Electronic Supplementary Material (ESI) for New Journal of Chemistry.

96 hour aerobic thermolysis of PPN^+X^- salts at 200 °C, 250 °C, and 300 °C. An evaluation of anion suitability for use in ionic liquids with long-term, high-temperature thermal stability

Adela Benchea,[a] Benjamin Siu,[b] Mohammad Soltani,[a] E. Alan Salter,[a] Andrzej Wierzbicki,[a] Kevin N. West,*[b] and James H. Davis, Jr.*[a]

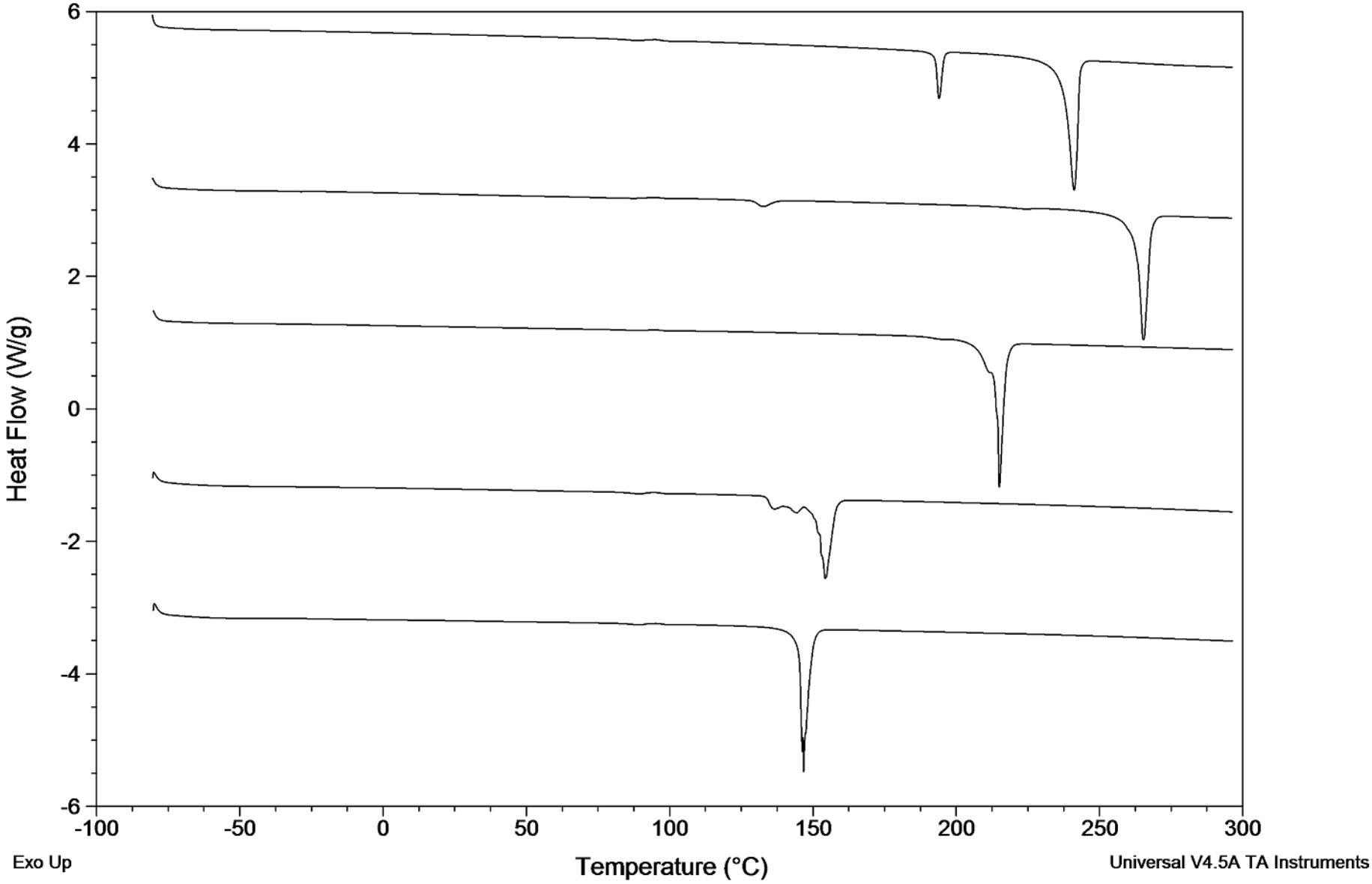
a Department of Chemistry, University of South Alabama, Mobile, Alabama 36688 USA.
b Department of Chemical & Biomolecular Engineering, University of South Alabama, Mobile, Alabama 36688 USA.

SUPPORTING INFORMATION

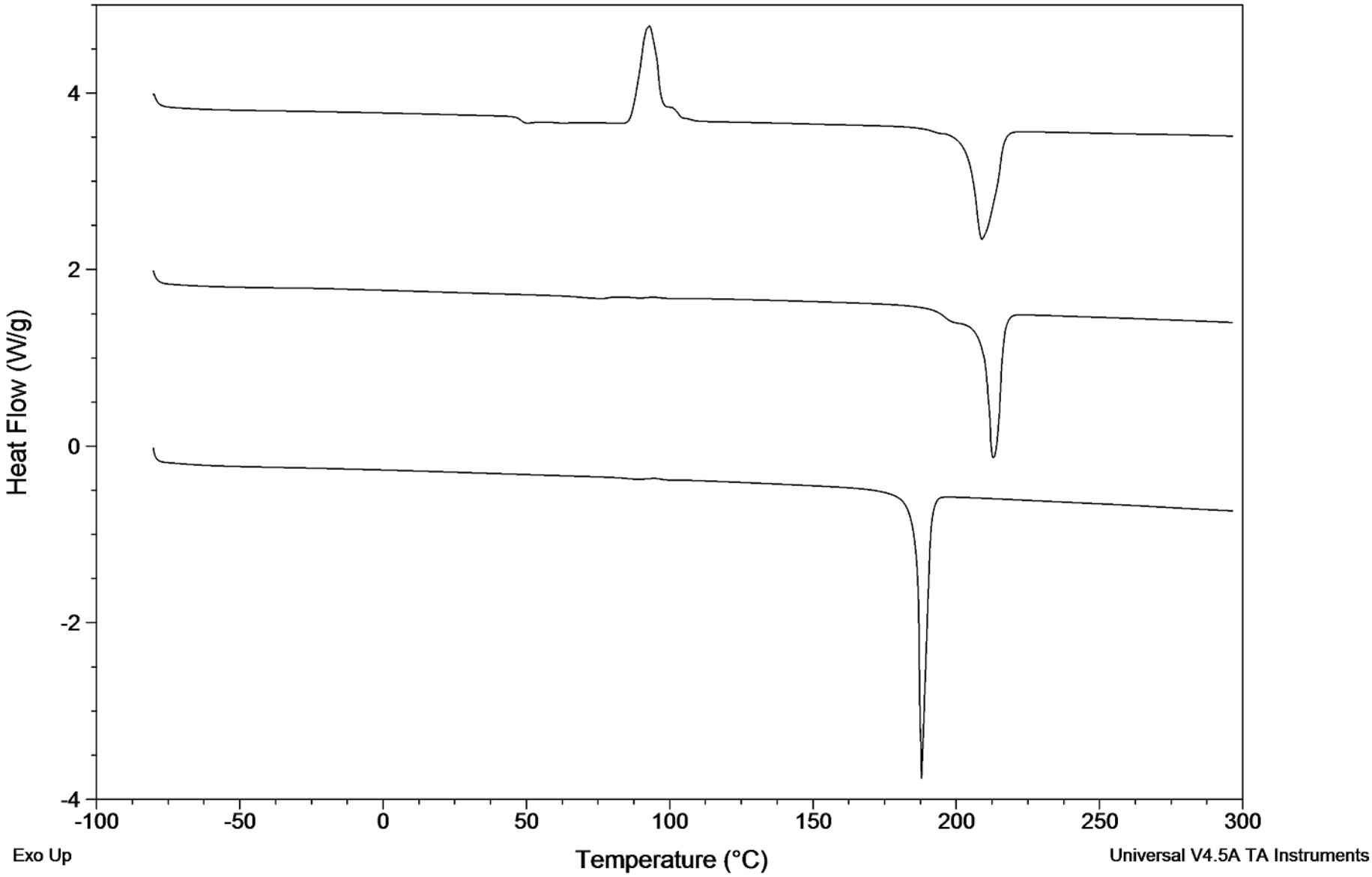
- DSC Traces for all salts (**1**-**14**)
- Electrostatic potential maps for the Sac^- and $BDSA^-$ anions, and computational details
- Multinuclear NMR spectra of all new salts (**5**, **6**, **8**, **10**, **11**, **14**)

Differential Scanning Calorimetry

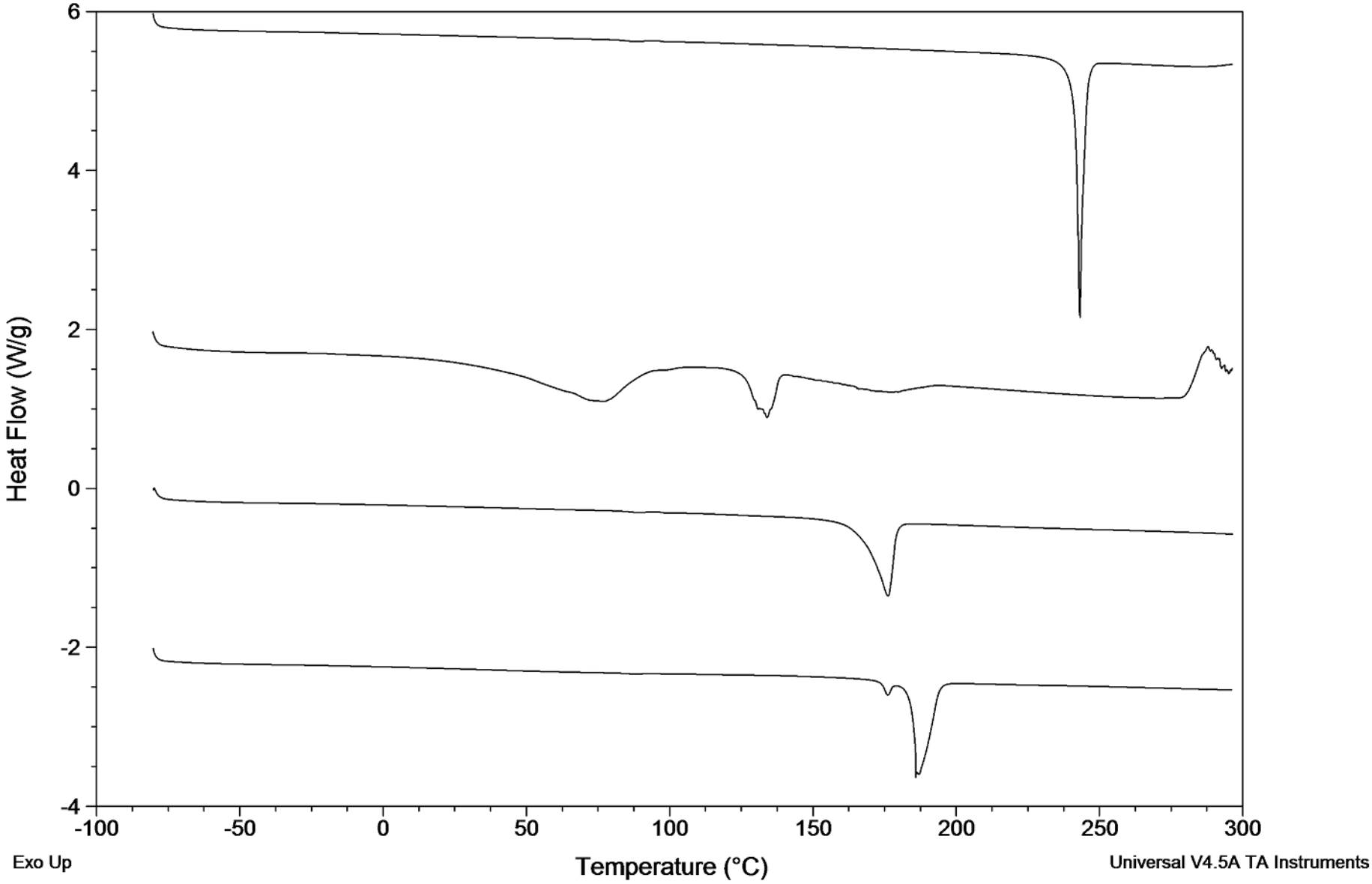
Top to Bottom: **1**, **2**, **3**, **4**, **5**.



Differential Scanning Calorimetry
Top to Bottom: **6**, **7**, **8**.

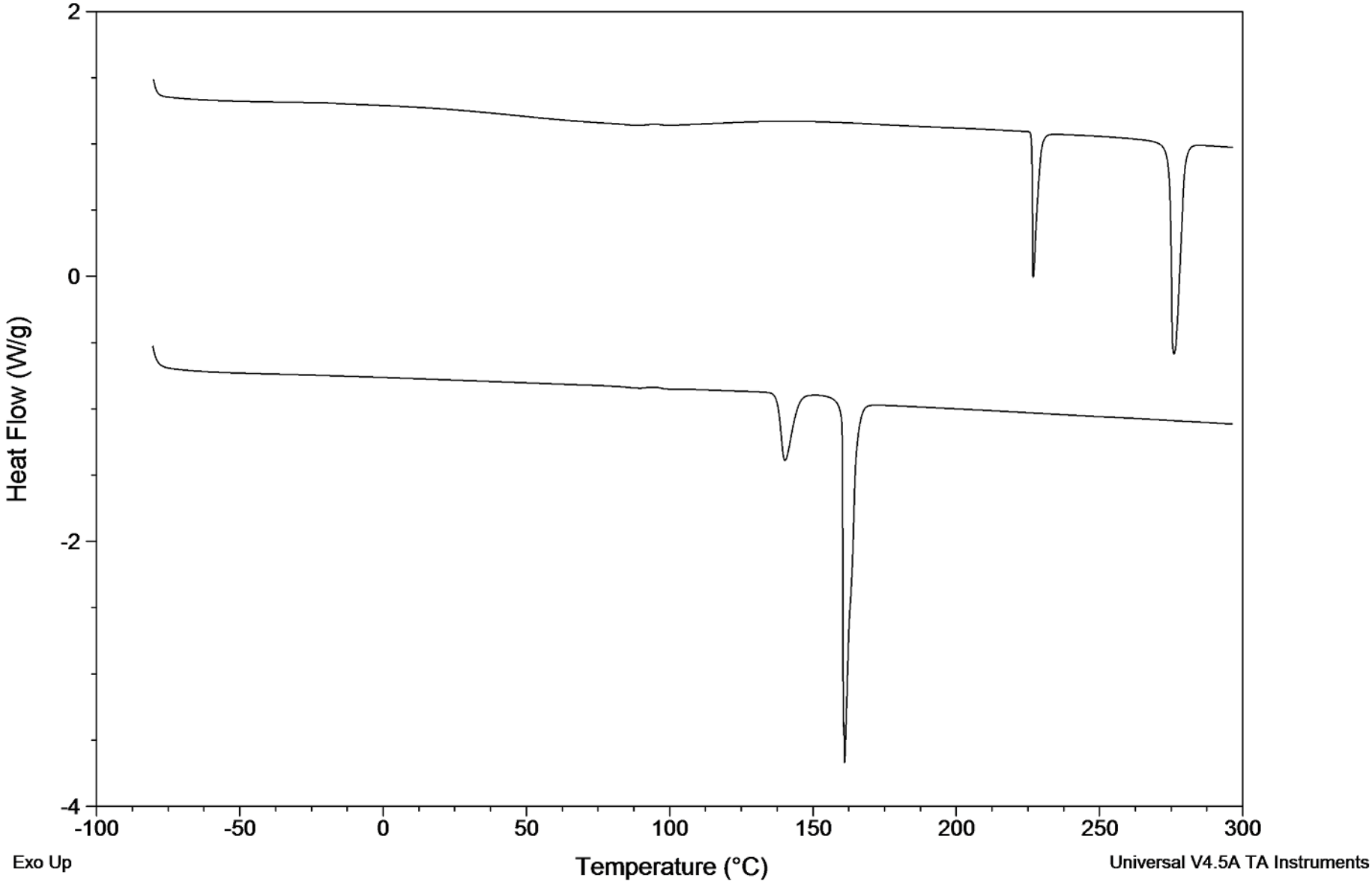


Differential Scanning Calorimetry
Top to Bottom: **9**, **10**, **11**, **12**.

