creation_Time     = 21-DEC-2013 11:23:32
Revision_Time     =  1-FEB-2014 11:39:02
Current_Time      =  5-FEB-2014 14:32:01

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 4.36731904[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 32768
X_Prescans        = 1
X_Resolution      = 0.22897343[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          = 19.2[dC]
X_90_Width        = 9.53[us]
X_Acq_Time        = 4.36731904[s]
X_Angle           = 45[deg]
X_Atn             = 0.4[dB]
X_Pulse           = 4.765[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 9.36731904[s]
```


5h

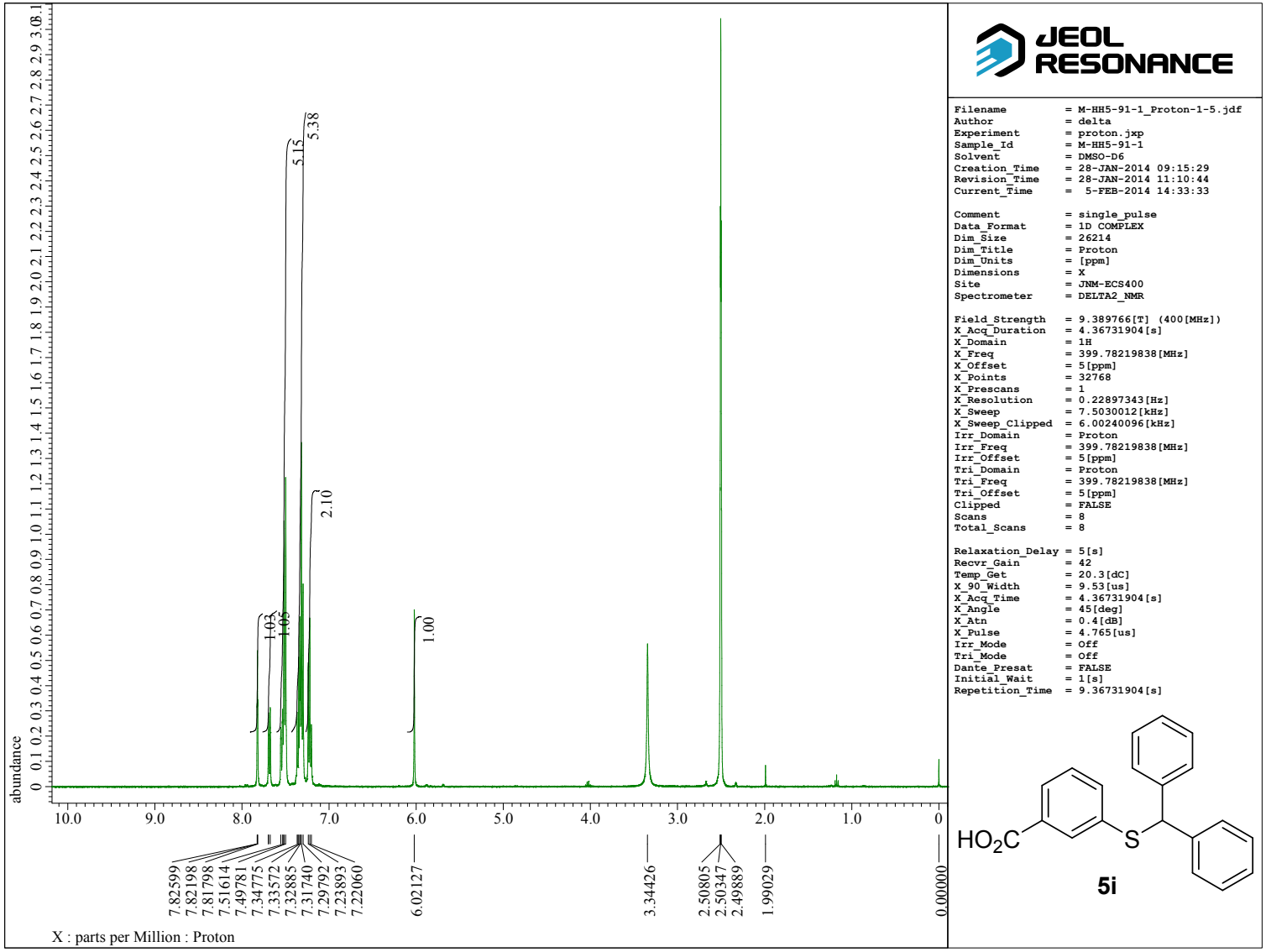


JEOL RESONANCE

