Electronic Supplementary Material (ESI) for RSC Advances.

Furopyridinediones as novel inhibitors of α-glucosidases

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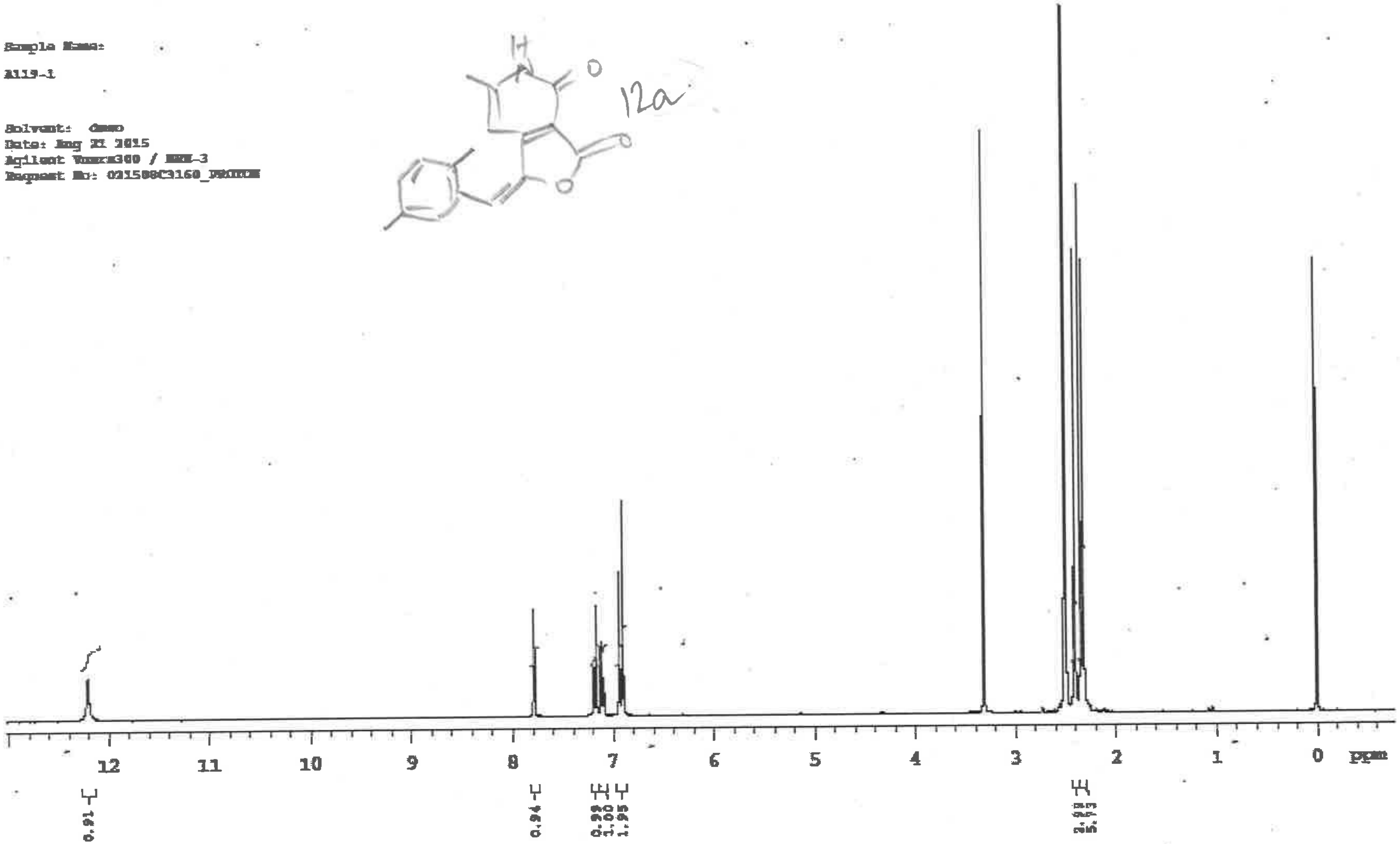
Contents

Sample Name:

A119-1

Solvent: dmso
Date: Aug 21 2015
Agilent Vnmrs300 / NMR-3
Request No: 021508C3160_PROTON



12a

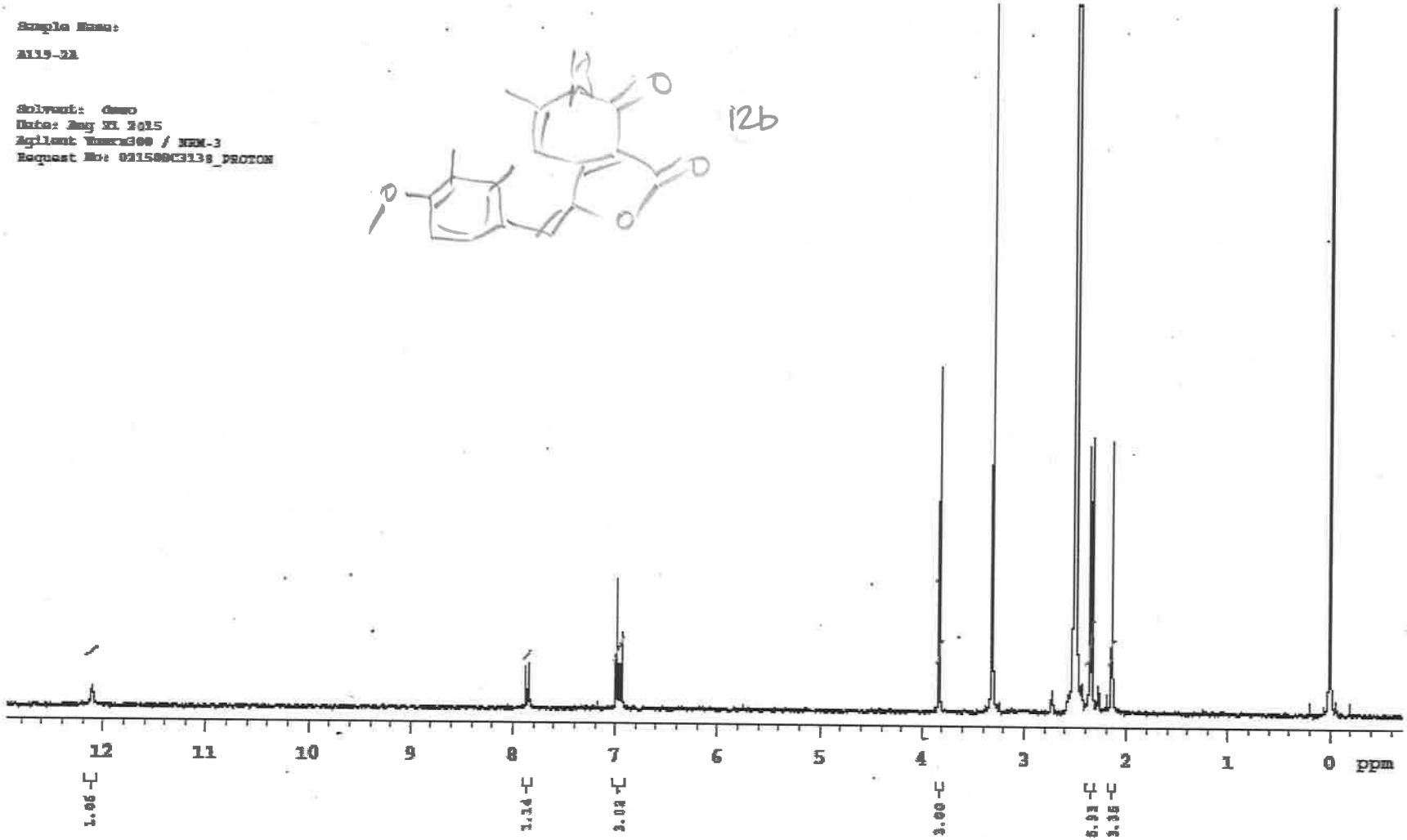
Plotname: 031509C3160_PROTON_01_plot01

Sample Name:

A119-2A

Solvent: dmso
Date: May 21 2015
Agilent Vnmrs600 / NEM-3
Request No: 021508C3138_PROTON

12b

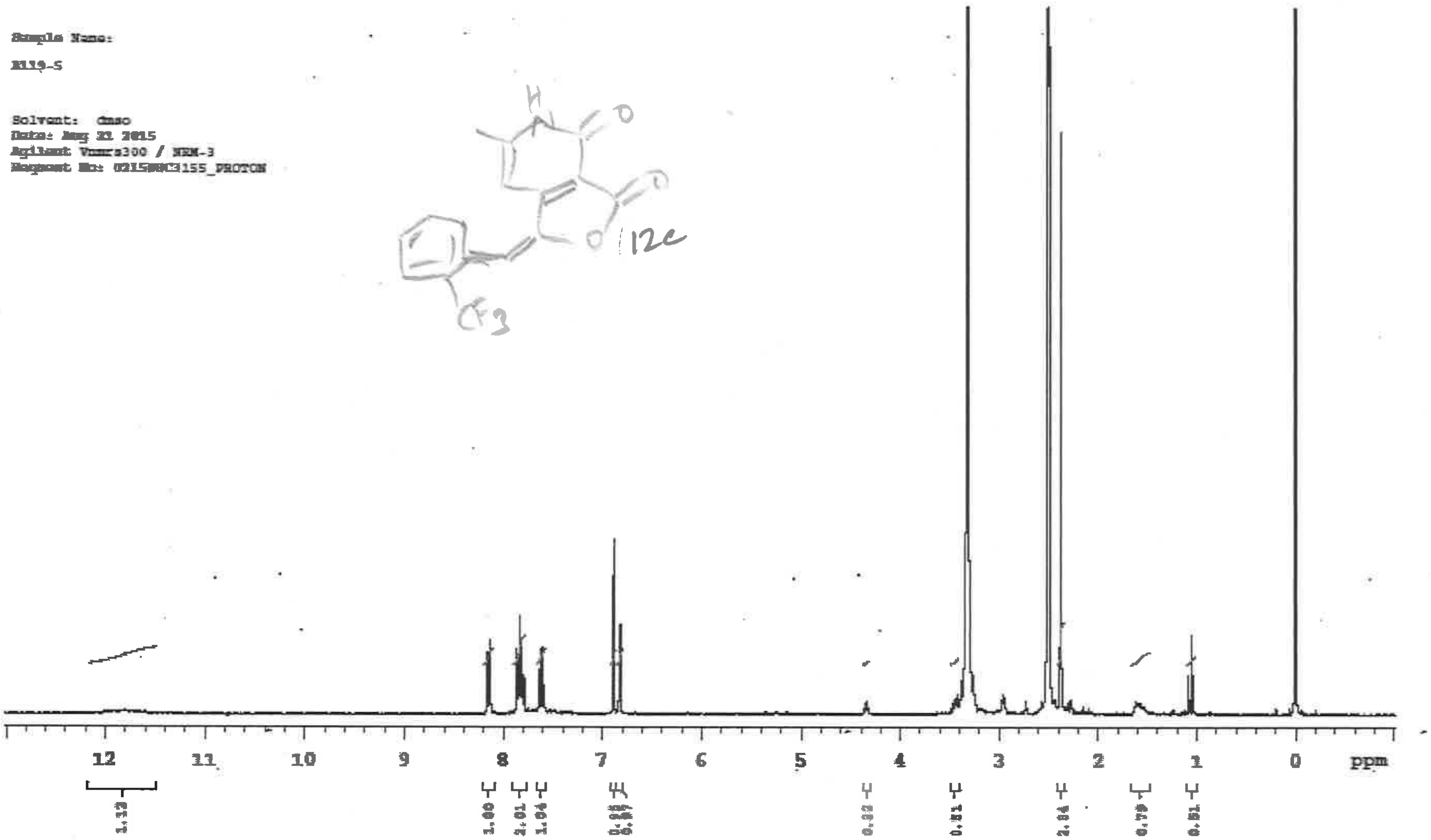


Filename: 021508C3138_PROTON_01_plot01

Sample Name:

B119-5

Solvent: dmso
Date: Aug 21 2015
Agilent Vnmrs300 / NRM-3
Request No: 021508C3155_PROTON

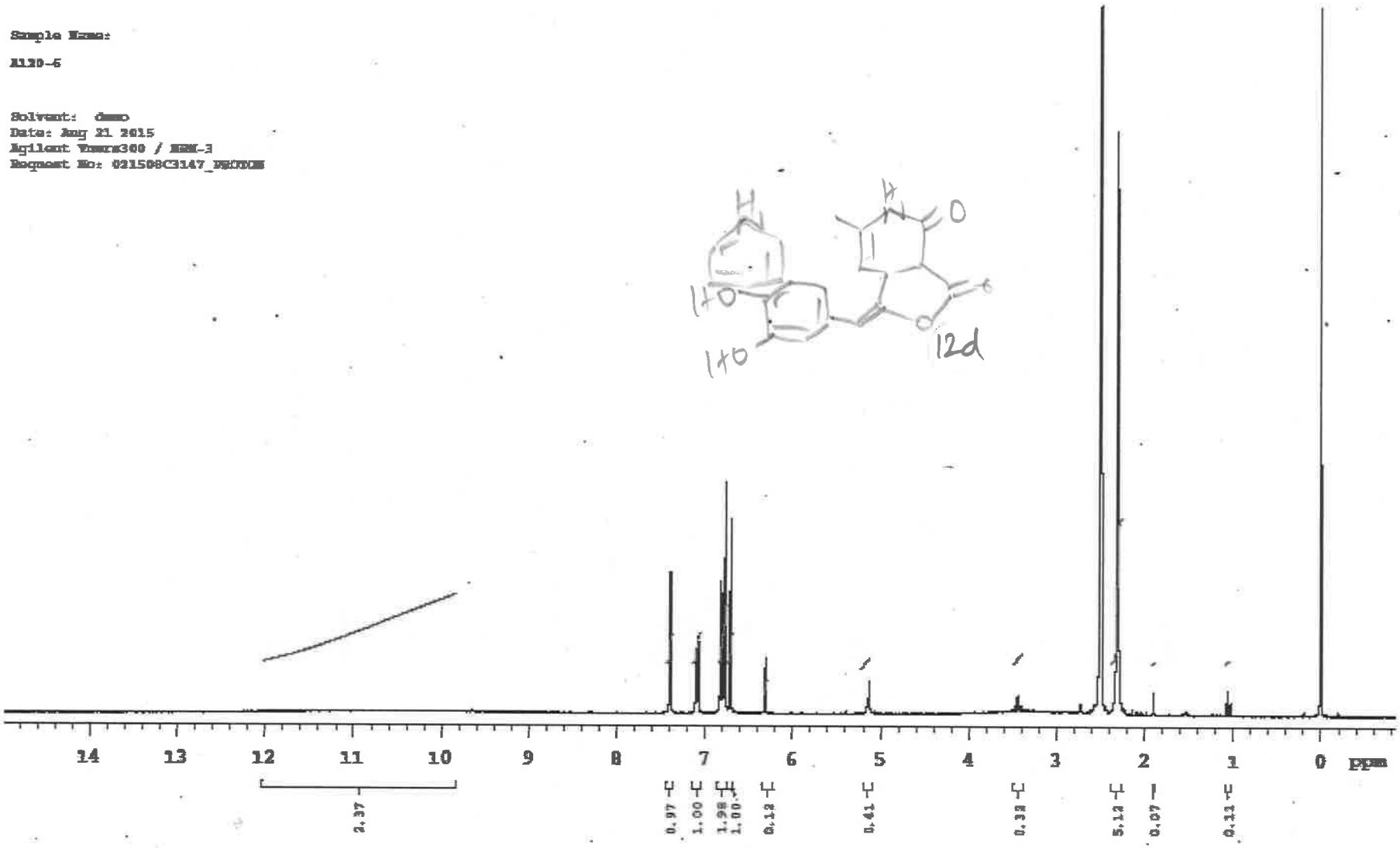


Plotname: 021508C3155_PROTON_01_plot01

Sample Name:

A130-6

Solvent: dmso
Date: Aug 21 2015
Agilent Vnmrs300 / NMR-3
Request No: 021508C3147_PROTON

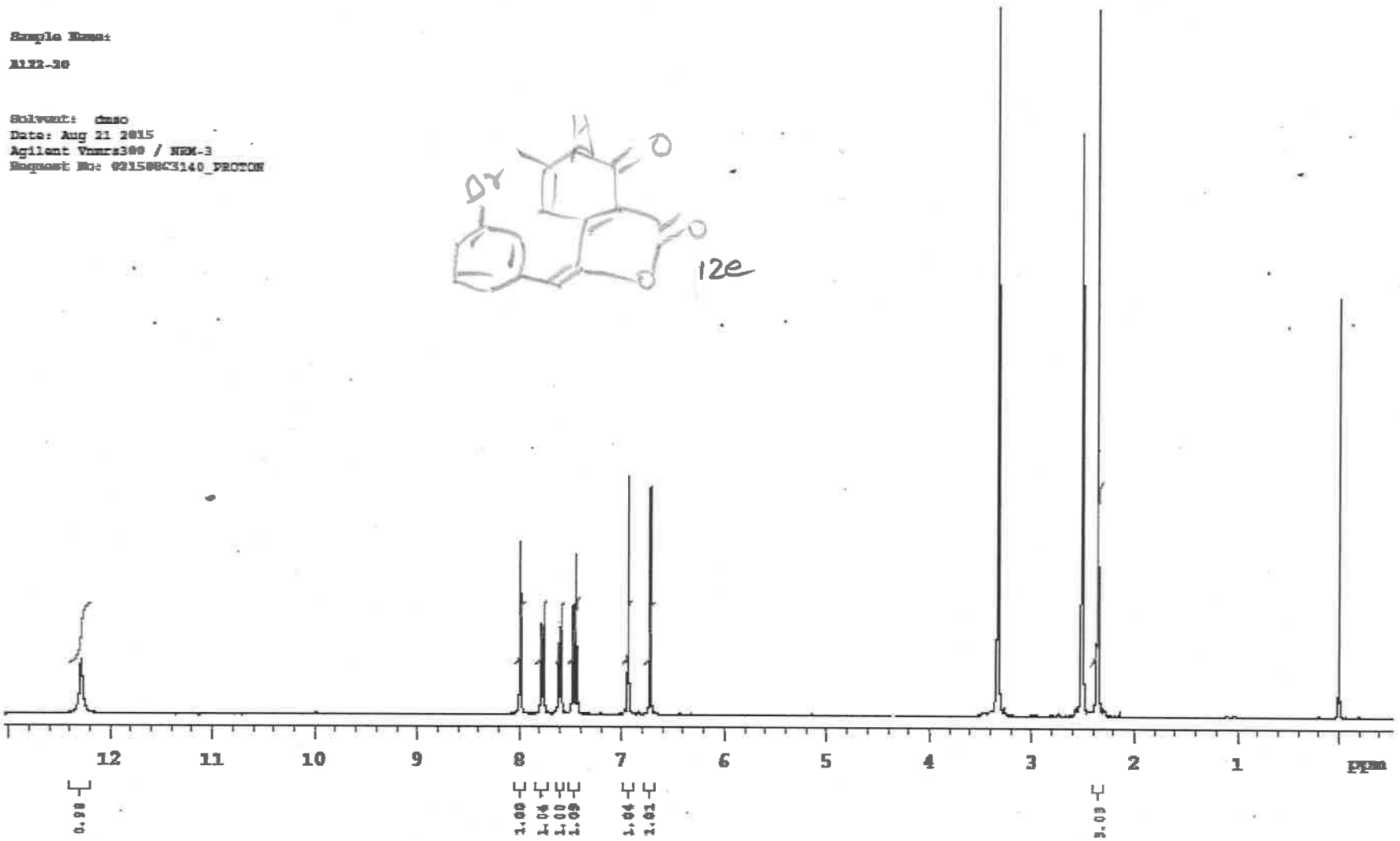


Plotname: 021508C3147_PROTON_01_plot01

Sample Name:

RJ22-30

Solvent: dmso
Date: Aug 21 2015
Agilent Vnmrs300 / NRM-3
Exposat No: 021508C3140_PROTON

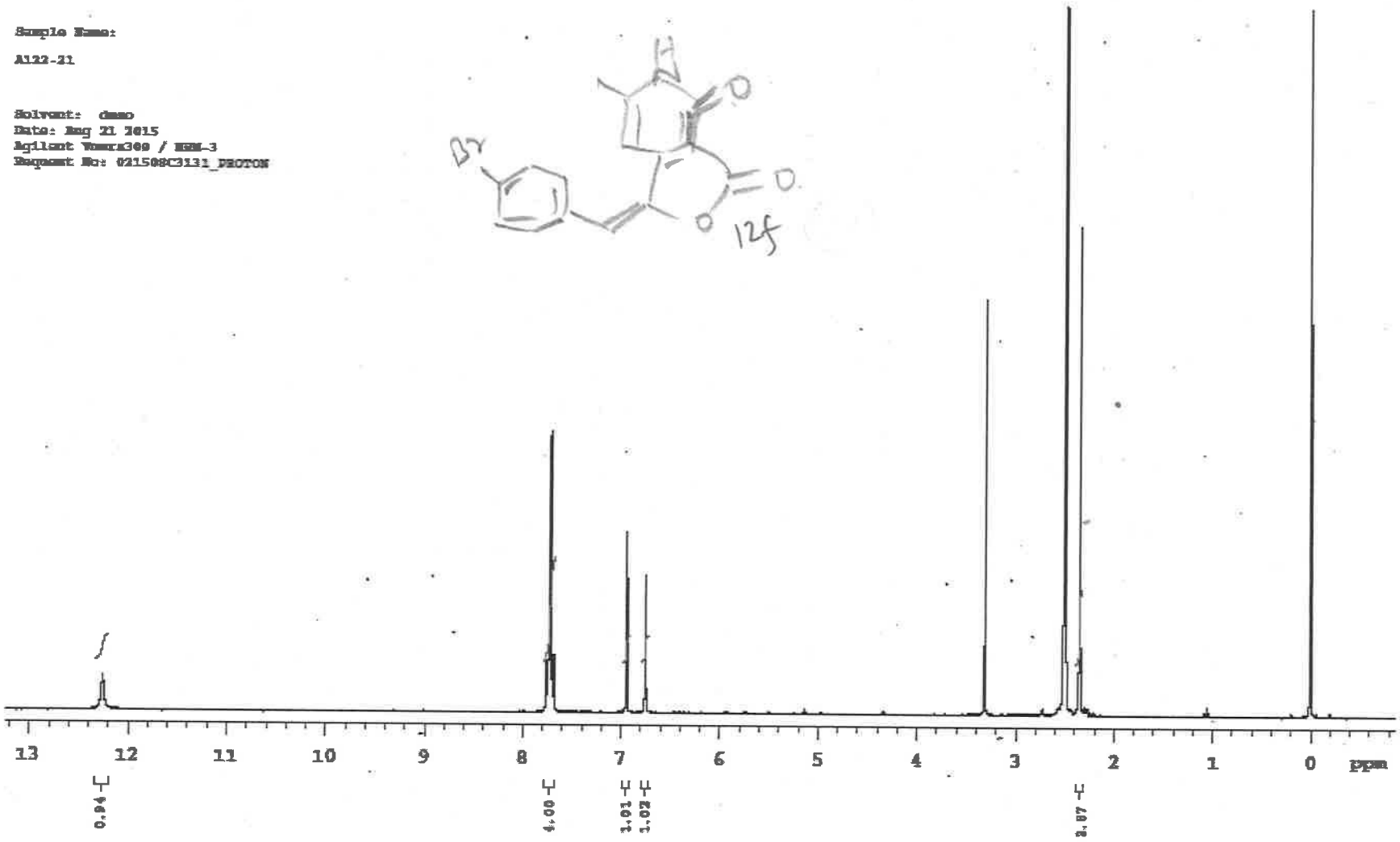


Plotname: 021508C3140_PROTON_01_plot01

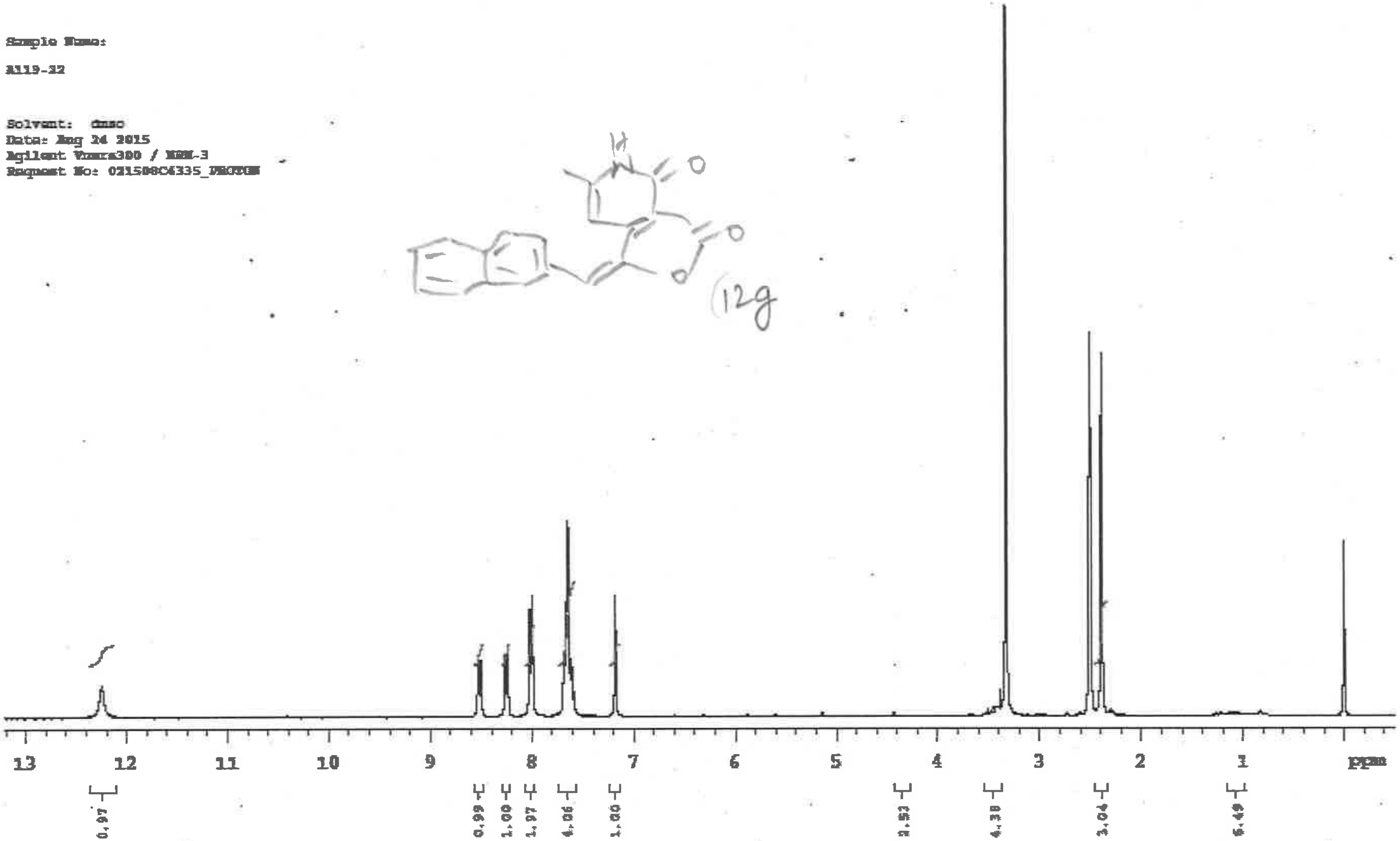
Sample Name:

A122-21

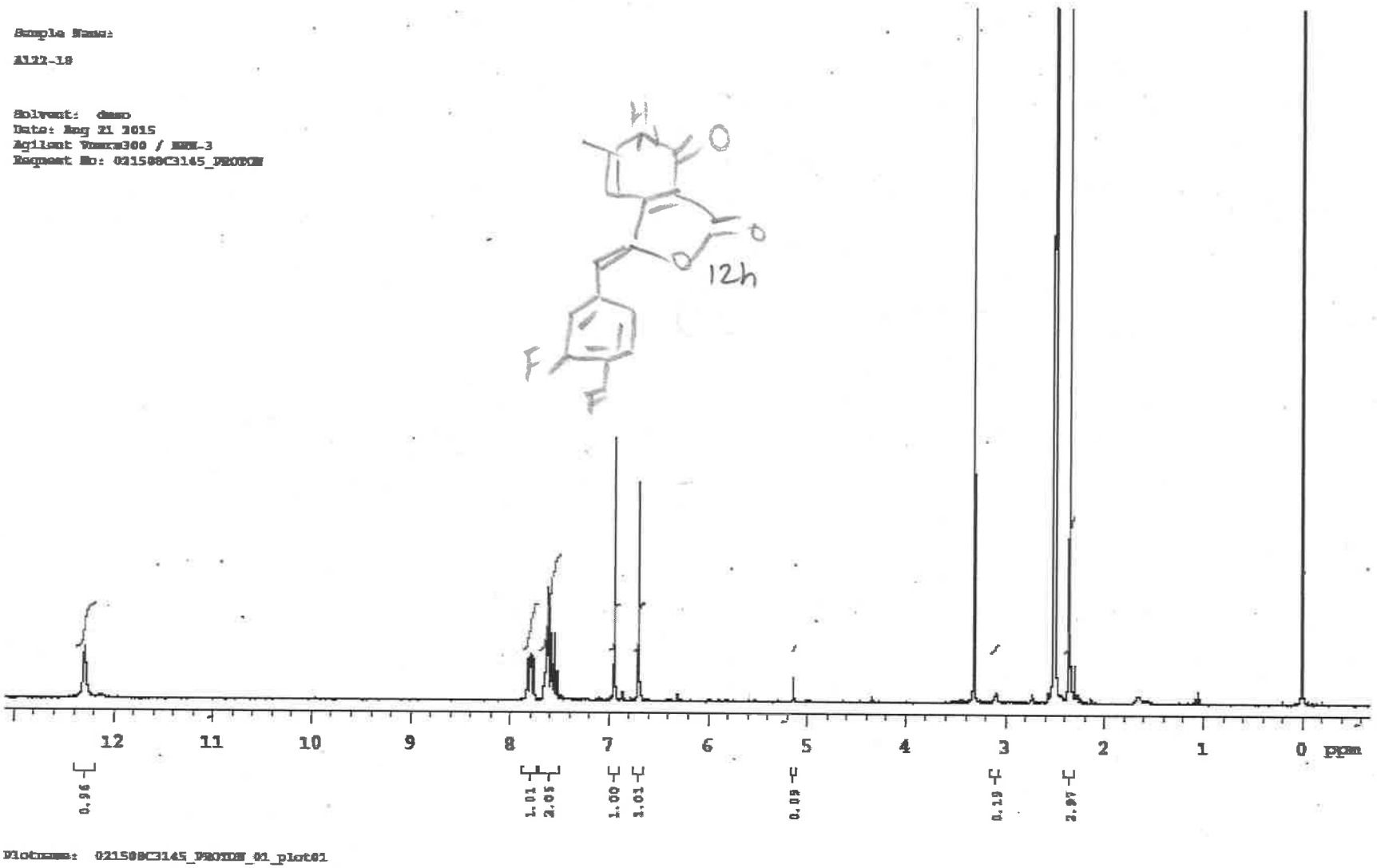
Solvent: dmso
Date: Aug 21 2015
Agilent Vnmrs300 / ESM-3
Request No: 021508C3131_PROTON

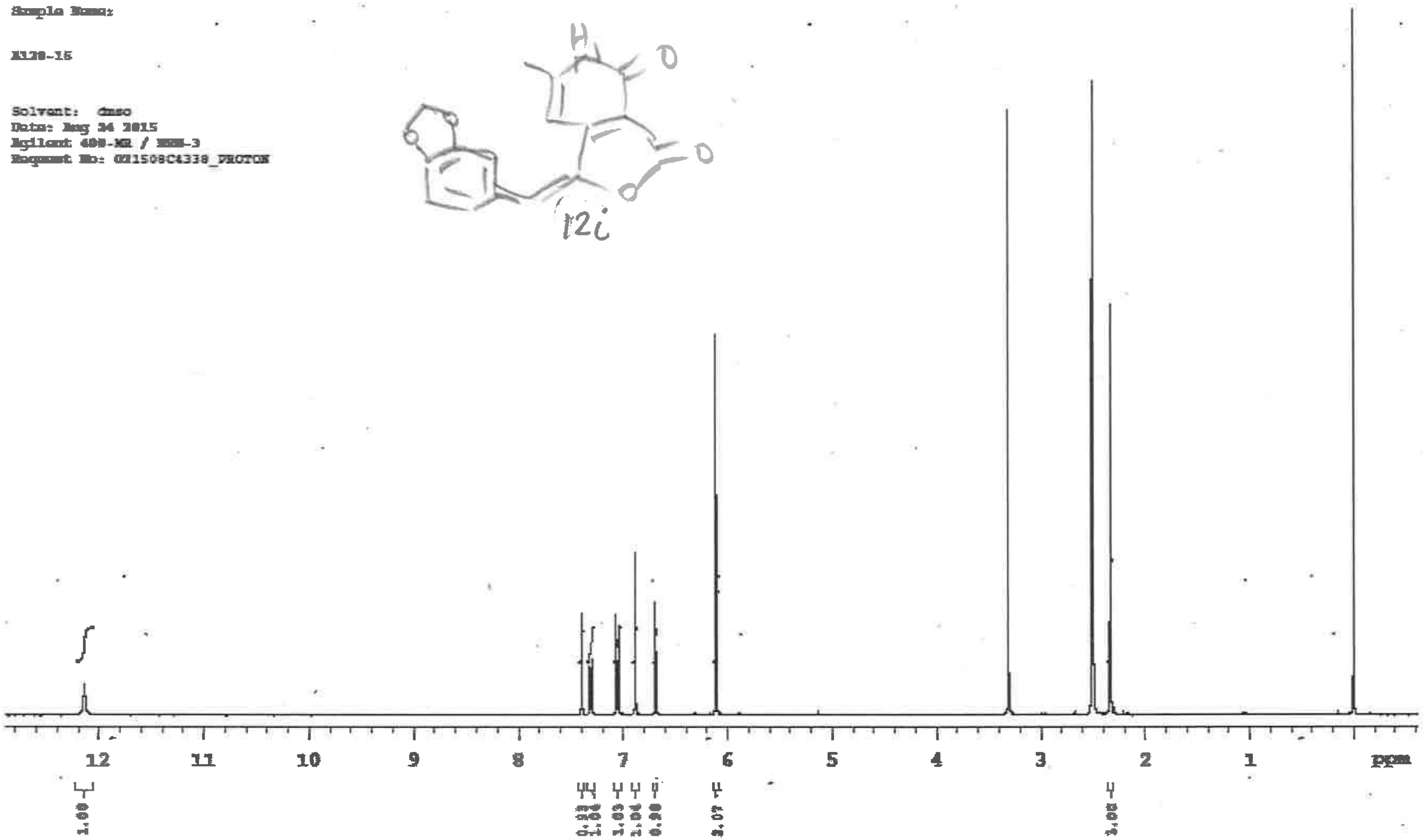


Plotname: 021508C3131_PROTON_01_plot01



Plotname: 021508C4335_PROTON_01_plot01

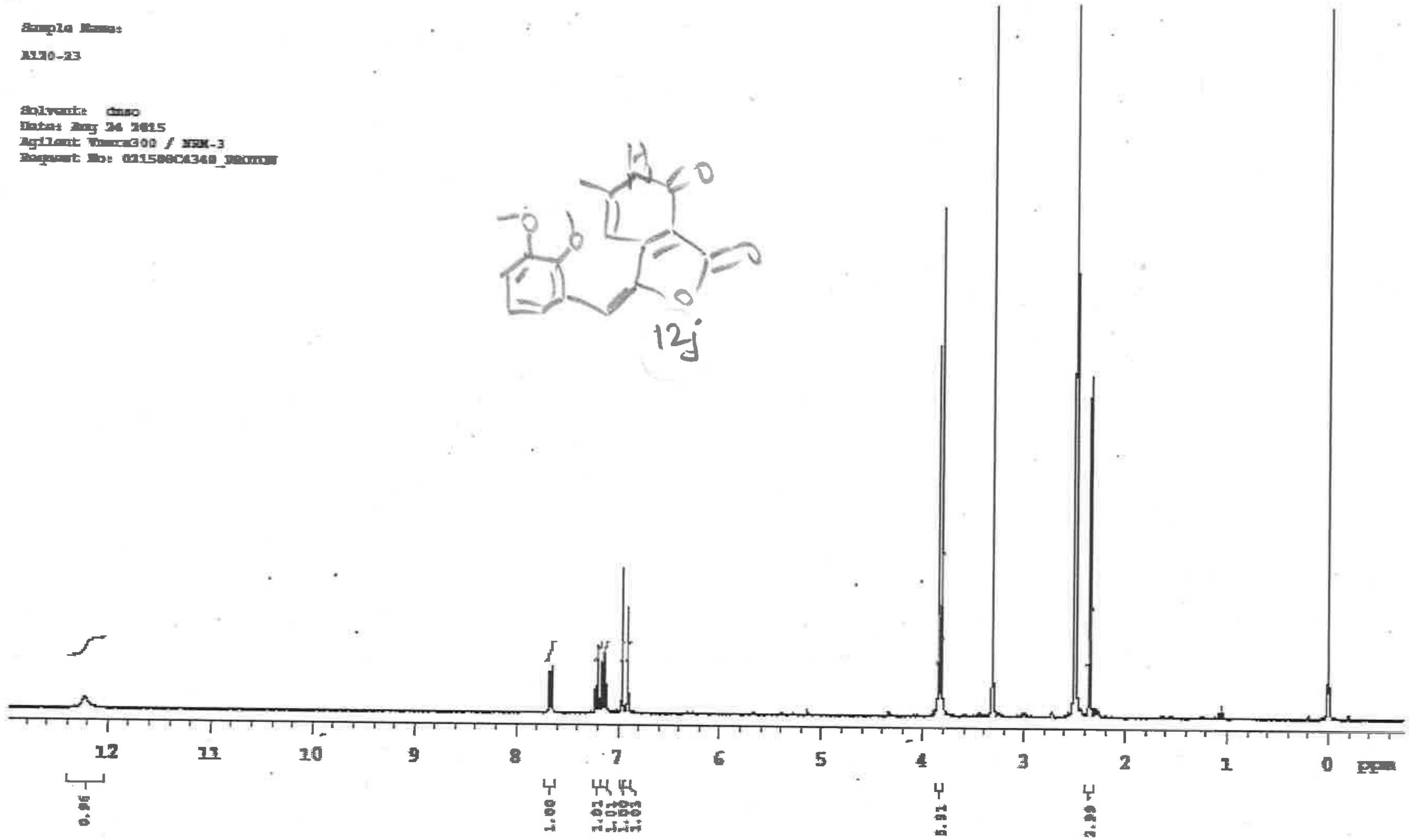

Sample Name:
A122-18
Solvent: dmso
Date: Aug 21 2015
Agilent Vnmrs300 / BBM-3
Request No: 021508C3145_PROTON
12h
F
F
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.96
1.01
2.05
1.00
1.01
0.09
0.19
2.97
Plotname: 021508C3145_PROTON_01_plot01


Sample Name:
Solvent: dmso
15508C4338_PROTON
12i
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00

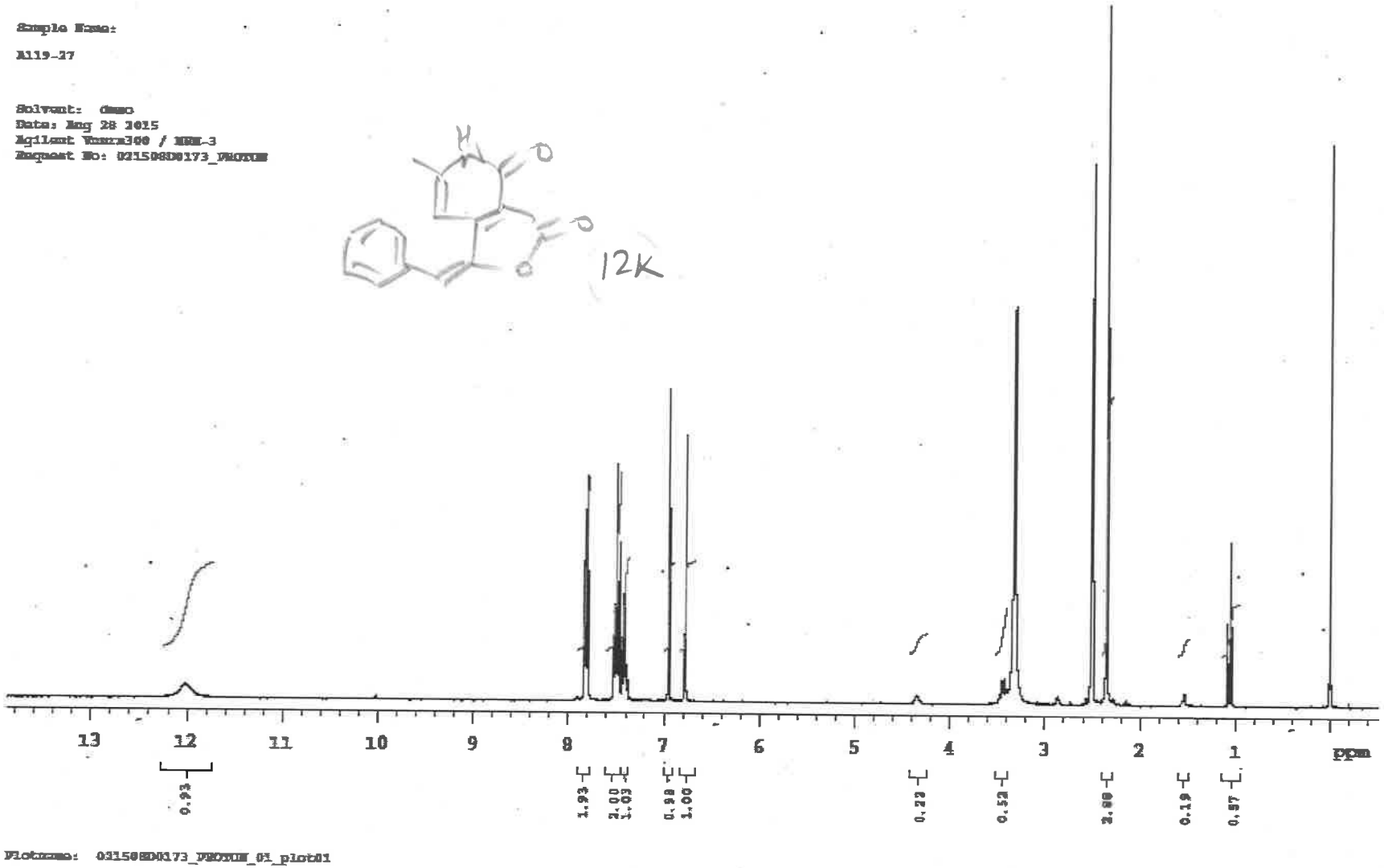
Sample Name:

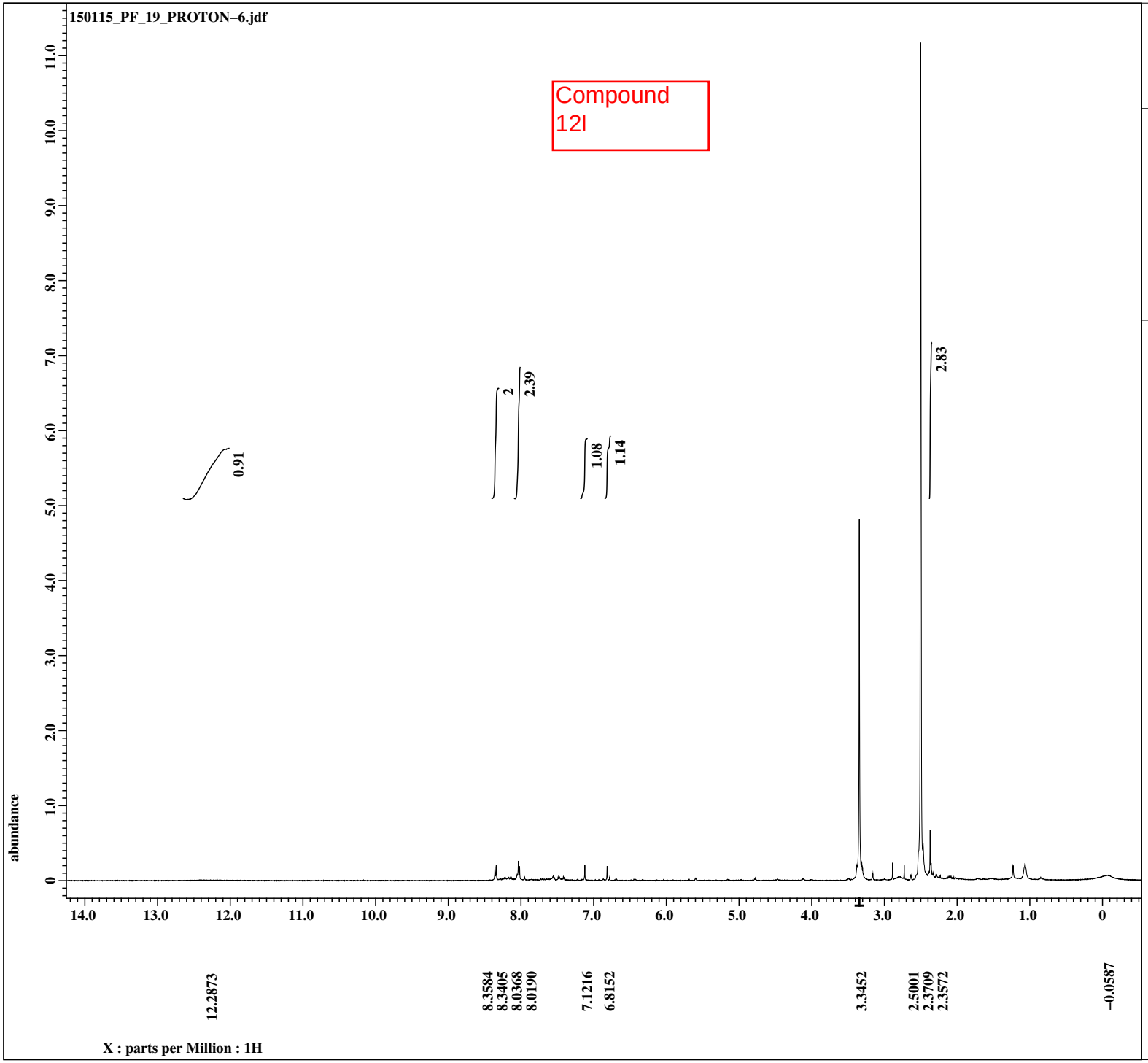
A120-23

Solvent: dmso
Date: Aug 24 2015
Agilent VnmrS300 / NMR-3
Request No: 021500C4340_PROTON



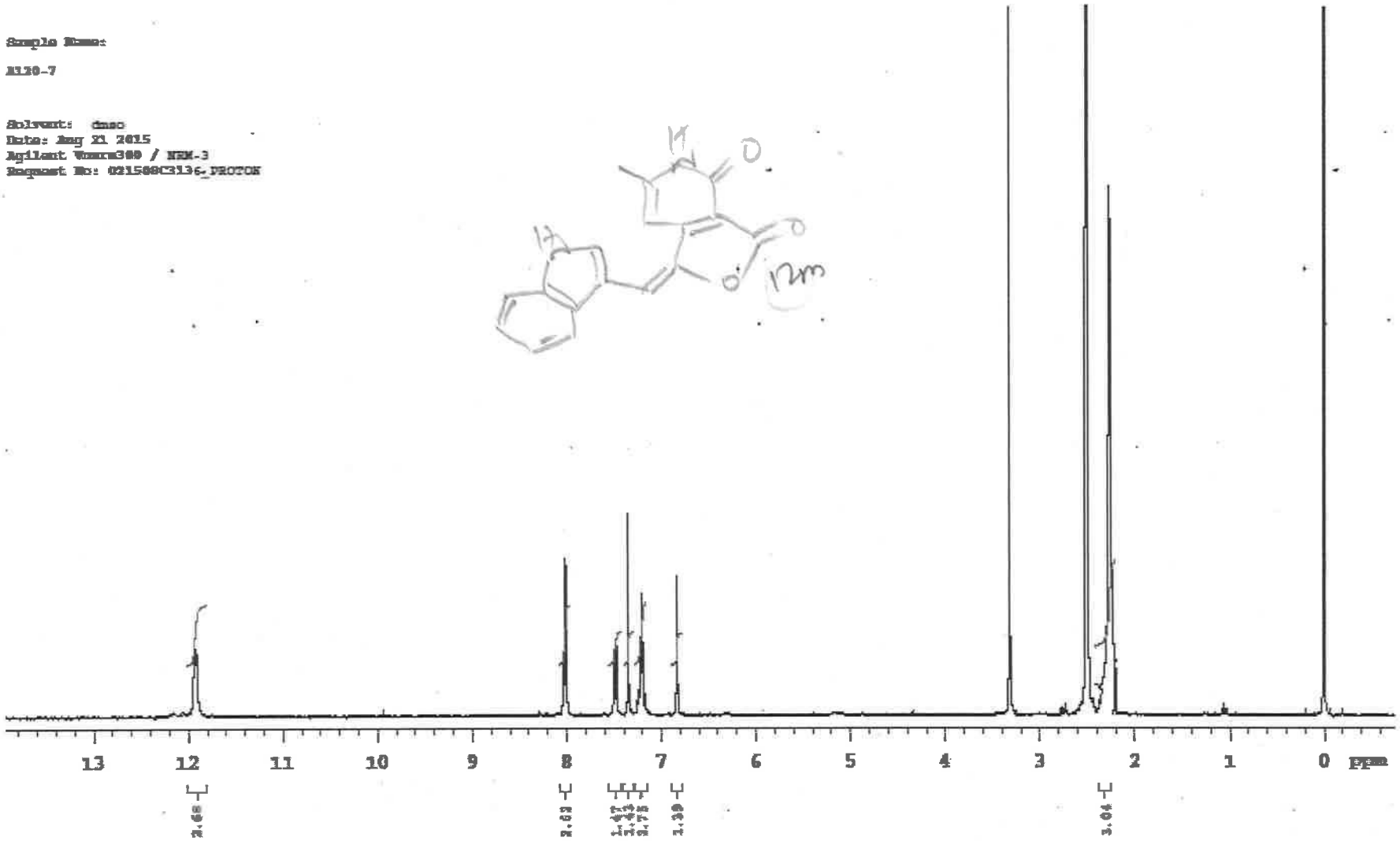
Plotname: 021500C4340_PROTON_01_plot01

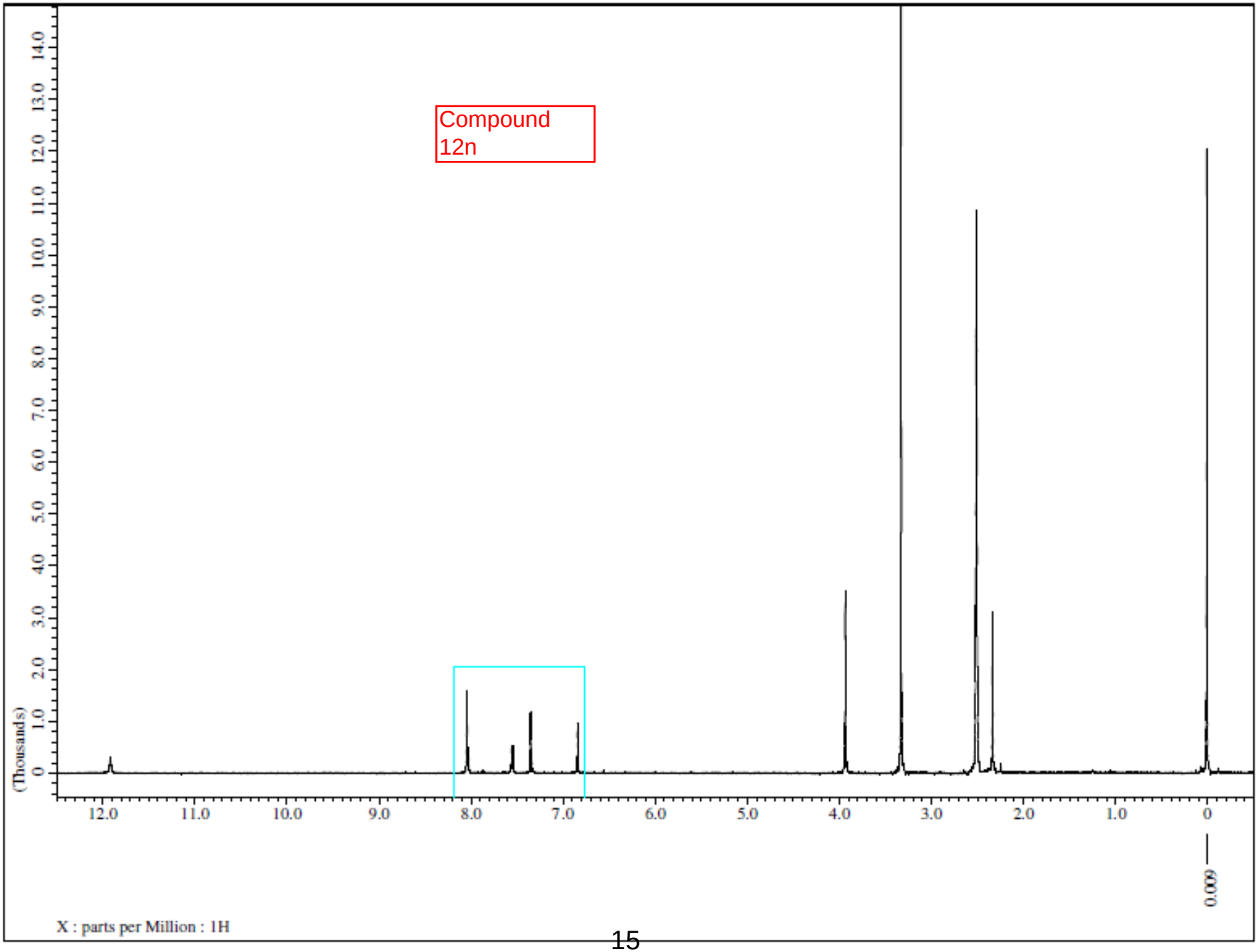

Sample Name:
A119-27
Solvent: dmso
Date: Aug 28 2015
Agilent Vnmrs400 / NMR-3
Request No: 0215082D0173_PROTON
12K
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.93
1.93
2.00
1.03
0.98
1.00
0.22
0.52
2.80
0.19
0.97
Plotname: 0215082D0173_PROTON_01_plot01