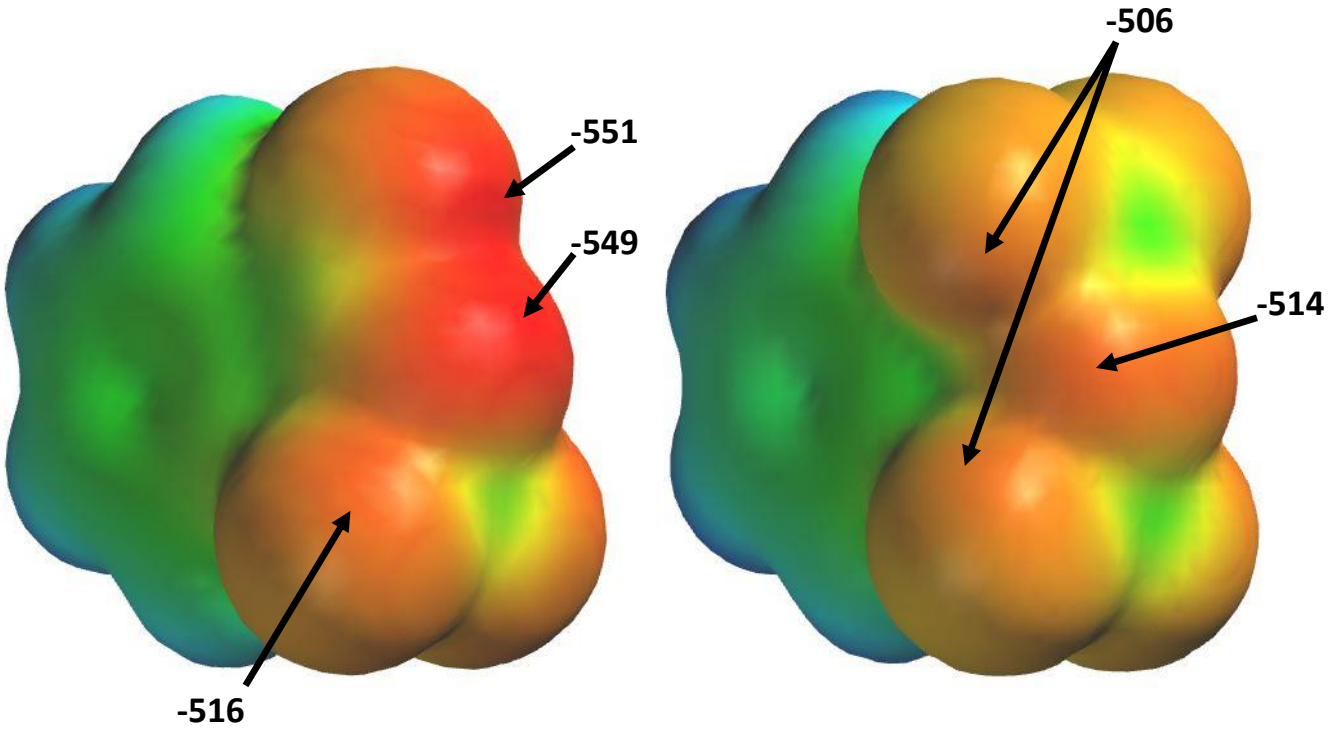


Differential Scanning Calorimetry

Top to Bottom: **13**, **14**.



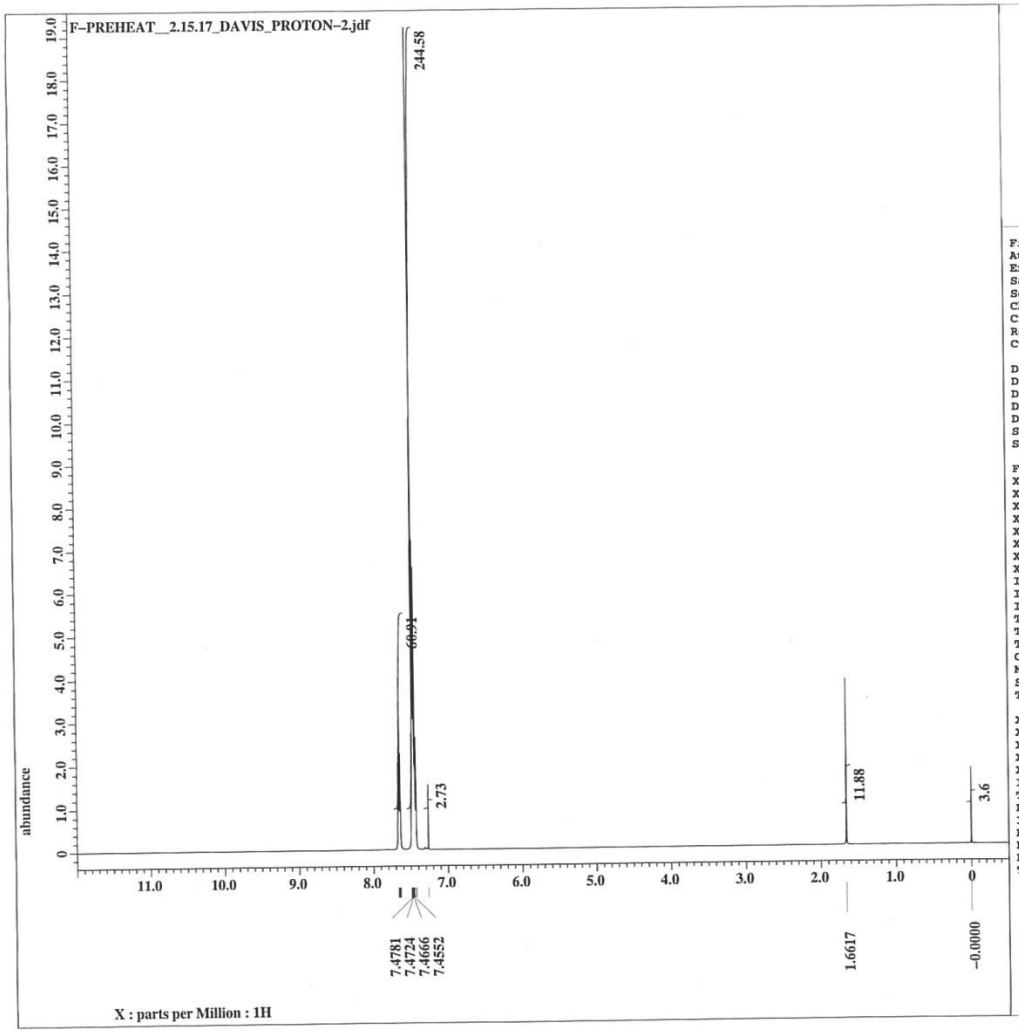
Computational Outcomes



Electrostatic potential energy surface plots for Sac^- (left) and $BDSA^-$ (right) generated by Spartan'08 [computational model: B3LYP/6-311+G(d,p)].

Color range: -551(red) to -102 (blue) kJ/mol. Selected local extrema are indicated. For Sac^-, the most negative site is associated with the carbonyl oxygen at -551 kJ/mol, followed closely by a site near the imidate N at -549 kJ/mol; the regions about the sulfonyl O atoms (orange) are generally not as negative as the imidate N or the carbonyl oxygen (red). The imidate moiety of $BDSA^-$ is comparatively less negative than its counterpart in Sac^-; the most negative site on Sac^- is near the imidate N at -514 kJ/mol.

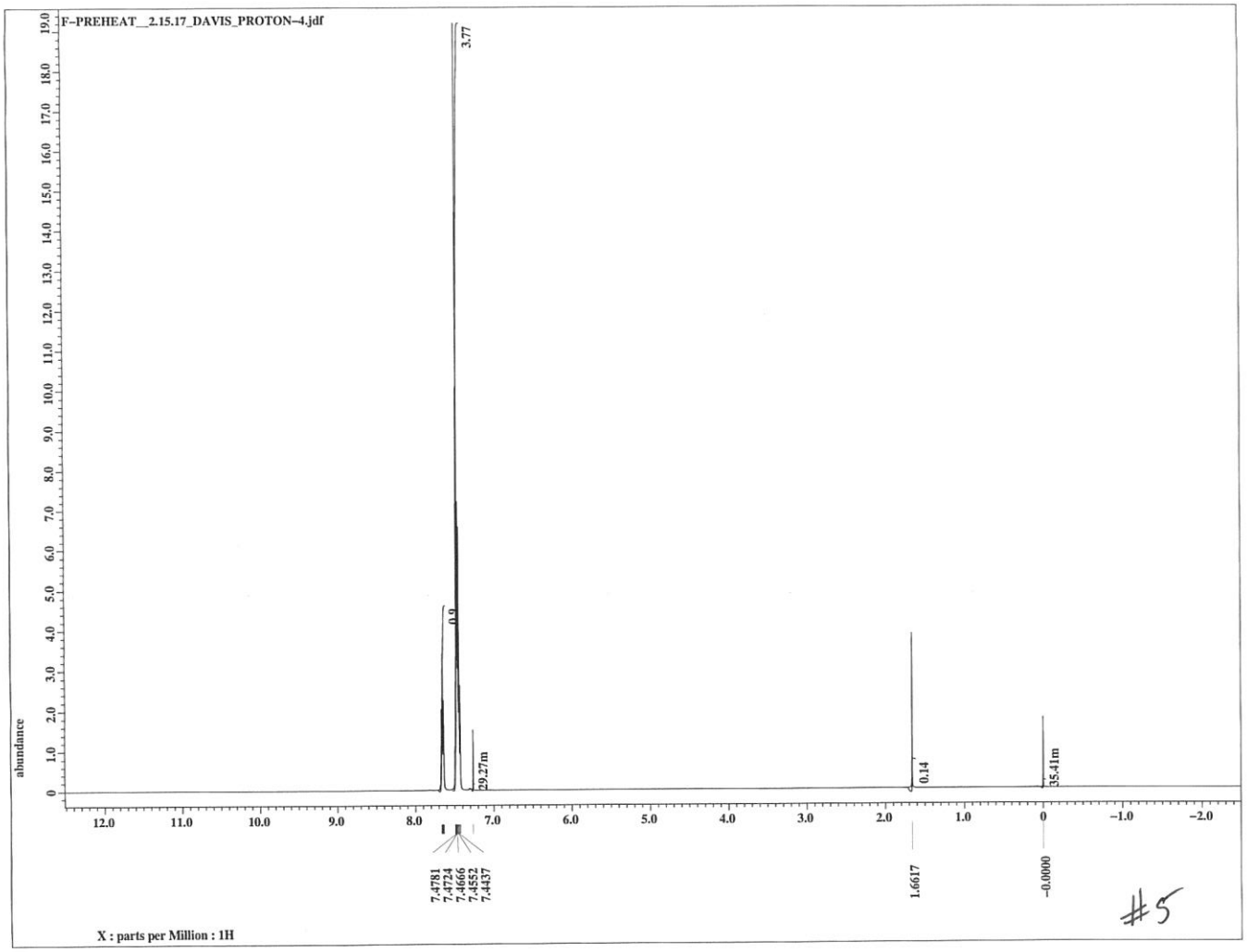
A.D. Becke, J. Chem. Phys. 98 (1993) 5648-5652;
C. Lee, W. Yang, R.G. Parr, Phys. Rev. B 37 (1988) 785-789;
S.H. Vosko, L. Wilk, M. Nusair, Can. J. Phys. 58 (1980) 1200-1211;
P.J. Stephens, F.J. Devlin, C.F. Chabalowski, M.J. Frisch, J. Phys. Chem. 98 (1994) 11623-11627.

