

Ionic liquids of superior thermal stability. Validation of PPh_4^+ as an organic cation of impressive thermodynamic durability

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Supporting Information

General Information:

Commercial reagents were obtained from Aldrich Chemical and Oakwood Chemicals and used without further purification. ^1H , ^{19}F , and ^{13}C NMR were recorded on a 500 MHz JEOL spectrometer using CDCl_3 as a solvent at room temperature. All chemical shifts for ^1H and ^{13}C NMR were reported downfield using tetramethylsilane (TMS, at δ 0.00 ppm).

General procedure for the synthesis of (4-methylphenyl)triphenylphosphonium (d_{15}) bromide**Method A:**

In a 50 ml heavy wall pressure vessel with an internal thread (Teflon cap) containing a stirbar, 4-bromotoluene (1.0 equiv), triphenylphosphine (d_{15}) (1.0 equiv), NiBr_2 (5.0 mol%) and ethylene glycol (15 ml) were added under nitrogen atmosphere. The reaction mixture was then stirred at 180 °C for 8 hours. The mixture was then cooled to room temperature, and aqueous NaBr added to dissolve the Ni salts and ethylene glycol. Dichloromethane was added to extract the desired phosphonium salt from the mixture. After two more extractions, the combined organic extracts were dried over anhydrous Na_2SO_4 ; solvents were removed under reduced pressure, and pure (4-methylphenyl)triphenylphosphonium bromide was isolated as a white solid. The same procedure was utilized for the non-deuterated triphenylphosphine derivatives.

Method B:

In a 50 ml heavy wall pressure vessels with an internal thread (Teflon cap) containing a stirbar, 4-bromotoluene (1.0 equiv), triphenylphosphine (d_{15}) (1.0 equiv), $\text{Pd}(\text{OAc})_2$ (1.5 mol%) and xylene (15 ml) were added under nitrogen atmosphere and reaction mixture stirred at 145 °C for 4 hours. The desired product precipitated as a white solid during the course of the reaction. The reaction mixture was cooled to the room temperature, filtered and washed with xylene and diethyl ether and pure product was isolated as a white solid. The same procedure is equally effective when using non-deuterated triphenylphosphine.

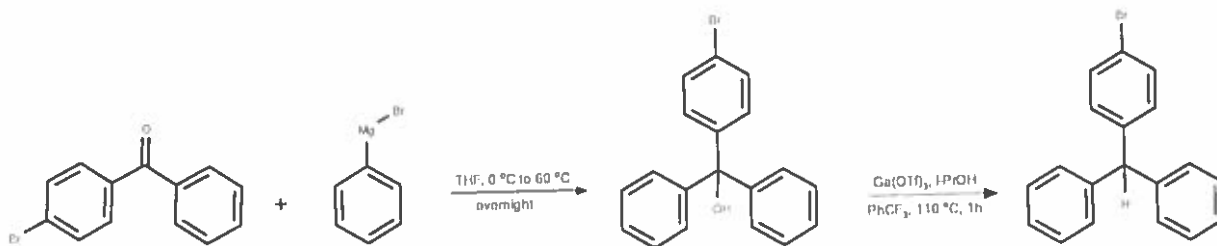
General procedure for the synthesis of (4-methylphenyl)triphenylphosphonium (d_{15}) bistriflimide

The bistriflimide salt was synthesized by an ion exchange of potassium bistriflimide (1.0 equiv) and phosphonium salt (1.0 equiv) in water for 15 min at room temperature. The reaction mixture was then extracted three times with dichloromethane. The combined organic extracts were dried

over anhydrous Na_2SO_4 , solvents were removed under reduced pressure, and pure (4-methylphenyl)triphenylphosphonium bistriflimide was isolated as a white solid.

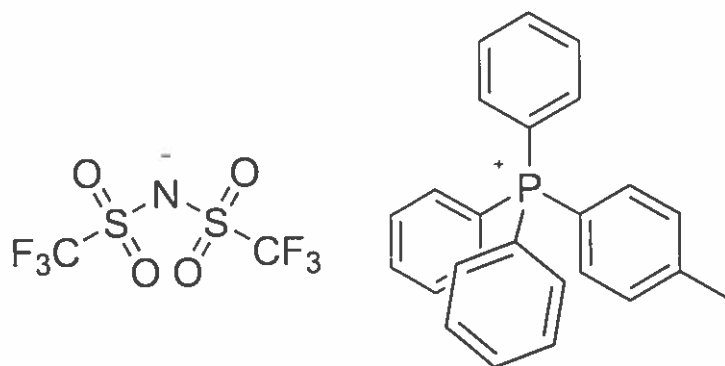
General procedure for the synthesis of 4-Bromophenyl diphenylmethane

In an oven-dried 100 mL flask, a solution of 4-bromobenzophenone (20 mmol, 1.0 equiv) in THF (50 mL) was prepared. Phenylmagnesium bromide solution (Aldrich; 3.0 M in Et_2O , 17 mL, 2.5 equiv) was added dropwise at 0 °C under nitrogen atmosphere and the resulting mixture was then stirred at 60 °C overnight. The reaction was then quenched with a saturated aqueous solution of NH_4Cl and extracted three times with dichloromethane. The organic extracts were combined, dried over Na_2SO_4 , and concentrated under reduced pressure. The residue was then purified by flash chromatography on silica gel (hexane) to give 4-Bromophenyl diphenylmethanol in 80% yield as colorless viscous liquid. The 4-bromophenyl diphenylmethanol (12 mmol, 1.0 equiv) was then transferred into an oven-dried 100 mL flask equipped with a stirring bar. $\text{Ga}(\text{OTf})_3$ (5.0 mol%), and isopropanol (60 mmol, 5.0 equiv) in PhCF_3 (20 mL) was added. The resulting mixture was stirred at 110 °C for 1 h. The mixture was then cooled to room temperature, diluted with Et_2O , filtered and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (hexane) to give the 4-bromophenyl diphenylmethane as a white pure product in 85% yield.



Compound 3 Pre- and Post-heating NMR Spectra

Temperature of Post-heating samples noted in upper left corner of each spectrum



X : parts per Million : 1H

7.5091
7.5022
7.4576
7.4312

2.4886

1.6984

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
-1.0
-2.0

abundance

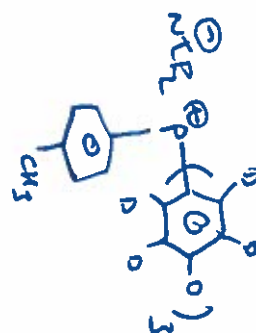
3.88

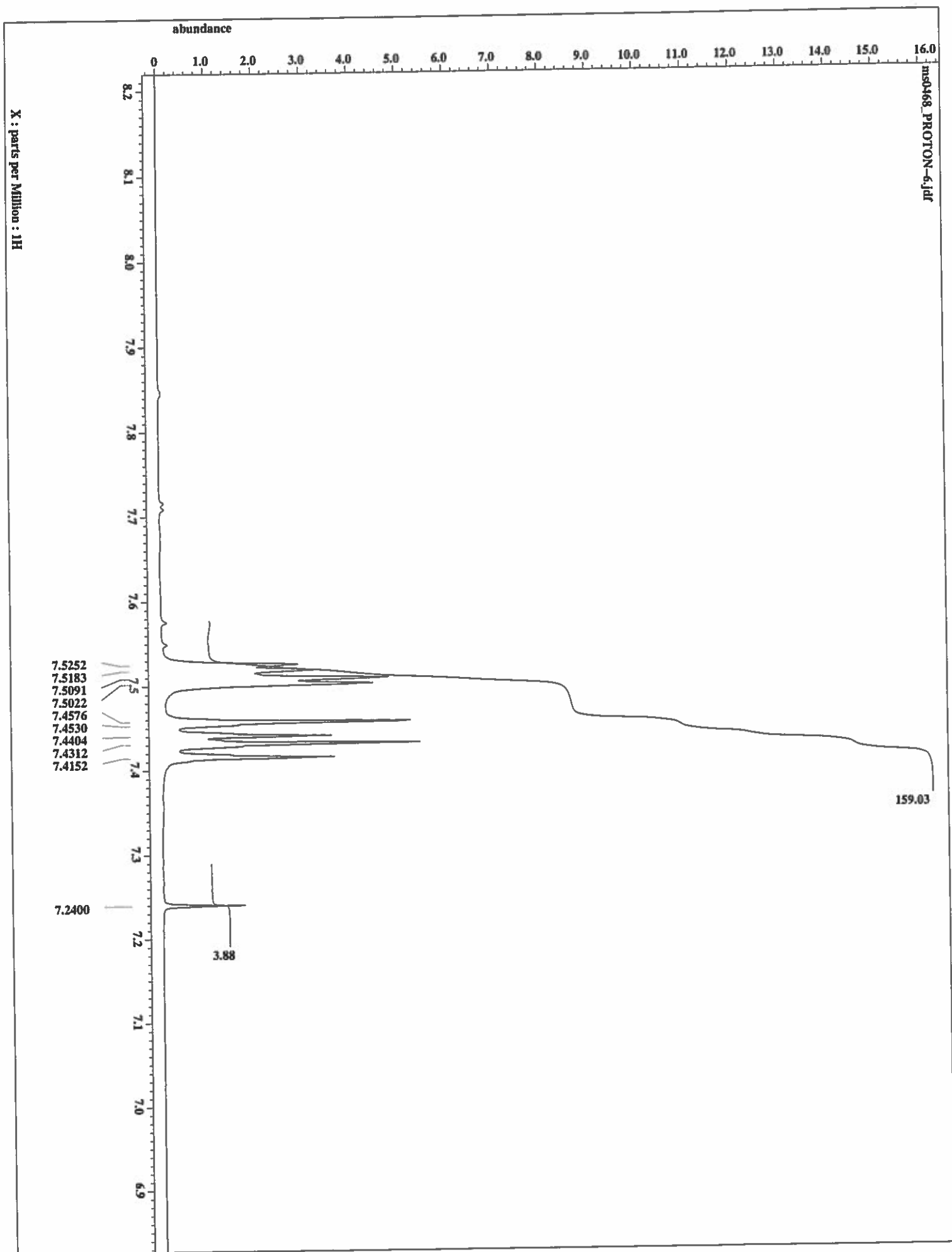
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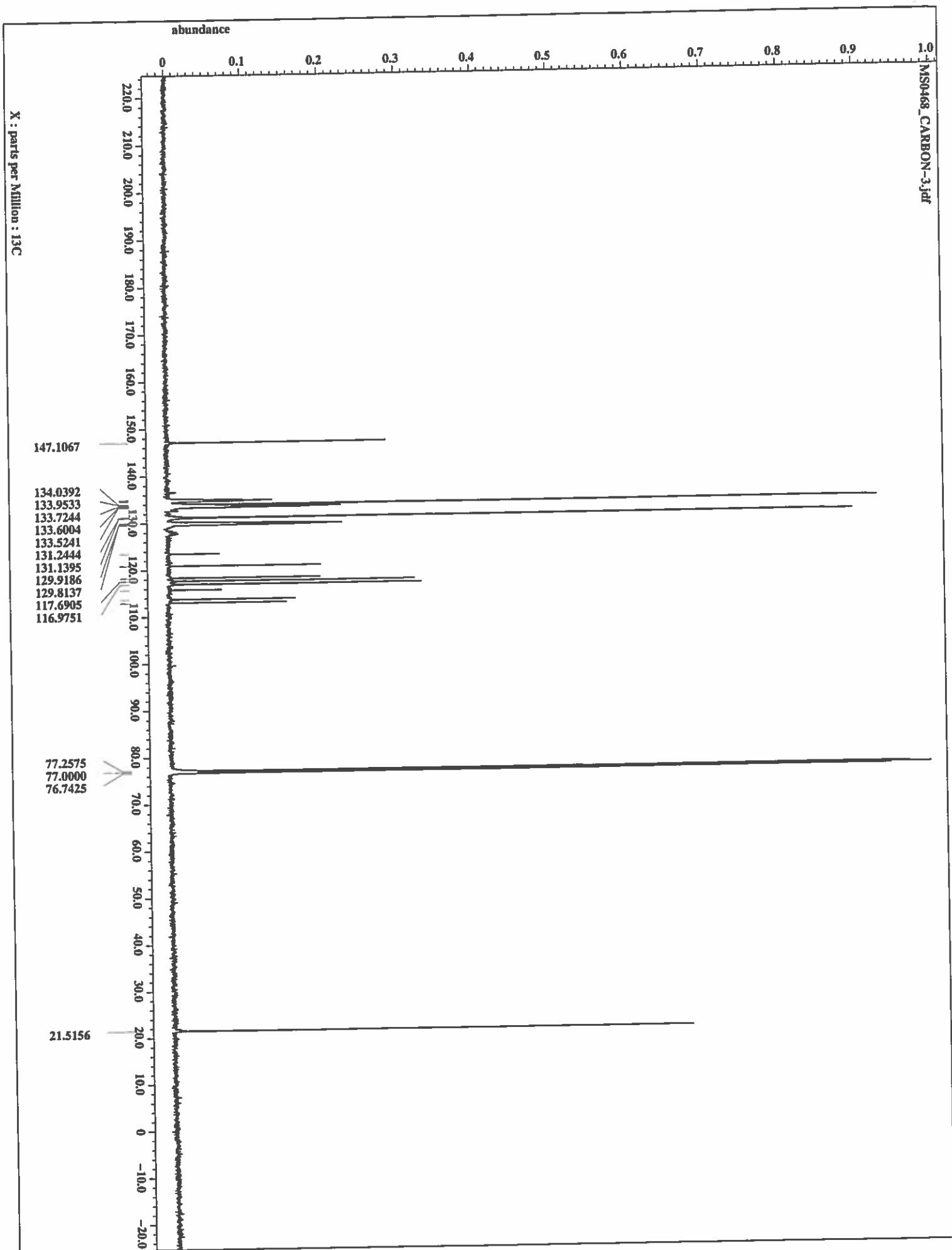
122.2

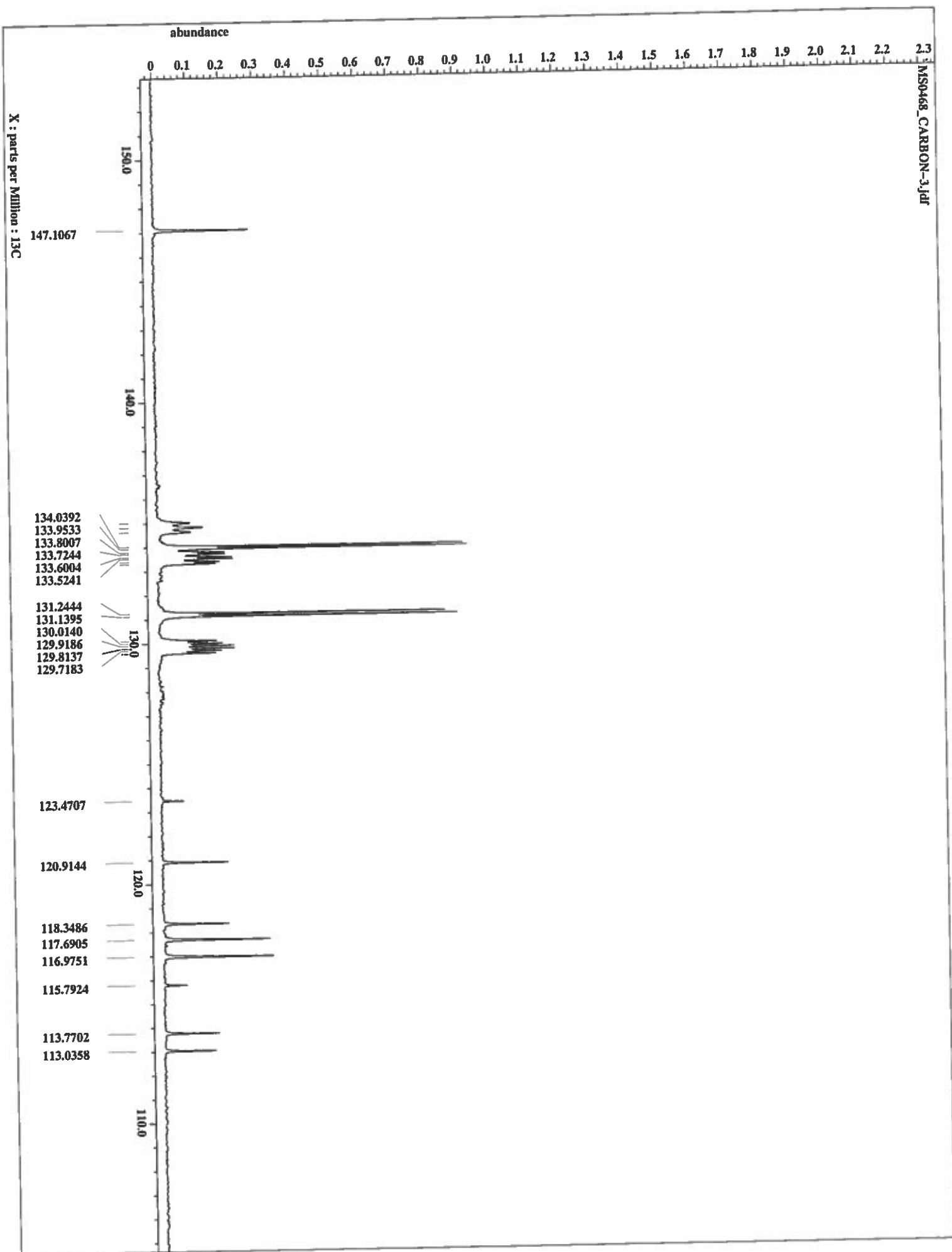
159.03

ms0468_PROTON-6.jdt

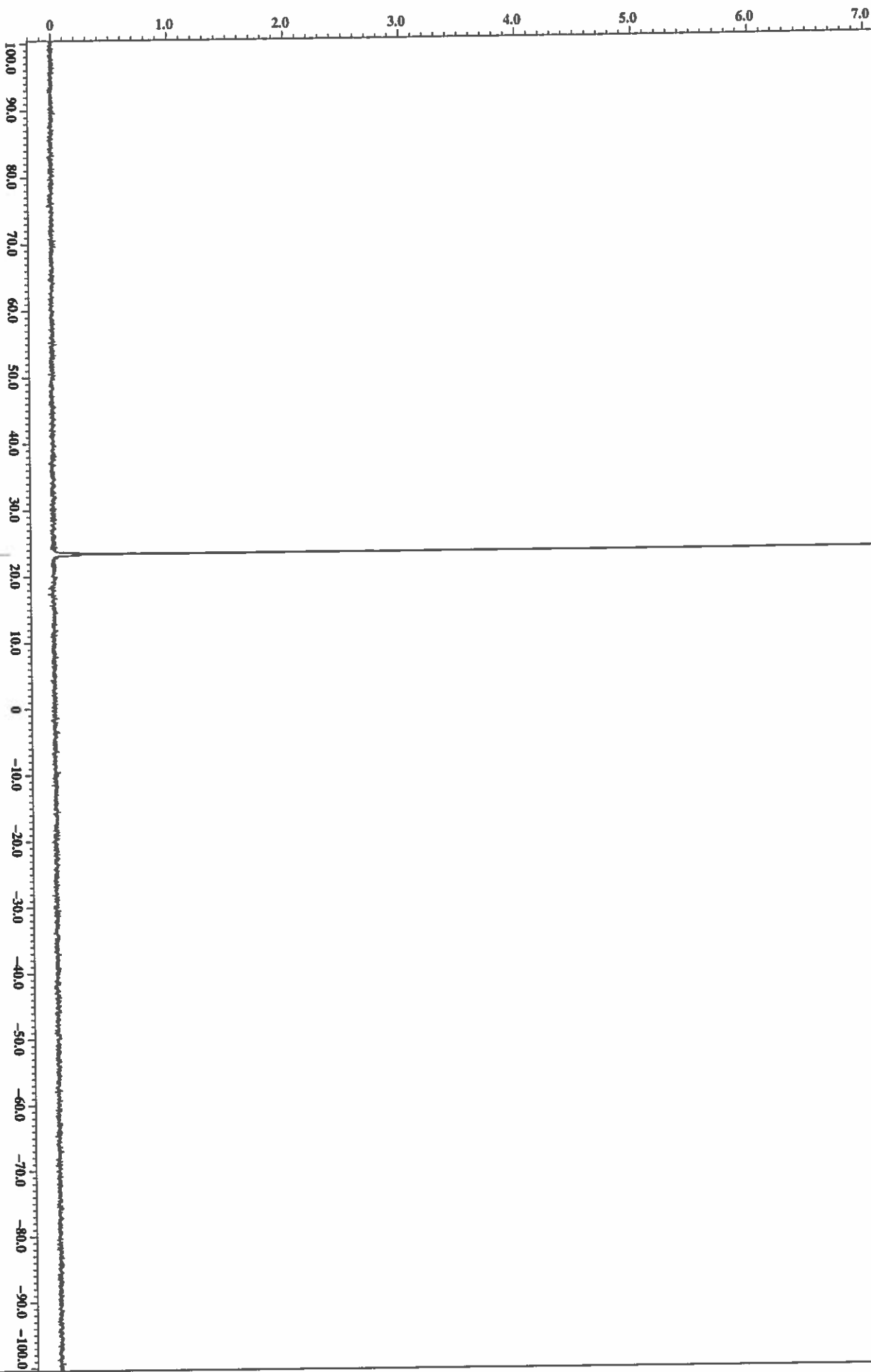








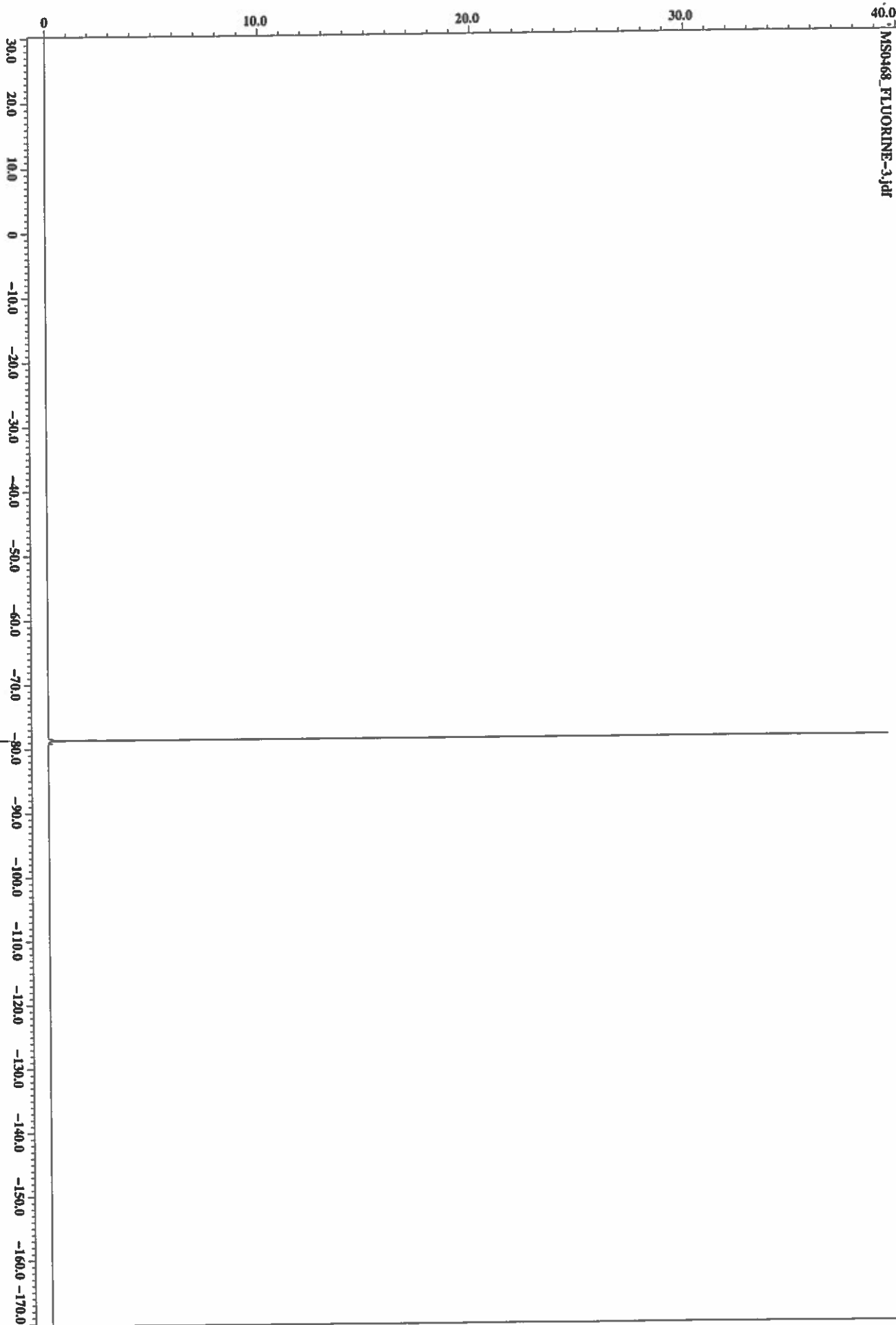
abundance



23.4287

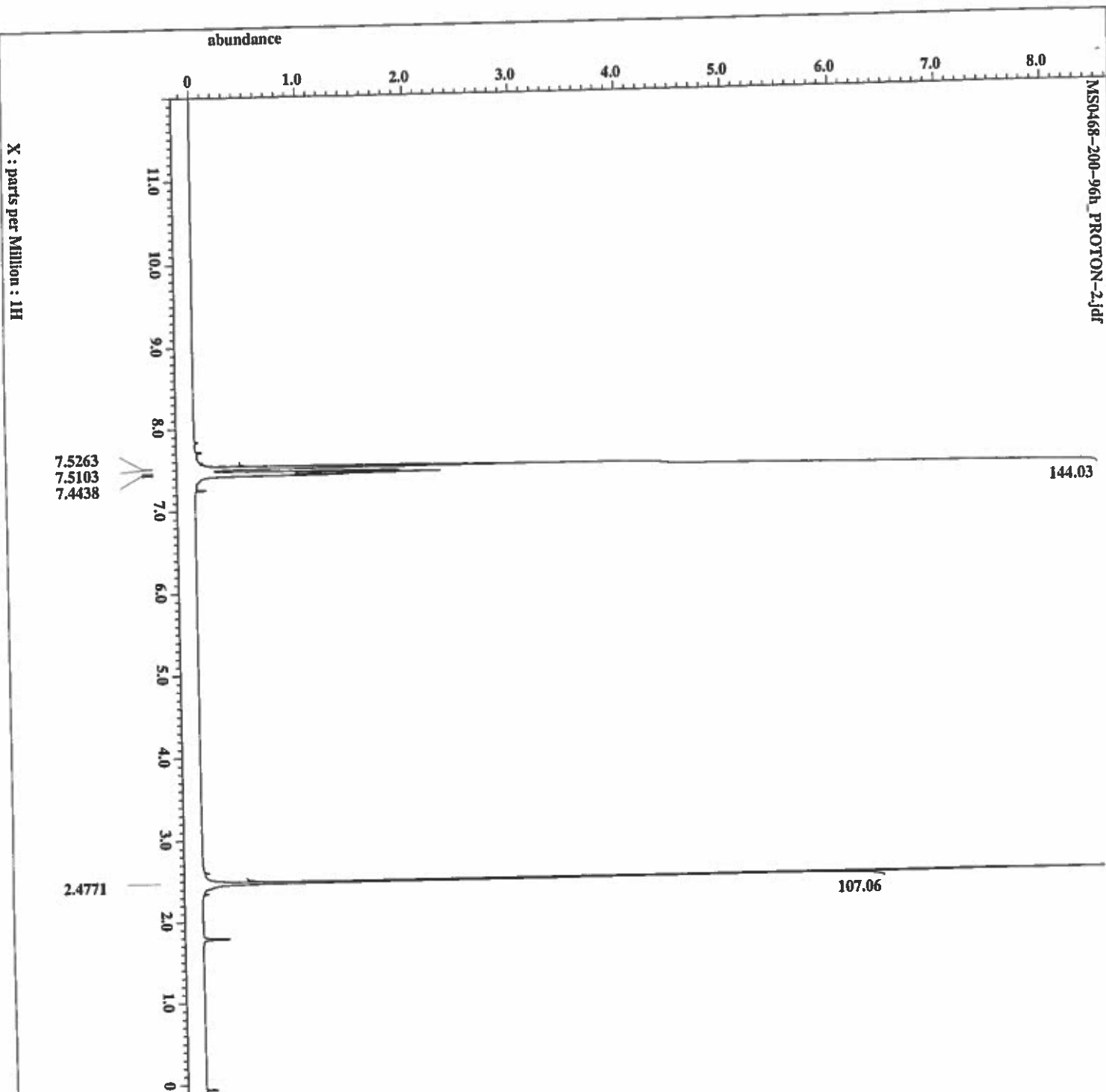
X : parts per Million : 31P

abundance



X : parts per Million : 19F

-78.6486



```

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Experiment: single_pulse_ex2
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Solvent: CHLOROFORM-D
Charger_sample: 17
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Revision_time: 12-JUN-2018 15:41:01
Current_time: 12-JUN-2018 15:41:02

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Dim. size: 13107
Dim. title: 1H
Dim. units: [ppm]
Dimensions: X
Site: RCA 500
Spectrometer: JNM-ECX500

=====
Field strength: 11.7473579 [T] (500 [MHz])
X_acq_duration: 1.74587904 [s]
X_domain: 1H
X_freq: 500.15991521 [MHz]
X_offset: 5.0 [ppm]
X_points: 16384
X_prescans: 1
X_resolution: 0.5737773 [Hz]
X_sweep: 9.3643848 [kHz]
1H_domain: 1H
1H_freq: 500.15991521 [MHz]
1H_offset: 5.0 [ppm]
1H_domain: 1H
1H_freq: 500.15991521 [MHz]
1H_offset: 5.0 [ppm]
Clipped: FALSE
Mod. return: 1
Scans: 16
Total_scans: 16

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X_90_width: 12.4 [us]
X_acq_time: 1.74587904 [s]
X_angle: 45 [deg]
X_atn: 4 [dB]
X_pulse: 6.2 [us]
1H_mode: OF2
1H_mode: OF2
Pulse_program: FALKE
Pulse_program: FALKE
Initial_wait: 1 [s]
Recvr_gain: 32
Relaxation_delay: 4 [s]
Relaxation_delay: 5.74587904 [s]
Relaxation_time: 22.1 [sec]
Temp_get:
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```

abundance

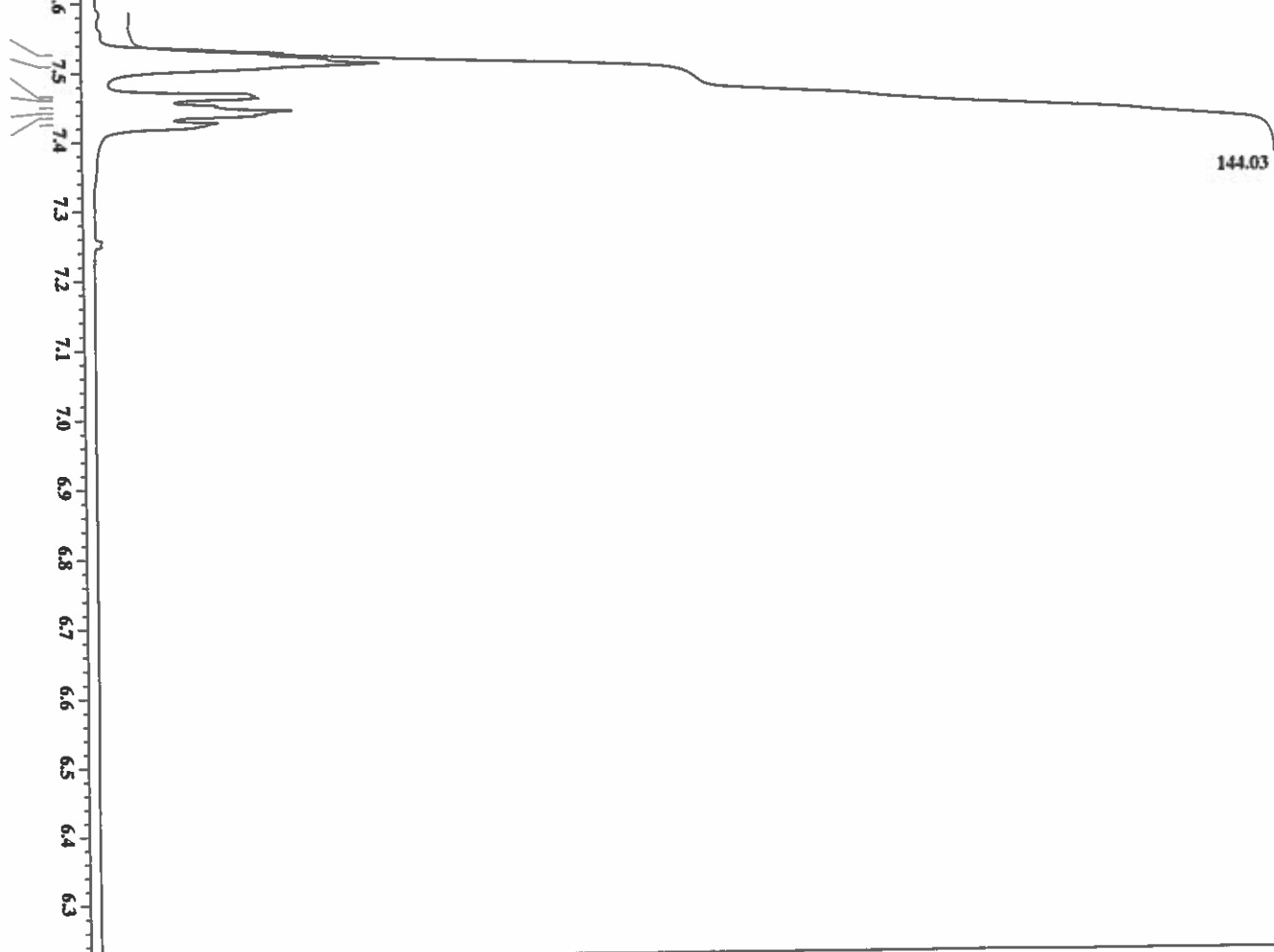
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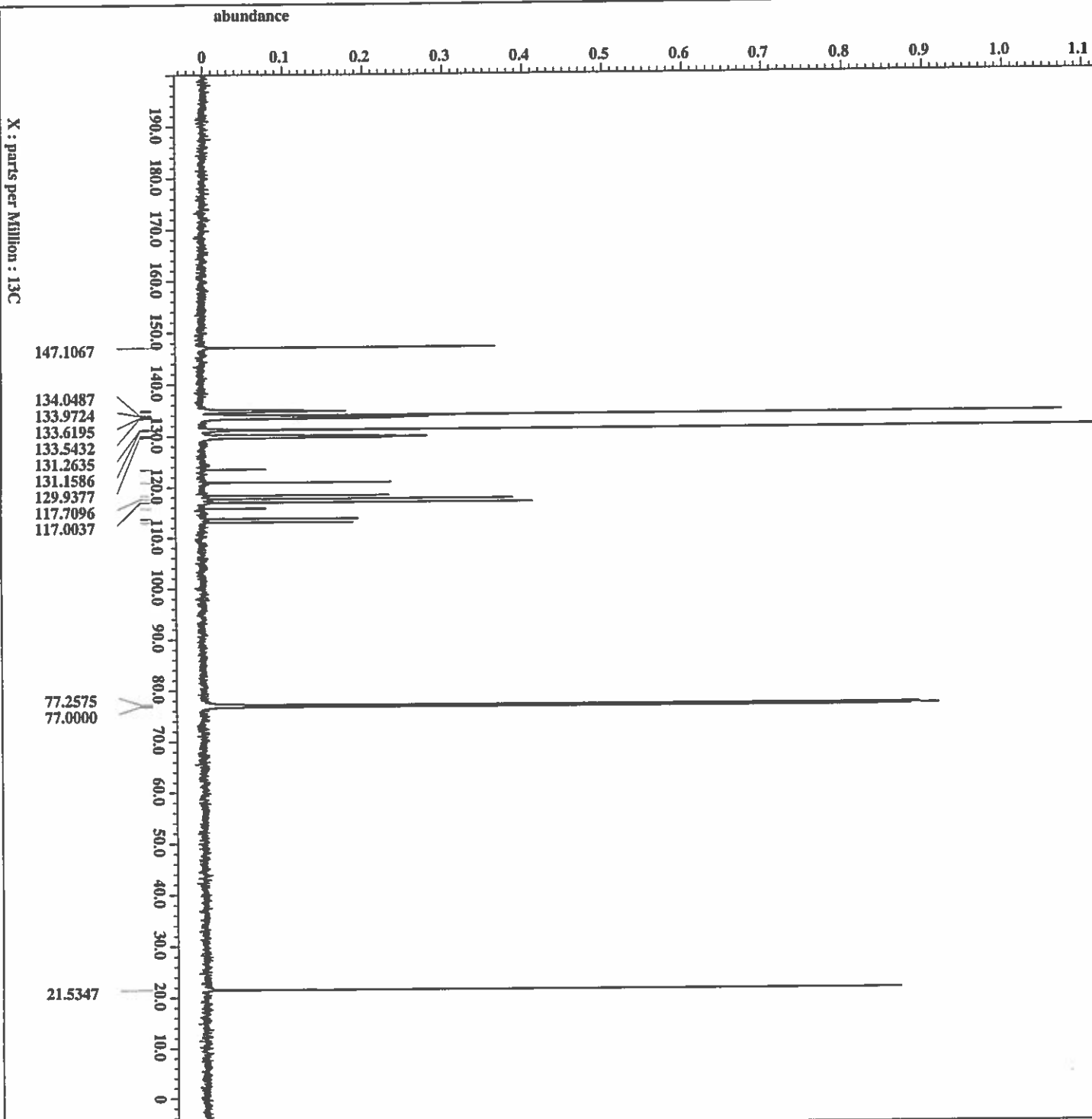
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3

X : parts per Million : 1H

7.5263
7.5103
7.4656
7.4622
7.4438
7.4370

144.03





```

Filename      = MS0468-200-96h_CARBON
Author        = Jim Davis
Experiment    = single-pulse-dec
Sample_id     = MS0468-200-96h
Solvent       = CHLOROFORM-D
ChangeX_sample = 17
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Revision_time  = 12-JUN-2018 16:02:13
Current_time   = 12-JUN-2018 16:02:14

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Dim_units     = [ppm]
Dimensions    = X
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Spectrometer  = JNM-KCA500

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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        = 1H
X_domain       = 1H
X_freq         = 39.3061761 [MHz]
X_offset       = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
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Mod_return     = 1
Scans          = 400
Total_scans    = 400

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
X_atn_dec      = 20.7 [dB]
X_atn_noe      = 20.7 [dB]
X_atn_noe      = TRUE
Decoupling     = 16s
Initial_wait   = 16s
Noe            = TRUE
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 22.6 [degC]
  
```

abundance

0 1.0 2.0 3.0 4.0

150.0 148.0 146.0 144.0 142.0 140.0 138.0 136.0 134.0 132.0 130.0 128.0 126.0 124.0 122.0 120.0 118.0 116.0 114.0 112.0 110.0 108.0

147.1067

134.0487
133.9724
133.8198
133.7339
133.6195
133.5432

131.2635
131.1586
130.0331
129.9377
129.8328
129.7374

123.4898

120.9335

118.3677

117.7096

117.0037

115.8114

113.7893

113.0644

X : parts per Million : 13C

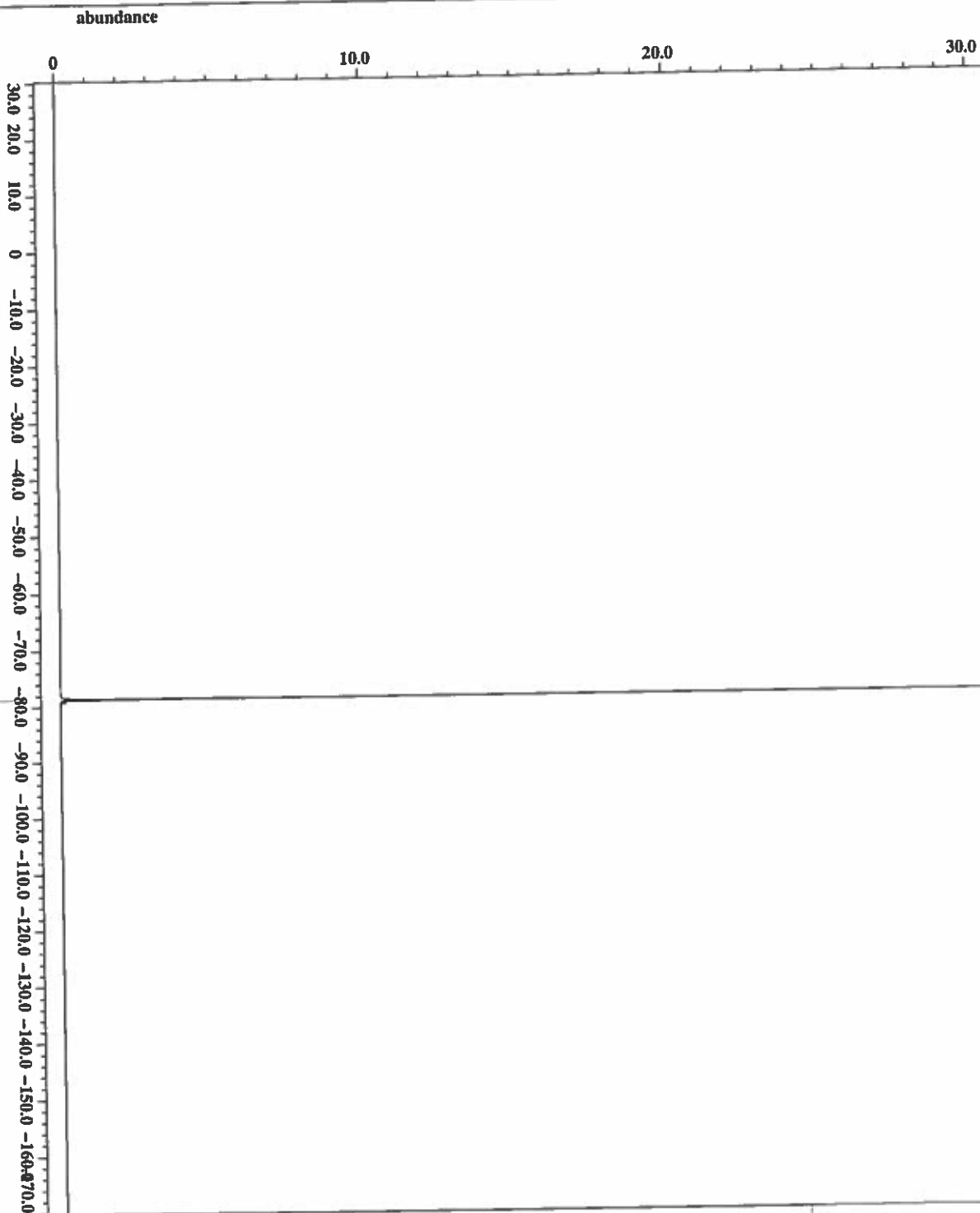


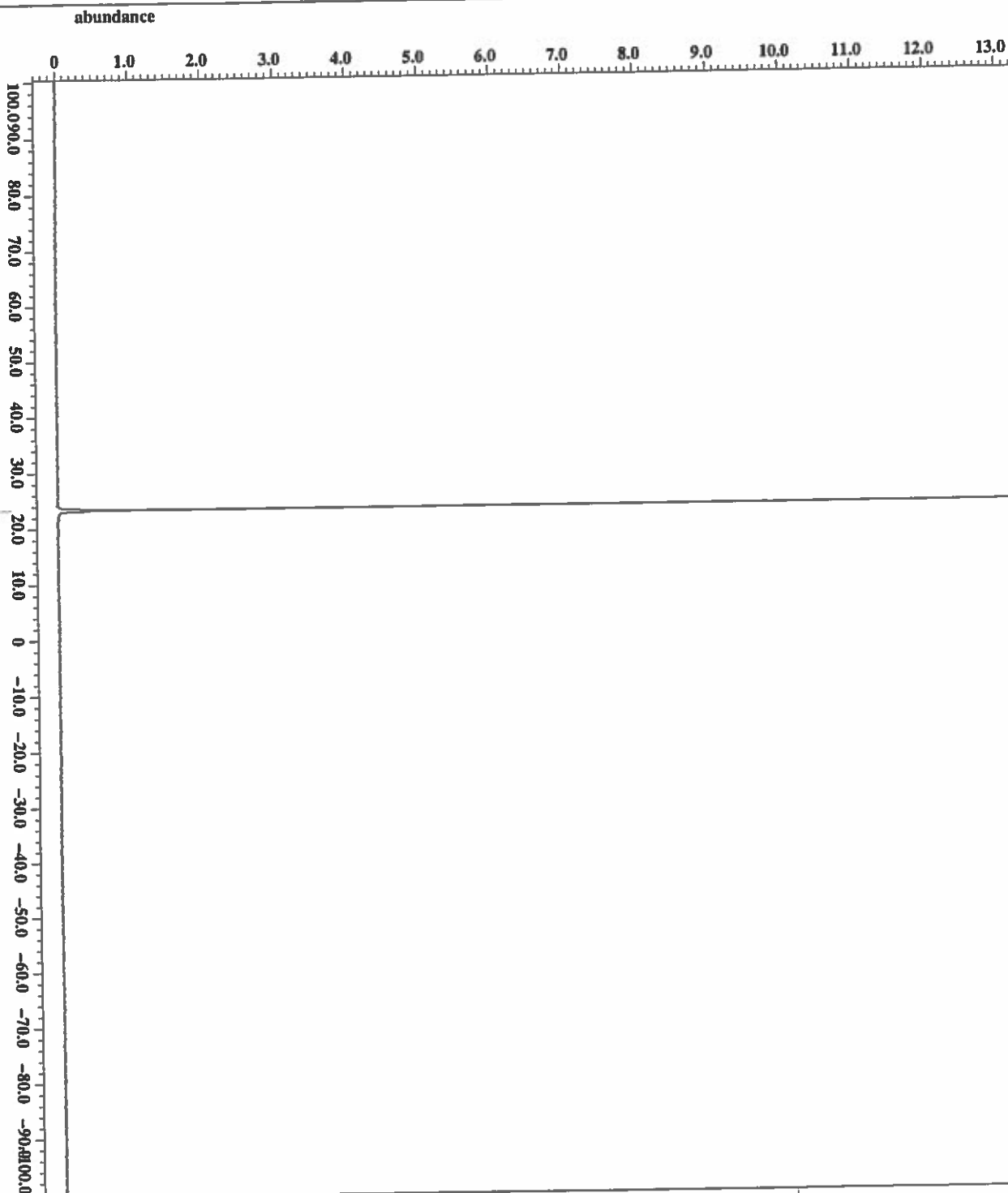
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 Author
 Jim Davis
 Experiment
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 Sample Id
 MS0468-200-96h
 Solvent
 CHLOROFORM-D
 Changer_sample
 17
 Creation_time
 12-JUN-2018 16:32:54
 Revision_time
 12-JUN-2018 16:05:26
 Current_time
 13-JUN-2018 16:05:26

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 Dim_file
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 Dim_units
 [ppm]
 Dimensions
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 Site
 ECA 500
 JNM-ECA500
 Spectrometer

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 X_domain
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 X_freq
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 X_offset
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 X_points
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 X_prescans
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 X_resolution
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 X_sweep
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 Irr_domain
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 Irr_freq
 470.62046084 [MHz]
 Irr_offset
 5 [ppm]
 Tr1_domain
 19F
 Tr1_freq
 470.62046084 [MHz]
 Tr1_offset
 5 [ppm]
 Cllpped
 FALSE
 Mod_return
 1
 Scans
 16
 Total_scans
 16

X_90_width
 13.1 [us]
 X_acq_time
 0.55574528 [s]
 X_angle
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 X_atn
 2.5 [dB]
 X_pulse
 6.55 [us]
 Irr_mode
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 Tr1_mode
 Off
 Dente_present
 FALSE
 Initial_wait
 1 [s]
 Recvr_gain
 34
 Relaxation_delay
 4 [s]
 Repetition_time
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 Temp_get
 22.3 [deg]





```

Filename      = MS0468-200-96h_PHOSPH
Author        = Jim Davis
Experiment    = single_pulse_dec
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Solvent       = CHLOROFORM-D
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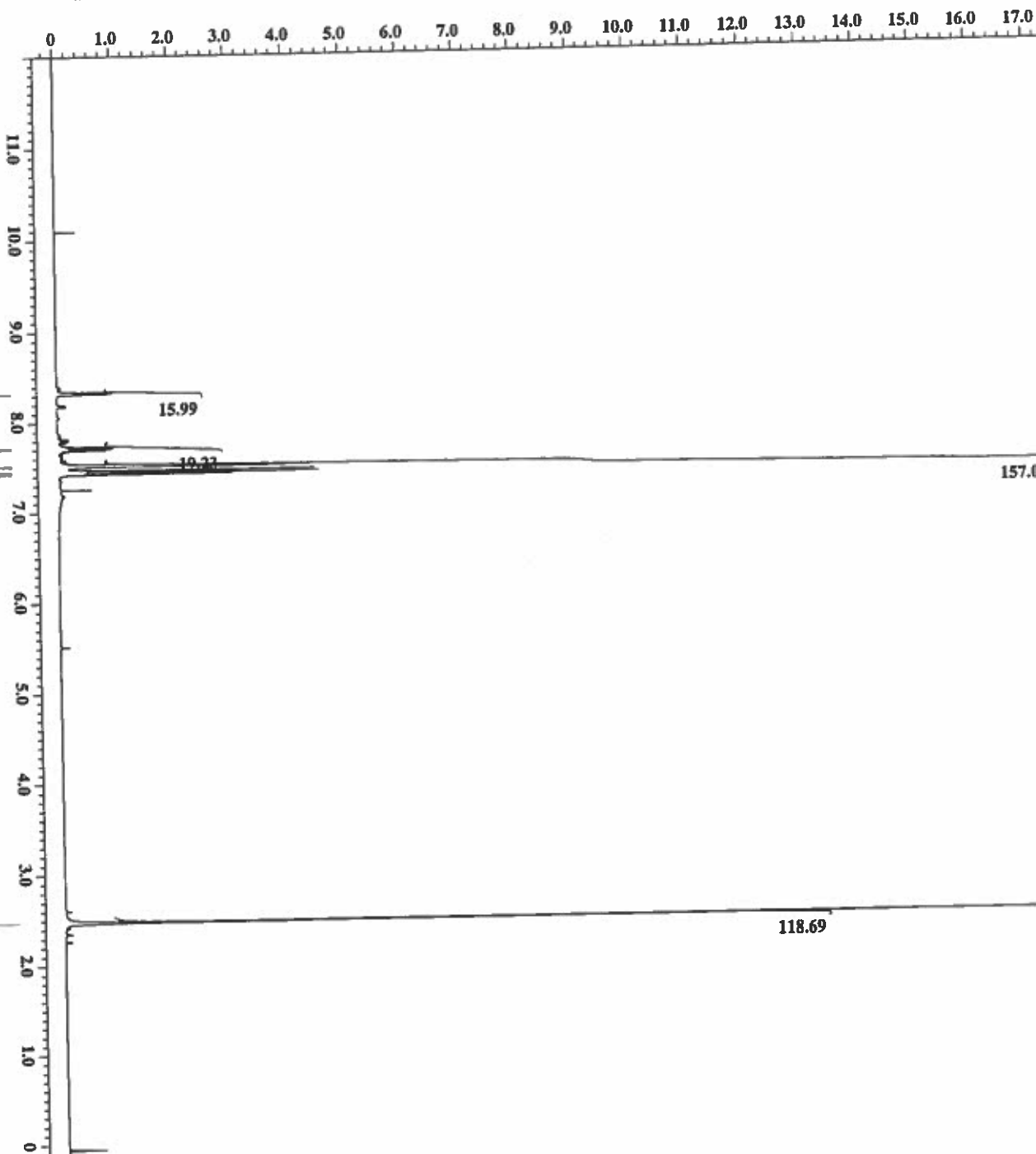
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X_offset       = 0 [ppm]
X_points       = 32768
X_prescans     = 4
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Xr_freq        = 500.15991521 [MHz]
Xr_offset      = 5.0 [ppm]
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Mod_return     = 1
Scans          = 50
Total_scans    = 50

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X_angle        = 30 [deg]
X_atn          = 5 [dB]
X_pulse        = 4.89566667 [us]
Xr_atn_dec     = 20.7 [dB]
Xr_atn_noe     = 20.7 [dB]
WALTZ          = TRUE
Decoupling     = TRUE
Inlet1_wait    = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Recvr_gain     = 56
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Temp_get       = 22.6 [degC]

```

abundance



X : parts per Million : 1H

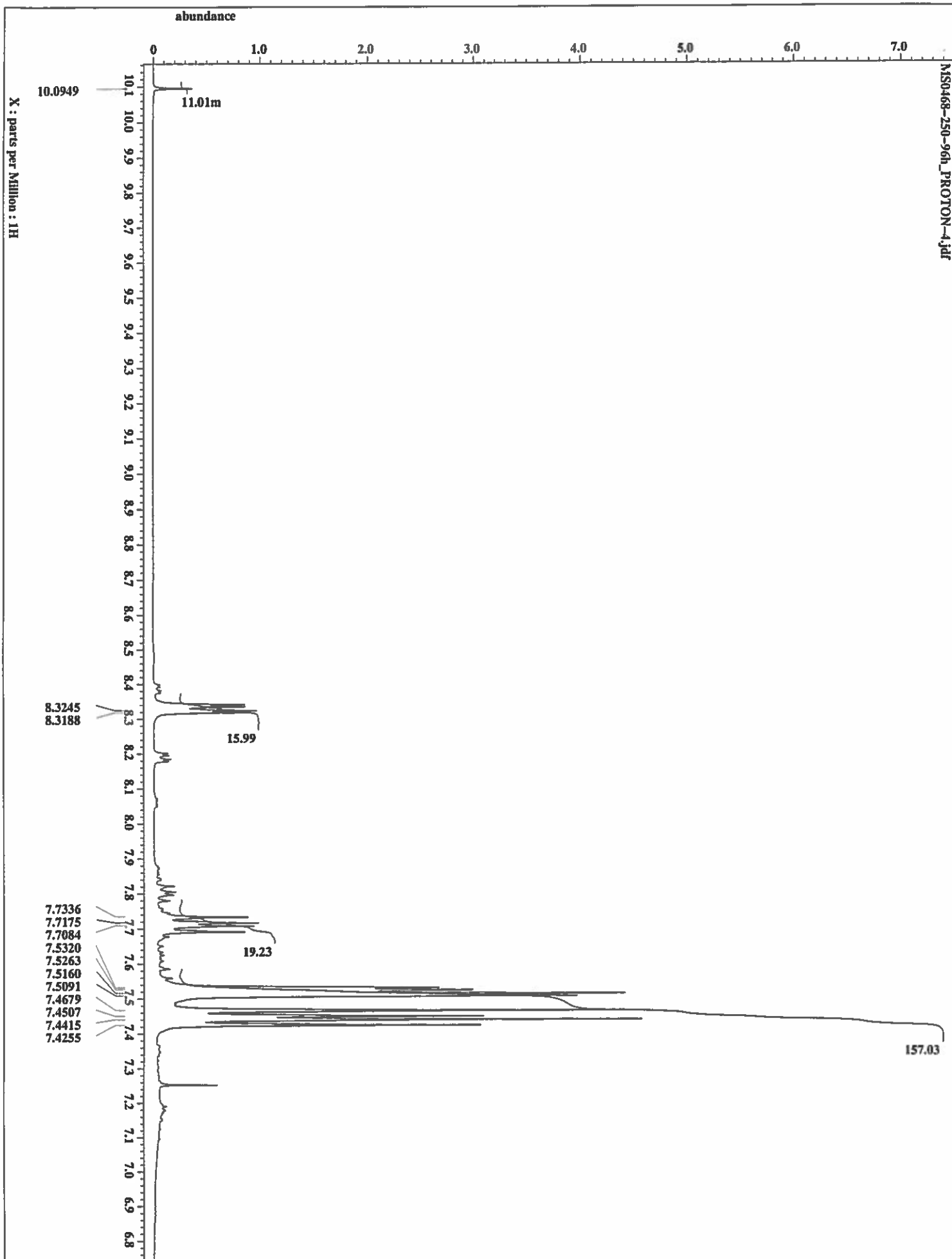


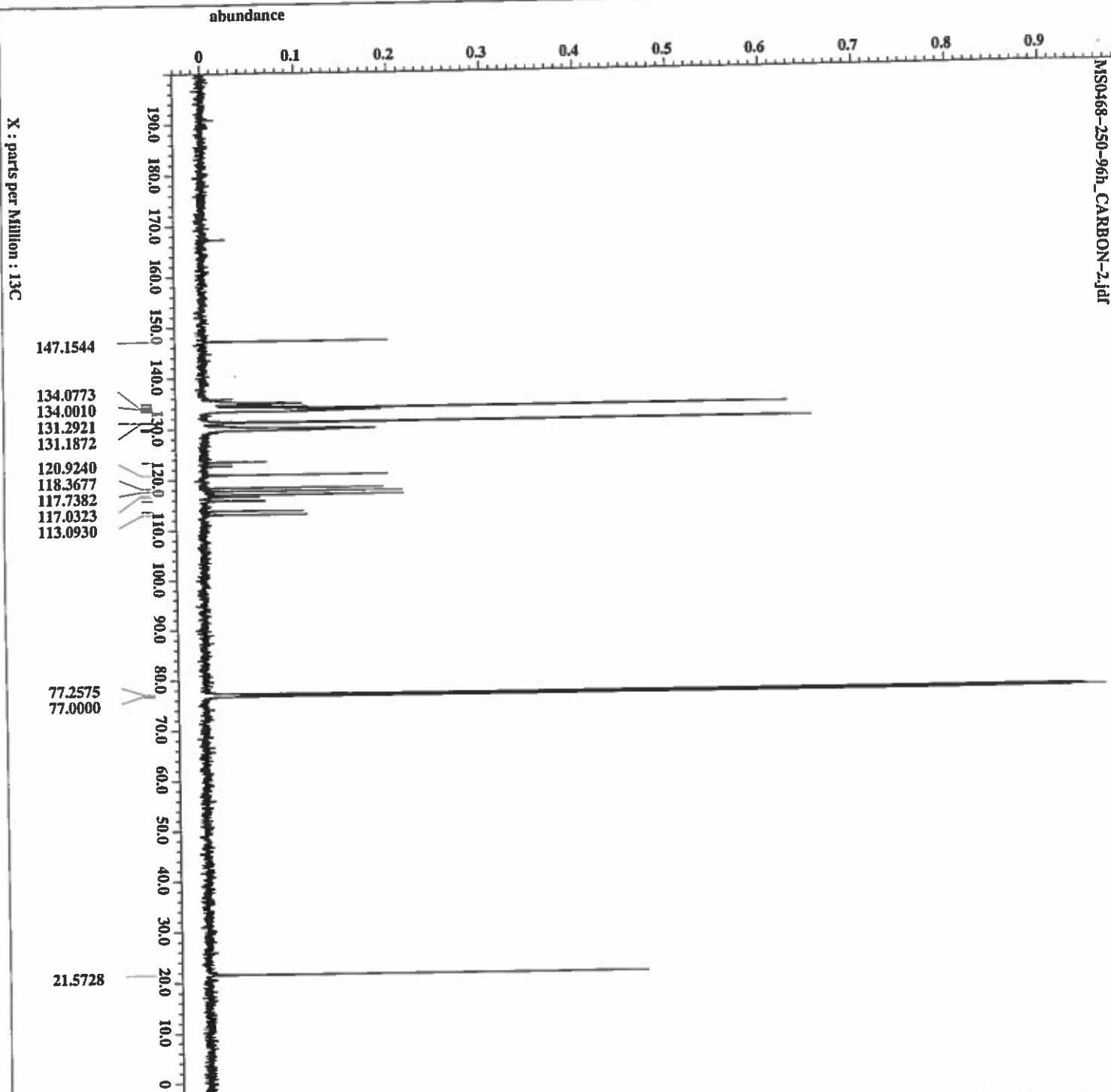
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Dimensions    = X
Site          = XCA 500
Spectrometer  = JNM-ECA500

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X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 9.38438438 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
T1_domain      = 1H
T1_freq        = 500.15991521 [MHz]
T1_offset      = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16
X_90_pulch     = 12.4 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [db]
X_pulse        = 6.2 [us]
Off            = OFF
T1_mode        = ORF
Dante_preset   = PALSZ
Initial_wait   = 1 [s]
Recvr_gain     = 36
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
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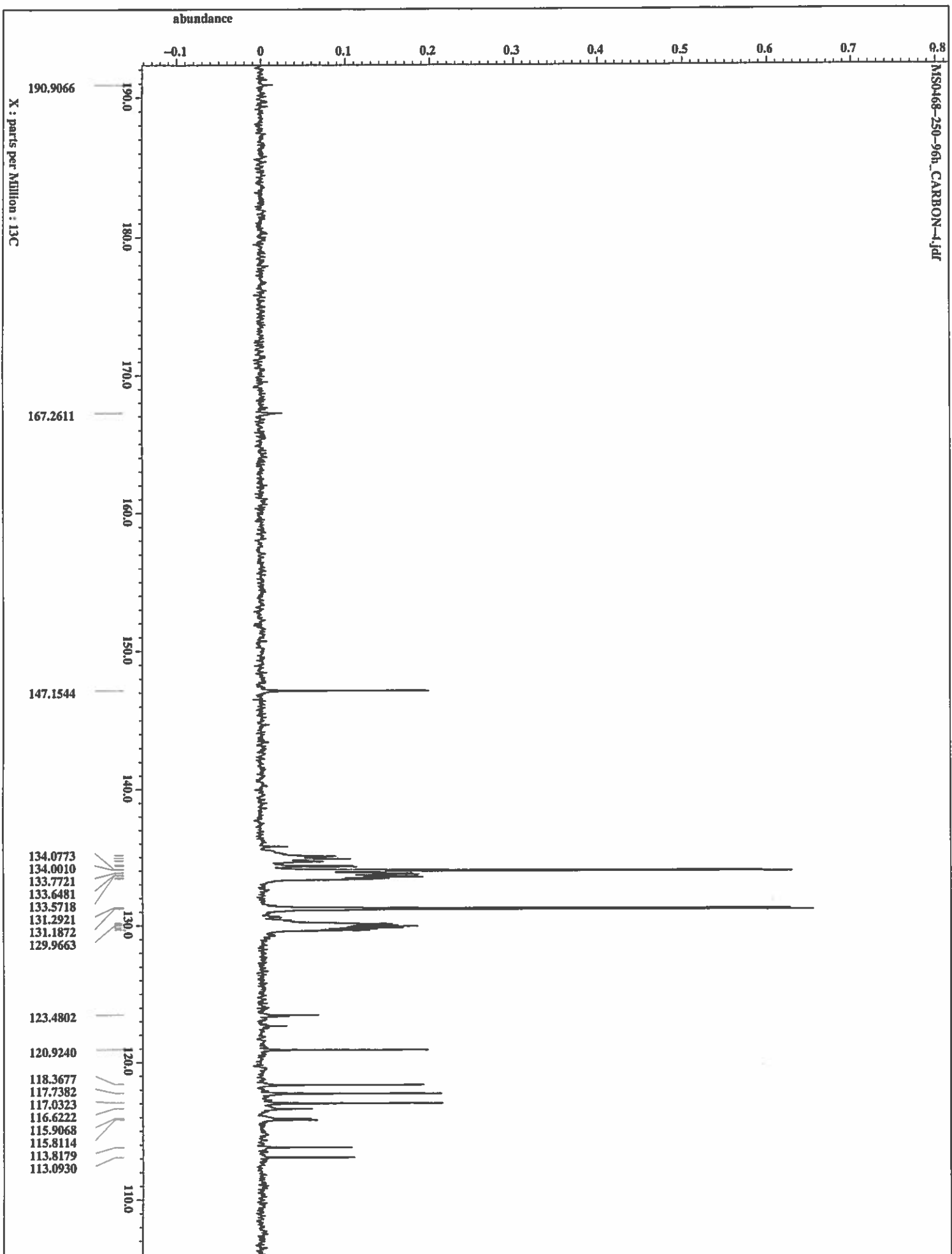
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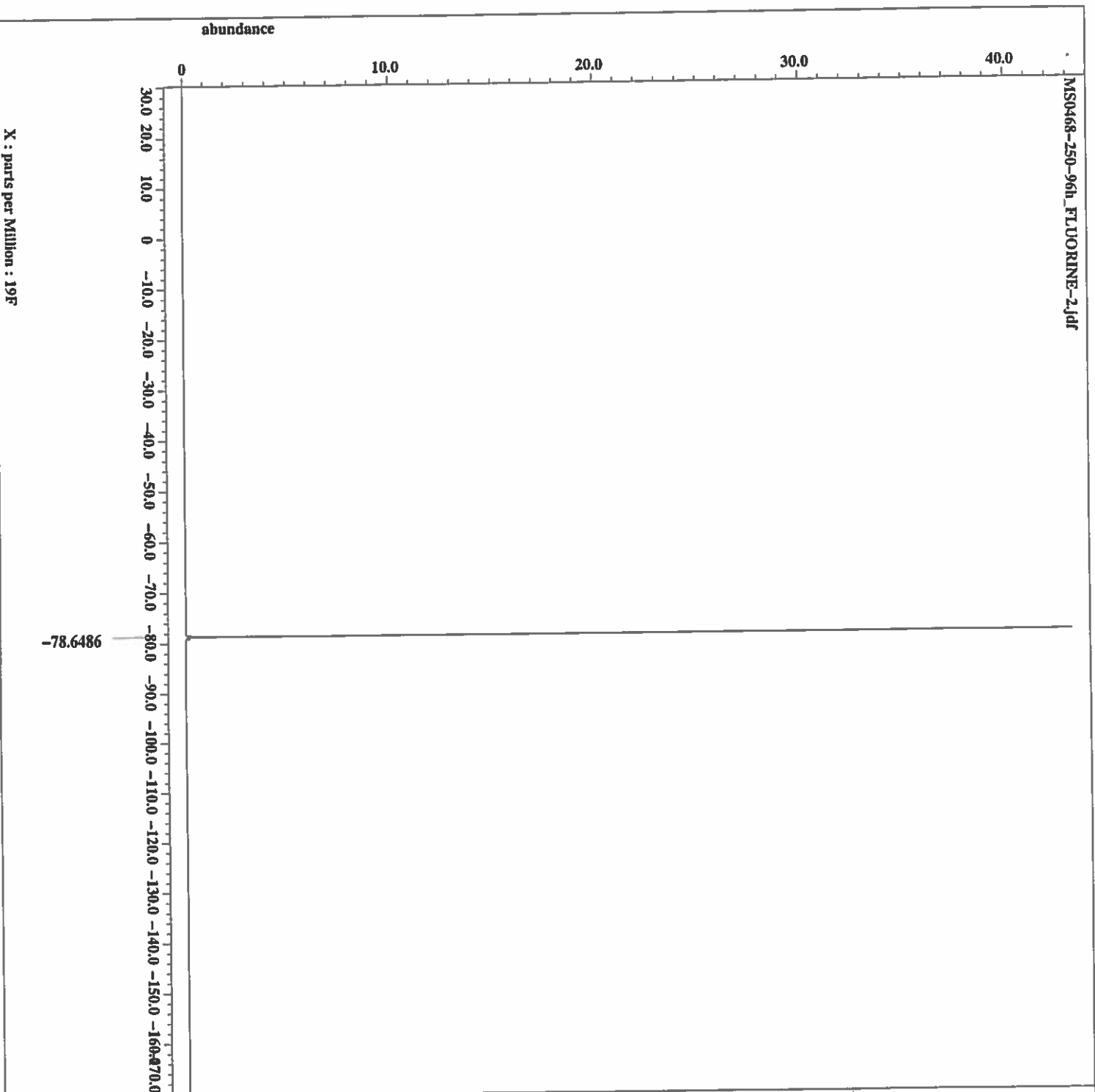
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Spectrometer

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X_offset       = 100 [ppm]
X_points       = 32768
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X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
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X_offset       = 5.0 [ppm]
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X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_doe    = 20.7 [dB]
Irr_noise      = WALTZ
Decoupling     = TRU2
Initial_wait   = 1 [s]
Noe            = TRU2
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 22.6 [dci]

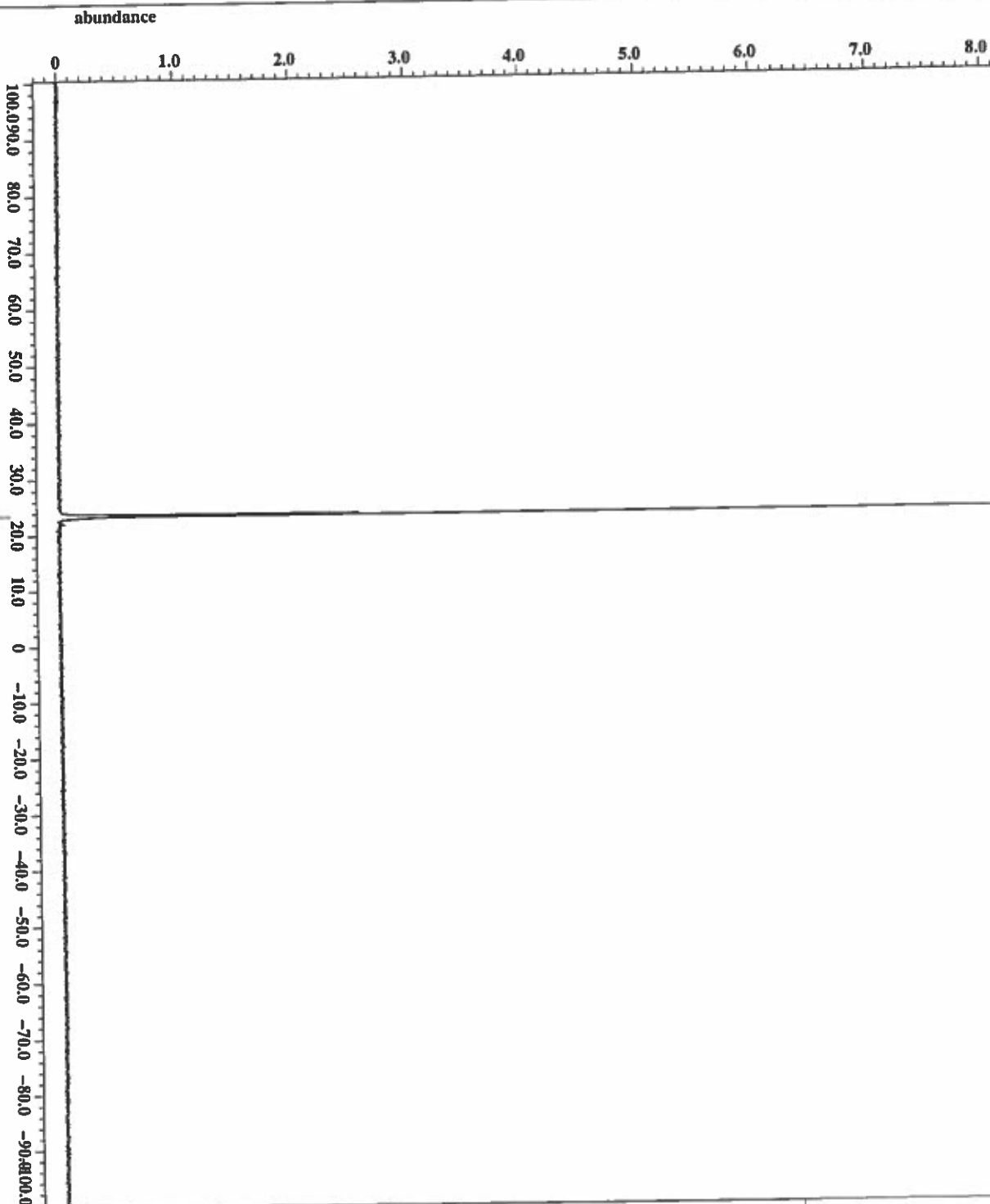
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MS0468 750 06b ET IIOPINE-2 14C

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experiment	=	single_pulse_ex2
sample_id	=	MS0668-250-96h
solvent	=	CHLOROFORM-D
Charger_sample	=	18
creation_time	=	12-JUN-2018 17:08:39
revision_time	=	12-JUN-2018 16:42:10
Current_time	=	12-JUN-2018 16:42:11
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Dim_size	=	52428
Dim_circle	=	19°
Dim_wlts	=	[ppm]
Dimensions	=	X
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Spectrometer	=	JNM-ECX500
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X_domain	=	19°
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X_offset	=	-70 [ppm]
X_pulses	=	65536
X_prescans	=	1
X_resolution	=	1.7933855 [Hz]
X_sweep	=	117.9245285 [kHz]
irr_domain	=	19°
irr_freq	=	470.62046084 [MHz]
irr_offset	=	5 [ppm]
irr_domain	=	19°
irr_freq	=	470.62046084 [MHz]
irr_offset	=	5 [ppm]
clipped	=	PALSI
Mod_return	=	1
Scans	=	16
Total_scans	=	16
X_90_width	=	13.1 [us]
X_acq_time	=	0.55574528 [s]
X_angle	=	45 [deg]
X_atn	=	2.5 [dB]
X_pulse	=	6.55 [us]
irr_mode	=	OFF
irr_mode	=	OFF
Dante_present	=	PALSI
Initial_walt	=	1 [s]
Recvr_gain	=	36
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Repetition_time	=	22.3 [s]
Temp_get	=	



X : parts per Million : 31P



```

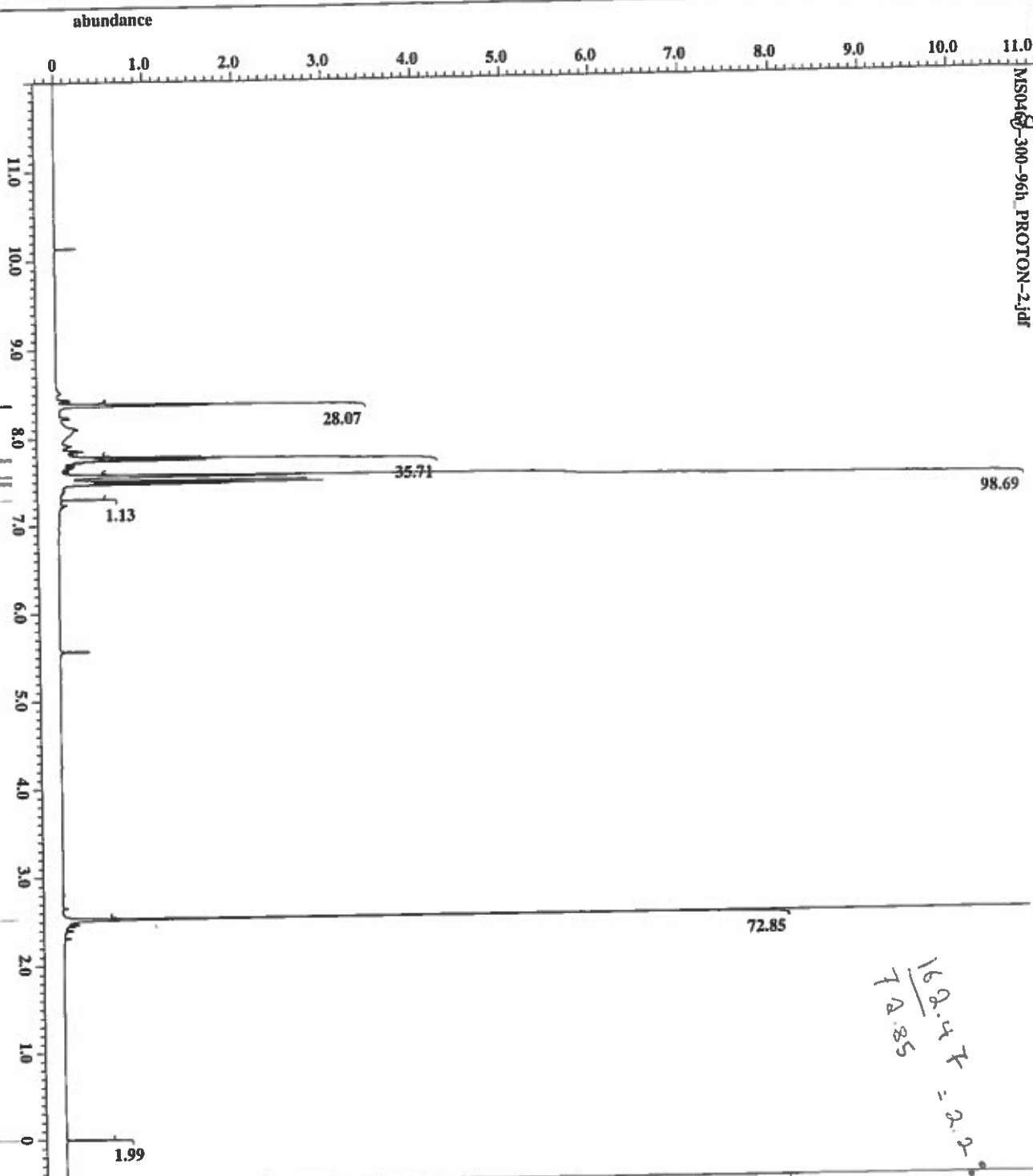
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Dim_units     = [ppm]
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Spectrometer  = JNM-ECA500

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X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.55068995 [Hz]
X_sweep        = 50.01300813 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 50
Total_scans    = 50

X_90_width     = 14.687 [us]
X_acq_time     = 0.64487424 [s]
X_angle        = 30 [deg]
X_atn          = 5 [dB]
Irr_atn_dec    = 4.89566667 [us]
Irr_atn_noe    = 20.7 [dB]
WALTZ          = WALTZ
Decoupling     = 1 [s]
Inlet1_wait    = 2 [s]
Noe_time       = 58
Recvr_gain     = 2 [s]
Relaxation_delay = 2.64487424 [s]
Repetition_time = 22.6 [dc]
Temp_get       = 22.6 [dc]

```



99.7
35.7
28.1
16.2
16.2

X : parts per Million : 1H

2400/6.25
molar
converted

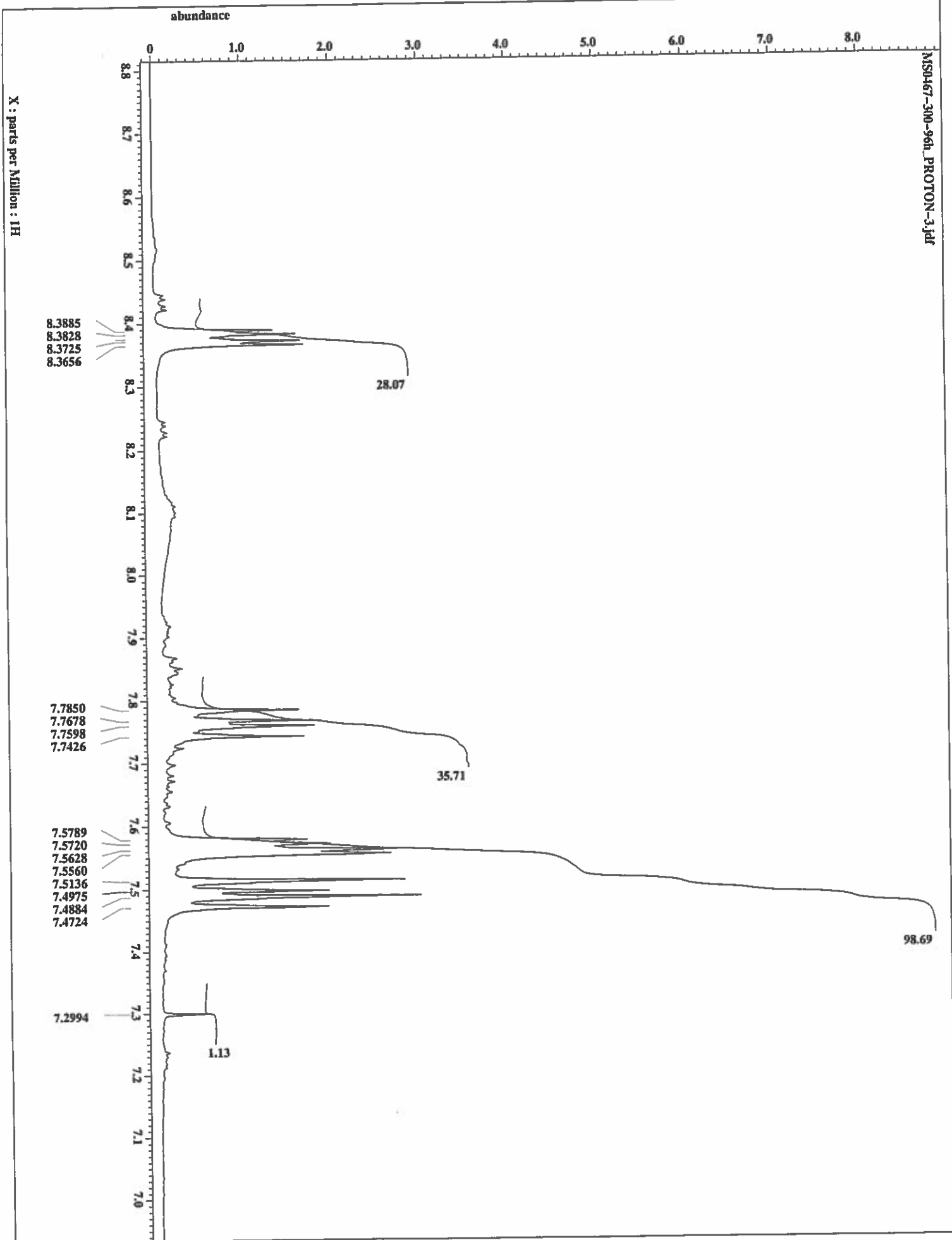
16.2.4 x = 2.2.1
7.2.85



SOUTH ALABAMA
JAGUARS

Filename
MS0467-300-96h_PROTON
Author
Jim Davis
Experiment
single_pulse.ex2
Sample_id
MS0467-300-96h
Solvent
CHLOROFORM-D
Charger_sample
7
Creation_time
12-JUN-2018 12:28:49
Revision_time
12-JUN-2018 12:02:22
Current_time
12-JUN-2018 12:02:22
Data_format
1D COMPLEX
Dim_size
13107
Dim_title
1H
Dim_units
[ppm]
Dimensions
X
SICA 500
SICA 500
Spectrometer
JNM-ECA500
Field_strength
11.7473579 [T] (500 [MH
X_acq_duration
1.74587904 [s]
X_domain
1H
X_freq
500.15391521 [MHz]
X_offset
5.0 [ppm]
X_points
16384
X_prescan
1
X_resolution
0.57277737 [Hz]
X_sweep
9.38438438 [kHz]
Xir_domain
1H
Xir_freq
500.15391521 [MHz]
Xir_offset
5.0 [ppm]
Xir_domain
1H
Xir_freq
500.15391521 [MHz]
Xir_offset
5.0 [ppm]
Clipped
FALSE
Mod_return
1
Scans
16
Total_scans
16
X_90_width
12.4 [us]
X_acq_time
1.74587904 [s]
X_angle
45 [deg]
X_atn
4 [dB]
X_pulse
6.2 [us]
Xir_mode
off
Xir_mode
off
Dente_presat
FALSE
Initial_wait
1 [s]
Recvr_gain
36
Relaxation_delay
4 [s]
Repetition_delay
5.74587904 [s]
Temp_get
21.7 [deg]

1 - received on 1 for unshared parameters

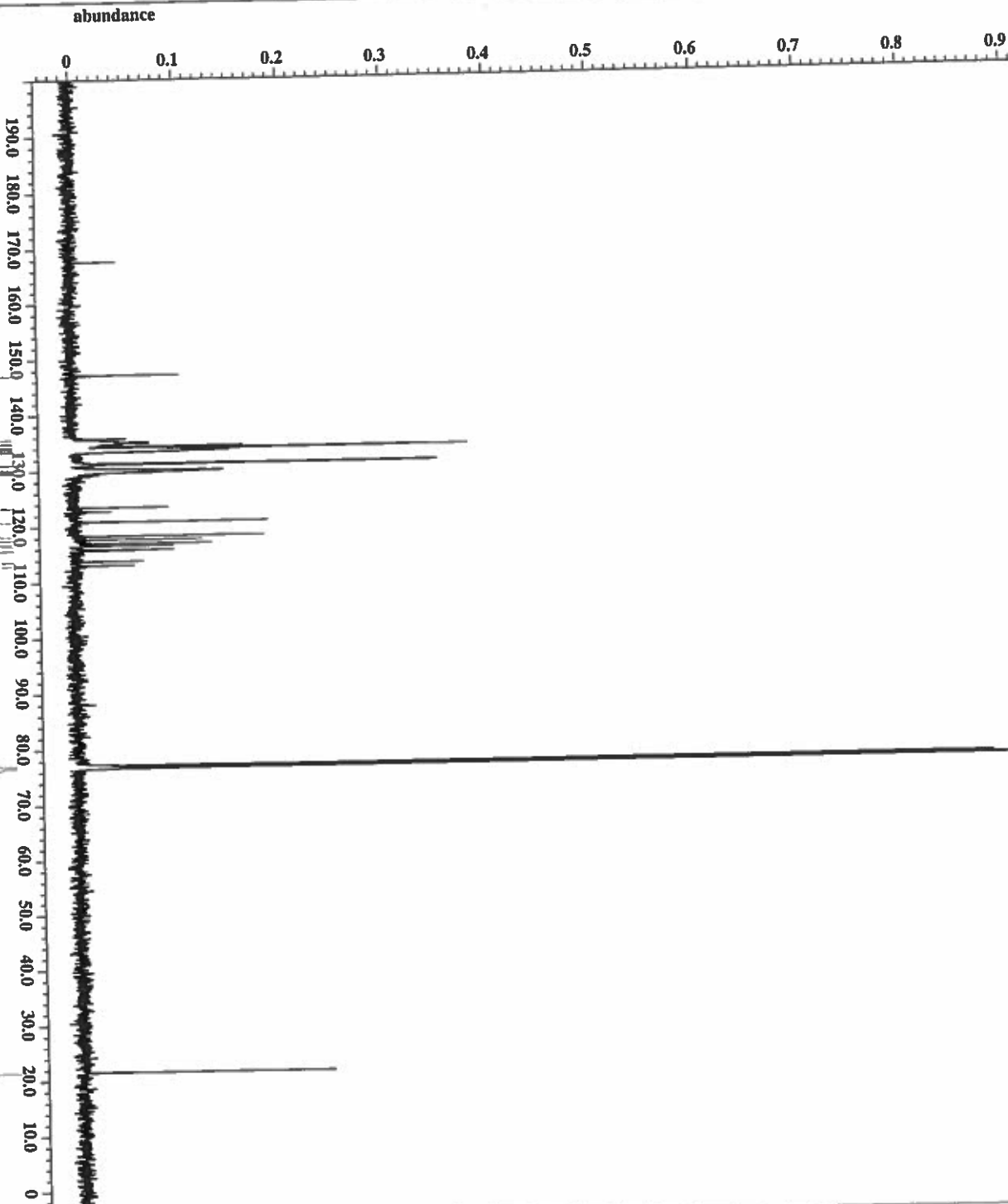


X : parts per Million : 13C

147.1639
134.0869
134.0010
131.3017
131.1872
120.8858
118.3296
117.7382
117.0228
115.9068

77.0000
76.7425

21.5823



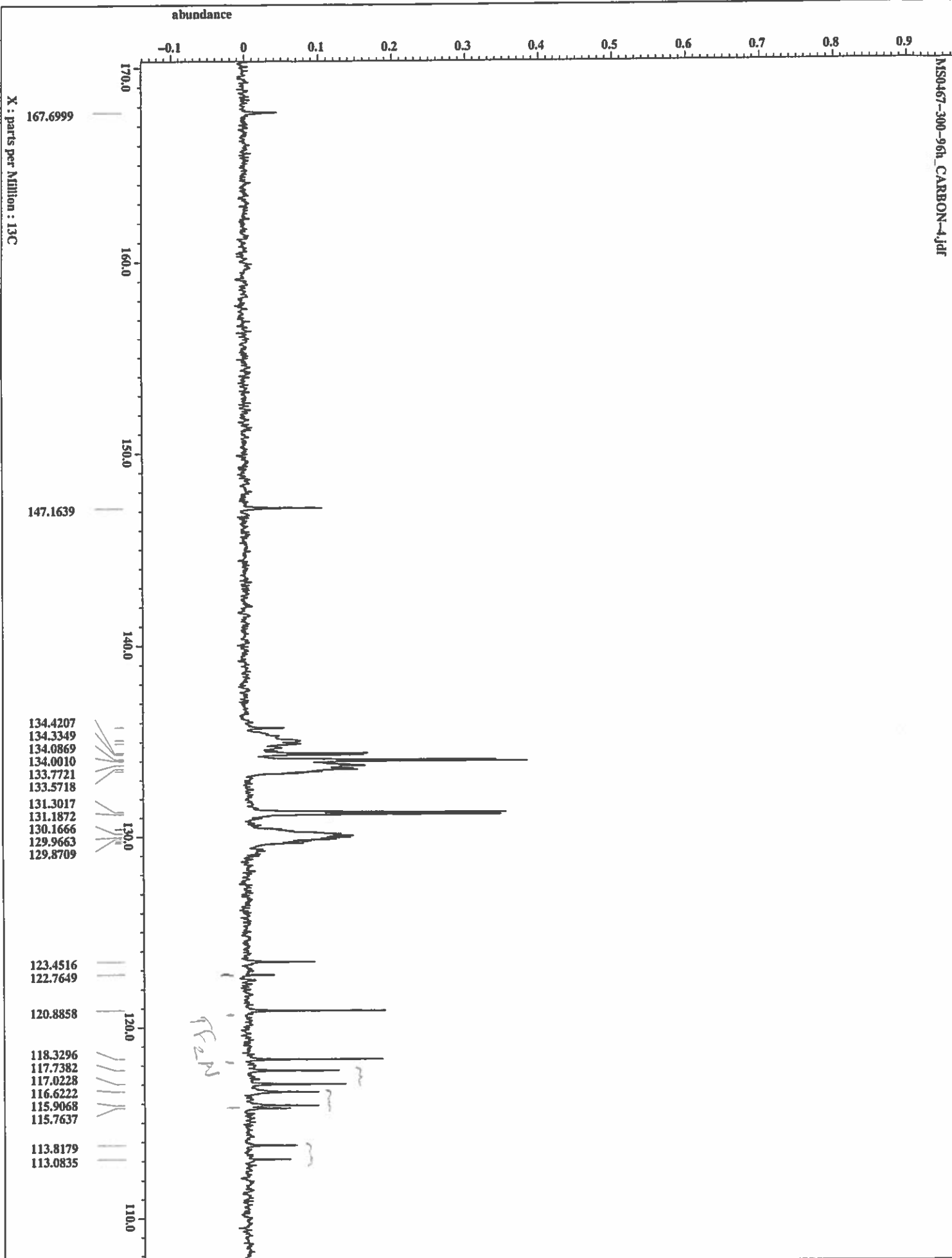
Filename = MS0467-300-96h CARBON
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = MS0467-300-96h
 Solvent = CHLOROFORM-D
 Changer_sample = 7
 Creation_time = 12-JUN-2018 12:44:00
 Revision_time = 12-JUN-2018 12:17:33
 Current_time = 12-JUN-2018 12:17:33

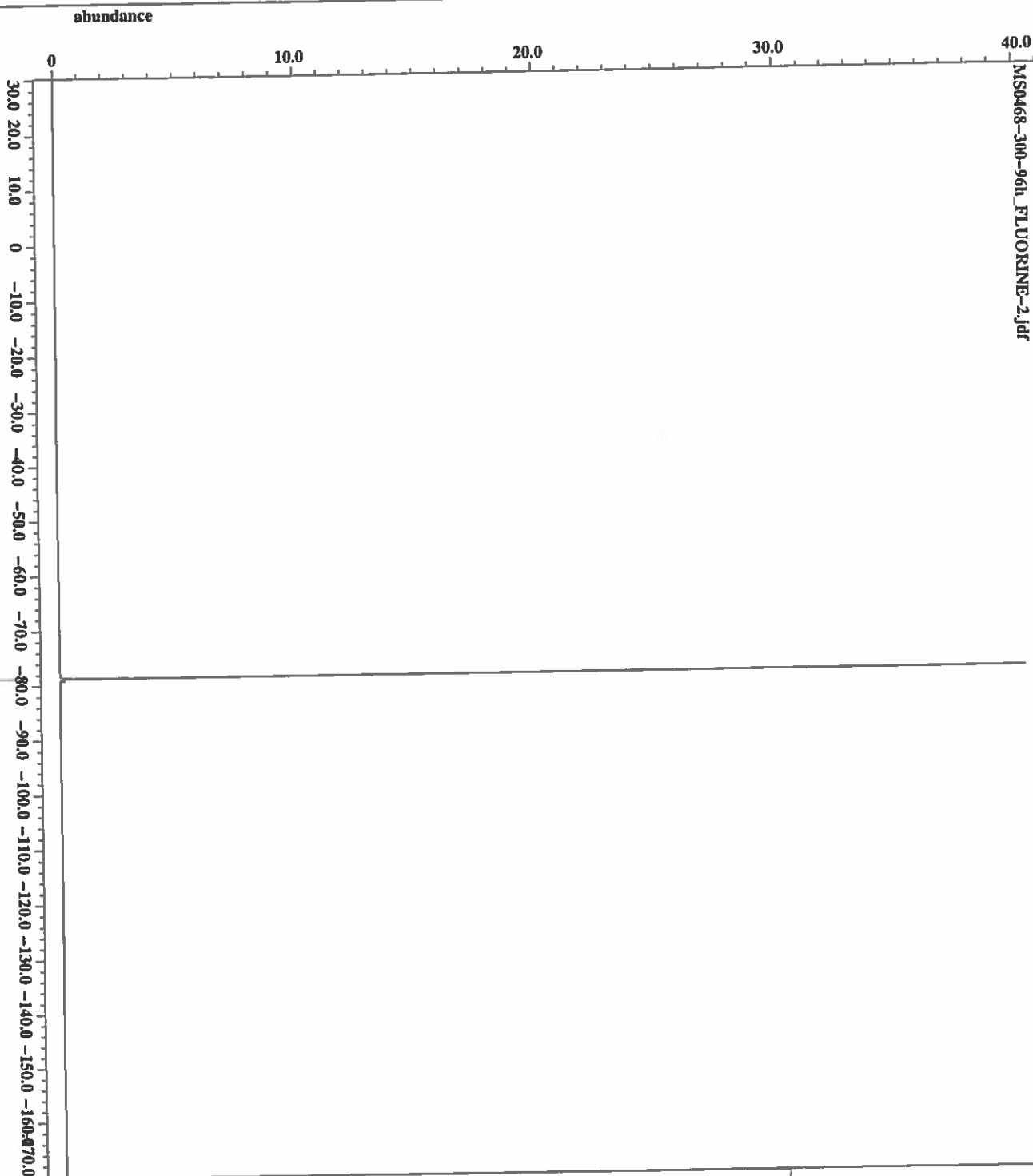
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_file = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

 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 = FALSTZ
 Mod_return = 1
 Scans = 256
 Total_scans = 256

 X_90_width = 13.2 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 6 [dB]
 X_pulse = 4.4 [us]
 Irr_atn_dec = 20.7 [dB]
 Irr_atn_psc = 20.7 [dB]
 Irr_noise = WALVZ
 Decoupling = TRUZ
 Initial_wait = 1 [s]
 Recv_time = TRUZ
 Recv_gain = 2 [s]
 Relaxation_delay = 2 [s]
 Repetition_time = 2.83361792 [s]
 Temp_get = 22.3 [deg]







X : parts per Million : 19F



SOUTH ALABAMA
JAGUARS

```

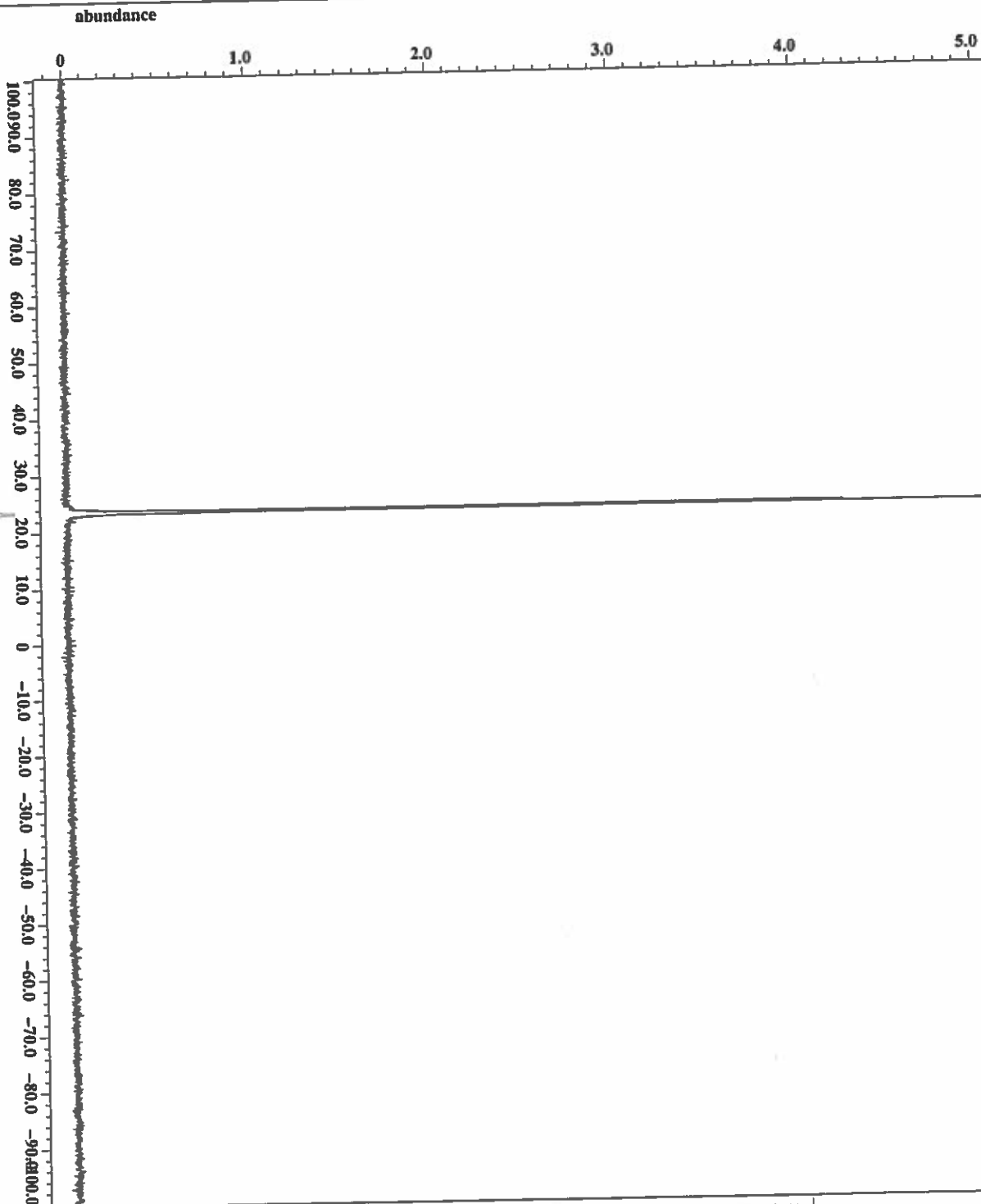
=====
Filename      = MS0468-300-96h_1D001
Author        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0468-300-96h
Solvent       = CHLOROFORM-D
Charger_sample = 7
Creation_time  = 12-JUN-2018 12:47:07
Revision_time  = 12-JUN-2018 12:20:40
Current_time   = 12-JUN-2018 12:20:41

=====
Data_format   = 1D COMPLEX
Dim_size      = 52428
Dim_unit      = 19F
Dim_title     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

=====
Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.55574528 [s]
X_domain       = 19F
X_freq         = 470.62046084 [MHz]
X_offset       = -70 [ppm]
X_points       = 65536
X_prescans     = 1
X_resolution   = 1.7993855 [Hz]
X_sweep        = 117.9245283 [MHz]
Irr_domain     = 19F
Irr_freq       = 470.62046084 [MHz]
Irr_offset     = 5 [ppm]
Irr_domain     = 19F
T1_domain      = 470.62046084 [MHz]
T1_freq        = 5 [ppm]
T1_offset      = 5 [ppm]
T1_offset      = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

=====
X_90_width     = 13.1 [us]
X_acq_time     = 0.55574528 [s]
X_angle        = 45 [deg]
X_atn          = 2.5 [dB]
X_pulse        = 6.55 [us]
Irr_mode       = Off
T1_mode        = Off
Pulse_program  = FALST
Initial_wait   = 1 [s]
Recvr_gain     = 36
Relaxation_delay = 4 [s]
Repetition_time = 4.55574528 [s]
Temp_get       = 22 [dc]
=====

```



X : parts per Million : 31P



```

Filename      = MS0468-300-96h_PHOSPH
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0468-300-96h
Solvent       = CHLOROFORM-D
Charger_sample = 7
Creation_time  = 12-JUN-2018 12:50:45
Revision_time  = 12-JUN-2018 12:24:17
Current_time   = 12-JUN-2018 12:24:17

Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 31P
Dim_units     = [ppm]
Dimensions    = X
Sfrc          = ECA 500
Sfrc          = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.64487424 [s]
X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution    = 1.55068995 [Hz]
X_sweep        = 50.81300813 [kHz]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 25
Total_scans    = 25

X_90_width     = 14.687 [us]
X_acq_time     = 0.64487424 [s]
X_angle        = 30 [deg]
X_atn          = 5 [dB]
X_pulse        = 4.8956667 [us]
X_atn_dec      = 20.7 [dB]
X_atn_pwr      = 20.7 [dB]
X_atn_pwr      = VAL/TZ
Decoupling     = TRUEZ
Initial_wait    = 1 [s]
Moe            = TRUEZ
Moe_time       = 2 [s]
Moe_time       = 58
Recv_gain      = 21 [s]
Relaxation_delay = 2.64487424 [s]
Repetition_time = 22.2 [s]
Temp_set       = 22.2 [dC]

```

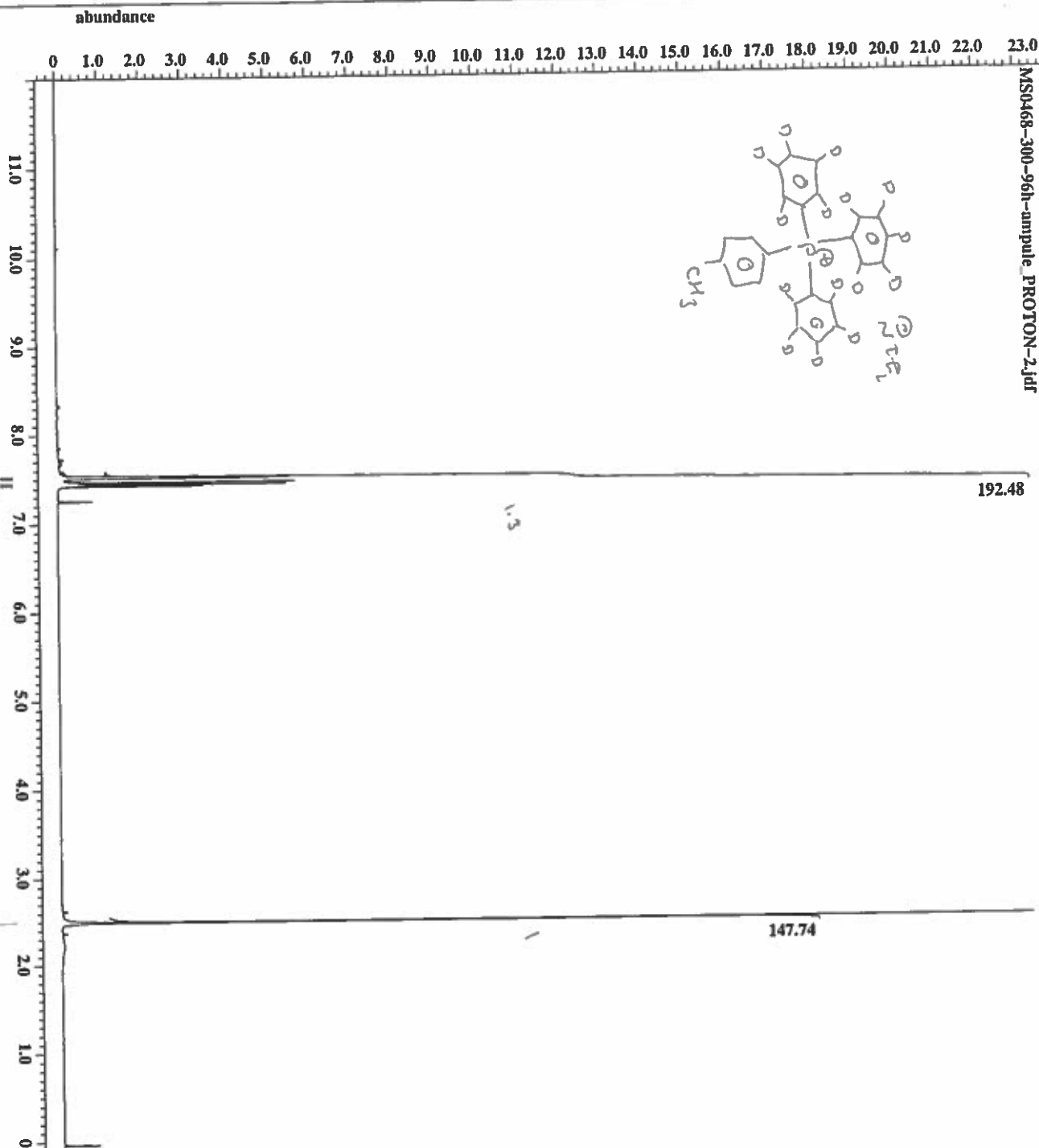
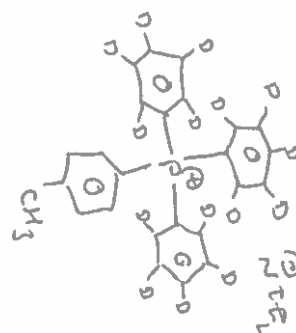
abundance

0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0

42.0 41.0 40.0 39.0 38.0 37.0 36.0 35.0 34.0 33.0 32.0 31.0 30.0 29.0 28.0 27.0 26.0 25.0 24.0 23.0 22.0 21.0 20.0 19.0 18.0 17.0 16.0 15.0 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

23.7274
23.4057

X : parts per Million : 31P



X : parts per Million : 1H

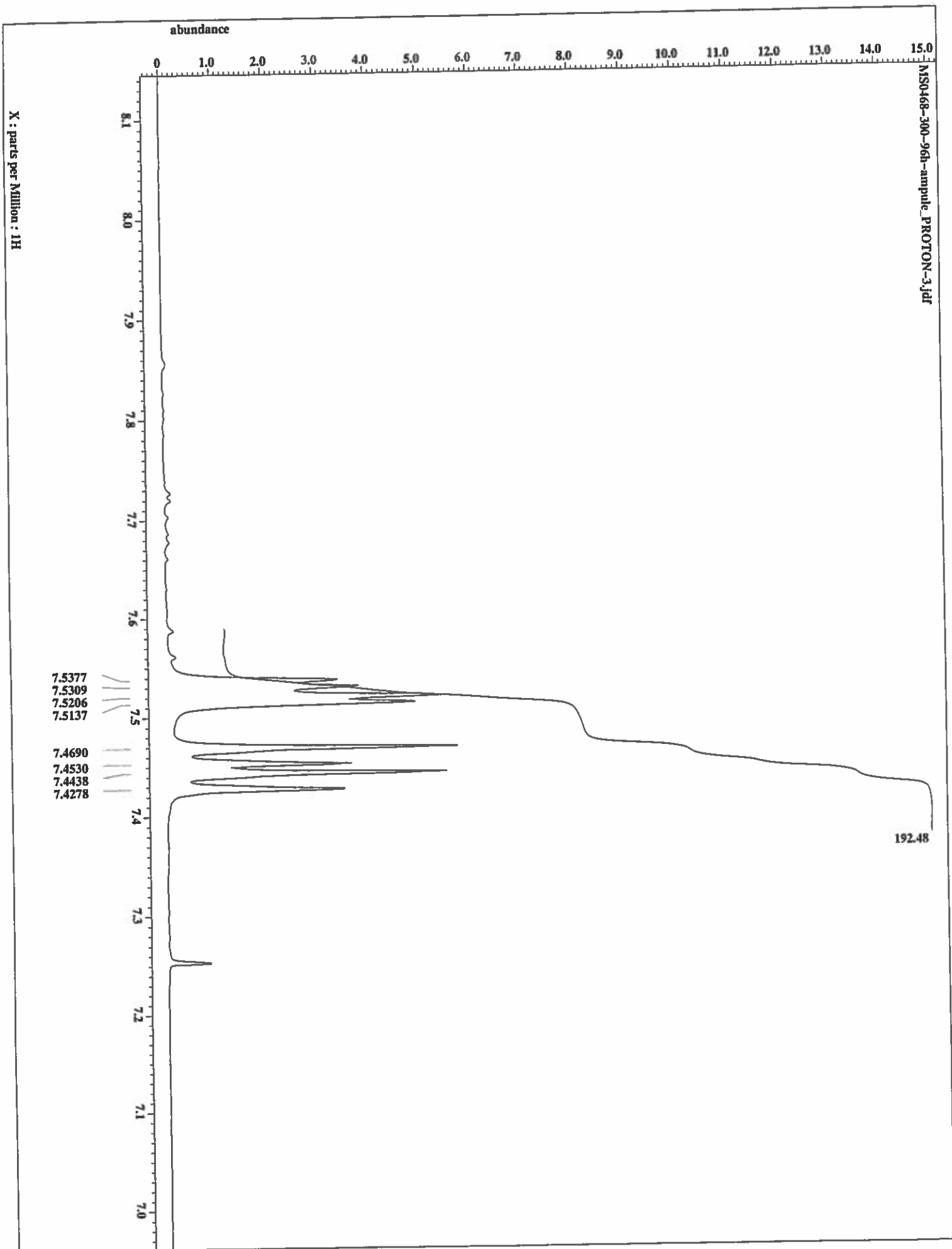


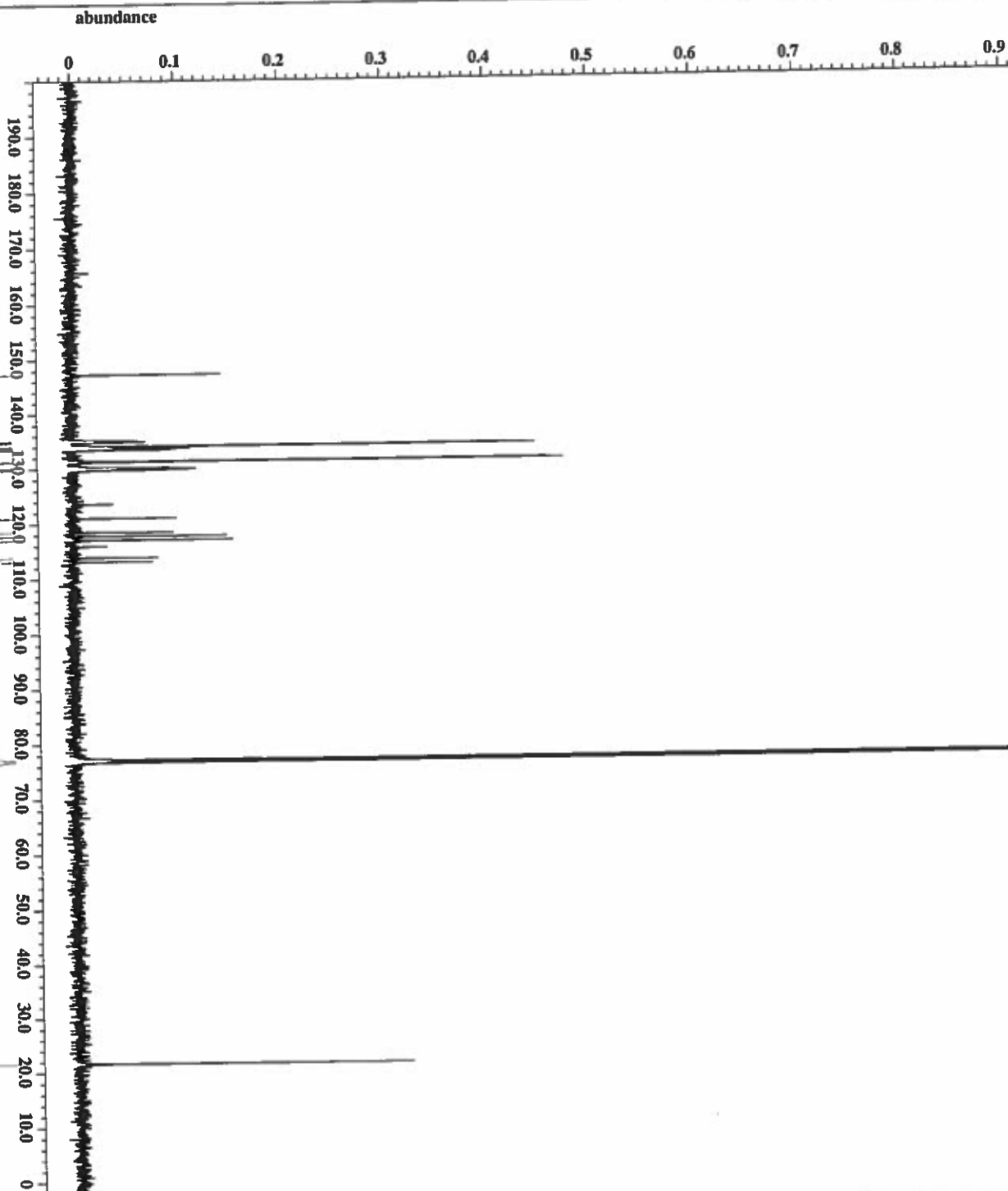
```

File Name      MS0468-300-96h-ampule
Author         Jim Davis
Experiment     single_pulse.ex2
Sample ID      MS0468-300-96h-ampule
Solvent        CHLOROFORM-D
Change Sample  9
Creation Time   25-JUN-2018 10:40:03
Revision Time   25-JUN-2018 10:17:21
Current Time    25-JUN-2018 10:17:21

Data Format     1D COMPLEX
Dir Size       13107
Dir Title      1H
Dir Units      [ppm]
Dimensions     X
Site           ECA 500
Spectrometer   JNM-ECA500

Field Strength 11.7473579 [T] (500 [MH
X_acq_duration 1.74587904 [s]
X_domain       1H
X_freq         500.15991521 [MHz]
X_offset       5.0 [ppm]
X_points       16384
X_prescans     1
X_resolution   0.5727737 [Hz]
X_sweep        9.38438438 [kHz]
Xr_domain      1H
Xr_freq        500.15991521 [MHz]
Xr_offset      5.0 [ppm]
Xr1_domain     1H
Xr1_freq       500.15991521 [MHz]
Xr1_offset     5.0 [ppm]
Clipped        FALSE
Mod_return     1
Scans          16
Total_scans    16
X_90_width     12.4 [us]
X_acq_time     1.74587904 [s]
X_angle        45 [deg]
X_atn          4 [dB]
X_pulse        6.2 [us]
Xr1_mode       ORF
Xr1_offset     ORF
Dante_preset   FALSTZ
Initfil_wait   1 [s]
Recvr_gain     40
Relaxation_delay 4 [s]
Repetition_time 5.74587904 [s]
Temp_set       21.8 [C]
  
```





X : parts per Million : 13C

147.2879

134.1823
134.0964
131.3971
131.2921
121.0480
118.4917
117.8336
117.1182
113.9133

77.2575
76.7520

21.6968

```

=====
Filename      = MS0468-300-96h-ampule
Author        = Jim Davis
Experiment     = single_pulse_dec
Sample_id     = MS0468-300-96h-ampule
Solvent       = CHLOROFORM-D
Charger_sample = 9
Creation_time  = 25-JUN-2018 10:54:25
Revision_time = 25-JUN-2018 10:51:43
Current_time   = 25-JUN-2018 10:31:43

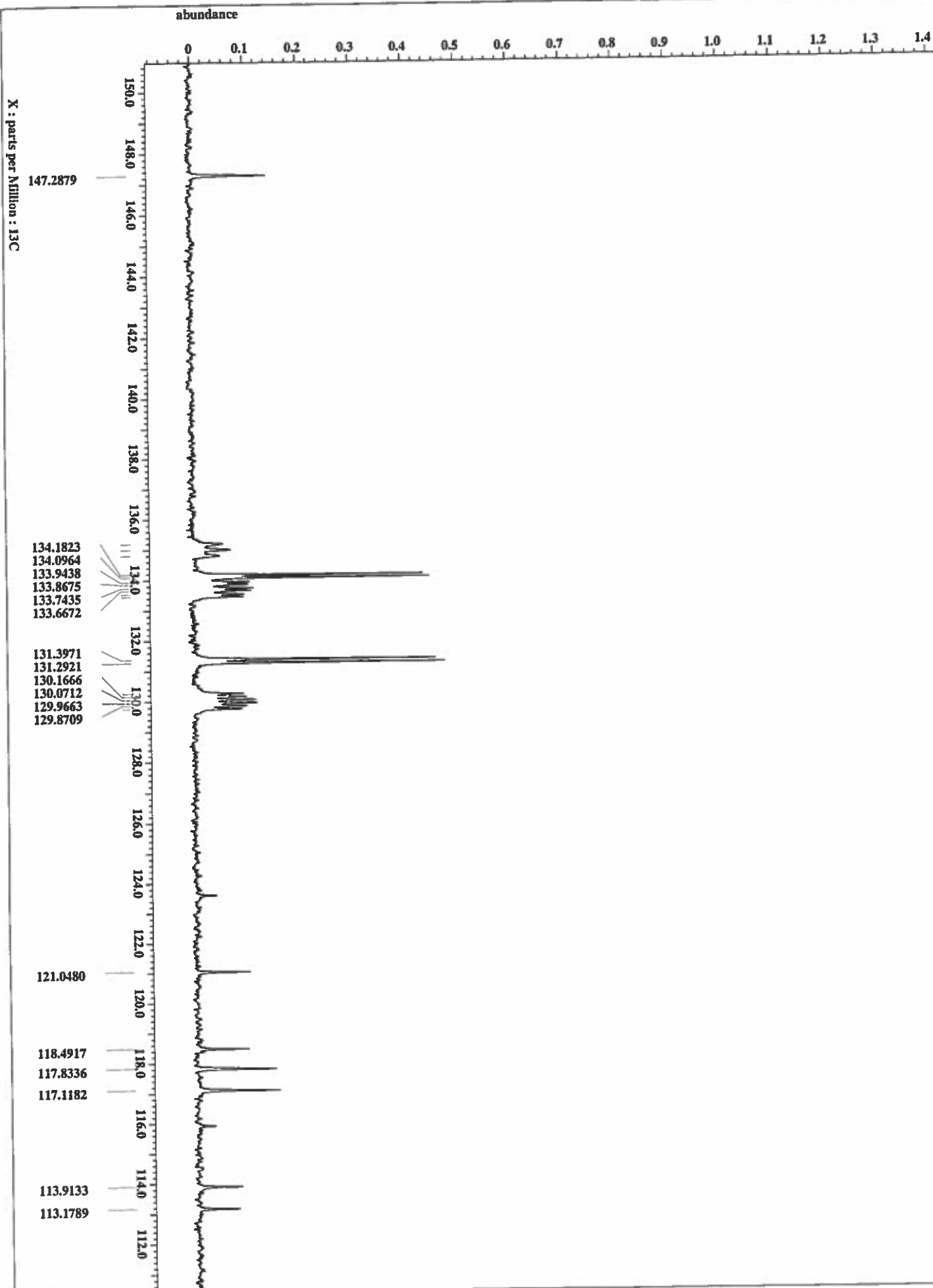
=====
Data_format   = 1D COMPLEX
Dir_size      = 26214
Dir_title     = 13C
Dir_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-EXA500

=====
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]
X_atn          = 1H
X_atn_freq     = 500.15991521 [MHz]
X_atn_offset   = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 256
Total_scans    = 256

=====
X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
X_atn_dec      = 20.7 [dB]
X_atn_poc      = 20.7 [dB]
X_noise        = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Hoe_time       = TRUE
Recur_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get       = 22.5 [dci]
=====

```





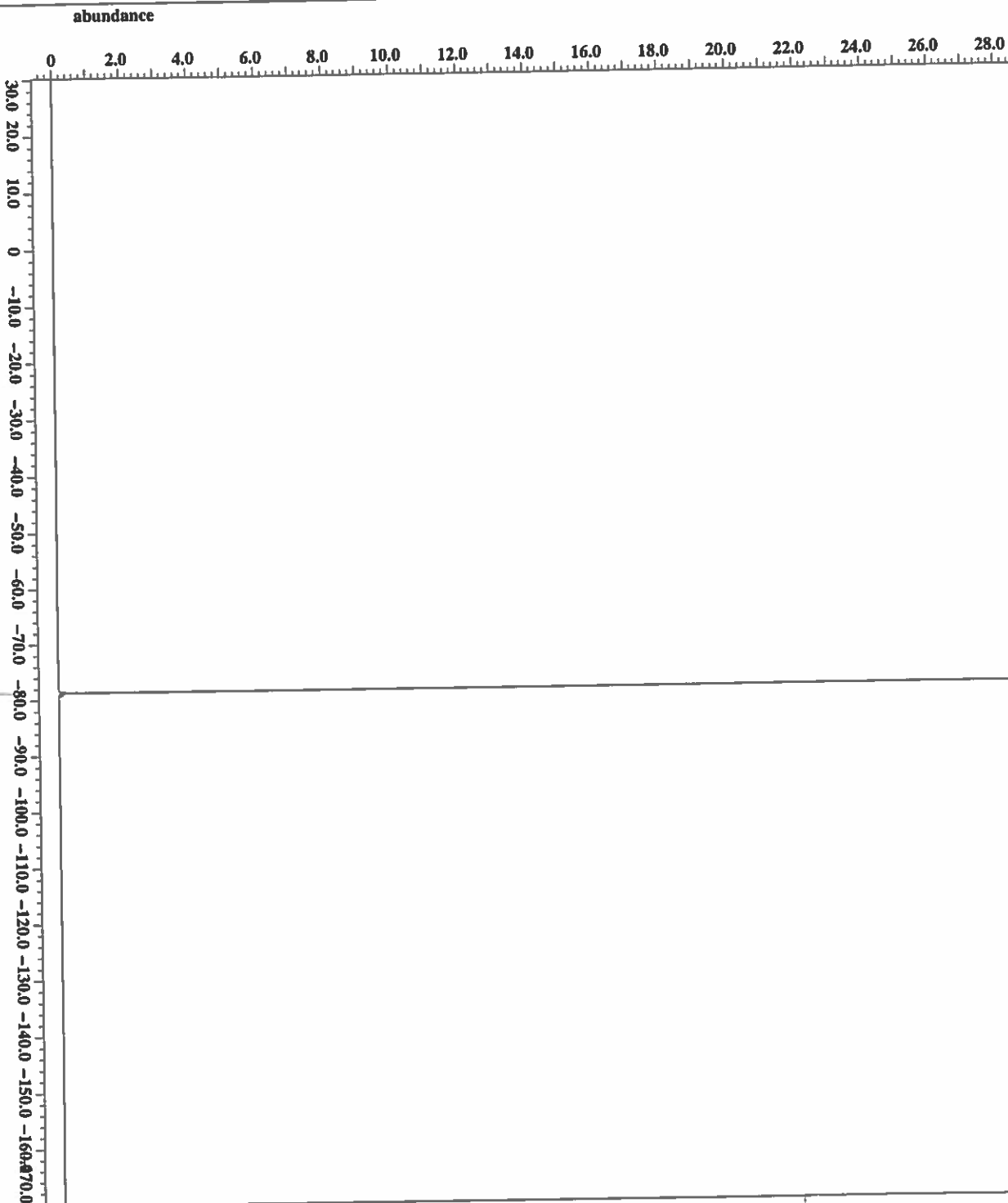


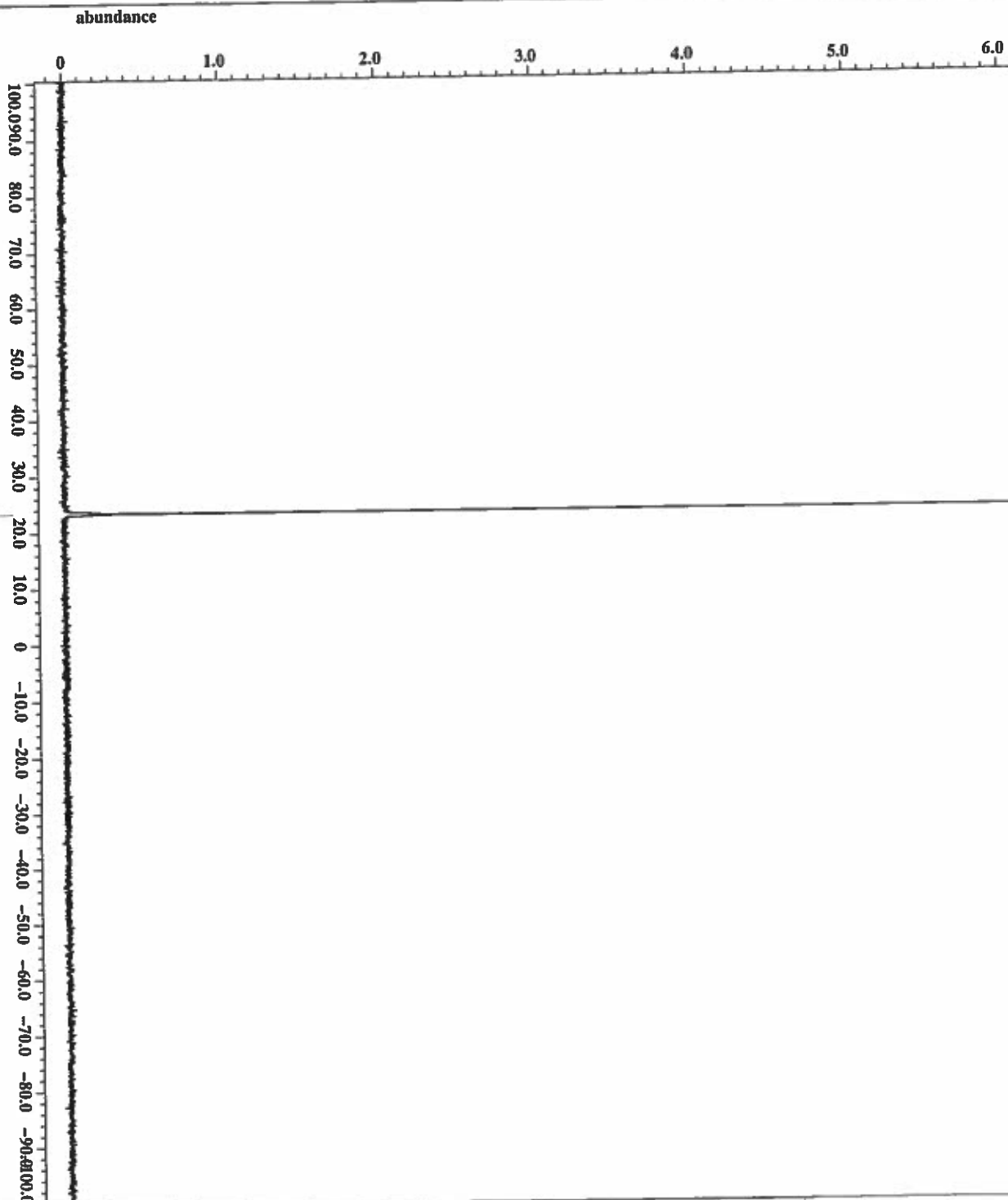
filename = MS0468-300-96h-ampule
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0468-300-96h-ampule
 Solvent = CHLOROFORM-D
 Changer_sample = 9
 Creation_time = 25-JUN-2018 10:57:31
 Revision_time = 25-JUN-2018 10:34:51
 Current_time = 25-JUN-2018 10:34:51

Data_format = 1D COMPLEX
 Dim_size = 52428
 Dim_title = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECX500

Field_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 0.55574528 [s]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = -70 [ppm]
 X_points = 65536
 X_prescans = 1
 X_resolution = 1.7993855 [Hz]
 X_sweep = 117.9245283 [kHz]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = 5 [ppm]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = 5 [ppm]
 Mod_return = FALSE
 Scans = 1
 Total_scans = 16

X_90_width = 13.1 [us]
 X_acq_time = 0.55574528 [s]
 X_angle = 45 [deg]
 X_atn = 2.5 [dB]
 X_pulse = 6.55 [us]
 Xrf_mode = OF2
 Xrf_mode = OF2
 Dente_presat = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 38
 Relaxation_delay = 4 [s]
 Repetition_time = 4.55574528 [s]
 Temp_get = 22.1 [dc]





```

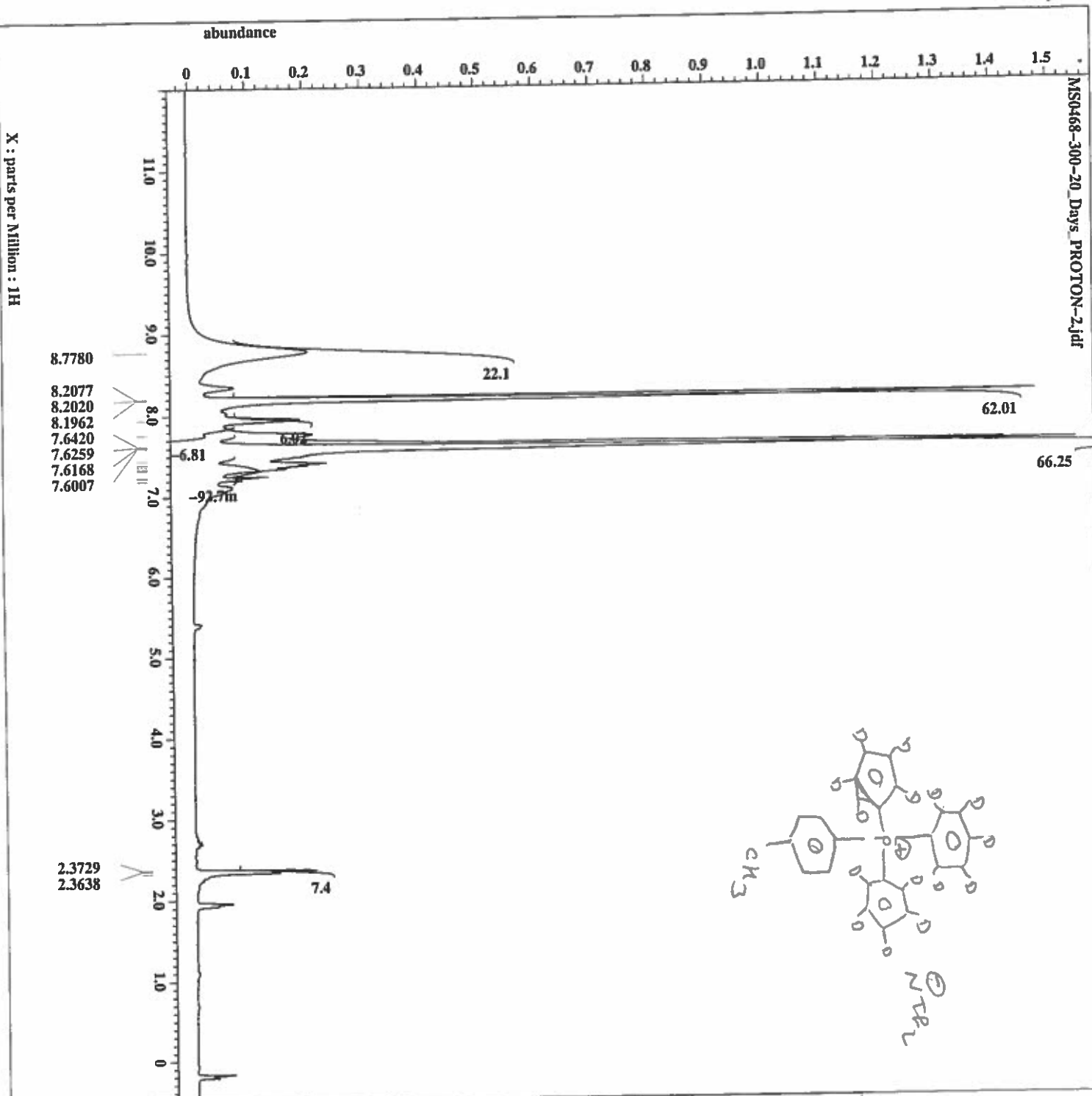
P1: name
  = MS0468-300-96h-ampule
Author
  = Jim Davis
Experiment
  = single_pulse_dec
Sample_id
  = MS0468-300-96h-ampule
Solvent
  = CHLOROFORM-D
Charger_sample
  = 9
Creation_time
  = 25-JUN-2018 11:01:05
Revision_time
  = 25-JUN-2018 10:38:23
Current_time
  = 25-JUN-2018 10:38:23

Data_format
  = 1D COMPLEX
Dim_size
  = 26214
Dim_title
  = 31P
Dim_units
  = [ppm]
Dimensions
  = X
Site
  = ECA 500
Spectrometer
  = JNM-EXA500

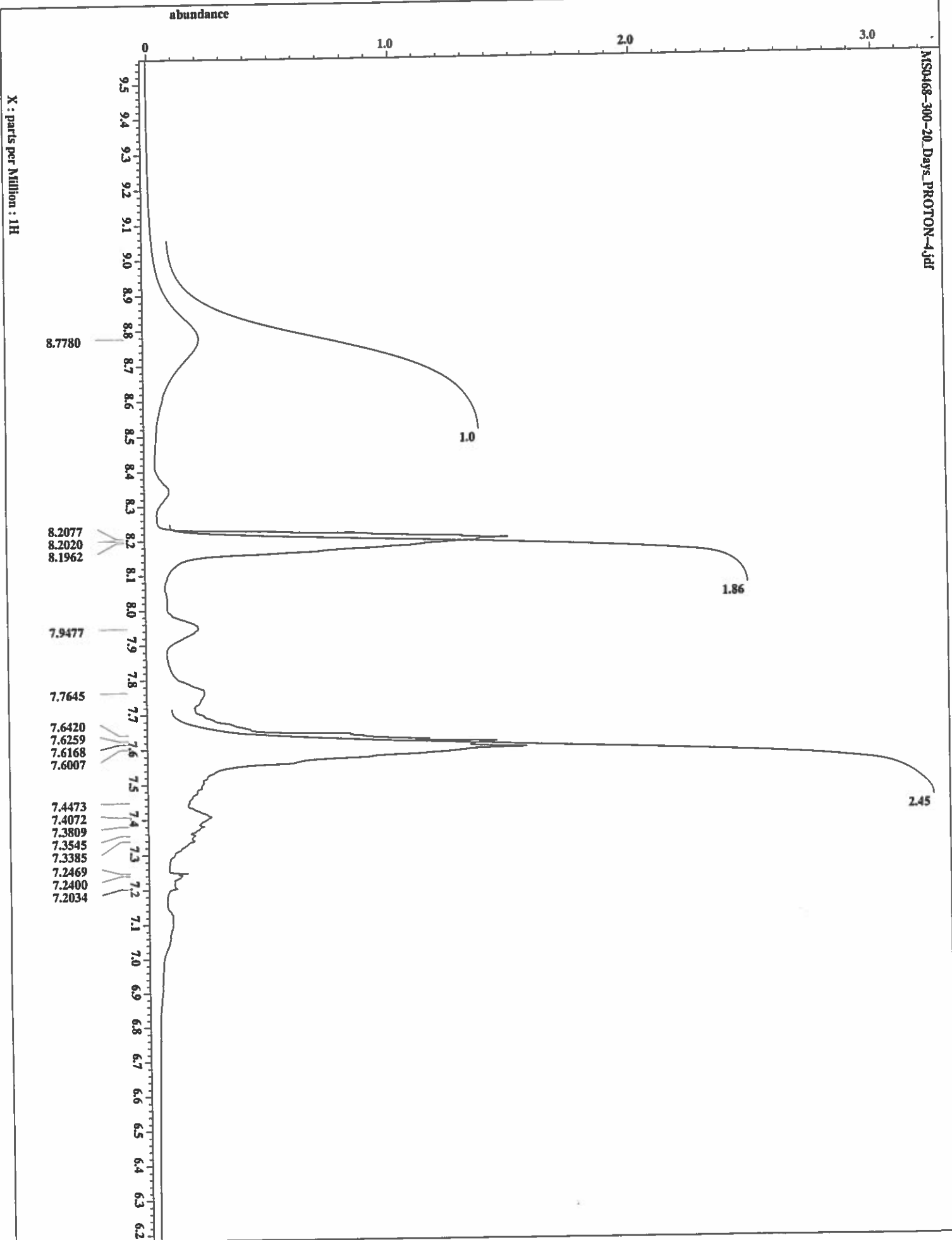
P1: field_strength
  = 11.7473579 [T] (500 [MH
X_acq_duration
  = 0.64487424 [s]
X_domain
  = 31P
X_freq
  = 202.46831075 [MHz]
X_offset
  = 0 [ppm]
X_points
  = 32768
X_prescans
  = 4
X_resolution
  = 1.55068995 [Hz]
X_sweep
  = 50.81300813 [kHz]
Irr_domain
  = 1H
Irr_freq
  = 500.15991521 [MHz]
Irr_offset
  = 5.0 [ppm]
Clipped
  = FALSE
Mod_return
  = 1
Scans
  = 25
Total_scans
  = 25

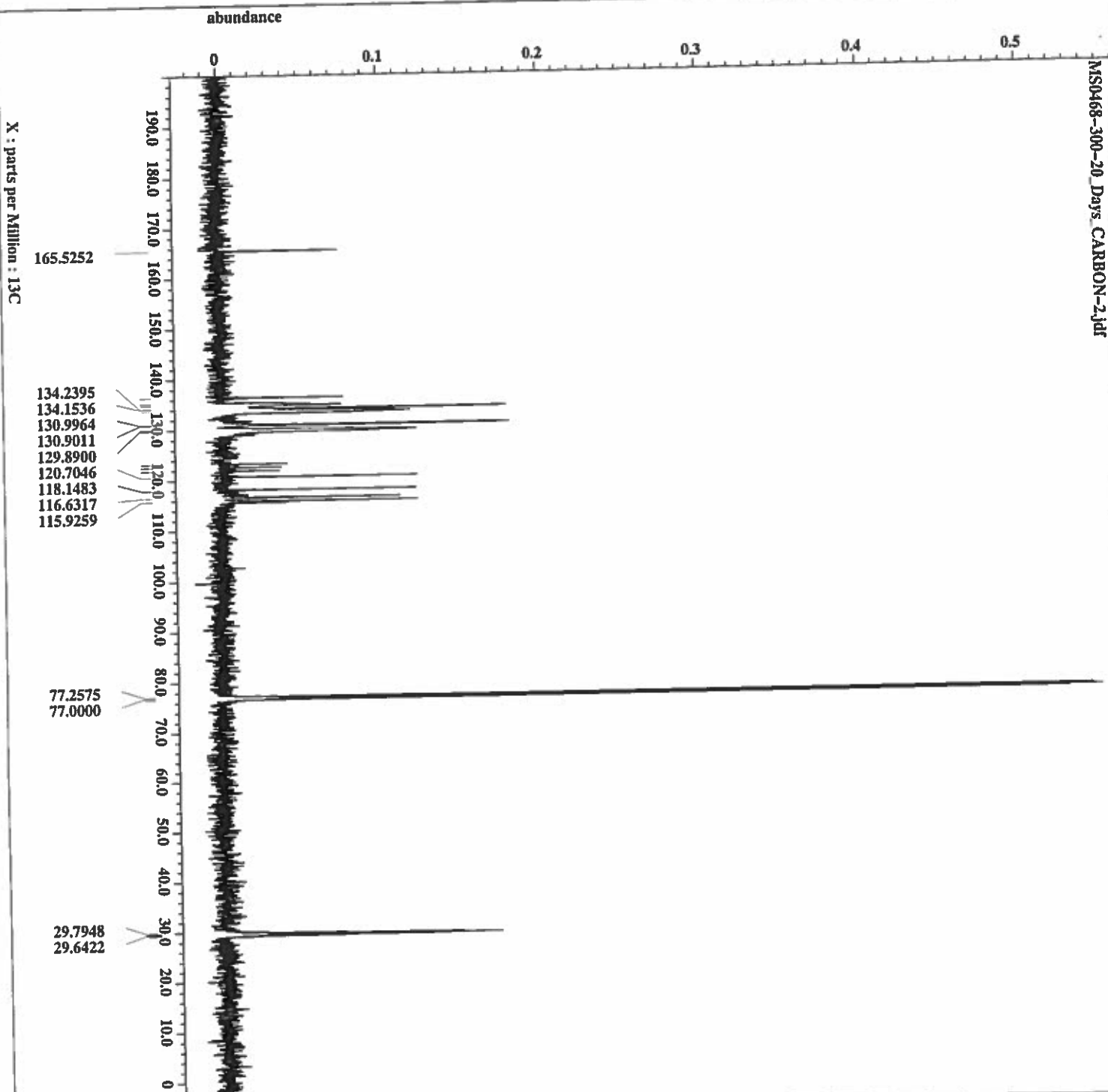
X_90_width
  = 14.687 [us]
X_acq_time
  = 0.64487424 [s]
X_angle
  = 30 [deg]
X_atn
  = 5 [dB]
X_pulse
  = 4.89566667 [us]
Irr_atn_dec
  = 20.7 [dB]
Irr_atn_noz
  = 20.7 [dB]
Irr_noise
  = WALTZ
Decoupling
  = TRUZ
Initial_wait
  = 1 [s]
Noe_time
  = 1 [s]
Recvr_gain
  = 58
Relaxation_delay
  = 2 [s]
Repetition_delay
  = 2.64487424 [s]
Repetition_time
  = 22.31 [dc]
Temp_get
  = 22.31 [dc]

```



Filename	MS0468-300-20_Day5.yr
Author	Jim Davis
Exponential	single_pulse.ex2
Sample_id	MS0468-300-20_Day5
Solvent	CHLOROFORM-D
Charger_sample	8
Creation time	27-JUN-2018 17:21:47
Revision time	27-JUN-2018 16:58:52
Current_time	27-JUN-2018 16:58:52
Data_format	= ID_COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= BCA 500
Spectrometer	= JNM-ECX500
Field_strength	= 11.7473579[G] (500[MHz]
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0 [ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57377737[Hz]
X_sweep	= 9.38638638[Hz]
Ir1_domain	= 1H
Ir1_freq	= 500.15991521[MHz]
Ir1_offset	= 5.0 [ppm]
Ir1_domain	= 1H
Ir1_freq	= 500.15991521[MHz]
Ir1_offset	= 5.0 [ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Ir1_mode	= Off
Tr1_mode	= FALSE
Dante_preset	= 1[s]
Initial_wait	= 38
Recev_gain	= 4[s]
Relaxation_delay	= 5.74587904[s]
Relaxation_time	= 22.5[dc]
Temp_get	





```

Filename      = MS0468-300-20_Days_CA
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0468-300-20_Days
Solvent       = CHLOROFORM-D
Charger_sample = 8
Creation_time  = 27-JUN-2018 17:36:07
Revision_time  = 27-JUN-2018 17:13:13
Current_time   = 27-JUN-2018 17:13:13

Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
ECA 500
Site          = JMR-ECA500
Spectrometer

Field_strength = 11.7473579 [G] (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        = 39.3081764 [kHz]
Xt_domain      = 1H
Xt_freq        = 500.15991521 [MHz]
Xt_offset      = 5.0 [ppm]
Mod_return     = FALSTZ
Scans          = 1
Total_scans    = 256

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_noe    = 20.7 [dB]
Irr_noise      = 20.7 [dB]
Decoupling     = WALTZ
Initial_valt   = TRUZ
Noe_time       = 1 [s]
Recvr_gain     = 2 [s]
Relaxation_delay = 2.83361792 [s]
Repetition_time = 23.2 [dc]
Temp_get       = 23.2 [dc]

```

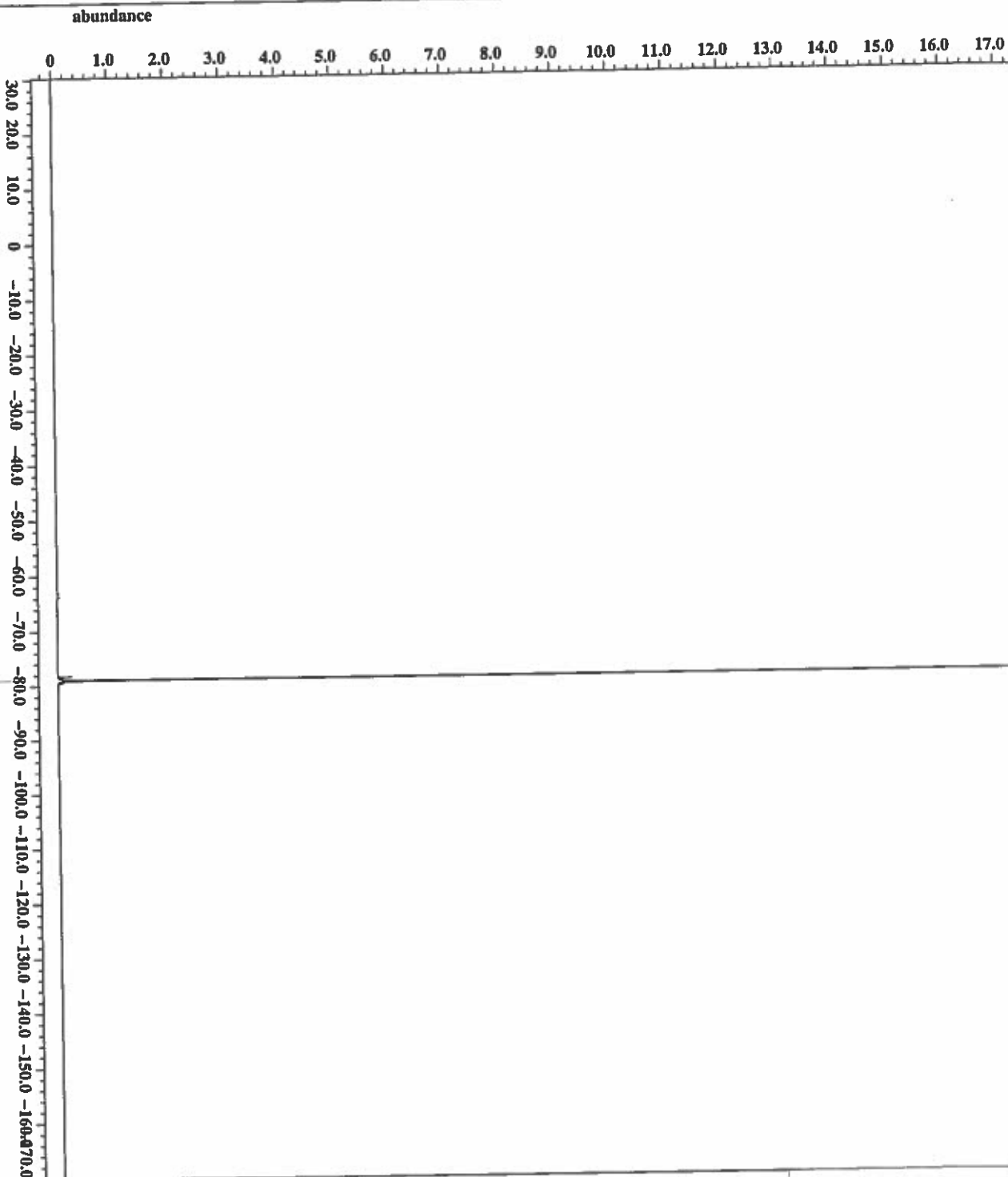


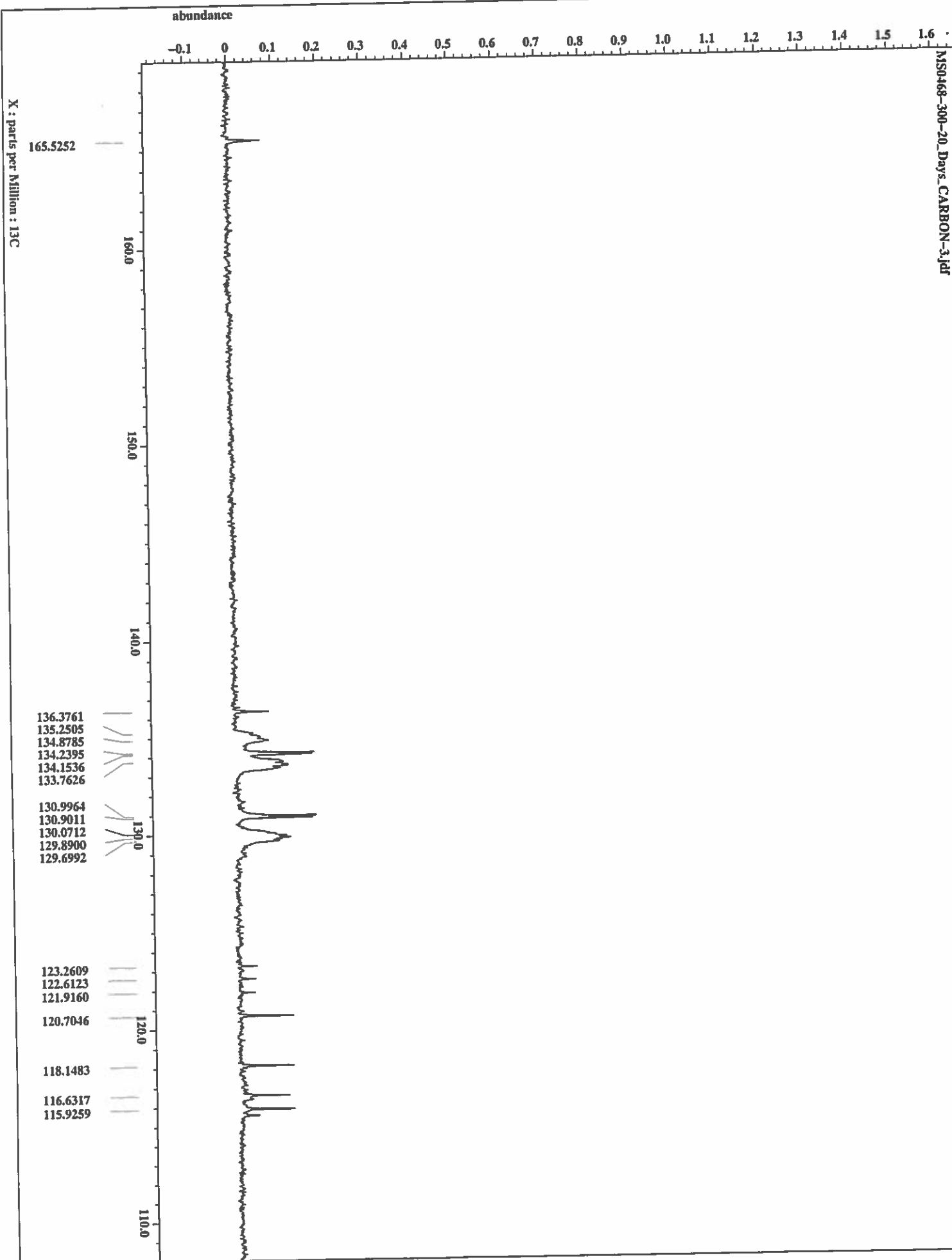
Filename = MS0468-300-20_Days_FL
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0468-300-20_Days
 Solvent = CHLOROFORM-D
 Changer_sample = 8
 Creation_time = 27-JUN-2018 17:39:03
 Revision_time = 27-JUN-2018 17:16:08
 Current_time = 27-JUN-2018 17:16:08

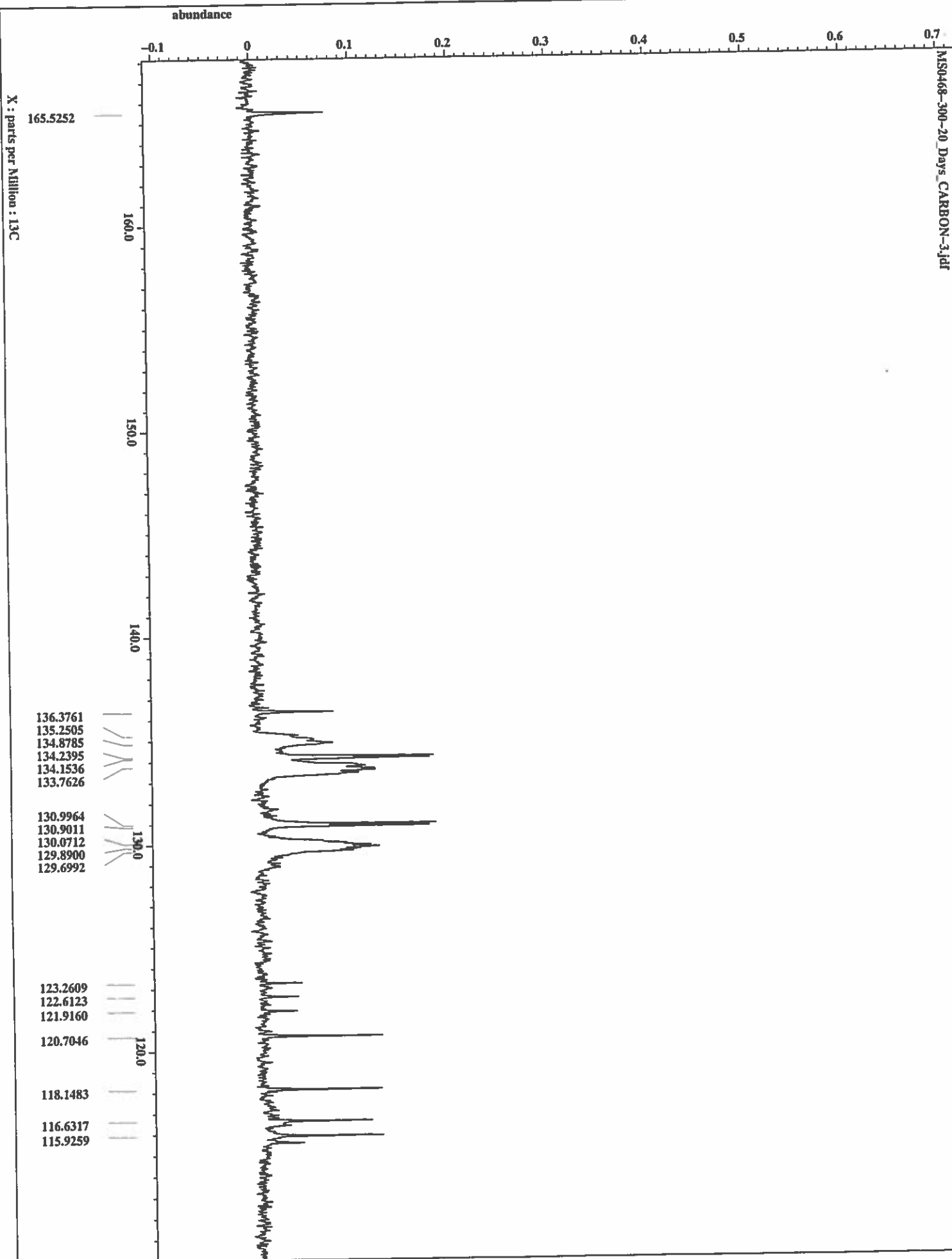
Data_format = 1D COMPLEX
 Dim_size = 52428
 Dim_title = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = EXA 500
 Spectrometer = JNM-ZCA500

Field_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 0.55574528 [s]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = -70 [ppm]
 X_points = 65536
 X_preampl = 1
 X_resolution = 1.7993855 [Hz]
 X_sweep = 117.9245283 [kHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084 [MHz]
 Irr_offset = 5 [ppm]
 Tr1_domain = 19F
 Tr1_freq = 470.62046084 [MHz]
 Tr1_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 13.1 [us]
 X_acq_time = 0.55574528 [s]
 X_angle = 45 [deg]
 X_atn = 2.5 [dB]
 X_pulse = 6.55 [us]
 OF = 0CF
 Tr1_mode = OF
 Dnate_preset = PALSE
 Initcl_wait = 1 [s]
 Recvr_gain = 36
 Relaxation_delay = 4 [s]
 Repetition_time = 4.55574528 [s]
 Temp_set = 22.8 [dc]





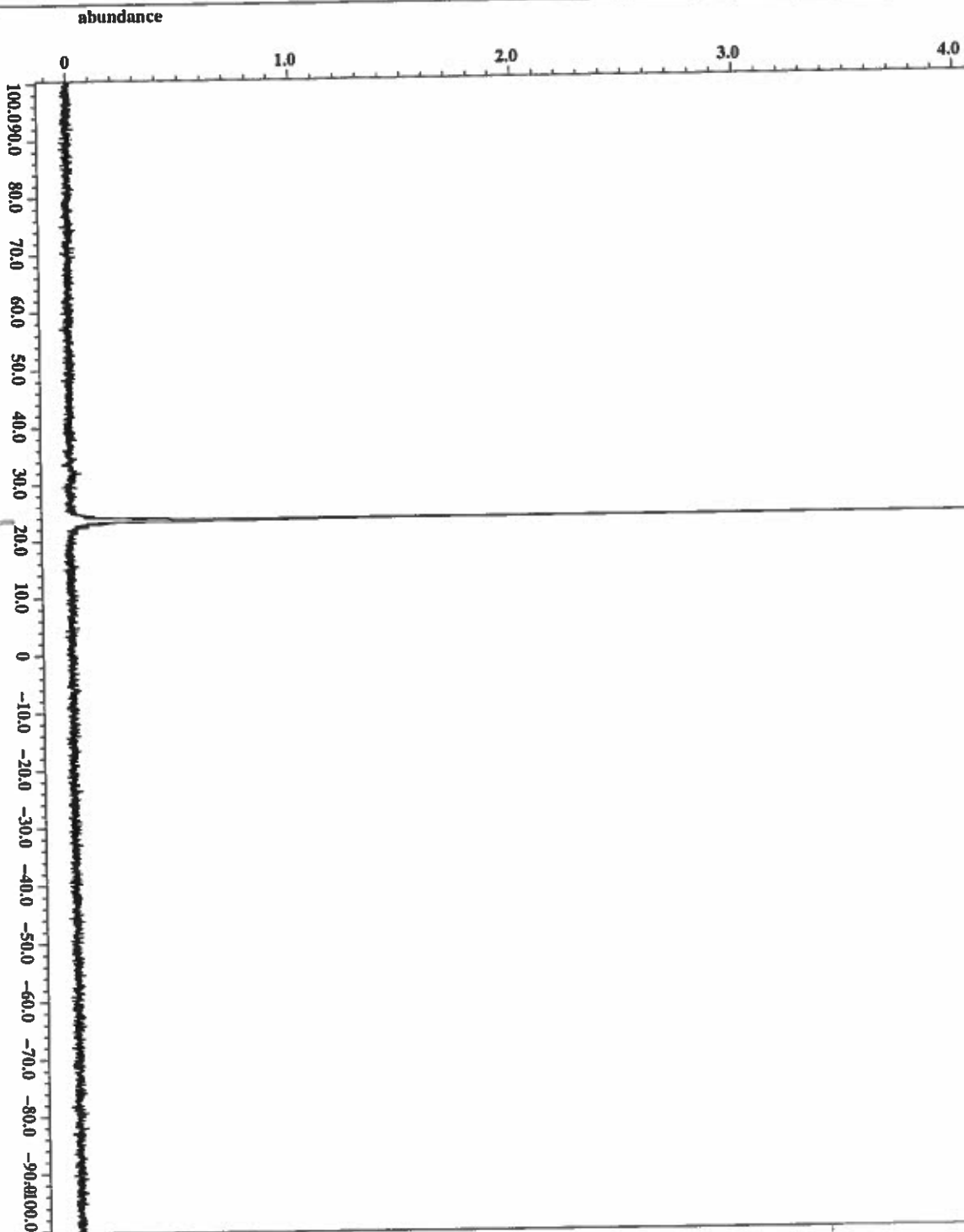




Filename MS0468-300-20_Days_PH
 Author Jim Davis
 Experiment single_pulse_dec
 Sample_id MS0468-300-20_Days
 Solvent CHLOROFORM-D
 Changer_sample 8
 Creation_time 27-JUN-2018 17:43:38
 Revision_time 27-JUN-2018 17:19:43
 Current_time 27-JUN-2018 17:19:44

Data_format 1D COMPLEX
 Dia_size 26214
 Dia_title 31P
 Dia_units [ppm]
 Dimensions X
 Site ECA 500
 Spectrometer JNM-ECA500

Field_strength 11.7473529 [G] (500 [MH
 X_acq_duration 0.64487424 [s]
 X_domain 31P
 X_freq 202.46831075 [MHz]
 X_offset 0 [ppm]
 X_points 32768
 X_prescans 4
 X_resolution 1.5506895 [Hz]
 X_sweep 50.81300813 [kHz]
 Irr_domain 1H
 Irr_freq 500.15991521 [MHz]
 Irr_offset 5.0 [ppm]
 Clipped FALSE
 Mod_return 1
 Scans 25
 Total_scans 25
 X_90_width 14.687 [us]
 X_acq_time 0.64487424 [s]
 X_angle 30 [deg]
 X_atn 5 [dB]
 X_pulse 4.89566667 [us]
 Irr_atn_dec 20.7 [dB]
 Irr_atn_noe 20.7 [dB]
 VALTZ VALTZ
 Decoupling TRUEZ
 Initial_wait 1 [s]
 Noe_time TRUEZ
 Noe_gain 2 [s]
 Relaxation_delay 2 [s]
 Repetition_time 2.64487424 [s]
 Temp_get 23 [deg]



X : parts per Million : 31P

abundance

0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0

40.0

30.0

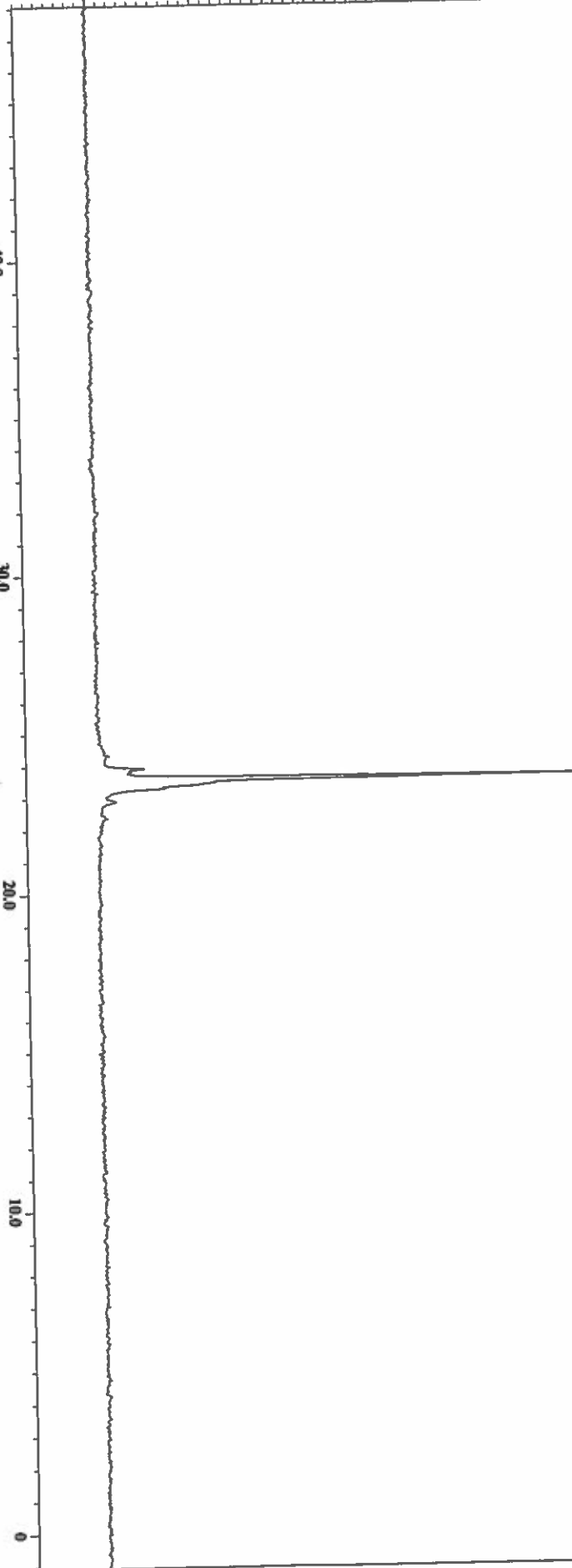
23.5895

20.0

10.0

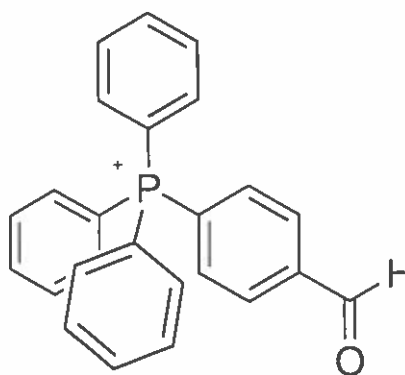
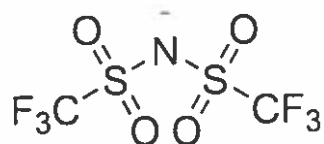
0

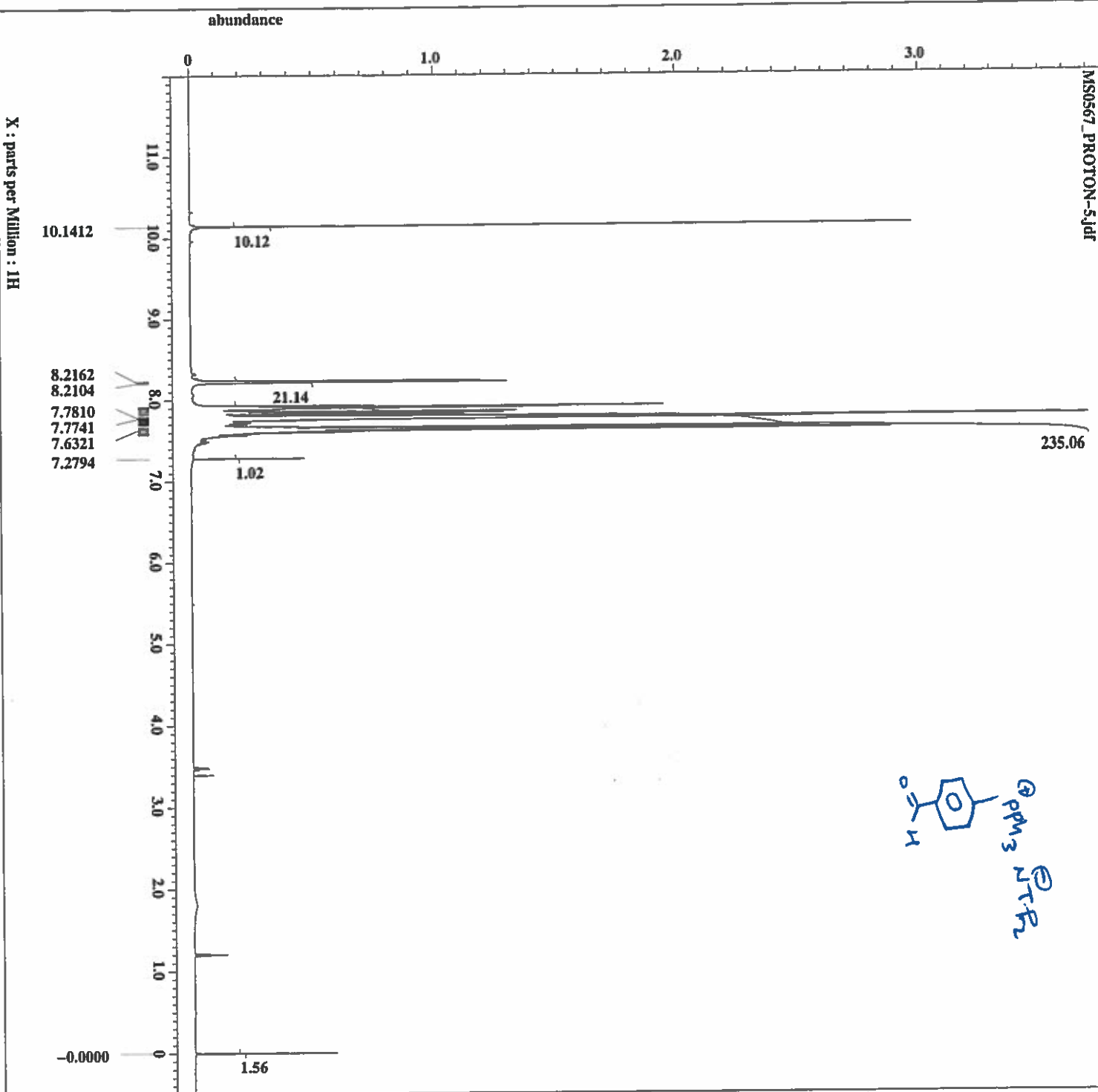
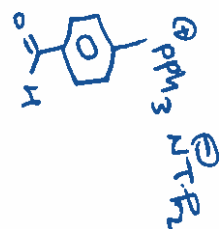
X : parts per Million : 31P



Compound 4 Pre- and Post-heating NMR Spectra

Temperature of Post-heating samples noted in upper left corner of each spectrum





```

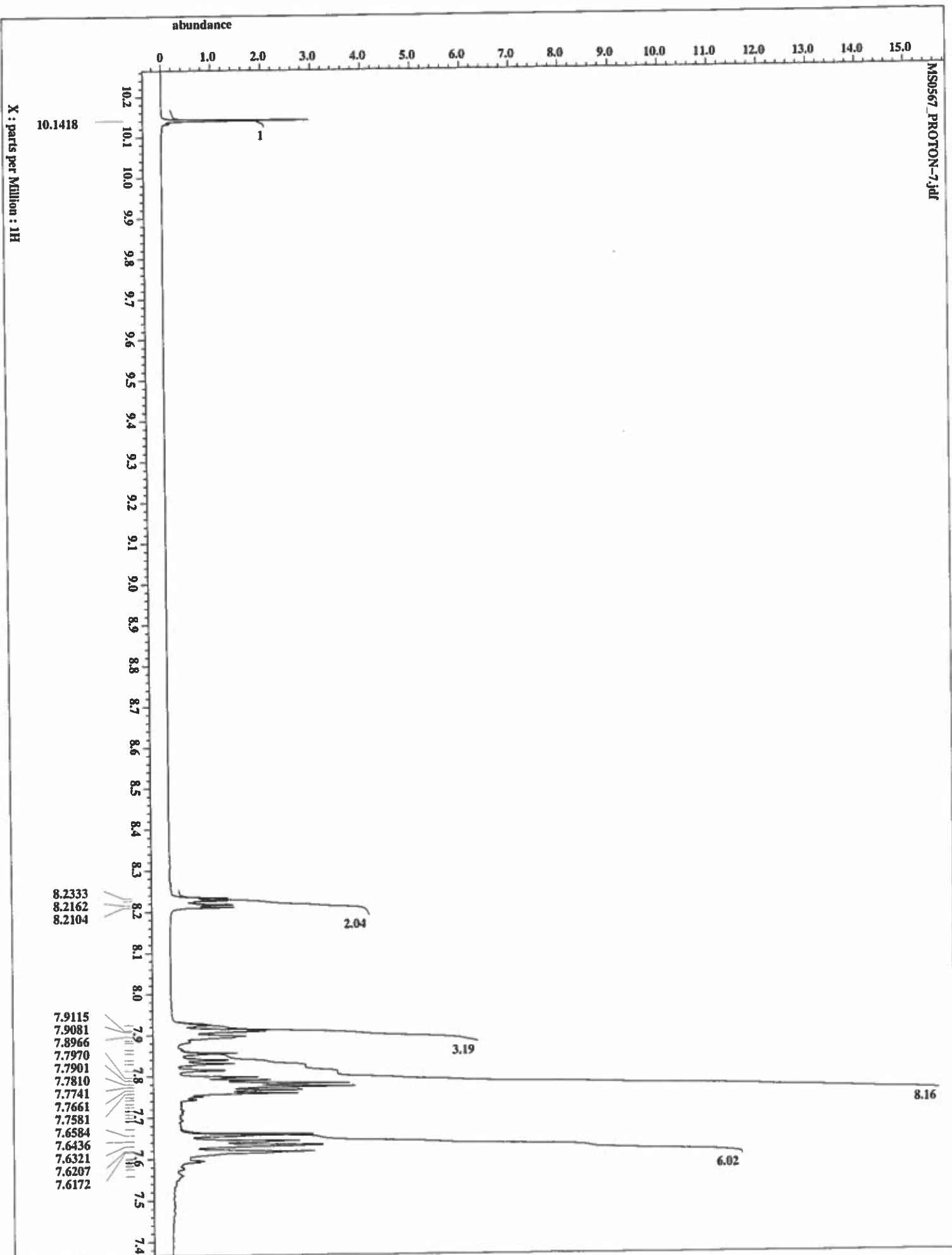
=====
Filename      MS0567_PROTON-5.jdt
Author        Jim Davis
Experiment     single_pulse.ex2
Sample_id      MS0567
Solvent        CHLOROFORM-D
Creation_time  3-OCT-2018 19:18:04
Revision_time  3-OCT-2018 18:53:06
Current_time   3-OCT-2018 18:53:06

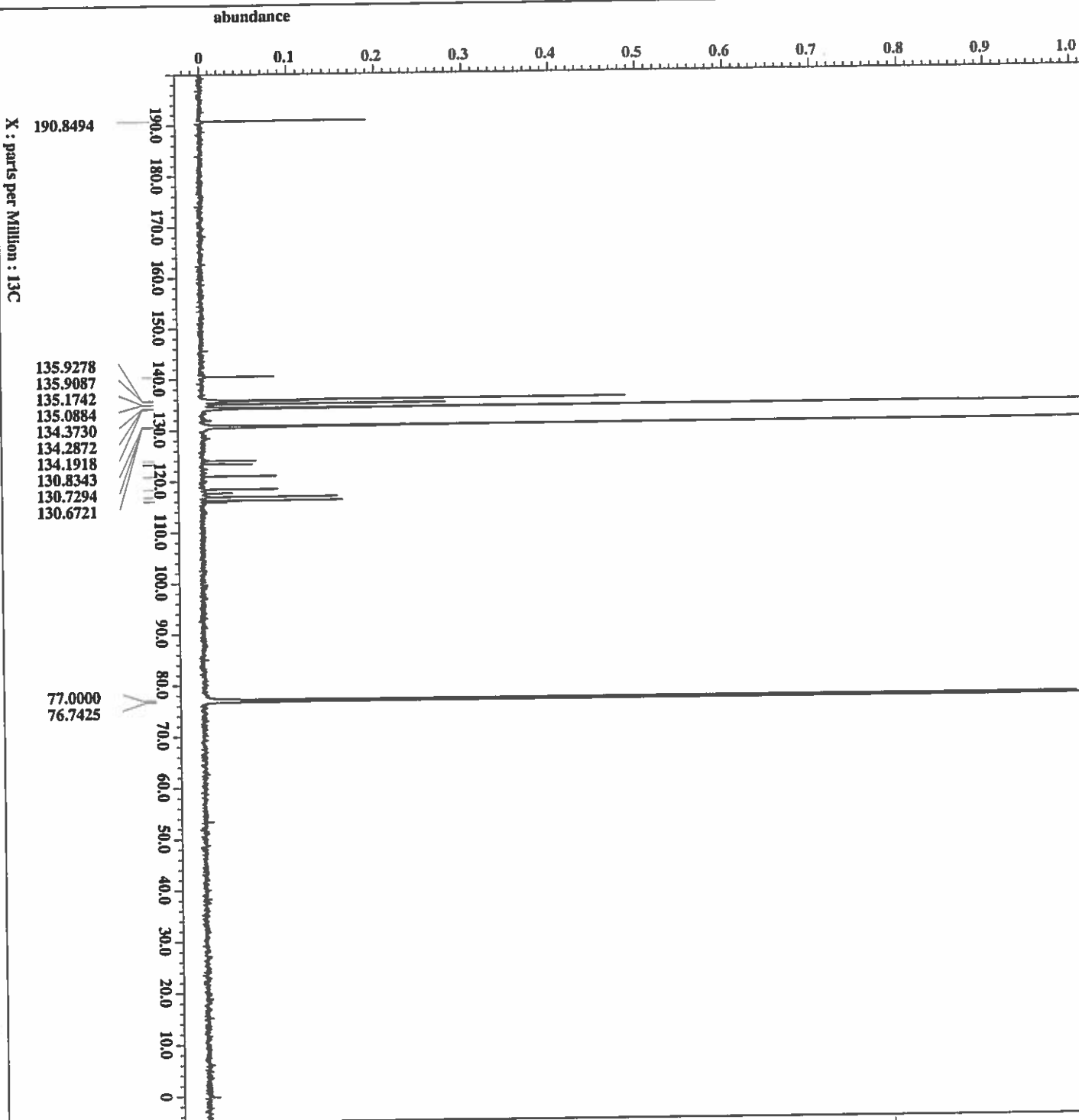
Data_format    ID COMPLEX
Dia_size       13107
Dim_title      1H
Dim_units      [ppm]
Dimensions     X
Site           ECA 500
Spectrometer   JNM-ECA500

Field_strength 11.743579 [T] (500 [MHz])
X_acq_duration 1.74587904 [s]
X_domain       1H
X_freq         500.15991521 [MHz]
X_offset       5.0 [ppm]
X_points       16384
X_prescans     1
X_resolution   0.57277737 [Hz]
X_sweep        9.38438438 [kHz]
Irr_domain     1H
Irr_freq       500.15991521 [MHz]
Irr_offset     5.0 [ppm]
T1r_domain     1H
T1r_freq       500.15991521 [MHz]
T1r_offset     5.0 [ppm]
Clipped        FALSE
Mod_return     1
Scans          16
Total_scans    16

X_90_width     12.4 [us]
X_acq_time      1.74587904 [s]
X_angle        45 [deg]
X_atn          4 [dB]
X_pulse        6.2 [us]
Irr_mode       off
T1r_mode       off
Dante_present  FALSE
Initial_wait   1 [s]
Recvr_gain     30
Relaxation_delay 4 [s]
Repetition_time 5.74587904 [s]
Temp_get       22.4 [C]
=====

```





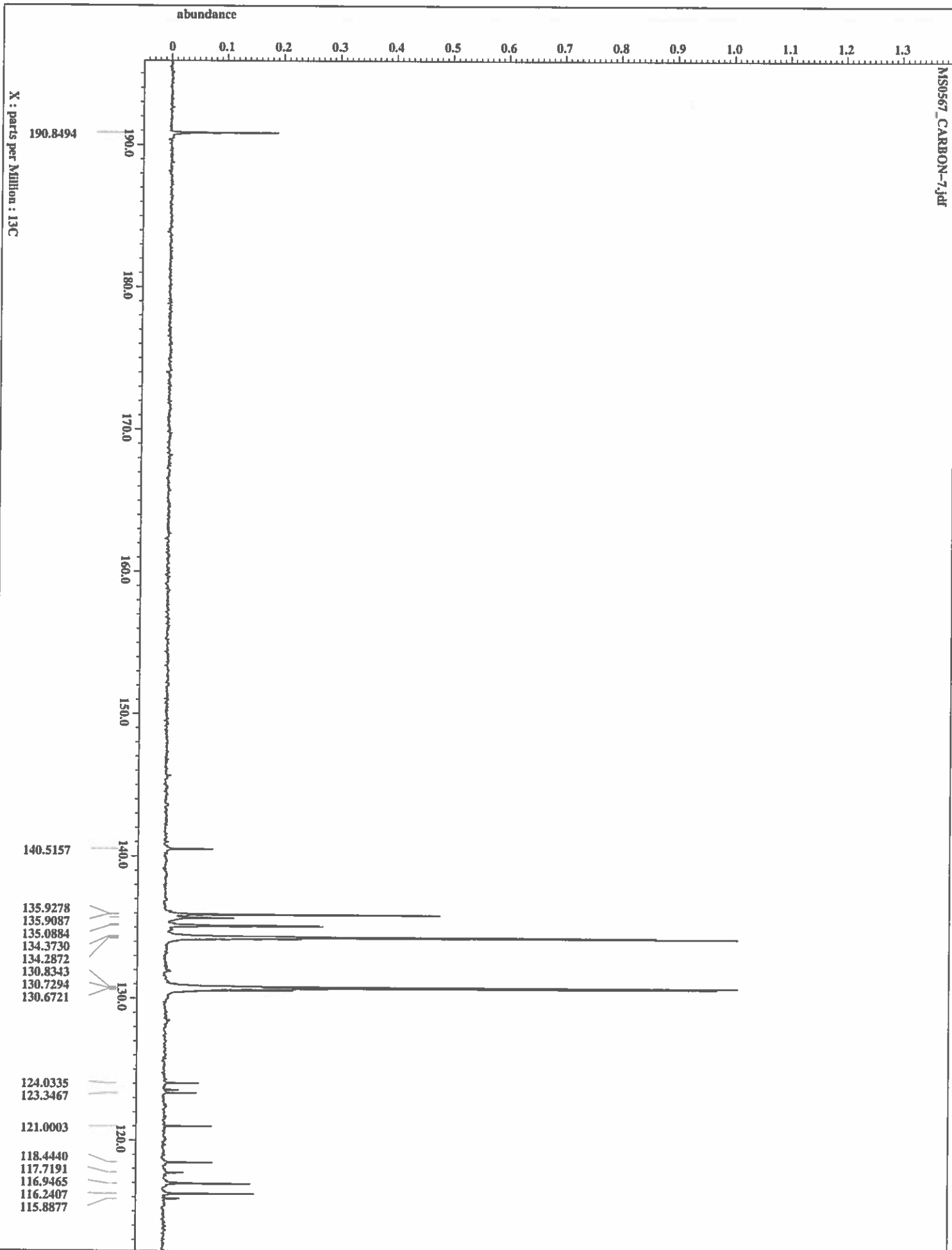
```

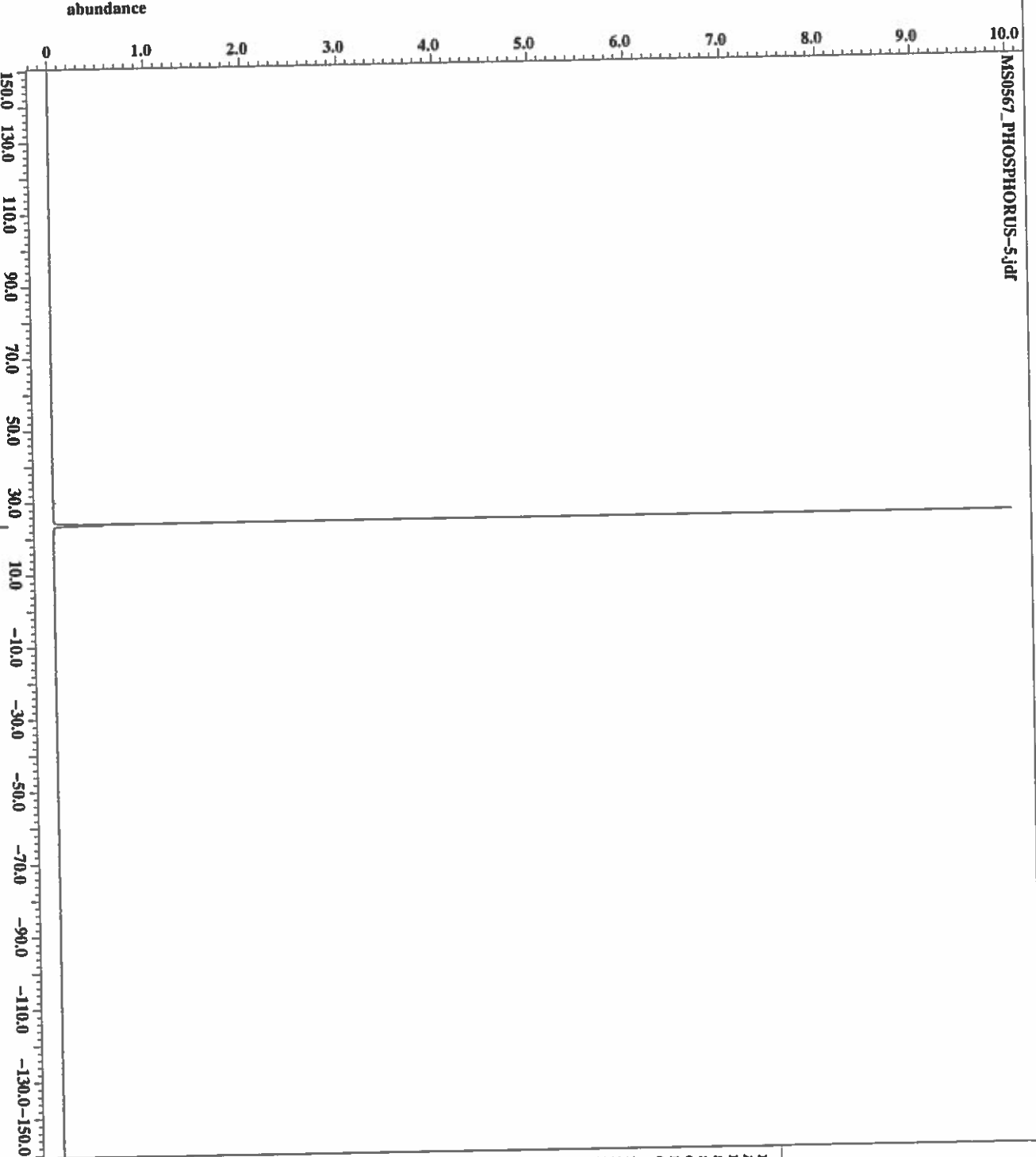
File Name      = MS0567_CARBON-5.jdt
Author         = Jim Davis
Experiment     = single_pulse_dec
Sample_id      = MS0567
Solvent        = CHLOROFORM-D
Creation time   = 3-OCT-2018 20:08:47
Revision time  = 3-OCT-2018 19:43:49
Current time    = 3-OCT-2018 19:43:49

Data Format     = 1D COMPLEX
Dim. size      = 26214
Dim. title     = 13C
Dim. units     = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-PCA500

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     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_soe    = 20.7 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Incl1d1_waltz  = 1 [s]
Noc            = TRUE
Noc_time       = 60
Recvr_gain     = 2 [s]
Relaxation_delay = 2.83361792 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 23.1 [degC]
  
```





X : parts per Million : 31P



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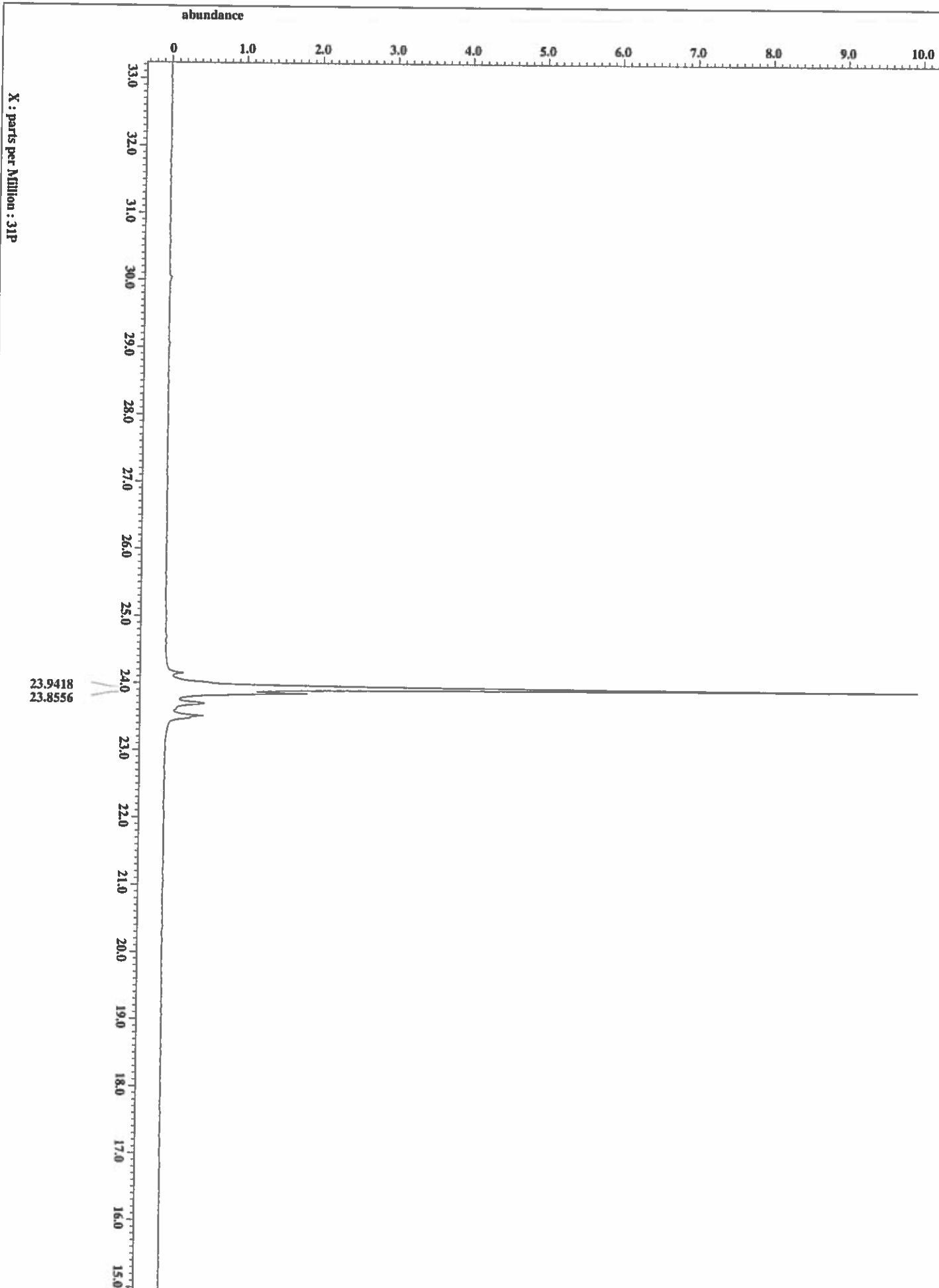
```

=====
Filename      = MS0567_PHOSPHORUS-5.j
Author        = Jim Davis
Experiment     = single_pulse_dec
Sample_id     = MS0567
Solvent       = CHLOROFORM-D
Creation_time  = 4-OCT-2018 01:35:23
Revision_time  = 4-OCT-2018 01:10:23
Current_time   = 4-OCT-2018 01:10:23

=====
Data_format   = 1D COMPLEX
Dim_size      = 52428
Dim_title     = 31P
Dim_units     = [ppm]
Dimensions    = X
Size          = 2CA 500
Spectrometer  = JNM-ECA500

=====
Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.85983232 [s]
X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 65536
X_prescans     = 4
X_resolution   = 1.16301746 [Hz]
X_sweep        = 76.2195122 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 128
Total_scans    = 128

=====
X_90_width     = 14.687 [us]
X_acq_time     = 0.85983232 [s]
X_angle        = 30 [deg]
X_atn          = 5 [dB]
X_pulse        = 4.89566667 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_noe    = 20.7 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUZ
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Recvt_gain     = 56
Relaxation_delay = 2 [s]
Repetition_time = 2.85983232 [s]
Temp_get       = 23.2 [dC]
    
```



abundance

10.0

20.0

30.0

50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0 -210.0 -220.0 -230.0 -240.0 -250.0

-78.6647

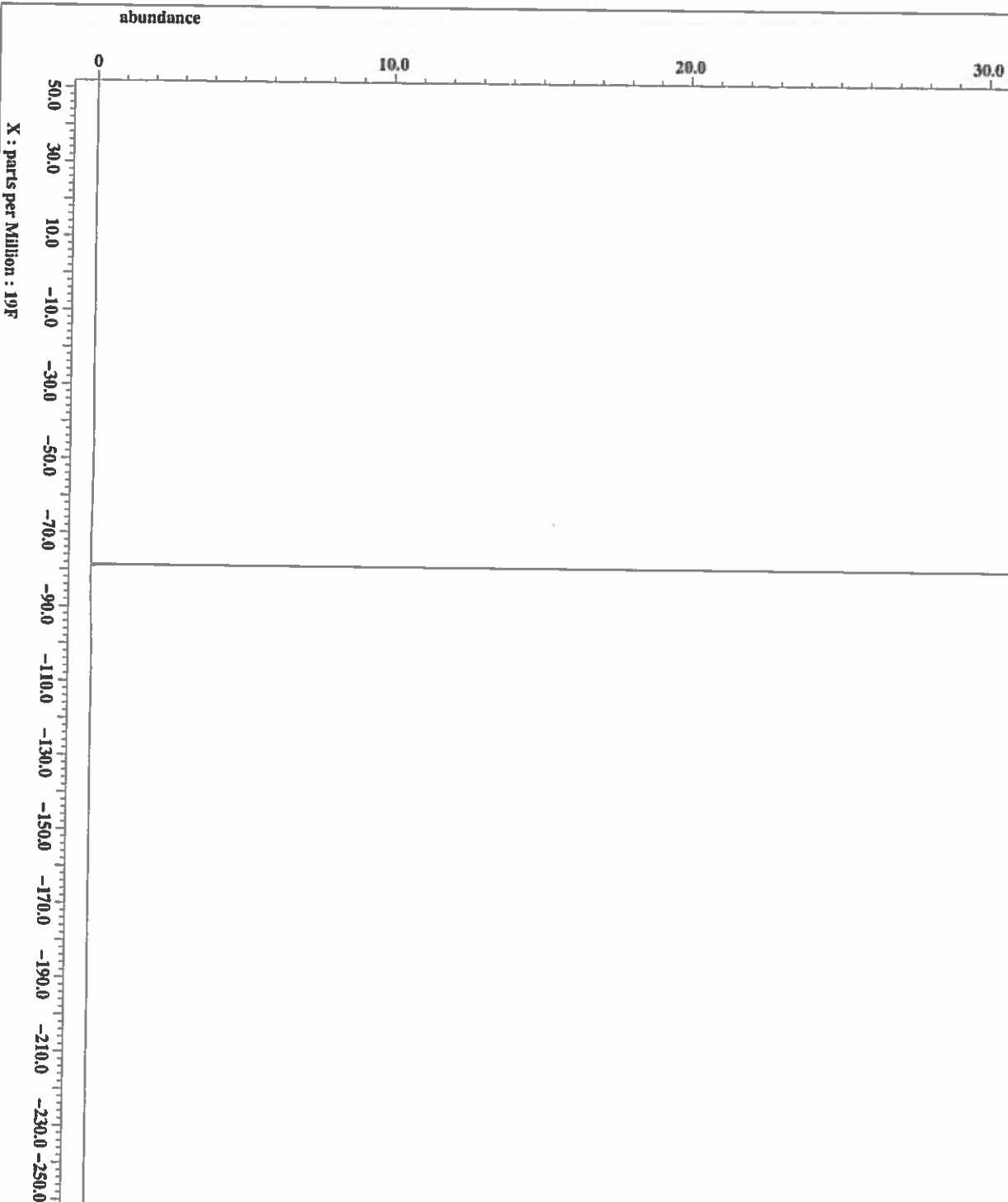
X : parts per Million : 19F

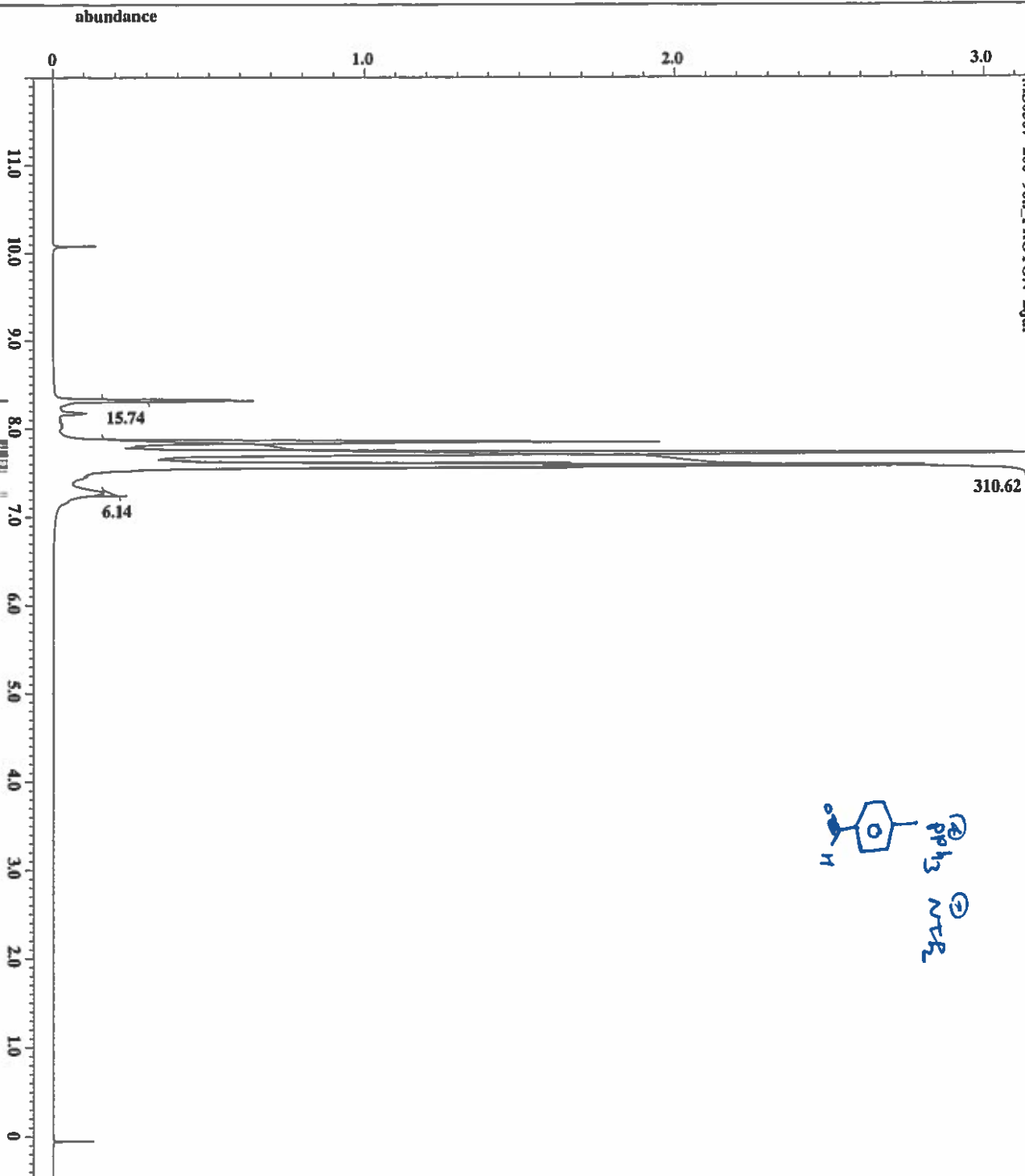
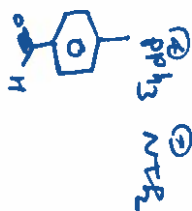


Filename MS0567_FLUORINE-5.jdt
 Author Jim Davis
 Experiment single_pulse.ex2
 Sample_id MS0567
 Solvent CHLOROFORM-D
 Creation_time 4-OCT-2018 01:41:31
 Revision_time 4-OCT-2018 01:16:32
 Current_time 4-OCT-2018 01:16:33

Data_format 1D COMPLEX
 Dia_size 104857
 Dia_title 19F
 Dia_units [ppm]
 Dimensions X
 Site ECA 500
 Spectrometer JNM-ECA500

Field_strength 11.7473579 [T] (500 [MH
 X_acq_duration 0.7340032 [s]
 X_domain 19F
 X_freq 470.62046084 [MHz]
 X_offset -100 [ppm]
 X_points 131072
 X_prescans 1
 X_resolution 1.36239188 [Hz]
 X_sweep 178.57142857 [kHz]
 Irt_domain 19F
 Irt_freq 470.62046084 [MHz]
 Irt_offset 5 [ppm]
 Tri_domain 19F
 Tri_freq 470.62046084 [MHz]
 Tri_offset 5 [ppm]
 Clipped FALSE
 Mod_return 1
 Scans 50
 Total_scans 50
 X_90_width 13.1 [us]
 X_acq_time 0.7340032 [s]
 X_angle 45 [deg]
 X_atn 2.5 [dB]
 X_pulse 6.55 [us]
 Irt_mode OET
 Tri_mode OET
 Dante_presat FALSE
 Initial_wait 1 [s]
 Recvr_gain 54
 Relaxation_delay 4 [s]
 Repetition_time 4.7340032 [s]
 Temp_get 22.8 [dC]





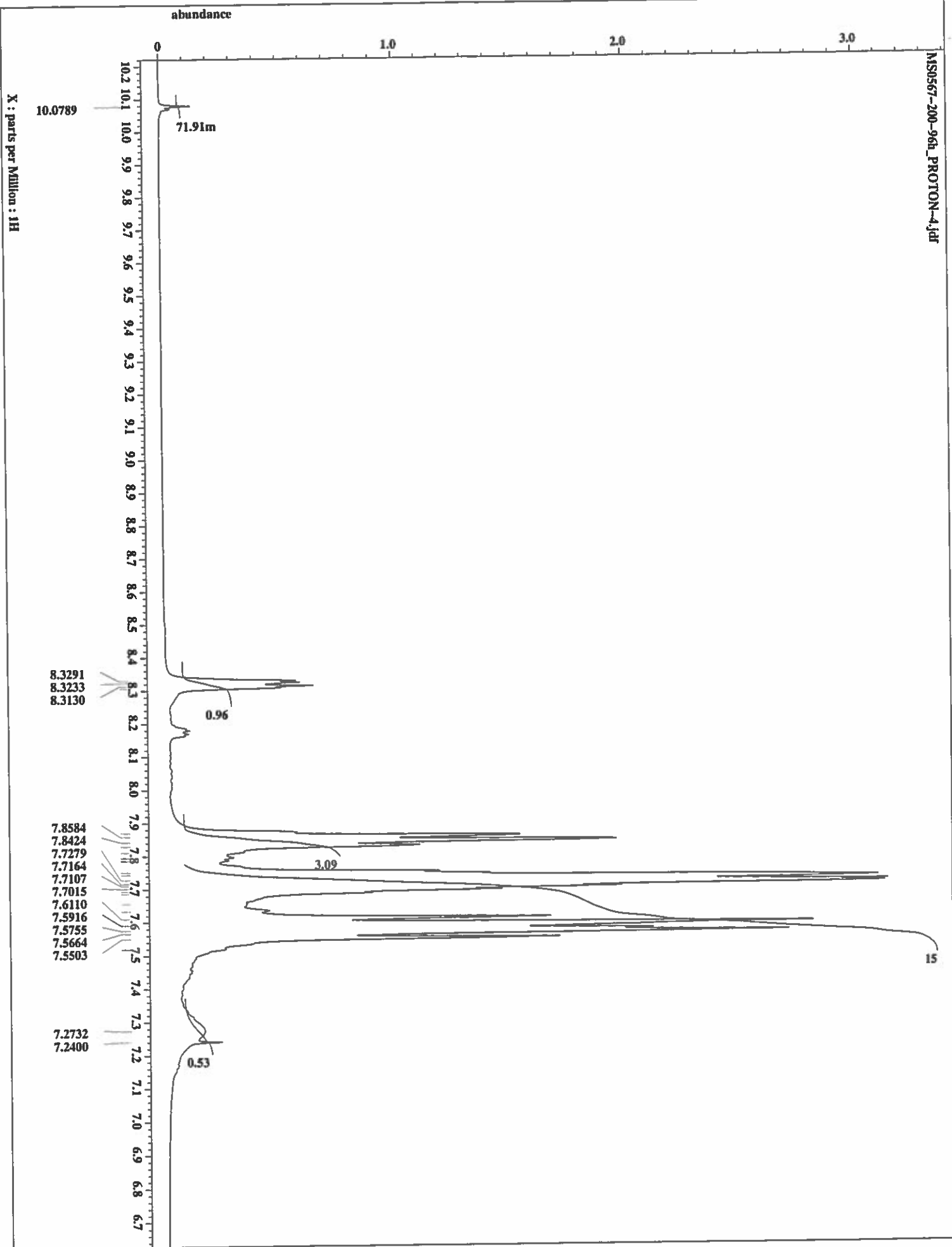
X : parts per Million : 1H

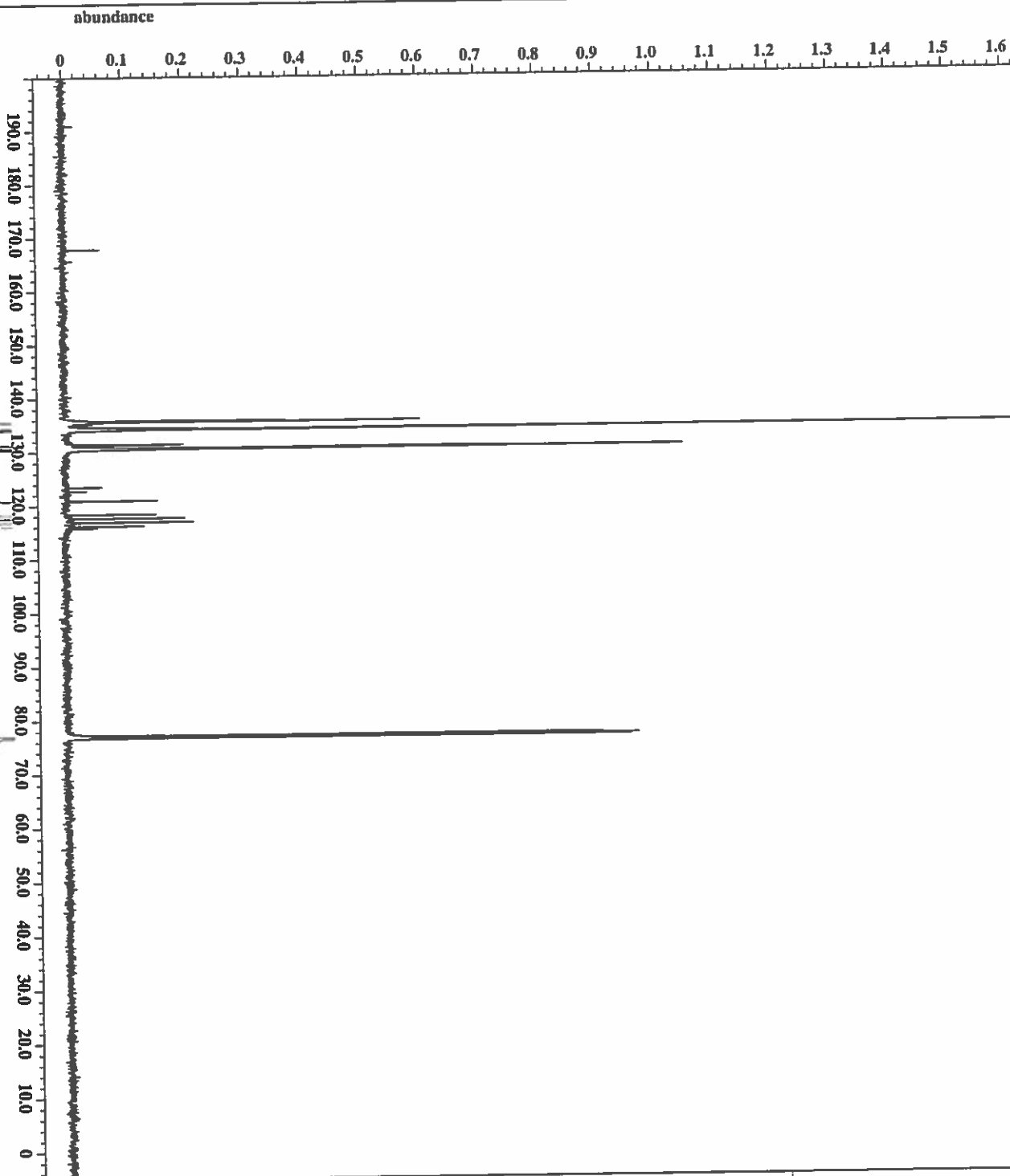
Filename = MS0567-200-96h_PROTON
 Author = Jim Davis
 Experiment = single_pulse_2x2
 Sample_id = MS0567-200-96h
 Solvent = CHLOROFORM-D
 Creation_time = 8-OCT-2018 09:48:43
 Revision_time = 8-OCT-2018 09:23:22
 Current_time = 8-OCT-2018 09:23:22

 Data_format = 1D COMPLEX
 Dir_size = 13107
 Dir_title = 1H
 Dir_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

 Field_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 1.74587904 [s]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.57277737 [Hz]
 X_sweep = 9.38438438 [kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 T1_domain = 1H
 T1_freq = 500.15991521 [MHz]
 T1_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

 X_90_width = 12.4 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_atn = 4 [dB]
 X_pulse = 6.2 [us]
 Irr_mode = OFZ
 T1_mode = FALSE
 Dante_presat = 1 [s]
 Initial_wait = 30
 Recvr_gain = 5.74587904 [s]
 Relaxation_delay = 4 [s]
 Repetition_time = 22.9 [s]
 Temp_get = 22.9 [C]