```
Filename          = M-HH5-78-2-2_Carbon-1-2.jd
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH5-78-2-2
Solvent           = DMSO-D6
Creation_Time     =  9-JAN-2014 15:12:51
Revision_Time     =  9-JAN-2014 17:56:42
Current_Time      =  5-FEB-2014 14:32:55

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             = 256
Total_Scans       = 256

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 20.8[dC]
X_90_Width        = 8[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.1[dB]
X_Pulse           = 2.66666667[us]
Irr_Atn_Dec       = 21.763[dB]
Irr_Atn_Noe       = 21.763[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]
```



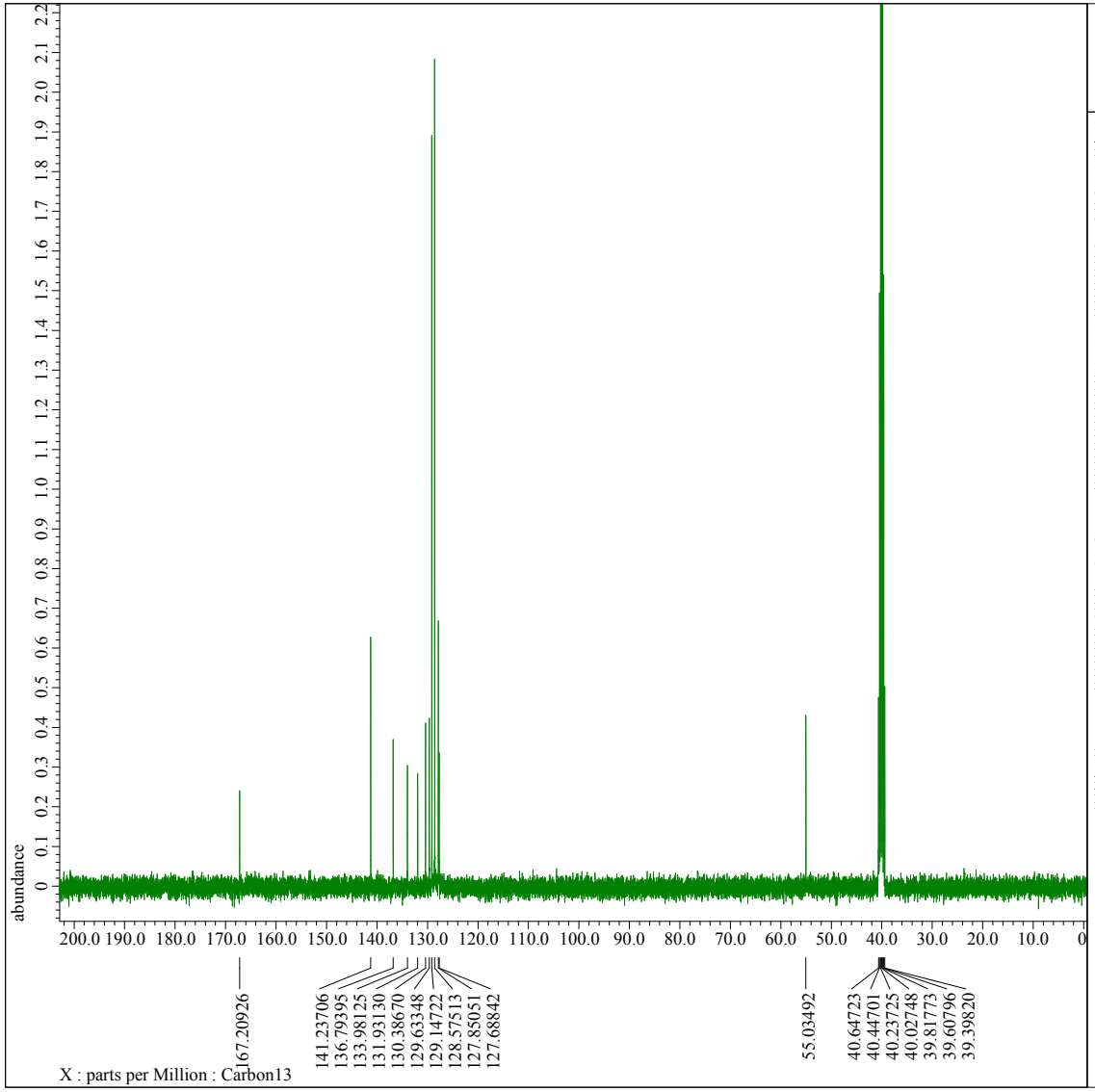
5h



JEOL RESONANCE

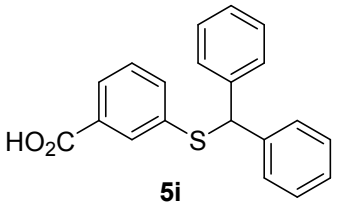
```
Filename          = M-HH5-91-1_Proton-1-5.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH5-91-1
Solvent           = DMSO-D6
Creation_Time     = 28-JAN-2014 09:15:29
Revision_Time     = 28-JAN-2014 11:10:44
Current_Time      =  5-FEB-2014 14:33:33

