

The effect of structural modifications on the thermal stability, melting points and ion interactions for a series of tetraaryl-phosphonium-based mesothermal[†] ionic liquids

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A family of mesothermal ionic liquids comprised of tetraarylphosphonium cations and the bis(trifluoromethanesulfonyl)amidate anion are shown to be materials of exceptional thermal stability, enduring (without decomposition) heating in air at 300°C for three months. It is further established that three specific structural elements – phenoxy, phenacyl, and phenyl sulfonyl – can be present in the cation structures without compromising their thermal stability, and that their incorporation has specific impacts on the melting points of the salts. Most importantly, it is shown that the ability of such a structural component to lower a salt melting point is tied to its ability to lower cation-cation repulsions in the material.

Supporting Information

Supporting Information

Entropy Calculations

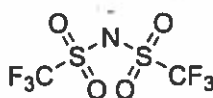
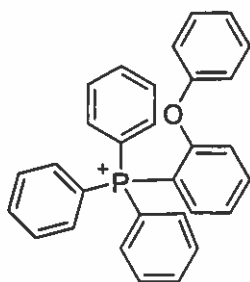
Liquid phase enthalpies were calculated using the two-phase thermodynamic (2PT) method,^{1, 2} which has been shown to accurately reproduce the standard molar entropies and heat capacities of a number of common solvents.³ Readers should refer to the original papers for the full details but the essence of the method is now described. First, the motions of each of the atoms are subdivided into translational, rotational and vibrational contributions. These components are then autocorrelated, summed and the results inverted in Fourier space to obtain the density of states (DOS), which relates the fraction of the total $3N$ degrees of freedom with a given vibrational frequency. Next, these vibrational frequencies are classified as either gas-like or solid-like via a key step in the 2PT method that is rooted in differences in their diffusivities. Finally, these gas-like and solid-like DOS of each of the translational, rotational and vibrational components are weighted by the theoretical entropy of the corresponding component of an ideal gas or a harmonic solid and integrated to obtain the total entropy.

In our work, separate simulations were run from saved states collected throughout the main simulation run. Initial configurations were taken at the specified temperature and the simulations performed in the *NPT* ensemble at that corresponding fixed temperature for a short period of 20 ps. During this run, atom positions and velocities were output every 4 fs and used for the actual 2PT analysis.

References

1. S.-T. Lin, M. Blanco and W. A. Goddard, III, *J. Chem. Phys.*, 2003, **119**, 11792-11805.
2. S.-T. Lin, P. K. Maiti and W. A. Goddard, III, *J. Phys. Chem. B*, 2010, **114**, 8191-8198.
3. T. A. Pascal, S.-T. Lin and W. A. Goddard, III, *Phys. Chem. Chem. Phys.*, 2011, **13**, 169-181.

COMPOUND 2



Atlantic Microlab, Inc.

Sample No. Phosphonium 51A

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Company/School U of South Alabama
 Dept. Chemistry
 Address Chem 223
 City, State, Zip Mobile AL 36688
 Name James Davis Date 10/31/2016
 Phone (251) 751-0520

Professor/Supervisor: James Davis
 PO# / CC# _____

Element	Theory	Found	Single ☒ Duplicate ☐
C	54.01	53.34	53.39
H	3.40	3.37	3.38
N	1.97	2.05	2.03
		NO CHARGE FOR DUPLICATES	

Elements CHNPOSF Present: _____
 Analyze CHN for: _____
 Hygroscopic ☐ Explosive ☐
 M.P. unk B.P. none
 To be dried: Yes ☒ No ☐
 Temp. 60C Vac. high Time 4h
 Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
 Include Email Address or FAX # Below
jdavis@southalabama.edu

NOV 01 2016

NOV 01 2016

Date Received _____ Date Completed _____

Remarks:

S1A_PROTON-2.jdf
yellow 3



SOUTH ALABAMA
JAGUARS

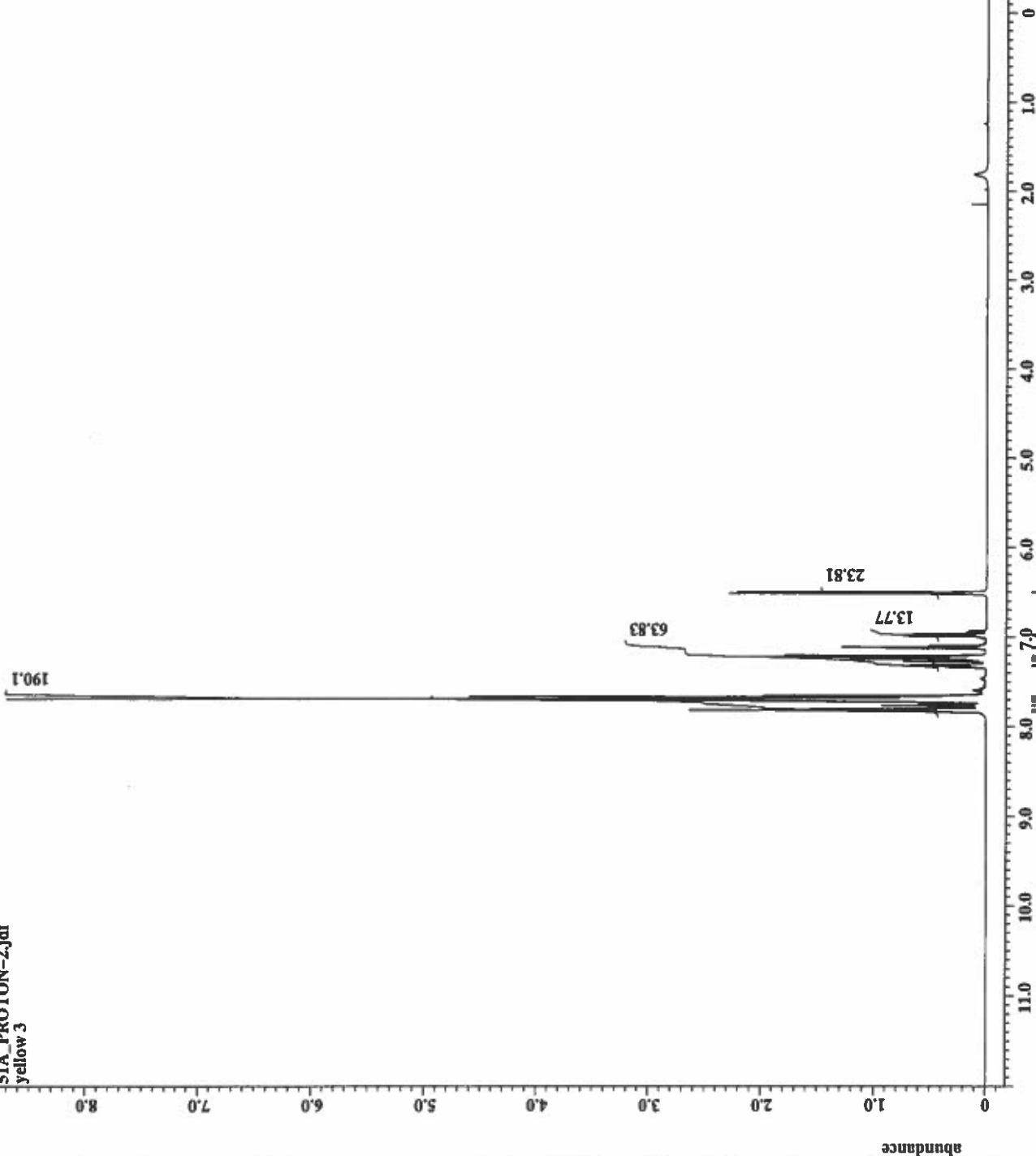
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Current_time   = 1-JUL-2016 13:41:38

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Spectrometer  = JNM-ECA500

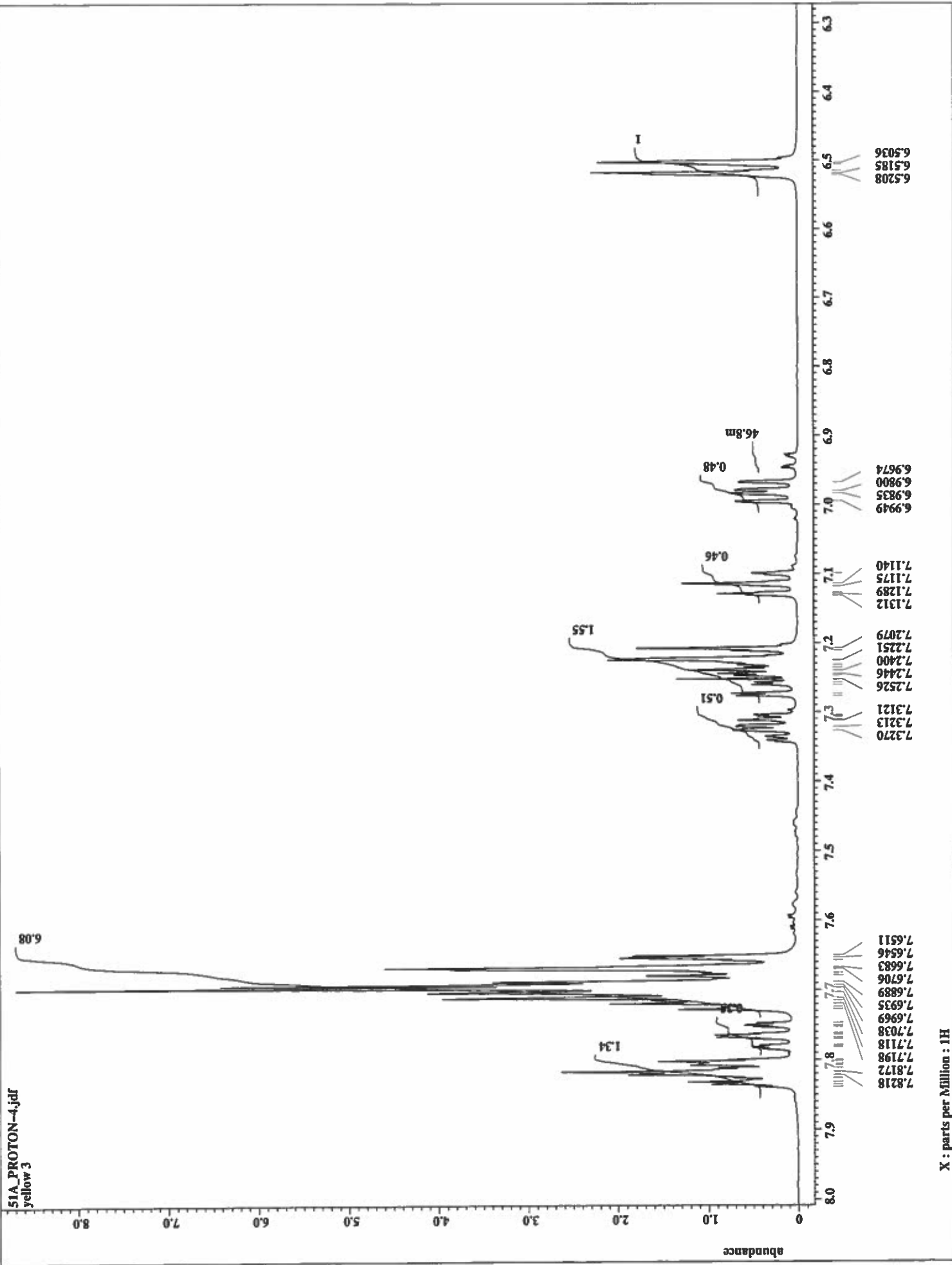
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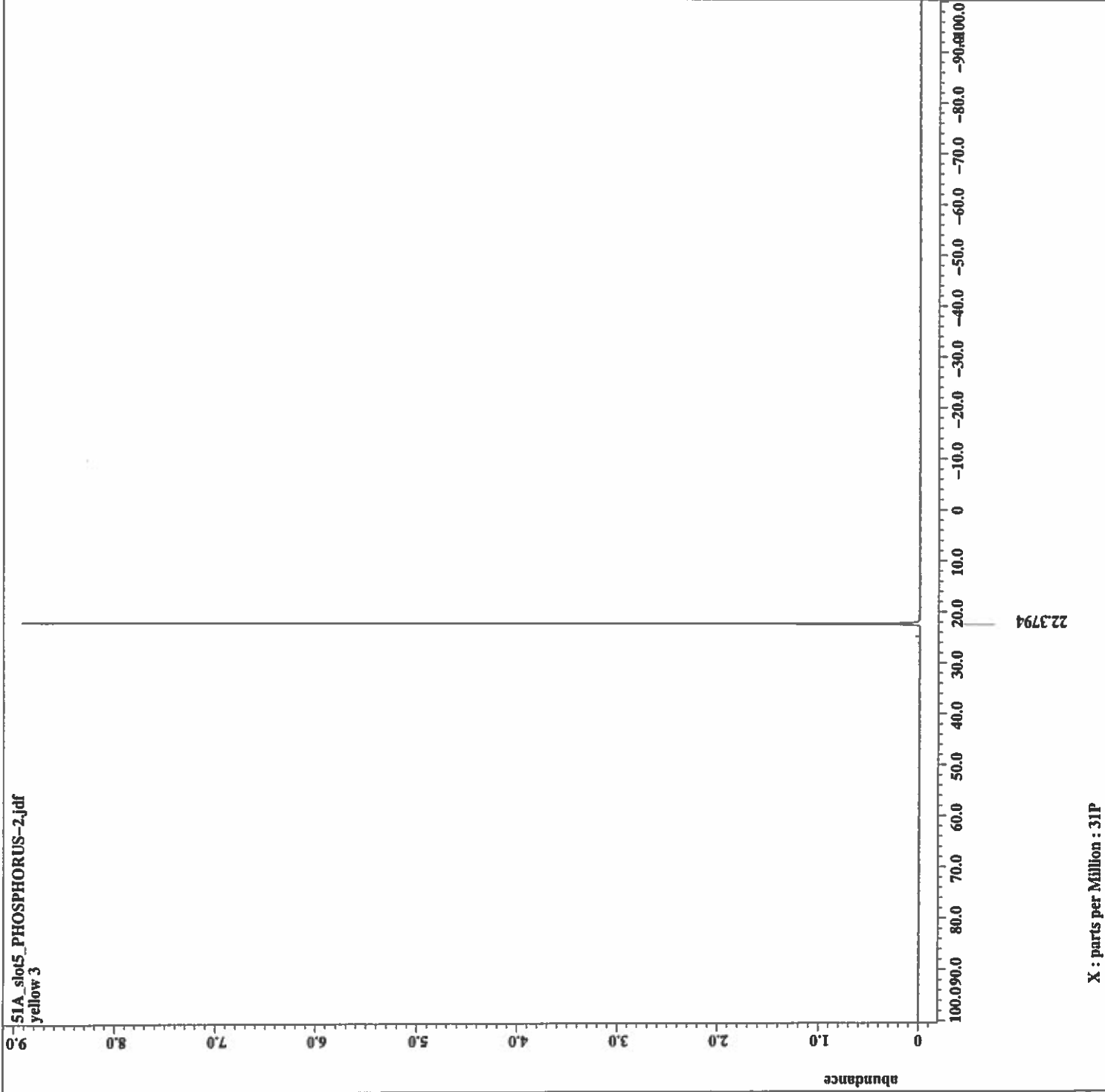
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Regrain_gain  = 32
Relaxation_delay = 4[s]
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7.6969
7.6935
7.6683
7.2526
7.2251
7.2079
6.5185
6.5036

X : parts per Million : 1H





SOUTH ALABAMA
JAGUARS

Filename = 51A_slot5_PHOSPHORUS-
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = 88631099
Solvent = CHLOROFORM-D
Changer_sample = 5
Creation_time = 1-JUL-2016 18:02:34
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X_prescans = 4
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X_sweep = 50.81300813[kHz]
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Irr_offset = 5.0[ppm]
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X_angle = 30[deg]
X_atn = 5[db]
X_pulse = 4.66666667[us]
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Decoupling = TRUEZ
Initial_wait = 1[s]
Noe_time = TRUE
Noe_time = 2[s]
Recvr_gain = 58
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Temp_get = 23.5[dc]

51A_slot5_FLUORINE-2.jdf
yellow 3



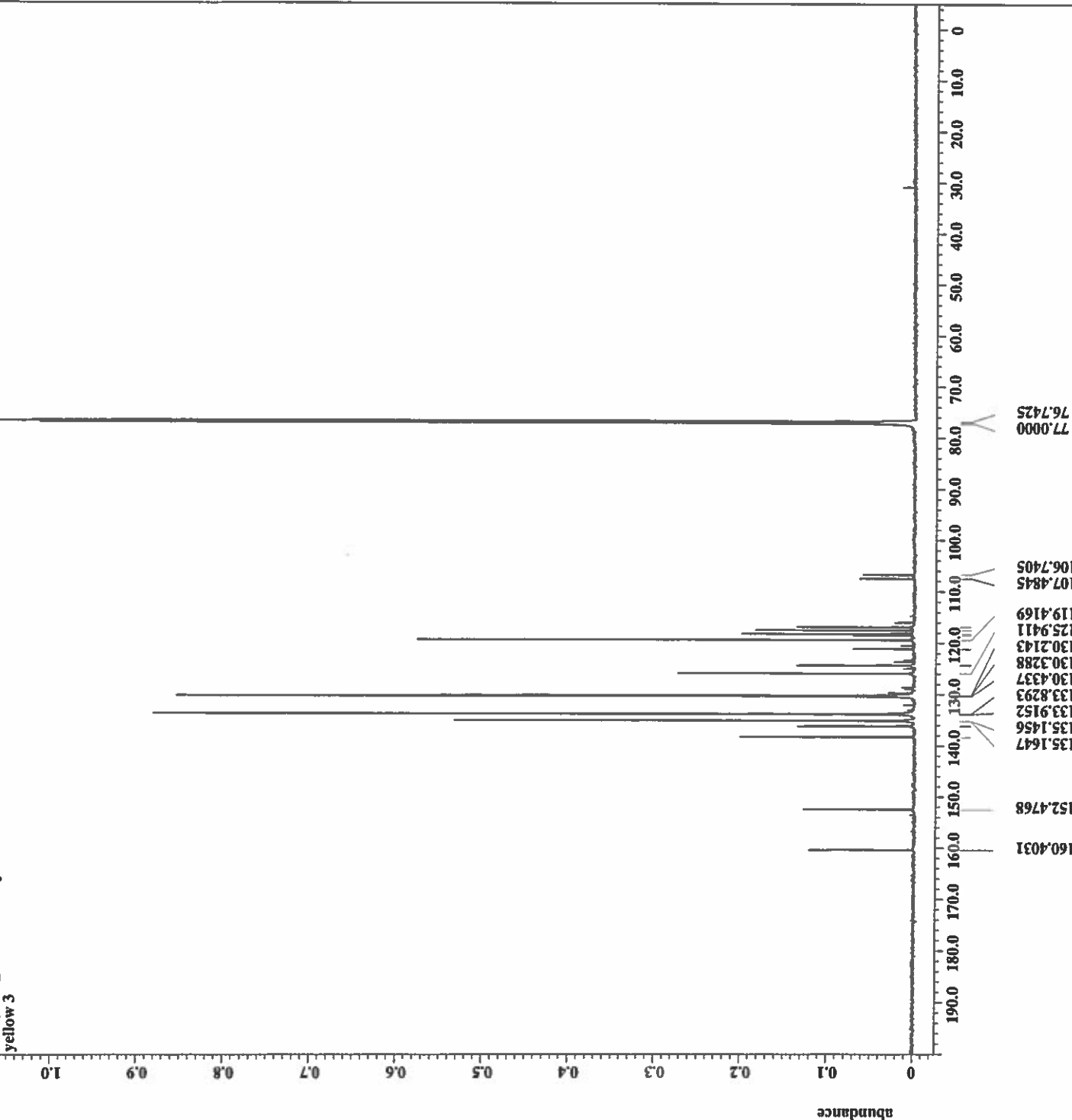
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Experiment = single_pulse.ex2
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Changer_sample = 5
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Spectrometer = JNM-ECA500
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X_freq = 470.62046084[MHz]
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X_points = 65536
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X_resolution = 1.7993855[Hz]
X_sweep = 117.9245283[kHz]
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Xrr_freq = 470.62046084[MHz]
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Xrr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 15.7[us]
X_acq_time = 0.55574528[s]
X_angle = 45[deg]
X_atn = 4[db]
X_pulse = 7.85[us]
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Pulse_preset = FALSE
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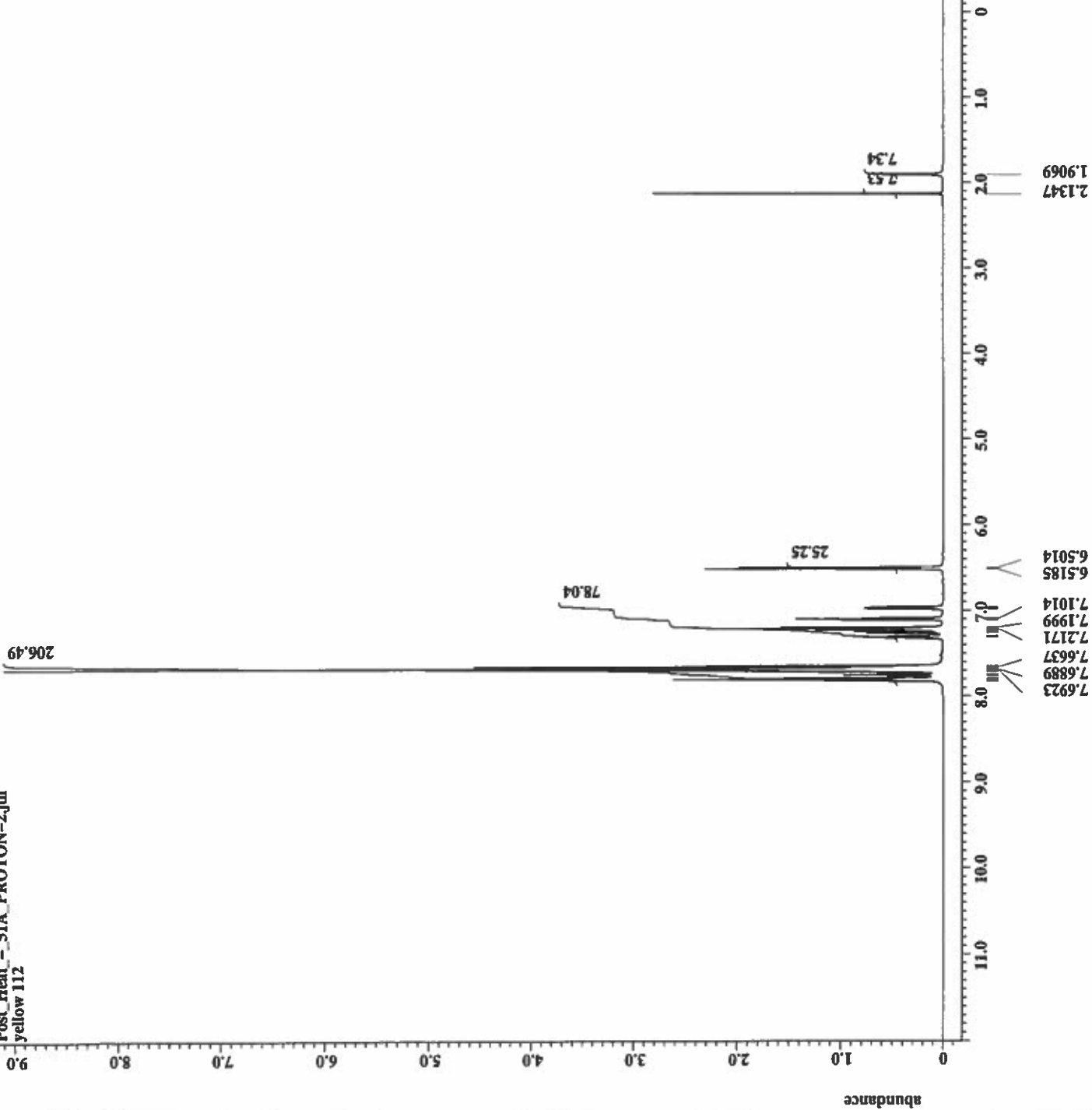
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S1A_slot5_CARBON-2.jdr
yellow 3



SOUTH ALABAMA
JAGUARS

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Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = 88162356
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Changer_sample = 5
Creation_time = 2-JUL-2016 07:16:27
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Dim_units = [ppm]
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Spectrometer = JNM-ECA500
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X_offset = 100[ppm]
X_points = 32768
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X_resolution = 1.19959034[MHz]
X_sweep = 39.3081761[MHz]
Irr_domain = 1H
Irr_freq = 500.15991521[MHz]
Irr_offset = 5.0[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 3100
Total_scans = 3100
X_90_width = 12.55[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 6[db]
X_pulse = 4.18333333[us]
Irr_atn_dec = 20.5[db]
Irr_atn_no = 20.5[db]
Irr_noise = WALTZ
Decoupling = TRU2
Initial_wait = 1[s]
Noe_time = 2[s]
Noe_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get = 23.6[degC]



X : parts per Million : 1H

```

Filename      = Post_Heat_-_51A_PROTO
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = Post_Heat_-_51A
Solvent       = CHLOROFORM-D
Charger_sample = 14
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Revision_time  = 1-JUL-2016 14:34:43
Current_time   = 1-JUL-2016 14:34:43

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Site          = ECA 500
Spectrometer  = JNM-ECA500

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X_acq_duration = 1.74587904[s]
X_domain       = 1H
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X_resolution   = 0.57277737[Hz]
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Mod_return     = 1
Scans          = 16
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X_acq_time     = 1.74587904[s]
X_angle        = 45[deg]
X_atn          = 4[db]
X_pulse        = 6.675[us]
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Relax_gain      = 20
Relaxation_delay = 4[s]
Repetition_time = 5.74587904[s]
Temp_get       = 22.5[dc]
    
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Post_Heat_-_51A_PROTON-4.jdr
yellow 112

9.0

8.0

7.0

6.0

5.0

4.0

3.0

2.0

1.0

0

abundance

0.6

0.8

7.0

6.0

5.0

4.0

3.0

2.0

0.2

7.6981

7.6923

7.6889

7.6832

7.6637

7.2526

7.2377

7.2320

7.2171

7.1999

7.1163

7.1014

6.5208

6.5185

6.5014

2.1347

1.9069

0.21

0.22

1.08

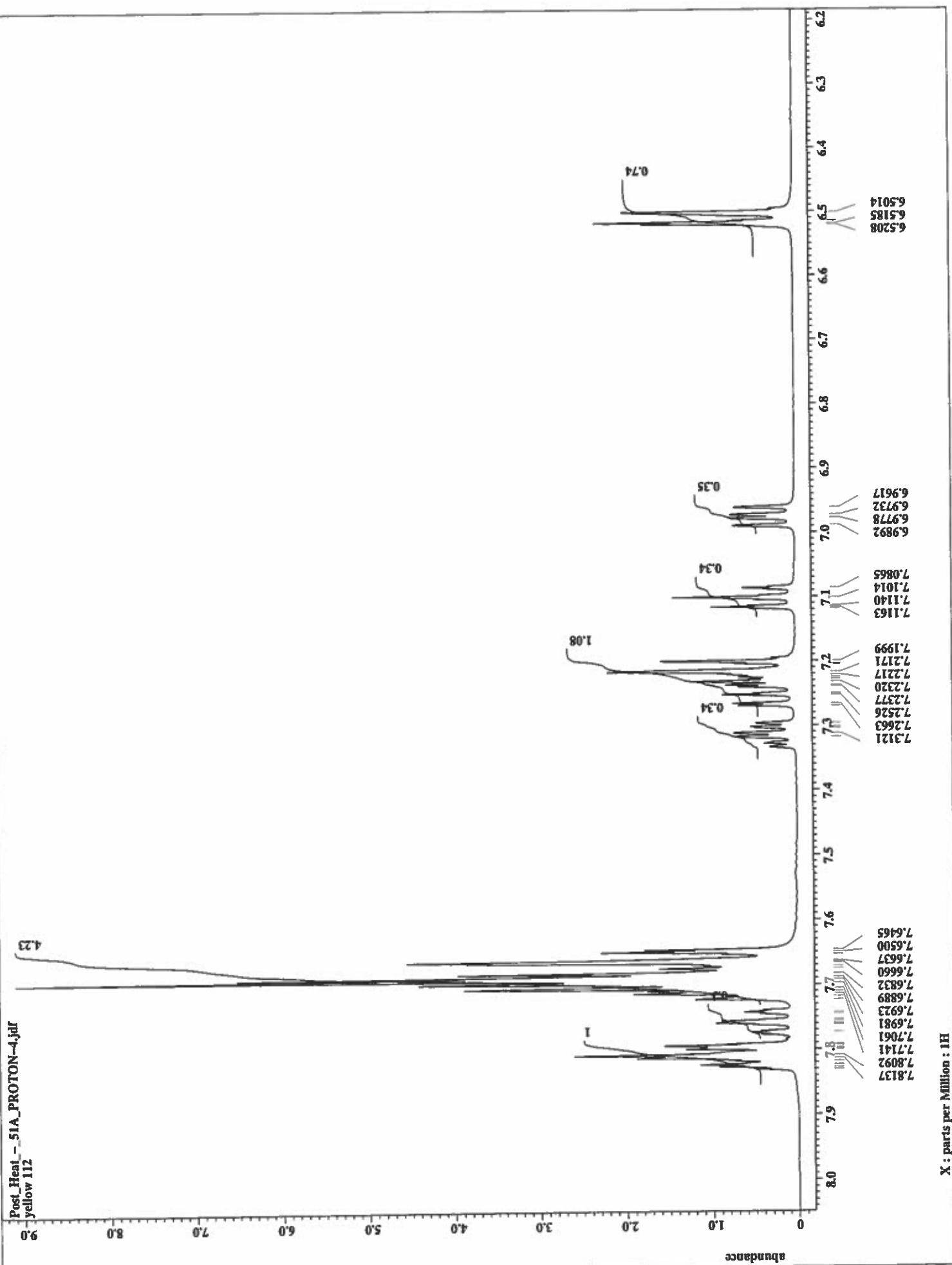
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0.35

0.74

4.23

X : parts per Million : 1H



Postheat - 51A_slot14_PHOSPHORUS-2.jdf
Yellow 12



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Experiment = single_pulse_dec
Sample_id = S8716124
Solvent = CHLOROFORM-D
Changer_sample = 14
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Revision_time = 1-JUL-2016 20:06:11
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Dim_units = [ppm]
Dimensions = X 500
Site = ECA 500
Spectrometer = JNM-ECA500
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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 = 256
Total_scans = 256
X_90_width = 14[us]
X_acq_time = 0.64487424[s]
X_angle = 30[deg]
X_atn = 5[db]
X_pulse = 4.66666667[us]
X_atn_dec = 20.5[db]
X_atn_noe = 20.5[db]
X_noise = TRUE
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 = 23.3[dc]

abundance

100.090.0 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 -90.0100.0

22.3641

X : parts per Million : 31P



Filename = Postheat - 51A_slot14
Author = Jim Davis
Experiment = single_pulse.ex2
Sample_id = S8587979
Solvent = CHLOROFORM-D
Changer_sample = 14
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Spectrometer = JNM-ECA500
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X_sweep = 117.9245283[kHz]
Irr_domain = 13F
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Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 470.62046084[MHz]
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Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 15.7[us]
X_acq_time = 0.55574528[s]
X_angle = 45[deg]
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X_pulse = 7.85[us]
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Recvr_gain = 40
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Temp_get = 22.6[dc]

-78.6104



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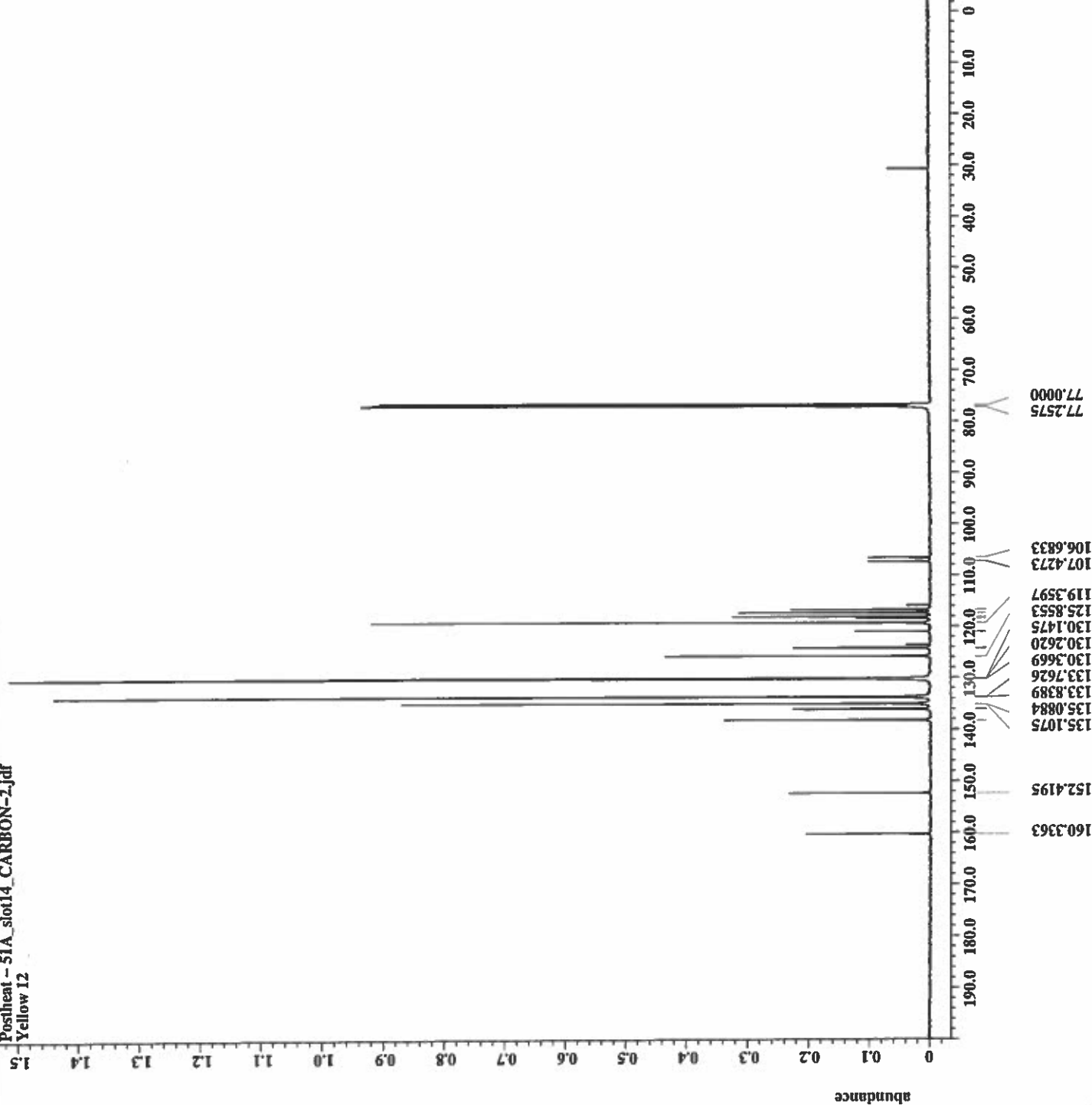
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Experiment     - single_pulse_dec
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Revision_time - 3-JUL-2016 05:35:38
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Spectrometer  - JNM-ECA500

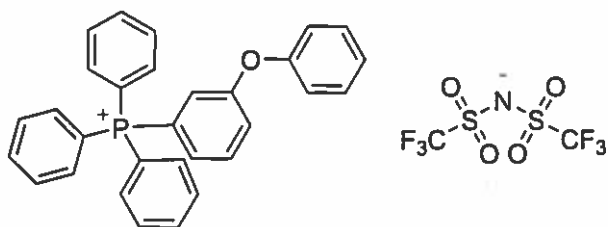
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X_offset       - 100[ppm]
X_points       - 32768
X_prescans     - 4
X_resolution   - 1.19959034[Hz]
X_sweep        - 39.3081761[MHz]
X_domain      - 1H
X_freq         - 500.15991521[MHz]
X_offset       - 5.0[ppm]
Clipped        - FALSE
Mod_return     - 1
Scans          - 3100
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X_90_width     - 12.55[us]
X_acq_time     - 0.83361792[s]
X_angle        - 30[deg]
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X_pulse        - 4.18333333[us]
X_atn_dec      - 20.5[db]
X_atn_noe      - 20.5[db]
X_noise        - WALTZ
Decoupling     - TRUE
Initial_wait   - 1[s]
Noe            - tau2
Noe_time       - 2[s]
Recovery_gain  - 60
Relaxation_delay - 2[s]
Repetition_time - 2.83361792[s]
Temp_get       - 23.3[dc]
    
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X : parts per Million : 13C

COMPOUND 3

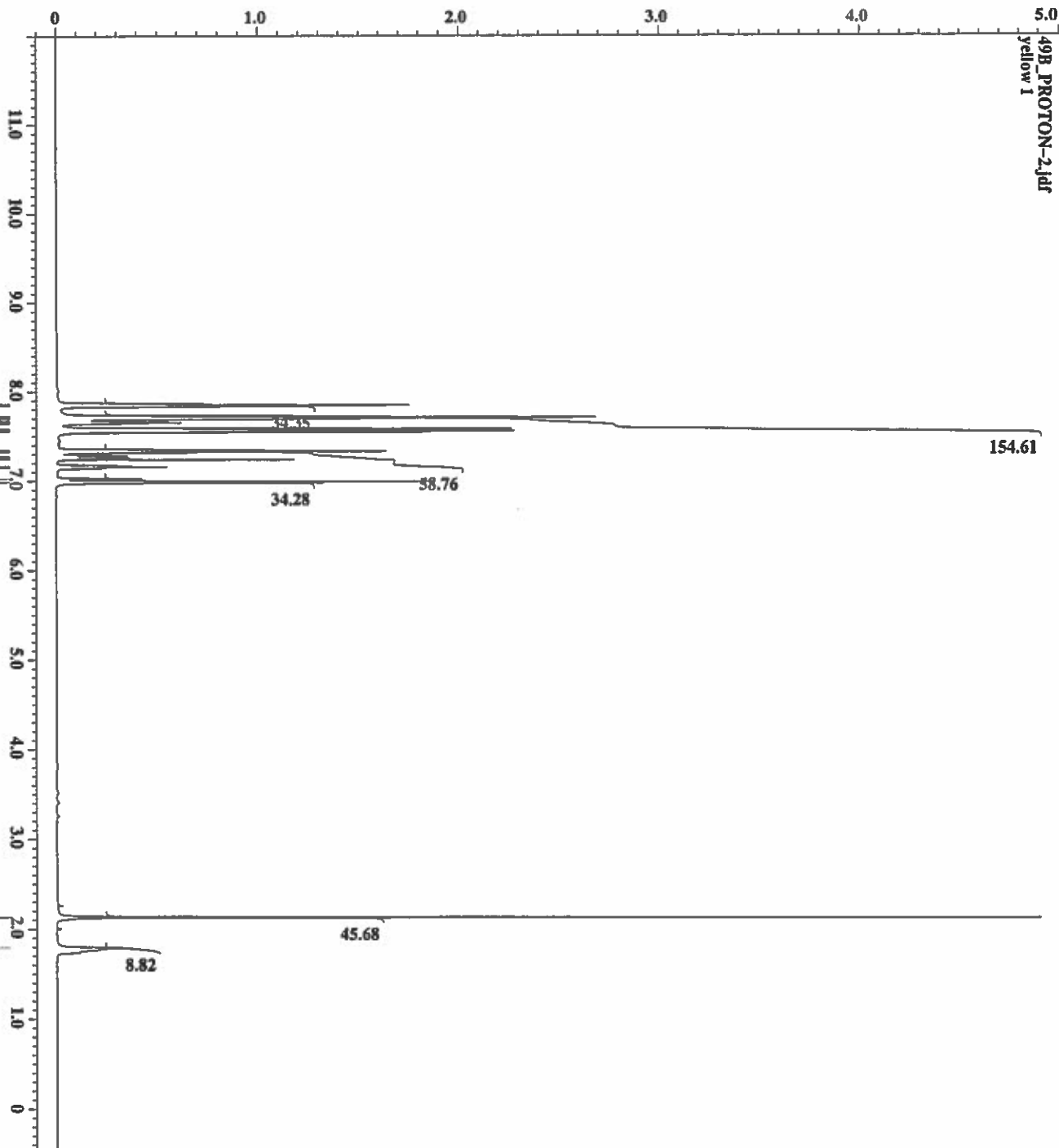


49B_PROTON-2.jdf
yellow 1

7.7141
7.7095
7.5881
7.5721
7.5618
7.5469
6.9961

2.1359
2.1302
1.7923

1H
1H
1H
1H
1H
1H
1H



X : parts per Million : 1H

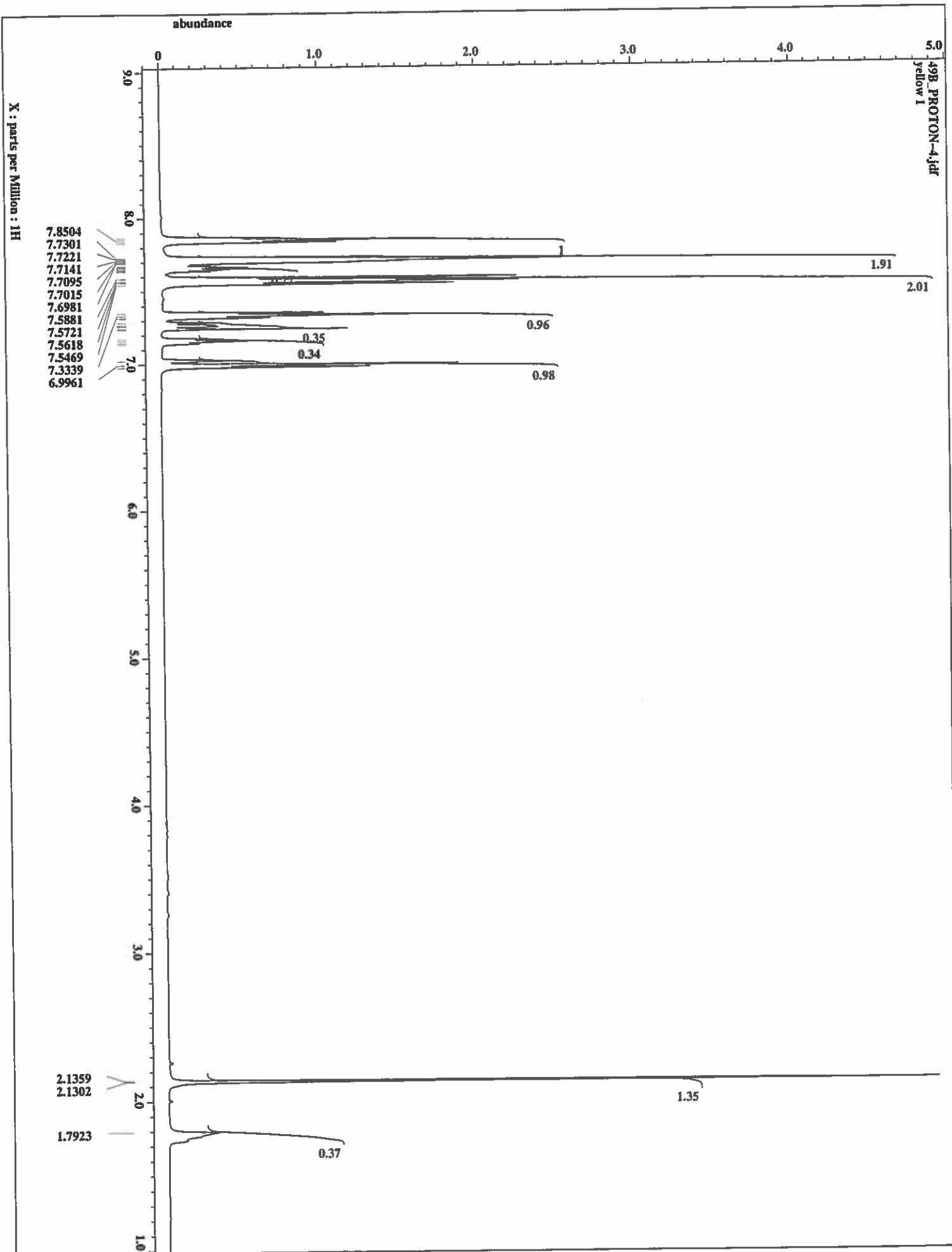


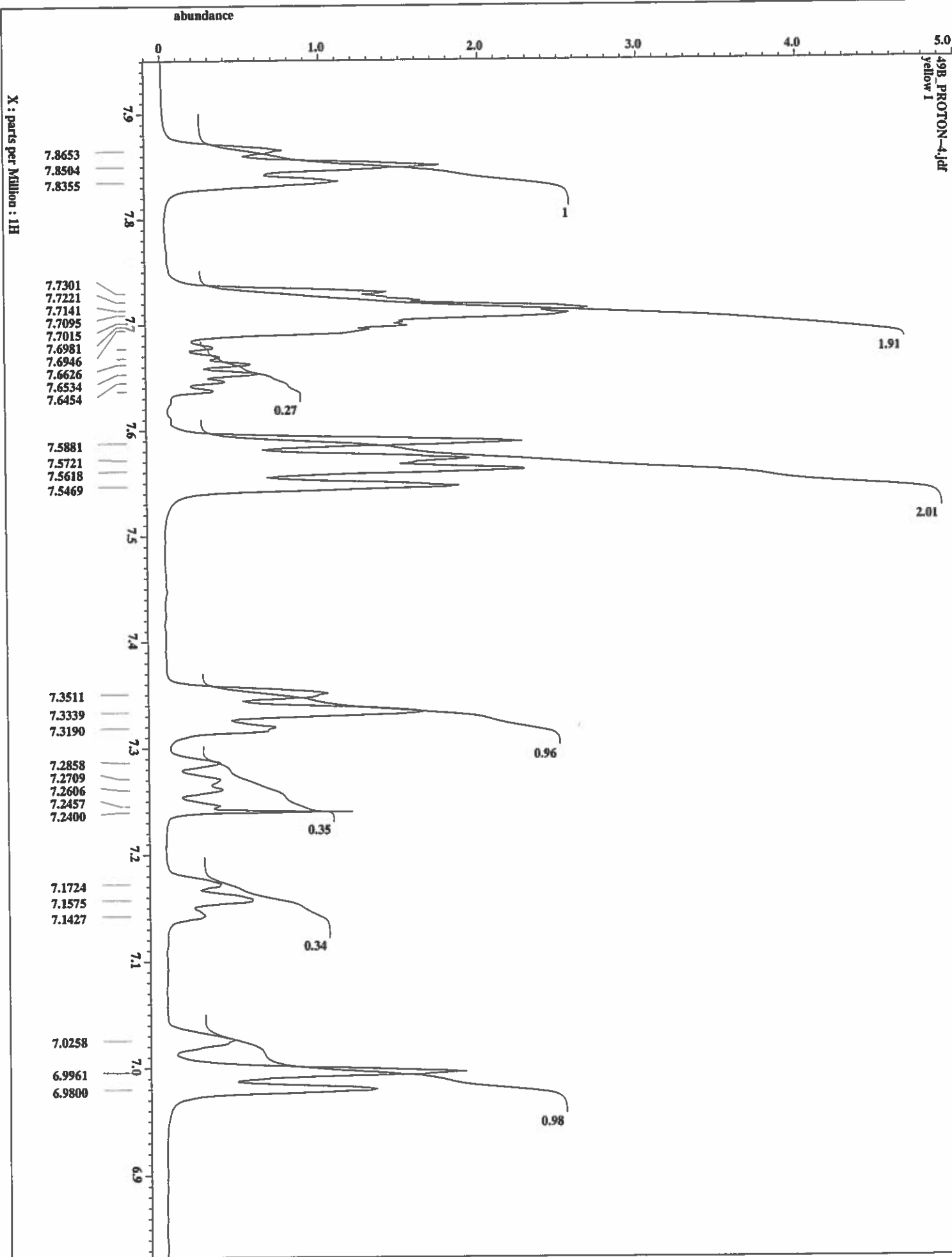
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Spectrometer = JNM-ECA500

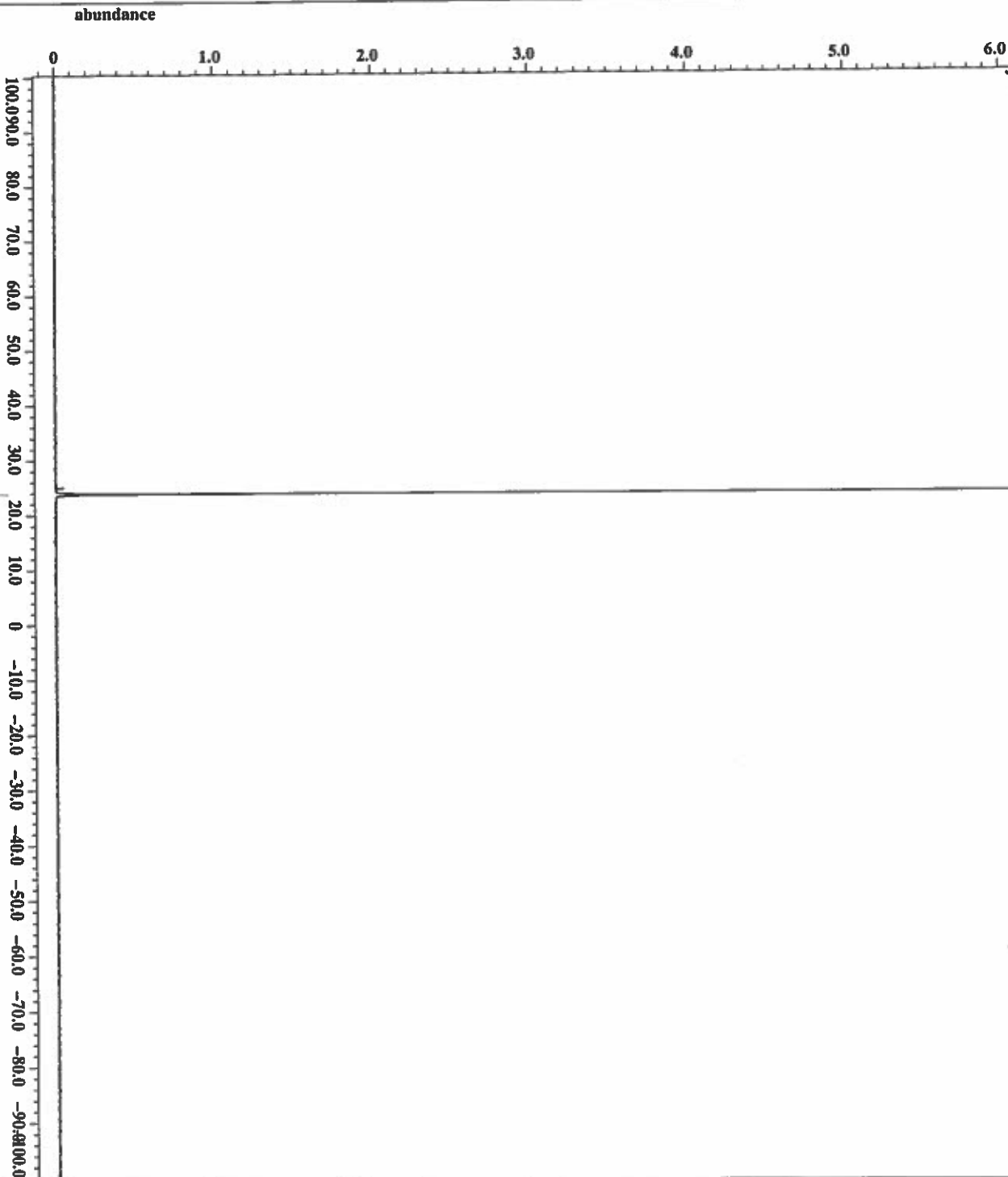
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X_freq = 500.15391521 [MHz]
X_offset = 5.0 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.57277737 [Hz]
X_sweep = 9.38438438 [kHz]
X_domain = 1H
X_freq = 500.15391521 [MHz]
X_offset = 5.0 [ppm]
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X1_freq = 500.15391521 [MHz]
X1_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 13.35 [us]
X_acq_time = 1.74587904 [s]
X_angle = 45 [deg]
X_atn = 4 [dB]
X_pulse = 6.675 [us]
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X1_offset = OF2
Dante_presat = FALSE
Initial_walt = 1 [s]
Recvr_gain = 34
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_set = 22.3 [deg]





49B_slot2_PHOSPHORUS-2.jdt
yellow 1



X : parts per Million : 31P



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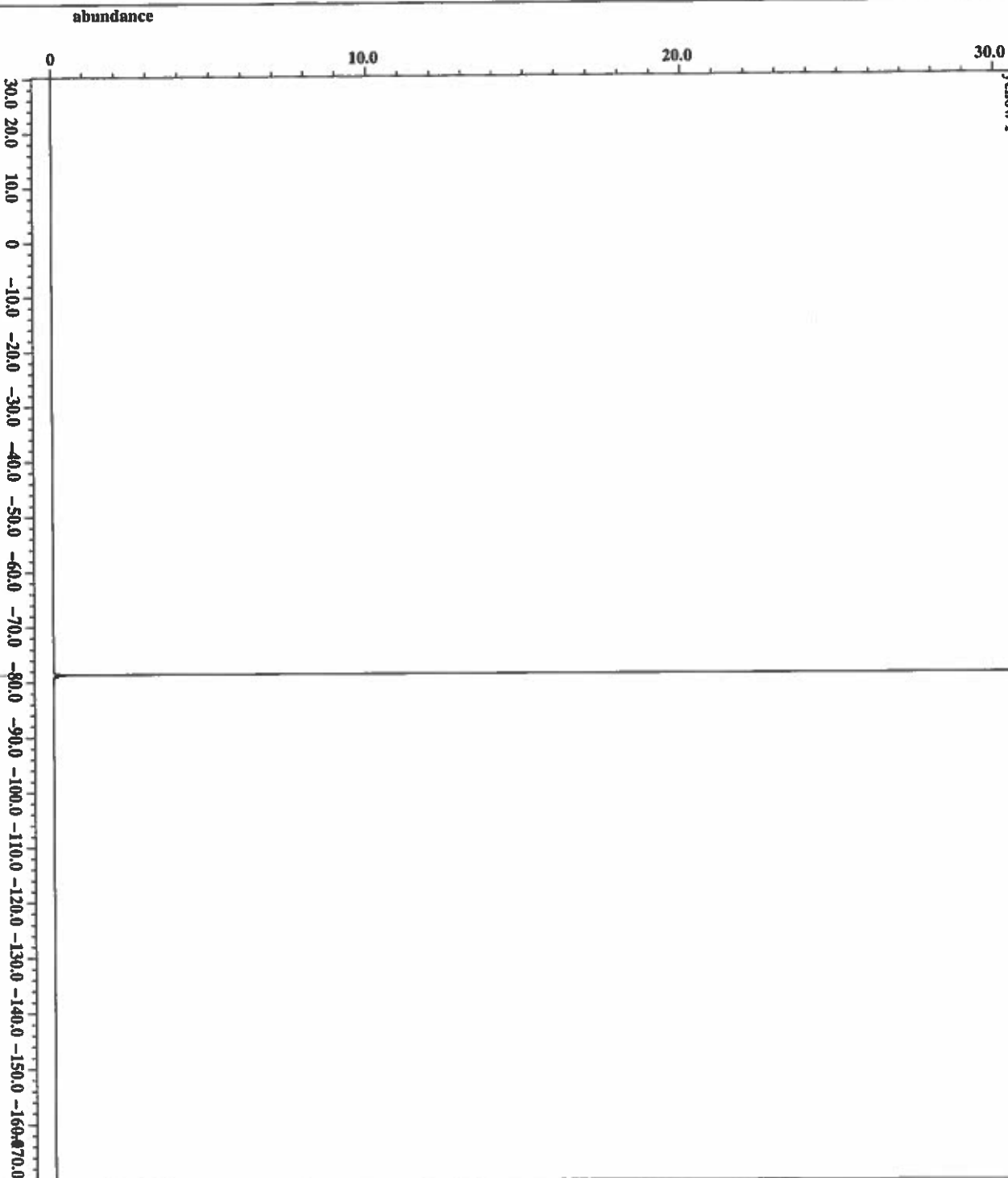
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Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = B#612304
Solvent       = CHLOROFORM-D
Charger_sample = 2
Creation_time  = 1-JUL-2016 17:31:05
Revision_time  = 1-JUL-2016 17:13:00
Current_time   = 1-JUL-2016 17:13:00

Comment
Data_format   = yellow 1
Dim_size      = 1D COMPLEX
Dim_title     = 26214
Dim_unit      = 31P
Dimensions    = [ppm]
Site          = X
Spectrometer  = ECA 500
              = 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          = 256
Total_scans    = 256

X_90_width     = 14 [us]
X_acq_time     = 0.64487424 [s]
X_angle        = 30 [deg]
X_atn          = 5 [dB]
X_pulse        = 4.66666667 [us]
X_atn_dec      = 20.5 [dB]
X_atn_poe      = 20.5 [dB]
Xr_pulse       = 10.125 [us]
Decoupling     = TRUZ
Initial_wait   = 1 [s]
Noe            = TRUZ
Noe_time       = 2 [s]
Recvr_gain     = 58
Relaxation_delay = 2 [s]
Repetition_time = 2.64487424 [s]
Temp_get       = 23.4 [degC]
  
```

49B_slot2_FLUORINE-2.jif
yellow 1



X : parts per Million : 19F



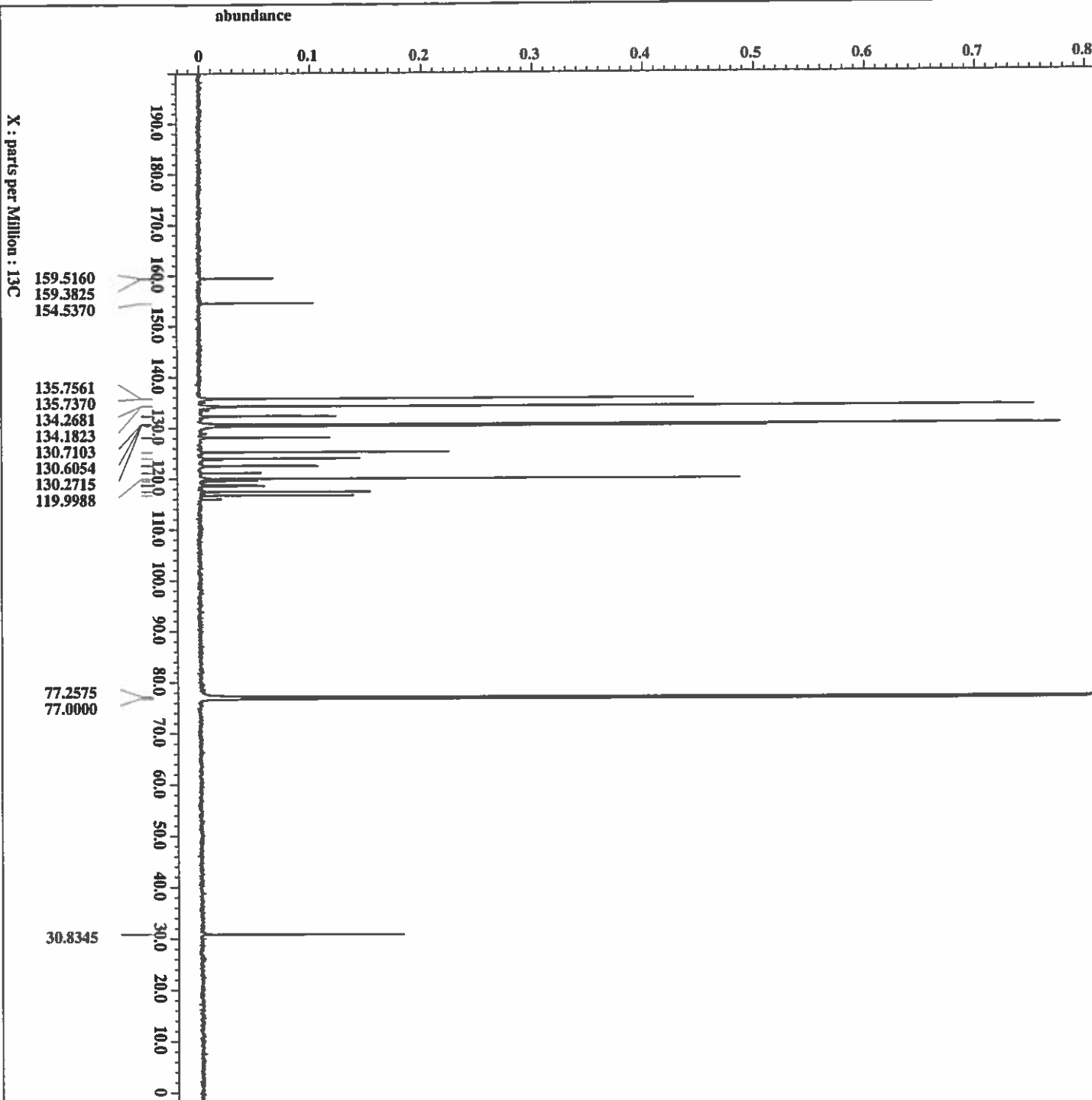
Filename = 49B_slot2_FLUORINE-2.
Author = Jim Davis
Experiment = single_pulse.ex2
Sample_id = 88549939
Solvent = CHLOROFORM-D
Charger_sample = 3
Creation_time = 1-JUL-2016 15:37:22
Revision_time = 1-JUL-2016 15:19:17
Current_time = 1-JUL-2016 15:19:17

Comment = yellow 1
Data_format = 1D COMPLEX
Dim_size = 32428
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 = 117.9245263 [Hz]
Irr_domain = 19F
Irr_freq = 470.62046084 [MHz]
Irr_offset = 5 [ppm]
Irr_domain = 19F
Irr_freq = 470.62046084 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 15.7 [us]
X_acq_time = 0.55574528 [s]
X_angle = 45 [deg]
X_atp = 4 [dB]
X_pulse = 7.85 [us]
Irr_mode = O2F
Irr_freq = O2F
Pulse = PALSE
Pulse = 1 [s]
Relaxation_delay = 44
Relaxation_delay = 4.55574528 [s]
Temp_get = 22.7 [deg]

49B_slot2_CARBON-2.jdt
yellow 1



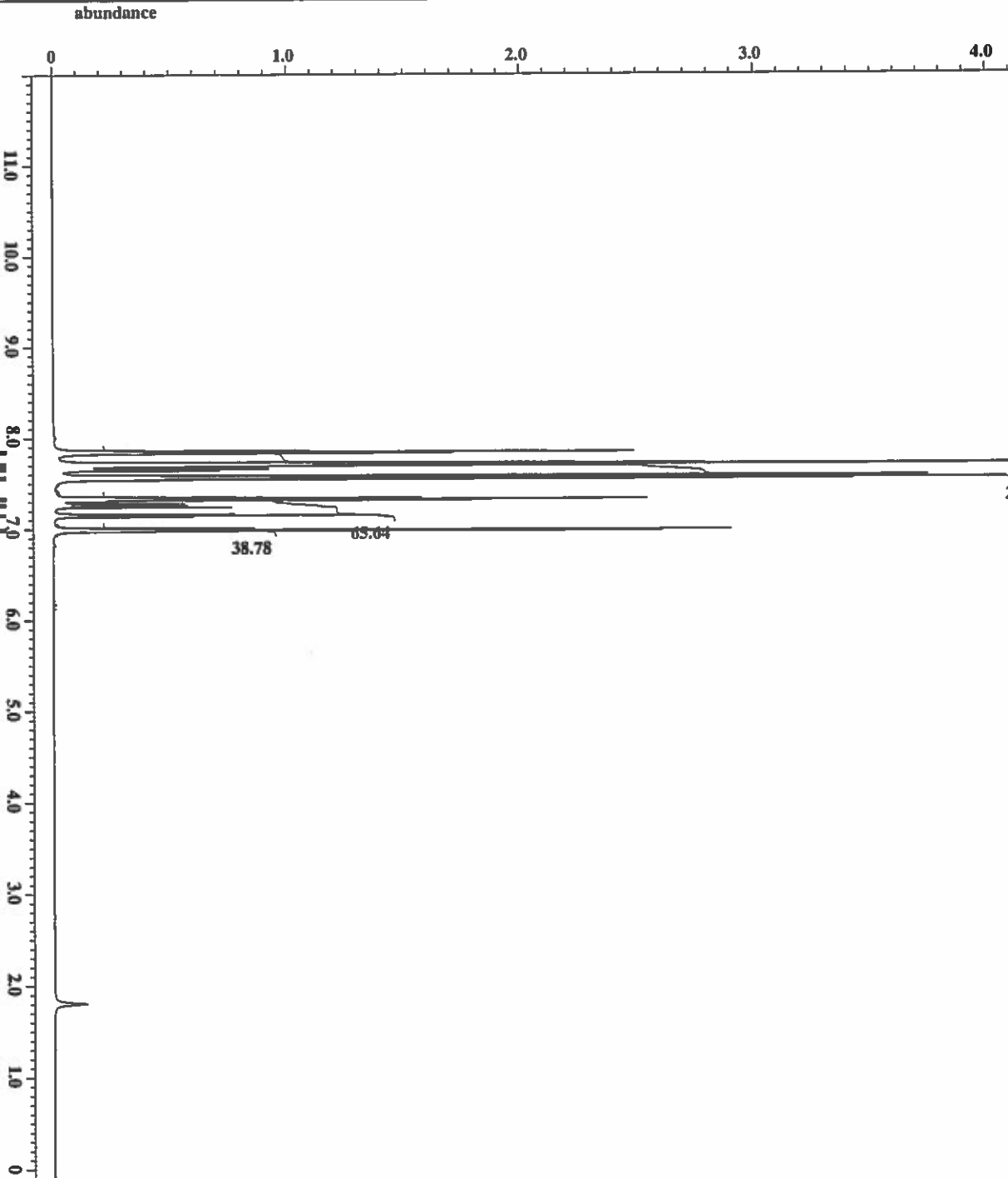
Filename = 49B_slot2_CARBON-2.jdt
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = 88845434
Solvent = CHLOROFORM-D
Charger_sample = 2
Creation_time = 2-JUL-2016 02:14:54
Revision_time = 2-JUL-2016 01:56:46
Current_time = 2-JUL-2016 01:56:46

Comment = yellow 1
Data_format = 1D COMPLEX
Dir_size = 26214
Dir_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 = 3100
Total_scans = 3100

X_90_width = 12.55 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 6 [dB]
X_pulse = 4.18333333 [us]
X_atn_dec = 20.5 [dB]
X_atn_noe = 20.5 [dB]
X_atn_noe = WALTZ
Decoupling = TRIZ
Initial_wait = 1 [s]
Noe_time = TRIZ
Noe_gain = 2 [s]
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get = 23.2 [deg]

Post_Heat_-_49B_PROTON-2.jdf
yellow 13



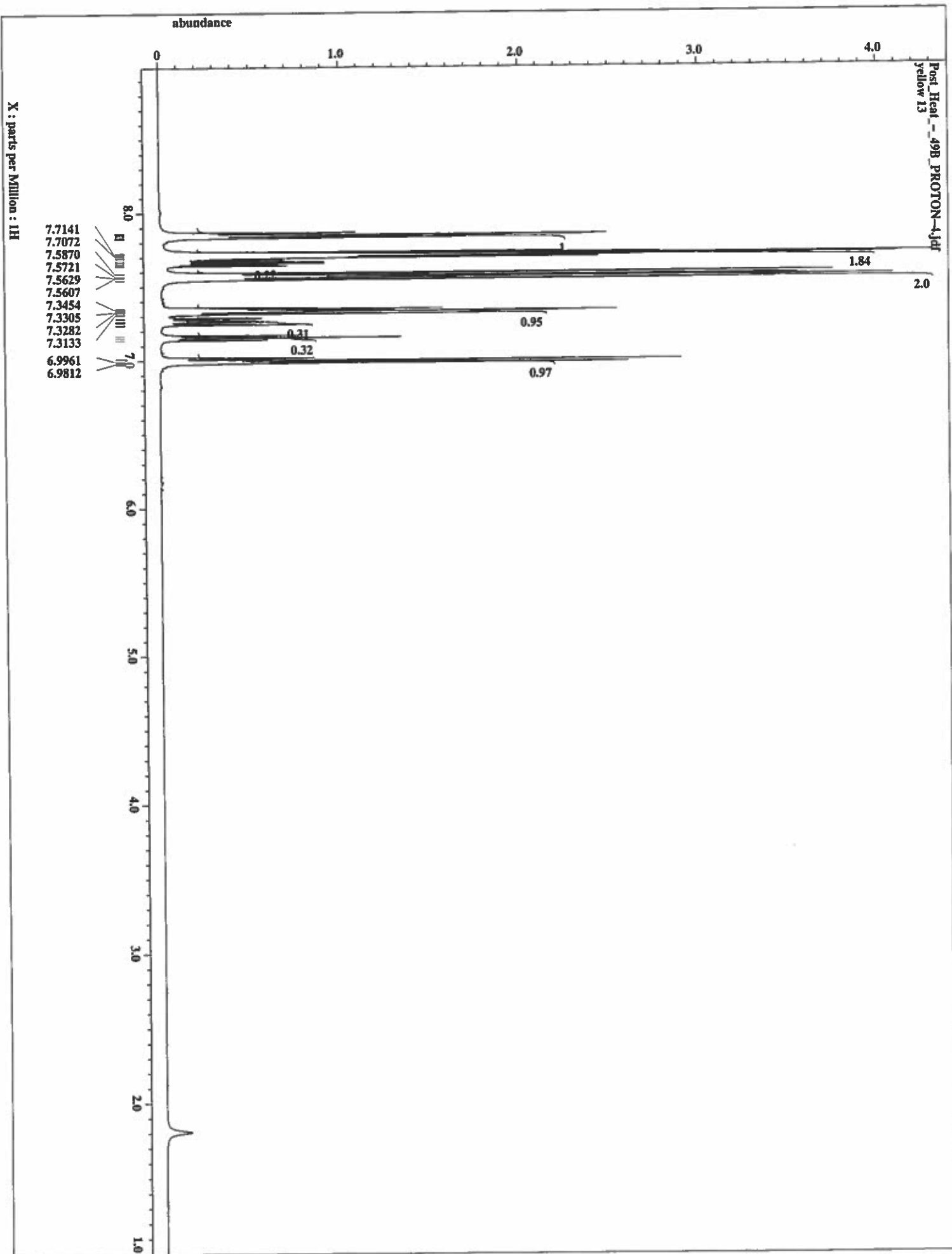
Filename = Post_Heat_-_49B_PROT
Author = Jim Davis
Experiment = single_pulse.ex2
Sample_id = Post_Heat_-_49B
Solvent = CHLOROFORM-D
Charger_sample = 15
Creation_time = 1-JUL-2016 14:58:51
Revision_time = 1-JUL-2016 14:40:46
Current_time = 1-JUL-2016 14:40:46