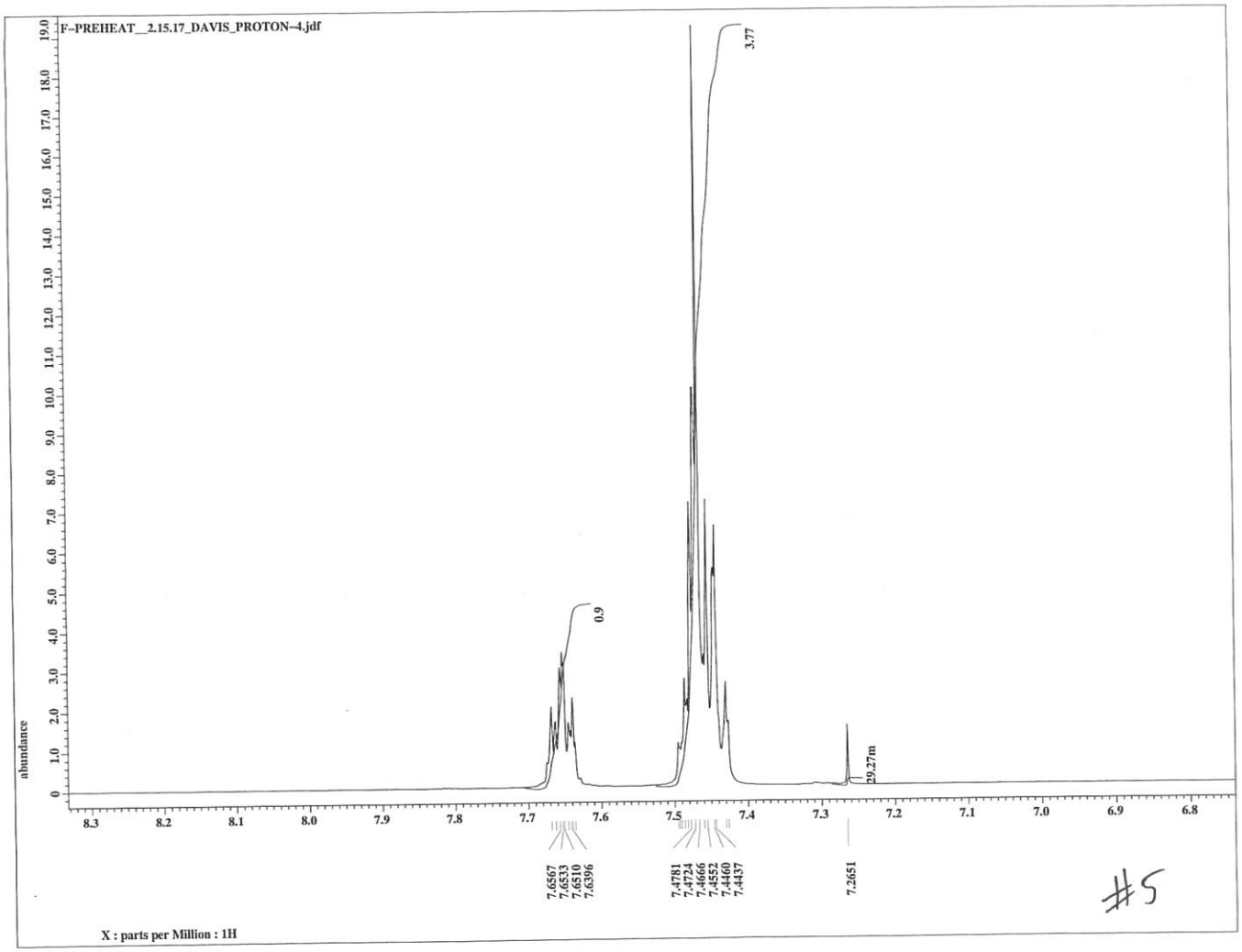


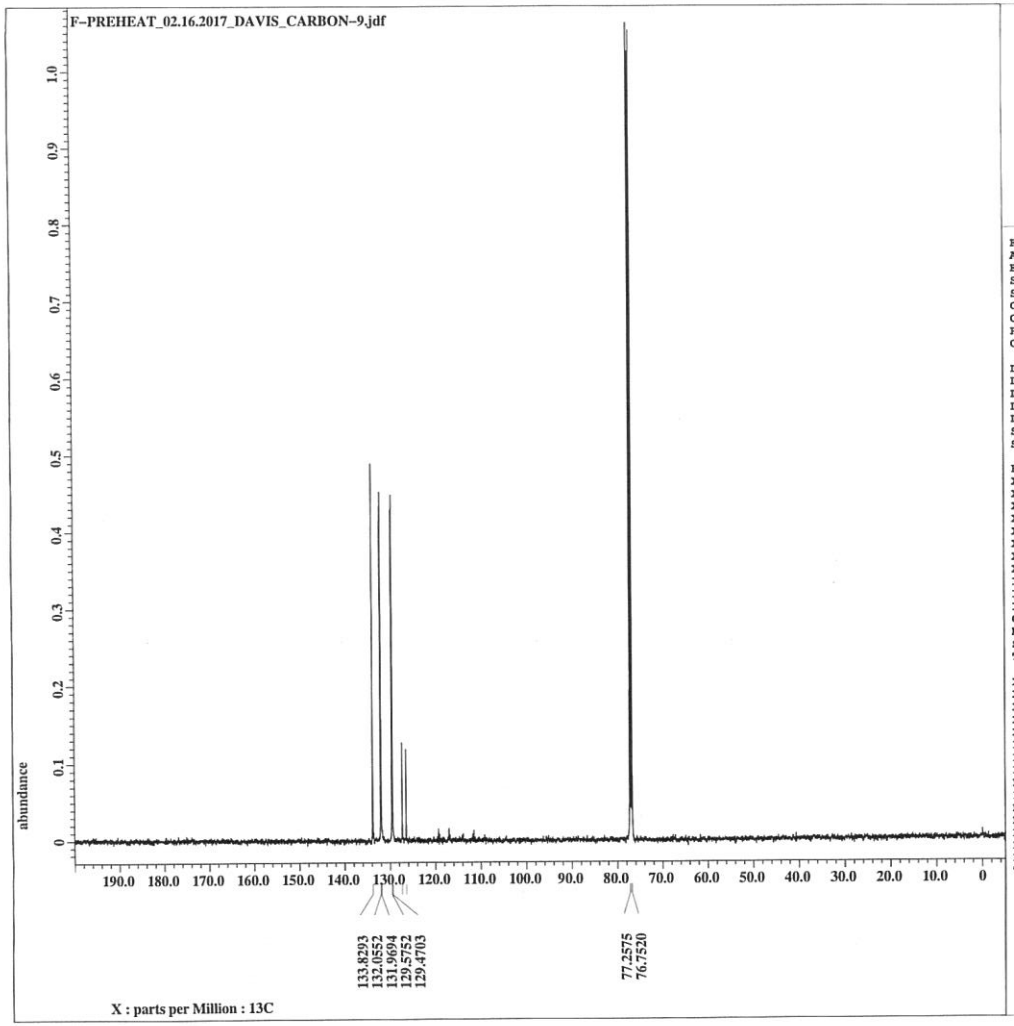
SOUTH ALABAMA JAGUARS

Filename	= F-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= F-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 22
Creation_time	= 15-FEB-2017 17:38:25
Revision_time	= 15-FEB-2017 17:22:08
Current_time	= 15-FEB-2017 17:22:08
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	= 13.07[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.535[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	= 20.9[dC]

PPN BETI,
IL#5


F-PREHEAT__2.15.17_DAVIS_PROTON-4.jdf
abundance
3.77
0.9
29.27m
0.14
35.41m
7.4781
7.4724
7.4666
7.4552
7.4437
1.6617
-0.0000
#5
X : parts per Million : 1H

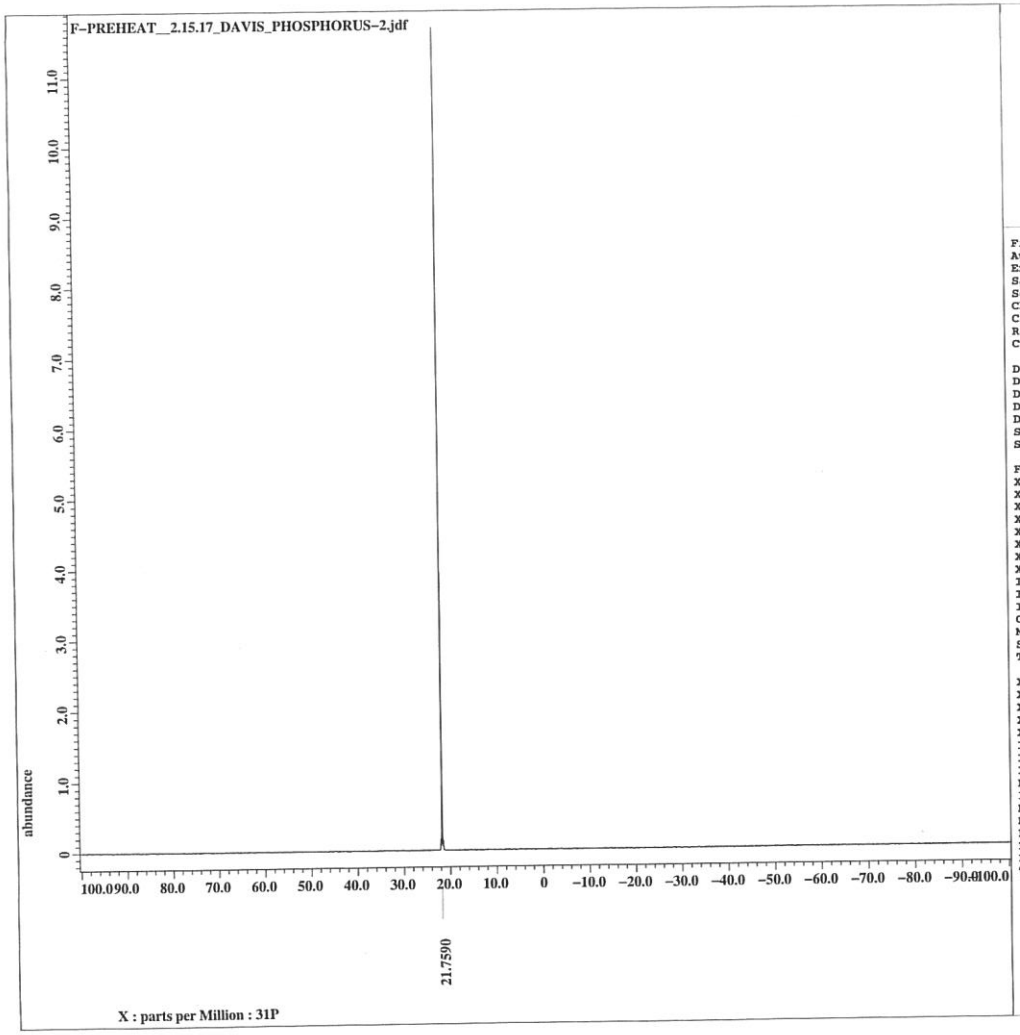

F-PREHEAT__2.15.17_DAVIS_PROTON-4.jdf
abundance
3.77
0.9
29.27m
7.6567
7.6533
7.6510
7.6396
7.4781
7.4724
7.4666
7.4552
7.4460
7.4437
7.2651
#5
X : parts per Million : 1H



SOUTH ALABAMA JAGUARS

Filename	= F-PREHEAT_02.16.2017_
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= F-PREHEAT_02.16.2017_
Solvent	= CHLOROFORM-D
Changer_sample	= 22
Creation_time	= 16-FEB-2017 15:29:04
Revision_time	= 16-FEB-2017 15:12:51
Current_time	= 16-FEB-2017 15:12:51
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 1024
Total_scans	= 1024
X_90_width	= 12.7[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.23333333[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	= 21.1[dC]

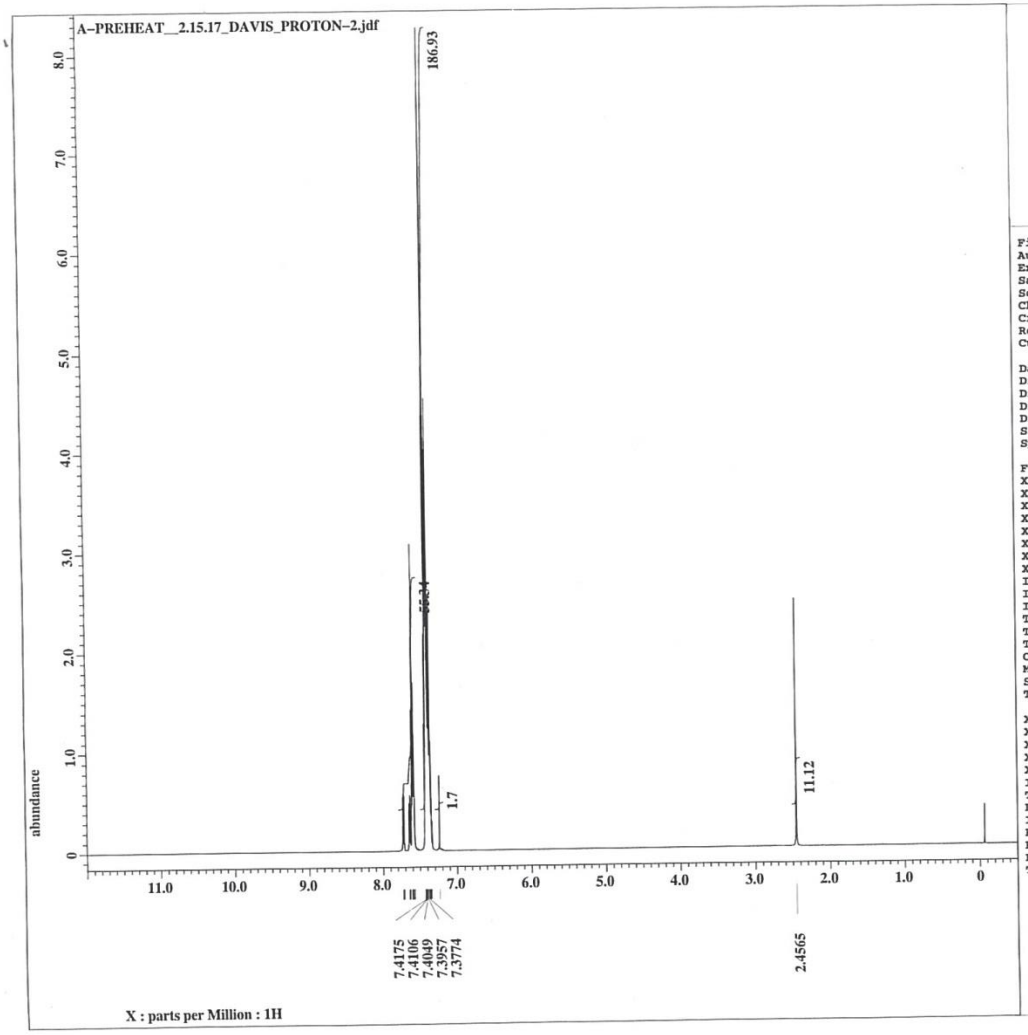
#5



SOUTH ALABAMA JAGUARS

Filename	= F-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= F-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 22
Creation_time	= 15-FEB-2017 19:16:50
Revision_time	= 15-FEB-2017 19:00:33
Current_time	= 15-FEB-2017 19:00:33
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	= 14.687[us]
X_acq_time	= 0.64487424[s]
X_angle	= 30[deg]
X_atn	= 5[dB]
X_pulse	= 4.89566667[us]
Irr_atn_dec	= 20.5[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	= 21.3[dC]

