Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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

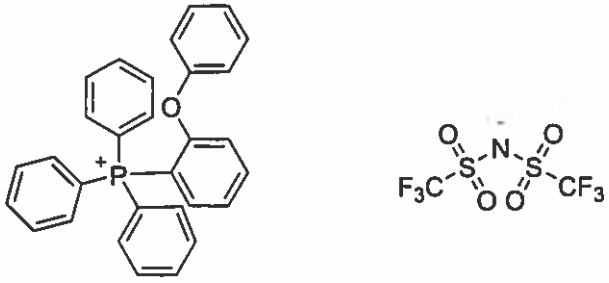
Liquid phase enthalpies were calculated using the two-phase thermodynamic (2PT) method,[1, 2] which has been shown to accurately reproduce the standard molar entropies and heat capacities of a number of common solvents.[3] Readers should refer to the original papers for the full details but the essence 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.

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

Sample No. Phosphonium 51A

Company/School U of South Alabama
Dept. Chemistry
Address Chem 223
City, State, Zip Mobile AL 36688

Professor/Supervisor: James Davis
Name James Davis Date 10/31/2016
PO# / CC#
Phone (251) 751-0520

Element	Theory	Found	
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	

Single ☒ Duplicate ☐

Elements Present: CHNPOSF

Analyze for: CHN

Hygroscopic ☐ Explosive ☐
M.P. unk B.P. none

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

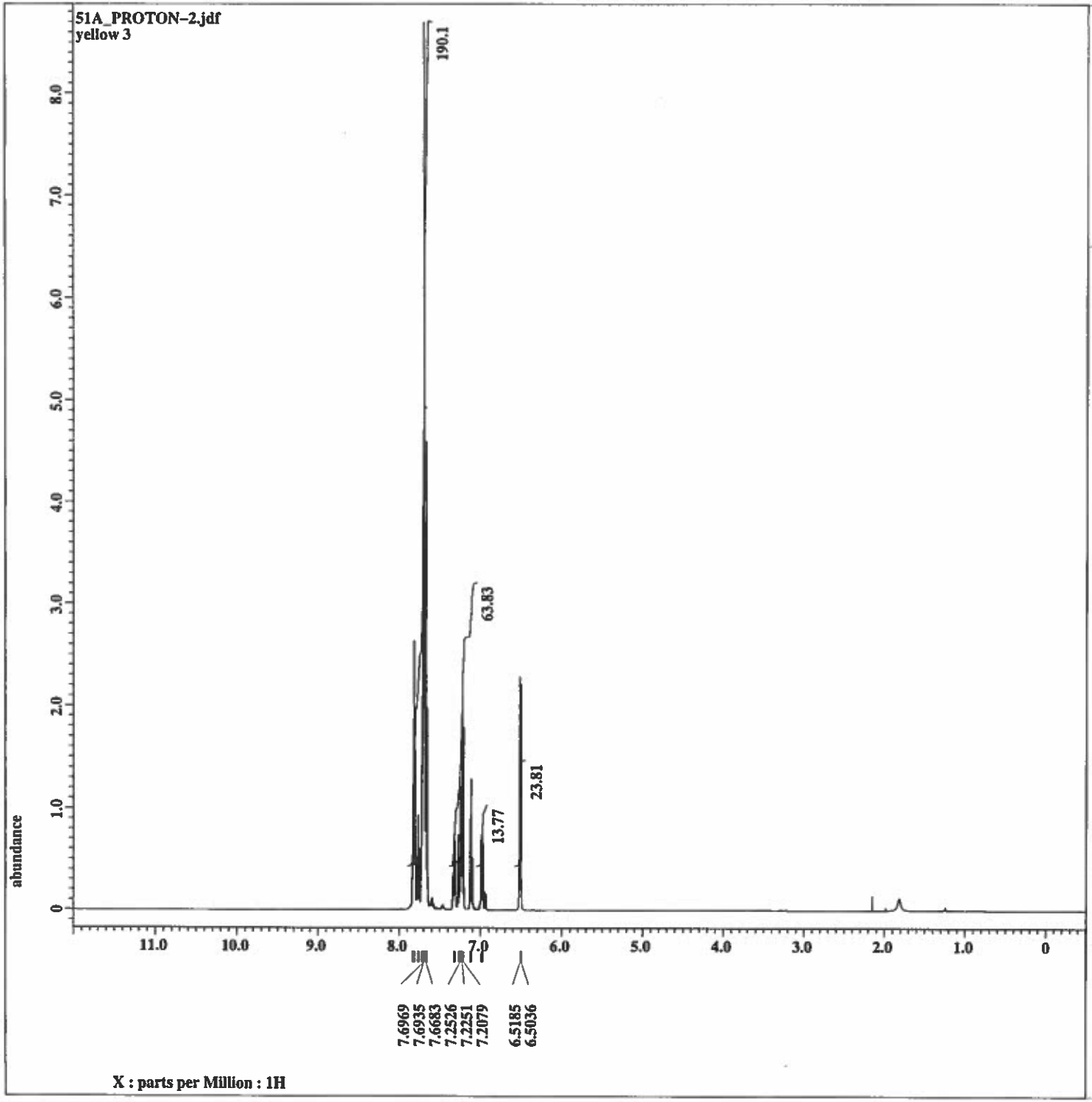
Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

Include Email Address or FAX # Below

jdavis@southalabama.edu

Date Received NOV 01 2016 Date Completed NOV 01 2016

Remarks:



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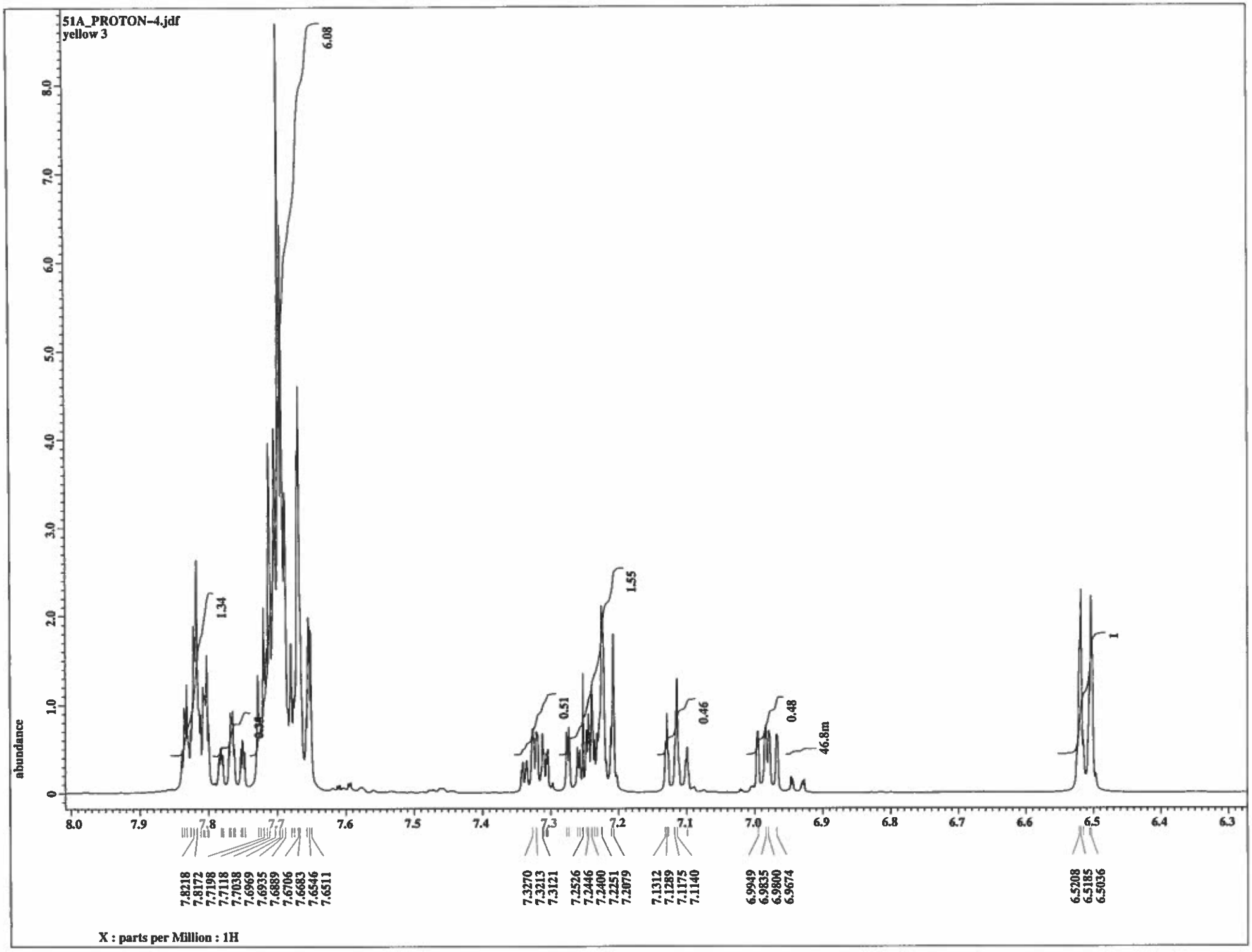
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0.51
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0.48
46.8m
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7.6546
7.6511
7.3270
7.3213
7.3121
7.2526
7.2446
7.2400
7.2251
7.2079
7.1312
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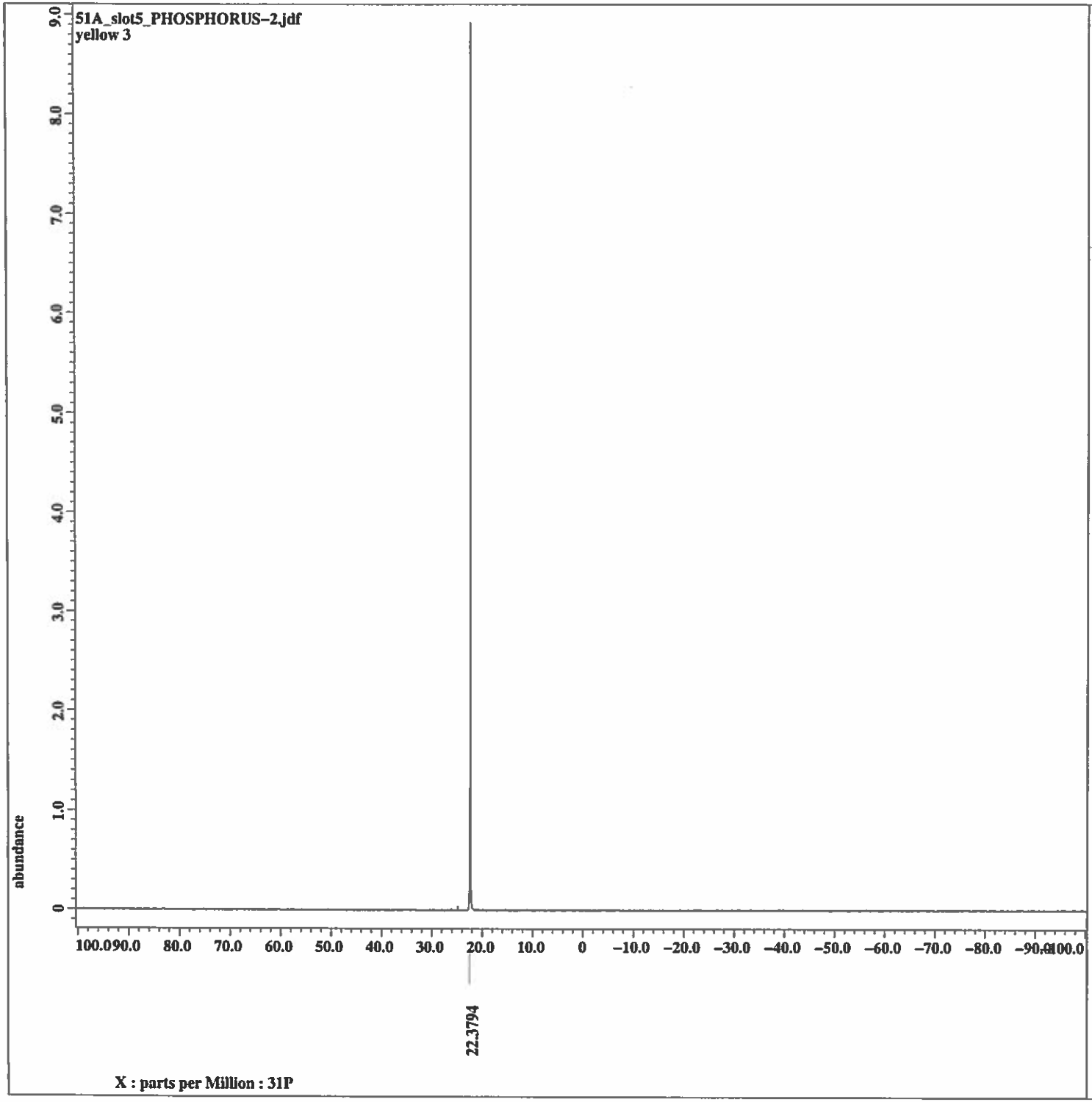

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X_offset	= 0[ppm]
X_points	= 32768
X_prescans	= 4
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X_sweep	= 50.81300813[kHz]
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Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
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Mod_return	= 1
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Noe	= TRUE
Noe_time	= 2[s]
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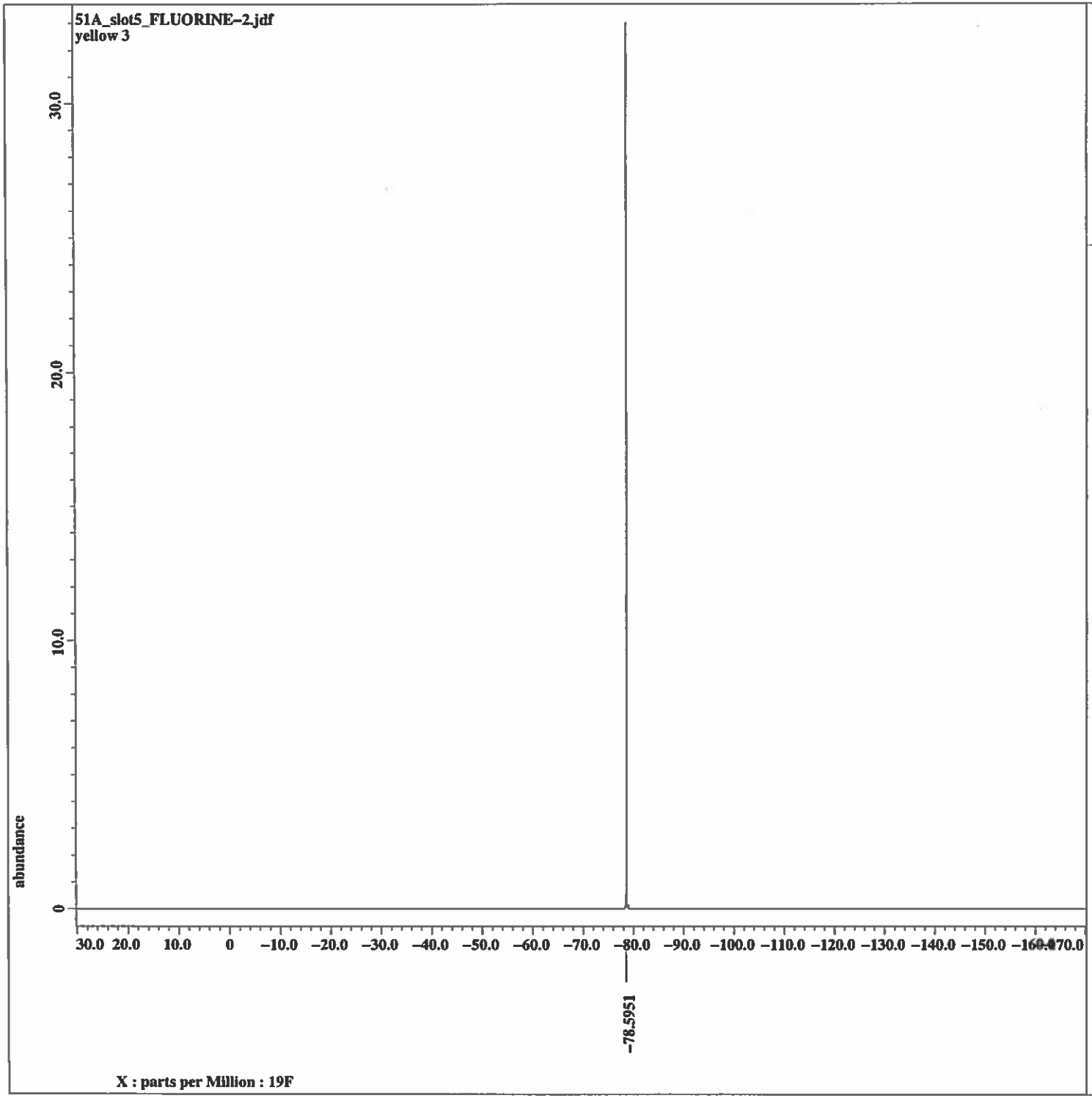

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X_domain	= 19F
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X_offset	= -70[ppm]
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X_resolution	= 1.7993855[Hz]
X_sweep	= 117.9245283[kHz]
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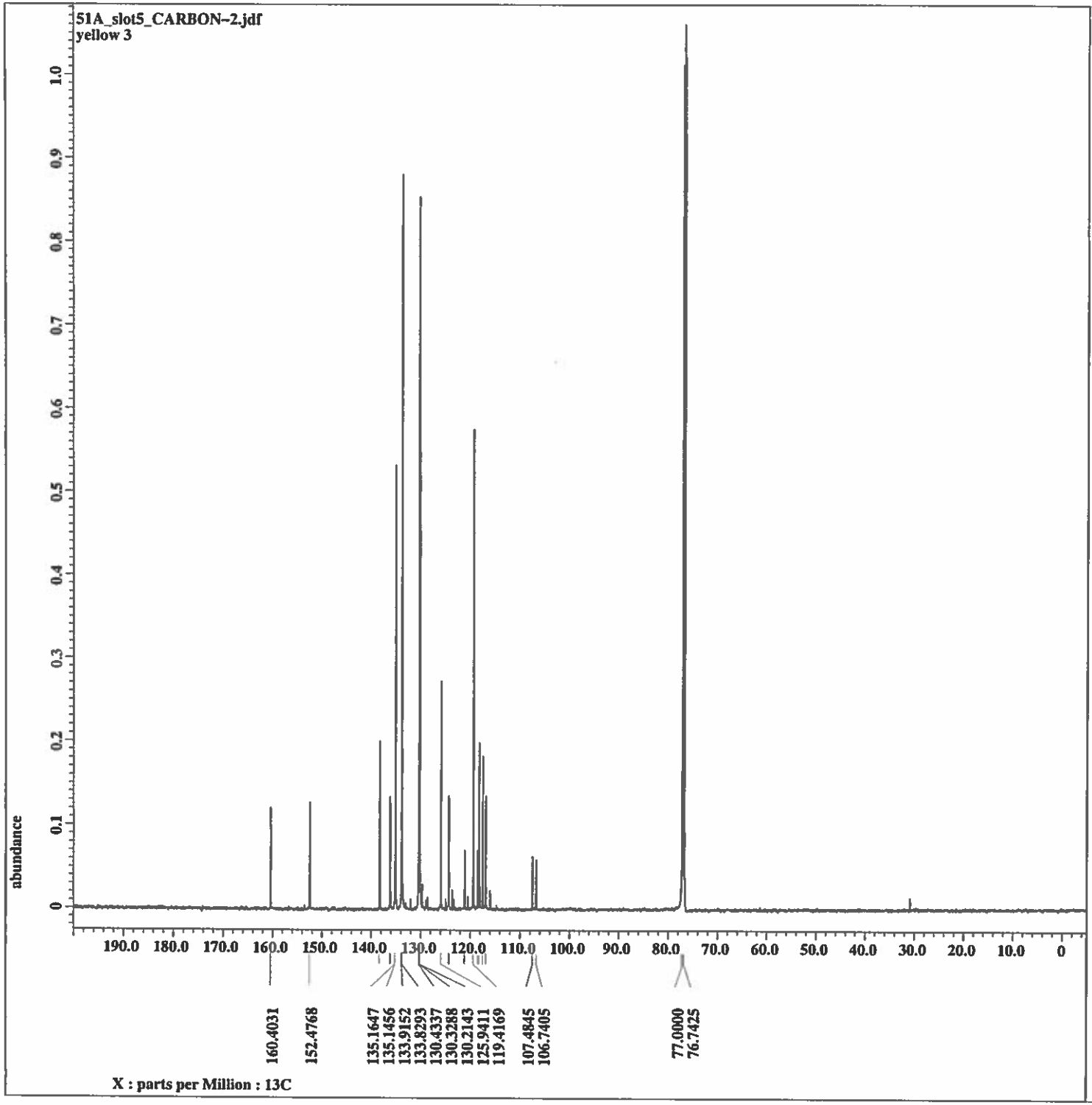

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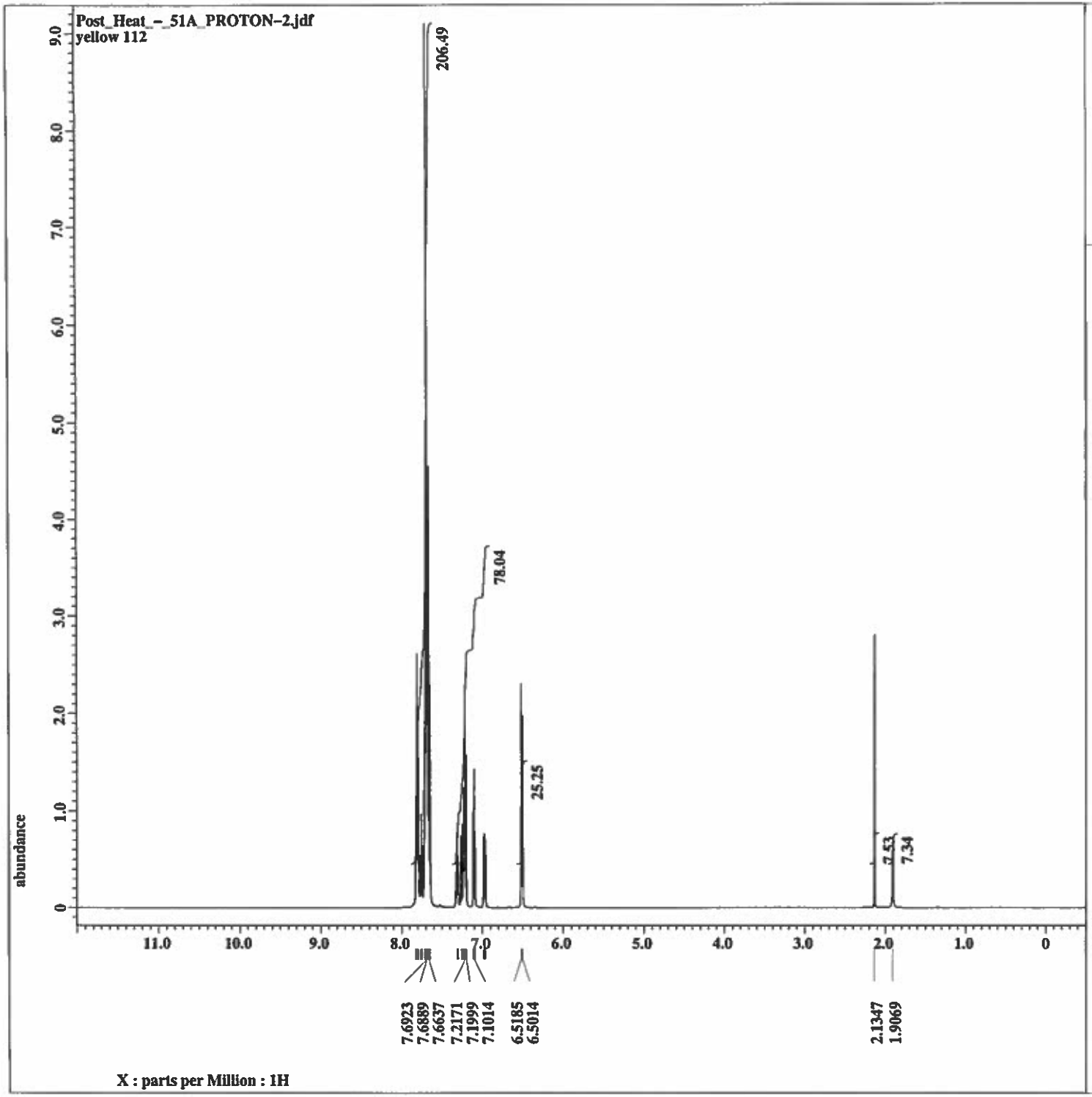

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Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
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X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.675[us]
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Tri_mode	= Off
Dante_presat	= FALSE
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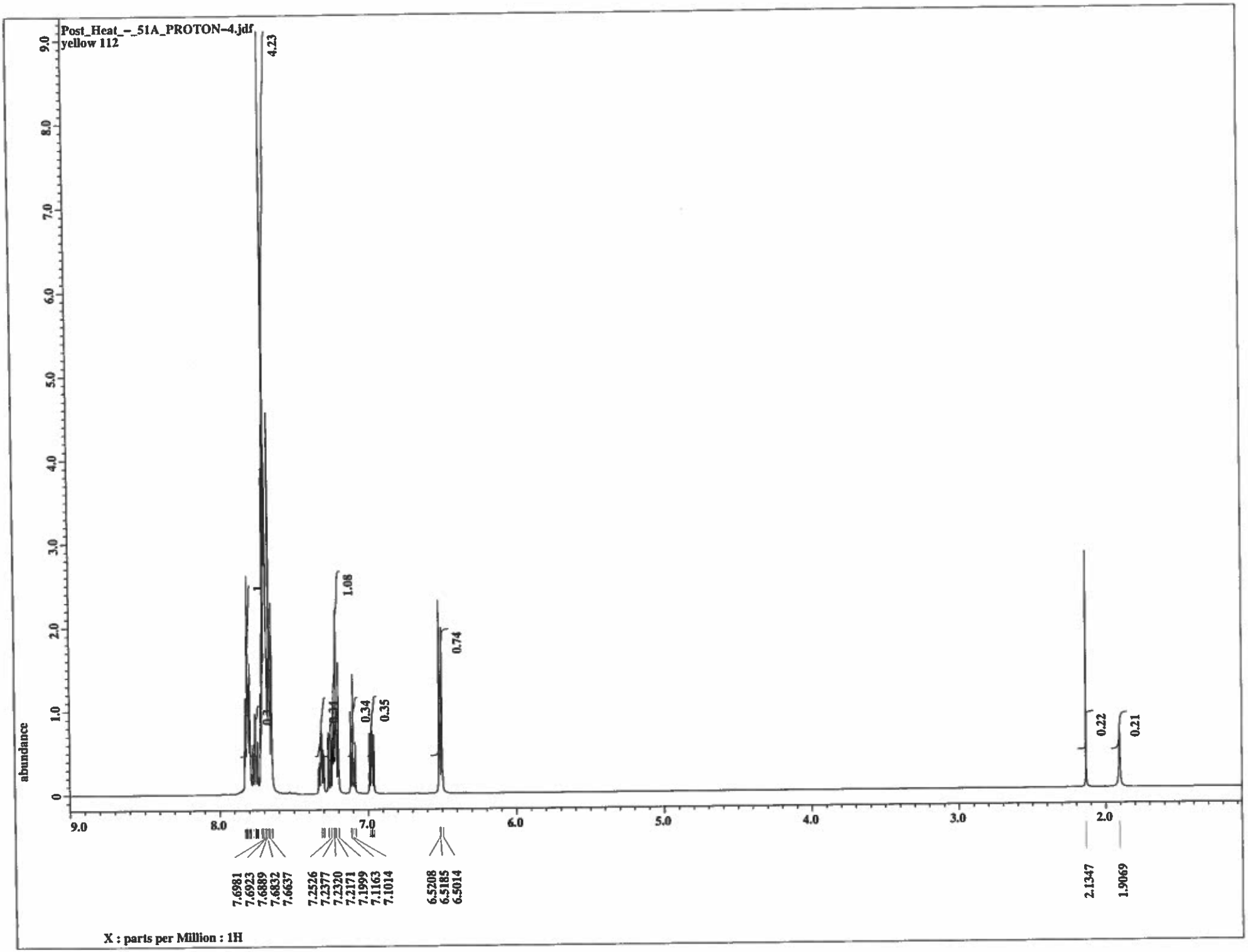
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0.22
0.21
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7.6889
7.6832
7.6637
7.2526
7.2377
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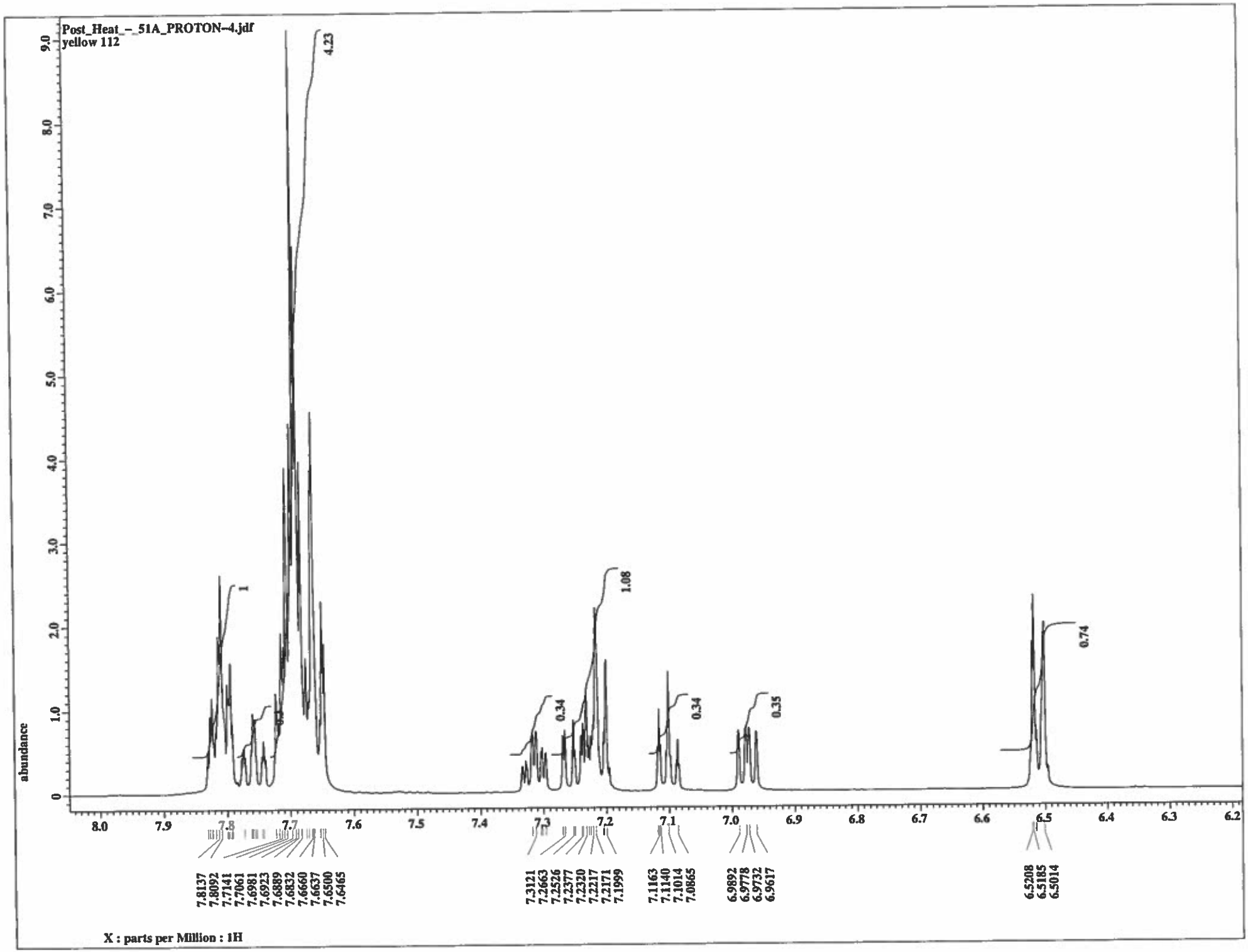
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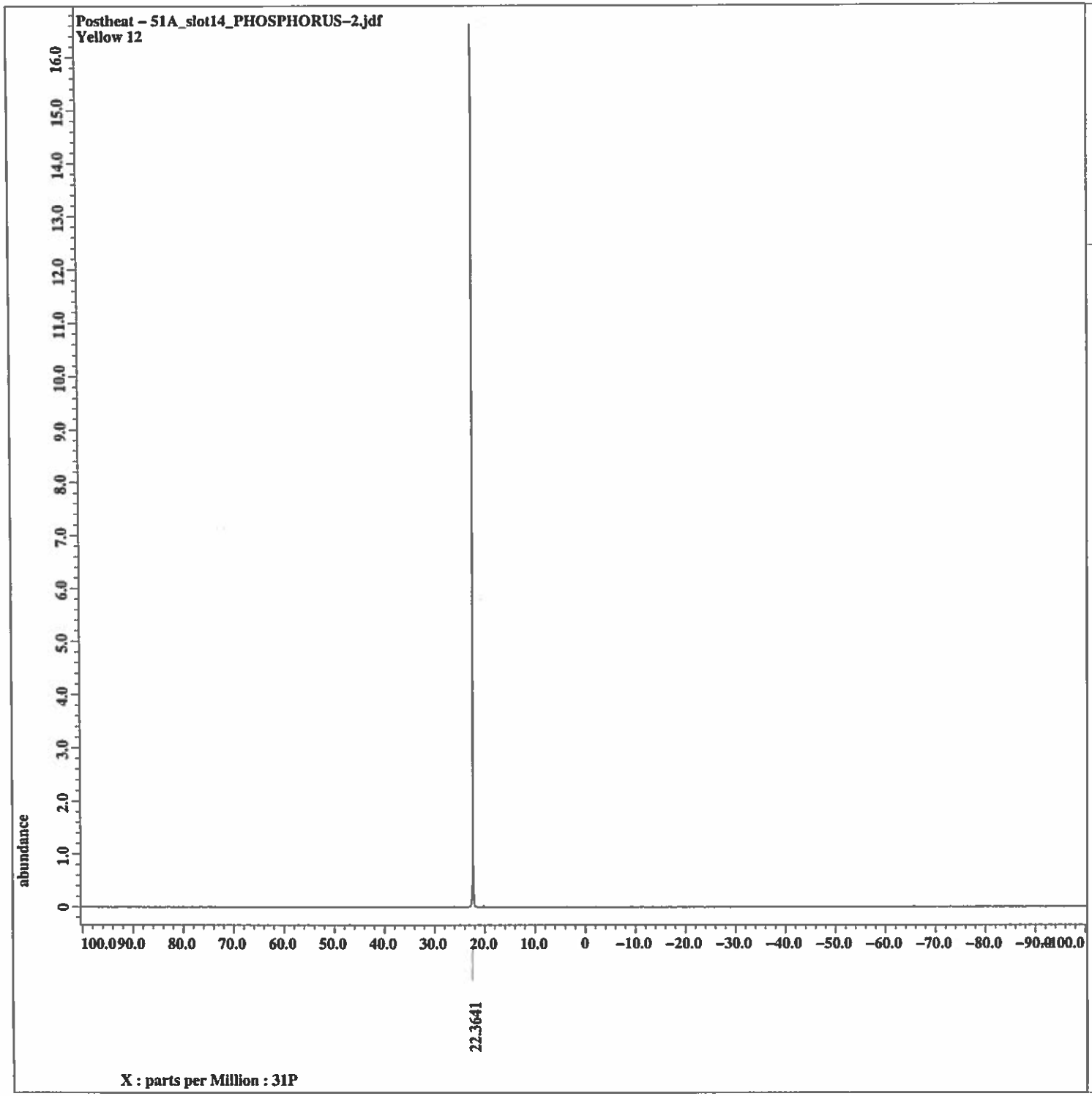

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Noe	= TRUE
Noe_time	= 2[s]
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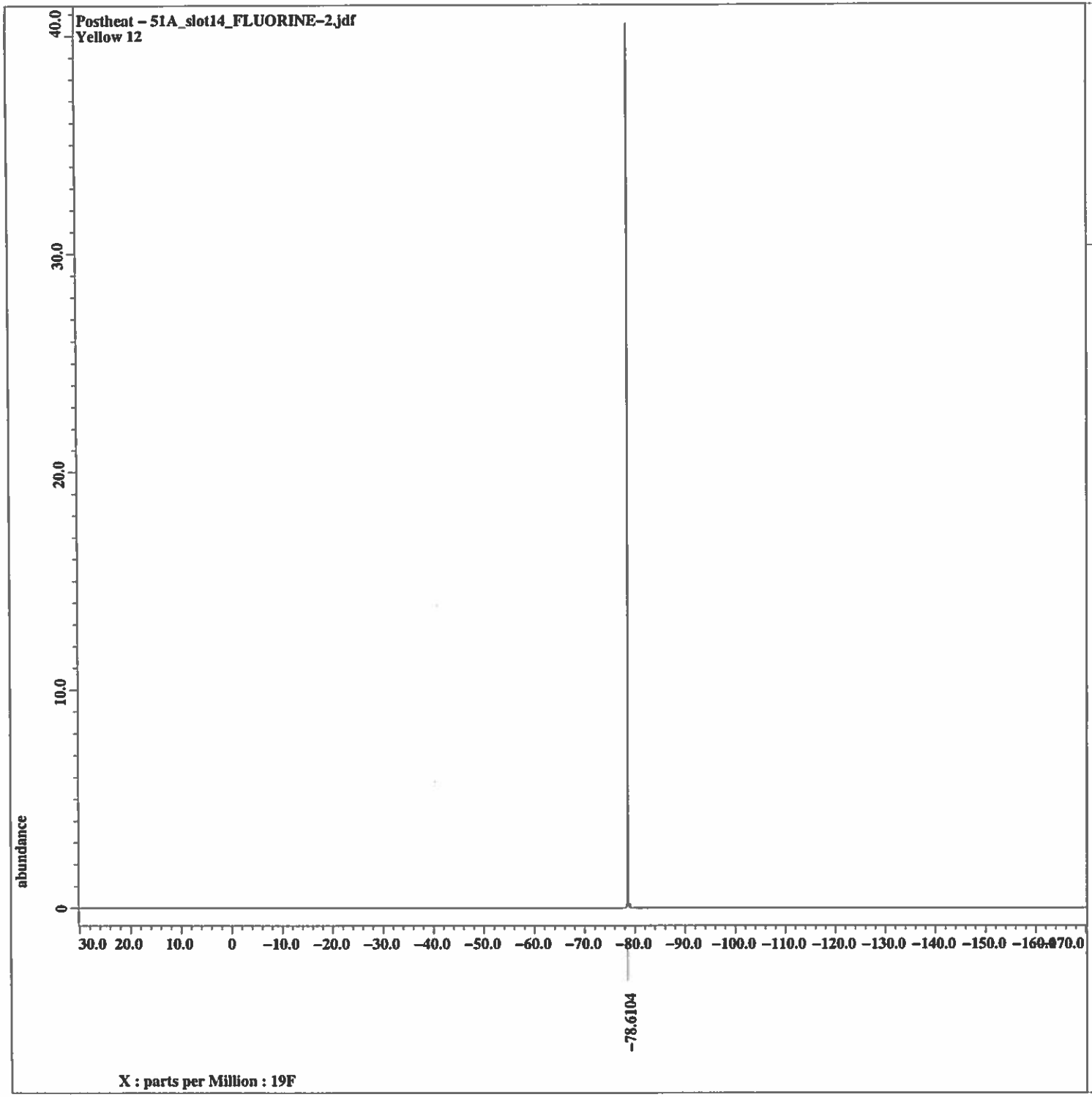

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X_sweep	= 117.9245283[kHz]
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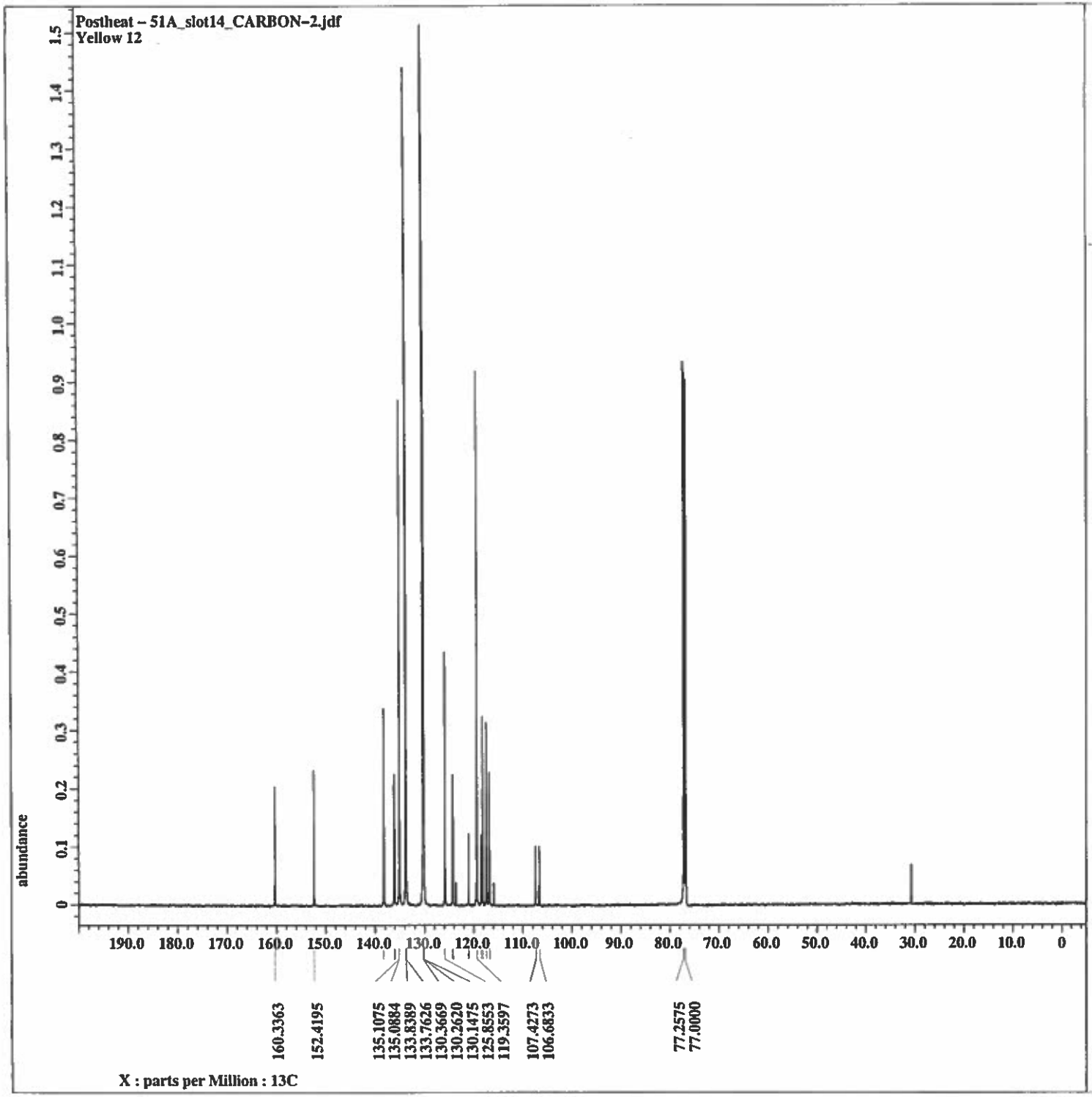

SOUTH ALABAMA JAGUARS

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X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
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Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
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X_pulse	= 4.18333333[us]
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Irr_atn_noe	= 20.5[dB]
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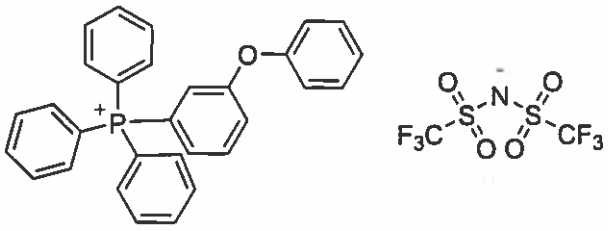
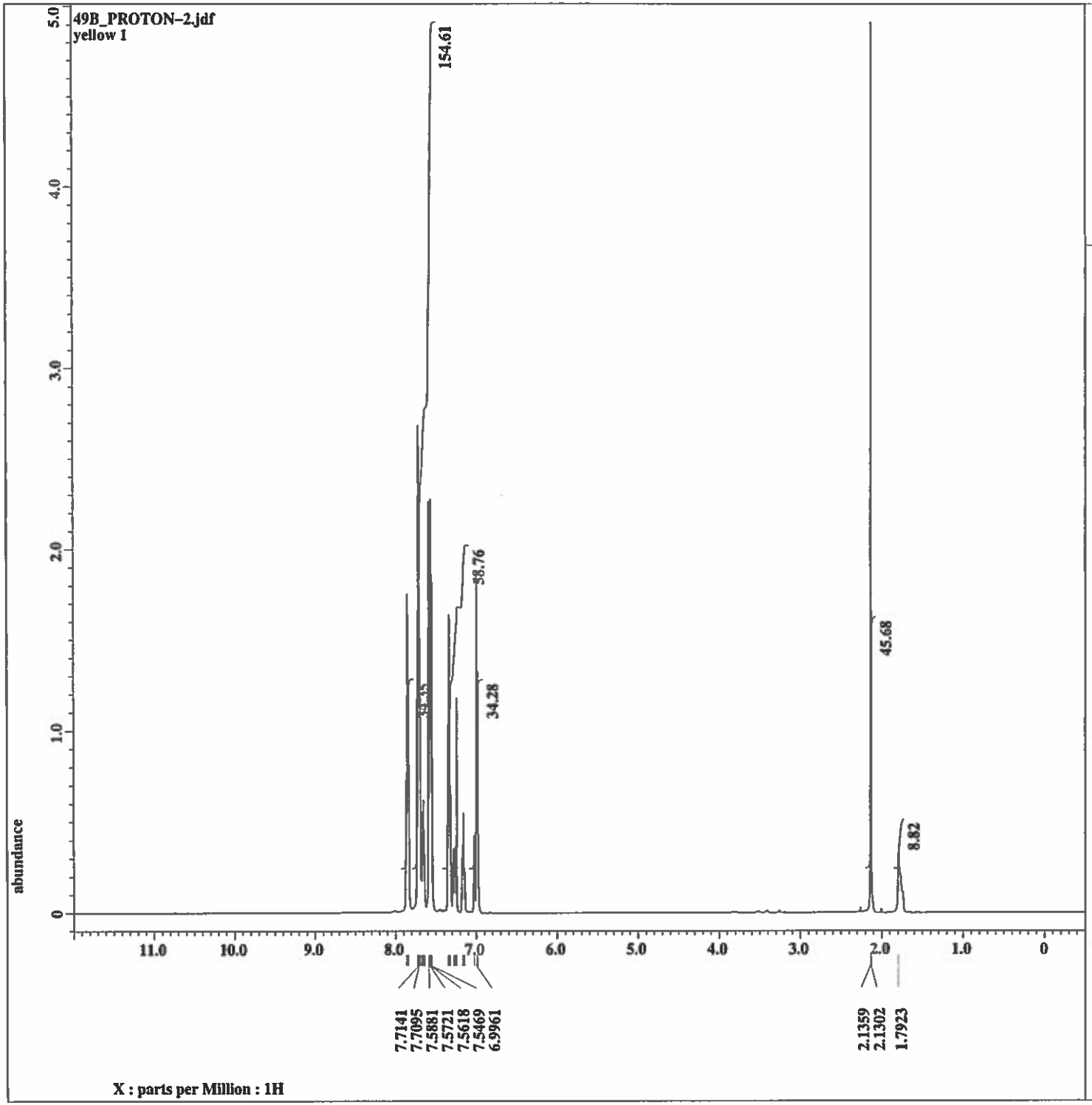
Temp_get	= 23.3[dC]

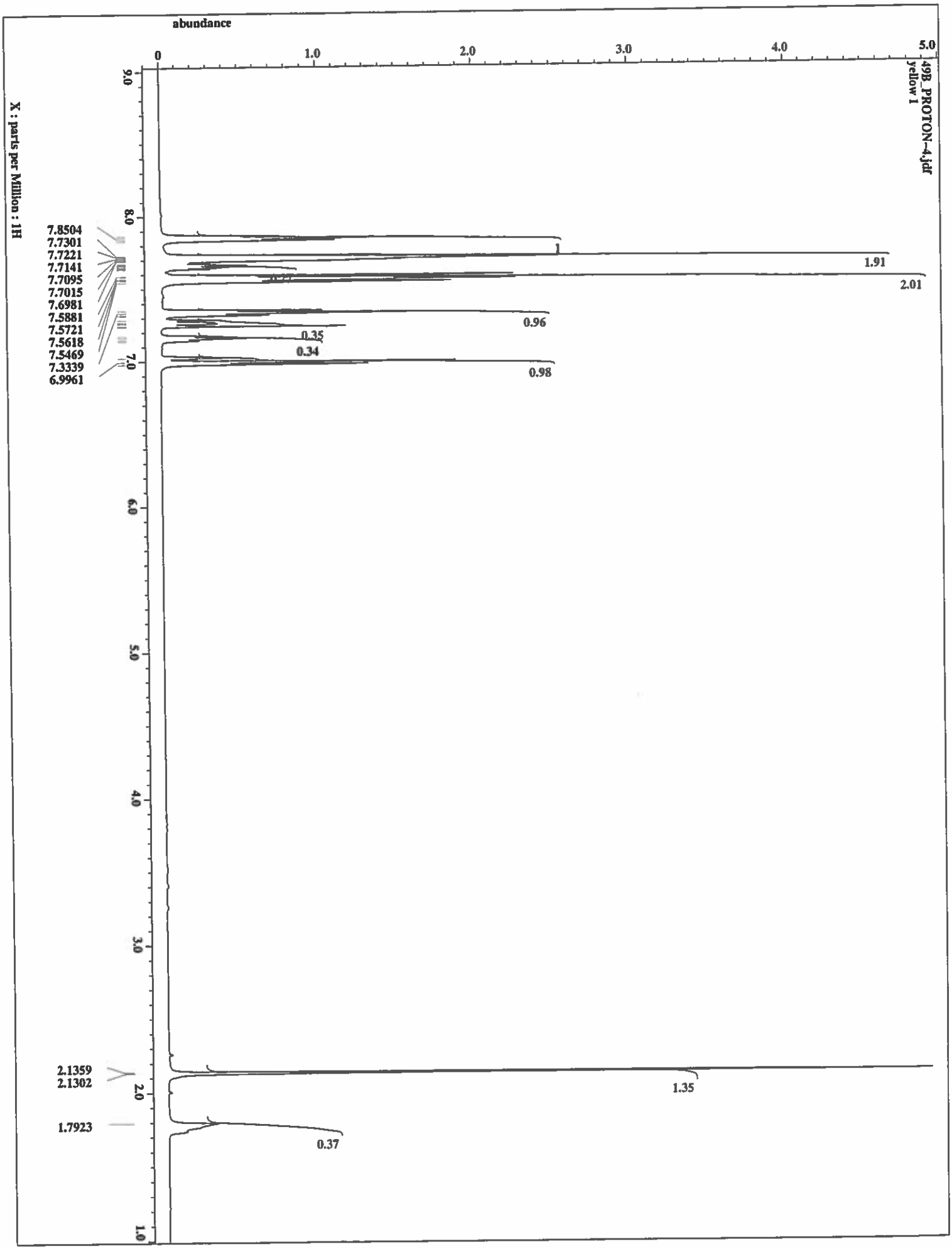
COMPOUND 3

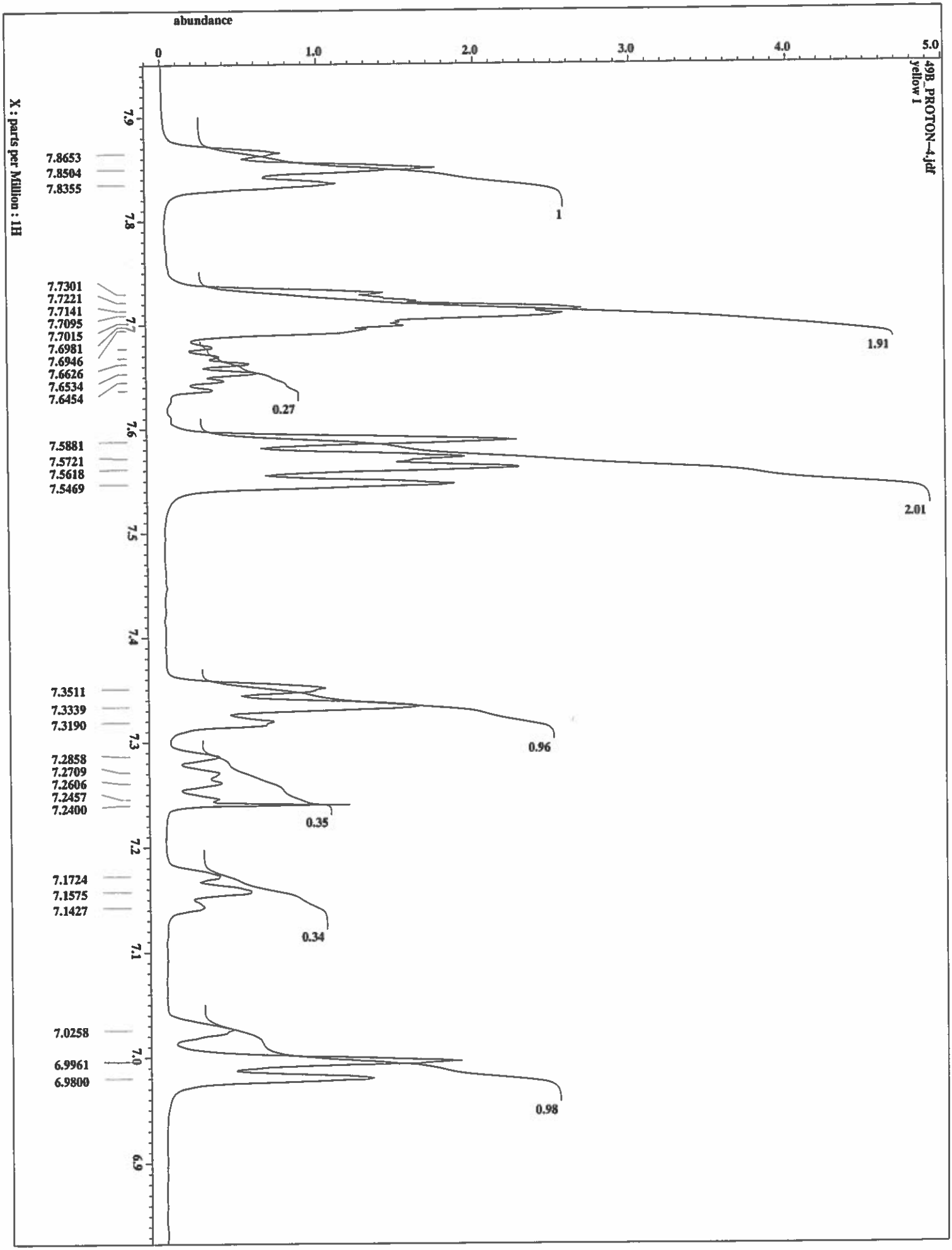


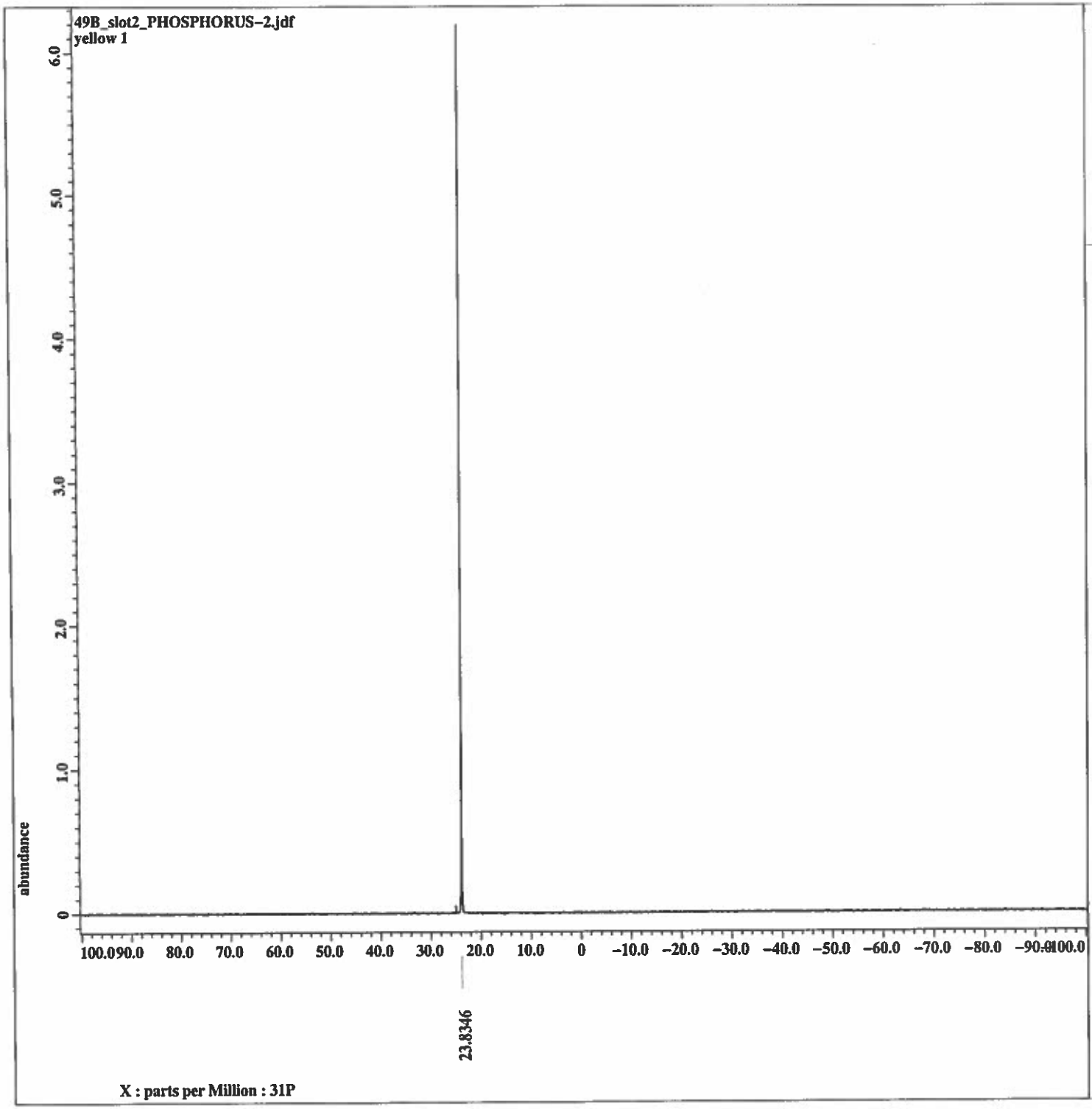


SOUTH ALABAMA JAGUARS

Filename	= 49B_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= 49B
Solvent	= CHLOROFORM-D
Changer_sample	= 2
Creation_time	= 1-JUL-2016 13:47:20
Revision_time	= 1-JUL-2016 13:29:15
Current_time	= 1-JUL-2016 13:29:15
Comment	= yellow 1
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
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_atn	= 4[dB]
X_pulse	= 6.675[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 34
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.3[dC]

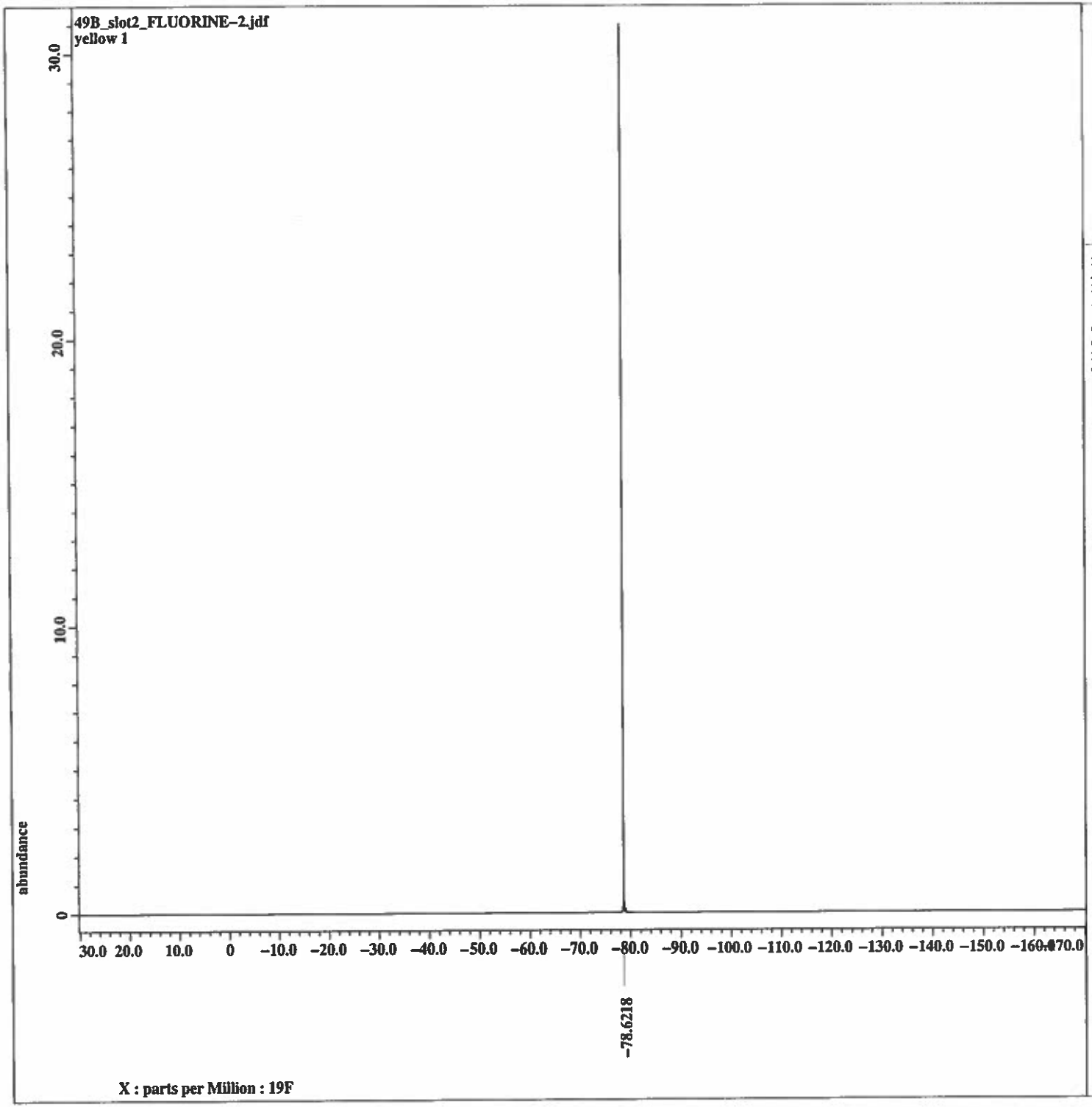

abundance
0
1.0
2.0
3.0
4.0
5.0
49B_PROTON-4.jdf
yellow 1
X : parts per Million : 1H
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.8504
7.7301
7.7221
7.7141
7.7095
7.7015
7.6981
7.5881
7.5721
7.5618
7.5469
7.3339
6.9961
1.91
2.01
0.96
0.35
0.34
0.98
2.1359
2.1302
1.7923
1.35
0.37


abundance
0
1.0
2.0
3.0
4.0
5.0
49B_PROTON-4.jdf
yellow 1
X : parts per Million : 1H
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
7.8653
7.8504
7.8355
7.7301
7.7221
7.7141
7.7095
7.7015
7.6981
7.6946
7.6626
7.6534
7.6454
7.5881
7.5721
7.5618
7.5469
7.3511
7.3339
7.3190
7.2858
7.2709
7.2606
7.2457
7.2400
7.1724
7.1575
7.1427
7.0258
6.9961
6.9800
1
1.91
0.27
2.01
0.96
0.35
0.34
0.98



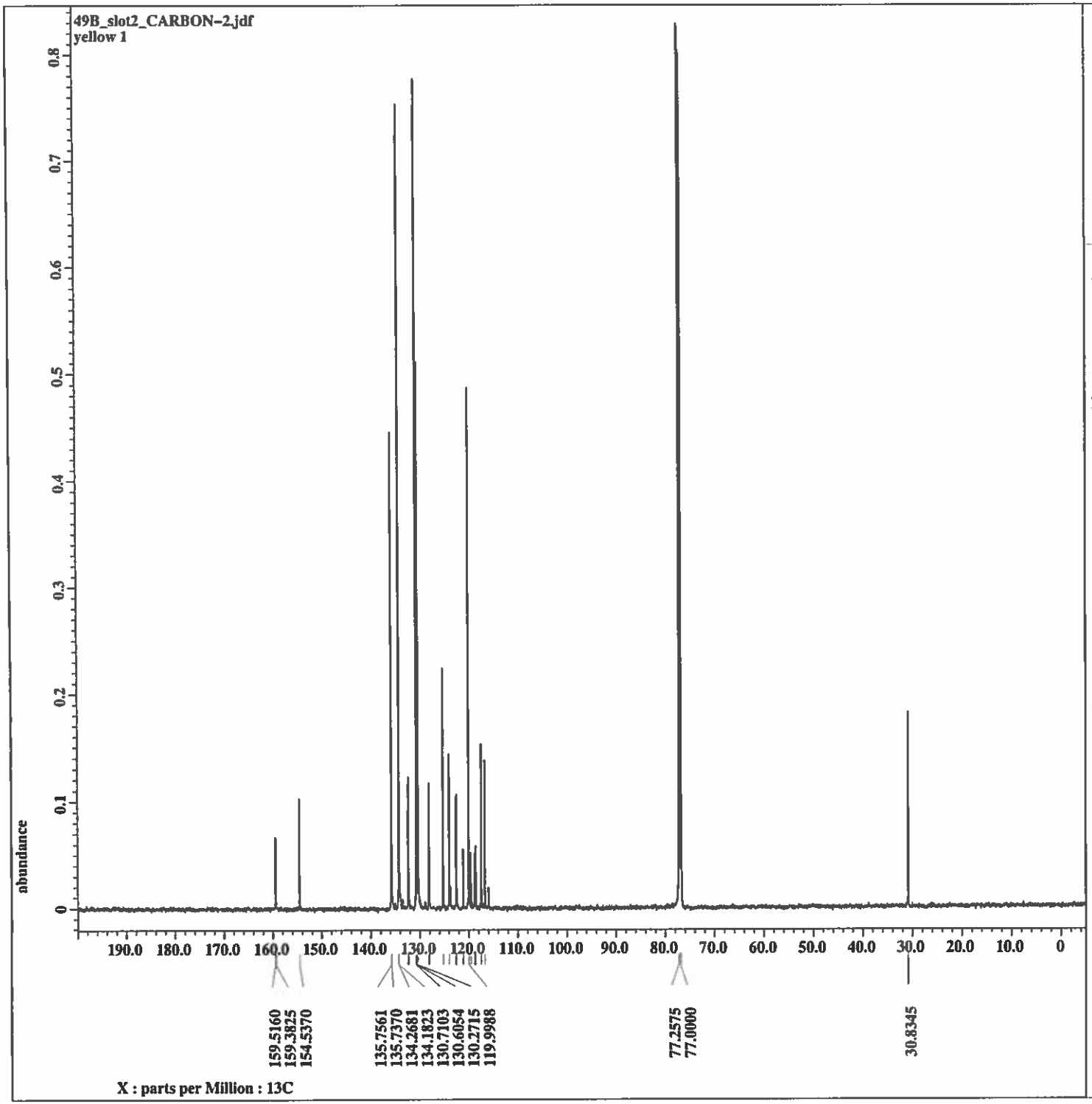
SOUTH ALABAMA JAGUARS

Filename	= 49B_slot2_PHOSPHORUS-
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#612204
Solvent	= CHLOROFORM-D
Changer_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	= yellow 1
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	= WALTZ
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	= 23.4[dC]