Comment = yellow 13
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

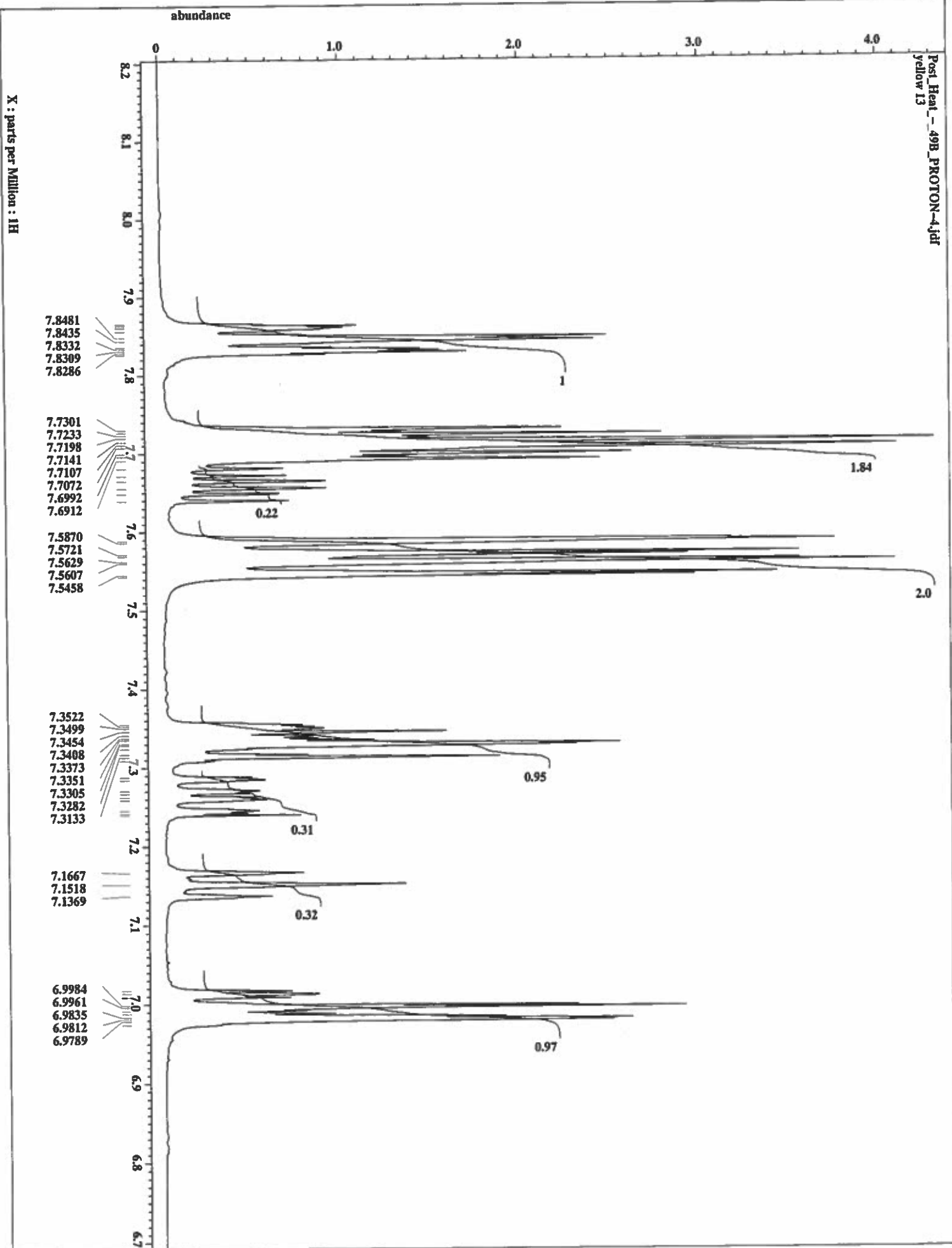
Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain = 1H
X_freq = 500.15991521 [MHz]
X_offset = 5.0 [ppm]
X_points = 16384
X_preampl = 1
X_resolution = 0.57277737 [Hz]
X_sweep = 9.38438438 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Irr_domain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

X_90_width = 13.35 [us]
X_acq_time = 1.74587904 [s]
X_angle = 45 [deg]
X_atn = 4 [dB]
X_pulse = 6.675 [us]
Irr_mode = OCE
Irr_mode = OCE
Dance_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 28
Relaxation_delay = 4 [s]
Relaxation_delay = 5.74587904 [s]
Temp_gpc = 23.7 [deg]

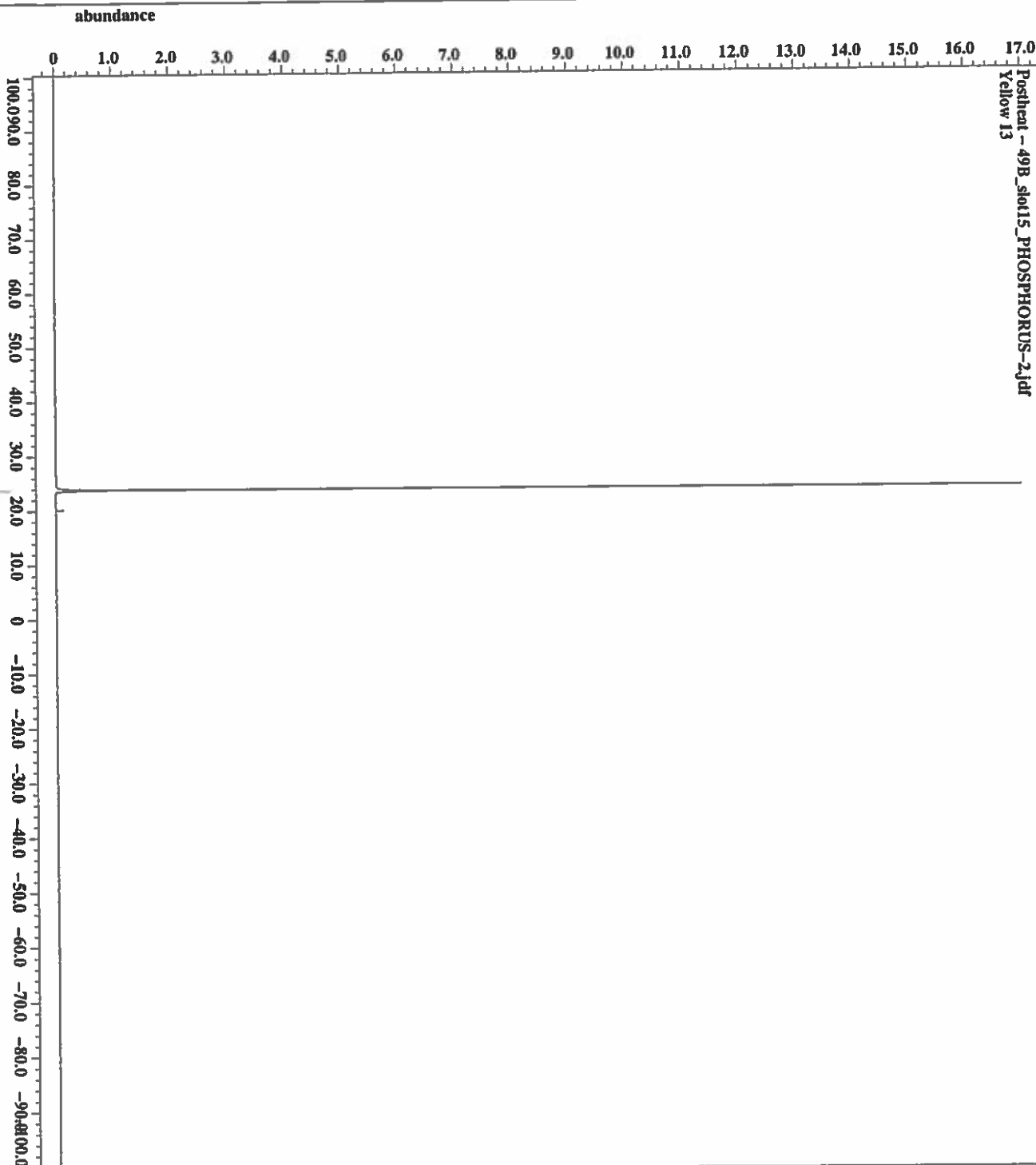




Post_Heat_49B_PROTON-4jdr
yellow 13



Postheat - 49B_slot15_PHOSPHORUS-2.jdt
Yellow 13



X : parts per Million : 31P



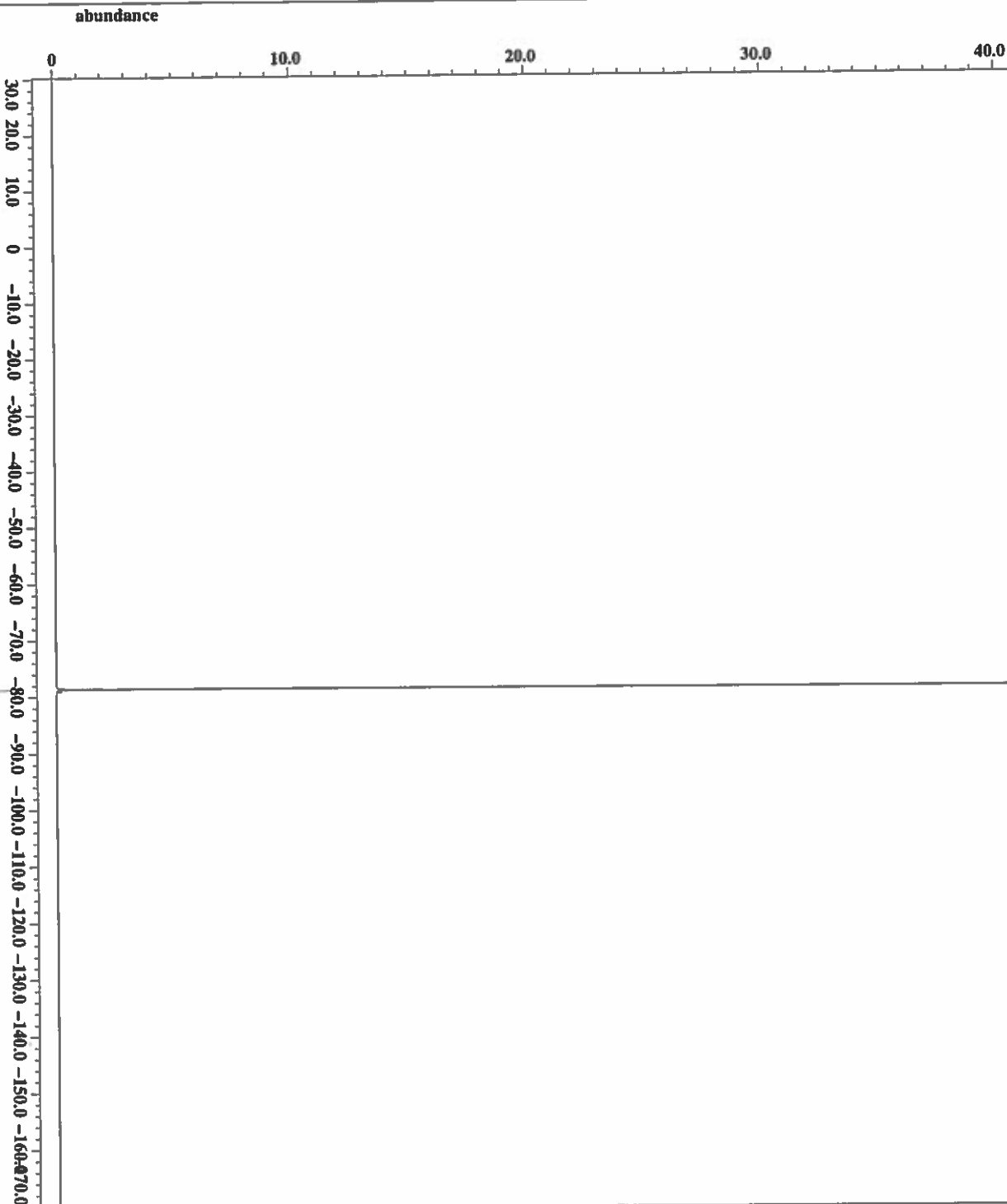
filename = Postheat - 49B_slot15
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = 8#725535
 Solvent = CHLOROFORM-D
 Changer_sample = 15
 Creation_time = 1-JUL-2016 20:39:53
 Revision_time = 1-JUL-2016 20:21:47
 Current_time = 1-JUL-2016 20:21:47

 Comment = Yellow 13
 Data_format = 1D COMPLEX
 Dm_size = 26214
 Dm_title = 31P
 Dm_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 = 202.46631075 [MHz]
 X_offset = 0 [ppm]
 X_pulses = 32768
 X_prescans = 4
 X_resolution = 1.55066895 [Hz]
 X_sweep = 50.81300813 [kHz]
 Itr_domain = 1H
 Itr_freq = 500.15991521 [MHz]
 Itr_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 256
 Total_scans = 256

 X_90_width = 14 [us]
 X_acq_time = 0.64487424 [s]
 X_angle = 30 [deg]
 X_atn = 5 [dB]
 X_pulse = 4.66666667 [us]
 Itr_atn_dec = 20.5 [dB]
 Itr_atn_noe = 20.5 [dB]
 Itr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 58
 Recvr_gain = 2 [s]
 Relaxation_delay = 2 [s]
 Repetition_time = 2.64487424 [s]
 Temp_get = 23.5 [degC]

Postheat - 49B_slot15_FLUORINE-2.jdr
Yellow 13



X : parts per Million : 19F



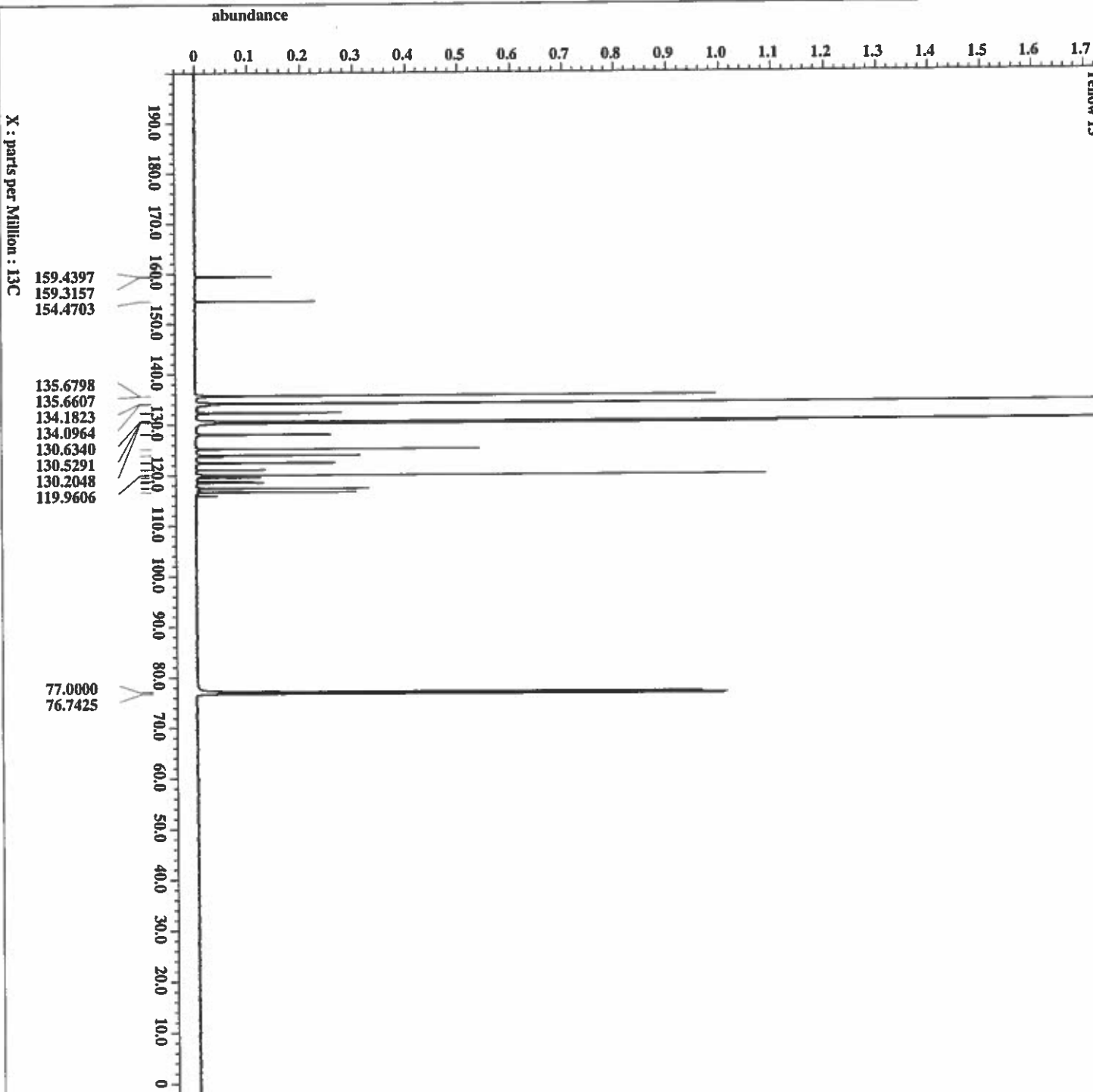
Filename Postheat - 49B_slot15
 Author Jim Davis
 Experiment single_pulse.ex2
 Sample_id S8591437
 Solvent CHLOROFORM-D
 Changer_sample 15
 Creation_time 1-01-2016 16:46:22
 Revision_time 1-01-2016 16:28:17
 Current_time 1-01-2016 16:28:17

 Comment Yellow 13
 Data_format 1D COMPLEX
 Data_size 52428
 Data_title 19F
 Data_units [ppm]
 Dimensions X
 Site ECA 500
 Spectrometer JNM-ECX500

 Field_strength 11.7473578 [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 [Hz]
 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 16
 Total_scans 16

 X_90_width 15.7 [us]
 X_acq_time 0.55574528 [s]
 X_angle 45 [deg]
 X_atn 4 [dB]
 X_pulse 7.85 [us]
 Xr_mode Off
 Xr_mode Dance_preset
 Initial_wait 40
 Relaxation_delay 4 [s]
 Repetition_time 22.7 [sec]
 Temp_get

Postheat - 49B_slot15 CARBON-2.jdr
Yellow 13



X : parts per Million : 13C



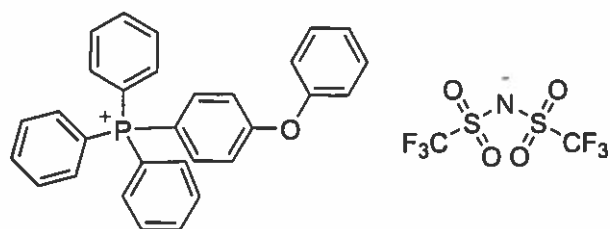
Filename = Postheat - 49B_slot15
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = S#203203
 Solvent = CHLOROFORM-D
 Changer_sample = 15
 Creation_time = 3-JUL-2016 08:24:29
 Revision_time = 3-JUL-2016 08:06:18
 Current_time = 3-JUL-2016 08:06:18

 Comment = Yellow 13
 Data_format = 1D COMPLEX
 Data_size = 26214
 Data_title = 13C
 Data_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECX500

 Field_strength = 11.7473578 [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 = 1H
 X_domain = 500.15991521 [MHz]
 X_freq = 5.0 [ppm]
 X_offset = FALSE
 Mod_return = 1
 Scans = 3100
 Total_scans = 3100

 X_90_width = 12.55 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 6 [dB]
 X_pulse = 4.18333333 [us]
 X_atn_dec = 20.5 [dB]
 X_atn_noe = 20.5 [dB]
 X_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 = 23.3 [deg]

COMPOUND 4



Atlantic Microlab, Inc.

No. Phosphonium 156A

Atlantic Blvd. Suite M
S, GA 30071
atlcmicrolab.com

Supervisor: James Davis

C#

Company/School U of South Alabama

Dept. Chemistry

Address Chem 223

City, State, Zip Mobile AL 36688

Name James Davis

Phone (251) 751-0520

Date 10/31/2016

Ant	Theory	Found	
54.01	54.27		
3.40	3.42		
1.97	1.96		

Single ☒

Duplicate ☐

Elements CHNPOSF
Present:

Analyze CHN
for:

Hygroscopic ☐

Explosive ☐

M.P. unk

B.P. none

To be dried: Yes ☒ No ☐
Temp. 60C Vac. high Time 4h

Rush Service ☒

Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

Include Email Address or FAX # Below

jdavis@southalabama.edu

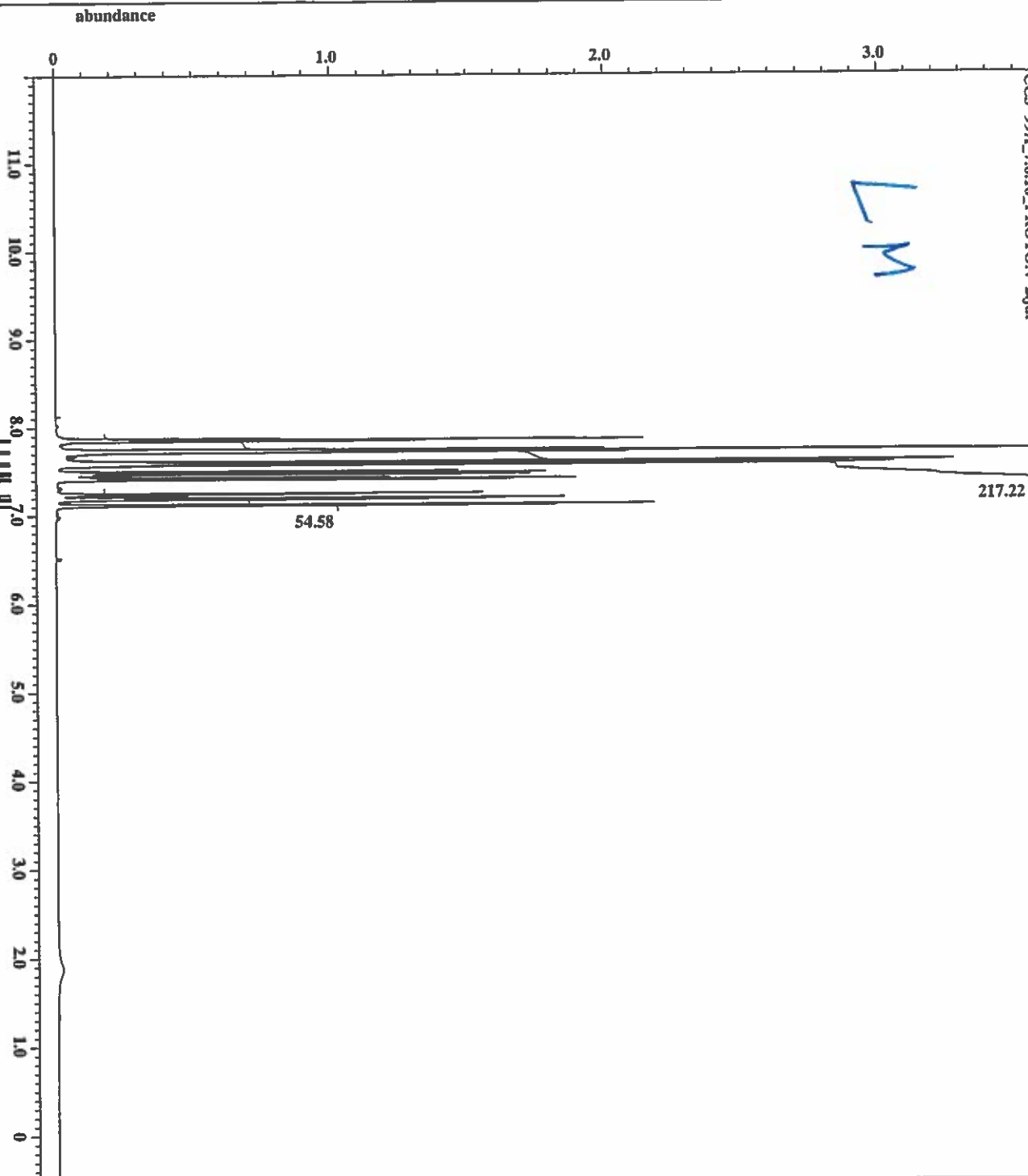
NOV 01 2016

Date Completed

NOV 01 2016

ks:

LM



X : parts per Million : 1H



Filename
Author
Experiment
Sample_1d
Solvent
Changer_sample
Creation_time
Revision_time
Current_time

Data_format
Dir_size
Dir_title
Dir_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
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_mode
Irr_mode
Dance_present
Initial_wait
Recvr_gain
Relaxation_delay
Repetition_time
Temp_get

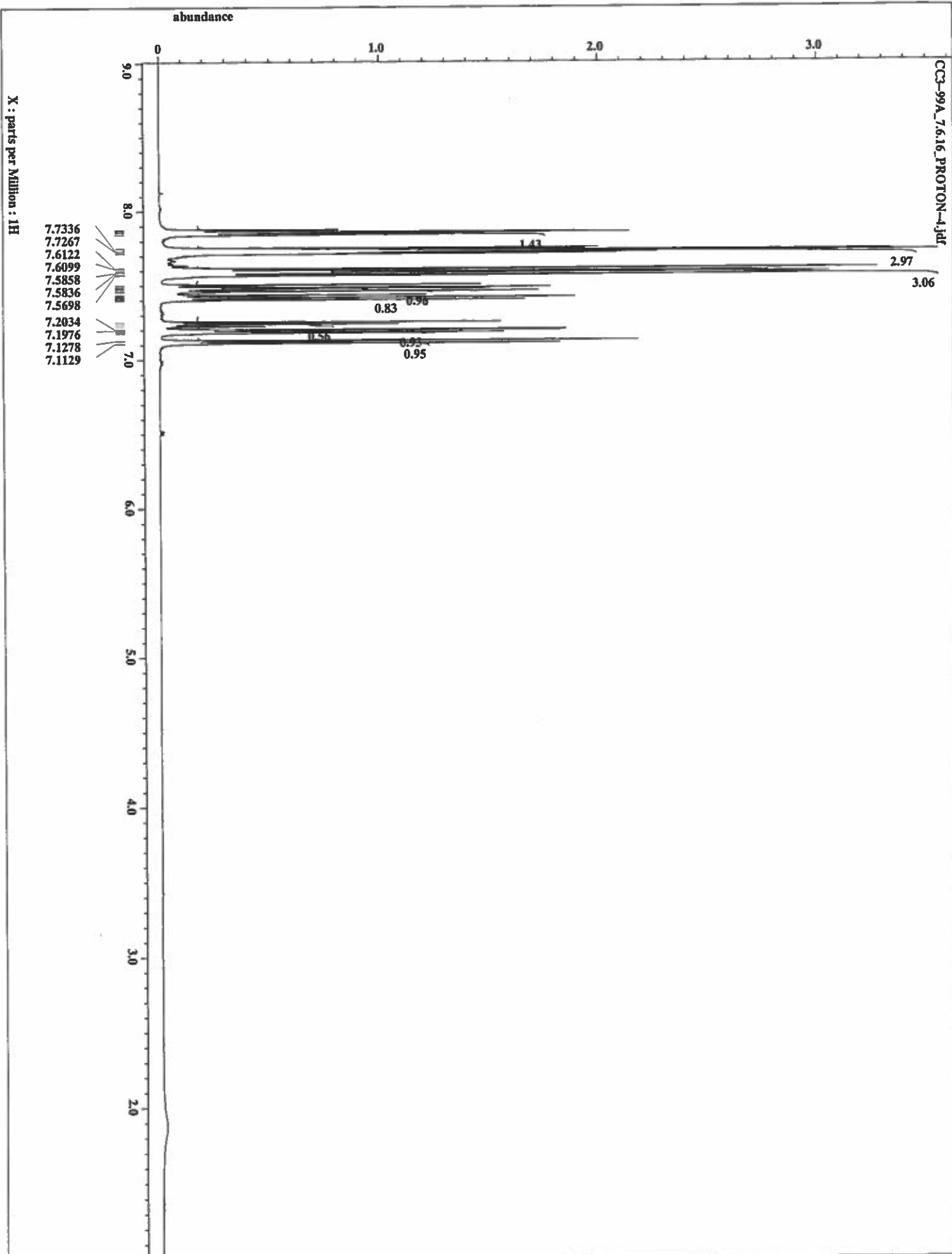
CC3-99A_7.6.16_PROTON
Jim Davis
single_pulse.ex2
CC3-99A_7.6.16
CHLOROFORM-D
6
6-JUL-2016 16:48:03
6-JUL-2016 16:29:36
6-JUL-2016 16:29:36

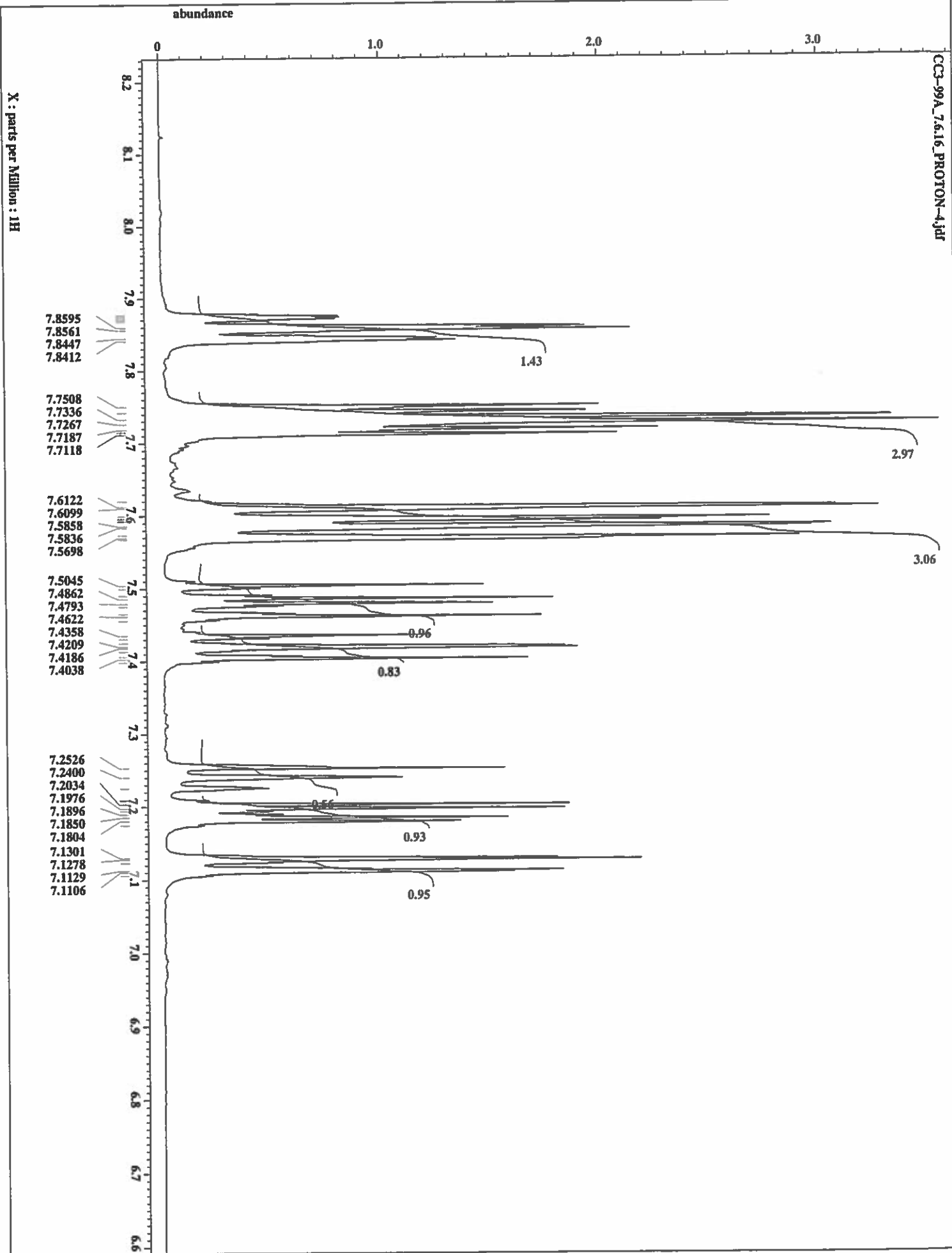
1D COMPLEX
13107
1H
[ppm]
X
ECA 500
JNM-ECA500

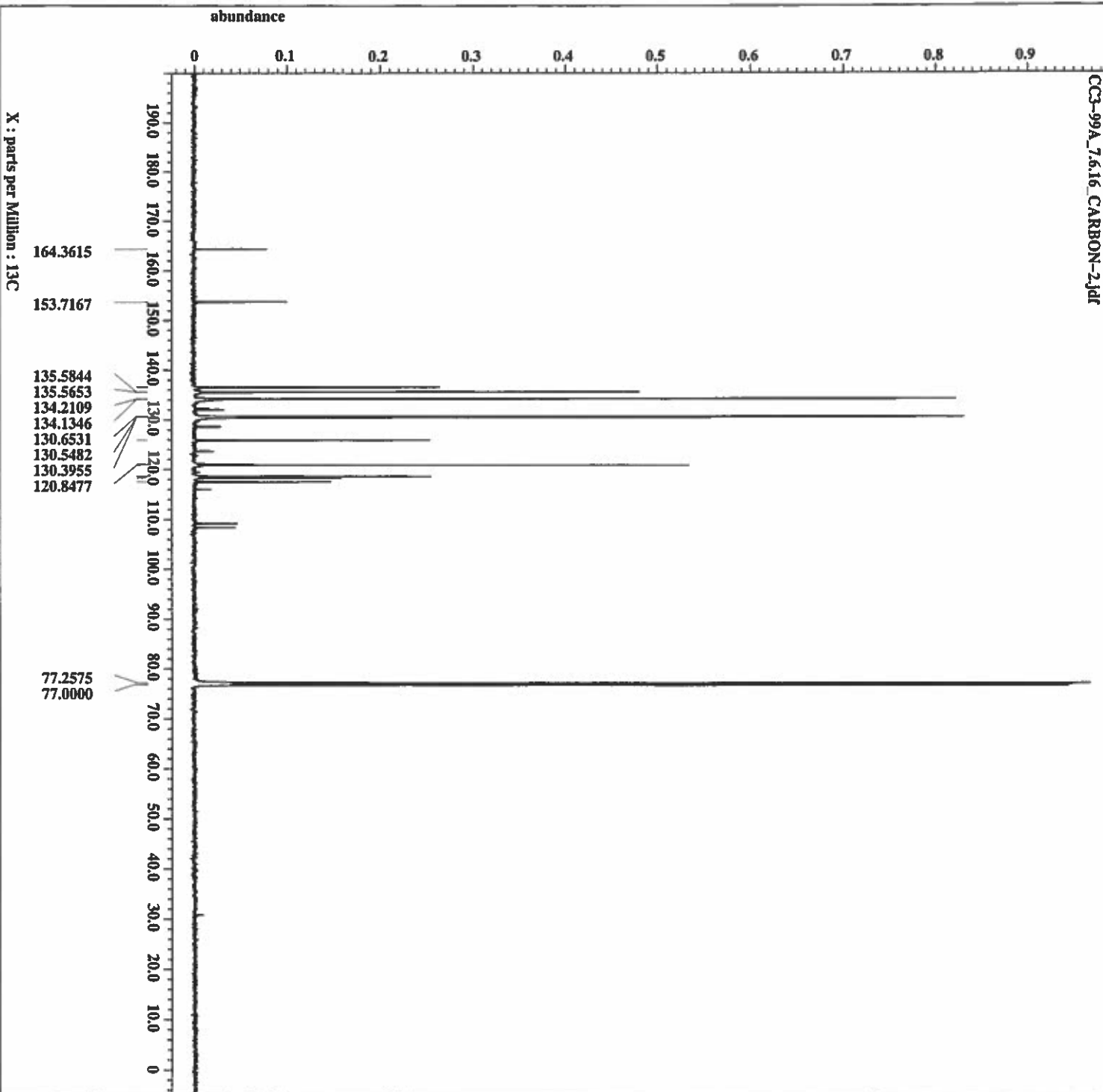
11.7473579 [Hz] (500 MHz)
1.74587904 [s]
1H
500.15991521 [MHz]
5.0 [ppm]
16384
1
0.57277737 [Hz]
9.38438438 [Hz]
1H
500.15991521 [MHz]
5.0 [ppm]
500.15991521 [MHz]
5.0 [ppm]
FALSTZ
1
32
32

13.35 [us]
1.74587904 [s]
45 [deg]
4 [dB]
6.675 [us]
OFF
OFF
FALSTZ
1 [s]
32
4 [s]
5.74587904 [s]
22.7 [s]









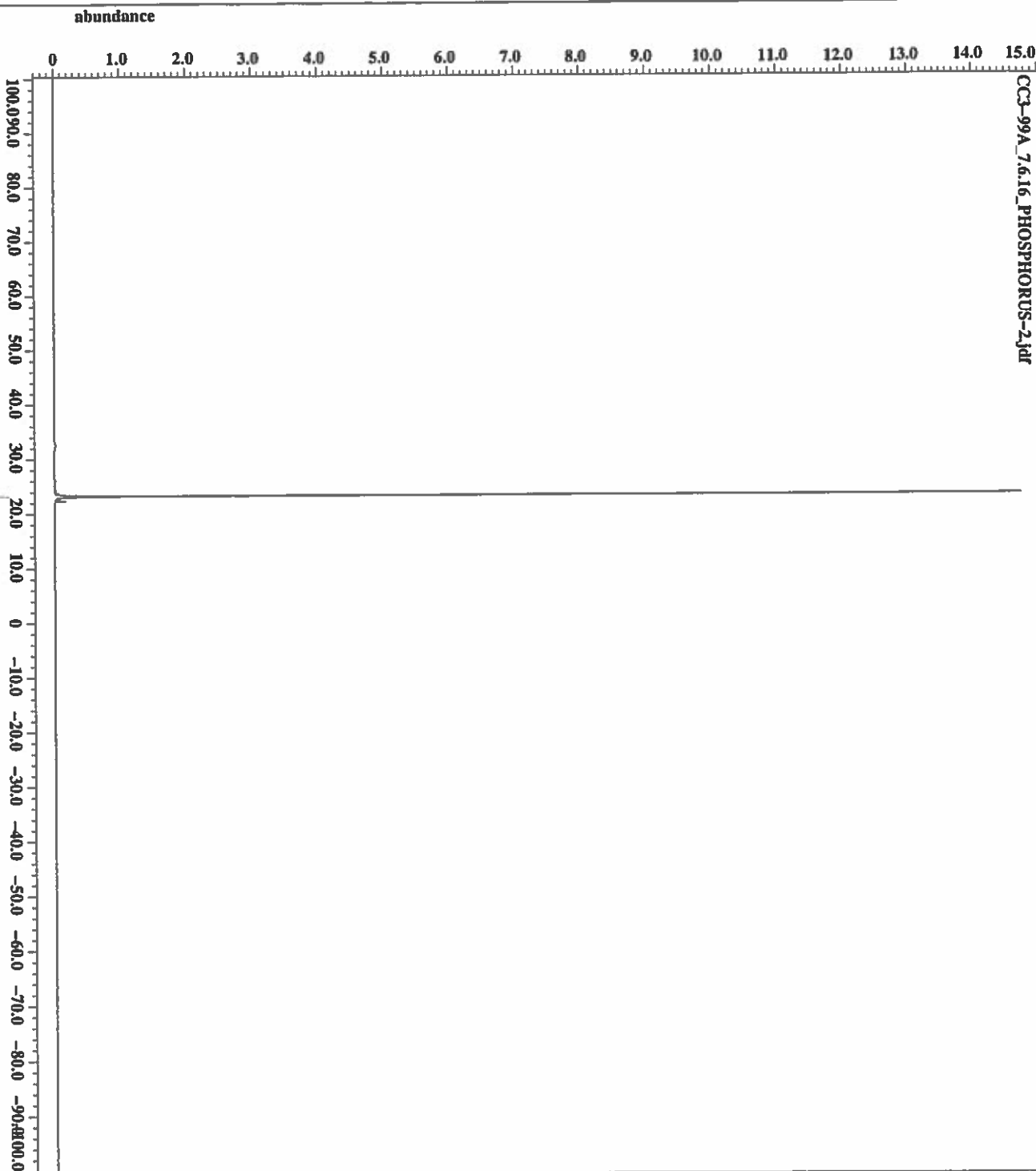
```

Filename      = CC3-99A_7.6.16_CARBON
Author        = Jim Davis
Experiment    = single_pulse_dec
Sample_id     = CC3-99A_7.6.16
Solvent       = CHLOROFORM-D
Charger_sample = 6
Creation_time  = 7-JUL-2016 07:10:07
Revision_time  = 7-JUL-2016 06:51:36
Current_time   = 7-JUL-2016 06:51:36

Data_format   = 1D COMPLEX
Dir_size      = 26214
Dir_file      = 13C
Dir_units     = [ppm]
Dimensions    = X
Size          = 6CA 500
Spectrometer  = JNM-ECA500

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_pulses       = 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]
Xir_offset     = FALSE
Mod_return     = 1
Gcans          = 2048
Total_scans    = 2048

X_90_width     = 12.55 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [db]
X_pulse        = 4.18333333 [us]
Xir_atn_dec    = 20.5 [db]
Xir_atn_noe    = 20.5 [db]
Xir_noise      = NMRZ
Decoupling     = TRIZ
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get       = 23.9 [dc]
  
```



```

=====
File Name      CC3-99A_7.6.16_PHOSPH
Author         Jim Davis
Experiment     single_pulse_dec
Sample ID      CC3-99A_7.6.16
Solvent        CHLOROFORM-D
Charger_Sample 6
Creation time  7-JUL-2016 07:35:04
Revision time  7-JUL-2016 07:16:35
Current time   7-JUL-2016 07:16:35

=====
Data Format
Data Size     26214
Data Title    31P
Data Units    [ppm]
Dimensions    X
Site          XCA 500
Spectrometer  JNM-ZCA500

=====
Field Strength 11.7473579 [G] (500 MHz)
Acq Duration    0.64487424 [s]
FID             31P
X Domain        202.46831075 [MHz]
X Freq          0 [ppm]
X Offset        32768
X Points        4
X Prescans      1.55068995 [Hz]
X Resolution    50.81300813 [kHz]
X Sweep         1H
X Domain        500.15991521 [MHz]
X Freq          5.0 [ppm]
X Offset        FALSE
C1 Type         1
Mod Return      512
Scans           512
Total Scans     512

=====
X 90 Width     16 [us]
X Acq Time     0.64487424 [s]
X Angle        30 [deg]
X Achn         5 [dB]
X Pulse        4.66666667 [us]
Xr Attn Dec    20.5 [dB]
Xr Attn Noe    20.5 [dB]
Xr Noise       VALVE
Decoupling     TRUE
Initial Wait    1 [s]
Noe            1 [s]
Noe Time       TRUE
Relaxation Delay 2 [s]
Repetition Time 23.6 [dc]
Temp Grad      23.6 [dc]
=====

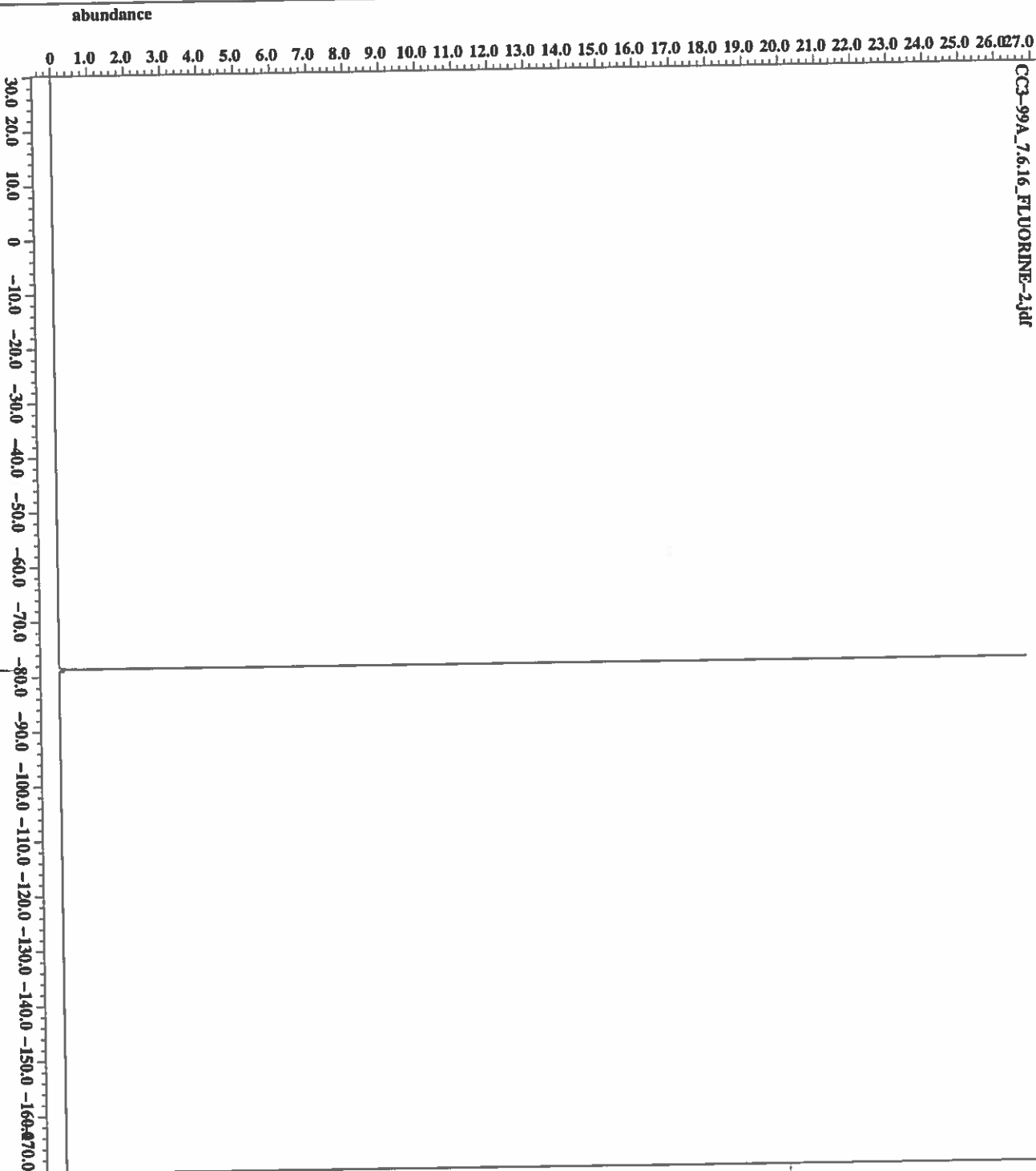
```

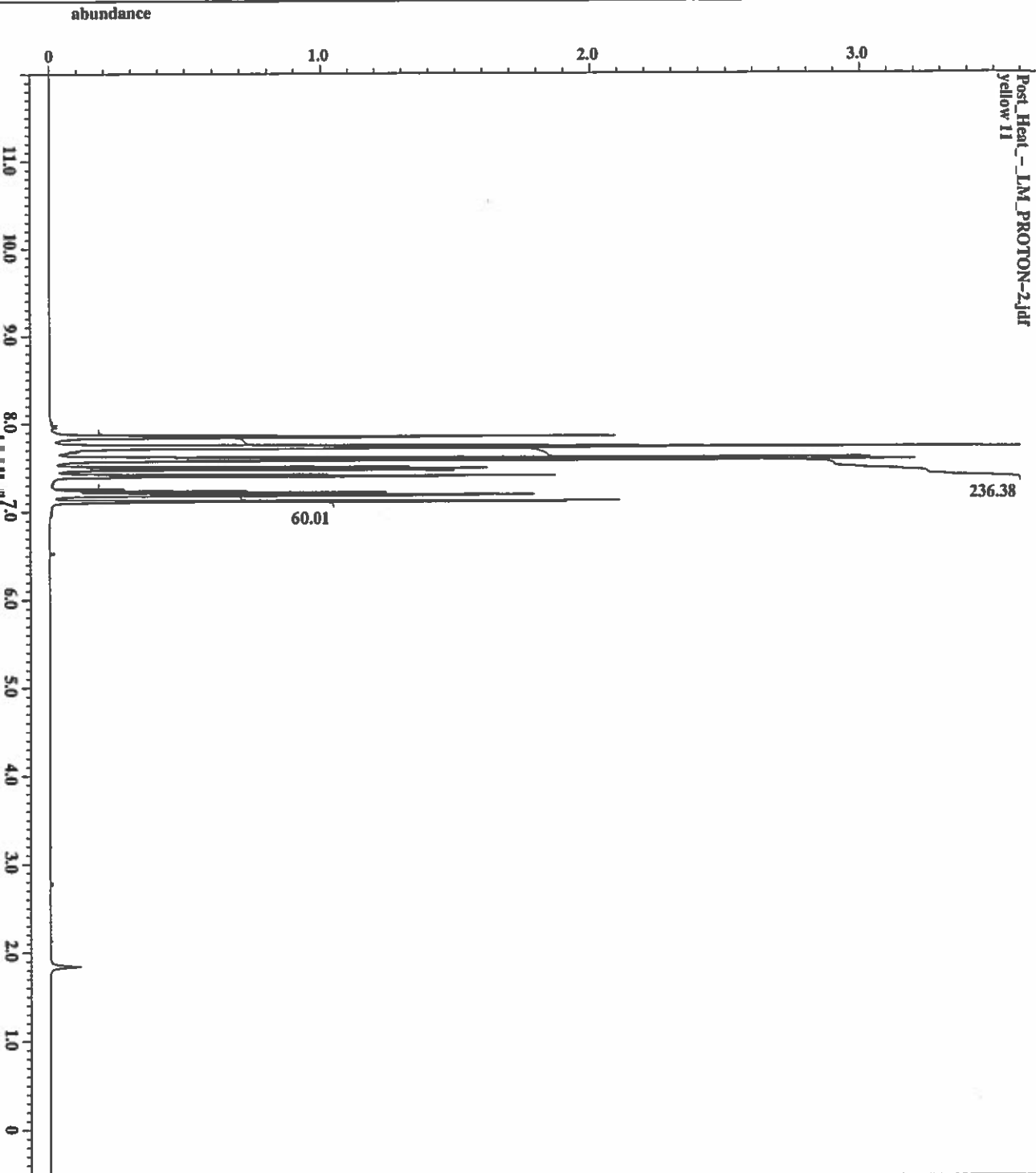


filename = CC3-99A_7.6.16_FLUORINE-2.jdt
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = CC3-99A_7.6.16
 Solvent = CHLOROFORM-D
 Changer_sample = 6
 Creation_time = 7-JUL-2016 07:39:26
 Revision_time = 7-JUL-2016 07:20:55
 Current_time = 7-JUL-2016 07:20:55

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]
 Irr_domain = 19F
 Irr_freq = 470.62046084 [MHz]
 Irr_offset = 5 [ppm]
 Trf_domain = 19F
 Trf_freq = 470.62046084 [MHz]
 Trf_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 32
 Total_scans = 32
 X_90_width = 15.7 [us]
 X_acq_time = 0.55574528 [s]
 X_angle = 45 [deg]
 X_atn = 4 [dB]
 X_pulse = 7.85 [us]
 Irr_mode = OFF
 Dantec_preset = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 42
 Relaxation_delay = 4 [s]
 Repetition_time = 4.55574528 [s]
 Temp_get = 23.1 [C]





X : parts per Million : 1H



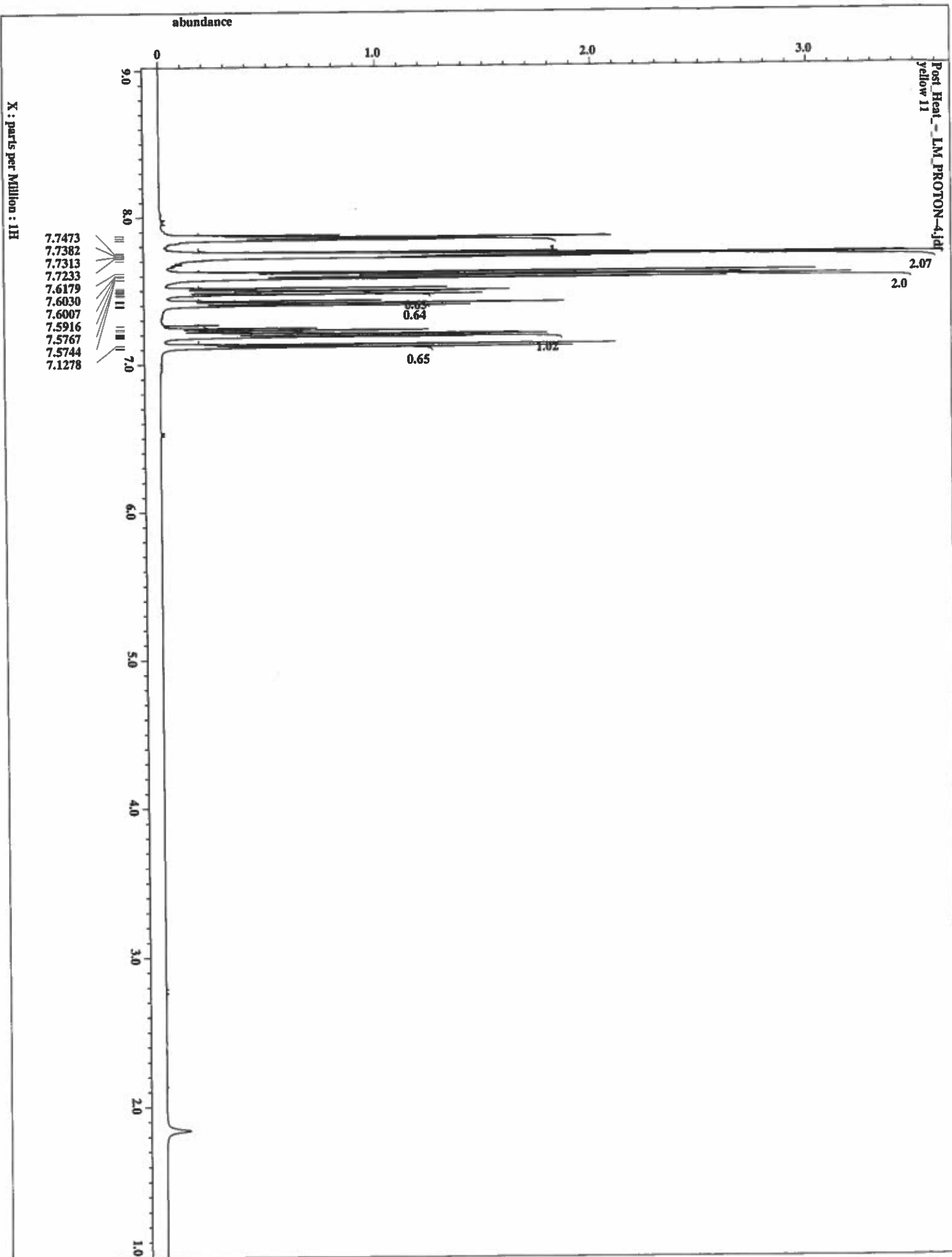
```

Filename
  = Post_Heat_-_1M_PROTON
Author
  = Jim Davis
Experiment
  = single_pulse.ex2
Sample_id
  = Post_Heat_-_1M
Solvent
  = CHLOROFORM-D
Charger_sample
  = 13
Creation_time
  = 1-JUL-2016 14:46:42
Revision_time
  = 1-JUL-2016 14:28:37
Current_time
  = 1-JUL-2016 14:28:37

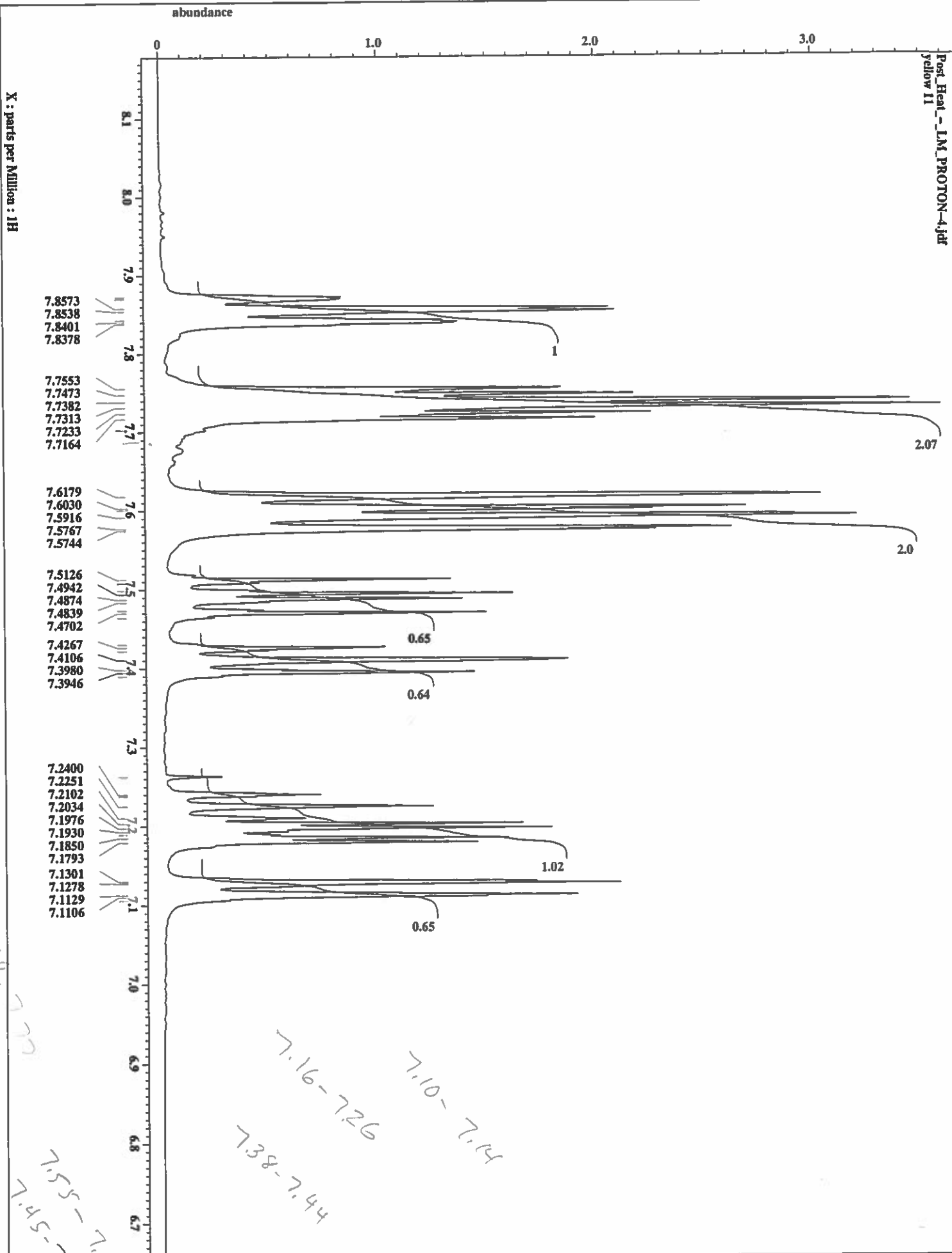
Comment
Data_format
  = yellow 11
Dir_size
  = 13107
Dir_title
  = 1H
Dim_units
  = [ppm]
Dimensions
  = X
Site
  = ECA 500
Spectrometer
  = JNM-ECA500

Field_strength
  = 11.7473579 [T] (500 [MH
X_acq_duration
  = 1.74567904 [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
Tr1_freq
  = 500.15991521 [MHz]
Tr1_offset
  = 5.0 [ppm]
Clipped
  = PALSE
Mod_return
  = 1
Scans
  = 16
Total_scans
  = 16

X_90_width
  = 13.35 [us]
X_acq_time
  = 1.74567904 [s]
X_angle
  = 45 [deg]
X_atn
  = 4 [dB]
X_pulse
  = 6.675 [us]
Irr_mode
  = Off
Tr1_mode
  = Off
Pulse_program
  = PALSE
Initial_wait
  = 1 [s]
Recvr_gain
  = 24
Relaxation_delay
  = 4 [s]
Repetition_time
  = 5.74567904 [s]
Temp_get
  = 22.3 [C]
  
```

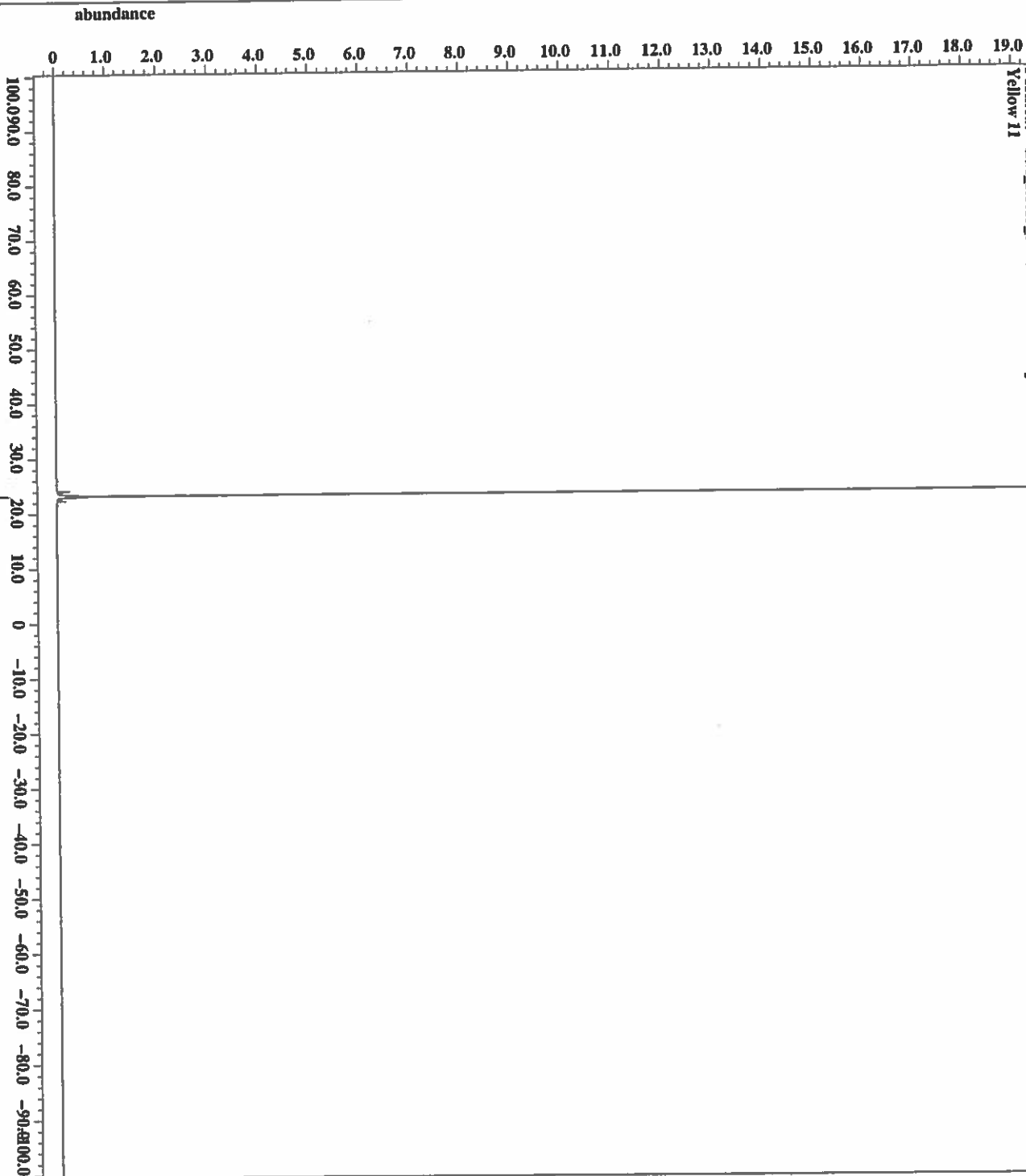


Post Heat - LM, PROTON-4.jdt
yellow 11



X : parts per Million : 1H

Postheat - LM_slot13_PHOSPHORUS-2.jdr
Yellow 11



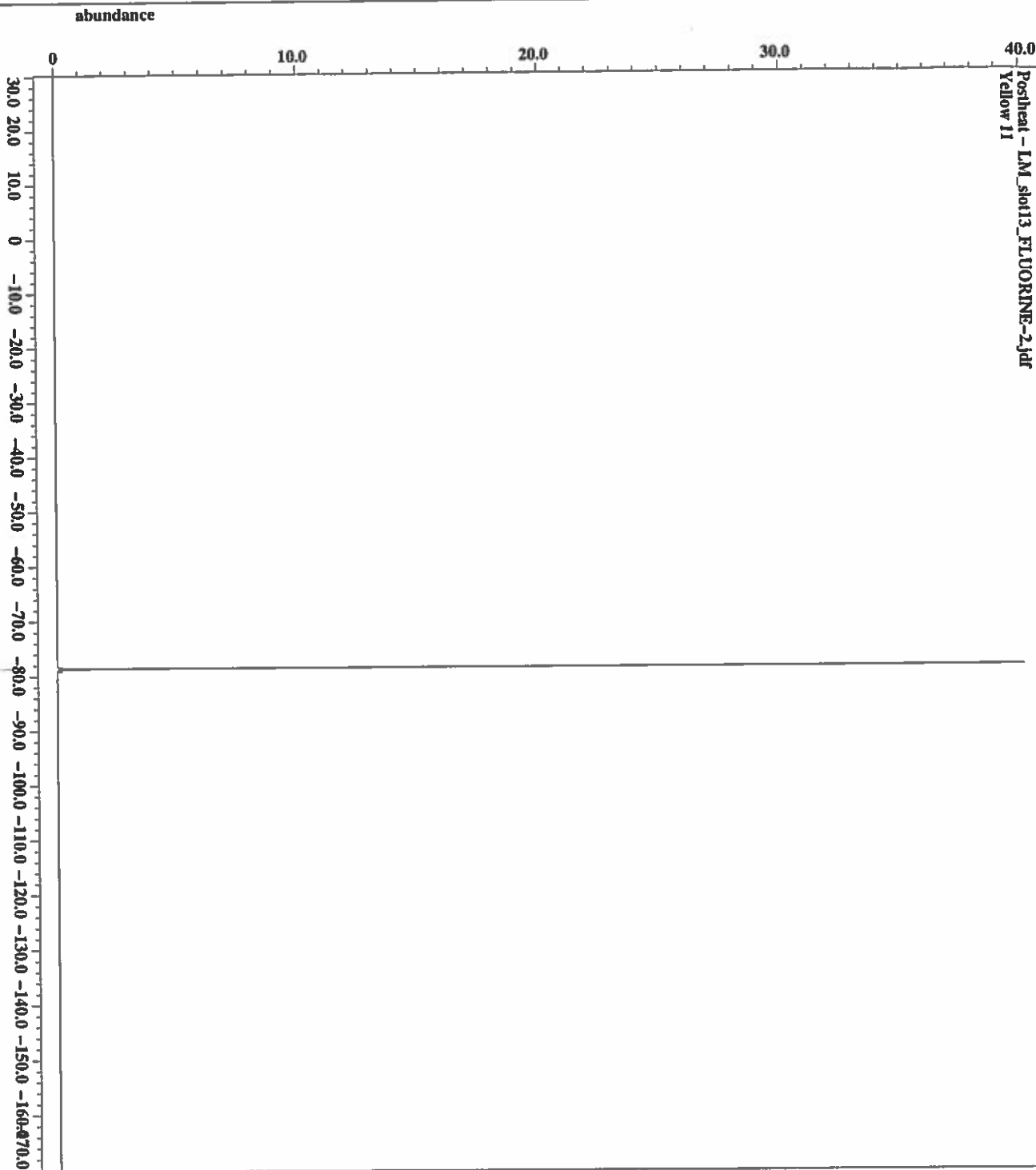
Filename = Postheat - LM_slot13-
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = #706760
Solvent = CHLOROFORM-D
Charger_sample = 13
Creation_time = 1-JUL-2016 20:08:36
Revision_time = 1-JUL-2016 19:50:30
Current_time = 1-JUL-2016 19:50:30

Comment = Yellow 11
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 [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 = 256
Total_scans = 256