```

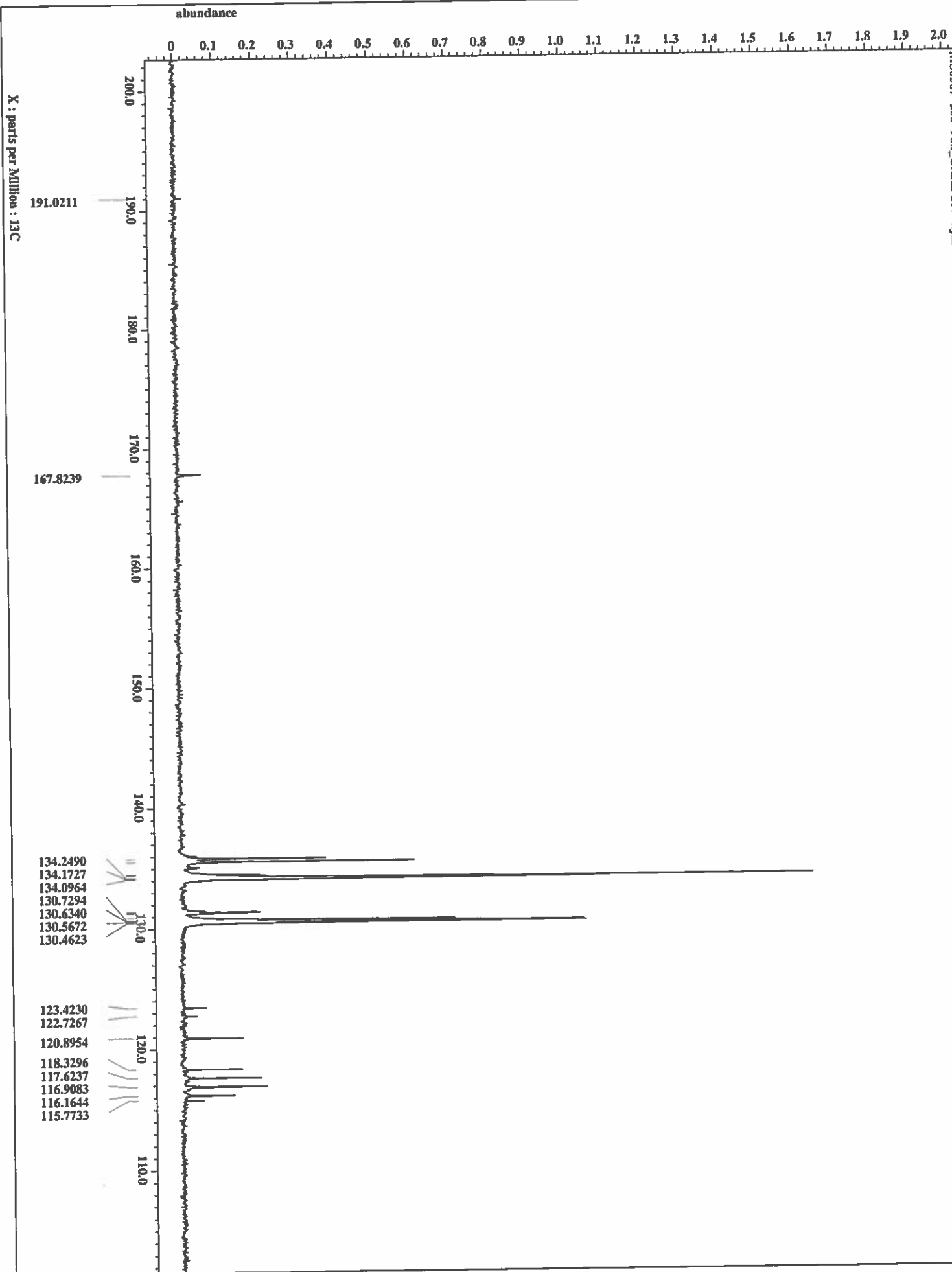
=====
Filename      = MS0567-200-96h_CARBON
Author        = Jim Davis
Experiment    = single-pulse-dec
Sample_id     = MS0567-200-96h
Solvent       = CHLOROFORM-D
Creation_time = 8-OCT-2018 10:02:05
Revision_time = 8-OCT-2018 09:36:43
Current_time  = 8-OCT-2018 09:36:43

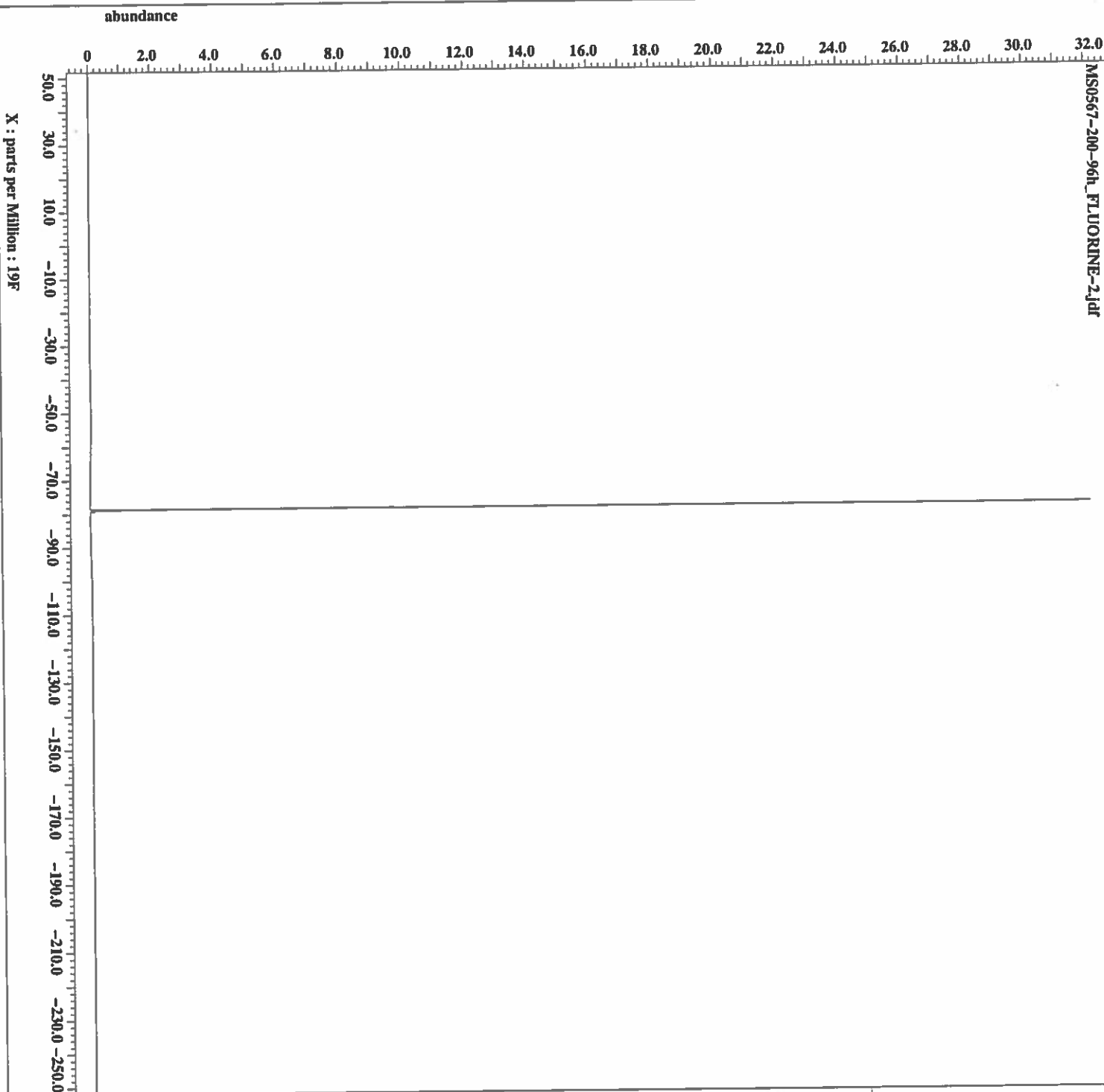
Data_format   = 1D COMPLEX
Data_size     = 26214
Data_title    = 13C
Data_units    = [ppm]
Dimensions    = X
Site          = QCA 500
Spectrometer  = QNP-ZCA500

Field_strength = 11.7473579 [T] (500 [MH]
Acq_duration   = 0.83361792 [s]
=====
X_domain      = 13C
X_freq        = 125.76529766 [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]
Mod_return    = VALSE
Scans         = 1
Total_scans   = 256

X_90_width    = 13.2 [us]
X_acq_time    = 0.83361792 [s]
X_angle       = 30 [deg]
X_atn         = 6 [dB]
X_pulse       = 4.4 [us]
Irr_atn_dec   = 20.7 [dB]
Irr_atn_noe   = 20.7 [dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1 [s]
Noe           = TRUE
Noe_time      = 2 [s]
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set      = 22.9 [deg]
=====

```





```

Filename      = MS0567-200-96h_FLUORI
Anchor        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0567-200-96h
Solvent       = CHLOROFORM-D
Creation_time  = 8-OCT-2018 10:05:45
Revision_time  = 8-OCT-2018 09:40:25
Current_time   = 8-OCT-2018 09:40:25

Data_format    = 1D COMPLEX
Dim_size       = 104857
Dim_title      = 19F
Dim_units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.7340032[s]
X_domain       = 19F
X_freq         = 470.62066084[MHz]
X_offset       = -100[ppm]
X_points       = 131072
X_prescans     = 1
X_resolution   = 1.36239188[Hz]
X_sweep        = 178.57142857[kHz]
Irr_domain     = 19F
Irr_freq       = 470.62066084[MHz]
Irr_offset     = 51[ppm]
Tri_domain     = 19F
Tri_freq       = 470.62066084[MHz]
Tri_offset     = 51[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 20
Total_scans    = 20

X_90_width     = 13.1[us]
X_acq_time     = 0.7340032[s]
X_angle        = 45[deg]
X_etn          = 2.5[ds]
X_pulse        = 6.55[us]
Irr_mode       = OFT
Tri_mode       = OFT
Dante_presat   = FALSE
Initial_wait   = 1[se]
Recvr_gain     = 54
Relaxation_delay = 4[se]
Repetition_delay = 4.7340032[s]
Temp_get       = 22.5[dc]

```

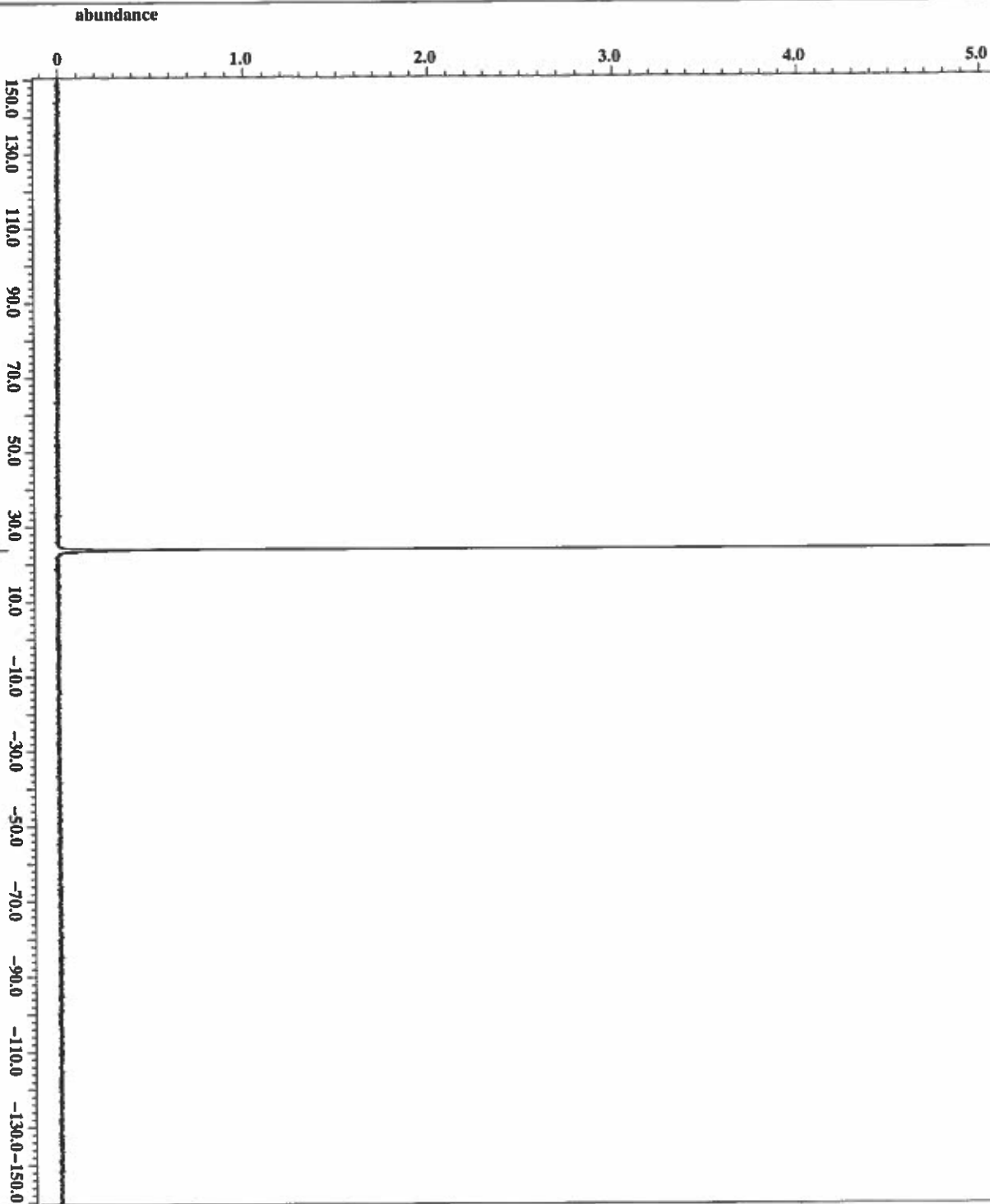


Filename = MS0567-200-96h_PHOSPH
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = MS0567-200-96h
 Solvent = CHLOROFORM-D
 Creation_time = 8-OCT-2018 10:09:52
 Revision_time = 8-OCT-2018 09:44:30
 Current_time = 8-OCT-2018 09:44:30

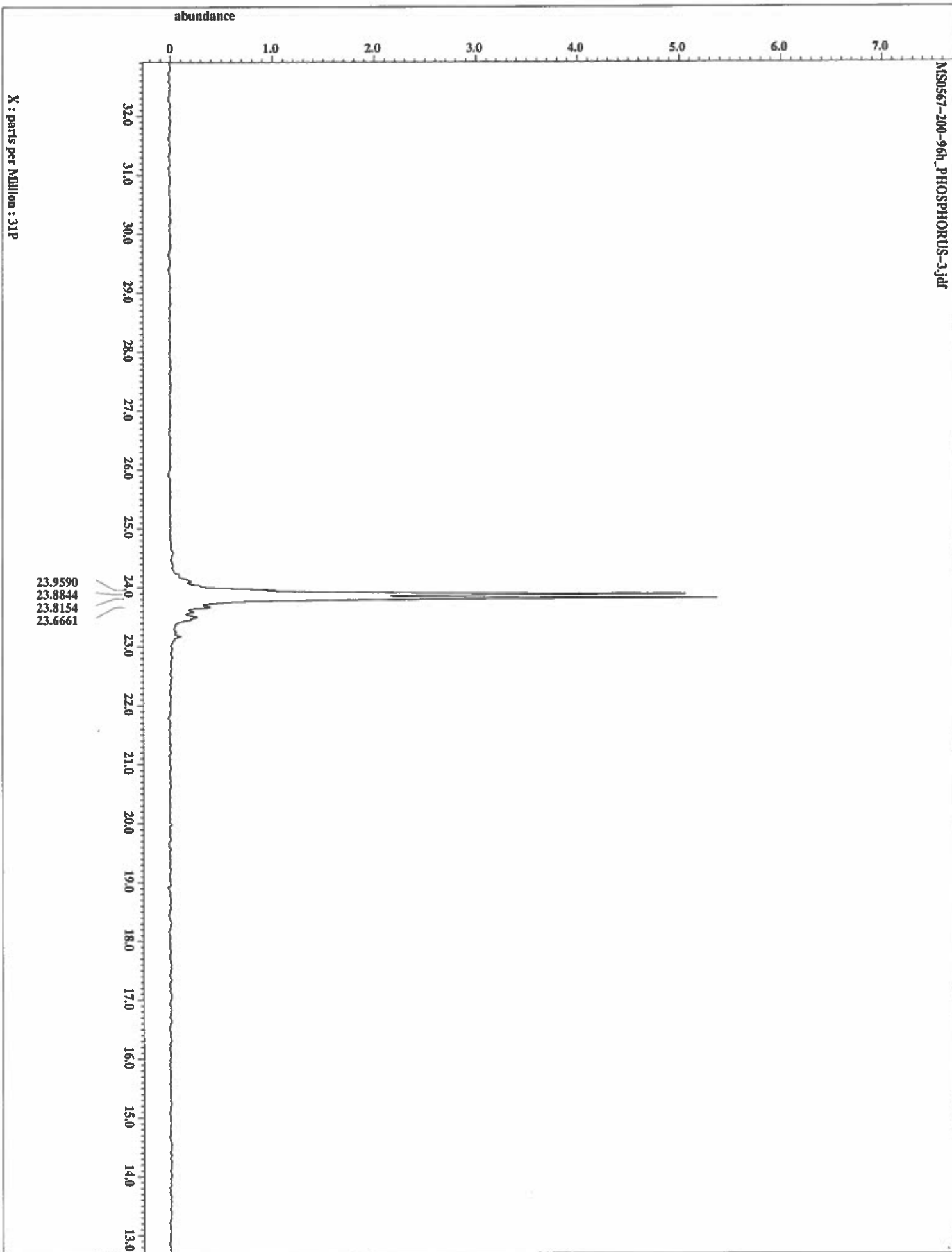
Data format = 1D COMPLEX
 Dim_size = 52428
 Dim_title = 31P
 Dim_units = [ppm]
 Dimensions = x
 Site = ECA 500
 Spectrometer = JNM-ECA500

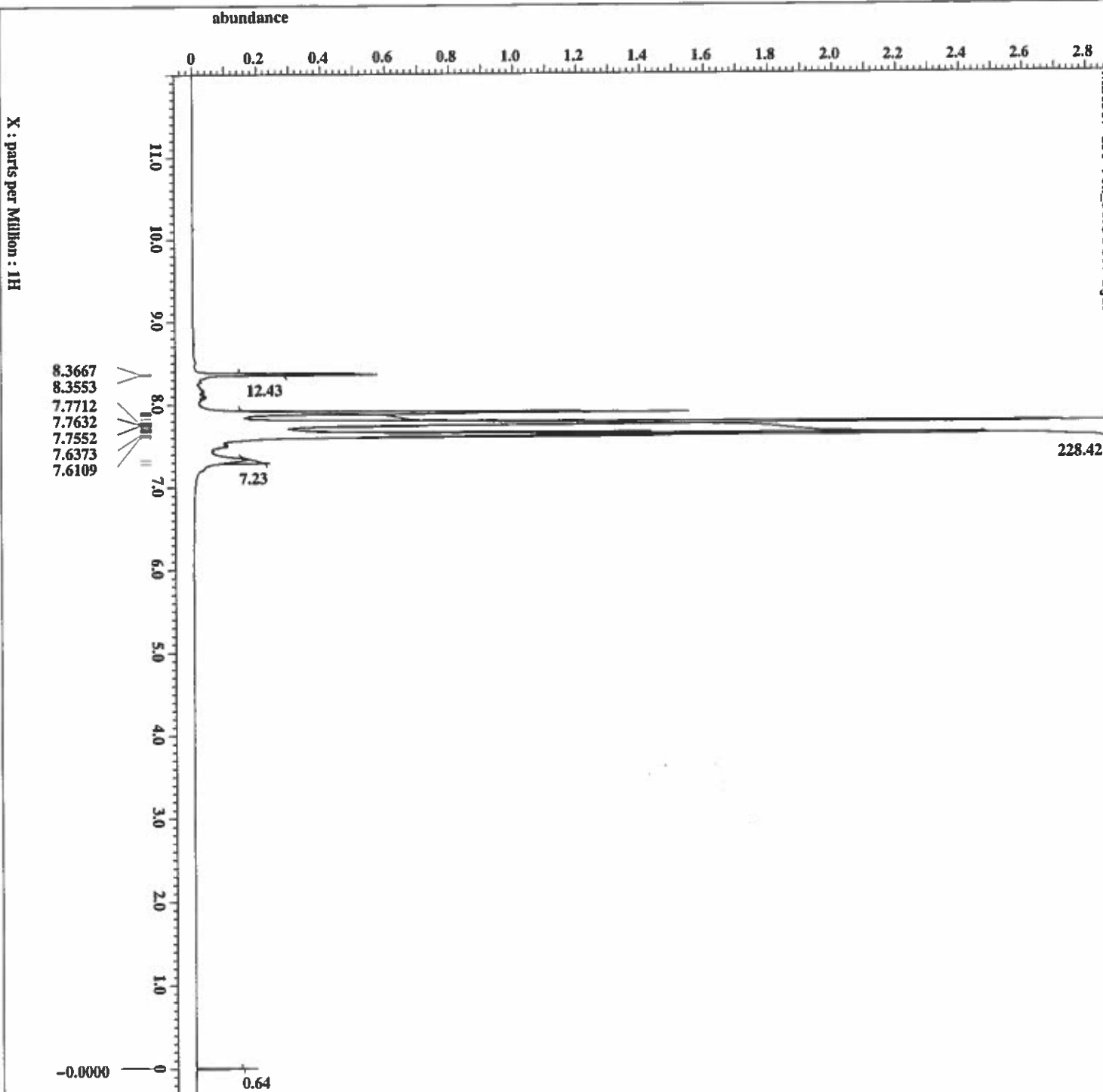
Pfield_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 0.8598332 [s]
 X_domain = 31P
 X_freq = 202.46831075 [MHz]
 X_offset = 0 [ppm]
 X_points = 65536
 X_prescans = 4
 X_resolution = 1.16301746 [Hz]
 X_sweep = 76.2195122 [kHz]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 30
 Total_scans = 30

X_90_width = 14.687 [us]
 X_acq_time = 0.8598332 [s]
 X_angle = 30 [deg]
 X_atn = 5 [dB]
 X_pulse = 4.89566667 [us]
 Xir_atn_dec = 20.7 [dB]
 Xir_atn_noe = 20.7 [dB]
 Xir_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 56
 Relaxation_delay = 2 [s]
 Repetition_time = 2.8598332 [s]
 Temp_get = 22.9 [dC]



X : parts per Million : 31P





228.42



SOUTH ALABAMA
JAGUARS

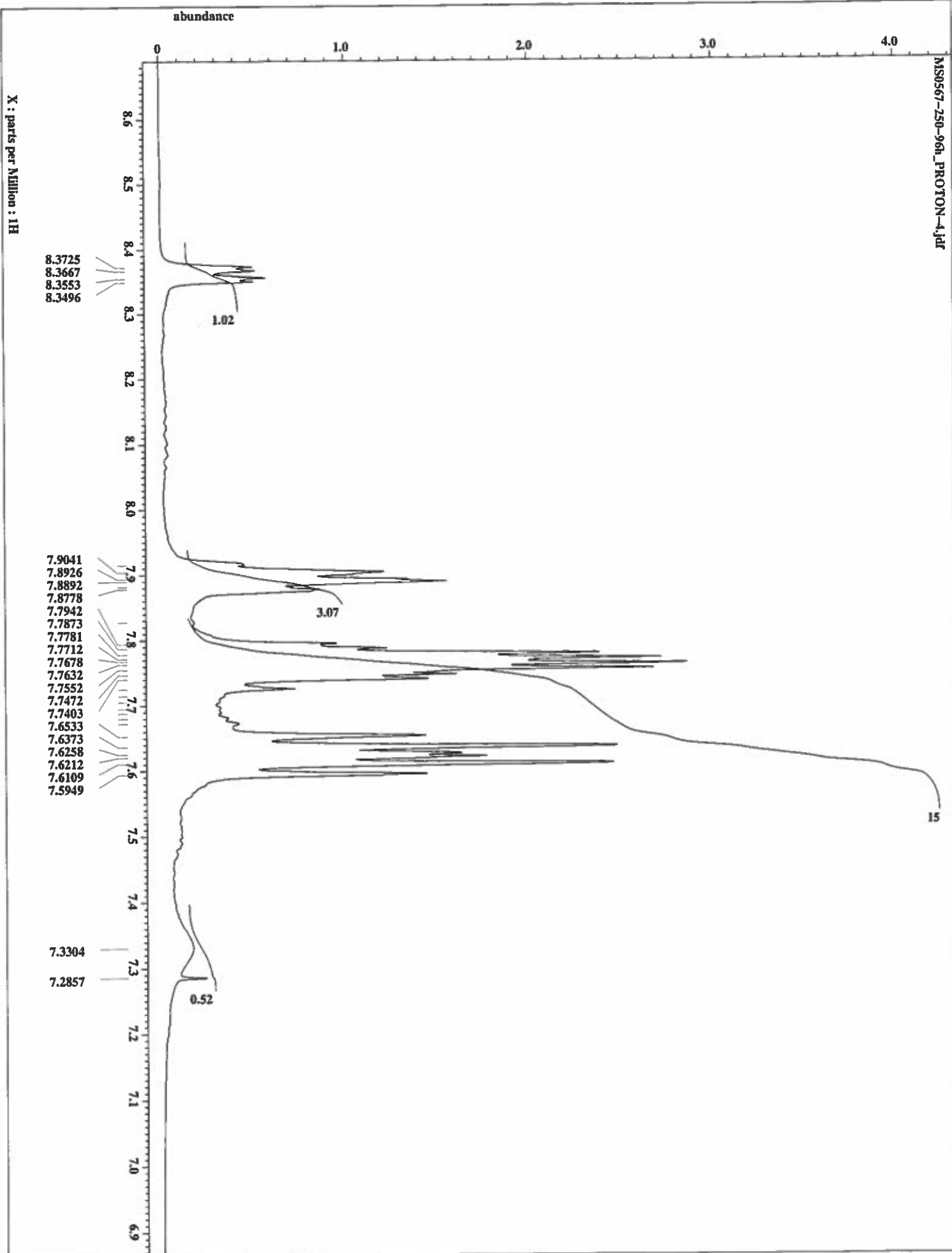
```

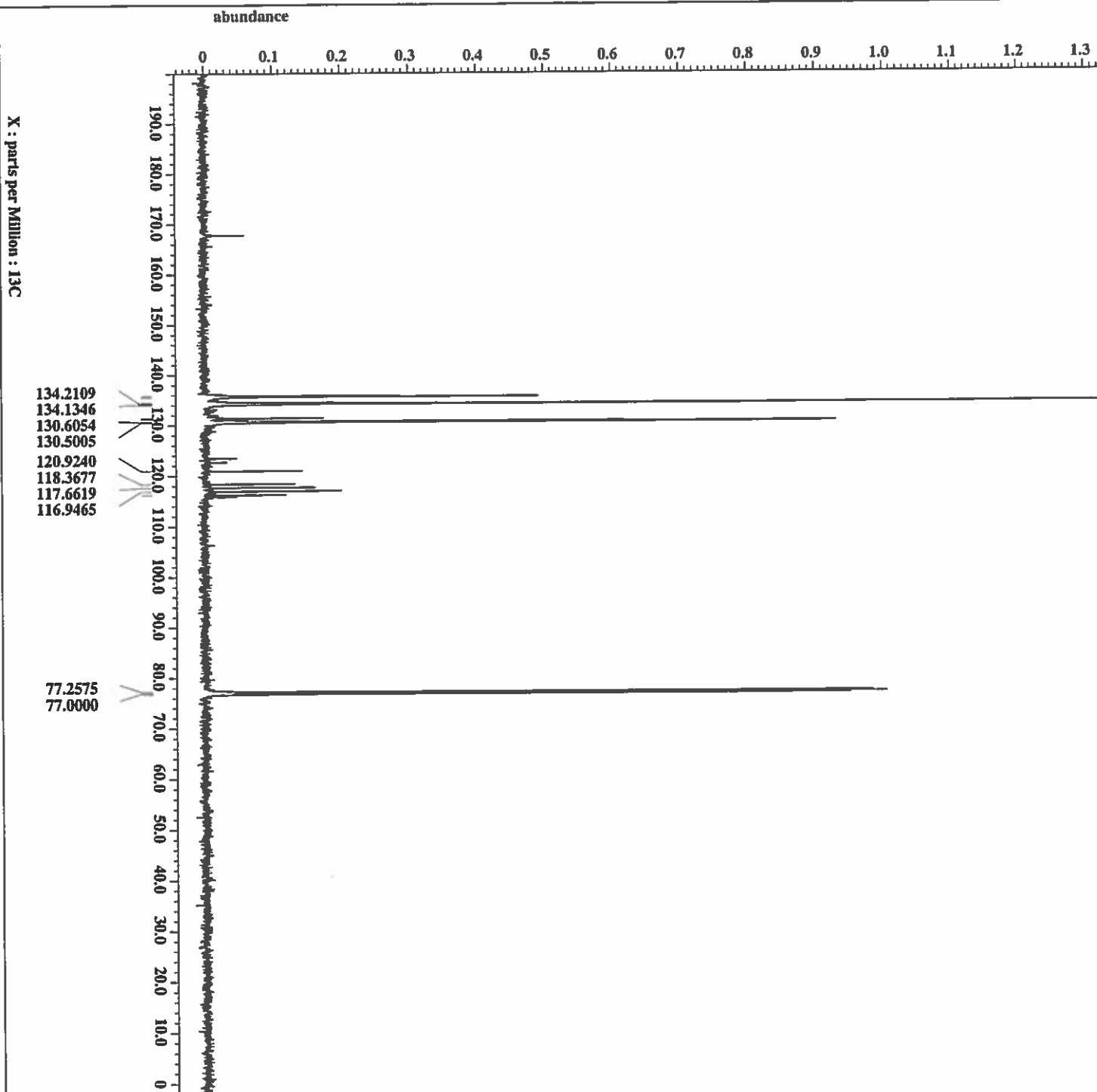
Filename      = MS0567-250-96h_PROTON
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = MS0567-250-96h
Solvent       = CHLOROFORM-D
Creation_time = 8-OCT-2018 10:17:25
Revision_time = 8-OCT-2018 09:52:04
Current_time  = 8-OCT-2018 09:52:04

Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 9.38438438 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Pulse          = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 12.4 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [db]
X_pulse        = 6.2 [us]
Irr_pulse      = 6.2 [us]
Irr_mode       = Off
Pulse_preset   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 26
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_set       = 22.7 [deg]
  
```





```

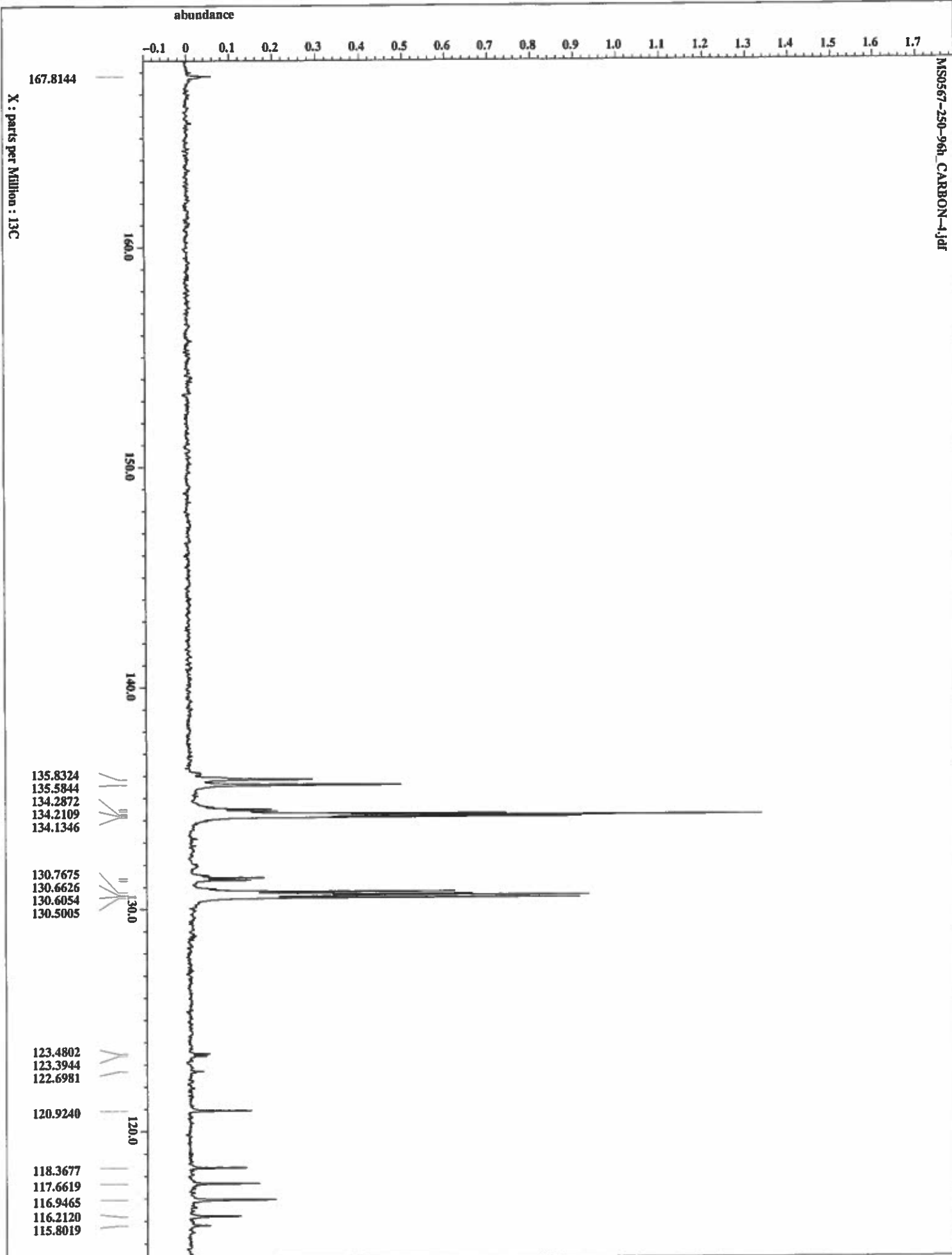
File name      = MS0567-250-96h_CARBON
Author         = Jim Davis
Experiment     = single_pulse_dec
Sample id      = MS0567-250-96h
Solvent        = CHLOROFORM-D
Creation time   = 8-OCT-2018 10:30:48
Revision time  = 8-OCT-2018 10:05:27
Current time   = 8-OCT-2018 10:05:27

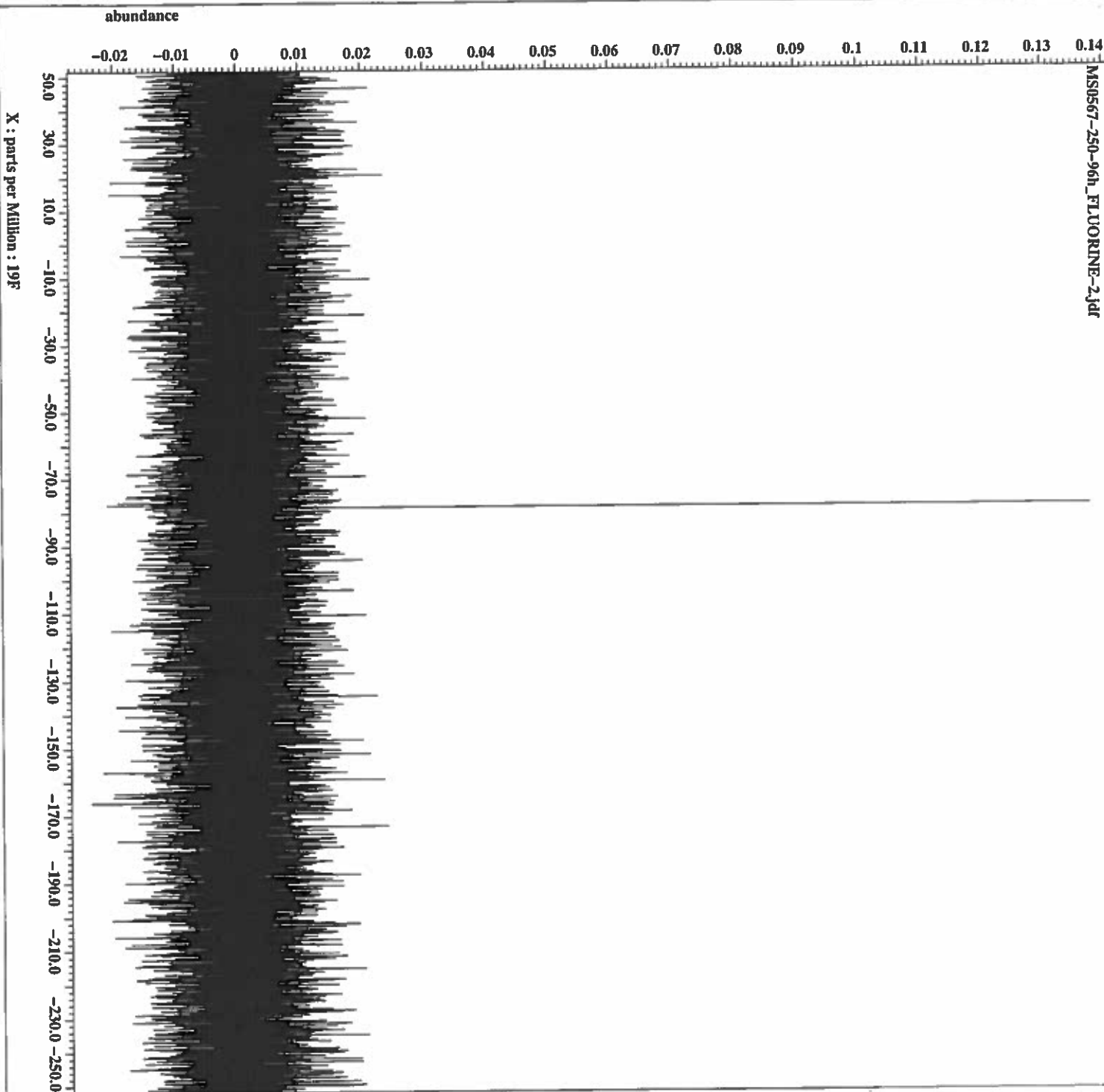
Data format    = 1D COMPLEX
Dim size       = 26214
Dim title      = 13C
Dim units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

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]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 256
Total_scans    = 256

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [db]
X_pulse        = 4.4 [us]
Xir_atn_dec    = 20.7 [db]
Xir_atn_noe    = 20.7 [db]
Xir_noise      = WALTZ
Decoupling     = TRUZ
Initial_wait   = 1 [s]
Noe            = TRUZ
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get       = 23.3 [degC]

```





```

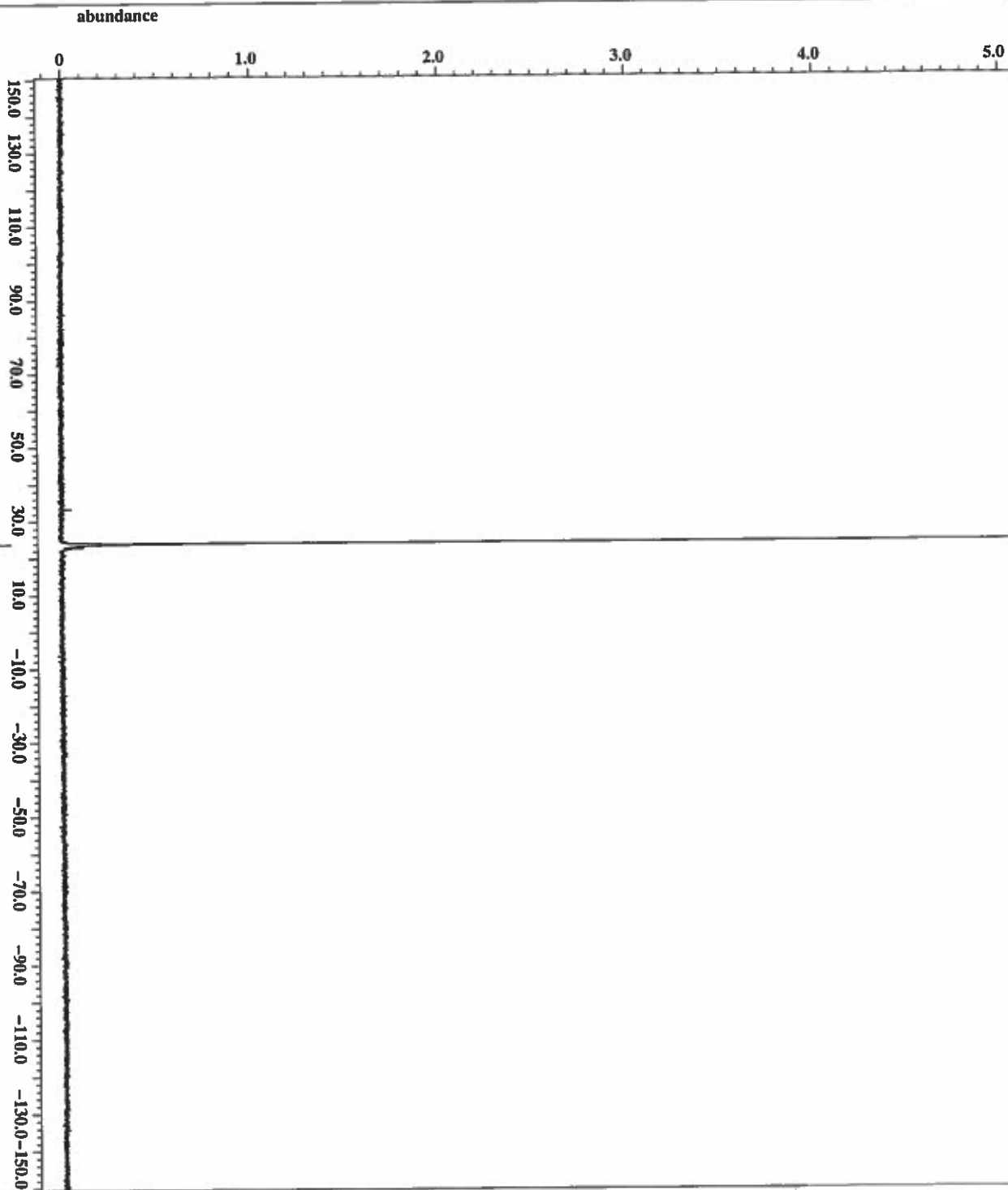
Filename      = MS0567-250-96h_FLUORINE
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = MS0567-250-96h
Solvent       = CHLOROFORM-D
Creation_time  = 8-OCT-2018 10:35:00
Revision_time = 8-OCT-2018 10:09:40
Current_time  = 8-OCT-2018 10:09:40

Data_format   = 1D COMPLEX
Dim_size      = 104857
Dim_title     = 19F
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.7340032[s]
X_domain       = 19F
X_freq         = 470.62046084[MHz]
X_offset       = -100[ppm]
X_points       = 131072
X_prescans     = 1
X_resolution   = 1.36239188[Hz]
X_sweep        = 178.57142857[kHz]
Xir_domain    = 19F
Xir_freq       = 470.62046084[MHz]
Xir_offset     = 5[ppm]
Xir_domain    = 19F
Xir_freq       = 470.62046084[MHz]
Xir_offset     = 5[ppm]
Xir_mode       = FALSE
Mod_return     = 1
Scans          = 20
Total_scans    = 20

X_90_pulch    = 13.1[us]
X_acq_time     = 0.7340032[s]
X_angle       = 45[deg]
X_atn         = 2.5[db]
X_pulse       = 6.55[us]
Xir_mode      = off
Xir_mode       = off
Pulse         = FALSE
Initial_wait   = 1[s]
Recvr_gain    = 70
Relaxation_delay = 4[s]
Repetition_time = 4.7340032[s]
Temp_get       = 22.9[degC]

```



X : parts per Million : 31P



```

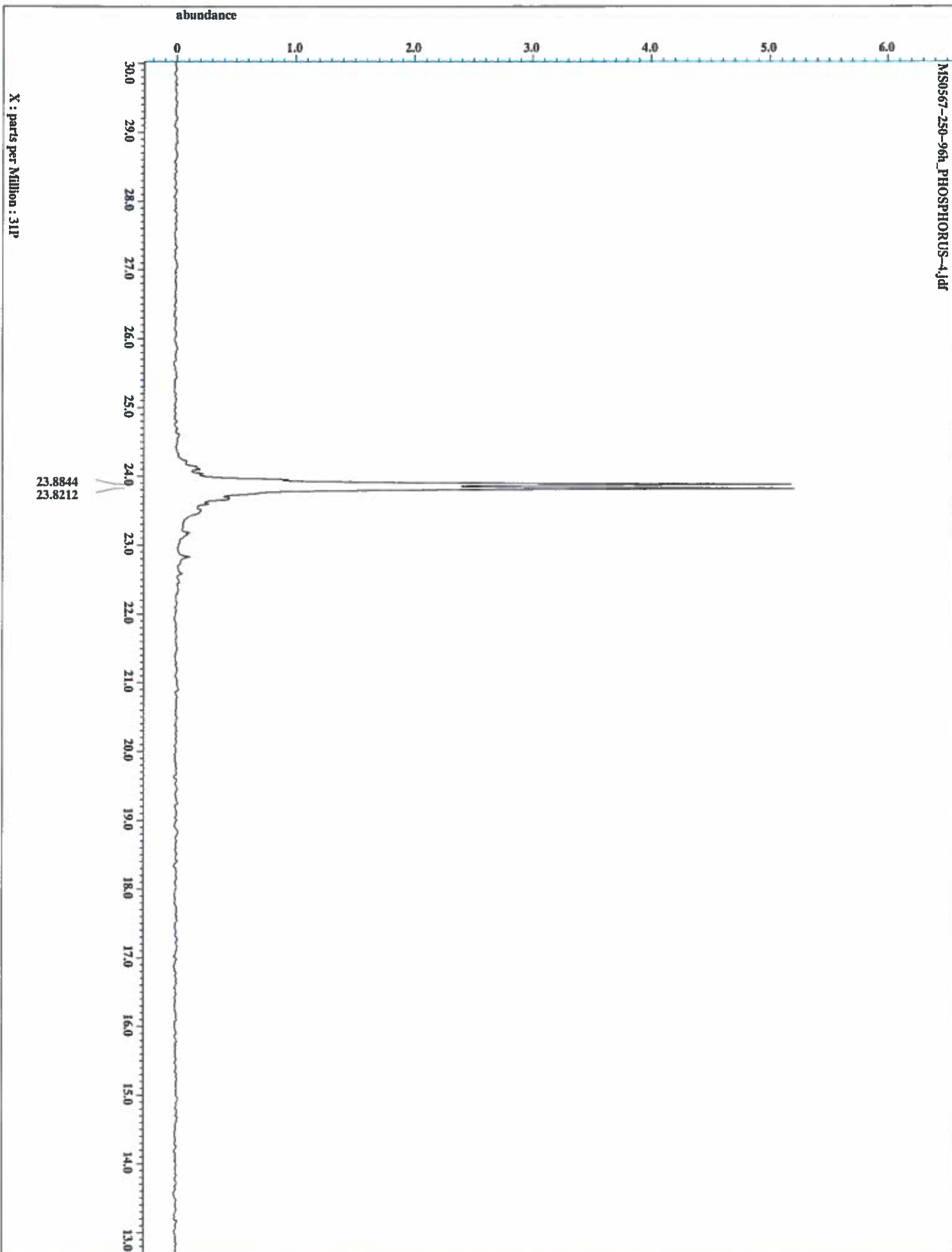
Filename      = MS0567-250-96h_PHOSPH
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0567-250-96h
Solvent       = CHLOROFORM-D
Creation_time = 8-OCT-2018 10:39:10
Revision_time = 8-OCT-2018 10:13:49
Current_time  = 8-OCT-2018 10:13:49

Data_format   = 1D COMPLEX
Dim_size      = 52428
Dim_title     = 31P
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500 [MH
X_acq_duration = 0.8598332[s]
X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 65536
X_prescans     = 4
X_resolution   = 1.16301746[Hz]
X_sweep        = 76.2195122[kHz]
Xt_domain      = 1H
Xt_freq        = 500.15991521 [MHz]
Xt_offset      = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 30
Total_scans    = 30

X_90_width     = 14.687[us]
X_acq_time     = 0.8598332[s]
X_angle        = 30[deg]
X_atn          = 5[db]
X_pulse        = 4.89566667[us]
Irr_atn_dec    = 20.7[db]
Irr_atn_noe    = 20.7[db]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe_time       = TRUE
Noe_delay      = 2[s]
Noe_gain       = 58
Relaxation_delay = 2[s]
Repetition_time = 2.8598322[s]
Temp_get       = 23.3[degC]

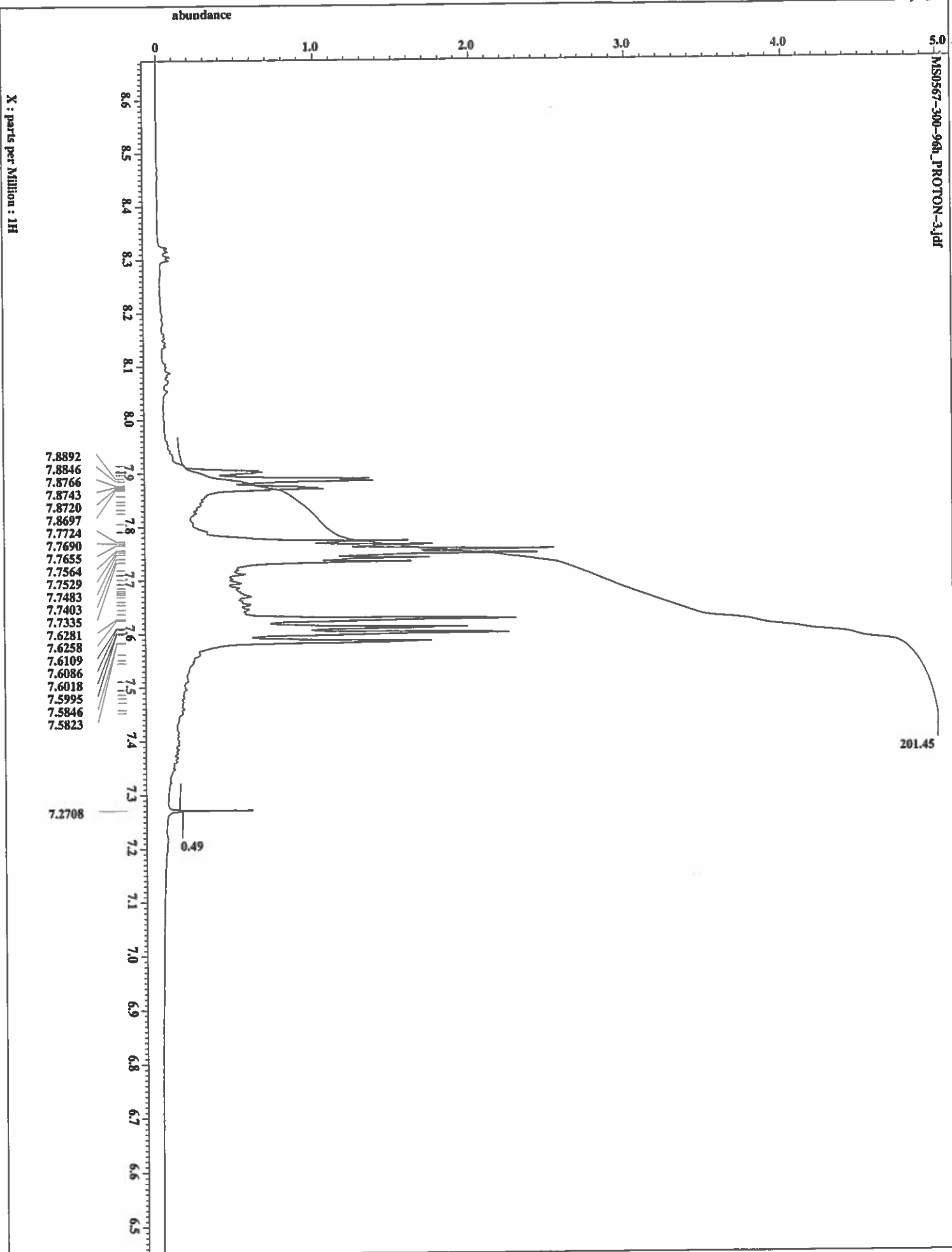
```

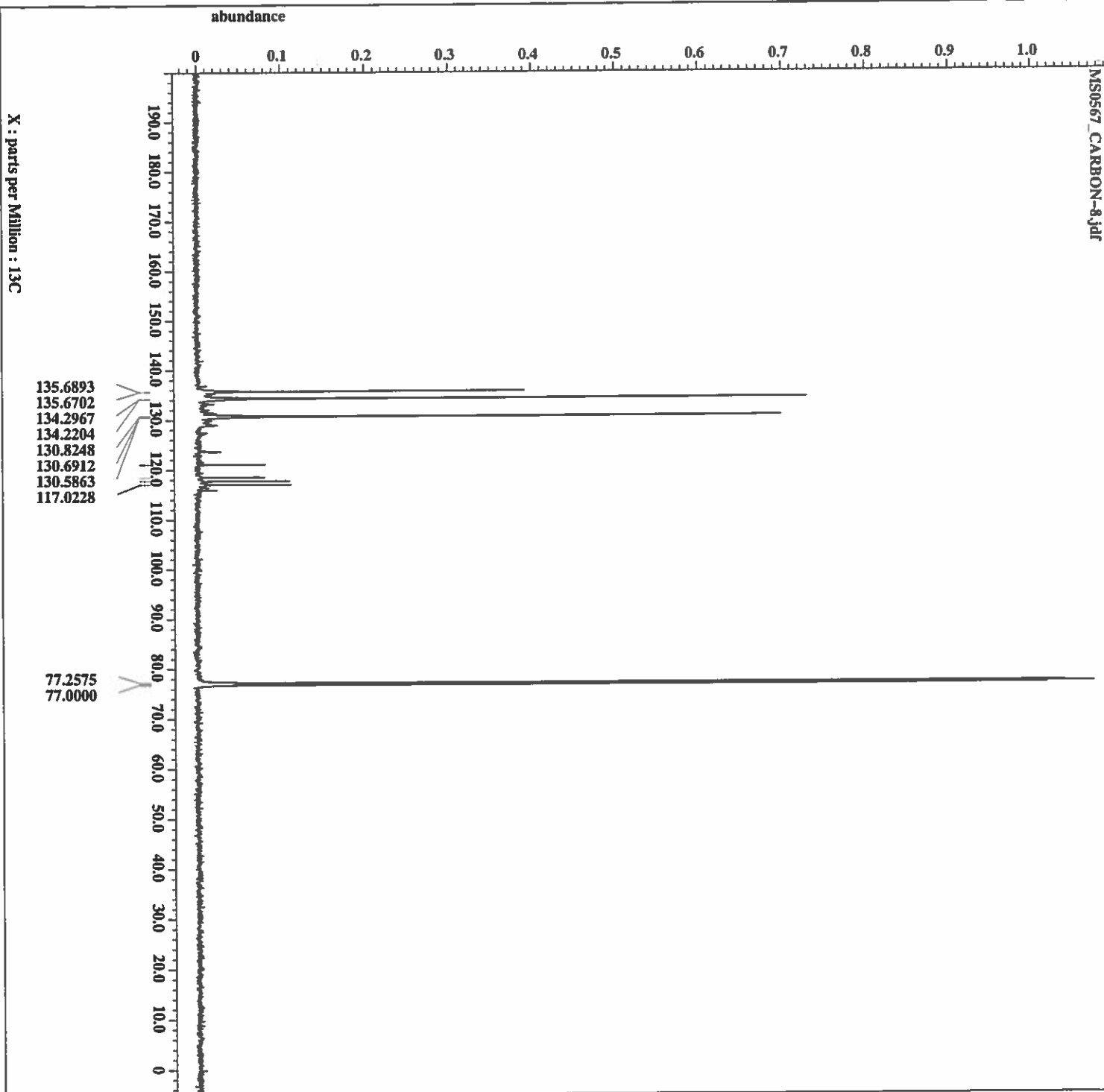




7.7564
7.7483
7.6281
7.6258
7.6018
7.5995

Filename	MS0567-300-96n_PROTON
Author	Jim Davis
Experiment	single_pulse.ex2
Sample_id	MS0567-300-96n
Solvent	CHLOROFORM-D
Creation_time	8-OCT-2018 10:46:10
Revision_time	8-OCT-2018 10:20:47
Current_time	8-OCT-2018 10:20:47
Date_format	1D COMPLEX
Dim_size	13107
Dim_title	1H
Dim_units	[ppm]
Dimensions	X
Size	2CA 500
Spectrometer	JNM-ZCA500
Field_strength	11.74735791[T] (500[MH
X_acq_duration	1.74587904[s]
X_domain	1H
X_freq	500.15991521[MHz]
X_offset	5.01[ppm]
X_points	16384
X_prescans	1
X_resolution	0.57277377[Hz]
X_sweep	9.3843838[kHz]
1H_domain	1H
1H_freq	500.15991521[MHz]
1H_offset	5.01[ppm]
1H_domain	1H
1H_freq	500.15991521[MHz]
1H_offset	5.01[ppm]
1H_domain	1H
1H_freq	500.15991521[MHz]
1H_offset	5.01[ppm]
Clipped	FALSTZ
Good_return	1
Scans	16
Total_scans	16
X_90_width	12.4[us]
X_acq_time	1.74587904[s]
X_angle	45[deg]
X_atn	4[db]
X_pulse	6.2[us]
1H_mode	OFF
1H_mode	OFF
Dante_preset	FALSTZ
Initial_wait	1[s]
Recv_gain	30
Relaxation_delay	4[s]
Repetition_time	5.74587904[s]
Temp_get	23[degC]





```

Filename      = MS0567 CARBON-8.jdr
Author        = Jim Davis
Experiment     = single_pulse_dec
Sample_id     = MS0567
Solvent       = CHLOROFORM-D
Creation_time  = 8-OCT-2018 18:35:33
Revision_time  = 8-OCT-2018 18:10:09
Current_time   = 8-OCT-2018 18:10:09

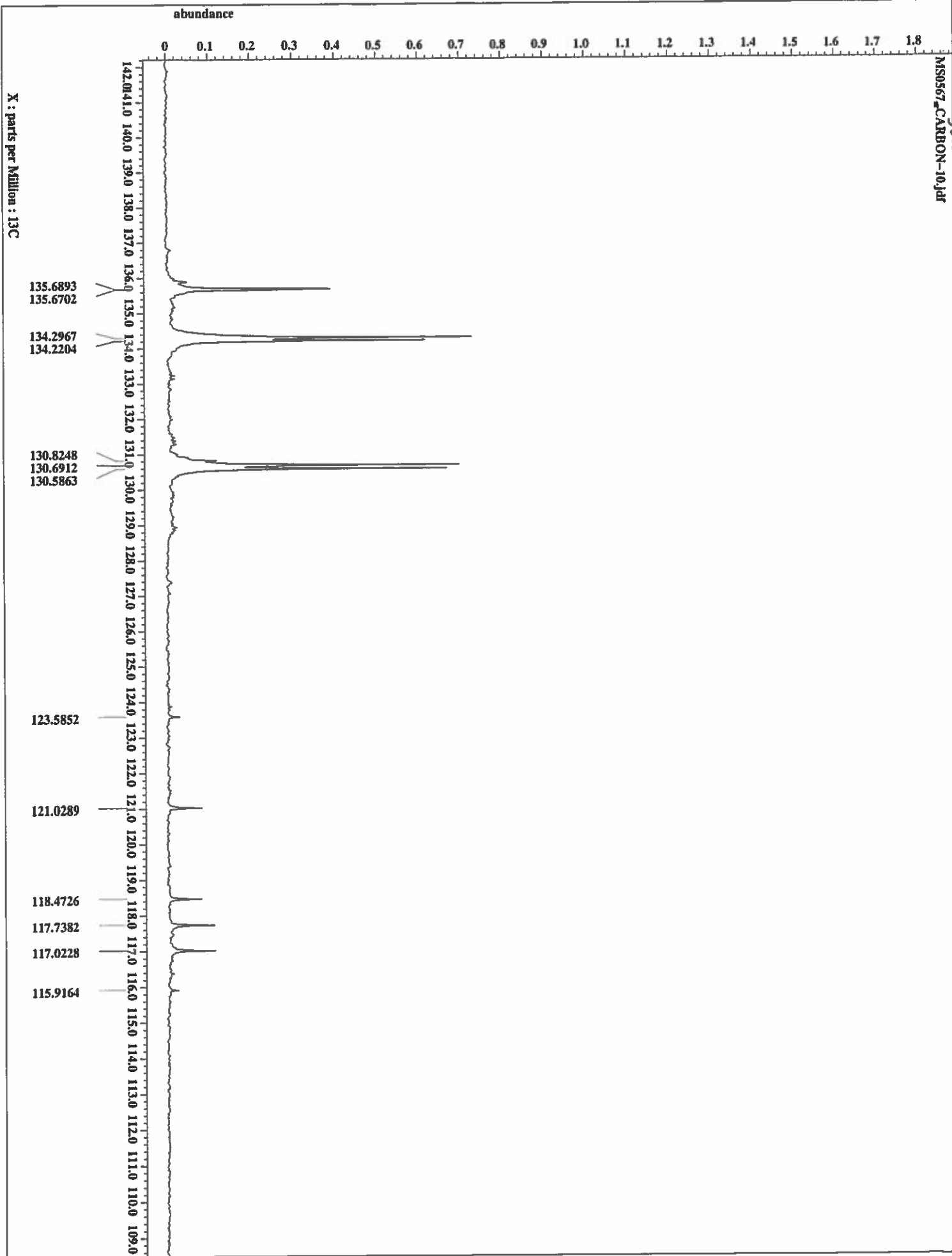
Data_format    = 1D COMPLEX
Dim_size       = 26214
Dim_title      = 13C
Dim_units      = [ppm]
Dimensions     = X
Site           = FCA 500
Spectrometer   = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76539768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Xr_domain      = 1H
Xr_freq        = 500.13991521 [MHz]
Xr_offset      = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 1024
Total_scans    = 1024

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn         = 6 [dB]
X_pulse        = 4.4 [us]
Xr_atn_dec     = 20.7 [dB]
Xr_atn_noe     = 20.7 [dB]
Xr_noise       = WALTZ
Decoupling     = TRUZ
Initial_wait   = 1 [s]
Noe            = TRUZ
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get       = 23.5 [degC]

```

20°C - 96h



abundance

0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0

50.0 30.0 10.0 -10.0 -30.0 -50.0 -70.0 -90.0 -110.0 -130.0 -150.0 -170.0 -190.0 -210.0 -230.0 -250.0

X : parts per Million : 19F


SOUTH ALABAMA
JAGUARS

```

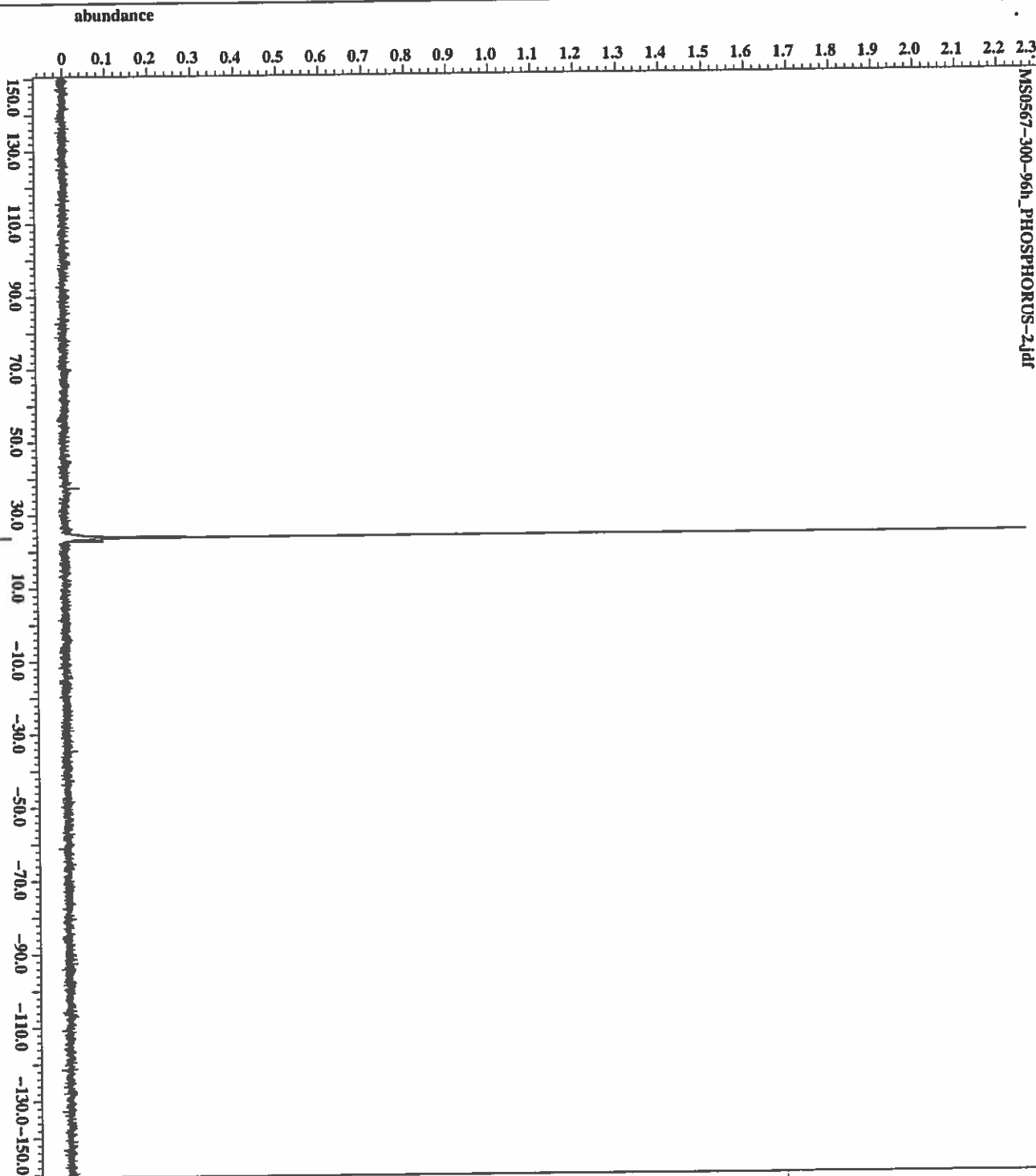
Filename      = MS0567-300-96h_FLUORINE
Author        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0567-300-96h
Solvent       = CHLOROFORM-D
Creation_time  = 8-OCT-2018 11:03:15
Revision_time  = 8-OCT-2018 10:37:54
Current_time   = 8-OCT-2018 10:37:54

Data_format    = 1D COMPLEX
Dim_size       = 104857
Dim_cfile     = 19F
Dim_units     = [ppm]
Dimensions     = X
Site          = ECA 500
Spectrometer   = JNM-ECA500

Field_strength = 11.7473579[G] (500[MHz]
X_acq_duration = 0.7340032[s]
X_domain       = 19F
X_freq         = 470.62046084 [MHz]
X_offset       = -100 [ppm]
X_points       = 131072
X_prescans     = 1
X_resolution   = 1.36239188 [Hz]
X_sweep        = 178.57142857 [kHz]
Xt_domain      = 19F
Xt_freq        = 470.62046084 [MHz]
Xt_offset      = 5 [ppm]
Xt_domain      = 19F
Xt_freq        = 470.62046084 [MHz]
Xt_offset      = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 20
Total_scans    = 20

X_90_width     = 13.1[us]
X_acq_time     = 0.7340032[s]
X_angle        = 45[deg]
X_atn          = 2.5[db]
X_pulse        = 6.5[us]
Xt_mode        = off
Xt_mode        = off
Dante preset   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 64
Relaxation_delay = 4[s]
Repetition_time = 4.7340032[s]
Temp_get       = 22.8[degC]

```



X : parts per Million : 31P



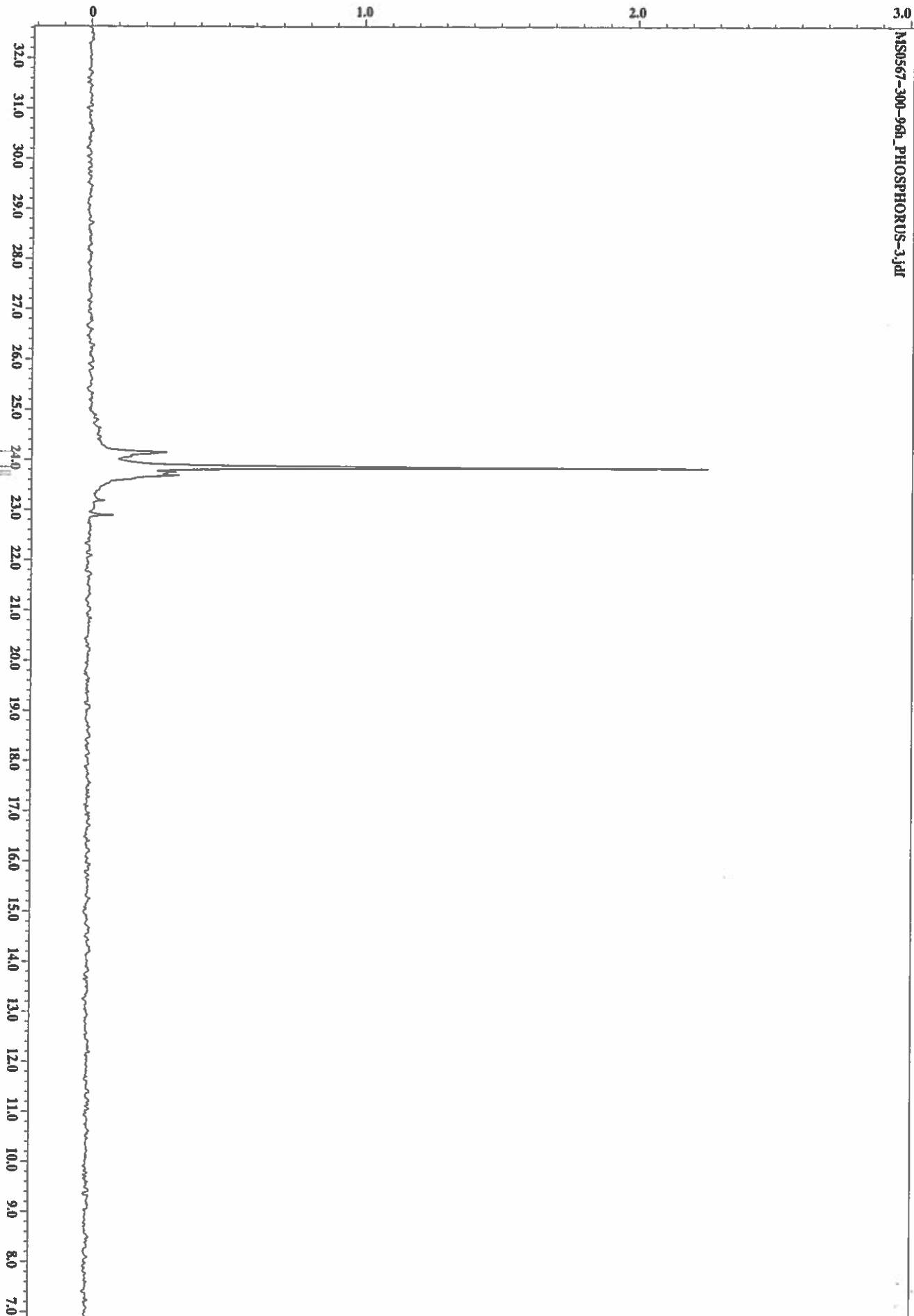
```

Filename      = MS0567-300-96h_PHOSPH
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0567-300-96h
Solvent       = CHLOROFORM-D
Creation_time  = 8-OCT-2018 11:07:22
Revision_time  = 8-OCT-2018 10:42:00
Current_time   = 8-OCT-2018 10:42:00

Data_format   = 1D COMPLEX
Dim_size      = 52428
Dim_title     = 31P
Dim_units     = [ppm]
Dimensions    = X
Site          = FCA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 0.8598332 [s]
X_domain      = 31P
X_freq        = 202.46831075 [MHz]
X_offset      = 0 [ppm]
X_points      = 65536
X_prescans    = 4
X_resolution  = 1.16301746 [Hz]
X_sweep       = 76.2195122 [kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521 [MHz]
Irr_offset    = 5.0 [ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 30
Total_scans   = 30

X_90_width    = 14.687 [us]
X_acq_time     = 0.8598332 [s]
X_angle       = 30 [deg]
X_atn         = 5 [dB]
X_pulse       = 4.89566667 [us]
Irr_atn_dec   = 20.7 [dB]
Irr_atn_noe   = 20.7 [dB]
Irr_noise     = VALTZ
Decoupling    = TRUE
Initial_wait  = 1 [s]
Hoe_time      = TRUE
Hoe_time      = 21 [s]
Recvr_gain    = 56
Relaxation_delay = 21 [s]
Repetition_time = 2.8598332 [s]
Temp_get      = 23.2 [C]
  
```

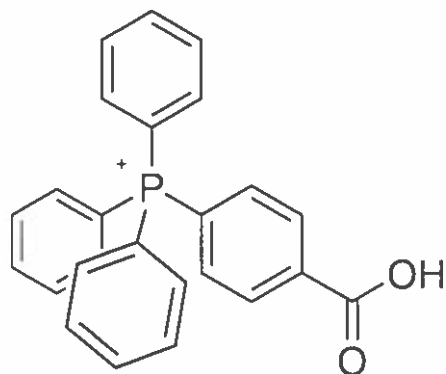
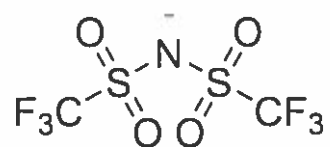


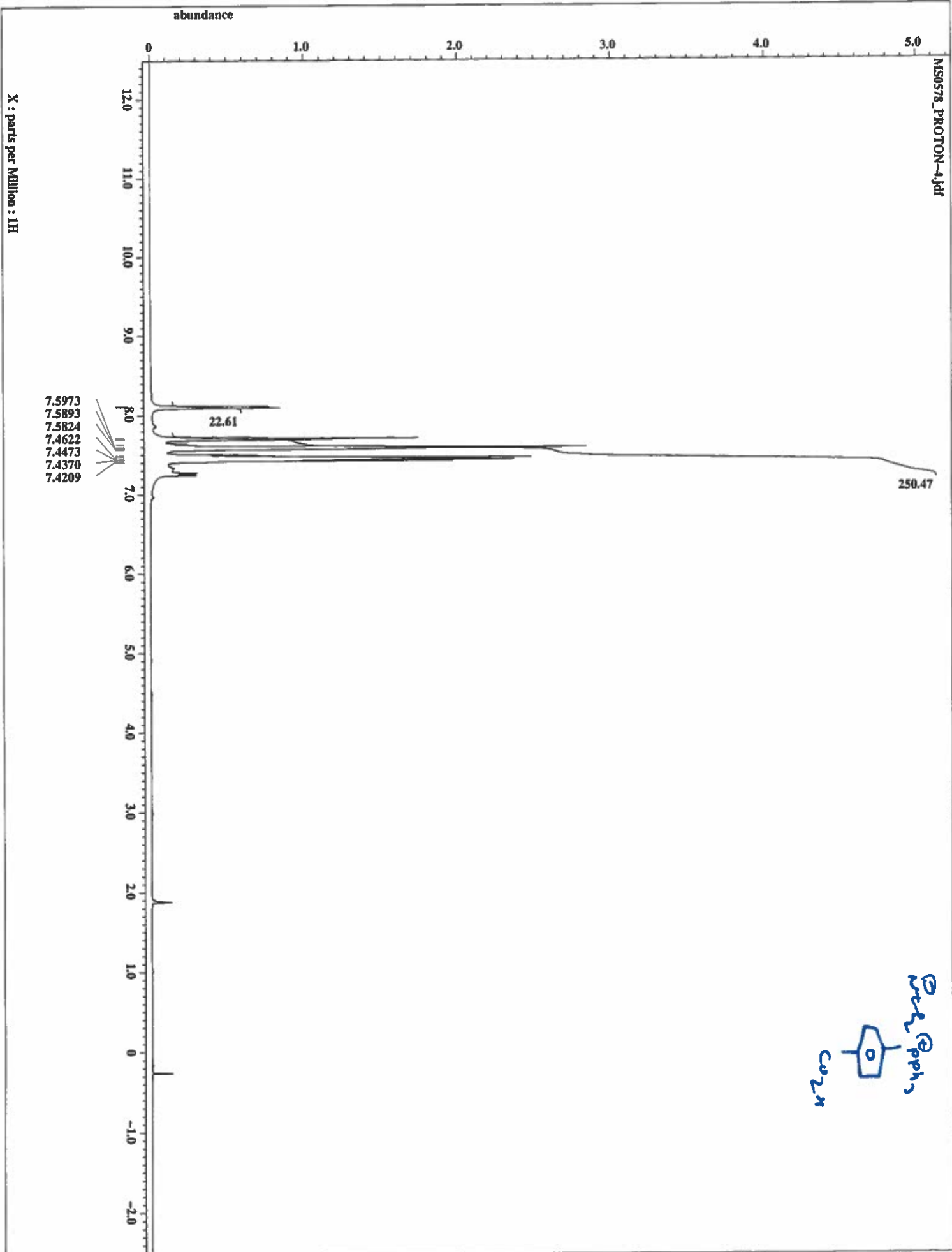
24.1543
23.8499
23.7580
23.6948

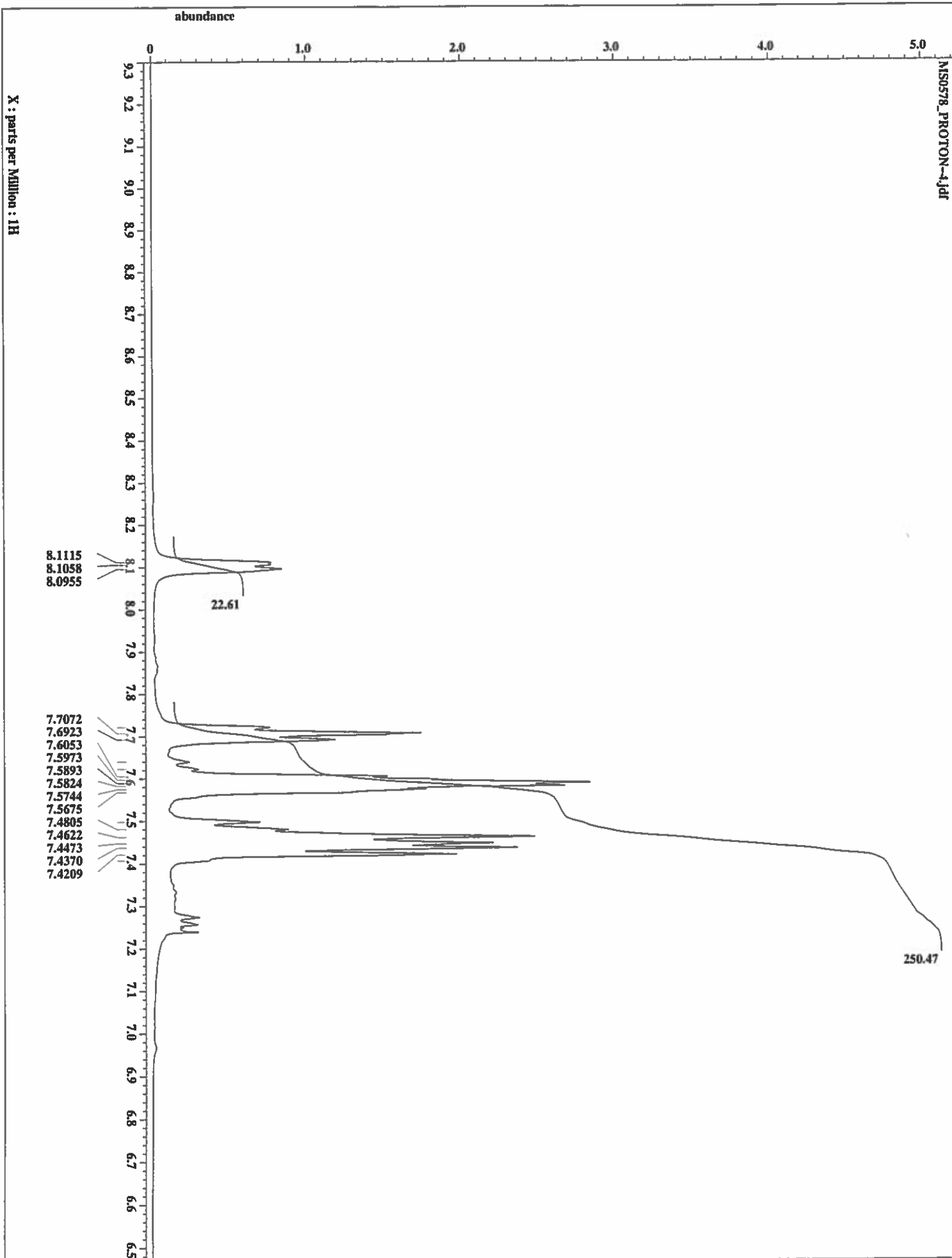
X : parts per Million : 31P

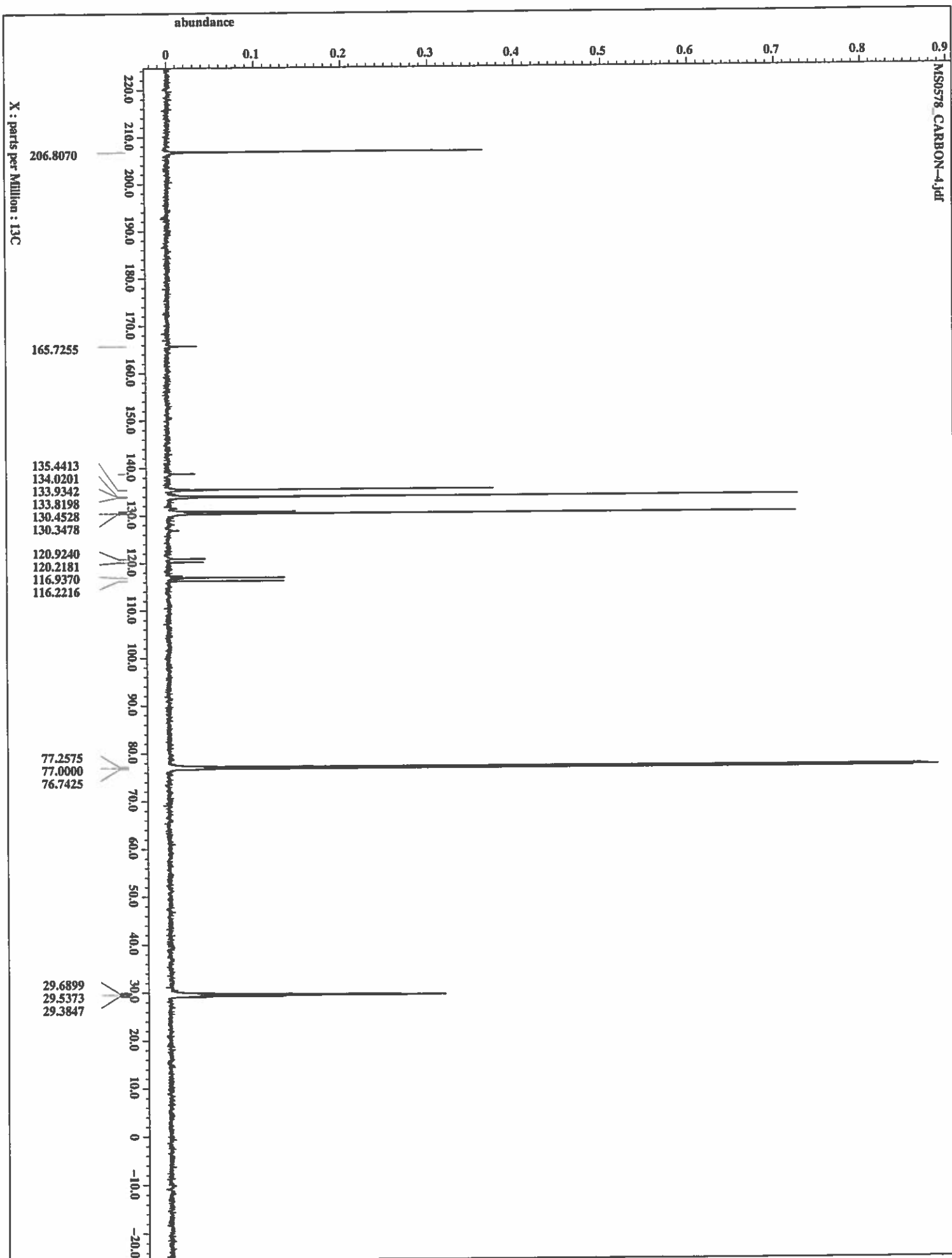
Compound 5 Pre- and Post-heating NMR Spectra

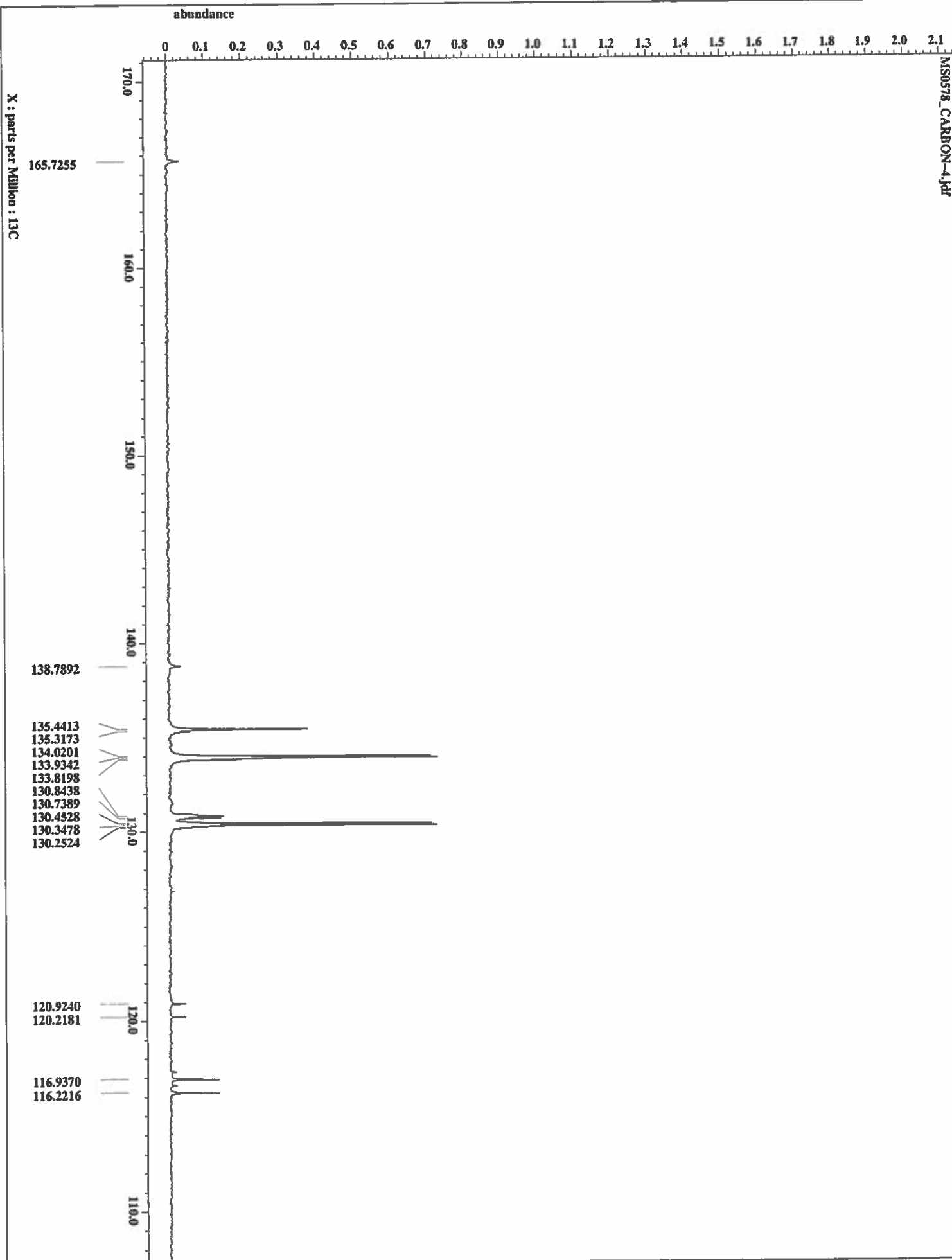
Temperature of Post-heating samples noted in upper left corner of each spectrum

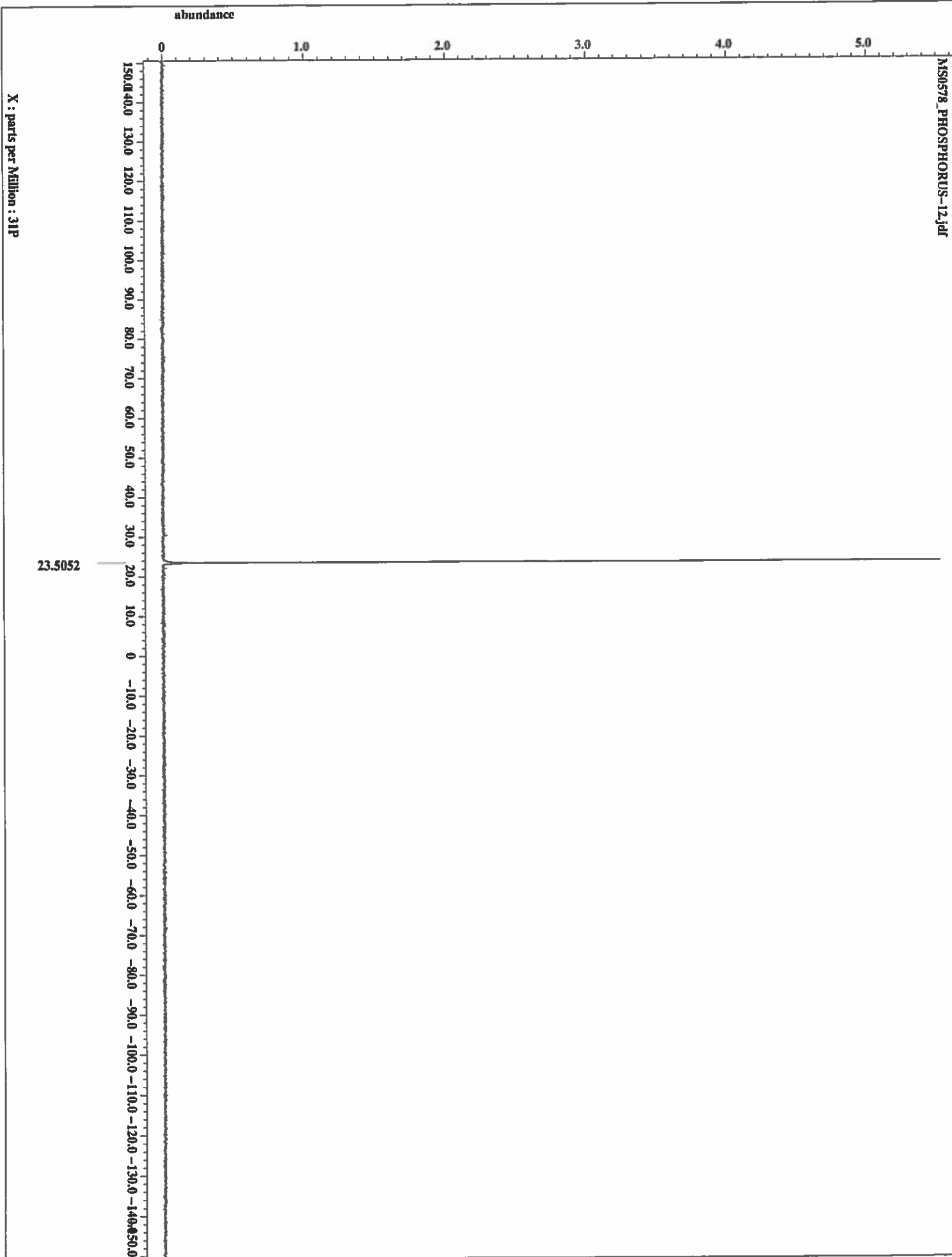


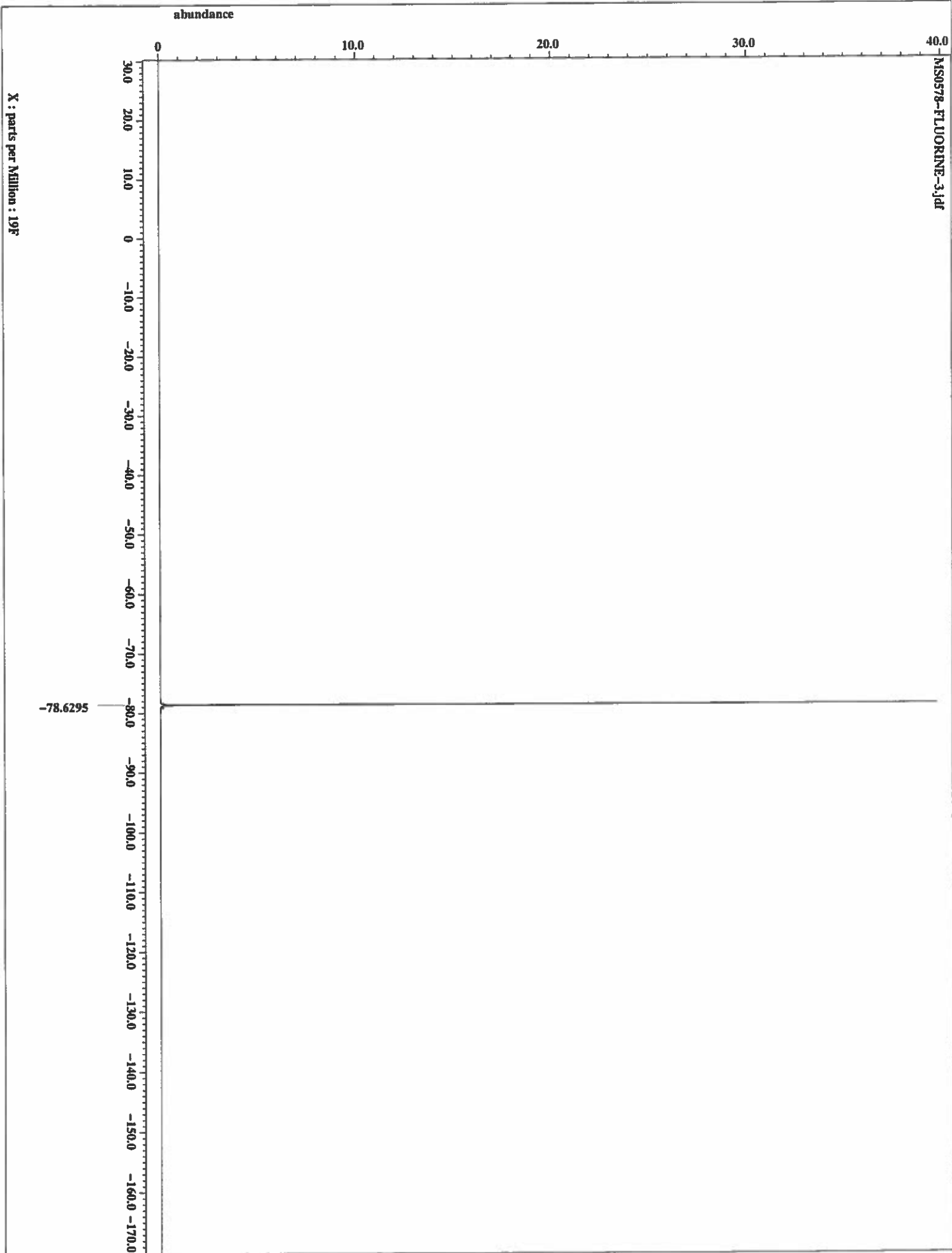






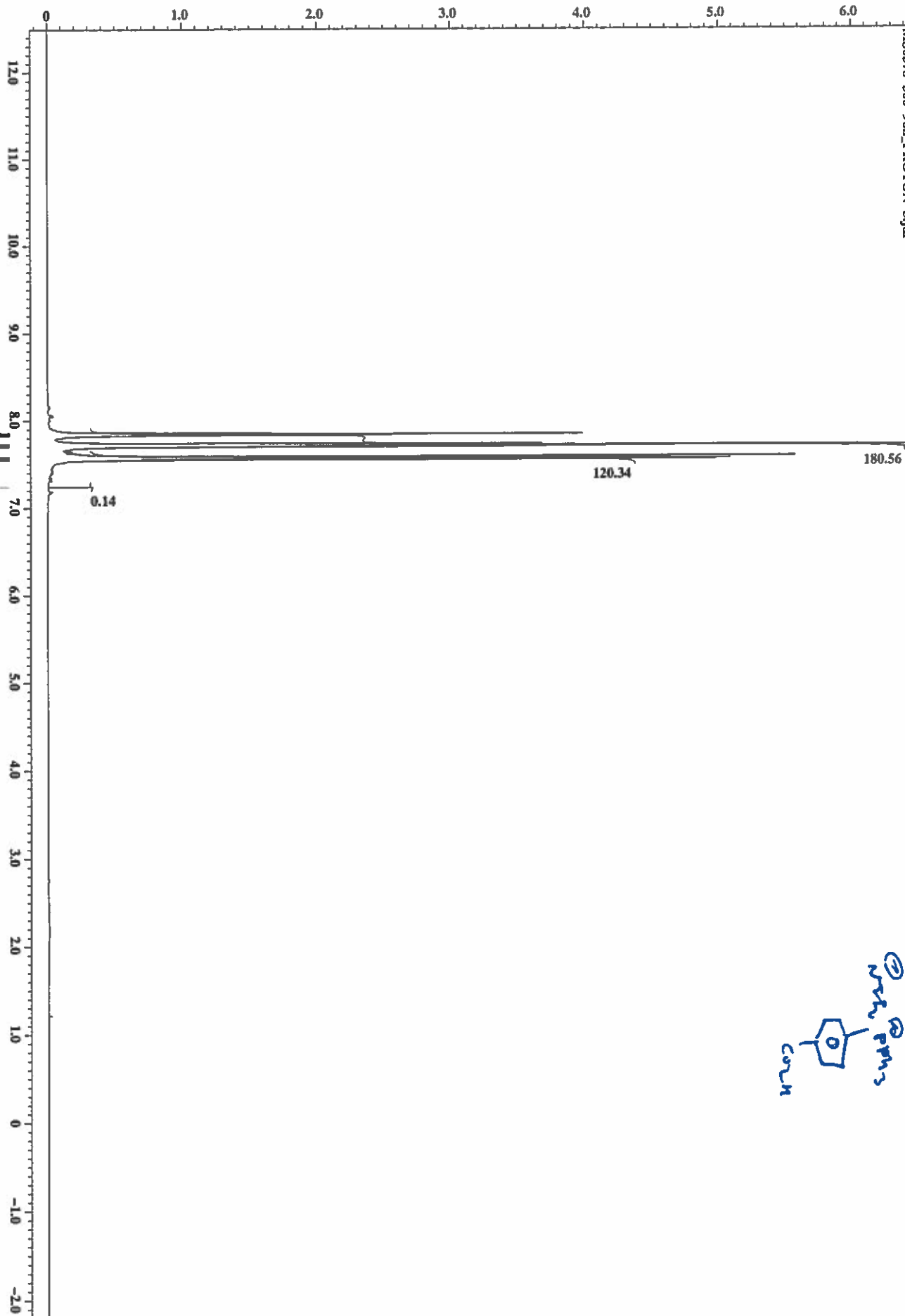


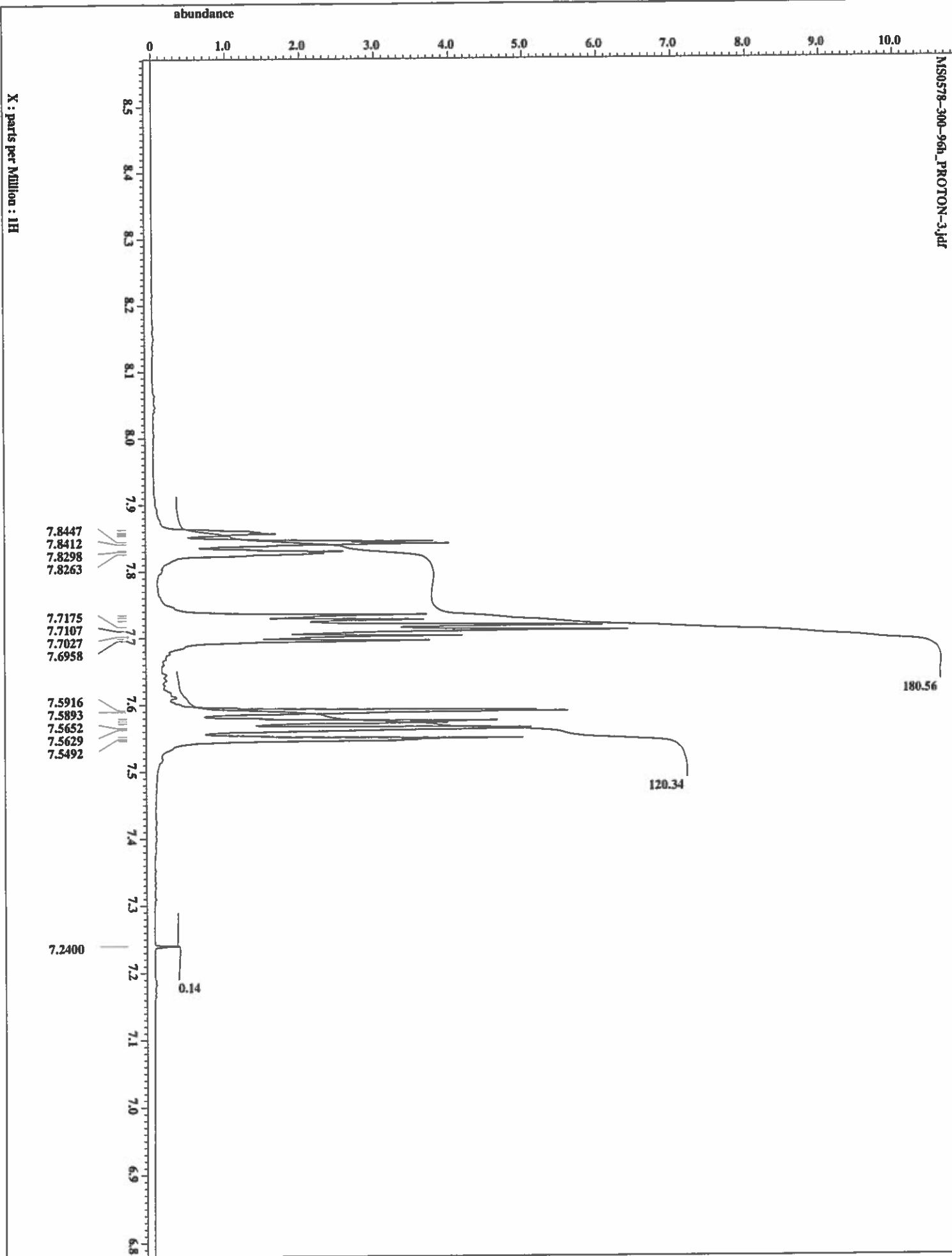


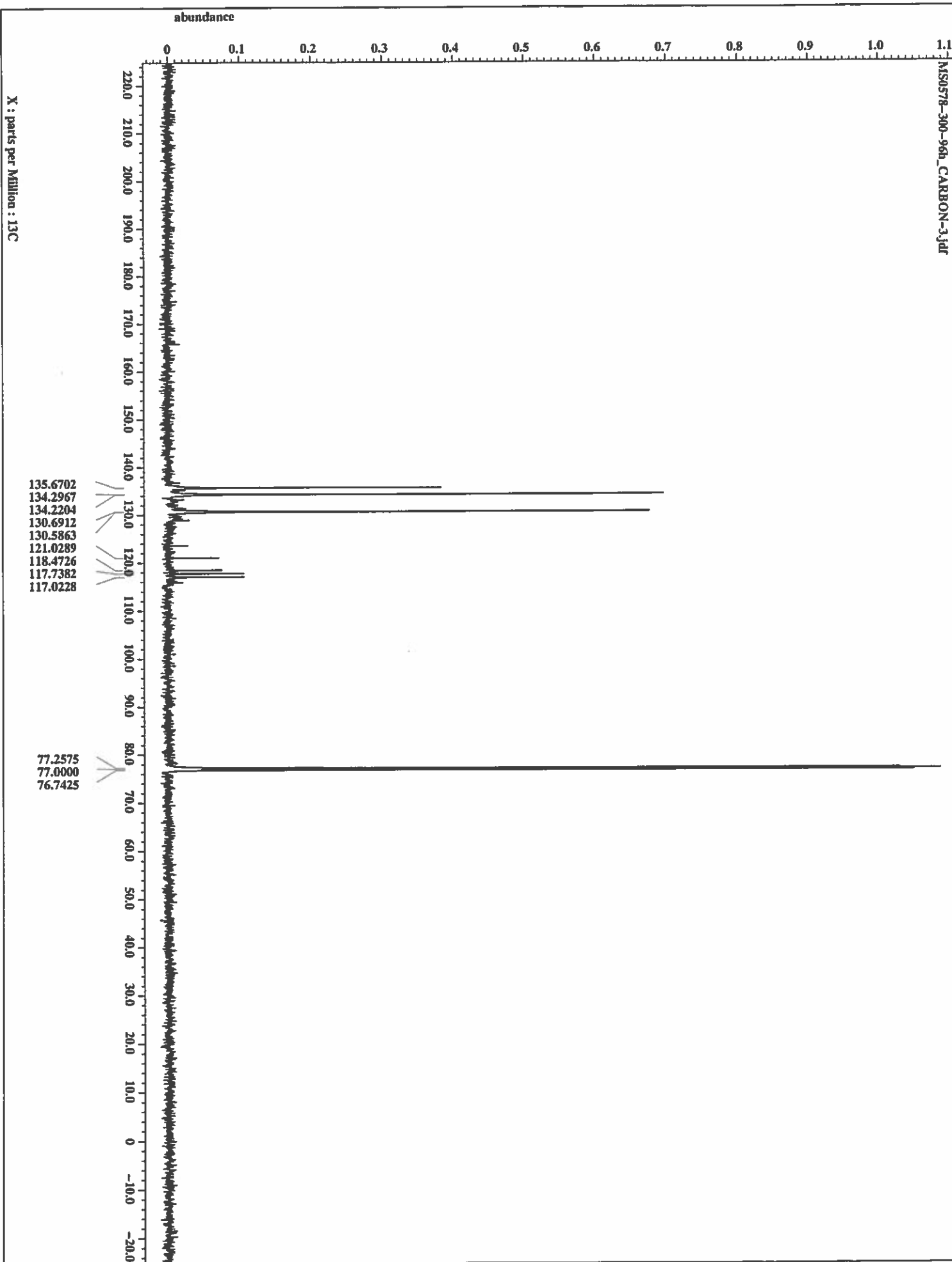


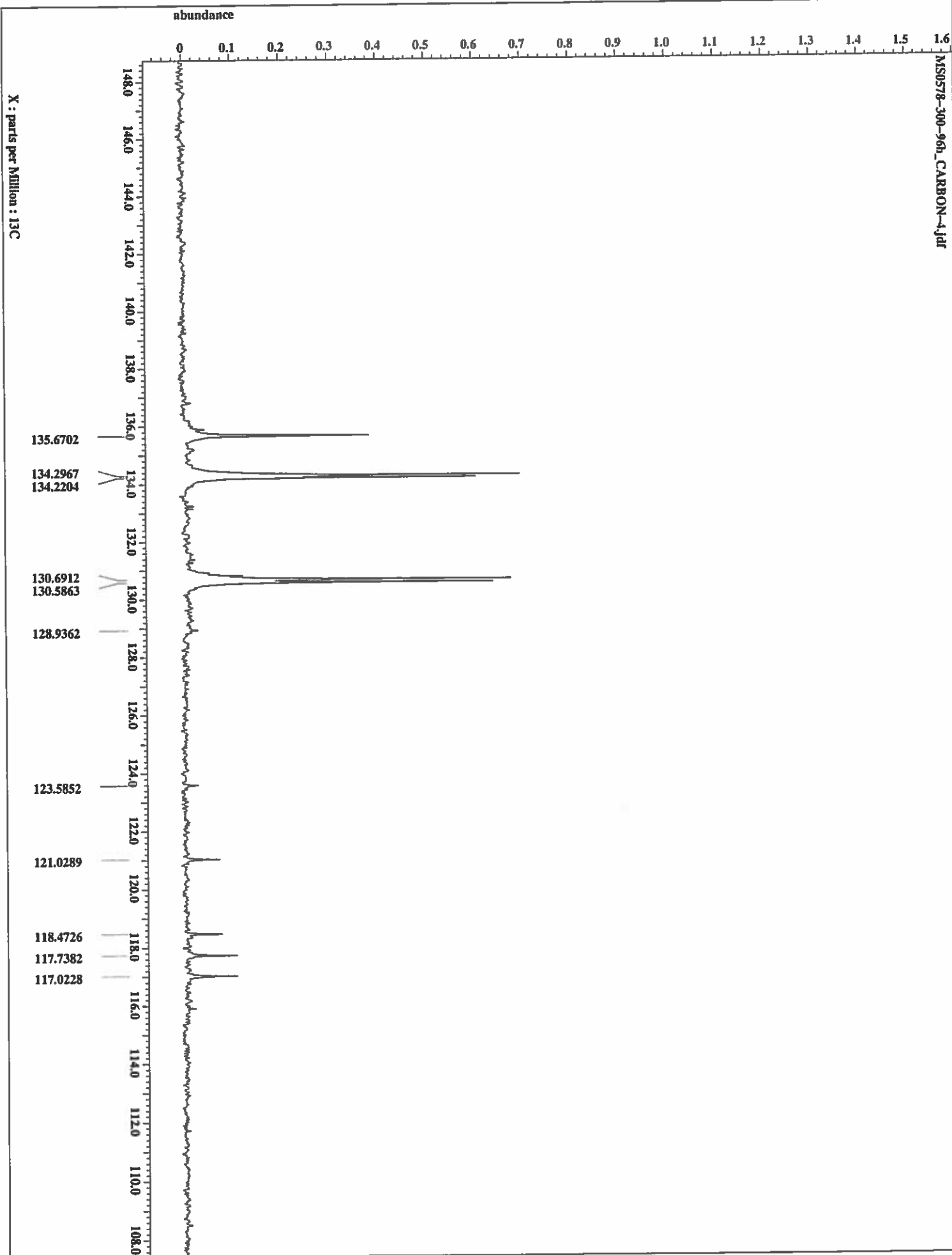
X : parts per Million : 1H

7.7175
7.7107
7.5916
7.5893
7.5652
7.5629









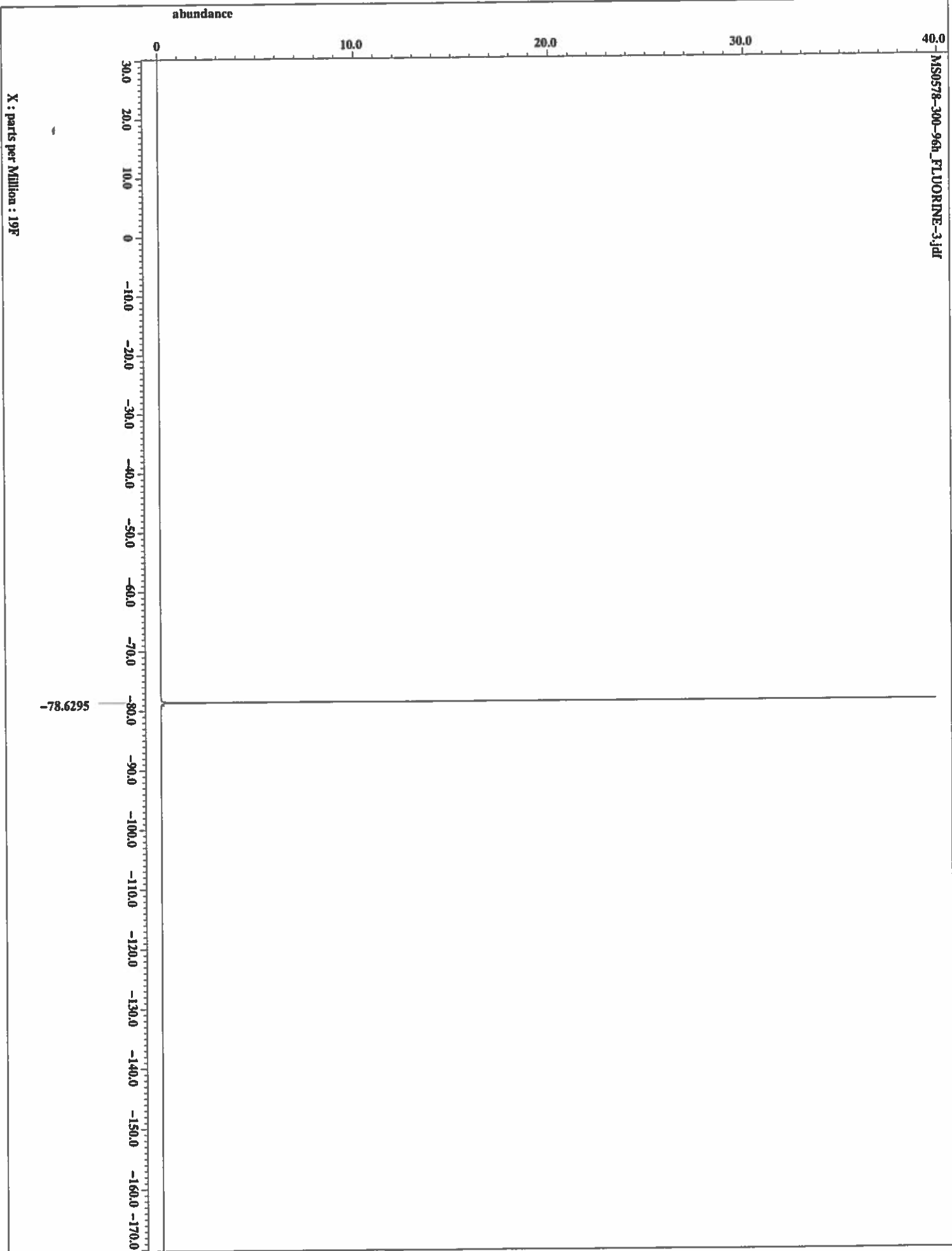
abundance

0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0

100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0

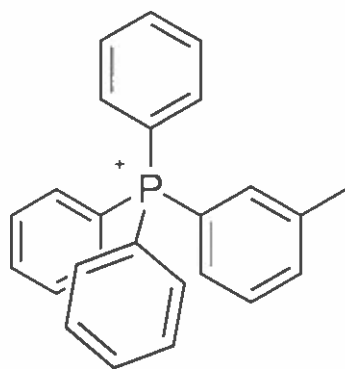
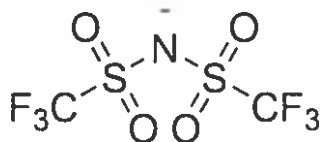
23.8039

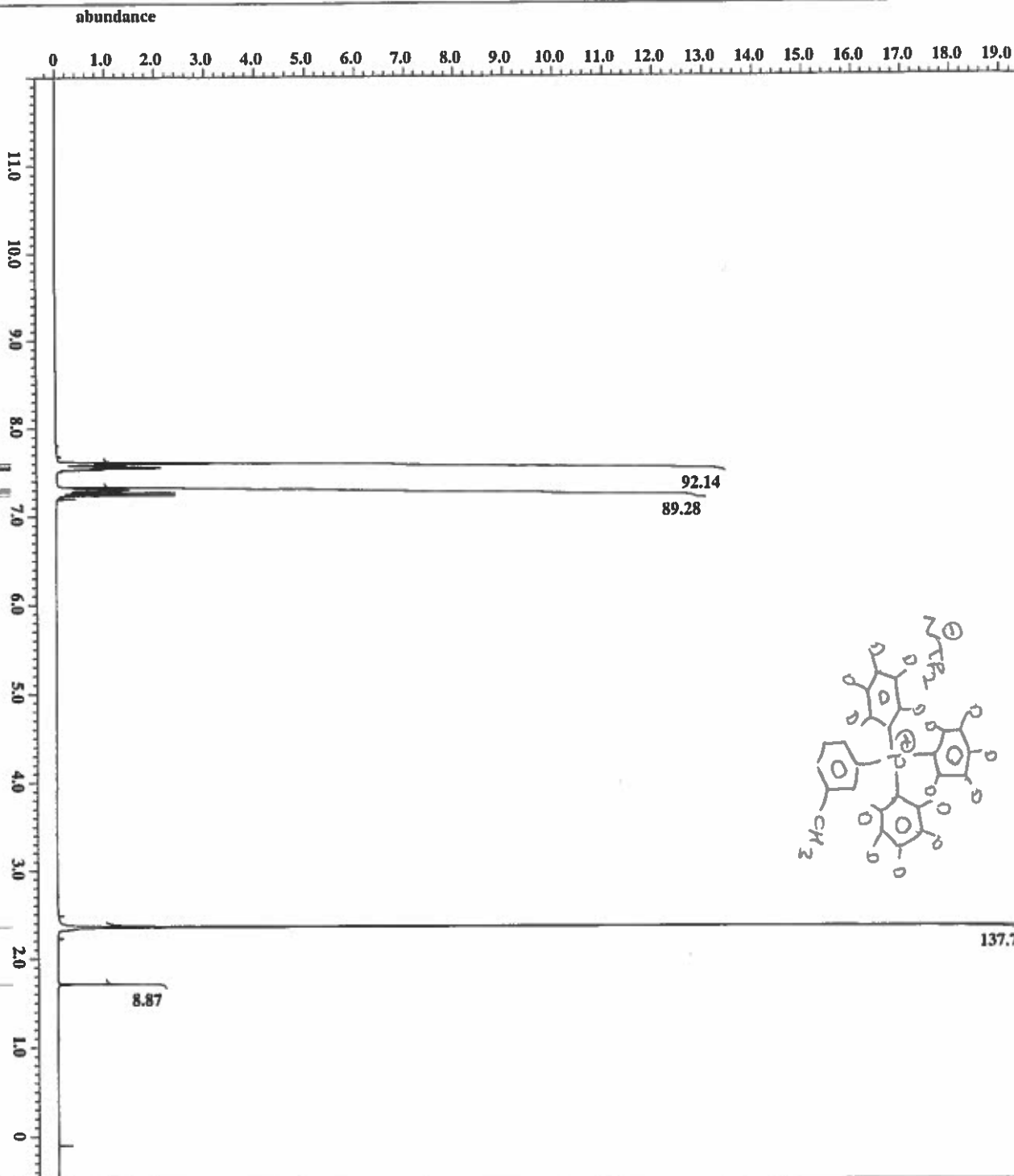
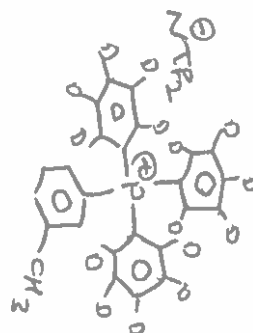
X : parts per Million : 31P



Compound 6 Pre- and Post-heating NMR Spectra

Temperature of Post-heating samples noted in upper left corner of each spectrum



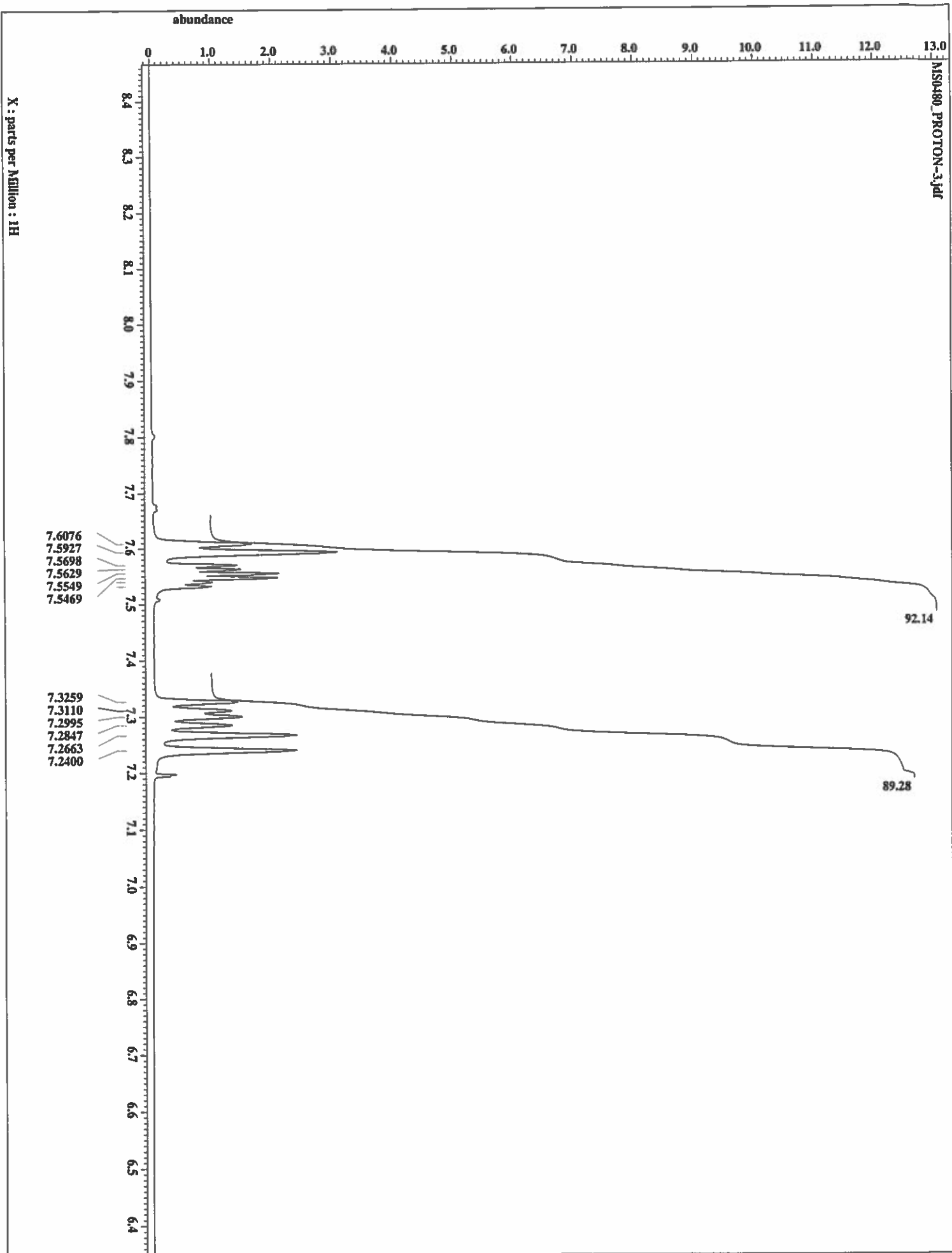


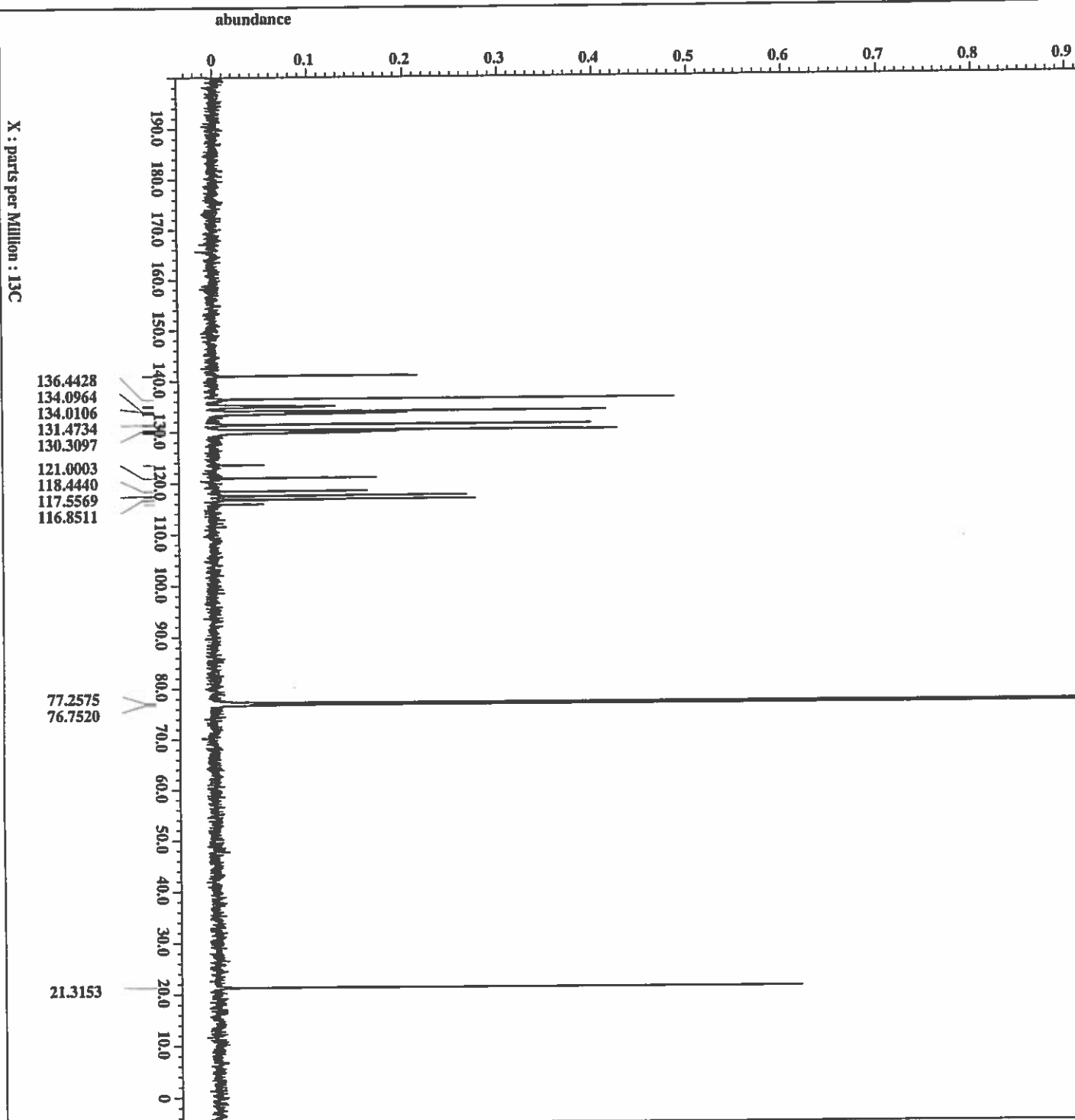
```

Filename      = MS0480_PROTON-2.jdt
Author        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0480
Solvent       = CHLOROFORM-D
Charger_sample = 2
Creation_time  = 22-JUN-2018 16:28:37
Revision_time  = 22-JUN-2018 16:07:10
Current_time   = 22-JUN-2018 16:07:10

Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 9.38438438 [kHz]
Xr_domain      = 1H
Xr_freq        = 500.15991521 [MHz]
Xr_offset      = 5.0 [ppm]
Xr1_domain     = 1H
Xr1_freq       = 500.15991521 [MHz]
Xr1_offset     = 5.0 [ppm]
Clipped        = PULSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16
X_g0_width     = 12.4 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 6.2 [us]
Xr_mode        = Off
Dante_presat   = PULSE
Initial_pelt   = 1 [s]
Relaxation_delay = 36
Recovery_gain   = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_get       = 22 [C]
  
```





```

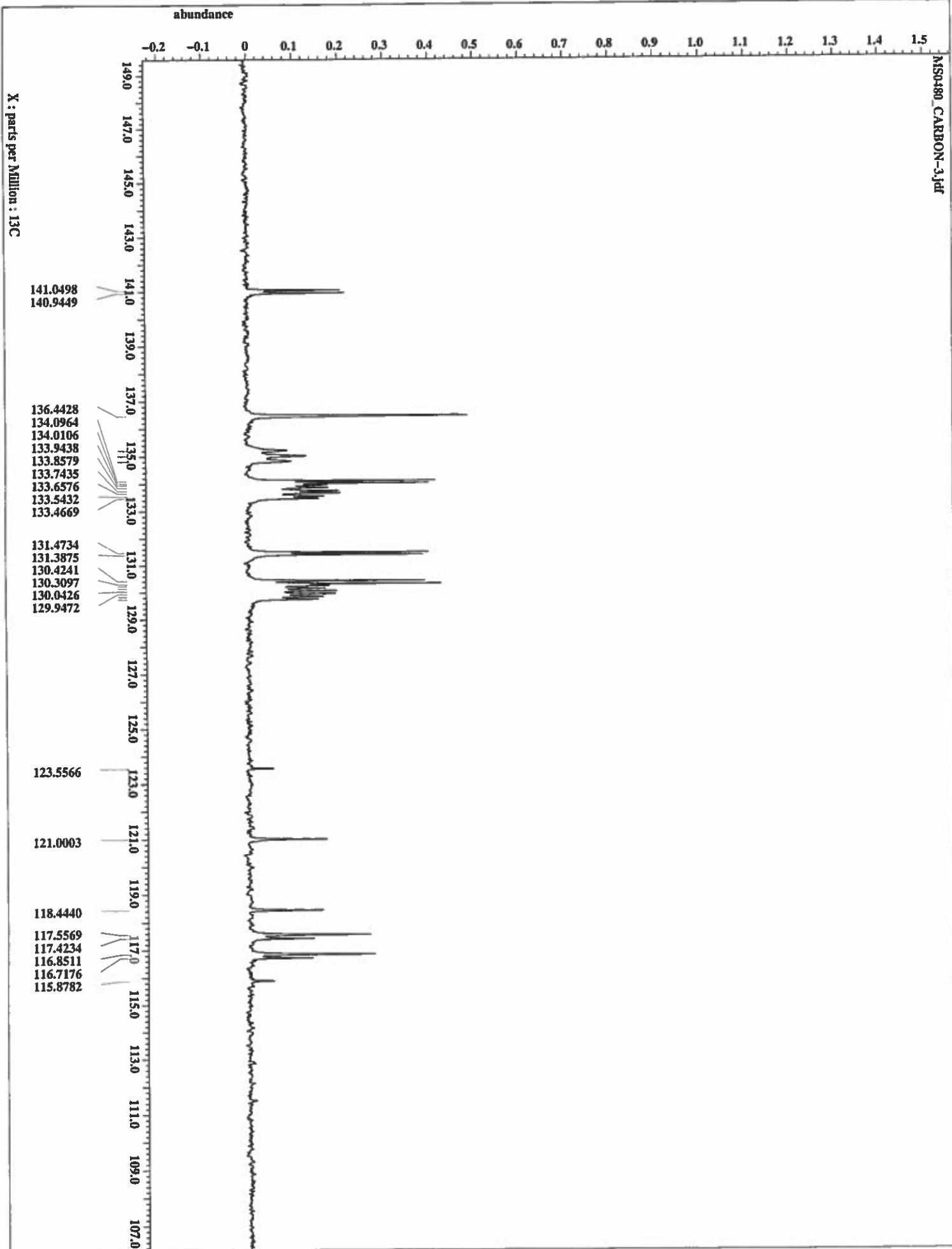
=====
File Name      MS0480_CARBON-2.jdt
Author         Jim Davis
Experiment     Single_Pulse_Dec
Sample ID      MS0480
Solvent        CHLOROFORM-D
Change Sample  2
Creation Time   22-JUN-2018 16:44:03
Revision Time   22-JUN-2018 16:21:36
Current Time    22-JUN-2018 16:21:36

=====
Data Format     1D COMPLEX
Dir Size       26214
Dir Title      13C
Dir Units      [ppm]
Dimensions     X
Site           ECA 500
Spectrometer   JNM-ECX500

=====
Field Strength 11.7673579 [T] (500 [MHZ])
Acq Duration   0.83361792 [s]
Domain         13C
Freq           125.76529768 [MHz]
Offset         100 [ppm]
Points         32768
Prescans       4
Resolution     1.19959034 [Hz]
Sweep          39.3081761 [kHz]
Irr Domain     1H
Irr Freq       500.15991521 [MHz]
Irr Offset     5.0 [ppm]
Clipped        FALSE
Mod Return     1
Scans          256
Total Scans    256

=====
X 90 Width     13.2 [us]
X Acq Time     0.83361792 [s]
X Angle        30 [deg]
X Atrn         6 [dB]
X Pulse        4.4 [us]
Irr Attn Dec   20.7 [dB]
Irr Attn Noe   20.7 [dB]
Irr Noise      WALTZ
Decoupling     TRUE
Initial Wait    1 [s]
Noe Time       TRUE
Recr Gain      2 [s]
Relaxation Delay 2.83361792 [s]
Repetition Time 22.6 [s]
Temp Set       22.6 [C]
=====

```





```

=====
Filename      MS0480_PHOSPHORUS-2.j
Author        Jim Davis
Experiment    single_pulse_dec
Sample_id     MS0480
Solvent       CHLOROFORM-D
Charger_sample 2
Creation_time 22-JUN-2018 16:25:52
Revision_time 22-JUN-2018 16:03:24
Current_time  22-JUN-2018 16:03:24
=====

```

```

=====
Data_format   1D COMPLEX
Dim_size      26214
Dim_cicle     31P
Dim_units     [ppm]
Dimensions    X
Site          FCA 500
Spectrometer  JNM-ECX500
=====

```

```

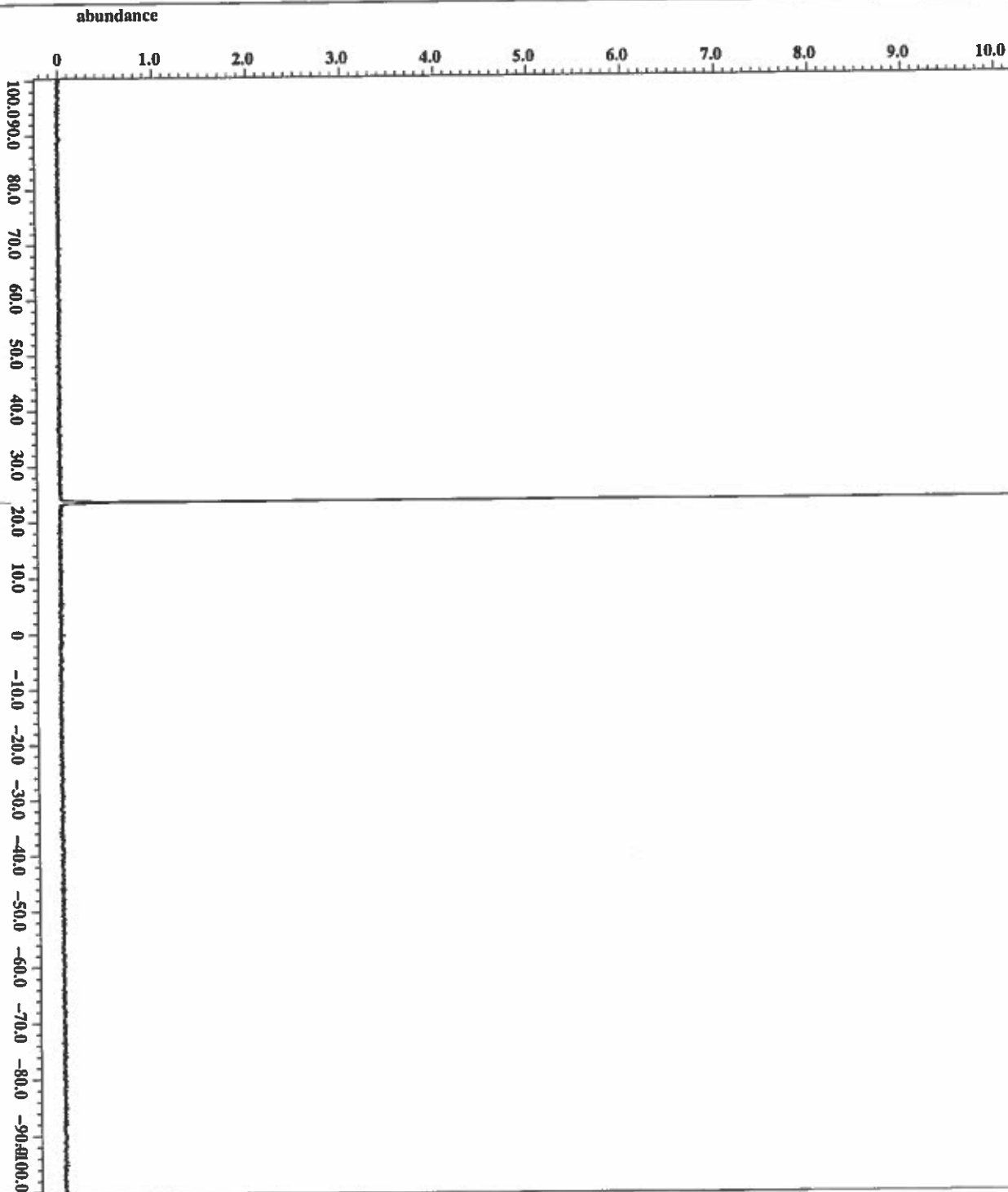
=====
Field_strength 11.7473579[T] (500 [MHz]
X_acq_duration 0.64487424[s]
X_domain       31P
X_freq         202.46831075 [MHz]
X_offset       0 [ppm]
X_points       32768
X_preamplifier 4
X_resolution    1.55068995 [Hz]
X_sweep         50.81300813 [kHz]
X_domain       1H
X_freq         500.15991521 [MHz]
X_offset       5.0 [ppm]
X_offset       FALSE
Mod_return     1
Scans          25
Total_scans    25
=====

```

```

=====
X_90_width     14.687 [us]
X_acq_time     0.64487424 [s]
X_angle        30 [deg]
X_atn          5 [dB]
X_pulse        4.89566667 [us]
X_atn_dec      20.7 [dB]
X_atn_poe      20.7 [dB]
X_noise        VALVE
Decoupling     TRUE
Initial_wait   1 [s]
Noe_time       TRUE
Noe_delay      2 [s]
Relaxation_delay 2.64487424 [s]
Repetition_time 22.31 [dc]
Temp_set       22.31 [dc]
=====

```



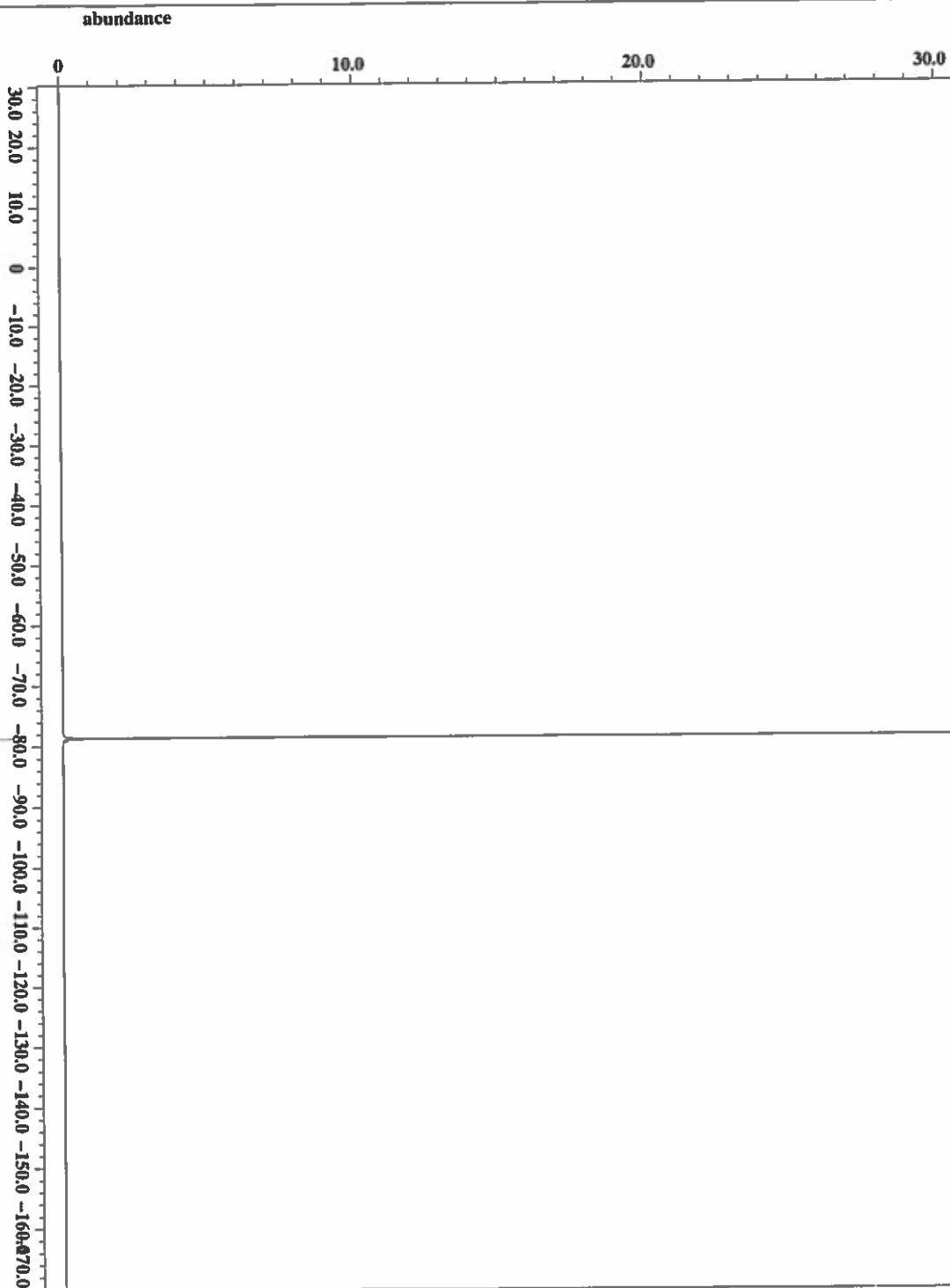


Filename = MS0480_FLUORINE-2.jdf
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0480
 Solvent = CHLOROFORM-D
 Change sample = 2
 Creation_time = 22-JUN-2018 16:46:59
 Revision_time = 22-JUN-2018 16:24:31
 Current_time = 22-JUN-2018 16:24:31

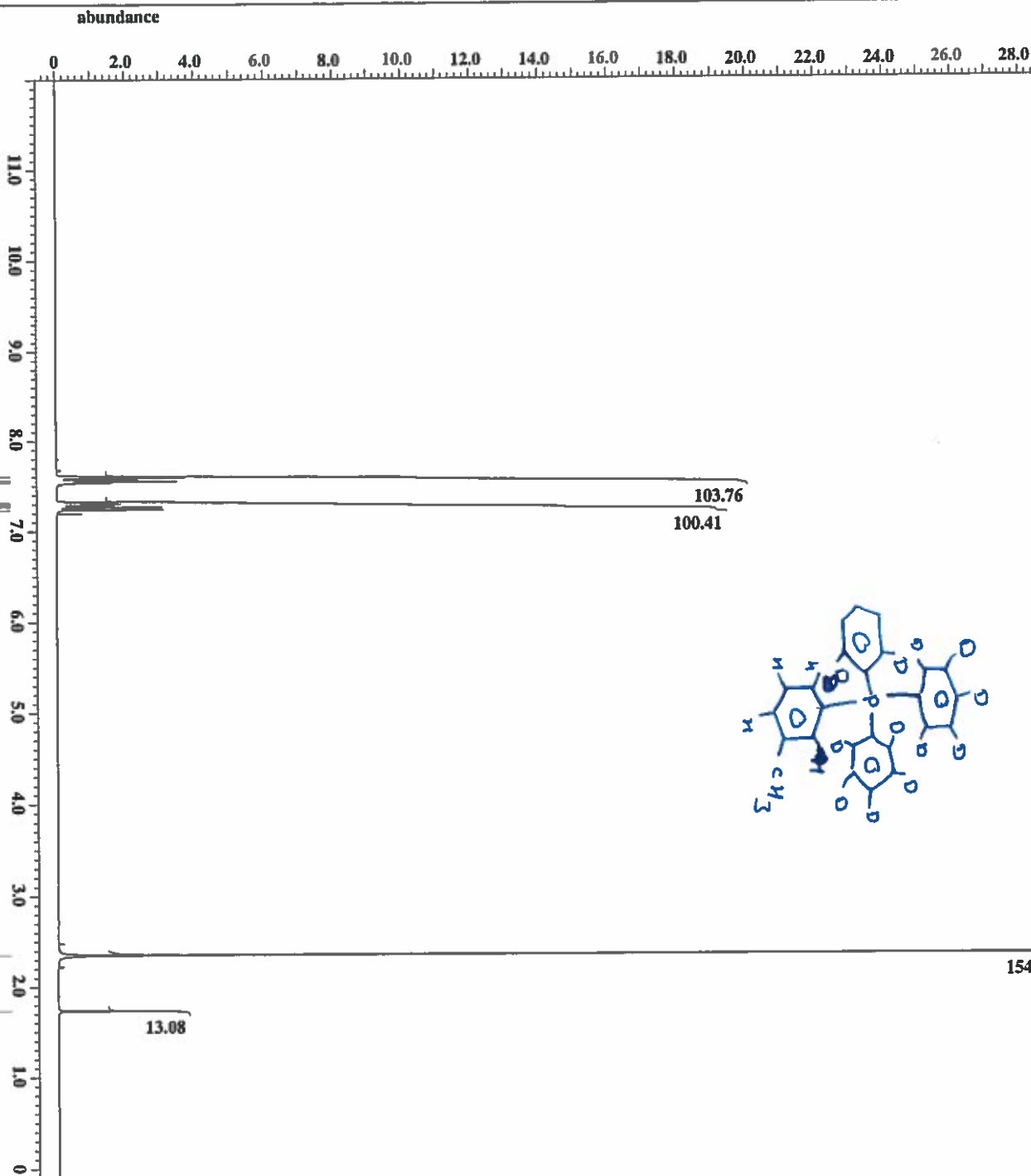
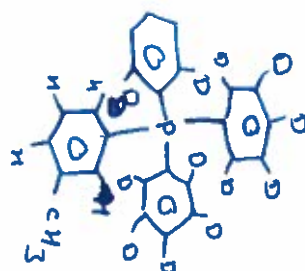
Data format = 1D COMPLEX
 Dim_size = 52428
 Dim_file = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 0.55574528 [s]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = -70 [ppm]
 X_points = 65536
 X_prescans = 1
 X_resolution = 1.7993855 [Hz]
 X_sweep = 117.9245283 [kHz]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = 19F
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = 5 [ppm]
 Mod_return = PULSE
 Scans = 1
 Total_scans = 16

X_90_width = 13.1 [us]
 X_acq_time = 0.55574528 [s]
 X_angle = 45 [deg]
 X_atn = 2.5 [dB]
 X_pulse = 6.5 [us]
 Xr_mode = off
 Tx1_mode = PULSE
 Dante_preset = 1 [a]
 Initial_wait = 38
 Recvr_gain = 4 [a]
 Relaxation_delay = 4.55574528 [s]
 Repetition_time = 22.2 [dc]



X : parts per Million : 19F



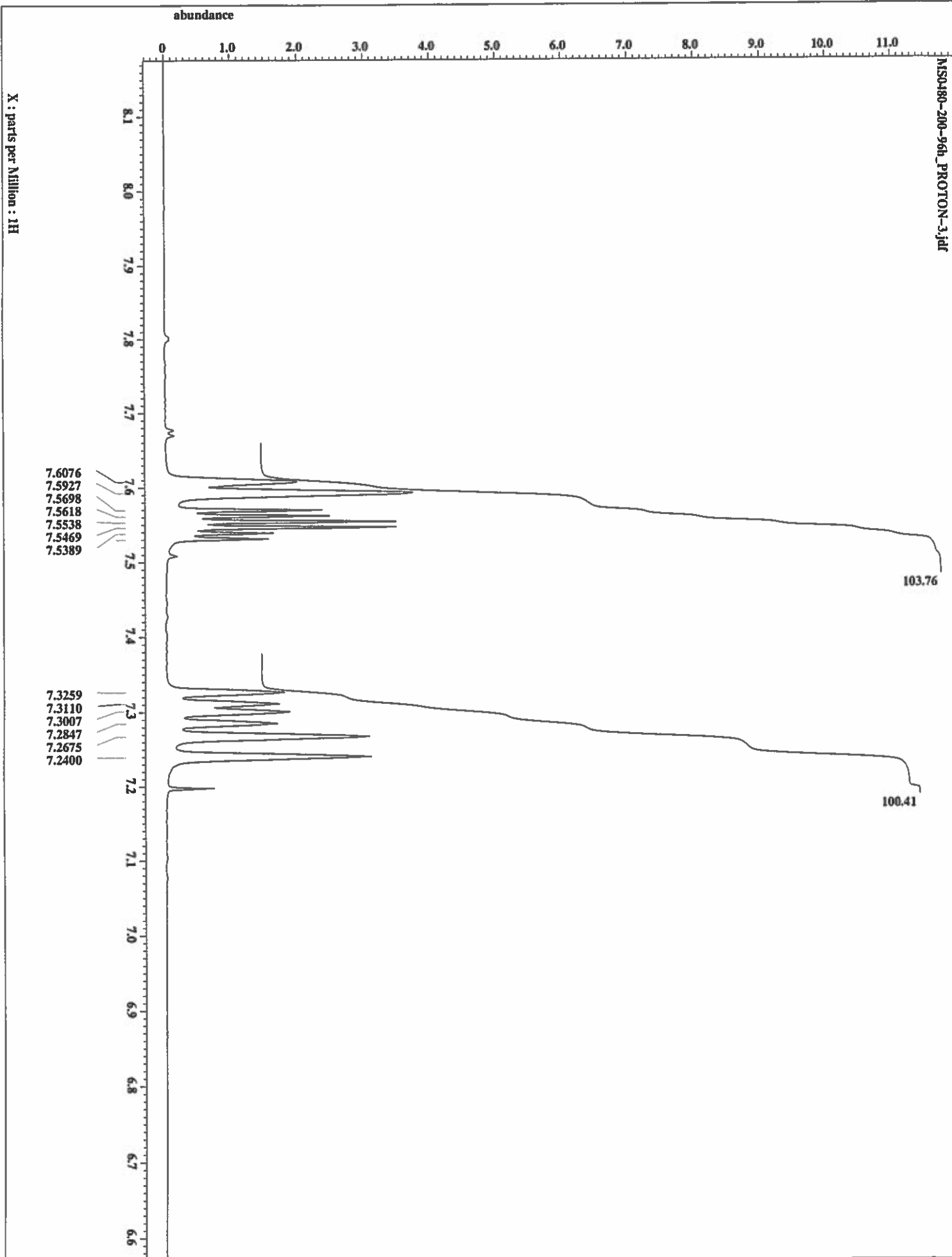
```

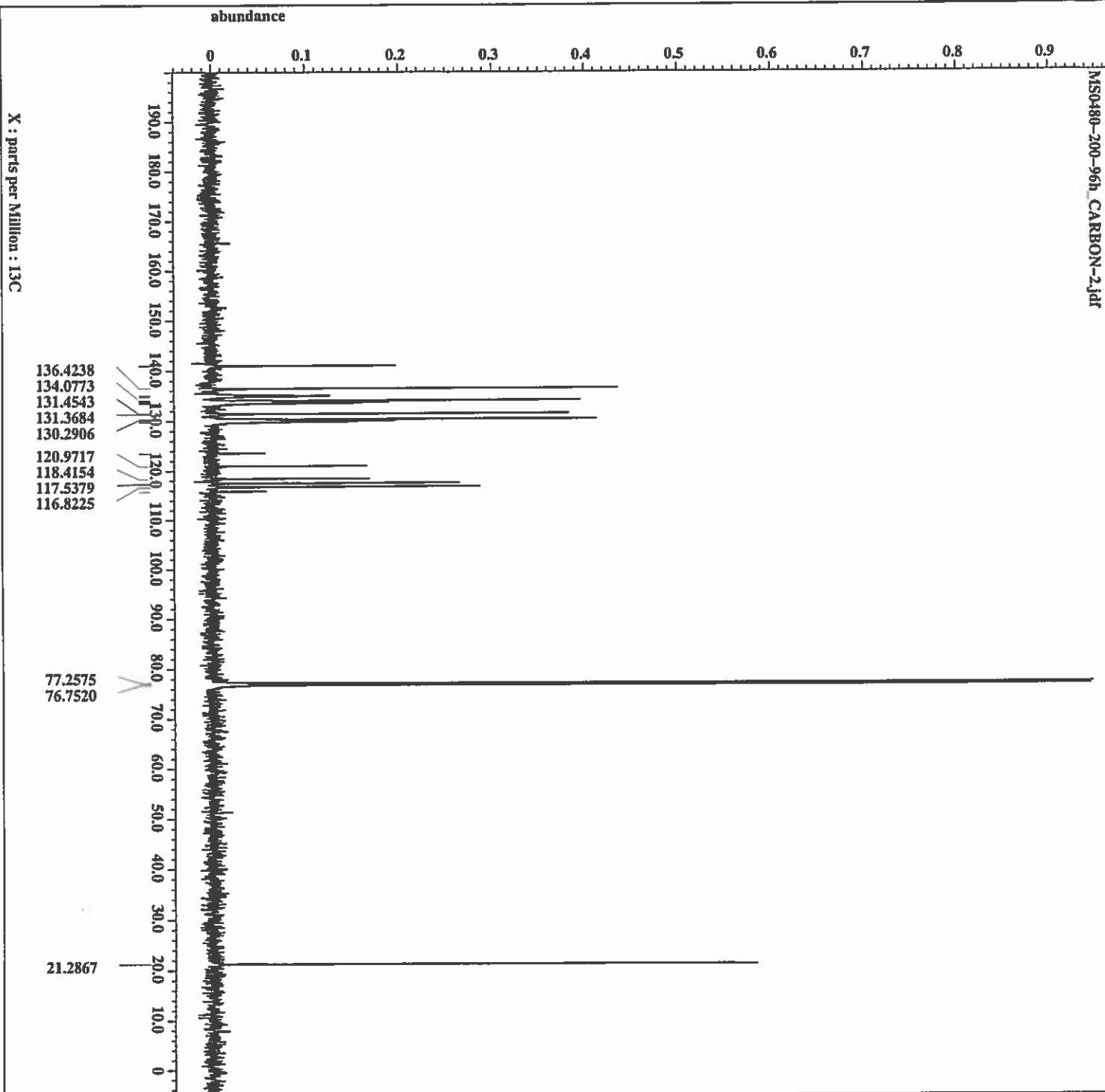
Filename      = MS0480-200-96h_PROTON
Anchor        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0480-200-96h
Solvent       = CHLOROFORM-D
Changer_sample = 6
Creation_time  = 27-JUN-2018 08:42:39
Revision_time  = 27-JUN-2018 08:19:47
Current_time   = 27-JUN-2018 08:19:47

Data_format    = 1D COMPLEX
Dim_size       = 13107
Dim_title      = 1H
Dim_units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

P1d_strength   = 11.74735797 (500 MHz)
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 9.38438438 [kHz]
Xt_domain      = 1H
Xt_freq        = 500.15991521 [MHz]
Xt_offset      = 5.0 [ppm]
Xt_domain      = 1H
Xt_freq        = 500.15991521 [MHz]
Xt_offset      = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 12.4 [us]
X_acq_time      = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse         = 6.2 [us]
Xt_pulse        = 6.2 [us]
Xt_mode         = OFZ
Pulse_program   = FALGE
Initial_wait    = 1 [s]
Recvr_gain     = 36
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_get       = 21.6 [C]
  
```





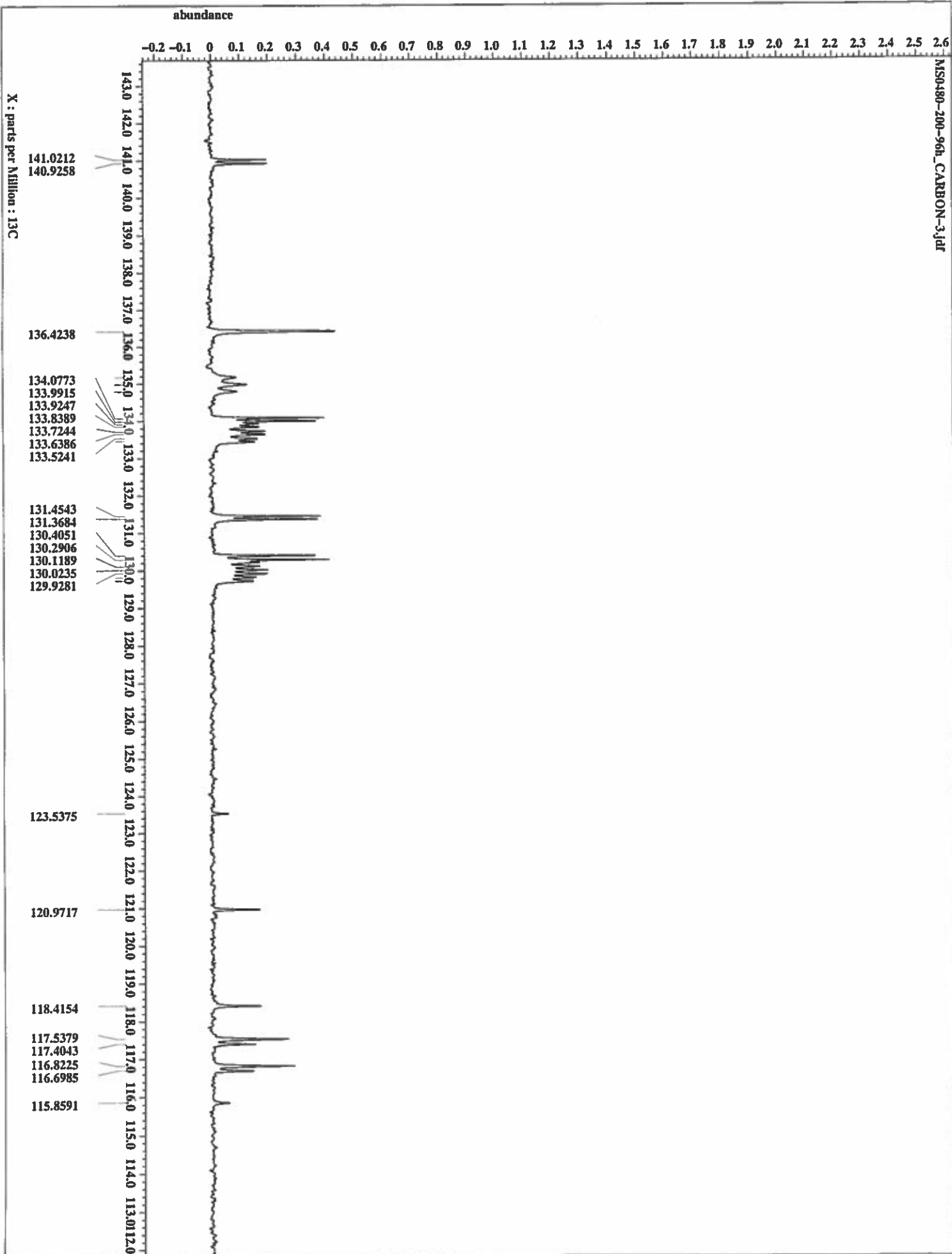
```

Filename      = MS0480-200-96h CARBON
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0480-200-96h
Solvent       = CHLOROFORM-D
Charger       = 6
Creation_time  = 27-JUN-2018 08:51:14
Revision_time = 27-JUN-2018 08:28:22
Current_time  = 27-JUN-2018 08:28:22

Date_format   = DD MM YY
Dim_size      = 26214
Dim_file      = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

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   = 1.1959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Xt_domain      = 1H
Xt_freq        = 500.15991521 [MHz]
Xt_offset      = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 134
Total_scans    = 134

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Xt_atn_dec     = 20.7 [dB]
Xt_atn_noe     = 20.7 [dB]
Irr_decouple   = WALTZ
Decoupling     = TRUE
Initial_volt   = 2 [s]
Noe_time       = 2 [s]
Rever_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 22.3 [dC]
  
```



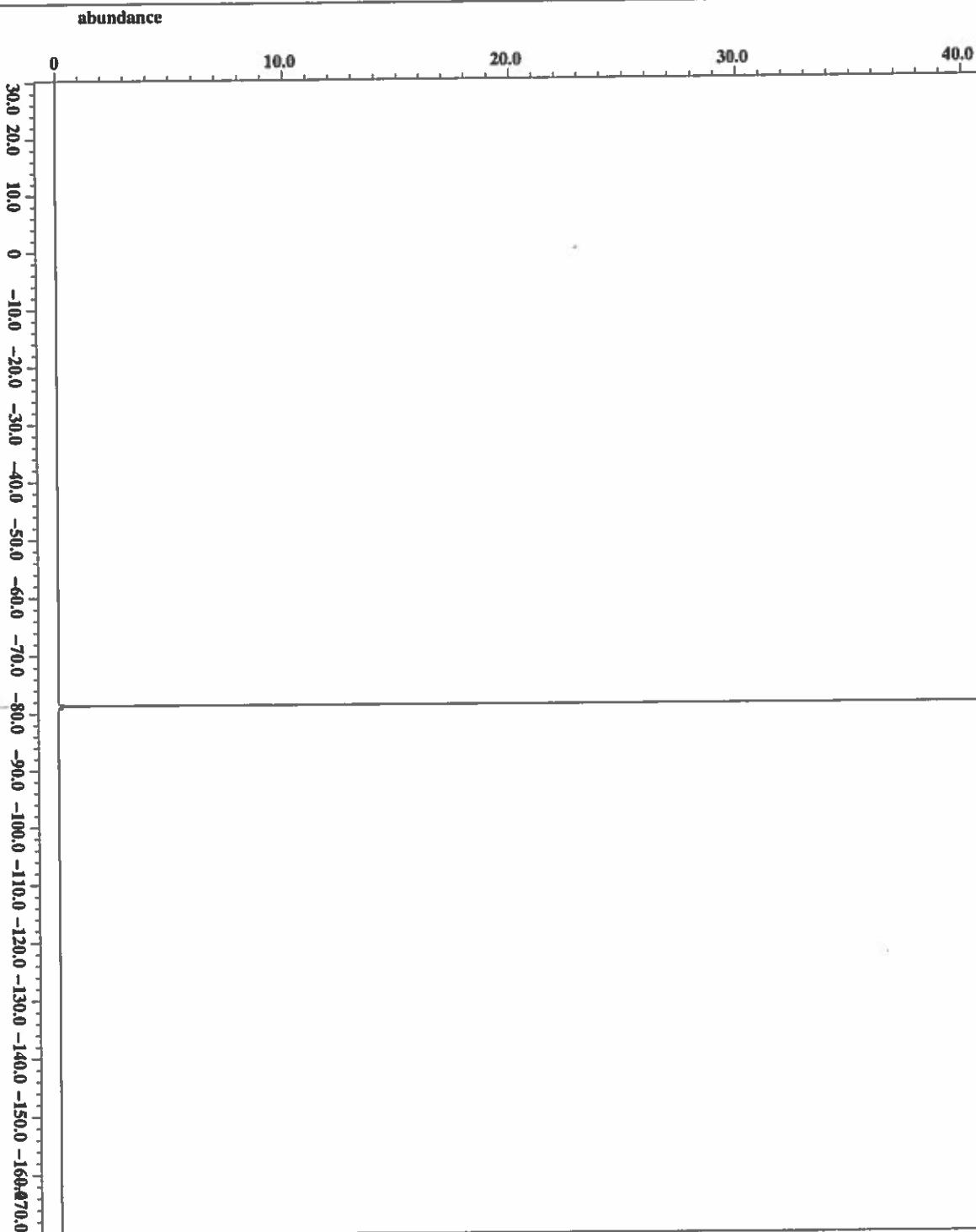


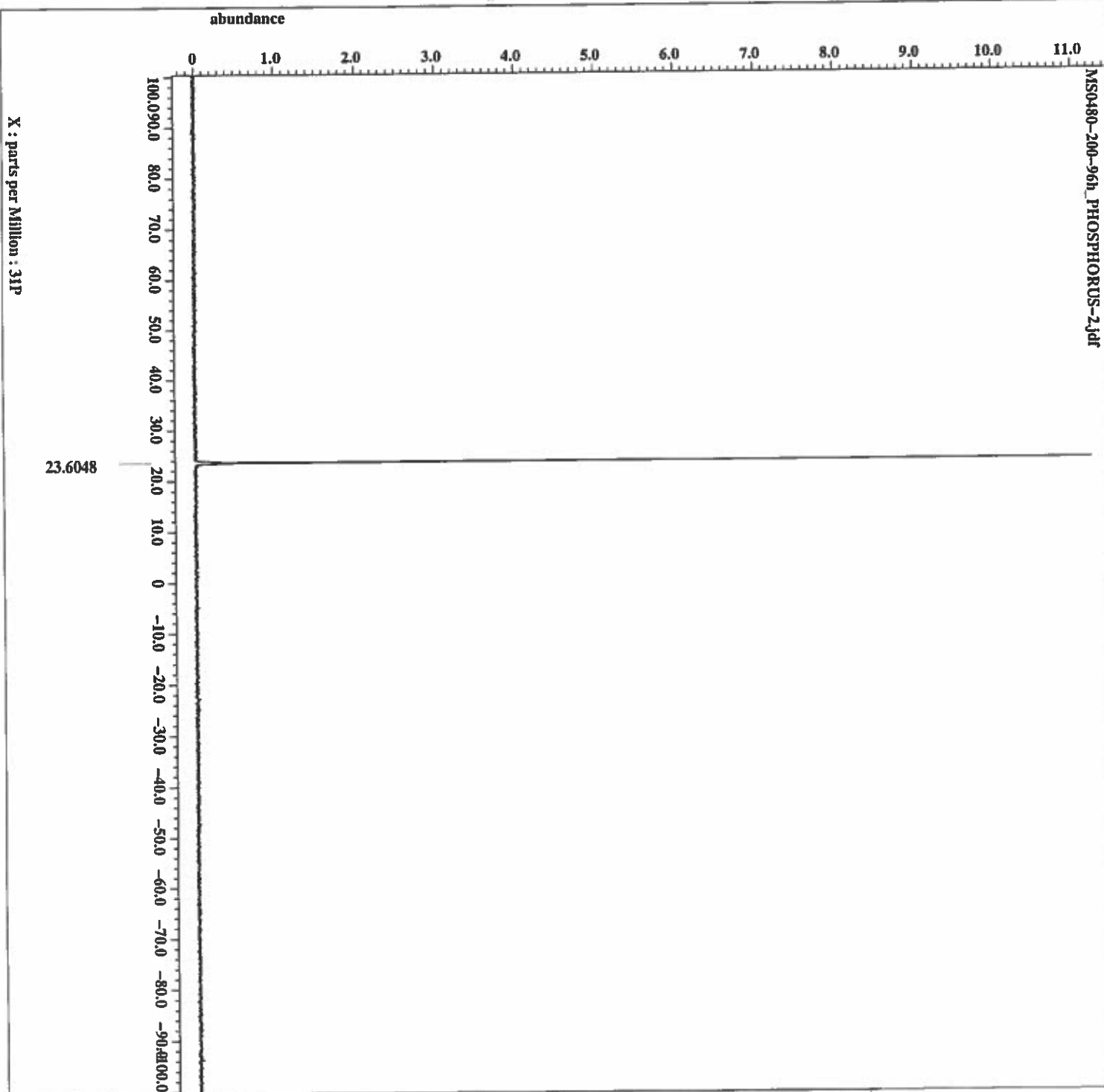
P11name MS0480-200-96h_FLUORINE
 Author Jim Davis
 Experiment single_pulse.ex2
 Sample_id MS0480-200-96h
 Solvent CHLOROFORM-D
 Changer_sample 6
 Creation_time 27-JUN-2018 08:54:05
 Revision_time 27-JUN-2018 08:31:12
 Current_time 27-JUN-2018 08:31:12

Data_format 1D COMPLEX
 Dim_size 52428
 Dim_title 19F
 Dim_units [ppm]
 Dimensions X
 Site ECA 500
 Spectrometer JNM-ECA500

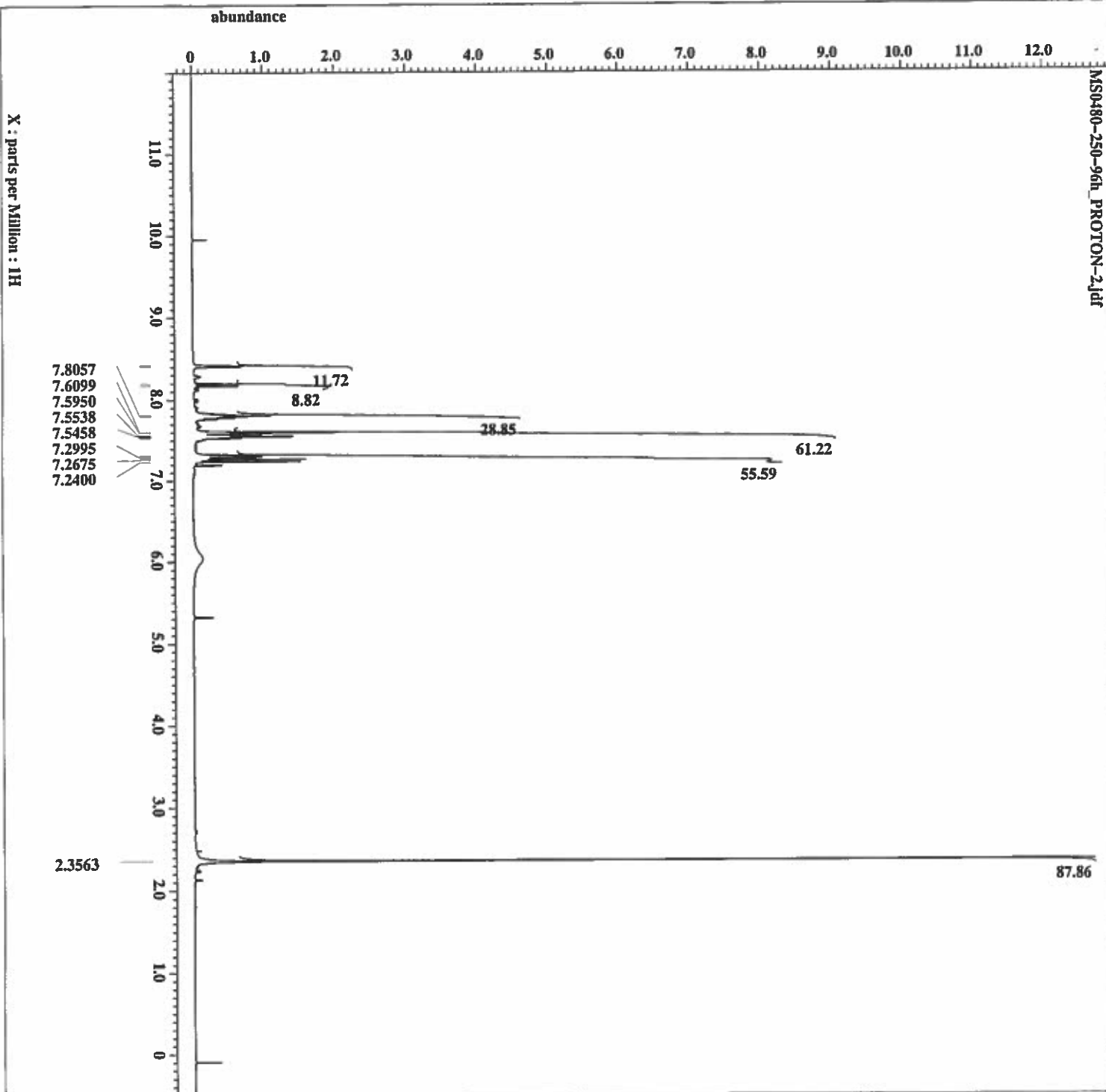
Field_strength 11.7473579 [T] (500 [MH
 X_acq_duration 0.55574528 [s]
 X_domain 19F
 X_freq 470.62046084 [MHz]
 X_offset -70 [ppm]
 X_points 65536
 X_prescans 1
 X_resolution 1.7993855 [Hz]
 X_sweep 117.9245283 [kHz]
 X_domain 19F
 X_freq 470.62046084 [MHz]
 X_offset 5 [ppm]
 X1_domain 19F
 X1_freq 470.62046084 [MHz]
 X1_offset 5 [ppm]
 Clipped FALSE
 Mod_return 1
 Scans 16
 Total_scans 16

X_90_width 13.1 [us]
 X_acq_time 0.55574528 [s]
 X_angle 45 [deg]
 X_atn 2.5 [dB]
 X_pulse 6.55 [us]
 X_offset OFF
 X1_mode OFF
 Dante_preset FALSE
 Initial_wait 1 [s]
 Recvz_gain 38
 Relaxation_delay 4 [s]
 Repetition_time 4.55574528 [s]
 Temp_get 21.9 [dc]





Filename	= MS0480-200-96h_PROBSP
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0480-200-96h
Solvent	= CHLOROFORM-D
Charger_sample	= 6
Creation time	= 27-JUN-2018 08:57:49
Revision time	= 27-JUN-2018 08:34:56
Current_time	= 27-JUN-2018 08:34:58
Date_format	= DD.MM.YYYY
Dim_size	= 26214
Dim_title	= 31P
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579 [T] (500 [MH
X_acq_duration	= 0.64487424 [s]
X_domain	= 31P
X_freq	= 202.4681075 [MHz]
X_offset	= 0 [ppm]
X_points	= 32768
X_pulses	= 4
X_resolution	= 1.5506895 [Hz]
X_sweep	= 50.81300813 [kHz]
irr_domain	= 1H
irr_freq	= 500.15991521 [MHz]
irr_offset	= 5.0 [ppm]
clipped	= FALSE
Mod_return	= 1
Seams	= 25
Total_scans	= 25
X_90_width	= 14.687 [us]
X_acq_time	= 0.64487424 [s]
X_angle	= 30 [deg]
X_atn	= 5 [dB]
X_pulse	= 4.89566667 [us]
irr_atn_dec	= 20.7 [dB]
irr_atn_poe	= 20.7 [dB]
irr_noise	= WALTZ
Decoupling	= TRUE
initial_walt	= 1 [s]
Noe	= TRUE
Noe_time	= 2 [s]
Recvr_gain	= 58
Relaxation_delay	= 2 [s]
Repetition_time	= 2.64487424 [s]
Temp_get	= 22.21 [dC]



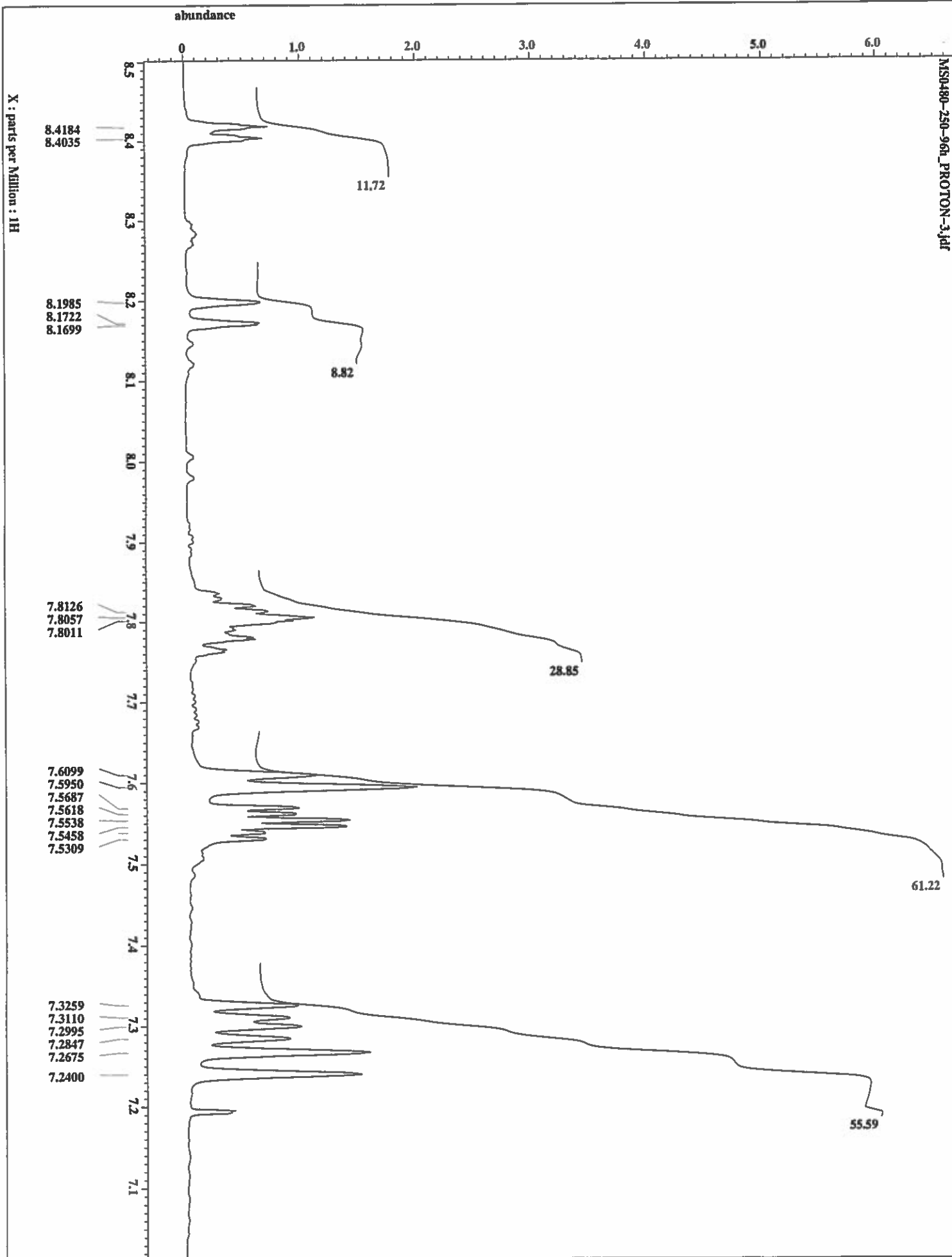
```

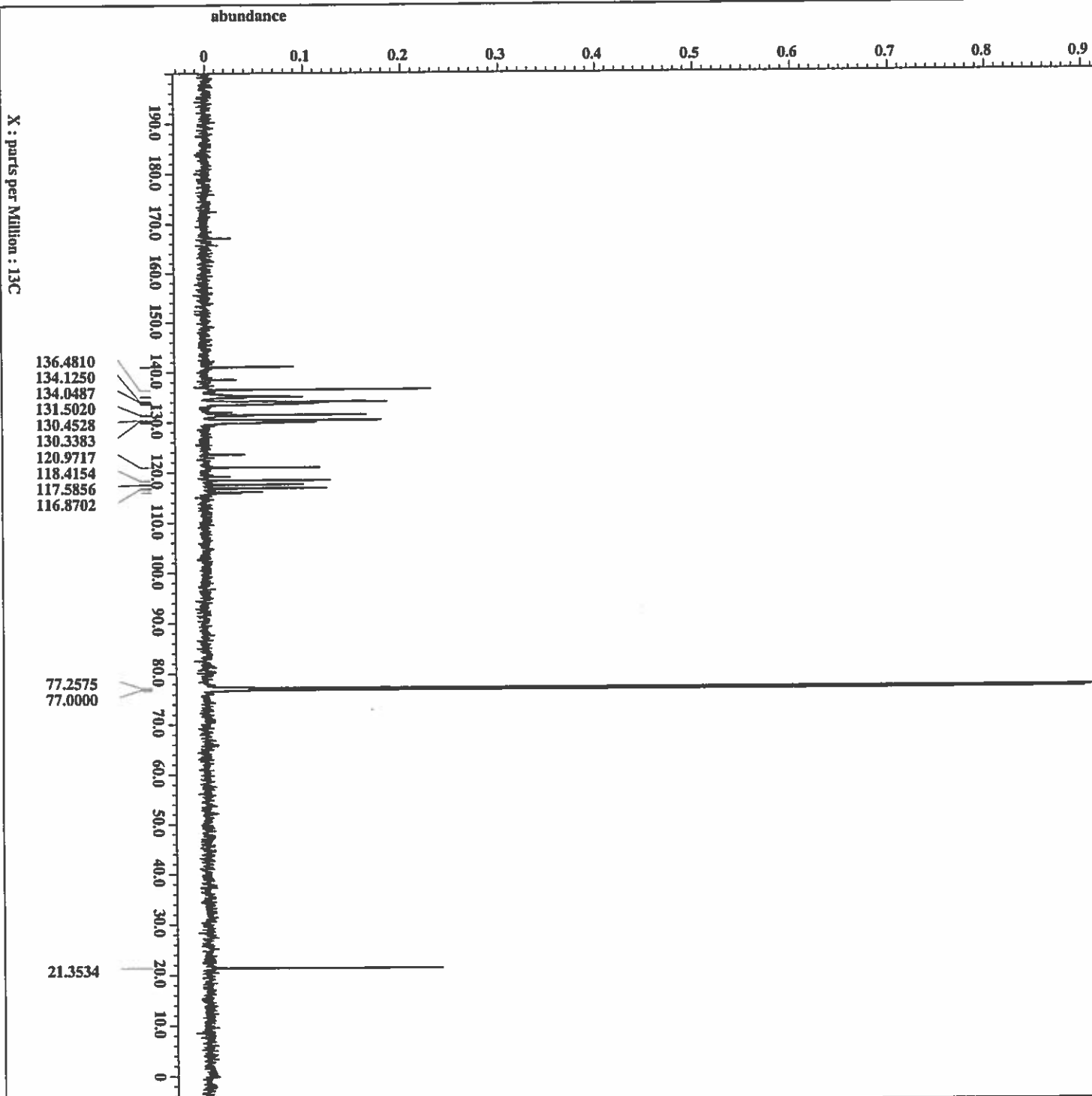
Filename      = MS0480-250-96h_PROTON
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = MS0480-250-96h
Solvent       = CHLOROFORM-D
Charger_sample = 7
Creation_time  = 27-JUN-2018 09:05:00
Revision_time  = 27-JUN-2018 08:42:07
Current_time   = 27-JUN-2018 08:42:07

Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_circle    = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = XCA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 9.36436436 [kHz]
Xt_domain      = 1H
Xt_freq        = 500.15991521 [MHz]
Xt_offset      = 5.0 [ppm]
Xt_domain      = 1H
Xt_freq        = 500.15991521 [MHz]
Xt_offset      = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Total_scans    = 16

X_90_width     = 12.4 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 6.2 [us]
Xt_mode        = OFC
Pulse_program  = PULSE
Initial_wait   = 1 [s]
Relaxation_delay = 38
Recovery_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_get       = 21.9 [C]
  
```





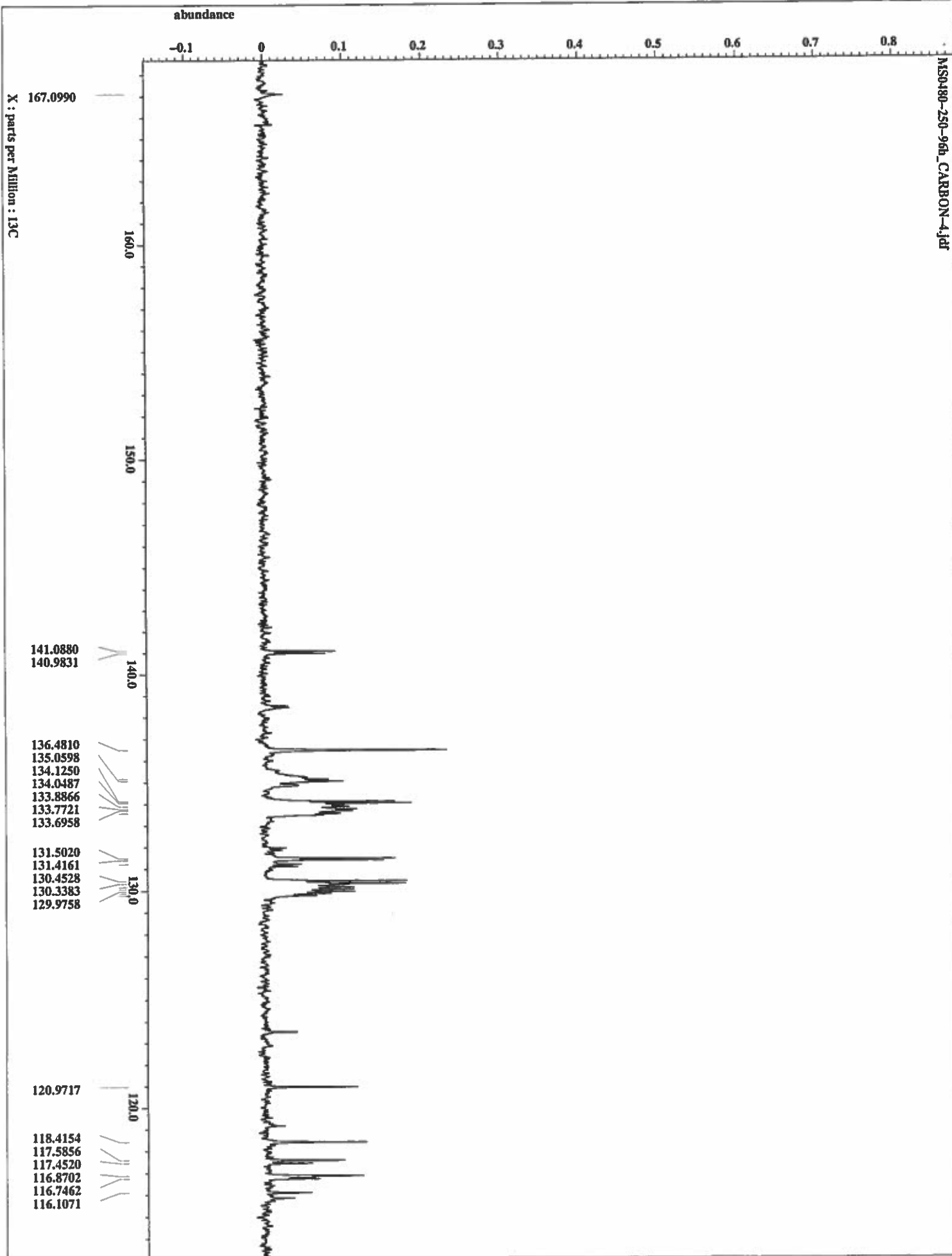
```

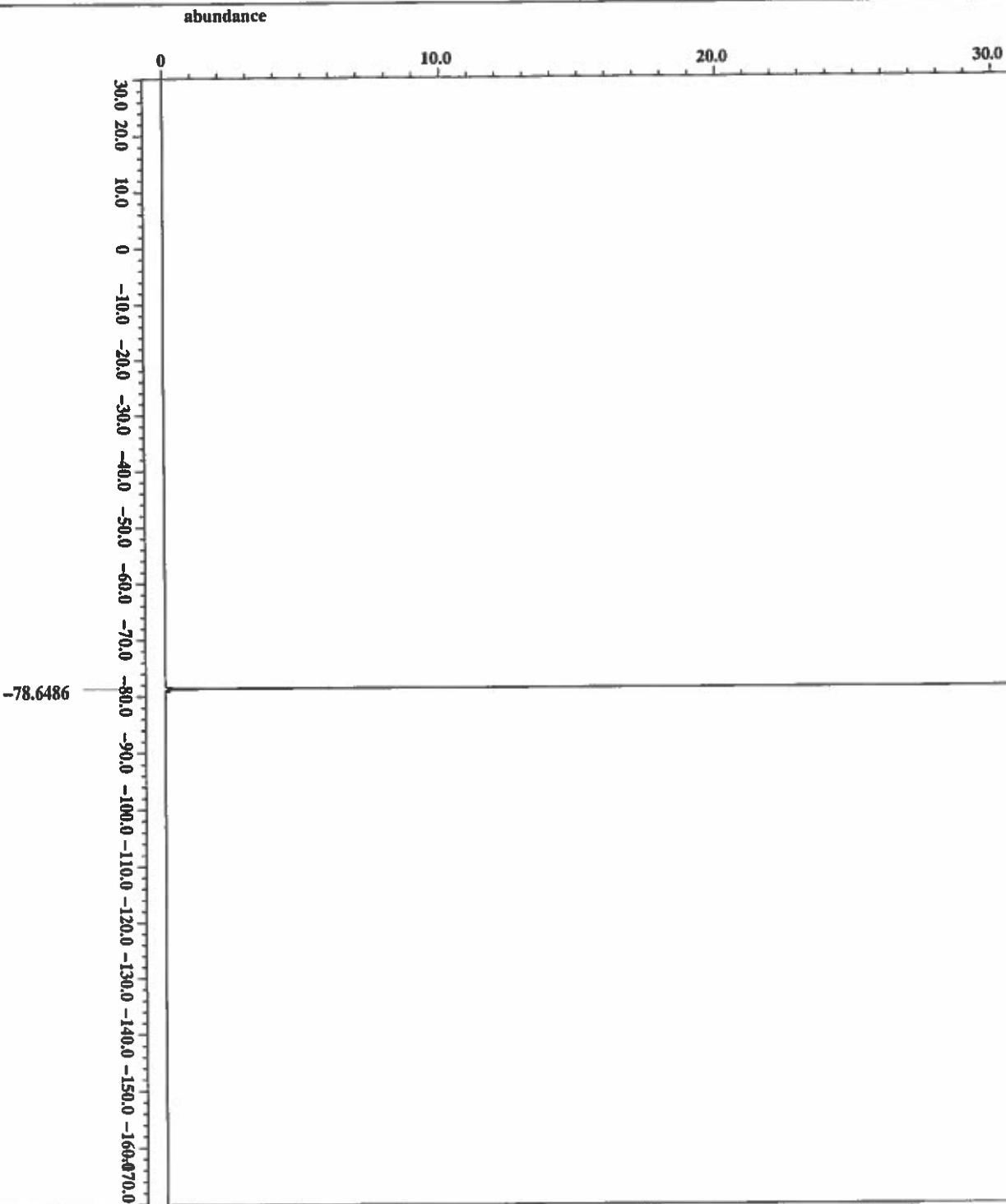
Filename      = MS0480-250-96h CARBON
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0480-250-96h
Solvent       = CHLOROFORM-D
Charger_sample = 7
Creation_time  = 27-JUN-2018 09:21:34
Revision_time  = 27-JUN-2018 08:58:41
Current_time   = 27-JUN-2018 08:58:41

Data_format    = 1D COMPLEX
Dim_size       = 26214
Dim_title      = 13C
Dim_units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

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        = 39.3081764 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 300
Total_scans    = 300

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_noe    = 20.7 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe_time       = TRUE
Noe            = 2 [s]
Nocv_grdn      = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 22.6 [deg]
  
```





X : parts per Million : 19F



SOUTH ALABAMA
JAGUARS

```

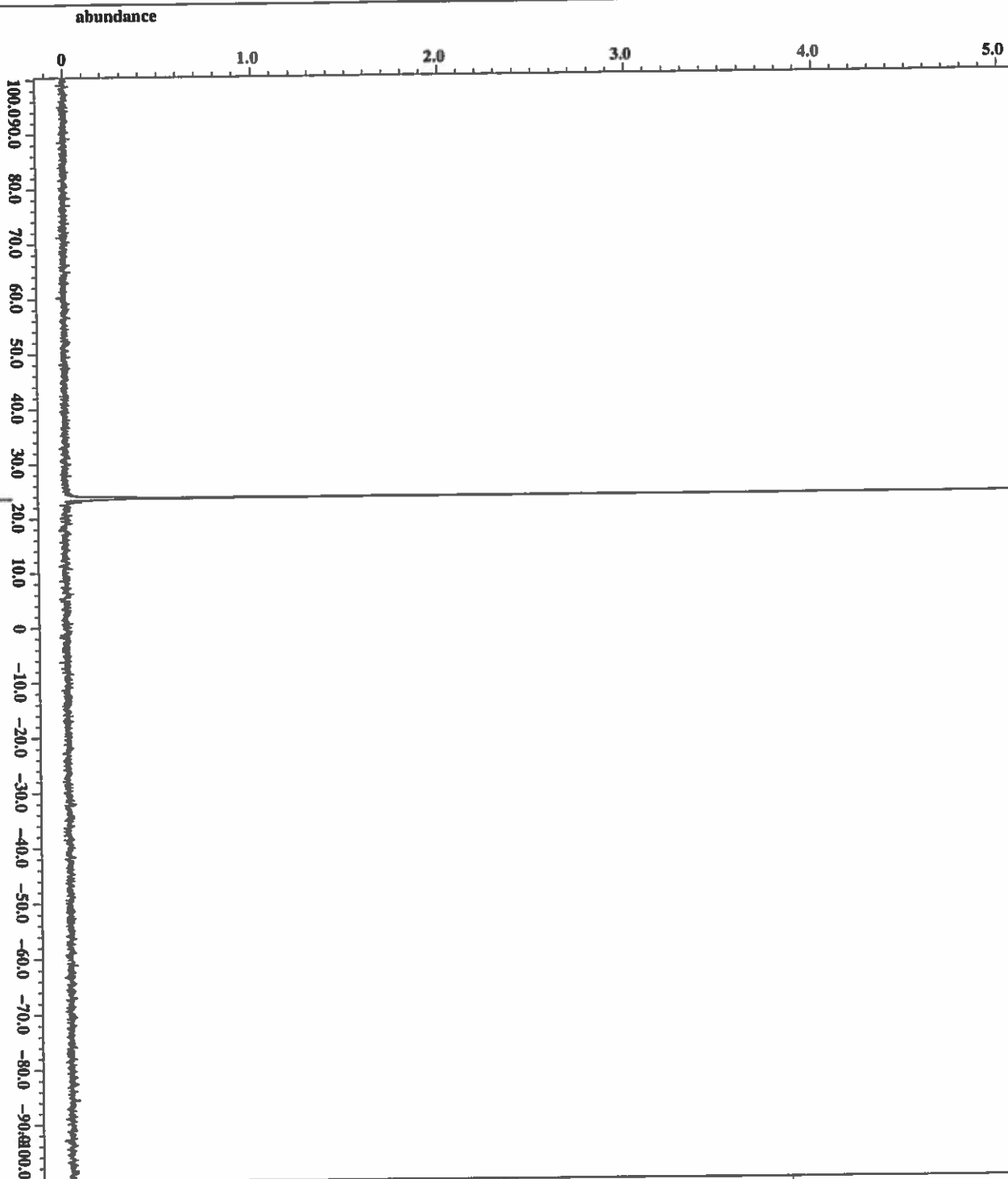
Filename      = MS0480-250-96h_FLUORINE
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = MS0480-250-96h
Solvent       = CHLOROFORM-D
Charger_sample = 7
Creation_time  = 27-JUN-2018 09:24:29
Revision_time  = 27-JUN-2018 09:01:37
Current_time   = 27-JUN-2018 09:01:38

Date_format   = 1D COMPLEX
Dim_size      = 52428
Dim_title     = 19F
Dim_units     = [ppm]
Dimensions    = X
Sfca          = ECA 500
Sfca          = JNM-ECA500

Spectrometer  =

Pfield_strength = 11.7473579 [T] (500 [MH
X_acq_duration  = 0.55574528 [s]
X_domain        = 19F
X_freq          = 470.62046084 [MHz]
X_offset        = -70 [ppm]
X_points        = 65536
X_prescans      = 1
X_resolution    = 1.799385 [Hz]
X_sweep         = 117.9245283 [kHz]
X_domain        = 19F
X_freq          = 470.62046084 [MHz]
X_offset        = 5 [ppm]
X1_freq         = 19F
X1_domain       = 470.62046084 [MHz]
X1_offset       = 5 [ppm]
Clipped        = FALSE
Mod_return      = 1
Total_scans     = 16

X_90_width      = 13.1 [us]
X_acq_time       = 0.55574528 [s]
X_angle         = 45 [deg]
X_axn           = 2.5 [dB]
X_pulse         = 6.55 [us]
X1_mode         = OF2
Pulse           = FALSE
Pulse           = 1 [s]
Pulse           = 38
Relaxation_delay = 4 [s]
Repetition_time  = 4.55574528 [s]
Temp_get        = 22.2 [dc]
  
```



filename
 Author
 Experiment
 Sample_id
 solvent
 changer_sample
 Creation_time
 Revision_time
 Current_time

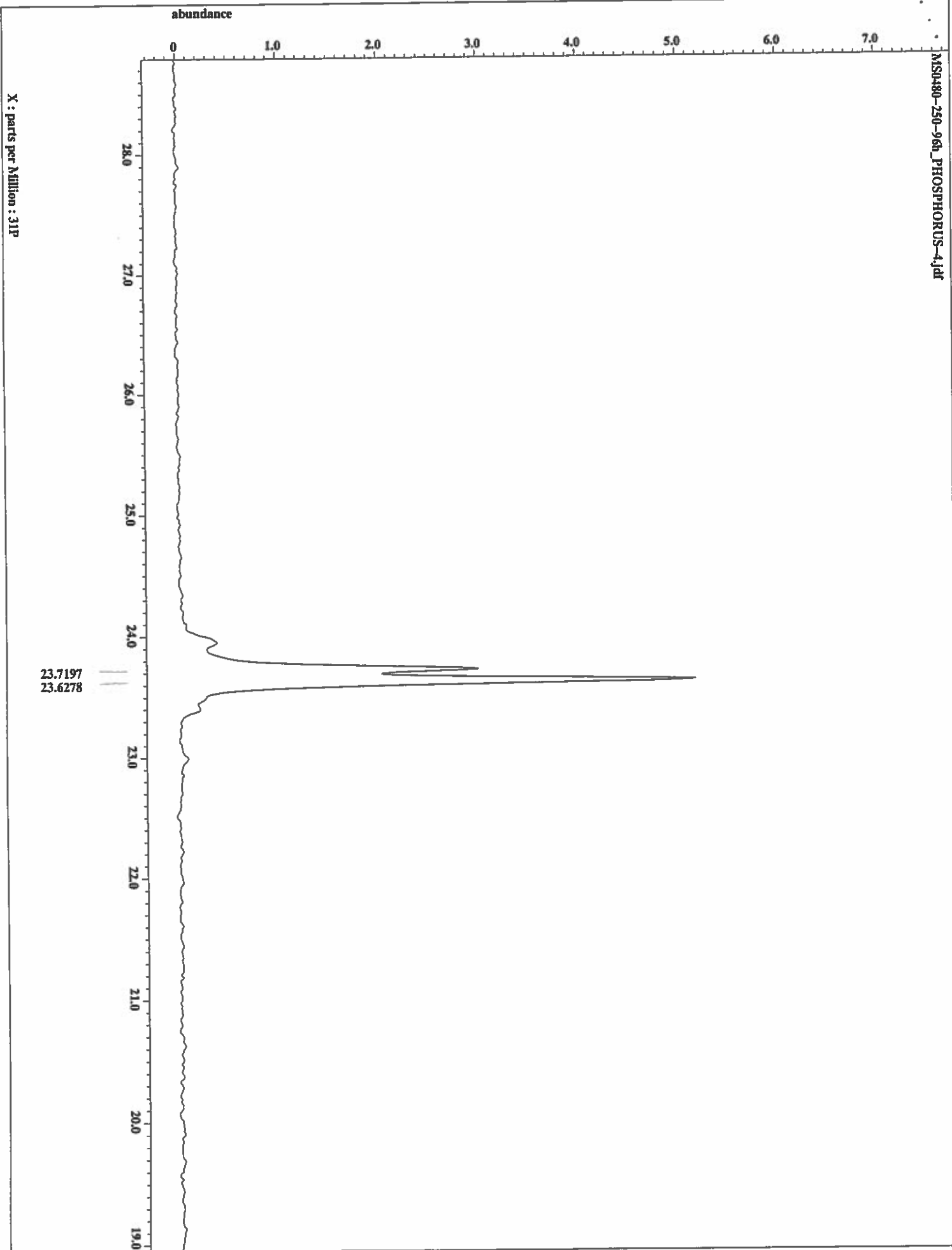
= MS0480-250-96h_PHOSPH
 = Jim Davis
 = single_pulse_dec
 = MS0480-250-96h
 = CHLOROFORM-D
 = 7
 = 27-JUN-2018 09:28:13
 = 27-JUN-2018 09:05:21
 = 27-JUN-2018 09:05:21

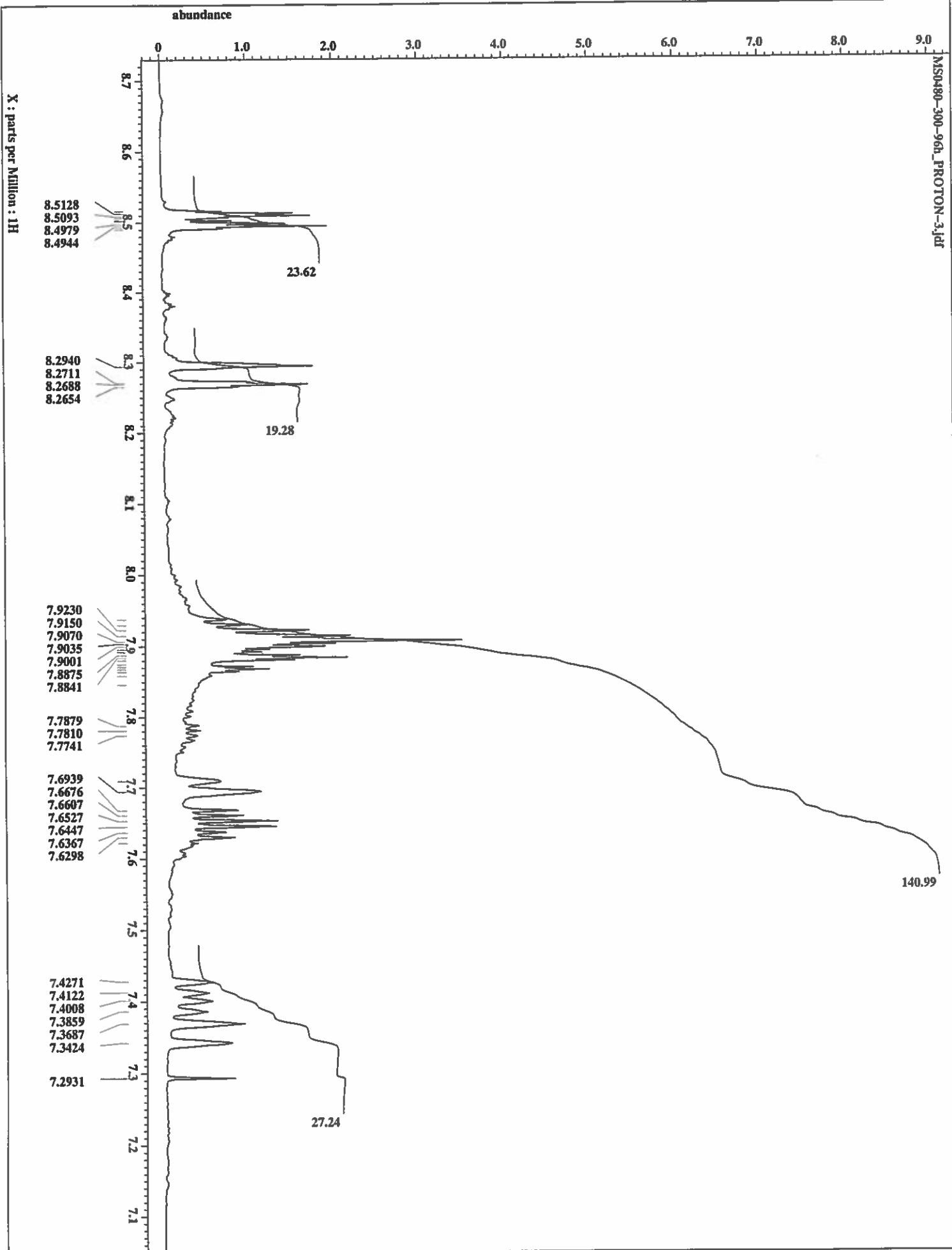
Data_format
 Dim_size
 Dim_title
 Dim_units
 Dimensions
 Site
 Spectrometer

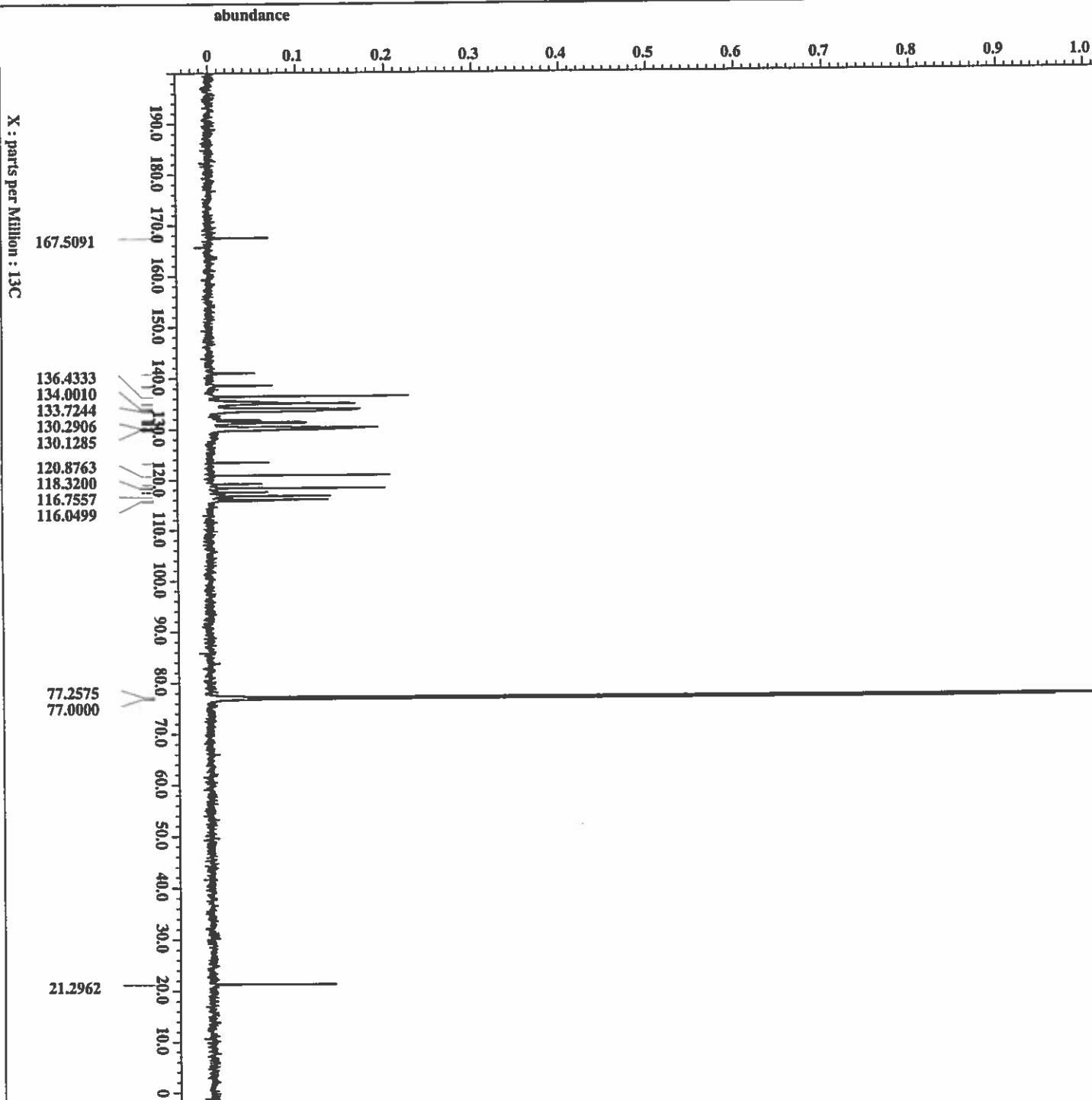
= 1D COMPLEX
 = 26214
 = 31P
 = [ppm]
 = X
 = FCA 500
 = JNM-ECA500

Field_strength
 X_acq_duration
 X_domain
 X_freq
 X_offset
 X_points
 X_prescans
 X_resolution
 X_sweep
 Irr_domain
 Irr_freq
 Irr_offset
 Clipped
 Mod_return
 Scans
 Total_scans
 X_90_width
 X_acq_time
 X_angle
 X_atn
 X_pulse
 Irr_atn_dec
 Irr_atn_noe
 Irr_noise
 Decoupling
 Initial_wait
 Noe
 Noe_time
 Recvr_gain
 Relaxation_delay
 Repetition_time
 Temp_get

= 11.7473579 [T] (500 [MH
 = 0.64487424 [s]
 = 31P
 = 202.46831075 [MHz]
 = 0 [ppm]
 = 32768
 = 4
 = 1.55068995 [Hz]
 = 50.81300813 [kHz]
 = 1H
 = 500.15991521 [MHz]
 = 5.0 [ppm]
 = FALSE
 = 1
 = 25
 = 25
 = 14.687 [us]
 = 0.64487424 [s]
 = 30 [deg]
 = 5 [db]
 = 4.89566667 [us]
 = 20.7 [dB]
 = 20.7 [dB]
 = WALTZ
 = TRUE
 = 1 [s]
 = TRUE
 = 2 [s]
 = 58
 = 2 [s]
 = 2.64487424 [s]
 = 22.4 [deg]





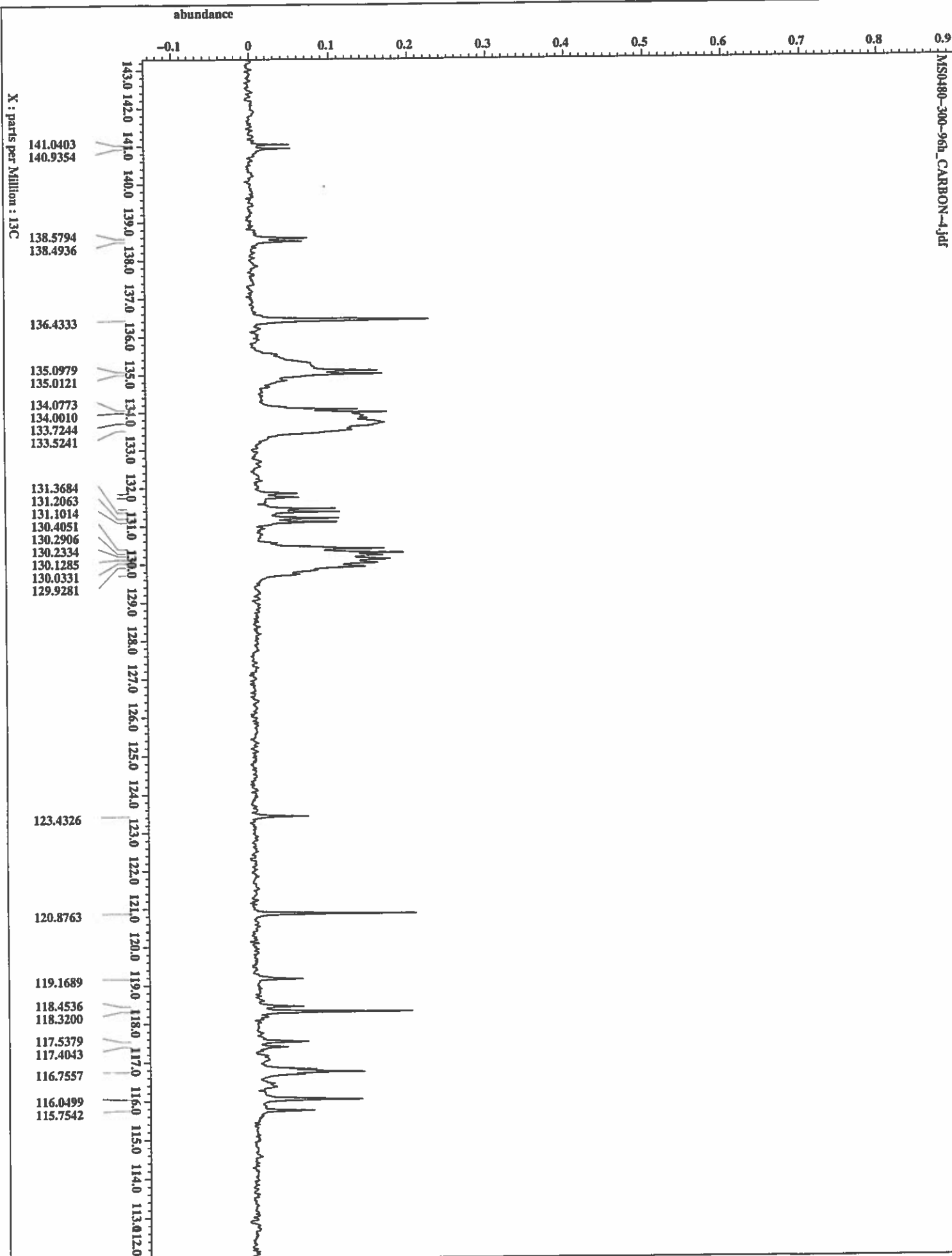


filename = MS0480-300-96h_CARBON
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = MS0480-300-96h
 Solvent = CHLOROFORM-D
 Changer_sample = 8
 Creation_time = 27-JUN-2018 09:56:43
 Revision_time = 27-JUN-2018 09:33:51
 Current_time = 27-JUN-2018 09:33:51

Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

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 = 400
 Total_scans = 400

X_90_width = 13.2 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 6 [dB]
 X_pulse = 4.4 [us]
 Irr_atn_dec = 20.7 [dB]
 Irr_atn_poe = 20.7 [dB]
 Decoupling = WALTZ
 Initial_wait = TRUE
 Noe = 1 [s]
 Noe_time = 60
 Recvr_gain = 2 [s]
 Relaxation_delay = 2.83361792 [s]
 Repetition_time = 22.8 [dc]
 Temp_get = 22.8 [dc]