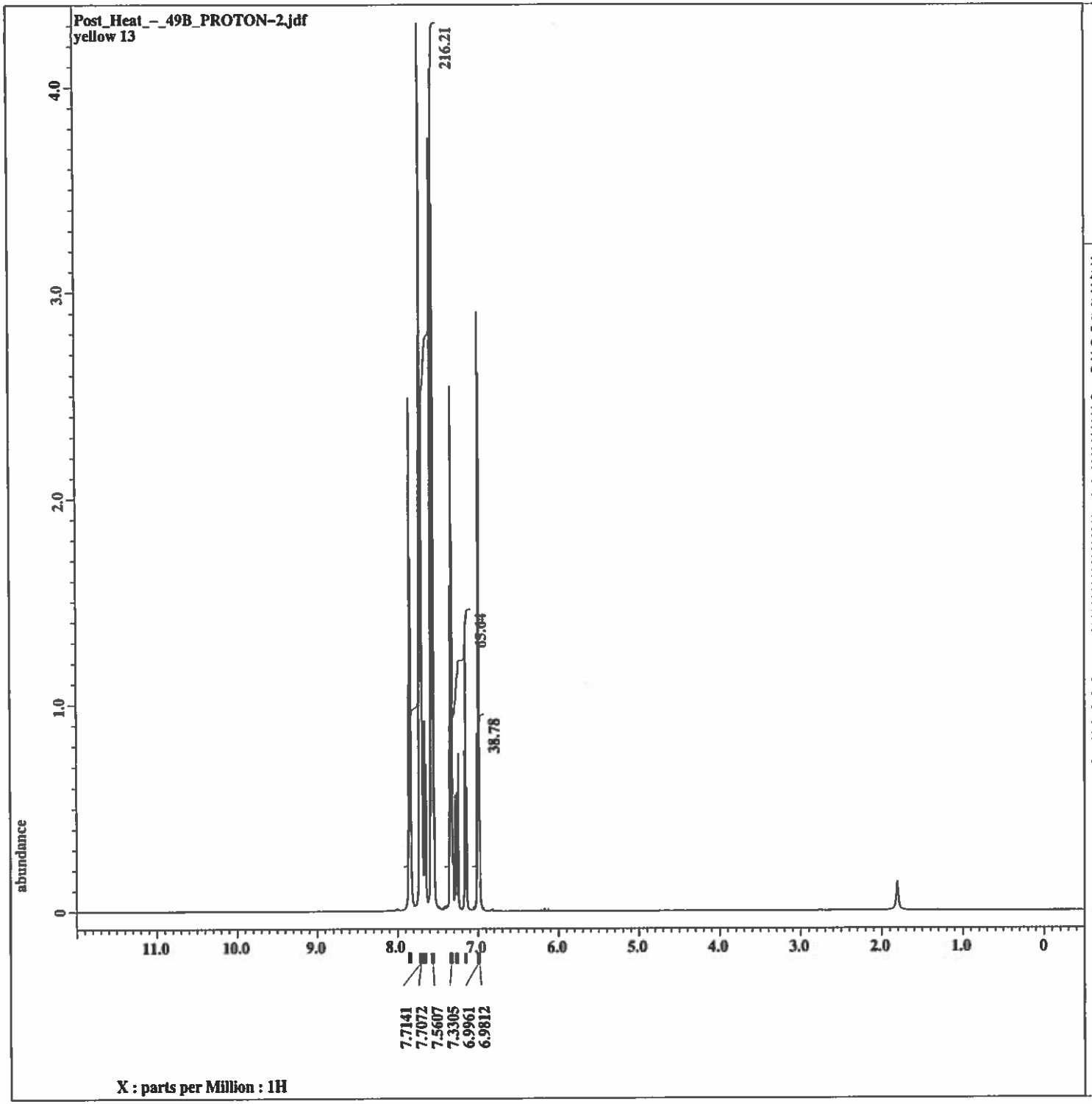
SOUTH ALABAMA JAGUARS

Filename	= 49B_slot2_FLUORINE-2.
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= S#549939
Solvent	= CHLOROFORM-D
Changer_sample	= 2
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	= 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]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 44
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.7[dC]



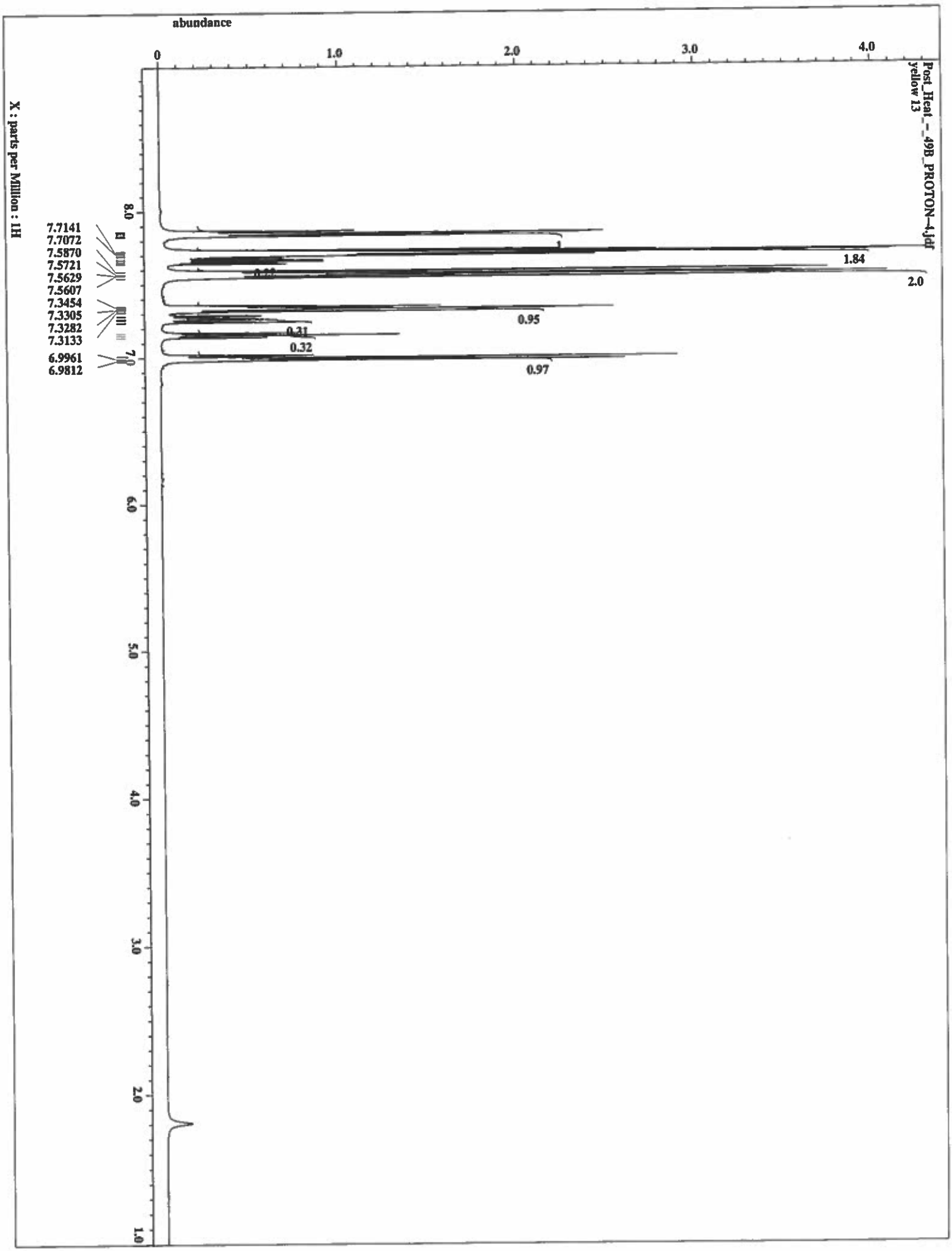
SOUTH ALABAMA JAGUARS

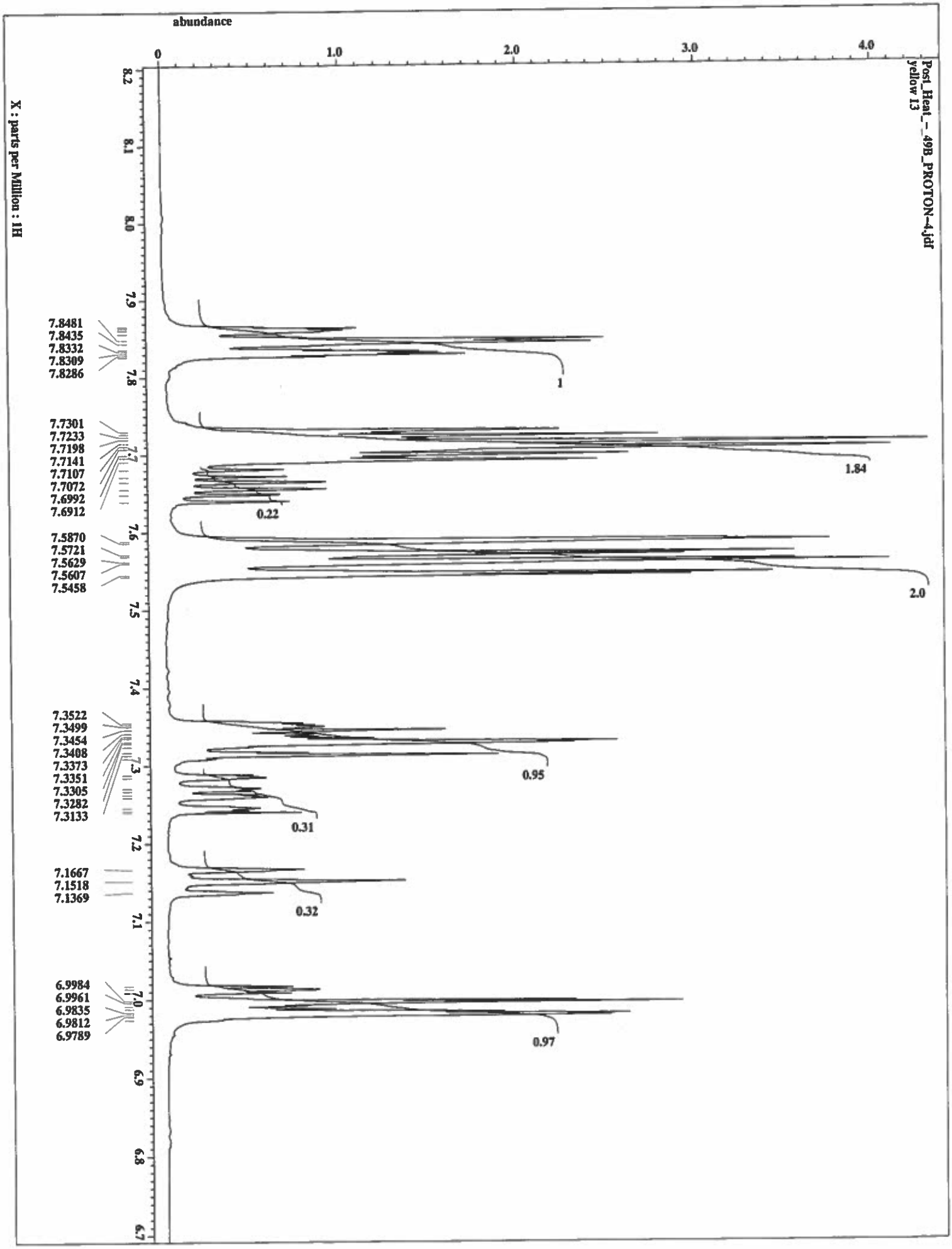
Filename	= 49B_slot2_CARBON-2.jd
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#845434
Solvent	= CHLOROFORM-D
Changer_sample	= 2
Creation_time	= 2-JUL-2016 02:14:54
Revision_time	= 2-JUL-2016 01:56:46
Current_time	= 2-JUL-2016 01:56:46
Comment	= yellow 1
Data_format	= 1D COMPLEX
Dim_size	= 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	= 23.2[dC]

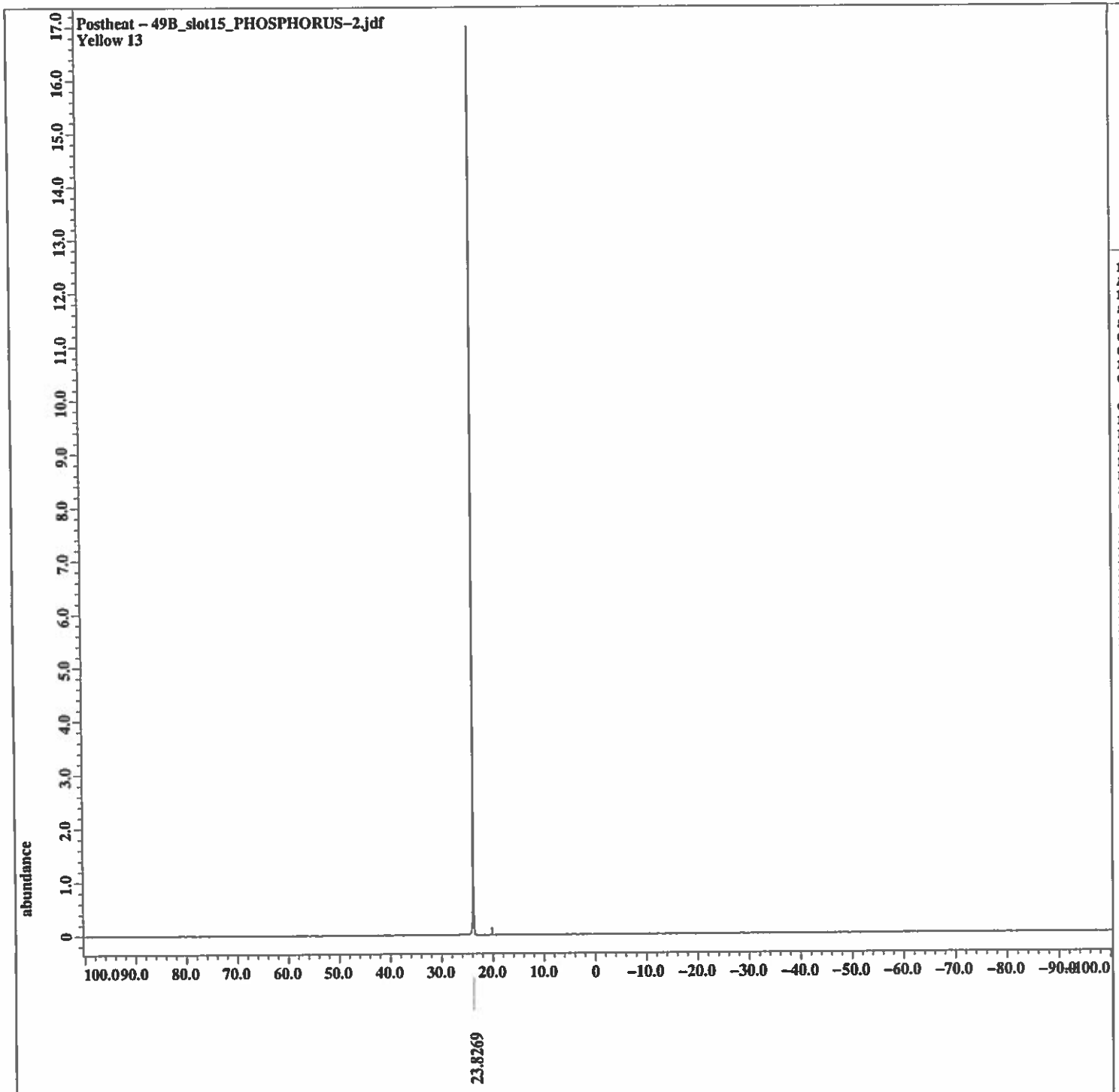


SOUTH ALABAMA JAGUARS

Filename	= Post_Heat_-_49B_PROTO
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= Post_Heat_-_49B
Solvent	= CHLOROFORM-D
Changer_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_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]
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_atn	= 4[dB]
X_pulse	= 6.675[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 28
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.7[dC]

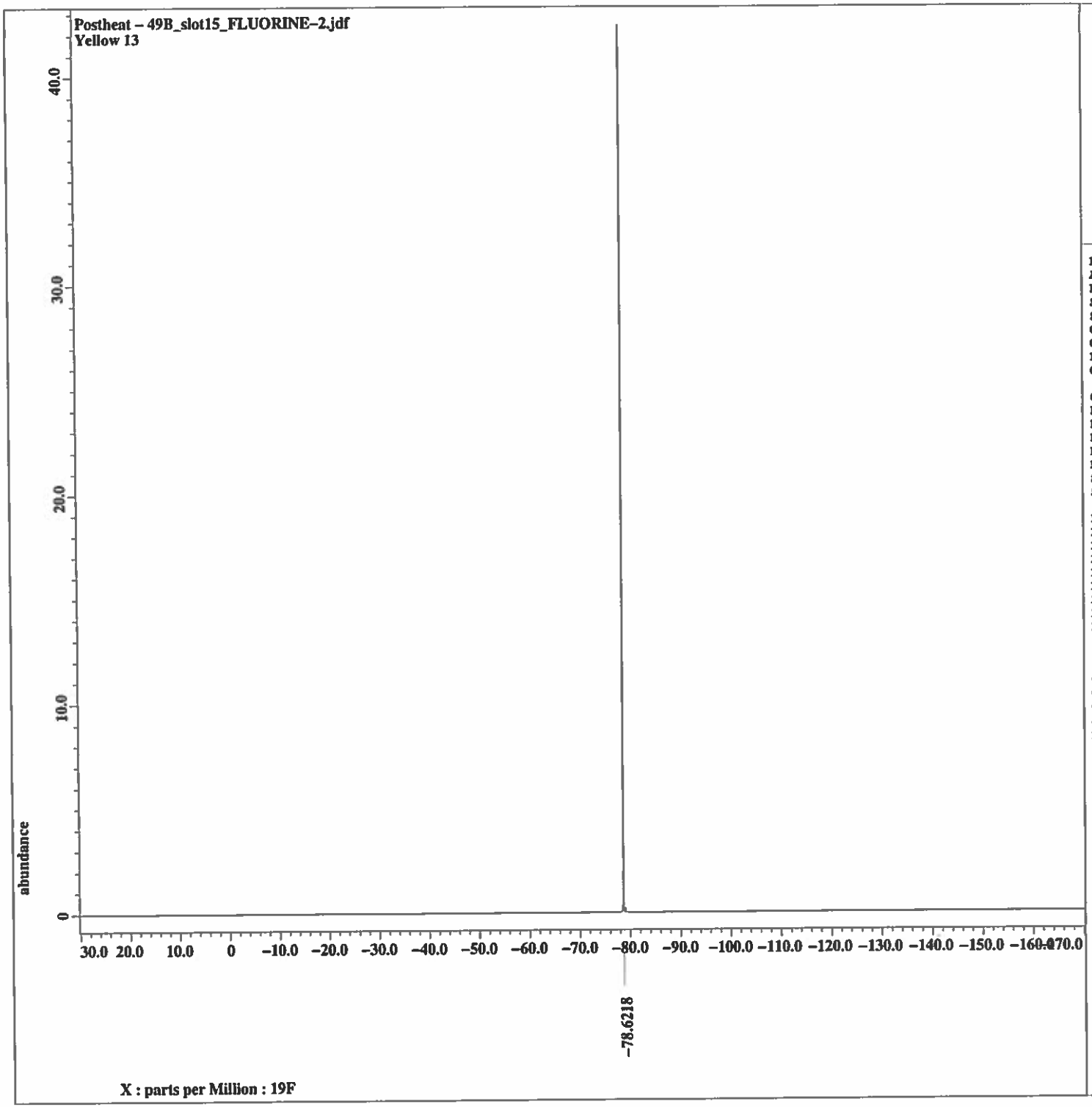

abundance
0
1.0
2.0
3.0
4.0
Post_Heat_-_49B_PROTON-4.jdf
yellow 13
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.7141
7.7072
7.5870
7.5721
7.5629
7.5607
7.3454
7.3305
7.3282
7.3133
6.9961
6.9812
1
1.84
2.0
0.95
0.31
0.32
0.97


abundance
0
1.0
2.0
3.0
4.0
Post_Heat_-_49B_PROTON-4.jdf
yellow 13
X : parts per Million : 1H
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
7.8481
7.8435
7.8332
7.8309
7.8286
1
7.7301
7.7233
7.7198
7.7141
7.7107
7.7072
7.6992
7.6912
1.84
0.22
7.5870
7.5721
7.5629
7.5607
7.5458
2.0
7.3522
7.3499
7.3454
7.3408
7.3373
7.3351
7.3305
7.3282
7.3133
0.95
0.31
7.1667
7.1518
7.1369
0.32
6.9984
6.9961
6.9835
6.9812
6.9789
0.97



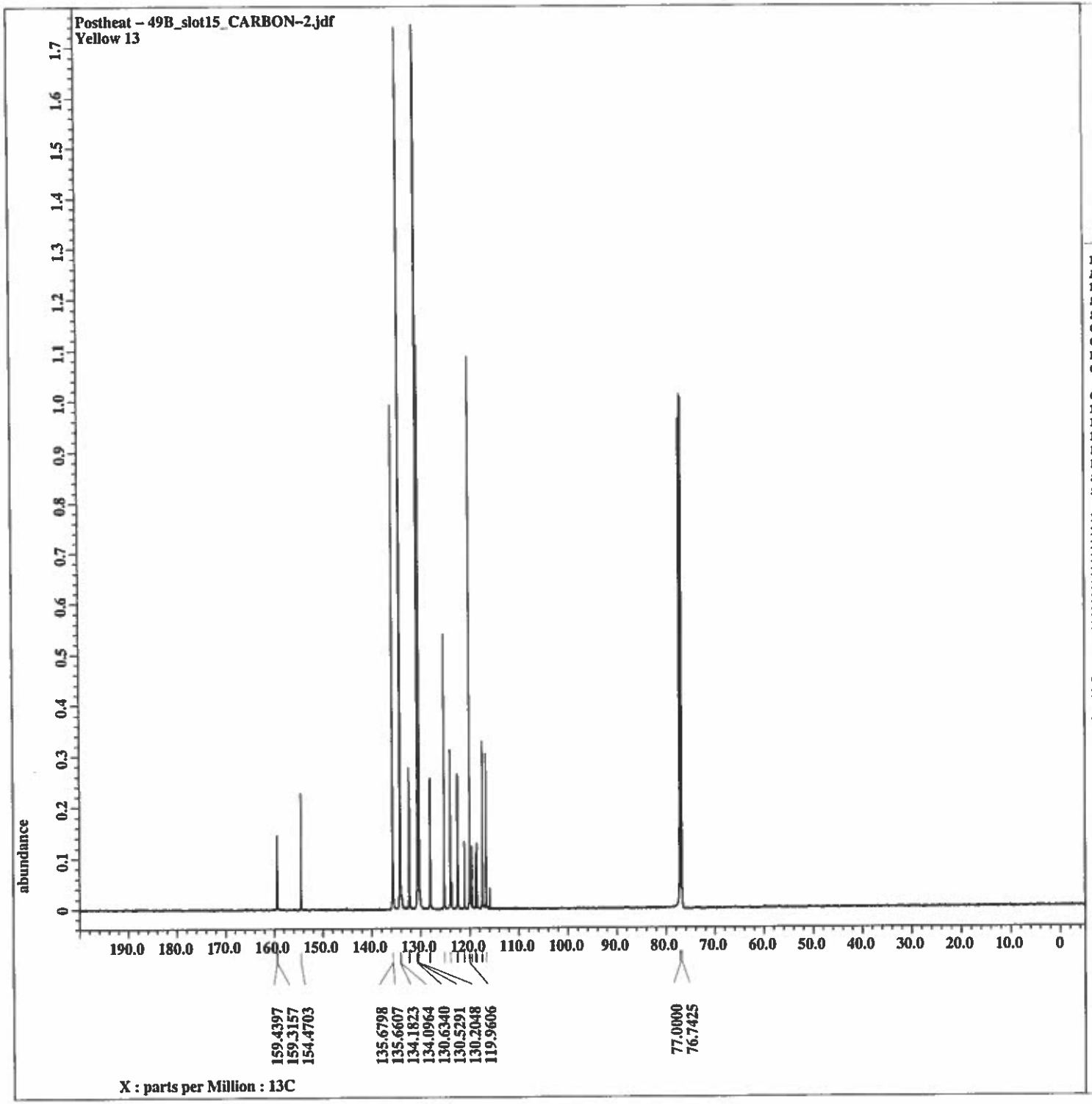
SOUTH ALABAMA JAGUARS

Filename	= Postheat - 49B_slot15
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#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
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	= WALTZ
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	= 23.5[dC]



SOUTH ALABAMA JAGUARS

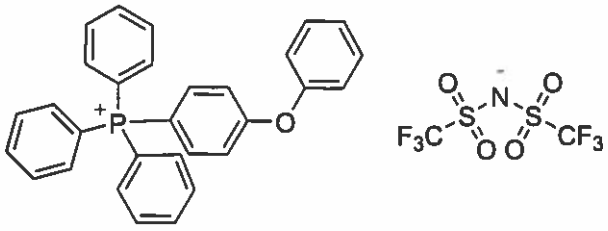
Filename	= Postheat - 49B_slot15
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= S#591437
Solvent	= CHLOROFORM-D
Changer_sample	= 15
Creation_time	= 1-JUL-2016 16:46:22
Revision_time	= 1-JUL-2016 16:28:17
Current_time	= 1-JUL-2016 16:28:17
Comment	= Yellow 13
Data_format	= 1D COMPLEX
Dim_size	= 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]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.7[dC]



SOUTH ALABAMA JAGUARS

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
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	= 23.3[dC]

COMPOUND 4



Atlantic Microlab, Inc.

No. Phosphonium 156A

lantic Blvd. Suite M
s, GA 30071
'anticmicrolab.com

Company/School U of South Alabama
Dept. Chemistry
Address Chem 223
City, State, Zip Mobile AL 36688

or/Supervisor: James Davis
C#

Name James Davis
Date 10/31/2016
Phone (251) 751-0520

ent	Theory	Found	
;	54.01	54.27	
l	3.40	3.42	
l	1.97	1.96	

Single ☒ Duplicate ☐

Elements Present: CHNPOSF

Analyze for: CHN

Hygroscopic ☐ Explosive ☐
M.P. unk B.P. none

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

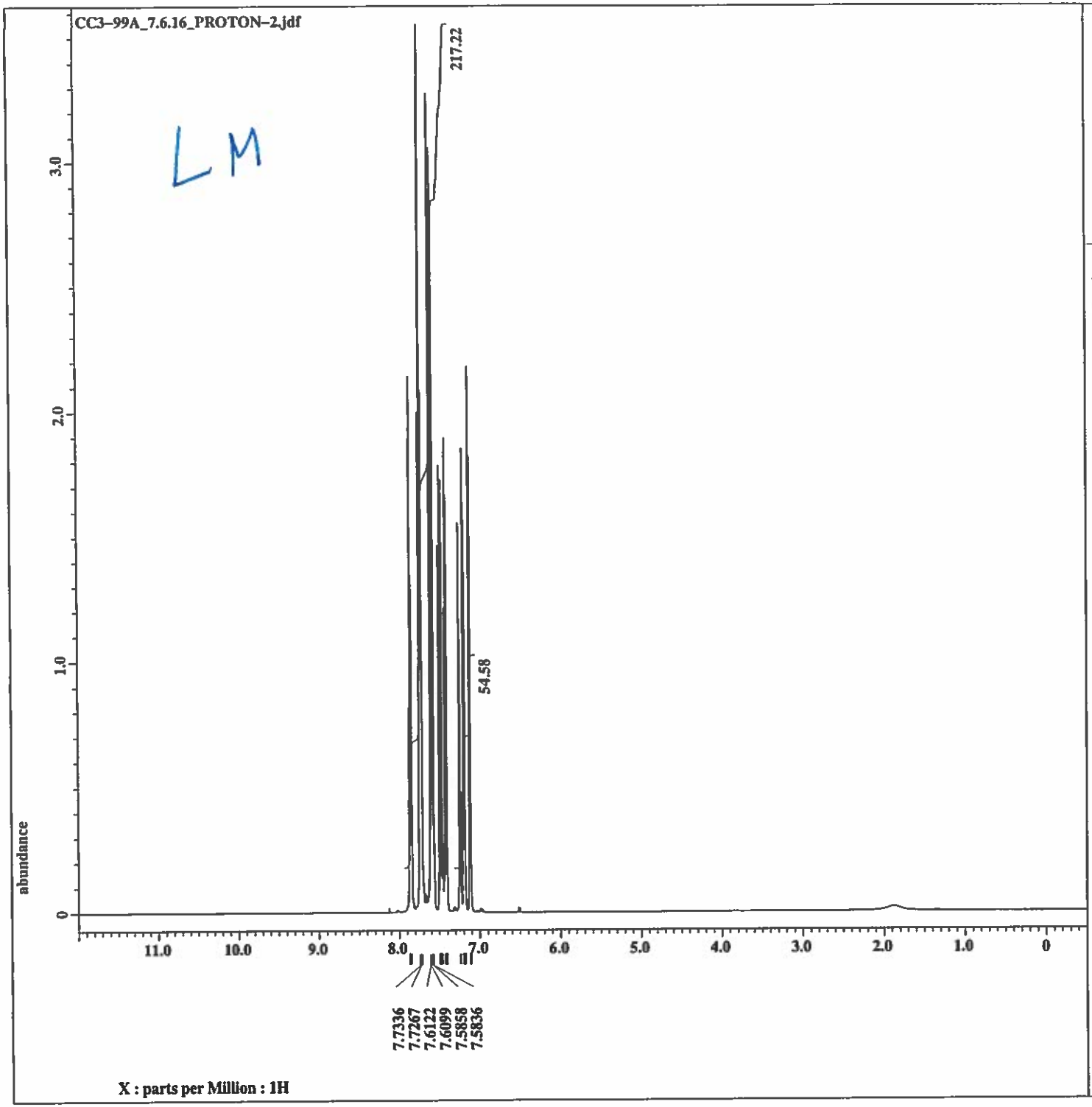
Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

Include Email Address or FAX # Below

jdavis@southalabama.edu

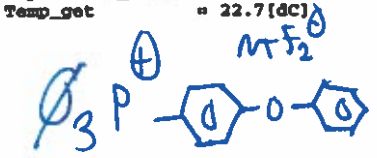
Received NOV 01 2016
Date Completed NOV 01 2016

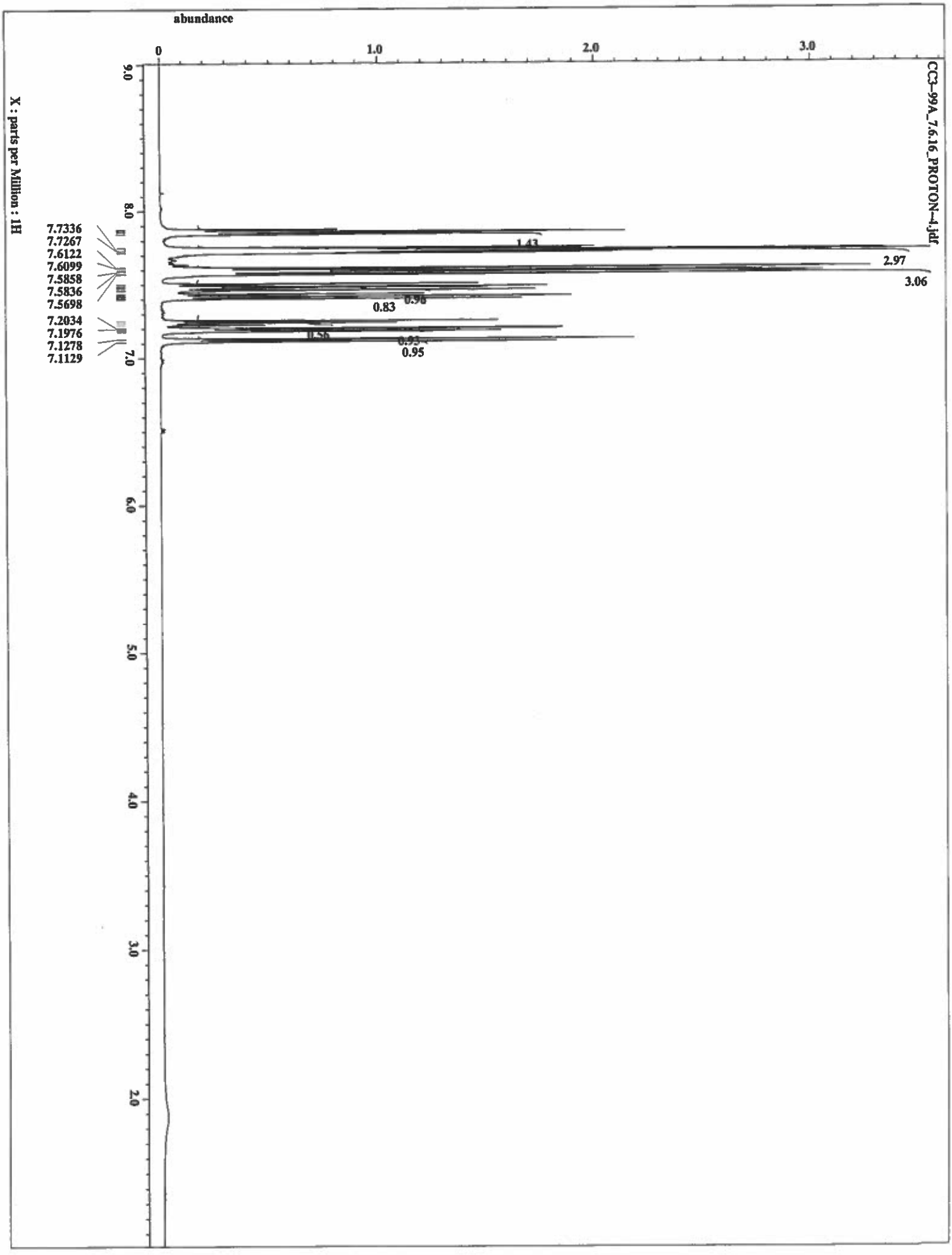
ks:

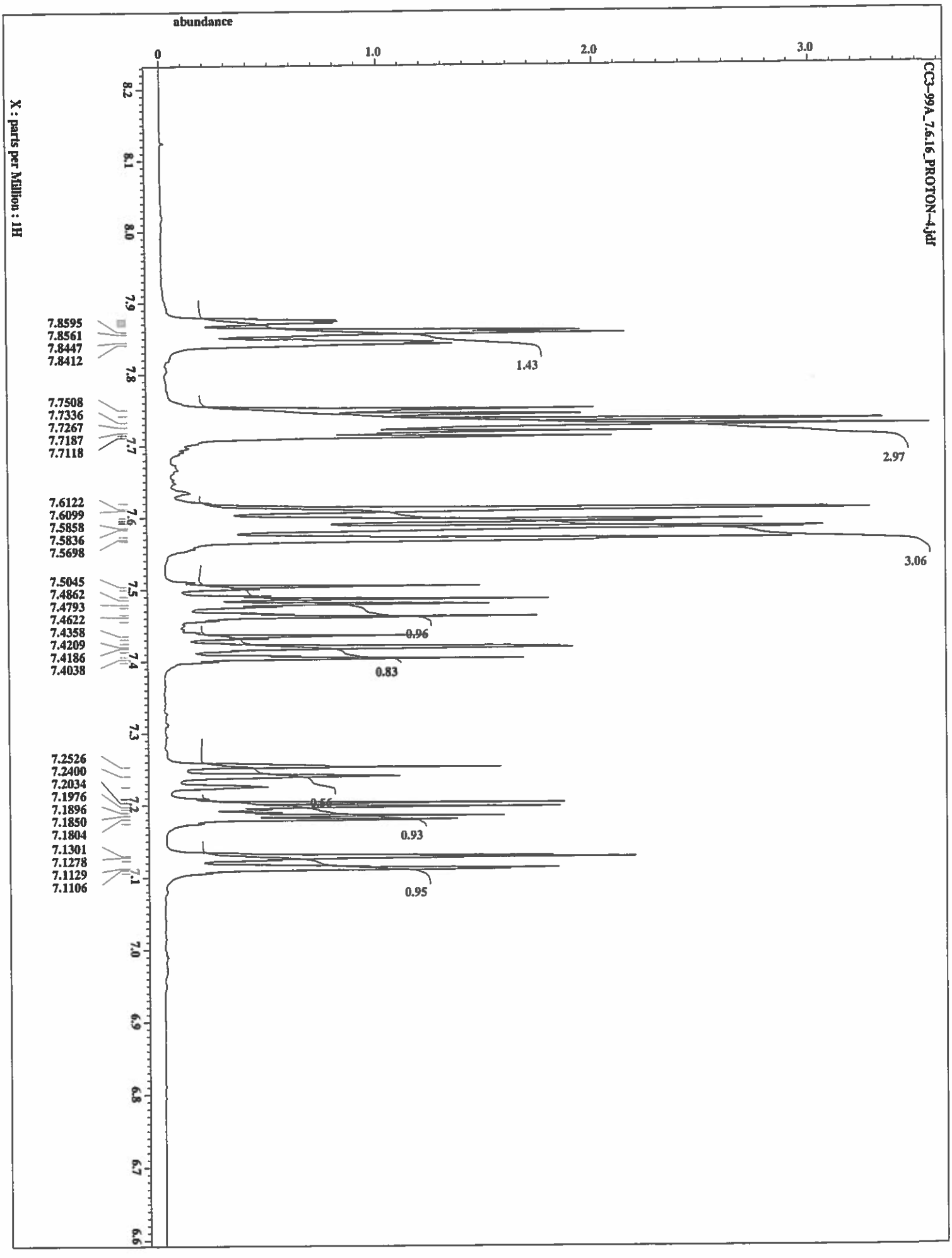


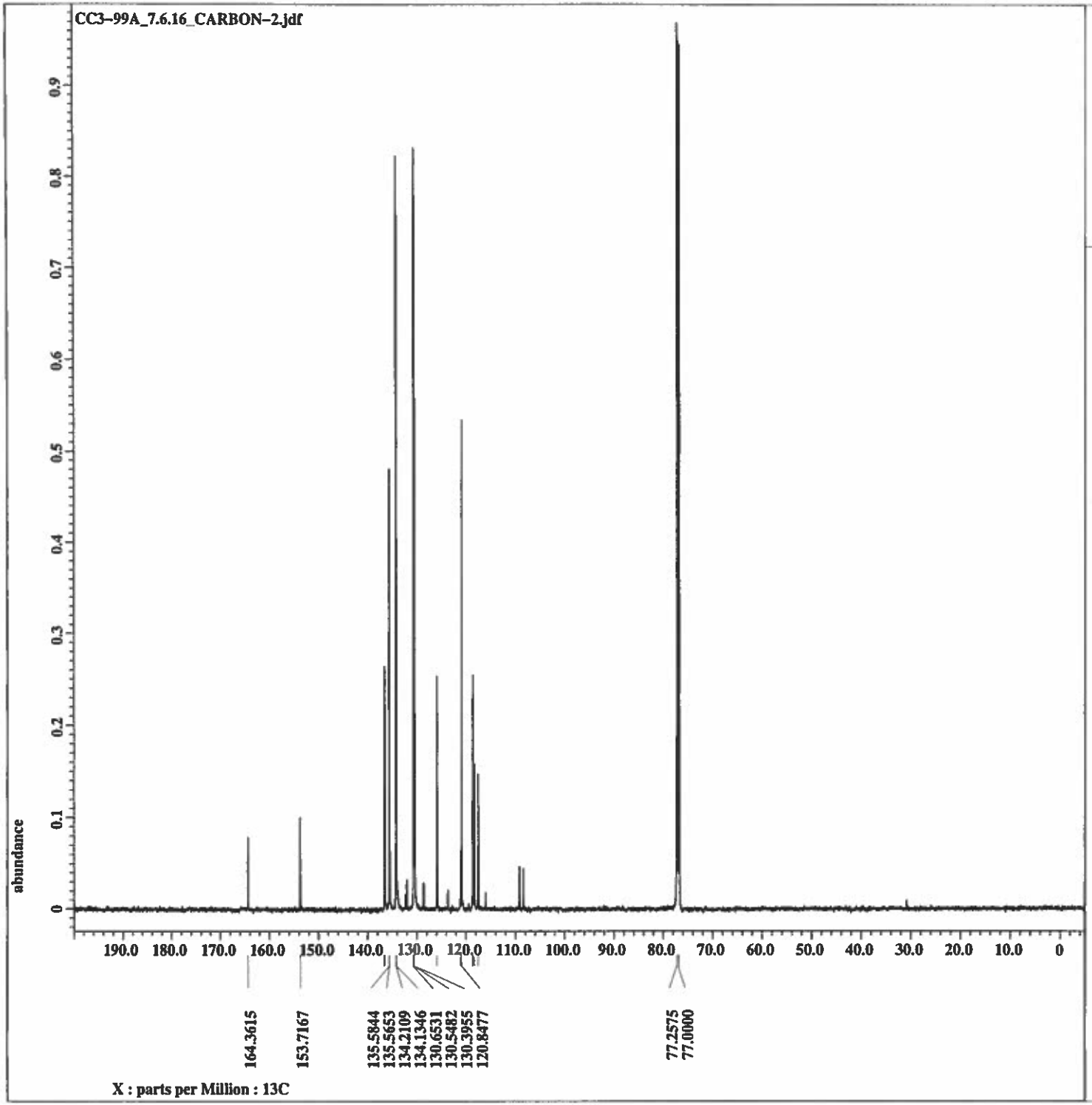
SOUTH ALABAMA JAGUARS

Filename	= CC3-99A_7.6.16_PROTON
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= CC3-99A_7.6.16
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 6-JUL-2016 16:48:03
Revision_time	= 6-JUL-2016 16:29:36
Current_time	= 6-JUL-2016 16:29:36
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 32
Total_scans	= 32
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
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 32
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.7[dC]



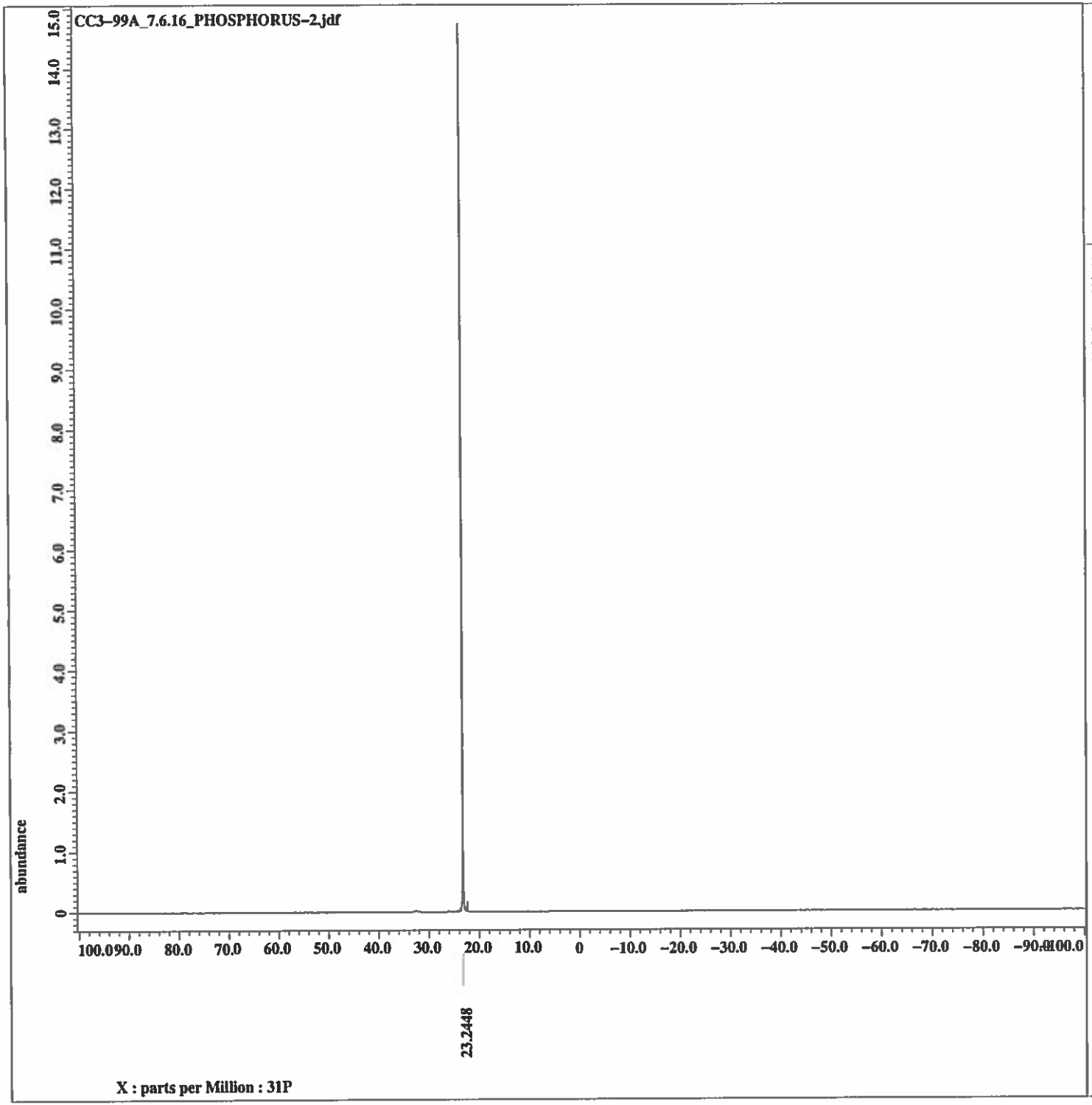

abundance
0
1.0
2.0
3.0
CC3-99A_7.6.16_PROTON-4.jdf
X : parts per Million : 1H
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
7.7336
7.7267
7.6122
7.6099
7.5858
7.5836
7.5698
7.2034
7.1976
7.1278
7.1129
1.43
2.97
3.06
0.83
0.96
0.56
0.93
0.95


abundance
0
1.0
2.0
3.0
CC3-99A_7.6.16_PROTON-4.jdf
X : parts per Million : 1H
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
7.8595
7.8561
7.8447
7.8412
1.43
7.7508
7.7336
7.7267
7.7187
7.7118
2.97
7.6122
7.6099
7.5858
7.5836
7.5698
3.06
7.5045
7.4862
7.4793
7.4622
7.4358
7.4209
7.4186
7.4038
0.96
0.83
7.2526
7.2400
7.2034
7.1976
7.1896
7.1850
7.1804
7.1301
7.1278
7.1129
7.1106
0.56
0.93
0.95



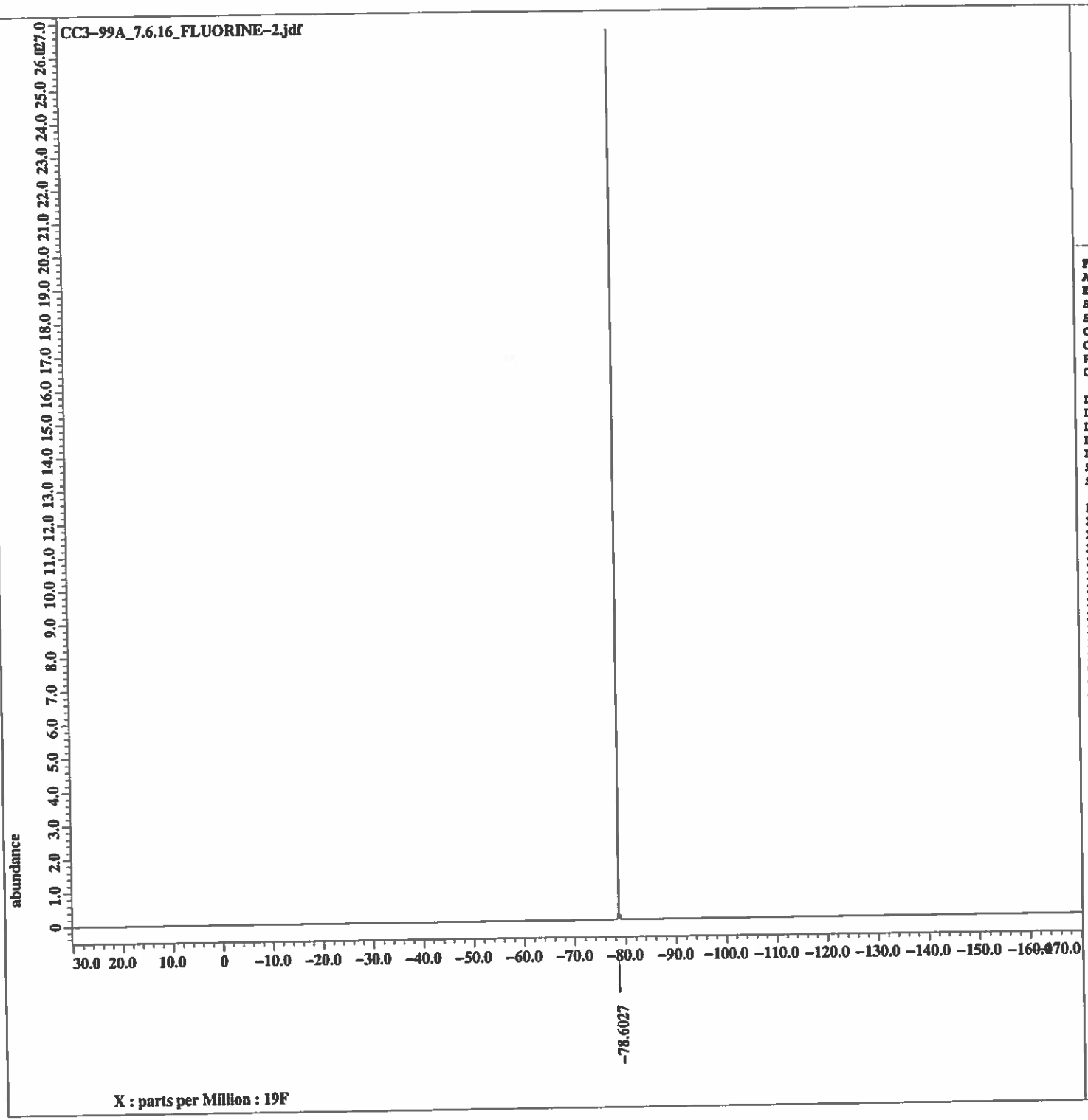
SOUTH ALABAMA JAGUARS

Filename	= CC3-99A_7.6.16_CARBON
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= CC3-99A_7.6.16
Solvent	= CHLOROFORM-D
Changer_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
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	= 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]
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	= 23.9[dC]

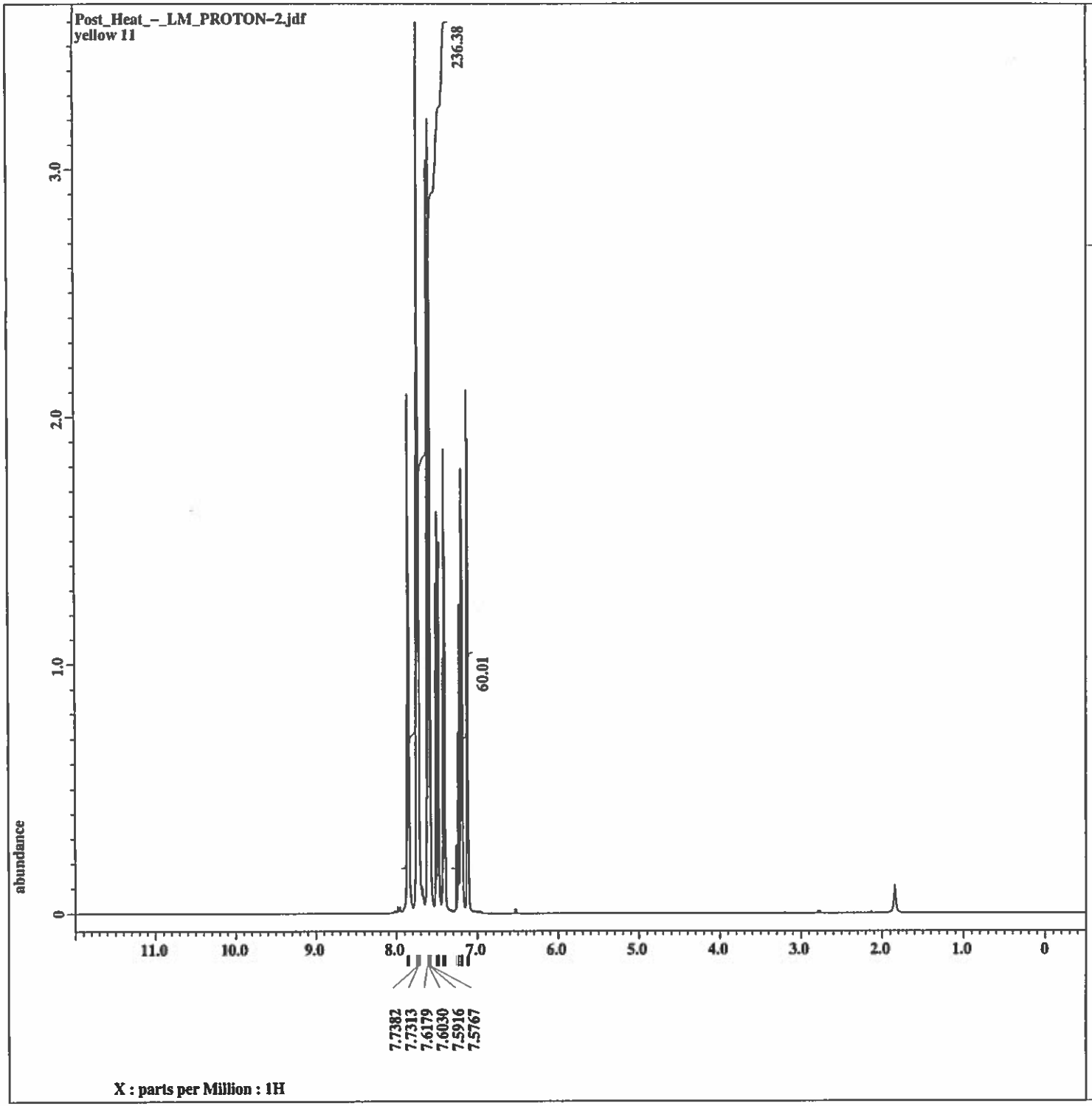


SOUTH ALABAMA JAGUARS

Filename	= CC3-99A_7.6.16_PHOSPH
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= CC3-99A_7.6.16
Solvent	= CHLOROFORM-D
Changer_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	= 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	= 512
Total_scans	= 512
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	= 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	= 23.6[dC]

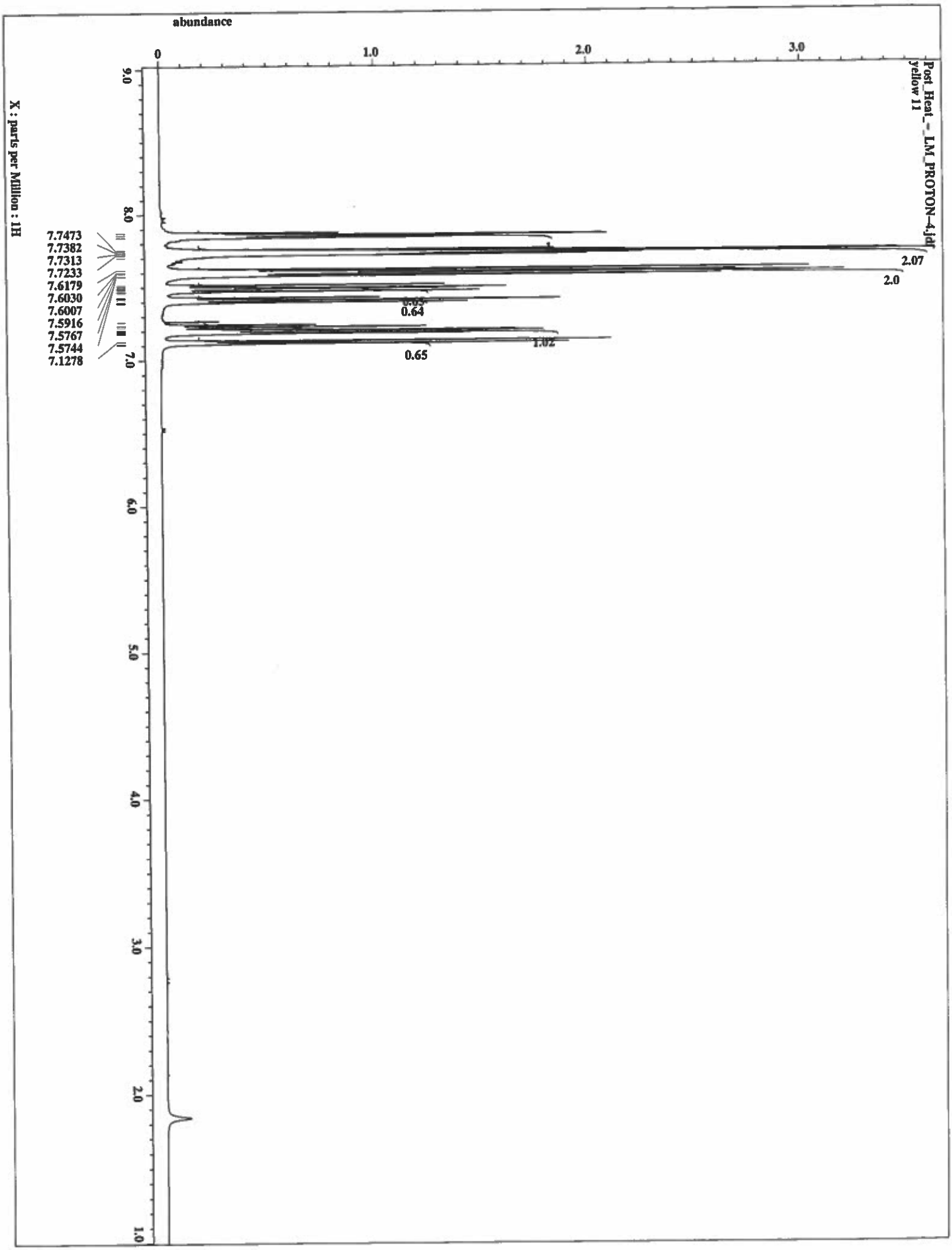


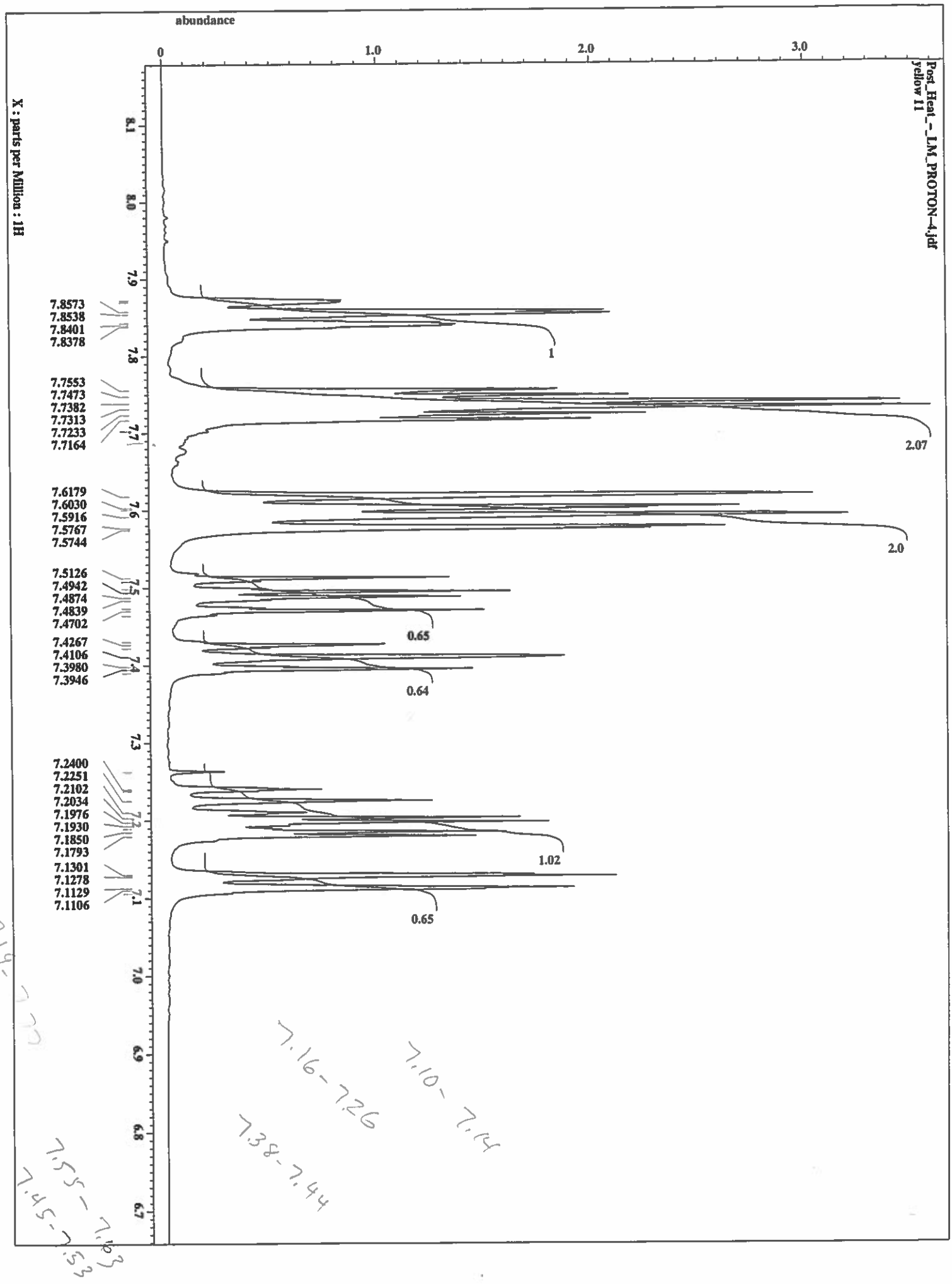
Filename	= CC3-99A_7.6.16_FLUORI
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= CC3-99A_7.6.16
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 7-JUL-2016 07:39:26
Revision_time	= 7-JUL-2016 07:20:55
Current_time	= 7-JUL-2016 07:20:55
Data_format	= 1D COMPLEX
Dim_size	= 52428
Dim_title	= 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]
Tri_domain	= 19F
Tri_freq	= 470.62046084[MHz]
Tri_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
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 42
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 23.1[dC]

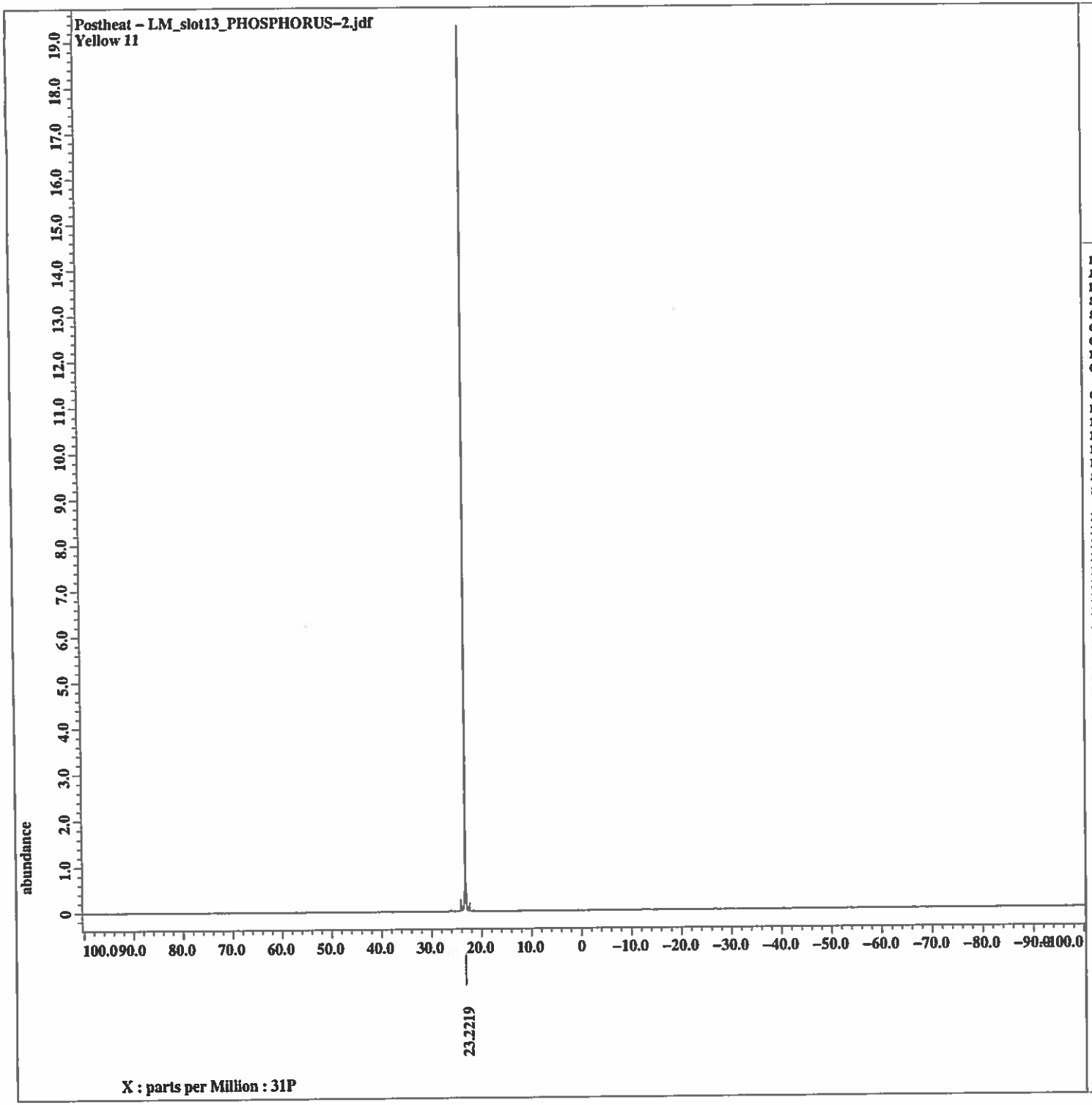


SOUTH ALABAMA JAGUARS

Filename	= Post_Heat_-_LM_PROTON
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= Post_Heat_-_LM
Solvent	= CHLOROFORM-D
Changer_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	= yellow 11
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
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_atn	= 4[dB]
X_pulse	= 6.675[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 24
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.3[dC]

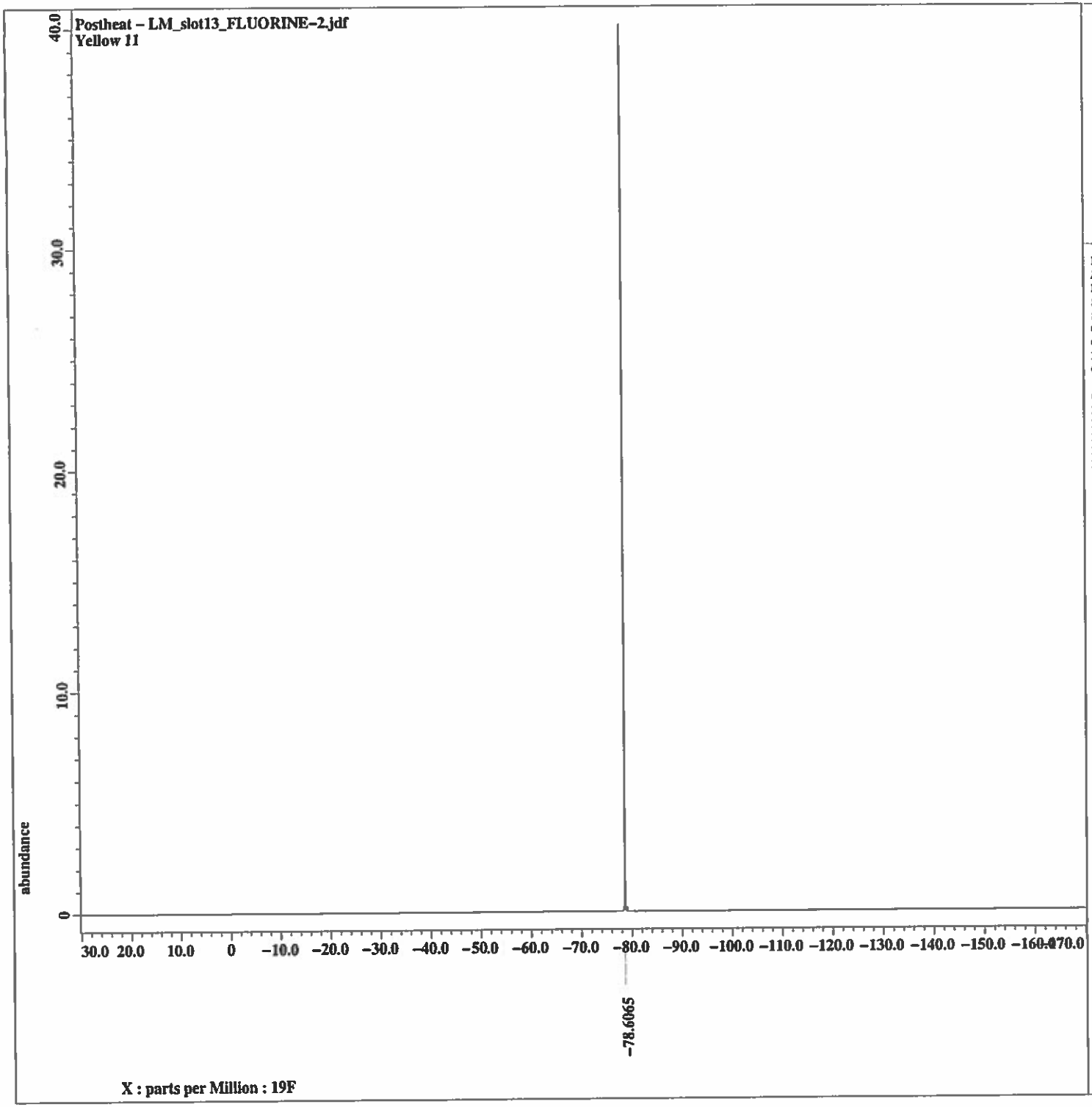

abundance
0
1.0
2.0
3.0
Post_Heat_-_LM_PROTON-4.jdf
yellow 11
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.7473
7.7382
7.7313
7.7233
7.6179
7.6030
7.6007
7.5916
7.5767
7.5744
7.1278
2.07
2.0
0.64
1.02
0.65
X : parts per Million : 1H


abundance
0
1.0
2.0
3.0
Post_Heat_-_LM_PROTON-4.jdf
yellow 11
X : parts per Million : 1H
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
7.8573
7.8538
7.8401
7.8378
7.7553
7.7473
7.7382
7.7313
7.7233
7.7164
7.6179
7.6030
7.5916
7.5767
7.5744
7.5126
7.4942
7.4874
7.4839
7.4702
7.4267
7.4106
7.3980
7.3946
7.2400
7.2251
7.2102
7.2034
7.1976
7.1930
7.1850
7.1793
7.1301
7.1278
7.1129
7.1106
1
2.07
2.0
0.65
0.64
1.02
0.65