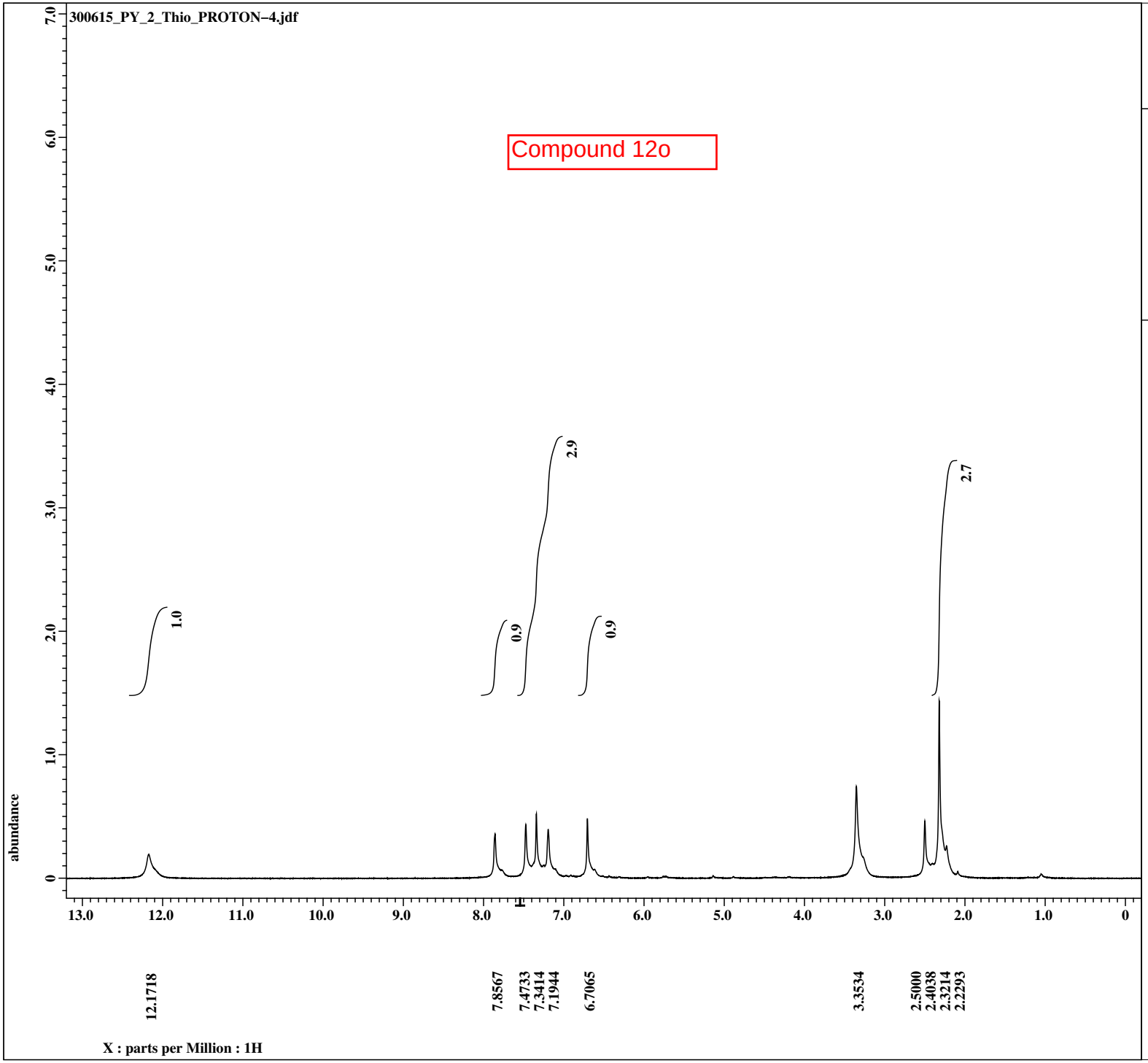



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
phase : 4.25 : -14 : 73.28704[%]
reference : 2.462[ppm] : 2.5[ppm]

Derived from: 150115_PF_19_PROTON-1.jdf
```

```
Filename          = 150115_PF_19_PROTON-6
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = 150115_PF_19
Solvent           = DMSO-D6
Creation_time     = 15-JAN-2015 19:45:38
Revision_time     = 16-JAN-2015 10:44:10
Current_time      = 16-JAN-2015 10:44:37

Comment           = 150115_PF_19
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = JNM-ECX500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.4548992[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 7.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.68733284[Hz]
X_sweep           = 11.26126126[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 11.21[us]
X_acq_time        = 1.4548992[s]
X_angle           = 45[deg]
X_atn             = 3.4[dB]
X_pulse           = 5.605[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 48
Relaxation_delay  = 4[s]
Repetition_time   = 5.4548992[s]
Temp_get          = 18[dC]
```


Sample Name:
A130-7
Solvent: dmso
Date: Aug 21 2015
Agilent Vnmrs300 / NRM-3
Request No: 0215S0C3136_PROTON
12m
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.68
2.03
3.04
1.39
Plotname: 0215S0C3136_PROTON_01_plot01


Compound
12n
(Thousands)
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.000
X : parts per Million : 1H

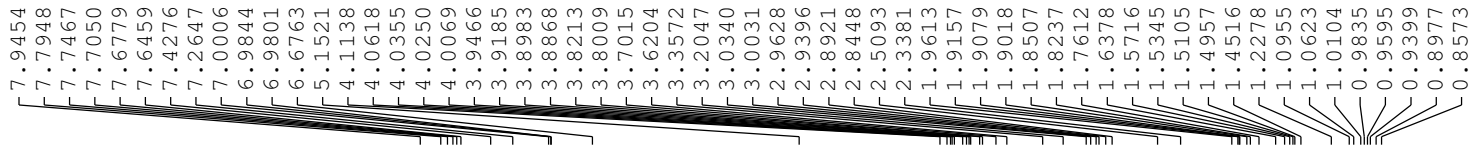



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 300615_PY_2_Thio_PROTON-1.
```

```
Filename          = 300615_PY_2_Thio_PROT
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = 300615_PY_2_Thio
Solvent           = DMSO-D6
Creation_time     =  1-JUL-2015 09:50:53
Revision_time     =  1-JUL-2015 11:48:15
Current_time      =  1-JUL-2015 11:48:48

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = JNM-ECX500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.4548992[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 7.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.68733284[Hz]
X_sweep           = 11.26126126[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.6[us]
X_acq_time        = 1.4548992[s]
X_angle           = 45[deg]
X_atn             = 3.4[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 4[s]
Repetition_time   = 5.4548992[s]
Temp_get          = 18.4[dC]
```

1 H NMR of PF-17

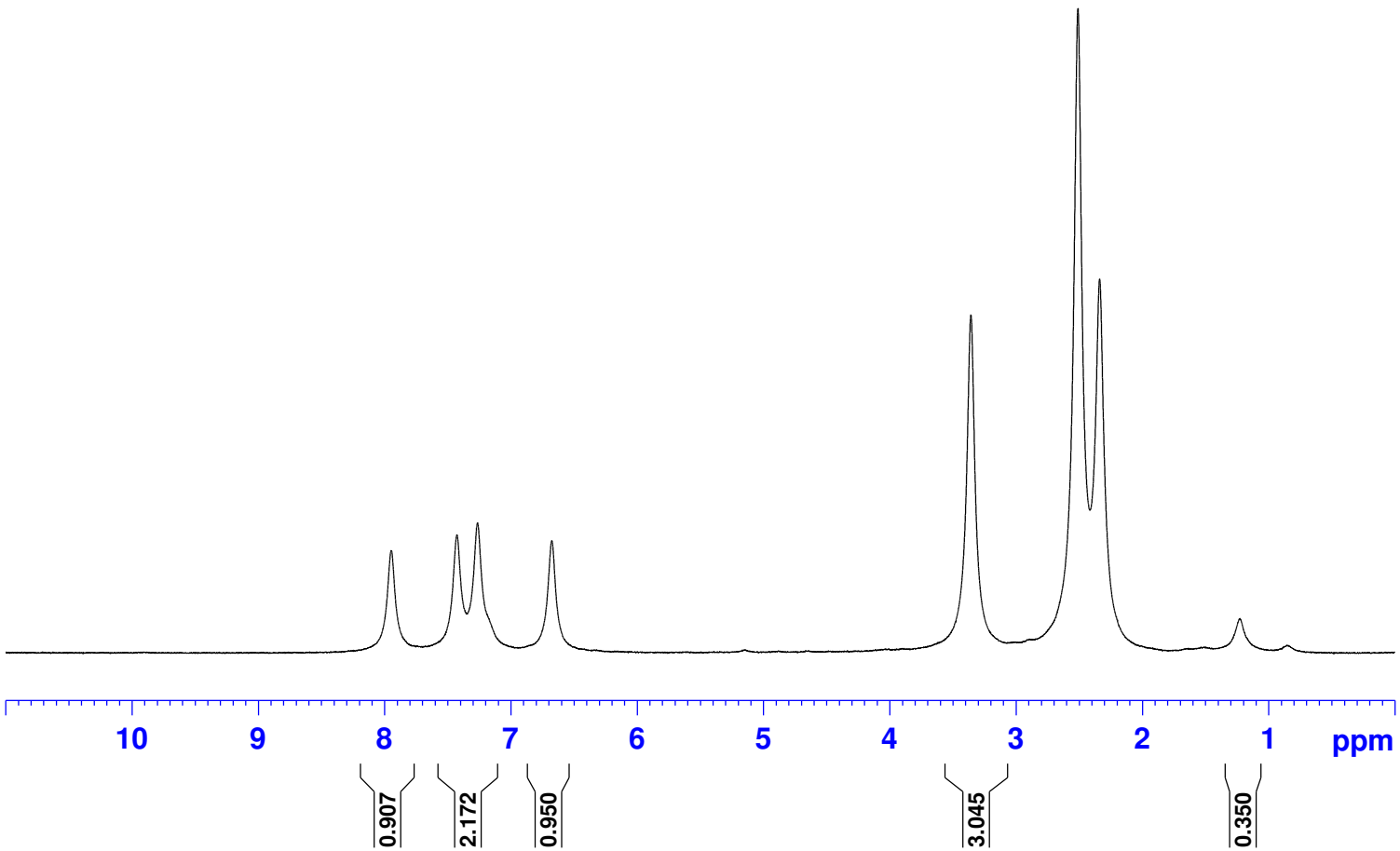
Compound 12p

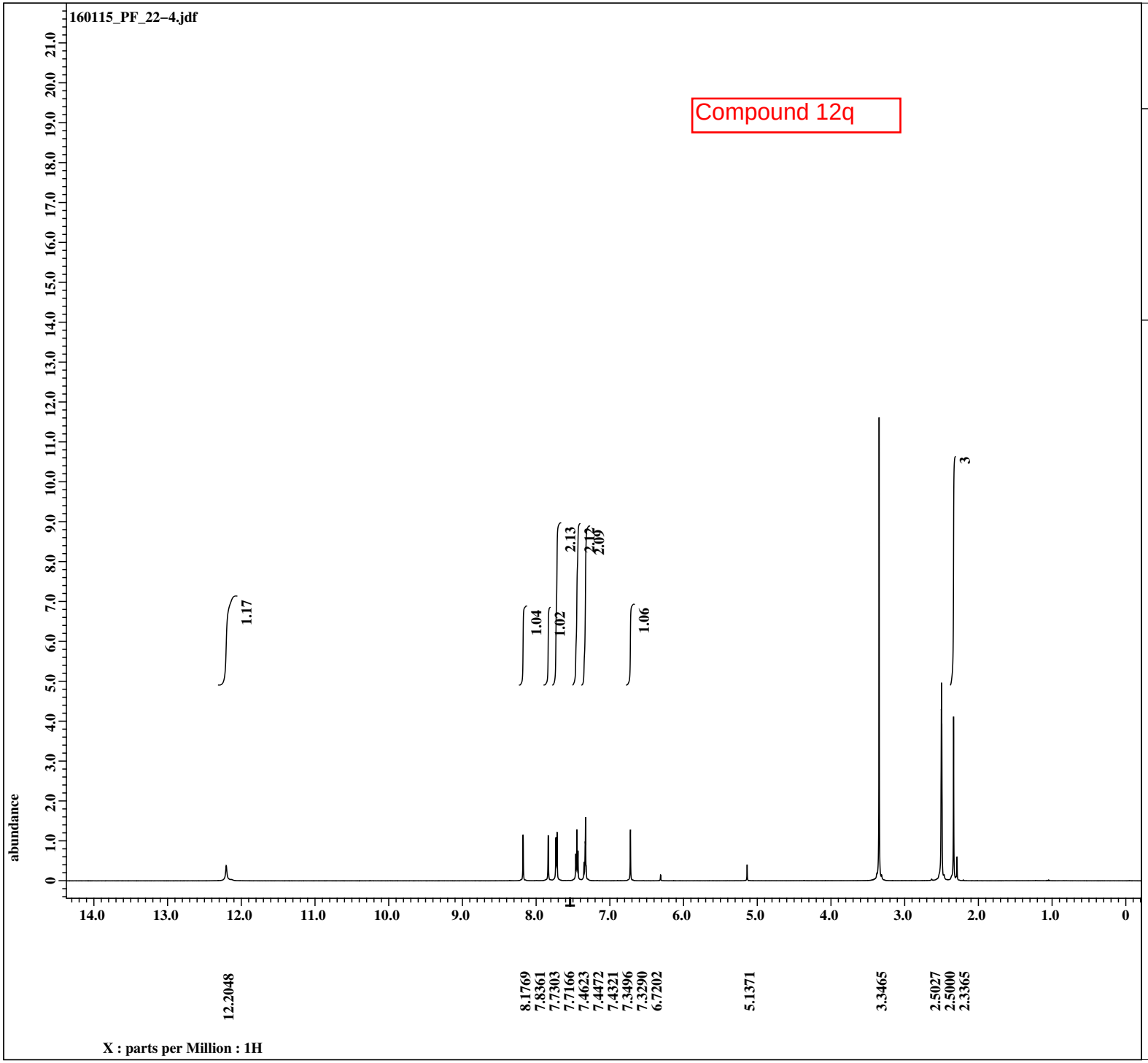


NAME	Shantanu
EXPNO	2
PROCNO	1
Date_	20150515
Time	11.41
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	144
DW	48.400 usec
DE	6.50 usec
TE	299.1 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

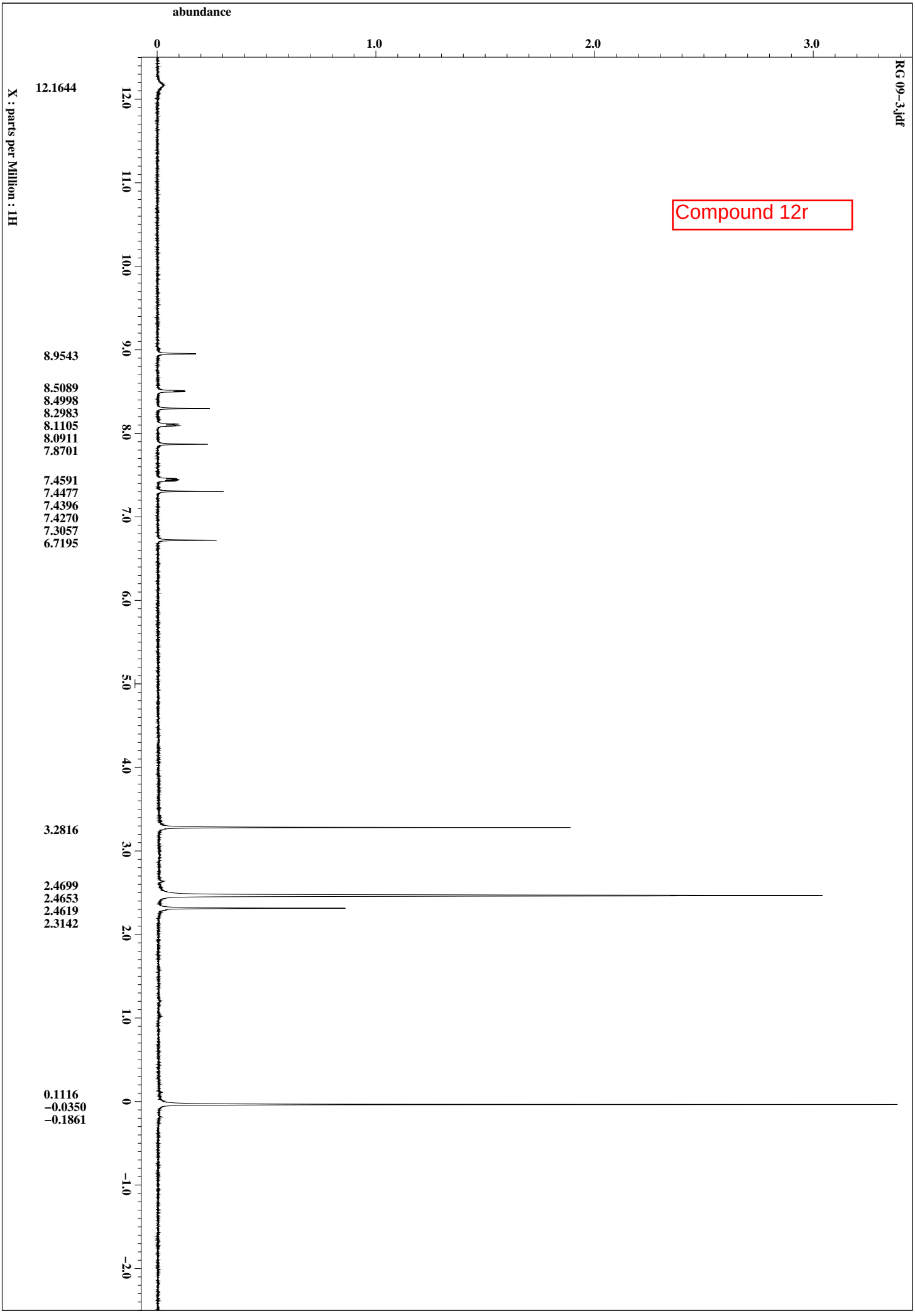
NUC1	1H
P1	10.90 usec
PL1	1.10 dB
PL1W	18.99148560 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

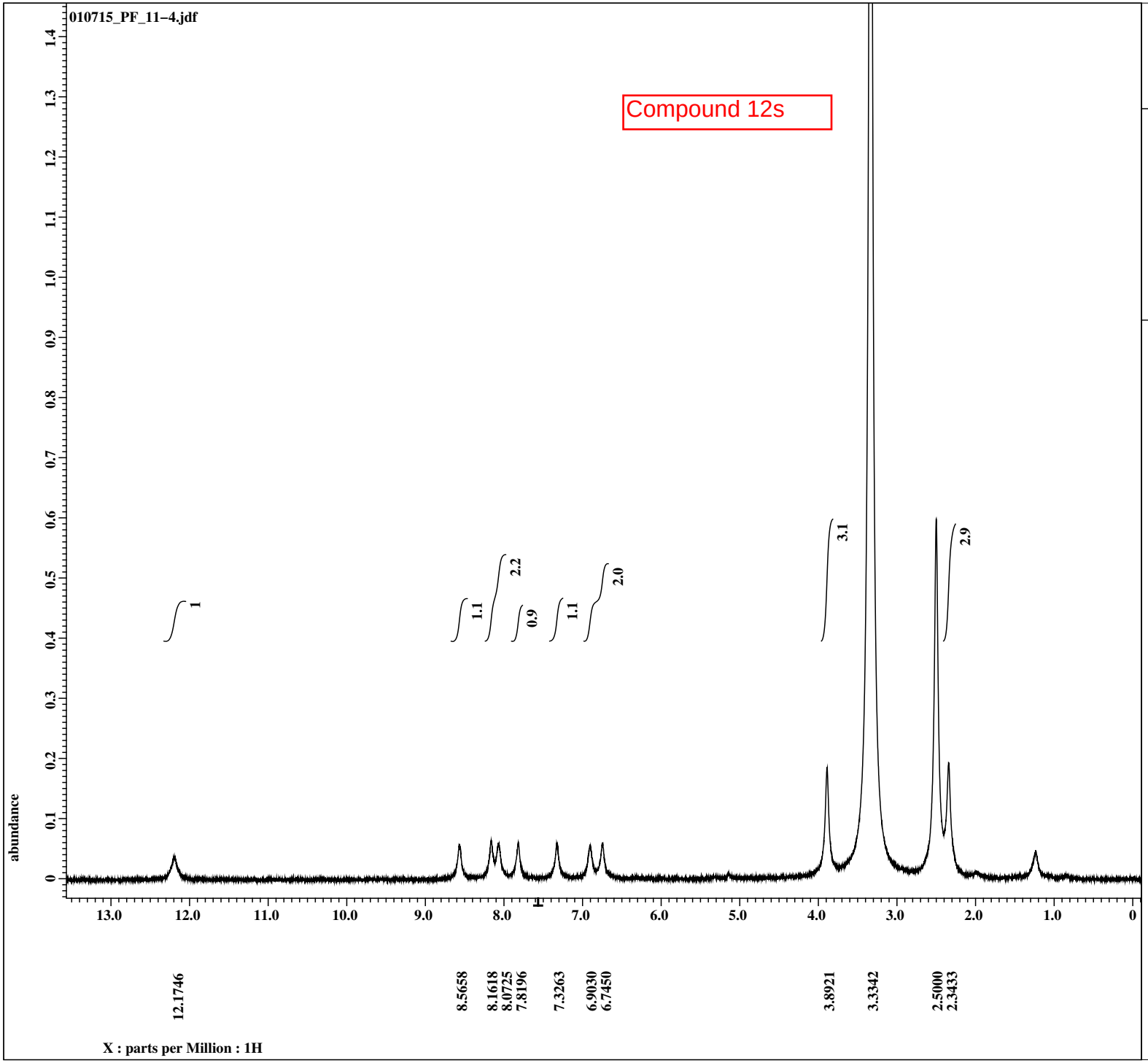





```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 160115_PF_22-1.jdf
```

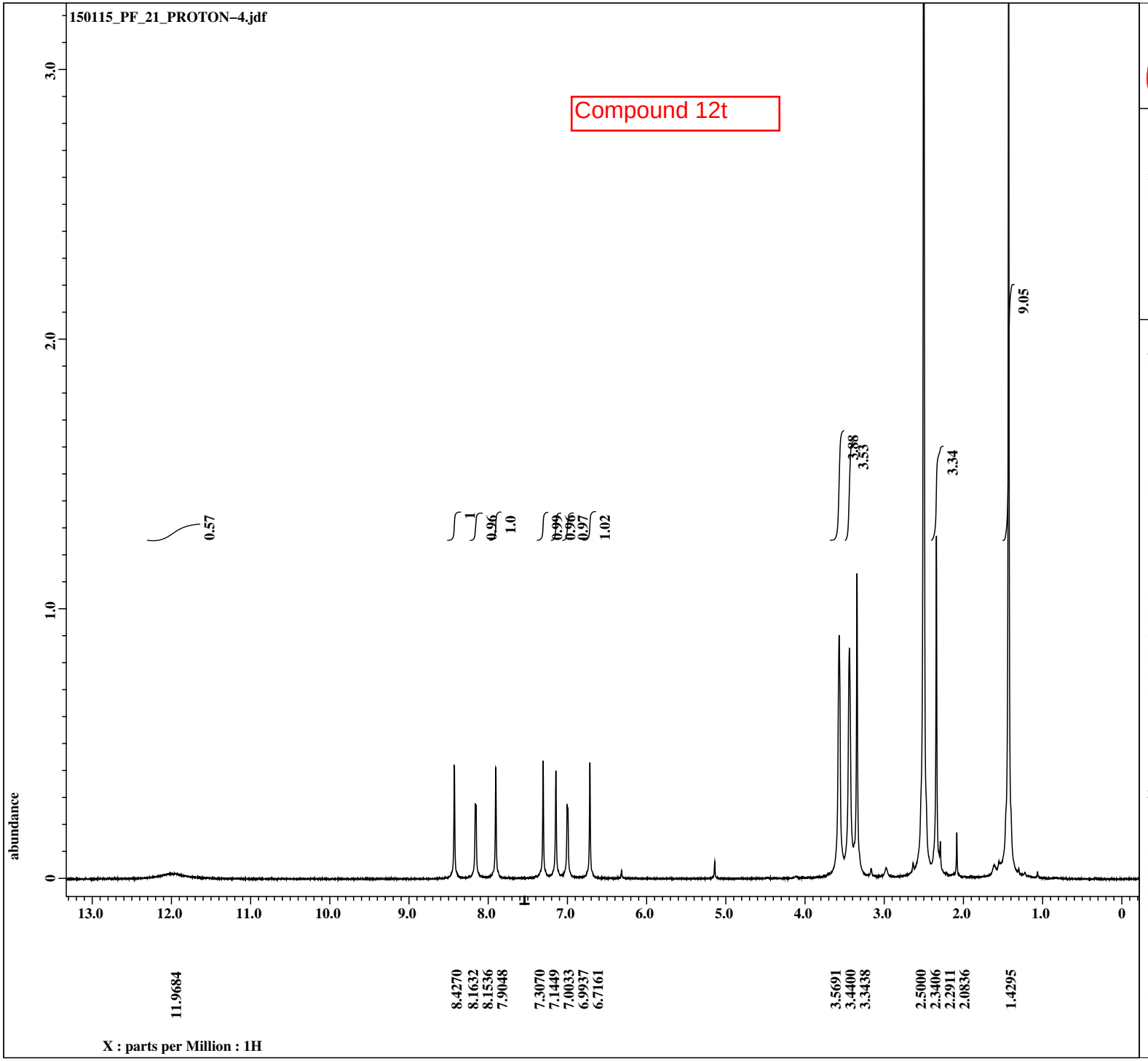
```
Filename          = 160115_PF_22-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = 160115_PF_22
Solvent           = DMSO-D6
Creation_time     = 16-JAN-2015 17:38:10
Revision_time     = 17-JAN-2015 09:38:05
Current_time      = 17-JAN-2015 09:38:29

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = JNM-ECX500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.4548992[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 7.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.68733284[Hz]
X_sweep           = 11.26126126[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 11.21[us]
X_acq_time        = 1.4548992[s]
X_angle           = 45[deg]
X_atn             = 3.4[dB]
X_pulse           = 5.605[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 6.4548992[s]
Temp_get          = 19.5[dC]
```


abundance
0
1.0
2.0
3.0
RG 09–3.jdf
X : parts per Million : 1H
12.1644
8.9543
8.5089
8.4998
8.2983
8.1105
8.0911
7.8701
7.4591
7.4477
7.4396
7.4270
7.3057
6.7195
3.2816
2.4699
2.4653
2.4619
2.3142
0.1116
−0.0350
−0.1861
Compound 12r