```

Filament      = M50480-300-96h_FILAMENT
Author        = Jim Davis
Experiment     = single_pulse_ex2
Sample_id     = M50480-300-96h
Solvent       = CHLOROFORM-D
Charger_sample = 8
Creation_time  = 27-JUN-2018 09:59:49
Creation_time  = 27-JUN-2018 09:36:57
Current_time   = 27-JUN-2018 09:36:57

```

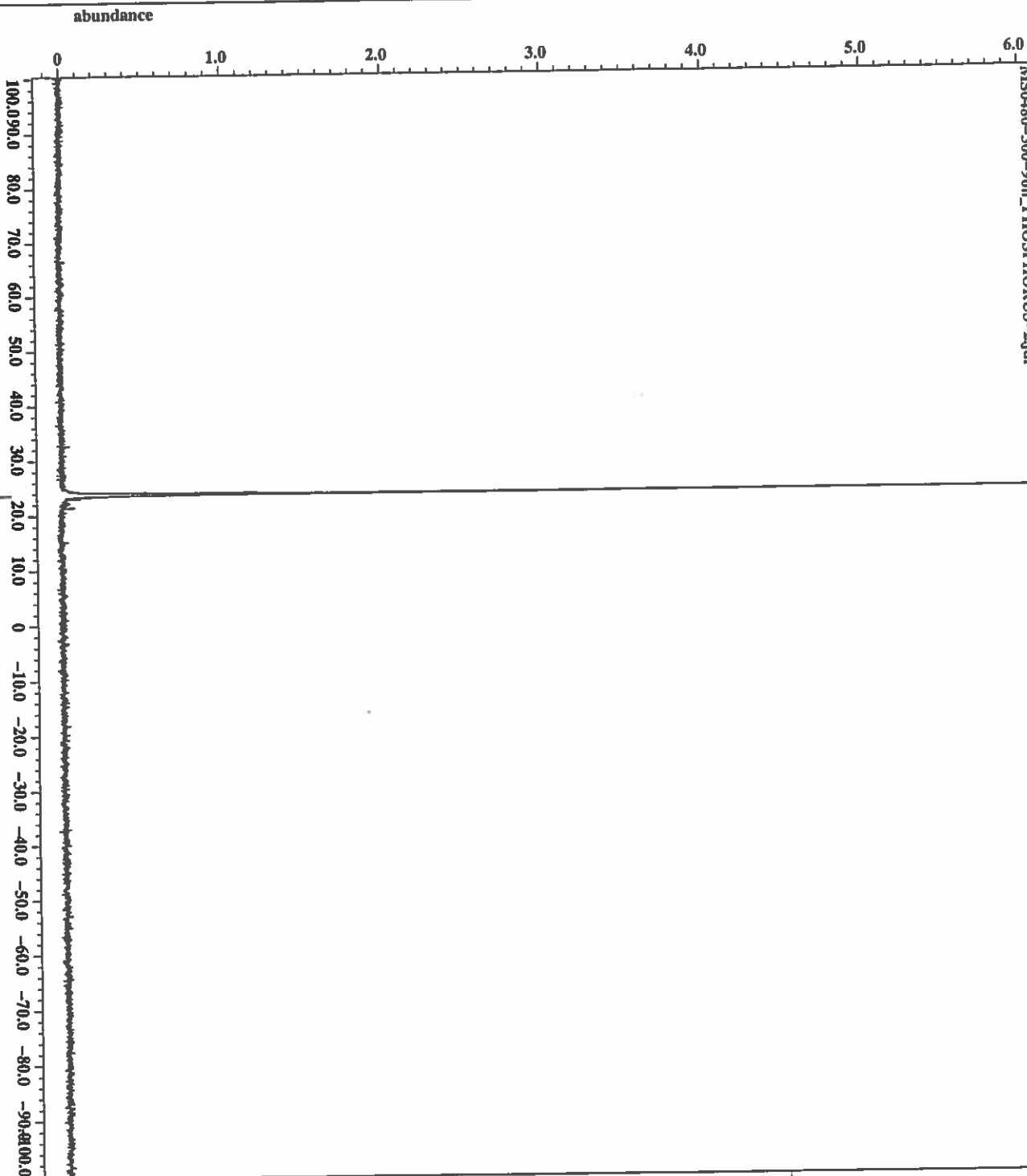
```

Data_format      = ID_COMPLEX
Dim_size         = 52428
Dim_title        = 19F
Dim_units        = [ppm]
Dimensions       = x
                 = ECA 500
                 = JNM-ECA500
Spectrometer

```

field_strength	= 11.7475379 [G]	(500 [MHz])
X_acq_duration	= 0.55574528 [s]	
X_domain	= 19°	
X_freq	= 470.62046084 [MHz]	
X_offset	= -70 [Dppm]	
X_points	= 65536	
X_prescans	= 1	
X_resolution	= 1.7993855 [Hz]	
X_sweep	= 117.9245283 [kHz]	
irr_domain	= 19°	
irr_freq	= 470.62046084 [MHz]	
irr_offset	= 5 [Dppm]	
irr_domain	= 19°	
trf_freq	= 470.62046084 [MHz]	
trf_offset	= 5 [Dppm]	
clipped	= FALSE	
mod_return	= 1	
scans	= 16	
total_scans	= 16	
X_90_width	= 13.1 [µs]	
X_acq_time	= 0.55574528 [s]	
X_angle	= 45 [deg]	
X_atn	= 2.5 [dB]	
X_pulse	= 6.55 [µs]	
irr_mode	= OFE	
trf_mode	= OFE	
pulse_presat	= FALSE	
initial_wait	= 1 [s]	
recvr_gain	= 36	
relaxation_delay	= 4 [µs]	
Repetition_time	= 4.55574528 [s]	
Temp_get	= 22.4 [°C]	





X : parts per Million : 31P

23.7197
23.6201SOUTH ALABAMA
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```

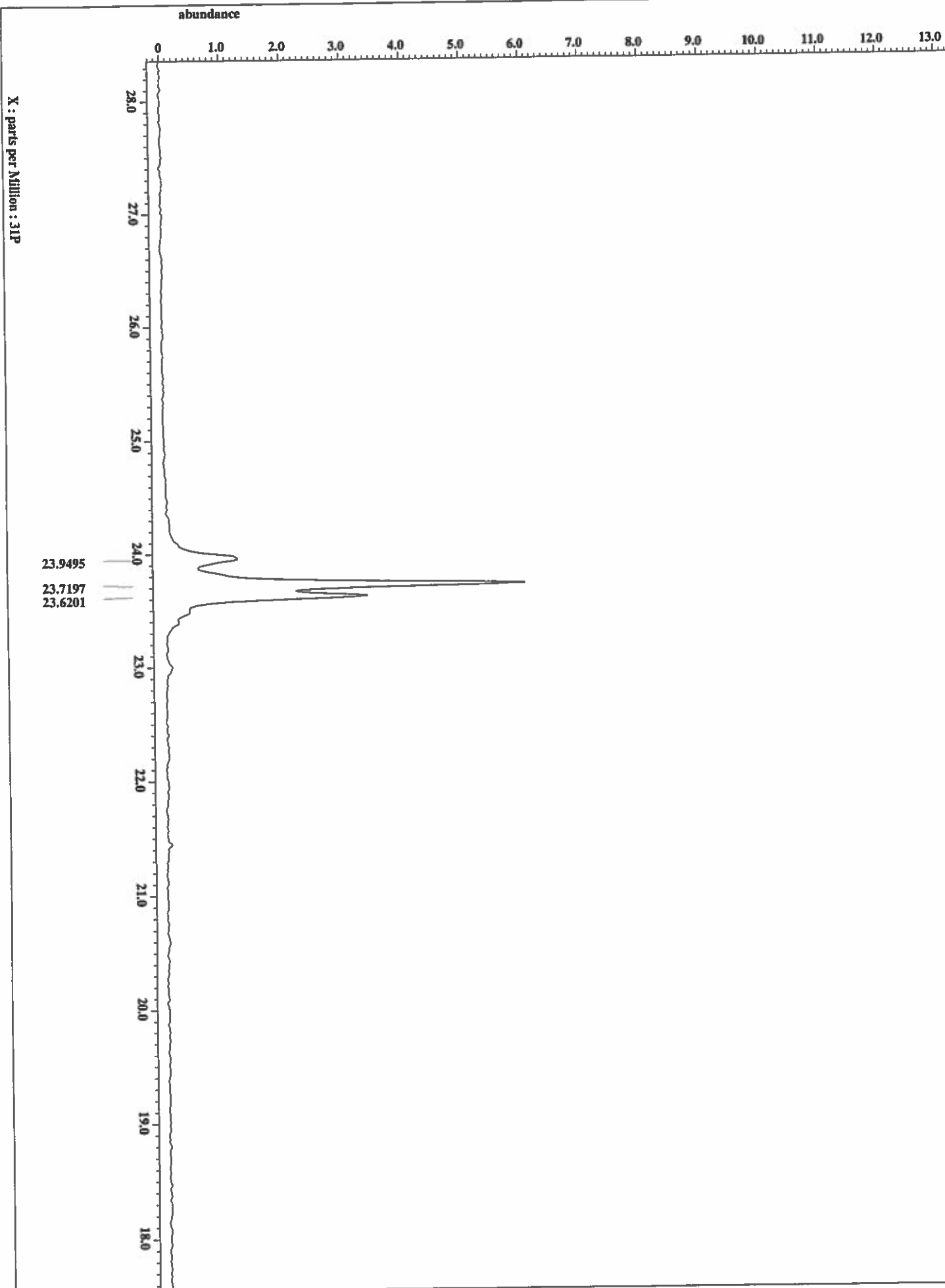
Filename      = MS0480-300-96h_PHOSPH
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0480-300-96h
Solvent       = CHLOROFORM-D
Charger_sample = 8
Creation_time  = 27-JUN-2018 10:03:29
Revision_time  = 27-JUN-2018 09:40:36
Current_time   = 27-JUN-2018 09:40:36

Data_format    = 1D COMPLEX
Dim_size       = 26214
Dim_title      = 31P
Dim_units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

P1,pld_strength = 11.7473579 [?] (500 [MHz]
X_acq_duration  = 0.64487424 [s]
X_domain        = 31P
X_freq          = 202.46931075 [MHz]
X_offset        = 0 [ppm]
X_points        = 32768
X_prescans      = 4
X_resolution    = 1.55068995 [Hz]
X_sweep         = 50.81300813 [kHz]
X_domain        = 1H
X_freq          = 500.15991521 [MHz]
X_offset        = 5.0 [ppm]
X_return        = FALSE
Mod_return      = 1
Scans           = 25
Total_scans     = 25

X_90_width      = 14.687 [us]
X_acq_time      = 0.64487424 [s]
X_angle         = 30 [deg]
X_atn           = 5 [dB]
X_pulse         = 4.89566667 [us]
X_pulse_dec     = 20.7 [dB]
X_atn_dec       = 20.7 [dB]
X_atn_poe       = 20.7 [dB]
X_noise         = WALTZ
Decoupling      = TRUE
Initial_wait    = 1 [s]
Noe             = TRUE
Noe_time        = 2 [s]
Relaxation_delay = 2.64487424 [s]
Repetition_time = 2.64487424 [s]
Temp_get        = 22.6 [ac]

```



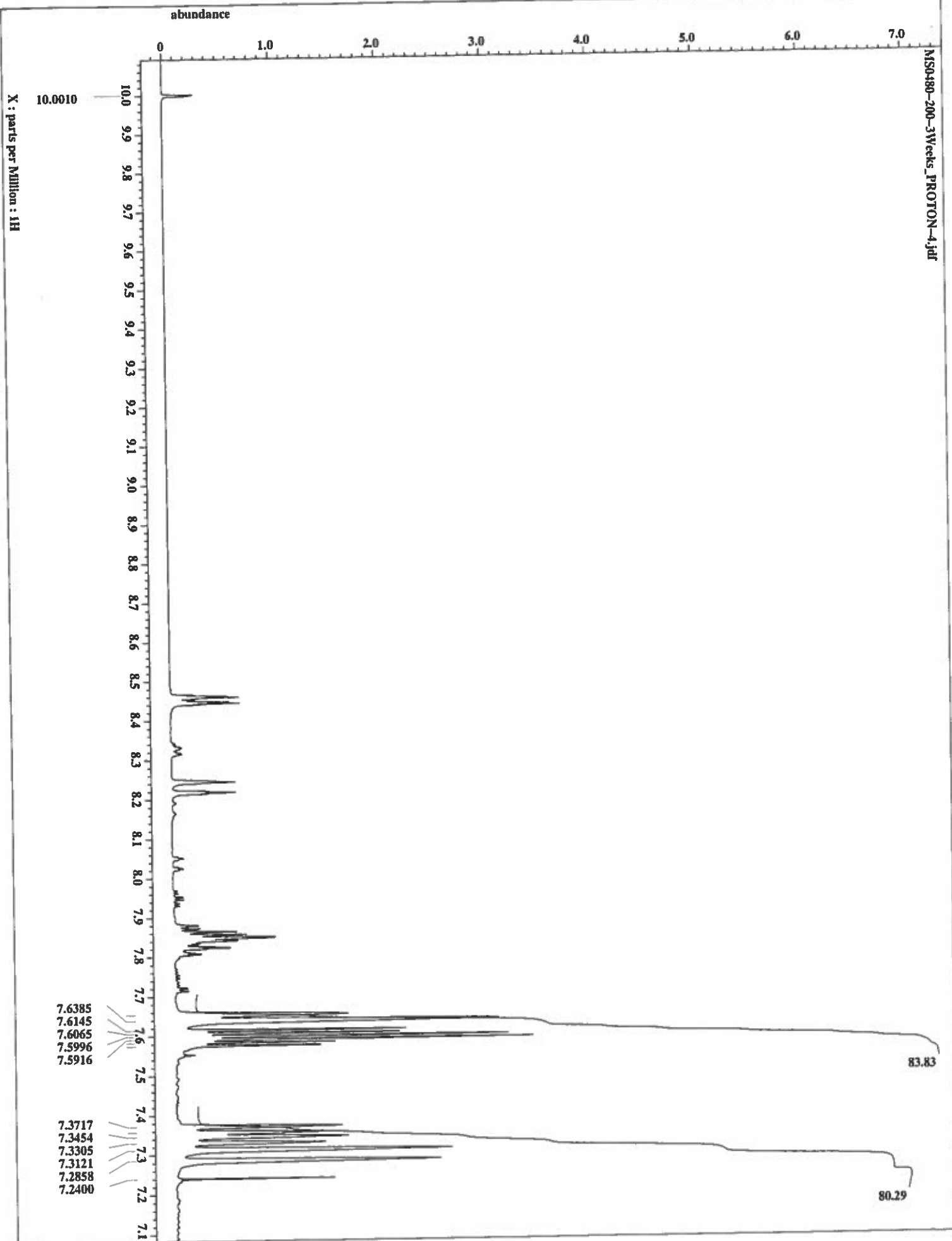


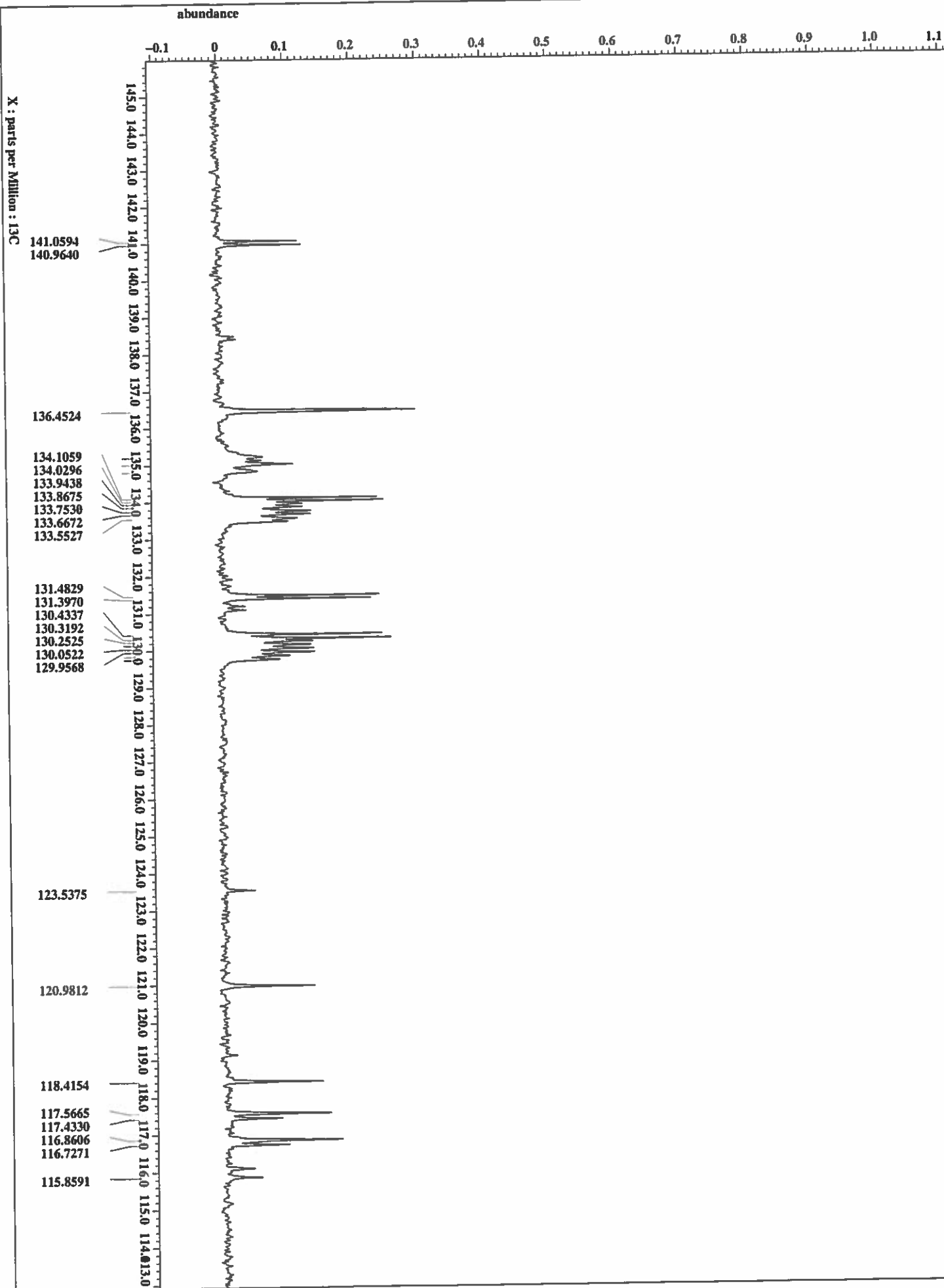
7.6385
7.5996
7.5916
7.3121

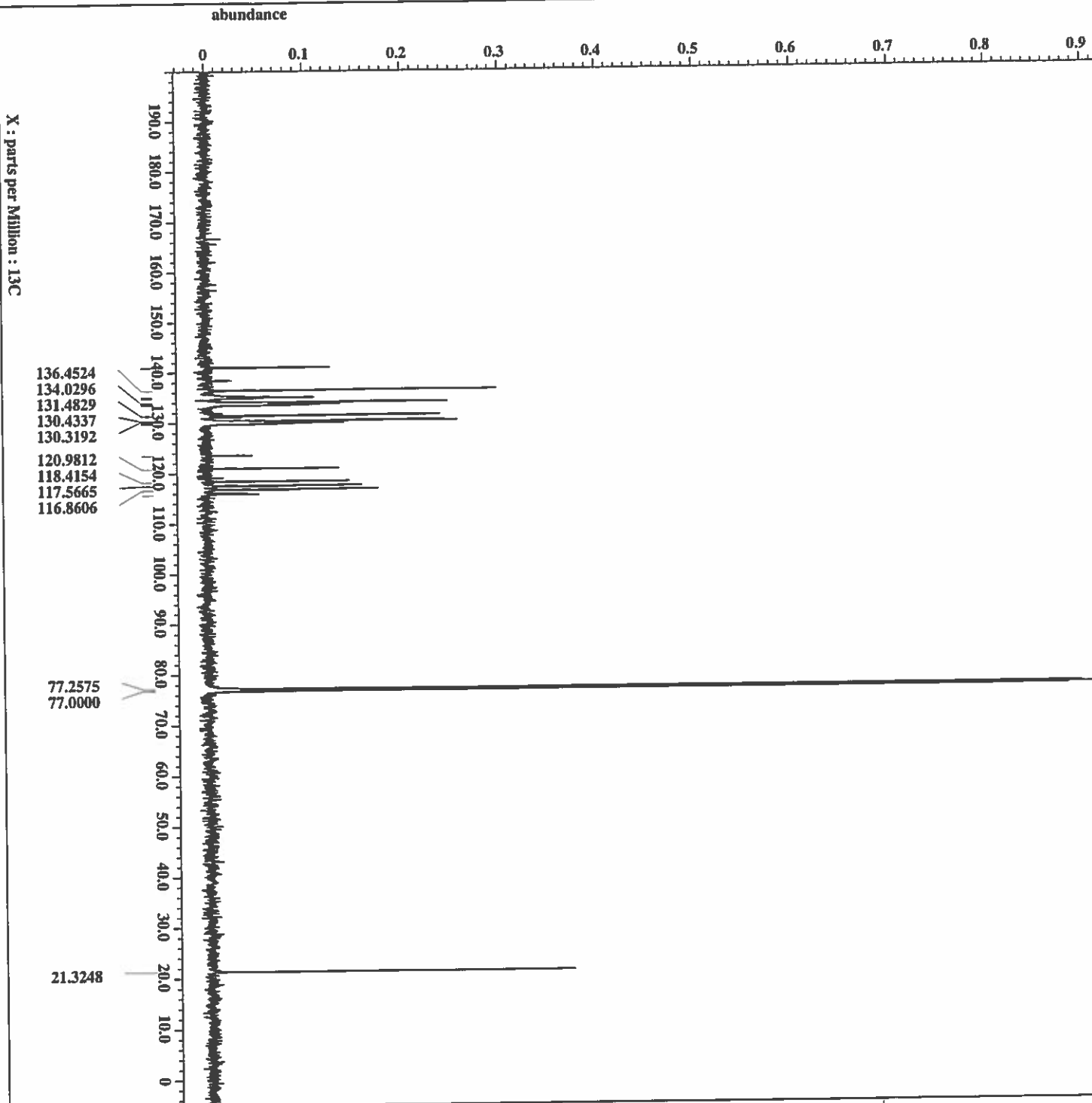
2.4004

Filename	= MS0480-200-3Weeks_Pro
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0480-200-3Weeks
Solvent	= CHLOROFORM-D
Charger_sample	= 21
Creation time	= 13-JUL-2018 10:20:02
Revision time	= 13-JUL-2018 09:57:35
Current time	= 13-JUL-2018 09:57:35
Data_format	= ID_COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579 [T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521 [MHz]
X_offset	= 5.0 [ppm]
X_points	= 16384
X_resolution	= 1
X_resolutions	= 0.57277737 [Hz]
X_sweep	= 9.38638638 [kHz]
Iter_domain	= 1H
Iter_freq	= 500.15991521 [MHz]
Iter_offset	= 5.0 [ppm]
Iter_domain	= 1H
Tr1_freq	= 500.15991521 [MHz]
Tr1_offset	= 5.0 [ppm]
Clipped	= PULSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_g0_width	= 12.4 [us]
X_acq_time	= 1.74587904[s]
X_angle	= 45 [deg]
X_atn	= 4 [da]
X_pulse	= 6.2 [us]
Iter_mode	= OFF
Tr1_mode	= OFF
Dance_preset	= PRIZR
Initial_wait	= 1[s]
Relax_gain	= 38
Relaxation_delay	= 4[s]
Relaxation_time	= 5.74587904[s]
Temp_get	= 22.7 [dC]

X: parts per Million: 1H







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```

Filename      = MS0480-200-3weeks_CAR
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0480-200-3weeks
Solvent       = CHLOROFORM-D
Charger_sample = 21
Creation_time  = 13-JUL-2018 10:34:27
Revision_time  = 13-JUL-2018 10:11:58
Current_time   = 13-JUL-2018 10:11:58

Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

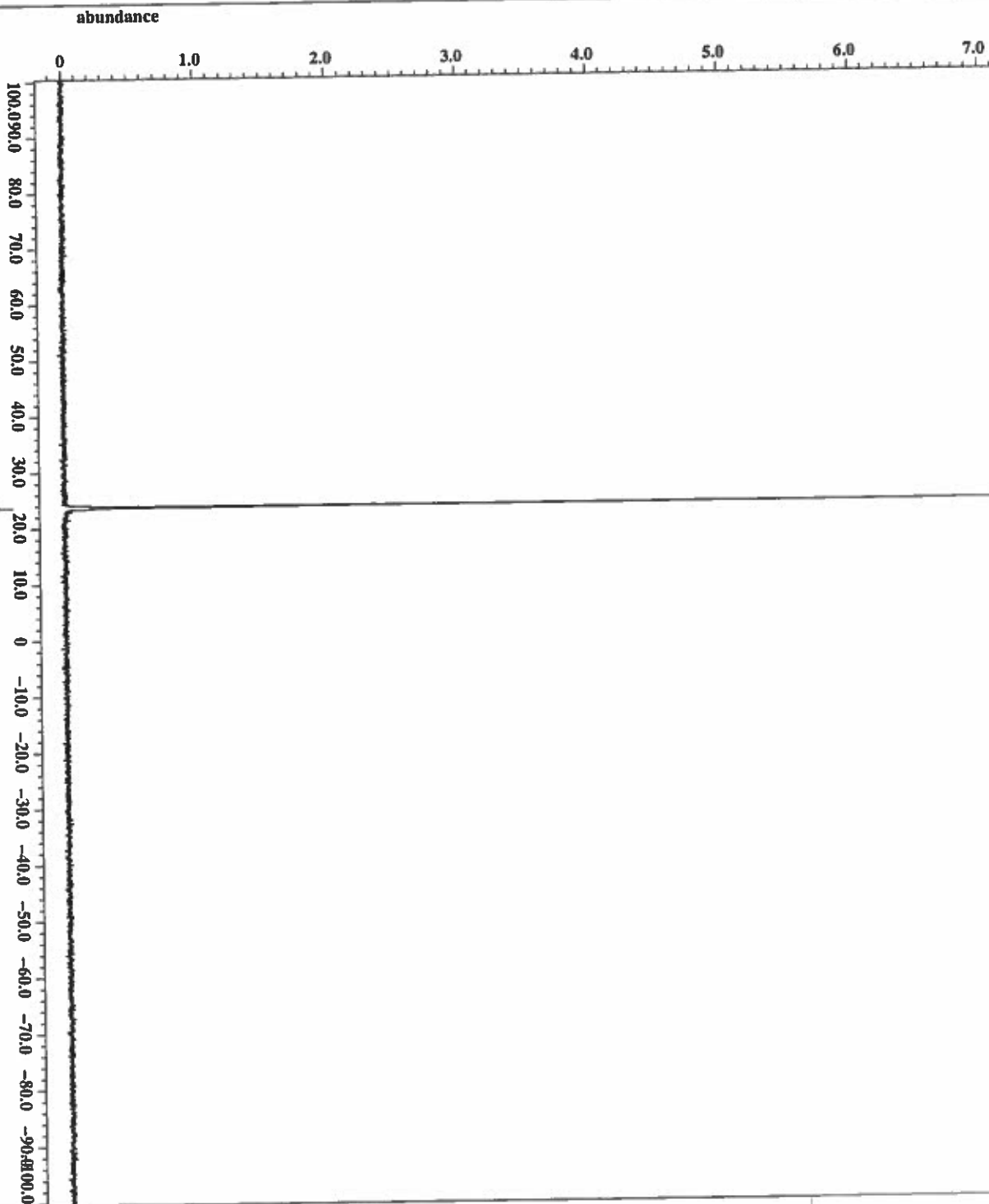
Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain      = 13C
X_freq        = 125.76529768 [MHz]
X_offset      = 100 [ppm]
X_points      = 32768
X_prescans    = 4
X_resolution  = 1.19959034 [Hz]
X_sweep       = 39.3081761 [Hz]
X_domain      = 1H
Xir_freq      = 500.15991521 [MHz]
Xir_offset    = 5.0 [ppm]
Mod_return    = FALSTZ
Total_scans   = 1
              = 256
              = 256

X_90_width    = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle       = 30 [deg]
X_atn         = 6 [dB]
X_pulse       = 4.4 [us]
Xir_atn_dec   = 20.7 [dB]
Xir_atn_poe   = 20.7 [dB]
Xir_noise     = KALFZ
Decoupling    = TRUZ
Initital_wait = TRUZ
Noe           = TRUZ
Noe_time      = 60
Recvr_gain    = 21 [e]
Relaxation_delay = 2.83361792 [s]
Repetition_time = 23.2 [dc]
Temp_get      = 23.2 [dc]

```



Fieldname	
Author	= MS0480-200-3Weeks_F10D
Experiment	= Jim Davis
Sample_id	= single_pulse.exe2
Solvent	= MS0480-200-3Weeks
Change_sample	= CHLOROPORM-D
Creation_time	= 13-JUL-2018 10:37:37
Revision_time	= 13-JUL-2018 10:15:09
Current_time	= 13-JUL-2018 10:15:09
Data_format	= 1D_COMPLEX
Dim_size	= 52428
Dim_title	= 19F
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[F] (500[MH
X_acq_duration	= 0.55574528[s]
X_domain	= 19F
X_freq	= 470.62046084[MHz]
X_offset	= -70 [ppm]
X_points	= 65536
X_prescans	= 1
X_resolution	= 1.7993855 [Hz]
X_sweep	= 117.9245283 [kHz]
irr_domain	= 470.62046084 [MHz]
irr_freq	= 19F
irr_offset	= 19F
irr_domain	= 470.62046084 [MHz]
irr_freq	= 19F
irr_offset	= 19F
Clipped	= 1
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 13.1 [us]
X_acq_time	= 0.55574528[s]
X_angle	= 45 [deg]
X_atn	= 2.5 [dB]
X_pulse	= 6.55 [us]
irr_mode	= Off
Tri_mode	= Off
Donce_presat	= FALST
Initial_wait	= 1[s]
Recvr_gain	= 38
Relaxation_delay	= 4[s]
Relaxation_time	= 4.55574528[s]
Temp_Get	= 22.8 [dC]

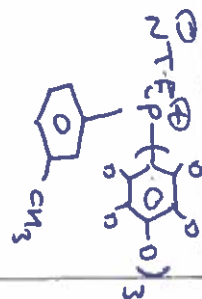
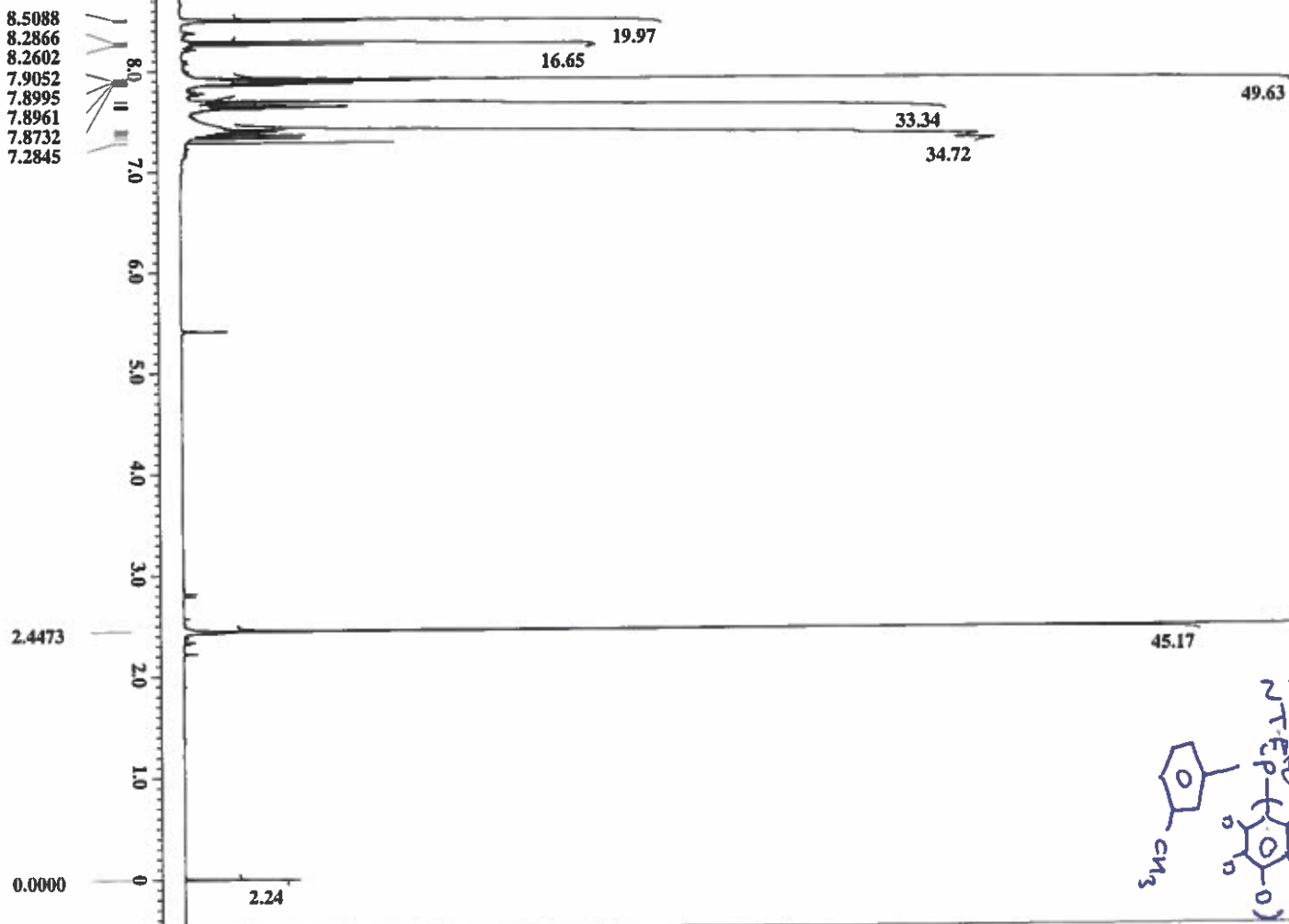


Filename MS0480-200-3Weeks_PHO
 Author Jim Davis
 Experiment single_pulse_dec
 Sample_id MS0480-200-3Weeks
 Solvent CHLOROFORM-D
 Changer_sample 21
 Creation_time 13-JUL-2018 10:41:16
 Revision_time 13-JUL-2018 10:18:48
 Current_time 13-JUL-2018 10:18:48

Data_format 1D COMPLEX
 Dia_size 26214
 Dia_title 31P
 Dia_units [ppm]
 Dimensions X
 Site ECA 500
 Spectrometer JNM-ECA500

Field_strength 11.7473579 [T] (500 [MH
 X_acq_duration 0.64487424 [s]
 X_domain 31P
 X_freq 202.46831075 [MHz]
 X_offset 0 [ppm]
 X_points 32768
 X_prescans 4
 X_resolution 1.55068995 [Hz]
 X_sweep 50.81300813 [kHz]
 Irr_domain 1H
 Irr_freq 500.15991521 [MHz]
 Irr_offset 5.0 [ppm]
 Clipped FALSE
 Mod_return 1
 Scans 25
 Total_scans 25

X_90_width 14.687 [us]
 X_acq_time 0.64487424 [s]
 X_angle 30 [deg]
 X_atn 5 [dB]
 X_pulse 4.89566667 [us]
 Irr_atn_dec 20.7 [dB]
 Irr_atn_noi 20.7 [dB]
 Irr_noise KALTRZ
 Decoupling TR02
 Initial_wait 1 [s]
 Noe TR02
 Noe_time 2 [s]
 Recv_gain 58
 Relaxation_delay 2 [s]
 Repetition_time 2.64487424 [s]
 Temp_get 23 [dC]



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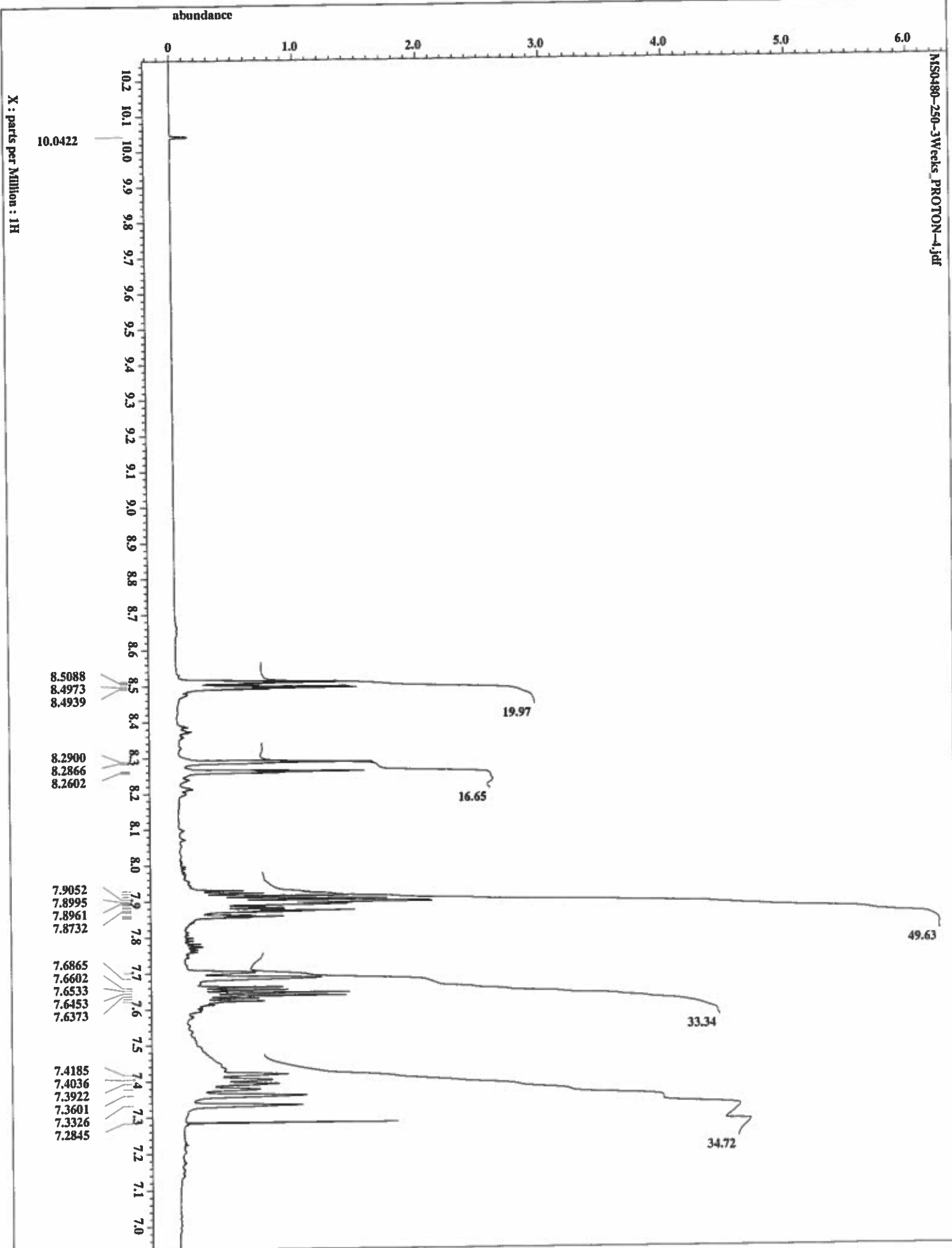


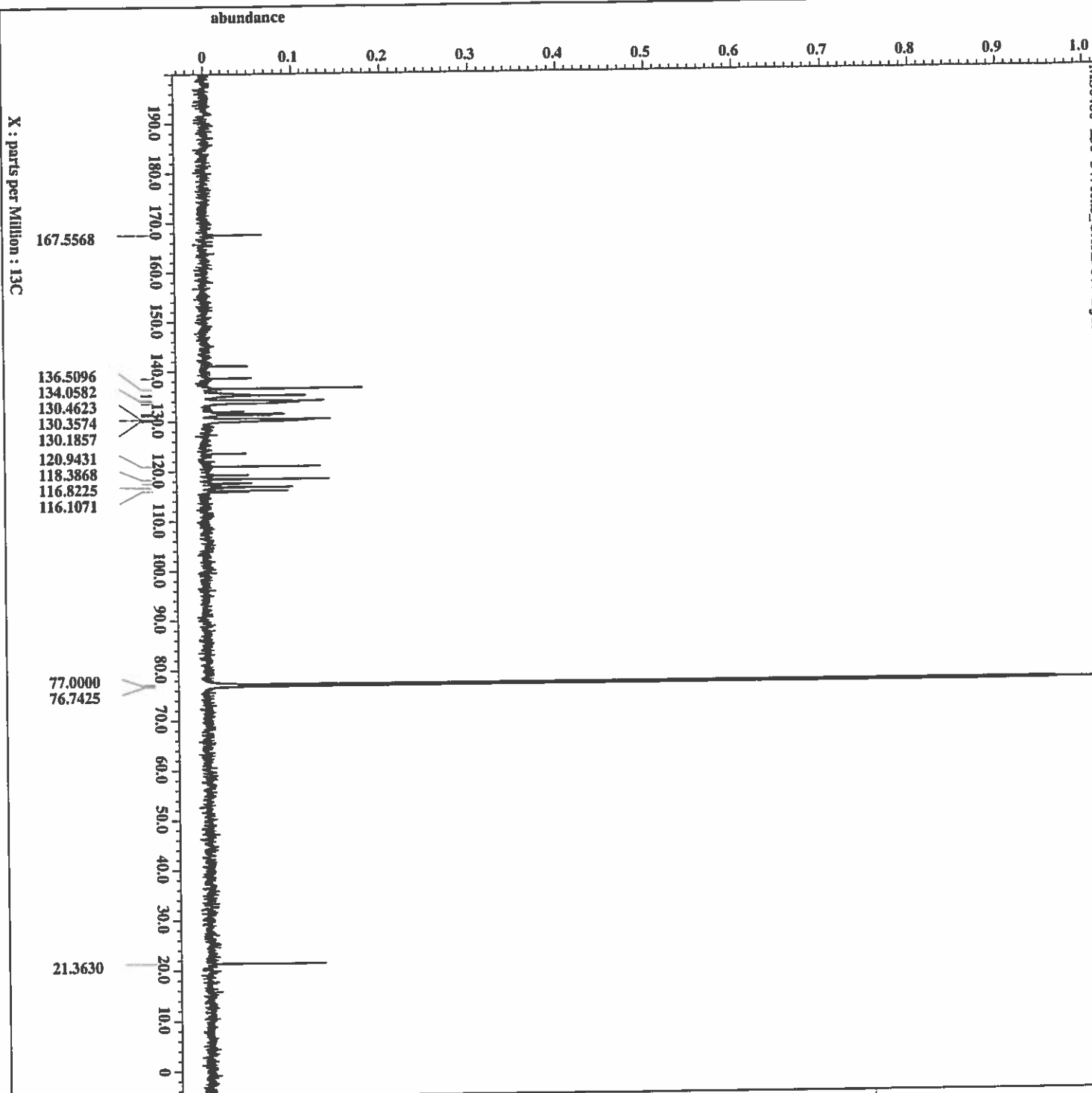
Filename = MS0480-250-3Weeks_PRO
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0480-250-3Weeks
 Solvent = CHLOROFORM-D
 Change_sample = 22
 Creation_time = 13-JUL-2018 10:48:37
 Revision_time = 13-JUL-2018 10:26:10
 Current_time = 13-JUL-2018 10:26:10

Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_file = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[G] (500 [MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.57277737 [Hz]
 X_sweep = 9.38438438 [kHz]
 Irf_domain = 1H
 Irf_freq = 500.15991521 [MHz]
 Irf_offset = 5.0 [ppm]
 Trf_domain = 1H
 Trf_freq = 500.15991521 [MHz]
 Trf_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 12.4 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_atn = 4 [db]
 X_pulse = 6.2 [us]
 Irf_mode = OFZ
 Trf_mode = OFZ
 Dacite_preset = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 38
 Relaxation_delay = 4 [s]
 Repetition_time = 5.74587904 [s]
 Temp_get = 22.7 [C]





```

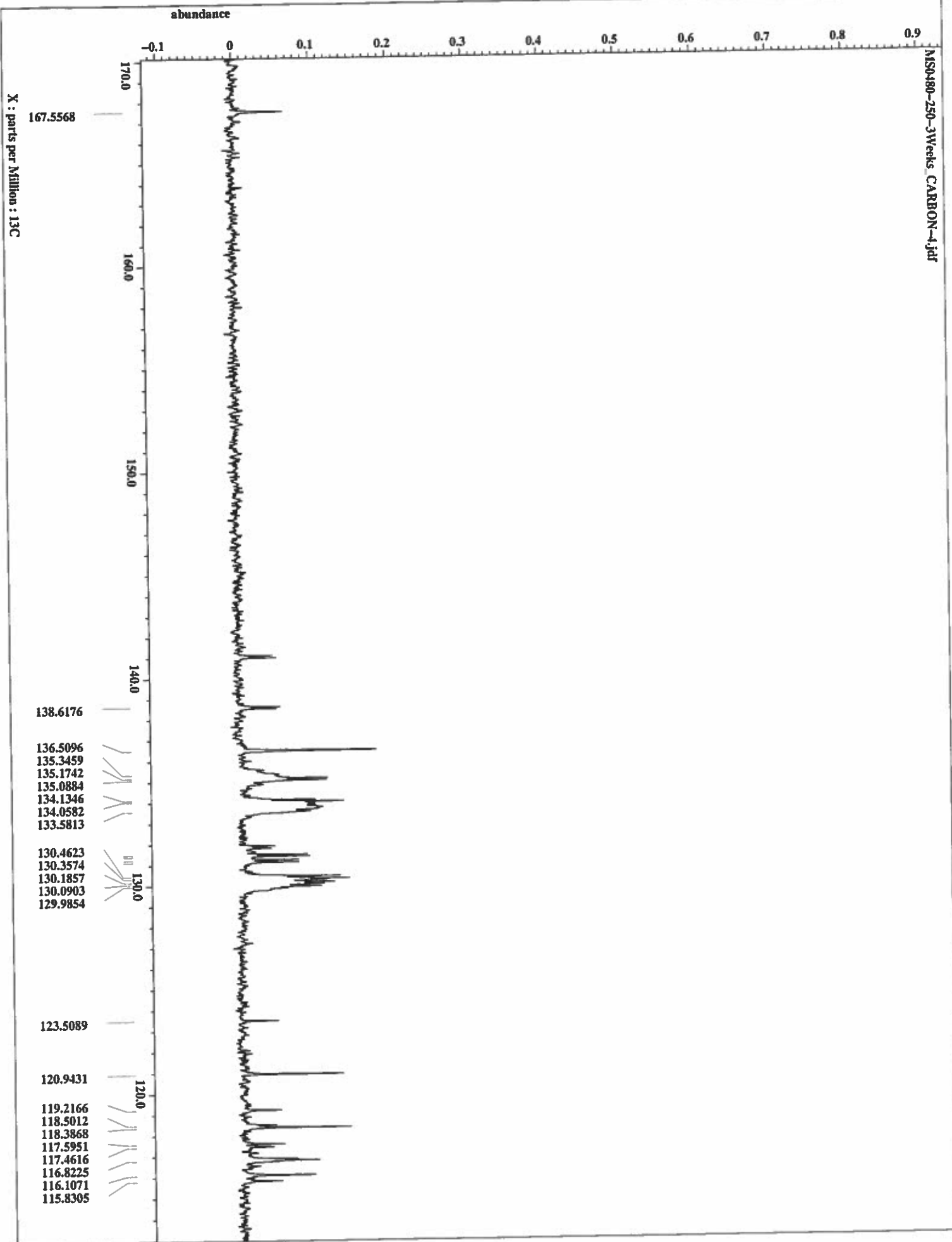
=====
File      MS0480-250-3Weeks_CAR
Author    Jim Davis
Experiment single_pulse_dec
Sample_id MS0480-250-3Weeks
Solvent    CHLOROFORM-D
Charger_sample
Creation_time 13-JUL-2018 11:03:06
Revision_time 13-JUL-2018 10:40:37
Current_time 13-JUL-2018 10:40:37

=====
Data_format 1D COMPLEX
Dim_size    26214
Dim_title   13C
Dim_units   [ppm]
Dimensions  1
Site        ECA 500
Spectrometer JNM-ECA500

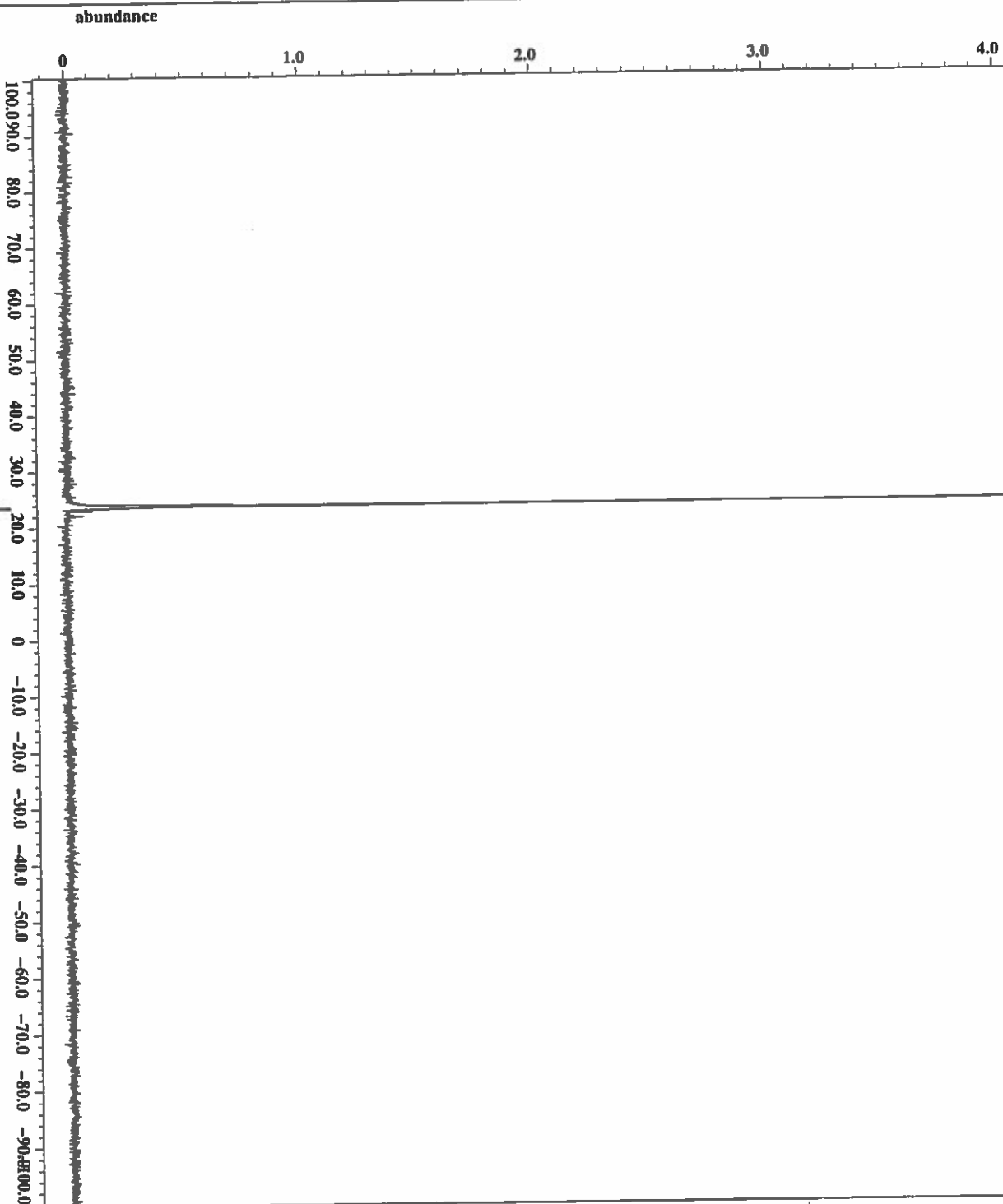
=====
Field_strength 11.7473579 [T] (500 MHz)
Acq_duration    0.83361792 [s]
X_domain        13C
X_freq          125.76529768 [MHz]
X_offset        100 [ppm]
X_points        32768
X_prescans      4
X_sweeps        1.19959034 [Hz]
X_resolution    39.3081761 [Hz]
X_domain        1H
X_freq          500.15991521 [MHz]
X_offset        5.0 [ppm]
X_domain        FALSE
Mod_return      1
Scans           256
Total_scans     256

=====
X_90_width      13.2 [us]
X_acq_time      0.83361792 [s]
X_angle         30 [deg]
X_atn           6 [dB]
X_pulse         4.4 [us]
Irr_atn_dec     20.7 [dB]
Irr_atn_noe     20.7 [dB]
Irr_noise       WALTZ
Decoupling      TRUE
Initial_wait    1 [s]
Noe_time        TRUE
Relaxation_delay 21 [s]
Repetition_time 2.83361792 [s]
Temp_get        23.2 [degC]
=====

```



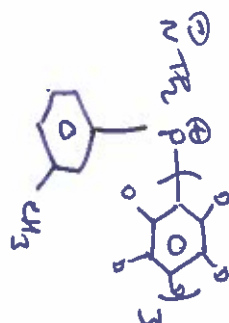
```
X_90_width = 1.3 [us]
X_acq_time = 0.55574528 [s]
X_angle = 45 [deg]
X_atn = 2.5 [dB]
X_pulse = 6.55 [us]
Itr_mode = OFF
Itr_mode = PALSZ
Dante_preset = 1[s]
Initial_wait = 38
Recvr_gain = 4[s]
Relaxation_delay = 4.55574528 [s]
Repetition_time = 22.8 [dc]
Temp_get
```



filename = MS0480-250-3Weeks_PBO
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = MS0480-250-3Weeks
 Solvent = CHLOROFORM-D
 Changer_sample = 22
 Creation_time = 13-JUL-2018 11:10:13
 Revision_time = 13-JUL-2018 10:47:44
 Current_time = 13-JUL-2018 10:47:44

Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 31P
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

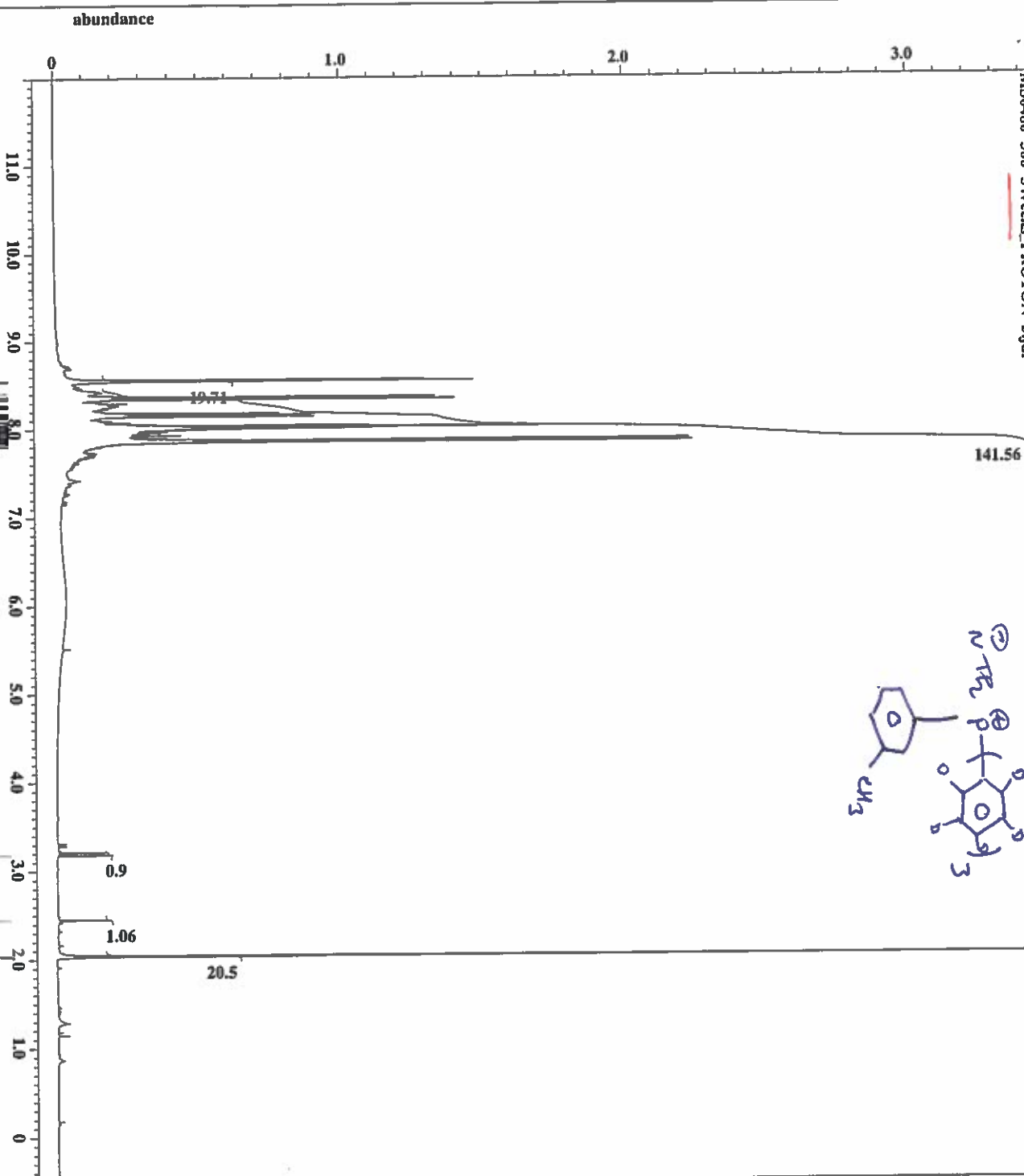
Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 0.64487424[s]
 X_domain = 31P
 X_freq = 302.46831075 [MHz]
 X_offset = 0 [ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.55068995 [Hz]
 X_sweep = 50.81300813 [kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 Clipped = FALSZ
 Mod_return = 1
 Scans = 25
 Total_scans = 25
 X_90_width = 14.587 [us]
 X_acq_time = 0.64487424 [s]
 X_angle = 30 [deg]
 X_atn = 5 [dB]
 X_pulse = 4.89566667 [us]
 Irr_atn_dec = 20.7 [dB]
 Irr_atn_noe = 30.7 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUZ
 Initial_walt = TRUZ
 Noe_time = 1[s]
 Recv_gain = TRUZ
 Relaxation_delay = 2[s]
 Repetition_time = 2.64487424 [s]
 Temp_set = 23 [degC]



8.5481
8.3385
8.0270
8.0213
7.8736
7.8484

3.1840
2.4511
2.0446
2.0400

X : parts per Million : 1H

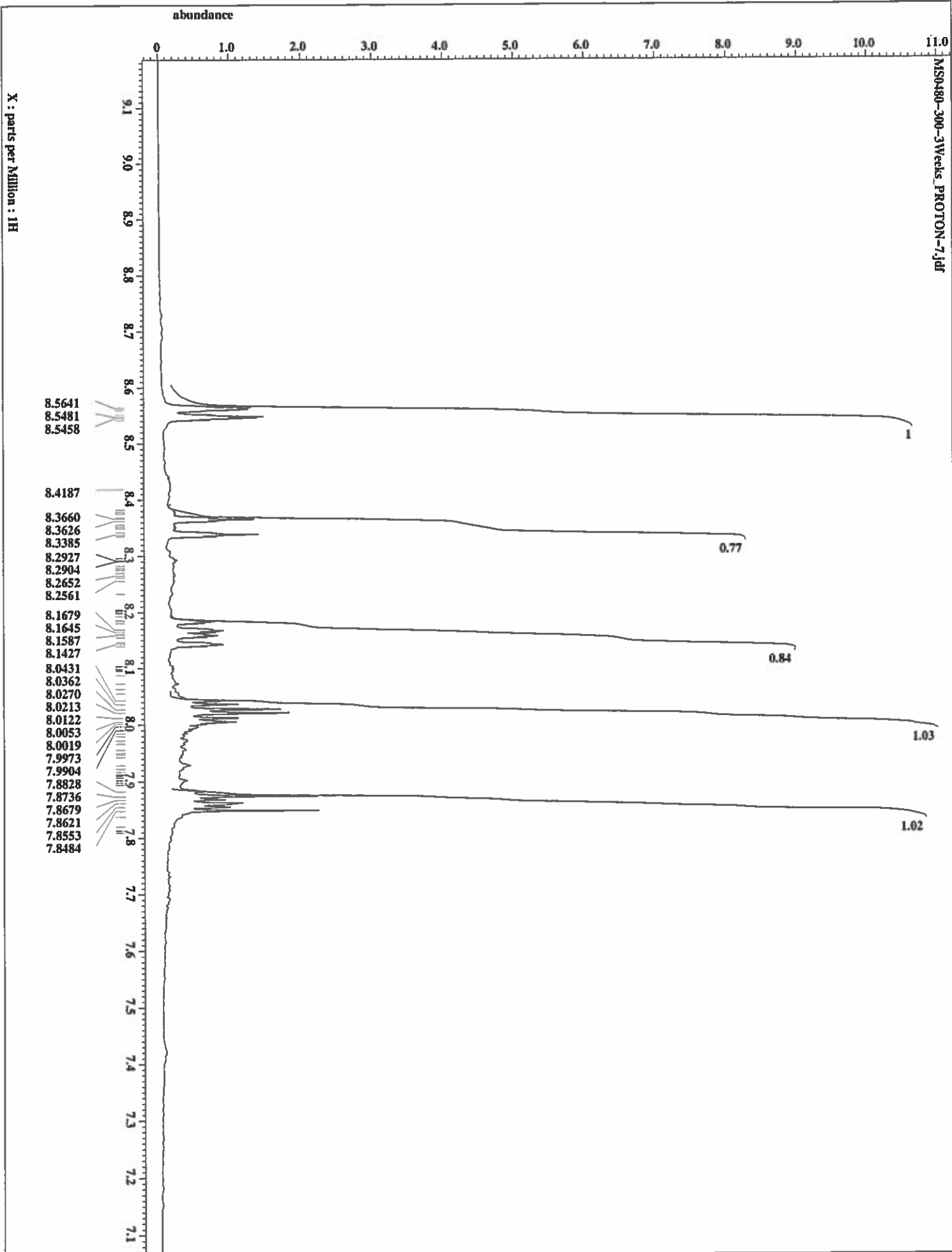


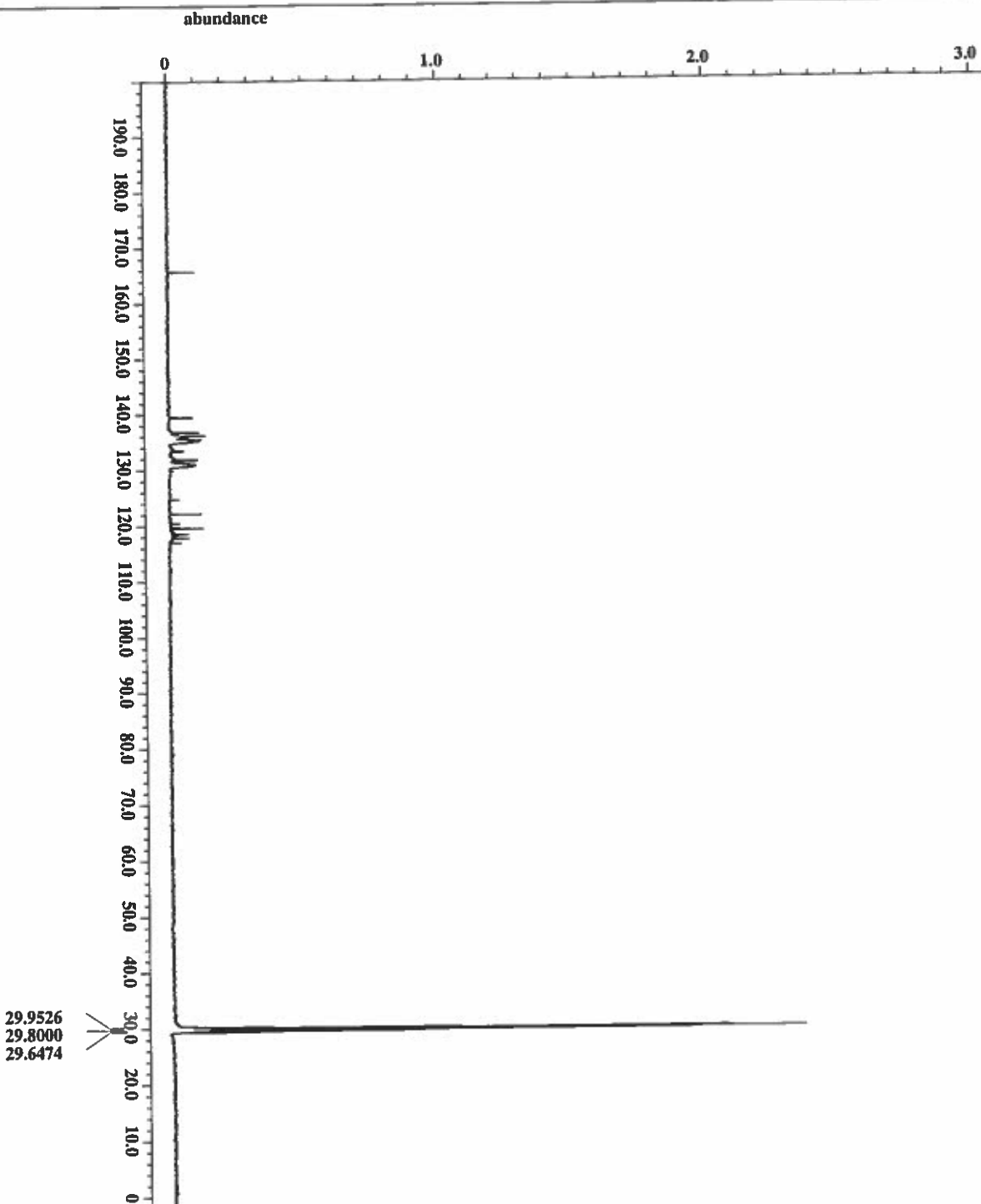
Filename = MS0480-300-3Weeks_PRO
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0480-300-3Weeks
 Solvent = ACETONE-D6
 Changer_sample = 6
 Creation_time = 14-JUL-2018 11:14:36
 Revision_time = 14-JUL-2018 10:52:04
 Current_time = 14-JUL-2018 10:52:04

 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

 Field_strength = 11.747379 [T] (500 [MH
 X_acq_duration = 1.74587904 [s]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.5727737 [Hz]
 X_sweep = 9.38438438 [kHz]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X1_domain = 1H
 X1_freq = 500.15991521 [MHz]
 X1_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

 X_90_width = 12.4 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_acn = 4 [dB]
 X_pulse = 6.2 [us]
 X1_mode = OFF
 Dante_preset = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 40
 Relaxation_delay = 4 [s]
 Repetition_time = 5.74587904 [s]
 Temp_get = 22.5 [dC]





X : parts per Million : 13C



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```

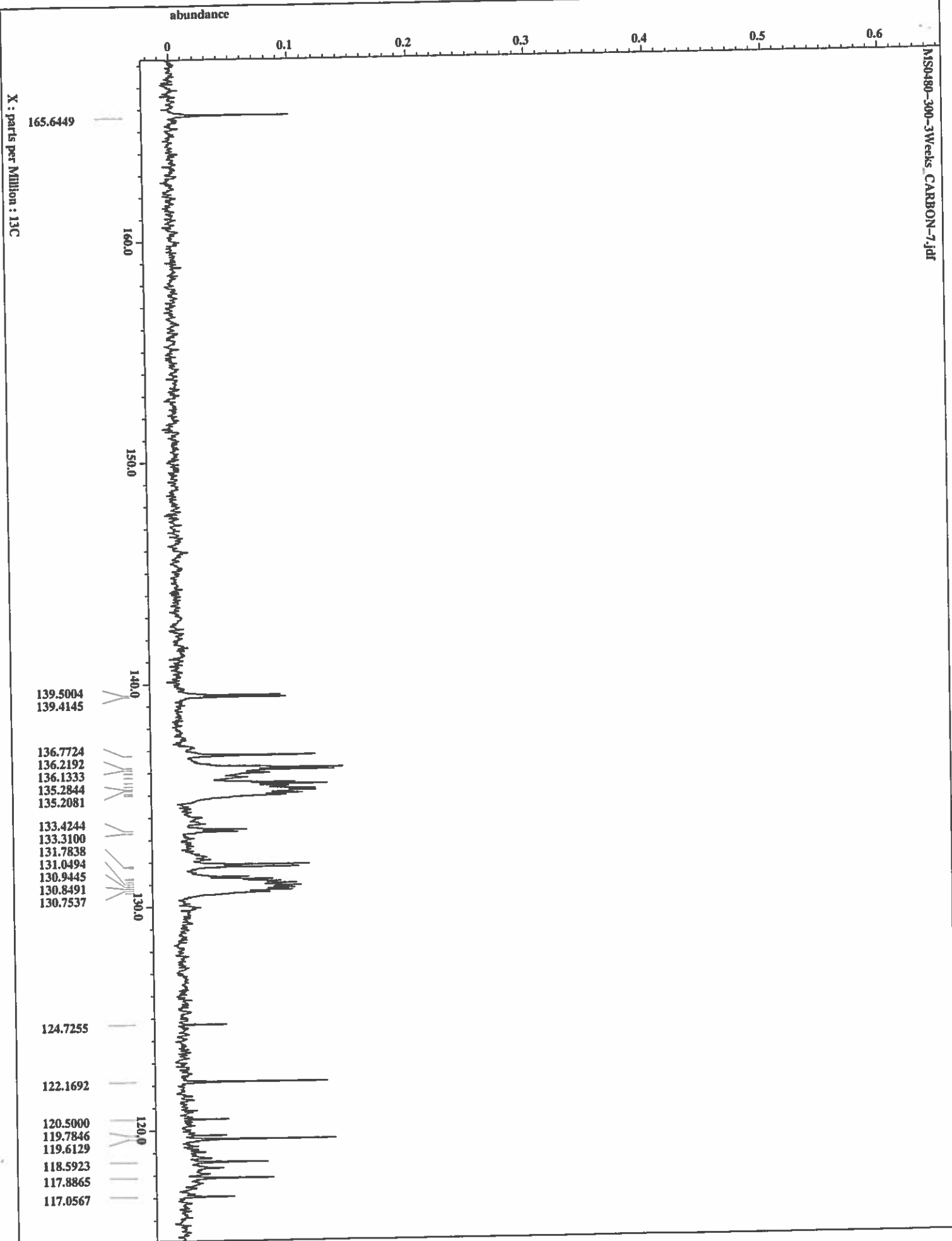
filename      = MS0480-300-3Weeks_CAR
author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0480-300-3Weeks
Solvent       = ACETONE-D6
Changer_sample = 6
Creation_time  = 14-JUL-2018 11:36:02
Revision_time = 14-JUL-2018 11:13:31
Current_time  = 14-JUL-2018 11:13:31

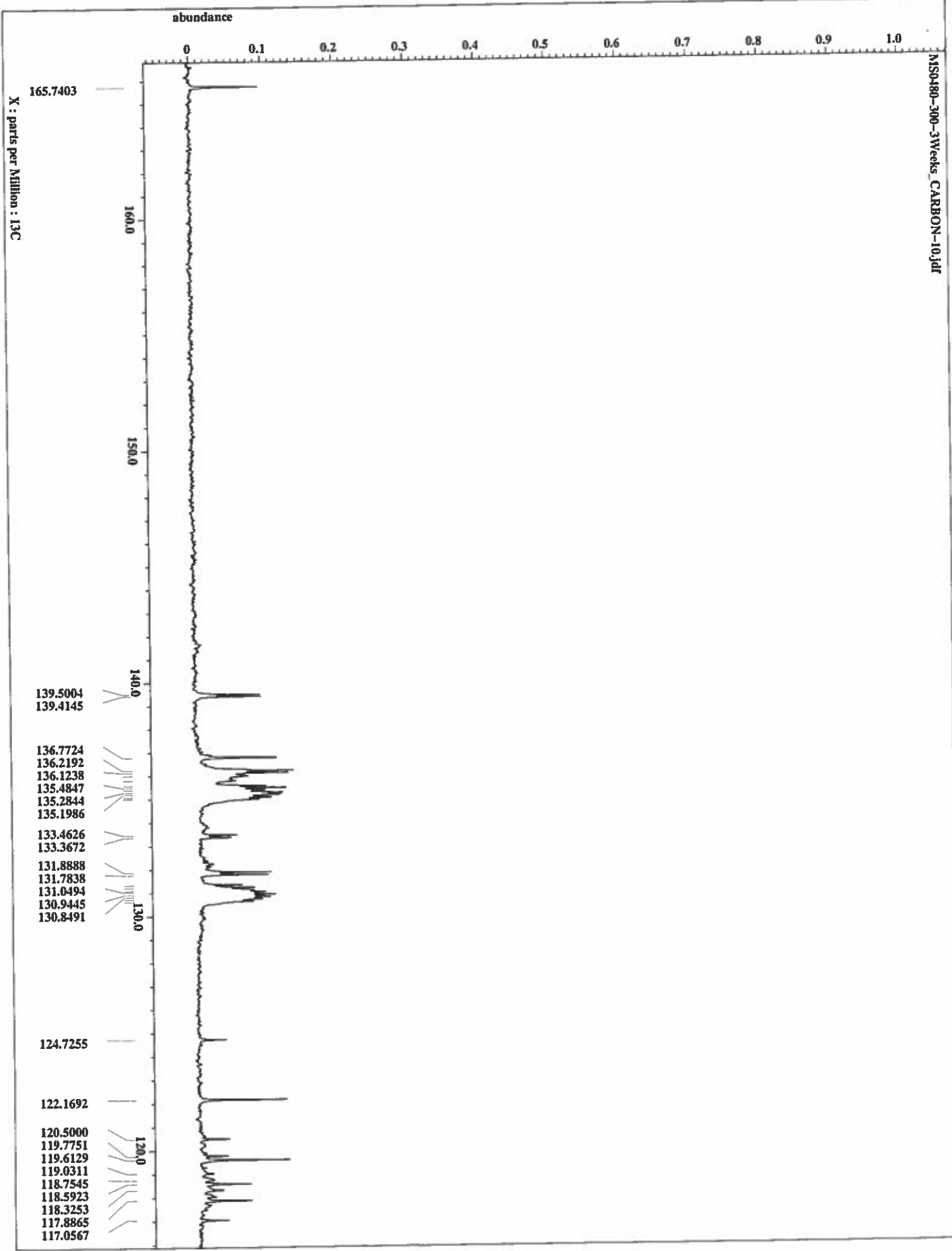
Data_format   = 1D COMPLEX
Dir_size      = 26214
Dir_title     = 13C
Dir_units     = [ppm]
Dimensions    = X
Site          = PQA 500
Spectrometer  = JNM-ECA500

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          = 400
Total_scans    = 400

X_90_pwidth    = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_noe    = 20.7 [dB]
Irr_noise      = WALTZ
Decoupling     = TRIZ
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 21 [s]
Noe_delay      = 60
Relaxation_delay = 21 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 23.1 [deg]

```



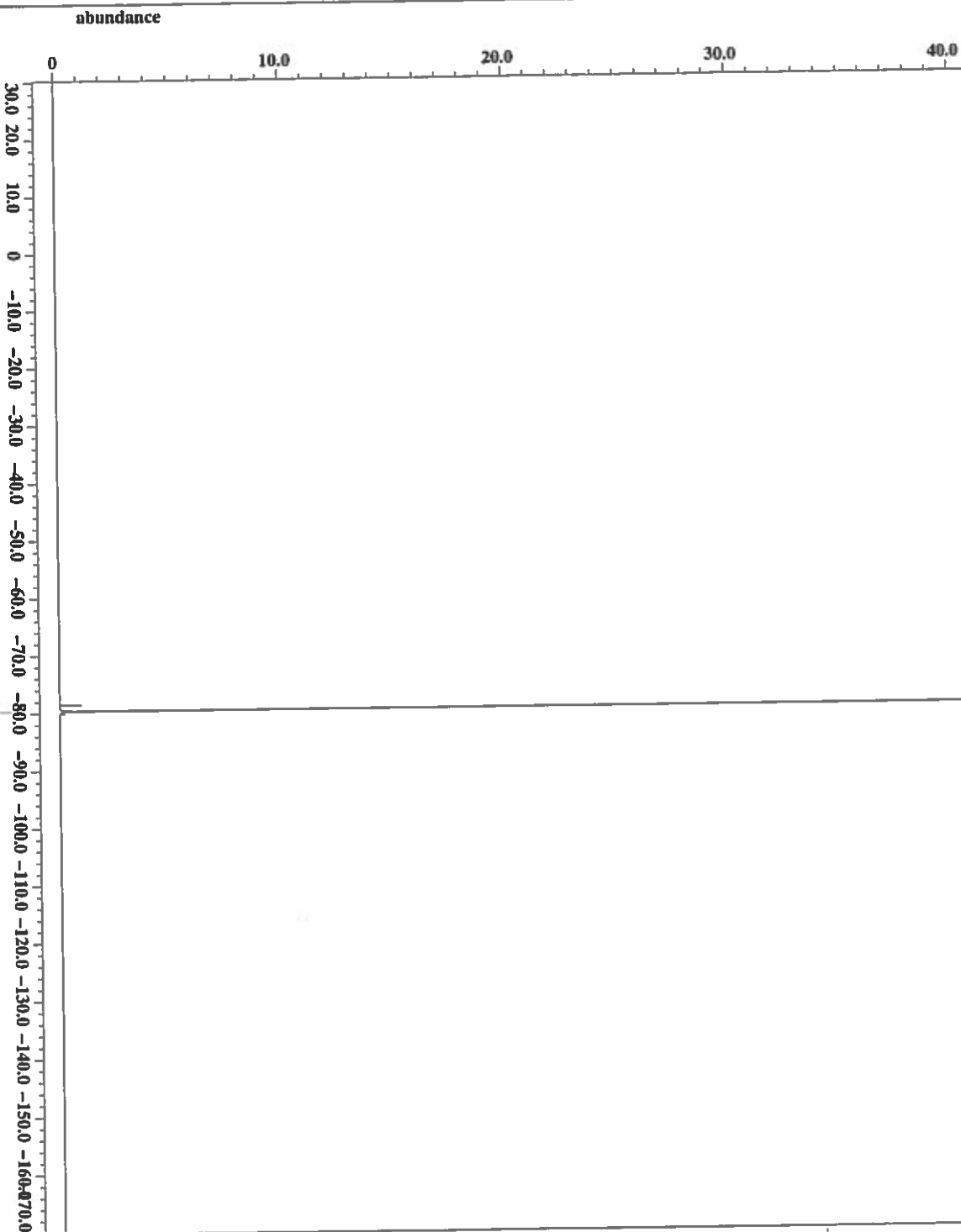


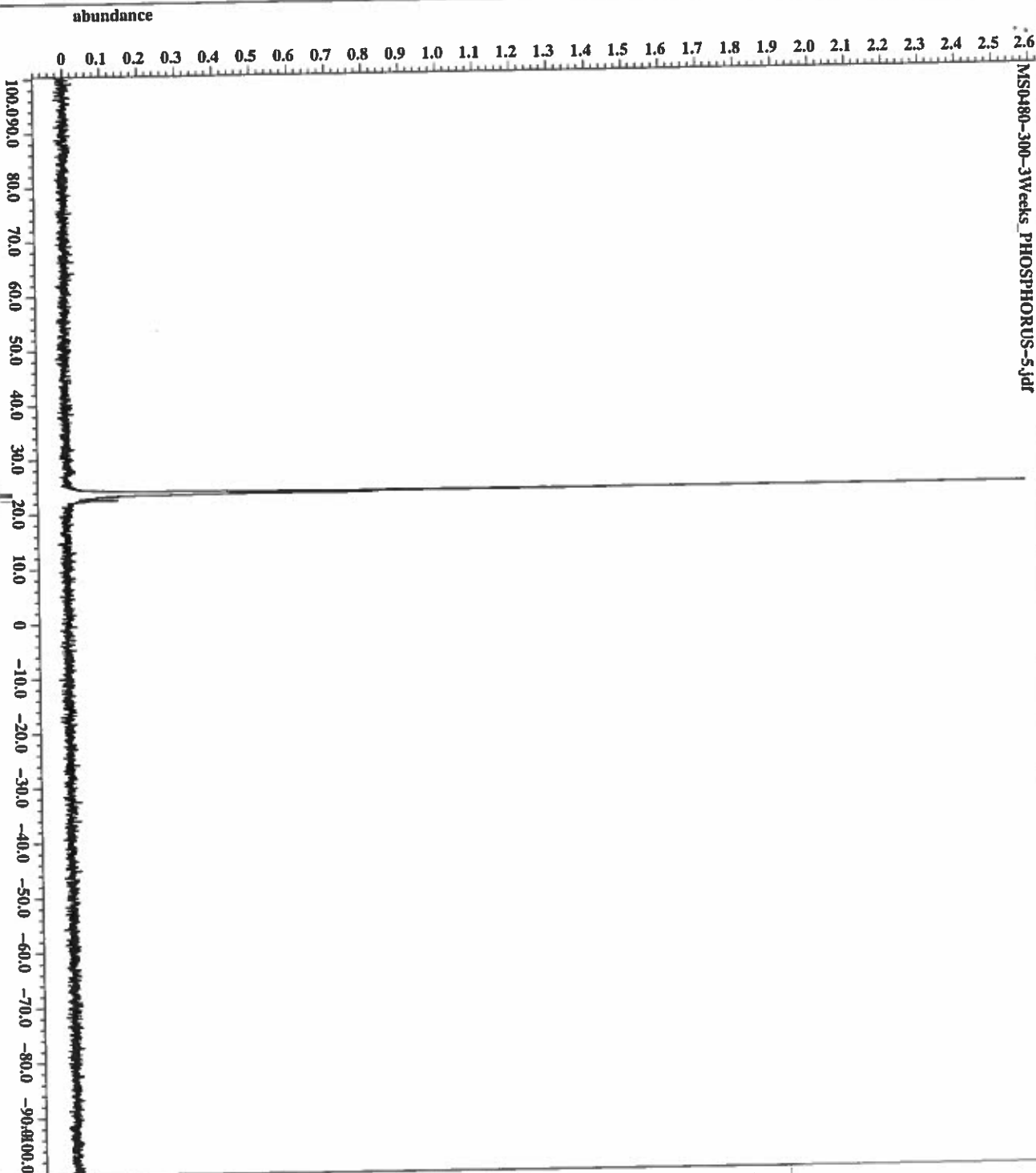


Filename = MS0480-300-3Weeks_FLU
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0480-300-3Weeks
 Solvent = ACETONE-D6
 Changer_sample = 6
 Creation_time = 14-JUL-2018 11:39:17
 Revision_time = 14-JUL-2018 11:16:46
 Current_time = 14-JUL-2018 11:16:47

Data_format = 1D COMPLEX
 Dia_size = 52428
 Dia_title = 19F
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.747357917 (500)MH
 X_acq_duration = 0.55574528[s]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = -70 [ppm]
 X_points = 6536
 X_prescans = 1
 X_resolution = 1.7993855 [Hz]
 X_sweep = 117.9245283 [kHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084 [MHz]
 Irr_offset = 5 [ppm]
 Tr1_domain = 19F
 Tr1_freq = 470.62046084 [MHz]
 Tr1_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 13.1 [us]
 X_acq_time = 0.55574528 [s]
 X_angle = 45 [deg]
 X_atn = 2.5 [dB]
 X_pulse = 6.55 [us]
 Irr_mode = OF2
 Dante preset = FALSE
 Initial wait = 1 [s]
 Recvr_gain = 42
 Relaxation_delay = 4 [s]
 Repetition_time = 4.55574528 [s]
 Temp_get = 22.7 [deg]





23.8959
23.6891
23.4746



SOUTH ALABAMA
JAGUARS

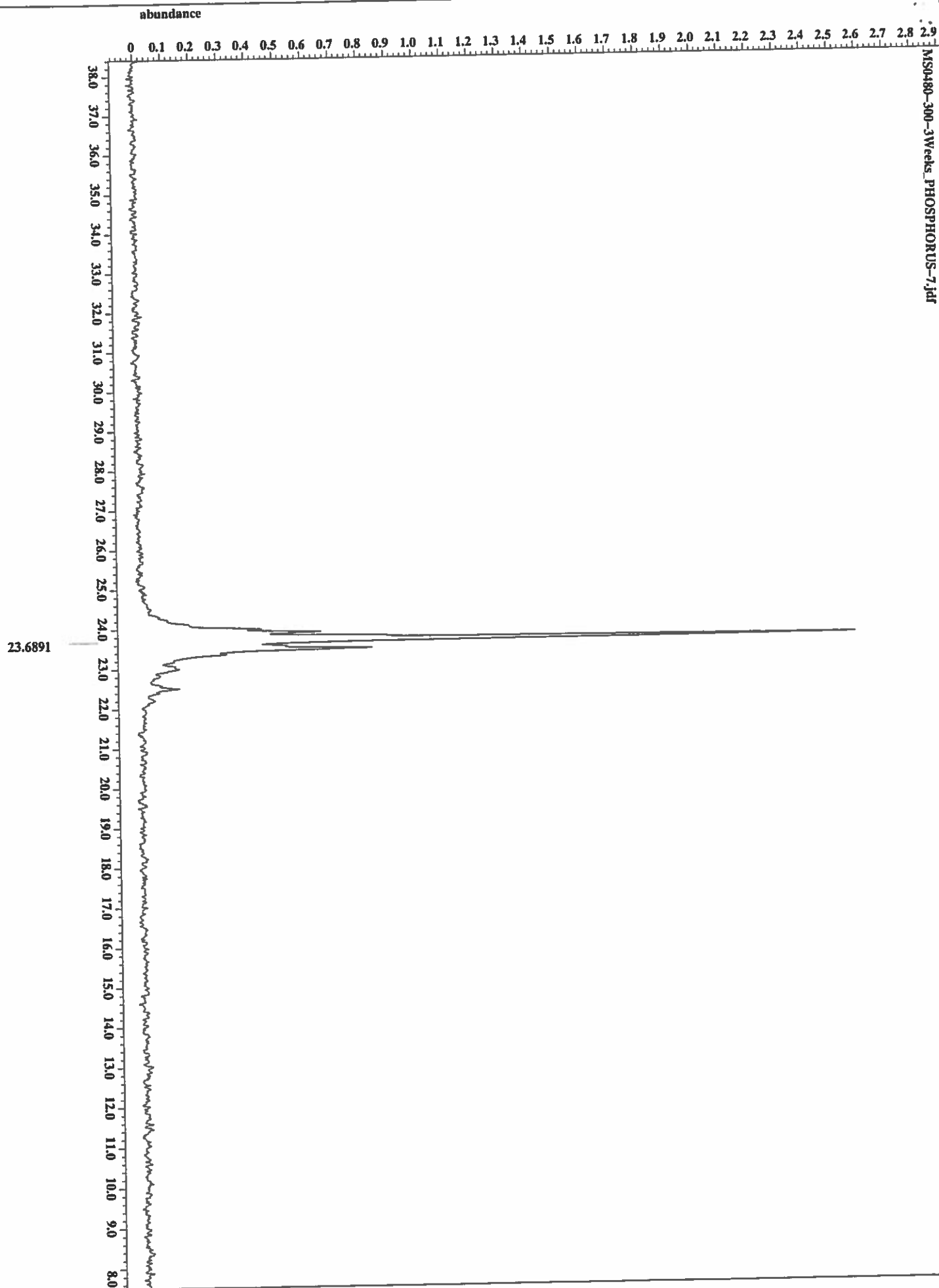
```

Filename      = MS0480-300-3weeks_PRO
Author        = Jim Davis
Experiment     = single_pulse_dec
Sample_id     = MS0480-300-3weeks
Solvent       = ACETONE-D6
Charger_sample = 6
Creation_time  = 14-JUL-2018 11:44:00
Revision_time  = 14-JUL-2018 11:21:28
Current_time   = 14-JUL-2018 11:21:28

Data_format    = 1D COMPLEX
Dim_size       = 26214
Dim_title      = 31P
Dim_units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

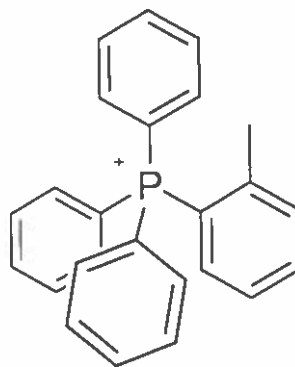
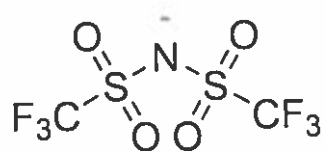
Field_strength = 11.7473579 [T] (500 [MHz]
X_acq_duration = 0.64487424 [s]
X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.55068995 [Hz]
X_sweep        = 50.81300813 [Hz]
Irr_domain     = 1H
Irr_freq       = 500.1591521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 50
Total_scans    = 50

X_90_width     = 14.687 [us]
X_acq_time     = 0.64487424 [s]
X_angle        = 30 [deg]
X_atn          = 5 [dB]
X_pulse        = 4.89566667 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_noe    = 20.7 [dB]
Irr_noise      = WALFZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Recvr_gain     = 58
Relaxation_delay = 2 [s]
Repetition_time = 2.64487424 [s]
Temp_get       = 23 [C]
  
```



Compound 7 Pre- and Post-heating NMR Spectra

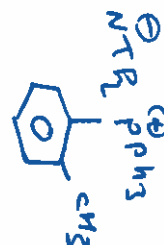
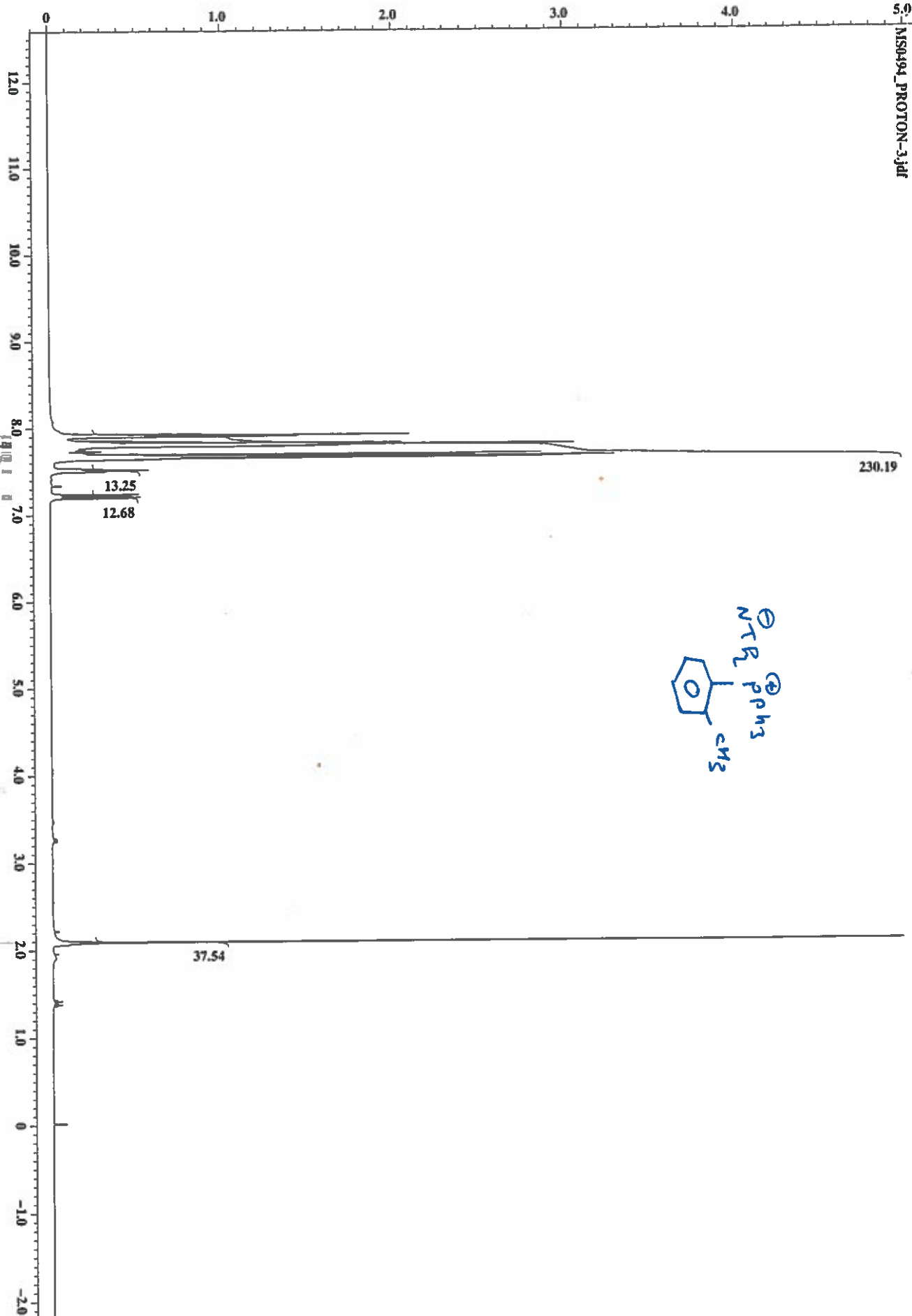
Temperature of Post-heating samples noted in upper left corner of each spectrum

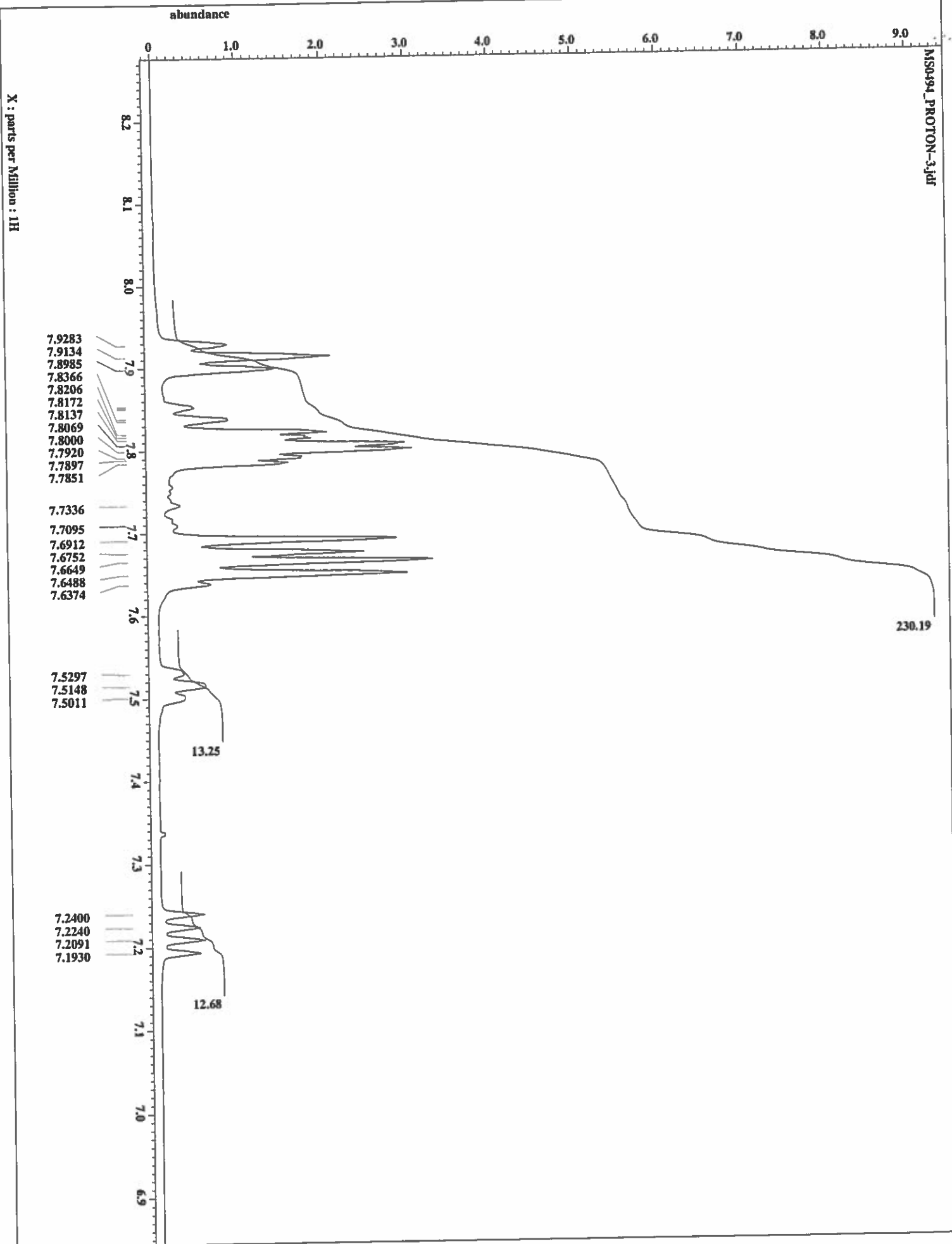


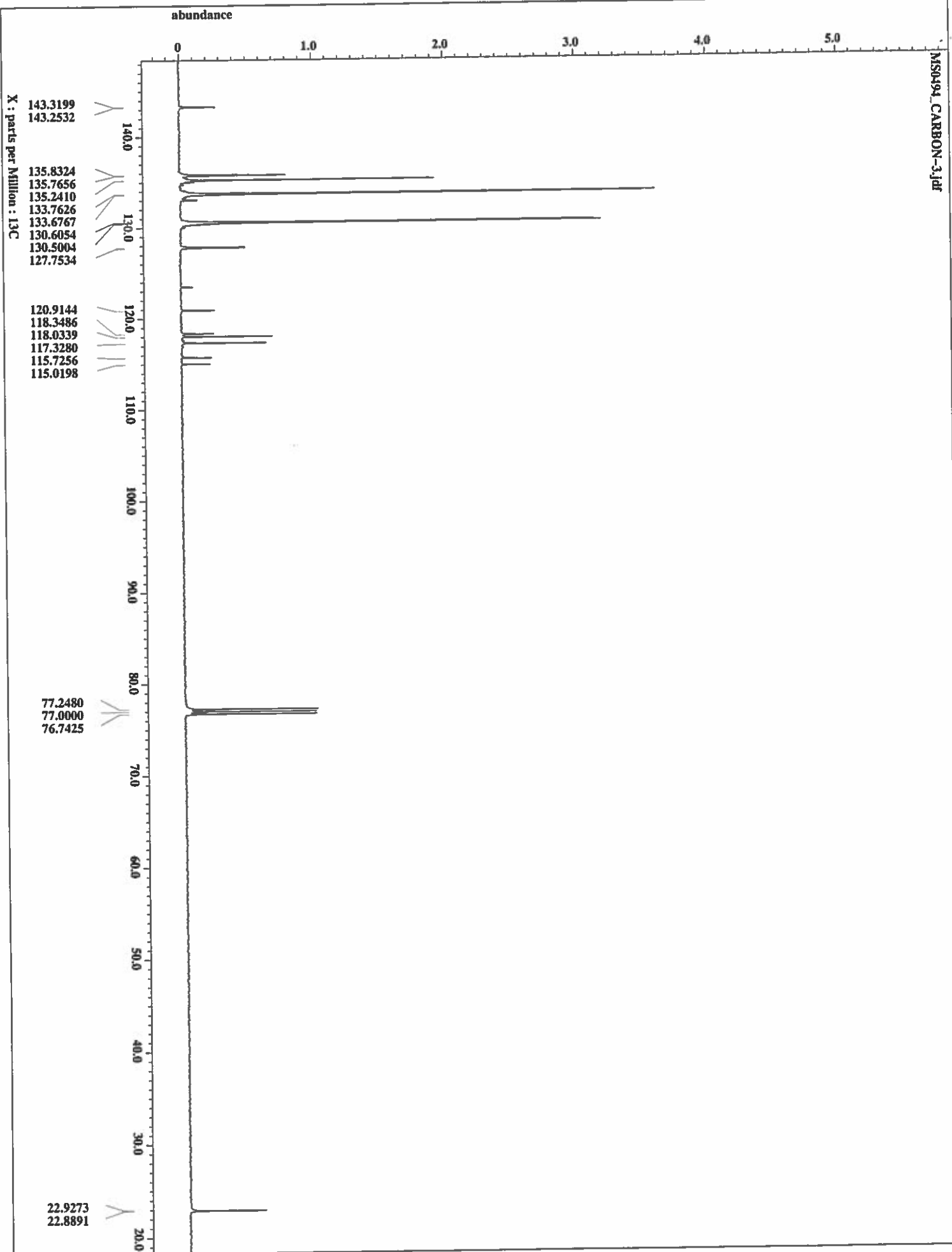
X : parts per Million : 1H

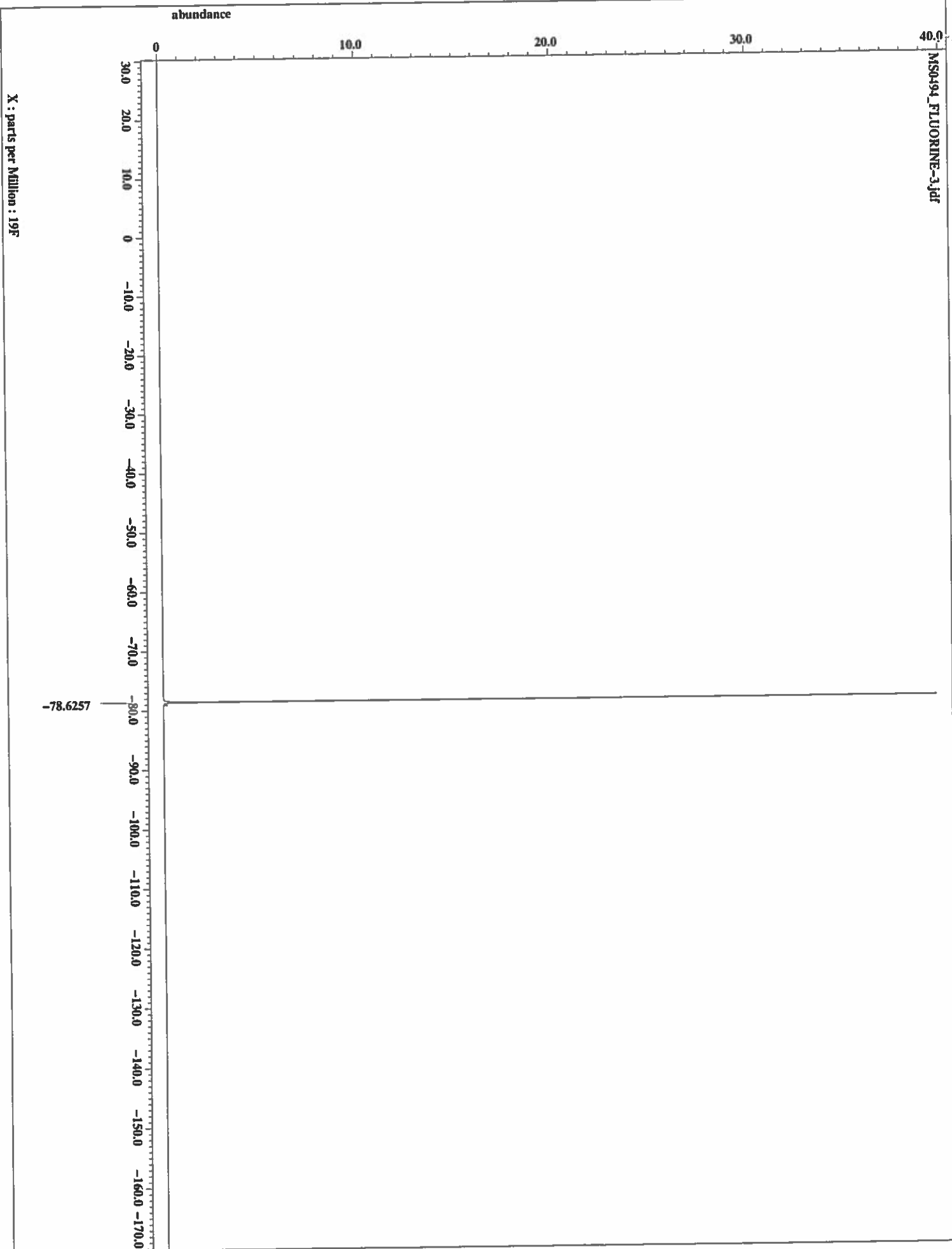
7.9134
7.8069
7.8000
7.6912
7.6752
7.6649
7.6488

abundance









MS0494_PHOSPHORUS-3.jdt

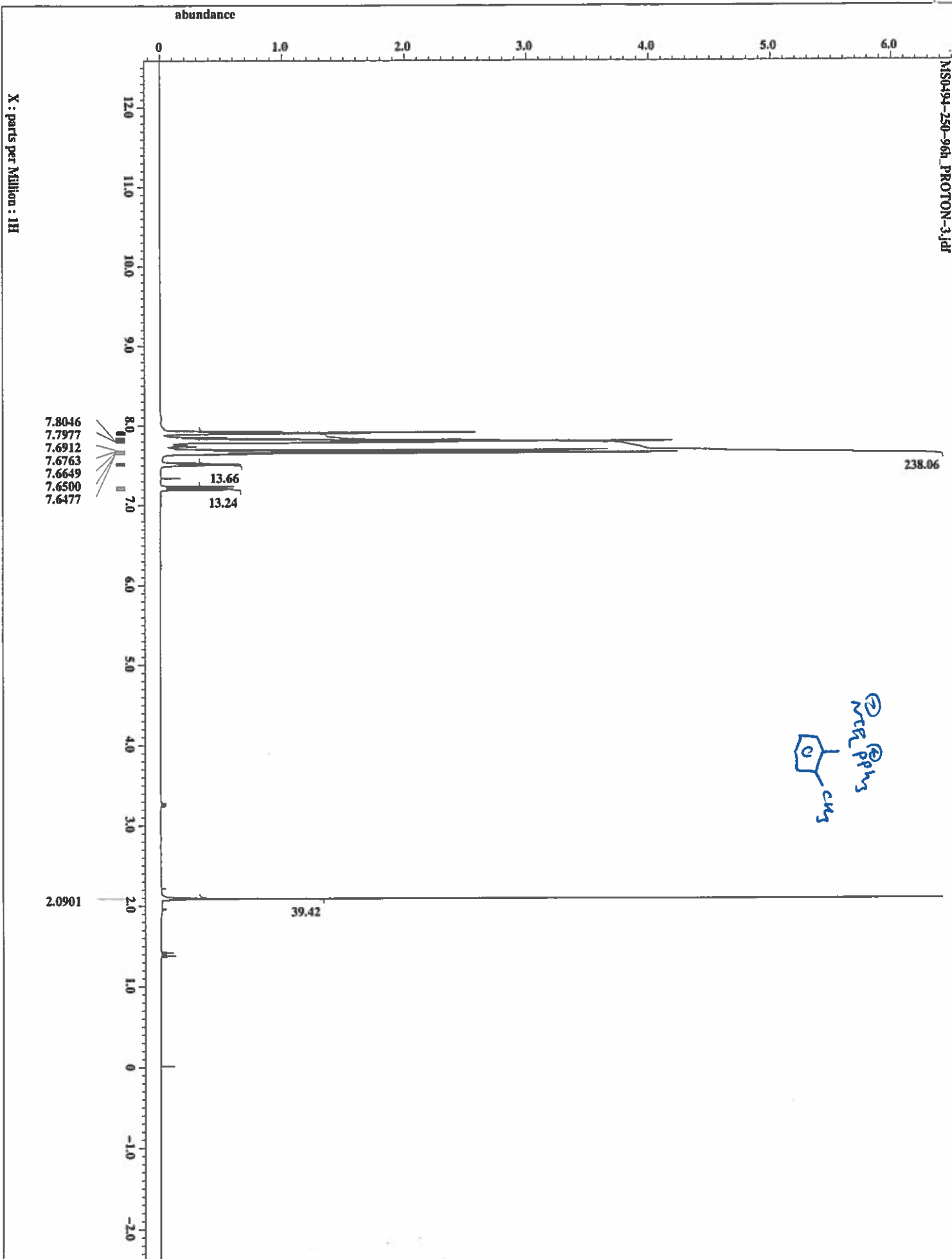
abundance

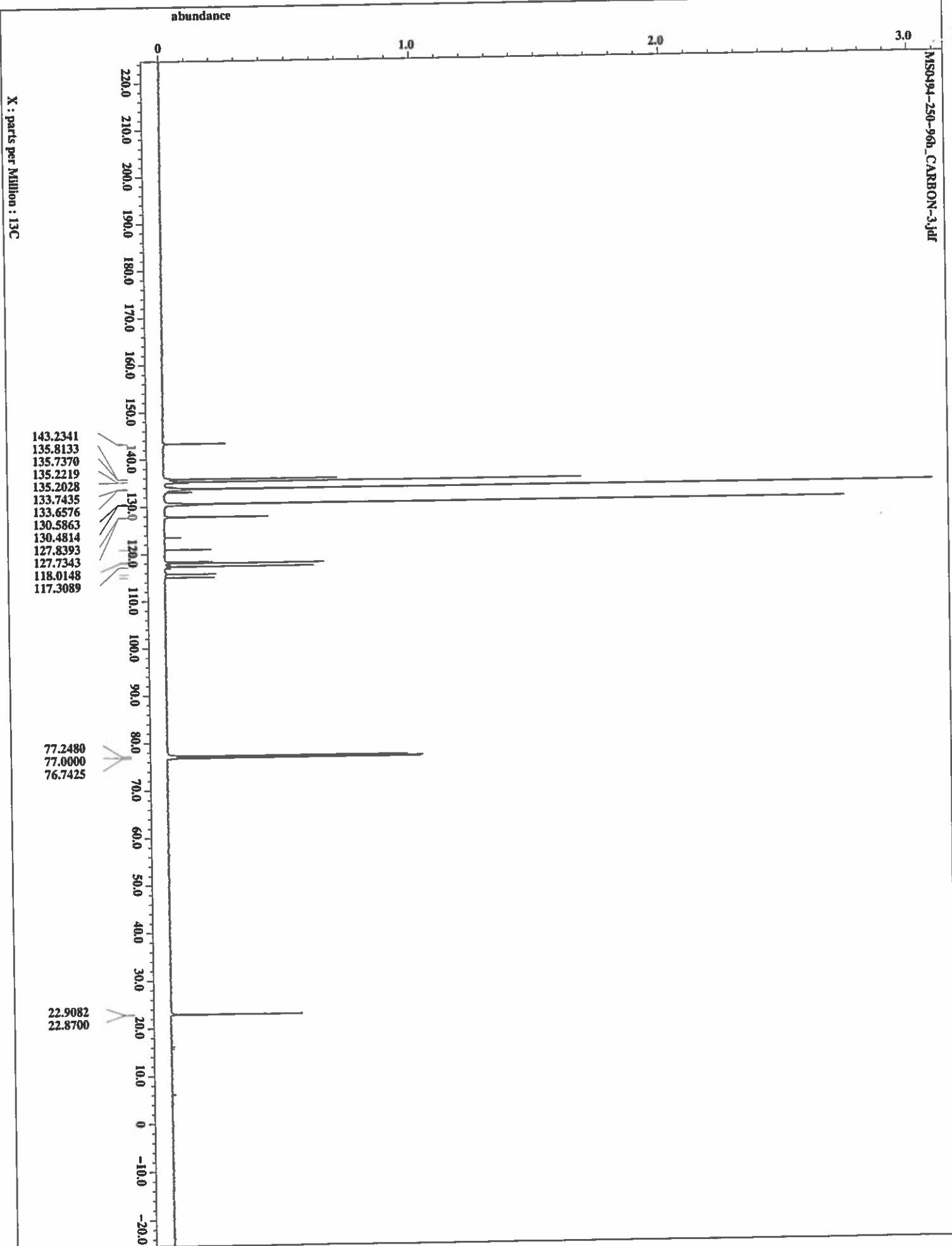
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0 25.0

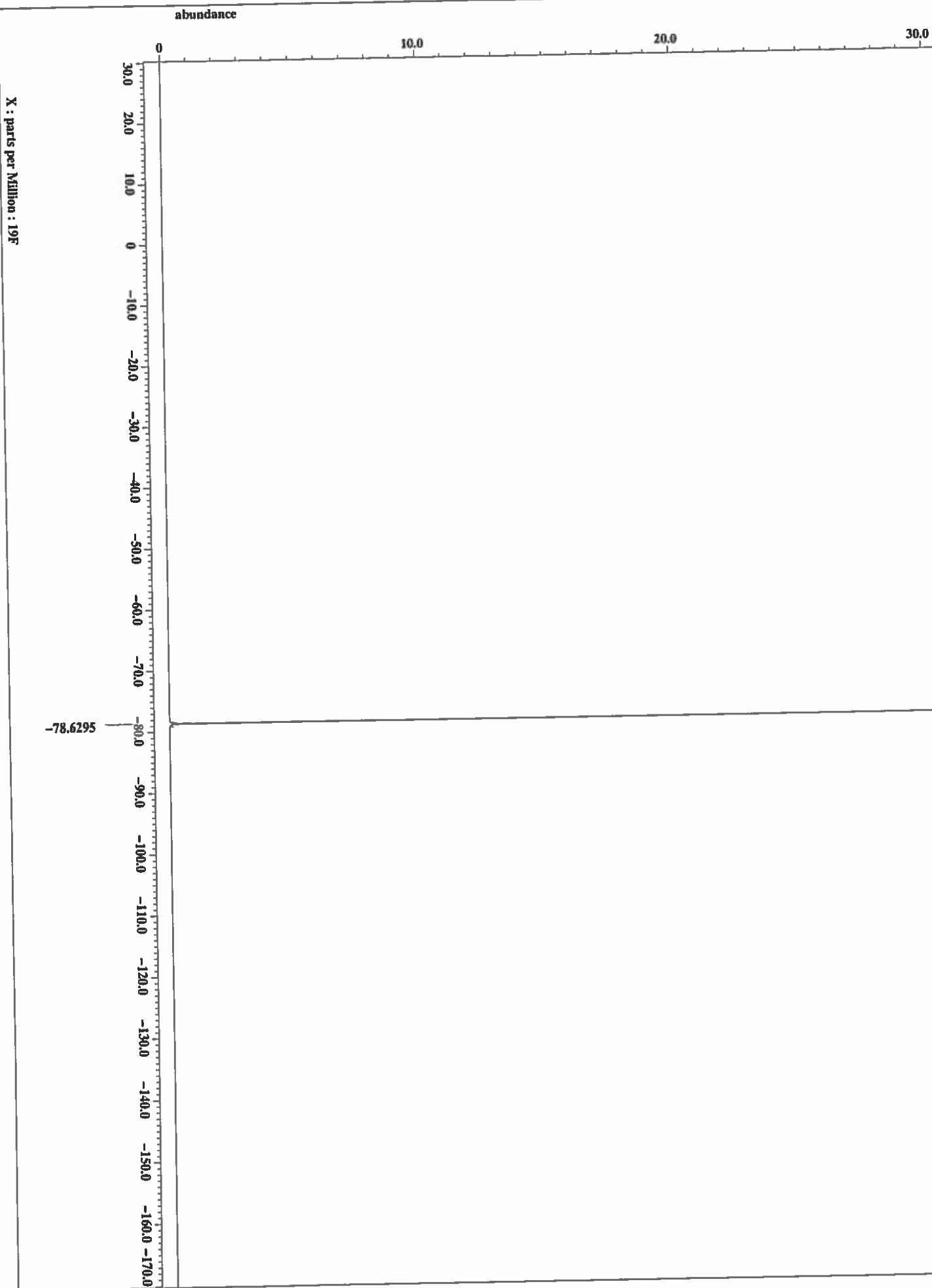
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0

22.7623

X : parts per Million : 31P







abundance

0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0 25.0 26.0 27.0

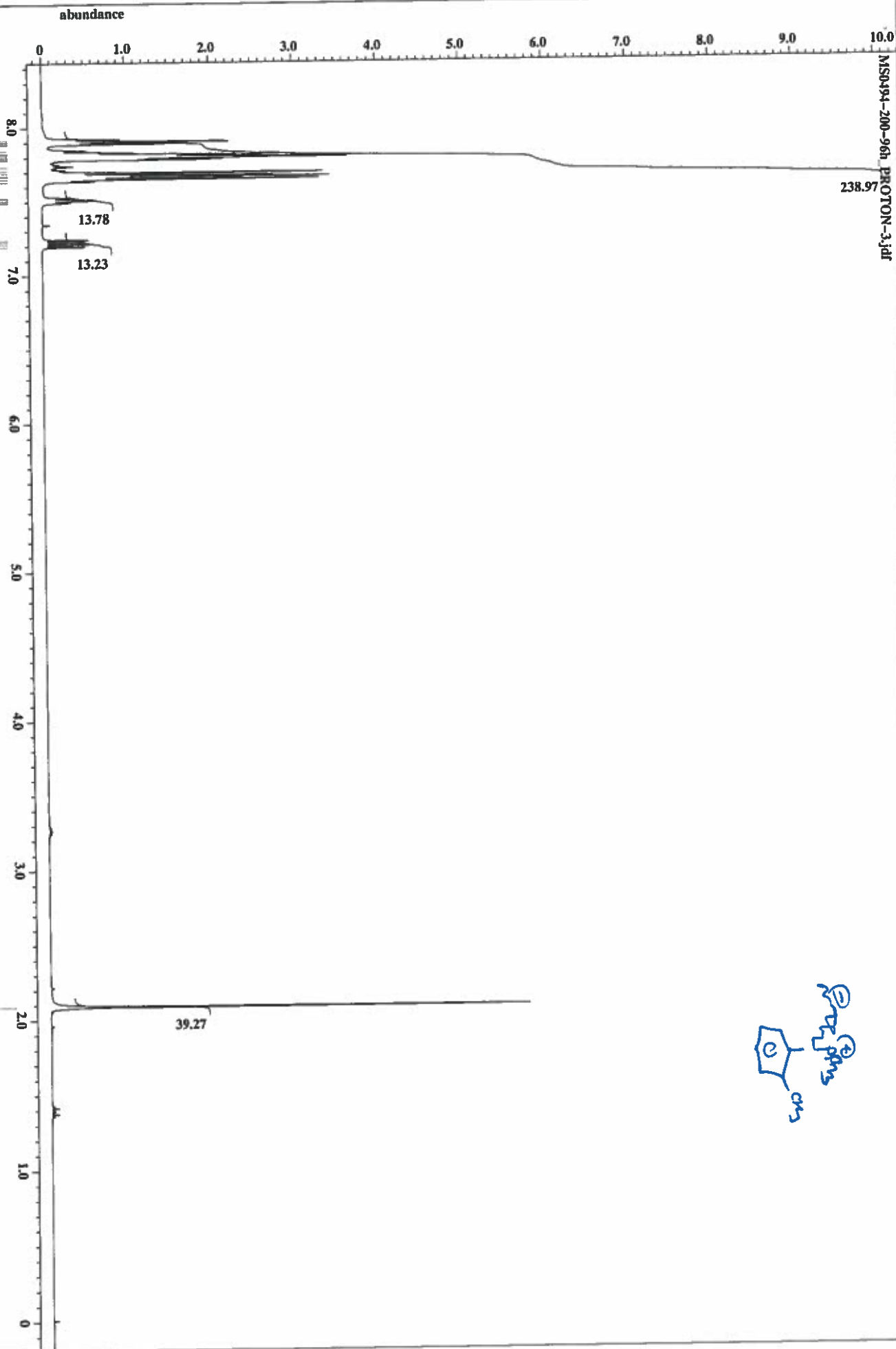
100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0

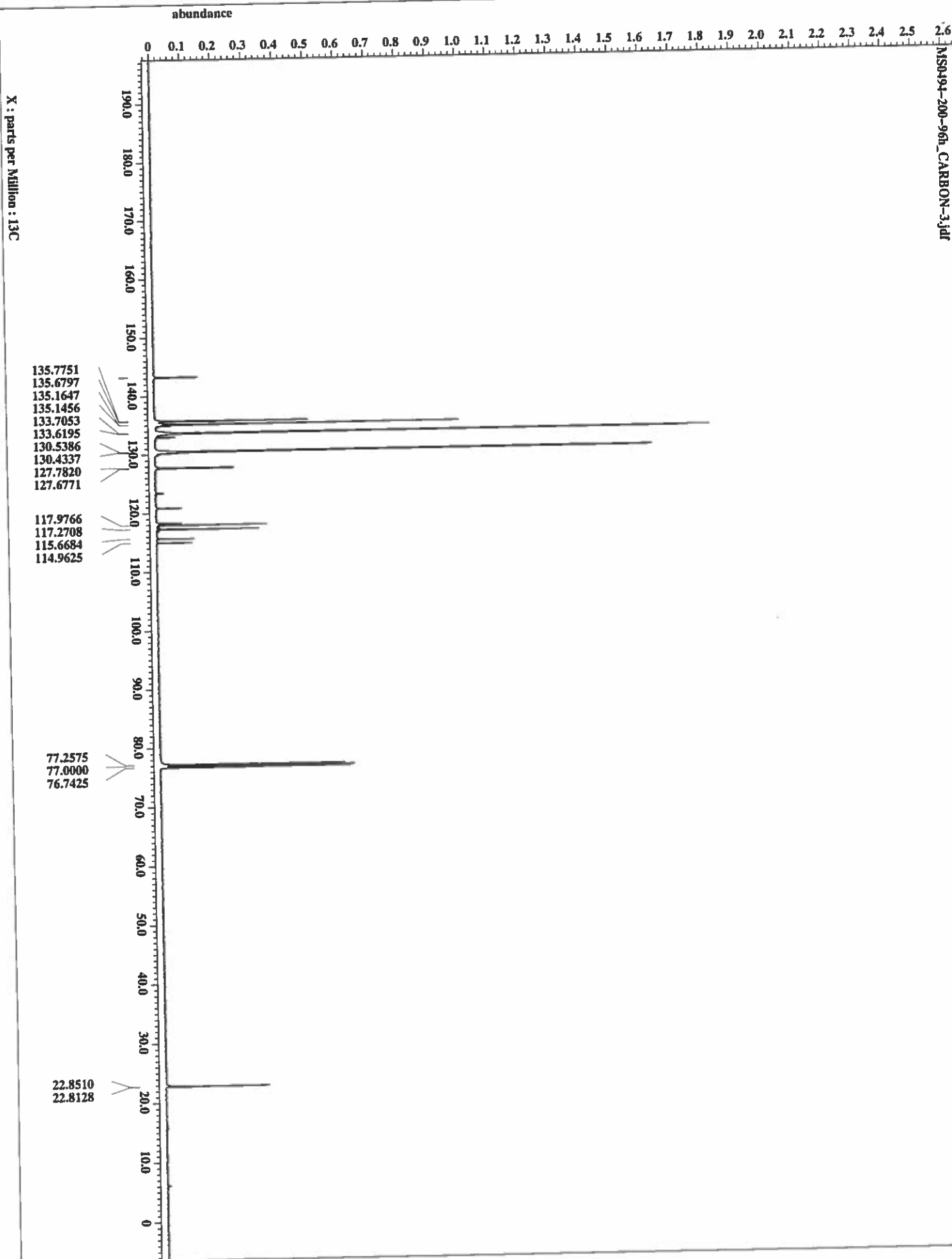
22.7547

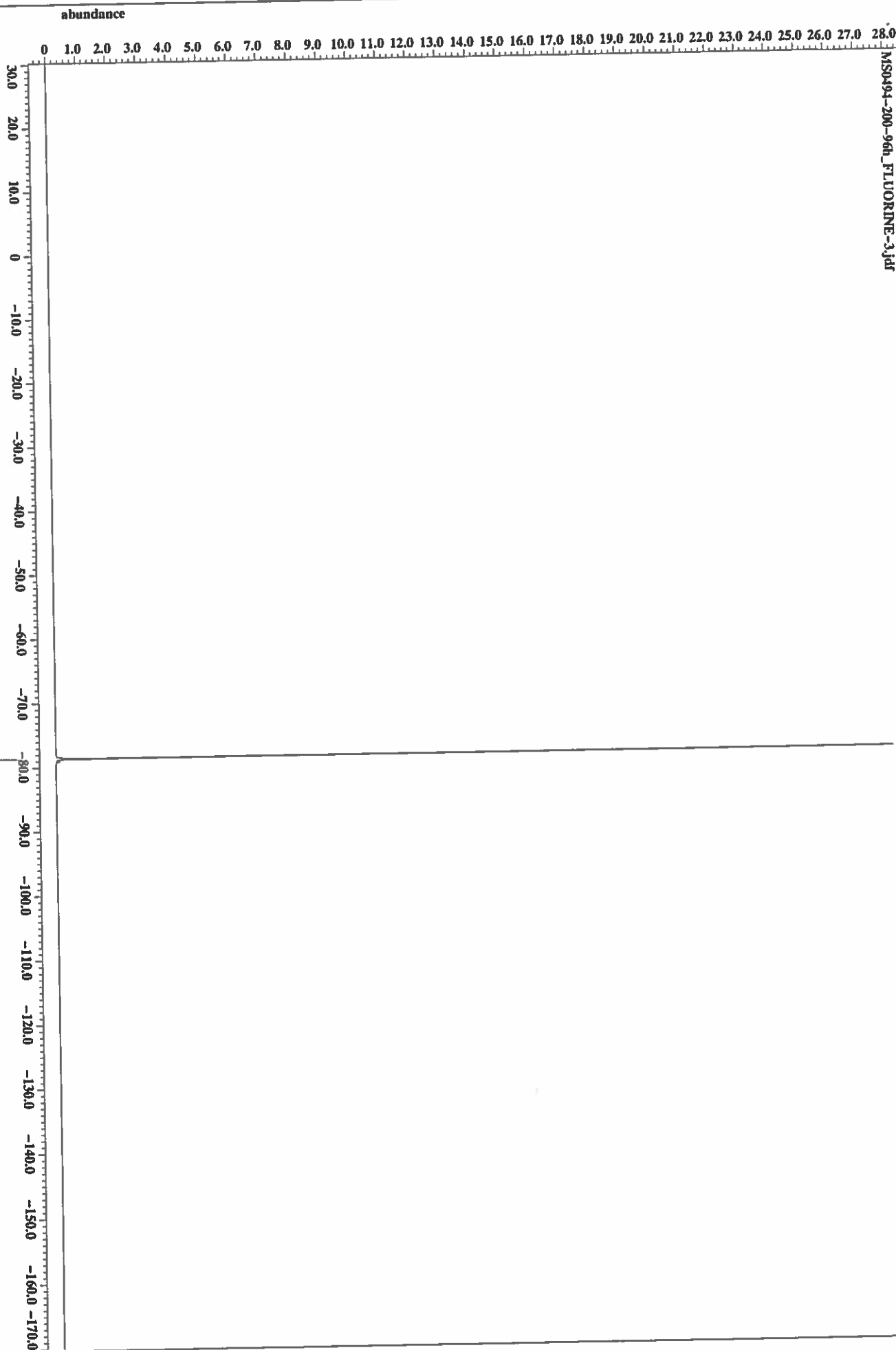
X : parts per Million : 31P

X : parts per Million : 1H

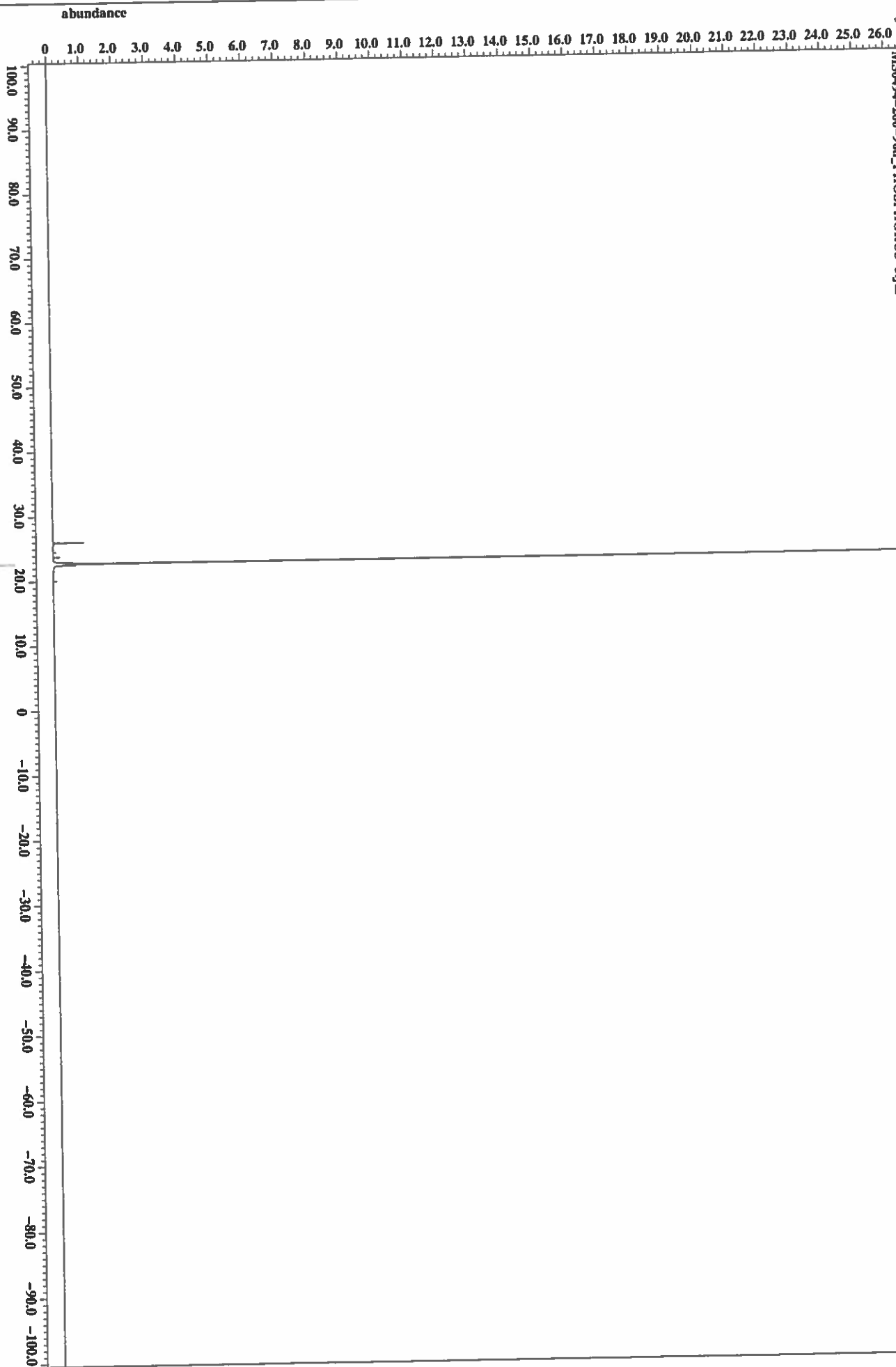
7.9042
7.8206
7.8137
7.8046
7.7977
7.6946
7.6798
7.6775
7.6694
7.6546







X : parts per Million : 19F



X : parts per Million : 31P

abundance

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9

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 -1.0 -2.0

X : parts per Million : 1H

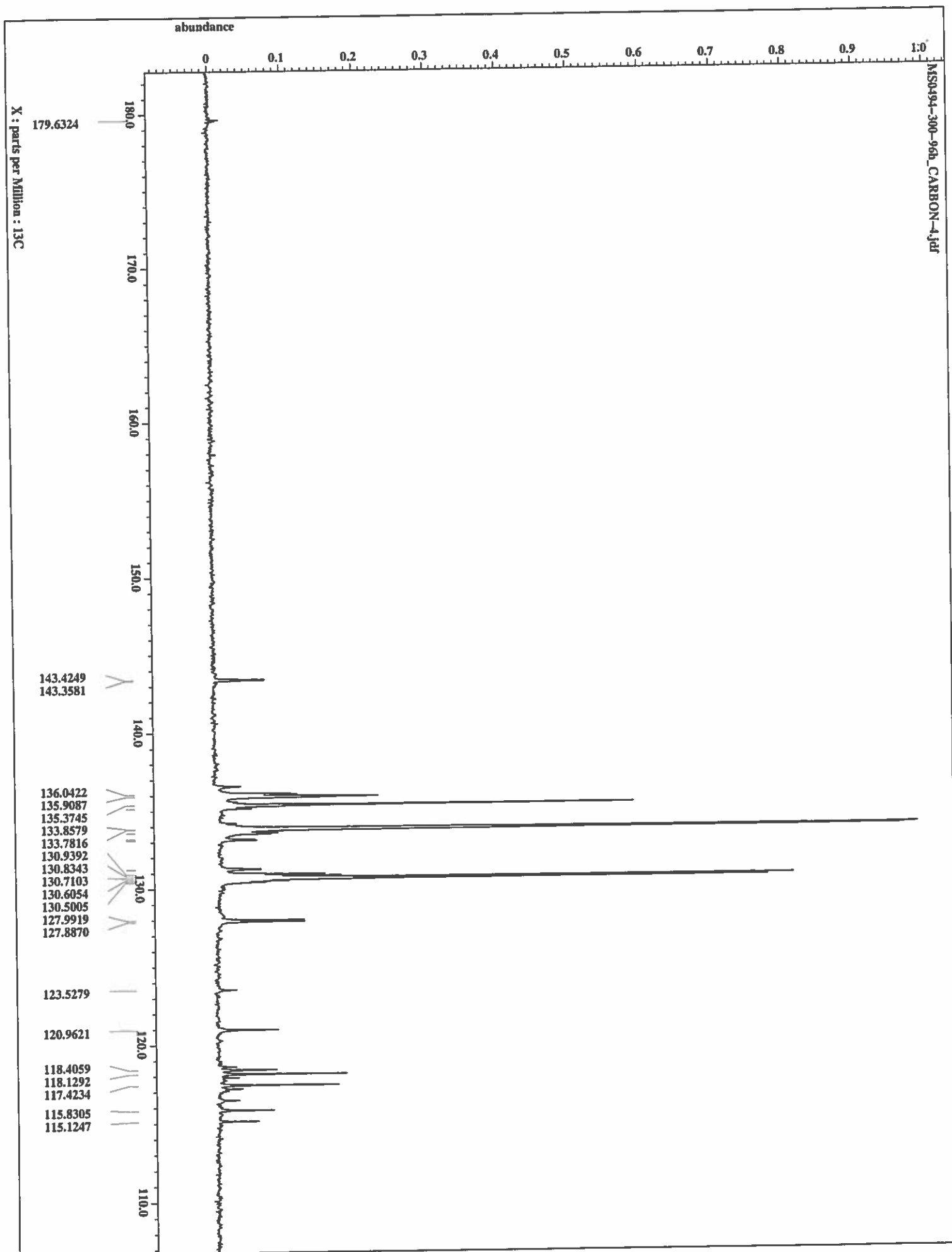
8.6680
8.1115
7.9225
7.8057
7.6866
7.6672
7.5240
7.2400
7.2251
7.2114

2.0958

9.97

1





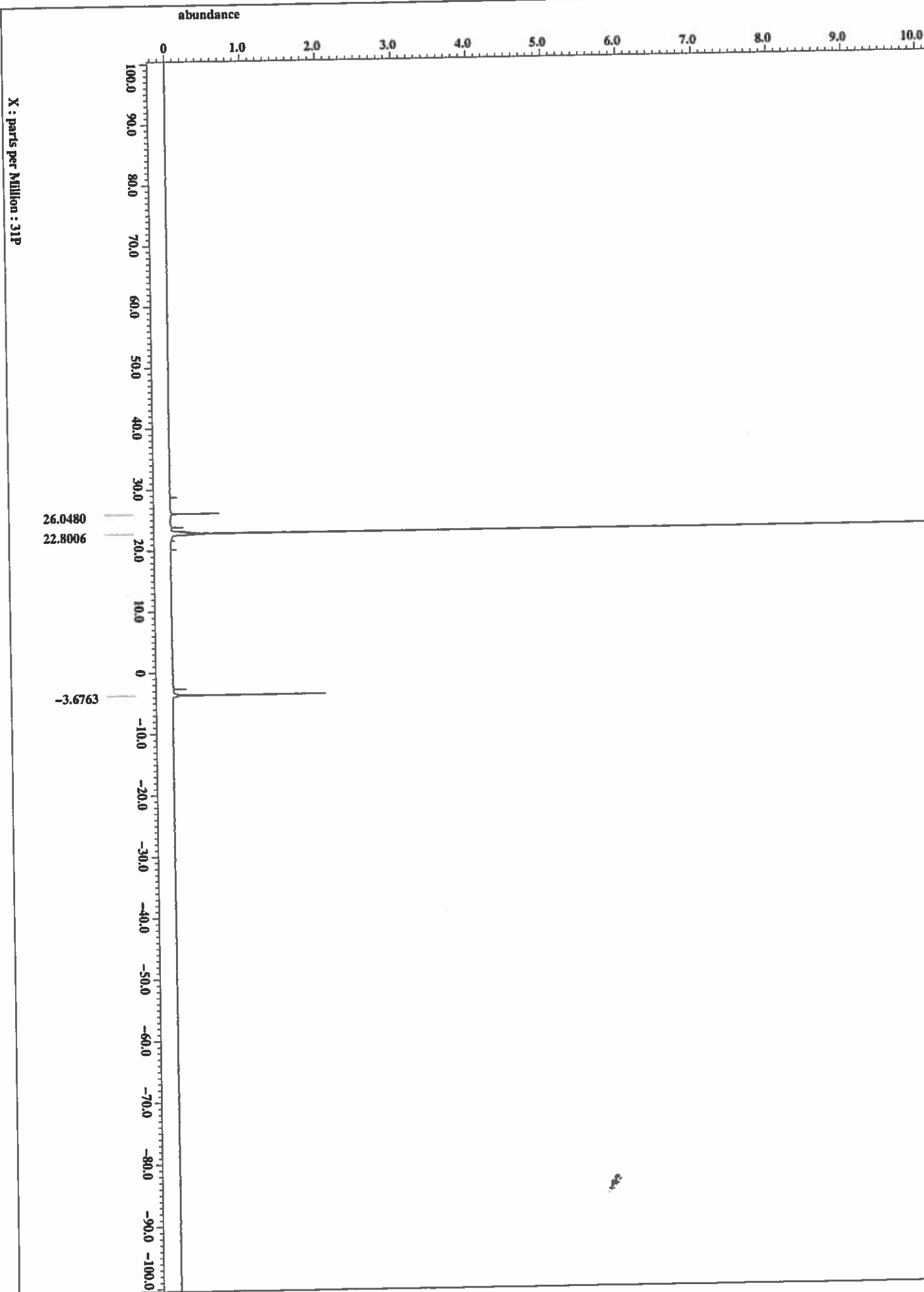
abundance

0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0

30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0

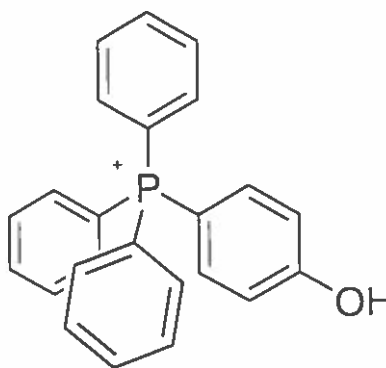
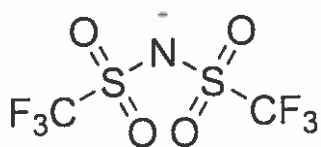
-78.6295

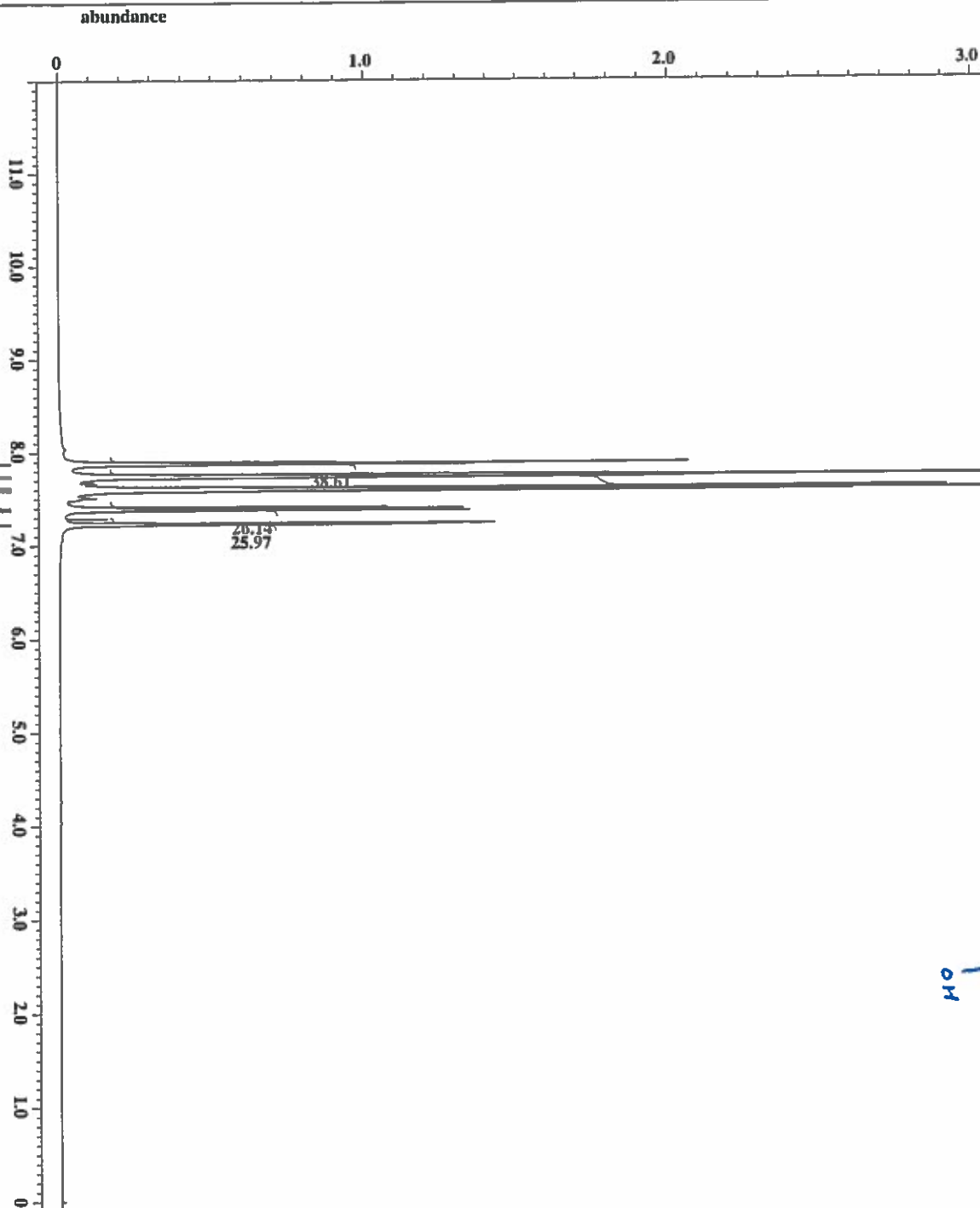
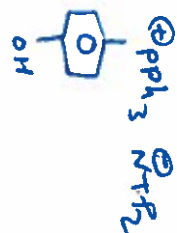
X : parts per Million : 19F



Compound 11 Pre- and Post-heating NMR Spectra

Temperature of Post-heating samples noted in upper left corner of each spectrum





X : parts per Million : 1H



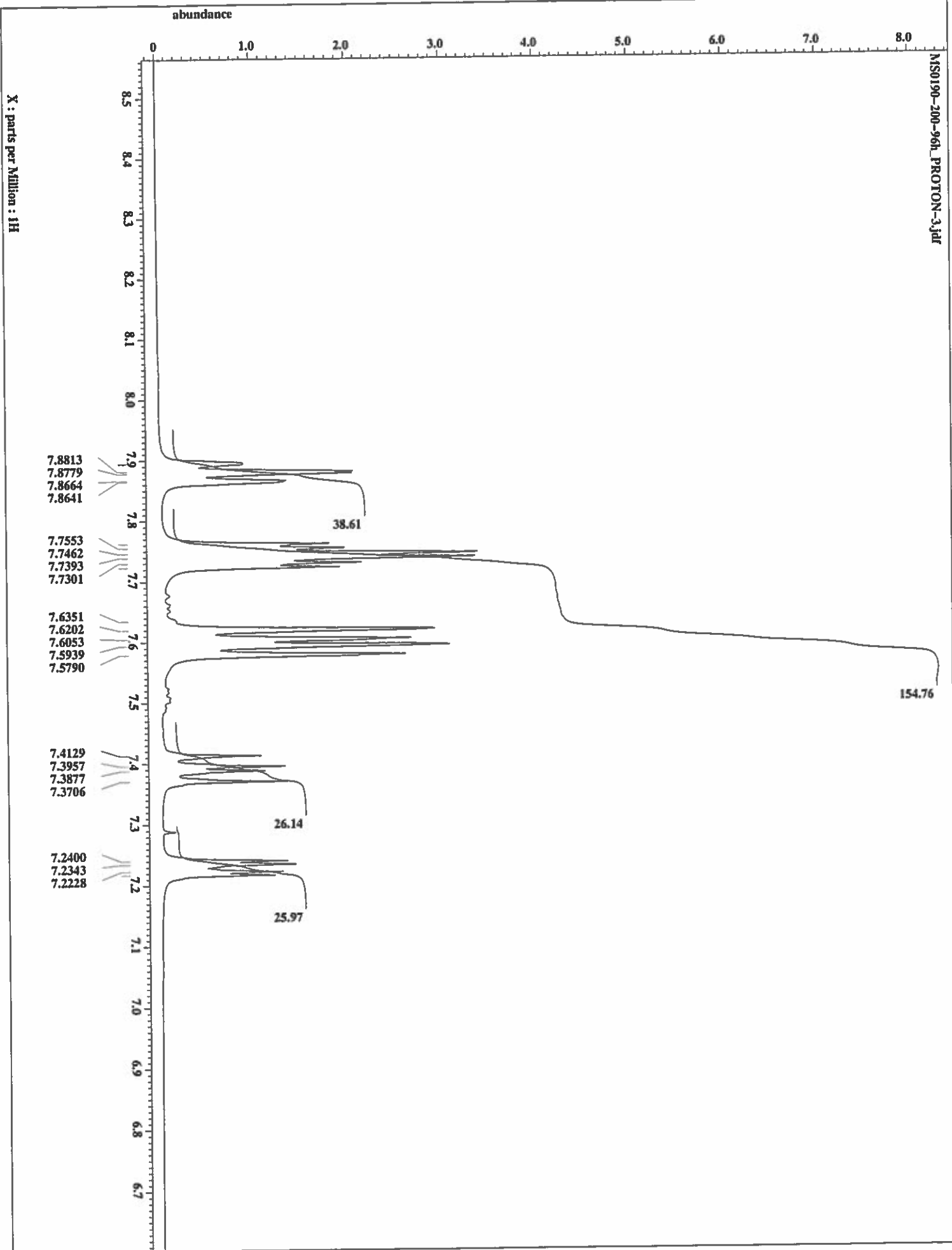
```

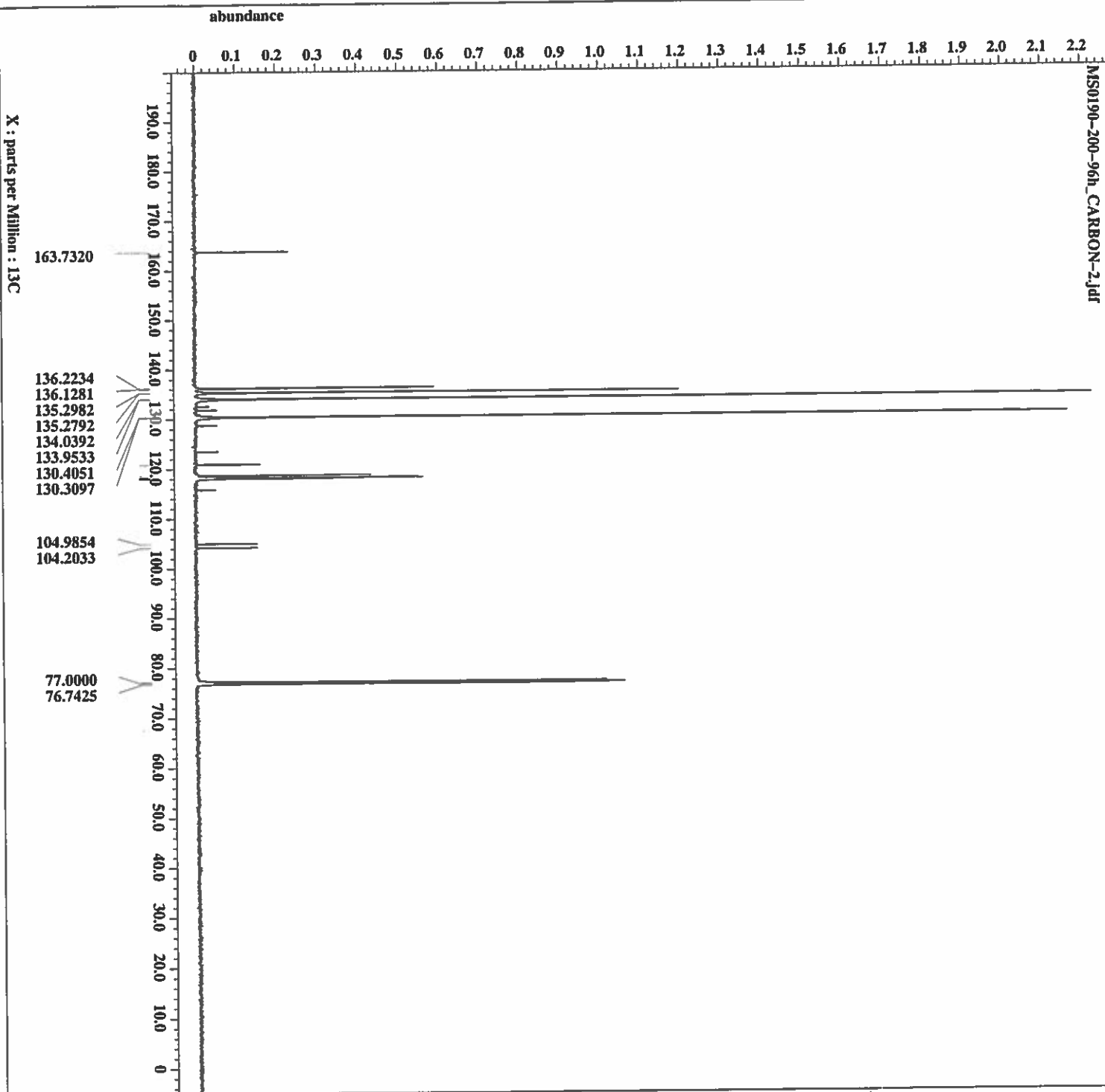
Filename      = MS0190-200-96h_PROTON
Author        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0190-200-96h
Solvent       = CHLOROFORM-D
Creation_time  = 6-JAN-2019 14:41:07
Revision_time = 6-JAN-2019 14:15:56
Current_time  = 6-JAN-2019 14:15:56

Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = RCA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.743579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_swap         = 9.38636638 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
T1_domain      = 1H
T1_freq        = 500.15991521 [MHz]
T1_offset      = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 12.4 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [db]
X_pulse        = 6.2 [us]
Off            = OFF
T1_mode        = 02F
Dante_preset   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 24
Relaxation_delay = 4 [s]
Repetition_delay = 5.74587904 [s]
Temp_get       = 19.9 [C]
  
```





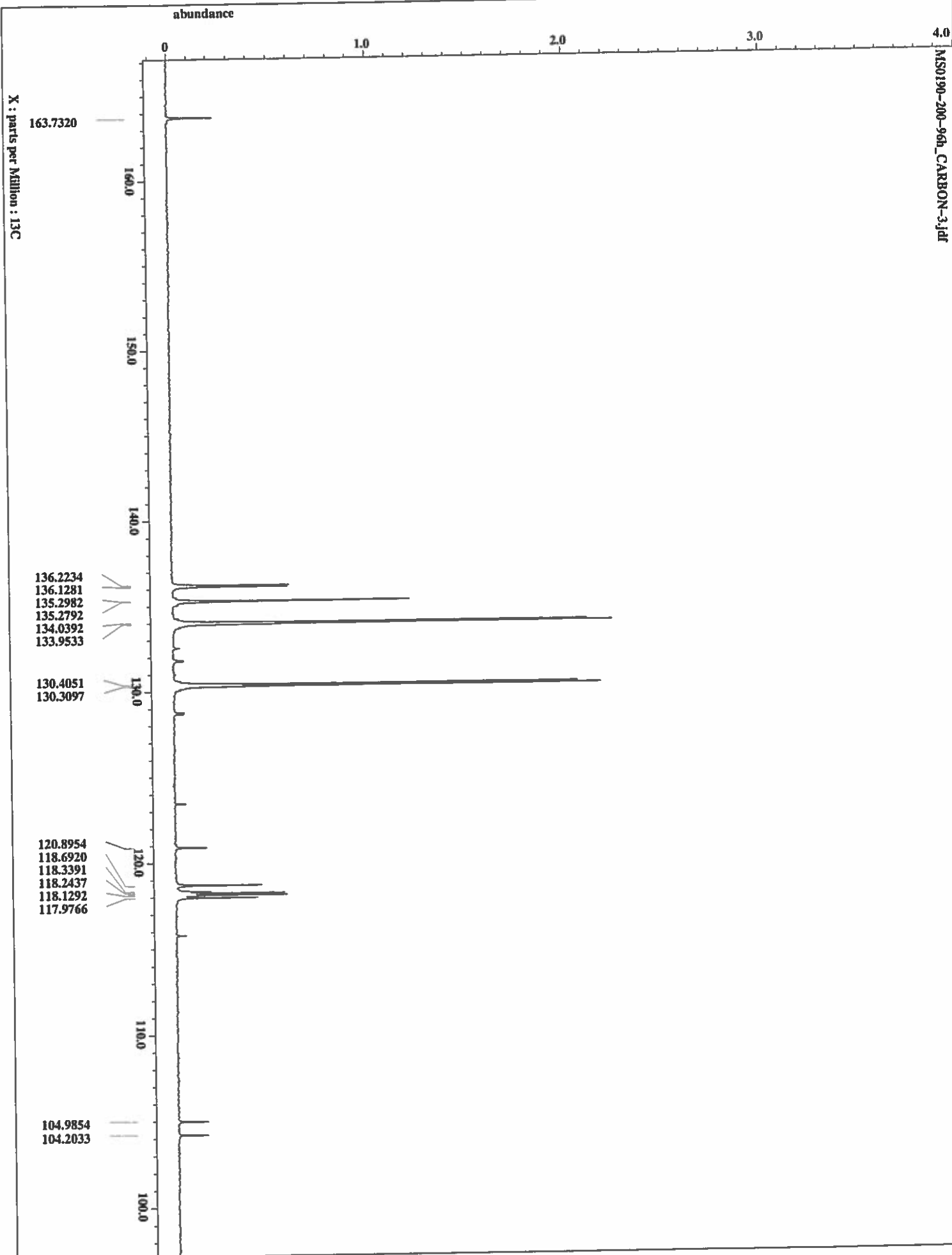
```

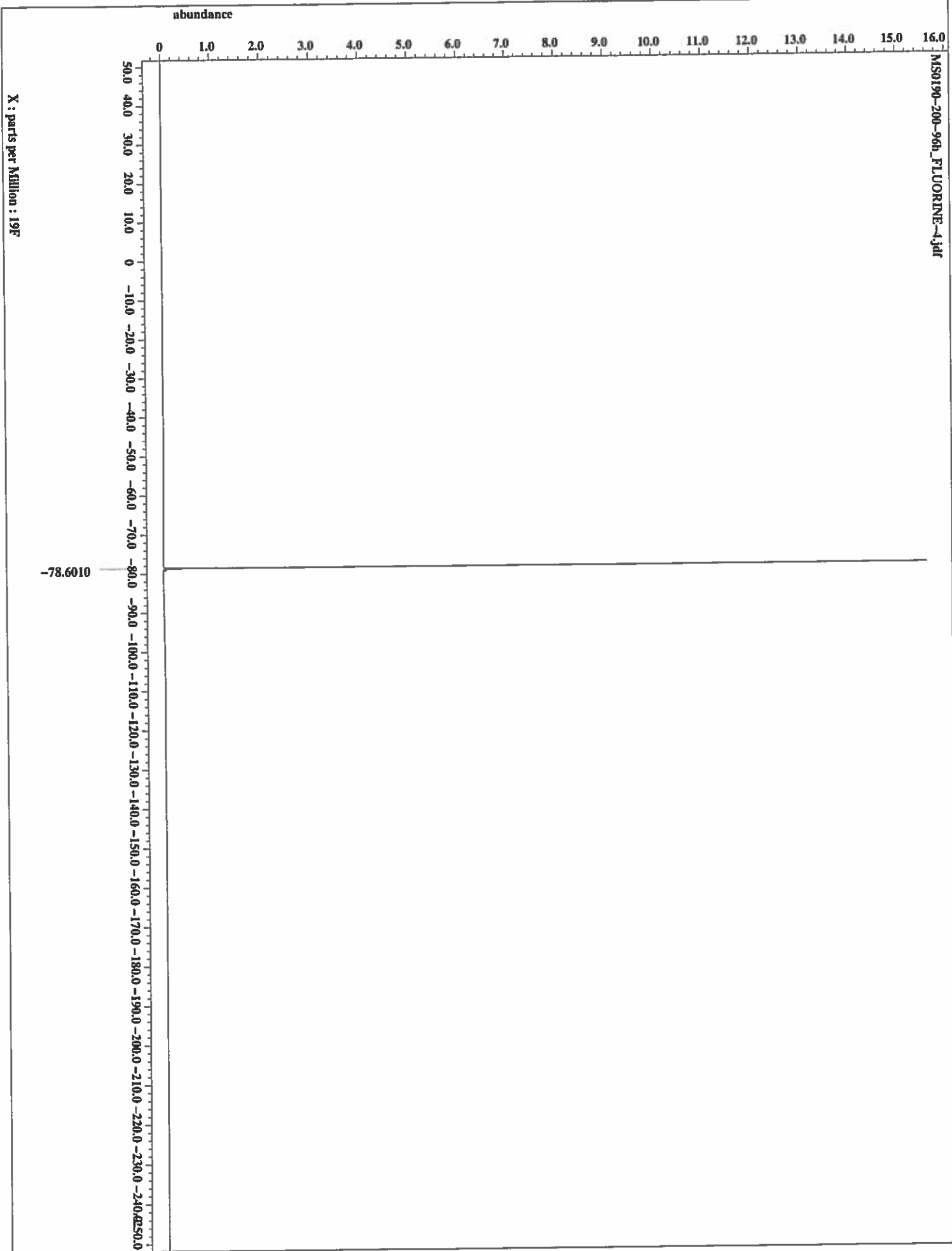
Filename      = MS0190-200-96h_CARBON
Author        = Jim Davis
Experiment    = single-pulse-dec
Sample_id     = MS0190-200-96h
Solvent       = CHLOROFORM-D
Creation_time  = 6-JAN-2019 15:11:58
Revision_time  = 6-JAN-2019 14:46:47
Current_time   = 6-JAN-2019 14:46:47

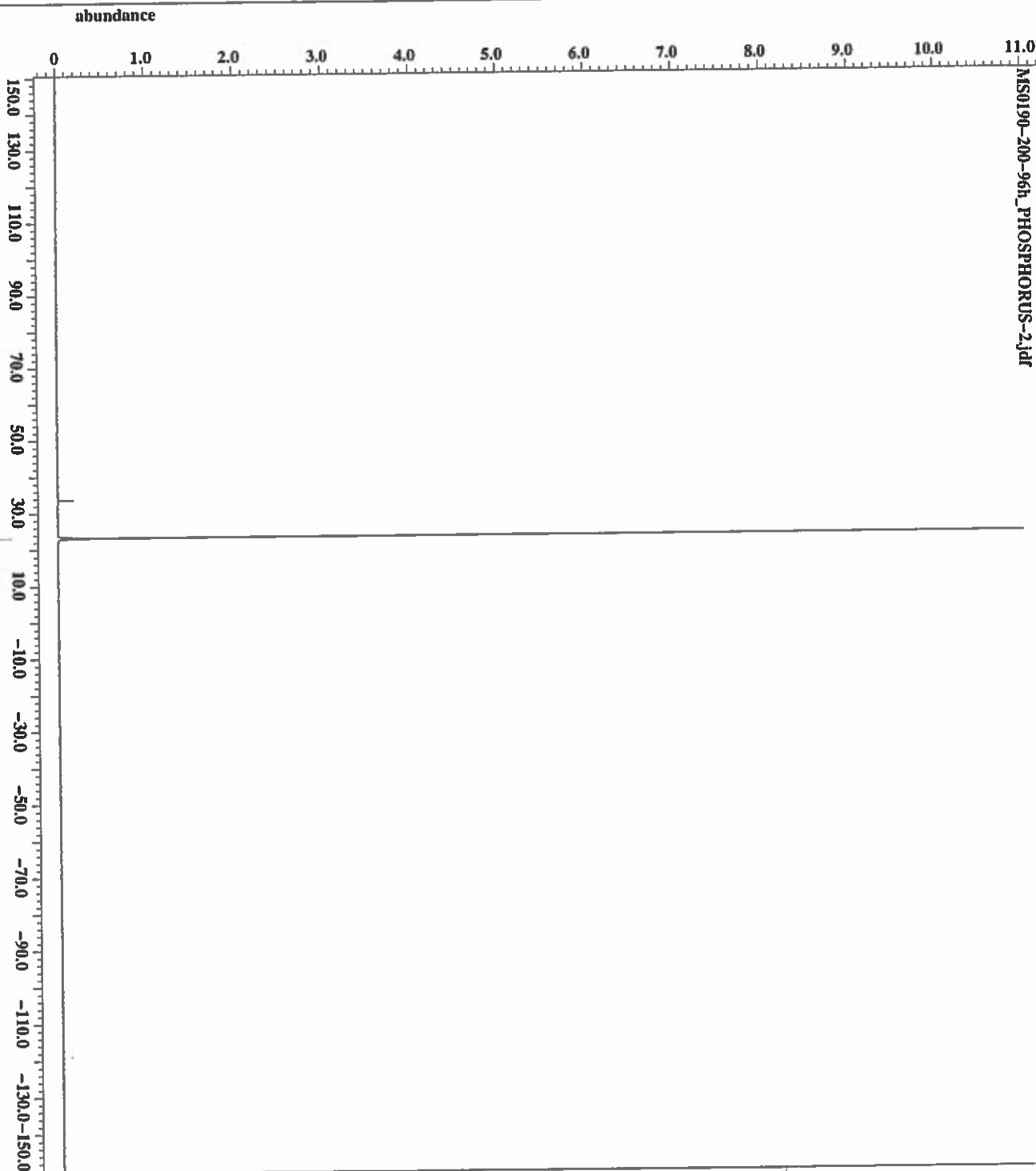
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_c1size    = 13C
Dim_c1title   = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

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]
X_domain       = 1H
Xir_freq       = 500.15991521 [MHz]
Xir_offset     = 5.0 [ppm]
Mod_return     = FALSE
Scans          = 1
Total_scans    = 600

X_90_p1dch    = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Xir_atn_dec    = 20.7 [dB]
Xir_atn_noe    = 20.7 [dB]
Xir_noise      = KALTZ
Decoupling     = TRUZ
Inital_wait    = 1 [s]
Noe            = TRUZ
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 20.7 [C]
  
```







SOUTH ALABAMA
JAGUARS

```

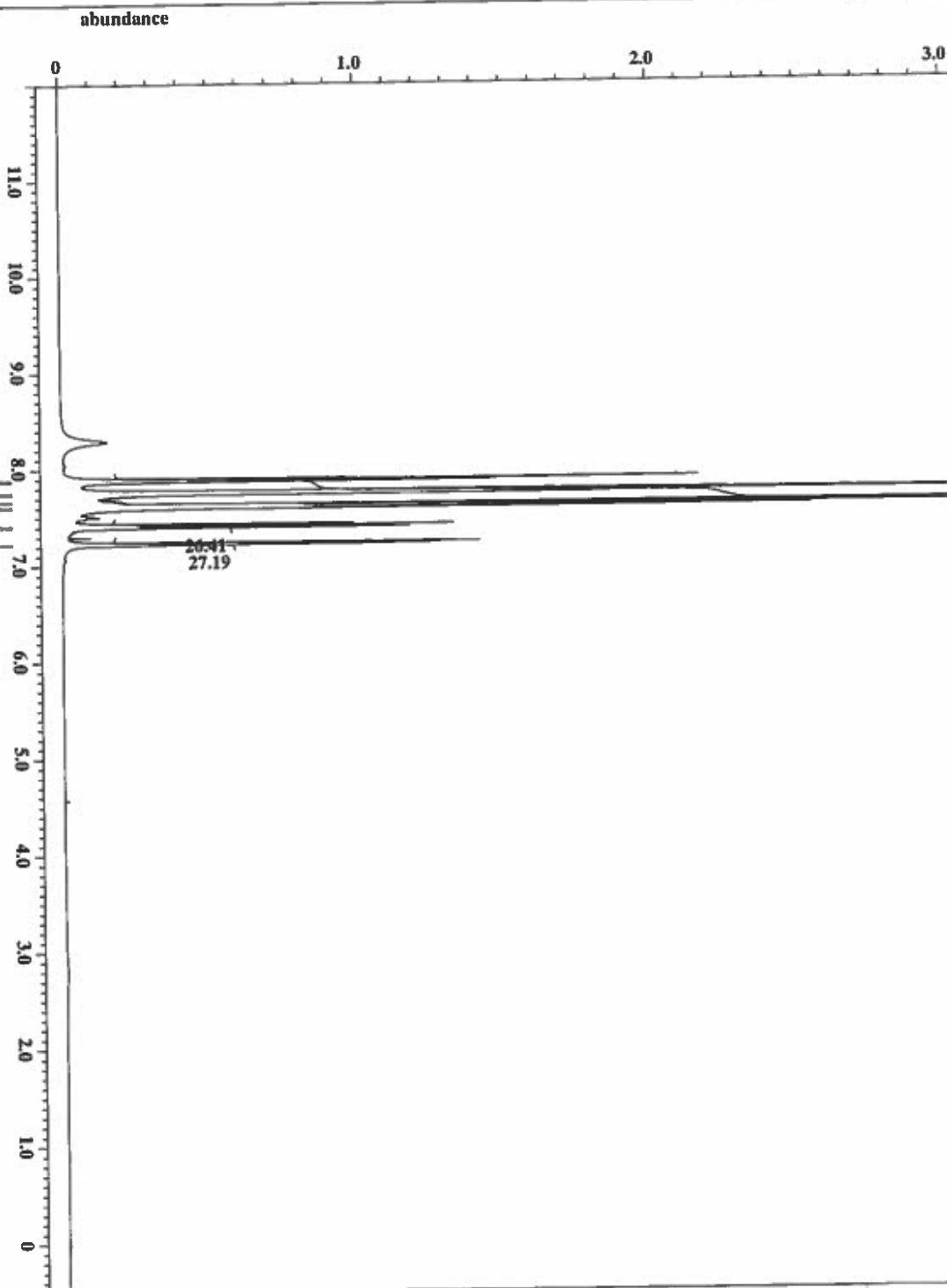
Filename      = MS0190-200-96h_PROSPH
Author        = Jim Davis
Experiment    = single-pulse-dec
Sample_id     = MS0190-200-96h
Solvent       = CHLOROFORM-D
Creation_time = 6-JAN-2019 15:33:59
Revision_time = 6-JAN-2019 15:08:48
Current_time  = 6-JAN-2019 15:08:48

Data_format   = 1D COMPLEX
Dim_size      = 52428
Dim_c1cle     = 31P
Dim_units     = [ppm]
Dimensions    = X
Sice          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.85983232[s]
X_domain      = 31P
X_freq        = 202.46831075[MHz]
X_offset      = 0.1[ppm]
X_points      = 65536
X_prescans    = 4
X_resolution  = 1.16301746[Hz]
X_sweep       = 76.2195122[KHz]
X_domain      = 1H
Irr_freq      = 500.15991522[MHz]
Irr_offset    = 5.0[ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 128
Total_scans   = 128

X_90_width    = 14.687[us]
X_acq_time     = 0.85983232[s]
X_angle       = 30[deg]
X_atn         = 5[dB]
X_pulse       = 4.89566667[us]
Irr_atn_dec   = 20.7[dB]
Irr_atn_poe   = 20.7[dB]
Irr_noise     = WALTZ
Decoupling    = WROX
Initial_wait   = 1[s]
Noe           = TRUE
Noe_time      = 2[te]
Noe_gain      = 58
Relaxation_delay = 2[te]
Repetition_time = 2.85983232[s]
Temp_get      = 20.4[dc]
  
```

230.94



SOUTH ALABAMA
JAGUARS

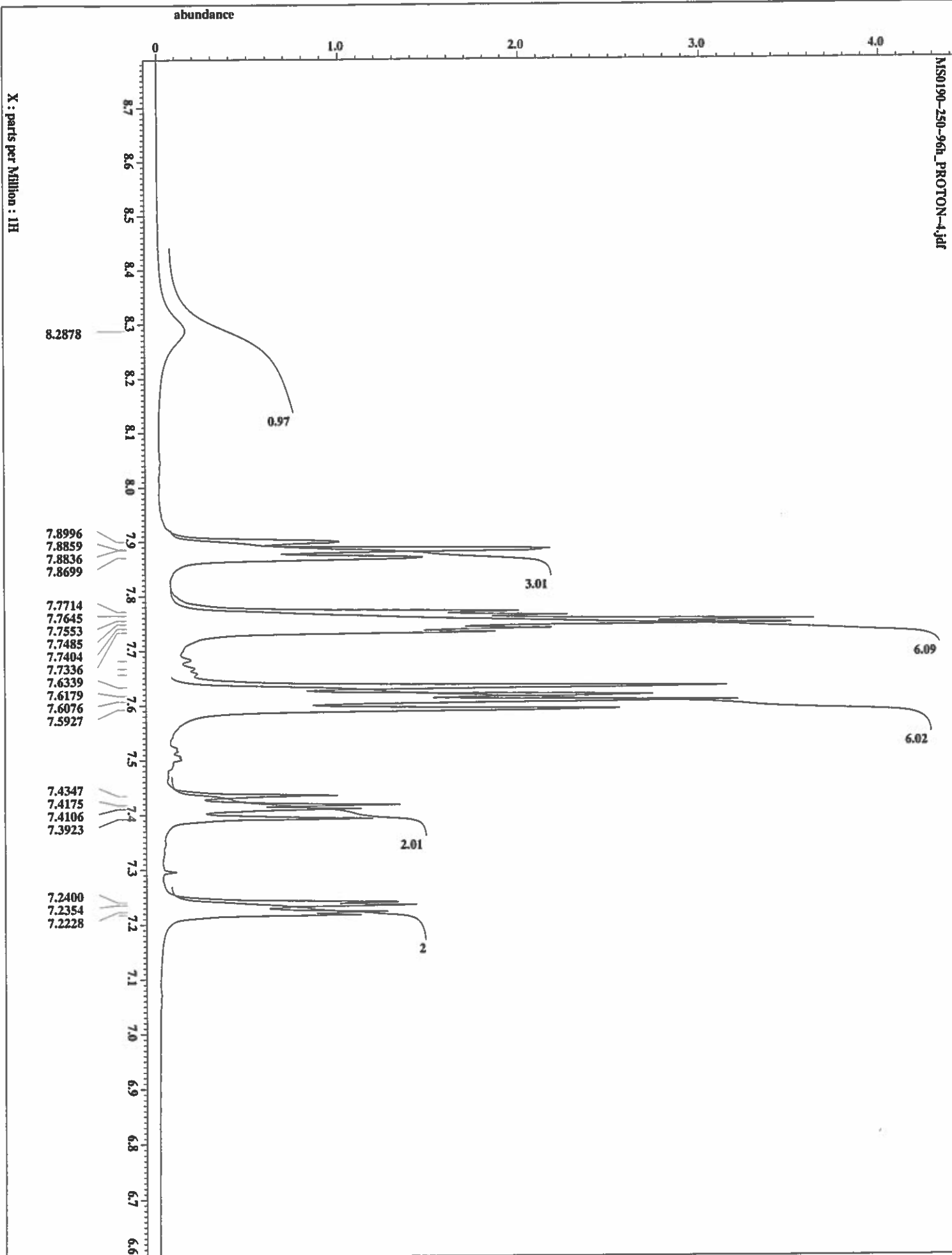
```

Filename      = MS0190-250-96h_PROTON
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = MS0190-250-96h
Solvent       = CHLOROFORM-D
Creation_time = 6-JAN-2019 15:41:34
Revision_time = 6-JAN-2019 15:16:23
Current_time  = 6-JAN-2019 15:16:23

Data_format   = 1D COMPLEX
Dir_size      = 13107
Dir_title     = 1H
Dir_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 9.38438438 [Hz]
Xt1_domain     = 1H
Xt1_freq       = 500.15991521 [MHz]
Xt1_offset     = 5.0 [ppm]
Xt1_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 12.4 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 6.2 [us]
Xt1_pulse      = 6.2 [us]
Xt1_offset     = 0.0 [ppm]
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 28
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_set       = 20.3 [degC]
  
```





```

File Name      MS0190-250-96h CARBON
Author         Jim Davis
Experiment     single pulse dec
Sample ID      MS0190-250-96h
Solvent        CHLOROFORM-D
Creation time   6-JAN-2019 16:12:33
Revision time   6-JAN-2019 15:47:22
Current time    6-JAN-2019 15:47:22

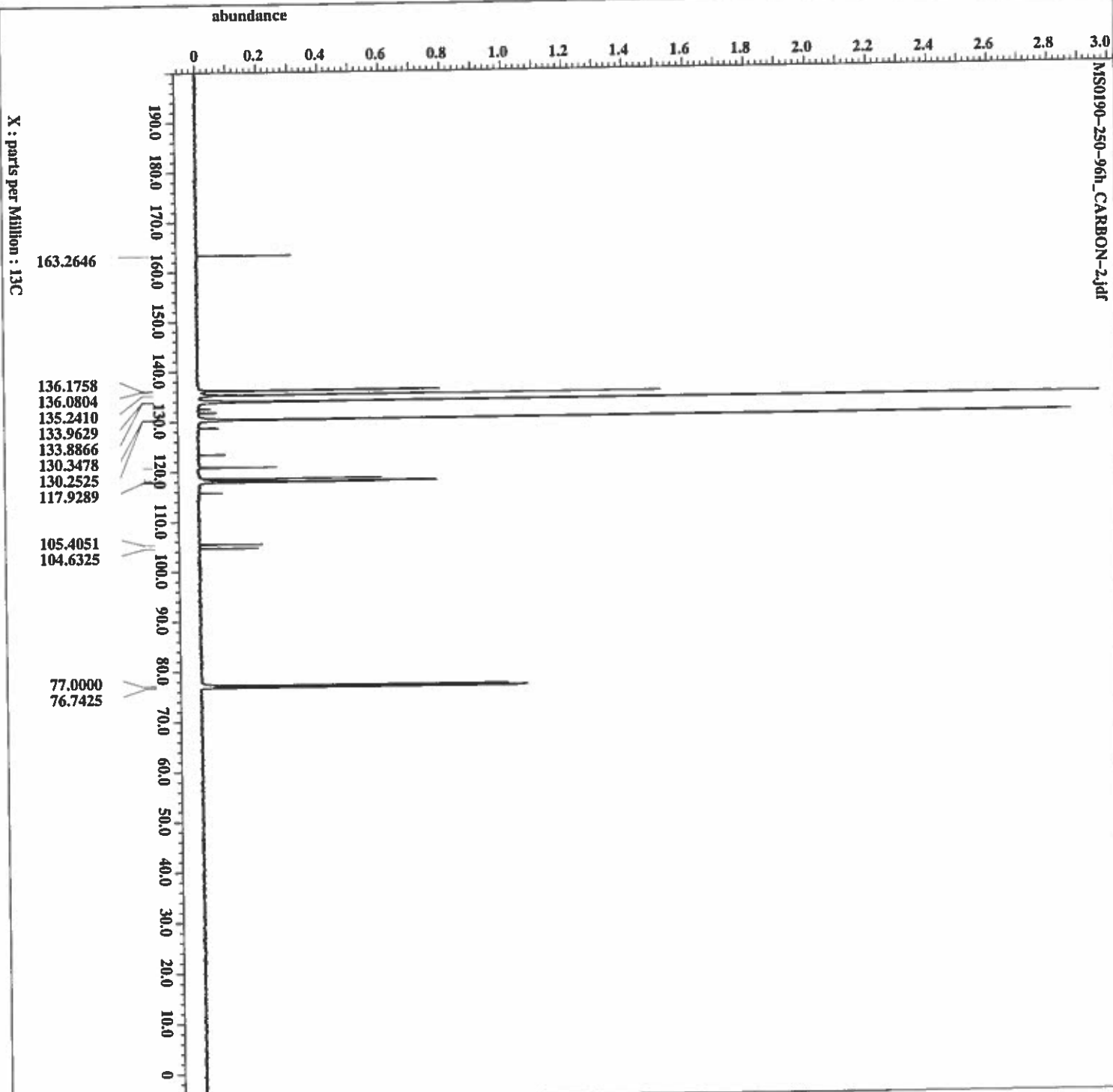
Data Format     1D COMPLEX
Dir Size       26214
Dir Cntle      13C
Dir Units      [ppm]
Dimensions     X
ECA 500
Site           JNM-ECA500

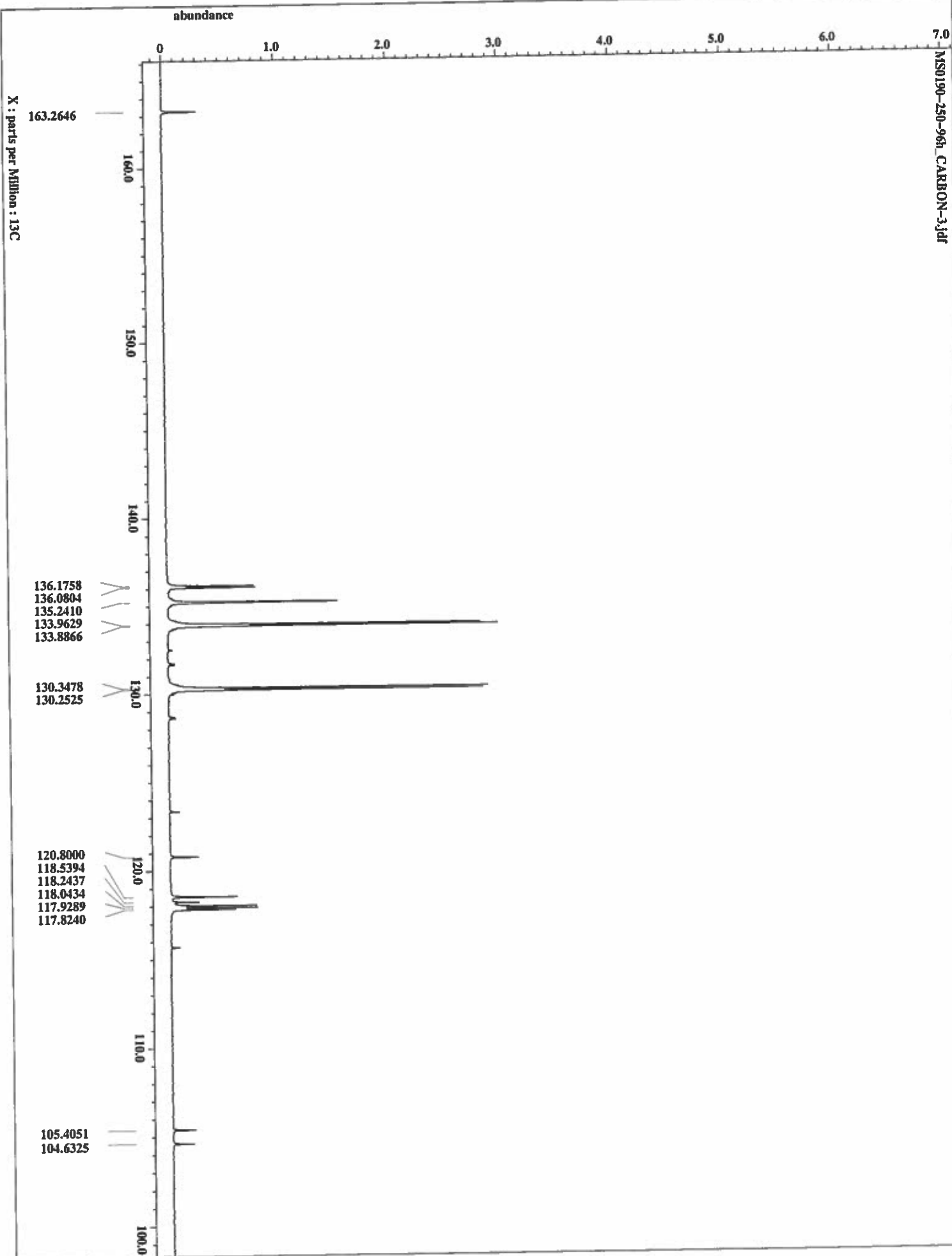
Spectrometer

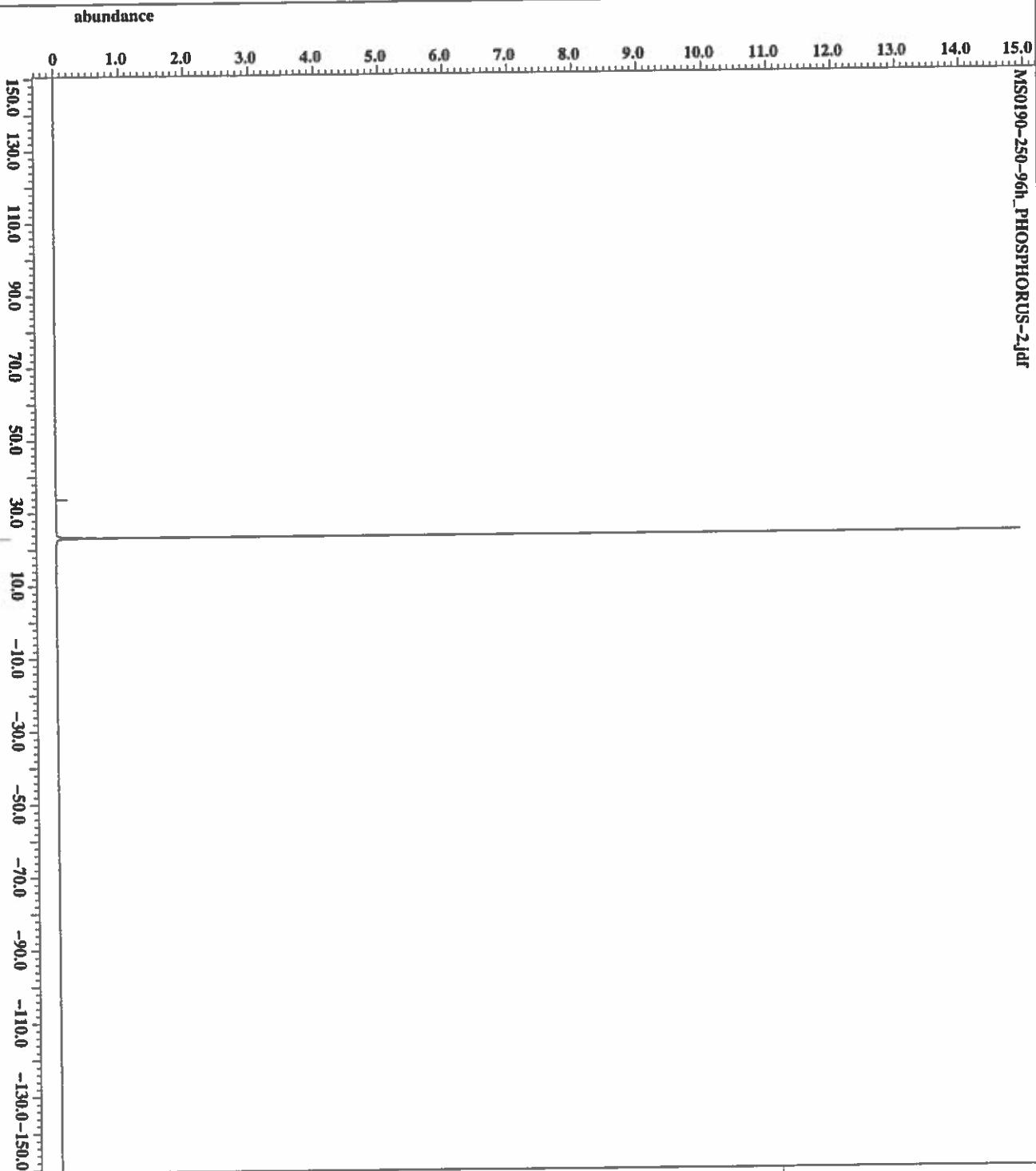
Field strength 11.7473579 [T] (500 [MH
X_acq_duration 0.83361792 [s]
X_domain       13C
X_freq         125.76529768 [MHz]
X_offset       100 [ppm]
X_points       32768
X_prescans     4
X_resolution   1.13959034 [Hz]
X_sweep        39.3081761 [kHz]
X_domain       1H
X_freq         500.15991521 [MHz]
X_offset       5.0 [ppm]
X_pulse        FALSE
Mod_return     1
Scans          600
Total_scans    600

X_90_width     13.2 [us]
X_acq_time      0.83361792 [s]
X_angle        30 [deg]
X_atn          6 [dB]
X_pulse        4.4 [us]
Xr_atn_dec     20.7 [dB]
Xr_atn_noe     20.7 [dB]
Xr_noise       MALTRZ
Decoupling     TRUE
Initial_wait    1 [s]
Noc            TRUE
Noc_time       2 [s]
Recvr_gain     60
Relaxation_delay 2 [s]
Repetition_time 2.83361792 [s]
Temp_set       20.9 [deg]

```







```

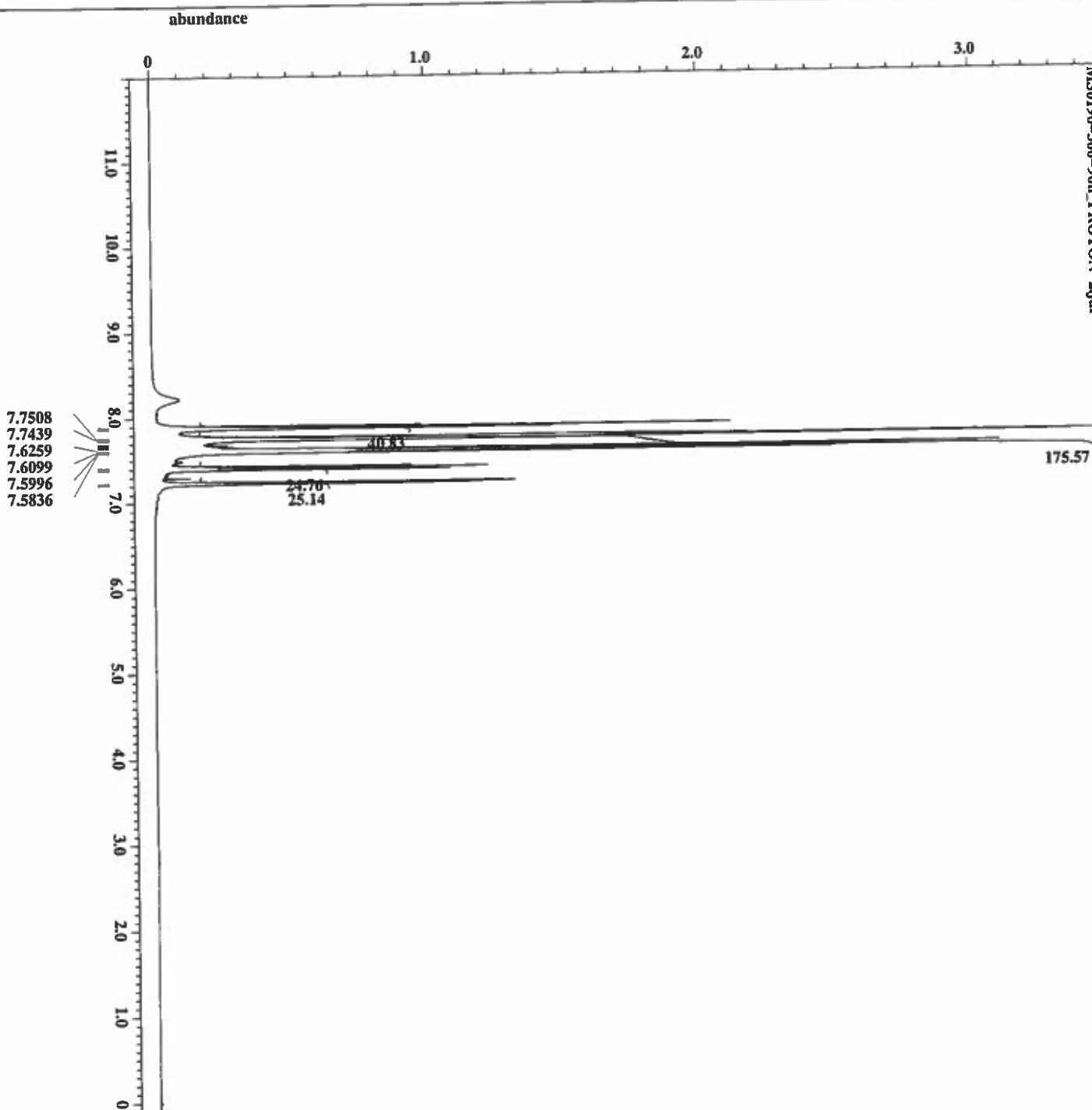
Filename      = MS0190-250-96h_PROSPH
Author        = Jim Davis
Experiment    = single-pulse_dec
Sample_id     = MS0190-250-96h
Solvent       = CHLOROFORM-D
Creation_time = 6-JAN-2019 16:33:32
Revision_time = 6-JAN-2019 16:08:21
Current_time  = 6-JAN-2019 16:08:21

Date_format   = 1D COMPLEX
Dim_size      = 52428
Dim_title     = 31P
Dim_units     = [ppm]
Dimensions    = X
Site          = FCA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500 [MH
X_acq_duration = 0.85983232[s]
X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 65336
X_prescans     = 4
X_rescans      = 1.16301746 [Hz]
X_resolution   = 76.2195122 [Hz]
X_sweep        = 1H
X_domain       = 500.15991521 [MHz]
X_freq         = 5.0 [ppm]
X_offset       = TRU2
X_resolution   = 1
Mod_return     = 128
Total_scans    = 128

X_90_width     = 14.687 [us]
X_acq_time     = 0.85983232 [s]
X_angle        = 30 [deg]
X_atn          = 5 [dB]
X_pulse        = 4.89566667 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_noe    = 20.7 [dB]
Irr_noise      = WALTZ
Decoupling     = TRU2
Initial_wait   = 1 [s]
Noe            = TRU2
Noe_time       = 2 [s]
Recvr_gain     = 54
Relaxation_delay = 2 [s]
Repetition_time = 2.85983232 [s]
Temp_get       = 20.7 [dc]

```



X : parts per Million : 1H



SOUTH ALABAMA
JAGUARS

```

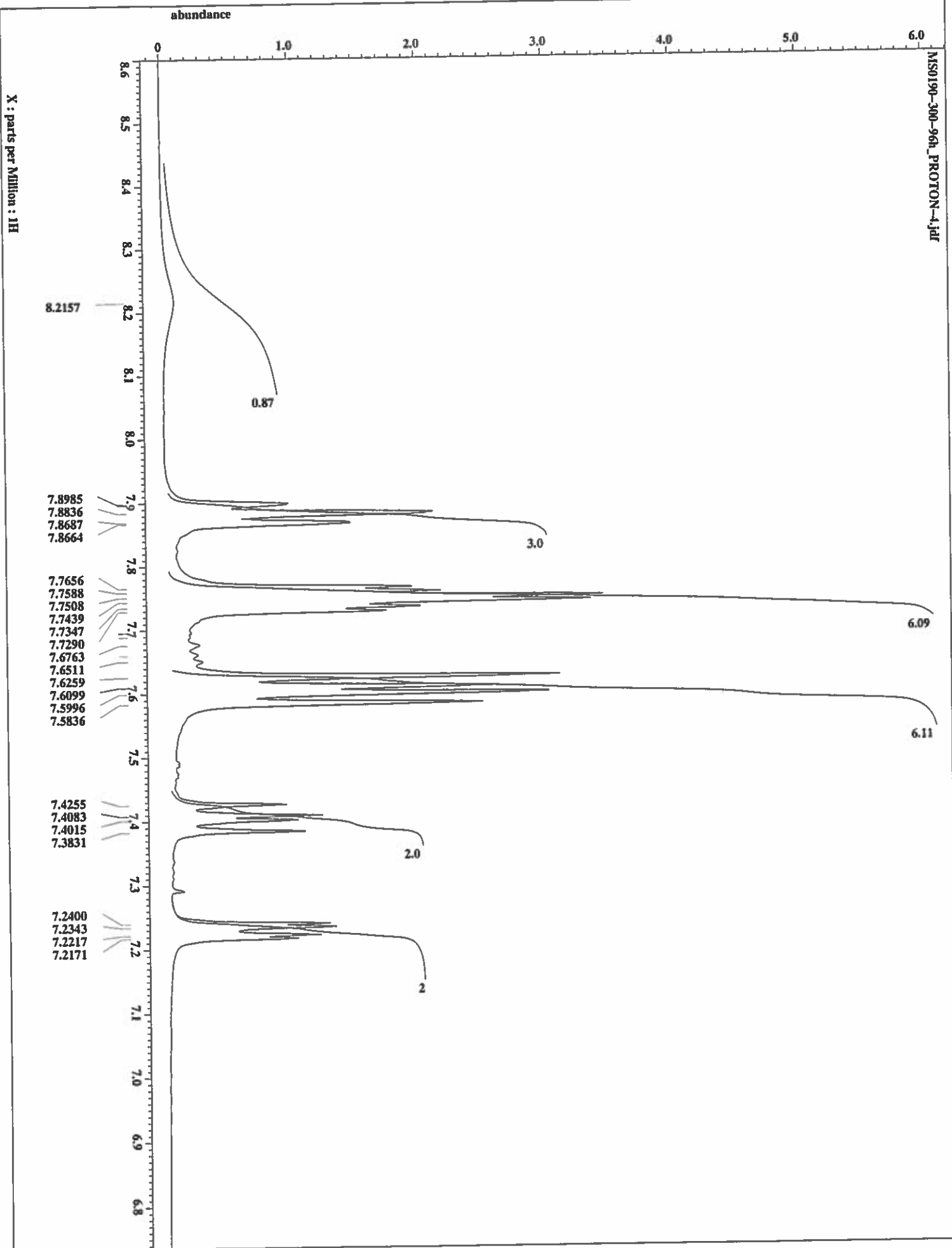
Filename      MS0190-300-96h_PROTON
Author        Jim Davis
Experiment    single_pulse.ex2
Sample_id     MS0190-300-96h
Solvent       CHLOROFORM-D
Creation_time 6-JAN-2019 16:40:50
Revision_time 6-JAN-2019 16:15:39
Current_time  6-JAN-2019 16:15:39

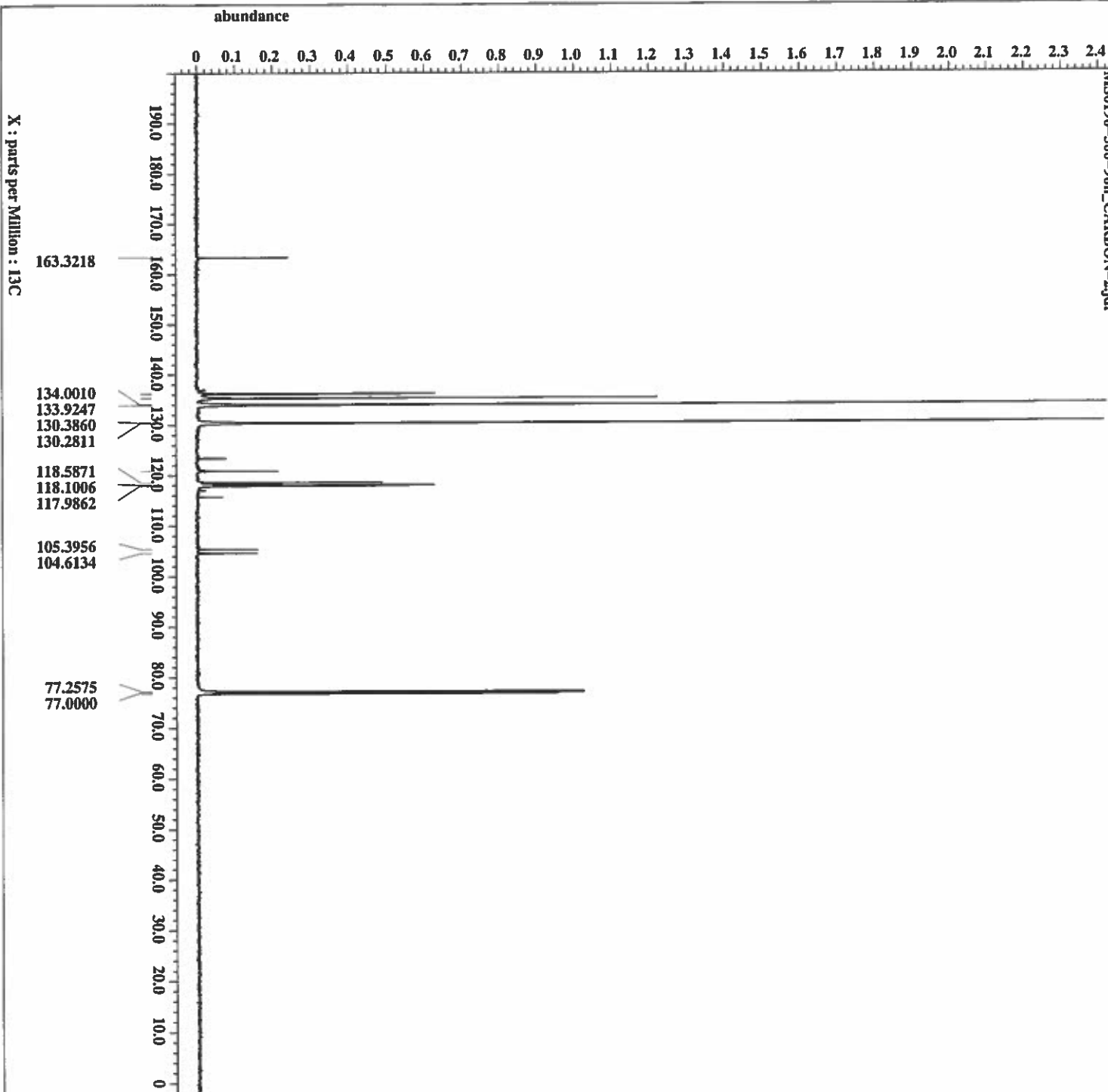
Data_format   1D COMPLEX
Dir_size      13107
Dir_cfile     1H
Dir_units     [ppm]
Dimensions    X
Site          RCA 500
Spectrometer  JNM-ECA500

Field_strength 11.7473579 [T] (500 [MH
X_acq_duration 1.74587904 [s]
X_domain       1H
X_freq         500.1591521 [MHz]
X_offset       5.0 [ppm]
X_points       16384
X_prescans     1
X_resolution   0.5727737 [Hz]
X_sweep        9.38438438 [kHz]
X_domain       1H
Xir_domain     500.1591521 [MHz]
Xir_freq       5.0 [ppm]
Xir_offset     1H
Xir_domain     500.1591521 [MHz]
Xir_freq       5.0 [ppm]
Xir_offset     FALSE
Mod_return     1
Scans          16
Total_scans    16

X_90_width     12.4 [us]
X_acq_time      1.74587904 [s]
X_angle        45 [deg]
X_atn          4 [dB]
X_pulse        6.21 [us]
Xir_mode       Off
Xir_mode       Off
Pulse_program  DANTE_presat
Initial_wait    1 [s]
Recvr_gain     28
Relaxation_delay 4 [s]
Repetition_time 5.74587904 [s]
Temp_get       20.5 [degC]