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 4.36731904[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 32768
X_Prescans        = 1
X_Resolution      = 0.22897343[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          = 20.3[dC]
X_90_Width        = 9.53[us]
X_Acq_Time        = 4.36731904[s]
X_Angle           = 45[deg]
X_Atn             = 0.4[dB]
X_Pulse           = 4.765[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 9.36731904[s]
```


5i

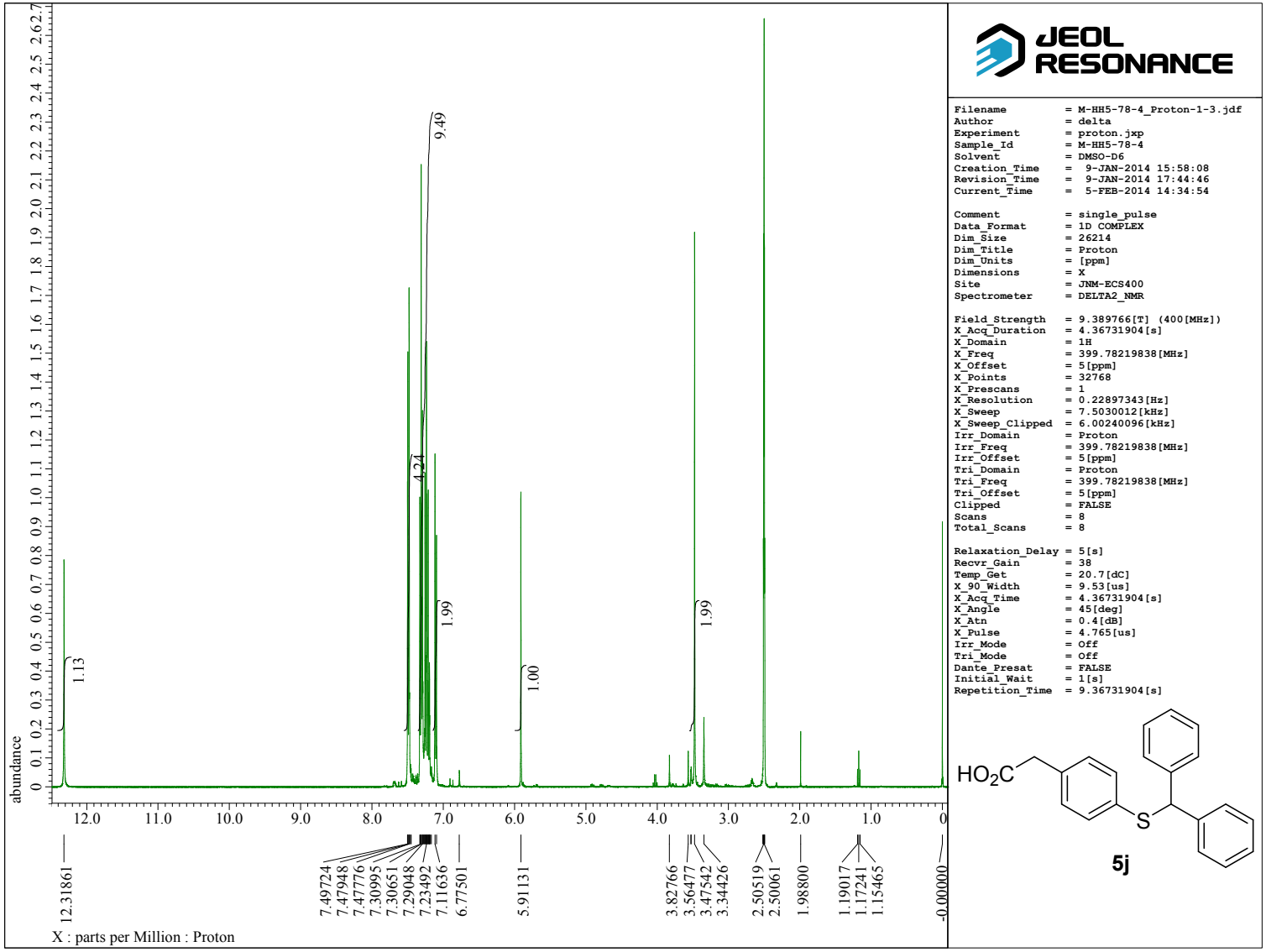


JEOL RESONANCE