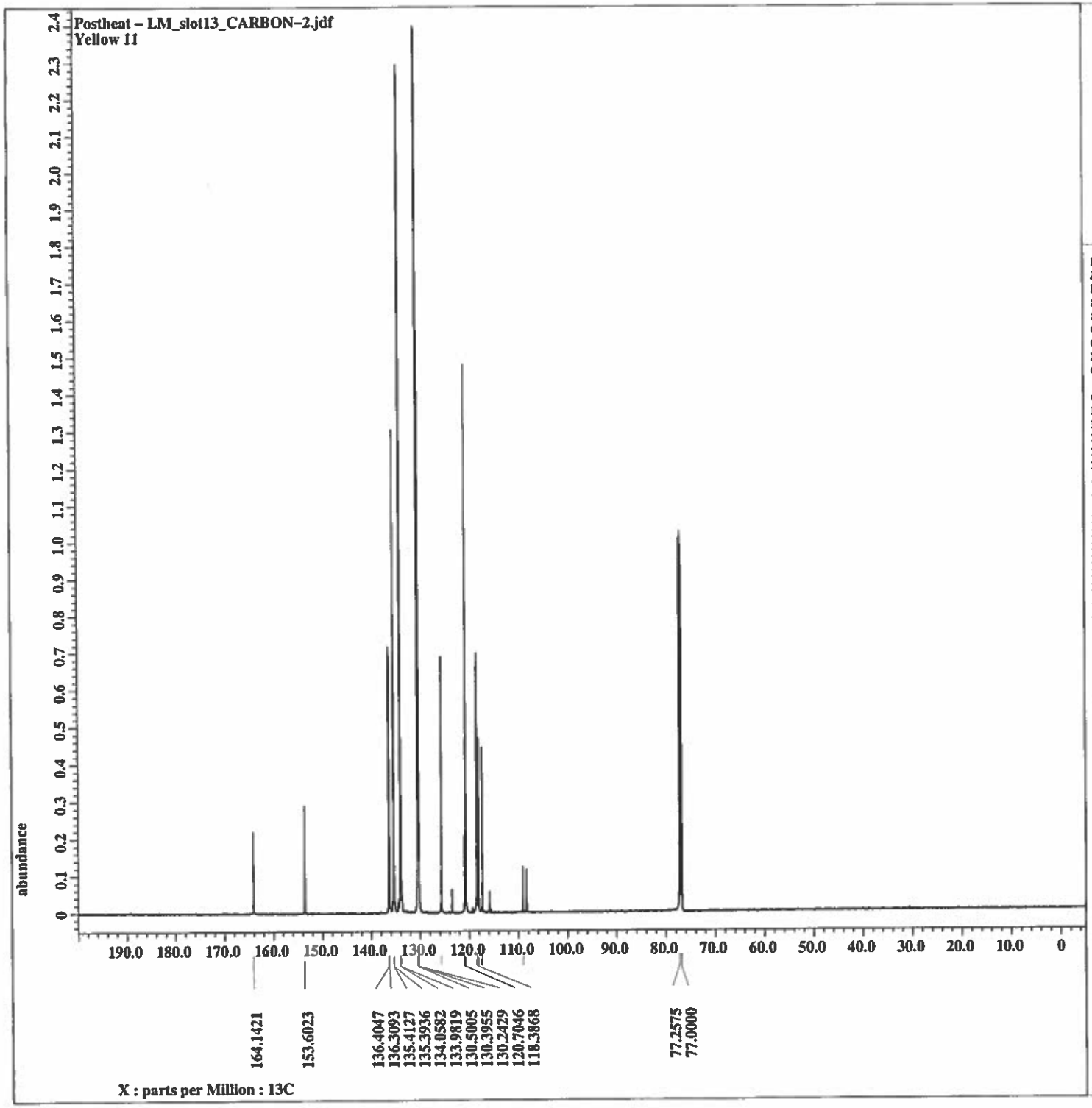
SOUTH ALABAMA JAGUARS

Filename	= Postheat - LM_slot13_
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#706760
Solvent	= CHLOROFORM-D
Changer_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_noe	= 20.5[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 56
Relaxation_delay	= 2[s]
Repetition_time	= 2.64487424[s]
Temp_get	= 23.1[dC]



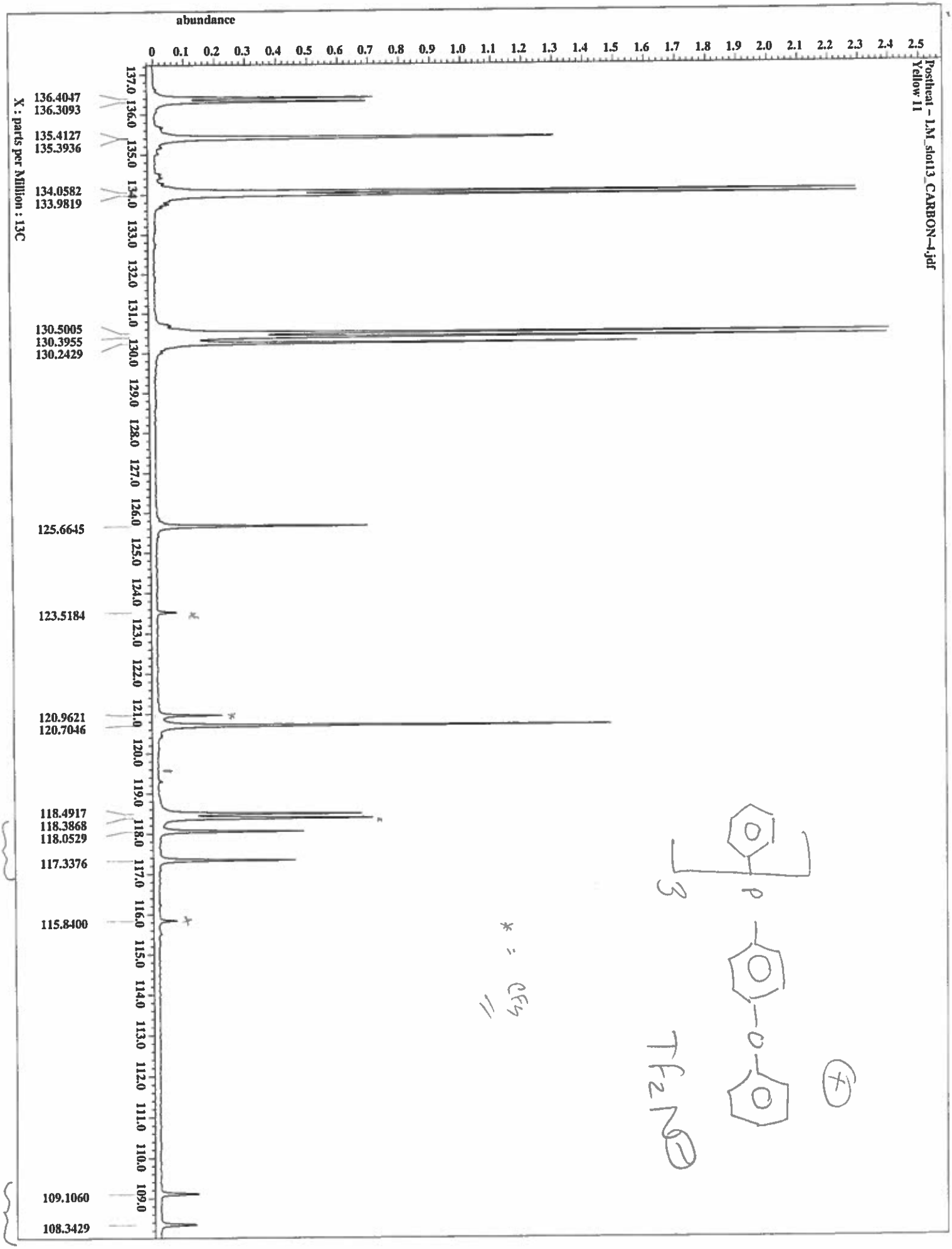
SOUTH ALABAMA JAGUARS

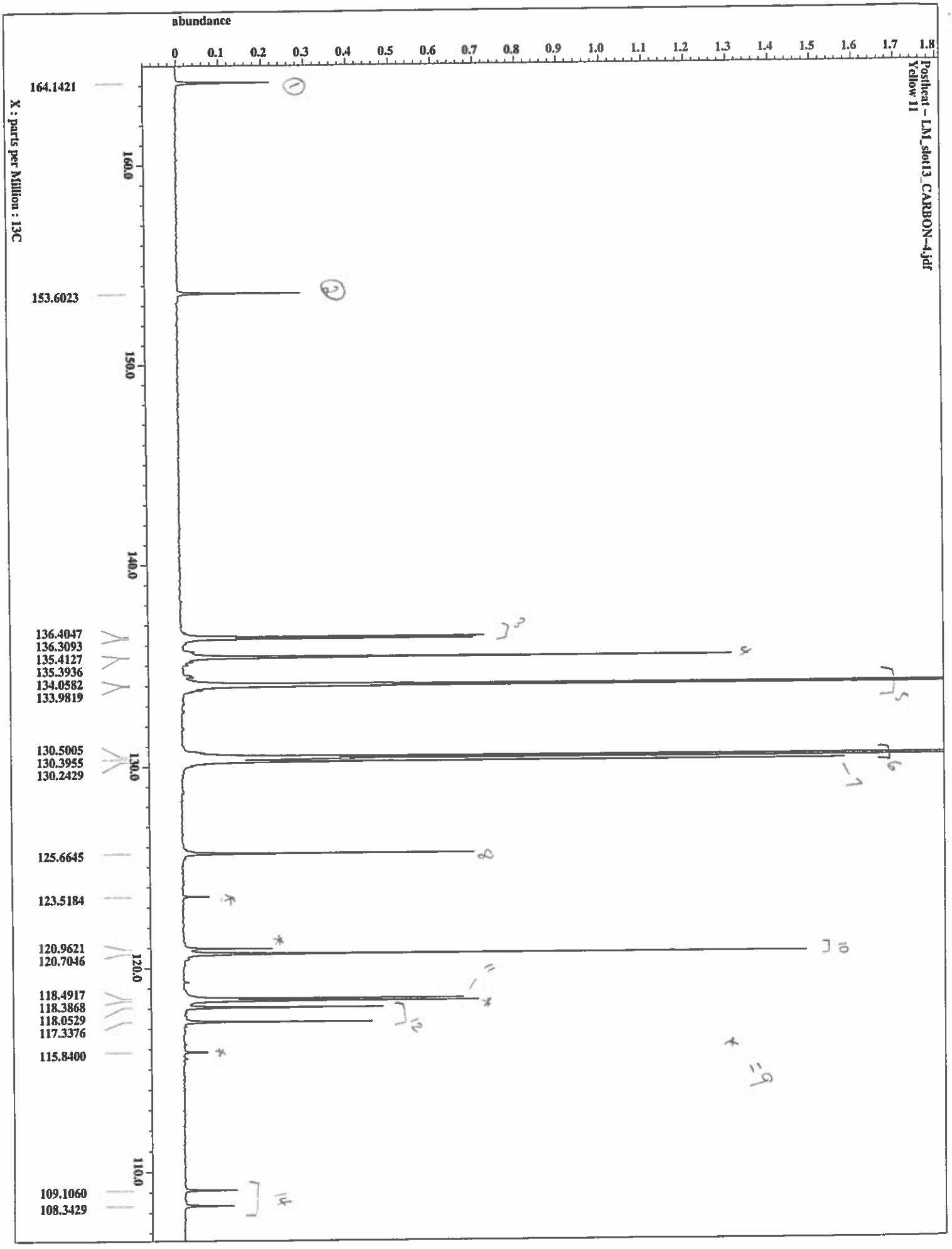
Filename	= Postheat - LM_slot13_
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= S#584563
Solvent	= CHLOROFORM-D
Changer_sample	= 13
Creation_time	= 1-JUL-2016 16:35:04
Revision_time	= 1-JUL-2016 16:16:59
Current_time	= 1-JUL-2016 16:16:59
Comment	= Yellow 11
Data_format	= 1D COMPLEX
Dim_size	= 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]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.6[dC]



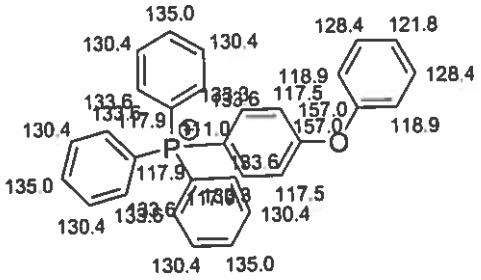
SOUTH ALABAMA JAGUARS

Filename	= Postheat - LM_slot13_
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#22217
Solvent	= CHLOROFORM-D
Changer_sample	= 13
Creation_time	= 3-JUL-2016 03:23:03
Revision_time	= 3-JUL-2016 03:04:54
Current_time	= 3-JUL-2016 03:04:54
Comment	= Yellow 11
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	= 23.9[dC]

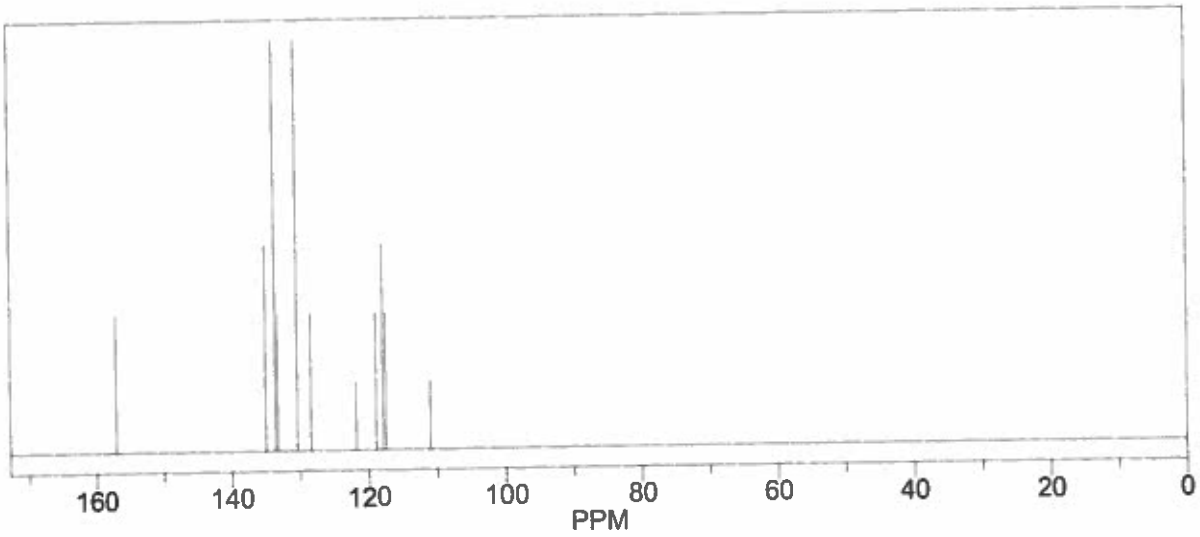

abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3 2.4 2.5
Postheat - LM_slot13_CARBON-4.jdf
Yellow 11
X : parts per Million : 13C
136.4047
136.3093
135.4127
135.3936
134.0582
133.9819
130.5005
130.3955
130.2429
125.6645
123.5184
120.9621
120.7046
118.4917
118.3868
118.0529
117.3376
115.8400
109.1060
108.3429
137.0 136.0 135.0 134.0 133.0 132.0 131.0 130.0 129.0 128.0 127.0 126.0 125.0 124.0 123.0 122.0 121.0 120.0 119.0 118.0 117.0 116.0 115.0 114.0 113.0 112.0 111.0 110.0 109.0
* : CF3
TFMO
(x)
TP-C
T-PC


abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8
Postheat – LM_slot13_CARBON-4.jdf
Yellow 11
X : parts per Million : 13C
164.1421
153.6023
136.4047
136.3093
135.4127
135.3936
134.0582
133.9819
130.5005
130.3955
130.2429
125.6645
123.5184
120.9621
120.7046
118.4917
118.3868
118.0529
117.3376
115.8400
109.1060
108.3429
160.0
150.0
140.0
130.0
120.0
110.0

ChemNMR ^{13}C Estimation



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

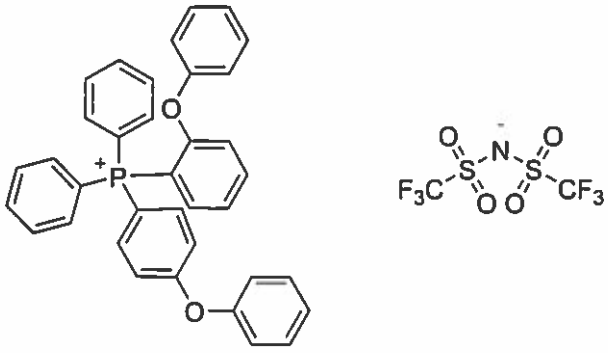


Protocol of the C-13 NMR Prediction: (Lib=S)

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*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*C*1
		0.9	general corrections
C	157.0	128.5	1-benzene
		27.6	1 -O-1:C*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*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*C*1
		0.2	general corrections
CH	118.9	128.5	1-benzene
		-11.2	1 -O-1:C*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*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*C*1
		0.2	general corrections
CH	118.9	128.5	1-benzene
		-11.2	1 -O-1:C*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*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*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*C*1
		0.2	general corrections

COMPOUND 5



Atlantic Microlab, Inc.

No. Phosphonium 49C

lantic Blvd. Suite M
ss, GA 30071
lanticmicrolab.com

Company/School U of South Alabama
Dept. Chemistry
Address Chem 223
City, State, Zip Mobile AL 36688

or/Supervisor: James Davis
C#

Name James Davis Date 10/31/2016
Phone (251) 751-0520

ent	Theory	Found	
C	56.79	56.58	
H	3.51	3.56	
N	1.74	1.76	

Single ☐ Duplicate ☐

Elements Present: CHNPOSF

Analyze for: CHN

Hygroscopic ☐ Explosive ☐
M.P. unk B.P. none

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

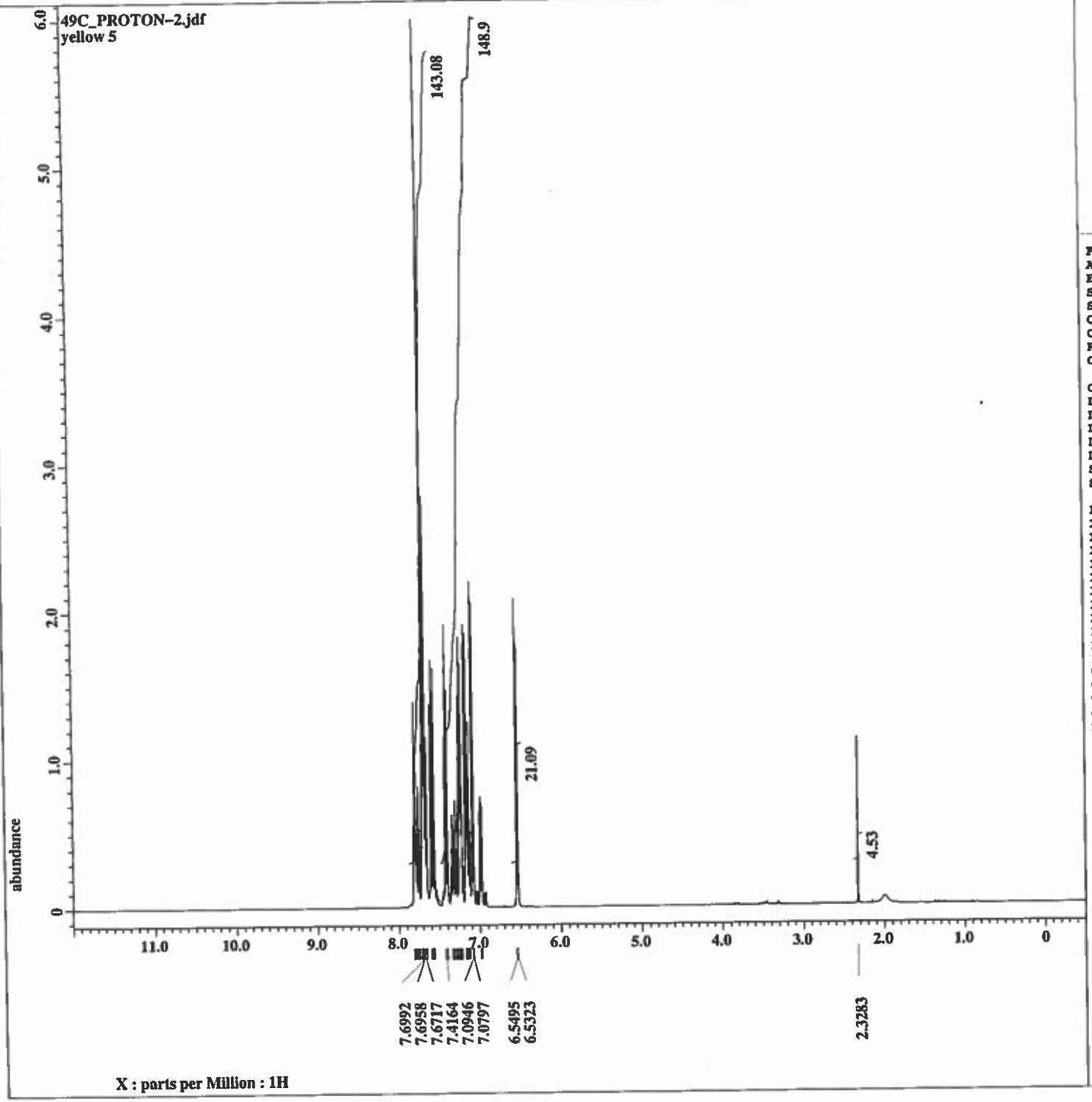
Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

Include Email Address or FAX # Below

jdavis@southalabama.edu

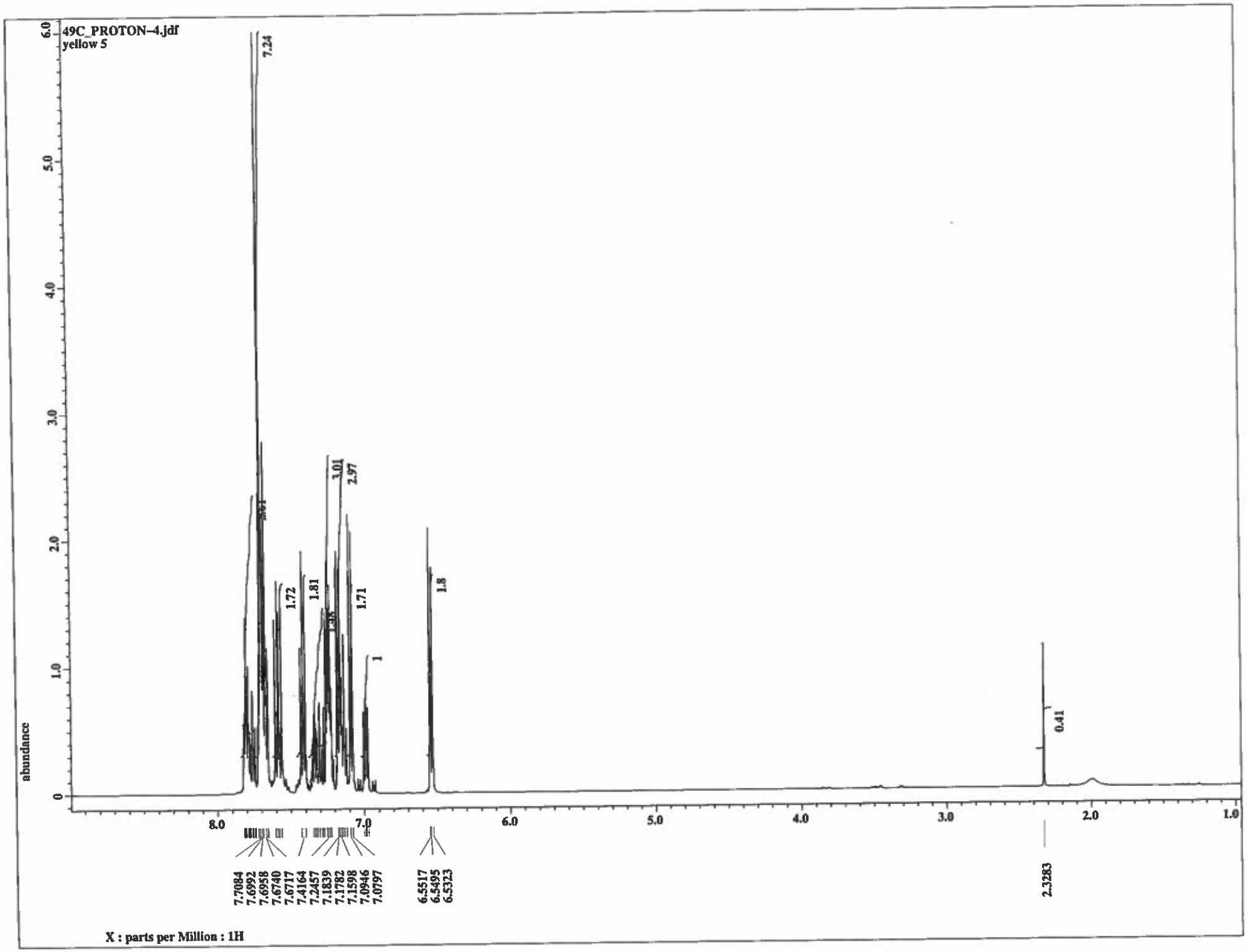
Received NOV 01 2016 Date Completed NOV 01 2016

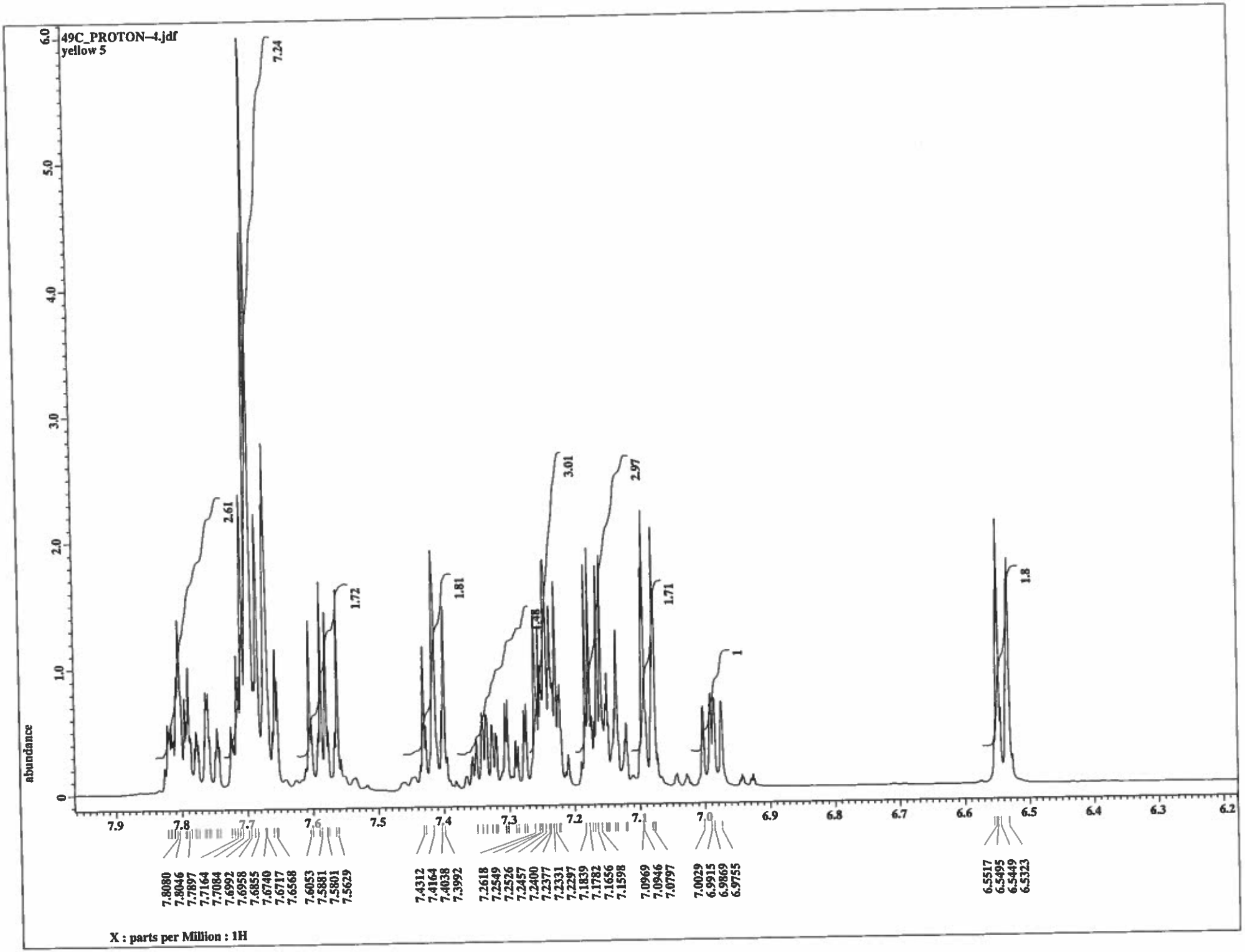
arks:



SOUTH ALABAMA JAGUARS

Filename	= 49C_PROTON-2.jdf
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[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 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
Tri_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
abundance
7.24
3.01
2.97
1.72
1.81
1.71
1.8
1
0.41
7.7084
7.6992
7.6958
7.6740
7.6717
7.4164
7.2457
7.1839
7.1782
7.1598
7.0946
7.0797
6.5517
6.5495
6.5323
2.3283
X : parts per Million : 1H


49C_PROTON-4.jdf
yellow 5
abundance
X : parts per Million : 1H
7.24
2.61
1.72
1.81
3.01
2.97
1.71
1
1.8
7.8080
7.8046
7.7897
7.7164
7.7084
7.6992
7.6958
7.6855
7.6740
7.6717
7.6568
7.6053
7.5881
7.5801
7.5629
7.4312
7.4164
7.4038
7.3992
7.2618
7.2549
7.2526
7.2457
7.2400
7.2377
7.2331
7.2297
7.1839
7.1782
7.1656
7.1598
7.0969
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7.0029
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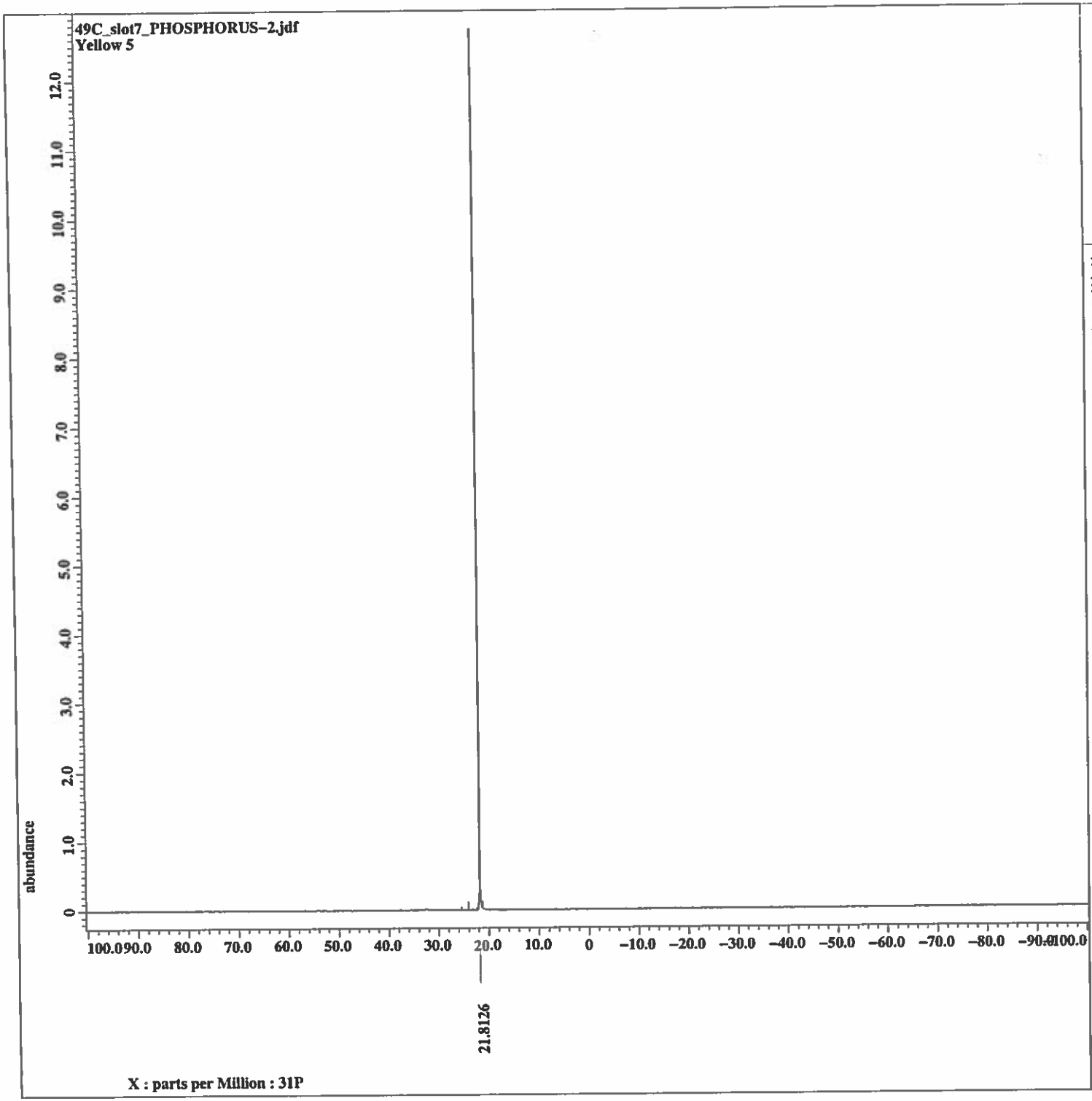
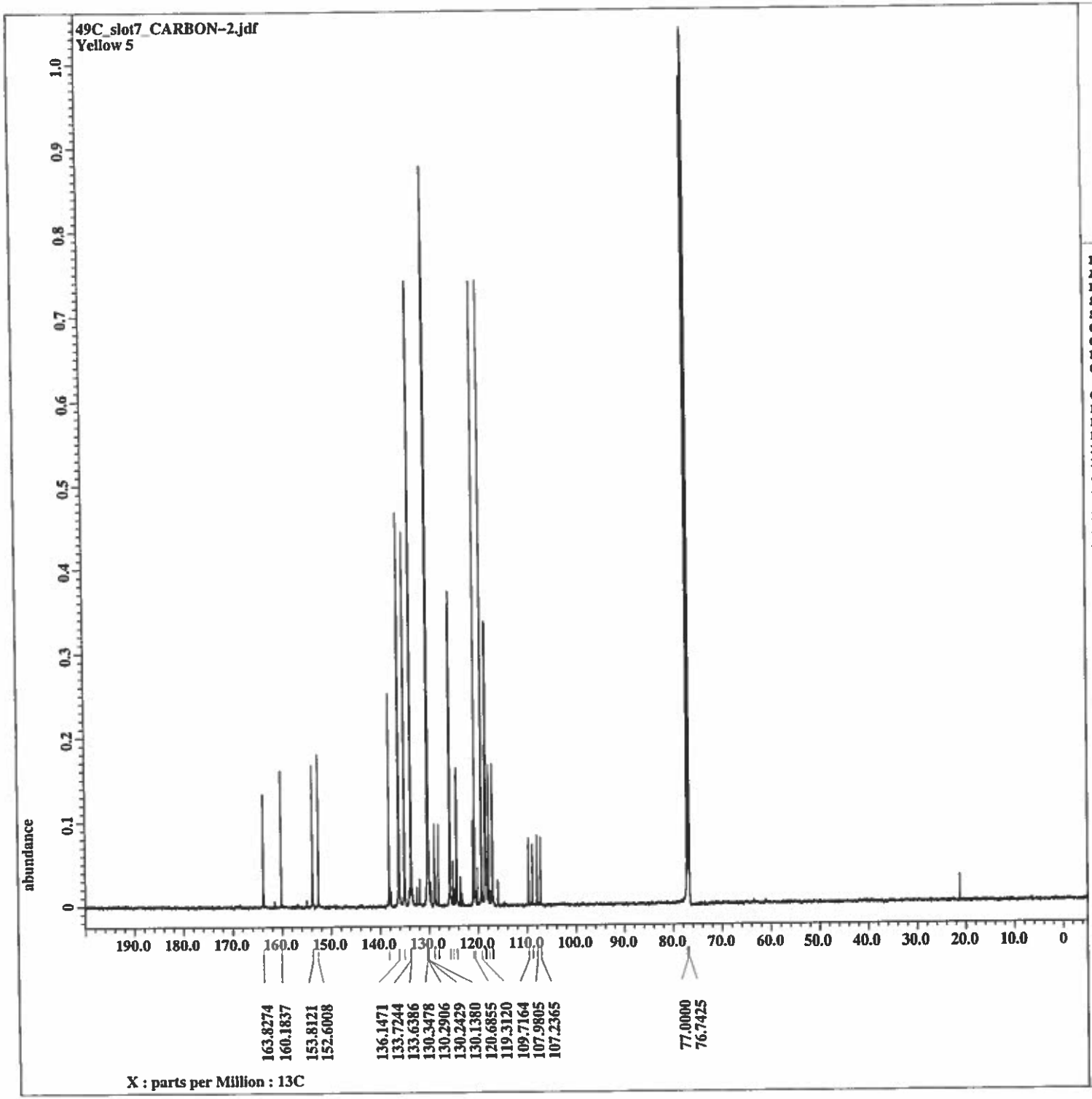
6.9755
6.5517
6.5495
6.5449
6.5323

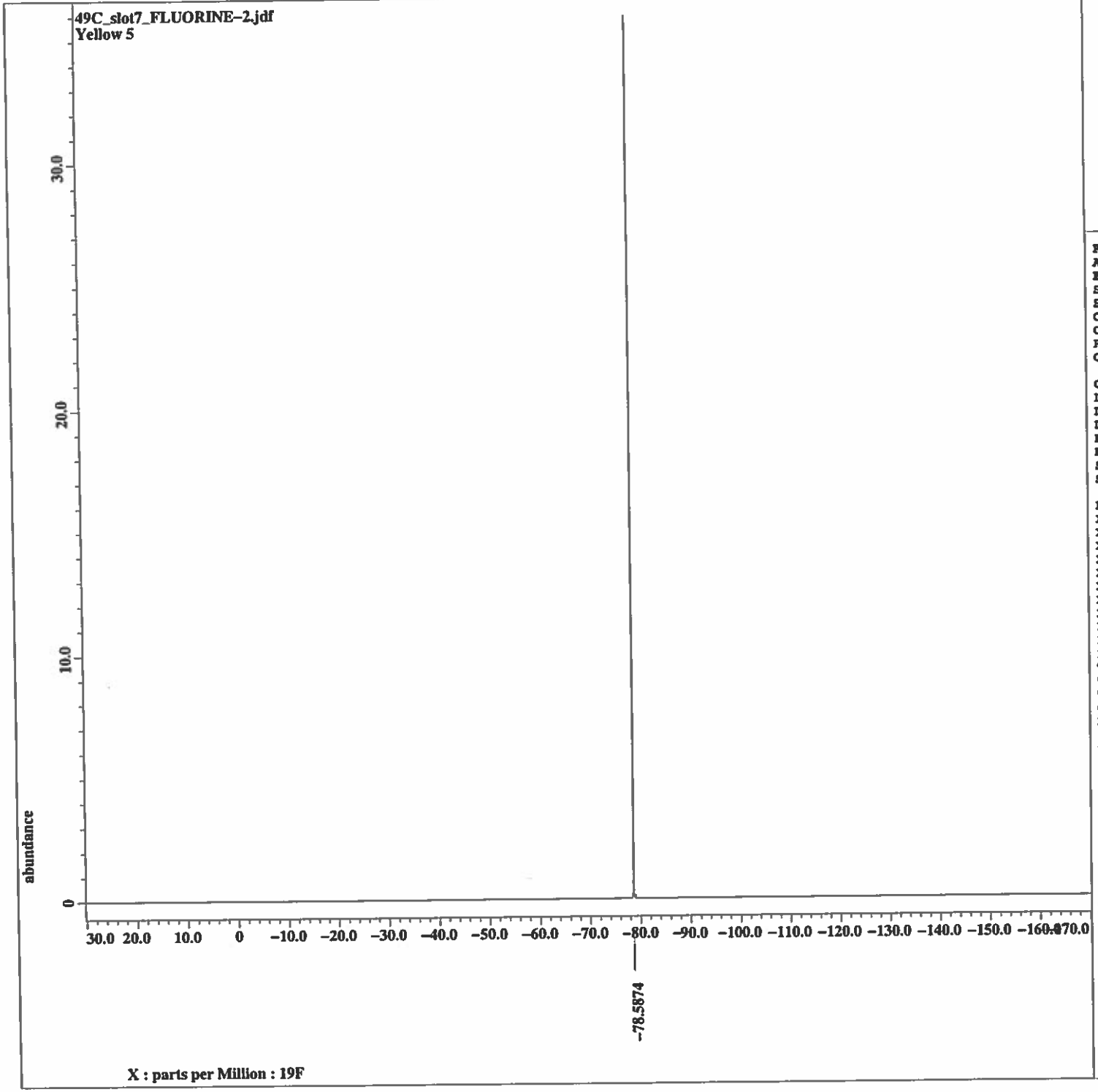


Filename	= 49C_slot7_PHOSPHORUS-
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#649941
Solvent	= CHLOROFORM-D
Changer_sample	= 7
Creation_time	= 1-JUL-2016 18:33:54
Revision_time	= 1-JUL-2016 18:15:48
Current_time	= 1-JUL-2016 18:15:48
Comment	= Yellow 5
Data_format	= 1D COMPLEX
Dim_size	= 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	= WALTZ
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	= 23.5[dC]

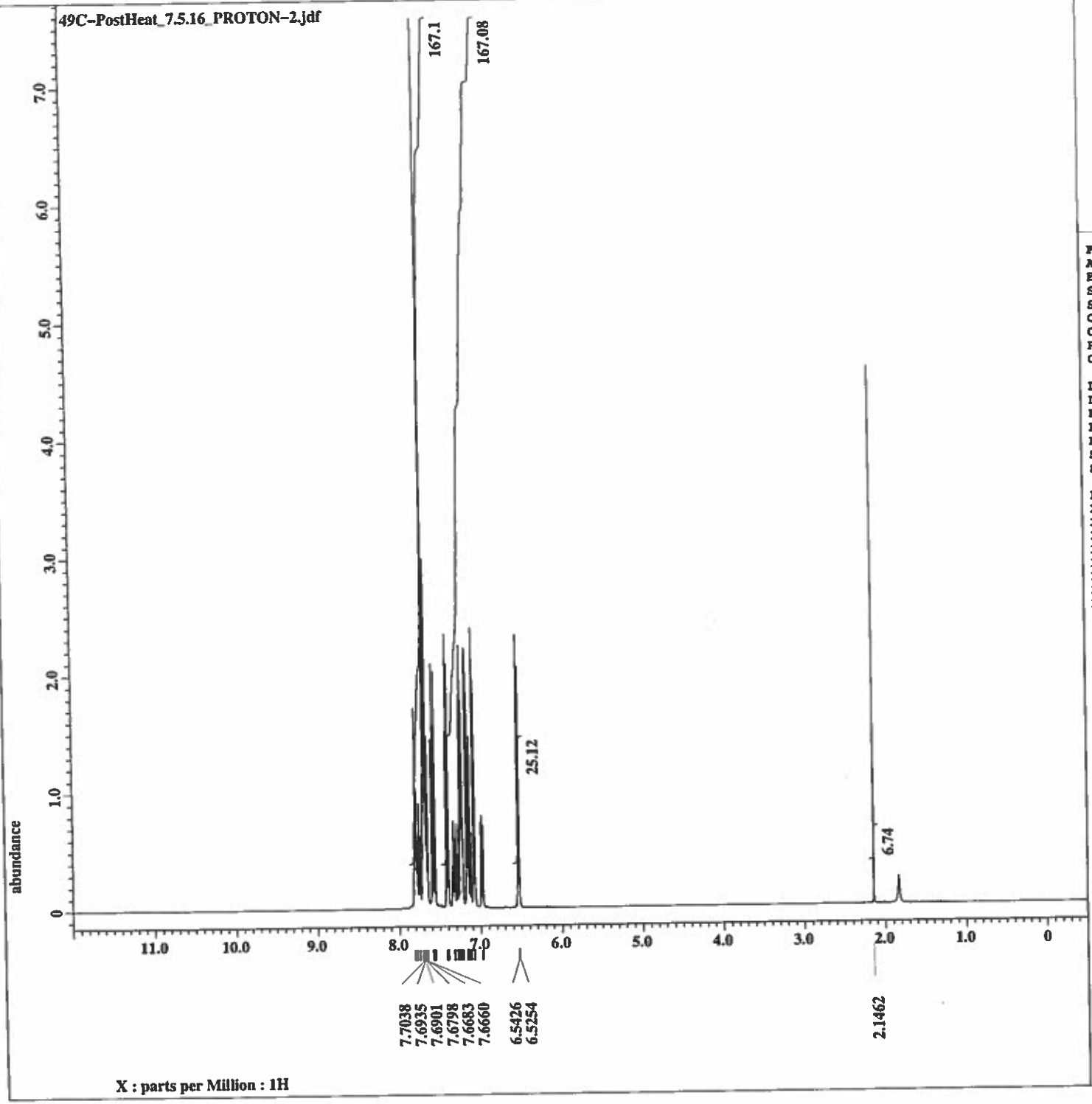


SOUTH ALABAMA JAGUARS

Filename	= 49C_slot7_CARBON-2.jd
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#343224
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]

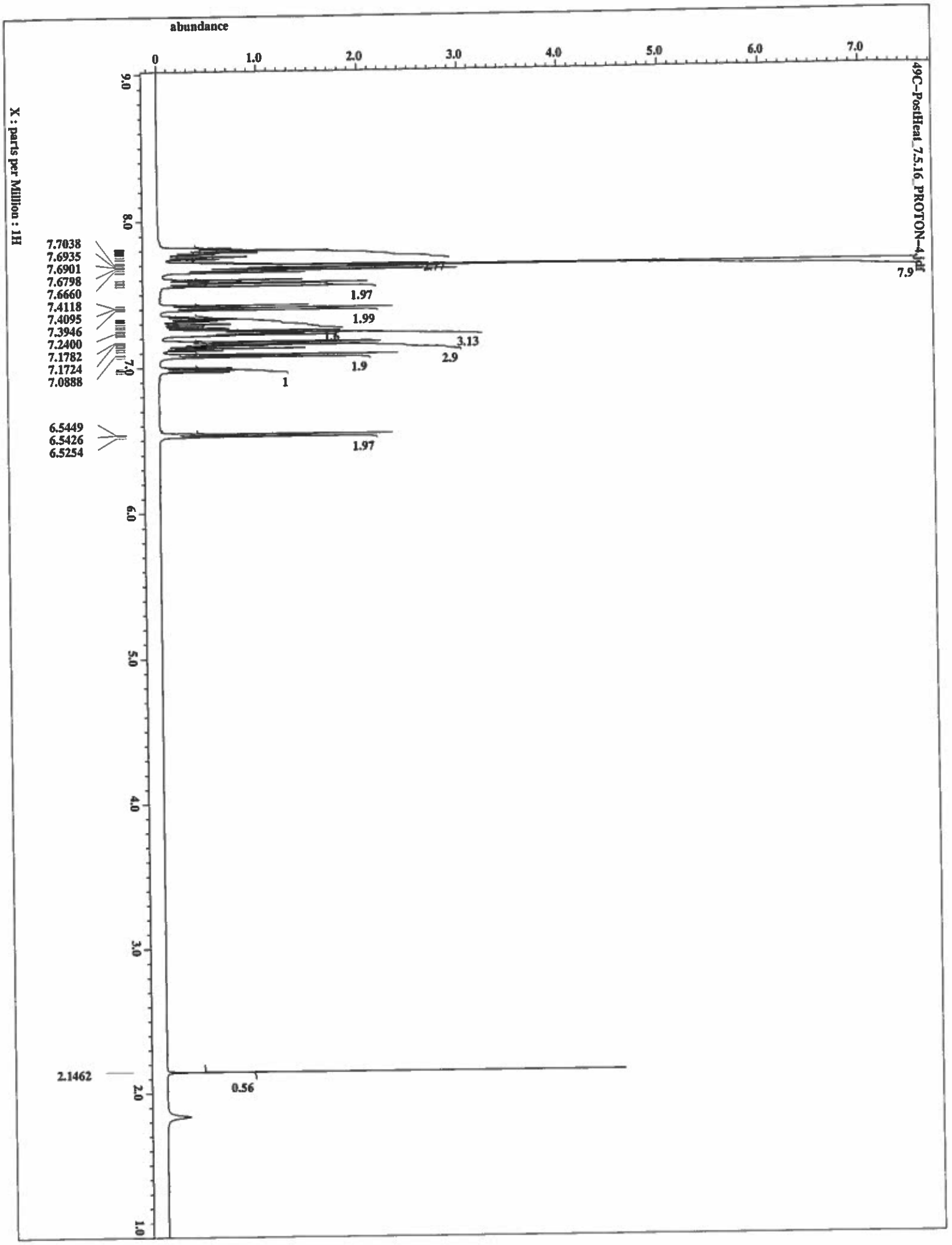


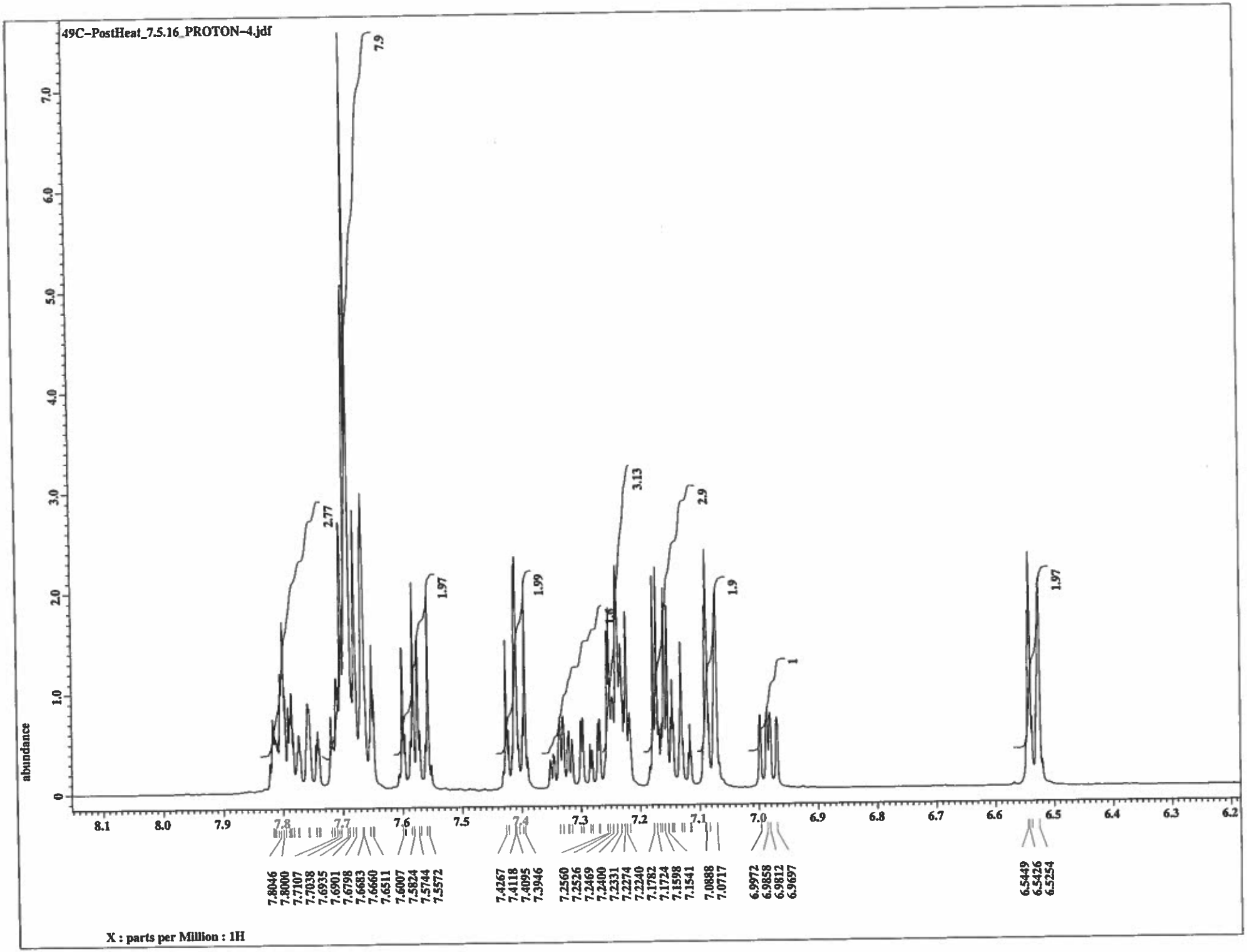
Filename	= 49C_slot7_FLUORINE-2.
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= S#563729
Solvent	= CHLOROFORM-D
Changer_sample	= 7
Creation_time	= 1-JUL-2016 16:00:20
Revision_time	= 1-JUL-2016 15:42:15
Current_time	= 1-JUL-2016 15:42:15
Comment	= Yellow 5
Data_format	= 1D COMPLEX
Dim_size	= 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[kHz]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.9[dC]

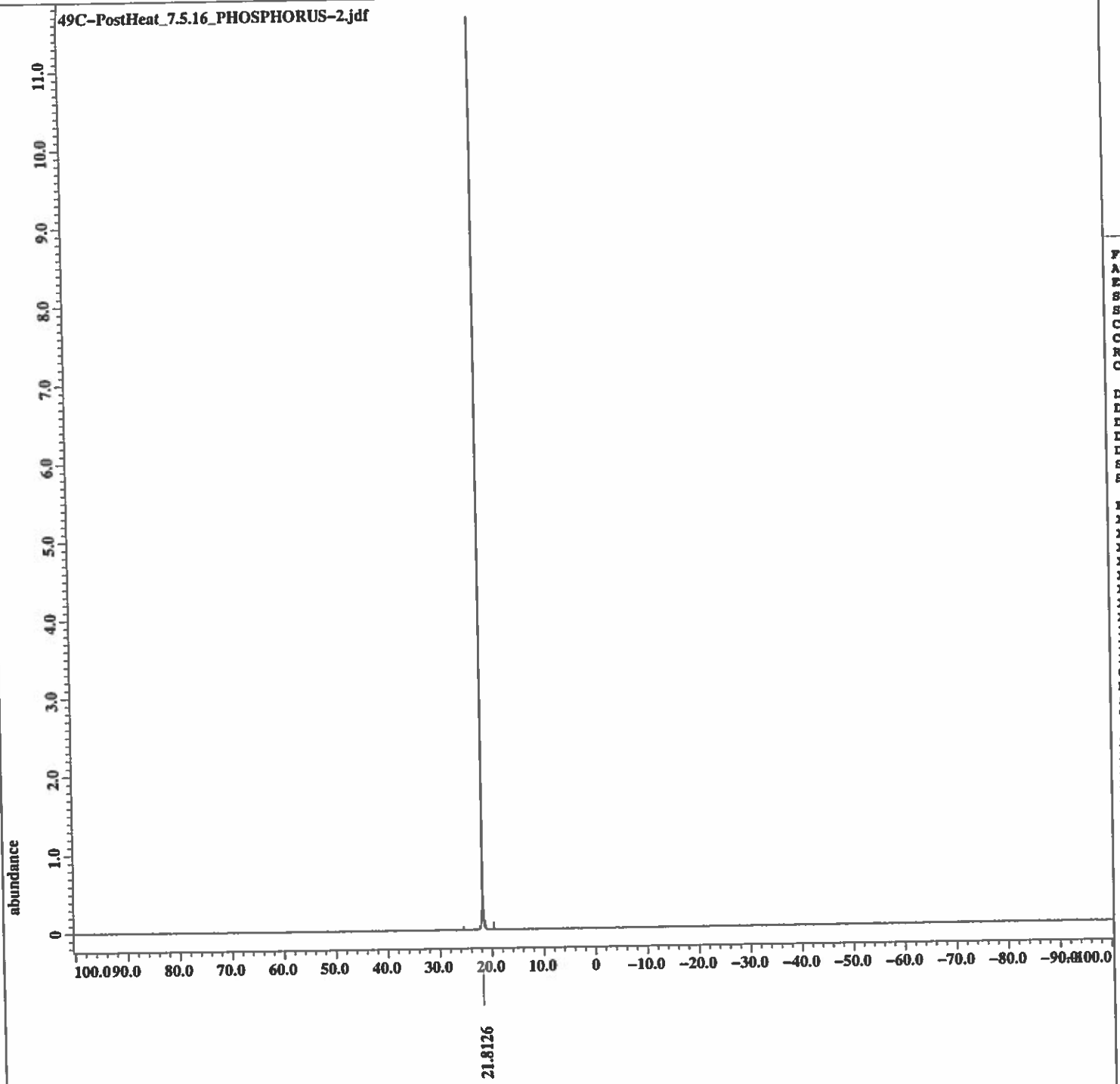


SOUTH ALABAMA JAGUARS

Filename	= 49C-PostHeat_7.5.16_P
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= 49C-PostHeat_7.5.16
Solvent	= CHLOROFORM-D
Changer_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	= 11.7473579[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]
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_atn	= 4[dB]
X_pulse	= 6.675[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 30
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.6[dC]

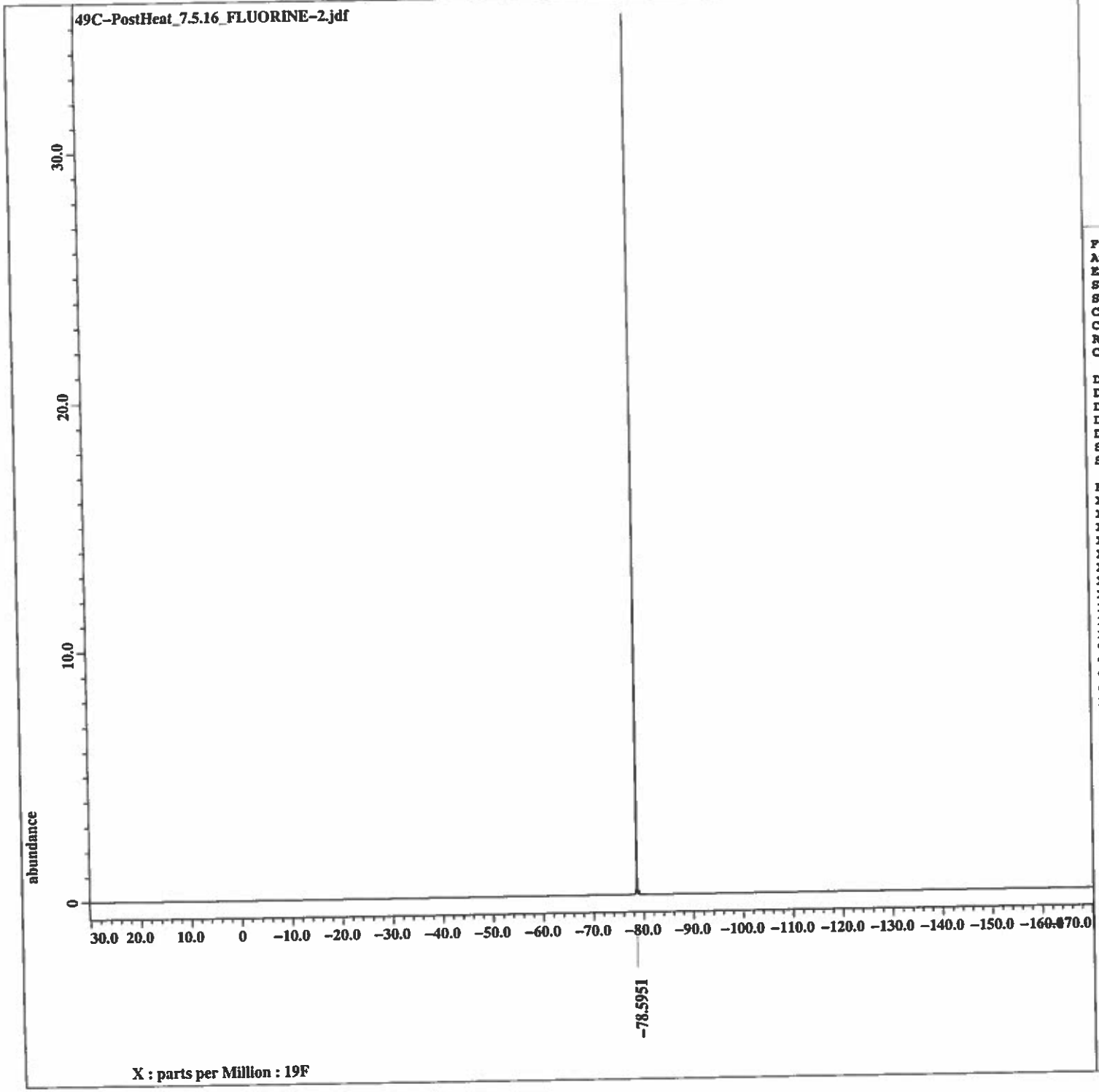

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
49C-PostHeat_7.5.16_PROTON-4.jdf
X : parts per Million : 1H
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.7038
7.6935
7.6901
7.6798
7.6660
7.4118
7.4095
7.3946
7.2400
7.1782
7.1724
7.0888
6.5449
6.5426
6.5254
2.1462
7.9
1.97
1.99
3.13
2.9
1.9
1
1.97
0.56


49C-PostHeat_7.5.16_PROTON-4.jdf
abundance
X : parts per Million : 1H
7.9
2.77
1.97
1.99
3.13
2.9
1.9
1
1.97
7.8046
7.8000
7.7107
7.7038
7.6935
7.6901
7.6798
7.6683
7.6660
7.6511
7.6007
7.5824
7.5744
7.5572
7.4267
7.4118
7.4095
7.3946
7.2560
7.2526
7.2469
7.2400
7.2331
7.2274
7.2240
7.1782
7.1724
7.1598
7.1541
7.0888
7.0717
6.9972
6.9858
6.9812
6.9697
6.5449
6.5426
6.5254



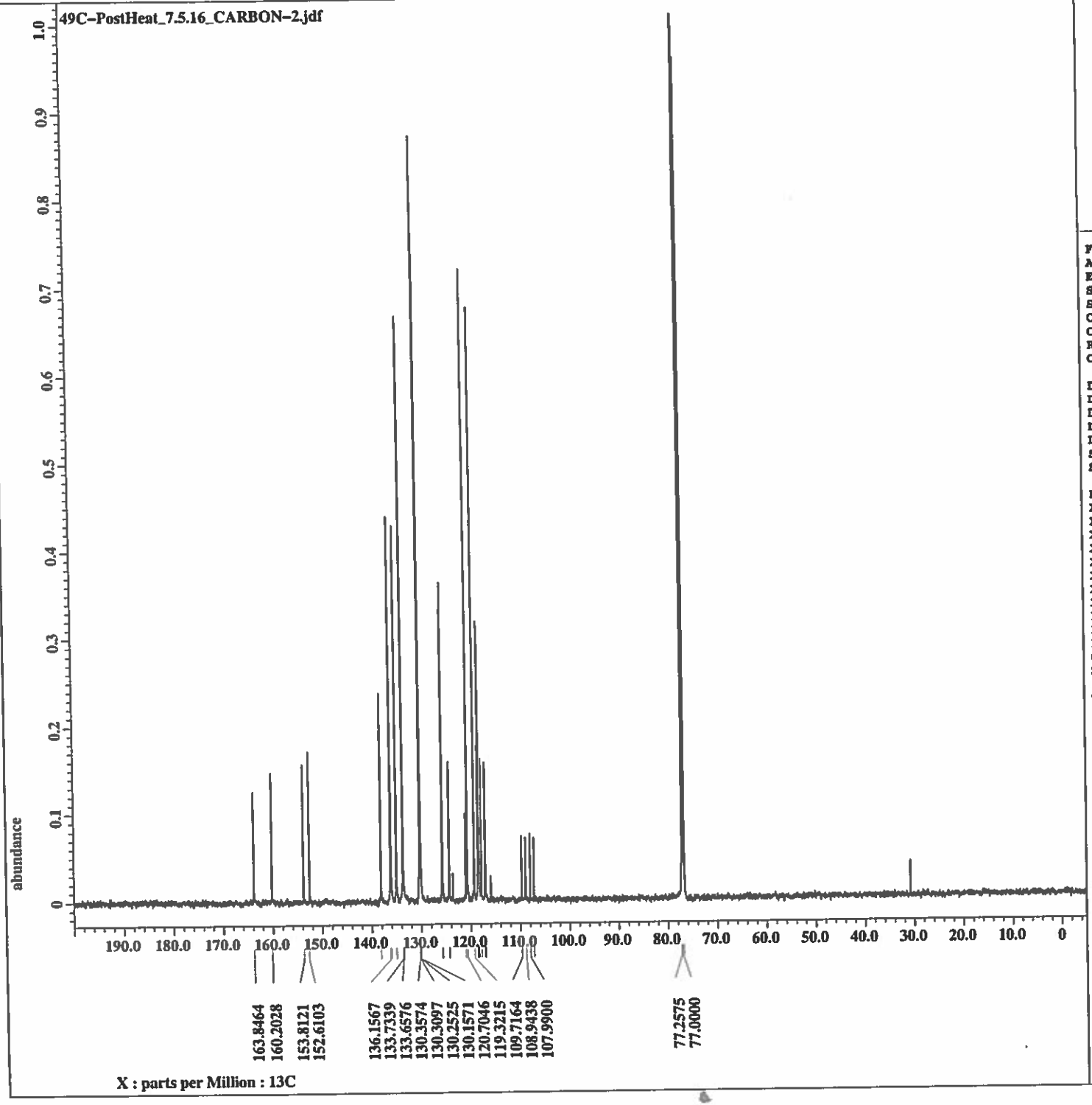
SOUTH ALABAMA JAGUARS

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	= 9
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
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	= WALTZ
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	= 23.5[dC]



SOUTH ALABAMA JAGUARS

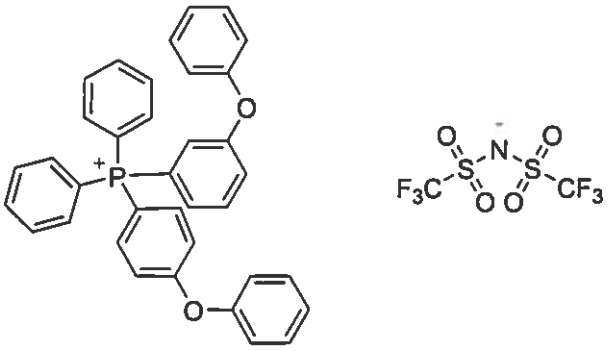
Filename	= 49C-PostHeat_7.5.16_F
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= 49C-PostHeat_7.5.16
Solvent	= CHLOROFORM-D
Changer_sample	= 9
Creation_time	= 5-JUL-2016 23:01:50
Revision_time	= 5-JUL-2016 22:43:27
Current_time	= 5-JUL-2016 22:43:27
Data_format	= 1D COMPLEX
Dim_size	= 52428
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[kHz]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.8[dC]



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]

COMPOUND 6



Atlantic Microlab, Inc.