#5

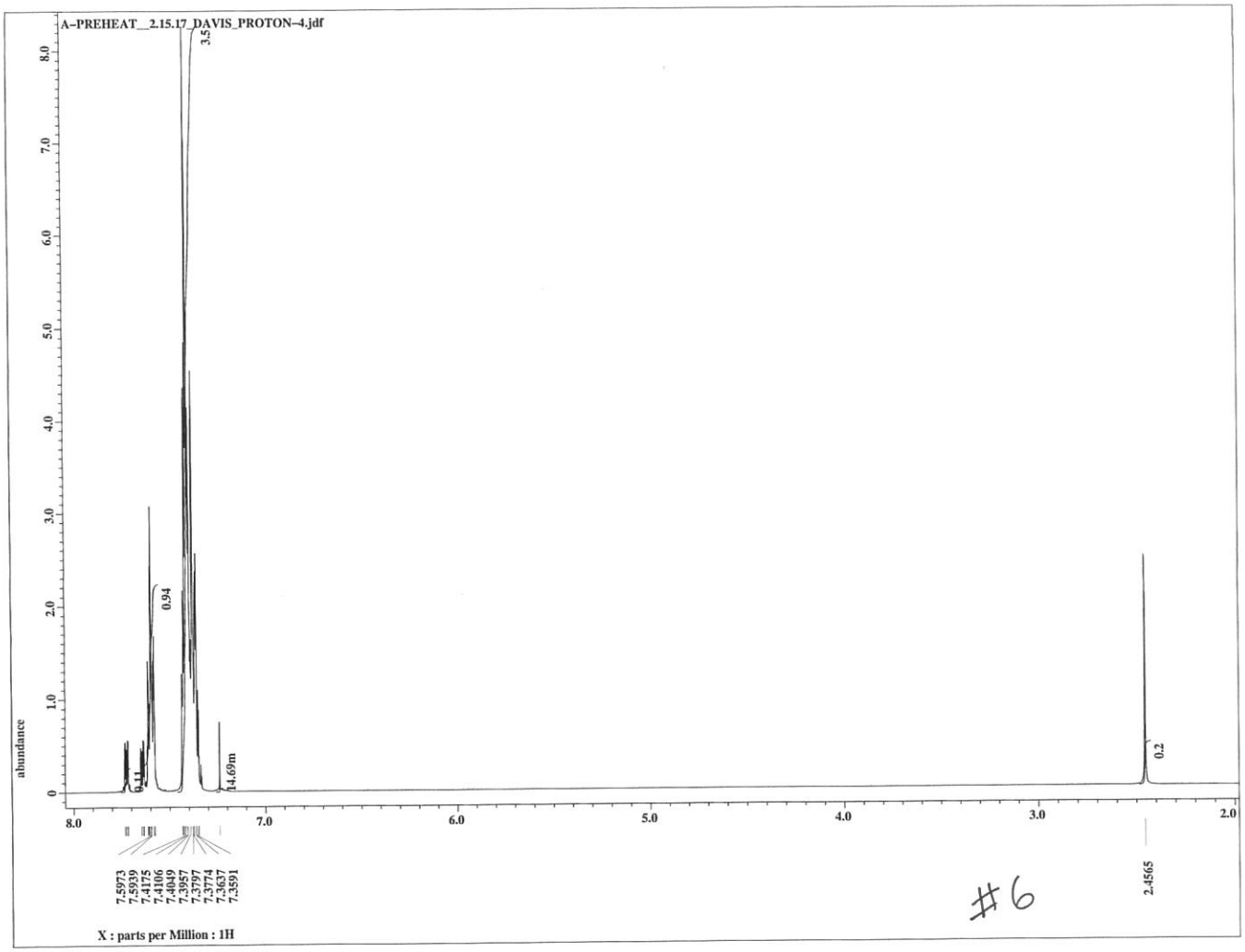


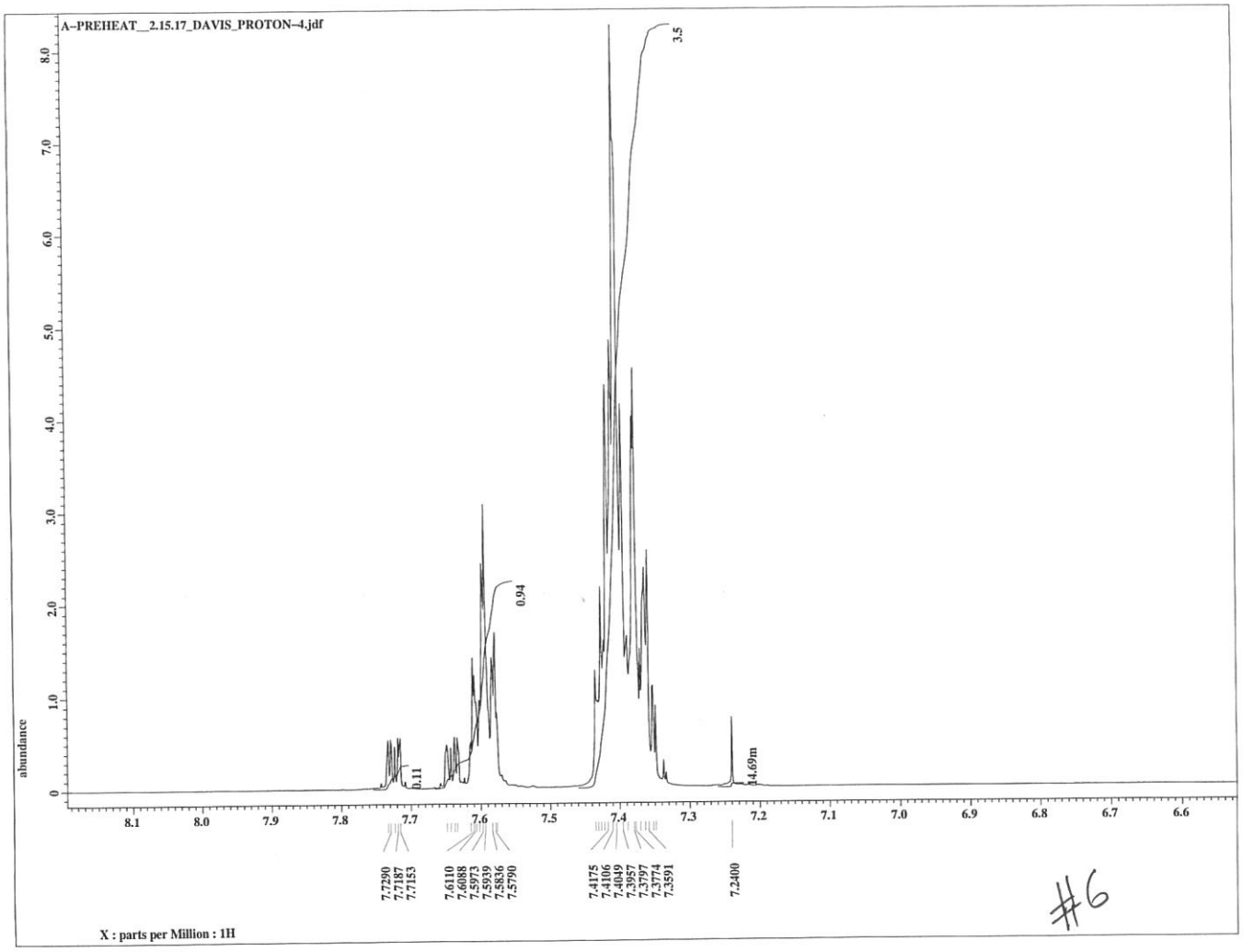
SOUTH ALABAMA JAGUARS

Filename	= A-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= A-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 17
Creation_time	= 15-FEB-2017 17:07:25
Revision_time	= 15-FEB-2017 16:51:08
Current_time	= 15-FEB-2017 16:51:08
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	= 13.07[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.535[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	= 21[dC]

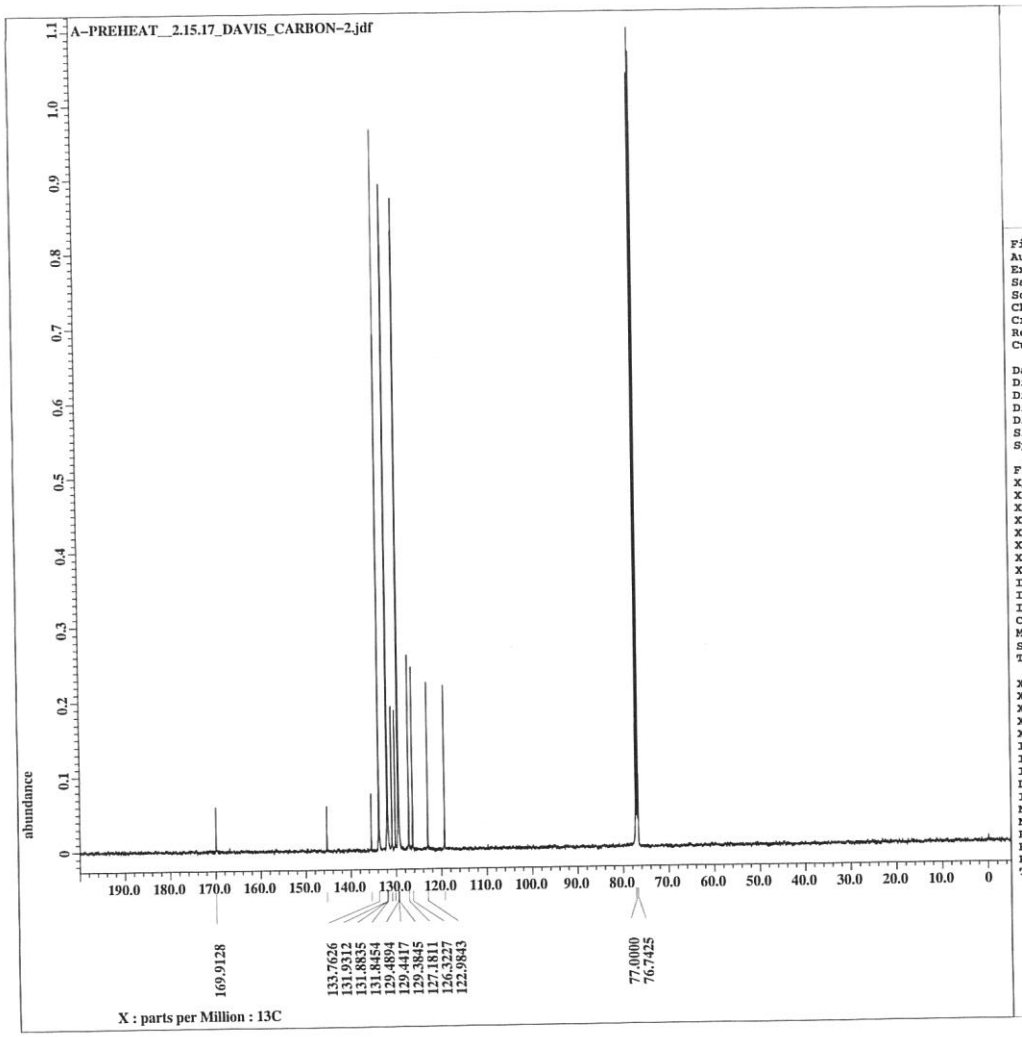
PPN SAC)

IL #6


A-PREHEAT__2.15.17_DAVIS_PROTON-4.jdf
abundance
3.5
0.94
0.11
4.69m
0.2
2.4565
7.5973
7.5929
7.4175
7.4106
7.4049
7.3957
7.3797
7.3774
7.3637
7.3591
X : parts per Million : 1H
#6

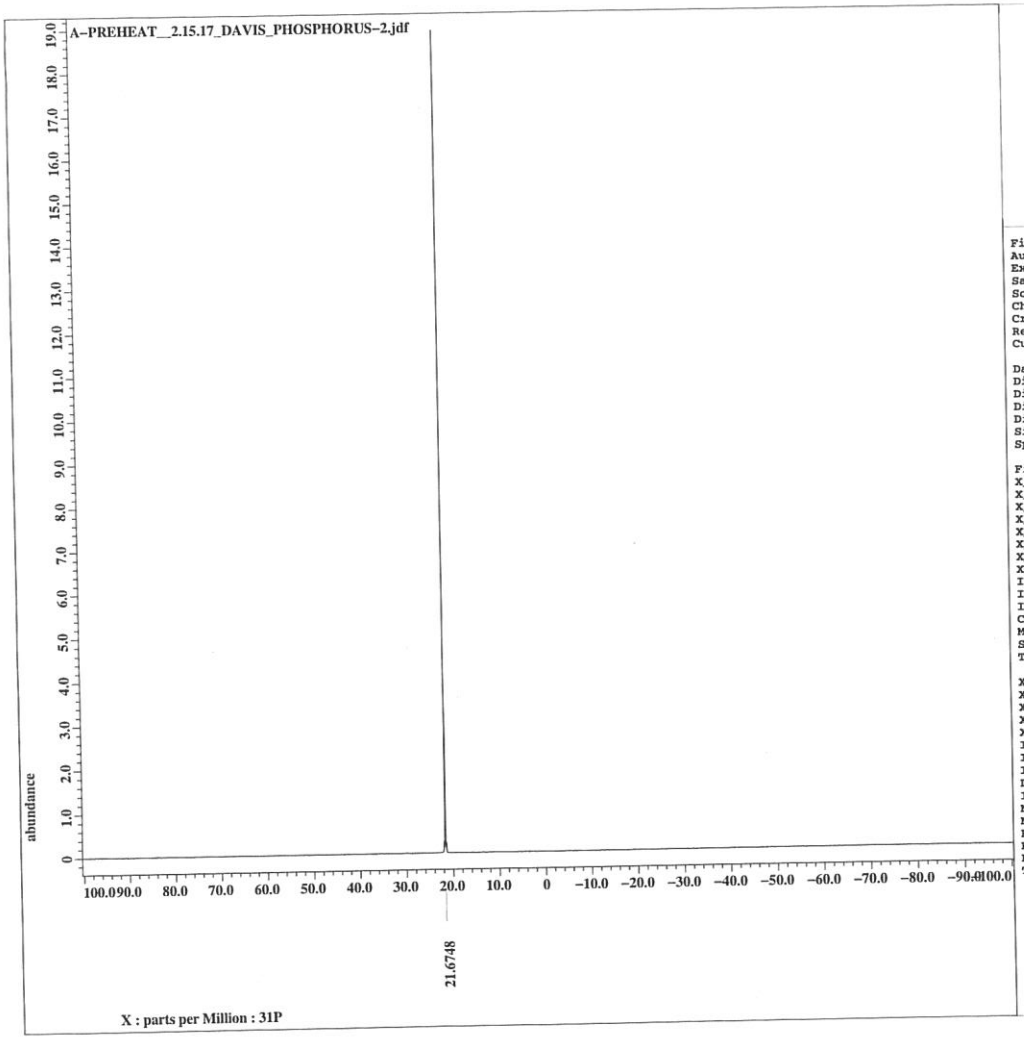

A-PREHEAT__2.15.17_DAVIS_PROTON-4.jdf
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
3.5
0.94
0.11
4.69m
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
7.7290
7.7187
7.7153
7.6110
7.6088
7.5973
7.5939
7.5836
7.5790
7.4175
7.4106
7.4049
7.3957
7.3797
7.3774
7.3591
7.2400
X : parts per Million : 1H

#6



Filename	= A-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= A-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 17
Creation_time	= 15-FEB-2017 20:57:59
Revision_time	= 15-FEB-2017 20:41:40
Current_time	= 15-FEB-2017 20:41:42
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	= 2000
Total_scans	= 2000
X_90_width	= 12.7[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.23333333[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	= 21.1[dC]

