

Supporting Information

Thermal extremophiles: Triarylsulfonium ionic liquids stable in air for 90 days at 300 °C

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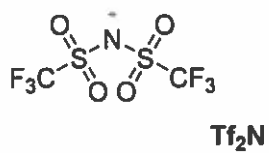
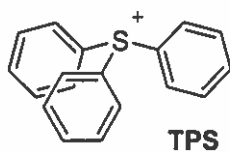
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b Department of Chemistry, University of South Alabama

Compound 1

Elemental Analysis

^1H -, ^{13}C -, and ^{19}F -NMR Spectra



Atlantic Microlab, Inc.

to. JD-SULFONIUM-1 Company/School U. SOUTH ALABAMA
 antic Blvd. Suite M Dept. CHEMISTRY
 s, GA 30071 Address CHEM BLDG 223
 anticmicrolab.com City, State, Zip MOBILE, AL, 36688
 r/Supervisor: JAMES DAVIS Name JAMES DAVIS Date 10/12/2016
 # Phone (251) 751-0520

Ant	Theory	Found	Single <input checked="" type="checkbox"/>	Duplicate <input type="checkbox"/>
	44.20	44.10		
	2.78	2.70		
	2.58	2.64		
Elements CHNOSF Present: _____ Analyze CHN for: _____ Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/> M.P. <u>UNK</u> B.P. <u>NONE</u> To be dried: Yes <input checked="" type="checkbox"/> No <input type="checkbox"/> Temp. <u>100C</u> Vac. <u>HIGH</u> Time <u>4H</u> Rush Service <input checked="" type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small>				
Include Email Address or FAX # Below <u>jdavis@southalabama.edu</u>				

Received OCT 14 2016 Date Completed OCT 14 2016
 rks: _____



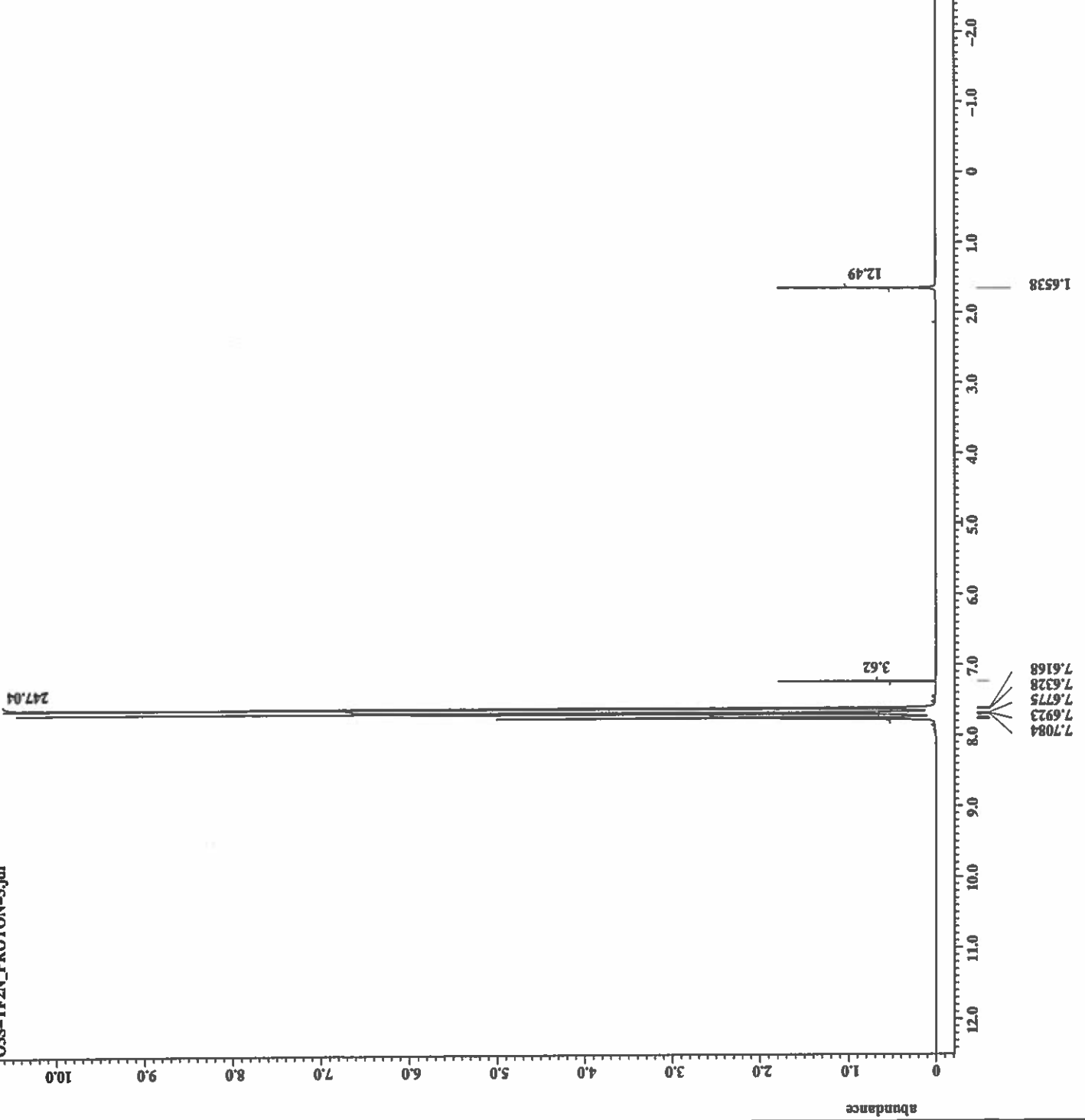
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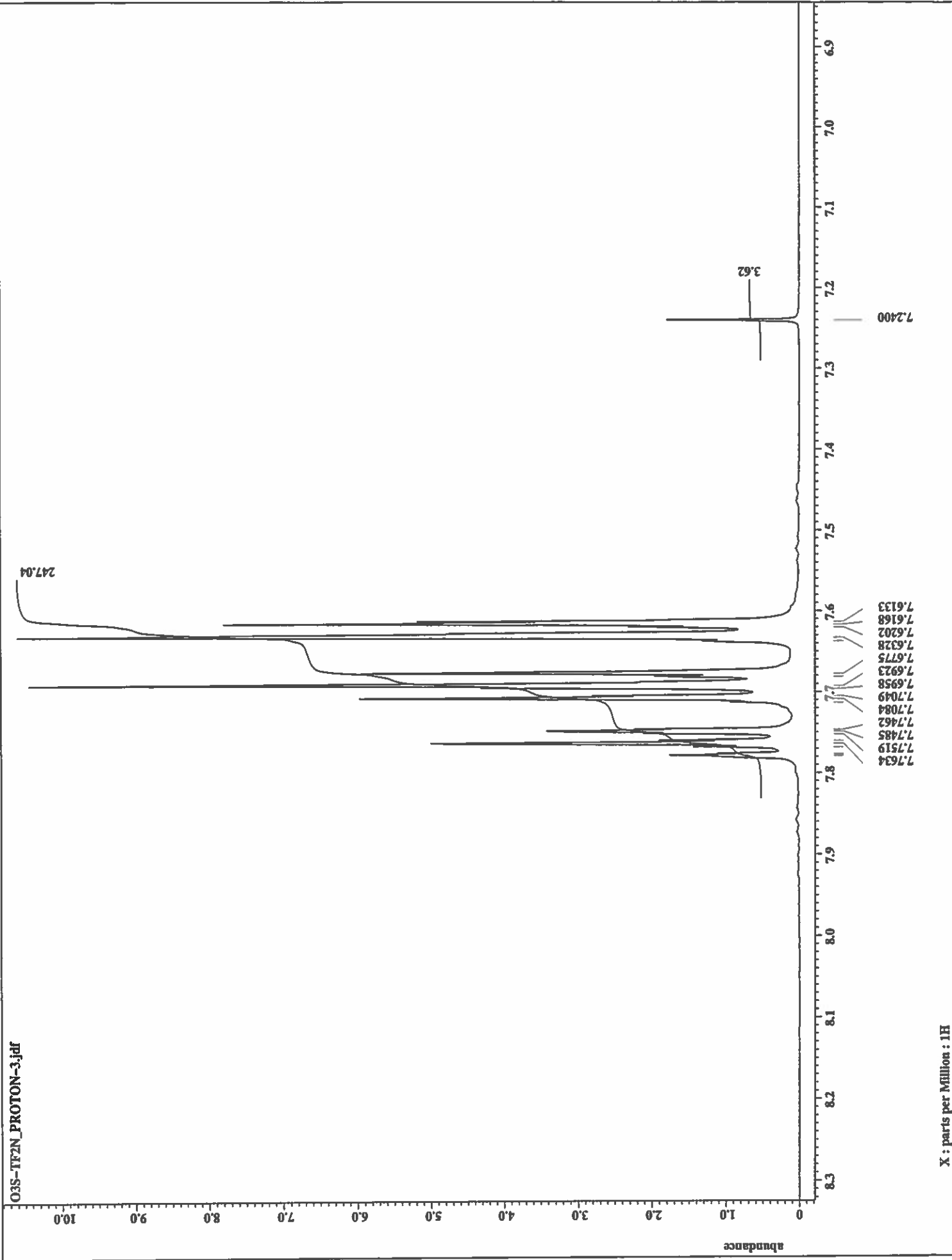
Filename = O3S-TF2N_PROTON-3.jdf
Author = Jim Davis
Experiment = single_pulse.ex2
Sample_id = O3S-TF2N
Solvent = CHLOROFORM-D
Changer_sample = 5
Creation_time = 16-JUN-2016 10:26:45
Revision_time = 16-JUN-2016 10:09:50
Current_time = 14-OCT-2016 08:13:21

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

Field_strength = 11.7473579 [T] (500 [MHZ])
X_acq_duration = 1.74587904 [s]
X_domain = 1H
X_freq = 500.15991521 [MHz]
X_offset = 5.0 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.57277737 [Hz]
X_sweep = 9.38438438 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
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
Daube_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 38
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_get = 22 [C]
    
```







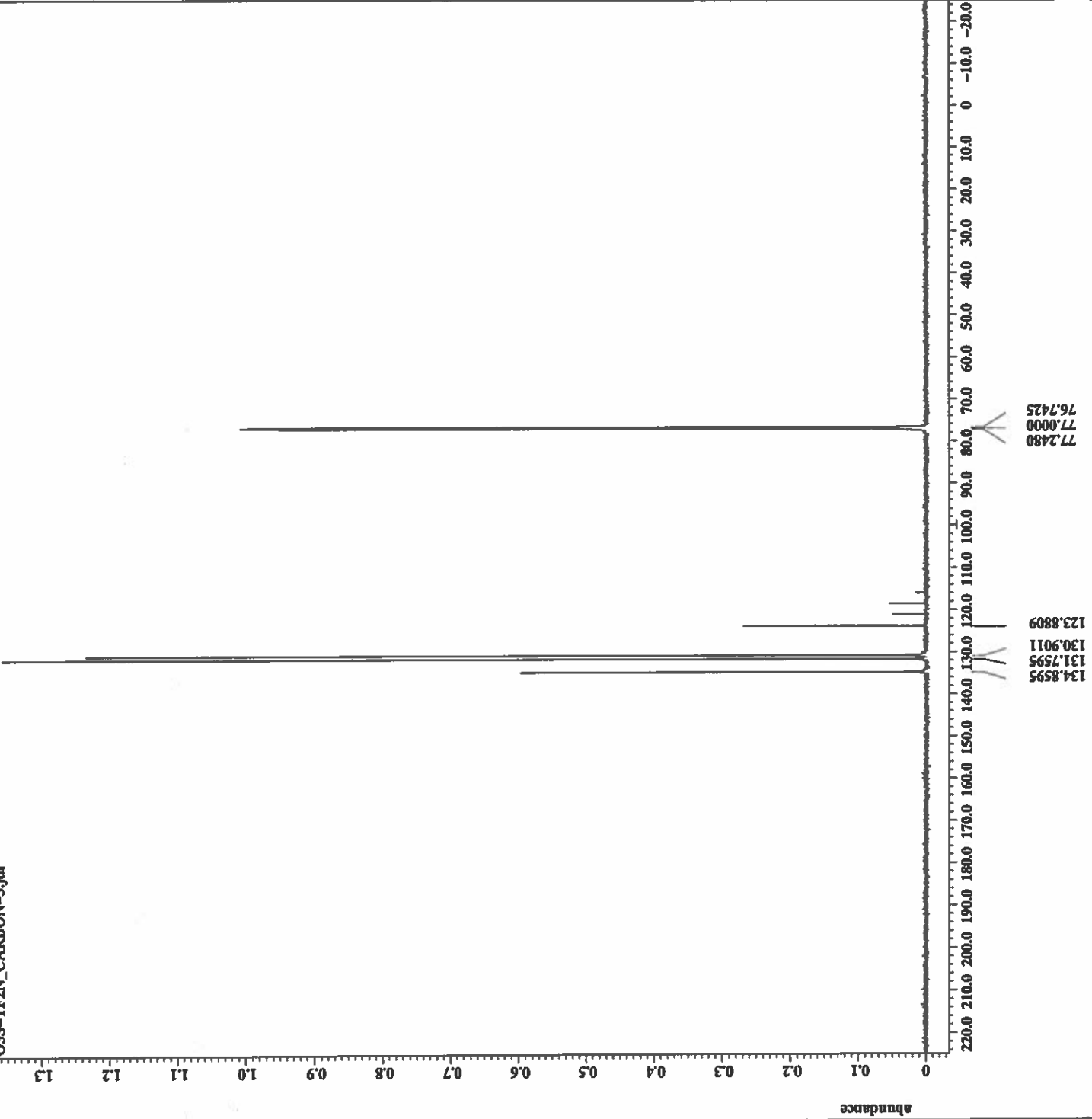
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Filename = 03S-TFZN_CARBON-3.jdf
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = 03S-TFZN
Solvent = CHLOROFORM-D
Changer_sample = 5
Creation_time = 16-JUN-2016 20:50:25
Revision_time = 16-JUN-2016 20:33:27
Current_time = 14-OCT-2016 08:10:41

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[F] (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 = 1.15959034[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_poc = 20.5[db]
Irr_pulse = WALTZ
Decoupling = TRUZ
Initial_wait = 1[s]
Noe = TRUZ
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get = 22.8[dc]
    
```