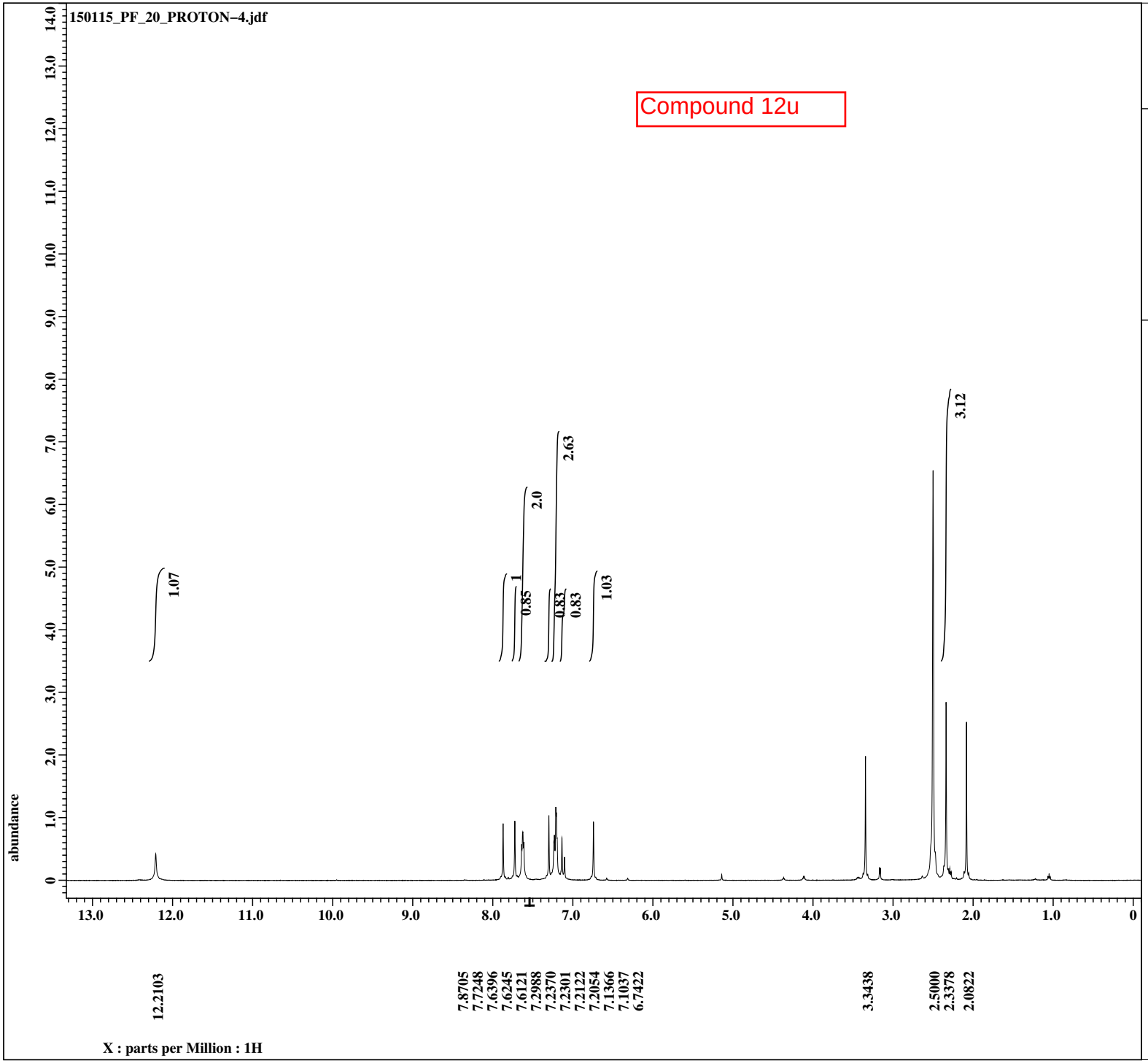

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 010715_PF_11-1.jdf
```

```
Filename          = 010715_PF_11-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = 010715_PF_11
Solvent           = DMSO-D6
Creation_time     =  1-JUL-2015 15:58:42
Revision_time     =  1-JUL-2015 15:19:05
Current_time      =  1-JUL-2015 15:19:16

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = JNM-ECX500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.4548992[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 7.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.68733284[Hz]
X_sweep           = 11.26126126[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 11.6[us]
X_acq_time        = 1.4548992[s]
X_angle           = 45[deg]
X_atn             = 3.4[dB]
X_pulse           = 5.8[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 46
Relaxation_delay  = 5[s]
Repetition_time   = 6.4548992[s]
Temp_get          = 22.1[dC]
```




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 150115_PF_21_PROTON-1.jdf
```

```
Filename          = 150115_PF_21_PROTON-4
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = 150115_PF_21
Solvent           = DMSO-D6
Creation_time     = 15-JAN-2015 17:48:37
Revision_time     = 16-JAN-2015 10:22:34
Current_time      = 16-JAN-2015 10:23:11

Comment           = 150115_PF_21
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = JNM-ECX500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.4548992[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 7.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.68733284[Hz]
X_sweep           = 11.26126126[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 11.21[us]
X_acq_time        = 1.4548992[s]
X_angle           = 45[deg]
X_atn             = 3.4[dB]
X_pulse           = 5.605[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
Relaxation_delay  = 4[s]
Repetition_time   = 5.4548992[s]
Temp_get          = 18.2[dC]
```

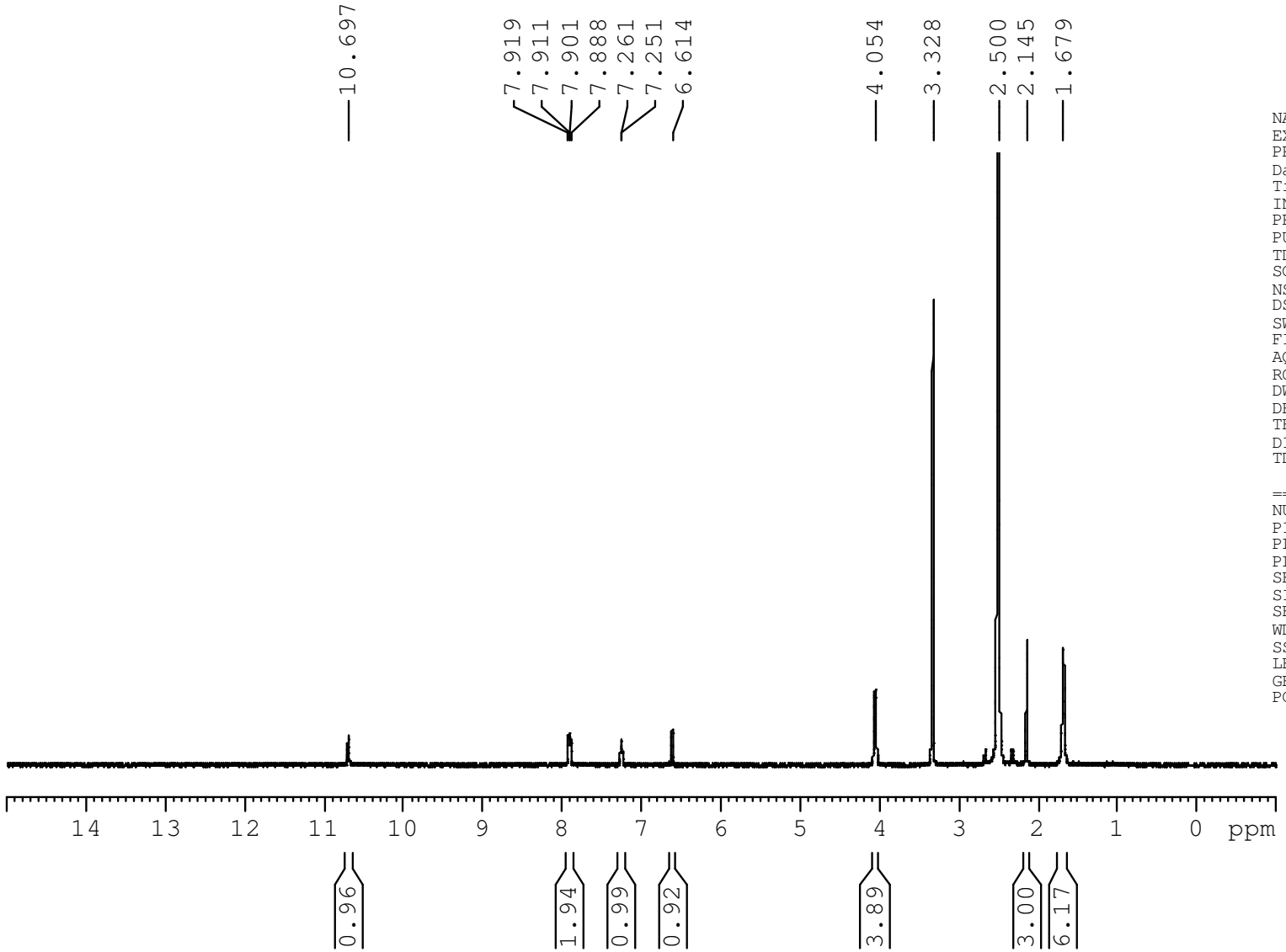



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 150115_PF_20_PROTON-1.jdf
```

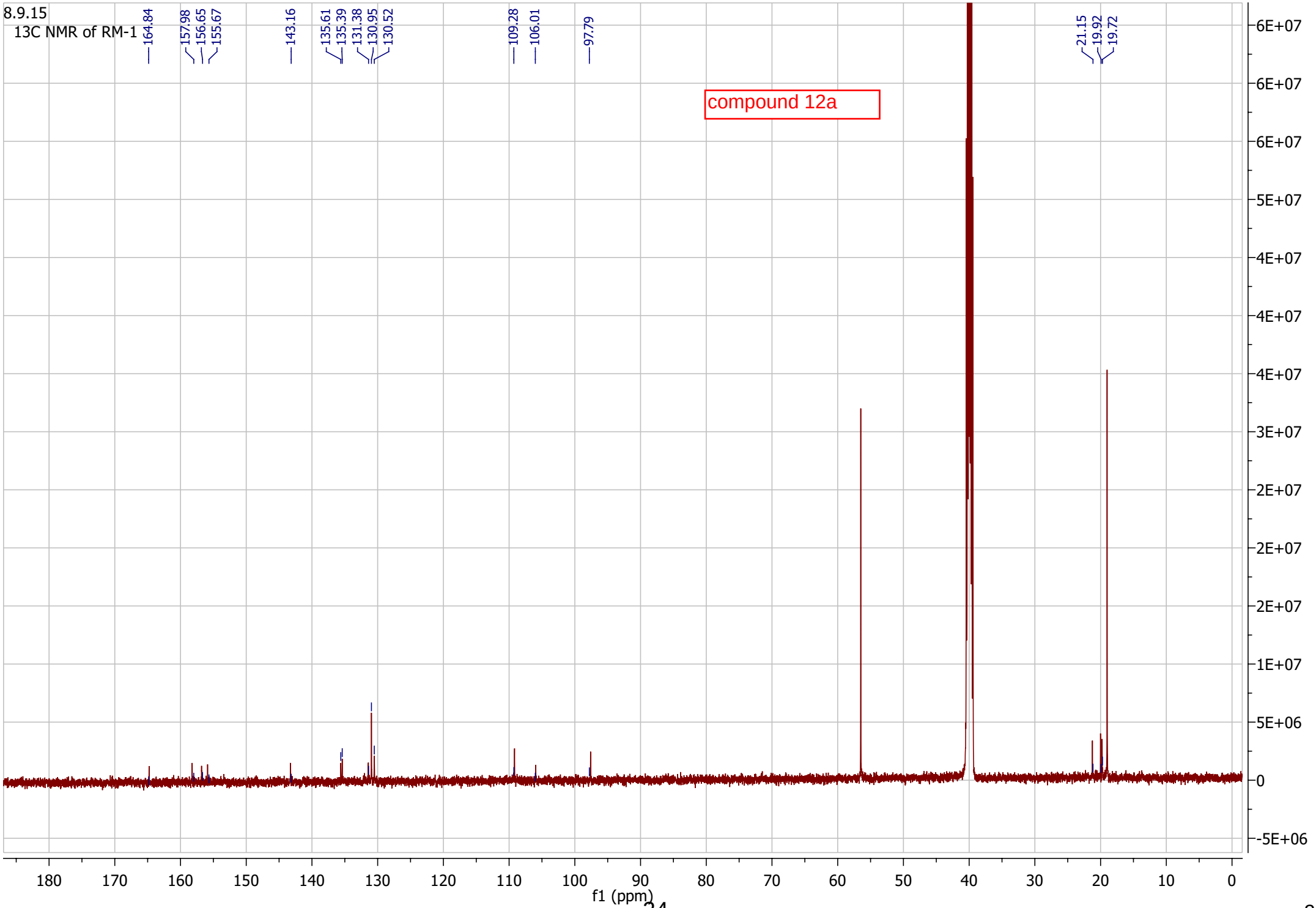
```
Filename          = 150115_PF_20_PROTON-4
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = 150115_PF_20
Solvent           = DMSO-D6
Creation_time     = 15-JAN-2015 21:41:25
Revision_time     = 16-JAN-2015 10:53:34
Current_time      = 16-JAN-2015 10:54:00