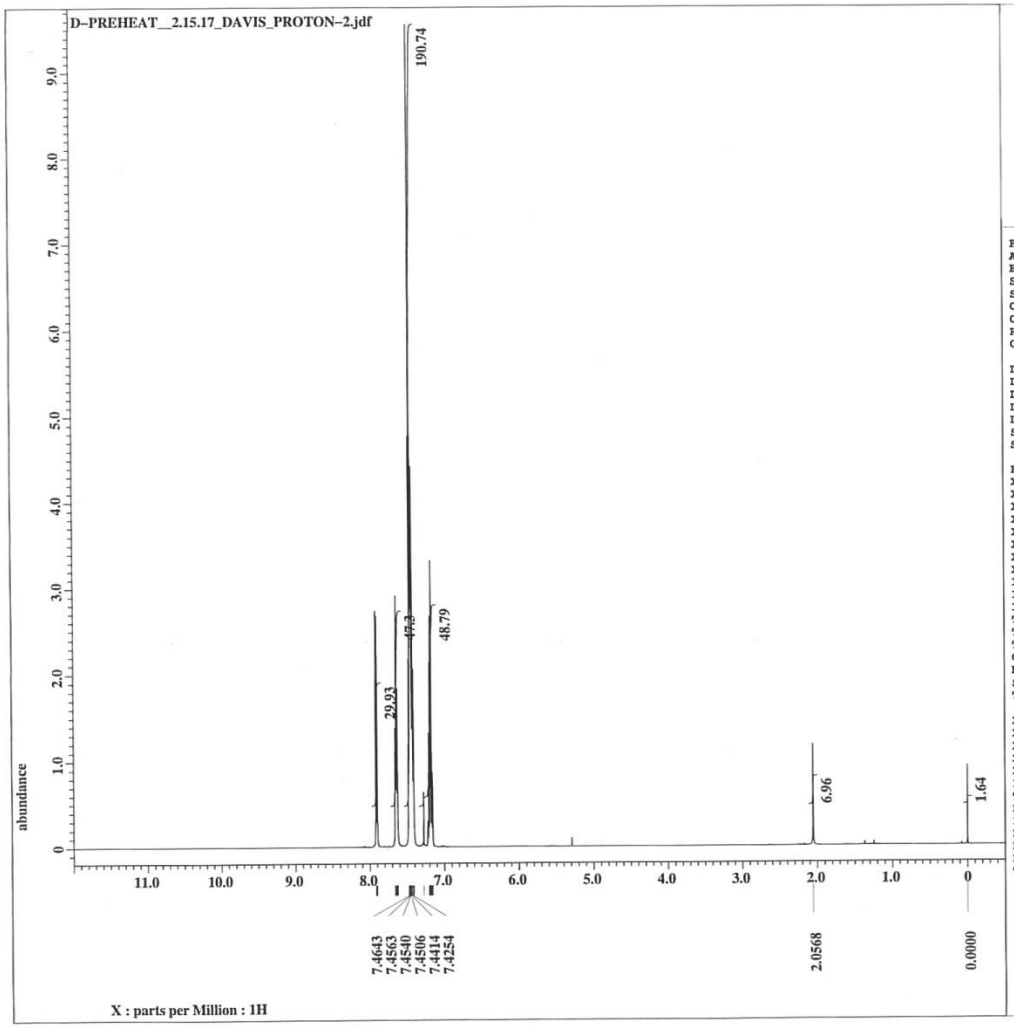
#6



SOUTH ALABAMA JAGUARS

Filename	= A-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= A-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 17
Creation_time	= 15-FEB-2017 17:56:22
Revision_time	= 15-FEB-2017 17:40:05
Current_time	= 15-FEB-2017 17:40:05
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	= 14.687[us]
X_acq_time	= 0.64487424[s]
X_angle	= 30[deg]
X_atn	= 5[dB]
X_pulse	= 4.89566667[us]
Irr_atn_dec	= 20.5[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	= 21.4[dC]

#6

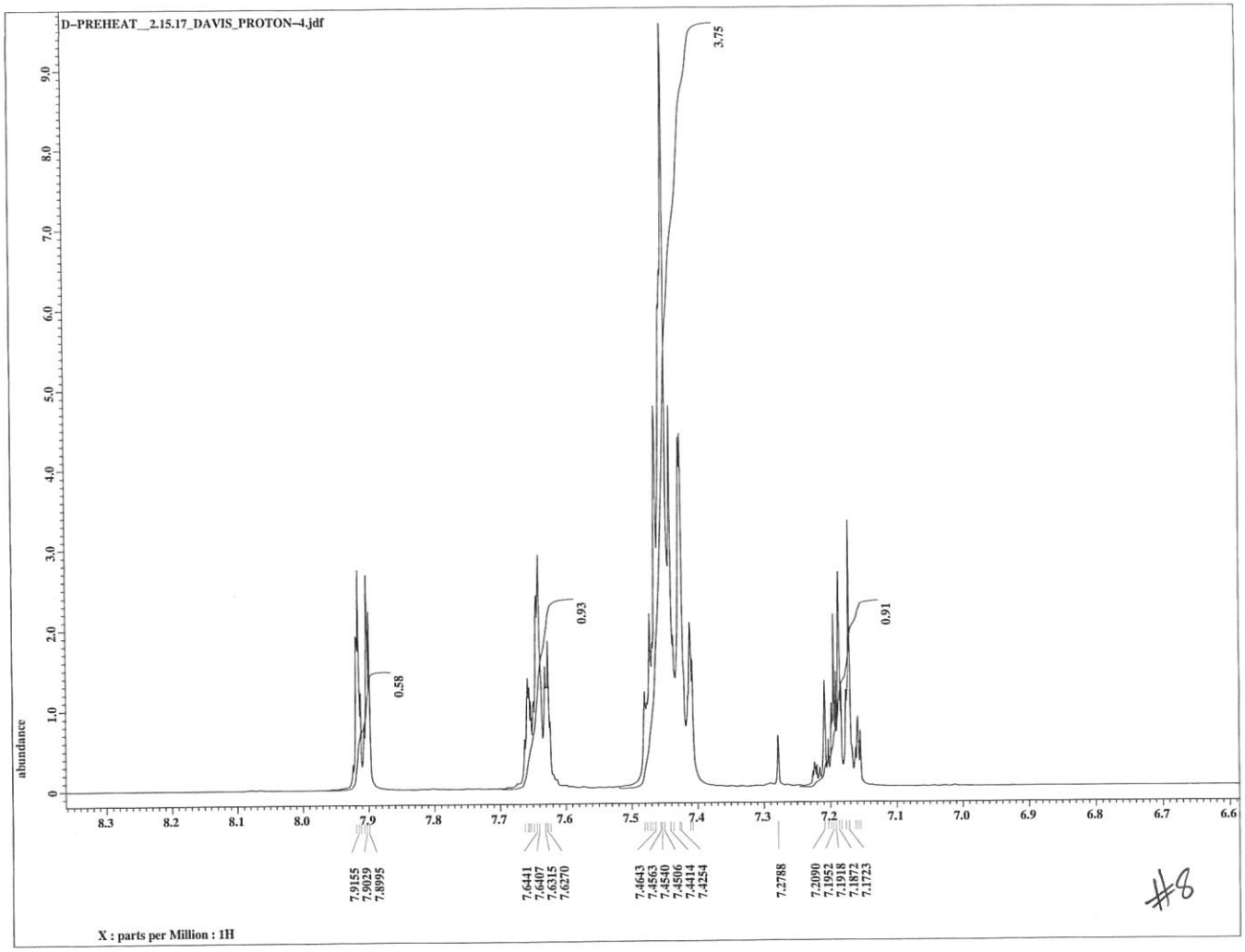


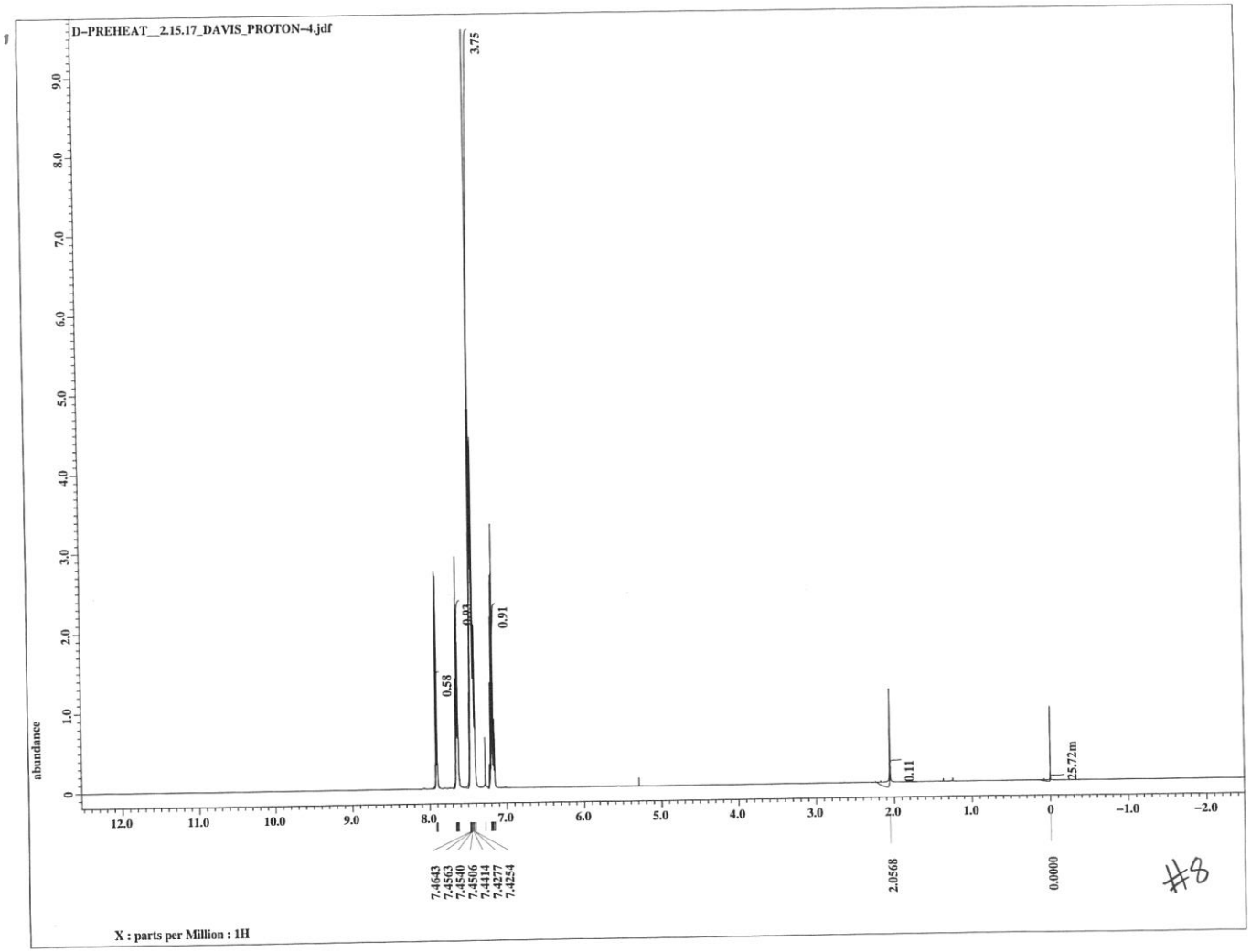
SOUTH ALABAMA JAGUARS

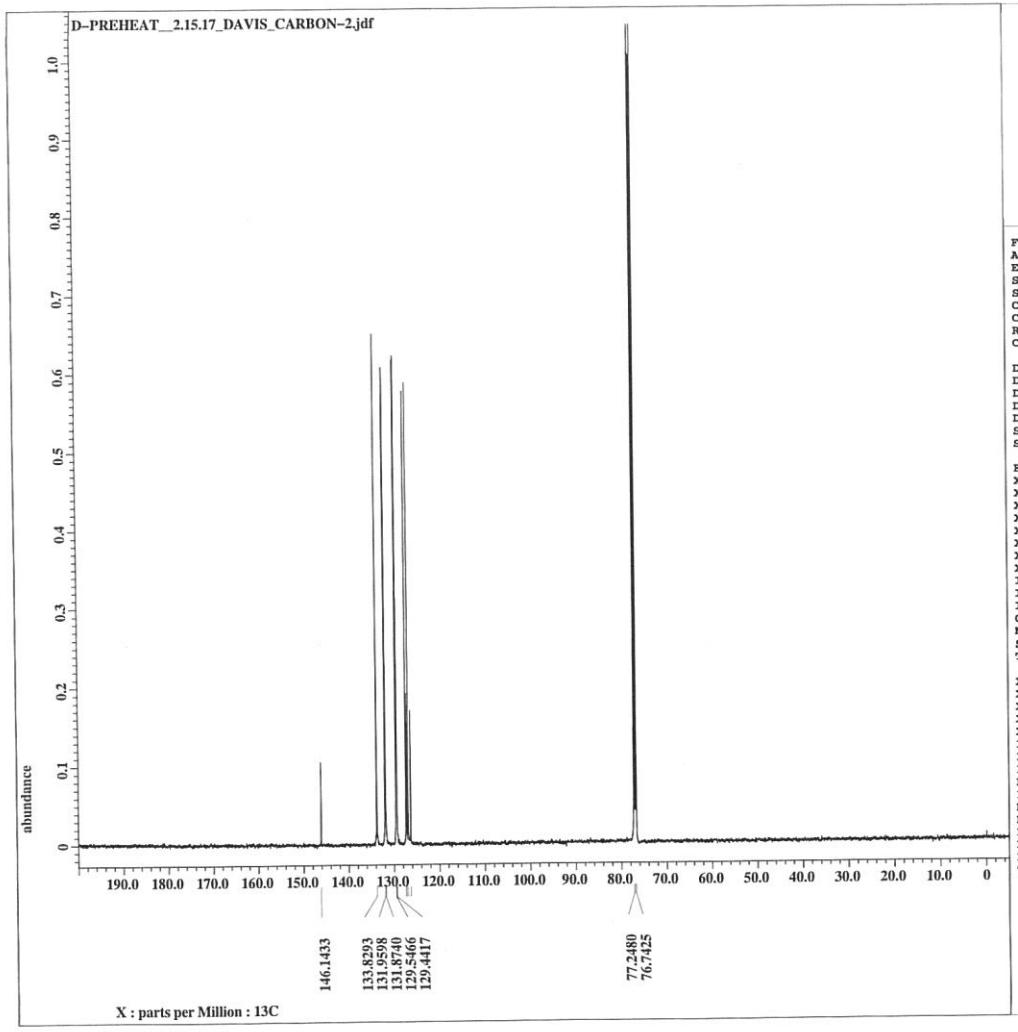
Filename	= D-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= D-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 20
Creation_time	= 15-FEB-2017 17:25:56
Revision_time	= 15-FEB-2017 17:09:39
Current_time	= 15-FEB-2017 17:09:39
Data_format	= 1D COMPLEX
Dim_size	= 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	= 13.07[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.535[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	= 20.9[dC]

PPN $\phi\text{-}SO_2\text{-}\overset{\ominus}{N}\text{-}SO_2\text{-}\phi$

IL #8


D-PREHEAT__2.15.17_DAVIS_PROTON-4.jdf
abundance
3.75
0.93
0.91
0.58
7.9155
7.9029
7.8995
7.6441
7.6407
7.6315
7.6270
7.4643
7.4563
7.4540
7.4506
7.4414
7.4254
7.2788
7.2090
7.1952
7.1918
7.1872
7.1723
X : parts per Million : 1H
#8

