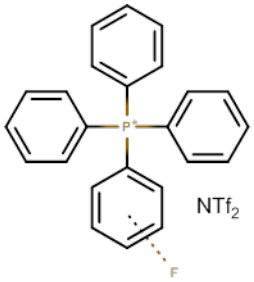
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Tuning the Melting Point of Selected Ionic Liquids Through Adjustment of the Cation's Dipole Moment

General Information:

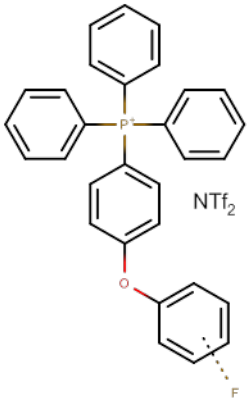
Commercial reagents were obtained from Aldrich Chemical and Oakwood Chemicals and used without further purification. ^{1}H, ^{19}F, ^{31}P and ^{13}C NMR was recorded on a 500 MHz JEOL spectrometer using $CDCl_3$ as a solvent at room temperature.

General Procedure for the Synthesis of Fluorophenyltriphenyl Phosphonium [NTf_2^-] ILs



In a 50 ml heavy wall pressure vessels with an internal thread containing steering bar, Fluoro-iodobenzene (1.0 equiv), triphenyl phosphine (1.0 equiv), $Pd(OAc)_2$ (1.5 mol%) and Xylene (15 ml) were added under nitrogen atmosphere and the reaction mixture stirred at 140 °C for 2 hours. The reaction mixture was then cooled down to the room temperature and filtered to yield pure fluorophenyltriphenyl phosphonium iodide as a pale-white solid. The [NTf_2^-] salt was obtained by anion exchange of $KNTf_2$ (1.0 equiv) and phosphonium salt (1.0 equiv) in water for 15 min at room temperature. The reaction mixture was then extracted three times with DCM and brine solution. The combined organic extracts were dried over anhydrous Na_2SO_4 and solvents were removed under reduced pressure to furnish desired fluorophenyltriphenyl phosphonium [NTf_2^-] as a white solid.

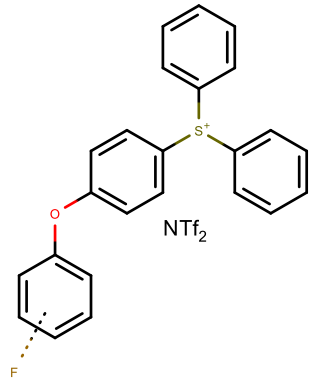
General Procedure for the Synthesis of (fluorophenoxy)phenyltriphenylphosphanium [NTf_2^-] ILs



First 3-(fluorophenoxy)bromobenzene was prepared using following method: In a 100 ml heavy wall pressure vessels with an internal thread containing steering bar, 3-fluorophenylboronic acid (2.0 equiv, 10 g)), 4-bromophenol (1.0 equiv), triethylamine (5.0 equiv), Copper(II) acetate (1.0 equiv), and MS 4Å(2.0 g) powder and the reaction mixture stirred for 5 hours at room temperature. After the completion of reaction the mixture was filtered through a filter paper and concentrated under reduced pressure. Further purification with column chromatography (Hexane/EtOAc) resulted pure 3-(fluorophenoxy)bromobenzene. Next step, In a 50 ml heavy wall pressure vessels with an internal thread containing steering bar, 3-(fluorophenoxy)bromobenzene (1.0 equiv), triphenyl phosphine (1.0 equiv), $NiCl_2.6H_2O$ (10 mole%) ethylene glycol (10 ml) were added under nitrogen atmosphere and the reaction mixture stirred at 160 °C for 12 hours. The reaction mixture was then extracted three times with DCM and brine solution and concentrated under reduced pressure to yield pure 3-(fluorophenoxy)phenyltriphenylphosphanium bromide. The [NTf_2^-] salt was obtained by anion exchange of $KNTf_2$ (1.0 equiv) and phosphonium salt (1.0 equiv) in water for 15 min at room temperature. The reaction mixture was then extracted three times with DCM and brine solution. The combined organic extracts were dried over anhydrous Na_2SO_4 and solvents were removed

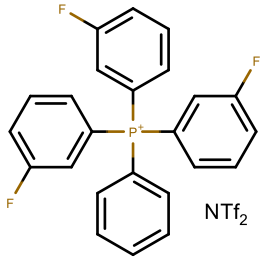
under reduced pressure to furnish pure 3-(fluorophenoxy)phenyltriphenylphosphanium [NTf_2^-] as a white solid. Same procedure was applied for the synthesis of 2-(fluorophenoxy)phenyltriphenylphosphanium [NTf_2^-] and 4-(fluorophenoxy)phenyltriphenylphosphanium [NTf_2^-].

General Procedure for the Synthesis of triphenylsulfonium [NTf_2^-] ILs



In a 100 ml round bottom flask containing a steering bar, Diphenyl Sulfoxide (1.0 equiv, 5g) and Fluorophenoxyl benzene (1.1 equiv) in DCM (50 ml) was stirred for 10 minutes at room temperature. Triflic anhydride solution (1.05 equiv) in DCM was added dropwise to the reaction mixture at room temperature and reaction mixture stirred for overnight at room temperature. After completion of the reaction, solvent was removed under vacuum and washed with ether to remove the unreacted materials to furnish the desired sulfonium product. The [NTf_2^-] salt was obtained by anion exchange of excess $KNTf_2$ (5 equiv) and sulfonium salt (1.0 equiv) in water-methanol for 30 min at room temperature. The reaction mixture was then extracted three times with DCM and brine solution and the combined organic extracts were dried over anhydrous Na_2SO_4. Then solvents were removed under reduced pressure to result desired triphenylsulfonium [NTf_2^-].

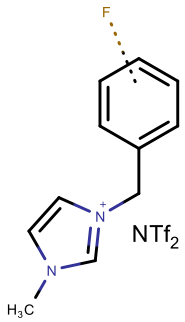
Synthesis of tris(3-fluorophenyl)(phenyl)phosphonium [NTf_2^-] IL



In a 50 ml heavy wall pressure vessels with an internal thread containing steering bar, Bromobenzene (1.0 equiv), Tris(3-fluorophenyl)phosphine (1.0 equiv), $NiCl_2.6H_2O$ (10 mole%) ethylene glycol (10 ml) were added under nitrogen atmosphere and the reaction mixture stirred at 180 °C for 15 hours. The reaction mixture was then cooled down to the room temperature and was extracted three times with DCM / brine solution and concentrated under reduced pressure to yield tris(3-fluorophenyl)(phenyl)phosphonium bromide. The [NTf_2^-] salt was obtained by anion exchange of $KNTf_2$ (1.0 equiv) and phosphonium salt (1.0 equiv) in water for 15 min at room temperature. The reaction mixture was then extracted three times with DCM and brine solution. The combined organic extracts were dried over anhydrous Na_2SO_4 and solvents were removed under reduced pressure to furnish pure of tris(3-fluorophenyl)(phenyl)phosphonium [NTf_2^-].

Same method was applied for the synthesis of tris(4-fluorophenyl)(phenyl)phosphonium [NTf_2^-].

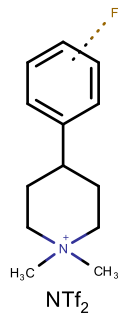
Synthesis of 3-benzyl-1-methyl-imidazolium [NTf_2^-] ILs



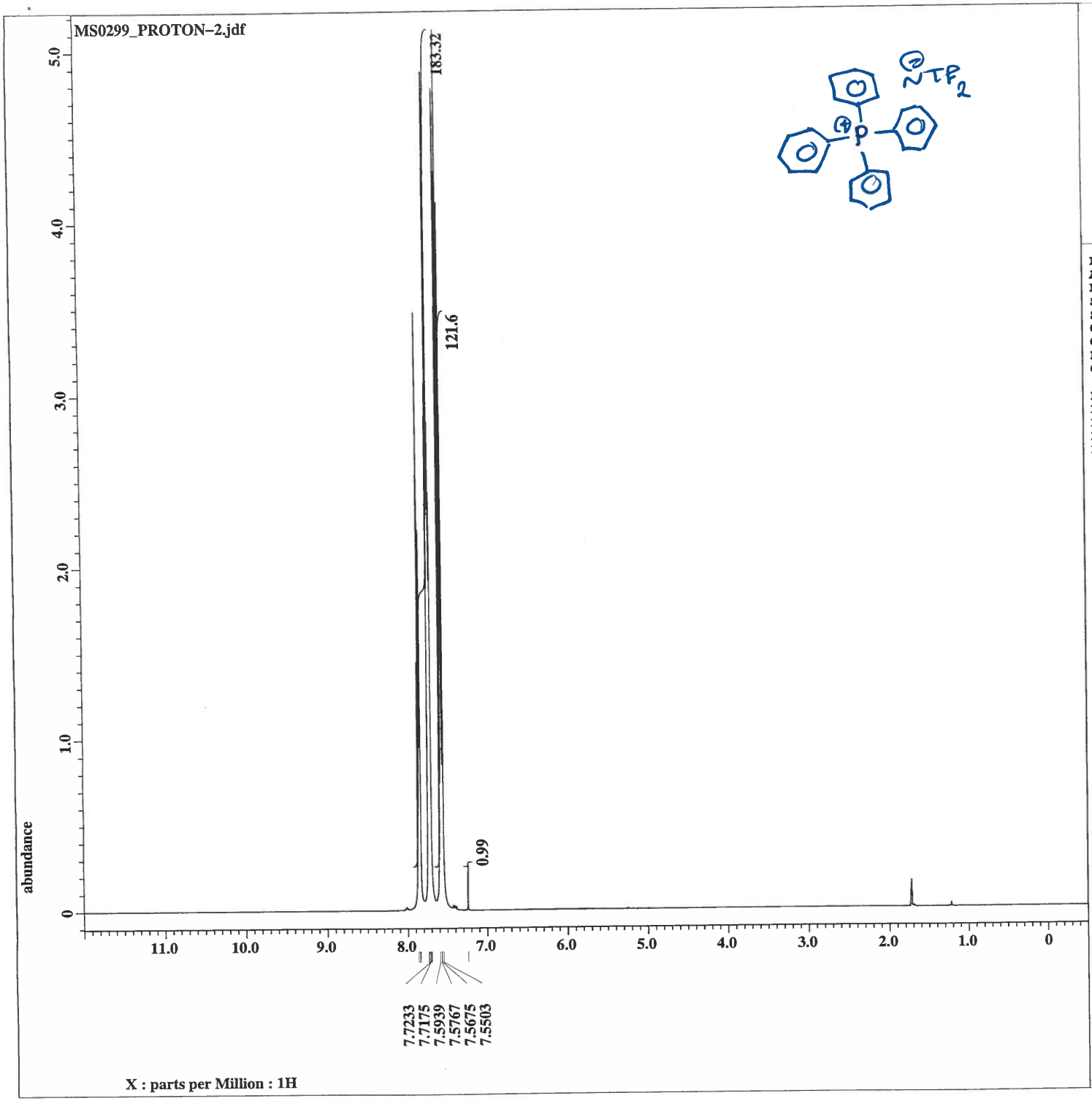
In a 100 ml round bottom flask containing a steering bar, 1-methylimidazol (1.0 equiv, 5g) and Benzyl Bromide (1.0 equiv) in THF (50 ml) was stirred for overnight at 40 °C. Then the reaction mixture was filtered and white solid yielded as a pure product. Anion exchange with $KNTf_2$ (1.0 equiv) carried out in water and stirred for 30 min at room temperature. The reaction mixture was then extracted three times with DCM and brine solution and the combined organic extracts were dried

over anhydrous Na_2SO_4. Then solvents were removed under reduced pressure to produce pure 3-benzyl-1-methyl-imidazolium [NTf_2^-] as a colorless liquid.

1,1-dimethyl-4-phenylpiperidinium [NTf_2^-] ILs



For the synthesis of 1,1-dimethyl-4-phenylpiperidin-1-ium [NTf_2^-], first 1,1-dimethyl-4-phenylpiperidinium iodide salt was prepared using following method. In a 100 ml round bottom flask containing a steering bar, 4-phenylpiperidine (1.0 equiv, 2 g), iodomethane (5.0 equiv), and potassium bicarbonate (1.5 equiv) in methanol (50 ml) was stirred for 24 hours at room temperature. Then solvent was removed under vacuum and the mixture was dissolved in DCM and filtered through filter paper. Filtrate was concentrated under reduced pressure and pure product was obtained in high yield. Anion exchange with $KNTf_2$ in water furnished 1,1-dimethyl-4-phenylpiperidinium [NTf_2^-]. The reaction mixture was then extracted with DCM and the combined organic extracts were dried over anhydrous Na_2SO_4. Then solvents were removed under reduced pressure to produce pure 1,1-dimethyl-4-phenylpiperidinium [NTf_2^-] as a white solid.



SOUTH ALABAMA JAGUARS

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Solvent	= CHLOROFORM-D
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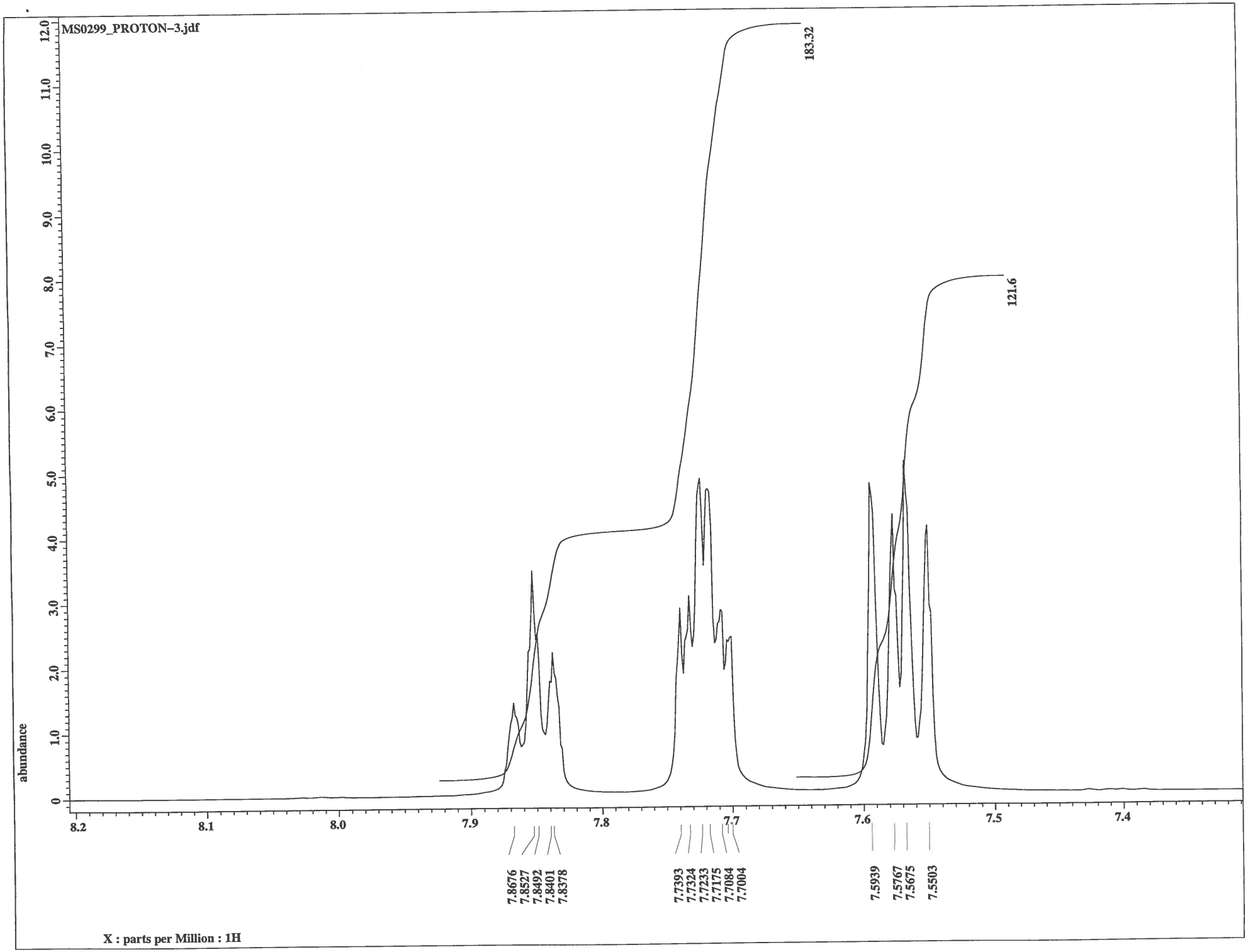
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7.0
8.0
9.0
10.0
11.0
12.0
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.8676
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7.7393
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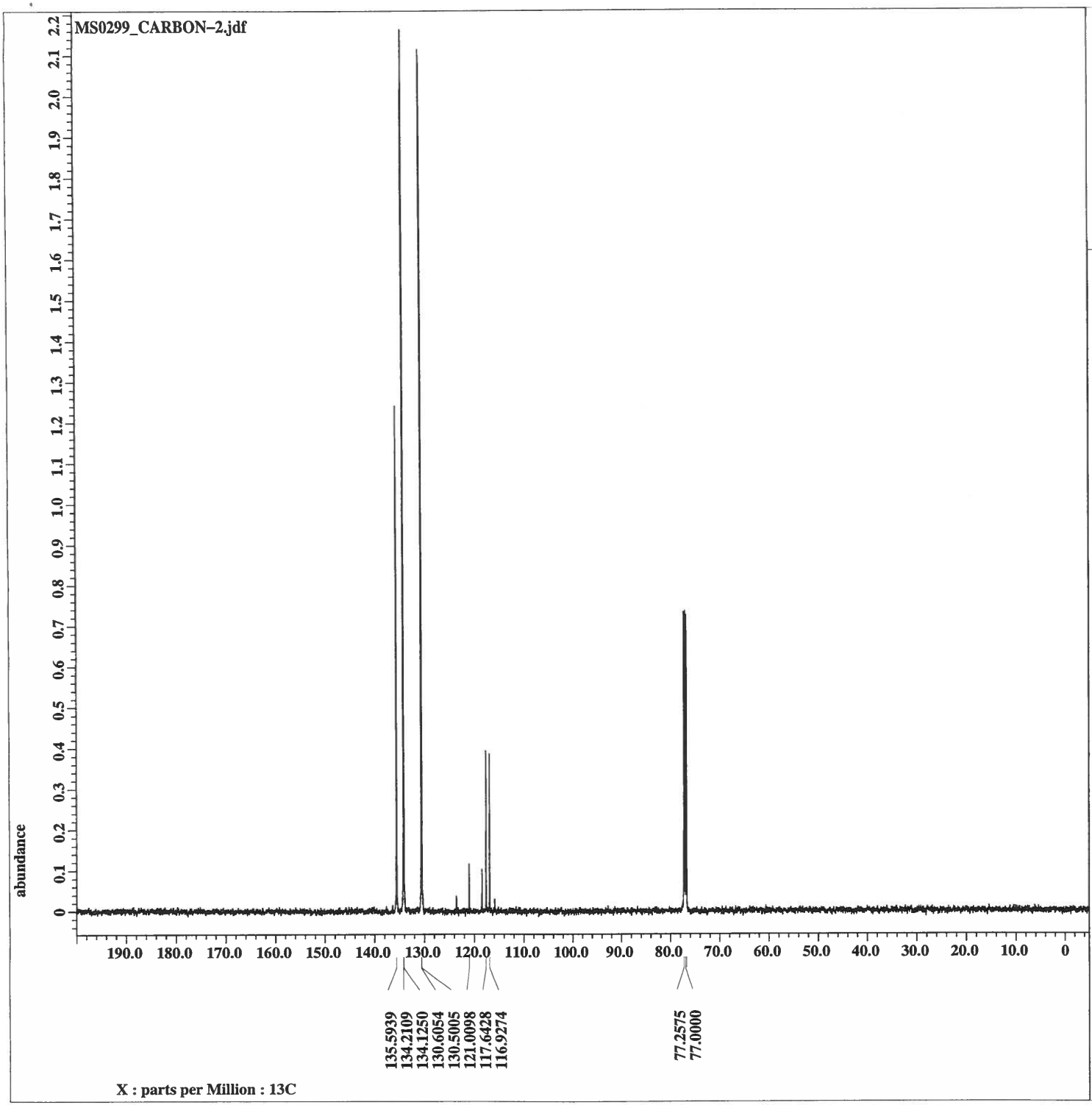

SOUTH ALABAMA JAGUARS

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Solvent	= CHLOROFORM-D
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Mod_return	= 1
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Noe	= TRUE
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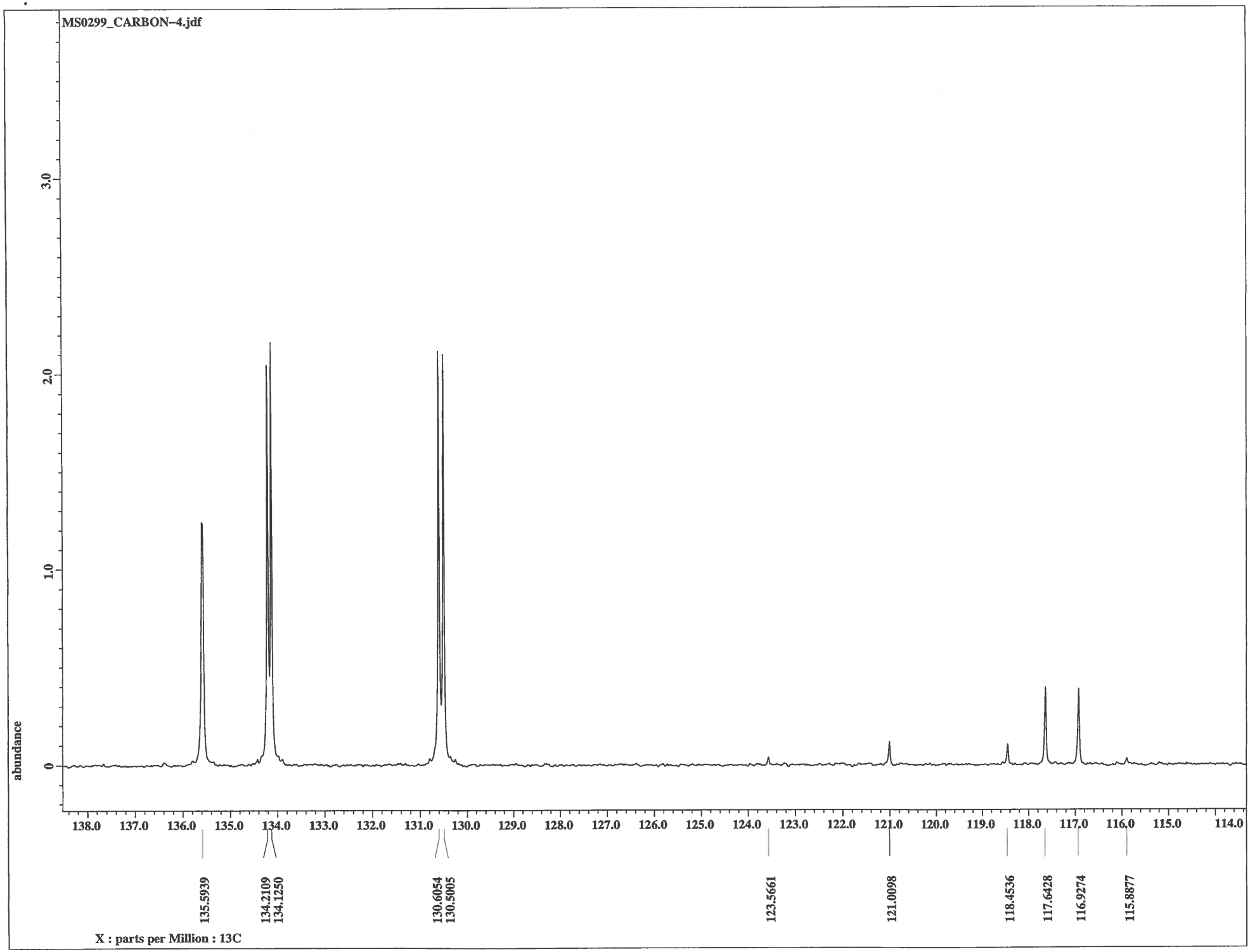
MS0299_CARBON-4.jdf
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126.0
125.0
124.0
123.0
122.0
121.0
120.0
119.0
118.0
117.0
116.0
115.0
114.0
135.5939
134.2109
134.1250
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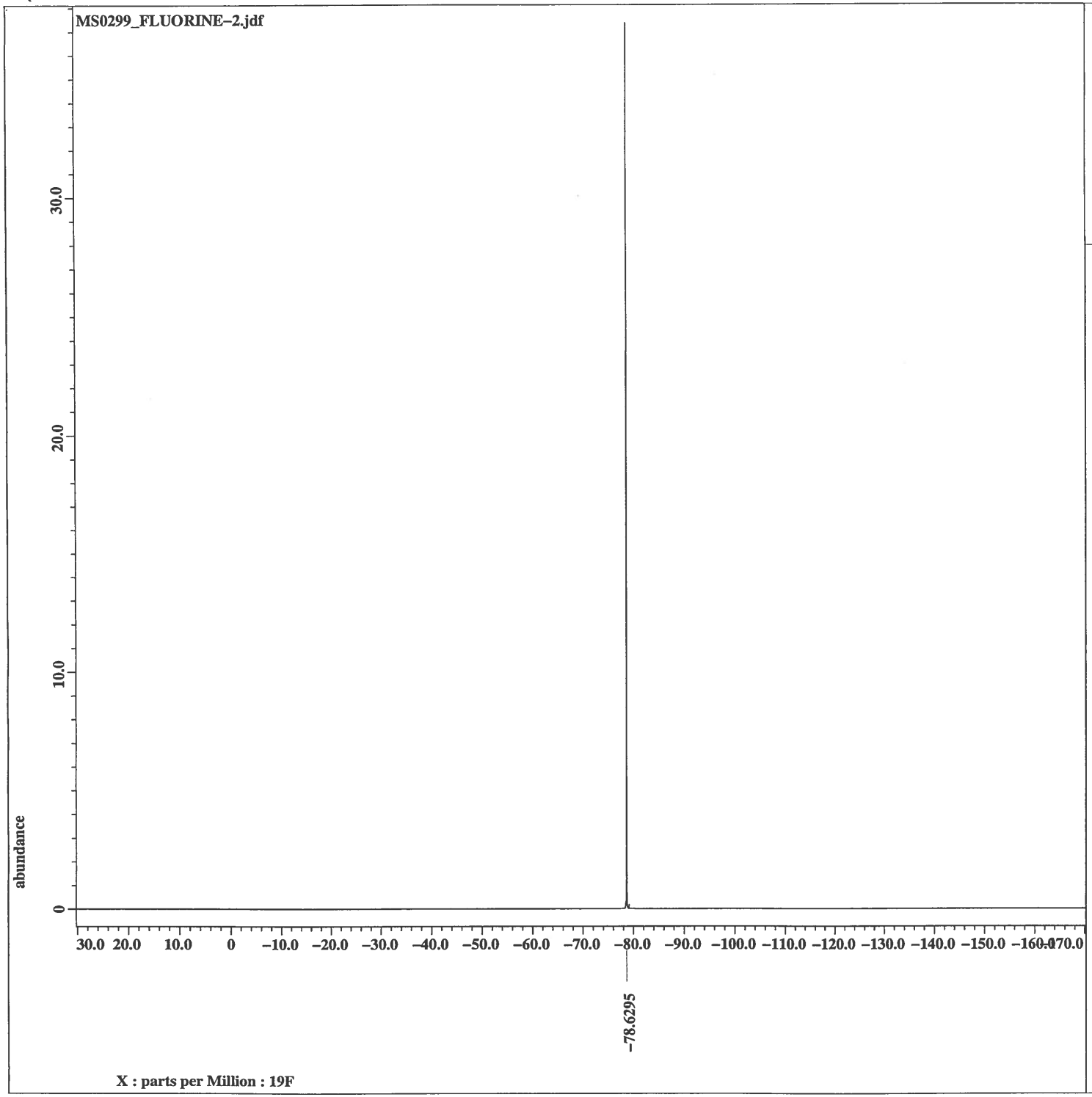
116.9274
115.8877
X : parts per Million : 13C



SOUTH ALABAMA JAGUARS™

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Solvent	= CHLOROFORM-D
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Dante_presat	= FALSE
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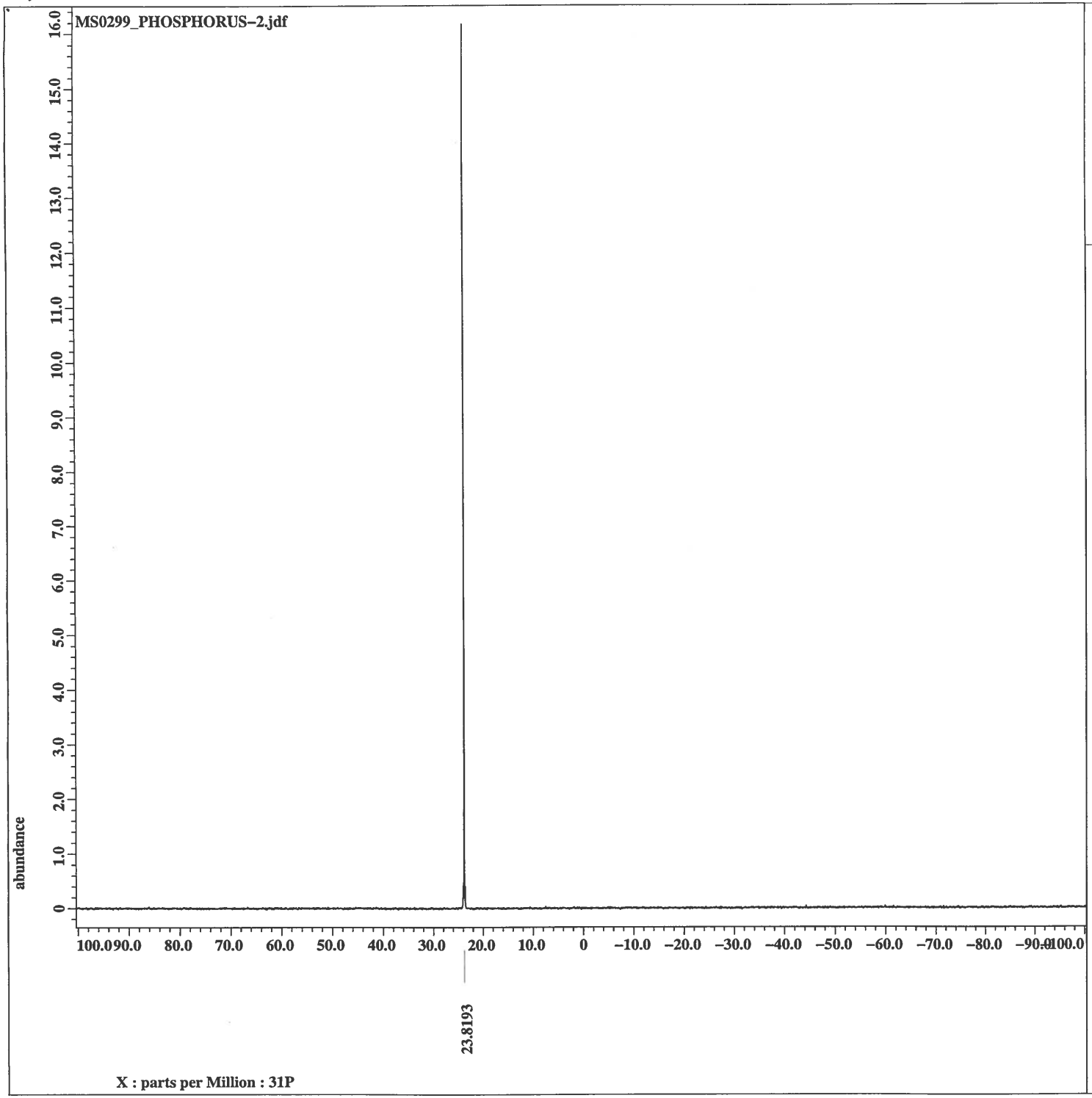