```





```

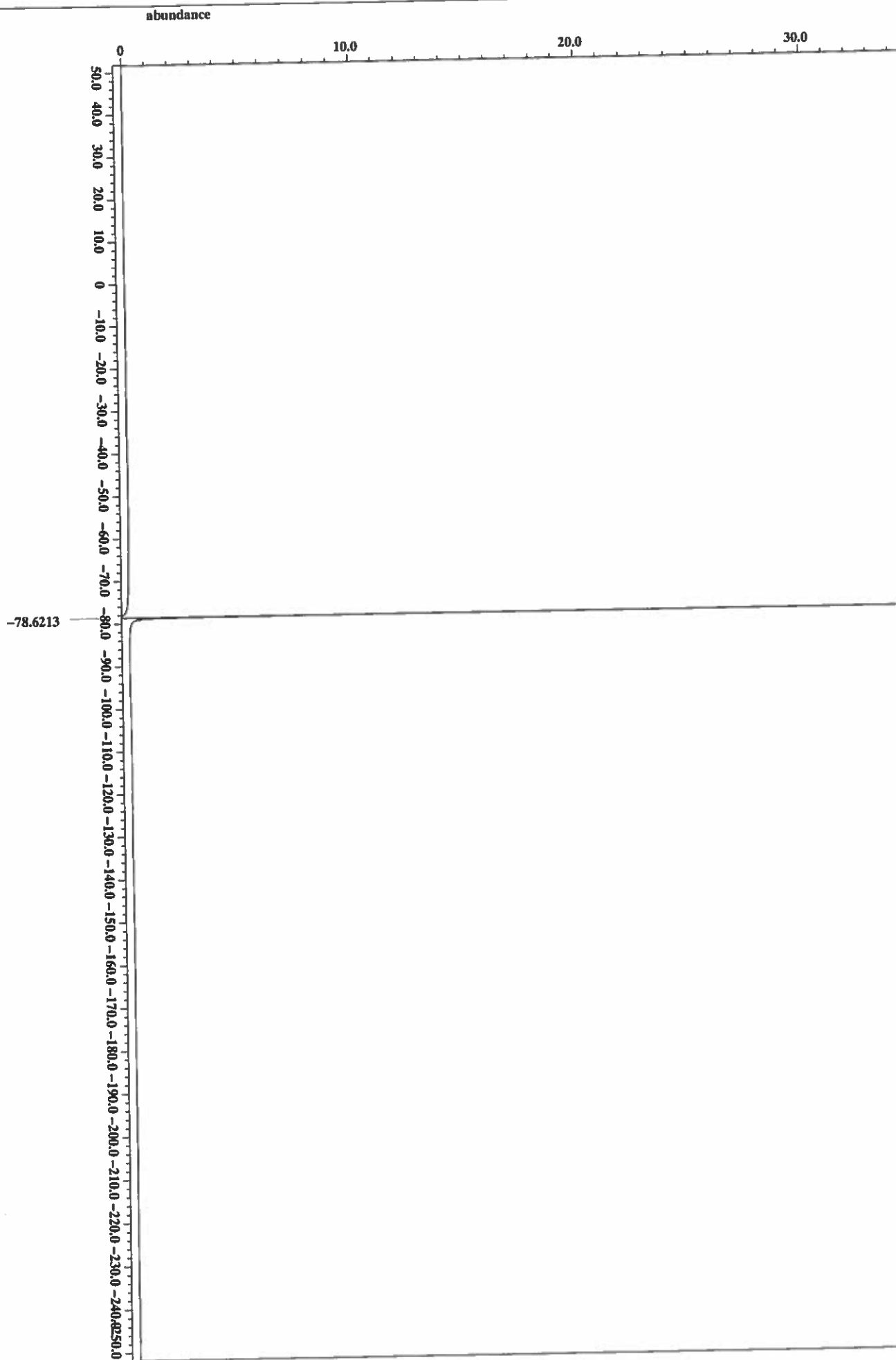
Filename      = MS0190-300-96h_CARBON
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0190-300-96h
Solvent       = CHLOROFORM-D
Creation_time  = 6-JAN-2019 17:11:33
Revision_time  = 6-JAN-2019 16:46:20
Current_time   = 6-JAN-2019 16:46:22

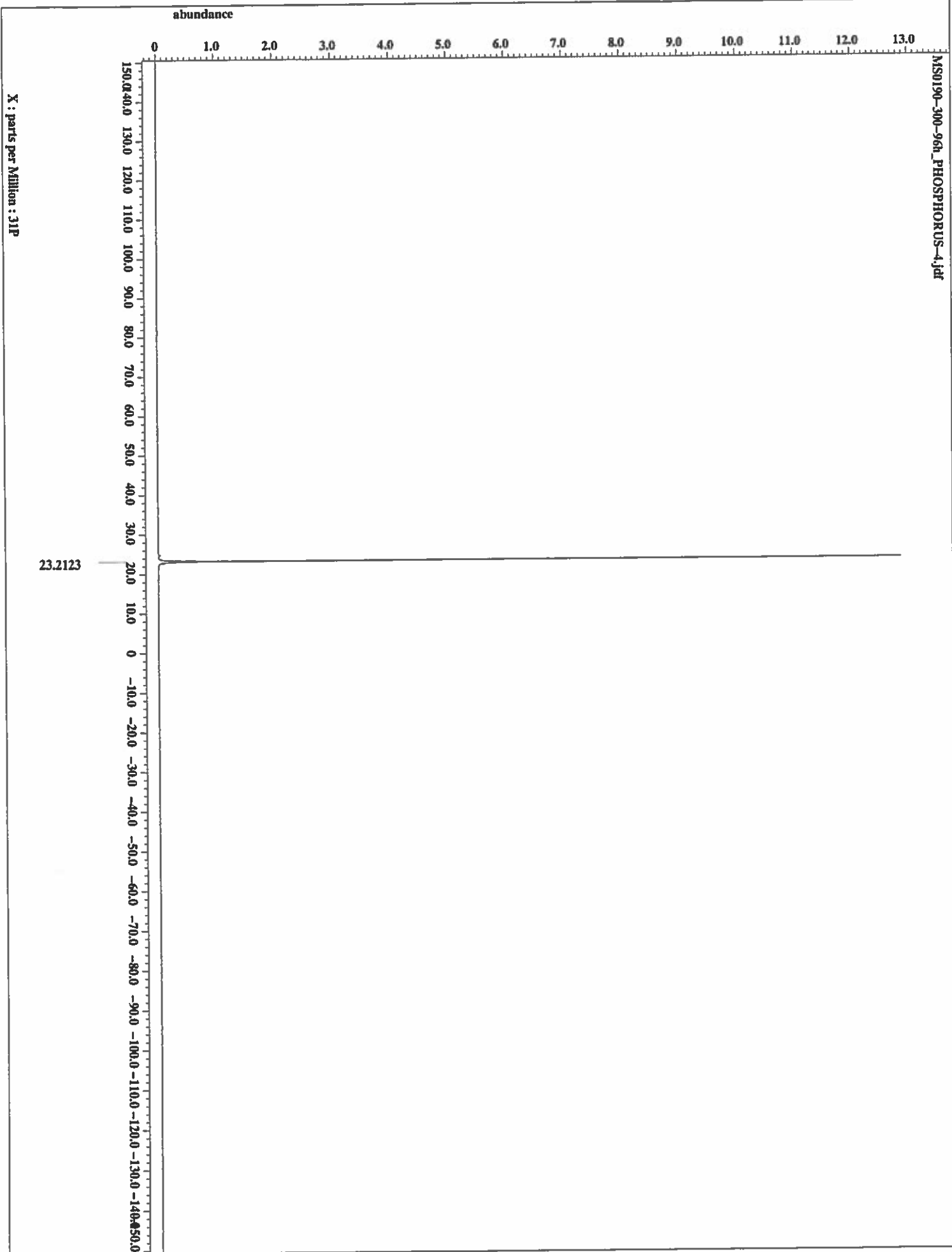
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

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]
Xt_domain      = 1H
Xt_freq        = 500.15991521 [MHz]
Xt_offset      = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 600
Total_scans    = 600

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_noe    = 20.7 [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_set       = 21 [C]

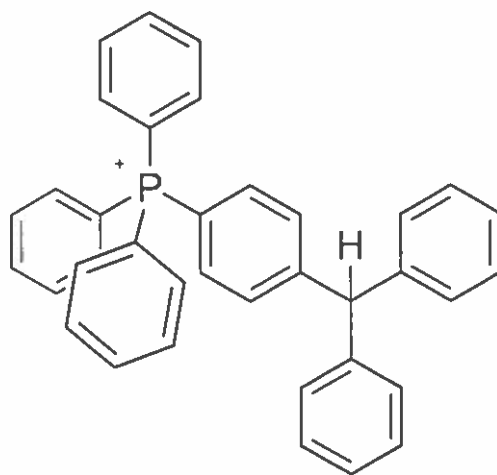
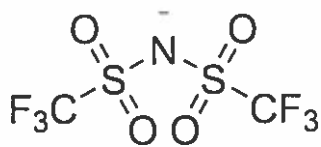
```

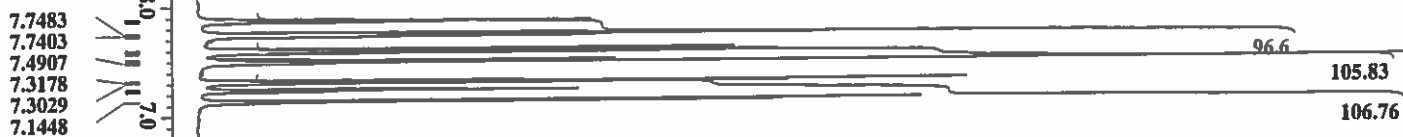




Compound 18 Pre- and Post-heating NMR Spectra

Temperature of Post-heating samples noted in upper left corner of each spectrum

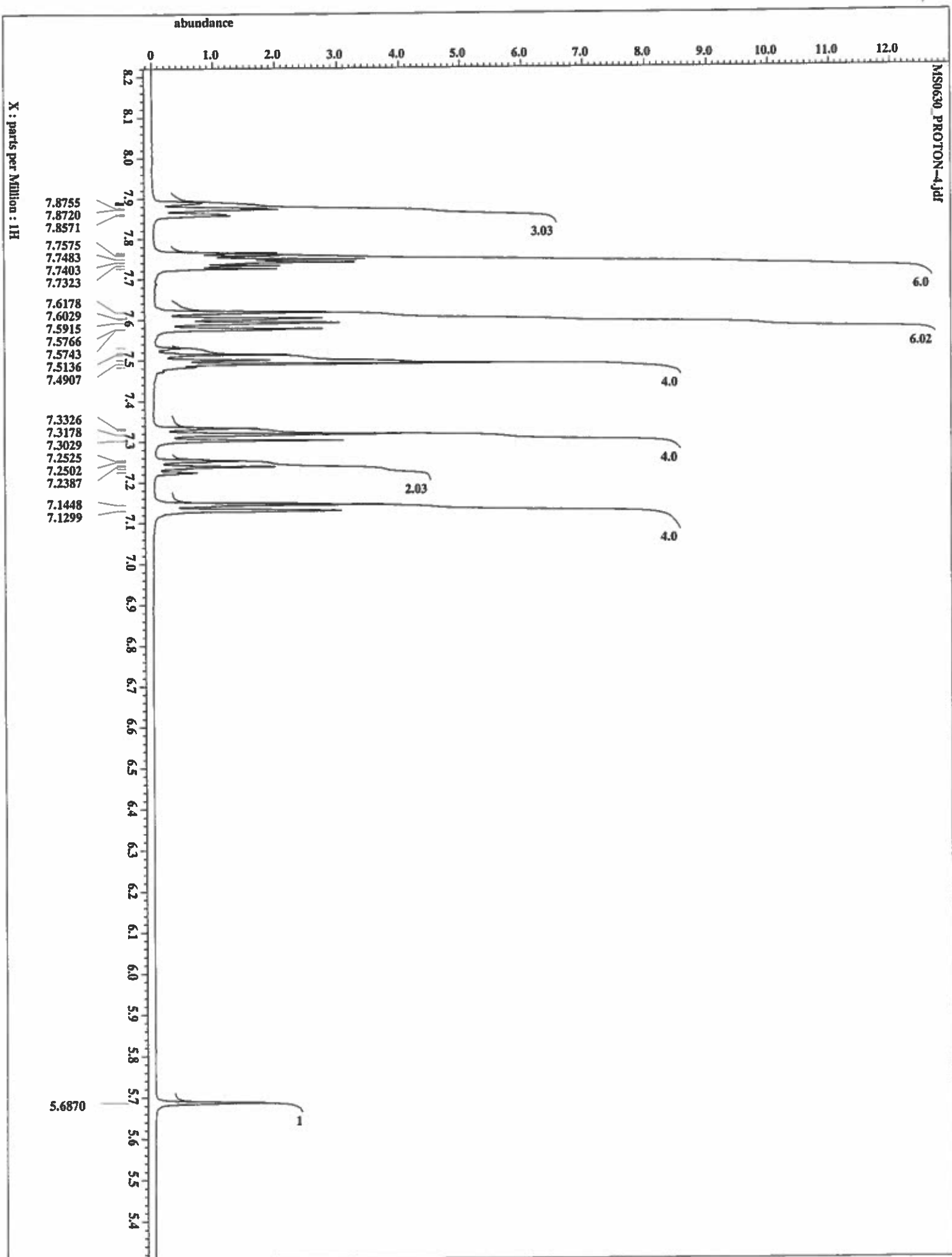


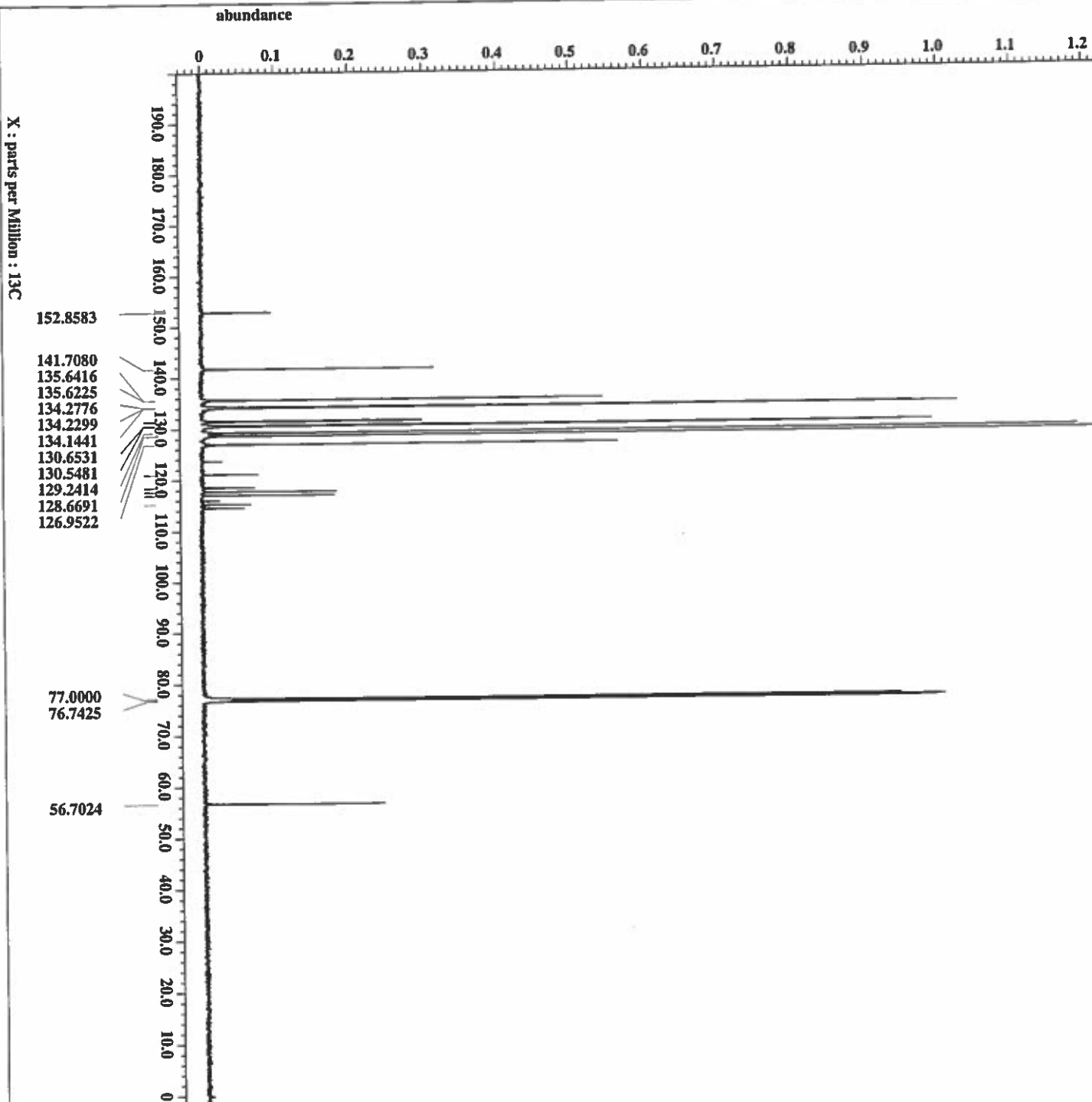


X : parts per Million : 1H



Filename = MS0630_PROTON-2.jdt
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0630
 Solvent = CHLOROFORM-D
 Creation_time = 13-DEC-2018 14:06:58
 Revision_time = 13-DEC-2018 13:39:03
 Current_time = 13-DEC-2018 13:39:03
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500
 Pfield_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 1.74587904 [s]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X_points = 16384
 X_resolution = 0.57277737 [Hz]
 X_sweep = 9.38438438 [kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 Trf_domain = 1H
 Trf_freq = 500.15991521 [MHz]
 Trf_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 13.4 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_atn = 4 [db]
 X_pulse = 6.2 [us]
 Irr_mode = OF2
 Trf_mode = OF2
 Dante_presat = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 30
 Relaxation_delay = 4 [s]
 Repetition_time = 5.74587904 [s]
 Temp_get = 20.1 [deg]





```

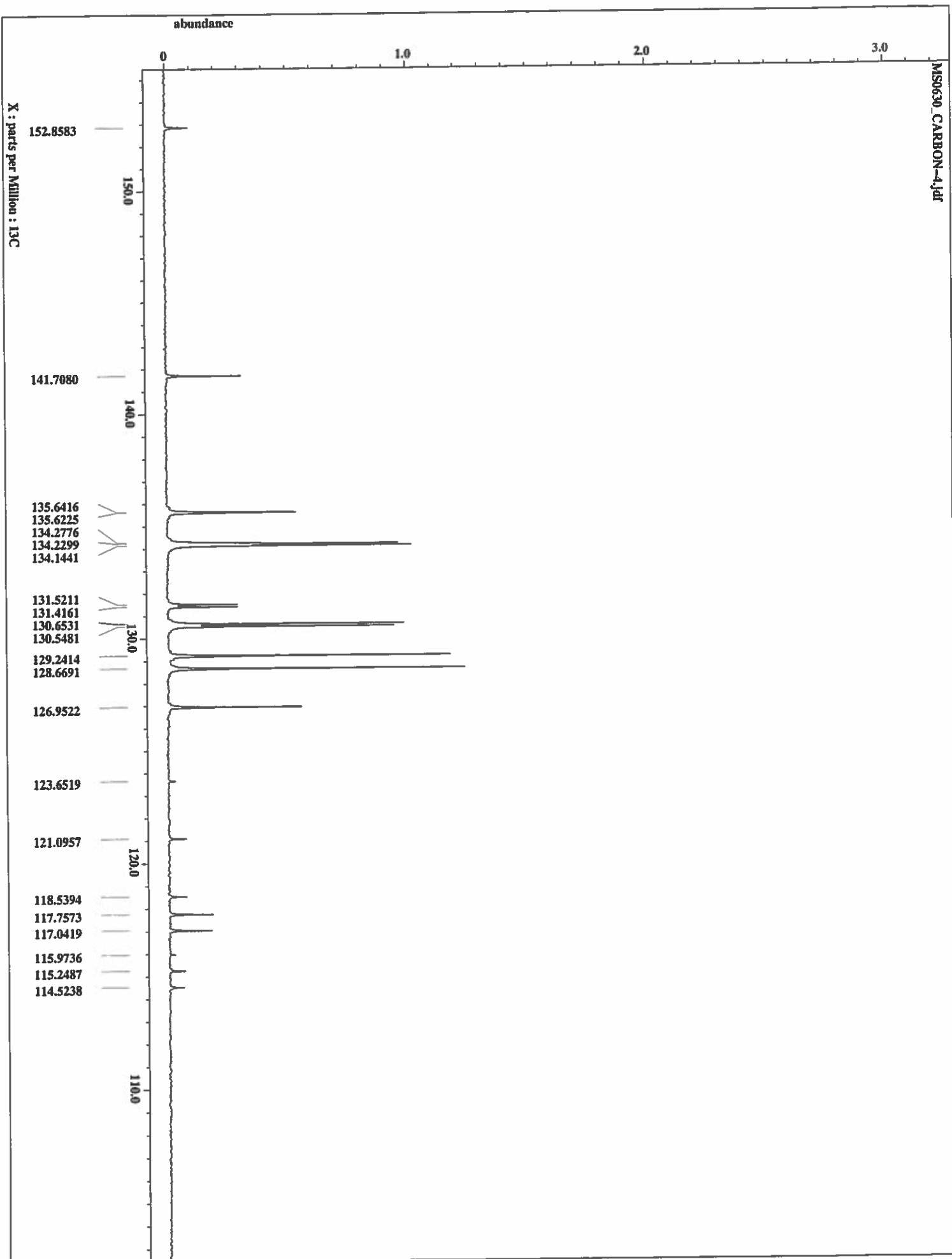
Filename      MS0630 CARBON-5.jdr
Author        Jim Davis
Experiment     single_pulse_dec
Sample_id      MS0630
Solvent        CHLOROFORM-D
Creation_time  13-DEC-2018 16:30:15
Reviation_time 13-DEC-2018 16:04:18
Current_time   13-DEC-2018 16:04:18

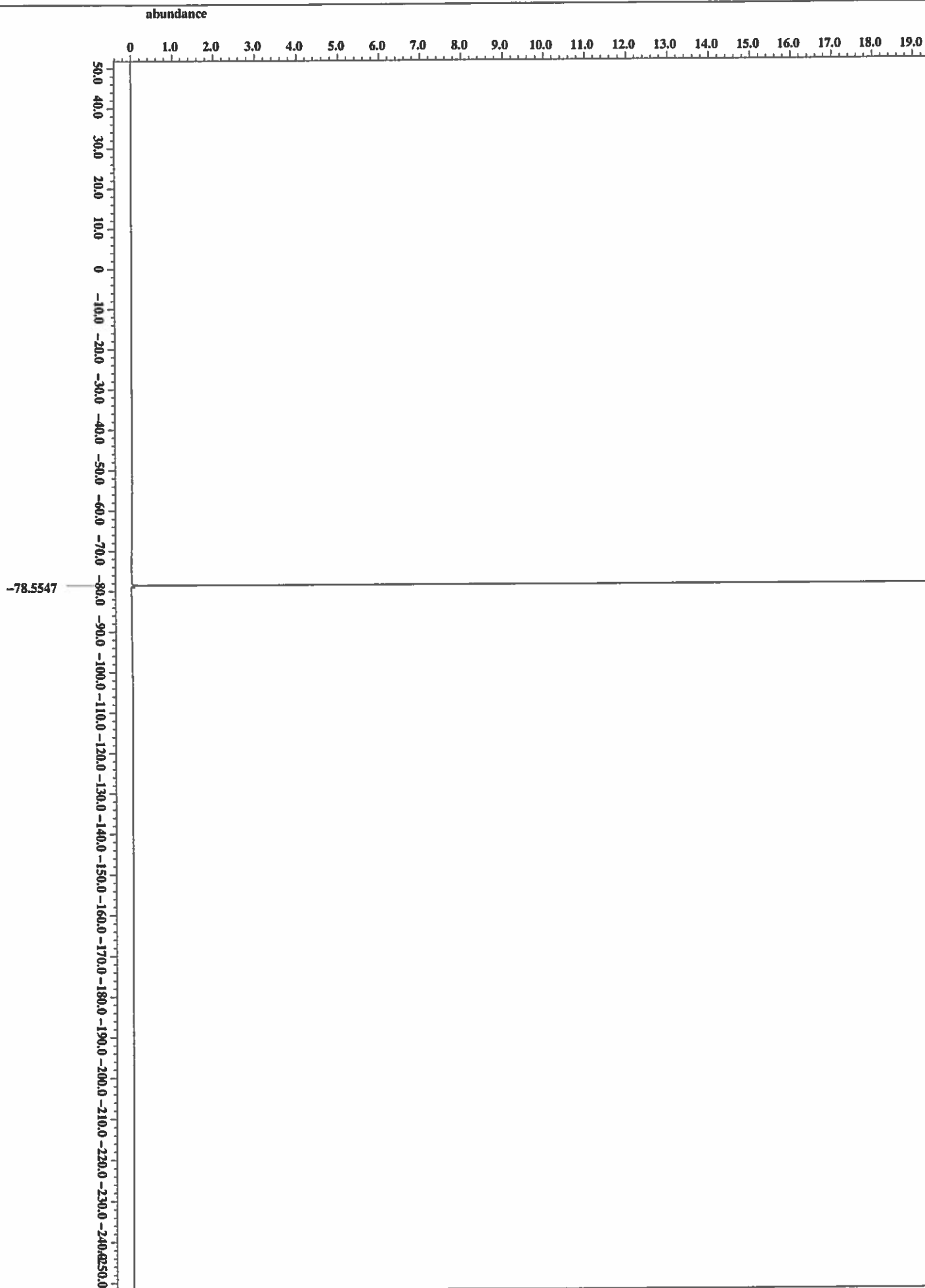
Data_format    1D COMPLEX
Dim_size       26214
Dim_title      13C
Dim_units      [ppm]
Dimensions     X
Site           RCA 500
Spectrometer   JNM-ZCA500

Field_strength 11.74735791[V] (500 [MHz]
X_acq_duration 0.833617921[s]
X_domain       13C
X_freq         125.76529768 [MHz]
X_offset       100.1 [ppm]
X_points       32768
X_prescans     4
X_resolution   1.19959634 [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          1500
Total_scans    1500

X_90_width     13.2 [us]
X_acq_time     0.833617921[s]
X_angle        30 [deg]
X_atn          6 [dB]
X_pulse        4.4 [us]
Irr_atn_dec    20.7 [dB]
Irr_atn_noe    20.7 [dB]
Irr_noise      WALTZ
Decoupling     FNUZ
Initial_wait    1 [s]
Noe            FNUZ
Noe_time       2 [s]
Recvr_gain     60
Relaxation_delay 2 [s]
Repetition_time 2.833617921[s]
Temp_get       20.6 [C]

```





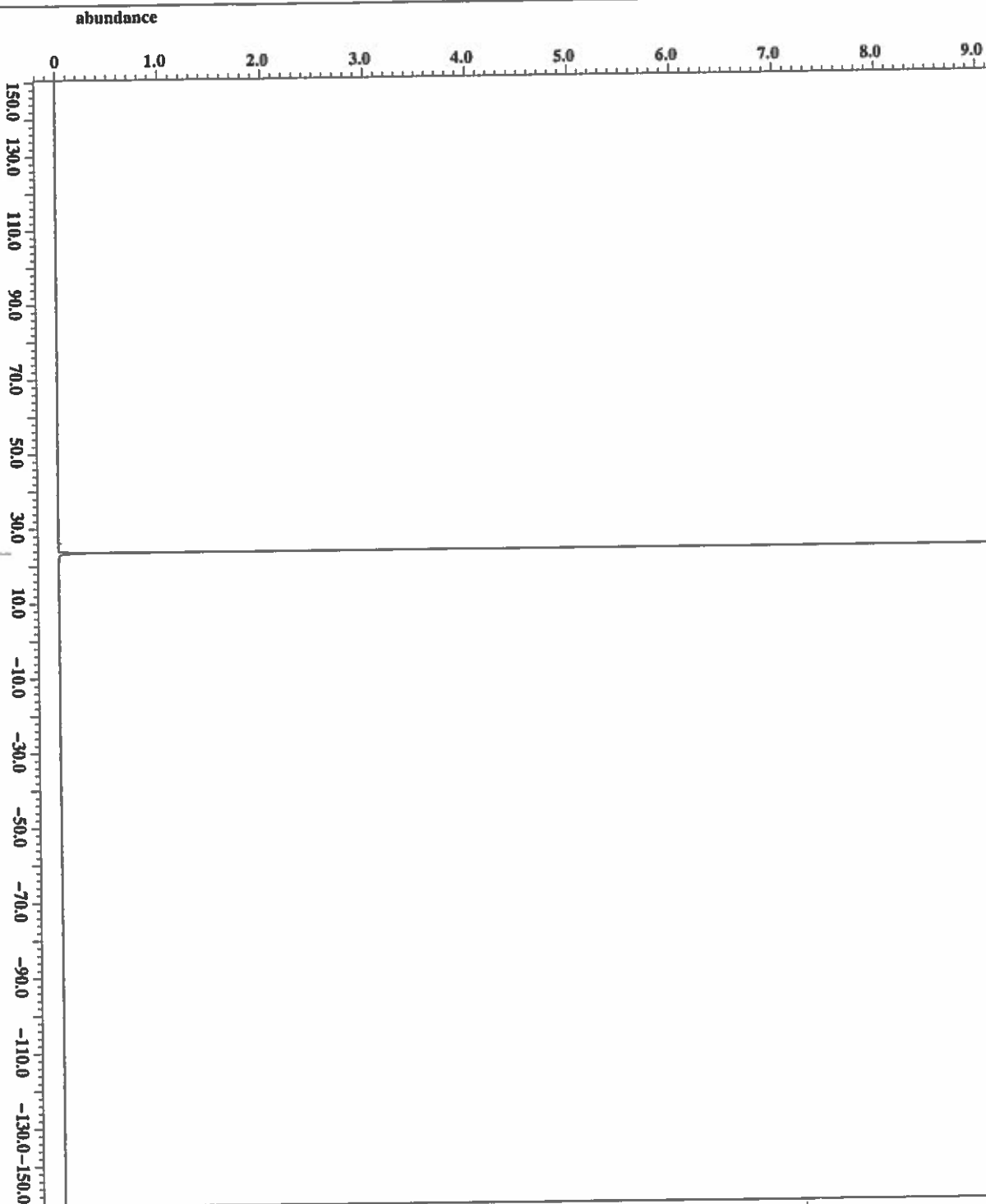


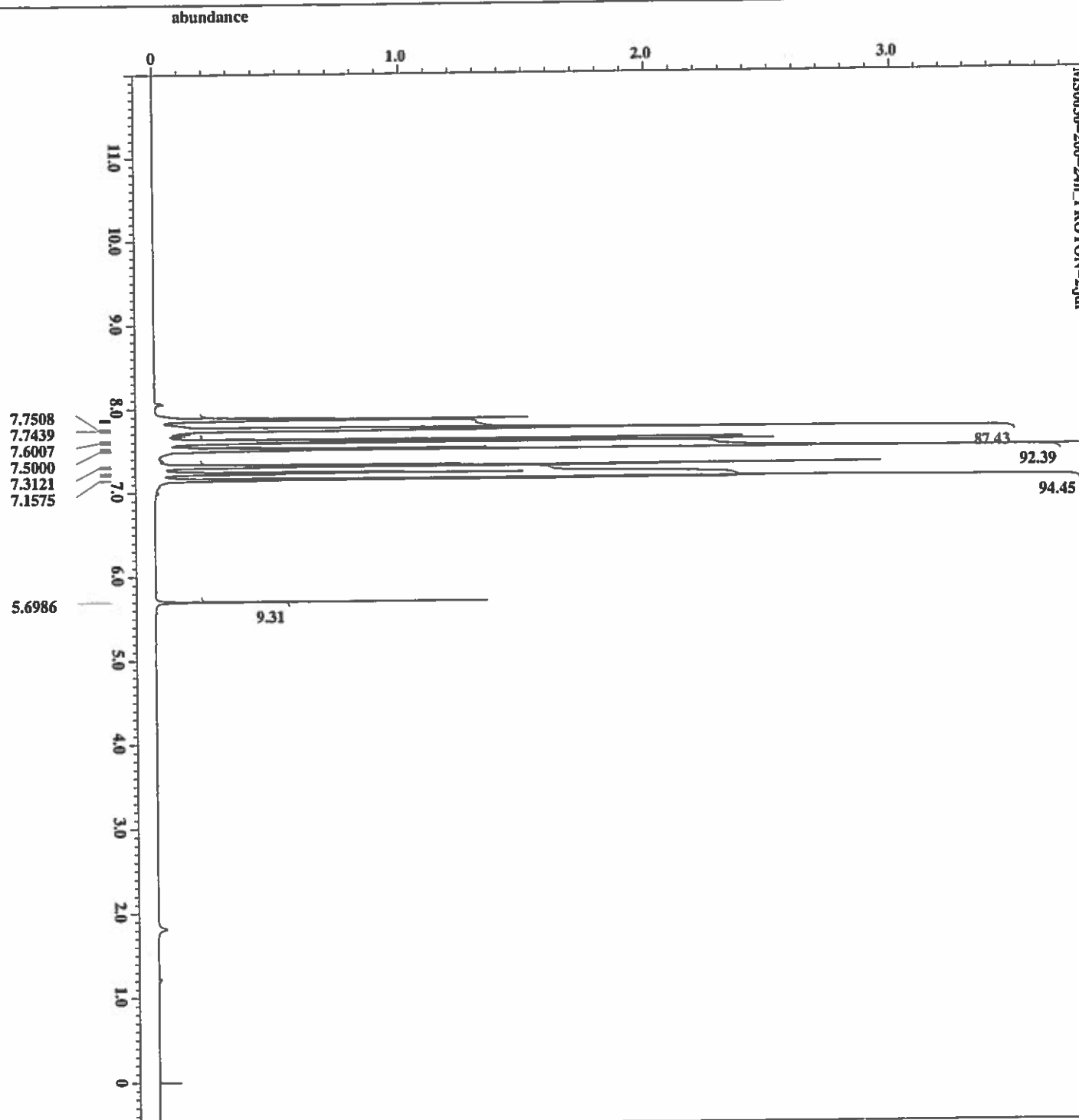
Filename MS0630_PHOSPHORUS-8.j
 Author Jim Davis
 Experiment single_pulse_dec
 Sample_id MS0630
 Solvent CHLOROFORM-D
 Creation_time 13-DEC-2018 16:38:55
 Revision_time 13-DEC-2018 16:12:58
 Current_time 13-DEC-2018 16:12:58

Data_format 1D COMPLEX
 Dia_size 52428
 Dia_title 31P
 Dia_units [ppm]
 Dimensions X
 Bits XCA 500
 Spectrometer JNM-ECA500

Field_strength 11.7473579 [G] (500 [MH
 X_acq_duration 0.85983232 [s]
 X_domain 31P
 X_freq 202.46831075 [MHz]
 X_offset 0 [ppm]
 X_points 65536
 X_prescans 4
 X_resolutions 1.16301746 [Hz]
 X_sweep 76.2195122 [Hz]
 Irr_domain 1H
 Irr_freq 500.15991521 [MHz]
 Irr_offset 5.0 [ppm]
 Clipped FALSE
 Mod_return 1
 Scans 128
 Total_scans 128

X_90_width 14.687 [us]
 X_acq_time 0.85983232 [s]
 X_angle 30 [deg]
 X_eta 5 [dB]
 X_pulse 4.89566667 [us]
 Irr_atn_dec 20.7 [dB]
 Irr_atn_noe 20.7 [dB]
 Irr_noise WALTZ
 Decoupling TRIZ
 Initial_wait 1 [s]
 Noe TRIZ
 Noe_time 2 [s]
 Noe 54
 Recvr_gain 21 [e]
 Relaxation_delay 2.85983232 [s]
 Repetition_time 20.6 [s]
 Temp_get 20.6 [C]





```

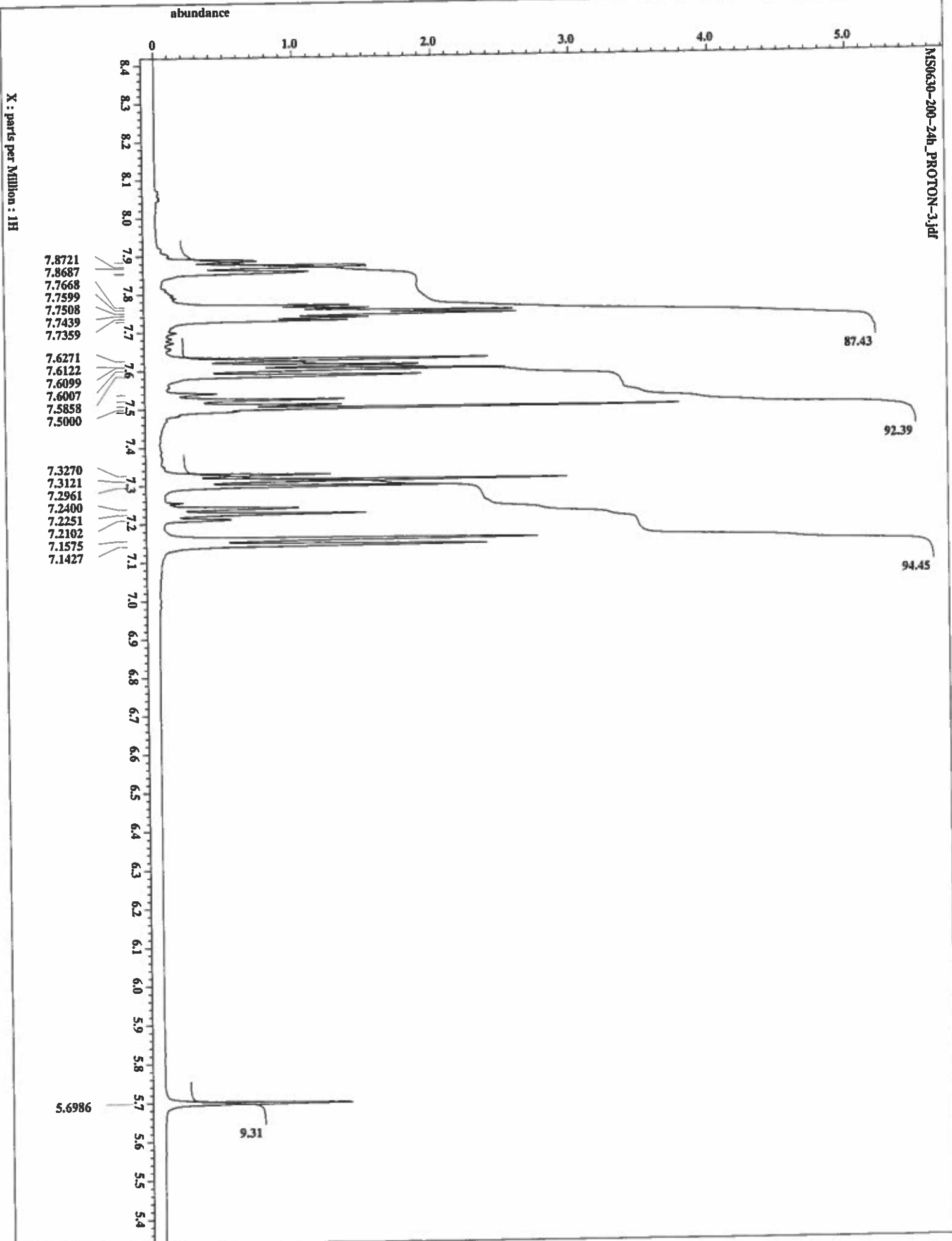
Filename      = MS0630-200-24h_PROTON
Author        = Jim Davie
Experiment    = single_pulse-ex2
Sample_id     = MS0630-200-24h
Solvent       = CHLOROFORM-D
Creation_time  = 14-DEC-2018 14:09:36
Revision_time  = 14-DEC-2018 13:43:35
Current_time   = 14-DEC-2018 13:43:35

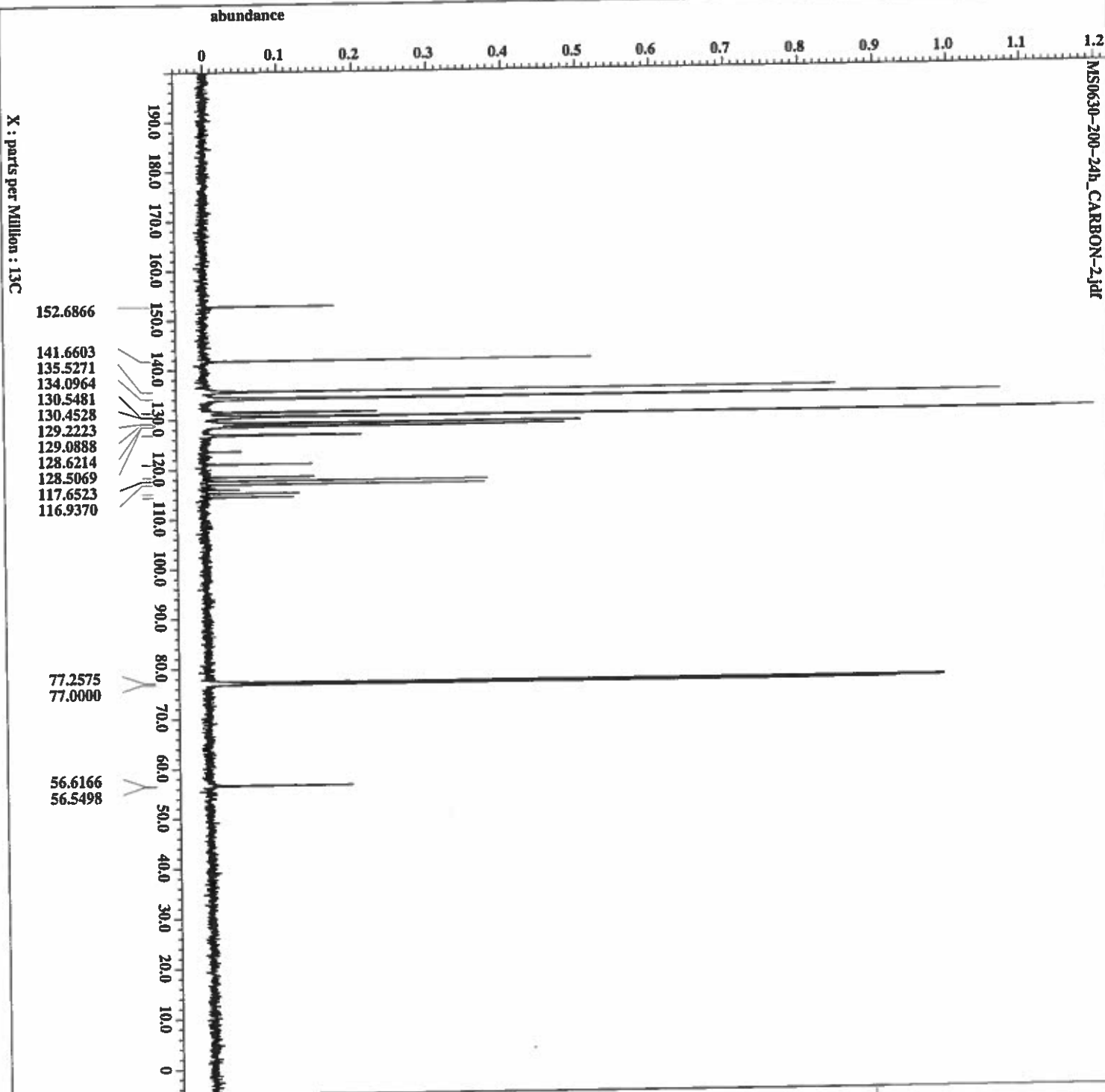
Data_format   = 1D COMPLEX
Dir_size      = 13107
Dir_title     = 1H
Dir_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500[MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_pointsize    = 16384
X_prescans     = 1
X_resolution    = 0.57277737 [Hz]
X_sweep        = 9.38438438 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Tr1_domain     = 1H
Tr1_freq       = 500.15991521 [MHz]
Tr1_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 12.4 [us]
X_acq_time      = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 6.2 [us]
Irr_mode       = Off
Tr1_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 34
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_set       = 19.9 [degC]

```





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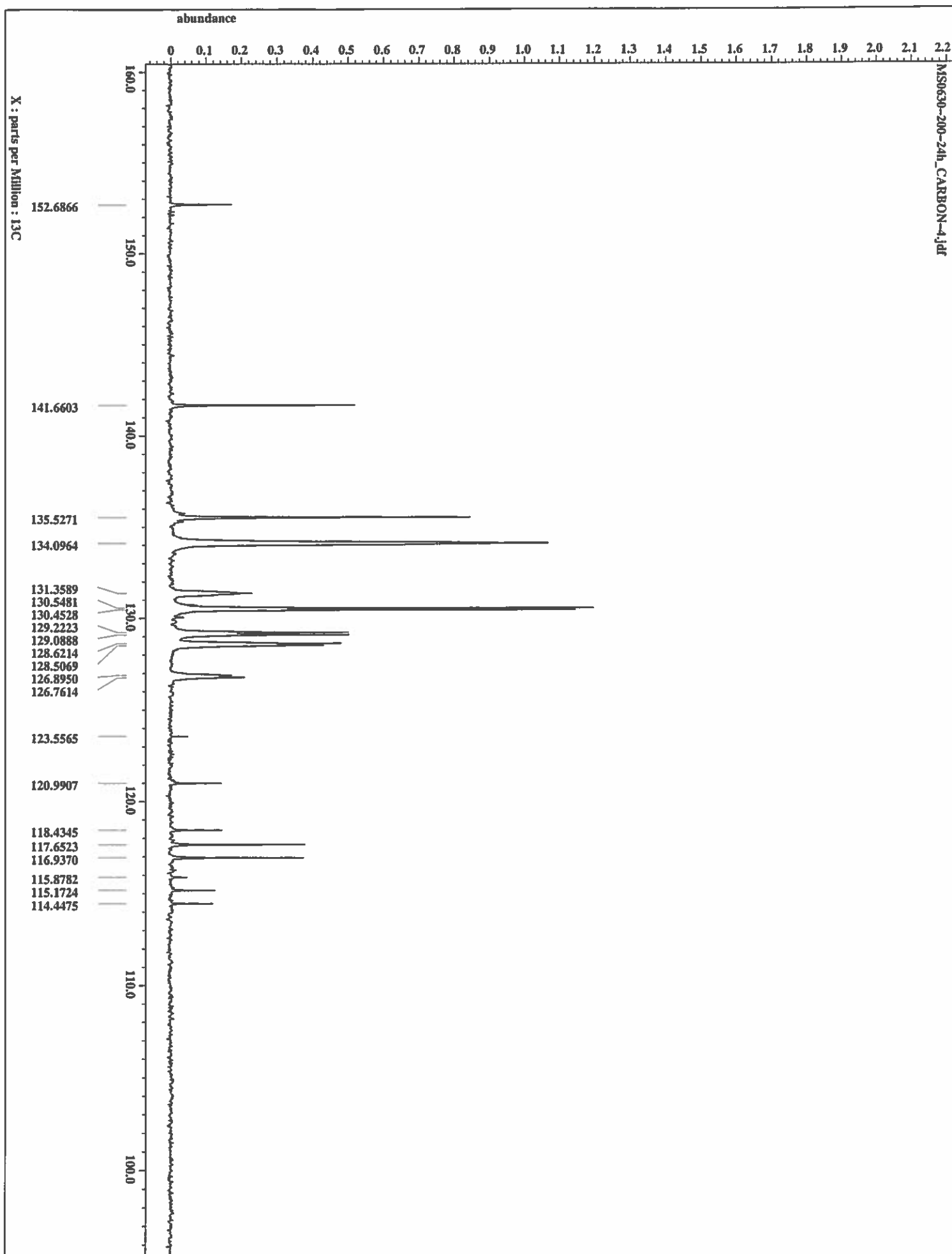
Filename      = MS0630-200-24h_CARBON
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0630-200-24h
Solvent       = CHLOROFORM-D
Creation_time = 14-DEC-2018 14:23:49
Revision_time = 14-DEC-2018 13:57:48
Current_time  = 14-DEC-2018 13:57:48

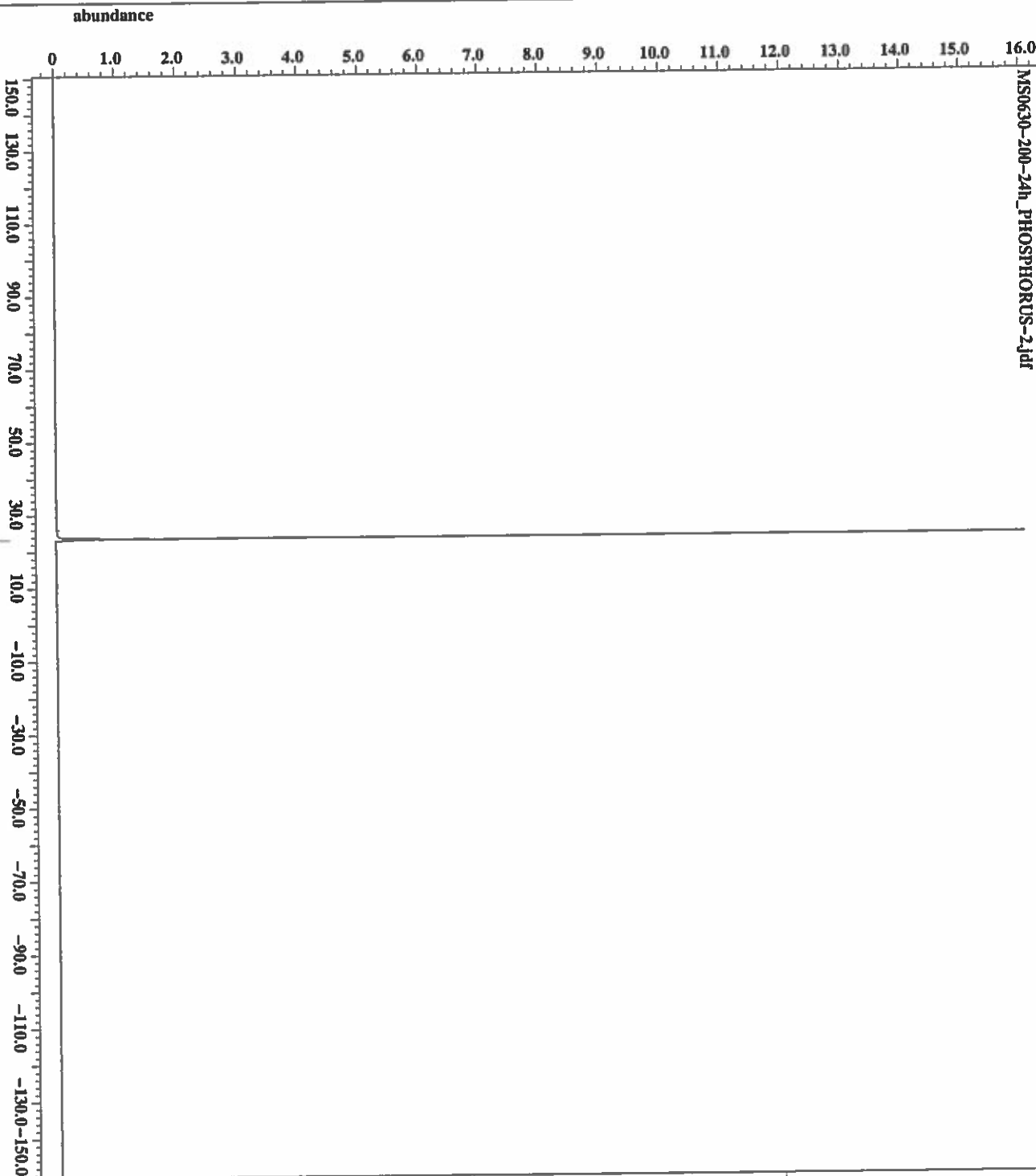
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

field_strength = 11.74735791[M] (500 MHz)
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prgname      = 4
X_resolution   = 1.19959034[Hz]
X_sweep        = 39.3081761[Hz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 1
Bcans          = 256
Total_scans    = 256

X_90_width     = 13.2[us]
X_acq_time     = 0.83361792[s]
X_angle        = 30[deg]
X_atn          = 6[db]
X_pulse        = 4.4[us]
Irr_atn_dec    = 20.7[db]
Irr_atn_poe    = 20.7[db]
Irr_pulse      = VOLTZ
Decoupling     = TRUZ
Initial_wait   = 1[s]
Roe           = PRUZ
Roe_time       = 2[s]
Recvr_gain     = 60
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get       = 20.2[degC]

```





X : parts per Million : 31P



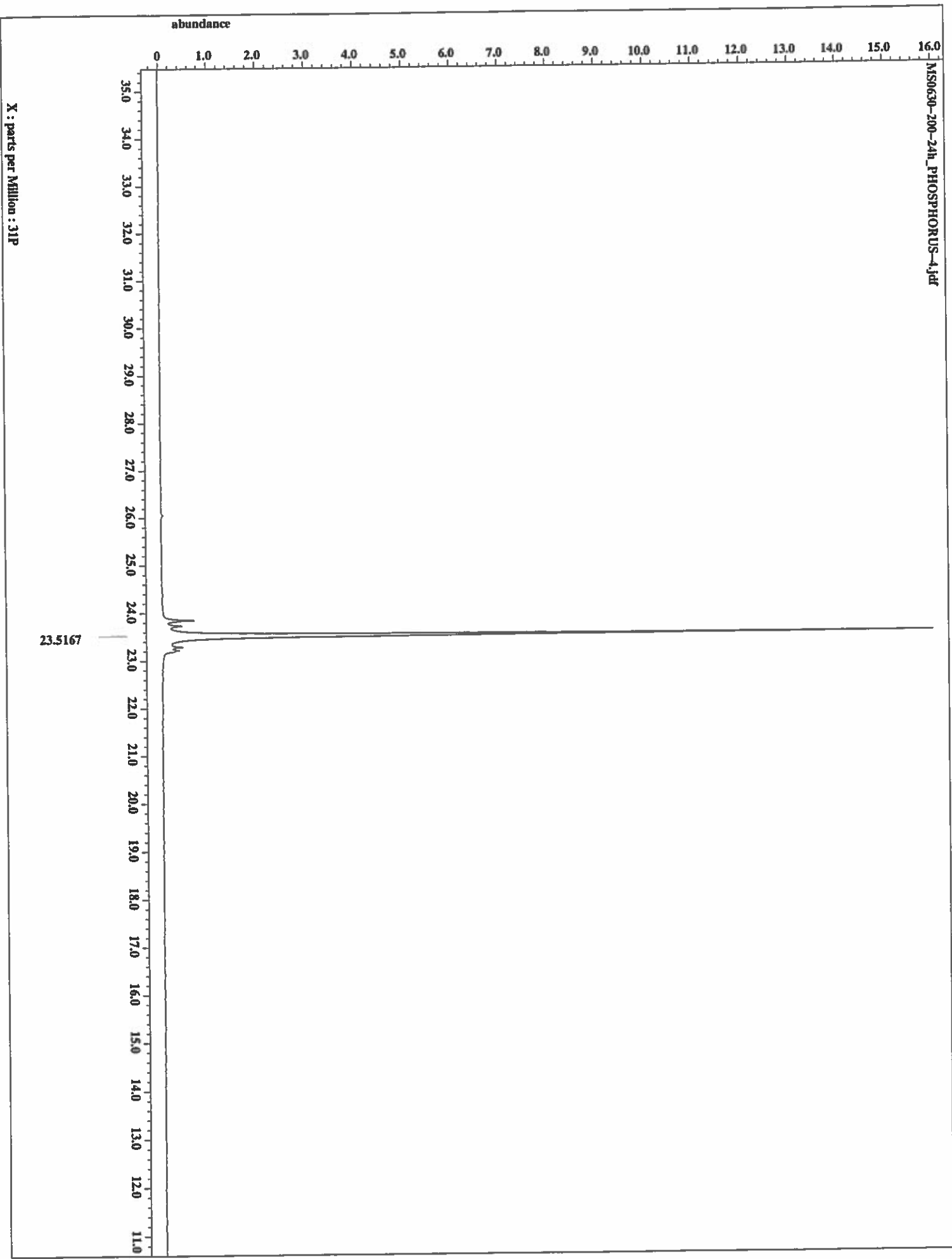
SOUTH ALABAMA
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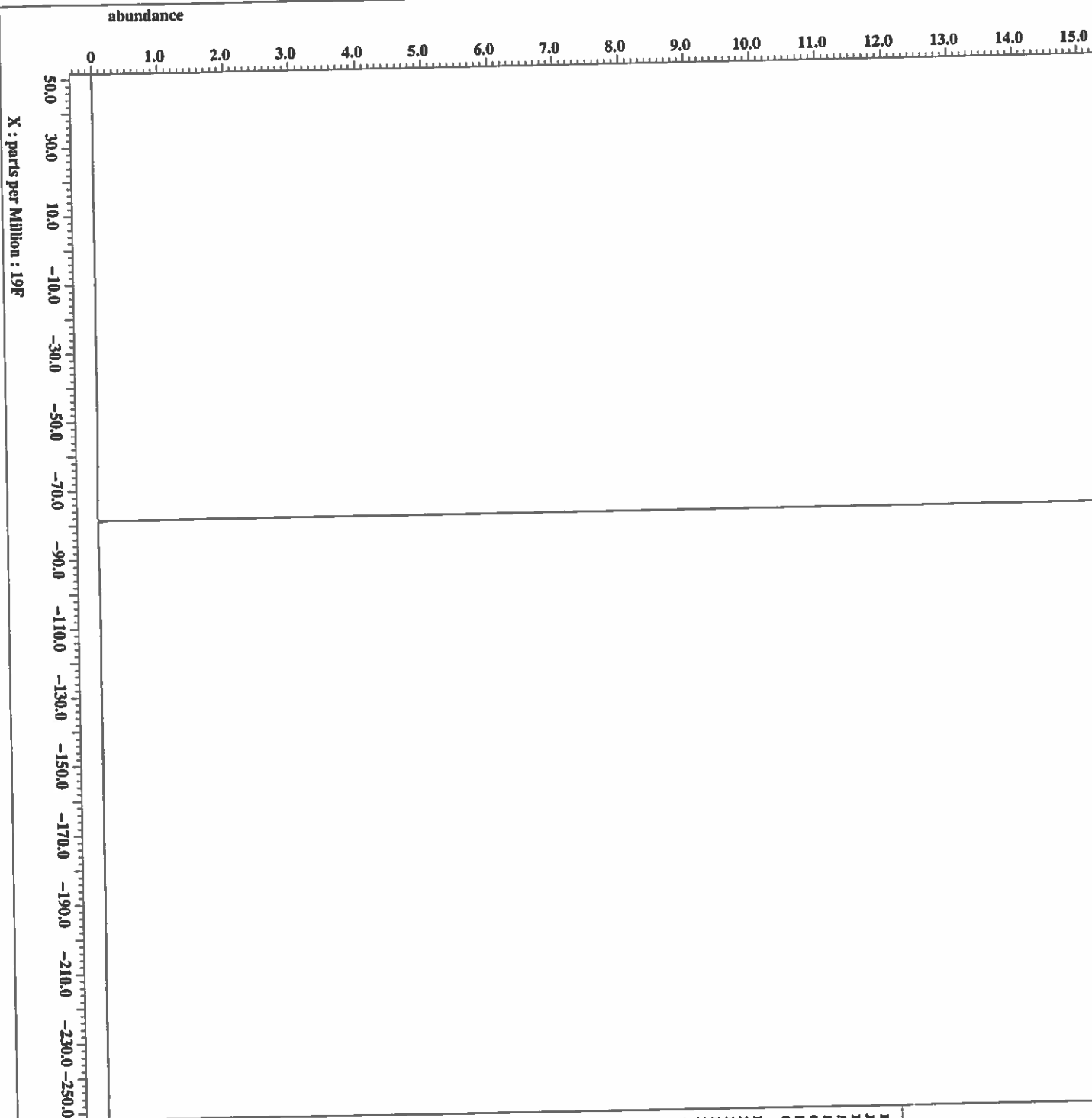
Filename MS0630-200-24h_PHOSPH
Author Jim Davis
Experiment single_pulse_dec
Sample_id MS0630-200-24h
Solvent CHLOROFORM-D
Creation_time 14-DEC-2018 14:29:22
Revision_time 14-DEC-2018 14:03:21
Current_time 14-DEC-2018 14:03:21

Data_format 1D COMPLEX
Dir_size 52428
Dir_title 31P
Dir_units (ppm)
Dimensions X
Site ECA 500
Spectrometer JNM-ECA500

Field_strength 11.7673579 [T] (500 MHz)
Acq_duration 0.85983232 [s]
X_domain 31P
X_freq 202.46831075 [MHz]
X_offset 0 [ppm]
X_points 65536
X_prescans 4
X_resolution 2.16301746 [Hz]
X_sweep 76.2195122 [Hz]
X_domain 18
X_freq 500.15991521 [MHz]
X_offset 5.0 [ppm]
Clipped FALSE
Mod_return 1
Scans 60
Total_scans 60

X_90_width 14.687 [us]
X_acq_time 0.85983232 [s]
X_angle 30 [deg]
X_atn 5 [dB]
X_pulse 4.89566667 [us]
Irr_atn_dec 20.7 [dB]
Irr_atn_pwr 20.7 [dB]
WALTZ TRUE
Decoupling 1 [s]
Initial_wait TRUE
Hoe_time 2 [s]
Recvr_gain 54
Relaxation_delay 2 [s]
Repetition_time 2.85983232 [s]
Temp_get 20.2 [C]





SOUTH ALABAMA
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```

File Name      = MS0630-200-24h_FLUORINE
Author         = Jim Devils
Experiment     = single_pulse.ex2
Sample ID     = MS0630-200-24h
Solvent       = CHLOROFORM-D
Creation Time  = 14-DEC-2018 14:36:28
Revision Time  = 14-DEC-2018 14:10:27
Current Time   = 14-DEC-2018 14:10:27

Data Format
Dim Size      = 1D COMPLEX
Dim 1 Size    = 104857
Dim 1 Title   = 19F
Dim 2 Size    = 19F
Dim 2 Title   = {ppm}
Dim Units     = X
Dimensions    = ECA 500
Site          = JNM-ECA500
Spectrometer

P1:pd.strength = 11.7473579[F] (500[MH
X:acq.duration = 0.7340032[s]
X:domain       = 19F
X:f1req        = 470.62046084[MHz]
X:offset       = -100[ppm]
X:points       = 131072
X:prescans     = 1
X:resolution   = 1.36239188[Hz]
X:sweep        = 178.57142857[Hz=1]
X:domain       = 19F
X:f2req        = 470.62046084[MHz]
X:offset       = 5[ppm]
X:f1domain     = 19F
X:f2domain     = 470.62046084[MHz]
X:f1freq       = 5[ppm]
X:f2freq       = 470.62046084[MHz]
X:f1offset     = FALSE
X:clipped      = 1
X:mod_return   = 1
X:scans        = 60
Total_scans    = 60

X:q1_width     = 13.1[us]
X:acq_time     = 0.7340032[s]
X:angle        = 45[deg]
X:atn         = 2.5[db]
X:pulse        = 6.55[us]
X:mode         = OFF
X:tri_mode     = OFF
X:irradiation  = PULSE
X:relaxation    = 70
X:relaxation_delay = 4[s]
X:relaxation_wait = 4.7340032[s]
X:repetition_time = 20.1[dc]
X:temp_get     = 20.1[dc]

```

3.0

2.0

1.0

abundance

0

11.0

10.0

9.0

8.0

7.0

6.0

5.0

4.0

3.0

2.0

1.0

0

201.88

75.85

7.68

7.7576
7.7508
7.6099
7.5103
7.3144
7.1667

5.7077

X : parts per Million : 1H



SOUTH ALABAMA
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```

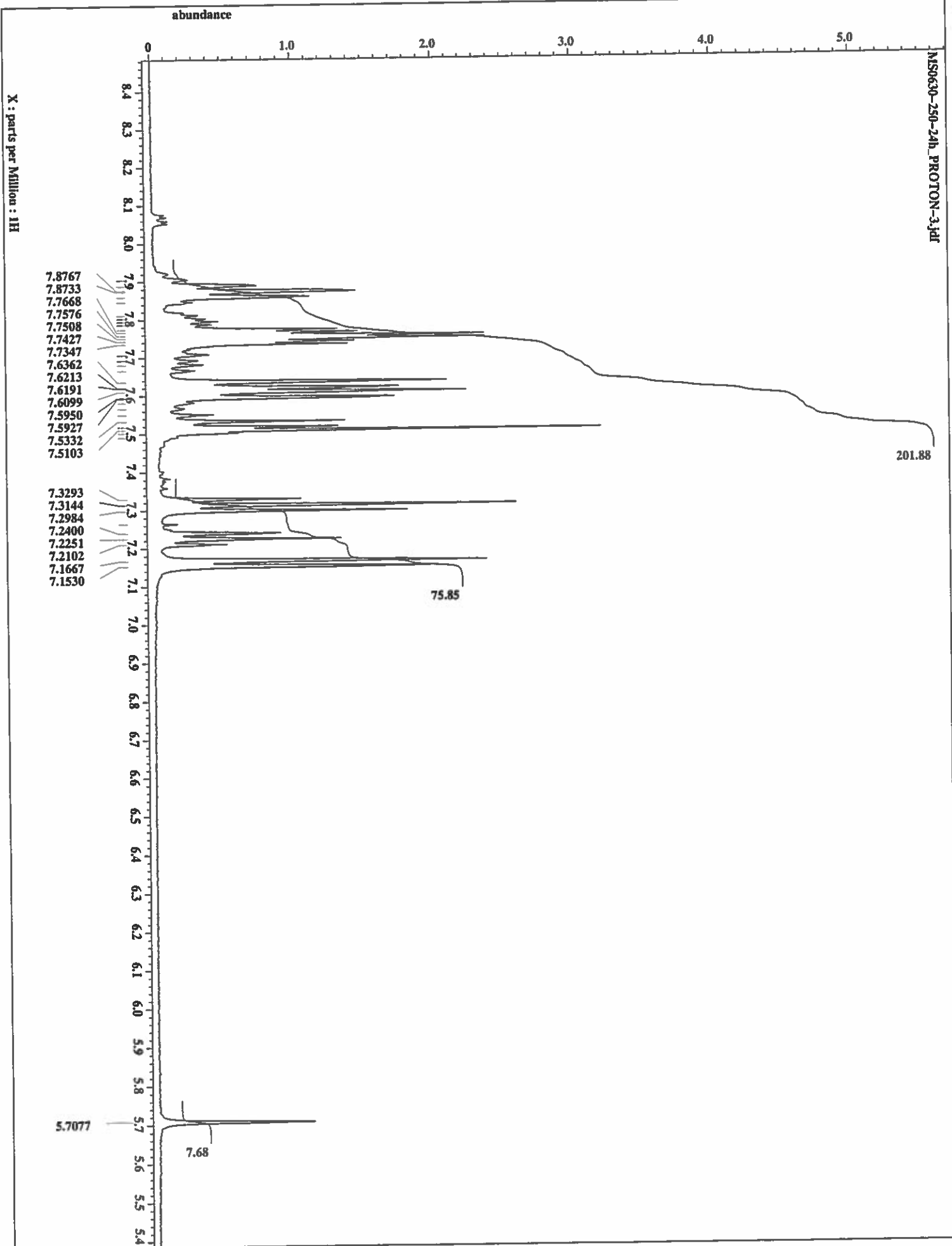
=====
File name      MS0630-250-24h_PROTON
Author         Jim Davis
Experiment     single_pulse.ex2
Sample_id      MS0630-250-24h
Solvent        CHLOROFORM-D
Creation_time  14-DEC-2018 14:51:58
Revision_time  14-DEC-2018 14:25:57
Current_time   14-DEC-2018 14:25:57

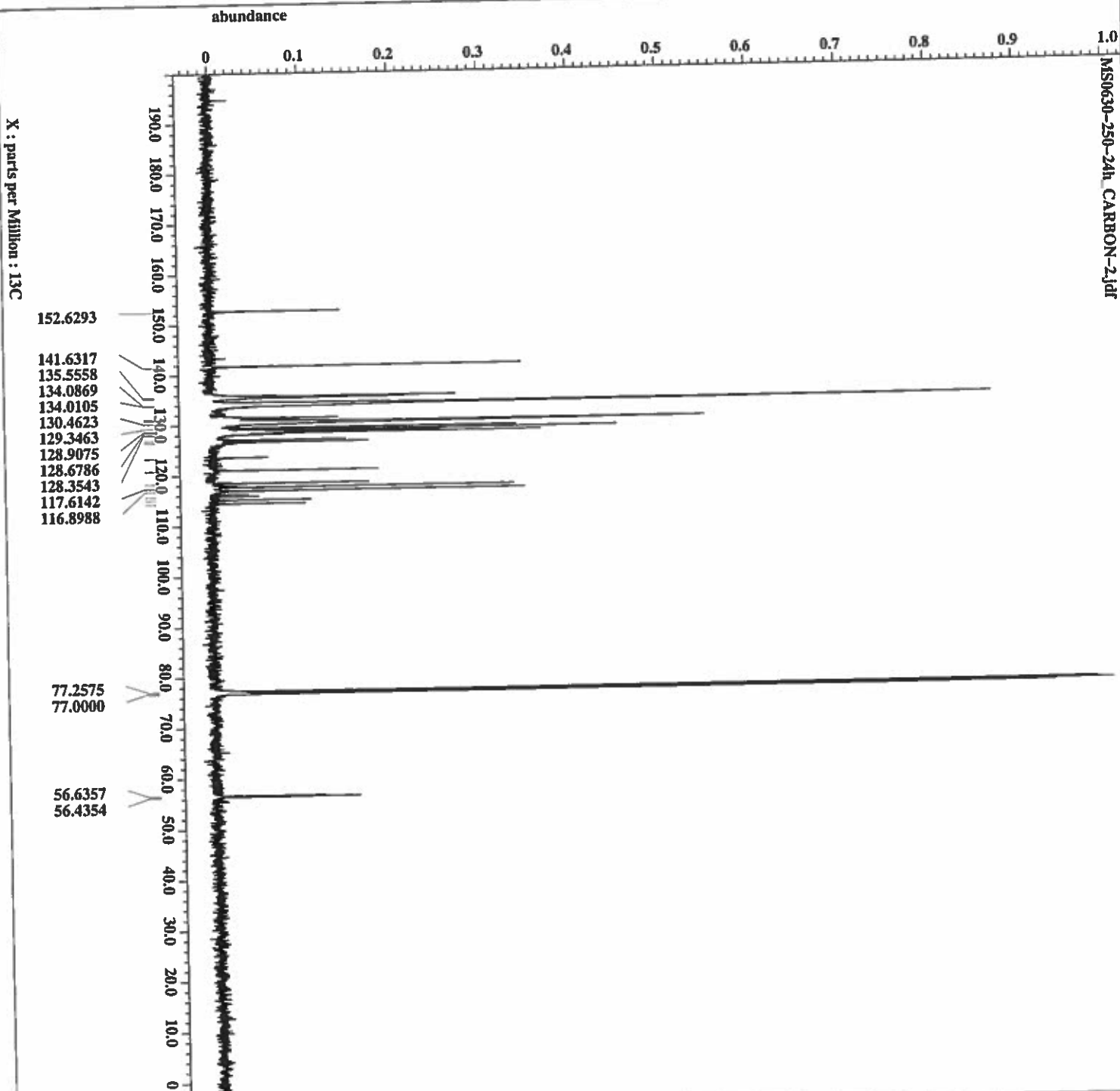
=====
Data format    1D COMPLEX
Dim_size       13107
Dim_title      1H
Dim_units      (ppm)
Dimensions     X
Site           ECA 500
Spectrometer   JNM-ECA500

=====
Field_strength 11.7473579 [T] (500 [MH
X_acq_duration 1.74587904 [s]
X_domain       1H
X_freq         500.15991521 [MHz]
X_offset       5.0 [ppm]
X_points       16384
X_prescans     1
X_resolution   0.57277737 [Hz]
X_sweep        9.38438438 [kHz]
Xr_domain      1H
Xr_freq        500.15991521 [MHz]
Xr_offset      5.0 [ppm]
Xr1_domain     1H
Xr1_freq       500.15991521 [MHz]
Xr1_offset     5.0 [ppm]
Clipped        FALSE
Mod_return     1
Scans          16
Total_scans    16

=====
X_90_width     12.4 [us]
X_acq_time     1.74587904 [s]
X_angle        45 [deg]
X_atn          4 [dB]
X_pulse        6.3 [us]
Xr1_mode       OF2
Xr1_offset     0 [Hz]
Dante_preset   FALSE
Initial_wait   1 [s]
Recvr_gain     62
Relaxation_delay 4 [s]
Repetition_time 5.74587904 [s]
Temp_get       20.1 [deg]
=====

```





```

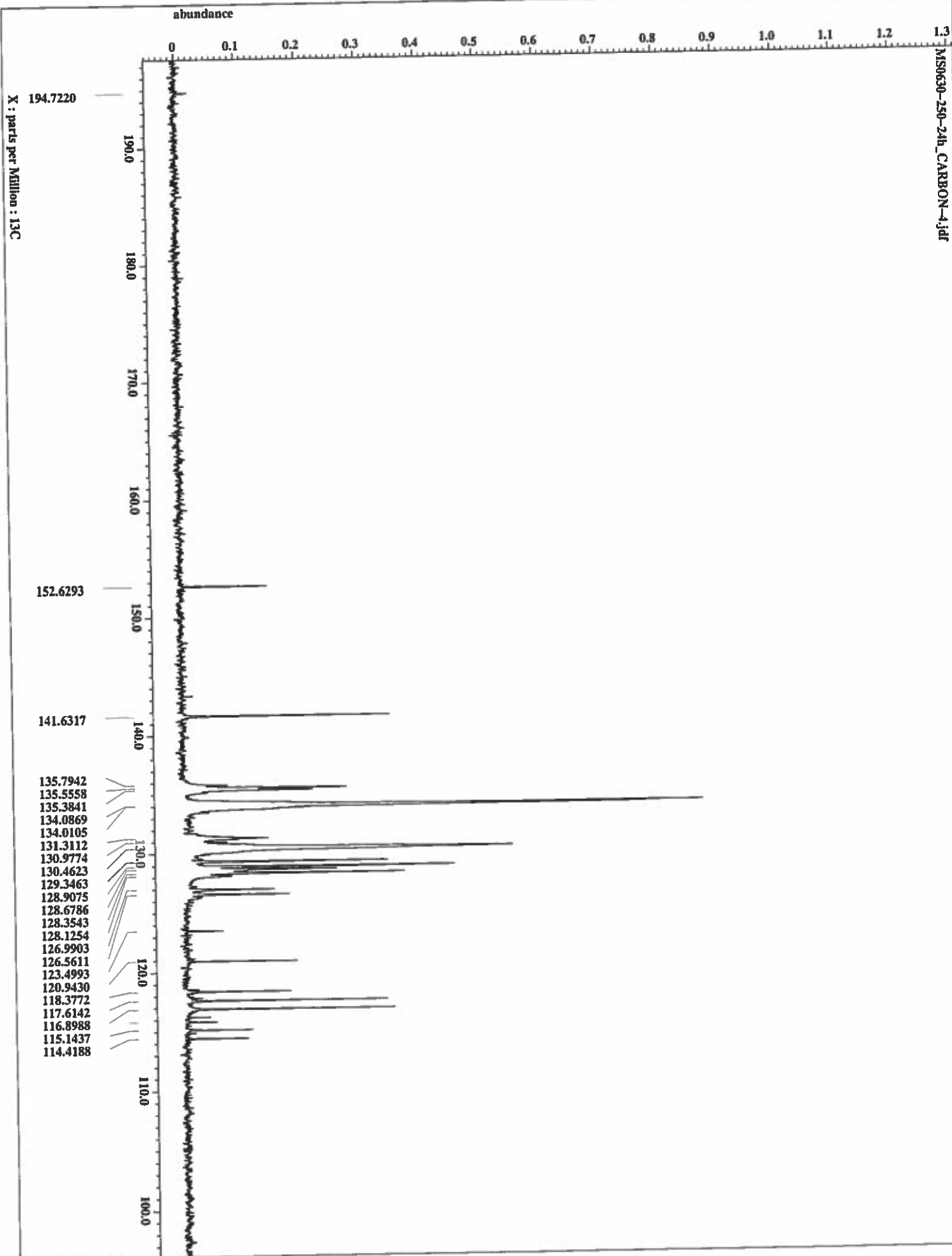
File Name      = MS0630-250-24h CARBON
Author         = Jim Davis
Experiment     = single_pulse_dec
Sample ID      = MS0630-250-24h
Solvent        = CHLOROFORM-D
Creation Time   = 14-DEC-2018 15:07:36
Revision Time  = 14-DEC-2018 14:41:35
Current Time    = 14-DEC-2018 14:41:35

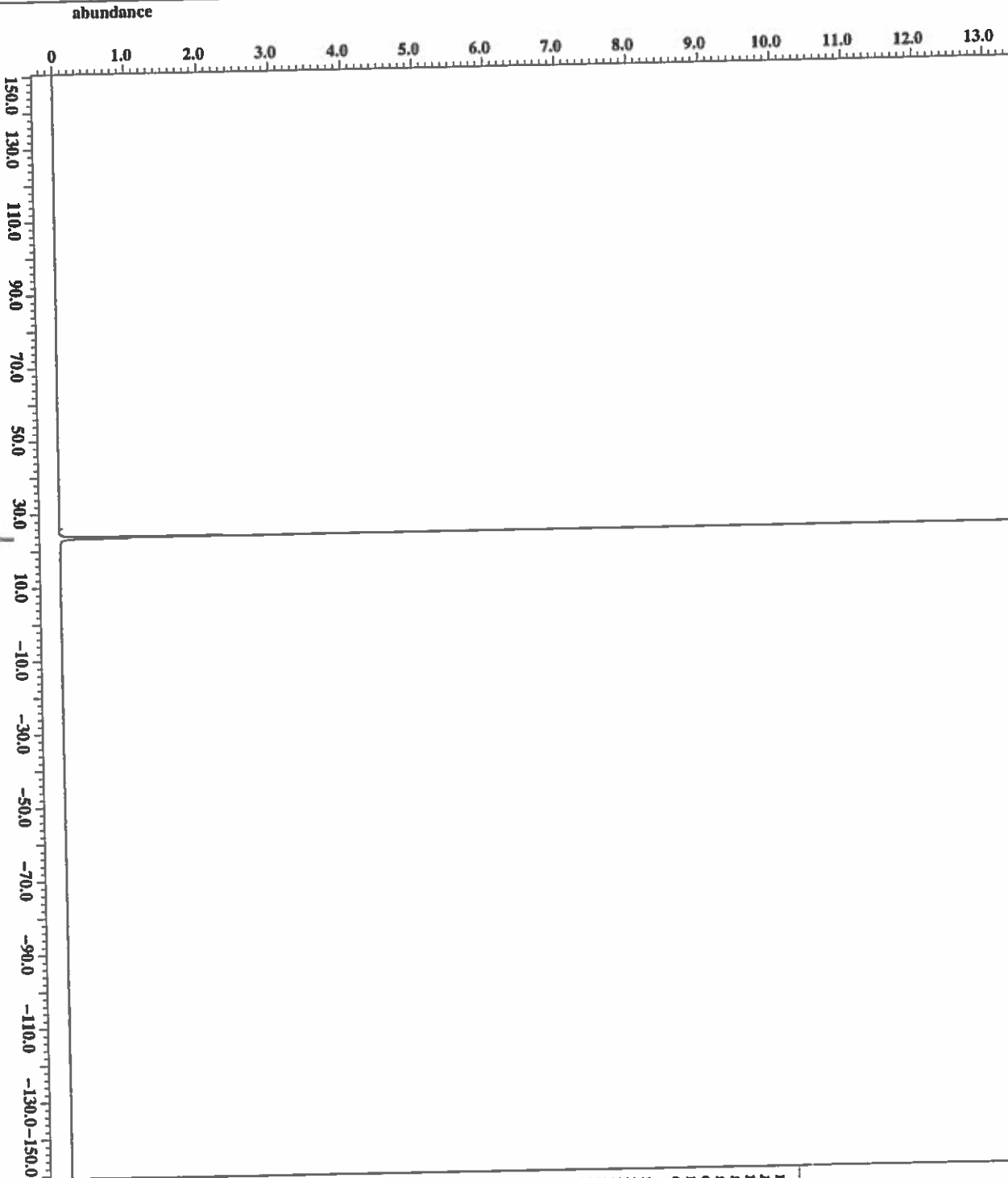
Data Format     = 1D COMPLEX
Dim Size       = 26214
Dim Title      = 13C
Dim Units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

Field Strength = 11.7473579 [T] (500 [MH
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        = 500.15891521 [MHz]
Irr Offset      = 5.0 [ppm]
Clipped         = FALSE
Mod Return      = 1
Scans           = 256
Total Scans     = 256

X 90 Width      = 13.2 [us]
X Acq Time      = 0.83361792 [s]
X Angle         = 30 [deg]
X Attn          = 6 [dB]
X Pulse         = 4.4 [us]
Irr Attn Dec    = 20.7 [dB]
Irr Attn Noe    = 20.7 [dB]
Irr Noise       = WALTZ
Decoupling      = TRUE
Initial Volt    = TRUE
Noe Time        = 2 [s]
Noe             = 60
Recvr Gain      = 21 [s]
Relaxation Delay = 2.83361792 [s]
Repetition Time = 20.2 [dc]
Temp Set        = 20.2 [dc]

```





SOUTH ALABAMA
JAGUARS

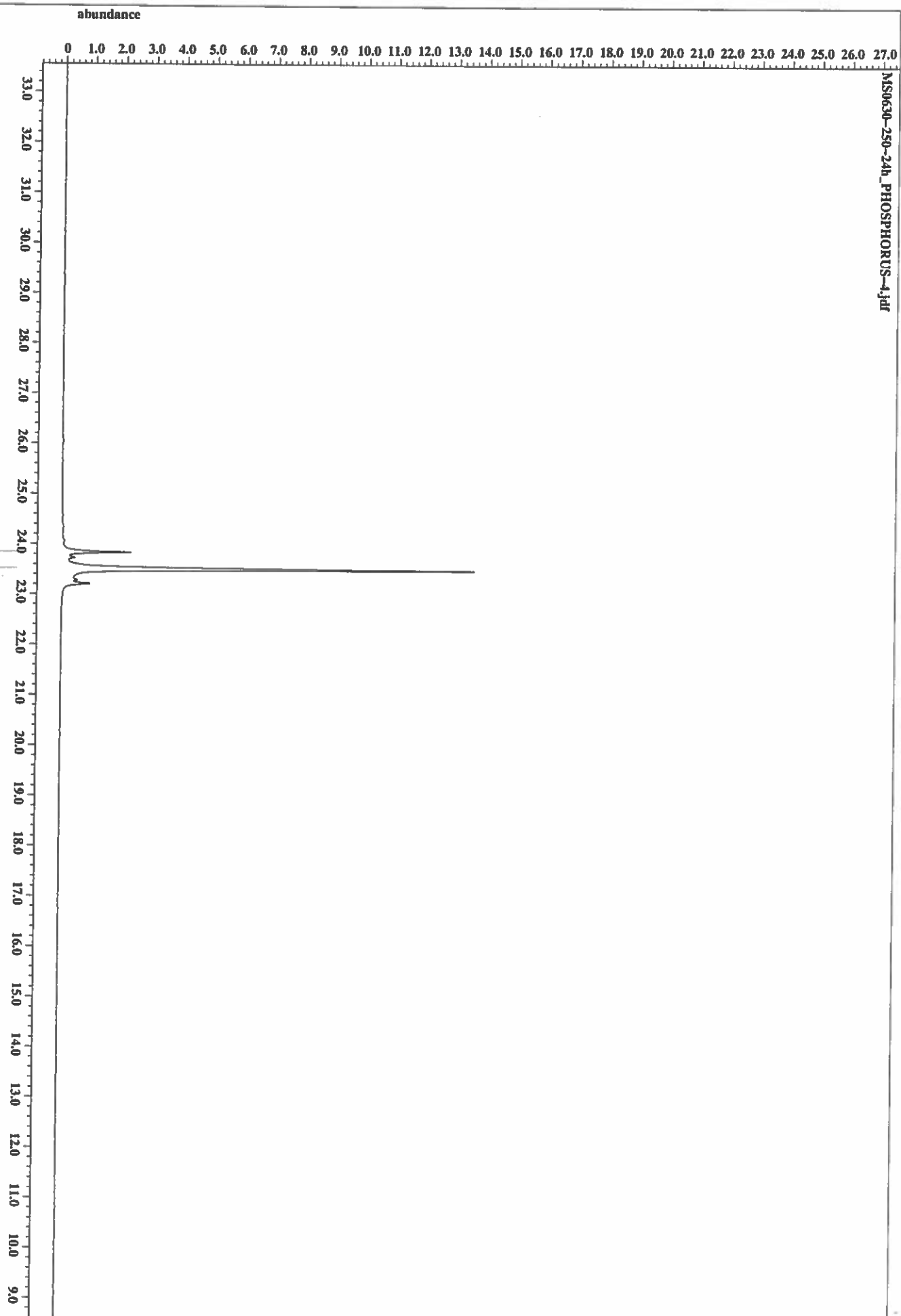
```

File Name      = MS0630-250-24h_PHOSPH
Author         = Jim Davis
Experiment     = single_pulse_dec
Sample_1d     = MS0630-250-24h
Solvent       = CHLOROFORM-D
Creation_time  = 14-DEC-2018 15:12:45
Revision_time  = 14-DEC-2018 14:46:45
Current_time   = 14-DEC-2018 14:46:45

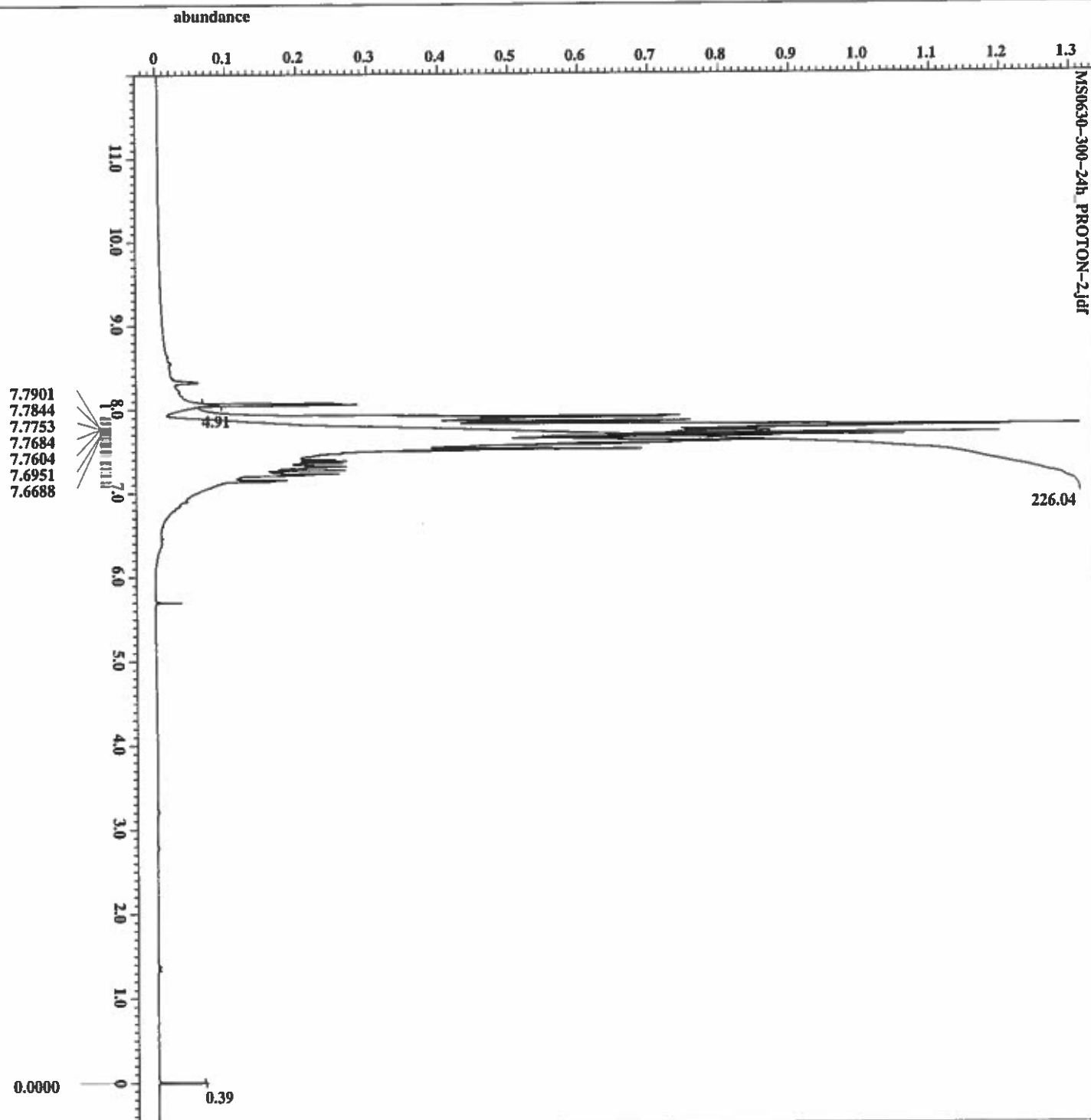
Data Format     = 1D COMPLEX
Dim Size       = 52428
Dim Title      = 31P
Dim Units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

Field Strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.85983232 [s]
X_domain       = 31P
X_freq         = 203.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 65536
X_prescans     = 4
X_resolution   = 1.16301746 [Hz]
X_sweep        = 76.2195122 [kHz]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 60
Total_scans    = 60

X_90_width     = 14.687 [us]
X_acq_time     = 0.85983232 [s]
X_angle        = 30 [deg]
X_pulse        = 5 [ds]
X_atn          = 4.8956667 [us]
Irr_atn_dec    = 20.7 [ds]
Irr_atn_noe    = 20.7 [ds]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Recvr_gain     = 54
Relaxation_delay = 2 [s]
Repetition_time = 2.85983232 [s]
Temp_get       = 20.3 [dc]
  
```



X : parts per Million : 31P



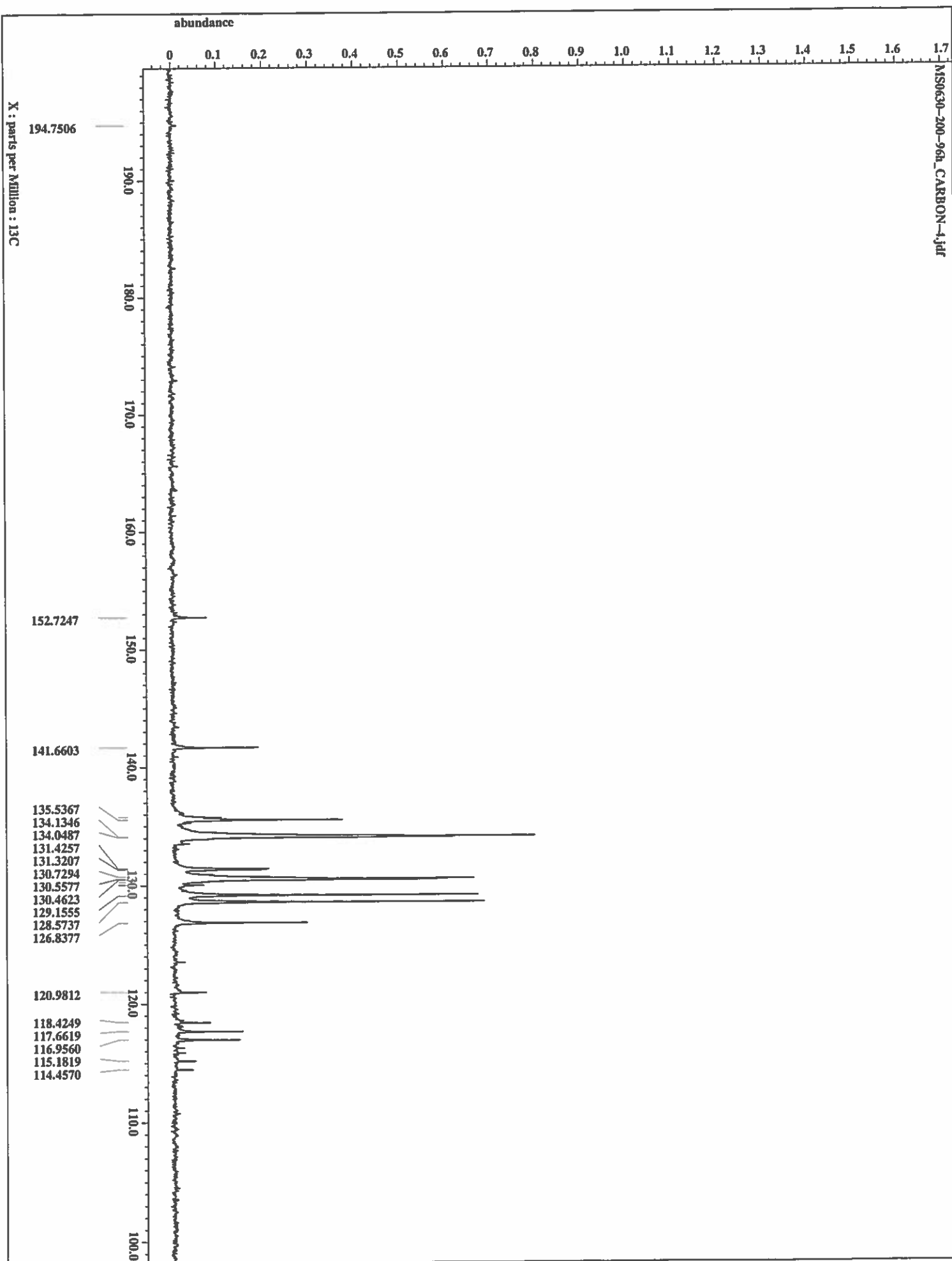
```

Filename      MS0630-300-24h_PROTON
Author        jim Davis
Experiment    single_pulse.exe
Sample_id     MS0630-300-24h
Solvent       CHLOROFORM-D
Creation_time  14-DEC-2018 15:25:13
Revision_time 14-DEC-2018 14:59:11
Current_time   14-DEC-2018 14:59:11

Data_format   2D COMPLEX
Dim_size      13107
Dim_c1c1e     1H
Dim_units     [ppm]
Dimensions    X
Site          ECA 500
Spectrometer  JNM-ZCA500

Field_strength 11.7473579 [T] (500 [MH
X_acq_duration 1.74587904 [s]
X_domain       1H
X_freq         500.15991521 [MHz]
X_offset       5.0 [ppm]
X_points       16384
X_prescans     1
X_resolution   0.57277737 [Hz]
X_sweep        9.38438438 [kHz]
Xr_domain      1H
Xr_freq        500.15991521 [MHz]
Xr_offset      5.0 [ppm]
Xr1_domain     1H
Xr1_freq       500.15991521 [MHz]
Xr1_offset     5.0 [ppm]
Clipped        FALSE
Mod_return     1
Scans          16
Total_scans    16
X_90_width     12.4 [us]
X_acq_time     1.74587904 [s]
X_angle        45 [deg]
X_atn          4 [dB]
X_pulse        6.2 [us]
Xr1_mode       OET
Xr1_offset     0.5 [ppm]
Pulse          OET
Pulse2         FALSE
Initial_wait   1 [s]
Recvr_gain     30
Relaxation_delay 4 [s]
Repetition_time 5.74587904 [s]
Temp_get       20.2 [dc]
  
```





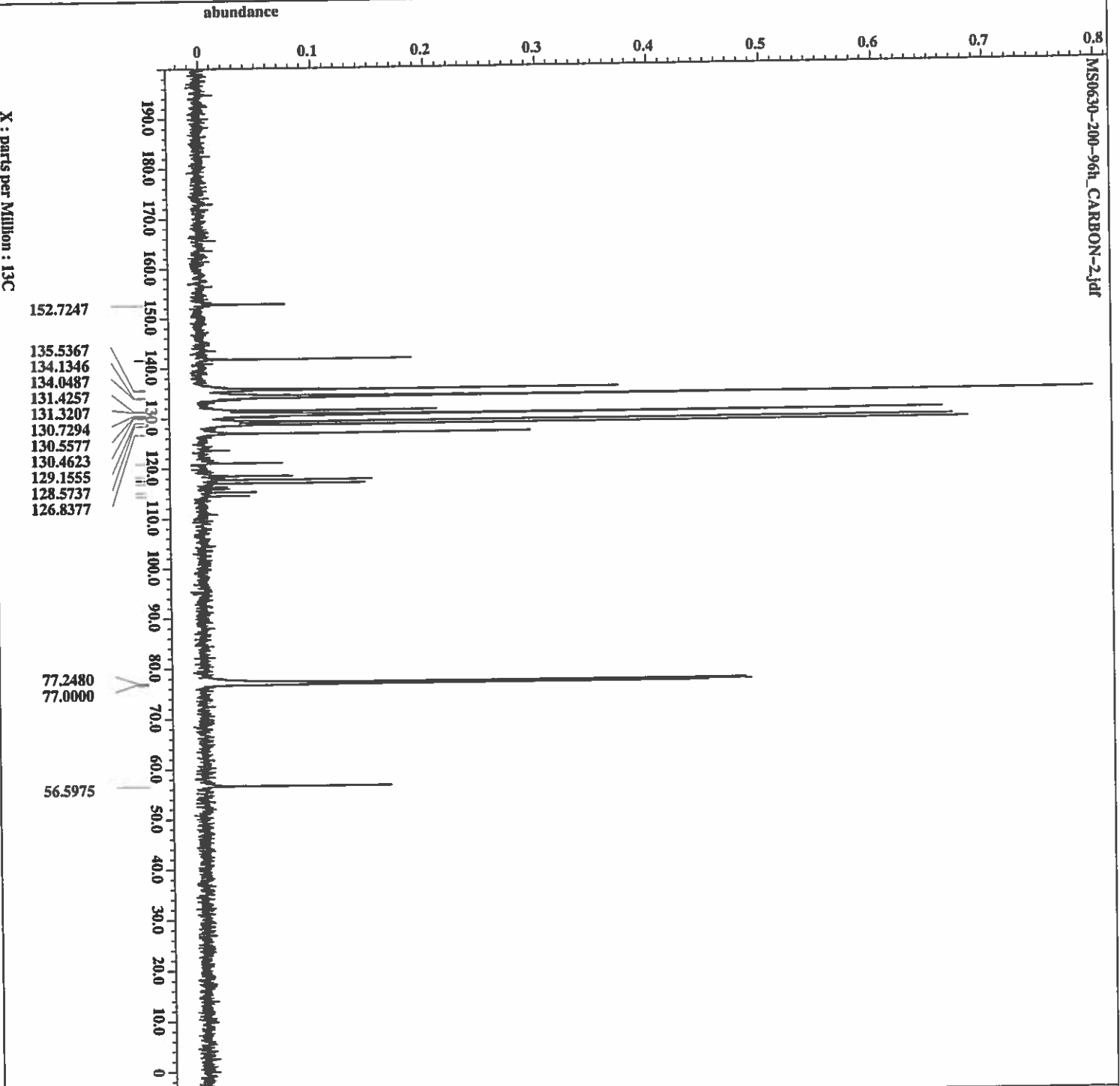


Filename = MS0630-200-96h_CARBON
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = MS0630-200-96h
Solvent = CHLOROFORM-D
Creation_time = 18-DEC-2018 09:34:34
Revision_time = 18-DEC-2018 09:08:15
Current_time = 18-DEC-2018 09:08:15

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

Field_strength = 11.747379 [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]
Xt_domain = 1H
Xt_freq = 500.15891521 [MHz]
Xt_offset = 5.0 [ppm]
Mod_return = FALSE
Scans = 1
Total_scans = 300

X_90_width = 13.2 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 6 [dB]
X_pulse = 4.4 [us]
Xt_atn_dec = 20.7 [dB]
Xt_atn_noe = 20.7 [dB]
Decoupling = WALTZ
Initial_wait = TRUE
Nuc = 13C
Nuc_time = 2 [s]
Nuc_recv_gain = 20 [dB]
Relaxation_delay = 2.83361792 [s]
Repetition_time = 20 [dc]
Temp_get



abundance

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3 2.4 2.5

9.4 9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 5.9 5.8 5.7 5.6 5.5 5.4 5.3 5.2 5.1 5.0 4.9

8.0600
8.0496
8.0439
7.8710
7.7645
7.7565
7.7485
7.7416
7.7324
7.6225
7.6076
7.5962
7.5813
7.4965

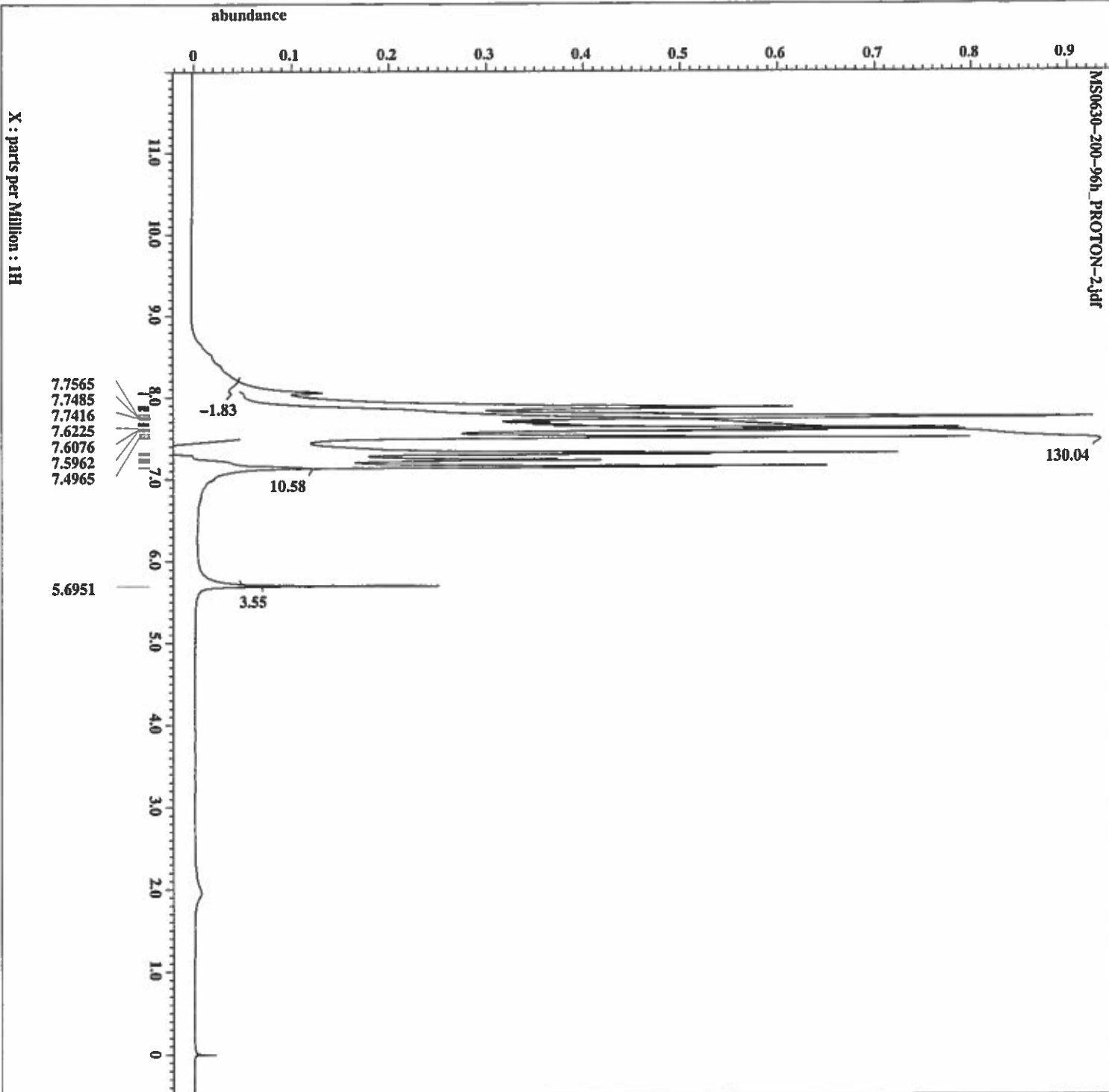
7.3247
7.3099
7.2950
7.2251
7.1518
7.1381

13.82

0.25

5.6951

X : parts per Million : 1H



```

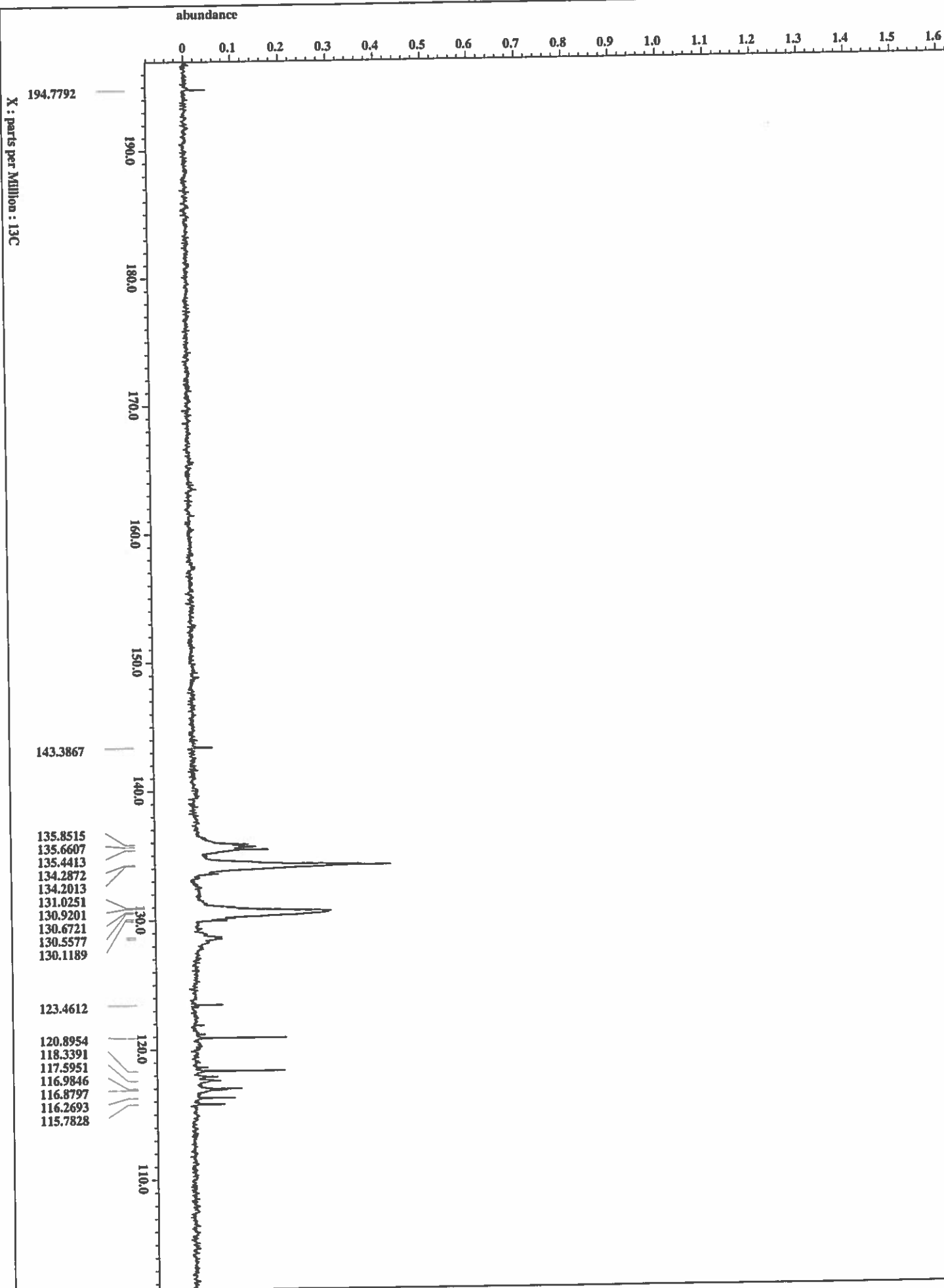
File: MS0630-200-96h_PROTON
Author: Jim Davis
Experiment: single_pulse.exe2
Sample_ID: MS0630-200-96h
Solvent: CHLOROFORM-D
Creation_time: 18-DEC-2018 09:17:38
Revision_time: 18-DEC-2018 08:51:20
Current_time: 18-DEC-2018 08:51:20

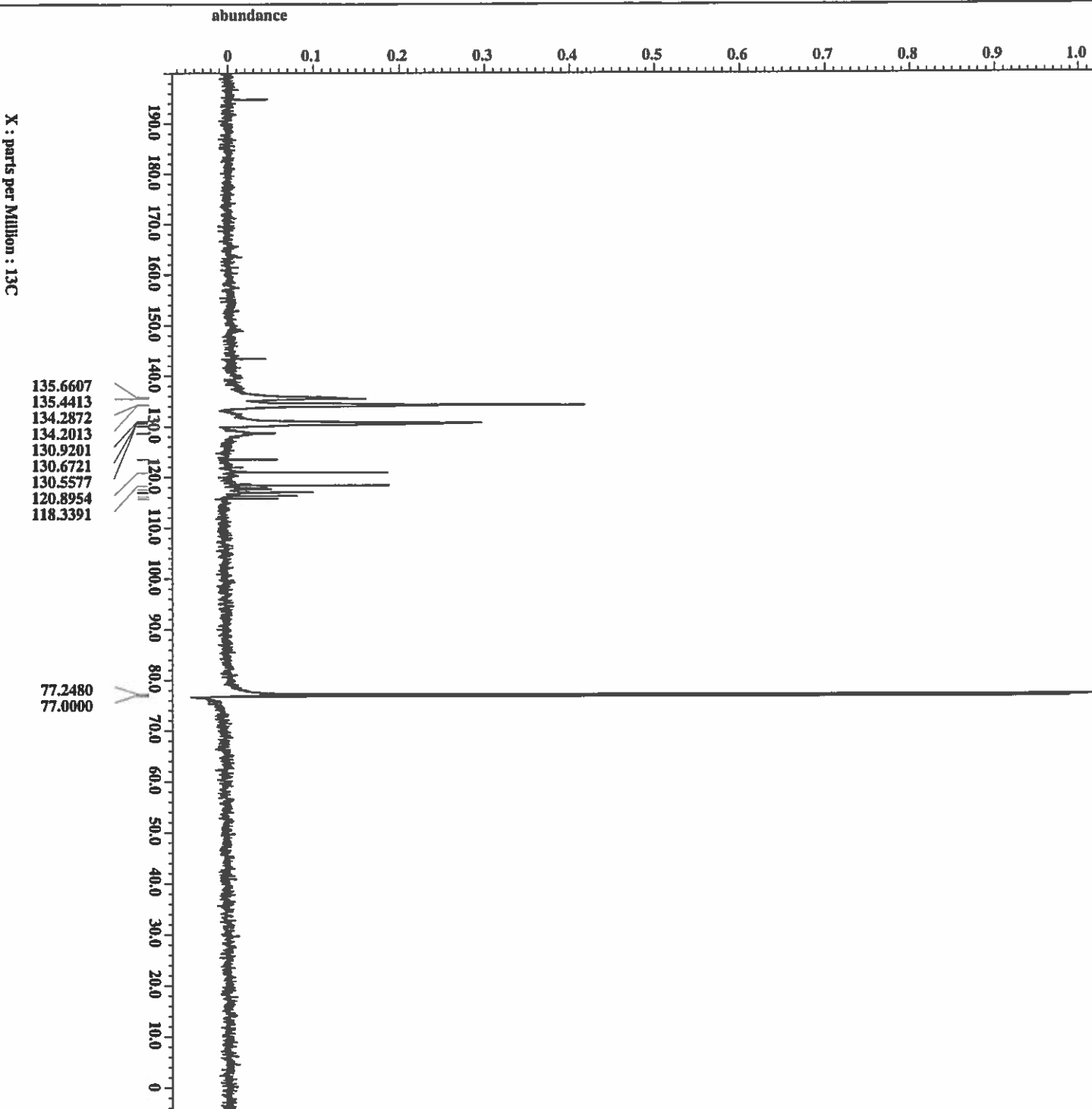
Data_format: 1D COMPLEX
Dir_size: 13107
Dir_title: 1H
Dir_units: [ppm]
Dimensions: X
Site: ECA 500
Spectrometer: JNM-ECA500

P1: 11.7473579 [s] (500 MHz)
X_acq_duration: 1.74587904 [s]
X_domain: 1H
X_freq: 500.15991521 [MHz]
X_offset: 5.0 [ppm]
X_points: 16384
X_prescans: 1
X_resolution: 0.57277737 [Hz]
X_sweep: 9.38438438 [kHz]
1H_domain: 1H
1H_freq: 500.15991521 [MHz]
1H_offset: 5.0 [ppm]
1H_domain: 1H
1H_freq: 500.15991521 [MHz]
1H_offset: 5.0 [ppm]
Mod_return: FALSTZ
Total_scans: 16

X_90_width: 12.4 [us]
X_acq_time: 1.74587904 [s]
X_angle: 45 [deg]
X_acn: 4 [dB]
X_pulse: 6.2 [us]
1H_mode: OF2
1H_mode: FALSTZ
Dance_preset: 1 [s]
Initial_wait: 32
Recvr_gain: 4 [s]
Relaxation_delay: 5.74587904 [s]
Repetition_time: 19.3 [s]
Temp_get: 19.3 [C]

```





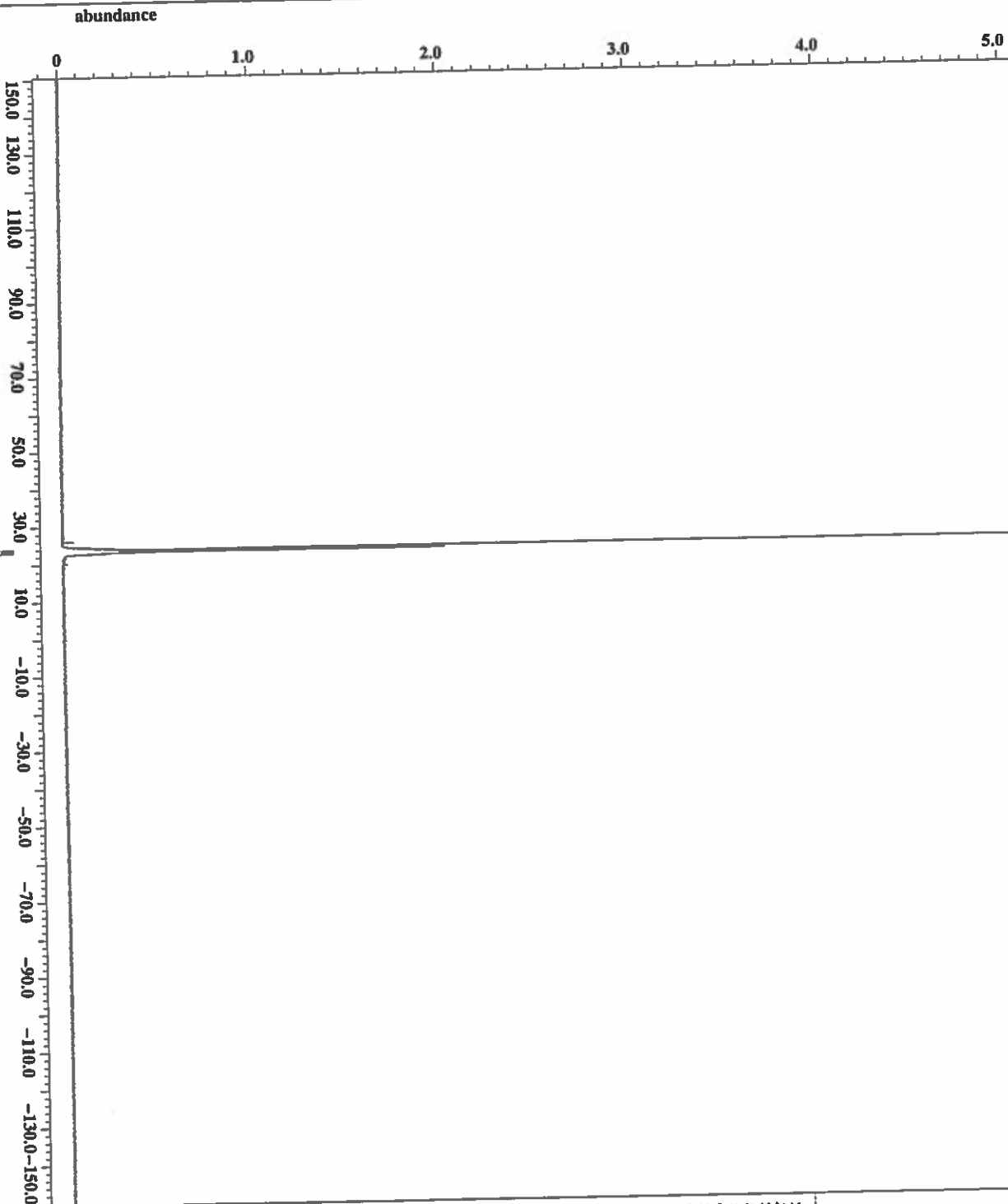
```

File Name      = MS0630-300-24h_CARBON
Author         = Jim Davis
Experiment     = 8single_pulse_dec
Sample_id      = MS0630-300-24h
Solvent        = CHLOROFORM-D
Creation_time   = 14-DEC-2018 15:39:46
Revision_time  = 14-DEC-2018 15:13:45
Current_time   = 14-DEC-2018 15:13:45

Data Format
Dim_size       = 1D COMPLEX
Dim_size       = 26214
Dim_c1         = 13C
Dim_c2         = 13C
Dim_units      = [ppm]
Dimensions     = X
Sca           = FCA 500
Site           = DNM-ECA500
Spectrometer   =

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     = 3.0 [ppm]
Mod_return     = FALST
Scans          = 1
Total_scans    = 256

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_noe    = 20.7 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUZ
Initial_wait   = 1 [s]
Noe            = TRUZ
Noe_time       = 2 [s]
Recr_gain      = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 20.3 [C]
  
```



X : parts per Million : 31P



```

=====
File: MS0630-300-24h_PHOSPH
Author: Jim Davis
Experiment: single_pulse_dec
Sample ID: MS0630-300-24h
Solvent: CHLOROFORM-D
Creation time: 14-DEC-2018 15:32:03
Revision time: 14-DEC-2018 14:56:01
Current time: 14-DEC-2018 14:56:01

=====
Data format: 1D COMPLEX
Dim size: 52428
Dim title: 31P
Dim units: [ppm]
Dimensions: X
Spectrum: ECA 500
Spectrometer: JNM-ECA500

=====
Field strength: 11.7473579 [T] (500 [MH
X_acq_duration: 0.8598332 [s]
X_domain: 31P
X_freq: 202.46831075 [MHz]
X_offset: 0 [ppm]
X_points: 65536
X_prescans: 4
X_resolution: 1.16301746 [Hz]
X_sweep: 76.2195122 [kHz]
Xr_domain: 1H
Xr_freq: 500.15991521 [MHz]
Xr_offset: 5.0 [ppm]
Clipped: FALSE
Mod_return: 1
Scans: 60
Total_scans: 60

=====
X_90_width: 14.687 [us]
X_acq_time: 0.8598332 [s]
X_angle: 30 [deg]
X_atn: 5 [dB]
X_pulse: 4.8956667 [us]
Xr_atn_dec: 20.7 [dB]
Xr_atn_noe: 20.7 [dB]
Xr_noise: WALTZ
Decoupling: TRUE
Initial_volt: 1 [s]
Noe_time: 2 [s]
Noe_gain: 54
Relaxation_delay: 2 [s]
Repetition_time: 2.8598332 [s]
Temp_get: 20.4 [C]
=====

```

abundance

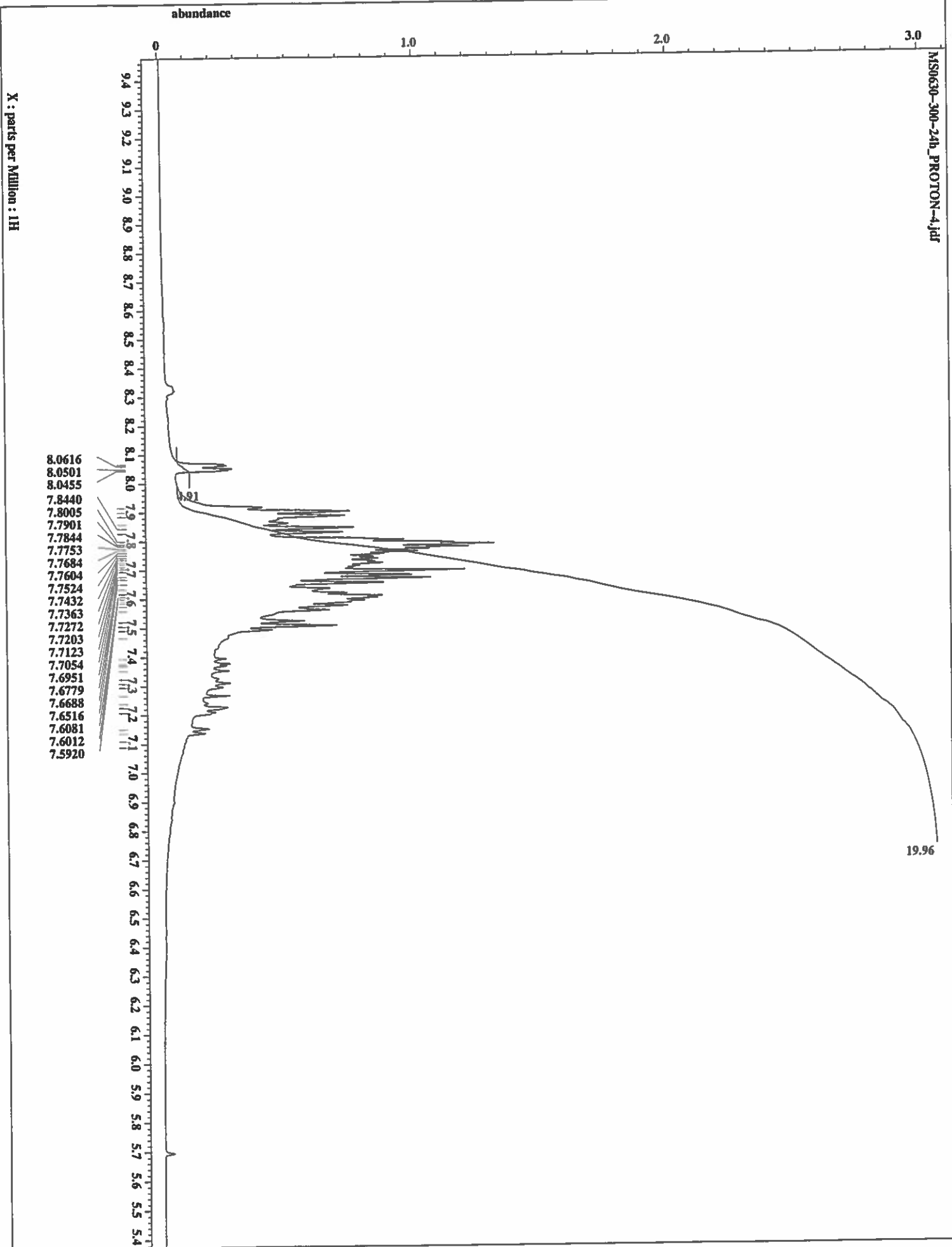
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0

40.0 39.0 38.0 37.0 36.0 35.0 34.0 33.0 32.0 31.0 30.0 29.0 28.0 27.0 26.0 25.0 24.0 23.0 22.0 21.0 20.0 19.0 18.0 17.0 16.0 15.0 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

23.8442
23.2065

X : parts per Million : 31P







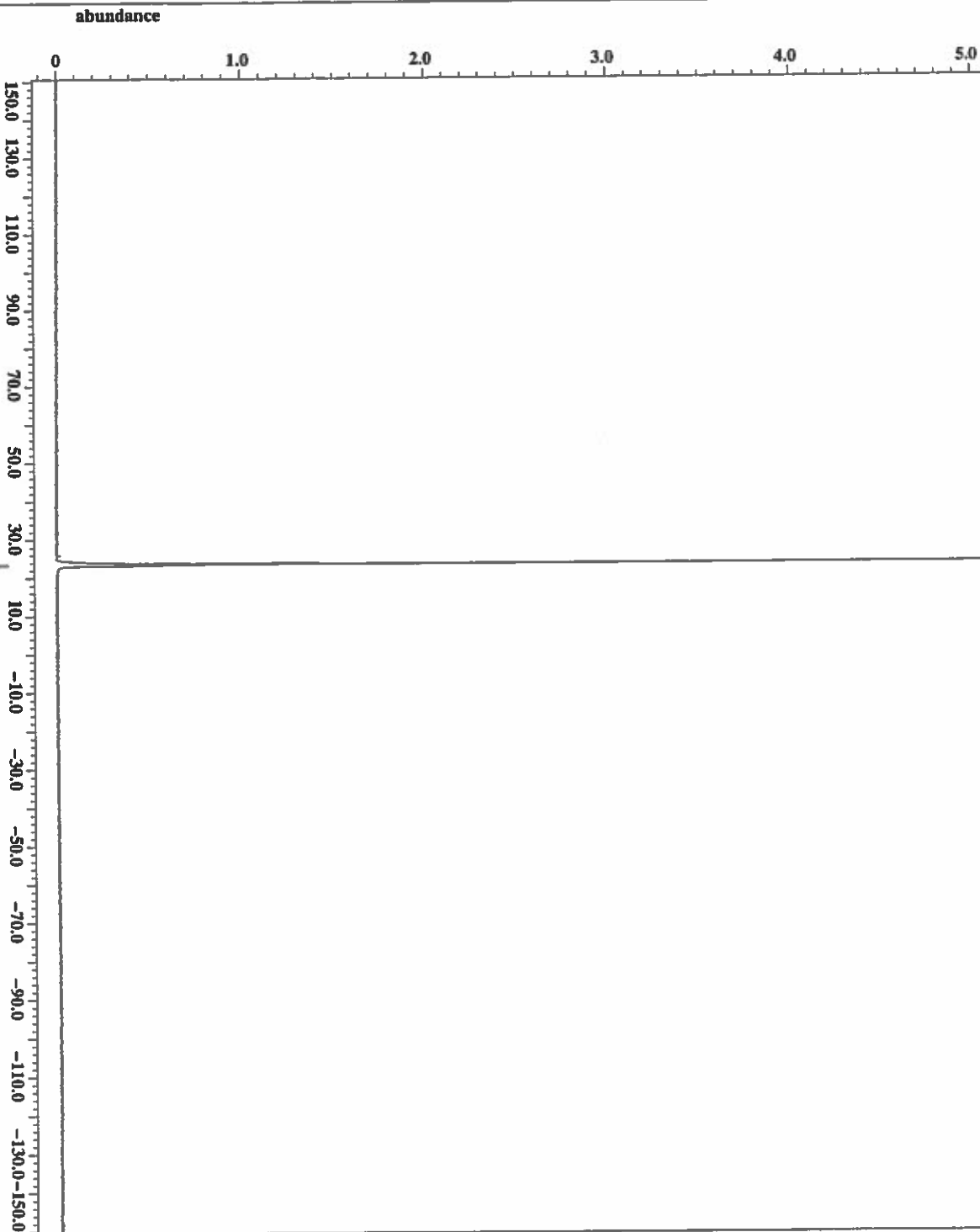
SOUTH ALABAMA
JAGUARS

Filename = MS0630-200-96h_PHOSPH
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = MS0630-200-96h
 Solvent = CHLOROFORM-D
 Creation_time = 18-DEC-2018 09:40:42
 Revision_time = 18-DEC-2018 09:14:24
 Current_time = 18-DEC-2018 09:14:24

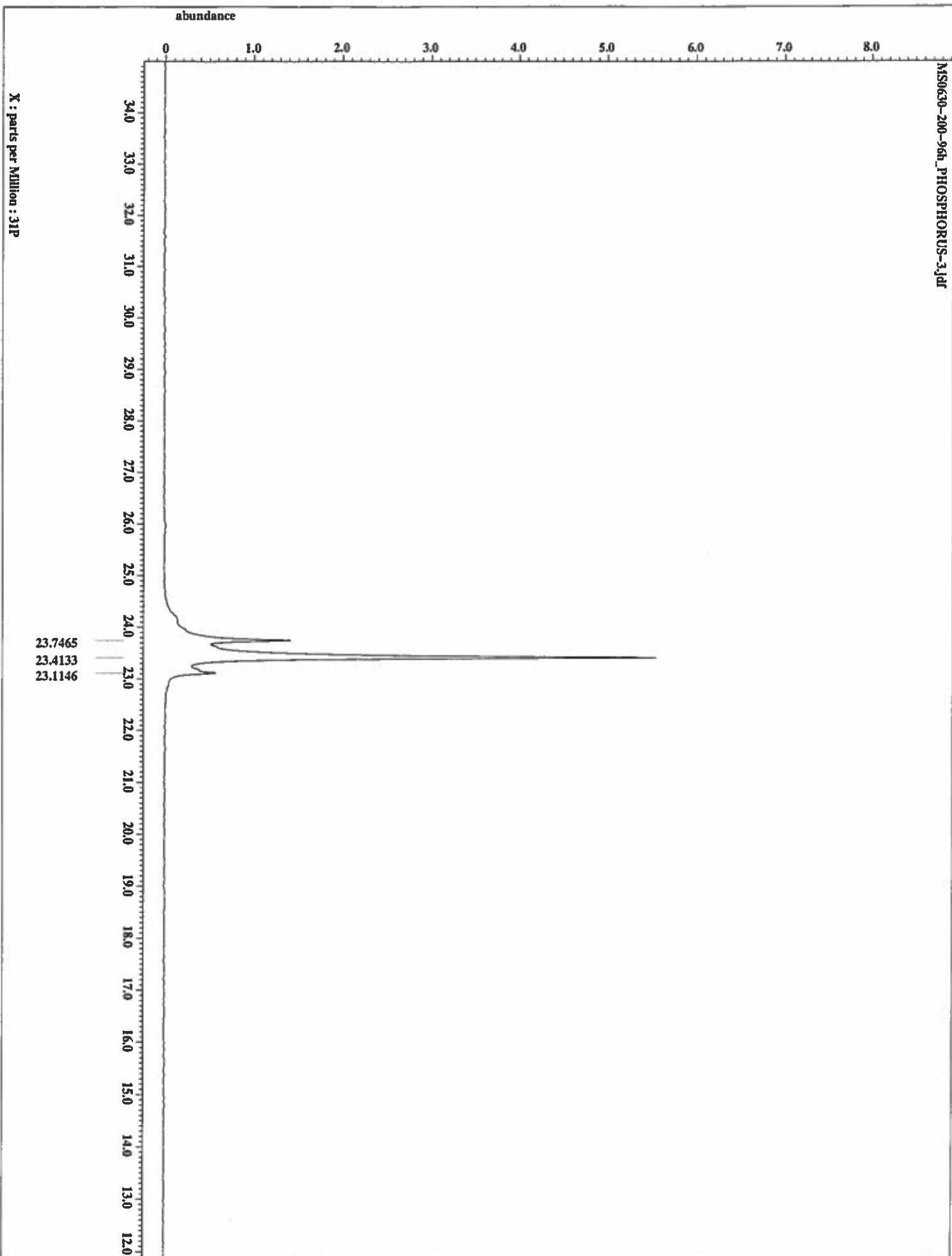
Data format = 1D COMPLEX
 Dim_size = 52428
 Dim_title = 31P
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [KH
 X_acq_duration = 0.85983232 [s]
 X_domain = 31P
 X_freq = 202.46831075 [MHz]
 X_offset = 0 [ppm]
 X_points = 65536
 X_prescans = 4
 X_resolution = 1.16301746 [Hz]
 X_sweep = 76.2195122 [kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 70
 Total_scans = 70

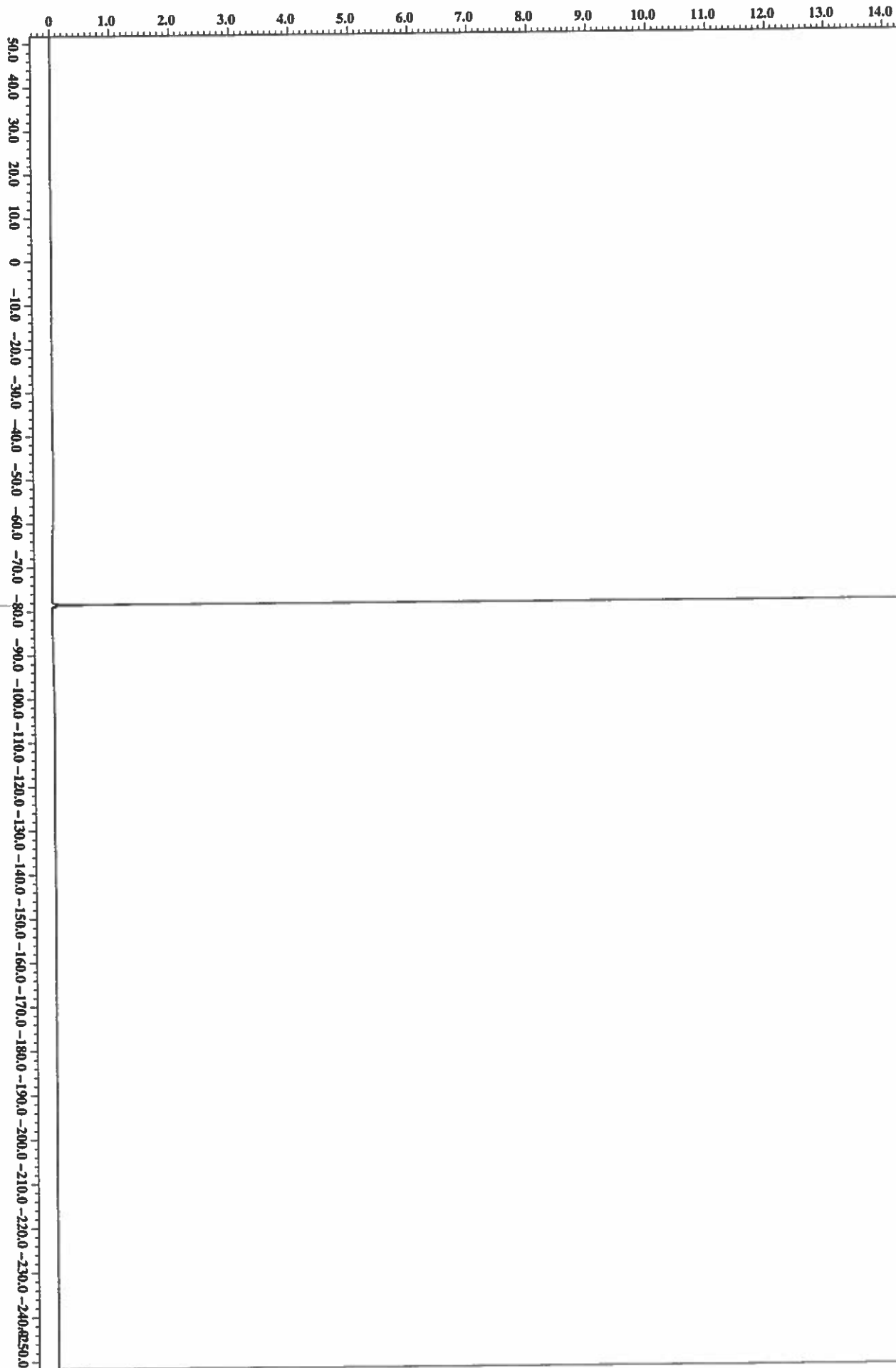
X_90_width = 14.687 [us]
 X_acq_time = 0.85983232 [s]
 X_angle = 30 [deg]
 X_atn = 5 [dB]
 X_pulse = 4.8956667 [us]
 Irr_atn_dec = 20.7 [dB]
 Irr_atn_poe = 20.7 [dB]
 Irr_noise = VALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Irruz = TRUE
 Hse_time = 2 [s]
 Recvr_gain = 54
 Relaxation_delay = 2 [s]
 Repetition_time = 2.85983232 [s]
 Temp_get = 19.8 [C]



X : parts per Million : 31P

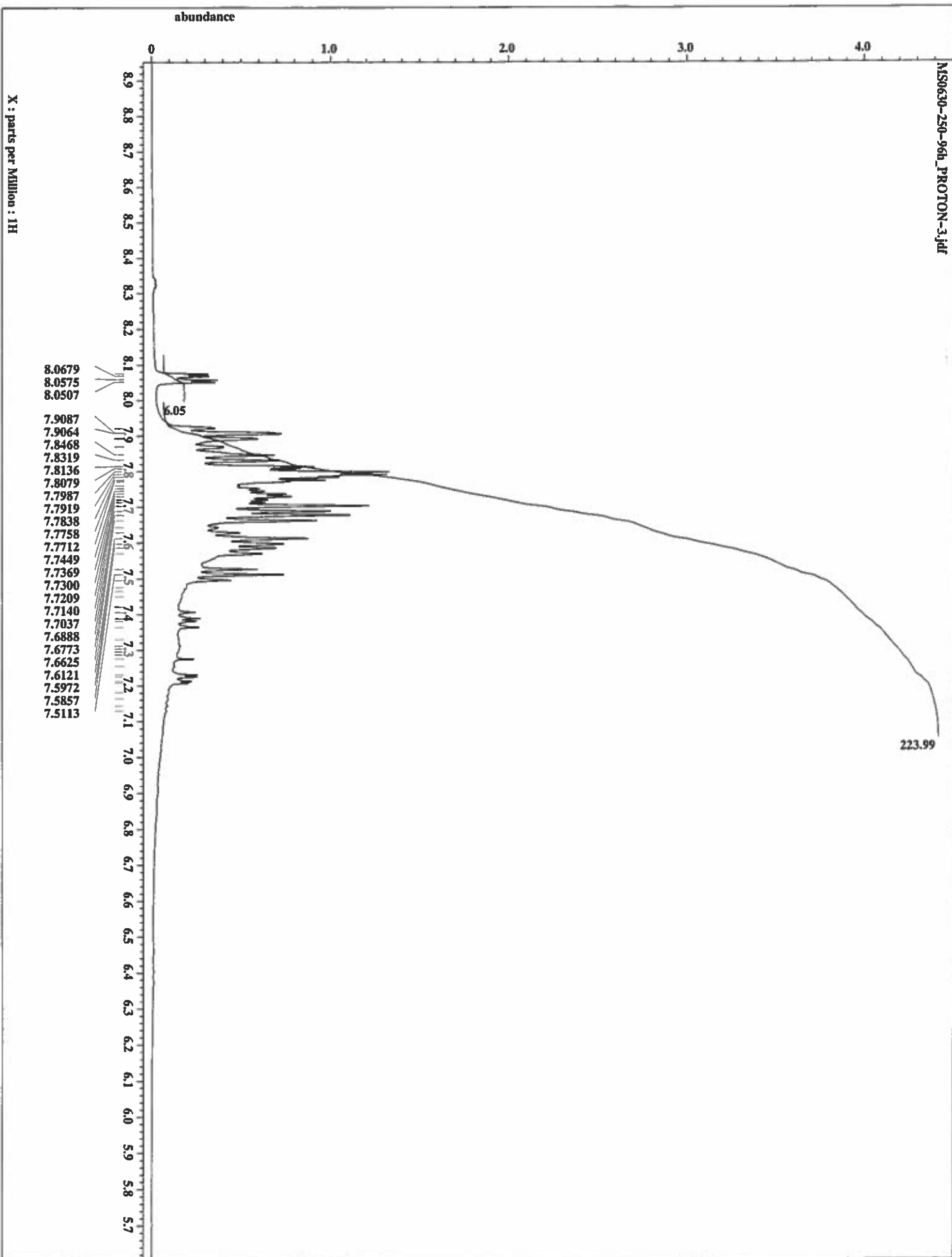


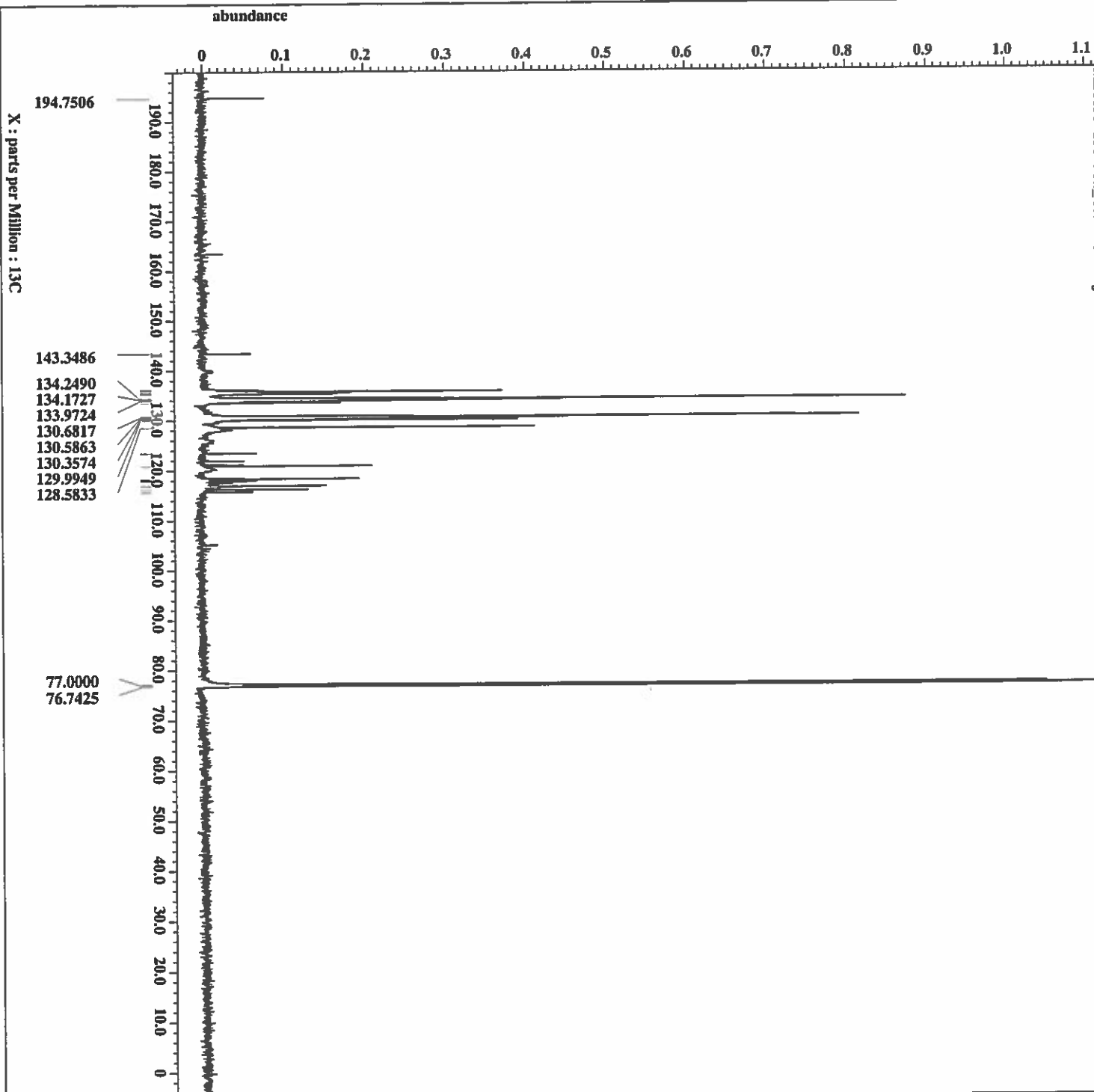
abundance



-78.5460

X : parts per Million : 19F





```

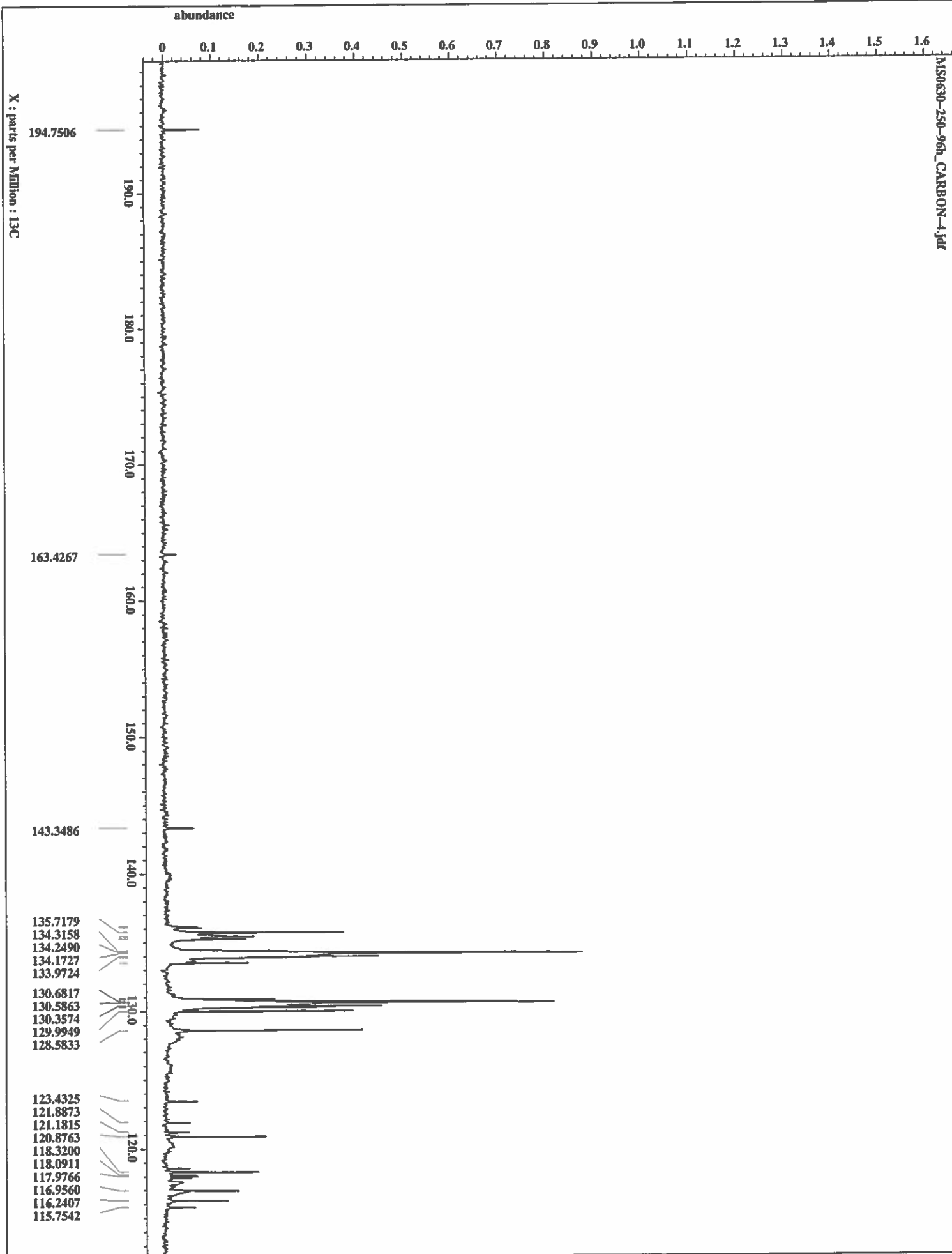
Filename      = MS0630-250-96h_CARBON
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0630-250-96h
Solvent       = CHLOROFORM-D
Creation_time = 18-DEC-2018 11:57:53
Revision_time = 18-DEC-2018 11:31:35
Current_time  = 18-DEC-2018 11:31:35

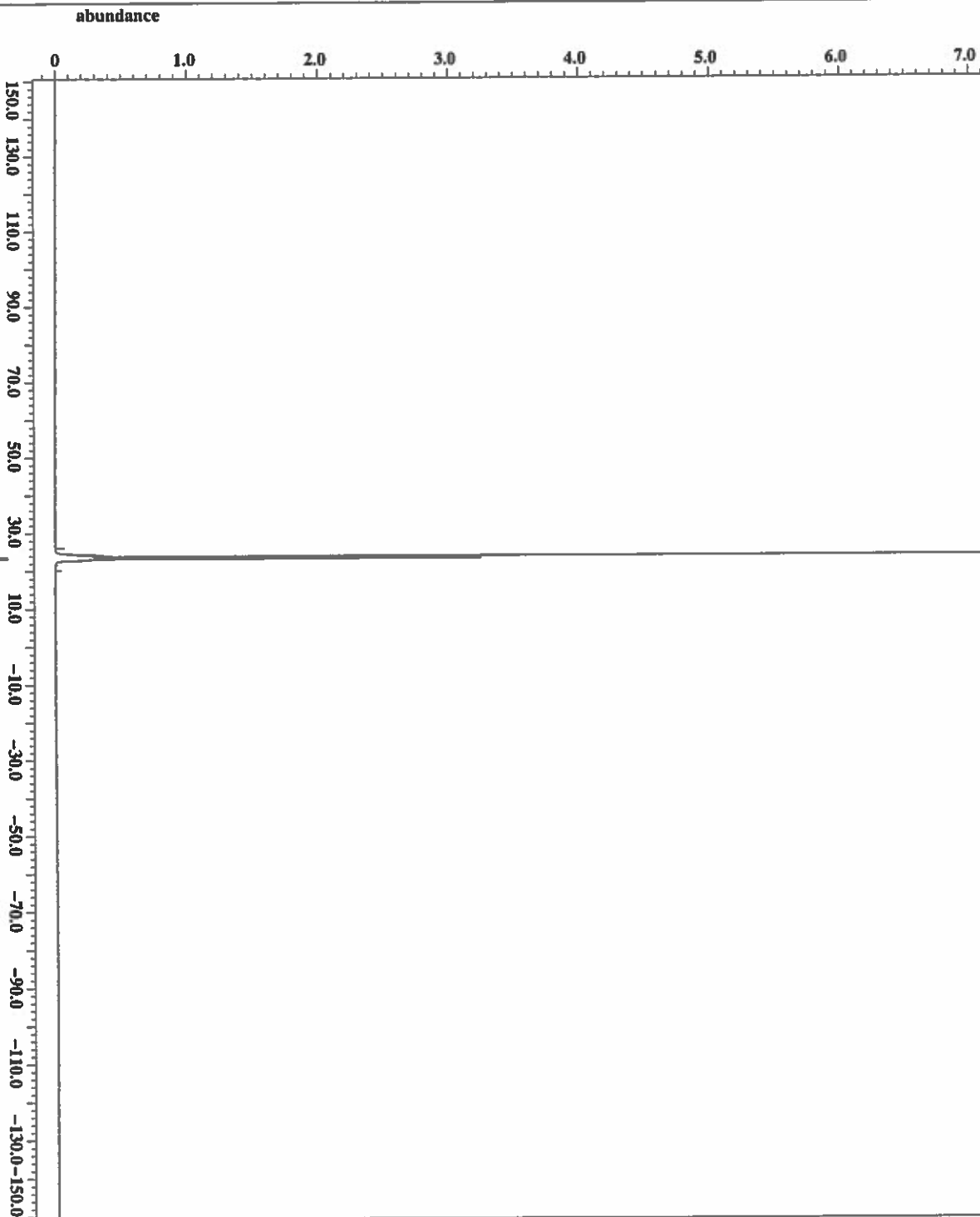
Data_format   = 1D COMPLEX
Dim_size      = 32714
Dim_c1size    = 13C
Dim_u1size    = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7471579 [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]
Xr_domain      = 1H
Xr_freq        = 500.15991521 [MHz]
Xr_offset      = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 400
Total_scans    = 400

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Xr_atn_dec     = 20.7 [dB]
Xr_atn_noe     = 20.7 [dB]
Xr_noise       = WALTZ
Decoupling     = TRIZ
Initial_wait   = 1 [s]
Noe_time       = TRIZ
Noe_gain       = 2 [s]
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 20.7 [deg]

```





SOUTH ALABAMA
JAGUARS

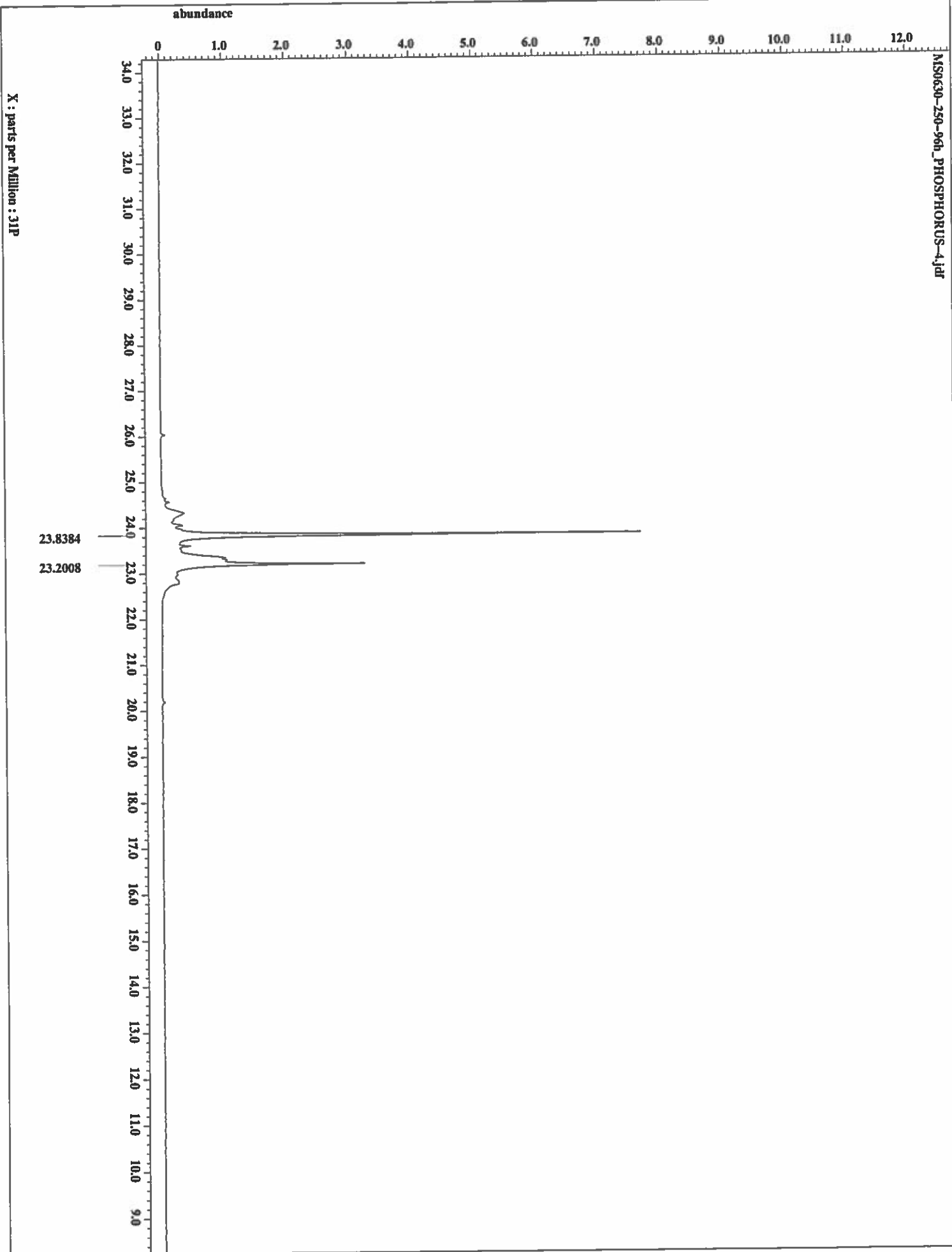
```

Filename      = MS0630-250-96h_PHOSPH
Author        = Jim Davila
Experiment    = single_pulse_dec
Sample_id     = MS0630-250-96h
Solvent       = CHLOROFORM-D
Creation_time = 18-DEC-2018 12:06:35
Revision_time = 18-DEC-2018 11:40:17
Current_time  = 18-DEC-2018 11:40:17

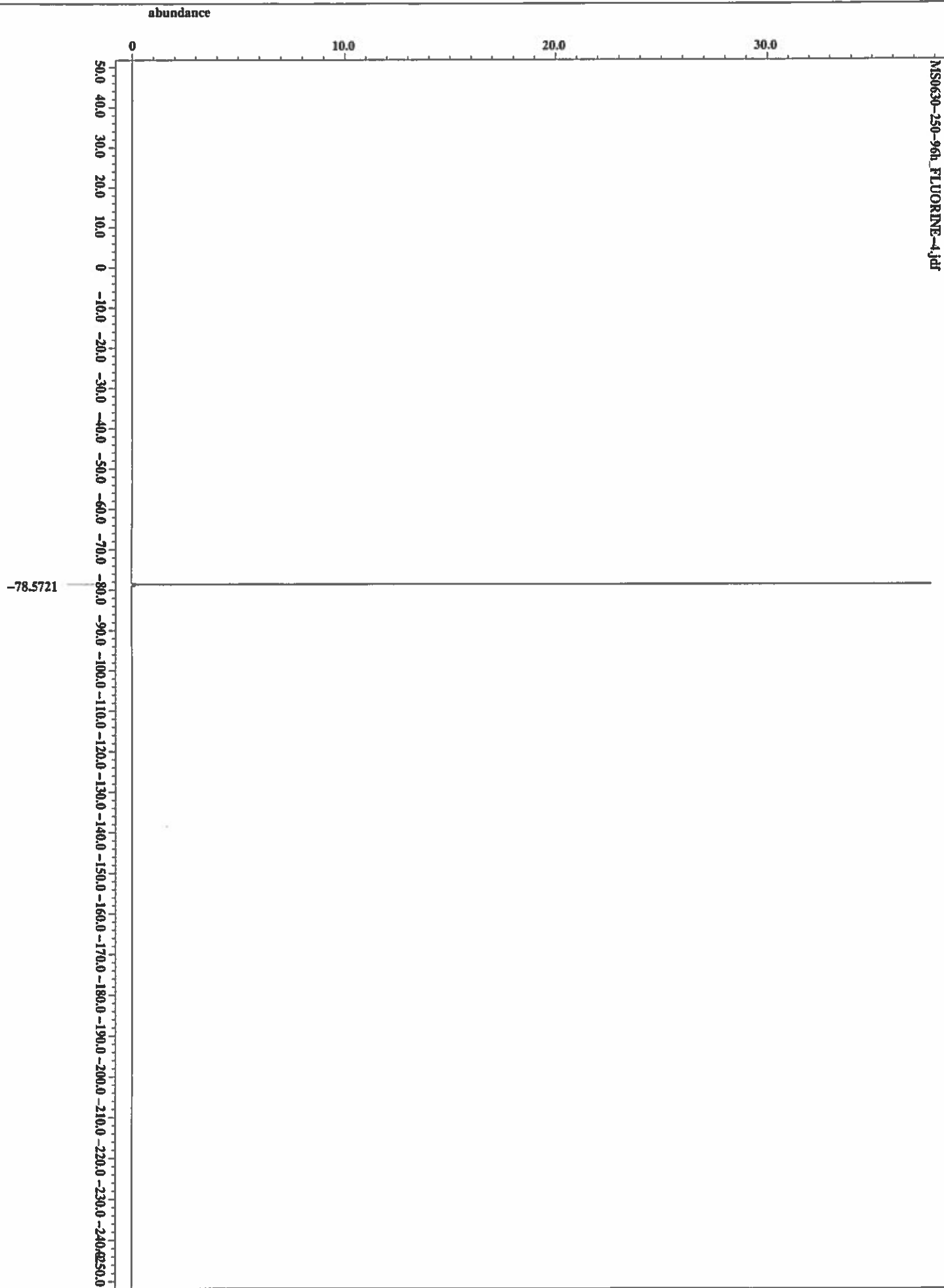
Data format   = 1D COMPLEX
Dir_size      = 52428
Dir_title     = 31P
Dir_units     = [ppm]
Dimensions    = X
Sfca          = SCA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MHz])
X_acq_duration = 0.85983232 [s]
X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 65536
X_prescans     = 4
X_resolution   = 1.16303746 [Hz]
X_sweep        = 18
Xir_domain     = 76.2195122 [MHz]
Xir_freq       = 500.15991521 [MHz]
Xir_offset     = 5.0 [ppm]
Clipped        = TRUEZ
Mod_return     = 1
Scans          = 128
Total_scans    = 128

X_90_width     = 14.687 [us]
X_acq_time      = 0.85983232 [s]
X_angle        = 30 [deg]
X_atn          = 5 [dB]
X_pulse        = 4.89566667 [us]
Xir_atn_dec    = 20.7 [dB]
Xir_atn_noe    = 20.7 [dB]
Xir_noise      = VALTZ
Decoupling     = TRUEZ
Initial_wait    = 1 [s]
Noe_time       = TRUEZ
Noe_delay      = 2 [s]
Relaxation_delay = 2 [s]
Repetition_time = 2.85983232 [s]
Temp_get       = 20.6 [C]
  
```

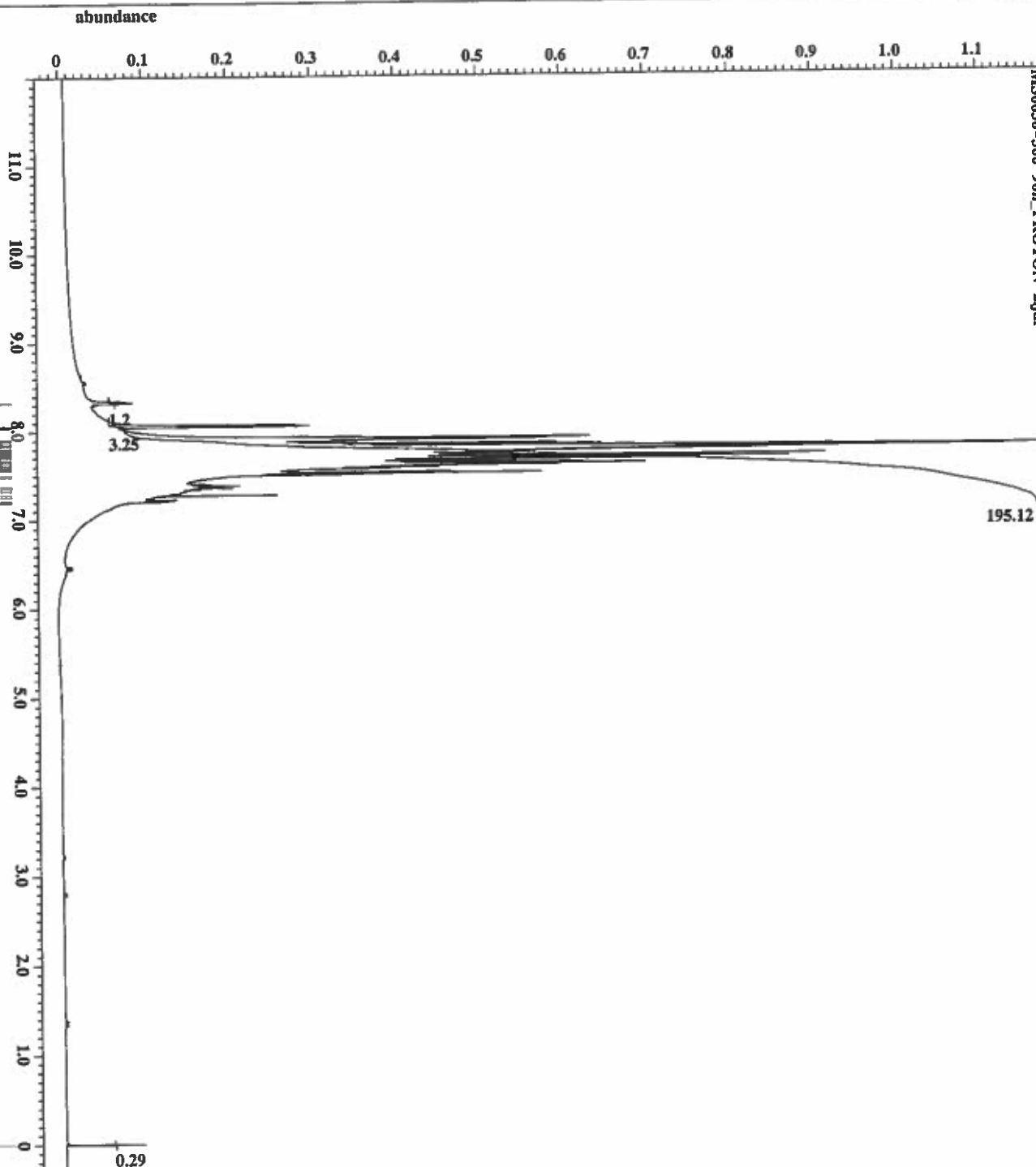


X : parts per Million : ^{31}P





SOUTH ALABAMA
JAGUARS



X : parts per Million : 1H

```

Filename      = MS0630-300-96h_PROTON
Author        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0630-300-96h
Solvent       = CHLOROFORM-D
Creation_time  = 18-DEC-2018 12:26:17
Revision_time  = 18-DEC-2018 11:59:58
Current_time   = 18-DEC-2018 11:59:58

Data_format   = 1D COMPLEX
Dir_size      = 13107
Dir_title     = 1H
Dir_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 9.38438438 [kHz]
Xt_domain      = 1H
Xt_freq        = 500.15991521 [MHz]
Xt_offset      = 5.0 [ppm]
Xt_domain      = 1H
Xt_freq        = 500.15991521 [MHz]
Xt_offset      = 5.0 [ppm]
Mod_return     = FALSE
Total_scans    = 16

X_90_width     = 12.4 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_atn          = 6.3 [us]
X_pulse        = Off
Xt_mode        = Off
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 24
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_set       = 20.3 [deg]

```

abundance

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3 2.4 2.5

10.201 10.0 9.9 9.8 9.7 9.6 9.5 9.4 9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0

8.3341
8.3227

1.2

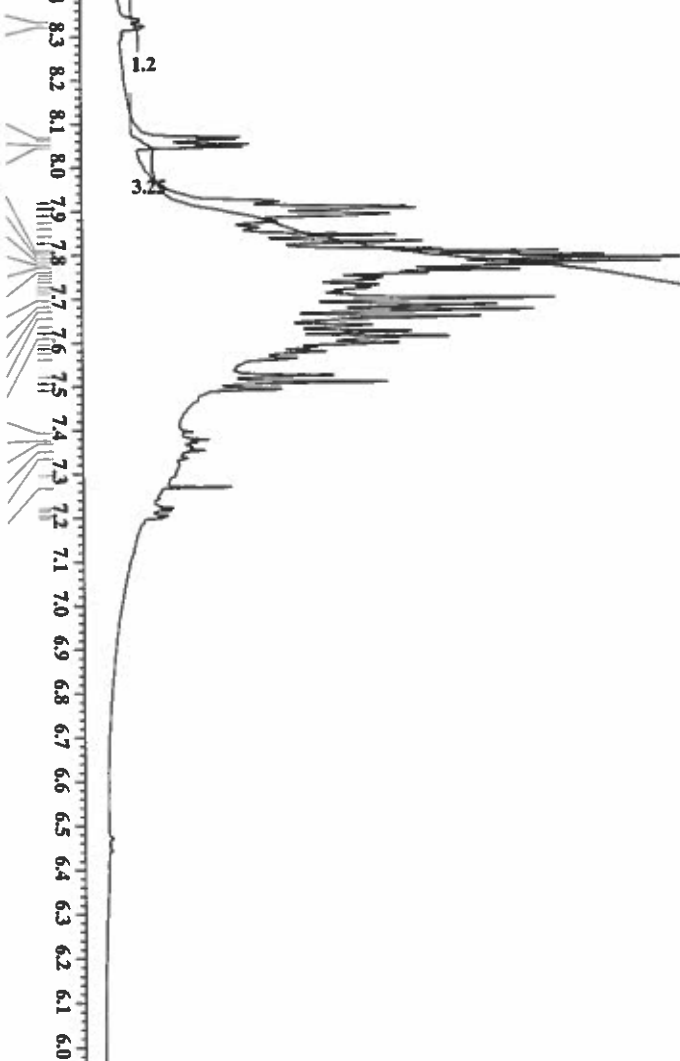
8.0684
8.0524
8.0455

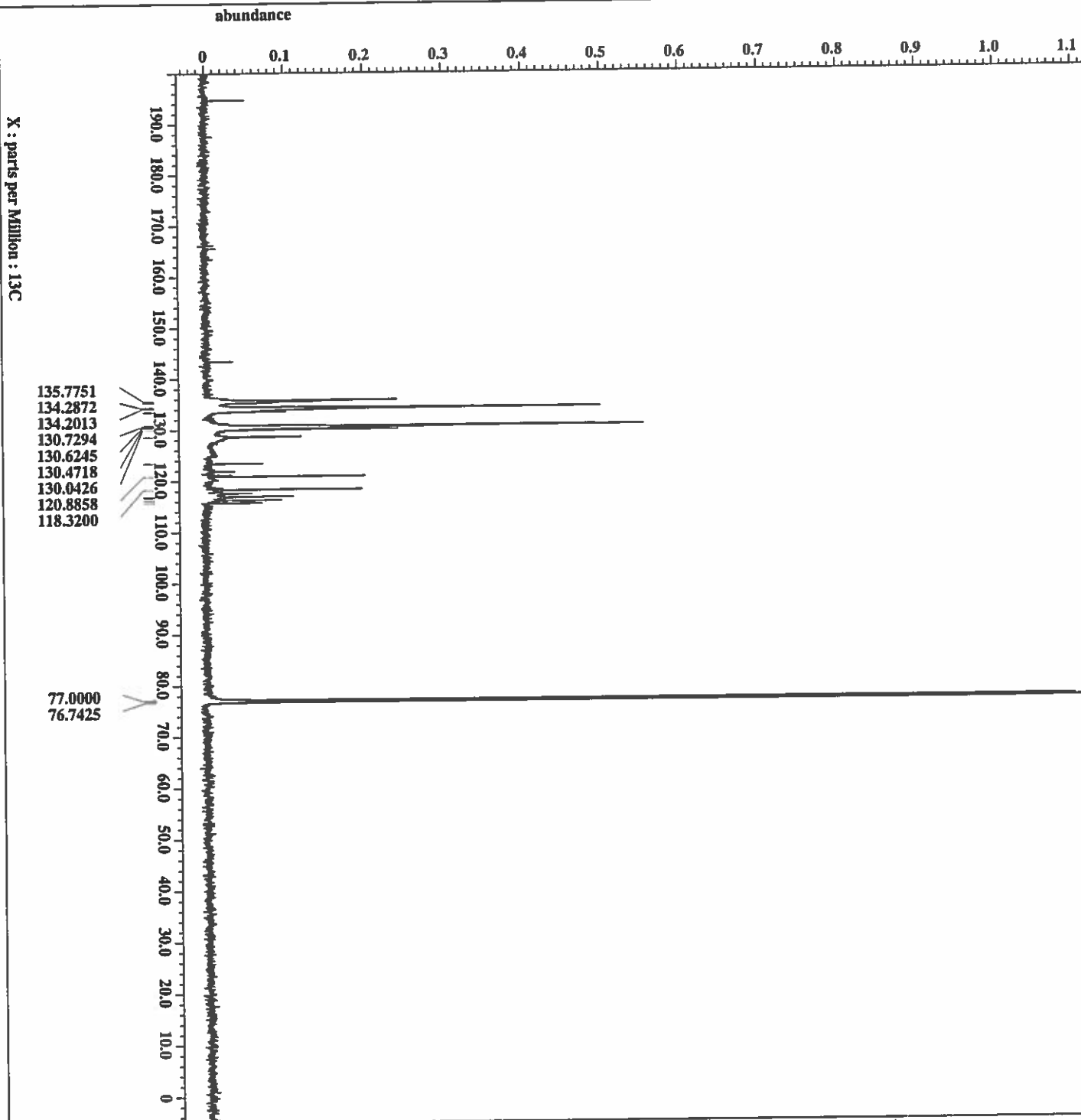
3.25

7.8039
7.7947
7.7867
7.7787
7.7718
7.7615
7.6974
7.6825
7.6710
7.6562
7.6104
7.3951
7.3779
7.3710
7.3527
7.3355
7.2691

195.12

X : parts per Million : 1H





SOUTH ALABAMA
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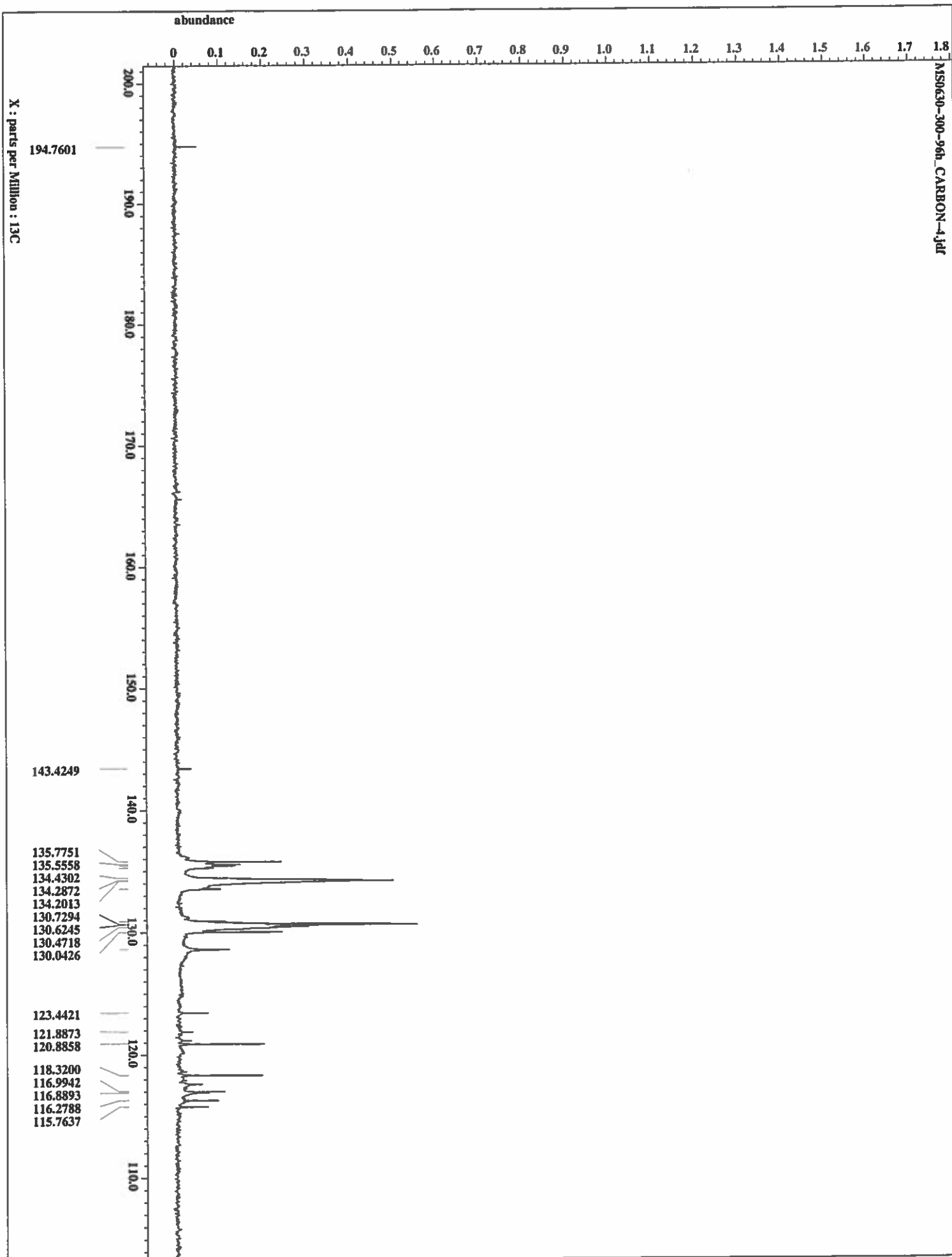
```

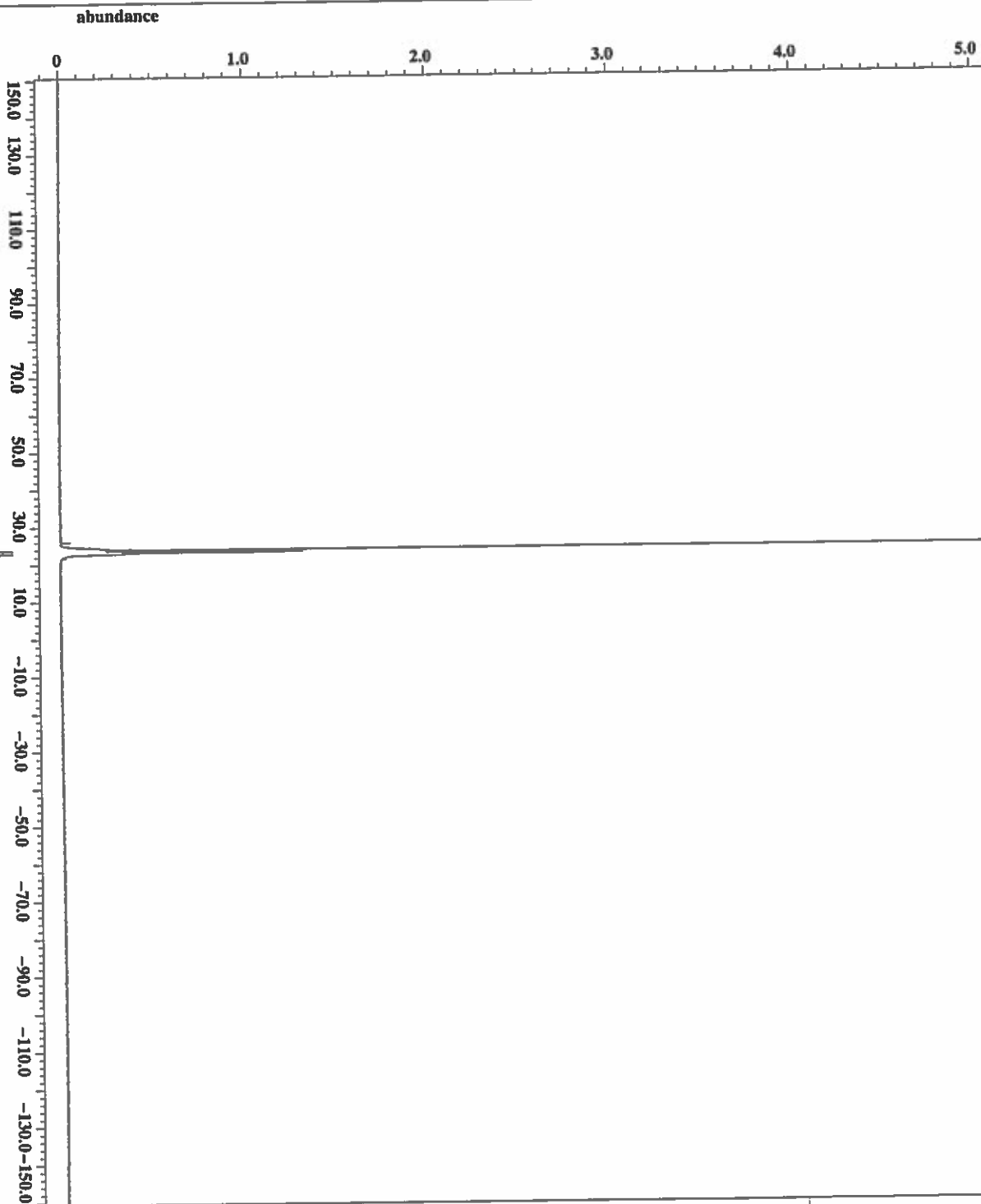
Filename      = MS0630-300-96h_CARBON
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0630-300-96h
Solvent       = CHLOROFORM-D
Creation_time = 18-DEC-2018 12:47:22
Revision_time = 18-DEC-2018 12:21:02
Current_time  = 18-DEC-2018 12:21:02

Data_format   = 1D COMPLEX
Dir_size      = 26214
Dir_cfile     = 13C
Dir_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

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]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 400
Total_scans    = 400

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
X_atn_dec      = 20.7 [dB]
X_atn_noe      = 20.7 [dB]
X_nu1tz        = TRUE
Decoupling     = INH1
Initial_wait   = 1 [s]
Noe            = 1 [s]
Noe_time       = 2 [s]
Nuc1           = 13C
Nuc2           = 13C
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get       = 20.6 [C]
  
```





X : parts per Million : 31P


SOUTH ALABAMA
JAGUARS

```

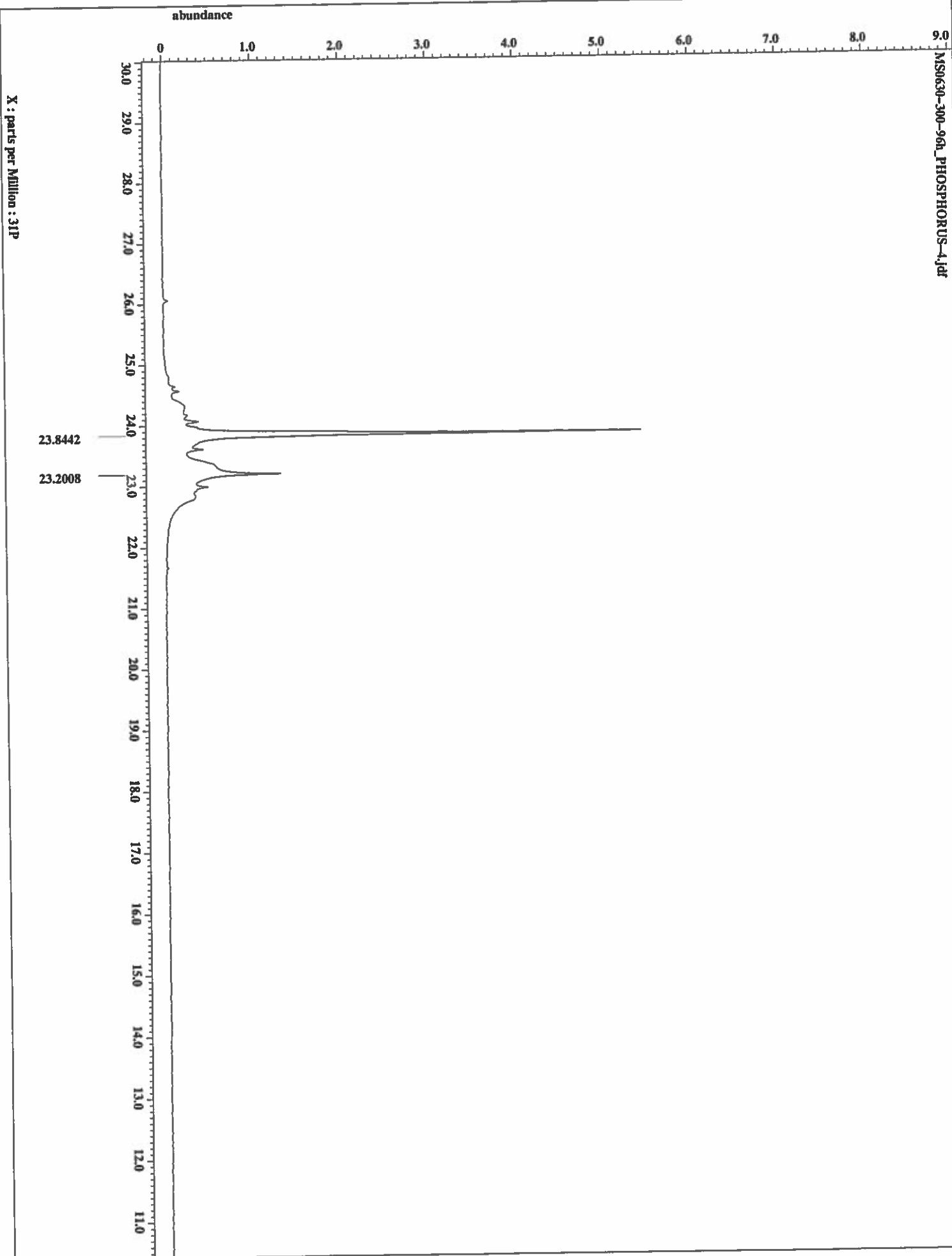
Filename      = MS0630-300-96h_PHOSPH
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0630-300-96h
Solvent       = CHLOROFORM-D
Creation_time = 18-DEC-2018 12:55:48
Revision_time = 18-DEC-2018 12:29:29
Current_time  = 18-DEC-2018 12:29:29

Data_format   = 1D COMPLEX
Dir_size      = 53428
Dir_cttsize   = 31P
Dir_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

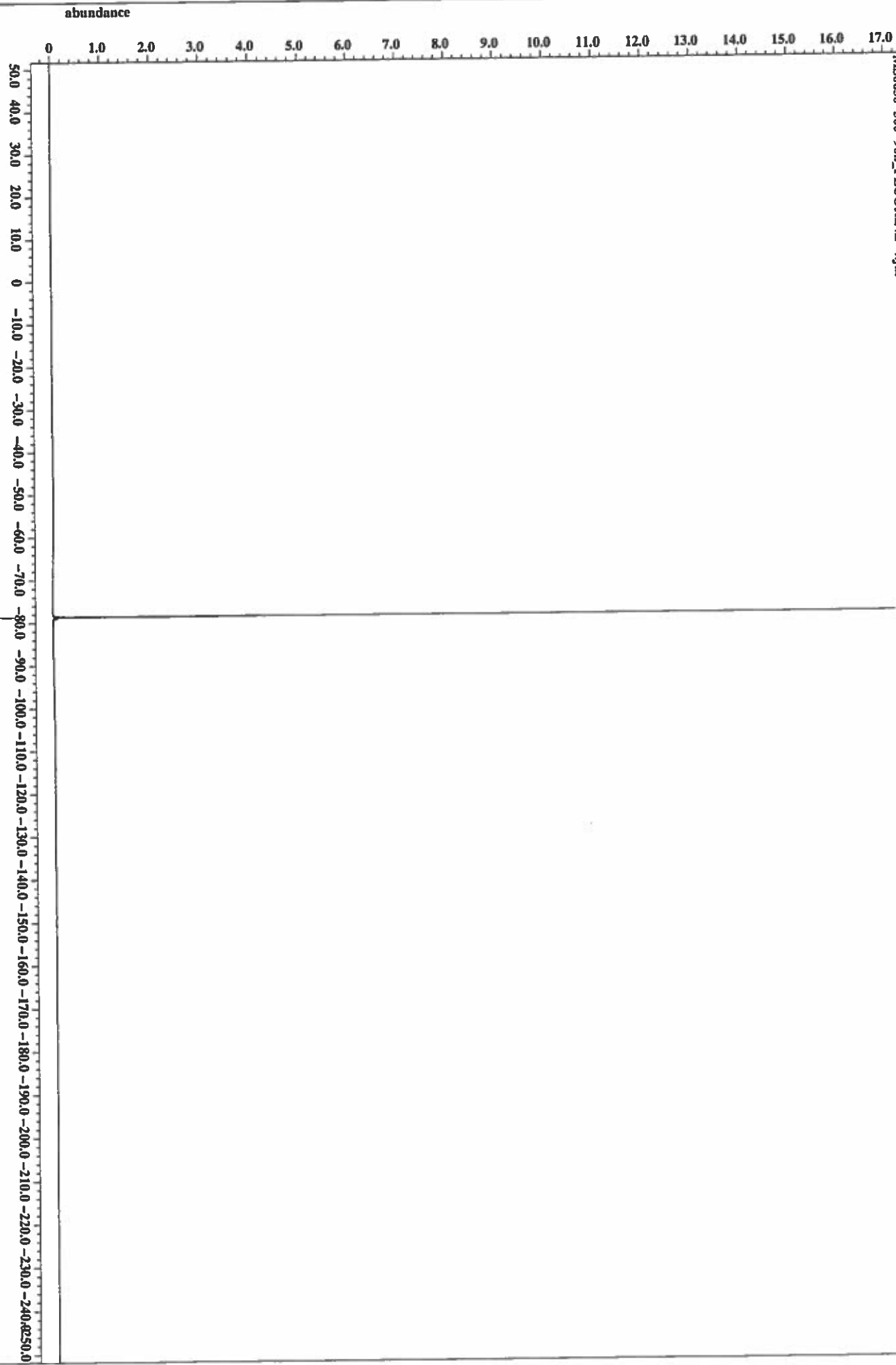
Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.85983232 [s]
X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 65536
X_prescans     = 4
X_resolution   = 1.16301746 [Hz]
X_sweep        = 76.2195122 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = TRUE
Mod_return     = 1
Scans          = 128
Total_scans    = 128

X_90_width     = 14.687 [us]
X_acq_time     = 0.85983232 [s]
X_angle        = 30 [deg]
X_atn          = 5 [db]
X_pulse        = 4.89566667 [us]
Irr_atn_dec    = 20.7 [db]
Irr_atn_noe    = 20.7 [db]
WALTZ          = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Recvr_gain     = 54
Relaxation_delay = 2 [s]
Repetition_time = 2.85983232 [s]
Temp_get       = 20.9 [deg]

```



MS0630-300-96H_FLUORINE-4.jdt

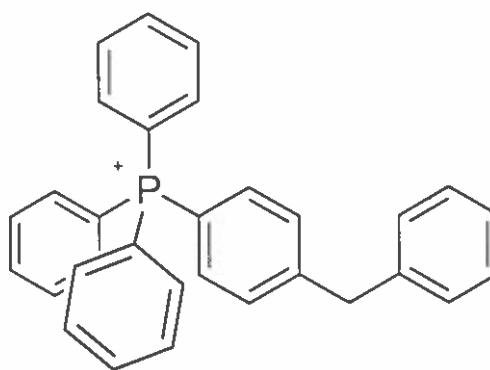
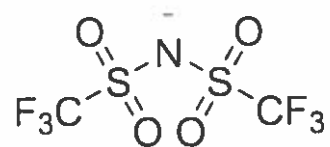


X : parts per Million : 19F

-78.5894

Compound 14 Pre- and Post-heating NMR Spectra

Temperature of Post-heating samples noted in upper left corner of each spectrum



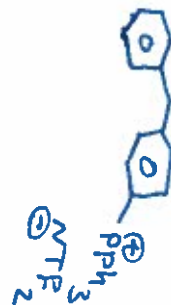
7.7462
7.7382
7.6156
7.5893
7.5744
7.5721

100.05

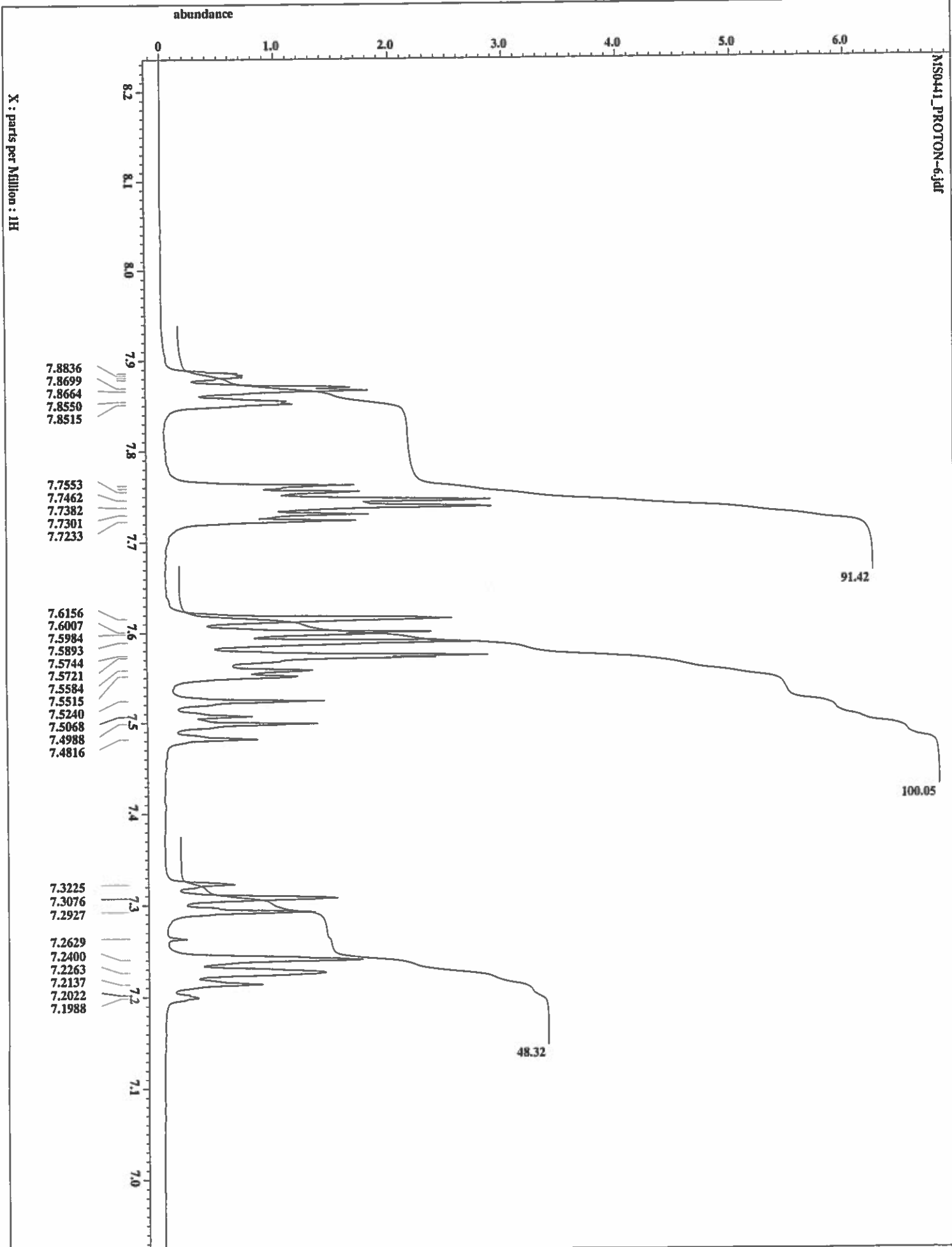
48.32

20.18

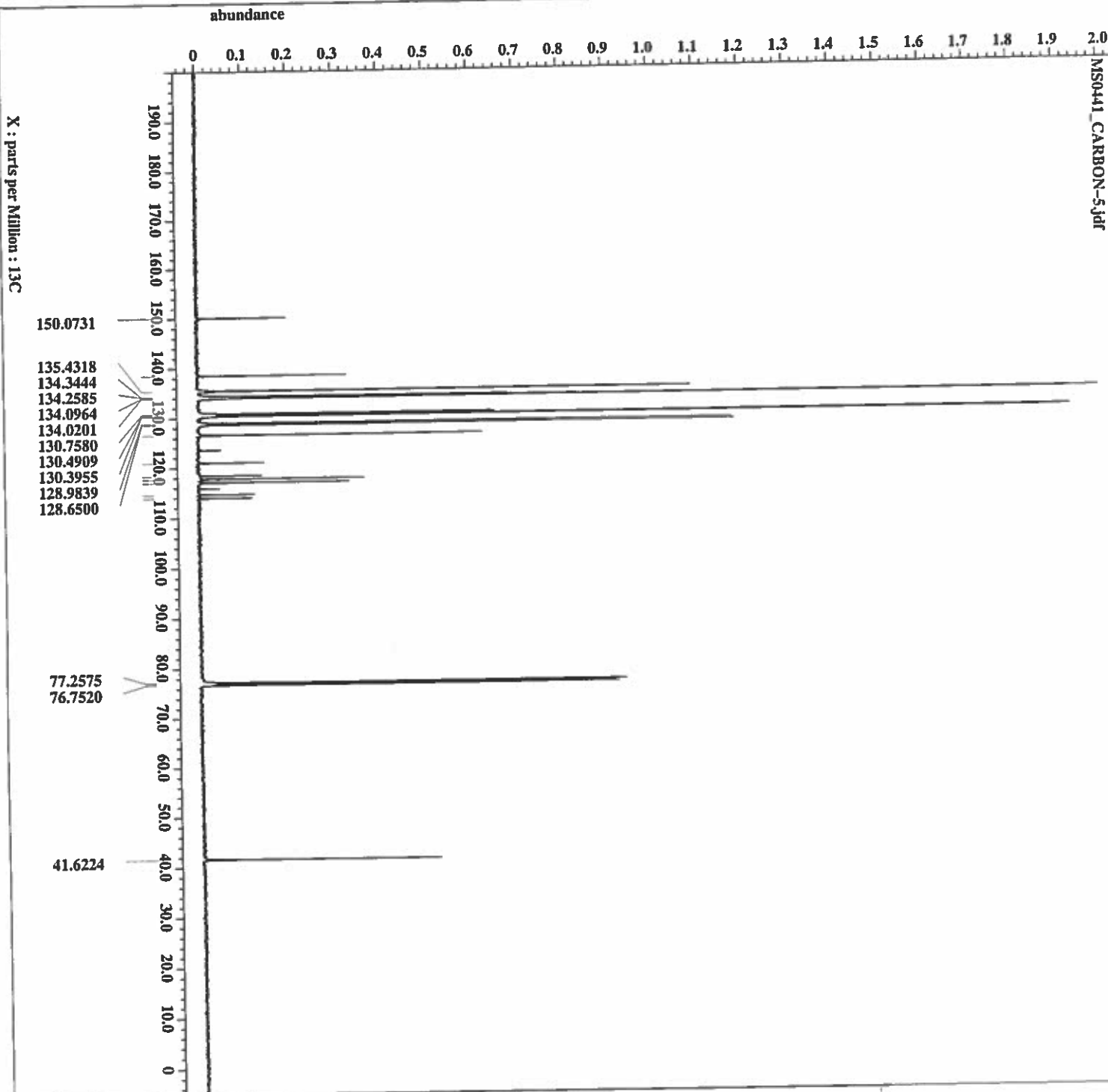
4.1251



filename MS0441_PROTON-5.jdf
 Author Jim Davis
 Experiment single_pulse.ex2
 Sample_id MS0441
 Solvent CHLOROFORM-D
 Changer_sample 15
 Creation_time 9-MAY-2018 19:31:18
 Revision_time 9-MAY-2018 19:07:27
 Current_time 9-MAY-2018 19:07:27
 Data_format 1D COMPLEX
 Dim_size 13107
 Dim_title 1H
 Dim_units [ppm]
 Dimensions X
 Site ECA 500
 Spectrometer JNM-ECA500
 Field_strength 11.747357917 (500 MHz)
 X_acq_duration 1.74587904[s]
 X_domain 1H
 X_freq 500.15991521 [MHz]
 X_offset 5.0 [ppm]
 X_points 16384
 X_prescans 1
 X_resolution 0.57277737 [Hz]
 X_sweep 9.38638638 [kHz]
 Irr_domain 1H
 Irr_freq 500.15991521 [MHz]
 Irr_offset 5.0 [ppm]
 Tr1_domain 1H
 Tr1_freq 500.15991521 [MHz]
 Tr1_offset 5.0 [ppm]
 Clipped FALSE
 Mod_return 1
 Scans 16
 Total_scans 16
 X_90_width 12.4 [us]
 X_acq_time 1.74587904[s]
 X_angle 45 [deg]
 X_atn 4 [dB]
 X_pulse 6.2 [us]
 Tr1_mode OCF
 Dante_preset FALSE
 Initial_wait 1 [s]
 Relaxation_delay 4 [s]
 Repetition_time 5.74587904[s]
 Temp_get 22.9 [degC]



MS0441 CARBON-5.jdt



Filename = MS0441 CARBON-5.jdt
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = MS0441
 Solvent = CHLOROFORM-D
 Change_sample = 15
 Creation_time = 9-MAY-2018 20:21:48
 Revision_time = 9-MAY-2018 19:57:58
 Current_time = 9-MAY-2018 19:57:58

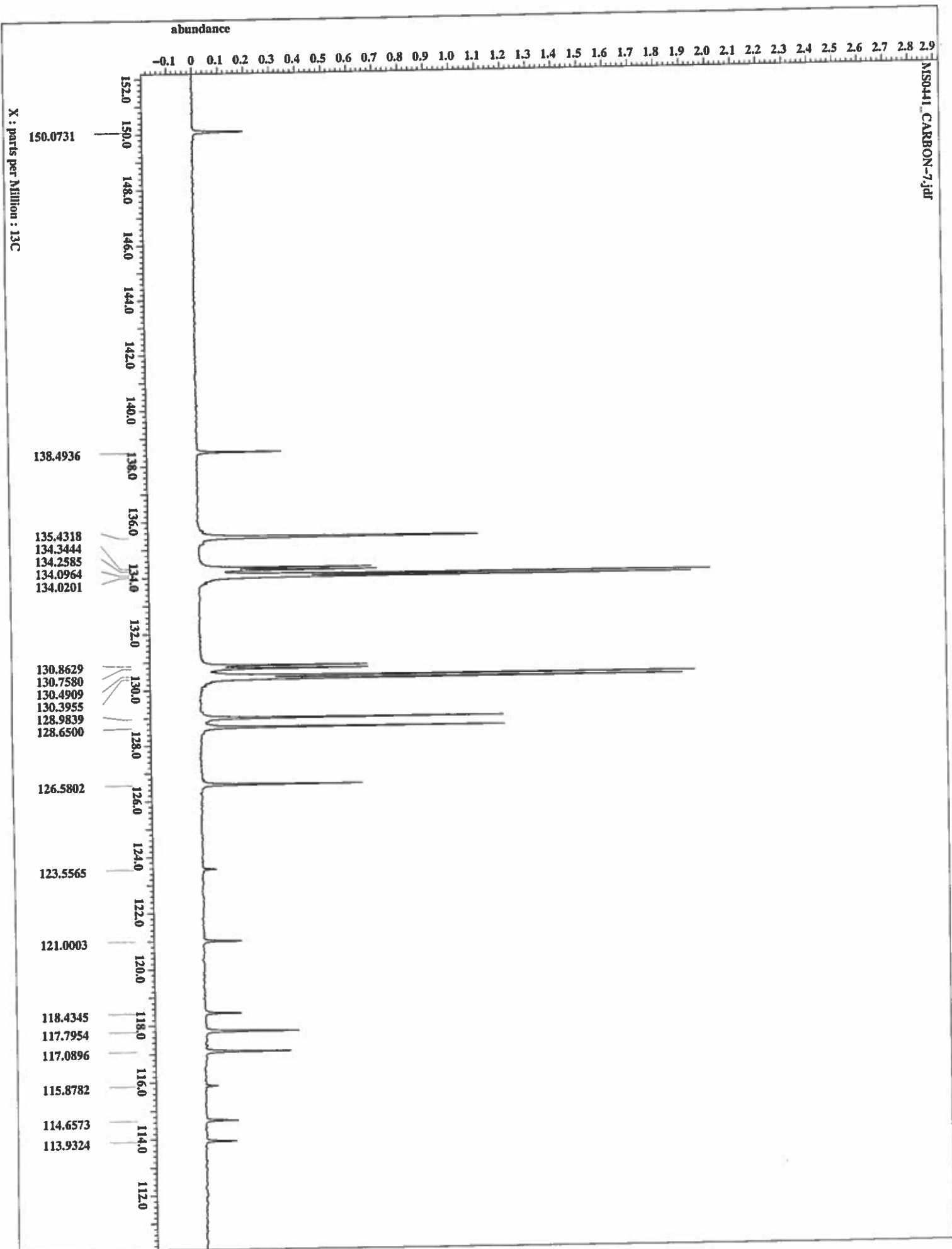
 Data_format = 1D COMPLEX
 Dir_size = 26214
 Dir_name = 13C
 Dir_title = [ppm]
 Dir_units = X
 Dimensions = ECA 500
 Size = JNM-ECA500

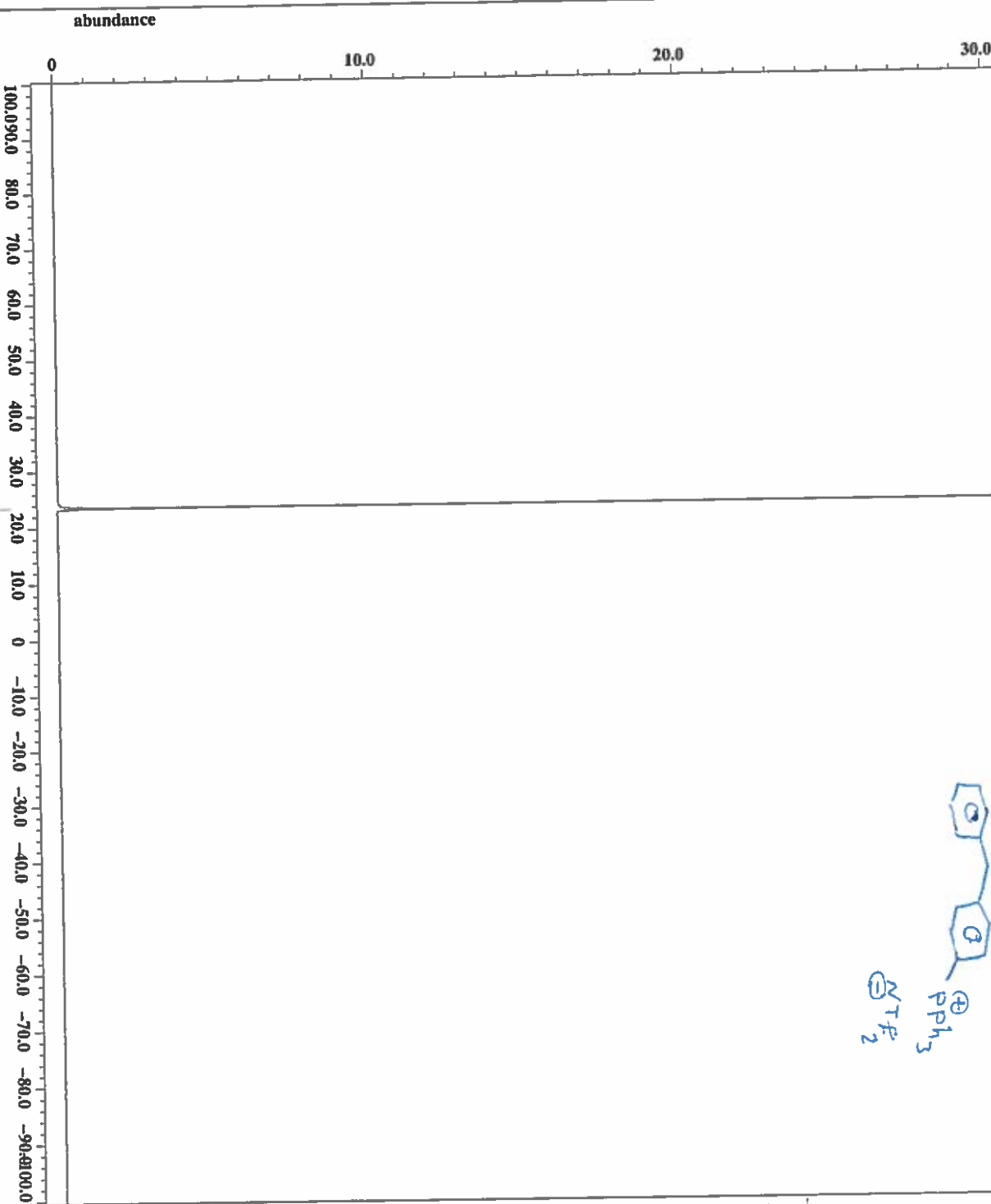
 Spectrometer =

 Field_strength = 11.7473579 [T] (500 [MHZ])
 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]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X_offset = FALSE
 Mod_return = 1
 Scans = 1024
 Total_scans = 1024

 X_90_width = 13.2 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 6 [dB]
 X_atn = 4.4 [us]
 X_pulse = 20.7 [dB]
 X_atn_dec = 20.7 [dB]
 X_atn_noe = 20.7 [dB]
 X_noise = NALFZ
 Decoupling = TRUZ
 Initial_wait = 1 [s]
 Noe = TRUZ
 Noe_time = 2 [s]
 Recv_gain = 60
 Relaxation_delay = 2 [s]
 Repetition_time = 2.83361792 [s]
 Temp_set = 23.4 [degC]







X : parts per Million : 31P

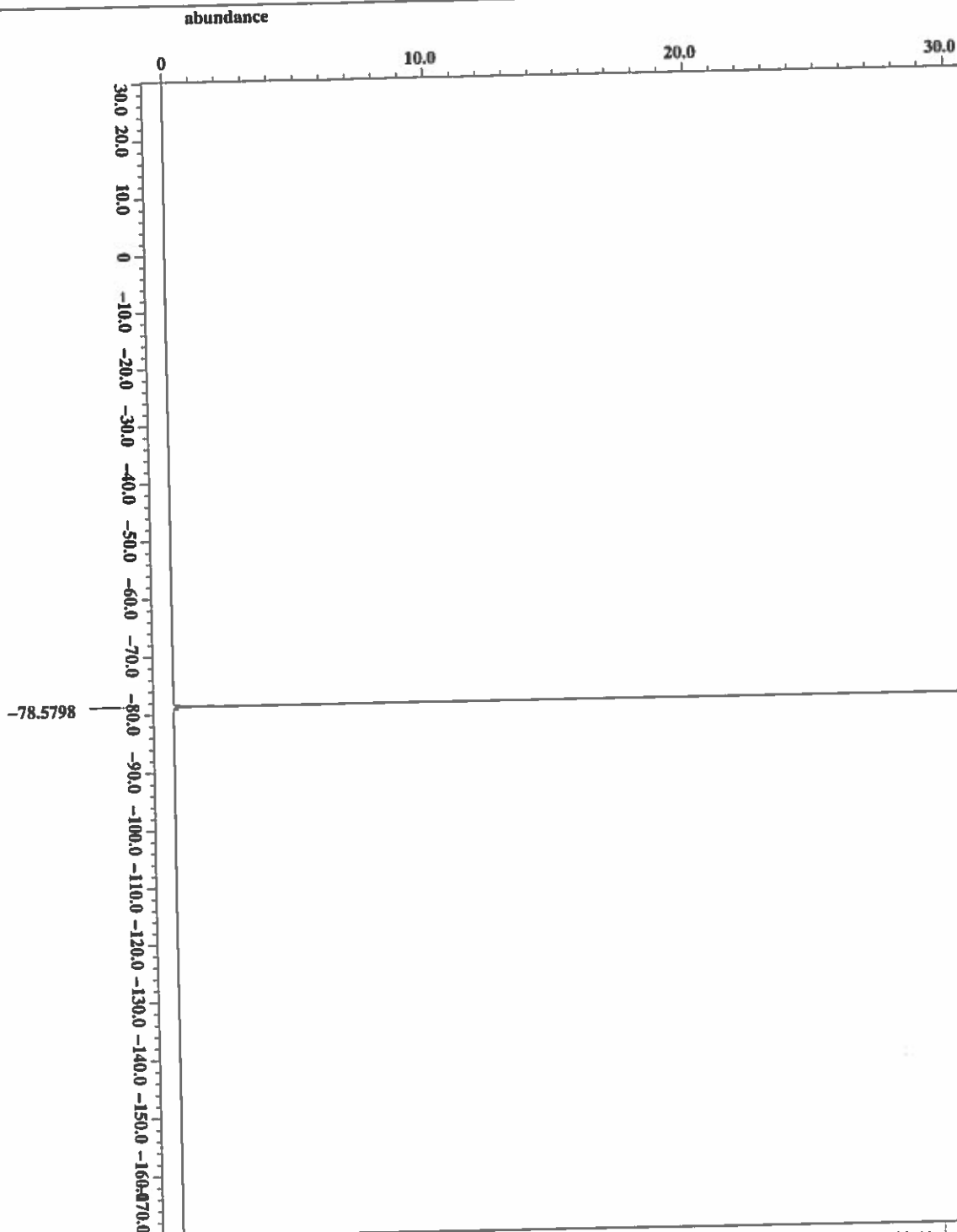
```