0.3

0.2

0.1

abundance

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

116.0213

118.5776

121.1338

123.6901

123.8809

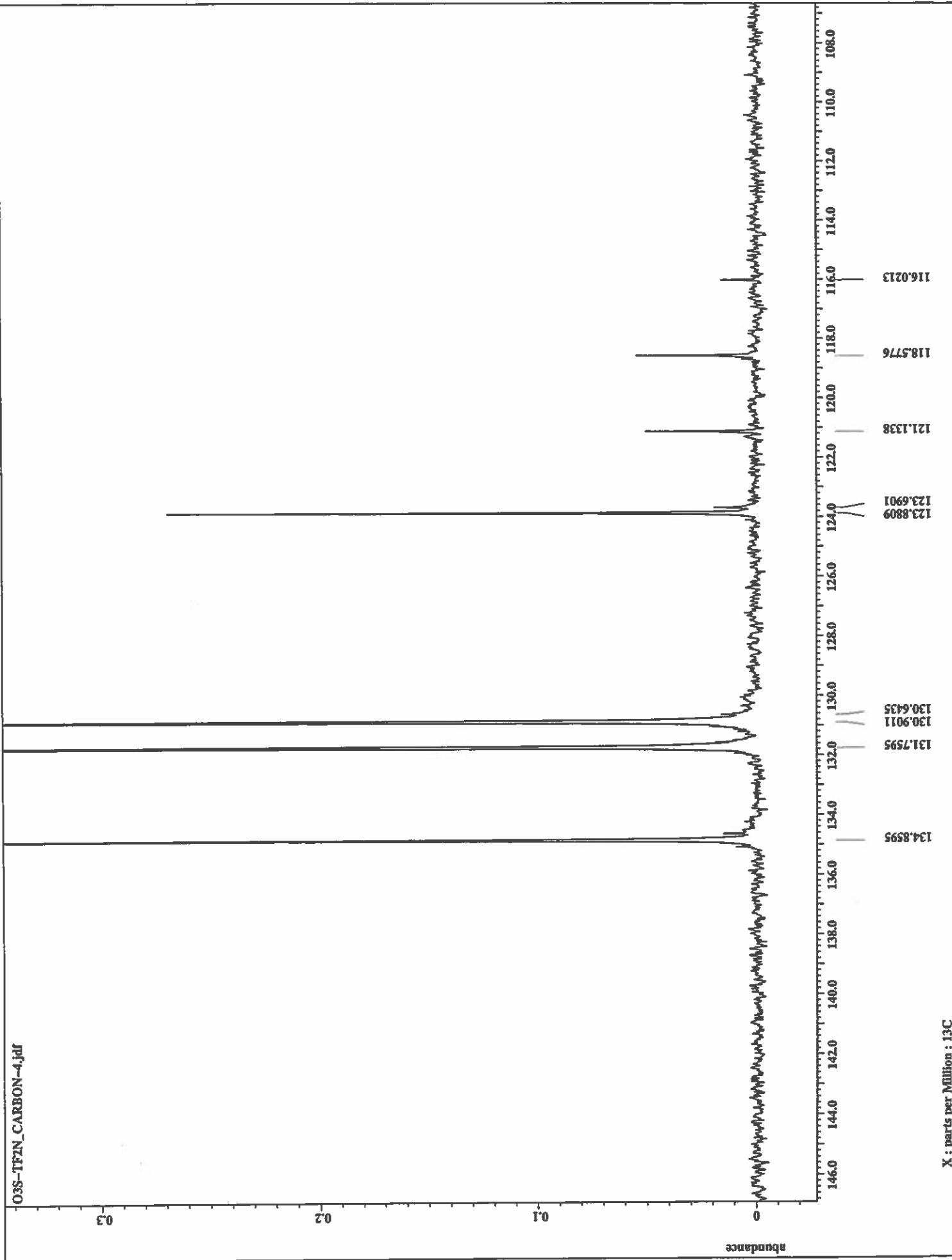
130.6435

130.9011

131.7595

134.8595

X : parts per Million : 13C





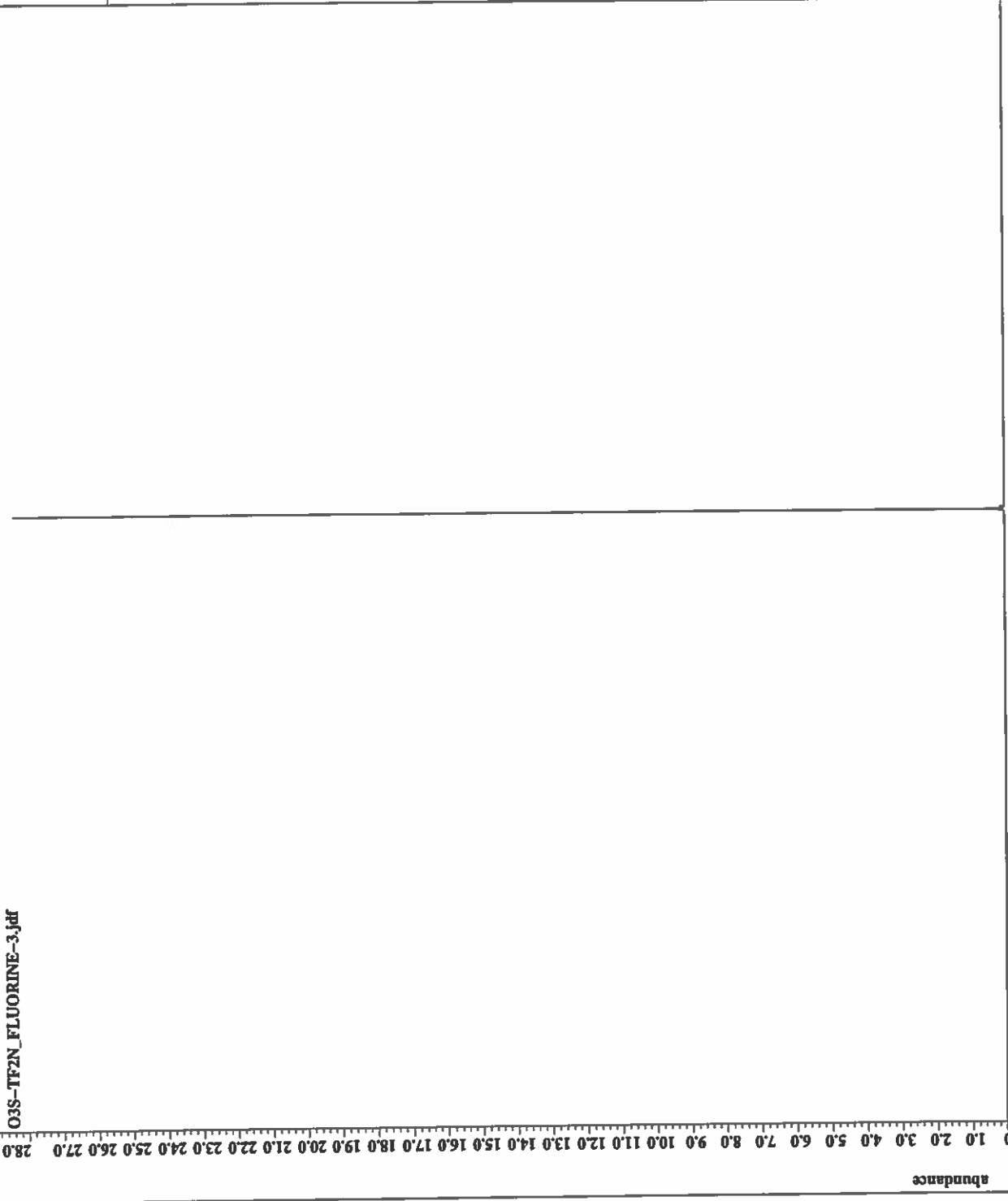
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Filename = 038-TF2N_FLUORINE-3.j
Author = Jim Davis
Experiment = single_pulse.ex2
Sample_id = 038-TF2N
Solvent = CELEOROFORM-D
Changer_sample = 5
Creation_time = 16-JUN-2016 10:56:57
Revision_time = 16-JUN-2016 10:40:02
Current_time = 14-OCT-2016 08:09:45

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 [MHZ])
X_acq_duration = 0.55574528 [s]
X_domain = 19F
X_freq = 470.62046084 [MHZ]
X_offset = -70 [ppm]
X_points = 65536
X_prescans = 1
X_resolution = 1.7993855 [Hz]
X_sweep = 117.9245283 [MHZ]
Irr_domain = 19F
Irr_freq = 470.62046084 [MHZ]
Irr_offset = 5 [ppm]
Tri_domain = 19F
Tri_freq = 470.62046084 [MHZ]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 15.7 [us]
X_acq_time = 0.55574528 [s]
X_angle = 45 [deg]
X_atn = 4 [dB]
X_pulse = 7.85 [us]
Irr_mode = Off
Tri_mode = Off
Pulse_preset = FALSE
Initial_wait = 1 [s]
Recvt_gain = 44
Relaxation_delay = 4 [s]
Repetition_time = 4.55574528 [s]
Temp_get = 22 [dC]
    
```



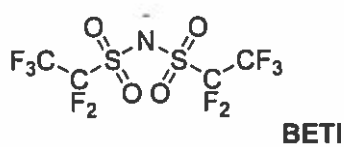
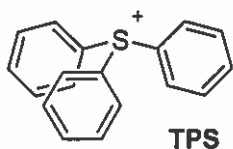
Abundance vs. Chemical Shift (ppm) scale: 30.0, 20.0, 10.0, 0, -10.0, -20.0, -30.0, -40.0, -50.0, -60.0, -70.0, -80.0, -90.0, -100.0, -110.0, -120.0, -130.0, -140.0, -150.0, -160.0

-78.6180

Compound 2

Elemental Analysis

^1H -, ^{13}C -, and ^{19}F -NMR Spectra



Atlantic Microlab, Inc.

No. JD-SULFONIUM 2 - RECRYSTALLIZED

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Dept. CHEMISTRY

Address CHEM BLDG 223

City, State, Zip MOBILE AL 36688

Name JAMES DAVIS Date 10/17/2016

Phone (251) 751-0520

Supervisor: DAVIS

C#

Element	Theory	Found	Single <input checked="" type="checkbox"/>	Duplicate <input type="checkbox"/>
C	41.06	41.09		
H	2.35	2.31		
N	2.18	2.24		
Elements CHNOSF Present: Analyze CHN for:				
Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/> M.P. UNK B.P. NONE				
To be dried: Yes <input checked="" type="checkbox"/> No <input type="checkbox"/> Temp. 60C Vac. HIGH Time 4 H				
Rush Service <input checked="" type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small>				
Include Email Address or FAX # Below jdavis@southalabama.edu				

Received OCT 18 2016

Date Completed

OCT 18 2016

Remarks:



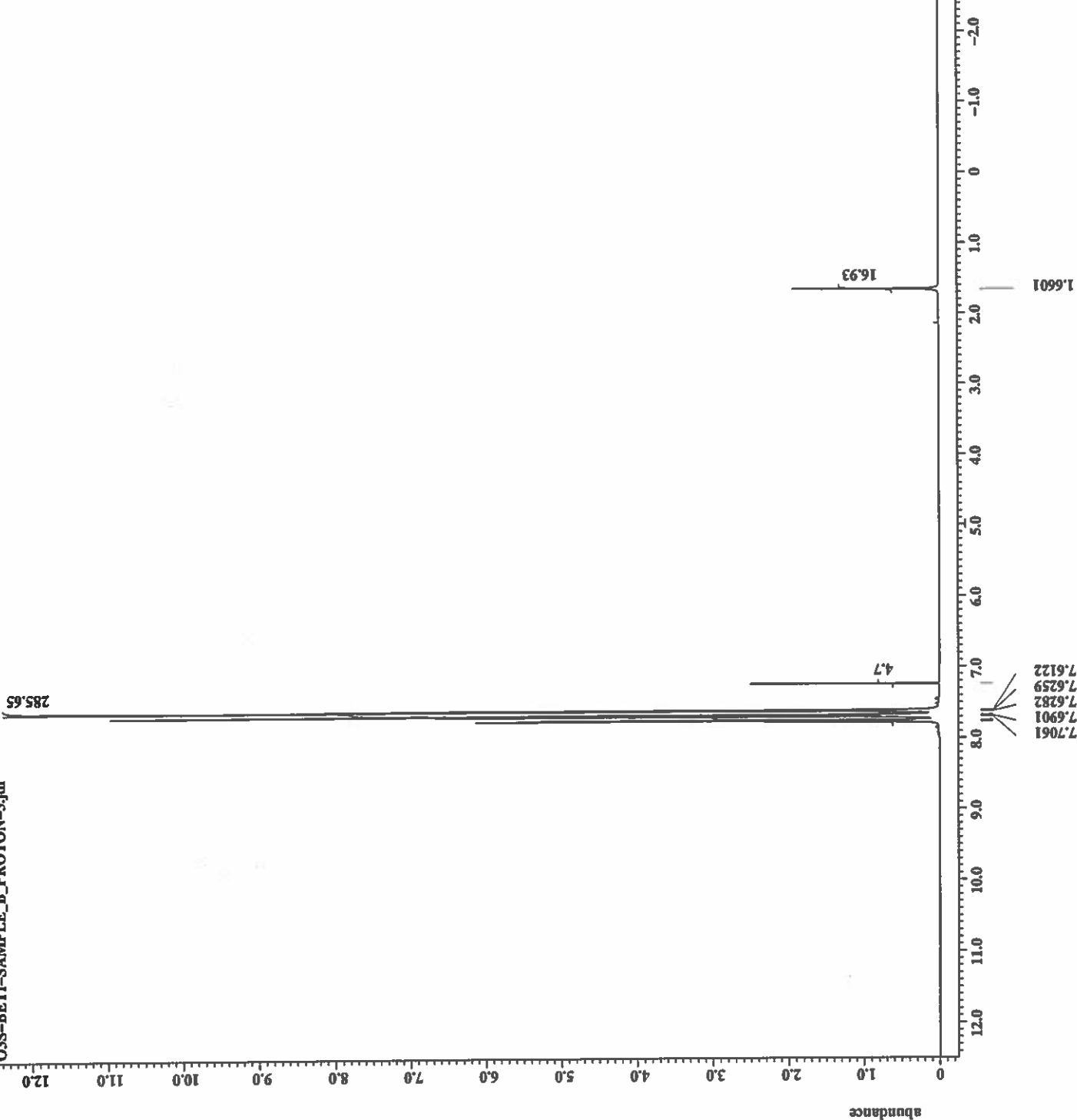
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File: O3S-BETI-SAMPLE_B_PRO
Author: Jim Davis
Experiment: single_pulse.ex2
Sample ID: O3S-BETI-SAMPLE_B
Solvent: CELEOROFORM-D
Charger_sample: 6
Creation_time: 16-JUN-2016 10:32:53
Revision_time: 16-JUN-2016 10:15:58
Current_time: 14-OCT-2016 08:06:45

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

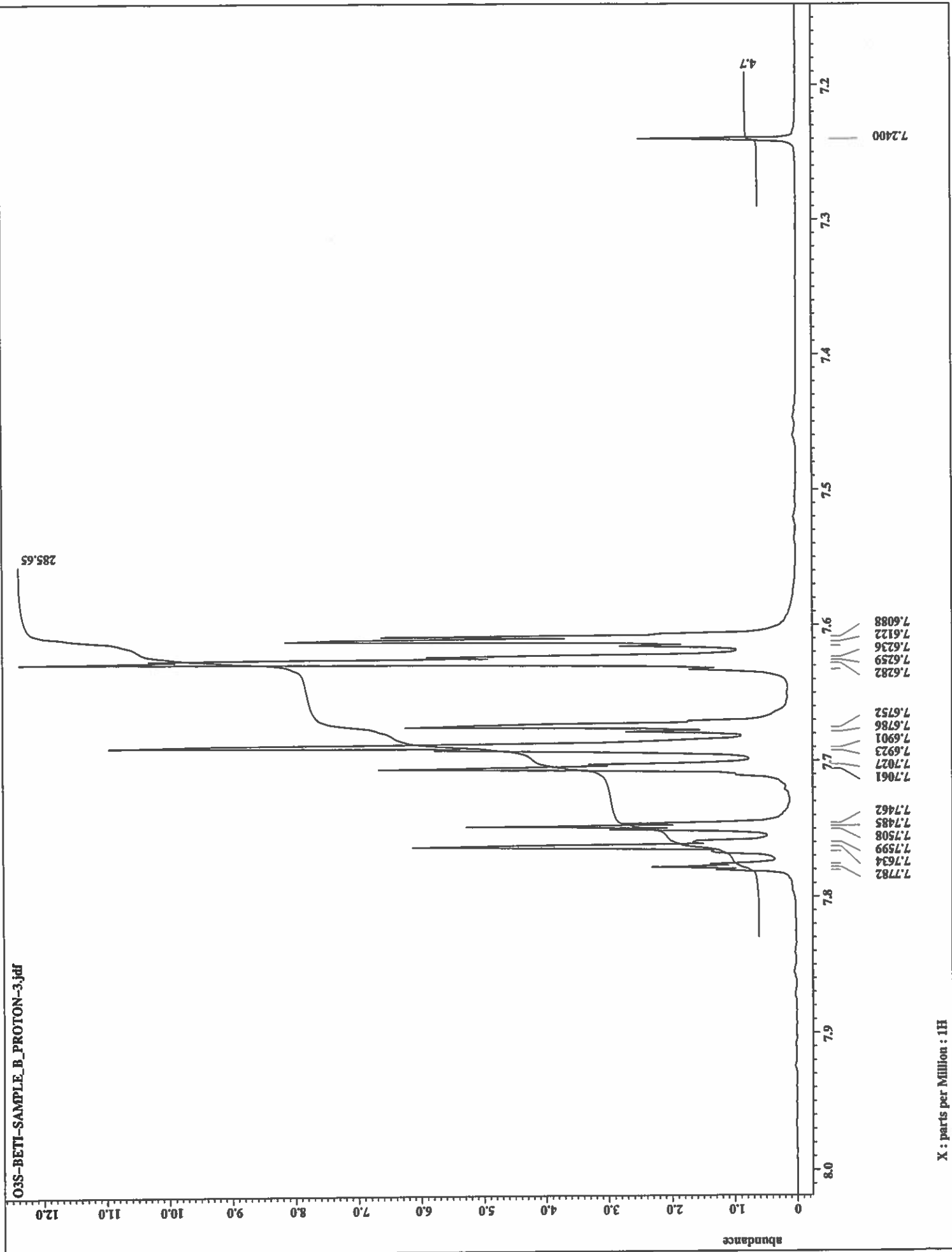
Field_strength: 11.7473579 [T] (500 [MHZ])
X_acq_duration: 1.74587904 [s]
X_domain: 1H
X_freq: 500.15991521 [MHz]
X_offset: 5.0 [ppm]
X_points: 16384
X_prescans: 1
X_resolution: 0.57277737 [kHz]
X_sweep: 9.38638438 [kHz]
Irr_domain: 1H
Irr_freq: 500.15991521 [MHz]
Irr_offset: 5.0 [ppm]
Tri_domain: 1H
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
Date_presat: FALSE
Initial_wait: 1 [s]
Recvr_gain: 40
Relaxation_delay: 4 [s]
Repetition_time: 5.74587904 [s]
Temp_get: 22.2 [dC]
    
```