No. Phosphonium 49A

antic Blvd. Suite M
s, GA 30071
anticmicrolab.com

Company/School U of South Alabama
Dept. Chemistry
Address Chem 223
City, State, Zip Mobile AL 36688

r/Supervisor: James Davis
C#

Name James Davis Date 10/31/2016
Phone (251) 751-0520

ent	Theory	Found	
;	56.79	56.63	
ł	3.51	3.49	
l	1.74	1.77	

Single ☒ Duplicate ☐

Elements Present: CHNPOSF

Analyze for: CHN

Hygroscopic ☐ Explosive ☐
M.P. unk B.P. none

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

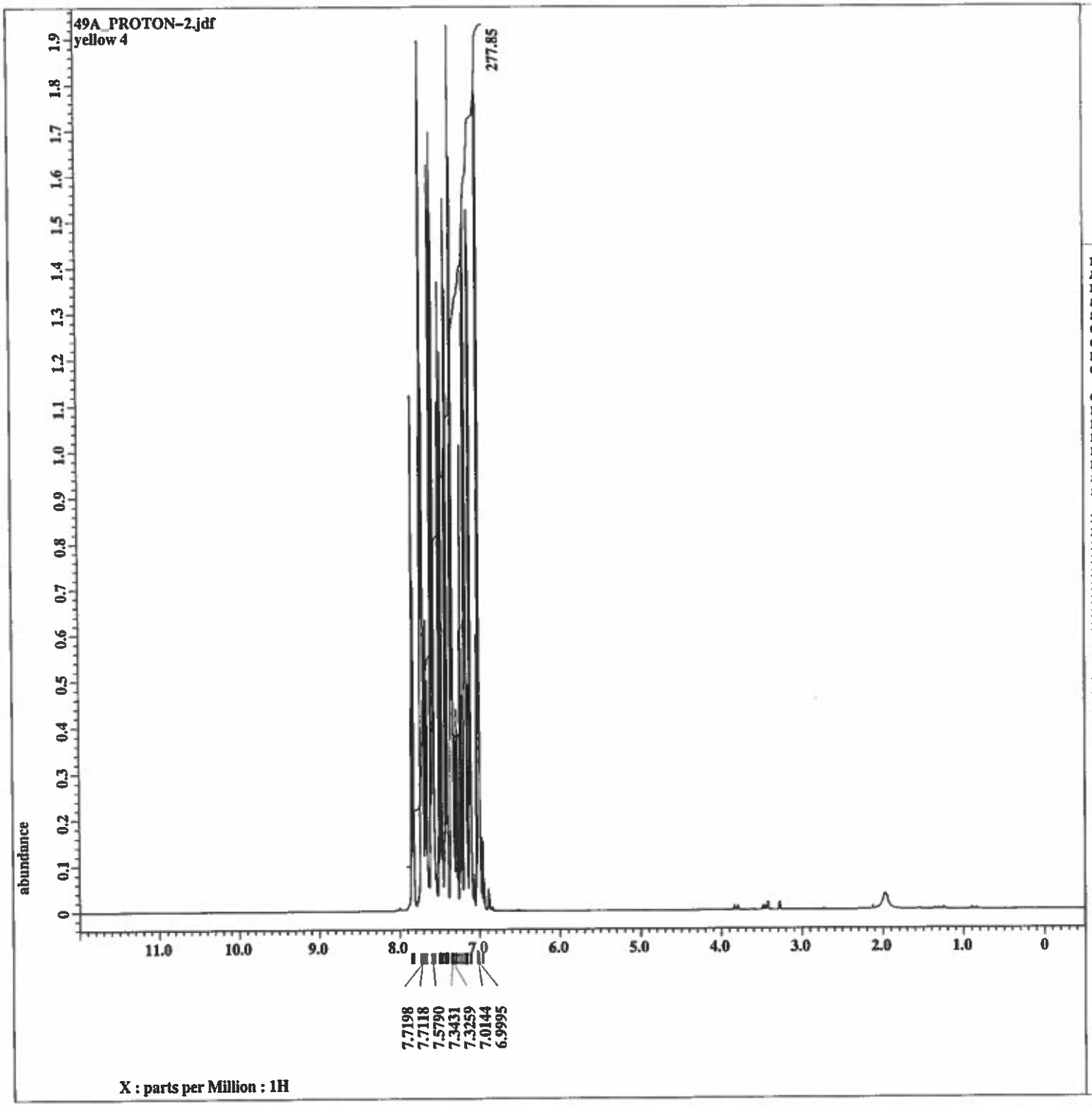
Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

Include Email Address or FAX # Below

jdavis@southalabama.edu

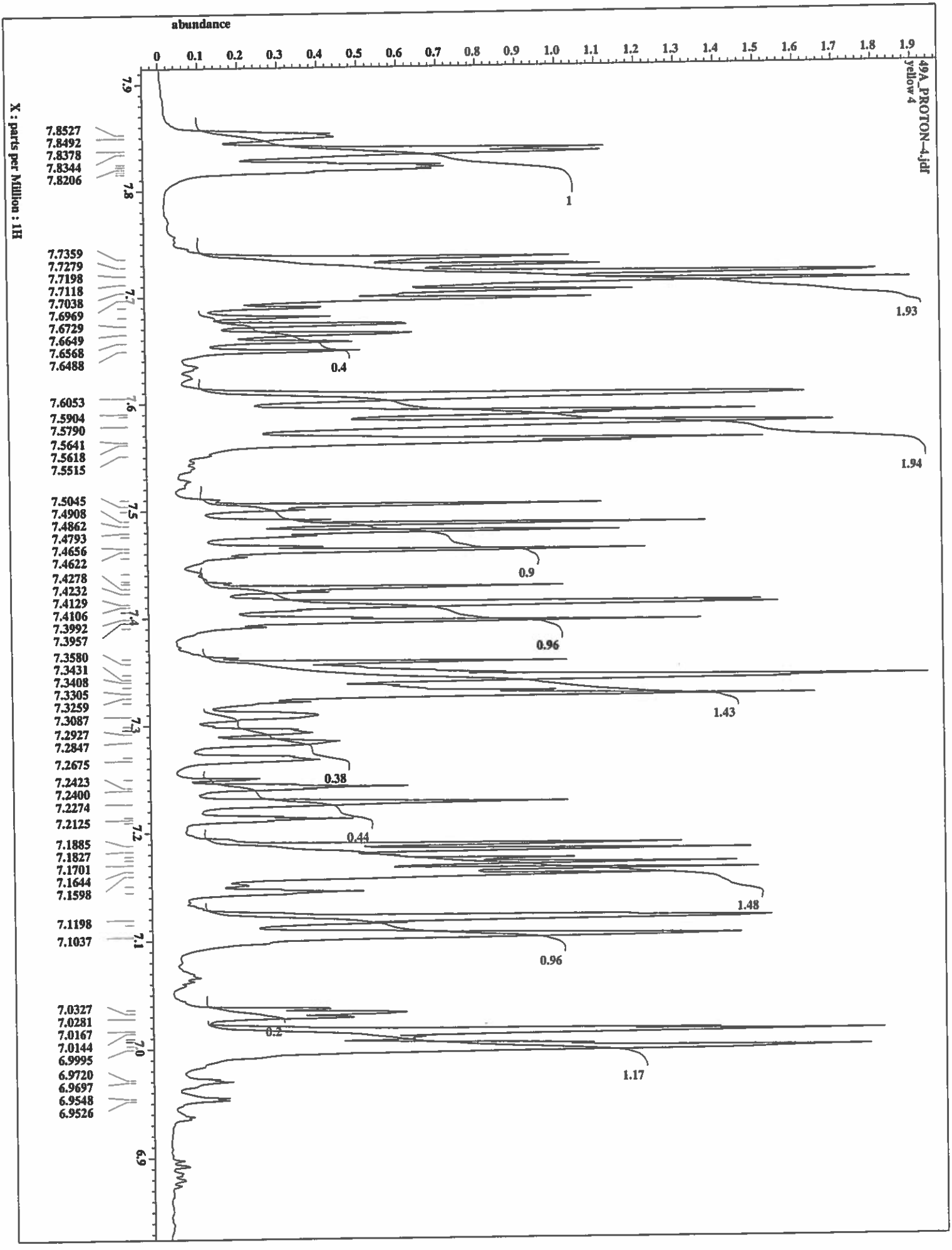
Received NOV 01 2016 Date Completed NOV 01 2016

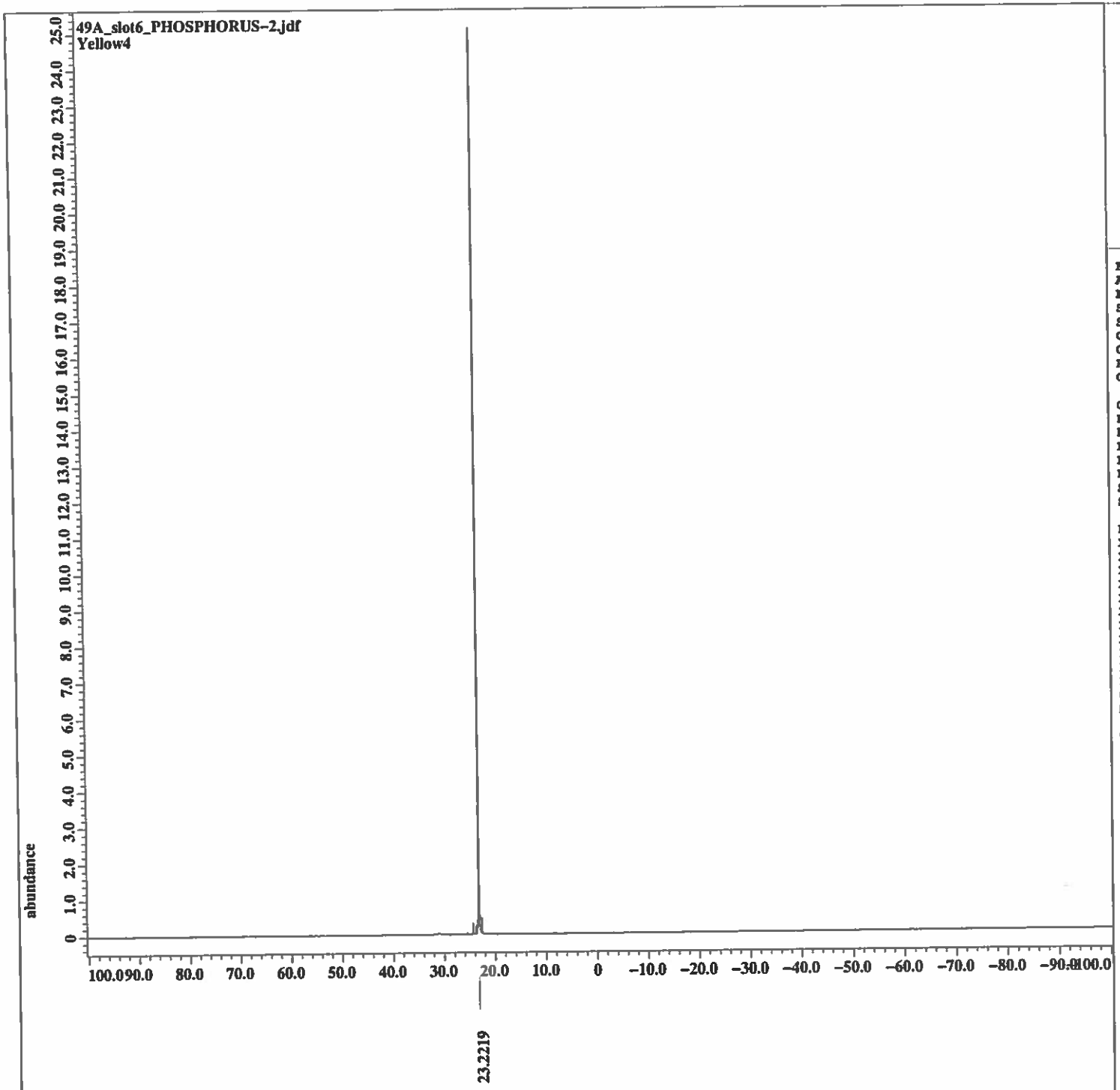
ks:



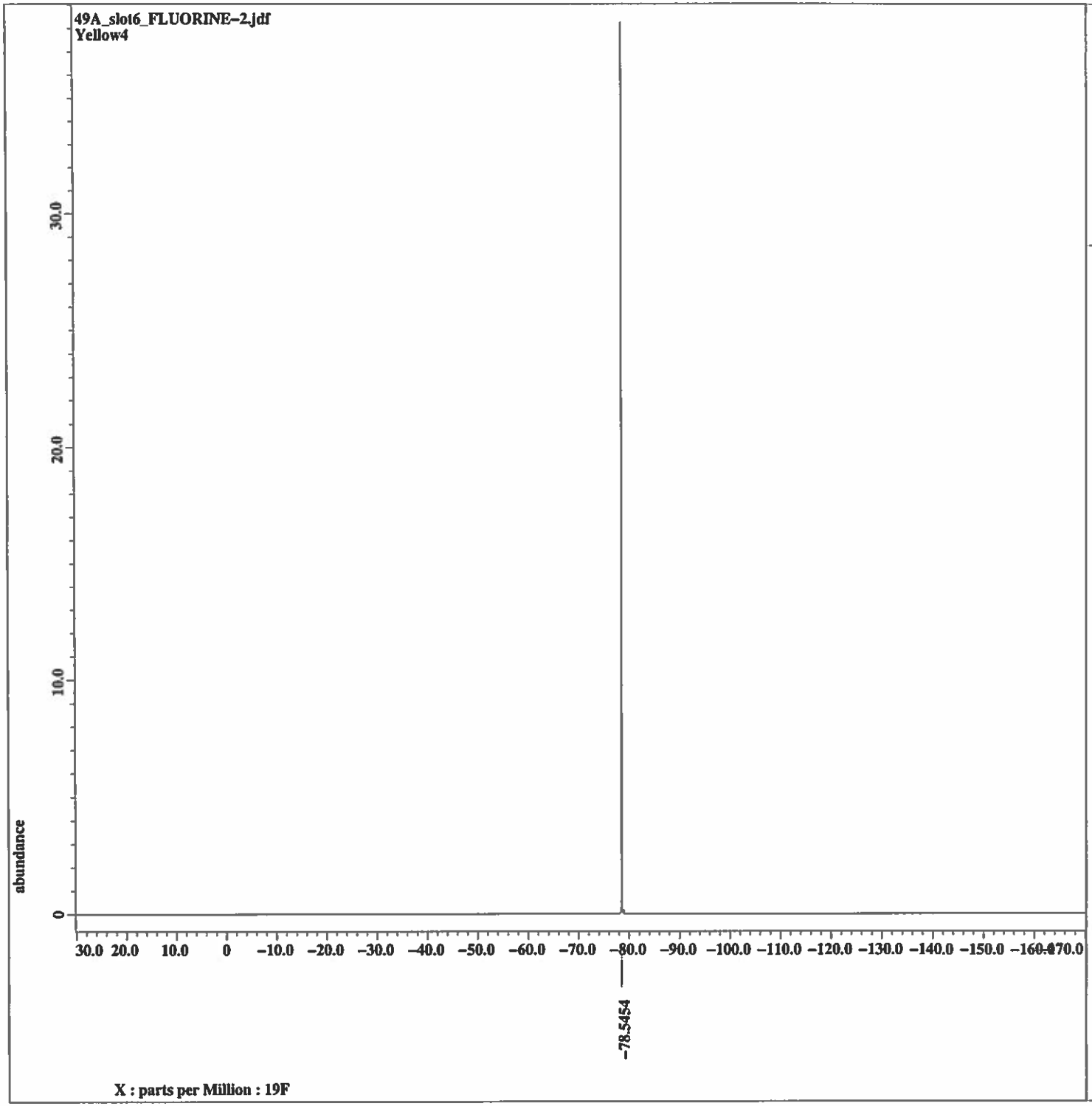
SOUTH ALABAMA JAGUARS

Filename	= 49A_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= 49A
Solvent	= CHLOROFORM-D
Changer_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	= yellow 4
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
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_atn	= 4[dB]
X_pulse	= 6.675[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 22
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.5[dC]

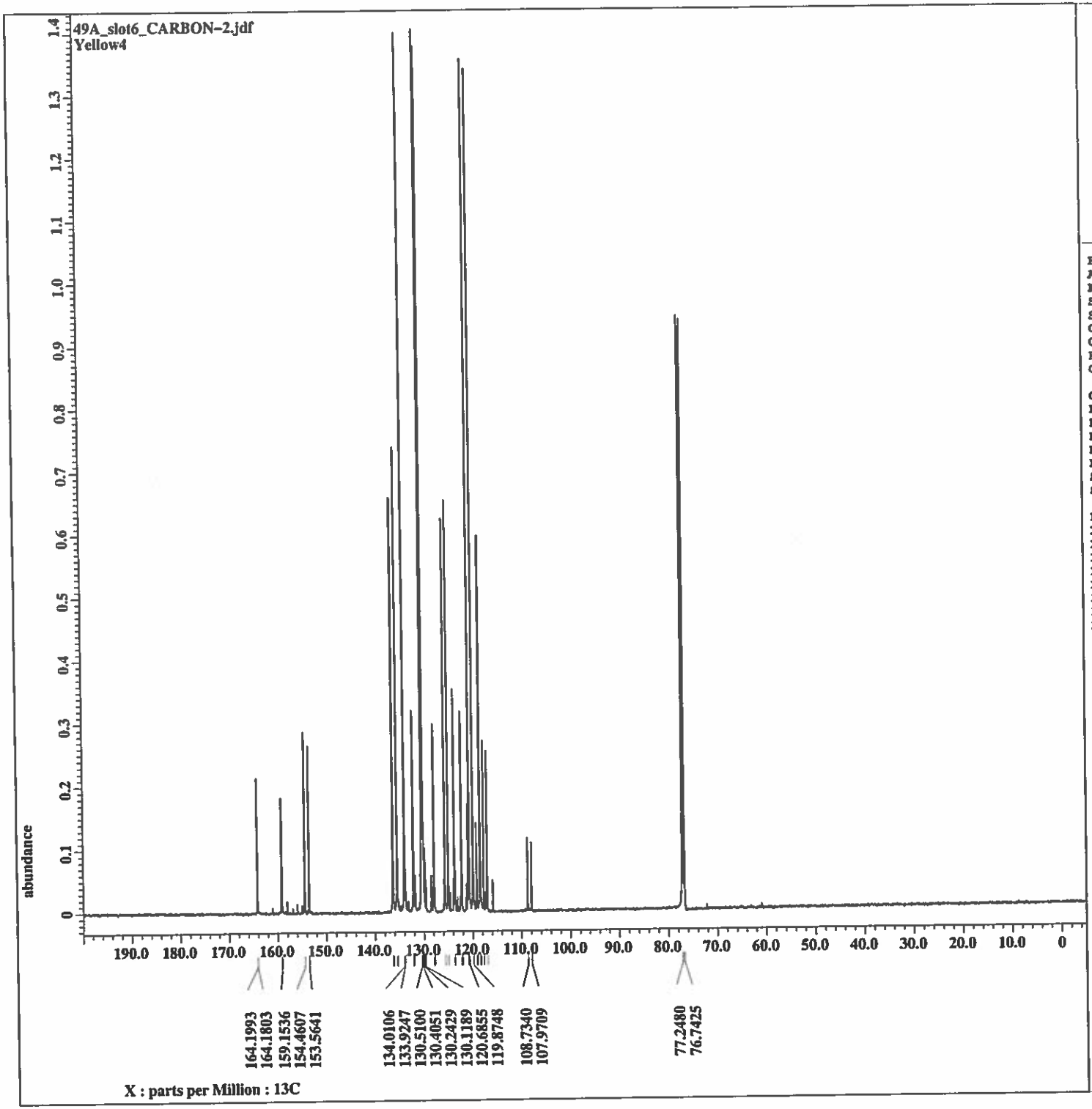

abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9
49A_PROTON-4.jdf
yellow 4
X : parts per Million : 1H
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
7.8527
7.8492
7.8378
7.8344
7.8206
1
7.7359
7.7279
7.7198
7.7118
7.7038
7.6969
7.6729
7.6649
7.6568
7.6488
1.93
0.4
7.6053
7.5904
7.5790
7.5641
7.5618
7.5515
1.94
7.5045
7.4908
7.4862
7.4793
7.4656
7.4622
0.9
7.4278
7.4232
7.4129
7.4106
7.3992
7.3957
0.96
7.3580
7.3431
7.3408
7.3305
7.3259
7.3087
1.43
7.2927
7.2847
7.2675
0.38
7.2423
7.2400
7.2274
7.2125
0.44
7.1885
7.1827
7.1701
7.1644
7.1598
1.48
7.1198
7.1037
0.96
7.0327
7.0281
7.0167
7.0144
6.9995
6.9720
6.9697
6.9548
6.9526
0.2
1.17



Filename	= 49A_slot6_PHOSPHORUS-
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#640571
Solvent	= CHLOROFORM-D
Changer_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
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	= WALTZ
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	= 23.5[dC]

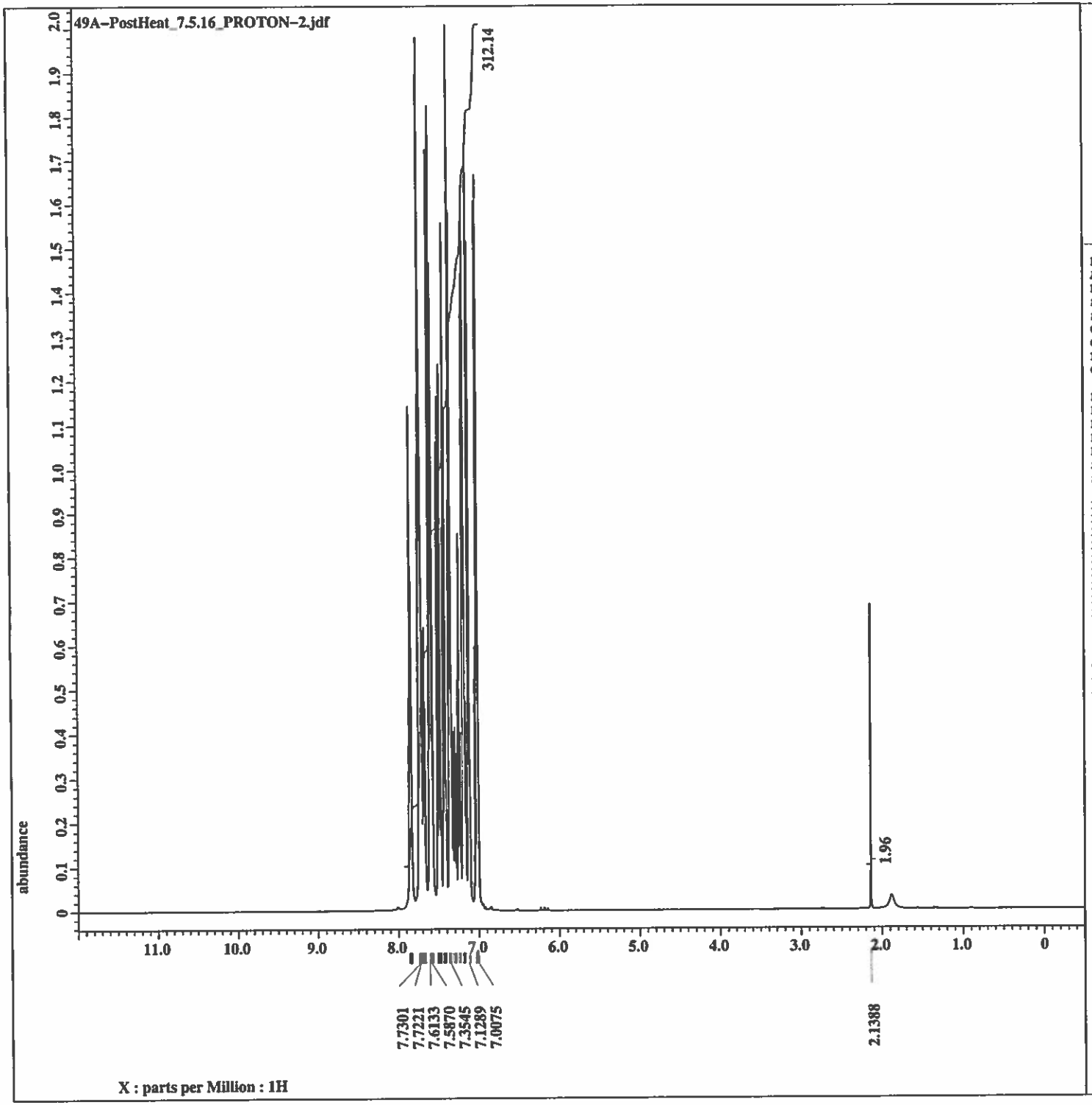


Filename	= 49A_slot6_FLUORINE-2.
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= S#560379
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 1-JUL-2016 15:54:36
Revision_time	= 1-JUL-2016 15:36:31
Current_time	= 1-JUL-2016 15:36:31
Comment	= Yellow4
Data_format	= 1D COMPLEX
Dim_size	= 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]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.9[dC]



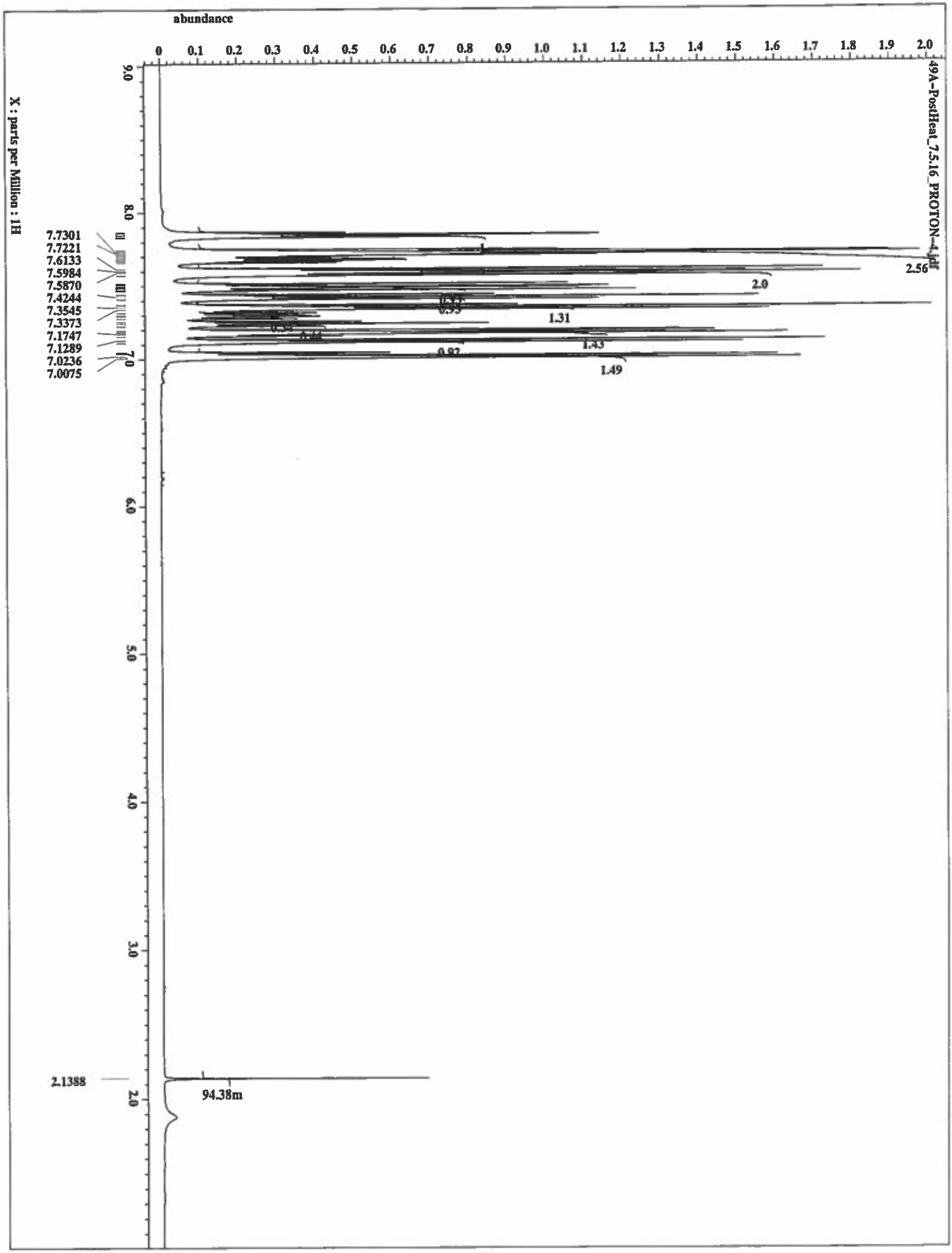
SOUTH ALABAMA JAGUARS

Filename	= 49A_slot6_CARBON-2.jd
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#252811
Solvent	= CHLOROFORM-D
Changer_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
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	= 23.7[dC]



SOUTH ALABAMA JAGUARS

Filename	= 49A-PostHeat_7.5.16_P
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= 49A-PostHeat_7.5.16
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 5-JUL-2016 16:08:41
Revision_time	= 5-JUL-2016 15:50:19
Current_time	= 5-JUL-2016 15:50:19
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
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_atn	= 4[dB]
X_pulse	= 6.675[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 24
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.5[dC]


abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0
49A-PostHeat_7.5.16_PROTON-4.jdf
X : parts per Million : 1H
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0
7.7301
7.7221
7.6133
7.5984
7.5870
7.4244
7.3545
7.3373
7.1747
7.1289
7.0236
7.0075
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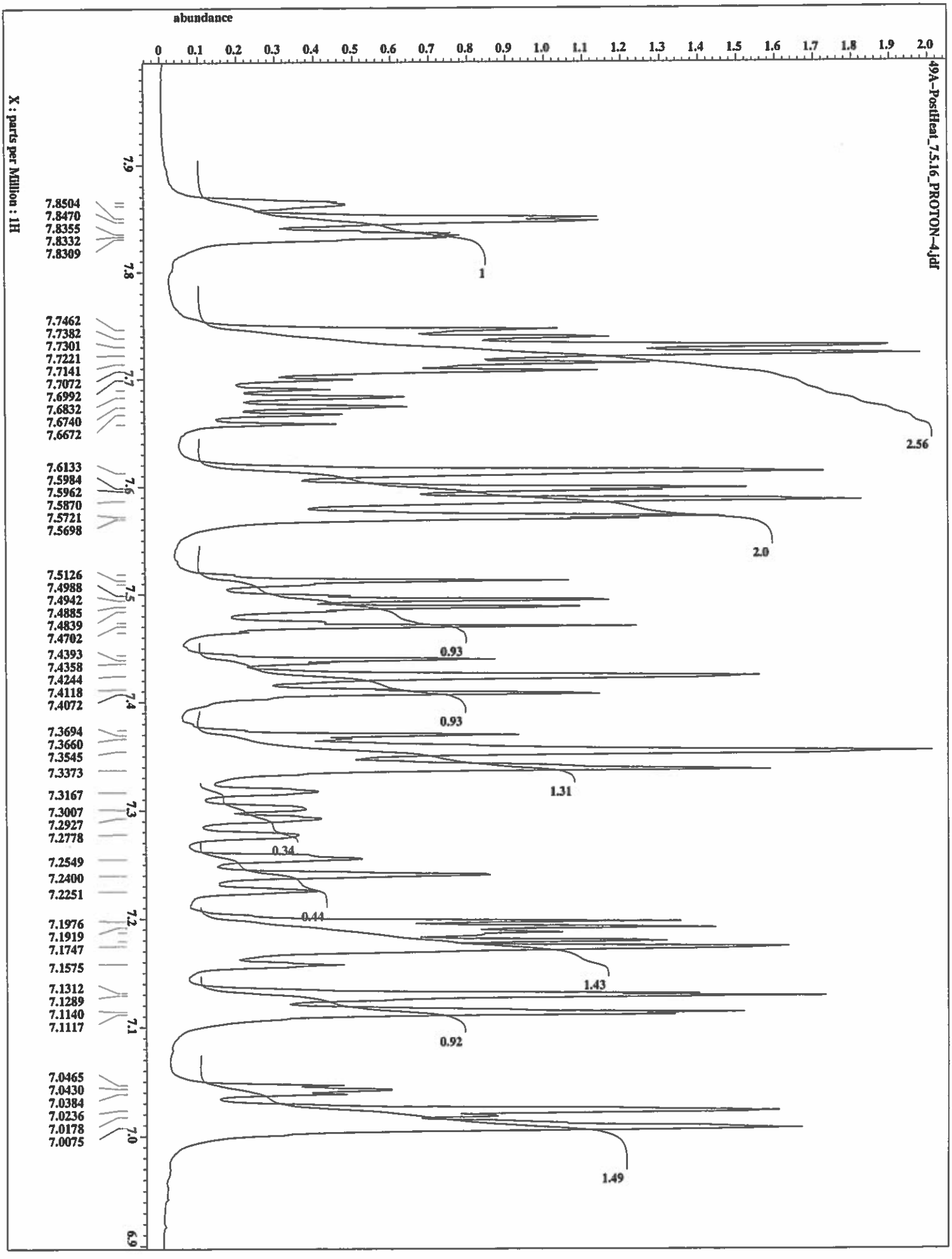
2.0
1.31
1.43
1.49
2.1388
94.38m


abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0
49A-PostHeat_7.5.16_PROTON-4.jdf
X : parts per Million : 1H
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
7.8504
7.8470
7.8355
7.8332
7.8309
1
7.7462
7.7382
7.7301
7.7221
7.7141
7.7072
7.6992
7.6832
7.6740
7.6672
2.56
7.6133
7.5984
7.5962
7.5870
7.5721
7.5698
2.0
7.5126
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7.4885
7.4839
7.4702
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7.4393
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7.1312
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7.0236
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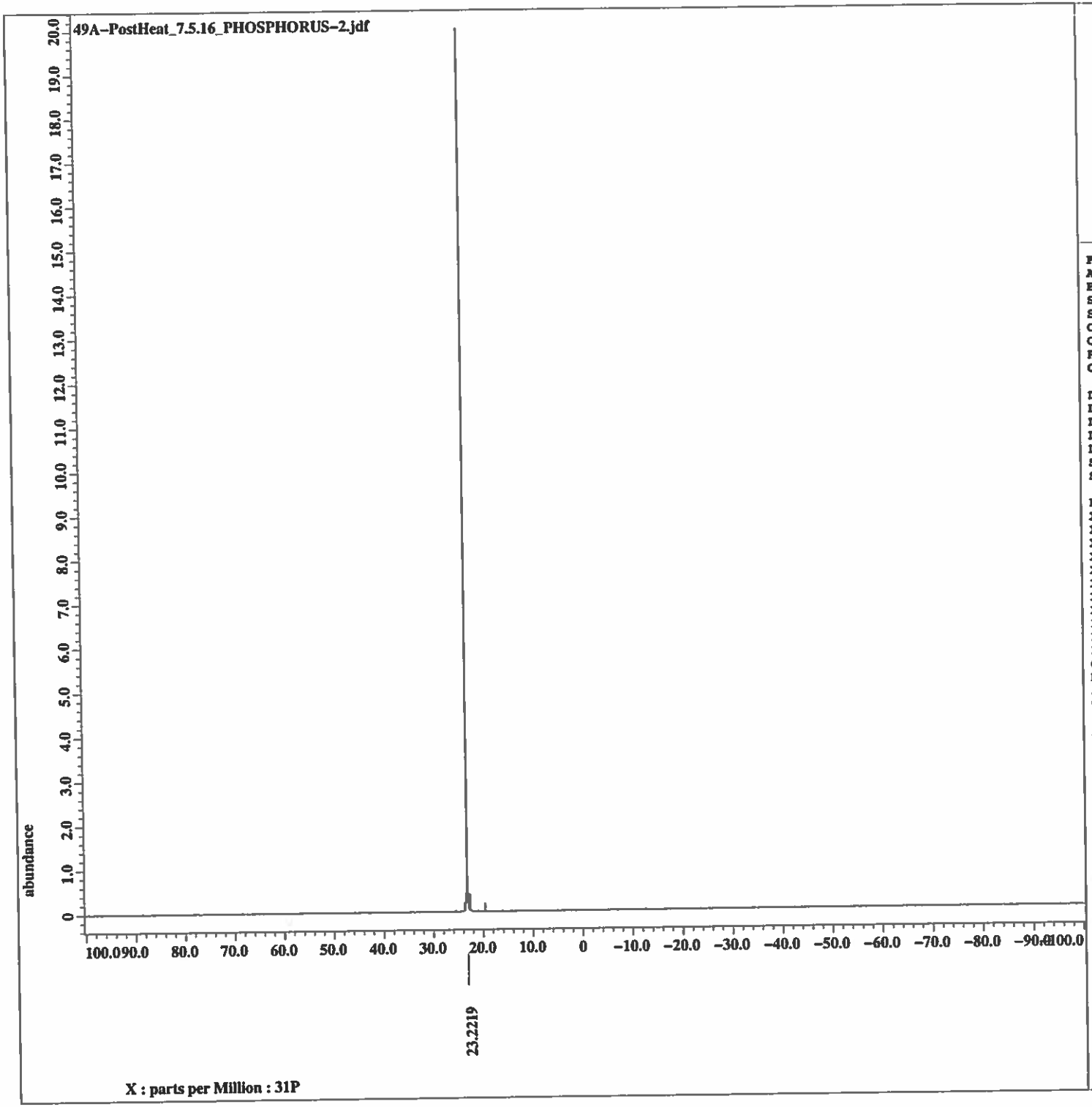
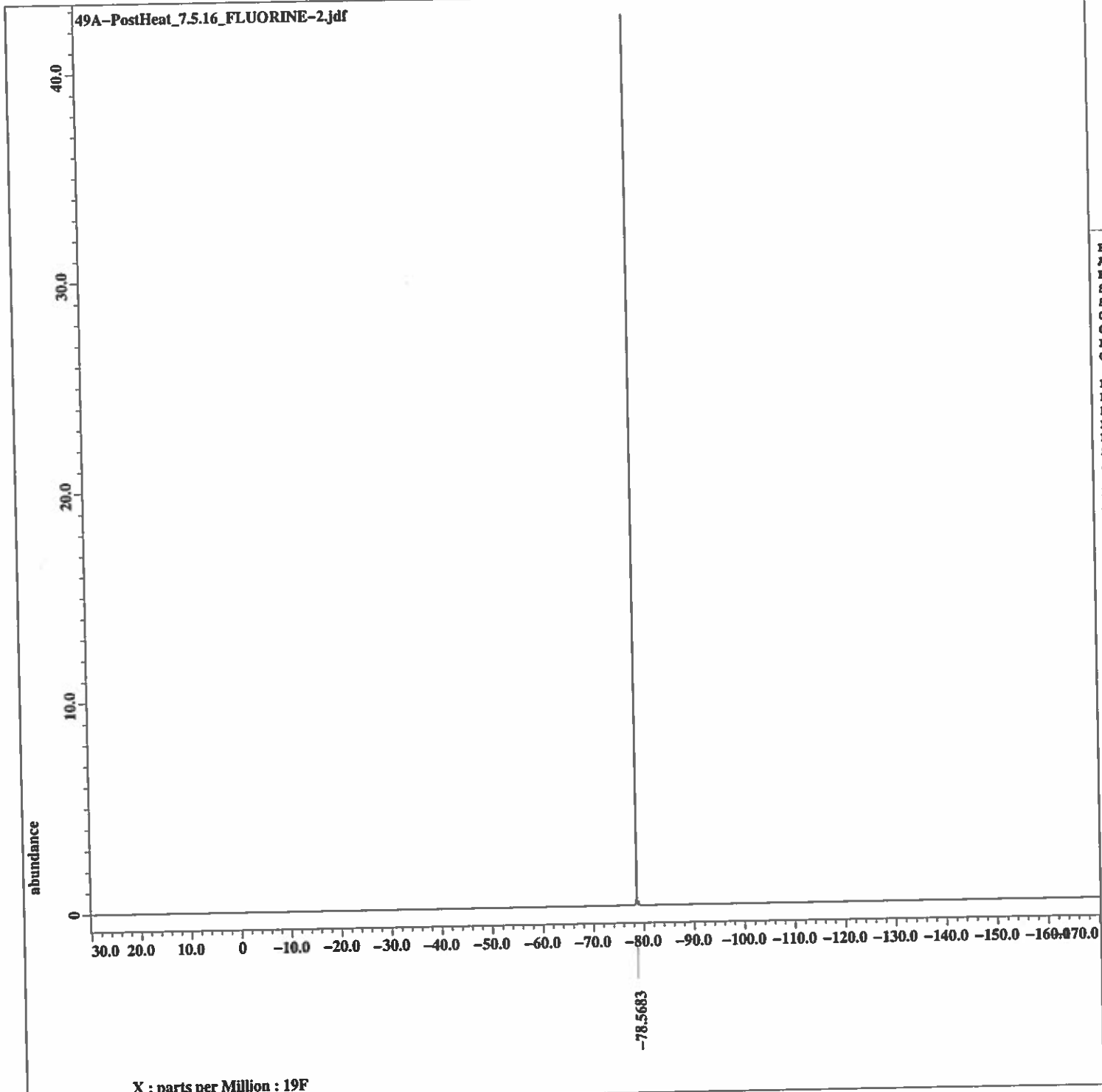
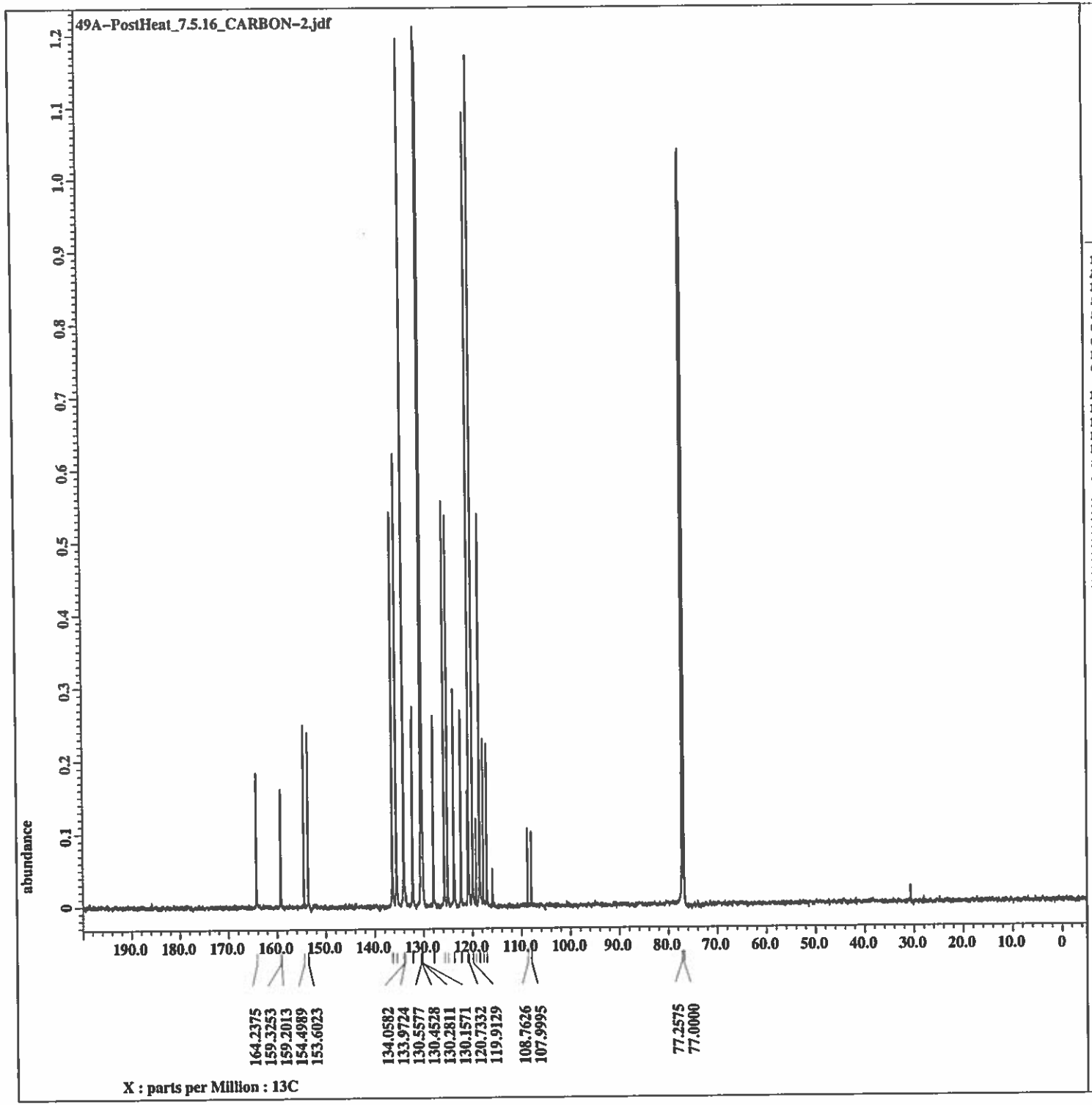
7.0075
1.49



Filename	= 49A-PostHeat_7.5.16_P
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= 49A-PostHeat_7.5.16
Solvent	= CHLOROFORM-D
Changer_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
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	= WALTZ
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[dC]



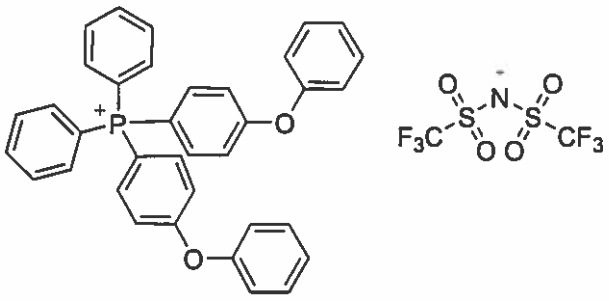
Filename	= 49A-PostHeat_7.5.16_F
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= 49A-PostHeat_7.5.16
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 5-JUL-2016 20:39:15
Revision_time	= 5-JUL-2016 20:20:53
Current_time	= 5-JUL-2016 20:20:53
Data_format	= 1D COMPLEX
Dim_size	= 52428
Dim_title	= 19F
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[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]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 38
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 23.2[dC]



SOUTH ALABAMA JAGUARS

Filename	= 49A-PostHeat_7.5.16_C
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= 49A-PostHeat_7.5.16
Solvent	= CHLOROFORM-D
Changer_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-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	= 23.5[dC]

COMPOUND 7



Atlantic Microlab, Inc.

No. Phosphonium 141A

lantic Blvd. Suite M
s, GA 30071
lanticmicrolab.com

Company/School U of South Alabama
Dept. Chemistry
Address Chem 223
City, State, Zip Mobile AL 36688

or/Supervisor: James Davis
C#

Name James Davis Date 10/31/2016
Phone (251) 751-0520

ent	Theory	Found	
C	56.79	57.08	
H	3.51	3.51	
N	1.74	1.75	

Single ☐ Duplicate ☐

Elements Present: CHNPOSF

Analyze for: CHN

Hygroscopic ☐ Explosive ☐
M.P. unk B.P. none

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

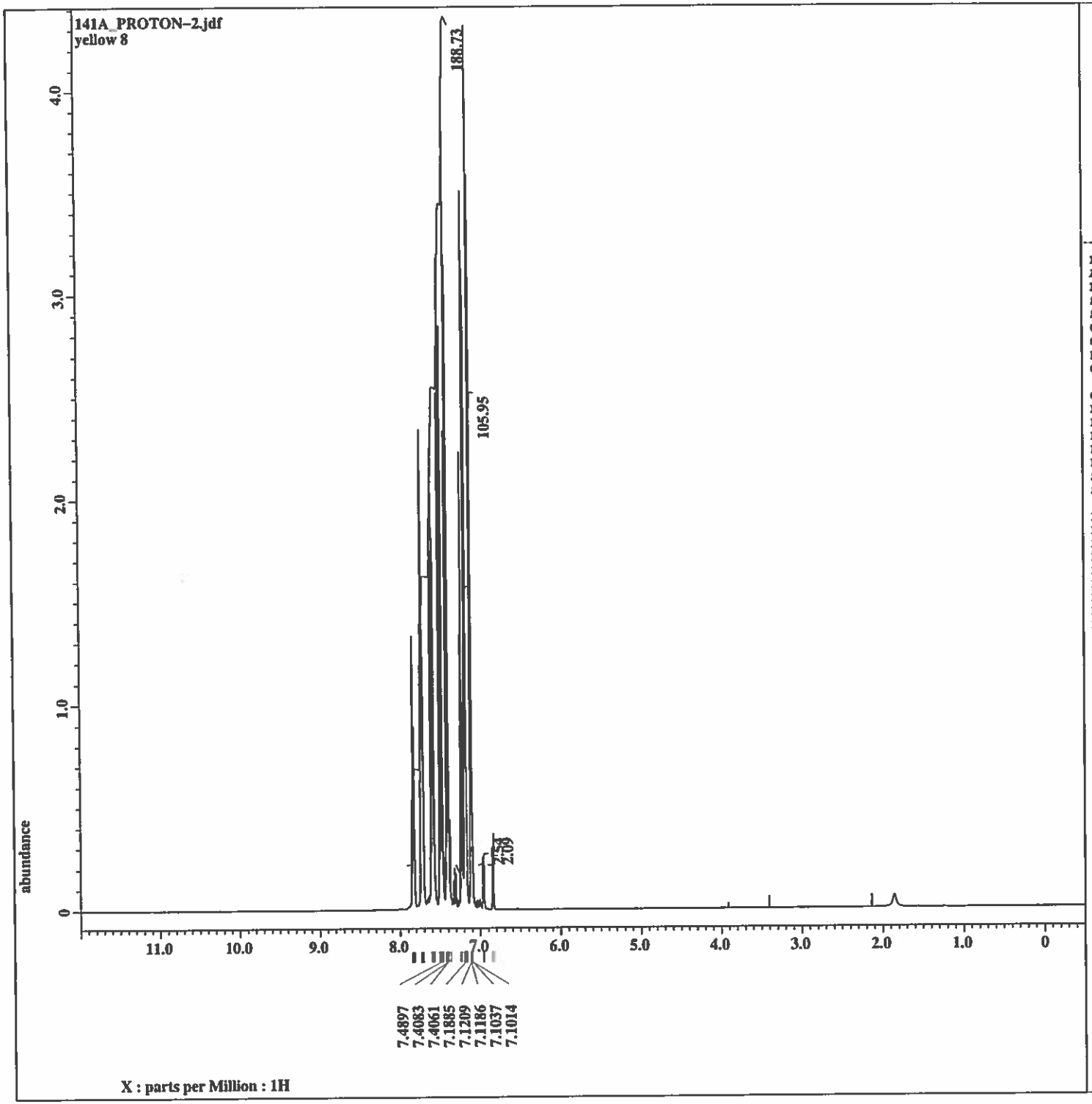
Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

Include Email Address or FAX # Below

jdavis@southalabama.edu

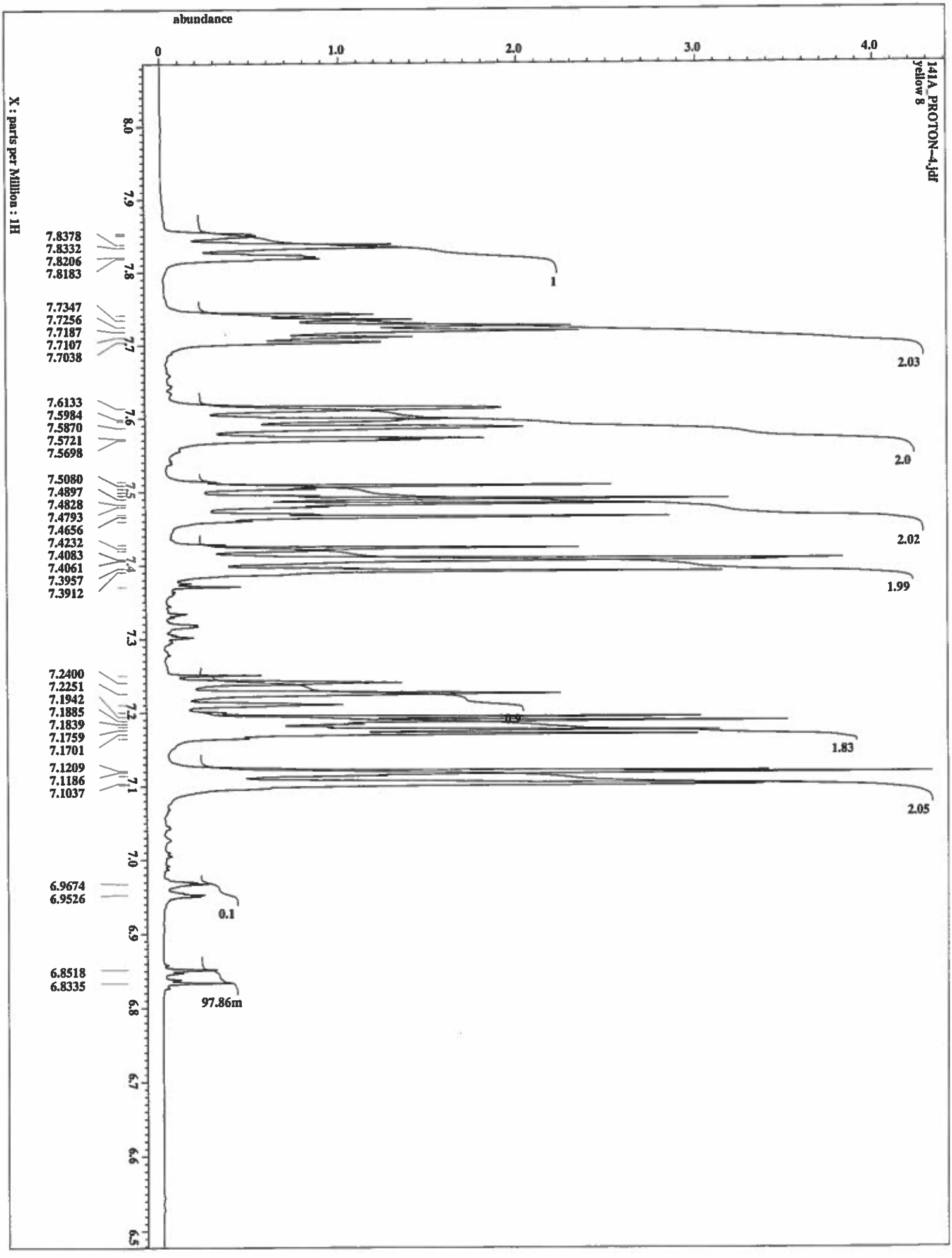
Received NOV 01 2016 Date Completed NOV 01 2016

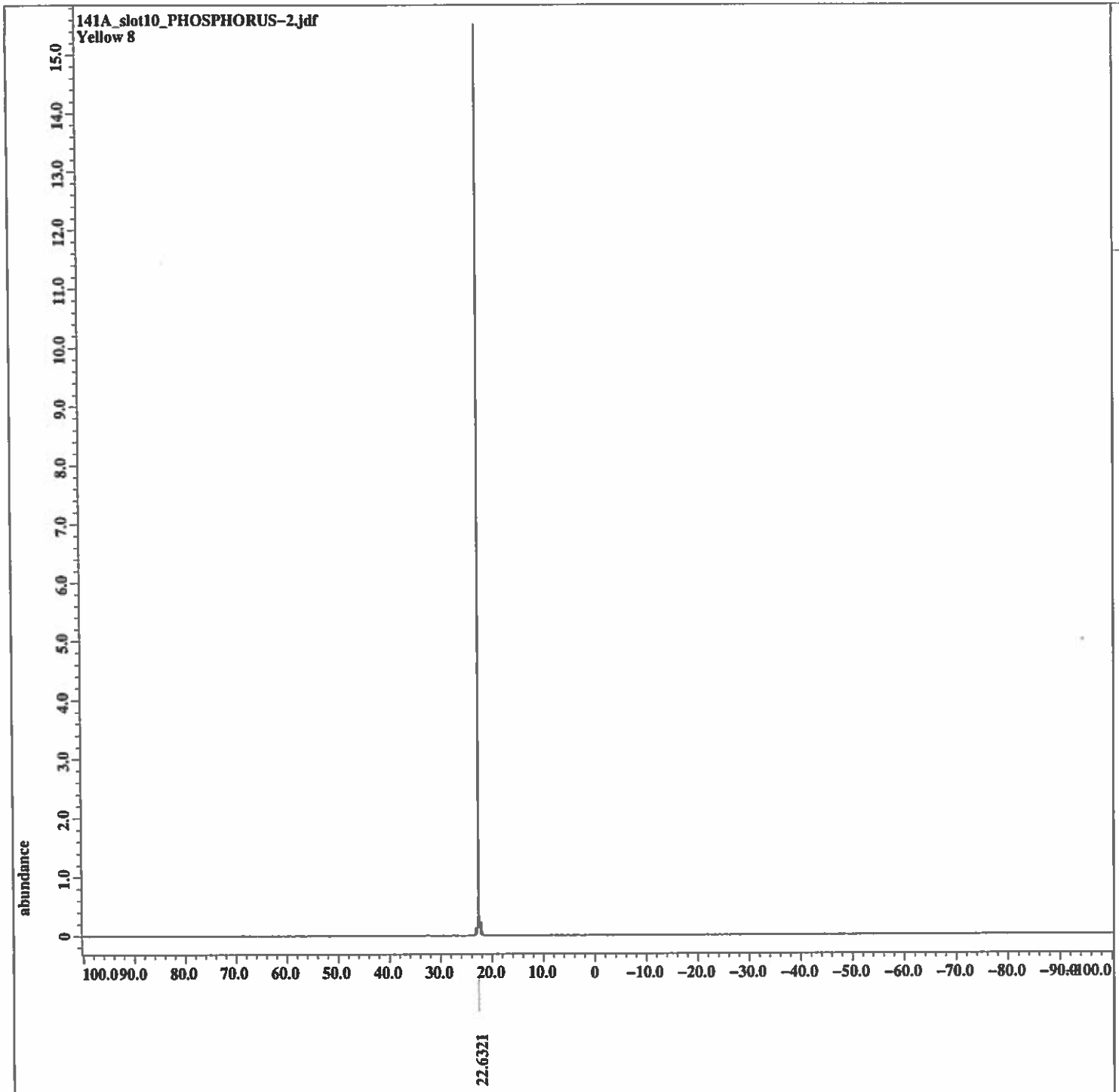
rks:



SOUTH ALABAMA JAGUARS

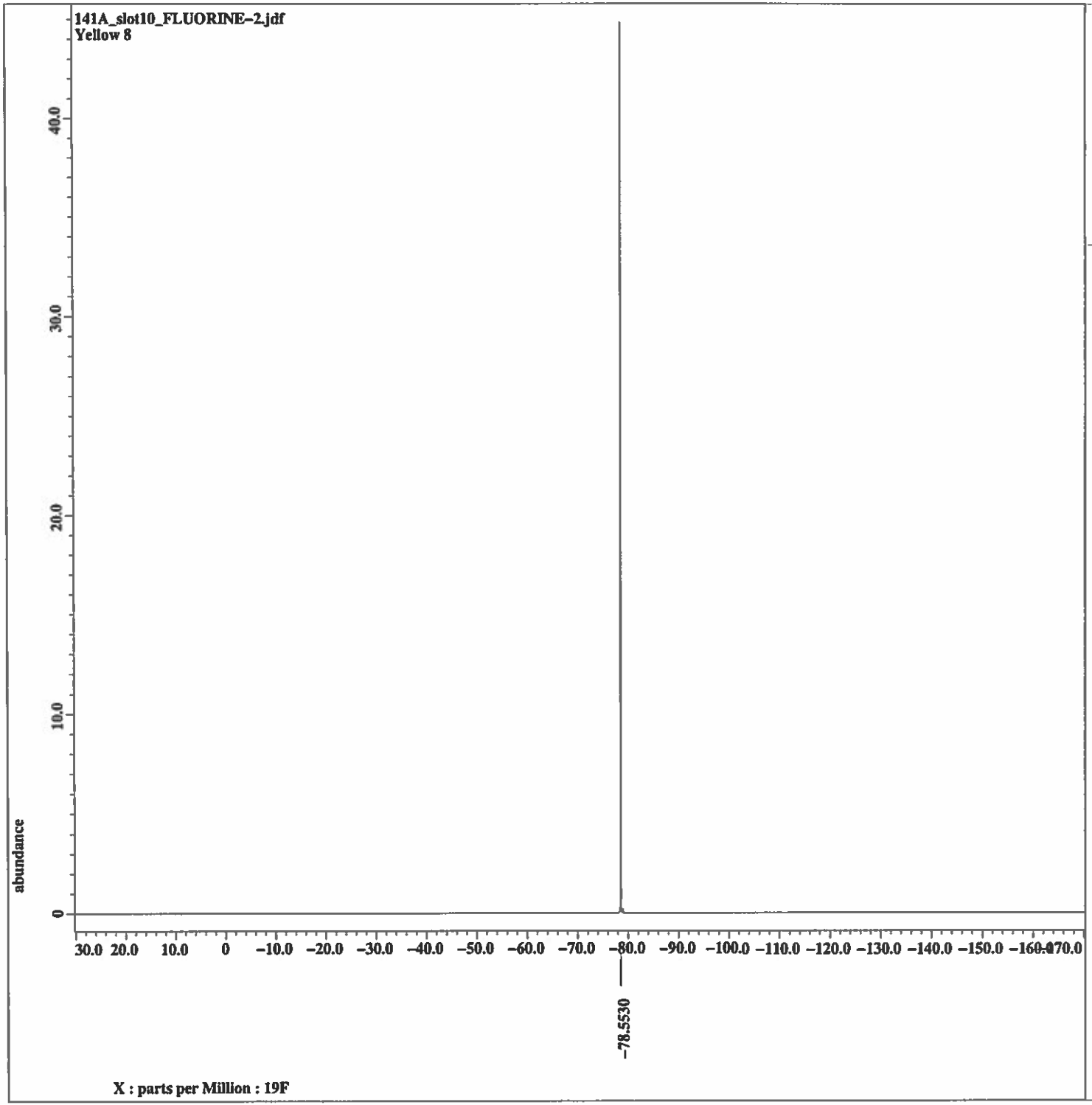
Filename	= 141A_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= 141A
Solvent	= CHLOROFORM-D
Changer_sample	= 10
Creation_time	= 1-JUL-2016 14:21:38
Revision_time	= 1-JUL-2016 14:03:33
Current_time	= 1-JUL-2016 14:03:33
Comment	= yellow 8
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
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_atn	= 4[dB]
X_pulse	= 6.675[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 26
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.4[dC]


abundance
0
1.0
2.0
3.0
4.0
141A_PROTON-4.jdf
yellow 8
X : parts per Million : 1H
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
7.8378
7.8332
7.8206
7.8183
7.7347
7.7256
7.7187
7.7107
7.7038
7.6133
7.5984
7.5870
7.5721
7.5698
7.5080
7.4897
7.4828
7.4793
7.4656
7.4232
7.4083
7.4061
7.3957
7.3912
7.2400
7.2251
7.1942
7.1885
7.1839
7.1759
7.1701
7.1209
7.1186
7.1037
6.9674
6.9526
6.8518
6.8335
1
2.03
2.0
2.02
1.99
1.83
2.05
0.1
97.86m



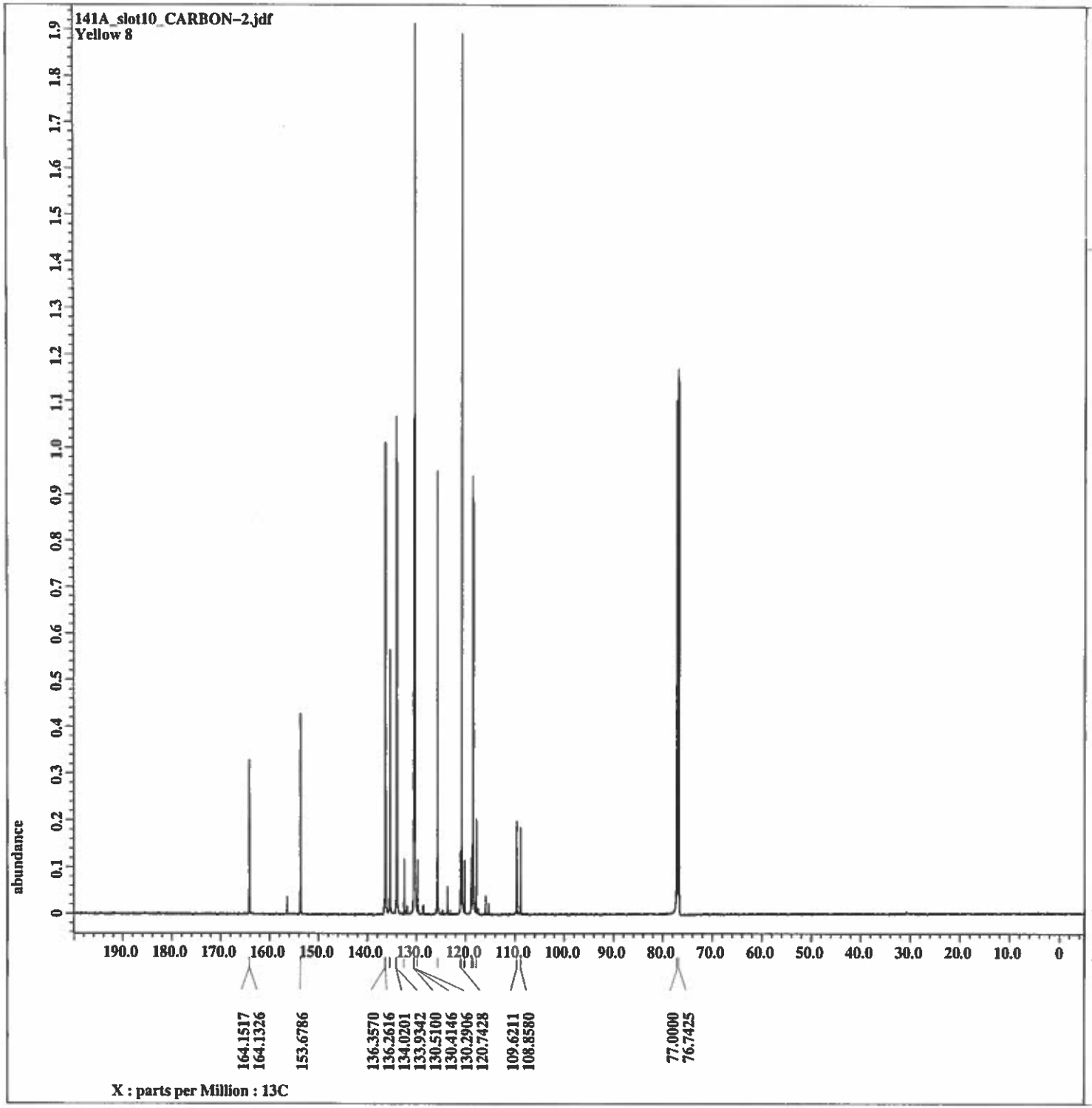
SOUTH ALABAMA JAGUARS

Filename	= 141A_slot10_PHOSPHORU
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#668763
Solvent	= CHLOROFORM-D
Changer_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	= Yellow 8
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	= WALTZ
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	= 23.6[dC]

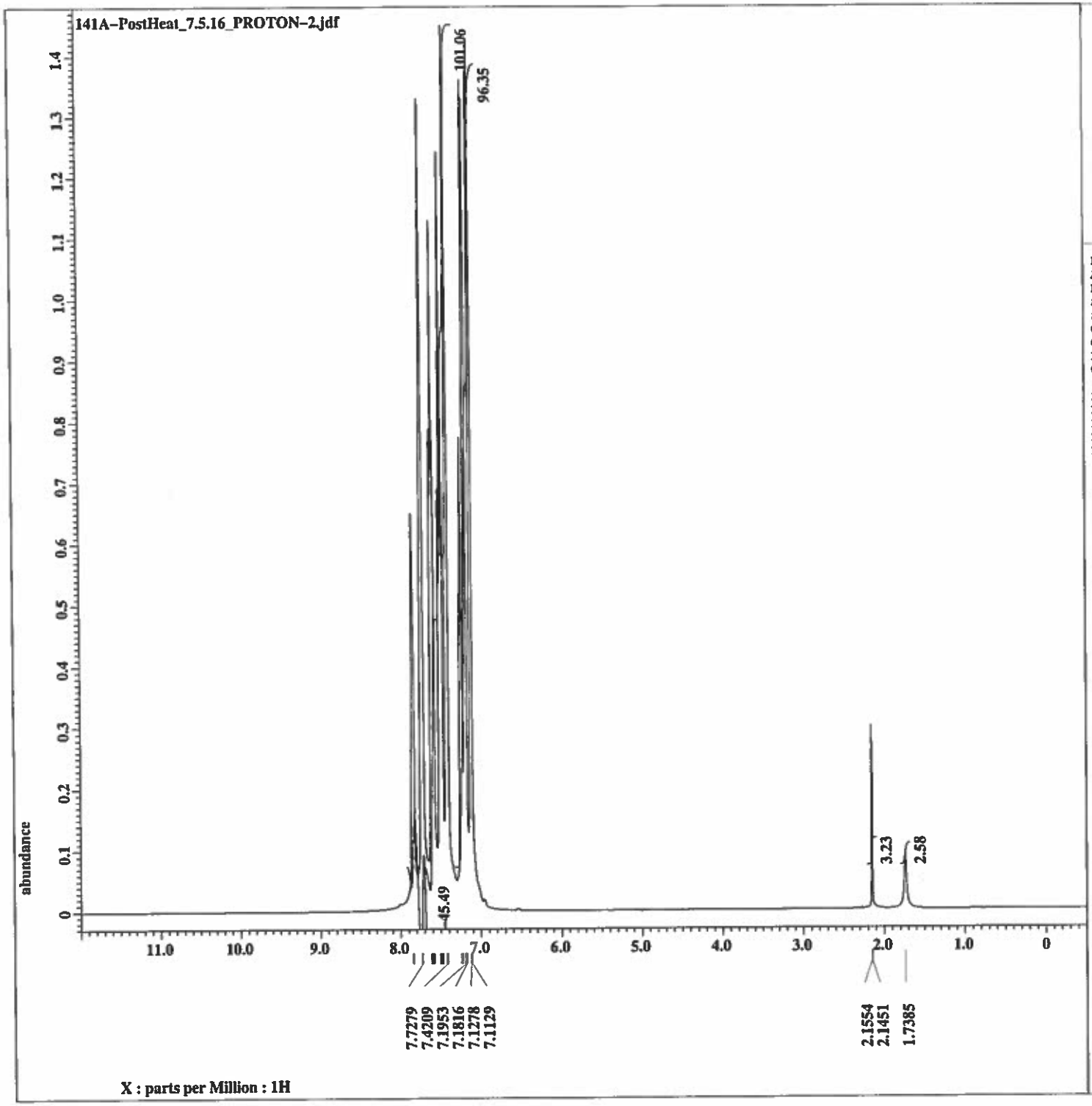


SOUTH ALABAMA JAGUARS

Filename	= 141A_slot10_FLUORINE-
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= S#570563
Solvent	= CHLOROFORM-D
Changer_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	= Yellow 8
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]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 23[dC]