File: MS0441_PHOSPHORUS-2.j
Author: Jim Davis
Experiment: single_pulse_dec
Sample_ID: MS0441
Solvent: CHLOROFORM-D
Change: sample
Creation_time: 9-MAY-2018 17:17:05
Revision_time: 9-MAY-2018 16:53:16
Current_time: 9-MAY-2018 16:53:16

Data:
  Format: 1D COMPLEX
  Dir_size: 26214
  Dim_title: 31P
  Dim_units: [ppm]
  Dimensions: X
  Site: XCA 500
  Spectrometer: JNM-EXA500

Field_strength: 11.7473579 [T] (500 [MH
X_acq_duration: 0.64487424 [s]
X_domain: 31P
X_freq: 202.46831075 [MHz]
X_offset: 0 [ppm]
X_points: 32768
X_prescans: 4
X_resolution: 1.55068995 [Hz]
X_sweep: 50.81300813 [kHz]
Irr_domain: 1H
Irr_freq: 500.15991521 [MHz]
Irr_offset: 5.0 [ppm]
Clipped: FALSE
Mod_return: 1
Scans: 25
Total_scans: 25

X_90_width: 14.687 [us]
X_acq_time: 0.64487424 [s]
X_angle: 30 [deg]
X_atn: 5 [dB]
X_pulse: 4.89566667 [us]
Irr_atn_dec: 20.7 [dB]
Irr_atn_poe: 20.7 [dB]
Irr_noise: WALTZ
Decoupling: TRDZ
Initial_wait: 1 [s]
Noe: TRDZ
Noe_time: 2 [s]
Noe_gain: 54
Relaxation_delay: 2 [s]
Relaxation_time: 2.64487424 [s]
Temp_get: 22.6 [degC]
    
```



```

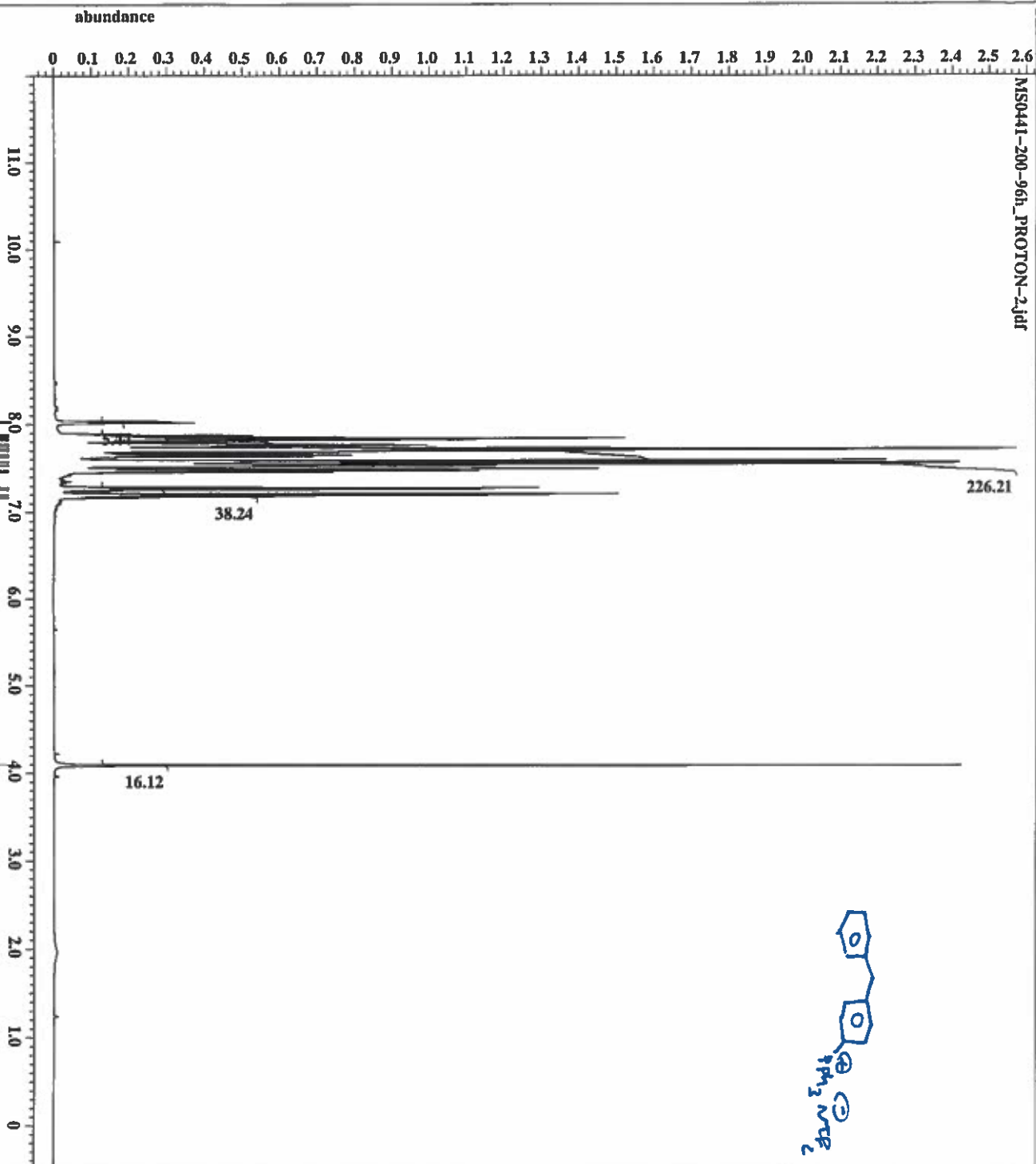
=====
File: MS0441_FLUORINE-2.jdt
Author: Jim Davis
Experiment: single_pulse.ex2
Sample ID: MS0441
Solvent: CHLOROFORM-D
Charger_sample: 15
Creation_time: 9-MAY-2018 17:19:52
Revision_time: 9-MAY-2018 16:56:03
Current_time: 9-MAY-2018 16:56:03

=====
Data:
  Data_format: 1D COMPLEX
  Dir_size: 52428
  Dir_title: 19F
  Dim_units: [ppm]
  Dimensions: X
  Site: ECA 500
  Spectrometer: JNM-ECA500

=====
Field_strength: 11.7473579 [T] (500 [MH
X_acq_duration: 0.55574528 [s]
X_domain: 19F
X_freq: 470.62046084 [MHz]
X_offset: -76 [ppm]
X_points: 65536
X_prescans: 1
X_resolution: 1.7993855 [Hz]
X_sweep: 117.9245283 [kHz]
Xr_domain: 19F
Xr_freq: 470.62046084 [MHz]
Xr_offset: 5 [ppm]
Xr1_domain: 19F
Xr1_freq: 470.62046084 [MHz]
Xr1_offset: 5 [ppm]
Mod_return: FALSE
Mod_return: 1
Scans: 16
Total_scans: 16

=====
X_90_width: 13.1 [us]
X_acq_time: 0.55574528 [s]
X_angle: 45 [deg]
X_atn: 2.5 [dB]
X_pulse: 6.55 [us]
Xr_mode: OCE
Xr1_mode: OCE
Dante_presat: FALSE
Initial_wait: 1 [s]
Recvr_gain: 36
Relaxation_delay: 4 [s]
Repetition_time: 4.55574528 [s]
Temp_get: 22.4 [dC]
=====

```



```

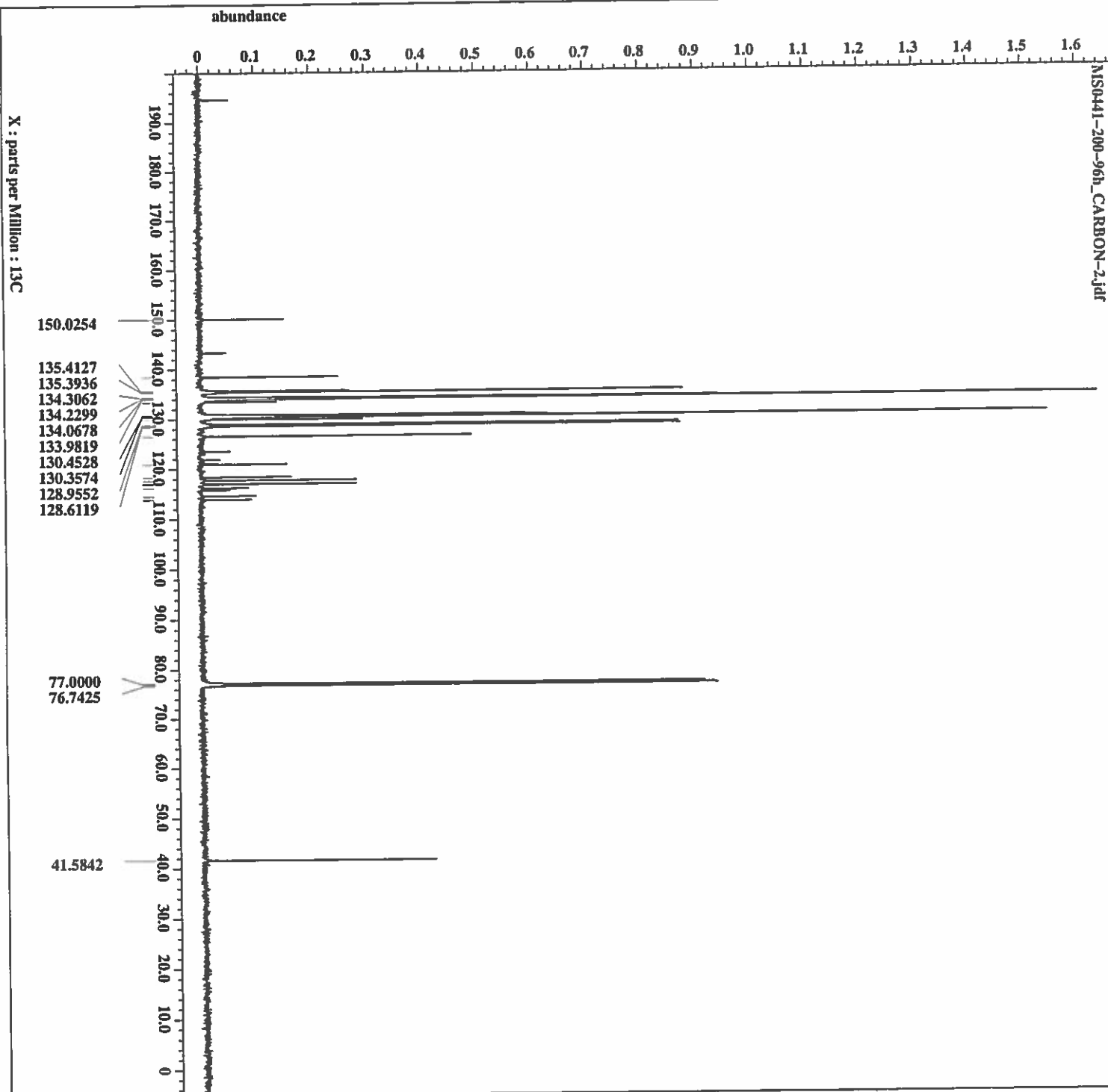
Filename      = MS0441-200-96h_PROTON
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = MS0441-200-96h
Solvent       = CHLOROFORM-D
Charger_sample = 2
Creation_time  = 14-MAY-2018 23:01:47
Revision_time  = 14-MAY-2018 21:37:32
Current_time   = 14-MAY-2018 21:37:32

Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15391521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 9.38438438 [kHz]
Xr_domain      = 1H
Xr_freq        = 500.15391521 [MHz]
Xr_offset      = 5.0 [ppm]
Xr1_domain     = 1H
Xr1_freq       = 500.15391521 [MHz]
Xr1_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Total_scans    = 16

X_90_width     = 12.4 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 6.2 [us]
Xr1_mode       = OFF
Xr1_offset     = OFF
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 22
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_set       = 23.2 [deg]

```



Filename
 Author
 Experiment
 Sample_id
 Solvent
 Changer_sample
 Creation_time
 Revision_time
 Current_time

= MS0441-200-96h_CARBON
 = Jim Davis
 = single_pulse_dec
 = MS0441-200-96h
 = CHLOROFORM-D
 = 2
 = 14-MAY-2018 22:22:55
 = 14-MAY-2018 21:58:40
 = 14-MAY-2018 21:58:40

Data_format
 Dim_size
 Dim_title
 Dim_units
 Dimensions
 Site
 Spectrometer

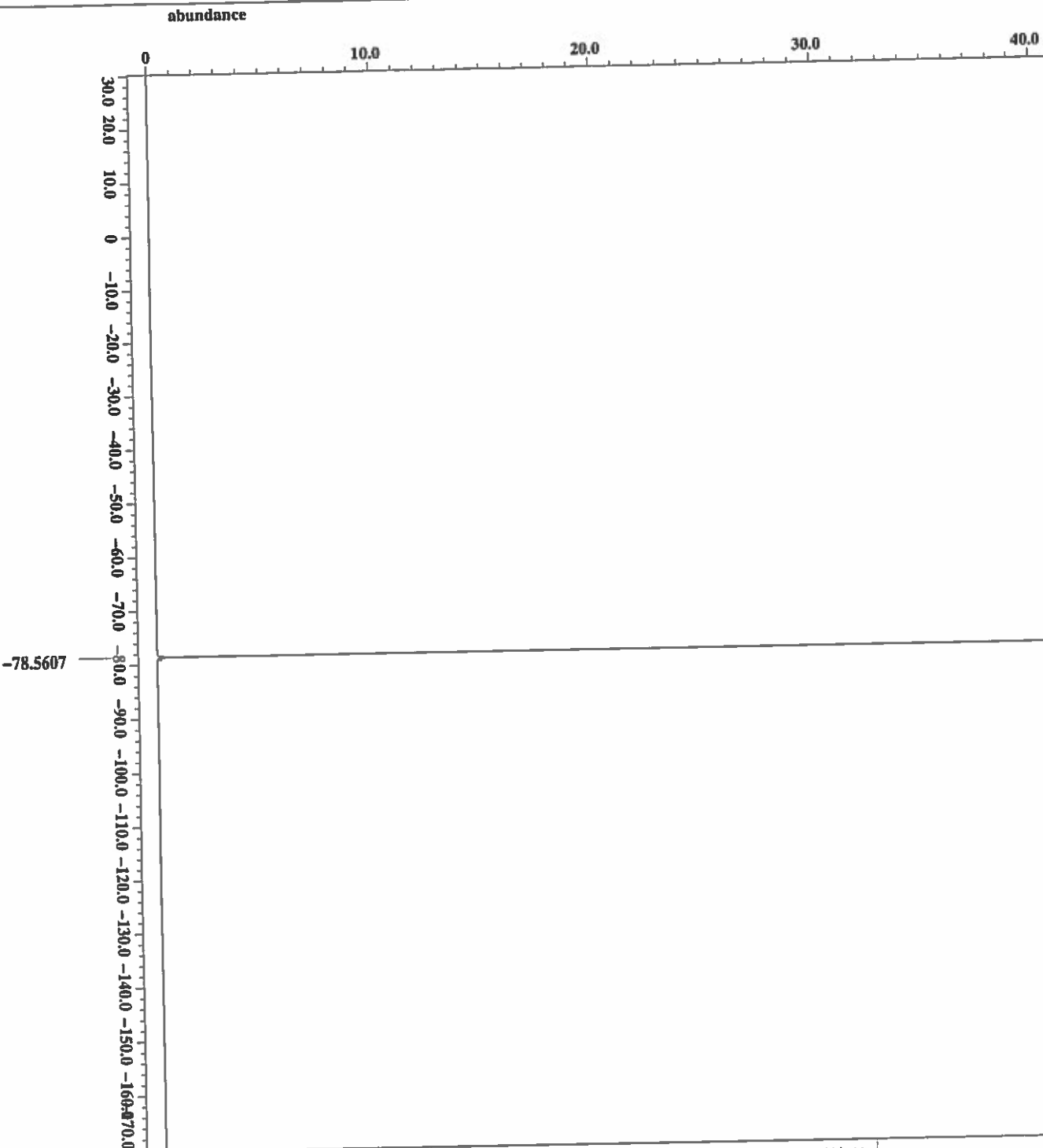
= 1D COMPLEX
 = 26214
 = 13C
 = [ppm]
 = X
 = ECA 500
 = JNM-ECA500

Field_strength
 X_acq_duration
 X_domain
 X_freq
 X_offset
 X_points
 X_prescans
 X_resolution
 X_sweep
 Irr_domain
 Irr_freq
 Irr_offset
 Clipped
 Mod_return
 Scans
 Total_scans

= 11.7473579 [V] (500 [MH
 = 0.83361792 [s]
 = 13C
 = 125.76529768 [MHz]
 = 100 [ppm]
 = 32768
 = 4
 = 1.19959034 [Hz]
 = 39.3081761 [kHz]
 = 1H
 = 500.15991521 [MHz]
 = 5.0 [ppm]
 = FALSE
 = 1
 = 400
 = 400

X_90_width
 X_acq_time
 X_angle
 X_atn
 X_pulse
 Irr_atn_dec
 Irr_atn_noe
 Irr_noise
 Decoupling
 Initial_volt
 Noe
 Noe_time
 Recv_gain
 Relaxation_delay
 Repetition_time
 Temp_get

= 13.2 [us]
 = 0.83361792 [s]
 = 30 [deg]
 = 6 [dB]
 = 4.4 [us]
 = 20.7 [dB]
 = 20.7 [dB]
 = WALTZ
 = TRUE
 = 1 [s]
 = TRUE
 = 2 [s]
 = 60
 = 2 [s]
 = 2.83361792 [s]
 = 23.3 [deg]



SOUTH ALABAMA
JAGUARS

```

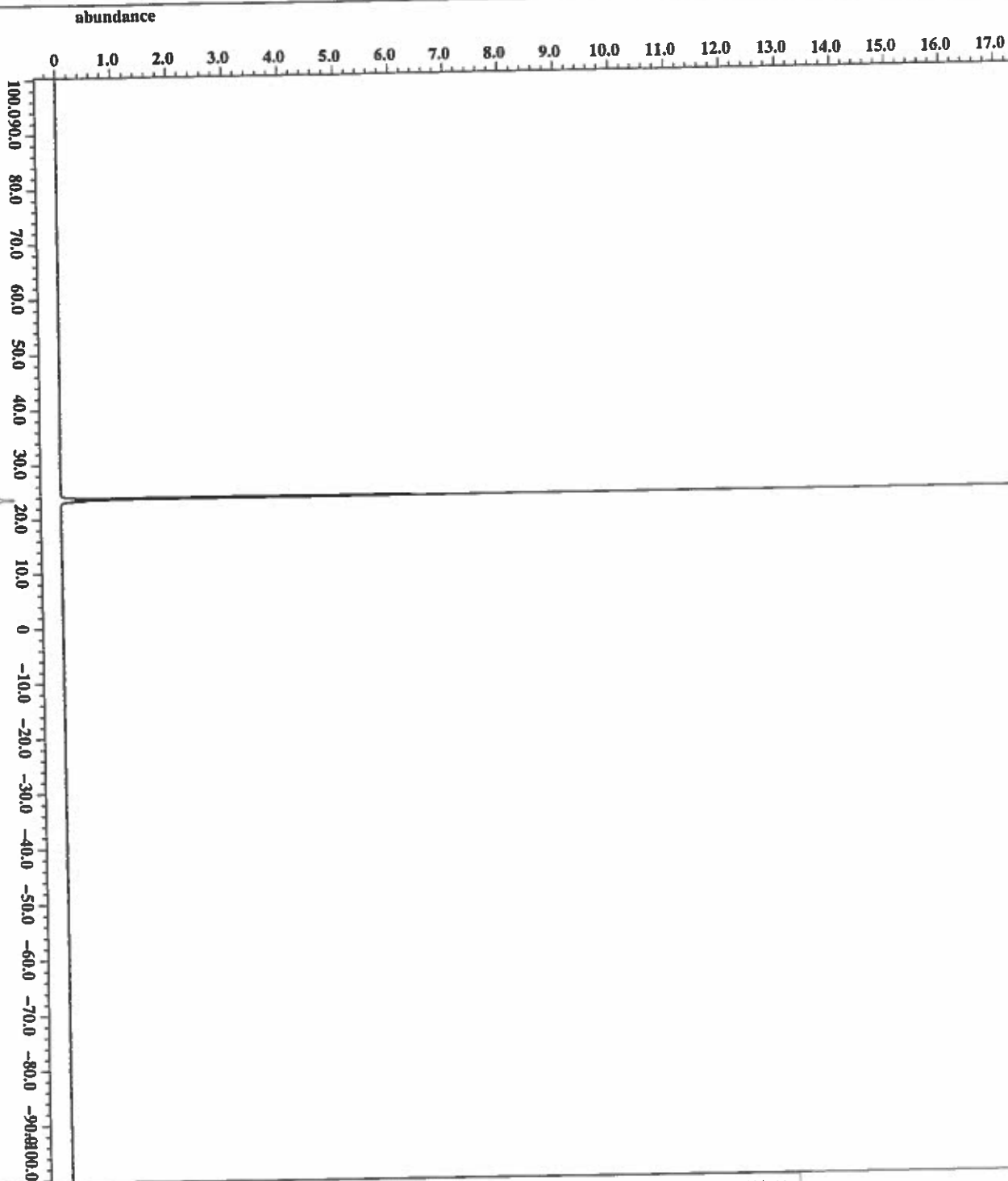
=====
Filename      = MS0441-200-96h_FLUORI
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = MS0441-200-96h
Solvent       = CHLOROFORM-D
Charger_sample = 2
Creation_time  = 16-MAY-2018 22:25:53
Revision_time  = 16-MAY-2018 22:01:37
Current_time   = 16-MAY-2018 22:01:37

Data_format   = 1D COMPLEX
Dim_size      = 52428
Dim_title     = 19F
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECX500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.55574528 [s]
X_domain       = 19F
X_freq         = 470.62046084 [MHz]
X_offset       = -70 [ppm]
X_points       = 65536
X_prescans     = 1
X_resolution   = 1.7993855 [Hz]
X_sweep        = 117.9245283 [kHz]
Xr_domain      = 19F
Xr_freq        = 470.62046084 [MHz]
Xr_offset      = 5 [ppm]
Xr1_domain     = 19F
Xr1_freq       = 470.62046084 [MHz]
Xr1_offset     = 5 [ppm]
Xr1_offset     = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 13.1 [us]
X_acq_time     = 0.55574528 [s]
X_angle        = 45 [deg]
X_atn          = 2.5 [dB]
X_pulse        = 6.55 [us]
Xr_mode        = OCF
Xr1_mode       = FALSE
Dante_present  = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 38
Relaxation_delay = 4 [s]
Repetition_time = 4.55574528 [s]
Temp_get       = 22.9 [degC]
=====

```



SOUTH ALABAMA
JAGUARSTM

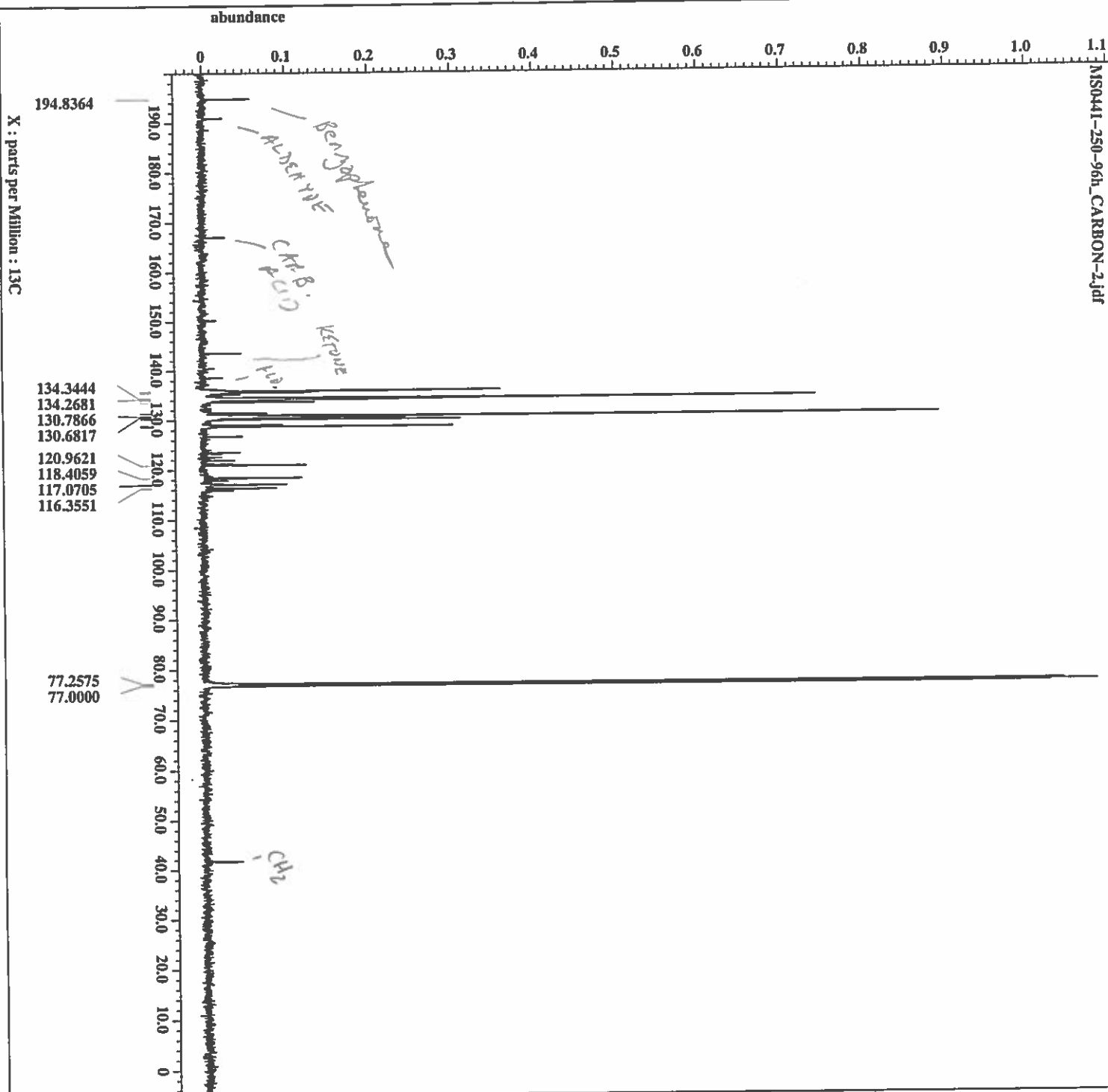
```

Filename      = MS0441-200-96h_PHOSPH
Author        = Jim Davis
Experiment     = single_pulse_dec
Sample_id     = MS0441-200-96h
Solvent       = CHLOROFORM-D
Charger_sample = 2
Creation_time  = 14-MAY-2018 22:30:32
Revision_time = 14-MAY-2018 22:06:15
Current_time   = 14-MAY-2018 22:06:15

Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 31P
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.64487424[s]
X_domain       = 31P
X_freq         = 202.46831075[MHz]
X_offset       = 0[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.55068995[MHz]
X_sweep        = 50.81308131[MHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 50
Total_scans    = 50

X_90_width     = 14.687[us]
X_acq_time     = 0.64487424[s]
X_angle        = 30[deg]
X_atn          = 5[db]
X_pulse        = 4.89566667[us]
Irr_atn_dec    = 20.7[db]
Irr_atn_doe    = 20.7[db]
Irr_pulse      = WALFz
Decoupling     = GRUZ
Initiael_wait  = 1[s]
Noe            = TROZ
Noe_time       = 2[s]
Recvr_gain     = 56
Relaxation_delay = 2[s]
Repetition_time = 2.64487424[s]
Temp_set       = 23.1[deg]
  
```

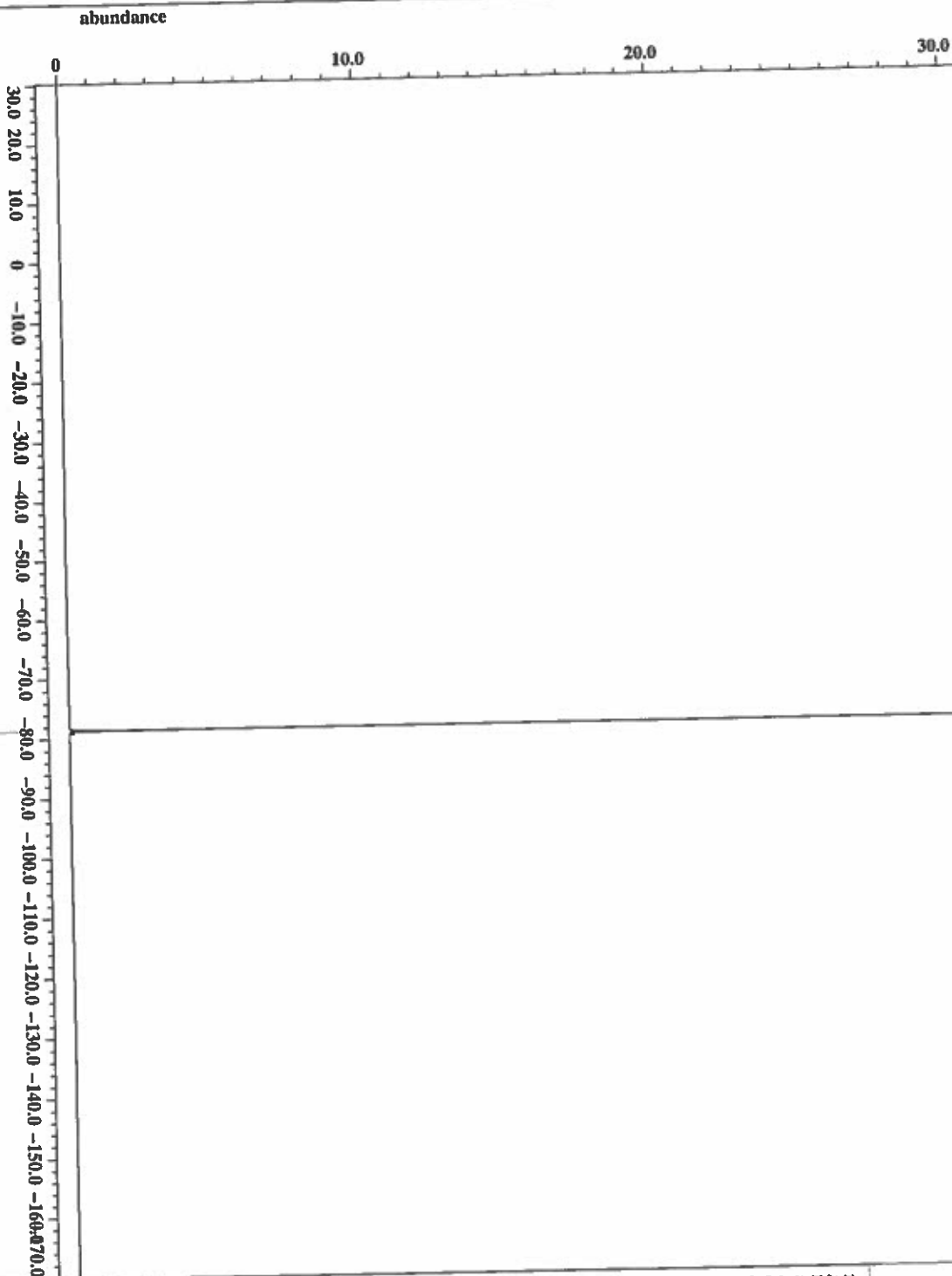
Filename
 MS0441-250-96h_CARBON
 Author
 Jim Davis
 Experiment
 Single_pulse_dec
 Sample_id
 MS0441-250-96h
 Solvent
 CHLOROFORM-D
 Change_sample
 3
 Creation_time
 14-MAY-2018 22:58:55
 Revision_time
 14-MAY-2018 22:34:38
 Current_time
 14-MAY-2018 22:34:38

Data_format
 1D COMPLEX
 Dir_size
 26214
 Dir_title
 13C
 Dir_units
 [ppm]
 Dimensions
 X
 Site
 ECA 500
 Spectrometer
 UNM-ECA500

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]
 Itr_domain
 1H
 Itr_freq
 500.15991521 [MHz]
 Itr_offset
 5.0 [ppm]
 Clipped
 FALSE
 Mod_return
 1
 Scans
 400
 Total_scans
 400

X_90_width
 13.2 [us]
 X_acq_time
 0.83361792 [s]
 X_angle
 30 [deg]
 X_atn
 6 [dB]
 X_pulse
 4.4 [us]
 Itr_atn_dec
 20.7 [dB]
 Itr_atn_noise
 20.7 [dB]
 Itr_noise
 WALTZ
 Decoupling
 TRUZ
 Initial_wait
 1 [s]
 Noe_time
 2 [s]
 Noe_wait
 60
 Recv_gain
 2 [s]
 Relaxation_delay
 2 [s]
 Repetition_time
 2.83361792 [s]
 Temp_set
 23.3 [deg]





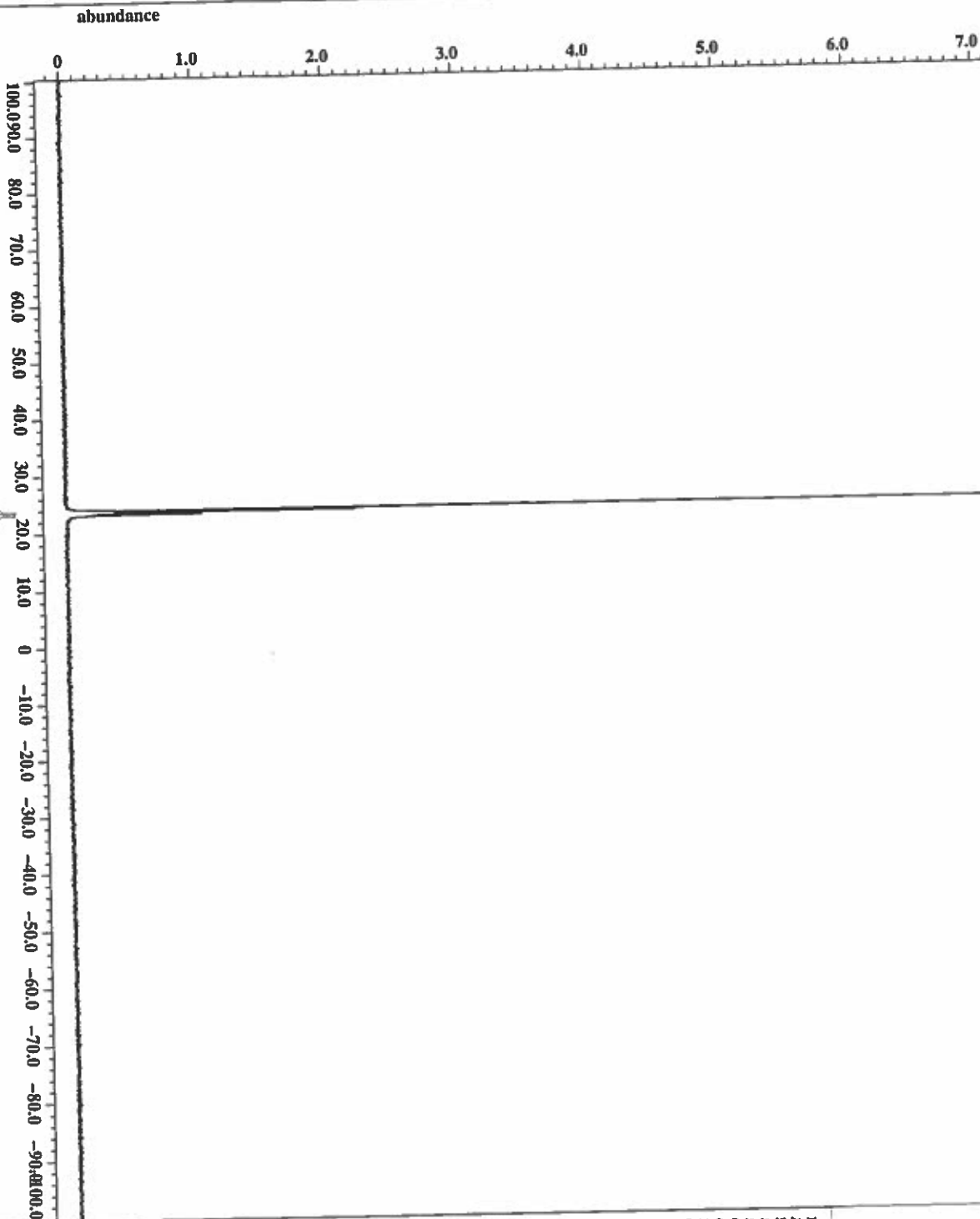
SOUTH ALABAMA
JAGUARSTM

```

Filename      = MS0441-250-96h_FLUORI
Author        = Jim Devils
Experiment    = single_pulse.ex2
Sample_id     = MS0441-250-96h
Solvent       = CHLOROFORM-D
Charger_sample = 3
Creation_time  = 14-MAY-2018 23:01:53
Revision_time  = 14-MAY-2018 22:37:37
Current_time   = 14-MAY-2018 22:37:37

Data_format   = 1D COMPLEX
Dim_size      = 52428
Dim_cfile     = 19F
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ZCA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.55574528 [s]
X_domain       = 19F
X_freq         = 470.62046084 [MHz]
X_offset       = -70 [ppm]
X_points       = 65536
X_prescans     = 1
X_resolution   = 1.7993655 [Hz]
X_sweep        = 117.9245263 [kHz]
Irr_domain     = 19F
Irr_freq       = 470.62046084 [MHz]
Irr_offset     = 5 [ppm]
Irr_domain     = 19F
Irr_freq       = 470.62046084 [MHz]
Irr_offset     = 5 [ppm]
Mod_return     = FALSE
Mod_return     = 1
Mod_return     = 16
Total_scans    = 16
X_90_width     = 13.1 [us]
X_acq_time     = 0.55574528 [s]
X_angle        = 45 [deg]
X_atn          = 2.5 [dB]
X_pulse        = 6.55 [us]
Irr_mode       = OF
Irr_mode       = OF
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 38
Relaxation_delay = 4 [s]
Repetition_time = 4.55574528 [s]
Temp_get       = 22.9 [dc]
  
```



X : parts per Million : 31P

23.9035
23.8346
23.5512

```

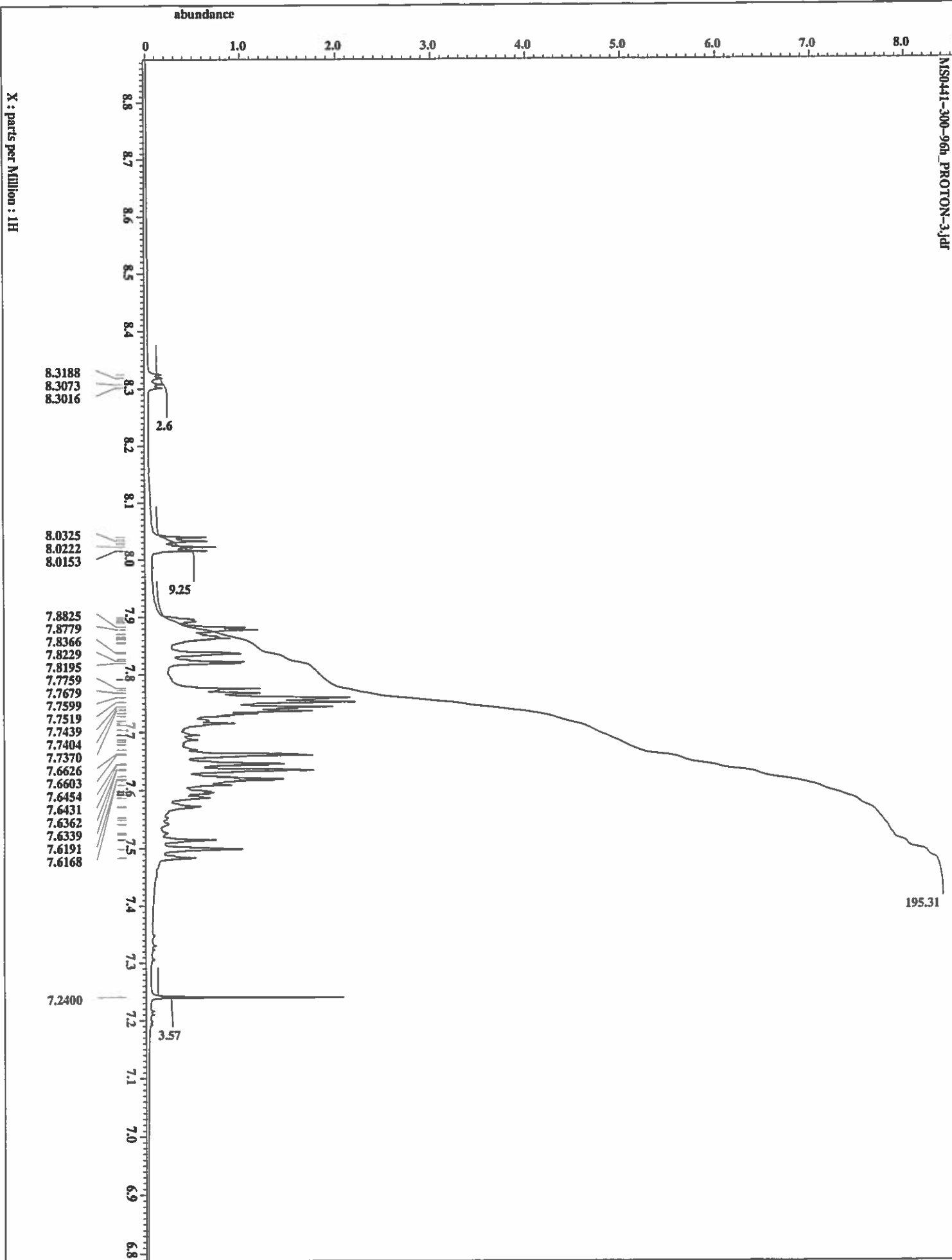
File Name      = MS0441-250-96h_PHOSPH
Author         = Jim Davis
Experiment     = single_pulse_dec
Sample ID      = MS0441-250-96h
Solvent        = CHLOROFORM-D
Change Sample  = 3
Creation Time  = 14-MAY-2018 23:06:31
Revision Time  = 14-MAY-2018 22:42:14
Current Time   = 14-MAY-2018 22:42:14

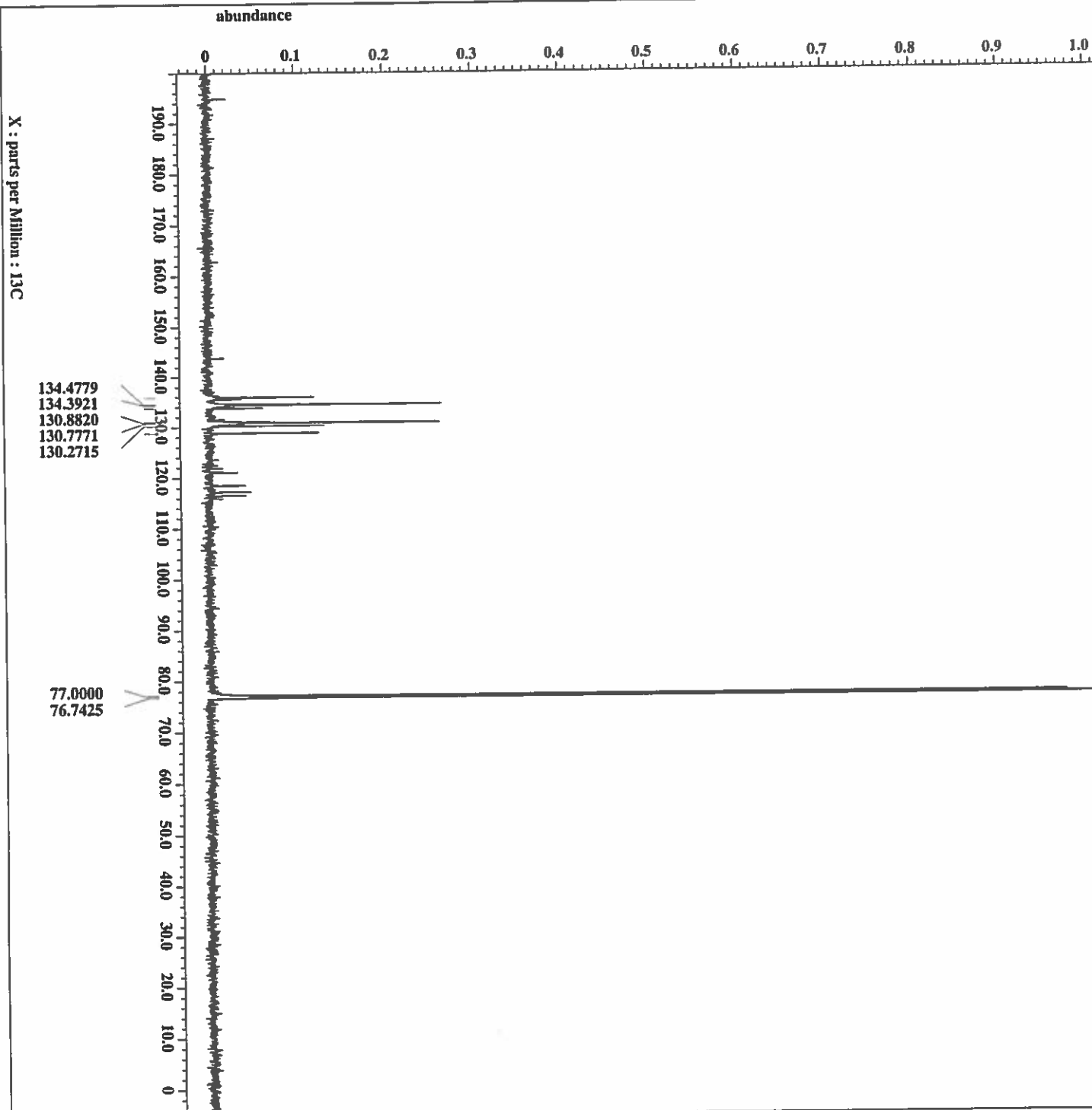
Data Format     = 1D COMPLEX
Dir Size       = 26214
Dir Cycle      = 31P
Dir Units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

Field Strength = 11.743579 [T] (500 [MH
Acq Duration    = 0.64487424 [s]
Domain          = 31P
Freq            = 202.46831075 [MHz]
Offset          = 0 [ppm]
Points          = 33768
Preprocs        = 4
Resolution      = 1.55068995 [Hz]
Sweep           = 50.81300813 [kHz]
Irr Domain      = 1H
Irr Freq        = 500.15991521 [MHz]
Irr Offset      = 5.0 [ppm]
Clipped         = FALSE
Mod Return      = 1
Scans           = 50
Total Scans     = 50

X 90 Width      = 14.687 [us]
X Acq Time      = 0.64487424 [s]
X Angle         = 30 [deg]
X Attn          = 5 [dB]
Irr Pulse       = 4.89566667 [us]
Irr Attn Dec    = 20.7 [dB]
Irr Attn Noe    = 20.7 [dB]
WALTZ           = WALTZ
Decoupling      = TRUZ
Incl Incl Wait  = 1 [s]
Noe             = TRUZ
Noe Time        = 2 [s]
Recvr Gain      = 58
Relaxation Delay = 2 [s]
Repetition Time = 2.64487424 [s]
Temp Set        = 23 [C]
    
```







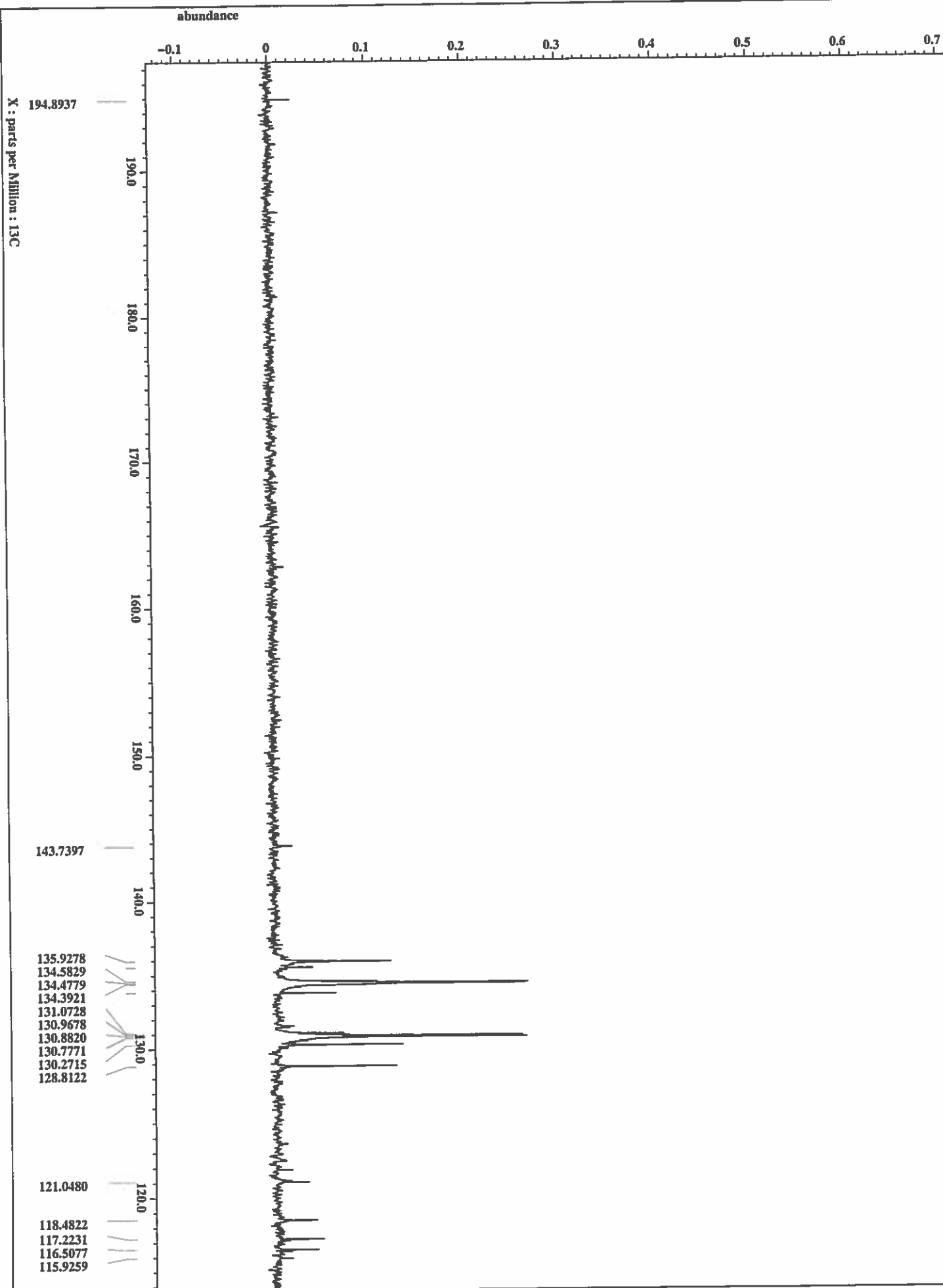
```

File name      = MSD441-300-96h_CARBON
Author         = Jim Davis
Experiment     = single_pulse_dec
Sample_id      = MSD441-300-96h
Solvent        = CHLOROFORM-D
Change_sample  = 4
Creation time   = 14-MAY-2018 23:35:02
Revision time  = 14-MAY-2018 23:10:45
Current_time   = 14-MAY-2018 23:10:45

Data format    = 1D COMPLEX
Dim_size       = 26214
Dim_cfile      = 13C
Dim_units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = QNP-ECA500

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 108 [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          = 400
Total_scans    = 400

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_noe    = 20.7 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUZ
Initial_wait   = 1 [s]
Noe            = TRUZ
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 23.3 [deg]
  
```



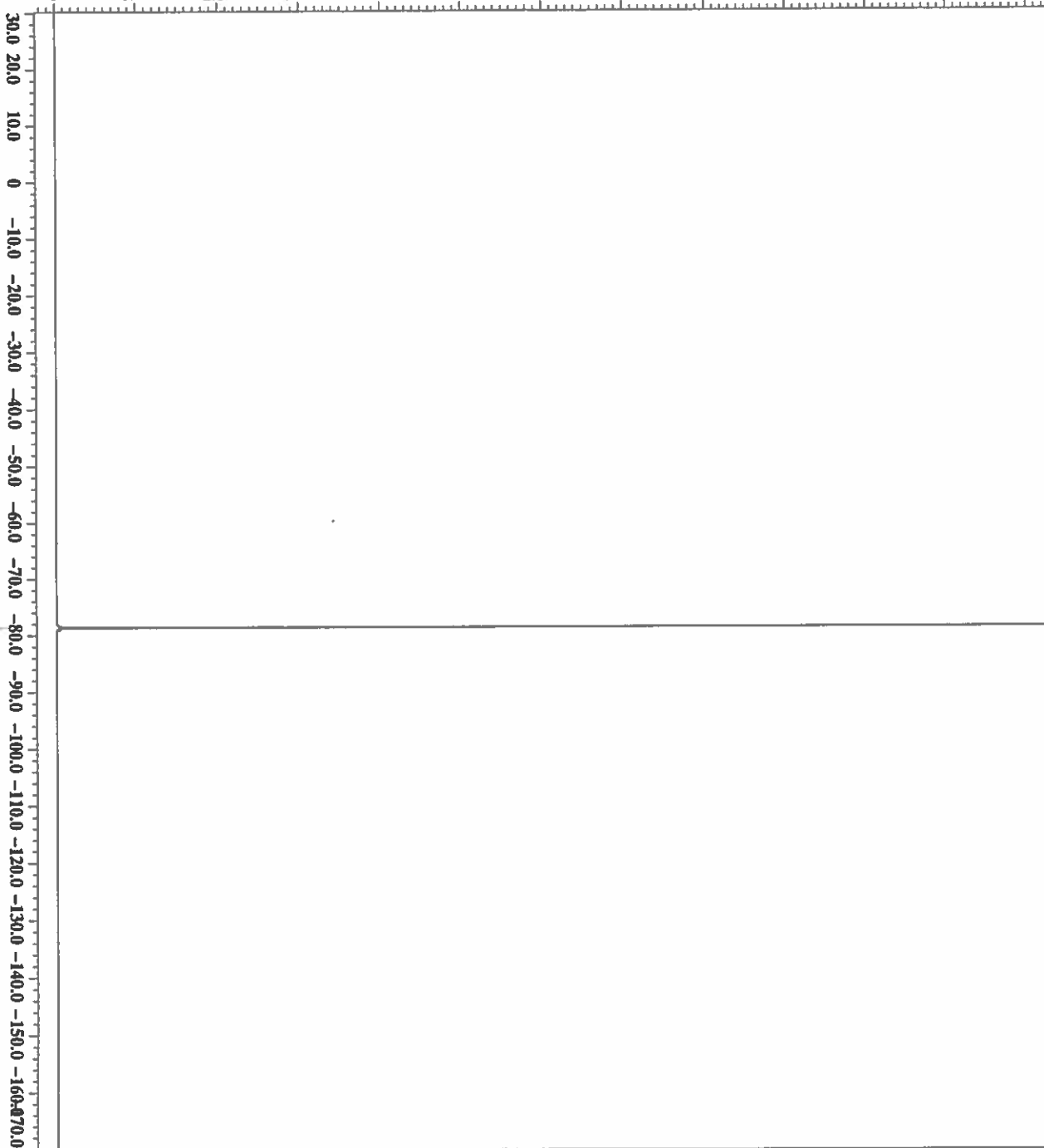


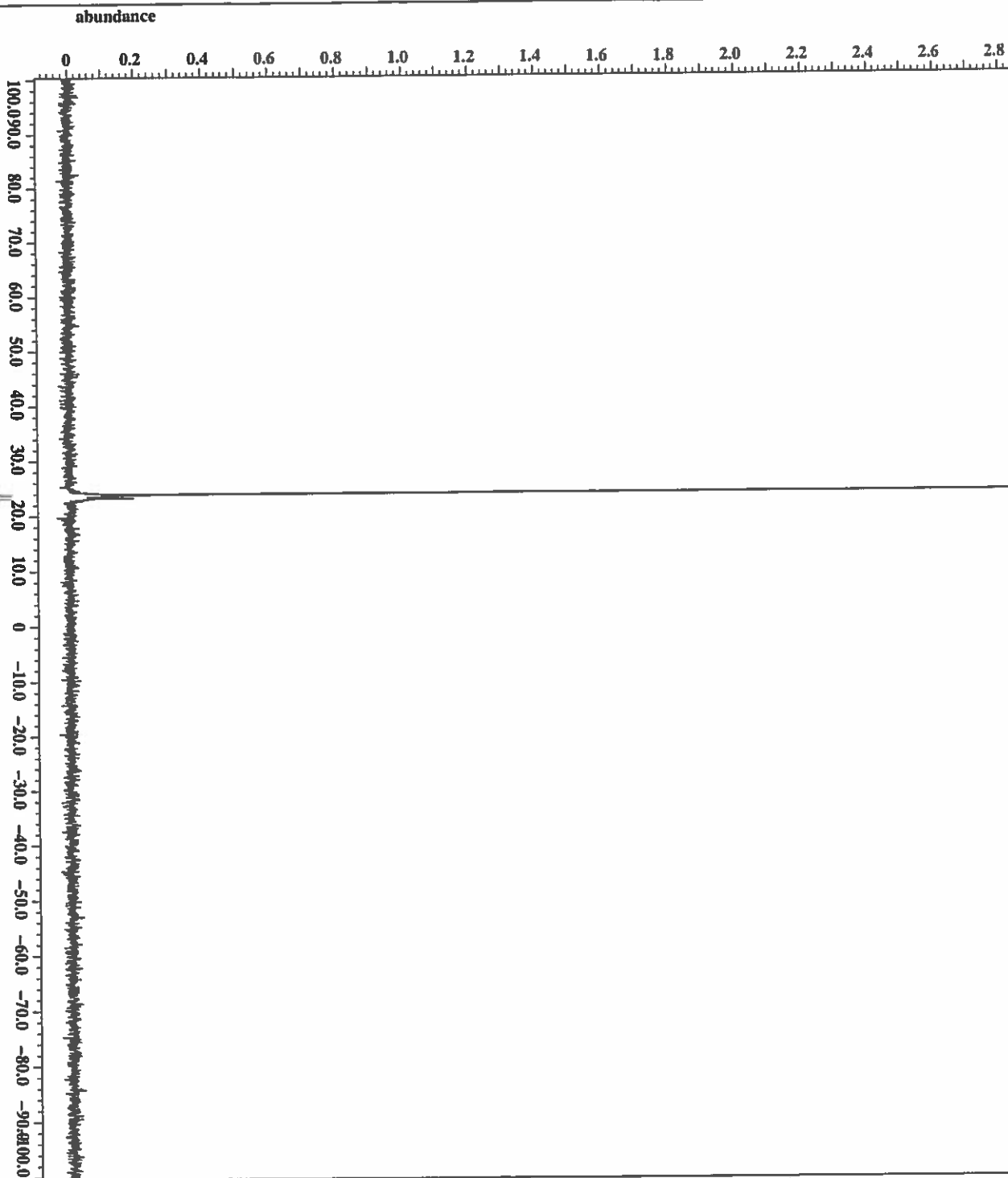
Filename
 Author
 Experiment
 Sample_id
 Solvent
 Changer_sample
 Creation_time
 Revision_time
 Current_time

Data_format
 Dim_size
 Dim_circle
 Dim_units
 Dimensions
 Site
 Spectrometer

Field_strength
 X_acq_duration
 X_domain
 X_freq
 X_offset
 X_points
 X_prescans
 X_resolution
 X_sweep
 Itr_domain
 Itr_freq
 Itr_offset
 Tr1_domain
 Tr1_freq
 Tr1_offset
 Clipped
 Mod_return
 Scans
 Total_scans

X_90_width
 X_acq_time
 X_angle
 X_atn
 X_pulse
 Itr_mode
 Tr1_mode
 Dancet_preset
 Initial_wait
 Recvr_gain
 Relaxation_delay
 Repetition_time
 Temp_get





```

Filename      = MS0441-300-96h_PHOSPH
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0441-300-96h
Solvent       = CHLOROFORM-D
Charger_sample = 4
Creation_time  = 14-MAY-2018 23:42:58
Revision_time  = 14-MAY-2018 23:18:43
Current_time   = 14-MAY-2018 23:16:43

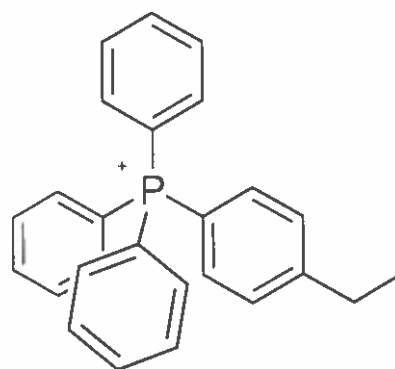
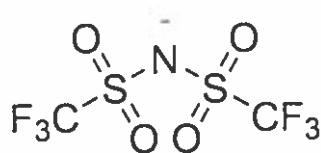
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_t1       = 31P
Dim_t2       = [ppm]
Dimensions    = X
PQA 500
Site          = JNM-ECA500
Spectrometer

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.64487424 [s]
X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 33768
X_prescans     = 4
X_resolution   = 1.55068995 [Hz]
X_sweep        = 50.81300813 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 50
Total_scans    = 50

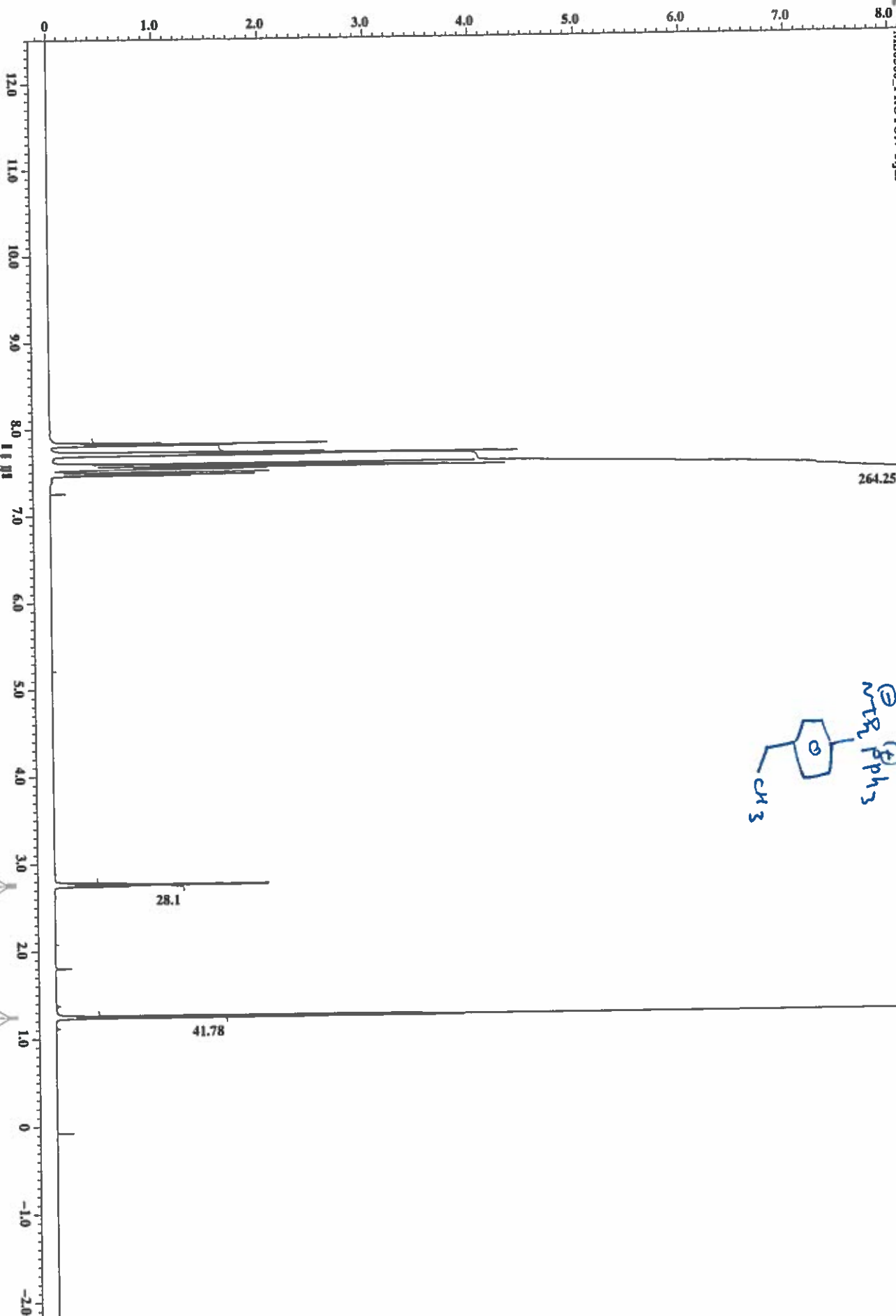
X_90_width     = 14.687 [us]
X_acq_time     = 0.64487424 [s]
X_angle        = 30 [deg]
X_atn          = 5 [dB]
X_pulse        = 4.89566667 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_hoe    = 20.7 [dB]
Irr_noise      = VALVE
Decoupling     = TRUZ
Initial_wait    = TRUZ
Nuc_time       = 2 [s]
Nuc             = 31P
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.64487424 [s]
Temp_set       = 22.9 [C]
  
```

Compound 12 Pre- and Post-heating NMR Spectra

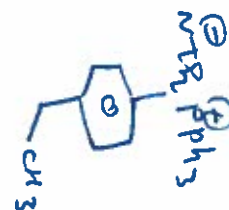
Temperature of Post-heating samples noted in upper left corner of each spectrum

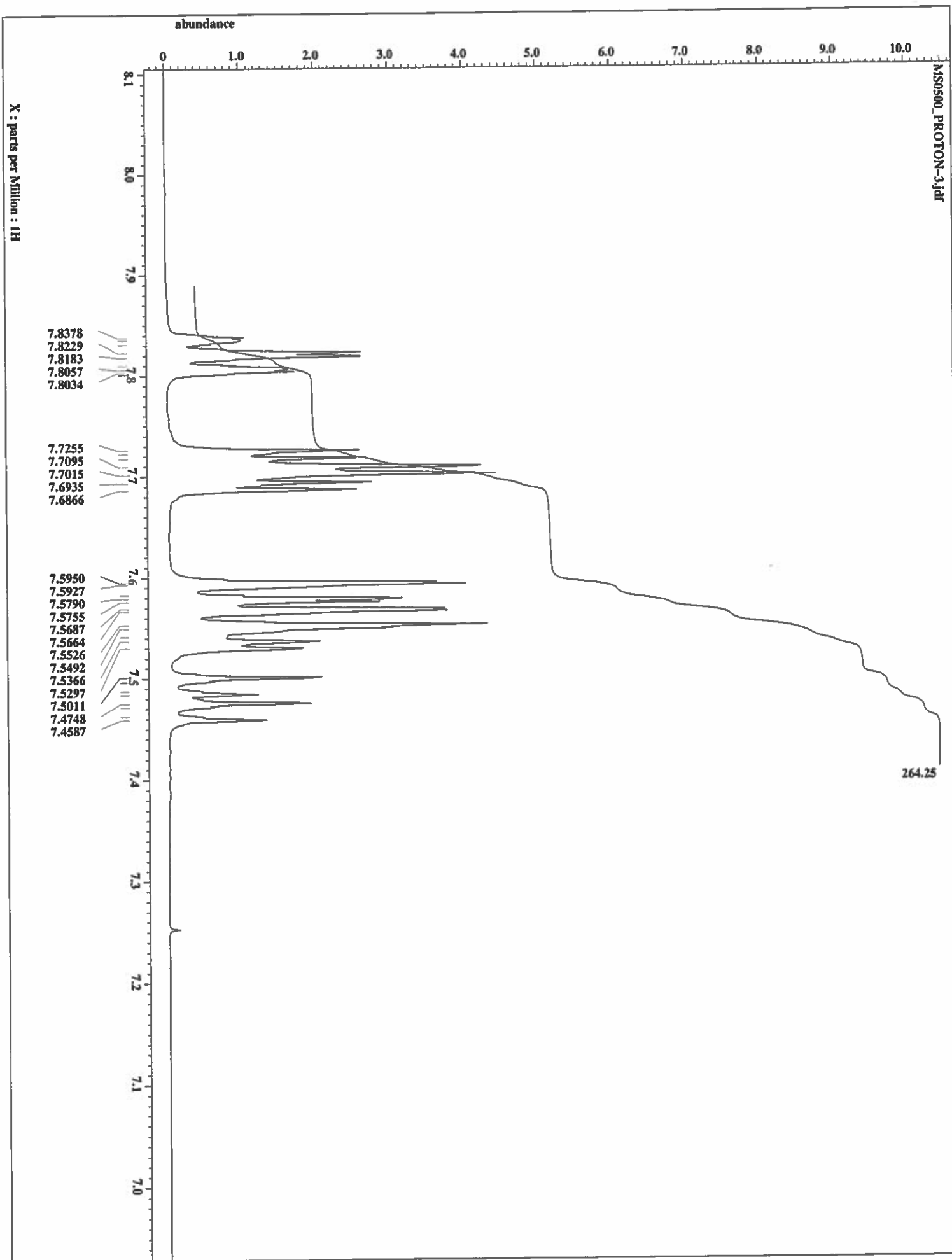


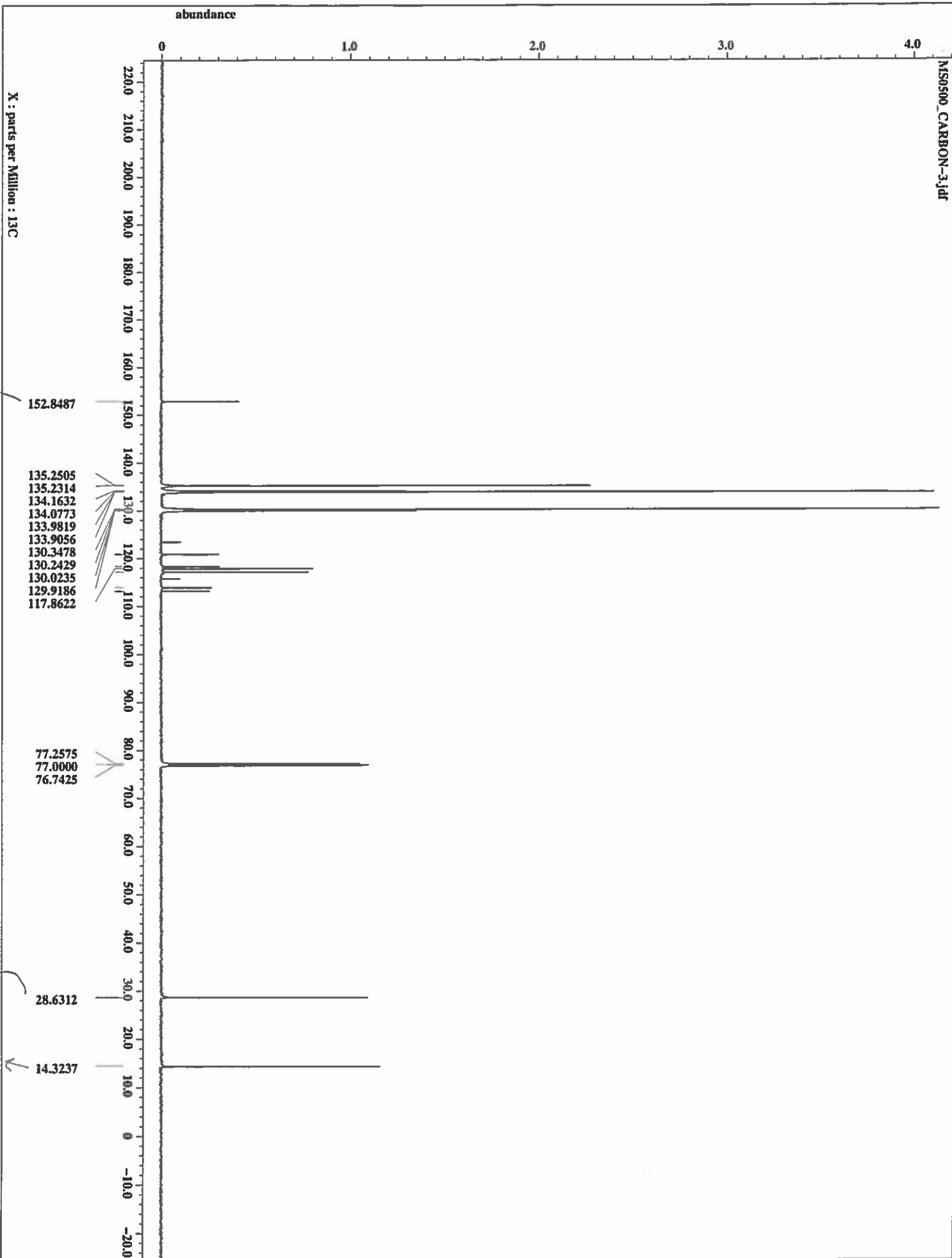
abundance

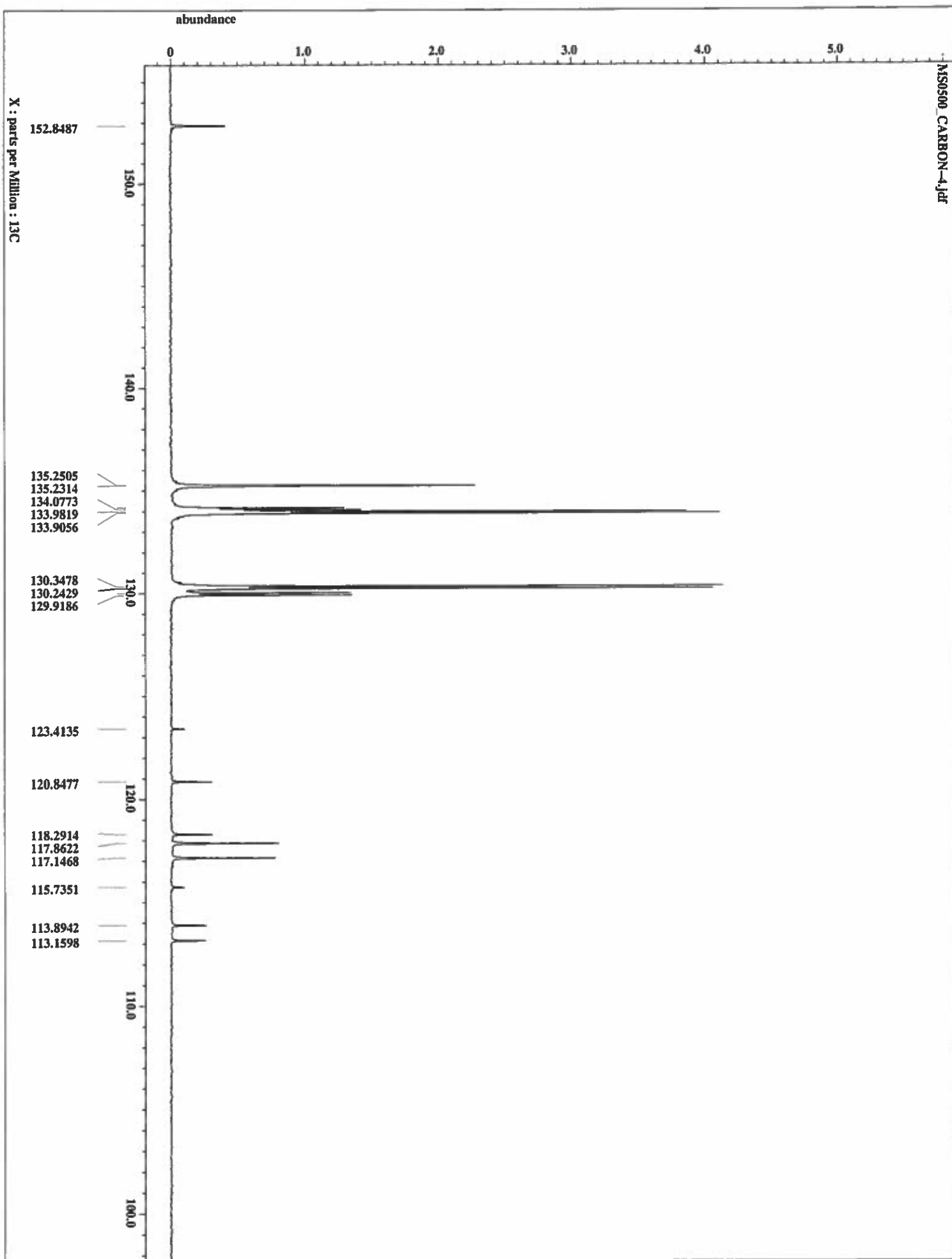


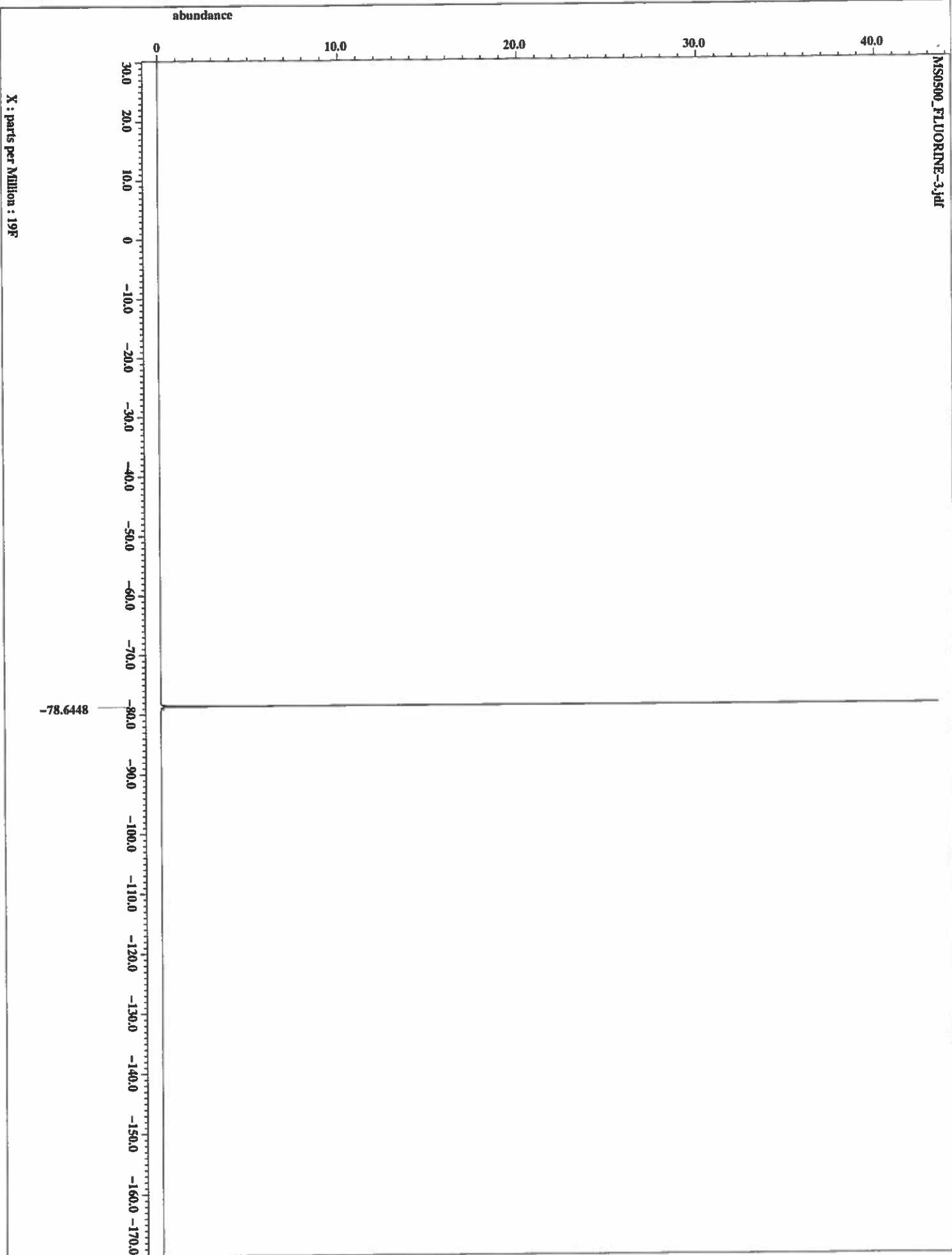
X : parts per Million : 1H











abundance

30.0

20.0

10.0

0

100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0

23.4516

X : parts per Million : 31P

abundance

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3 2.4 2.5 2.6 2.7 2.8

X : parts per Million : 1H

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
-1.0
-2.08.2191
8.2123
7.7107
7.7038
7.5939
7.5778
7.5687

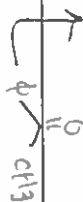
2.95

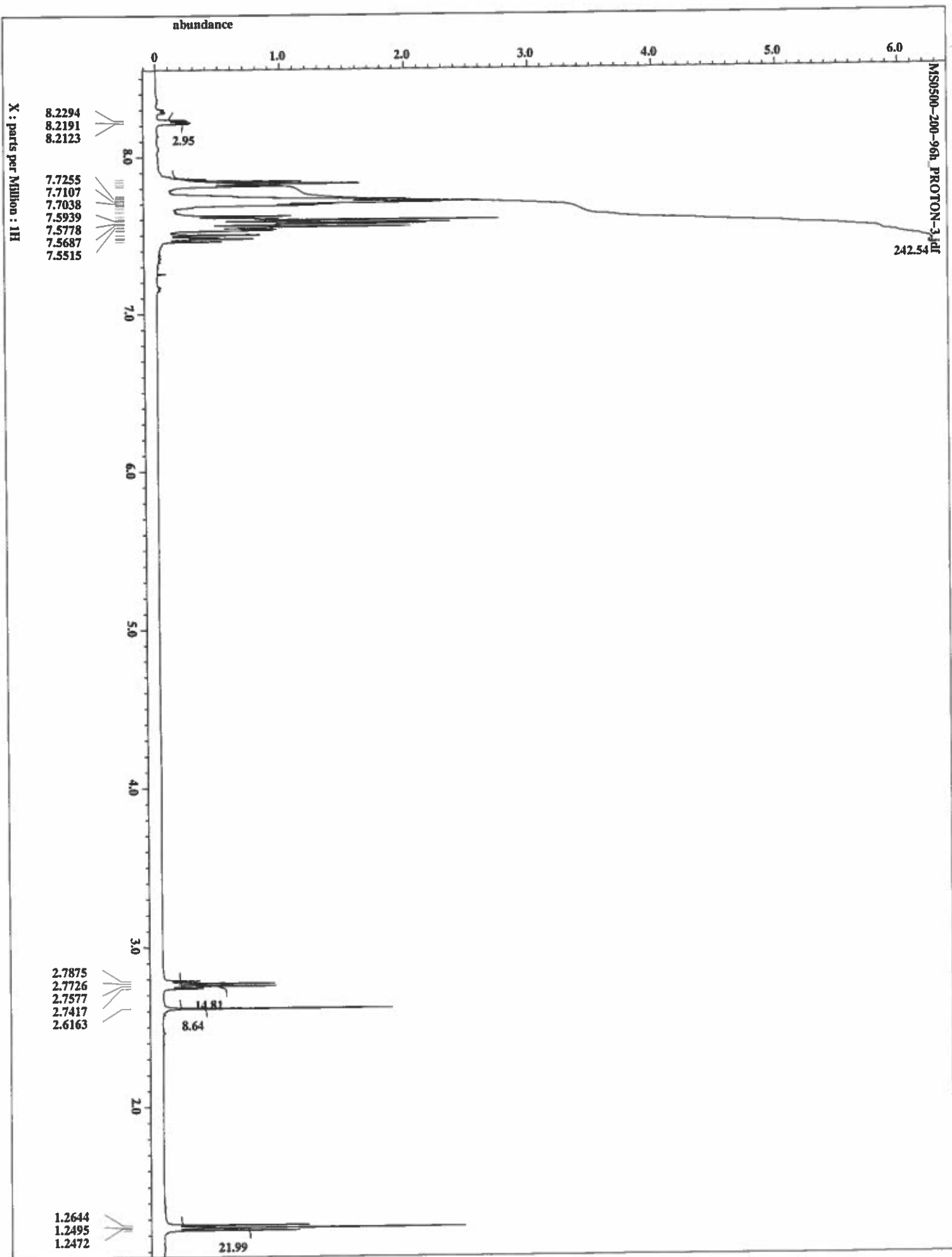
242.54

2.7726
2.7577
2.616313.81
8.641.2644
1.2495
1.2472

21.99

14.00 - 14.50 Hz





abundance

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6

196.8681

X : parts per Million : 13C

190.0

180.0

170.0

160.0

152.8964

150.0

141.5649

140.0

134.1250

134.0487

134.0010

133.9247

130.5577

130.4528

130.3669

130.2620

130.0

123.3753

122.4215

121.7252

120.8190

120.0

118.2628

117.8717

117.1563

116.9083

116.2025

113.9133

113.1789

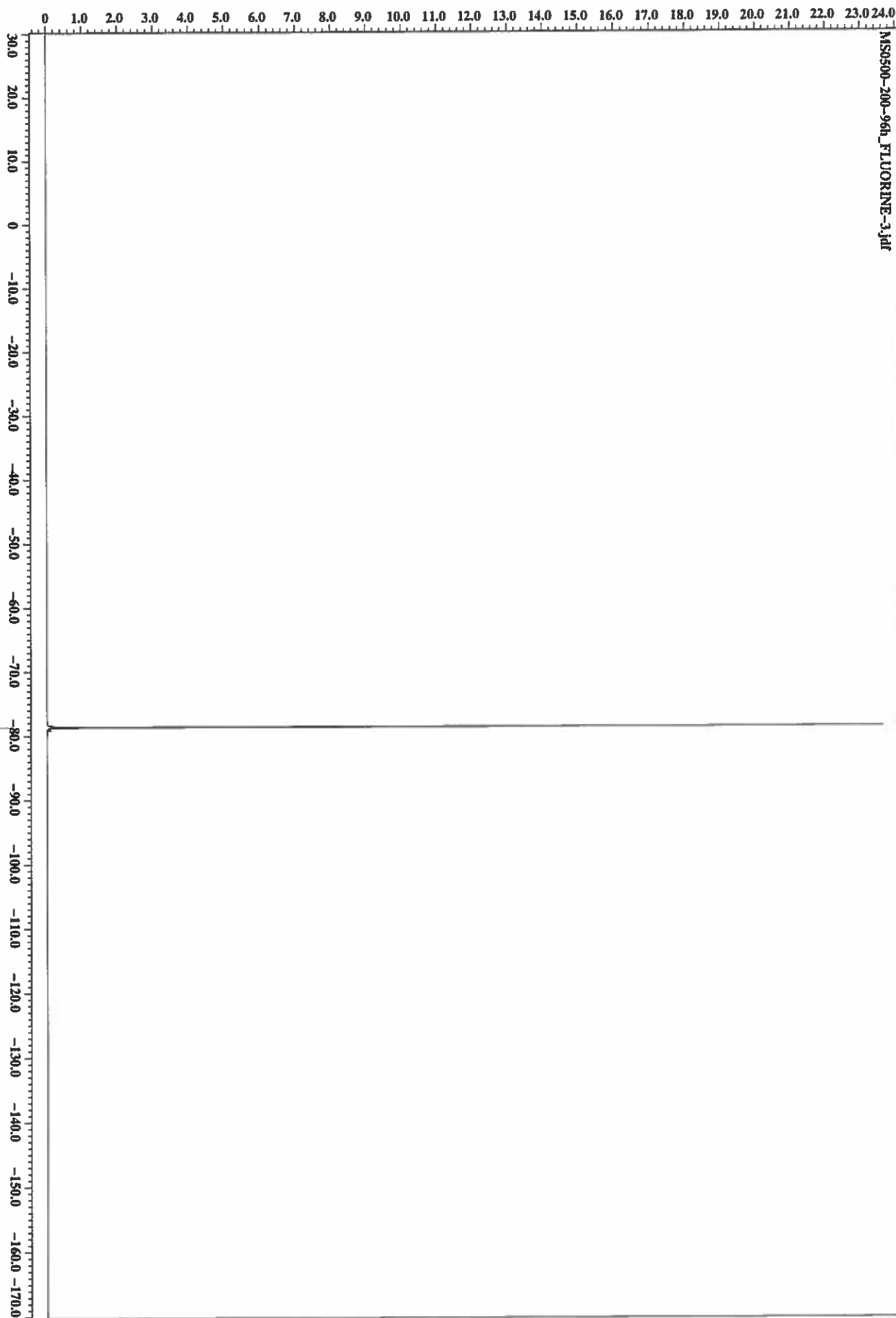
110.0

KETON 3

CARB. 2



abundance



X : parts per Million : 19F

-78.6601

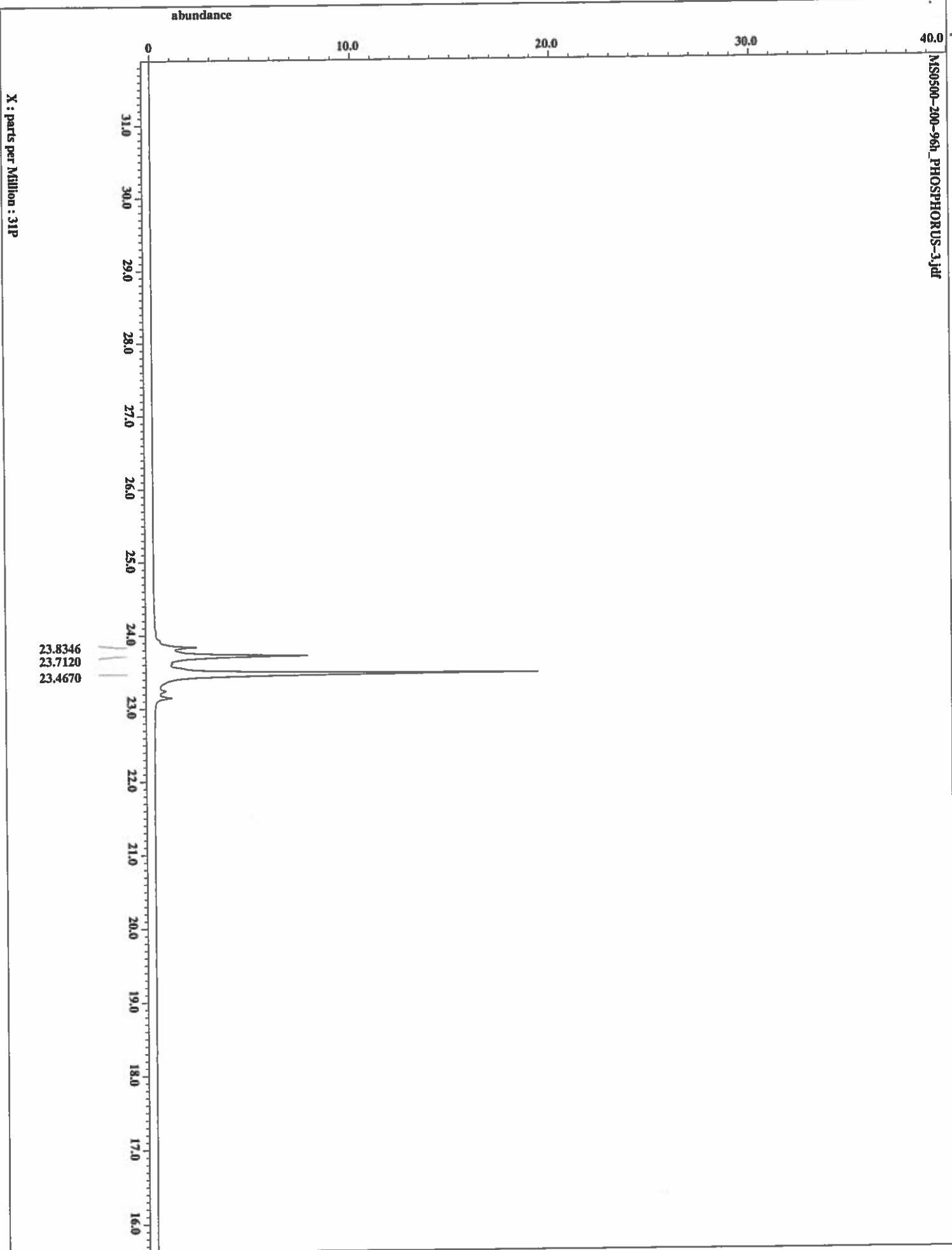
abundance

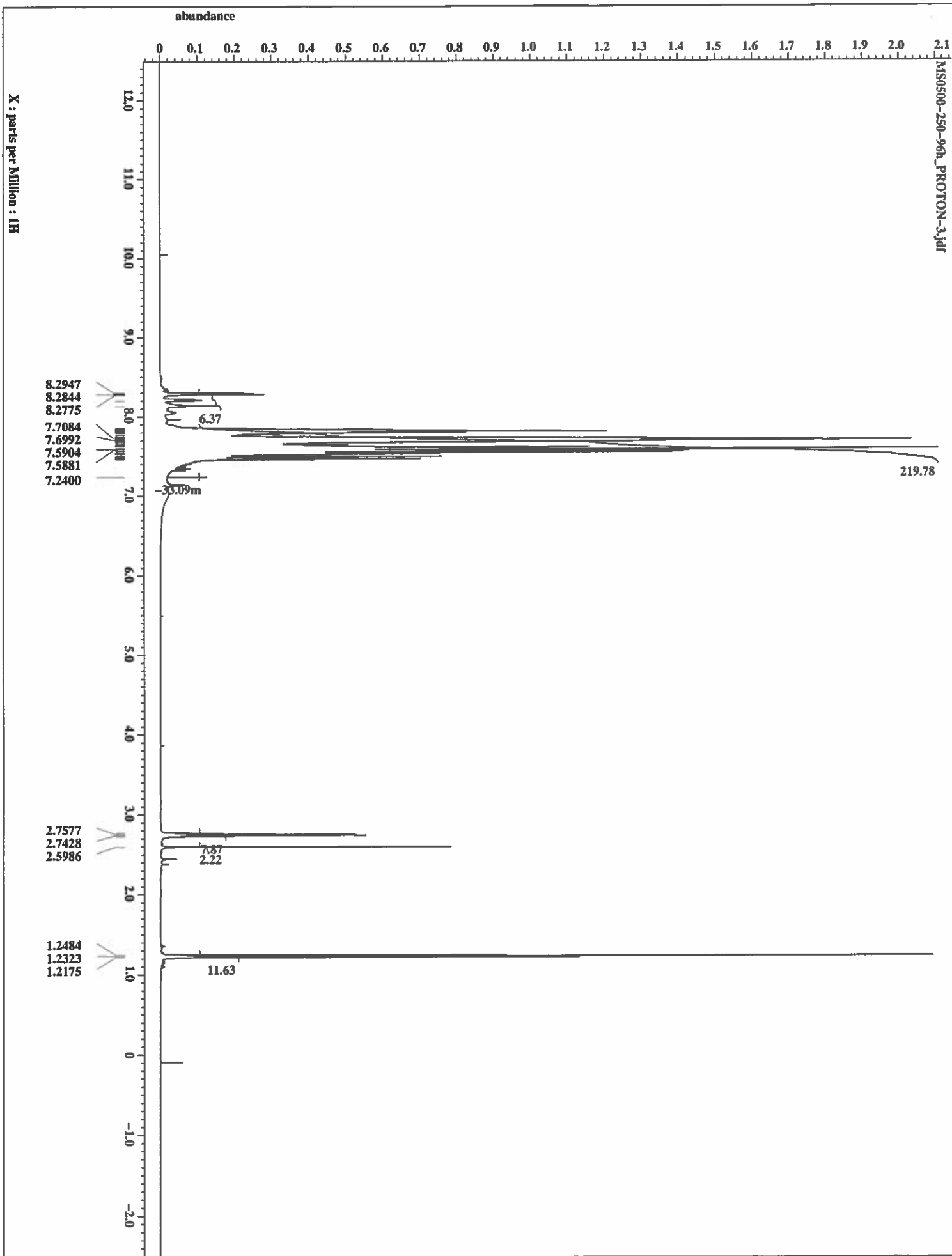
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0

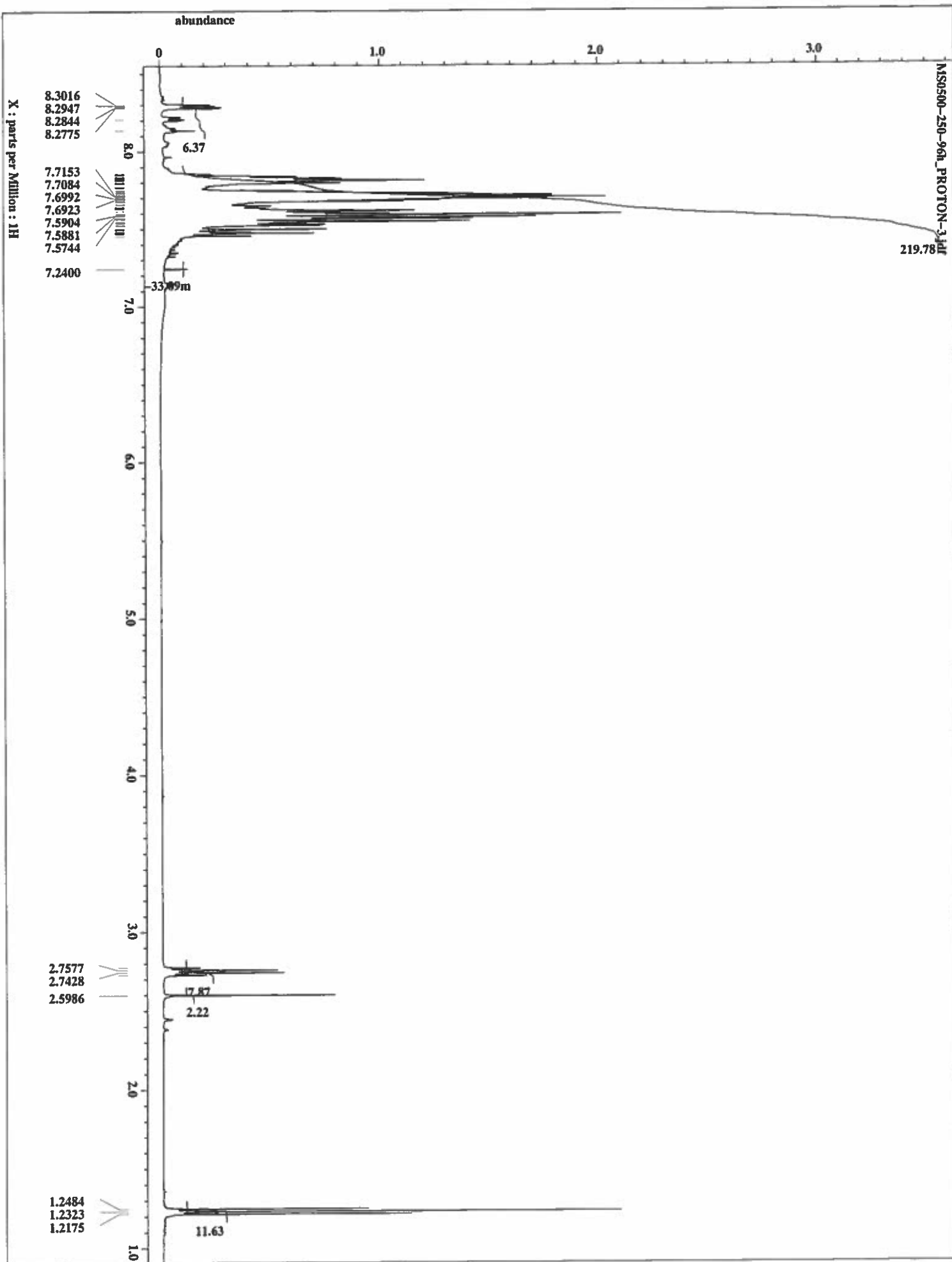
100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0

23.8346
23.7120
23.4670

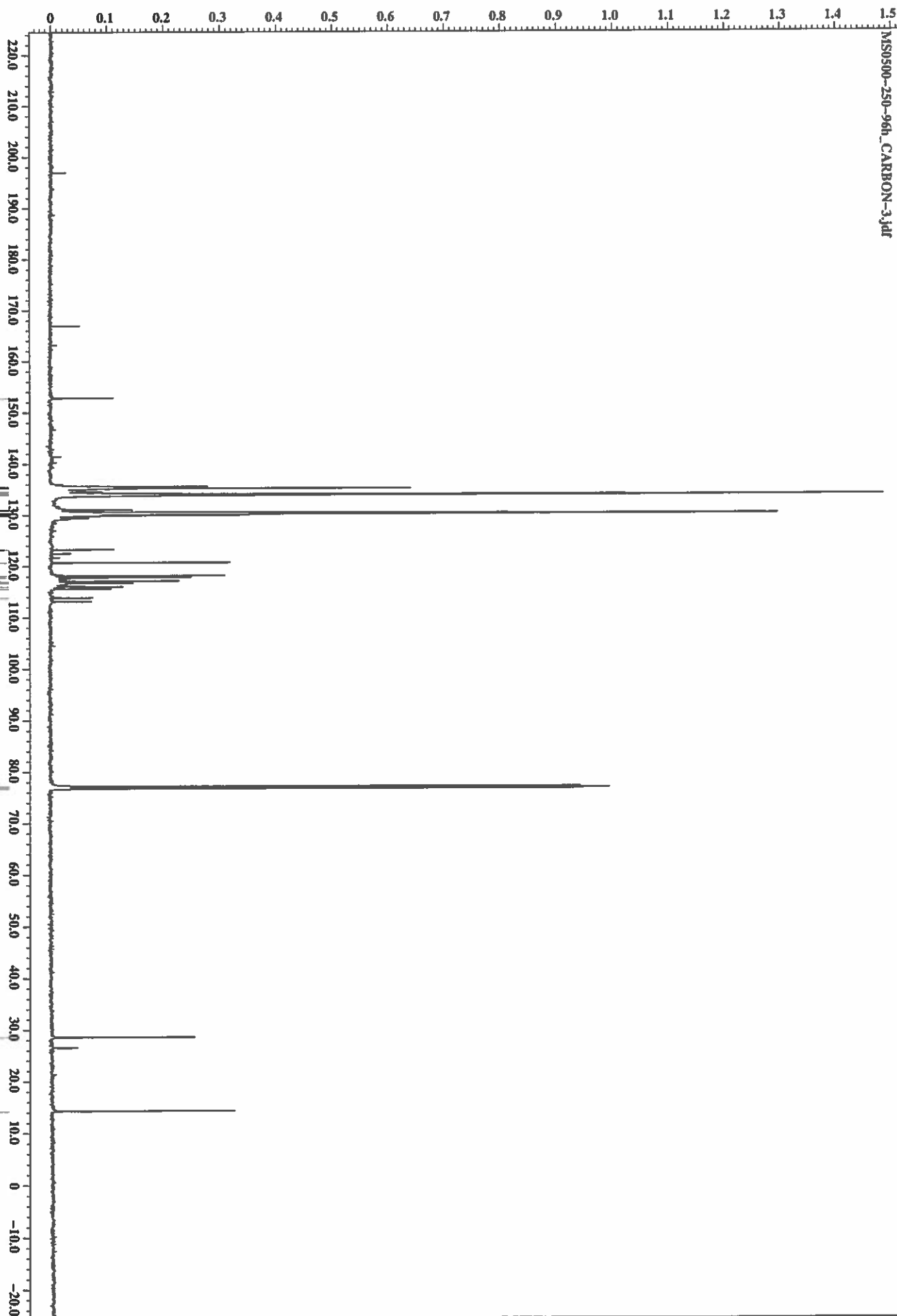
X : parts per Million : 31P





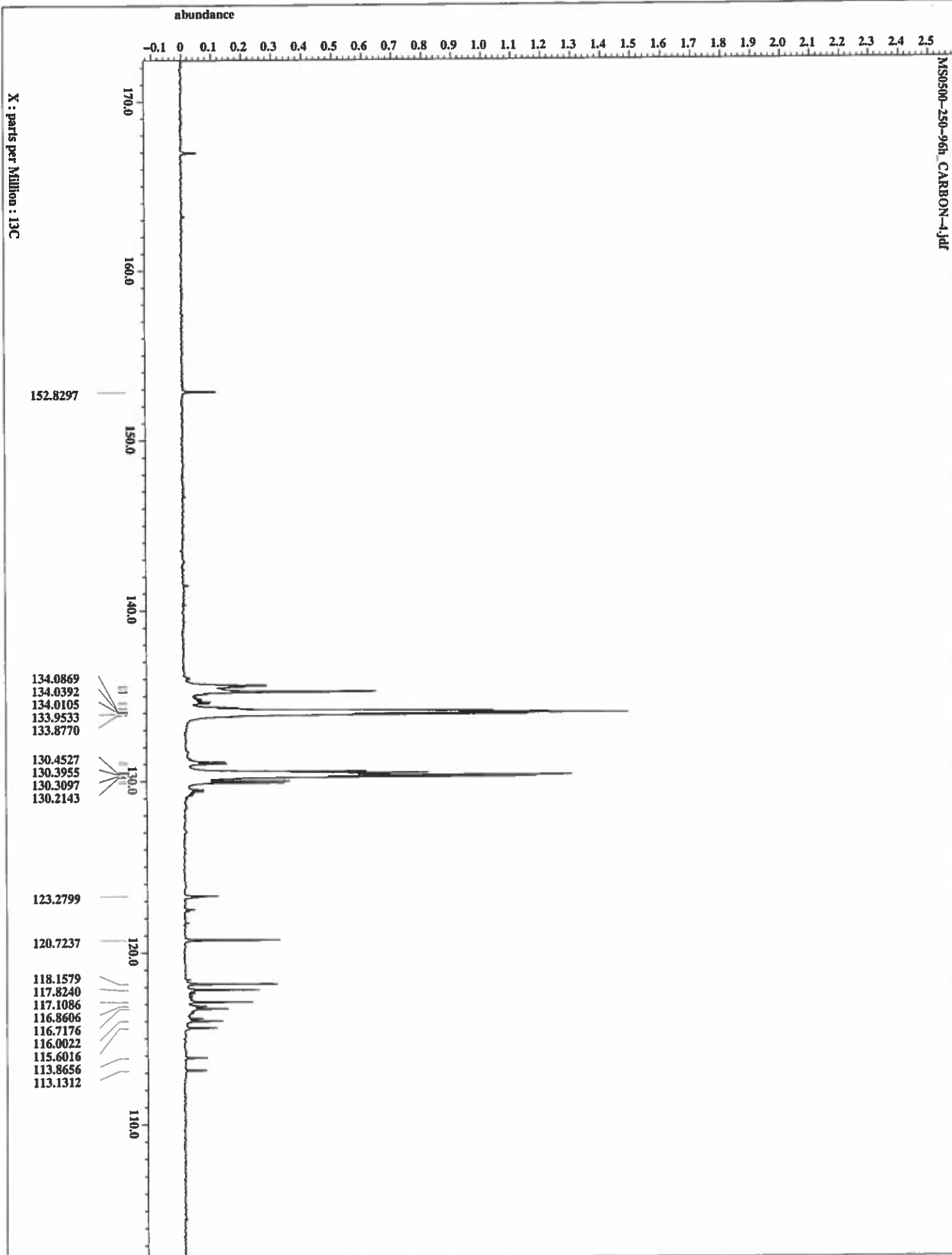


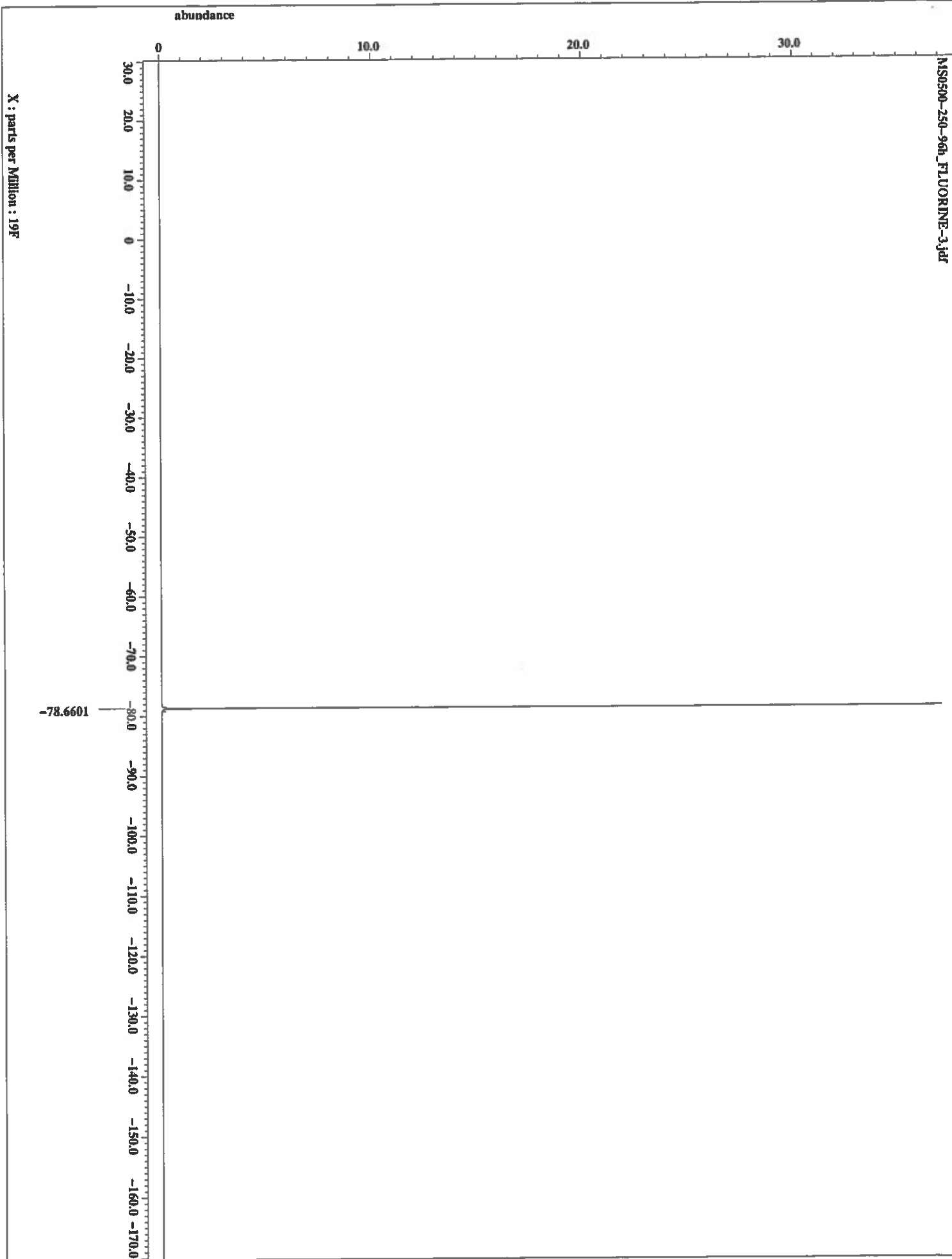
abundance

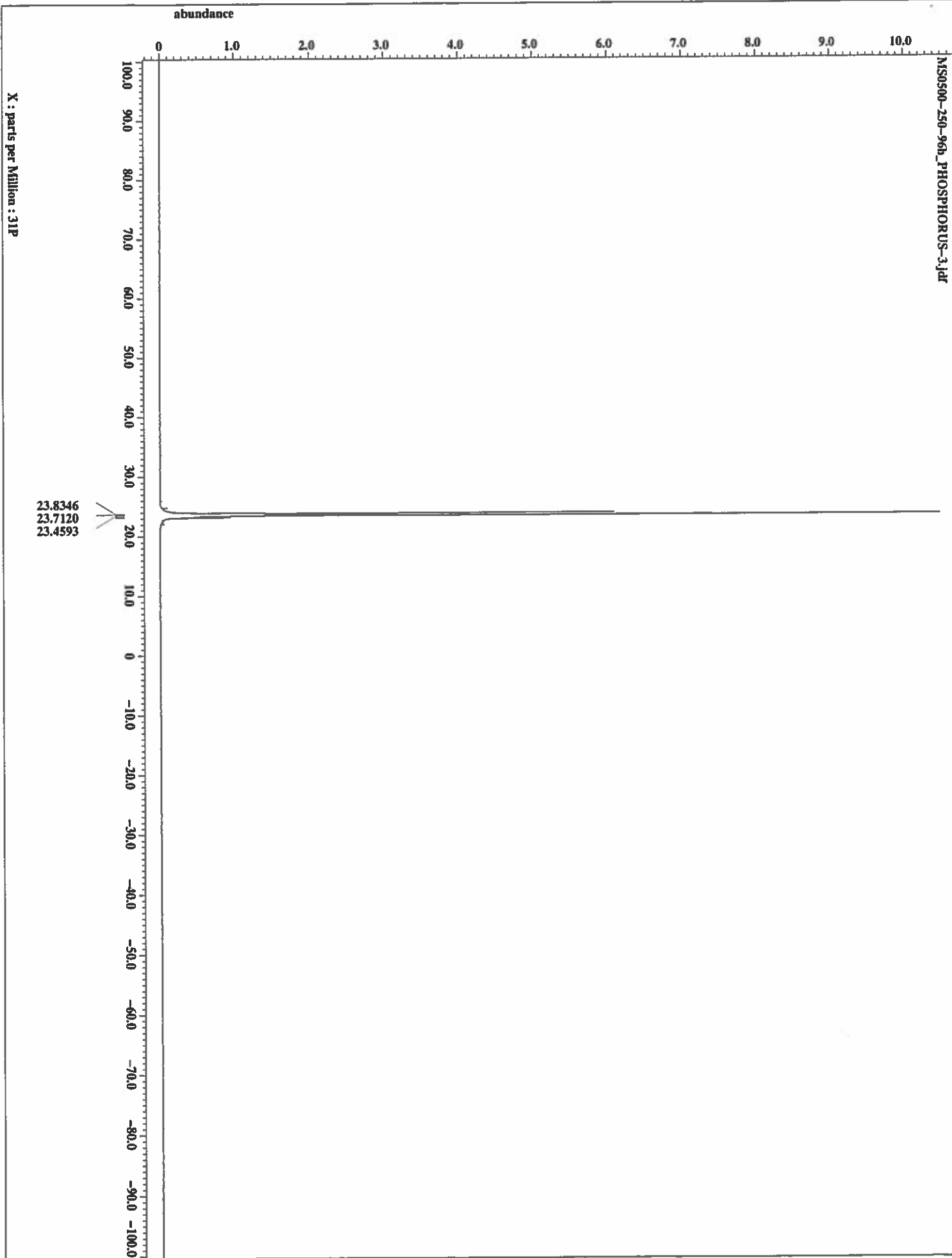


X : parts per Million : 13C

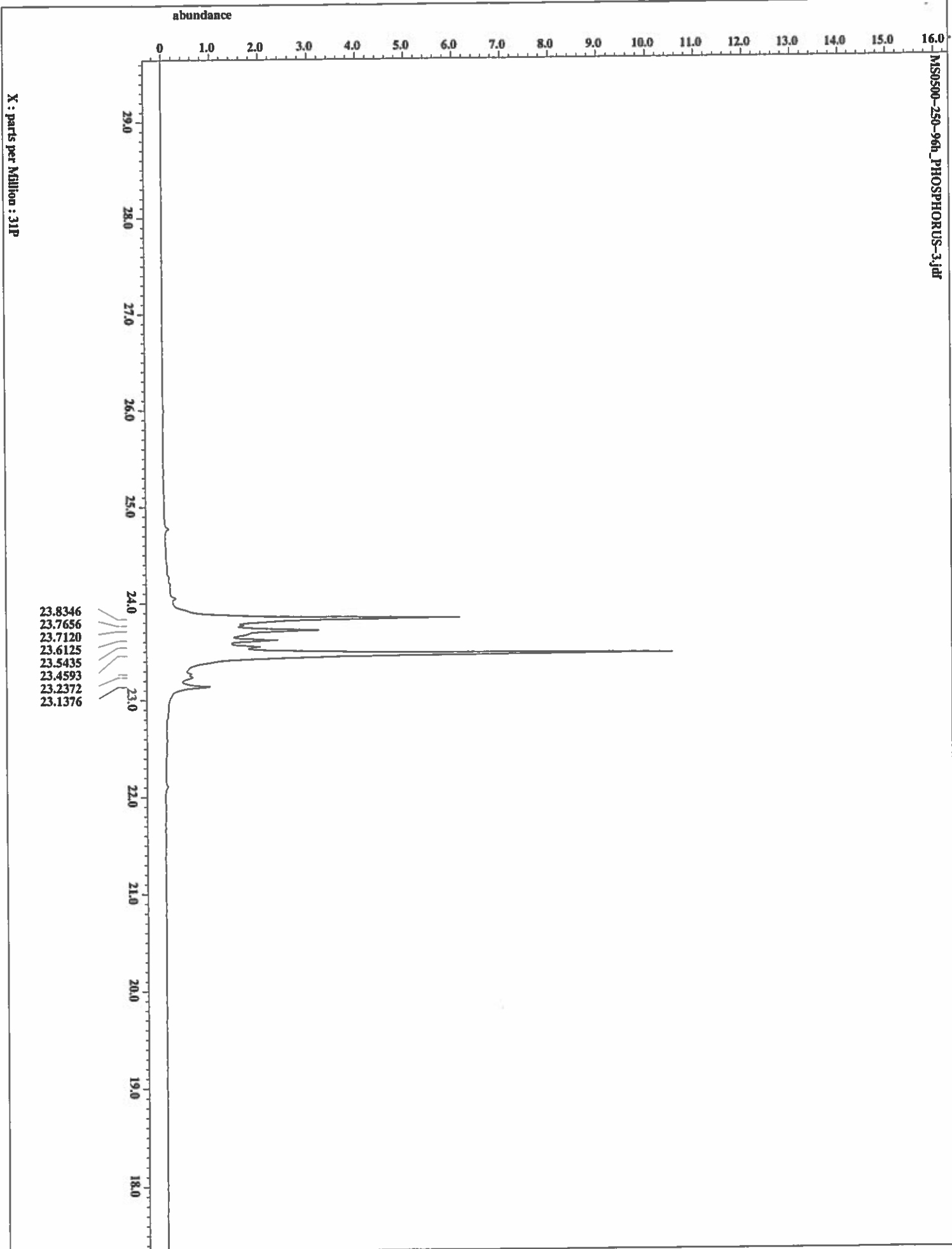


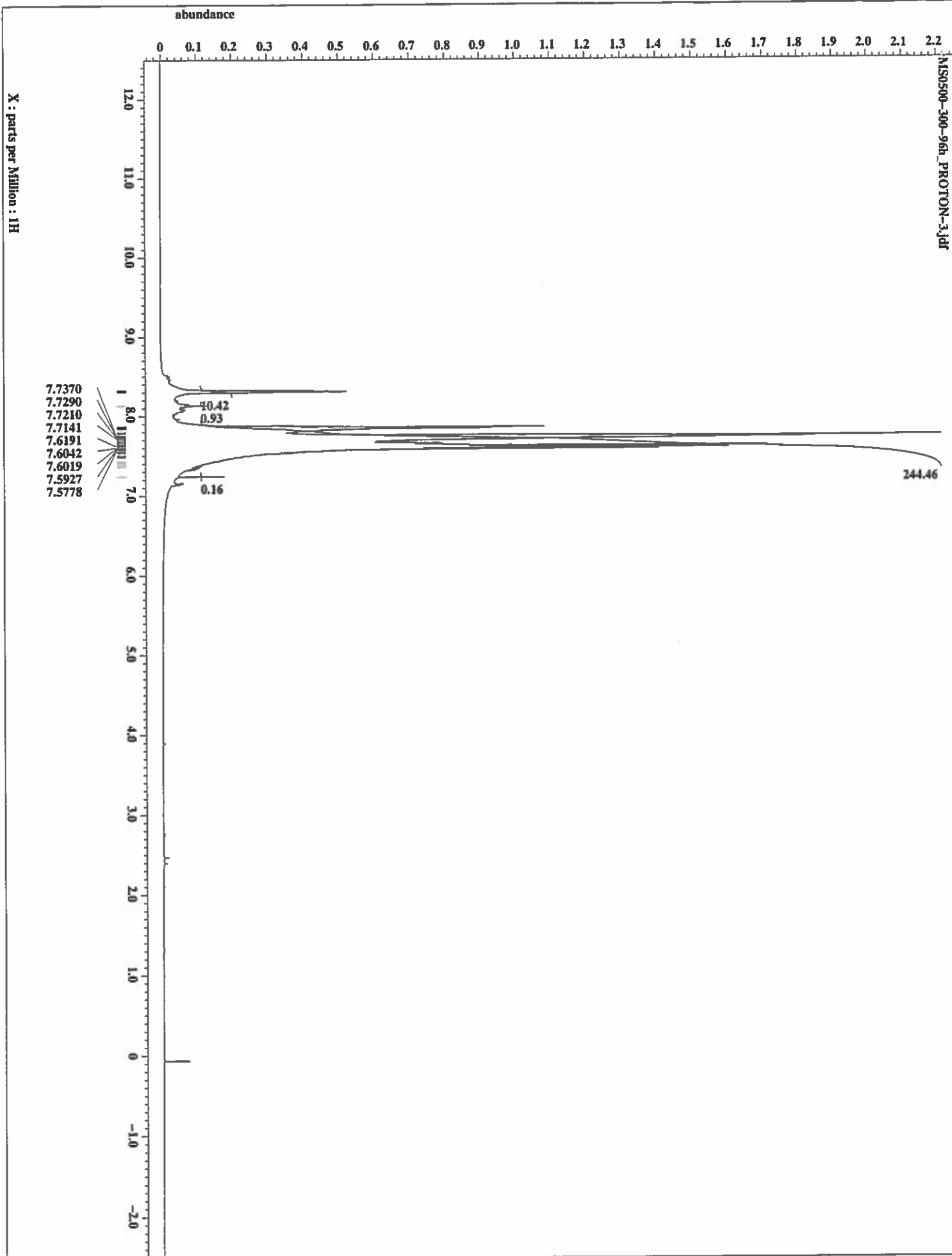


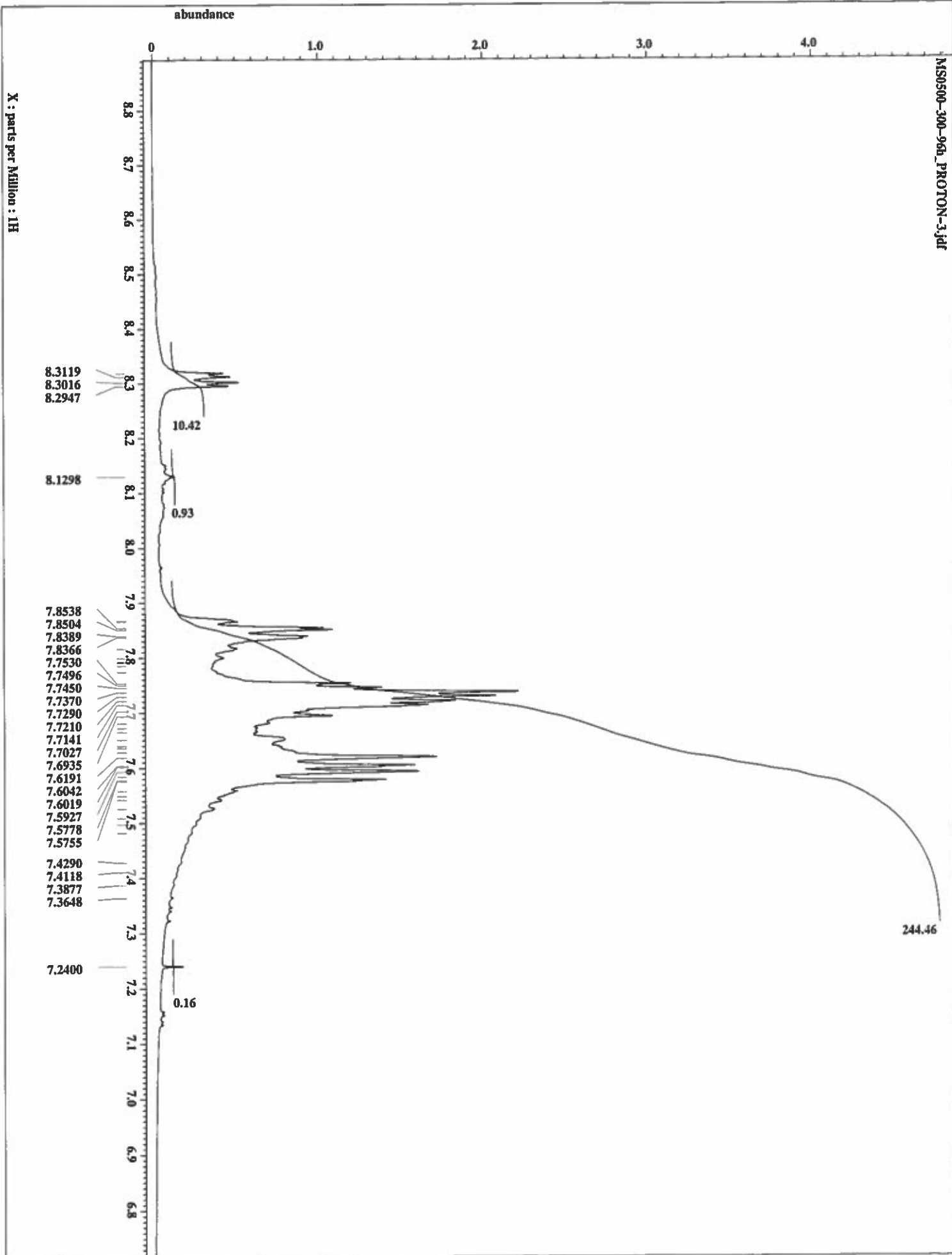


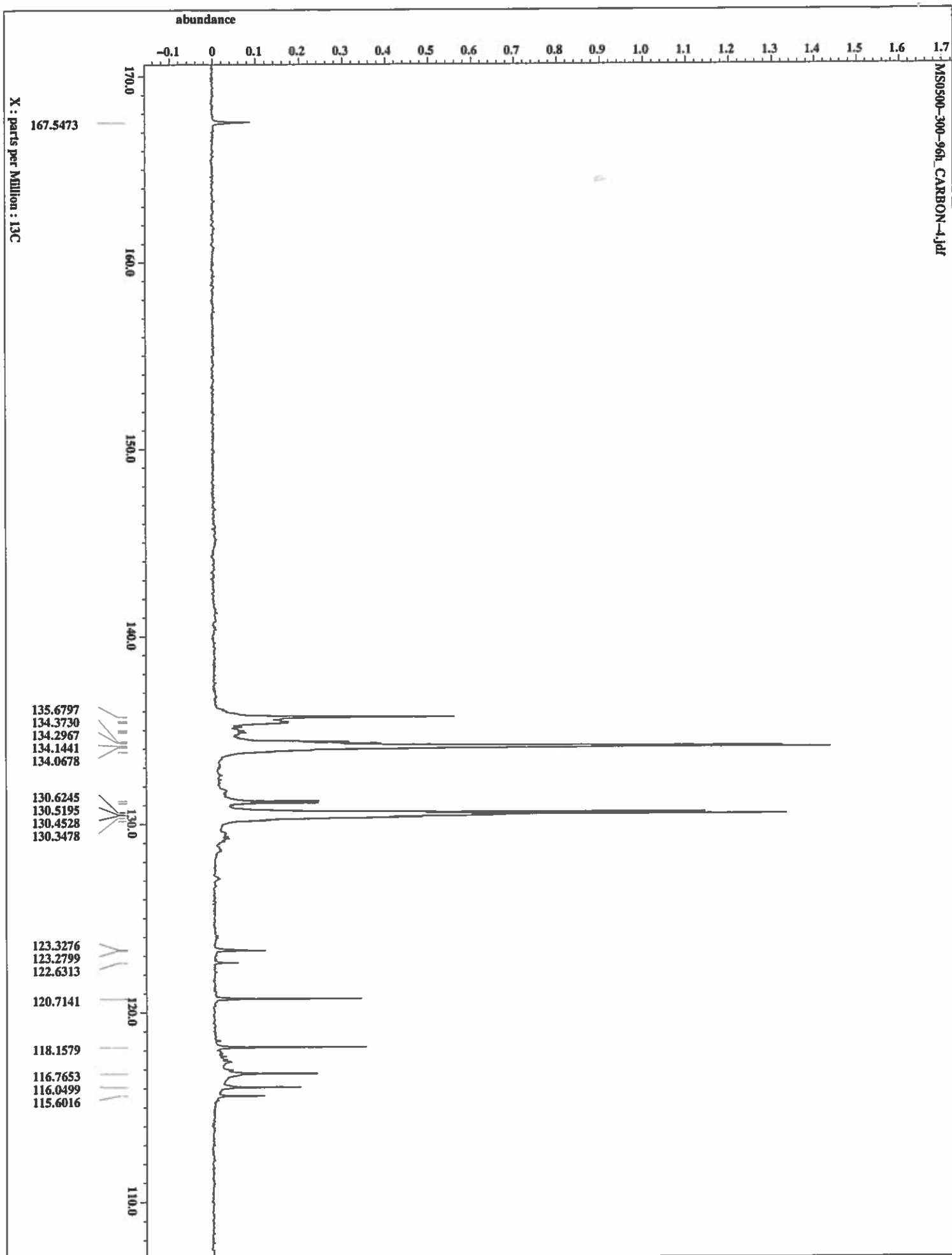


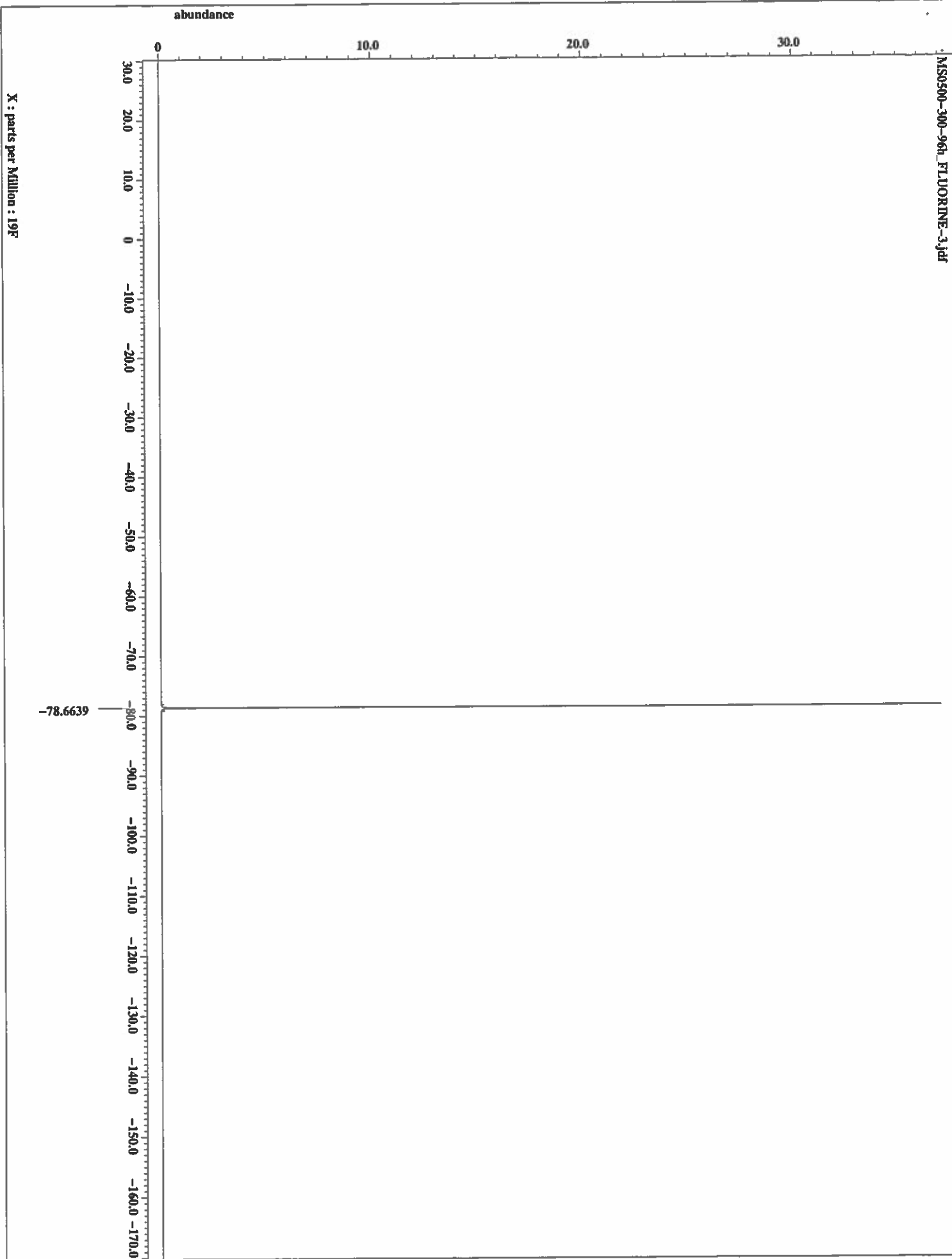
X : parts per Million : 31P

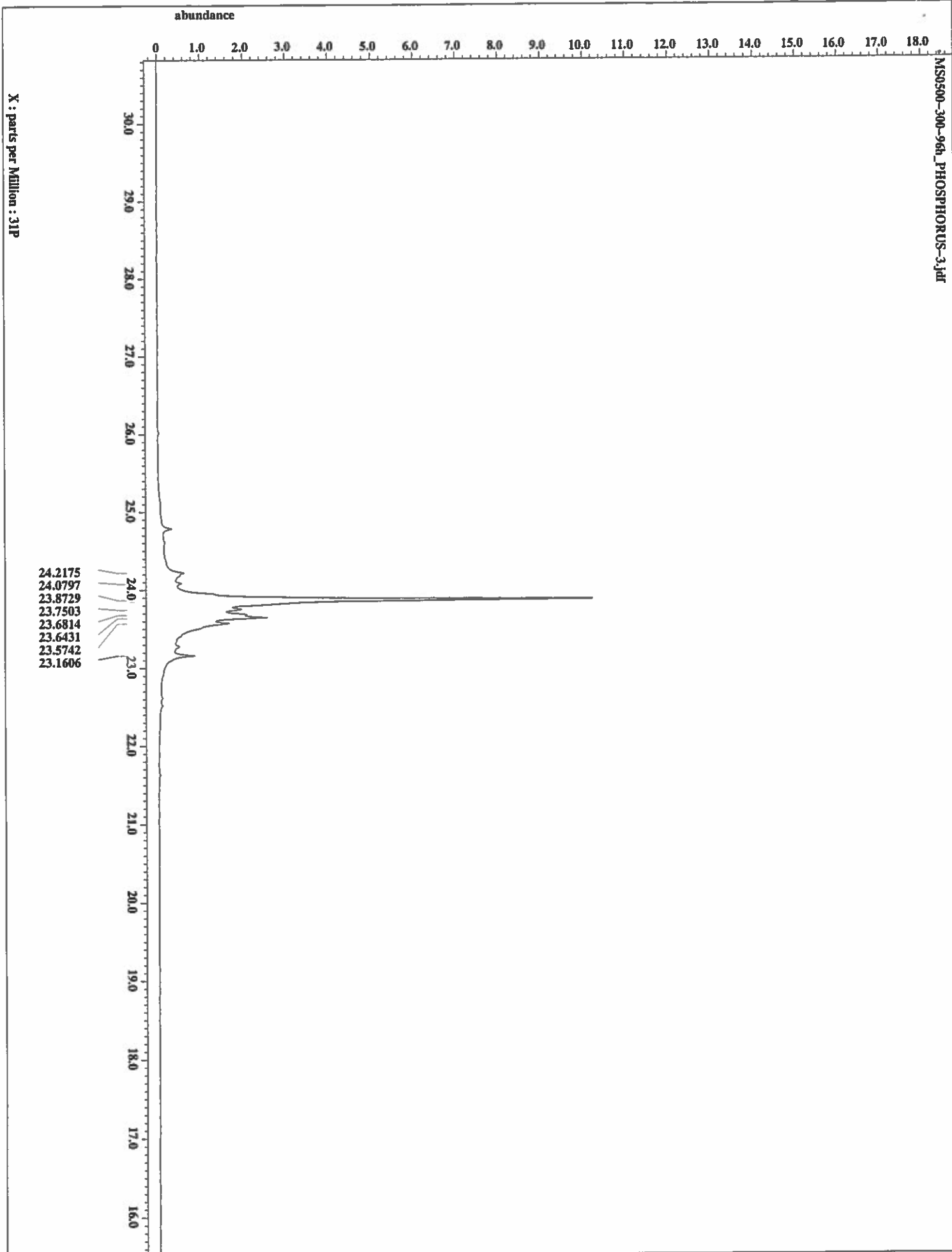






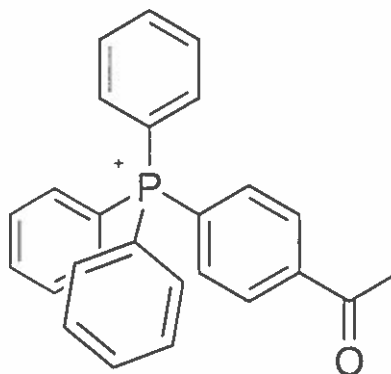
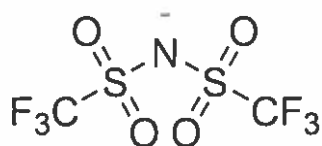


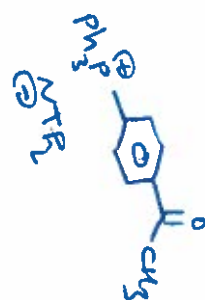




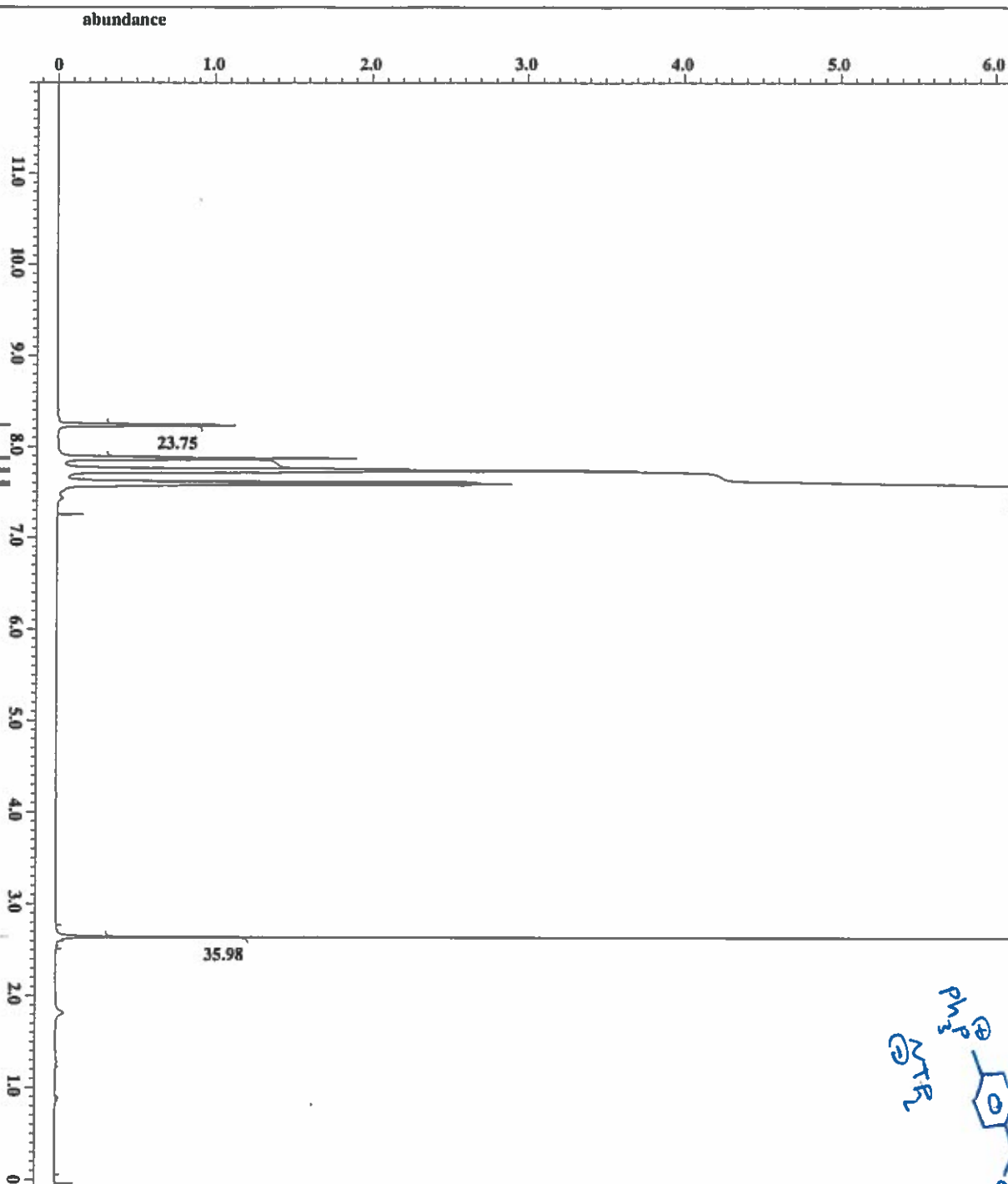
Compound 13 Pre- and Post-heating NMR Spectra

Temperature of Post-heating samples noted in upper left corner of each spectrum





SOUTH ALABAMA
JAGUARS



X : parts per Million : 1H

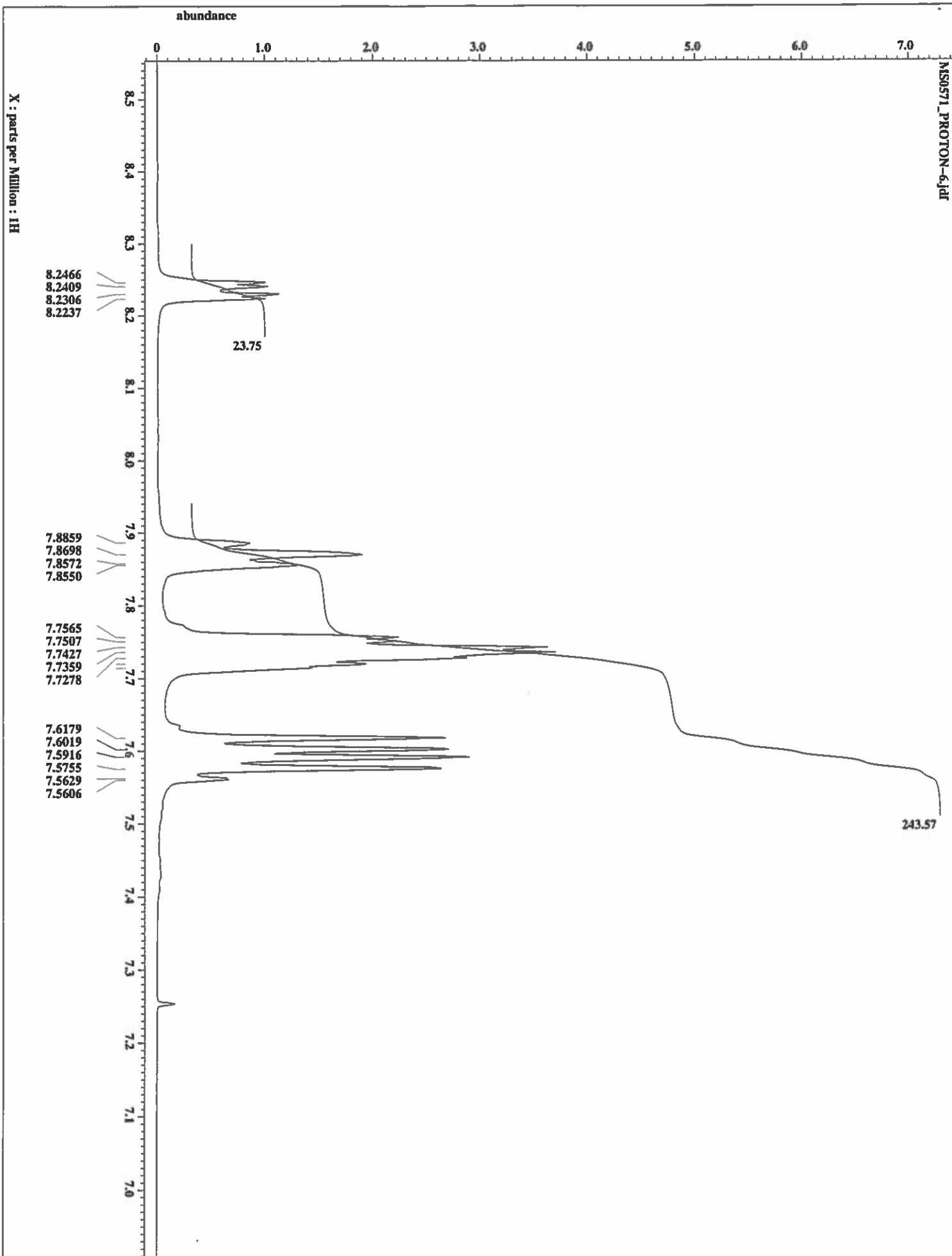
```

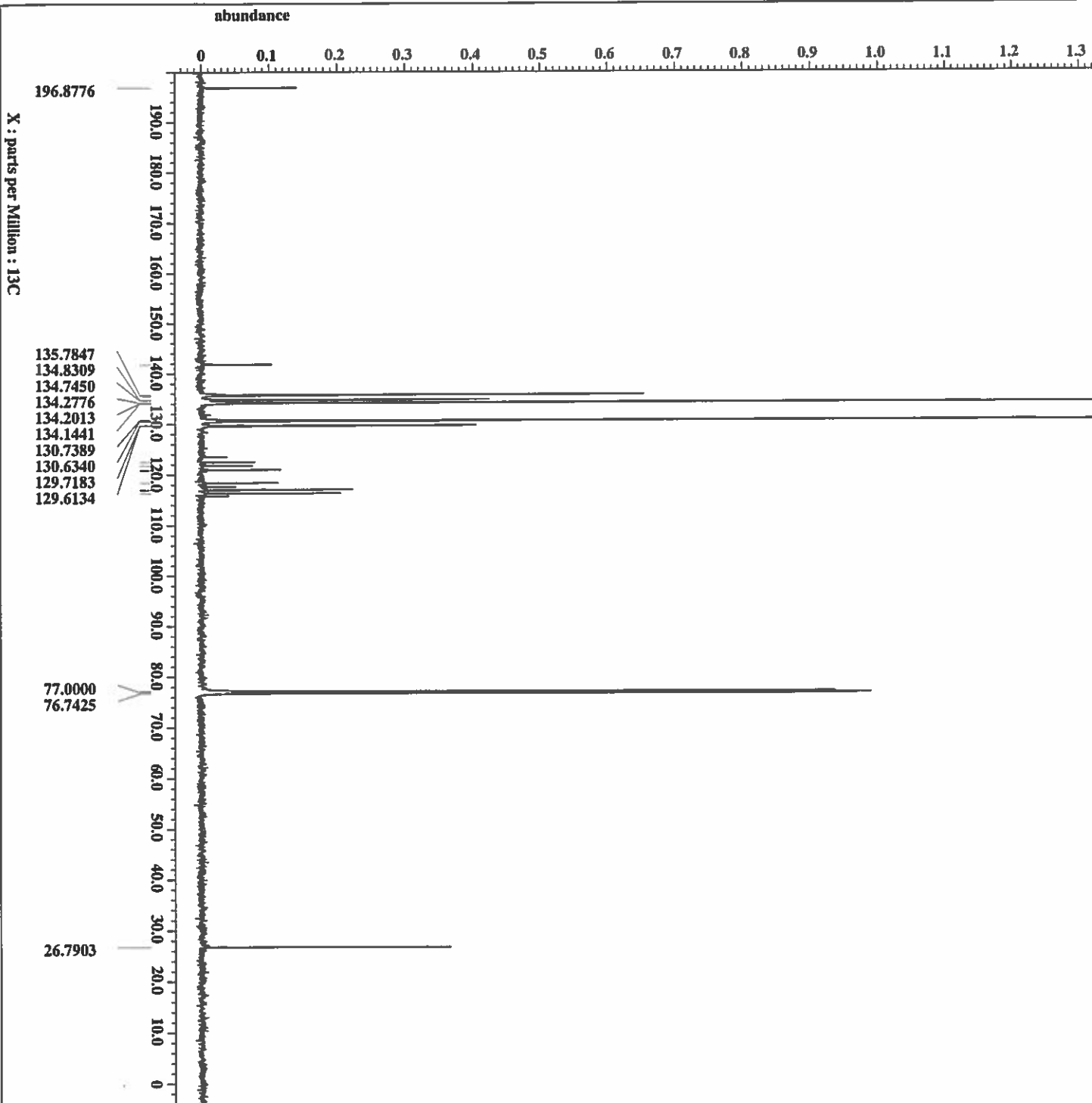
File: MS0571_PROTON-5.jdt
Author: Jim Davis
Experiment: single_pulse.ex2
Sample ID: MS0571
Solvent: CHLOROFORM-D
Creation time: 24-OCT-2018 11:17:36
Revision time: 24-OCT-2018 10:54:07
Current time: 24-OCT-2018 10:54:07

Data format: 1D COMPLEX
Dim size: 13107
Dim title: 1H
Dim units: [ppm]
Dimensions: X
Site: ECA 500
Spectrometer: JNM-ECA500

Field strength: 11.7473579 [T] (500 [MH
X_acq_duration: 1.74587904 [s]
X_domain: 1H
X_freq: 500.15991521 [MHz]
X_offset: 5.0 [ppm]
X_points: 16384
X_prescans: 1
X_resolution: 0.57277737 [Hz]
X_sweep: 9.38438436 [kHz]
X_domain: 1H
X_freq: 500.15991521 [MHz]
X_offset: 5.0 [ppm]
X1_domain: 1H
X1_freq: 500.15991521 [MHz]
X1_offset: 5.0 [ppm]
X1_offset: 5.0 [ppm]
Mod return: FALSE
Scans: 1
Total_scans: 16

X_90_width: 12.4 [us]
X_acq_time: 1.74587904 [s]
X_angle: 45 [deg]
X_atn: 4 [dB]
X_pulse: 6.2 [us]
X_mode: OFE
X1_mode: OFE
Pulse_program: DANTE_PRESAT
Initial wait: 1 [s]
Recvr_gain: 28
Relaxation_delay: 4 [s]
Relaxation_time: 5.74587904 [s]
Temp_get: 21.5 [degC]
  
```





```

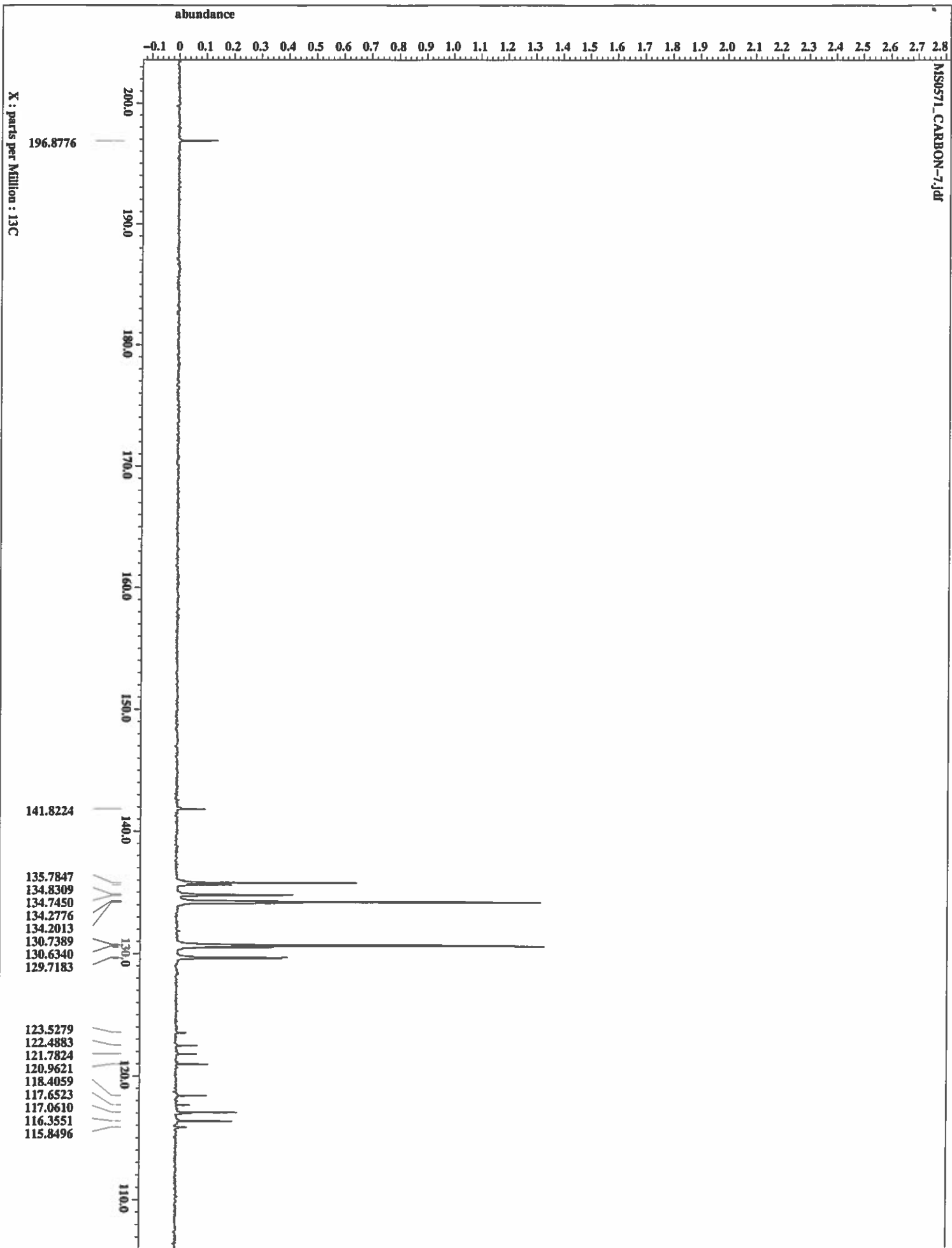
Filename      = MS0571 CARBON-5.jdt
Author        = Jim Davis
Experiment     = single_pulse_dec
Sample_id     = MS0571
Solvent       = CHLOROFORM-D
Creation_time  = 24-OCT-2018 11:39:16
Revision_time = 24-OCT-2018 11:15:47
Current_time  = 24-OCT-2018 11:15:47

Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

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]
Xir_domain     = 1H
Xir_freq       = 500.15991521 [MHz]
Xir_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 400
Total_scans    = 400

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Xir_atn_dec    = 20.7 [dB]
Xir_atn_noe    = 20.7 [dB]
Xir_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Recvt_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get       = 22.1 [dC]

```





```

Filename      = MS0571_FLUORINE-2.jdt
Author        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0571
Solvent       = CHLOROFORM-D
Creation_time  = 5-OCT-2018 12:15:39
Revision_time  = 5-OCT-2018 11:50:32
Current_time   = 5-OCT-2018 11:50:34

Data_format   = 1D COMPLEX
Dim_size      = 104857
Dim_title     = 19F
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.7340032 [s]
X_domain       = 19F
X_freq         = 470.62046084 [MHz]
X_offset       = -100 [ppm]
X_points       = 131072
X_prescans     = 1
X_resolution   = 1.36239188 [Hz]
X_sweep        = 178.57142857 [Hz]
Xr_domain      = 19F
Xr_freq        = 470.62046084 [MHz]
Xr_offset      = 5 [ppm]
Xr1_domain     = 19F
Xr1_freq       = 470.62046084 [MHz]
Xr1_offset     = 5 [ppm]
Xr1_offset     = FALSE
Mod_return     = 1
Scans          = 32
Total_scans    = 32

X_90_width     = 13.1 [us]
X_acq_time     = 0.7340032 [s]
X_angle        = 45 [deg]
X_atn          = 2.5 [dB]
X_pulse        = 6.55 [us]
Xr1_mode       = OCE
Xr1_mode       = FALSE
Dante_preset   = 1 [s]
Initial_wait   = 62
Recev_gain     = 4 [s]
Relaxation_delay = 4.7340032 [s]
Repetition_time = 22.9 [dc]
Temp_get       = 22.9 [dc]

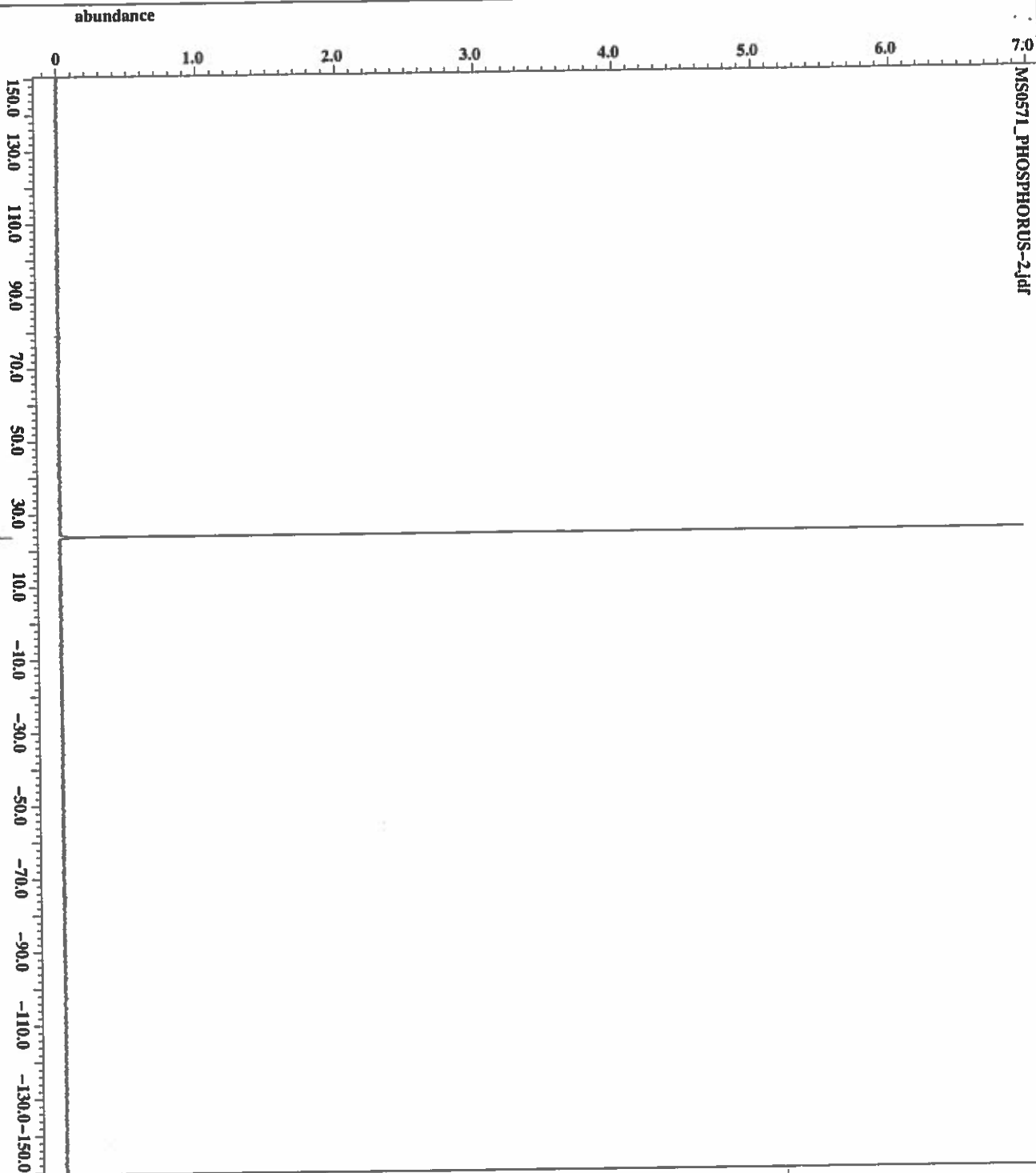
```

abundance

0 2.0 4.0 6.0 8.0 10.0 12.0 14.0 16.0 18.0 20.0 22.0 24.0 26.0 28.0 30.0 32.0

50.0 30.0 10.0 -10.0 -30.0 -50.0 -70.0 -90.0 -110.0 -130.0 -150.0 -170.0 -190.0 -210.0 -230.0 -250.0

X : parts per Million : 19F



```

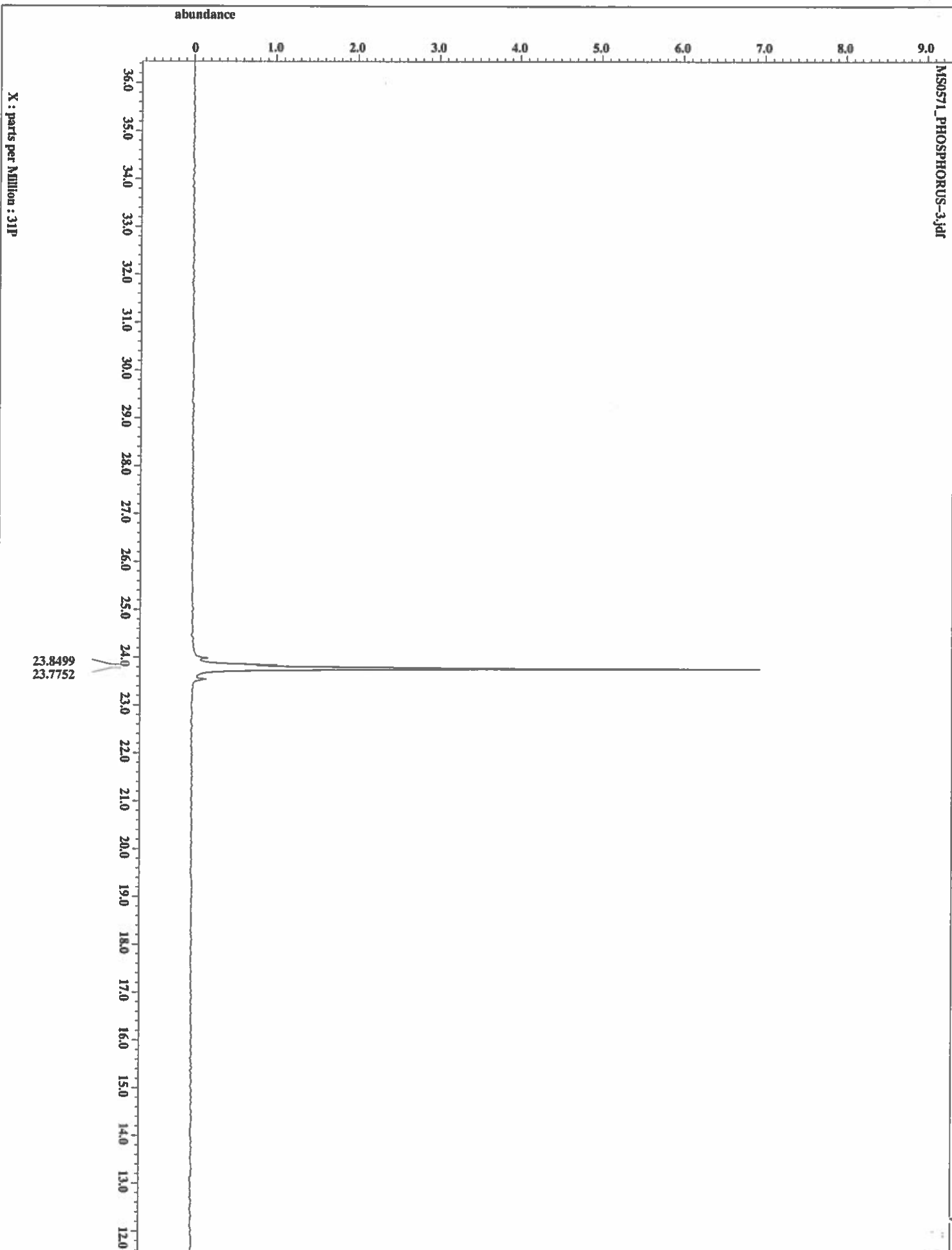
Filename      = MS0571_PHOSPHORUS-2.j
Author        = Jia Davis
Experiment    = single_pulse_dec
Sample_id     = MS0571
Solvent       = CHLOROFORM-D
Creation_time  = 5-OCT-2018 12:19:45
Revision_time  = 5-OCT-2018 11:54:39
Current_time   = 5-OCT-2018 11:54:39

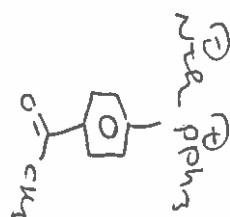
Data_format   = 1D COMPLEX
Dim_size      = 52428
Dim_title     = 31P
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.6598332[s]
X_domain       = 31P
X_freq         = 202.46831075[MHz]
X_offset       = 0[ppm]
X_points       = 65336
X_prescans     = 4
X_resolution   = 1.16301746[Hz]
X_sweep        = 76.2195122[kHz]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_return       = FALSZ
Mod_return     = 1
Scans          = 30
Total_scans    = 30

X_90_width    = 14.687[us]
X_acq_time     = 0.8598332[s]
X_angle       = 30[deg]
X_atn         = 5[db]
X_pulse       = 4.89566667[us]
Irr_atn_dec   = 20.7[db]
Irr_atn_noe   = 20.7[db]
Irr_noise     = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe_time       = TRUE
Noe           = 2[s]
Recvr_gain     = 56
Relaxation_delay = 2[s]
Repetition_delay = 2.85983322[s]
Repetition_time = 23.21[dc]
Temp_get       = 23.21[dc]

```



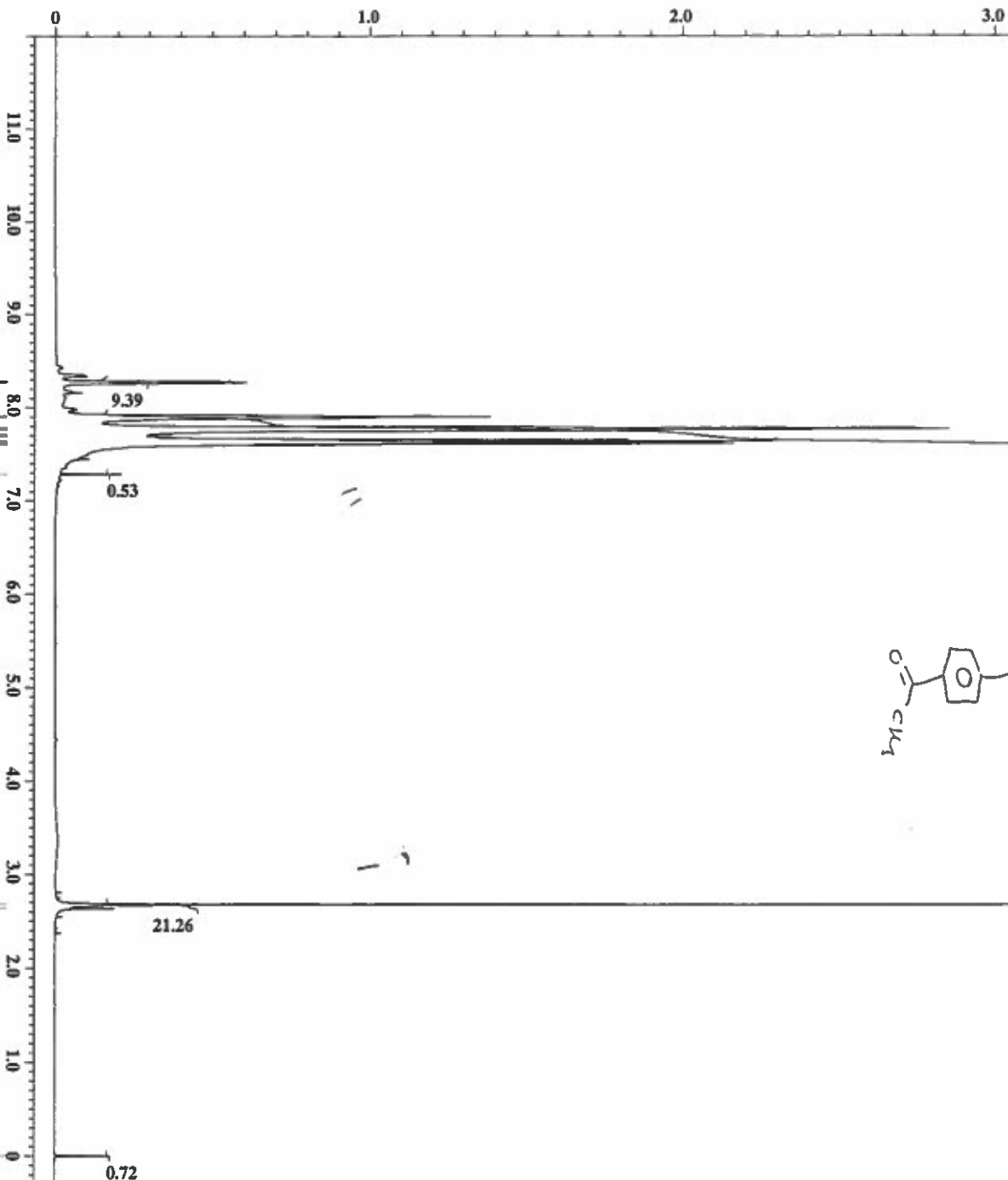


7.7770
7.7690
7.7609
7.7541
7.6384
7.6270
7.6121

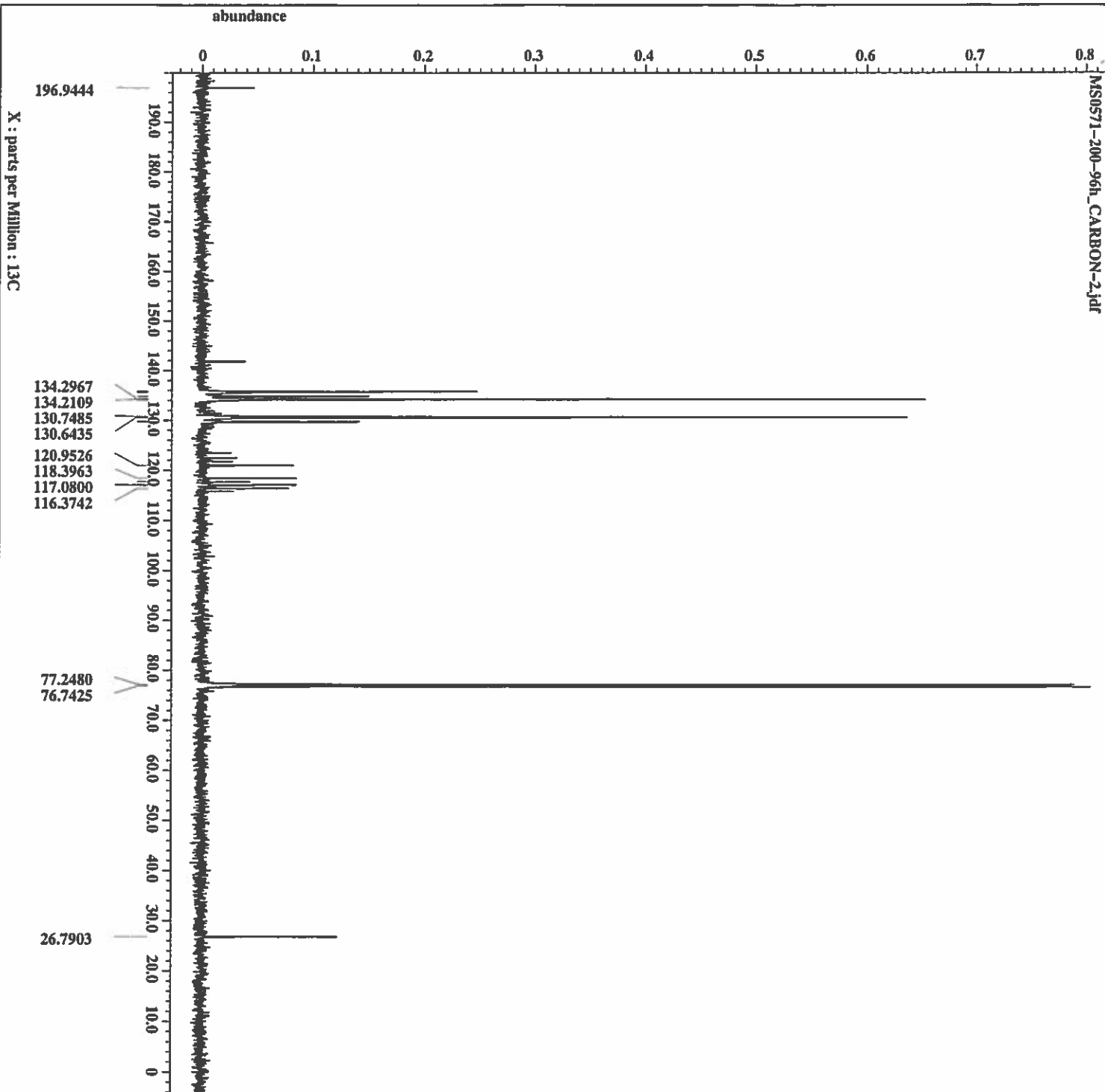
2.6786
2.6362

-0.0000

abundance



Filename = MS0571-200-96h_PROTON
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0571-200-96h
 Solvent = CHLOROFORM-D
 Creation_time = 9-OCT-2018 17:03:20
 Revision_time = 9-OCT-2018 16:37:49
 Current_time = 9-OCT-2018 16:37:49
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 1H
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500
 Field_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 1.74587904 [s]
 X_domain = 1H
 X_freq = 500.15891521 [MHz]
 X_offset = 5.0 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.5727737 [Hz]
 X_sweep = 9.38438438 [kHz]
 Itr_domain = 1H
 Itr_freq = 500.15891521 [MHz]
 Itr_offset = 5.0 [ppm]
 Itr_domain = 1H
 Itr_freq = 500.15891521 [MHz]
 Itr_offset = 5.0 [ppm]
 Mod_return = FALSE
 Scans = 1
 Total_scans = 16
 X_90_width = 12.4 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_atn = 4 [dB]
 X_pulse = 6.2 [us]
 Itr_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 28
 Relaxation_delay = 4 [s]
 Repetition_time = 5.74587904 [s]
 Temp_get = 23.7 [degC]



```

File Name      = MS0571-200-96h_CARBON
Author         = Jim Davis
Experiment     = single_pulse_dec
Sample ID      = MS0571-200-96h
Solvent        = CHLOROFORM-D
Creation Time   = 9-OCT-2018 17:15:55
Revision Time  = 9-OCT-2018 16:50:24
Current Time   = 9-OCT-2018 16:50:24

Data Format     = 1D COMPLEX
Dim Size       = 26214
Dim Title      = 13C
Dim Units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECX500

F1d1_strength  = 11.7473579 [V] (500 MHz)
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]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_offset       = FALSE
Mod_return     = 1
Scans          = 256
Total_scans    = 256

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
X_atn_dec      = 20.7 [dB]
X_atn_noe      = 20.7 [dB]
X_noise        = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = 1 [s]
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get       = 23 [degC]

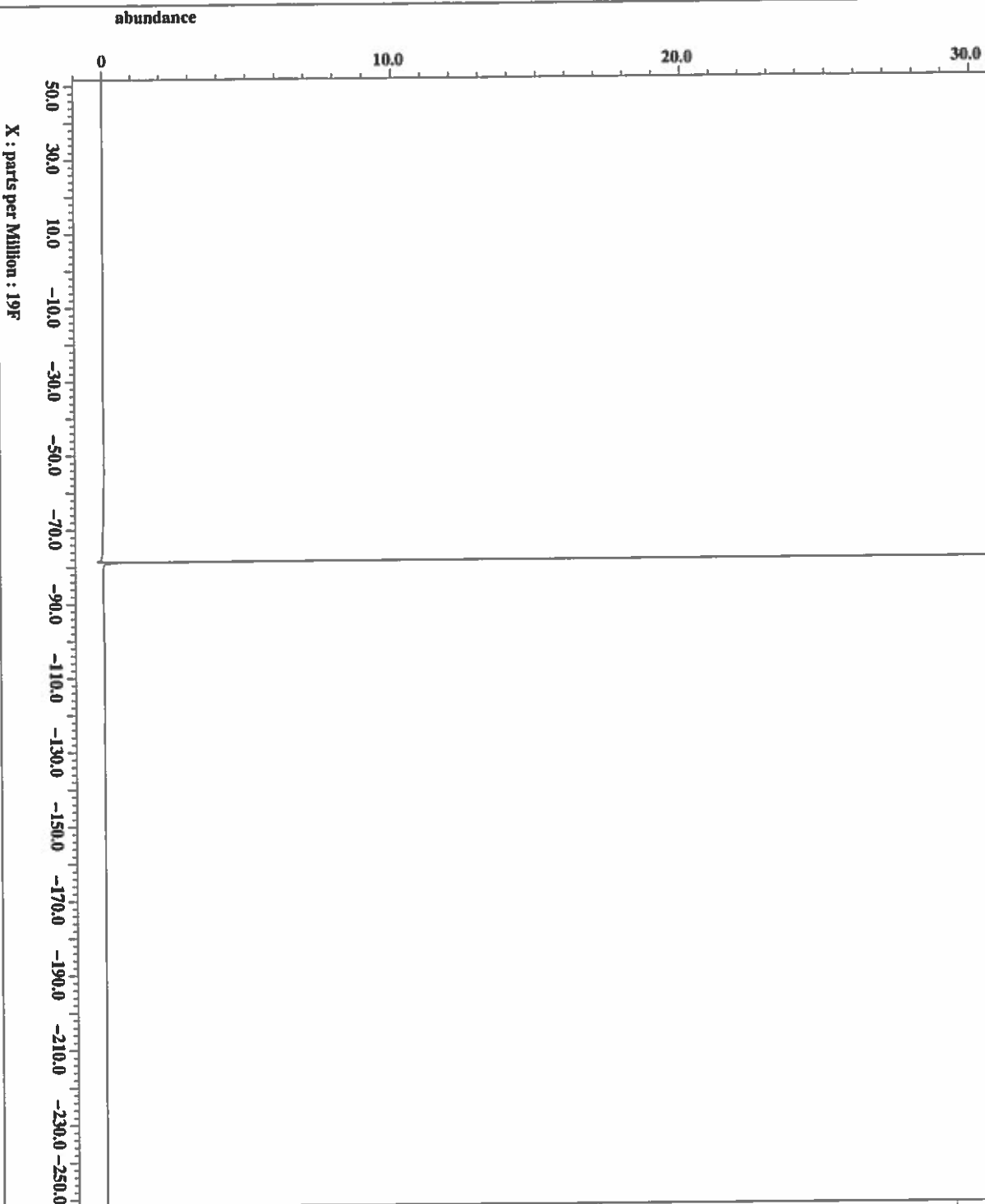
```



Filename = MS0571-200-96h_FLUORINE
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0571-200-96h
 Solvent = CHLOROFORM-D
 Creation_time = 9-OCT-2018 17:20:21
 Revision_time = 9-OCT-2018 16:54:52
 Current_time = 9-OCT-2018 16:54:52

Data_format = 1D COMPLEX
 Dim_size = 104857
 Dim_title = 19F
 Dim_unit = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 0.7340032 [s]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = -100 [ppm]
 X_points = 131072
 X_prescans = 1
 X_resolution = 1.36239188 [Hz]
 X_sweep = 178.57142857 [kHz]
 Xr_domain = 19F
 Xr_freq = 470.62046084 [MHz]
 Xr_offset = 5 [ppm]
 Xr_domain = 19F
 Xr_freq = 470.62046084 [MHz]
 Xr_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 32
 Total_scans = 32
 X_90_width = 13.1 [us]
 X_acq_time = 0.7340032 [s]
 X_angle = 45 [deg]
 X_atn = 2.5 [dB]
 X_pulse = 6.55 [us]
 Xr_mode = Off
 Dantec_preset = PALSE
 Initial_wait = 1 [s]
 Recvr_gain = 40
 Relaxation_delay = 4 [s]
 Repetition_time = 4.7340032 [s]
 Temp_get = 22.7 [C]



23.8442
23.7695

X : parts per Million : 31P



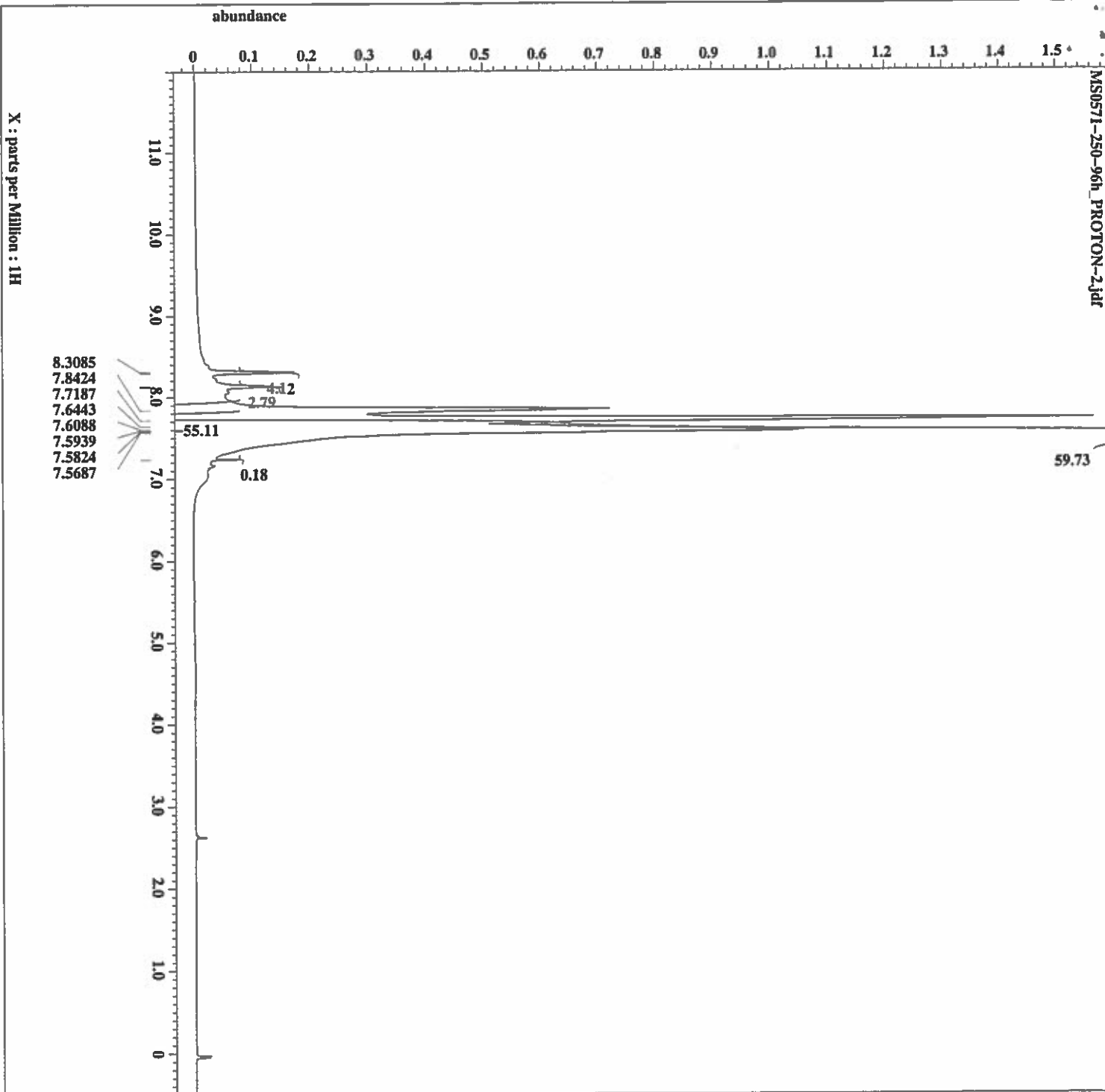
```

File Name      MS0571-200-96h_PHOSPH
Author         Jim Davis
Experiment     single_pulse_dec
Sample Id      MS0571-200-96h
Solvent        CHLOROFORM-D
Creation time   9-OCT-2018 17:24:42
Revision time   9-OCT-2018 16:59:12
Current time    9-OCT-2018 16:59:12

Data Format     1D COMPLEX
Dia Size       52428
Dia Title      31P
Dia Units      [ppm]
Dimensions     X
Site           RCA 500
Spectrometer   JNM-ECA500

Field Strength 11.7473579 [T] (500 [MH
Acq Duration    0.85983232 [s]
Domain          31P
Freq           202.46831075 [MHz]
Offset          0 [ppm]
Points         65536
Prescans        4
Resolution      1.16301746 [Hz]
Sweep          76.2195122 [Hz]
IRF Domain      1H
IRF Freq        500.15991521 [MHz]
IRF Offset      3.0 [ppm]
Clipped         FALSE
Mod Return      1
Scans           35
Total Scans     35

X_90_width      14.687 [us]
X_acq_time      0.85983232 [s]
X_angle         30 [deg]
X_db            5 [dB]
X_pulse         4.89566667 [us]
IRF_atn_dec     20.7 [dB]
IRF_atn_noe     20.7 [dB]
IRF_noise       20.7 [dB]
Decoupling      WALTZ
Initial Wait     TRU2
Noc             1 [s]
Noc2            TRU2
Noc3            2 [s]
Noc4            56
Recvr_gain      21 [s]
Relaxation delay 2.85983232 [s]
Repetition time 23.1 [s]
Temp_set        23.1 [C]
  
```



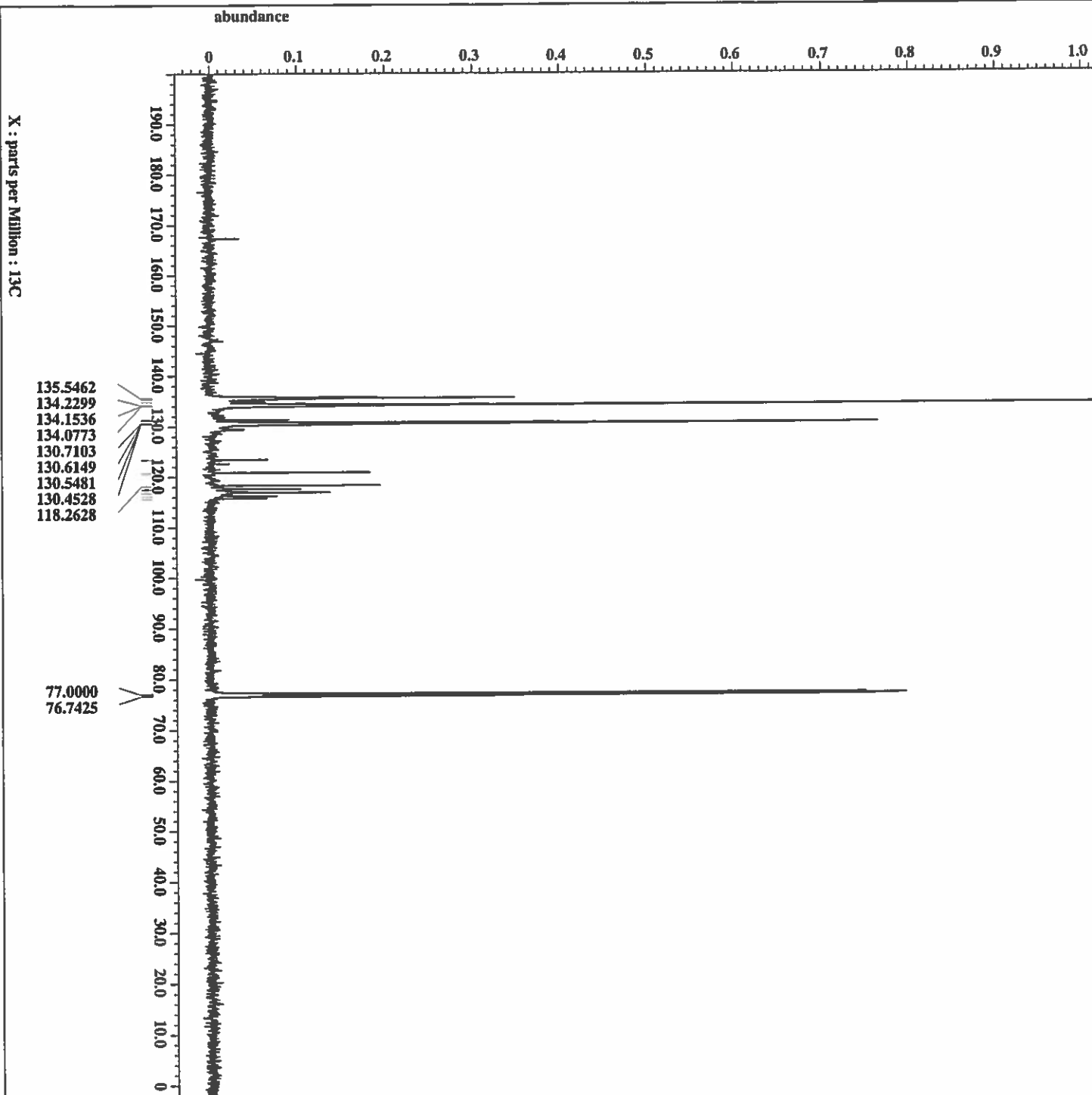
```

Pilename      = MS0571-250-96h_PROTON
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = MS0571-250-96h
Solvent       = CHLOROFORM-D
Creation_time  = 9-OCT-2018 17:31:57
Revision_time  = 9-OCT-2018 17:06:28
Current_time   = 9-OCT-2018 17:06:28

Data_format    = 1D COMPLEX
Dim_size       = 13107
Dim_c1         = 1H
Dim_u1         = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_rec_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 9.38438438 [kHz]
Xir_domain    = 1H
Xir_freq       = 500.15991521 [MHz]
Xir_offset     = 5.0 [ppm]
Xri_domain    = 1H
Xri_freq       = 500.15991521 [MHz]
Xri_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 12.4 [us]
X_aqc_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 6.2 [us]
Xri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 24
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_get       = 22.8 [dc]
  
```



```

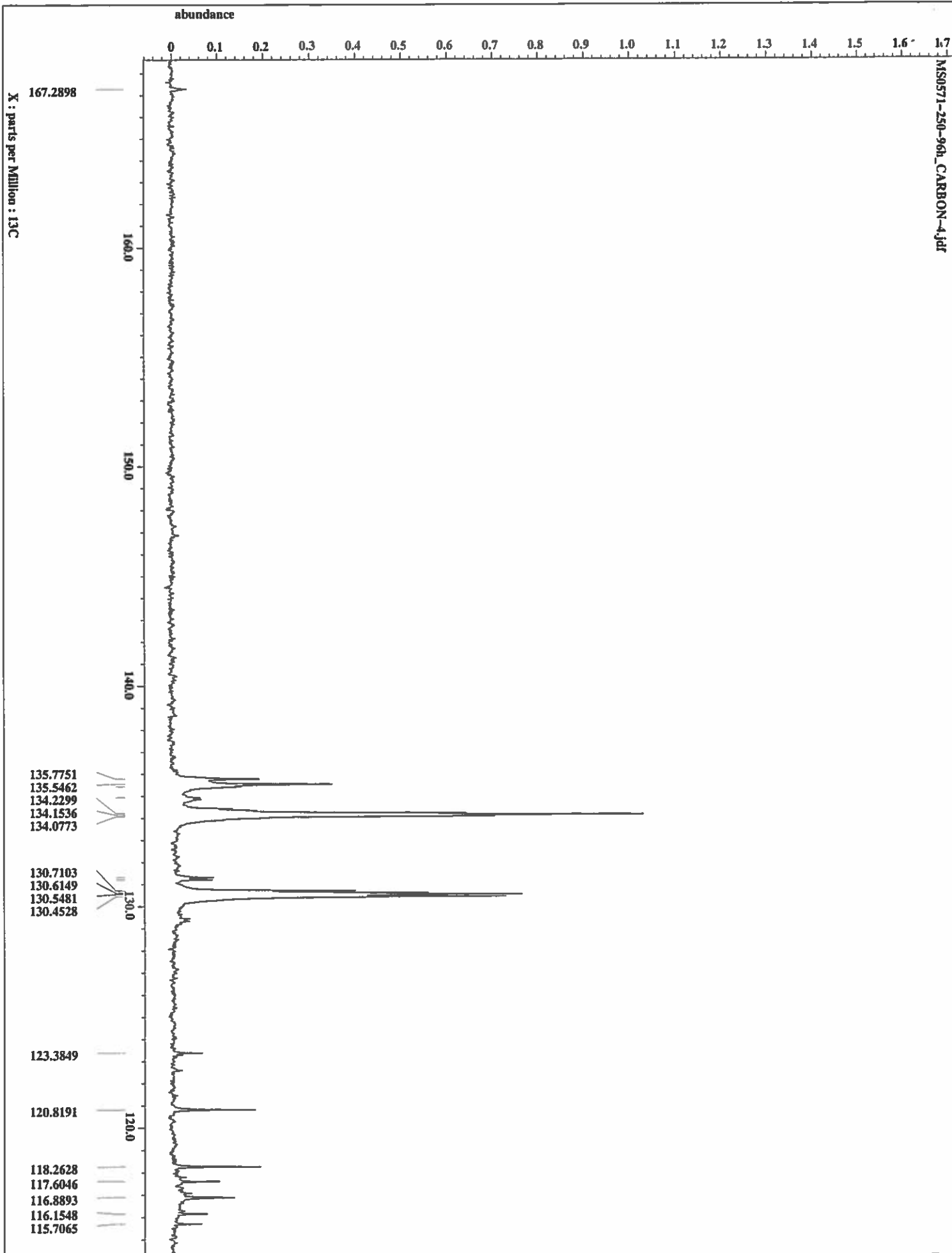
Filename      = MS0571-250-96h CARBON
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0571-250-96h
Solvent       = CHLOROFORM-D
Creation_time = 9-OCT-2018 17:45:20
Revision_time = 9-OCT-2018 17:19:30
Current_time  = 9-OCT-2018 17:19:51

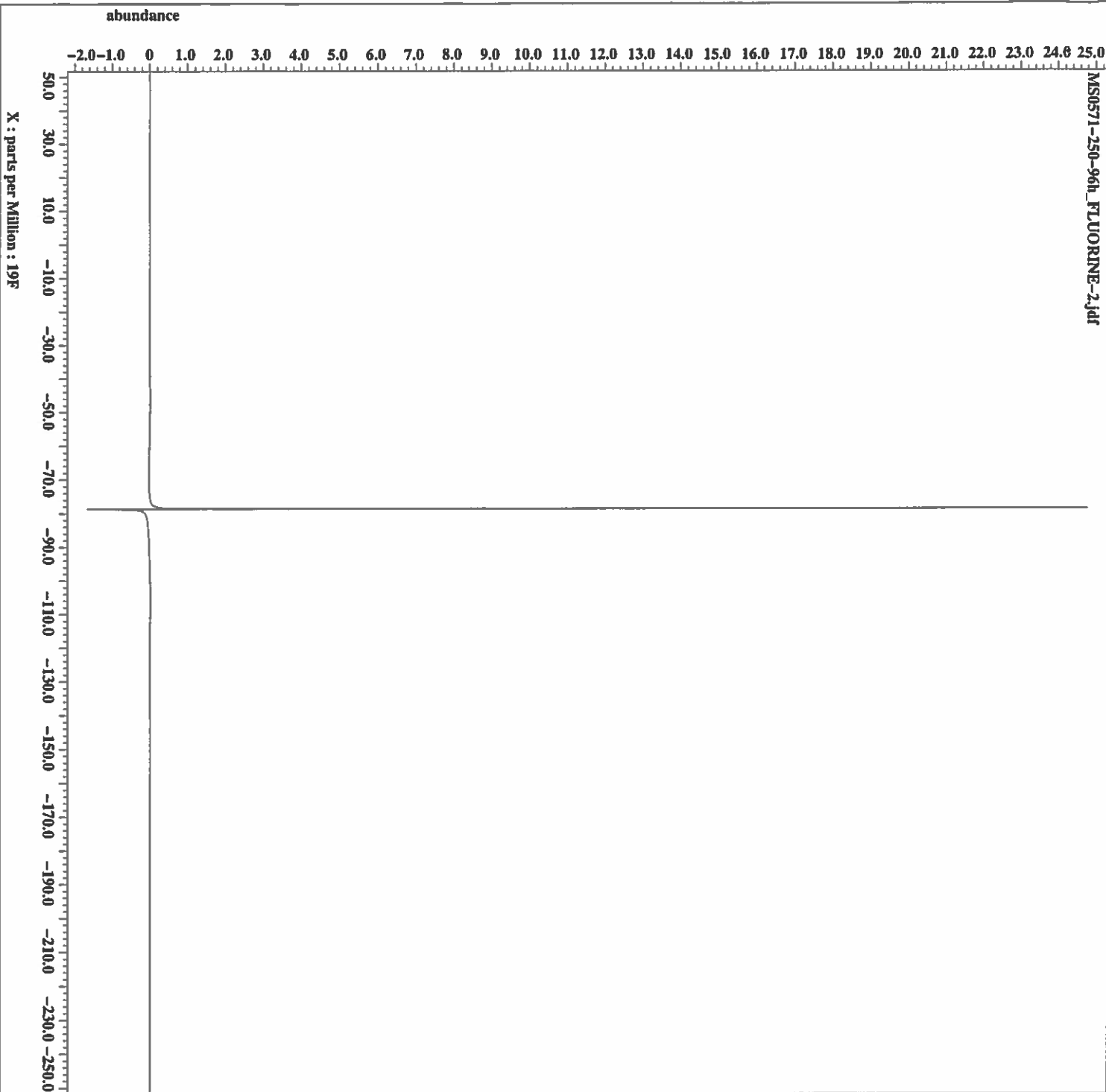
Data format
Dim_size      = 1D COMPLEX
Dim_c1size    = 26214
Dim_c1size    = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

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]
X1H            = 1H
X1H_domain     = 500.15991521 [MHz]
X1H_freq       = 5.0 [ppm]
X1H_offset     = FALSE
Clipped        = 1
Mod_return     = 256
Scans          = 256
Total_scans    = 256

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [db]
X_pulse        = 4.4 [us]
X1H_atn_dec    = 20.7 [db]
X1H_atn_noe    = 20.7 [db]
X1H_noise      = WALYZ
Decoupling     = TRUE
Inlet1_waltc   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Nacq_gain      = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get       = 23 [dc]

```





```

Filename      = MS0571-250-96h_FLUORINE-2.jdt
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = MS0571-250-96h
Solvent       = CHLOROFORM-D
Creation_time = 9-OCT-2018 17:49:41
Revision_time = 9-OCT-2018 17:24:12
Current_time  = 9-OCT-2018 17:24:12

Data_format   = 1D COMPLEX
Dia_size      = 104857
Dia_title     = 19F
Dia_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.7340032[s]
X_domain       = 19F
X_freq         = 470.62046084[MHz]
X_offset       = -100[ppm]
X_points       = 131072
X_prescans     = 1
X_resolution   = 1.36239188[Hz]
X_sweep        = 178.57142857[MHz]
Irr_domain     = 19F
Irr_freq       = 470.62046084[MHz]
Irr_offset     = 5[ppm]
Irr_domain     = 19F
T1_freq        = 470.62046084[MHz]
T1_offset      = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 32
Total_scans    = 32

X_90_width     = 13.1[us]
X_acq_time      = 0.7340032[s]
X_angle        = 45[deg]
X_atn          = 2.5[dB]
X_pulse        = 6.55[us]
Irr_mode       = Off
T1_mode        = Off
Dante_preset   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 36
Relaxation_delay = 4[s]
Repetition_time = 4.7340032[s]
Temp_get       = 22.7[degC]

```

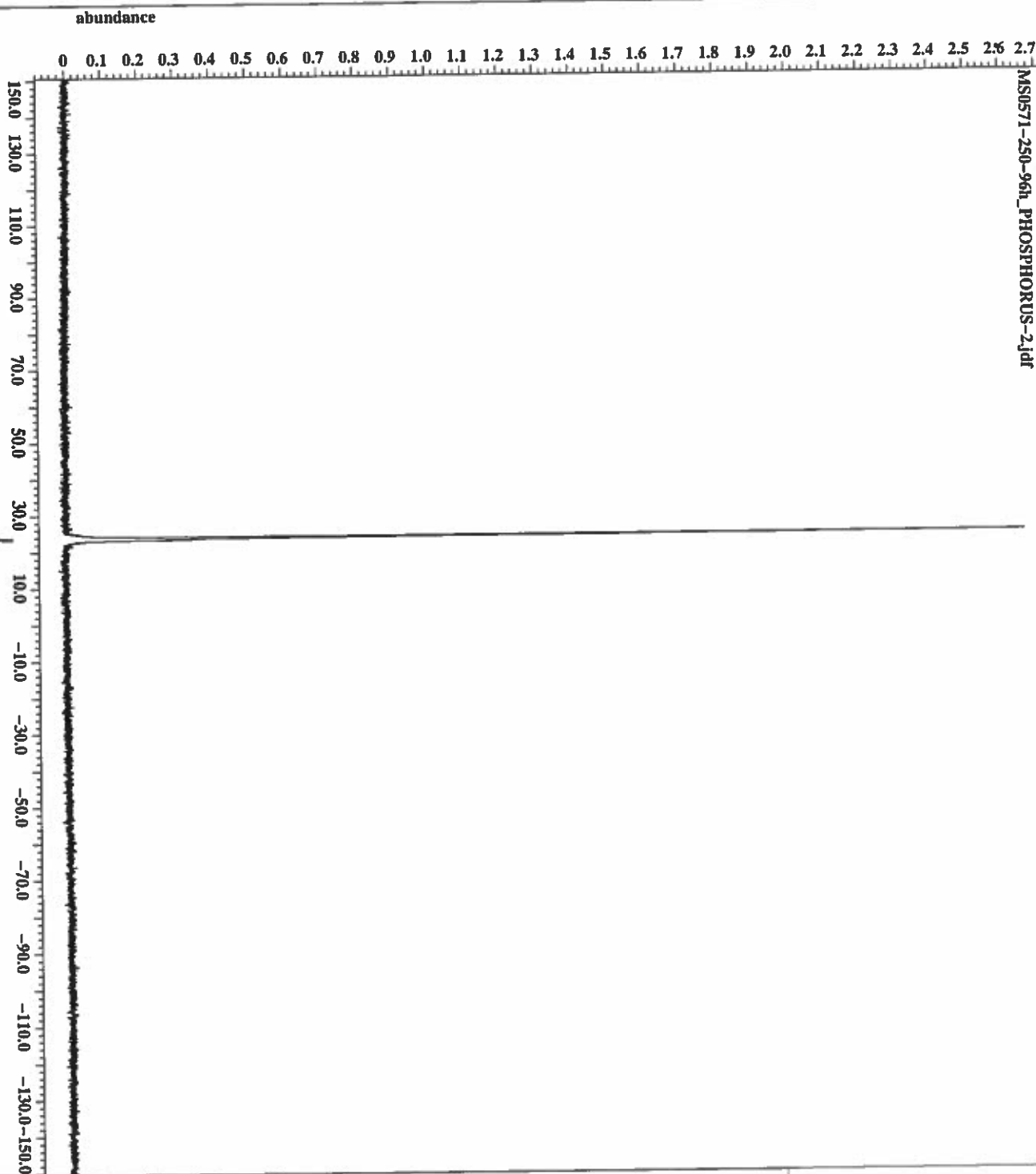


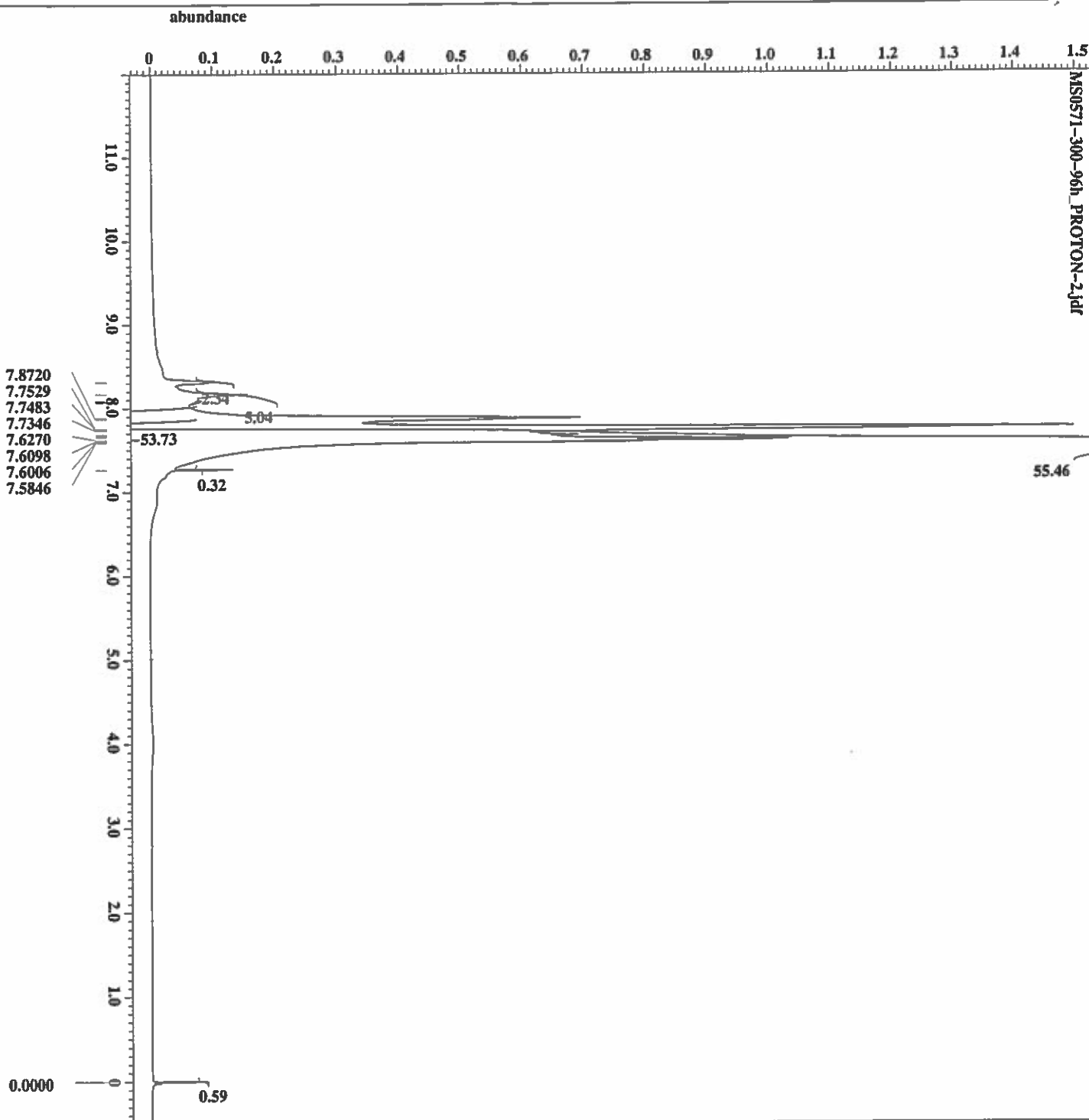
Filename MS0571-250-96h_PHOSPH
 Author Jim Davis
 Experiment single_pulse_dec
 Sample_id MS0571-250-96h
 Solvent CHLOROFORM-D
 Creation_time 9-OCT-2018 17:53:48
 Revision_time 9-OCT-2018 17:28:19
 Current_time 9-OCT-2018 17:28:19

Data_format 1D COMPLEX
 Dim_size 52428
 Dim_title 31P
 Dim_units [ppm]
 Dimensions X
 Site KCA 500
 Spectrometer JNM-ECA500

Field_strength 11.7473579[T] (500[MH
 X_acq_duration 0.85983232[s]
 X_domain 31P
 X_freq 202.46831075[MHz]
 X_offset 0[ppm]
 X_points 65336
 X_prescans 4
 X_resolution 1.16301746[Hz]
 X_sweep 76.2195122[KHz]
 X_domain 1H
 X_freq 500.15991521[MHz]
 X_offset 5.0[ppm]
 Clipped FALSE
 Mod_return 1
 Scans 35
 Total_scans 35

X_90_width 14.687[us]
 X_acq_time 0.85983232[s]
 X_angle 30[deg]
 X_atn 5[db]
 X_pulse 4.89566667[us]
 Iir_atn_dec 20.7[db]
 Iir_atn_noe 20.7[db]
 Iir_noise WALTZ
 Decoupling TRUE
 Initial_wait 1[s]
 Noe_time TRUE
 Recvr_gain 2[s]
 Relaxation_delay 2.85983232[s]
 Repetition_time 23[dc]
 Temp_get