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Noe	= TRUE
Noe_time	= 2[s]
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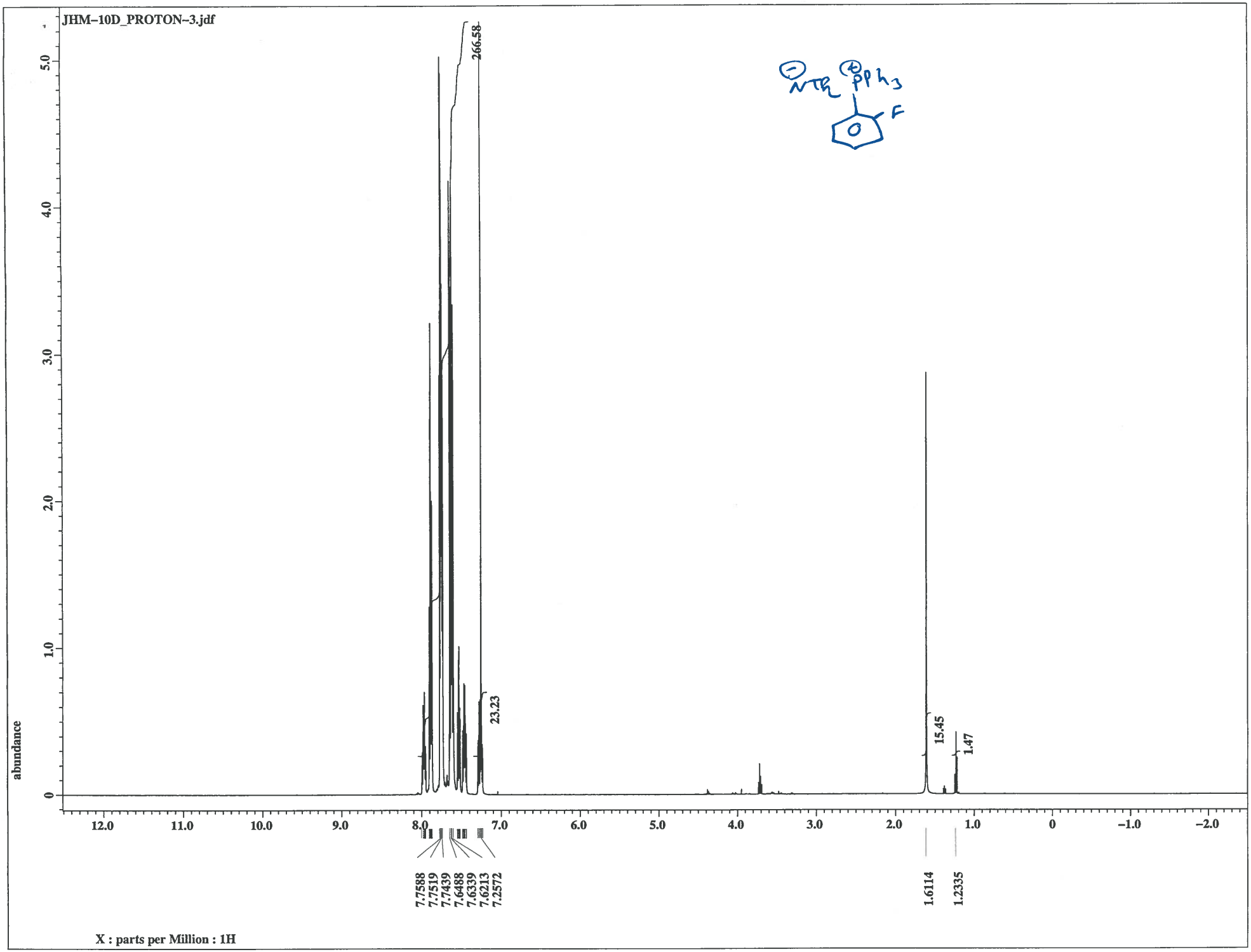
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12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
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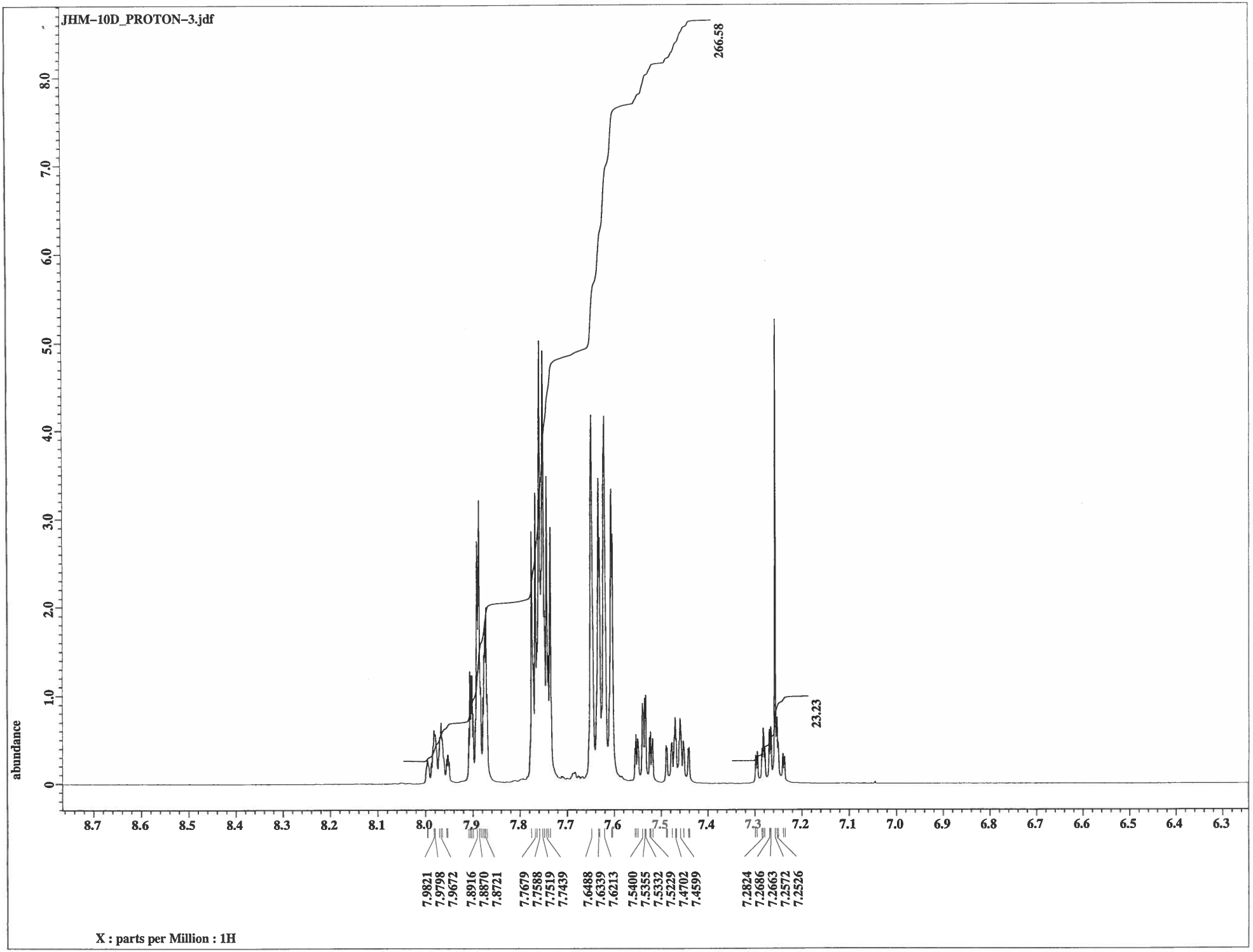
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8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
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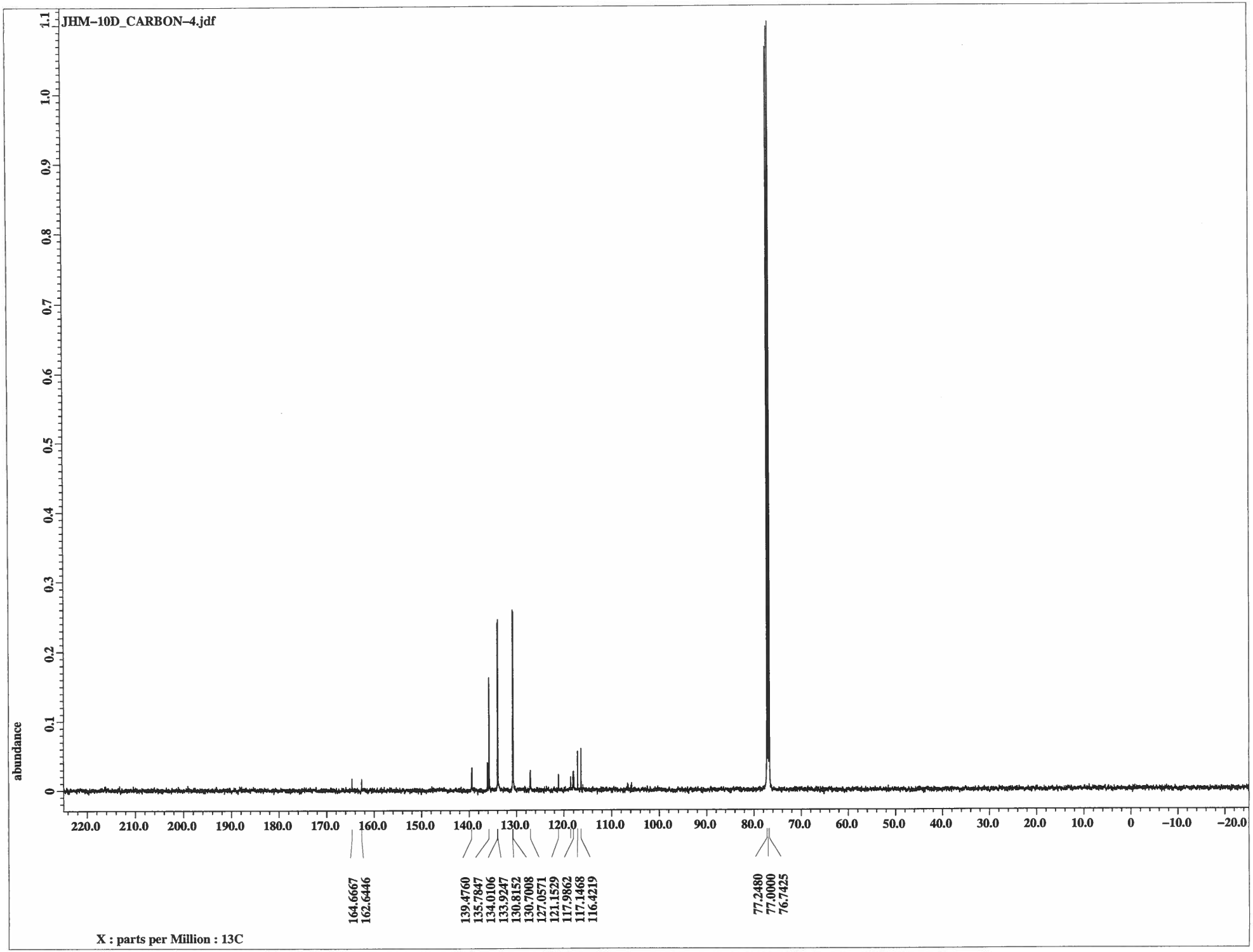
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0.4
0.3
0.2
0.1
0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
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162.6446
139.4760
135.7847
134.0106
133.9247
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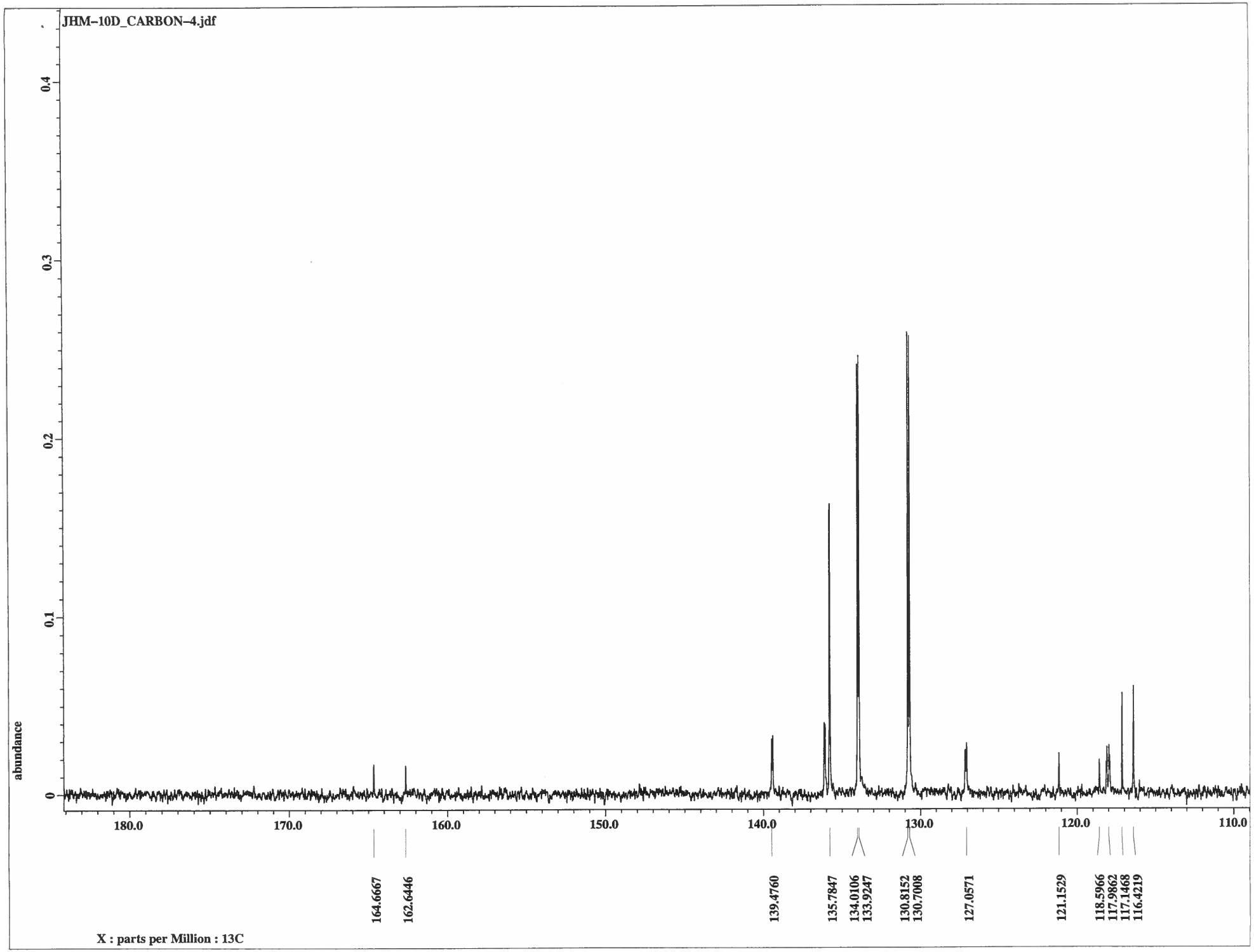
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120.0
110.0
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162.6446
139.4760
135.7847
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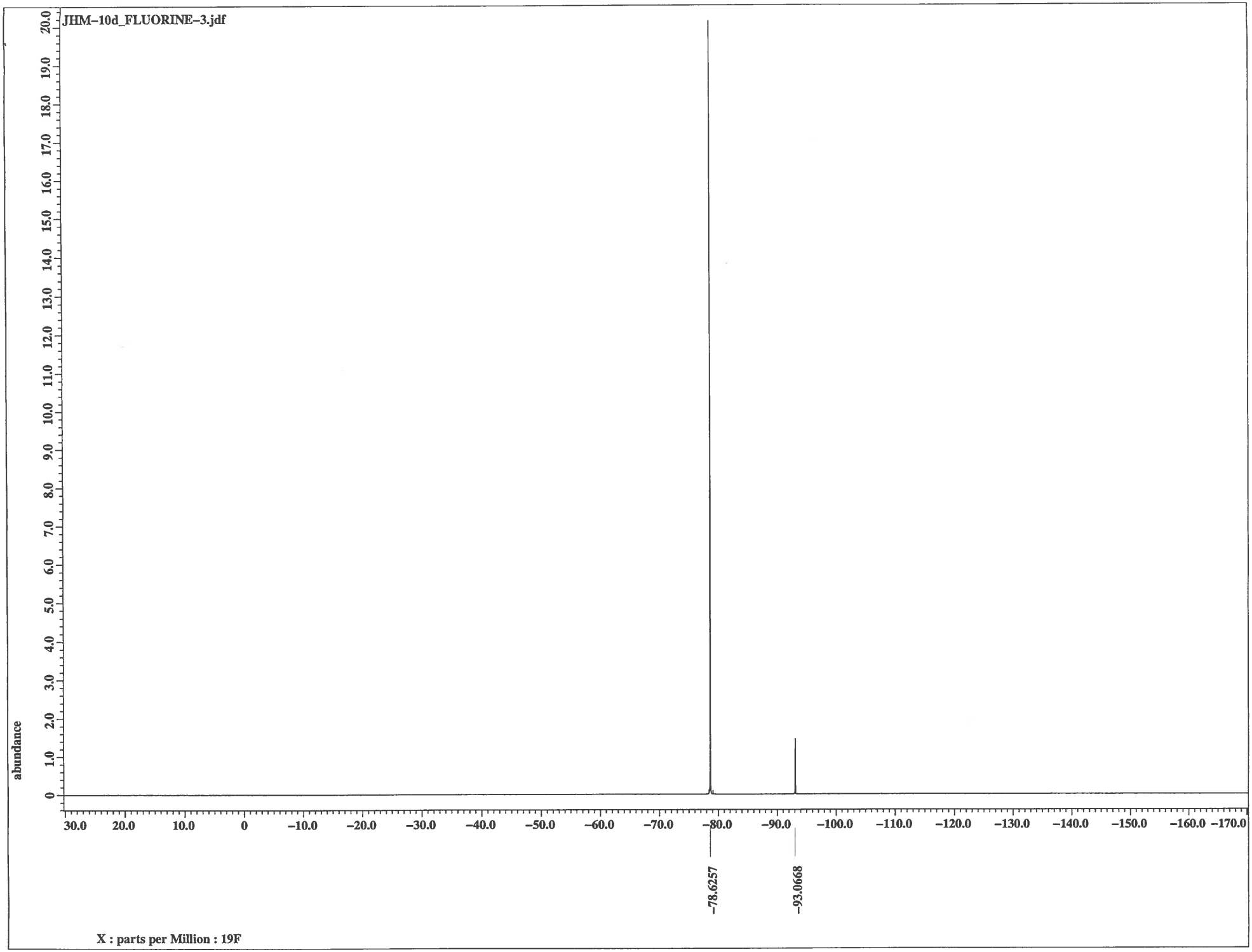
X : parts per Million : 13C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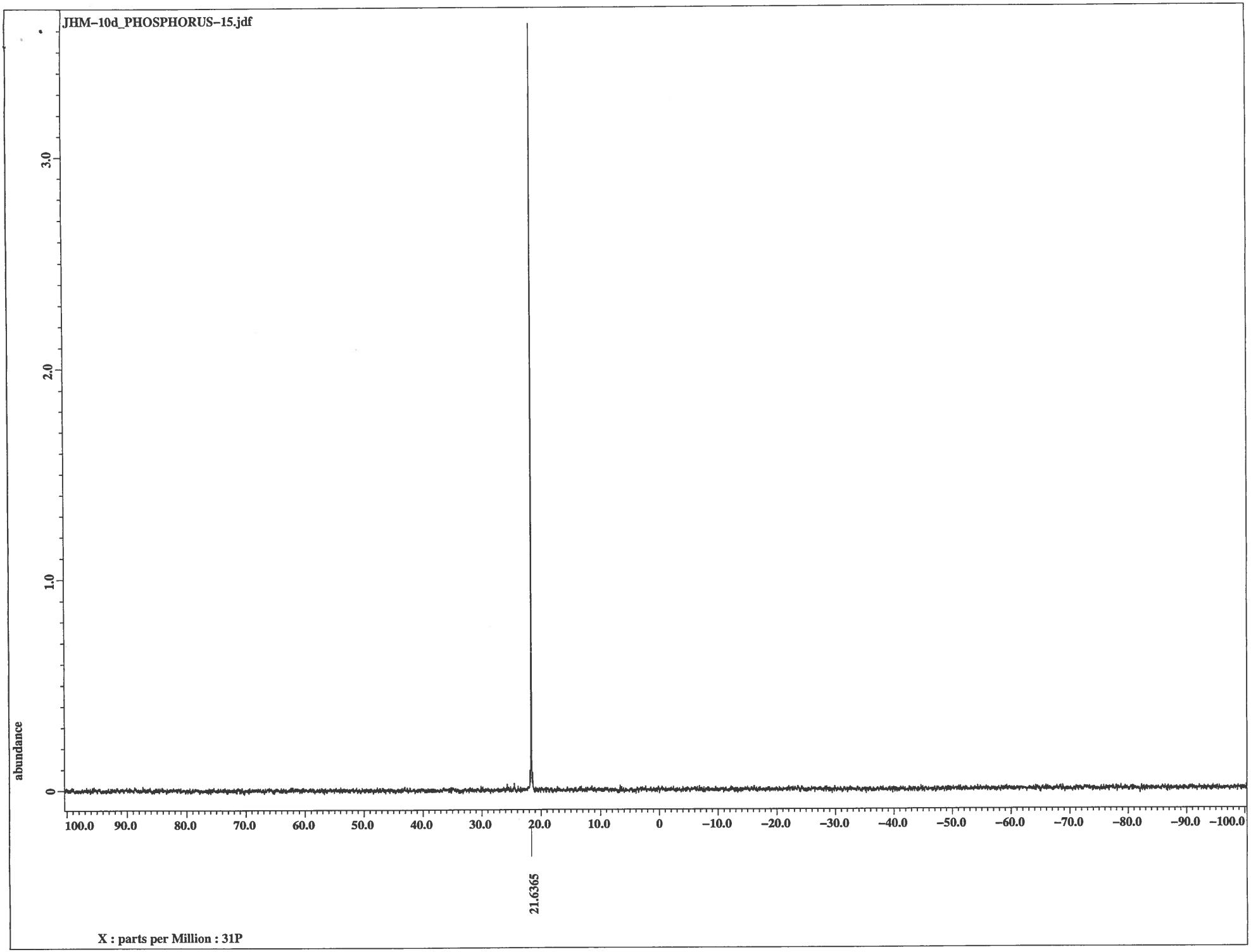
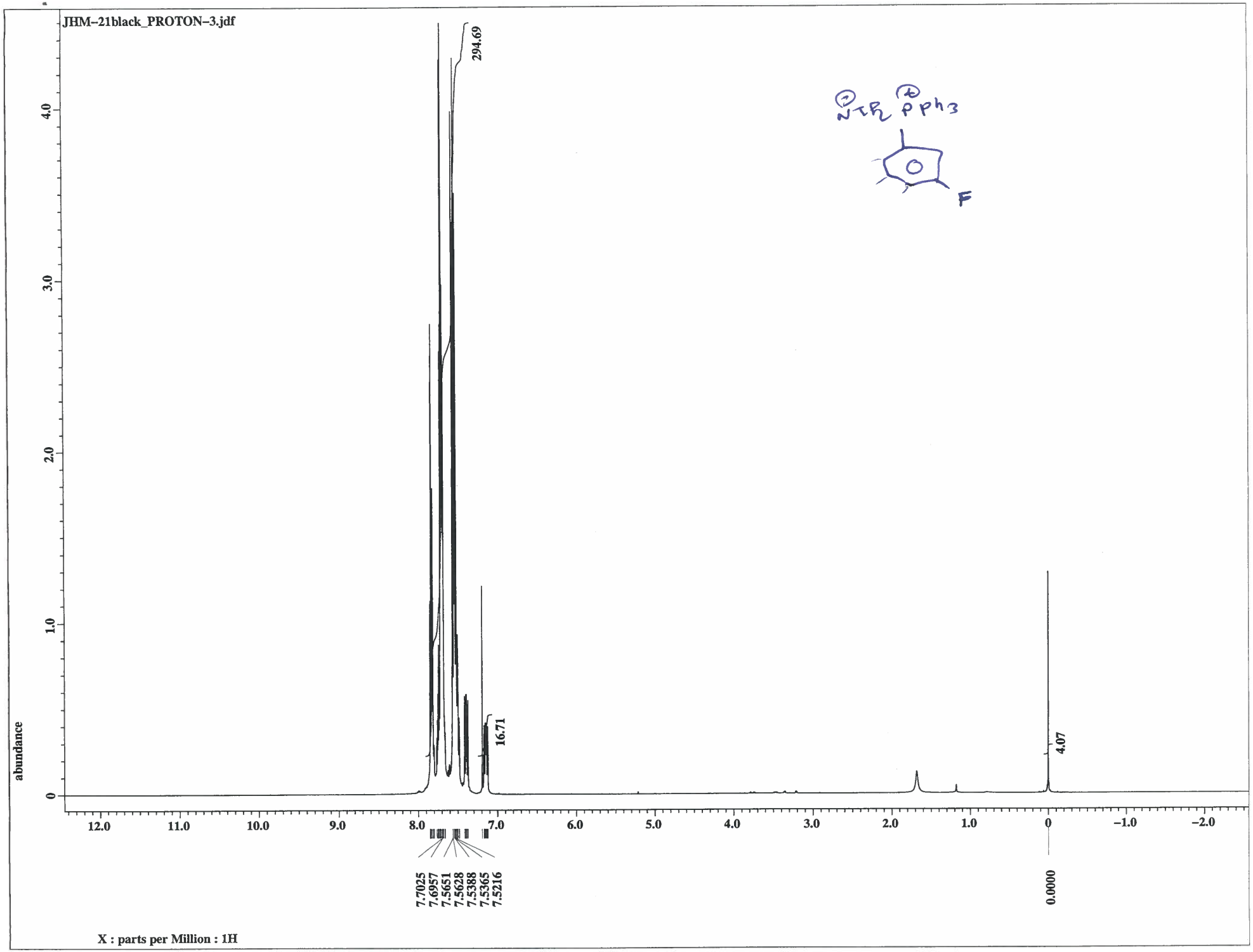
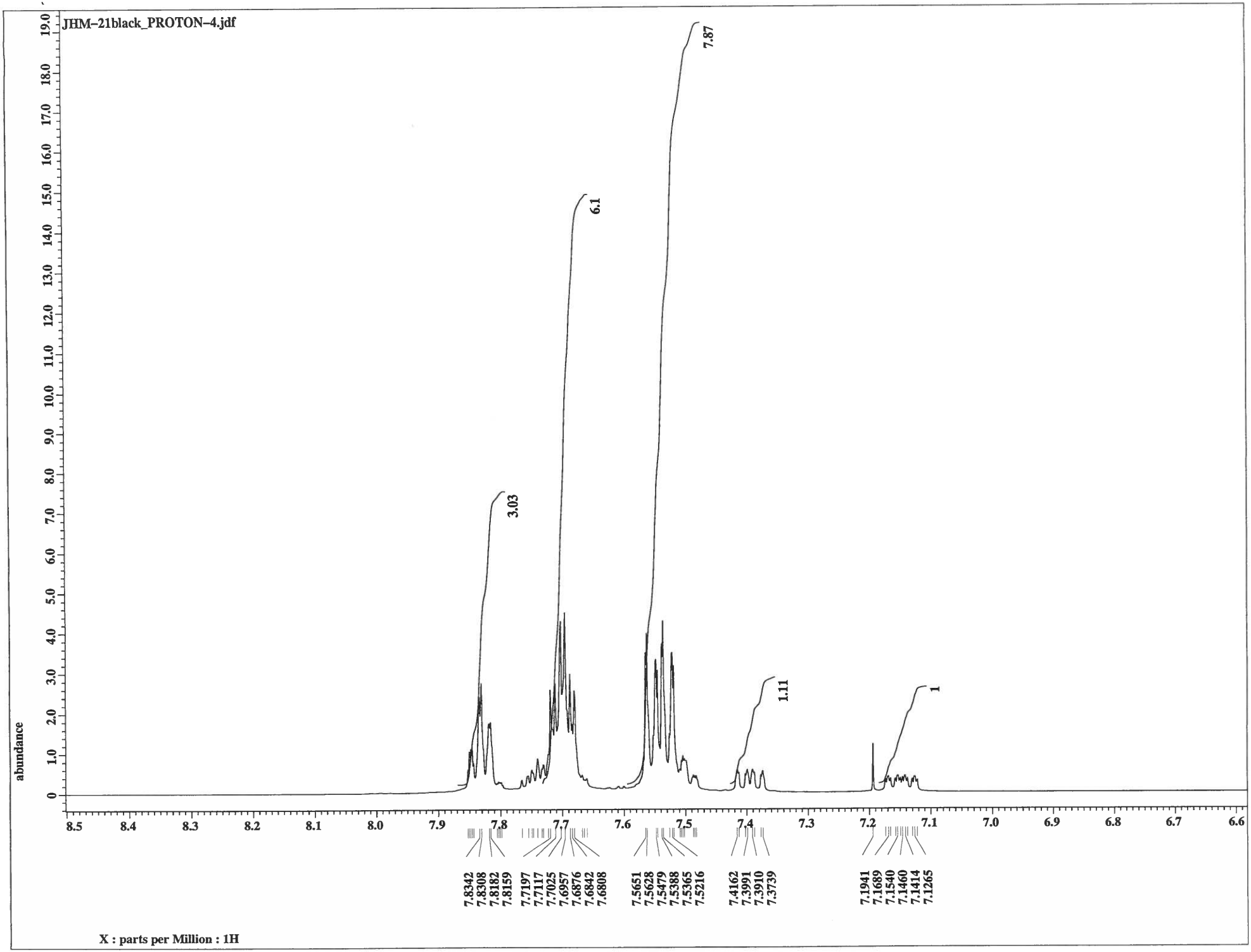
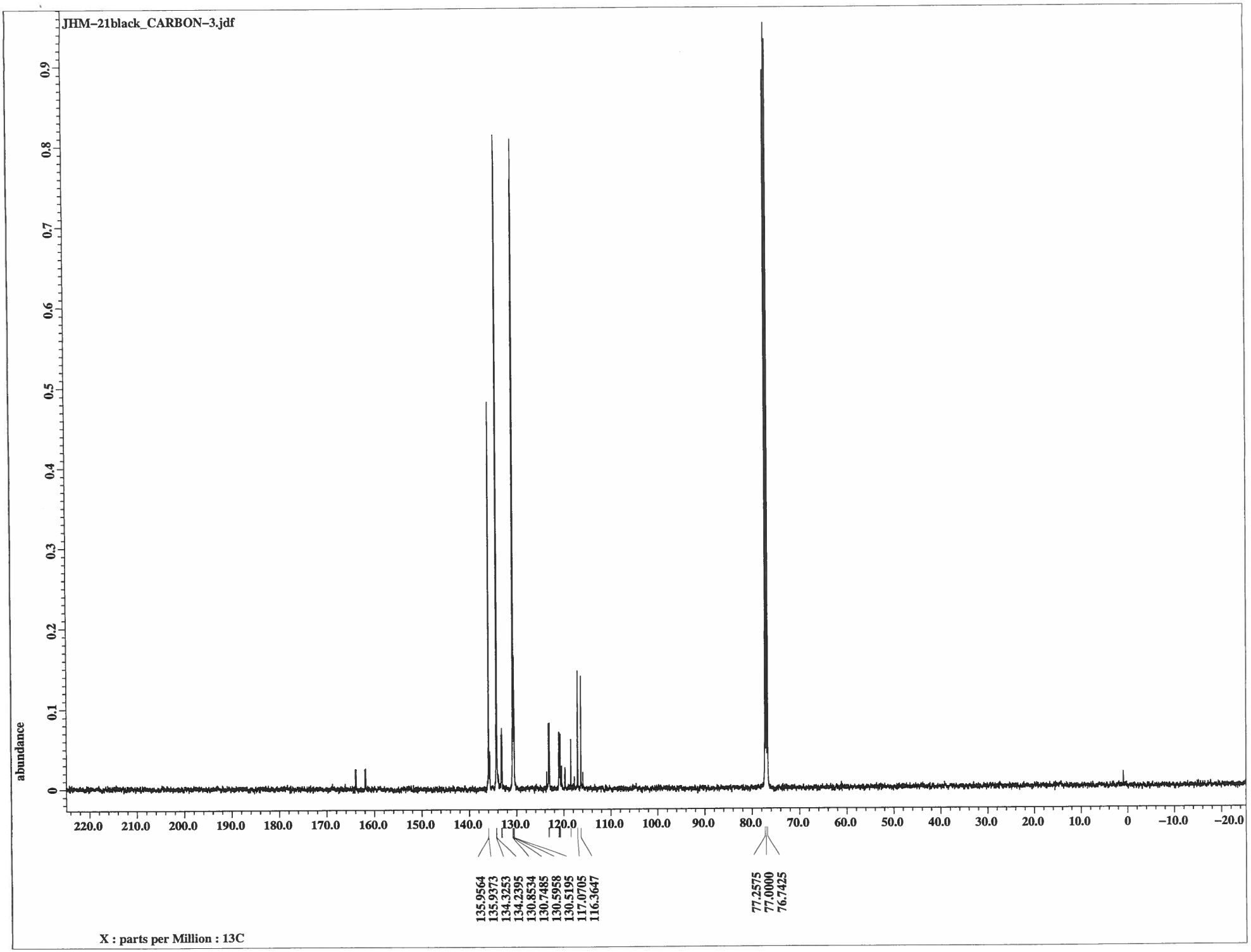
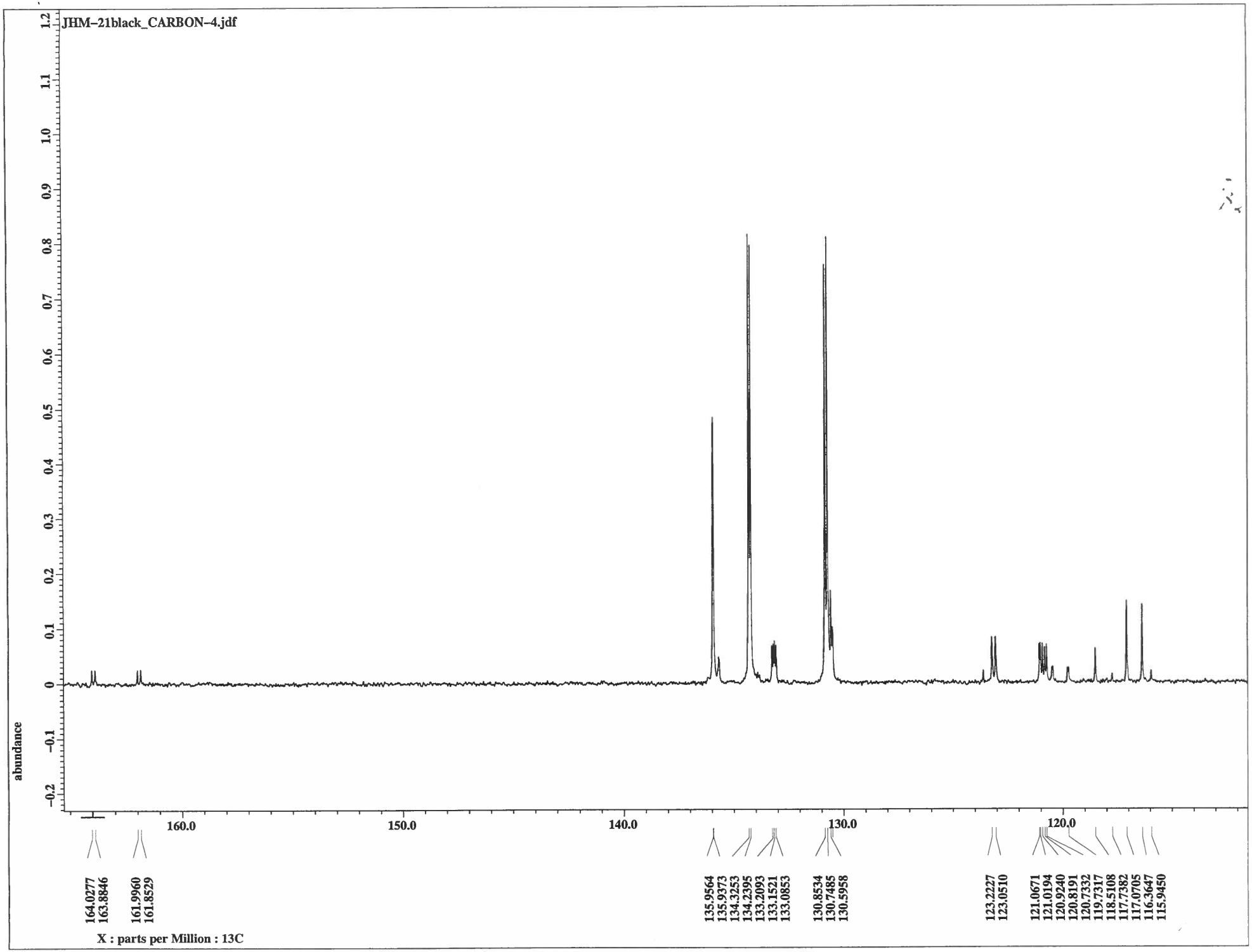
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-150.0
-160.0
-170.0
-78.6257
-93.0668
X : parts per Million : 19F