X : parts per Million : 1H

OSS-BETT-SAMPLE_B_PROTON-3.jfif



X : parts per Million : 1H



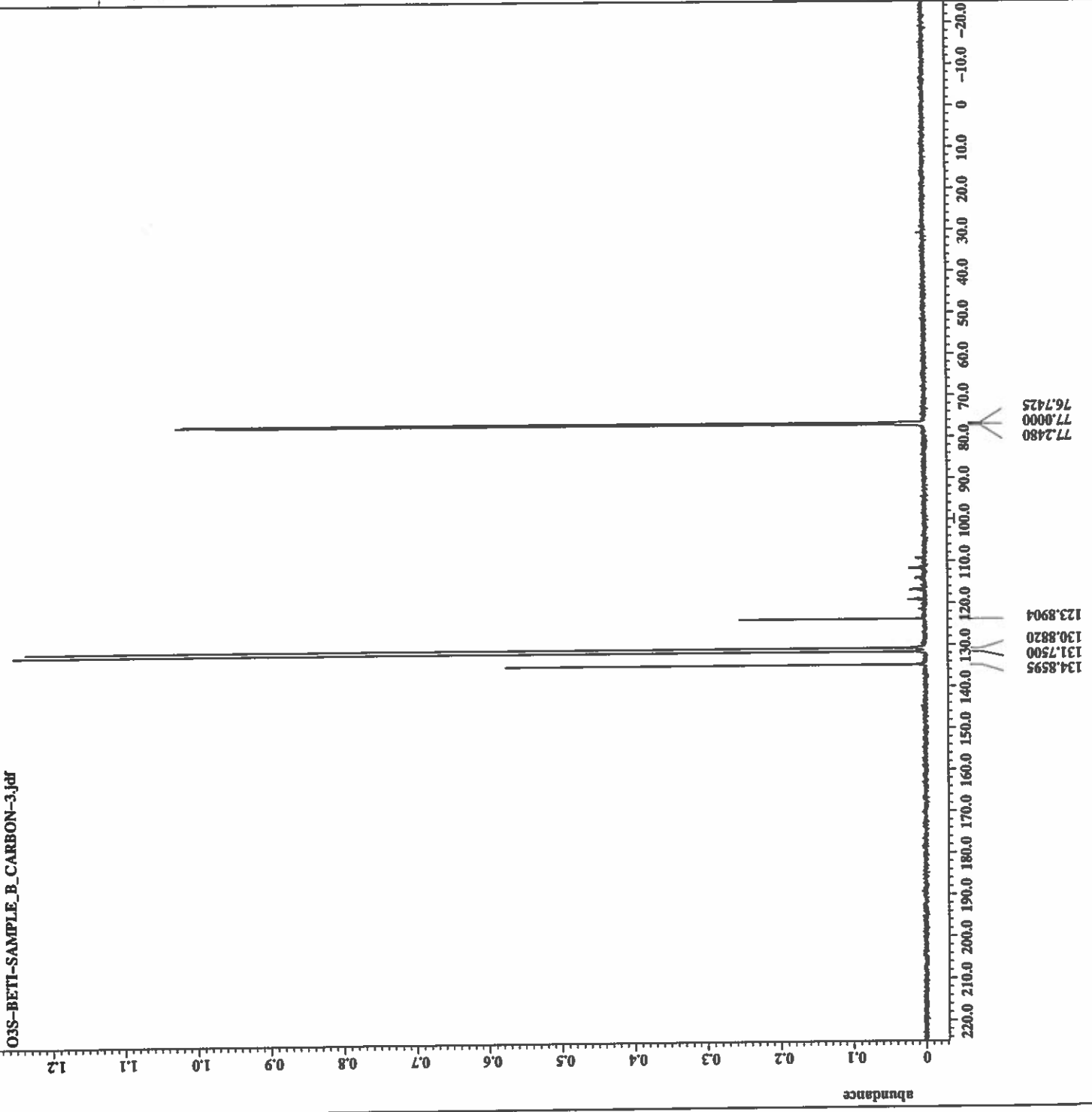
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Filename = 038-BETI-SAMPLE_B_CAR
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = 038-BETI-SAMPLE_B
Solvent = CHLOROFORM-D
Changer_sample = 6
Creation_time = 16-JUN-2016 21:43:04
Revision_time = 16-JUN-2016 21:26:05
Current_time = 14-OCT-2016 08:04:30

Data_format = 1D COMPLEX
Dia_size = 26214
Dia_title = 13C
Dia_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

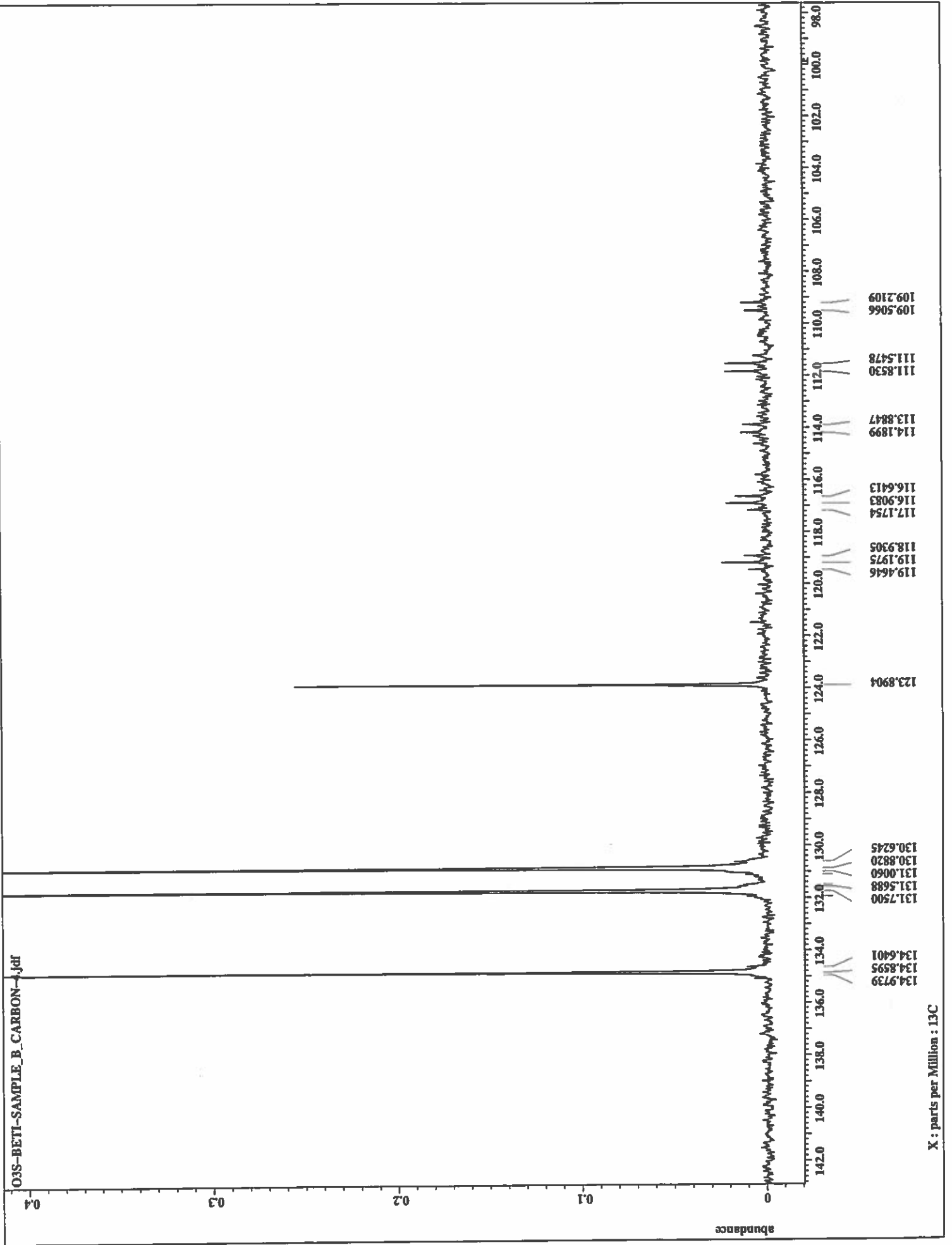
Field_strength = 11.7473579[T] (500 [MH
X_acq_duration = 0.83361792[s]
X_domain = 13C
X_freq = 125.76529768 [MHz]
X_offset = 32768
X_points = 4
X_prescans = 1
X_resolution = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
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 = WALVE
Decoupling = TRUEZ
Initial_wait = 1 [s]
Noe = TRUEZ
Noe_time = 2 [s]
Recvr_gain = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get = 22.6 [DC]
    
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X : parts per Million : 13C

OSS-BETT-SAMPLE_B. CARBON-jdi





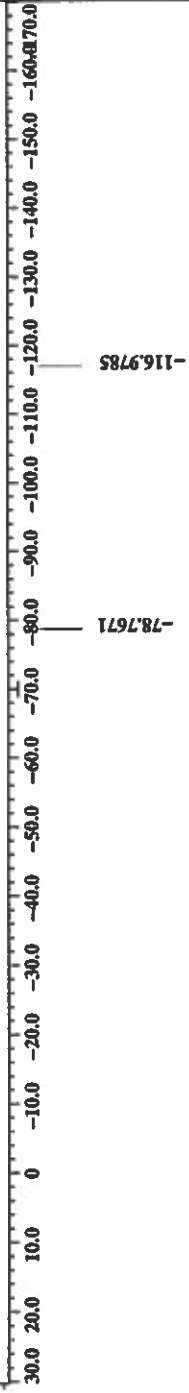
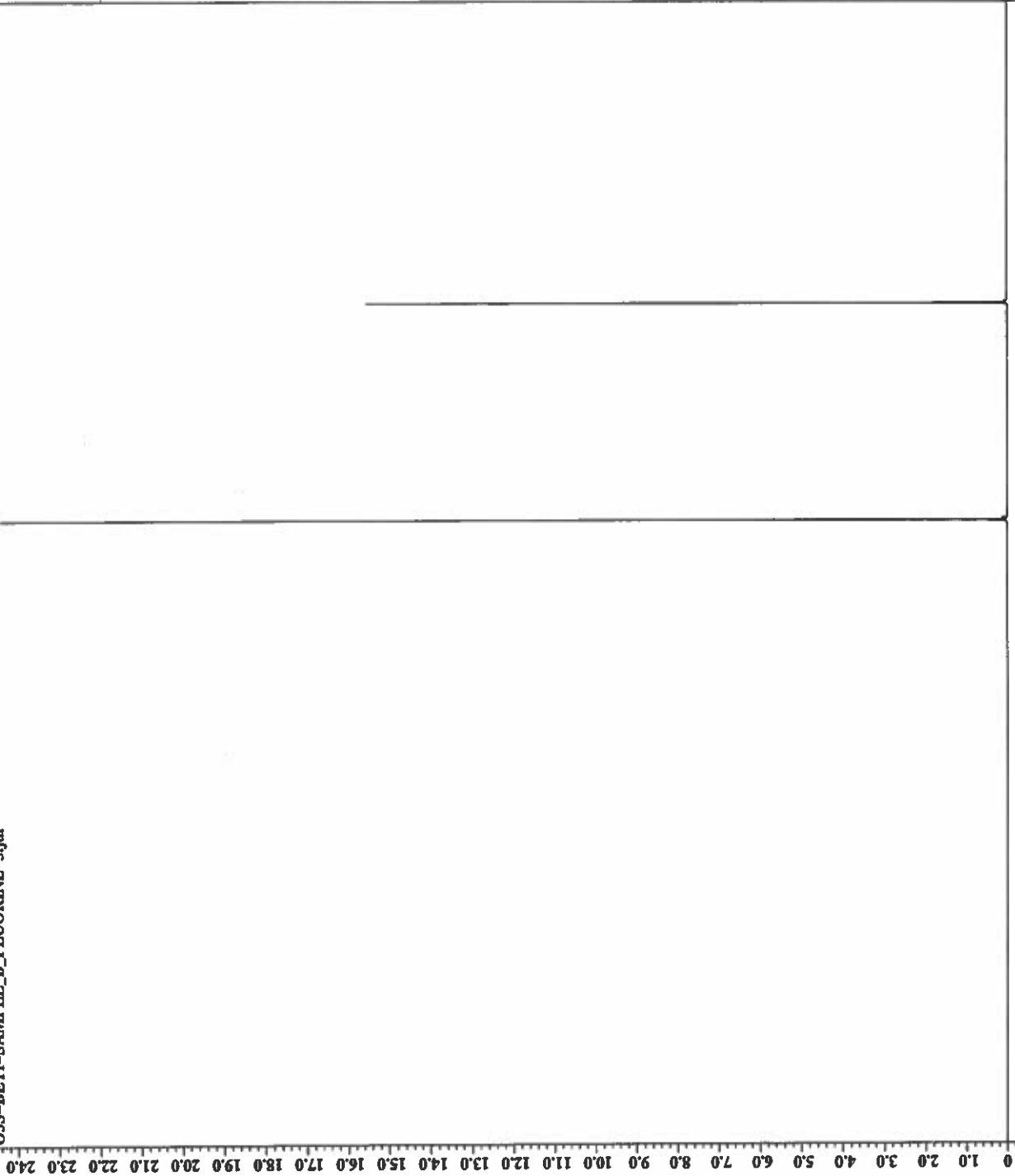
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Filename = 03S-BETI-SAMPLE_B_FLU
Author = Jim Davis
Experiment = single_pulse.ex2
Sample_id = 03S-BETI-SAMPLE_B
Solvent = CHLOROFORM-D
Changer_sample = 6
Creation_time = 16-JUN-2016 11:02:33
Revision_time = 16-JUN-2016 10:45:38
Current_time = 14-OCT-2016 08:03:27

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

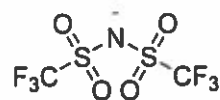
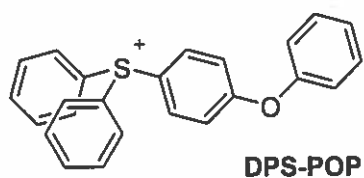
X_90_width = 15.7[us]
X_acq_time = 0.55574528[s]
X_angle = 45[deg]
X_atn = 4[dB]
X_pulse = 7.85[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 4[s]
Repetition_time = 4.55574528[s]
Temp_get = 22.1[DC]
    