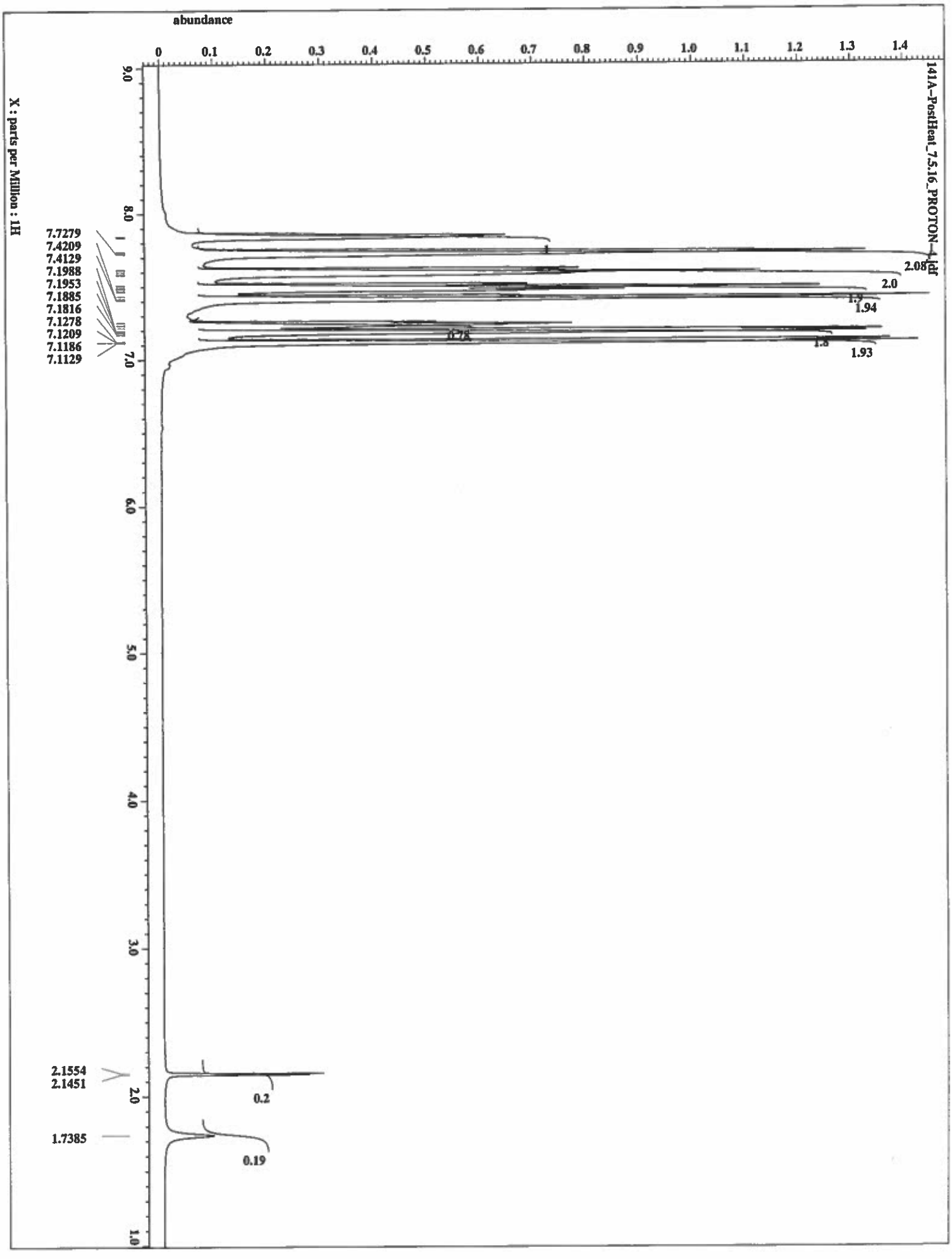


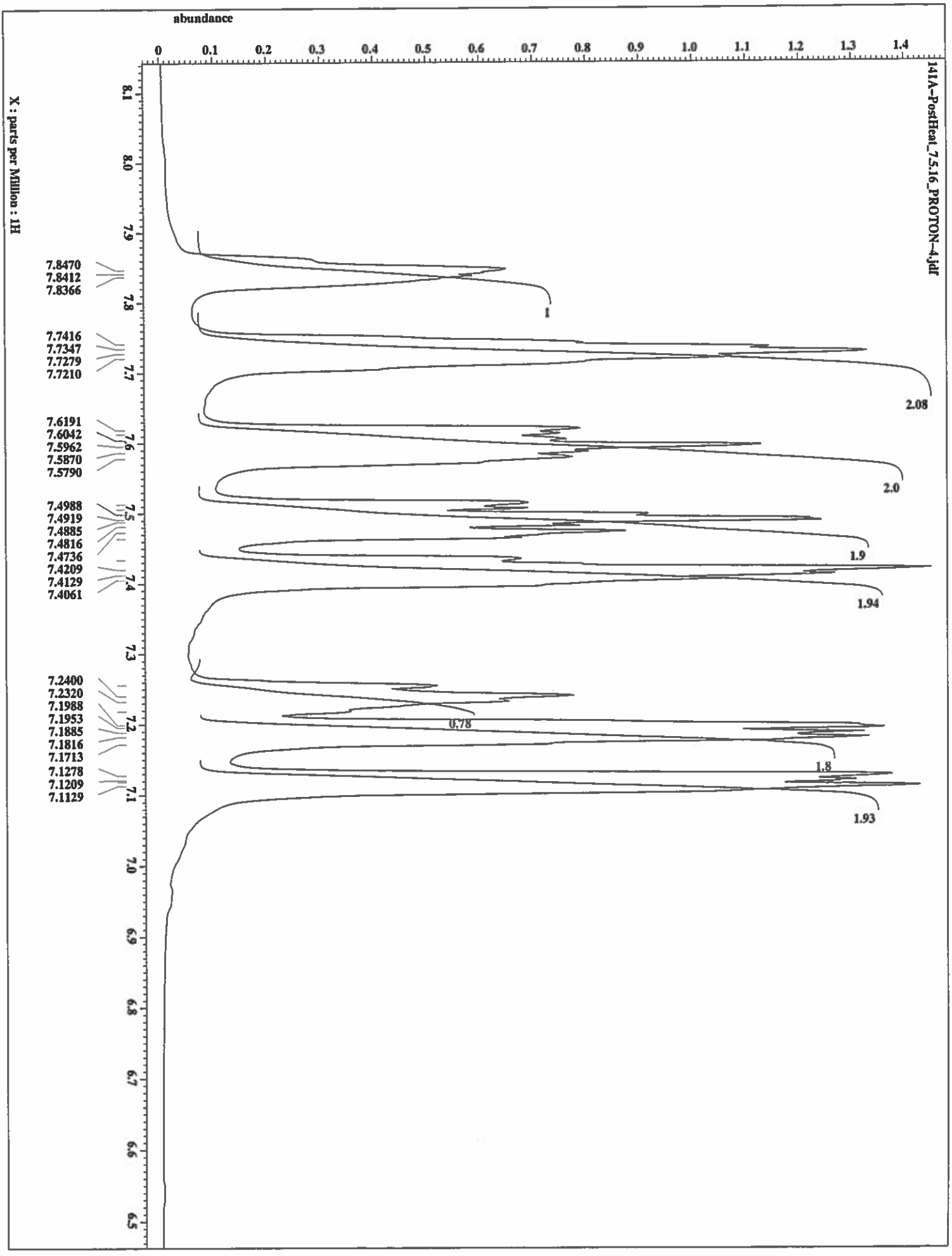
Filename	= 141A_slot10_CARBON-2.
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#524117
Solvent	= CHLOROFORM-D
Changer_sample	= 10
Creation_time	= 2-JUL-2016 17:19:26
Revision_time	= 2-JUL-2016 17:01:14
Current_time	= 2-JUL-2016 17:01:14
Comment	= Yellow 8
Data_format	= 1D COMPLEX
Dim_size	= 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]

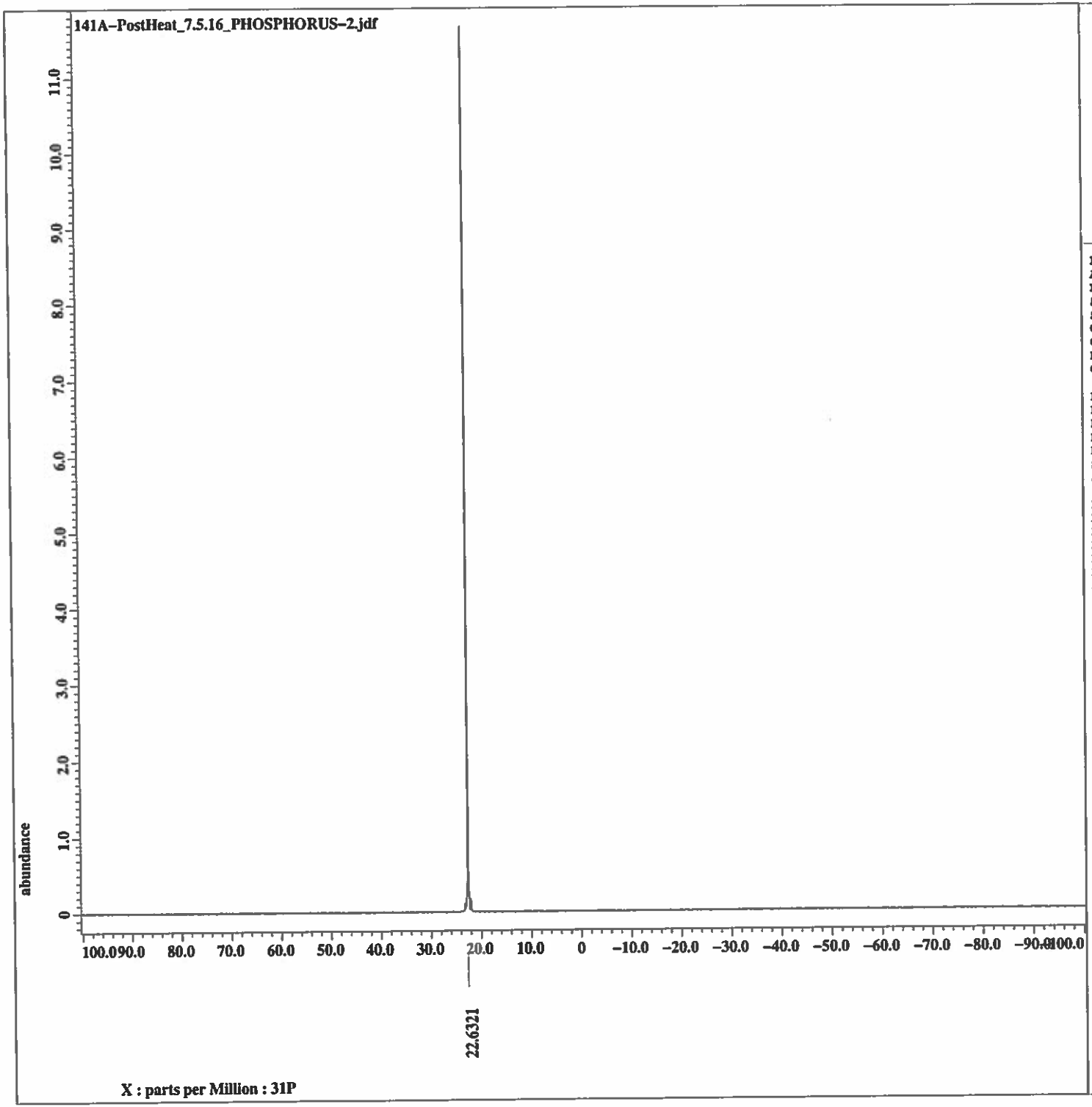


SOUTH ALABAMA JAGUARS

Filename	= 141A-PostHeat_7.5.16_
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= 141A-PostHeat_7.5.16
Solvent	= CHLOROFORM-D
Changer_sample	= 4
Creation_time	= 5-JUL-2016 15:55:44
Revision_time	= 5-JUL-2016 15:37:22
Current_time	= 5-JUL-2016 15:37:22
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
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_atn	= 4[dB]
X_pulse	= 6.675[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 28
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.7[dC]

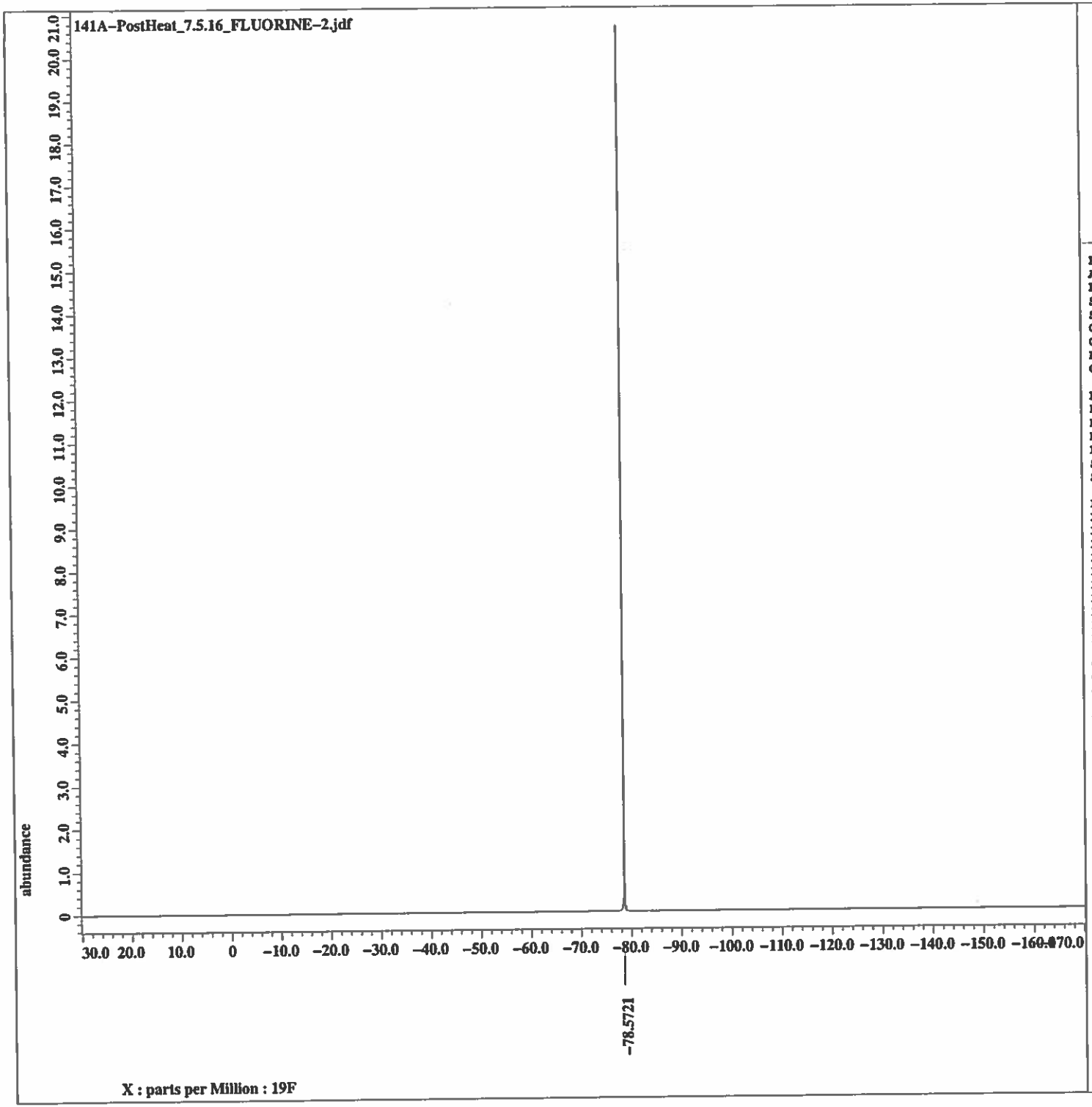

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
141A-PostHeat_7.5.16_PROTON-1.jdf
X : parts per Million : 1H
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.7279
7.4209
7.4129
7.1988
7.1953
7.1885
7.1816
7.1278
7.1209
7.1186
7.1129
2.08
2.0
1.94
0.78
1.93
2.1554
2.1451
0.2
1.7385
0.19


abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4
141A-PostHeat_7.5.16_PROTON-4.jdf
X : parts per Million : 1H
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5
7.8470
7.8412
7.8366
1
7.7416
7.7347
7.7279
7.7210
2.08
7.6191
7.6042
7.5962
7.5870
7.5790
2.0
7.4988
7.4919
7.4885
7.4816
7.4736
7.4209
7.4129
7.4061
1.9
1.94
7.2400
7.2320
7.1988
7.1953
7.1885
7.1816
7.1713
7.1278
7.1209
7.1129
0.78
1.8
1.93



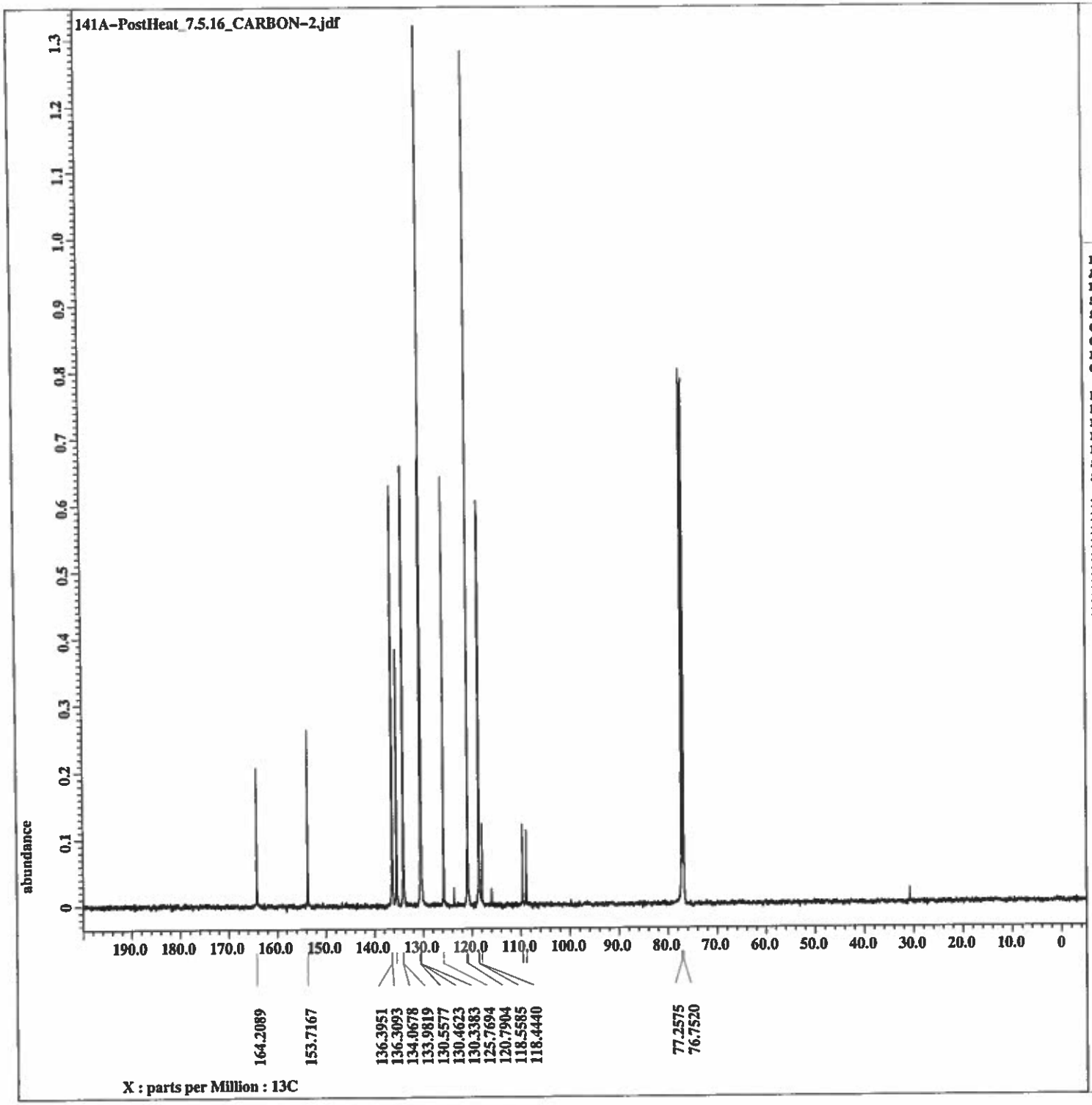
SOUTH ALABAMA JAGUARS

Filename	= 141A-PostHeat_7.5.16_
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= 141A-PostHeat_7.5.16
Solvent	= CHLOROFORM-D
Changer_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	= 202.46831075[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	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.64487424[s]
Temp_get	= 23.4[dC]



SOUTH ALABAMA JAGUARS

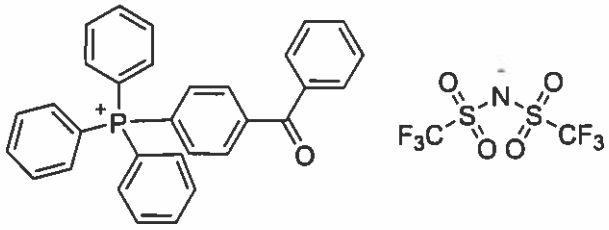
Filename	= 141A-PostHeat_7.5.16_
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= 141A-PostHeat_7.5.16
Solvent	= CHLOROFORM-D
Changer_sample	= 4
Creation_time	= 5-JUL-2016 18:16:22
Revision_time	= 5-JUL-2016 17:58:00
Current_time	= 5-JUL-2016 17:58:00
Data_format	= 1D COMPLEX
Dim_size	= 52428
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]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.9[dC]



SOUTH ALABAMA JAGUARS

Filename	= 141A-PostHeat_7.5.16_
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= 141A-PostHeat_7.5.16
Solvent	= CHLOROFORM-D
Changer_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
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	= 23.6[dC]

COMPOUND 8



Atlantic Microlab, Inc.

:lantic Blvd. Suite M
ss, GA 30071
lanticmicrolab.com

No. Phosphonium NEW1

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

ient	Theory	Found	
C	54.77	54.64	
H	3.34	3.38	
N	1.94	1.94	

Single ☒ Duplicate ☐

Elements Present: CHNPOSF

Analyze for: CHN

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.

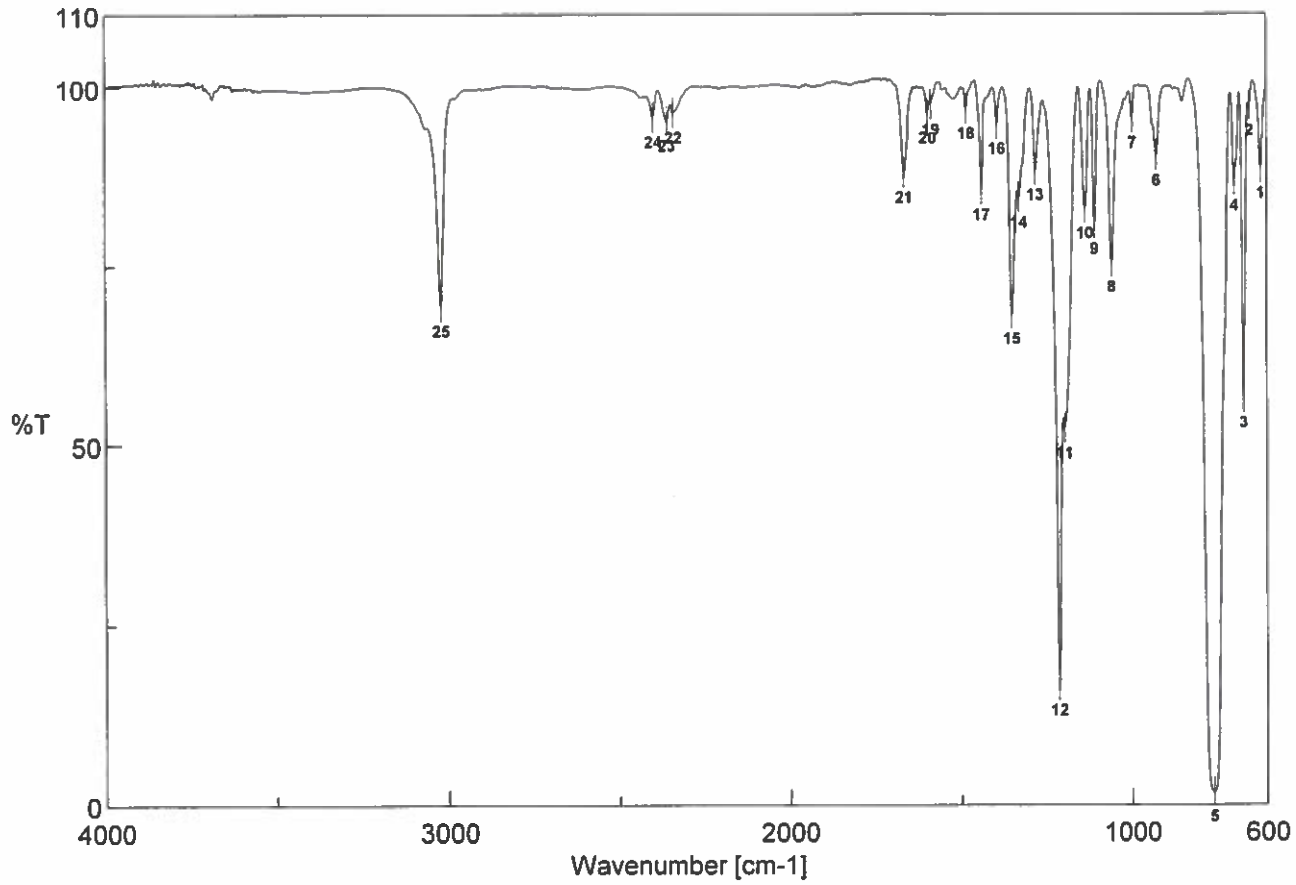
Include Email Address or FAX # Below

jdavis@southalabama.edu

Received NOV 01 2016 Date Completed NOV 01 2016

arks:

FREEDOM - FREHEAT 04/08/2014



Result of Peak Picking

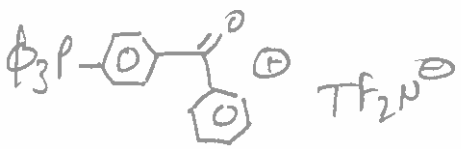
No.	Position	Intensity	No.	Position	Intensity
1	617.109	88.453	2	650.858	97.1388
3	668.214	56.3186	4	697.141	86.7757
5	757.888	1.74588	6	926.628	90.2178
7	997.982	95.417	8	1058.73	75.3689
9	1108.87	80.6851	10	1136.83	82.9582
11	1198.54	52.1195	12	1215.9	16.5624
13	1282.43	88.2943	14	1331.61	84.4817
15	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]

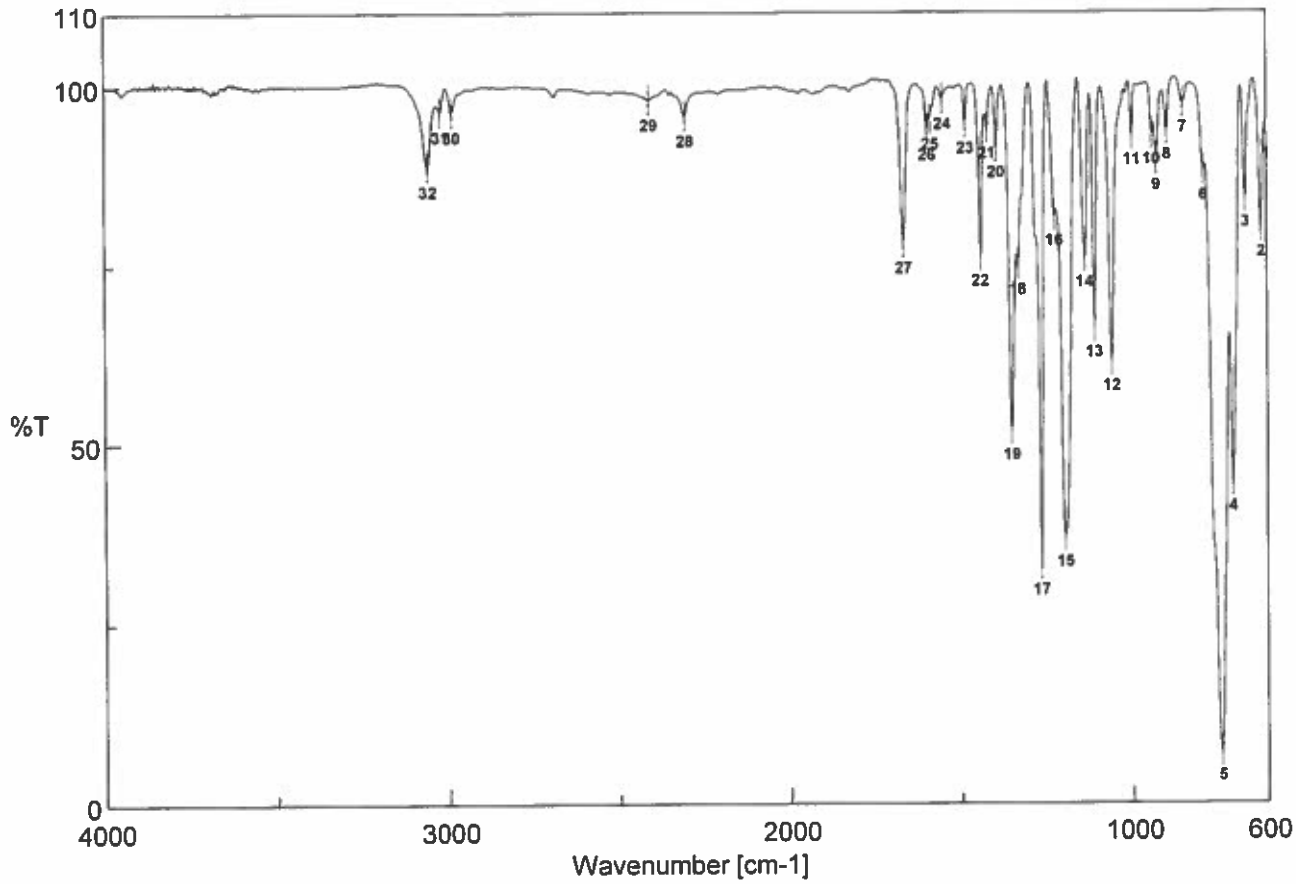
Sample Name	
Comment	
User	
Division	
Company	University of South Alabama

[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 heat



Result of Peak Picking

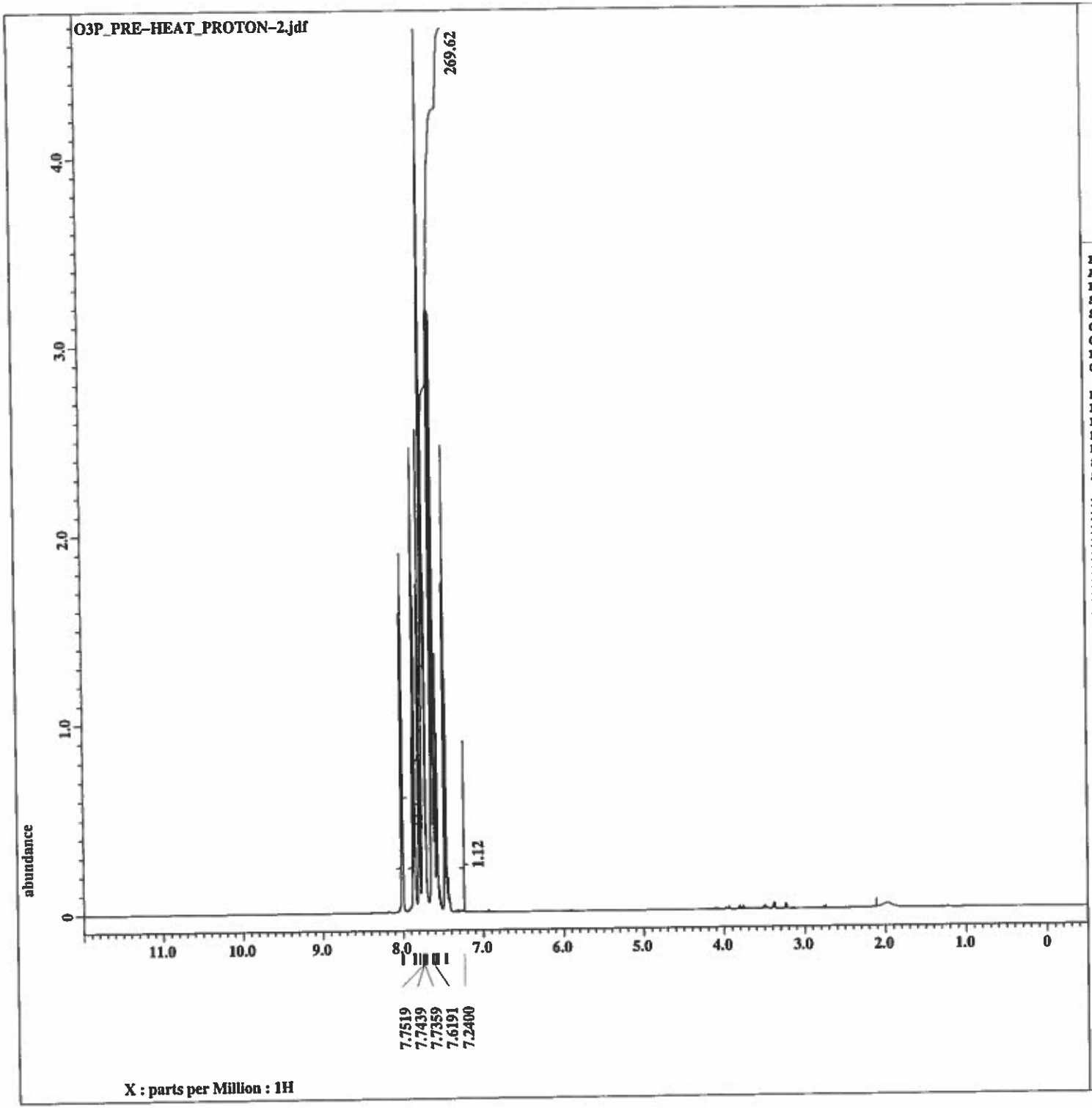
No.	Position	Intensity	No.	Position	Intensity
1	600.717	93.6423	2	617.109	79.9825
3	663.393	84.2213	4	702.926	44.5407
5	738.603	7.16906	6	787.779	87.9998
7	847.561	97.4499	8	895.773	93.6442
9	926.628	89.4414	10	939.163	93.0852
11	997.982	92.9605	12	1059.69	61.4873
13	1108.87	66.2023	14	1136.83	75.9367
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

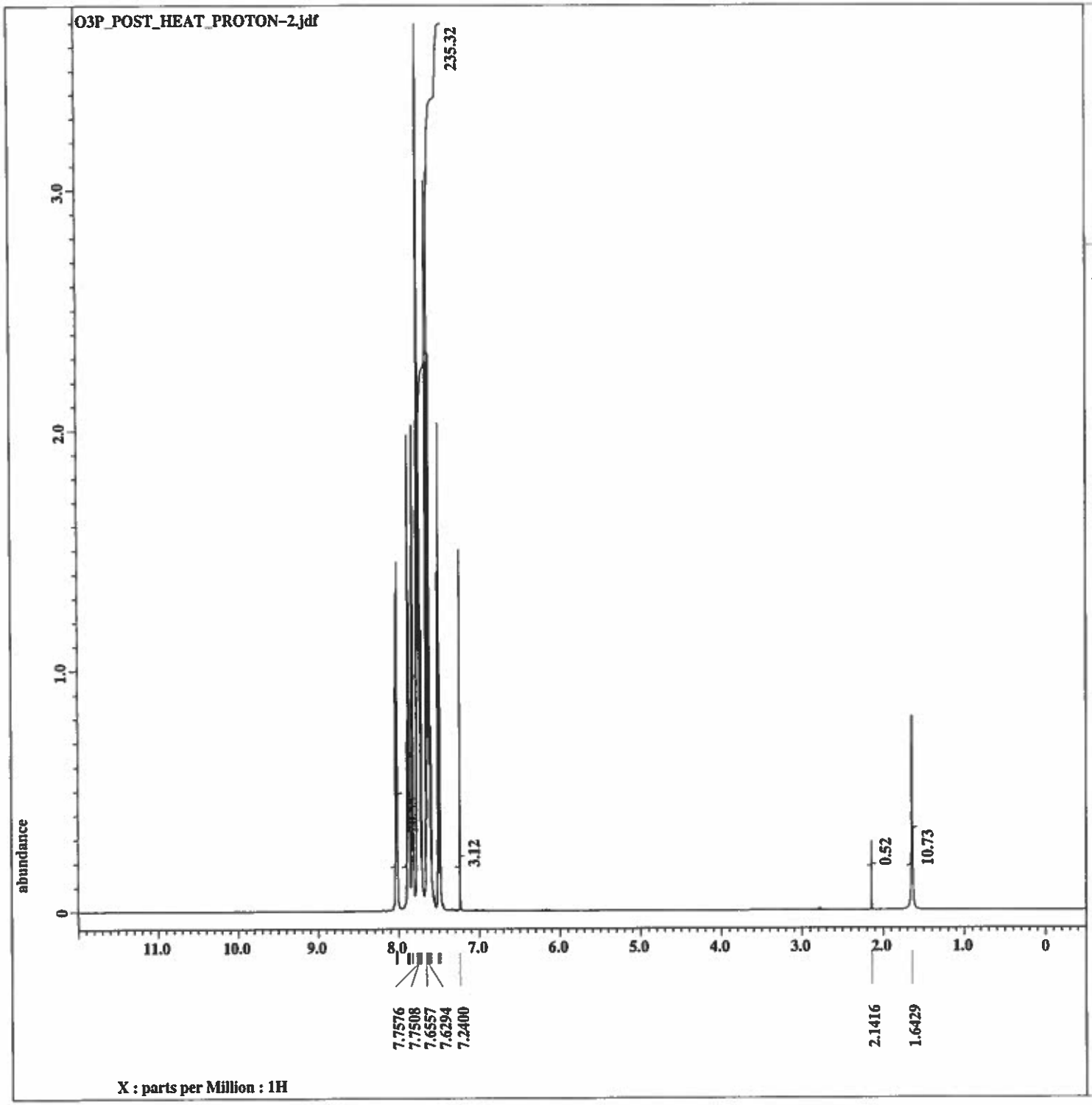
[Measurement Information]

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)



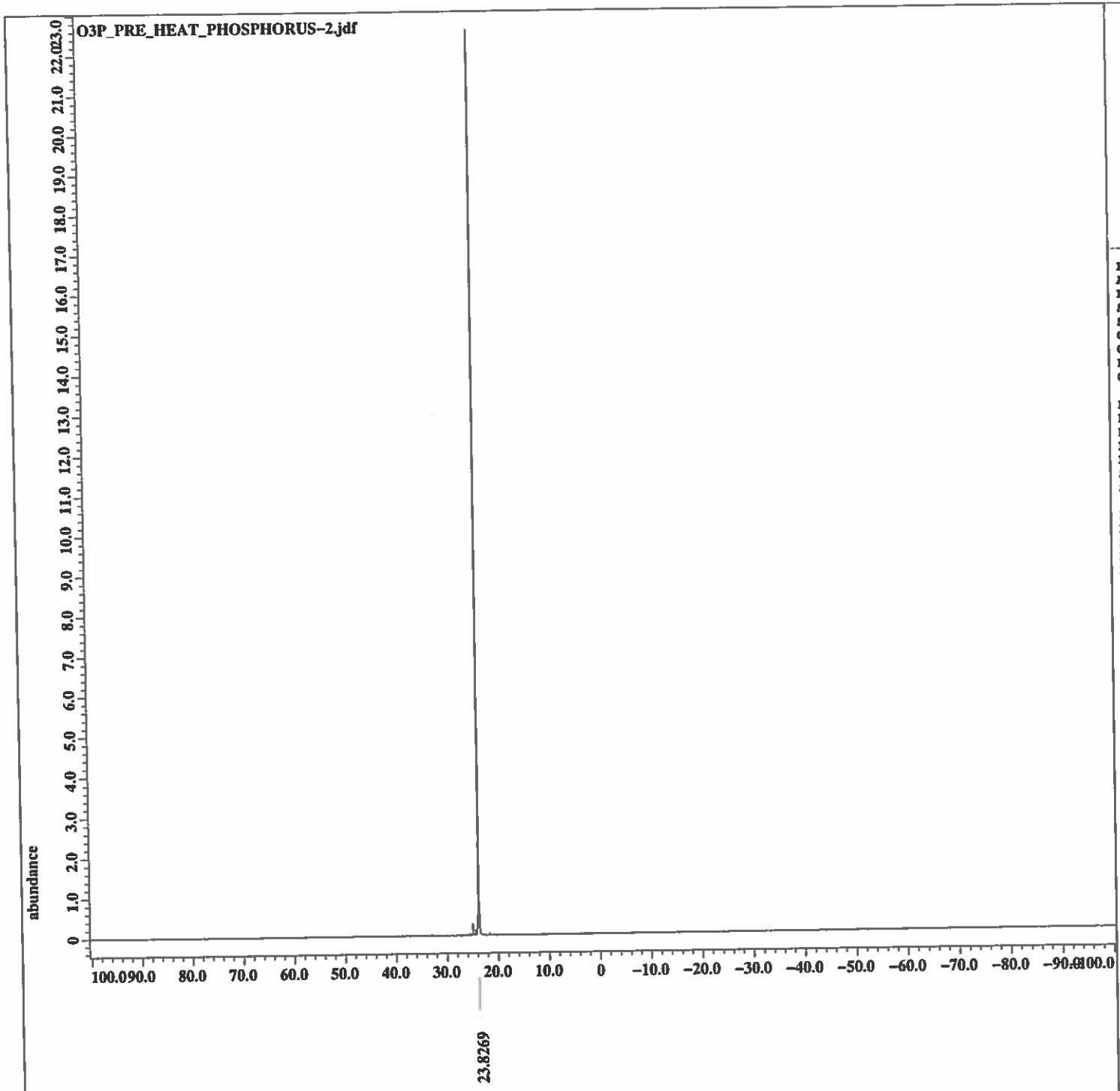
SOUTH ALABAMA JAGUARS

Filename	= O3P_PRE-HEAT_PROTON-2
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= O3P_PRE-HEAT
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 8-JUL-2016 13:53:23
Revision_time	= 8-JUL-2016 13:34:47
Current_time	= 8-JUL-2016 13:34:47
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
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_atn	= 4[dB]
X_pulse	= 6.675[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 26
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.3[dC]

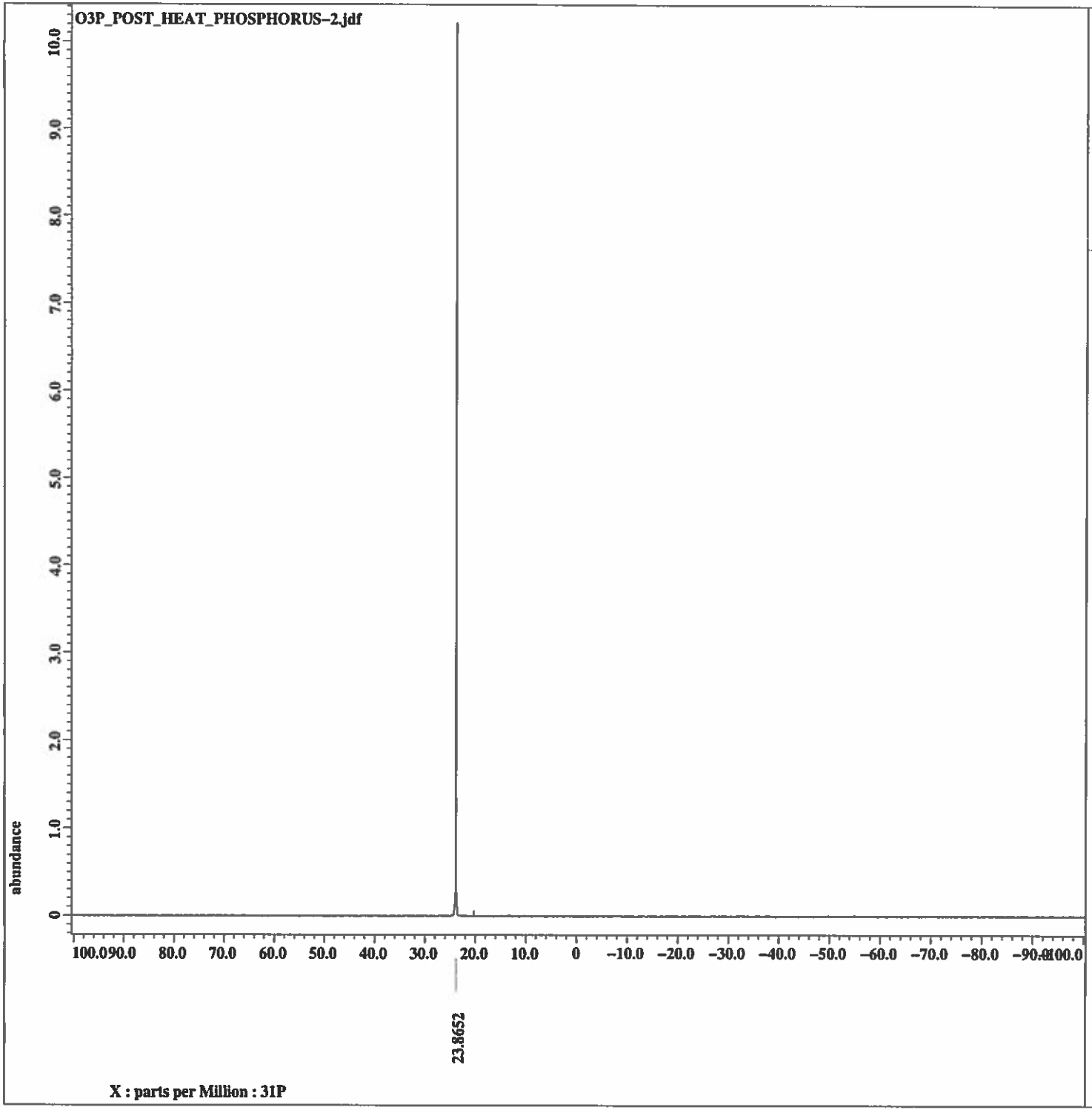


SOUTH ALABAMA JAGUARS

Filename	= O3P_POST_HEAT_PROTON-
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= O3P_POST_HEAT
Solvent	= CHLOROFORM-D
Changer_sample	= 7
Creation_time	= 8-JUL-2016 13:59:31
Revision_time	= 8-JUL-2016 13:40:53
Current_time	= 8-JUL-2016 13:40:53
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
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_atn	= 4[dB]
X_pulse	= 6.675[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.4[dC]

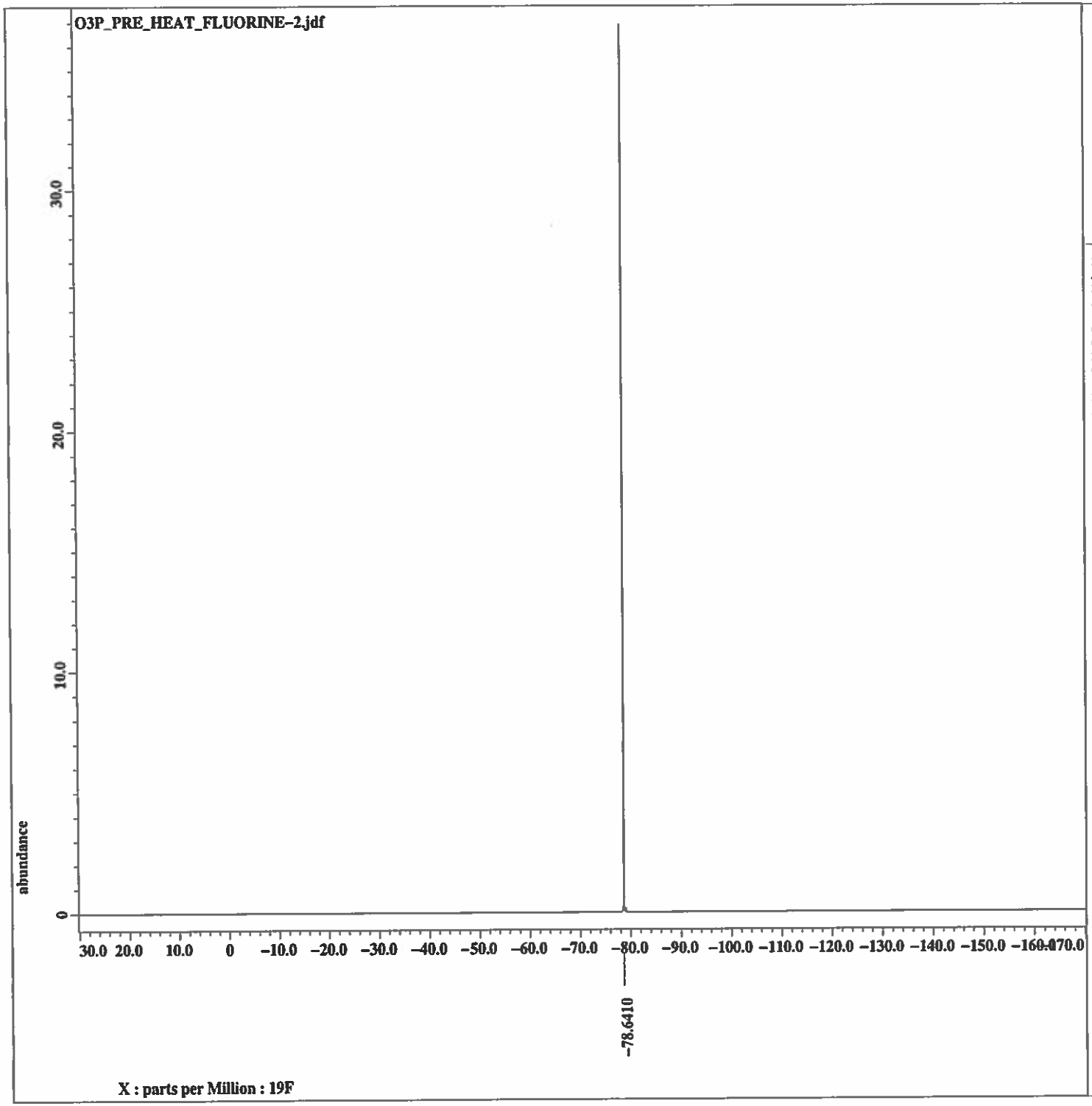


Filename	= O3P_PRE_HEAT_PHOSPHOR
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= O3P_PRE_HEAT
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 8-JUL-2016 14:29:24
Revision_time	= 8-JUL-2016 14:10:48
Current_time	= 8-JUL-2016 14:10:48
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 31P
Dim_units	= [ppm]
Dimensions	= X
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	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 54
Relaxation_delay	= 2[s]
Repetition_time	= 2.64487424[s]
Temp_get	= 23.5[dC]



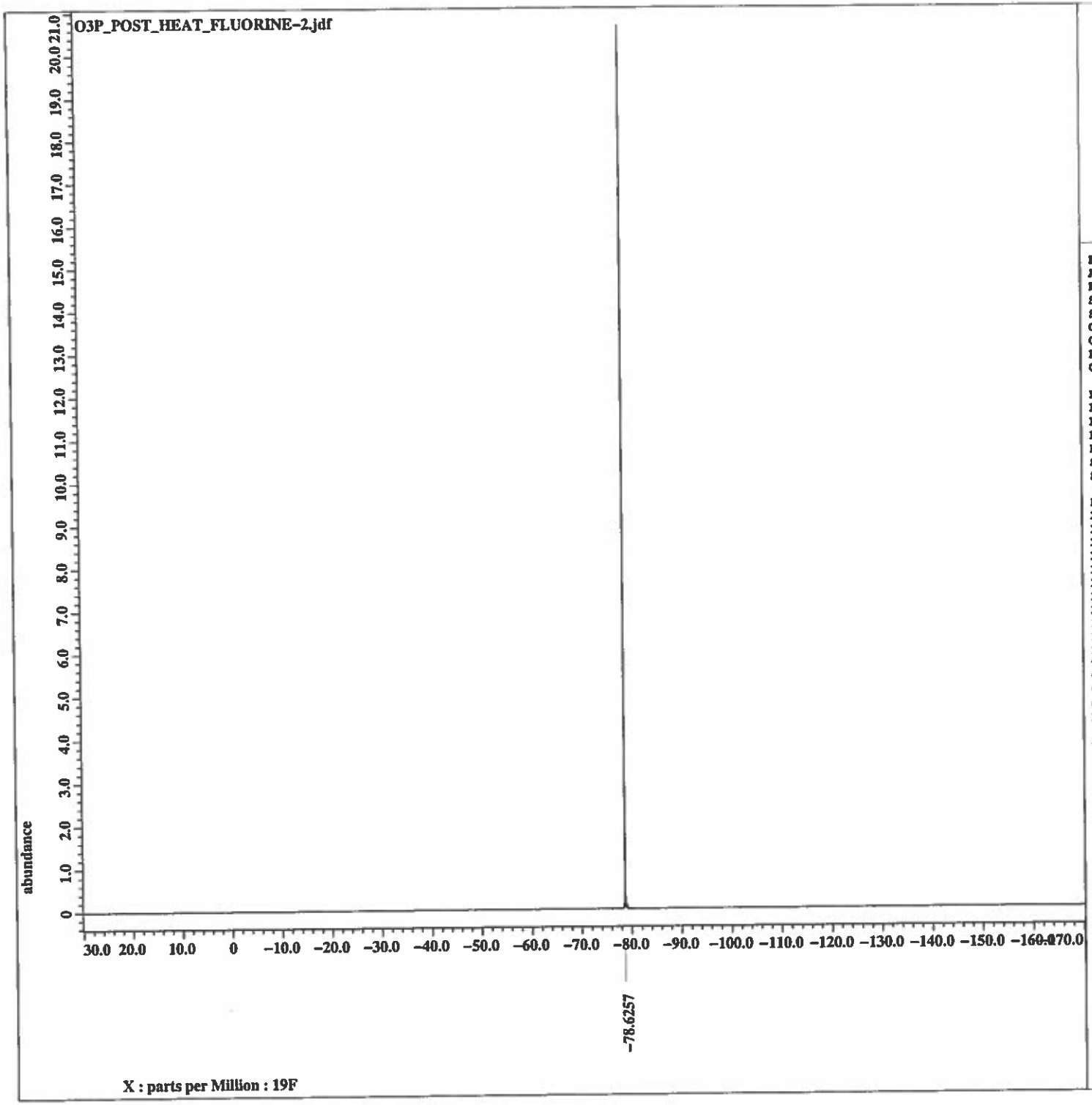
SOUTH ALABAMA JAGUARS

Filename	= O3P_POST_HEAT_PHOSPHO
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= O3P_POST_HEAT
Solvent	= CHLOROFORM-D
Changer_sample	= 7
Creation_time	= 8-JUL-2016 14:13:09
Revision_time	= 8-JUL-2016 13:54:31
Current_time	= 8-JUL-2016 13:54:31
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	= WALTZ
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]



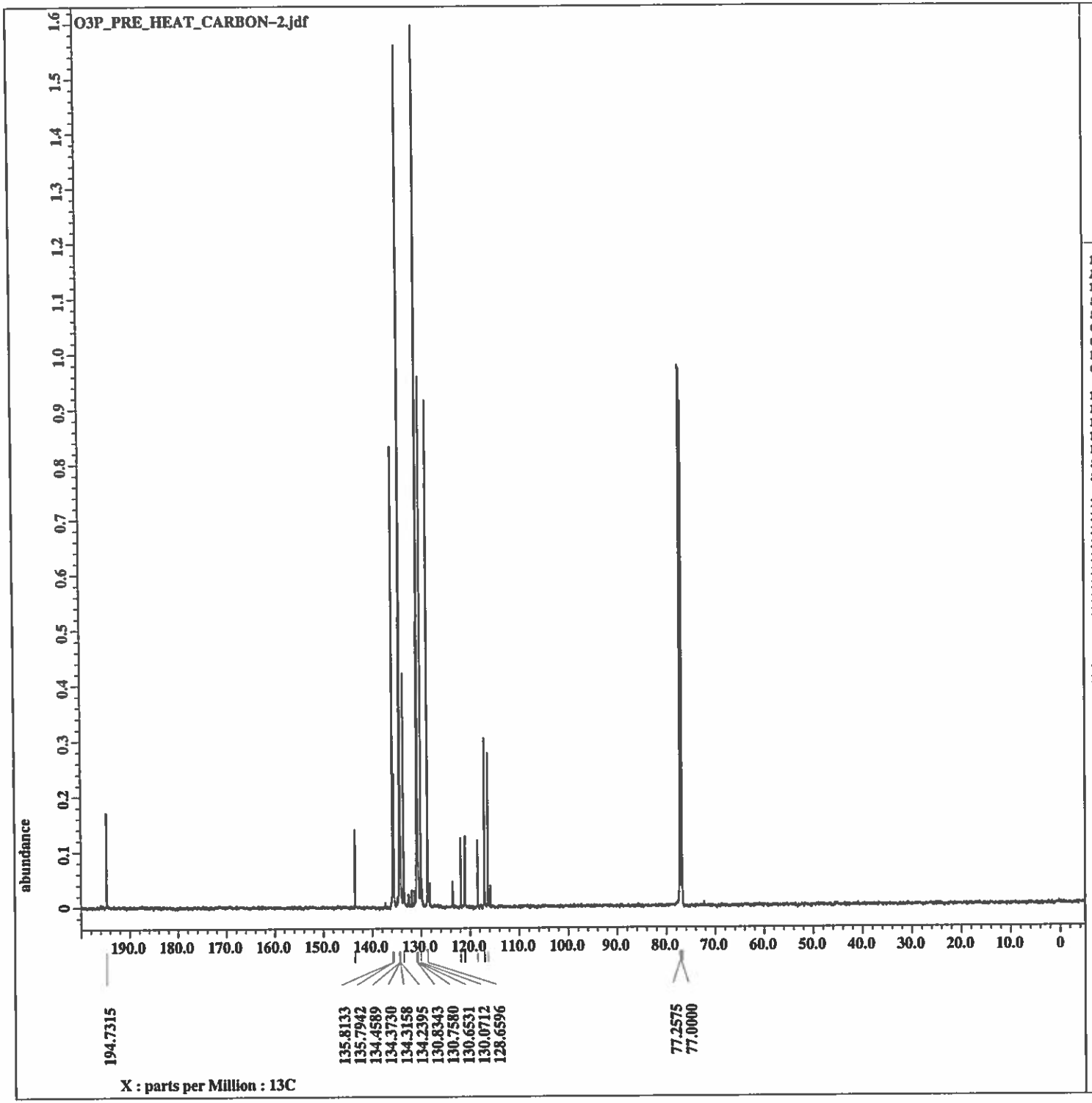
SOUTH ALABAMA JAGUARS

Filename	= O3P_PRE_HEAT_FLUORINE
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= O3P_PRE_HEAT
Solvent	= CHLOROFORM-D
Changer_sample	= 6
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_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]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 38
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.5[dC]



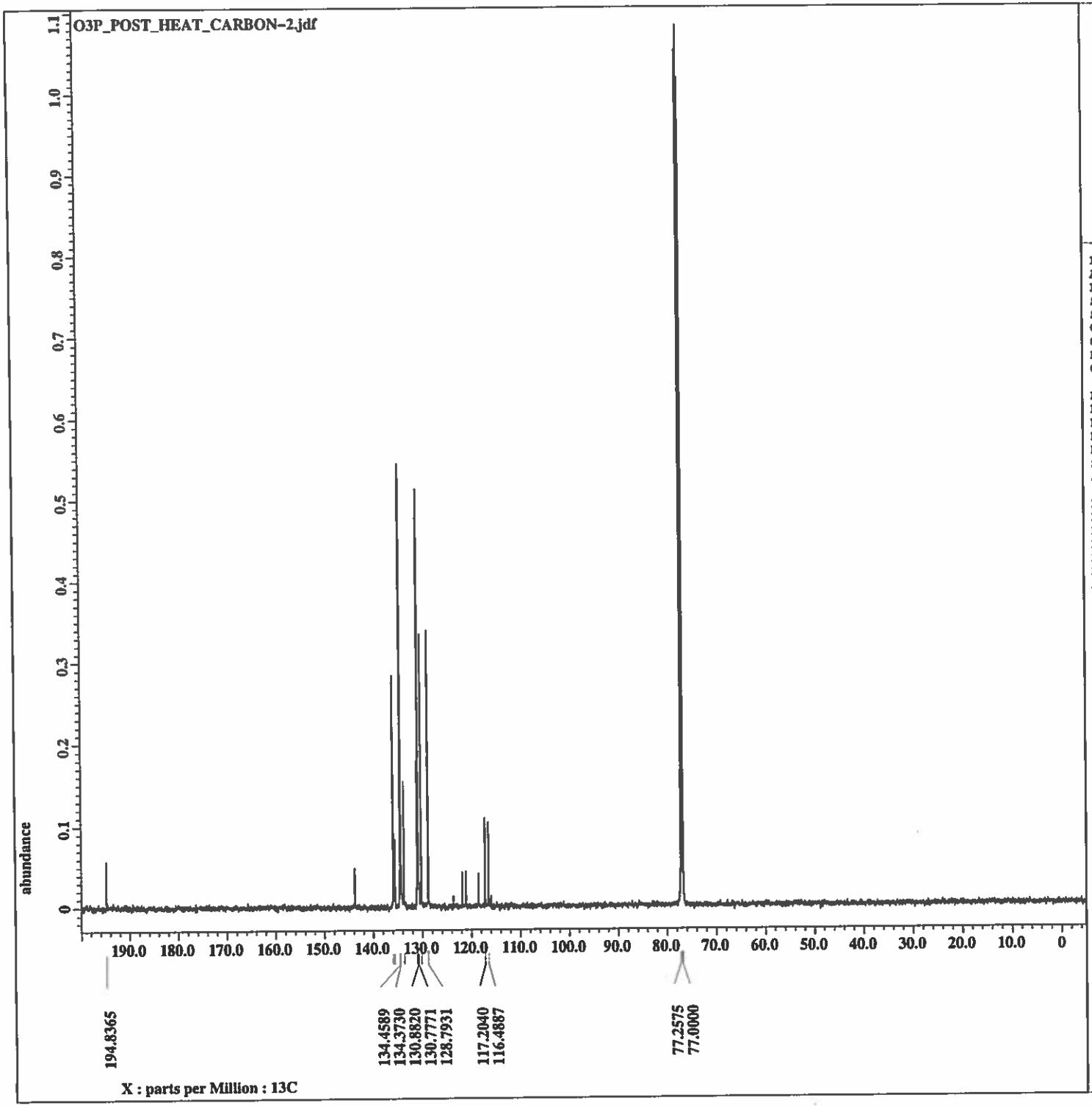
SOUTH ALABAMA JAGUARS

Filename	= O3P_POST_HEAT_FLUORIN
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= O3P_POST_HEAT
Solvent	= CHLOROFORM-D
Changer_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	= 470.62046084[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]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 44
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.6[dC]



SOUTH ALABAMA JAGUARS

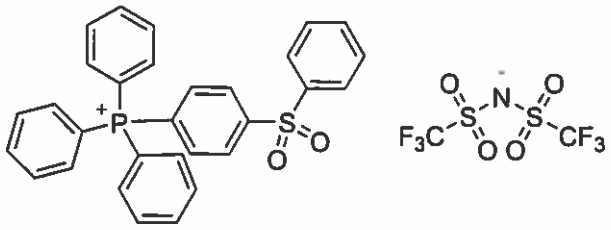
Filename	= O3P_PRE_HEAT_CARBON-2
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= O3P_PRE_HEAT
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 8-JUL-2016 19:06:38
Revision_time	= 8-JUL-2016 18:47:59
Current_time	= 8-JUL-2016 18:47:59
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 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	= 23.5[dC]

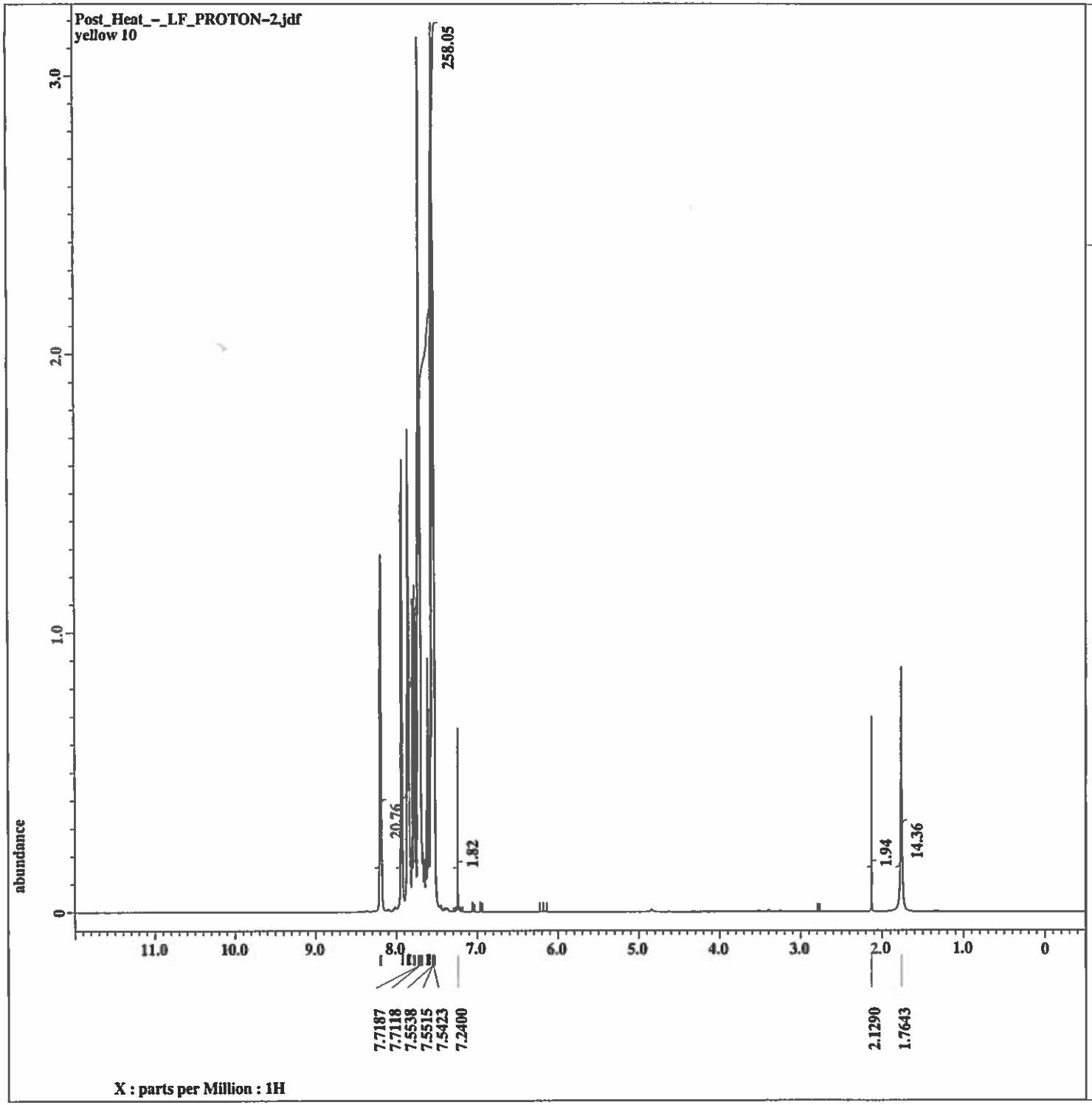


SOUTH ALABAMA JAGUARS

Filename	= O3P_POST_HEAT_CARBON-
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= O3P_POST_HEAT
Solvent	= CHLOROFORM-D
Changer_sample	= 7
Creation_time	= 8-JUL-2016 18:13:19
Revision_time	= 8-JUL-2016 17:54:41
Current_time	= 8-JUL-2016 17:54:41
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= TRUE
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	= 23.5[dC]