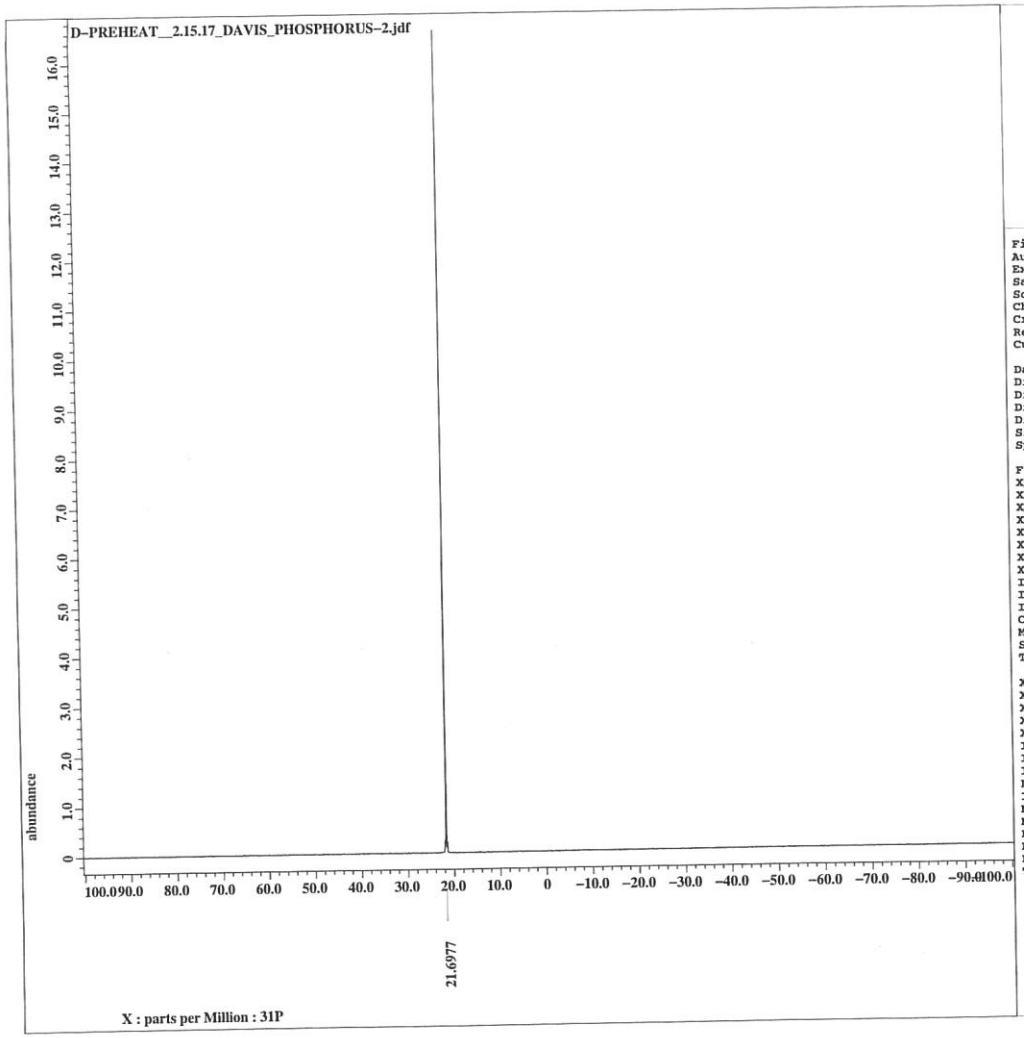

D-PREHEAT__2.15.17_DAVIS_PROTON-4.jdf
abundance
3.75
0.58
0.93
0.91
0.11
25.72m
7.4643
7.4563
7.4540
7.4506
7.4414
7.4277
7.4254
2.0568
0.0000
#8
X : parts per Million : 1H



SOUTH ALABAMA JAGUARS

Filename	= D-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= D-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 20
Creation_time	= 16-FEB-2017 01:54:34
Revision_time	= 16-FEB-2017 01:38:16
Current_time	= 16-FEB-2017 01:38:16
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	= 2000
Total_scans	= 2000
X_90_width	= 12.7[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.23333333[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	= 20.9[dC]

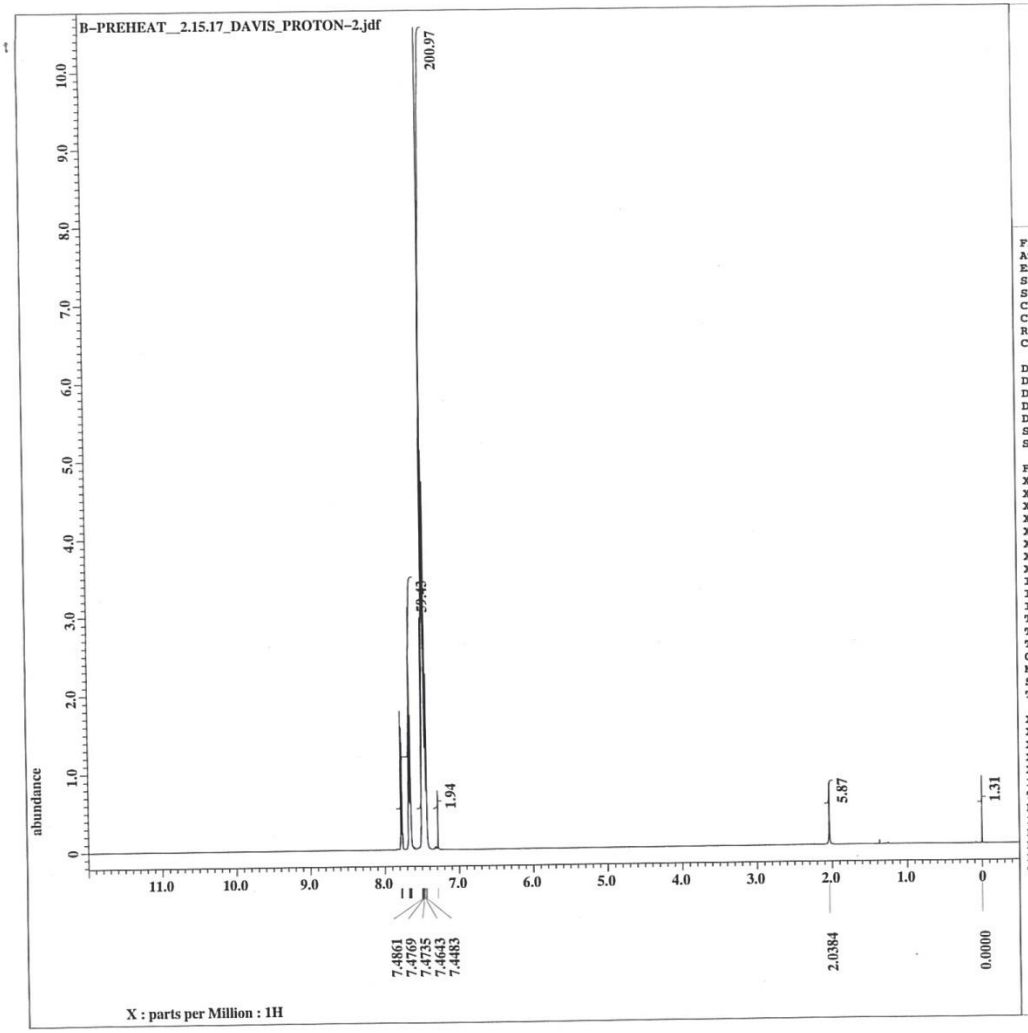
#8



SOUTH ALABAMA JAGUARS

Filename	= D-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= D-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 20
Creation_time	= 15-FEB-2017 18:45:12
Revision_time	= 15-FEB-2017 18:28:55
Current_time	= 15-FEB-2017 18:28:55
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	= 14.687[us]
X_acq_time	= 0.64487424[s]
X_angle	= 30[deg]
X_atn	= 5[dB]
X_pulse	= 4.89566667[us]
Irr_atn_dec	= 20.5[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	= 21.3[dC]

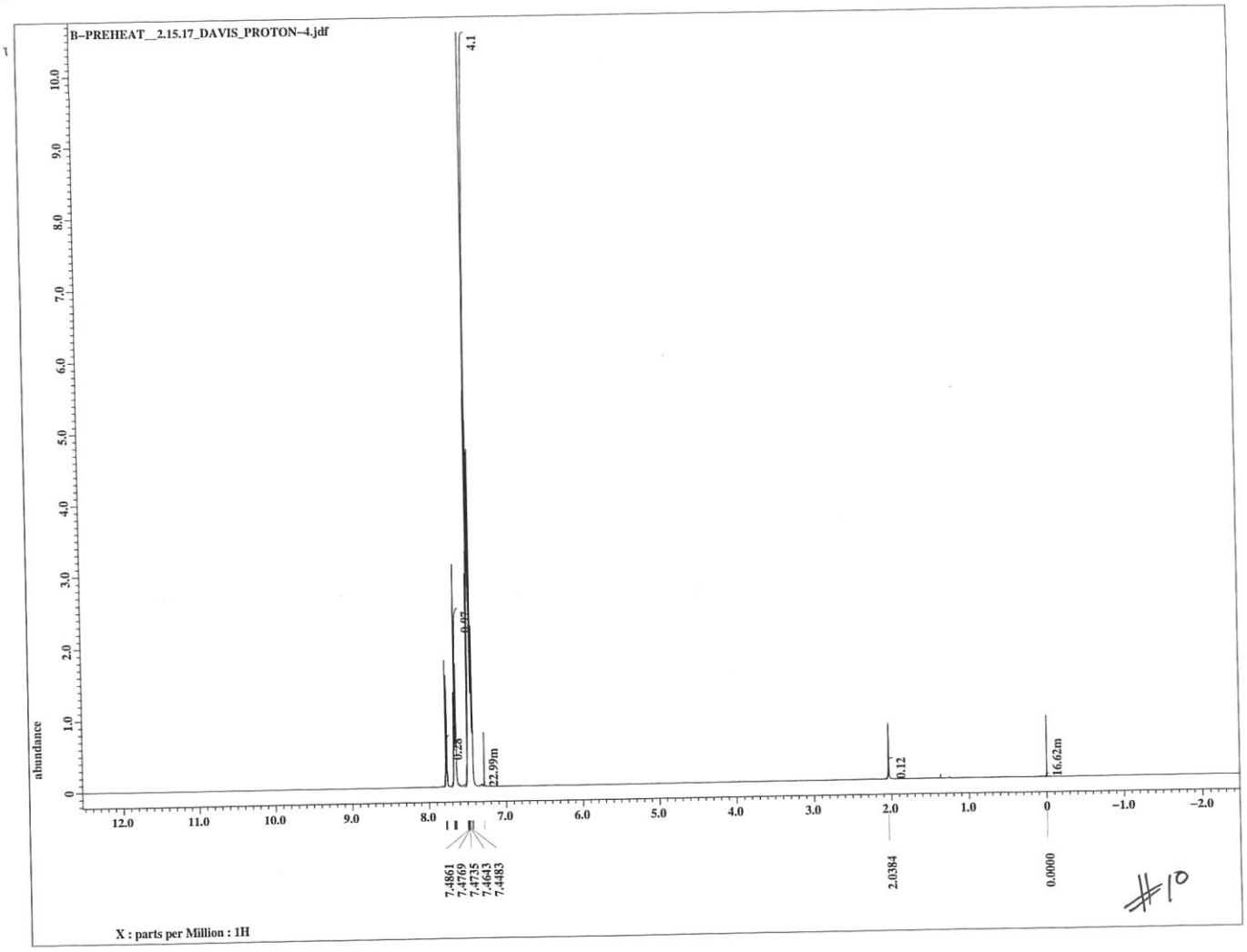
#8



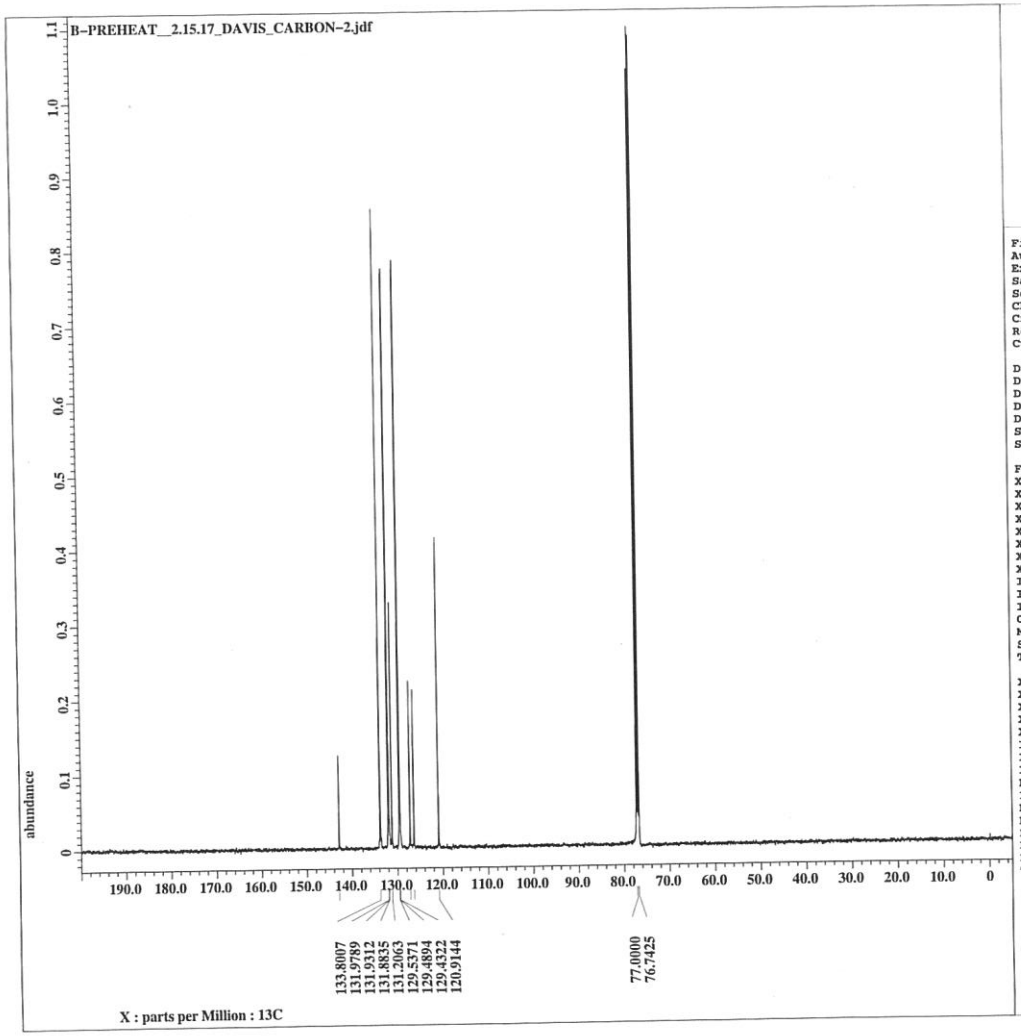
SOUTH ALABAMA JAGUARS

Filename	= B-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= B-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 18
Creation_time	= 15-FEB-2017 17:13:37
Revision_time	= 15-FEB-2017 16:57:20
Current_time	= 15-FEB-2017 16:57:20
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	= 13.07[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.535[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	= 20.9[dC]