X_90_width = 14 [us]
X_acq_time = 0.64487424 [s]
X_angle = 30 [deg]
X_atn = 5 [dB]
X_pulse = 4.66666667 [us]
irr_atn_dec = 20.5 [dB]
irr_atn_noi = 20.5 [dB]
irr_noise = VALVE
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 2 [s]
Recvr_gain = 56
Relaxation_delay = 2 [s]
Relaxation_time = 2.64487424 [s]
Temp_get = 23.1 [dC]

Postheat - LM_slot13_FLUORINE-2.jdr
Yellow 11



X : parts per Million : 19F



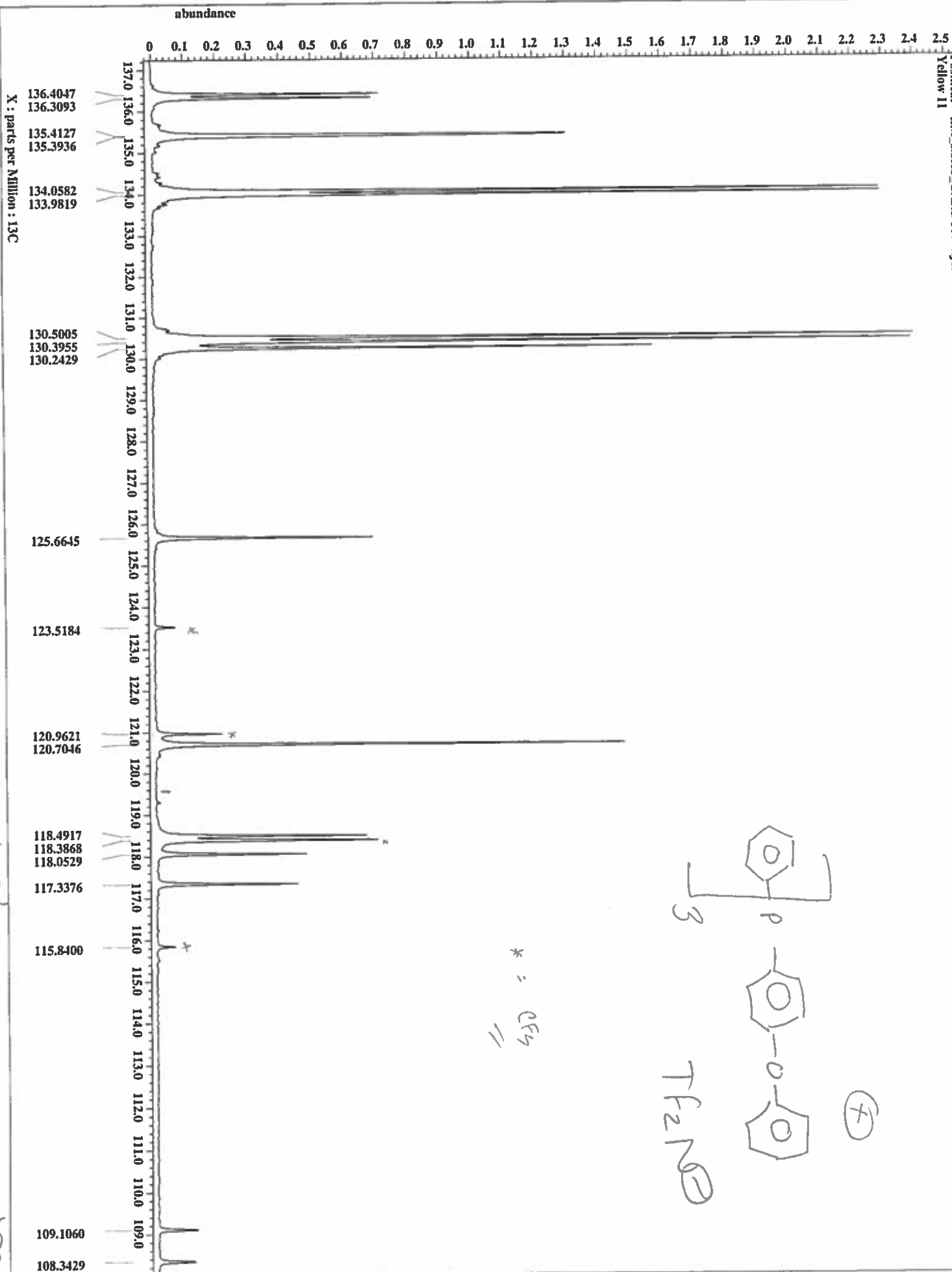
```

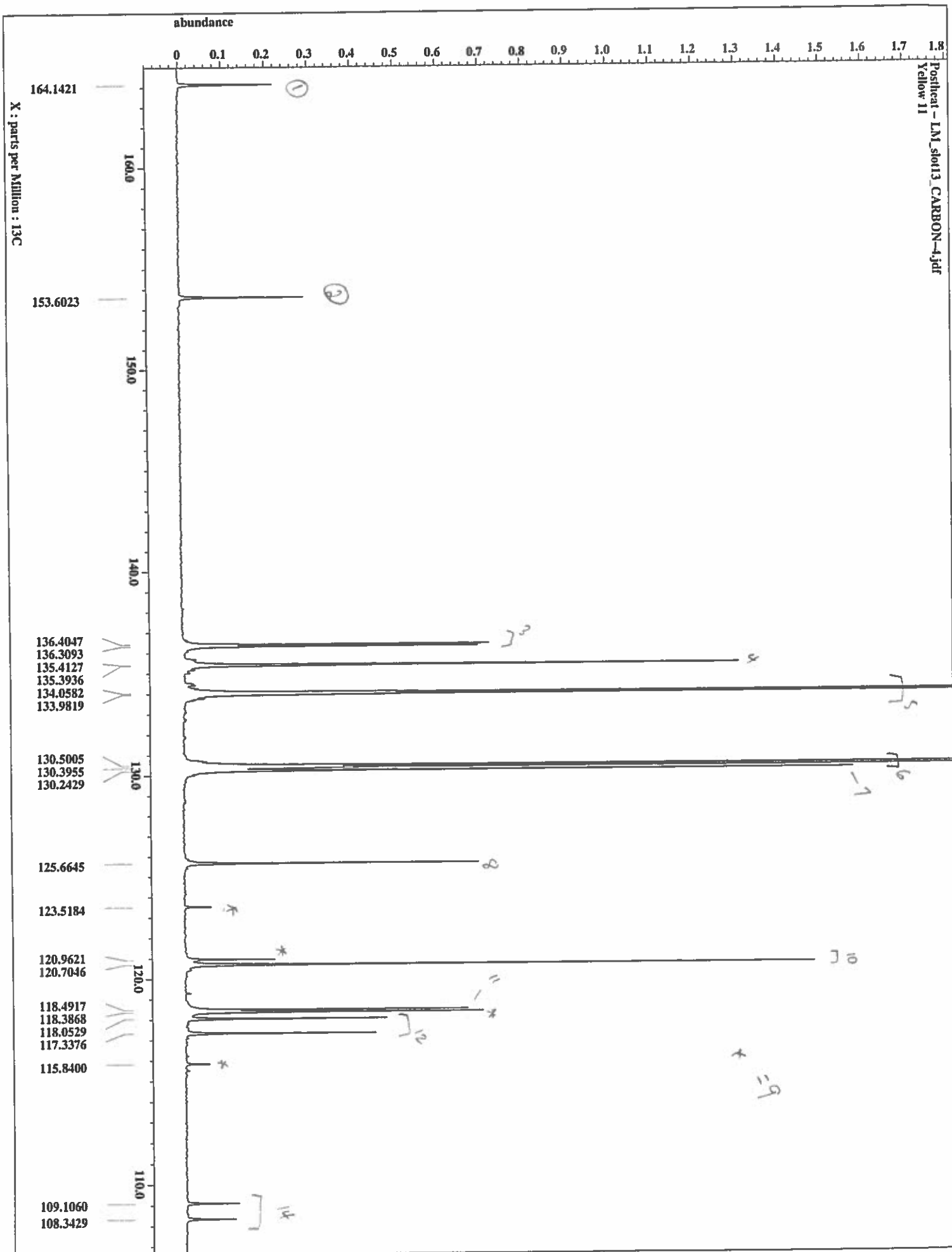
Filename      = Postheat - LM_slot13_
Author        = Jim Davis
Experiment     = single_pulse.ex2
Sample_id     = S#584563
Solvent       = CHLOROFORM-D
Charger_sample = 13
Creation_time  = 1-JUL-2016 16:35:04
Revision_time = 1-JUL-2016 16:16:59
Current_time   = 1-JUL-2016 16:16:59

Comment
Data_format   = Yellow 11
Dia_size      = 1D COMPLEX
Dia_title     = 52428
Dia_units     = 19F
Dimensions    = [ppm]
Site          = X
Spectrometer  = ECA 500
              = JNM-ECA500

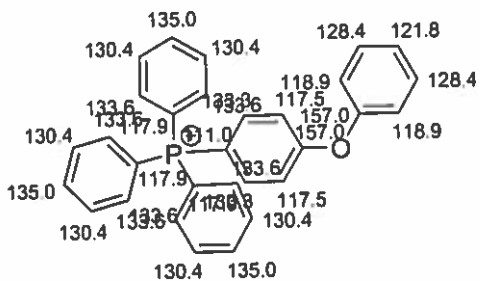
Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.55574528 [s]
X_domain       = 19F
X_freq         = 470.62046084 [MHz]
X_offset       = -70 [ppm]
X_points       = 65536
X_prescans     = 1
X_resolution   = 1.7993855 [Hz]
X_sweep        = 117.9245283 [kHz]
Xr_domain      = 19F
Xr_freq        = 470.62046084 [MHz]
Xr_offset      = 5 [ppm]
Xr1_domain     = 19F
Xr1_freq       = 470.62046084 [MHz]
Xr1_offset     = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16
X_90_width     = 15.7 [us]
X_acq_time     = 0.55574528 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 7.85 [us]
Xr_mode        = Off
Xr1_mode       = OFF
Dance_present  = FALSE
Initial_wait   = 1 [s]
Reover_gain    = 36
Relaxation_delay = 4 [s]
Repetition_time = 4.55574528 [s]
Temp_get       = 22.6 [degC]

```

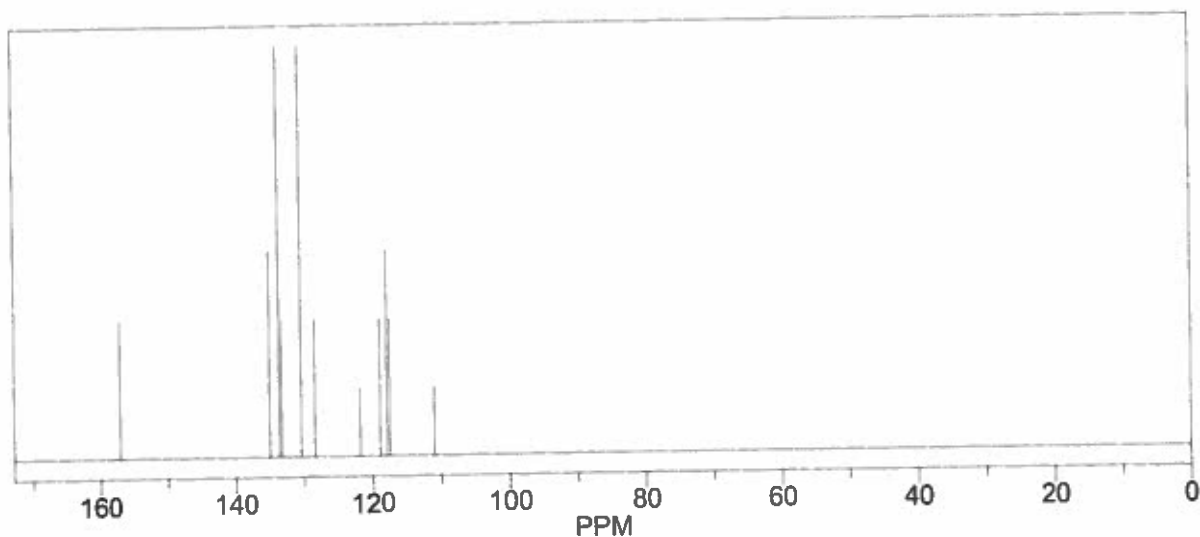





ChemNMR ¹³C Estimation



Estimation quality is indicated by color: good, medium, rough

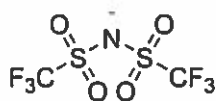
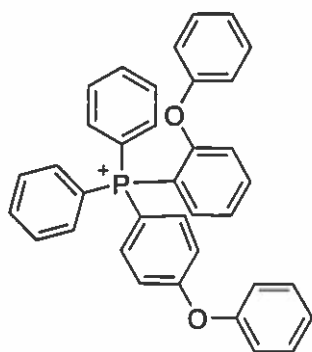


Protocol of the C-13 NMR Prediction: (Lib=S)

Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
C	111.0	128.5	1-benzene
		?	1 unknown substituent(s)
		-6.9	1 -O-1:C*C*C*C*C*1
		-10.6	general corrections
C	117.9	128.5	1-benzene
		?	1 unknown substituent(s)
		-10.6	general corrections
C	117.9	128.5	1-benzene
		?	1 unknown substituent(s)
		-10.6	general corrections
C	117.9	128.5	1-benzene
		?	1 unknown substituent(s)
		-10.6	general corrections
C	157.0	128.5	1-benzene
		?	1 unknown substituent(s)
		27.6	1 -O-1:C*C*C*C*C*1
		0.9	general corrections
C	157.0	128.5	1-benzene
		27.6	1 -O-1:C*C*C*C*C*1
		0.9	general corrections
CH	133.3	128.5	1-benzene
		?	1 unknown substituent(s)
		-0.3	1 -O-1:C*C*C*C*C*1
		5.1	general corrections
CH	133.6	128.5	1-benzene
		?	1 unknown substituent(s)
		5.1	general corrections
CH	133.6	128.5	1-benzene
		?	1 unknown substituent(s)

		1	UNKNOWN SUBSTITUENT(S)
	5.1		general corrections
CH 133.6	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	5.1		general corrections
CH 117.5	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	-11.2	1	-O-1:C*C*C*C*C*1
	0.2		general corrections
CH 118.9	128.5	1	benzene
	-11.2	1	-O-1:C*C*C*C*C*1
	1.6		general corrections
CH 133.3	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	-0.3	1	-O-1:C*C*C*C*C*1
	5.1		general corrections
CH 133.6	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	5.1		general corrections
CH 133.6	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	5.1		general corrections
CH 133.6	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	5.1		general corrections
CH 117.5	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	-11.2	1	-O-1:C*C*C*C*C*1
	0.2		general corrections
CH 118.9	128.5	1	benzene
	-11.2	1	-O-1:C*C*C*C*C*1
	1.6		general corrections
CH 130.4	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	1.9		general corrections
CH 130.4	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	1.9		general corrections
CH 130.4	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	1.9		general corrections
CH 128.4	128.5	1	benzene
	-0.3	1	-O-1:C*C*C*C*C*1
	0.2		general corrections
CH 130.4	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	1.9		general corrections
CH 130.4	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	1.9		general corrections
CH 130.4	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	1.9		general corrections
CH 128.4	128.5	1	benzene
	-0.3	1	-O-1:C*C*C*C*C*1
	0.2		general corrections
CH 135.0	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	6.5		general corrections
CH 135.0	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	6.5		general corrections
CH 135.0	128.5	1	benzene
	?	1	UNKNOWN SUBSTITUENT(S)
	6.5		general corrections
CH 121.8	128.5	1	benzene
	-6.9	1	-O-1:C*C*C*C*C*1
	0.2		general corrections

COMPOUND 5



Atlantic Microlab, Inc.

No. Phosphonium 49C

Atlantic Blvd. Suite M
 ss, GA 30071
 atlanticmicrolab.com

Company/School U of South Alabama

Dept. Chemistry

Address Chem 223

City, State, Zip Mobile AL 36688

or/Supervisor: James Davis

Name James Davis

Date 10/31/2016

C#

Phone (251) 751-0520

Element	Theory	Found	Single ☐	Duplicate ☐
C	56.79	56.58		
H	3.51	3.56		
N	1.74	1.76		
Elements CHNPOSF Present: _____ Analyze CHN for: _____ Hygroscopic ☐ Explosive ☐ M.P. <u>unk</u> B.P. <u>none</u> To be dried: Yes ☒ No ☐ Temp. <u>60C</u> <u>Vac.</u> <u>high</u> Time <u>4 h</u> Rush Service ☒ Rush service guarantee analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM. Include Email Address or FAX # Below jdavis@southalabama.edu				

Received NOV 01 2016

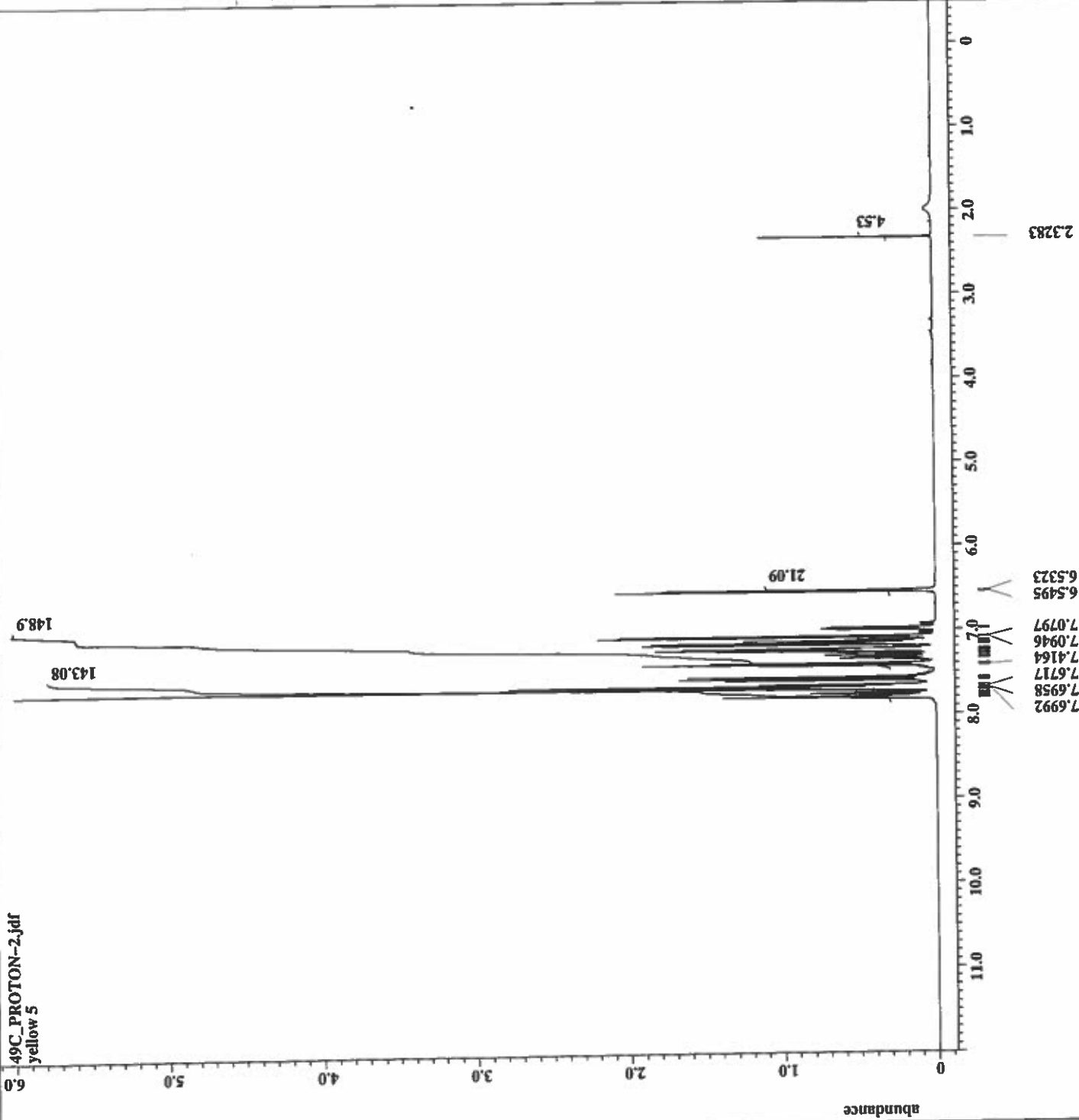
Date Completed

NOV 01 2016

arks:

49C_PROTON-2.jdr
yellow 5

148.9
143.08

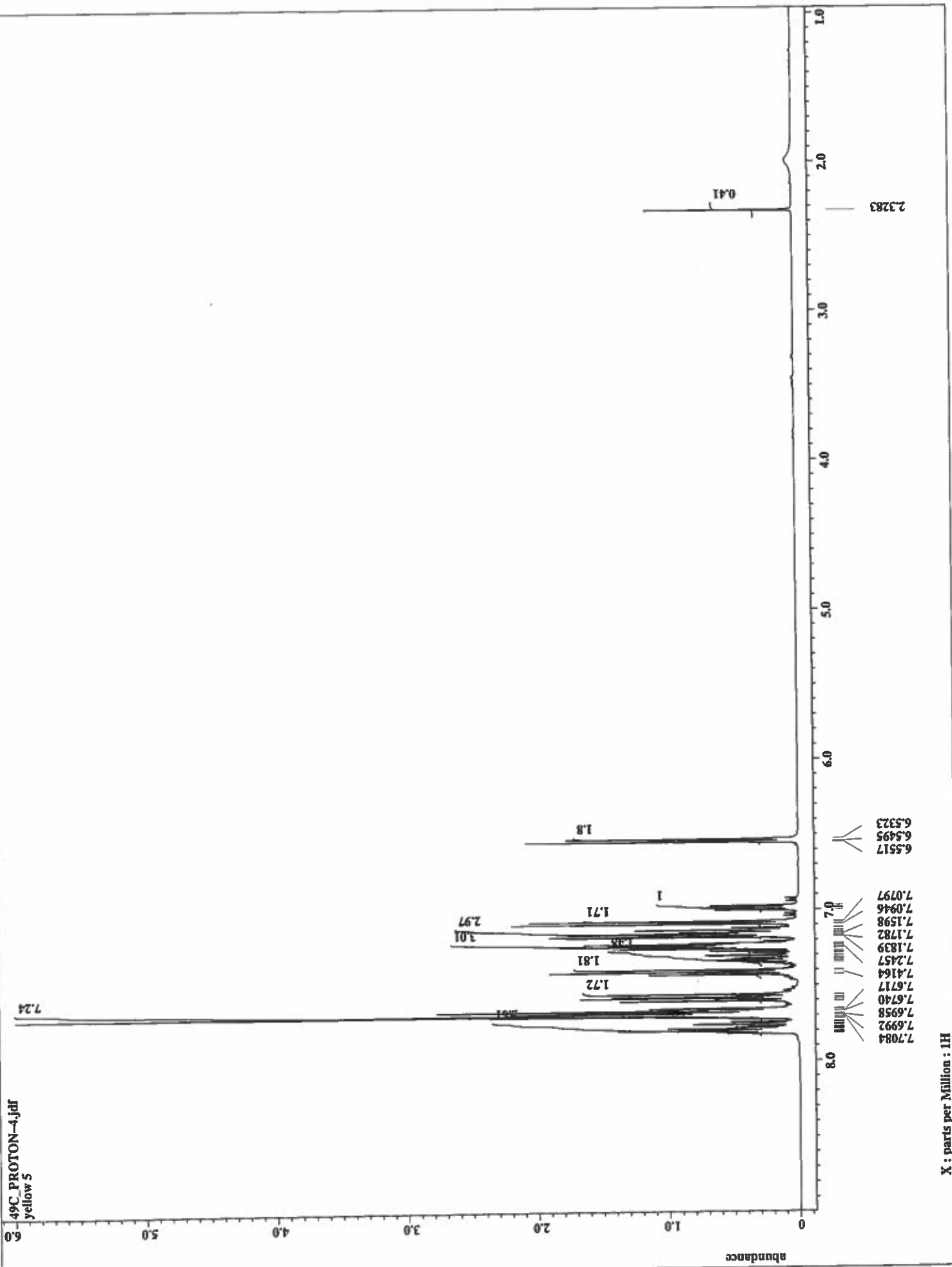


X : parts per Million : 1H

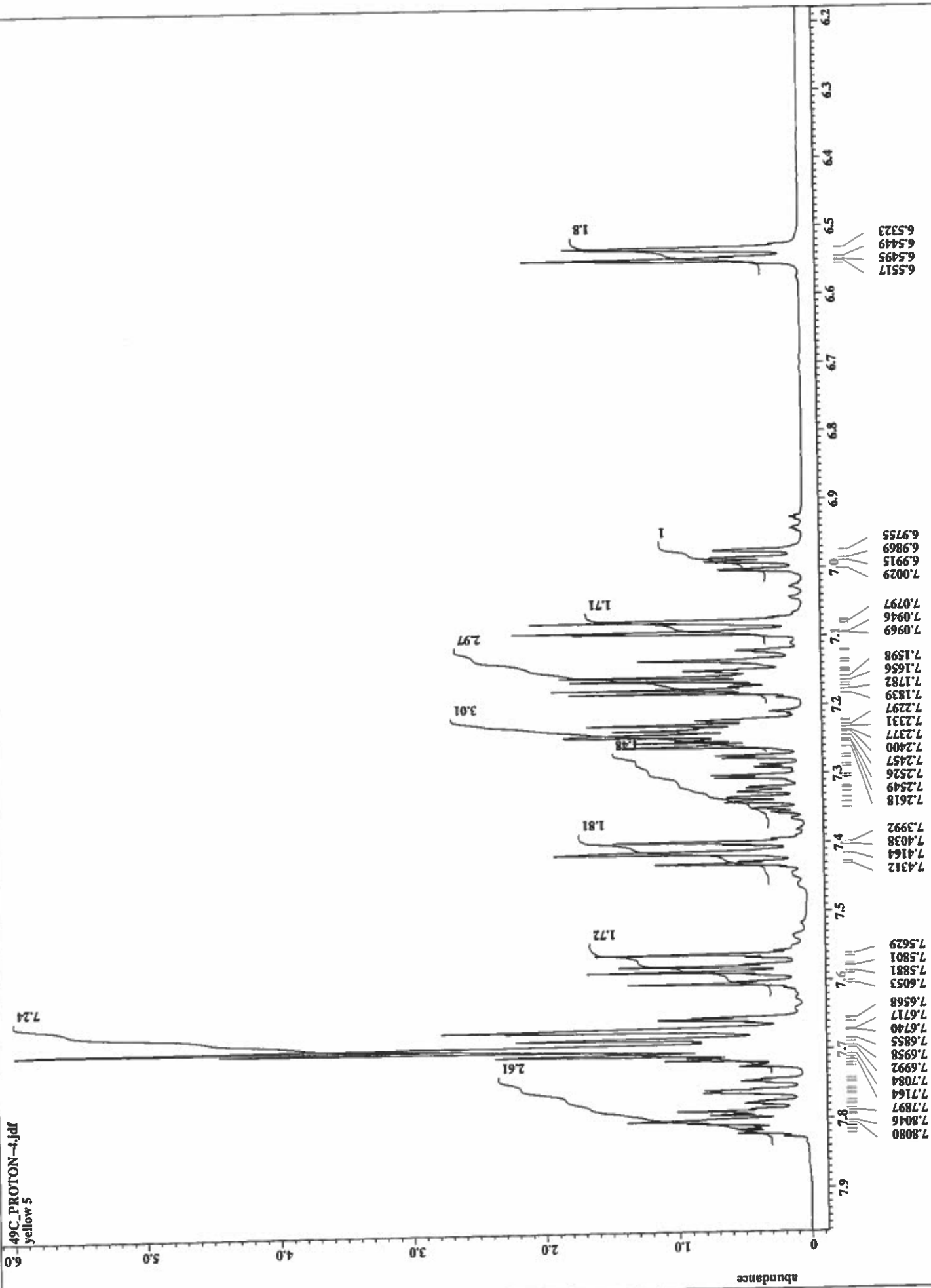


Filename = 49C_PROTON-2.jdr
Author = Jim Davis
Experiment = single_pulse.ex2
Sample_id = 49C
Solvent = CHLOROFORM-D
Changer_sample = 7
Creation_time = 1-JUL-2016 15:17:53
Revision_time = 1-JUL-2016 14:59:48
Current_time = 1-JUL-2016 14:59:48
Comment = yellow 5
Data_format = 1D COMPLEX
Dim_size = 13107
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 [MHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Tri_domain = 1H
Tri_freq = 500.15991521 [MHz]
Tri_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 13.35 [us]
X_acq_time = 1.74587904 [s]
X_angle = 45 [deg]
X_db = 4 [dB]
X_atn = 6.675 [us]
Irr_pulse = Off
Irr_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 28
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_get = 22.3 [dC]

49C PROTON-4.jdf
yellow 5



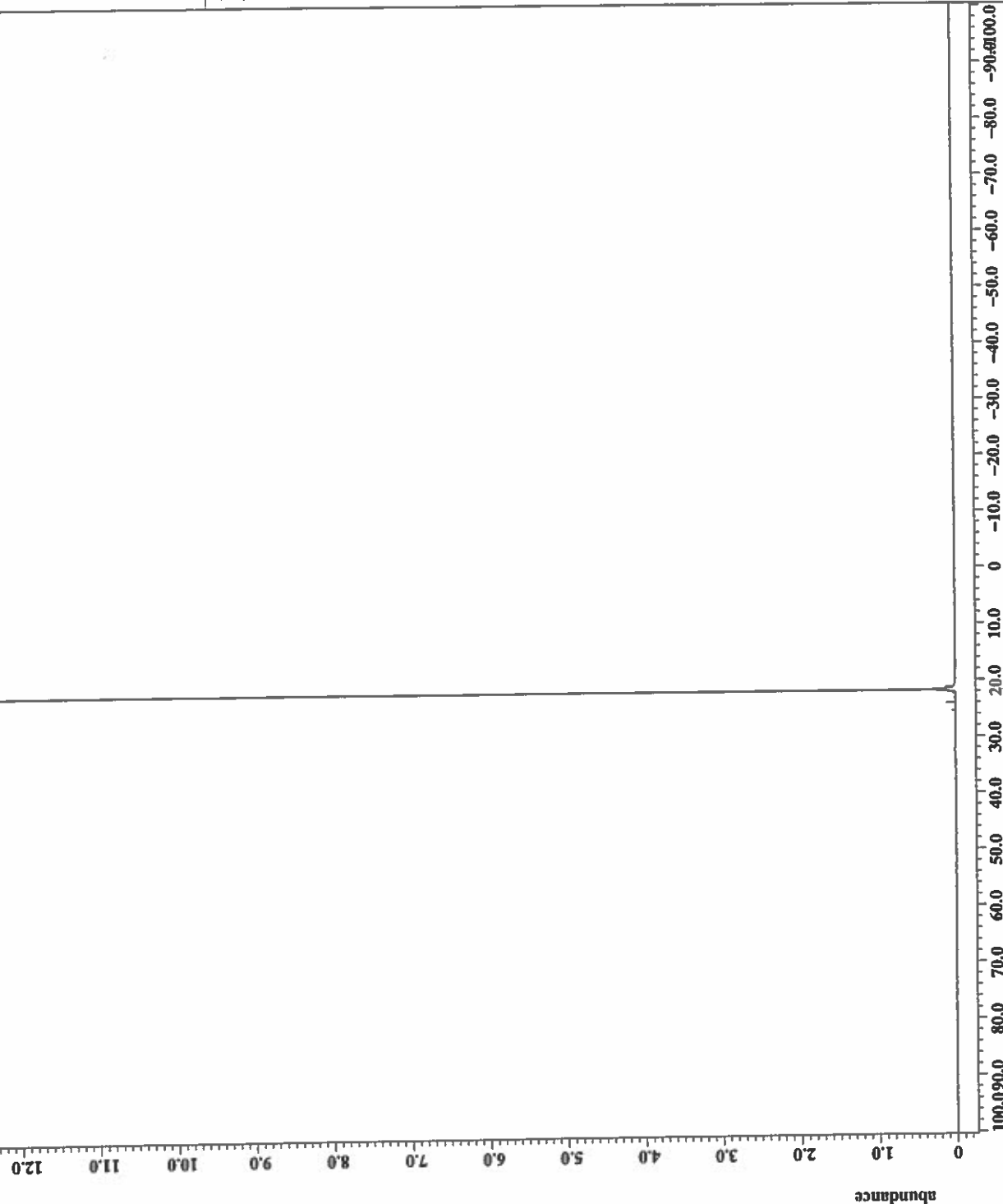
X : parts per Million : 1H





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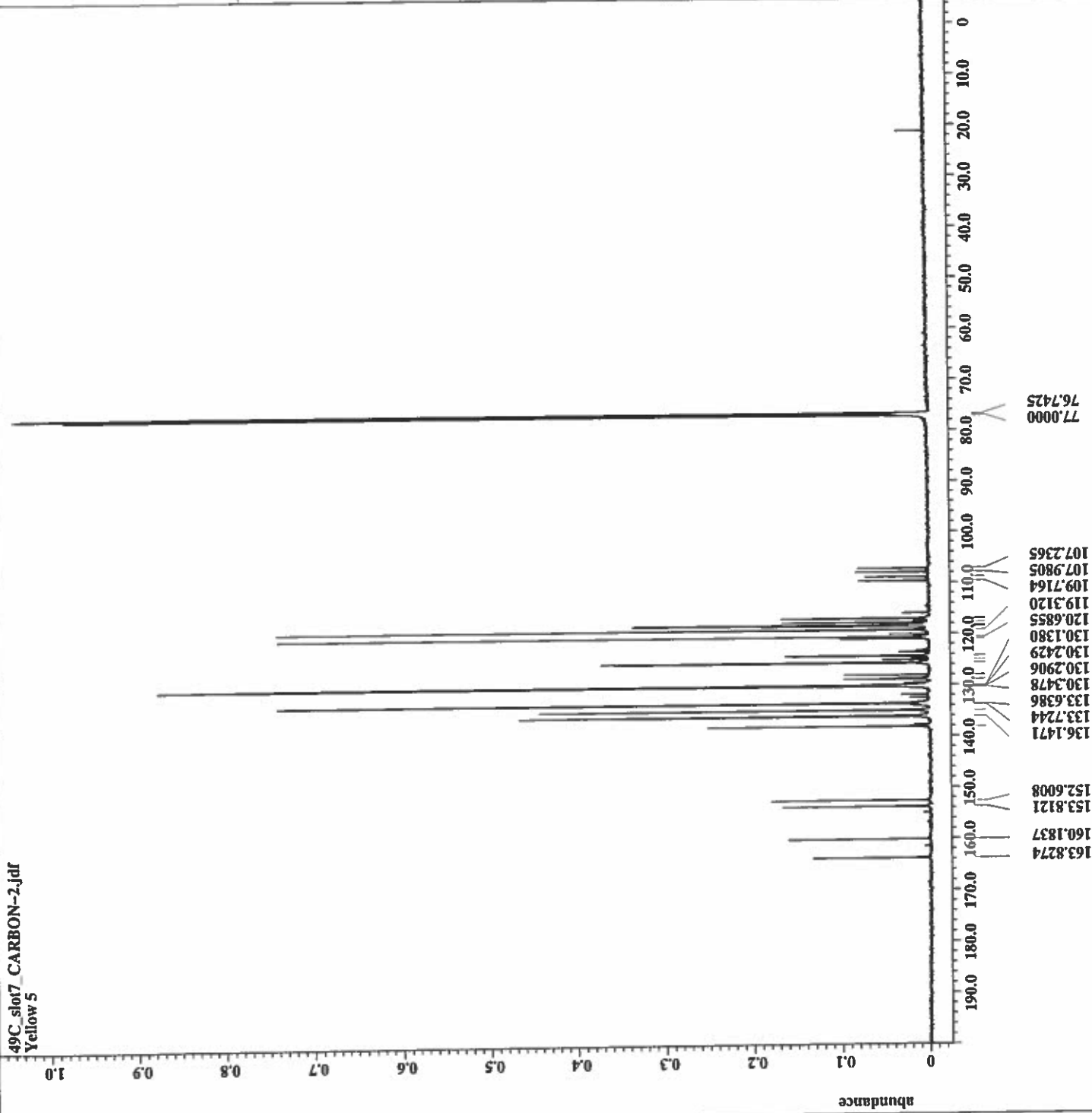
Filename = 49C_slot7_PHOSPHORUS-
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = S8649941
 Solvent = CHLOROFORM-D
 Changer_sample = 7
 Creation_time = 1-JUL-2016 18:33:54
 Revision_time = 1-JUL-2016 18:15:48
 Current_time = 1-JUL-2016 18:15:48
 Comment = Yellow 5
 Date_format = DD MMYY
 Dim_size = 26214
 Dim_title = 31P
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500
 Field_strength = 11.74737579 [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 = 256
 Total_scans = 256
 X_90_width = 14 [us]
 X_acq_time = 0.64487424 [s]
 X_angle = 30 [deg]
 X_atn = 5 [dB]
 X_pulpr = 4.66666667 [us]
 Irr_atn_dec = 20.5 [dB]
 Irr_atn_poe = 20.5 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUEZ
 Initial_wait = 1 [s]
 Noe = TRUEZ
 Noe_time = 2 [s]
 Recvr_gain = 58
 Relaxation_delay = 2 [s]
 Repetition_time = 2.64487424 [s]
 Temp_get = 23.5 [dC]



21.8126



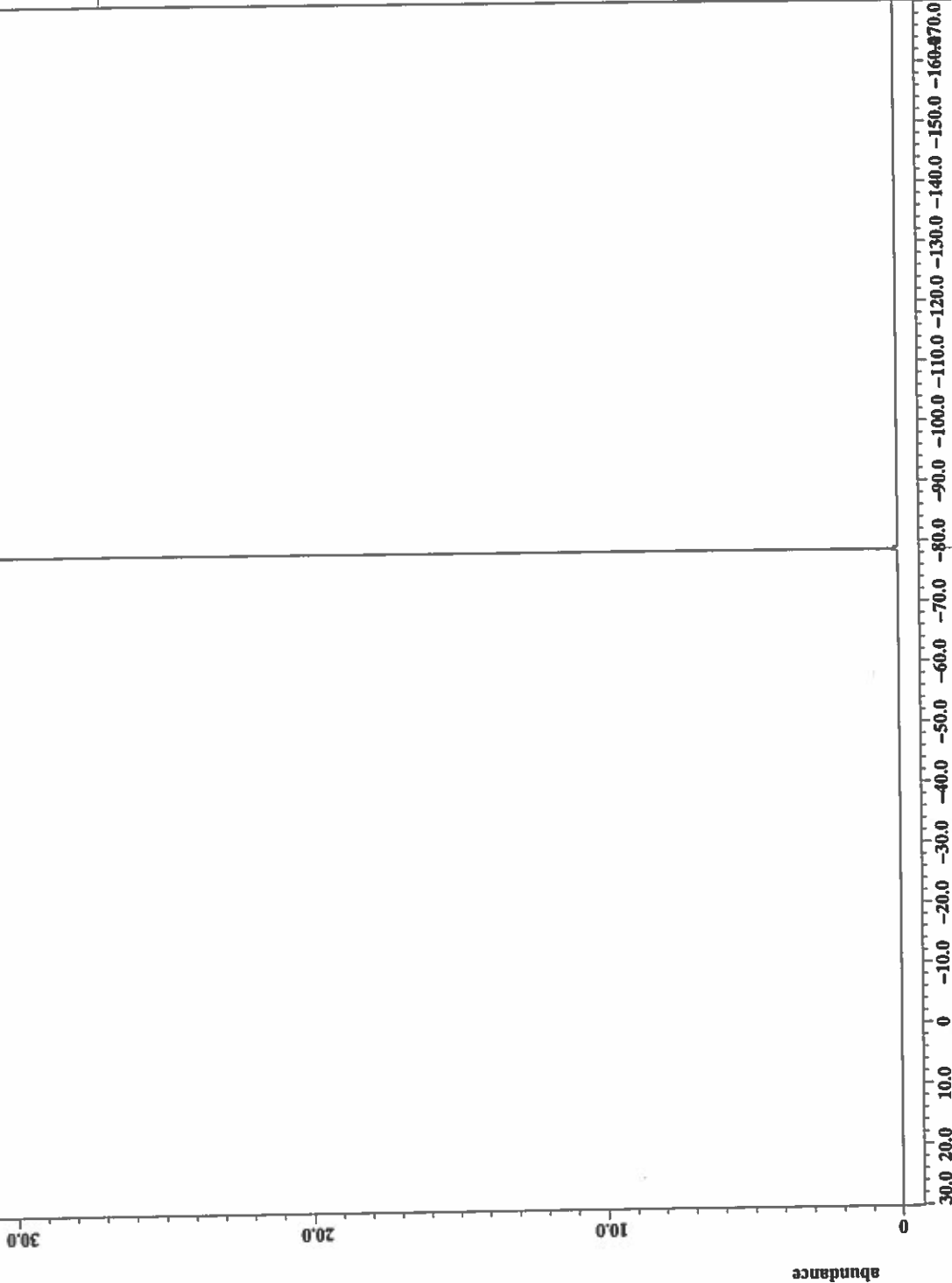
Filename = 49C_slot7_CARBON-2.jd
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = S8343224
 Solvent = CHLOROFORM-D
 Changer_sample = 7
 Creation_time = 2-JUL-2016 12:17:51
 Revision_time = 2-JUL-2016 11:59:40
 Current_time = 2-JUL-2016 11:59:40
 Comment = Yellow 5
 Data_format = 1D COMPLEX
 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 = 3100
 Total_scans = 3100
 X_90_width = 12.55 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 6 [dB]
 X_pulse = 4.18333333 [us]
 Irr_atn_dec = 20.5 [dB]
 Irr_atn_noe = 20.5 [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 = 23.8 [dC]





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Filename = 49C_slot7_FLUORINE-2.
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = S8563729
 Solvent = CHLOROFORM-D
 Changer_sample = 7
 Creation_time = 1-JUL-2016 16:00:20
 Revision_time = 1-JUL-2016 15:42:15
 Current_time = 1-JUL-2016 15:42:15
 Comment = Yellow 5
 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 [MHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084 [MHz]
 Irr_offset = 5 [ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084 [MHz]
 Tri_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 15.7 [us]
 X_acq_time = 0.55574528 [s]
 X_angle = 45 [deg]
 X_atn = 4 [dB]
 X_pulse = 7.85 [us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 40
 Relaxation_delay = 4 [s]
 Repetition_time = 4.55574528 [s]
 Temp_get = 22.9 [C]





SOUTH ALABAMA
JAGUARS

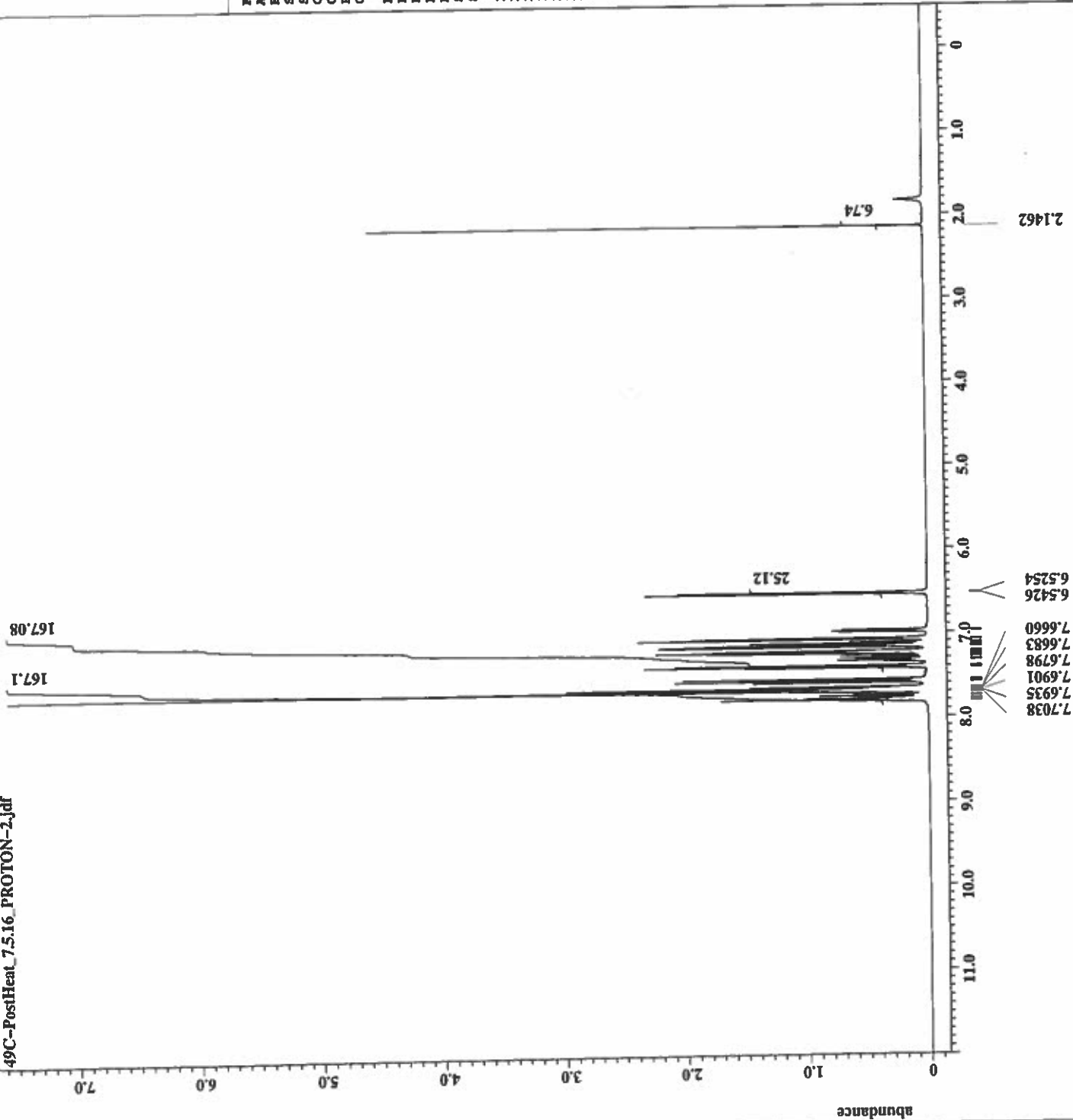
```

Filename      = 49C-PostHeat_7.5.16_P
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = 49C-PostHeat_7.5.16
Solvent       = CHLOROFORM-D
Charger_sample = 9
Creation_time  = 5-JUL-2016 15:49:03
Revision_time  = 5-JUL-2016 15:30:41
Current_time   = 5-JUL-2016 15:30:41

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

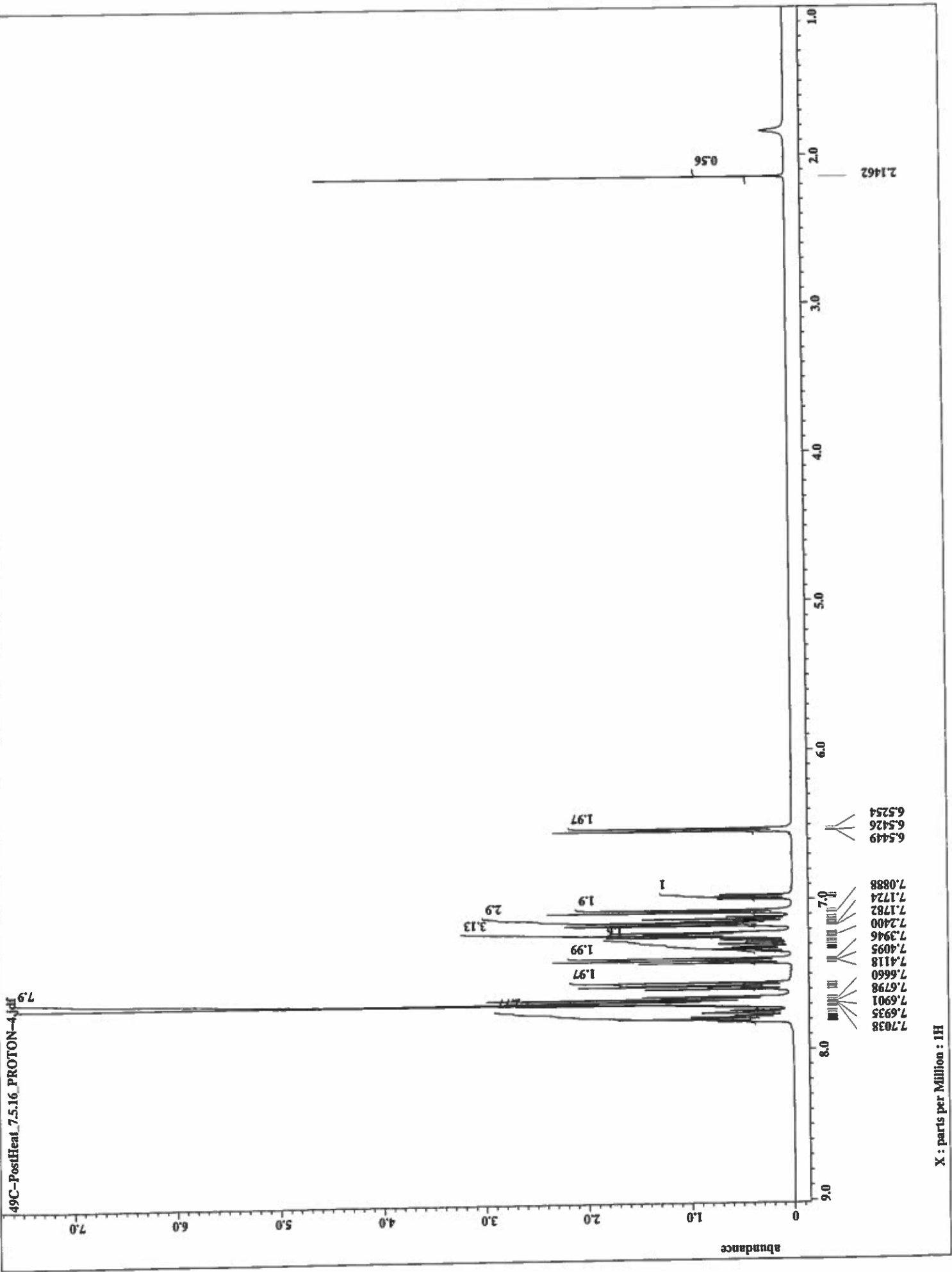
Field_strength = 11.7471579[T] (500[MH
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[KHz]
Xr_domain      = 1H
Xr_freq        = 500.15991521[MHz]
Xr_offset      = 5.0[ppm]
Xr_domain      = 1H
Xr_freq        = 500.15991521[MHz]
Xr_offset      = 5.0[ppm]
Tri_offset     = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 13.35[us]
X_acq_time     = 1.74587904[s]
X_angle        = 45[deg]
X_atn          = 4[dB]
X_pulse        = 6.675[us]
Xr_pulse       = Off
Xr_mode        = Off
Tri_mode       = FALSE
Dante_preset   = 1[s]
Initial_wait   = 30
Recvr_gain     = 5.74587904[s]
Relaxation_delay = 4[s]
Repetition_time = 22.6[dc]
Temp_get       =
  
```

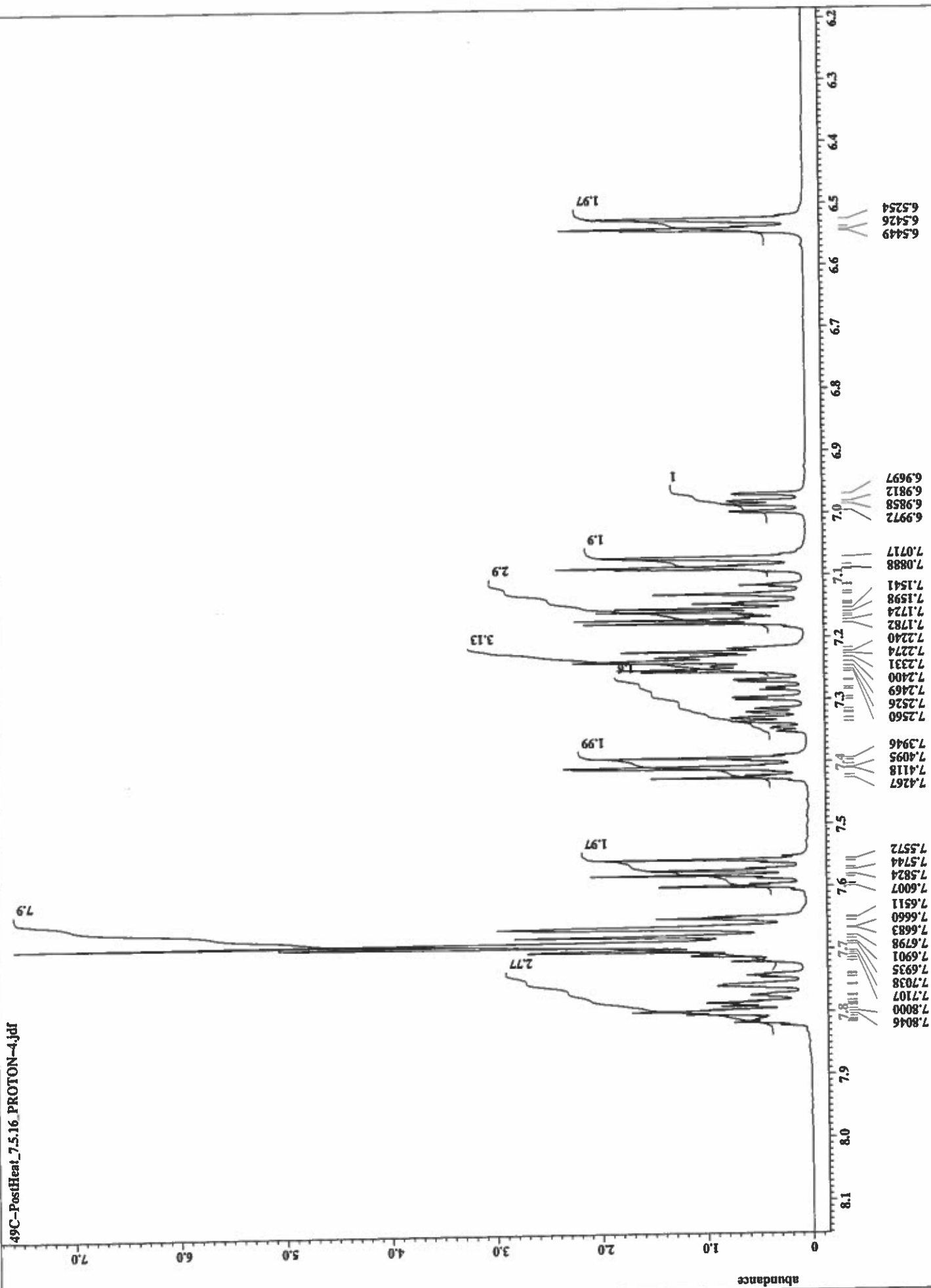


X : parts per Million : 1H

49C-PostHeat_7.5.16_PROTON-4.jdf



X : parts per Million : 1H





SOUTH ALABAMA
JAGUARS

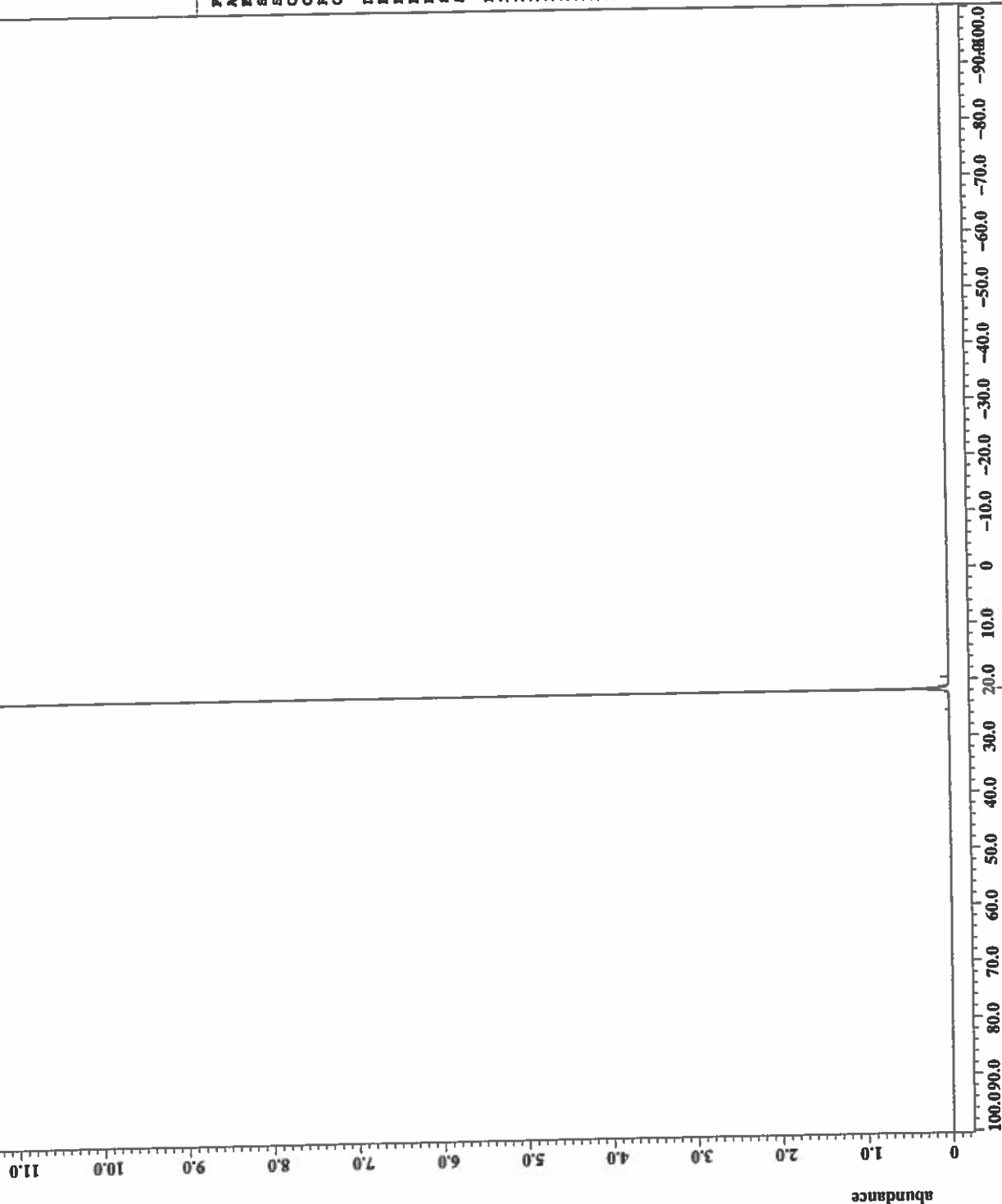
```

Filename      = 49C-PostHeat_7.5.16_P
Author       = Jim Davis
Experiment   = single_pulse_dec
Sample_id    = 49C-PostHeat_7.5.16
Solvent      = CHLOROFORM-D
Changer_sample
Creation_time 5-JUL-2016 23:15:45
Revision_time 5-JUL-2016 22:57:20
Current_time  5-JUL-2016 22:57:21

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

Field_strength
X_acq_duration 11.7473579[X] (500[MH
X_domain       = 0.64487424[s]
X_freq         = 31P
X_offset       = 202.46831075 [MHz]
X_points       = 0 [ppm]
X_prescans     = 32768
X_resolution   = 4
X_sweep        = 1.55068995 [Hz]
X_domain       = 50.81300813 [MHz]
X_freq         = 1H
X_offset       = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 256
Total_scans    = 256

X_90_width     = 14 [us]
X_acq_time     = 0.64487424 [s]
X_angle        = 30 [deg]
X_atn          = 5 [dB]
X_pulse        = 4.66666667 [us]
X_atn_dec      = 20.5 [dB]
X_atn_noe      = 20.5 [dB]
X_noise        = VAL72
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Revr_gain      = 58
Relaxation_delay = 2 [s]
Repetition_time = 2.64487424 [s]
Temp_get       = 23.5 [dC]
  
```



21.8126

X : parts per Million : 31P



SOUTH ALABAMA
JAGUARS

```

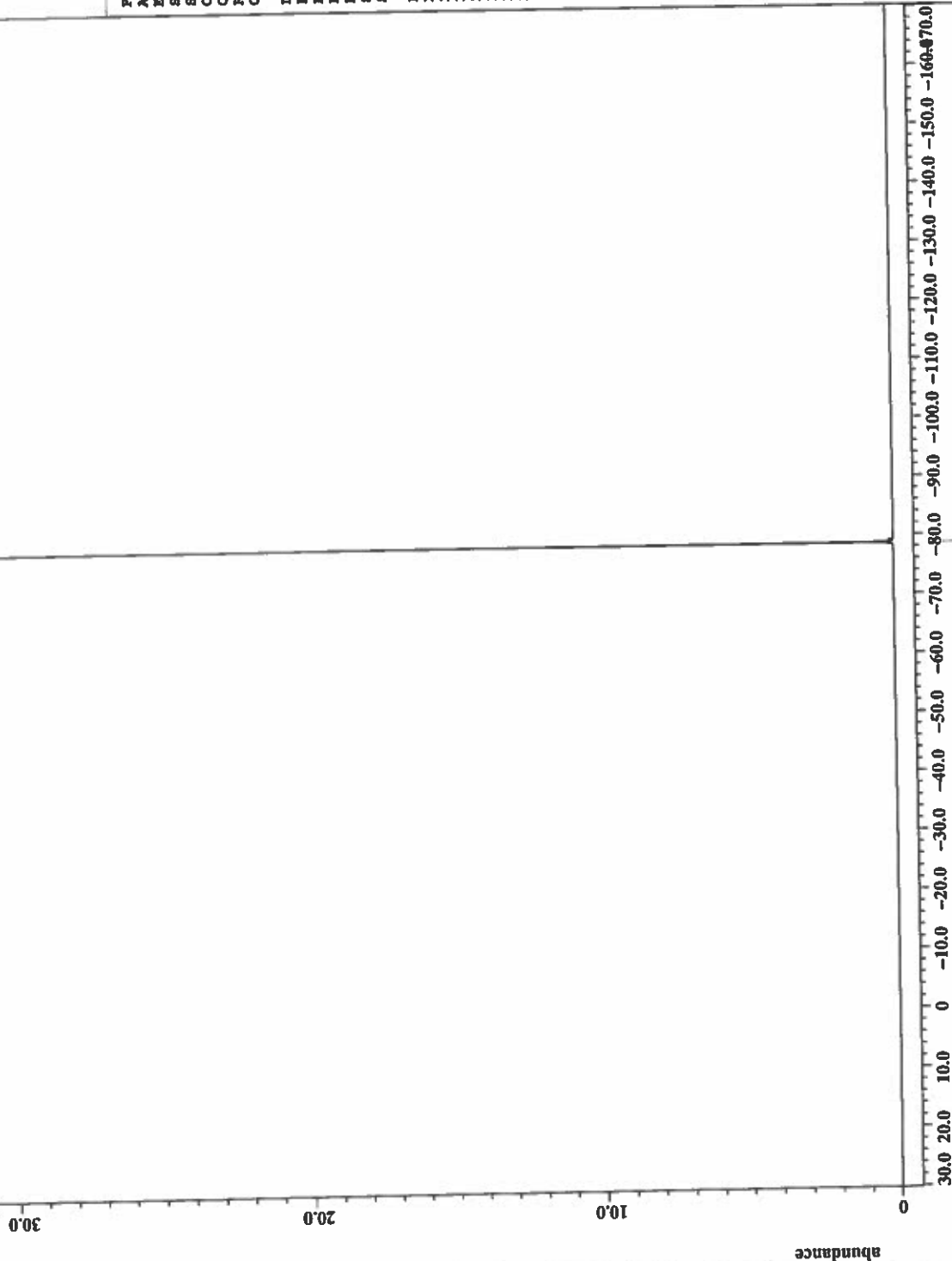
Filename      = 49C-PostHeat_7.5.16_F
Author       = Jim Davis
Experiment   = single_pulse.ex2
Sample_id    = 49C-PostHeat_7.5.16
Solvent      = CHLOROFORM-D
Changer_sample = 9
Creation_time   = 5-JUL-2016 23:01:50
Revision_time  = 5-JUL-2016 22:43:27
Current_time   = 5-JUL-2016 22:43:27

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[MHz]
Irr_domain     = 19F
Irr_freq       = 470.62046084[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 19F
Tri_freq       = 470.62046084[MHz]
Tri_offset     = 5[ppm]
Mod_return     = FALSE
Scans          = 1
Total_scans    = 16

X_90_width     = 15.7[us]
X_acq_time     = 0.55574528[s]
X_angle        = 45[deg]
X_atn          = 4[db]
X_pulse        = 7.85[us]
Irr_pulse      = Off
Irr_mode       = Off
Tri_mode       = FALSE
Dante_preset   = 40
Initial_wait   = 1[s]
Recvr_gain     = 4[s]
Relaxation_delay = 4[s]
Repetition_time = 4.55574528[s]
Temp_get       = 22.8[dc]

```

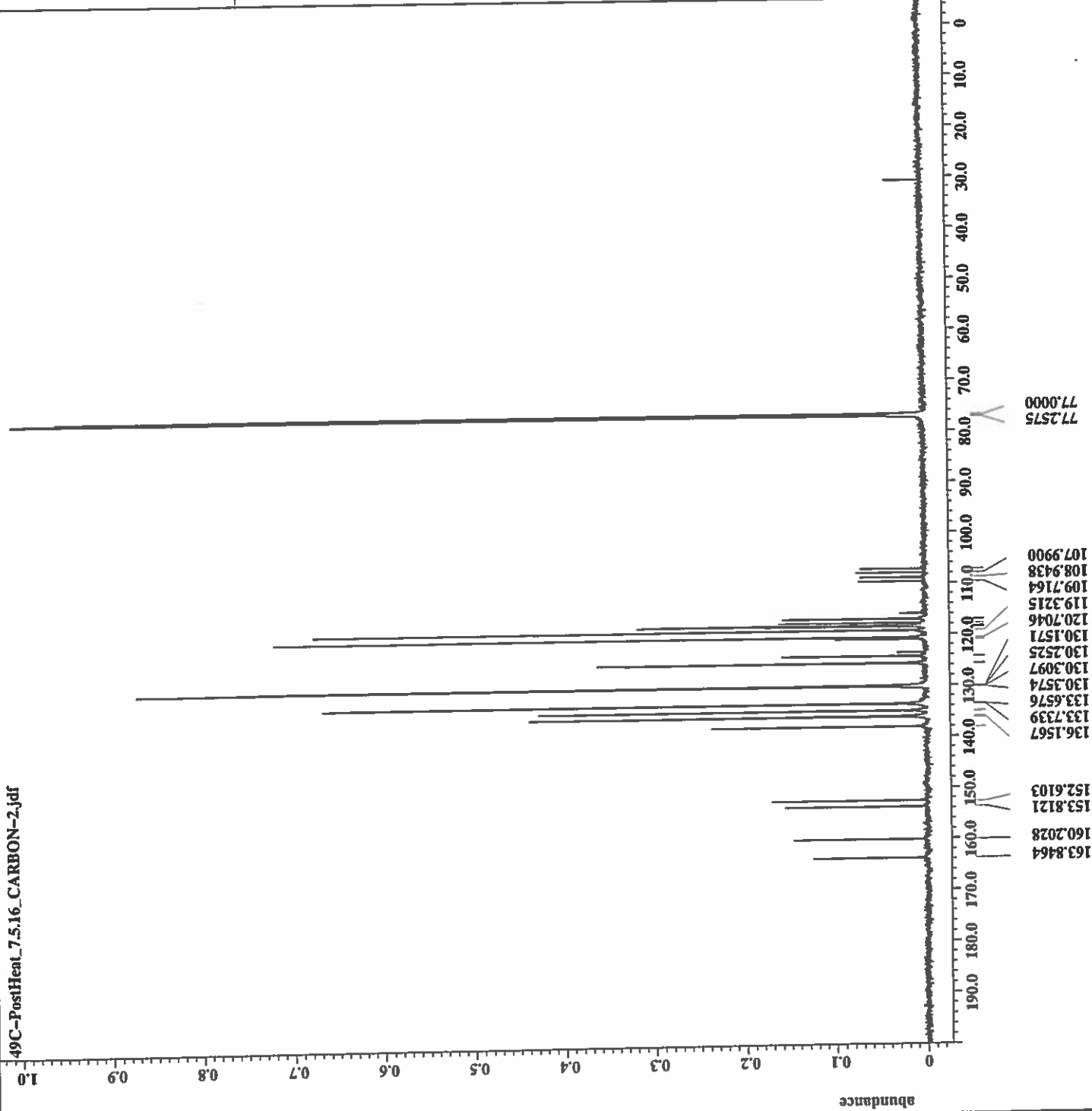


-78.5951



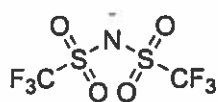
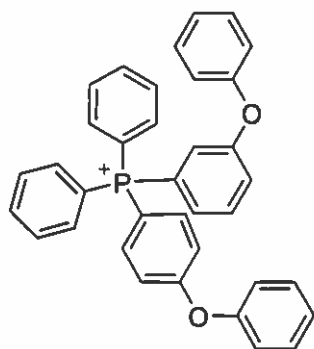
SOUTH ALABAMA
JAGUARS

Filename = 49C-PostHeat_7.5.16_C
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = 49C-PostHeat_7.5.16
 Solvent = CHLOROFORM-D
 Changer_sample = 9
 Creation_time = 5-JUL-2016 22:58:46
 Revision_time = 5-JUL-2016 22:40:21
 Current_time = 5-JUL-2016 22:40:21
 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 = 1024
 Total_scans = 1024
 X_90_width = 12.55[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 6[db]
 X_pulse = 4.18333333[us]
 Irr_atn_dec = 20.5[db]
 Irr_atn_noe = 20.5[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 = 23.1[dc]



X : parts per Million : 13C

COMPOUND 6



Atlantic Microlab, Inc.