```
Filename          = M-HH5-91-1-C_Carbon-1-2.jd
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH5-91-1-C
Solvent           = DMSO-D6
Creation_Time     = 28-JAN-2014 09:36:04
Revision_Time     = 28-JAN-2014 11:13:19
Current_Time      =  5-FEB-2014 14:34:14

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             = 118
Total_Scans       = 118

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 20.5[dC]
X_90_Width        = 8[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.1[dB]
X_Pulse           = 2.66666667[us]
Irr_Atn_Dec       = 21.763[dB]
Irr_Atn_Noe       = 21.763[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]
```



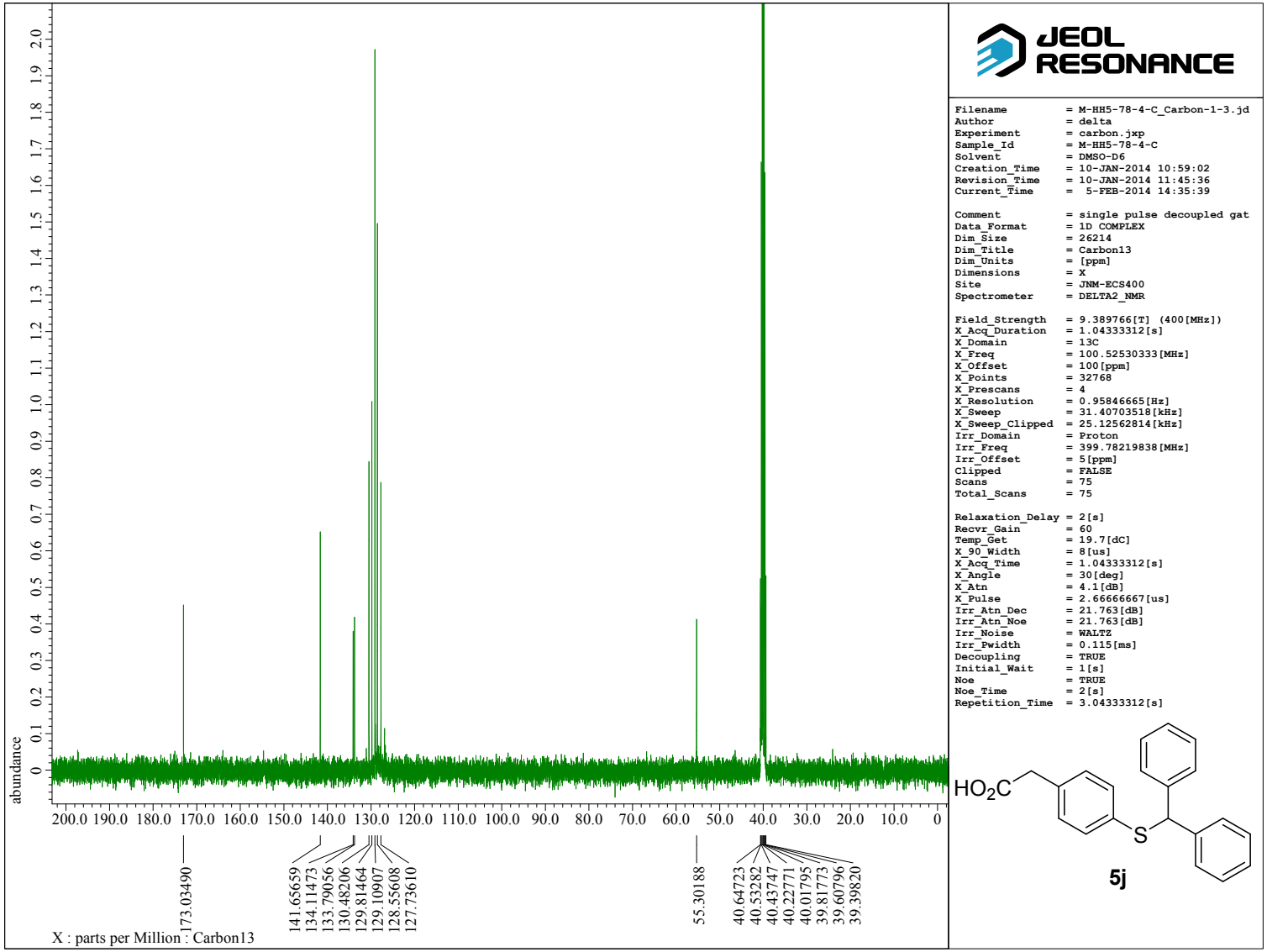
5i



JEOL RESONANCE