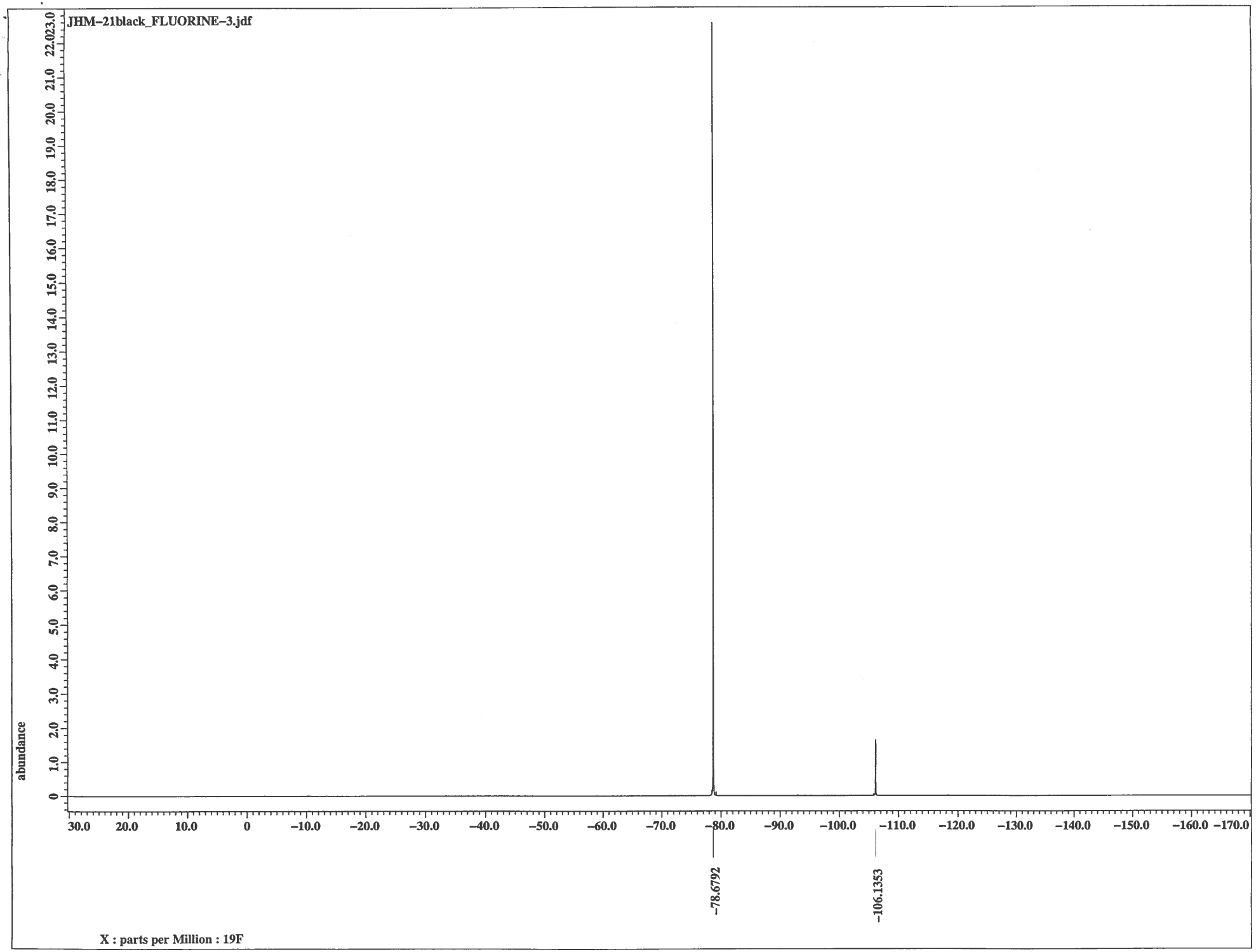

JHM-10d_PHOSPHORUS-15.jdf
abundance
3.0
2.0
1.0
0
100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0
21.6365
X : parts per Million : 31P

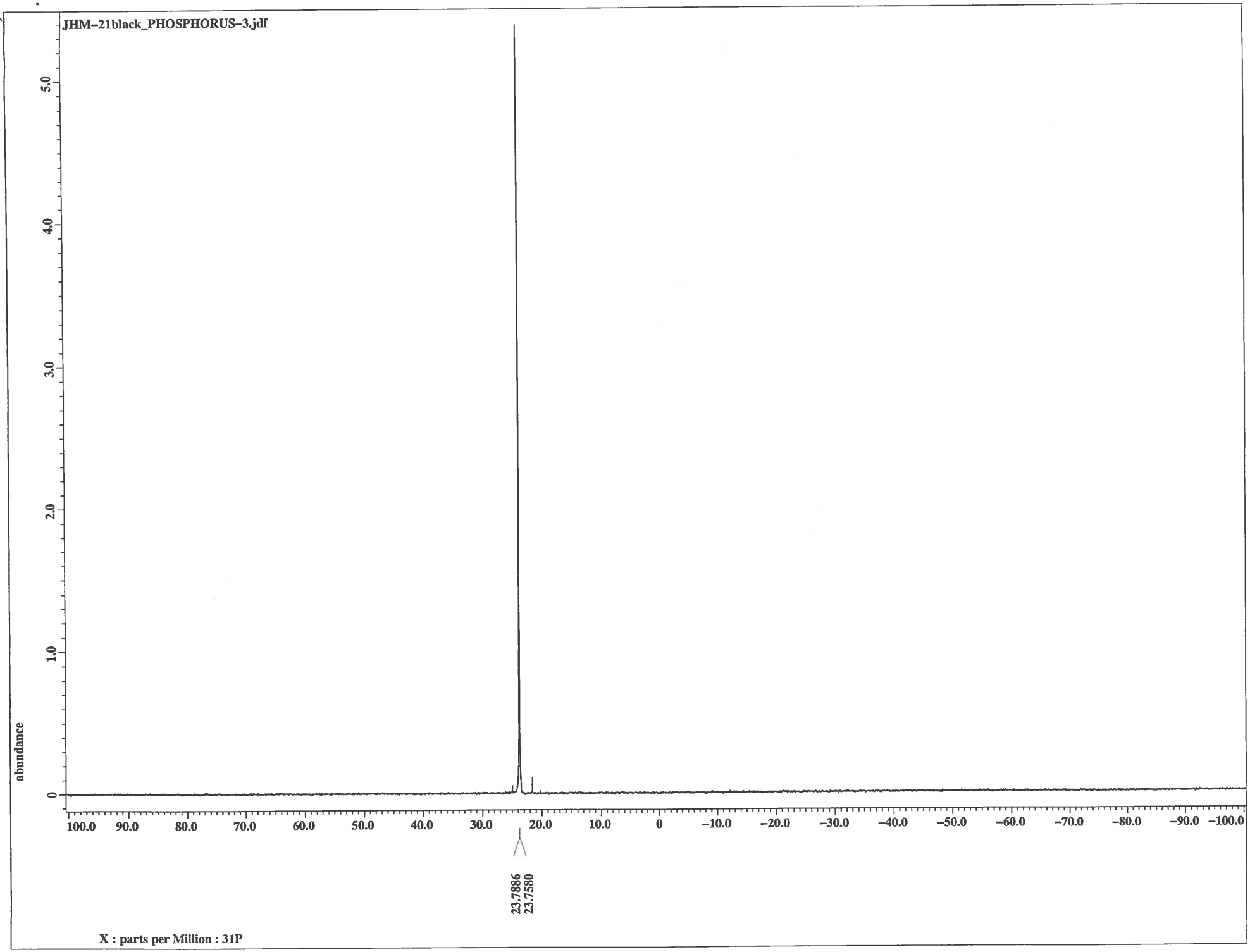

JHM-21black_PROTON-3.jdf
294.69
16.71
4.07
abundance
4.0
3.0
2.0
1.0
0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
7.7025
7.6957
7.5651
7.5628
7.5388
7.5365
7.5216
0.0000
X : parts per Million : 1H
NTf2
PPh3
F

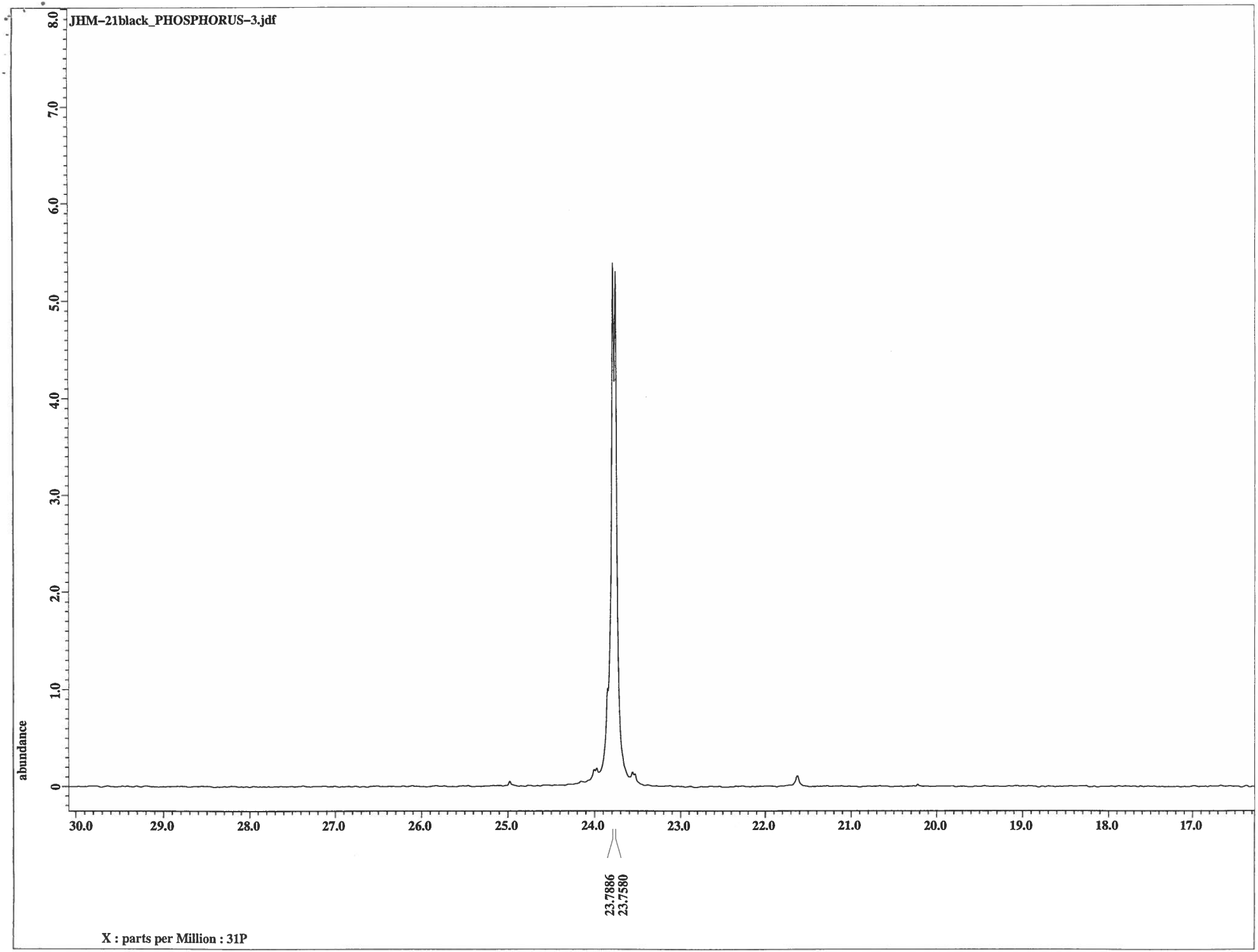

JHM-21black_PROTON-4.jdf
abundance
7.87
6.1
3.03
1.11
1
7.8342
7.8308
7.8182
7.8159
7.7197
7.7117
7.7025
7.6957
7.6876
7.6842
7.6808
7.5651
7.5628
7.5479
7.5388
7.5365
7.5216
7.4162
7.3991
7.3910
7.3739
7.1941
7.1689
7.1540
7.1460
7.1414
7.1265
X : parts per Million : 1H

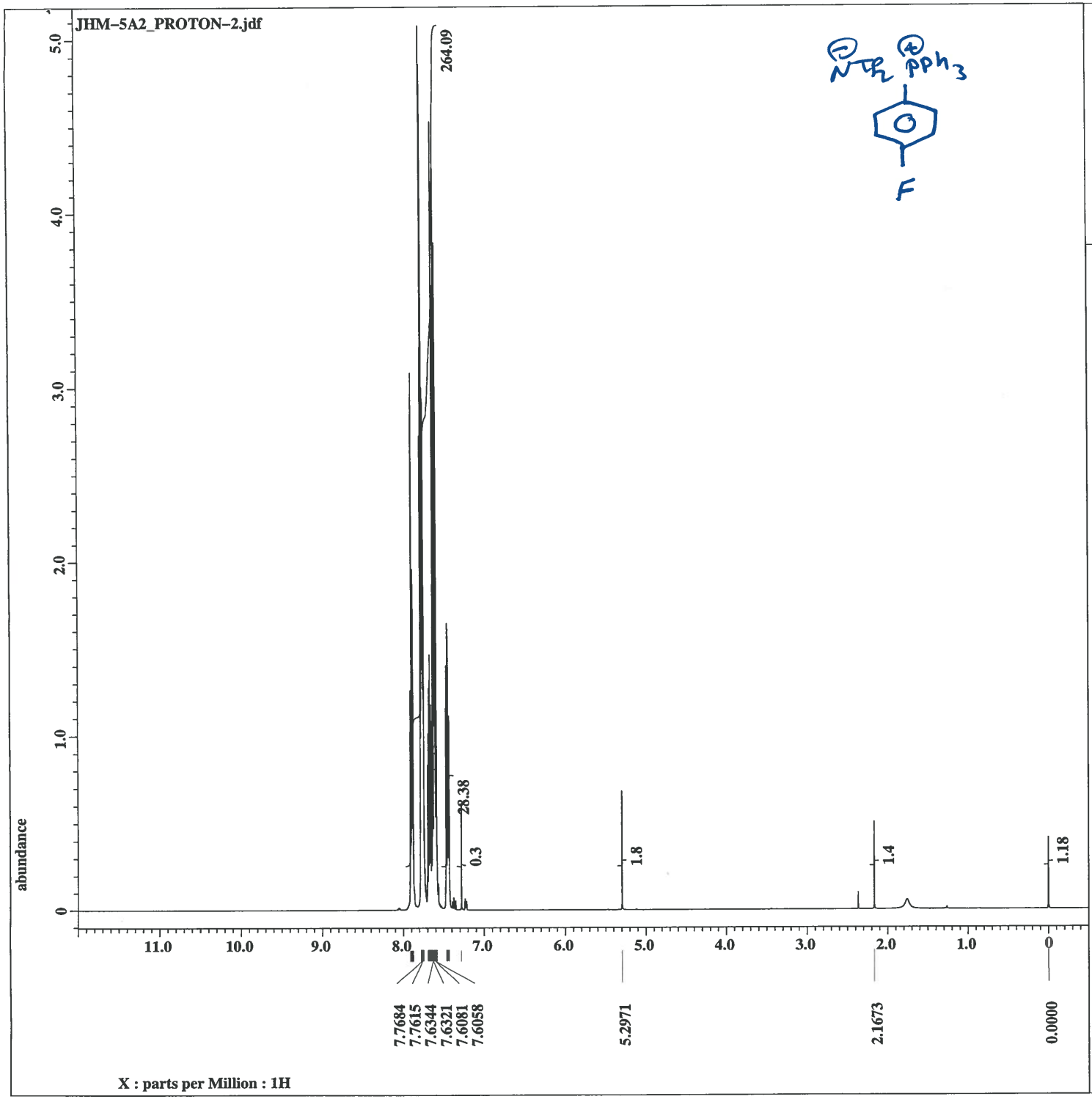

JHM-21black_CARBON-3.jdf
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
135.9564
135.9373
134.3253
134.2395
130.8534
130.7485
130.5958
130.5195
117.0705
116.3647
77.2575
77.0000
76.7425
X : parts per Million : 13C


JHM-21black_CARBON-4.jdf
abundance
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
160.0
150.0
140.0
130.0
120.0
164.0277
163.8846
161.9960
161.8529
135.9564
135.9373
134.3253
134.2395
133.2093
133.1521
133.0853
130.8534
130.7485
130.5958
123.2227
123.0510
121.0671
121.0194
120.9240
120.8191
120.7332
119.7317
118.5108
117.7382
117.0705
116.3647
115.9450
X : parts per Million : 13C


JHM-21black_FLUORINE-3.jdf
abundance
23.0
22.0
21.0
20.0
19.0
18.0
17.0
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
30.0
20.0
10.0
0
-10.0
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-150.0
-160.0
-170.0
-78.6792
-106.1353
X : parts per Million : 19F

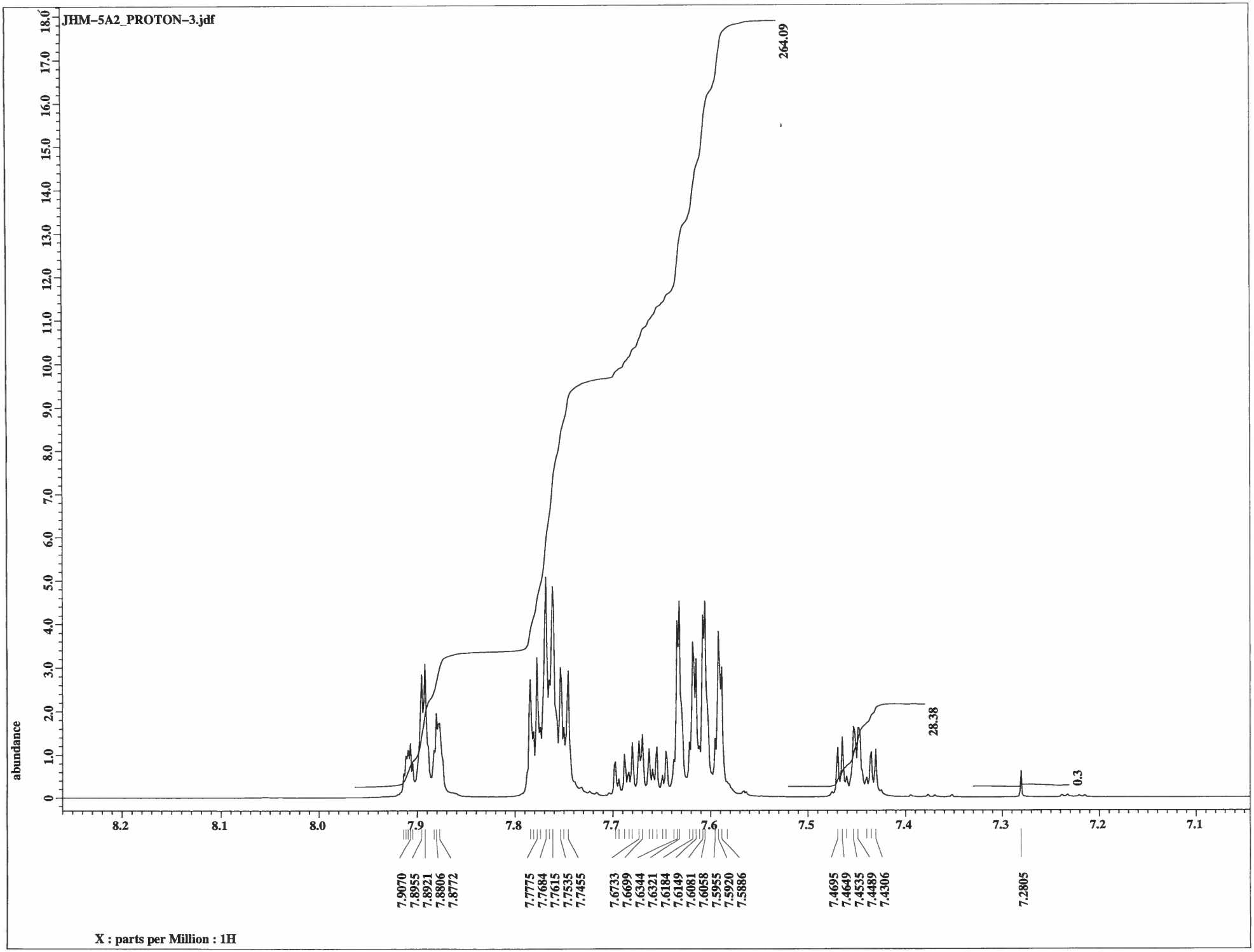

JHM-21black_PHOSPHORUS-3.jdf
abundance
5.0
4.0
3.0
2.0
1.0
0
100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0
23.7886
23.7580
X : parts per Million : 31P

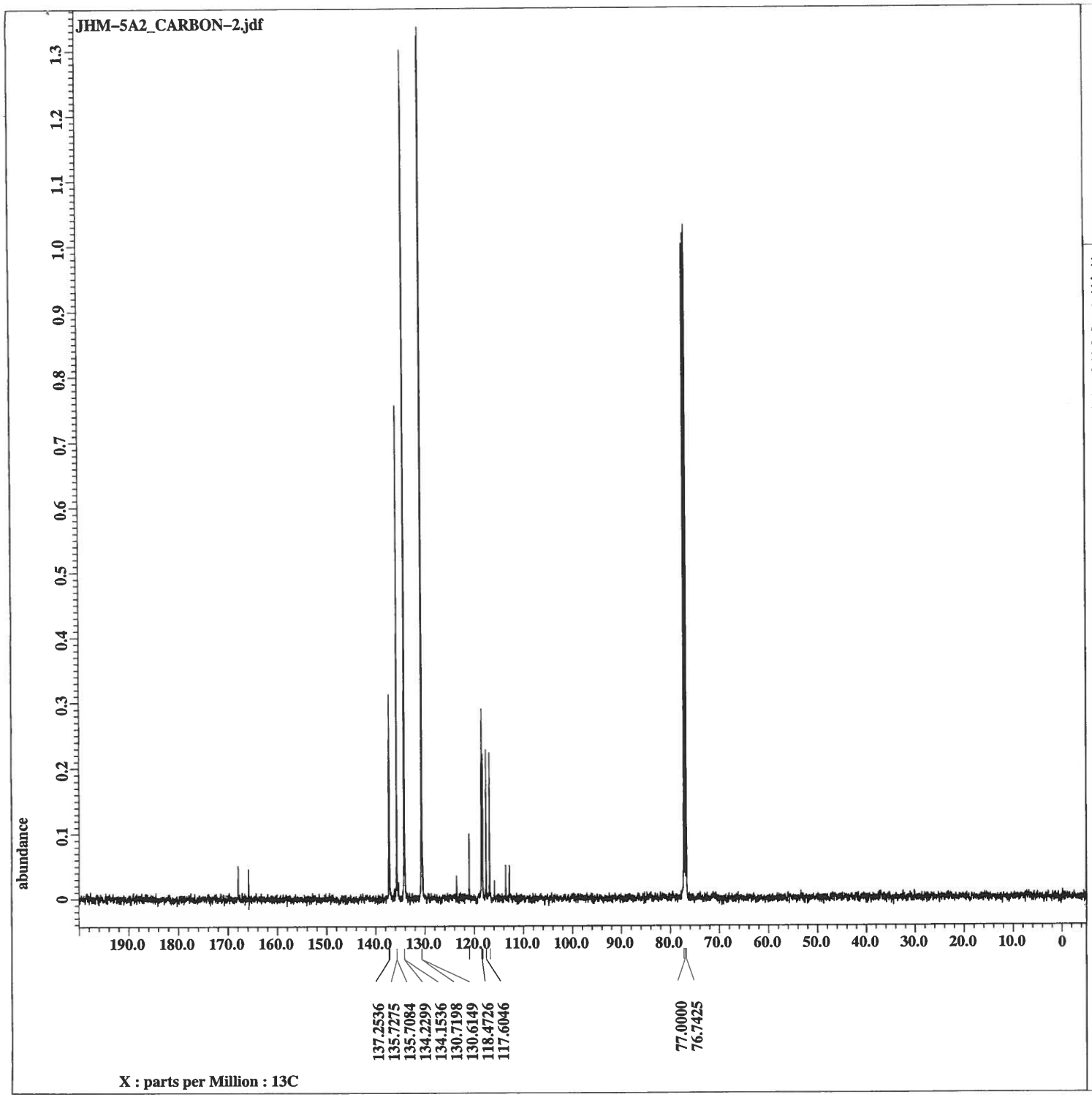

JHM-21black_PHOSPHORUS-3.jdf
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
30.0
29.0
28.0
27.0
26.0
25.0
24.0
23.0
22.0
21.0
20.0
19.0
18.0
17.0
23.7886
23.7580
X : parts per Million : 31P