```



Compound 3

Elemental Analysis

^1H -, ^{13}C -, and ^{19}F -NMR Spectra



Tf₂N

Atlantic Microlab, Inc.

No. JD-SULFONIUM-3-RECRYSTALLIZED
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 Company/School U SOUTH ALABAMA
 Dept. CHEMISTRY
 Address CHEM BLDG 223
 City, State, Zip MOBILE AL 36688
 Name JAMES DAVIS Date 10/17/2016
 Supervisor: DAVIS
 Phone (251) 751-0520
 CC# _____

Element	Theory	Found	Single <input checked="" type="checkbox"/>	Duplicate <input type="checkbox"/>
C	49.13	49.27		
H	3.01	2.98		
N	2.20	2.21		
Elements CHNOSF Present: _____ Analyze CHN for: _____ Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/> M.P. <u>UNK</u> B.P. <u>NONE</u> To be dried: Yes <input checked="" type="checkbox"/> No <input type="checkbox"/> Temp. <u>60</u> Vac. <u>HIGH</u> Time <u>4H</u> Rush Service <input checked="" type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small> Include Email Address or FAX # Below <u>jdavis@southalabama.edu</u>				

Sample Received OCT 18 2016 Date Completed OCT 18 2016
 Remarks: _____

PRINT HERE



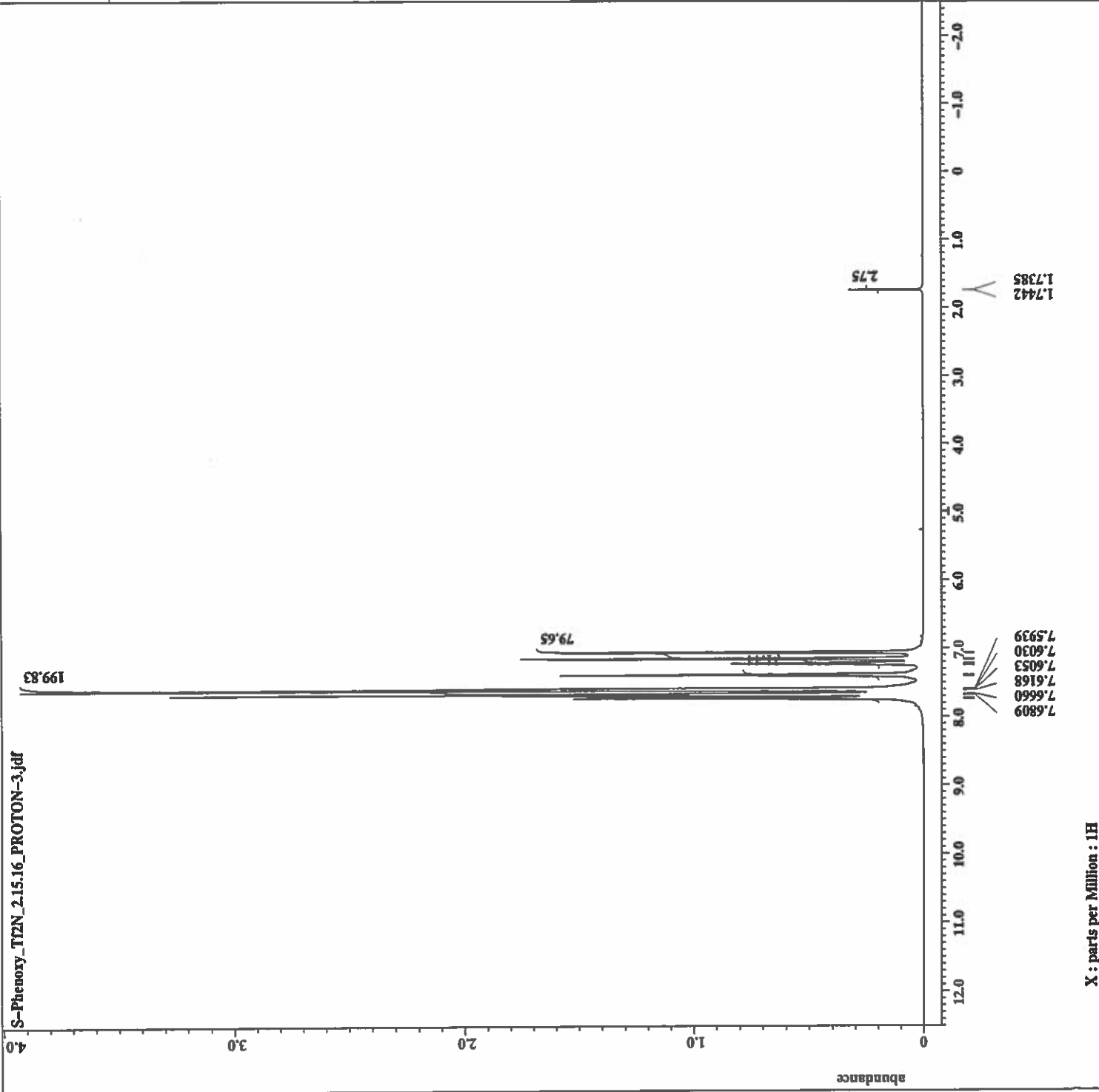
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Filename = S-Phenoxy_T2N_2.15.1
Author = Jim Davis
Experiment = single_pulse.ex2
Sample_id = S-Phenoxy_T2N_2.15.1
Solvent = CELEROFORM-D
Charger_sample = 18
Creation_time = 15-FEB-2016 17:08:16
Revision_time = 15-FEB-2016 16:54:28
Current_time = 14-OCT-2016 07:57:05

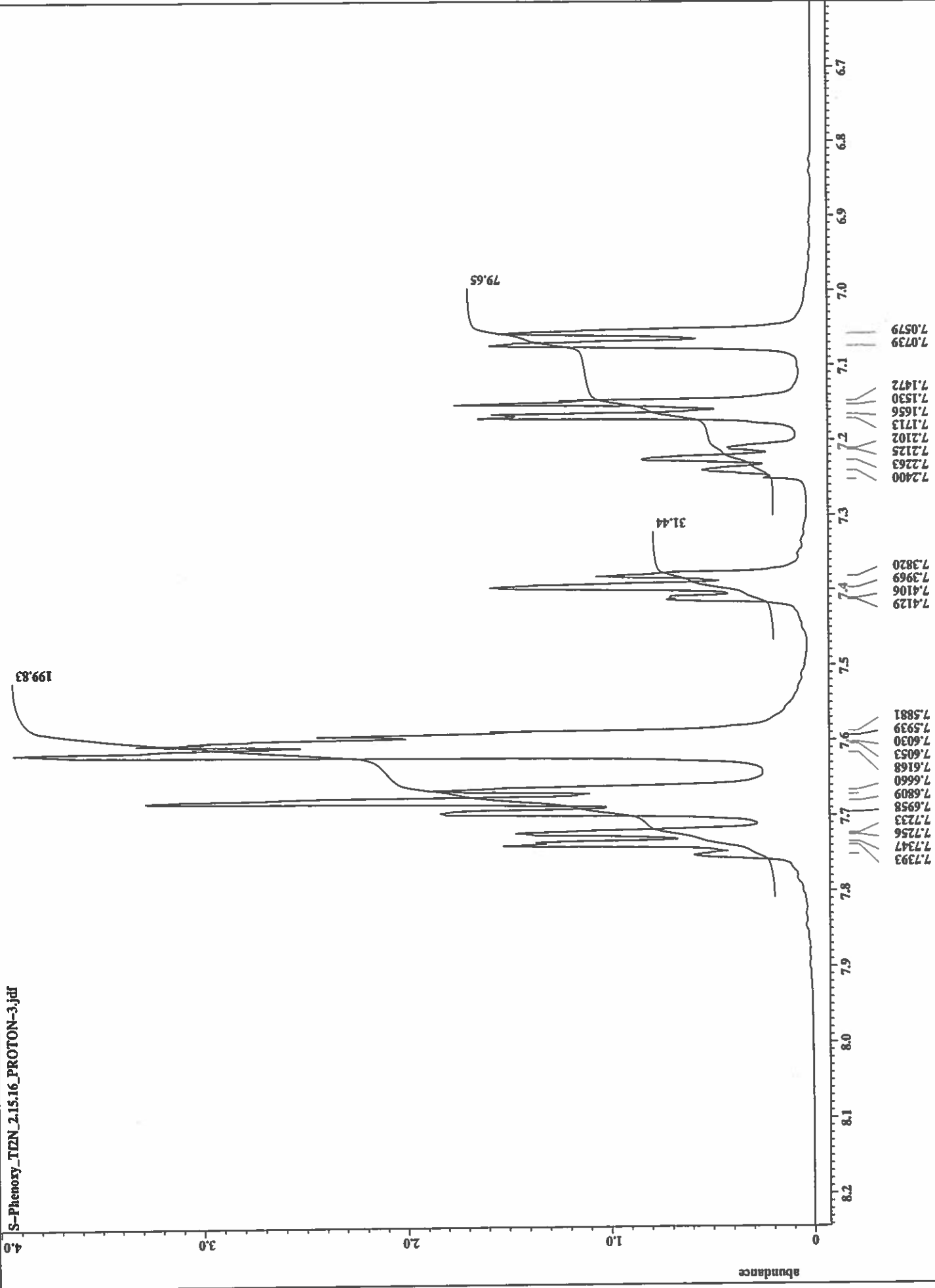
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = JNM-ECA500

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

X_90_width = 13.35 [us]
X_acq_time = 1.74587904 [s]
X_angle = 45 [deg]
X_atn = 4 [dB]
X_pulse = 6.675 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 30
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_get = 19.5 [dc]
    
```



S-Phenoxy_T12N_2.15.16_PROTON-3.jdf



X : parts per Million : 1H



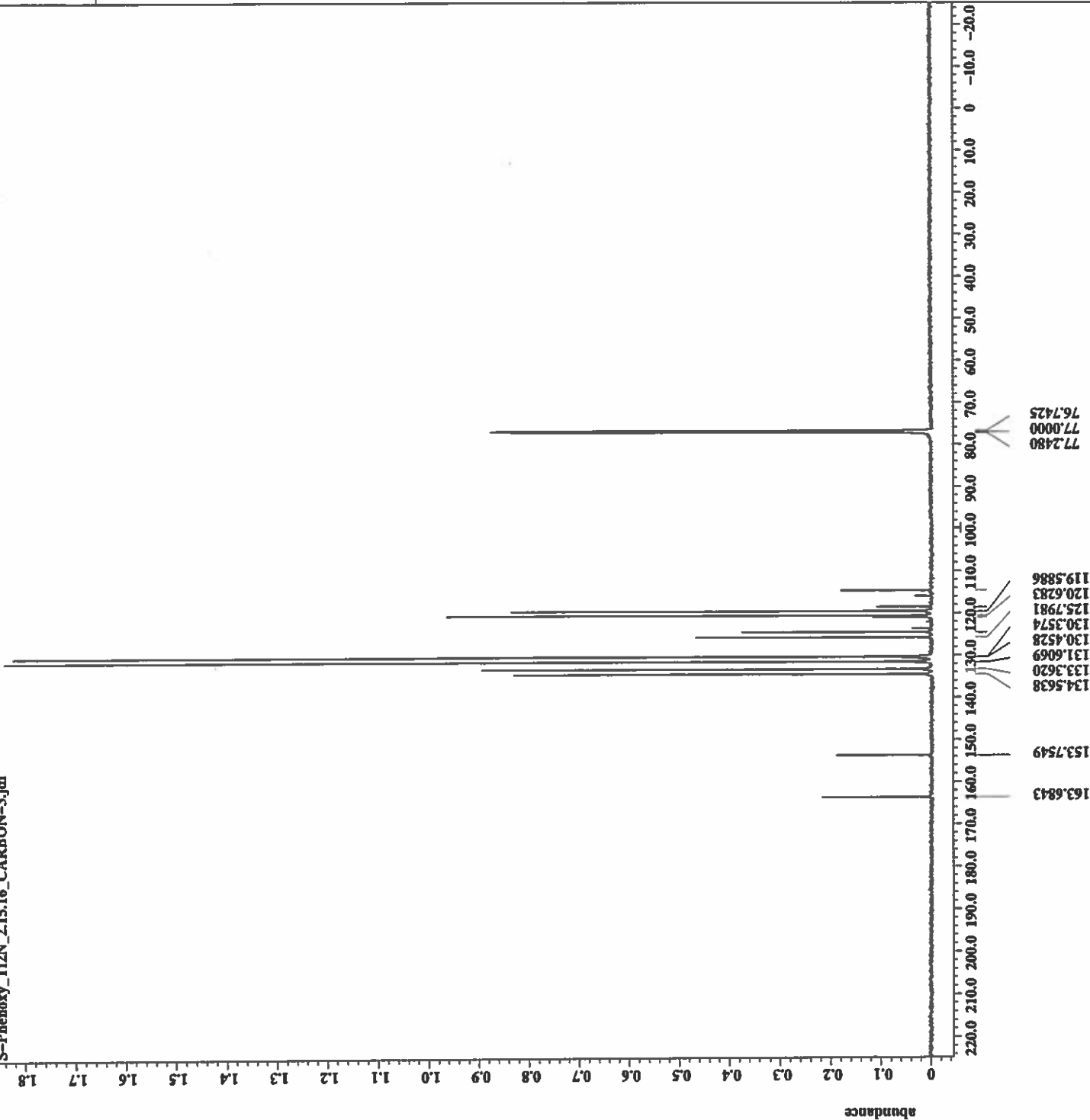
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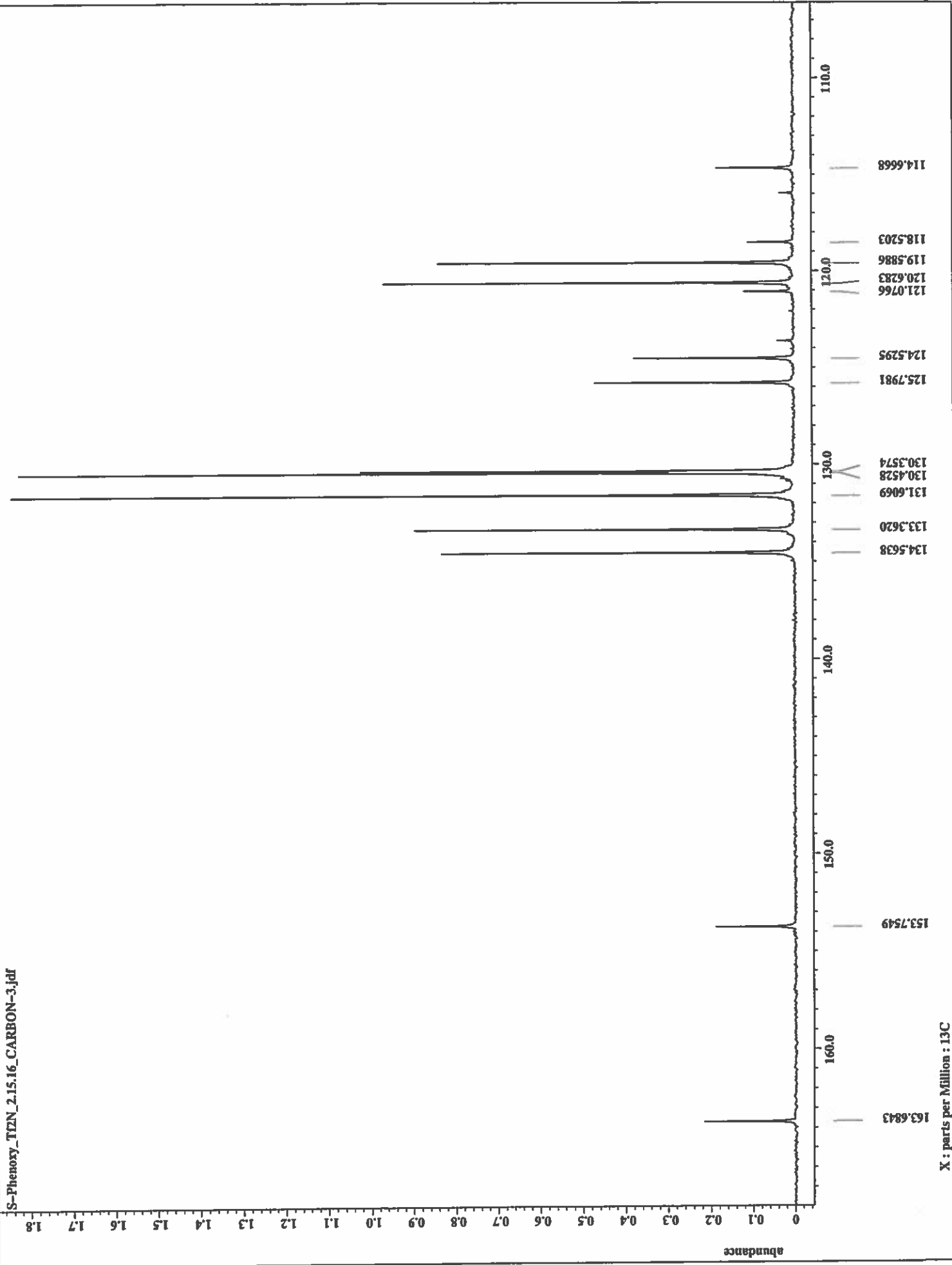
Filename = S-Phenoxy_T12N_2.15.1
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = S-Phenoxy_T12N_2.15.1
Solvent = CHLOROFORM-D
Channels = 18
Creation_time = 15-YES-2016 20:49:41
Revision_time = 15-FZB-2016 20:35:52
Current_time = 14-OCT-2016 07:54:12

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

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76529768 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991531 [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 = TRUZ
Initial_wait = 1 [s]
Noe = TRUZ
Noe_time = 2 [s]
Recvr_gain = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get = 20.6 [dC]
    