```
Filename          = M-HH5-78-4_Proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH5-78-4
Solvent           = DMSO-D6
Creation_Time     =  9-JAN-2014 15:58:08
Revision_Time     =  9-JAN-2014 17:44:46
Current_Time      =  5-FEB-2014 14:34:54

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 4.36731904[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 32768
X_Prescans        = 1
X_Resolution      = 0.22897343[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          = 20.7[dC]
X_90_Width        = 9.53[us]
X_Acq_Time        = 4.36731904[s]
X_Angle           = 45[deg]
X_Atn             = 0.4[dB]
X_Pulse           = 4.765[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 9.36731904[s]
```

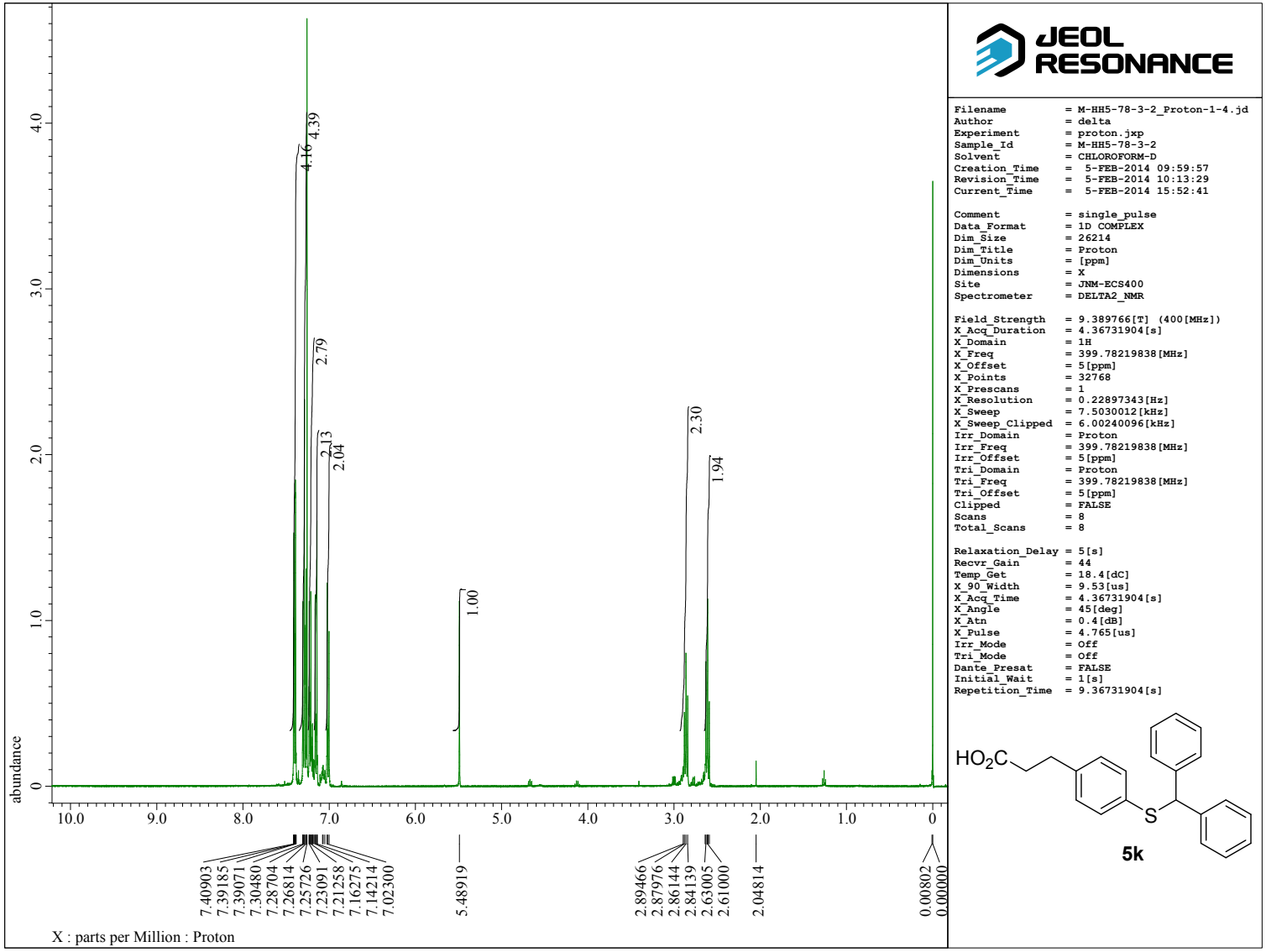

5j



JEOL RESONANCE

```
Filename          = M-HH5-78-4-C_Carbon-1-3.jd
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH5-78-4-C
Solvent           = DMSO-D6
Creation_Time     = 10-JAN-2014 10:59:02
Revision_Time     = 10-JAN-2014 11:45:36
Current_Time      =  5-FEB-2014 14:35:39

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             = 75
Total_Scans       = 75