No. Phosphonium 49A

Atlantic Blvd. Suite M
S, GA 30071
atlanticmicrolab.com

Company/School U of South Alabama

Dept. Chemistry

Address Chem 223

City, State, Zip Mobile AL 36688

Name James Davis

Date 10/31/2016

Phone (251) 751-0520

Supervisor: James Davis

C#

Test	Theory	Found		Single ☒ Duplicate ☐
	56.79	56.63		Elements CHNPOSF Present:
	3.51	3.49		Analyze CHN for:
	1.74	1.77		Hygroscopic ☐ Explosive ☐ M.P. <u>unk</u> B.P. <u>none</u>
				To be dried: Yes ☒ No ☐ Temp. <u>60C</u> Vac. <u>high</u> Time <u>4h</u>
				Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
				Include Email Address or FAX # Below <u>jdavis@southalabama.edu</u>

Received NOV 01 2016

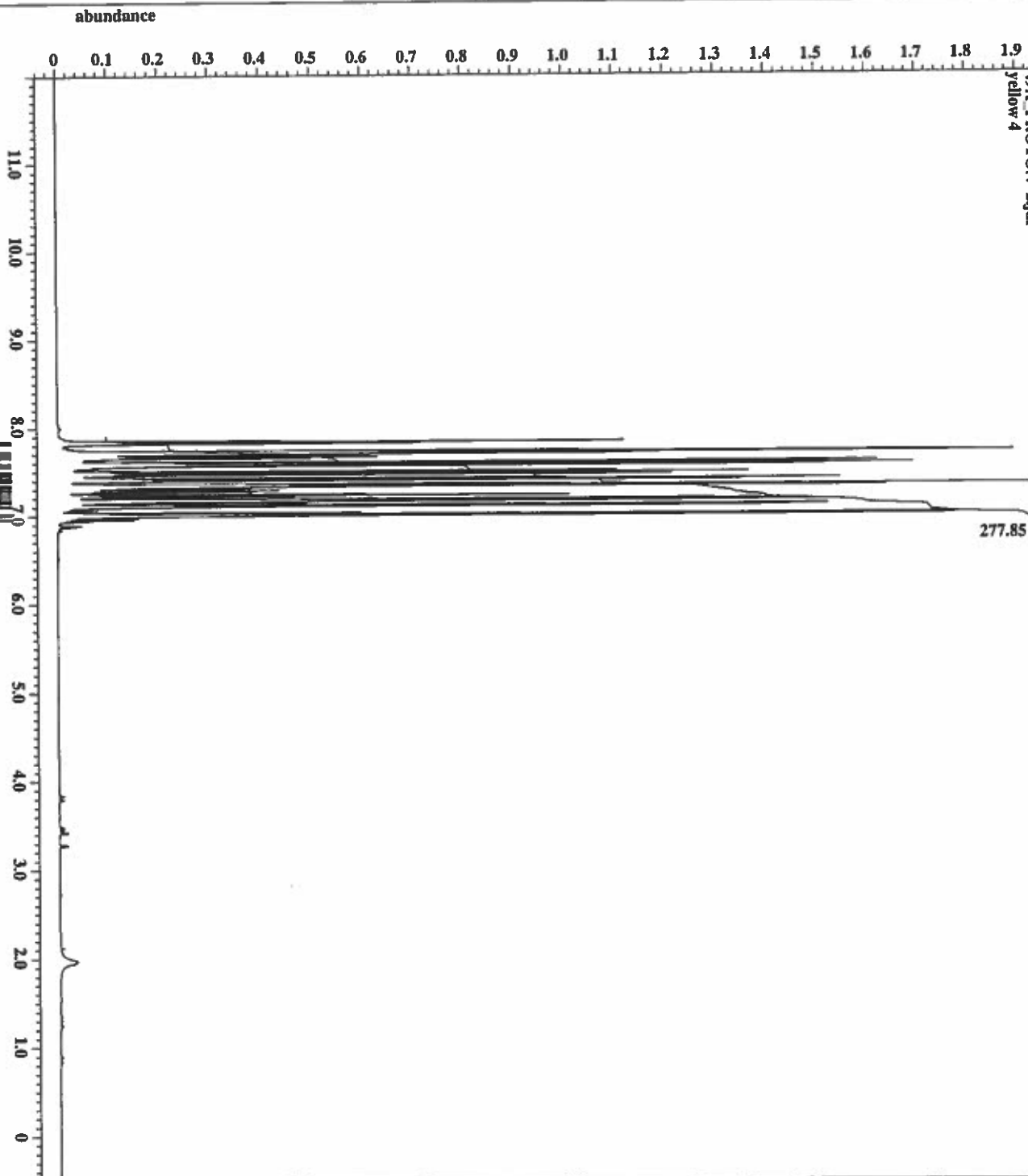
Date Completed

NOV 01 2016

Notes:

49A_PROTON-2.jdt
yellow 4

277.85



7.7198
7.7118
7.5790
7.3431
7.3259
7.0144
6.9995

X : parts per Million : 1H



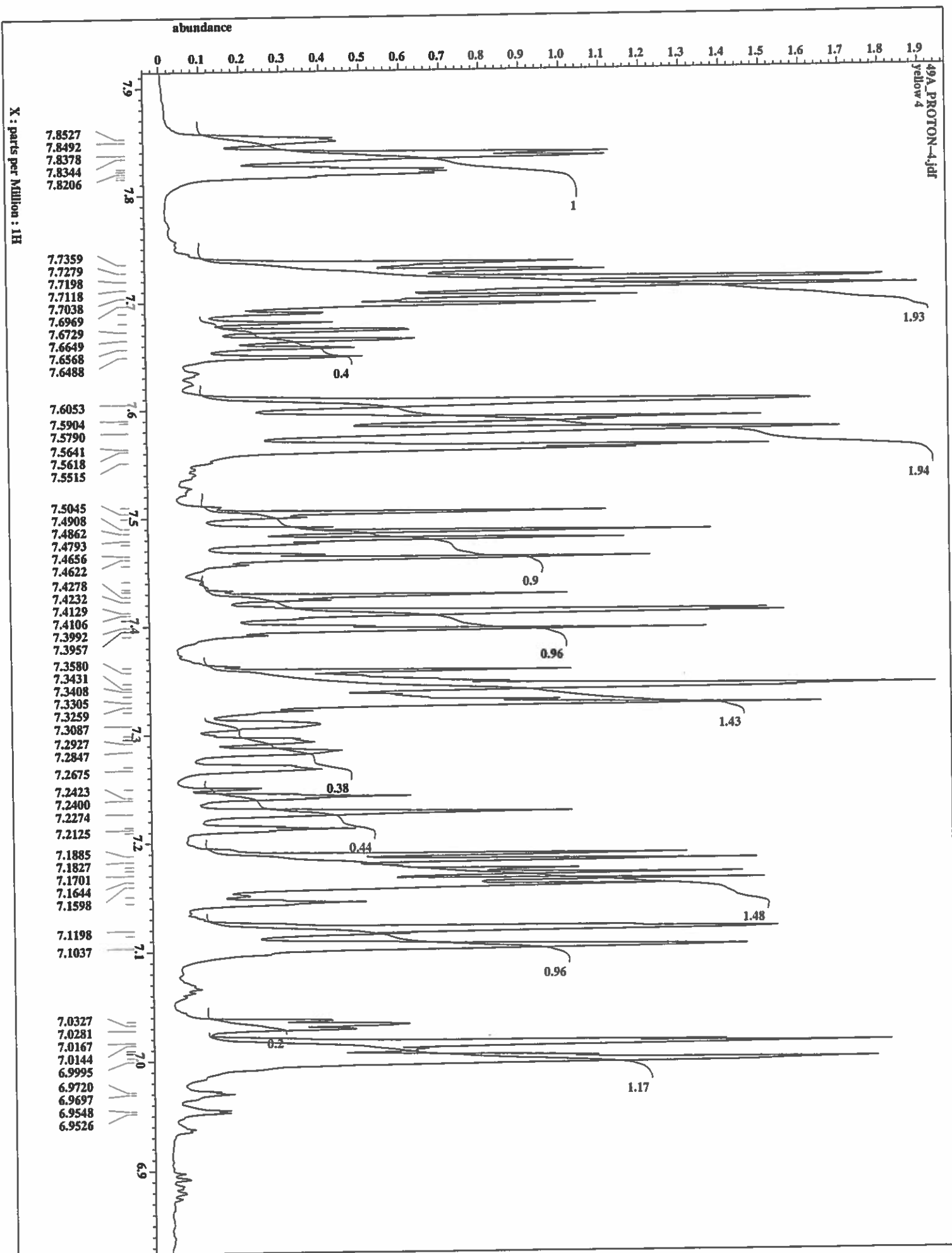
```

Filename      = 49A_PROTON-2.jdt
Author       = Jim Davis
Experiment   = single_pulse.ex2
Sample_id    = 49A
Solvent      = CHLOROFORM-D
Charger_sample = 6
Creation_time = 1-JUL-2016 14:06:02
Revision_time = 1-JUL-2016 13:47:57
Current_time  = 1-JUL-2016 13:47:57

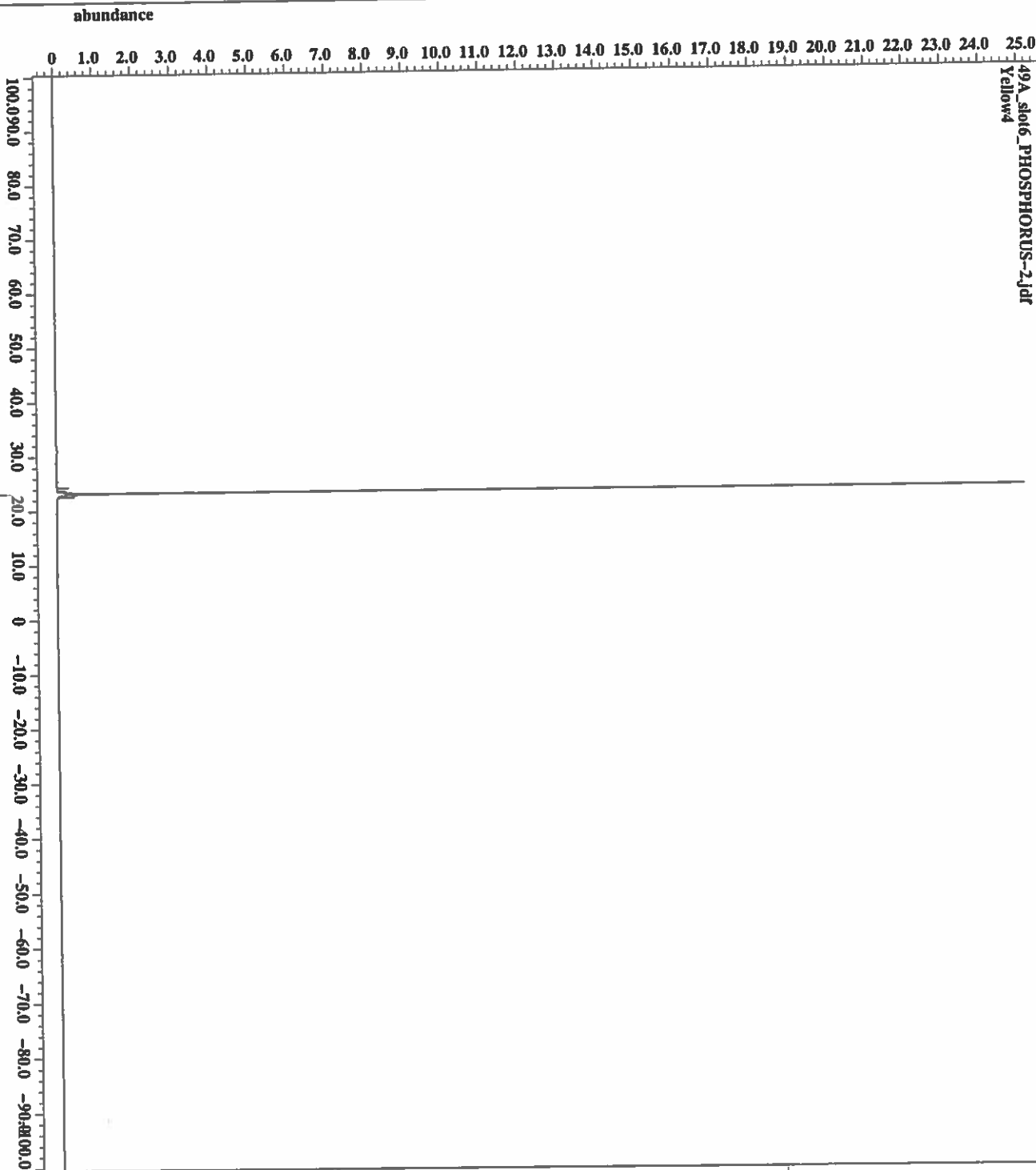
Comment
Data_format = 1D COMPLEX
Dir_size    = 13107
Dir_name    = 1H
Dir_units   = [ppm]
Dimensions  = X
Site        = ECA 500
Spectrometer = JNM-ECA500

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]
Xt1_domain    = 1H
Xt1_freq      = 500.15991521 [MHz]
Xt1_offset     = 5.0 [ppm]
Xt1_domain    = 1H
Xt1_freq      = 500.15991521 [MHz]
Xt1_offset     = 5.0 [ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 16
Total_scans   = 16

X_90_width    = 13.35 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 6.675 [us]
Xt1_mode       = ORF
Xt1_mode       = ORF
Dante_preset   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 22
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_get       = 22.5 [dC]
  
```



49A_slot6_PHOSPHORUS-2.jdr
Yellow4



X : parts per Million : 31P



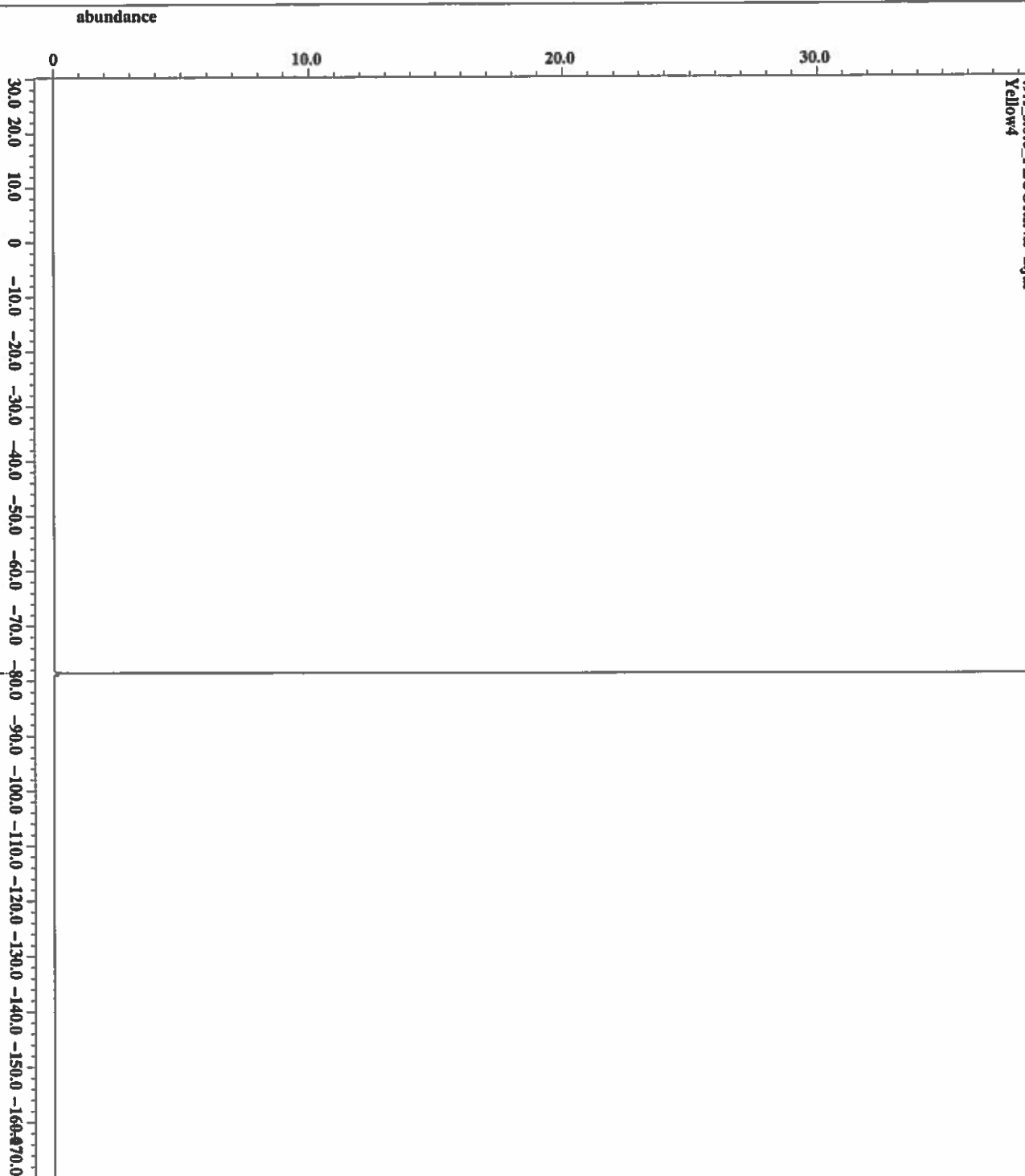
Filename = 49A_slot6_PHOSPHORUS-
Author = Jim Davis
Experiment = single-pulse_dec
Sample_id = S#640571
Solvent = CHLOROFORM-D
Charger_sample = 6
Creation_time = 1-JUL-2016 18:18:17
Revision_time = 1-JUL-2016 18:00:10
Current_time = 1-JUL-2016 18:00:12

Comment = Yellow4
Data_format = 1D COMPLEX
Data_size = 26214
Data_title = 31P
Data_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 = 33768
X_prescans = 4
X_resolution = 1.55068995 [Hz]
X_sweep = 50.81300813 [kHz]
Xr_domain = 1H
Xr_freq = 500.15991521 [MHz]
Xr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 256
Total_scans = 256

X_90_width = 14 [us]
X_acq_time = 0.64487424 [s]
X_angle = 30 [deg]
X_atn = 5 [dB]
X_pulse = 4.66666667 [us]
Xr_atn_dec = 20.5 [dB]
Xr_atn_poe = 20.5 [dB]
Xr_noise = VALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 2 [s]
Noe_gain = 58
Relaxation_delay = 2 [s]
Repetition_time = 2.64487424 [s]
Temp_get = 23.5 [deg]

49A_slot6_FLUORINE-2.jdt
Yellow4



X : parts per Million : 19F



```

=====
File      49A_slot6_FLUORINE-2.
Author    Jim Davis
Experiment single_pulse.ex2
Sample_id 85560379
Solvent    CHLOROFORM-D
Changer_sample 6
Creation_time 1-JUL-2016 15:54:36
Revision_time 1-JUL-2016 15:36:31
Current_time 1-JUL-2016 15:36:31

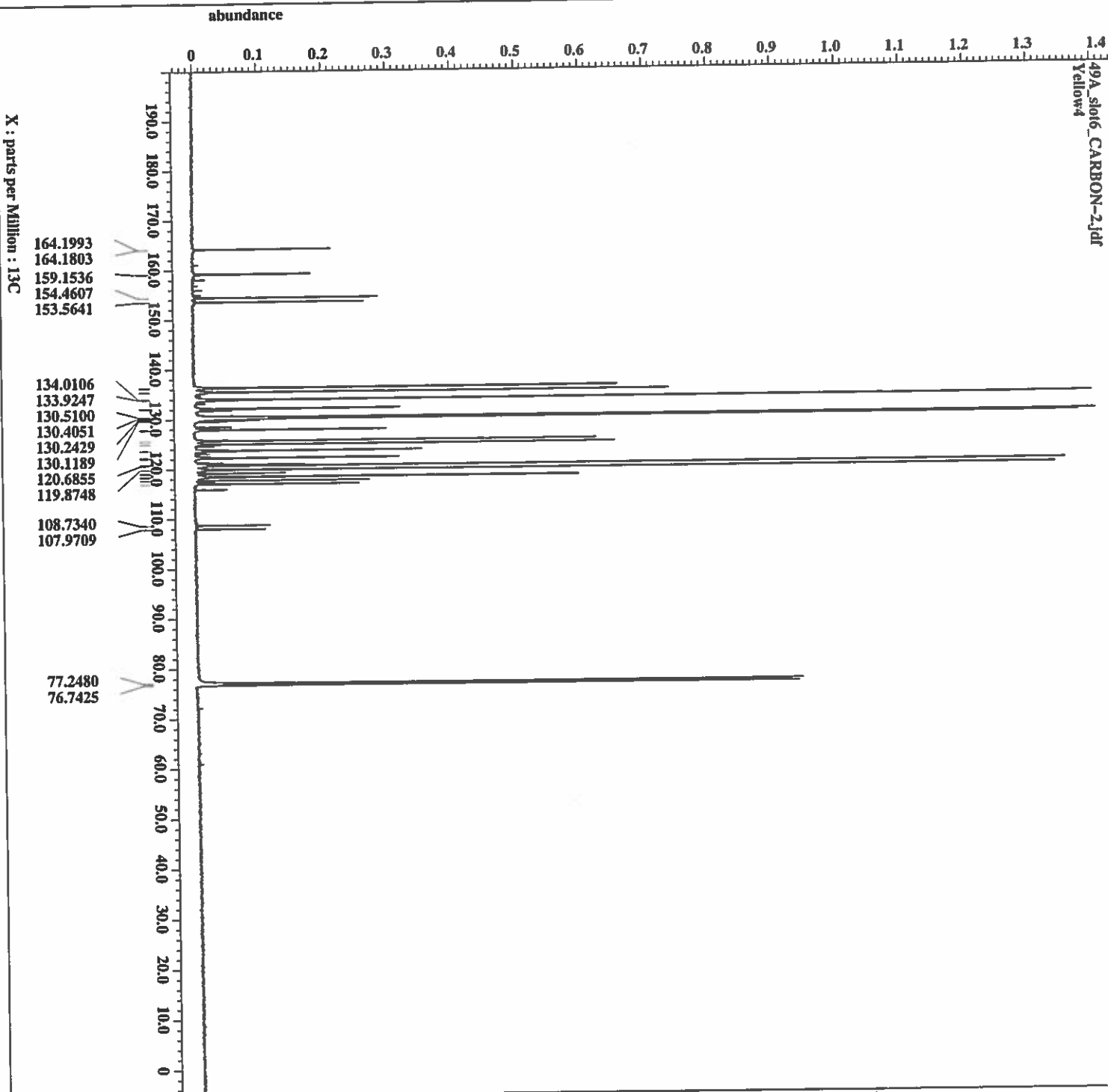
=====
Comment
Data_format ID COMPLEX
Dim_size     52428
Dim_title    19F
Dim_units    [ppm]
Dimensions   X
Site         FCA 500
Spectrometer JNM-ECX500

=====
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       65336
X_prescans     1
X_resolution   1.7993855 [Hz]
X_sweep        117.9245283 [kHz]
X_domain       19F
Xir_freq       470.62046084 [MHz]
Xir_offset     5 [ppm]
Xir_domain     19F
Xrl_freq       470.62046084 [MHz]
Xrl_offset     5 [ppm]
Clipped        FALSE
Mod_return     1
Bcans          16
Total_scans    16

=====
X_g0_width     15.7 [us]
X_acq_time     0.55574528 [s]
X_angle        45 [deg]
X_atn          4 [dB]
X_pulse        7.85 [us]
Xir_mode       OF
Xrl_mode       OF
Dance_preset   FALSE
Initial_wait   1 [s]
Recev_gain     36
Relaxation_delay 4 [s]
Repetition_time 2.35574528 [s]
Temp_set       22.9 [deg]
=====

```

49A_slot6_CARBON-2.j4
Yellow4



X : parts per Million : 13C

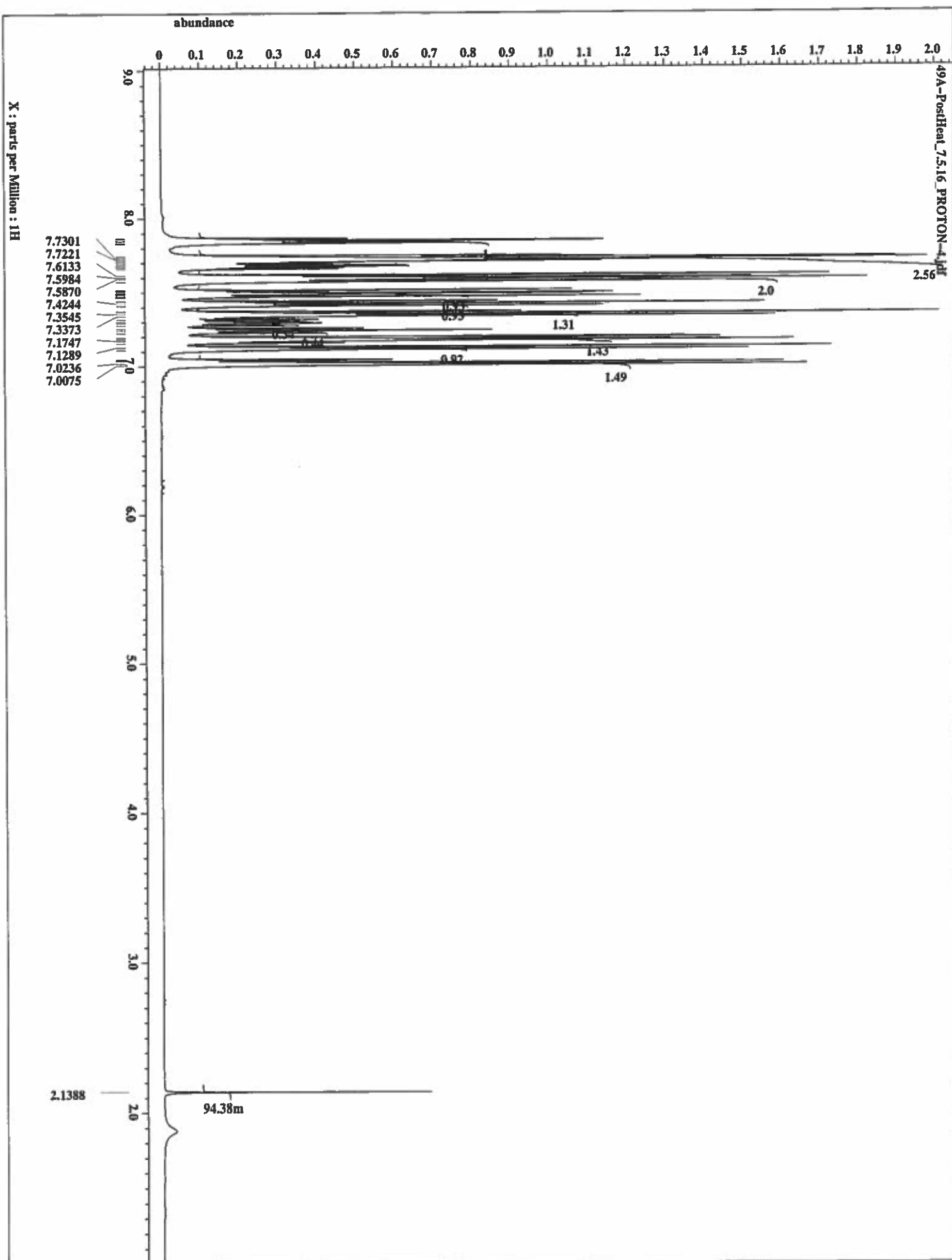


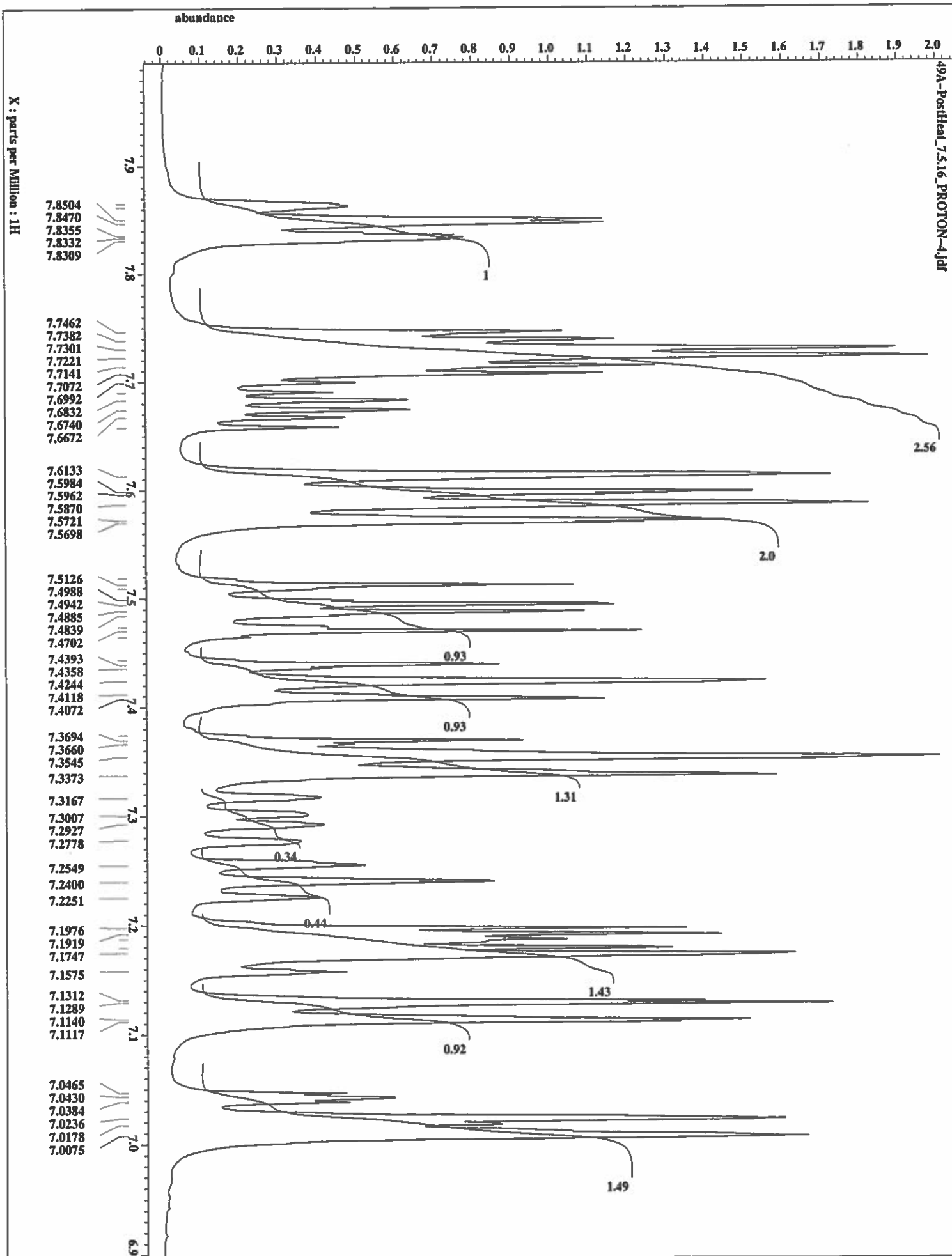
Filename = 49A_slot6_CARBON-2.j4
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = S#252811
 Solvent = CHLOROFORM-D
 Change_sample = 6
 Creation_time = 2-JUL-2016 09:47:08
 Revision_time = 2-JUL-2016 09:28:58
 Current_time = 2-JUL-2016 09:28:58

 Comment = Yellow4
 Data_format = 1D COMPLEX
 Data_size = 26214
 Data_title = 13C
 Data_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

 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]
 Xt_domain = 1H
 Xt_freq = 500.15991521 [MHz]
 Xt_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 3100
 Total_scans = 3100

 X_90_width = 12.55 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 6 [dB]
 X_pulse = 4.18333333 [us]
 Xt_atn_dec = 20.5 [dB]
 Xt_atn_noe = 20.5 [dB]
 Xt_noise = VAL7Z
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe_time = TRUE
 Noe_time = 21 [s]
 Recvr_gain = 60
 Relaxation_delay = 2 [s]
 Repetition_time = 2.83361792 [s]
 Temp_set = 23.7 [deg]





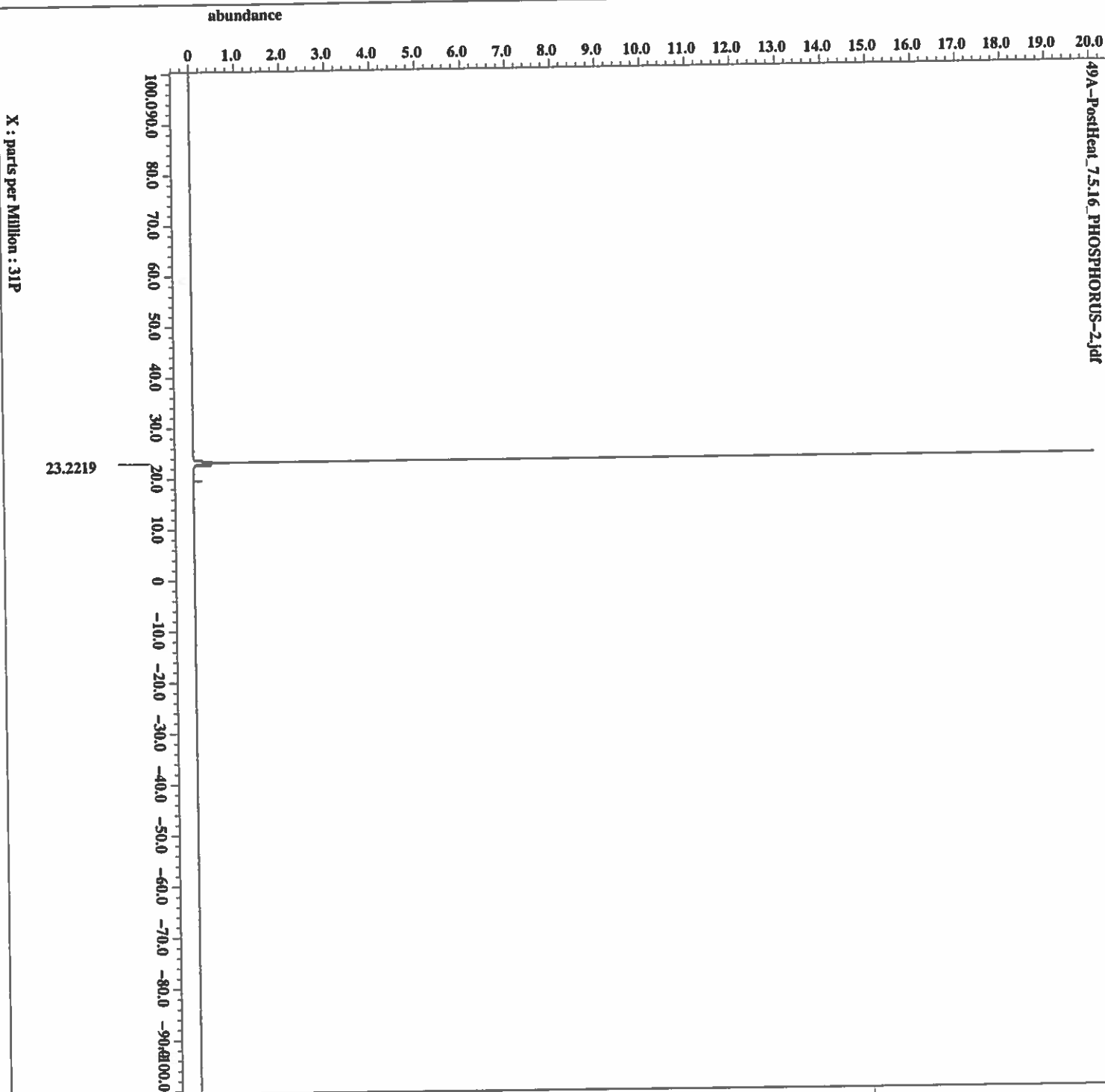


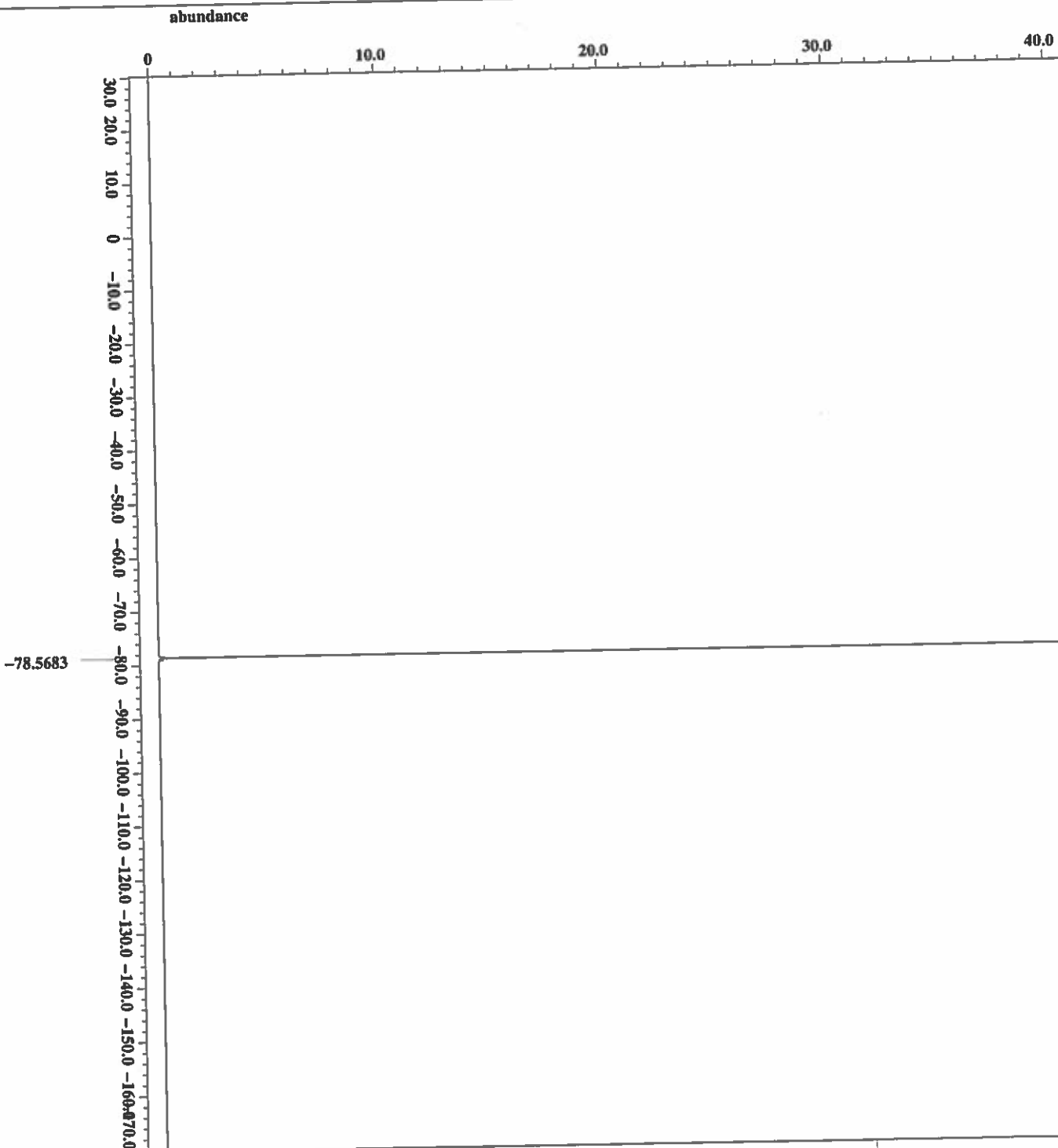
Filename = 49A-PostHeat_7.5.16_P
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = 49A-PostHeat_7.5.16
Solvent = CHLOROFORM-D
Charger_sample = 6
Creation_time = 5-JUL-2016 20:53:11
Revision_time = 5-JUL-2016 20:34:48
Current_time = 5-JUL-2016 20:34:48

Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 31P
Dim_units = [ppm]
Dimensions = X
ECA 500
Site = JNM-ECA500
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 = 256
Total_scans = 256

X_90_width = 14 [us]
X_acq_time = 0.64487424 [s]
X_angle = 30 [deg]
X_atn = 5 [dB]
X_pulse = 4.66666667 [us]
Irr_atn_dec = 20.5 [dB]
Irr_atn_noe = 20.5 [dB]
Irr_noise = WALTZ
Decoupling = TRU2
Initial_wait = 1 [s]
Noe = TRU2
Noe_time = 2 [s]
Noe_gain = 2 [s]
Relaxation_delay = 2.64487424 [s]
Temp_get = 23 [C]





X : parts per Million : 19F



SOUTH ALABAMA
JAGUARS

```

Filename      = 49A-PostHeat_7.5.16_F
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = 49A-PostHeat_7.5.16
Solvent       = CHLOROFORM-D
Charger_sample = 6
Creation_time  = 5-JUL-2016 20:39:15
Revision_time = 5-JUL-2016 20:20:53
Current_time   = 5-JUL-2016 20:20:53

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 [G] (500 [MHz]
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        = 117.9345283 [kHz]
Xt1_domain    = 19F
Xt1_freq      = 470.62046084 [MHz]
Xt1_offset     = 5 [ppm]
Xt1_domain    = 19F
Xt1_freq      = 470.62046084 [MHz]
Xt1_offset     = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_g0_width    = 15.7 [us]
X_acq_time     = 0.55574528 [s]
X_angle       = 45 [deg]
X_atn         = 4 [dB]
X_pulse       = 7.85 [us]
Xt1_mode      = OFZ
Xt1_offset    = OFZ
Pulse         = PULSE
Pulse_delay   = 1 [s]
Pulse_gain    = 38
Relaxation_delay = 4 [s]
Repetition_time = 4.55574528 [s]
Temp_cel      = 23.2 [degC]
  
```



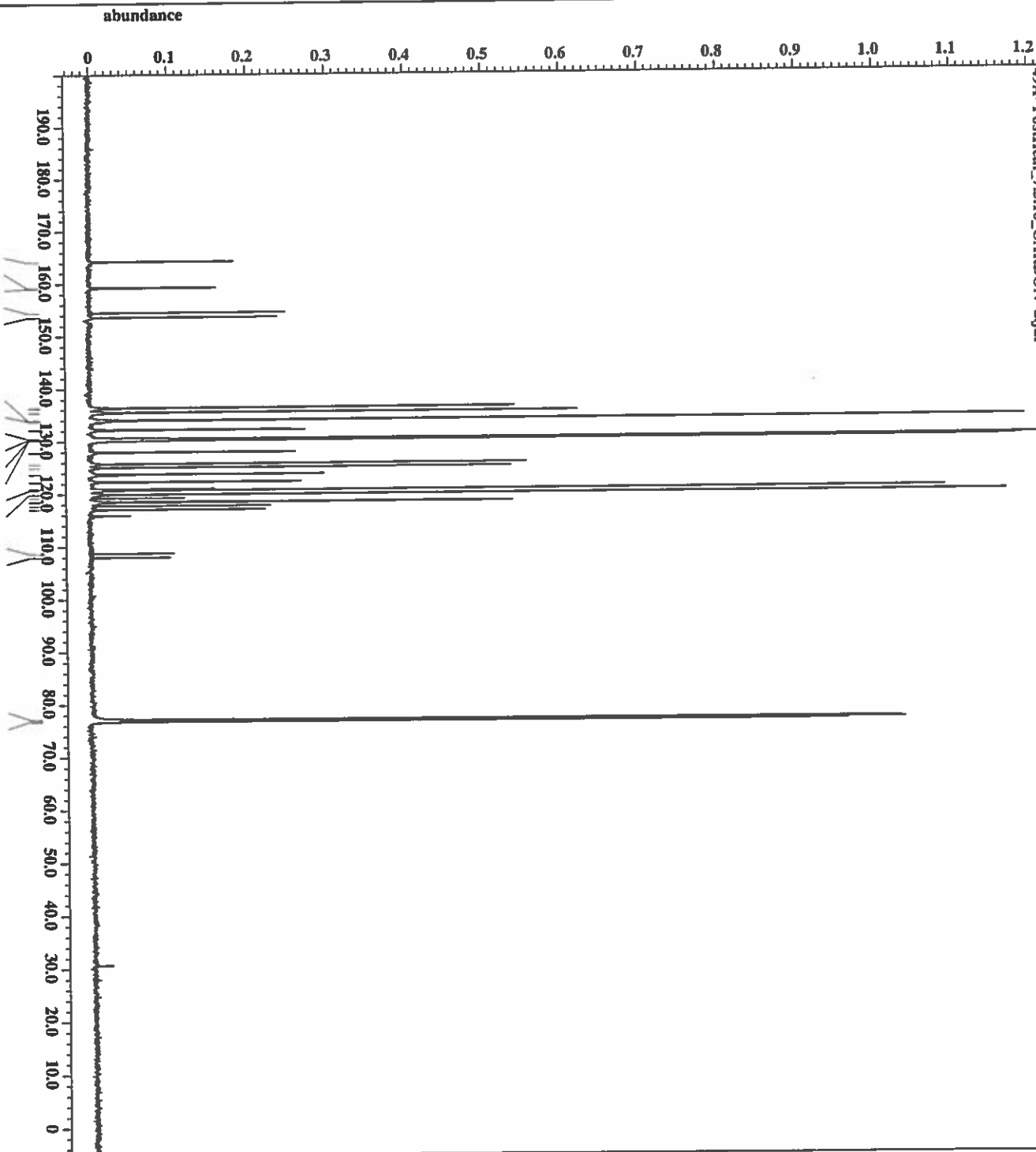

Filename = 49A-PostHeat_7.5.16_C
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = 49A-PostHeat_7.5.16
Solvent = CHLOROFORM-D
Charger_sample = 6
Creation_time = 5-JUL-2016 20:36:20
Revision_time = 5-JUL-2016 20:17:56
Current_time = 5-JUL-2016 20:17:56

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 = 125.76529766 [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]
Clipped = PULS2
Mod_return = 1
Scans = 1024
Total_scans = 1024

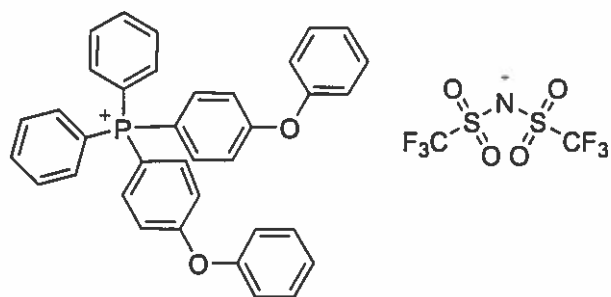
X_90_width = 12.55 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 6 [dB]
X_pulse = 4.18333333 [us]
Irr_atn_dec = 20.5 [dB]
Irr_atn_noe = 20.5 [dB]
Irr_noise = 20.5 [dB]
Decoupling = WALTZ
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 2 [s]
Recvr_gain = 60
Relaxation_delay = 2.83361792 [s]
Repetition_time = 23.5 [s]
Temp_set = 23.5 [degC]

49A-PostHeat_7.5.16_CARBON-2.jdt



X : parts per Million : 13C

COMPOUND 7



Atlantic Microlab, Inc.

No. Phosphonium 141A

Atlantic Blvd. Suite M
S, GA 30071
atlanticmicrolab.com

Company/School U of South Alabama

Dept. Chemistry

Address Chem 223

City, State, Zip Mobile AL 36688

Name James Davis

Date 10/31/2016

Supervisor: James Davis

Phone (251) 751-0520

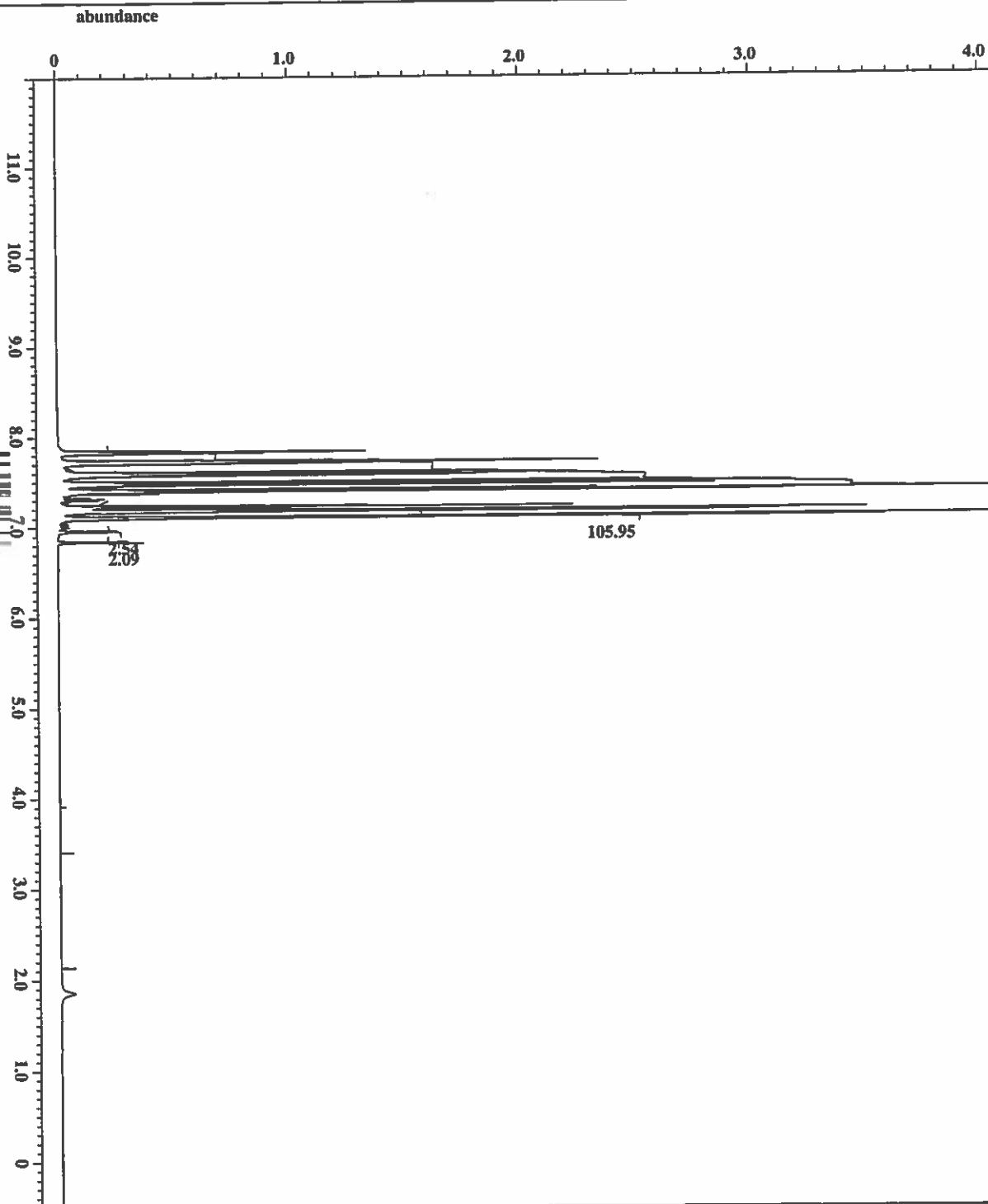
Test	Theory	Found	Single ☐	Duplicate ☐
1	56.79	57.08	Elements CHNPOSF Present:	
1	3.51	3.51	Analyze CHN for:	
1	1.74	1.75	Hygroscopic ☐ Explosive ☐ M.P. <u>unk</u> B.P. <u>none</u>	
			To be dried: Yes ☒ No ☐ Temp. <u>60C</u> Vac. <u>high</u> Time <u>4 h</u>	
			Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.	
			Include Email Address or FAX # Below jdavis@southalabama.edu	

Received NOV 01 2016

Date Completed NOV 01 2016

Notes:

141A_PROTON-2.jdt
yellow 8



X : parts per Million : 1H



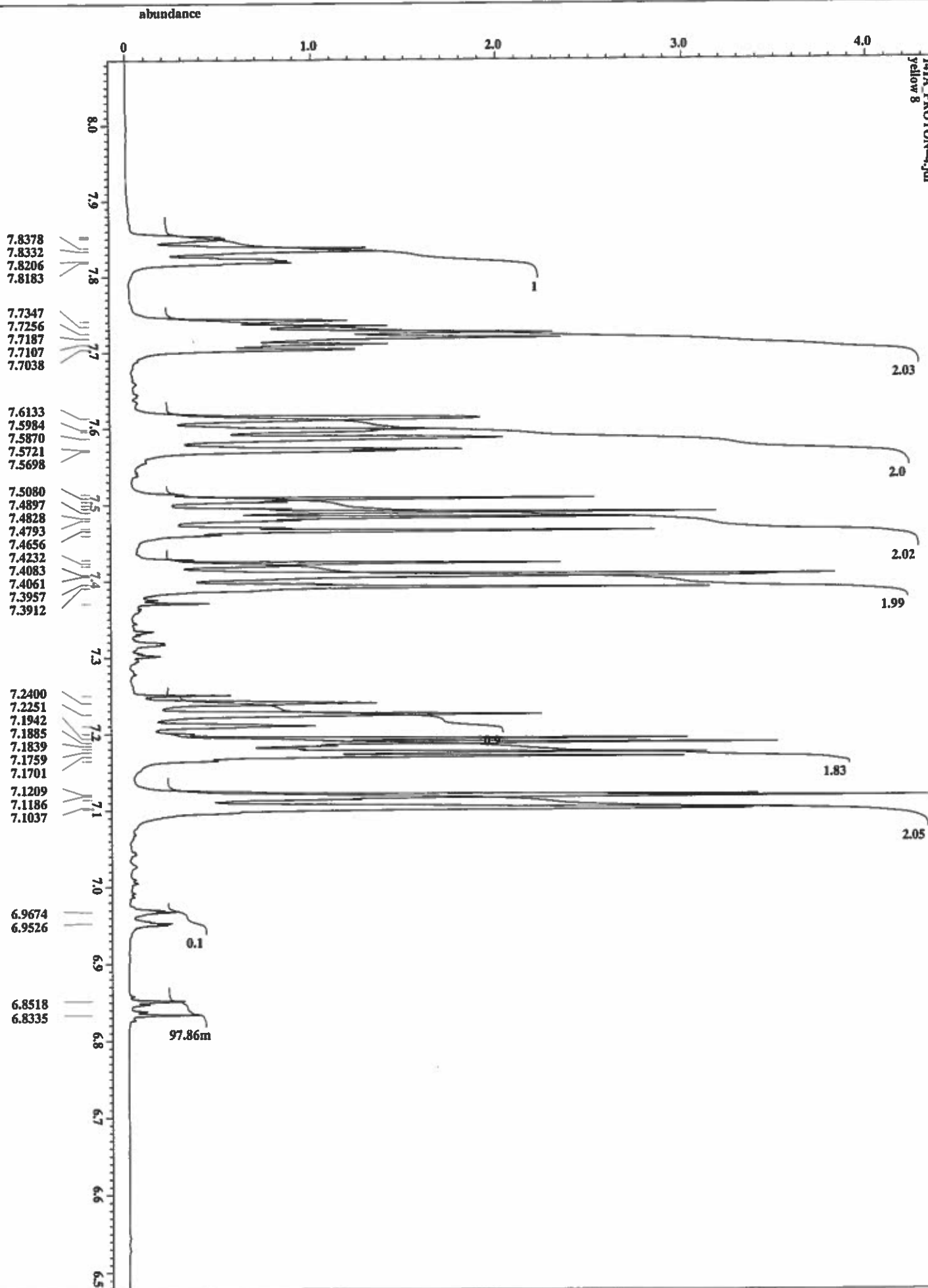
Filename 141A_PROTON-2.jdt
Author Jim Davis
Experiment single_pulse.ex2
Sample_id 141A
Solvent CHLOROFORM-D
Charger_sample 10
Creation_time 1-07-2016 14:21:38
Revision_time 1-07-2016 14:03:33
Current_time 1-07-2016 14:03:33

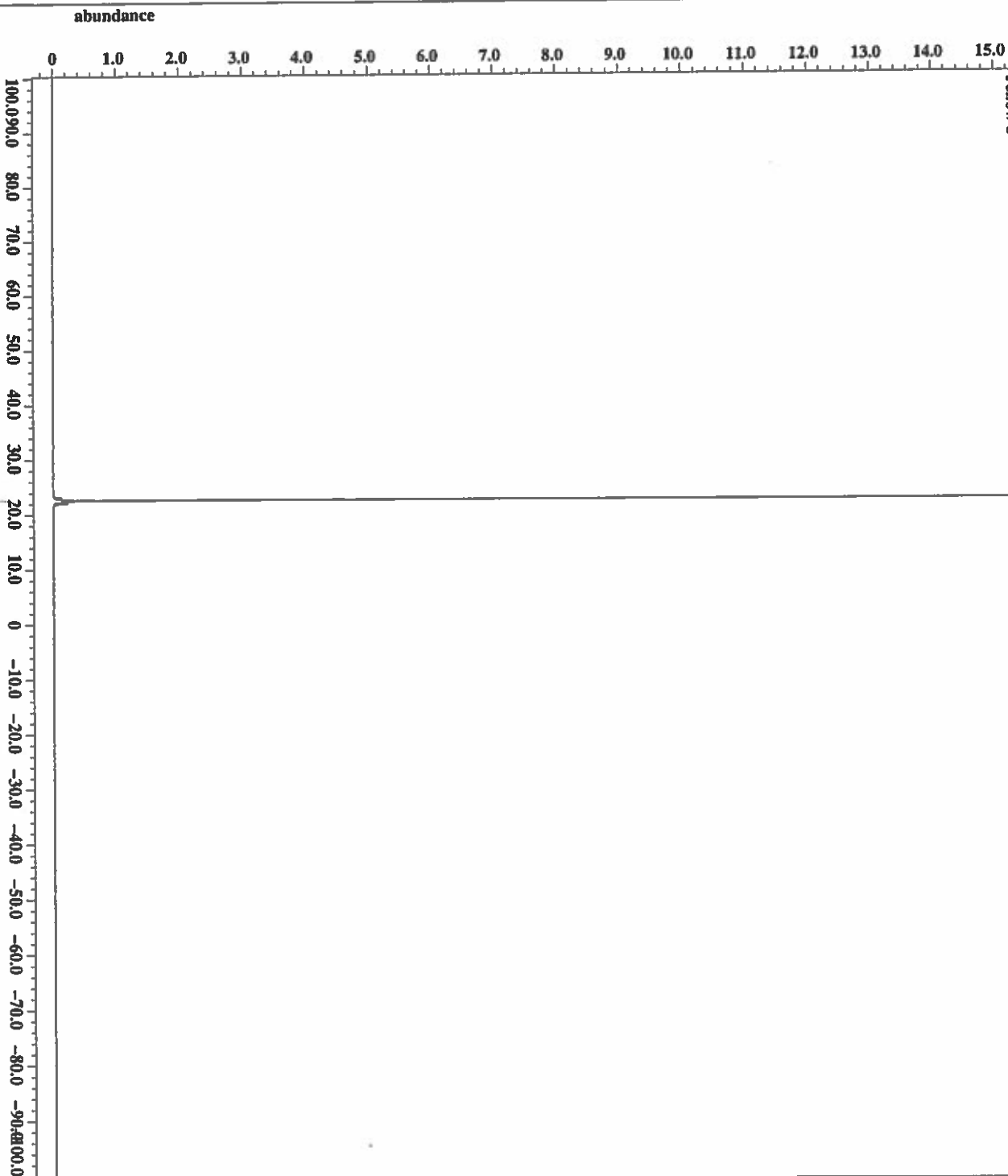
Comment
Data_format yellow 8
Data_size 13107
Dim_title 1H
Dim_units [ppm]
Dimensions X
Site ECA 500
Spectrometer JNM-ECA500

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
Prl_freq 500.15991521 [MHz]
Prl_offset FALSE
Mod_return 1
Mod_return 1
Mod_return 16
Total_scans 16

X_90_width 13.35 [us]
X_acq_time 1.74587904 [s]
X_angle 45 [deg]
X_atn 4 [dB]
X_pulse 6.675 [us]
Irr_mode Off
Prl_mode Off
Pulse FALSE
Pulse 26
Relaxation_delay 4 [s]
Relaxation_delay 5.74587904 [s]
Temp_get 23.4 [deg]

X : parts per Million : 1H





X : parts per Million : 31P



```

Filename      = 141A_stat10_PHOSPHORUS
Author        = Jim Davis
Experiment    = single pulse_dec
Sample_id     = 88689763
Solvent       = CHLOROFORM-D
Charger_sample = 10
Creation_time  = 1-JUL-2016 19:05:24
Revision_time  = 1-JUL-2016 18:47:18
Current_time   = 1-JUL-2016 18:47:18

Comment
Data_format   = Yellow 8
Dim_size      = 1D COMPLEX
Dim_title     = 26214
Dim_units     = 31P
Dimensions    = [ppm]
Site          = X
Spectrometer  = ECA 500
              = 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_rescans      = 1.55068995 [Hz]
X_resolution   = 50.81300813 [Hz]
X_sweep        = 1H
Xf1_domain     = 500.15991521 [MHz]
Xf1_freq       = 5.0 [ppm]
Xf1_offset     = FALSE
Xf1_return     = 1
Xf1_mod_return = 256
Xf1_scans      = 256
Xf1_total_scans = 256

X_90_width     = 14 [us]
X_acq_time      = 0.64487424 [s]
X_angle         = 30 [deg]
X_atn           = 5 [dB]
X_pulse         = 4.66666667 [us]
Xf1_atn_dec     = 20.5 [dB]
Xf1_atn_noe     = 20.5 [dB]
Xf1_noise       = MAX2Z
Xf1_decoupling  = TRU2
Xf1_initf1_wait = 1 [s]
Xf1_noe         = TRU2
Xf1_noe_time    = 2 [s]
Xf1_noe_delay   = 58
Xf1_noe_rep_time = 2.64487424 [s]
Xf1_noe_rep_delay = 23.6 [dc]
Xf1_noe_temp_get = 23.6 [dc]

```

141A_slot10_FLUORINE-2.jdr
Yellow 8



X : parts per Million : 19F



SOUTH ALABAMA
JAGUARS

```

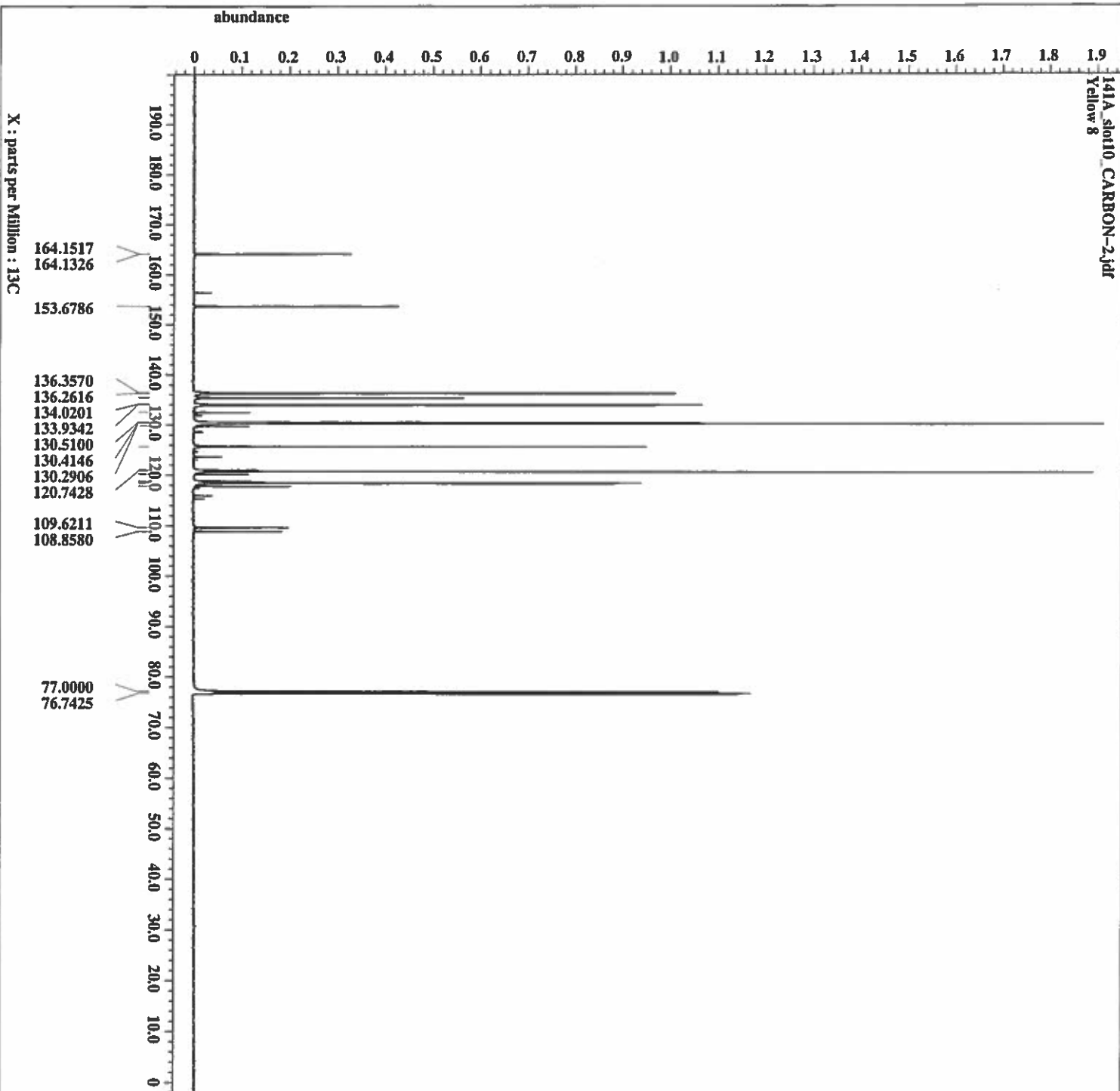
Filename      = 141A_slot10_FLUORINE-
Author        = Jim Davis
Experiment     = single_pulse.exe2
Sample_id     = 88570563
Solvent       = CHLOROFORM-D
ChangeX_sample = 10
Creation_time  = 1-JUL-2016 16:11:48
Revision_time = 1-JUL-2016 15:53:43
Current_time  = 1-JUL-2016 15:53:43

Comment
Data_format   = ID 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        = 117.9345283 [kHz]
Irr_domain     = 19F
Irr_freq       = 470.62046084 [MHz]
Irr_offset     = 5 [ppm]
Irr_domain     = 19F
T1_domain      = 19F
T1_freq        = 470.62046084 [MHz]
T1_offset      = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 15.7 [us]
X_acq_time     = 0.55574528 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 7.85 [us]
Irr_mode       = OEG
T1_mode        = OEG
PulseProgram   = FALSR
Initial_puls   = 1 [s]
Recvr_gain     = 40
Relaxation_delay = 4 [s]
Repetition_time = 4.55574528 [s]
Temp_get       = 23 [dc]
  
```

141A_slot10_CARBON-2.jdt
Yellow 8



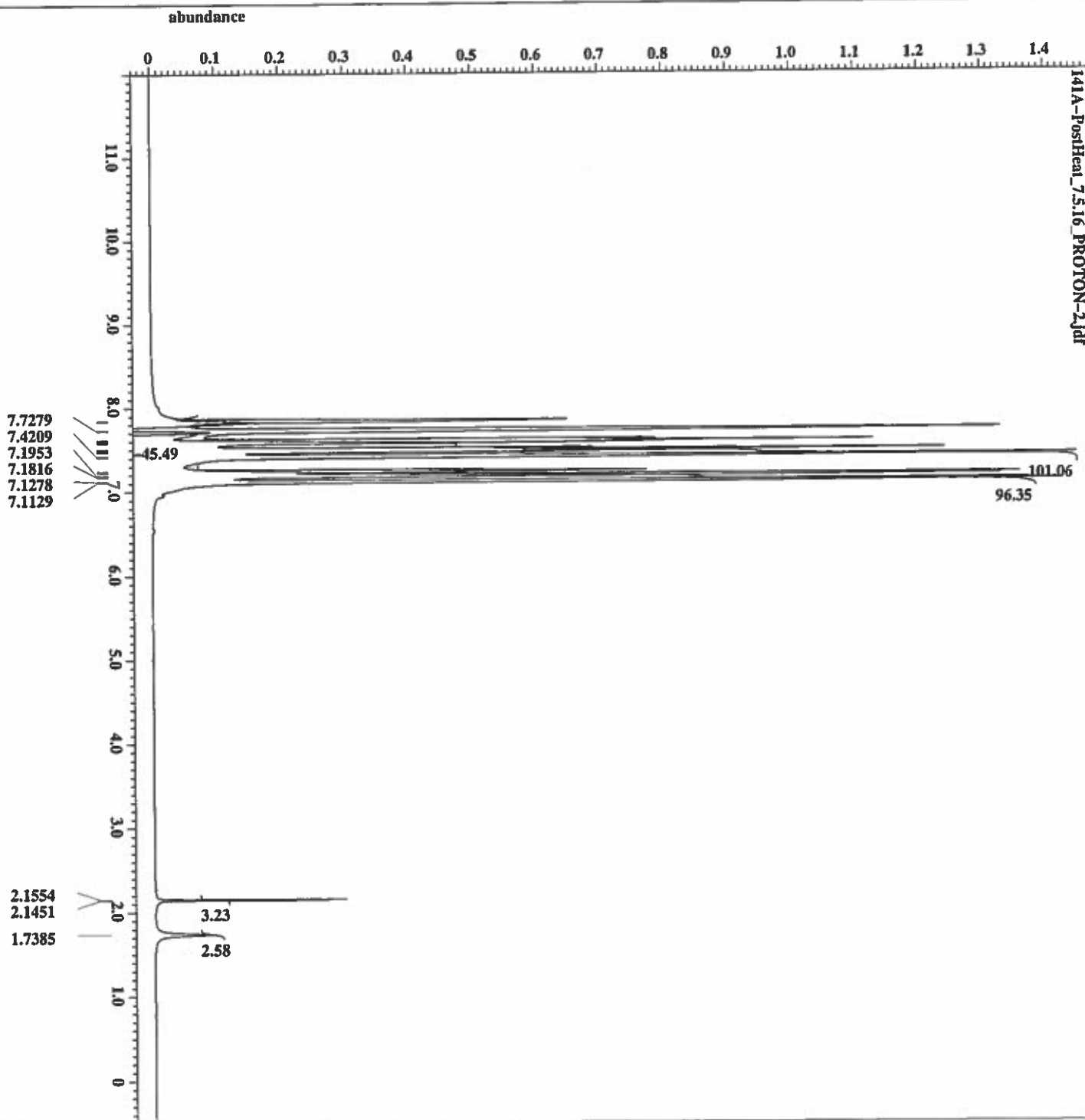
```

Filename      = 141A_slot10_CARBON-2.
Author       = Jim Davis
Experiment   = single_pulse_dec
Sample_id    = S#524117
Solvent      = CHLOROFORM-D
Charger_sample = 10
Creation_time = 2-JUL-2016 17:19:26
Revision_time = 2-JUL-2016 17:01:14
Current_time  = 2-JUL-2016 17:01:14

Comment
Data_format  = Yellow 8
Dim_size     = 1D COMPLEX
Dim_title    = 26214
Dim_units    = 13C
Dimensions   = [ppm]
Site         = X
Spectrometer = ECA 500
              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         = 500.15891521 [MHz]
X_offset       = 5.0 [ppm]
X_resolution   = FALSE
Mod_return     = 1
Scans          = 3100
Total_scans    = 3100

X_90_width     = 12.55 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 6 [dB]
X_pulse        = 4.18333333 [us]
Irr_atn_dec    = 20.5 [dB]
Irr_atn_noe    = 20.5 [dB]
Irr_noise      = WALTEZ
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       = 23.8 [deg]
  