```

Filename      = MS0571-300-96h_PROTON
Author        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0571-300-96h
Solvent       = CHLOROFORM-D
Creation_time  = 9-OCT-2018 18:01:12
Revision_time  = 9-OCT-2018 17:35:42
Current_time   = 9-OCT-2018 17:35:43

Data_format   = 1D COMPLEX
Dia_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57377737 [Hz]
X_sweep        = 9.38638438 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Tr1_domain     = 1H
Tr1_freq       = 500.15991521 [MHz]
Tr1_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_pulch    = 12.4 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [db]
X_pulse        = 6.2 [us]
Off            = Off
Tr1_mode       = Off
Dante_present  = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 26
Relaxation_delay = 4 [s]
Repetition_delay = 5.74587904 [s]
Temp_get       = 22.7 [dc]
  
```

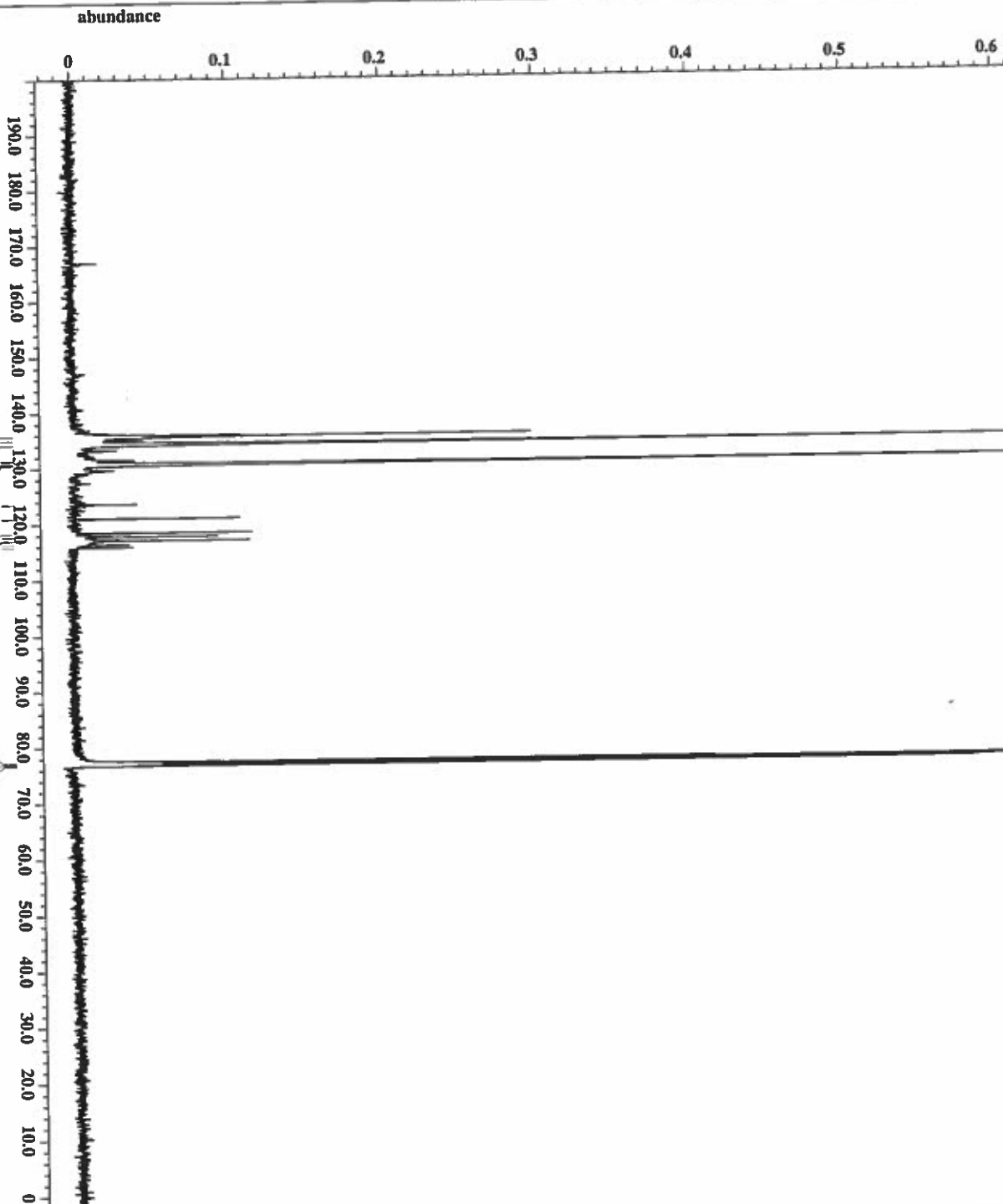


Filename = MS0571-300-96h CARBON
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = MS0571-300-96h
 Solvent = CHLOROFORM-D
 Creation_time = 9-OCT-2018 18:50:52
 Revision_time = 9-OCT-2018 18:25:22
 Current_time = 9-OCT-2018 18:25:22

Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

P1field_strength = 11.7473579[V] (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

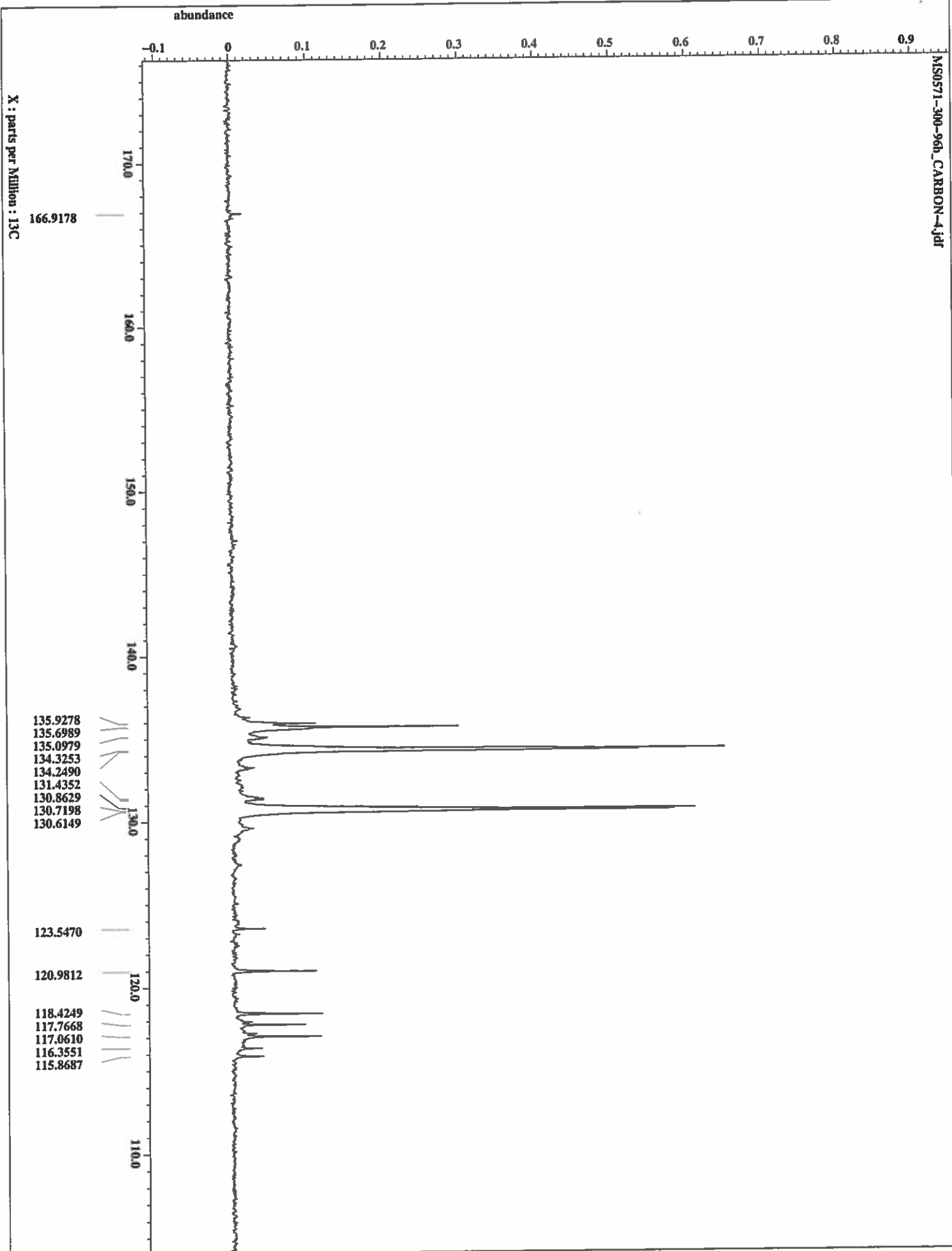
X_90_width = 13.2 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 6 [dB]
 X_pulse = 4.4 [us]
 Irr_atn_dec = 20.7 [dB]
 Irr_atn_noe = 20.7 [dB]
 Irr_noise = WALTZ
 Decoupling = FLOZ
 Initial_wait = 1[s]
 Noe = FLOZ
 Noe_time = 2[s]
 Relaxation_delay = 2.83361792 [s]
 Repetition_time = 2.83361792 [s]
 Temp_get = 23.4 [C]



135.9278
 135.6989
 134.3253
 134.2490
 130.8629
 130.7198
 130.6149
 118.4249
 117.0610

77.2480
 77.0000
 76.7425

X : parts per Million : 13C



abundance

0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0

50.0 30.0 10.0 -10.0 -30.0 -50.0 -70.0 -90.0 -110.0 -130.0 -150.0 -170.0 -190.0 -210.0 -230.0 -250.0

X : parts per Million : 19F



```

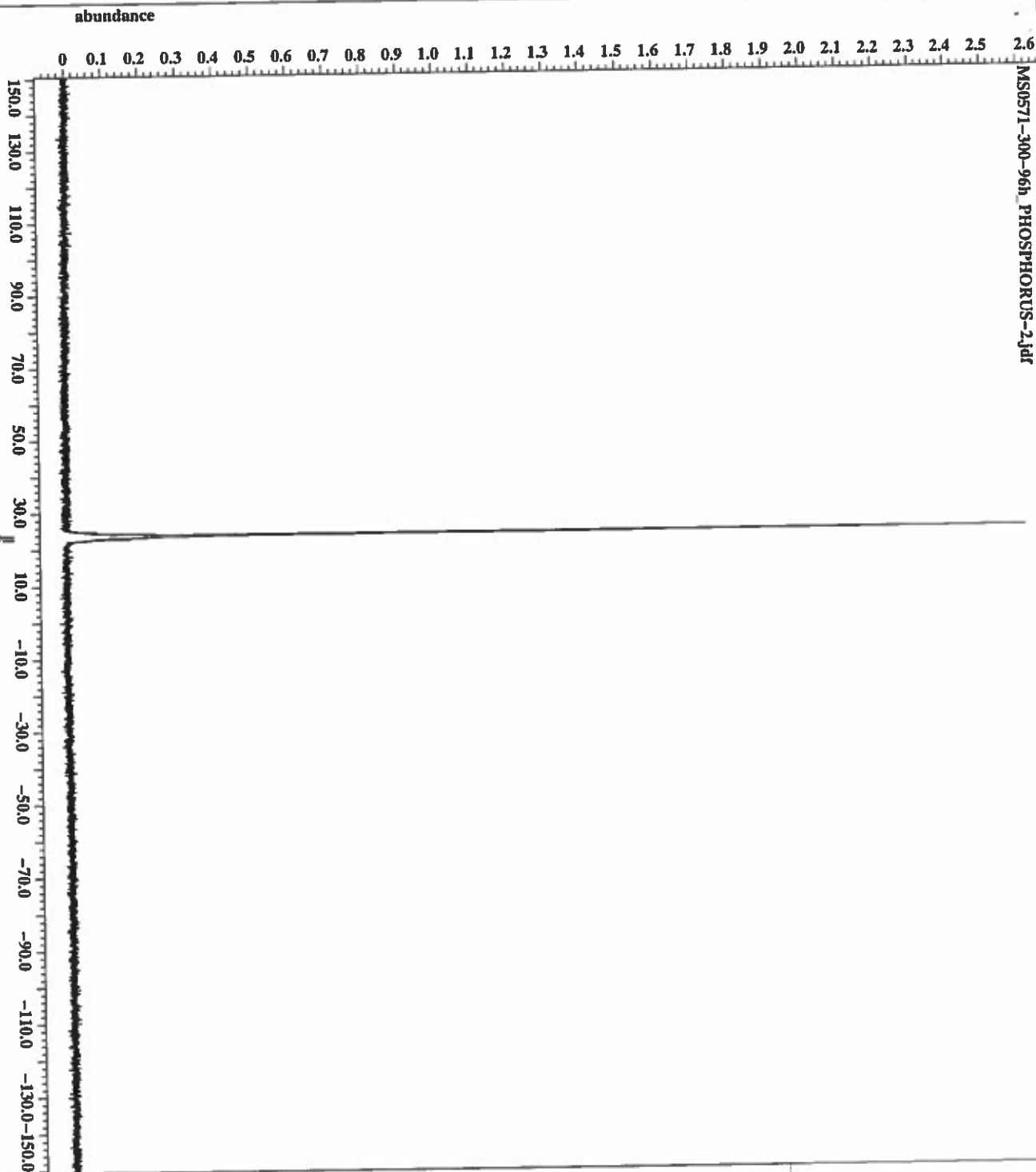
Filename      = MS0571-300-96h_FLUORINE
Author        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0571-300-96h
Solvent       = CHLOROFORM-D
Creation_time  = 9-OCT-2018 18:55:50
Revision_time  = 9-OCT-2018 18:30:20
Current_time   = 9-OCT-2018 18:30:20

Data_format    = 1D COMPLEX
Dim_size       = 104857
Dim_file       = 19F
Dim_units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.7340032[s]
X_domain       = 19F
X_freq         = 470.62046084[MHz]
X_offset       = -100[ppm]
X_points       = 131072
X_prescans     = 1
X_resolution   = 1.36239188[MHz]
X_sweep        = 178.57142857[MHz]
Xir_domain     = 19F
Xir_freq       = 470.62046084[MHz]
Xir_offset     = 5[ppm]
Xir_domain     = 19F
Xir_freq       = 470.62046084[MHz]
Xir_offset     = 5[ppm]
Mod_return     = FALSK
Scans          = 1
Total_scans    = 40

X_90_width     = 13.1[us]
X_acq_time     = 0.7340032[s]
X_angle        = 45[deg]
X_atn          = 2.5[db]
X_pulse        = 6.55[us]
Xir_mode       = OF2
Xir_mode       = OF2
Dance_presat   = FALSK
Initial_puls   = 1[s]
Recvr_gain     = 40
Relaxation_delay = 4[s]
Relaxation_delay = 4.7340032[s]
Repetition_time = 23[dc]
Temp_get       = 23[dc]

```



SOUTH ALABAMA
JAGUARS



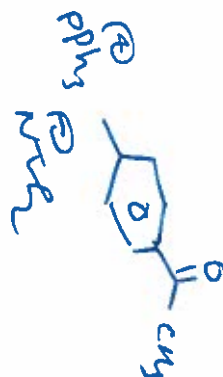
```

Filename      MS0571-300-96h_PHOSPH
Author        Jim Davis
Experiment    single_pulse_dec
Sample_id     MS0571-300-96h
Solvent       CHLOROFORM-D
Creation_time 9-OCT-2018 19:00:54
Revision_time 9-OCT-2018 18:35:25
Current_time  9-OCT-2018 18:35:25

Data_format   1D COMPLEX
Dim_size      32428
Dim_title     31P
Dim_units     [ppm]
Dimensions    X
Site          ECA 500
Spectrometer  JNM-ECA500

Field_strength 11.7473579 [T] (500 [MH
X_acq_duration 0.85983232 [s]
X_domain      31P
X_freq        202.46831075 [MHz]
X_offset      0 [ppm]
X_points      65536
X_prescans    4
X_rescans     1.16301746 [Hz]
X_resolution  76.2195122 [Hz]
X_sweep       1H
Irr_domain    500.15991521 [MHz]
Irr_freq      5.0 [ppm]
Irr_offset    PALSE
Clipped       1
Mod_return    50
Scans         50
Total_scans   50

X_90_width    14.687 [us]
X_acq_time     0.85983232 [s]
X_angle       30 [deg]
X_atn         5 [dB]
X_pulse       4.89566667 [us]
Irr_atn_dec   20.7 [dB]
Irr_atn_noe   20.7 [dB]
Irr_noise     KALTZ
Decoupling    TRUZ
Initial_wait   1 [s]
Noe           TRUZ
Noe_time       2 [s]
Recovery_gain  58
Relaxation_delay 2 [s]
Repetition_time 2.85983232 [s]
Temp_get      23.3 [degC]
  
```



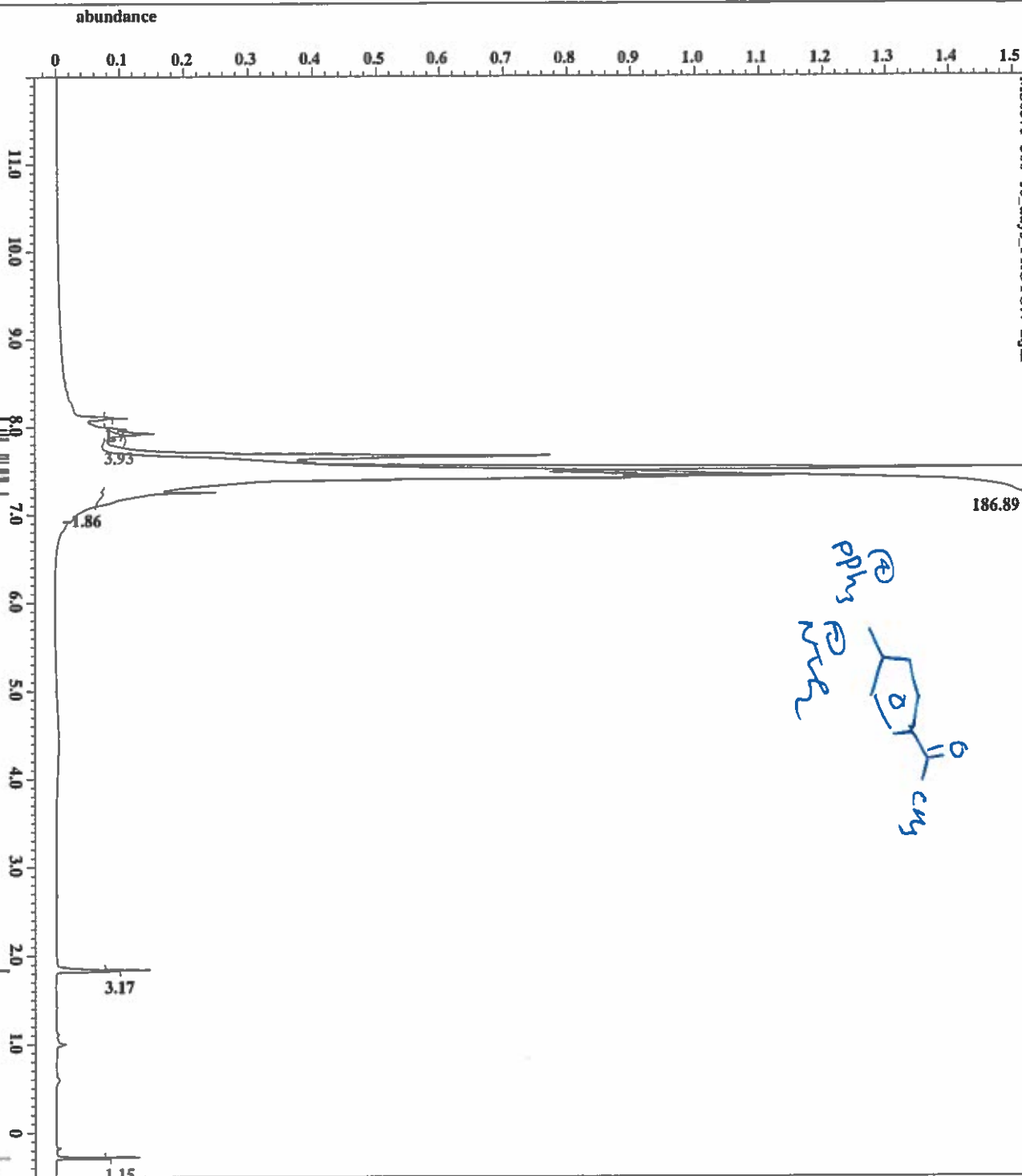
7.5286
7.5217
7.5126
7.5068
7.4416
7.4255
7.4164

186.89

1.8427
1.8393

-0.2736
-0.2930

X : parts per Million : 1H



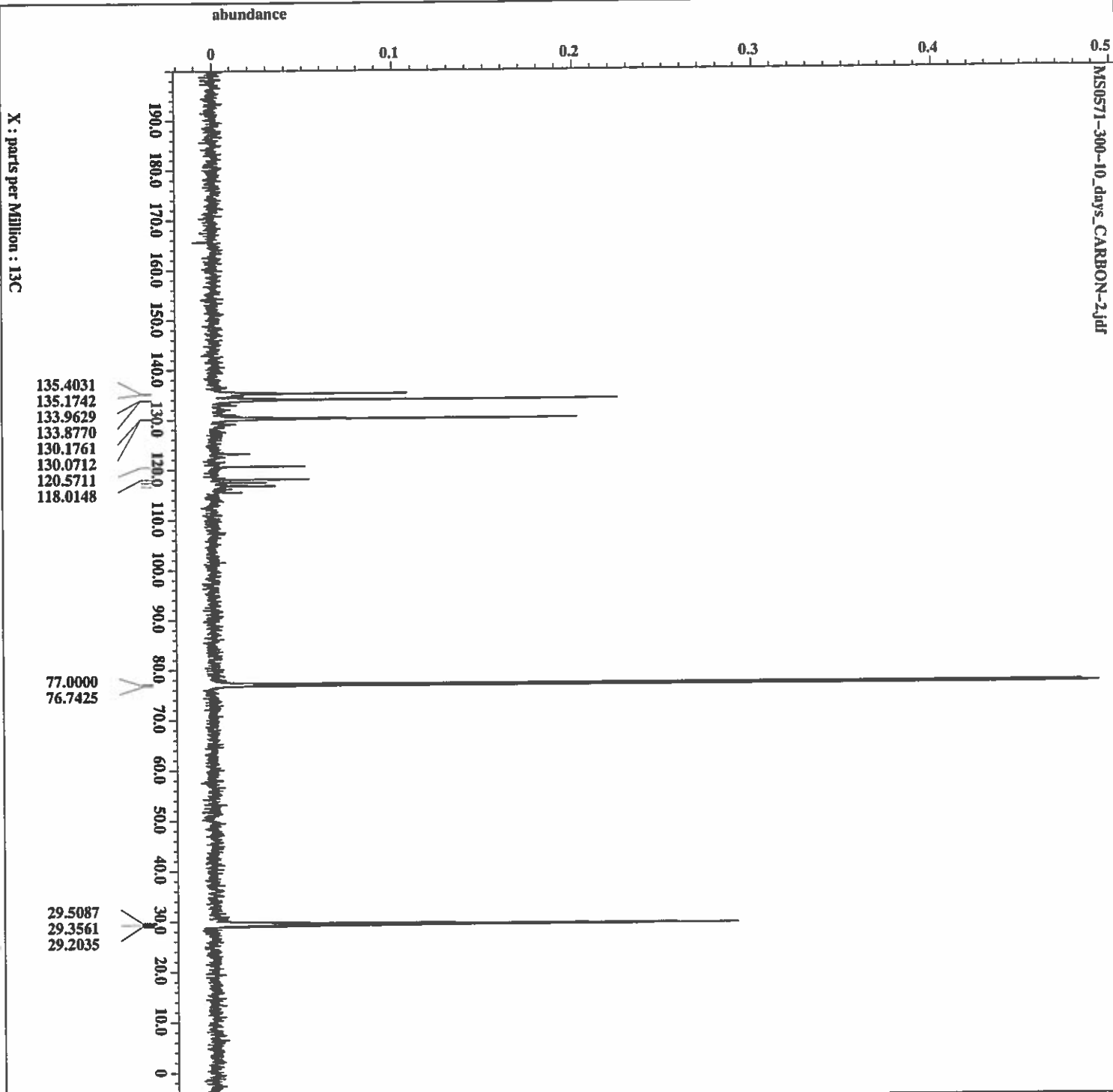
Filename = MS0571-300-10_days_PR
 Author = Jim Davis
 Experiment = single_pulse-ec2
 Sample_id = MS0571-300-10_days
 Solvent = CHLOROFORM-D
 Creation_time = 19-OCT-2018 10:46:06
 Revision_time = 19-OCT-2018 10:19:50
 Current_time = 19-OCT-2018 10:19:50

 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

 Field_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 1.74587904 [s]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.57277737 [Hz]
 X_sweep = 1H
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

 X_90_width = 12.4 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_atn = 4 [dB]
 X_pulse = 6.2 [us]
 X_mode = Off
 X_prescans = FALSE
 X_acq_time = 1 [s]
 Initial_wait = 32
 Recvr_gain = 4 [e]
 Relaxation_delay = 5.74587904 [s]
 Temp_set = 22.3 [C]





```

Filename      = MS0571-300-10_days_CA
Author        = Jim Davis
Experiment     = single_pulse_dec
Sample_id     = MS0571-300-10_days
Solvent       = CHLOROFORM-D
Creation_time  = 19-OCT-2018 11:05:28
Revision_time  = 19-OCT-2018 10:39:14
Current_time   = 19-OCT-2018 10:39:14

Data_format    = 1D COMPLEX
Dim_size       = 26214
Dim_title      = 13C
Dim_units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

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]
Xt_domain      = 1H
Xt_freq        = 500.13591521 [MHz]
Xt_offset      = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 400
Total_scans    = 400

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Xt_atn_dec     = 20.7 [dB]
Xt_atn_noe     = 20.7 [dB]
Xt_noise       = WALTZ
Decoupling     = TRUZ
Initial_wait    = 1 [s]
Noe_time       = TRUZ
Noe_delay      = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 22.9 [degC]

```

abundance

X : parts per Million : 13C

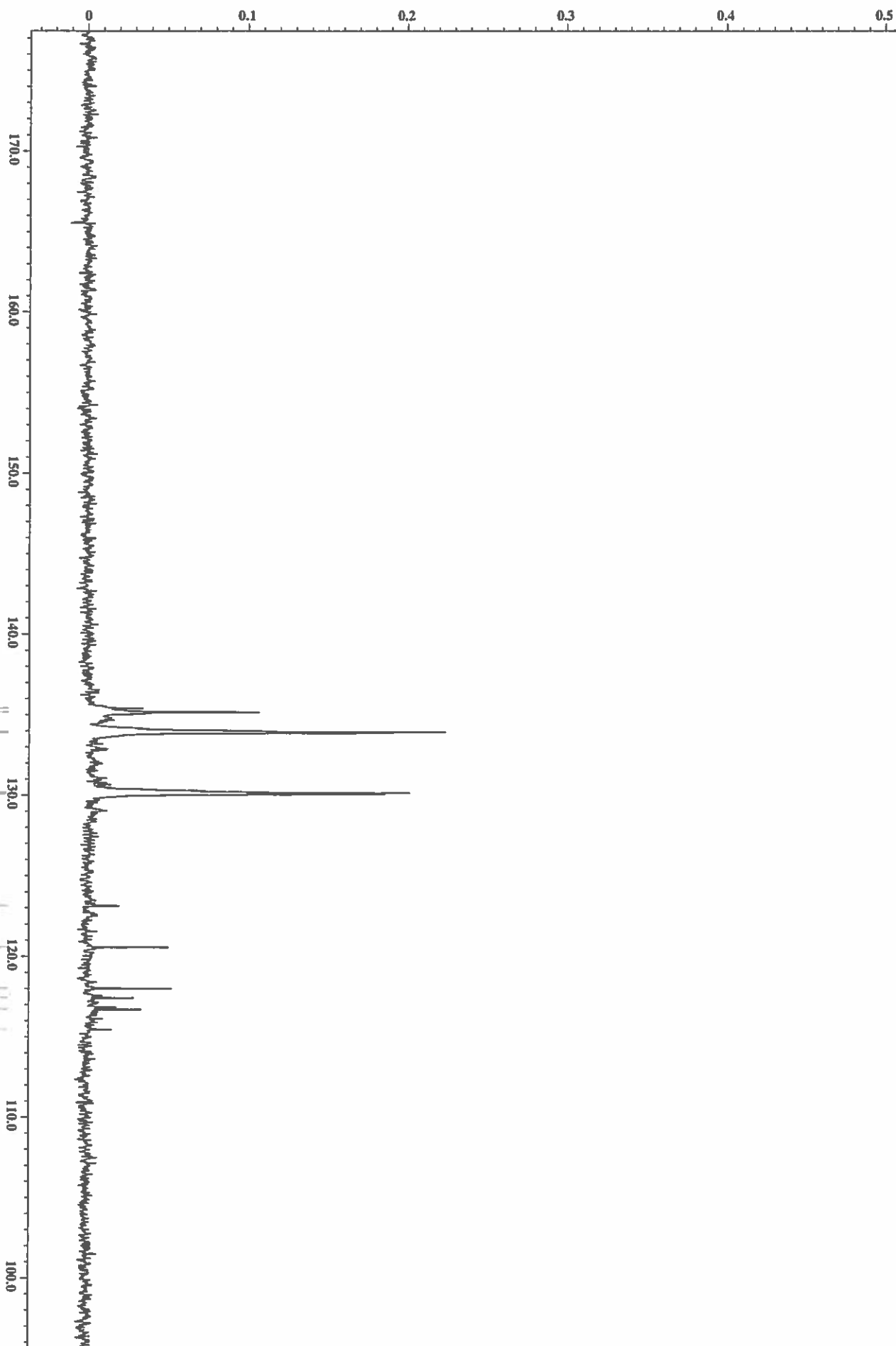
135.4031
135.1742
133.9629
133.8770

130.1761
130.0712

123.1369

120.5711

118.0148
117.4329
116.7176
115.4585





Filename = MS0571-300-10_days_FL
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0571-300-10_days
 Solvent = CHLOROFORM-D
 Creation_time = 19-OCT-2018 11:10:46
 Revision_time = 19-OCT-2018 10:44:32
 Current_time = 19-OCT-2018 10:44:32

Data_format = 1D COMPLEX
 Dim_size = 104857
 Dim_title = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 0.7340032 [s]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = -100 [ppm]
 X_points = 131072
 X_prescans = 1
 X_resolution = 1.36239188 [Hz]
 X_sweep = 178.57142857 [kHz]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = 5 [ppm]
 X1_domain = 19F
 X1_freq = 470.62046084 [MHz]
 X1_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 40
 Total_scans = 40

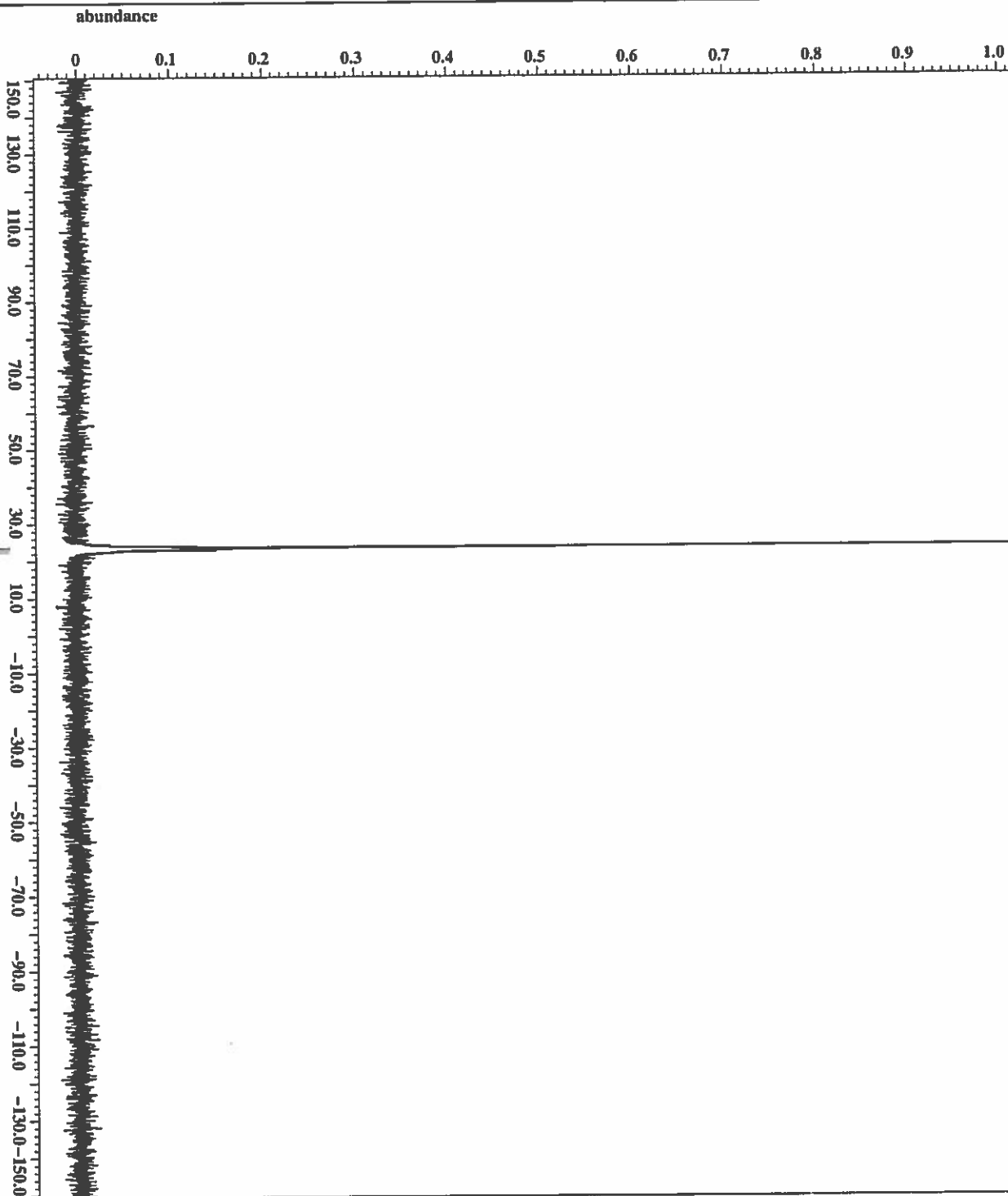
X_90_width = 13.1 [us]
 X_acq_time = 0.7340032 [s]
 X_angle = 45 [deg]
 X_eta = 2.5 [dB]
 X_pulse = 6.55 [us]
 X1_mode = OFF
 Dante_presat = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 62
 Relaxation_delay = 4 [s]
 Repetition_time = 4.7340032 [s]
 Temp_get = 22.5 [deg]

abundance

0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0

50.0 30.0 10.0 -10.0 -30.0 -50.0 -70.0 -90.0 -110.0 -130.0 -150.0 -170.0 -190.0 -210.0 -230.0 -250.0

X : parts per Million : 19F



X : parts per Million : 31P

23.5914
23.4076
22.7298

```

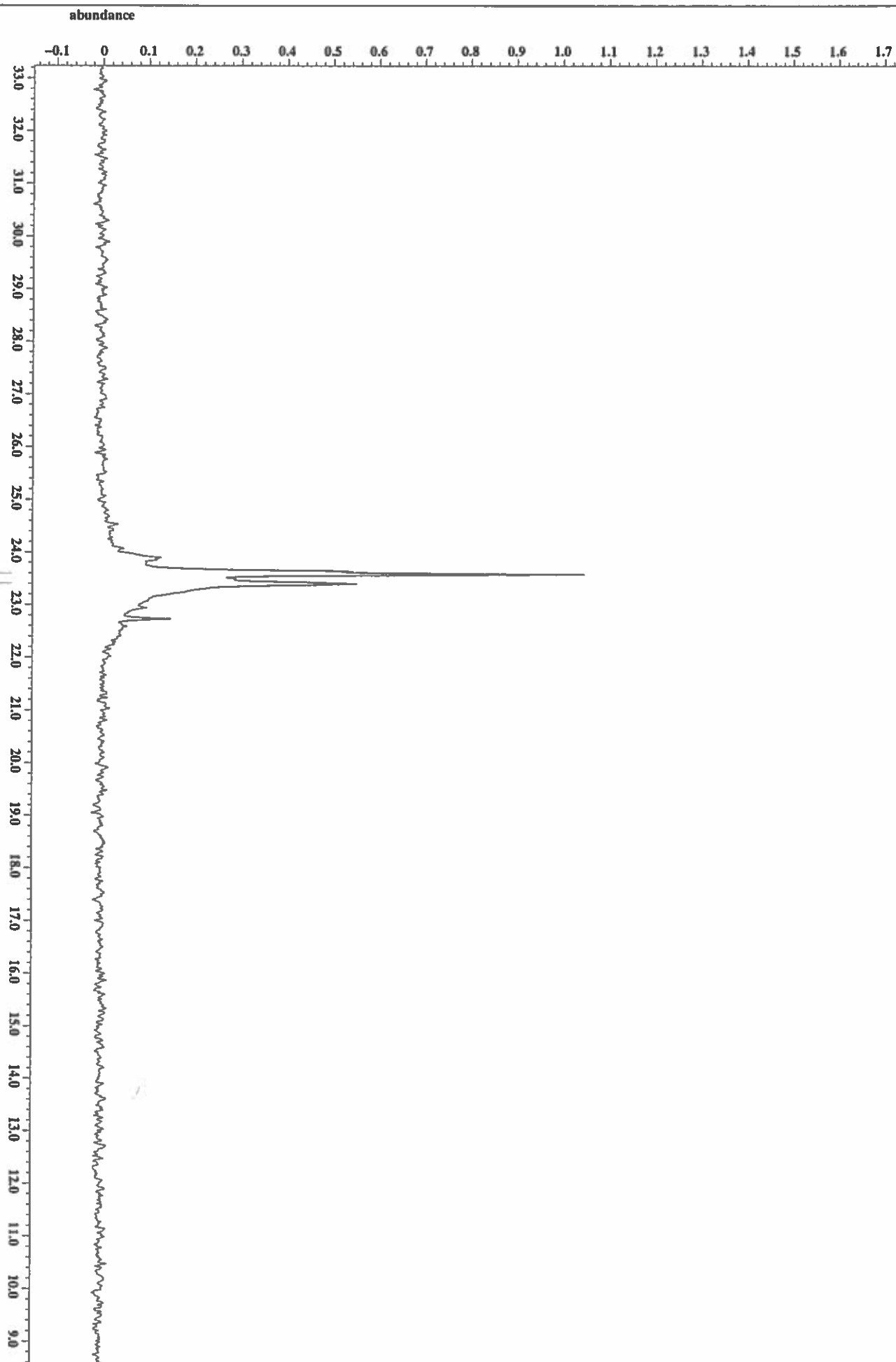
Filename      = MS0571-300-10_days_PH
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0571-300-10_days
Solvent       = CHLOROPFORM-D
Creation_time = 19-OCT-2018 11:15:16
Revision_time = 19-OCT-2018 10:48:02
Current_time  = 19-OCT-2018 10:49:02

Data_format   = 1D COMPLEX
Dim_size      = 52428
Dim_title     = 31P
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-EX500

Field_strength = 11.747379[T] (500[MH
X_acq_duration = 0.8598323[se]
X_domain       = 31P
X_freq         = 202.46831075[MHz]
X_offset       = 0[ppm]
X_points       = 65536
X_prescans     = 4
X_resolution   = 1.16301746[MHz]
X_sweep        = 76.2195122[kHz]
Irr_domain     = 1H
Irr_freq       = 500.13591571[MHz]
Irr_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 40
Total_scans    = 40

X_90_width     = 14.687[us]
X_acq_time     = 0.8598323[se]
X_angle        = 30[deg]
X_atn          = 5[db]
X_pulse        = 4.89566667[us]
Irr_atn_dec    = 20.7[db]
Irr_atn_pwr    = 20.7[db]
Irr_pwr        = WALTZ
Decoupling     = TRUZ
Initial_wait    = 1[se]
Noe            = TRUZ
Noe_time       = 2[se]
Recvr_gain     = 58
Relaxation_delay = 2[se]
Repetition_time = 2.8598323[se]
Temp_sec       = 22.6[dc]

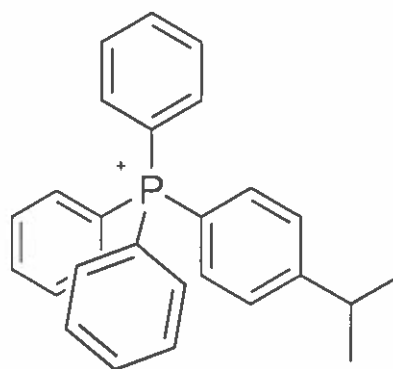
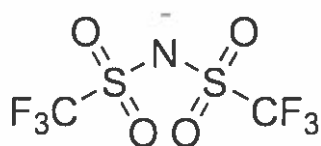
```

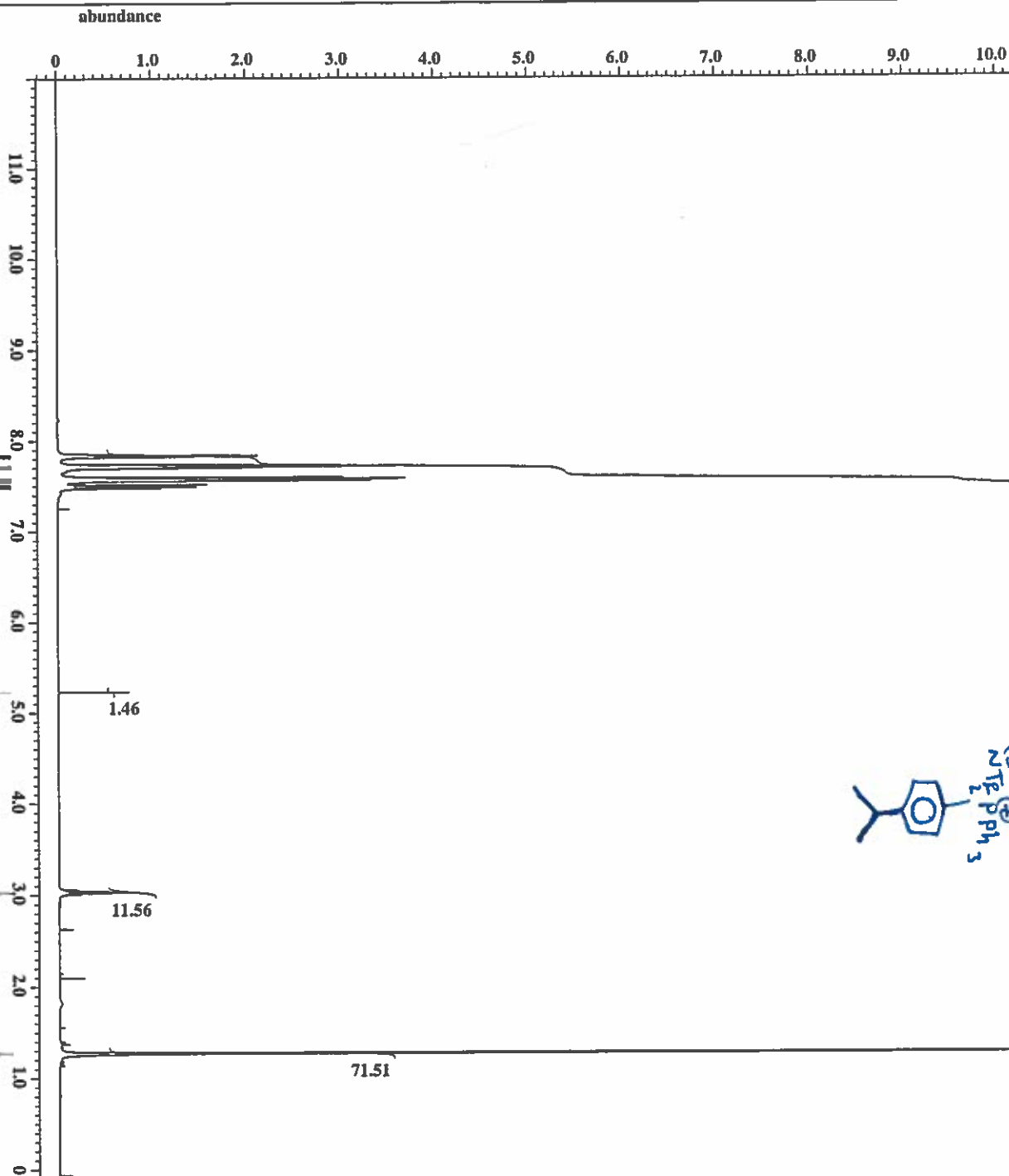
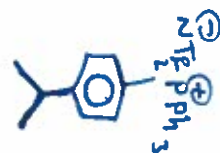


X : parts per Million : 31P

Compound 17 Pre- and Post-heating NMR Spectra

Temperature of Post-heating samples noted in upper left corner of each spectrum





X : parts per Million : 1H



SOUTH ALABAMA
JAGUARS

```

=====
File Name      = MS0503_PROTON-2.jdf
Author         = Jim Davis
Experiment     = single_pulse.ex2
Sample ID      = MS0503
Solvent        = CHLOROFORM-D
Charger Sample = 1
Creation Time   = 6-JUL-2018 16:26:04
Revision Time  = 6-JUL-2018 16:02:29
Current Time   = 6-JUL-2018 16:02:29

Data Format
Dim Size      = 1D COMPLEX
Dim 1 Size    = 13107
Dim 1 Unit    = 1H
Dim 2 Size    = 1
Dim 2 Unit    = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = UNM-ECA500

Field Strength = 11.7473579 [T] (500 [MH
Acq Duration   = 1.74587904 [s]
Domain         = 1H
Freq          = 500.15991521 [MHz]
Offset        = 5.0 [ppm]
Points        = 16384
Prescans      = 1
Resolution    = 0.5727737 [Hz]
Sweep         = 9.38438438 [kHz]
Iter Domain   = 1H
Iter Freq     = 500.15991521 [MHz]
Iter Offset   = 5.0 [ppm]
F1 Domain     = 1H
F1 Freq       = 500.15991521 [MHz]
F1 Offset     = 5.0 [ppm]
Clipped       = FALSE
Mod Return    = 1
Scans         = 16
Total Scans   = 16

X_90_Width    = 12.4 [us]
X_Acq_Time    = 1.74587904 [s]
X_Angle       = 45 [deg]
X_Alt         = 4 [dB]
X_Pulse       = 6.2 [us]
X_Pulse_Prog  = OF2
X1_Mode       = OF2
Pulse_Prog    = FALSE
Initial Wait  = 1 [s]
Relaxation Delay = 22
Relaxation Delay = 5.74587904 [s]
Repetition Time = 22.6 [s]
Temp Set      = 22.6 [C]
=====

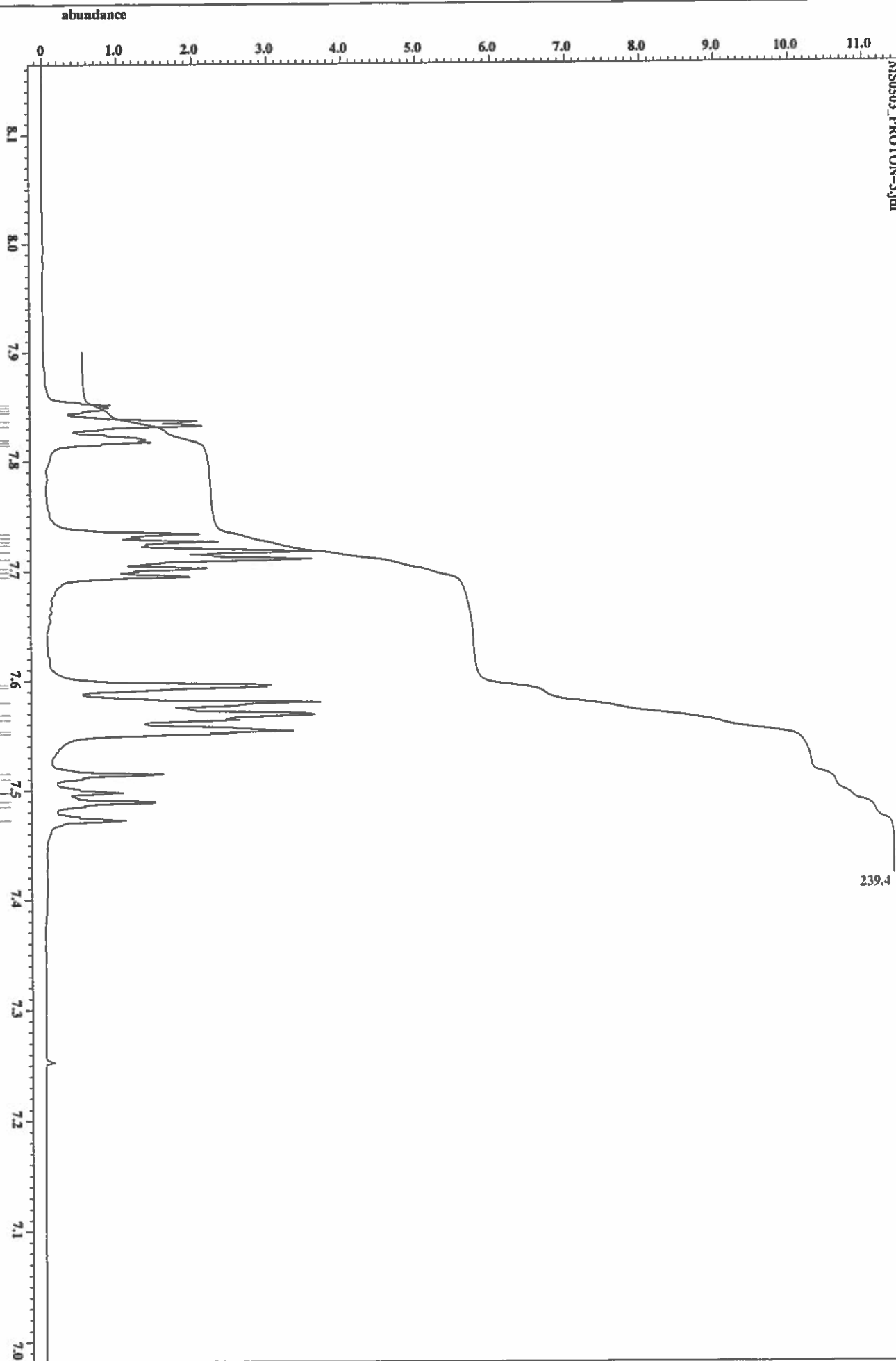
```

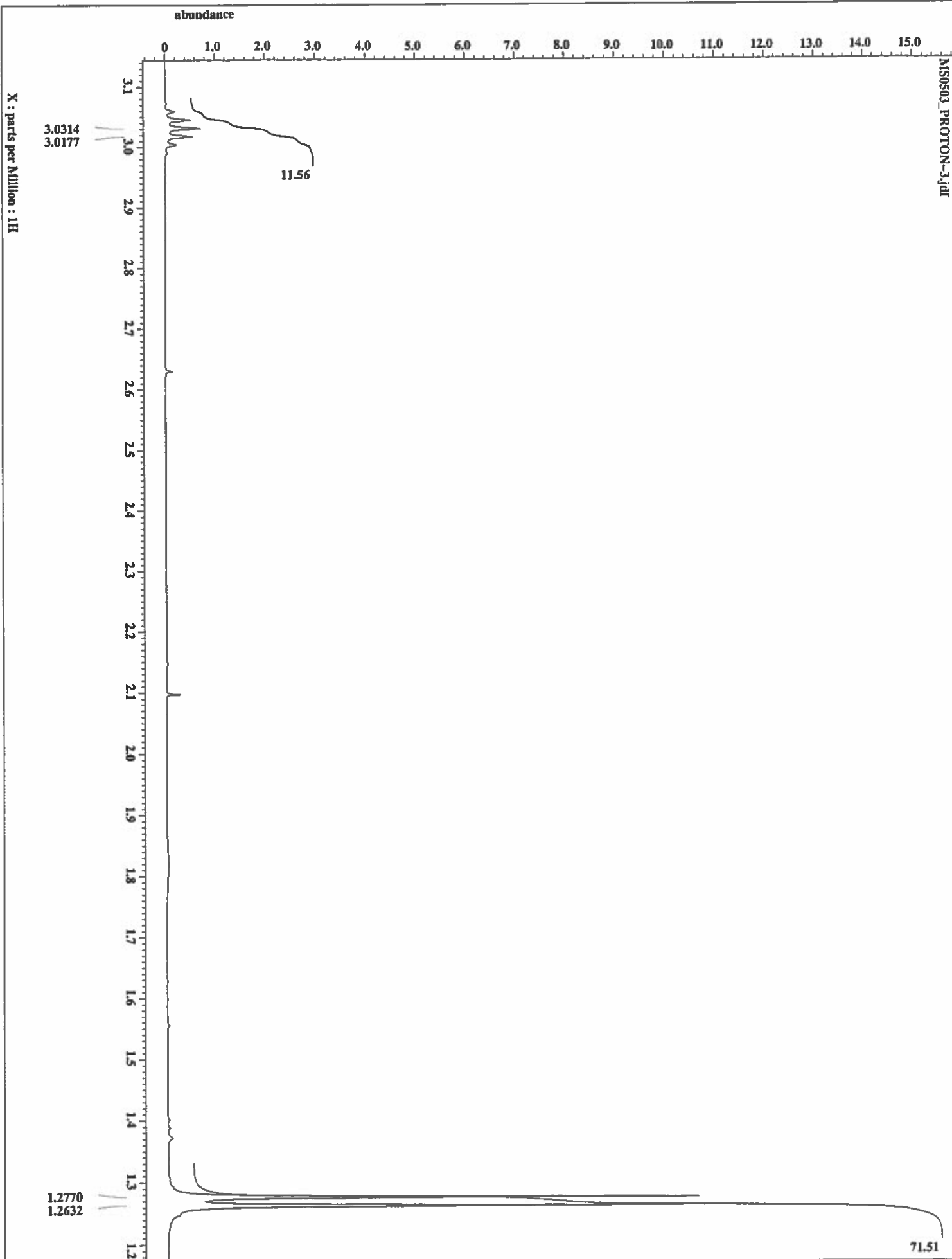
X : parts per Million : 1H

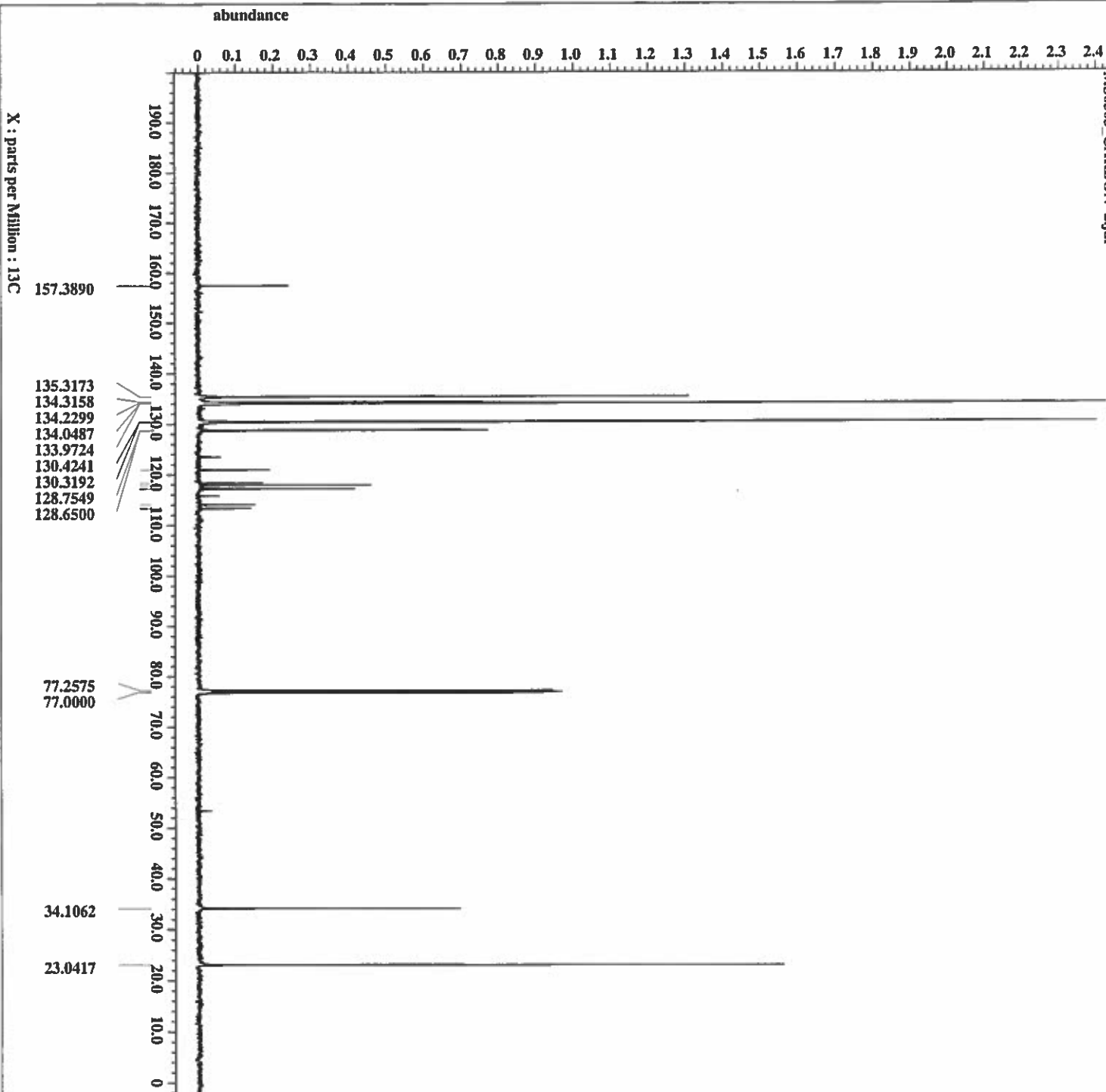
7.8515
7.8366
7.8321
7.8195
7.8172

7.7336
7.7267
7.7175
7.7107
7.7026

7.5961
7.5939
7.5801
7.5687
7.5641
7.5538
7.5515
7.5148
7.4977
7.4896
7.4851
7.4725







```

Filename      = MS0503-CARBON-2.jdt
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample Id     = MS0503
Solvent       = CHLOROFORM-D
Change_sample = 1
Creation_time  = 6-JUL-2018 16:39:26
Revision_time  = 6-JUL-2018 16:15:53
Current_time   = 6-JUL-2018 16:15:53

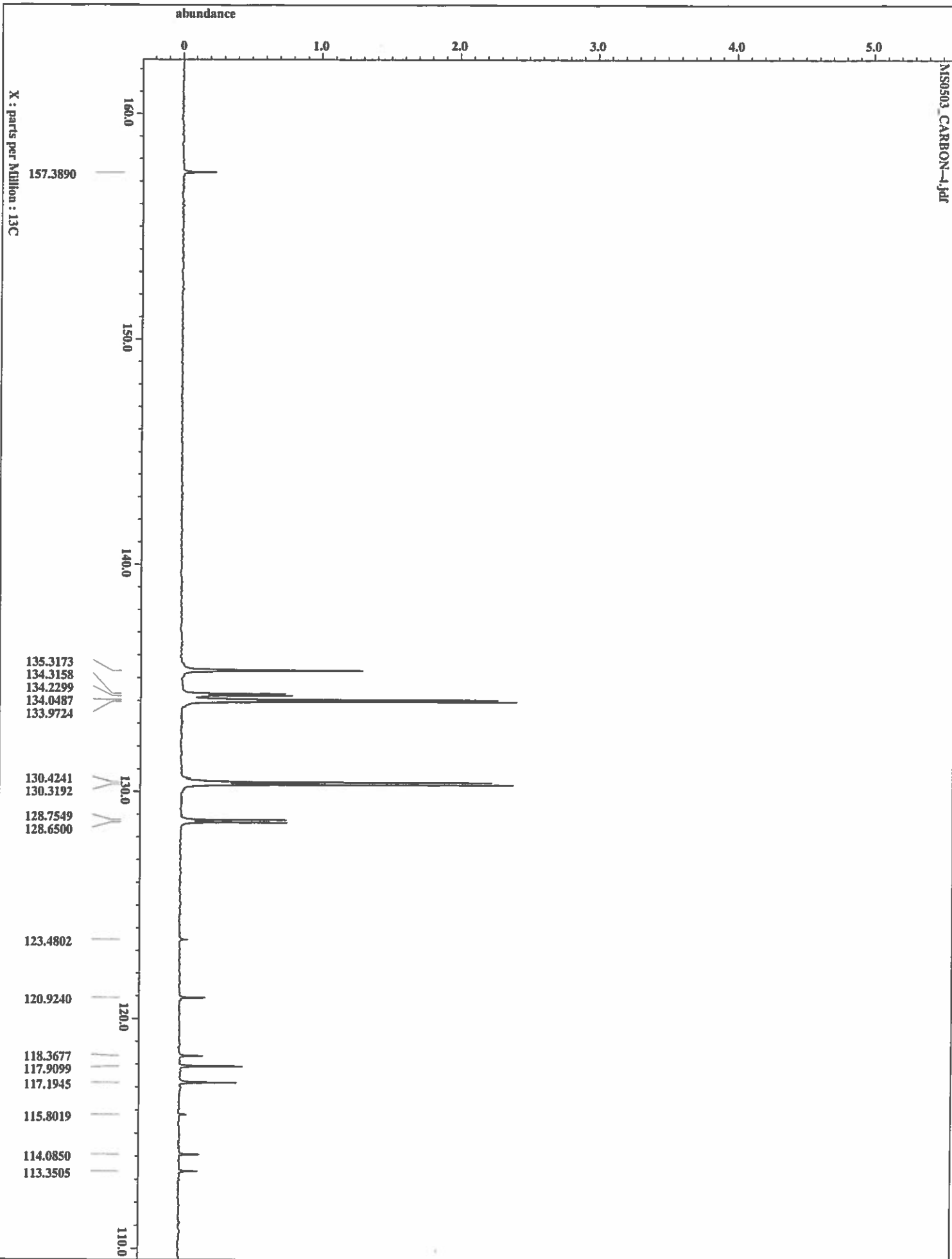
Data_format   = 1D COMPLEX
Dlm_size      = 26214
Dlm_title     = 13C
Dlm_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

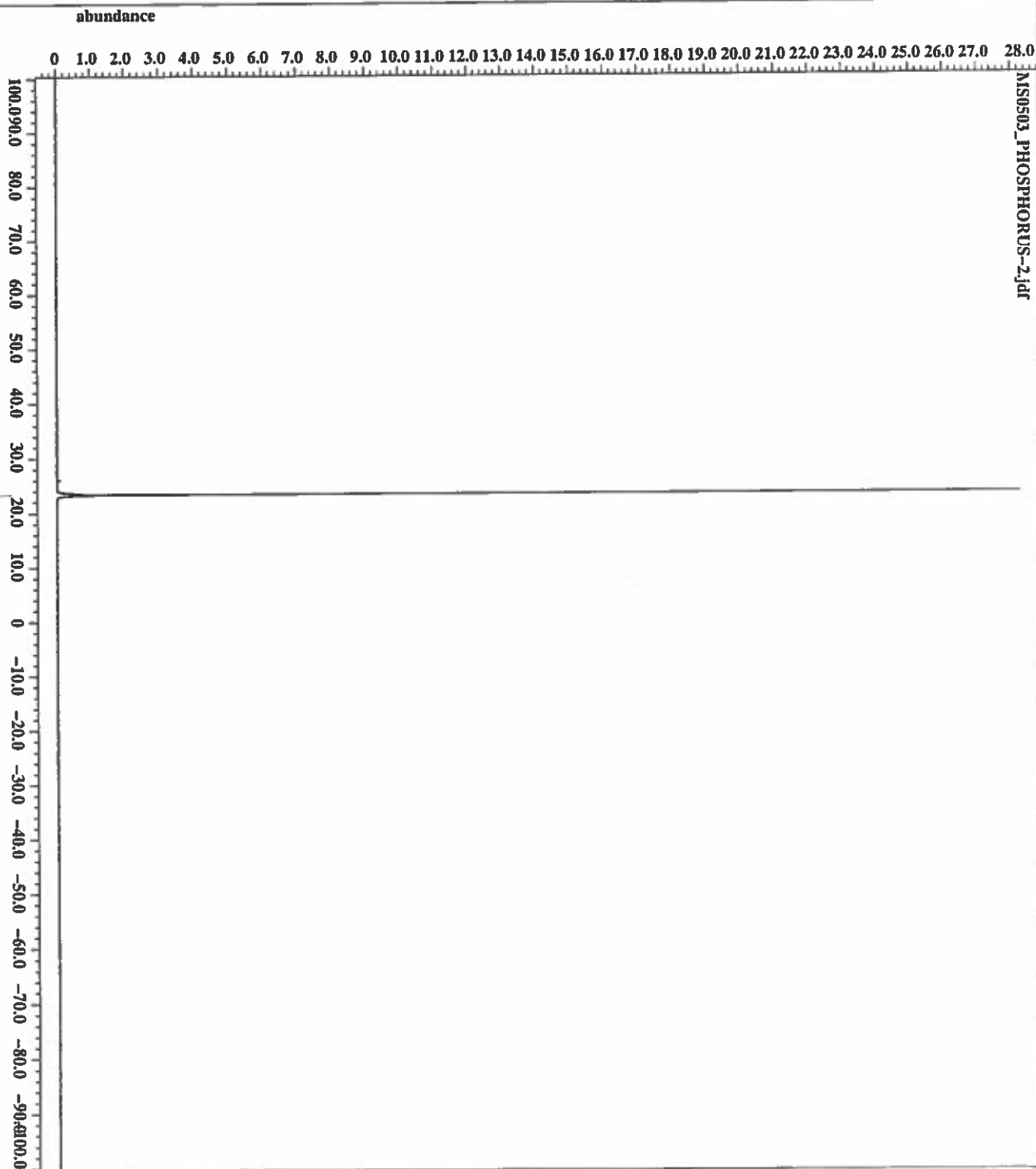
Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_offset       = FALSE
Mod_return     = 1
Scans          = 256
Total_scans    = 256

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
X_atn_dec      = 20.7 [dB]
X_atn_noe      = 20.7 [dB]
X_noise        = VALTZ
Decoupling     = gPRG
Initial_wait    = 1 [s]
Nuc1           = 13C
Nuc2           = 13C
Nuc3           = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 23 [C]
  
```

SOUTHERN
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```

Filename      = MS0503_PHOSPHORUS-2.j
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0503
Solvent       = CHLOROFORM-D
Charger_sample = 1
Creation_time  = 6-JUL-2018 16:18:19
Revision_time  = 6-JUL-2018 15:55:44
Current_time   = 6-JUL-2018 15:55:44

Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_c1title   = 31P
Dim_units     = [ppm]
Dimensions    = X
Site          = FCA 500
Spectrometer  = JNM-ECX500

Field_strength = 11.747379 [T] (500 [MH
X_acq_duration = 0.64487424 [s]
X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 32768
X_breathans     = 4
X_resolution    = 1.55068995 [Hz]
X_sweep         = 50.81300813 [kHz]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_offset       = FALSE
Mod_return     = 1
Scans          = 25
Total_scans    = 25

X_90_width     = 14.687 [us]
X_acq_time      = 0.64487424 [s]
X_angle        = 30 [deg]
X_atn          = 5 [dB]
X_pulse        = 4.89566667 [us]
Xir_atn_dec    = 20.7 [dB]
Xir_atn_noe    = 20.7 [dB]
Xir_noise      = FALSE
Decoupling     = TRUE
Initial_wait    = 1 [s]
Noe_time       = TRUE
Noe_time       = 2 [s]
Recur_gain     = 54
Relaxation_delay = 2 [s]
Repetition_time = 2.64487424 [s]
Temp_get       = 22.9 [degC]
  
```

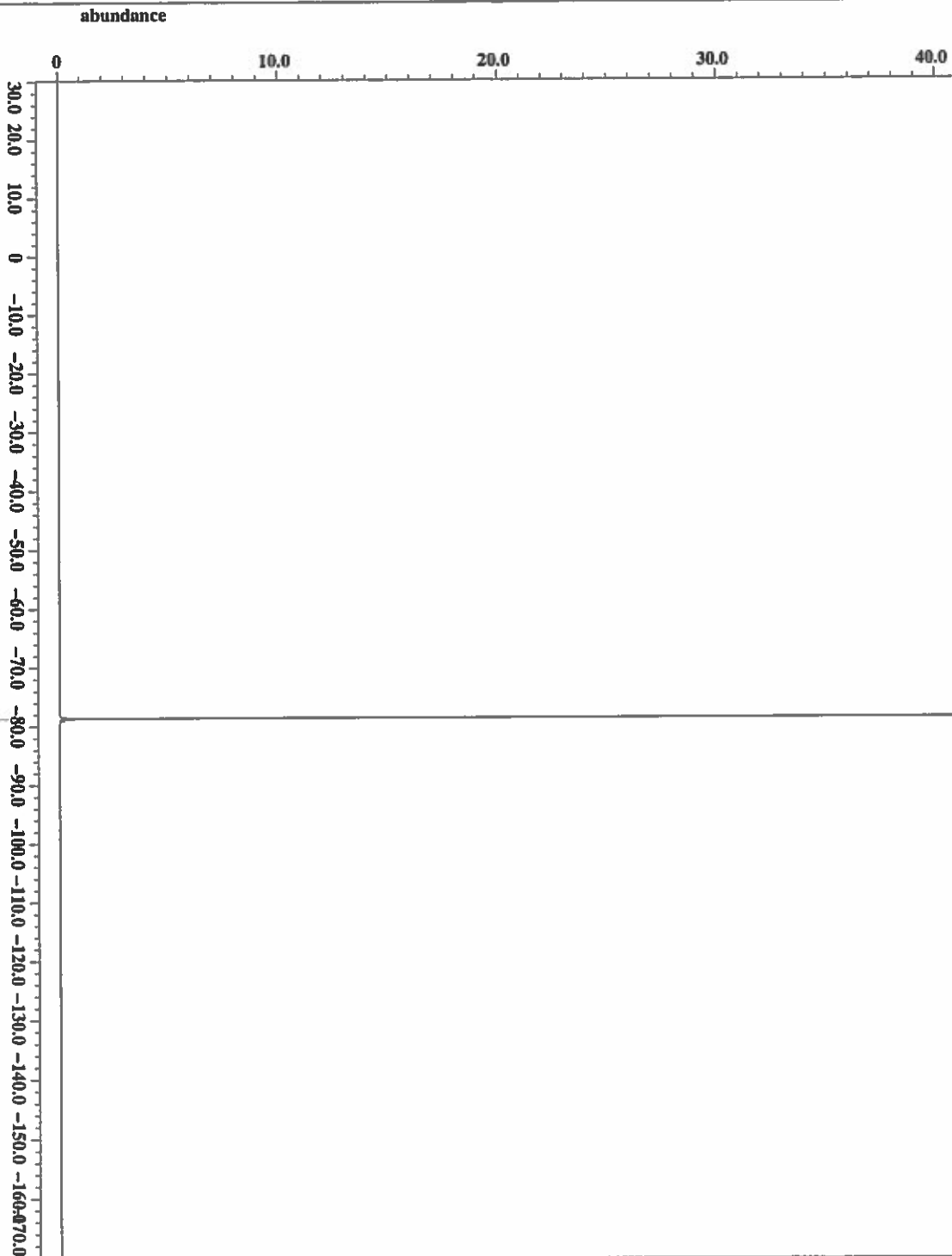


Filename = MS0503_FLUORINE-2.jdf
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0503
 Solvent = CHLOROFORM-D
 Changer_sample = 1
 Creation_time = 6-JUL-2018 16:23:31
 Revision_time = 6-JUL-2018 15:58:58
 Current_time = 6-JUL-2018 15:58:58

Data_format = 1D COMPLEX
 Dim_size = 52428
 Dim_title = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 0.55574528[s]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = -70[ppm]
 X_points = 65536
 X_prescans = 1
 X_resolution = 1.7993855[Hz]
 X_sweep = 117.9245283[kHz]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 5[ppm]
 X1_domain = 19F
 X1_freq = 470.62046084[MHz]
 X1_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 13.1[us]
 X_acq_time = 0.55574528[s]
 X_angle = 45[deg]
 X_atn = 2.5[db]
 X_pulse = 6.55[us]
 X1_mode = OF
 X1_presat = OF
 Initial_puls = 1[s]
 Relaxation_delay = 36
 Relaxation_delay = 4[s]
 Repetition_time = 4.55574528[s]
 Temp_get = 22.7[deg]



X : parts per Million : 19F

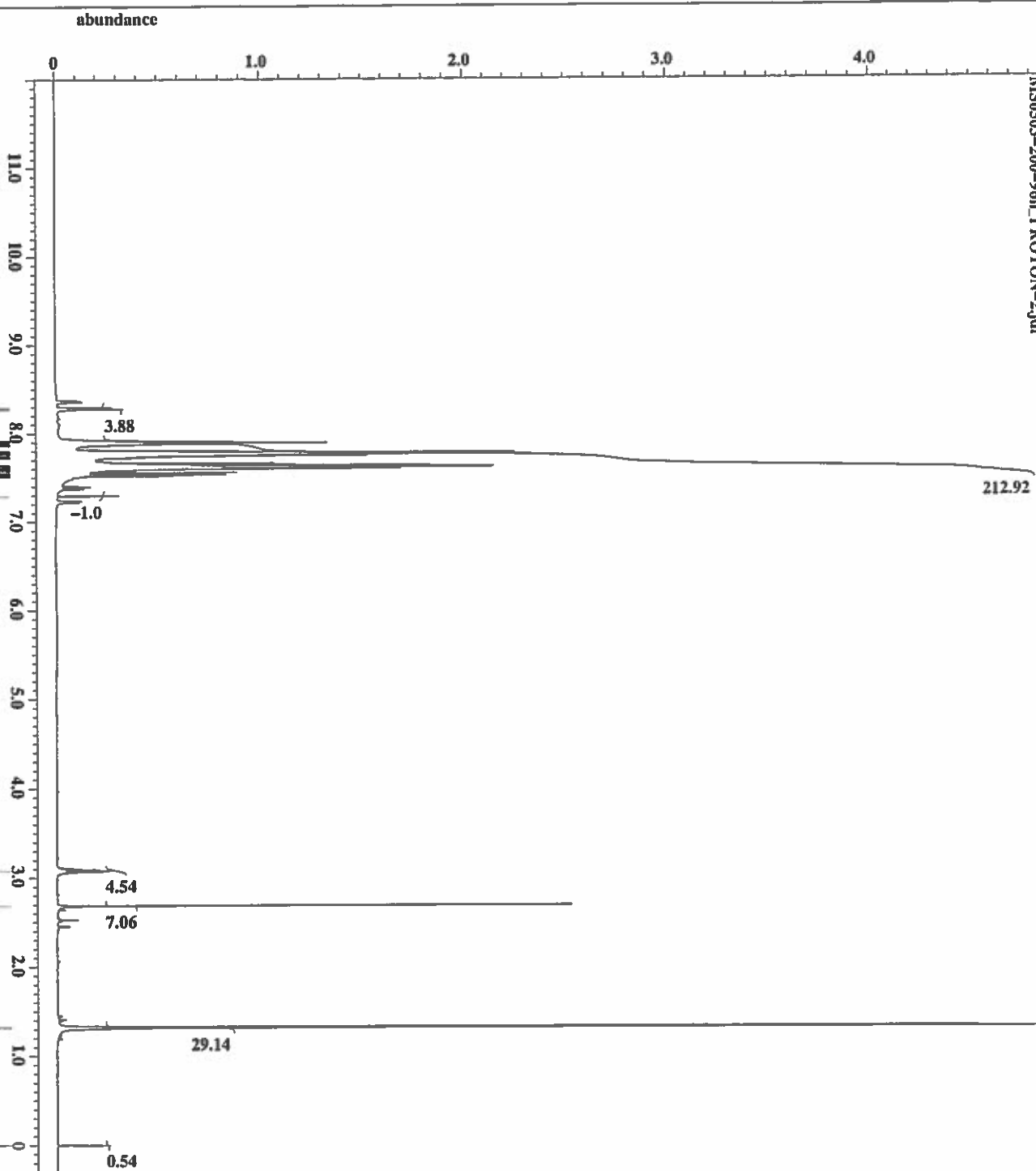
X : parts per Million : 1H

8.2751
8.2694
7.7827
7.7667
7.7598
7.2926

3.0823
2.6866

1.3296
1.3158

0.0000



Filename = MS0503-200-96h_PROTON
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0503-200-96h
 Solvent = CHLOROFORM-D
 Changer_sample = 4
 Creation_time = 11-JUL-2018 01:51:20
 Revision_time = 11-JUL-2018 01:29:03
 Current_time = 11-JUL-2018 01:29:05

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

 Field_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 1.74587904 [s]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.57277737 [Hz]
 X_sweep = 9.38438438 [kHz]
 Xr_domain = 1H
 Xr_freq = 500.15991521 [MHz]
 Xr_offset = 5.0 [ppm]
 Xr1_domain = 1H
 Xr1_freq = 500.15991521 [MHz]
 Xr1_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

 X_90_width = 12.4 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_atn = 4 [dB]
 X_pulse = 6.2 [us]
 Xr_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1 [s]
 Recv_gain = 24
 Relaxation_delay = 4 [s]
 Repetition_time = 5.74587904 [s]
 Temp_get = 22.2 [dc]

X : parts per Million : 1H

8.2923
8.2866
8.2751
8.2694

3.88

7.9075
7.9029
7.8949
7.8903
7.8778
7.8755

7.7827
7.7793
7.7758
7.7667
7.7598
7.7506
7.7438

7.6407
7.6384
7.6361
7.6235
7.6212
7.6166
7.6144
7.6121
7.6075
7.5972
7.5949

7.2926

1.0

212.92

abundance

0

1.0

2.0

3.0

4.0

5.0

8.6

8.5

8.4

8.3

8.2

8.1

8.0

7.9

7.8

7.7

7.6

7.5

7.4

7.3

7.2

7.1

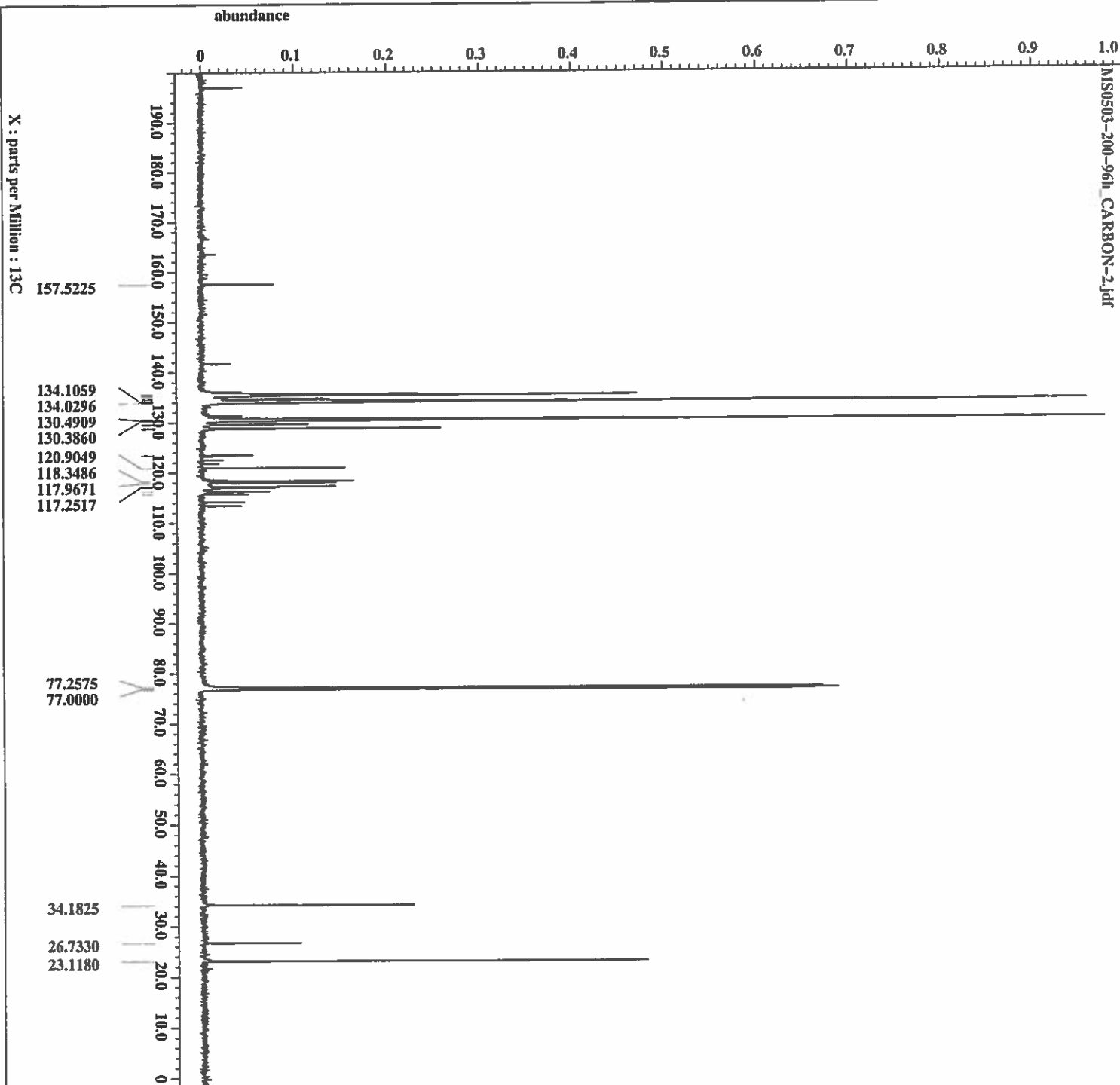


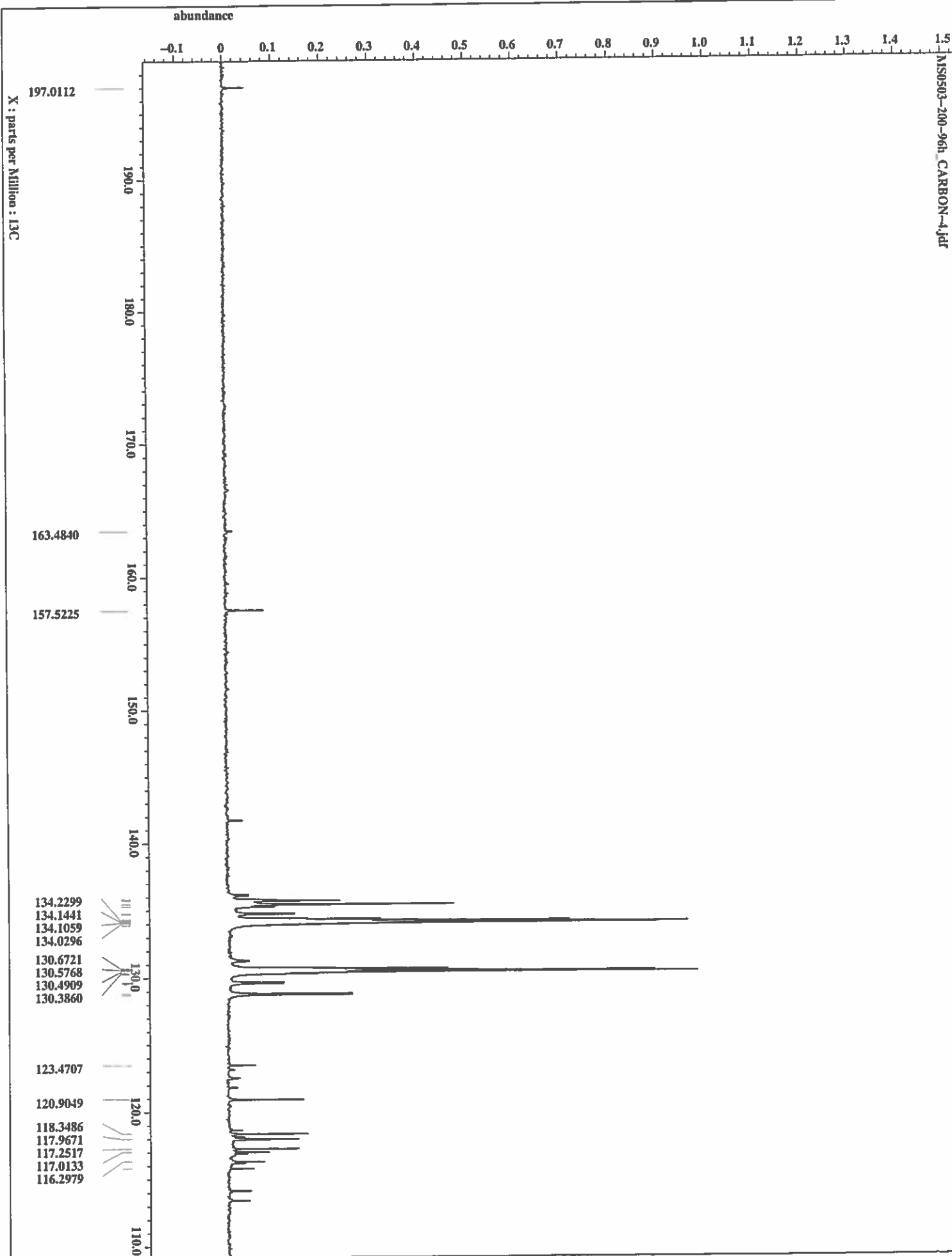
Filename = MS0503-200-96h_CARBON
Author = Jim Davis
Experiment = single-pulse_dec
Sample_id = MS0503-200-96h
Solvent = CHLOROFORM-D
Charger_sample = 4
Creation_time = 11-JUN-2018 02:42:11
Revision_time = 11-JUN-2018 02:19:54
Current_time = 11-JUN-2018 02:19:54

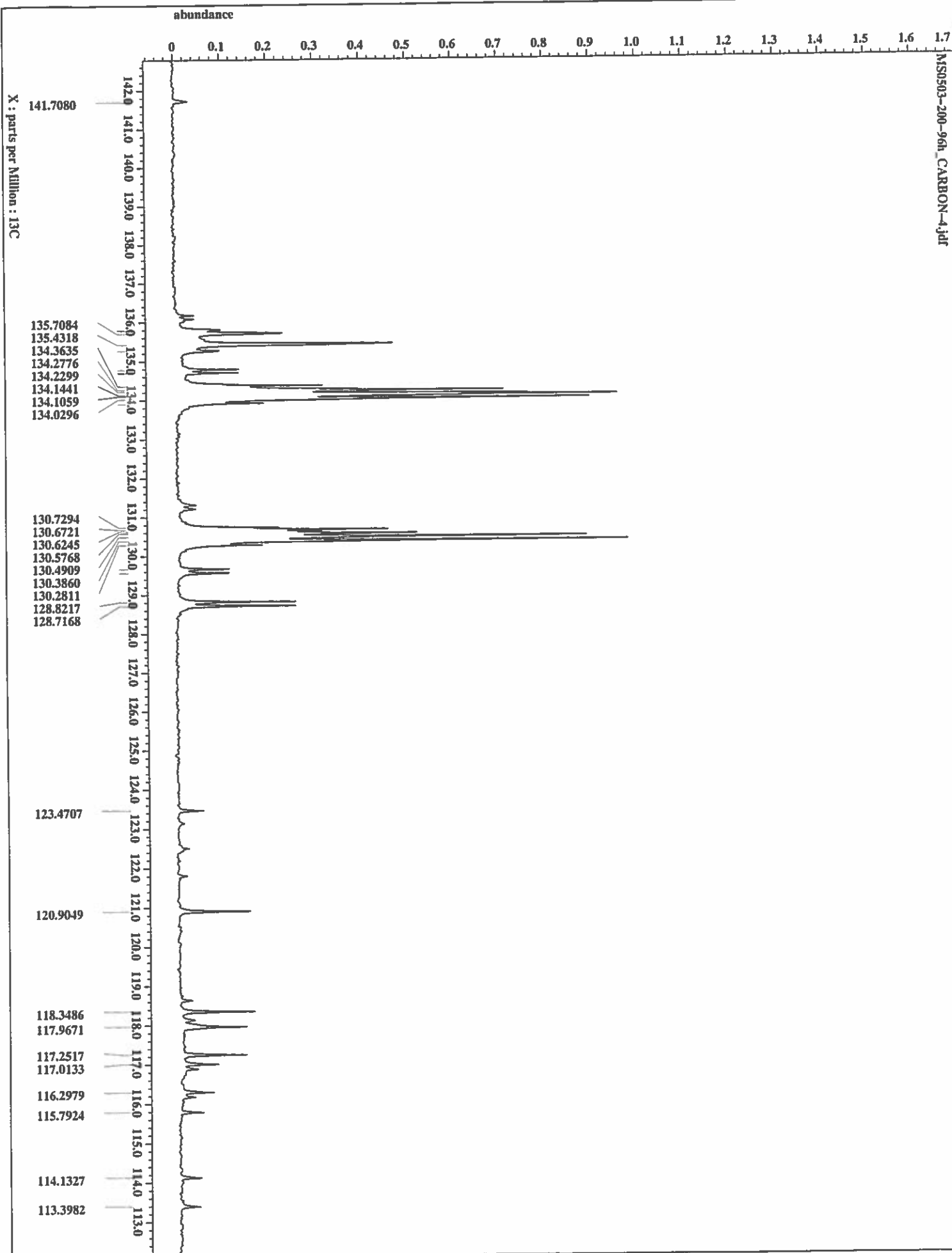
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.747379 [G] (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_resolution = 39.3081761 [kHz]
X_sweep = 1H
Irr_domain = 500.15891521 [MHz]
Irr_freq = 5.0 [ppm]
Irr_offset = FALSE
Mod_return = 1
Scans = 1024
Total_scans = 1024

X_90_width = 13.2 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 6 [dB]
X_pulse = 4.4 [us]
Irr_atn_dec = 20.7 [dB]
Irr_atn_noe = 20.7 [dB]
Decoupling = WALTZ
Initial_wait = TRUZ
Noe_time = TRUZ
Reverz_gain = 1 [s]
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set = 22.8 [dc]







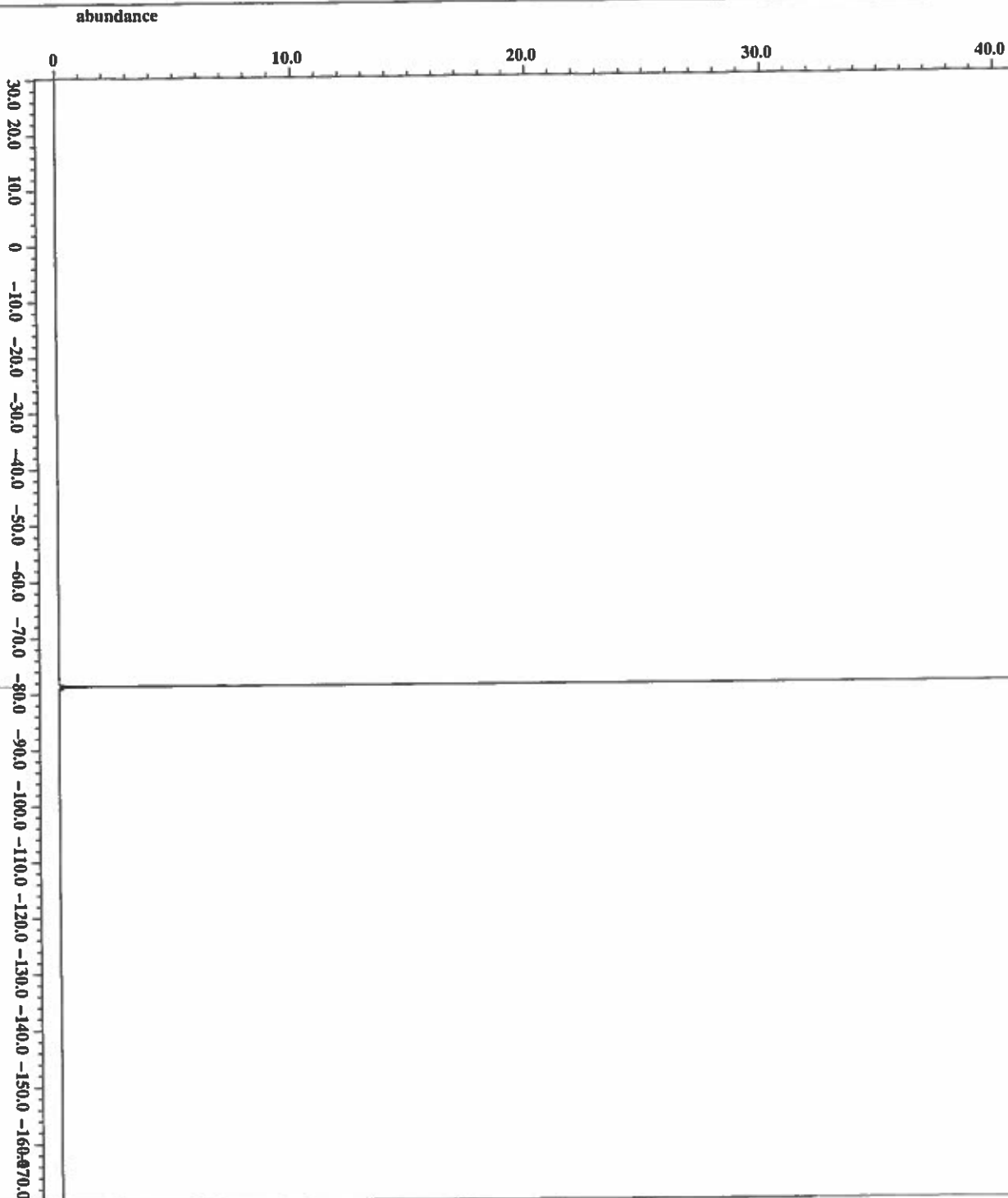


Pilename = MS0503-200-96h_FLUORINE
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0503-200-96h
 Solvent = CHLOROFORM-D
 Changer_sample = 4
 Creation_time = 11-JUL-2018 02:45:18
 Revision_time = 11-JUL-2018 02:23:01
 Current_time = 11-JUL-2018 02:23:01

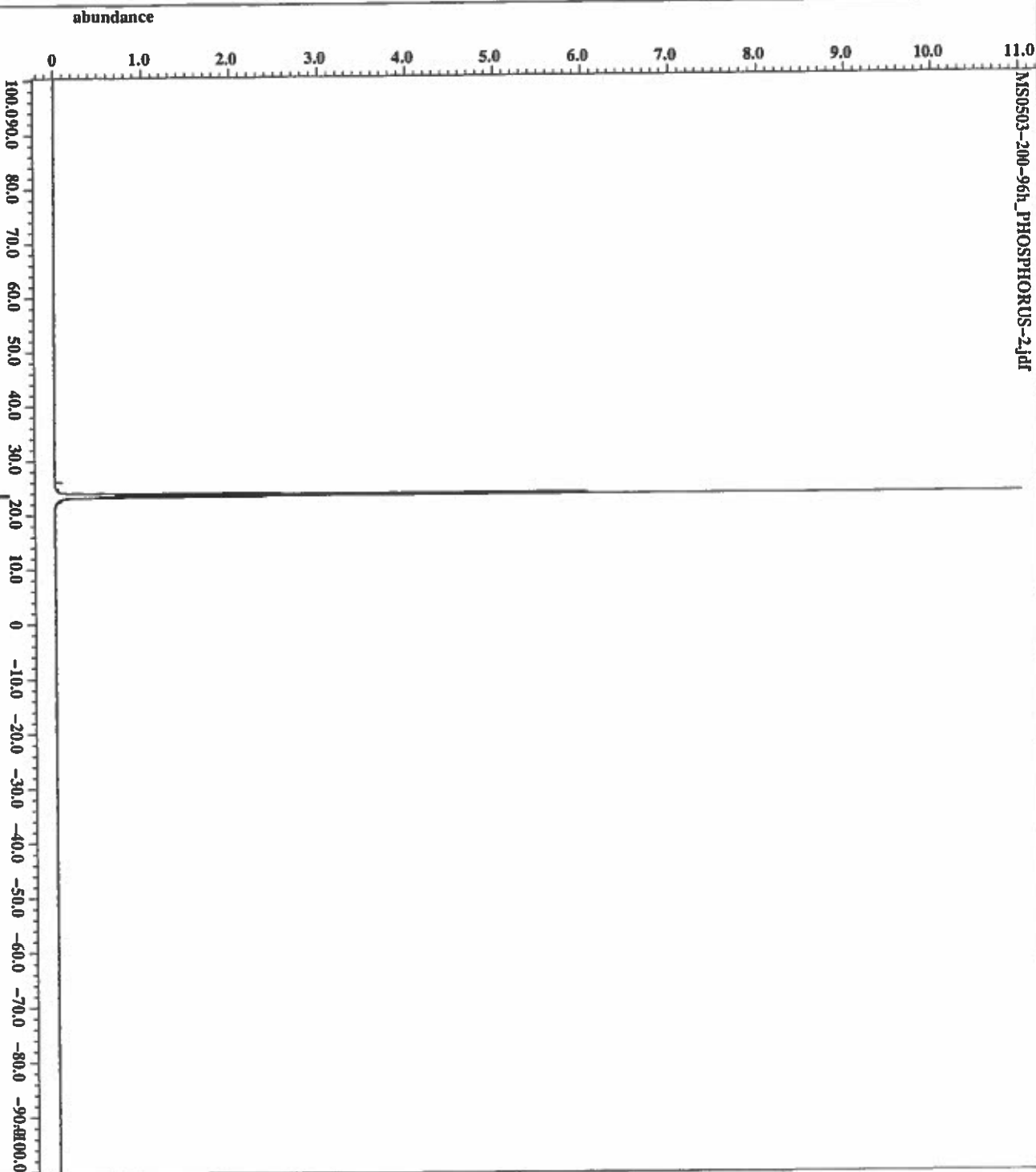
Data_format = 1D COMPLEX
 Dim_size = 52428
 Dim_title = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 0.55574528 [s]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = -70 [ppm]
 X_points = 65536
 X_prescans = 1
 X_resolution = 1.799385 [Hz]
 X_sweep = 117.9245283 [kHz]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = 5 [ppm]
 X1_domain = 19F
 X1_freq = 470.62046084 [MHz]
 X1_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 13.1 [us]
 X_acq_time = 0.55574528 [s]
 X_angle = 45 [deg]
 X_atn = 2.5 [dB]
 X_pulse = 6.55 [us]
 X1_mode = OF
 Dantec_preset = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 36
 Relaxation_delay = 4 [s]
 Repetition_time = 4.55574528 [s]
 Temp_90c = 22.4 [deg]



X : parts per Million : 19F



SOUTH ALABAMA
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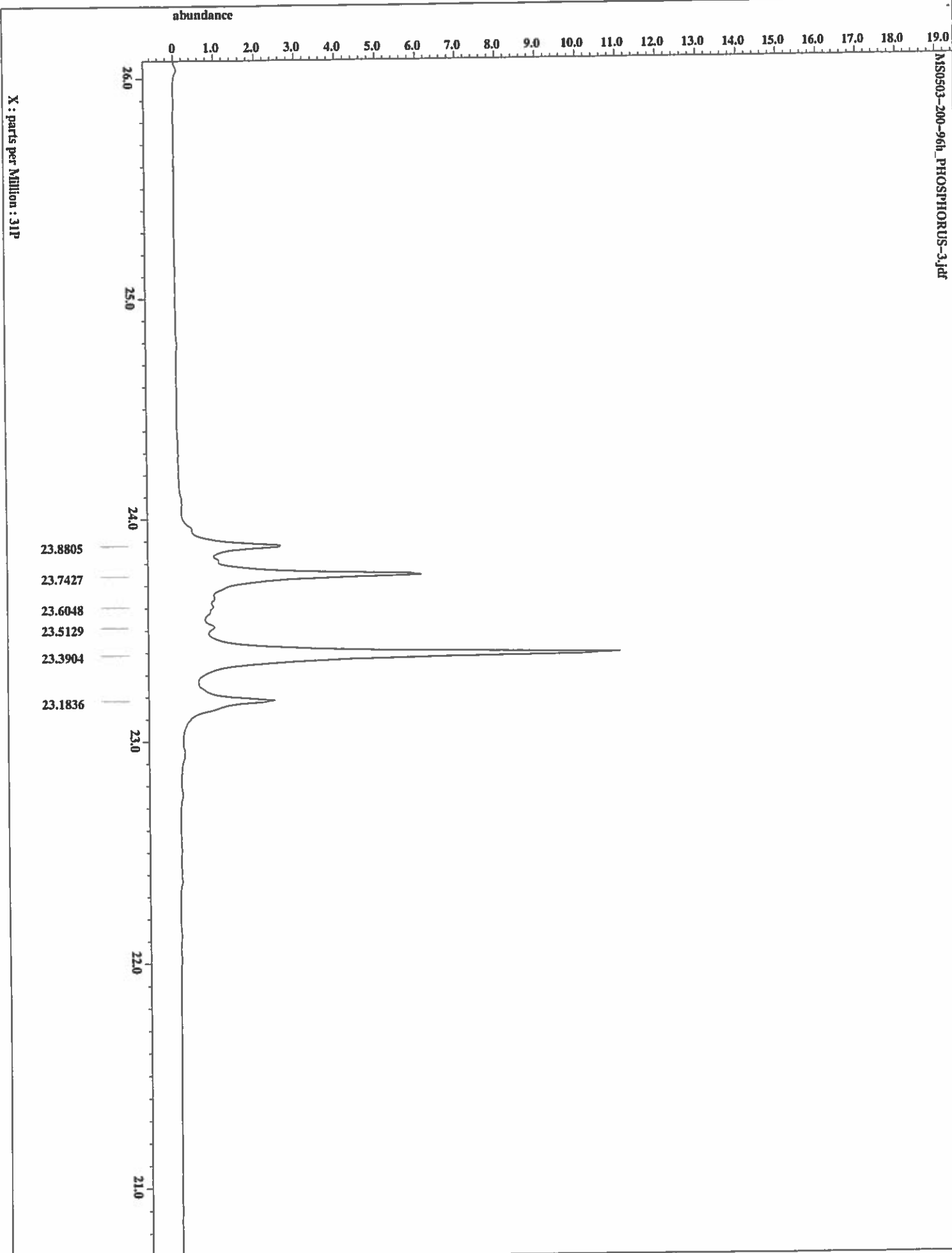
```

Filename      = MS0503-200-96h_PHOSPH
Author        = Jim Davis
Experiment    = 81nqle_pulse_dec
Sample_id     = MS0503-200-96h
Solvent       = CHLOROFORM-D
Charger_sample = 4
Creation_time  = 11-JUL-2018 02:59:05
Revision_time  = 11-JUL-2018 02:36:48
Current_time   = 11-JUL-2018 02:36:48

Date_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 31P
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = QNP-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.64487424 [s]
X_domain      = 31P
X_freq        = 202.46831075 [MHz]
X_offset      = 0 [ppm]
X_points      = 32768
X_prescans    = 4
X_resolution  = 1.55068995 [Hz]
X_sweep       = 50.81300813 [kHz]
X_domain      = 1H
X_freq        = 500.13591521 [MHz]
X_offset      = 5.0 [ppm]
X_resolution  = 5.0 [ppm]
Mod_return    = FALSTZ
Scans         = 1
Total_scans   = 256

X_90_width    = 14.687 [us]
X_acq_time     = 0.64487424 [s]
X_angle       = 30 [deg]
X_atn         = 5 [dB]
X_pulse       = 4.89566667 [us]
X_atn_dec     = 20.7 [dB]
X_atn_noe     = 20.7 [dB]
X_atn_noe     = 20.7 [dB]
Decoupling    = WALTZ
Initial_wait   = TRU2
Noc           = 1 [s]
Noc_time      = TRU2
Noc_time      = 2 [s]
Noc_time      = 58
Relaxation_delay = 2 [s]
Repetition_time = 2.64487424 [s]
Temp_get      = 22.8 [dC]
  
```

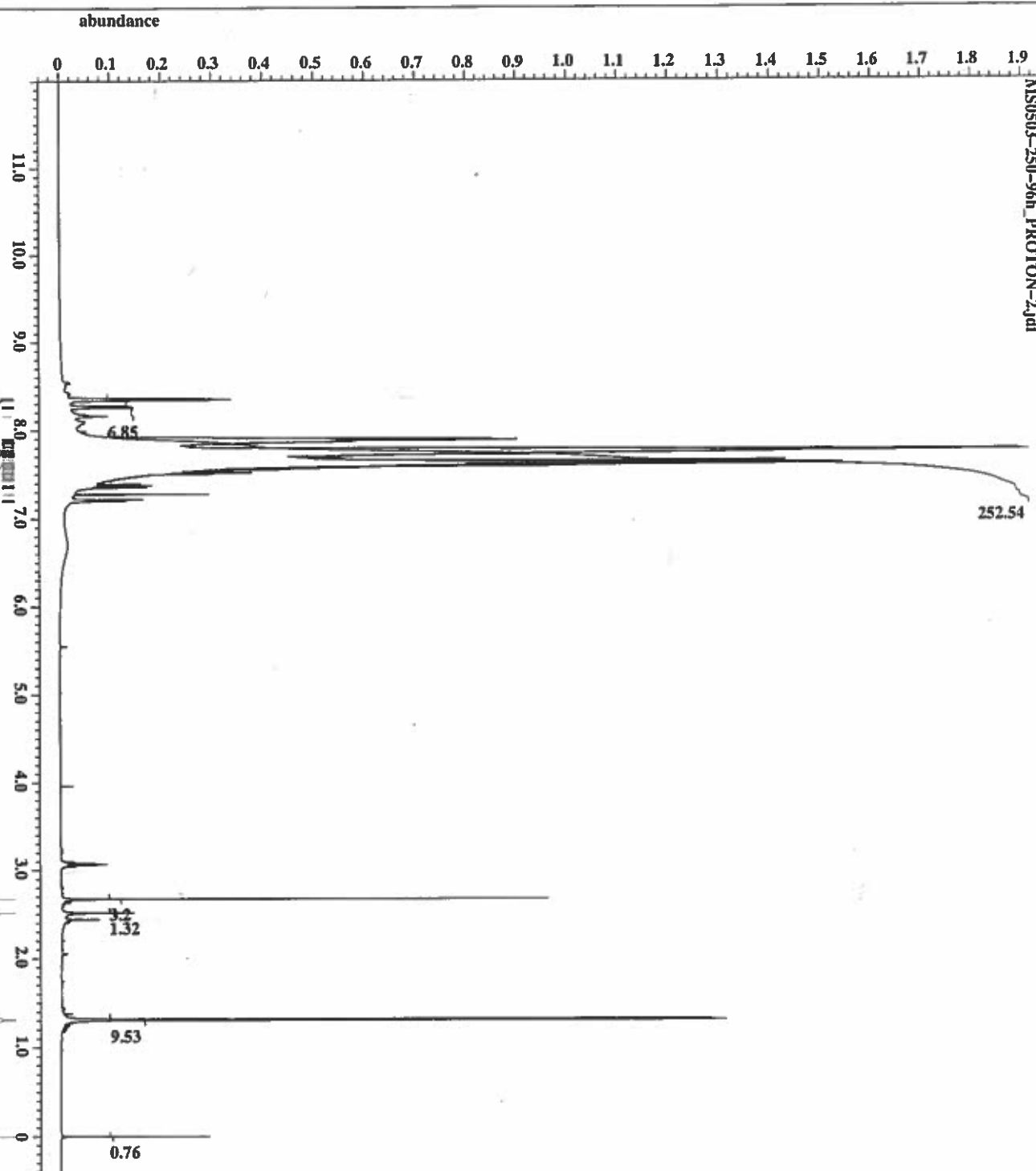


8.3553
8.3450
8.3393
7.7747
7.7678
7.7598
7.7518
7.6212

2.6740
2.5171

1.3193
1.3055

-0.0000



X : parts per Million : 1H



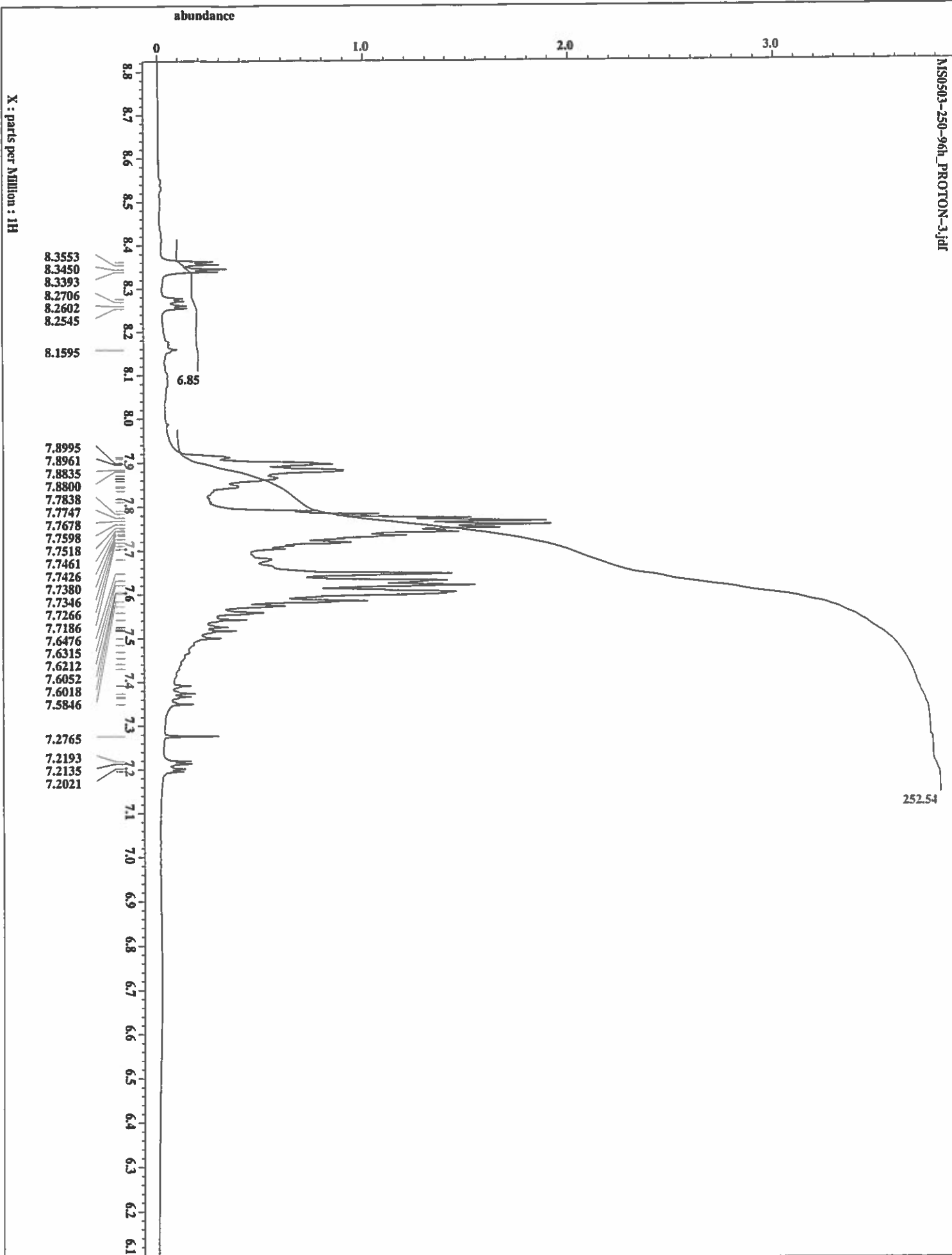
```

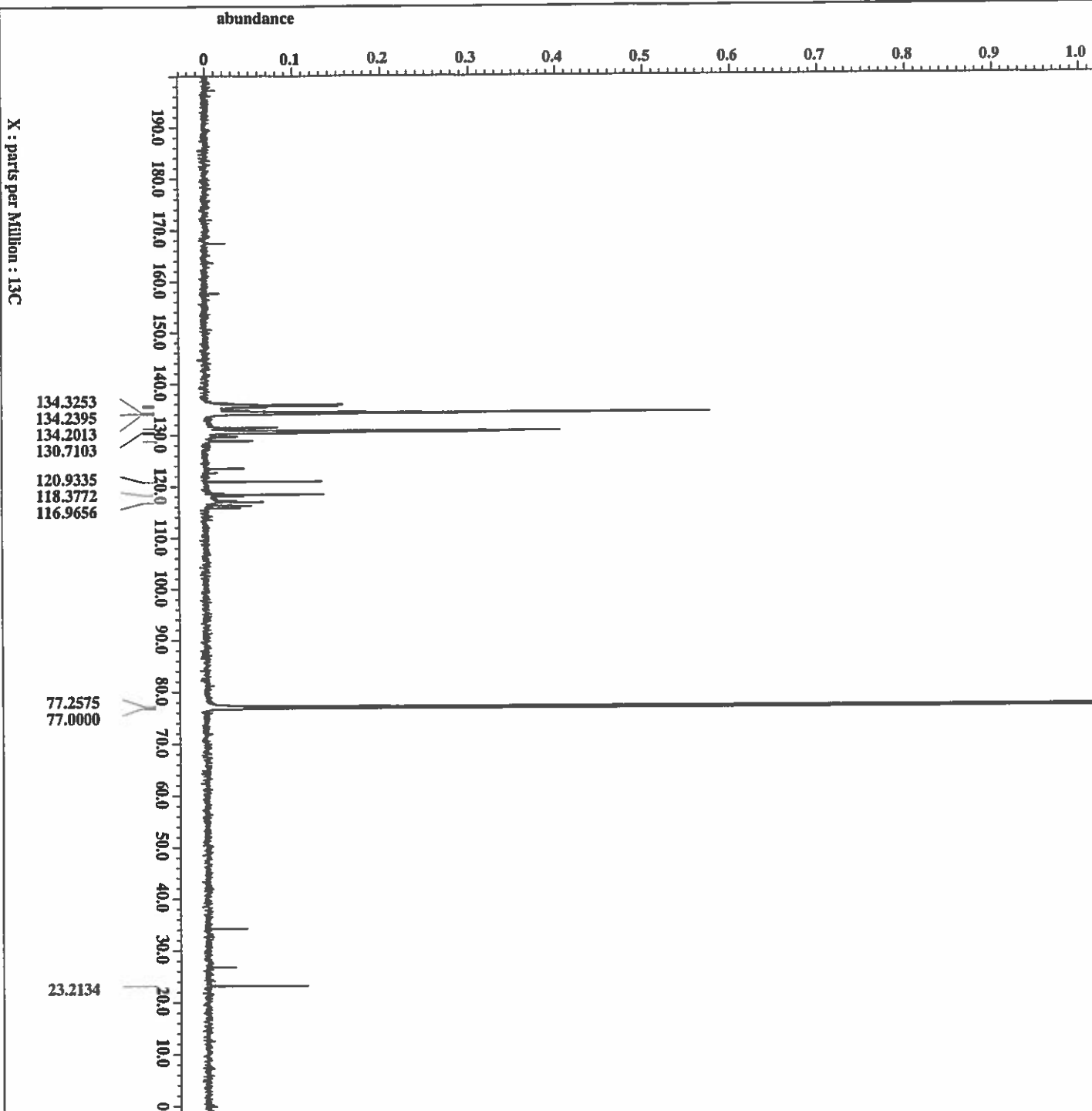
=====
File: MS0503-250-96h_PROTON
Author: Jia Davis
Experiment: single_pulse.ex2
Sample ID: MS0503-250-96h
Solvent: CHLOROFORM-D
Charger: sample
Creation time: 10-JUN-2018 18:34:37
Revision time: 10-JUN-2018 18:34:23
Current time: 10-JUN-2018 18:12:23

Data format: 1D COMPLEX
Dim size: 13107
Dim title: 1H
Dim units: [ppm]
Dimensions: X
Site: ECA 500
Spectrometer: JNM-ECA500

Field strength: 11.7473579 [T] (500 [MH
X_acq_duration: 1.74587904 [s]
X_domain: 1H
X_freq: 500.15991521 [MHz]
X_offset: 5.0 [ppm]
X_points: 16384
X_prescans: 1
X_resolution: 0.57277737 [Hz]
X_sweep: 9.38438438 [kHz]
Xr_domain: 1H
Xr_freq: 500.15991521 [MHz]
Xr_offset: 5.0 [ppm]
Xr1_domain: 1H
Xr1_freq: 500.15991521 [MHz]
Xr1_offset: 5.0 [ppm]
Clipped: FALSE
Mod_return: 1
Total_scans: 16

X_90_width: 12.4 [us]
X_acq_time: 1.74587904 [s]
X_angle: 45 [deg]
X_atn: 4 [dB]
X_pulse: 6.3 [us]
Xr_mode: OF2
Xr1_mode: OF2
Pulse program: FALGE
Initial wait: 1 [s]
Recvr_gain: 28
Relaxation delay: 4 [s]
Repetition time: 5.74587904 [s]
Temp_get: 22.8 [deg]
    
```





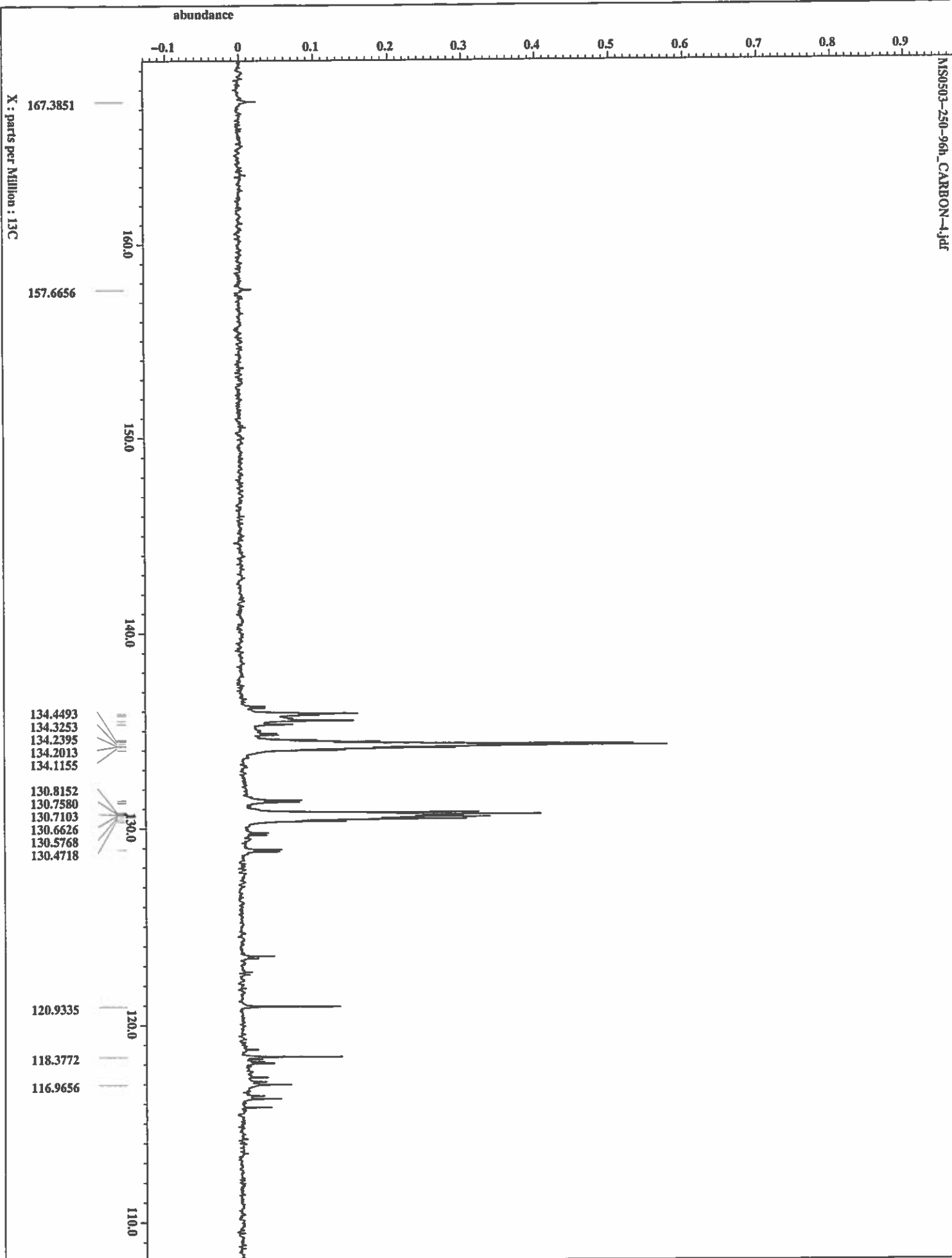
```

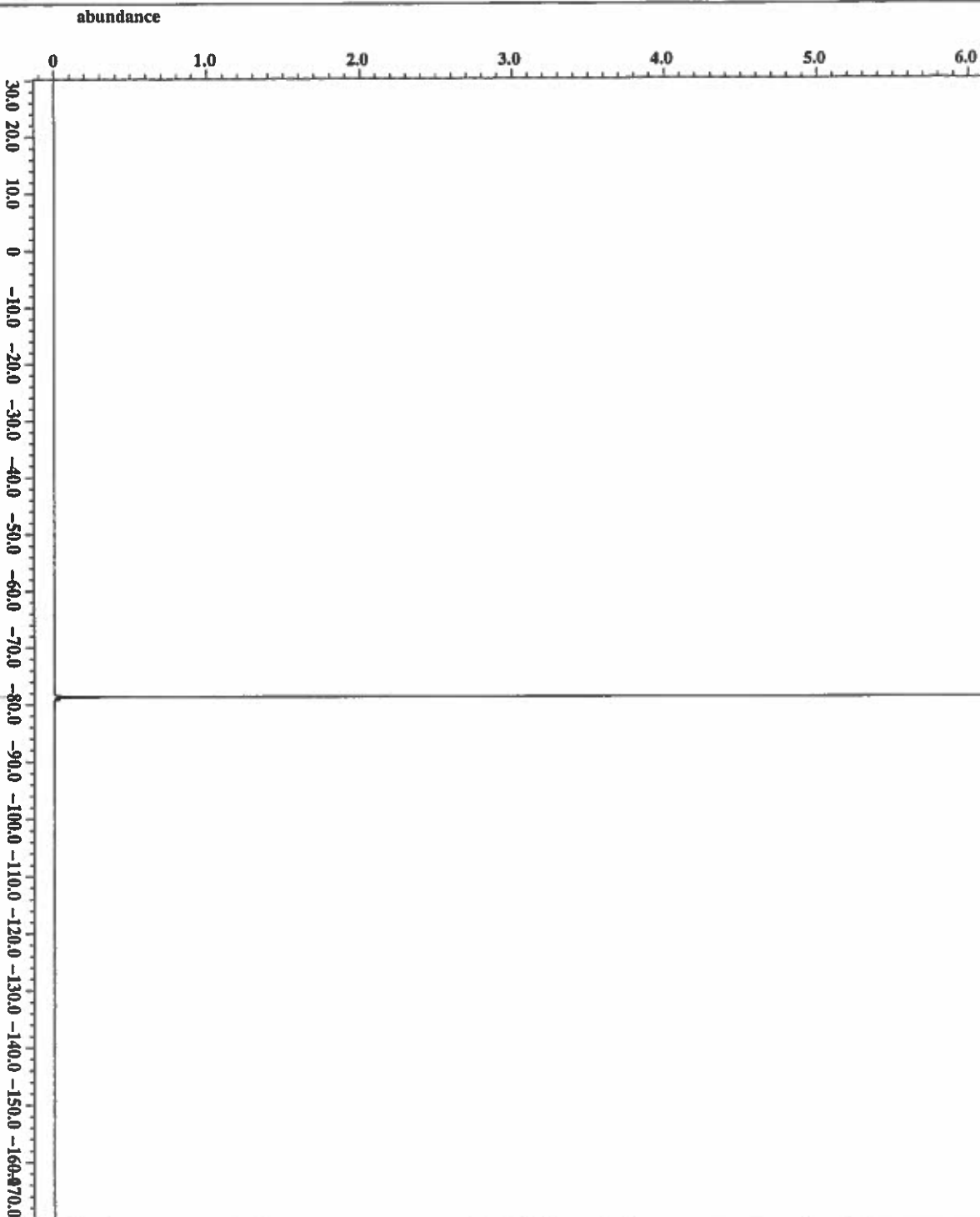
Filename      = MS0503-250-96h_CARBON
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0503-250-96h
Solvent       = CHLOROFORM-D
Charger_sample = 5
Creation_time  = 10-JUL-2018 19:05:21
Revision_time = 10-JUL-2018 18:43:05
Current_time  = 10-JUL-2018 18:43:05

Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 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          = 600
Total_scans    = 600

X_90_width     = 13.2 [us]
X_acq_time      = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_hoe    = 20.7 [dB]
Irr_noise      = VALVE
Decoupling     = TRUE
Initial_wait   = 1 [s]
Hoe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 23.4 [degC]
  
```





X : parts per Million : 19F

```

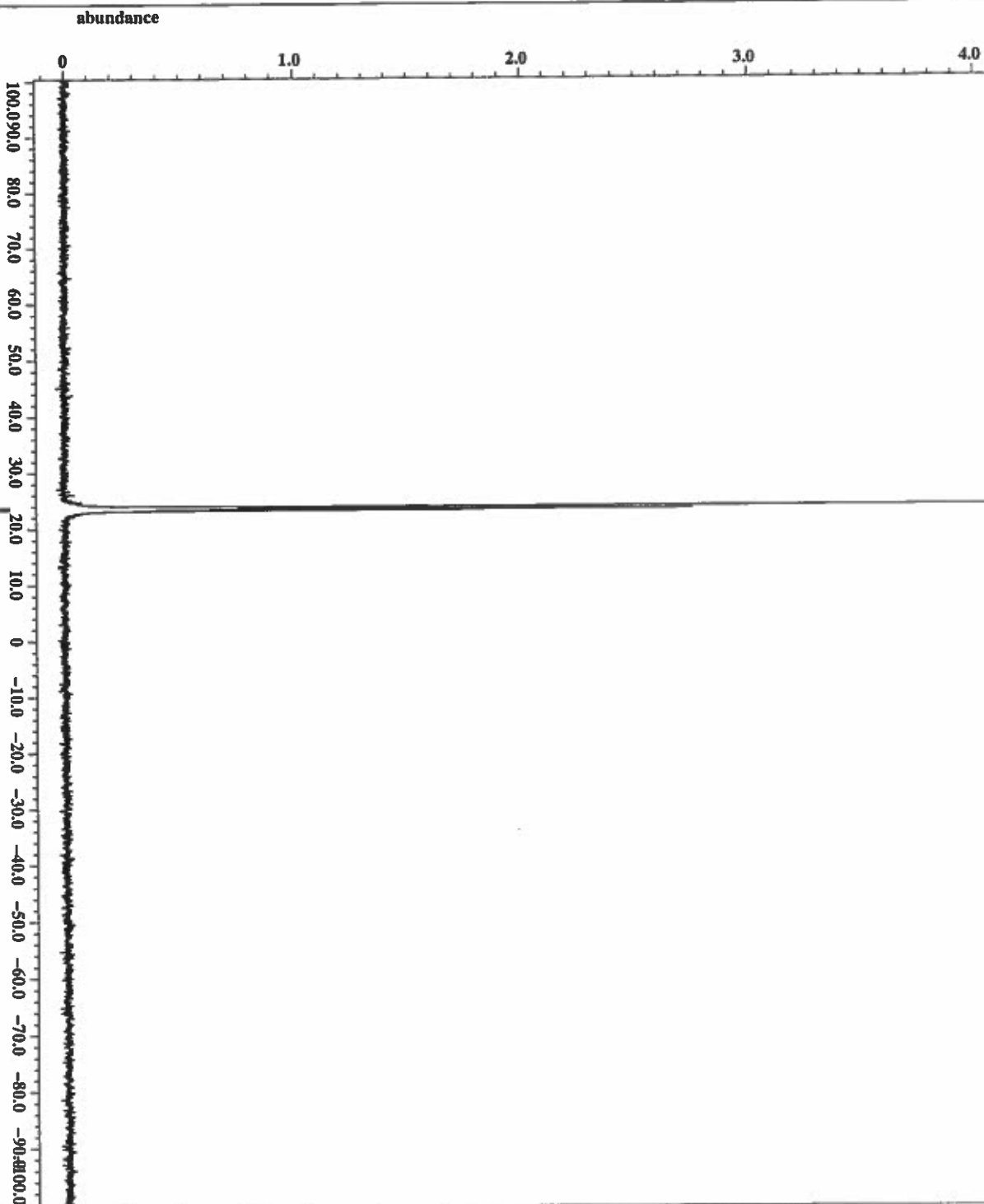
Filename      = MS0503-250-96h_FLUORINE
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = MS0503-250-96h
Solvent       = CHLOROFORM-D
Charger_sample = 5
Creation_time  = 10-JUN-2018 19:08:18
Revision_time  = 10-JUN-2018 18:46:04
Current_time   = 10-JUN-2018 18:46:04

Data_format    = 1D COMPLEX
Dim_size       = 52428
Dim_title      = 19F
Dim_units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

Field_strength = 11.747379 [T] (500 [MH
X_acq_duration = 0.55574528 [s]
X_domain       = 19F
X_freq         = 470.62046084 [MHz]
X_offset       = -70 [ppm]
X_points       = 65536
X_procscans    = 1
X_resolution    = 1.7993855 [Hz]
X_sweep        = 117.9245283 [Hz]
Xr_domain      = 19F
Xr_freq        = 470.62046084 [MHz]
Xr_offset      = 5 [ppm]
Xr1_domain     = 19F
Xr1_freq       = 470.62046084 [MHz]
Xr1_offset     = 5 [ppm]
Xr1_offset     = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 13.1 [us]
X_acq_time     = 0.55574528 [s]
X_angle        = 45 [deg]
X_atn          = 2.5 [dB]
X_pulse        = 6.55 [us]
Xr1_mode       = Off
Pulse_program  = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 38
Relaxation_delay = 4 [s]
Repetition_time = 4.55574528 [s]
Temp_set       = 23 [dC]

```



X : parts per Million : 31P



```

P1: name
Author
Experiment
Sample_id
Solvent
Charger_sample
Creation_time
Revision_time
Current_time

Data_format
Dim_size
Dim_title
Dim_units
Dimensions
Site
Spectrometer

Field_strength
X_acq_duration
X_domain
X_freq
X_offset
X_points
X_prescans
X_resolution
X_sweep
X_domain
X_freq
X_offset
Clipped
Mod_return
Scans
Total_scans

X_90_width
X_acq_time
X_angle
X_atn
X_pulse
Xr_atn_dec
Xr_atn_poe
Xr_noise
Decoupling
Initial_wait
Noe_time
Recvr_gain
Relaxation_delay
Repetition_time
Temp_set

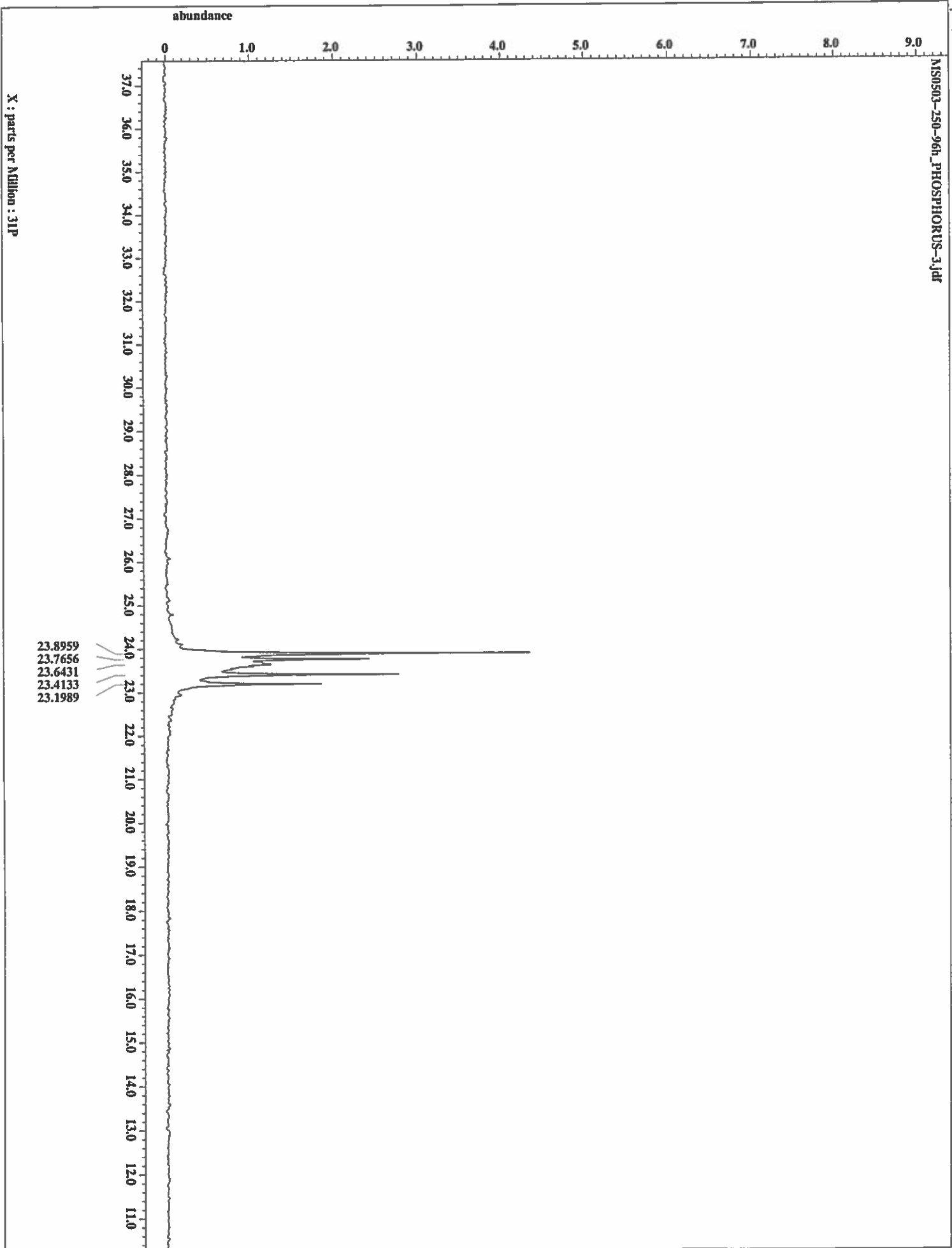
= MS0503-250-96h_PHOSPH
= Jim Davis
= single_pulse_dec
= MS0503-250-96h
= CHLOROFORM-D
= 5
= 10-JUL-2018 19:13:18
= 10-JUL-2018 18:51:02
= 10-JUL-2018 18:51:02

= 1D COMPLEX
= 26214
= 31P
= [ppm]
= X
= ECA 500
= JNM-ECA500

= 11.7473579 [T] (500 [MH
= 0.64467424 [s]
= 31P
= 202.46831075 [MHz]
= 0 [ppm]
= 32768
= 4
= 1.55068995 [Hz]
= 50.81300813 [kHz]
= 1H
= 500.15991521 [MHz]
= 5.0 [ppm]
= FALSE
= 1
= 50
= 50

= 14.687 [us]
= 0.64467424 [s]
= 30 [deg]
= 5 [dB]
= 4.89566667 [us]
= 20.7 [dB]
= 20.7 [dB]
= TRUE
= WALTZ
= 1 [s]
= TRUE
= 2 [s]
= 60
= 2.64467424 [s]
= 23.2 [deg]

```





SOUTH ALABAMA
JAGUARS

```

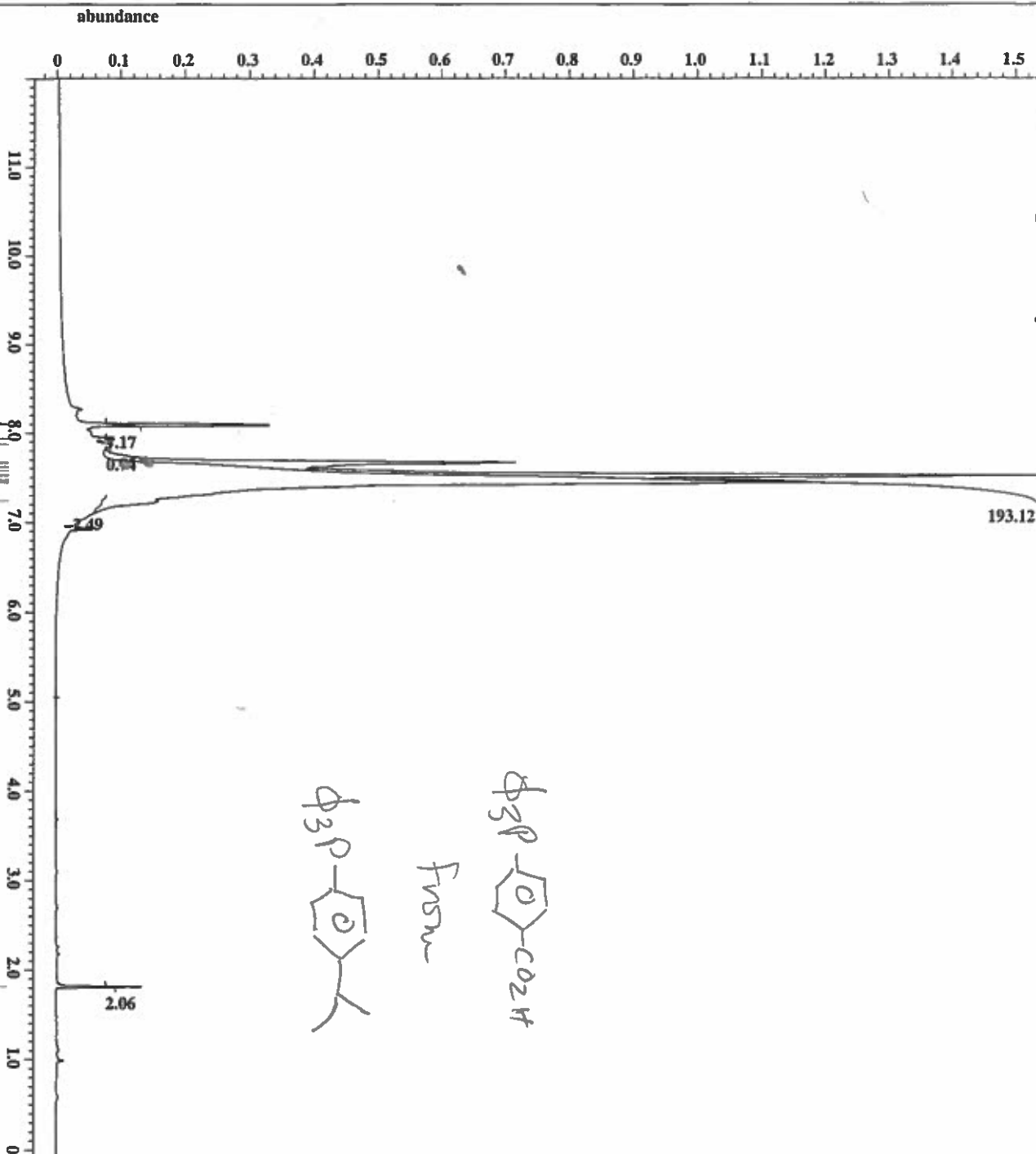
Filename      MS0503-300-96h_PROTON
Author        Jim Davis
Experiment     single_pulse.ex2
Sample_id      MS0503-300-96h
Solvent        CHLOROFORM-D
Charger_sample 6
Creation_time  10-JUL-2018 19:20:04
Revision_time  10-JUL-2018 18:57:48
Current_time   10-JUL-2018 18:57:48

Data_format    1D COMPLEX
Dir_size       13107
Dir_cfile      1H
Dir_units      [ppm]
Dimensions     X
Site           XCA 500
Spectrometer   JNM-ECA500

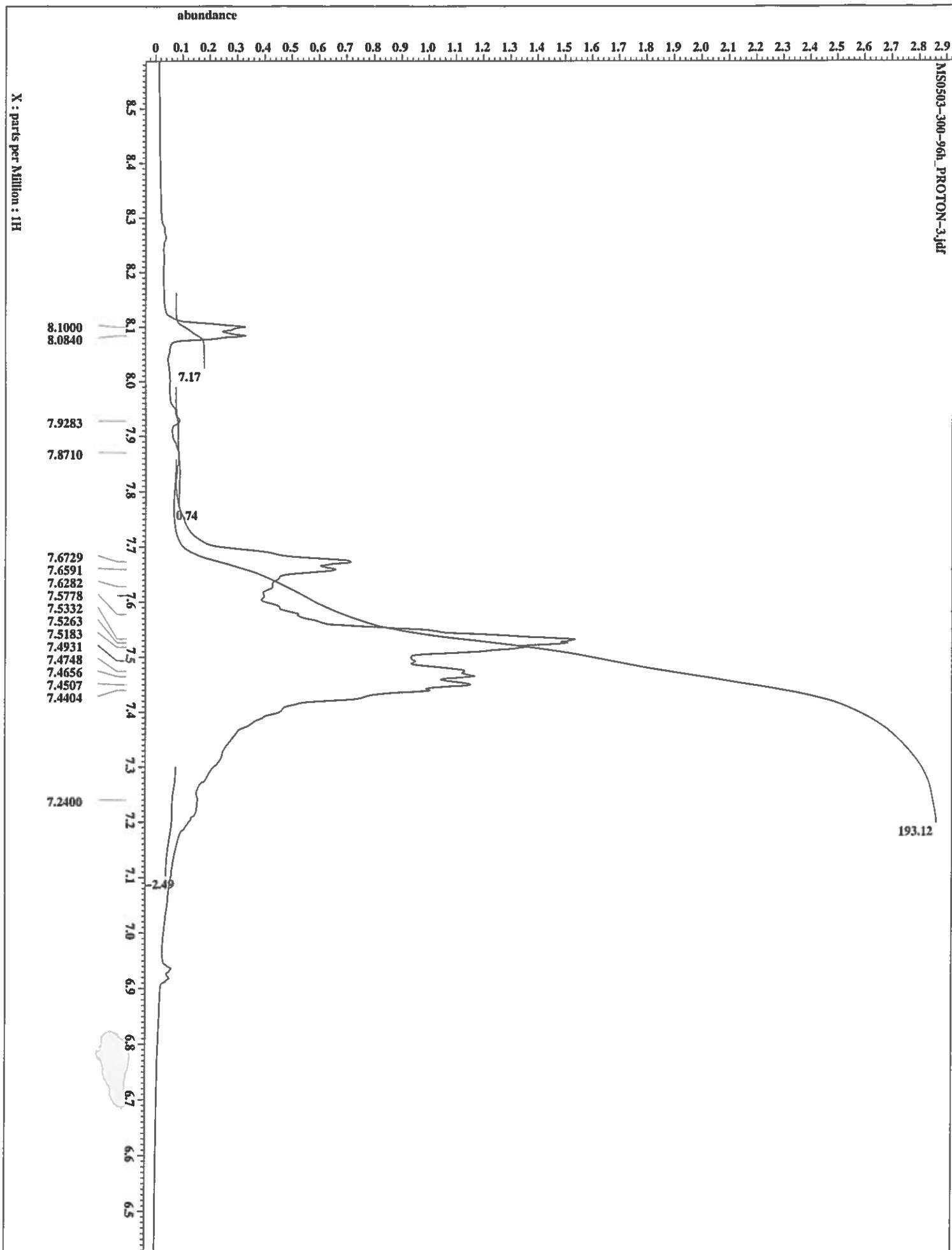
Field_strength 11.7473579 [T] (500 [MH
X_acq_duration 1.74587904 [s]
X_domain       1H
X_freq         500.15991521 [MHz]
X_offset       5.0 [ppm]
X_points       16384
X_prescans     1
X_resolution   0.5727737 [Hz]
X_sweep        9.38438438 [kHz]
Xr_domain      1H
Xr_freq        500.15991521 [MHz]
Xr_offset      5.0 [ppm]
Xr_domain      1H
Xr_freq        500.15991521 [MHz]
Xr_offset      5.0 [ppm]
Xr_offset      PALSE
Mod_return     1
Scans          16
Total_scans    16
X_90_width     12.4 [us]
X_acq_time     1.74587904 [s]
X_angle        45 [deg]
X_atn          4 [dB]
X_pulse        6.2 [us]
Xr_mode        ORG
Dance_preset   PALSE
Initial_wait   1 [s]
Recvr_gain     28
Relaxation_delay 4 [s]
Repetition_time 5.74587904 [s]
Temp_get       22.8 [dc]
  
```

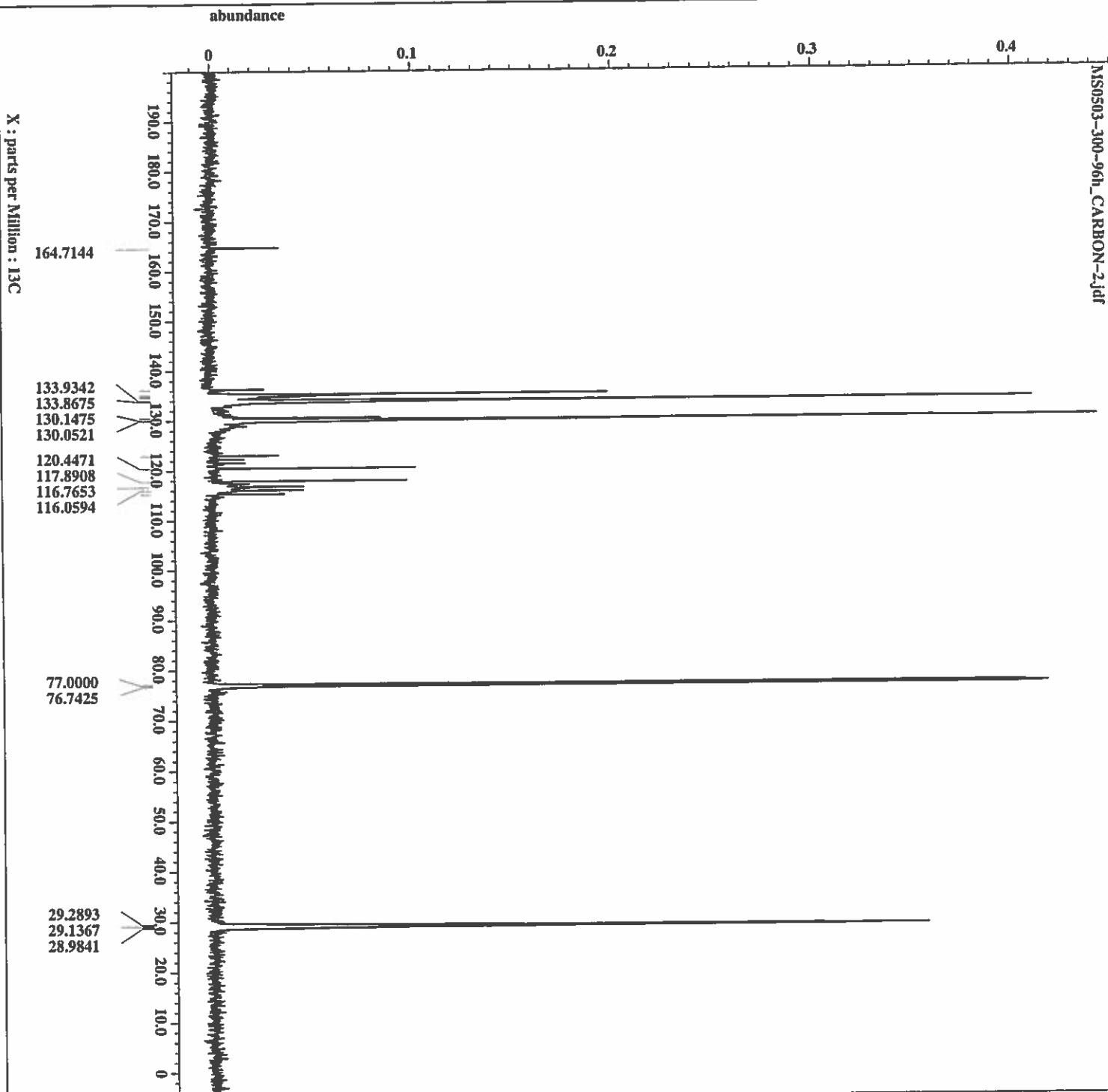
7.5332
7.5263
7.5183
7.4748
7.4656
7.4507
7.4404

1.8130

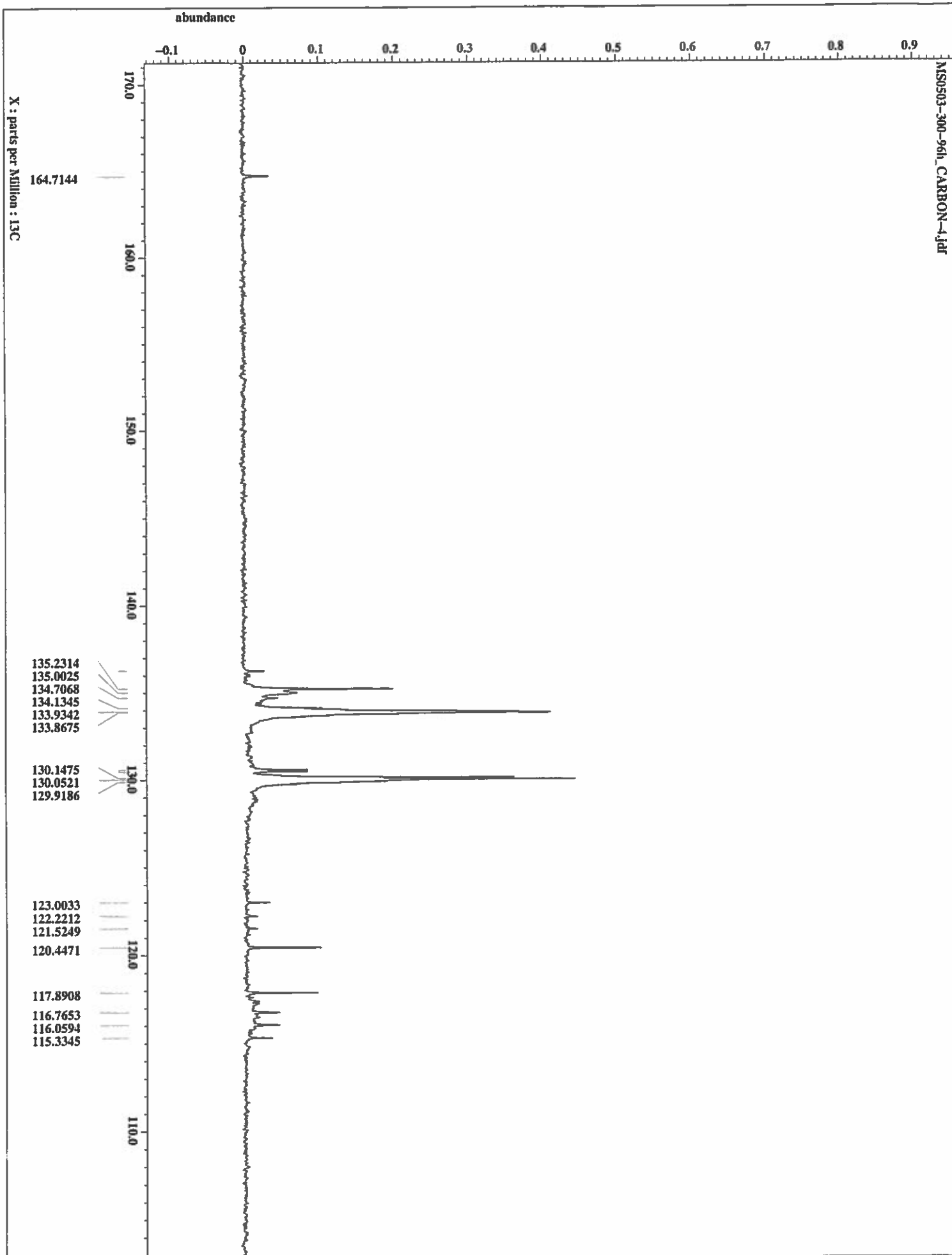


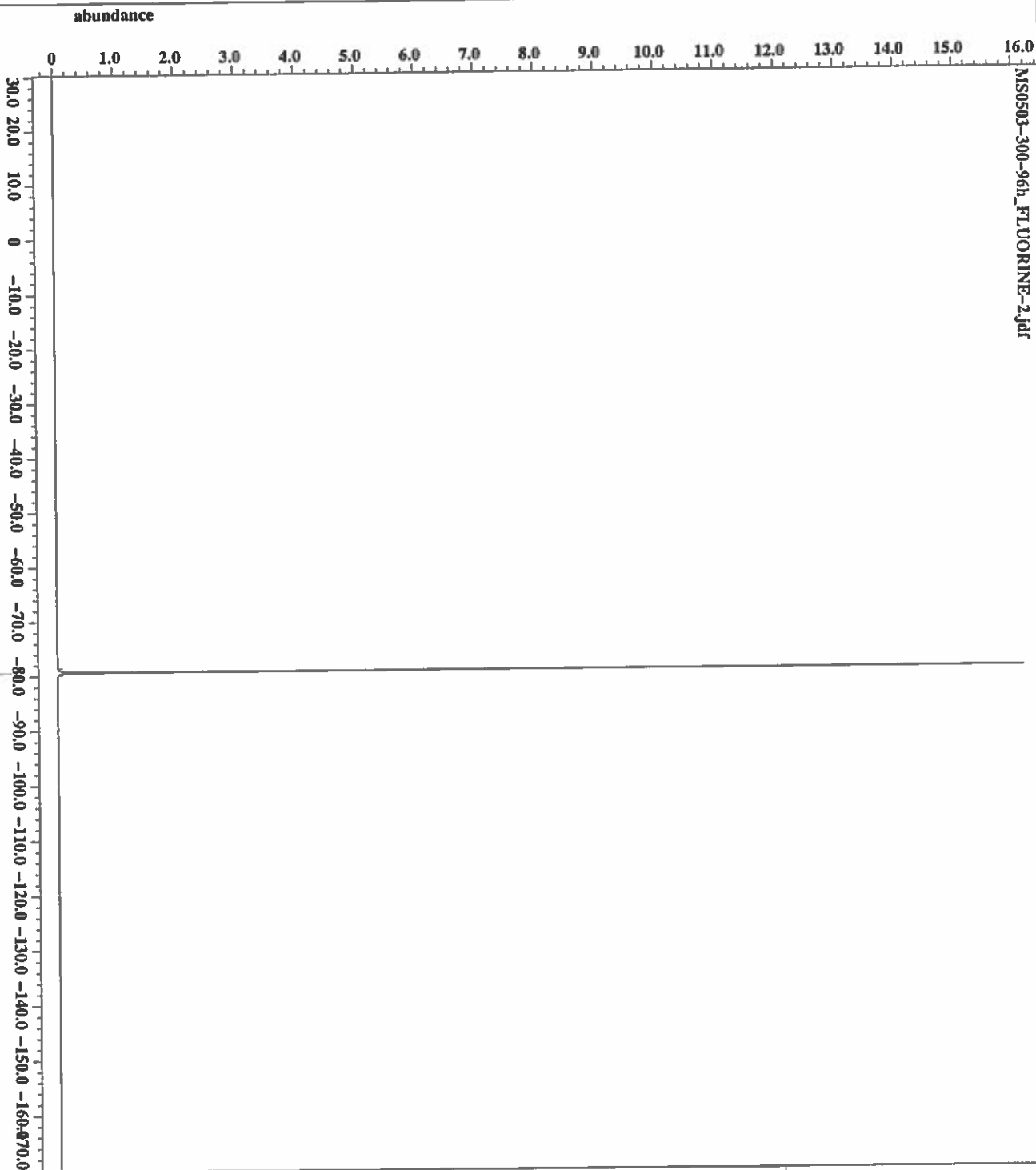
X : parts per Million : 1H





Filename	= M80503-300-96h_CARBON
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= M80503-300-96h
Solvent	= CHLOROFORM-D
Charger_sample	= 6
Creation_time	= 10-JUL-2018 20:10:45
Revision_time	= 10-JUL-2018 19:48:30
Current_time	= 10-JUL-2018 19:48:30
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECX500
Field_strength	= 11.74735791[T] (500[MHz])
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 1001[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.30817621[kHz]
Iter_domain	= 1H
Iter_freq	= 500.15991521[MHz]
Iter_offset	= 5.01[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 1024
Total_scans	= 1024
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[db]
X_pulse	= 4.4[us]
Iter_atn_dec	= 20.7[db]
Iter_atn_poe	= 20.7[db]
Iter_noise	= NALFZ
Decoupling	= TRUEZ
Initial_wait	= 1[s]
Noise	= TRUEZ
Noise_time	= 21[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 23.21[degC]





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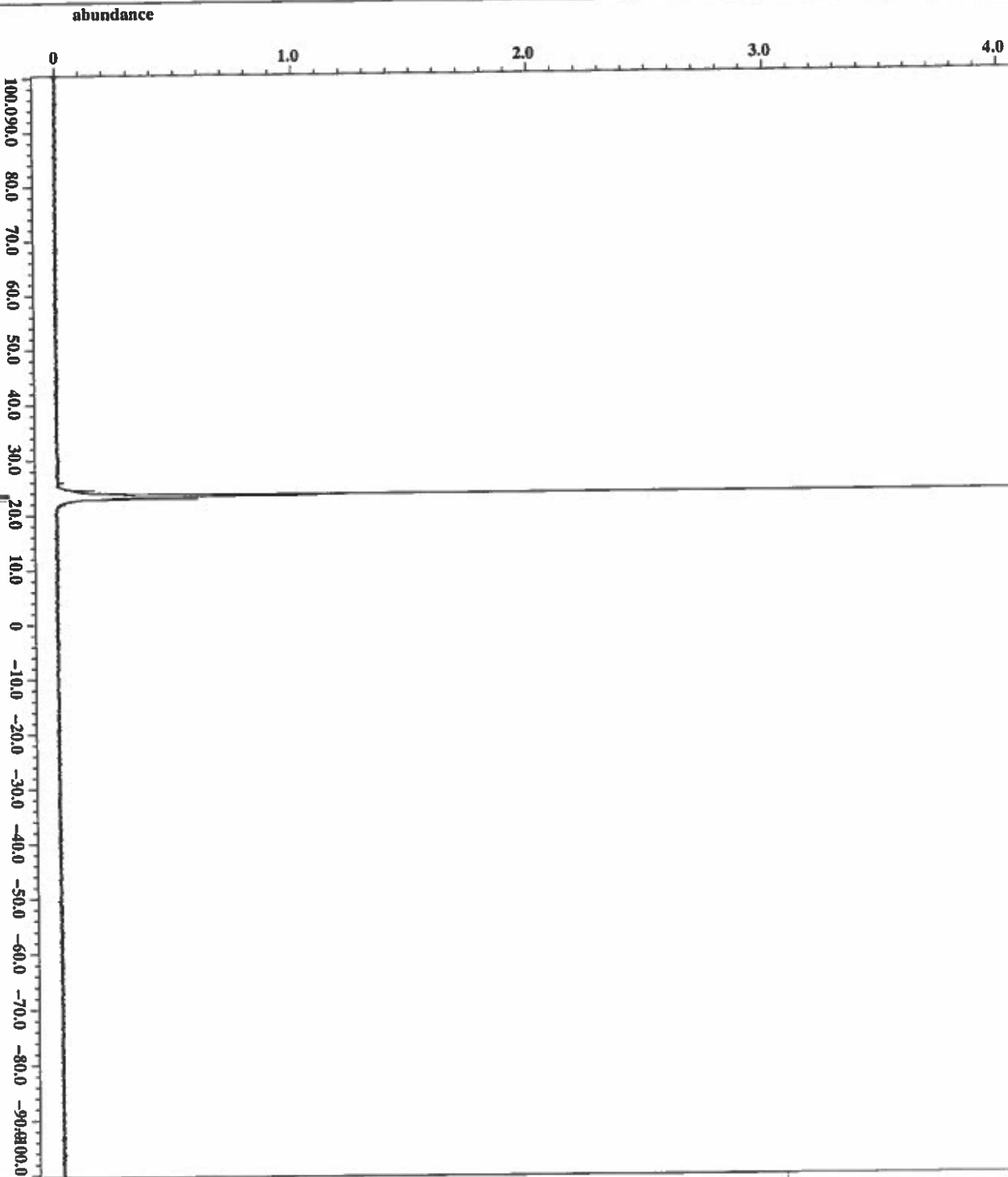
```

File Name      = MS0503-300-96h_FLUORINE
Author         = Jim Davis
Experiment     = 1dmg1e_pulse.ex2
Sample_ID      = MS0503-300-96h
Solvent        = CHLOROFORM-D
Charger_Sample = 6
Creation_Time   = 11-JUL-2018 00:23:39
Revision_Time  = 11-JUL-2018 00:01:23
Current_Time   = 11-JUL-2018 00:01:23

Data Format
Dim Size      = 1D COMPLEX
Dim Title     = 52428
Dim Units     = 19F
Dimensions    = [ppm]
Site          = X
Spectrometer  = ECA 500
              = JNM-ECA500

Field Strength = 11.7473579 [T] (500 [MH
X Acq Duration = 0.55574528 [s]
X Domain      = 19F
X Freq        = 470.62046084 [MHz]
X Offset      = -70 [ppm]
X Points      = 65536
X Prescans    = 1
X Resolution  = 1.7993855 [Hz]
X Slew        = 117.9245283 [kHz]
X Domain      = 19F
X Freq        = 470.62046084 [MHz]
X Offset      = 5 [ppm]
X1 Domain     = 19F
X1 Freq       = 470.62046084 [MHz]
X1 Offset     = 5 [ppm]
X1 Freq       = 470.62046084 [MHz]
X1 Offset     = FALSE
Clipped       = 1
Mod_Return    = 16
Scans         = 16
Total_Scans   = 16

X 90 Width    = 13.1 [us]
X Acq Time    = 0.55574528 [s]
X Angle       = 45 [deg]
X Aqn         = 2.5 [dB]
X Pulse       = 6.55 [us]
X1 Mode       = Off
X1 Mode       = Off
Pulse Presat  = FALSE
Initial Wait  = 1 [s]
Recvr Gain    = 38
Relaxation Delay = 4 [s]
Repetition Time = 4.55574528 [s]
Temp Set      = 22.2 [dC]
  
```



X : parts per Million : 31P

23.5512
23.4057
23.3214



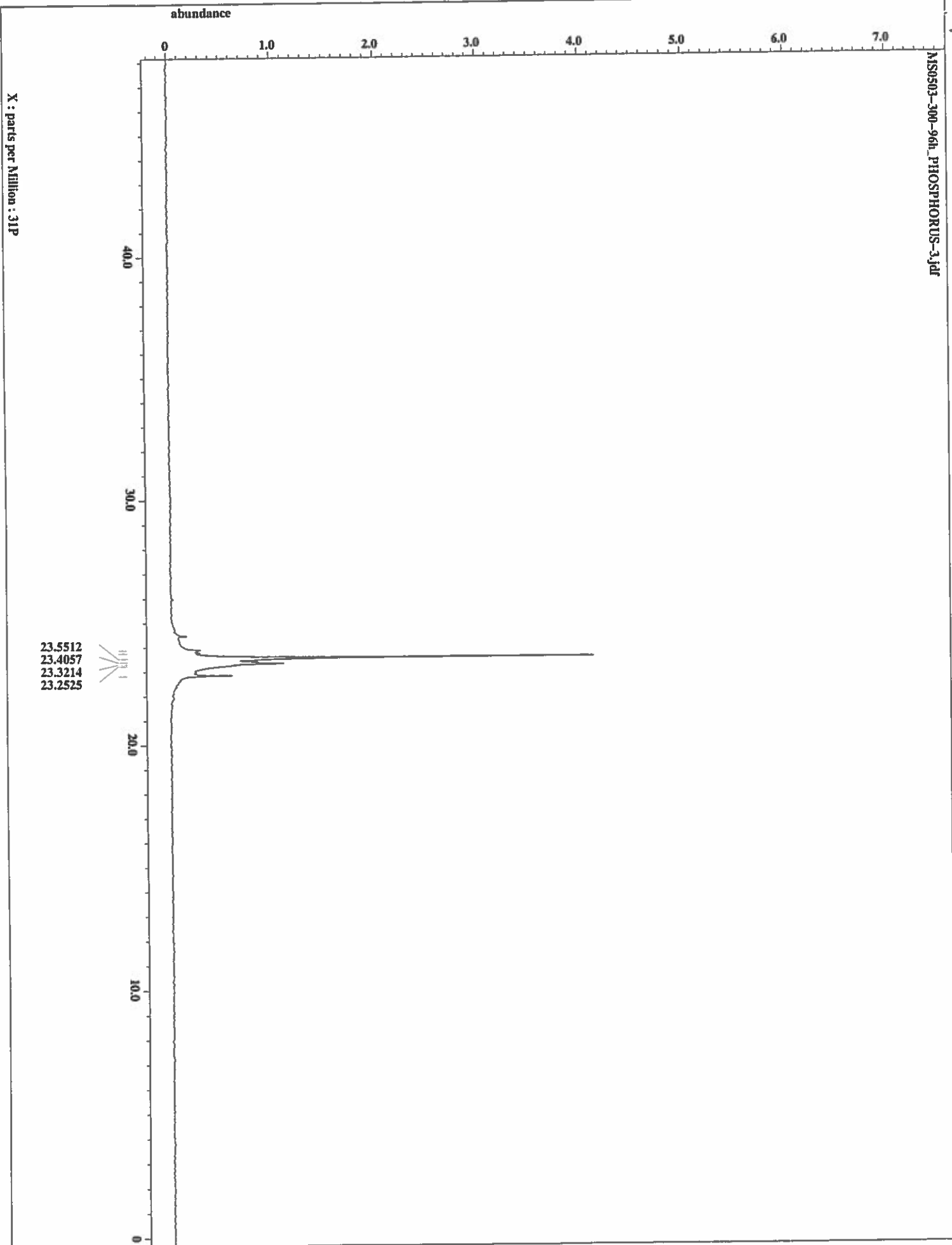
```

Filename      = MS0503-300-96h_PHOSPH
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0503-300-96h
Solvent       = CHLOROFORM-D
Charger_sample = 6
Creation_time  = 11-JUL-2018 00:37:42
Revision_time  = 11-JUL-2018 00:15:27
Current_time   = 11-JUL-2018 00:15:27

Date_format   =
Dim_size      = 1D COMPLEX
Dim_title     = 26214
Dim_units     = 31P
Dimensions    = [ppm]
Site          = X
Spectrometer  = ECA 500
              = JNM-ECA500

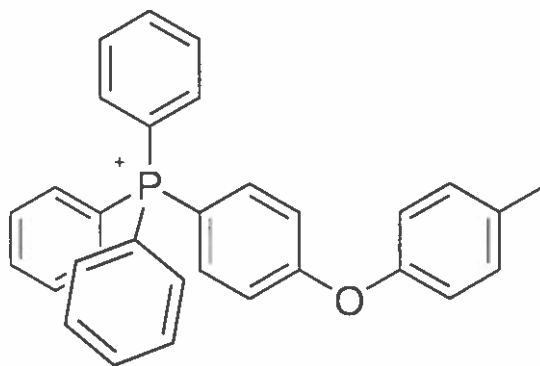
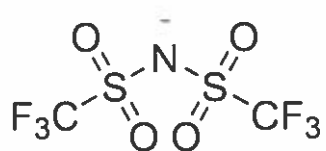
P1         = 11.7473579 [s] (500 MHz)
P1_dwell   = 0.64487424 [s]
X_domain   = 31P
X_freq     = 202.46831075 [MHz]
X_offset   = 0 [ppm]
X_points   = 32768
X_prescans = 4
X_resolution = 1.55068995 [Hz]
X_sweep     = 50.81300813 [kHz]
IRF_domain  = 1H
IRF_freq    = 500.15991521 [MHz]
IRF_offset  = 5.0 [ppm]
Mod_return  = FALSE
Scans       = 1
Total_scans = 256

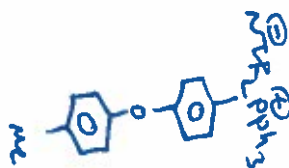
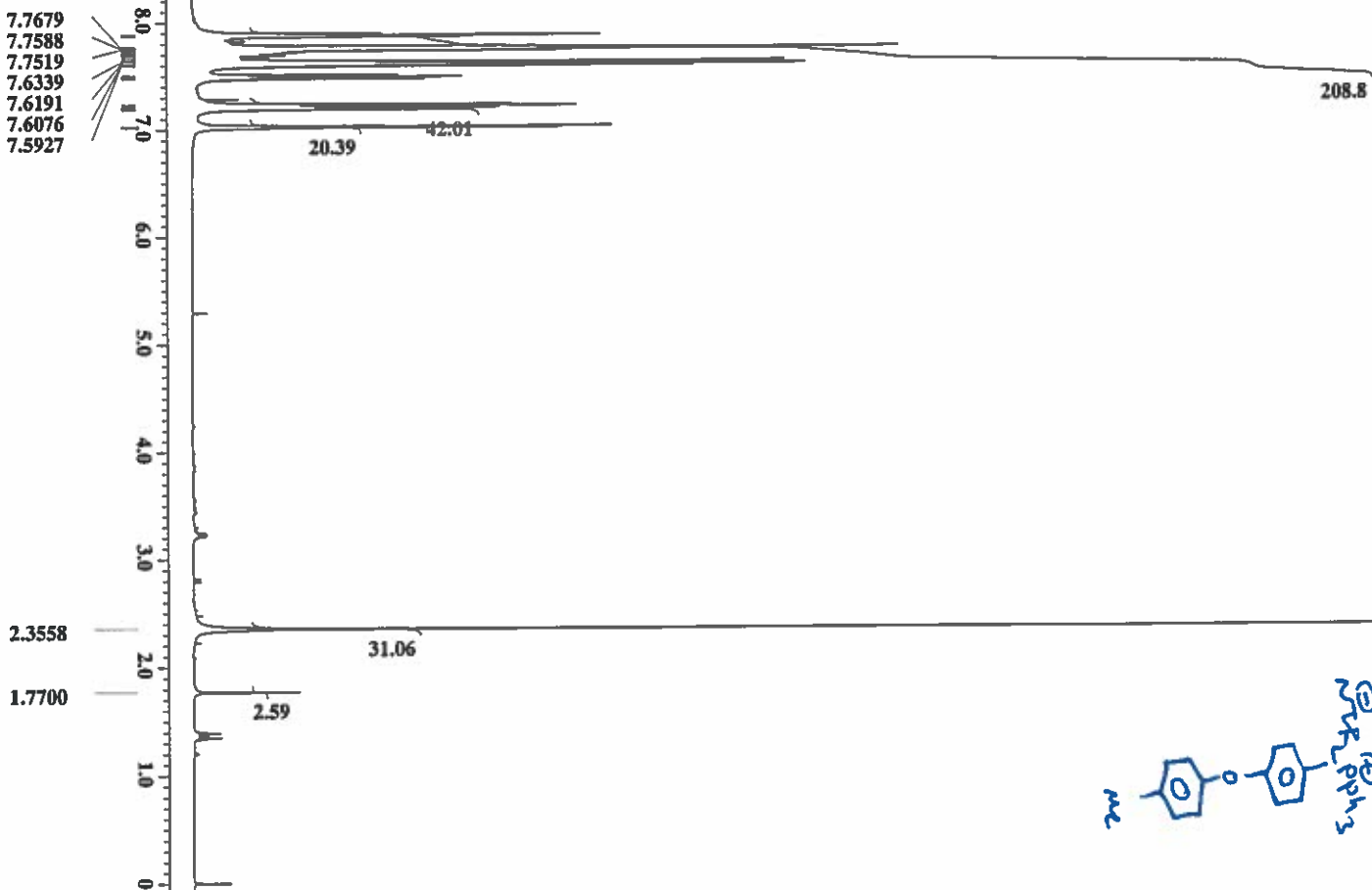
X_90_width  = 14.687 [us]
X_acq_time  = 0.64487424 [s]
X_angle     = 30 [deg]
X_atn       = 5 [dB]
X_pulse     = 4.89566667 [us]
IRF_atn_dec = 20.7 [dB]
IRF_atn_noe = 20.7 [dB]
IRF_noise   = WALTZ
Decoupling  = TRUE
Initial_wait = 1 [s]
Noe         = TRUE
Noe_time    = 2 [s]
Recvr_gain  = 21 [s]
Relaxation_delay = 2.64487424 [s]
Repetition_time = 22.7 [dc]
Temp_get    =
    
```



Compound 8 Pre- and Post-heating NMR Spectra

Temperature of Post-heating samples noted in upper left corner of each spectrum

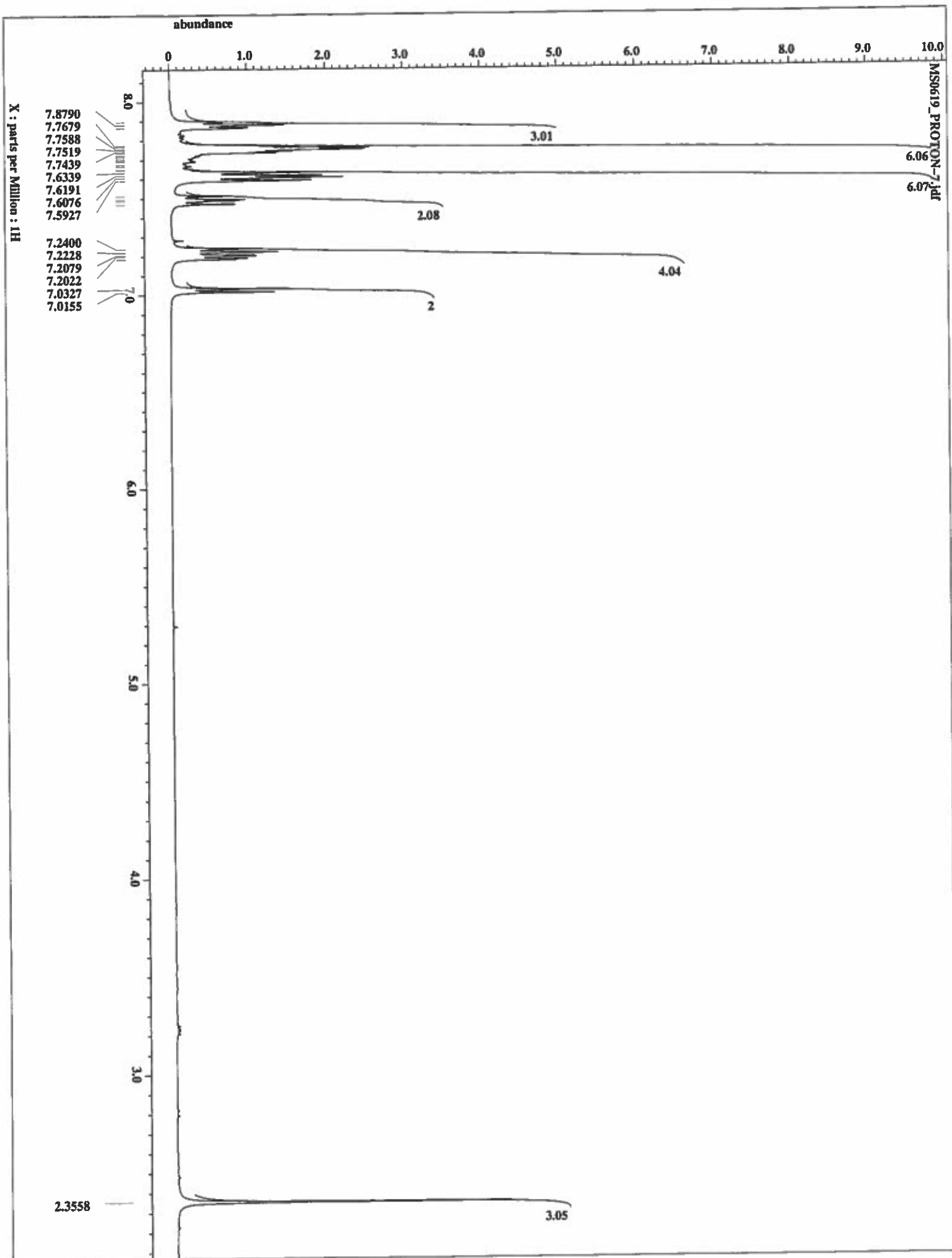


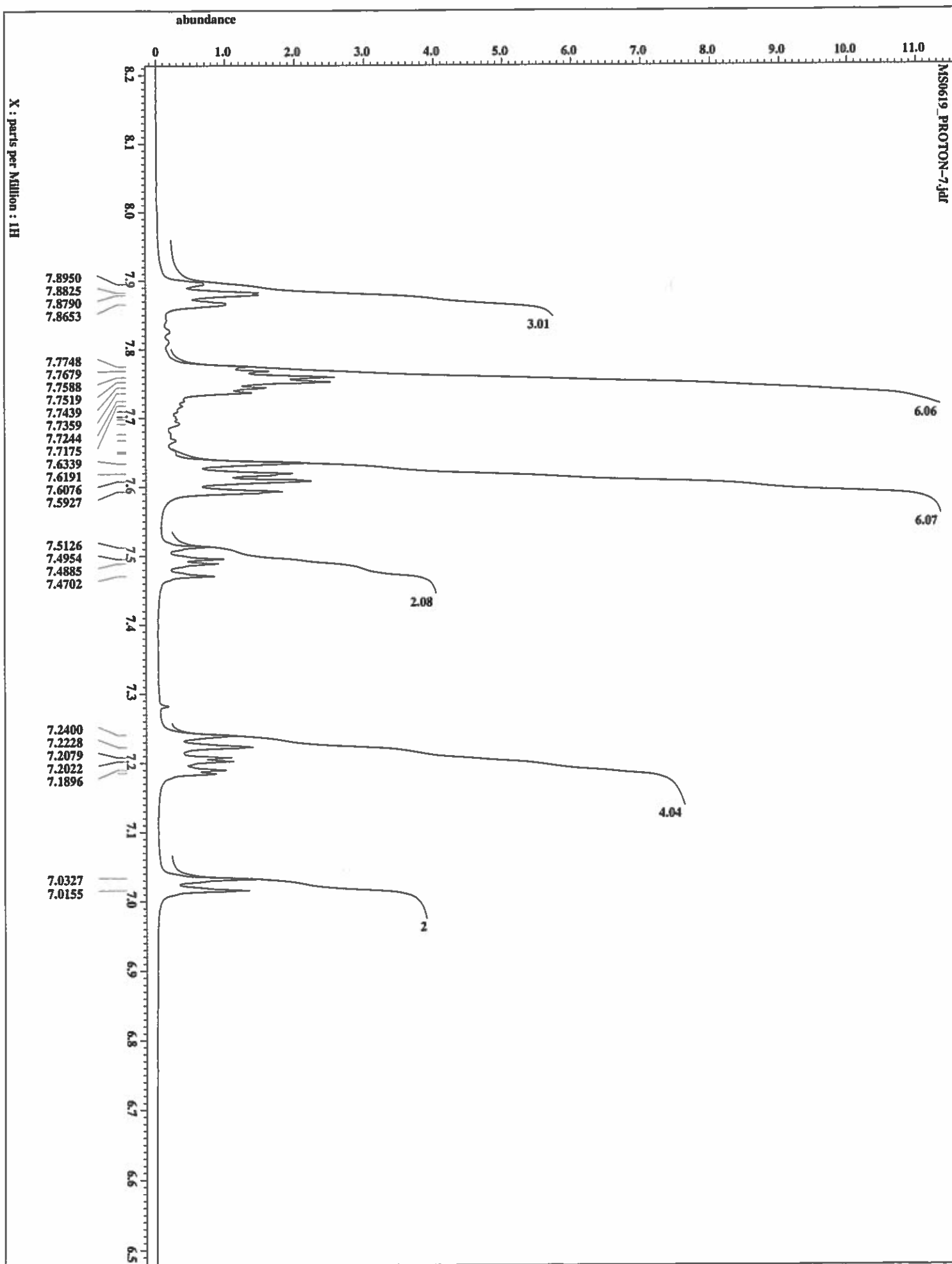


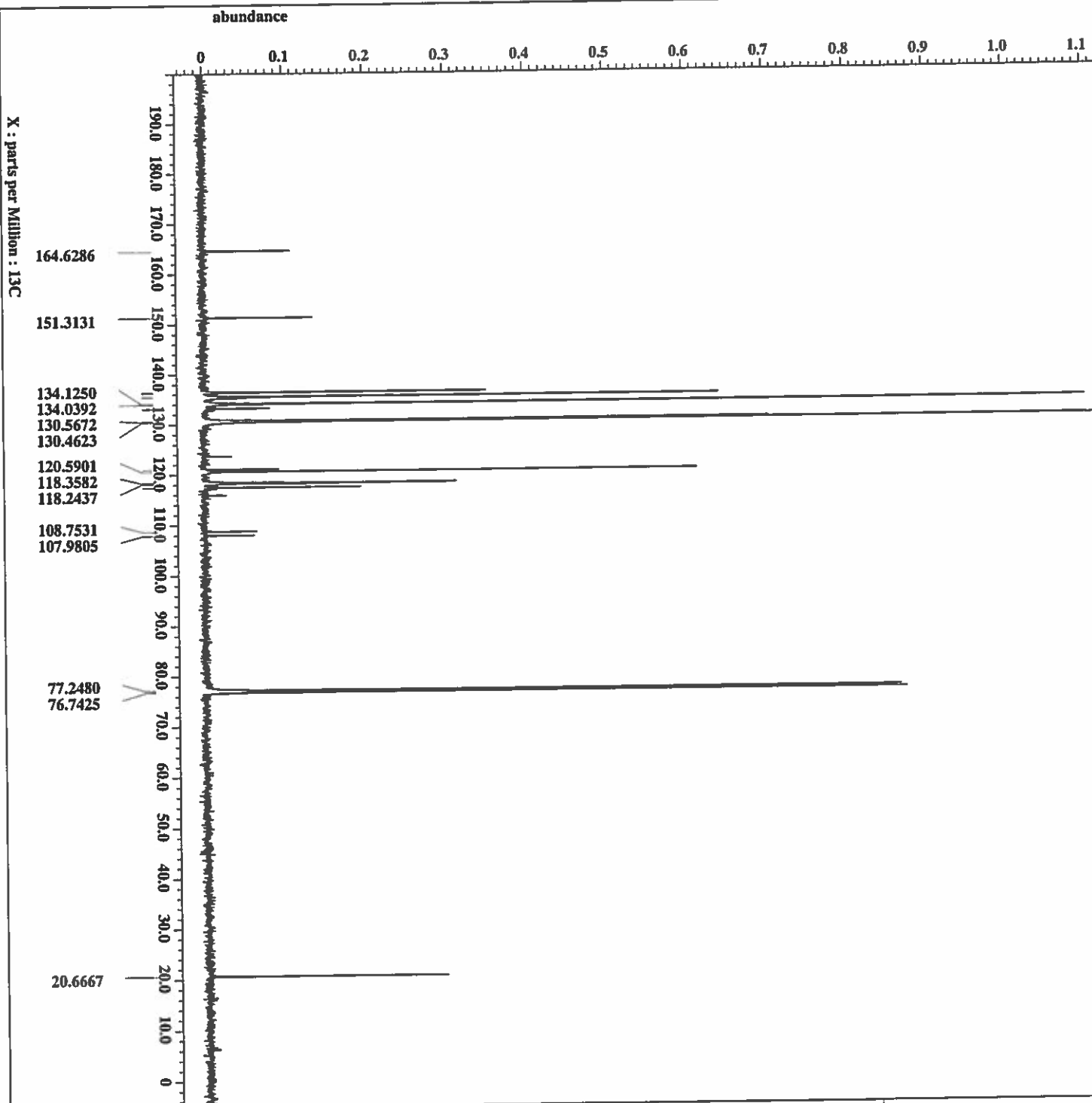
Filename
 Author
 Experiment
 Sample_id
 Solvent
 Creation_time
 Revision_time
 Current_time
 Data_format
 Dim_size
 Dim_c1c1s
 Dim_units
 Dimensions
 Site
 Spectrometer
 Field_strength
 X_acq_duration
 X_domain
 X_freq
 X_offset
 X_points
 X_prescans
 X_resolution
 X_sweep
 Irr_domain
 Irr_freq
 Irr_offset
 Tr1_domain
 Tr1_freq
 Tr1_offset
 Clipped
 Mod_return
 Scans
 Total_scans
 X_90_width
 X_acq_time
 X_angle
 X_atn
 X_pulse
 Irr_mode
 Tr1_mode
 Dante_presat
 Initial_waltz
 Recr_gain
 Relaxation_delay
 Repetition_time
 Temp_get

MS0619_PROTON-5.jdf
 Jim Davis
 single_pulse.ex2
 MS0619
 CHLOROFORM-D
 30-NOV-2018 15:05:13
 30-NOV-2018 14:40:17
 30-NOV-2018 14:40:17
 1D COMPLEX
 13107
 1H
 [ppm]
 X
 ECA 500
 JNM-ECA500
 11.7473579 [Hz] (500 MHz)
 1.74587904 [s]
 1H
 500.15991521 [MHz]
 5.0 [ppm]
 16384
 1
 0.57277737 [Hz]
 9.38438438 [Hz]
 1H
 500.15991521 [MHz]
 5.0 [ppm]
 500.15991521 [MHz]
 5.0 [ppm]
 FALSE
 1
 16
 16
 12.4 [us]
 1.74587904 [s]
 45 [deg]
 4 [dB]
 6.2 [us]
 O2
 FALSE
 1 [s]
 28
 4 [s]
 5.74587904 [s]
 22.1 [s]









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```

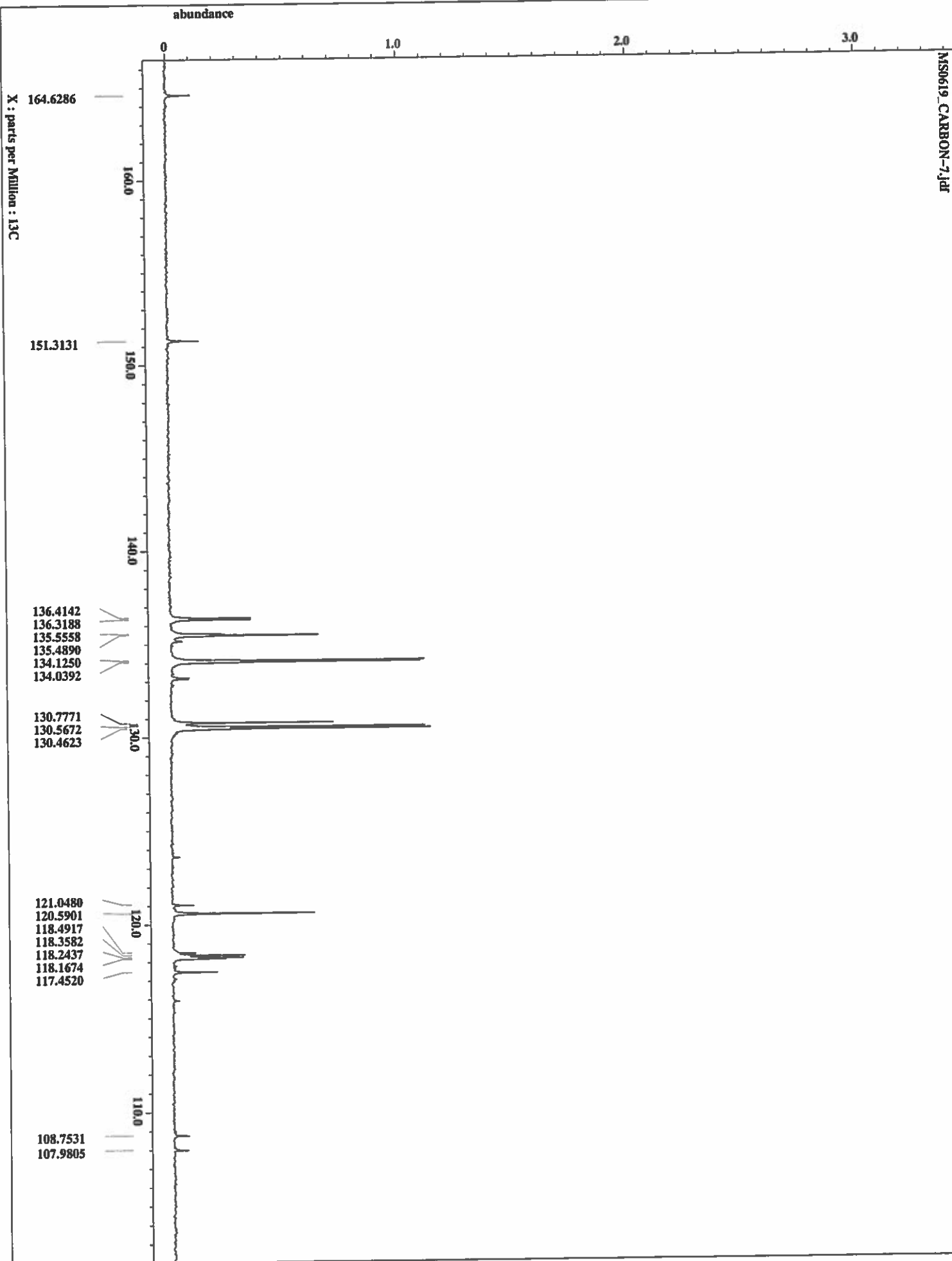
=====
File Name      MS0619_CARBON-5.jdt
Author        Jim Davis
Experiment     single_pulse_dec
Sample ID     MS0619
Solvent        CHLOROFORM-D
Creation Time  30-NOV-2018 15:26:35
Revision Time  30-NOV-2018 15:01:38
Current Time   30-NOV-2018 15:01:38

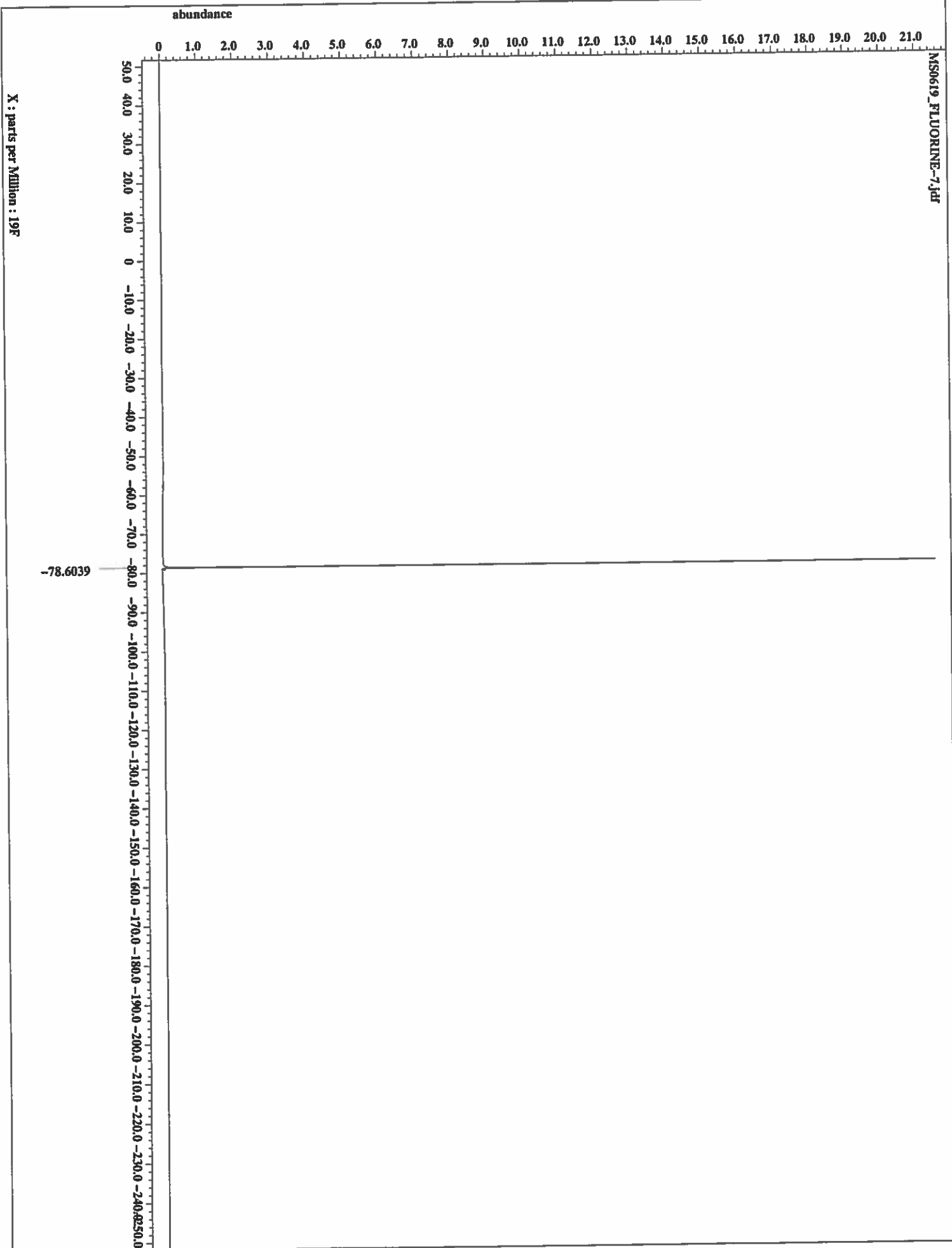
=====
Data Format     1D COMPLEX
Dir Size       26214
Dir Title      13C
Dir Units      [ppm]
Dimensions     X
Site           ECA 500
Spectrometer   JNM-ECX500

=====
Field Strength 11.7473579 [T] (500 MHz)
Acq Duration    0.83361792 [s]
Domain         13C
Freq           125.76529768 [MHz]
Offset         100 [ppm]
Points         32768
PreScans        4
Resolution      1.19959034 [Hz]
Sweep           39.3081761 [Hz]
IRF Domain      1H
IRF Freq        500.15991523 [MHz]
IRF Offset      5.0 [ppm]
Clipped         FALSE
Mod Return      1
Scans           400
Total Scans     400