Comment           = 150115_PF_20
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = JNM-ECX500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.4548992[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 7.5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.68733284[Hz]
X_sweep           = 11.26126126[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 11.21[us]
X_acq_time        = 1.4548992[s]
X_angle           = 45[deg]
X_atn             = 3.4[dB]
X_pulse           = 5.605[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 46
Relaxation_delay  = 4[s]
Repetition_time   = 5.4548992[s]
Temp_get          = 18.3[dC]
```

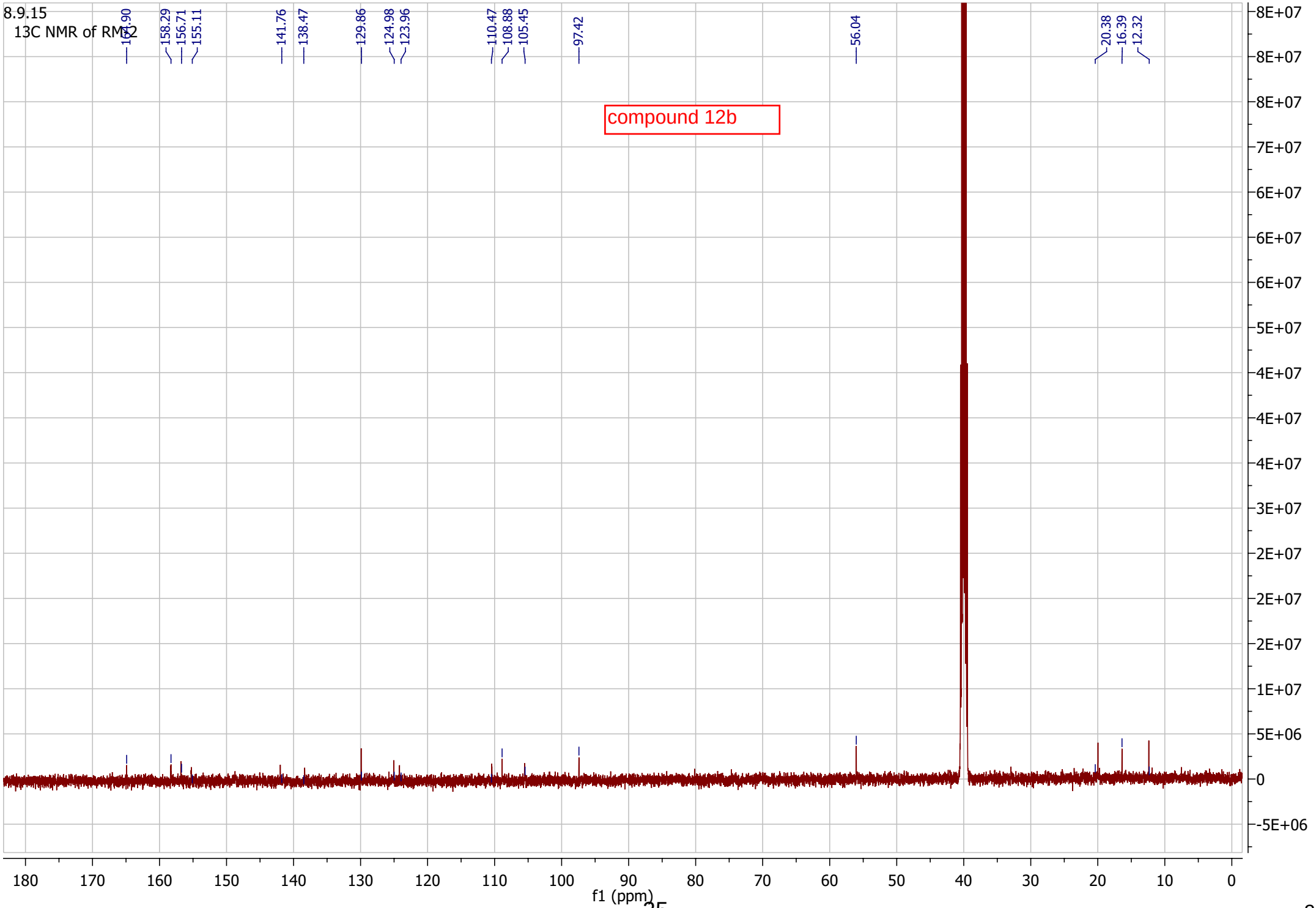
Compound 12v

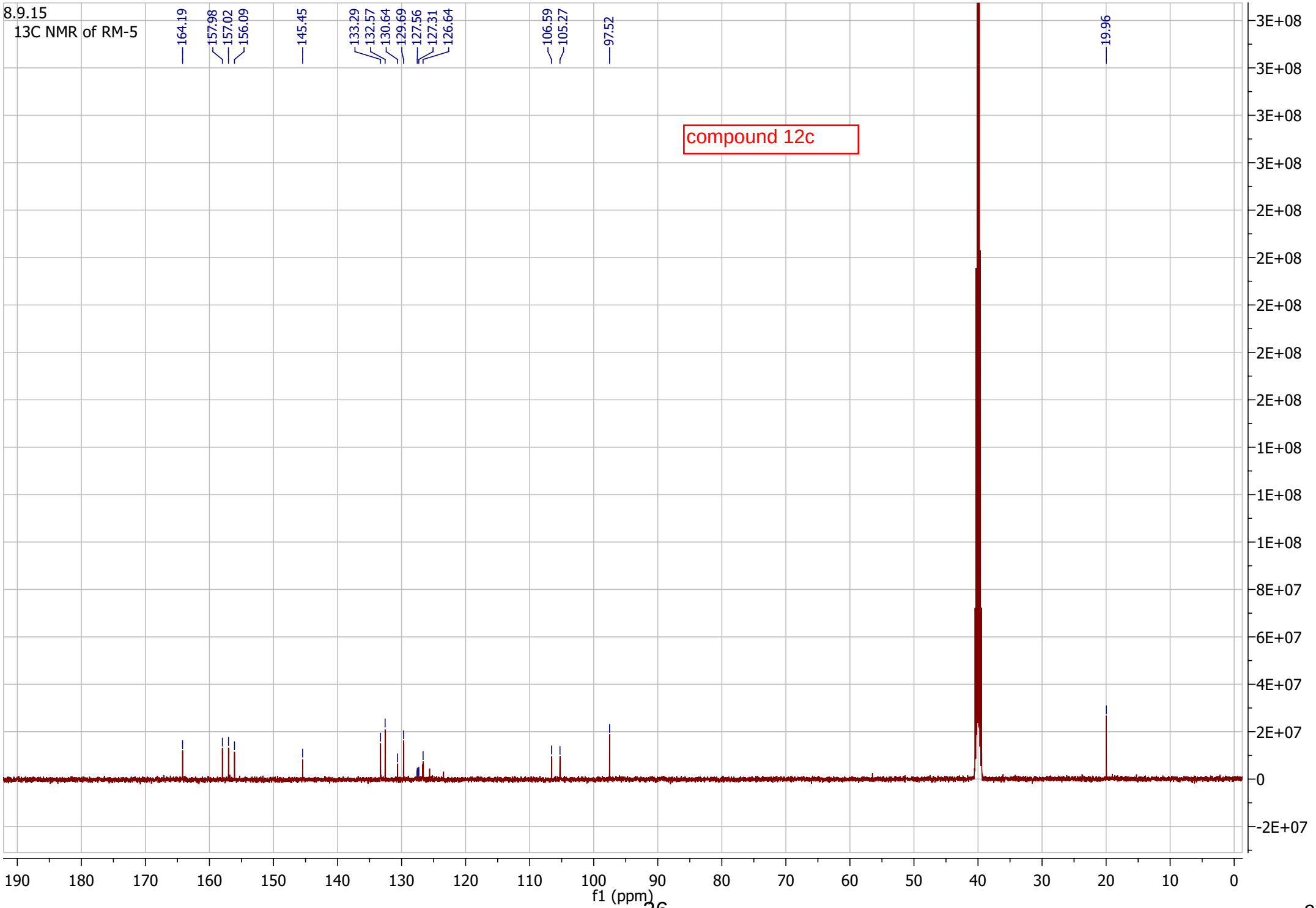
P165GB-Z00763-045-A DMSO P.S

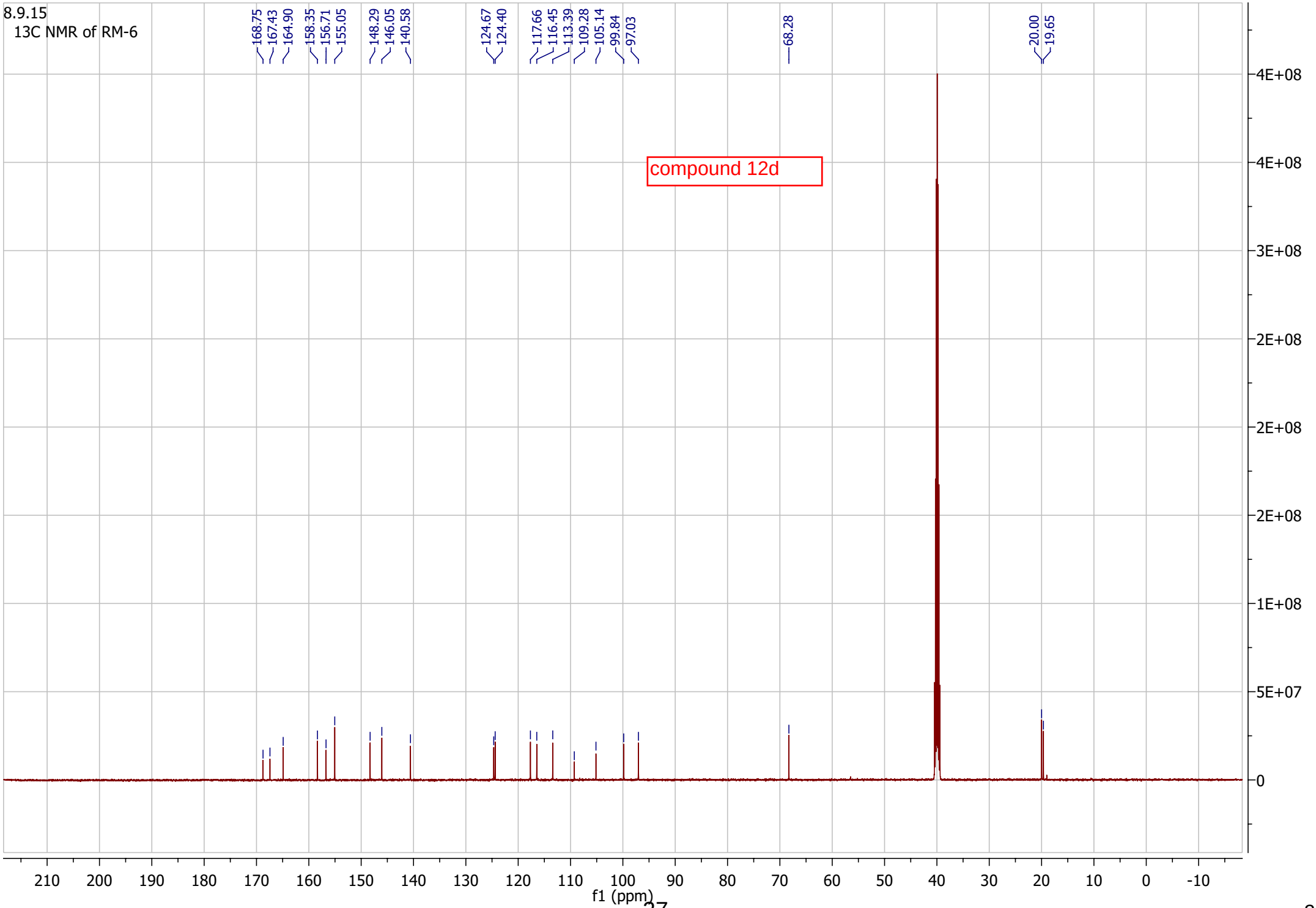


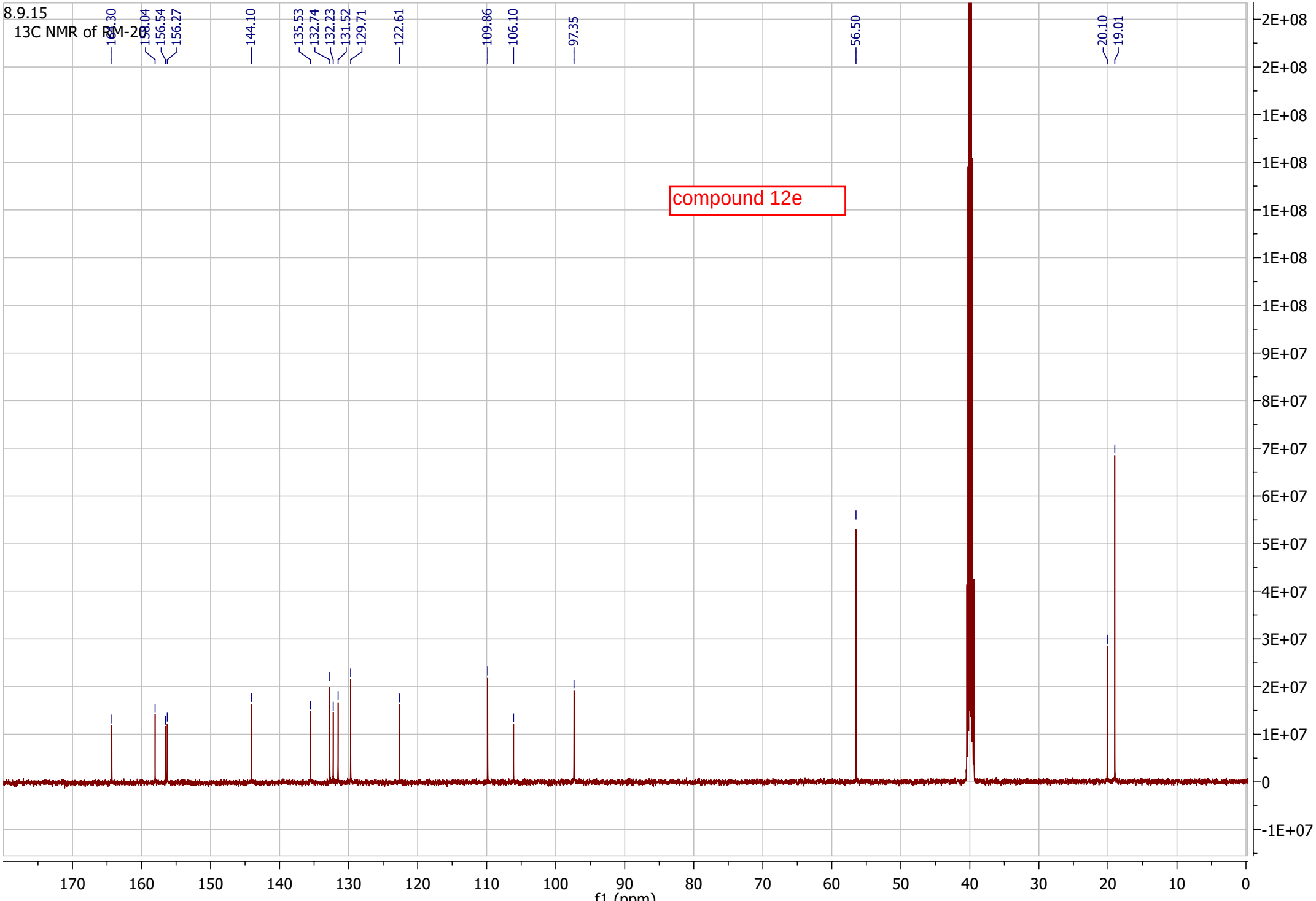
NAME	P165CB-Z00763-045-A
EXPNO	1
PROCNO	1
Date_	20140328
Time	16.48
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	8
DS	0
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	128
DW	60.800 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	9.90 usec
PL1	-2.80 dB
PL1W	20.58109283 W
SFO1	400.2624718 MHz
SI	65536
SF	400.2600044 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

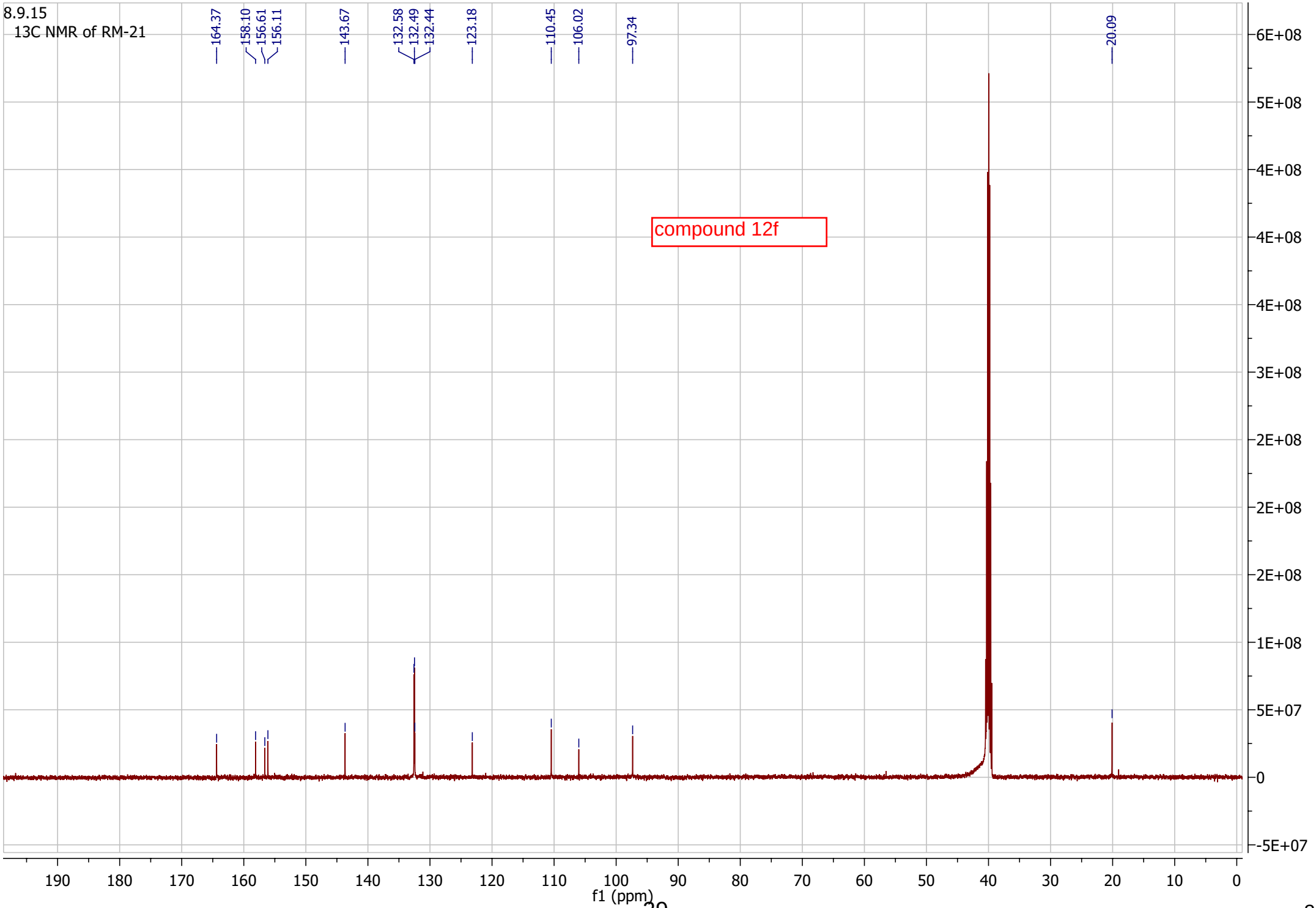

8.9.15
13C NMR of RM-1
164.84
157.98
156.65
155.67
143.16
135.61
135.39
131.38
130.95
130.52
109.28
106.01
97.79
21.15
19.92
19.72
compound 12a
6E+07
6E+07
6E+07
5E+07
4E+07
4E+07
4E+07
3E+07
2E+07
2E+07
2E+07
1E+07
5E+06
0
-5E+06
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

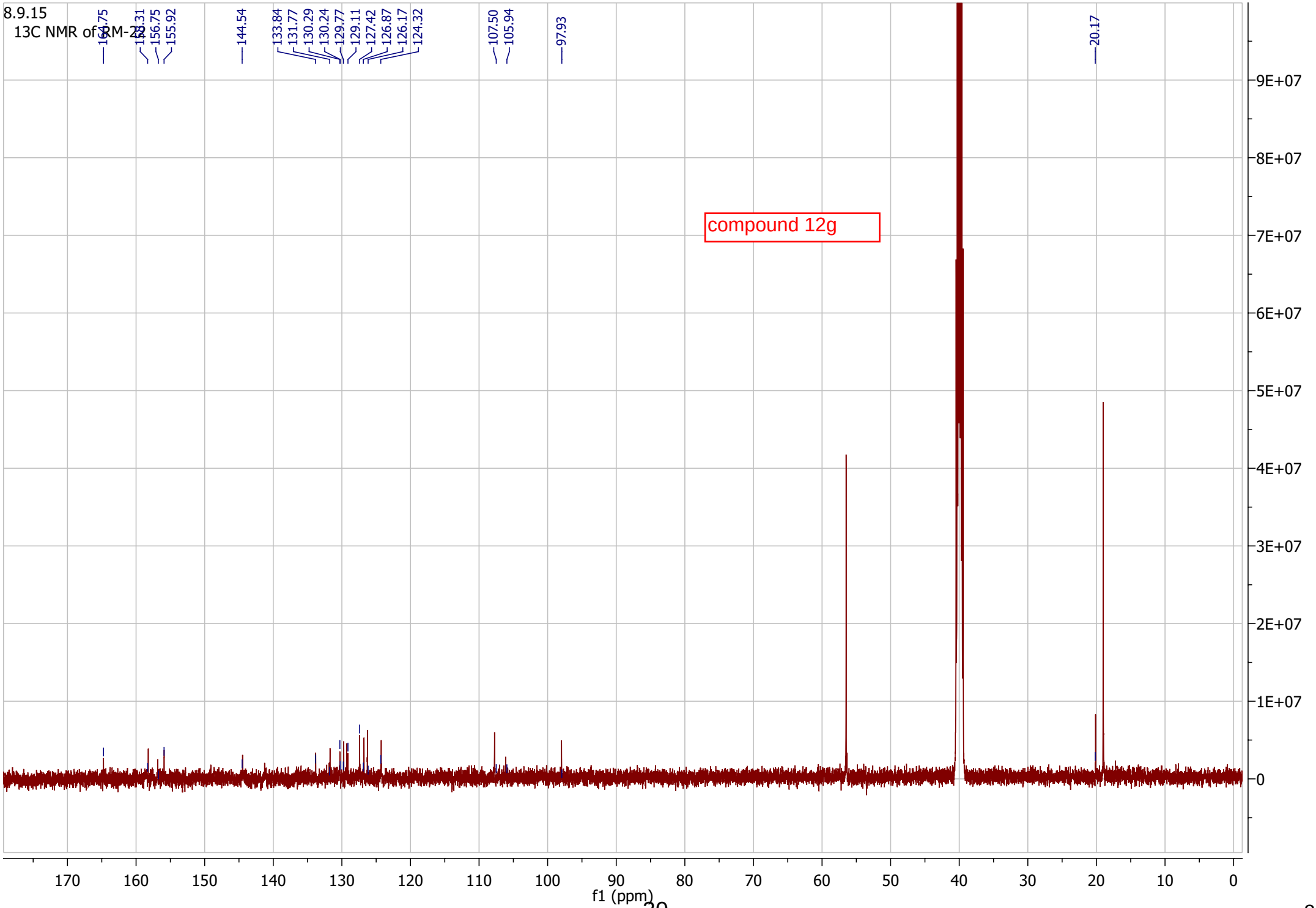

8.9.15
13C NMR of RM12
164.90
158.29
156.71
155.11
141.76
138.47
129.86
124.98
123.96
110.47
108.88
105.45
97.42
56.04
20.38
16.39
12.32
compound 12b
8E+07
8E+07
8E+07
7E+07
6E+07
6E+07
6E+07
5E+07
4E+07
4E+07
4E+07
3E+07
2E+07
2E+07
2E+07
1E+07
5E+06
0
-5E+06
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

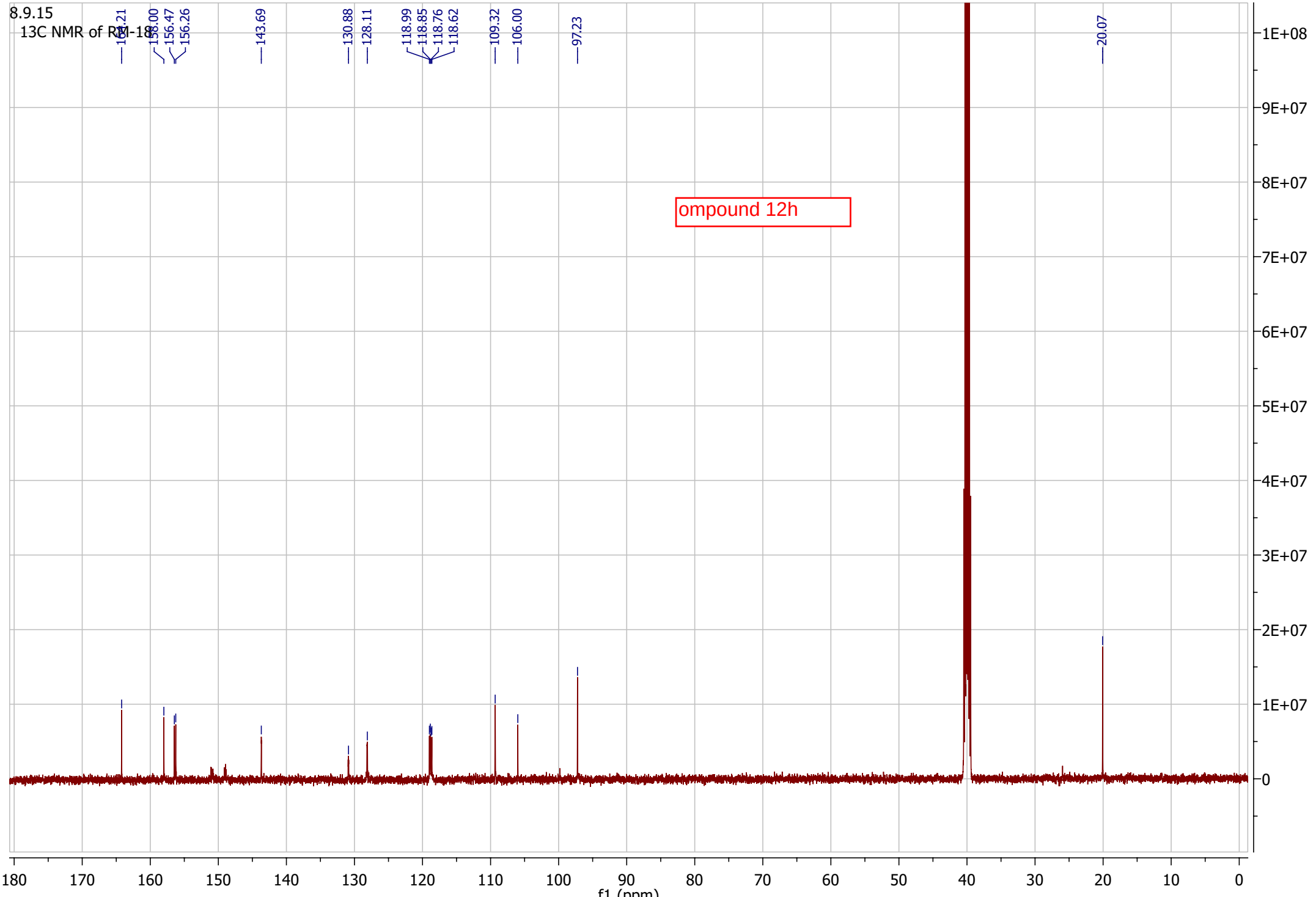

8.9.15
13C NMR of RM-5
164.19
157.98
157.02
156.09
145.45
133.29
132.57
130.64
129.69
127.56
127.31
126.64
106.59
105.27
97.52
19.96
compound 12c
3E+08
2E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

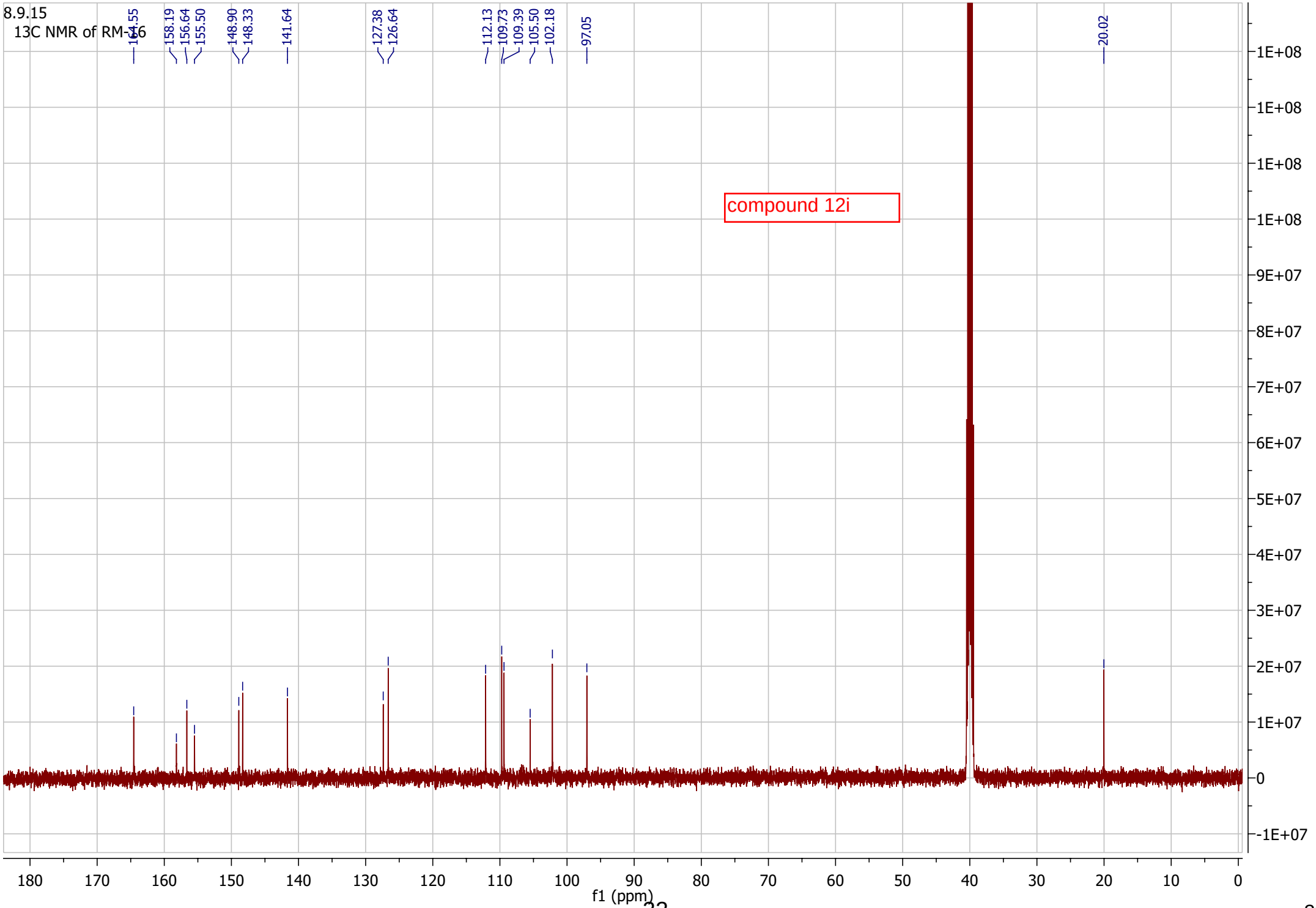

8.9.15
13C NMR of RM-6
168.75
167.43
164.90
158.35
156.71
155.05
148.29
146.05
140.58
124.67
124.40
117.66
116.45
113.39
109.28
105.14
99.84
97.03
68.28
20.00
19.65
compound 12d
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

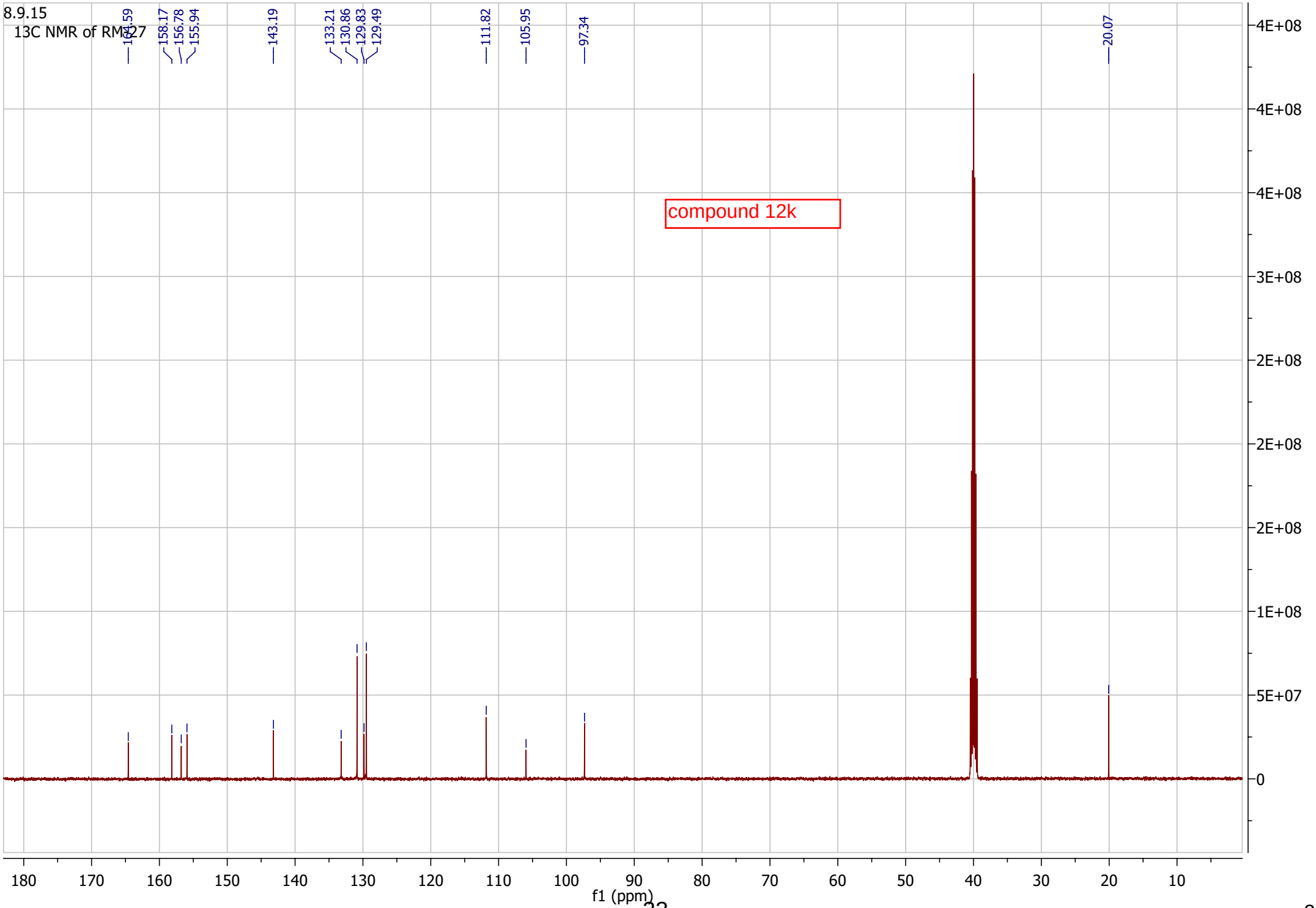

8.9.15
13C NMR of RM-28
164.30
158.04
156.54
156.27
144.10
135.53
132.74
132.23
131.52
129.71
122.61
109.86
106.10
97.35
56.50
20.10
19.01
compound 12e
2E+08
2E+08
1E+08
1E+08
1E+08
1E+08
1E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

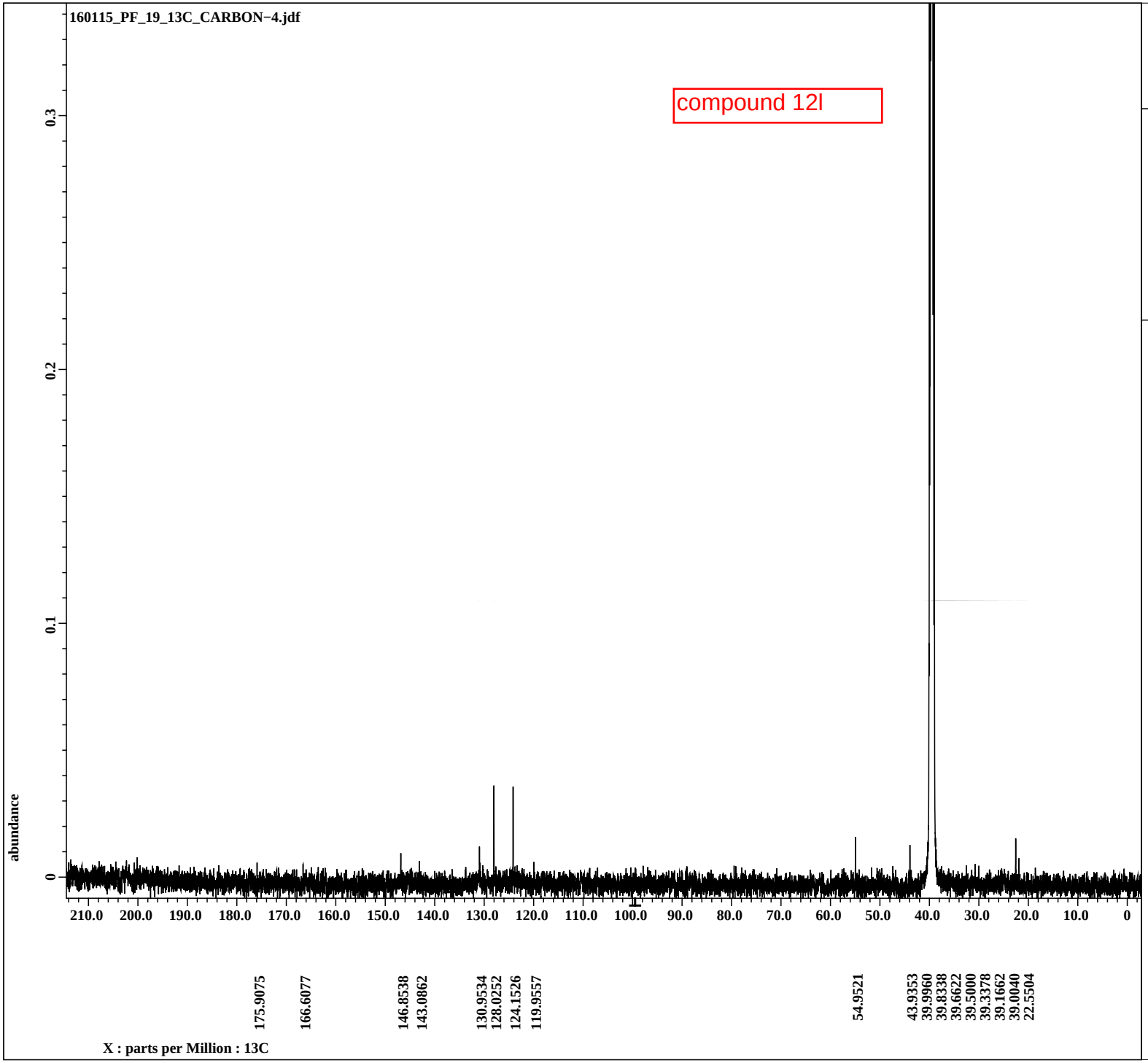

8.9.15
13C NMR of RM-21
164.37
158.10
156.61
156.11
143.67
132.58
132.49
132.44
123.18
110.45
106.02
97.34
20.09
compound 12f
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.9.15
13C NMR of RM-22
164.75
158.31
156.75
155.92
144.54
133.84
131.77
130.29
130.24
129.77
129.11
127.42
126.87
126.17
124.32
107.50
105.94
97.93
20.17
compound 12g
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.9.15
13C NMR of RM-18
163.21
158.00
156.47
156.26
143.69
130.88
128.11
118.99
118.85
118.76
118.62
109.32
106.00
97.23
20.07
ompound 12h
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.9.15
13C NMR of RM-16
164.55
158.19
156.64
155.50
148.90
148.33
141.64
127.38
126.64
112.13
109.73
109.39
105.50
102.18
97.05
20.02
compound 12i
1E+08
1E+08
1E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

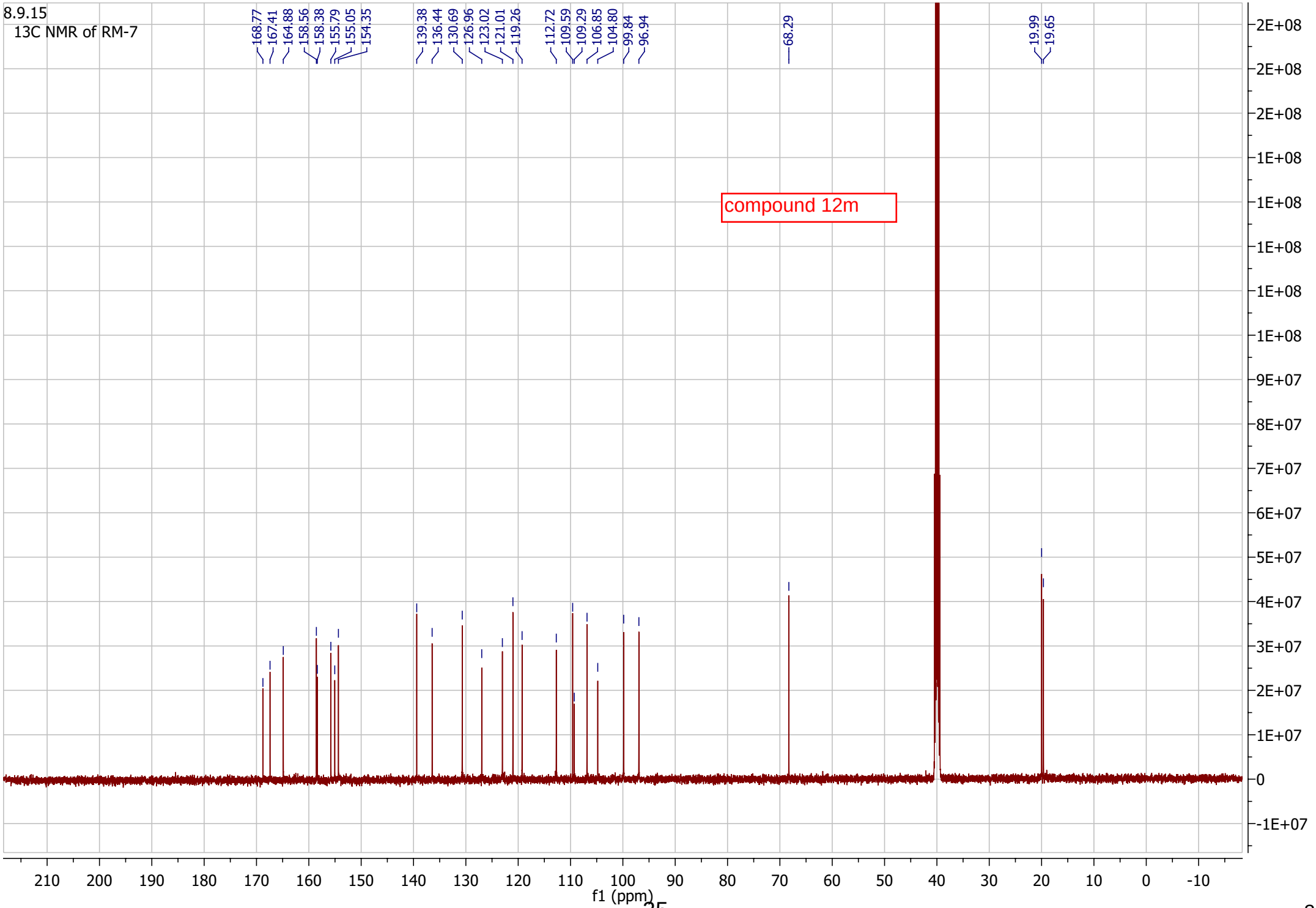

8.9.15
13C NMR of RM227
164.59
158.17
156.78
155.94
143.19
133.21
130.86
129.83
129.49
111.82
105.95
97.34
20.07
compound 12k
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

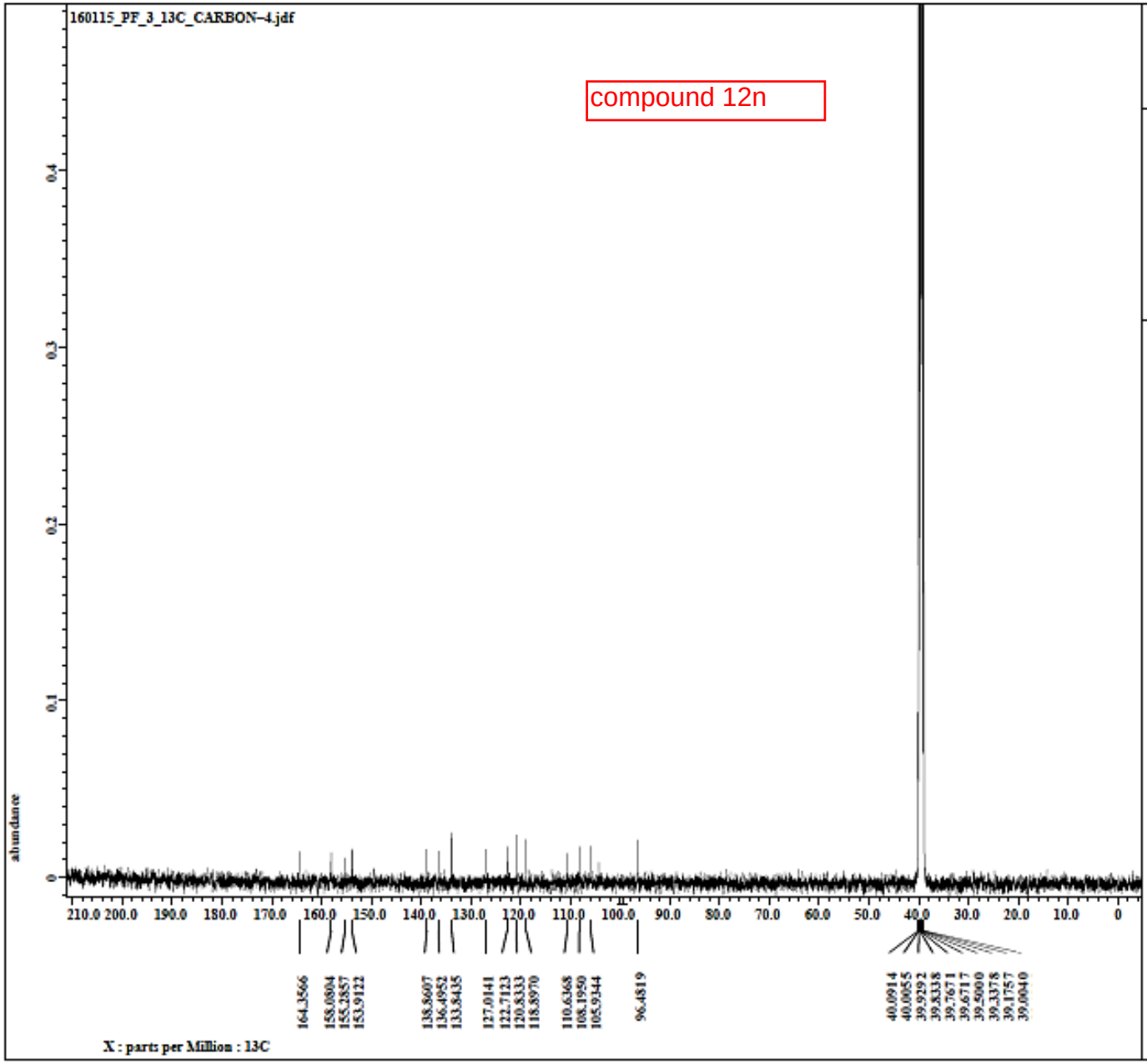


JEOL

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 160115_PF_19_13C_CARBON-1.
```