```

```

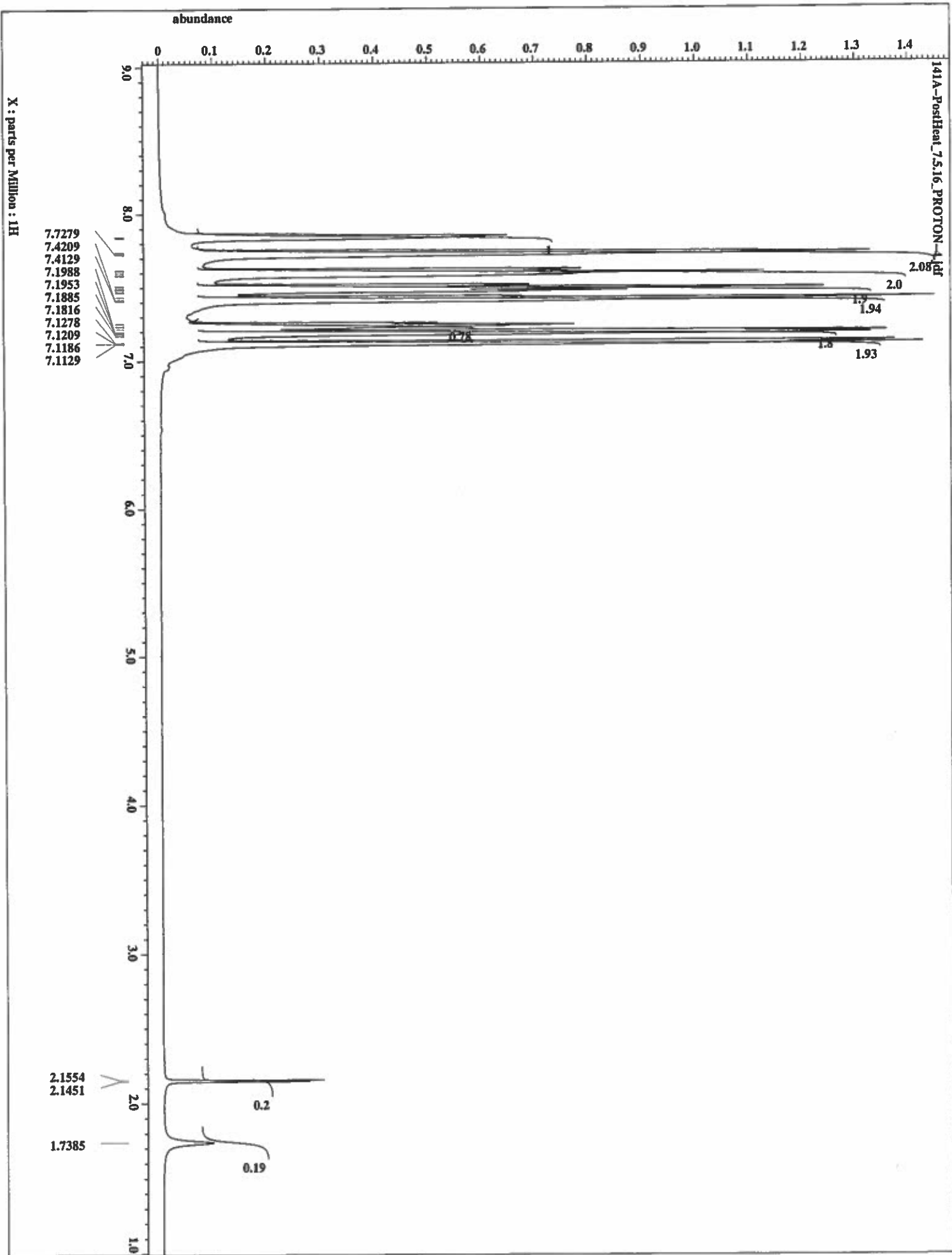
Filename      = 141A-PostHeat_7.5.16_
Author       = Jim Davis
Experiment   = single_pulse.ex2
Sample_id    = 141A-PostHeat_7.5.16
Solvent      = CHLOROFORM-D
Charger_name = 4
Creation_time = 5-JUL-2016 15:55:44
Revision_time = 5-JUL-2016 15:37:22
Current_time  = 5-JUL-2016 13:37:22

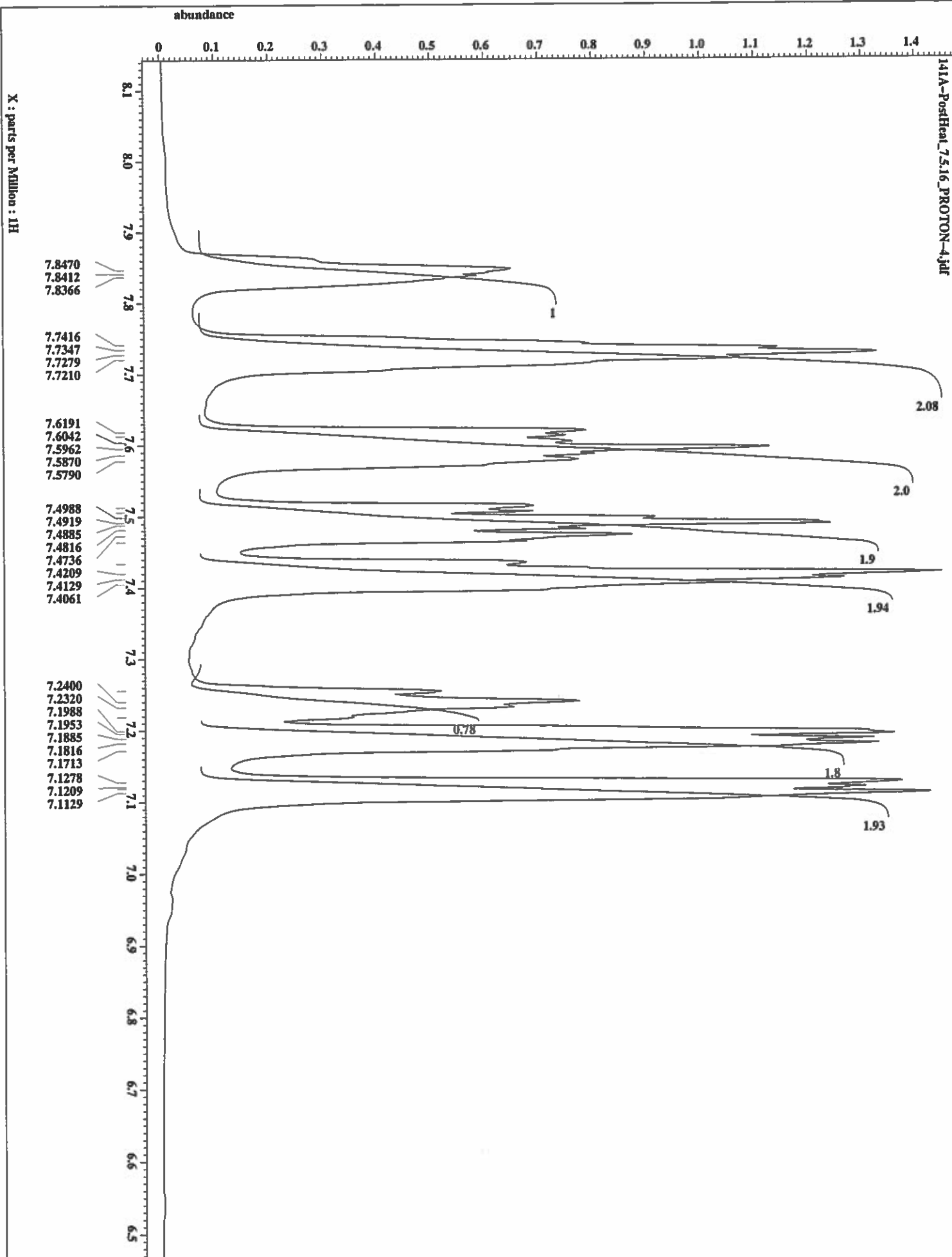
Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer = JNM-KCA500

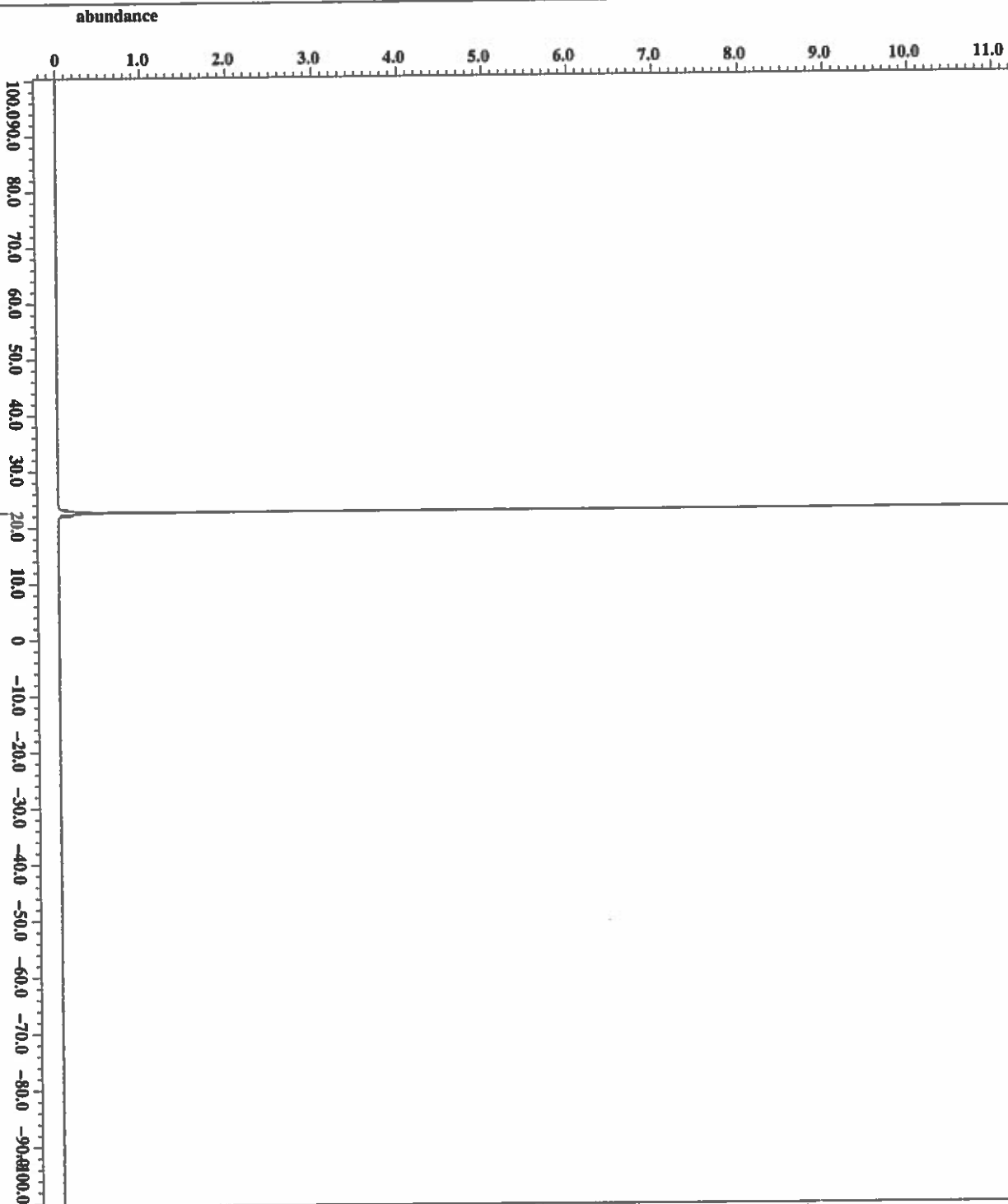
Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 9.38438438 [kHz]
Xr_domain      = 1H
Xr_freq        = 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     = 13.35 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulpr        = 6.675 [us]
Xr_mode        = OFC
Xr1_mode       = OFC
Pulse_program  = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 28
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_set       = 22.7 [degC]

```







X : parts per Million : 31P



```

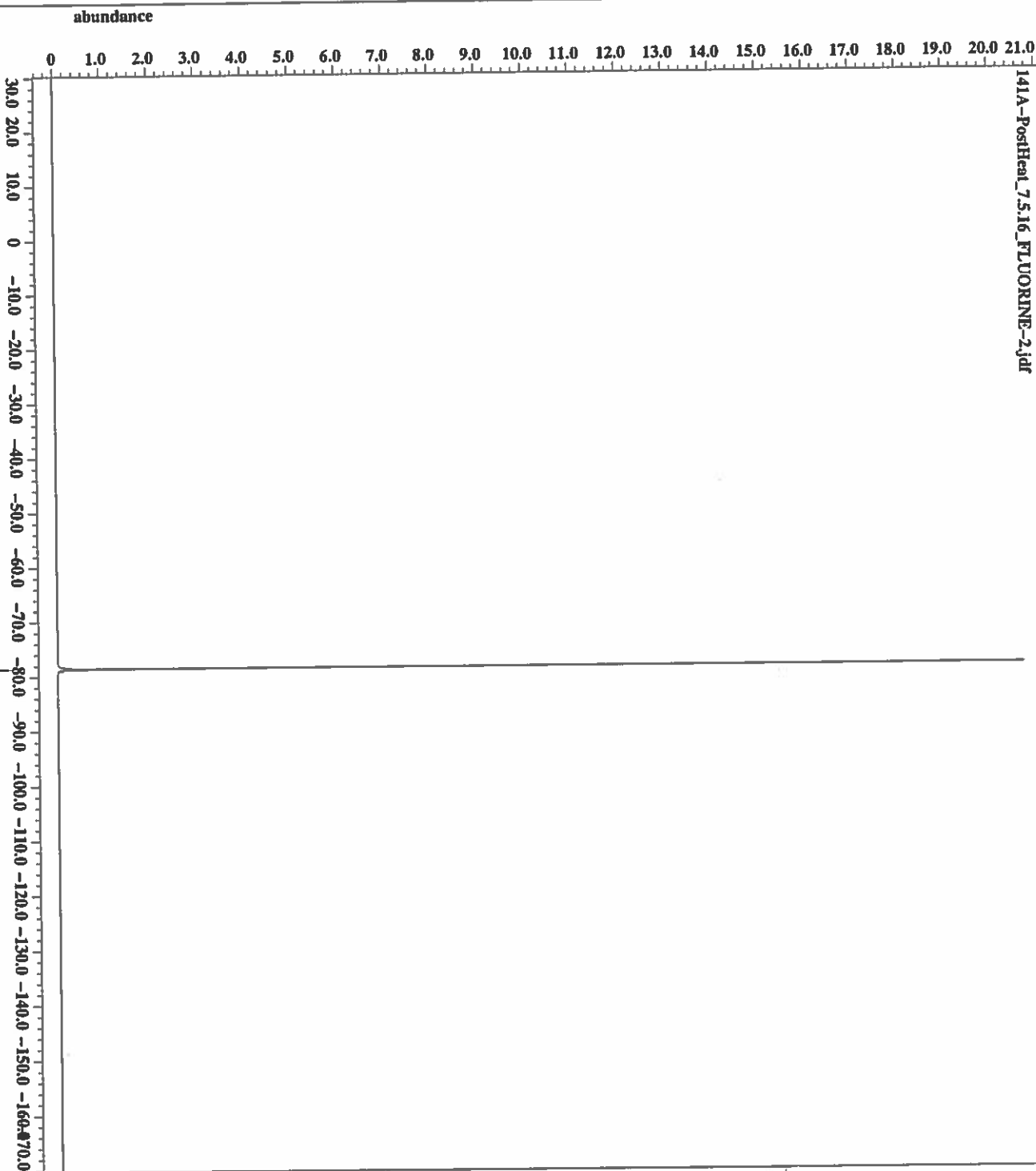
Filename      = 141A-PostHeat_7.5.16_
Author        = Jim Davis
Experiment     = single_pulse_dec
Sample_id     = 141A-PostHeat_7.5.16
Solvent       = CHLOROFORM-D
Charger_sample = 4
Creation_time  = 5-JUL-2016 18:30:36
Revision_time  = 5-JUL-2016 18:12:13
Current_time   = 5-JUL-2016 18:12:13

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         = 202.46631075 [MHz]
X_offset       = 0 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.55068995 [Hz]
X_sweep        = 50.81300913 [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     = 14 [us]
X_acq_time     = 0.64487424 [s]
X_angle        = 30 [deg]
X_atn          = 5 [dB]
X_pulse        = 4.66666667 [us]
Irr_atn_dec    = 20.5 [dB]
Irr_atn_noe    = 20.5 [dB]
Irr_noise      = WALTEZ
Decoupling     = TRU2
Initial_wait   = 1 [s]
Noe            = TRU2
Noe_time       = 2 [s]
Recovery_gain   = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.64487424 [s]
Temp_set       = 23.4 [degC]

```



X : parts per Million : 19F



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```

=====
File Name      = 141A-PostHeat_7.5.16_
Author         = Jim Davis
Experiment     = single-pulse.exe
Sample_Id      = 141A-PostHeat_7.5.16
Solvent        = CHLOROFORM-D
Charger_Sample = 4
Creation_Time   = 5-JUL-2016 18:16:22
Revision_Time  = 5-JUL-2016 17:58:00
Current_Time   = 5-JUL-2016 17:58:00

=====
Data Format
Dim_size      = 1D COMPLEX
Dim_size      = 52428
Dim_title     = 19F
Dim_units     = [ppm]
Dimensions    = X
Site          = QCA 500
Spectrometer  = QNP-PCAS00

=====
Field Strength = 11.7473579 [T] (500 [MH
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    = 19F
Irr_freq      = 470.62046084 [MHz]
Irr_offset    = 5 [ppm]
Irr_domain    = 19F
Irr_freq      = 470.62046084 [MHz]
Tri_domain    = 19F
Tri_freq      = 470.62046084 [MHz]
Tri_offset    = 5 [ppm]
Clipped       = FALSE
Mod_Return    = 1
Scans         = 16
Total_Scans   = 16

=====
X_90_Width     = 15.7 [us]
X_acq_Time     = 0.55574528 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 7.85 [us]
Irr_mode       = Off
Pulse_Program  = FALSE
Pulse_Program  = 1 [s]
Recvr_Gain     = 40
Relaxation_Delay = 4 [s]
Repetition_Time = 4.55574528 [s]
Temp_Set       = 22.9 [dc]
=====

```



Filename = 141A-PostHeat_7.5.16_
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = 141A-PostHeat_7.5.16
Solvent = CHLOROFORM-D
Charger_sample = 4
Creation_time = 5-JUL-2016 18:13:12
Revision_time = 5-JUL-2016 17:54:49
Current_time = 5-JUL-2016 17:54:49

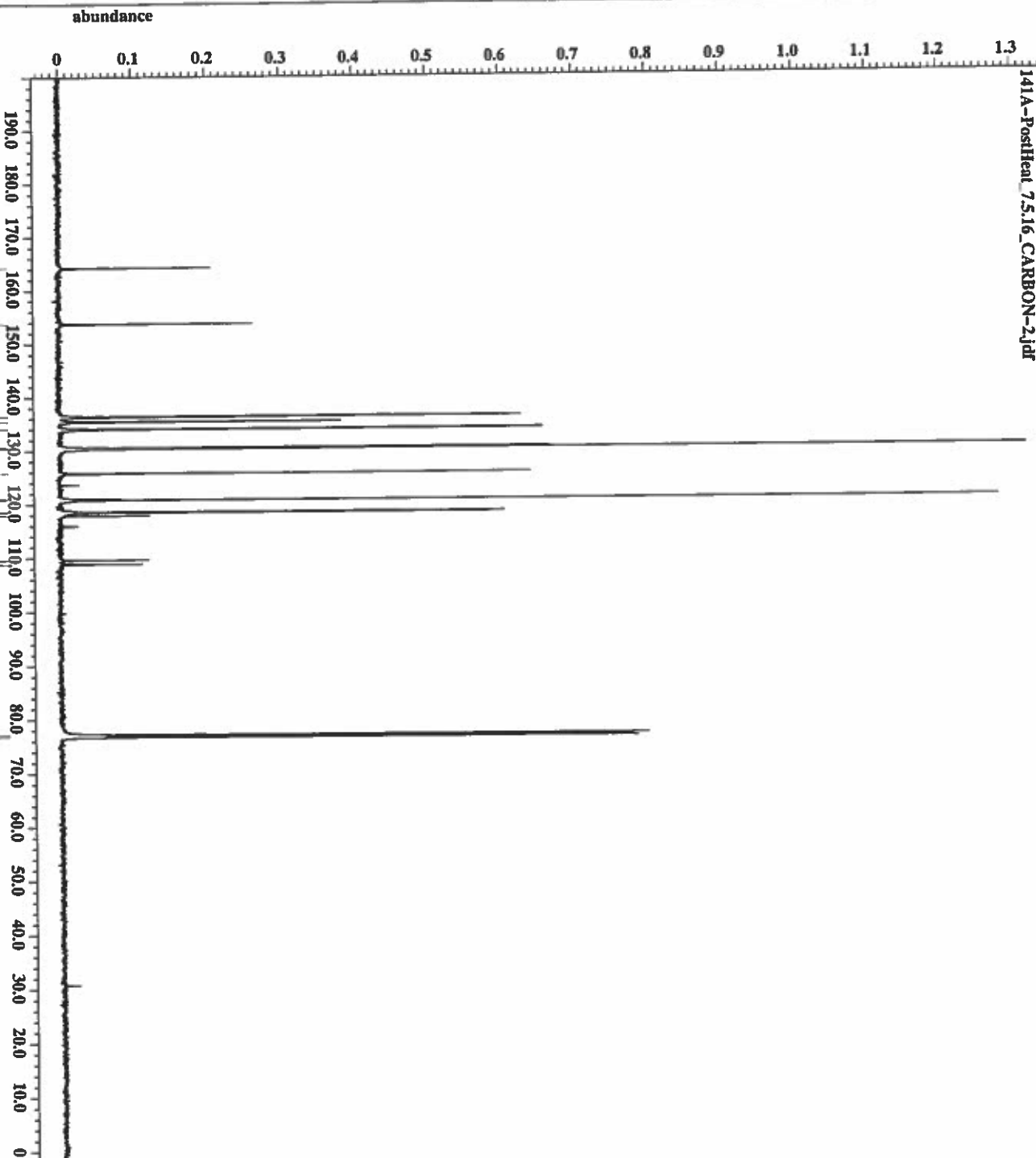
Date_format = 1D COMPLEX
Dm_size = 26214
Dm_title = 13C
Dm_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain = 13C
X_freq = 125.76529768[MHz]
X_offset = 100.1ppm
X_points = 32768
X_prescans = 4
X_resolution = 1.19959036[MHz]
X_sweep = 39.3081761[kHz]
X_domain = 18
X_freq = 500.15891521[MHz]
X_offset = 5.0[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1024
Total_scans = 1024

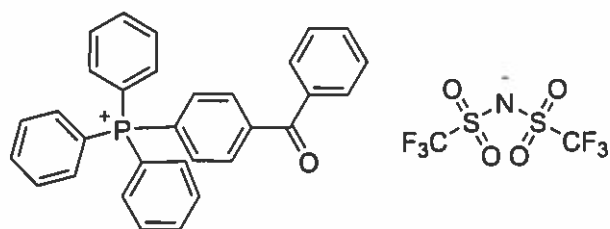
X_90_width = 12.55[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 6[db]
X_pulse = 4.18333333[us]
X_atn_dec = 20.5[db]
X_atn_noe = 20.5[db]
Decoupling = WALTZ
Initial_wait = TRUE
Noc = 2[s]
Noc_time = 60
Recvr_gain = 2[s]
Relaxation_delay = 2.83361792[s]
Repetition_time = 23.6[ac]

X : parts per Million : 13C

164.2089
153.7167
136.3951
136.3093
134.0678
133.9819
130.5577
130.4623
130.3383
125.7694
120.7904
118.5585
118.4440
77.2575
76.7520



COMPOUND 8



Atlantic Microlab, Inc.

No. Phosphonium NEW1

Atlantic Blvd. Suite M
 ss, GA 30071
 atlanticmicrolab.com

Company/School U of South Alabama

Dept. Chemistry

Address Chem 223

City, State, Zip Mobile AL 36688

Name James Davis Date 10/31/2016

Phone (251) 751-0520

or/Supervisor: James Davis

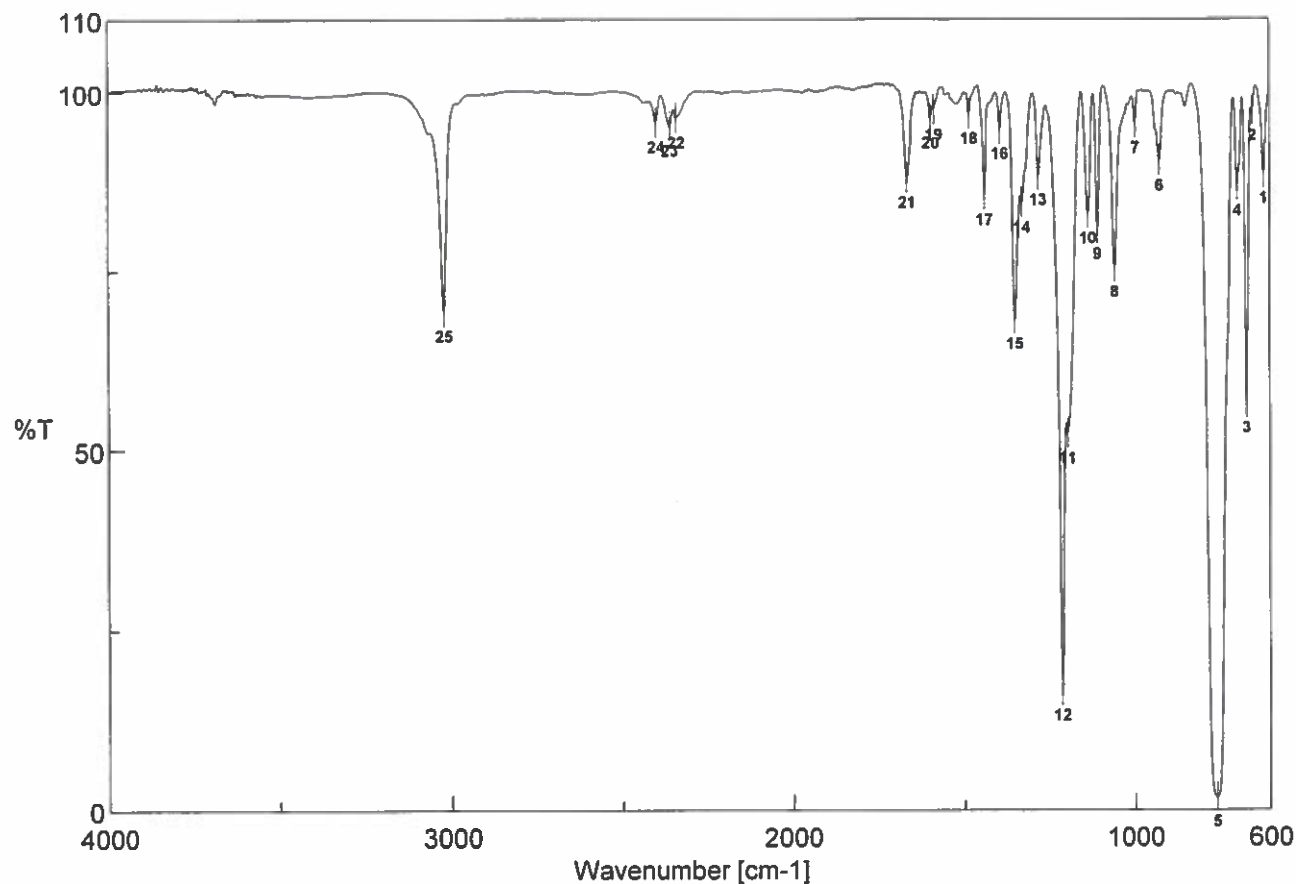
IC#: _____

ient	Theory	Found		Single ☒ Duplicate ☐	Elements CHNPOSF Present:	Analyze CHN for:	Hygroscopic ☐ Explosive ☐ M.P. <u>unk</u> B.P. <u>note</u>	To be dried: Yes ☒ No ☐ Temp. <u>60C</u> Vac. <u>high</u> Time <u>4h</u>	Rush Service ☒	Include Email Address or FAX # Below
C	54.77	54.64								
H	3.34	3.38								
N	1.94	1.94								

Rush service guarantees analysis will be completed and results available by 6 PM EST on the day the sample is received by 11 AM.

Received NOV 01 2016 Date Completed NOV 01 2016

arks:



Result of Peak Picking

No.	Position	Intensity	No.	Position	Intensity
1	617.109	88.453	2	650.858	97.1388
3	668.214	56.3186	4	697.141	86.7757
5	757.888	1.74588	6	926.628	90.2178
7	997.982	95.417	8	1058.73	75.3689
9	1108.87	80.6851	10	1136.83	82.9582
11	1198.54	52.1195	12	1215.9	16.5624
13	1282.43	88.2943	14	1331.61	84.4817
15	1351.86	68.1231	16	1395.25	94.6703
17	1439.6	85.5166	18	1485.88	96.8182
19	1588.09	97.3581	20	1597.73	96.1355
21	1665.23	87.8876	22	2340.19	96.2347
23	2359.48	95.0586	24	2399.98	95.6504
25	3019.98	69.3201			

[Comment]

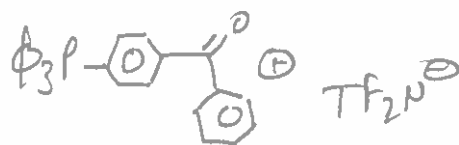
Sample Name
Comment
User
Division
Company

University of South Alabama

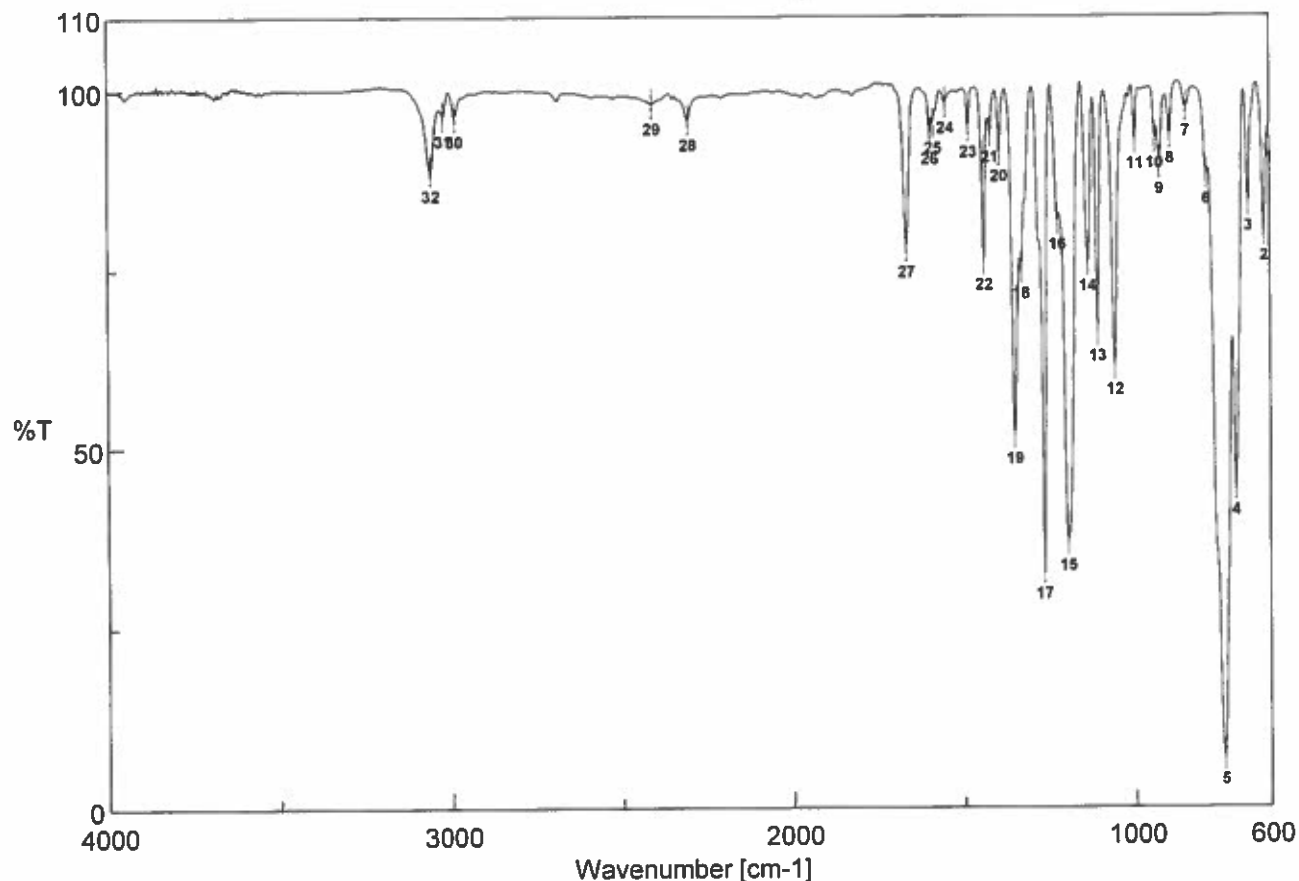
[Measurement Information]

Model Name FT/IR-4100typeA
Serial Number B013761016
Light Source Source #1
Detector Detector #1

Accumulation 8
Resolution 4 cm-1
Zero Filling On
Apodization Cosine
Gain Auto (1)
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (30000 Hz)



Post Leaf



Result of Peak Picking

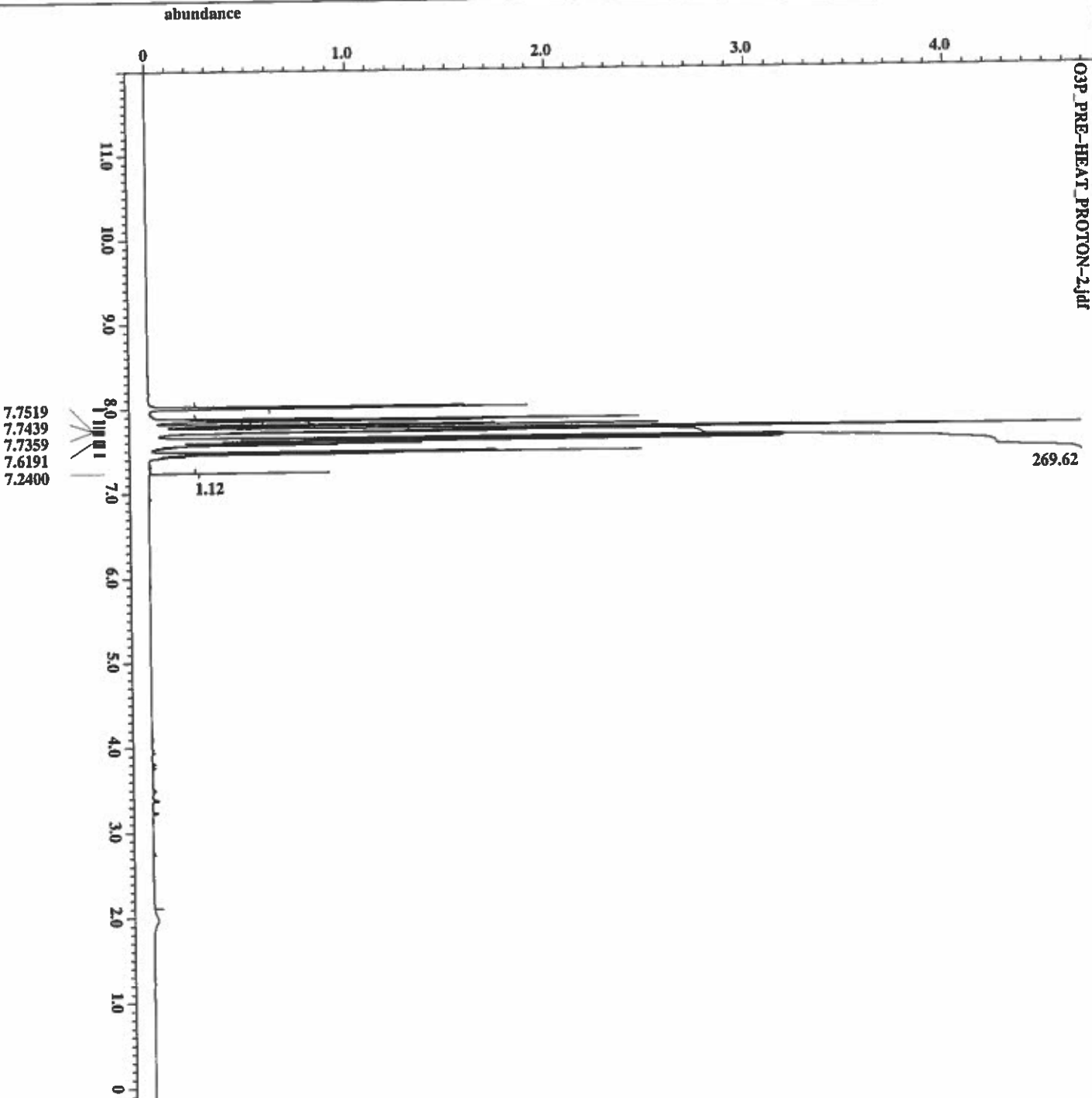
No.	Position	Intensity	No.	Position	Intensity
1	600.717	93.6423	2	617.109	79.9825
3	663.393	84.2213	4	702.926	44.5407
5	738.603	7.16906	6	787.779	87.9998
7	847.561	97.4499	8	895.773	93.6442
9	926.628	89.4414	10	939.163	93.0852
11	997.982	92.9605	12	1059.69	61.4873
13	1108.87	66.2023	14	1136.83	75.9367
15	1196.61	36.9475	16	1225.54	81.7338
17	1266.04	32.9806	18	1332.57	74.8423
19	1352.82	51.7959	20	1395.25	91.3053
21	1422.24	93.9211	22	1439.6	76.0923
23	1485.88	94.6772	24	1552.42	98.0516
25	1588.09	95.1557	26	1597.73	93.6591
27	1666.2	77.8443	28	2305.48	95.709
29	2410.58	97.913	30	2986.23	96.2079
31	3020.94	96.3787	32	3056.62	88.6928

[Comment]

Sample Name
 Comment
 User
 Division
 Company University of South Alabama

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B013761016
 Light Source Source #1
 Detector Detector #1
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (1)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)



```

Filename      = O3P_PRE-HEAT_PROTON-2
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = O3P_PRE-HEAT
Solvent       = CHLOROFORM-D
Charger_sample = 6
Creation_time  = 8-JUL-2016 13:53:23
Revision_time = 8-JUL-2016 13:34:47
Current_time  = 8-JUL-2016 13:36:47

Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X 500
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]
Irr_domain     = 1H
Irr_freq       = 500.15891521 [MHz]
Irr_offset     = 5.0 [ppm]
Prl_domain     = 1H
Prl_freq       = 500.15891521 [MHz]
Prl_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 13.35 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 6.675 [us]
X_mode         = OCF
Pulse_mode     = OCF
Pulse_program  = PALSE
Initial_wait   = 1 [s]
Reover_gain    = 26
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_set       = 22.3 [dc]

```



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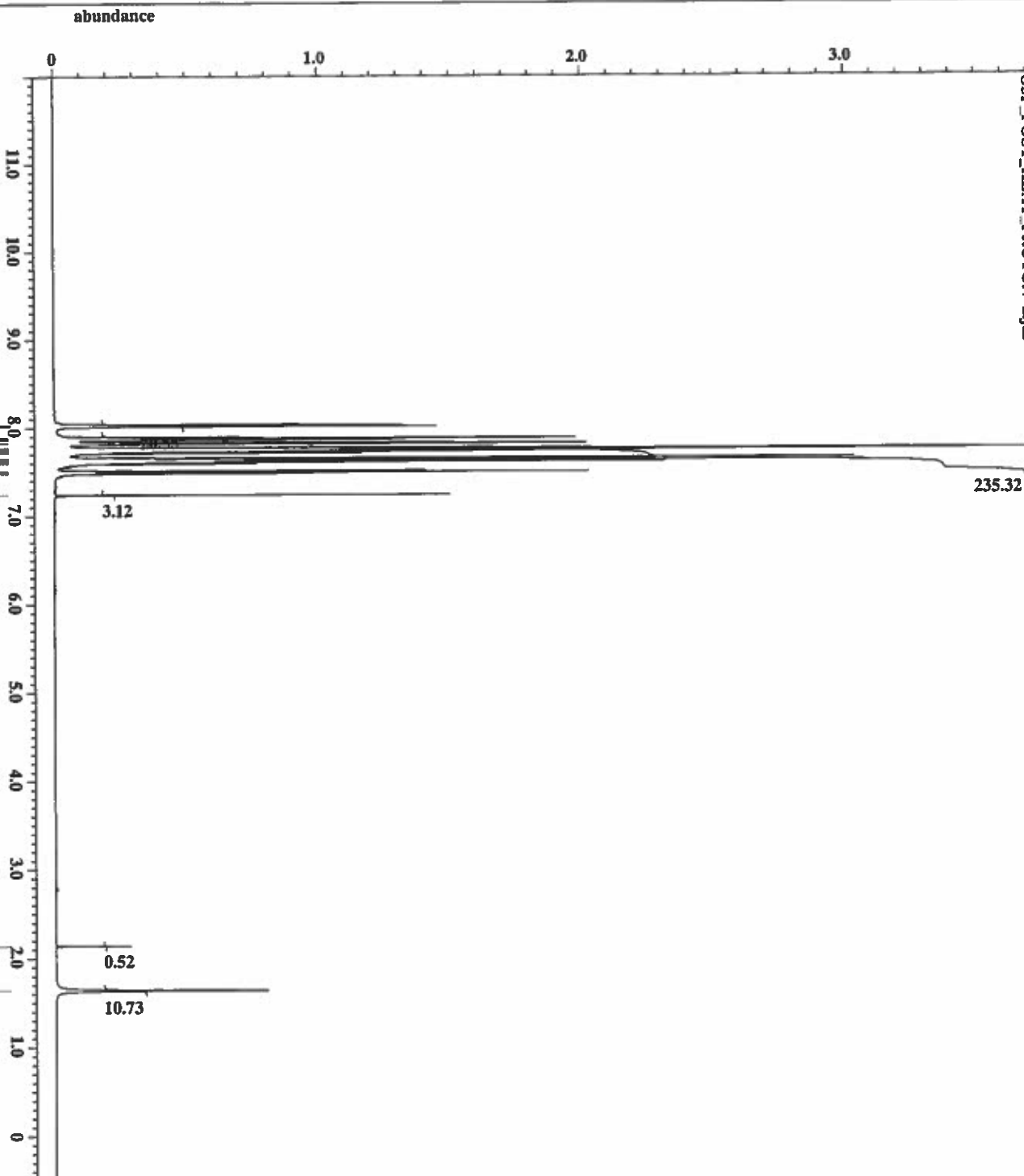


SOUTH ALABAMA
JAGUARSTM

Filename
Author
Experiment
Sample_id
Solvent
Changer_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
Irr_domain
Irr_freq
Irr_offset
Ttl_domain
Ttl_freq
Ttl_offset
Clipped
Mod_return
Scans
Total_scans
X_90_width
X_acq_time
X_angle
X_atn
X_pulse
Irr_mode
Ttl_mode
Dante_preset
Initial_wait
Recvr_gain
Relaxation_delay
Repetition_time
Temp_get



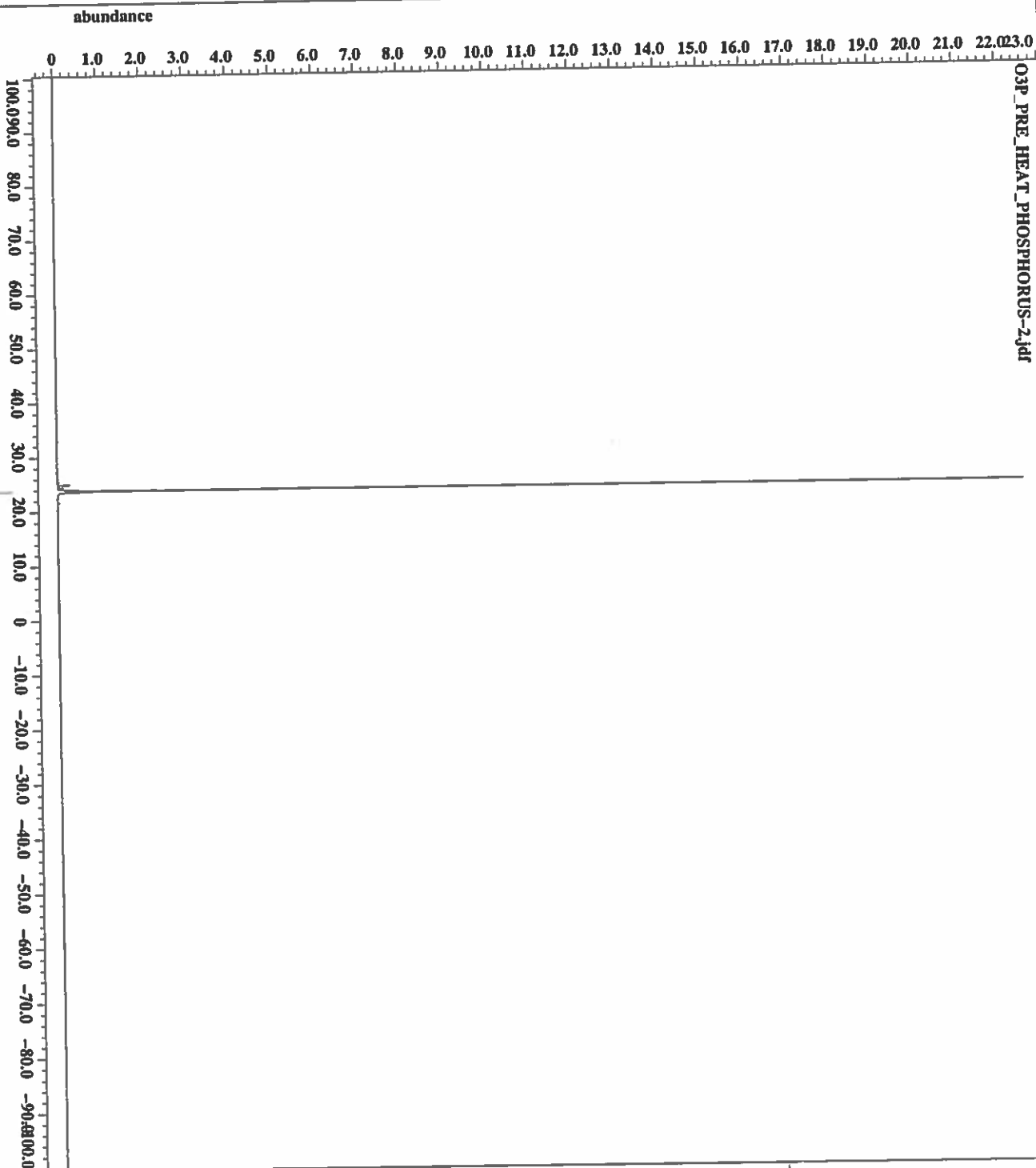


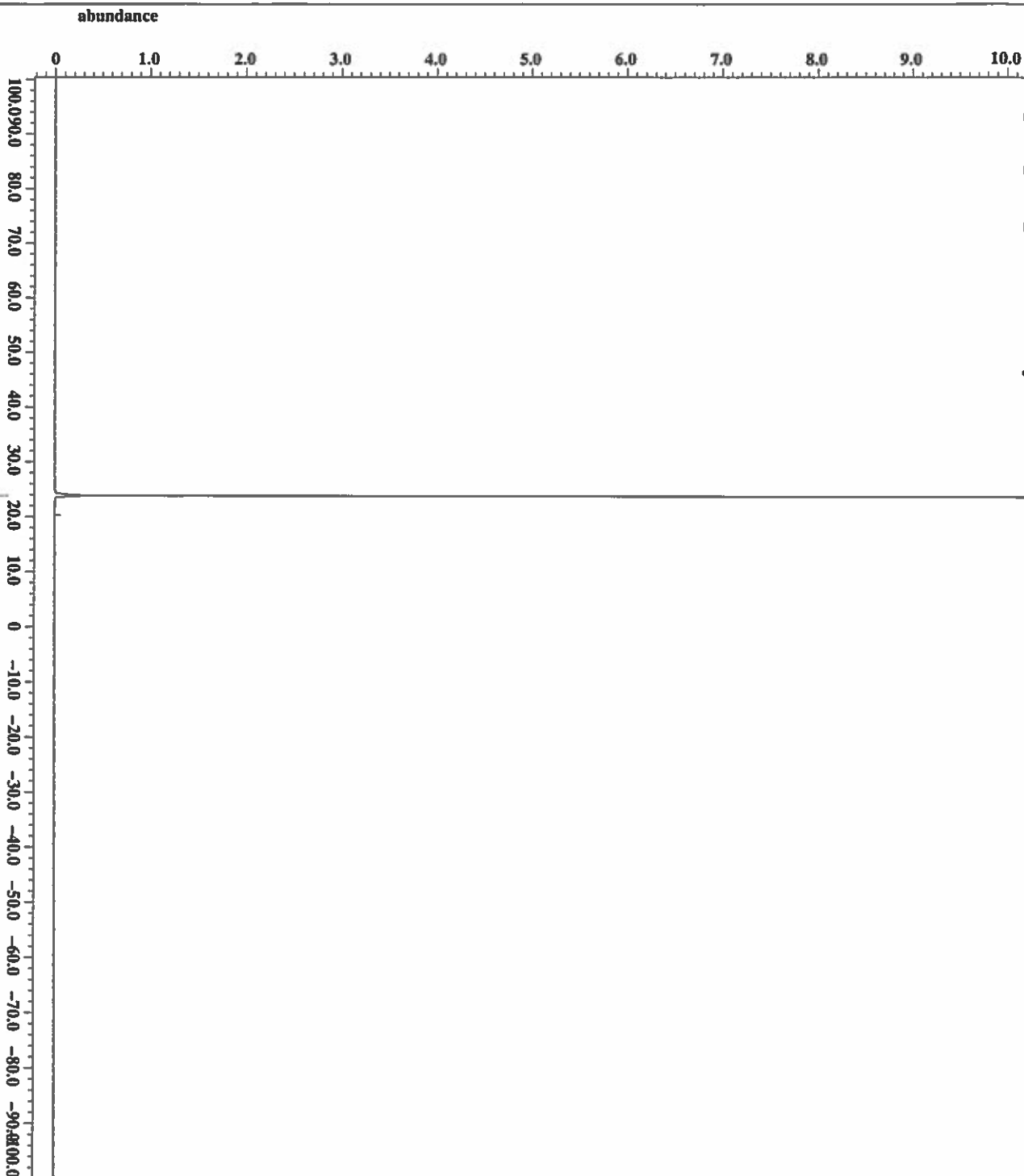
Filename = 03P_PRE_HEAT_PHOSPHOR
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = 03P_PRE_HEAT
Solvent = CHLOROFORM-D
Charger_sample = 6
Creation_time = 8-JUL-2016 14:29:24
Revision_time = 8-JUL-2016 14:10:48
Current_time = 8-JUL-2016 14:10:48

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

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_prescans = 4
X_resolution = 1.55068995 [Hz]
X_sweep = 50.81300813 [Hz]
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 = 14 [us]
X_acq_time = 0.64487424 [s]
X_angle = 30 [deg]
X_atn = 5 [dB]
Irr_atn_dec = 4.66666667 [us]
Irr_atn_dec = 20.5 [dB]
Irr_atn_noe = 20.5 [dB]
Irr_noise = 20.5 [dB]
Decoupling = WALTZ
Initial_wait = TRUE
Noe = 1 [s]
Noe_time = 2 [s]
Noe_gain = 54
Relaxation_delay = 2 [s]
Repetition_time = 2.64487424 [s]
Temp_set = 23.5 [dc]





X : parts per Million : 31P

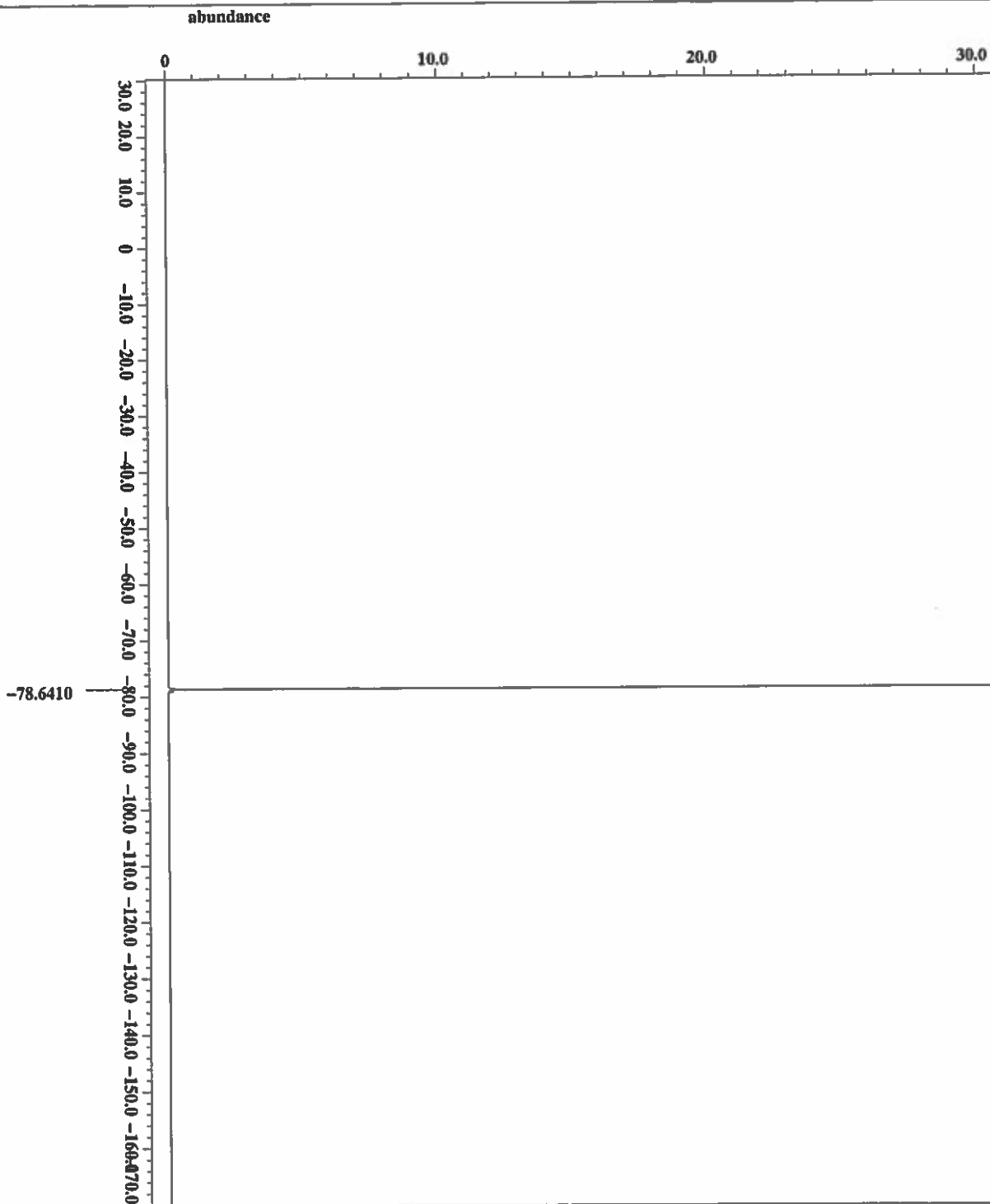


Filename = 03P_POST_HEAT_PHOSPHO
 Author = Jim Davis
 Experiment = single_pulse_dec
 Sample_id = 03P_POST_HEAT
 Solvent = CHLOROFORM-D
 Changer_sample = 7
 Creation_time = 8-JUN-2016 14:13:09
 Revision_time = 8-JUN-2016 13:56:31
 Current_time = 8-JUN-2016 13:56:31

 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 [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 = 256
 Total_scans = 256

 X_90_width = 14 [us]
 X_acq_time = 0.64487424 [s]
 X_angle = 30 [deg]
 X_atn = 5 [dB]
 X_pulse = 4.66666667 [us]
 Irr_atn_dec = 20.5 [dB]
 Irr_atn_noe = 20.5 [dB]
 Irr_noise = VAL7Z
 Decoupling = TRUEZ
 Initial_walt = 1 [s]
 Noe = TRUEZ
 Noe_time = 21 [s]
 Recvr_gain = 58
 Relaxation_delay = 2 [s]
 Repetition_time = 2.64487424 [s]
 Temp_set = 23.3 [dC]



X : parts per Million : 19F



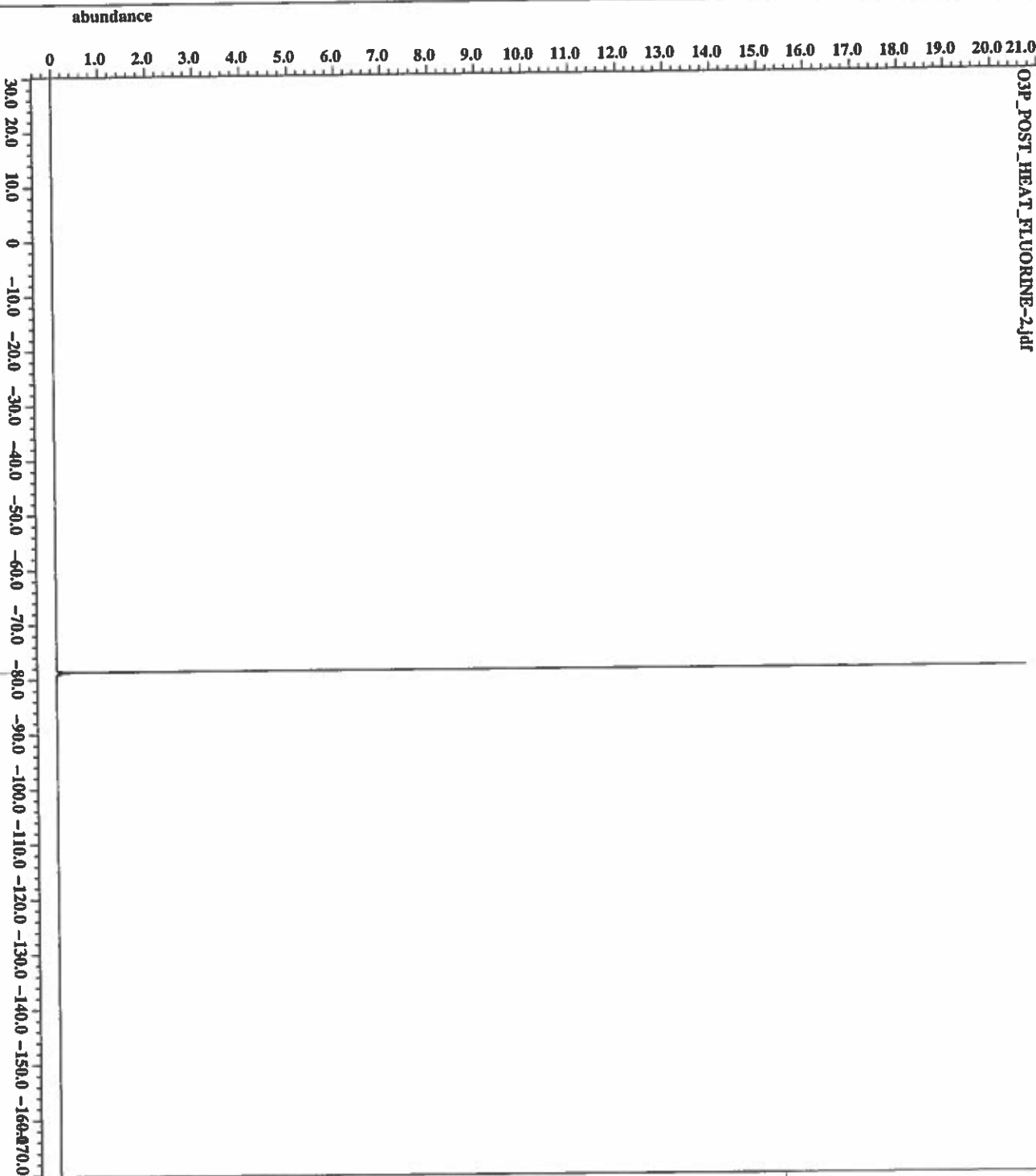
SOUTH ALABAMA
JAGUARS™

```

Filename      = 03P_PRE_HEAT_FLUORINE
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = 03P_PRE_HEAT
Solvent       = CHLOROFORM-D
Charger_sample
Creation_time  = 8-JUL-2016 15:07:54
Revision_time  = 8-JUL-2016 14:49:17
Current_time   = 8-JUL-2016 14:49:17

Data_format   = 1D COMPLEX
Dim_size      = 52428
Dim_c1       = 19F
Dim_c2       = 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_swept        = 117.9245283 [Hz]
Xr_domain      = 19F
Xr_freq        = 470.62046084 [MHz]
Xr_offset      = 5 [ppm]
Xr_domain      = 19F
Xr_freq        = 470.62046084 [MHz]
Xr_offset      = 5 [ppm]
Xr_offset      = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16
X_90_width     = 15.7 [us]
X_acq_time     = 0.55574528 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 7.85 [us]
Xr_mode        = OFC
Xr_mode        = OFC
Dante_preset   = FALSE
Initial_wait   = 38
Rever_gain     = 1 [s]
Relaxation_delay = 4 [s]
Repetition_time = 4.55574528 [s]
Temp_get       = 22.5 [degC]
  
```



X : parts per Million : 19F



```

Filename      = 03P_POST_HEAT_FLUORIN
Author        = Jim Davis
Experiment    = single_pulse.ex2
Sample_id     = 03P_POST_HEAT
Solvent       = CHLOROFORM-D
Change_sample = 7
Creation_time  = 8-JUL-2016 15:13:26
Revision_time  = 8-JUL-2016 14:54:50
Current_time   = 8-JUL-2016 14:54:50