SOUTH ALABAMA JAGUARS

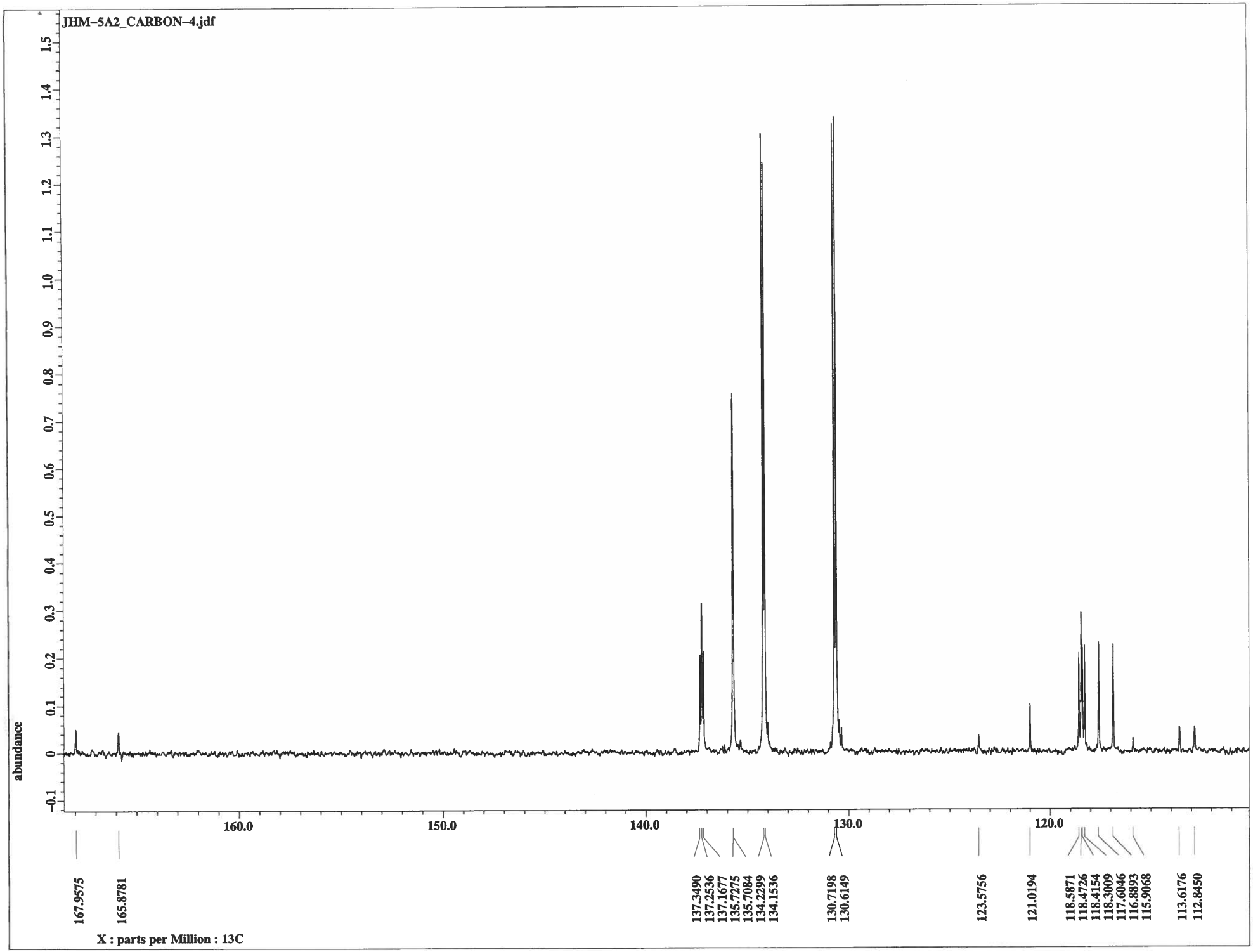
Filename	= JHM-5A2_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= JHM-5A2
Solvent	= CHLOROFORM-D
Changer_sample	= 11
Creation_time	= 25-JUL-2018 18:25:42
Revision_time	= 25-JUL-2018 18:02:17
Current_time	= 25-JUL-2018 18:02:17
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 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	= 100
Total_scans	= 100
X_90_width	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 30
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.2[dC]

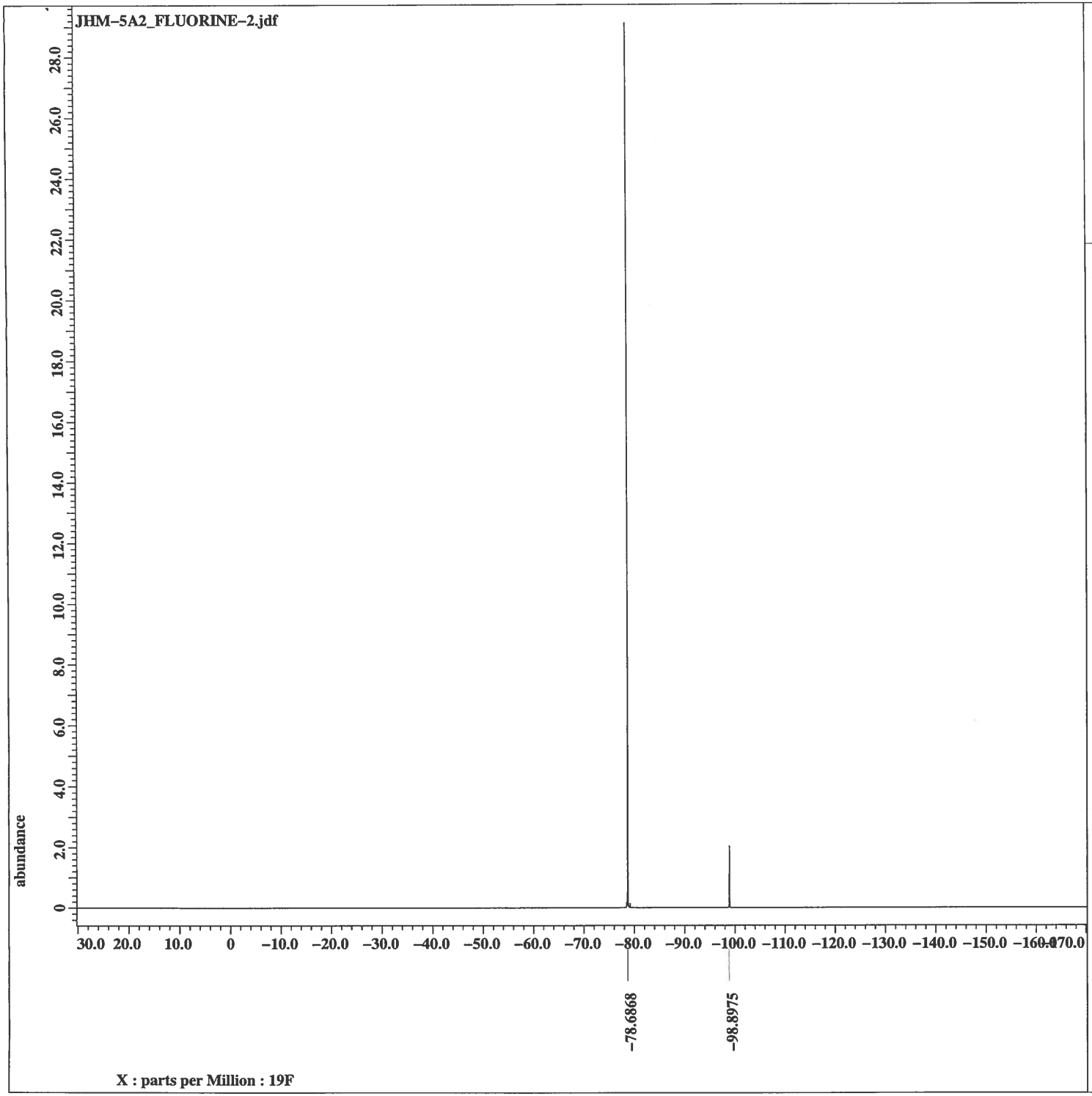

JHM-5A2_PROTON-3.jdf
abundance
264.09
28.38
0.3
7.9070
7.8955
7.8921
7.8806
7.8772
7.7775
7.7684
7.7615
7.7535
7.7455
7.6733
7.6699
7.6344
7.6321
7.6184
7.6149
7.6081
7.6058
7.5955
7.5920
7.5886
7.4695
7.4649
7.4535
7.4489
7.4306
7.2805
X : parts per Million : 1H



SOUTH ALABAMA JAGUARS

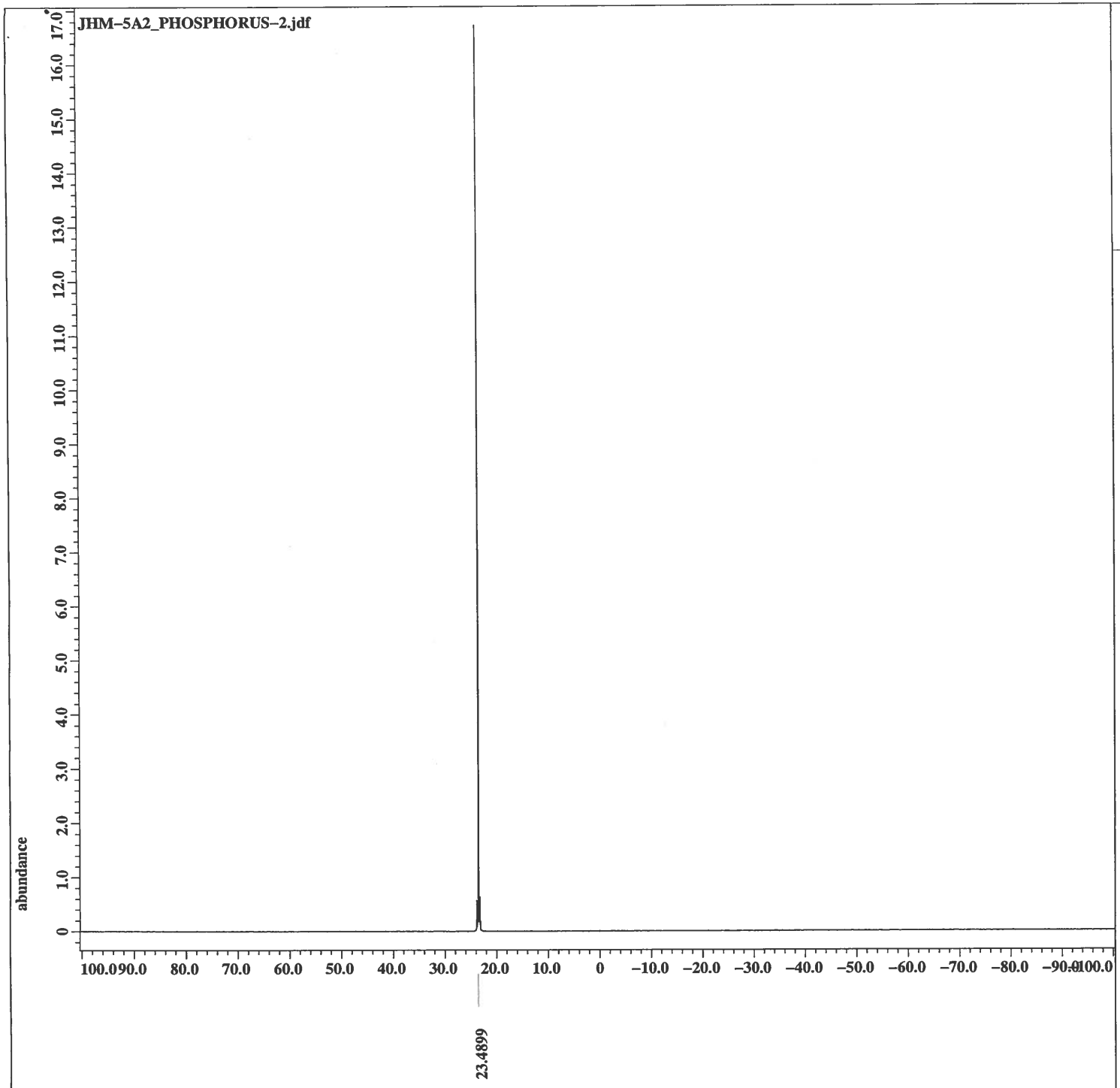
Filename	= JHM-5A2_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= JHM-5A2
Solvent	= CHLOROFORM-D
Changer_sample	= 11
Creation_time	= 25-JUL-2018 19:09:09
Revision_time	= 25-JUL-2018 18:45:43
Current_time	= 25-JUL-2018 18:45:43
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 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	= 300
Total_scans	= 300
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 22.9[dC]


JHM-5A2_CARBON-4.jdf
abundance
-0.1
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
160.0
150.0
140.0
130.0
120.0
167.9575
165.8781
137.3490
137.2536
137.1677
135.7275
135.7084
134.2299
134.1536
130.7198
130.6149
123.5756
121.0194
118.5871
118.4726
118.4154
118.3009
117.6046
116.8893
115.9068
113.6176
112.8450
X : parts per Million : 13C



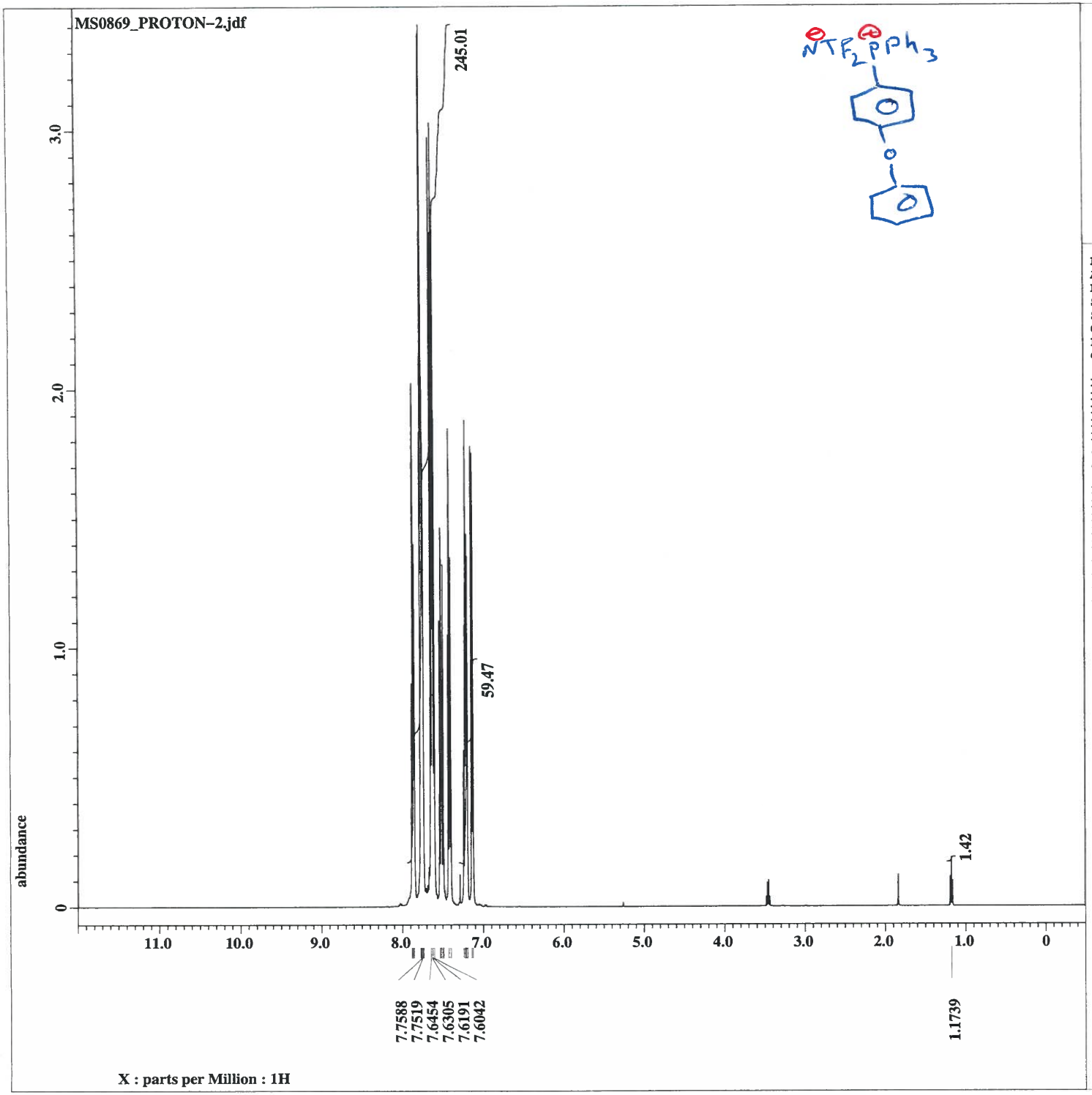
SOUTH ALABAMA JAGUARS

Filename	= JHM-5A2_FLUORINE-2.jd
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= JHM-5A2
Solvent	= CHLOROFORM-D
Changer_sample	= 11
Creation_time	= 25-JUL-2018 18:14:32
Revision_time	= 25-JUL-2018 17:51:07
Current_time	= 25-JUL-2018 17:51:07
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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 38
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.5[dC]



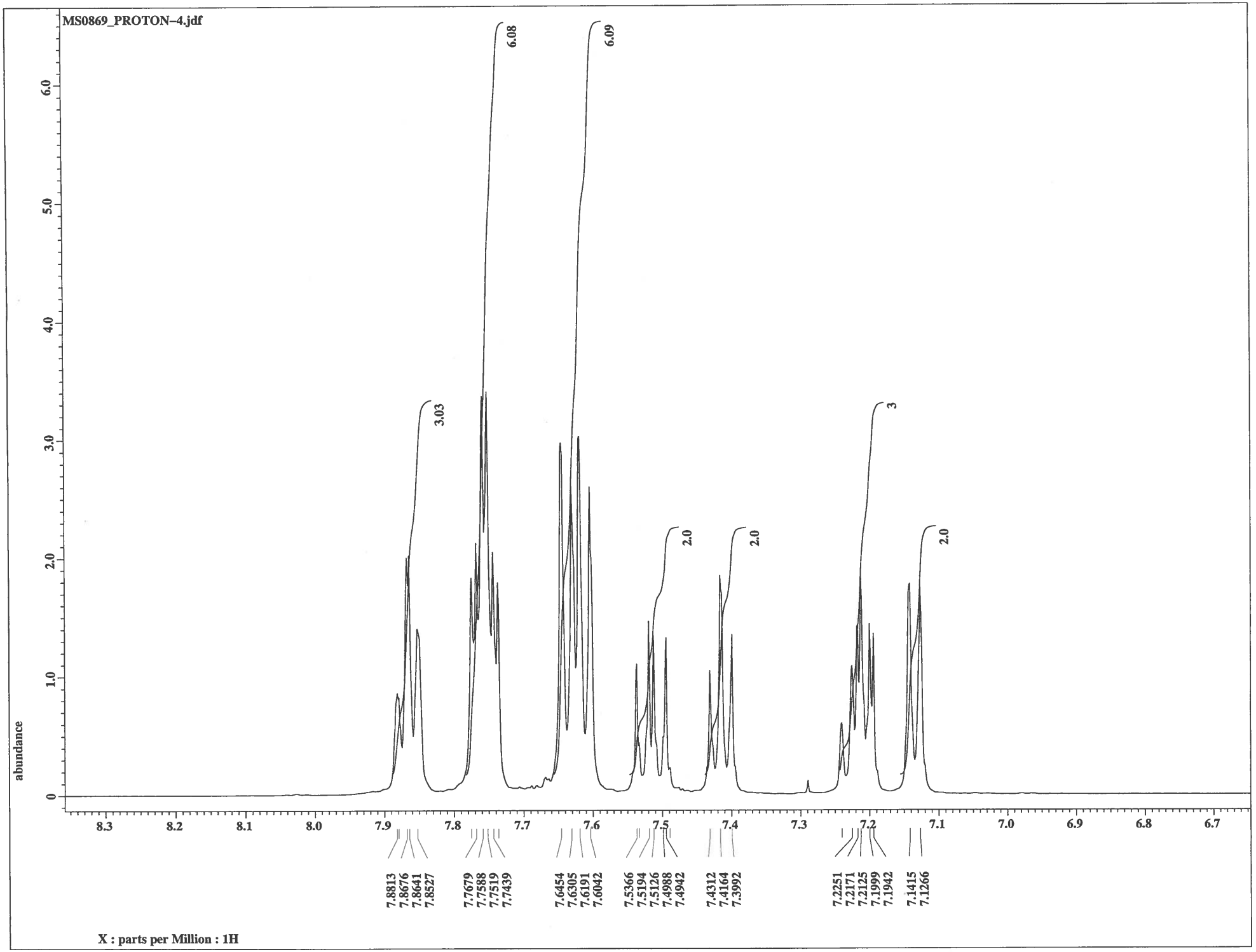
SOUTH ALABAMA JAGUARS

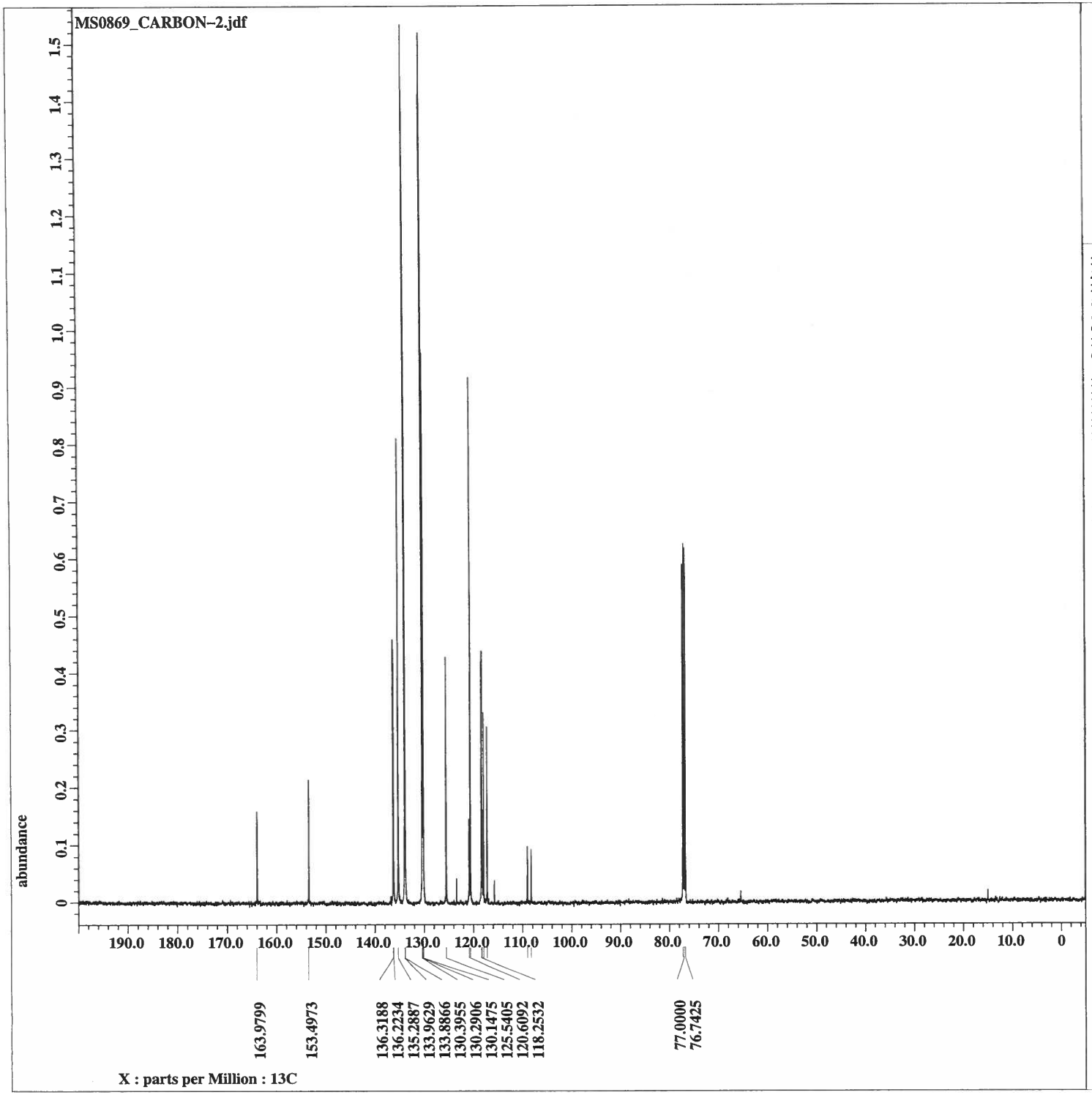
Filename	= JHM-5A2_PHOSPHORUS-2.
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= JHM-5A2
Solvent	= CHLOROFORM-D
Changer_sample	= 11
Creation_time	= 25-JUL-2018 18:38:23
Revision_time	= 25-JUL-2018 18:14:57
Current_time	= 25-JUL-2018 18:14:57
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 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	= 234
Total_scans	= 234
X_90_width	= 14.687[us]
X_acq_time	= 0.64487424[s]
X_angle	= 30[deg]
X_atn	= 5[dB]
X_pulse	= 4.89566667[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= 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	= 22.8[dC]



SOUTH ALABAMA JAGUARS

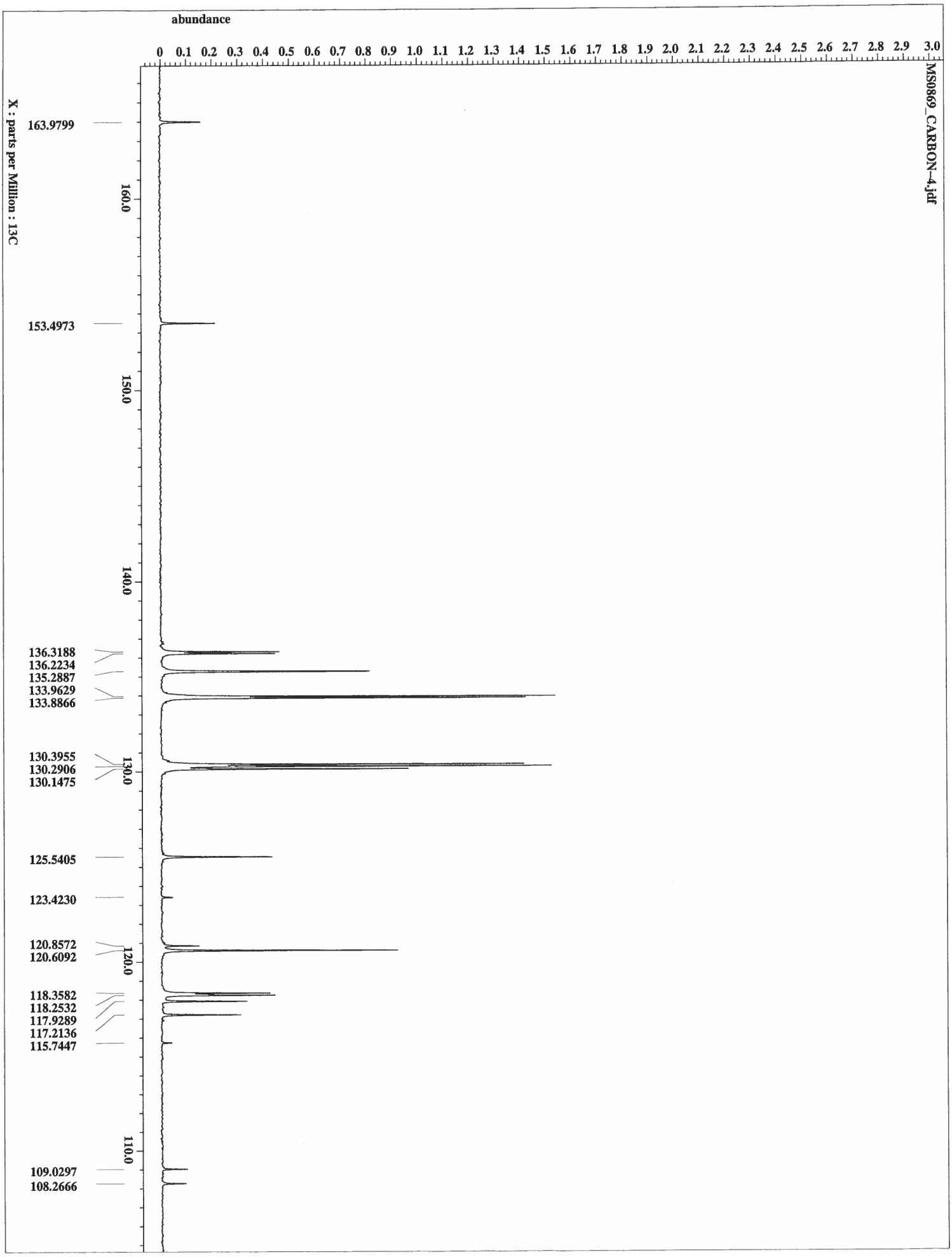
Filename	= MS0869_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0869
Solvent	= CHLOROFORM-D
Creation_time	= 26-NOV-2019 11:19:03
Revision_time	= 26-NOV-2019 10:49:59
Current_time	= 26-NOV-2019 10:49:59
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [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	= 11.3[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 5.65[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 20
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 19.3[dC]

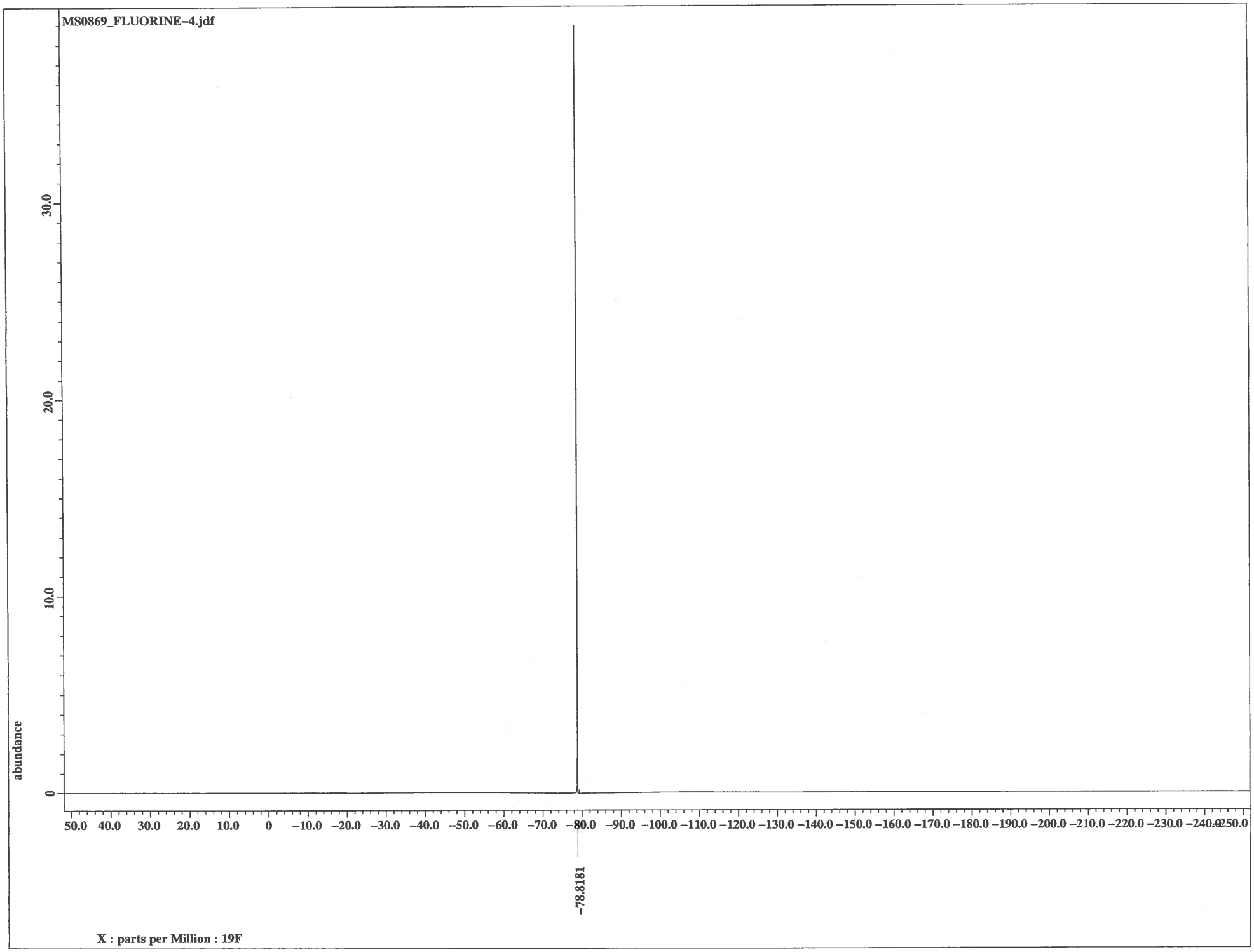

MS0869_PROTON-4.jdf
abundance
6.08
6.09
3.03
2.0
2.0
3
2.0
7.8813
7.8676
7.8641
7.8527
7.7679
7.7588
7.7519
7.7439
7.6454
7.6305
7.6191
7.6042
7.5366
7.5194
7.5126
7.4988
7.4942
7.4312
7.4164
7.3992
7.2251
7.2171
7.2125
7.1999
7.1942
7.1415
7.1266
X : parts per Million : 1H