=====
X 90 Width      13.2 [us]
Acq Time        0.83361792 [s]
Angle          30 [deg]
ACh            6 [dB]
X Pulse         4.4 [us]
IRF Attn Dec    20.7 [dB]
IRF Attn Noe    20.7 [dB]
VOLTz          TRUE
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 Set       23.1 [C]
=====

```





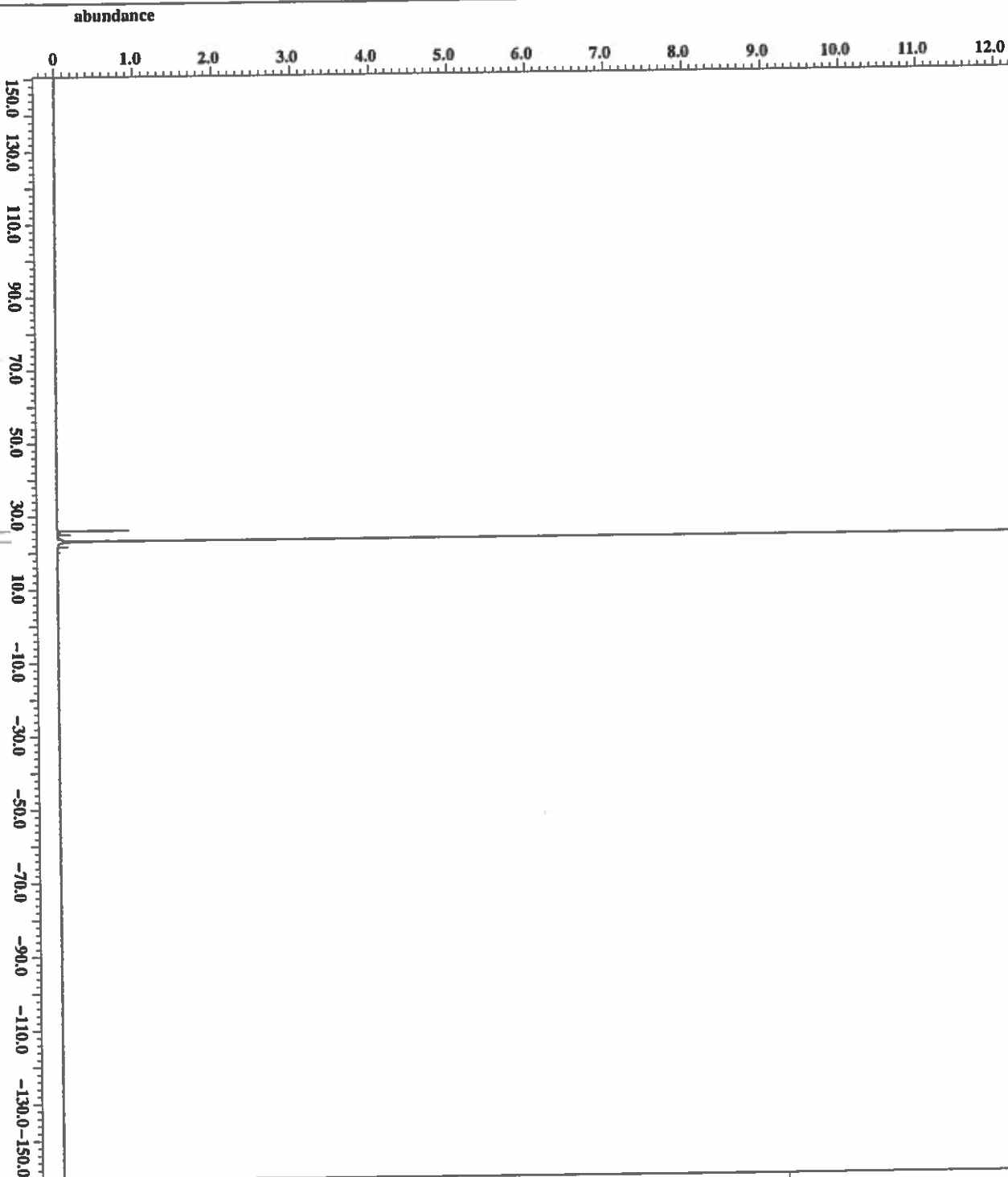


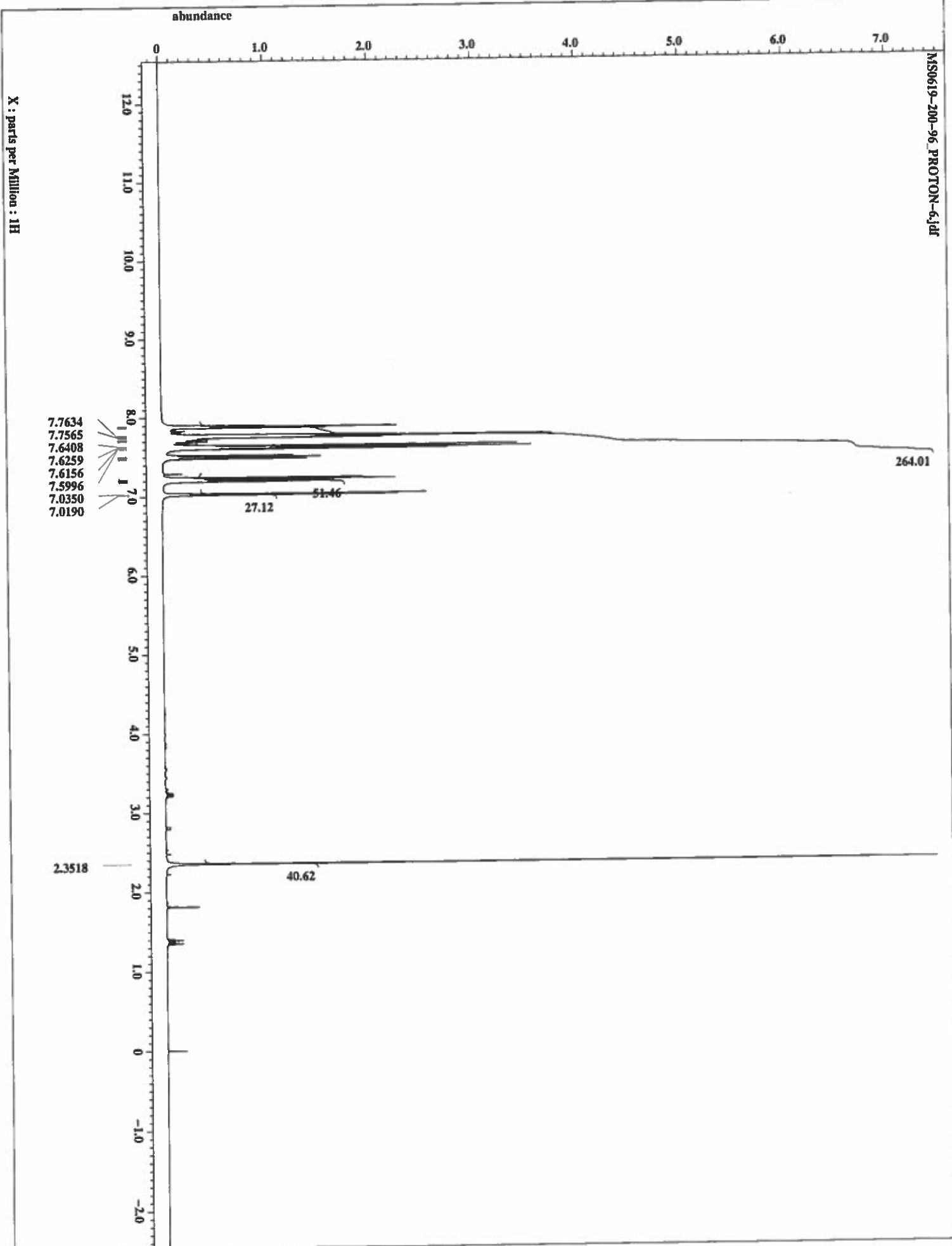
filename MS0619_PHOSPHORUS-5-J
 author Jim Davis
 experiment single_pulse_dec
 sample_id MS0619
 solvent CHLOROPFORM-D
 creation_time 30-NOV-2018 14:42:20
 revision_time 30-NOV-2018 14:17:23
 current_time 30-NOV-2018 14:17:24

Date_format 1D COMPLEX
 dim_size 52428
 dim_title 31P
 dim_units [ppm]
 dimensions X
 size ECA 500
 Spectrometer JNM-ECA500

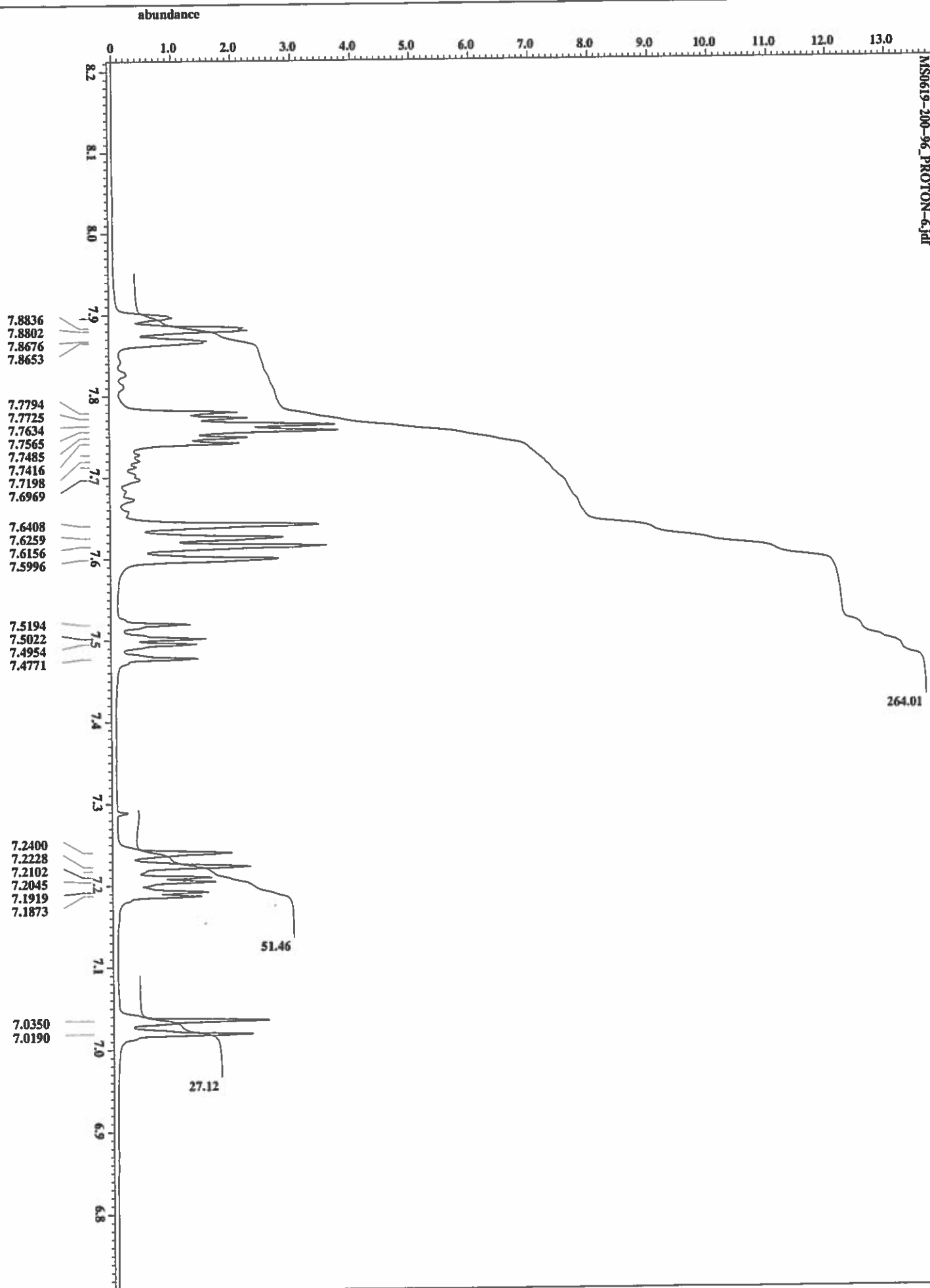
field_strength 11.7473579 [T] (500 [MH
 X_acq_duration 0.8598332 [s]
 X_domain 31P
 X_freq 202.46831075 [MHz]
 X_offset 0 [ppm]
 X_points 65536
 X_prescans 4
 X_resolution 1.16301746 [Hz]
 X_sweep 76.2195122 [Hz]
 X_domain 1H
 X_freq 500.15991521 [MHz]
 X_offset 5.0 [ppm]
 Clipped PALSE
 Mod_return 1
 Scans 50
 Total_scans 50

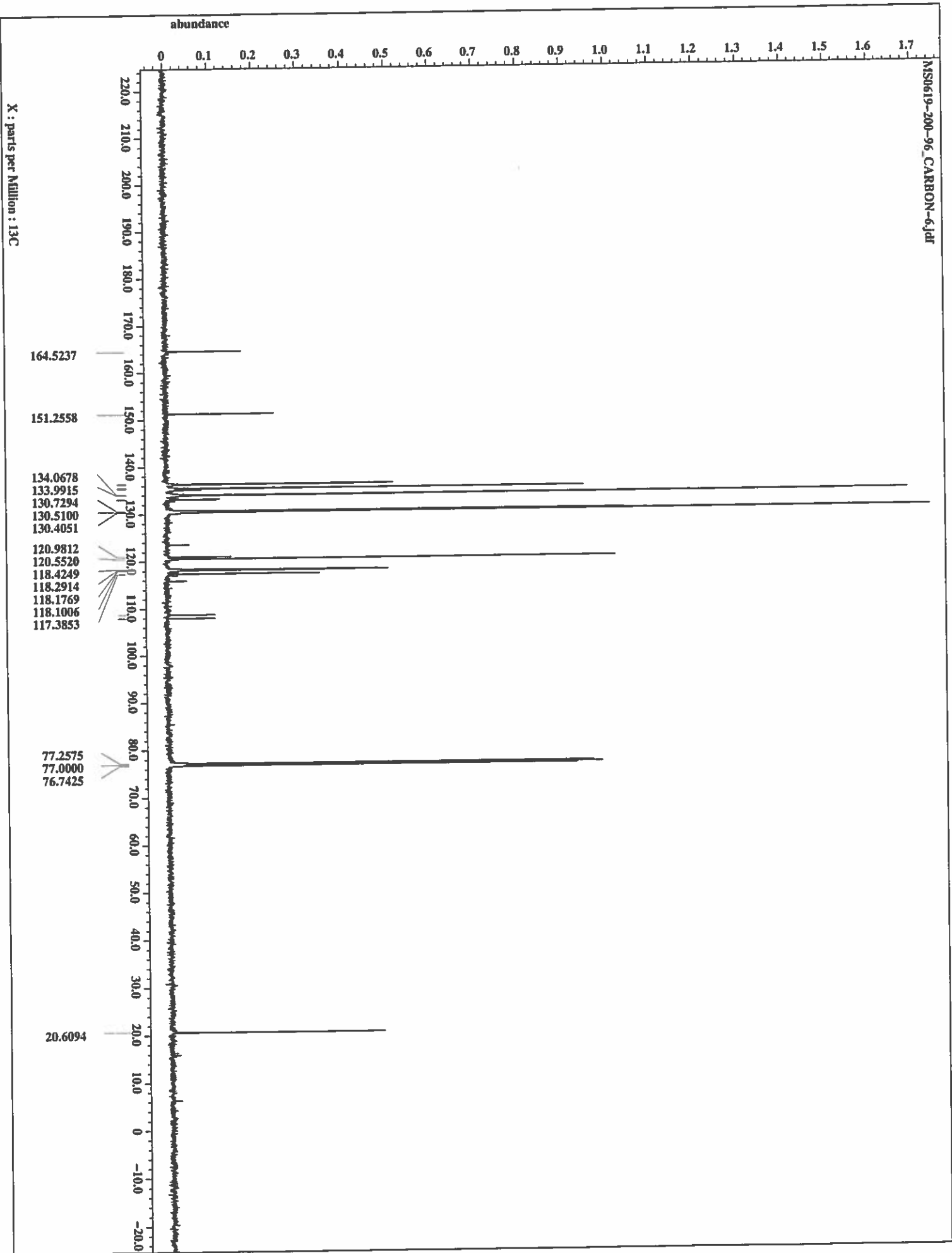
X_90_pulch 14.687 [us]
 X_acq_time 0.8598332 [s]
 X_angle 30 [deg]
 X_atn 5 [dB]
 X_pulse 4.89566667 [us]
 X_atn_dec 20.7 [dB]
 X_atn_noe 20.7 [dB]
 X_noise VALVE
 Decoupling TRUZ
 Initial_wait 1 [s]
 Noe 1 [s]
 Noe_time TRUZ
 Relaxr_gain 56
 Relaxation_delay 21 [s]
 Repetition_time 2.8598332 [s]
 Temp_get 22.7 [C]

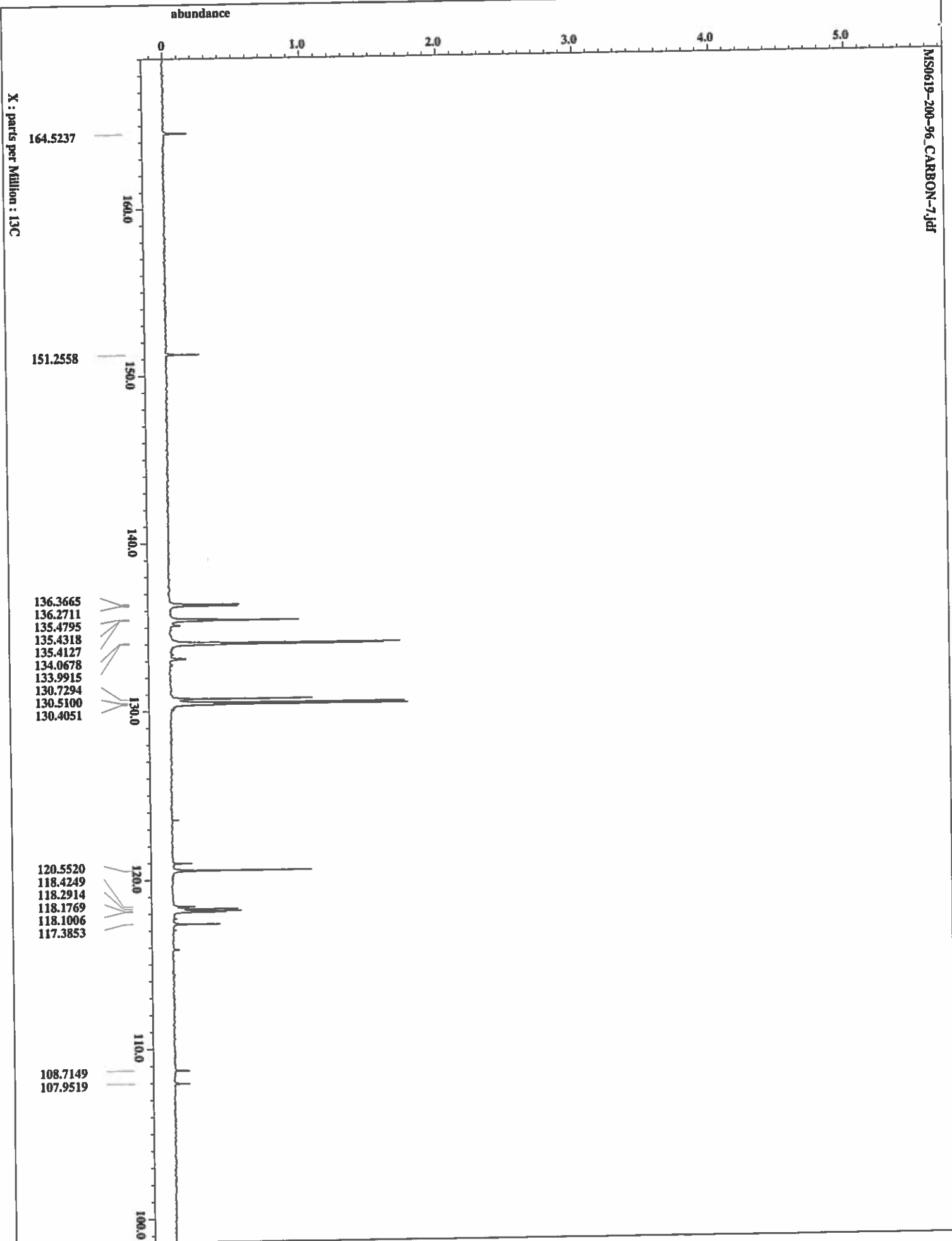


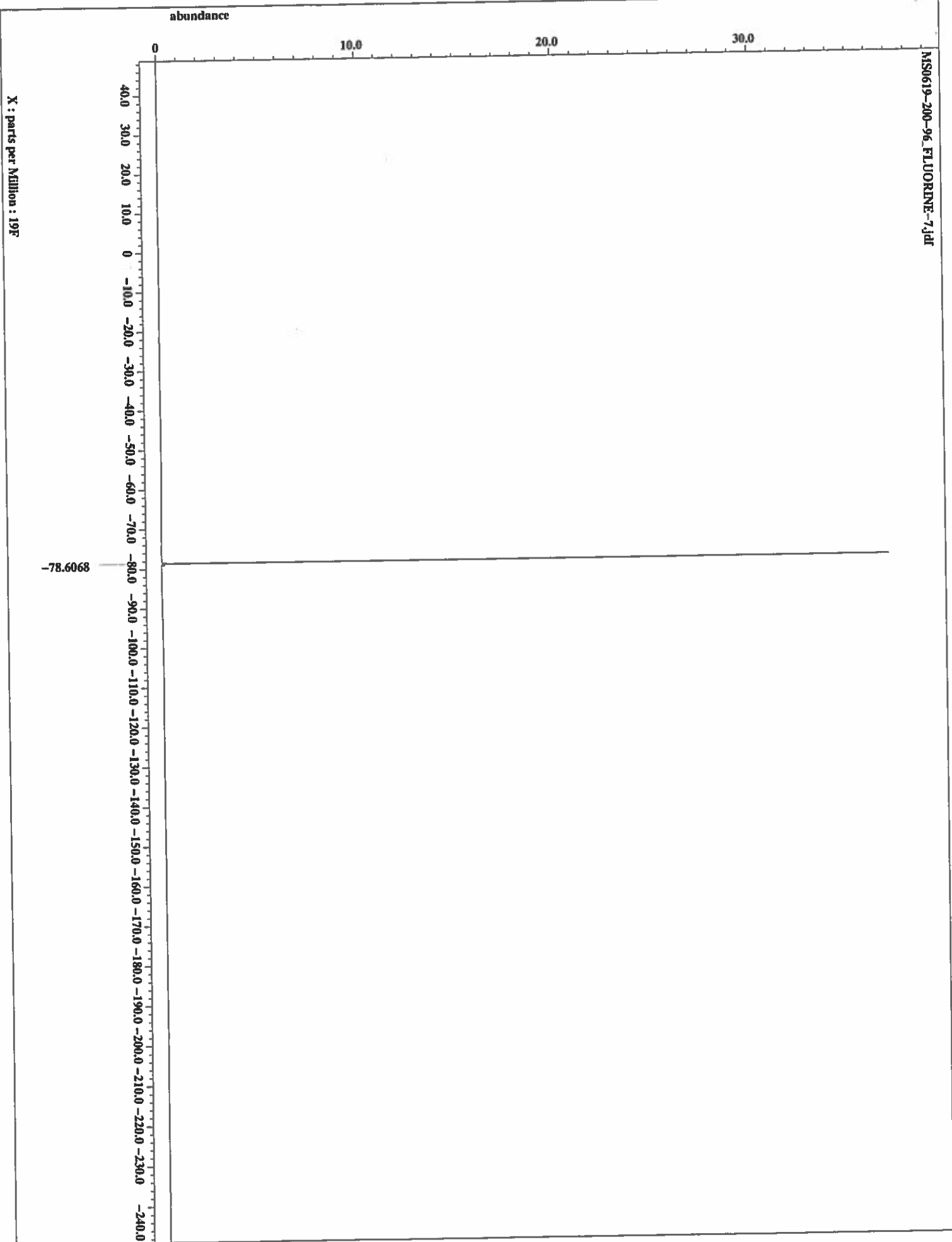


X : parts per Million : 1H









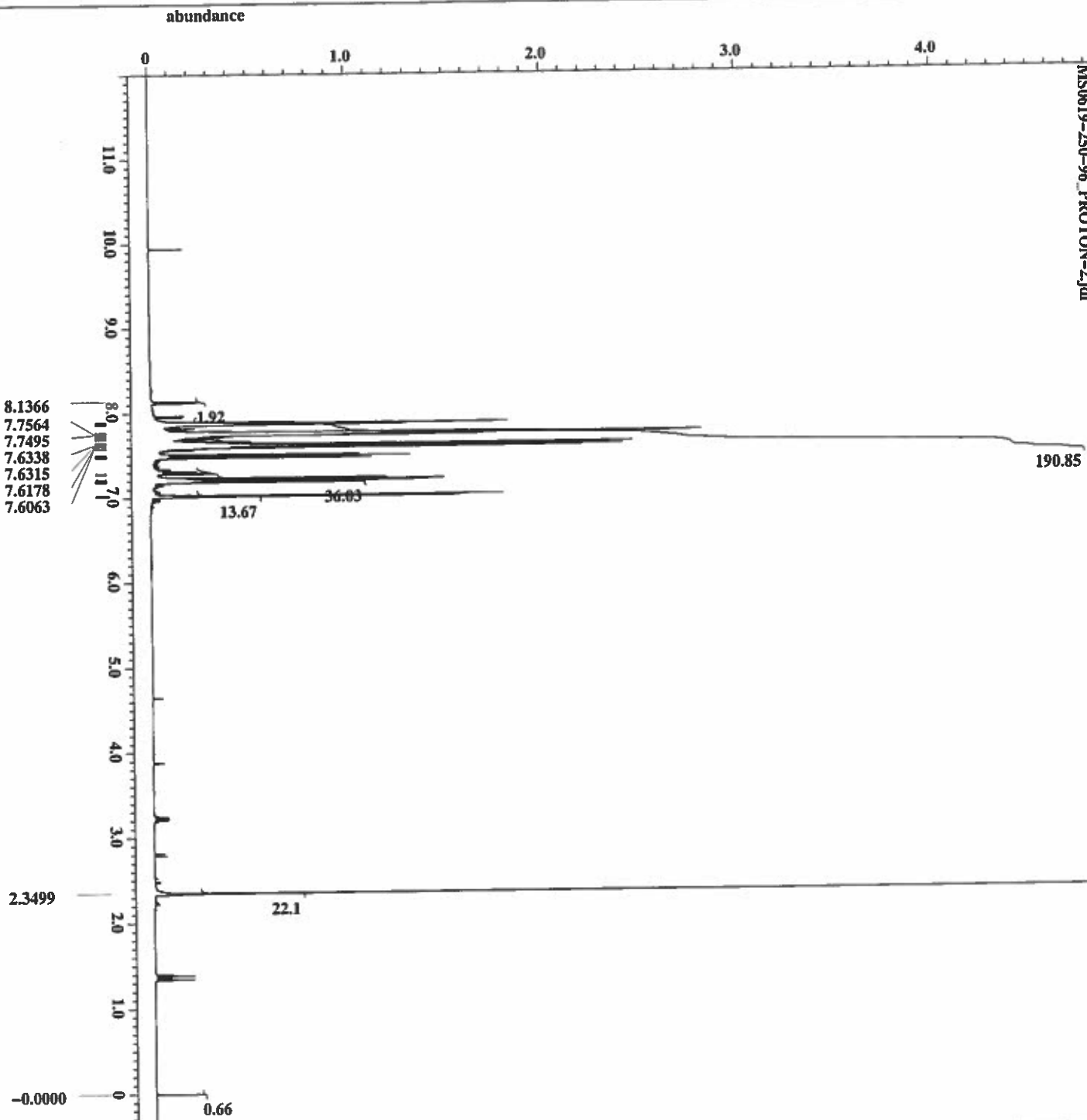
abundance

0 1.0 2.0 3.0 4.0 5.0 6.0 7.0

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 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0

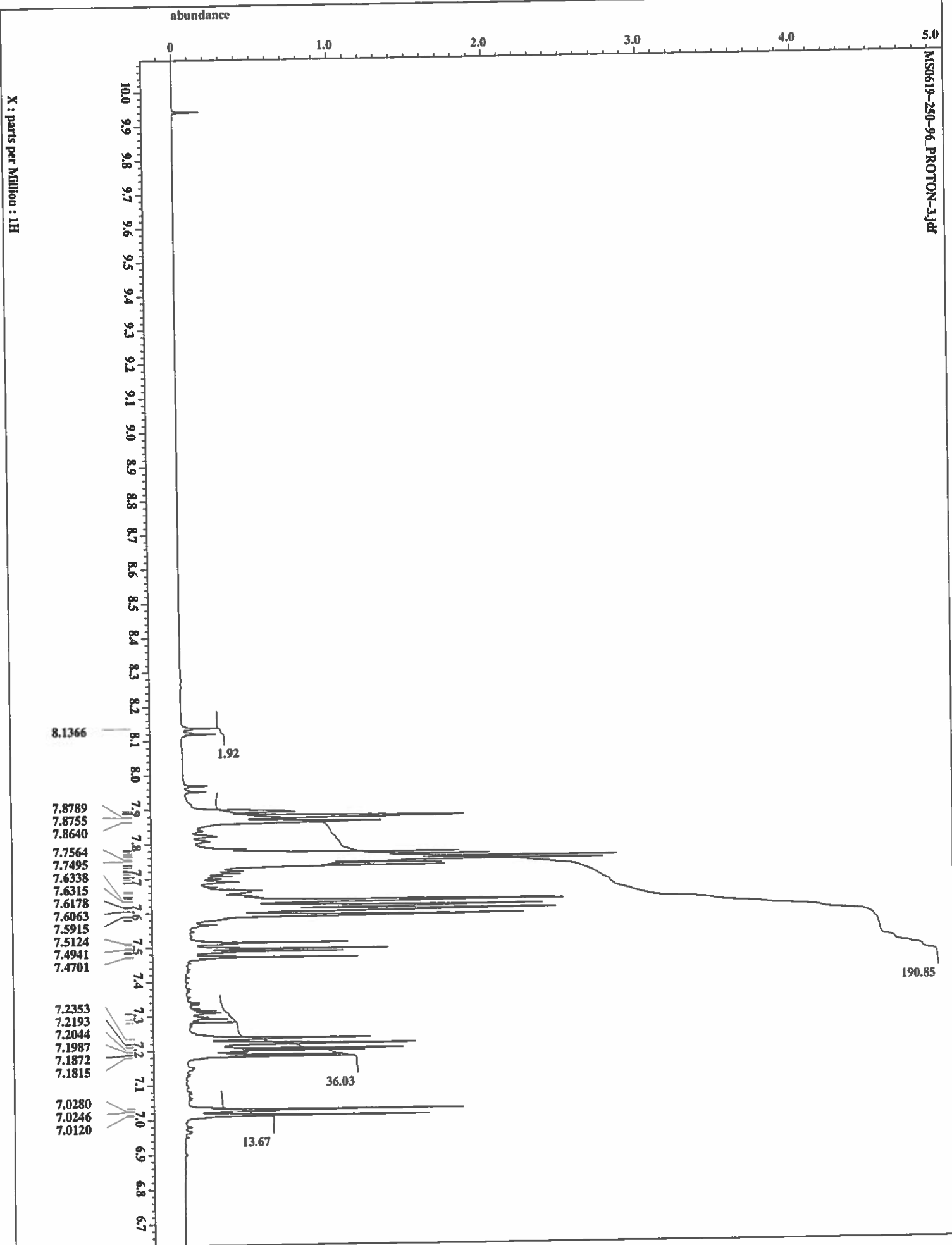
23.2065

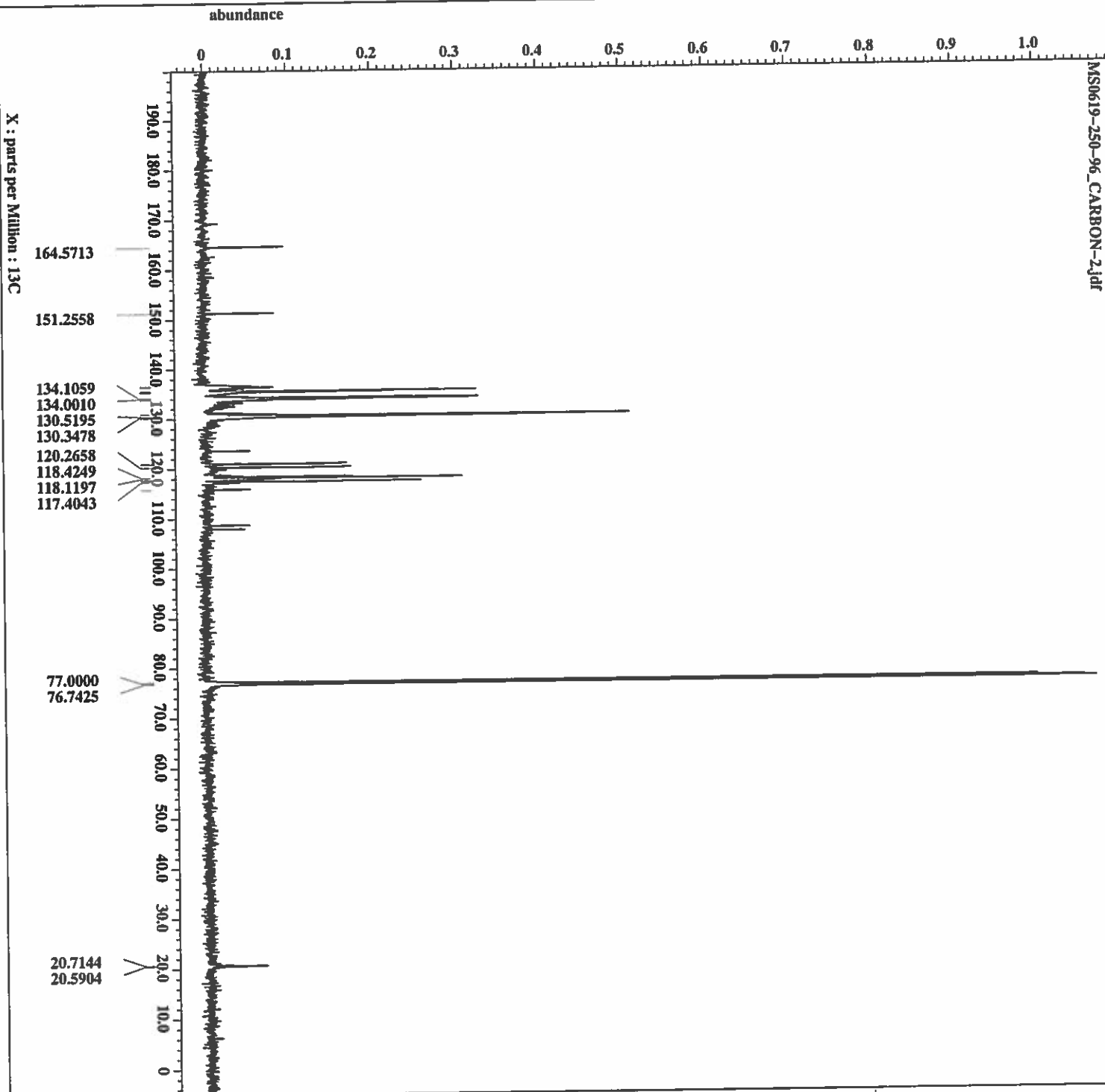
X : parts per Million : 31P



Filename	= MS0619-250-96_PROTON
Author	= JIN Devis
Experiment	= single_pulse.exe2
Sample_id	= MS0619-250-96
Solvent	= CHLOROFORM-D
Creation_time	= 4-DEC-2018 12:07:09
Revision_time	= 4-DEC-2018 11:41:52
Current_time	= 4-DEC-2018 11:41:52
Data_format	= 1D COMPLEX
Dir_size	= 13107
Dir_title	= 1H
Dir_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579 [T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0 [ppm]
X_points	= 16384
X_proscan	= 1
X_resolution	= 0.57277737 [Hz]
X_sweep	= 9.384338436 [kHz]
1st_domain	= 1H
1st_freq	= 500.15991521[MHz]
1st_offset	= 5.0 [ppm]
Tr1_domain	= 1H
Tr1_freq	= 500.15991521[MHz]
Tr1_offset	= 5.0 [ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 12.4 [us]
X_acq_time	= 1.74587904[s]
X_angle	= 45 [deg]
X_acn	= 4 [ds]
X_pulse	= 6.2 [us]
Trf_mode	= Off
Trf_mode	= Off
Dante_preset	= FALSE
Initial_wait	= 1 [s]
Recvr_gain	= 30
Relaxation_delay	= 4 [s]
Repetition_time	= 5.74587904[s]
Temp_get	= 20.6 [dc]







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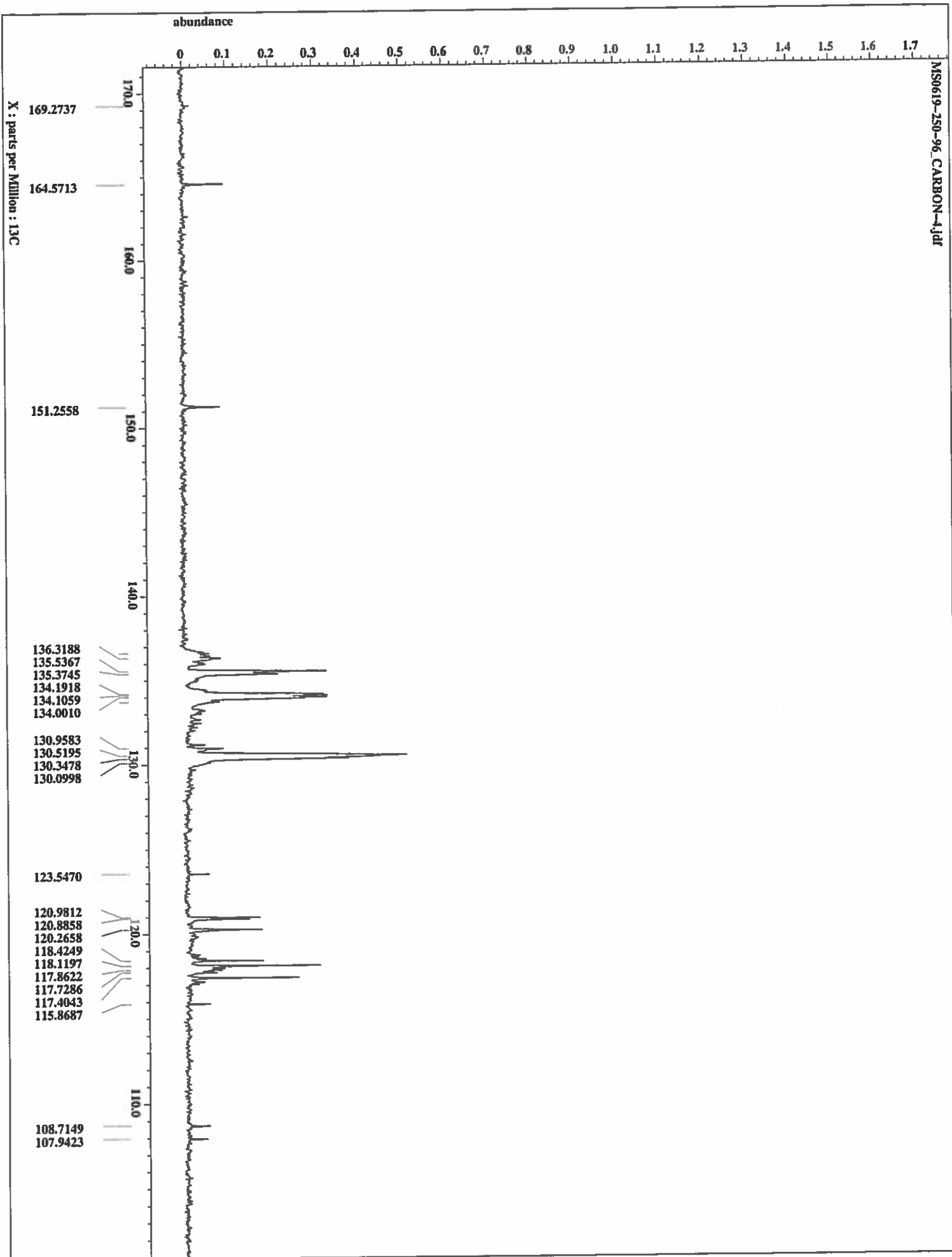
```

Filename      = MS0619-250-96_CARBON-
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0619-250-96
Solvent       = CHLOROFORM-D
Creation_time = 4-DEC-2018 12:21:52
Revision_time = 4-DEC-2018 11:56:35
Current_time  = 4-DEC-2018 11:56:35

Data_format   = 1D COMPLEX
Dir_size      = 26214
Dir_title     = 13C
Dir_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7673579 [G] (500 [MHz]
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]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 256
Total_scans    = 256

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Xr_atn_dec     = 20.7 [dB]
Xr_atn_doe     = 20.7 [dB]
Xr_noise       = VALVEZ
Decoupling     = TRUE
Inited_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 [C]
  
```



abundance

0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0 25.0 26.0 27.0 28.0 29.0

50.0 30.0 10.0 -10.0 -30.0 -50.0 -70.0 -90.0 -110.0 -130.0 -150.0 -170.0 -190.0 -210.0 -230.0 -250.0

X : parts per Million : 19F


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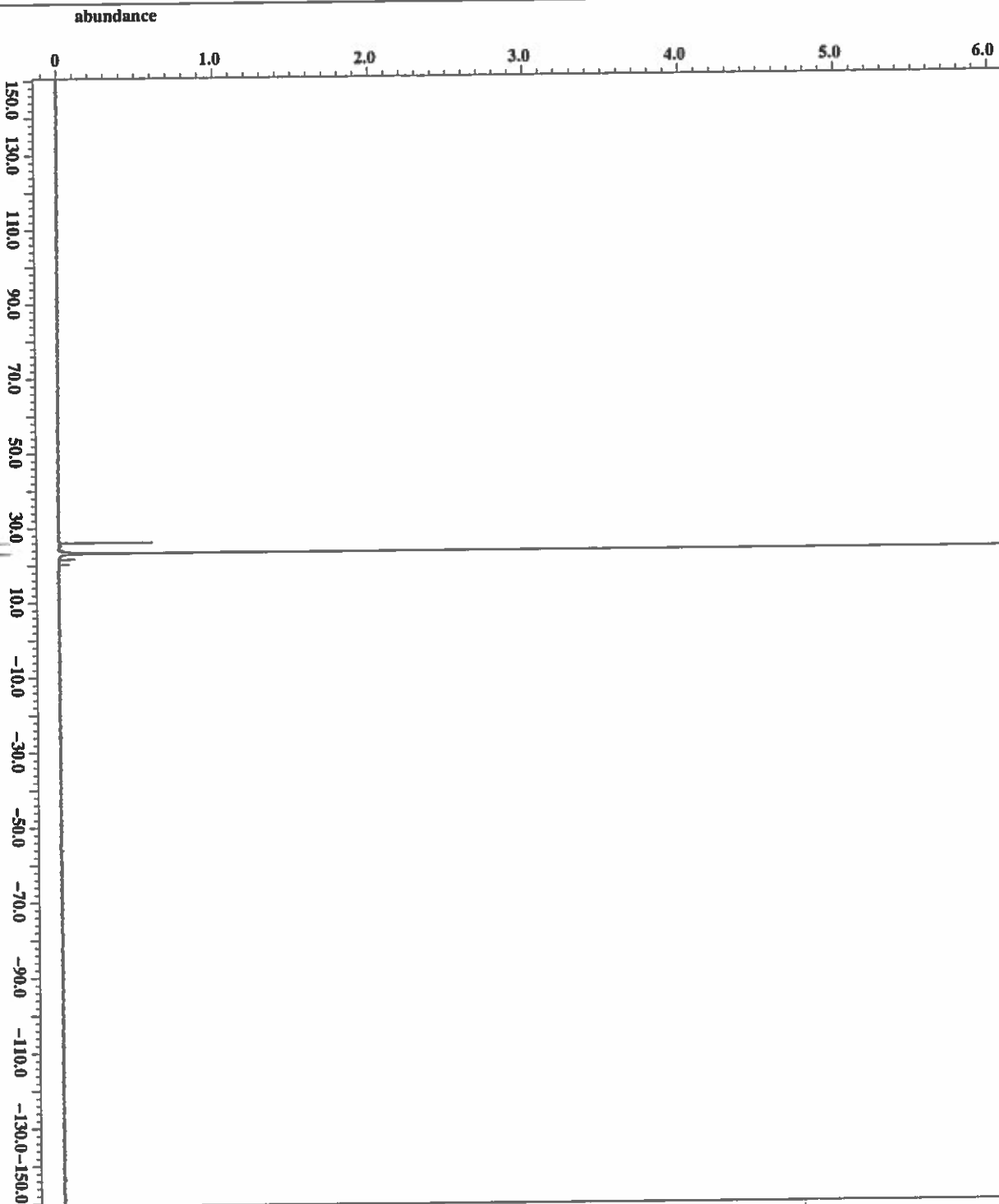
```

Filename      = MS0619-250-96_FLDORIN
Author        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0619-250-96
Solvent       = CHLOROFORM-D
Creation_time  = 4-DEC-2018 12:30:09
Revision_time  = 4-DEC-2018 12:04:53
Current_time   = 4-DEC-2018 12:04:53

Data_format   = 1D COMPLEX
Dlm_size      = 104857
Dlm_title     = 19F
Dlm_units     = 1ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.747357917 (500MHz)
X_acq_duration = 0.7340032[s]
X_domain       = 19F
X_freq         = 470.62046084 [MHz]
X_offset       = -100 [ppm]
X_points       = 131072
X_prescans     = 1
X_resolution   = 1.36239188 [Hz]
X_sweep        = 1
Xr_domain      = 19F
Xr_freq        = 470.62046084 [MHz]
Xr_offset      = 5 [ppm]
Xr1_domain     = 19F
Xr1_freq       = 470.62046084 [MHz]
Xr1_offset     = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 70
Total_scans    = 70

X_90_width     = 13.1 [us]
X_acq_time     = 0.7340032 [s]
X_angle        = 45 [deg]
X_atn          = 2.5 [dB]
X_pulse        = 6.55 [us]
Xr1_mode       = OF2
Xr1_mode       = OF2
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 66
Relaxation_delay = 4 [s]
Repetition_delay = 4.7340032 [s]
Temp_get       = 20.6 [degC]
  
```



X : parts per Million : 31P


SOUTH ALABAMA
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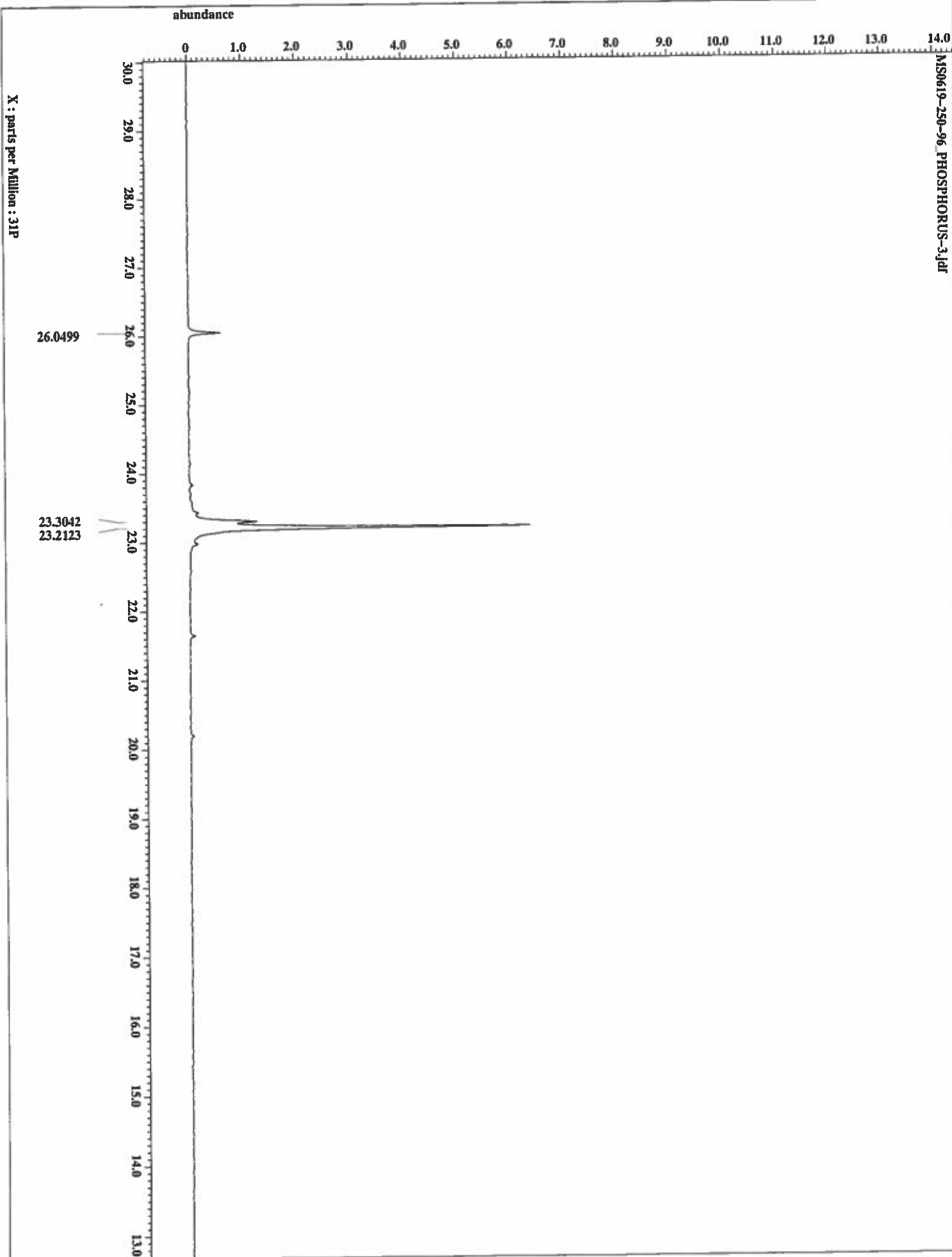
```

Filename      = MS0619-250-96_PHOSPHO
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0619-250-96
Solvent       = CHLOROFORM-D
Creation_time  = 4-DEC-2018 12:35:25
Revision_time  = 4-DEC-2018 12:10:07
Current_time   = 4-DEC-2018 12:10:07

Data_format   = 1D COMPLEX
Dim_size      = 52428
Dim_title     = 31P
Dim_units     = [ppm]
Dimensions    = X
Size          = 2048
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.85983232 [s]
X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 65536
X_prescans     = 4
X_resolution   = 1.16301746 [Hz]
X_sweep        = 76.2195122 [KHz]
X_domain      = 1H
Xir_freq       = 500.15991521 [MHz]
Xir_offset     = 5.0 [ppm]
Xir_return     = FALSTZ
Mod_return     = 1
Scans          = 50
Total_scans    = 50

X_90_width     = 14.687 [us]
X_acq_time      = 0.85983232 [s]
X_angle        = 30 [deg]
X_ech          = 5 [dB]
X_pulse        = 4.89566667 [us]
Xir_atn_dec    = 20.7 [dB]
Xir_atn_noe    = 20.7 [dB]
Xir_noise      = KALFZ
Decoupling     = TRUE
Initial_wait    = 1 [s]
Noe            = 1 [s]
Noe_time       = TRUE
Relaxation_delay = 2 [s]
Repetition_time = 2.85983232 [s]
Temp_get       = 20.9 [C]
  
```



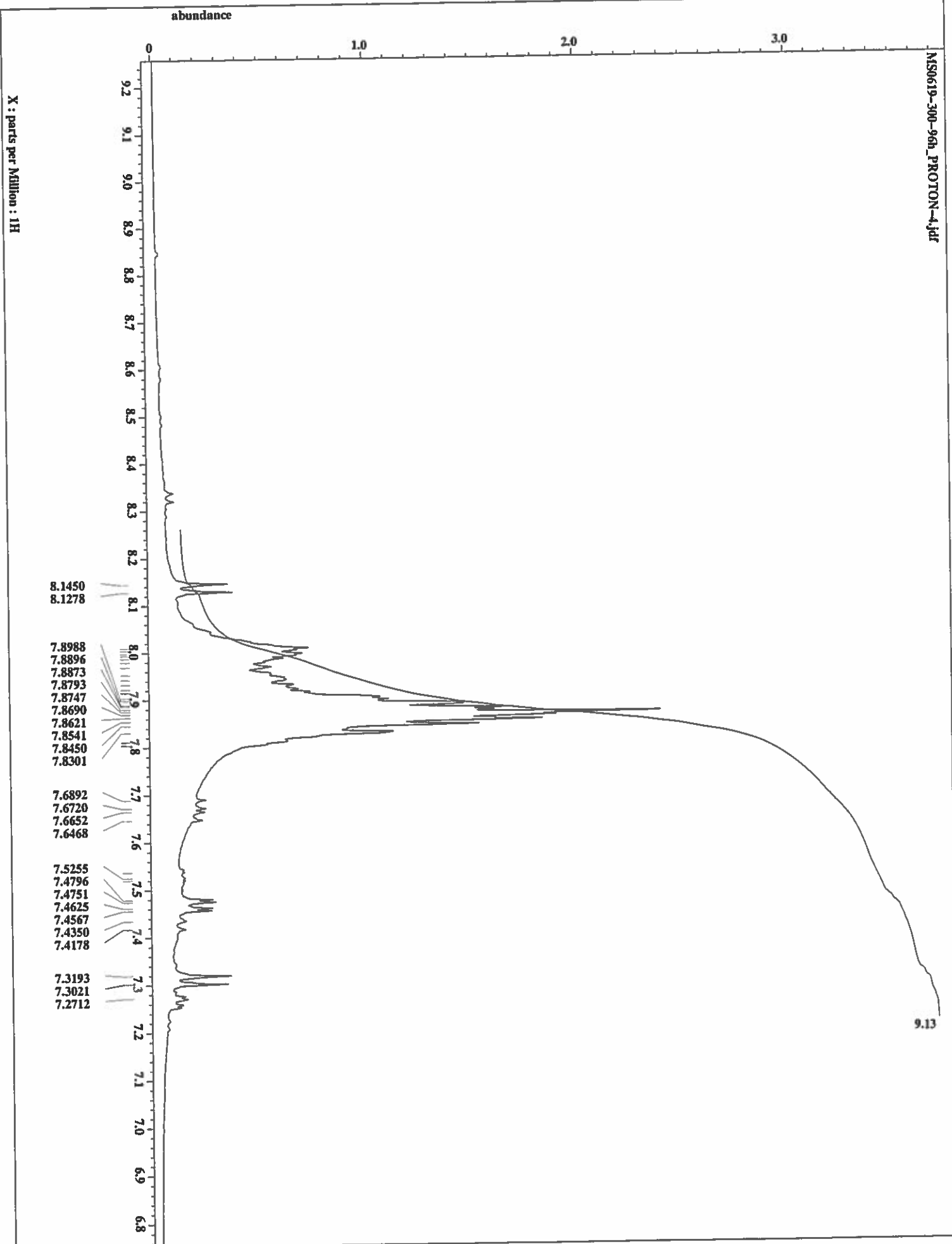
X: parts per Million: IH

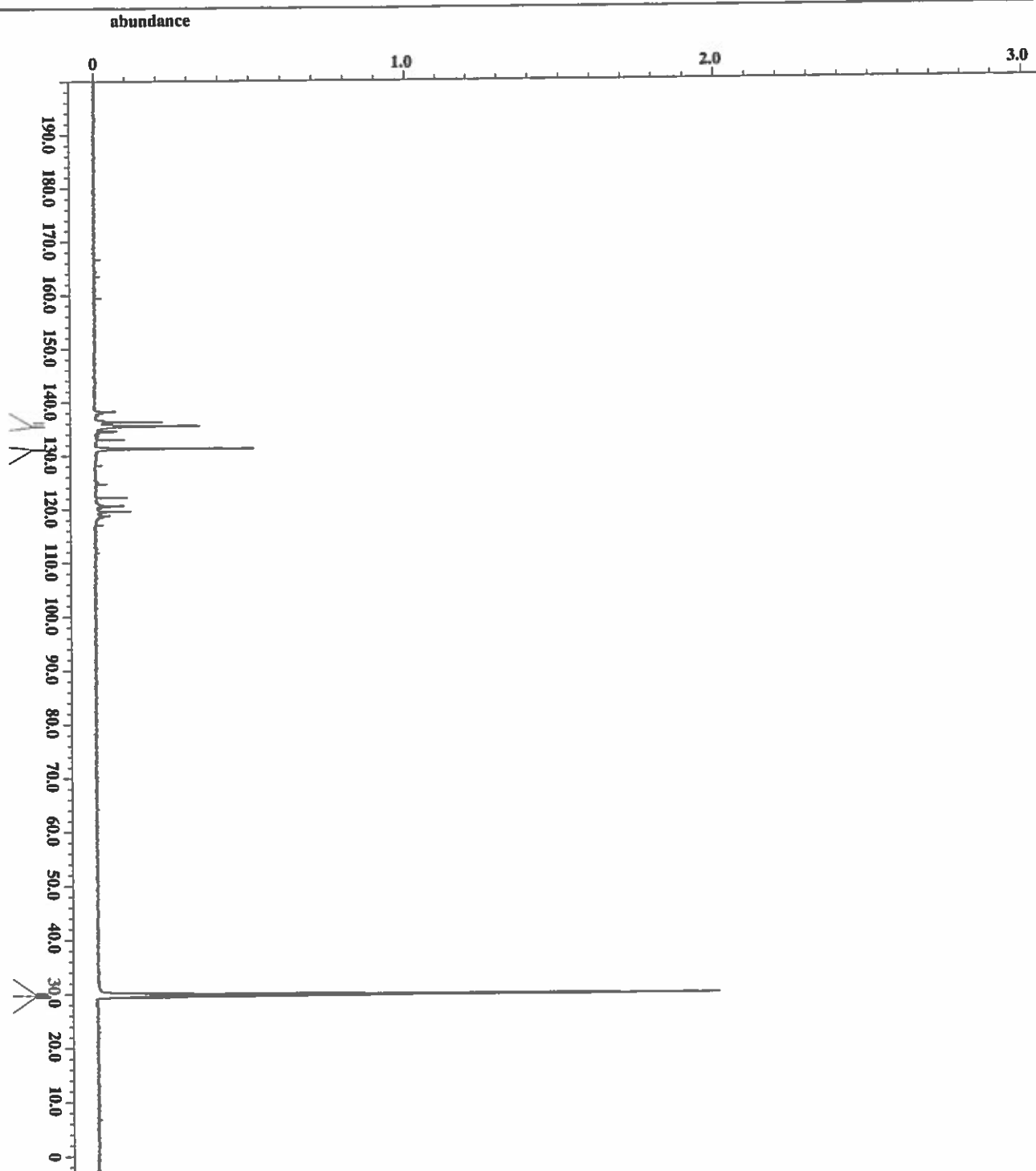


2.0446
2.0400
1.4285

Filename	= MS0619-300-96h_PROLOG
Author	= Jim Davis
Experiment	= single_pulse.exe2
Sample_id	= MS0619-300-96h
Solvent	= ACETONE-D6
Creation_time	= 4-DEC-2018 15:36:44
Revision_time	= 4-DEC-2018 15:11:24
Current_time	= 4-DEC-2018 15:11:25
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_cfile	= 1H
Dim_units	= [ppm]
Dimensions	= X
Size	= ECA 500
Spectrometer	= JNM-ECA500
Pulse_strength	= 11.7473579 [V] (500 [MHz])
X_acq_duration	= 1.76587904 [s]
X_domain	= 1H
X_freq	= 500.15991521 [MHz]
X_offset	= 5.01 [ppm]
X_pulprots	= 16384
X_prescans	= 1
X_resolution	= 0.57277737 [Hz]
X_sweep	= 9.38438438 [kHz]
1H_domain	= 1H
1H_freq	= 500.15991521 [MHz]
1H_offset	= 5.01 [ppm]
1H_domain	= 1H
1H_freq	= 500.15991521 [MHz]
1H_offset	= 5.01 [ppm]
clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 12.4 [us]
X_acq_time	= 1.74587904 [s]
X_angle	= 45 [deg]
X_atn	= 4 [dB]
X_pulse	= 6.2 [us]
1H_mode	= OFC
1H_mode	= OFC
Dante_presat	= FALSE
Initial_wait	= 1 [s]
Recvr_gain	= 30
Relaxation_delay	= 4 [s]
Relaxation_time	= 5.74587904 [s]
Temp_get	= 20.7 [dC]







X : parts per Million : 13C

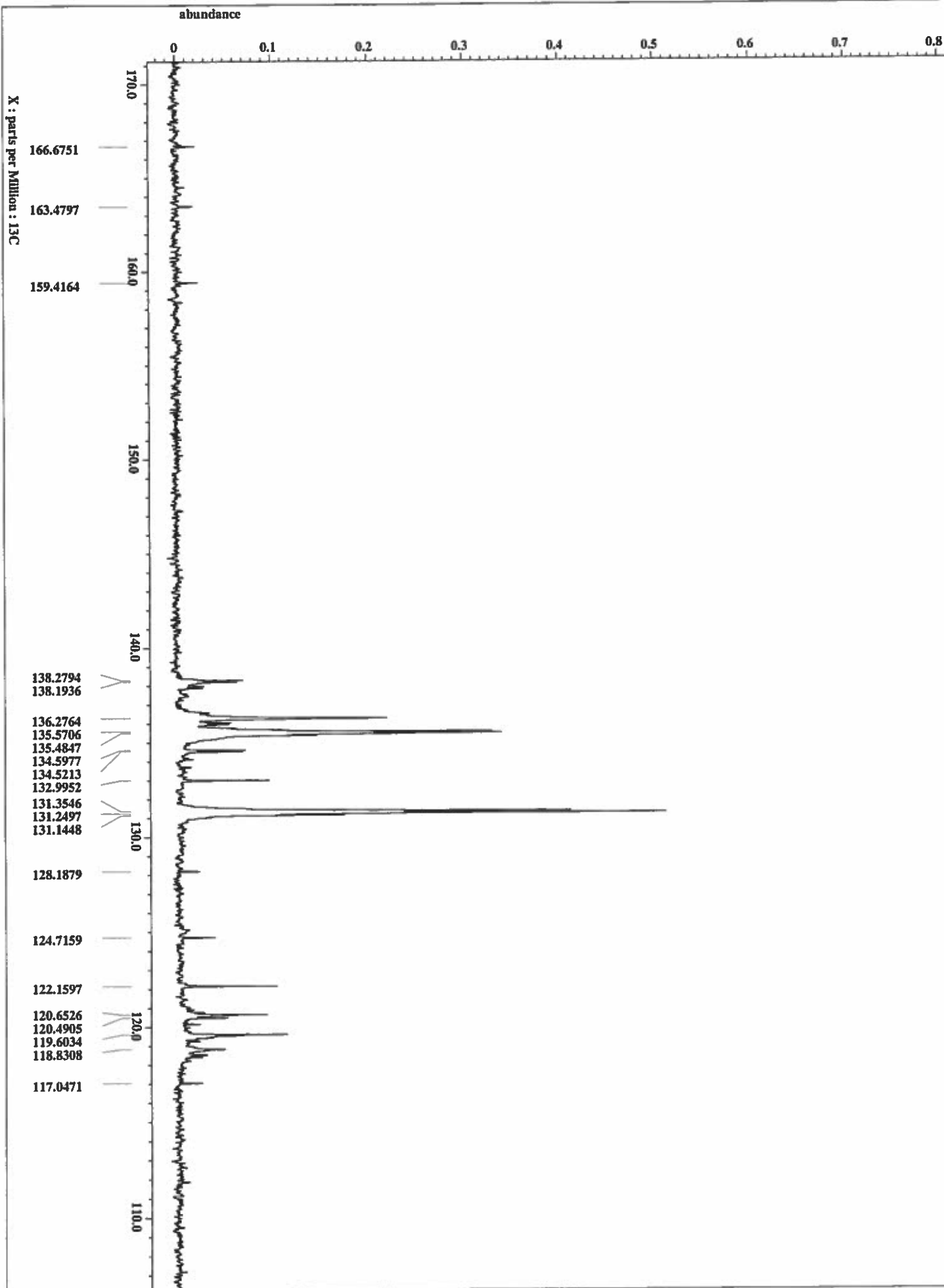


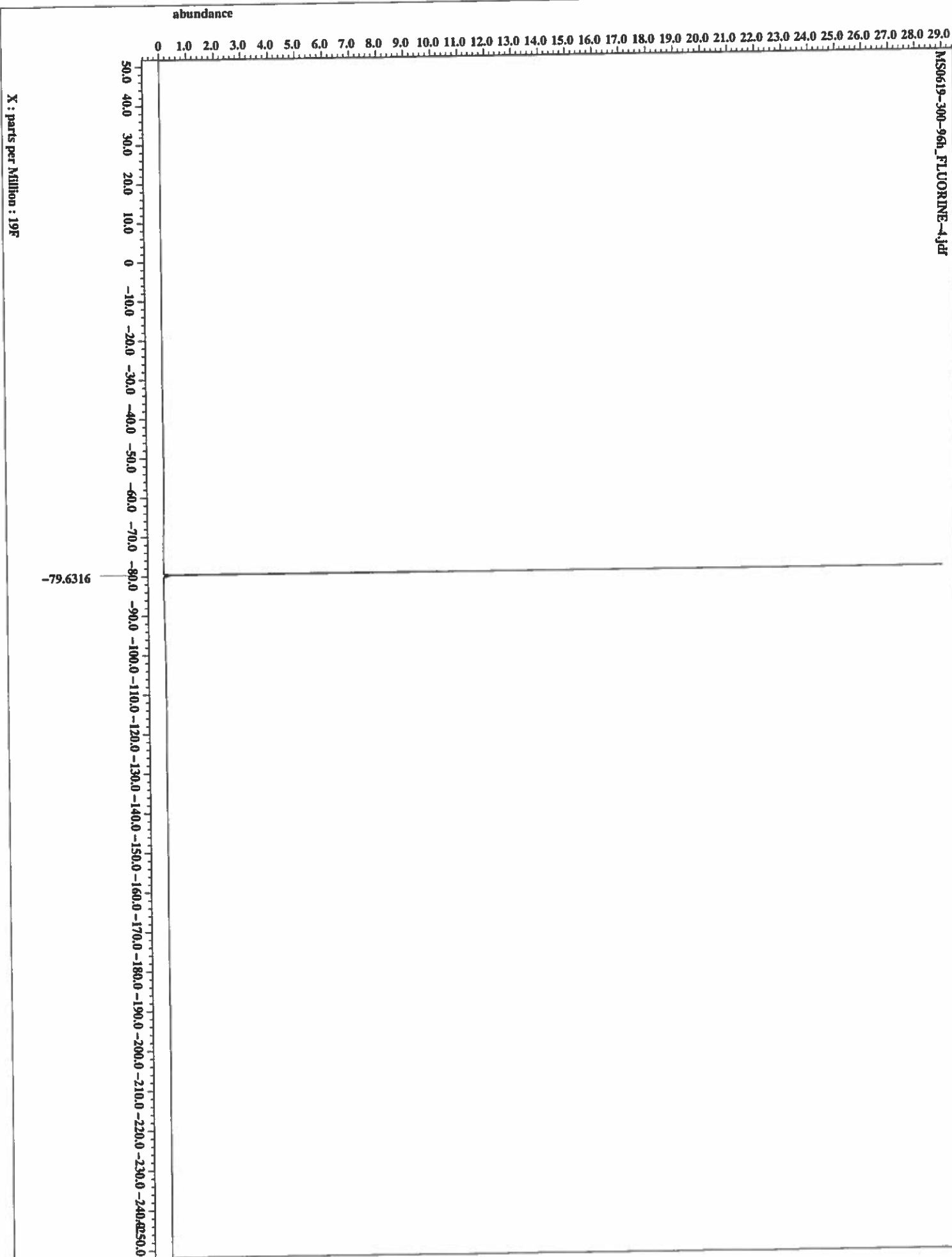
Filename = MS0619-300-96h_CARBON
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = MS0619-300-96h
 Solvent = ACETONE-D6
 Creation_time = 4-DEC-2018 16:08:01
 Revision_time = 4-DEC-2018 15:42:44
 Current_time = 4-DEC-2018 15:42:44

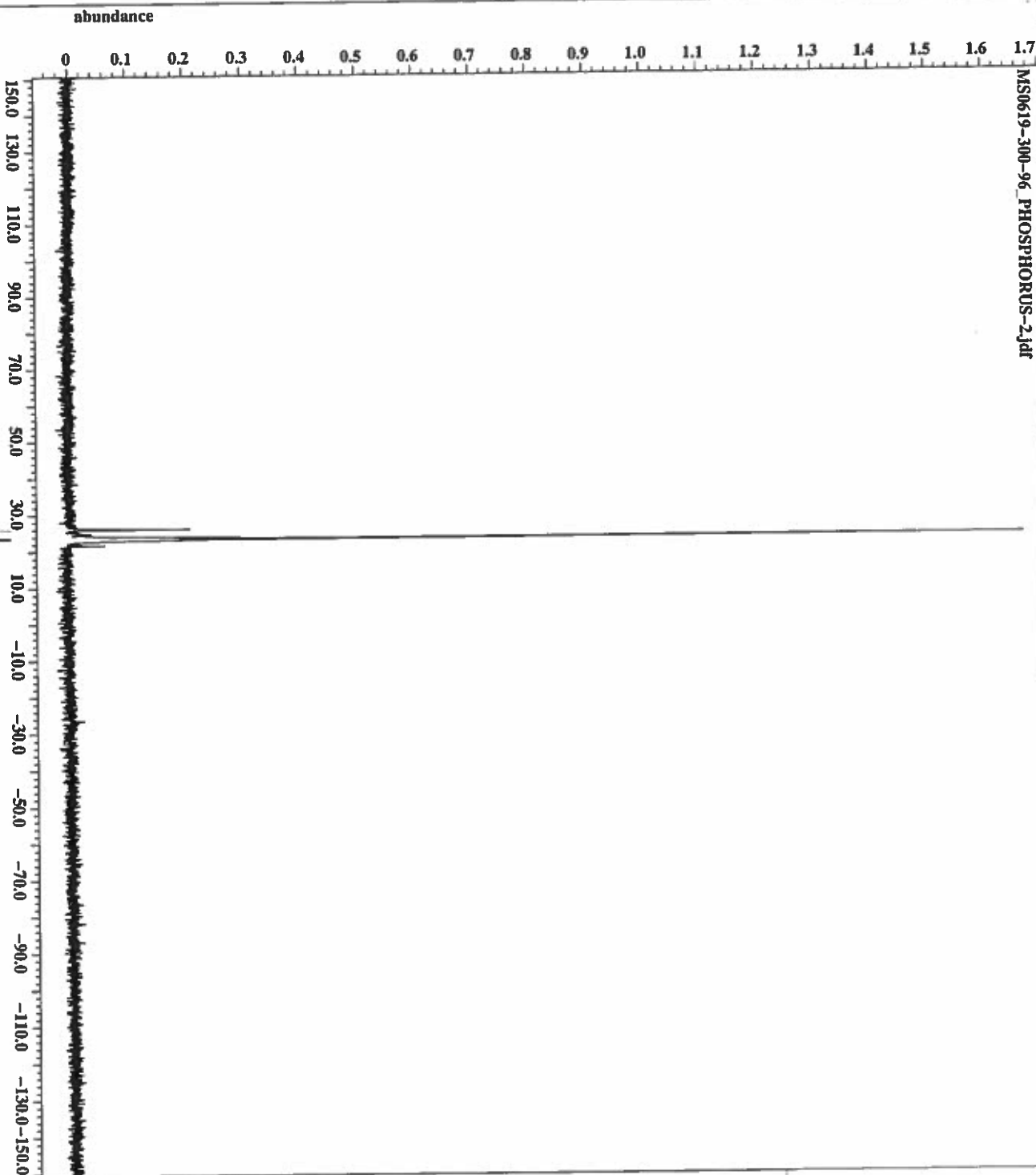
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECX500

 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]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 600
 Total_scans = 600

 X_90_width = 13.2 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 6 [db]
 X_pulse = 4.4 [us]
 Irr_atn_dec = 20.7 [db]
 Irr_atn_noe = 20.7 [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 = 21.1 [deg]







X : parts per Million : 31P



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=====
File name      MS0619-300-96_PHOSPHO
Author        Jim Davis
Experiment    single_pulse_dec
Sample_id     MS0619-300-96
Solvent       CHLOROFORM-D
Creation_time  4-DEC-2018 12:00:07
Revision_time 4-DEC-2018 11:34:50
Current_time   4-DEC-2018 11:34:50

=====
Data format
Dim_size      1D COMPLEX
Dim_title     52428
Dim_units     31P
Dimensions    [ppm]
Site          X
Spectrometer  ECA 500
              JNM-ECA500

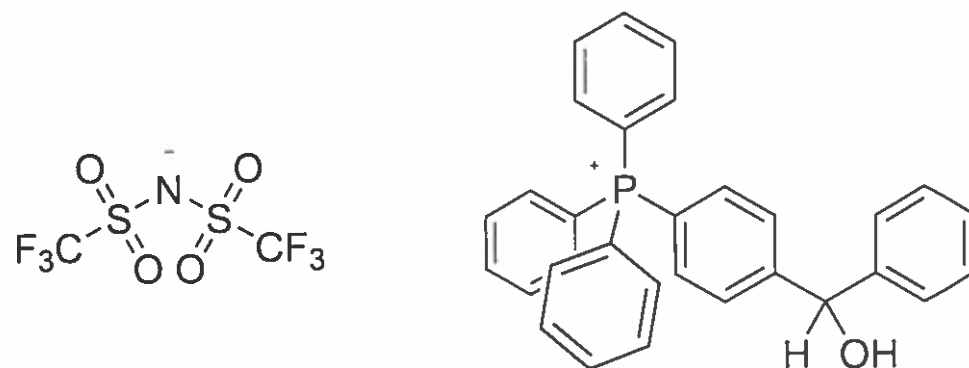
=====
Field_strength 11.7473579 [T] (500 MHz)
X_acq_duration 0.85983232 [s]
X_domain       31P
X_freq         202.46831075 [MHz]
X_offset       0 [ppm]
X_points       65536
X_prescans     4
X_resolution   1.163021746 [Hz]
X_sweep        76.2195122 [Hz]
X_domain       1H
Xir_freq       500.15991521 [MHz]
Xir_offset     5.0 [ppm]
Clipped        TRUE
Mod_return     1
Scans          50
Total_scans    50

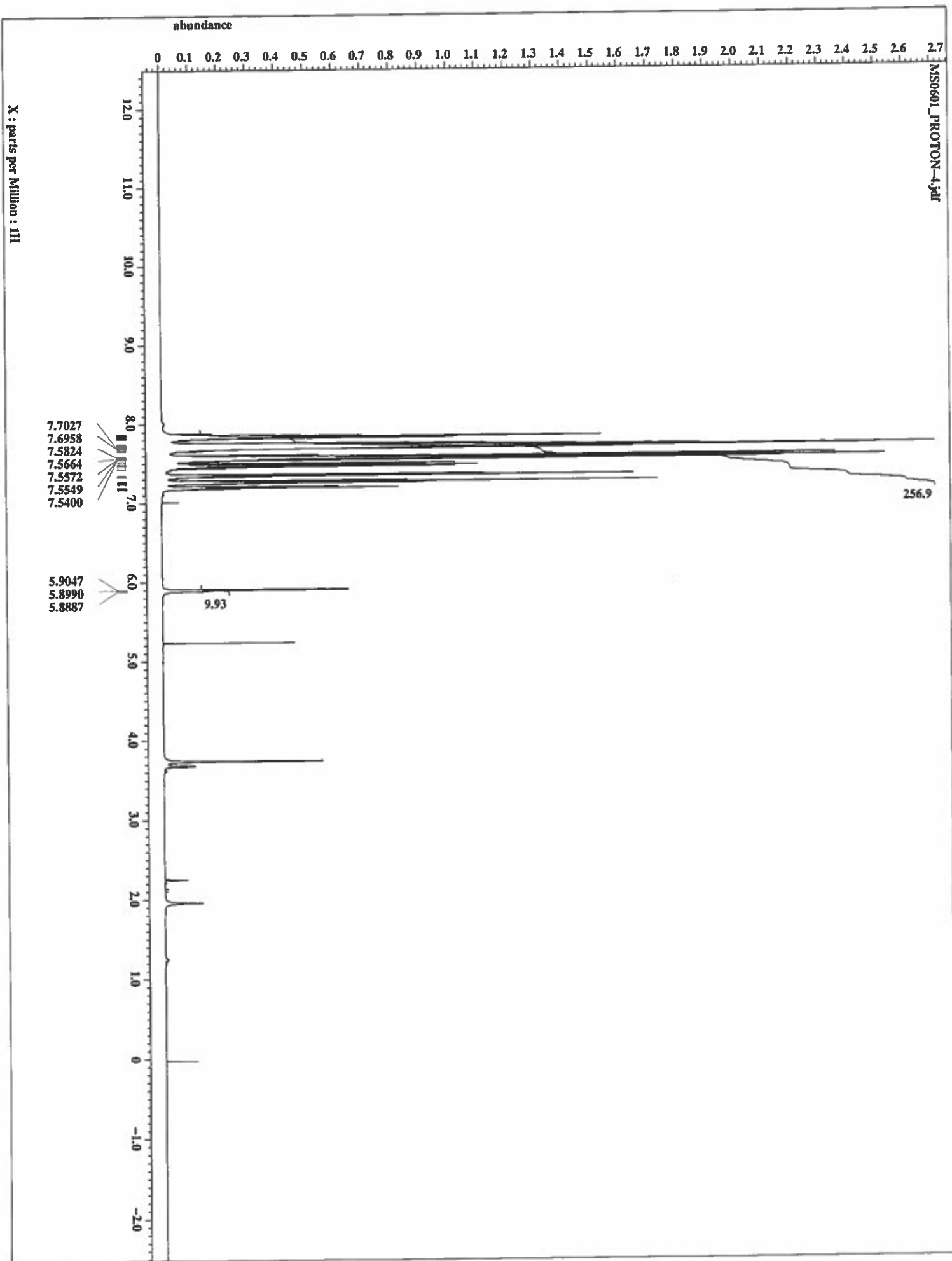
=====
X_90_width     14.687 [us]
X_acq_time     0.85983232 [s]
X_angle        30 [deg]
X_atn          5 [dB]
X_pulse        4.89566667 [us]
Xir_atn_dec    20.7 [dB]
Xir_atn_noe    20.7 [dB]
Xir_noise      VALVEZ
Decoupling     TRUE
Initial_wait    1 [s]
Hoe            1 [s]
Hoe_time       TRUE
Hoe            2 [s]
Relaxr_gain     58
Relaxation_delay 2 [s]
Repetition_time 2.85983233 [s]
Temp_get       20.7 [dC]
=====

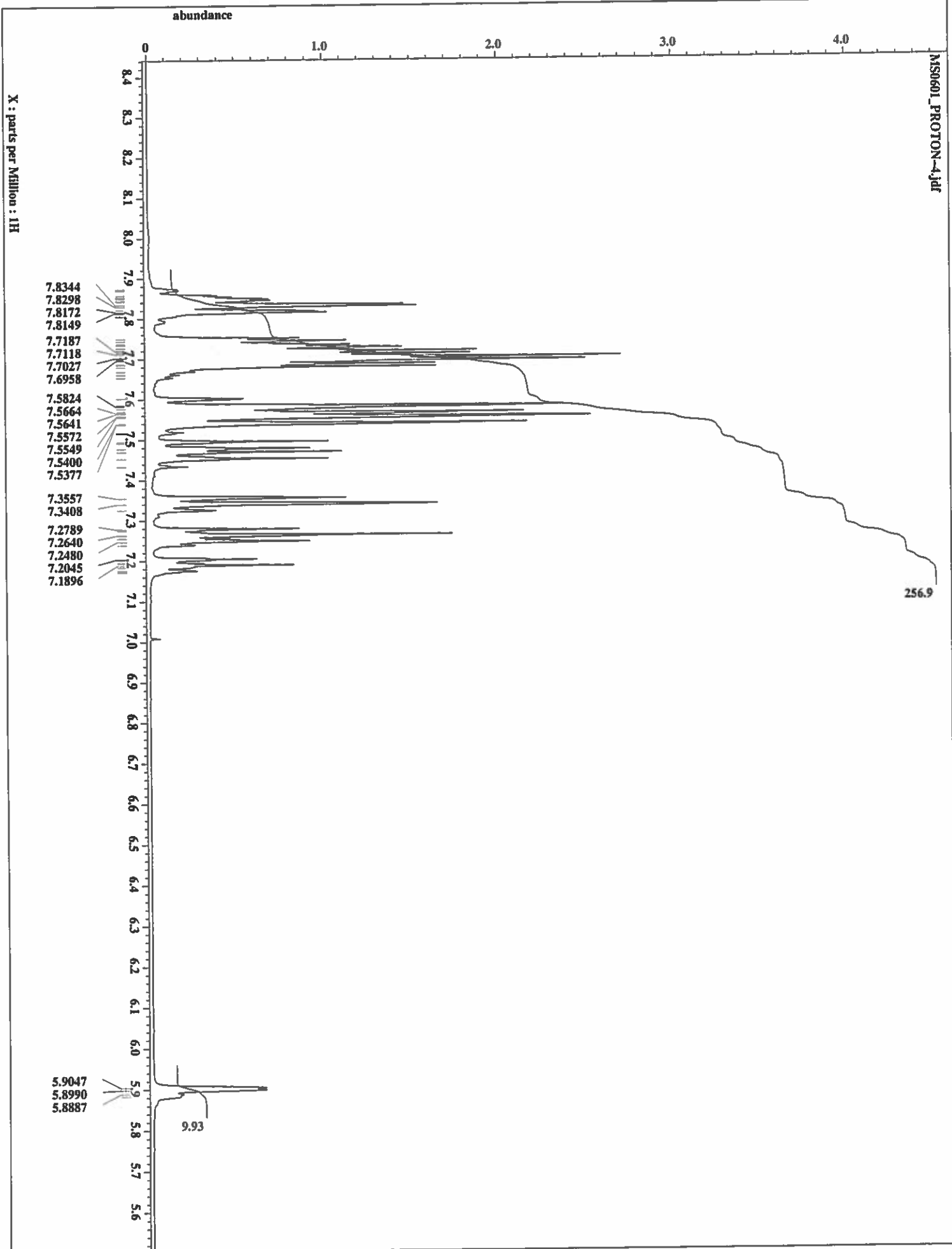
```

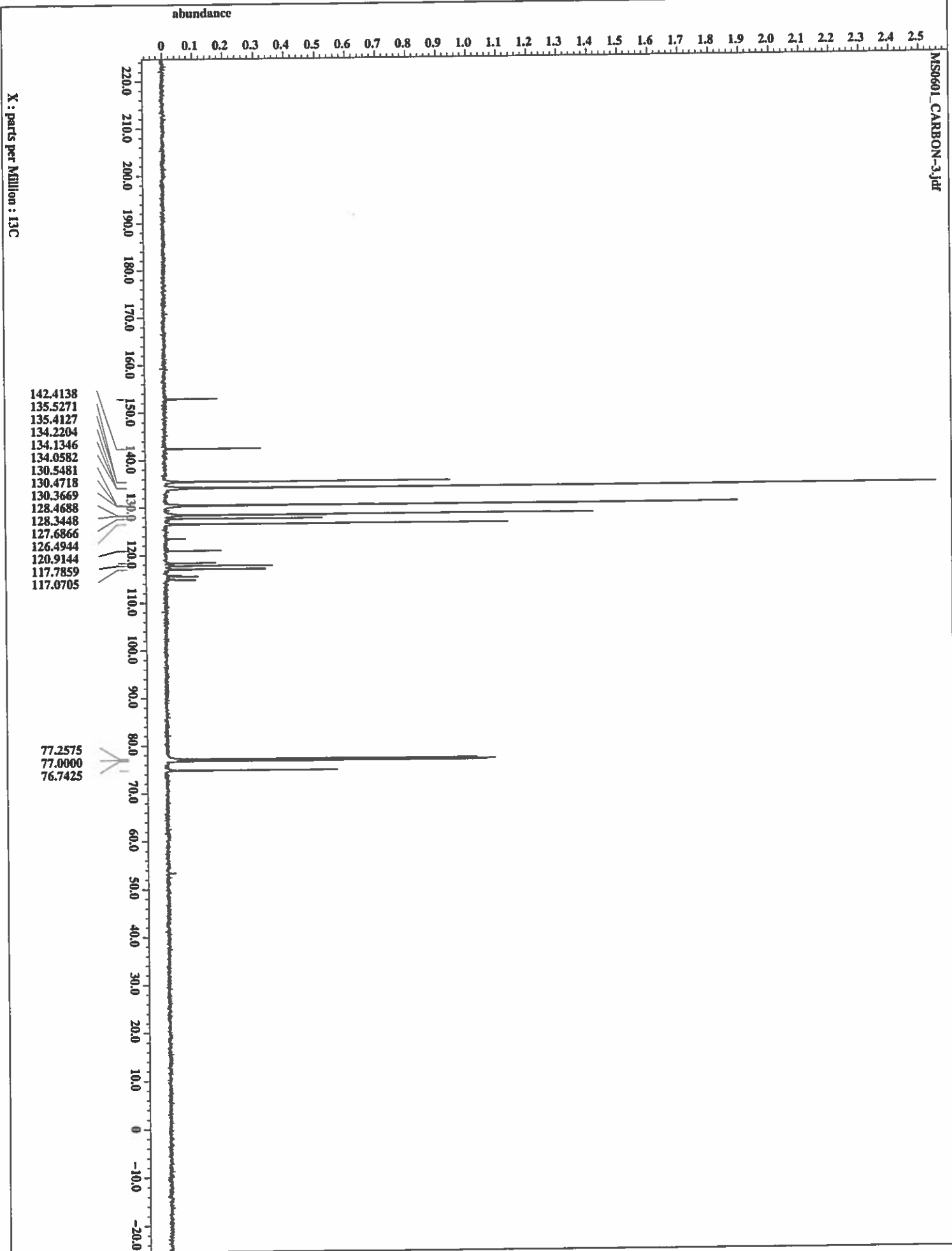
Compound 16 Pre- and Post-heating NMR Spectra

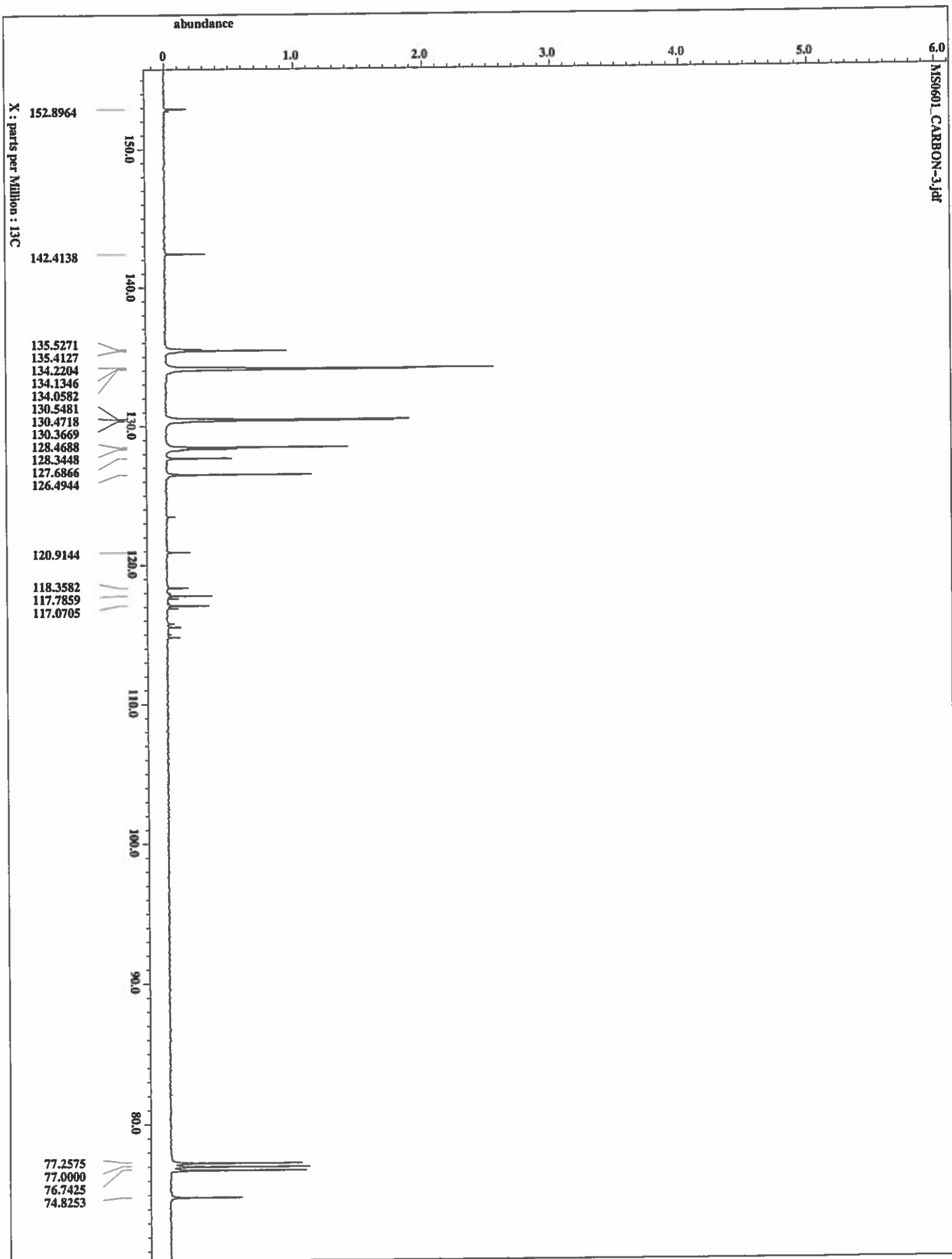
Temperature of Post-heating samples noted in upper left corner of each spectrum

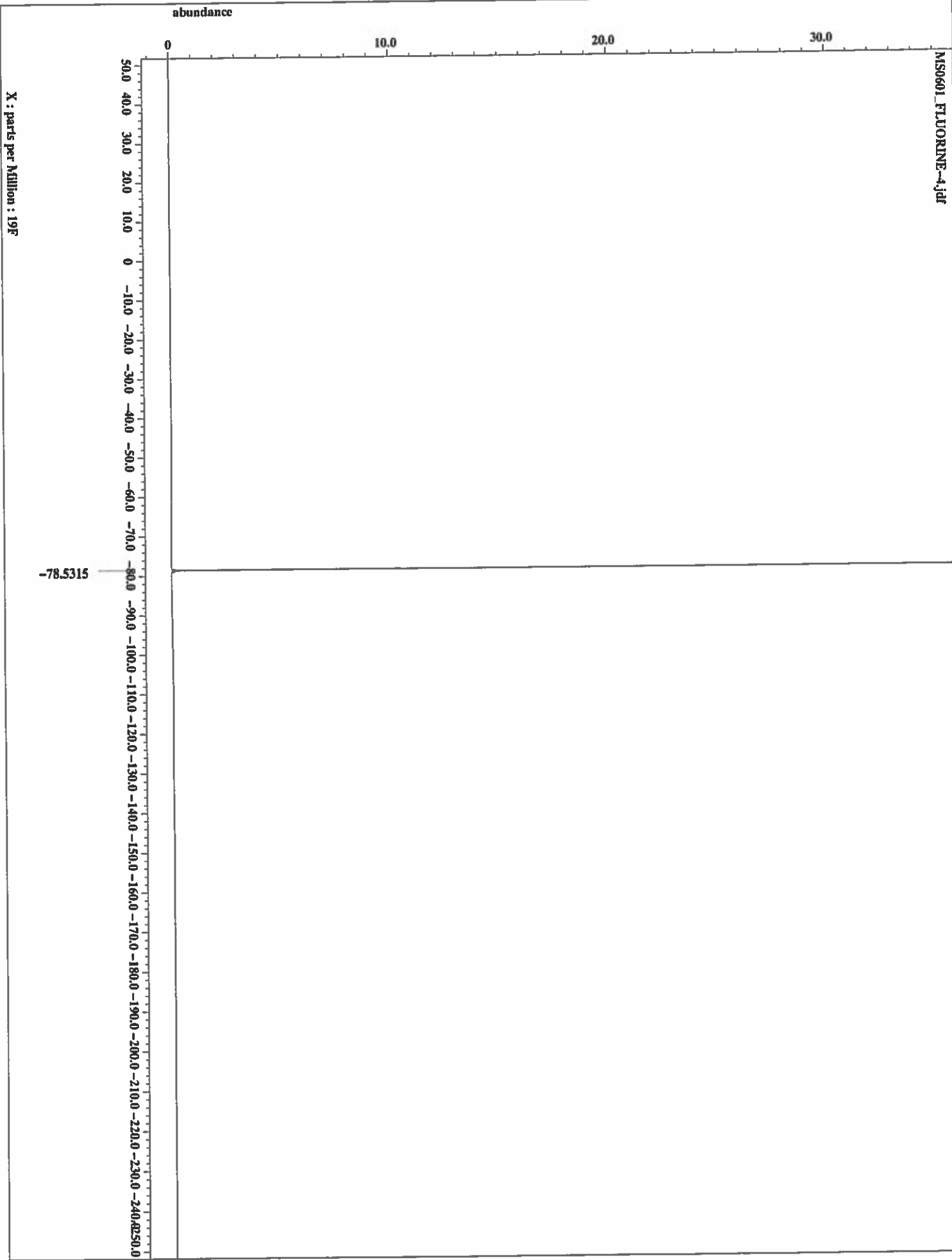


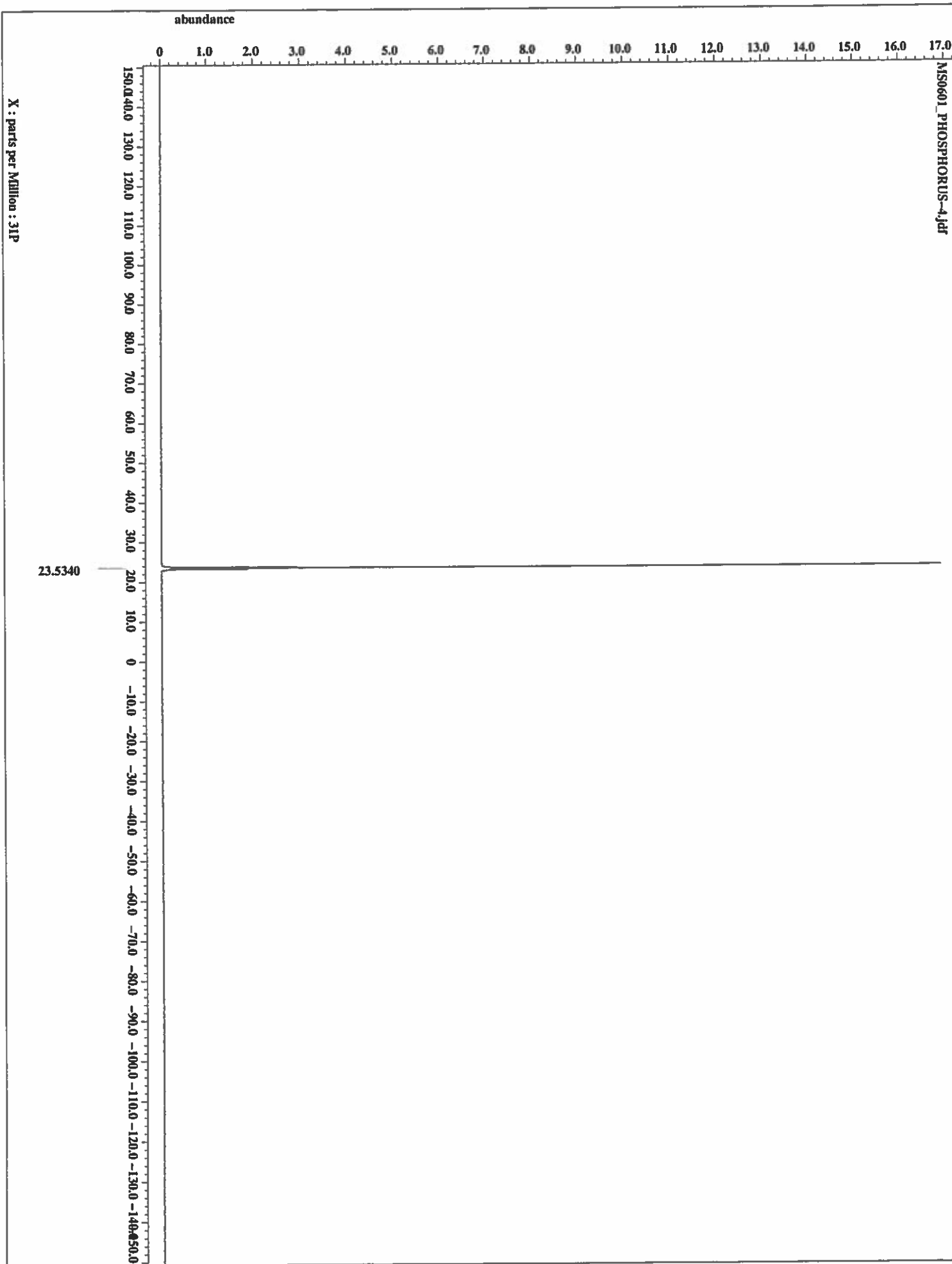


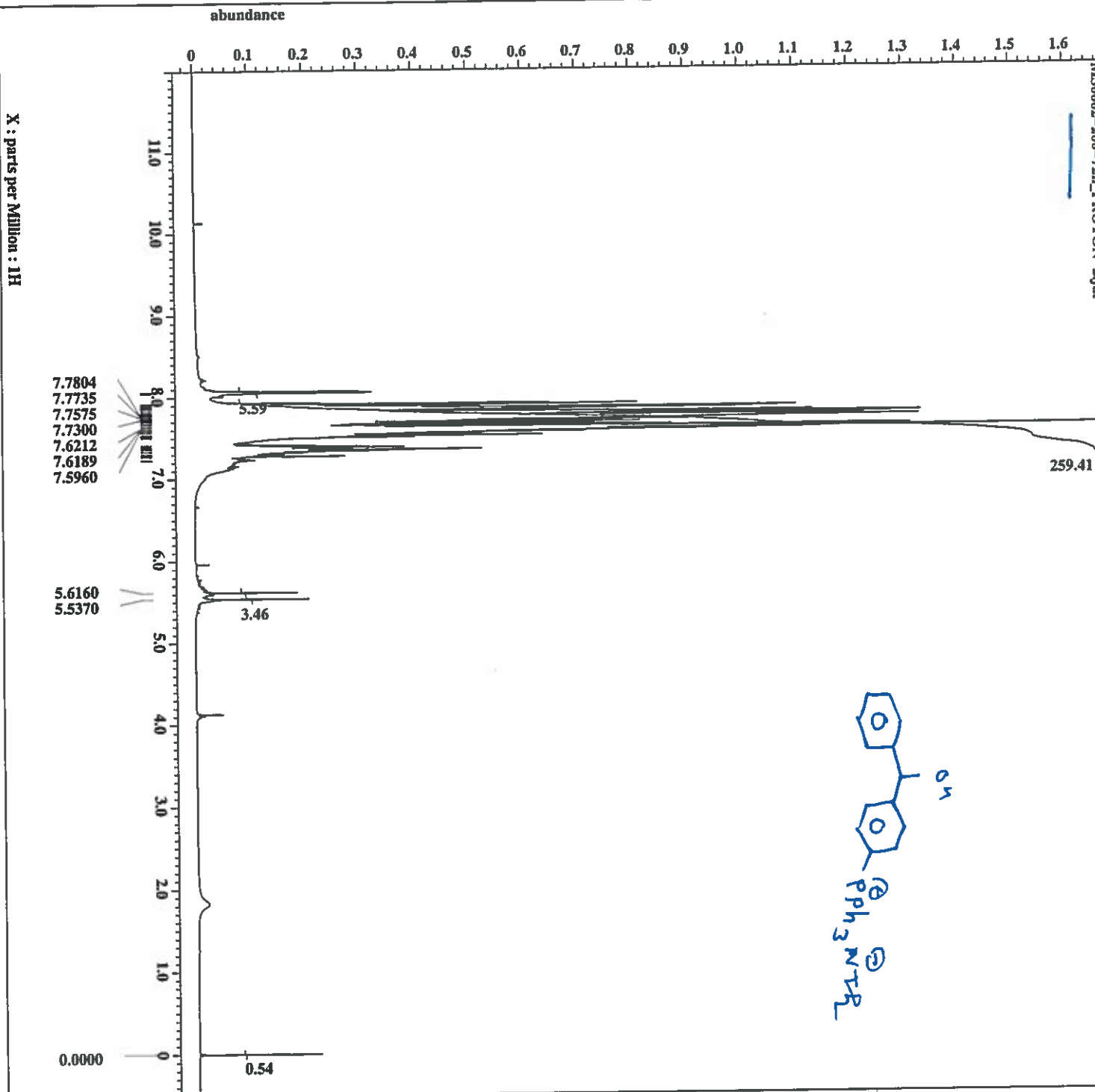








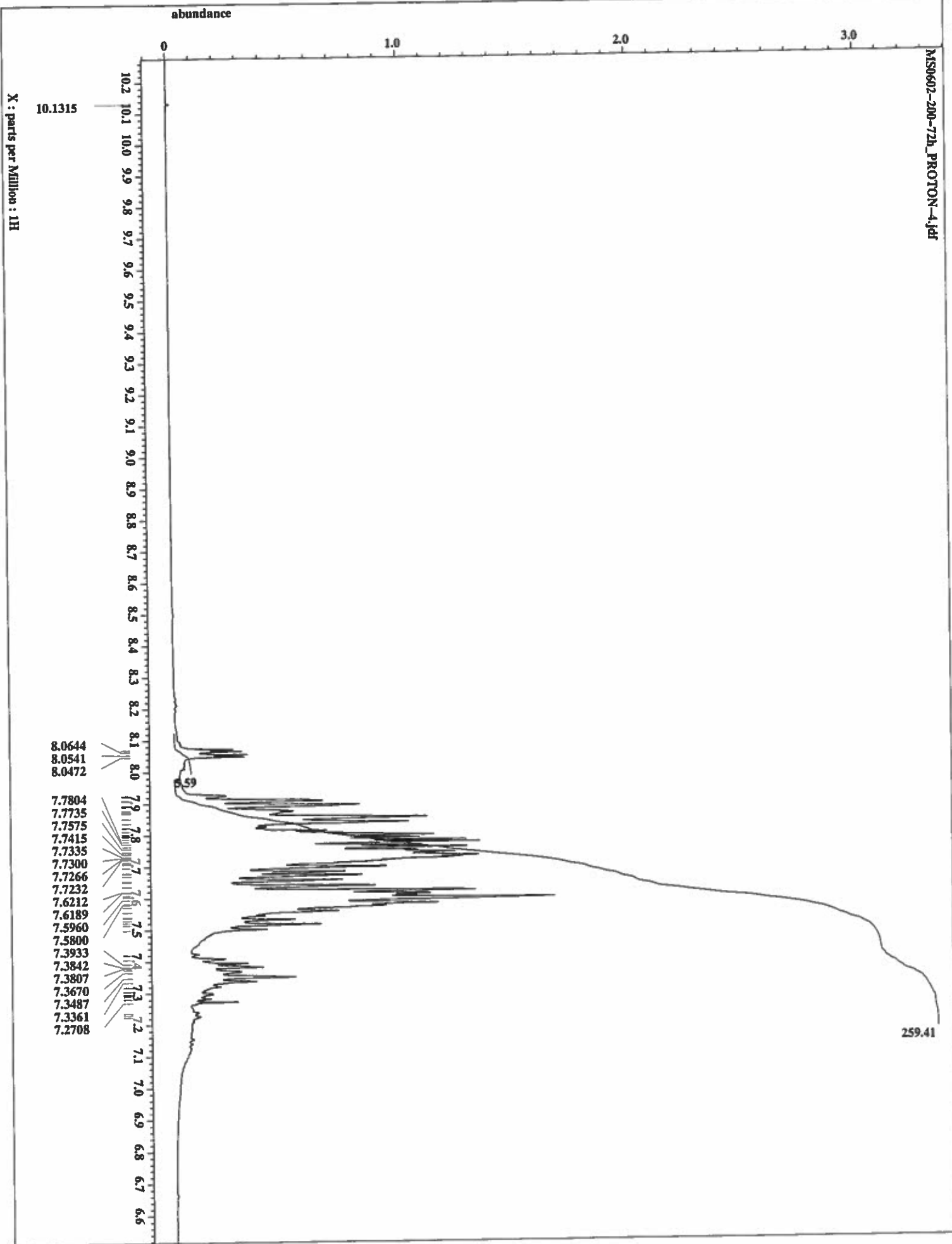


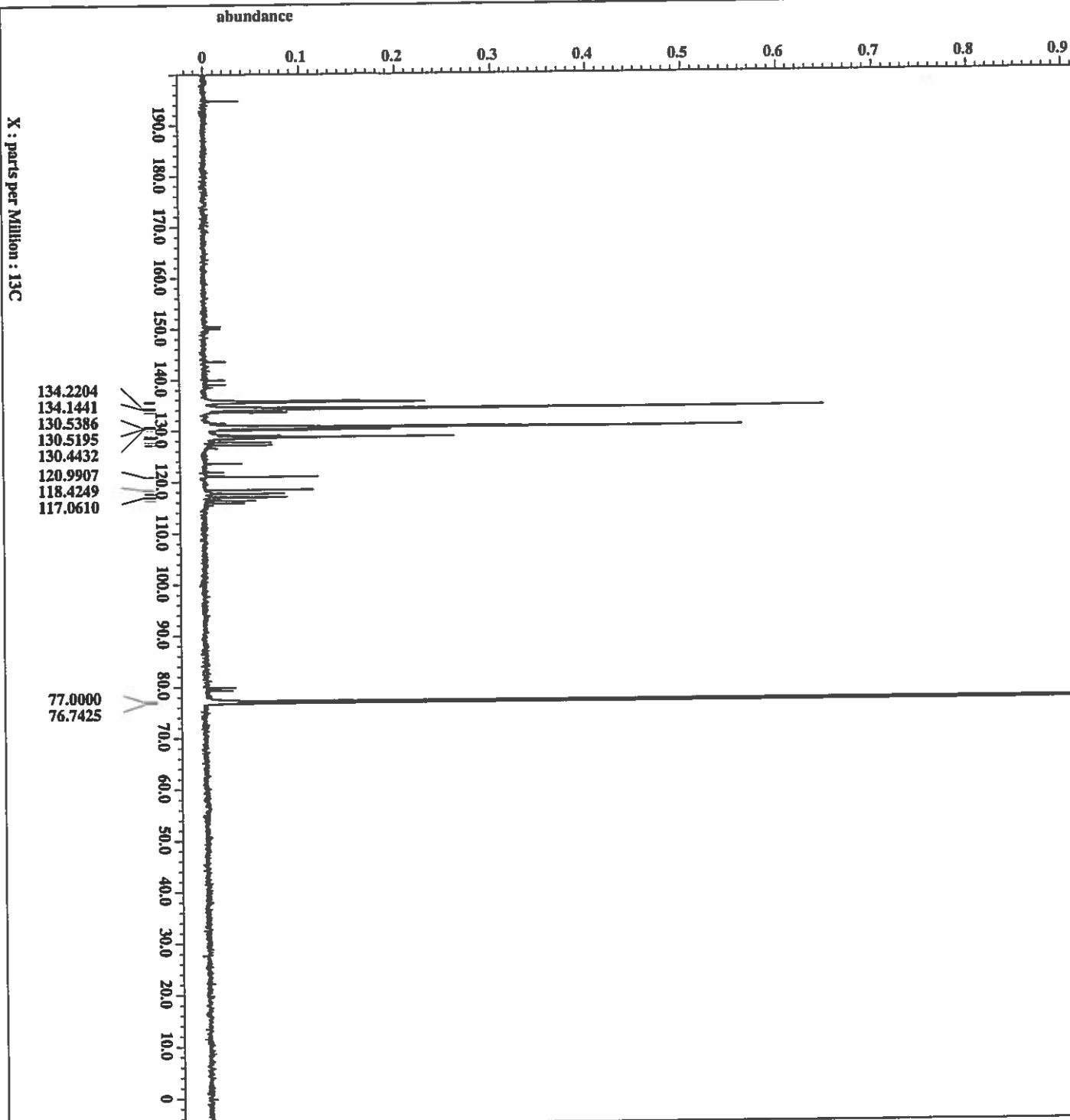


X : parts per Million : 1H



filename MS0602-200-72h_PROTON
 Author Jim Davis
 Experiment single_pulse.ex2
 Sample_id MS0602-200-72h
 Solvent CHLOROFORM-D
 Creation_time 8-NOV-2018 18:35:06
 Revision_time 8-NOV-2018 18:10:23
 Current_time 8-NOV-2018 18:10:23
 Data_format 1D COMPLEX
 Data_size 13107
 Data_file 1H
 Data_units [ppm]
 Dimensions 1
 Size X
 Spectrometer ECA 500
 JNM-ECA500
 Field_strength 11.7473579 [T] (500 [MHZ])
 X_acq_duration 1.74587904 [s]
 X_domain 1H
 X_freq 500.15991521 [MHZ]
 X_offset 5.0 [ppm]
 X_points 16384
 X_prescans 1
 X_resolution 0.5727737 [Hz]
 X_sweep 9.38438438 [Hz]
 Irr_domain 1H
 Irr_freq 500.15991521 [MHZ]
 Irr_offset 5.0 [ppm]
 Tr1_domain 1H
 Tr1_freq 500.15991521 [MHZ]
 Tr1_offset 5.0 [ppm]
 Clipped FALSE
 Mod_return 1
 Scans 16
 Total_scans 16
 X_90_width 12.4 [us]
 X_acq_time 1.74587904 [s]
 X_angle 45 [deg]
 X_atn 4 [dB]
 X_pulse 6.2 [us]
 Irr_mode OET
 Pulse_program PALSE
 Initial_wait 1 [s]
 Recv_gain 26
 Relaxation_delay 4 [s]
 Repetition_time 5.74587904 [s]
 Temp_get 22.8 [degC]





```

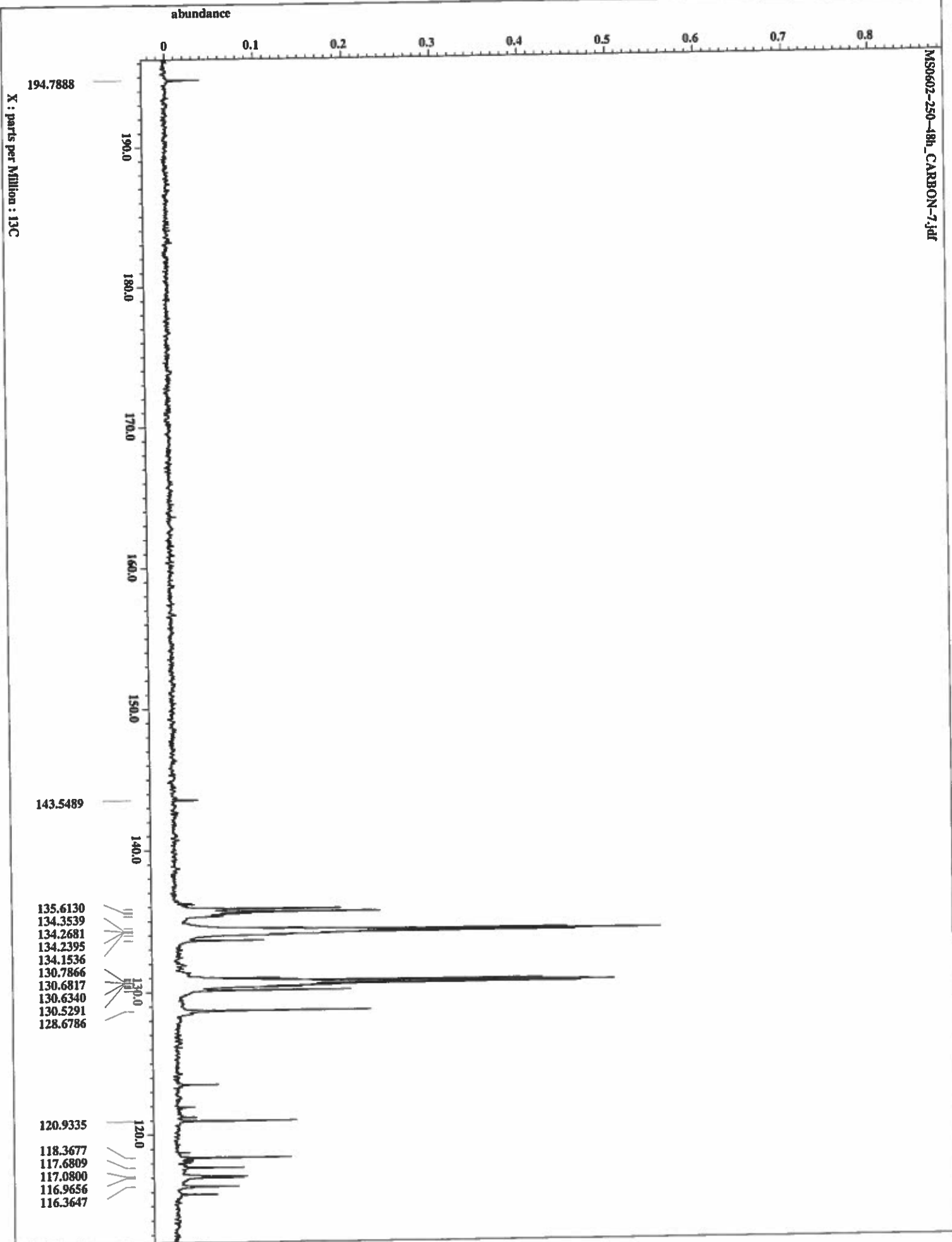
Filename      = MS0602-200-72h_CARBON
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0602-200-72h
Solvent       = CHLOROFORM-D
Creation_time  = 8-NOV-2018 19:23:57
Revision_time  = 8-NOV-2018 18:59:15
Current_time   = 8-NOV-2018 18:59:15

Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_cfile     = 13C
Dim_units     = [ppm]
Dimensions    = x
Size          = 8CA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain      = 13C
X_freq        = 125.76529768[MHz]
X_offset      = 100.1ppm]
X_points      = 32768
X_prescans    = 4
X_rescans     = 1.19959034[Hz]
X_sweep       = 39.3081761[MHz]
X_domain      = 1H
Xir_freq      = 500.15991521[MHz]
Xir_offset    = 5.0[ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 1024
Total_scans   = 1024

X_90_wdth     = 13.2[us]
X_acq_time    = 0.83361792[s]
X_angle       = 30[deg]
X_atn         = 6[db]
X_pulse       = 4.4[us]
Xir_atn_dec   = 20.7[db]
Xir_atn_doe   = 20.7[db]
Xir_noise     = NMRZ
Decoupling    = TRIZ
Inited1_wait  = 1[s]
Moe           = TRUZ
Moe_time      = 2[s]
Recur_galn    = 60
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_set      = 23.3[deg]

```



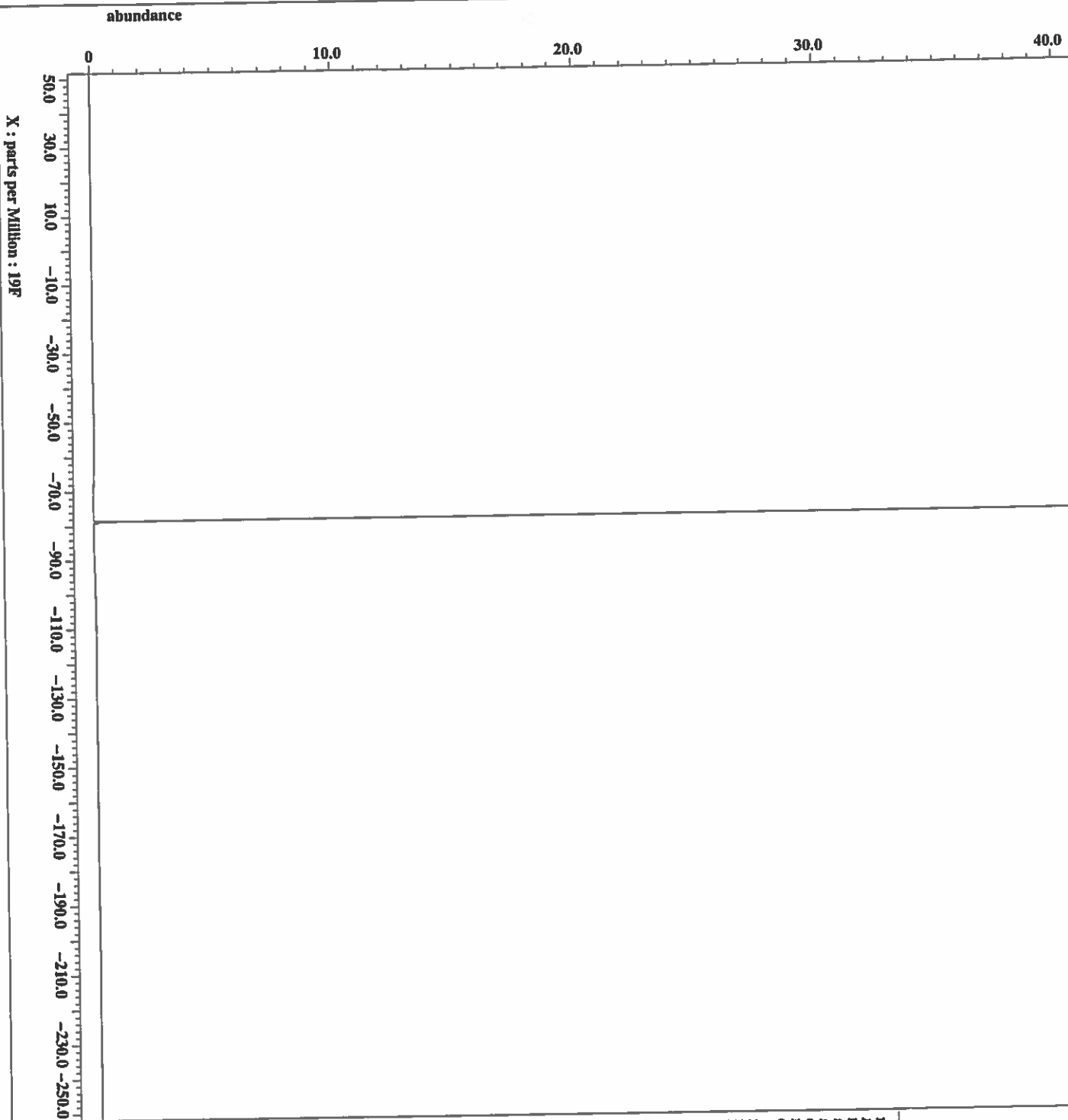


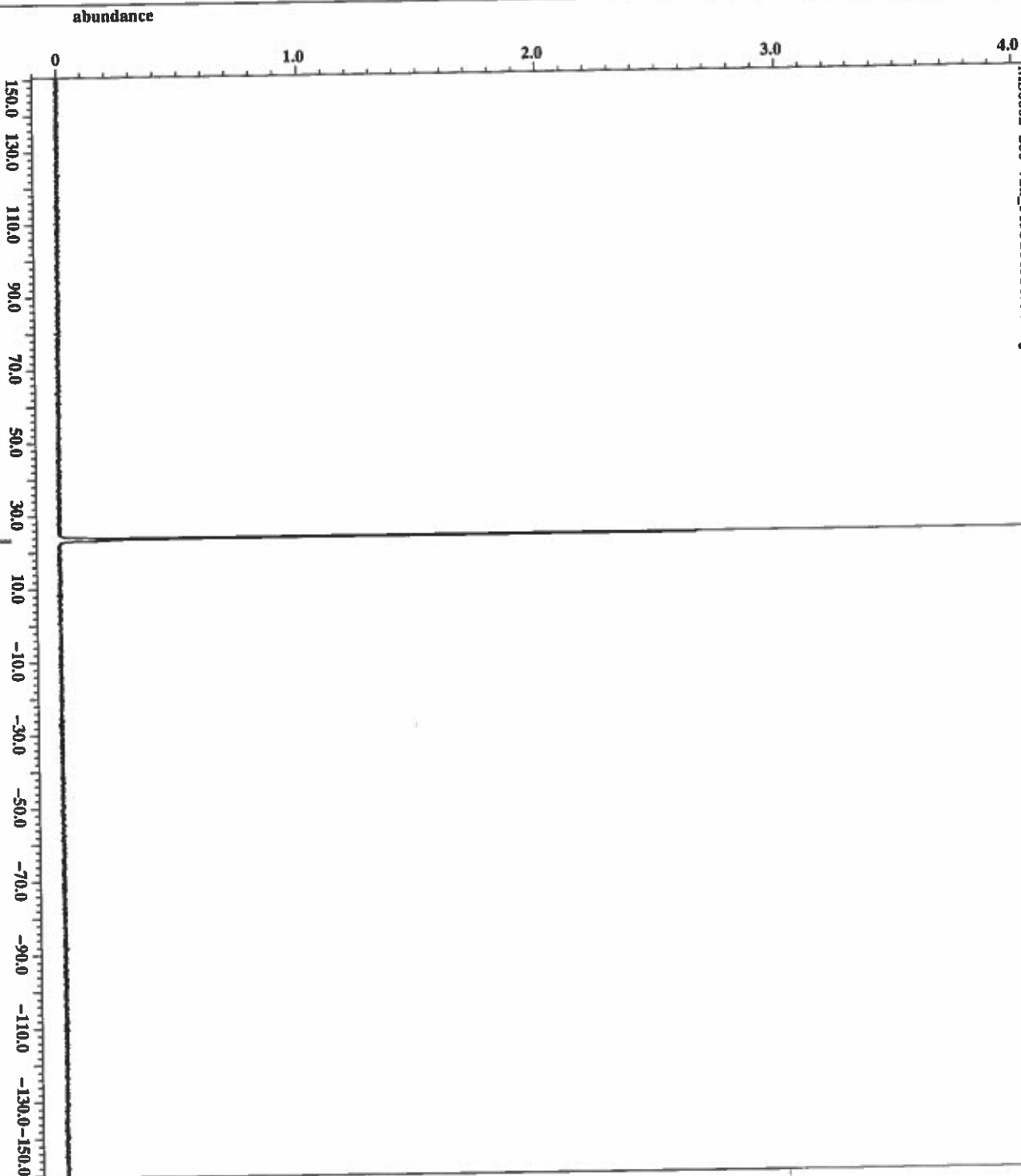
Filename = MS0602-200-72h_FLUORINE
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0602-200-72h
 Solvent = CHLOROFORM-D
 Creation_time = 8-NOV-2018 19:29:28
 Revision_time = 8-NOV-2018 19:04:45
 Current_time = 8-NOV-2018 19:04:45

Data_format = 1D COMPLEX
 Dir_size = 104857
 Dir_title = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

P101d_strength = 11.7473579 [r] (500 [kHz]
 X_acq_duration = 0.7340032 [s]
 X_domain = 19F
 X_freq = 470.62046084 [MHz]
 X_offset = -100 [ppm]
 X_points = 131072
 X_prescans = 1
 X_resolution = 1.36239186 [Hz]
 X_sweep = 178.57142857 [kHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084 [MHz]
 Irr_offset = 5 [ppm]
 Tr1_domain = 19F
 Tr1_freq = 470.62046084 [MHz]
 Tr1_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 40
 Total_scans = 40

X_90_width = 13.1 [us]
 X_acq_time = 0.7340032 [s]
 X_angle = 45 [deg]
 X_atn = 2.5 [dB]
 X_pulse = 6.55 [us]
 Irr_mode = Off
 Irr_mode = Off
 Pulse_presat = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 40
 Relaxation_delay = 4 [s]
 Repetition_time = 4.7340032 [s]
 Temp_get = 22.9 [degC]





X : parts per Million : 31P

23.8384
23.4593SOUTH ALABAMA
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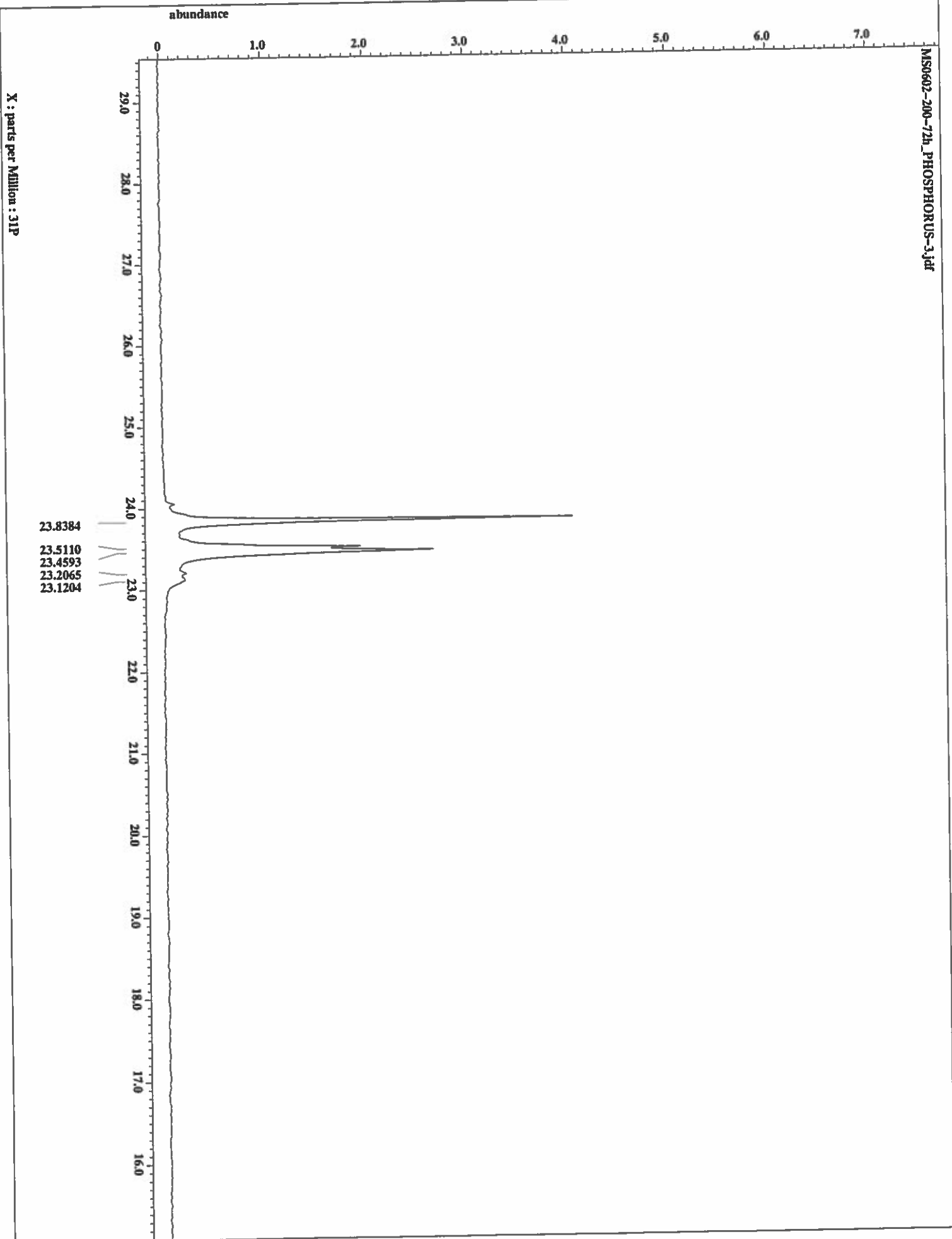
Filename      = MS0602-200-72h_PHOSPH
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0602-200-72h
Solvent       = CHLOROFORM-D
Creation_time  = 8-NOV-2018 19:34:39
Revision_time  = 8-NOV-2018 19:09:56
Current_time   = 8-NOV-2018 19:09:56

Data_format   = 1D COMPLEX
Dm_size       = 52428
Dm_cfile      = 31P
Dm_units      = [ppm]
Dimensions    = X
Site          = FCA 500
Spectrometer  = JNM-ECA500

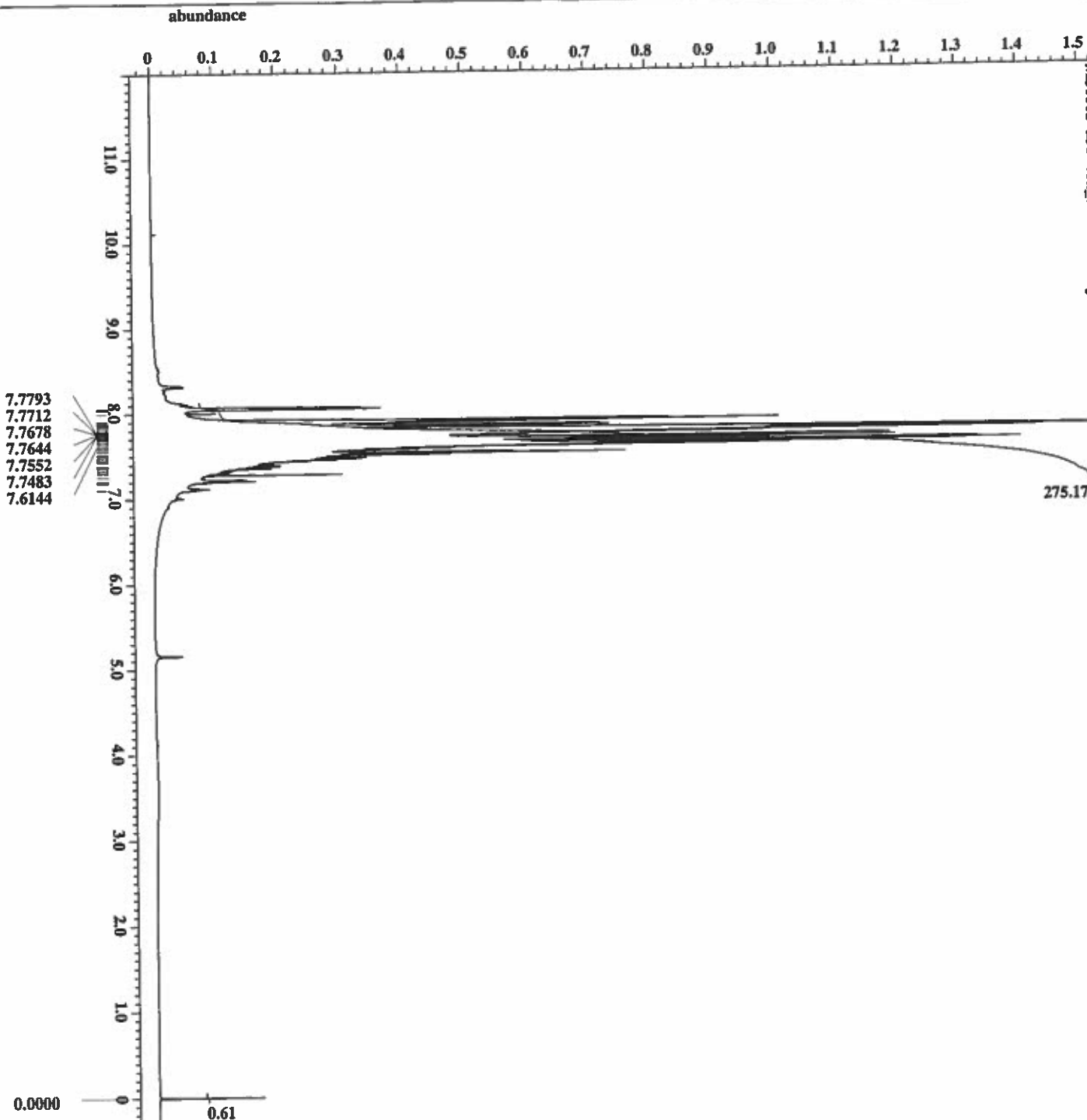
Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.85983232 [s]
X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 65536
X_prescans     = 4
X_resolution   = 1.16301746 [Hz]
X_sweep        = 76.2195122 [kHz]
X_domain      = 1H
Xrr_freq       = 500.15991521 [MHz]
Xrr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 50
Total_scans    = 50

X_90_pulch    = 14.687 [us]
X_acq_time     = 0.85983232 [s]
X_angle       = 30 [deg]
X_atn         = 5 [dB]
X_pulse       = 4.89566667 [us]
Xrr_atn_dec   = 20.7 [dB]
Xrr_atn_poe   = 20.7 [dB]
Xrr_noise     = VALVE
Decoupling     = TRIZ
Initial_wait   = 1 [s]
Noe           = TRIZ
Noe_time       = 2 [s]
Recvr_gain     = 56
Relaxation_delay = 2 [s]
Repetition_time = 2.85983232 [s]
Temp_get       = 23.2 [deg]

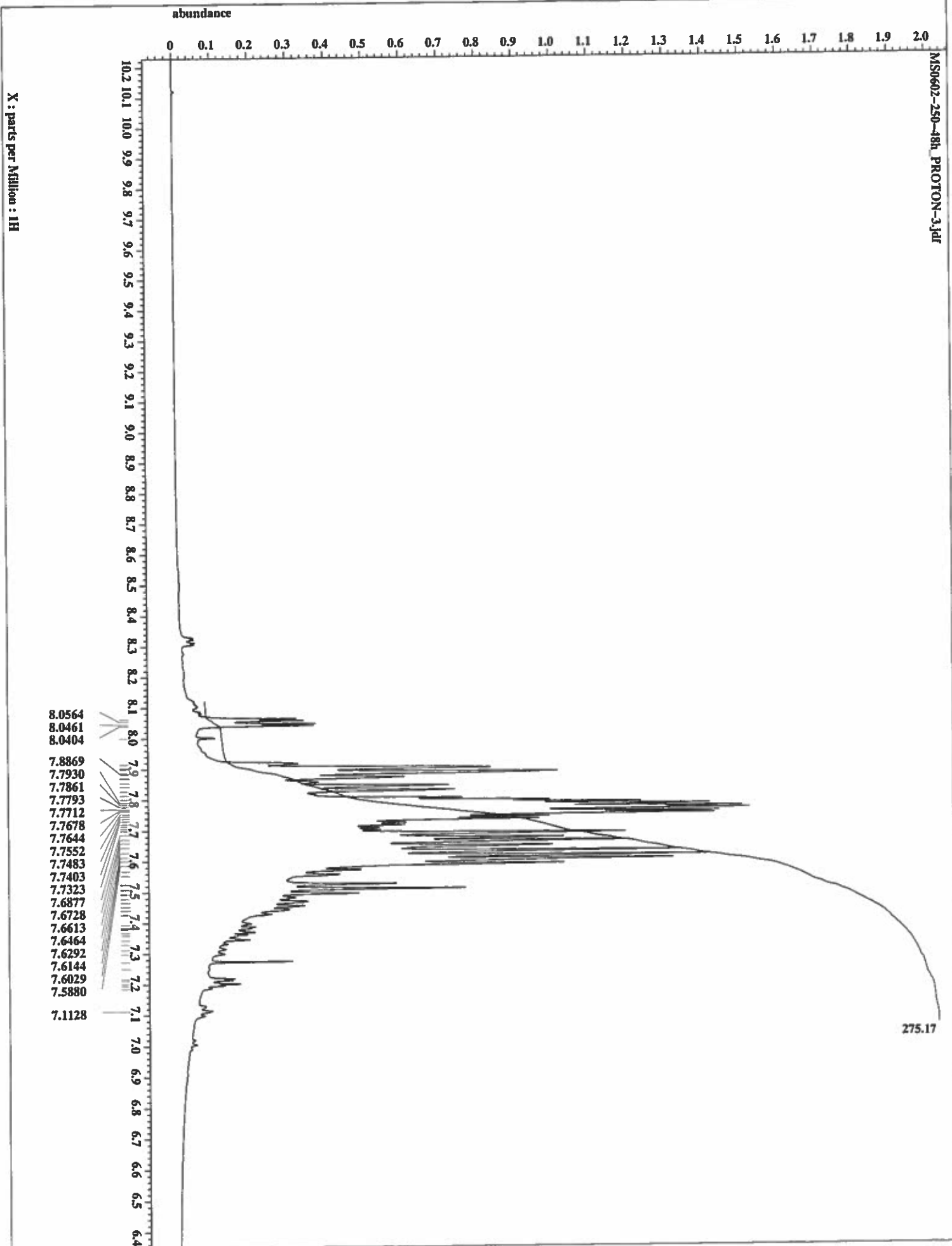
```



X: parts per Million: 1H



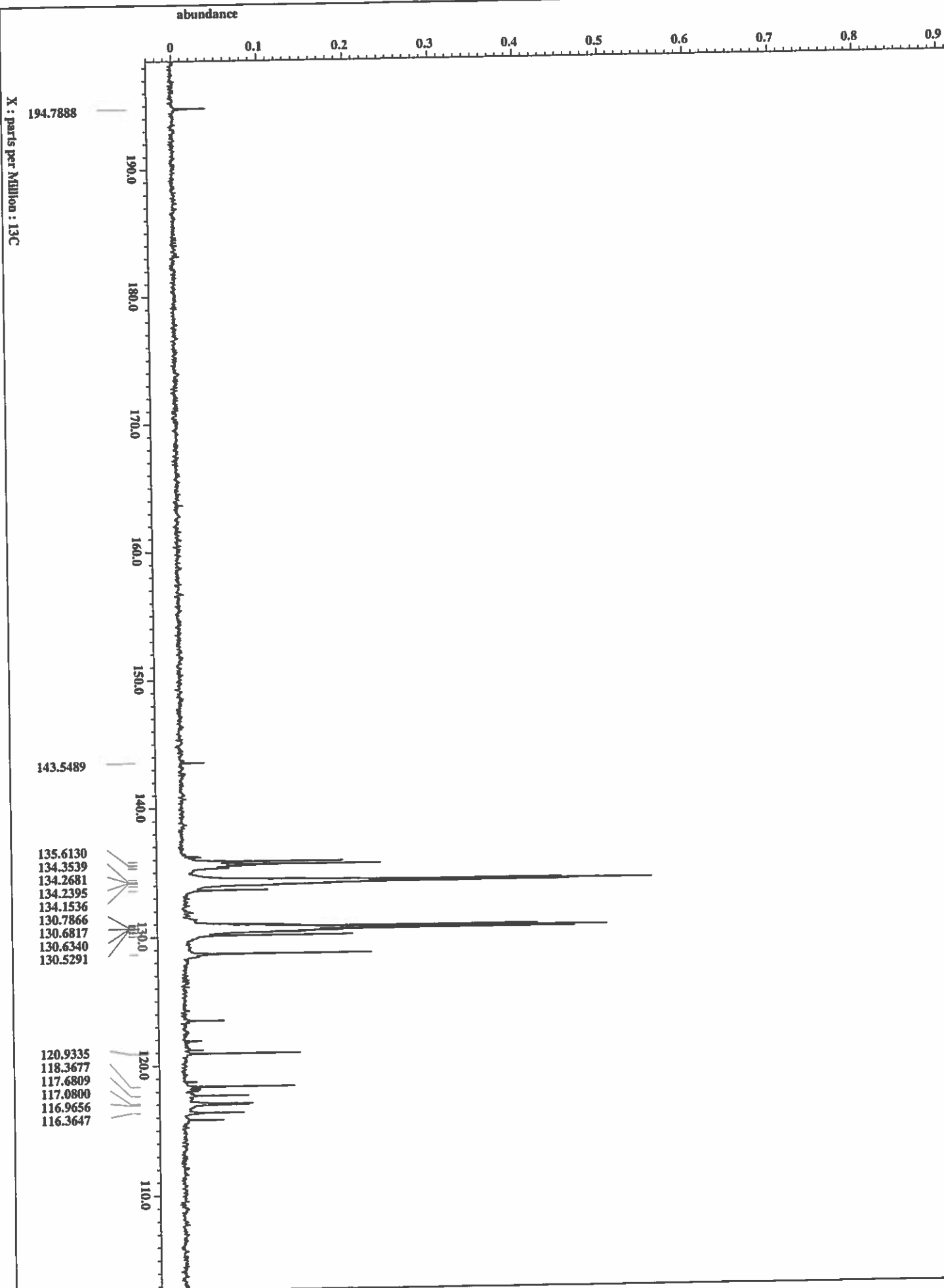
Filename	= JM0602-250-48h_PROTON
Author	= Jim Davis
Experiment	= single_pulse_wsz
Sample_id	= JM0602-250-48h
Solvent	= CHLOROFORM-D
Creation_time	= 8-NOV-2018 19:41:57
Revision_time	= 8-NOV-2018 19:17:14
Current_time	= 8-NOV-2018 19:17:14
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
X_acq_strength	= 11.7473579 [°] (500[MHz
X_acq_duration	= 1.74587904 [s]
X_domain	= 1H
X_freq	= 500.15991521 [MHz]
X_offset	= 5.0 [ppm]
X_puls1s	= 16384
X_pulses	= 1
X_prescans	= 0.57277737 [Hz]
X_resolution	= 9.384318438 [kHz]
X_sweep	= 1H
Iter_domain	= 500.15991521 [MHz]
Iter_freq	= 5.0 [ppm]
Iter_offset	= 1H
Tr1_domain	= 500.15991521 [MHz]
Tr1_freq	= 5.0 [ppm]
Tr1_offset	= PALSE
Clipped	= 1
Mod_return	= 16
Scans	= 16
Total_scans	= 16
X_90_width	= 12.4 [µs]
X_acq_time	= 1.74587904 [s]
X_angle	= 45 [deg]
X_atn	= 4 [dB]
X_pulse	= 6.2 [µs]
Tr_mode	= OF2
Tr1_mode	= OF2
Dante_presat	= PALSE
Initial_walt	= 1 [s]
Recvr_gain	= 28
Relaxation_delay	= 4 [µs]
Relaxation_time	= 5.74587904 [s]
Temp_get	= 22.8 [°C]

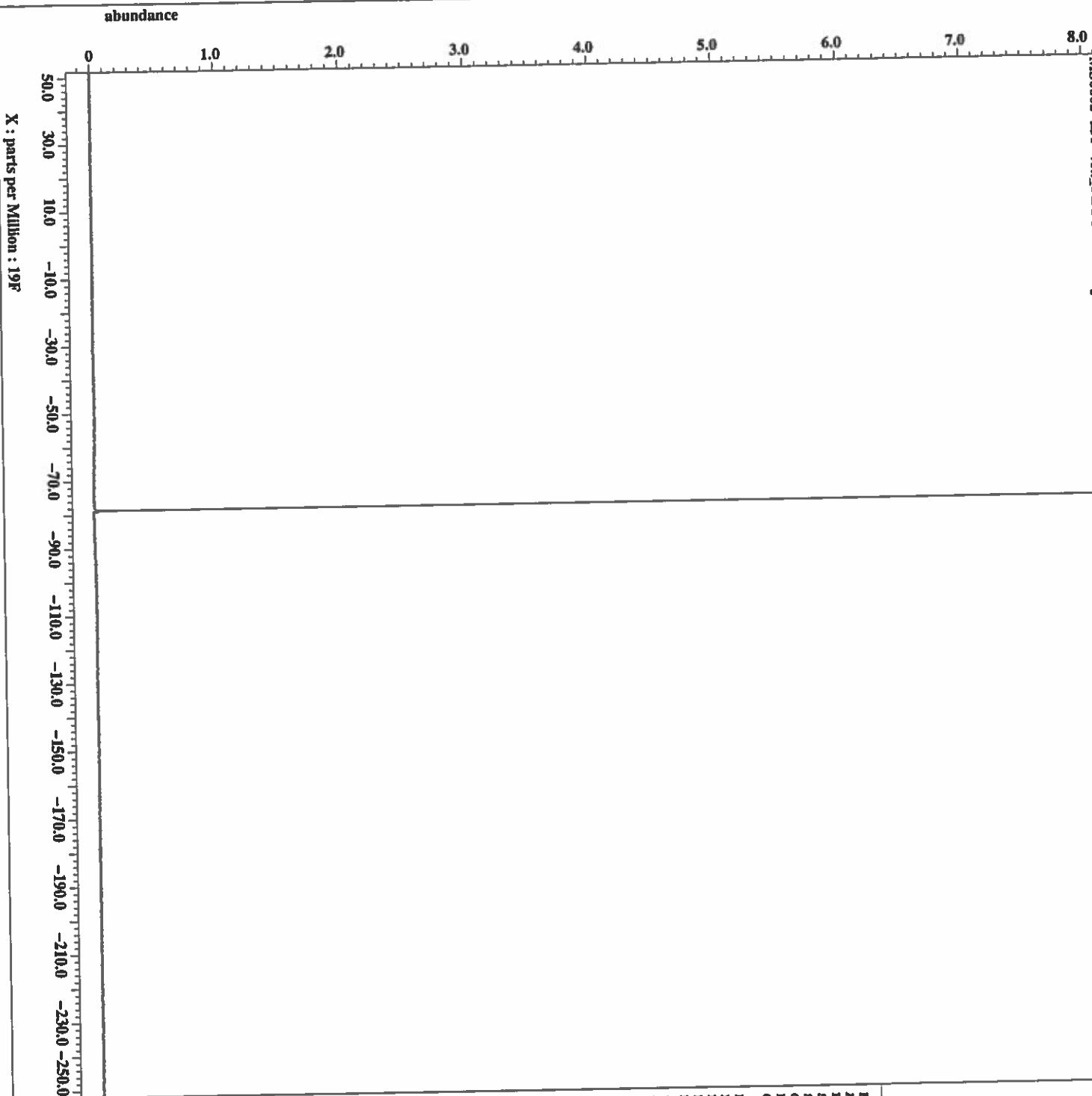




77.2480
76.7425

Filename	MS0602-250-48h_CARBON
Author	Jim Davis
Experiment	single_pulse_dec
Sample_id	MS0602-250-48h
Solvent	CHLOROFORM-D
Creation_time	8-NOV-2018 20:31:36
Revision_time	8-NOV-2018 20:06:52
Current_time	8-NOV-2018 20:06:53
Data_format	1D COMPLEX
Dir_size	26214
Dir_file	13C
Dir_units	[ppm]
Dimensions	X
Size	FCA 500
Spectrometer	JNM-ECX500
Field_strength	11.7473579 [T] (500 [MHz])
X_acq_duration	0.83361792[s]
X_domain	13C
X_freq	125.76529768 [MHz]
X_offset	100 [ppm]
X_pulses	32768
X_prescans	4
X_resolution	1.19959304 [Hz]
X_sweep	39.3081761 [kHz]
irr_domain	1H
irr_freq	500.15991521 [MHz]
irr_offset	5.0 [ppm]
Clipped	FALSE
Mod_return	1
Total_scans	1024
X_90_width	13.2 [us]
X_acq_time	0.83361792[s]
X_angle	30 [deg]
X_atn	6 [dB]
X_pulse	4.4 [us]
irr_atn_dec	20.7 [dB]
irr_atn_poe	20.7 [dB]
irr_noise	WALTZ
Decoupling	TRUZE
Initial_walt	1 [s]
Noe_time	TRUZE
Recvr_gain	21[s]
Relaxation_delay	2 [s]
Repetition_time	2.83361792[s]
Temp_get	23.3 [degC]





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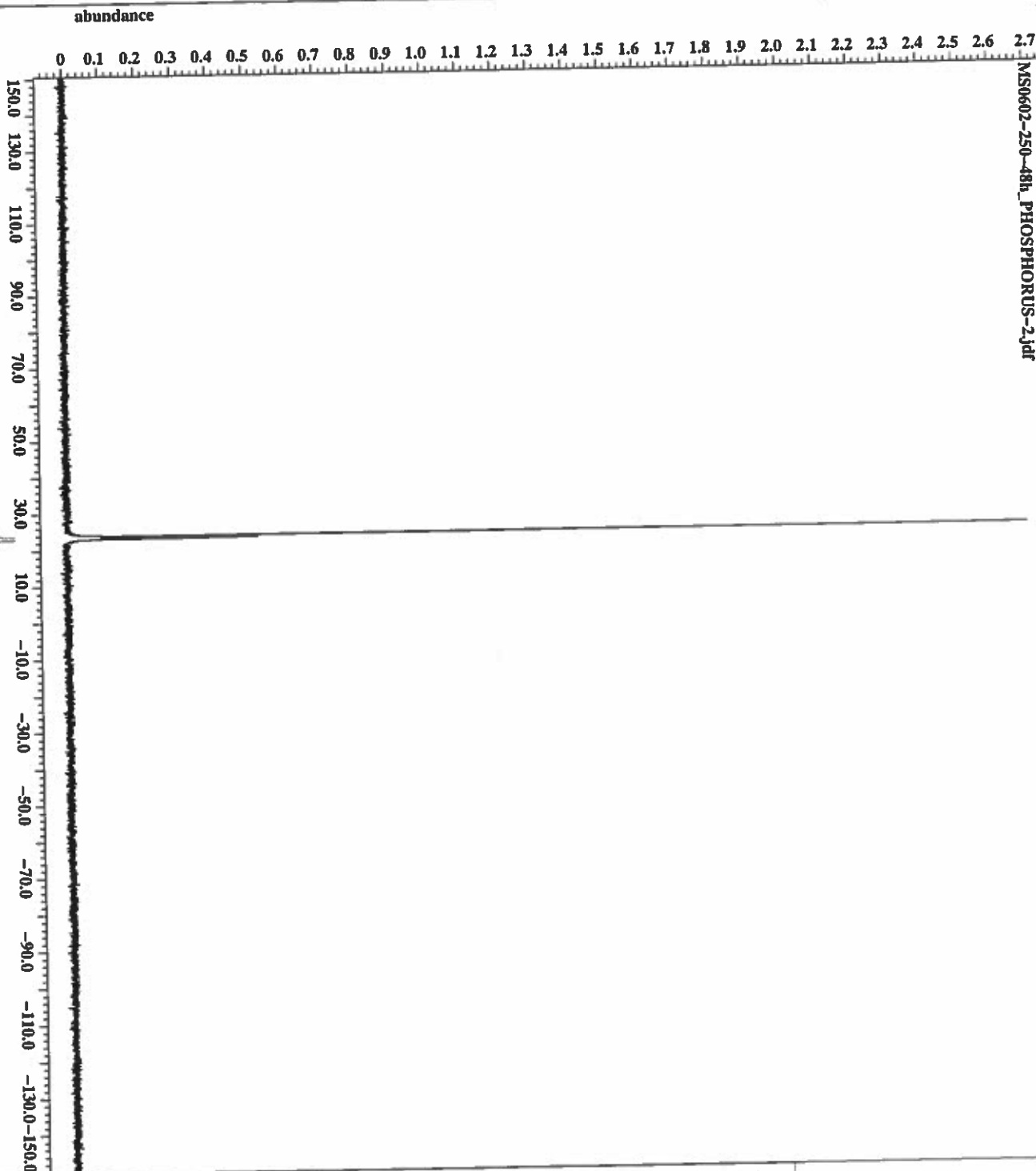
=====
Filename      = MS0602-250-48h_FLUORINE
Author        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0602-250-48h
Solvent       = CHLOROFORM-D
Creation_time  = 8-NOV-2018 20:37:30
Revision_time  = 8-NOV-2018 20:12:48
Current_time   = 8-NOV-2018 20:12:48

Data_format   = 1D COMPLEX
Dim_size      = 104857
Dir_title     = 19F
Dim_units     = (ppm)
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.7340032 [s]
X_domain       = 19F
X_freq         = 470.62046084 [MHz]
X_offset       = -100 [ppm]
X_points       = 131072
X_prescans     = 1
X_resolution   = 1.36239188 [Hz]
X_sweep        = 178.57142857 [kHz]
Xr_domain      = 19F
Xr_freq        = 470.62046084 [MHz]
Xr_offset      = 5 [ppm]
Xr1_domain     = 19F
Xr1_freq       = 470.62046084 [MHz]
Xr1_offset     = 5 [ppm]
Xr1_offset     = FALSE
Mod_return     = 1
Scans          = 40
Notch_scans    = 40

X_90_width     = 13.1 [us]
X_acq_time     = 0.7340032 [s]
X_angle        = 45 [deg]
X_atn          = 2.5 [dB]
X_pulse        = 6.55 [us]
Xr_mode        = OF
Xr1_mode       = FALSE
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 70
Relaxation_delay = 4 [s]
Repetition_time = 4.7340032 [s]
Temp_deg       = 22.8 [dC]
=====

```



X : parts per Million : 31P



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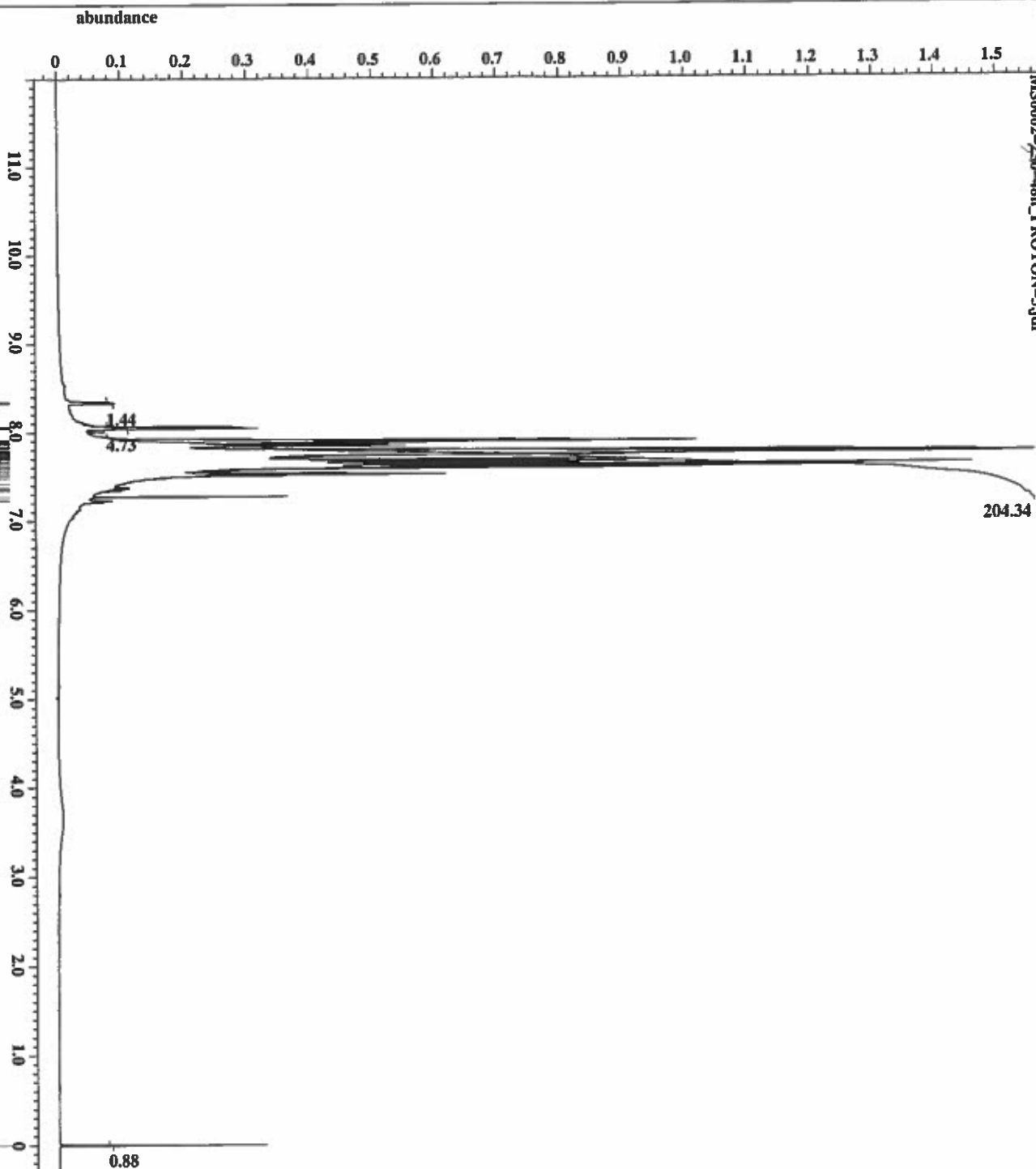
Filename      = MS0602-250-48h_PHOSPH
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0602-250-48h
Solvent       = CHLOROFORM-D
Creation_time = 8-NOV-2018 20:43:06
Revision_time = 8-NOV-2018 20:18:23
Current_time  = 8-NOV-2018 20:18:23

Data_format   = 1D COMPLEX
Dim_size      = 53428
Dir_cycle     = 31P
Dir_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECX500

P1         = 11.7473579 [s] (500 [kHz]
P2         = 0.85983232 [s]
X_domain   = 31P
X_freq     = 202.46831075 [MHz]
X_offset   = 0 [ppm]
X_points   = 65536
X_prescans = 4
X_resolution = 1.16301746 [Hz]
X_sweep    = 76.2195122 [kHz]
X_domain   = 1H
X_freq     = 500.15991521 [MHz]
X_offset   = 5.0 [ppm]
Clipped    = FALSE
Mod_return = 1
Scans      = 50
Total_scans = 50

X_90_width = 14.687 [us]
X_acq_time  = 0.85983232 [s]
X_angle     = 30 [deg]
X_atn       = 5 [db]
X_pulse     = 4.89566667 [us]
Xrtn_atn_dec = 20.7 [db]
Xrtn_atn_noe = 20.7 [db]
Xrtn_noise   = WALTZ
Decoupling   = TRUE
Initial_wait = 1 [s]
Nuc          = 31P
Nuc_time     = TRUE
Nuc_delay    = 2 [s]
Relaxation_delay = 2 [s]
Repetition_time = 2.85983232 [s]
Temp_get     = 23 [C]
  
```

8.3324
8.3267
7.7712
7.7632
7.7552
7.7483
7.6258
7.6109



X : parts per Million : 1H

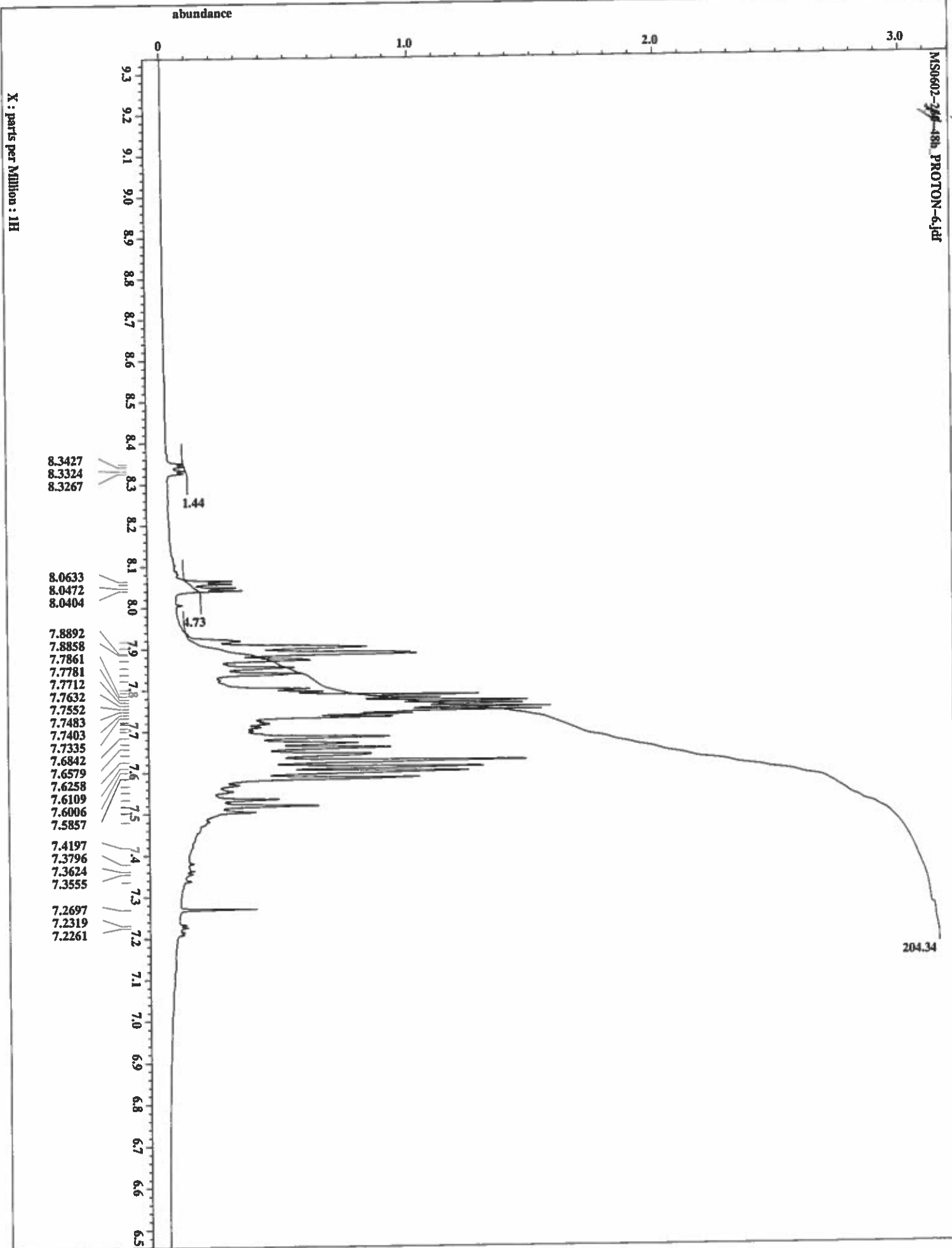


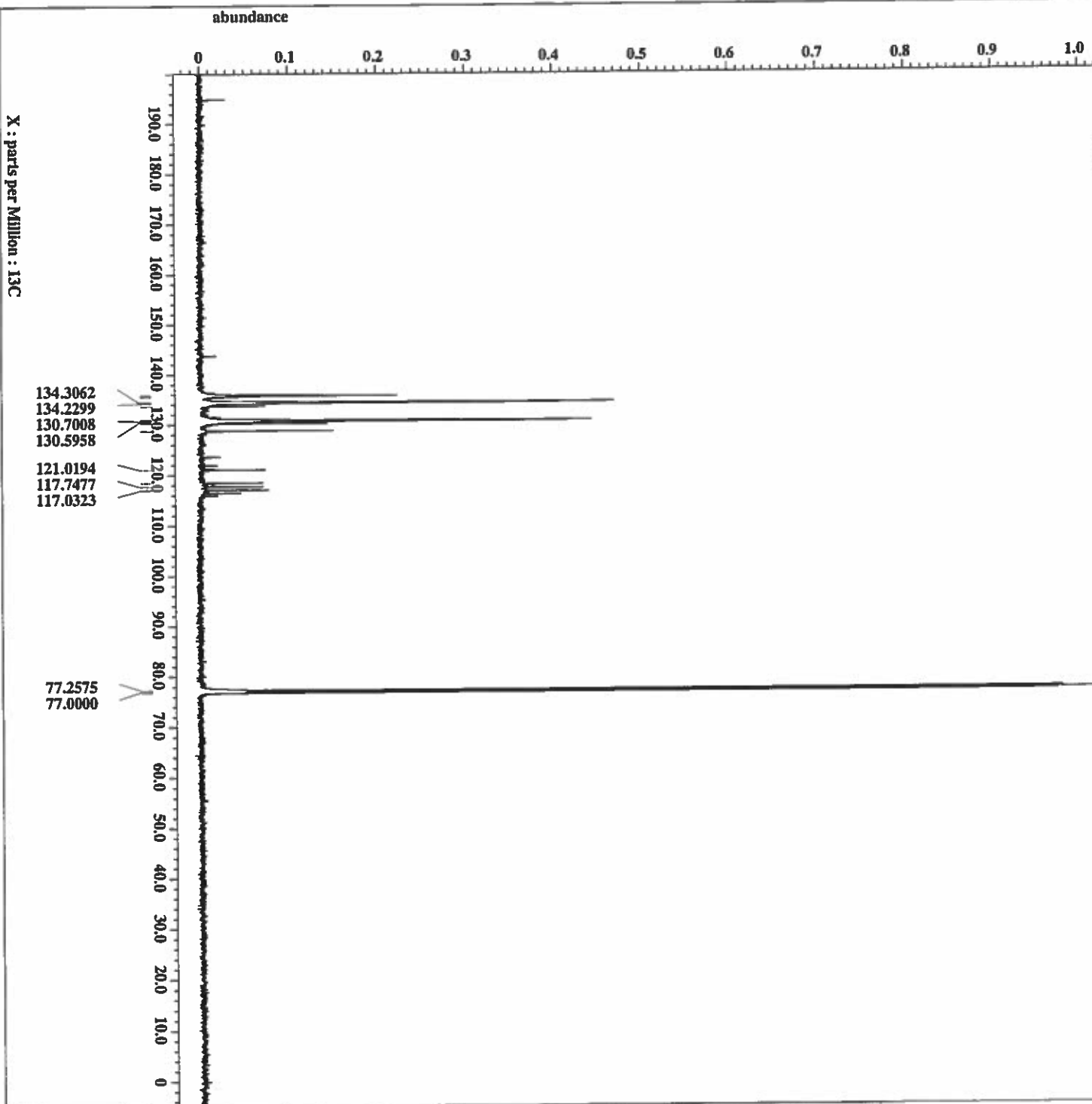
```

Filename      = MS0602-250-48h_PROTON
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = MS0602-250-48h
Solvent       = CHLOROFORM-D
Creation_time  = 8-NOV-2018 20:50:13
Revision_time = 8-NOV-2018 20:25:29
Current_time  = 8-NOV-2018 20:25:29

Data_format   = 1D COMPLEX
Dir_size      = 13107
Dir_cfile     = 1H
Dir_units     = [ppm]
Dimensions    = X
Site          = QCA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 9.38438438 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Tri_freq       = 500.15991521 [MHz]
Tri_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16
X_90_width     = 12.4 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [db]
X_pulse        = 6.2 [us]
Irr_mode       = OF2
Tri_mode       = OF2
Pulse_program  = FALST
Initial_wait   = 1 [s]
Recvr_gain     = 30
Relaxation_delay = 4 [s]
Repetition_delay = 5.74587904 [s]
Temp_get       = 22.7 [C]
  
```





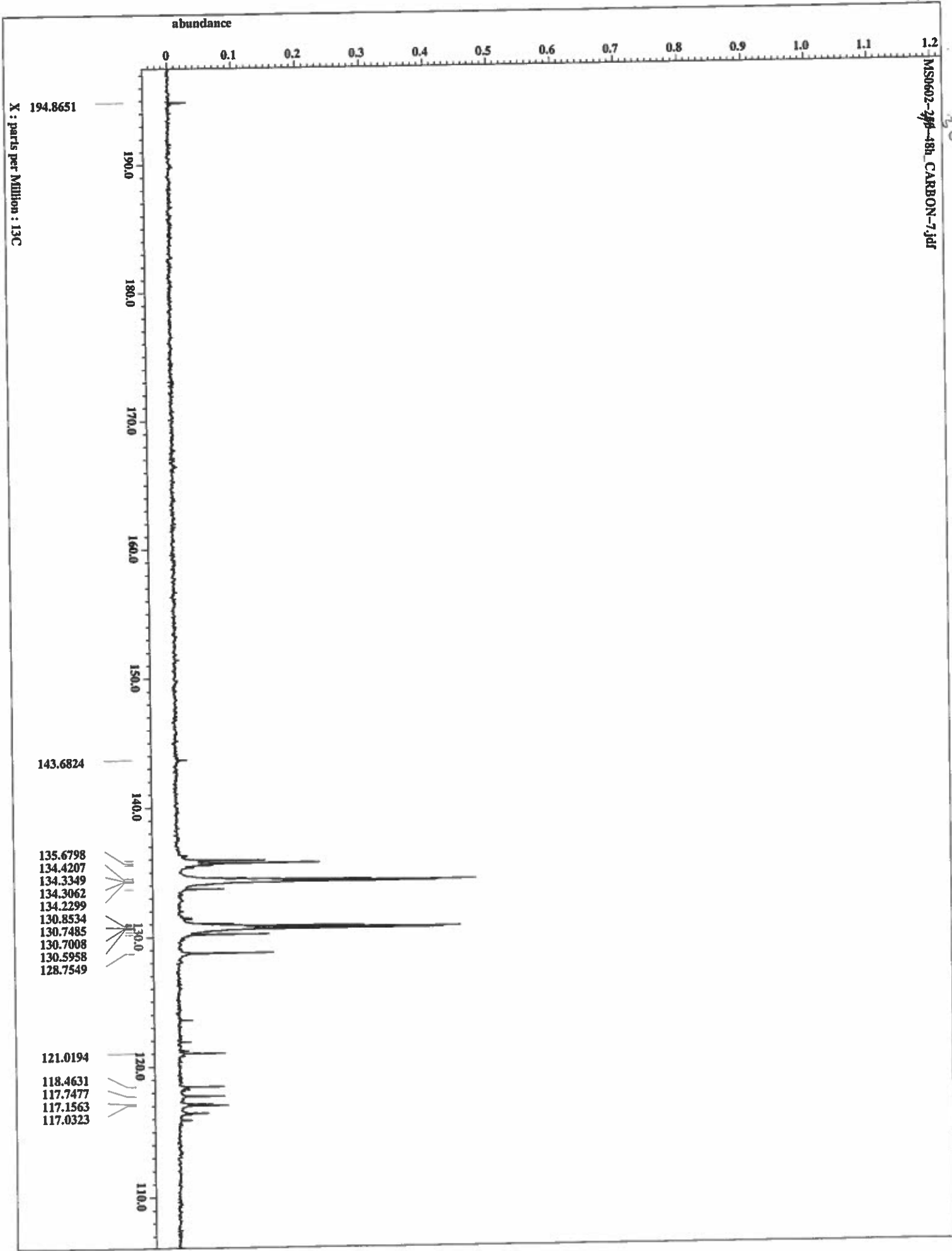
```

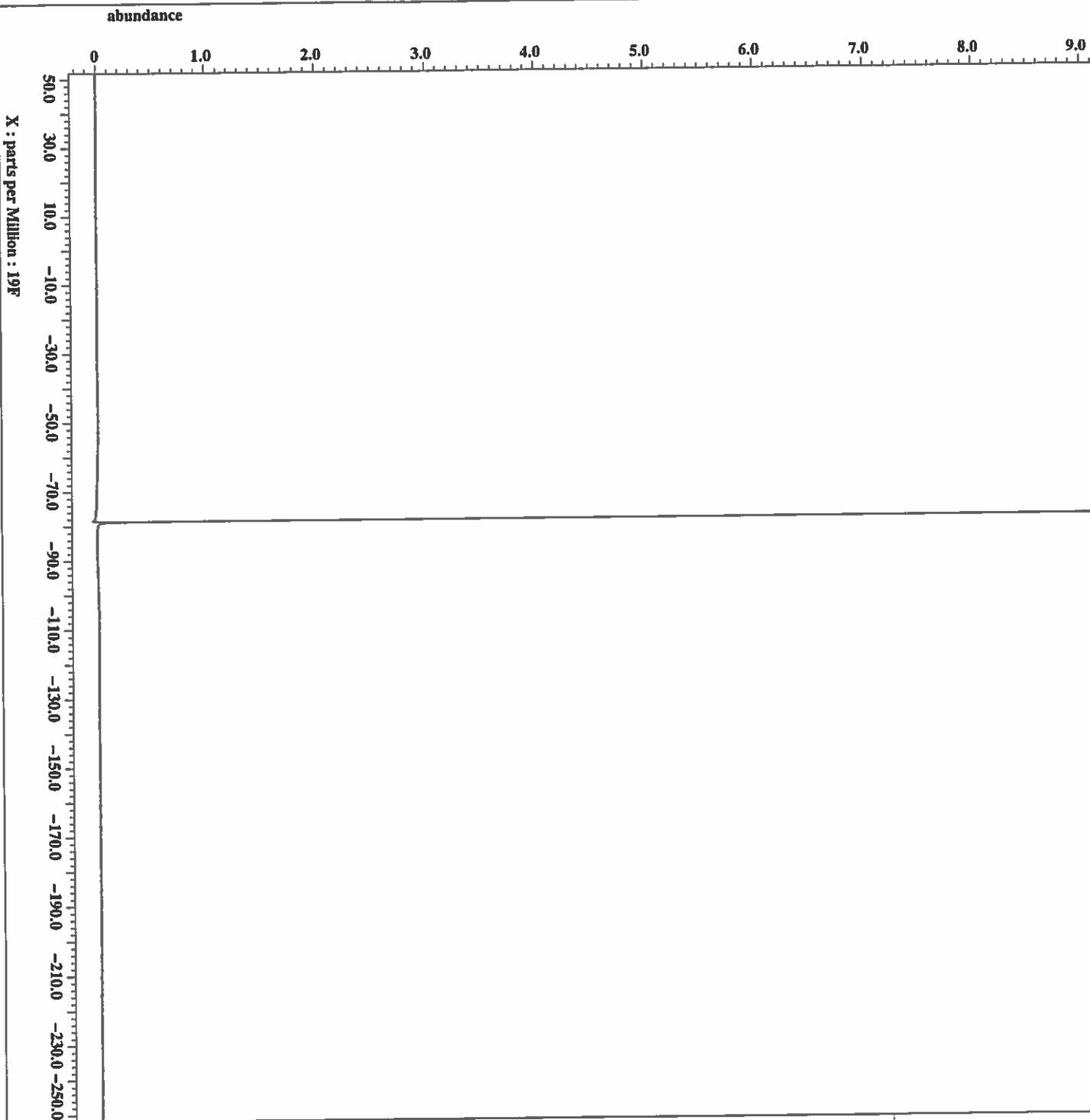
File Name      = MS0602-250-48h_CARBON
Author         = Jim Davis
Experiment     = single_pulse_dec
Sample_id      = MS0602-250-48h
Solvent        = CHLOROFORM-D
Creation_time   = 8-NOV-2018 21:39:53
Revision_time  = 8-NOV-2018 21:15:09
Current_time    = 8-NOV-2018 21:15:09

Data Format
Dim_size       = 1D COMPLEX
Dim_size       = 26214
Dim_title      = 13C
Dim_units      = [ppm]
Dimensions     = X
Site           = KCA 500
Spectrometer   = QNP-ZCA500

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]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_resolution   = FALSE
Mod_return     = 1
Scans          = 1034
Total_scans    = 1034

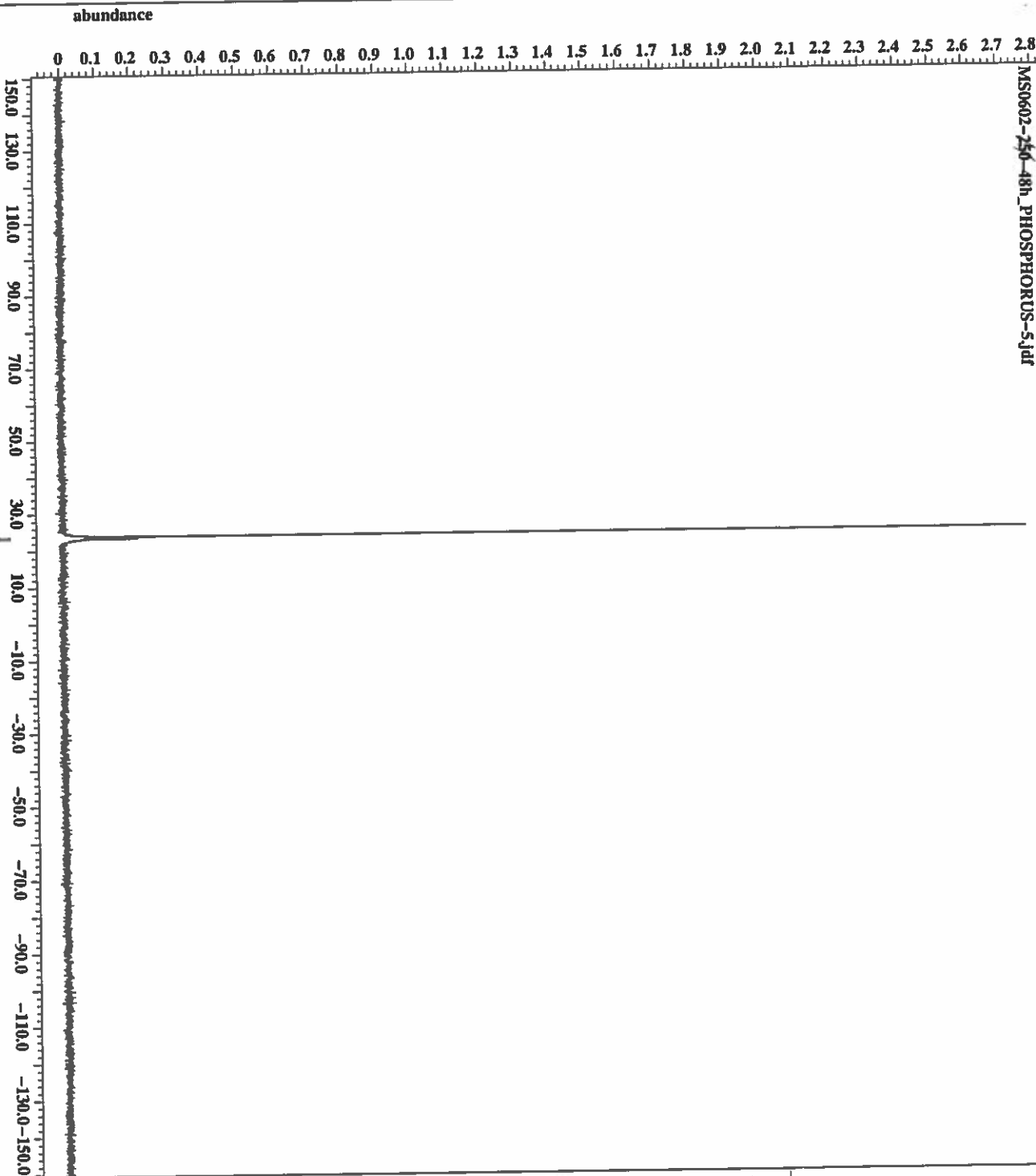
X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Xir_atn_dec    = 20.7 [dB]
Xir_atn_poe    = 20.7 [dB]
Xir_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noc            = TRUE
Noc_time       = 2 [s]
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get       = 23.1 [degC]
  
```





Filename	= MS0602-250-40h_17L0001
Author	= Jim Davis
Experiment	= single_pulse.exe2
Sample_id	= MS0602-250-40h
Solvent	= CHLOROFORM-D
Creation time	= 8-NOV-2018 21:45:50
Revision time	= 8-NOV-2018 21:21:08
Current_time	= 8-NOV-2018 21:21:08
Data_format	= 1D COMPLEX
Dim_size	= 104857
Dim_title	= 19F
Dim_units	= [ppm]
Dimensions	= X
Site	= FCA 500
Spectrometer	= JNM-ECX500
Field_strength	= 11.7473579 [T] (500 [MHz]
X_acq_duration	= 0.7340032 [s]
X_domain	= 19F
X_freq	= 470.62046084 [MHz]
X_offset	= -1001 [ppm]
X_pulses	= 131072
X_pulsescans	= 1
X_resolution	= 1.36739188 [Hz]
X_sweep	= 178.57142857 [kHz]
irf_domain	= 470.62046084 [MHz]
irf_freq	= 470.62046084 [MHz]
irf_offset	= 5 [ppm]
irf_domain	= 19F
irf_freq	= 470.62046084 [MHz]
irf_offset	= 5 [ppm]
trf_freq	= 470.62046084 [MHz]
trf_offset	= 5 [ppm]
Mod_return	= 1
Scans	= 40
Total_scans	= 40
X_90_width	= 13.1 [us]
X_acq_time	= 0.7340032 [s]
X_angle	= 45 [deg]
X_atn	= 2.5 [dB]
X_pulse	= 6.55 [us]
irf_mode	= Off
trf_mode	= Off
Dante_preset	= PALSE
Initial_wait	= 1 [s]
Recvr_gain	= 66
Relaxation_delay	= 4 [s]
Repetition_time	= 4.7340032 [s]
Temp_get	= 22.7 [degC]

300



23.8499
23.2123

X : parts per Million : 31P



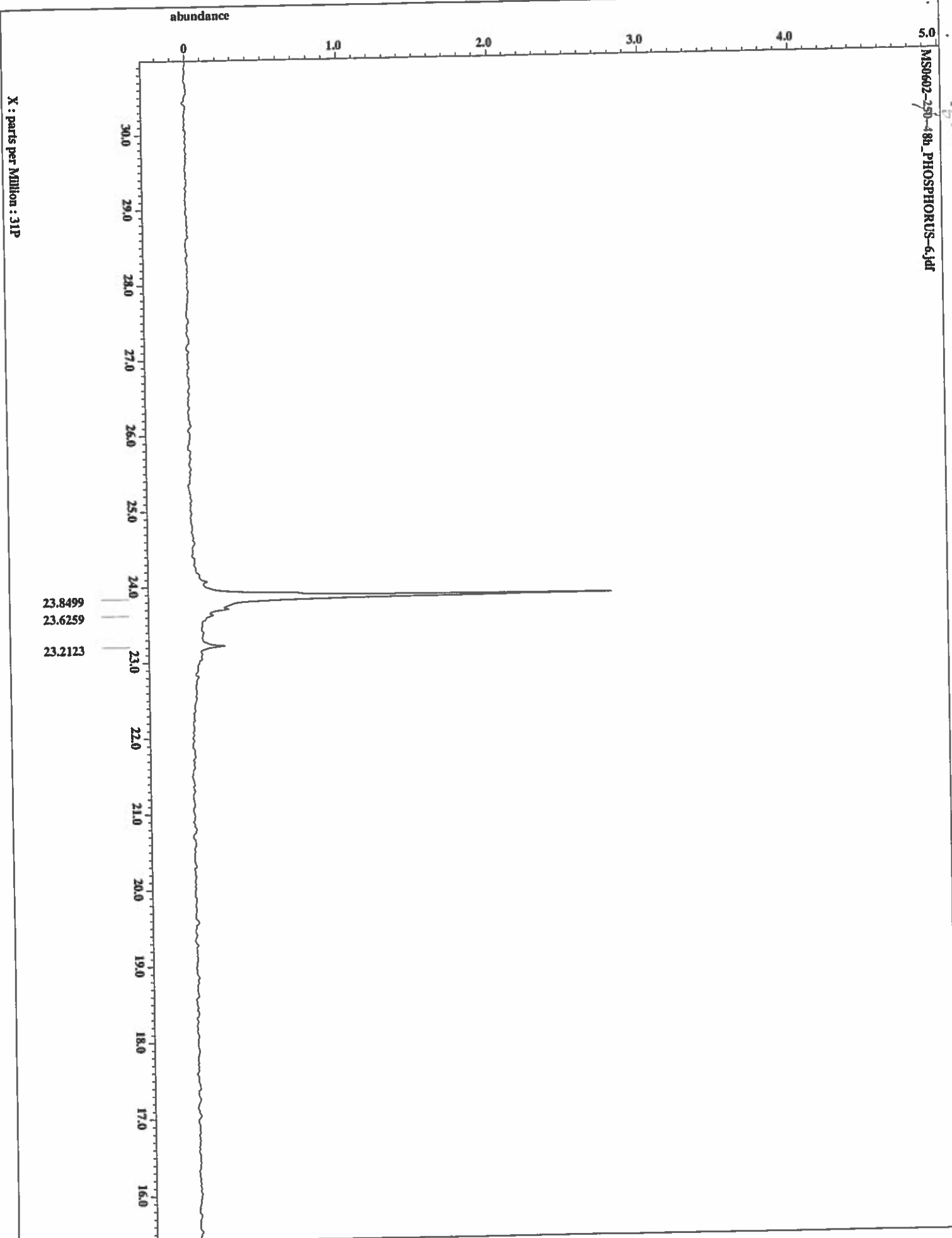
```

File Name      = MS0602-250-48h_PHOSPH
Author         = Jim Davis
Experiment     = single_pulse_dec
Sample ID      = MS0602-250-48h
Solvent        = CHLOROFORM-D
Creation Time   = 8-NOV-2018 21:50:58
Revision Time  = 8-NOV-2018 21:26:15
Current Time    = 8-NOV-2018 21:26:15

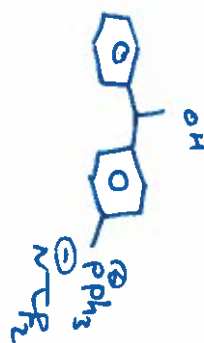
Data Format     = 1D COMPLEX
Dir Size       = 52428
Dir Title      = 31P
Dir Units      = [ppm]
Dimensions     = X
Size           = X
Spectrometer   = JNM-ECA500

Field Strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.85983332 [s]
X_domain       = 31P
X_freq         = 202.46831075 [MHz]
X_offset       = 0 [ppm]
X_points       = 65536
X_prescans     = 4
X_resolution   = 1.16301746 [Hz]
X_sweep        = 76.2195122 [Hz]
X_domain       = 18
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 50
Total_scans    = 50

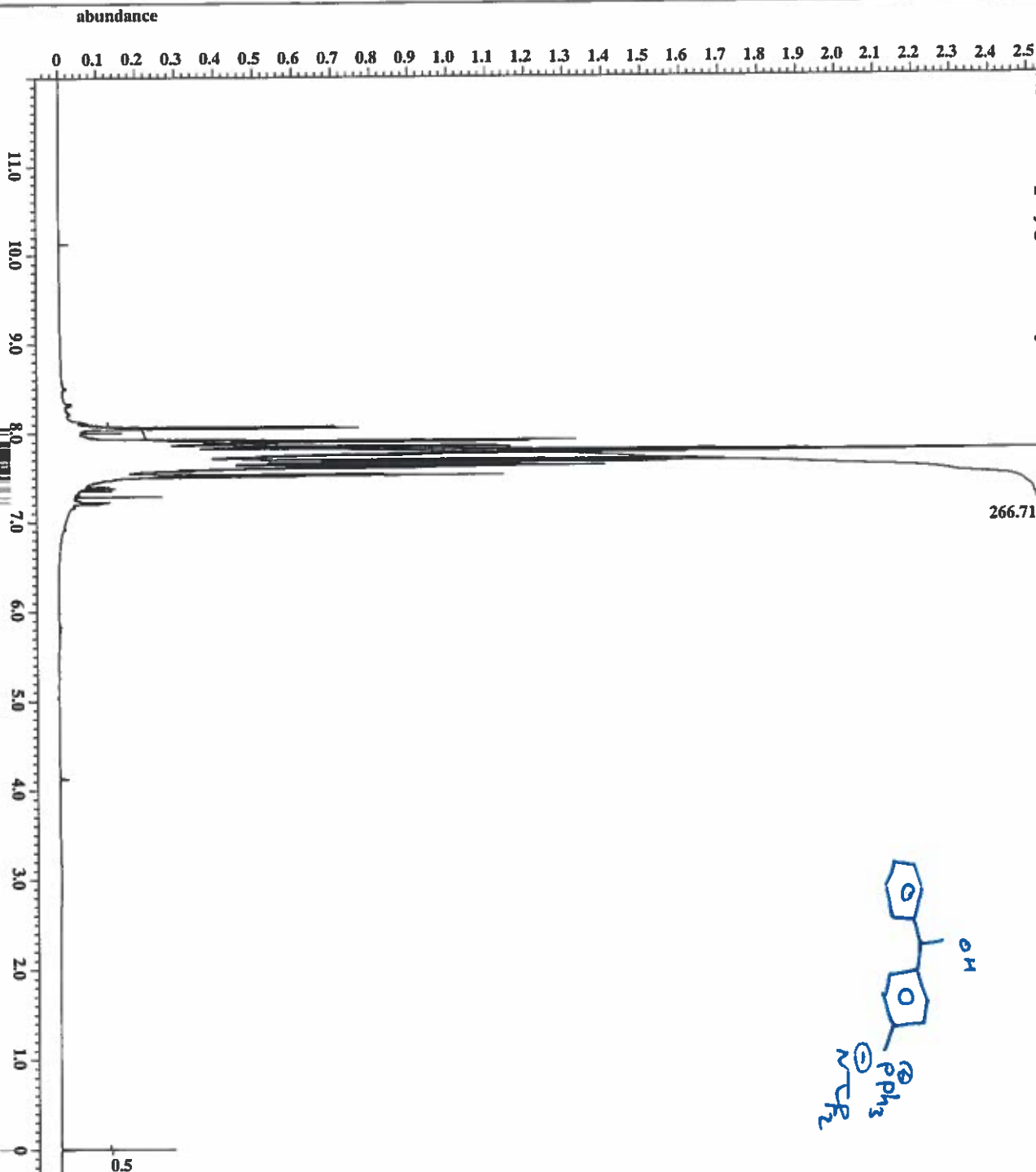
X_90_width     = 14.687 [us]
X_acq_time     = 0.85983332 [s]
X_angle        = 30 [deg]
X_atn          = 5 [dB]
X_pulse        = 4.89566667 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_pwr    = 20.7 [dB]
Irr_noise      = NALYZ
Decoupling     = TRUE
Inital_wait    = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Relaxation_delay = 58
Repetition_time = 2.85983333 [s]
Temp_set       = 23.1 [degC]
    
```



X : parts per Million : 31P



SOUTH ALABAMA
JAGUARS™

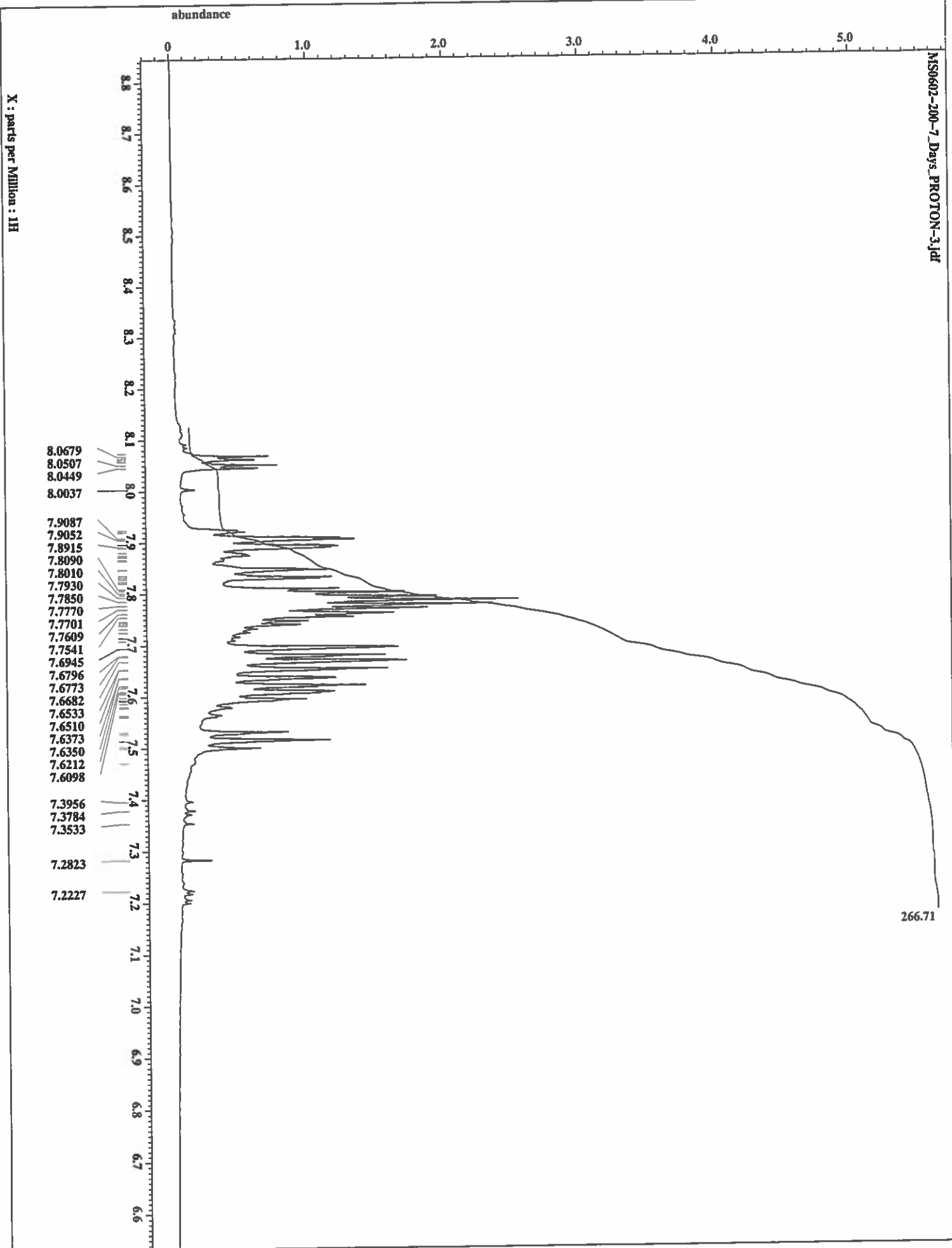


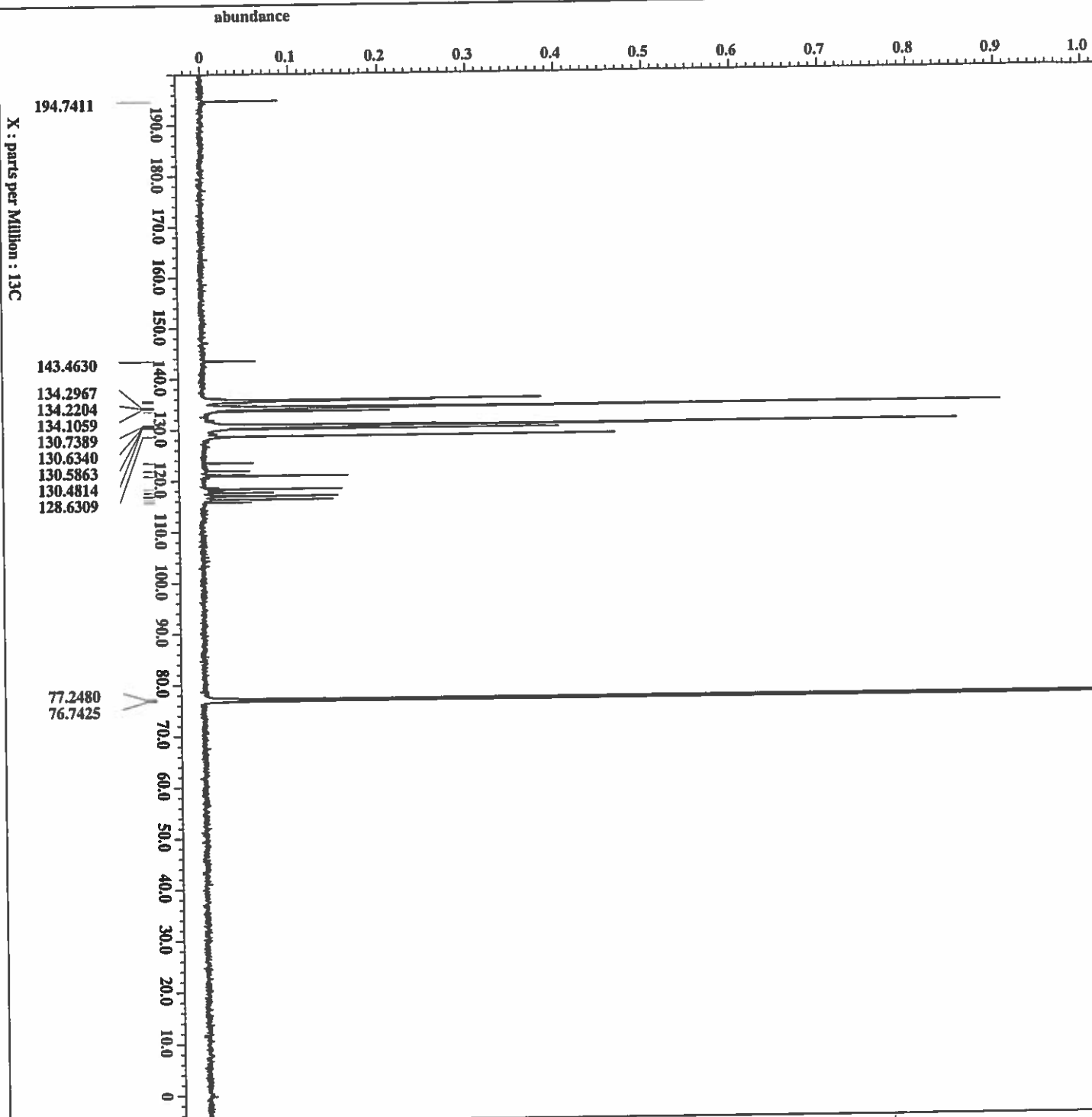
Filename = MS0602-200-7_Days_PRO
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = MS0602-200-7_Days
 Solvent = CHLOROFORM-D
 Creation_time = 19-NOV-2018 16:19:11
 Revision_time = 19-NOV-2018 15:55:02
 Current_time = 19-NOV-2018 15:55:02

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

Field_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 1.74587904 [s]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X_points = 16364
 X_prescans = 1
 X_resolution = 0.5727737 [Hz]
 X_sweep = 9.38438438 [kHz]
 Irf_domain = 1H
 Irf_freq = 500.15991521 [MHz]
 Irf_offset = 5.0 [ppm]
 Irf_domain = 1H
 Irf_freq = 500.15991521 [MHz]
 Irf_offset = 5.0 [ppm]
 C1ipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 12.4 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_atn = 4 [db]
 X_pulse = 6.2 [us]
 Irf_mode = OF
 Irf_mode = OF
 Dante_preset = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 26
 Relaxation_delay = 4 [s]
 Repetition_delay = 5.74587904 [s]
 Temp_get = 21.5 [C]





```

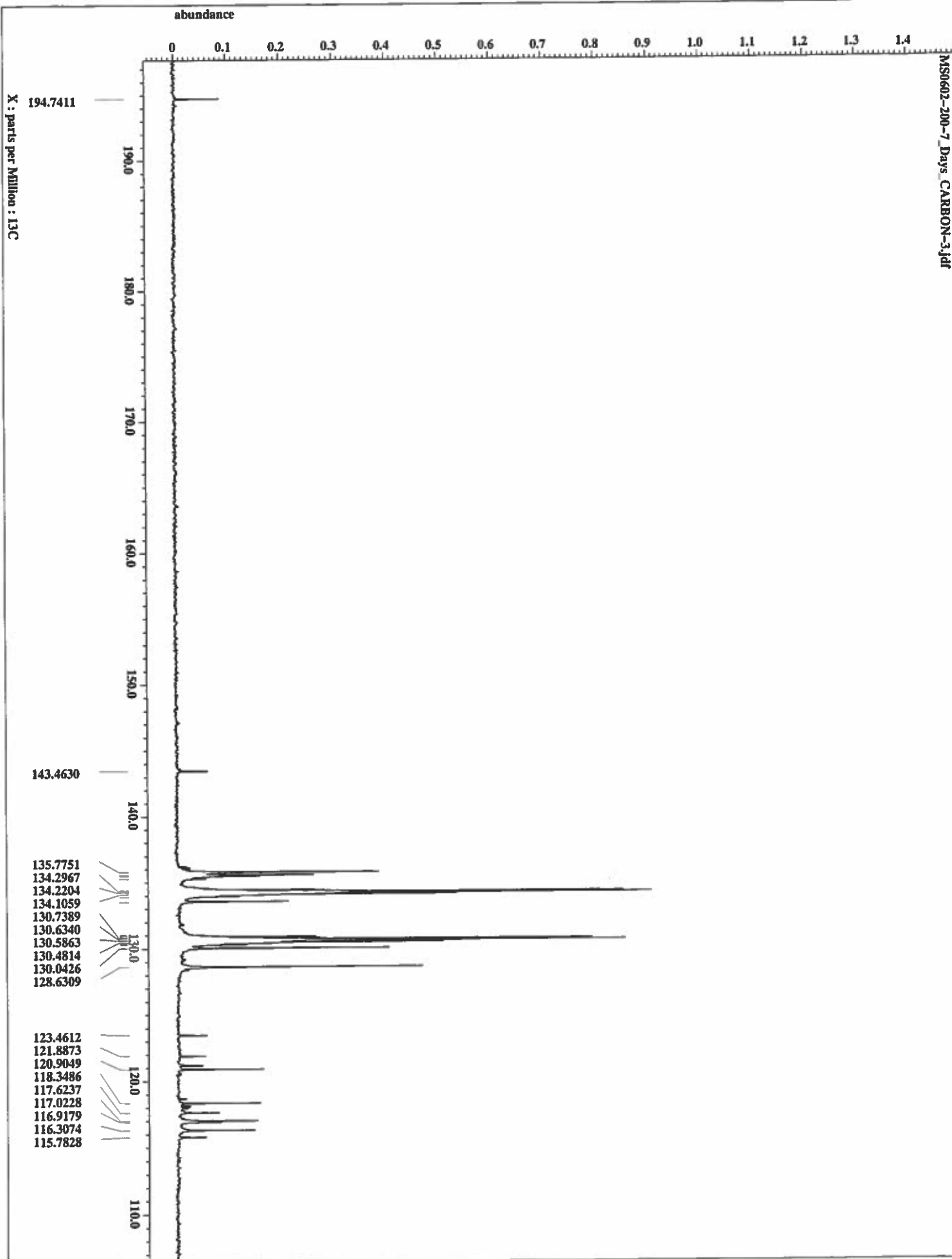
=====
Filename      = MS0602-200-7_Days_CAR
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = MS0602-200-7_Days
Solvent       = CHLOROFORM-D
Creation_time = 20-NOV-2018 00:22:06
Revision_time = 19-NOV-2018 23:57:56
Current_time  = 19-NOV-2018 23:57:56

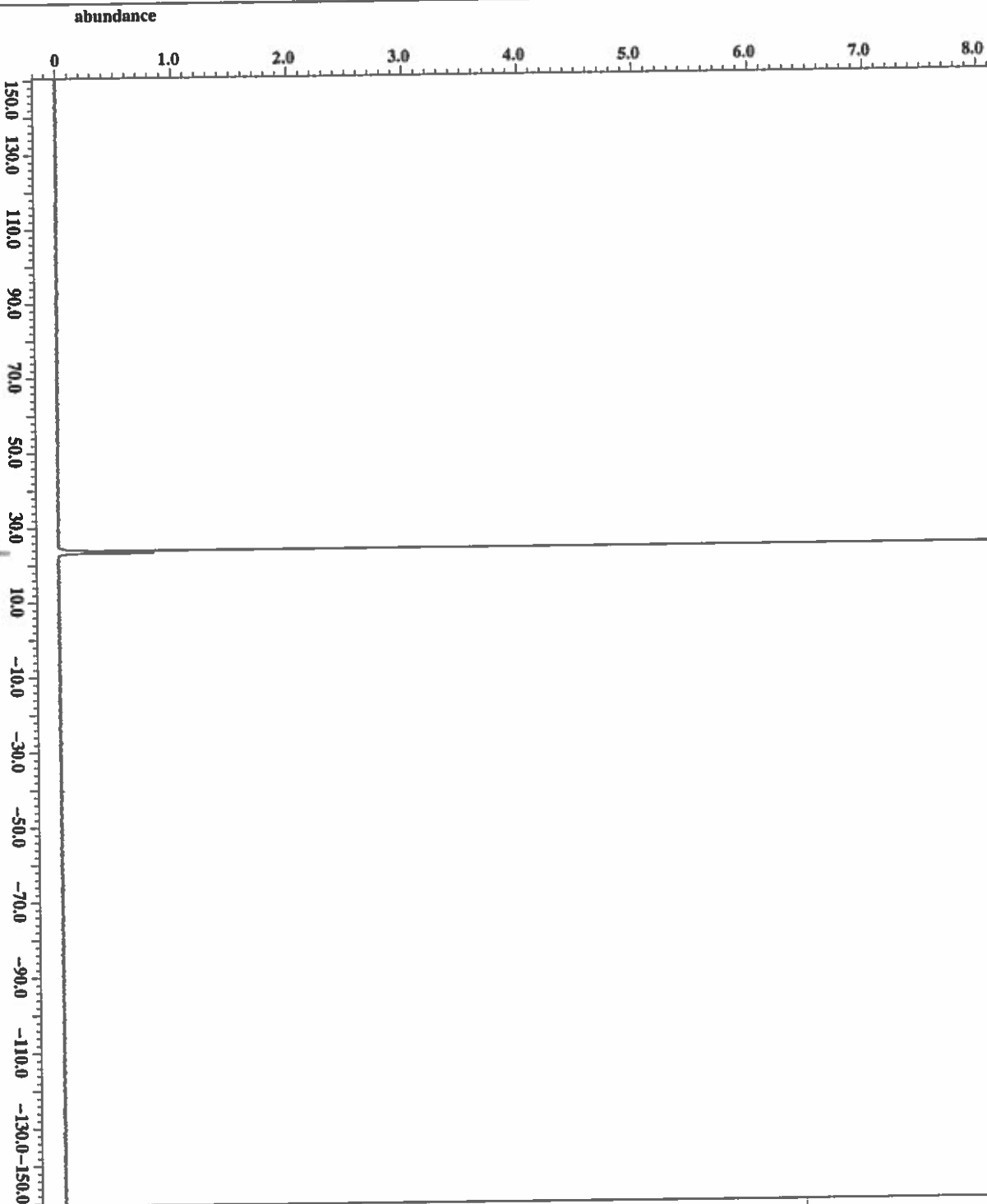
Data_format   = 1D COMPLEX
Dir_size      = 26214
Dir_ctitle    = 13C
Dir_units     = [ppm]
Dimensions    = X
Sfsize        = X
Sfcount       = RCA 500
Sfunit        = DMF-ECA500

Field_strength = 11.7473579 [T] (500 [MH
Acq_duration   = 0.83361792 [s]
Domain         = 13C
Freq           = 125.76529766 [MHz]
Offset         = 100 [ppm]
Points         = 32768
Prescans       = 4
Rescans        = 1.19959034 [Hz]
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     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
Irr_atn_dec    = 20.7 [dB]
Irr_atn_noe    = 20.7 [dB]
Irr_noise      = KALFZ
Decoupling     = TRUZ
Initial_wait   = 1 [s]
Noe            = TRUZ
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set       = 22.5 [deg]
=====

```





Filename MS0602-200-7_Days_PRO
 Author Jim Davis
 Experiment single_pulse_dec
 Sample_id MS0602-200-7_Days
 Solvent CHLOROFORM-D
 Creation_time 19-NOV-2018 16:28:59
 Revision_time 19-NOV-2018 16:04:50
 Current_time 19-NOV-2018 16:04:50

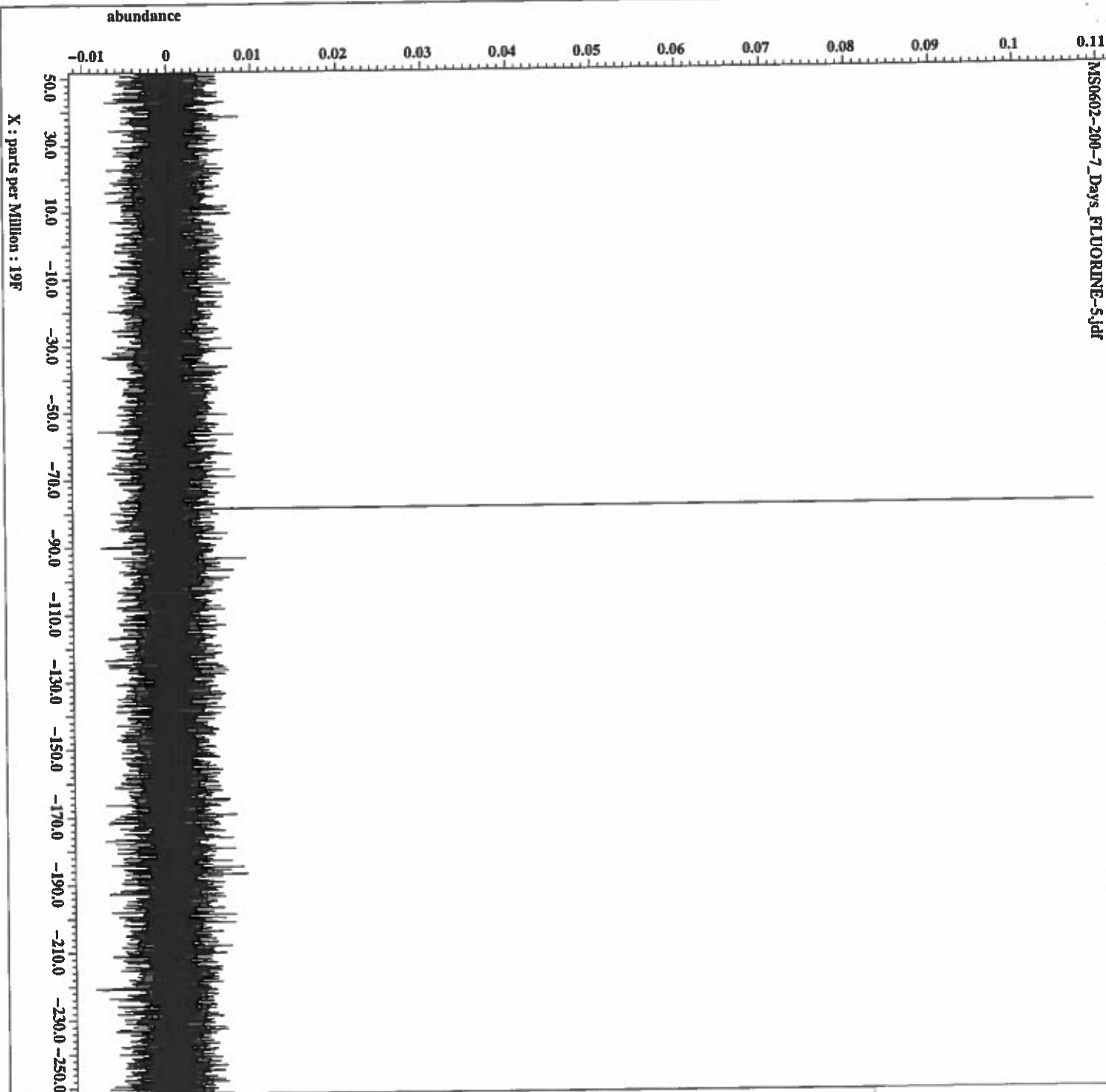
 Data_format 1D COMPLEX
 Dim_size 52428
 Dim_title 31P
 Dim_units [ppm]
 Dimensions X
 Site ECA 500
 Spectrometer JNM-ECA500

 Field_strength 11.7473579 [T] (500 [MH
 X_acq_duration 0.85983232 [s]
 X_domain 31P
 X_freq 202.46831075 [MHz]
 X_offset 0 [ppm]
 X_points 65336
 X_prescans 4
 X_resolution 1.16301746 [Hz]
 X_sweep 76.2195122 [kHz]
 Irr_domain 1H
 Irr_freq 500.15991521 [MHz]
 Irr_offset 5.0 [ppm]
 Clipped FALSE
 Mod_return 1
 Scans 40
 Total_scans 40

 X_90_width 14.687 [us]
 X_acq_time 0.85983232 [s]
 X_angle 30 [deg]
 X_atn 5 [dB]
 X_pulse 4.89566667 [us]
 Irr_atn_dec 20.7 [dB]
 Irr_atn_noe 20.7 [dB]
 Irr_noise WALTZ
 Decoupling TRU2
 Initial_wait 1 [s]
 Noe_time TRU2
 Recvr_gain 2 [s]
 Relaxation_delay 58
 Repetition_time 2.85983232 [s]
 Temp_get 23 [deg]

23.8327
23.1951

X : parts per Million : 31P



```

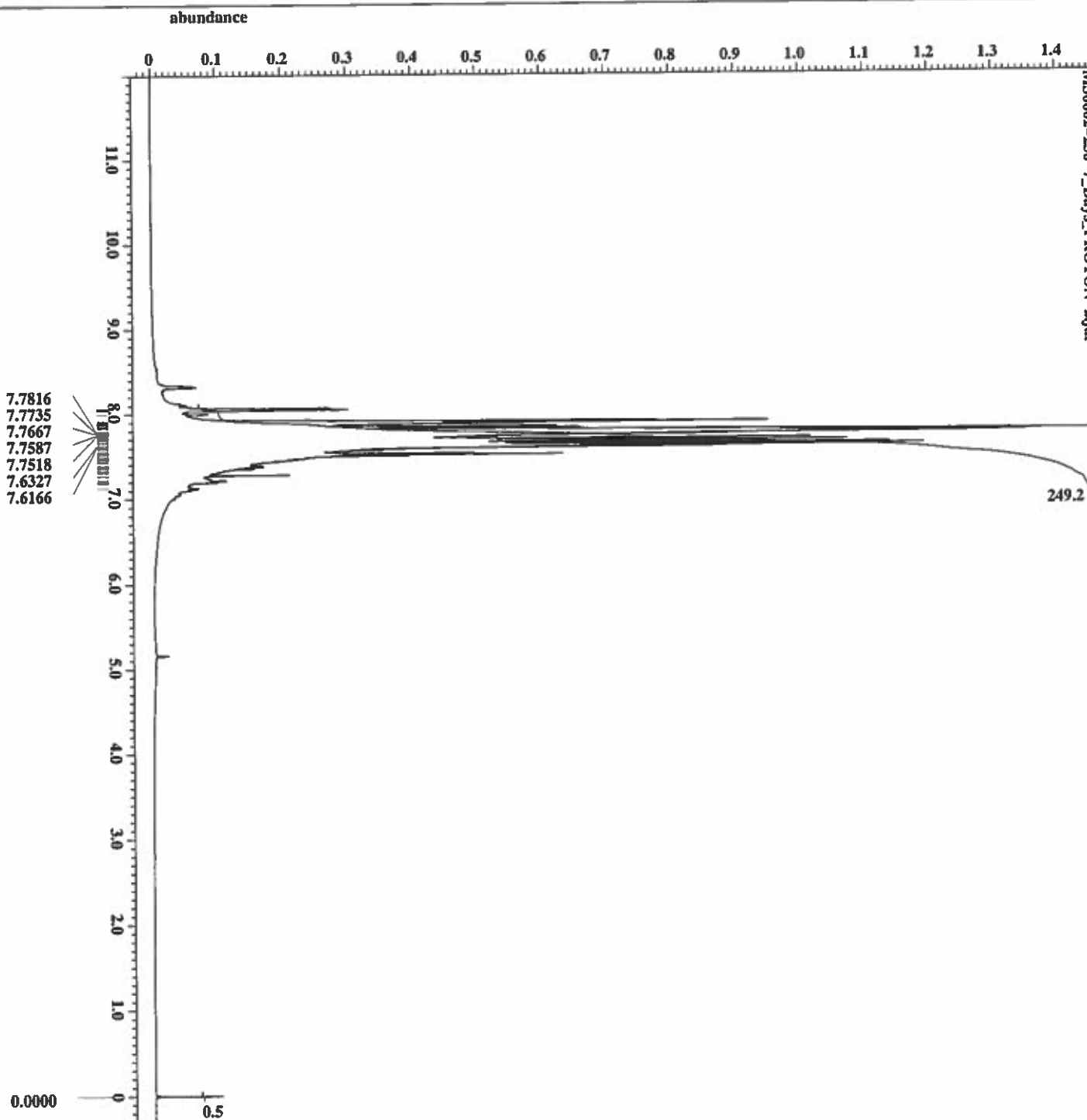
File Name      MS0602-200-7_Days_FLU
Author         Jim Davis
Experiment     single_pulse.exe
Sample_id      MS0602-200-7_Days
Solvent        CHLOROFORM-D
Creation time  20-NOV-2018 09:27:54
Revision time  20-NOV-2018 09:03:42
Current time   20-NOV-2018 09:03:43

Data Format
Data_size     = 1D COMPLEX
Dim_size      = 104857
Dim_title     = 19F
Dim_units     = [ppm]
Dimensions    = X
Site          = RCA 500
Spectrometer  = DNM-RCA500

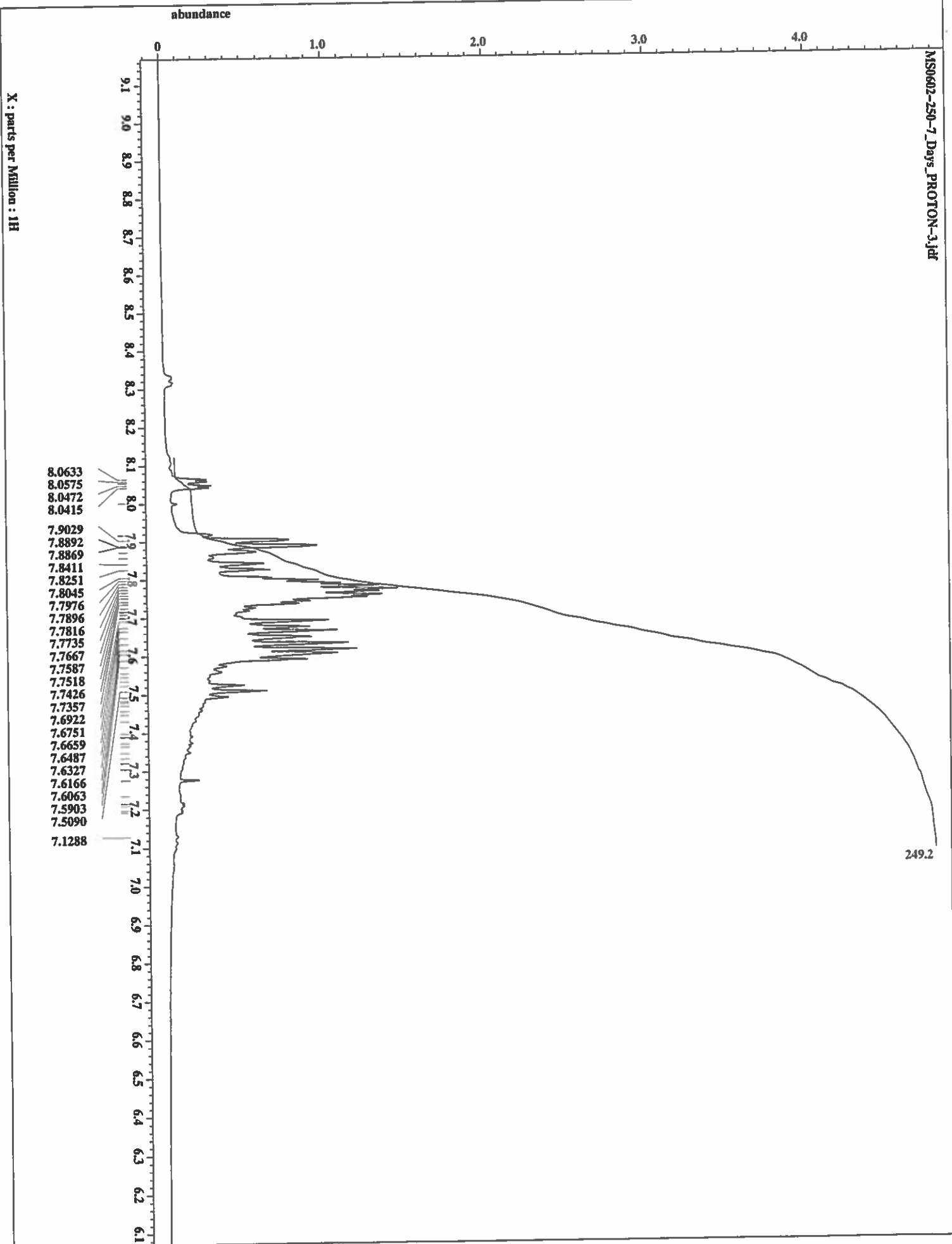
Field_strength 11.7473579 [T] (500 [MH
X_acq_duration 0.7340032 [s]
X_domain       = 19F
X_freq         = 470.62046084 [MHz]
X_offset       = -100 [ppm]
X_points       = 131072
X_prescans     = 1
X_resolution   = 1.36239188 [Hz]
X_sweep        = 178.57142857 [kHz]
X_domain      = 19F
Xir_freq       = 470.62046084 [MHz]
Xir_offset     = 19F
Xir_domain     = 19F
Xir_offset     = 5 [ppm]
Xir_freq       = 470.62046084 [MHz]
Xir_offset     = 5 [ppm]
Xir_domain     = FALSE
Clipped        = 1
Mod_return     = 128
Scans          = 128
Total_scans    = 128

X_90_width     = 13.1 [us]
X_acq_time     = 0.7340032 [s]
X_angle        = 45 [deg]
X_atn          = 2.5 [db]
X_pulse        = 6.55 [us]
Xir_pulse      = OFF
Xir_mode       = FALSE
Dante_presat   = 1 [s]
Initial_wait   = 70
Recvr_gain     = 4 [s]
Relaxation_delay = 4.7340032 [s]
Redetection_time = 21.9 [dc]
Temp_get       = 21.9 [dc]

```



Filename	= MS0602-250-7_Days_PRO
Author	= Jim Davis
Experiment	= single_pulse.exe2
Sample_id	= MS0602-250-7_Days
Solvent	= CHLOROFORM-D
Creation_time	= 19-NOV-2018 16:36:25
Revision_time	= 19-NOV-2018 16:12:14
Current_time	= 19-NOV-2018 16:12:14
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579 [T] (500 [MHz]
X_acq_duration	= 1.74587904 [s]
X_domain	= 1H
X_freq	= 500.15991521 [MHz]
X_offset	= 5.0 [ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.5727797 [Hz]
X_sweep	= 9.38638648 [kHz]
Ir1_domain	= 1H
Ir1_freq	= 500.15991521 [MHz]
Ir1_offset	= 5.0 [ppm]
Tr1_domain	= 1H
Tr1_freq	= 500.15991521 [MHz]
Tr1_offset	= 5.0 [ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 12.4 [us]
X_acq_time	= 1.74587904 [s]
X_angle	= 45 [deg]
X_atn	= 4 [dB]
X_pulse	= 6.2 [us]
Ir1_mode	= O22
Tr1_mode	= O22
Dante_preset	= PALSE
Initial_valt	= 1 [s]
Recvr_gain	= 26
Relaxation_delay	= 4 [s]
Relaxation_time	= 5.74567904 [s]
Temp_get	= 21.7 [C]



abundance

X : parts per Million : 19F



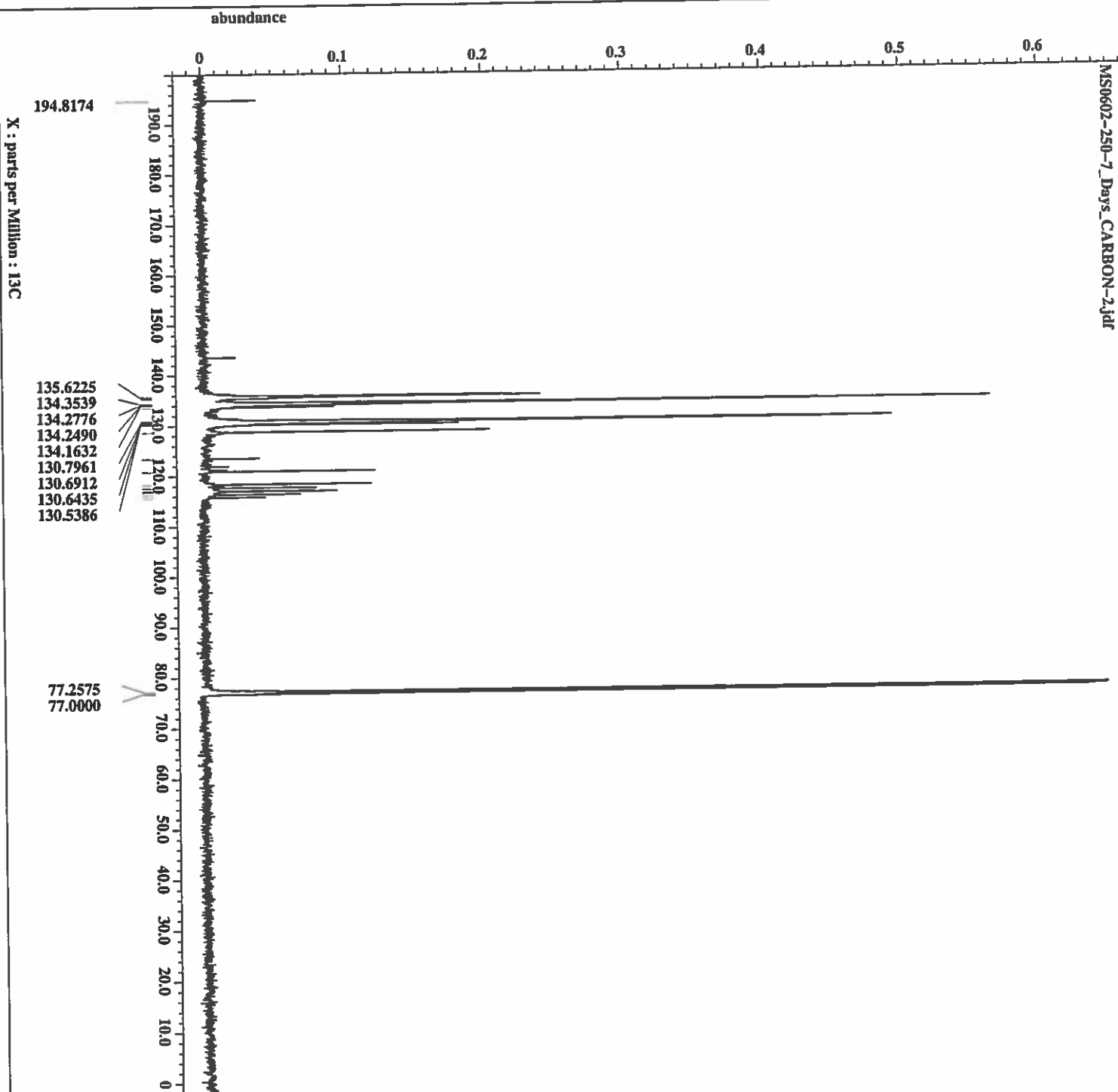
```