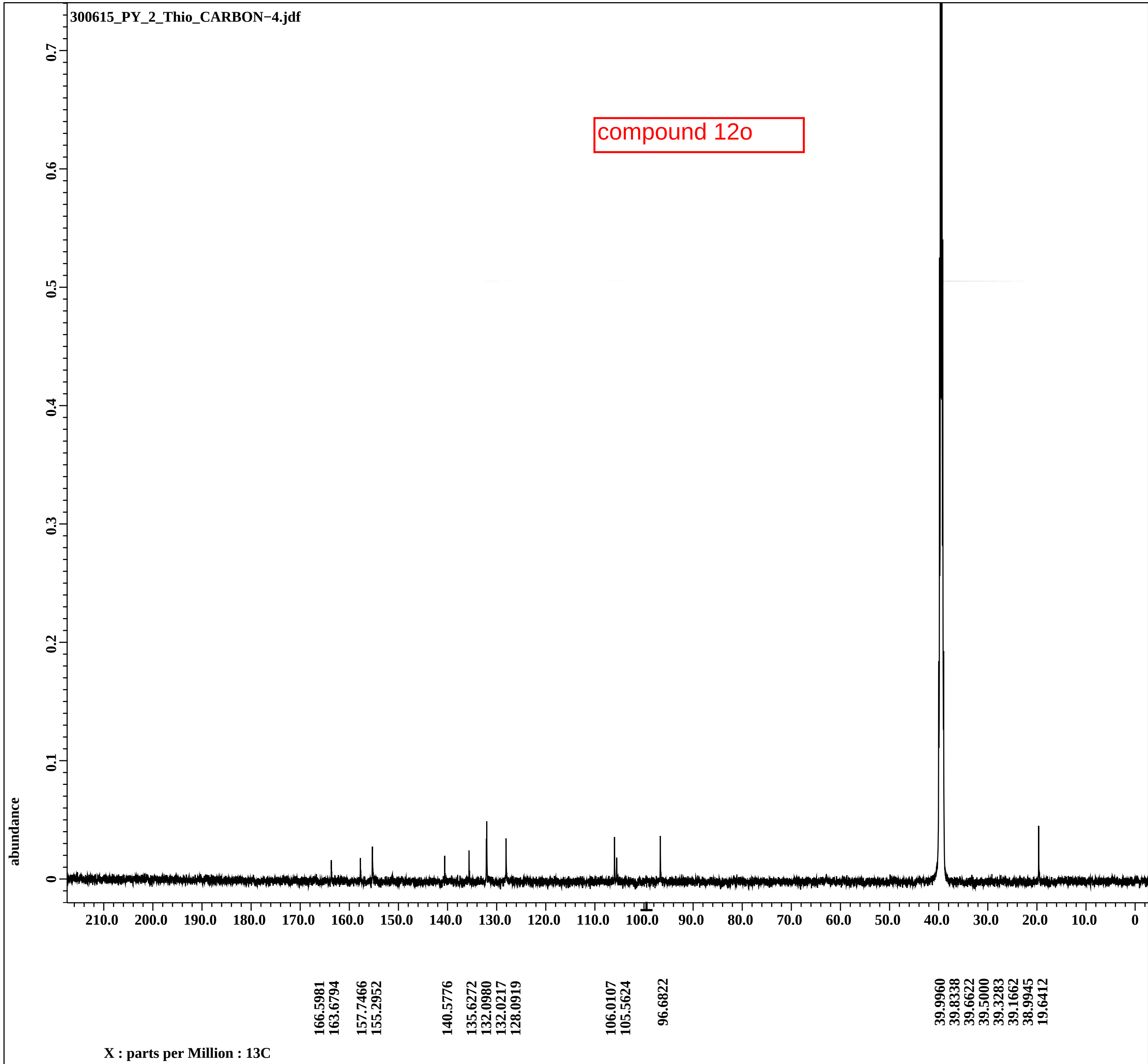
```
Filename          = 160115_PF_19_13C_CARB
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = 160115_PF_19_13C
Solvent           = DMSO-D6
Creation_time     = 17-JAN-2015 03:17:36
Revision_time     = 17-JAN-2015 09:53:20
Current_time      = 17-JAN-2015 09:53:43

Comment           = 160115_PF_19_13C
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = JNM-ECX500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1024
Total_scans       = 1024

X_90_width        = 8.62[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 6.4[dB]
X_pulse           = 2.87333333[us]
Irr_atn_dec       = 21.68[dB]
Irr_atn_noe       = 21.68[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.83361792[s]
Temp_get          = 18.1[dC]
```


8.9.15
13C NMR of RM-7
168.77
167.41
164.88
158.56
158.38
155.79
155.05
154.35
139.38
136.44
130.69
126.96
123.02
121.01
119.26
112.72
109.59
109.29
106.85
104.80
99.84
96.94
68.29
19.99
19.65
compound 12m
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
1E+08
1E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 160115_PF_3_13C_CARBON-1.j
```

```
Filename          = 160115_PF_3_13C_CARBO
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = 160115_PF_3_13C
Solvent           = DMSO-D6
Creation_time     = 17-JAN-2015 02:21:41
Revision_time     = 17-JAN-2015 09:48:38
Current_time      = 17-JAN-2015 09:48:58

Comment           = 160115_PF_3_13C
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = RCX 500
Spectrometer      = JNM-RCX500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1024
Total_scans       = 1024

X_90_width        = 8.62[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 6.4[dB]
X_pulse           = 2.87333333[us]
Irr_atn_dec       = 21.68[dB]
Irr_atn_noe       = 21.68[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.83361792[s]
Temp_get          = 18.3[dC]
```

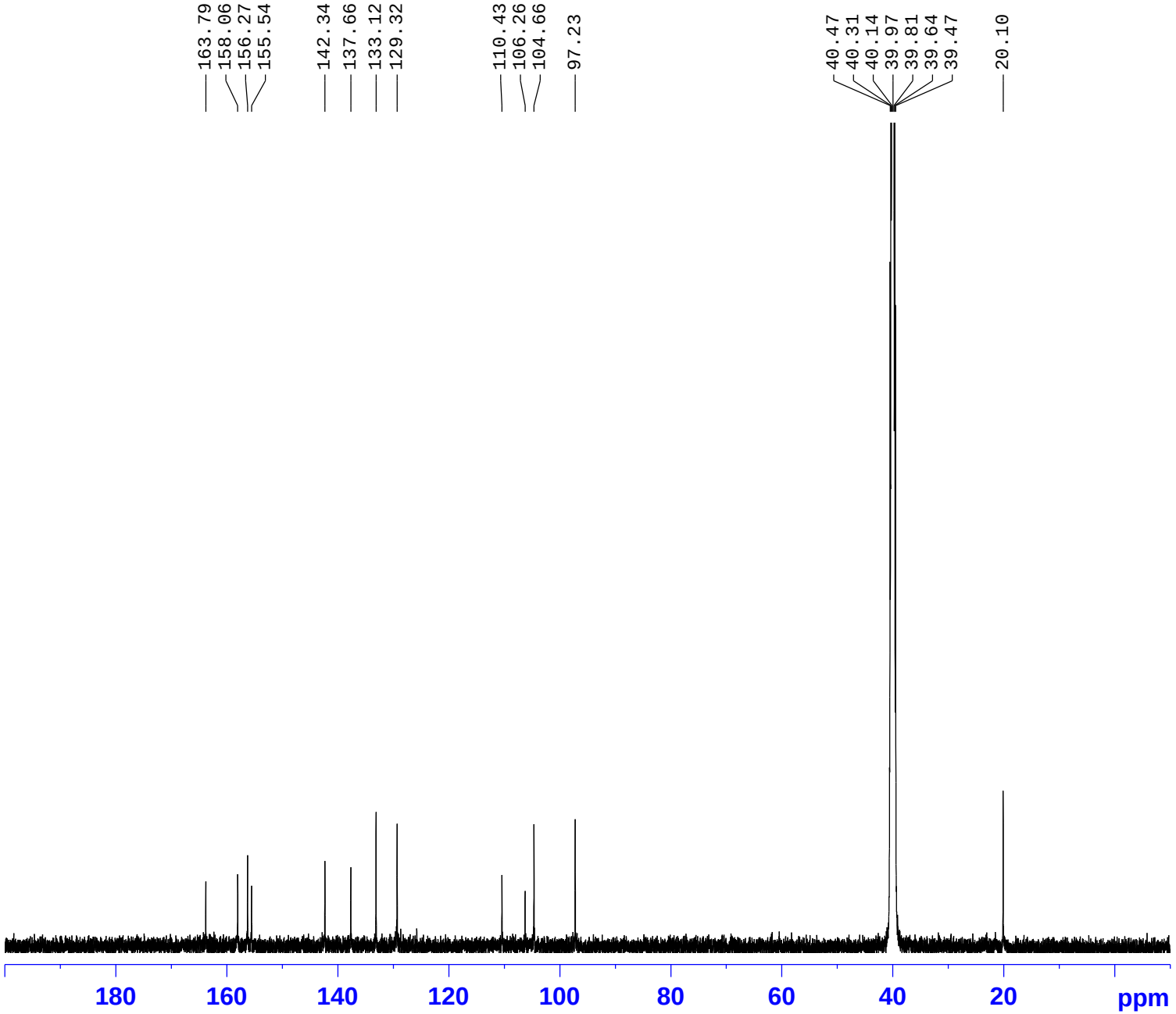


JEOL

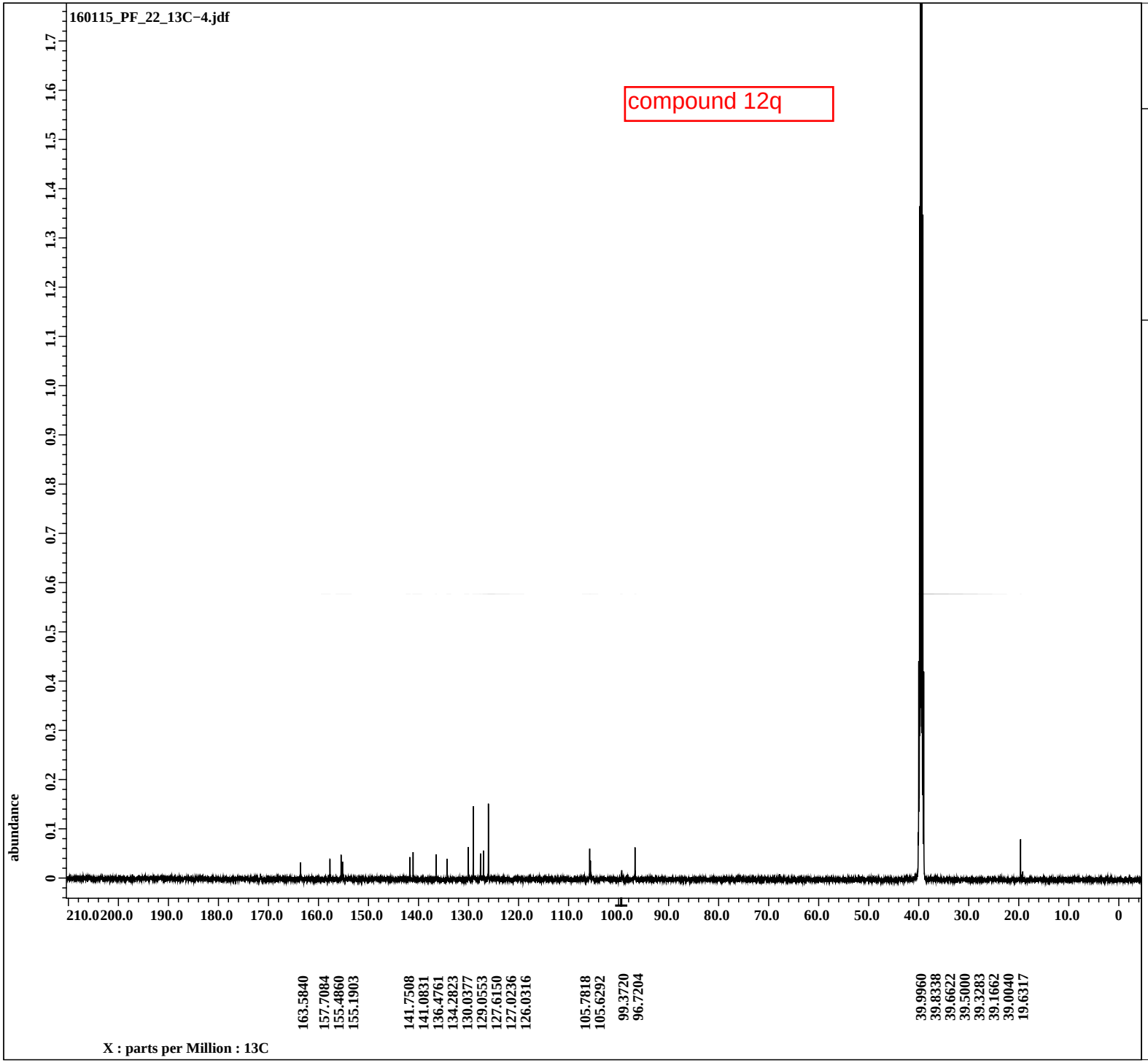
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 300615_PY_2_Thio_CARBON-1.

Filename           = 300615_PY_2_Thio_CARB
Author             = delta
Experiment         = single_pulse_dec
Sample_id          = 300615_PY_2_Thio
Solvent            = DMSO-D6
Creation_time      =  1-JUL-2015 10:39:45
Revision_time      =  1-JUL-2015 11:51:05
Current_time       =  1-JUL-2015 11:51:28

Data_format        = 1D COMPLEX
Dim_size           = 26214
Dim_title          = 13C
Dim_units          = [ppm]
Dimensions         = X
Site               = ECX 500
Spectrometer       = JNM-ECX500

Field_strength     = 11.7473579[T] (500[MH
X_acq_duration     = 0.83361792[s]
X_domain           = 13C
X_freq             = 125.76529768[MHz]
X_offset           = 100[ppm]
X_points           = 32768
X_prescans         = 4
X_resolution       = 1.19959034[Hz]
X_sweep            = 39.3081761[kHz]
Irr_domain         = 1H
Irr_freq           = 500.15991521[MHz]
Irr_offset         = 5.0[ppm]
Clipped            = FALSE
Mod_return         = 1
Scans              = 1024
Total_scans        = 1024

X_90_width         = 8.62[us]
X_acq_time         = 0.83361792[s]
X_angle            = 30[deg]
X_atn              = 6.4[dB]
X_pulse            = 2.87333333[us]
Irr_atn_dec        = 21.68[dB]
Irr_atn_noe        = 21.68[dB]
Irr_noise          = WALTZ
Decoupling         = TRUE
Initial_wait       = 1[s]
Noe                = TRUE
Noe_time           = 2[s]
Recvr_gain         = 60
Relaxation_delay   = 2[s]
Repetition_time    = 2.83361792[s]
Temp_get           = 19[dC]
```