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 19.7[dC]
X_90_Width        = 8[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.1[dB]
X_Pulse           = 2.66666667[us]
Irr_Atn_Dec       = 21.763[dB]
Irr_Atn_Noe       = 21.763[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]
```

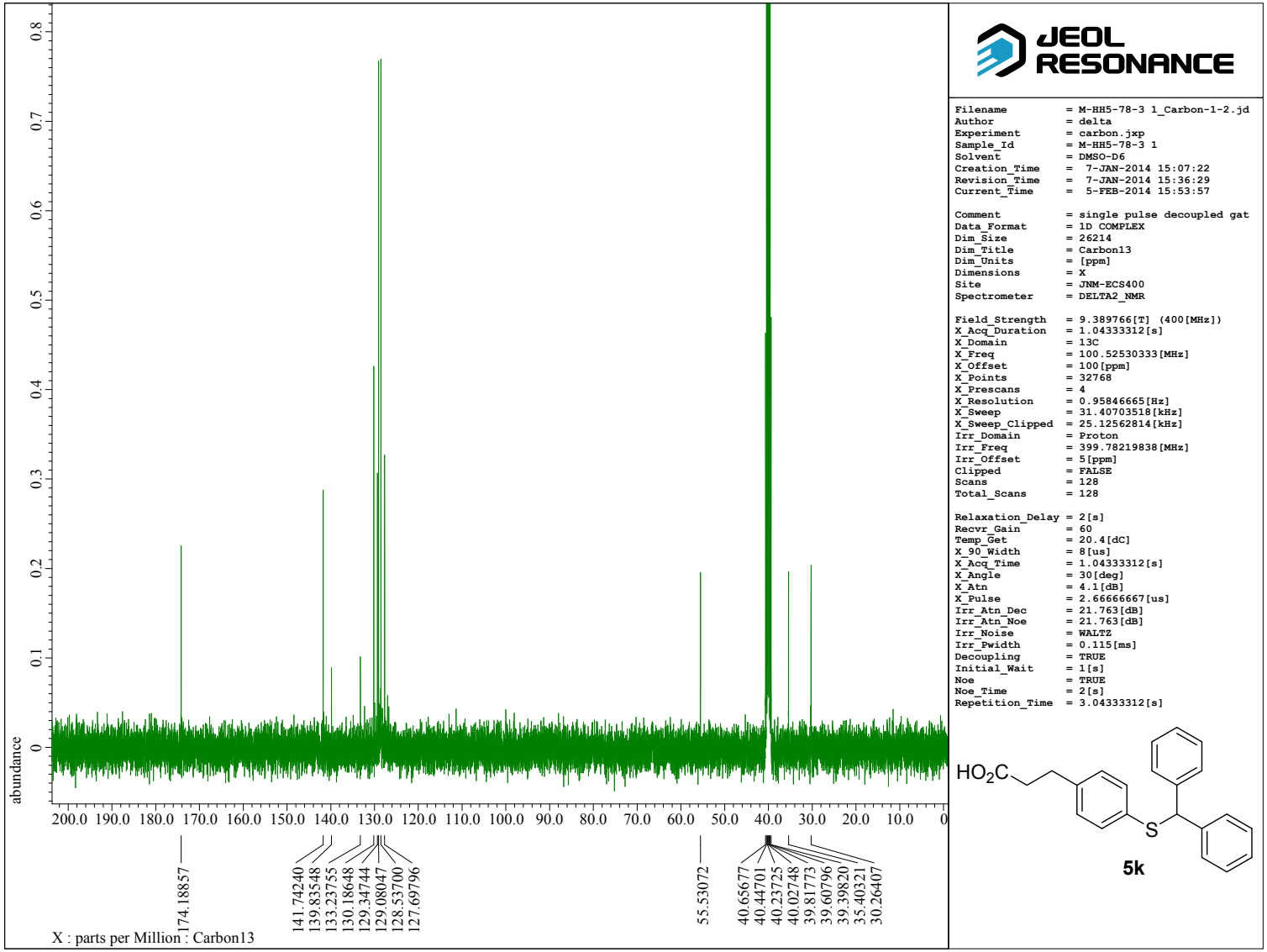

5j



JEOL RESONANCE

```
Filename          = M-HH5-78-3-2_Proton-1-4.jd
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH5-78-3-2
Solvent           = CHLOROFORM-D
Creation_Time     =  5-FEB-2014 09:59:57
Revision_Time     =  5-FEB-2014 10:13:29
Current_Time      =  5-FEB-2014 15:52:41

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 4.36731904[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 32768
X_Prescans        = 1
X_Resolution      = 0.22897343[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          = 18.4[dC]
X_90_Width        = 9.53[us]
X_Acq_Time        = 4.36731904[s]
X_Angle           = 45[deg]
X_Atn             = 0.4[dB]
X_Pulse           = 4.765[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 9.36731904[s]
```


5k



JEOL RESONANCE

```
Filename          = M-HH5-78-3 1_Carbon-1-2.jd
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH5-78-3 1
Solvent           = DMSO-D6
Creation_Time     =  7-JAN-2014 15:07:22
Revision_Time     =  7-JAN-2014 15:36:29
Current_Time      =  5-FEB-2014 15:53:57

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             = 128
Total_Scans       = 128

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 20.4[dC]
X_90_Width        = 8[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.1[dB]
X_Pulse           = 2.66666667[us]
Irr_Atn_Dec       = 21.763[dB]
Irr_Atn_Noe       = 21.763[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]
```


5k