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         = 470.6206084 [MHz]
X_offset       = -70 [ppm]
X_points       = 65536
X_prescans     = 1
X_resolution   = 1.799385 [Hz]
X_sweep        = 117.9245283 [kHz]
Irr_domain     = 19F
Irr_freq       = 470.6206084 [MHz]
Irr_offset     = 5 [ppm]
Irr_domain     = 19F
Irr_freq       = 470.6206084 [MHz]
Irr_offset     = 5 [ppm]
Txi_offset     = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 15.7 [us]
X_acq_time     = 0.55574528 [s]
X_angle        = 45 [deg]
X_atn          = 4 [dB]
X_pulse        = 7.85 [us]
Irr_mode       = OFF
Txi_mode       = OFF
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 44
Relaxation_delay = 4 [s]
Repetition_time = 4.55574528 [s]
Temp_get       = 22.6 [C]

```

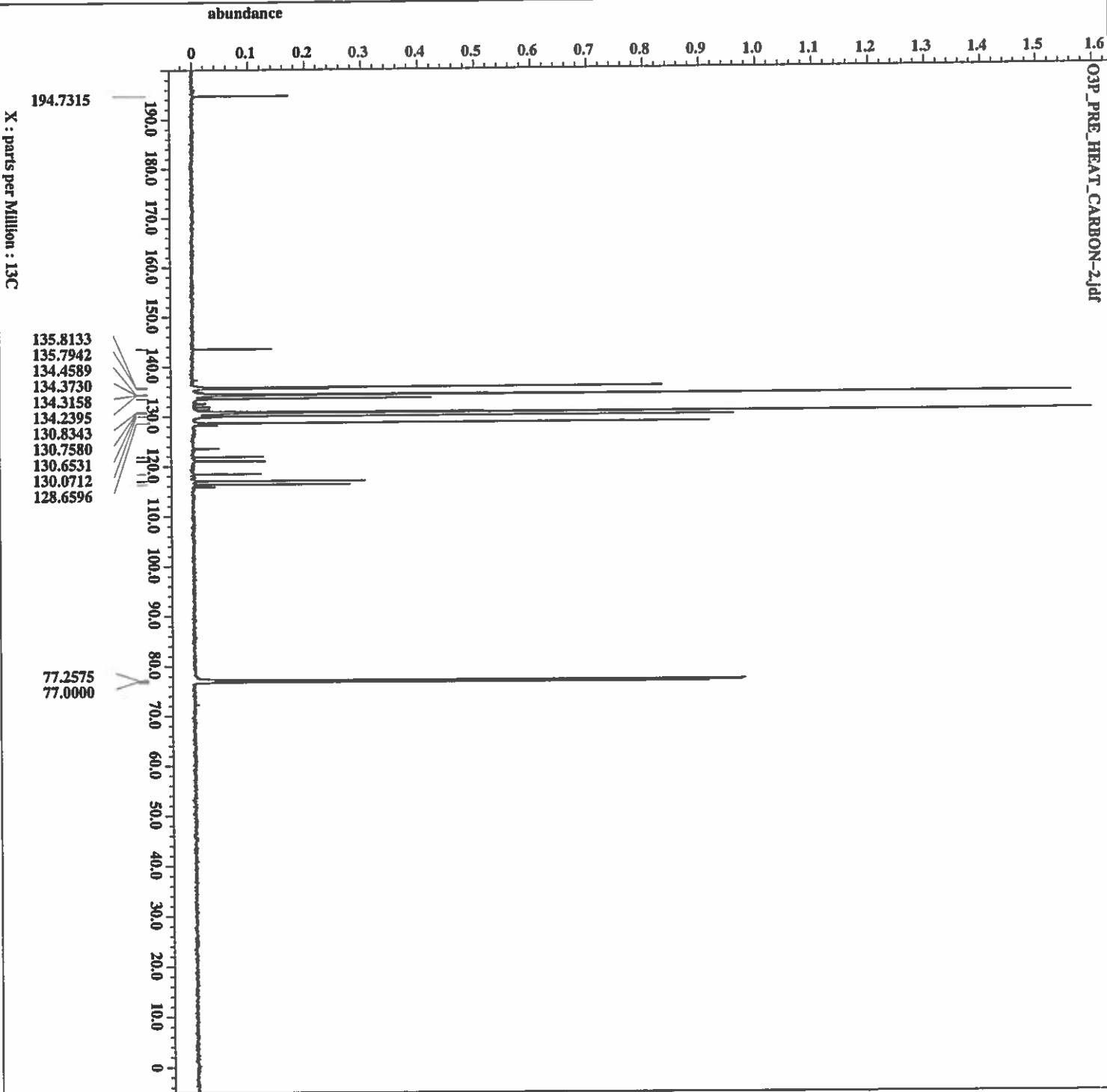



Filename = 03P_PRE_HEAT_CARBON-2
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = 03P_PRE_HEAT
Solvent = CHLOROFORM-D
Charger_sample = 6
Creation_time = 8-JUL-2016 19:06:38
Revision_time = 8-JUL-2016 18:47:59
Current_time = 8-JUL-2016 18:47:59

Data format = 1D COMPLEX
Dir_size = 26214
Dir_title = 13C
Dir_units = [ppm]
Dimensions = X
ECA 500
Site = JMW-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 [Hz]
X_domain = 1H
X_freq = 500.15991521 [MHz]
X_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1024
Total_scans = 1024

X_90_width = 12.55 [us]
X_acq_time = 0.83361792 [s]
X_angle = 30 [deg]
X_atn = 6 [dB]
X_pulse = 4.18333333 [us]
Xr_atn_dec = 20.5 [dB]
Xr_atn_noe = 20.5 [dB]
Xr_noise = WALTZ
Decoupling = WALTZ
Initial_wait = 1 [s]
Noe_time = 210 [s]
Noe_gain = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_set = 23.5 [C]





O3P_POST_HEAT_CARBON-
 Author
 Experiment
 Sample_id
 Solvent
 Changer_sample
 Creation_time
 Revision_time
 Current_time

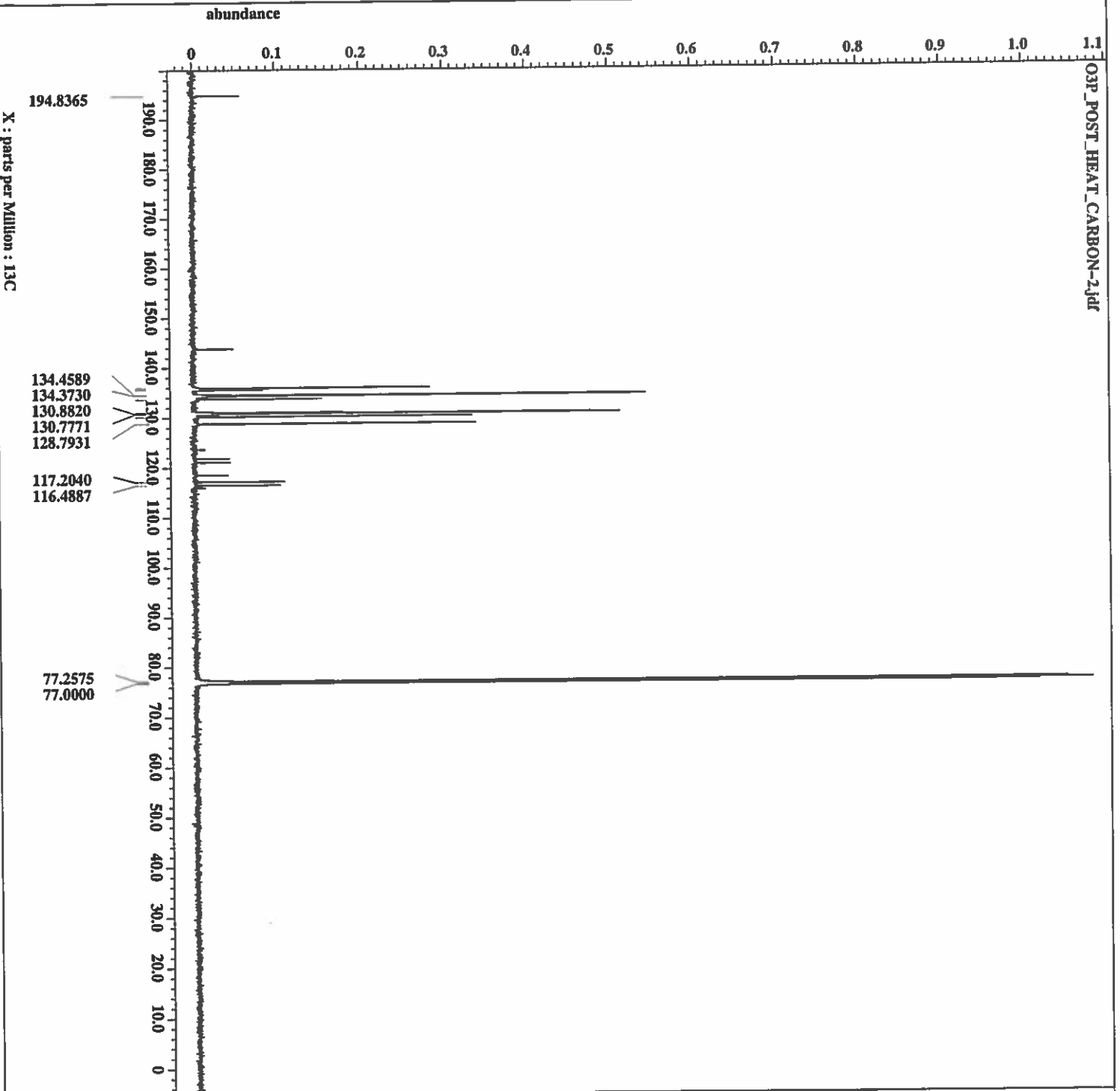
Data_format
 Dim_size
 Dim_title
 Dim_units
 Dimensions
 Site
 Spectrometer

Field_strength
 X_acq_duration
 X_domain
 X_freq
 X_offset
 X_points
 X_pulses
 X_resolution
 X_sweep

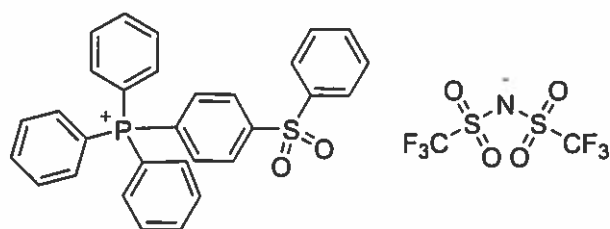
Iir_domain
 Iir_freq
 Iir_offset
 Clipped
 Mod_return
 Scans
 Total_scans

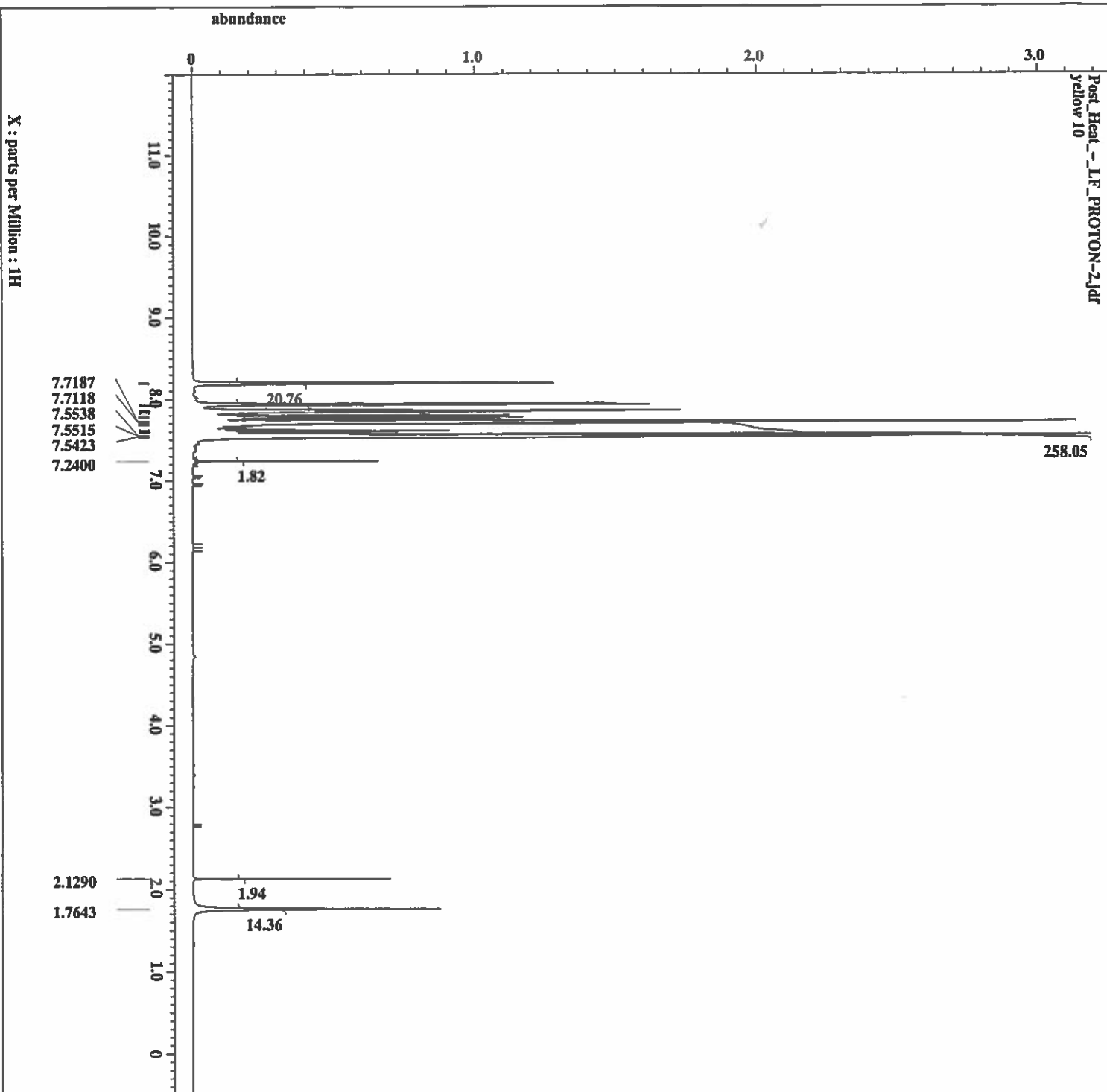
X_90_width
 X_acq_time
 X_angle
 X_atn
 X_pulse
 Iir_atn_dec
 Iir_atn_hoe
 Iir_noise
 Decoupling
 Initial_wait
 Hoe_time
 Recvr_gain
 Relaxation_delay
 Repetition_time
 Temp_set

= O3P_POST_HEAT_CARBON-
 = Jim Davis
 = single_pulse_dec
 = O3P_POST_HEAT
 = CHLOROFORM-D
 = 7
 = 8-JUL-2016 18:13:19
 = 8-JUL-2016 17:54:41
 = 8-JUL-2016 17:54:41
 = 2D COMPLEX
 = 26214
 = 13C
 = [ppm]
 = X
 = ECA 500
 = JNM-ECX500
 = 11.7473579 [T] (500 [MH
 = 0.83361792 [s]
 = 13C
 = 125.76529768 [MHz]
 = 100 [ppm]
 = 32768
 = 4
 = 1.1959034 [Hz]
 = 39.3081761 [kHz]
 = 1H
 = 500.15991521 [MHz]
 = 5.0 [ppm]
 = TRUE
 = 1
 = 1034
 = 1034
 = 12.55 [us]
 = 0.83361792 [s]
 = 30 [deg]
 = 6 [dB]
 = 4.18333333 [us]
 = 20.5 [dB]
 = 20.5 [dB]
 = WALTZ
 = TRUE
 = 1 [s]
 = TRUE
 = 2 [s]
 = 60
 = 2 [s]
 = 2.83361792 [s]
 = 23.5 [deg]

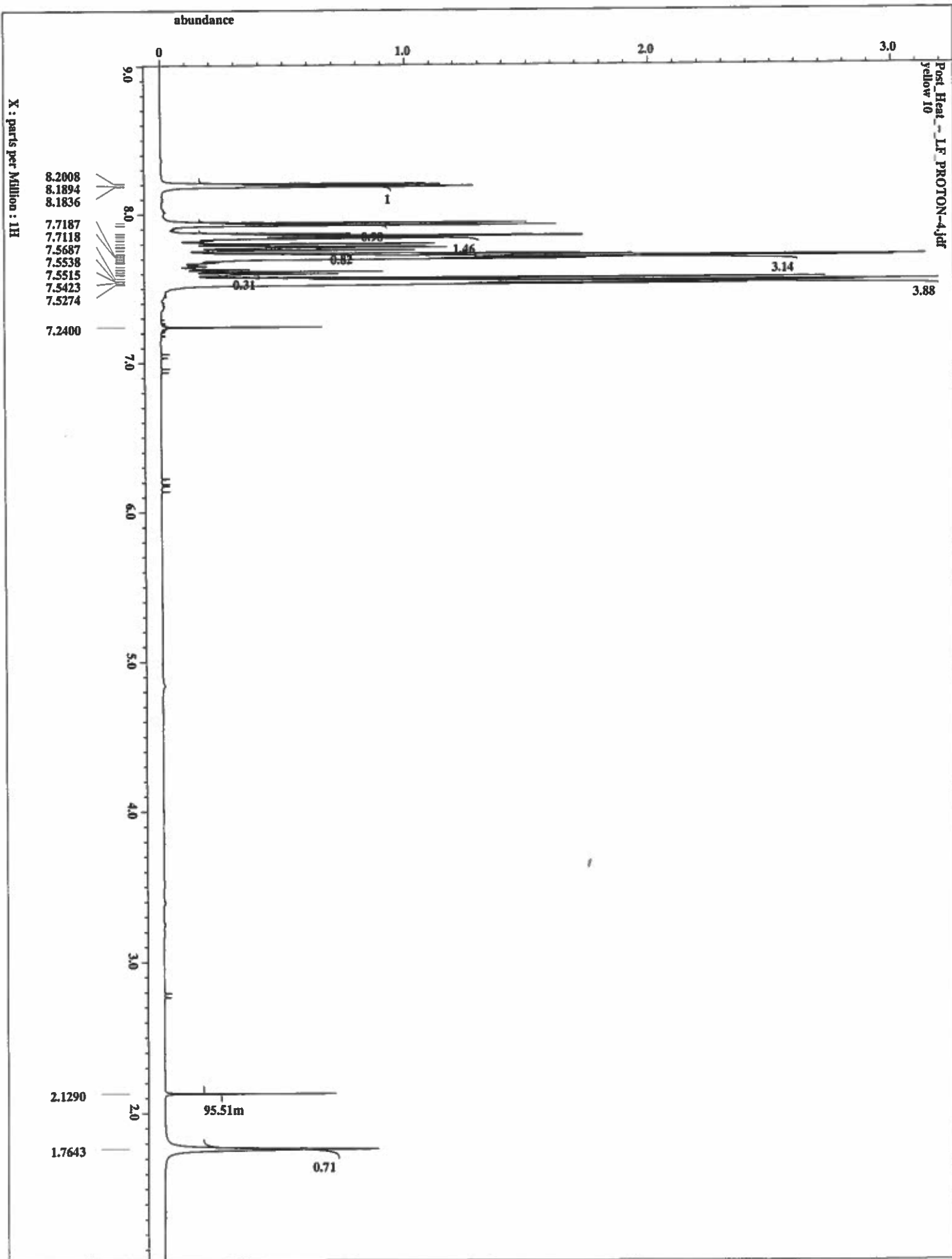


COMPOUND 9





Filename	Post_Heat_-_LF_PROTOCOL
Author	Jim Davis
Experiment	single_pulse.ex2
Sample_id	Post_Heat_-_LF
Solvent	CHROMOPORM-D
Changeover_sample	12
Creation_time	1-JUN-2016 14:40:35
Revision_time	1-JUN-2016 14:32:30
Current_time	1-JUL-2016 14:22:30
Comment	
Date_format	yellow 10
Dim_size	ID COMPLEX
Dim_title	13107
Dim_units	1H
Dimensions	[ppm]
Site	X
Spectrometer	ECA 500
	JNM-ECA500
Field_strength	11.7673579 [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_prgscans	1
X_resolution	0.57277737 [Hz]
X_sweep	9.36438438 [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
X_90_width	13.35 [us]
X_acq_time	1.74587904 [s]
X_angle	45 [deg]
X_atn	4 [dB]
X_pulse	6.675 [us]
1H_mode	O2F
1H_mode	O2F
Dante_preset	FALSE
Initial_wait	1 [s]
Recv_gain	32
Relaxation_delay	4 [s]
Repetition_time	5.774587904 [s]
Temp_get	22.21 [dC]



abundance

0 1.0 2.0 3.0

8.2065
8.2008
8.1894
8.1836

8.2

8.1

8.0

7.9409
7.9260
7.9237

7.9

0.98

7.8710
7.8687
7.8664
7.8550
7.8515
7.8401
7.8240

7.8

1.46

7.8000
7.7828
7.7748
7.7576

7.7

0.82

7.7347
7.7279
7.7187
7.7118
7.7027
7.6958
7.6866
7.6775
7.6717

7.7

3.14

7.6477
7.6282
7.6133
7.6099
7.5984
7.5962
7.5904

7.6

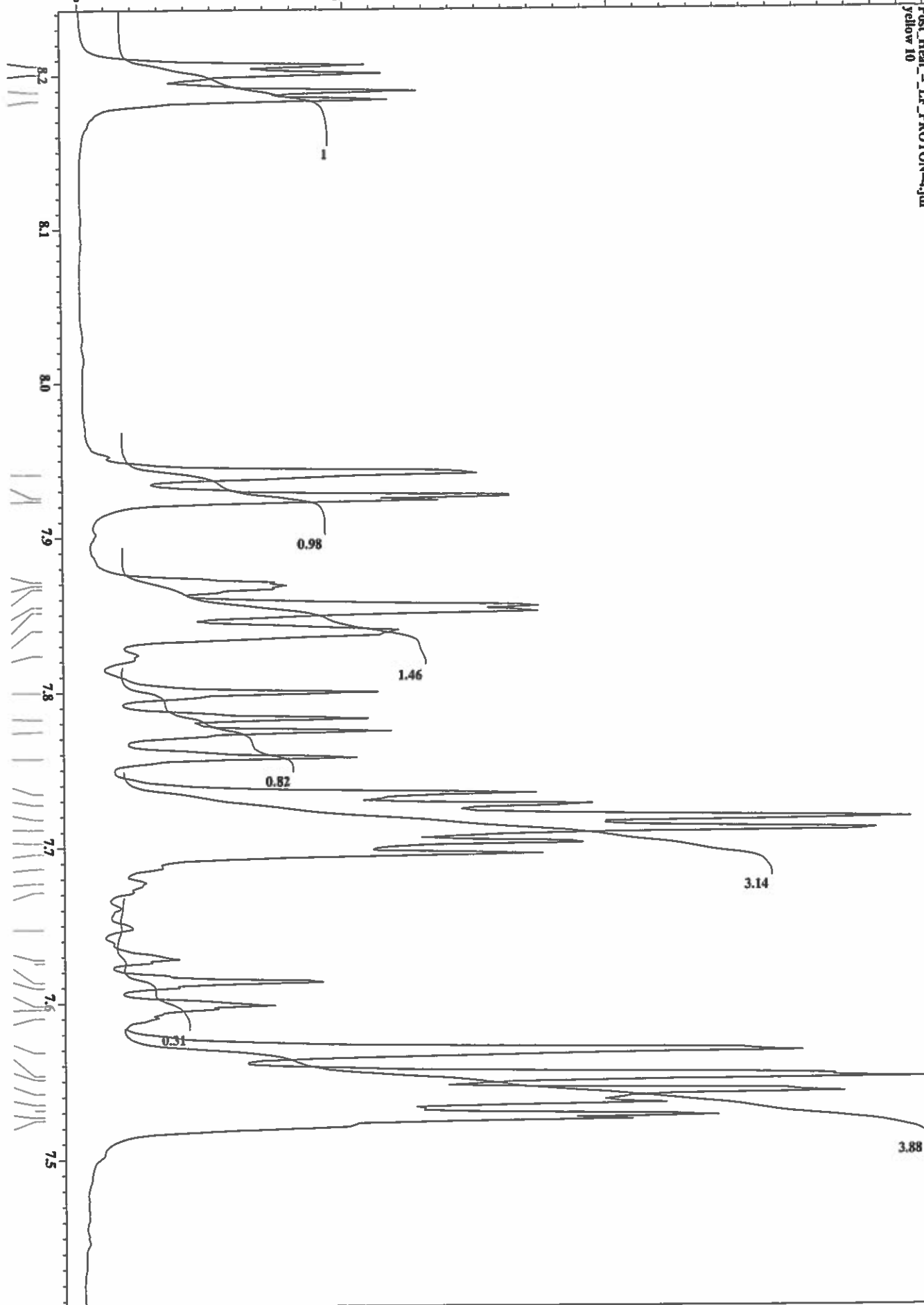
0.31

7.5687
7.5538
7.5515
7.5423
7.5355
7.5274
7.5252

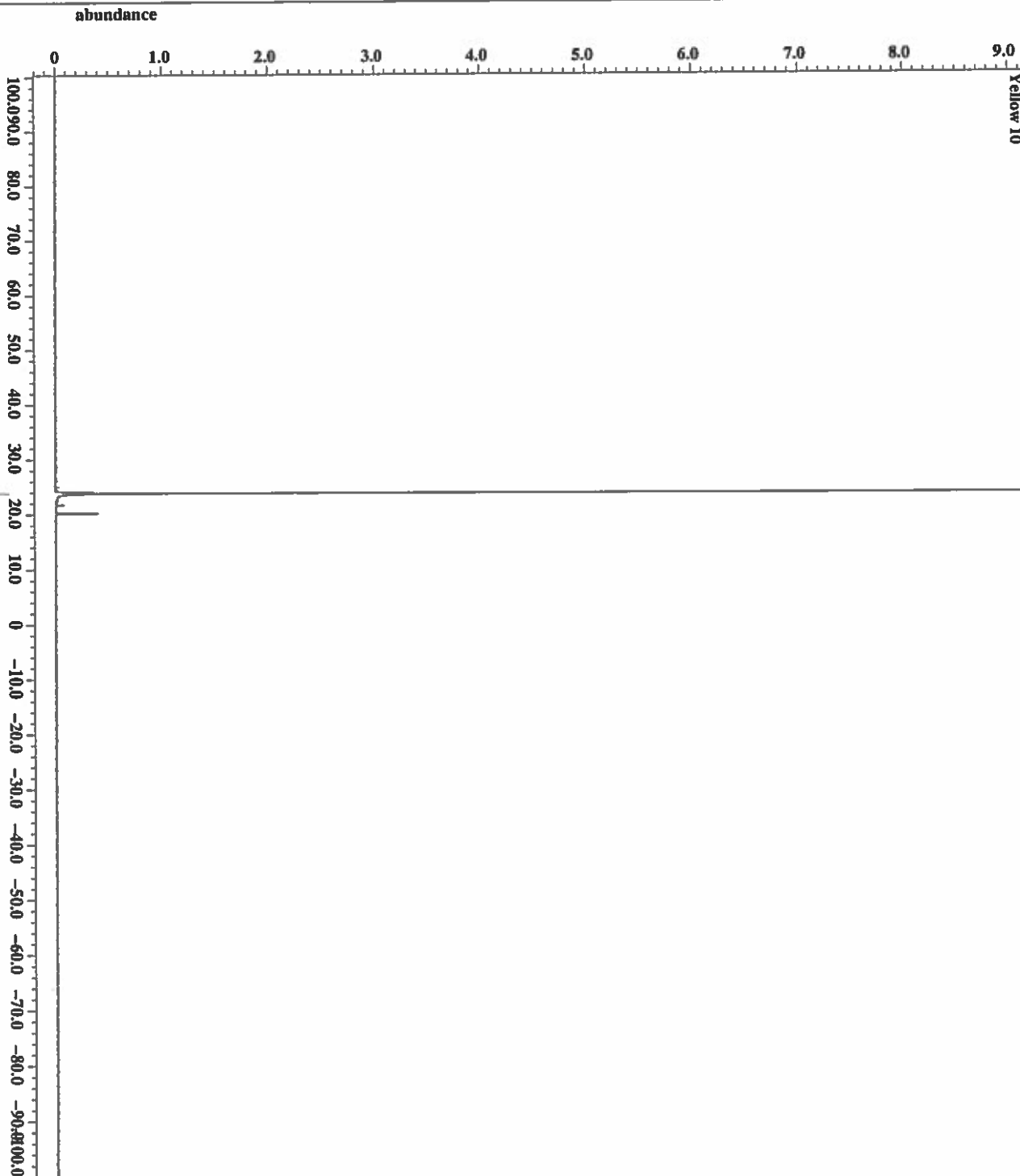
7.5

3.88

X : parts per Million : 1H



PostHeat - LF_slot12_PHOSPHORUS-2.jdt
Yellow 10



X : parts per Million : 31P



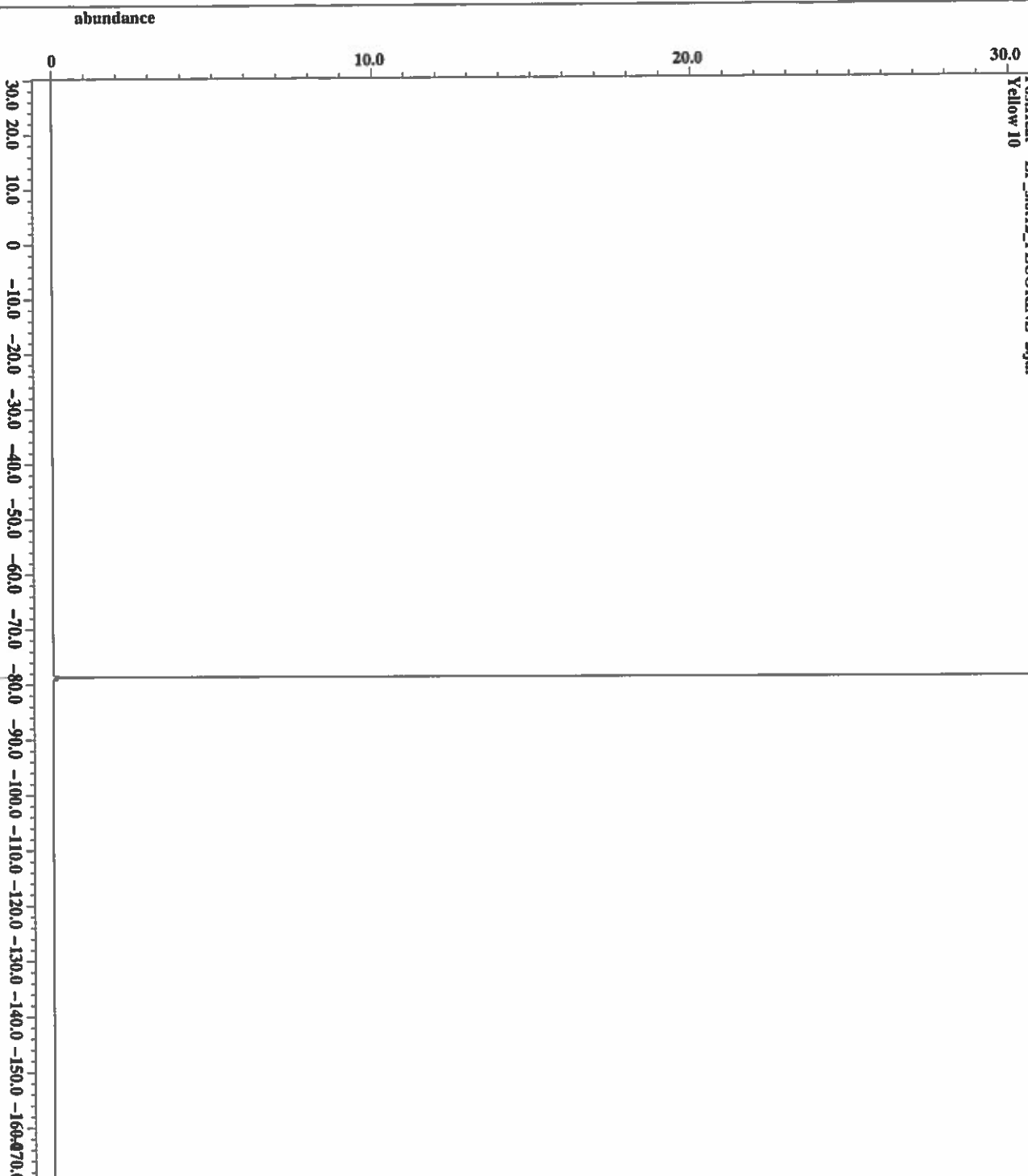
Filename = PostHeat - LF_slot12_
Author = Jim Davis
Experiment = single pulse_dec
Sample_id = S8697411
Solvent = CHLOROFORM-D
Charger_sample = 12
Creation_time = 1-JUL-2016 19:53:01
Revision_time = 1-JUL-2016 19:34:55
Current_time = 1-JUL-2016 19:34:55

Comment
Data_format = Yellow 10
Dim_size = 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_rescans = 1.55068995 [Hz]
X_resolution = 50.81300813 [Hz]
X_sweep = 1H
Xir_domain = 500.15991521 [MHz]
Xir_freq = 5.0 [ppm]
Xir_offset = FALSE
Xir_return = 1
Scans = 256
Total_scans = 256

X_90_width = 14 [us]
X_acq_time = 0.64487424 [s]
X_angle = 30 [deg]
X_atn = 5 [dB]
X_pulse = 4.66666667 [us]
Xir_atn_dec = 20.5 [dB]
Xir_atn_poe = 20.5 [dB]
Xir_poise = KALYZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 2 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 2.64487424 [s]
Temp_get = 23.7 [C]

PostHeat - LR_slot12_FLUORINE-2.jdr
Yellow 10



X : parts per Million : 19F

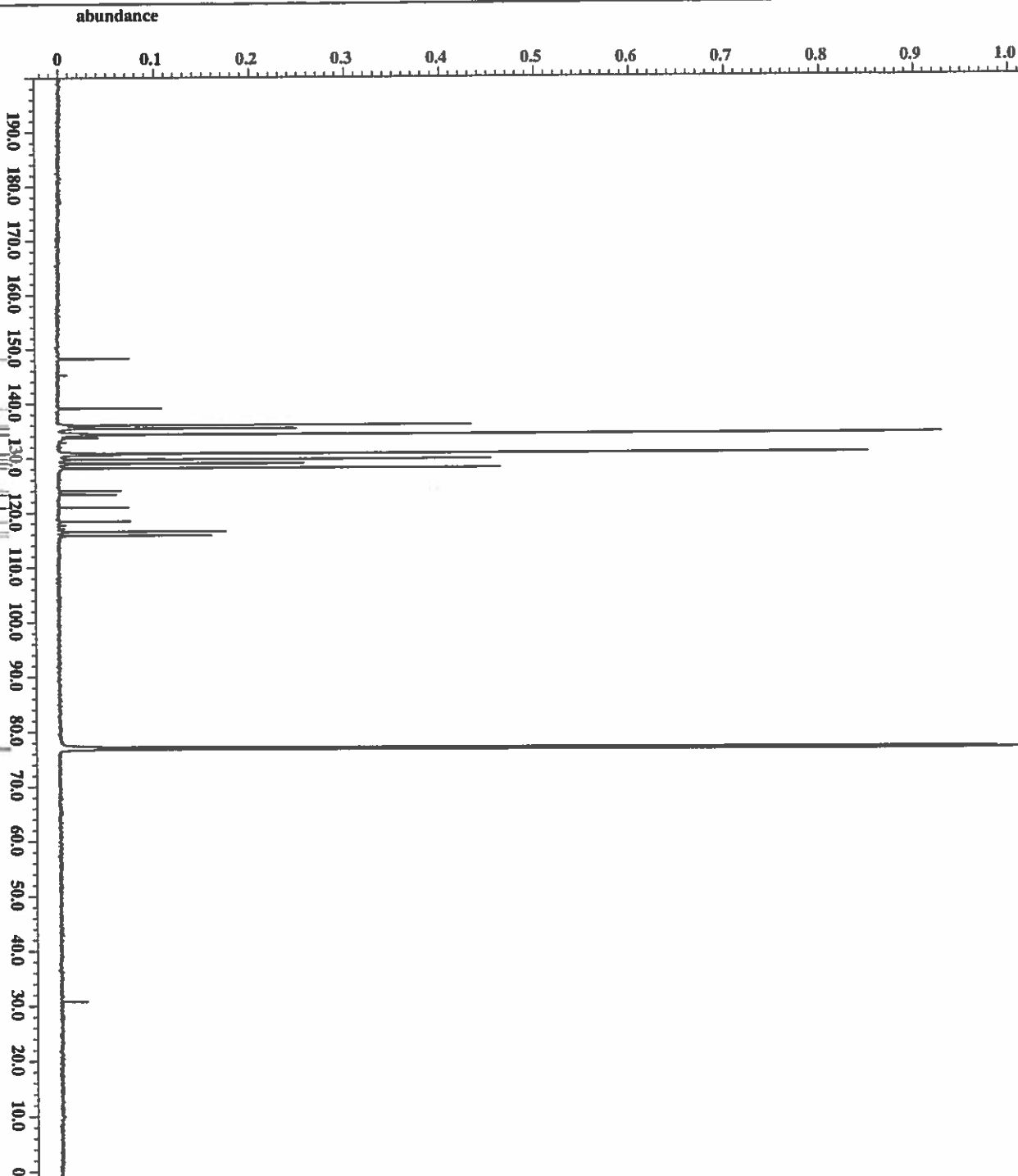


Filename PostHeat - LR_slot12-
Author Jim Davis
Experiment single_pulse.ex2
Sample_id S8581143
Solvent CHLOROFORM-D
Charger_sample 12
Creation_time 1-UTL-2016 16:29:21
Revision_time 1-UTL-2016 16:11:16
Current_time 1-UTL-2016 16:11:16

Comment
Data_Format Yellow 10
Dim_size 1D COMPLEX
Dim_title 52428
Dim_units 19F
Dimensions [ppm]
Site X
Spectrometer RCA 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_sweep 117.9245283 [kHz]
Irr_domain 19F
Irr_freq 470.62046084 [MHz]
Irr_offset 19F
T1_domain 19F
T1_freq 470.62046084 [MHz]
T1_offset 5 [ppm]
T1_offset VALIST
Clipped 1
Mod_return 16
Scans 16
Total_scans 16

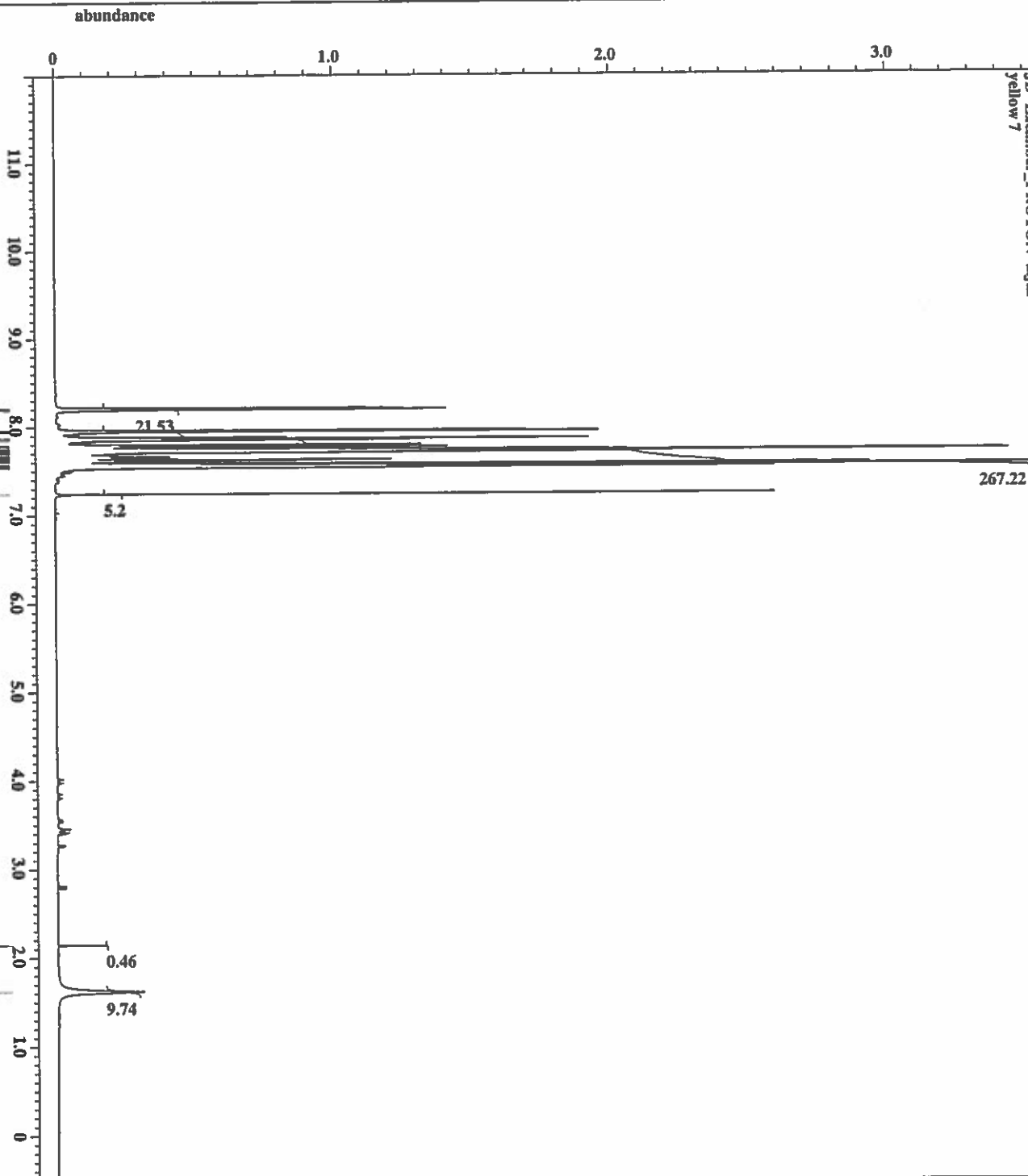
X_90_width 15.7 [us]
X_acq_time 0.55574528 [s]
X_angle 45 [deg]
X_atn 4 [dB]
X_pulse 7.85 [us]
Irr_mode ORF
T1_mode ORF
Dance_presat PALIST
Initial_walt 1 [s]
Recvr_gain 42
Relaxation_delay 4 [s]
Repetition_time 4.55574528 [s]
Temp_got 22.5 [degC]



X : parts per Million : 13C



Filename
 Author
 Experiment
 Sample_id
 Solvent
 Chamber_sample
 Creation_time
 Revision_time
 Current_time
 Comment
 Date_format
 Dia_size
 Dia_title
 Dia_units
 Dimensions
 Site
 Spectrometer
 Field_strength
 X_acq_duration
 X_domain
 X_freq
 X_offset
 X_points
 X_prescans
 X_resolution
 X_sweep
 Iir_domain
 Iir_freq
 Iir_offset
 Clipped
 Mod_return
 Scans
 Total_scans
 X_90_width
 X_acq_time
 X_angle
 X_atn
 X_pulse
 Iir_atn_dec
 Iir_atn_noe
 Iir_noise
 Decoupling
 Initial_wait
 Noe_time
 Noe_gain
 Relaxation_delay
 Repetition_time
 Temp_get
 PostHeat - LF_slot12_2
 Jim Davis
 single_pulse_dec
 88795819
 CHLOROFORM-D
 12
 3-JUL-2016 00:52:14
 3-JUL-2016 00:34:00
 3-JUL-2016 00:34:00
 Yellow 10
 ID COMPLEX
 26214
 13C
 [ppm]
 X
 ECA 500
 JNM-ECA500
 11.7473579 [T] (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]
 FALSZ
 1
 3100
 3100
 12.55 [us]
 0.83361792 [s]
 30 [deg]
 6 [dB]
 4.18333333 [us]
 20.5 [dB]
 20.5 [dB]
 VALDZ
 TRIZ
 1 [s]
 TRIZ
 2 [s]
 60
 2 [s]
 2.83361792 [s]
 23.9 [deg]



X : parts per Million : 1H

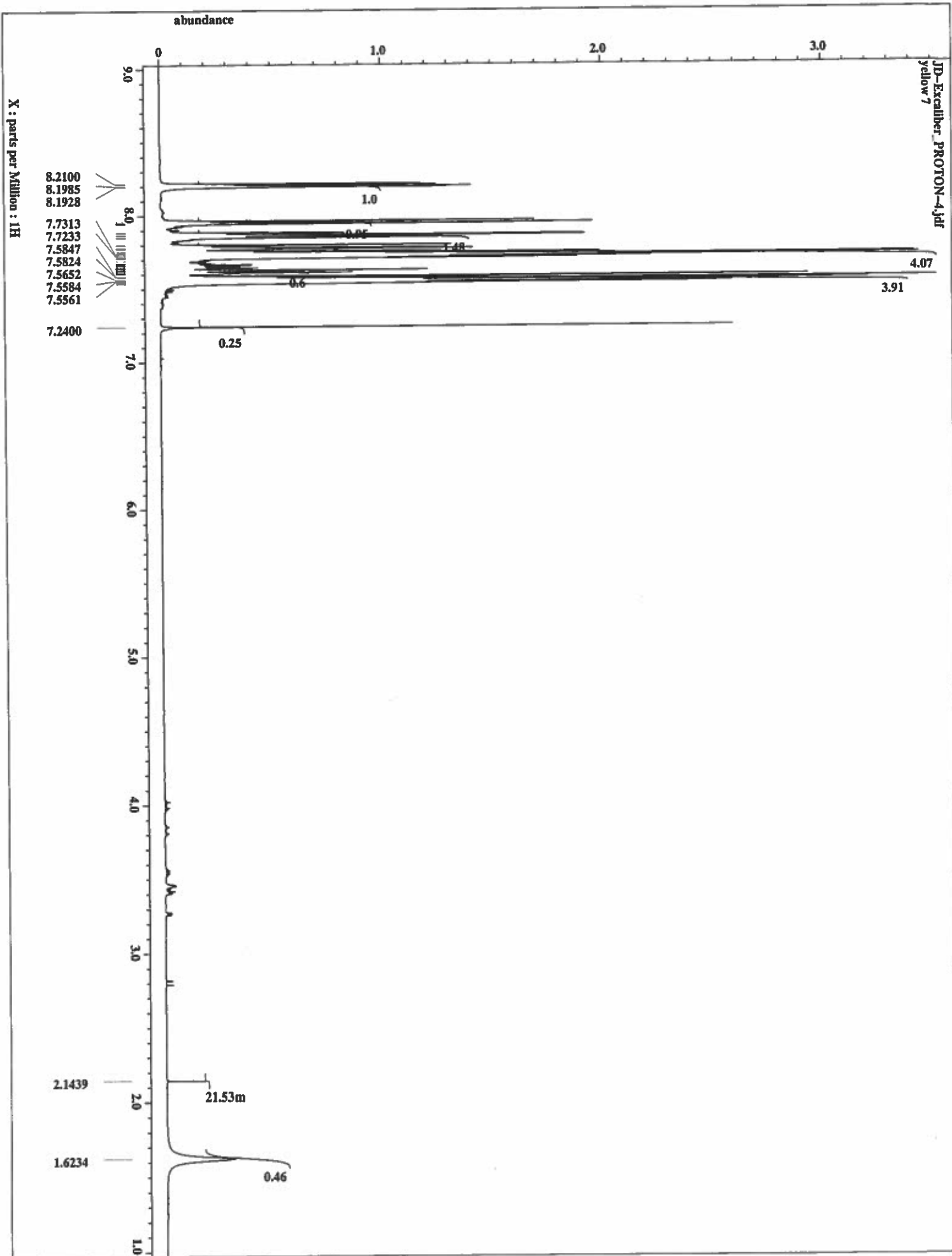


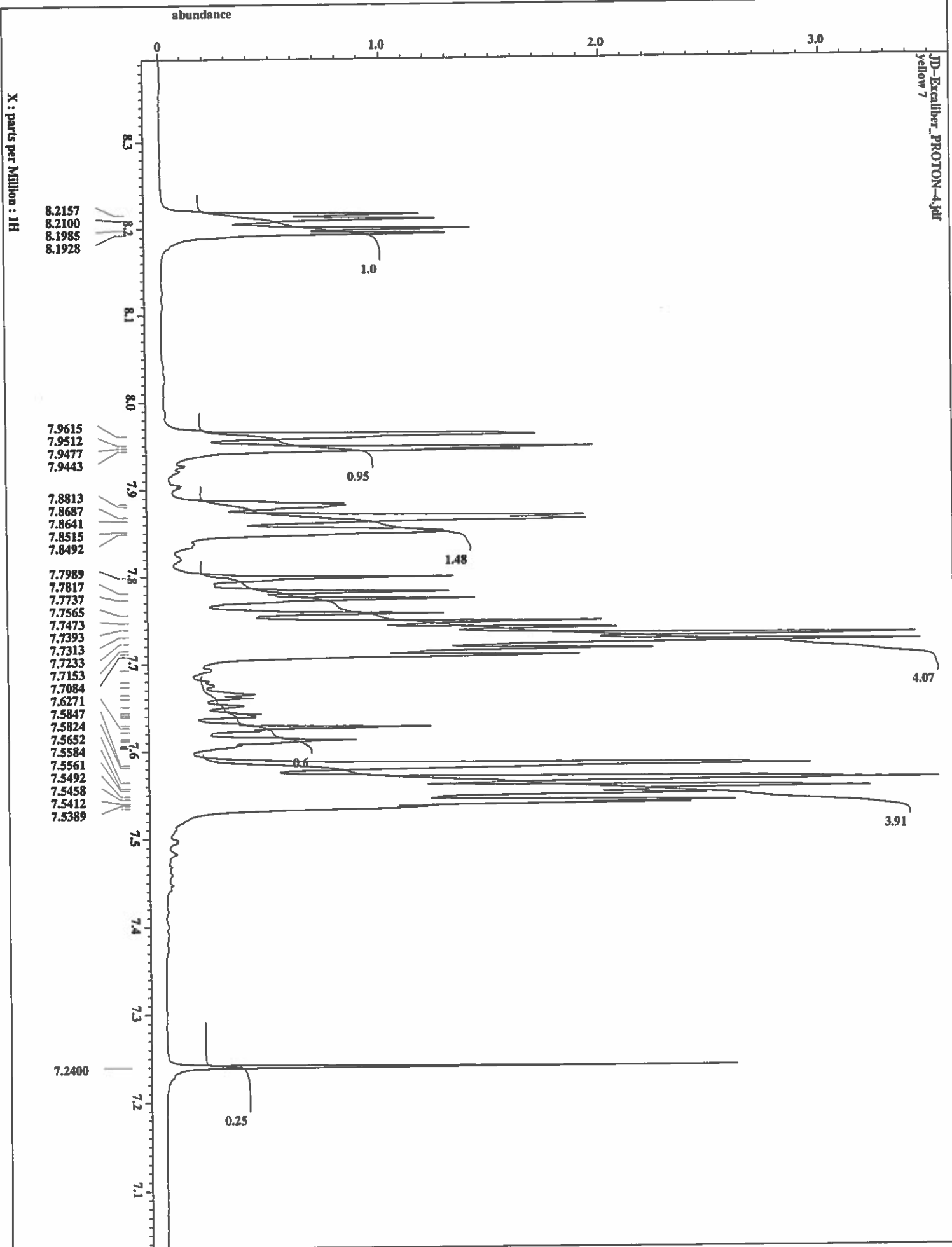
Filename = JD-Excaliber_PROTON-2
 Author = Jim Davis
 Experiment = single_pulse.ex2
 Sample_id = JD-Excaliber
 Solvent = CHLOROFORM-D
 Changer_sample = 9
 Creation_time = 1-JUL-2016 14:28:21
 Revision_time = 1-JUL-2016 14:10:16
 Current_time = 1-JUL-2016 14:10:16

 Comment = yellow 7
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 1H
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECX500

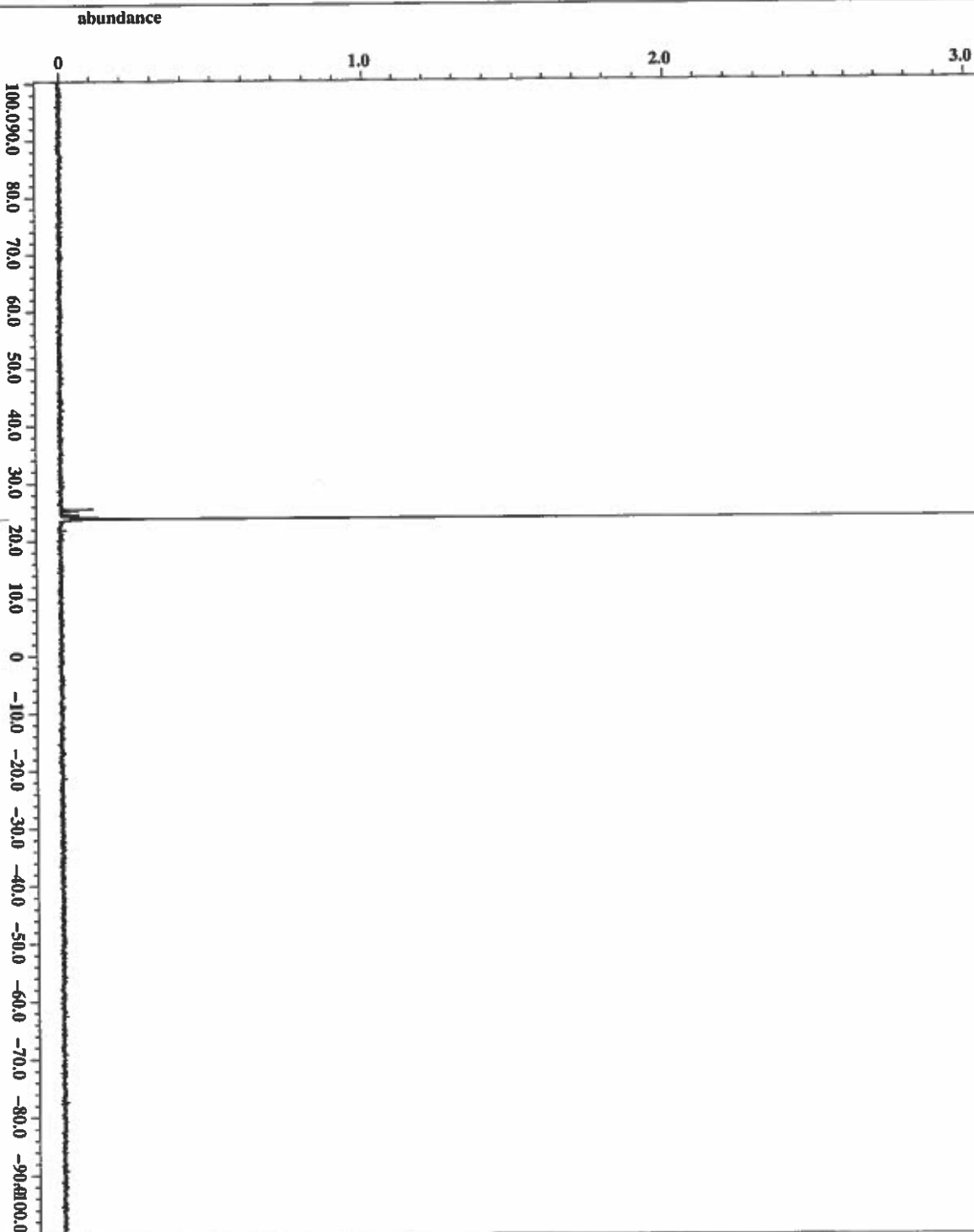
 Field_strength = 11.7473579 [T] (500 [MH
 X_acq_duration = 1.74587904 [s]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.57277737 [Hz]
 X_sweep = 9.38438438 [kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 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 = 13.35 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_axn = 4 [dB]
 X_pulse = 6.675 [us]
 Tr1_mode = Off
 Tr1_preset = FALSE
 Dente_preset = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 40
 Relaxation_delay = 4 [s]
 Repetition_time = 5.74587904 [s]
 Temp_get = 22.5 [C]





JD-Excaliber_slot9_PHOSPHORUS-2.jdt
Yellow 7



X : parts per Million : 31P

23.8576

```

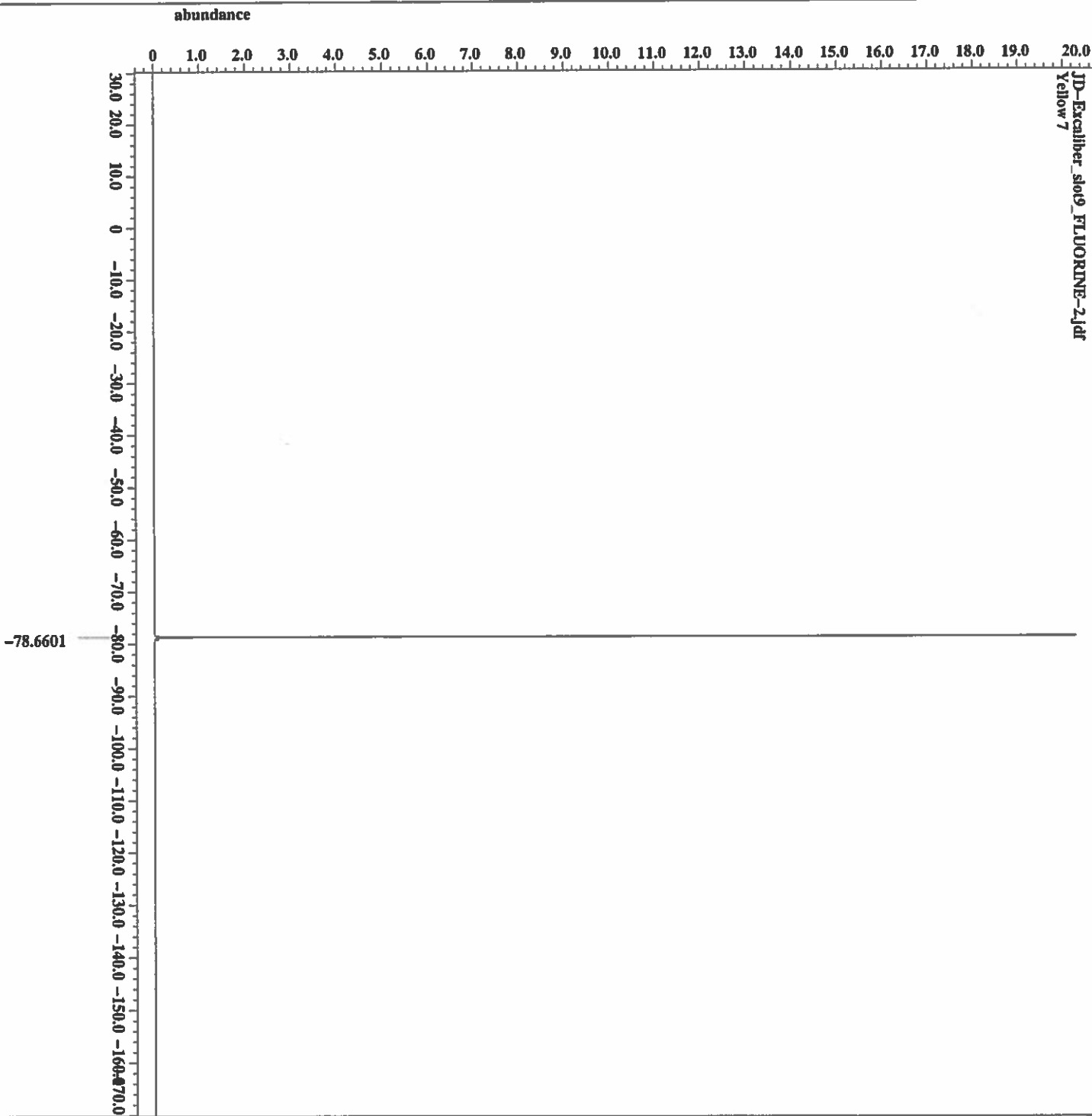
Filename      JD-Excaliber_slot9_PH
Author        Jim Davis
Experiment     single_pulse_dec
Sample_id      S#678612
Solvent        CHLOROFORM-D
Charger_sample 9
Creation_time  1-JUL-2016 19:21:40
Revision_time  1-JUL-2016 19:03:35
Current_time   1-JUL-2016 19:03:35

Comment
Data_format   = Yellow 7
Dlm_size       = 1D COMPLEX
Dlm_title      = 26214
Dlm_units      = 31P
Dimensions     = [ppm]
Site           = X
Spectrometer   = ECA 500
               = 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]
Xr_domain      1H
Xr_freq        500.15991521 [MHz]
Xr_offset       5.0 [ppm]
Clipped        FALSE
Mod_return      1
Scans           256
Total_scans     256