```







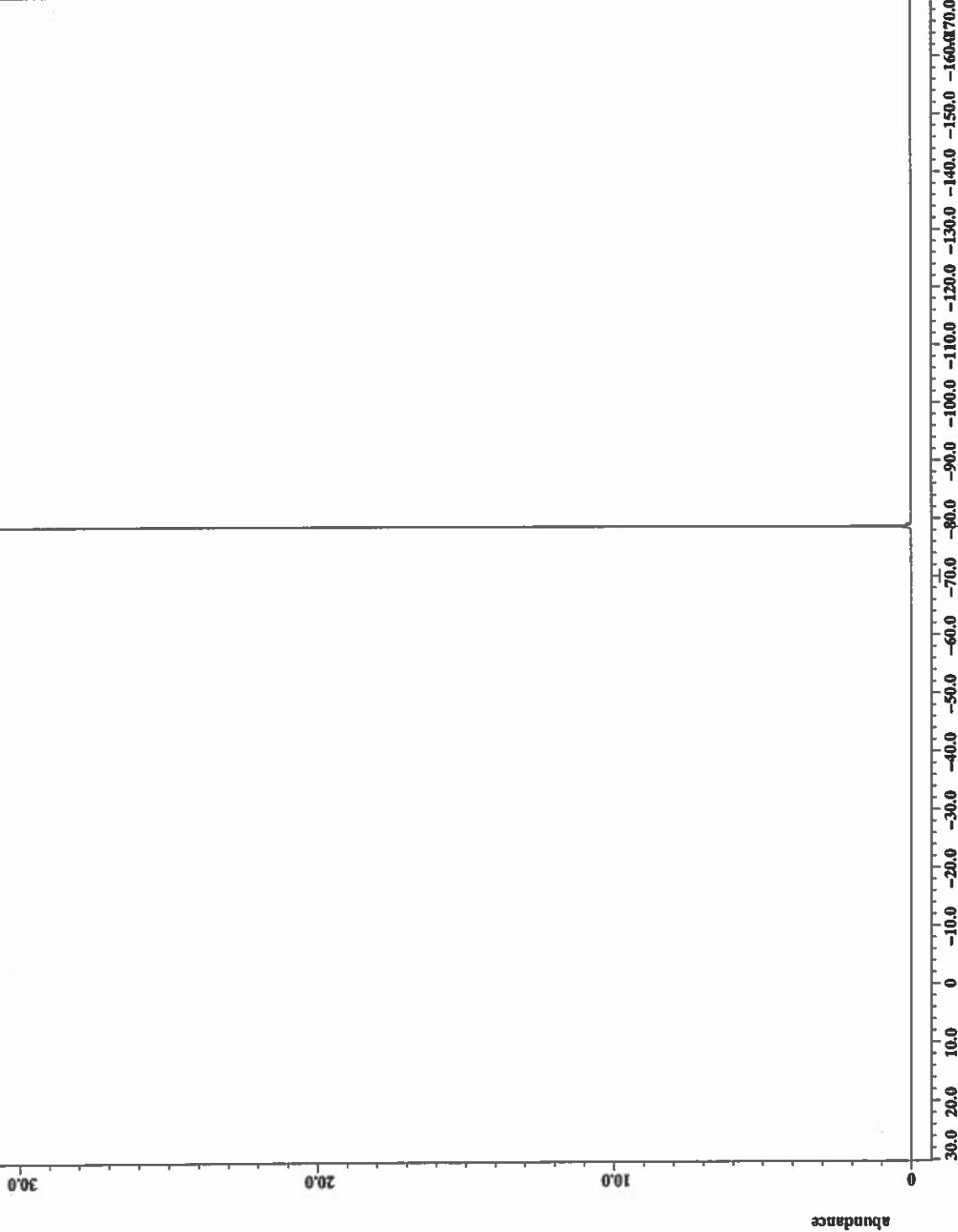
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Filename = S-Phenoxy_TF2N_FLUORINE
Author = Jim Davis
Experiment = single_pulse.ex2
Sample_id = S-Phenoxy_TF2N
Solvent = CHLOROFORM-D
Changer_sample = 18
Creation_time = 15-FEB-2016 16:34:35
Revision_time = 15-FEB-2016 16:20:48
Current_time = 14-OCT-2016 07:52:41

Data_format = 1D_COMPLEX
Dir_size = 52428
Dir_title = 19F
Dir_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 = 19.9 [DC]
    
```

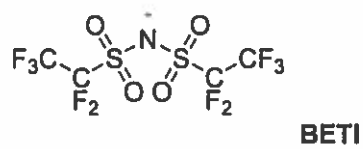
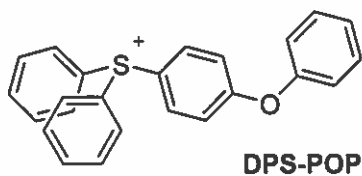


-78.5874

Compound 4

Elemental Analysis

^1H -, ^{13}C -, and ^{19}F -NMR Spectra



Atlantic Microlab, Inc.

Sample No. JD-SULFONIUM-4

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

Company/School U SOUTH ALABAMA

Dept. CHEMISTRY

Address CHEM BLDG 223

City, State, Zip MOBILE, AL, 36688

Professor/Supervisor: DAVIS

Name JAMES DAVIS

Date 10/12/2016

PO# / CC#

Phone (251) 751-0520

Element	Theory	Found	Single <input checked="" type="checkbox"/>	Duplicate <input type="checkbox"/>
C	45.72	45.66		
H	2.60	2.52		
N	1.90	1.94		
Elements CHNOSF Present: _____ Analyze CHN for: _____ Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/> M.P. <u>UNK</u> B.P. <u>NONE</u> To be dried: Yes <input checked="" type="checkbox"/> No <input type="checkbox"/> Temp. <u>100C</u> Vac. <u>HIGH</u> Time <u>4H</u> Rush Service <input checked="" type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 6 PM EST on the day the sample is received by 11 AM.</small> Include Email Address or FAX # Below <u>jdavis@southalabama.edu</u>				

Date Received OCT 14 2016

Date Completed OCT 14 2016

Remarks:



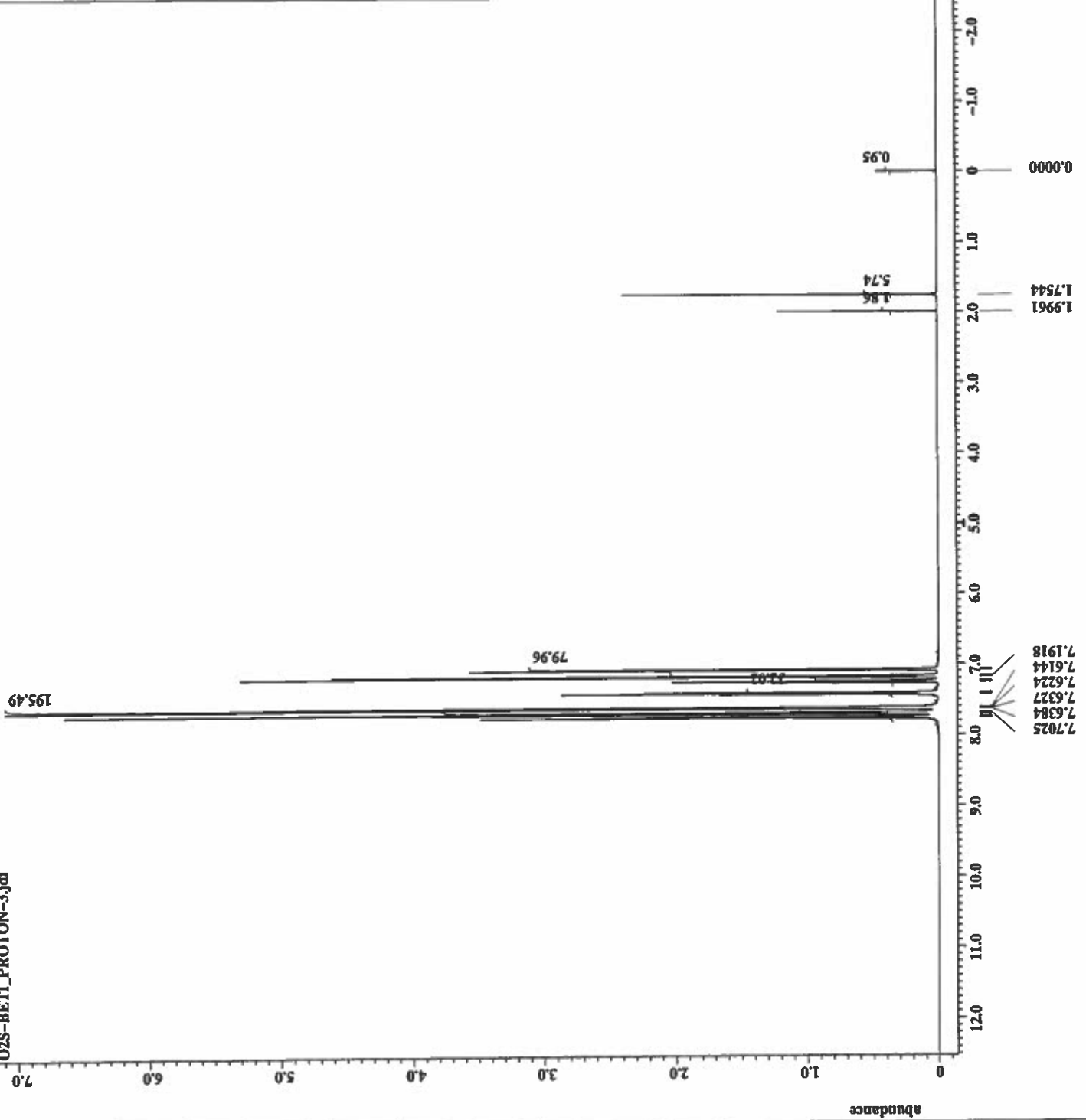
```

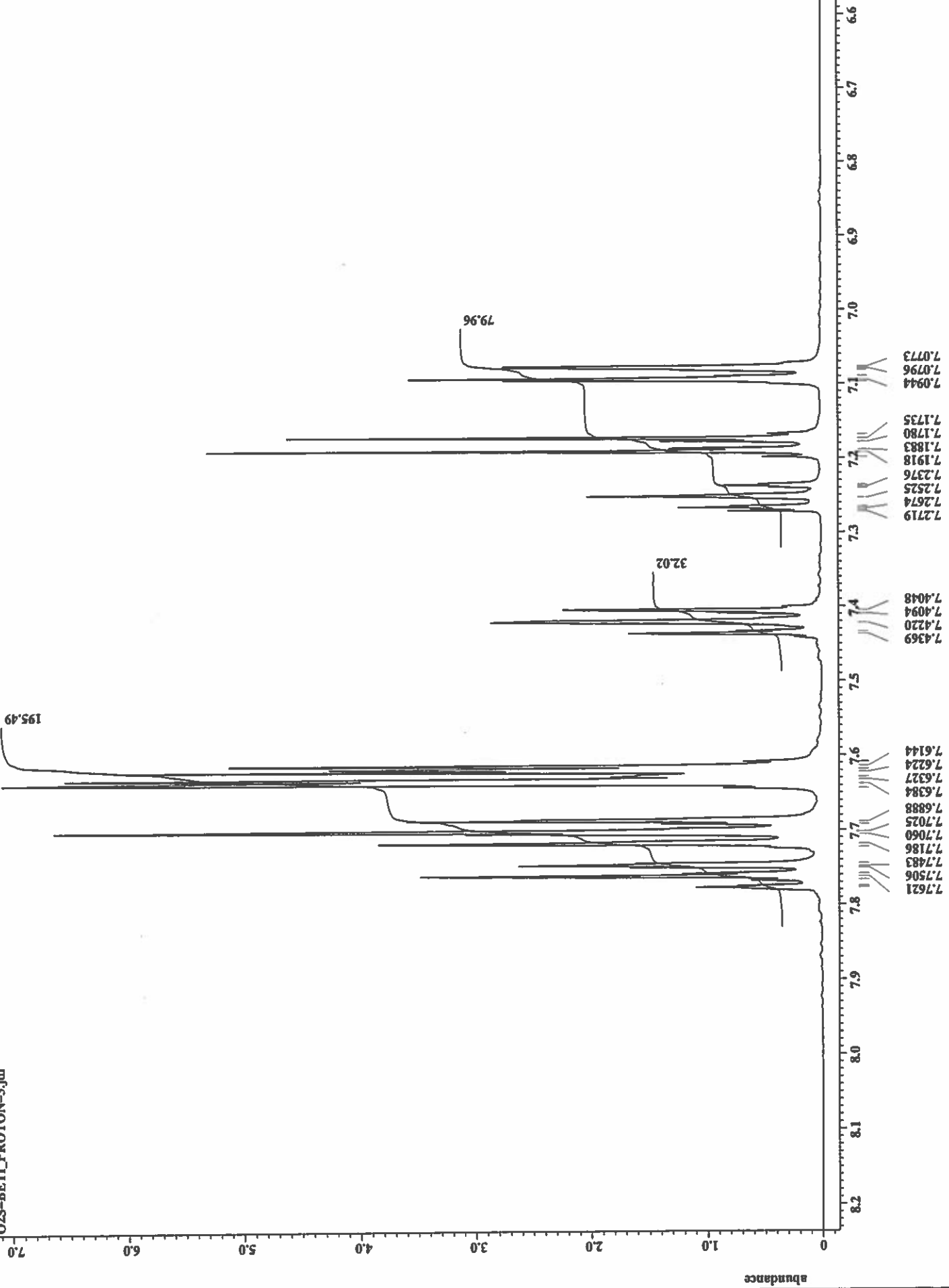
Filename = O2S-BETI_PROTON-3.jdf
Author = Jim Davis
Experiment = single_pulse.ex2
Sample_id = O2S-BETI
Solvent = CHLOROFORM-D
Changer_sample = 3
Creation_time = 12-OCT-2016 12:22:35
Revision_time = 12-OCT-2016 12:05:12
Current_time = 14-OCT-2016 07:48:29

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

Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain = 1H
X_freq = 500.15991521 [MHz]
X_offset = 5.0 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.57277737 [Hz]
X_sweep = 9.38438438 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
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_atn = 6.675 [us]
X_pulse = Off
Irr_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 30
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_get = 20.2 [dC]
    
```







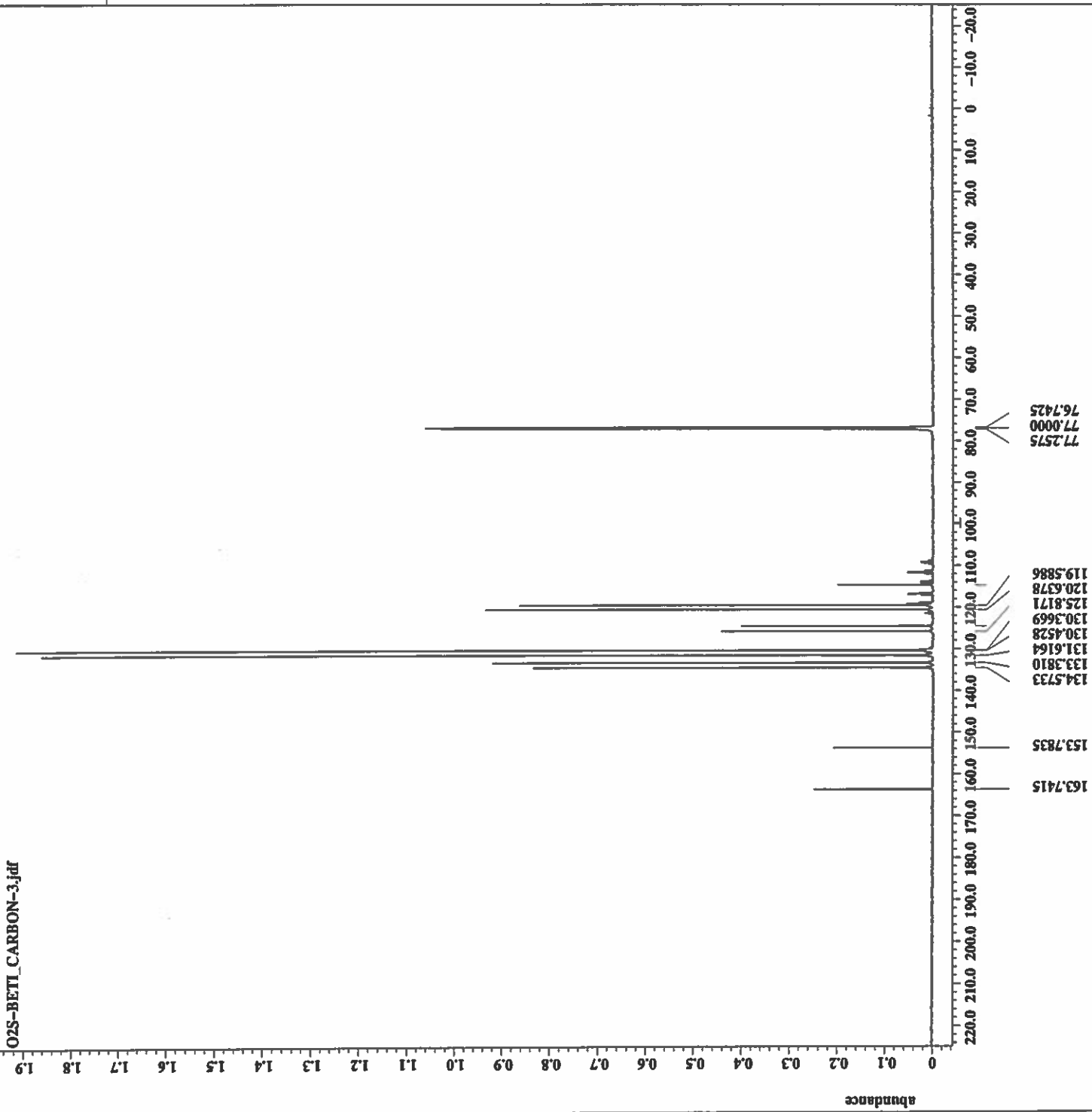
```

Filename = O2S-BETI CARBON-3.jdf
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = O2S-BETI
Solvent = CHLOROFORM-D
Changer_sample = 3
Creation_time = 12-OCT-2016 19:46:50
Revision_time = 12-OCT-2016 19:29:23
Current_time = 14-OCT-2016 07:45:32

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 [MHZ])
X_acq_duration = 0.83361792 [s]
X_domain = 13C
X_freq = 125.76529768 [MHZ]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034 [Hz]
X_sweep = 39.3081761 [kHz]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHZ]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 3000

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 = TRUZE
Initial_wait = 1 [s]
Noe = TRUZE
Noe_time = 2 [s]
Recvr_gain = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get = 21.3 [dC]
    
```