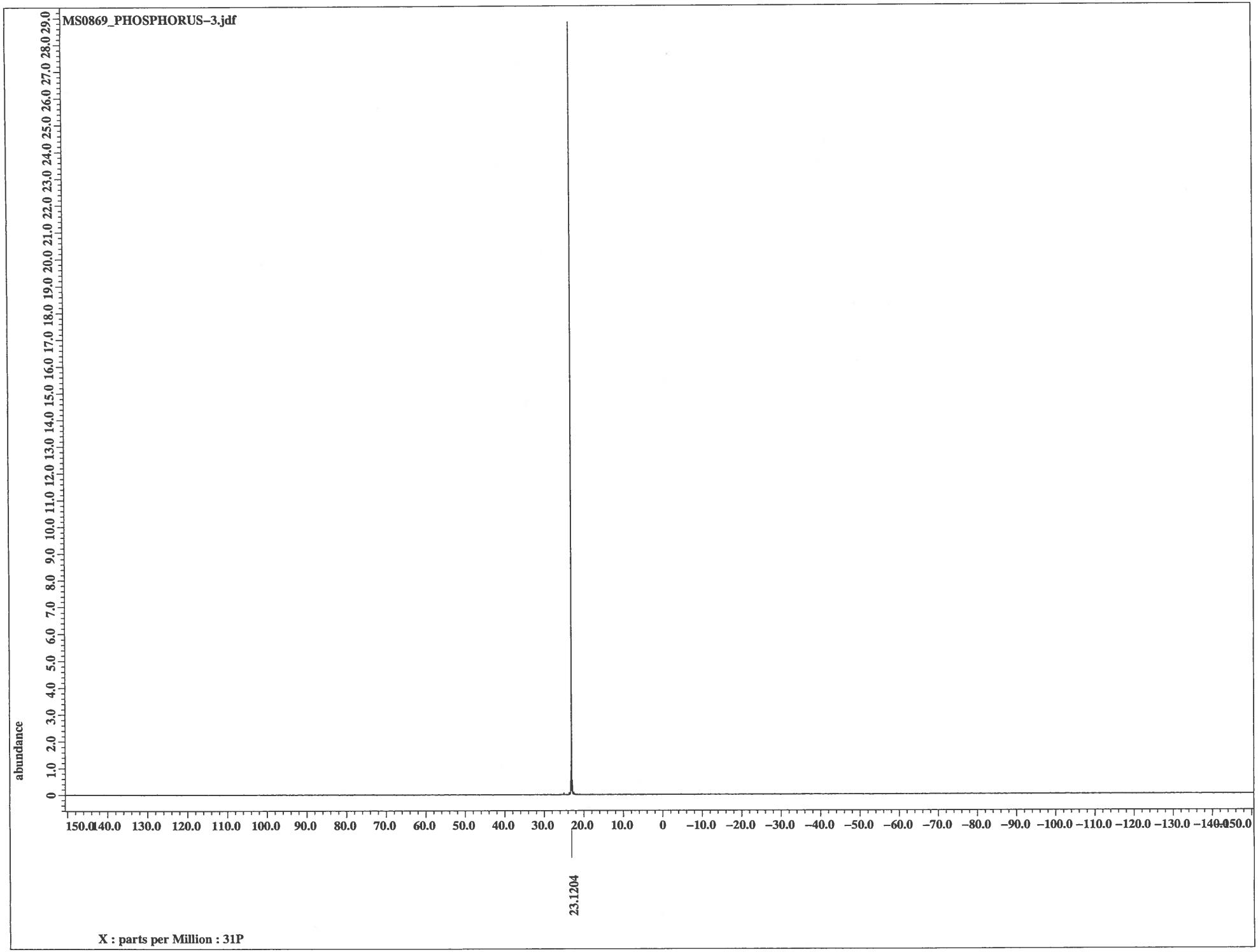


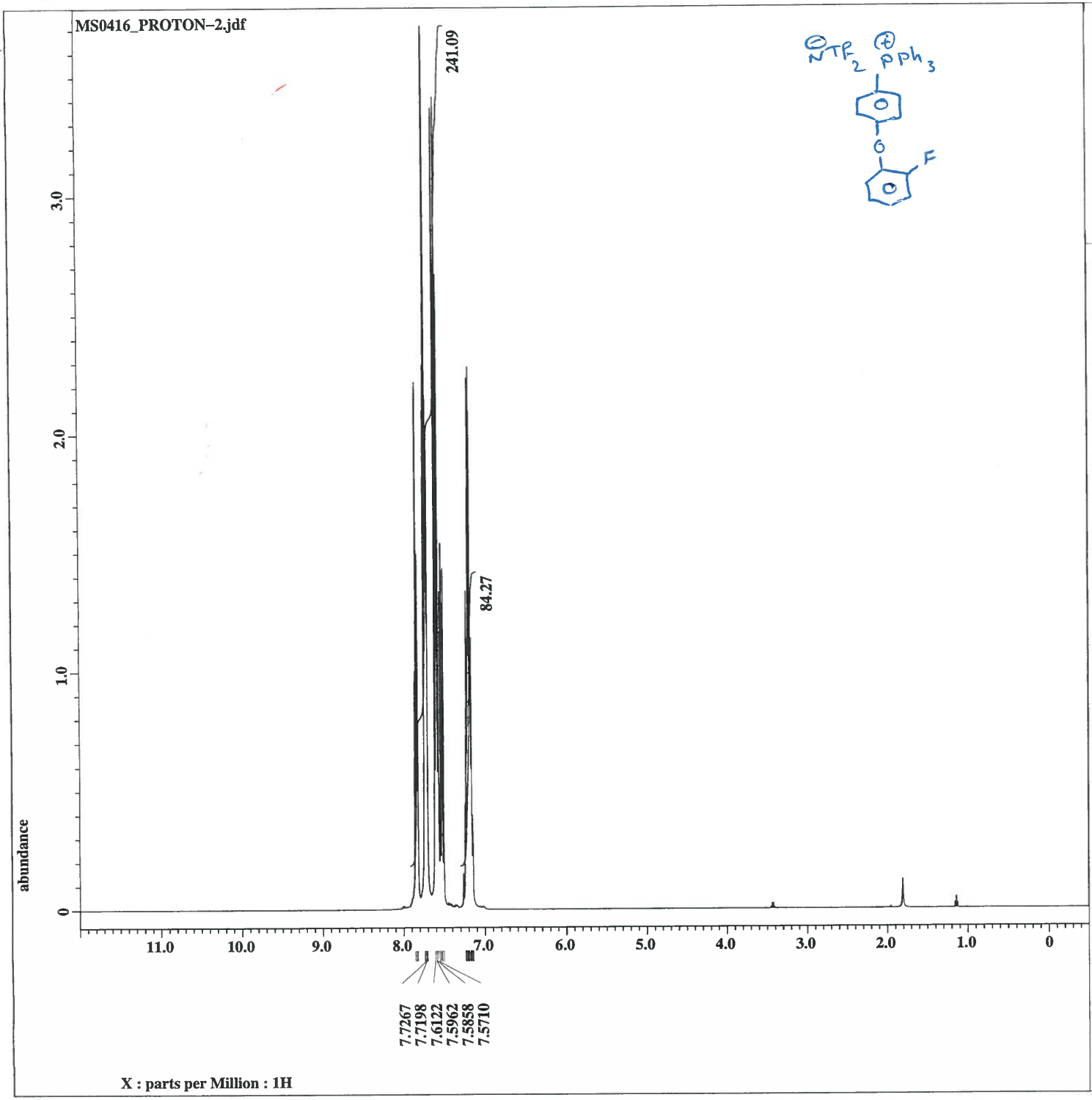
SOUTH ALABAMA JAGUARS

Filename	= MS0869_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0869
Solvent	= CHLOROFORM-D
Creation_time	= 26-NOV-2019 11:56:57
Revision_time	= 26-NOV-2019 11:27:52
Current_time	= 26-NOV-2019 11:27:53
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	= 449
Total_scans	= 449
X_90_width	= 13[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.33333333[us]
Irr_atn_dec	= 21.2[dB]
Irr_atn_noe	= 21.2[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	= 18.8[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 2.6 2.7 2.8 2.9 3.0
MS0869_CARBON-4.jdf
X : parts per Million : 13C
163.9799
153.4973
136.3188
136.2234
135.2887
133.9629
133.8866
130.3955
130.2906
130.1475
125.5405
123.4230
120.8572
120.6092
118.3582
118.2532
117.9289
117.2136
115.7447
109.0297
108.2666
160.0
150.0
140.0
130.0
120.0
110.0

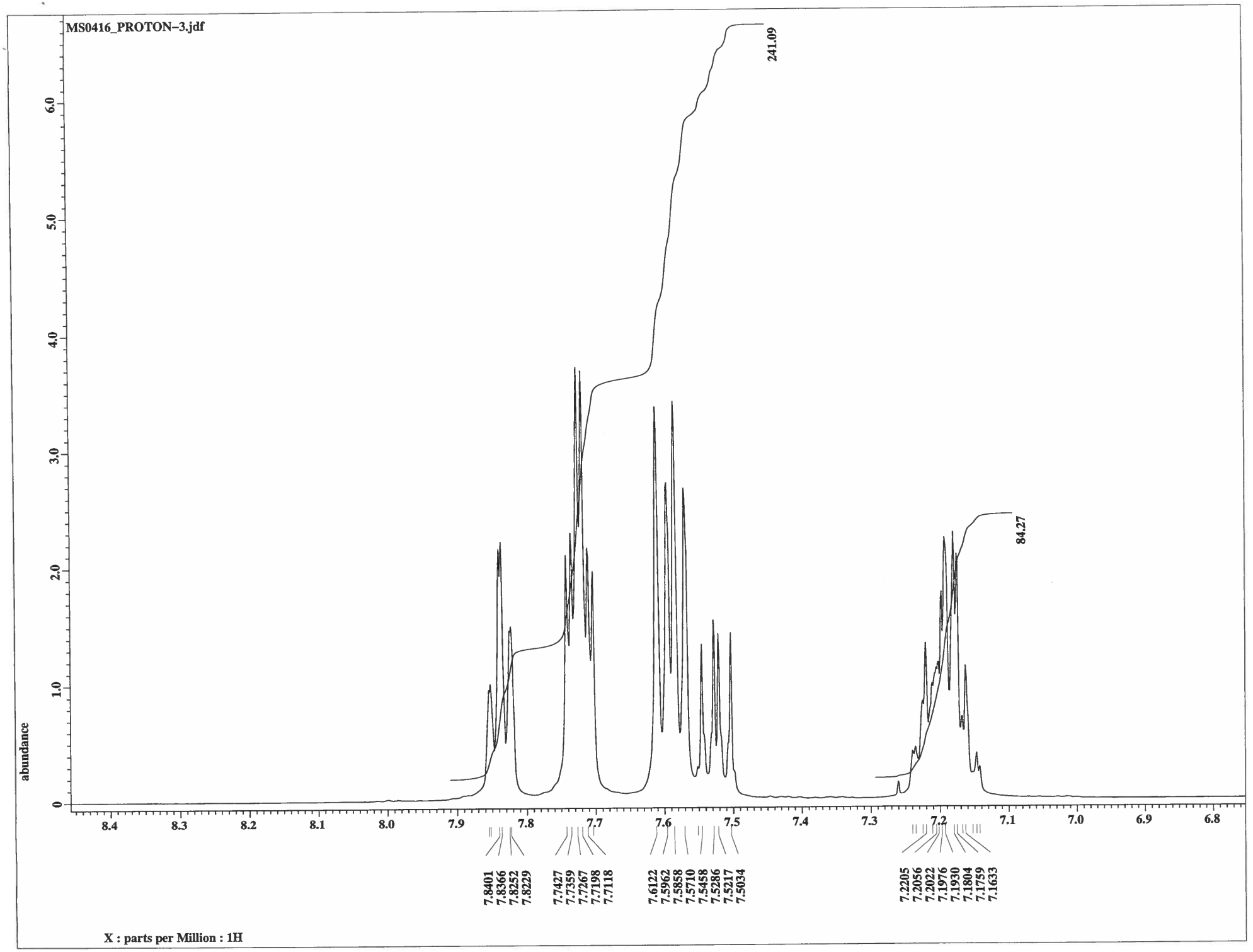

MS0869_FLUORINE-4.jdf
abundance
30.0
20.0
10.0
0
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0 -210.0 -220.0 -230.0 -240.0 -250.0
-78.8181
X : parts per Million : 19F

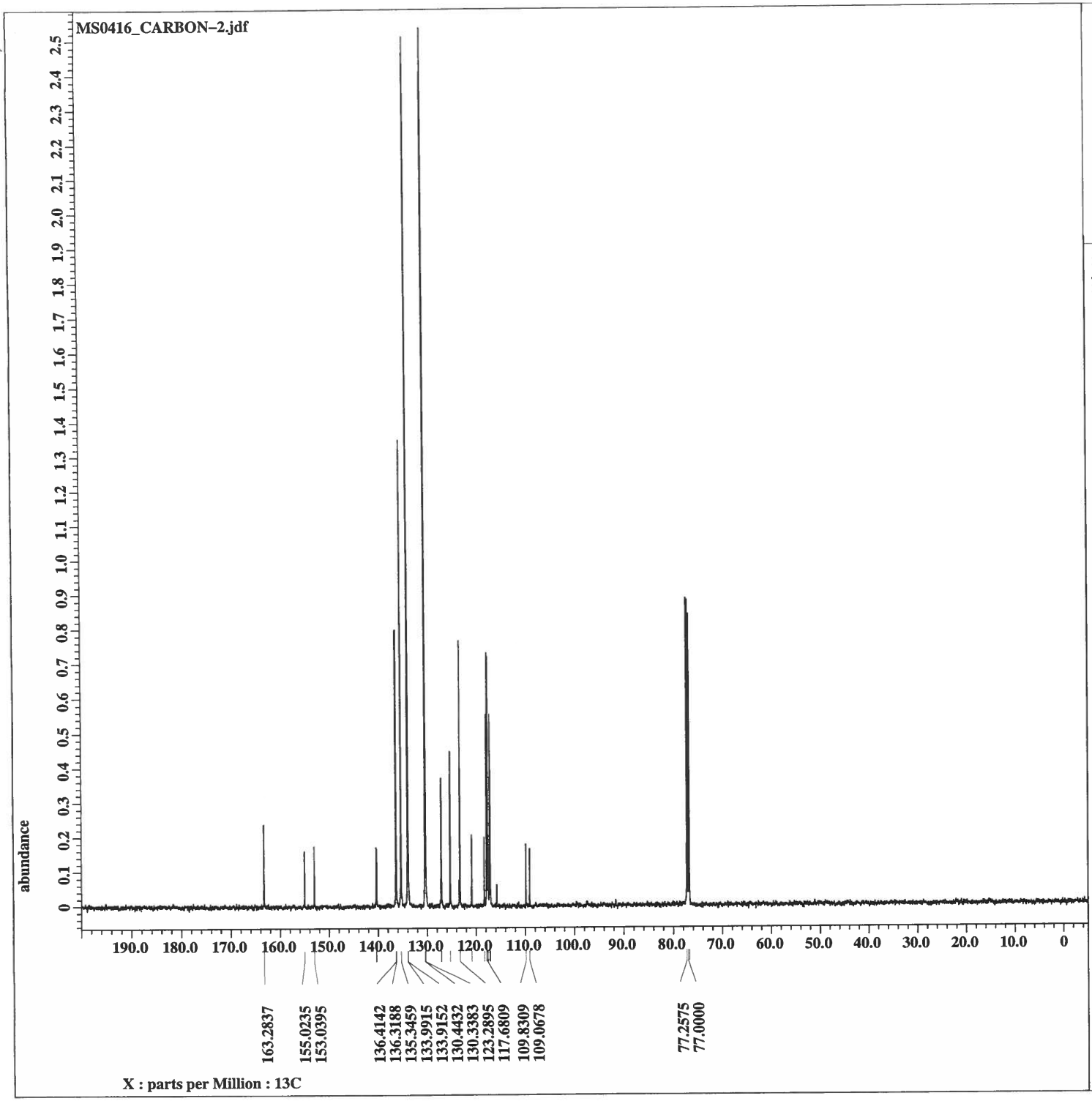

MS0869_PHOSPHORUS-3.jdf
abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0 25.0 26.0 27.0 28.0 29.0
150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0
23.1204
X : parts per Million : 31P



SOUTH ALABAMA JAGUARS

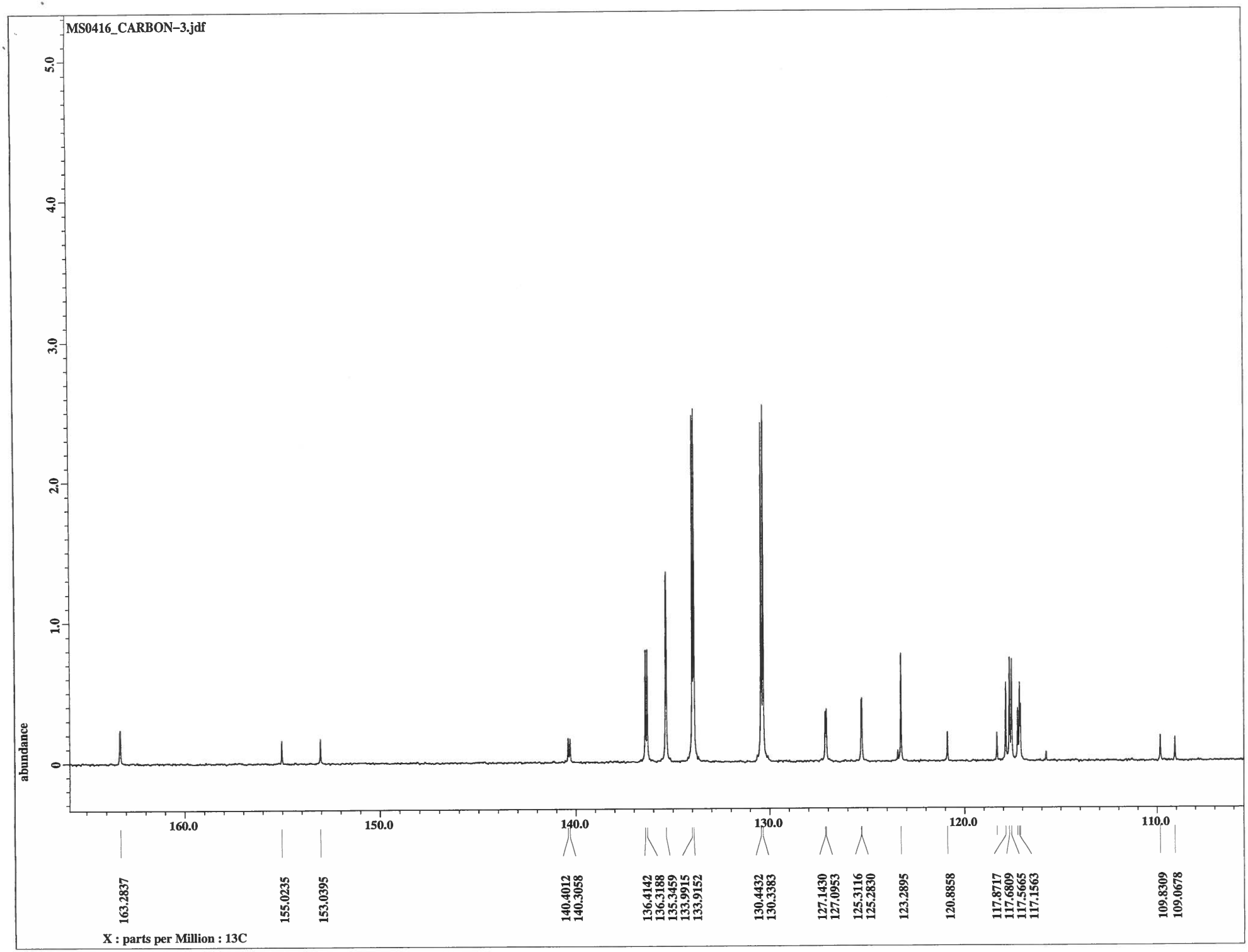
Filename	= MS0416_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0416
Solvent	= CHLOROFORM-D
Changer_sample	= 10
Creation_time	= 14-APR-2018 11:32:37
Revision_time	= 14-APR-2018 11:10:44
Current_time	= 14-APR-2018 11:10:44
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 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	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 24
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.8[dC]

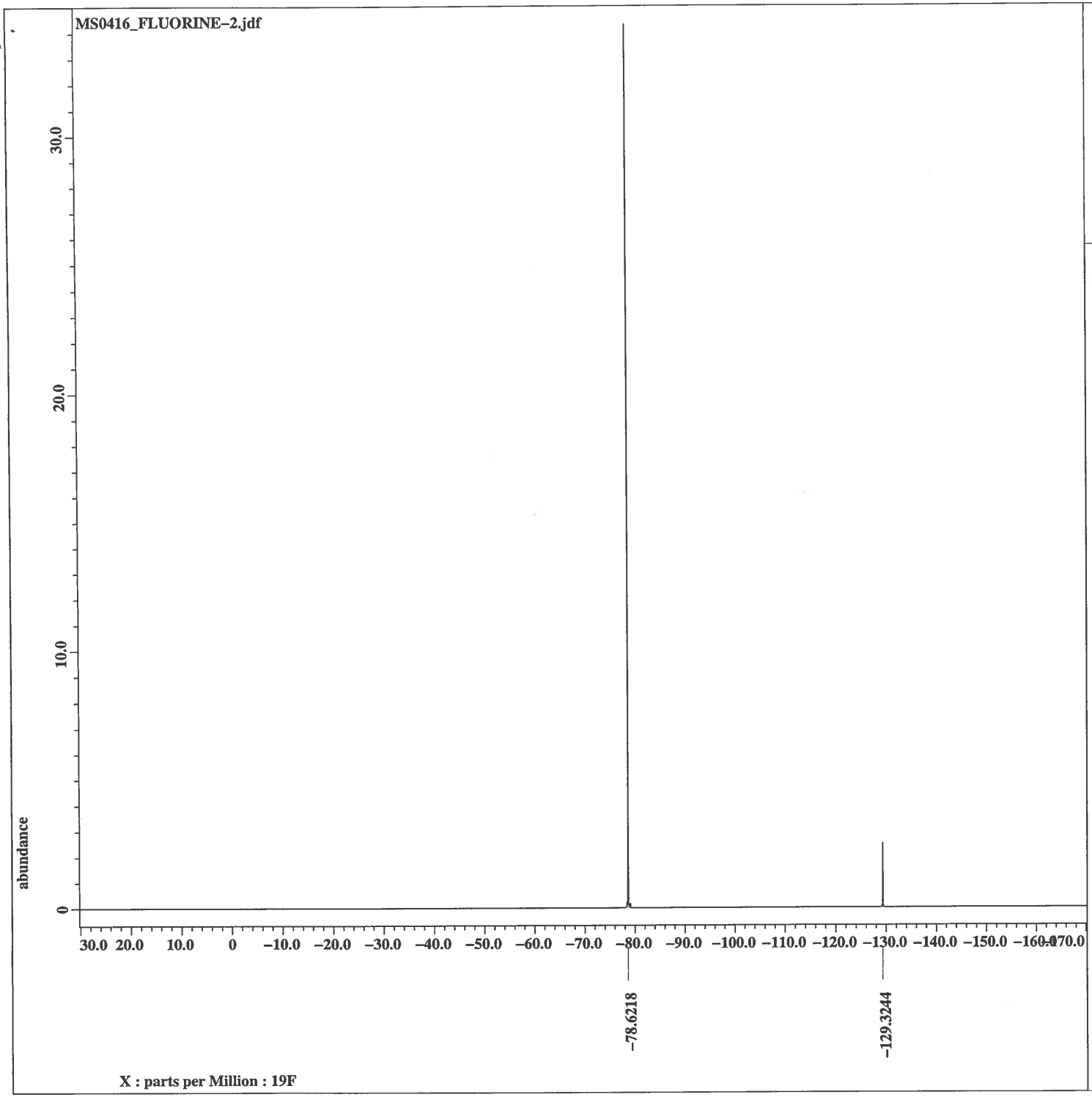

MS0416_PROTON-3.jdf
241.09
84.27
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
7.8401
7.8366
7.8252
7.8229
7.7427
7.7359
7.7267
7.7198
7.7118
7.6122
7.5962
7.5858
7.5710
7.5458
7.5286
7.5217
7.5034
7.2205
7.2056
7.2022
7.1976
7.1930
7.1804
7.1759
7.1633
X : parts per Million : 1H



SOUTH ALABAMA JAGUARS

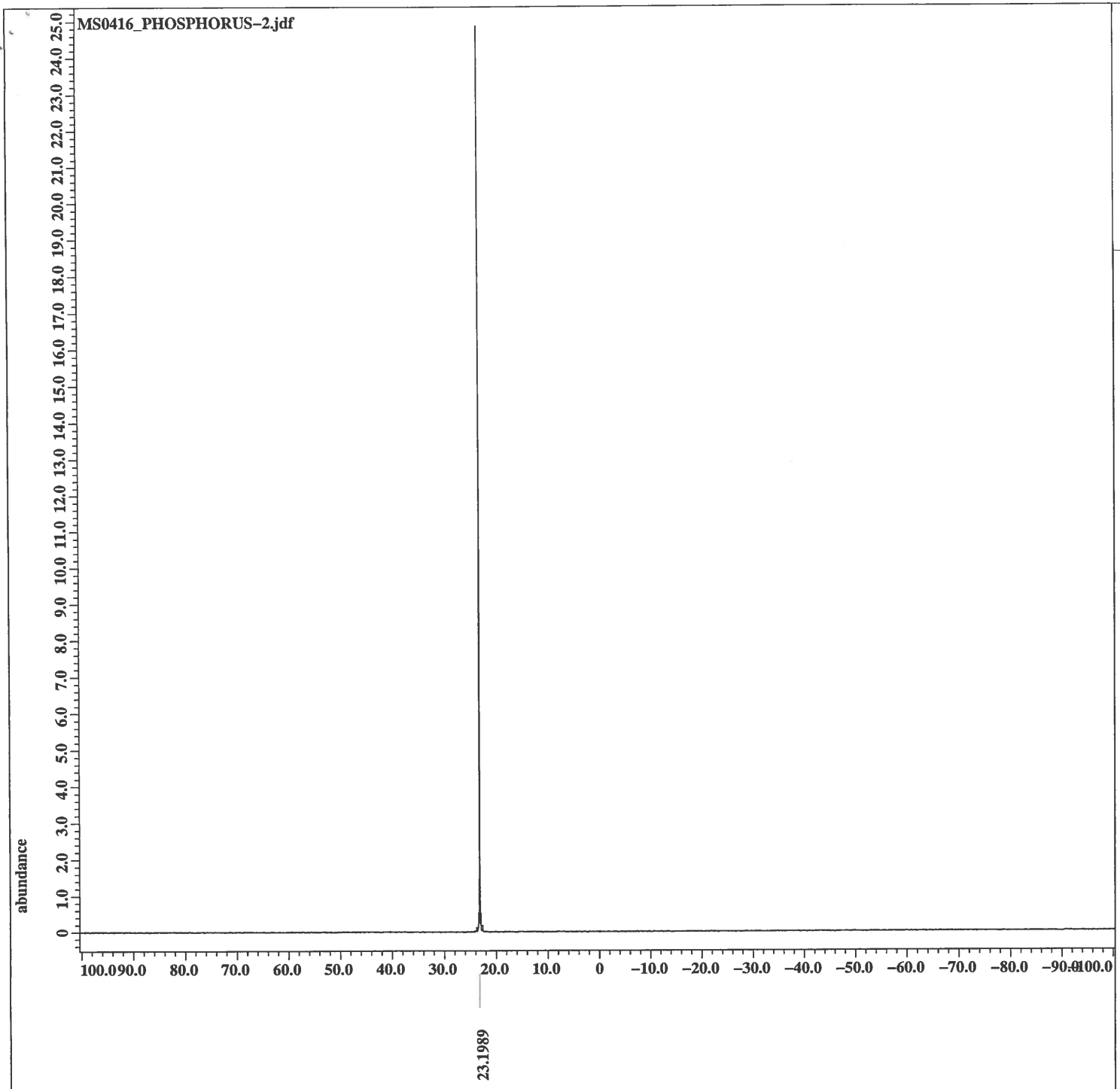
Filename	= MS0416_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0416
Solvent	= CHLOROFORM-D
Changer_sample	= 10
Creation_time	= 14-APR-2018 11:47:07
Revision_time	= 14-APR-2018 11:25:15
Current_time	= 14-APR-2018 11:25:15
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 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	= 256
Total_scans	= 256
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 23.2[dC]


MS0416_CARBON-3.jdf
abundance
5.0
4.0
3.0
2.0
1.0
0
160.0
150.0
140.0
130.0
120.0
110.0
163.2837
155.0235
153.0395
140.4012
140.3058
136.4142
136.3188
135.3459
133.9915
133.9152
130.4432
130.3383
127.1430
127.0953
125.3116
125.2830
123.2895
120.8858
117.8717
117.6809
117.5665
117.1563
109.8309
109.0678
X : parts per Million : 13C

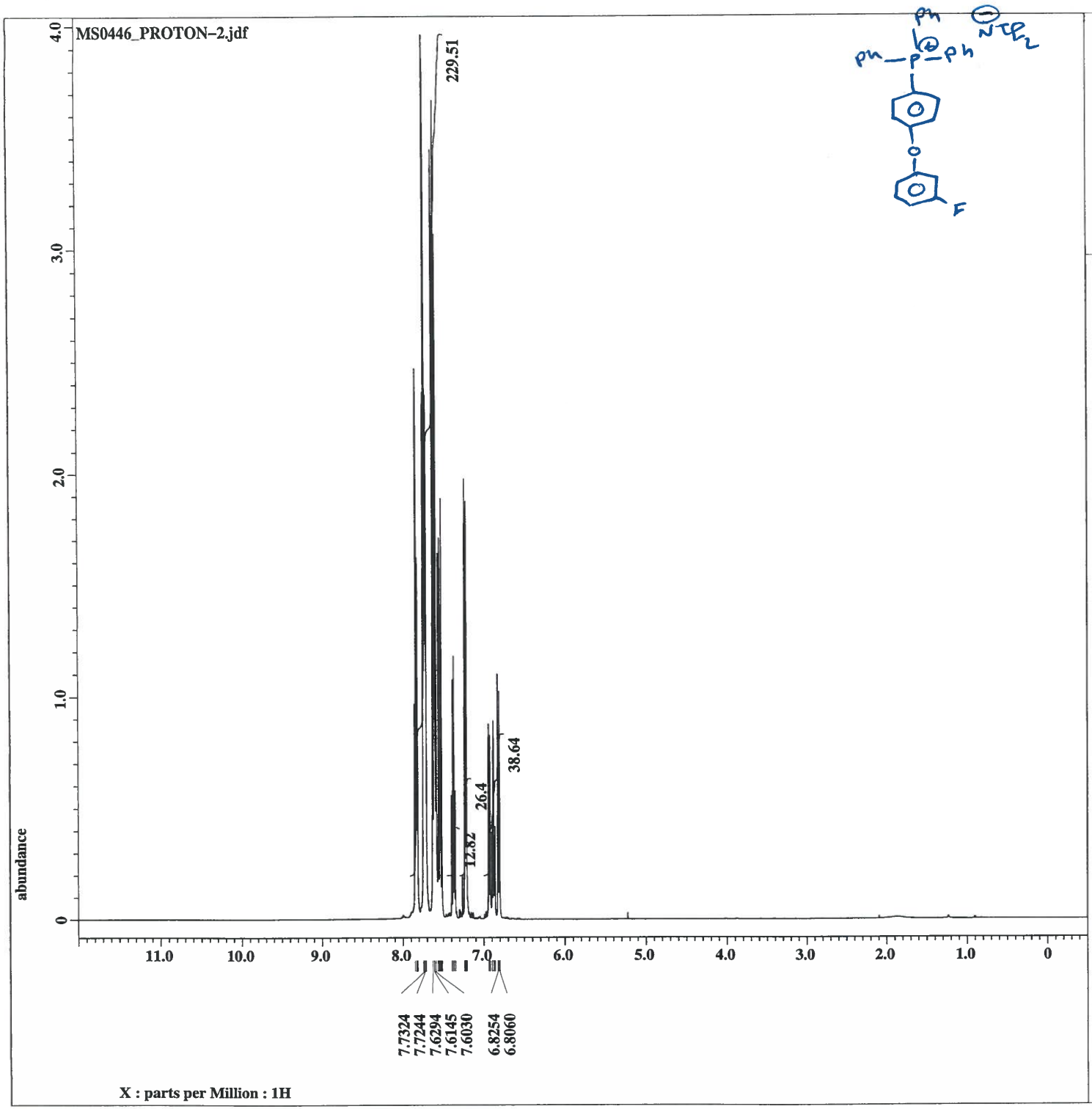


SOUTH ALABAMA JAGUARS

Filename	= MS0416_FLUORINE-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0416
Solvent	= CHLOROFORM-D
Changer_sample	= 10
Creation_time	= 14-APR-2018 11:25:31
Revision_time	= 14-APR-2018 11:03:39
Current_time	= 14-APR-2018 11:03:39
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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 34
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.6[dC]