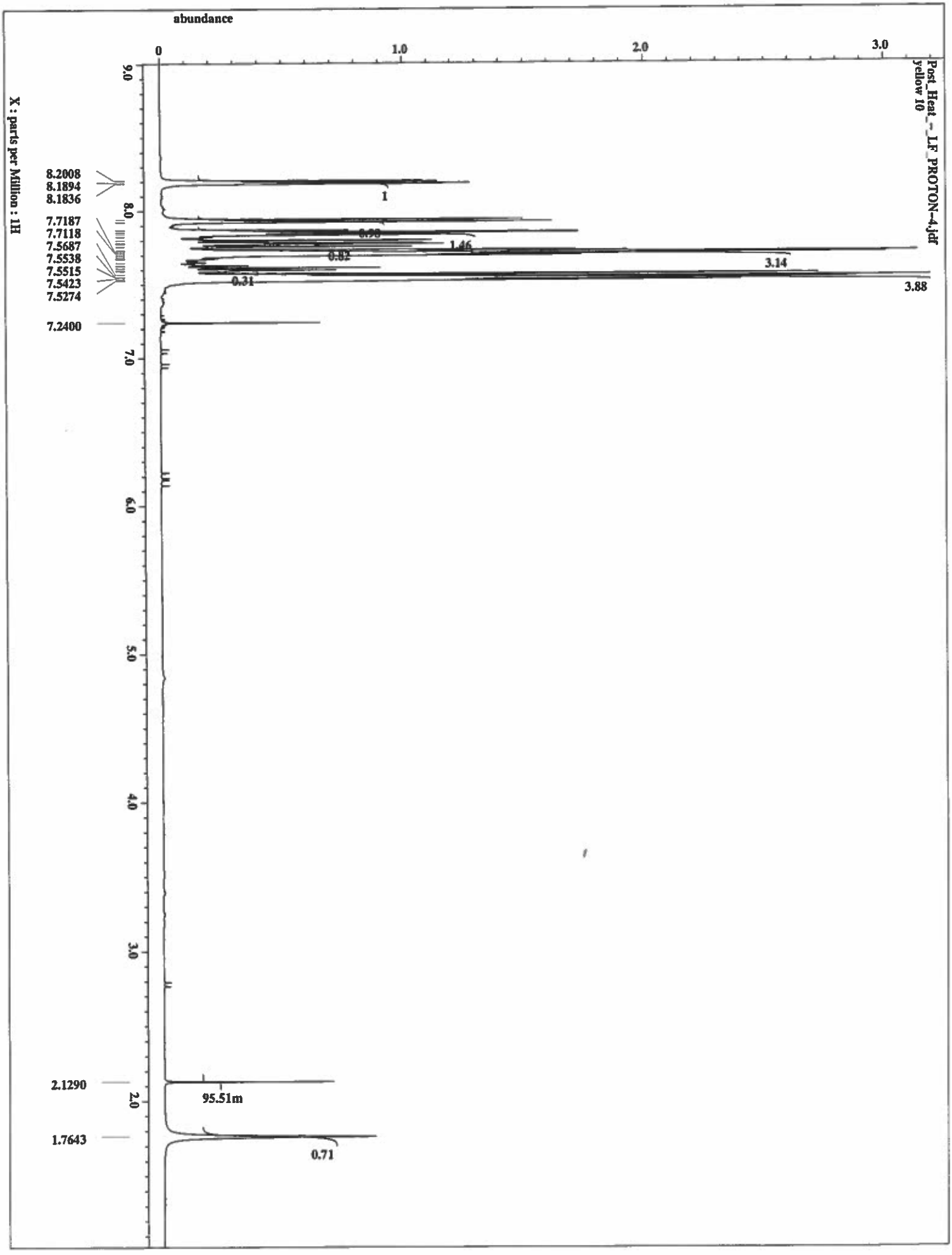
COMPOUND 9

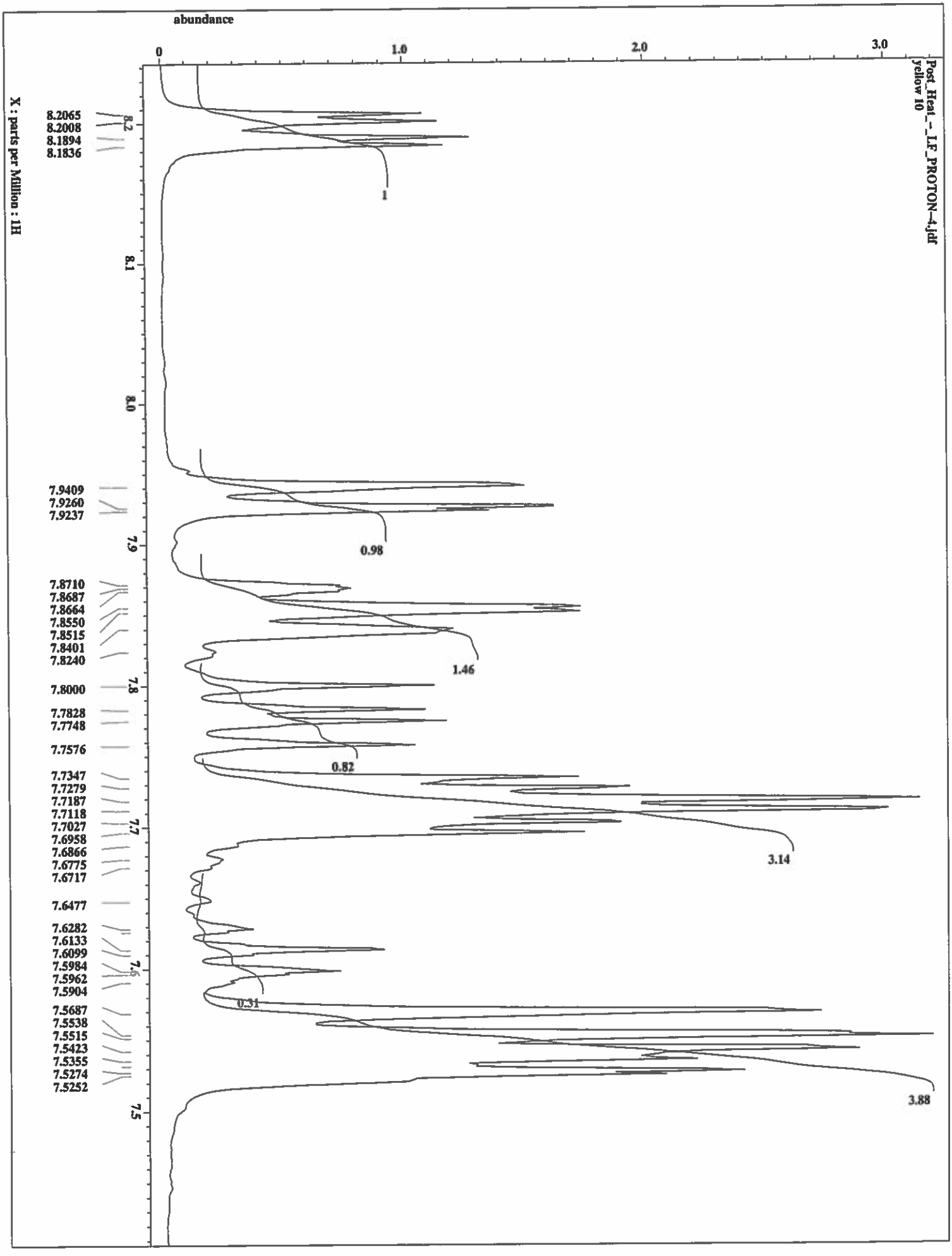


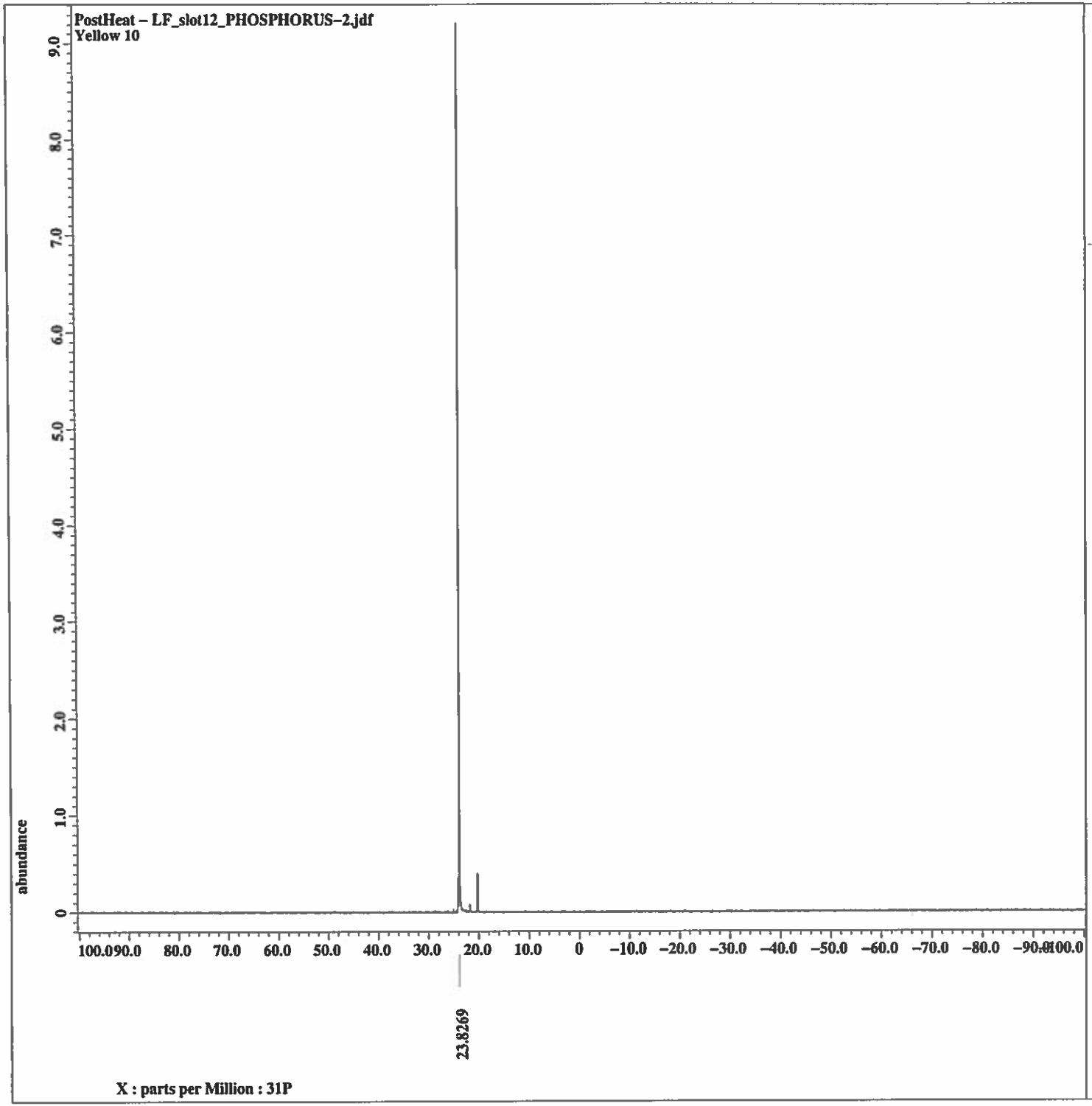


SOUTH ALABAMA JAGUARS

Filename	= Post_Heat_-_LF_PROTON
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= Post_Heat_-_LF
Solvent	= CHLOROFORM-D
Changer_sample	= 12
Creation_time	= 1-JUL-2016 14:40:35
Revision_time	= 1-JUL-2016 14:22:30
Current_time	= 1-JUL-2016 14:22:30
Comment	= yellow 10
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
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_atn	= 4[dB]
X_pulse	= 6.675[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 32
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.2[dC]

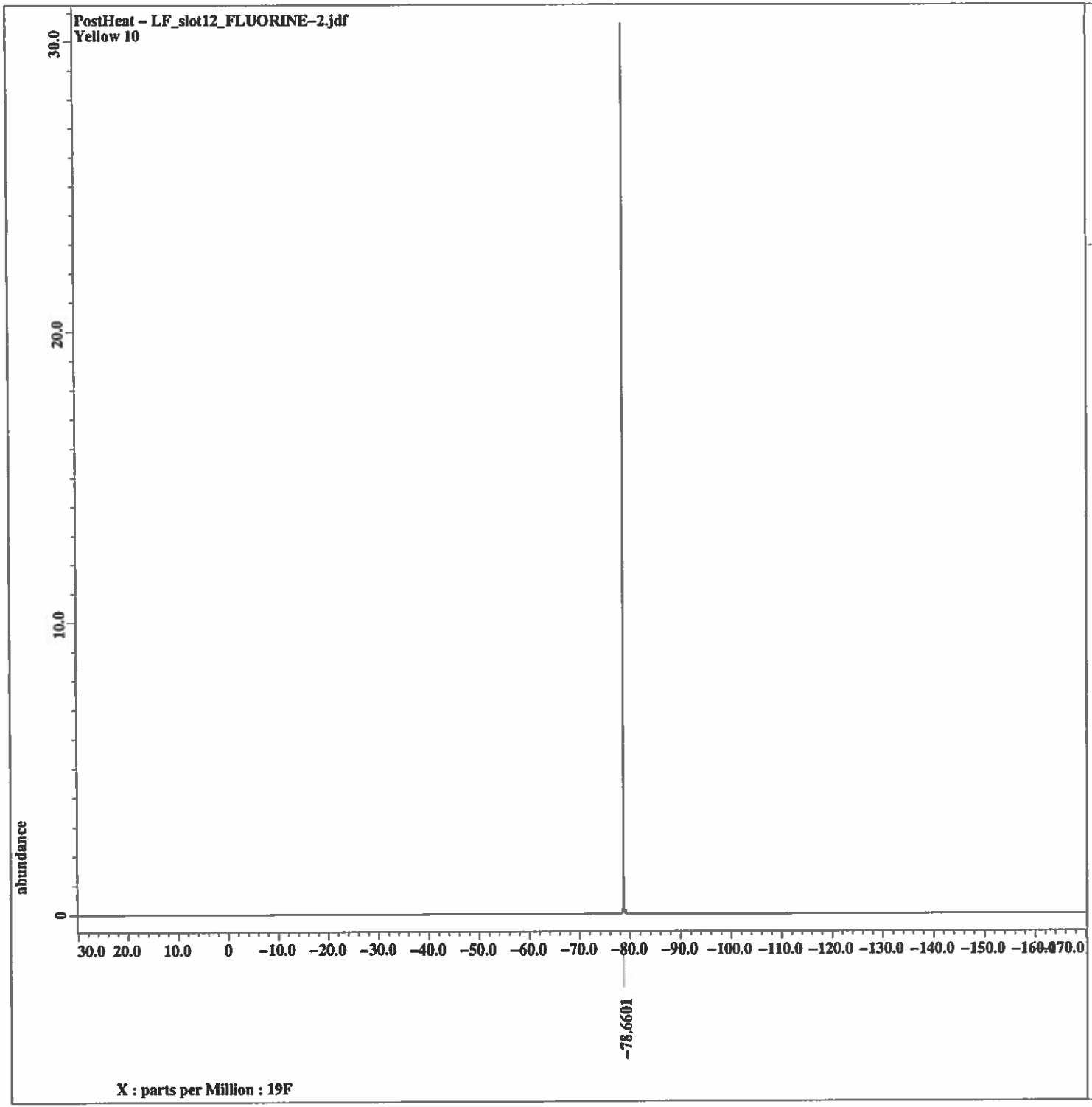

abundance
0
1.0
2.0
3.0
Post_Heat_-_LF_PROTON-4.jdf
yellow 10
X : parts per Million : 1H
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
8.2008
8.1894
8.1836
7.7187
7.7118
7.5687
7.5538
7.5515
7.5423
7.5274
7.2400
2.1290
1.7643
1
0.98
1.46
0.82
3.14
0.31
3.88
95.51m
0.71


abundance
0
1.0
2.0
3.0
Post_Heat_-_LF_PROTON-4.jdf
yellow 10
X : parts per Million : 1H
8.2065
8.2008
8.1894
8.1836
1
7.9409
7.9260
7.9237
0.98
7.8710
7.8687
7.8664
7.8550
7.8515
7.8401
7.8240
1.46
7.8000
7.7828
7.7748
7.7576
0.82
7.7347
7.7279
7.7187
7.7118
7.7027
7.6958
7.6866
7.6775
7.6717
3.14
7.6477
7.6282
7.6133
7.6099
7.5984
7.5962
7.5904
0.31
7.5687
7.5538
7.5515
7.5423
7.5355
7.5274
7.5252
3.88
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5



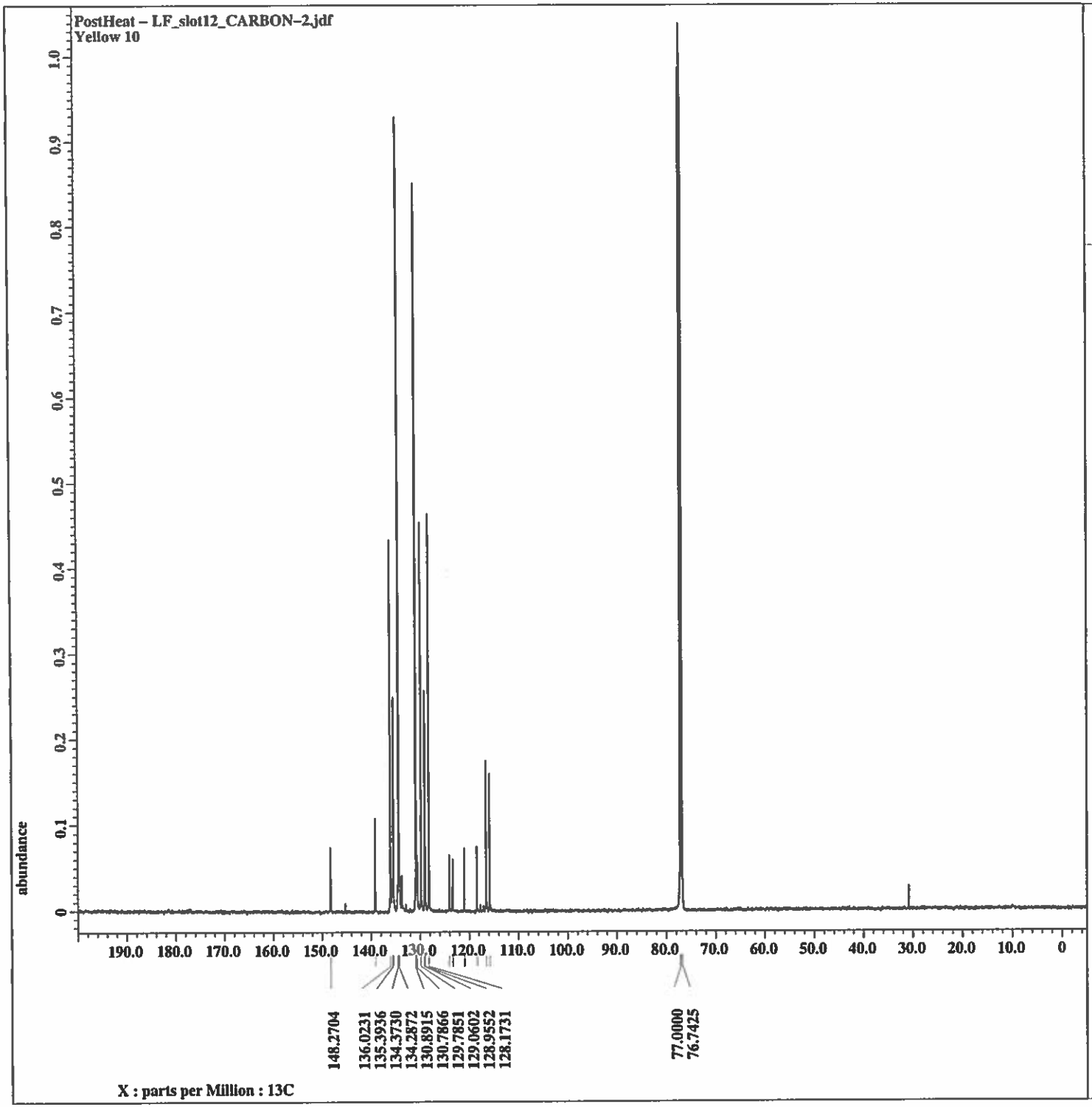
SOUTH ALABAMA JAGUARS

Filename	= PostHeat - LF_slot12_
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#697411
Solvent	= CHLOROFORM-D
Changer_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	= Yellow 10
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	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.64487424[s]
Temp_get	= 23.7[dC]



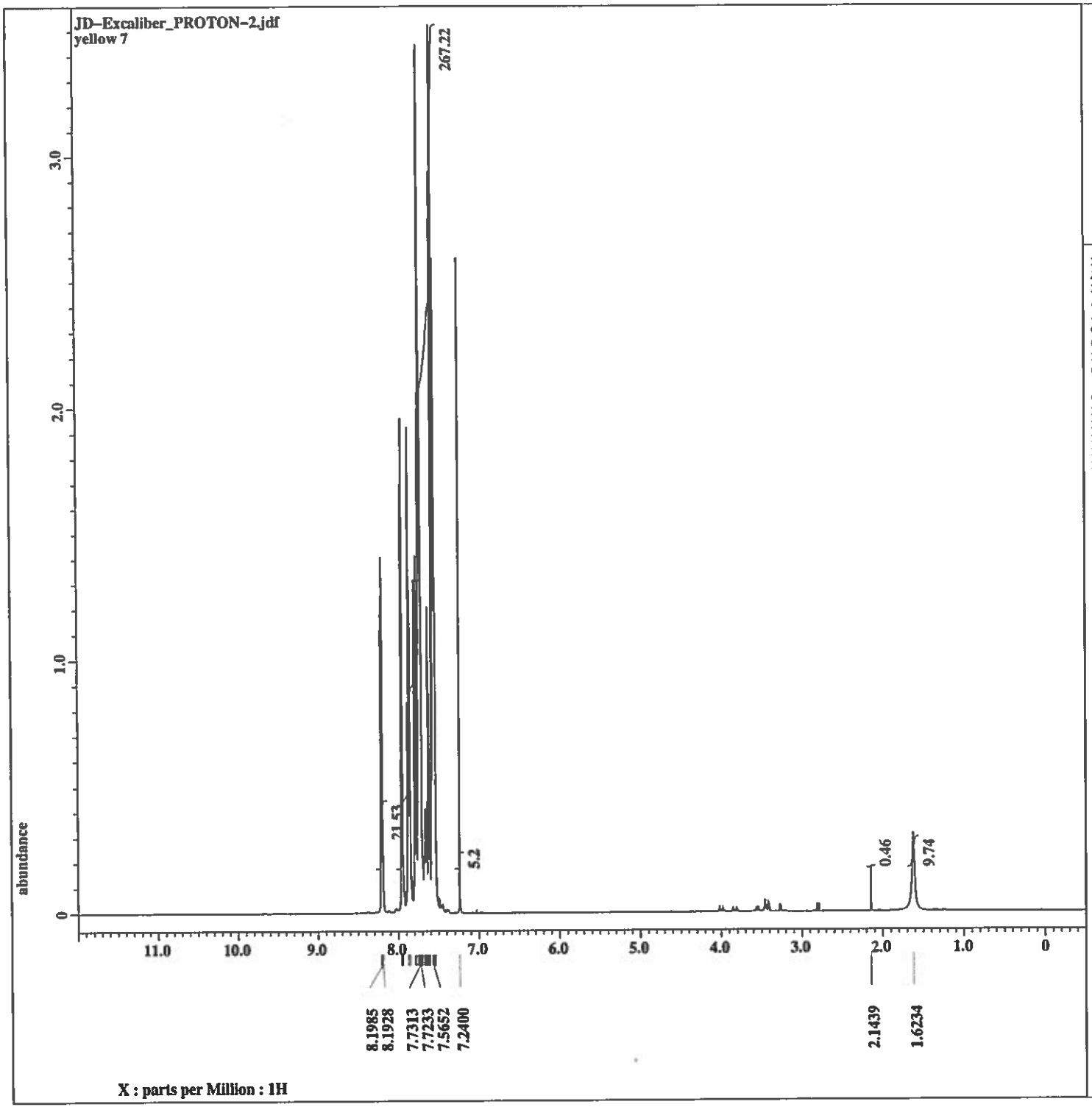
SOUTH ALABAMA JAGUARS

Filename	= PostHeat - LF_slot12_
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= S#581143
Solvent	= CHLOROFORM-D
Changer_sample	= 12
Creation_time	= 1-JUL-2016 16:29:21
Revision_time	= 1-JUL-2016 16:11:16
Current_time	= 1-JUL-2016 16:11:16
Comment	= Yellow 10
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]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 42
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.5[dC]



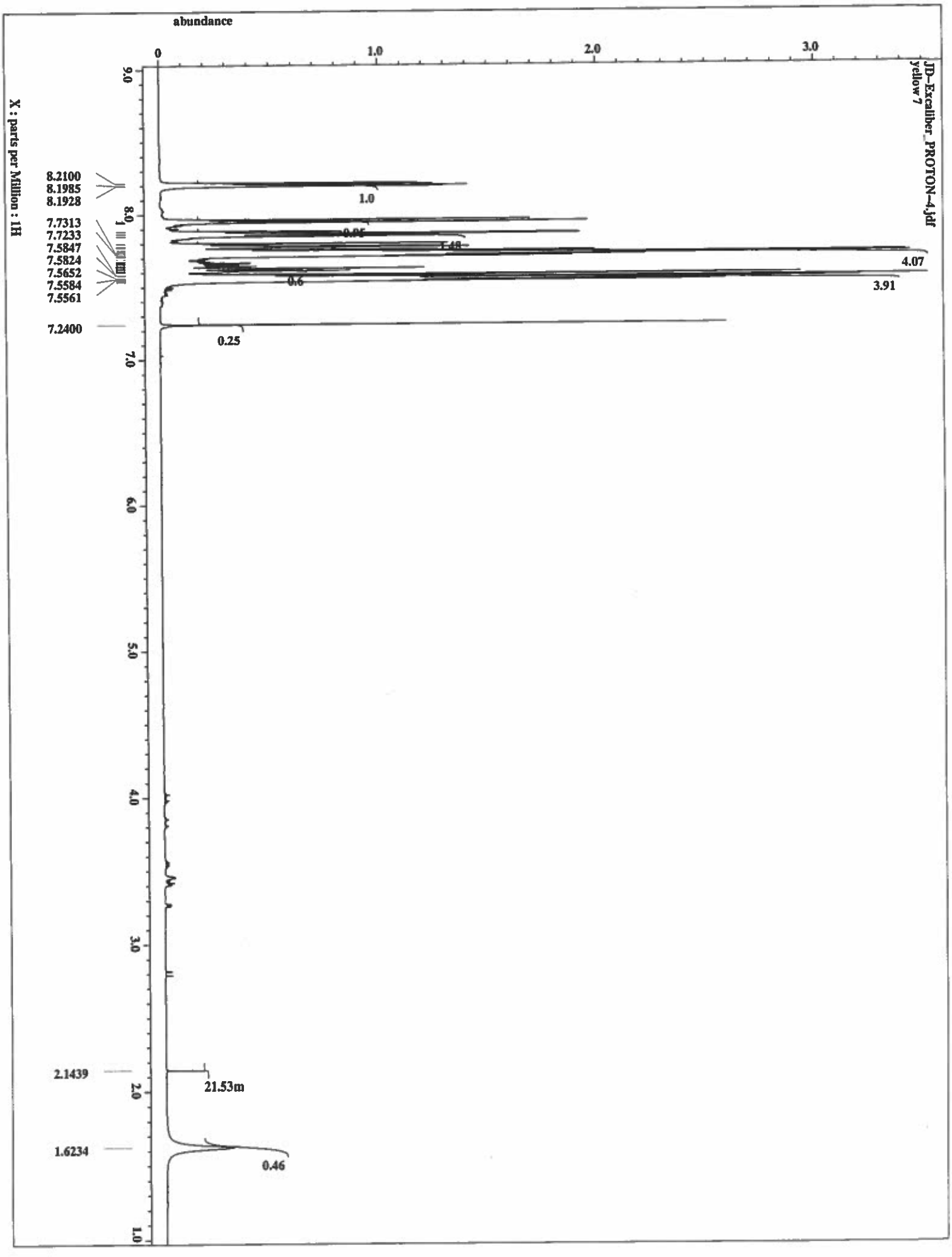
SOUTH ALABAMA JAGUARS

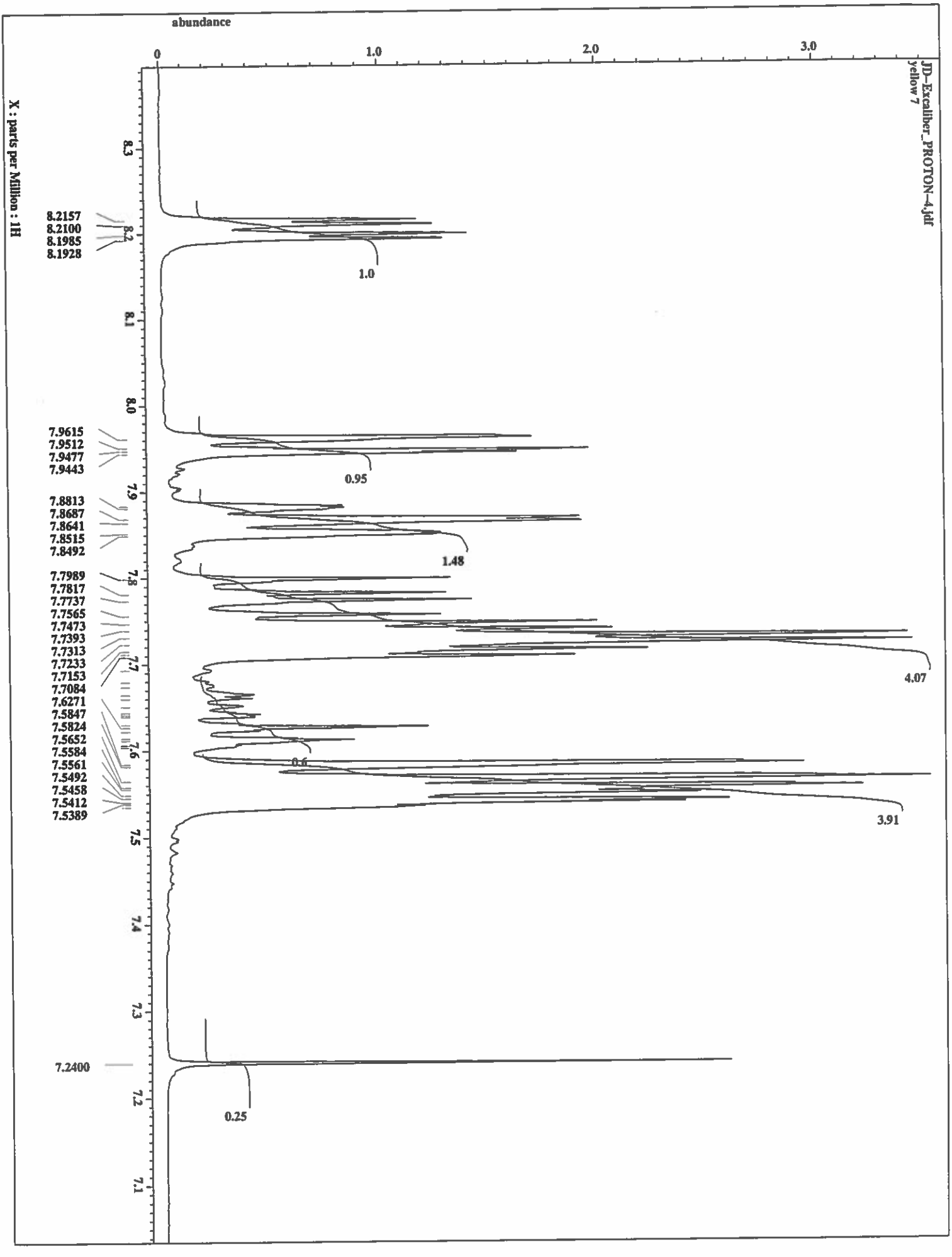
Filename	= PostHeat - LF_slot12_
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#795819
Solvent	= CHLOROFORM-D
Changer_sample	= 12
Creation_time	= 3-JUL-2016 00:52:14
Revision_time	= 3-JUL-2016 00:34:00
Current_time	= 3-JUL-2016 00:34:00
Comment	= Yellow 10
Data_format	= 1D COMPLEX
Dim_size	= 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	= 23.9[dC]

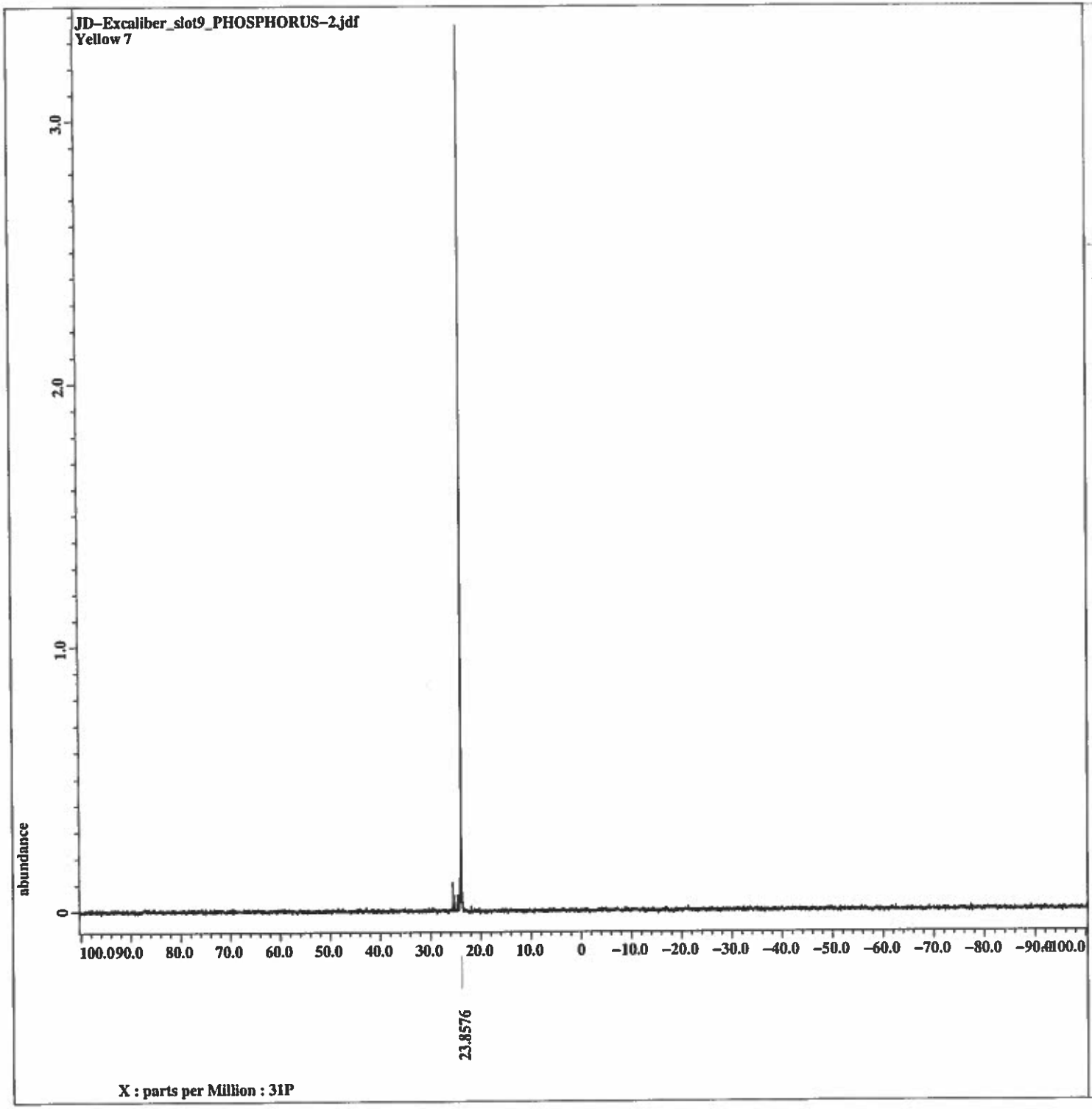


SOUTH ALABAMA JAGUARS

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
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
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_atn	= 4[dB]
X_pulse	= 6.675[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.5[dC]

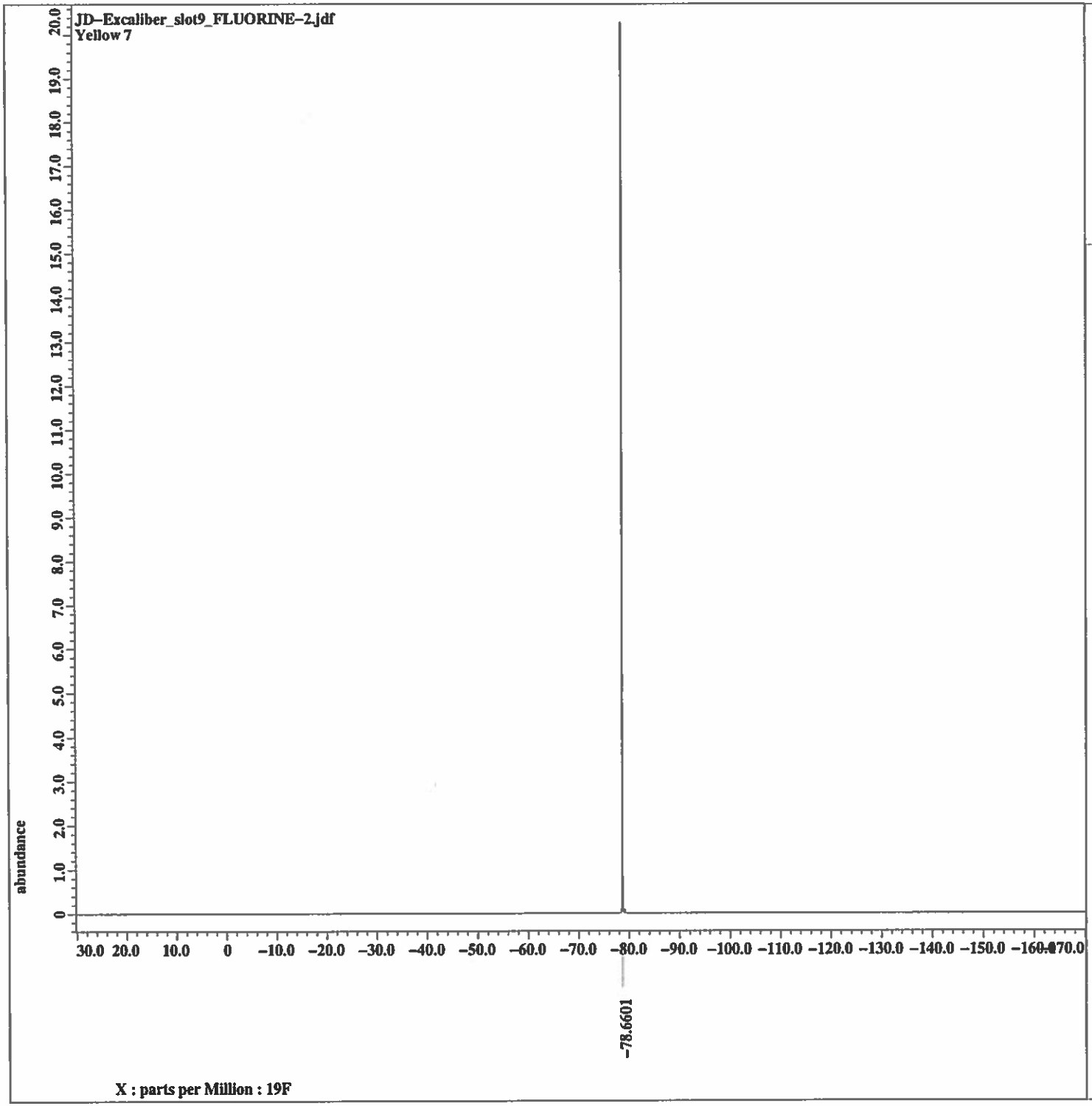

abundance
0
1.0
2.0
3.0
JD-Excaliber_PROTON-4.jdf
yellow 7
X : parts per Million : 1H
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.2100
8.1985
8.1928
7.7313
7.7233
7.5847
7.5824
7.5652
7.5584
7.5561
7.2400
2.1439
1.6234
1.0
0.05
1.48
4.07
0.6
3.91
0.25
21.53m
0.46


abundance
0
1.0
2.0
3.0
JD-Excaliber_PROTON-4.jdf
yellow 7
X : parts per Million : 1H
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
8.2157
8.2100
8.1985
8.1928
1.0
7.9615
7.9512
7.9477
7.9443
0.95
7.8813
7.8687
7.8641
7.8515
7.8492
1.48
7.7989
7.7817
7.7737
7.7565
7.7473
7.7393
7.7313
7.7233
7.7153
7.7084
4.07
7.6271
7.5847
7.5824
7.5652
7.5584
7.5561
7.5492
7.5458
7.5412
7.5389
0.6
3.91
7.2400
0.25



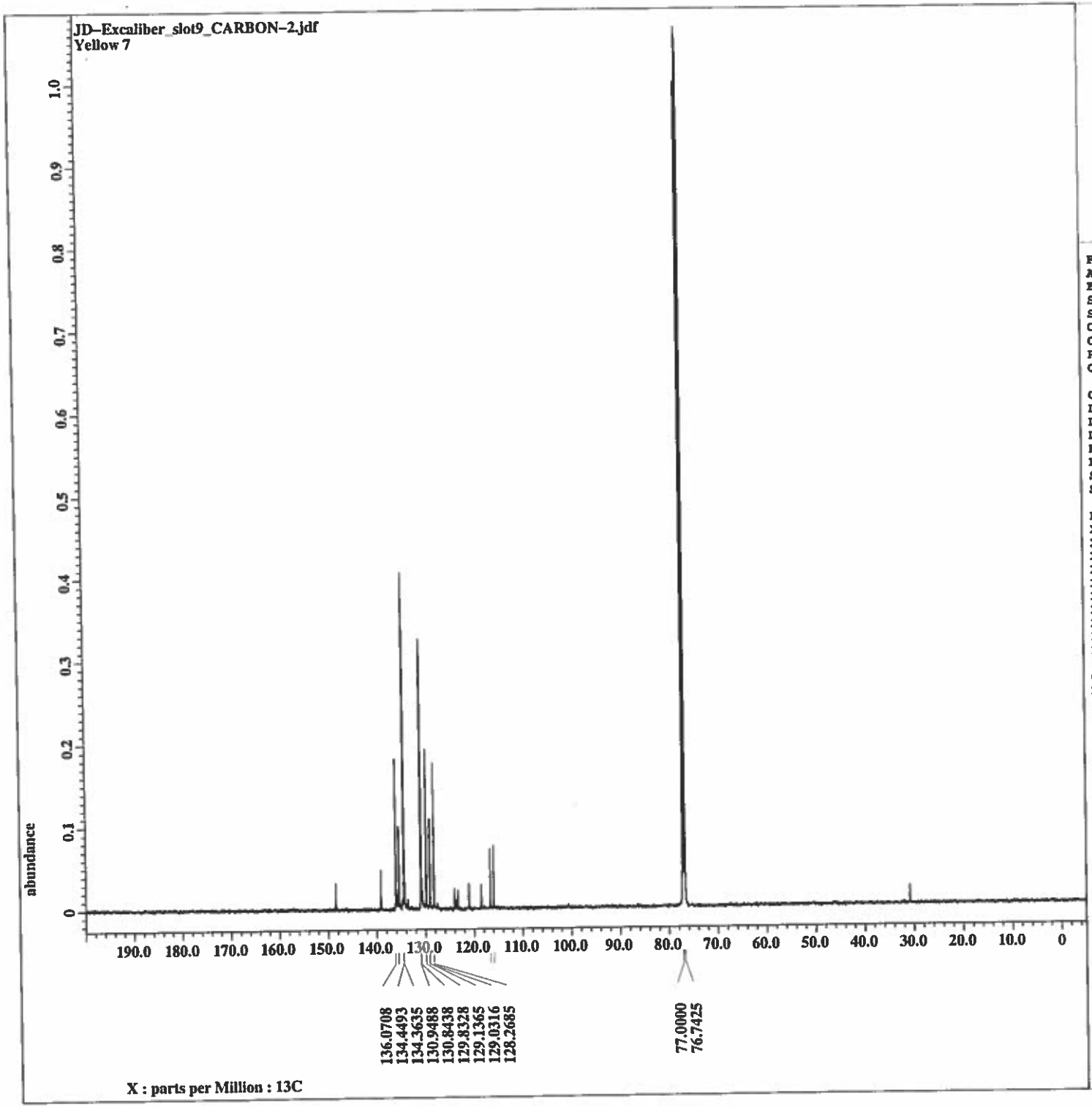
SOUTH ALABAMA JAGUARS

Filename	= JD-Excaliber_slot9_PH
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#678612
Solvent	= CHLOROFORM-D
Changer_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	= Yellow 7
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	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.64487424[s]
Temp_get	= 23.6[dC]



SOUTH ALABAMA JAGUARS

Filename	= JD-Excaliber_slot9_FL
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= S#574463
Solvent	= CHLOROFORM-D
Changer_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	= 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]
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_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 46
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.6[dC]



SOUTH ALABAMA JAGUARS

Filename	= JD-Excaliber_slot9_CA
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= S#614981
Solvent	= CHLOROFORM-D
Changer_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
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]