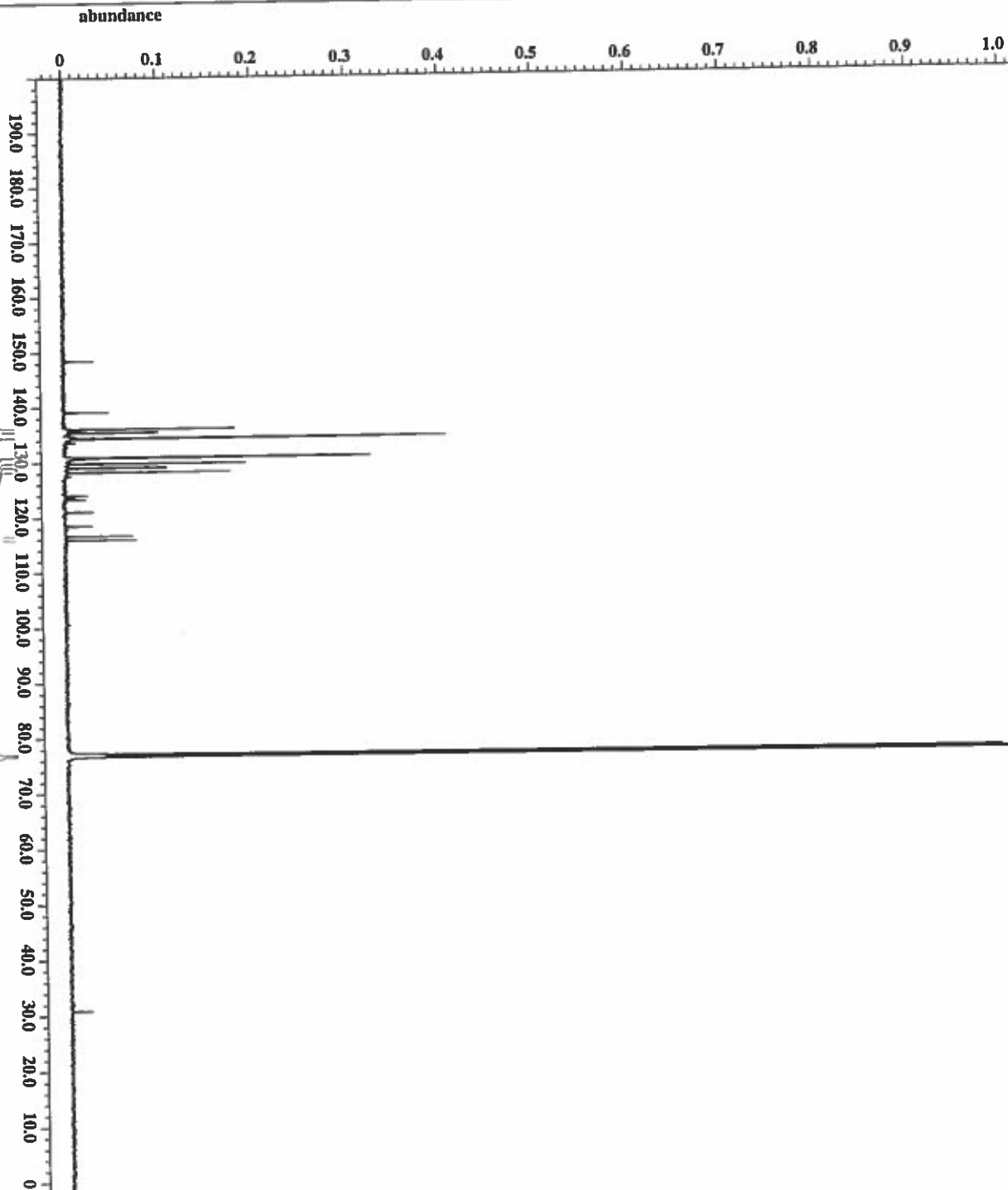
X_90_width     14 [us]
X_acq_time      0.64487424 [s]
X_angle        30 [deg]
X_atn          3 [dB]
X_pulse        4.66666667 [us]
Xr_atn_dec     20.5 [dB]
Xr_atn_noe     20.5 [dB]
Xr_noise       WALTZ
Decoupling      TRU2
Initial_wait    1 [s]
Noe            1 [s]
Noe_time        TRU2
Recvr_gain      2 [s]
Relaxation_delay 2 [s]
Repetition_time 2.64487424 [s]
Temp_get       23.6 [dC]

```



filname	=	jm-Excelsiber_slot9_fr
author	=	Jim Davis
Experiment	=	single_pulse.sw2
Sample_id	=	S#574463
Solvent	=	CHLOROFORM-D
Charger_sample	=	9
Creation_time	=	1-JUL-2016 16:17:54
Revision_time	=	1-JUL-2016 15:59:49
Current_time	=	1-JUL-2016 15:59:49
Comment	=	Yellow 7
Data_format	=	ID COMPLEX
Dim_size	=	52438
Dim_title	=	19F
Dim_units	=	[ppm]
Dimensions	=	X
Site	=	ECA 500
Spectrometer	=	JNM-ECA500
P1eq_strength	=	11.7473579 [w] (500 [kHz
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	=	1.7993885 [Hz]
X_sweep	=	117.9245283 [kHz]
1st_domain	=	19F
1st_freq	=	470.62046084 [MHz]
1st_offset	=	19F
1st_domain	=	19F
1st_freq	=	470.62046084 [MHz]
1st_offset	=	5 [ppm]
Clipped	=	FALST
Mod_return	=	1
Scans	=	16
Total_scans	=	16
X_90_width	=	15.7 [us]
X_acq_time	=	0.55574528 [s]
X_angle	=	45 [deg]
X_atn	=	4 [dB]
X_pulse	=	7.85 [us]
1st_mode	=	OFF
1st_mode	=	OFF
Dante_presat	=	FALST
Initial_wait	=	1 [s]
Recvr_gain	=	46
Relaxation_delay	=	4 [s]
Repetition_time	=	4.55574528 [s]
Temp_set	=	22.6 [deg]

JD-Excaliber_slot9_CARBON-2,1d1
Yellow 7



X : parts per Million : 13C



Filename JD-Excaliber_slot9_CA
 Author Jim Davis
 Experiment single-pulse-dec
 Sample_id 88614981
 Solvent CHLOROFORM-D
 Change sample 9
 Creation time 2-JUL-2016 19:50:47
 Revision time 2-JUL-2016 19:32:35
 Current time 2-JUL-2016 19:32:35

 Comment Yellow 7
 Data format 1D COMPLEX
 Data size 26214
 Data title 13C
 Dimensions [ppm]
 Site X
 Spectrometer ECA 500
 JNM-ECA500

 Field strength 11.763579 [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 3100
 Total_scans 3100

 X_90_width 12.55 [us]
 X_acq_time 0.83361792 [s]
 X_angle 30 [deg]
 X_atn 6 [dB]
 X_pulse 4.18333333 [us]
 Xt_atn_dec 20.5 [dB]
 Xt_atn_noe 20.5 [dB]
 Xt_noise WALTZ
 Decoupling TRUE
 Initial_wait 1 [s]
 Noe_time TRUE
 Noe_time 2 [s]
 Recvr_gain 60
 Relaxation_delay 2.63361792 [s]
 Repetition_time 23.8 [dc]
 Temp_get

Davis Collaboration

Method: Stenson_100MeOH

Tune File: C:\Xcalibur\methods\Stenson\JerryKoncarsSug
Neg to Pos.LITQTune

Spatula-tip of Samples dissolved in 1mL pure MeOH then
diluted 10000x with MeOH

Notebook: Collaborators Page 105

Compound 5

49-A
Before Δ

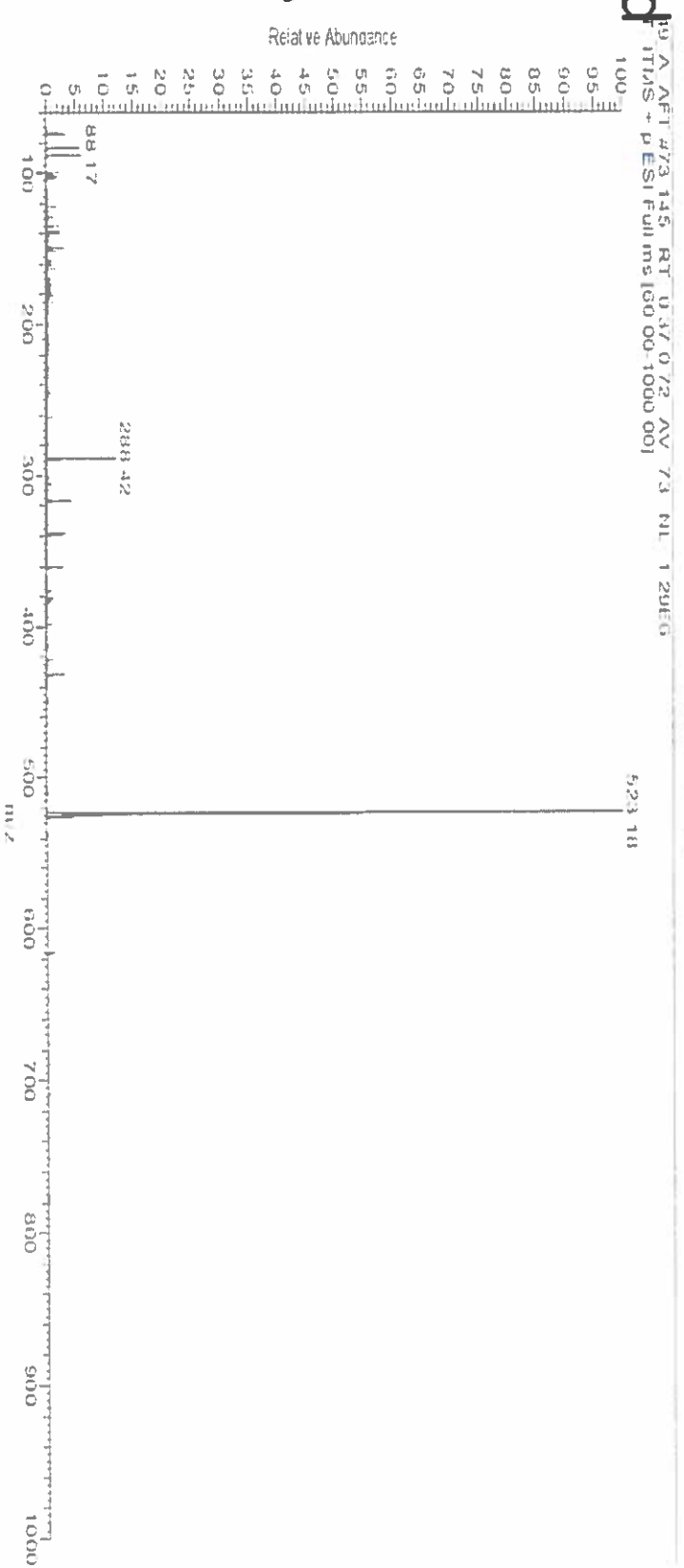
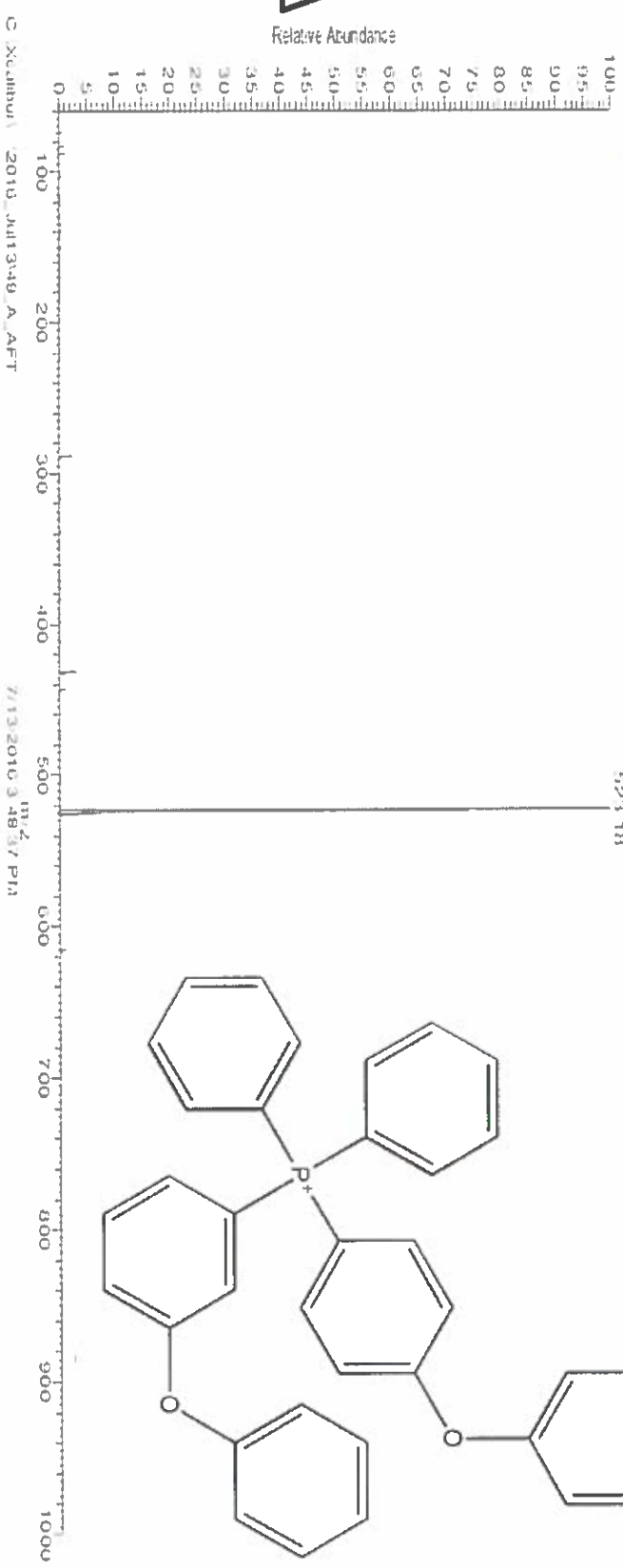
523.18

expected

49-A
After Δ

C:\MSDCHEM\DATA\2016_Jul19\4_A
E-A #73-114 RT 0.37-0.72 AV 7.3 NL 5.5176
TITMS + P ESI Full ms [60.00-1000.00]

7/13/2016 4:07:20 PM



Compare MS

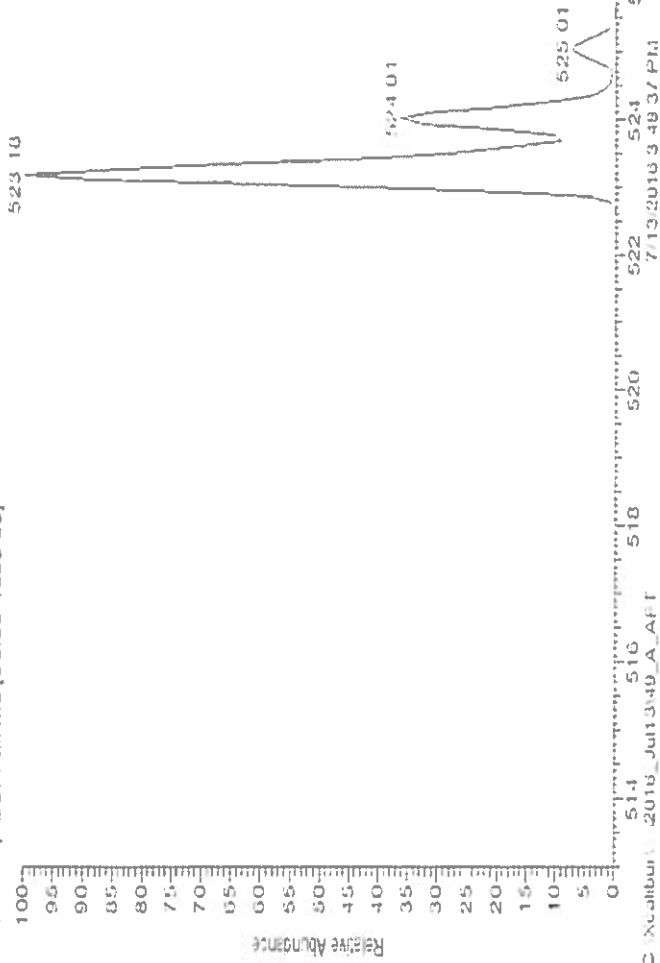
49-A
Before Δ

523.18
expected

49-A
After Δ

C:\Xcalibur Data\Davis\2016_Jul13\49-A

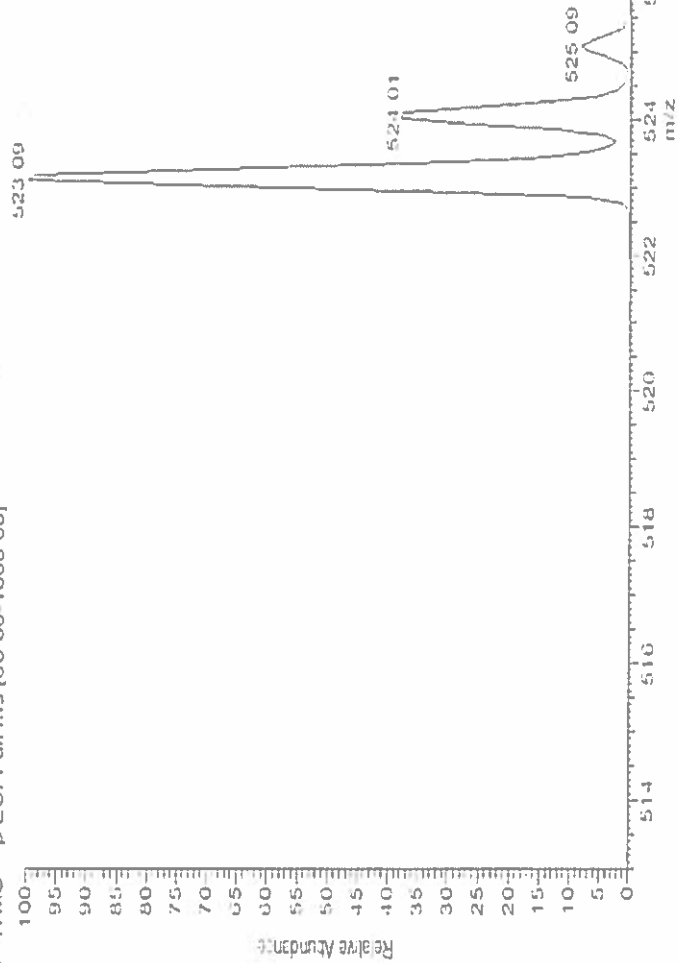
EA #68-181 RT: 0.35-0.90 AV 114 NL: 4 19E6
T: ITMS + p ESI Full ms (50.00-1000.00)



C:\Xcalibur\2016_Jul13\49-A_AFI

49-A_AFI #68-181 RT: 0.34-0.90 AV 114 NL: 9 71E5

T: ITMS + p ESI Full ms (50.00-1000.00)

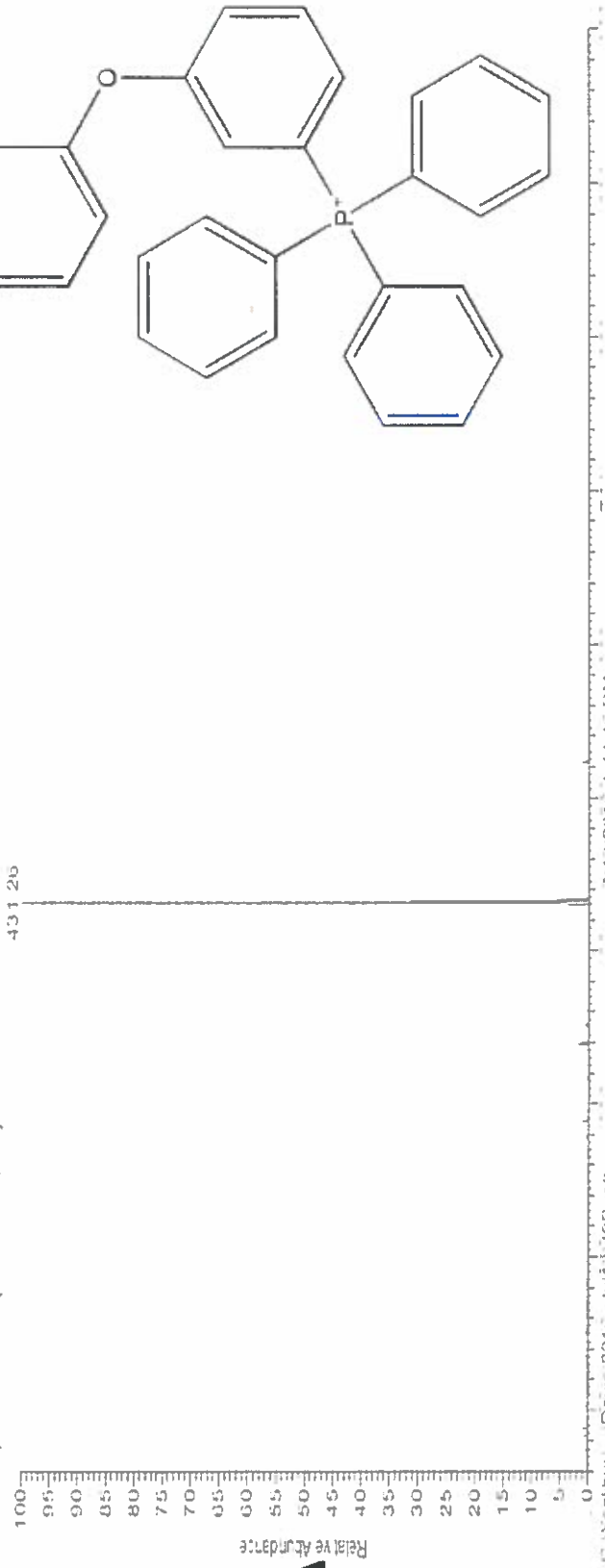


Compound

49-B
Before Δ

C:\Xcalibur\Data\Davis\2016_Jun\349_B

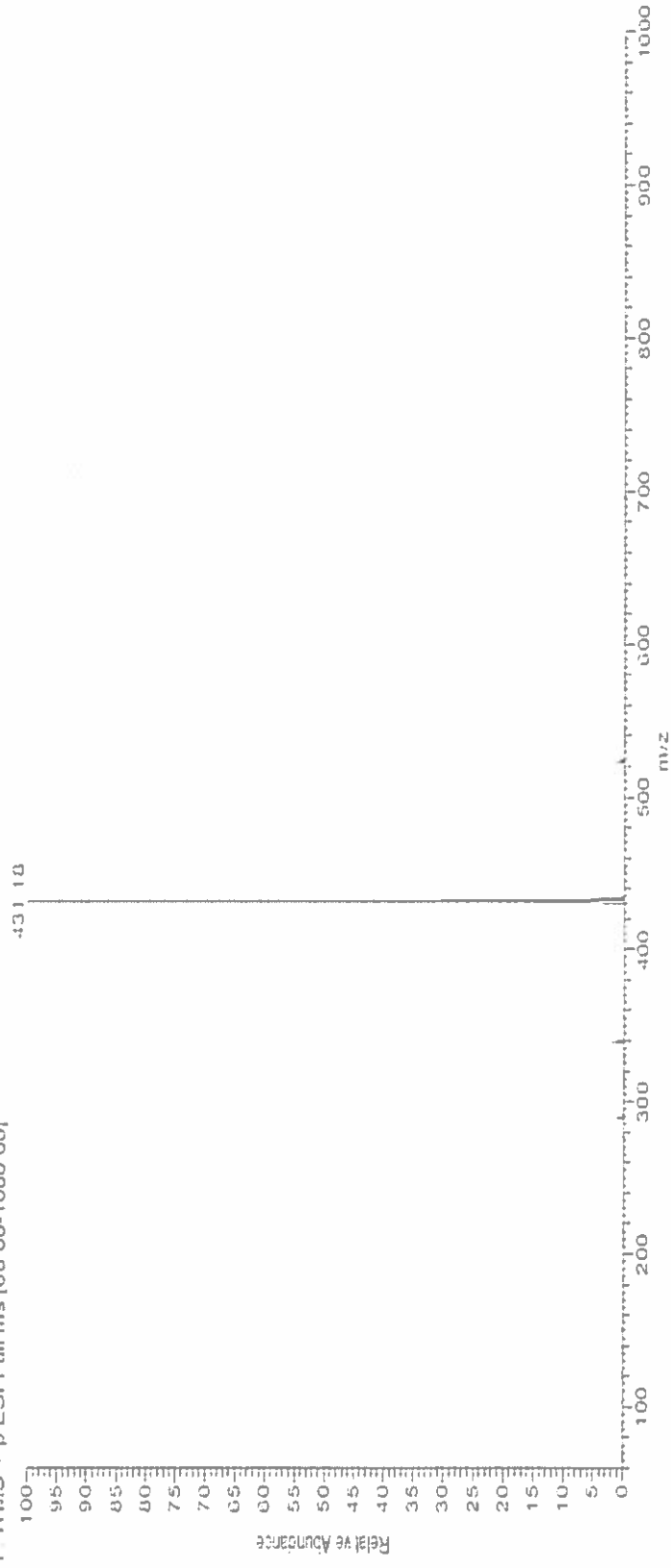
49-B #75-152 RT: 0.38-0.76 AV: 78 TIC: 5.57E9
T: ITMS + p ESI Full ms (60 00-1000 00)



431.16
expected

C:\Xcalibur\Data\Davis\2016_Jul\349B_at

49B at #73-145 RT: 0.37-0.72 AV: 73 TIC: 1.30E7
T: ITMS + p ESI Full ms (60 00-1000 00)



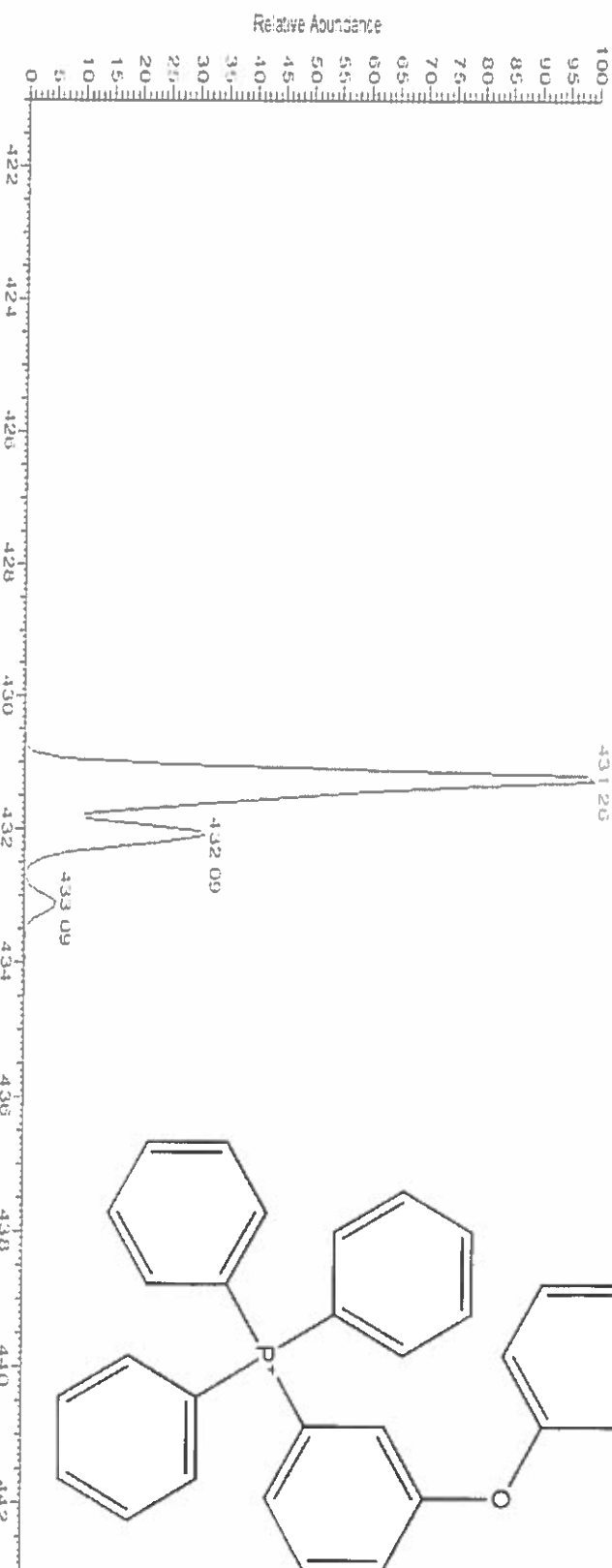
49-B
After Δ

10 U#68-195 RT: 0.35-0.97 AV: 126 HL: 3.98EG
T: 111MS + P ESI Full ms (60.00-1000.00)

49-B
Before Δ

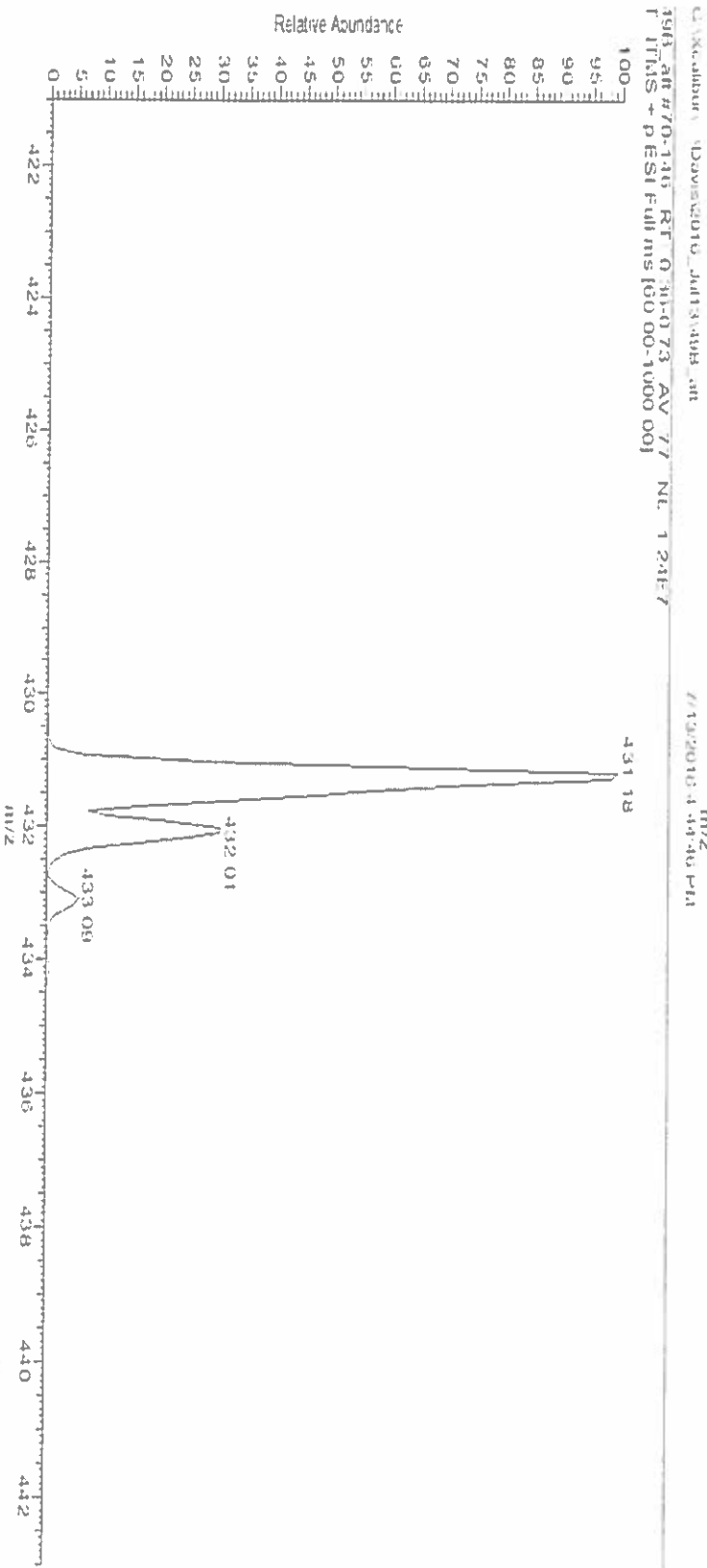
431.16

expected