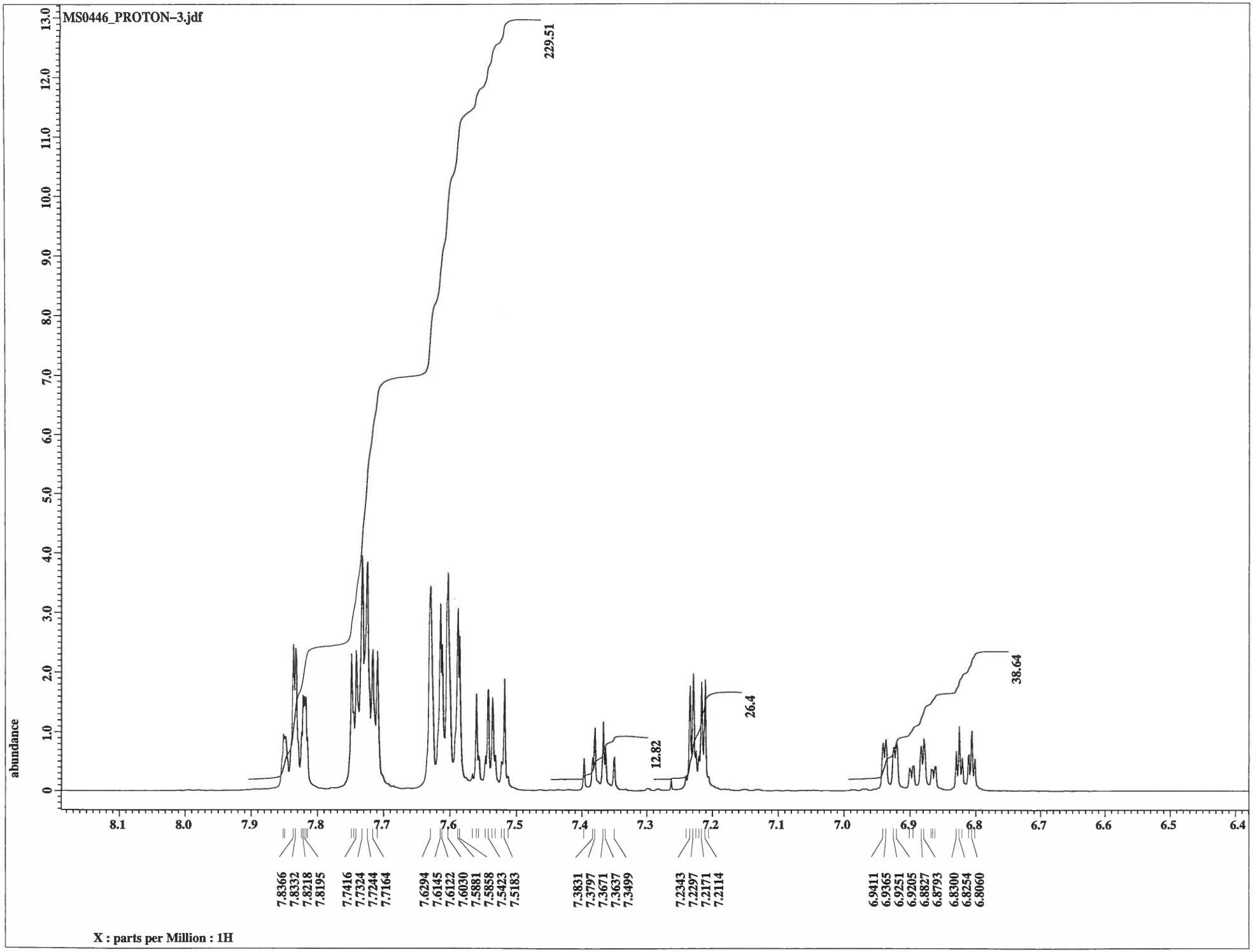


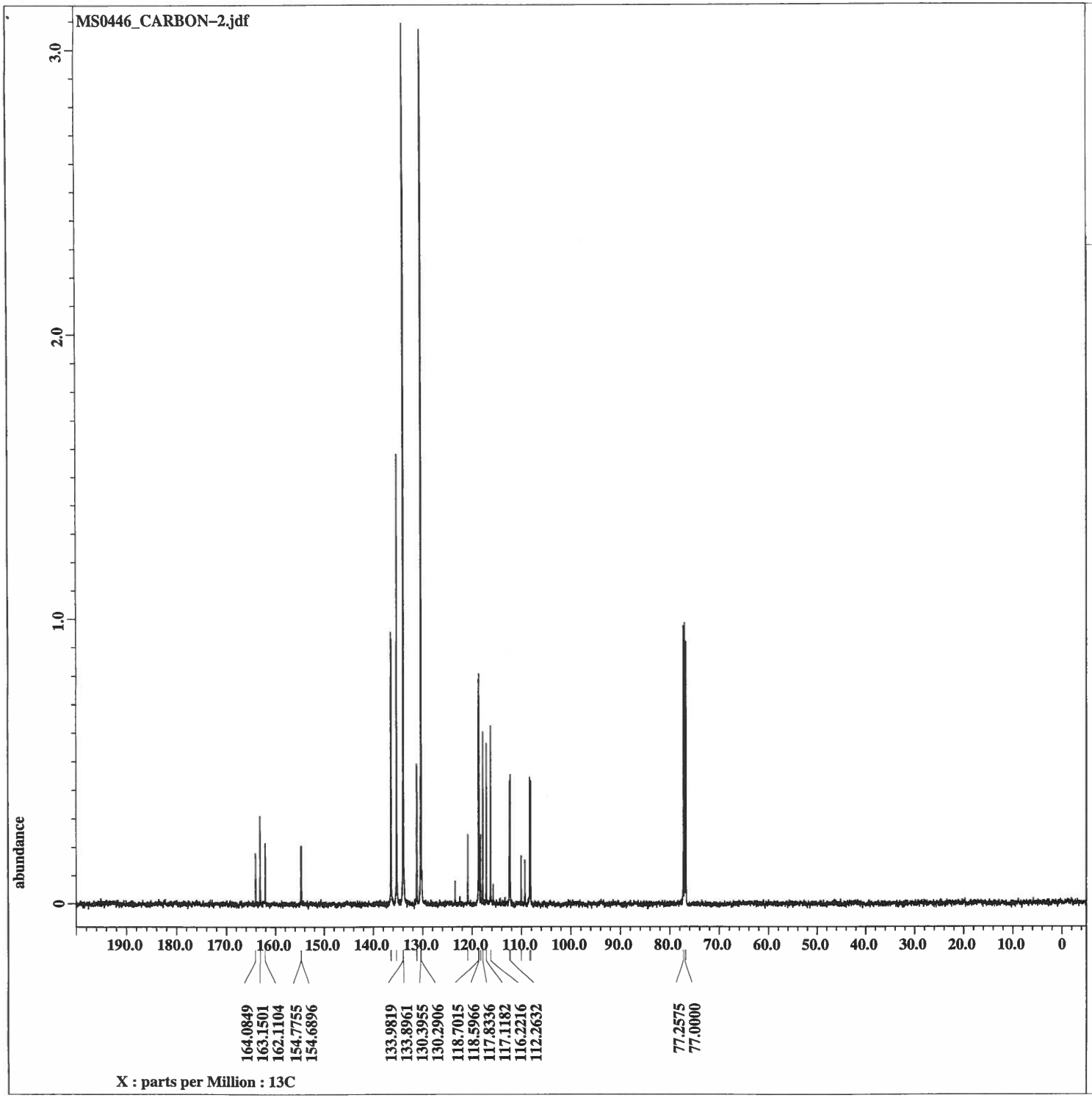
Filename	= MS0416_PHOSPHORUS-2.j
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0416
Solvent	= CHLOROFORM-D
Changer_sample	= 10
Creation_time	= 14-APR-2018 11:29:07
Revision_time	= 14-APR-2018 11:07:15
Current_time	= 14-APR-2018 11:07:15
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 31P
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.64487424[s]
X_domain	= 31P
X_freq	= 202.46831075[MHz]
X_offset	= 0[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.55068995[Hz]
X_sweep	= 50.81300813[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 25
Total_scans	= 25
X_90_width	= 14.687[us]
X_acq_time	= 0.64487424[s]
X_angle	= 30[deg]
X_atn	= 5[dB]
X_pulse	= 4.89566667[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
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[dC]



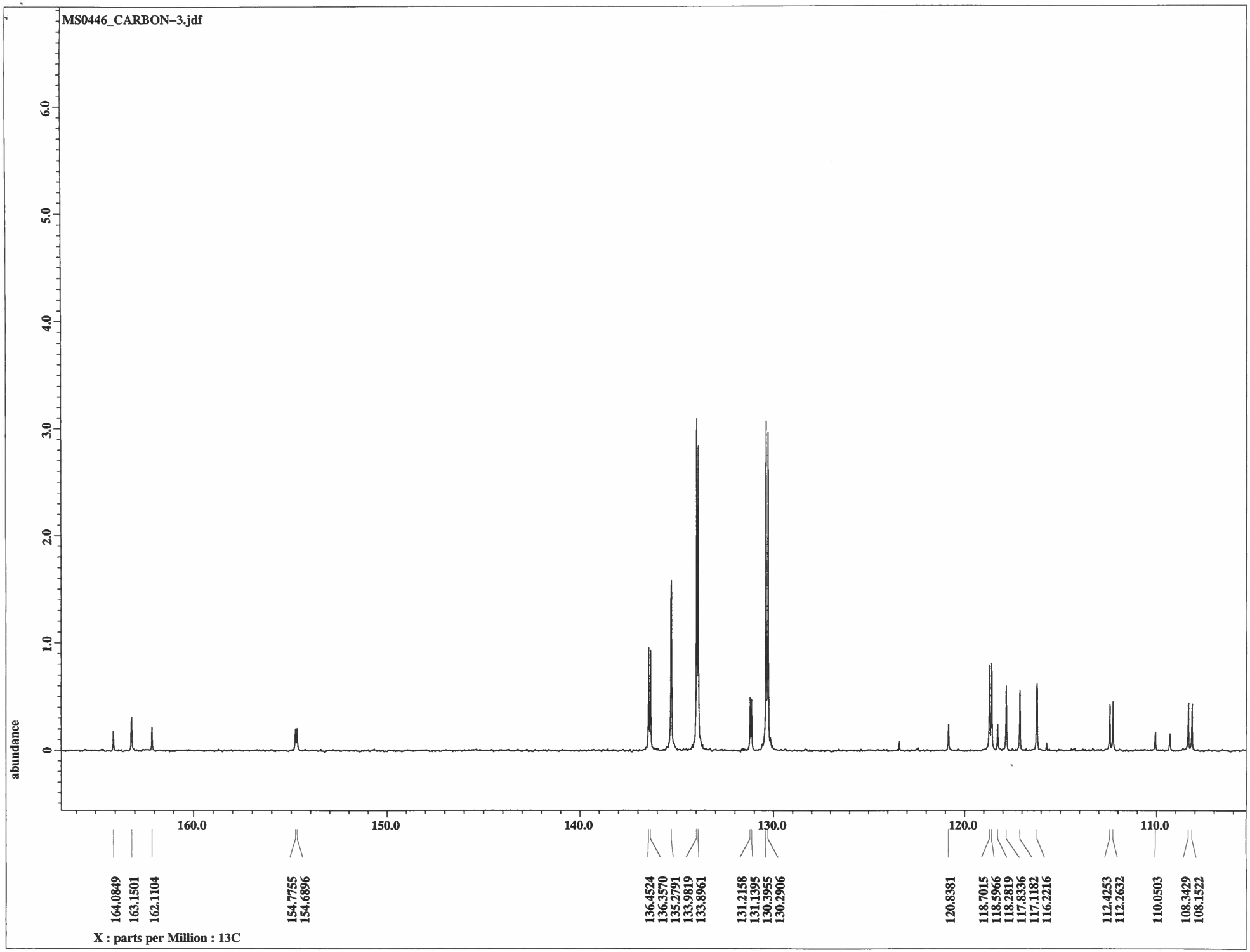
SOUTH ALABAMA JAGUARS

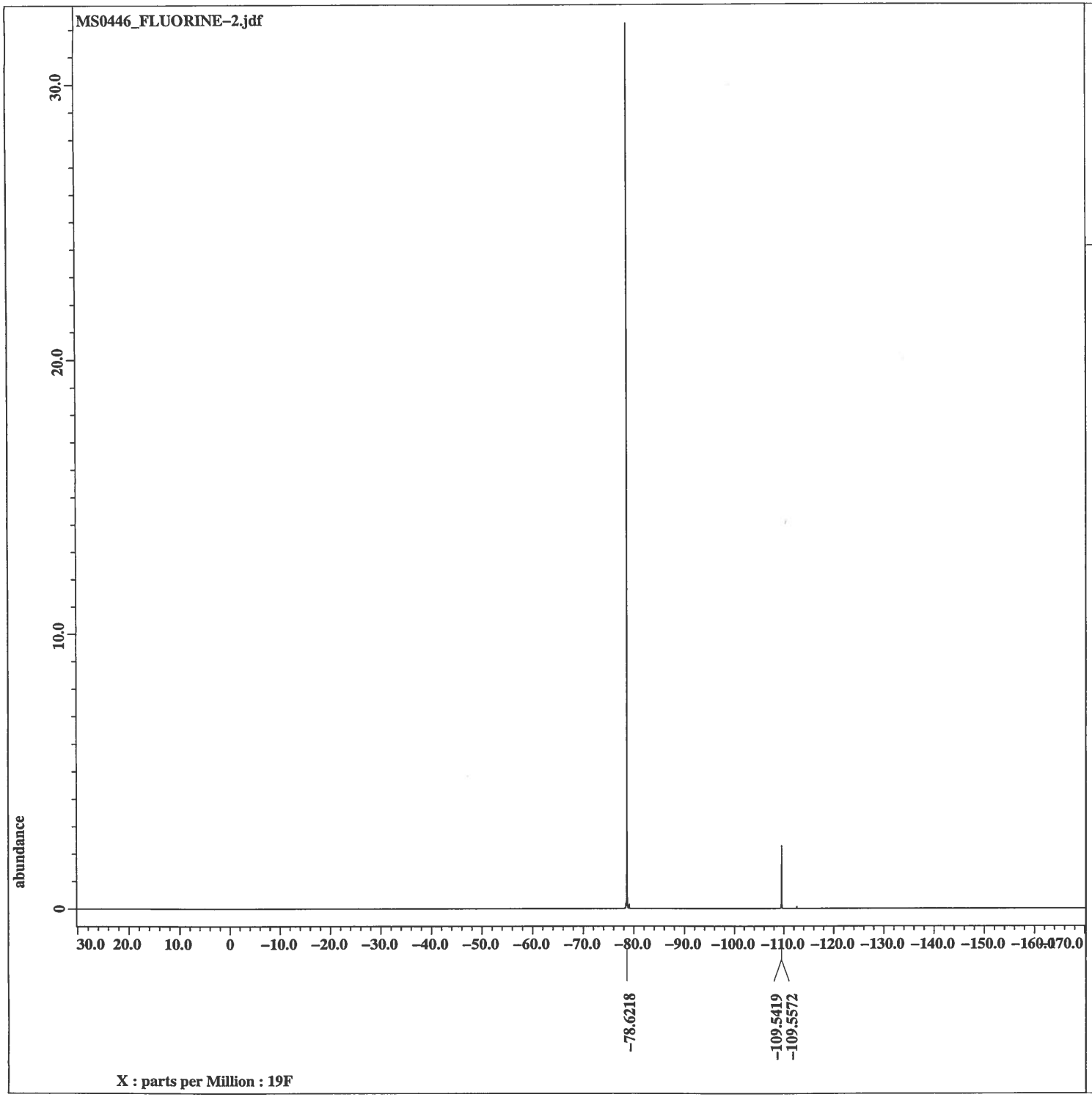
Filename	= MS0446_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0446
Solvent	= CHLOROFORM-D
Changer_sample	= 1
Creation_time	= 14-MAY-2018 12:32:44
Revision_time	= 14-MAY-2018 12:08:31
Current_time	= 14-MAY-2018 12:08:31
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 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	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 20
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.8[dC]


MS0446_PROTON-3.jdf
229.51
12.82
26.4
38.64
abundance
X : parts per Million : 1H
7.8366
7.8332
7.8218
7.8195
7.7416
7.7324
7.7244
7.7164
7.6294
7.6145
7.6122
7.6030
7.5881
7.5858
7.5423
7.5183
7.3831
7.3797
7.3671
7.3637
7.3499
7.2343
7.2297
7.2171
7.2114
6.9411
6.9365
6.9251
6.9205
6.8827
6.8793
6.8300
6.8254
6.8060



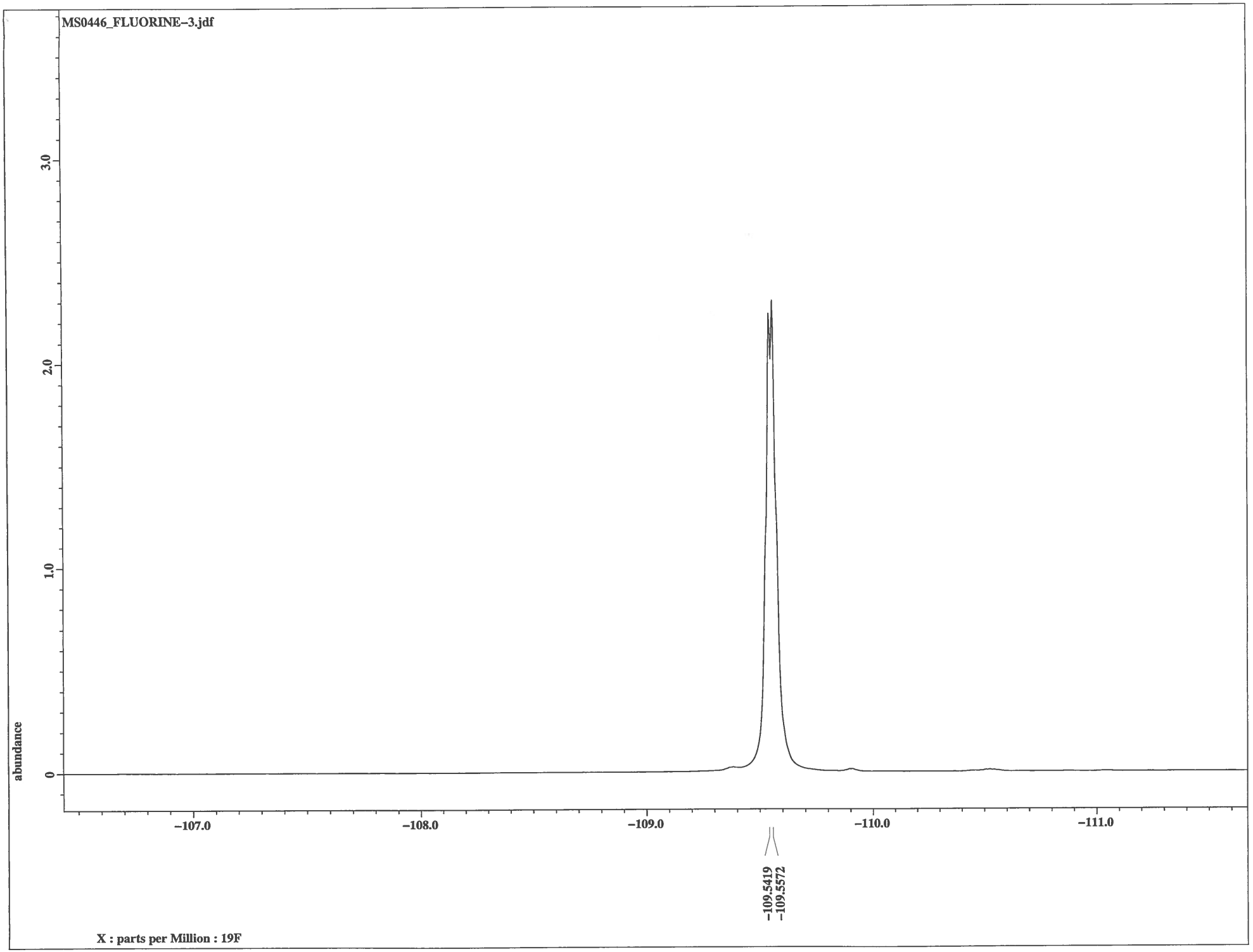
Filename	= MS0446_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0446
Solvent	= CHLOROFORM-D
Changer_sample	= 1
Creation_time	= 14-MAY-2018 12:41:05
Revision_time	= 14-MAY-2018 12:16:51
Current_time	= 14-MAY-2018 12:16:51
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 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	= 128
Total_scans	= 128
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 22.8[dC]

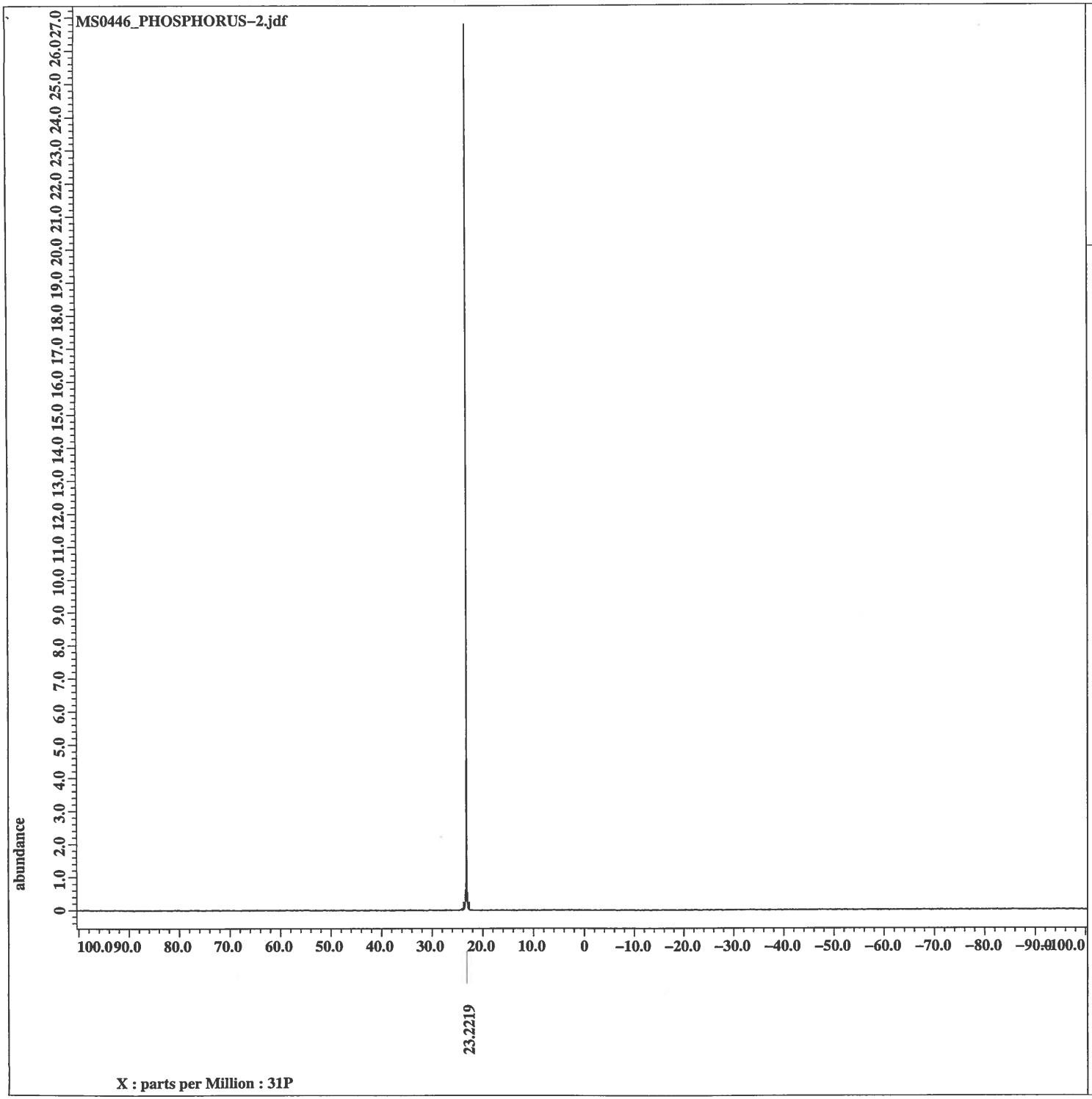

MS0446_CARBON-3.jdf
abundance
6.0
5.0
4.0
3.0
2.0
1.0
0
160.0
150.0
140.0
130.0
120.0
110.0
164.0849
163.1501
162.1104
154.7755
154.6896
136.4524
136.3570
135.2791
133.9819
133.8961
131.2158
131.1395
130.3955
130.2906
120.8381
118.7015
118.5966
118.2819
117.8336
117.1182
116.2216
112.4253
112.2632
110.0503
108.3429
108.1522
X : parts per Million : 13C



SOUTH ALABAMA JAGUARS™

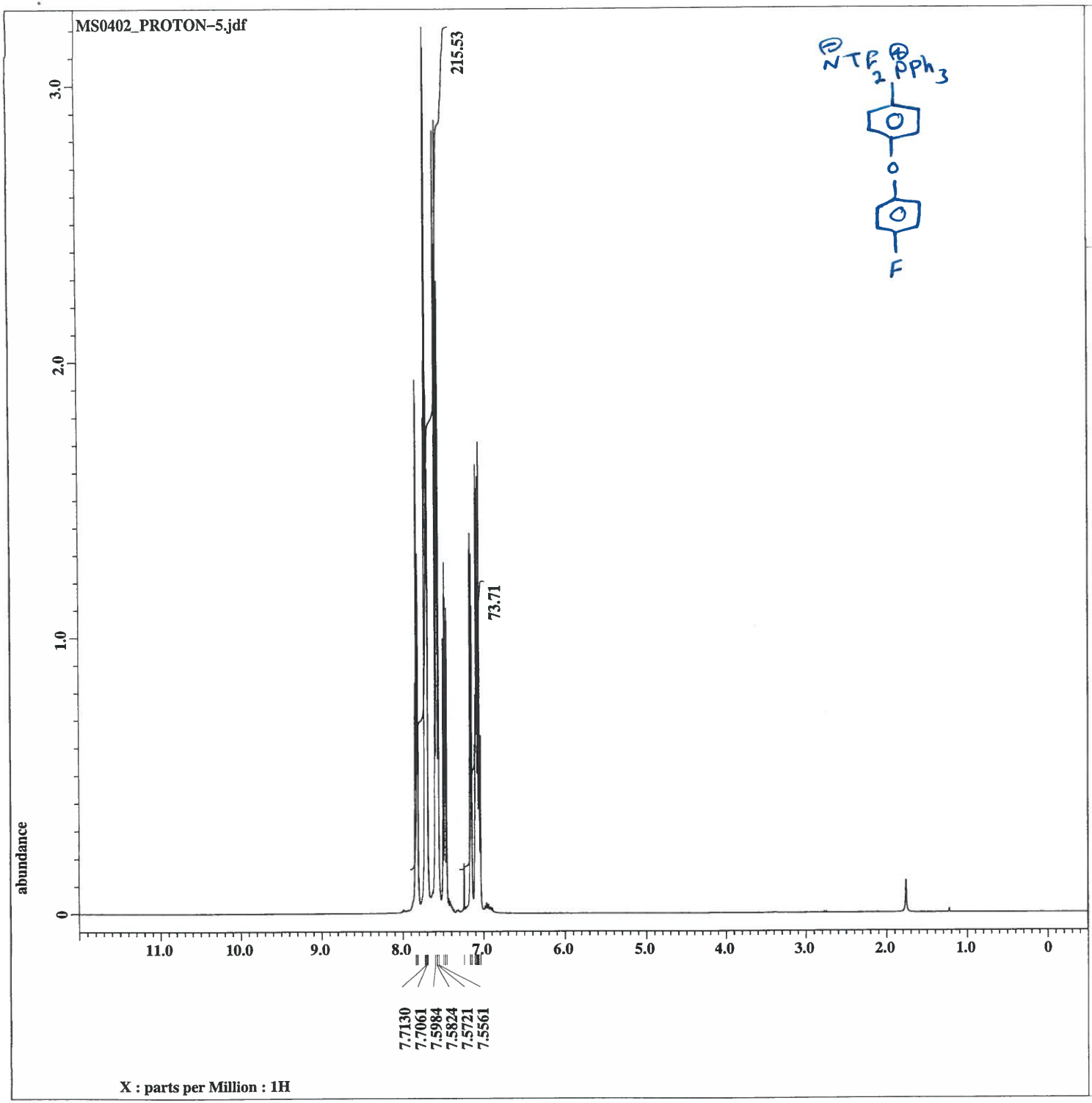
Filename	= MS0446_FLUORINE-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0446
Solvent	= CHLOROFORM-D
Changer_sample	= 1
Creation_time	= 14-MAY-2018 12:25:44
Revision_time	= 14-MAY-2018 12:01:32
Current_time	= 14-MAY-2018 12:01:32
Data_format	= 1D COMPLEX
Dim_size	= 52428
Dim_title	= 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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 30
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.7[dC]


MS0446_FLUORINE-3.jdf
3.0
2.0
1.0
0
abundance
-107.0
-108.0
-109.0
-110.0
-111.0
-109.5419
-109.5572
X : parts per Million : 19F