Davis Collaboration

Method: Stenson_100MeOH

Tune File: C:\Xcalibur\methods\Stenson\JerryKoncarSug Neg to Pos.LTQTune

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

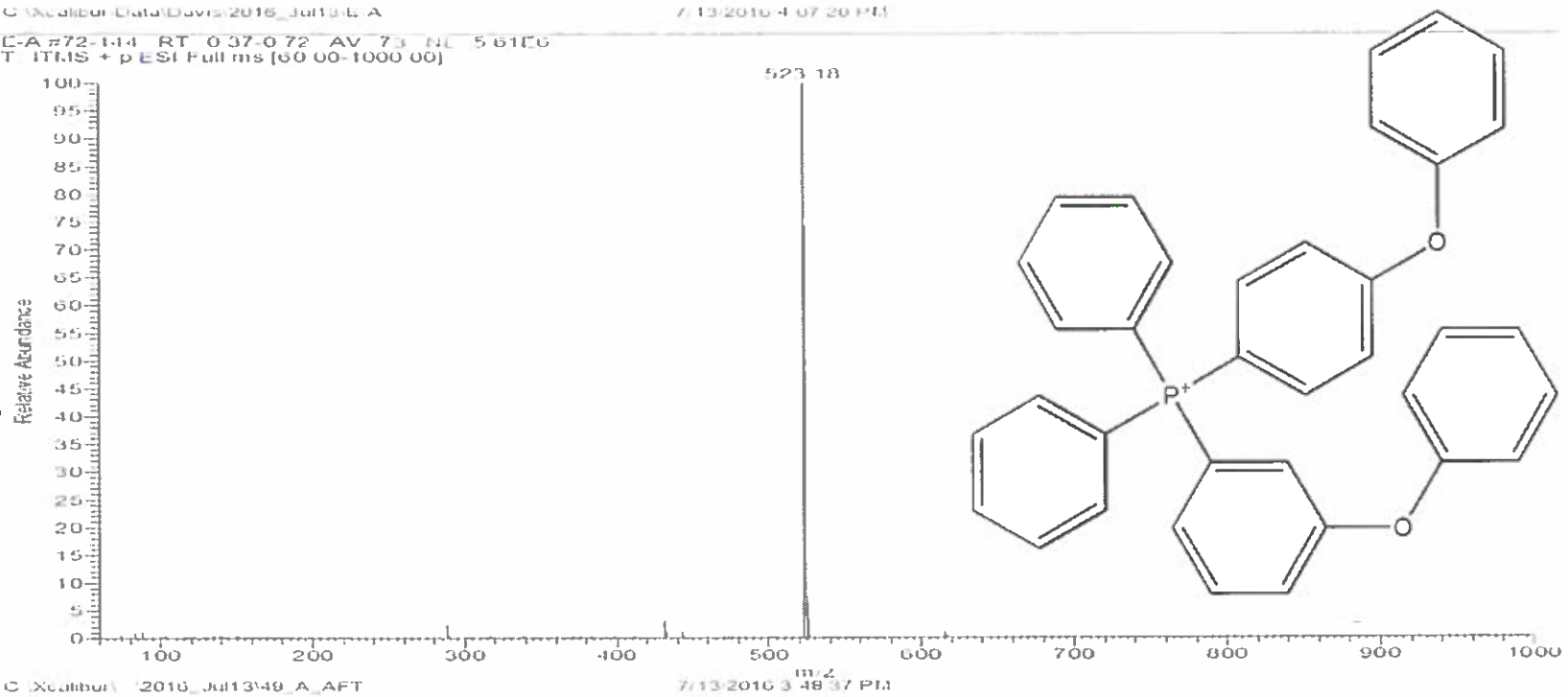
Notebook: Collaborators Page 105

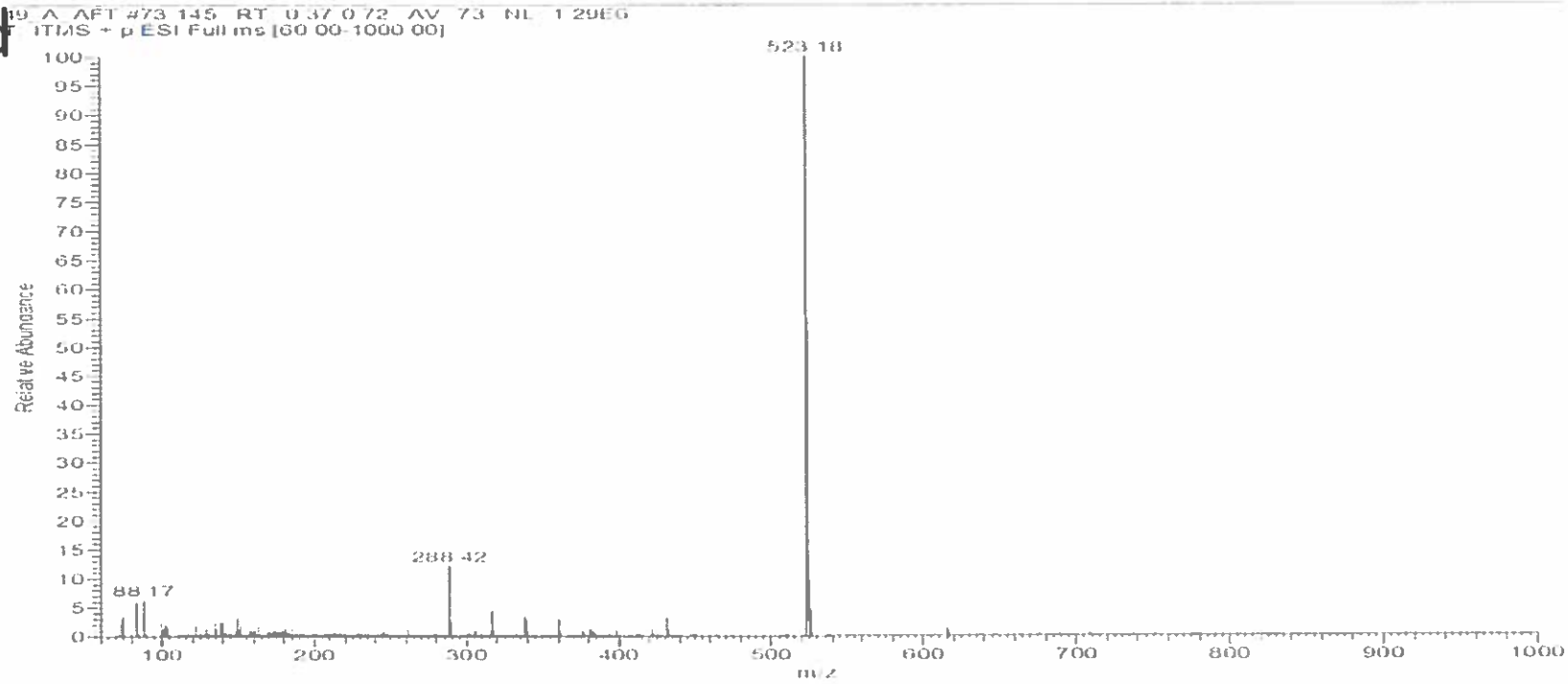
Compound 5

49-A
Before Δ

523.18
expected

49-A
After Δ



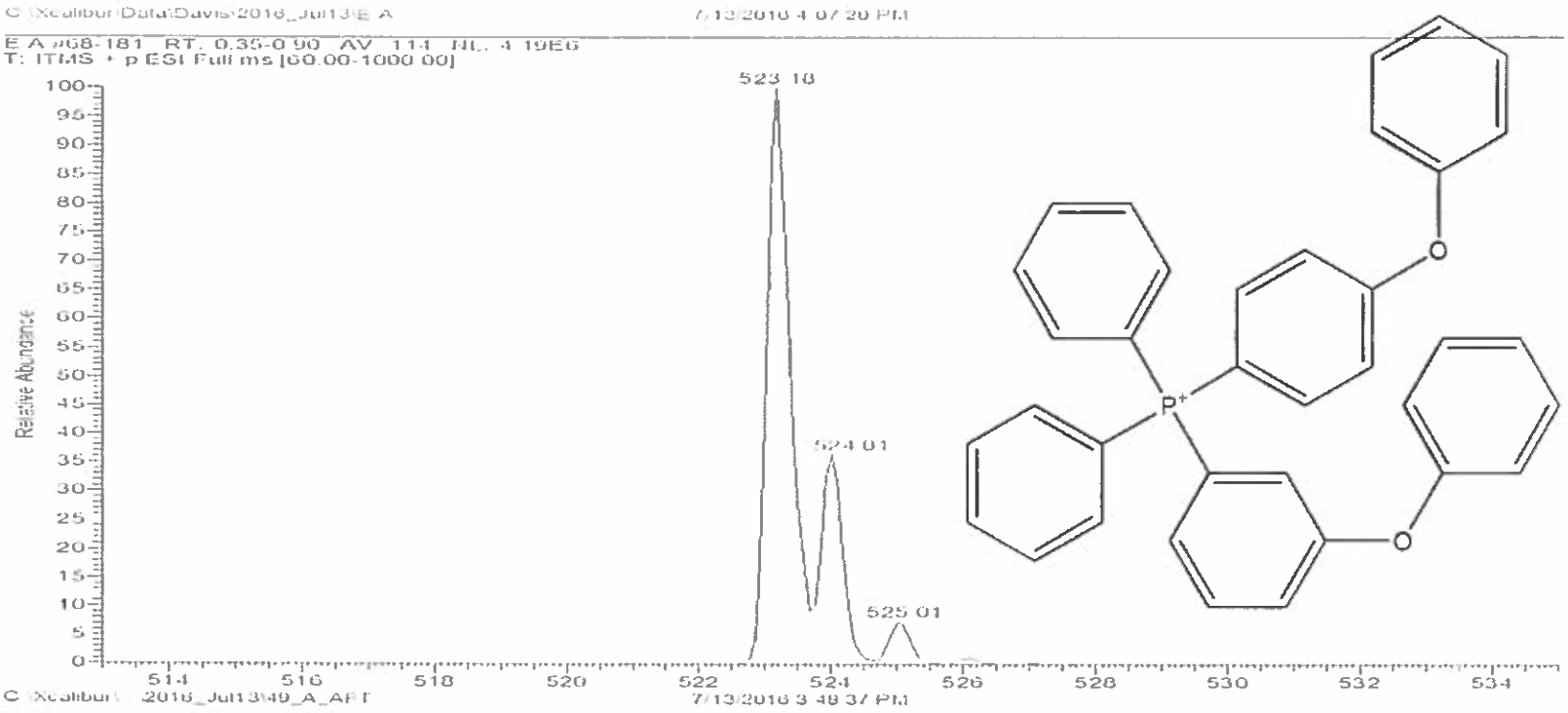


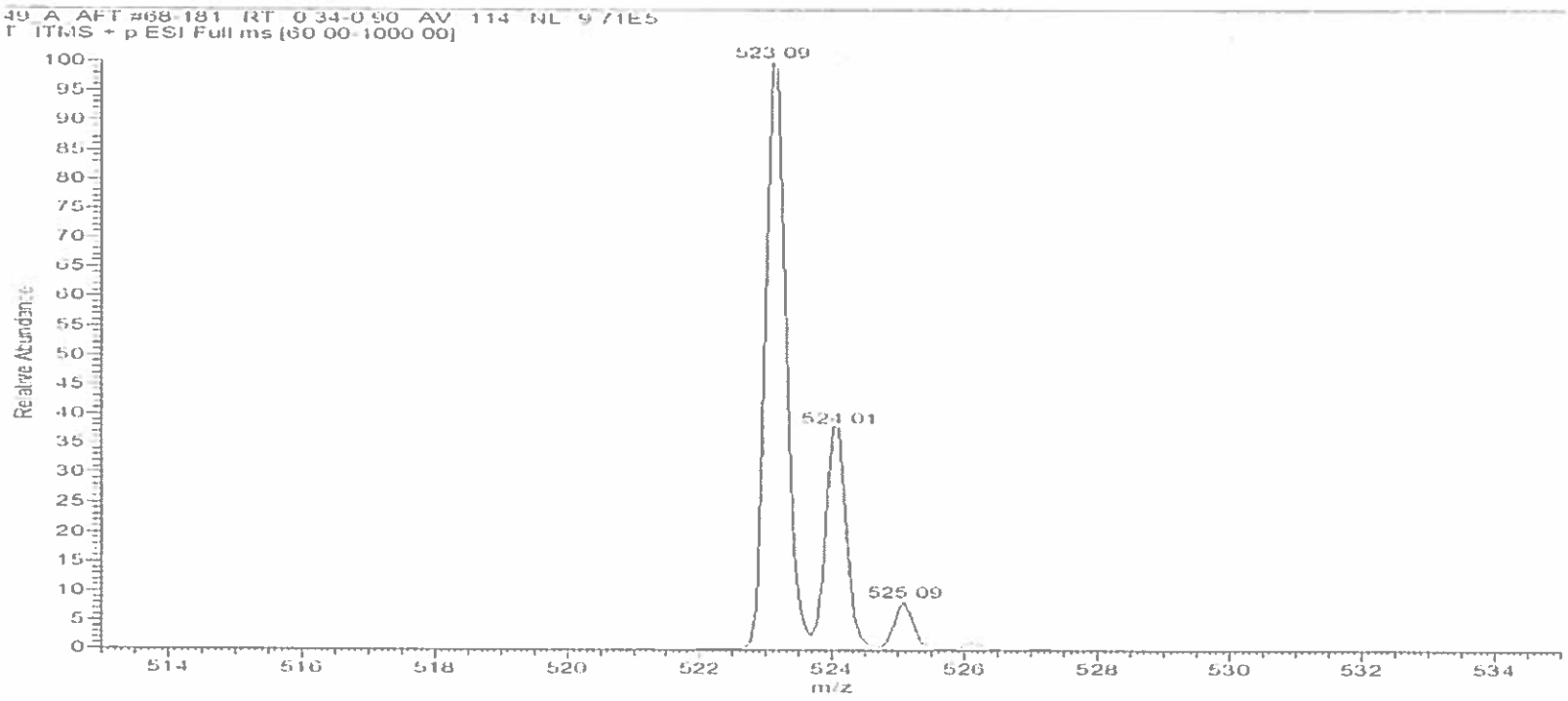
Compounds

49-A
Before Δ

523.18
expected

49-A
After Δ



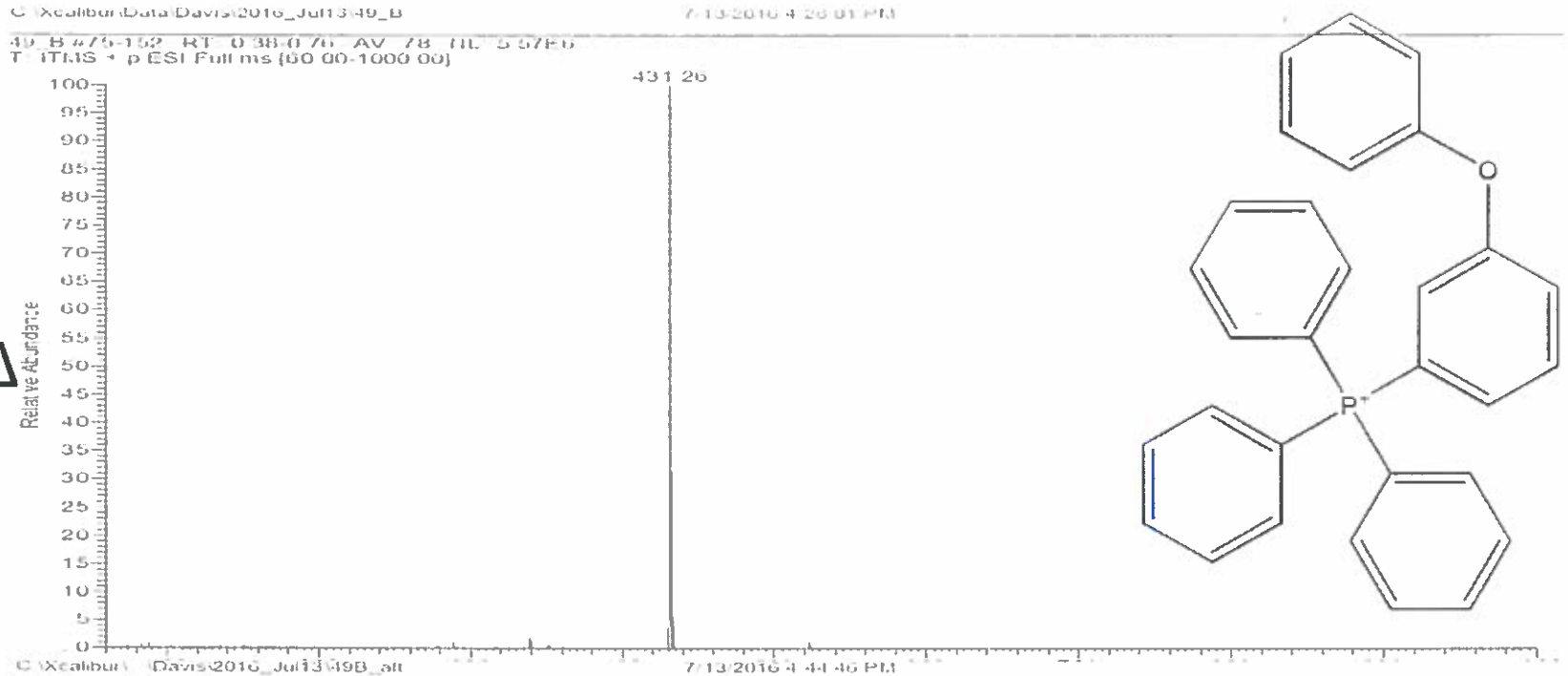


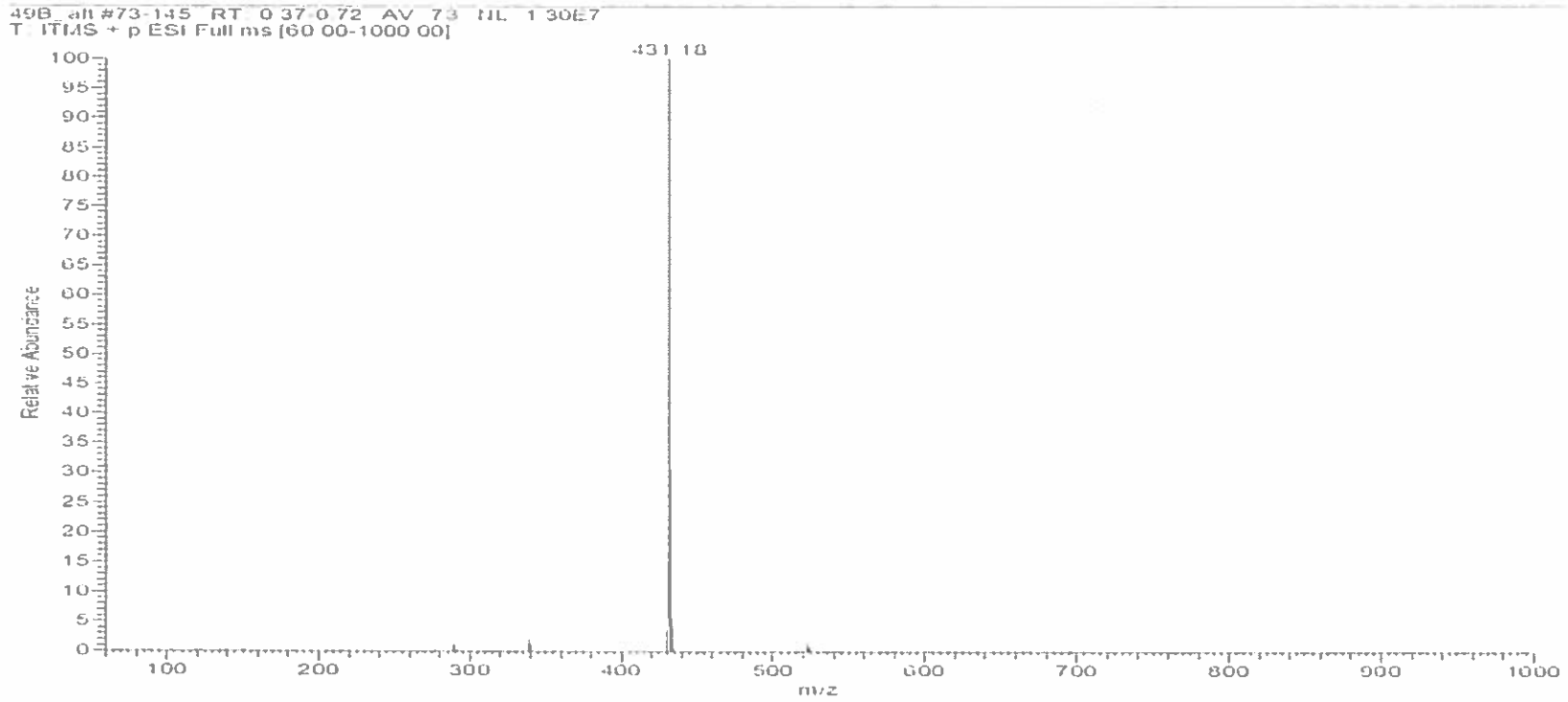
Compound 2

49-B
Before Δ

431.16
expected

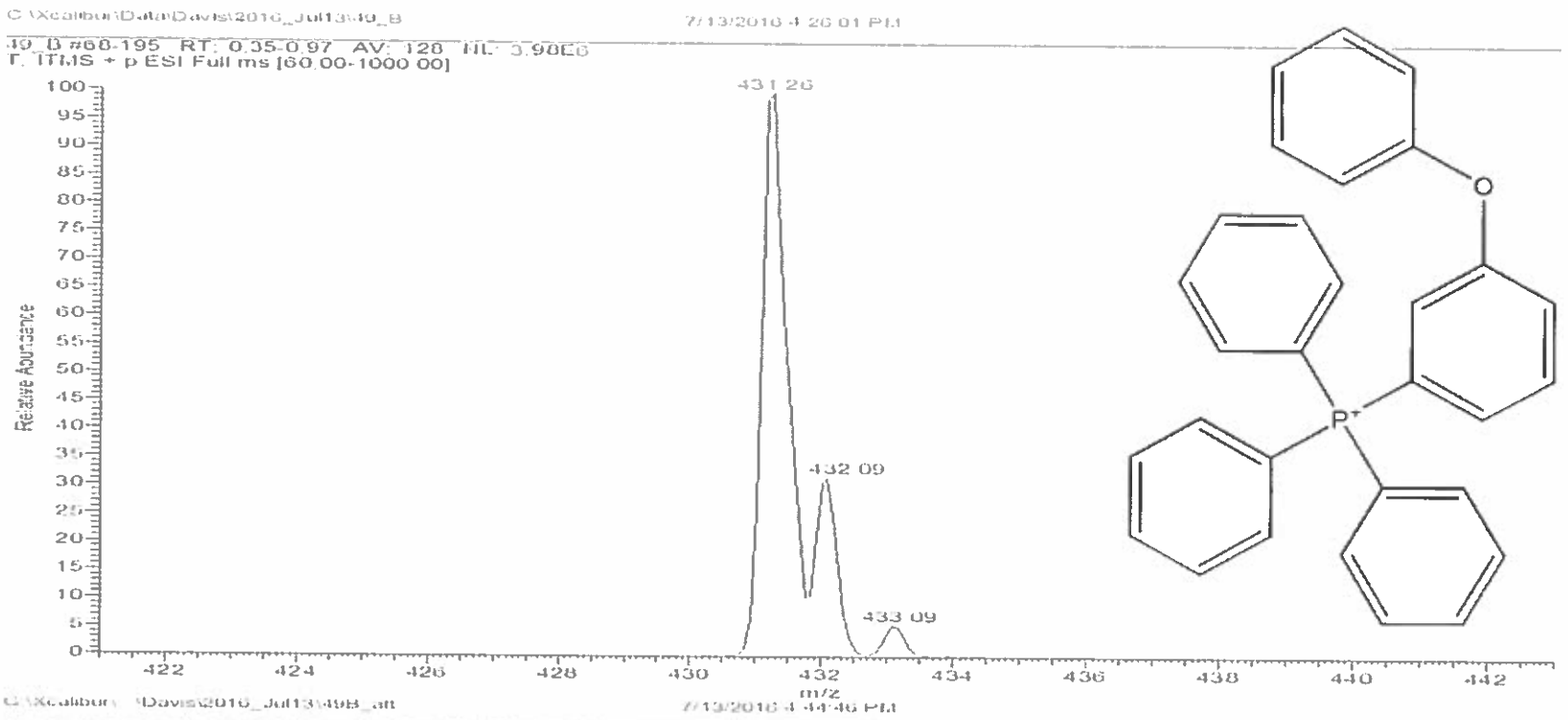
49-B
After Δ



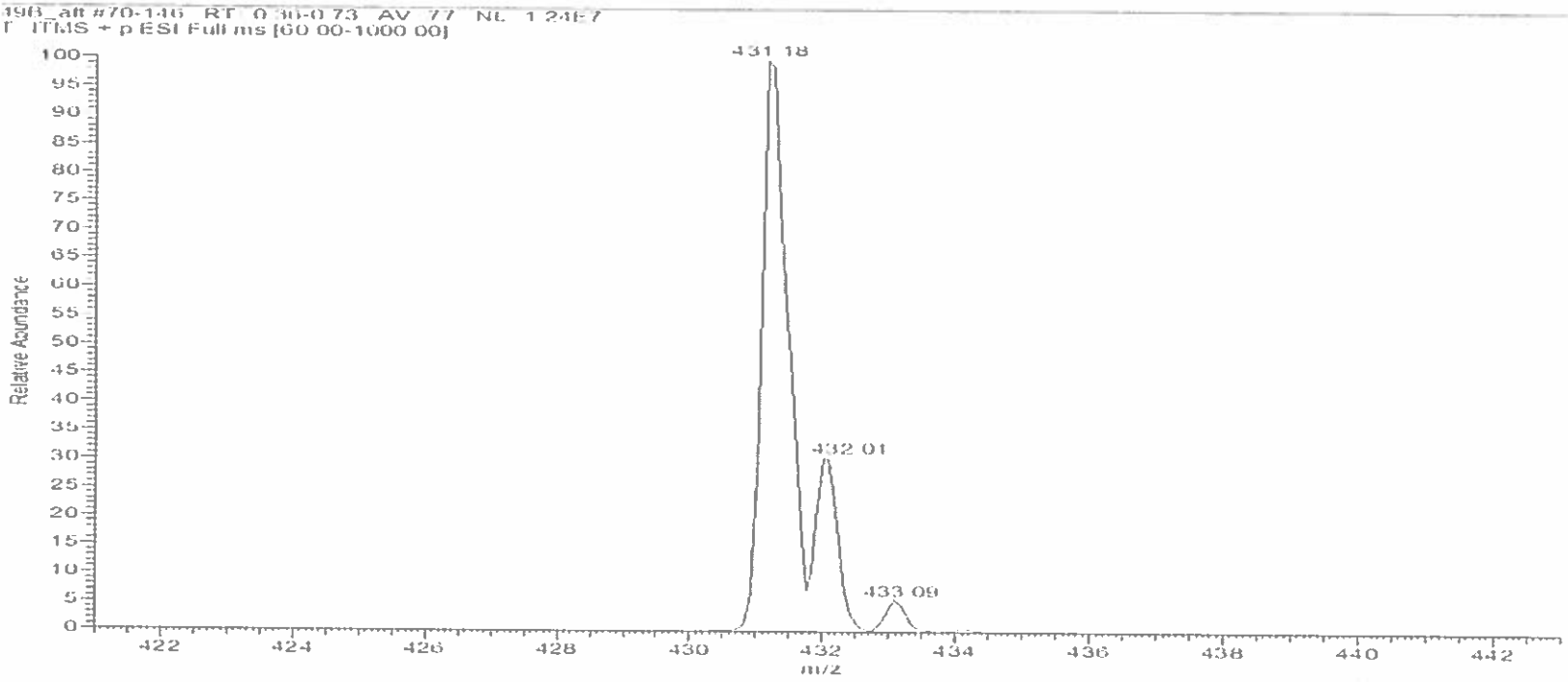


49-B
Before Δ

431.16
expected



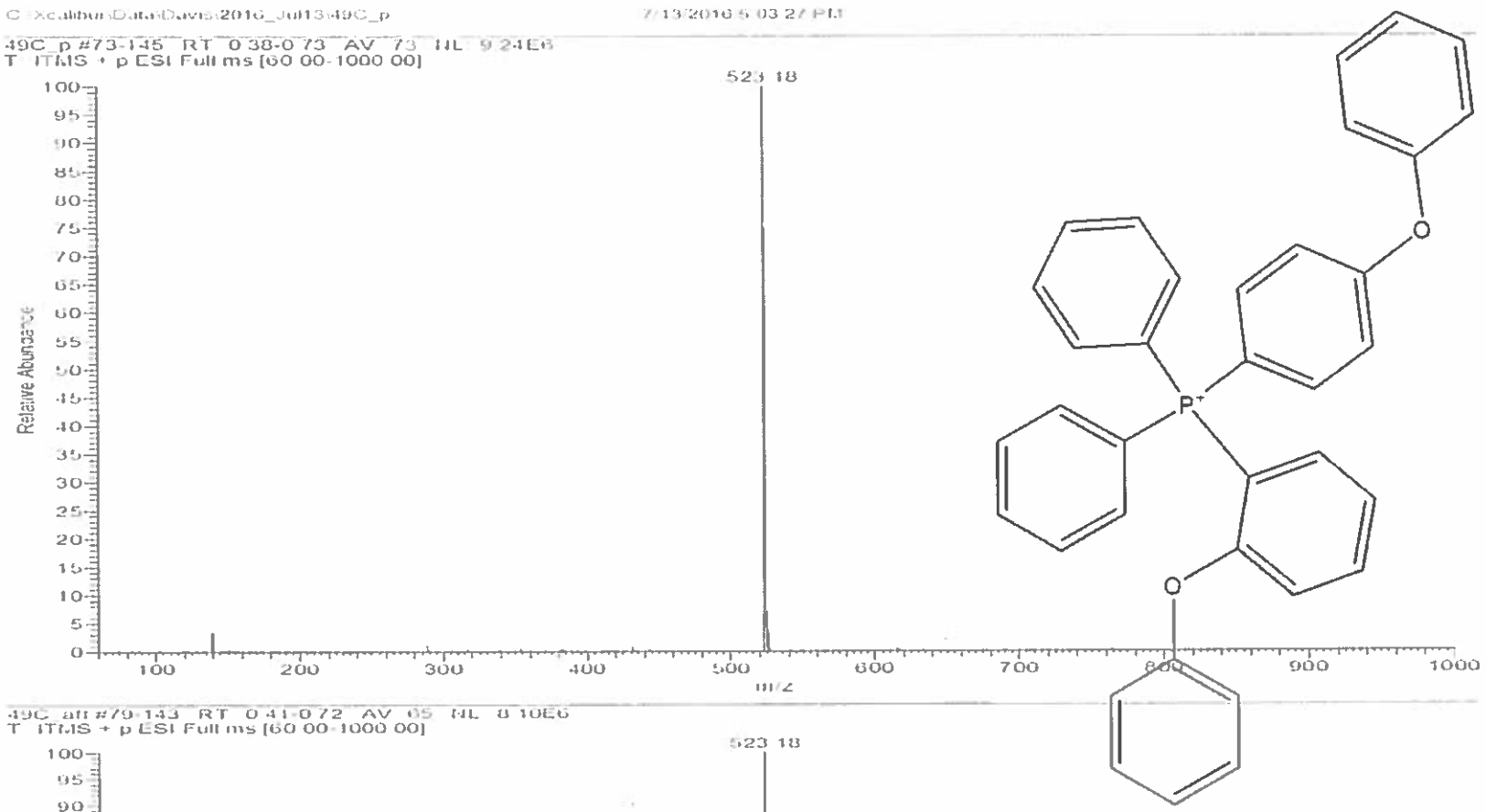
49-B
After Δ



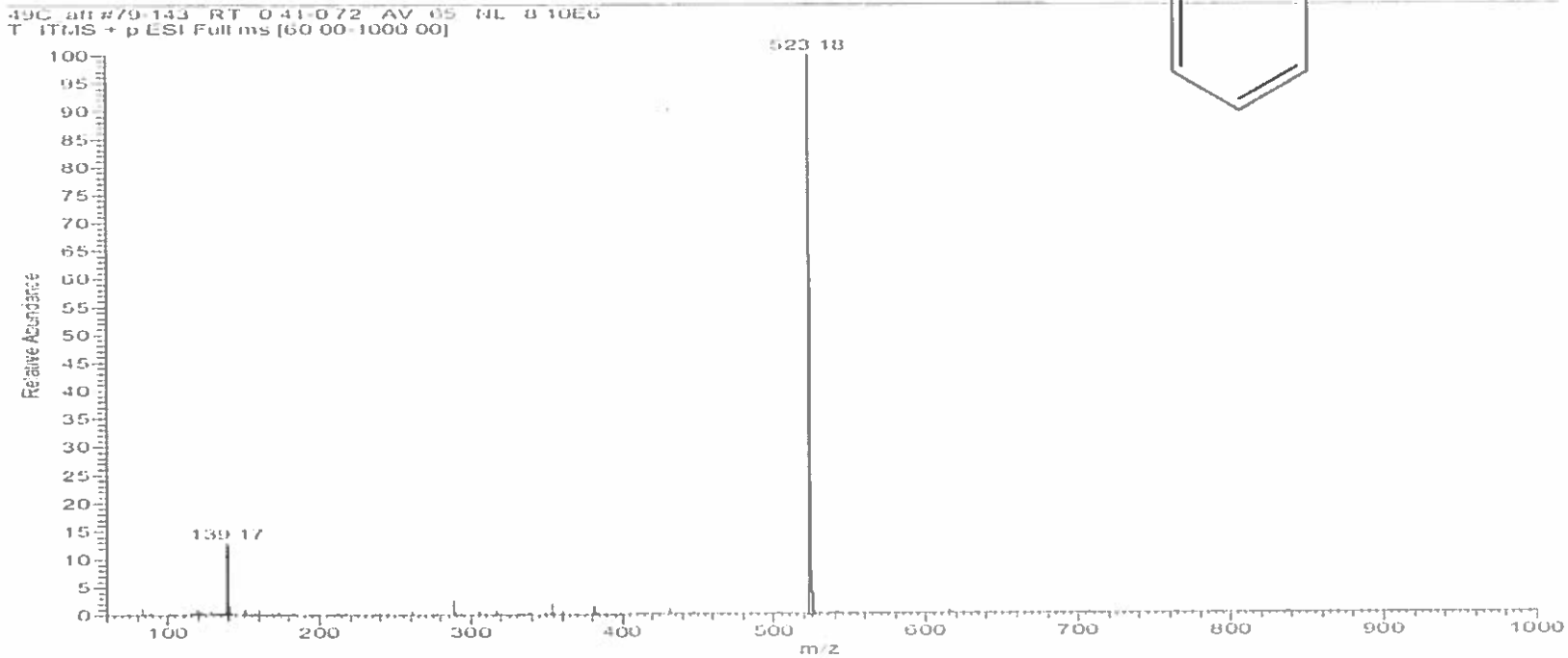
Compound 6

49-C
Before Δ

523.18
expected

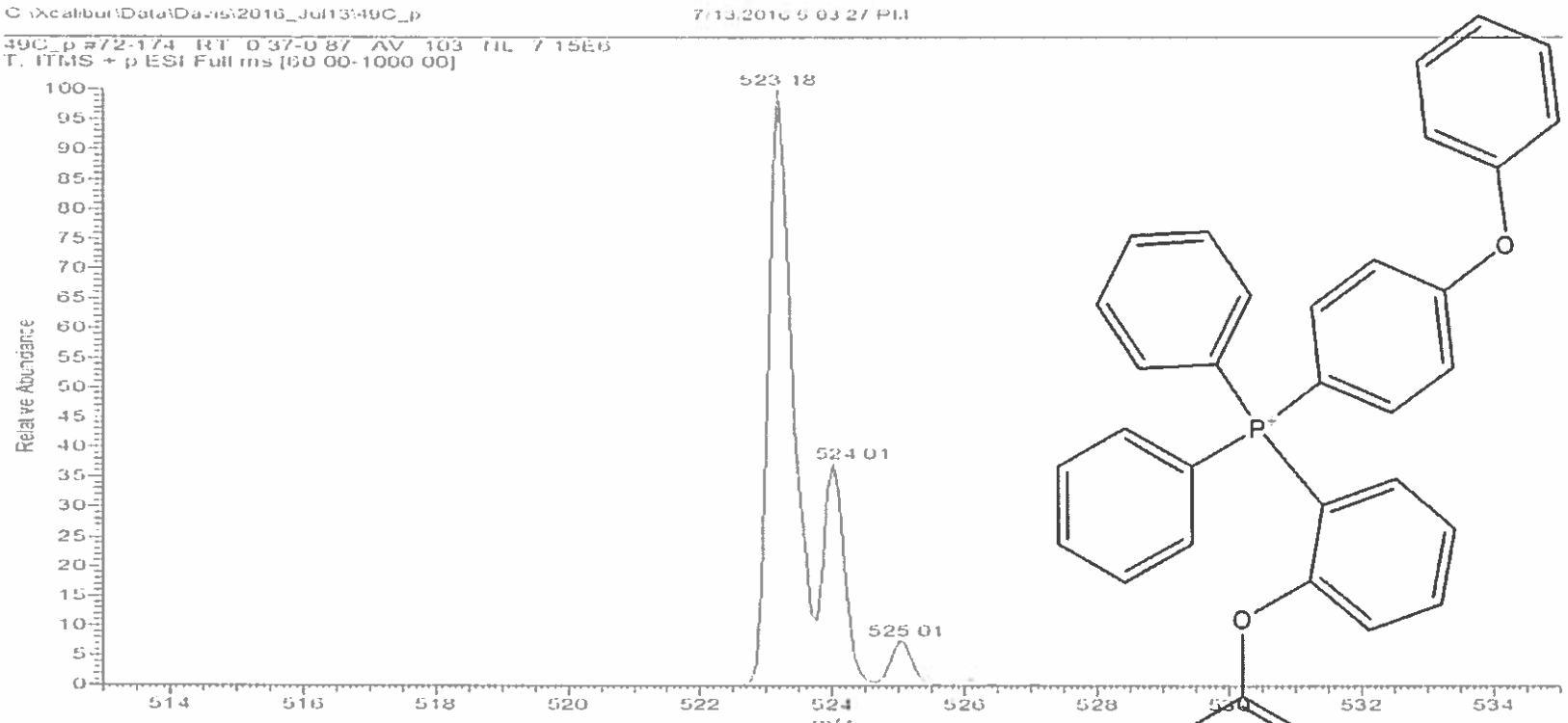


49-C
After Δ

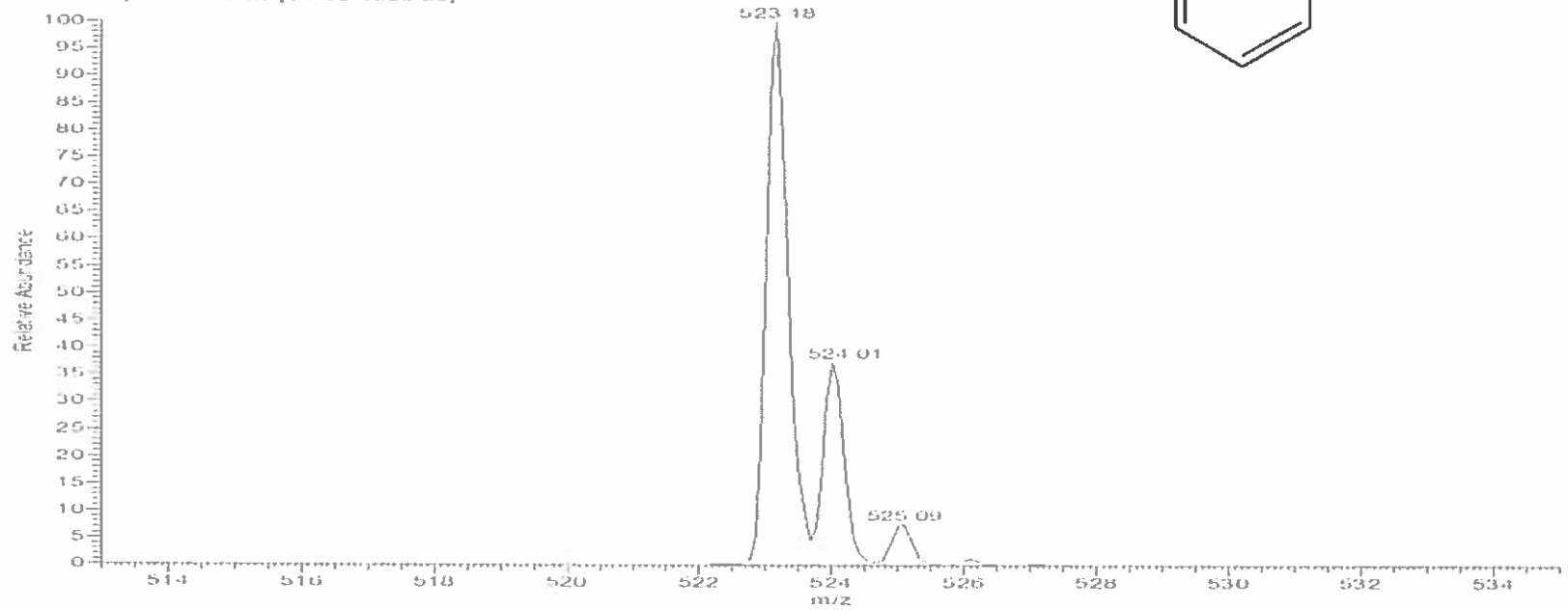


49-C
Before Δ

523.18
expected



49-C
After Δ

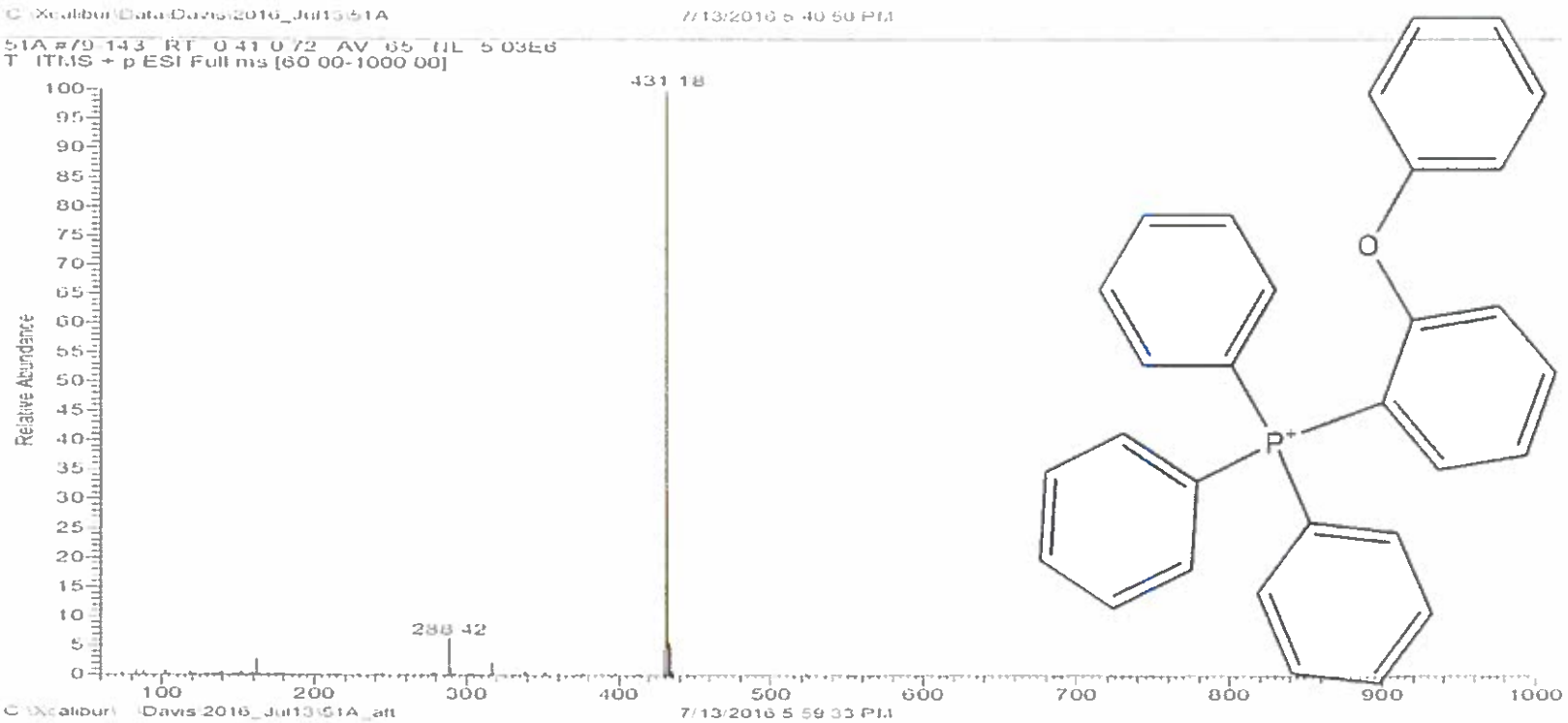


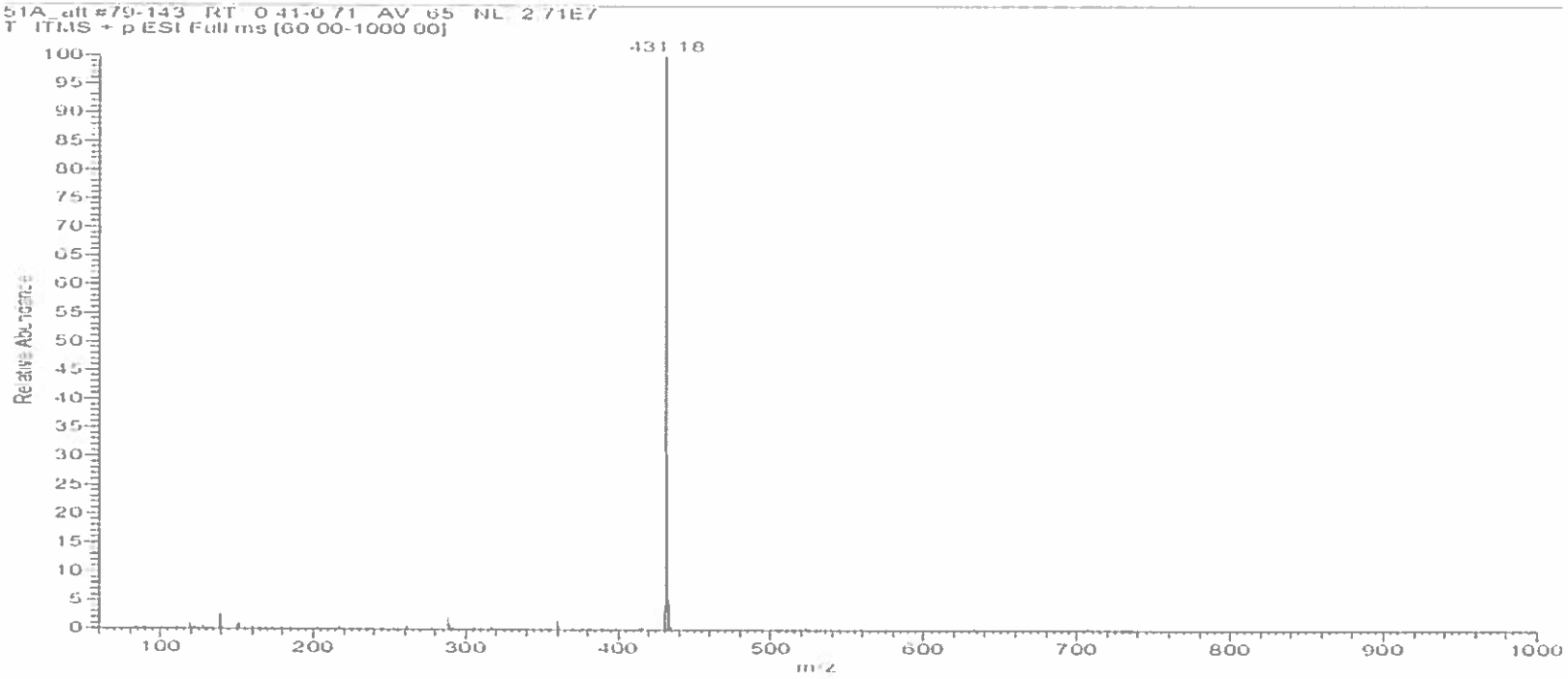
Compound 3

51-A
Before Δ

431.16
predicted

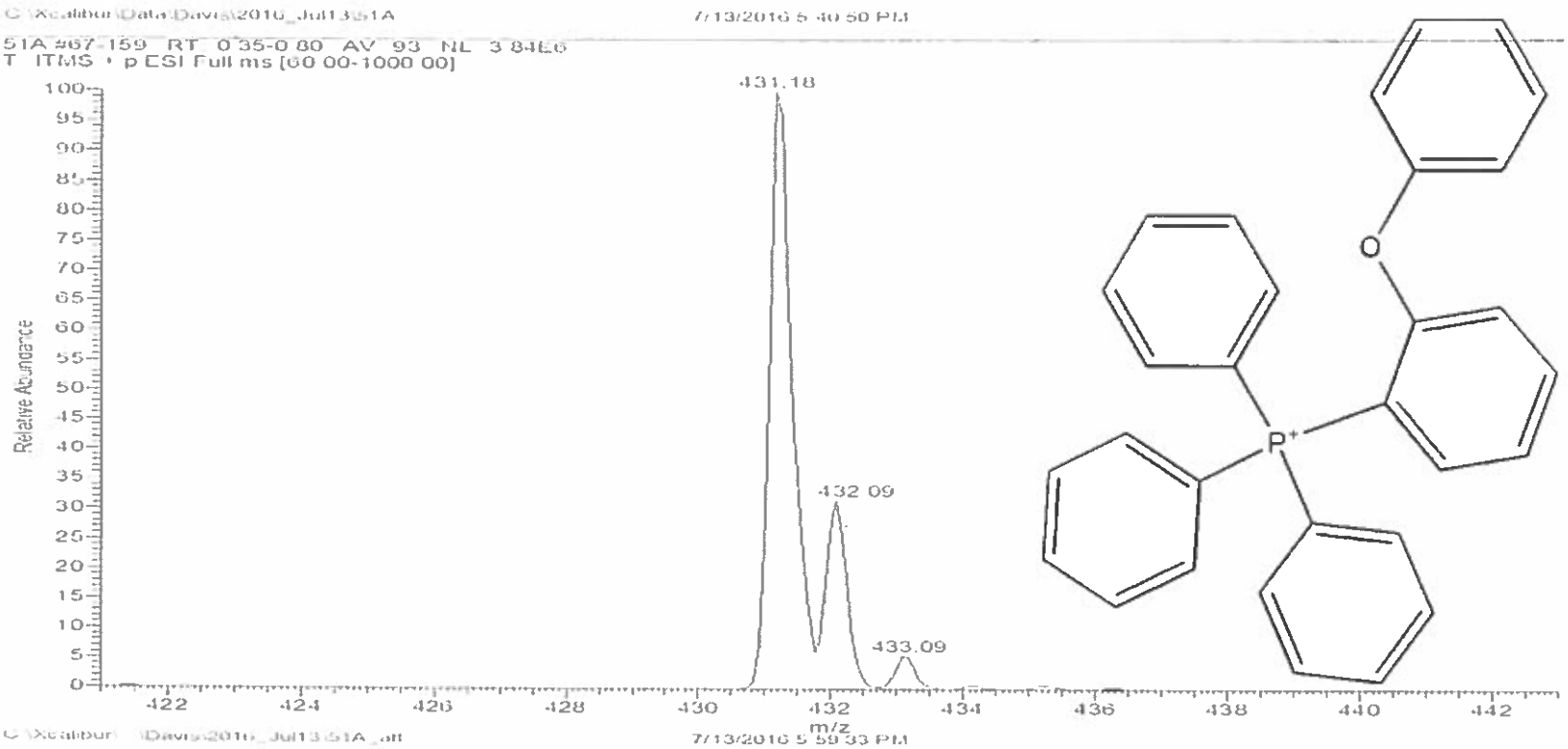
51-A
After Δ



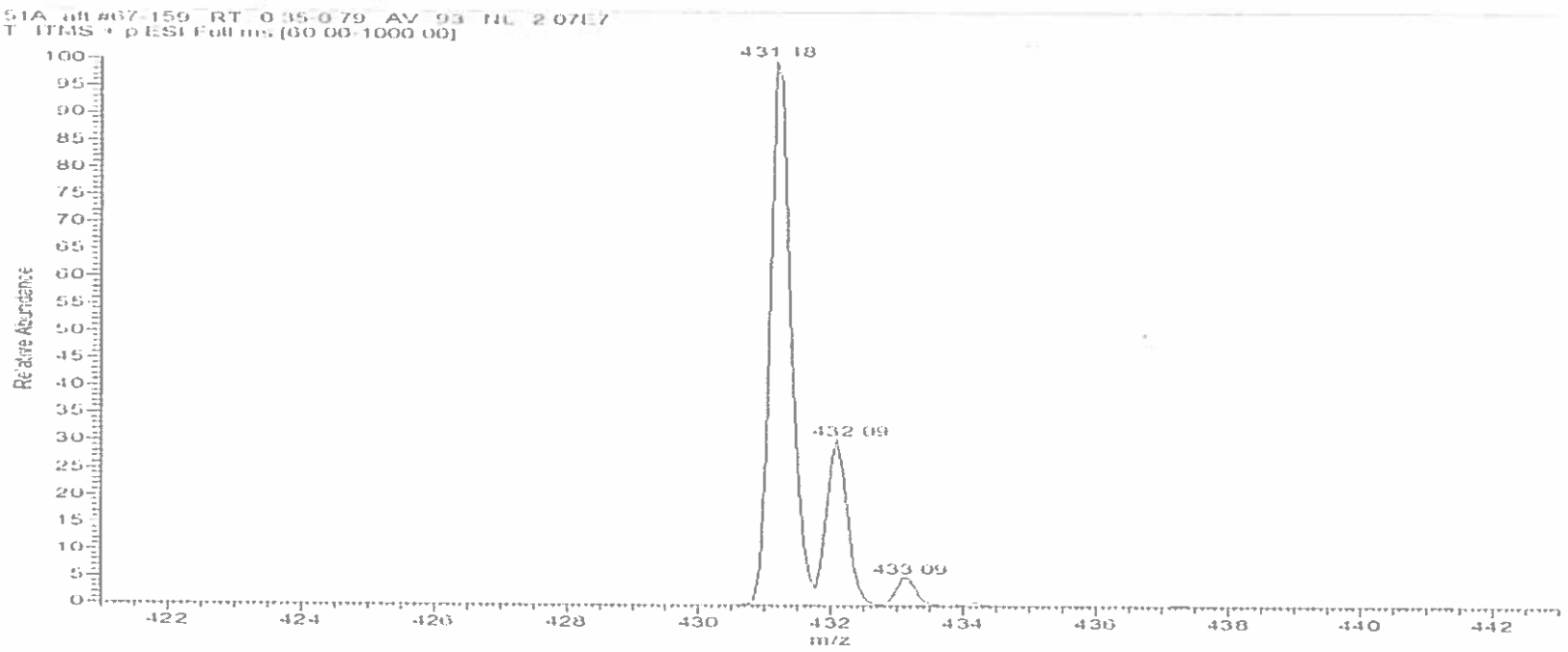


51-A
Before Δ

431.16
predicted



51-A
After Δ

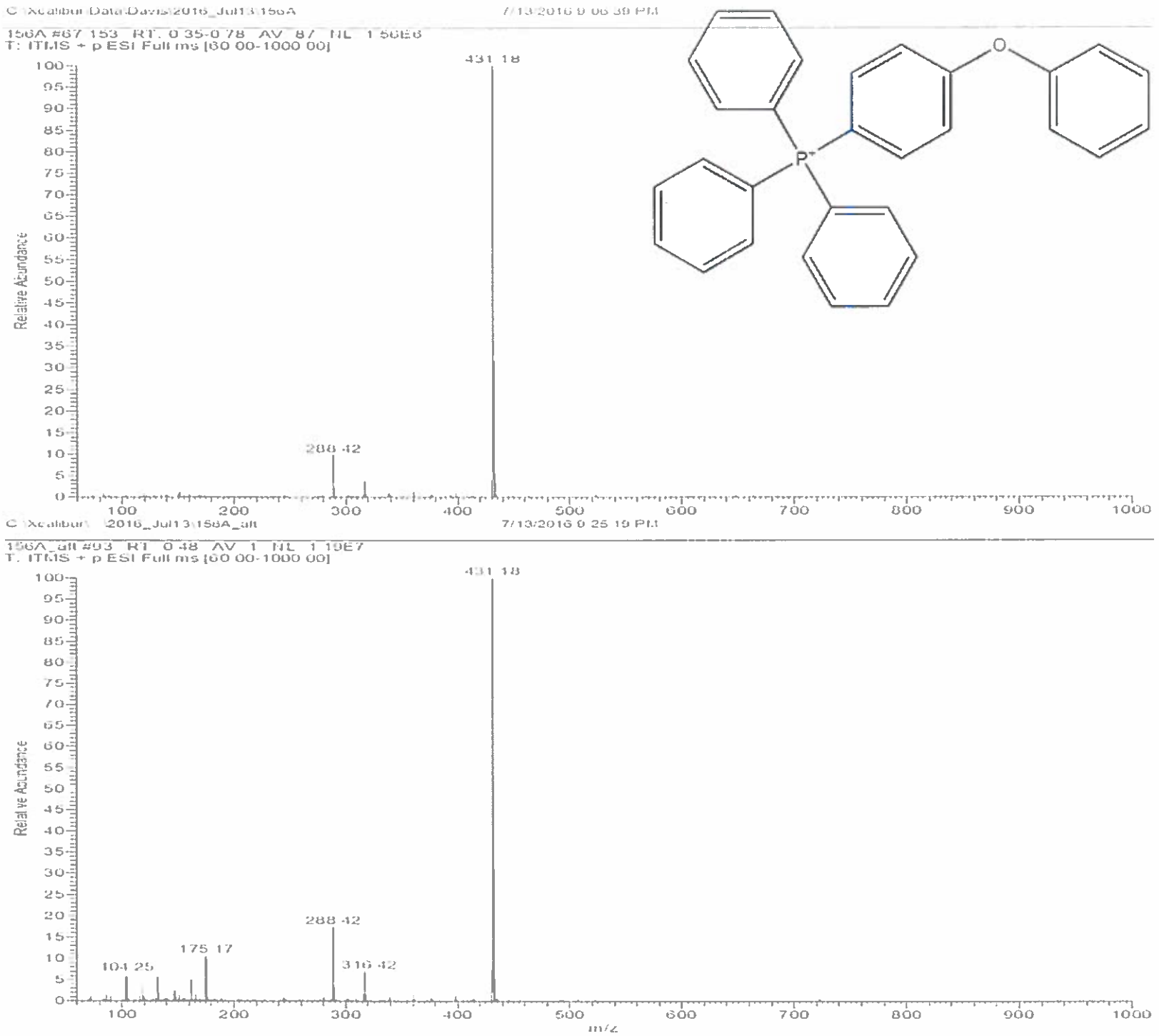


Compound 1

156-A
Before Δ

431.16
expected

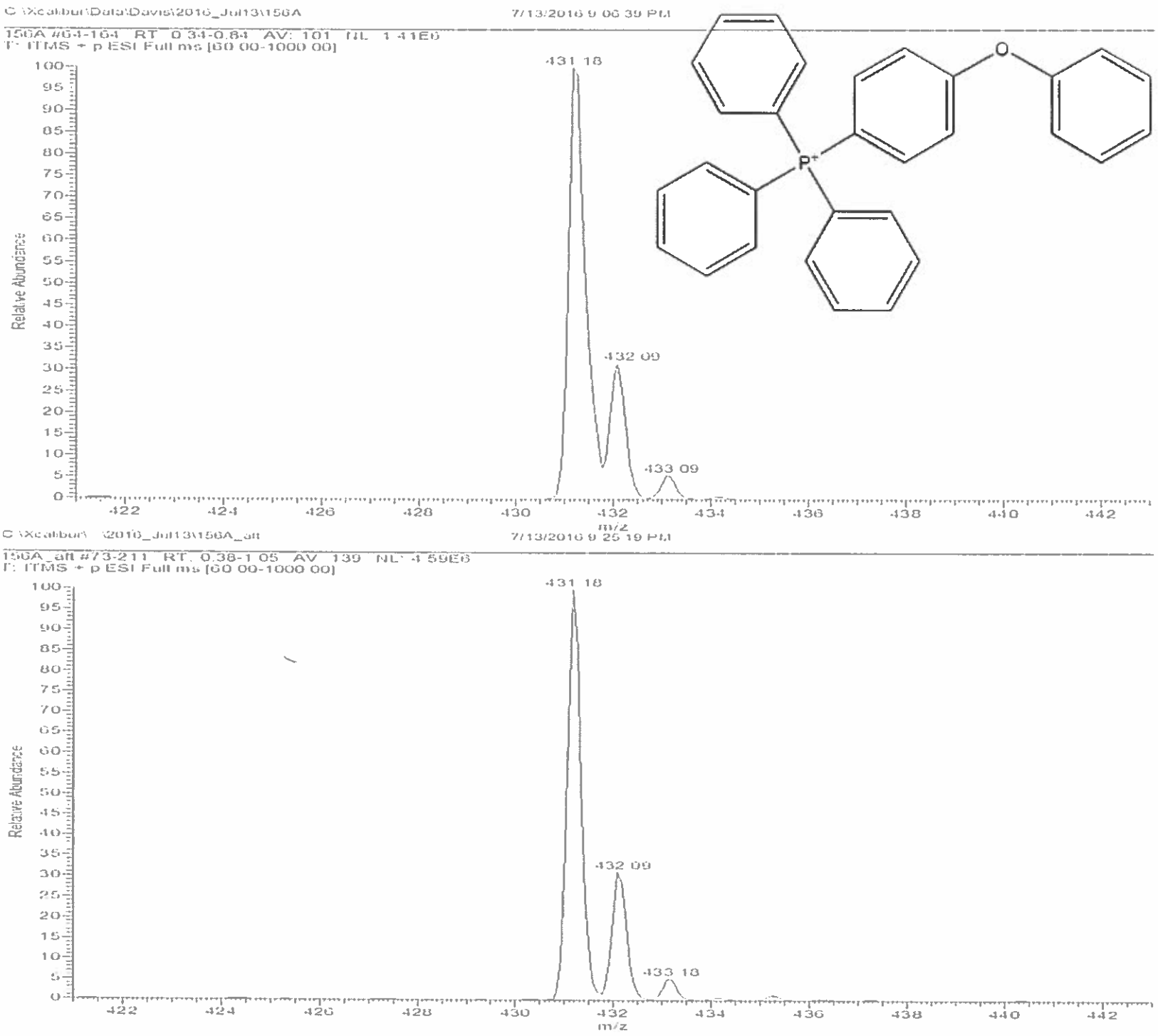
156-A
After Δ



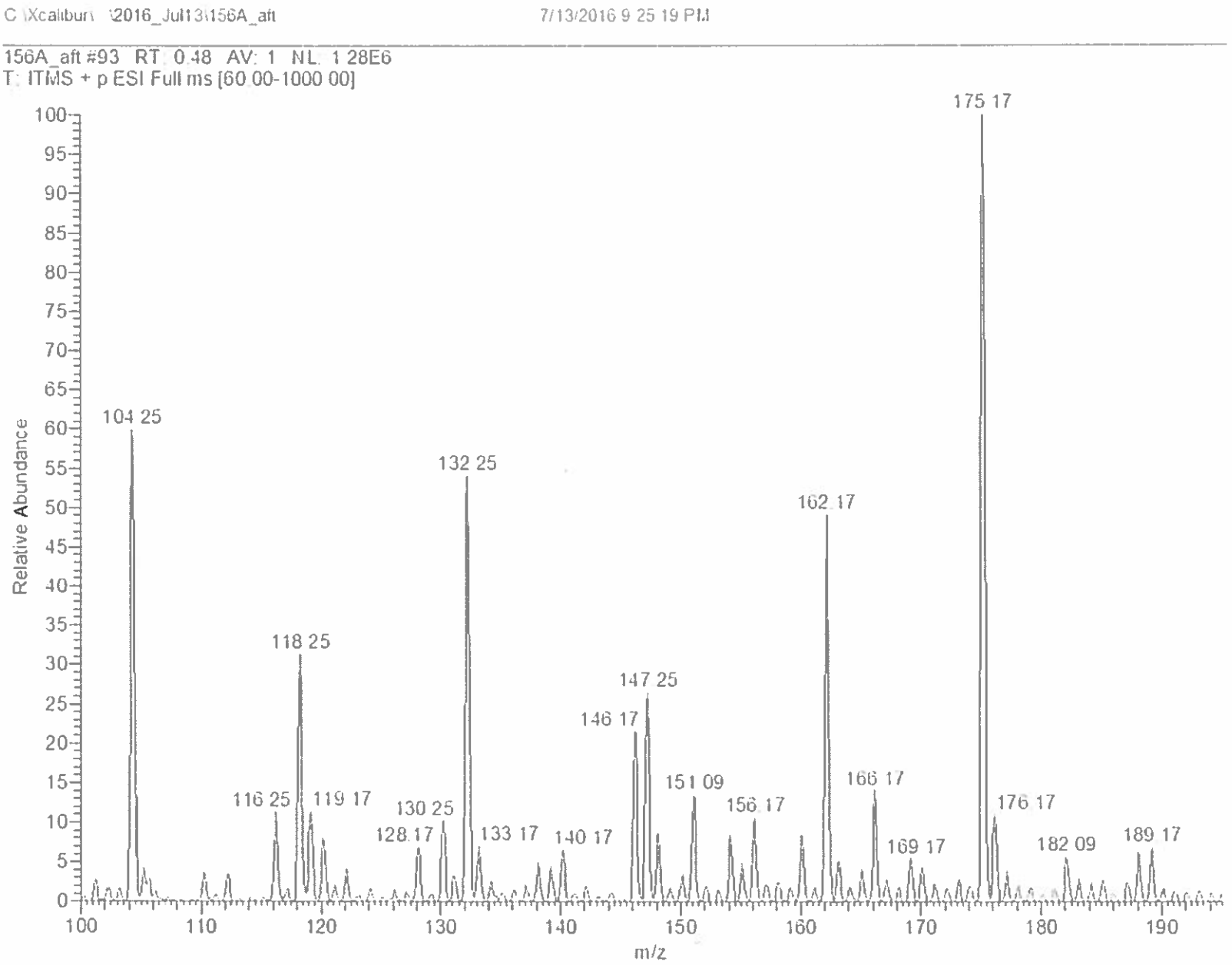
156-A
Before Δ

431.16
expected

156-A
After Δ



156-A New Peaks

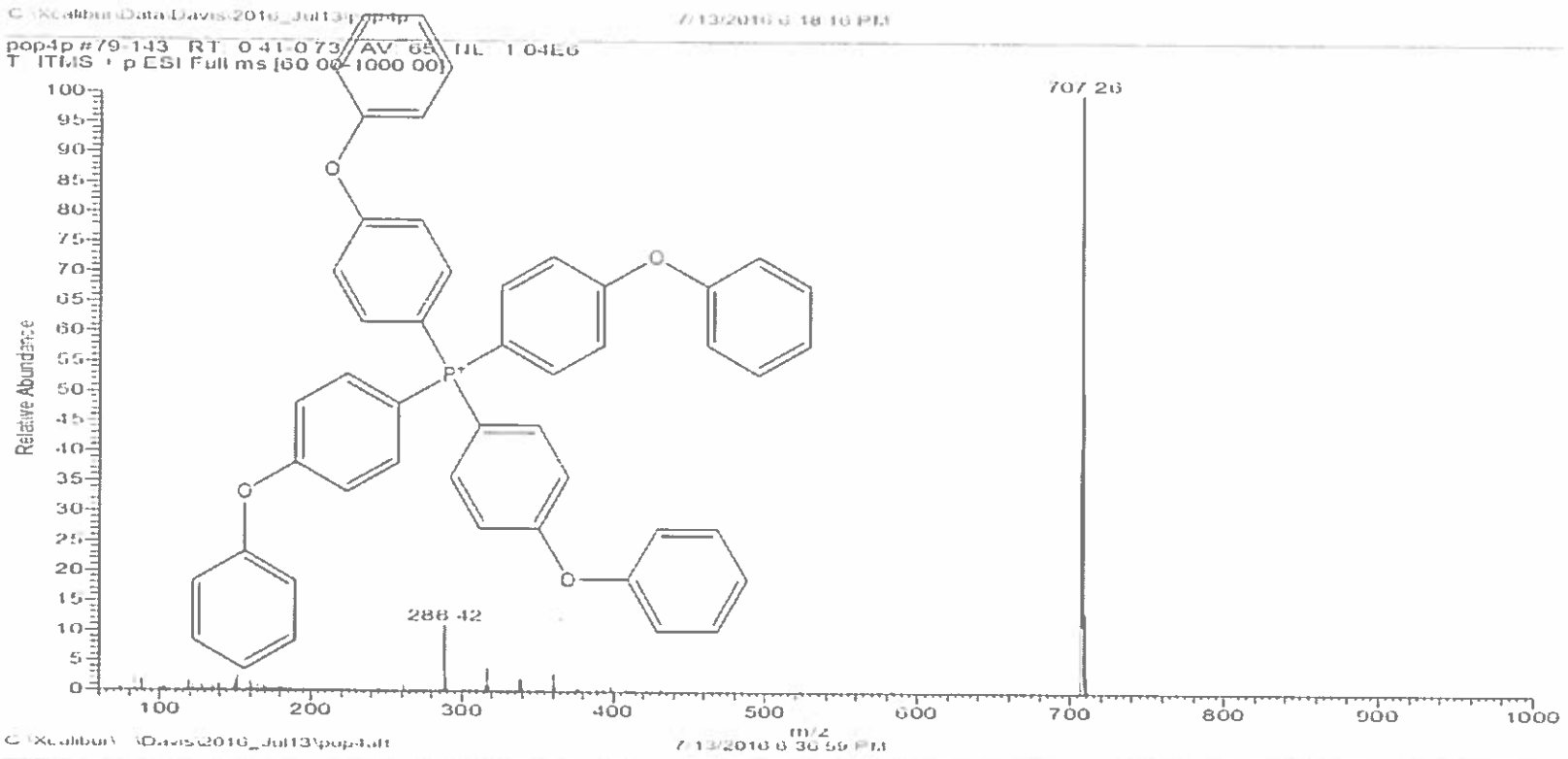


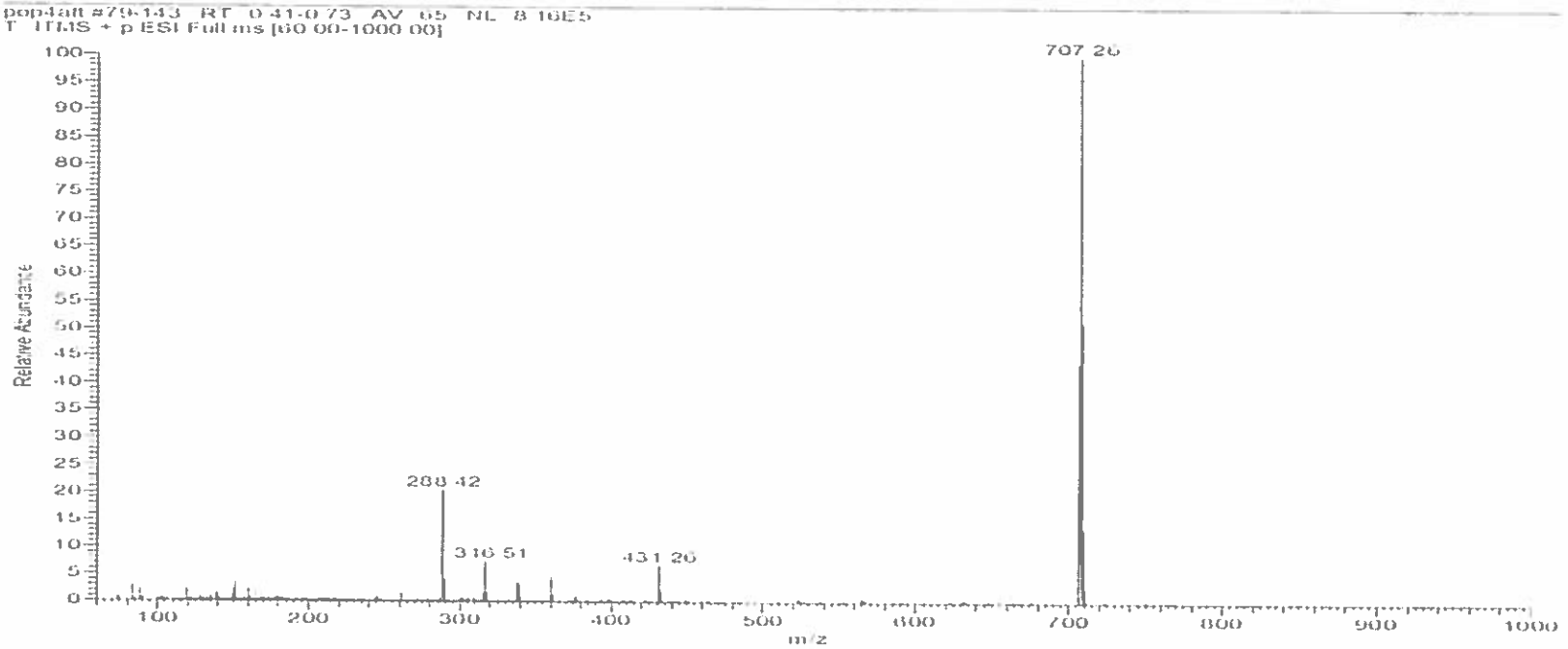
compound 7

POP4
Before Δ

707.23
expected

POP4
After Δ

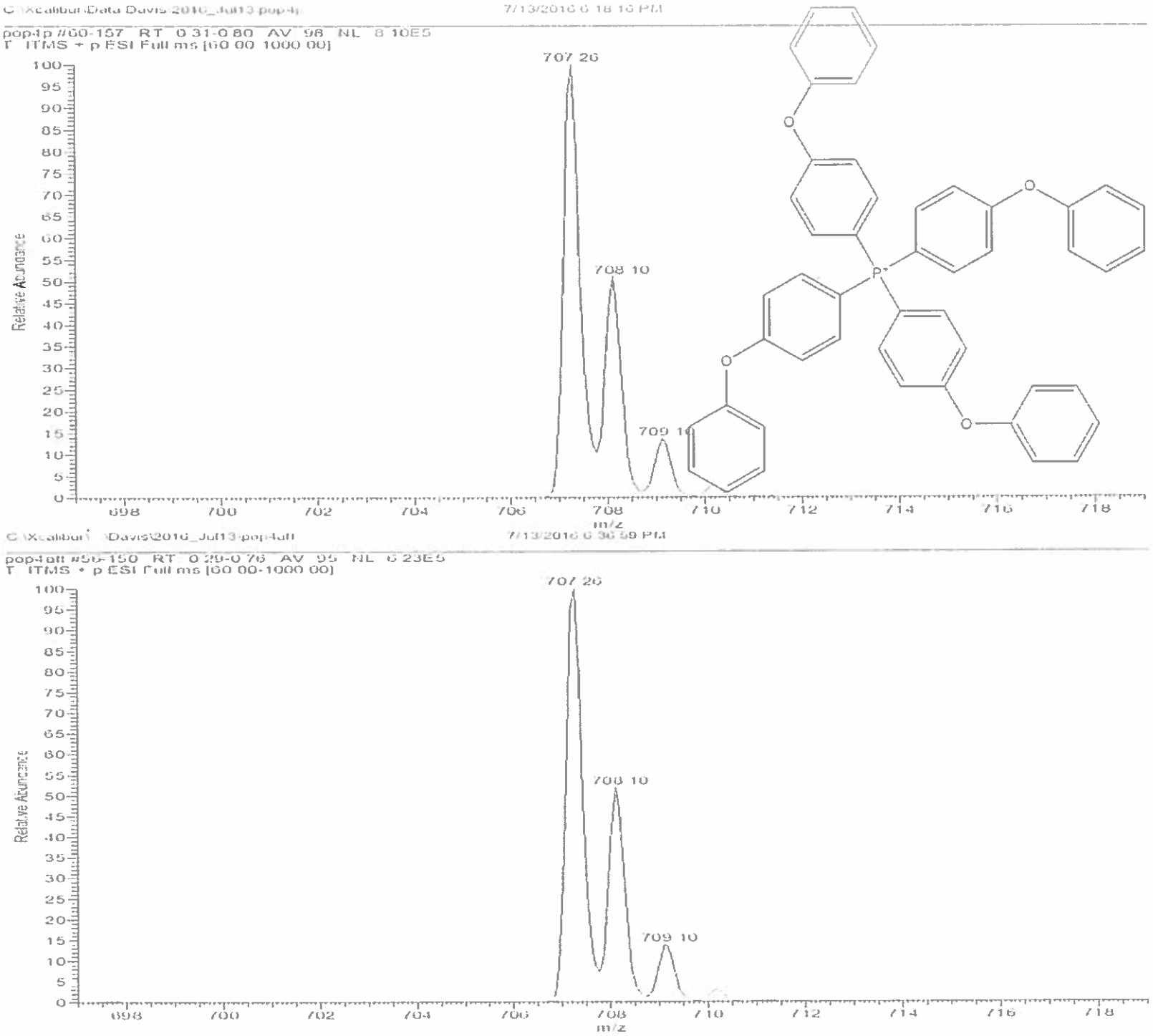




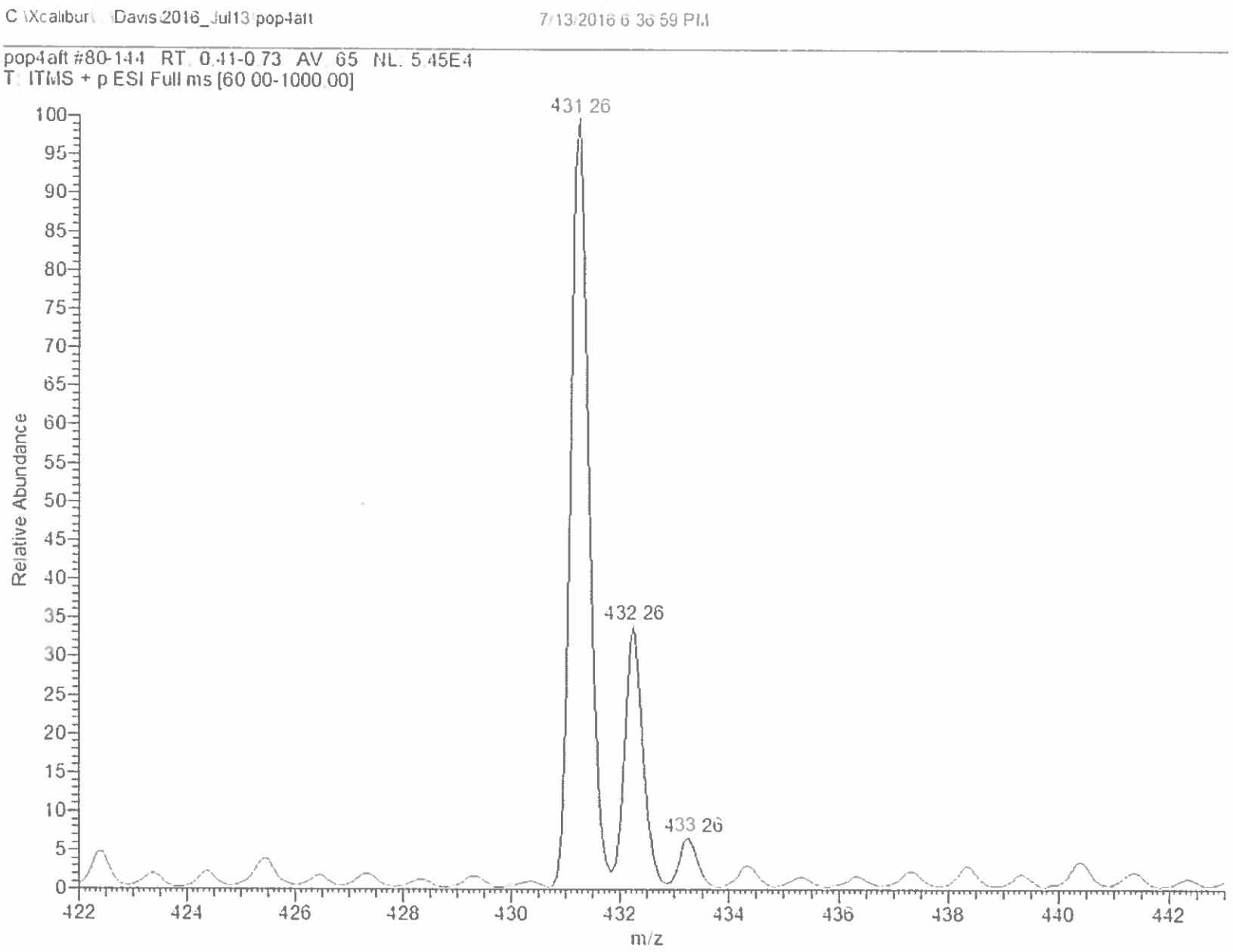
POP4
Before Δ

707.23
expected

POP4
After Δ



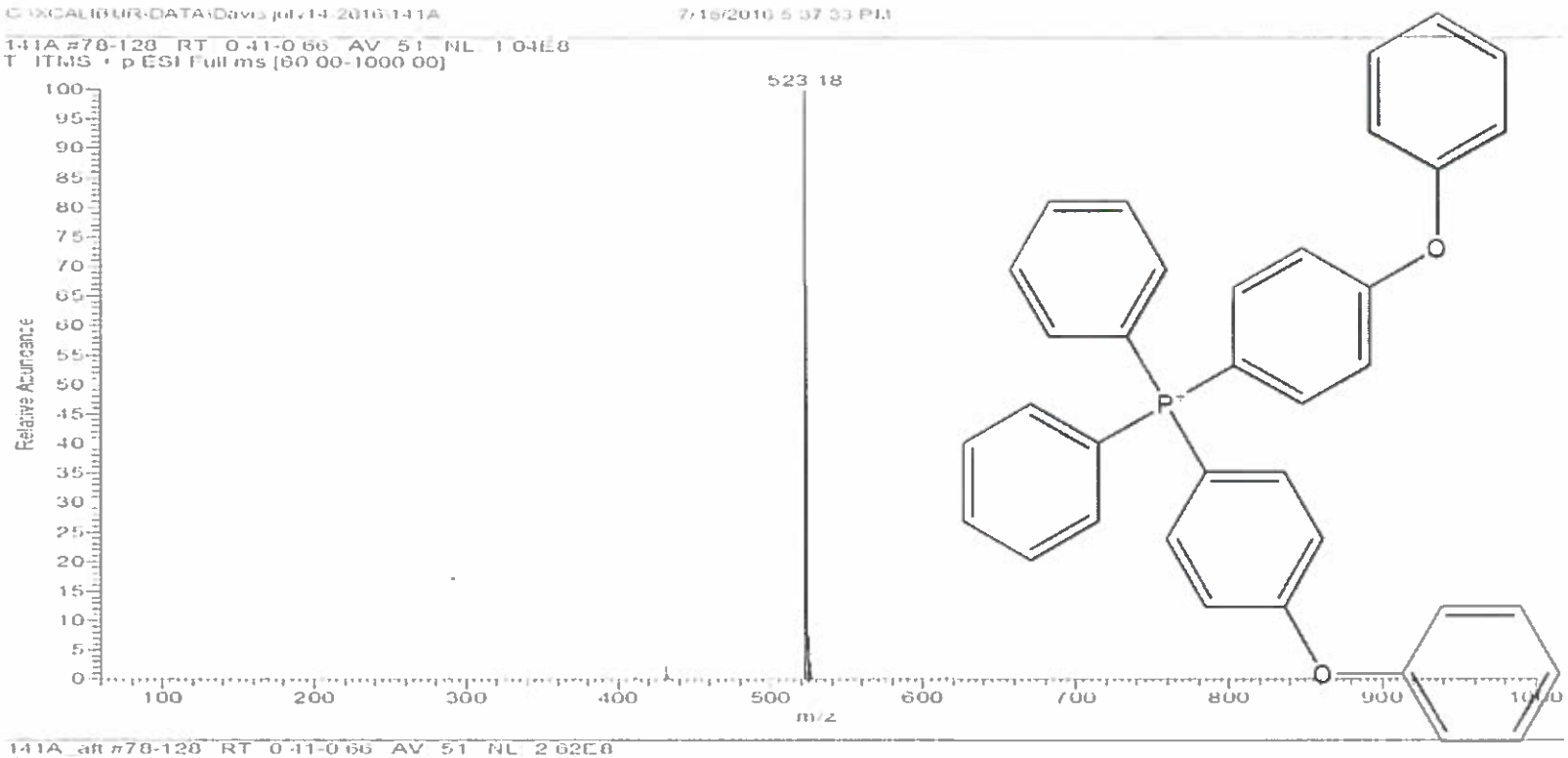
POP-4
New Peak



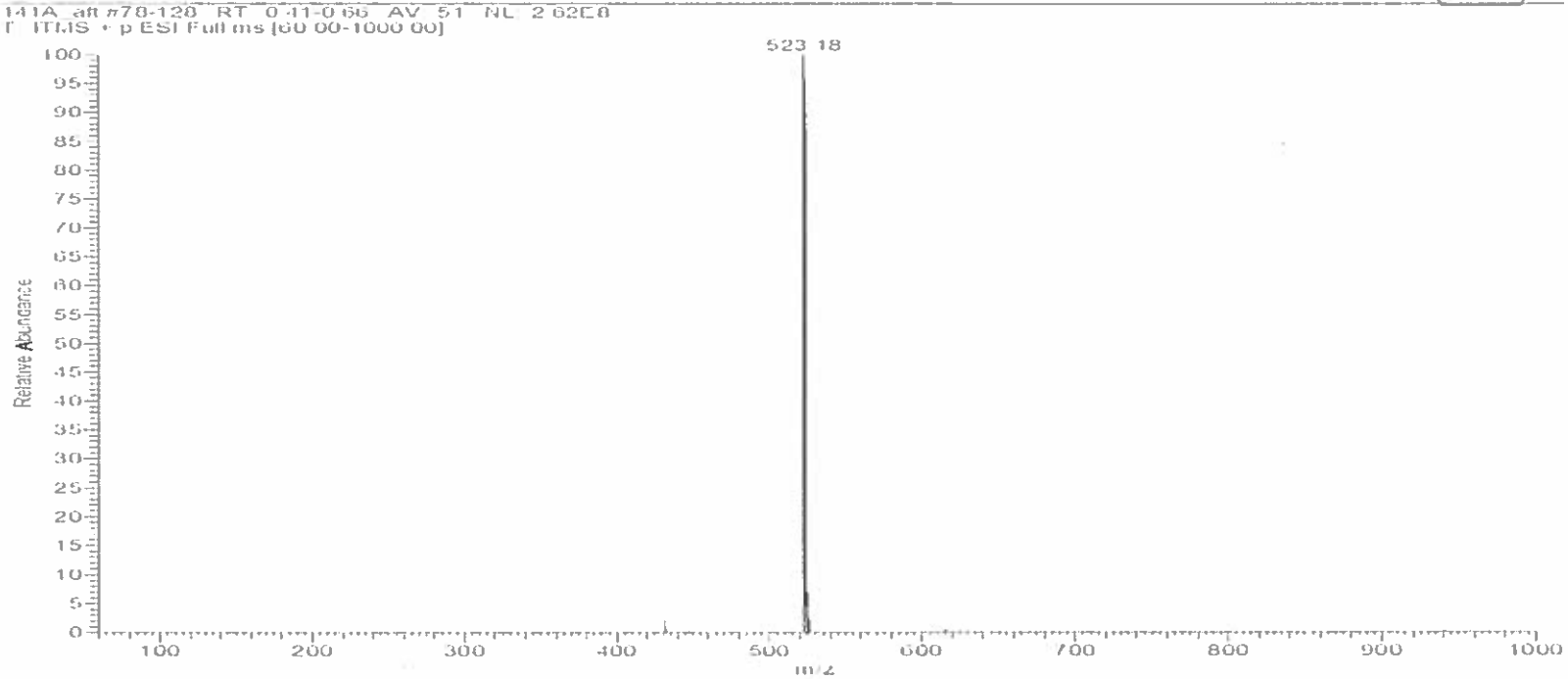
Compound 4

141-A
Before Δ

523.18
expected



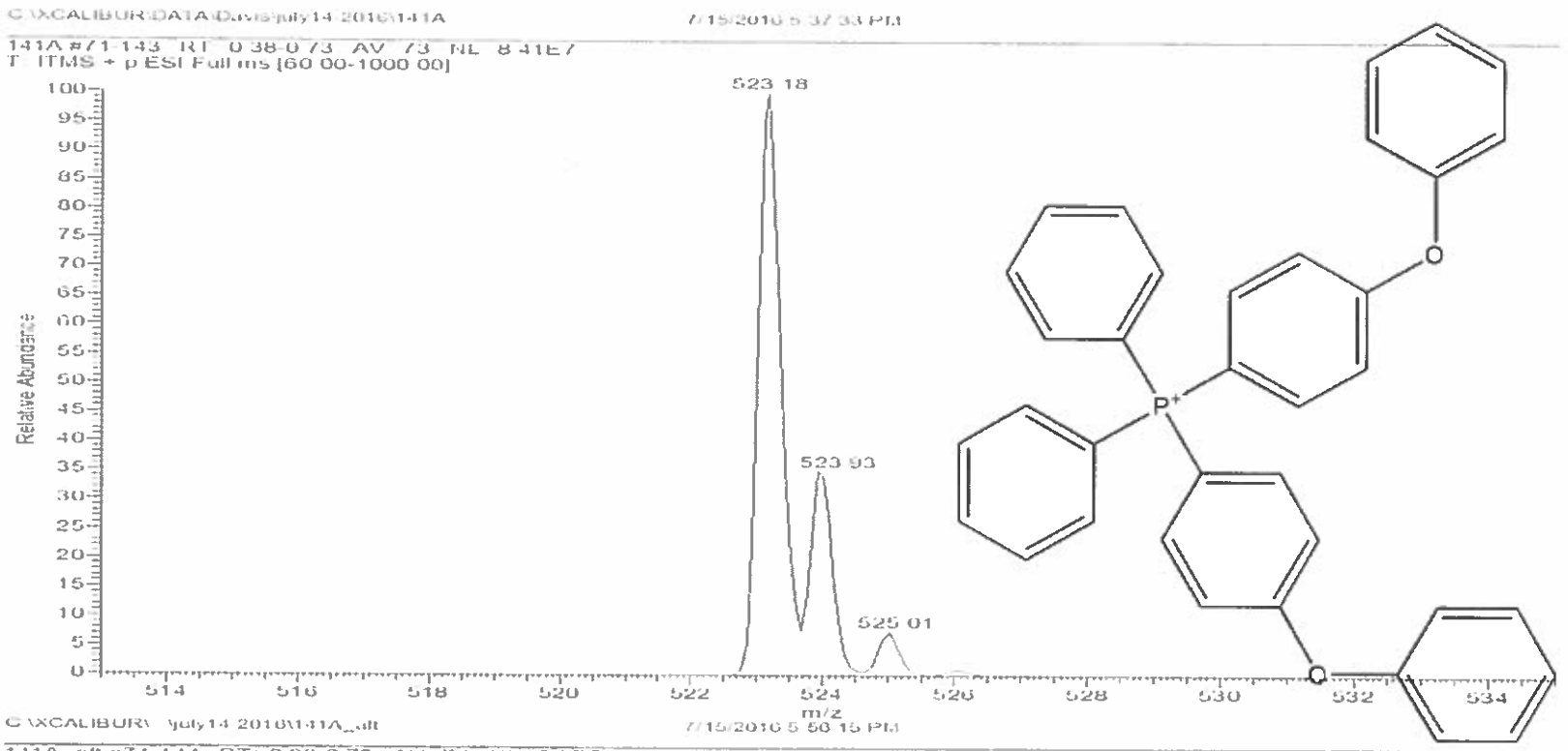