compound 12p

13C NMR of PF-17

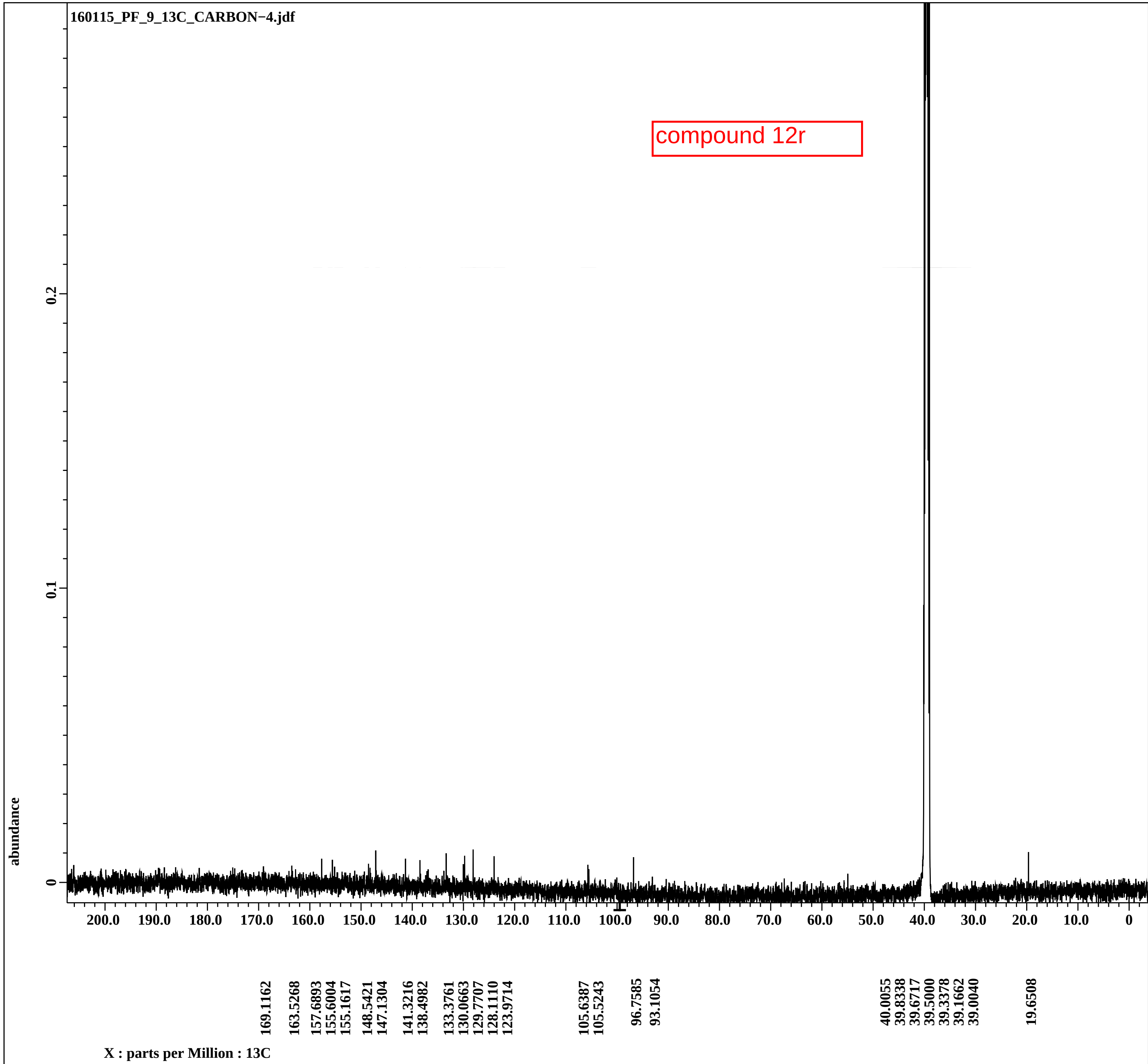



```
NAME            Shantanu
EXPNO                  3
PROCNO                 1
Date_           20150515
Time               13.31
INSTRUM             Spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT             DMSO
NS                  2048
DS                     4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010548 sec
RG                   144
DW                16.800 usec
DE                 6.50 usec
TE                299.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  8.75 usec
PL1                -2.20 dB
PL1W       116.72342682 W
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 1.10 dB
PL12               18.50 dB
PL13               18.50 dB
PL2W        18.99148560 W
PL12W        0.34558824 W
PL13W        0.34558824 W
SFO2        500.1320005 MHz
SI                 32768
SF          125.7577890 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

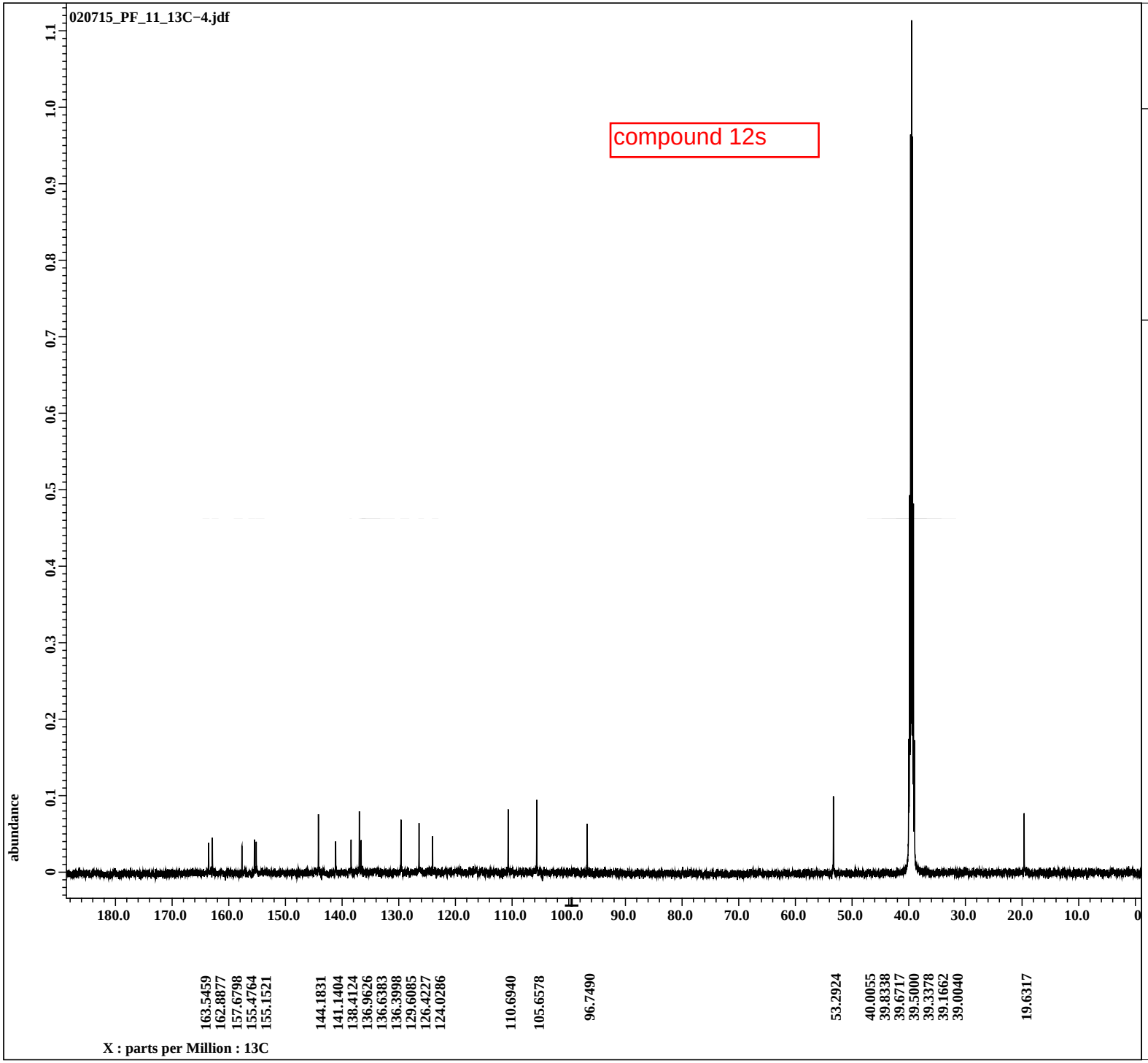



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 160115_PF_22_13C-1.jdf
```

```
Filename          = 160115_PF_22_13C-4.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = 160115_PF_22_13C
Solvent           = DMSO-D6
Creation_time     = 16-JAN-2015 18:27:09
Revision_time     = 17-JAN-2015 09:35:15
Current_time      = 17-JAN-2015 09:35:35

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = JNM-ECX500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1024
Total_scans       = 1024

X_90_width        = 8.62[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 6.4[dB]
X_pulse           = 2.87333333[us]
Irr_atn_dec       = 21.68[dB]
Irr_atn_noe       = 21.68[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.83361792[s]
Temp_get          = 19.3[dC]
```

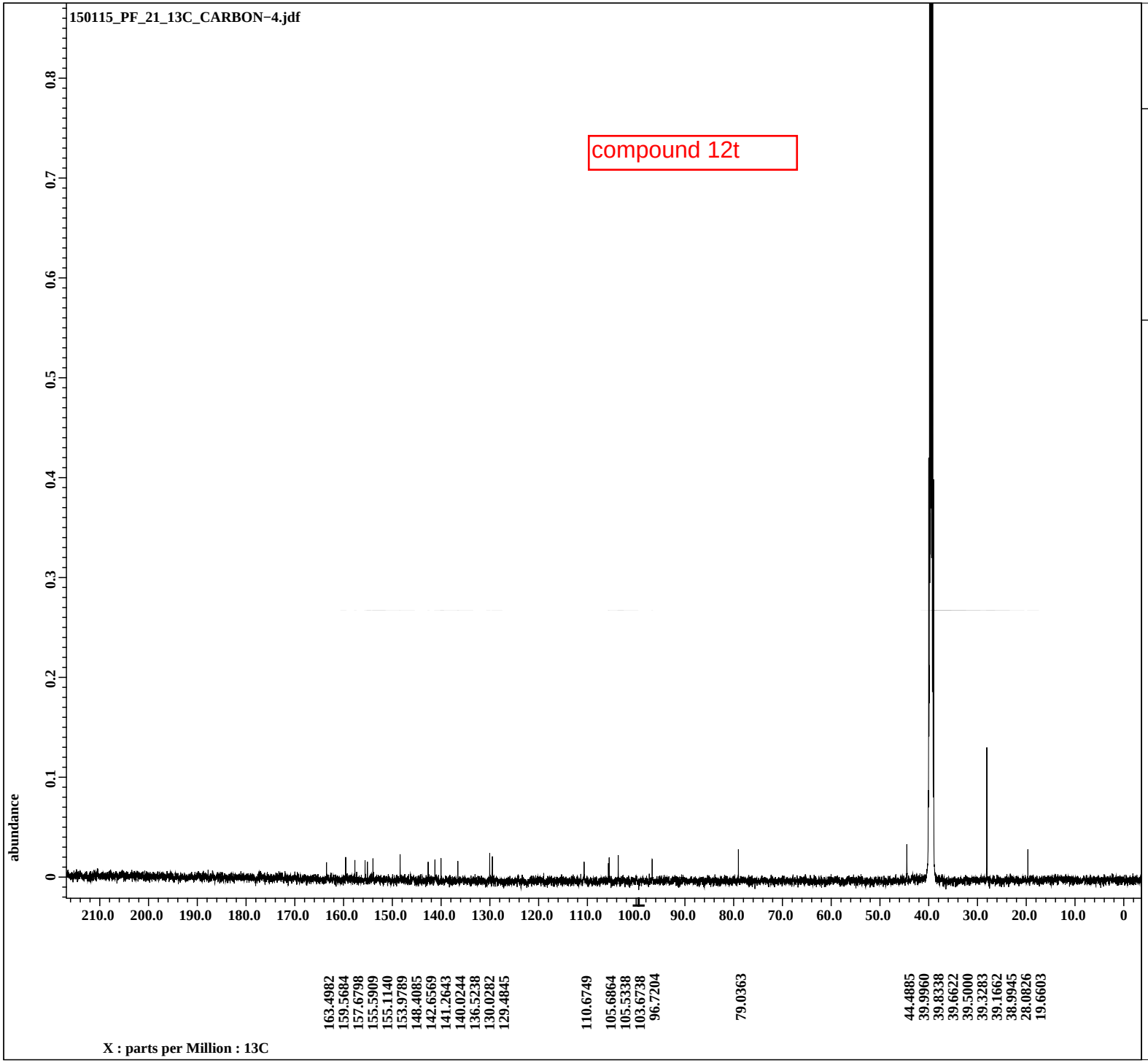



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 160115_PF_9_13C_CARBON-1.j

Filename          = 160115_PF_9_13C_CARBO
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = 160115_PF_9_13C
Solvent           = DMSO-D6
Creation_time     = 16-JAN-2015 20:12:19
Revision_time     = 17-JAN-2015 09:41:27
Current_time      = 17-JAN-2015 09:41:56

Comment           = 160115_PF_9_13C
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = JNM-ECX500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 2048
Total_scans       = 2048

X_90_width        = 8.62[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 6.4[dB]
X_pulse           = 2.87333333[us]
Irr_atn_dec       = 21.68[dB]
Irr_atn_noe       = 21.68[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.83361792[s]
Temp_get          = 19.2[dC]
```




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 020715_PF_11_13C-1.jdf
```

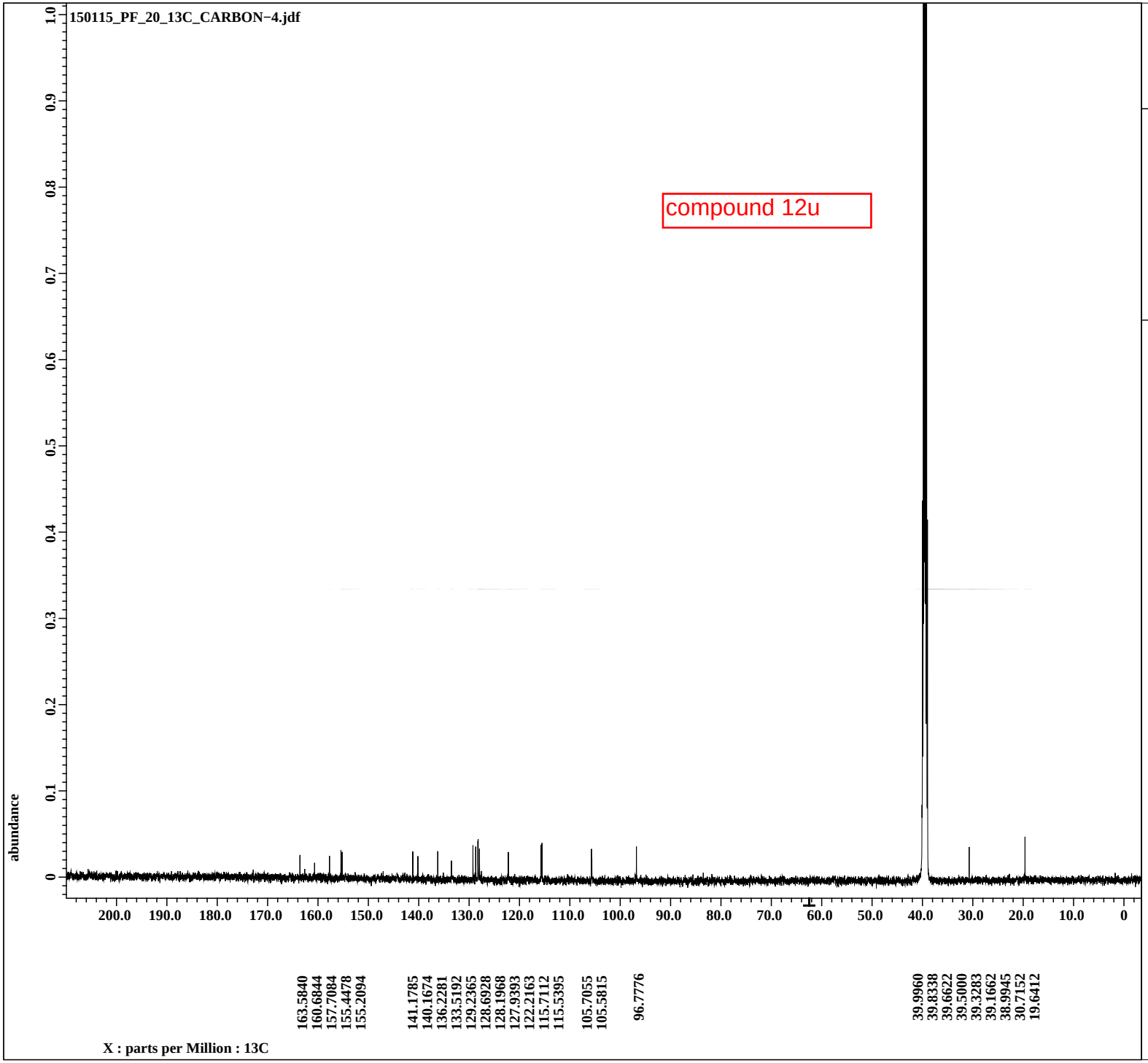
```
Filename          = 020715_PF_11_13C-4.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = 020715_PF_11_13C
Solvent           = DMSO-D6
Creation_time     =  2-JUL-2015 15:56:47
Revision_time     =  2-JUL-2015 15:18:03
Current_time      =  2-JUL-2015 15:18:18

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = JNM-ECX500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 442
Total_scans       = 442

X_90_width        = 8.62[us]
X_acq_time        = 0.83361792[s]
X_angle           = 90[deg]
X_atn             = 6.4[dB]
X_pulse           = 8.62[us]
Irr_atn_dec       = 21.68[dB]
Irr_atn_noe       = 21.68[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.83361792[s]
Temp_get          = 20.7[dC]
```



---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 150115_PF_21_13C_CARBON-1.

Filename	= 150115_PF_21_13C_CARB
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= 150115_PF_21
Solvent	= DMSO-D6
Creation_time	= 15-JAN-2015 18:37:35
Revision_time	= 16-JAN-2015 10:24:55
Current_time	= 16-JAN-2015 10:28:57
Comment	= 150115_PF_21_13C
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 500
Spectrometer	= JNM-ECX500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 1024
Total_scans	= 1024
X_90_width	= 8.62[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6.4[dB]
X_pulse	= 2.87333333[us]
Irr_atn_dec	= 21.68[dB]
Irr_atn_noe	= 21.68[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 18.1[dC]


150115_PF_20_13C_CARBON-4.jdf
compound 12u
abundance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
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
163.5840
160.6844
157.7084
155.4478
155.2094
141.1785
140.1674
136.2281
133.5192
129.2365
128.6928
128.1968
127.9393
122.2163
115.7112
115.5395
105.7055
105.5815
96.7776
39.9960
39.8338
39.6622
39.5000
39.3283
39.1662
38.9945
30.7152
19.6412
X : parts per Million : 13C

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

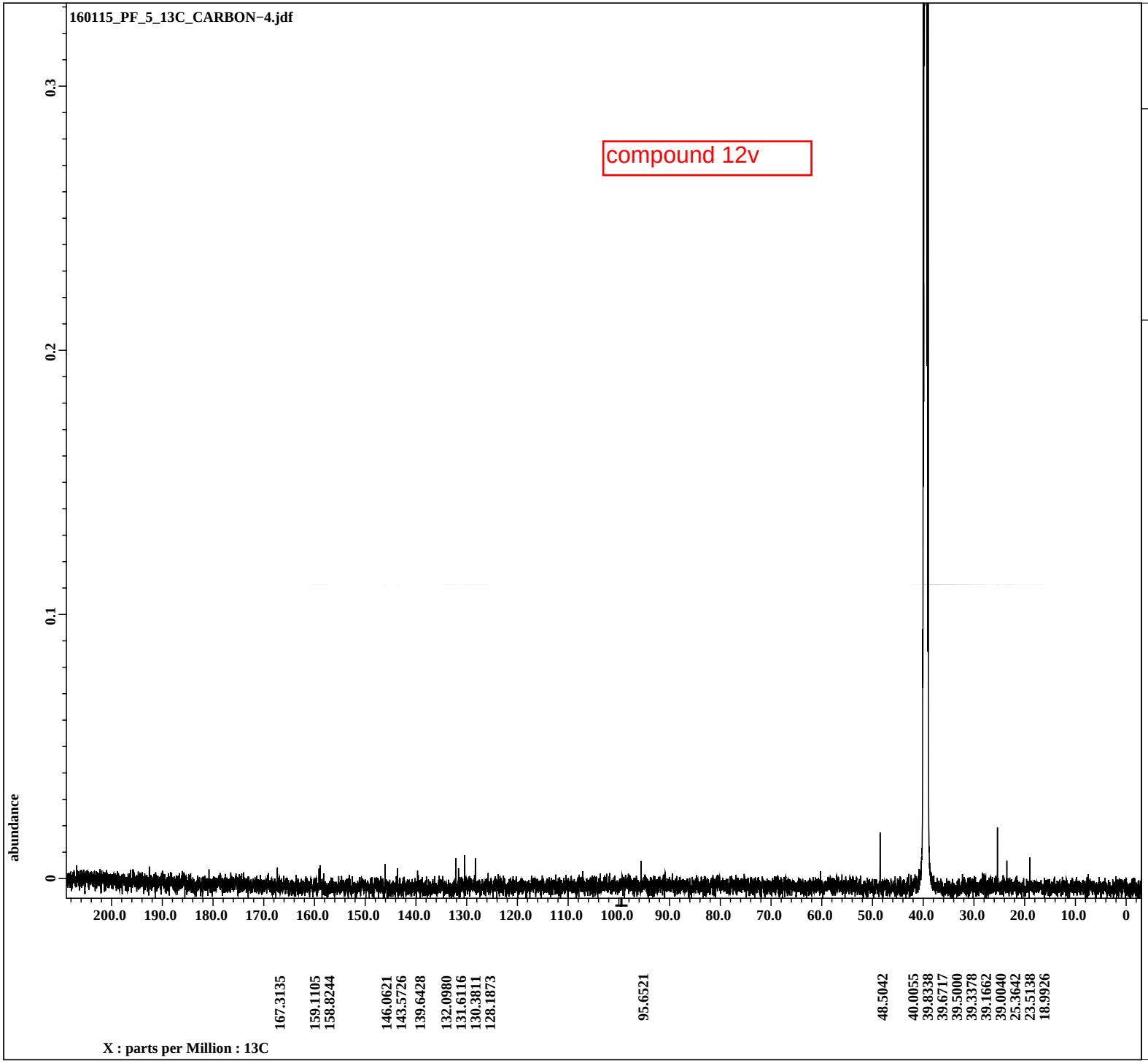
Derived from: 150115_PF_20_13C_CARBON-1.

Filename = 150115_PF_20_13C_CARB
Author = delta
Experiment = single_pulse_dec
Sample_id = 150115_PF_20
Solvent = DMSO-D6
Creation_time = 15-JAN-2015 22:30:17
Revision_time = 16-JAN-2015 10:48:54
Current_time = 16-JAN-2015 10:49:19

Comment = 150115_PF_20_13C
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX 500
Spectrometer = JNM-ECX500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain = 13C
X_freq = 125.76529768[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034[Hz]
X_sweep = 39.3081761[kHz]
Irr_domain = 1H
Irr_freq = 500.15991521[MHz]
Irr_offset = 5.0[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1024
Total_scans = 1024

X_90_width = 8.62[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 6.4[dB]
X_pulse = 2.87333333[us]
Irr_atn_dec = 21.68[dB]
Irr_atn_noe = 21.68[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get = 18.4[dC]

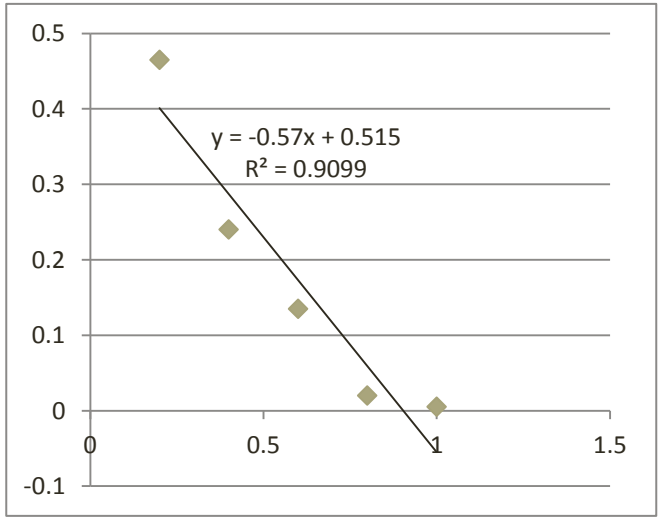


```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: 160115_PF_5_13C_CARBON-1.j
```

```
Filename          = 160115_PF_5_13C_CARBO
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = 160115_PF_5_13C
Solvent           = DMSO-D6
Creation_time     = 16-JAN-2015 23:41:22
Revision_time     = 17-JAN-2015 09:44:32
Current_time      = 17-JAN-2015 09:44:58

Comment           = 160115_PF_5_13C
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = JNM-ECX500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 2048
Total_scans       = 2048

X_90_width        = 8.62[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 6.4[dB]
X_pulse           = 2.87333333[us]
Irr_atn_dec       = 21.68[dB]
Irr_atn_noe       = 21.68[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.83361792[s]
Temp_get          = 18.1[dC]
```

α-glucosidase assay of **12p** using (p-nitro phenyl α-glucopyranoside)

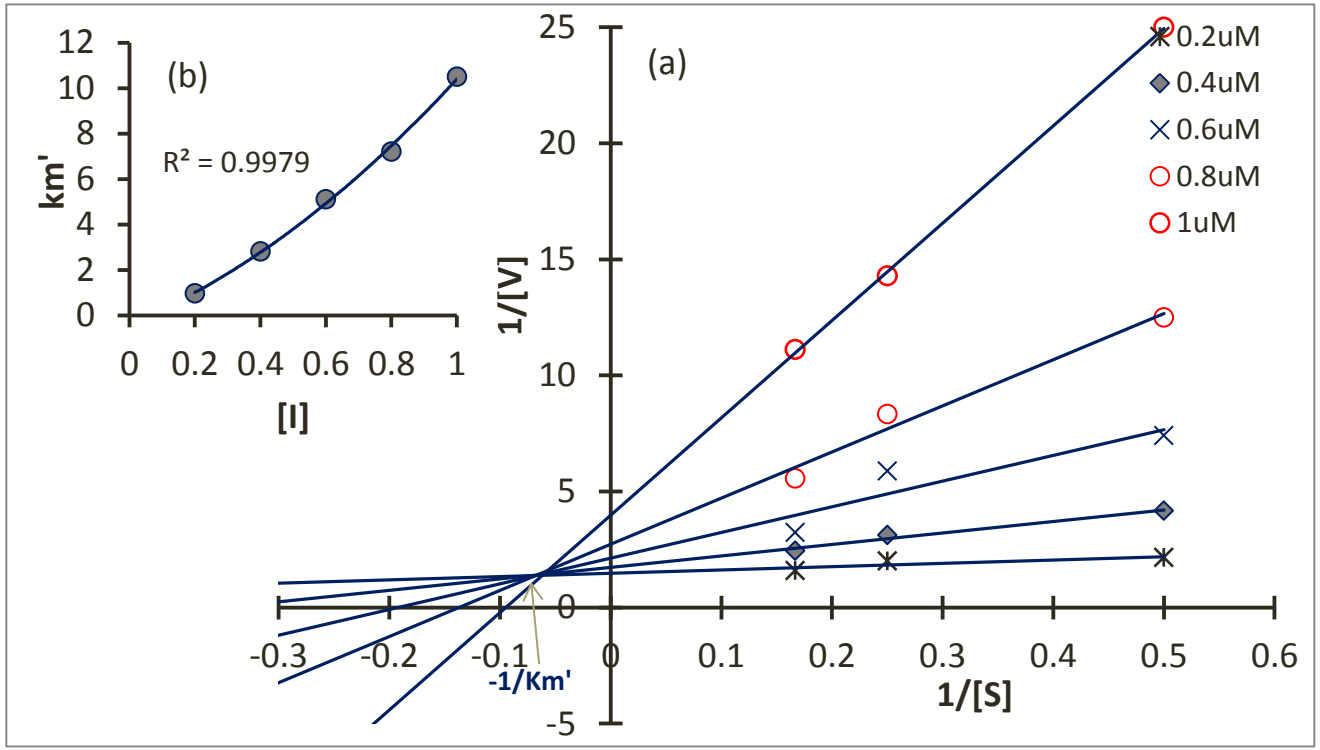
						control OD
Compound 12p	336			% of inhibition		0.9
Concentrations (µM)	R1	R2	average	C-T	IC_{50} (µg)	IC_{50} (µM)
0.2	0.48	0.45	0.465	**43.5**		
0.4	0.25	0.23	0.24	**66**	**0.82**	**0.244047619**
0.6	0.14	0.13	0.135	**76.5**		
0.8	0.03	0.01	0.02	**88**		
1	0	0.01	0.005	**89.5**		



α-glucosidase 12p-LB plot

So (mM)	mM of PNPG (substrate) 2	4	6		
Conc: of I (μM)	Vo(IU/ml)	Vo(IU/ml)	Vo(IU/ml)	km	(-1/km)
0.2	0.465	0.498	0.63	0.96	-1.04167
0.4	0.24	0.32	0.41	2.8	-0.35714
0.6	0.135	0.17	0.31	5.1	-0.19608
0.8	0.08	0.12	0.18	7.2	-0.13889
1	0.04	0.07	0.09	10.5	-0.09524