O2S-BETI_CARBON-4.jdf

abundance

0.5

0.4

0.3

0.2

0.1

0

170.0

160.0

150.0

140.0

130.0

120.0

110.0

109.4589

111.7958

114.1327

116.6031

117.1373

118.8923

119.1594

119.4265

119.5886

120.6378

124.5676

125.8171

130.2048

130.3669

130.4528

130.6149

131.6164

131.8072

133.3810

134.5733

153.7835

163.7415

X : parts per Million : 13C



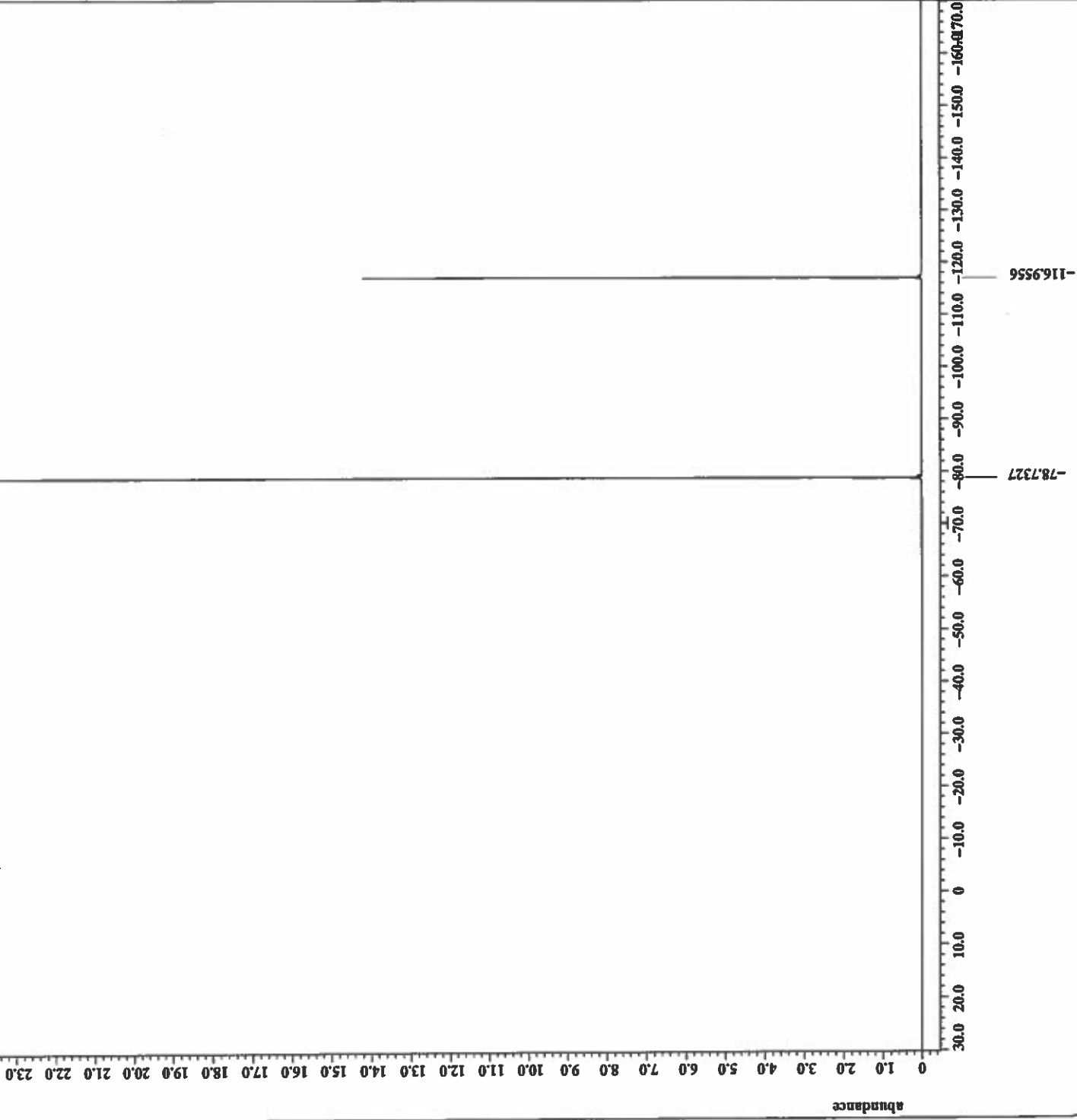
```

Filename = O2S-BETI_FLUORINE-3.j
Author = Jim Davis
Experiment = single_pulse.ex2
Sample_id = O2S-BETI
Solvent = CHLOROFORM-D
Changer_sample = 3
Creation_time = 12-OCT-2016 12:25:31
Revision_time = 12-OCT-2016 12:08:08
Current_time = 14-OCT-2016 07:44:52

Data_format = 1D COMPLEX
Dia_size = 52428
Dia_title = 19F
Dia_units = [ppm]
Dimensions = X
Site = XCA 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

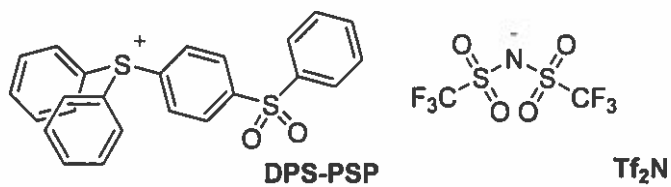
X_90_width = 15.7 [us]
X_acq_time = 0.55574528 [s]
X_angle = 45 [deg]
X_atn = 4 [dB]
X_pulse = 7.85 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 36
Relaxation_delay = 4 [s]
Repetition_time = 4.55574528 [s]
Temp_get = 20.3 [dC]
    
```



Compound 5

Elemental Analysis

^1H -, ^{13}C -, and ^{19}F -NMR Spectra



Atlantic Microlab, Inc.

Sample No. JD-SULFONIUM-5
 6180 Atlantic Blvd. Suite M
 Norcross, GA 30071
 www.atlanticmicrolab.com
 Company/School U. SOUTH ALABAMA
 Dept. CHEMISTRY
 Address CHEM BLDG 223
 City, State, Zip MOBILE, AL, 36688
 Professor/Supervisor: JAMES DAVIS Name JAMES DAVIS Date 10/12/2016
 PO# / CC# _____ Phone (251) 751-0520

Element	Theory	Found	Single <input checked="" type="checkbox"/>	Duplicate <input type="checkbox"/>
C	45.68	45.48	<input checked="" type="checkbox"/>	<input type="checkbox"/>
H	2.80	2.82	<input type="checkbox"/>	<input type="checkbox"/>
N	2.05	2.11	<input type="checkbox"/>	<input type="checkbox"/>
Elements CHNOSF Present: _____ Analyze CHN for: _____ Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/> M.P. <u>UNK</u> B.P. <u>NONE</u> To be dried: Yes <input checked="" type="checkbox"/> No <input type="checkbox"/> Temp. <u>100C</u> <u>Vac.</u> <u>HIGH</u> <u>Time</u> <u>4H</u> Rush Service <input checked="" type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small> Include Email Address or FAX # Below <u>jdavis@southalabama.edu</u>				

Date Received OCT 14 2016 Date Completed OCT 14 2016
 Remarks: _____



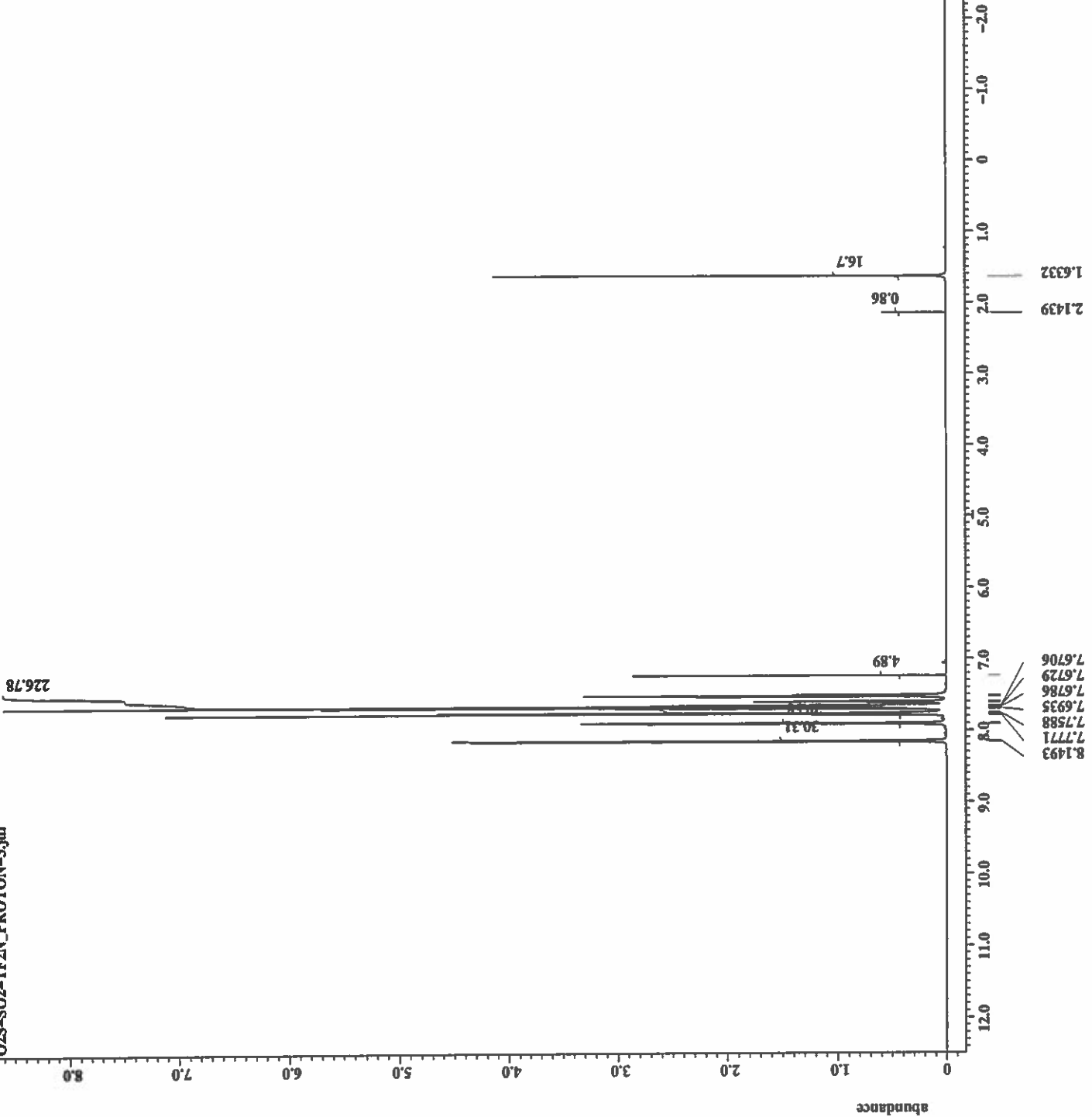
```

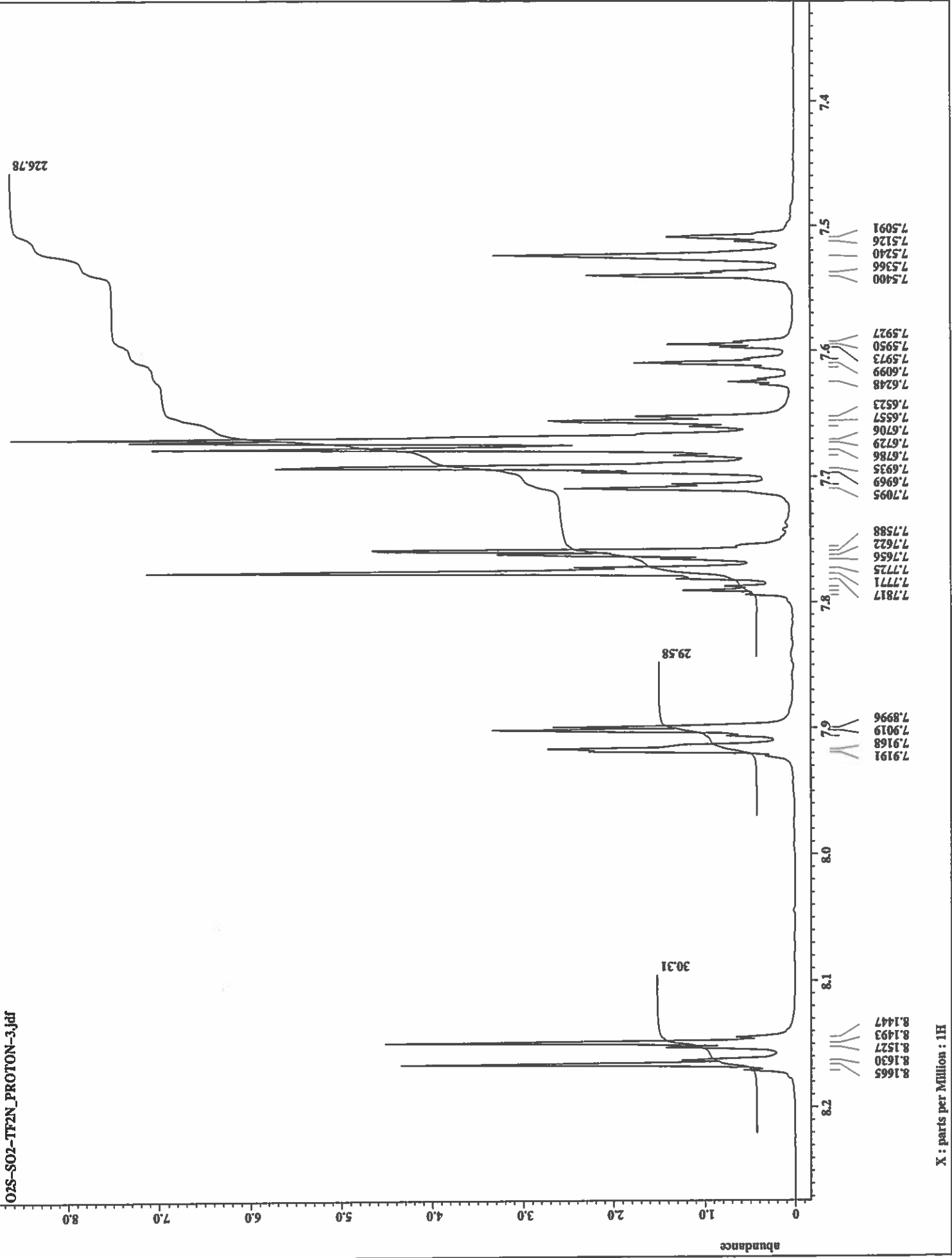
Filename = 02S-SO2-TF2N_PROTON-3
Author = Jim Davis
Experiment = single_pulse.ex2
Sample_id = 02S-SO2-TF2N
Solvent = CELEOROFORM-D
Channels = 4
Creation_time = 16-JUN-2016 10:28:39
Revision_time = 16-JUN-2016 10:03:44
Current_time = 14-OCT-2016 07:40:21

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_pcode = Off
Tri_mode = Off
Pulse_program = FALSE
Initial_wait = 1 [s]
Recvr_gain = 40
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_get = 22.1 [dC]
    
```