PPN BDSA, IL#10

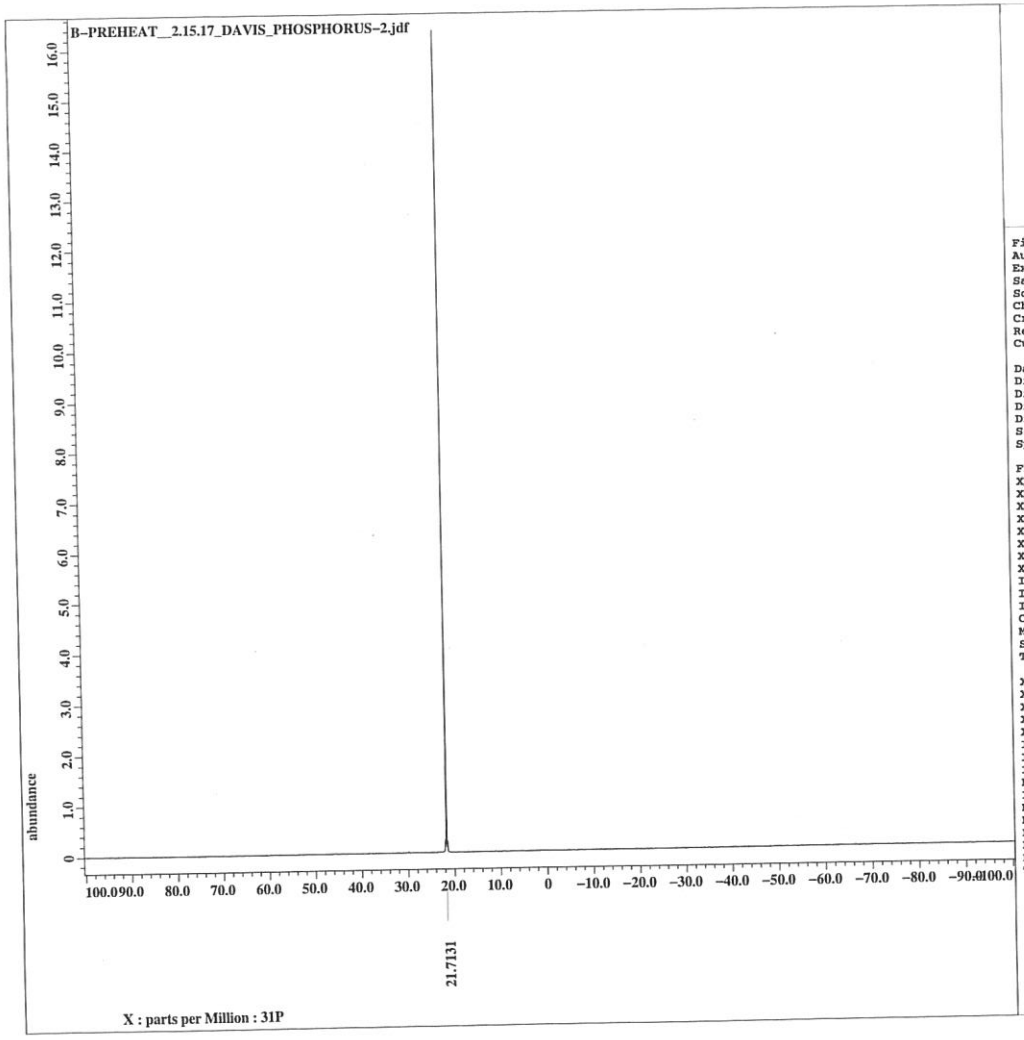

B--PREHEAT__2.15.17_DAVIS_PROTON--4.jdf
abundance
4.1
0.26
0.92
22.99m
0.12
16.62m
7.4861
7.4769
7.4735
7.4643
7.4483
2.0384
0.0000
X : parts per Million : 1H

#10



Filename	= B-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= B-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 18
Creation_time	= 15-FEB-2017 22:36:56
Revision_time	= 15-FEB-2017 22:20:38
Current_time	= 15-FEB-2017 22:20:38
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	= 2000
Total_scans	= 2000
X_90_width	= 12.7[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.23333333[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	= 20.9[dC]

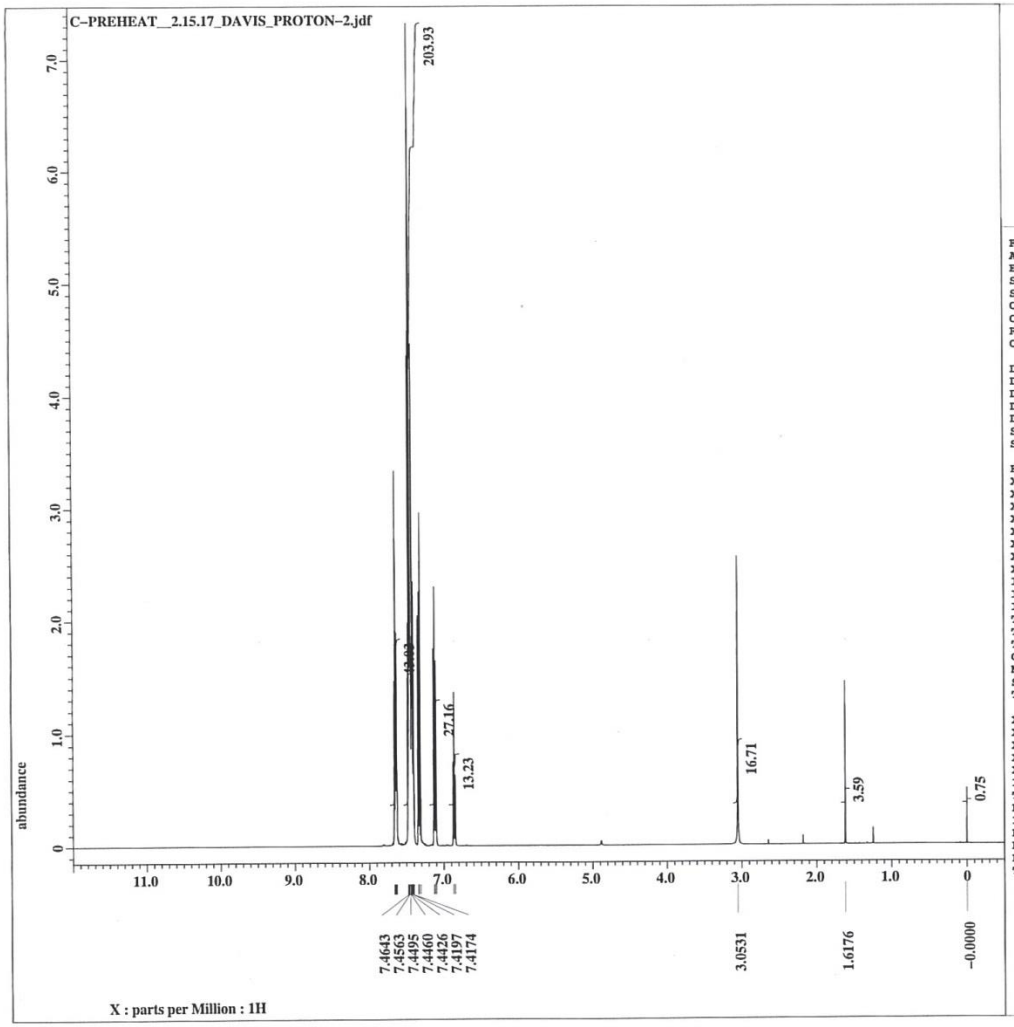
#10



SOUTH ALABAMA JAGUARS

Filename	= B-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= B-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 18
Creation_time	= 15-FEB-2017 18:13:44
Revision_time	= 15-FEB-2017 17:57:27
Current_time	= 15-FEB-2017 17:57:27
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	= 14.687[us]
X_acq_time	= 0.64487424[s]
X_angle	= 30[deg]
X_atn	= 5[dB]
X_pulse	= 4.89566667[us]
Irr_atn_dec	= 20.5[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	= 21.4[dC]

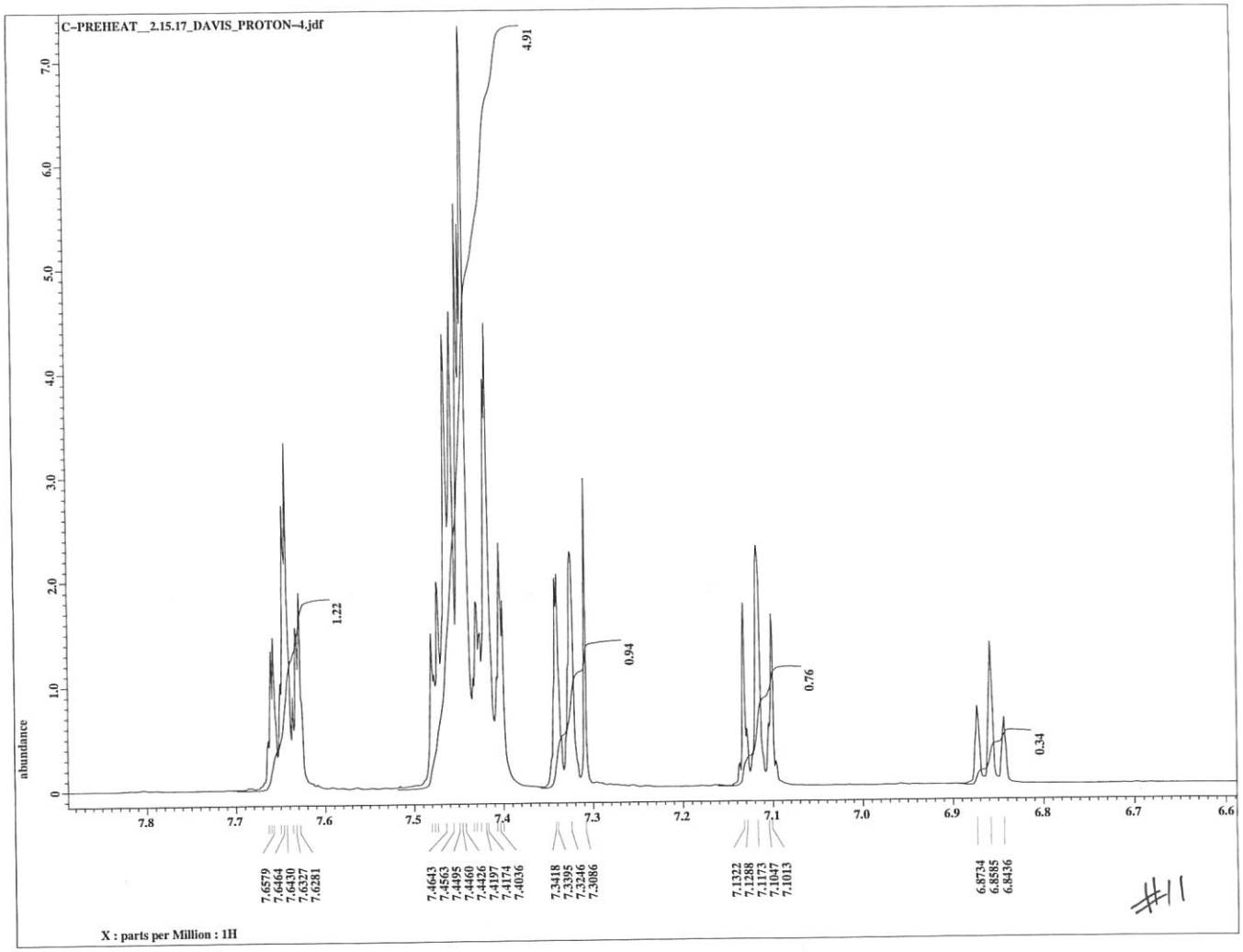
#10

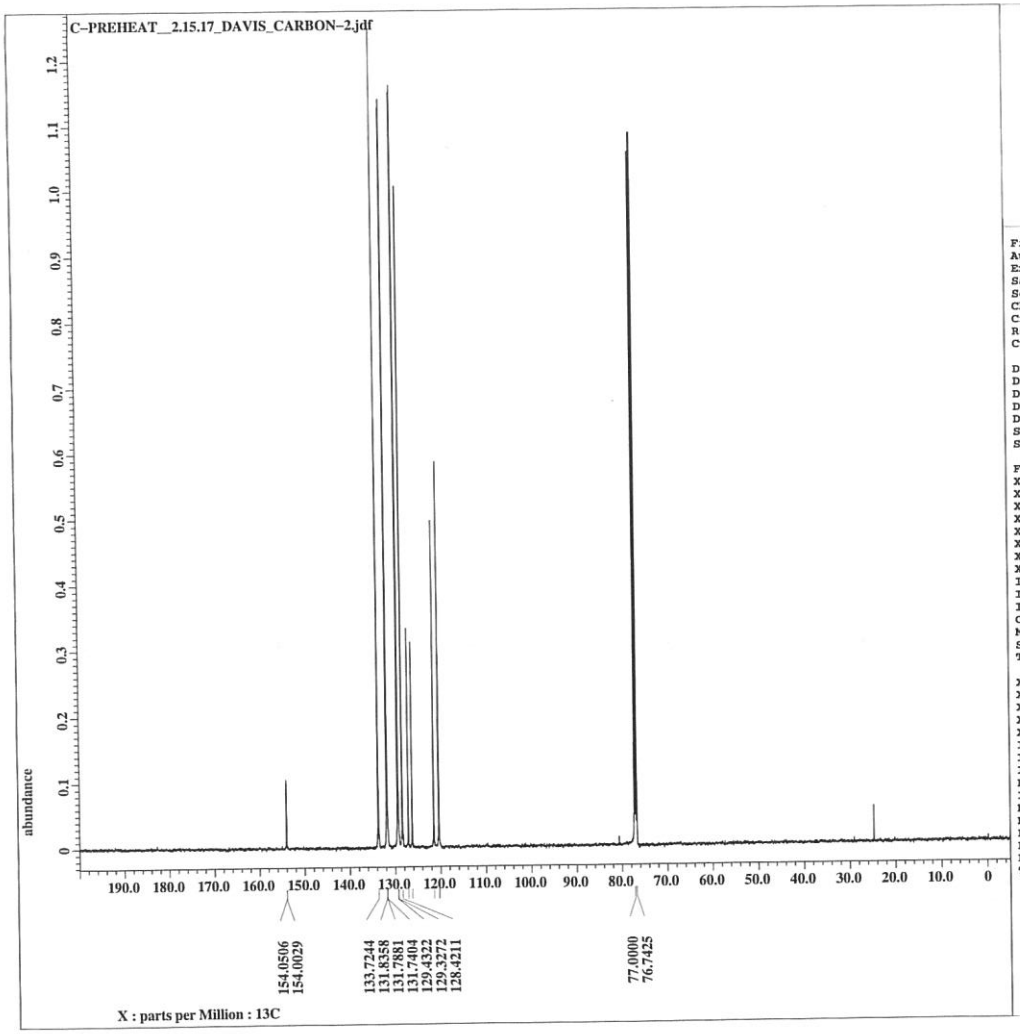


SOUTH ALABAMA JAGUARS

Filename	= C-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= C-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 19
Creation_time	= 15-FEB-2017 17:19:39
Revision_time	= 15-FEB-2017 17:03:22
Current_time	= 15-FEB-2017 17:03:22
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	= 13.07[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.535[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	= 20.9[dC]