Filename      = MS0602-250-7_Days_FLU
Author        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = MS0602-250-7_Days
Solvent       = CHLOROFORM-D
Creation_time  = 19-NOV-2018 16:41:38
Revision_time  = 19-NOV-2018 16:17:31
Current_time   = 19-NOV-2018 16:17:31

Data_format    = 1D COMPLEX
Dim_size       = 104857
Dim_title      = 19F
Dim_units      = [ppm]
Dimensions     = X
Site           = ECA 500
Spectrometer   = JNM-ECA500

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.7340032 [s]
X_domain       = 19F
X_freq         = 470.62046084 [MHz]
X_offset       = -100 [ppm]
X_points       = 131072
X_prescans     = 1
X_resolution   = 1.36239186 [Hz]
X_sweep        = 19F
Xr_domain      = 19F
Xr_freq        = 470.62046084 [MHz]
Xr_offset      = 5 [ppm]
Xr1_domain     = 19F
Xr1_freq       = 470.62046084 [MHz]
Xr1_offset     = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 32
Total_scans    = 32
X_90_width     = 13.1 [us]
X_acq_time     = 0.7340032 [s]
X_angle        = 45 [deg]
X_atn          = 2.5 [dB]
X_pulse        = 6.55 [us]
Xr_mode        = Off
Xr1_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 70
Relaxation_delay = 4 [s]
Repetition_delay = 4.7340032 [s]
Temp_get       = 21.7 [degC]

```



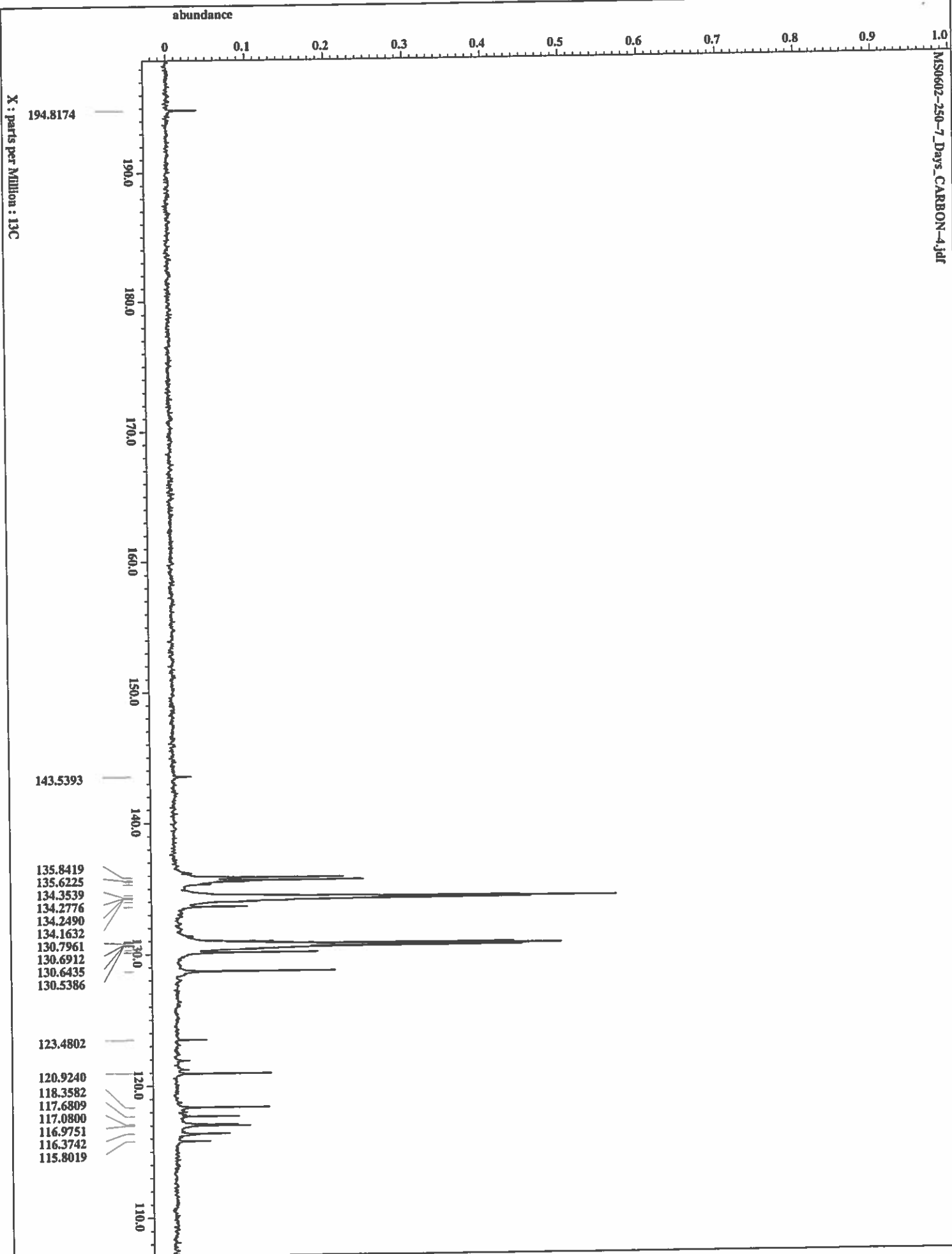
Filename
 MS0602-250-7_Days_CAR
 Author
 jim Davis
 Experiment
 single_pulse_dec
 Sample_id
 MS0602-250-7_Days
 Solvent
 CHLOROFORM-D
 Creation_time
 20-NOV-2018 01:16:33
 Revision_time
 20-NOV-2018 00:53:22
 Current_time
 20-NOV-2018 00:53:22

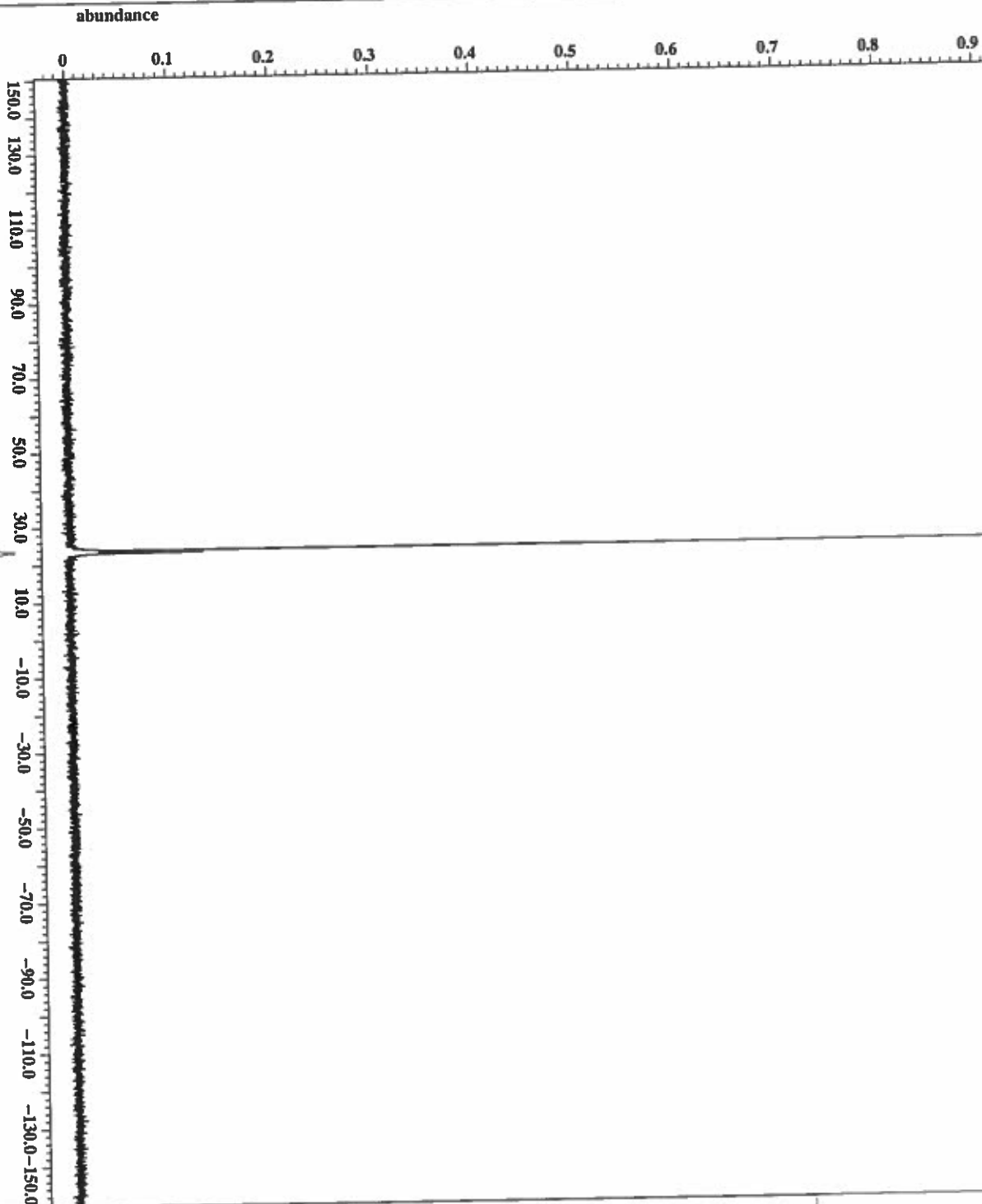
Data_format
 1D COMPLEX
 Dm_size
 26214
 Dm_title
 13C
 Dm_units
 [ppm]
 Dimensions
 X
 Site
 ECA 500
 Spectrometer
 JNM-ECA500

Field_strength
 11.747379 [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_rescans
 1.19959034 [Hz]
 X_resolution
 39.3081761 [kHz]
 X_sweep
 1H
 Irr_domain
 500.15991521 [MHz]
 Irr_freq
 5.0 [ppm]
 Irr_offset
 FALSE
 Mod_return
 1
 Scans
 1024
 Total_scans
 1024

X_90_width
 13.2 [us]
 X_acq_time
 0.83361792 [s]
 X_angle
 30 [deg]
 X_atn
 6 [db]
 X_pulse
 4.4 [us]
 Irr_atn_dec
 20.7 [db]
 Irr_atn_noe
 20.7 [db]
 Irr_noise
 WALTZ
 Decoupling
 TRUE
 Initial_wait
 1 [s]
 Noe
 TRUE
 Noe_time
 2 [s]
 Recvr_gain
 2 [s]
 Relaxation_delay
 2.83361792 [s]
 Repetition_time
 22.6 [dc]

Temp_get





```

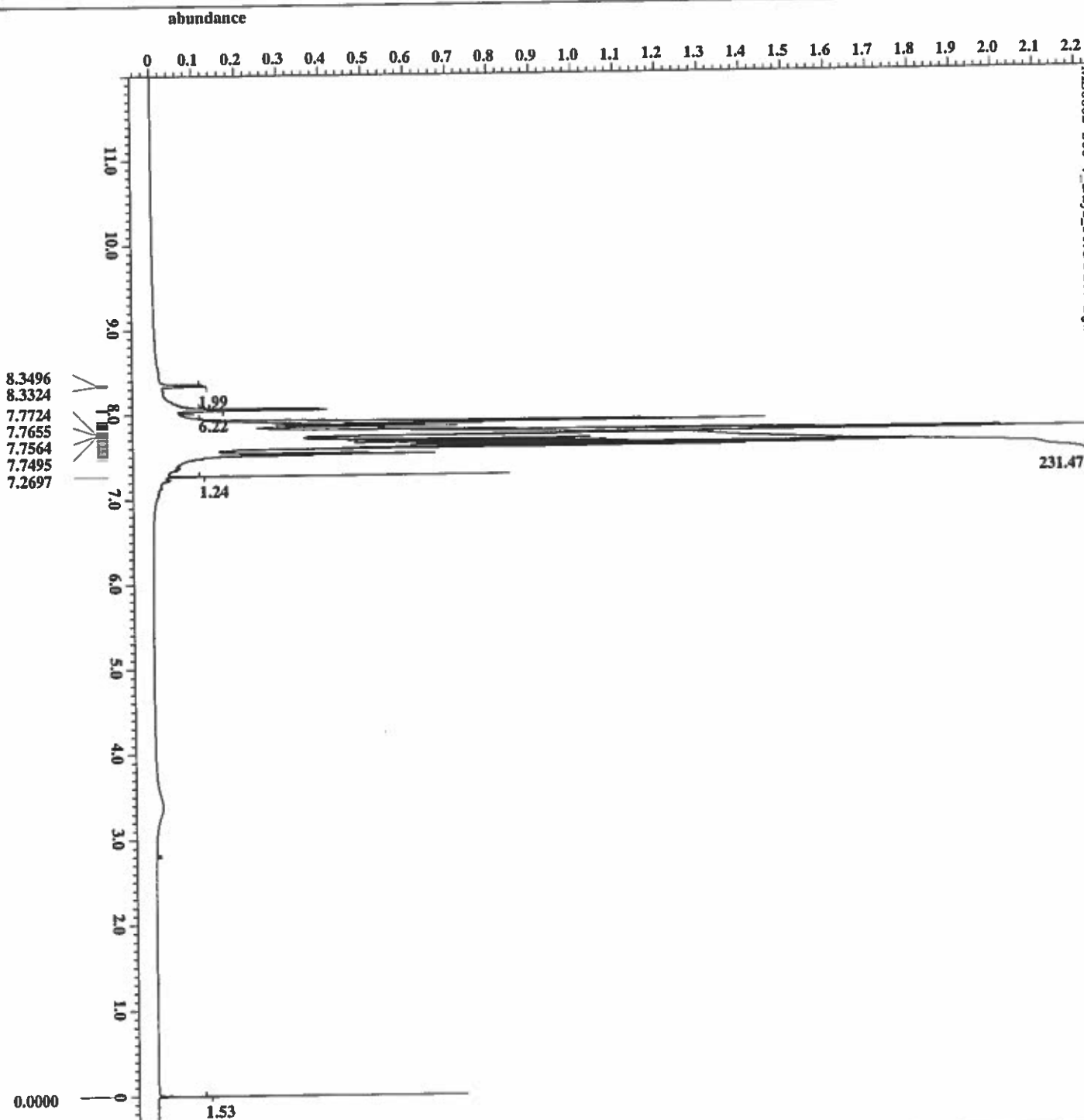
File Name      MS0602-250-7_Days_PRO
Author         Jim Davis
Experiment     Single_pulse_dec
Sample ID      MS0602-250-7_Days
Solvent       CHLOROFORM-D
Creation Time  19-NOV-2018 16:46:11
Revision Time  19-NOV-2018 16:42:02
Current Time   19-NOV-2018 16:42:02

Date Format     JD COMPLEX
Dim Size       52428
Dim Title      32P
Dim Units      [ppm]
Dimensions     1
Site           ECA 500
Spectrometer   JNM-ECA500

Field Strength 11.7473579 [T] (500 [MH
X_acq_duration 0.85983232 [s]
X_domain       31P
X_freq         202.46831075 [MHz]
X_offset       0 [ppm]
X_points       65536
X_prescans     4
X_resolution   1.16301746 [Hz]
X_sweep        76.2195122 [kHz]
X_domain       1H
X_freq         500.15991521 [MHz]
X_offset       5.0 [ppm]
Clipped        TRUE
Mod_return     1
Scans          40
Total_scans    40

X_90_width     14.687 [us]
X_acq_time     0.85983232 [s]
X_angle       30 [deg]
X_atn         5 [dB]
X_pulse       4.89566667 [us]
Irr_atn_dec   20.7 [dB]
Irr_atn_noe   20.7 [dB]
WALTZ         WALTZ
Decoupling     1 [s]
Initial_wait   TRUE
Noe_time       2 [s]
Noe           50
Recvr_gain     2 [s]
Relaxation_delay 2.85983232 [s]
Repetition_time 22.1 [dc]
Temp_get       22.1 [dc]

```



X : parts per Million : 1H

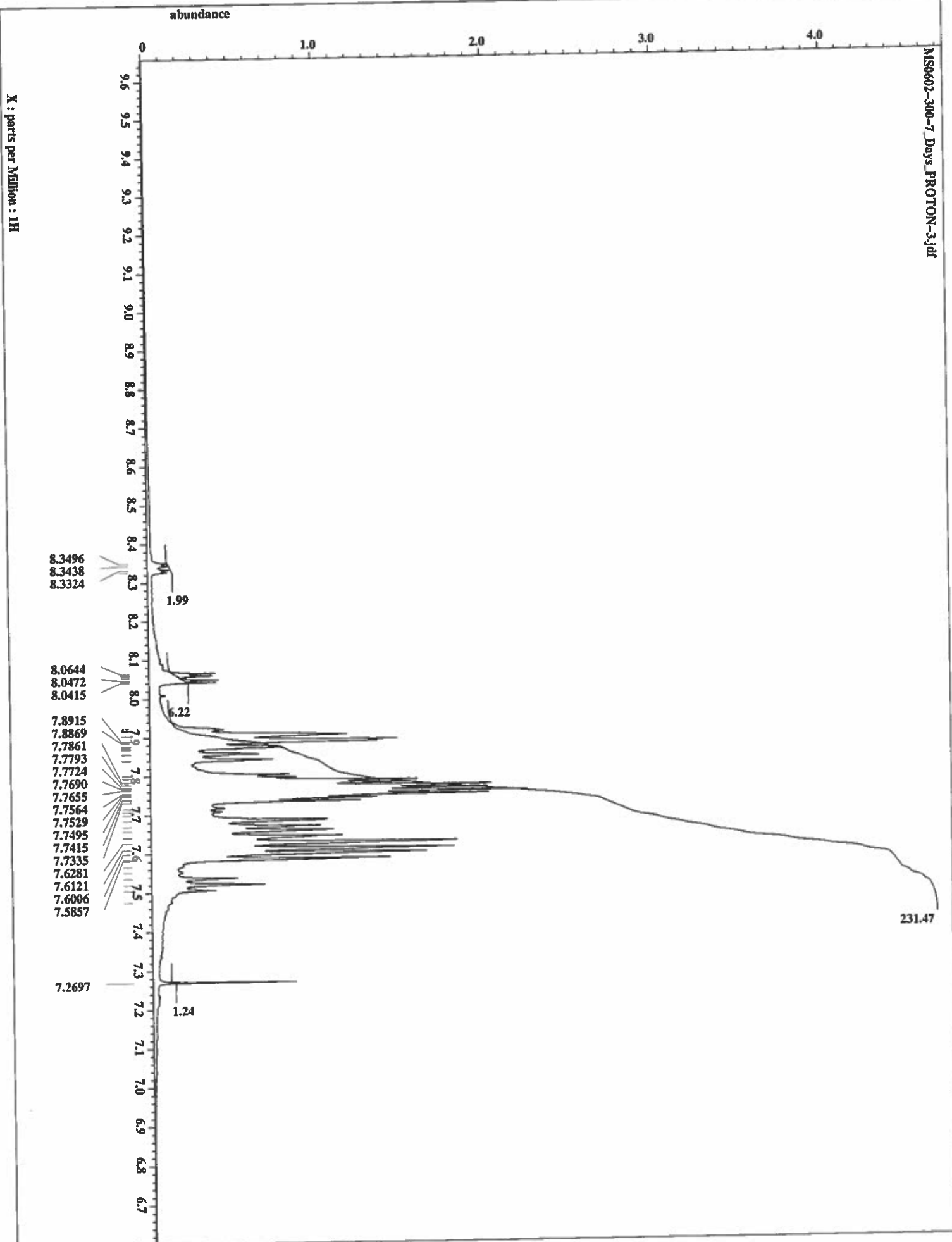


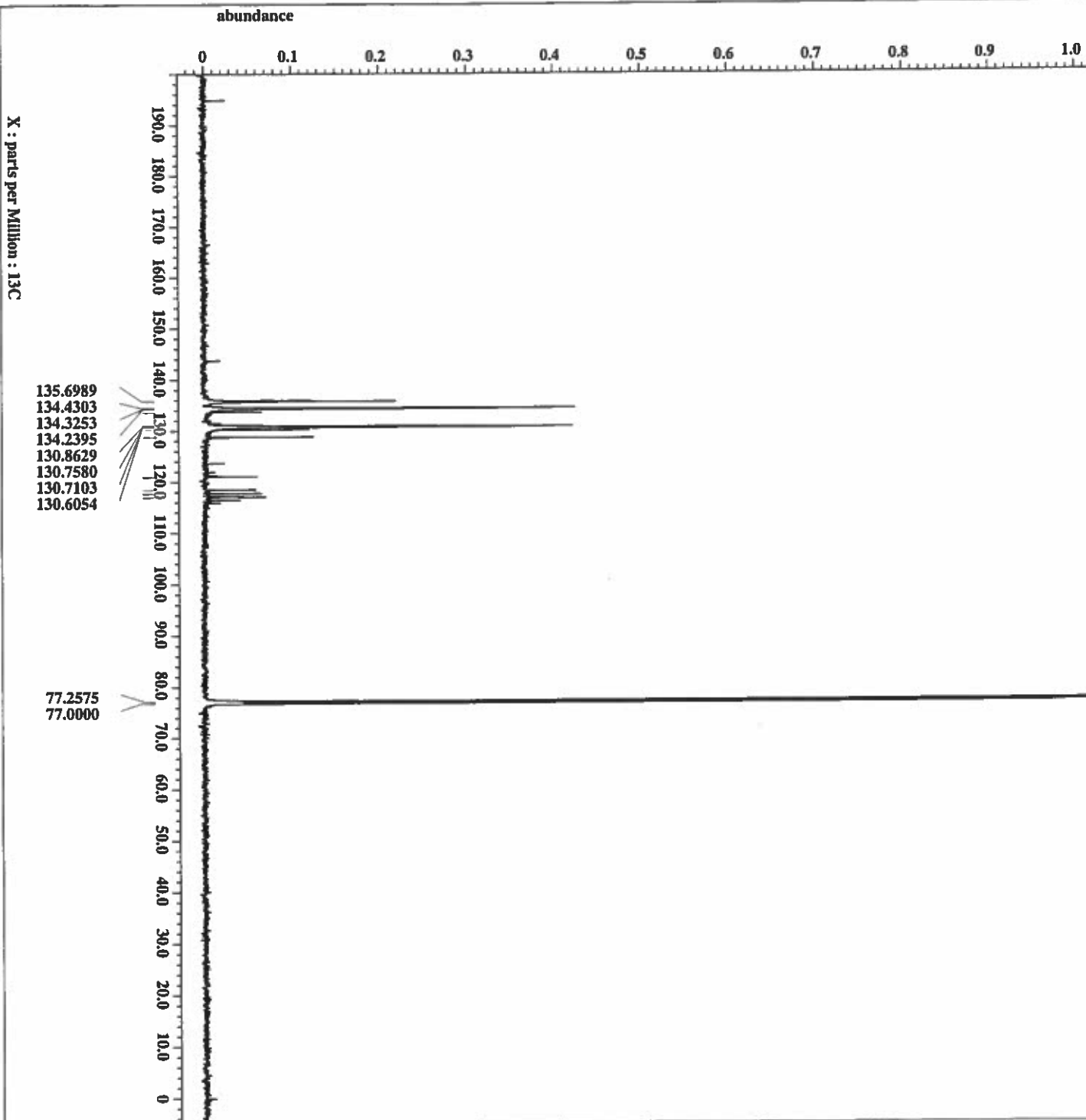
```

File Name      MS0602-300-7_Days_PRO
Author         Jim Davis
Experiment     *single_pulse.ex2
Sample ID     MS0602-300-7_Days
Solvent       CHLOROFORM-D
Creation Time  19-NOV-2018 16:53:34
Revision Time  19-NOV-2018 16:29:25
Current Time   19-NOV-2018 16:29:25

Data Format    1D COMPLEX
Dim Size      13107
Dim Title     1H
Dim Units     [ppm]
Dimensions    X
Site          ECA 500
Spectrometer  JNM-ECA500

Field Strength 11.7473579 [T] (500 [MH
X_acq_duration 1.74587904 [s]
X_domain       1H
X_freq         500.15991521 [MHz]
X_offset       5.01 [ppm]
X_points       16384
X_prescans     1
X_resolution   0.57277737 [Hz]
X_sweep        9.38438438 [kHz]
X_domain       1H
X_freq         500.15991521 [MHz]
X_offset       5.01 [ppm]
X1_domain      1H
X1_freq        500.15991521 [MHz]
X1_offset      5.01 [ppm]
Clipped        FALSE
Mod Return     1
Scans          16
Total Scans   16
X_90_width     12.4 [us]
X_acq_time     1.74587904 [s]
X_angle        45 [deg]
X_atn          4 [db]
X_pulse        6.2 [us]
Xir_mode       OF2
Xir_mode       OF2
Pulse Program  PULSE
Initial Value  1 [s]
Recvr Gain     36
Relaxation Delay 4 [s]
Repetition Time 5.74587904 [s]
Temp Set       21.8 [C]
  
```





```

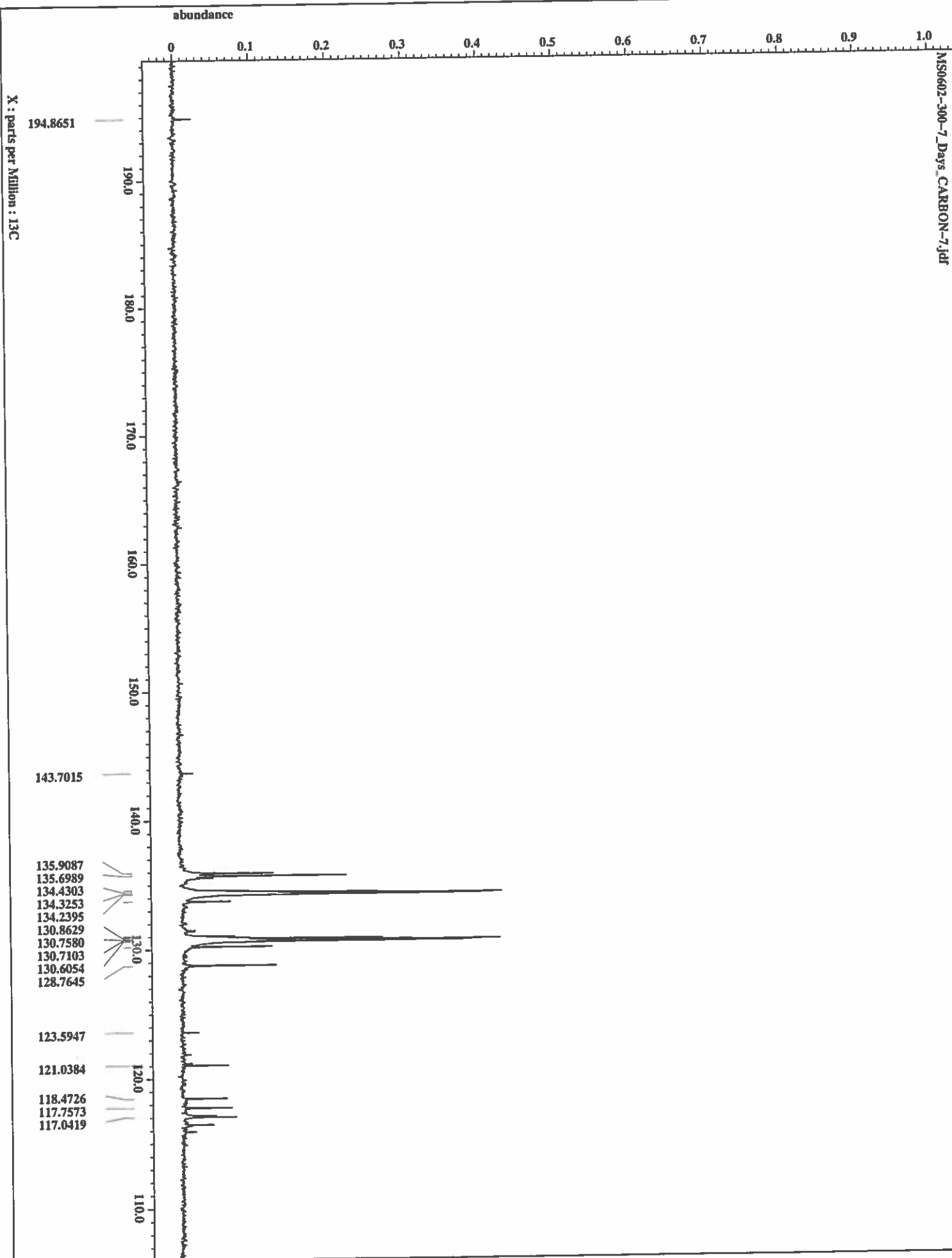
filename      = MS0602-300-7_Days_CAR
author        = Jim Davis
experiment    = single_pulse_dec
sample_id     = MS0602-300-7_Days
solvent       = CHLOROFORM-D
creation_time  = 20-NOV-2018 03:11:07
revision_time  = 20-NOV-2018 01:46:55
current_time   = 20-NOV-2018 01:46:55

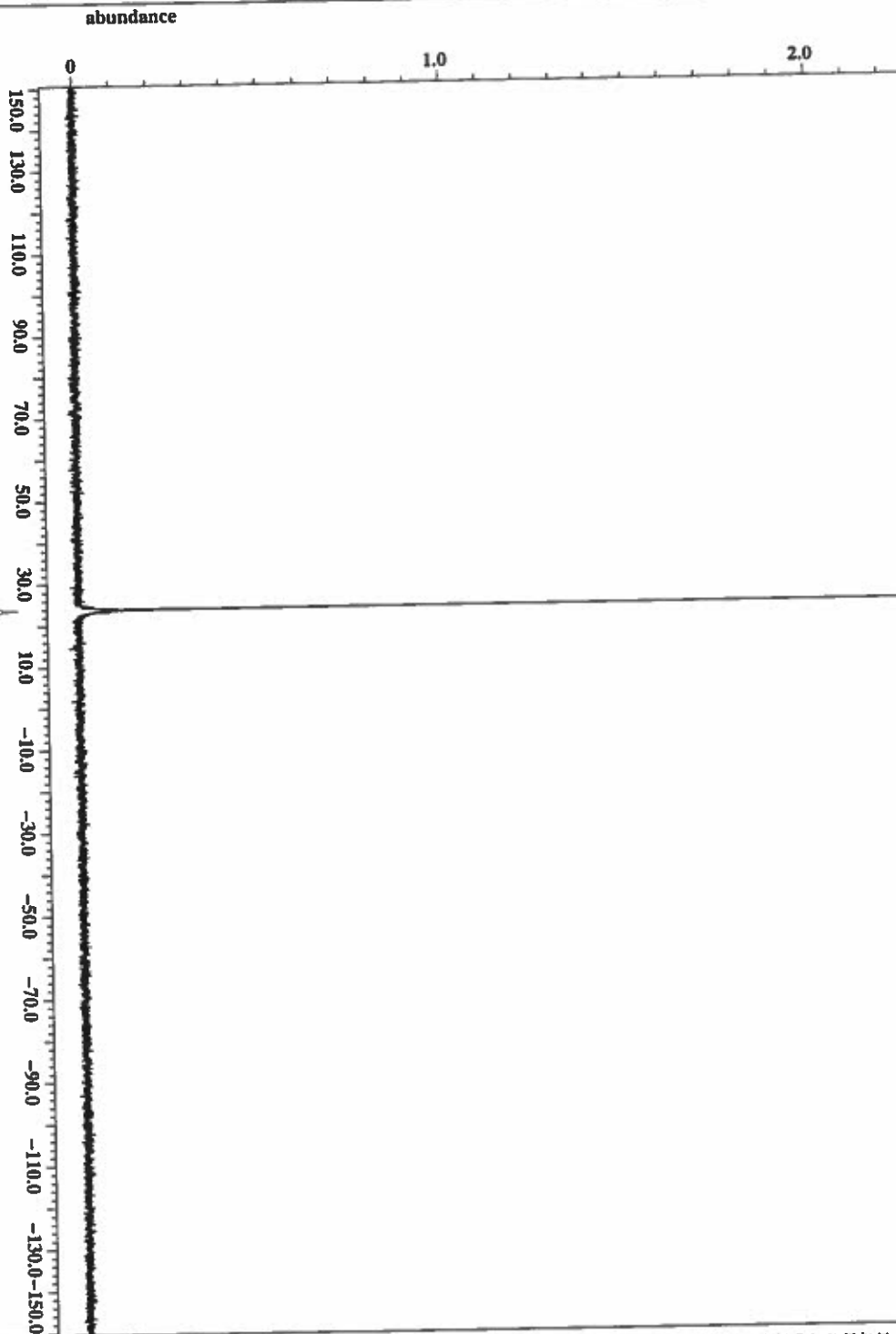
Data Format
dim_size      = 26214
dim_c1cle     = 13C
dim_units     = [ppm]
dimensions    = X
site          = ECA 500
spectrometer   = JNM-ECA500

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       = 33768
X_prescans     = 4
X_resolution    = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
irf_domain     = 1H
irf_freq       = 500.15991521 [MHz]
irf_offset     = 5.0 [ppm]
clipped        = FALSE
mod_return     = 1
scans          = 1024
total_scans    = 1024

X_90_width     = 13.2 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.4 [us]
irf_atn_dec    = 20.7 [dB]
irf_atn_noe    = 20.7 [dB]
irf_nolse      = VALTZ
decoupling     = TRUE
initial_walt    = 1 [e]
noe_time       = TRUE
noe_time       = 2 [e]
recvr_gain     = 60
relaxation_delay = 2 [e]
repetition_time = 2.83361792 [s]
temp_get       = 22.6 [C]

```





```

filename
  = MS0602-300-7_Days_PRO
Author
  = Jim Davis
Experiment
  = single_pulse_dec
Sample_id
  = MS0602-300-7_Days
Solvent
  = CHLOROFORM-D
Creation_time
  = 19-NOV-2018 17:03:08
Revision_time
  = 19-NOV-2018 16:38:59
Current_time
  = 19-NOV-2018 16:38:59

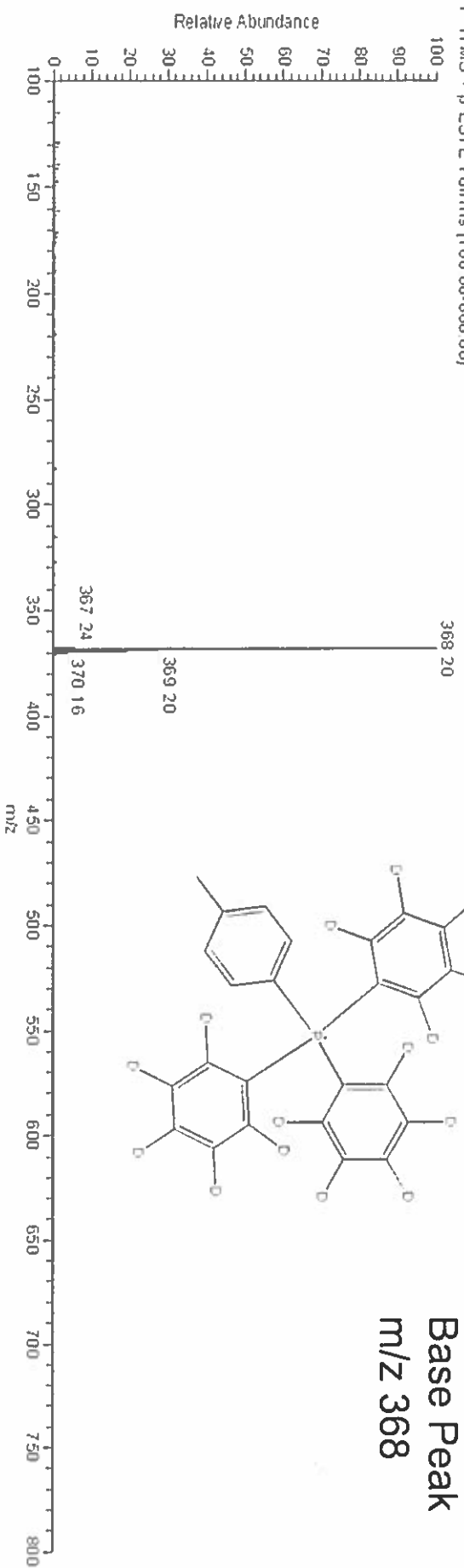
Date_format
  = DD MONTH
Dim_size
  = 52428
Dim_title
  = 31P
Dim_units
  = [ppm]
Dimensions
  = X
Site
  = ECA 500
Spectrometer
  = JNM-ECA500

Field_strength
  = 11.7473578 [T] (500 [MH
X_acq_duration
  = 0.85983232 [s]
X_domain
  = 31P
X_freq
  = 202.46831075 [MHz]
X_offset
  = 0 [ppm]
X_points
  = 6536
X_prescans
  = 4
X_rescans
  = 1.16301746 [Hz]
X_resolution
  = 76.2195122 [Hz]
X_sweep
  = 1H
X_domain
  = 500.15991521 [MHz]
X_freq
  = 5.0 [ppm]
X_offset
  = FALSE
Mod_return
  = 1
Scans
  = 40
Total_scans
  = 40

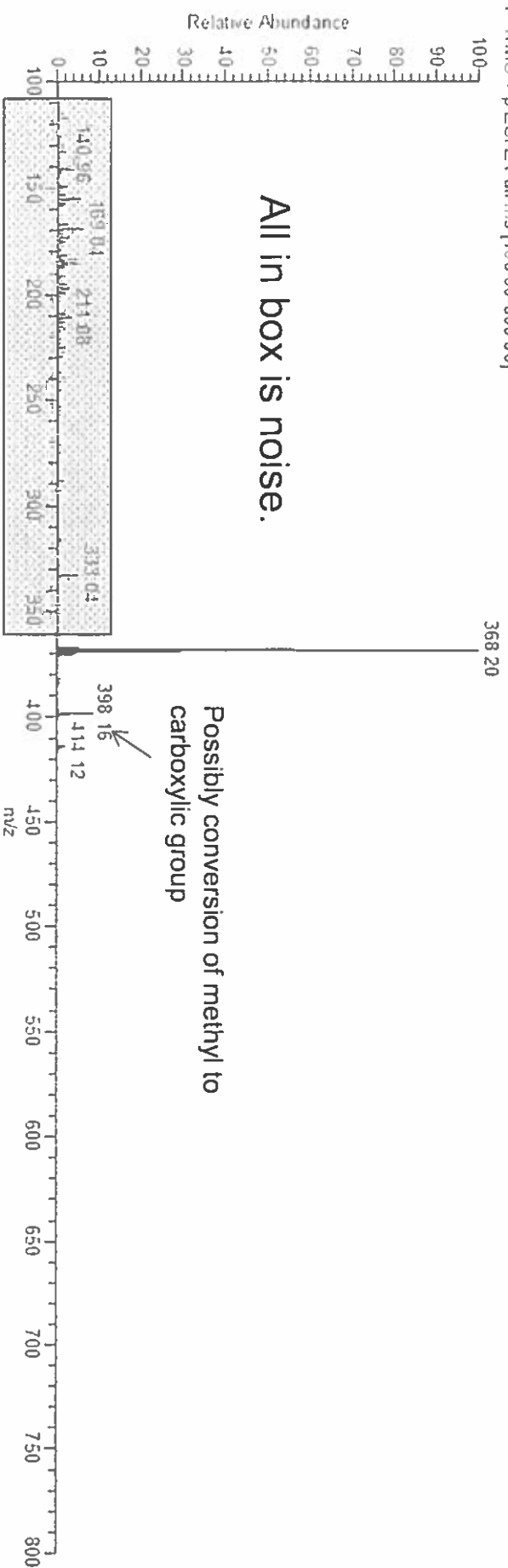
X_90_width
  = 14.687 [us]
X_acq_time
  = 0.85983232 [s]
X_angle
  = 30 [deg]
X_atn
  = 5 [dB]
X_pulse
  = 4.89566667 [us]
Irr_atn_dec
  = 20.7 [dB]
Irr_atn_noe
  = 20.7 [dB]
Irr_noise
  = VALTZ
Decoupling
  = TRUE
Initial_wait
  = 1 [s]
Noe_time
  = TRUE
Recvr_gain
  = 2 [s]
Relaxation_delay
  = 2 [s]
Repetition_delay
  = 2.85983232 [s]
Repetition_time
  = 22.21 [dc]
Temp_get
  = 22.21 [dc]

```

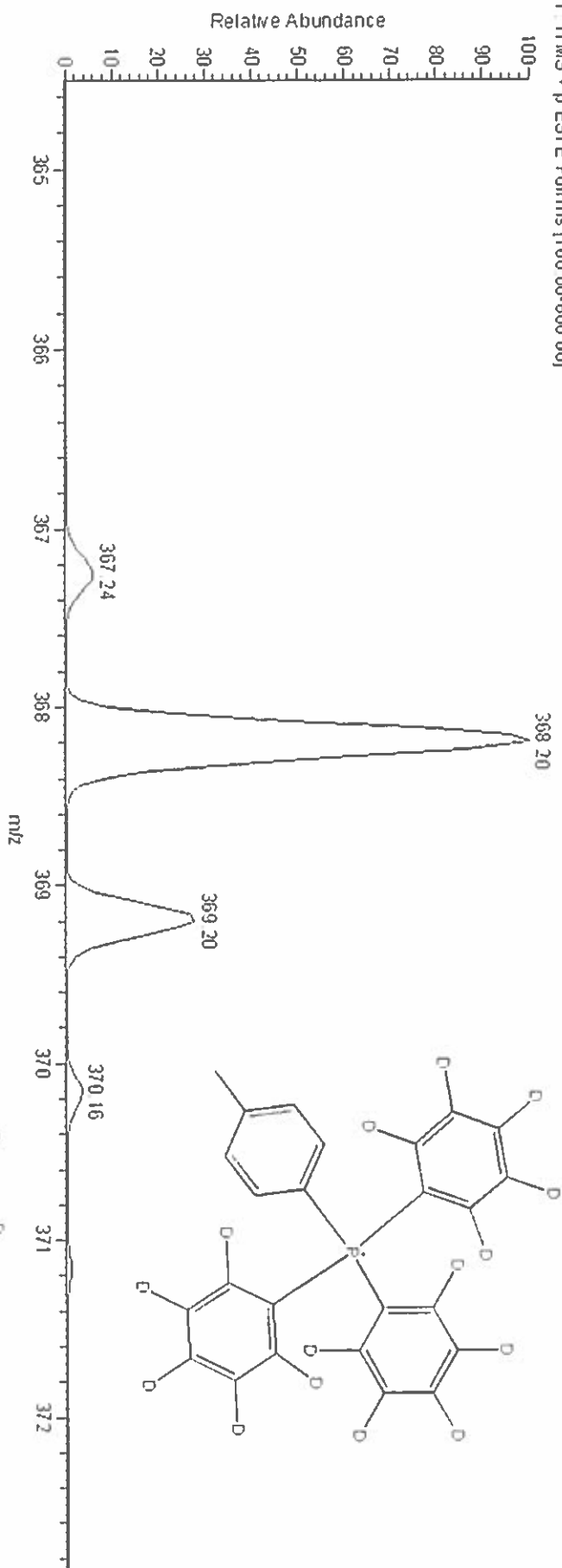
468_200 #137 RT 1.05 AV 1 NL 9.00E6
T ITMS + p ESI E Full ms [100.00-800.00]



468_250 #167-168 RT 1.31-1.32 AV 2 SB 96.004-0.79 IIL 5.97E5
T ITMS + p ESI E Full ms [100.00-800.00]

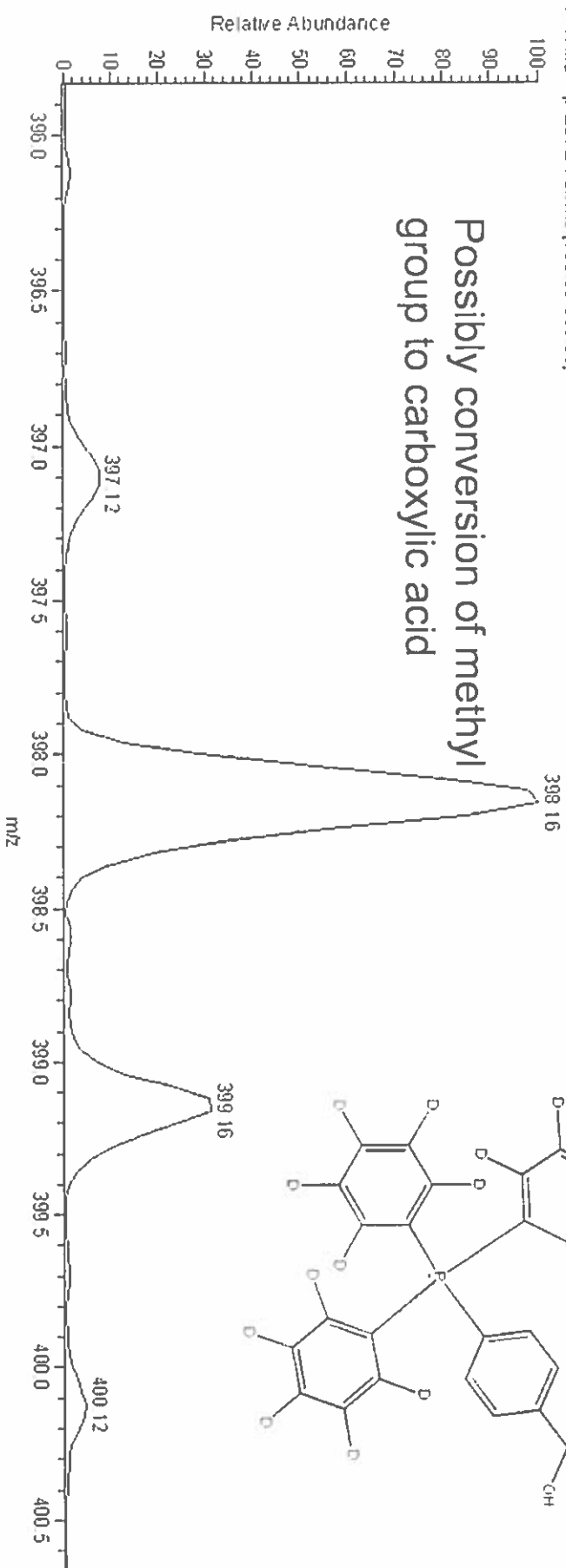


468_200 #140 RT: 1.07 AV: 1 NL: 8.70E6
T: ITMS + p ESI E Fullms (100.00-800.00)

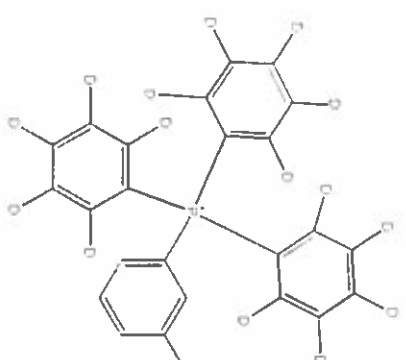


468_250 #166-169 RT: 1.30-1.32 AV: 4 SB: 109.006-0.91 NL: 3.56E4
T: ITMS + p ESI E Fullms (100.00-800.00)

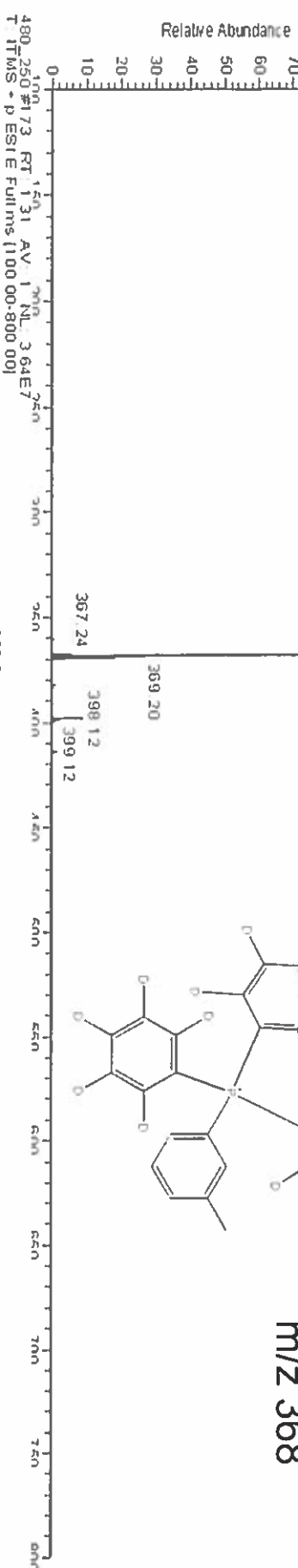
Possibly conversion of methyl
group to carboxylic acid



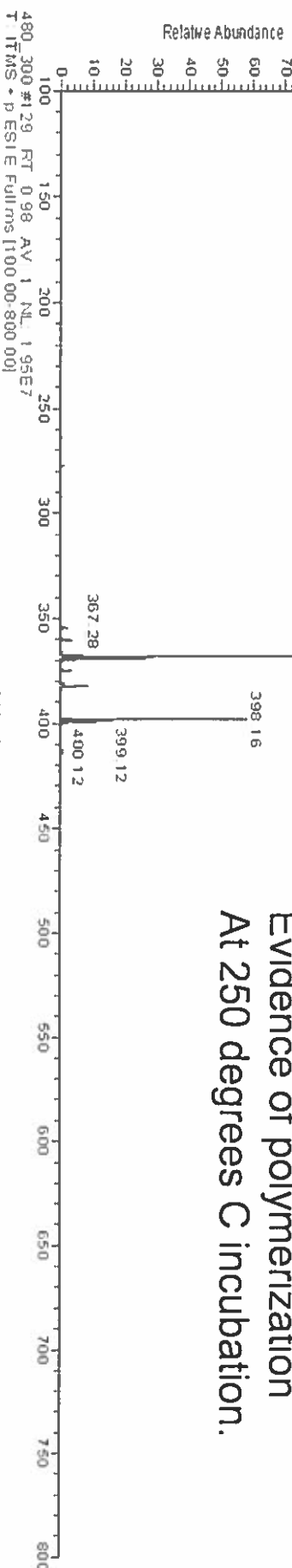
480 200 #134 RT 1.02 AV 1 NL 4.83E6
T:ITMS - p ESIE Fullms (100 00-800 00)



Base Peak
m/z 368



Evidence of polymerization
At 250 degrees C incubation.

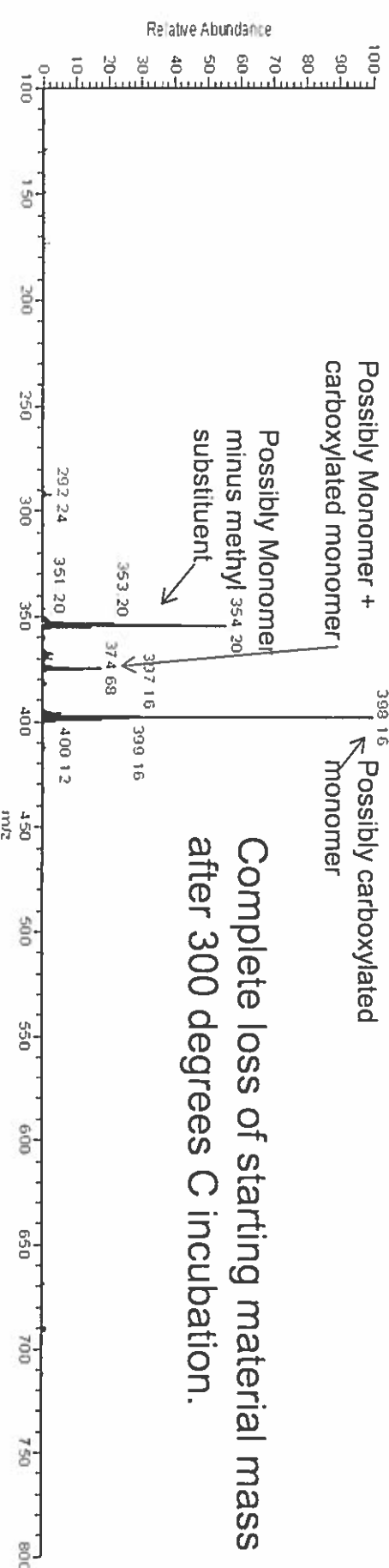


Possibly Monomer +
carboxylated monomer

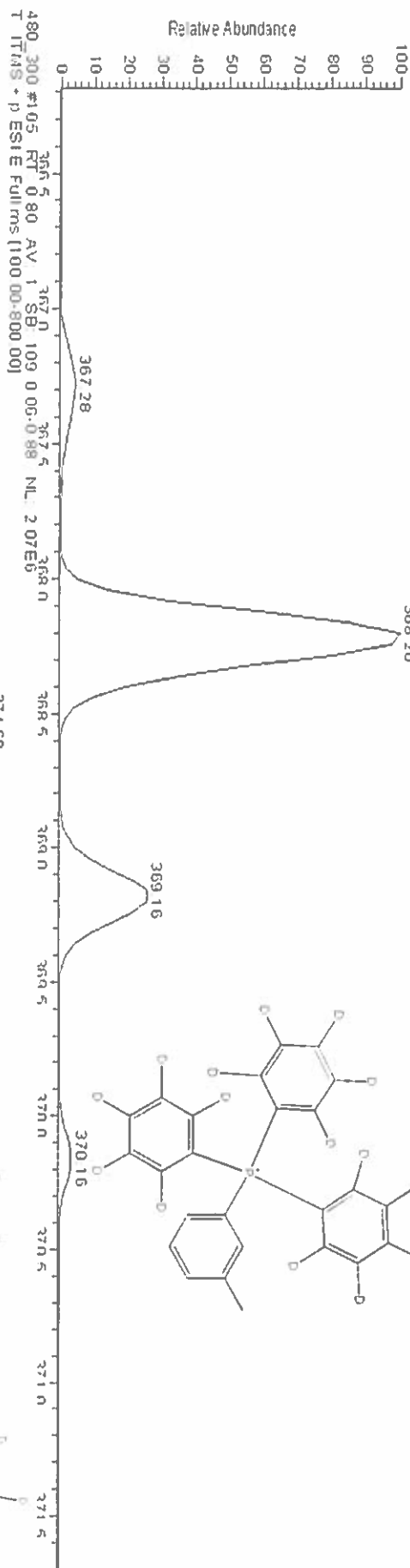
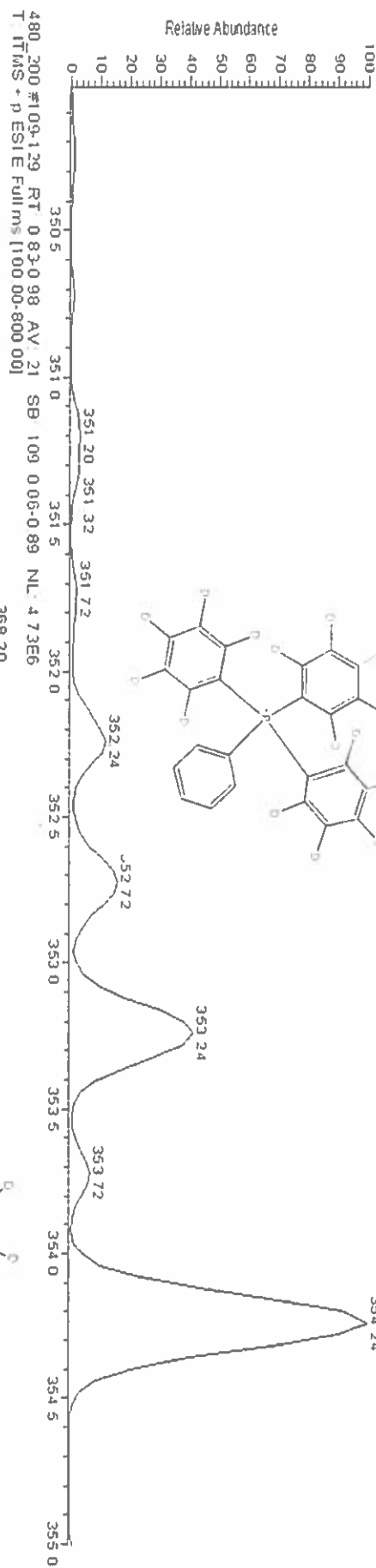
Possibly Monomer
minus methyl
substituent

Possibly carboxylated
monomer

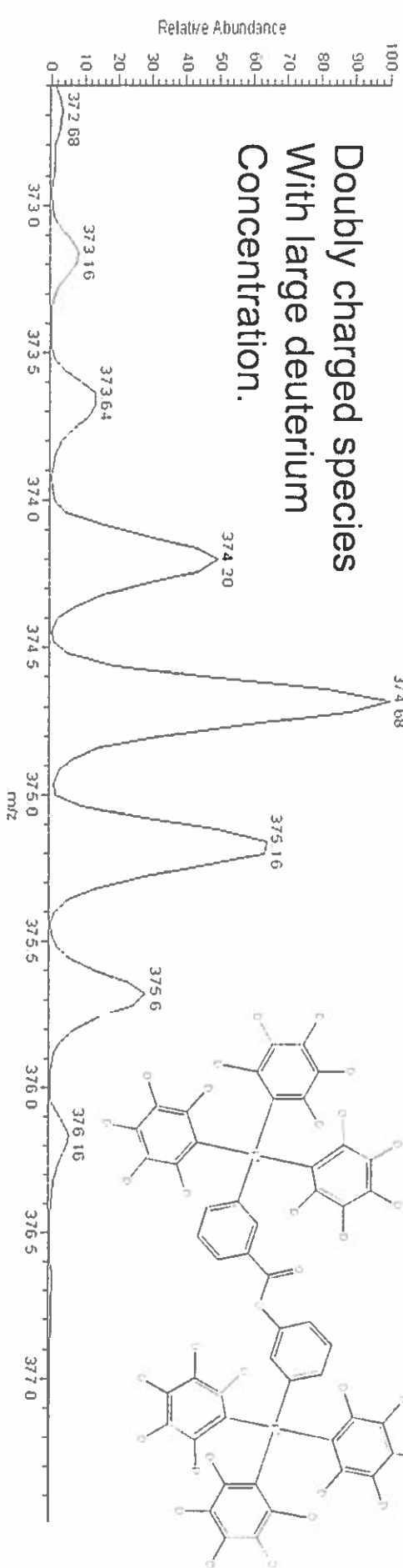
Complete loss of starting material mass
after 300 degrees C incubation.



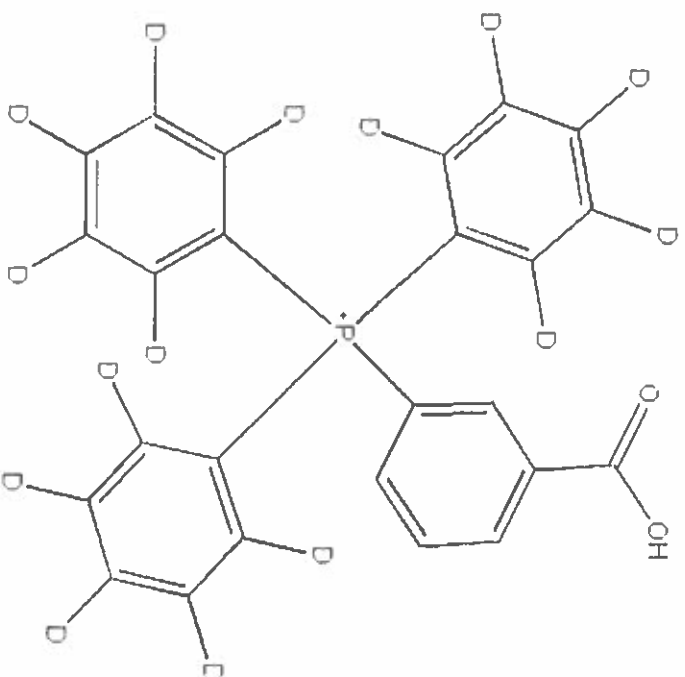
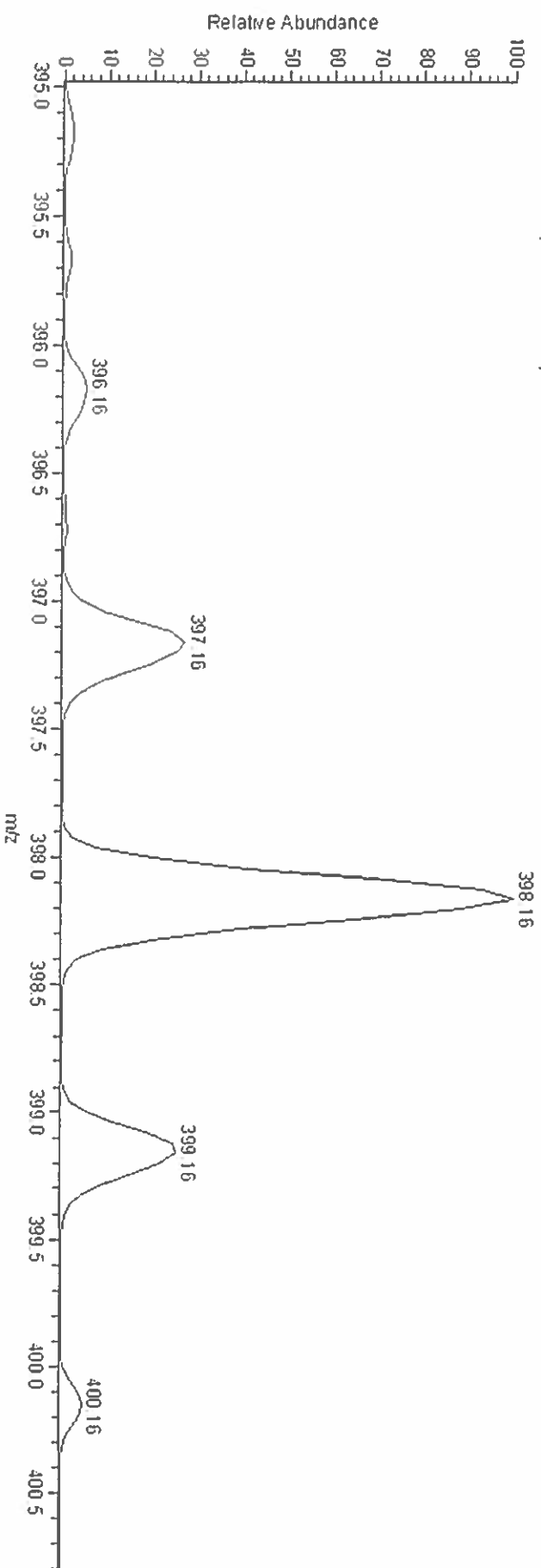
480 300 #105 RT 0.80 AV 1 SB 109 0.06-0.88 NL 5 19E6
T:ITMS - p ESIE Fullms (100.00-800.00)



**Doubly charged species
With large deuterium
Concentration.**

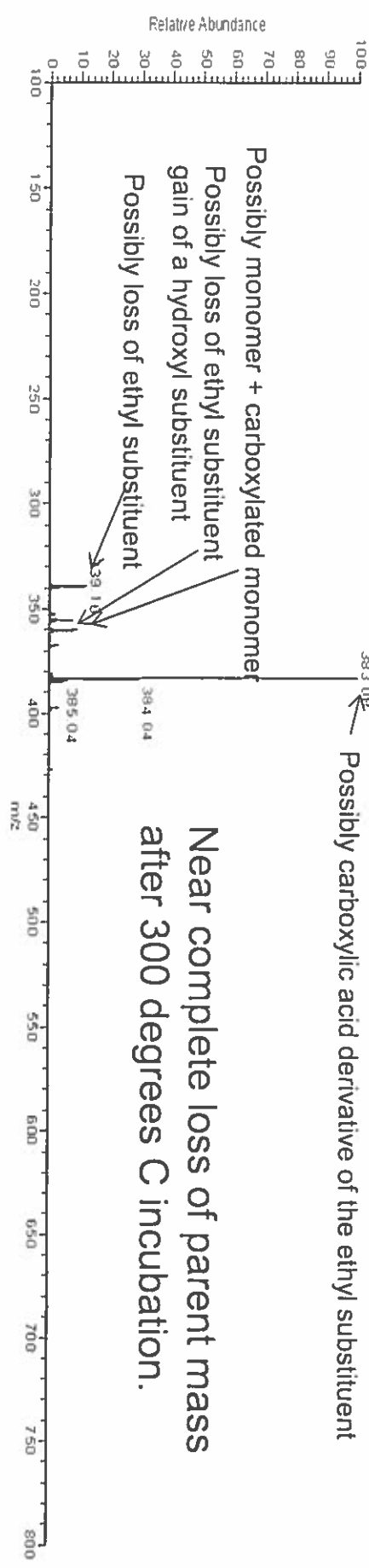
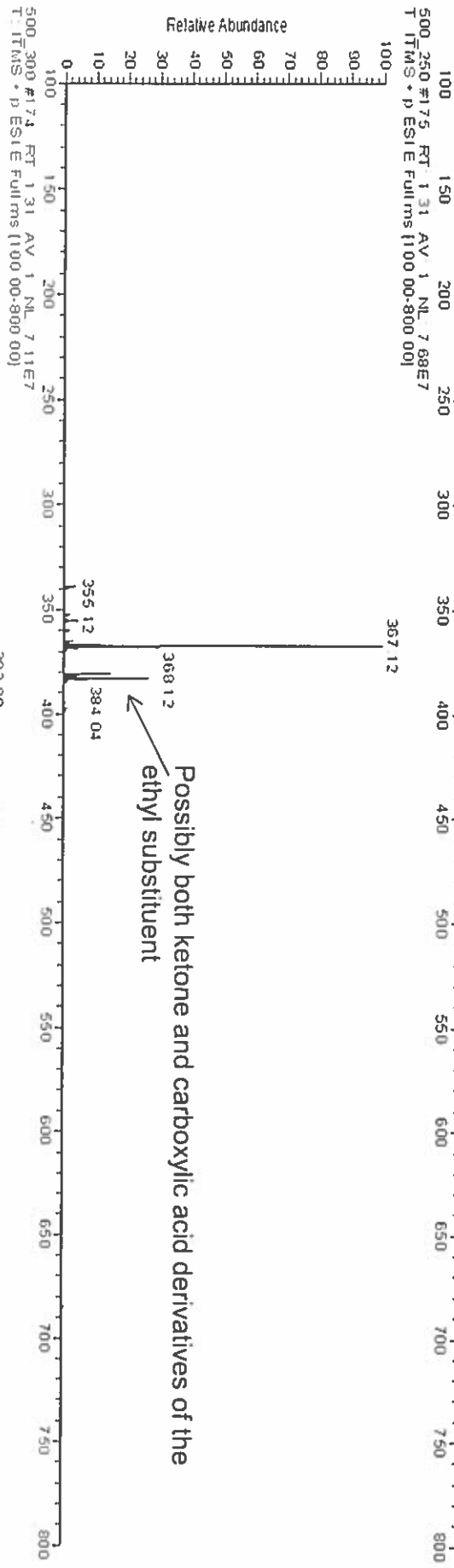
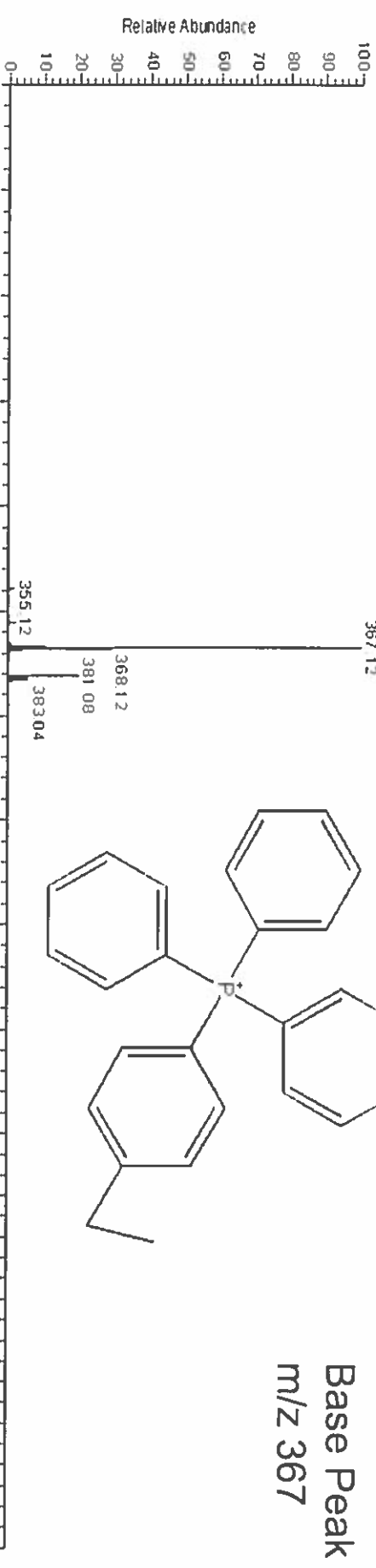


480 300 #105 RT 0.80 AV 1 SB 109 0.06-0.88 NL 8.32E6
T TMS + p ESIE Full ms (100.00-800.00)

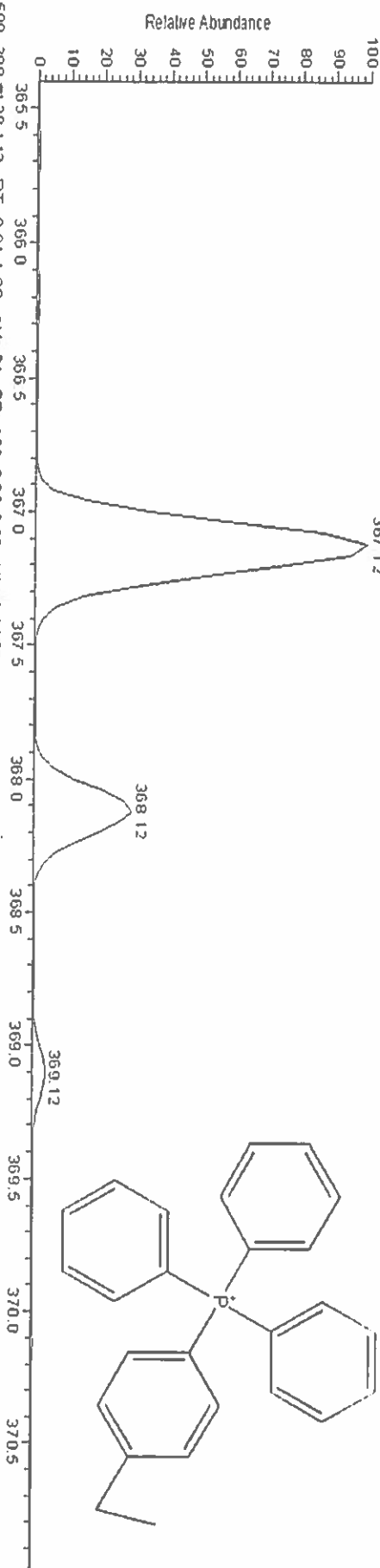


Conversion of methyl
group to carboxylic acid

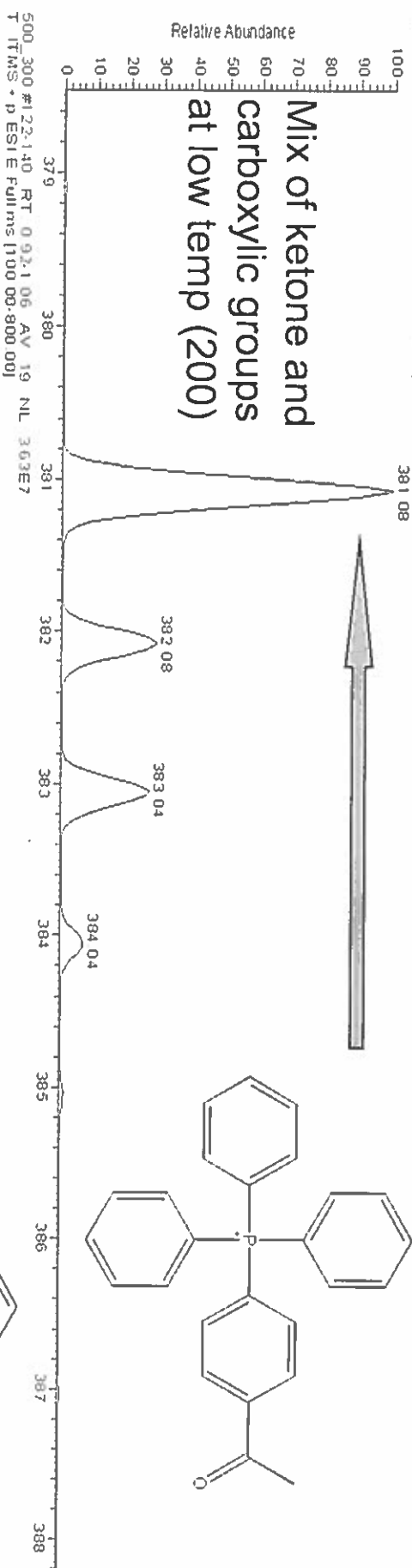
500_200 #145 RT 1.10 AV 1 NL 9.75E7
T ITMS + p ESI E Fullms [100 00-800 00]



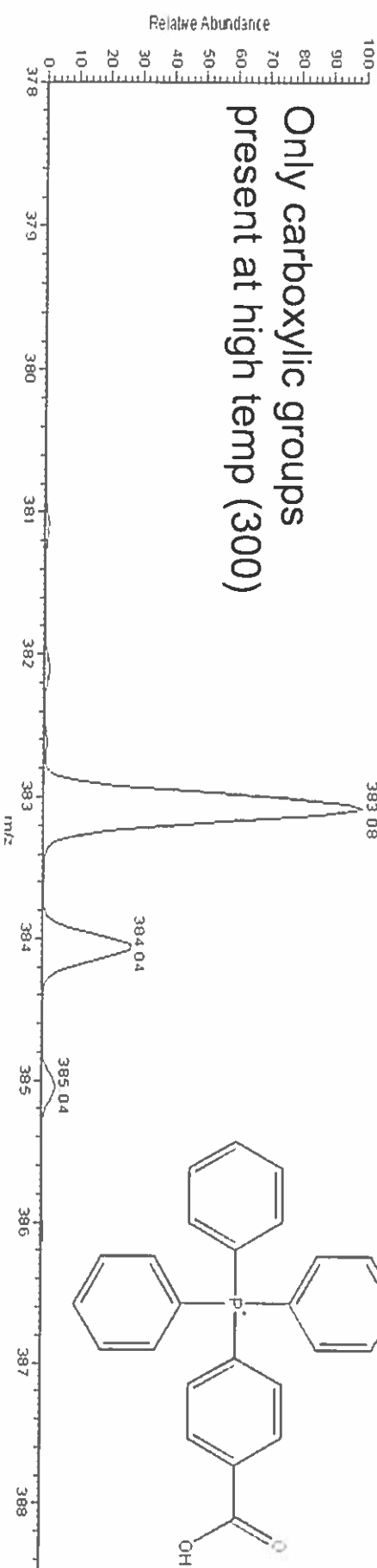
500_200 #120-143 RT 0 91-1 08 AV 24 SB 109 0 06-0 88 NL 1 03E8
T ITMS + P ESI E Fullms [100 00-800 00]



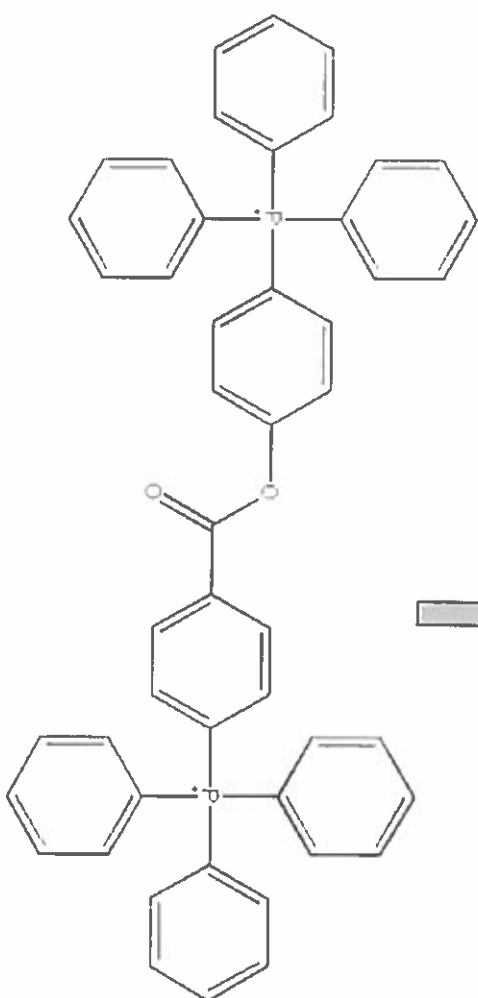
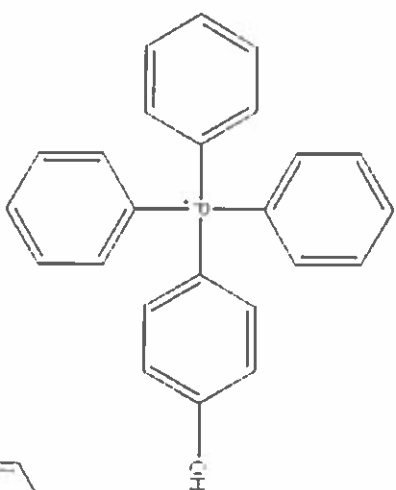
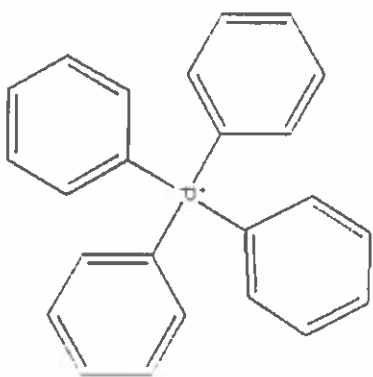
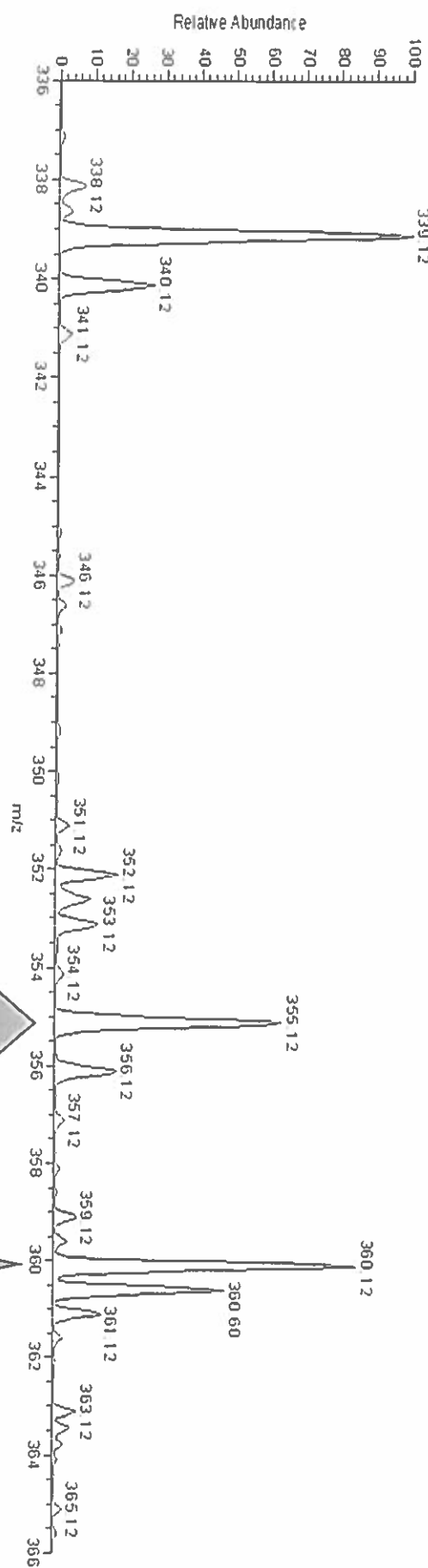
Mix of ketone and
carboxylic groups
at low temp (200)



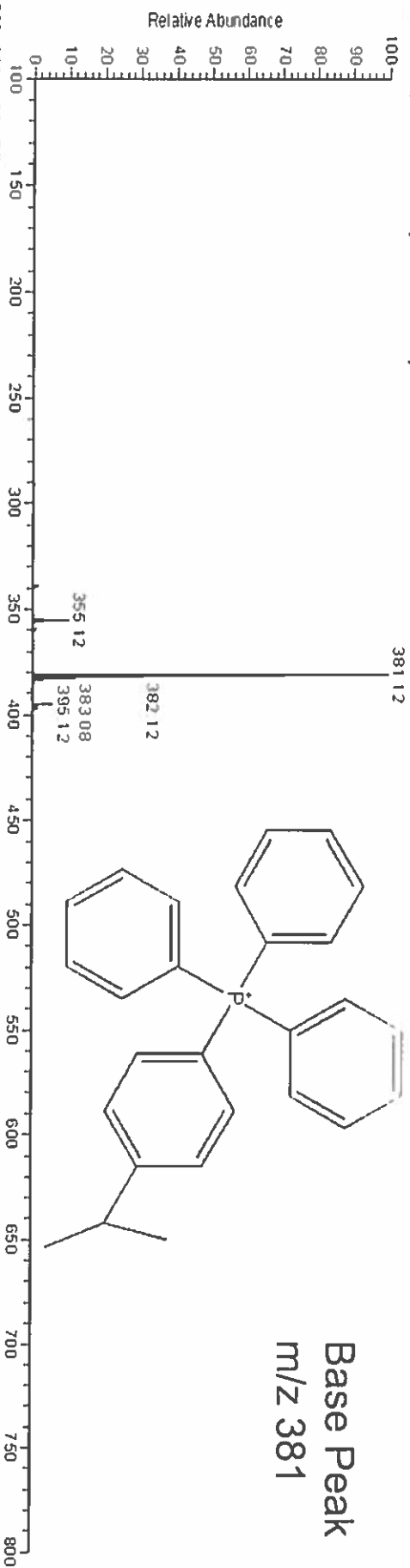
Only carboxylic groups
present at high temp (300)



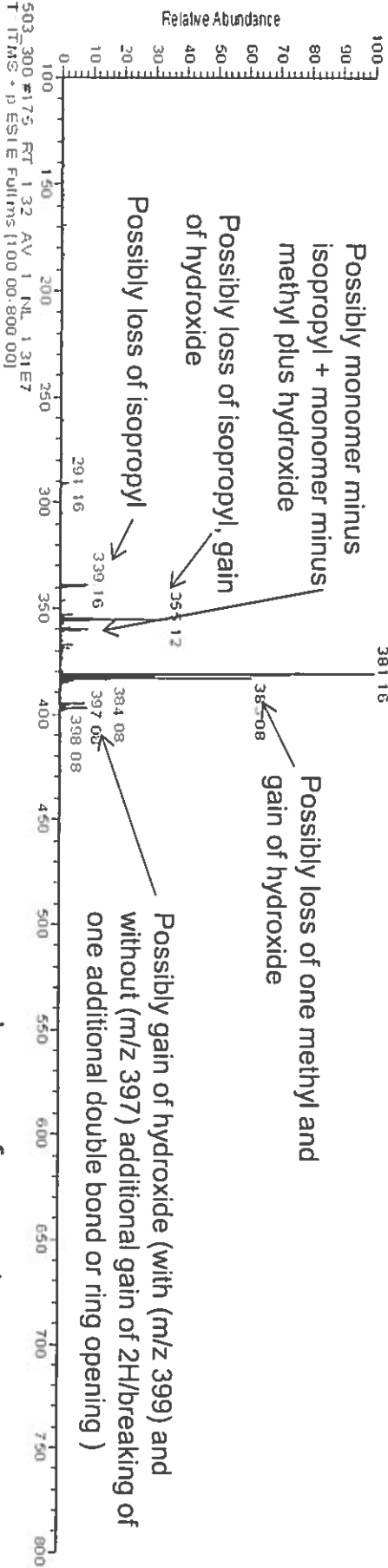
500 300 #1 22.140 RT: 0.92-1.06 AV: 19 NL: 531E6
T: FTMS + P ESI E Fullms (100 00-800 00)



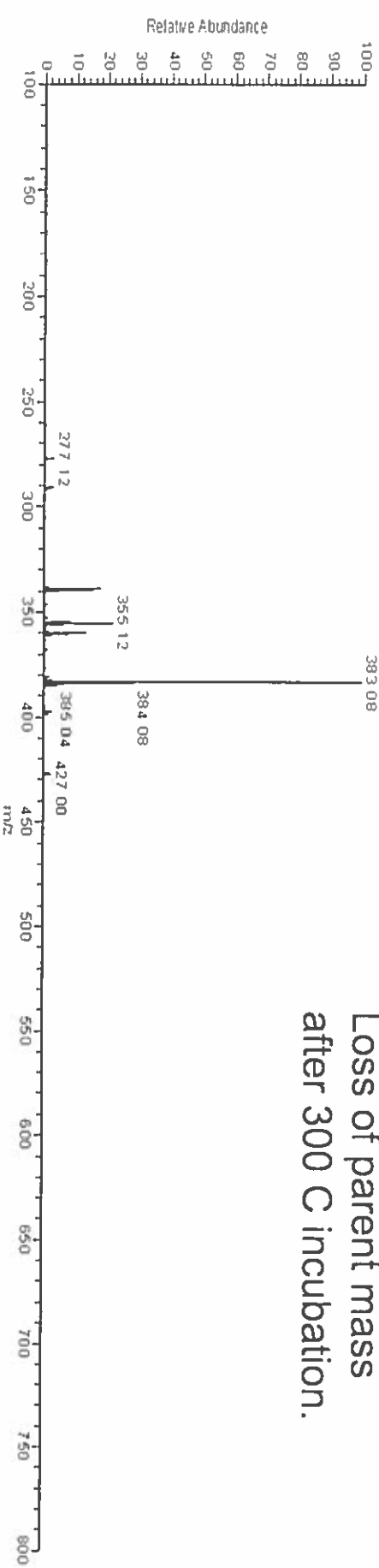
503_200 #173 RT 1.31 AV 1 NL 4.76E7
T ITMS • p ESI E Fullms (100 00-800 00)



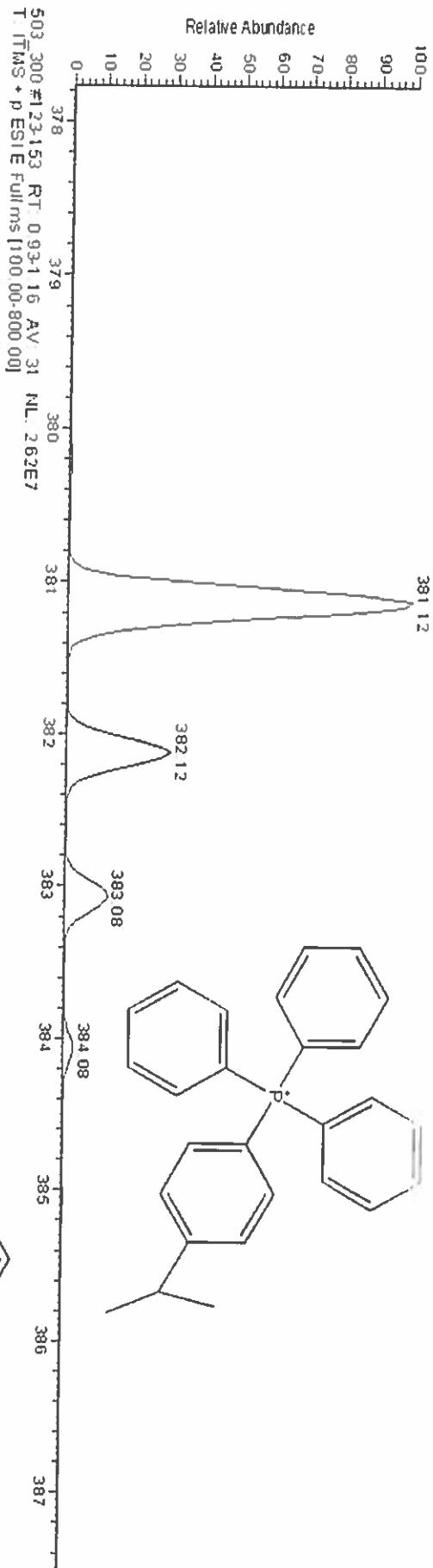
503_250 #166 RT 1.25 AV 1 NL 8.33E6
T ITMS • p ESI E Fullms (100 00-800 00)



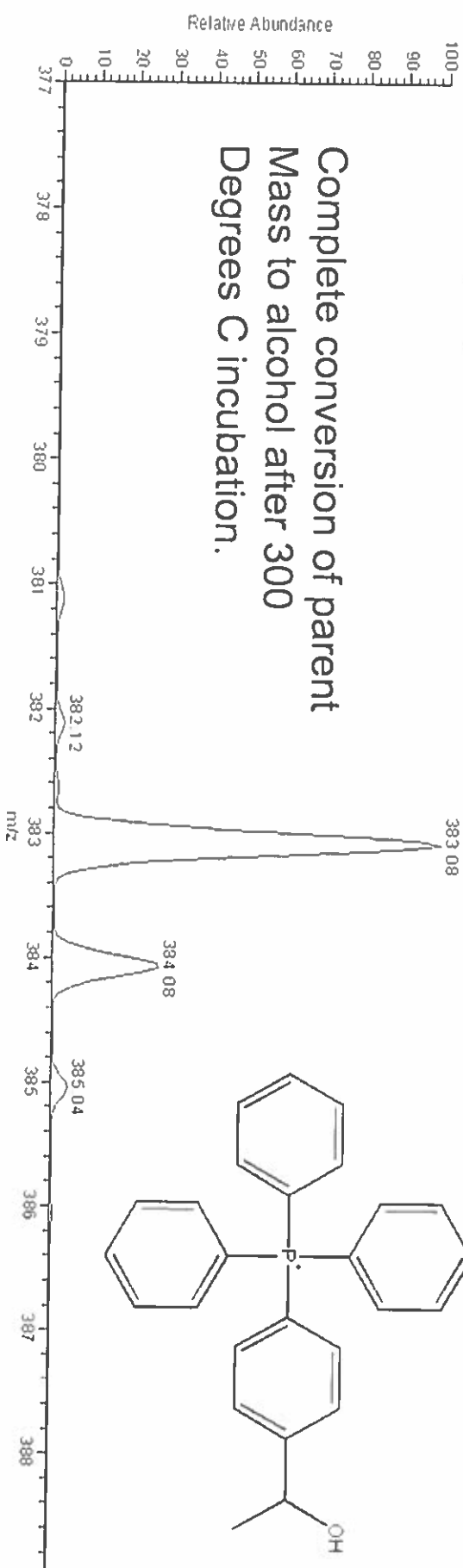
Loss of parent mass
after 300 C incubation.

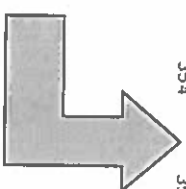
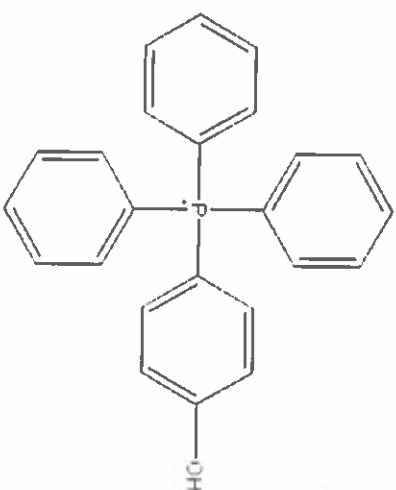
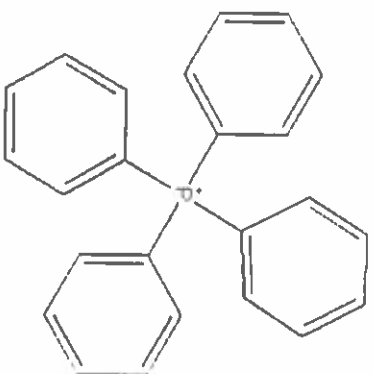
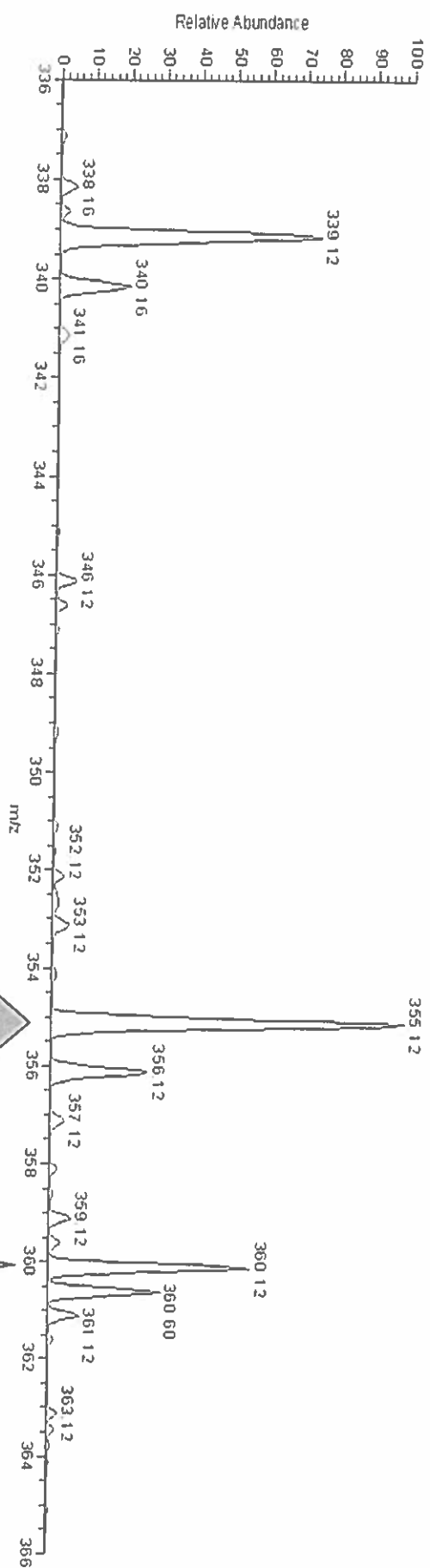


503_200 #120-147 RT 0.91-1.11 AV 28 NL 7.81E7
T TMS + P ESIE Full ms [100.00-800.00]

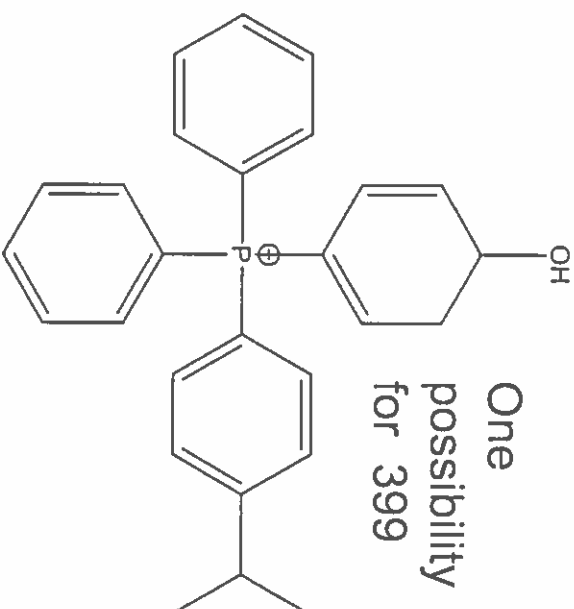
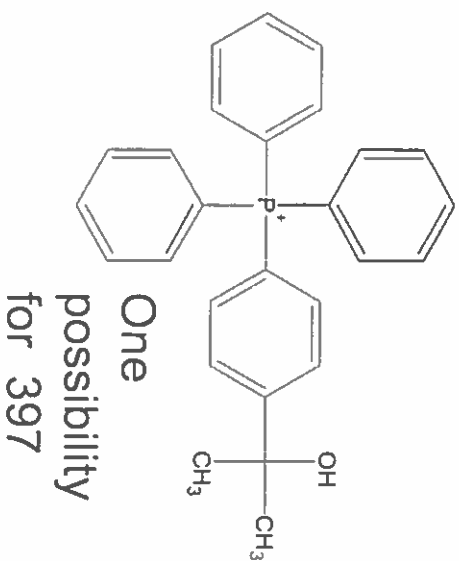
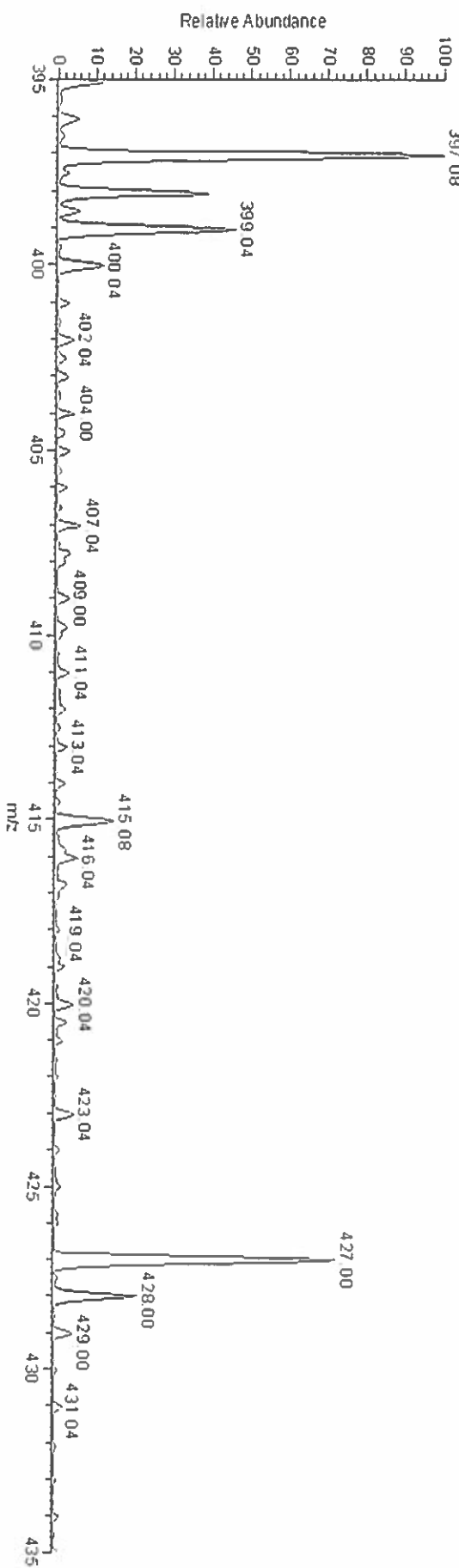


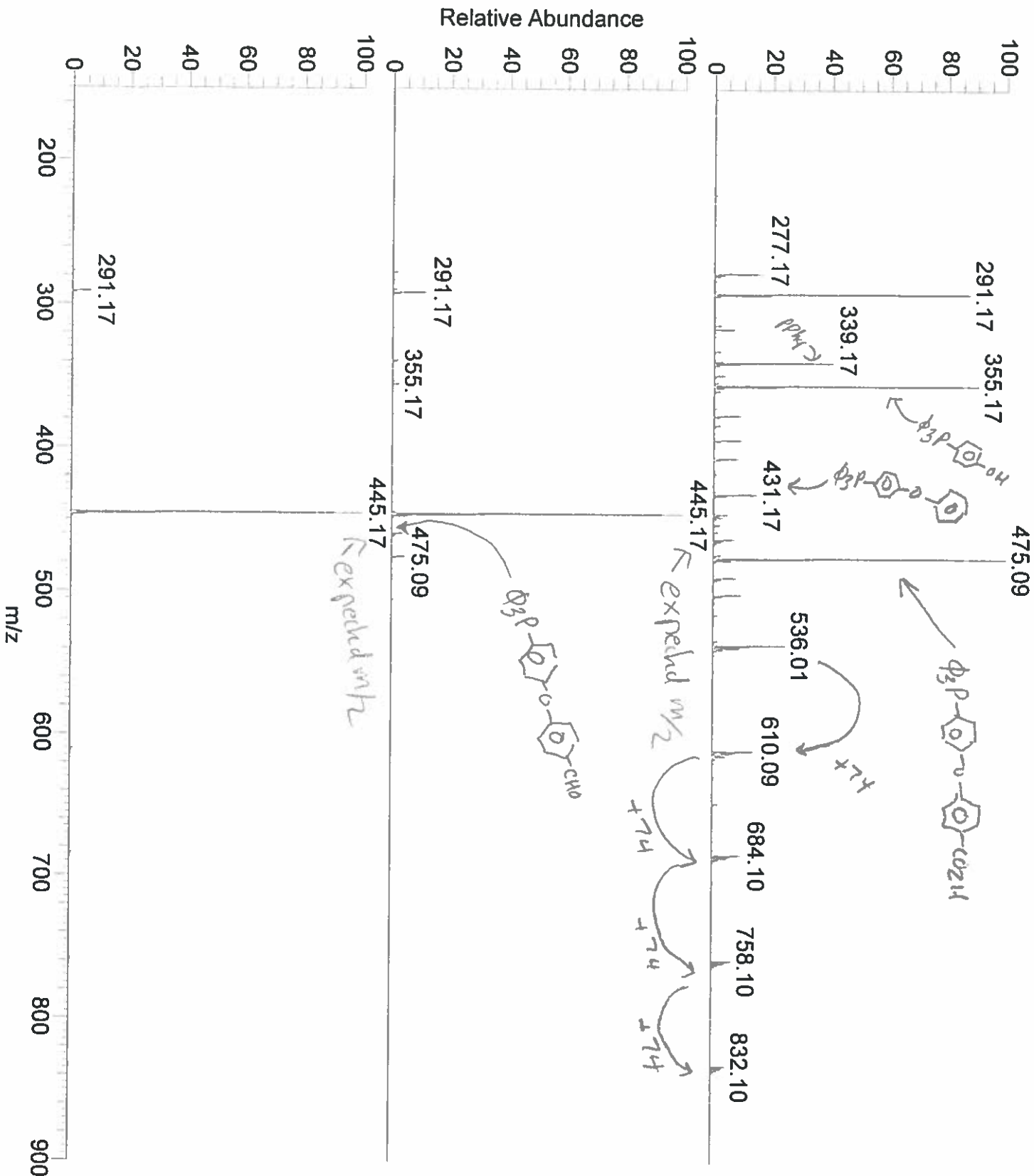
Complete conversion of parent
Mass to alcohol after 300
Degrees C incubation.





Very similar to 336-366 region for sample MSO 500





NL: 5.29E6
619-300#127-138 RT:
0.58-0.63 AV: 12 SB: 8
0.27-0.30 F: ITMS + p
ESI Full ms
[150.00-900.00]

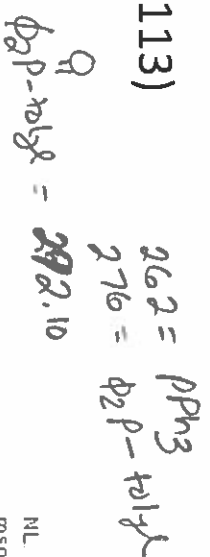
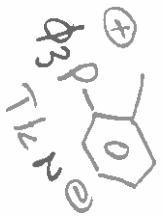
NL: 9.77E7
619-250#115-124 RT:
0.52-0.56 AV: 10 SB: 8
0.27-0.30 F: ITMS + p
ESI Full ms
[150.00-900.00]

NL: 1.06E8
619-200#128-139 RT:
0.58-0.63 AV: 12 SB: 8
0.27-0.30 F: ITMS + p
ESI Full ms
[150.00-900.00]

536
-475
61

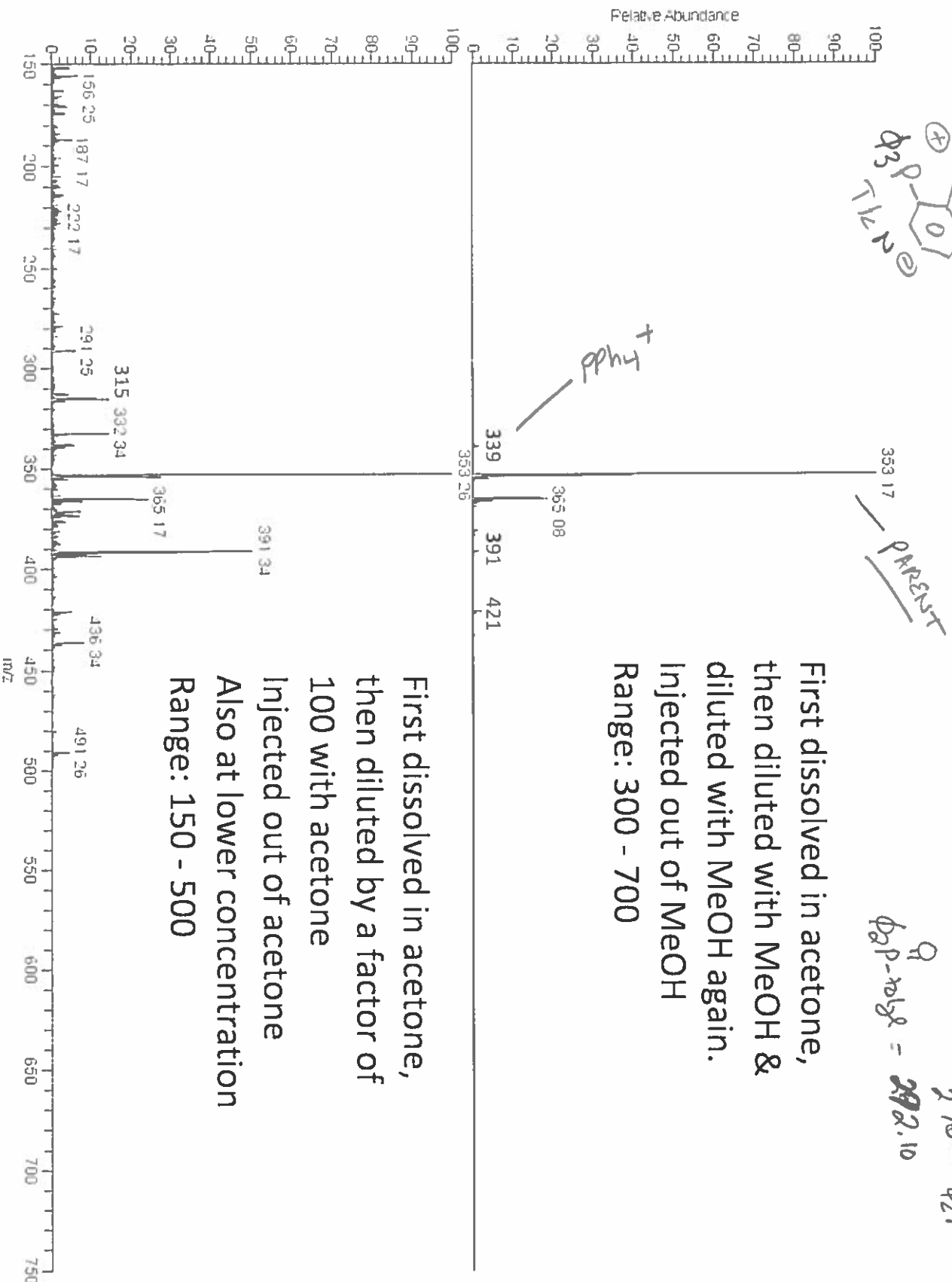
$$C = PPh_3 = 278.29$$

MS0494 (collab notebook pg 113)



NL 112E7
ms0494#182-204 PT
0 79-0 88 AV 23 SB
37 0 15-0 32 T ITMS +
PESIFULMS
[300 00-750 00]

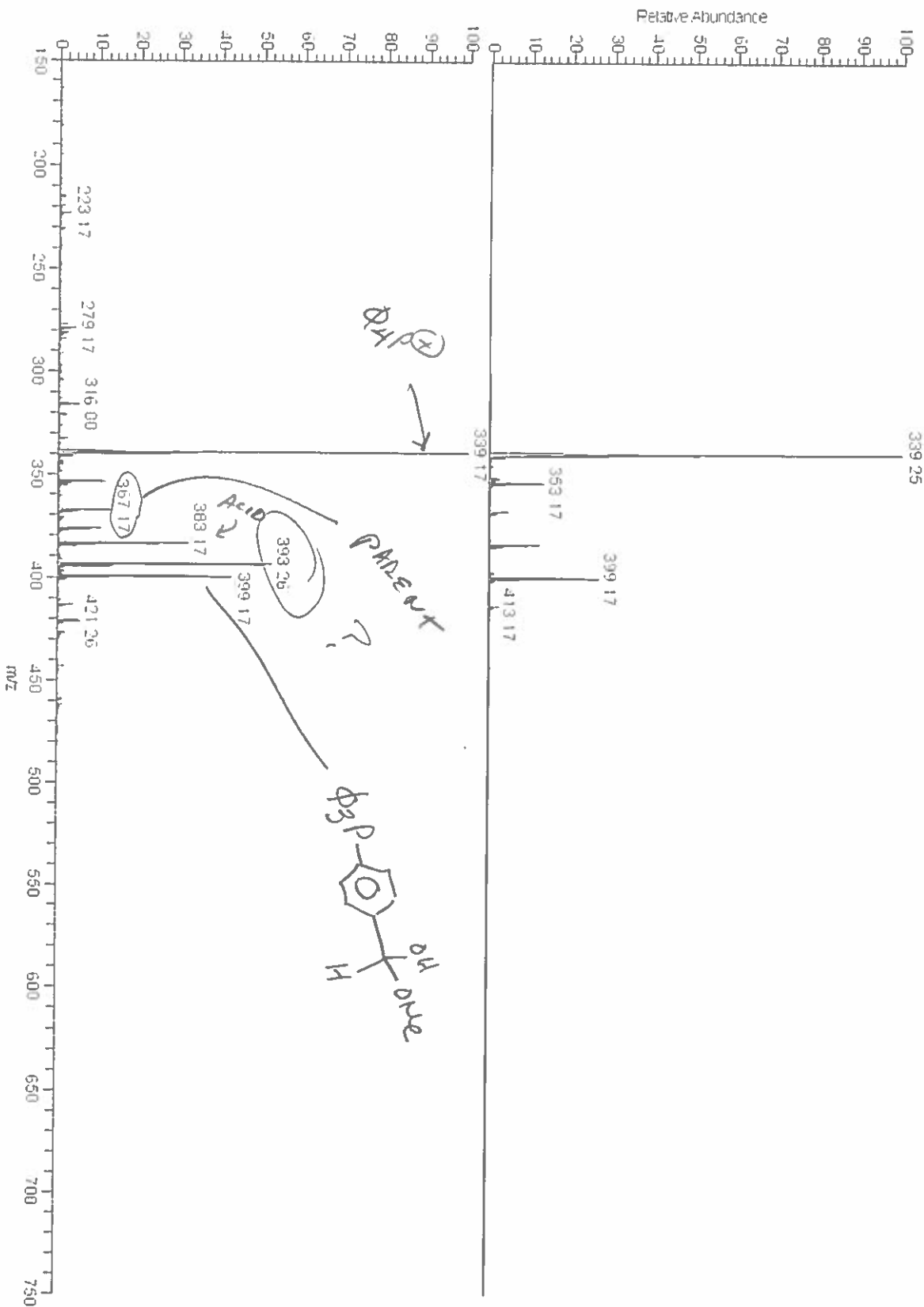
First dissolved in acetone,
then diluted with MeOH &
diluted with MeOH again.
Injected out of MeOH
Range: 300 - 700



NL 492E5
MS0494#133 PT 0 55
AV 1 T ITMS + PESI
Full ms [150 00-500 00]

First dissolved in acetone,
then diluted by a factor of
100 with acetone
Injected out of acetone
Also at lower concentration
Range: 150 - 500

"aldehyde" (collab notebook pg 111 & 113)



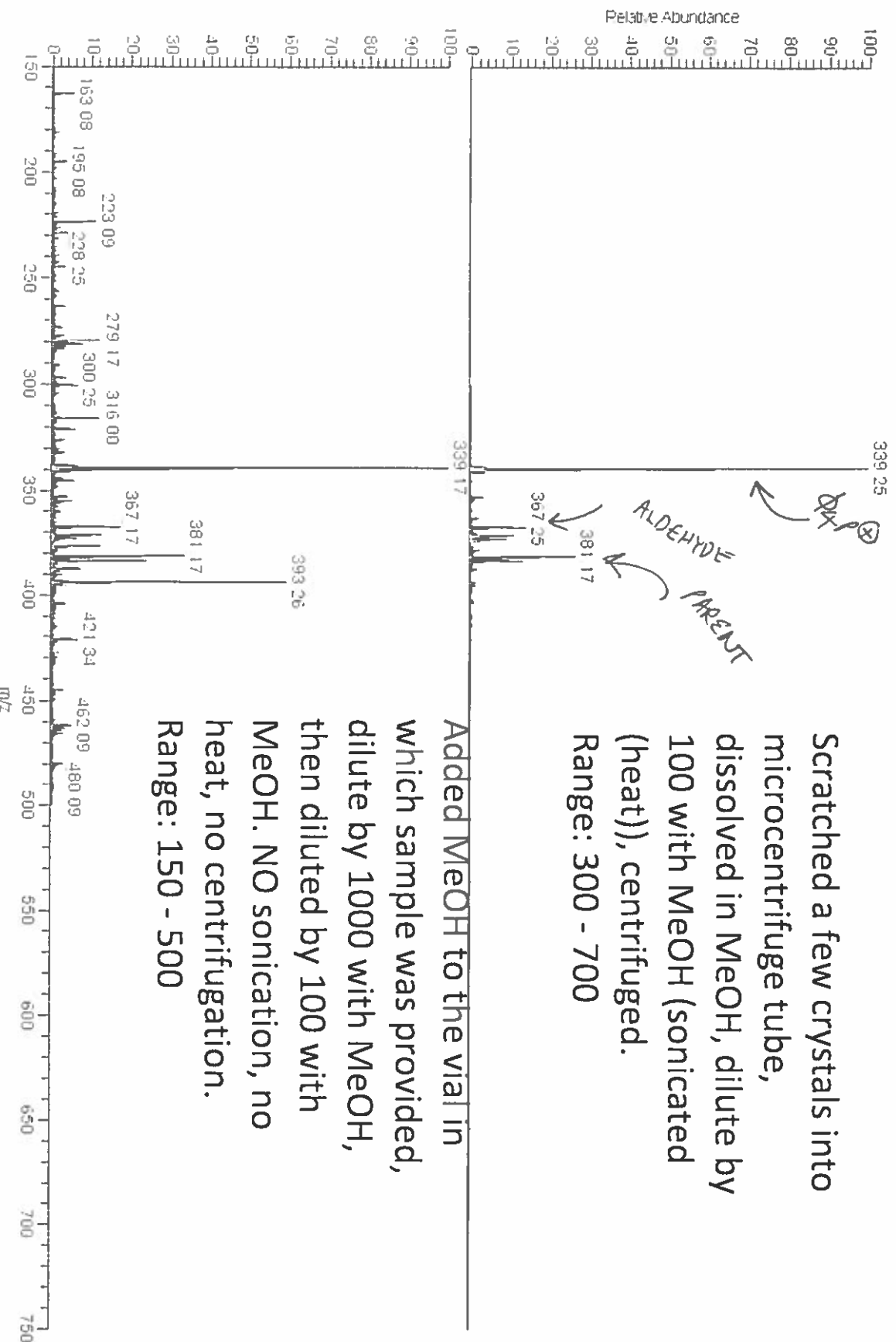
NL 3 38E6
 aldehyde#135-145 PT
 0.61-0.65 AV 11 SB 38
 0.15-0.32 T ITMS + p
 ESIFullms
 [300.00-750.00]

NL 6 55E5
 Aldehyde#142-154 PT
 0.57-0.62 AV 13 SB 38
 0.13-0.28 T ITMS + p
 ESIFullms
 [150.00-500.00]

"ketone" (collab notebook pg 111 & 113)

c:\ccalbur\mdays\2018_nov_20\ketone

11/20/2018 12:44:22 PM



Scatched a few crystals into microcentrifuge tube, dissolved in MeOH, dilute by 100 with MeOH (sonicated (heat)), centrifuged.
Range: 300 - 700

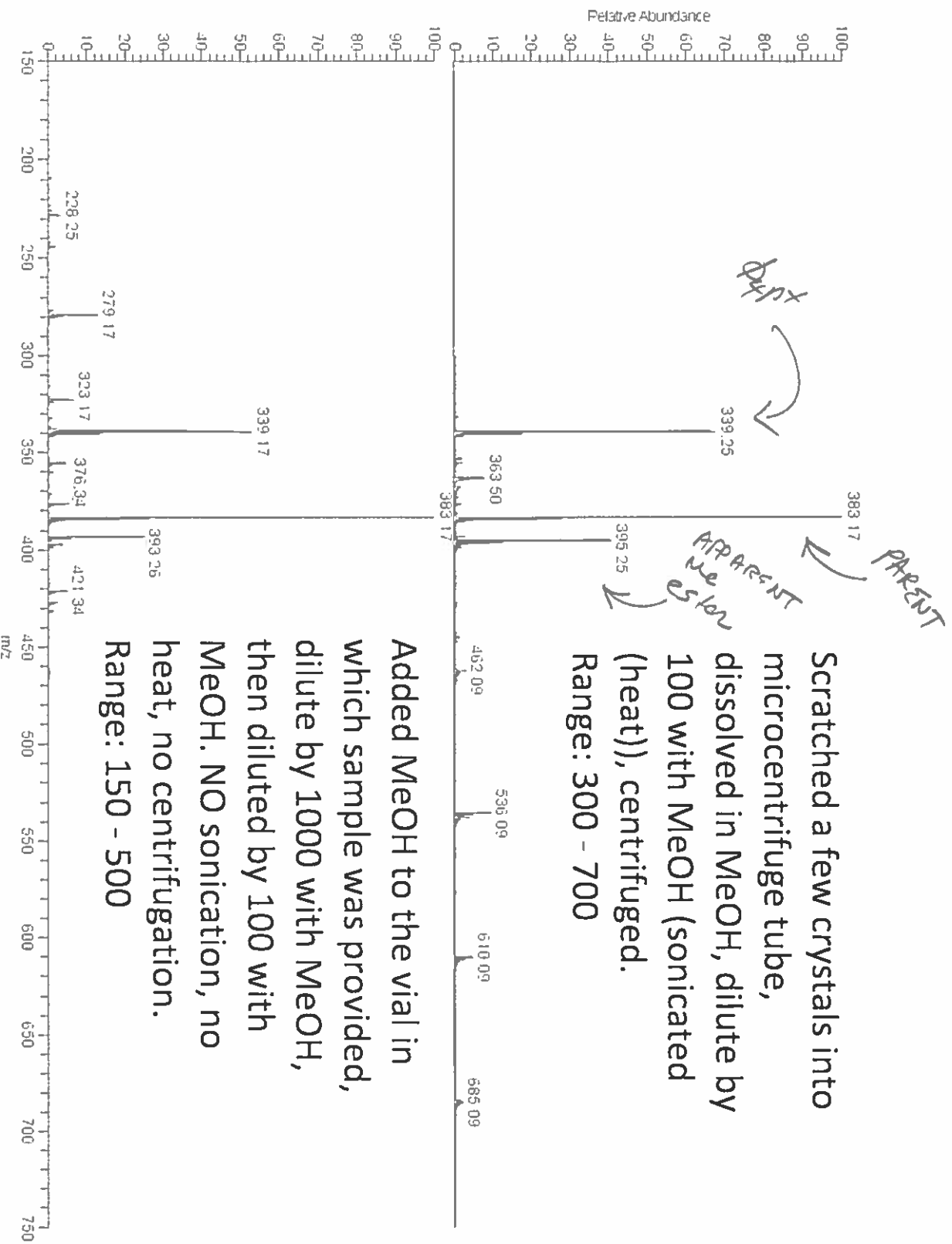
Added MeOH to the vial in which sample was provided, dilute by 1000 with MeOH, then diluted by 100 with MeOH. NO sonication, no heat, no centrifugation.
Range: 150 - 500

NL 1 03E6
ketone#127-142 PT
0 58-0 64 AV 16 SB
38 0 15-0 32 T ITMS +
P ESI Full ms
[300.00-750.00]

NL 7 16E5
ketone#136-152 PT
0 55-0 61 AV 17 SB
38 0 13-0 28 T ITMS +
P ESI Full ms
[150.00-500.00]

"acid" (collab notebook pg 111 & 113)

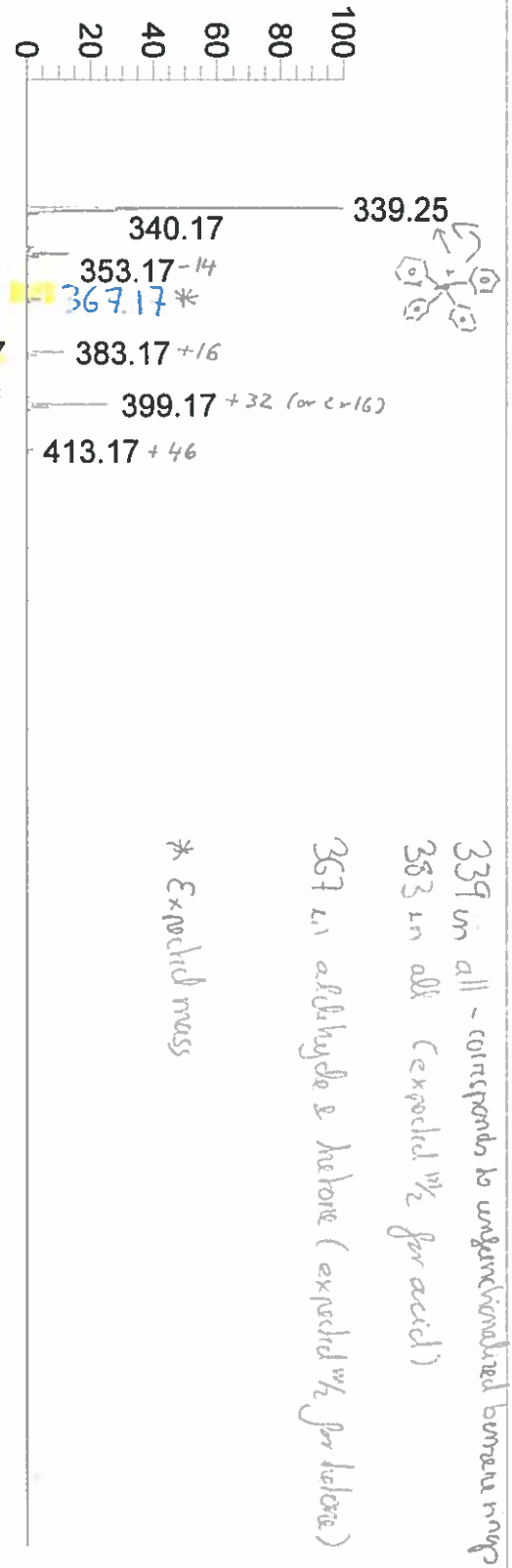
Scratched a few crystals into microcentrifuge tube, dissolved in MeOH, dilute by 100 with MeOH (sonicated (heat)), centrifuged.
Range: 300 - 700



NL 1 19E6
3cid#140-150 PT
0.63-0.67 AV 11 SB
36.0 07-0.23 T 1TMS +
p ESI Full ms
[300.00-750.00]

ML 1 60E6
Acid#140-158 PT
0.56-0.63 AV 19 SB
38.0 13-0.28 T 1TMS +
p ESI Full ms
[150.00-500.00]

Added MeOH to the vial in which sample was provided, dilute by 1000 with MeOH, then diluted by 100 with MeOH. NO sonication, no heat, no centrifugation.
Range: 150 - 500

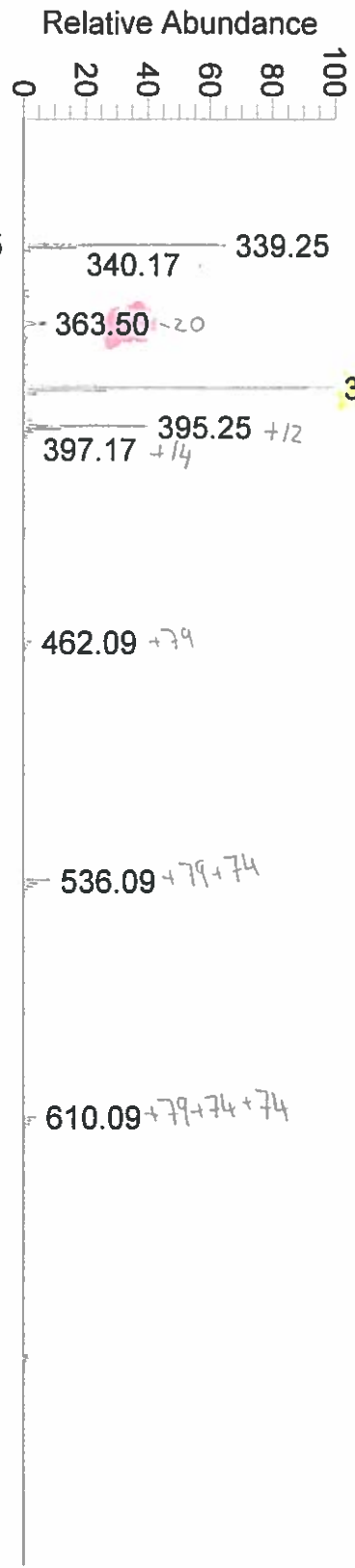


339 in all - corresponds to unfunctionalized benzene ring
383 in all (expected m/z for acid)
367 in aldehyde & ketone (expected m/z for ketone)

* Expected mass

$$\begin{array}{r} 462 \\ - 383 \\ \hline 79 \end{array}$$

NL: 3.38E6
Aldehyde#133-154 RT:
0.60-0.68 AV: 22 SB: 23
0.15-0.25 T: ITMS + p
ESI Full ms
[300.00-750.00]

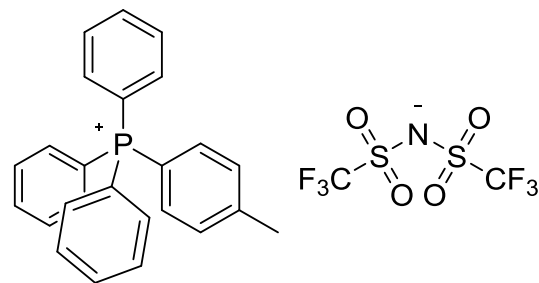


NL: 1.21E6
acid#140-156 RT:
0.63-0.70 AV: 17 SB: 22
0.15-0.25 T: ITMS + p
ESI Full ms
[300.00-750.00]



NL: 9.77E5
Ketone#122-146 RT:
0.56-0.66 AV: 25 SB: 23
0.15-0.25 T: ITMS + p
ESI Full ms
[300.00-750.00]

$$\begin{array}{r} 64 \\ - 67 \\ \hline 12 \end{array}$$



Pyrolysis off-gases

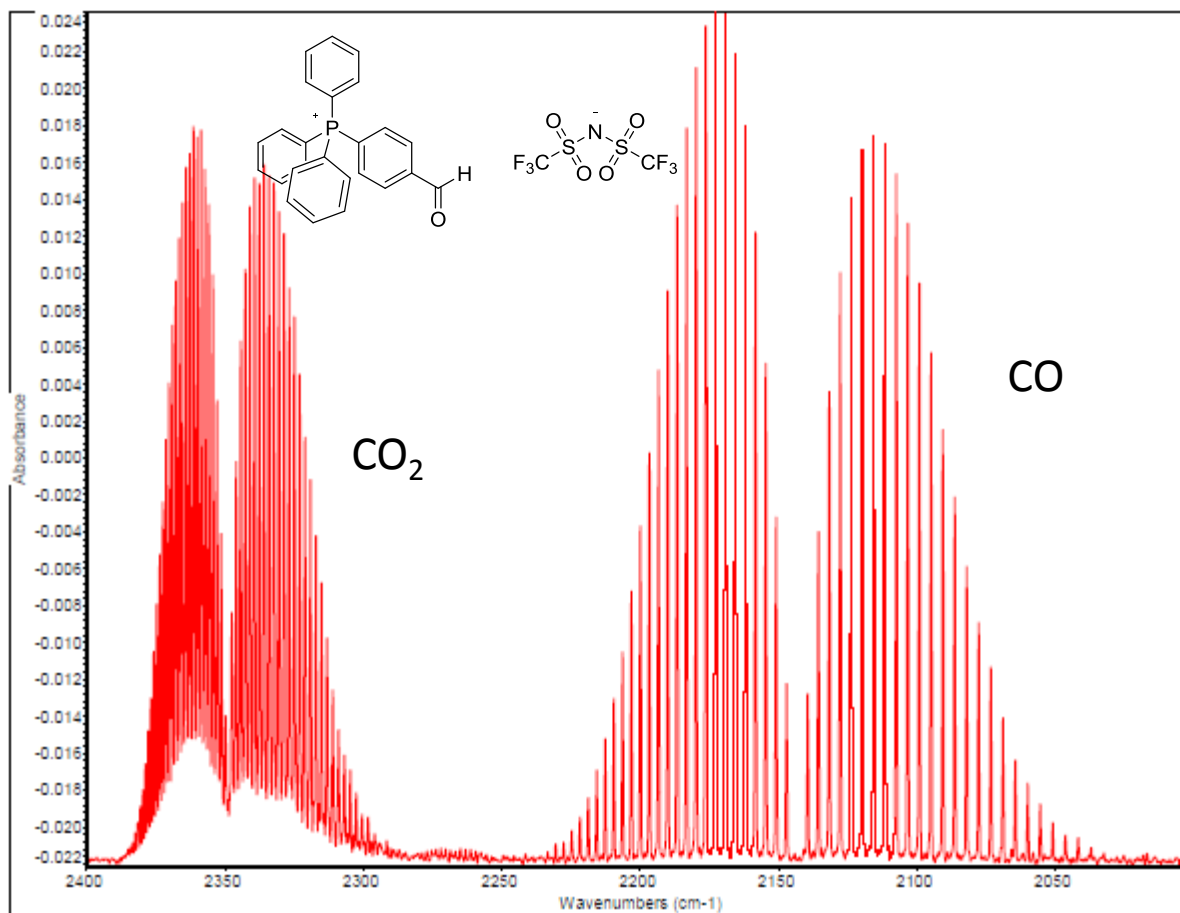
Absorbance

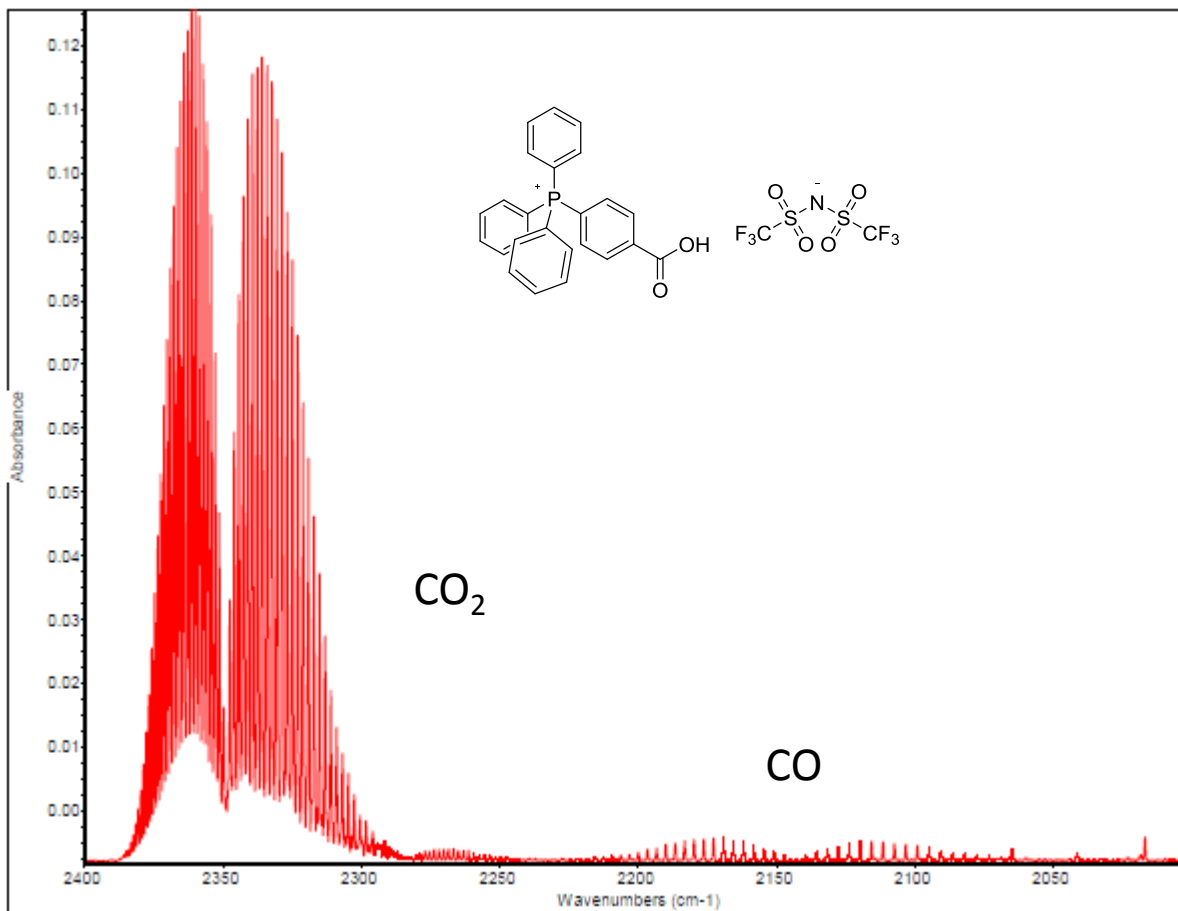
CO_2

Putative O-C-N containing
species from anion
decomposition

CO

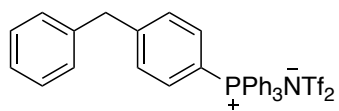
Wavenumbers (cm^{-1})



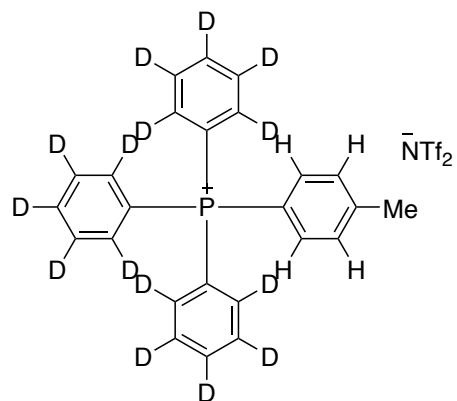


Key to structures for TGA scans

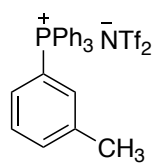
MS0441



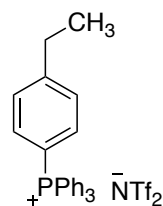
MS0468



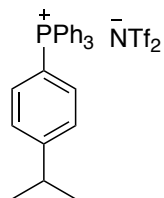
MS0477



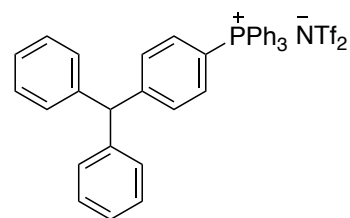
MS0500



MS0503



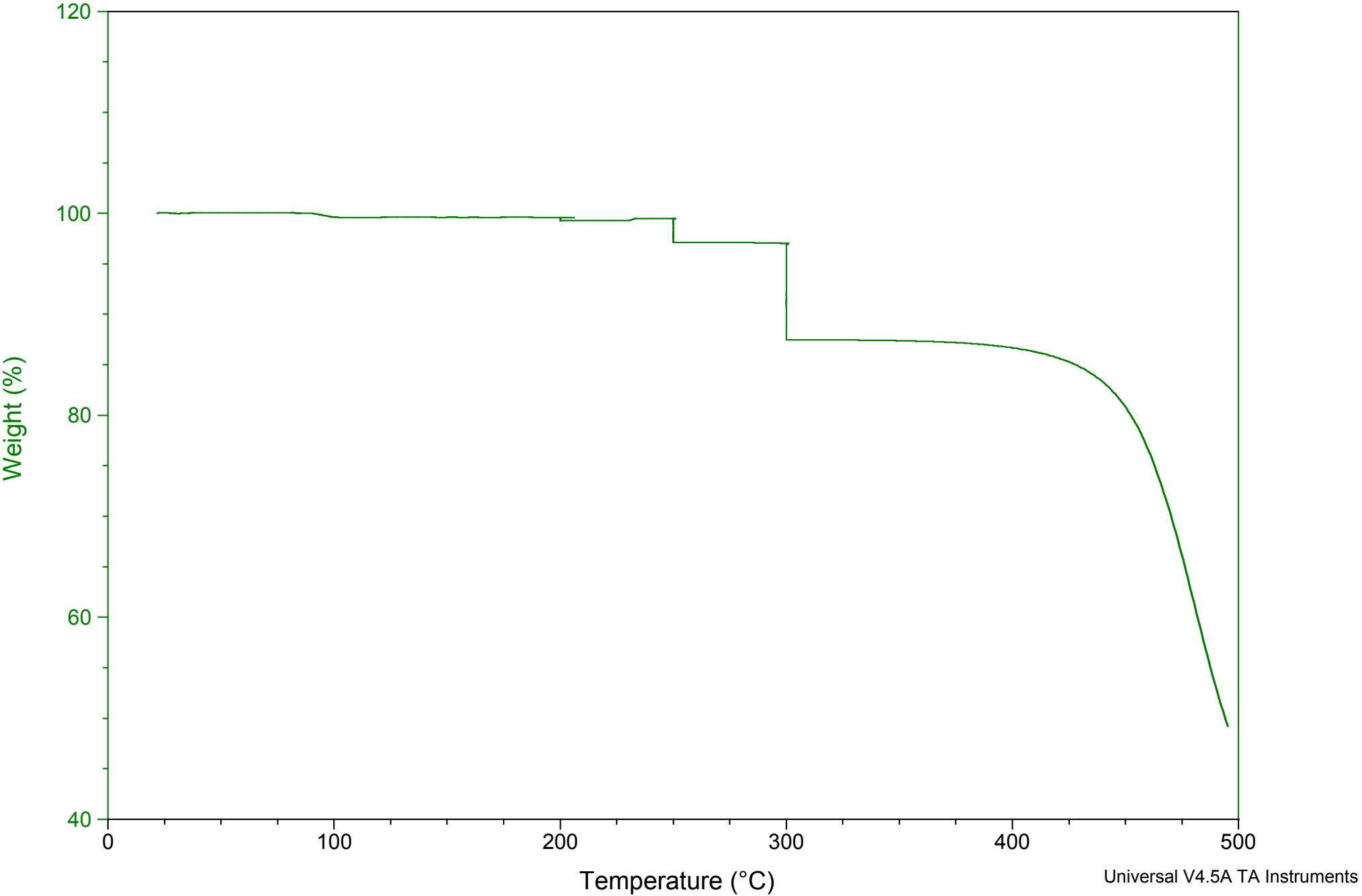
MS0630



Sample: 441
Size: 12.7630 mg
Method: test

TGA

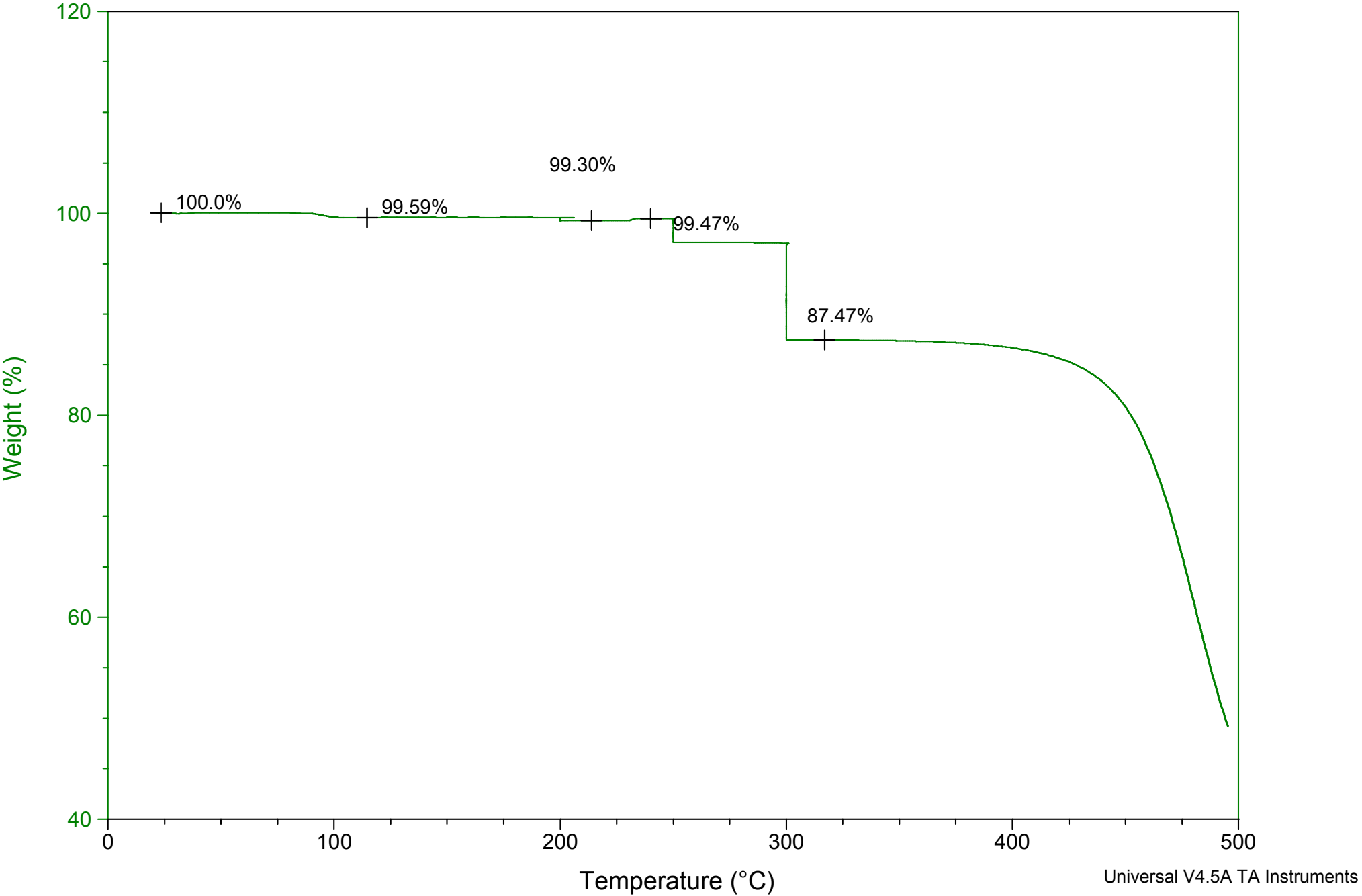
File: C:\...MS\1 min ramp rate\36 h\441.002
Run Date: 22-Apr-2019 08:28
Instrument: TGA Q500 V20.2 Build 27



Sample: 441
Size: 12.7630 mg
Method: test

TGA

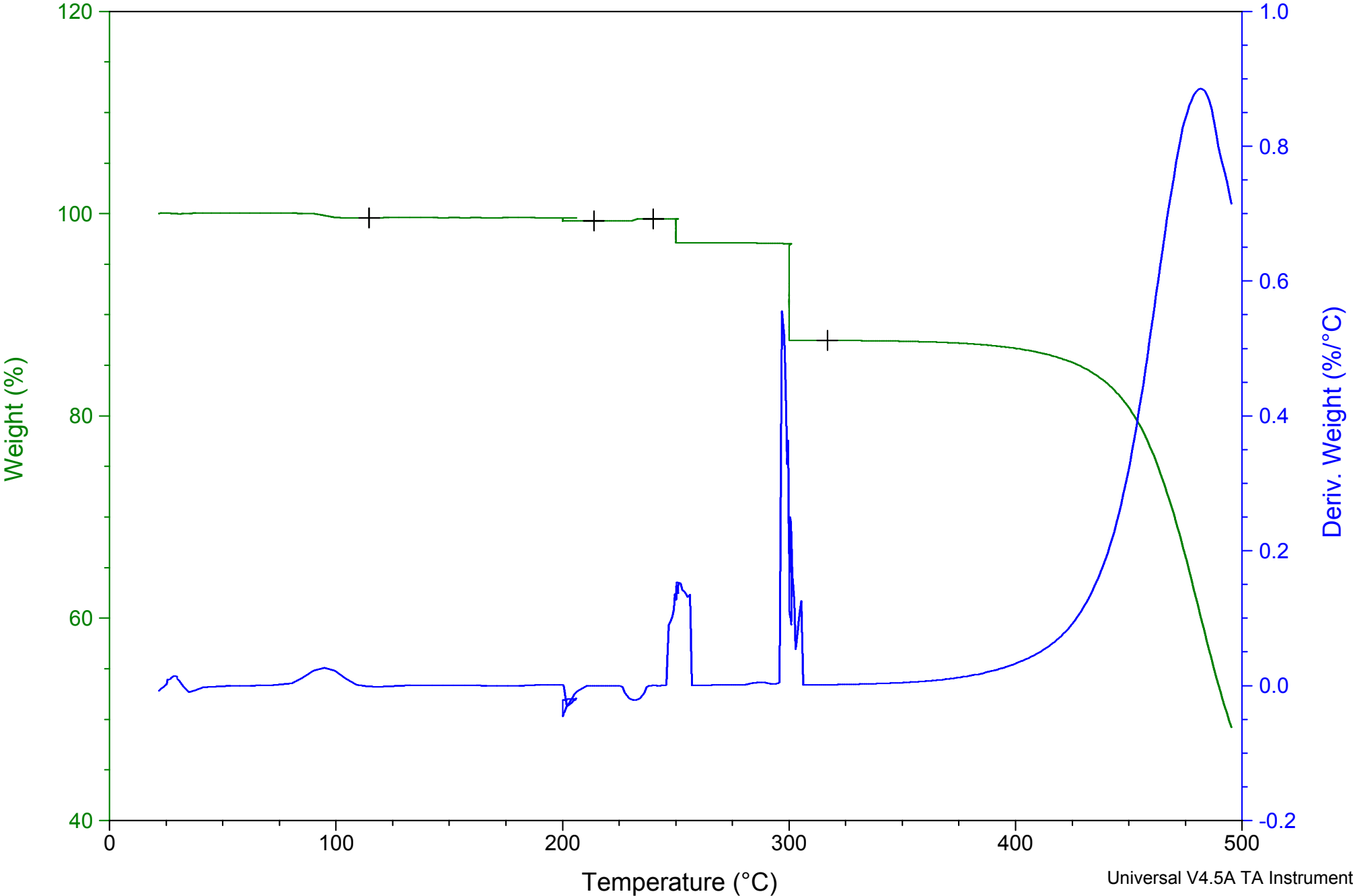
File: C:\...MS\1 min ramp rate\36 h\441.002
Run Date: 22-Apr-2019 08:28
Instrument: TGA Q500 V20.2 Build 27



Sample: 441
Size: 12.7630 mg
Method: test

TGA

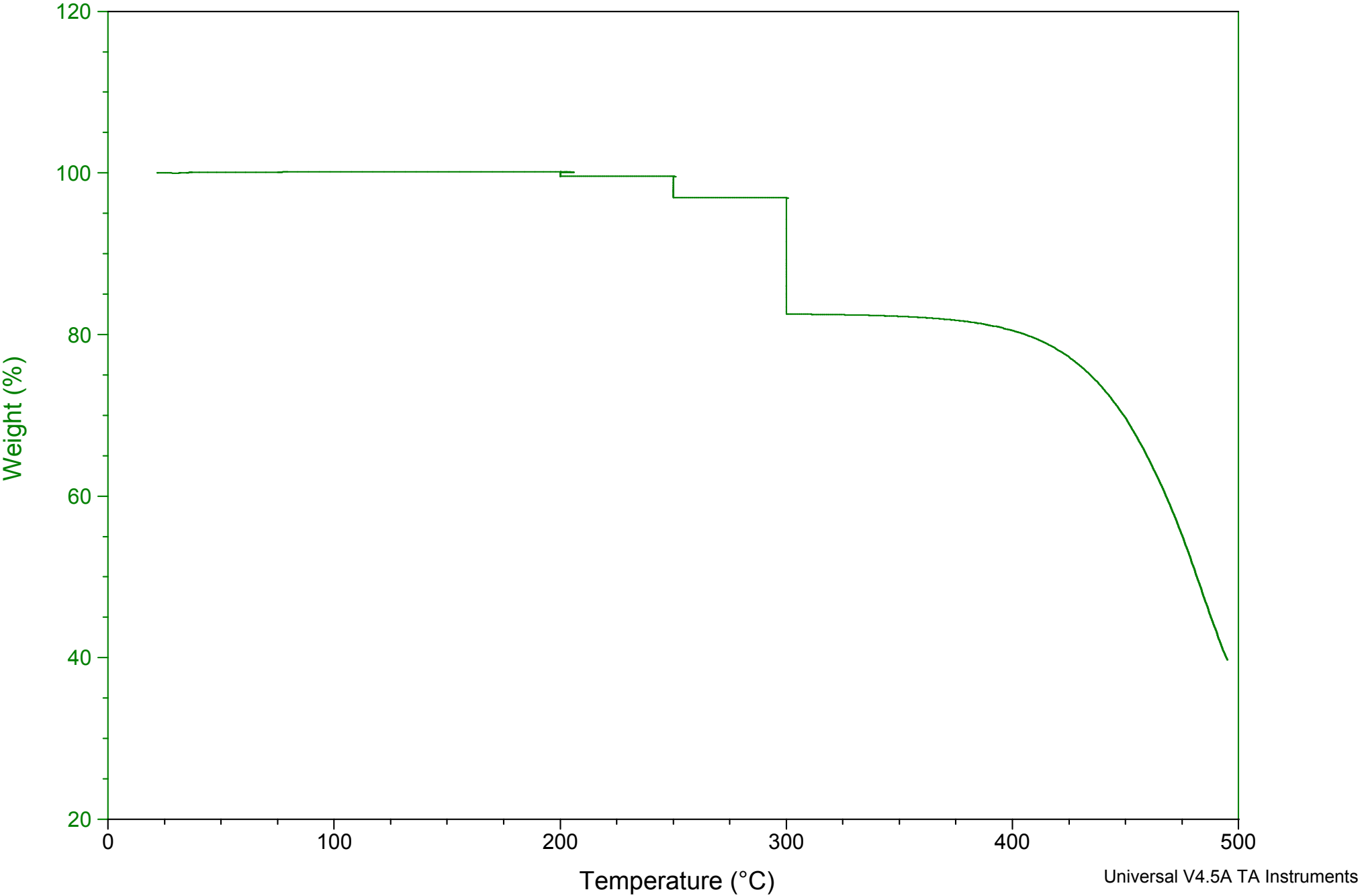
File: C:\...MS\1 min ramp rate\36 h\441.002
Run Date: 22-Apr-2019 08:28
Instrument: TGA Q500 V20.2 Build 27



Sample: 468
Size: 12.3470 mg
Method: test

TGA

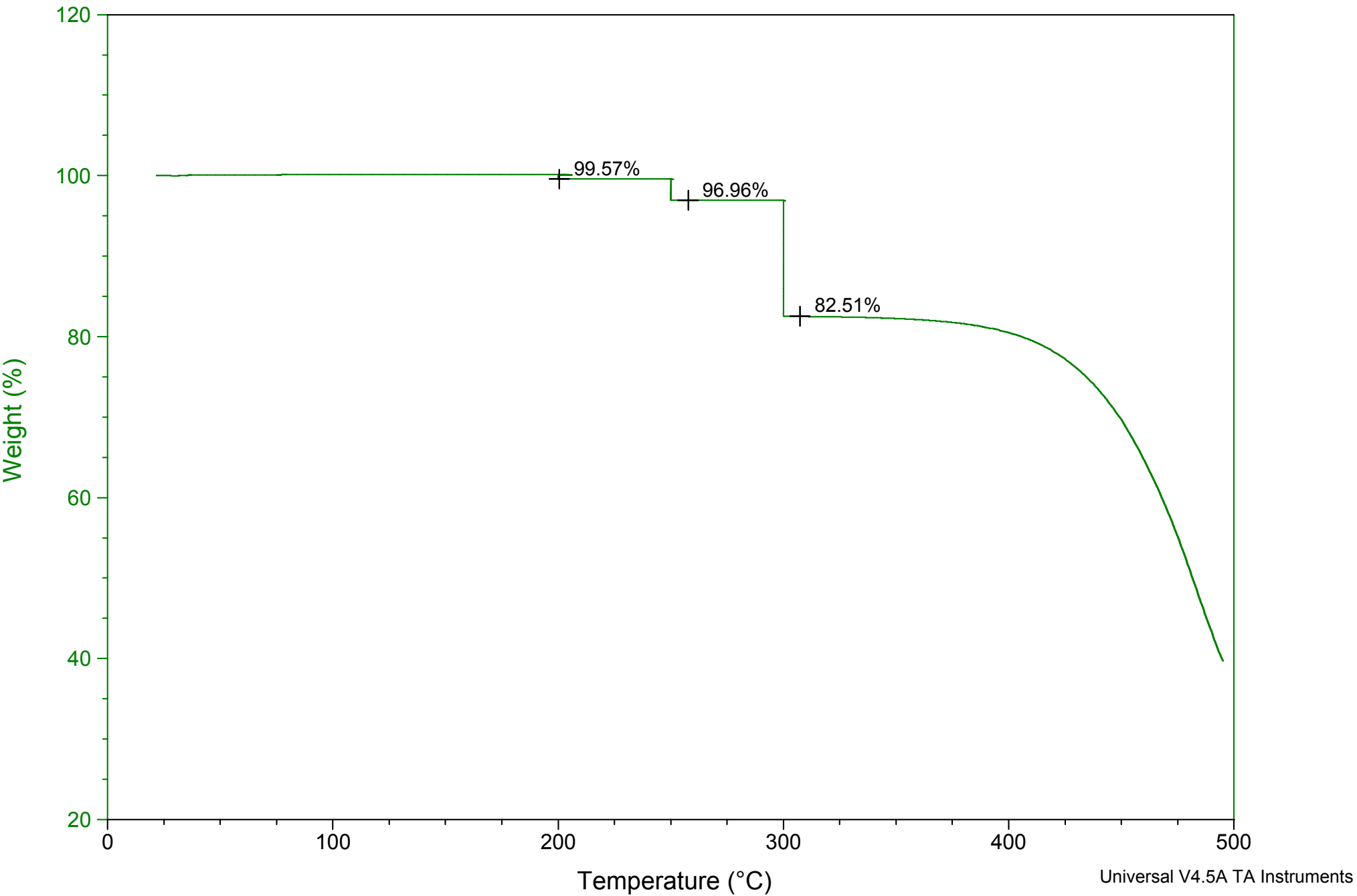
File: C:\...MS\1 min ramp rate\36 h\468.002
Run Date: 19-Apr-2019 09:07
Instrument: TGA Q500 V20.2 Build 27



Sample: 468
Size: 12.3470 mg
Method: test

TGA

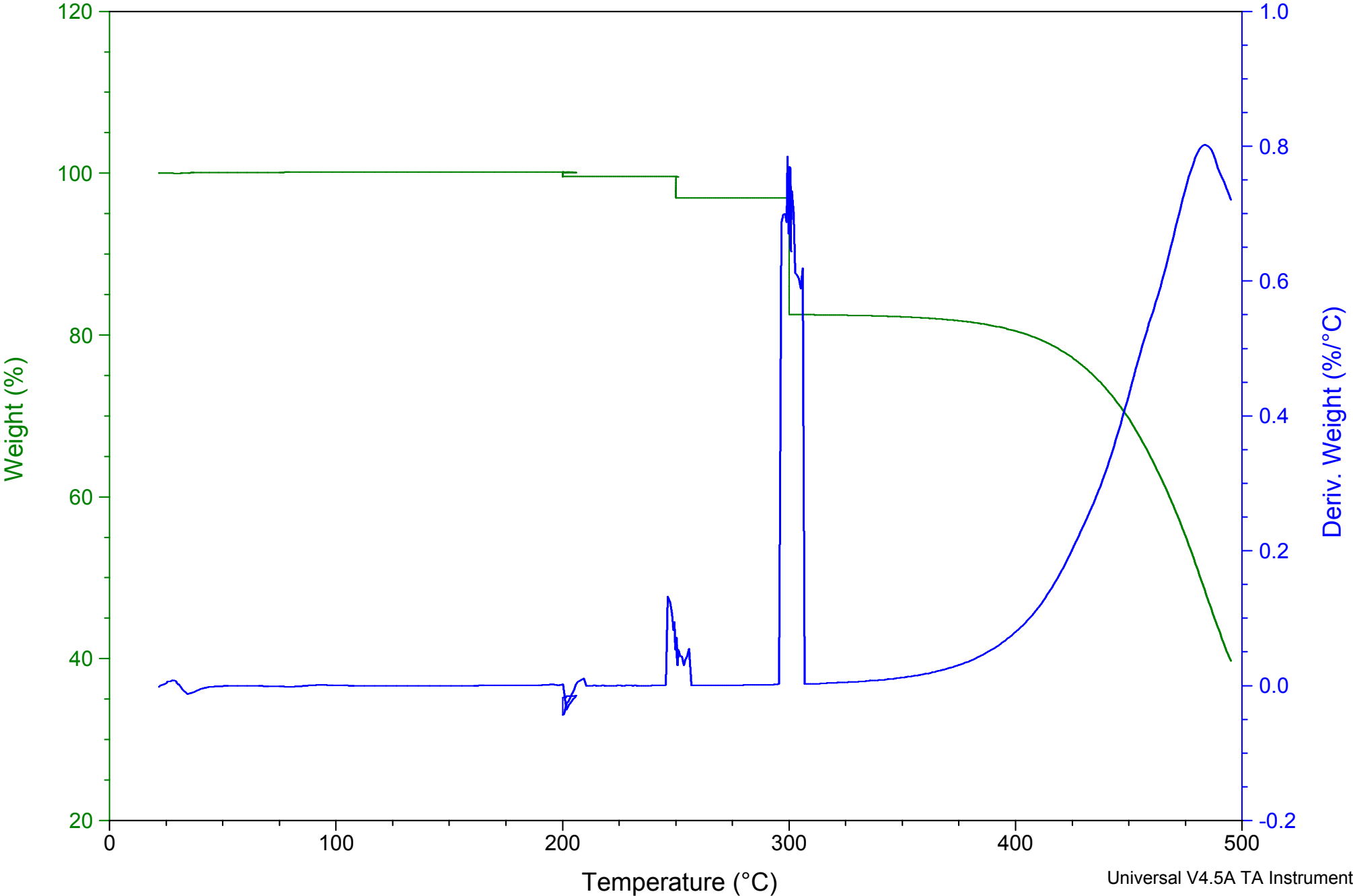
File: C:\...MS\1 min ramp rate\36 h\468.002
Run Date: 19-Apr-2019 09:07
Instrument: TGA Q500 V20.2 Build 27



Sample: 468
Size: 12.3470 mg
Method: test

TGA

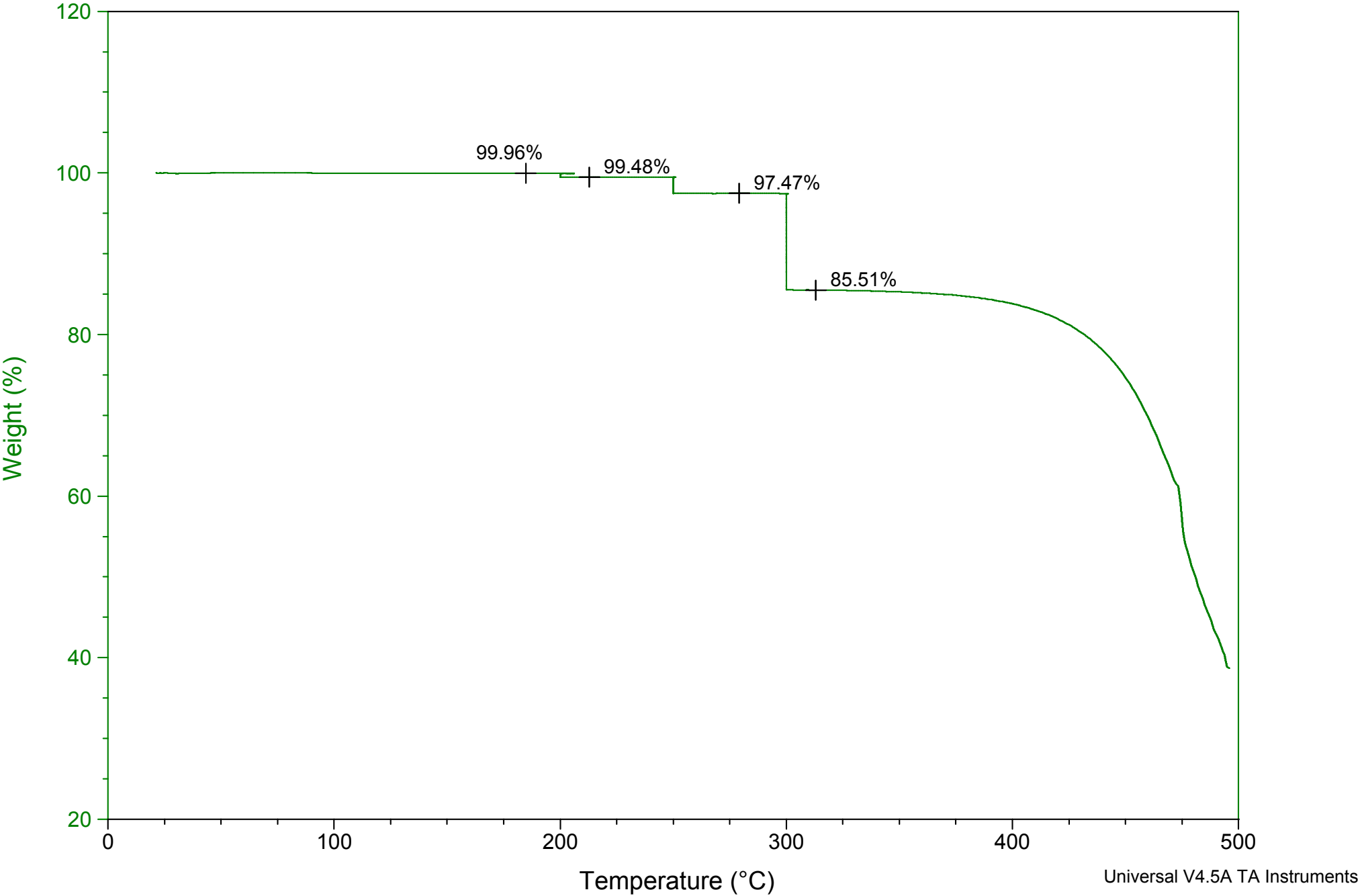
File: C:\...MS\1 min ramp rate\36 h\468.002
Run Date: 19-Apr-2019 09:07
Instrument: TGA Q500 V20.2 Build 27



Sample: 477
Size: 16.9800 mg
Method: test

TGA

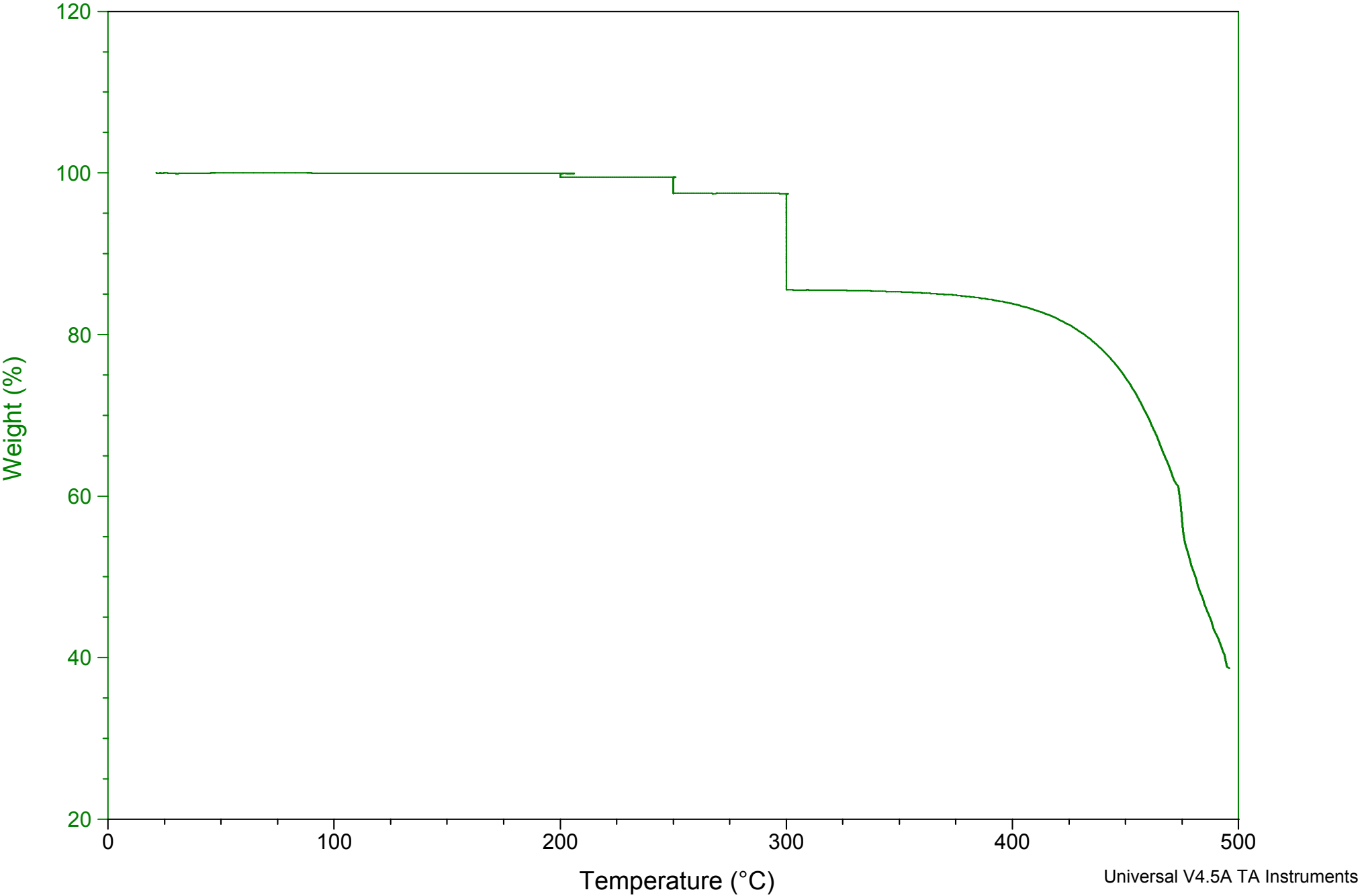
File: C:\...MS\1 min ramp rate\36 h\477.001
Run Date: 05-Apr-2019 09:34
Instrument: TGA Q500 V20.2 Build 27



Sample: 477
Size: 16.9800 mg
Method: test

TGA

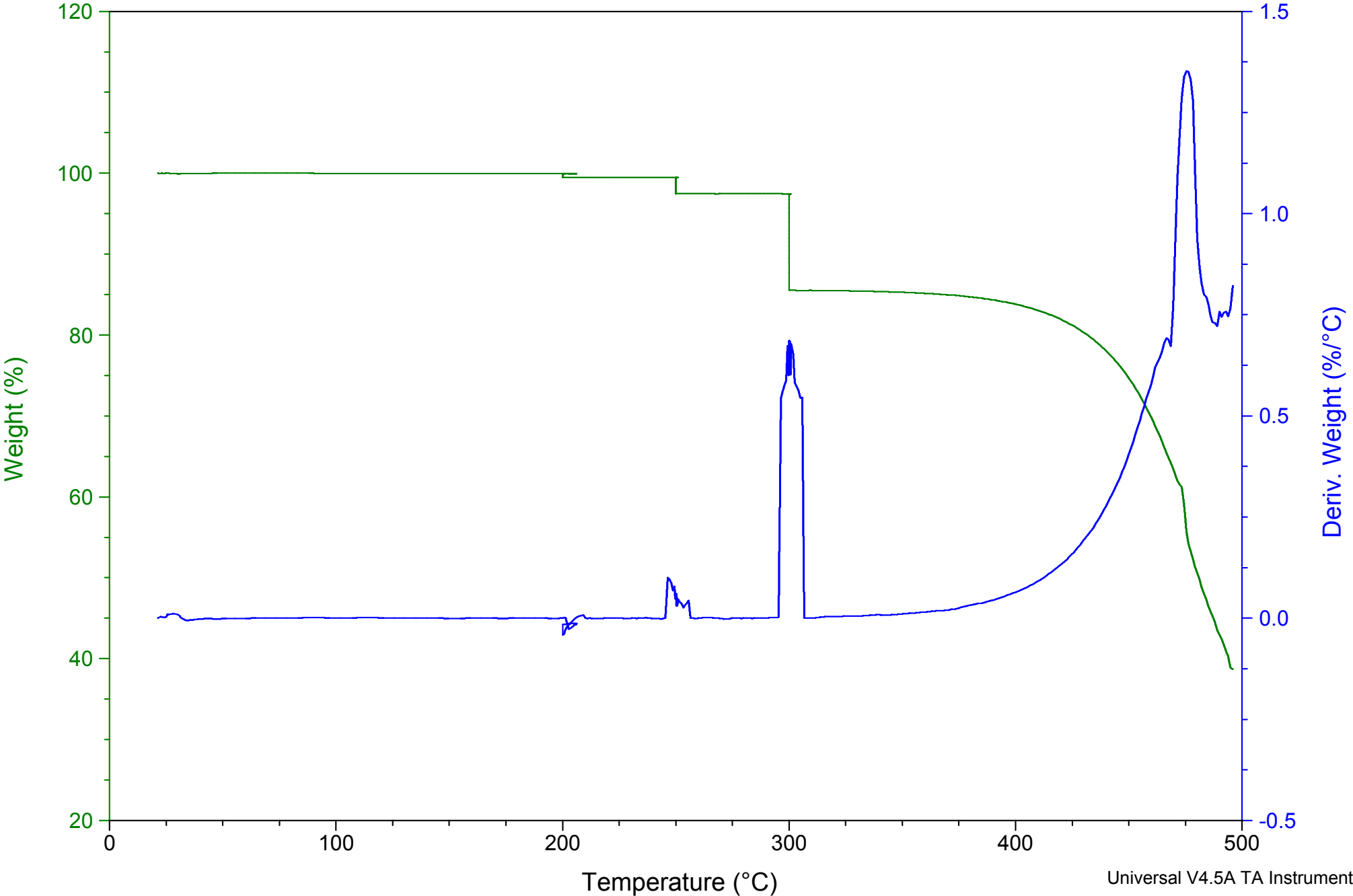
File: C:\...MS\1 min ramp rate\36 h\477.001
Run Date: 05-Apr-2019 09:34
Instrument: TGA Q500 V20.2 Build 27



Sample: 477
Size: 16.9800 mg
Method: test

TGA

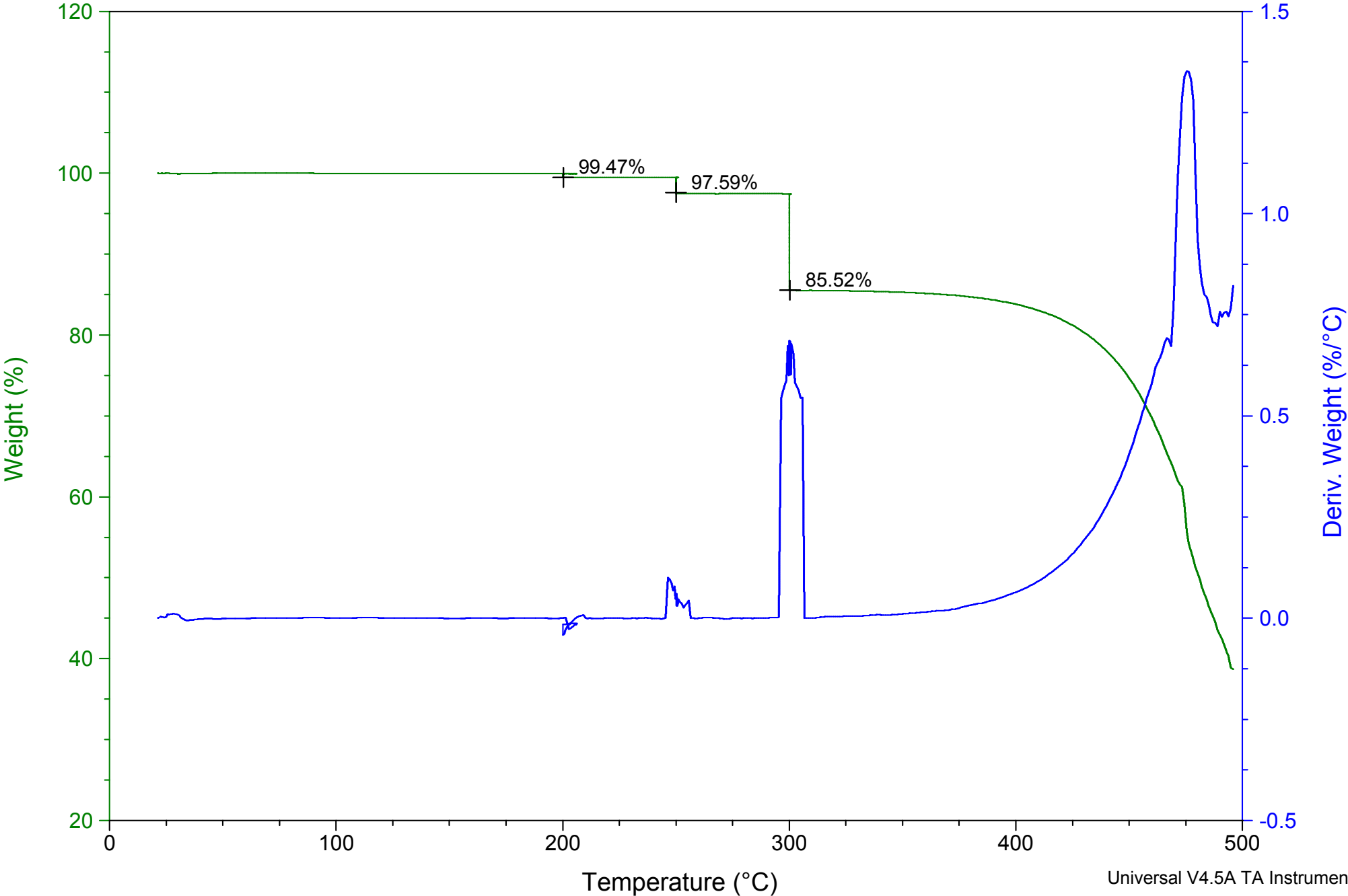
File: C:\...MS\1 min ramp rate\36 h\477.001
Run Date: 05-Apr-2019 09:34
Instrument: TGA Q500 V20.2 Build 27



Sample: 477
Size: 16.9800 mg
Method: test

TGA

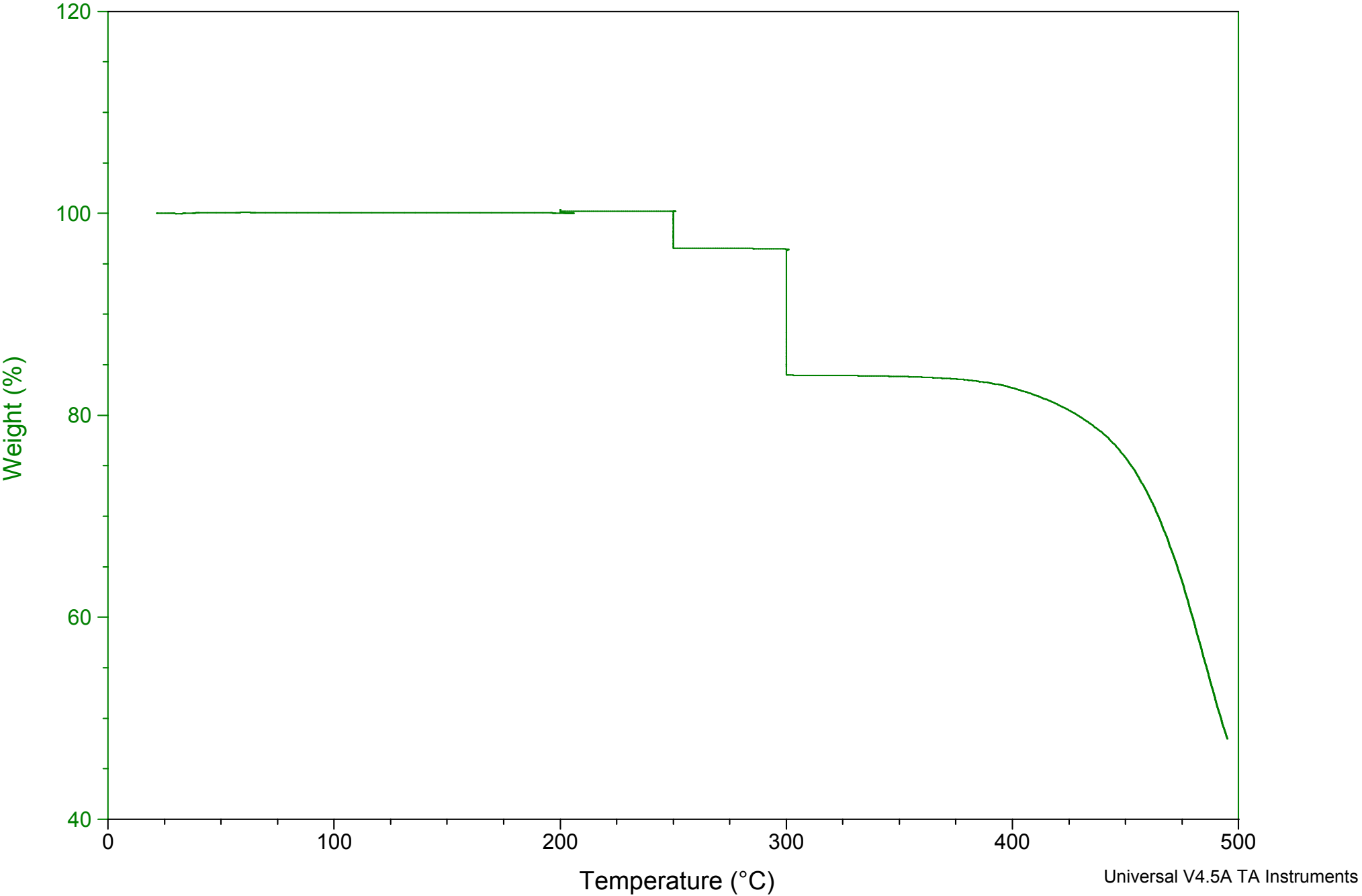
File: C:\...MS\1 min ramp rate\36 h\477.001
Run Date: 05-Apr-2019 09:34
Instrument: TGA Q500 V20.2 Build 27



Sample: 500
Size: 13.5770 mg
Method: test

TGA

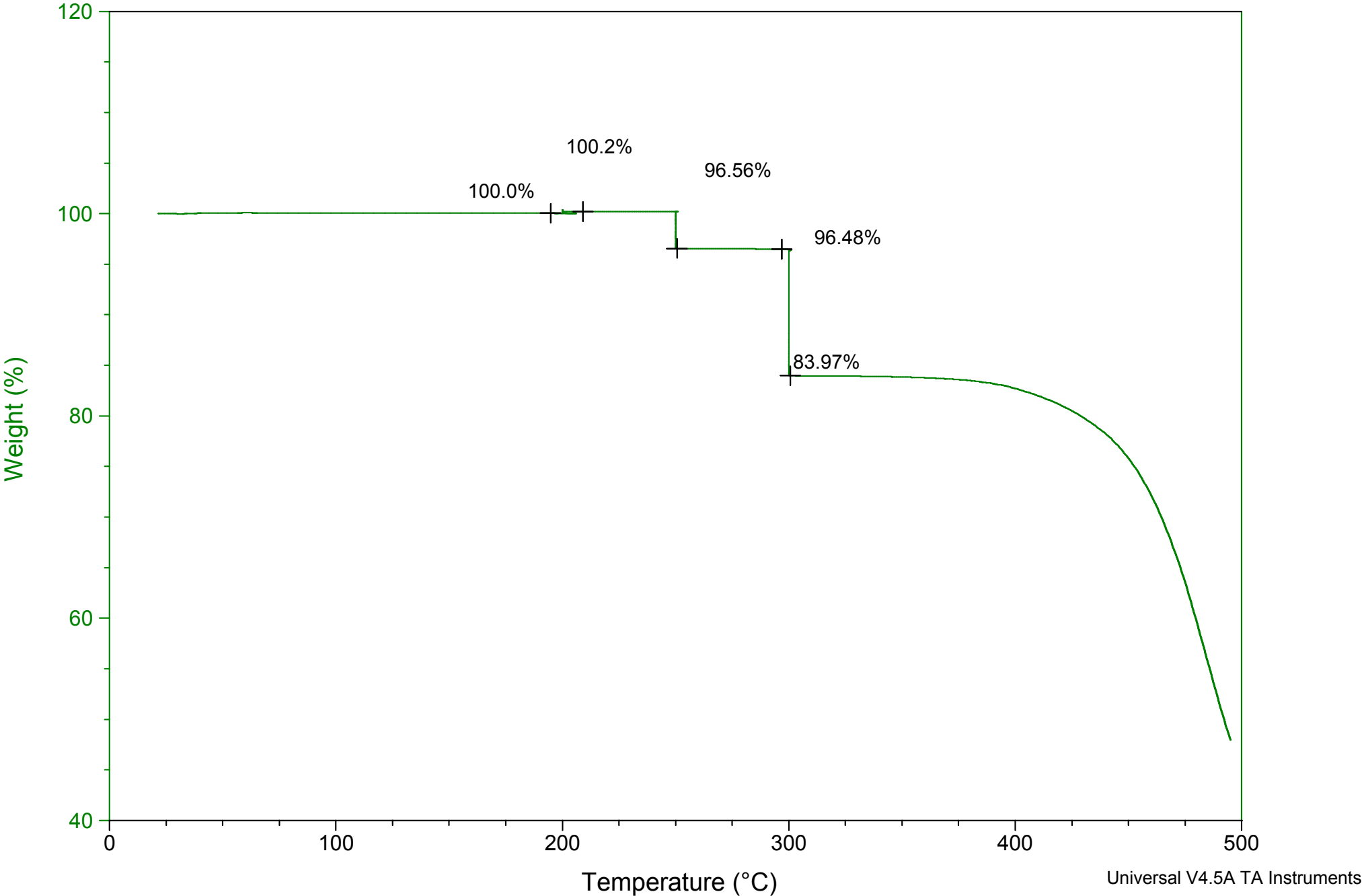
File: C:\...MS\1 min ramp rate\36 h\500.003
Run Date: 15-Apr-2019 10:36
Instrument: TGA Q500 V20.2 Build 27



Sample: 500
Size: 13.5770 mg
Method: test

TGA

File: C:\...MS\1 min ramp rate\36 h\500.003
Run Date: 15-Apr-2019 10:36
Instrument: TGA Q500 V20.2 Build 27



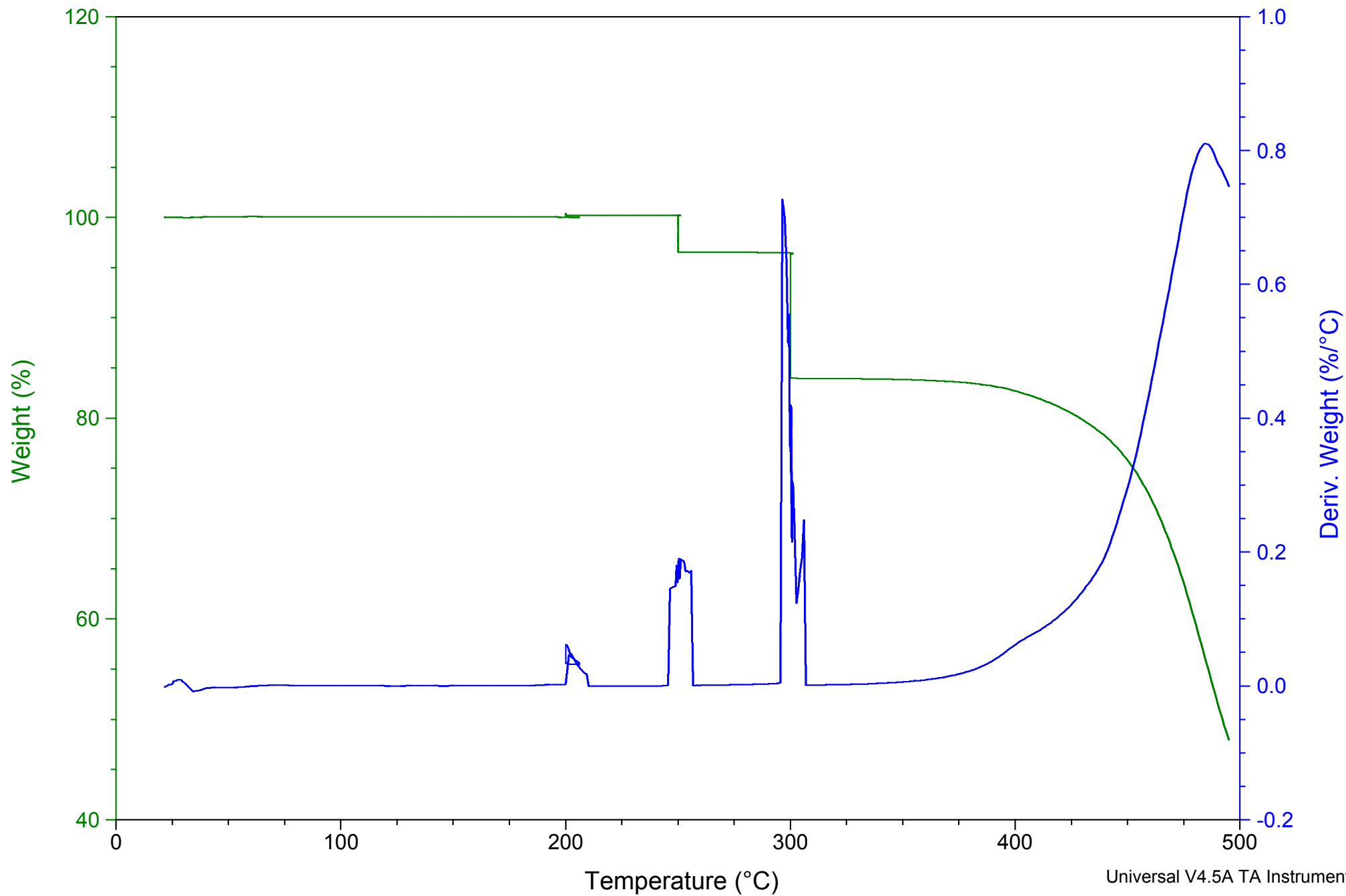
Sample: 500
Size: 13.5770 mg
Method: test

TGA

File: C:\...MS\1 min ramp rate\36 h\500.003

Run Date: 15-Apr-2019 10:36

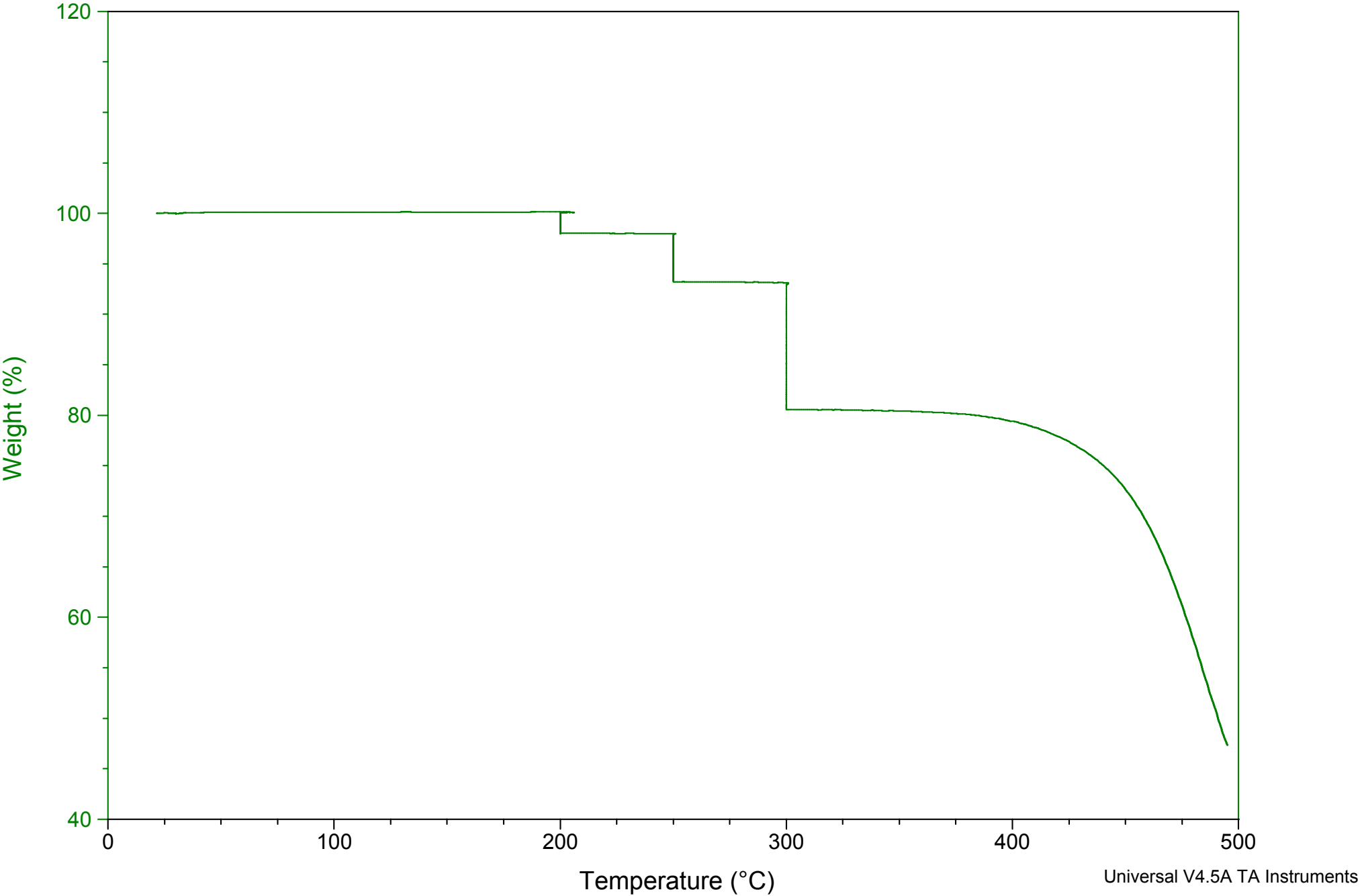
Instrument: TGA Q500 V20.2 Build 27



Sample: 503
Size: 10.3000 mg
Method: test

TGA

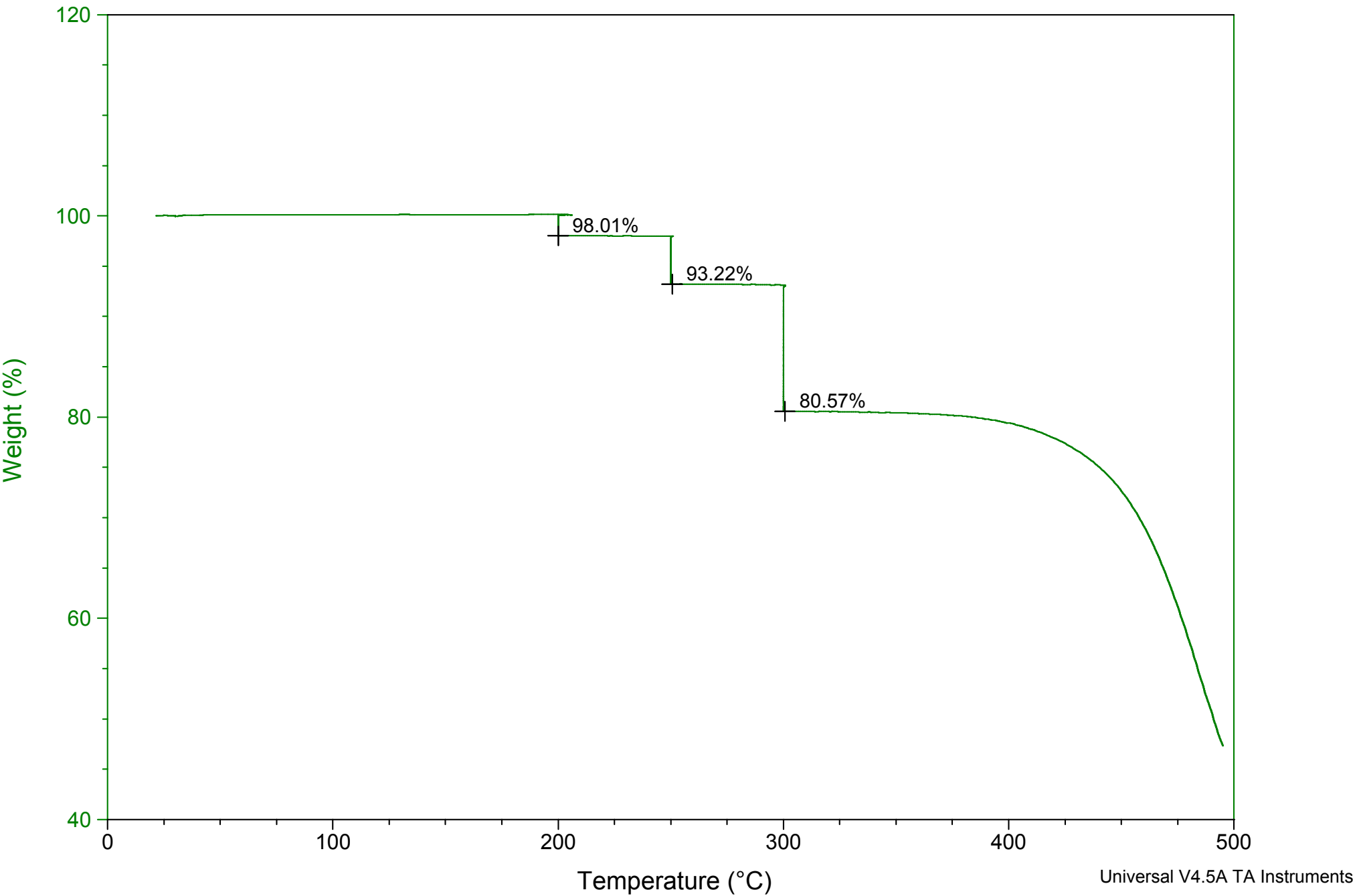
File: C:\...MS\1 min ramp rate\36 h\503.001
Run Date: 10-Apr-2019 09:17
Instrument: TGA Q500 V20.2 Build 27



Sample: 503
Size: 10.3000 mg
Method: test

TGA

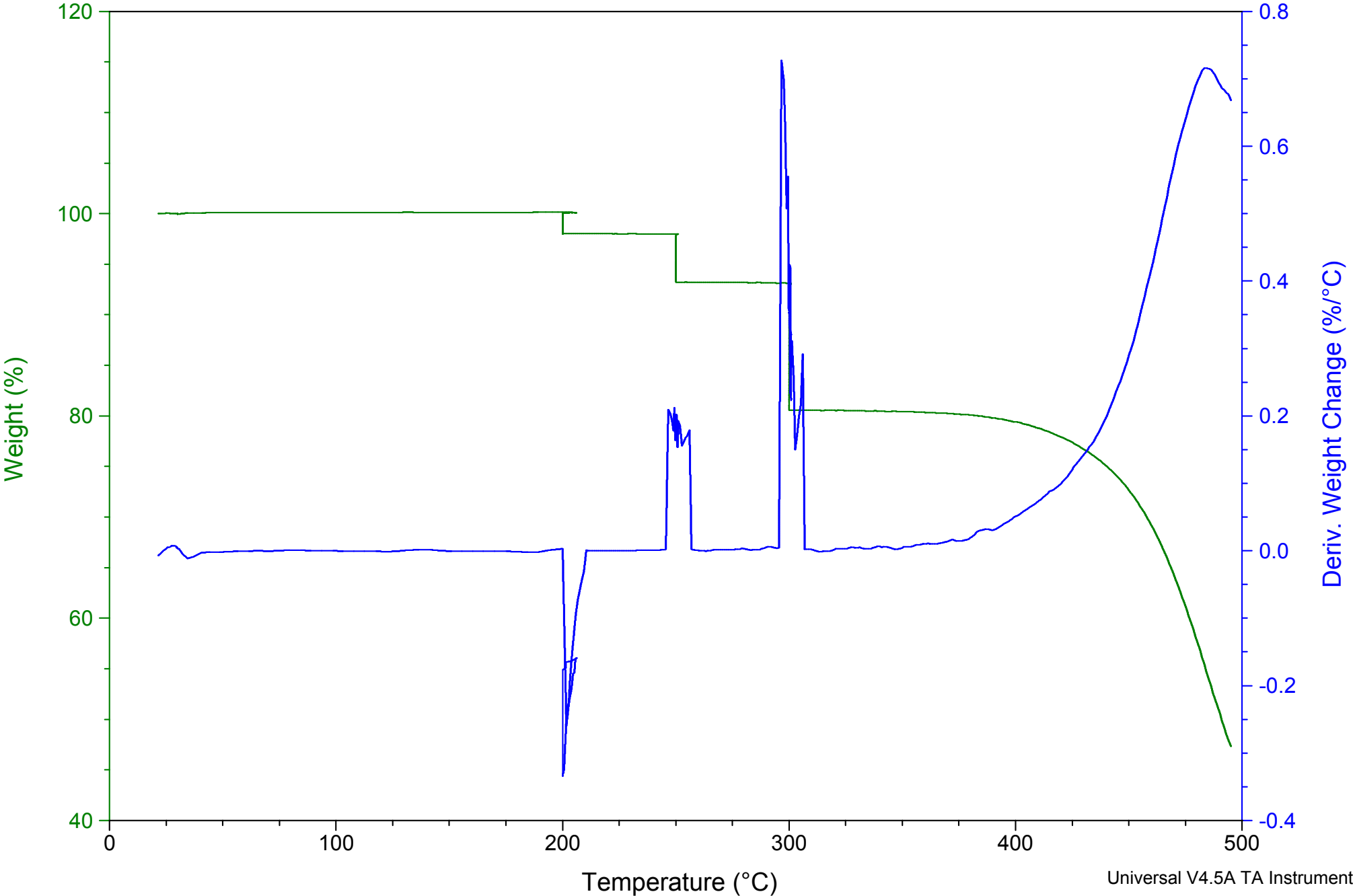
File: C:\...MS\1 min ramp rate\36 h\503.001
Run Date: 10-Apr-2019 09:17
Instrument: TGA Q500 V20.2 Build 27



Sample: 503
Size: 10.3000 mg
Method: test

TGA

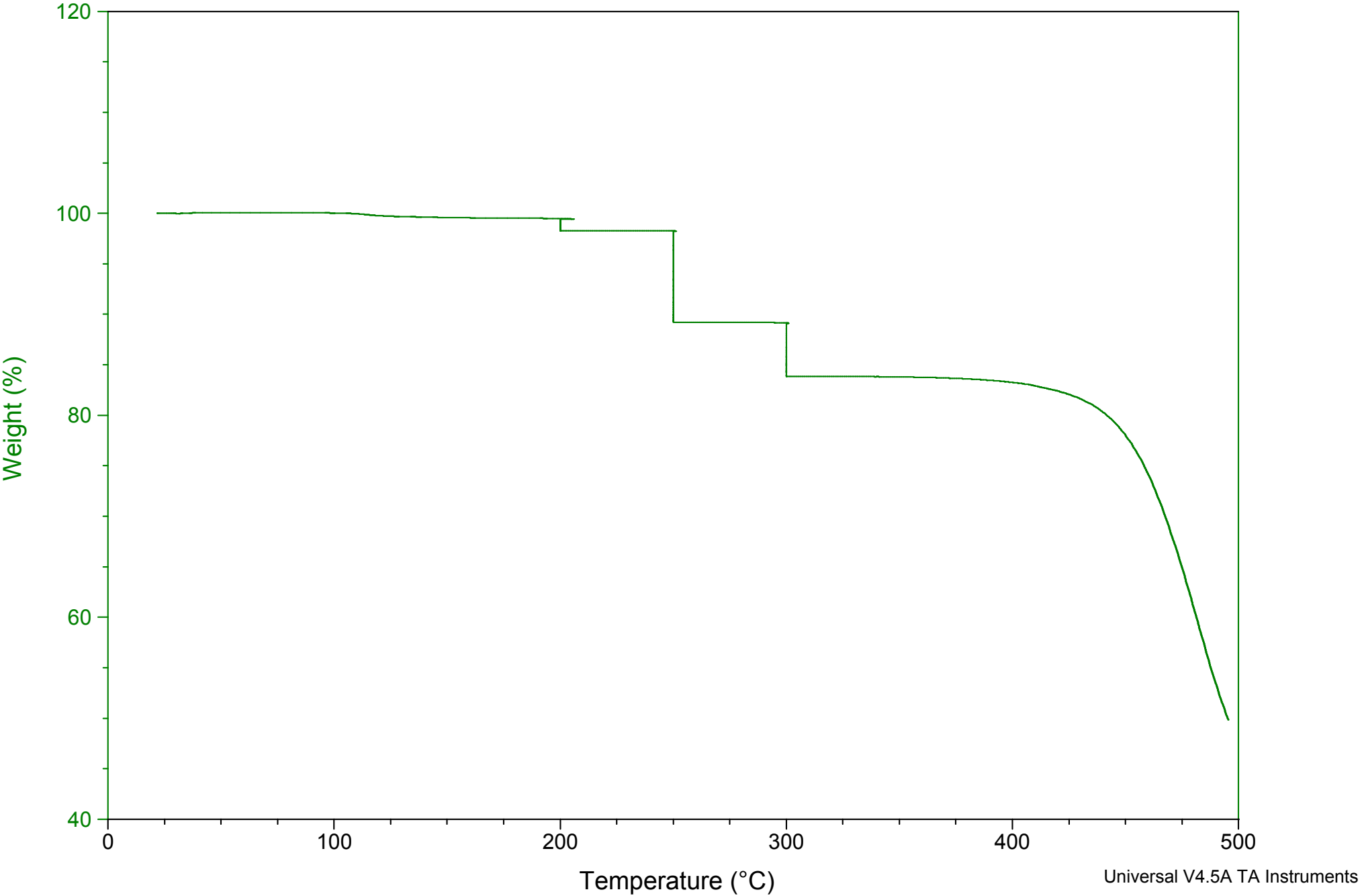
File: C:\...MS\1 min ramp rate\36 h\503.001
Run Date: 10-Apr-2019 09:17
Instrument: TGA Q500 V20.2 Build 27



Sample: 630
Size: 12.9130 mg
Method: test

TGA

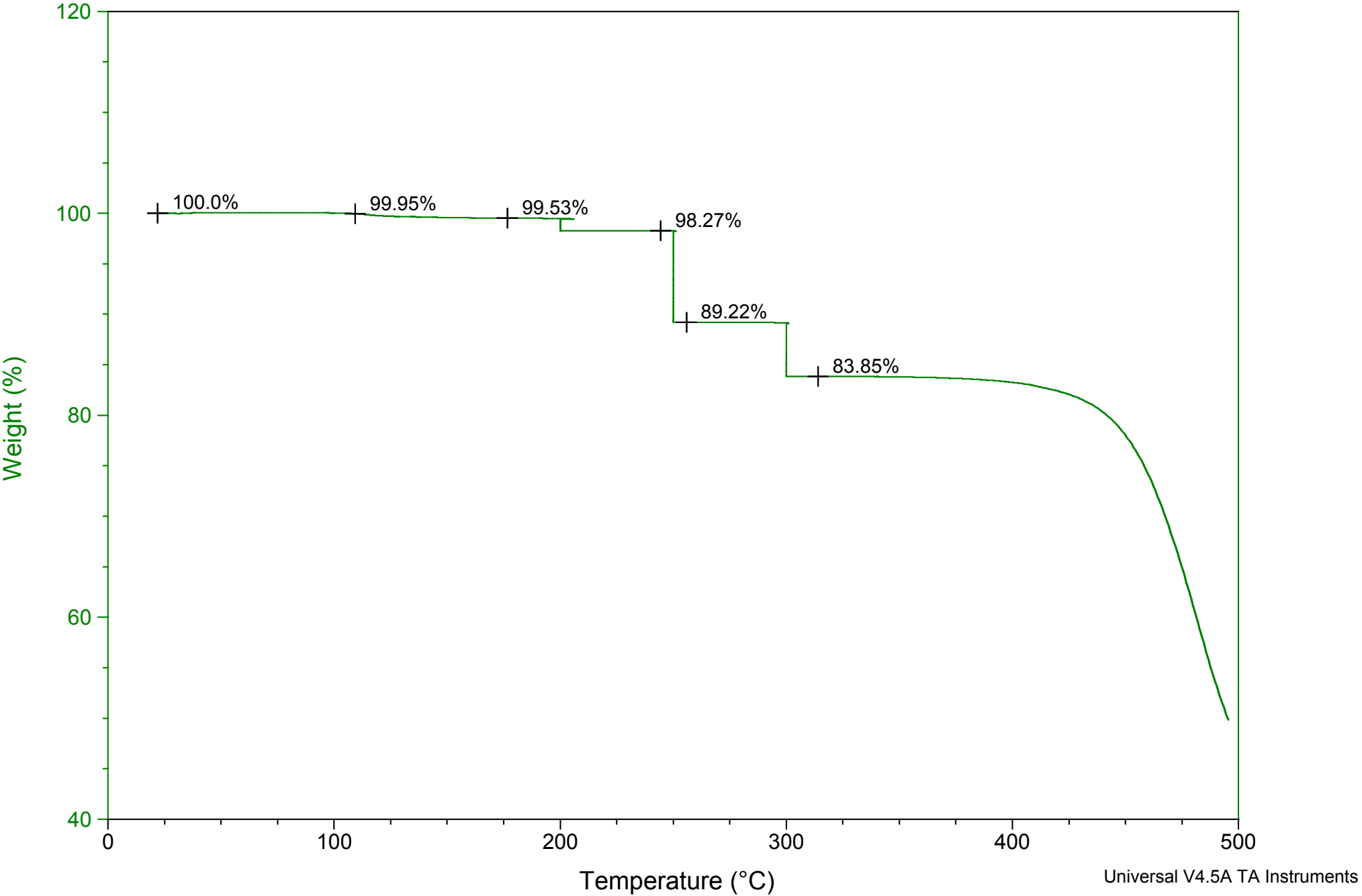
File: C:\...MS\1 min ramp rate\36 h\630.001
Run Date: 17-Apr-2019 09:01
Instrument: TGA Q500 V20.2 Build 27



Sample: 630
Size: 12.9130 mg
Method: test

TGA

File: C:\...MS\1 min ramp rate\36 h\630.001
Run Date: 17-Apr-2019 09:01
Instrument: TGA Q500 V20.2 Build 27



Sample: 630
Size: 12.9130 mg
Method: test

TGA

File: C:\...MS\1 min ramp rate\36 h\630.001
Run Date: 17-Apr-2019 09:01
Instrument: TGA Q500 V20.2 Build 27