141-A
After Δ

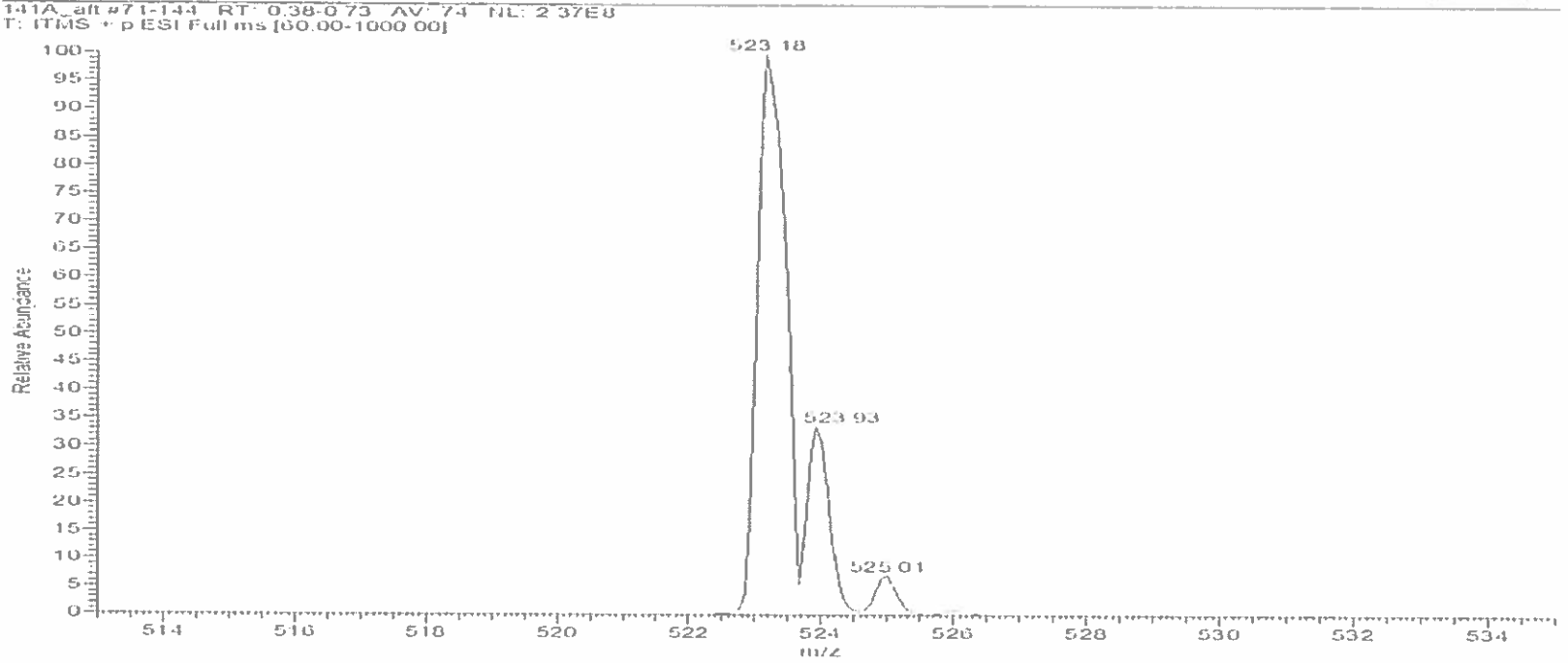


141-A
Before Δ

523.18
expected

141-A
After Δ



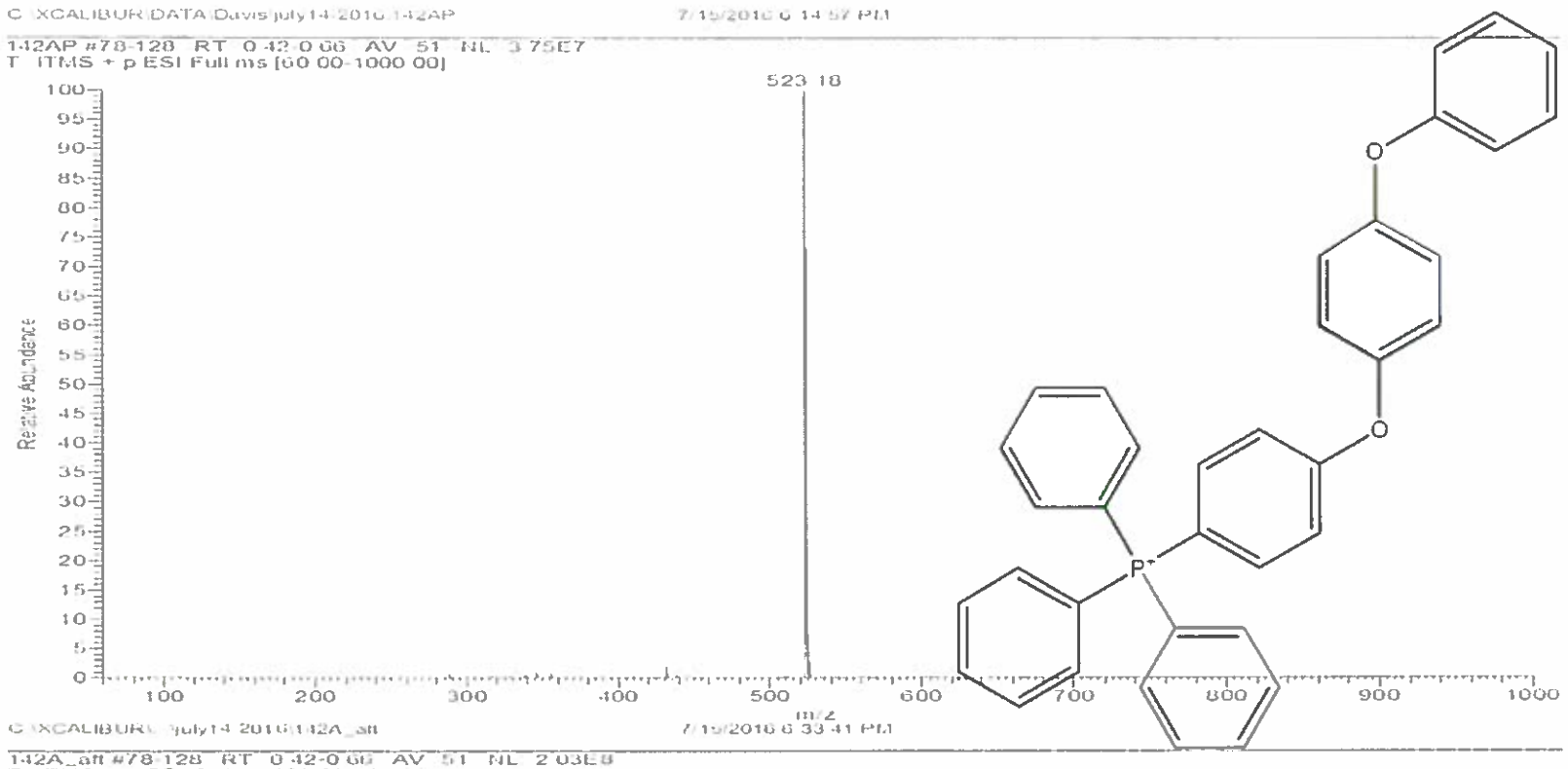


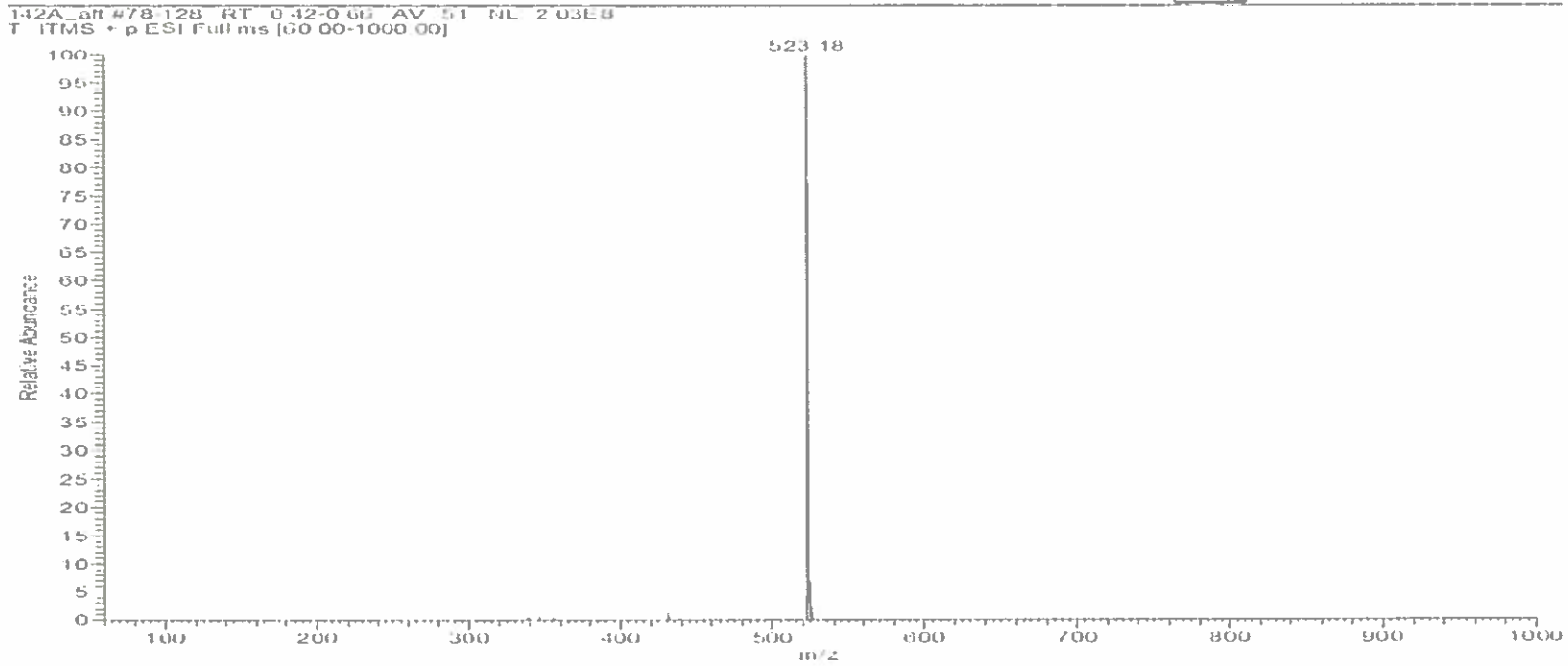
Compound 8

142-A
Before Δ

523.18
expected

142-A
After Δ

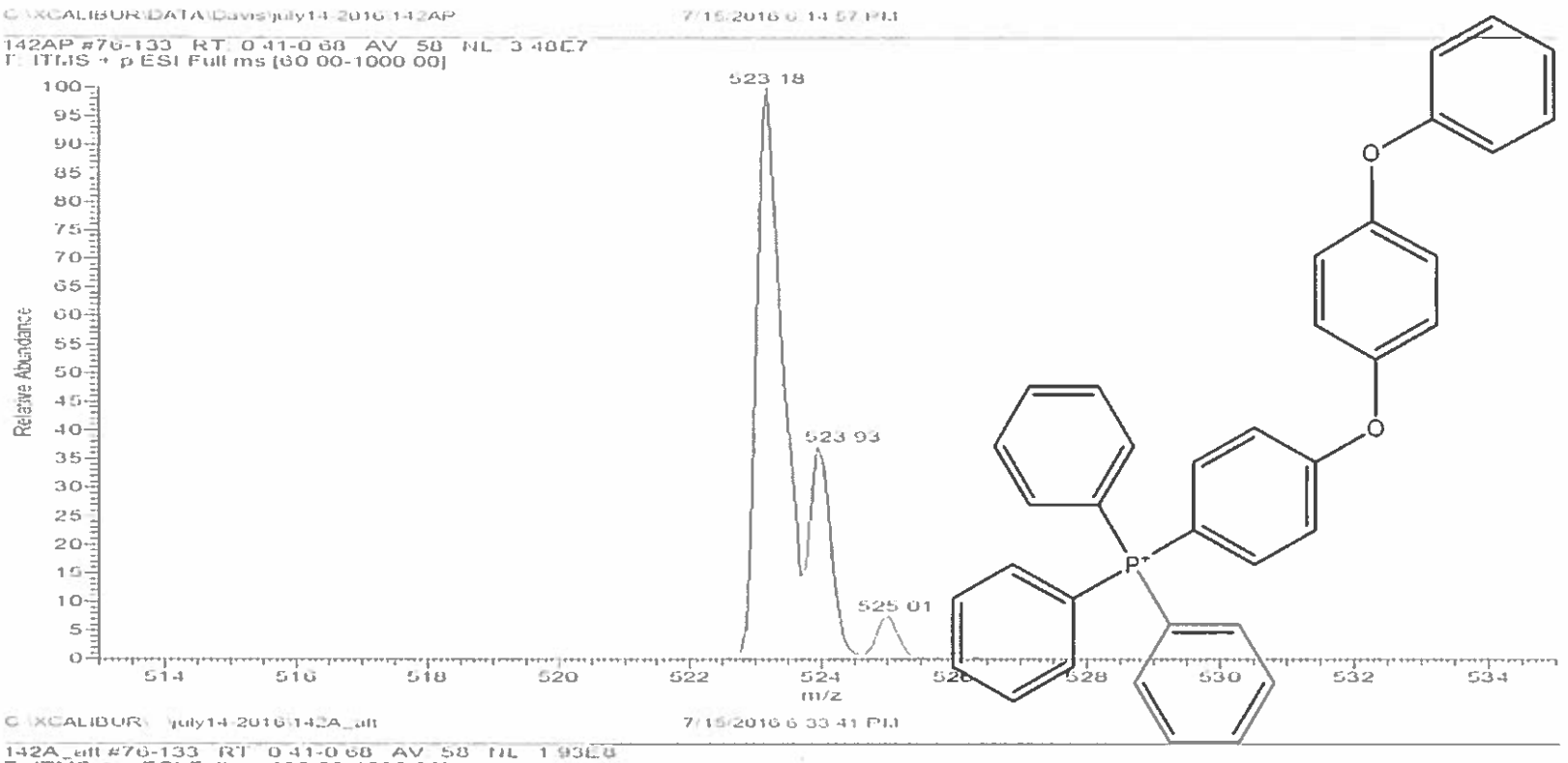


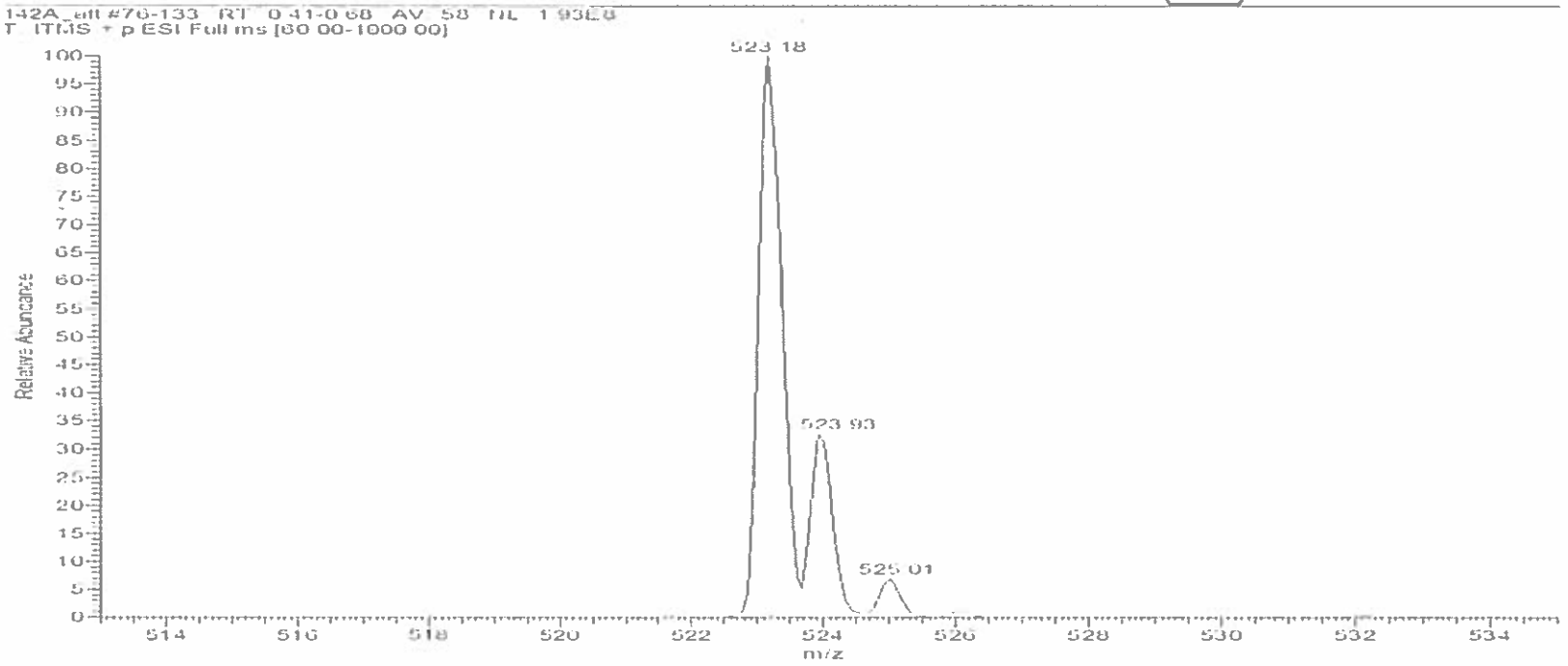


142-A
Before Δ

523.18
expected

142-A
After Δ



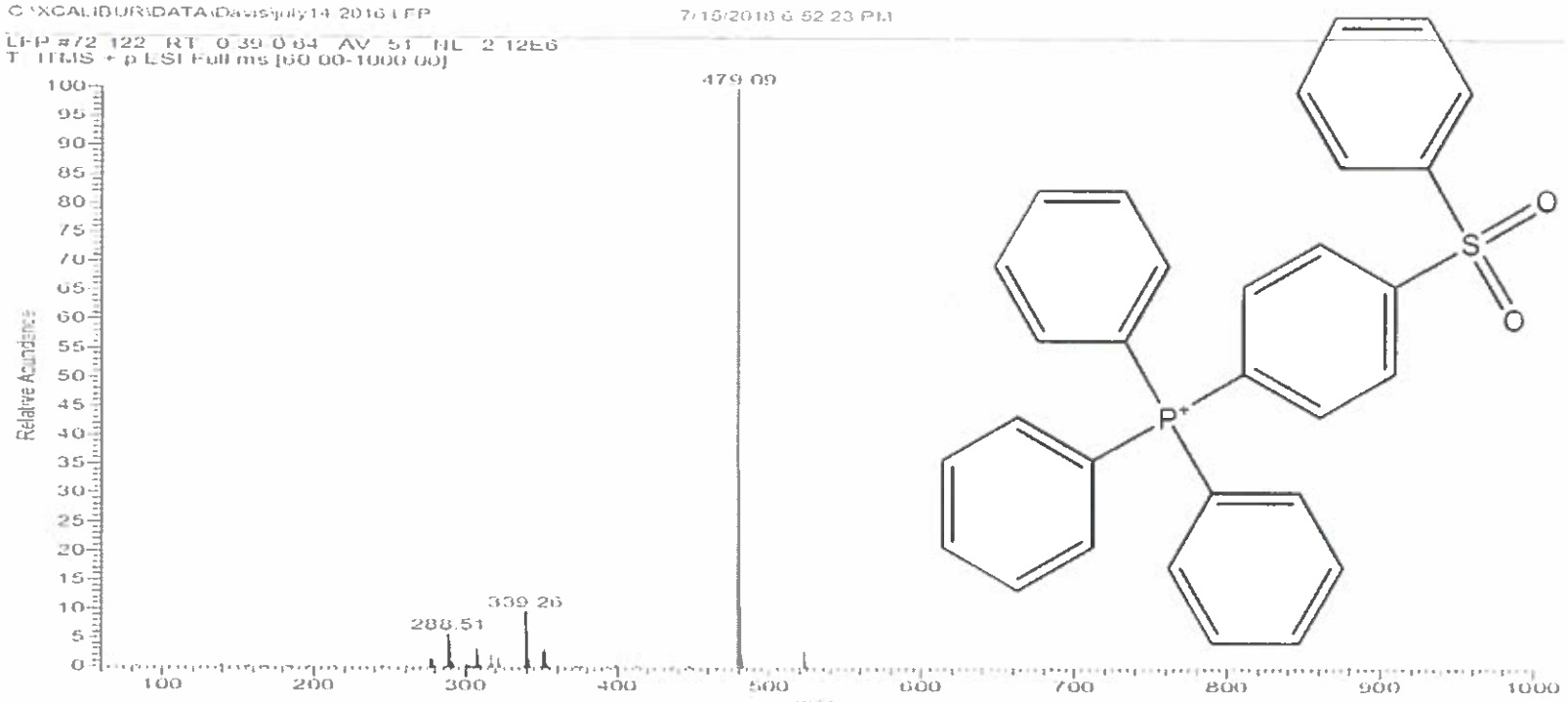


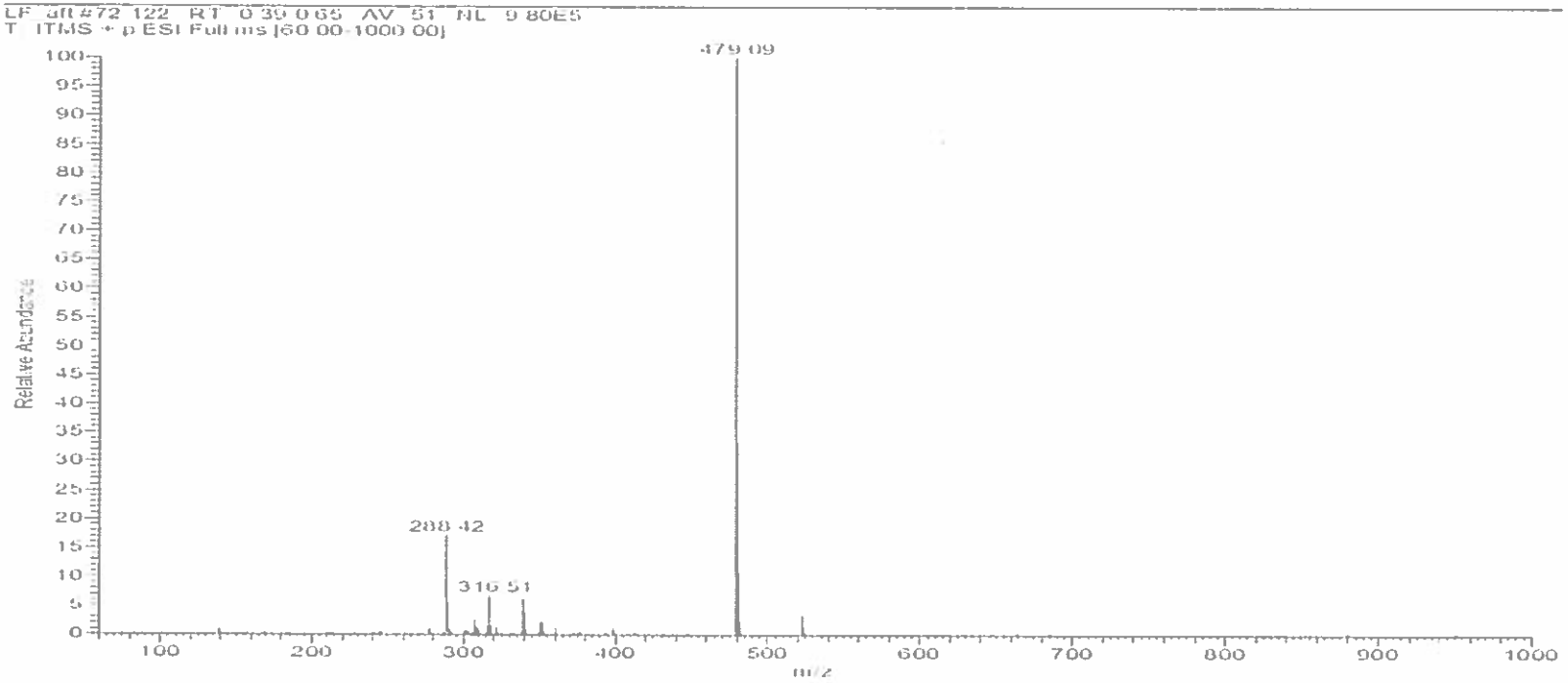
Compound 10

LF
Before Δ

479.12
expected

LF
After Δ

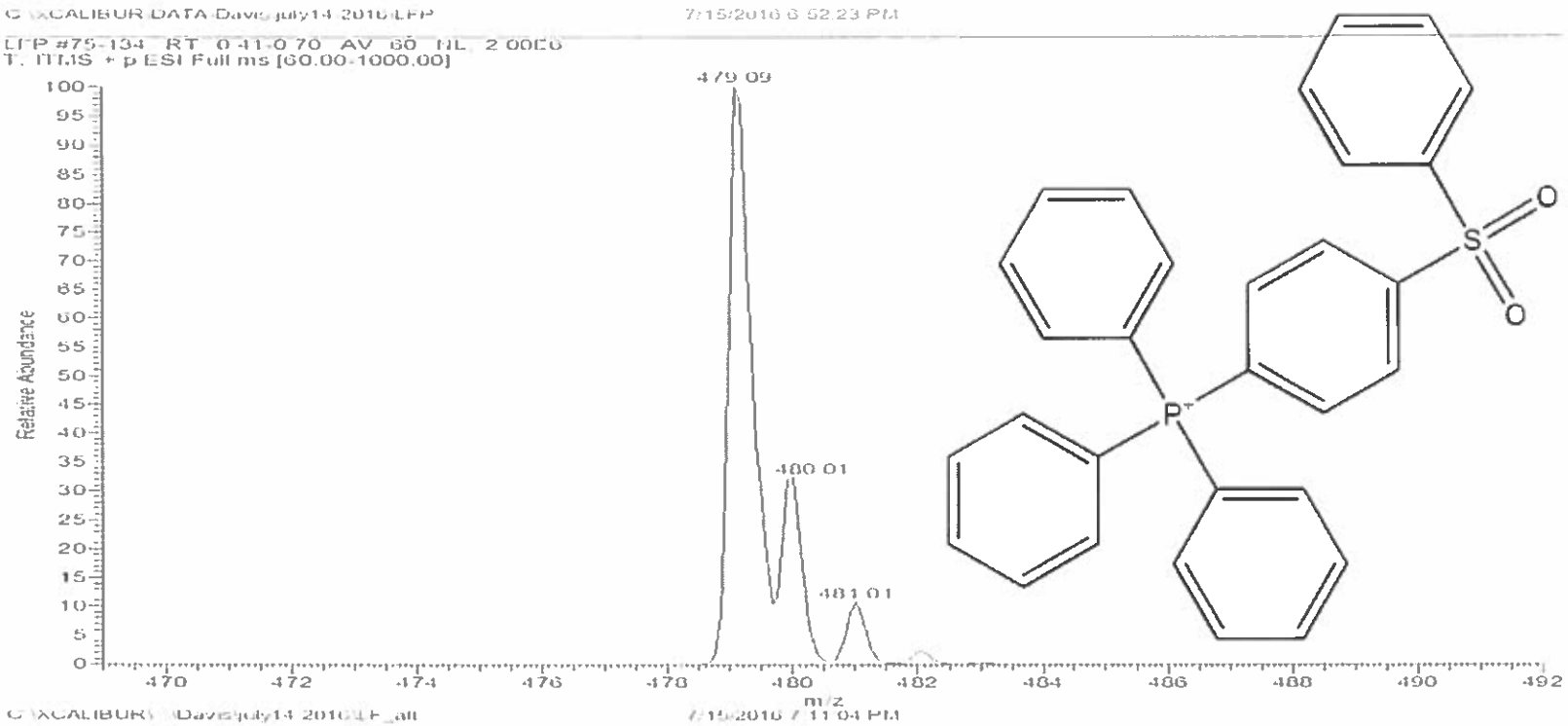


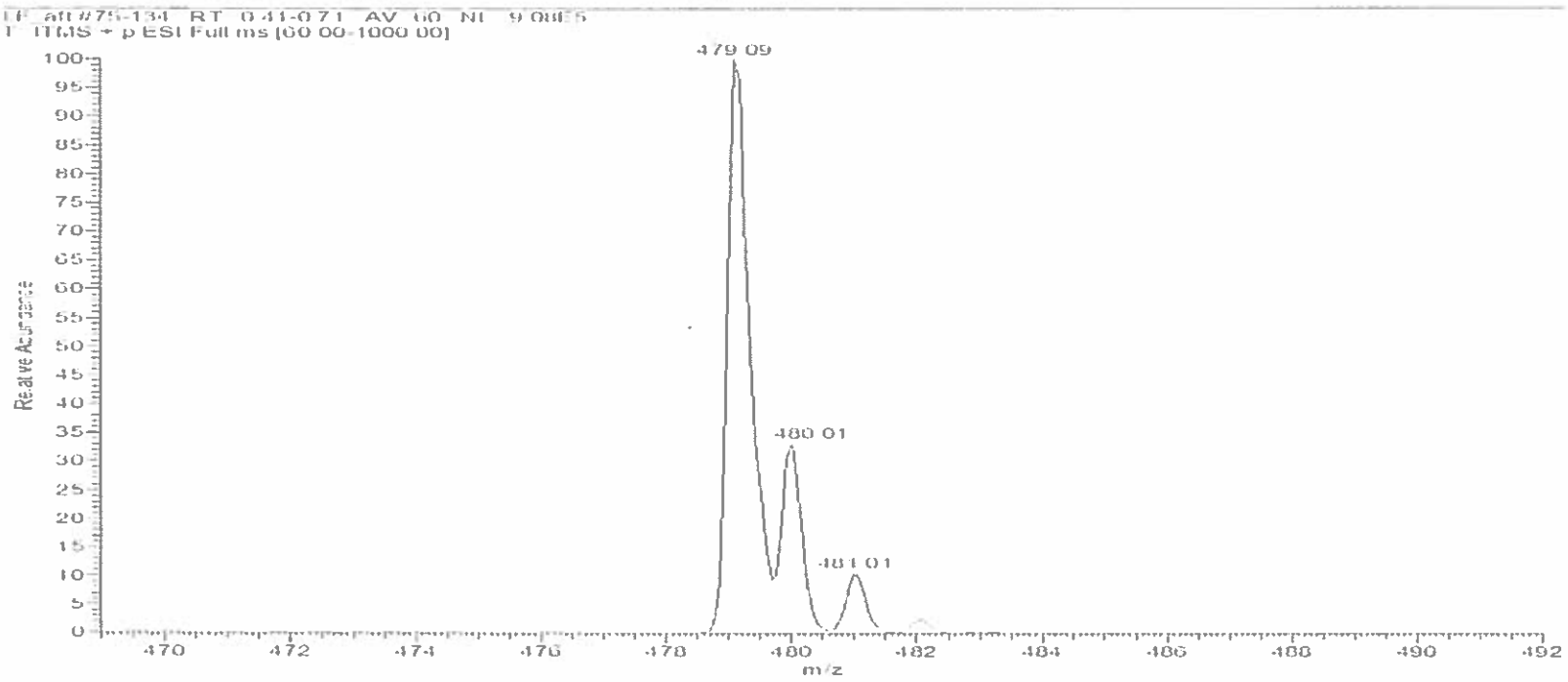


LF
Before Δ

479.12
expected

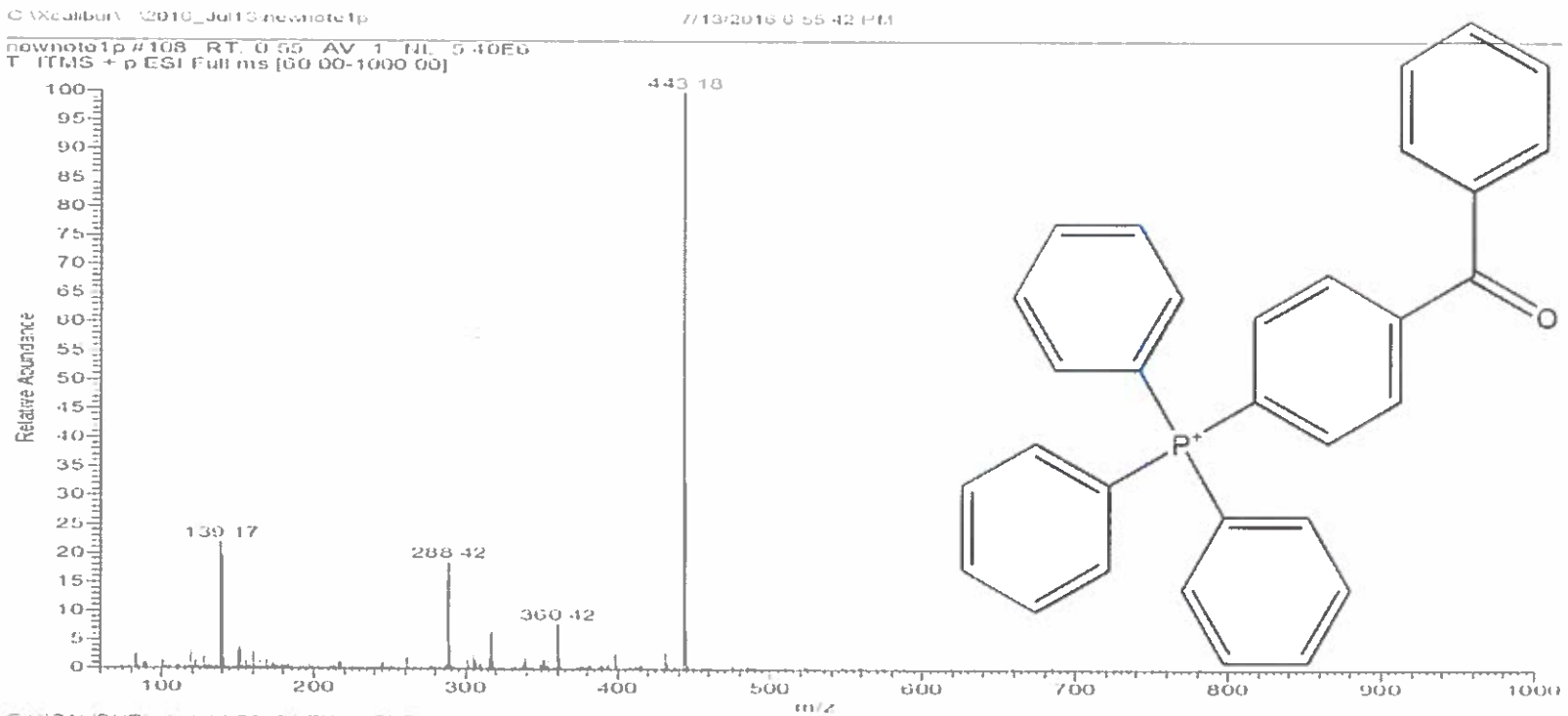
LF
After Δ





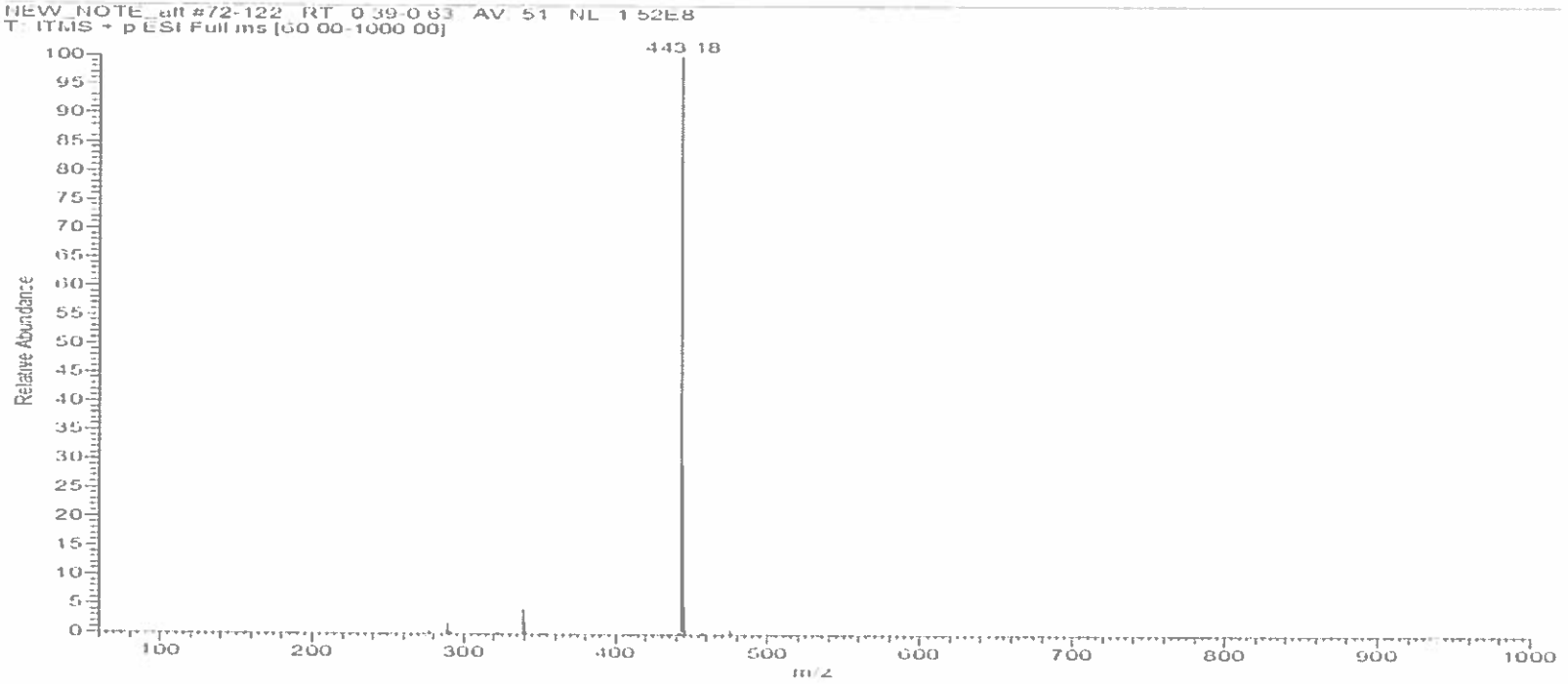
Compound 9

New Note 1 Before Δ



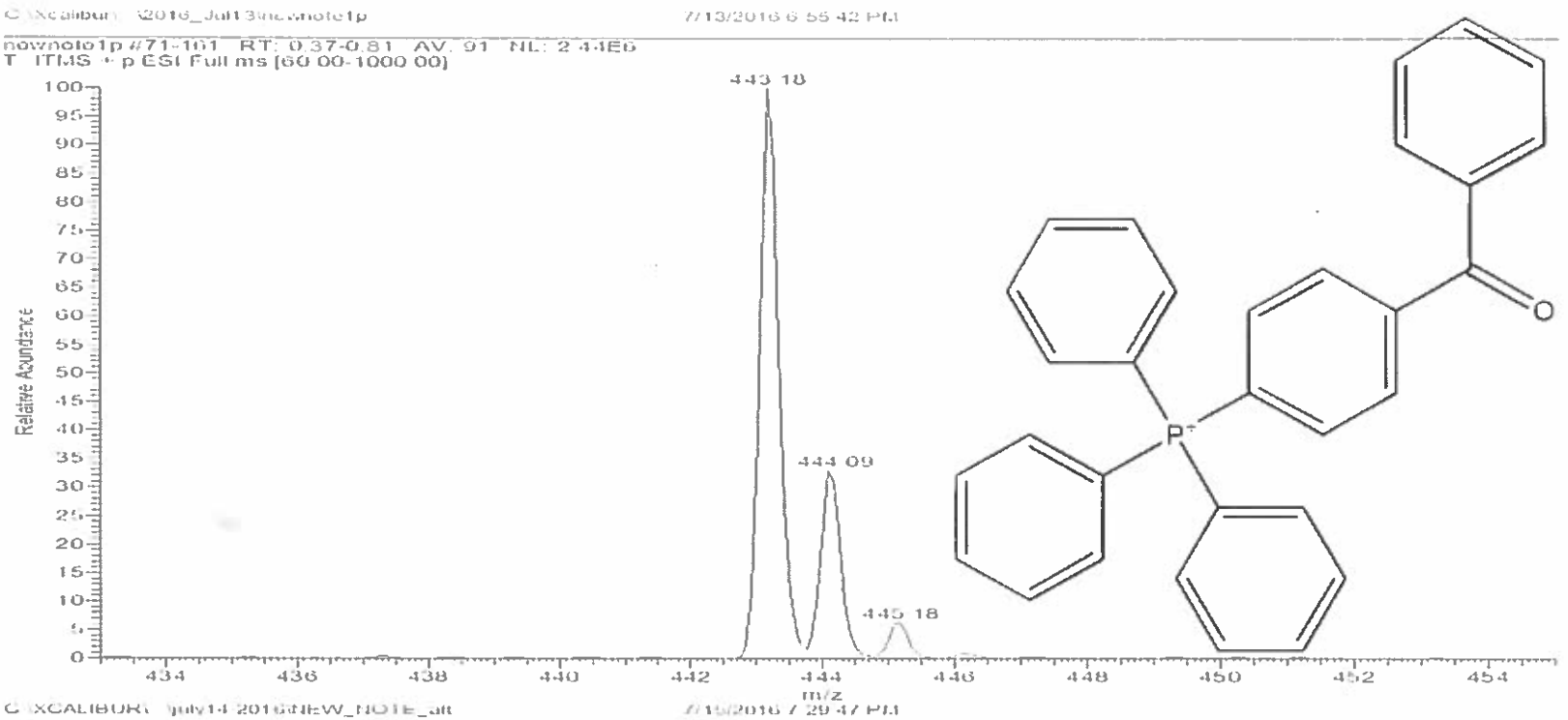
443.16 expected

New Note 1 After Δ

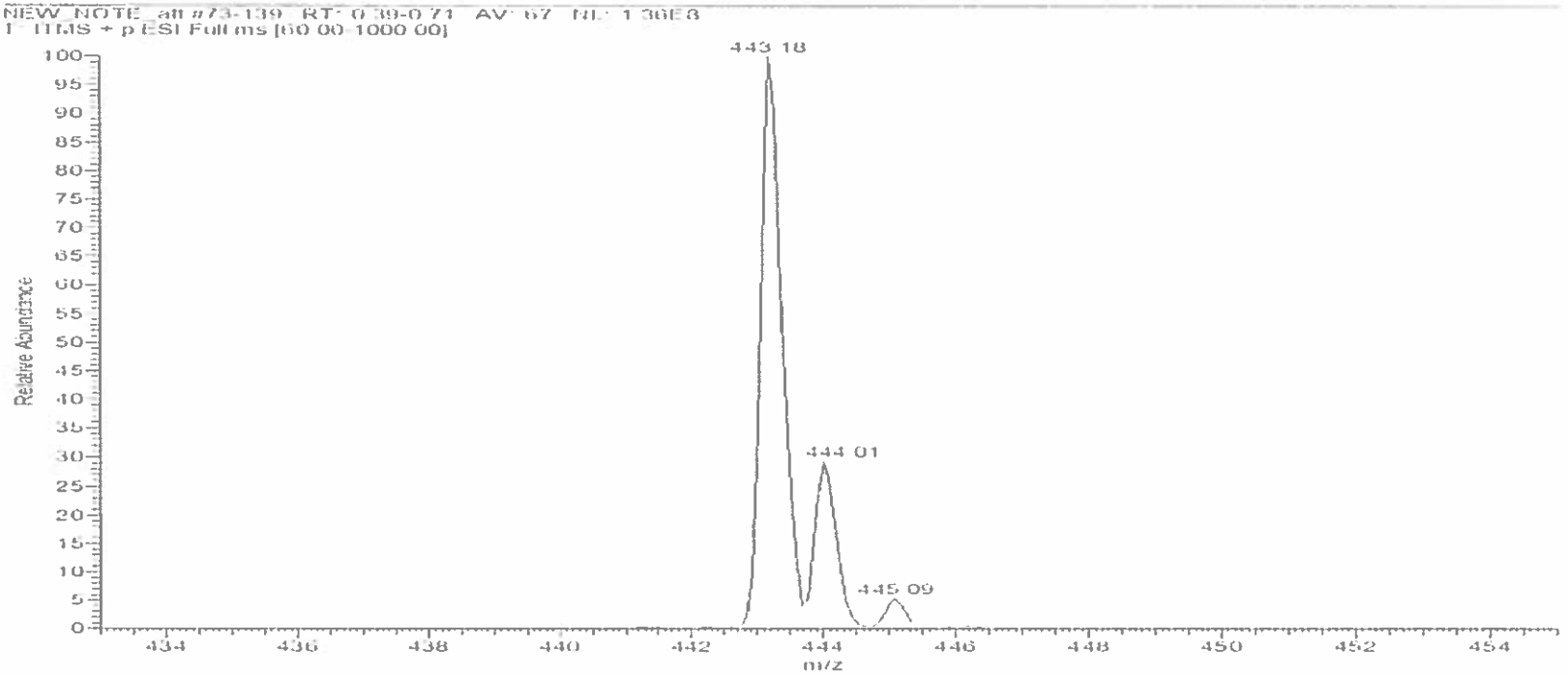


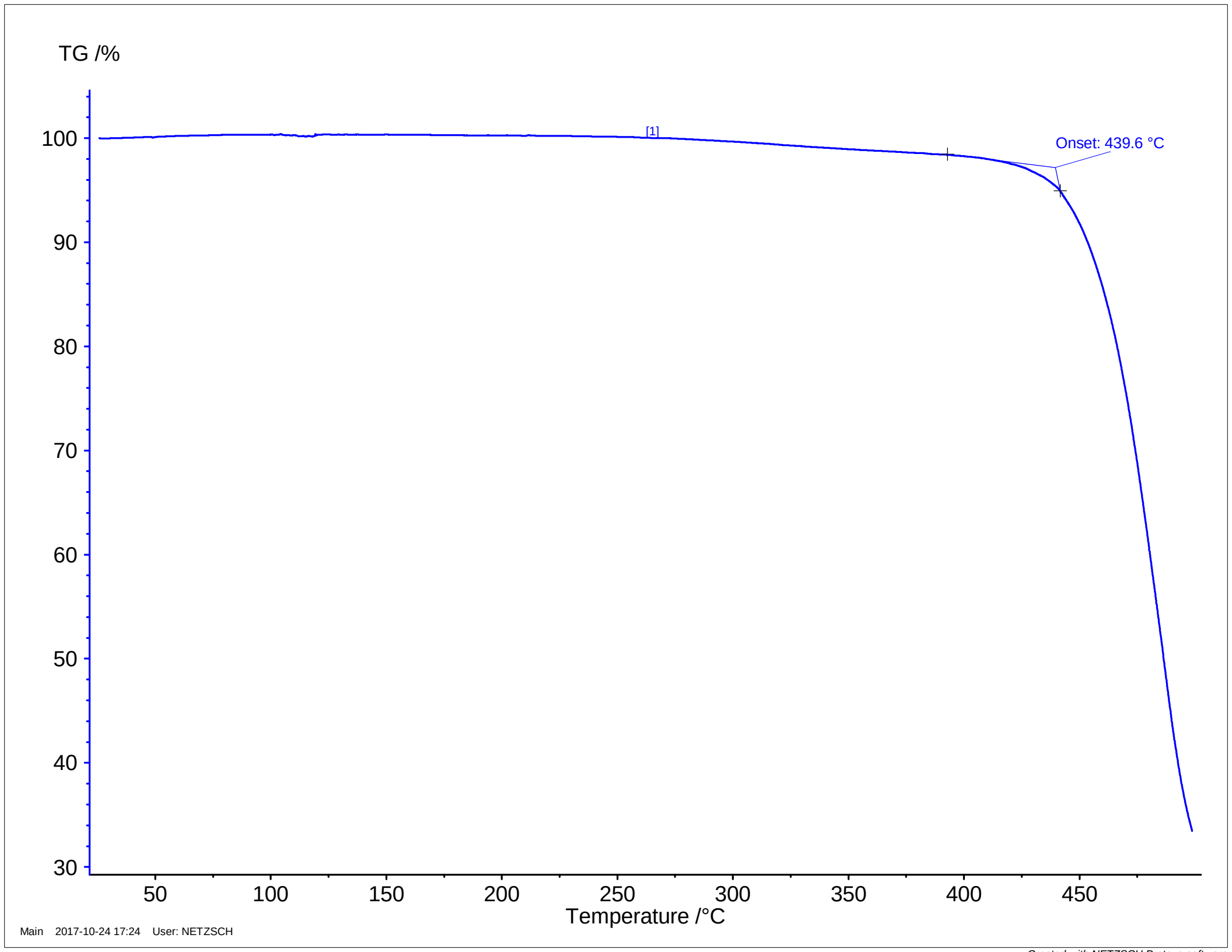
New Note 1 Before Δ

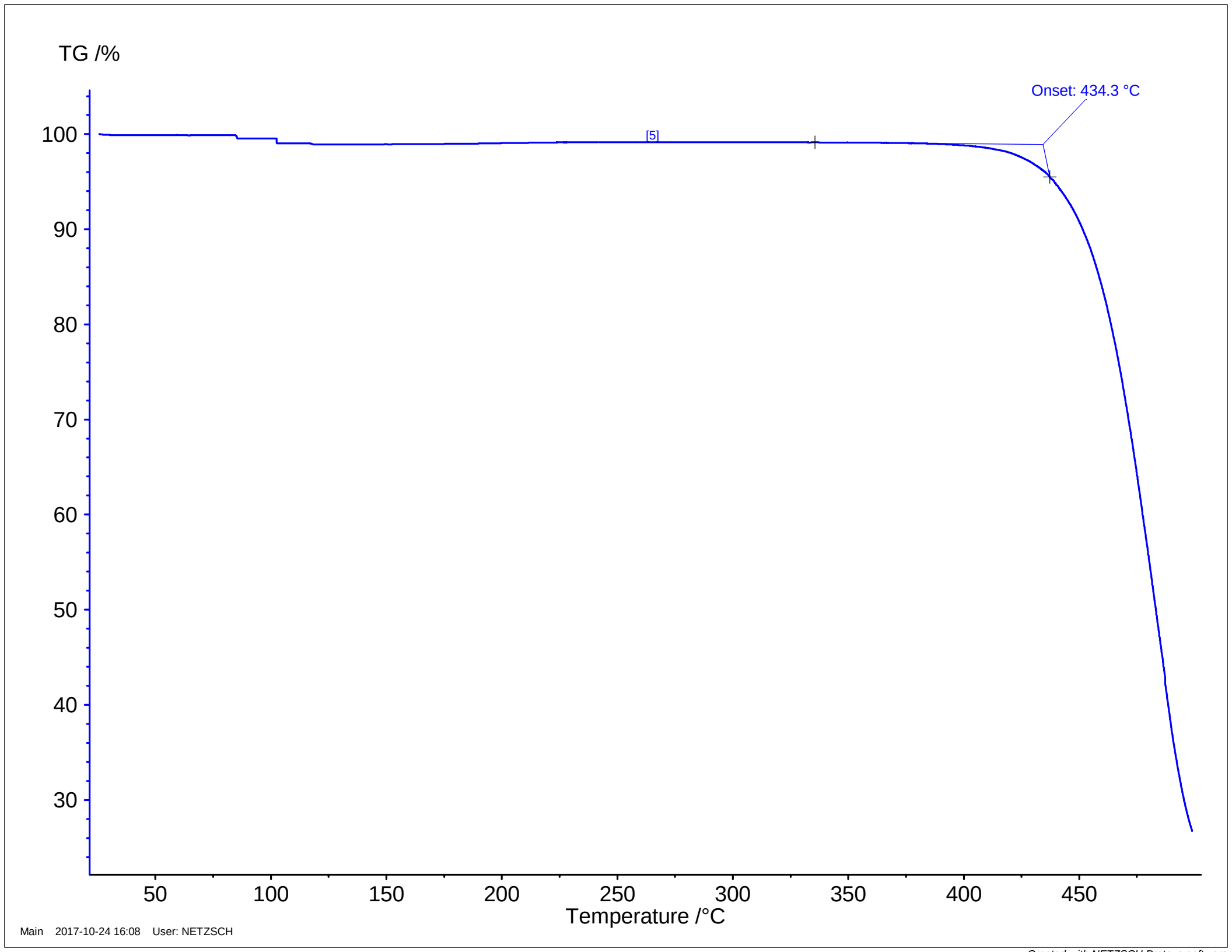
443.16 expected

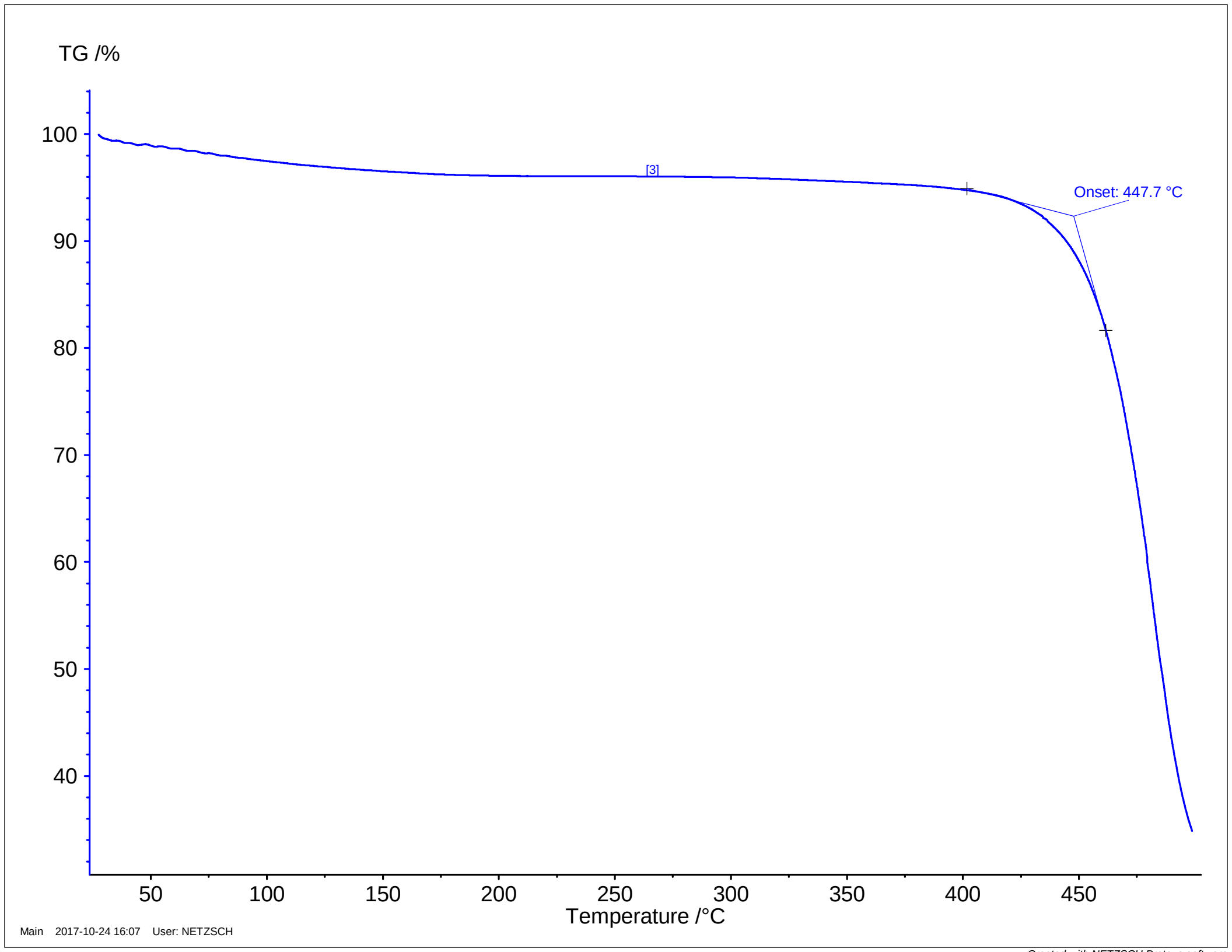


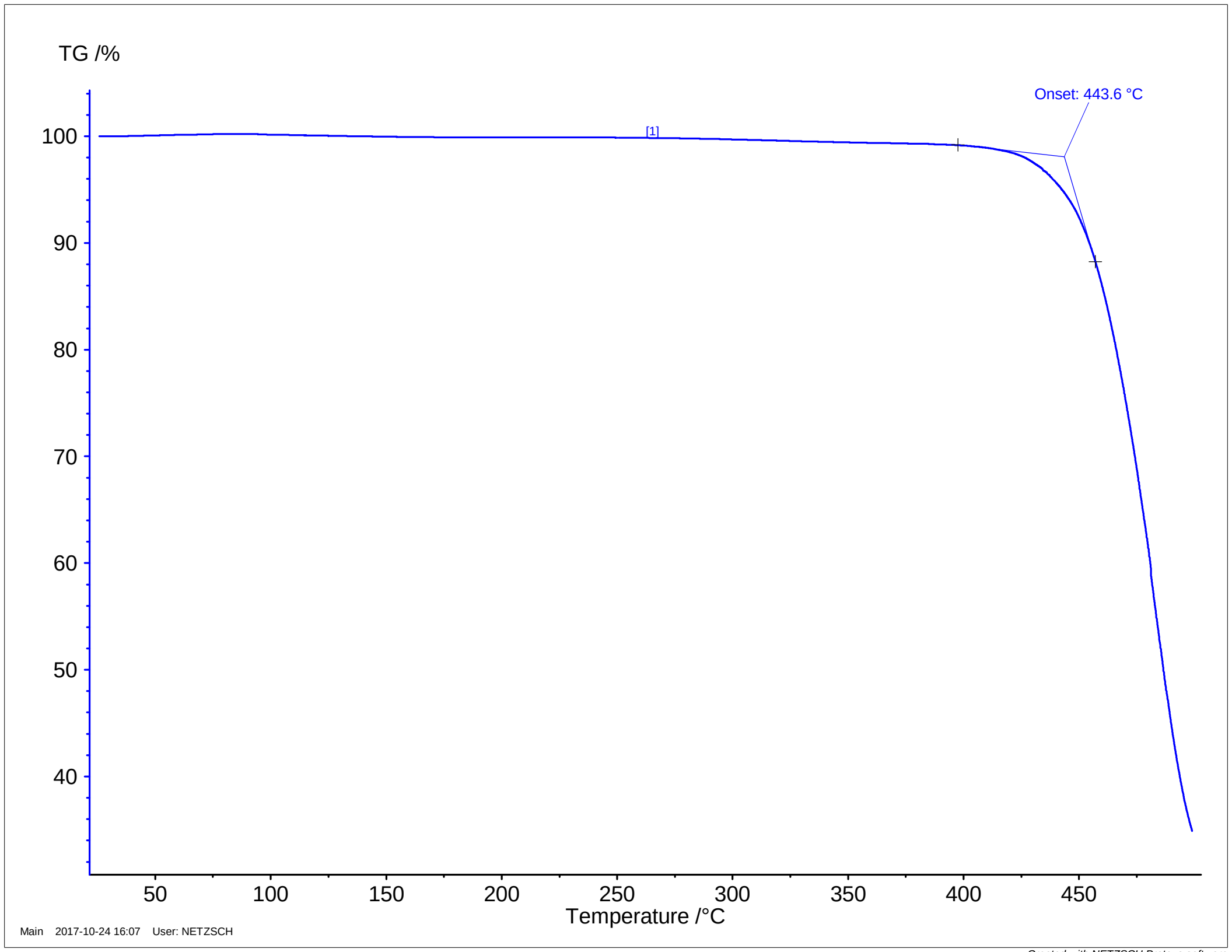
New Note 1 After Δ

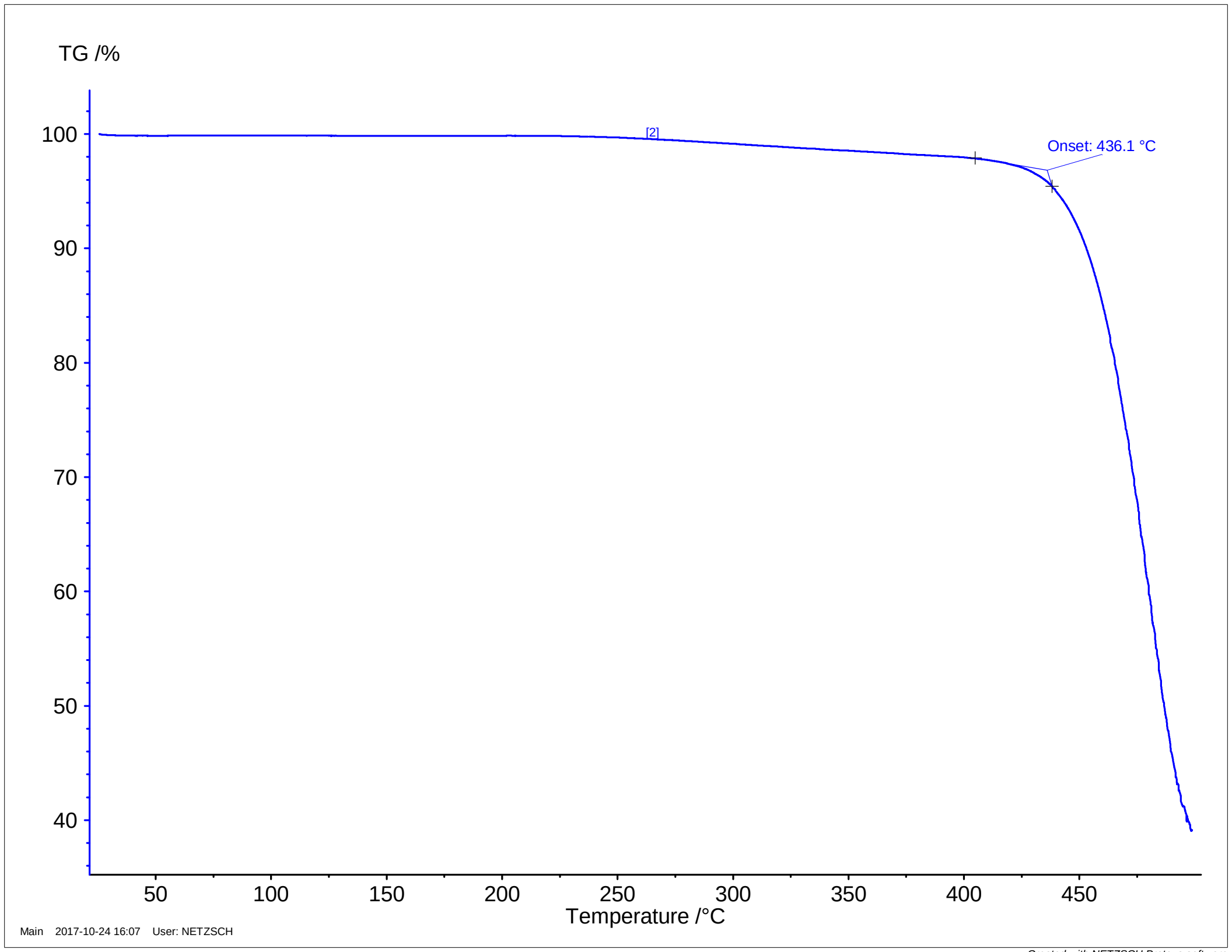


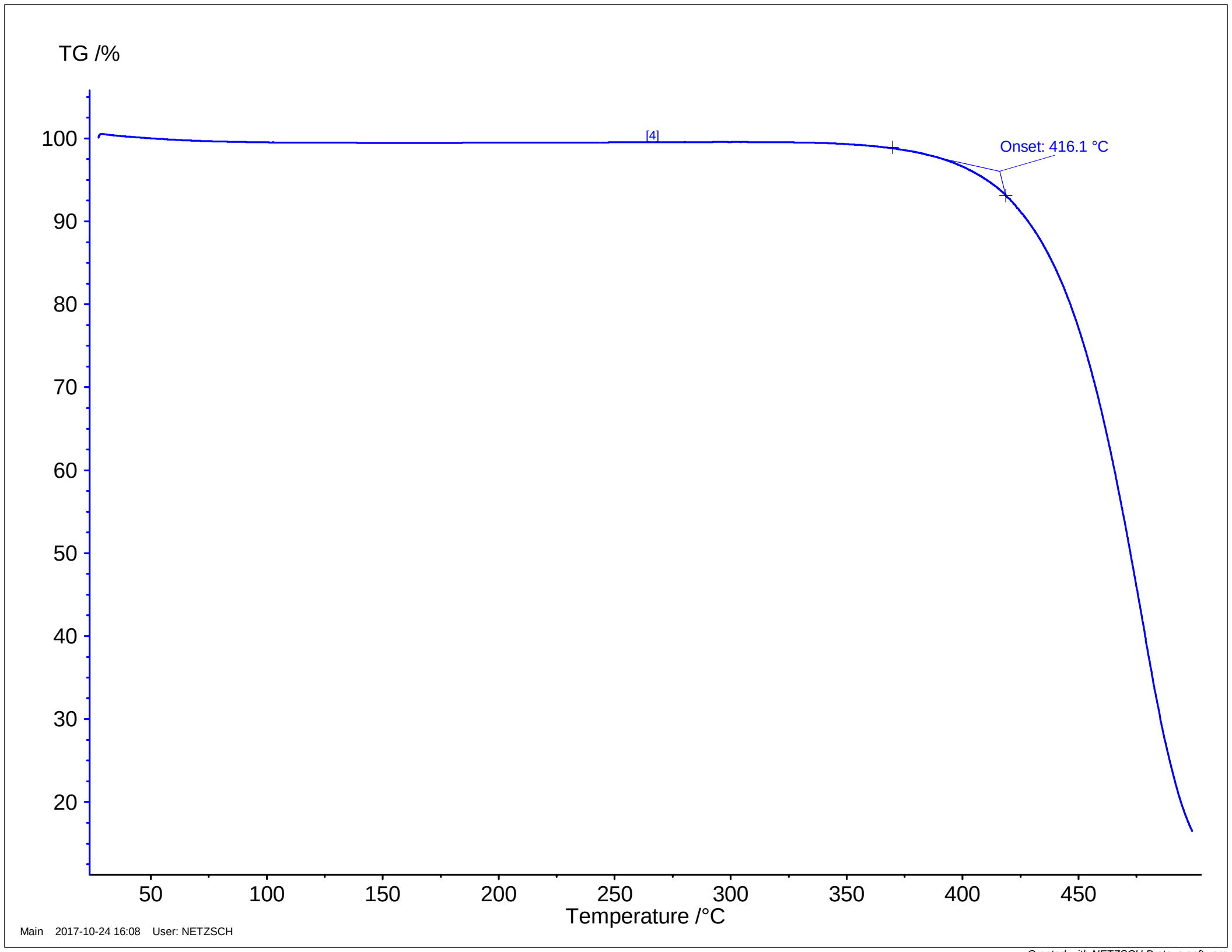

TG /%
100
90
80
70
60
50
40
30
[1]
Onset: 439.6 °C
50
100
150
200
250
300
350
400
450
Temperature /°C
Main 2017-10-24 17:24 User: NETZSCH


TG /%
Onset: 434.3 °C
[5]
100
90
80
70
60
50
40
30
50
100
150
200
250
300
350
400
450
Temperature /°C
Main 2017-10-24 16:08 User: NETZSCH


TG /%
100
90
80
70
60
50
40
[3]
Onset: 447.7 °C
50
100
150
200
250
300
350
400
450
Temperature /°C
Main 2017-10-24 16:07 User: NETZSCH


TG /%
Onset: 443.6 °C
[1]
100
90
80
70
60
50
40
50
100
150
200
250
300
350
400
450
Temperature /°C
Main 2017-10-24 16:07 User: NETZSCH


TG /%
100
90
80
70
60
50
40
[2]
Onset: 436.1 °C
50
100
150
200
250
300
350
400
450
Temperature /°C
Main 2017-10-24 16:07 User: NETZSCH


TG /%
100
90
80
70
60
50
40
30
20
[4]
Onset: 416.1 °C
50
100
150
200
250
300
350
400
450
Temperature /°C
Main 2017-10-24 16:08 User: NETZSCH