[S]	1/s	v10	v20	v30	v40	v50
2	0.5	0.465	0.24	0.135	0.08	0.04
4	0.25	0.498	0.32	0.17	0.12	0.07
6	0.166667	0.63	0.41	0.31	0.18	0.09
1/v		1/v10	1/v20	1/v30	1/v40	1/v50
	0.5	2.150538	4.166667	7.407407	12.5	25
	0.25	2.008032	3.125	5.882353	8.333333	14.28571
	0.166667	1.587302	2.439024	3.225806	5.555556	11.11111



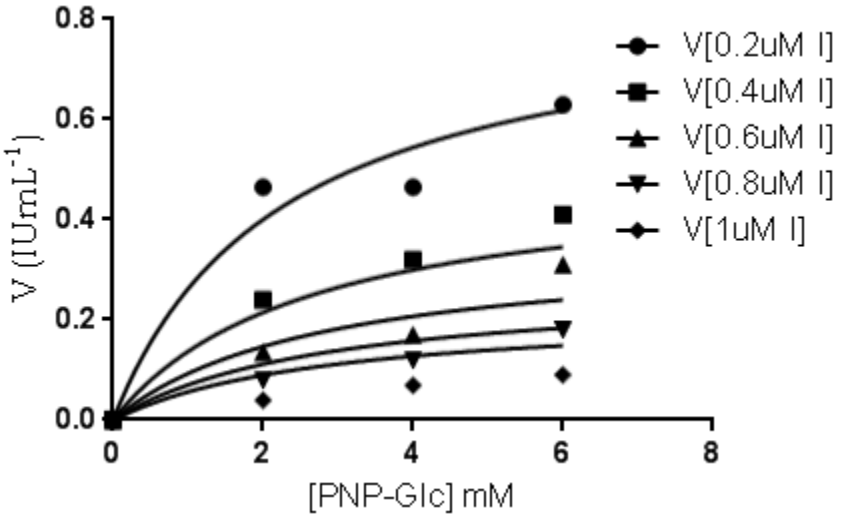
COS cell cytotoxicity screening

expt-1		O.D 1	O.D 2	avg	ctrl-avg	/ctrl	*100 or % inhibition
	control	0.765	0.723	0.744	0	0	0
	50	0.735	0.775	0.755	-0.011	-0.01478	-1.47849
	25	0.767	0.783	0.775	-0.031	-0.04106	-4.10596
	12.5	0.736	0.742	0.739	0.005	0.006452	0.645161
	6.25	0.779	0.788	0.7835	-0.0395	-0.05345	-5.34506
	3.125	0.743	0.741	0.742	0.002	0.002553	0.255265
	1.56	0.861	0.6	0.7305	0.0135	0.018194	1.819407
	0.78	0.685	0.752	0.7185	0.0255	0.034908	3.49076
	0.39	0.79	0.688	0.739	0.005	0.006959	0.695894
	0.195	0.716	0.704	0.71	0.034	0.046008	4.600812

Expt-2		O.D 1	O.D 2	avg	ctrl-avg	/ctrl	*100 or % inhibition
	control	1.039	1.259	1.149	0	0	0
	50	1.07	1.031	1.0505	0.0985	0.085727	8.572672
	25	1.197	1.353	1.275	-0.126	-0.10966	-10.9661
	12.5	1.211	1.208	1.2095	-0.0605	-0.05265	-5.26545
	6.25	1.073	1.126	1.0995	0.0495	0.043081	4.308094
	3.125	1.331	1.143	1.237	-0.088	-0.07659	-7.65883
	1.56	1.087	1.042	1.0645	0.0845	0.073542	7.354221
	0.78	1	1.073	1.0365	0.1125	0.097911	9.791123
	0.39	1.074	1.095	1.0845	0.0645	0.056136	5.613577
	0.195	1.089	1.076	1.0825	0.0665	0.057876	5.787641

To determine the kinetic parameters a linear regression analysis of **12p** against α-glucosidase was obtained (Michalis Menten plot)

We have performed a global non-linear regression analysis for different substrate concentrations in the presence of various concentrations of the potent mixed inhibitor (**12p**). Afterwards, the data was linearized and figured the binding constants (Ki) values. The regression plots were as follows



Substituted furopyridinediones as novel inhibitors of α-glucosidase

Chandramohan Bathula,[1, §] Rajanikanth Mamidala,[4, §] Chiranjeevi Thulluri,[3] Rahul Agarwal,[2], Kunal Kumar Jha,[1] Parthapratim Munshi,[1] Uma Adepally,[3] Ashutosh Singh,[2] M. Thirumalachary[4], Subhabrata Sen[1, *]

[1] *Department of Chemistry, School of Natural Sciences, Shiv Nadar University, Chithera, Dadri, UP 201314, India*

[2] *Department of Life Science, School of Natural Sciences, Shiv Nadar University, Chithera, Dadri, UP 201314, India*

[3] *Institute of Science and Technology, Jawaharlal Nehru Technological University Hyderabad, Kukatpally, Hyderabad500085, Telengana, India*

[4] *Department of Chemistry, Jawaharlal Nehru Technological University Hyderabad, Kukatpally, Hyderabad500085, Telengana, India*

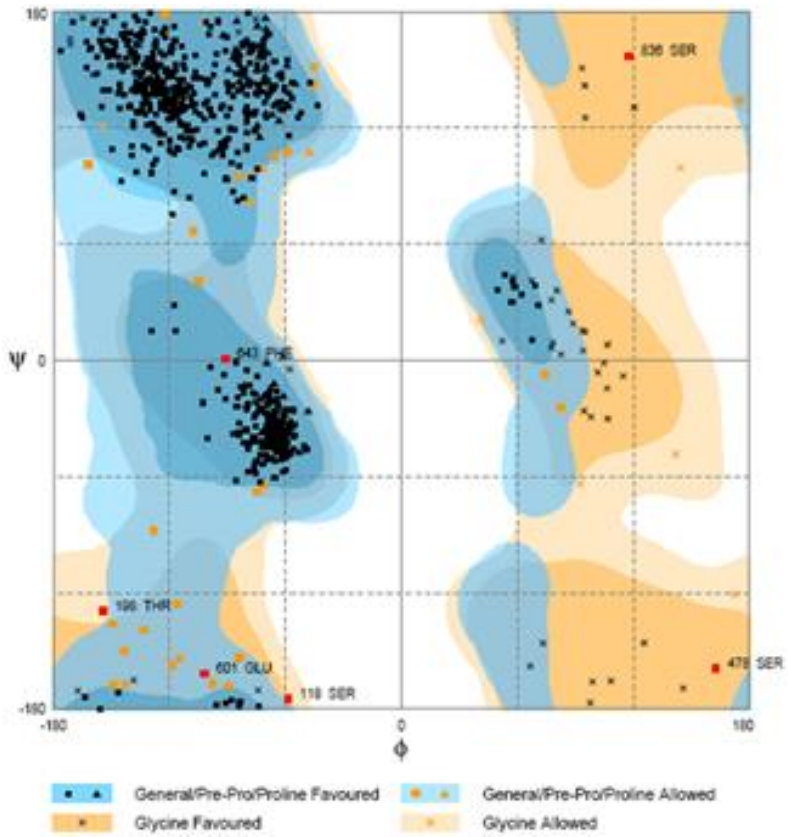


Figure 1. Ramachandran Plot of modelled α-glucosidase protein

For docking studies the modelled structures, **7a**, **9a**, **12d**, **12p**, acarbose and template structure (PDB ID: 3L4T) were aligned and the centroid coordinates of the complex ligand in the crystal structure (PDB ID: 3L4T) were used as the centre of the docking site. A grid of 60 x 60 x 60 with 0.375 A0 were constructed around the docking area using Autogrid v 4.2 software.

Docking analyses were done using Autodock v 4.2 software, in which top 10 docked conformation were taken using Genetic Algorithm. Each docking calculation consisted of 25 x 106 energy evaluations with 250 population size. A mutation rate of 0.02 and a crossover rate of 0.8 were used to generate new docking trials.

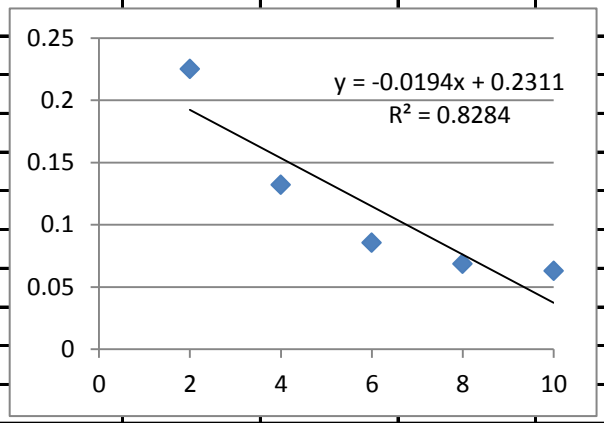
Docking interactions of 7a, 9a and 12d

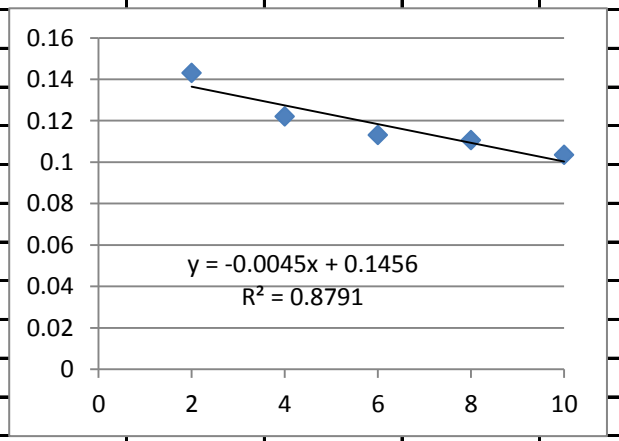
Table 1

Compound Name	**Residues involved in H-bond**	**Residues involved in other non-bonded interactions**
Compound **7a**	ARG 193, ARG 194, HIS 586	TRP 288, ASP 316, ILE 353, TRP 393, TRP 428, ASP 430, MET 431, PHE 437, ARG 512, TRP 525, ASP 528
Compound **9a**	ARG 193, ASP 528	ASP 194, TRP 393, ALA 467
Compound **12d**	SER 435, ARG 512	ARG 193, ASP 194, LEU 195, ALA 196, PHE 437, ALA 467, ASP 528, LEU 562

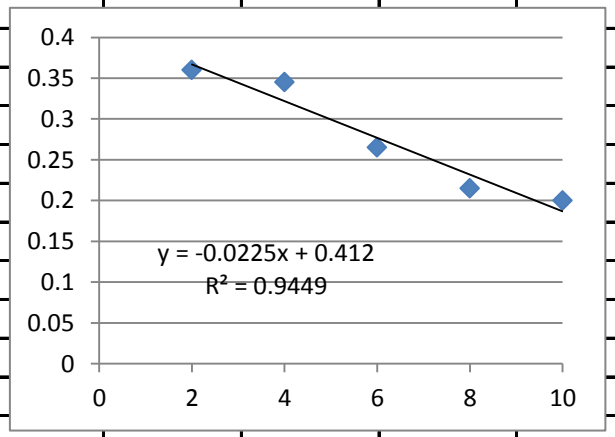
Note: Highlighted residues are important for alpha-glucosidase activity.

Alpha glucosidase assay screening using (p-Nitro phenyl alpha D- glucopyranoside)								
							control OD	
Compound 12a		281.31			% of inhibition		0.58	
Concentrations (µg)		R1	R2	average	C-T	Ic 50 (µg)	Ic 50 (µM)	
10		0.871	0.798	0.8345				
30		1.656	1.864	1.76				
50		1.505	2.313	1.909				
70		2.914	3.322	3.118				
100		3.691	3.613	3.652		**NOT ACTIVE**		
Compound 12c		321.25						
Concentrations (µg)		R1	R2					
2		0.24	0.21	0.225	35.5			
4		0.132	0.132	0.132	44.8	7.427835	23.12	
6		0.096	0.075	0.0855	49.45			
8		0.068	0.069	0.0685	51.15			
10		0.061	0.065	0.063	51.7			
Compound 12b		311.33						
Concentrations (µg)		R1	R2					
2		1.454	1.406	1.43				
4		2.8	2.454	2.627				
6		2.715	2.596	2.6555				
8		2.588	2.465	2.5265		**NOT ACTIVE**		
10		2.666	2.735	2.7005				
Compound 12e		332.15						
Concentrations (µg)		R1	R2					
2		0.171	0.115	0.143	43.7			
4		0.097	0.147	0.122	45.8	13.68889	41.21297272	
6		0.122	0.104	0.113	46.7			
8		0.137	0.084	0.1105	46.95			
10		0.079	0.128	0.1035	47.65			

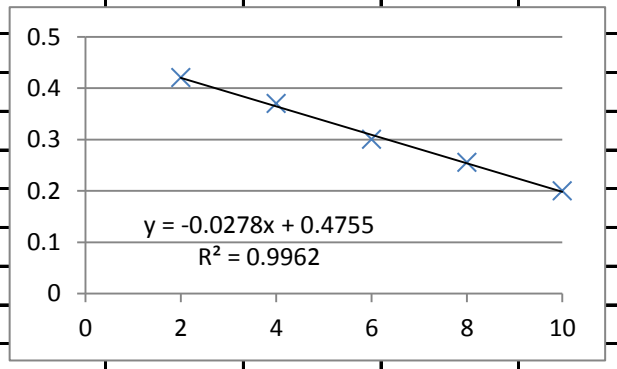




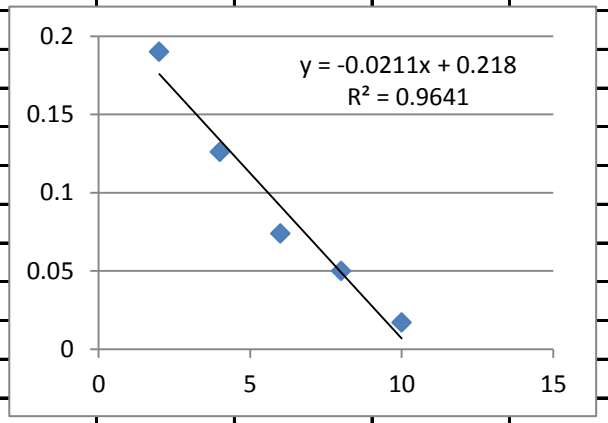
Compound 12g		303										
Concentrations (µg)		R1	R2									
2		0.573	1.405									
4		0.895	0.965	0.93								
6		1.375	1.546	1.4605								
8		2.435	2.46	2.4475		**NOT ACTIVE**						
10		2.64	2.628	2.634								
Compound 12i		297										
Concentrations (µg)		R1	R2									
2		0.681	0.784	0.7325								
4		1.797	1.784	1.7905								
6		2.876	2.804	2.84								
8		2.874	2.932	2.903								
10		2.88	2.96	2.92		**NOT ACTIVE**						
Compound 12j		313										
Concentrations (µg)		R1	R2									
2		0.43	0.449	0.4395								
4		0.906	0.873	0.8895								
6		1.753	2.337	2.045								
8		2.311	2.27	2.2905								
10		2.4	2.36	2.38		**NOT ACTIVE**						
Compound 12s		366										
Concentrations (µg)		R1	R2									
2		0.37	0.35	0.36	22.0							
4		0.36	0.33	0.345	23.5	11.2	30.6010929					
6		0.29	0.24	0.265	31.5							
8		0.21	0.22	0.215	36.5							
10		0.2	0.2	0.2	38.0							

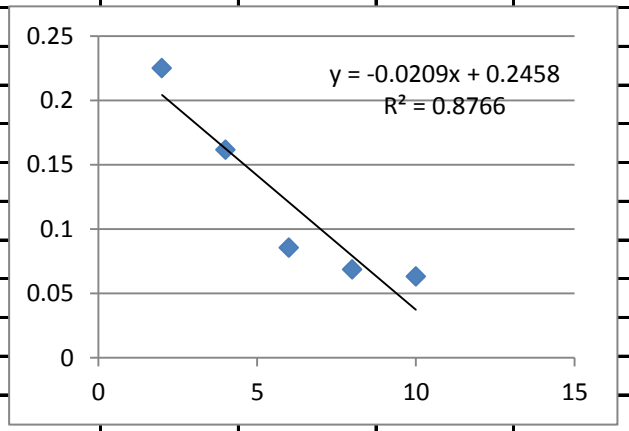


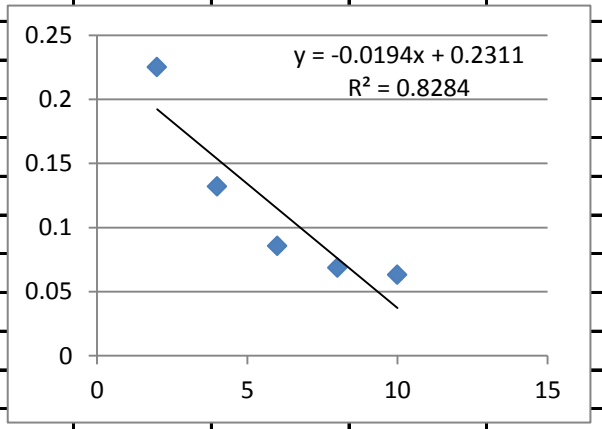
Compound 12r		336										
Concentrations (µg)		R1	R2									
2		0.396	0.339	0.3675								
4		0.798	0.504	0.651								
6		1.248	1.256	1.252								
8		1.872	1.913	1.8925		**NOT ACTIVE**						
10		2.102	2.225	2.1635								
Compound 12u		380										
Concentrations (µg)		R1	R2									
2		0.589	0.558	0.5735								
4		1.214	0.998	1.106								
6		2.141	2.233	2.187								
8		2.729	2.876	2.8025								
10		3.066	3.005	3.0355		**NOT ACTIVE**						
Compound 12v		343										
Concentrations (µg)		R1	R2									
2		0.672	0.744	0.708								
4		1.282	1.707	1.4945								
6		2.071	2.713	2.392								
8		2.921	2.888	2.9045								
10		3.1	2.886	2.993		**NOT ACTIVE**						
Compound 12k		253										
Concentrations (µg)		R1	R2									
2		0.44	0.4	0.42	16.0							
4		0.36	0.38	0.37	21.0	13.50719	53.38811954					
6		0.28	0.32	0.3	28.0							
8		0.25	0.26	0.255	32.5							
10		0.2	0.2	0.2	38.0							



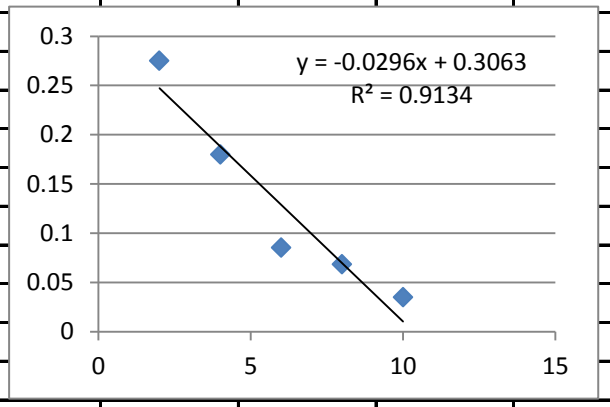
Compound 12d		285.25										
Concentrations (µg)		R1	R2		C-T	Ic 50 (µg)	Ic 50 (µM)					
2		0.18	0.2	0.19	50							
4		0.12	0.132	0.126	62	0.575916	2.02					
6		0.073	0.075	0.074	75							
8		0.04	0.06	0.05	88							
10		0.014	0.02	0.017	96							
Compound 12f		332.15										
Concentrations (µg)		R1	R2									
2		0.24	0.21	0.225	39							
4		0.155	0.168	0.1615	50.1	3.5311	10.63					
6		0.096	0.075	0.0855	69							
8		0.068	0.069	0.0685	88							
10		0.061	0.065	0.063	96							
Compound 12h		289.23										
Concentrations (µg)		R1	R2									
2		0.24	0.21	0.225	50.5							
4		0.132	0.132	0.132	59.8	0.314433	1.09					
6		0.096	0.075	0.0855	64.45							
8		0.068	0.069	0.0685	66.15							
10		0.061	0.065	0.063	66.7							

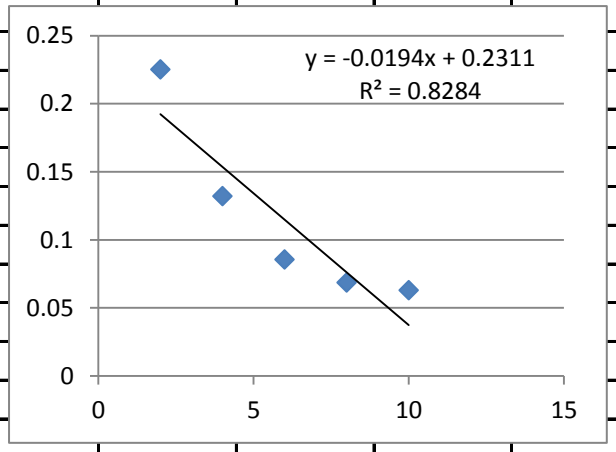


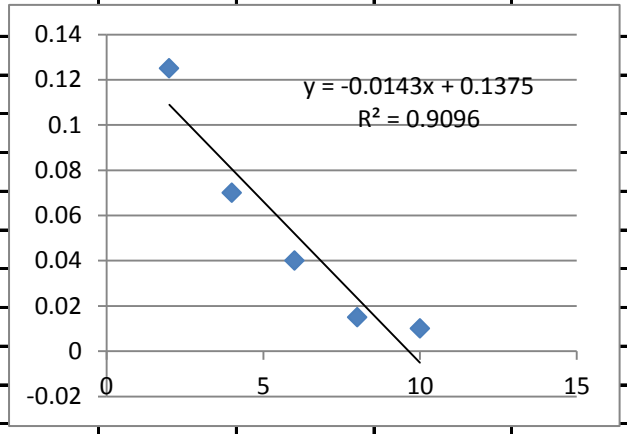




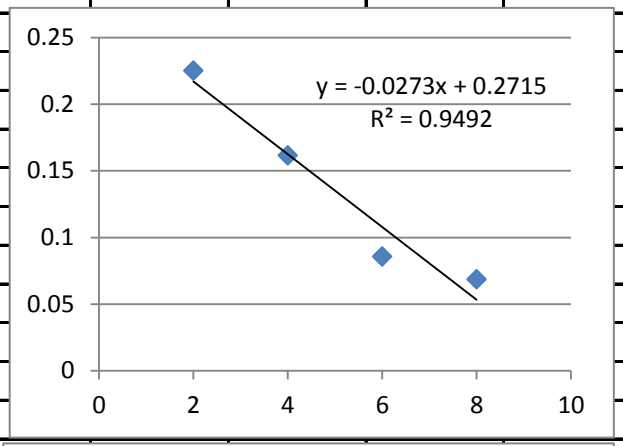
Compound 12l		298.25						
Concentrations (µg)		R1	R2					
2		0.28	0.27	0.275	47.5			
4		0.17	0.19	0.18	57	1.057432	3.55	
6		0.096	0.075	0.0855	66.45			
8		0.068	0.069	0.0685	68.15			
10		0.04	0.03	0.035	71.5			
Compound 12m		292.29						
Concentrations (µg)		R1	R2					
2		0.24	0.21	0.225	50			
4		0.132	0.132	0.132	62	0.628272	2.15	
6		0.096	0.075	0.0855	75			
8		0.068	0.069	0.0685	88			
10		0.061	0.065	0.063	96			
Compound 12n		243.22						
Concentrations (µg)		R1	R2					
2		0.11	0.14	0.125	45.5			
4		0.08	0.06	0.07	51	0.227642	0.94	
6		0.03	0.05	0.04	54			
8		0.01	0.02	0.015	56.5			
10		0.01	0.01	0.01	57			

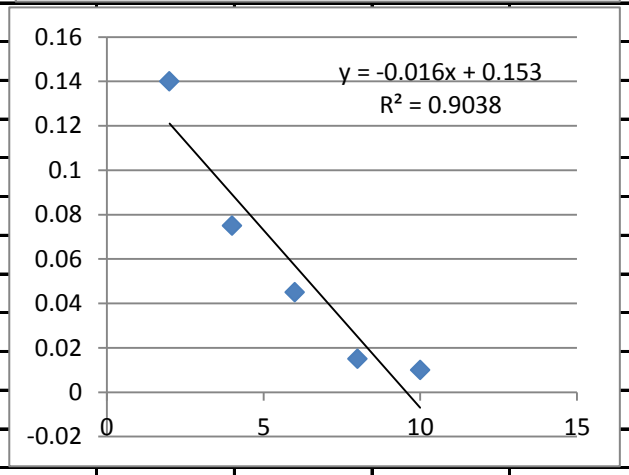


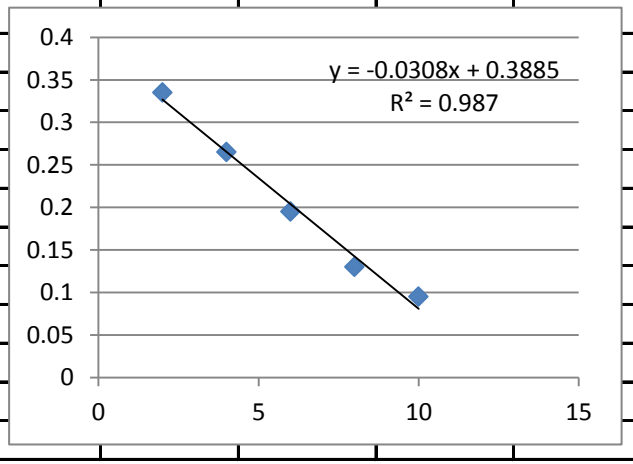




Compound 12o		259.28					
Concentrations (µg)		R1	R2				
2		0.24	0.21	0.225	39		
4		0.155	0.168	0.1615	50.1	2.669856	10.30
6		0.096	0.075	0.0855	69		
8		0.068	0.069	0.0685	88		
10		0.061	0.065	0.063	96		
Compound 12q		335.38					
Concentrations (µg)		R1	R2				
2		0.13	0.15	0.14	44		
4		0.07	0.08	0.075	50.5	2.8125	8.39
6		0.04	0.05	0.045	53.5		
8		0.01	0.02	0.015	56.5		
10		0.01	0.01	0.01	57		
Compound 12t		520.18					
Concentrations (µg)		R1	R2				
2		0.32	0.35	0.335	24.5		
4		0.28	0.25	0.265	31.5	45.05814	86.62
6		0.2	0.19	0.195	38.5		
8		0.12	0.14	0.13	45	86	
10		0.08	0.11	0.095	48.5		







Compound 2p		336			% of inhibition			control OD 0.9				
Concentrations (µM)		R1	R2	average	C-T	Ic 50 (µg)	Ic 50 (µM)					
0.2		0.48	0.45	0.465	**43.5**							
0.4		0.25	0.23	0.24	**66**	**0.82**	**0.244047619**					
0.6		0.14	0.13	0.135	**76.5**							
0.8		0.03	0.01	0.02	**88**							
1		0	0.01	0.005	**89.5**