PPN $\phi_2PO_2^{\ominus}$, IL# 11

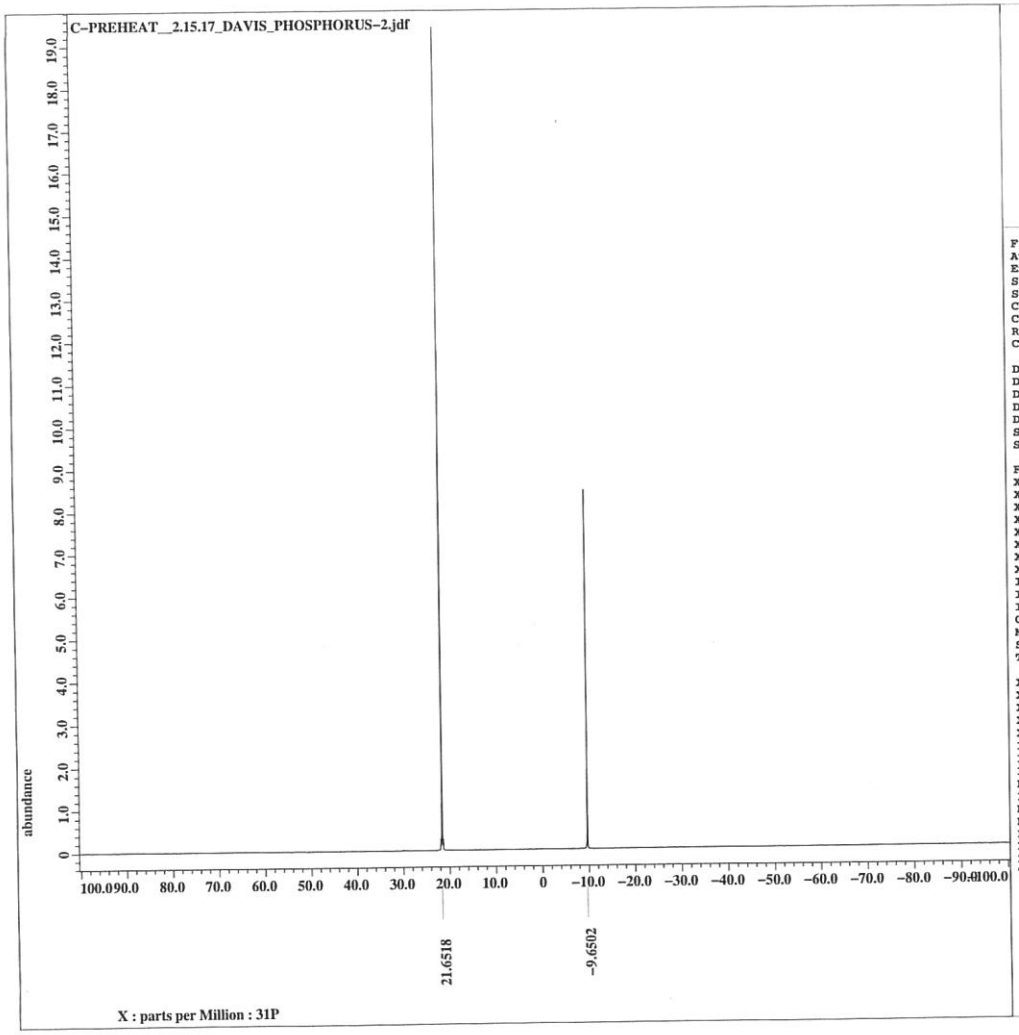

C-PREHEAT__2.15.17_DAVIS_PROTON-4.jdf
abundance
4.91
1.22
0.94
0.76
0.34
7.6579
7.6464
7.6430
7.6327
7.6281
7.4643
7.4563
7.4495
7.4460
7.4426
7.4197
7.4174
7.4036
7.3418
7.3395
7.3246
7.3086
7.1322
7.1288
7.1173
7.1047
7.1013
6.8734
6.8585
6.8436
#11
X : parts per Million : 1H



SOUTH ALABAMA JAGUARS

Filename	= C-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= C-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 19
Creation_time	= 16-FEB-2017 00:15:40
Revision_time	= 15-FEB-2017 23:59:22
Current_time	= 15-FEB-2017 23:59:22
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 2000
Total_scans	= 2000
X_90_width	= 12.7[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.23333333[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	= 21[dC]

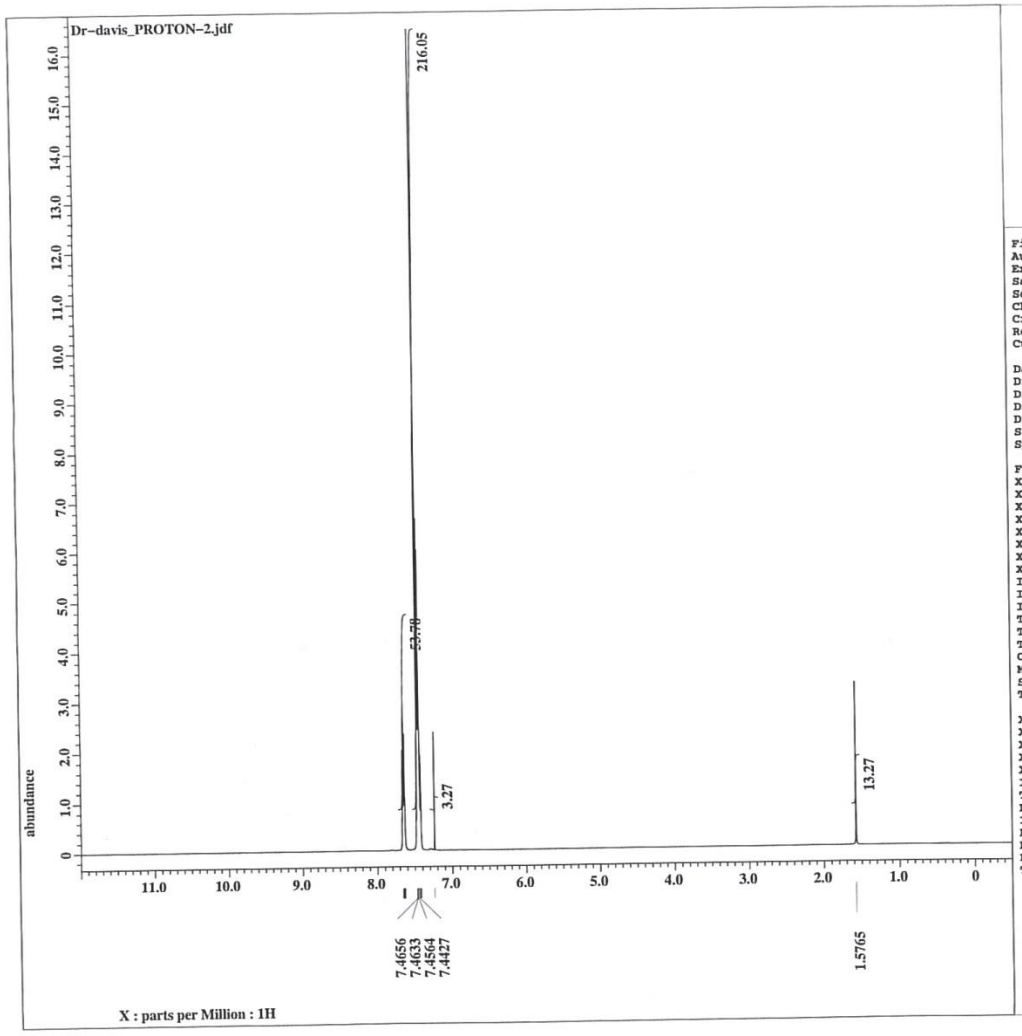
#11



SOUTH ALABAMA JAGUARS

Filename	= C-PREHEAT__2.15.17_DA
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= C-PREHEAT__2.15.17_DA
Solvent	= CHLOROFORM-D
Changer_sample	= 19
Creation_time	= 15-FEB-2017 18:29:20
Revision_time	= 15-FEB-2017 18:13:03
Current_time	= 15-FEB-2017 18:13:03
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	= 14.687[us]
X_acq_time	= 0.64487424[s]
X_angle	= 30[deg]
X_atn	= 5[dB]
X_pulse	= 4.89566667[us]
Irr_atn_dec	= 20.5[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	= 21.4[dC]

#11

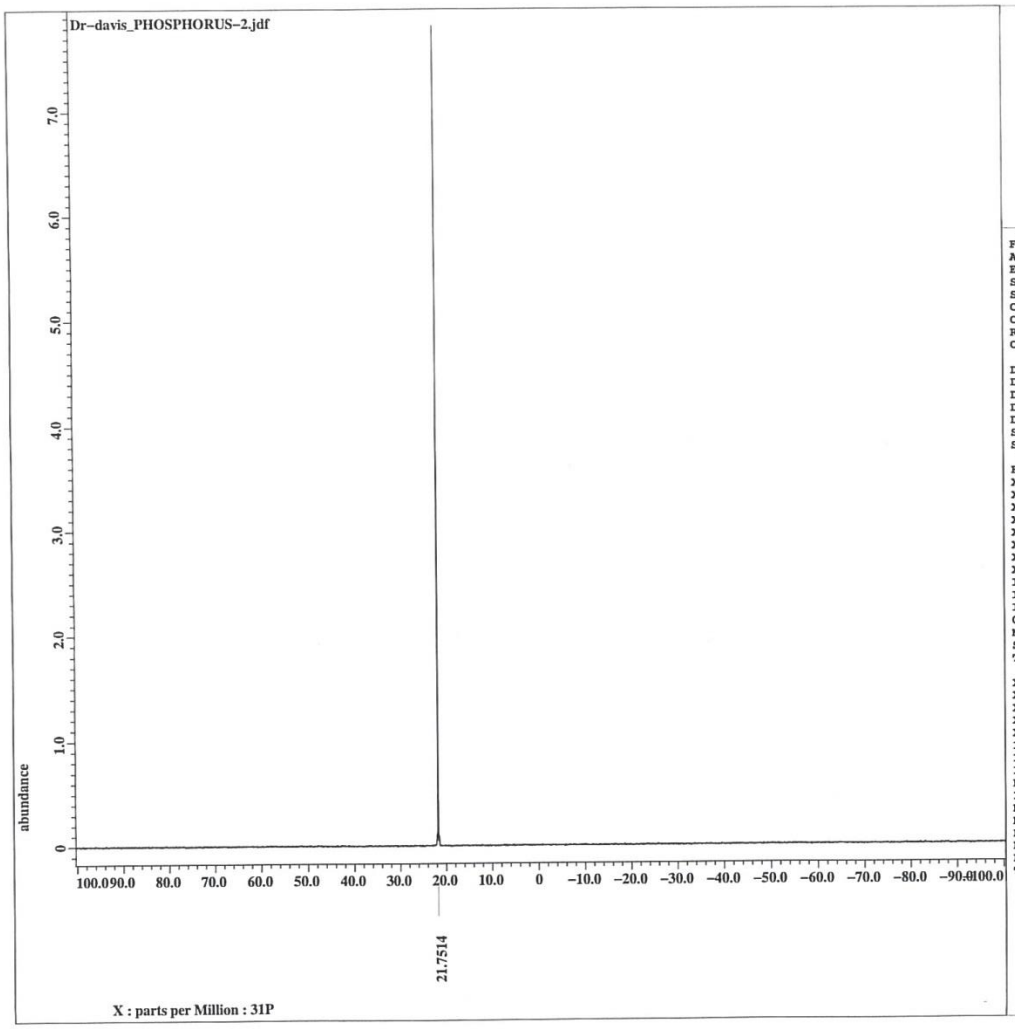


SOUTH ALABAMA JAGUARS

Filename	= Dr-davis_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= Dr-davis
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 22-MAY-2017 11:28:29
Revision_time	= 22-MAY-2017 11:05:52
Current_time	= 22-MAY-2017 11:05:52
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	= 13.07[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.535[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 42
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 21.9[dC]

$PNP^{\oplus}\ B(CN)_4^{\ominus}$

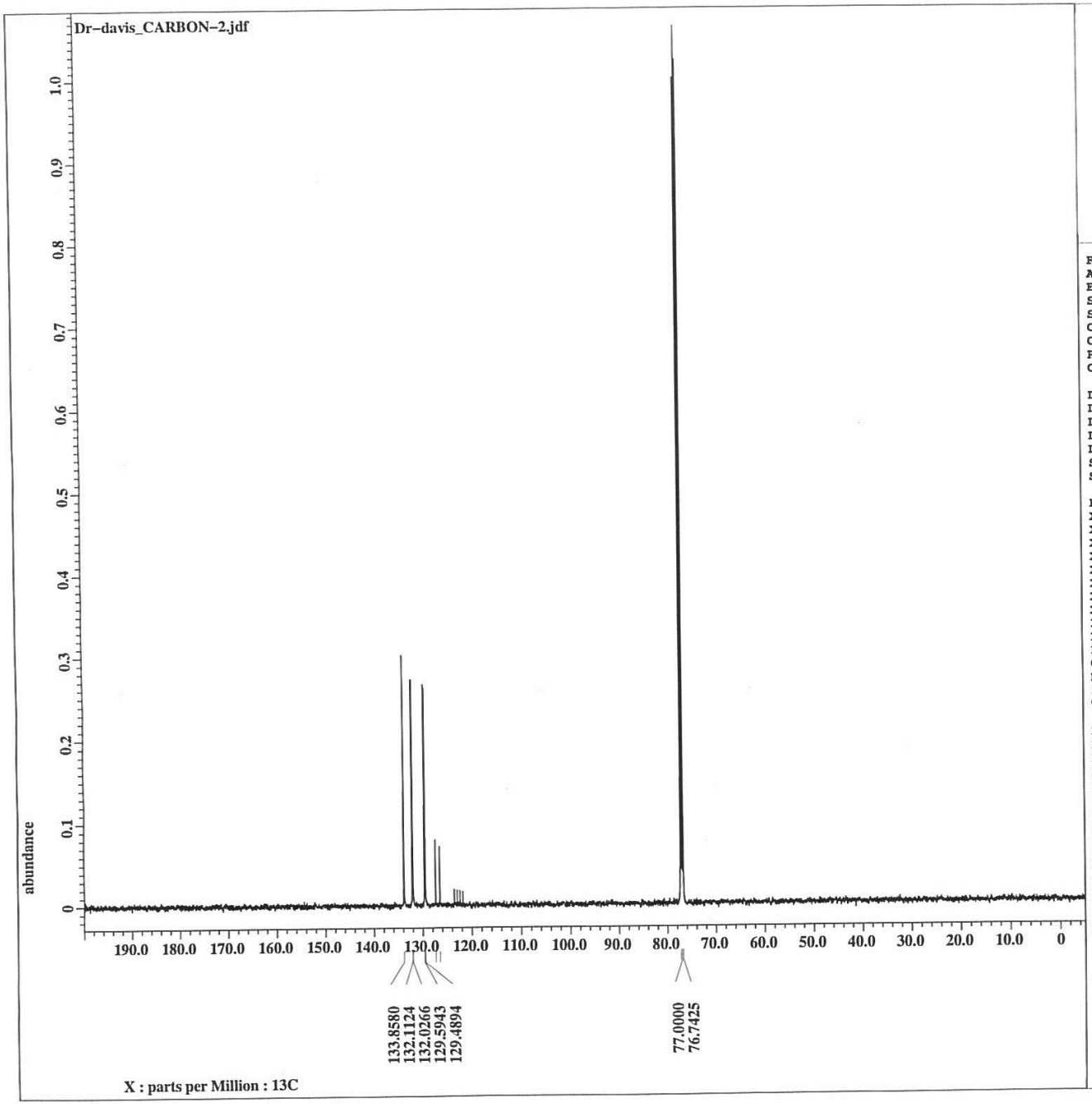
#14



SOUTH ALABAMA JAGUARS

Filename	= Dr-davis_PHOSPHORUS-2
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= Dr-davis
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 22-MAY-2017 11:25:00
Revision_time	= 22-MAY-2017 11:02:24
Current_time	= 22-MAY-2017 11:02:24
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	= 14.687[us]
X_acq_time	= 0.64487424[s]
X_angle	= 30[deg]
X_atn	= 5[dB]
X_pulse	= 4.89566667[us]
Irr_atn_dec	= 20.5[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	= 22.3[dC]

#14



SOUTH ALABAMA JAGUARS

Filename	= Dr-davis_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= Dr-davis
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 22-MAY-2017 12:18:25
Revision_time	= 22-MAY-2017 11:55:49
Current_time	= 22-MAY-2017 11:55:49
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	= 12.7[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.23333333[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	= 22.2[dC]

#14