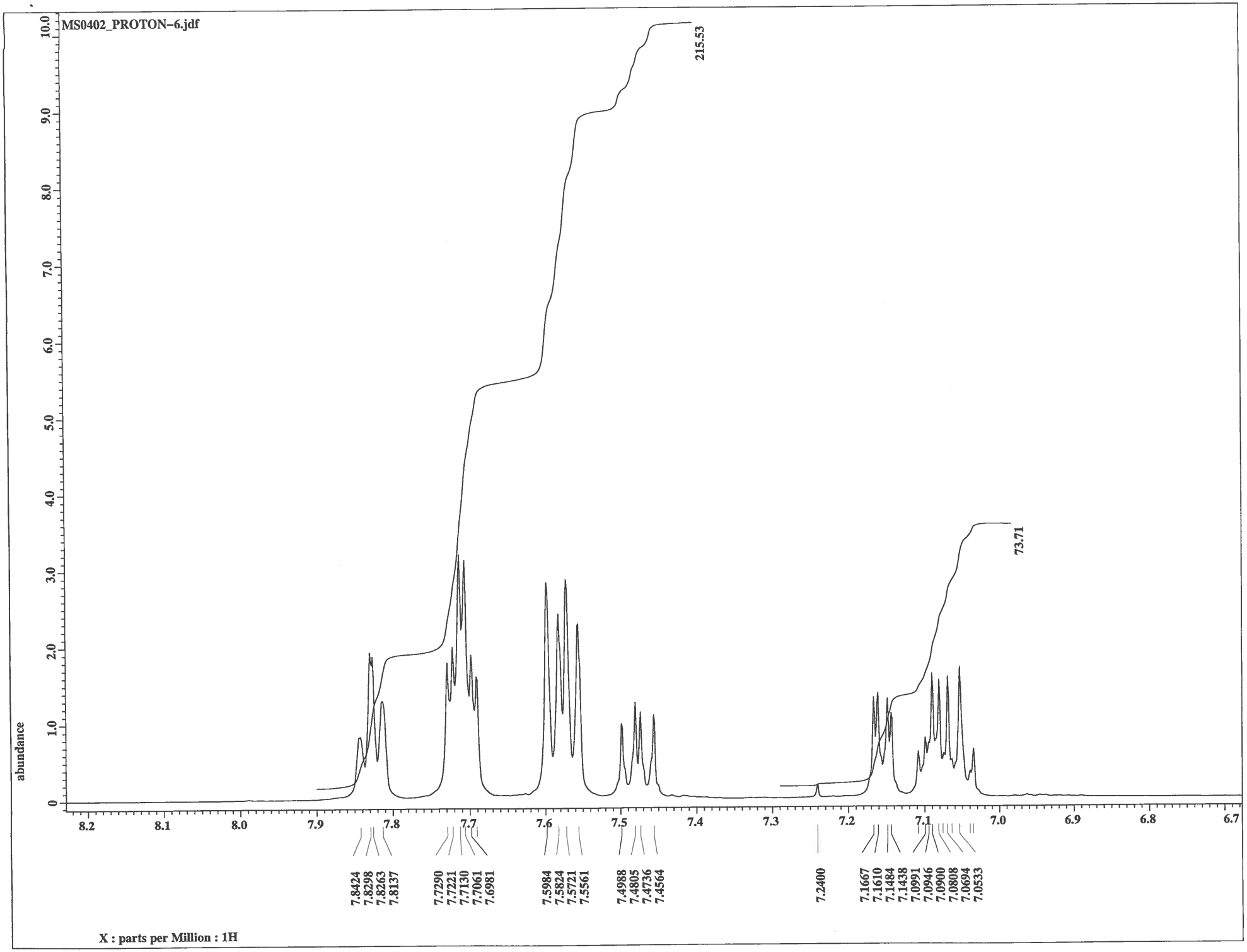


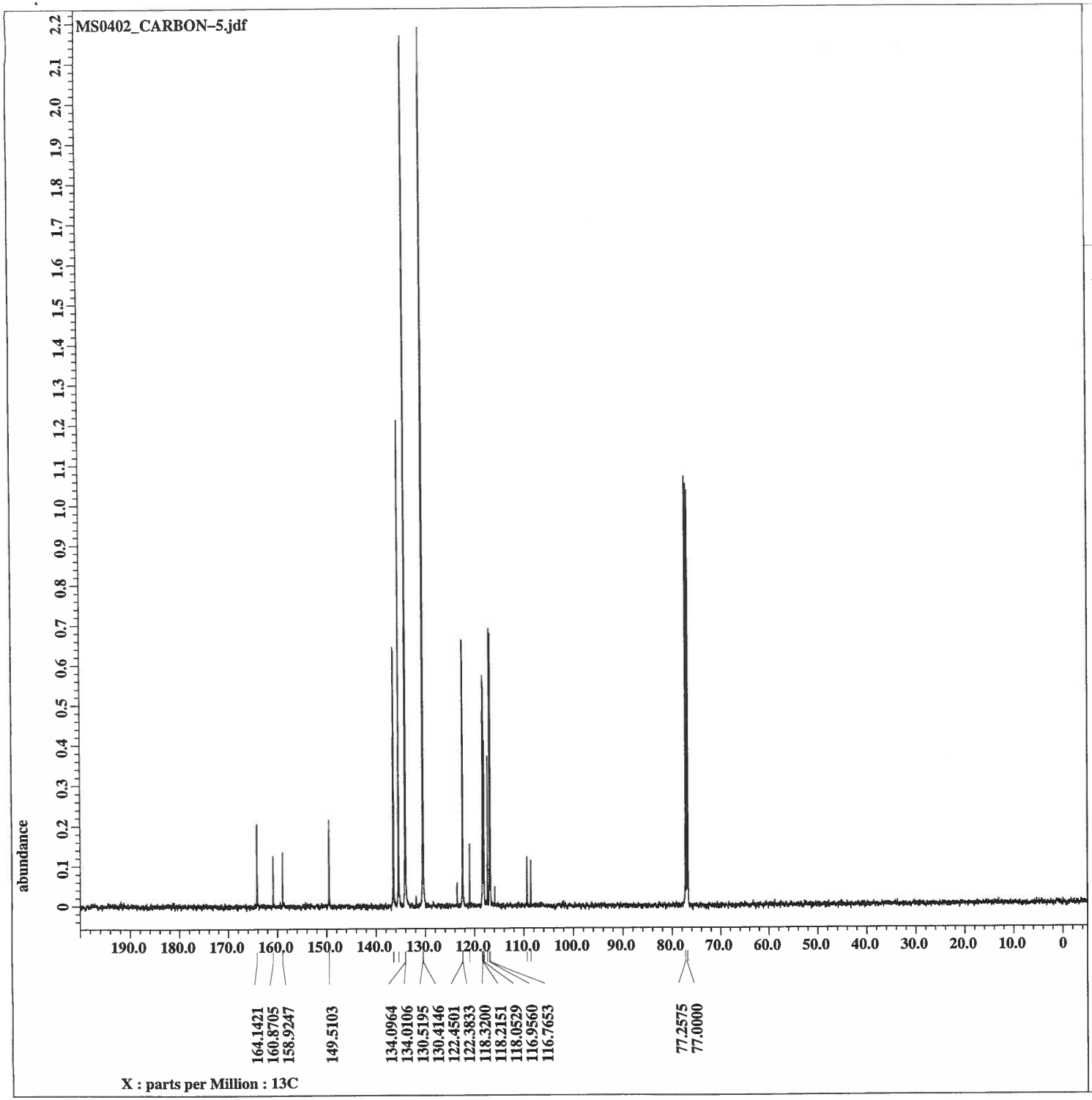
SOUTH ALABAMA JAGUARS™

Filename	= MS0446_PHOSPHORUS-2.j
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0446
Solvent	= CHLOROFORM-D
Changer_sample	= 1
Creation_time	= 14-MAY-2018 12:29:19
Revision_time	= 14-MAY-2018 12:05:05
Current_time	= 14-MAY-2018 12:05:05
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	= 25
Total_scans	= 25
X_90_width	= 14.687[us]
X_acq_time	= 0.64487424[s]
X_angle	= 30[deg]
X_atn	= 5[dB]
X_pulse	= 4.89566667[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
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[dC]



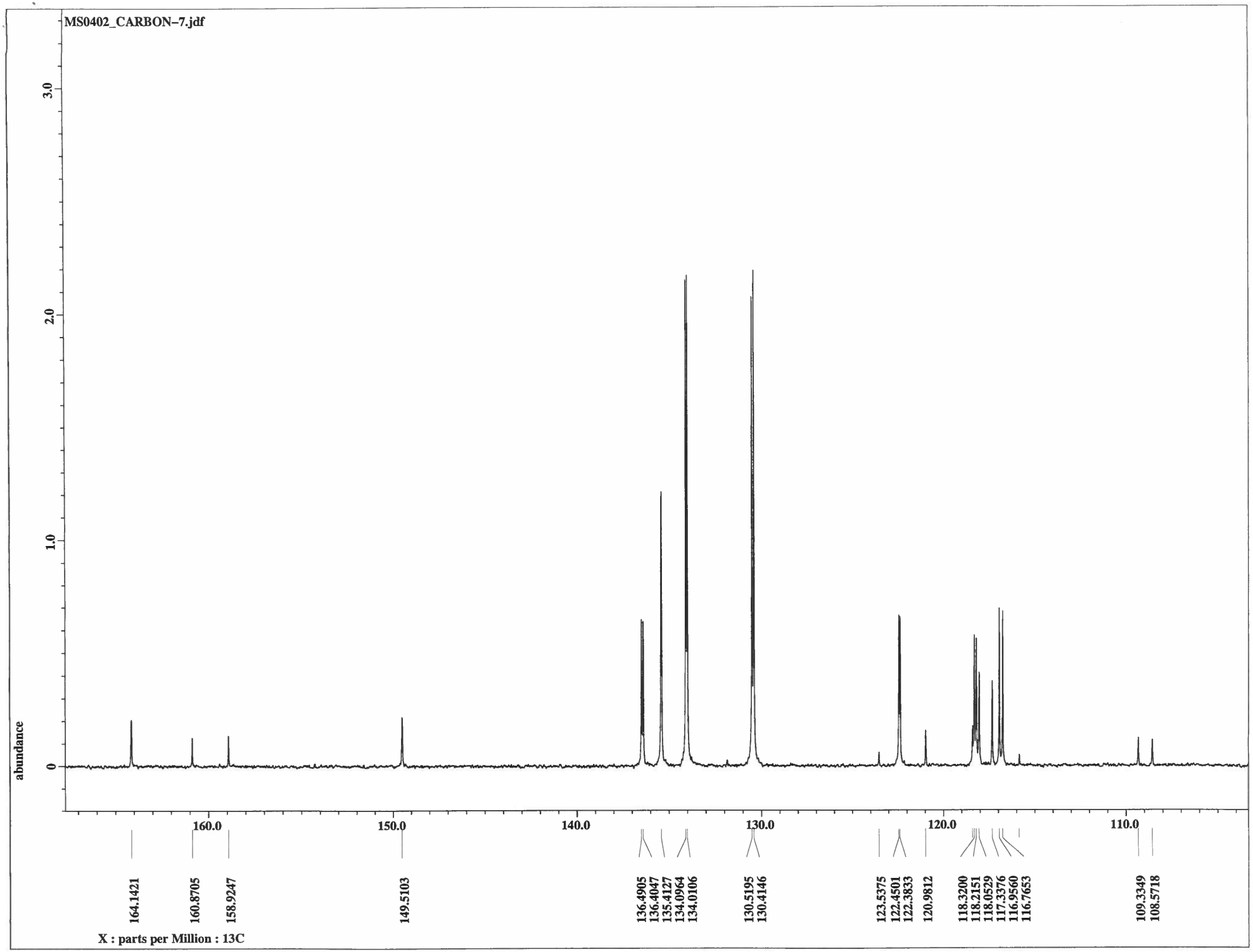
Filename	= MS0402_PROTON-5.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0402
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 18-MAY-2018 16:54:40
Revision_time	= 18-MAY-2018 16:30:05
Current_time	= 18-MAY-2018 16:30:05
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 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[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	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 24
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.8[dC]

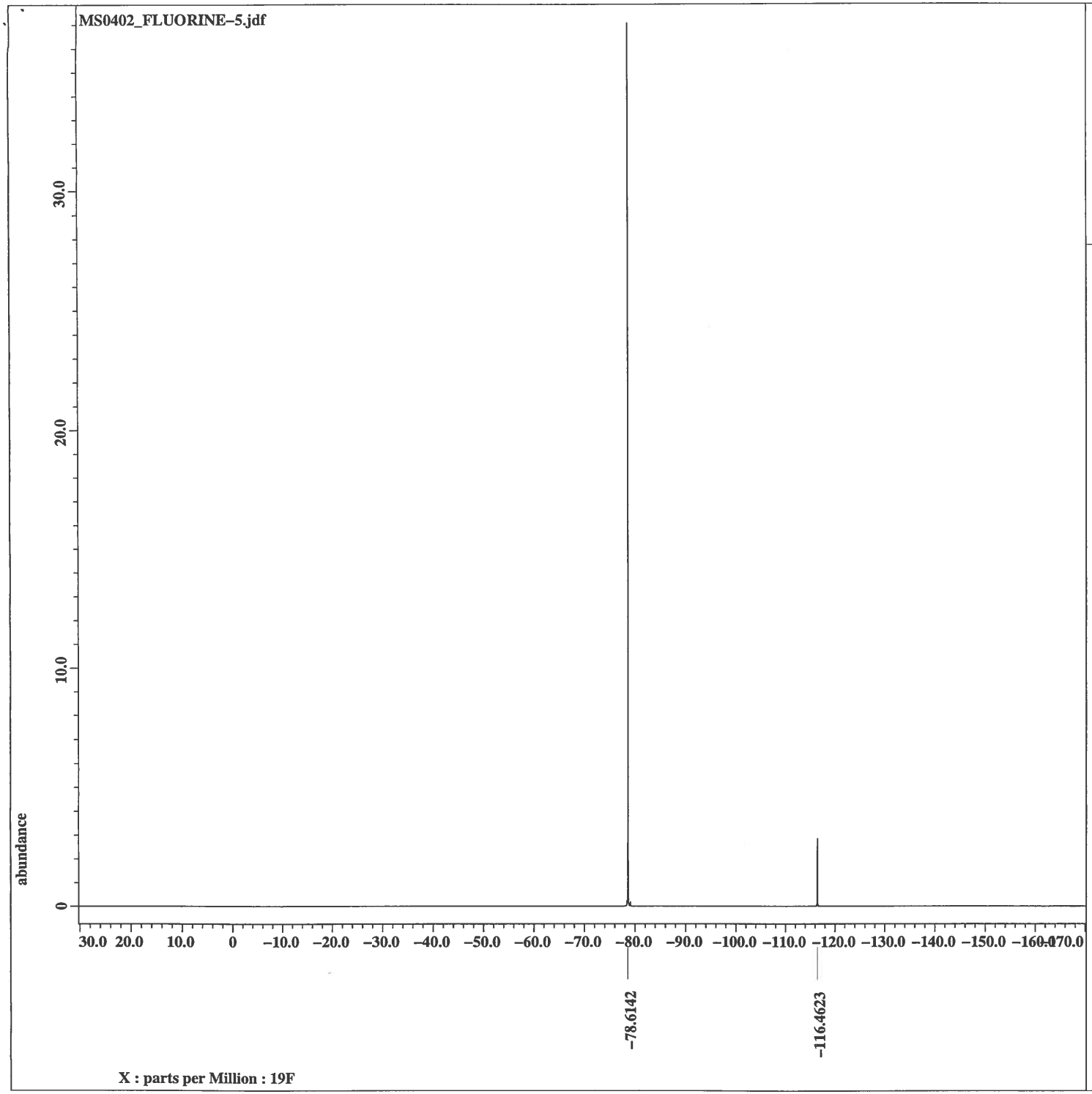

MS0402_PROTON-6.jdf
abundance
215.53
73.71
7.8424
7.8298
7.8263
7.8137
7.7290
7.7221
7.7130
7.7061
7.6981
7.5984
7.5824
7.5721
7.5561
7.4988
7.4805
7.4736
7.4564
7.2400
7.1667
7.1610
7.1484
7.1438
7.0991
7.0946
7.0900
7.0808
7.0694
7.0533
X : parts per Million : 1H



SOUTH ALABAMA JAGUARS

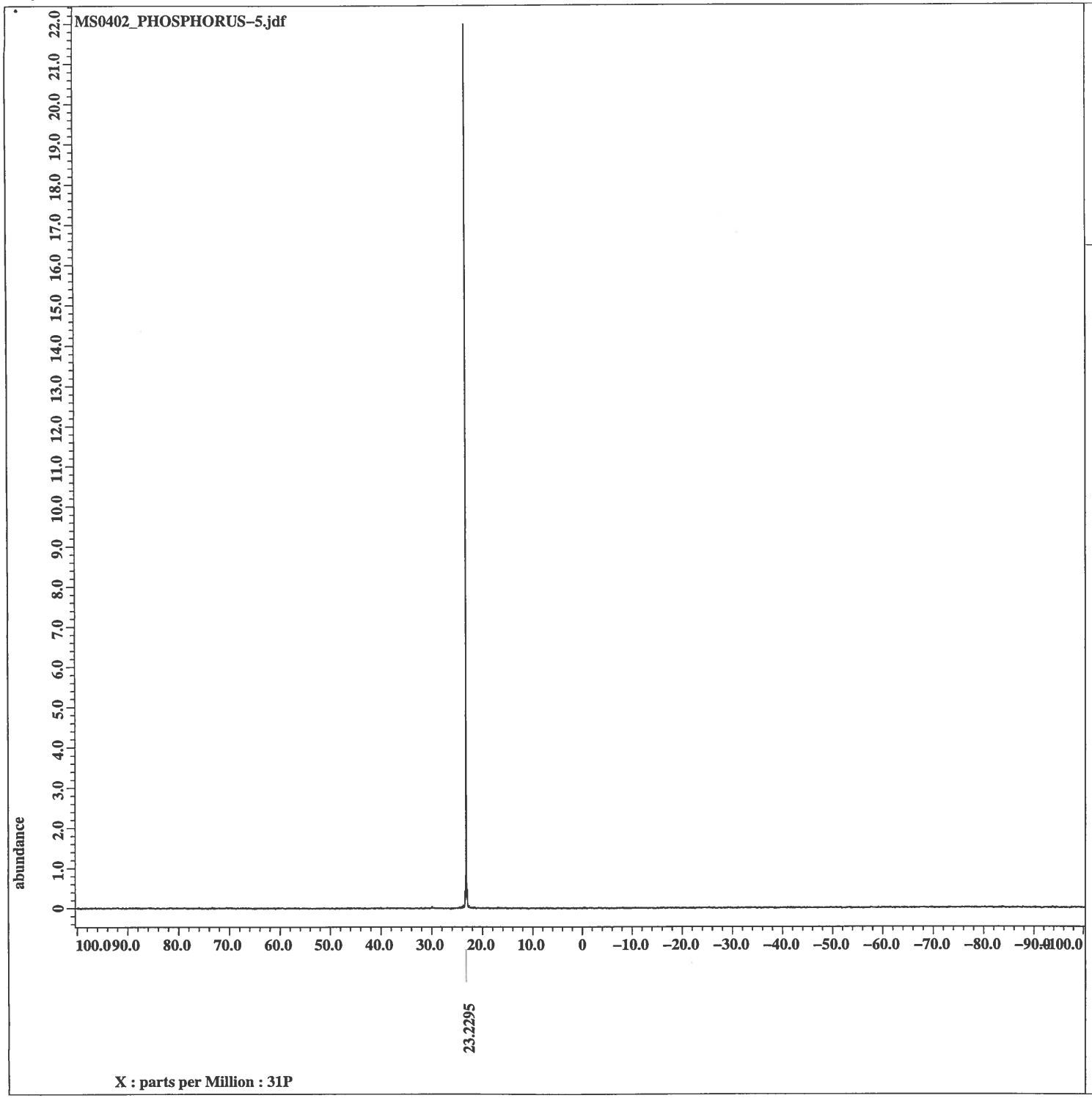
Filename	= MS0402_CARBON-5.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0402
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 18-MAY-2018 17:08:56
Revision_time	= 18-MAY-2018 16:44:20
Current_time	= 18-MAY-2018 16:44:20
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 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	= 256
Total_scans	= 256
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 22.9[dC]


MS0402_CARBON-7.jdf
abundance
3.0
2.0
1.0
0
160.0
150.0
140.0
130.0
120.0
110.0
164.1421
160.8705
158.9247
149.5103
136.4905
136.4047
135.4127
134.0964
134.0106
130.5195
130.4146
123.5375
122.4501
122.3833
120.9812
118.3200
118.2151
118.0529
117.3376
116.9560
116.7653
109.3349
108.5718
X : parts per Million : 13C



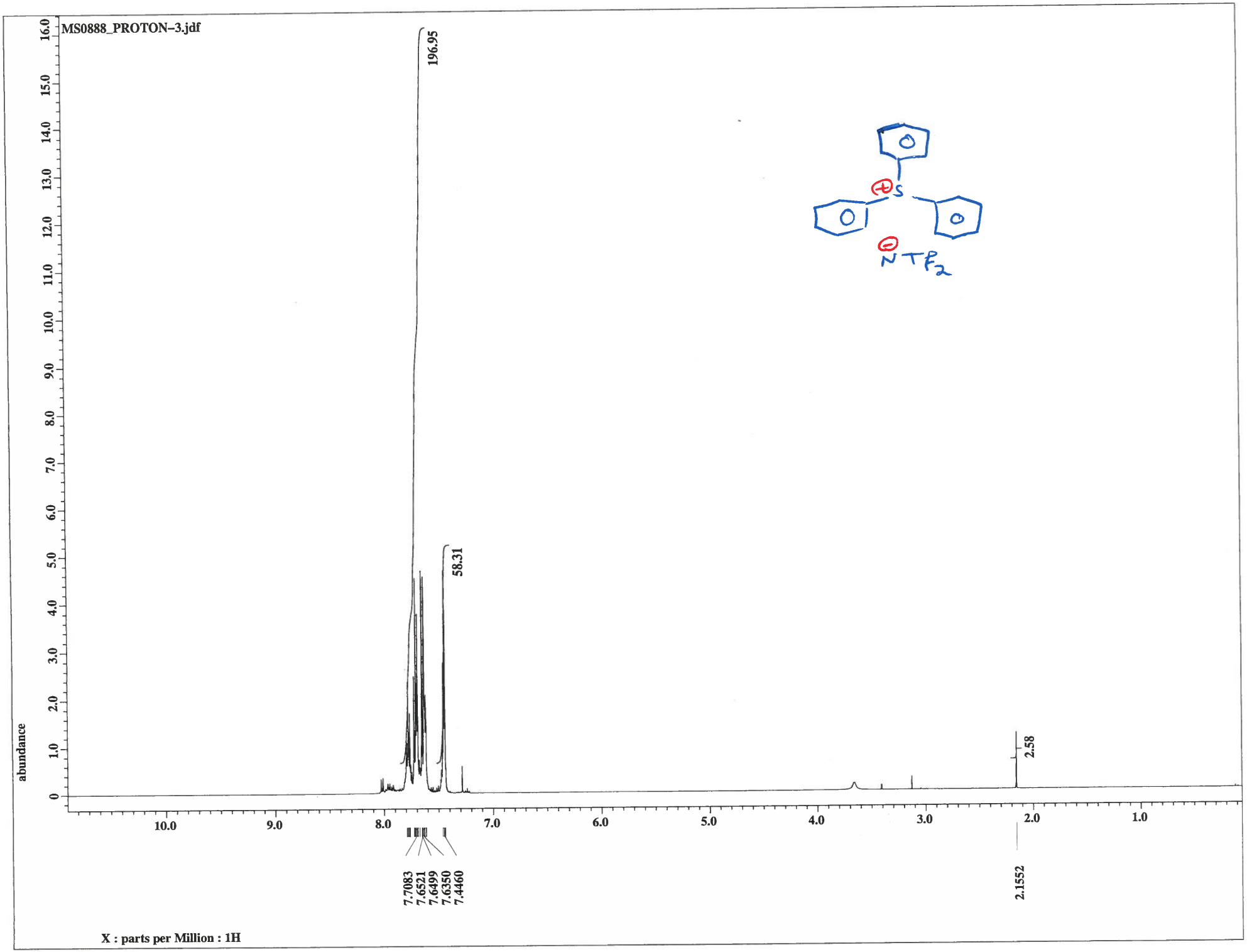
SOUTH ALABAMA JAGUARS™

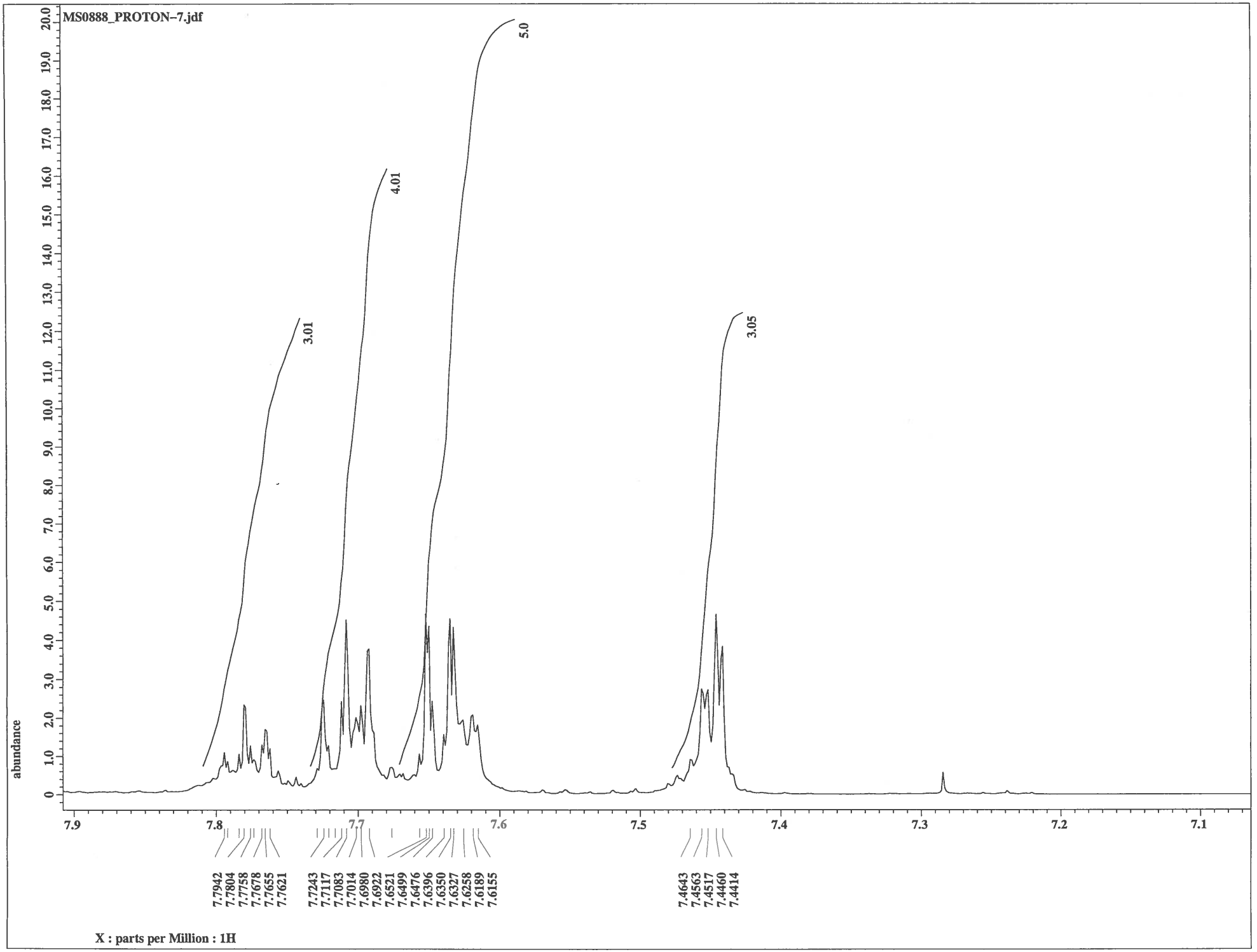
Filename	= MS0402_FLUORINE-5.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0402
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 18-MAY-2018 17:11:54
Revision_time	= 18-MAY-2018 16:47:18
Current_time	= 18-MAY-2018 16:47:18
Data_format	= 1D COMPLEX
Dim_size	= 52428
Dim_title	= 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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.6[dC]