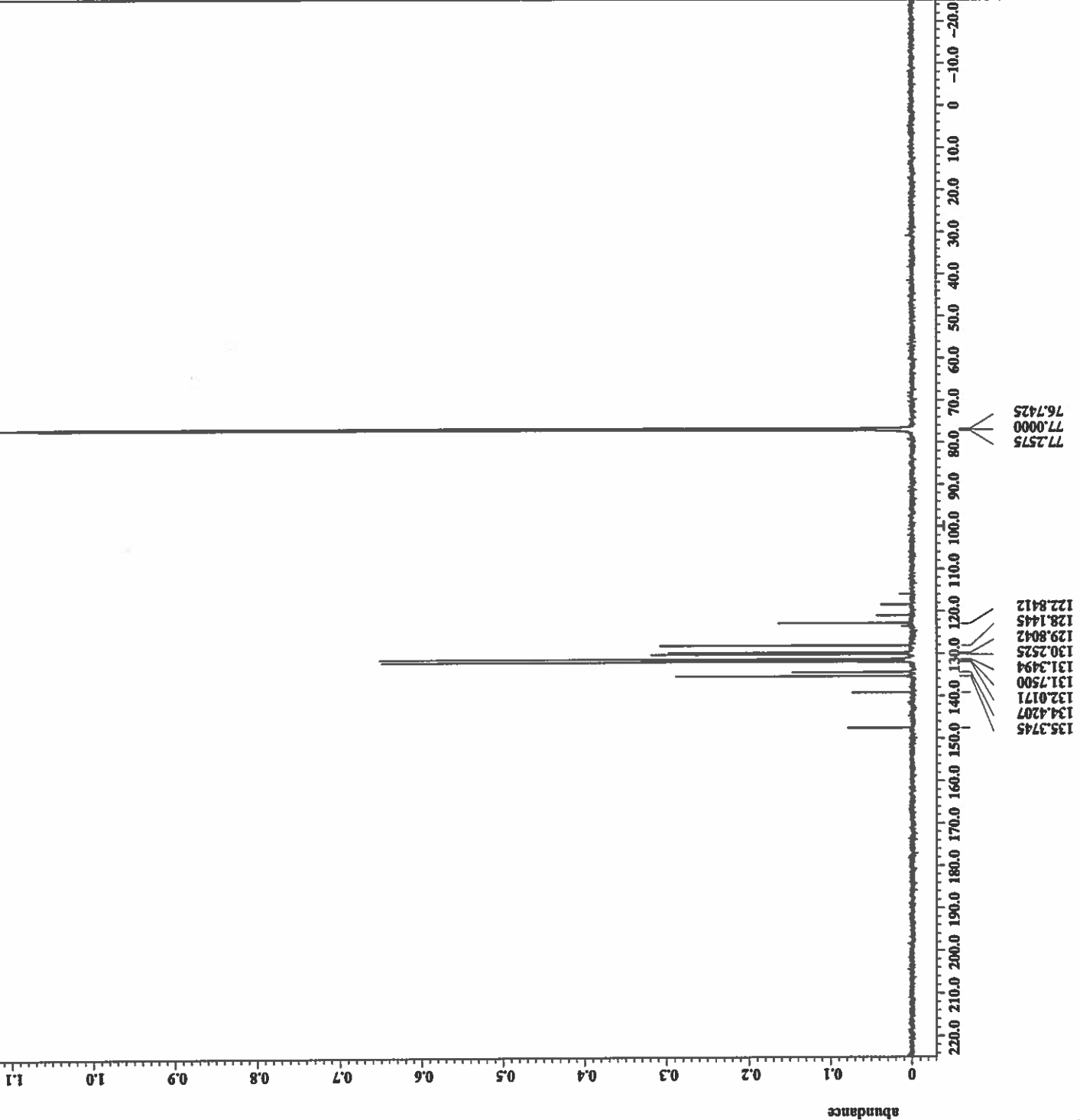
```

Filename = 02S-SO2-TF2N-CARBON-3
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = 02S-SO2-TF2N
Solvent = CHLOROFORM-D
Charger_sample = 4
Creation_time = 16-JUN-2016 19:57:49
Revision_time = 16-JUN-2016 19:40:51
Current_time = 14-OCT-2016 07:38:08

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 = 12768
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 = TRUZ
Initial_wait = 1 [s]
Noo = TRUZ
Noo_time = 2 [s]
Recvr_gain = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get = 22.7 [dC]
    
```



X : parts per Million : 13C

0.3

0.2

0.1

abundance

110.0

115.9164

118.4726

120.0

121.0384

122.8412

128.1445

130.0

129.8900

130.2525

131.3494

131.7500

132.0171

134.4207

135.3745

140.0

139.2090

150.0

147.5073



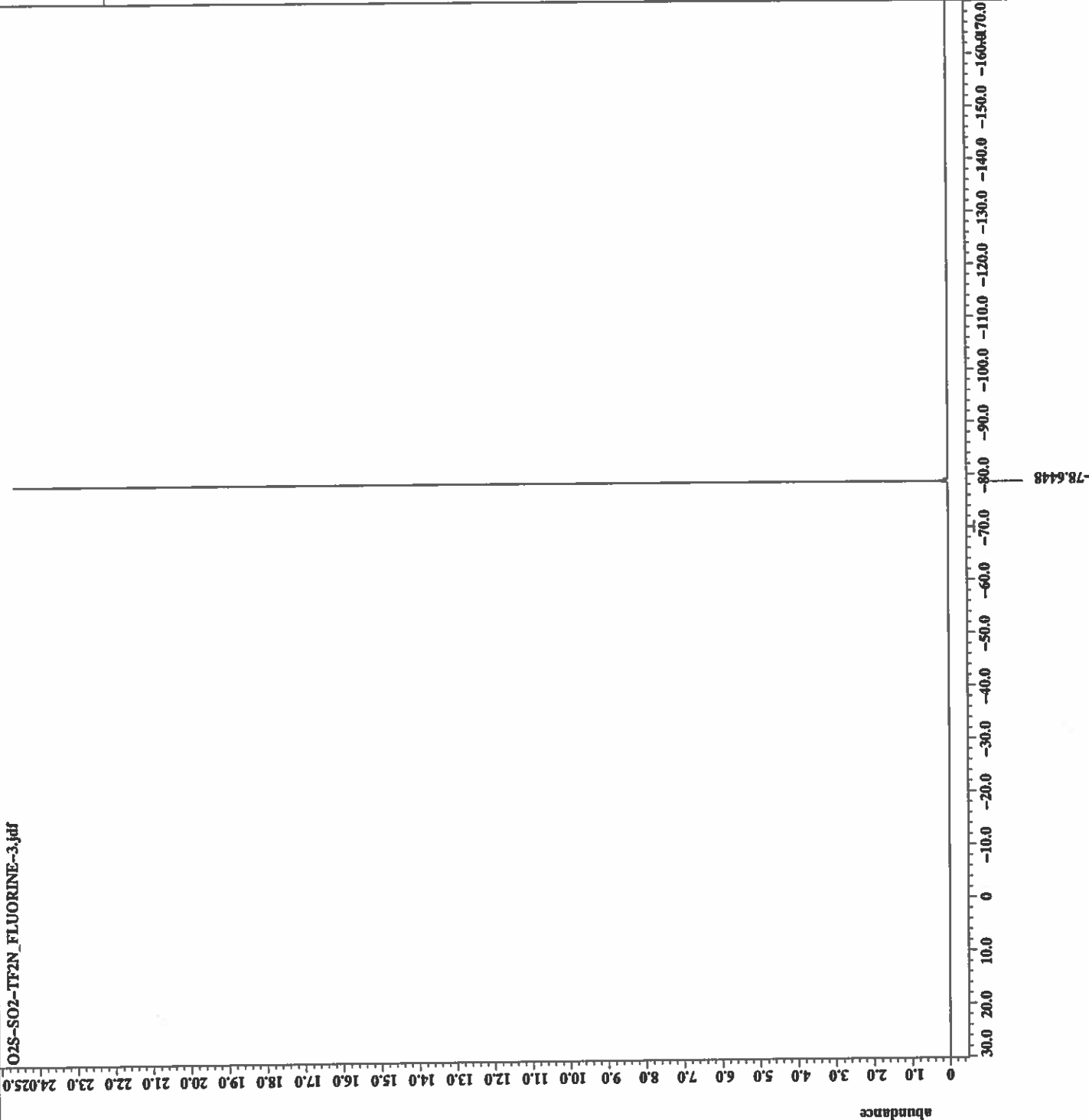
```

Filename = 02S-SO2-TF2N_FLUORINE
Author = Jim Davis
Experiment = single_pulse.exe2
Sample_id = 02S-SO2-TF2N
Solvent = CELEROFORM-D
Charger_sample = 4
Creation_time = 16-JUN-2016 10:51:22
Revision_time = 16-JUN-2016 10:34:27
Current_time = 14-OCT-2016 07:36:56

Data_format = 1D COMPLEX
Dim_size = 5248
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_pulse = Off
Tri_pulse = Off
Pente_preset = FALSE
Initial_wait = 1[s]
Recvr_gain = 46
Relaxation_delay = 4[s]
Repetition_time = 4.55574528[s]
Temp_get = 22.3[dc]
    
```

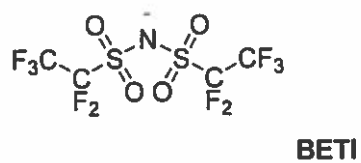
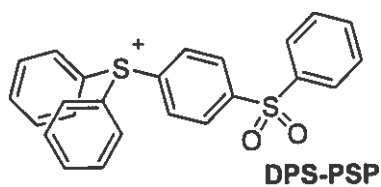


X : parts per Million : 19F

Compound 6

Elemental Analysis

^1H -, ^{13}C -, and ^{19}F -NMR Spectra



Atlantic Microlab, Inc.

Sample No. JD-SULFONIUM-6
 6180 Atlantic Blvd. Suite M
 Norcross, GA 30071
 www.atlanticmicrolab.com
 Company/School U SOUTH ALABAMA
 Dept. CHEMISTRY
 Address CHEM BLDG 223
 City, State, Zip MOBILE, AL, 36688
 Professor/Supervisor: DAVIS Name JAMES DAVIS Date 10/12/2016
 PO# / CC# _____ Phone (251) 751-0520

Element	Theory	Found	Single <input checked="" type="checkbox"/>	Duplicate <input type="checkbox"/>
C	42.91	42.95	Elements CHNOSF Present:	
H	2.44	2.44	Analyze CHN for:	
N	1.79	1.85	Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/> M.P. <u>UNK</u> B.P. <u>NONE</u> To be dried: Yes <input checked="" type="checkbox"/> No <input type="checkbox"/> Temp. <u>100C</u> Vac. <u>HIGH</u> Time <u>4H</u> Rush Service <input checked="" type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 6 PM EST on the day the sample is received by 11 AM.</small>	
Include Email Address or FAX # Below				
jdavis@southalabama.edu				

Date Received OCT 14 2016 Date Completed OCT 14 2016
 Remarks: _____



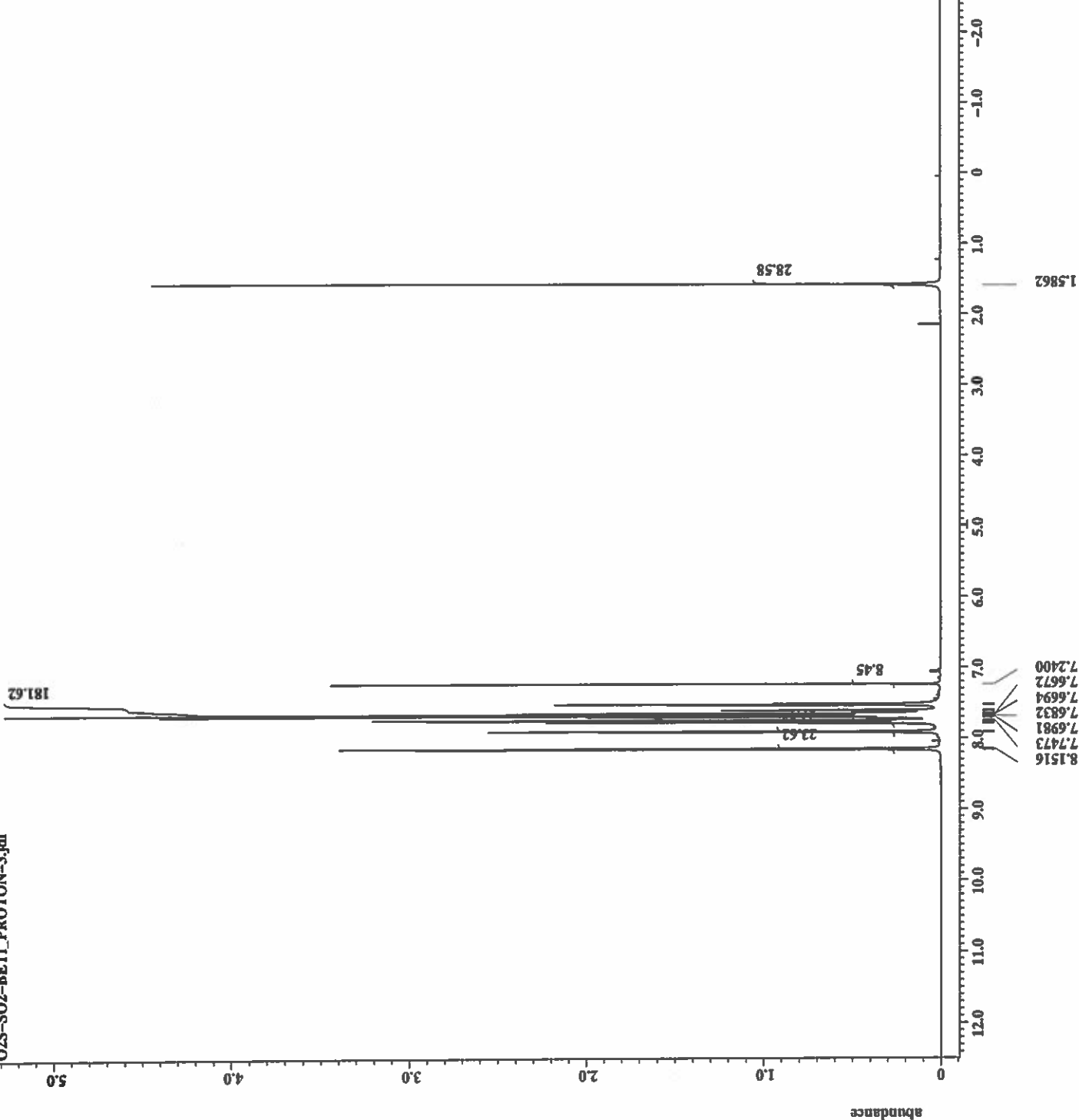
```

File: O2S-SO2-BETI_PROTON-3
Author: Jim Davis
Experiment: single_pulse.ex2
Sample ID: O2S-SO2-BETI
Solvent: CELOSOFORM-D
Changer Sample: 3
Creation Time: 16-JUN-2016 10:14:38
Revision Time: 16-JUN-2016 09:57:43
Current Time: 14-OCT-2016 07:30:18

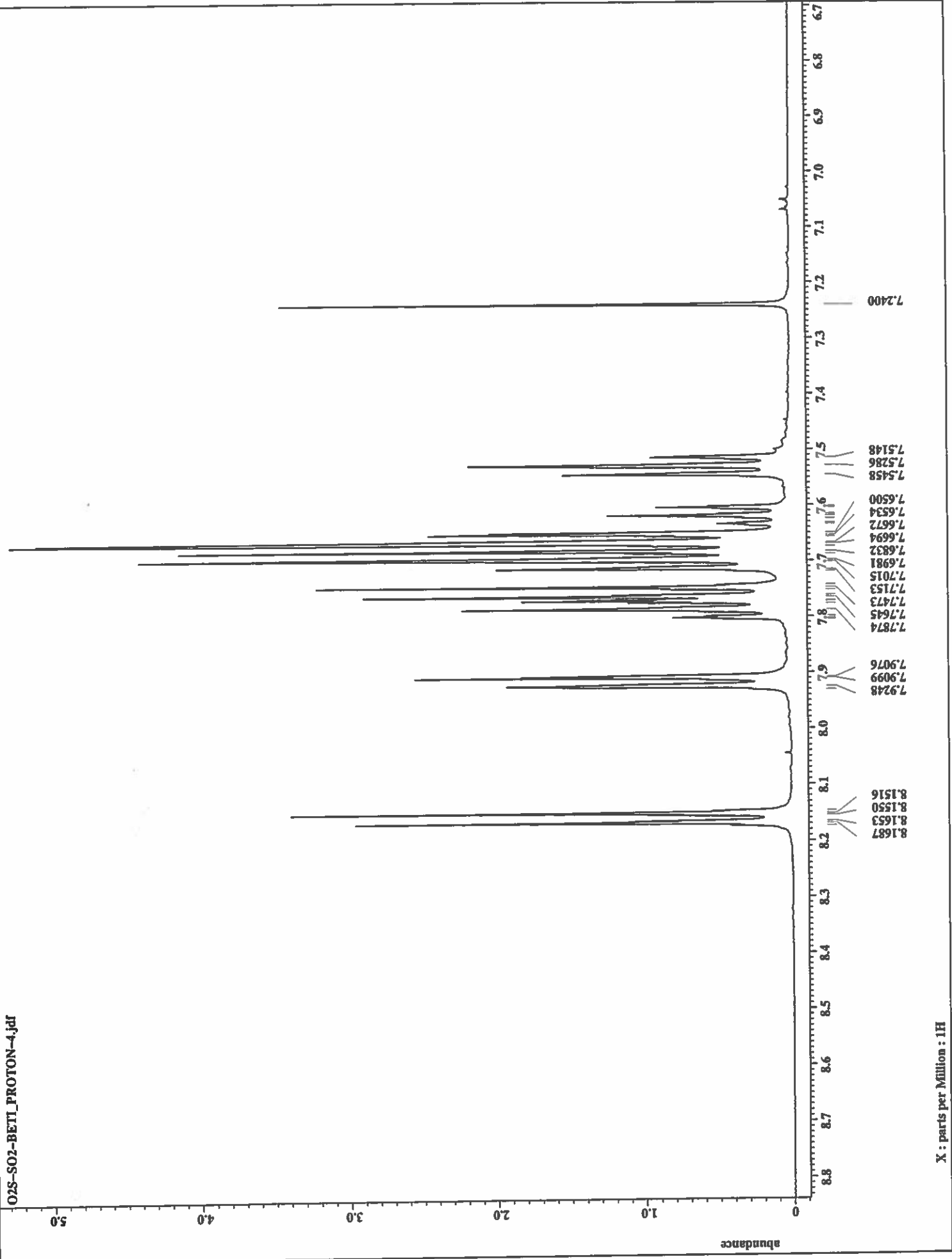
Data Format: 1D COMPLEX
Dir Size: 13107
Dir Title:
Dim Units: [ppm]
Dimensions: X
Site: ECA 500
Spectrometer: JNM-ECA500

Field Strength: 11.7473579 [F] (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

X90 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
Daube Presat: FALSE
Initial Wait: 1 [s]
Recvr Gain: 44
Relaxation Delay: 4 [s]
Repetition Time: 5.74587904 [s]
Temp Get: 22.3 [dC]
    
```