49-B

After Δ

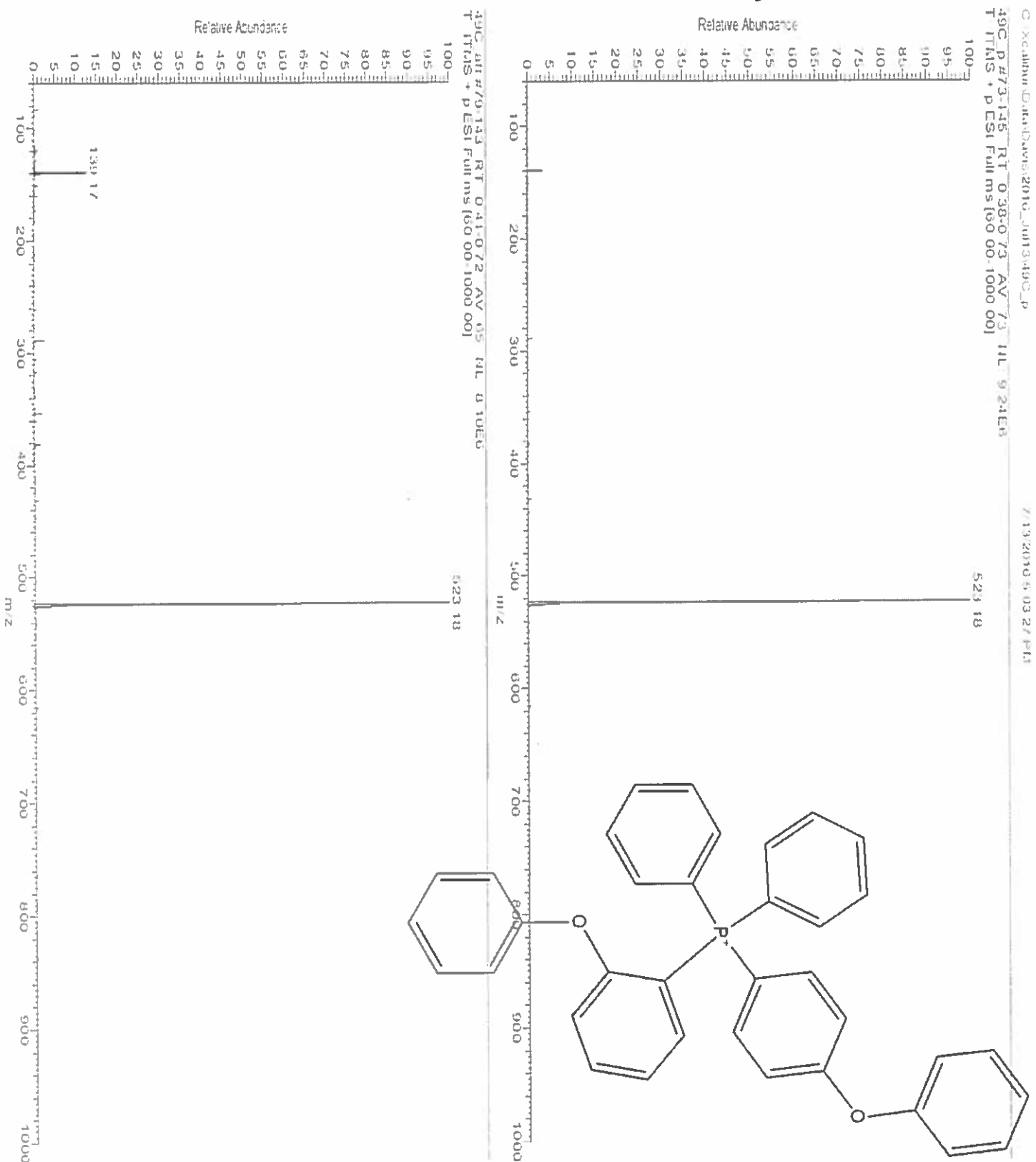


Compound 9

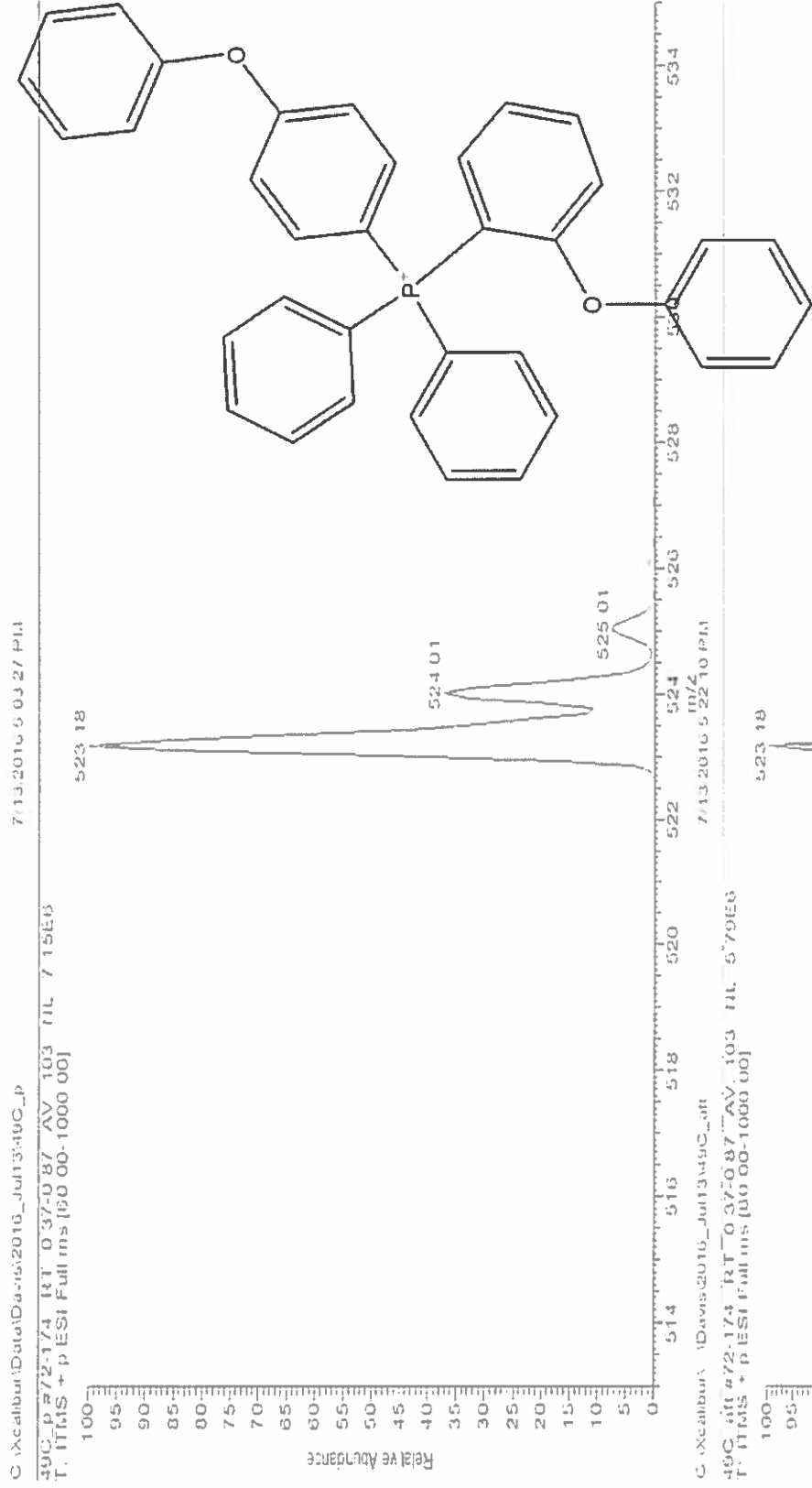
49-C
Before Δ

523.18
expected

49-C
After Δ

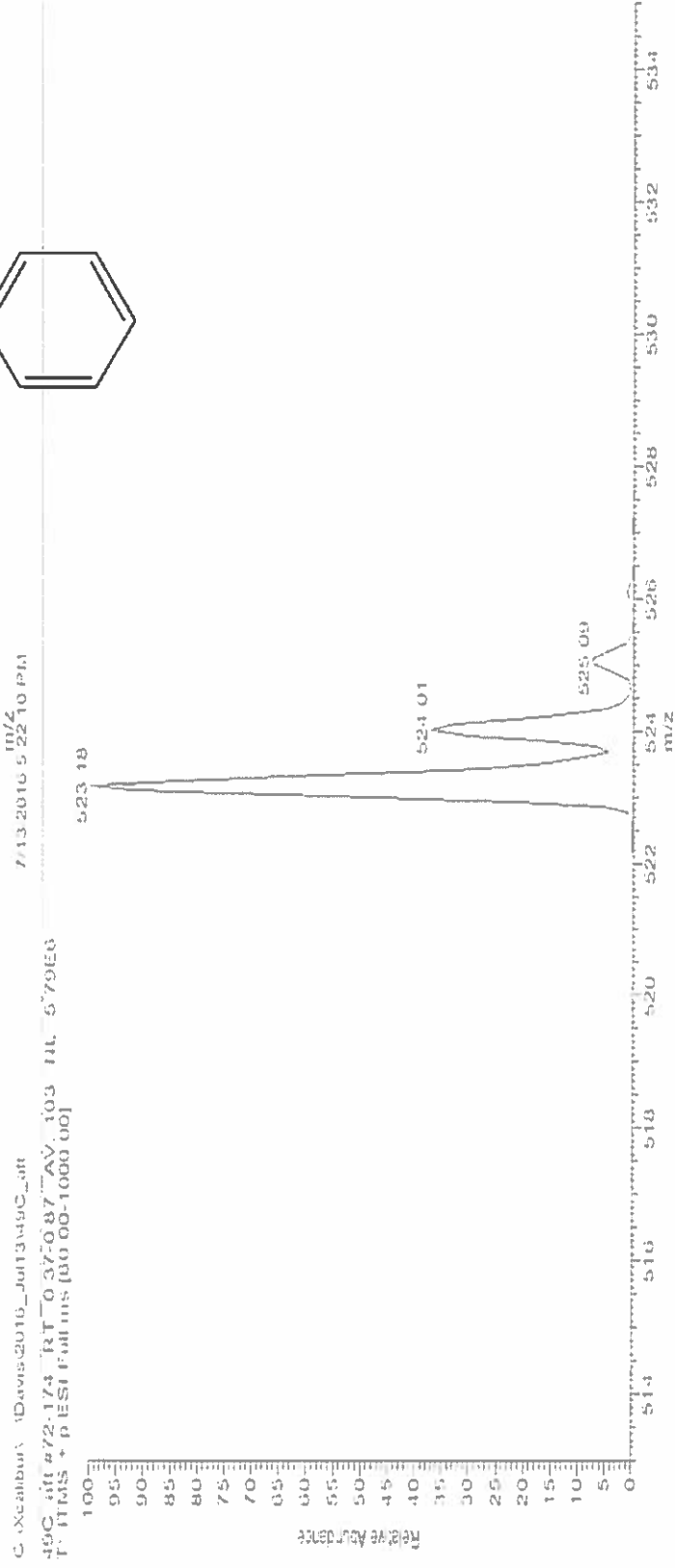


49-C
Before Δ



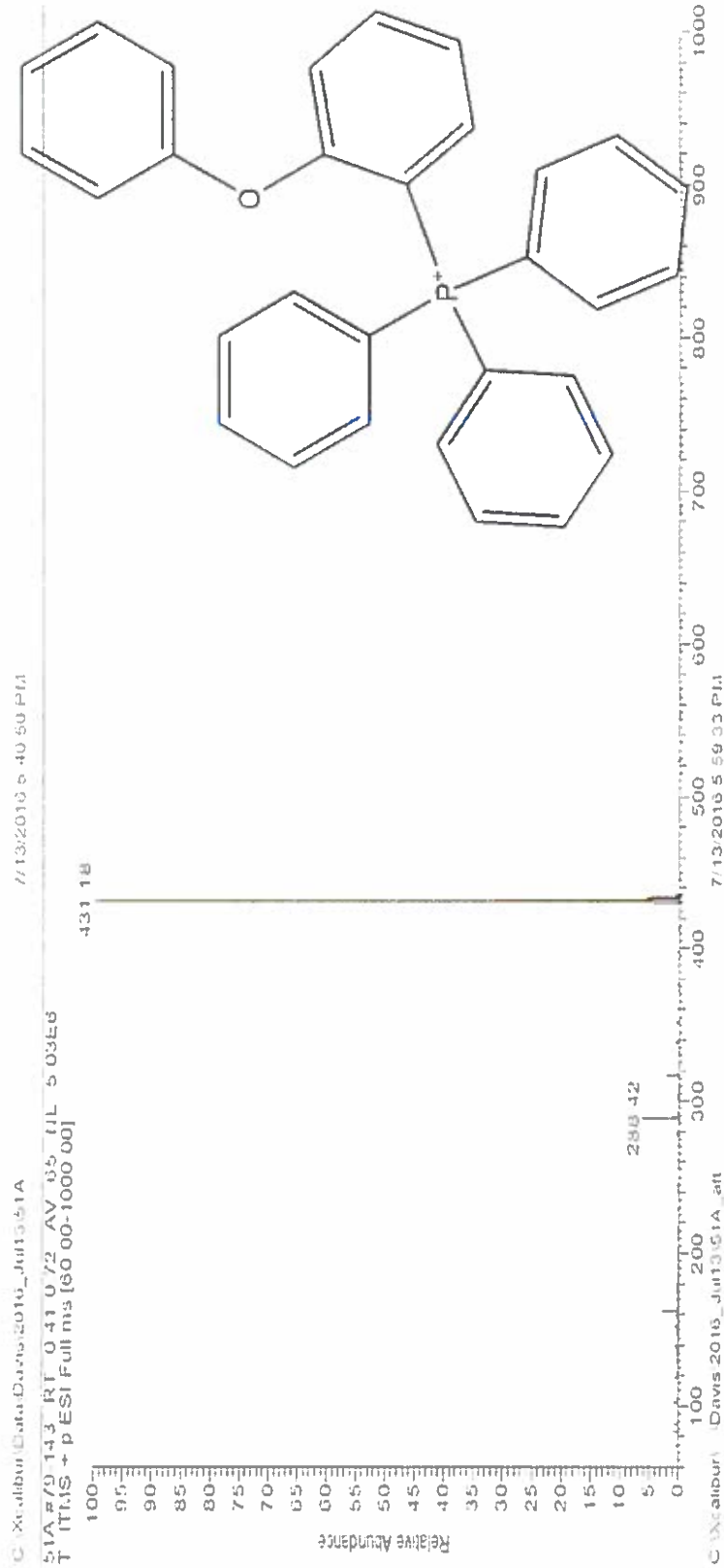
523.18
expected

49-C
After Δ

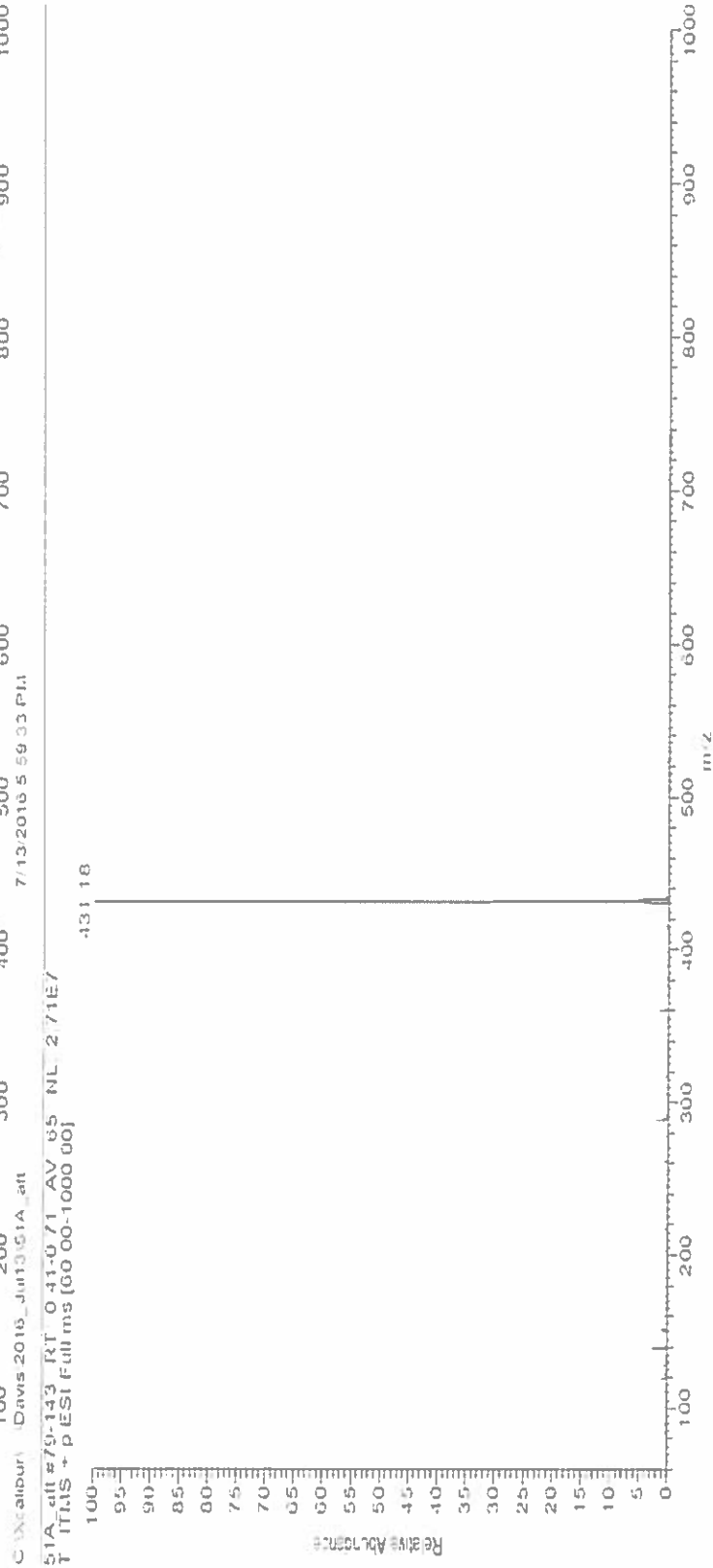


Compound 3

51-A
Before Δ

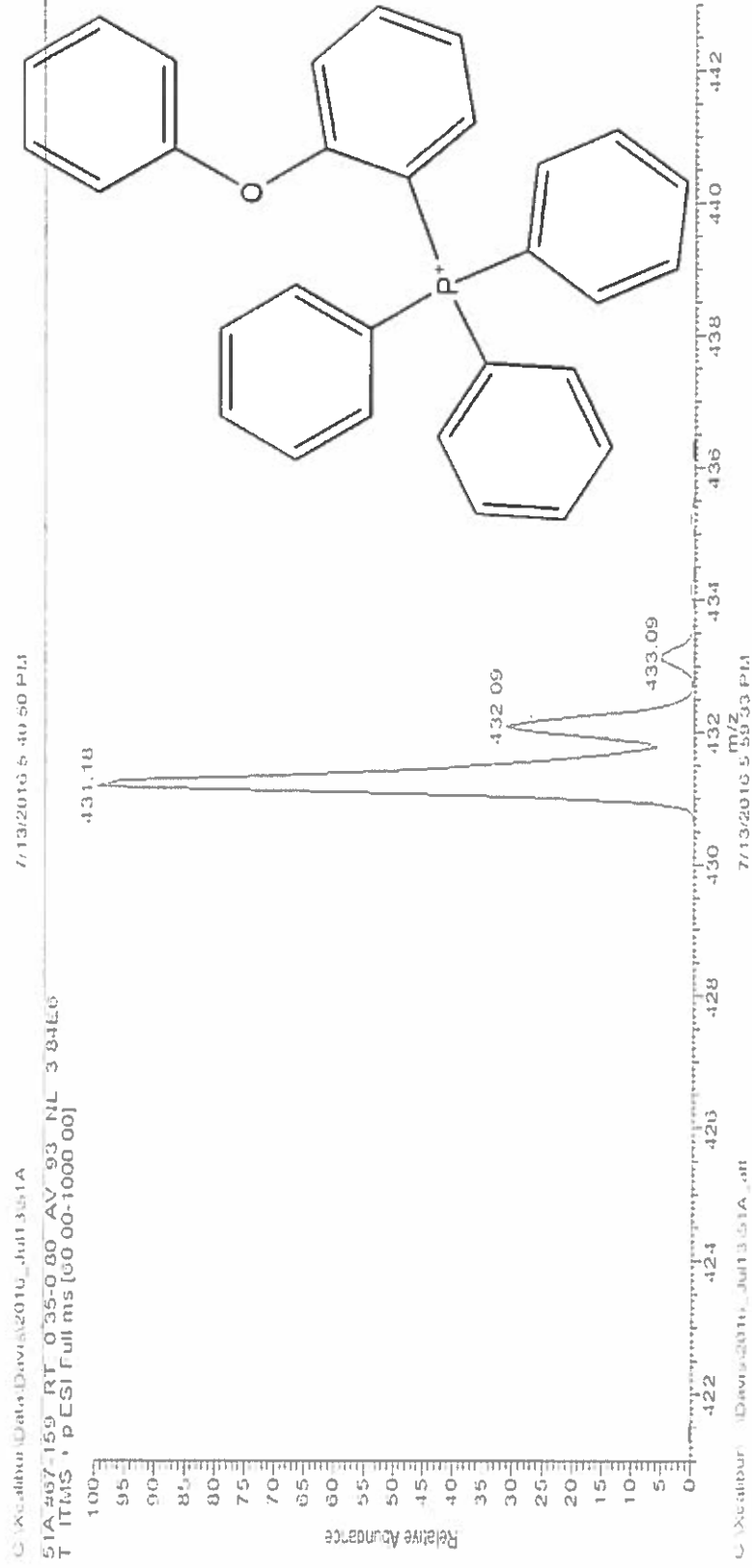


431.16
predicted



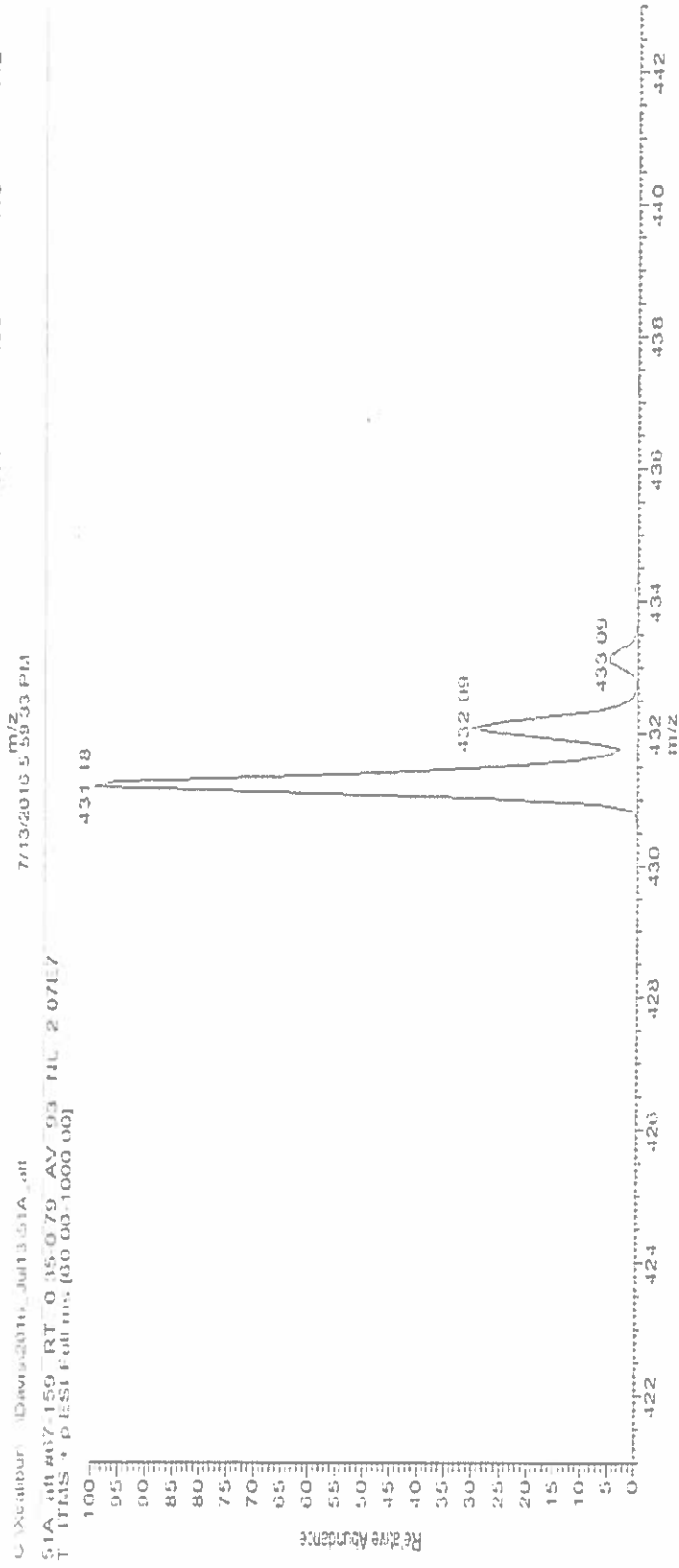
51-A
After Δ

51-A
Before Δ



431.16
predicted

51-A
After Δ

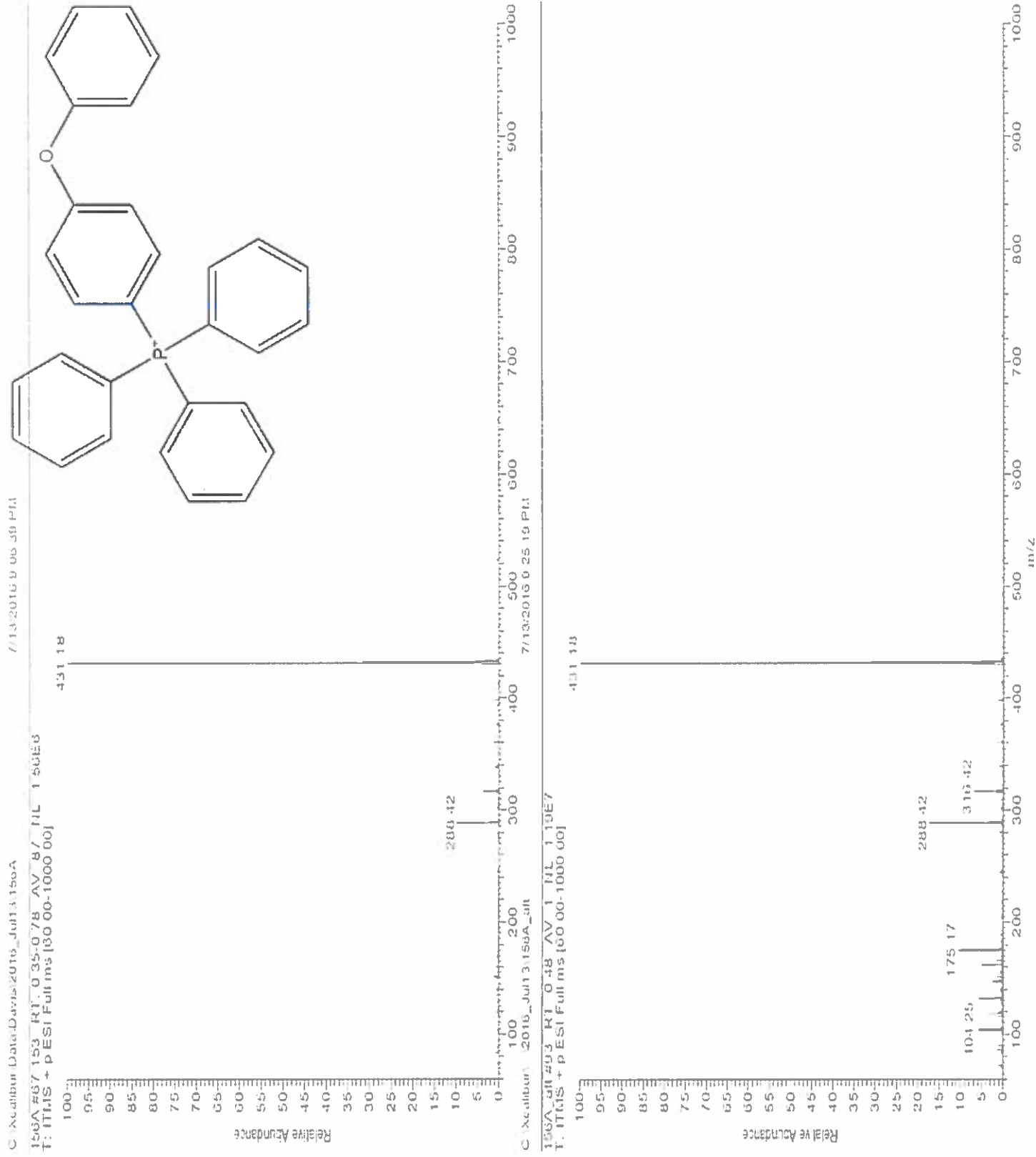


Compound

156-A
Before Δ

431.16
expected

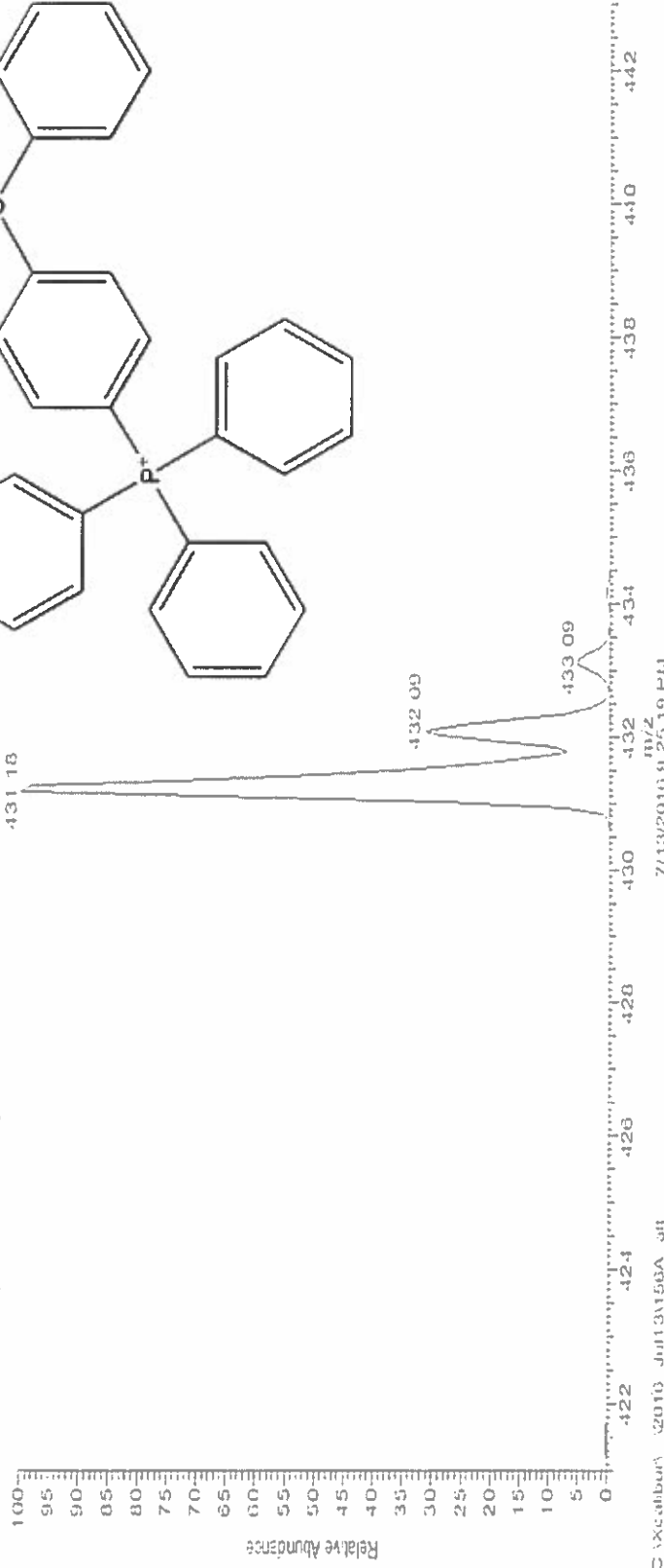
156-A
After Δ



C:\Xcalibur\Data\Davis\2016_Jul13\156A

7/13/2016 9 05 39 PM

156A_#03-164 RT: 0.34-0.84 AV: 101 (IL 1.41E5)
F: ITMS + PESI Full ms [50 00-1000 00]



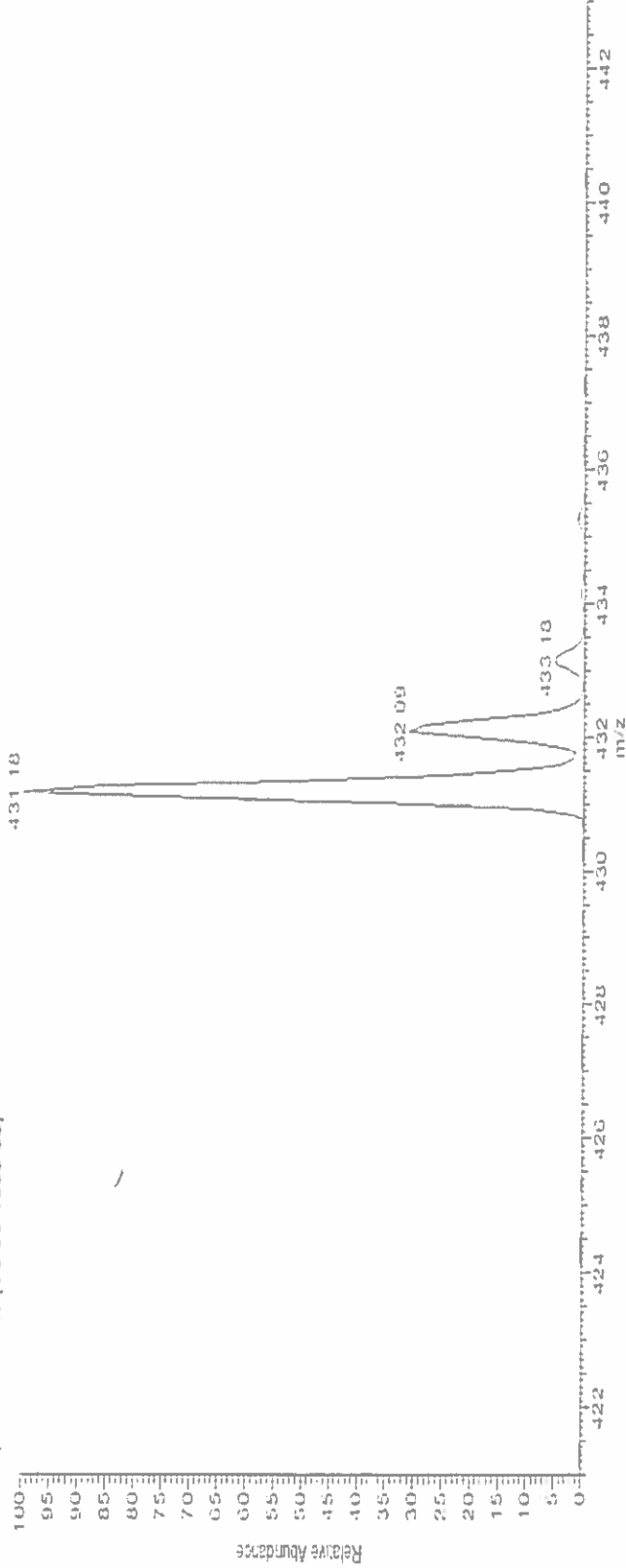
156-A
Before Δ

431.16
expected

C:\Xcalibur\2016_Jul13\156A_sit

7/13/2016 9 25 19 PM

156A_sit #73-211 RT: 0.38-1.05 AV: 139 NL: 4.59E5
F: ITMS + PESI Full ms [50 00-1000 00]

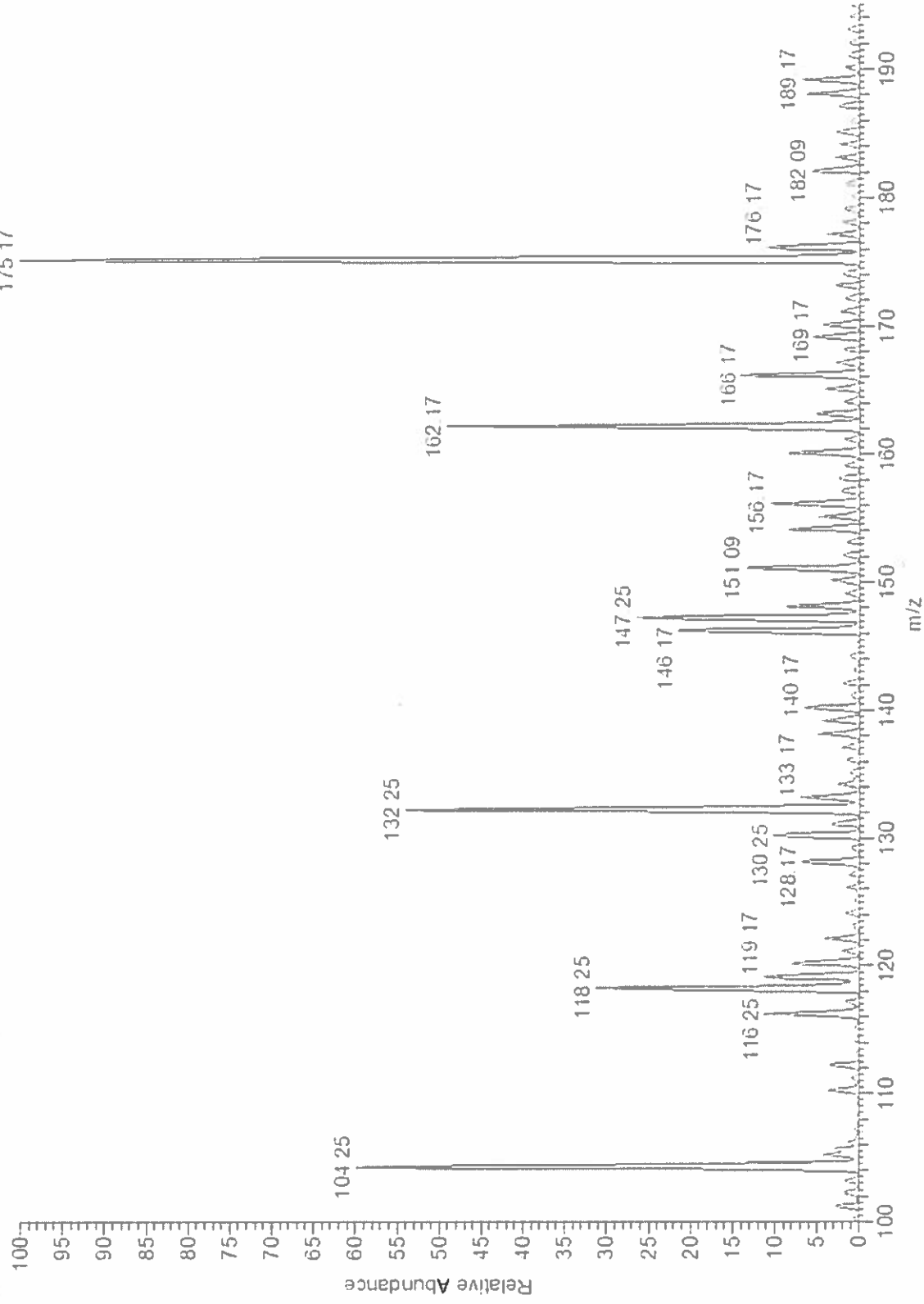


156-A
After Δ

C:\Xcalibur\2016_Jul13\156A_an

7/13/2016 9:25:19 PM

156A_an #93 RT: 0.48 AV: 1 NL: 128E6
T: ITMS + pESI Full ms [60.00-1000.00]



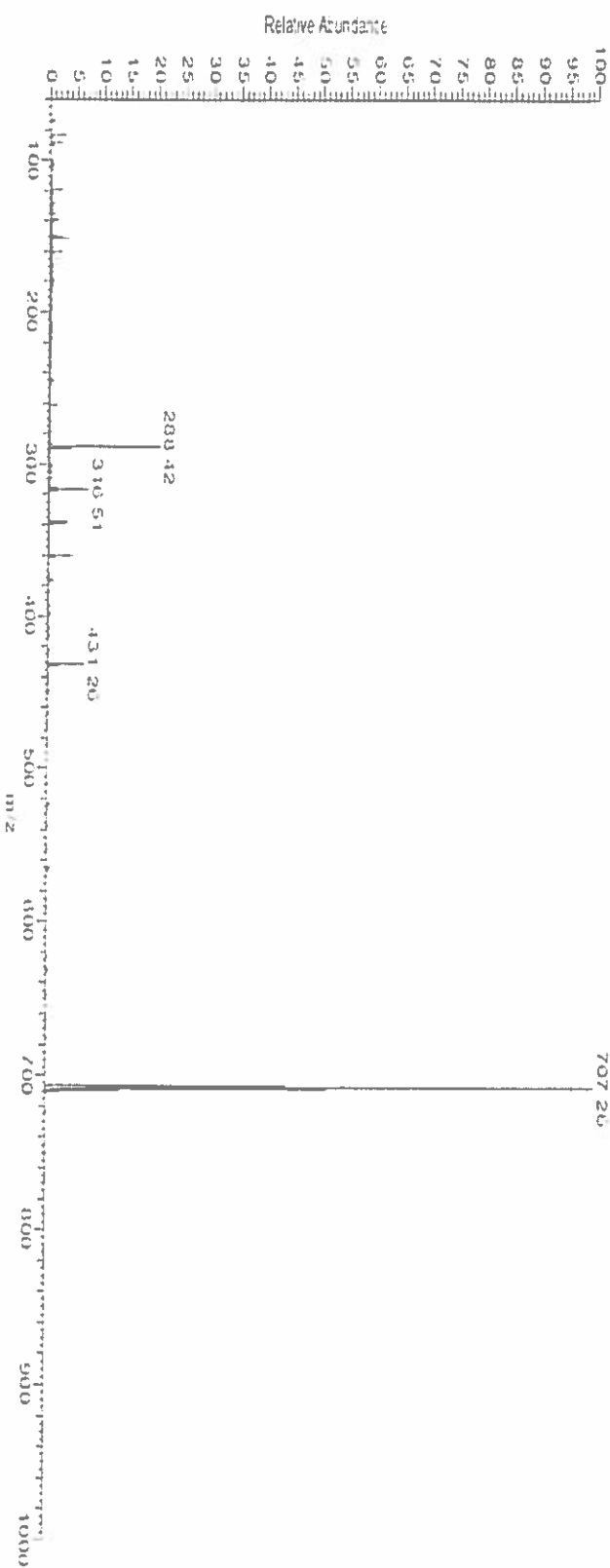
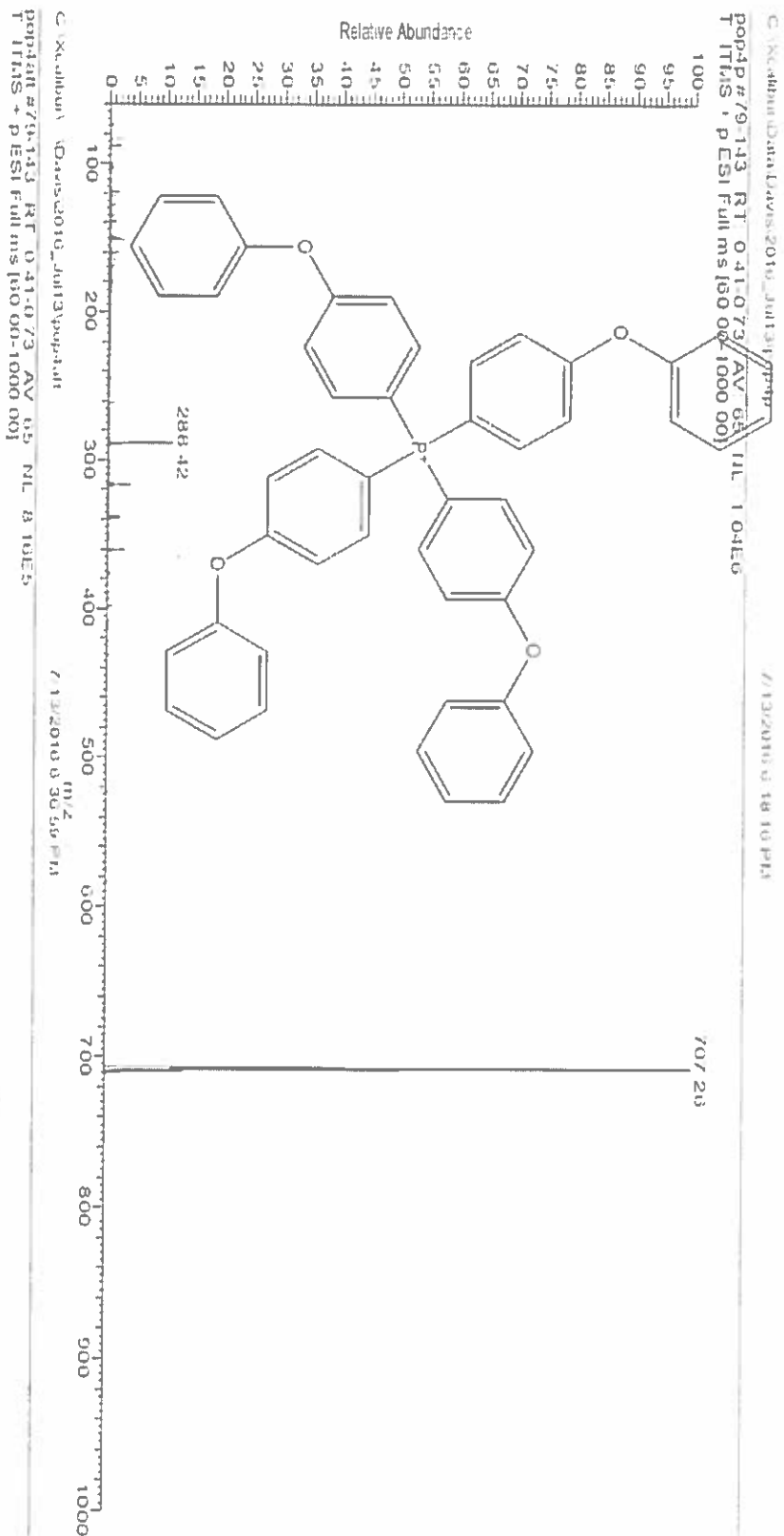
156-A
New Peaks

Compound X

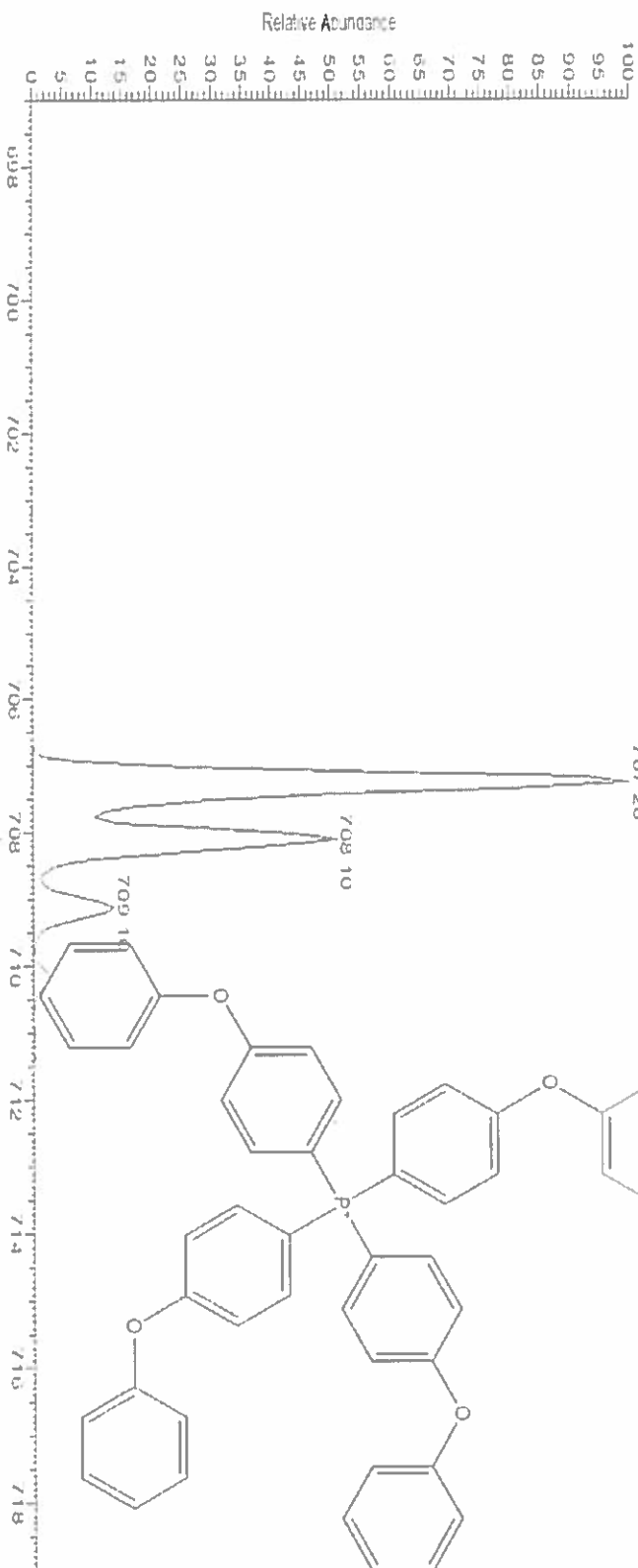
POP4
Before Δ

707.23
expected

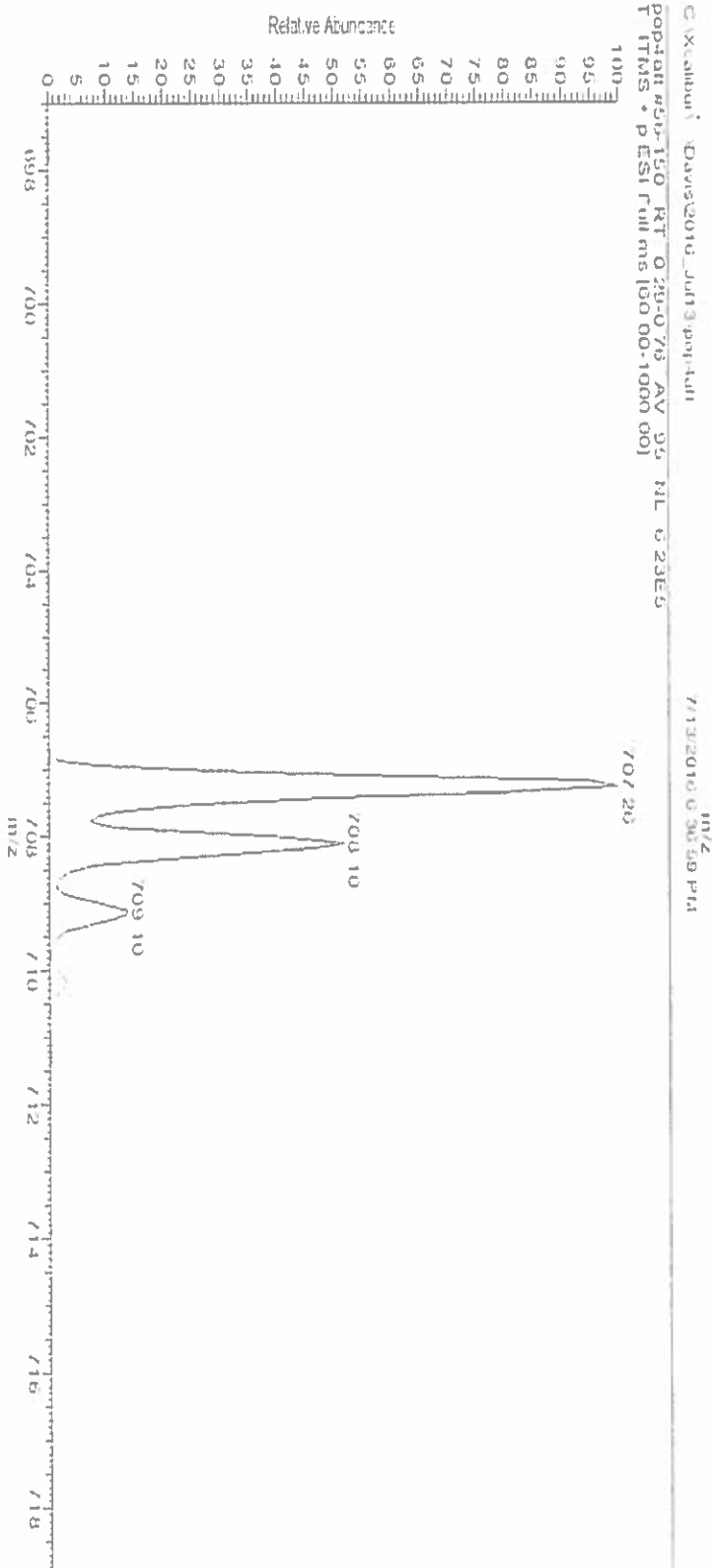
POP4
After Δ



POP4 #60-167 RT 0.31080 AV 98 NL 8 10ES
FTMS + P ESI Full ms (60.00-1000.00)

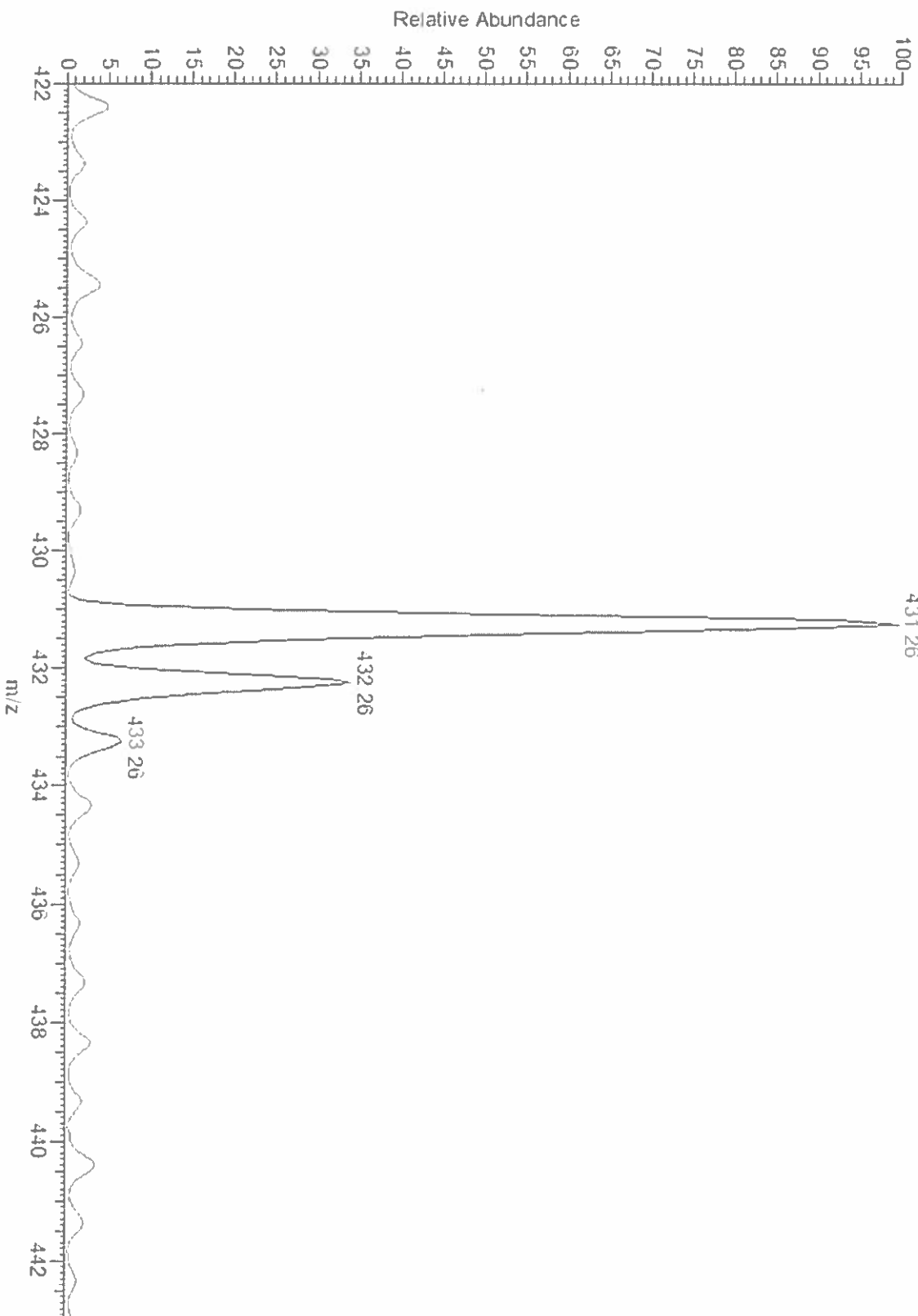


707.23
expected



pop-fall #80-144 RT: 0.41-0.73 AV: 65 NL: 5.45E4
T: ITMS + p ESI Full ms (60 00-1000 00)

POP-4 New Peak

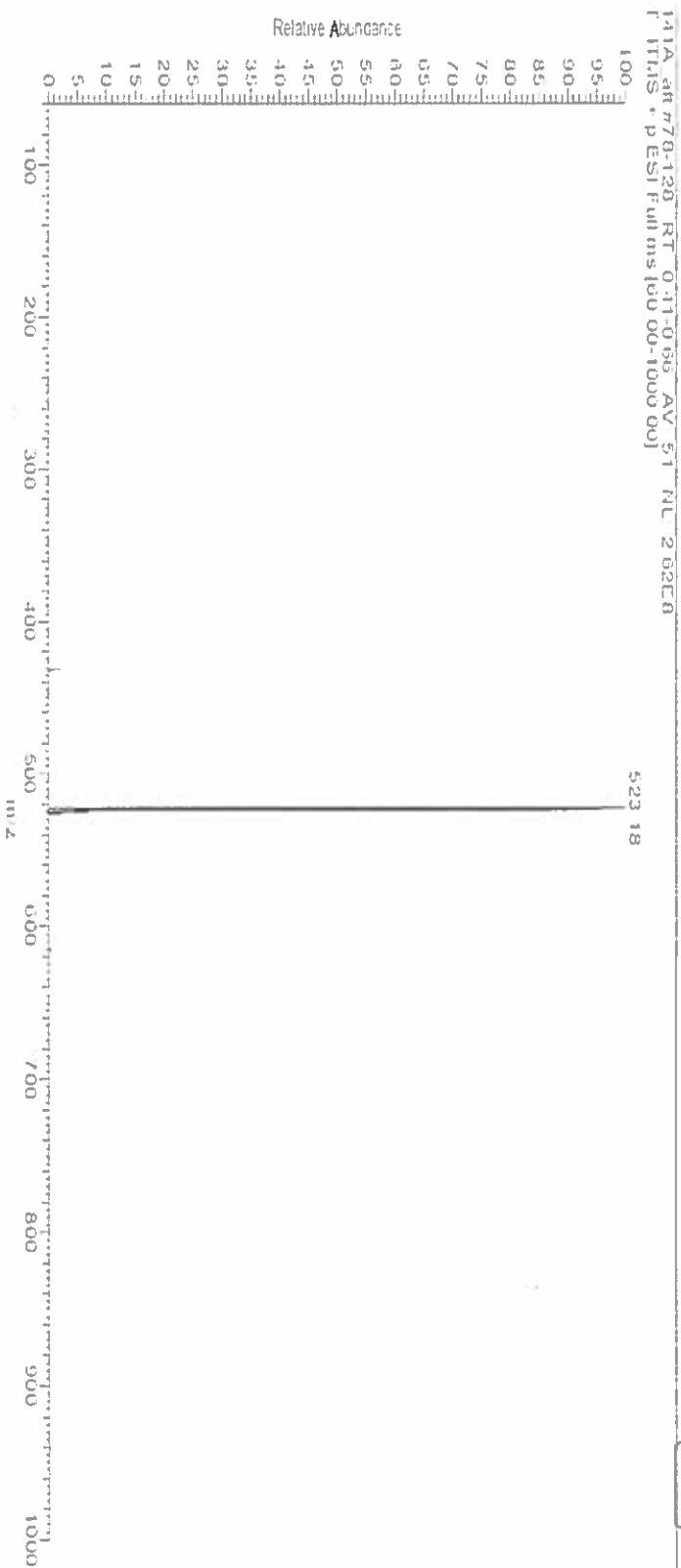
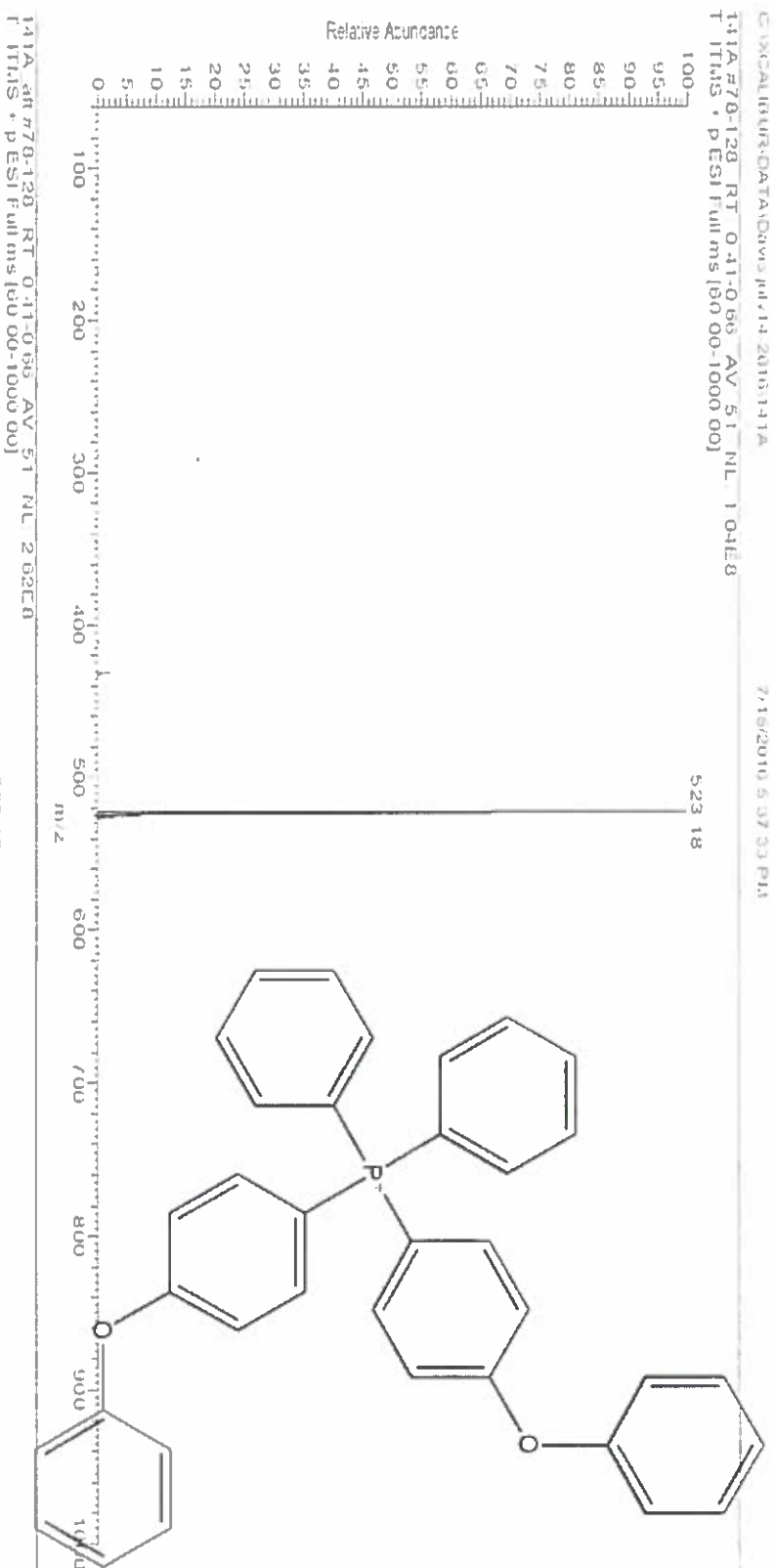


Compound X

141-A
Before Δ

523.18
expected

141-A
After Δ



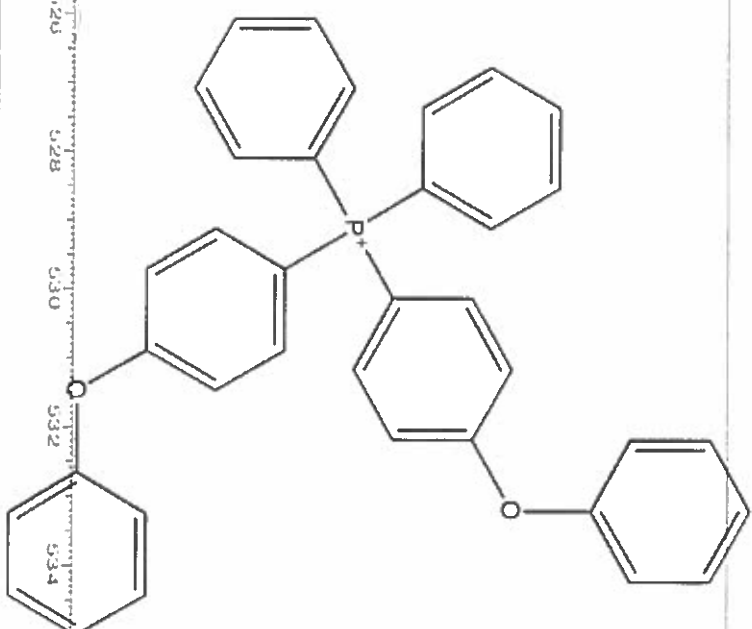
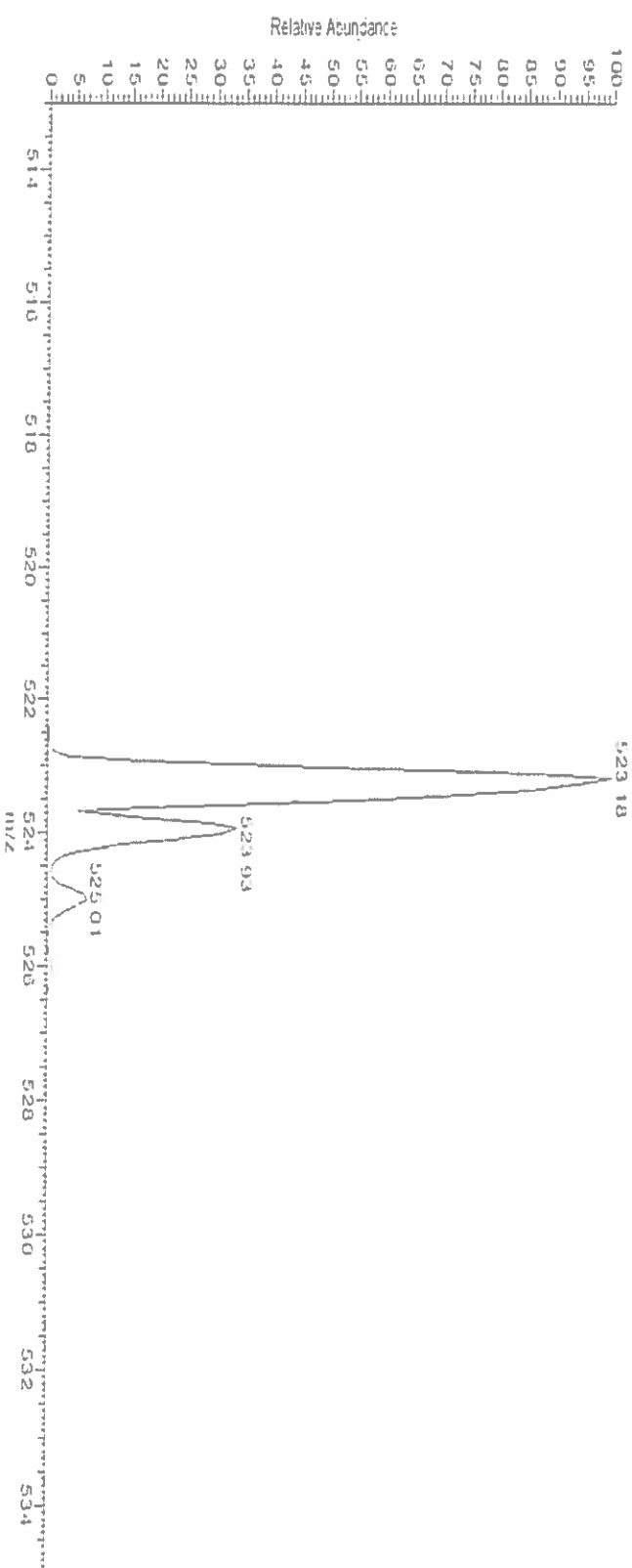
141A#71143 RT: 0.38-0.73 AV: 7.3 NL: 8.41E7
T: ITMS + P-ESI Full ms [60.00-1000.00]141-A
Before Δ

523.18

expected

C:\CALIBUR\ July14\2016\141A.vmr
141A#71143 RT: 0.38-0.73 AV: 7.4 NL: 2.37E8
T: ITMS + P-ESI Full ms [60.00-1000.00]

7/15/2016 5:50:15 PM

141-A
After Δ

Compound

142-A

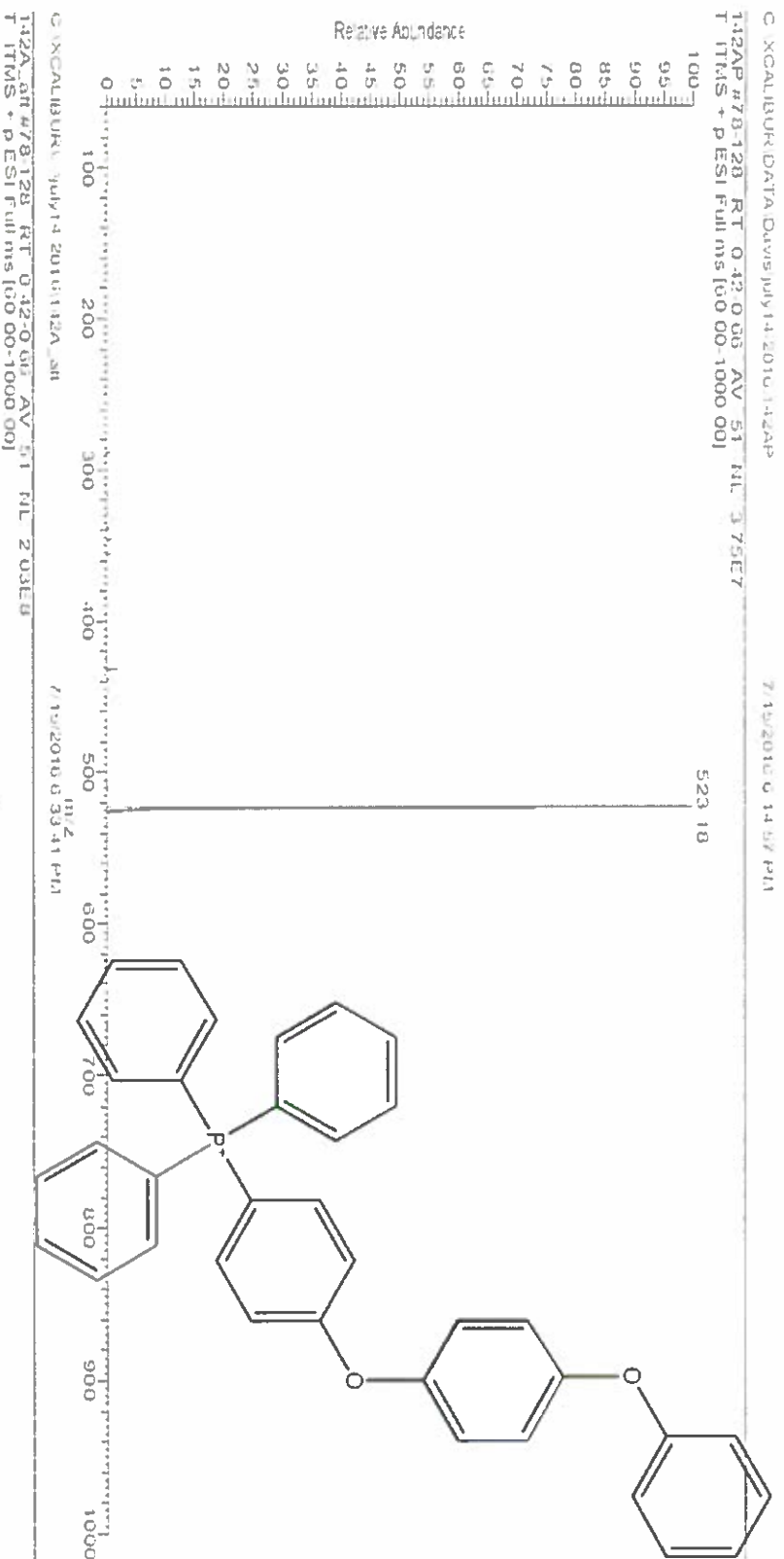
Before Δ

523.18

expected

142-A

After Δ



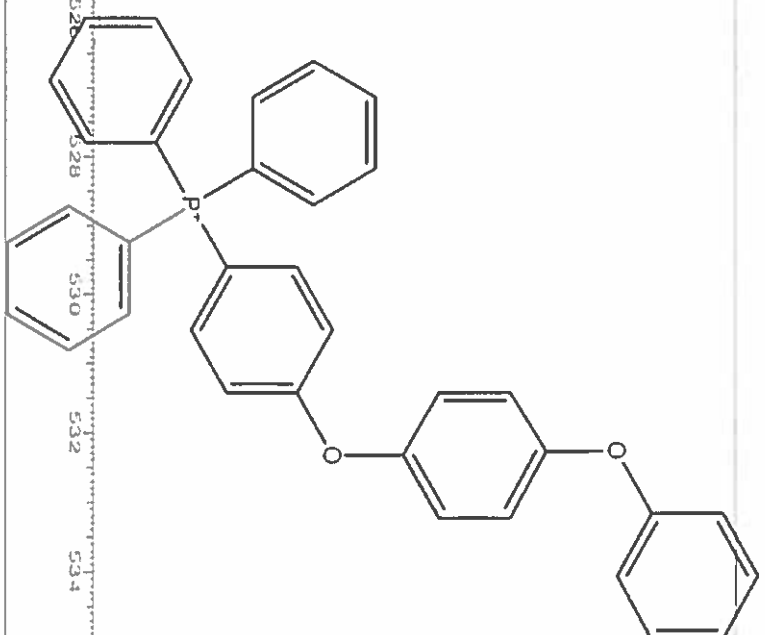
142AP #76-133 RT: 0.41-0.68 AV: 50 NL: 3.40E7
T: ITMS + pESI Full ms (50.00-1000.00)

142-A
Before Δ

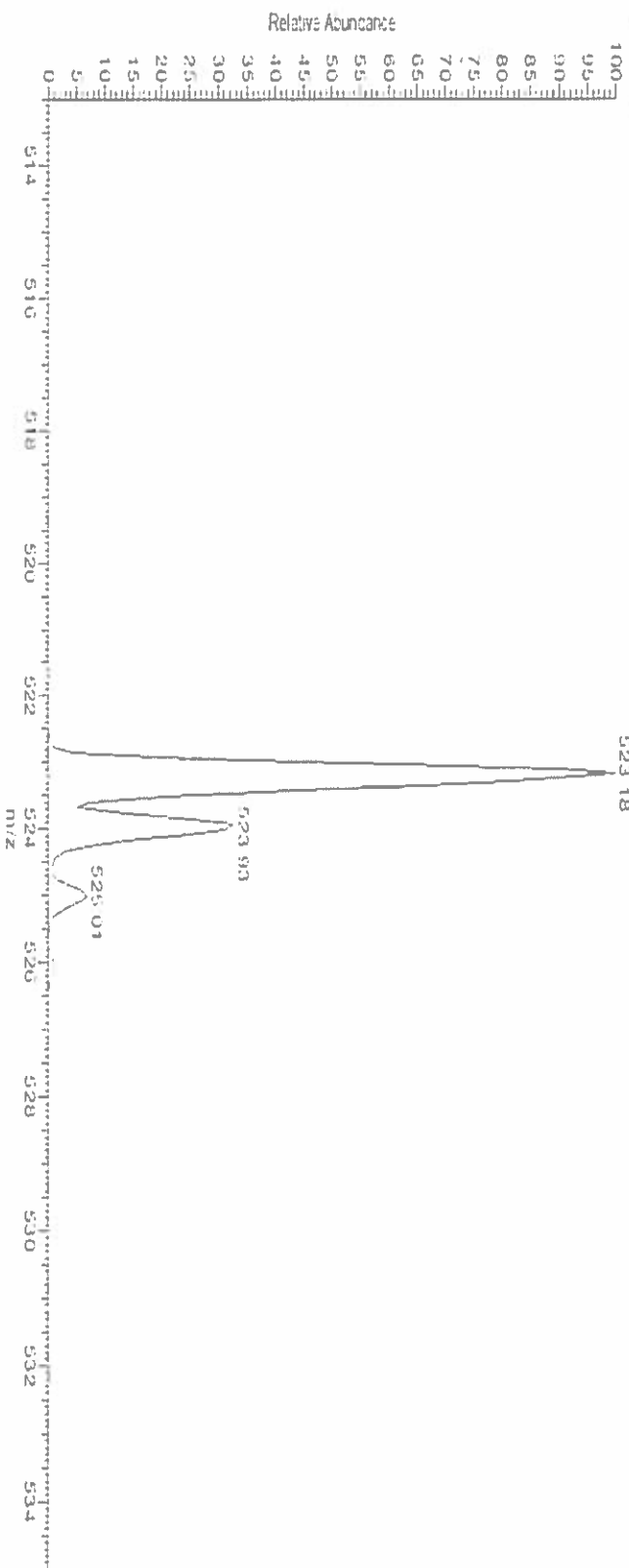
523.18

expected

C:\MSDCHEM\DATA\July14-2016\142A-all
142A all #76-133 RT: 0.41-0.68 AV: 50 NL: 1.93E6
T: ITMS + pESI Full ms (50.00-1000.00)



142-A
After Δ



Compound 1

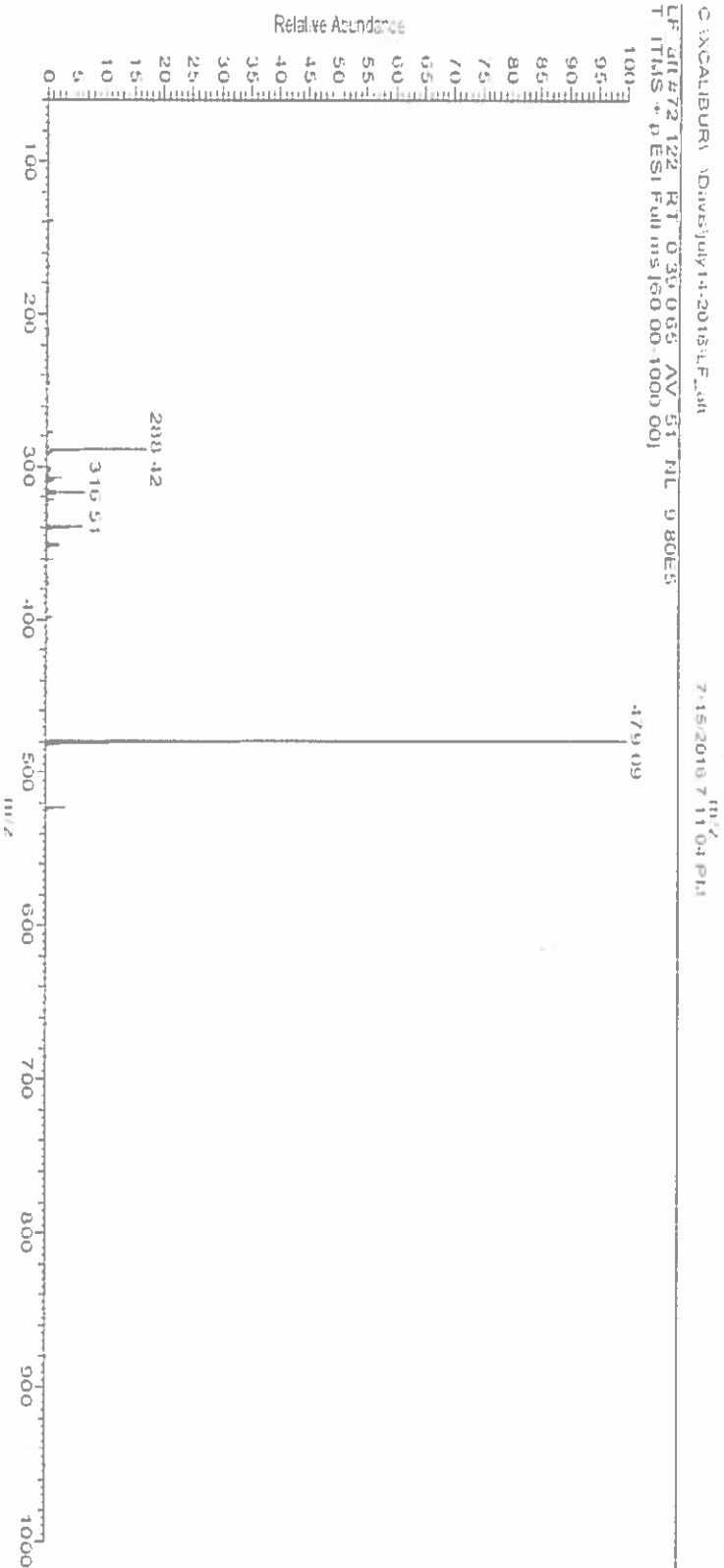
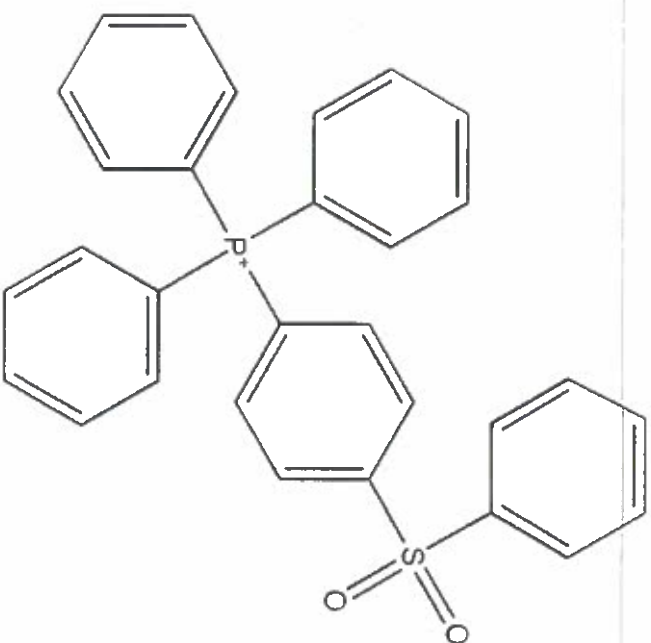
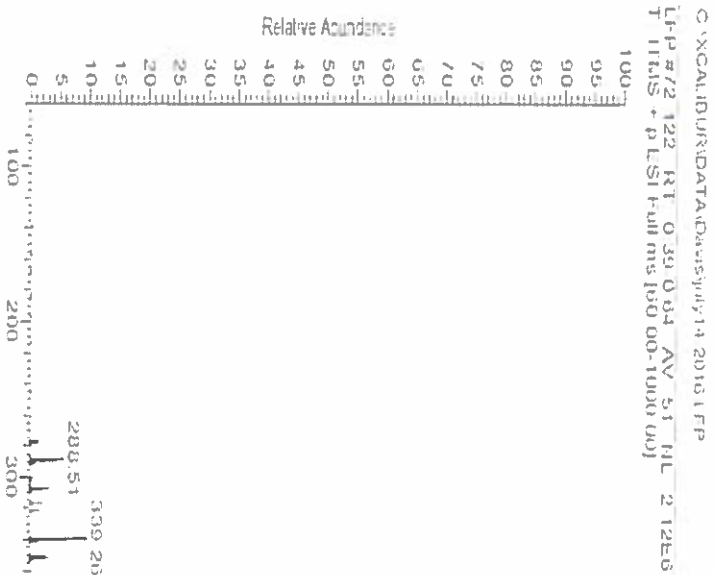
LF
Before Δ

479.12

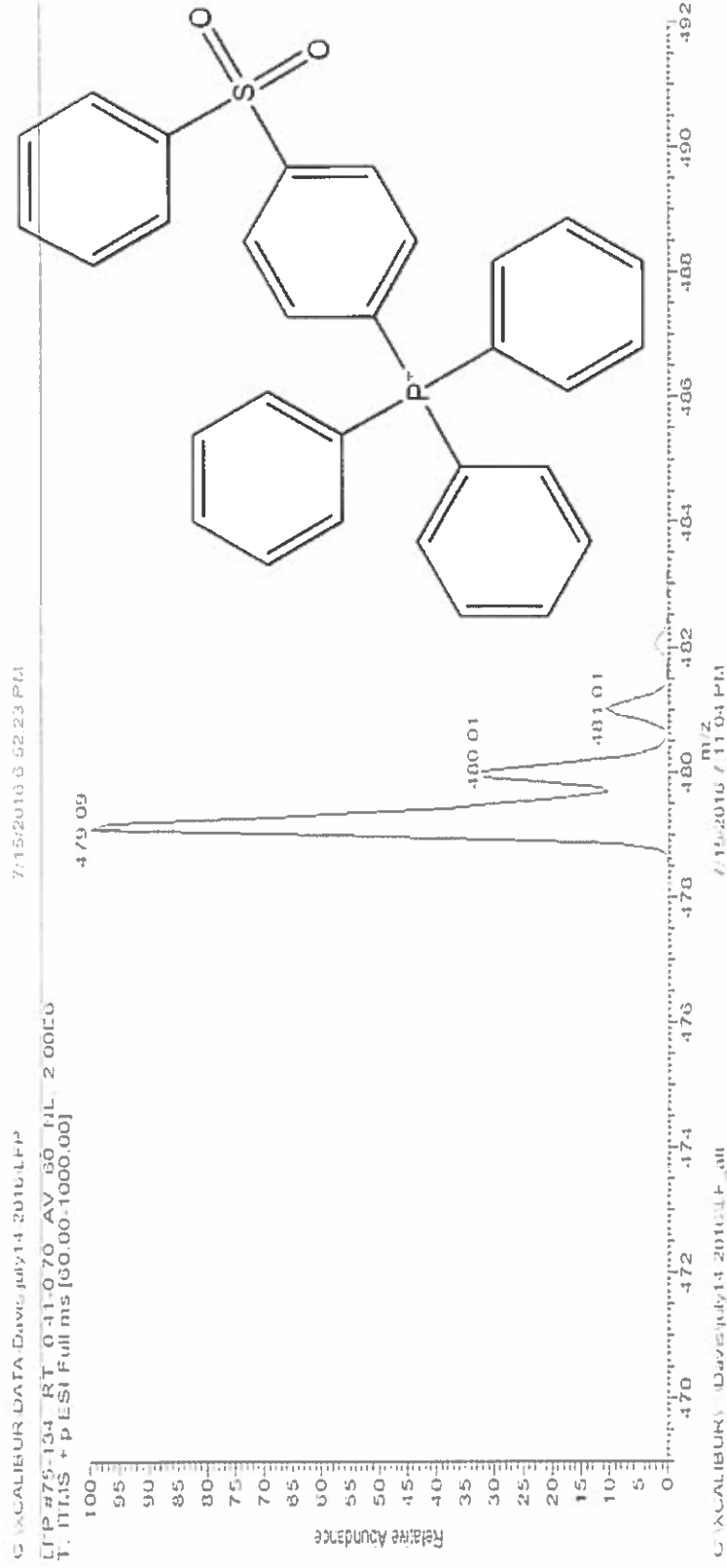
expected

LF

After Δ

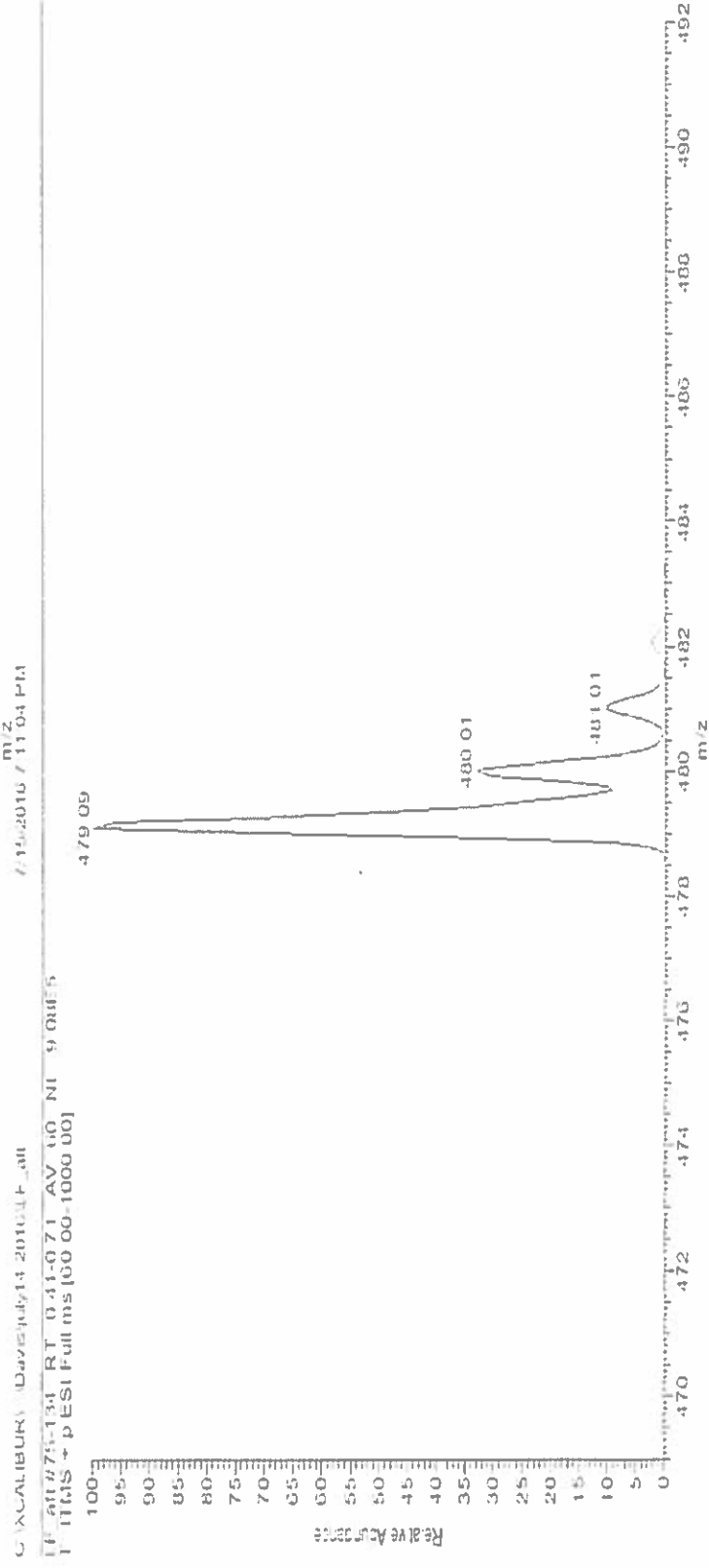


LF
Before Δ



479.12
expected

LF
After Δ

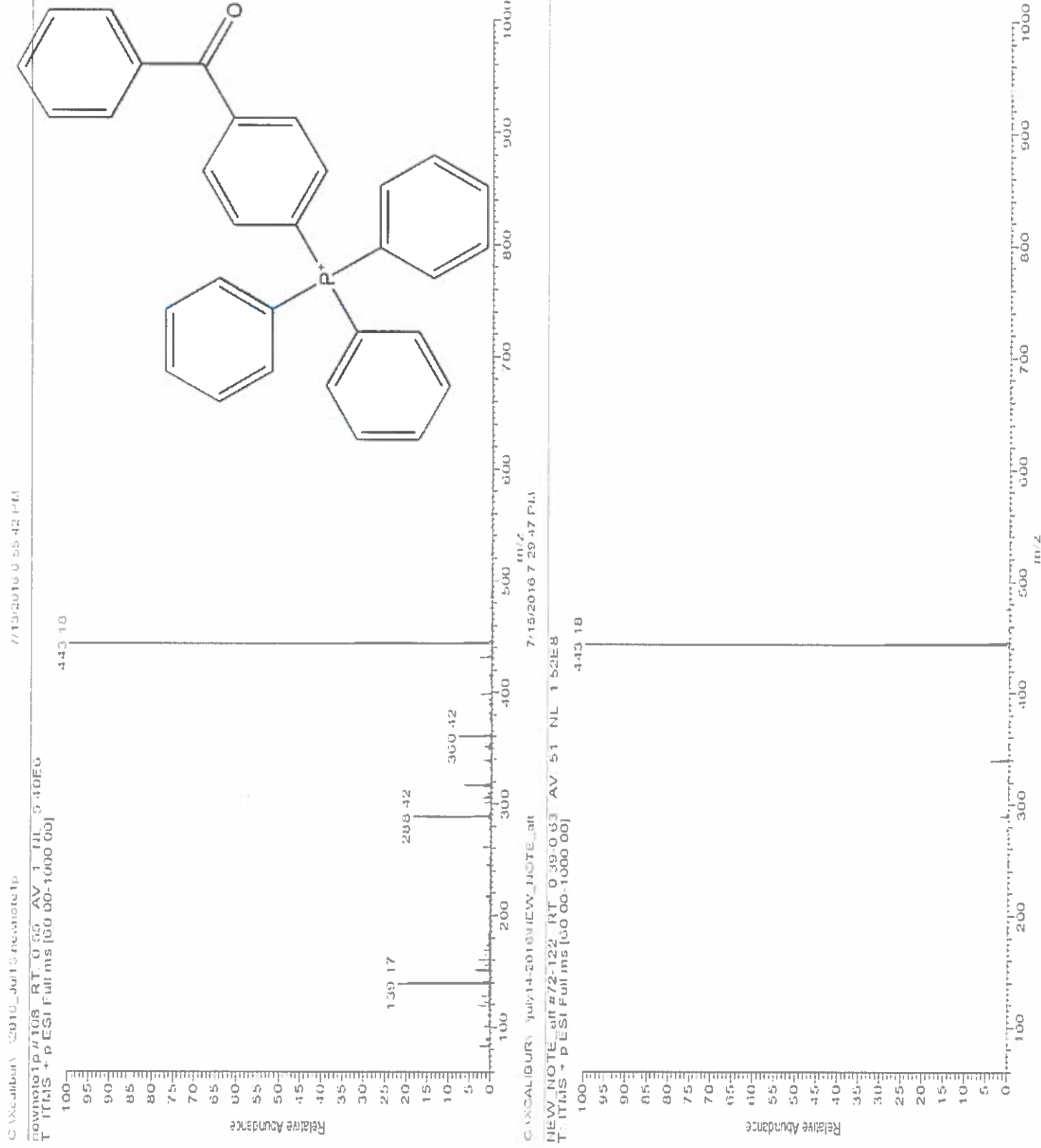


Compound

New Note
1
Before Δ

443.16
expected

New Note
1
After Δ



new_note1.p #71-101 RT: 0.37-0.81 AV: 91 FILE: 2-44EB
TITLES: + P ESI Full.ms (60.00-1000.00)

New Note

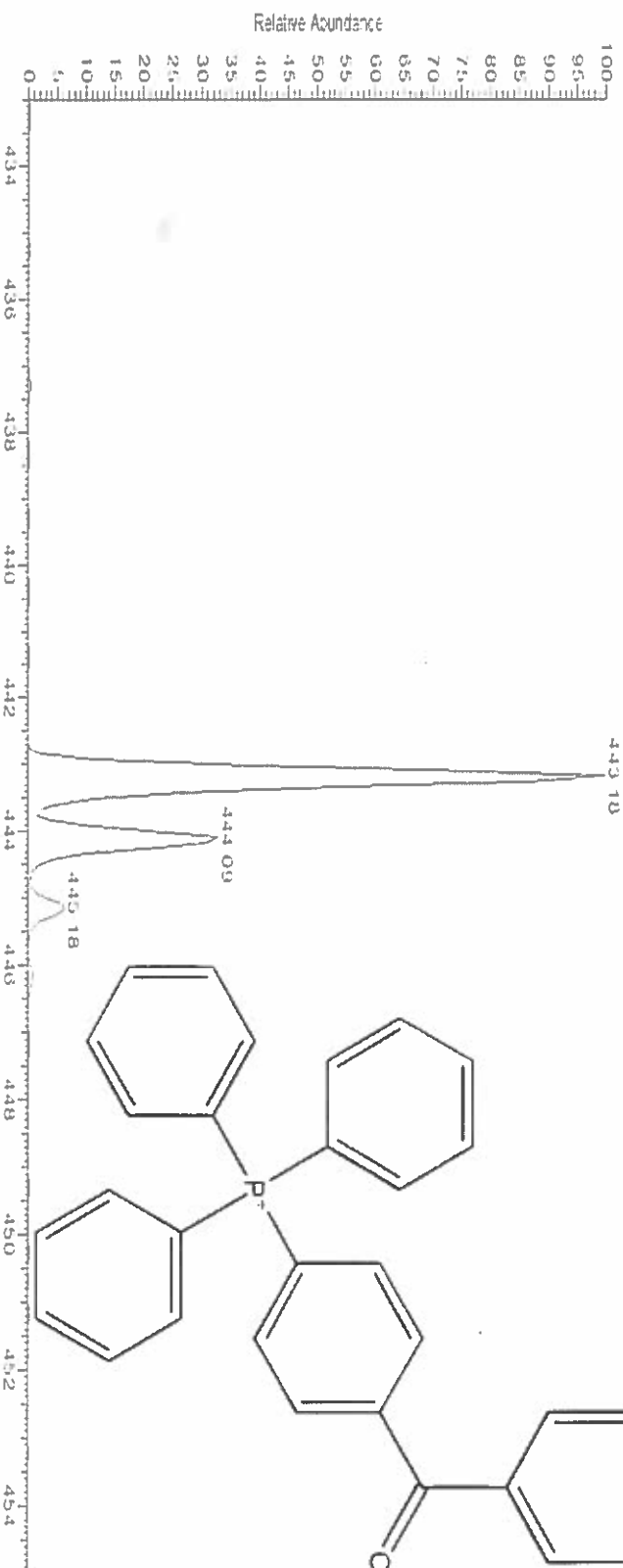
1

Before Δ

443.16

expected

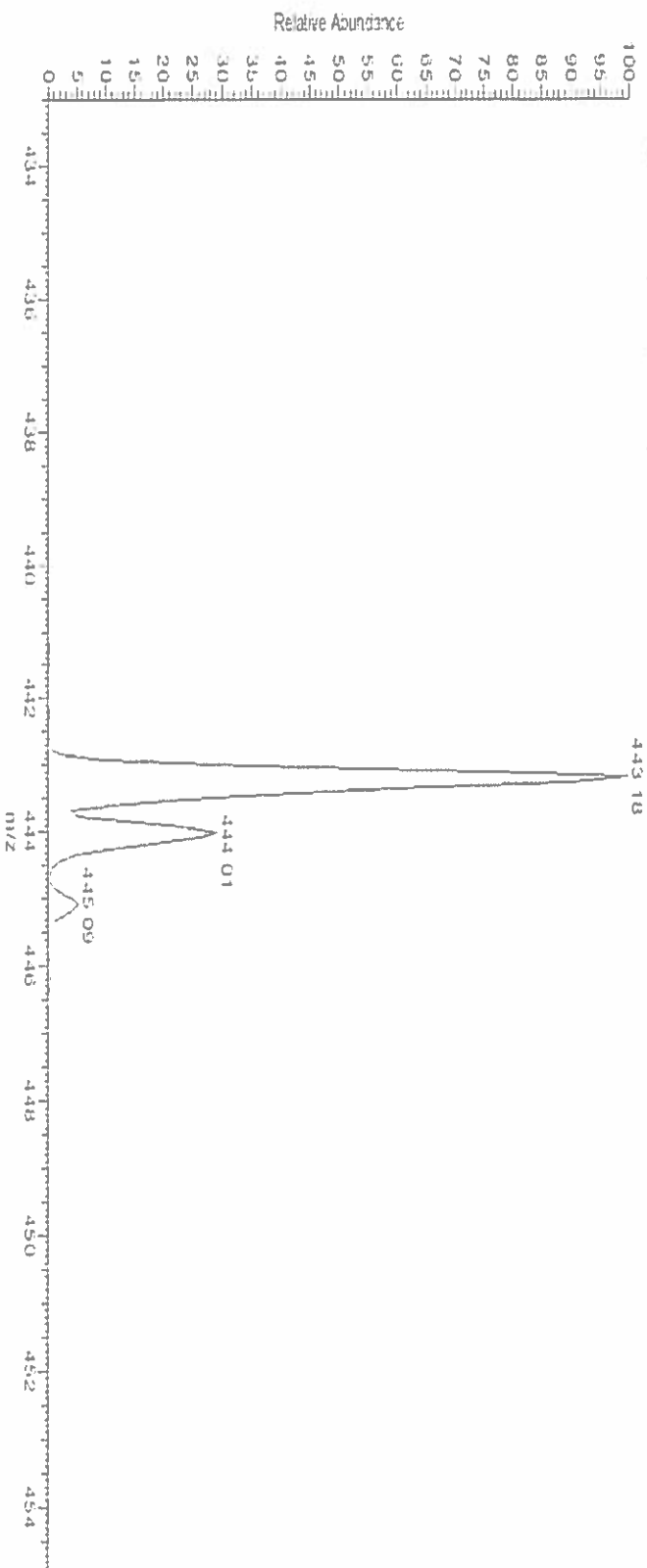
C:\MSDCHEM\2016_Jan13\new_note1.p
new_note1.p #71-139 RT: 0.39-0.71 AV: 97 FILE: 1-30EB
TITLES: + P ESI Full.ms (60.00-1000.00)



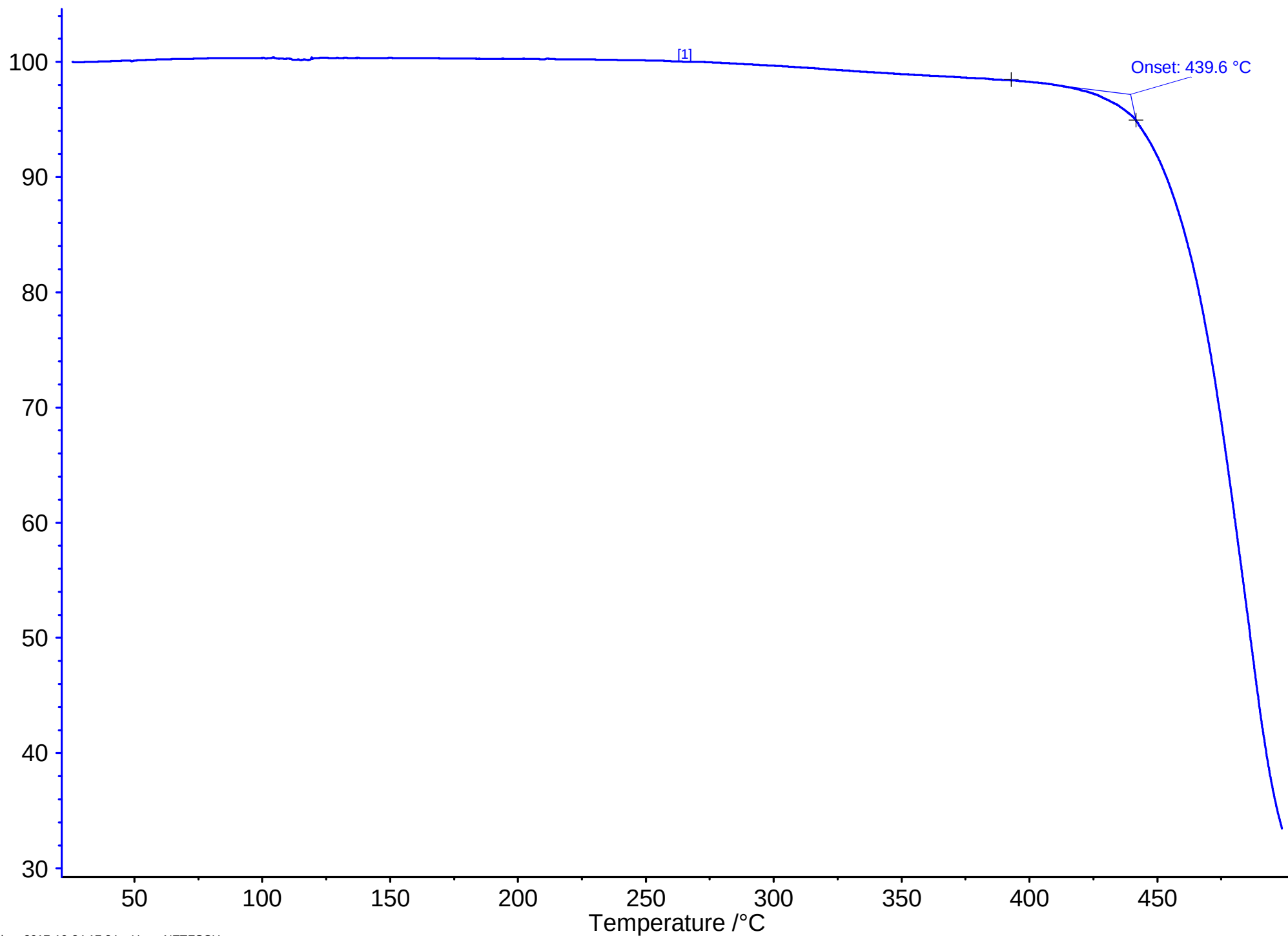
New Note

1

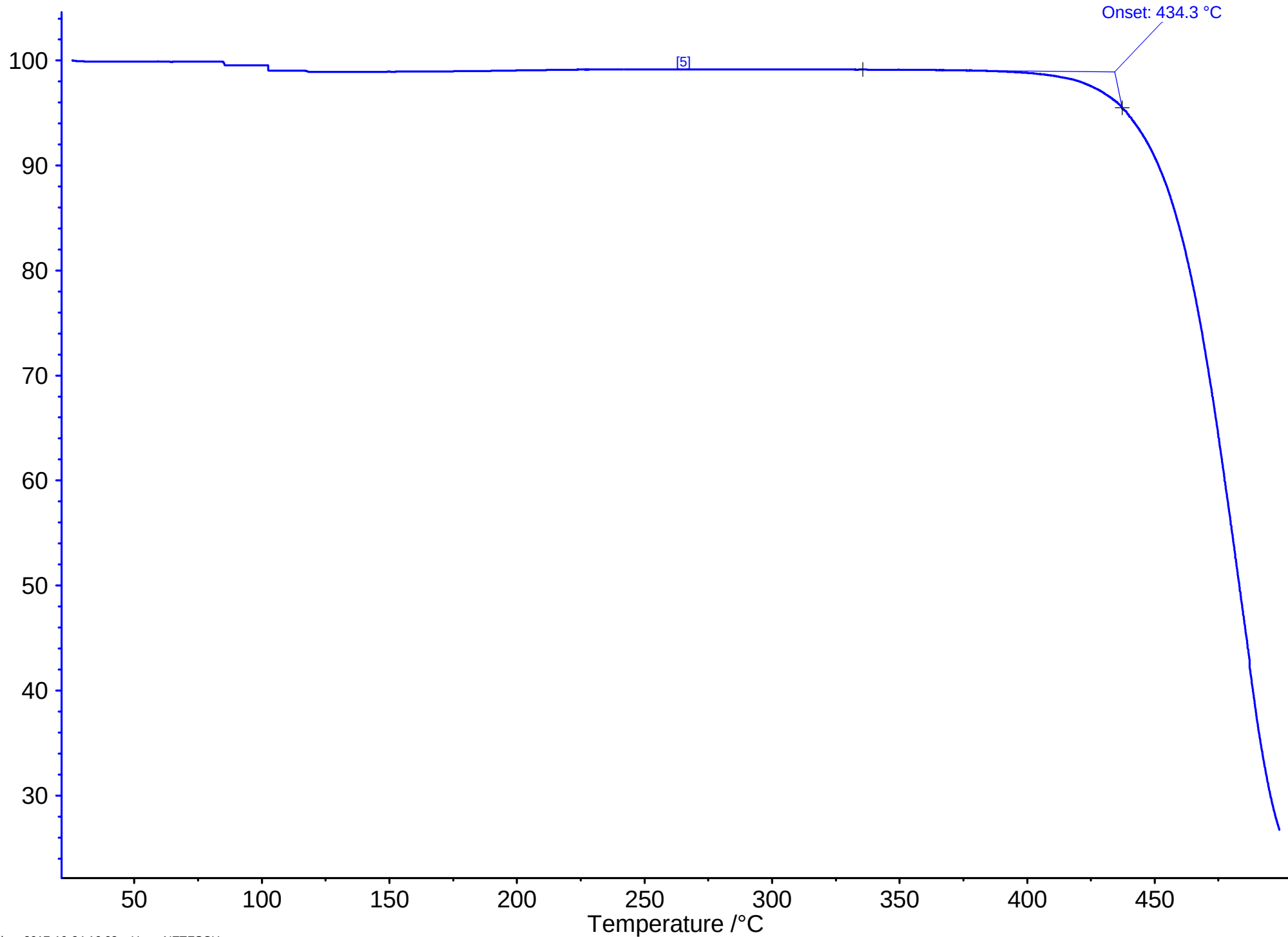
After Δ

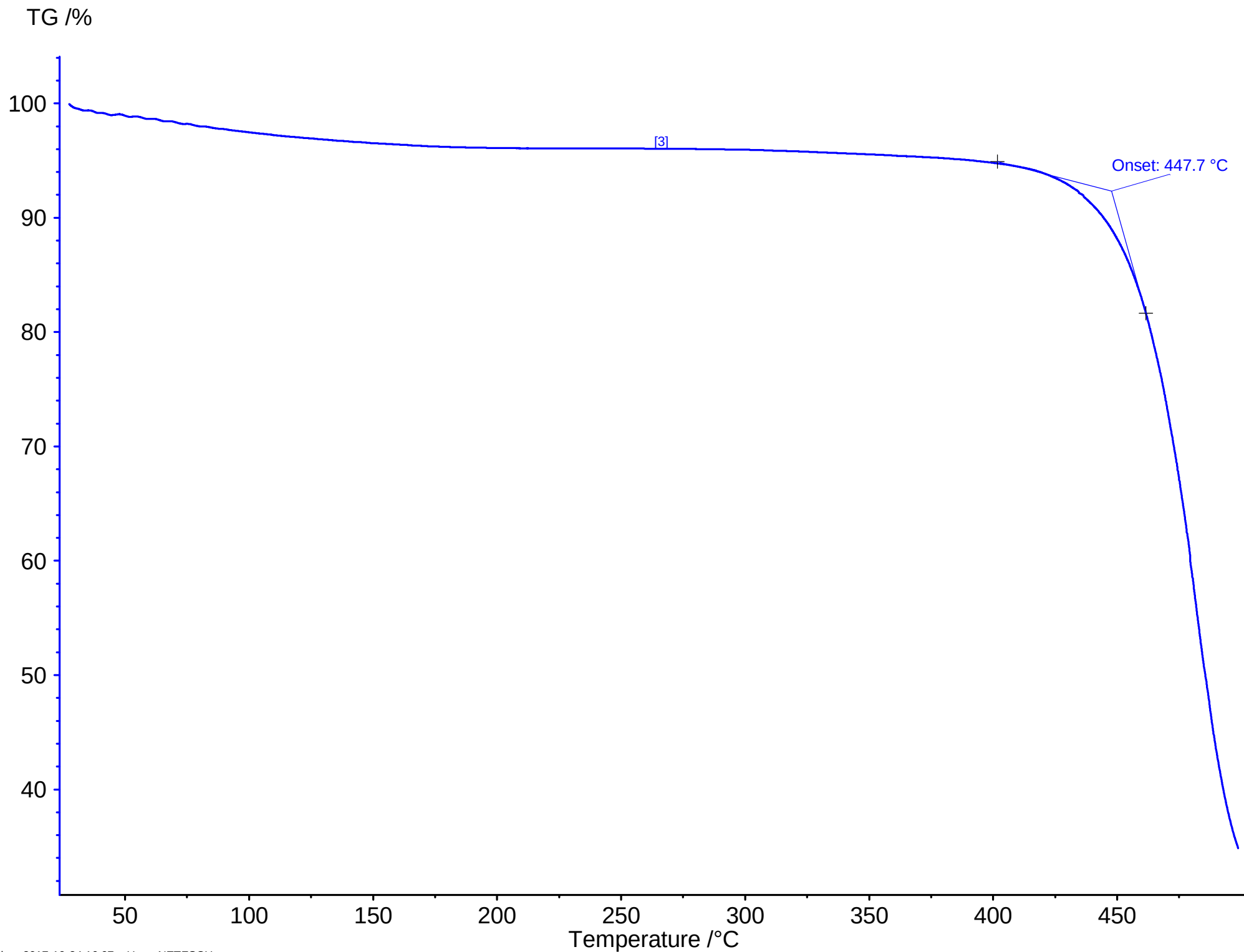


TG /%

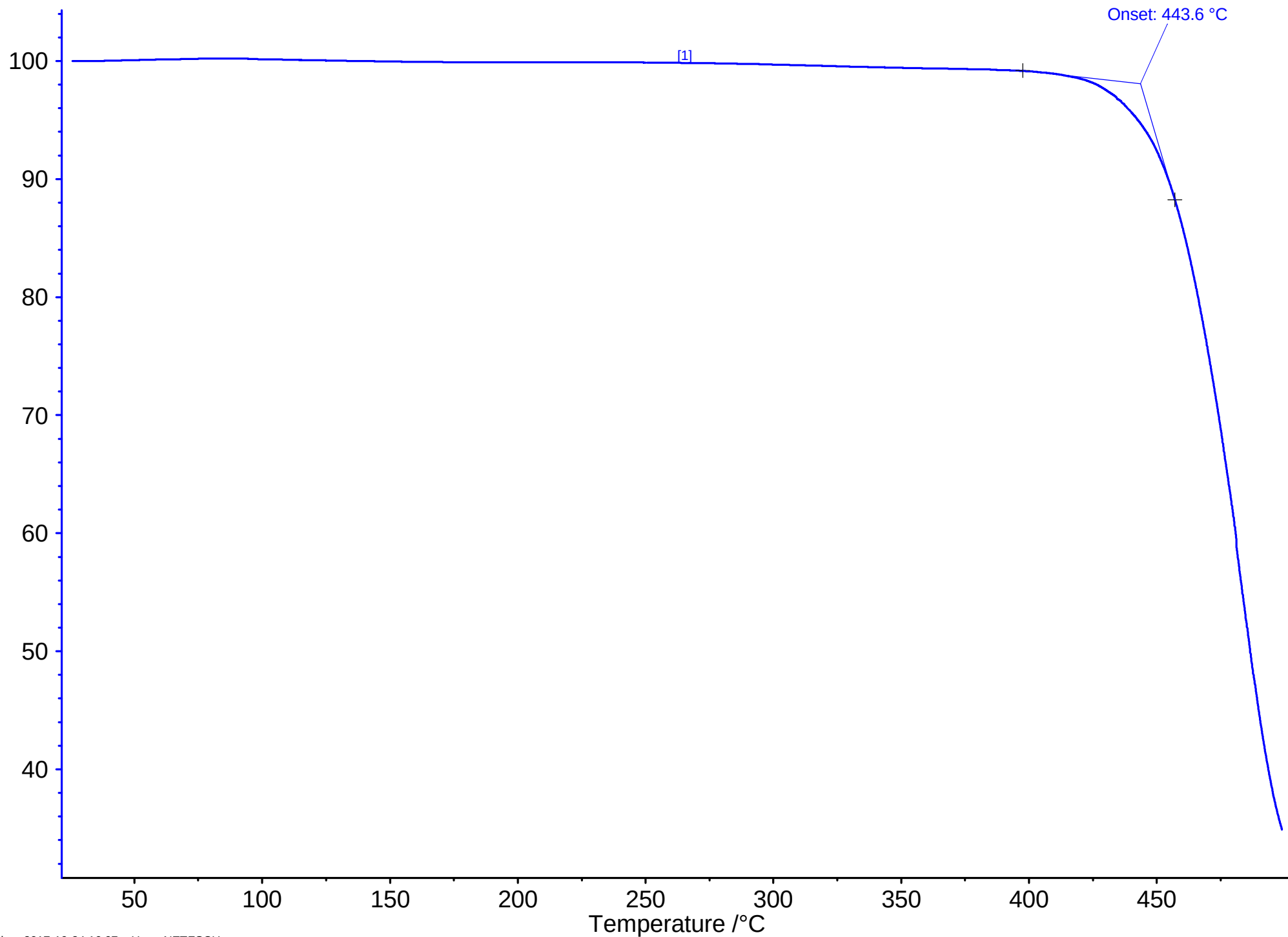


TG /%

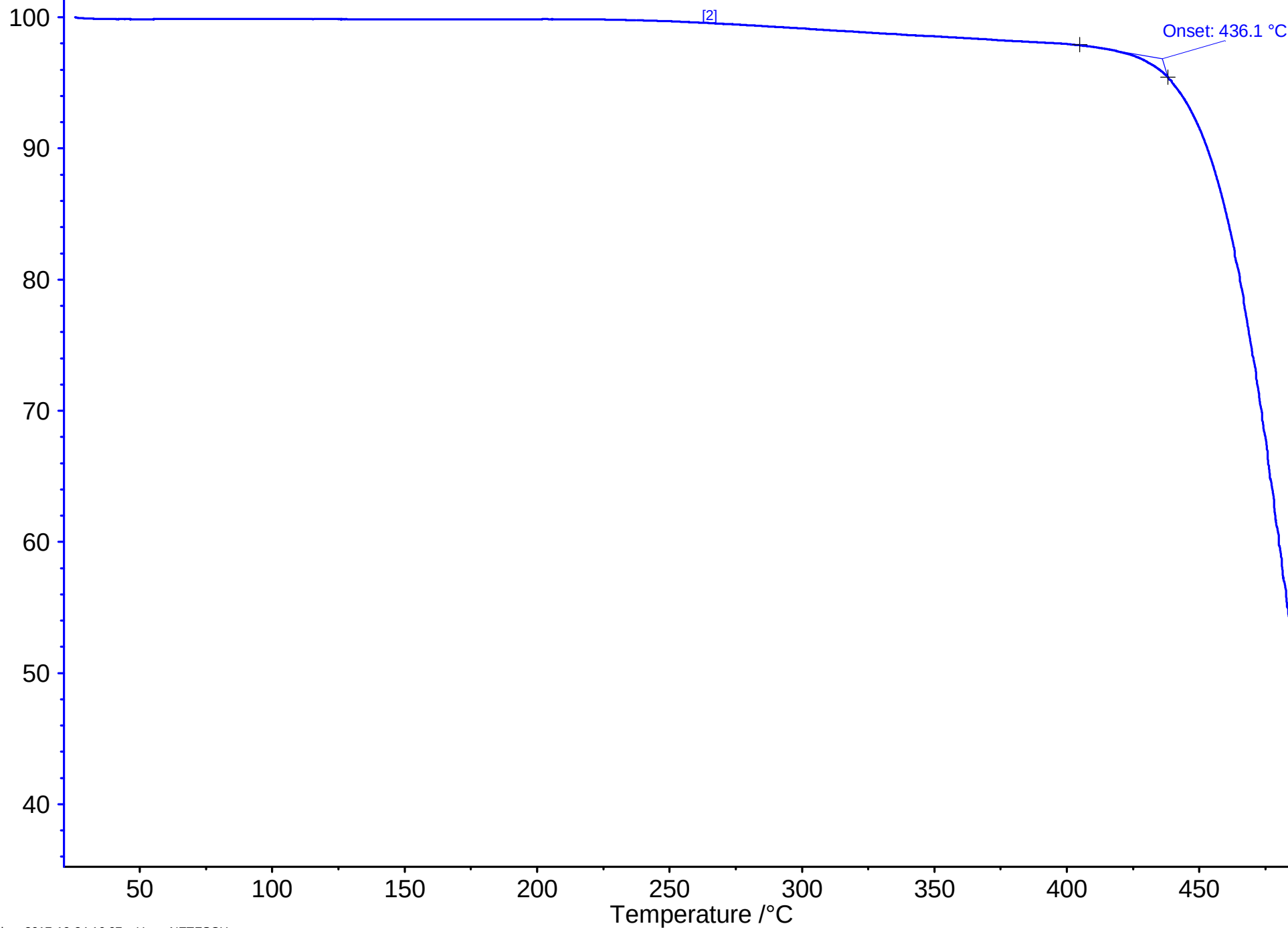




TG /%



TG /%



TG /%

100

90

80

70

60

50

40

30

20

50

100

150

200

250

300

350

400

450

Temperature /°C

[4]

Onset: 416.1 °C