025-SO2-BETI_PROTON-4.jdt



X : parts per Million : 1H



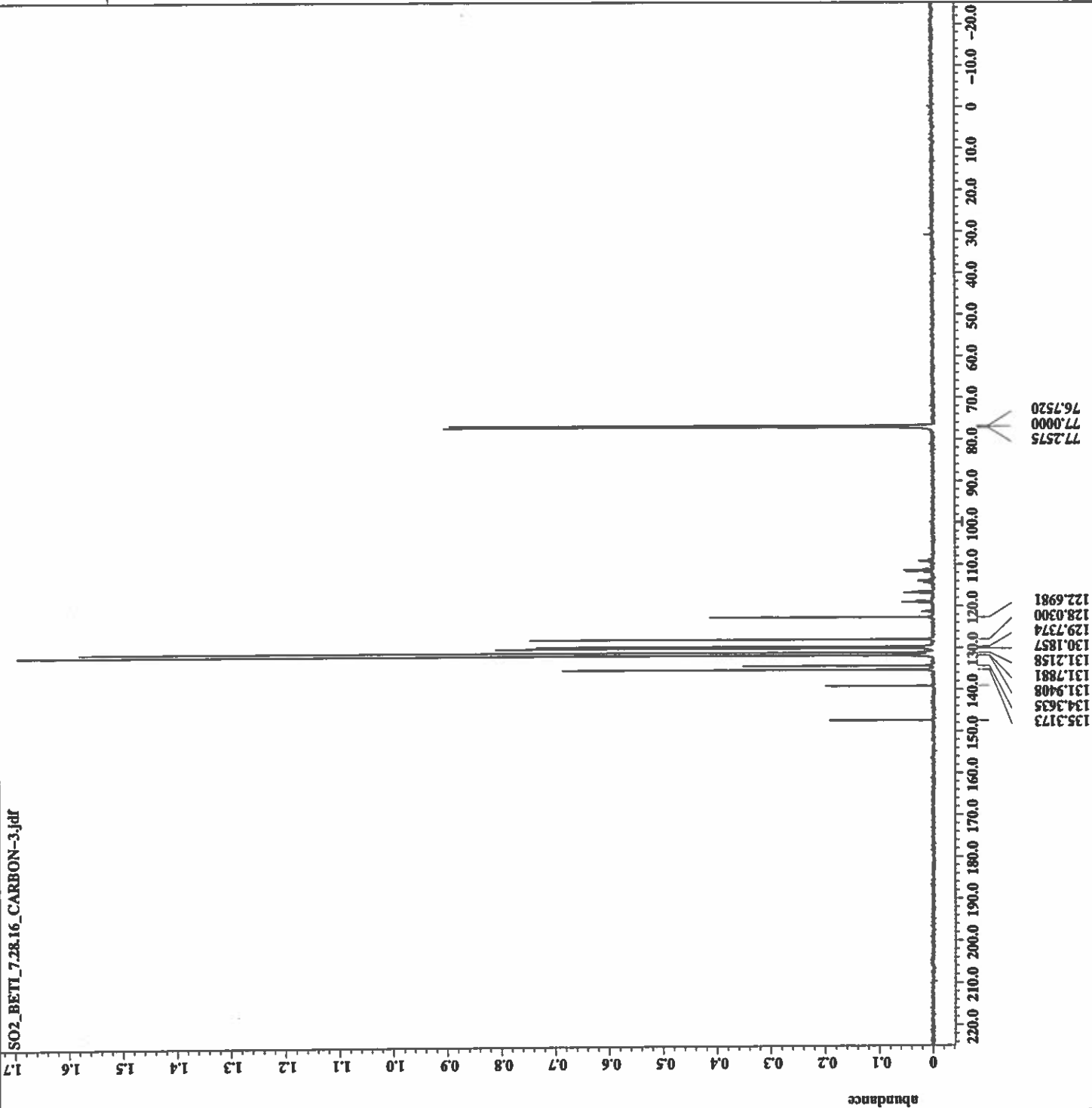
```

Filename = SO2_BETI_7.28.16_CARB
Author = Jim Davis
Experiment = single_pulse_dec
Sample_id = SO2_BETI_7.28.16
Solvent = CHLOROFORM-D
Changer_sample = 16
Creation_time = 28-JUL-2016 19:10:41
Revision_time = 28-JUL-2016 18:50:29
Current_time = 14-OCT-2016 07:32:56

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[MHz]
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_poc = 20.5[db]
Irr_poise = WAJRT
Decoupling = TRU2
Initial_wait = 1[s]
Noe = TRU2
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get = 21.7[dc]
    
```



0.5

0.4

0.3

0.2

0.1

abundance

150.0

140.0

147.4024

139.1994

135.5367

135.3173

135.0884

134.3635

131.9408

131.7881

131.5783

131.2158

130.1857

129.8614

129.7374

128.0300

122.6981

121.3341

121.0671

119.3120

119.0449

118.7779

117.0228

116.7557

116.4887

114.6665

114.3807

114.0755

113.7702

112.0438

111.7386

111.4238

111.1186

109.3922

109.0869

X : parts per Million : 13C



```

= 02S-SO2-BETI_FLUORINE
= Jim Davis
= single_pulse.ex2
= 02S-SO2-BETI
= CHLOROFORM-D
= 3
= 16-JUN-2016 10:45:16
= 16-JUN-2016 10:28:22
= 14-OCT-2016 07:29:13

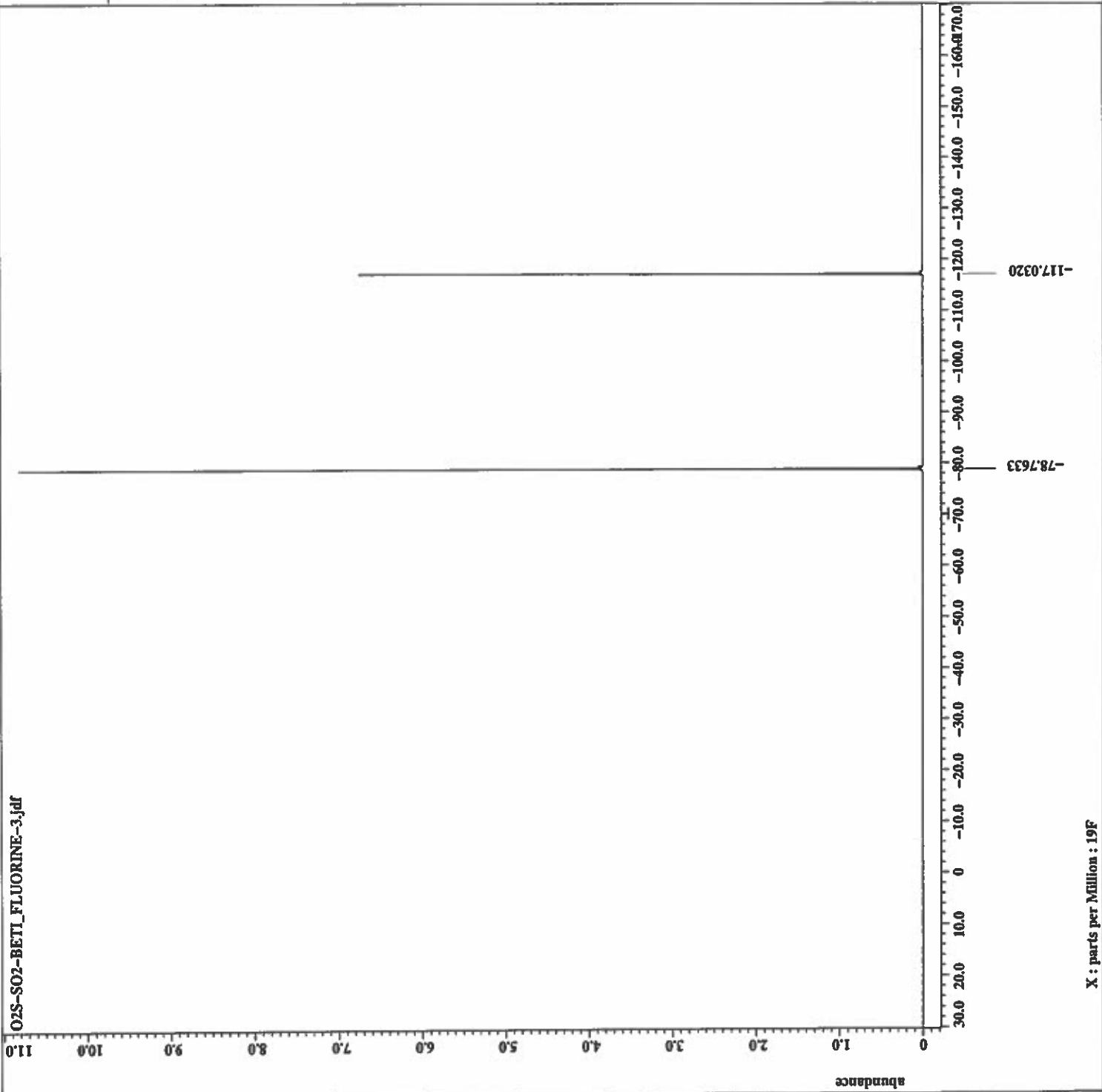
= 1D COMPLEX
= 52428
= 19F
= [ppm]
= X
= ECA 500
= JNM-ECA500

Spectrometer

Data_format
Dia_size
Dia_title
Dia_units
Dimensions
Site

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

X_90_width
X_acq_time
X_angle
X_stn
X_pulse
Irr_mode
Tri_mode
Dante_presat
Initial_wait
Recvr_gain
Relaxation_delay
Repetition_time
Temp_get
    
```



Compiled NMR Data

Compound 1 (TPS Tf₂N):

¹H (CDCl₃, 500 MHz): δ 7.35-7.79 (m, 3H), 7.66-7.72 (m, 6H), and 7.60-7.65 (m, 6H) ppm.

¹³C (CDCl₃, 125 MHz): δ 134.86, 131.76, 130.90, 123.98, 123.69, 121.14, 118.58 and 116.02 ppm.

¹⁹F (CDCl₃, 470 MHz): δ -78.62 ppm.

Compound 2 (TPS BETI):

¹H (CDCl₃, 500 MHz): δ 7.74-7.78 (m, 3H), 7.66-7.72 (m, 6H), and 7.60-7.64 (m, 6H) ppm.

¹³C (CDCl₃, 125 MHz): δ 134.97, 131.75, 130.88, 123.89, 119.46, 119.20, 118.93, 117.17, 116.91, 116.64, 114.19, 113.88, 111.85, 111.55, 109.51, and 109.21 ppm.

¹⁹F (CDCl₃, 470 MHz): δ -78.77 and -116.98 ppm.

Compound 3 (DPS-POP Tf₂N):

¹H (CDCl₃, 500 MHz): δ 7.73-7.79 (m, 2H), 7.67-7.73 (m, 4H), 7.60-7.65 (m, 6H), 7.40-7.44 (tt, 2H), 7.23-7.28 (m, 1H), 7.16-7.21 (m, 2H), and 7.07-7.11 (m, 2H) ppm.

¹³C (CDCl₃, 125 MHz): δ 163.68, 153.75, 134.56, 133.36, 131.61, 130.45, 130.36, 125.80, 124.53, 123.63, 121.08, 120.62, 119.59, 118.52, 115.96, and 114.67 ppm.

¹⁹F (CDCl₃, 470 MHz): δ - 78.59 ppm.

Compound 4 (DPS-POP BETI):

¹H (CDCl₃, 500 MHz): δ 7.73-7.79 (m, 2H), 7.67-7.73 (m, 4H), 7.60-7.66 (m, 6H), 7.40-7.45 (tt, 2H), 7.23-7.28 (m, 1H), 7.16-7.20 (m, 2H), and 7.07-7.11 (m, 2H) ppm.

¹³C (CDCl₃, 125 MHz): δ 163.74, 153.78, 134.57, 133.38, 131.62, 130.45, 130.37, 125.82, 124.57, 120.64, 121.70, 121.45, 121.20, 119.79, 119.59, 119.43, 119.16, 118.89, 117.13, 116.87, 116.60, 114.80, 114.69, 114.40, 114.13, 113.83, 112.10, 111.80, 111.49, 111.18, 109.80, 109.46, and 109.45 ppm.

¹⁹F (CDCl₃, 470 MHz): δ -78.73 and -116.96 ppm.

Compound 5 (DPS-PSP Tf₂N):

¹H (CDCl₃, 500 MHz): δ 8.14-8.18 (dd, 2H), 7.88-7.92 (dd, 2H), 7.74-7.80 (m, 4H), 7.64-7.72 (m, 8H), 7.58-7.63 (m, 1H), and 7.50-7.55 (m, 2H) ppm.

¹³C (CDCl₃, 125 MHz): δ 147.51, 139.21, 135.37, 134.42, 132.02, 131.75, 131.35, 130.25, 129.89, 129.80, 128.14, 123.20, 122.84, 121.03, 118.47, and 115.92 ppm.

¹⁹F (CDCl₃, 470 MHz): δ -78.64 ppm.

Compound 6 (DPS-PSP BETI):

¹H (CDCl₃, 500 MHz): δ 8.14-8.19 (dd, 2H), 7.88-7.92 (dd, 2H), 7.74-7.82 (m, 4H), 7.64-7.72 (m, 8H), 7.58-7.63 (m, 1H), and 7.49-7.54 (m, 2H) ppm.

¹³C (CDCl₃, 125 MHz): δ 147.40, 139.20, 135.20, 134.36, 131.94, 131.79, 131.22, 130.19, 129.86, 129.74, 128.03, 122.70, 121.60, 121.33, 121.07, 119.31, 119.05, 118.78, 117.02, 116.75, 116.49, 114.47, 114.20, 113.77, 112.04, 11.74, 111.42, 111.12, 109.39, and 109.09 ppm.

¹⁹F (CDCl₃, 470 MHz): δ -78.74 and -117.01 ppm.