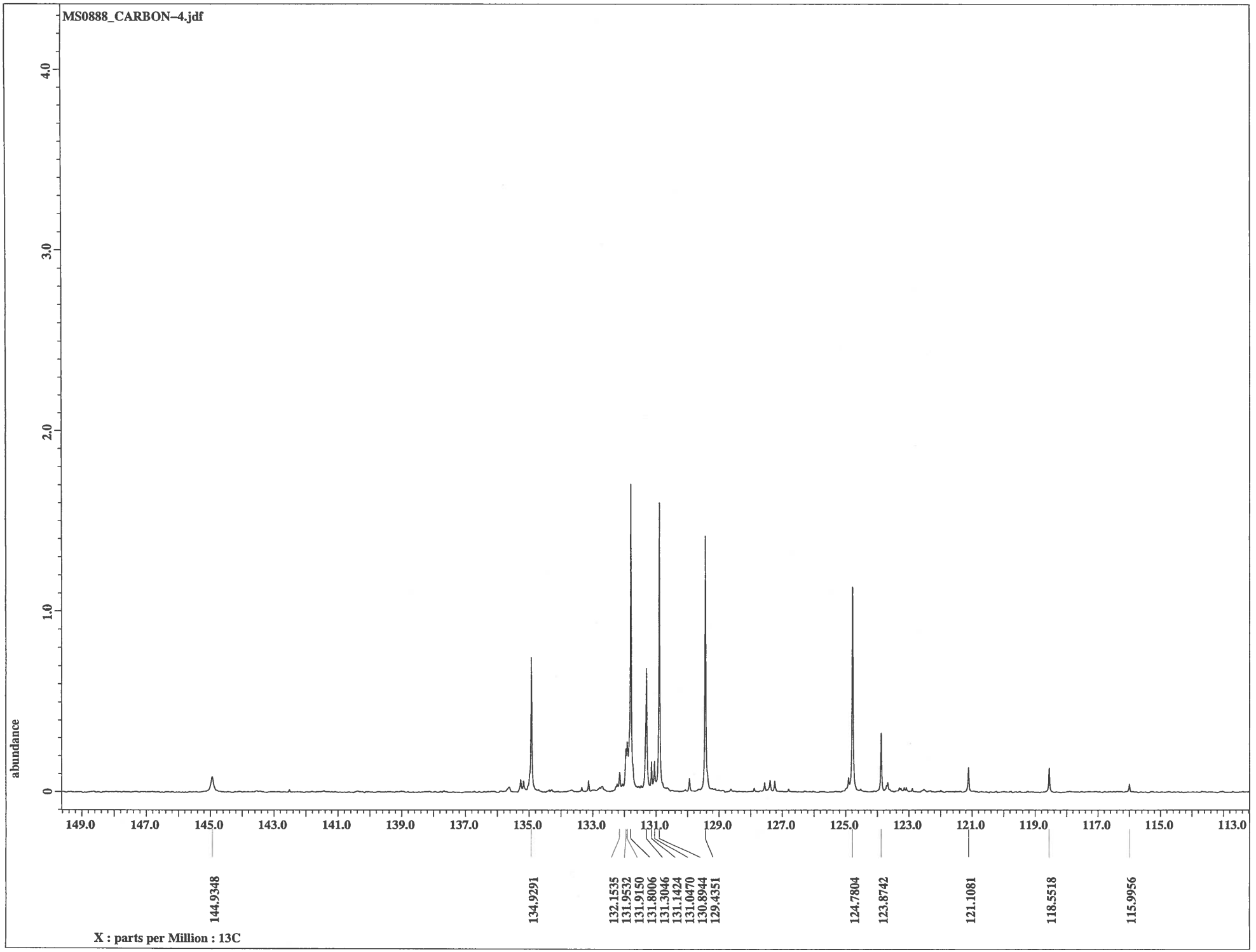


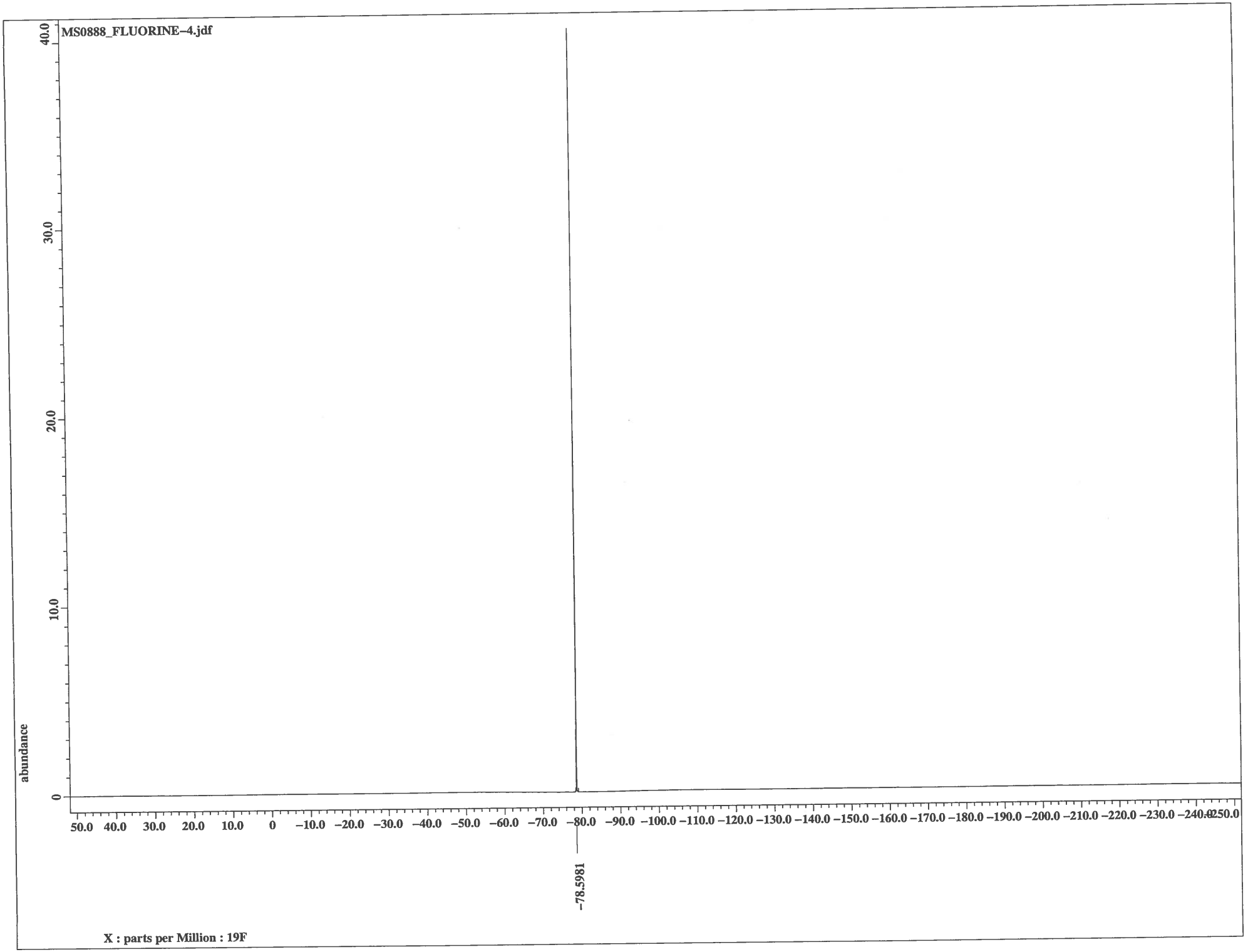
SOUTH ALABAMA JAGUARS™

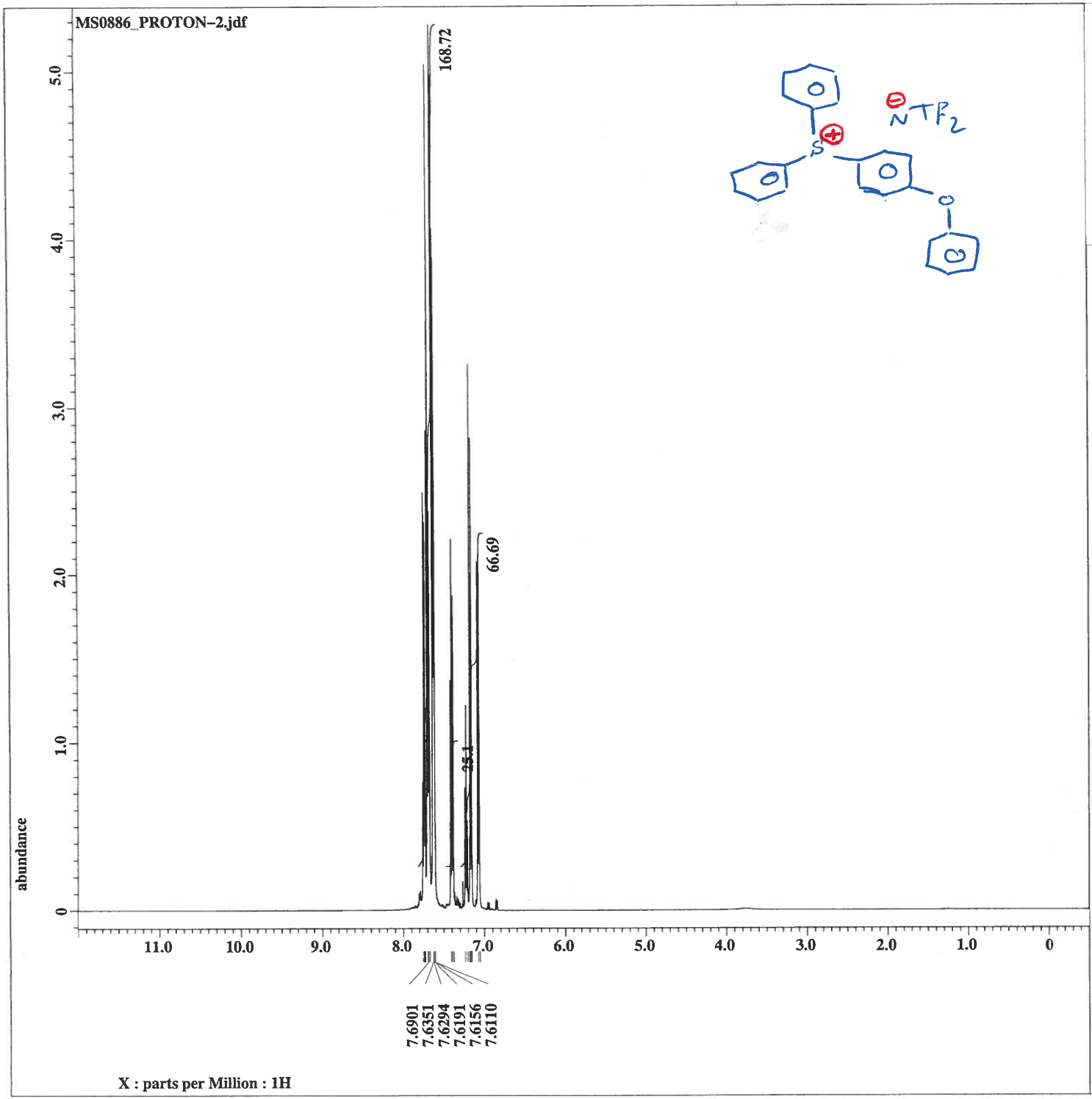
Filename	= MS0402_PHOSPHORUS-5.j
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0402
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 18-MAY-2018 17:15:26
Revision_time	= 18-MAY-2018 16:50:51
Current_time	= 18-MAY-2018 16:50:51
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 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	= 25
Total_scans	= 25
X_90_width	= 14.687[us]
X_acq_time	= 0.64487424[s]
X_angle	= 30[deg]
X_atn	= 5[dB]
X_pulse	= 4.89566667[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
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	= 22.9[dC]


MS0888_PROTON-3.jdf
196.95
58.31
2.58
2.1552
7.7083
7.6521
7.6499
7.6350
7.4460
abundance
X : parts per Million : 1H


MS0888_PROTON-7.jdf
abundance
3.01
4.01
5.0
3.05
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.7942
7.7804
7.7758
7.7678
7.7655
7.7621
7.7243
7.7117
7.7083
7.7014
7.6980
7.6922
7.6521
7.6499
7.6476
7.6396
7.6350
7.6327
7.6258
7.6189
7.6155
7.4643
7.4563
7.4517
7.4460
7.4414
X : parts per Million : 1H

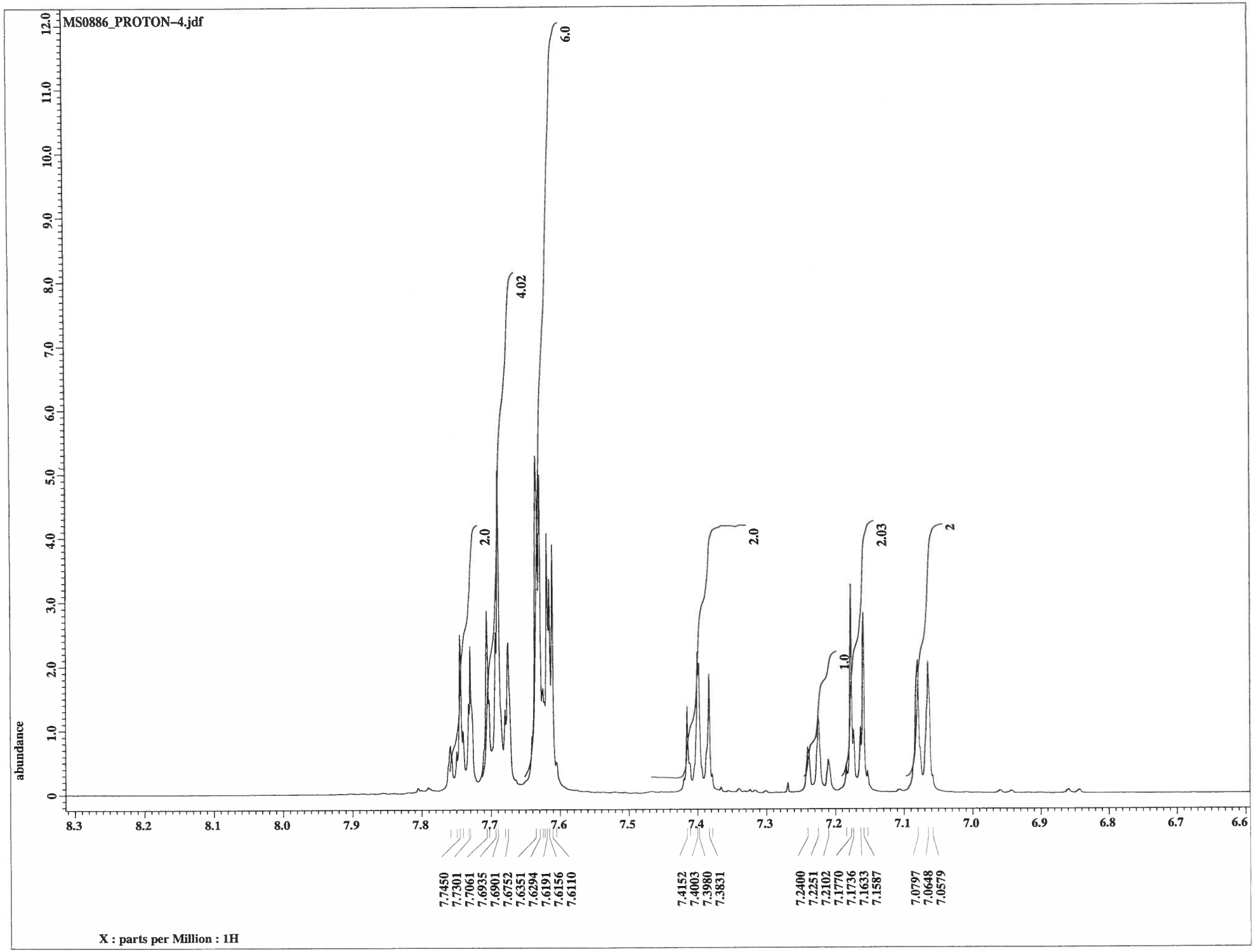

MS0888_CARBON-4.jdf
abundance
4.0
3.0
2.0
1.0
0
149.0
147.0
145.0
143.0
141.0
139.0
137.0
135.0
133.0
131.0
129.0
127.0
125.0
123.0
121.0
119.0
117.0
115.0
113.0
144.9348
134.9291
132.1535
131.9532
131.9150
131.8006
131.3046
131.1424
131.0470
130.8944
129.4351
124.7804
123.8742
121.1081
118.5518
115.9956
X : parts per Million : 13C

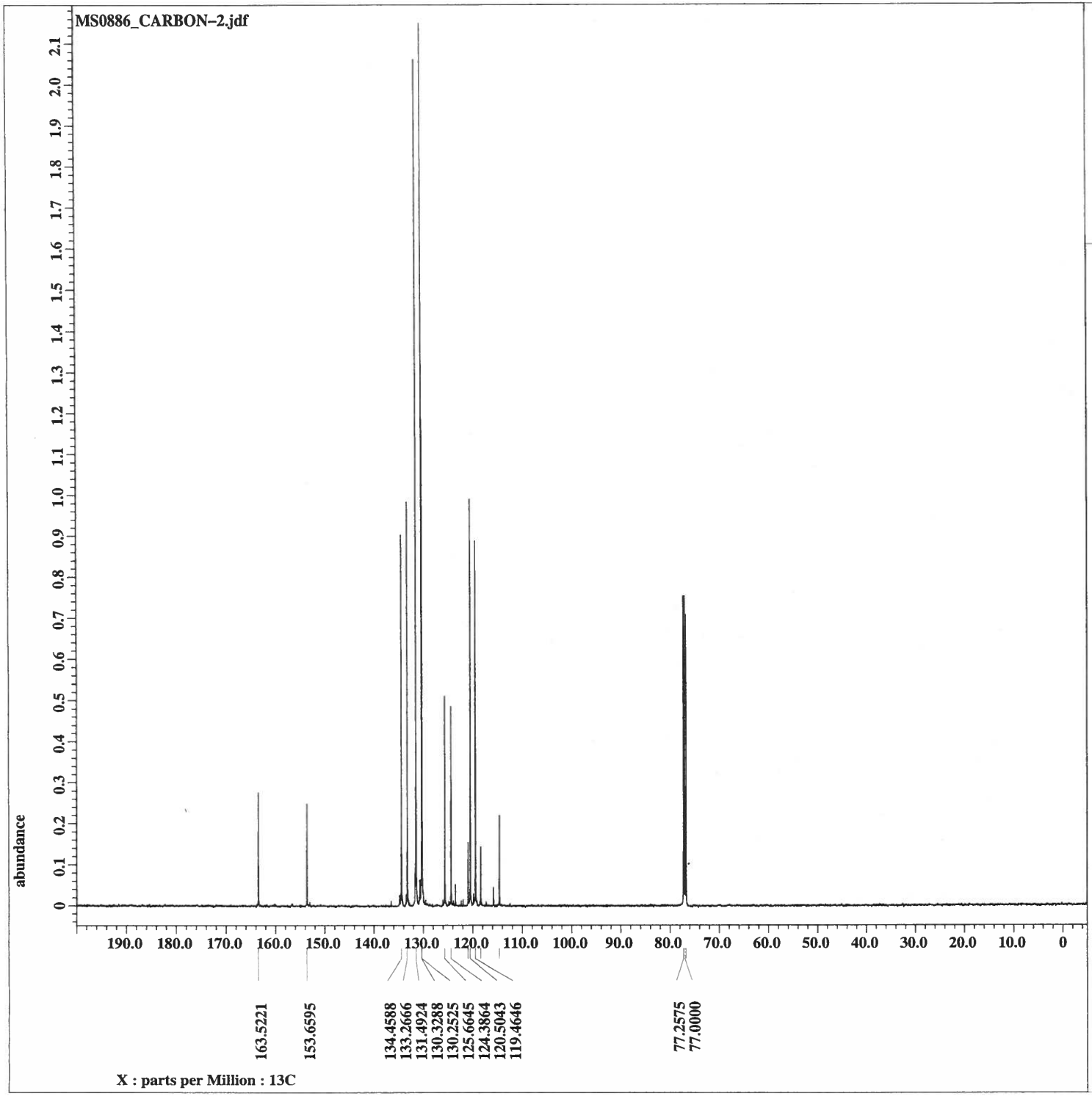

MS0888_FLUORINE-4.jdf
40.0
30.0
20.0
10.0
0
abundance
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0 -210.0 -220.0 -230.0 -240.0 -250.0
-78.5981
X : parts per Million : 19F



SOUTH ALABAMA JAGUARS

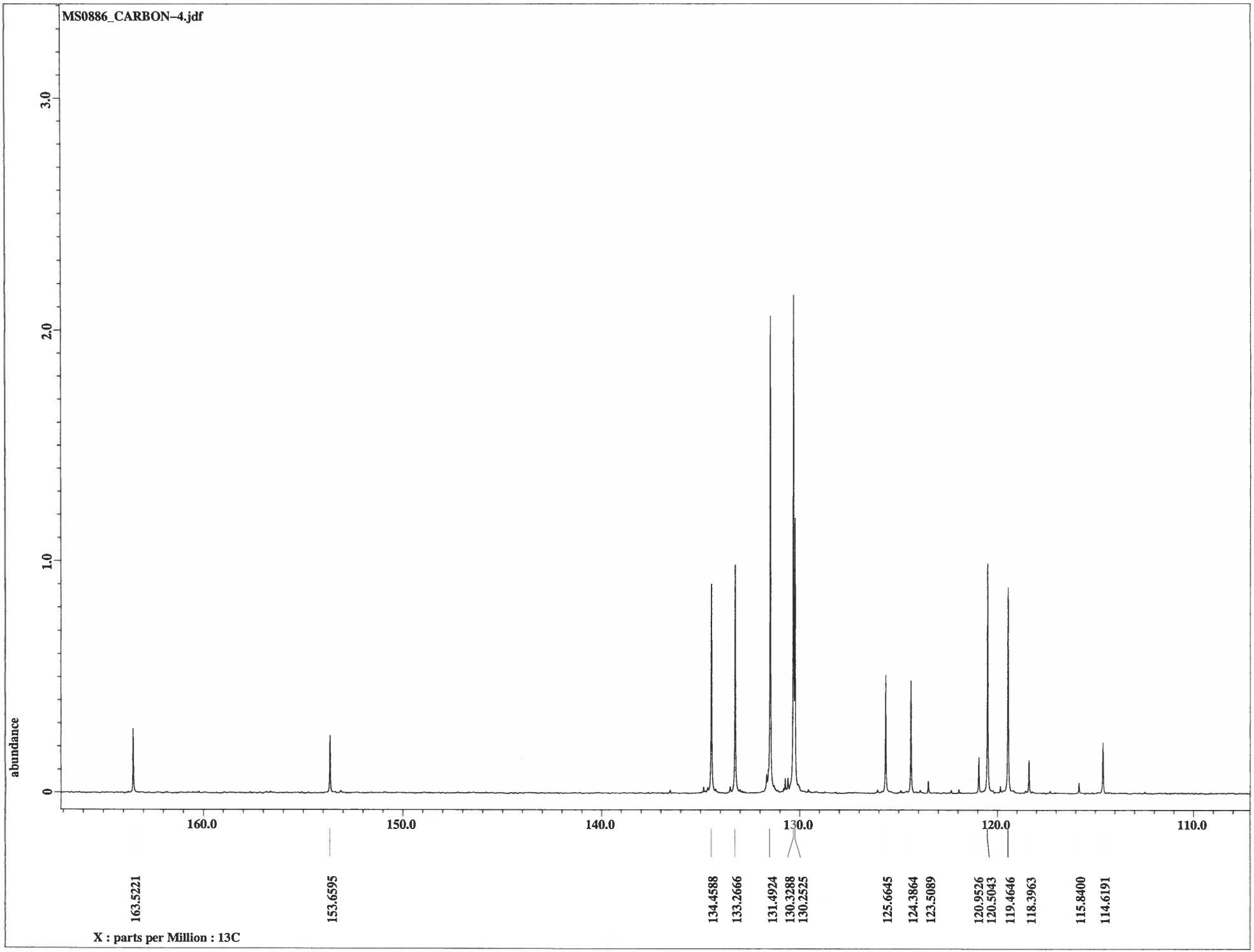
Filename	= MS0886_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0886
Solvent	= CHLOROFORM-D
Creation_time	= 29-NOV-2019 12:51:31
Revision_time	= 29-NOV-2019 12:22:15
Current_time	= 29-NOV-2019 12:22:15
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [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	= 11.3[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 5.65[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	= 19[dC]

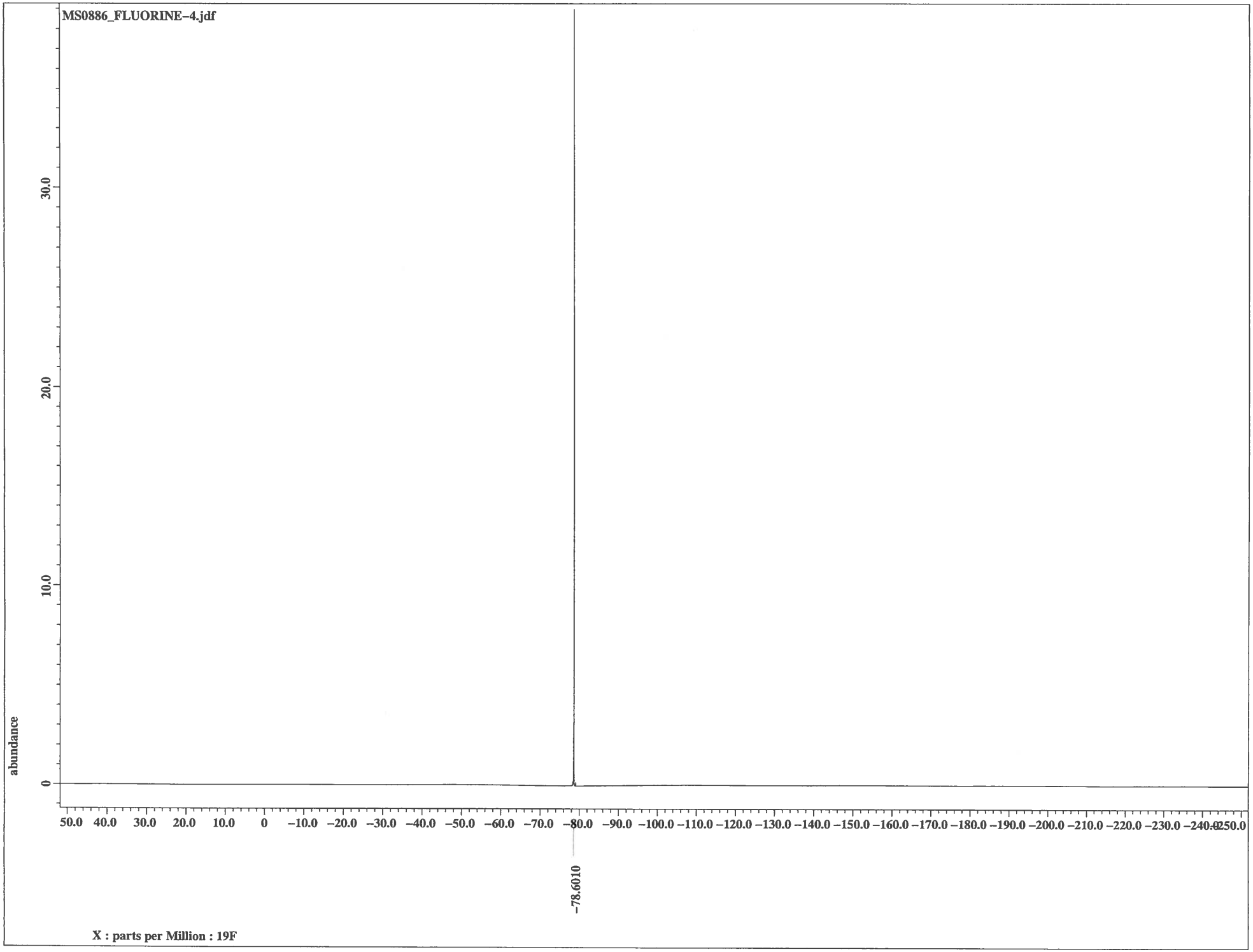

MS0886_PROTON-4.jdf
abundance
X : parts per Million : 1H
6.0
4.02
2.0
2.0
1.0
2.03
2
7.7450
7.7301
7.7061
7.6935
7.6901
7.6752
7.6351
7.6294
7.6191
7.6156
7.6110
7.4152
7.4003
7.3980
7.3831
7.2400
7.2251
7.2102
7.1770
7.1736
7.1633
7.1587
7.0797
7.0648
7.0579

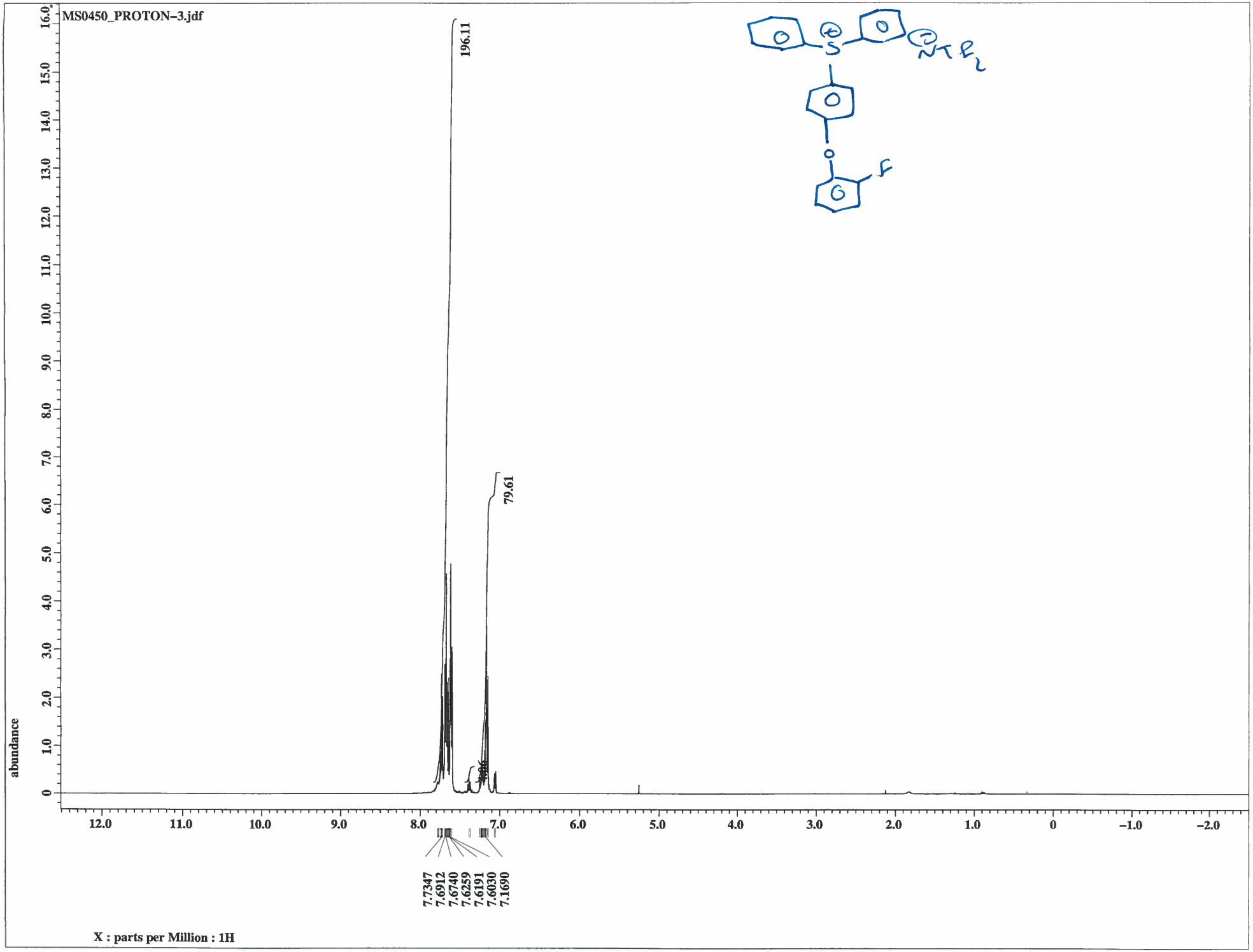


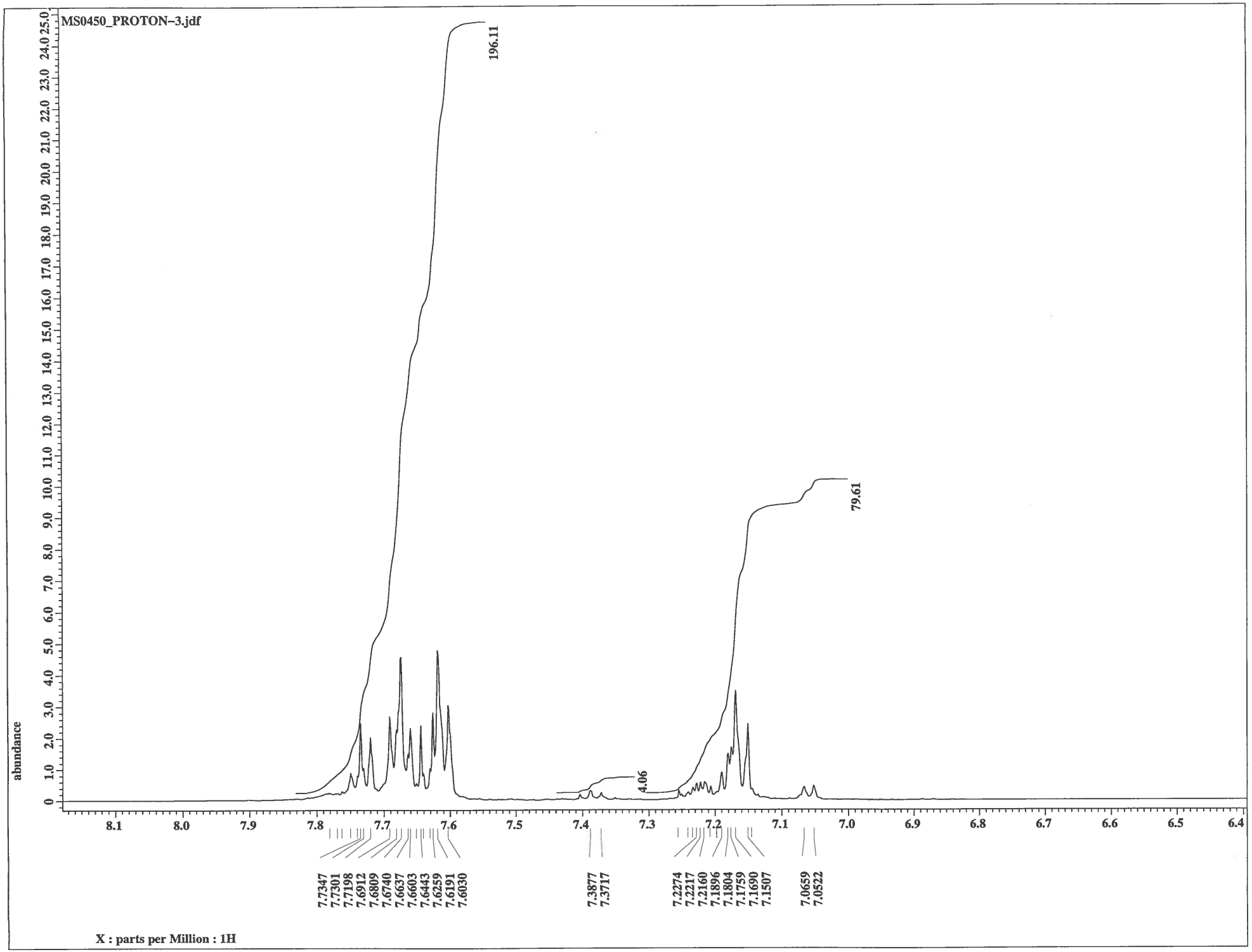
SOUTH ALABAMA JAGUARS

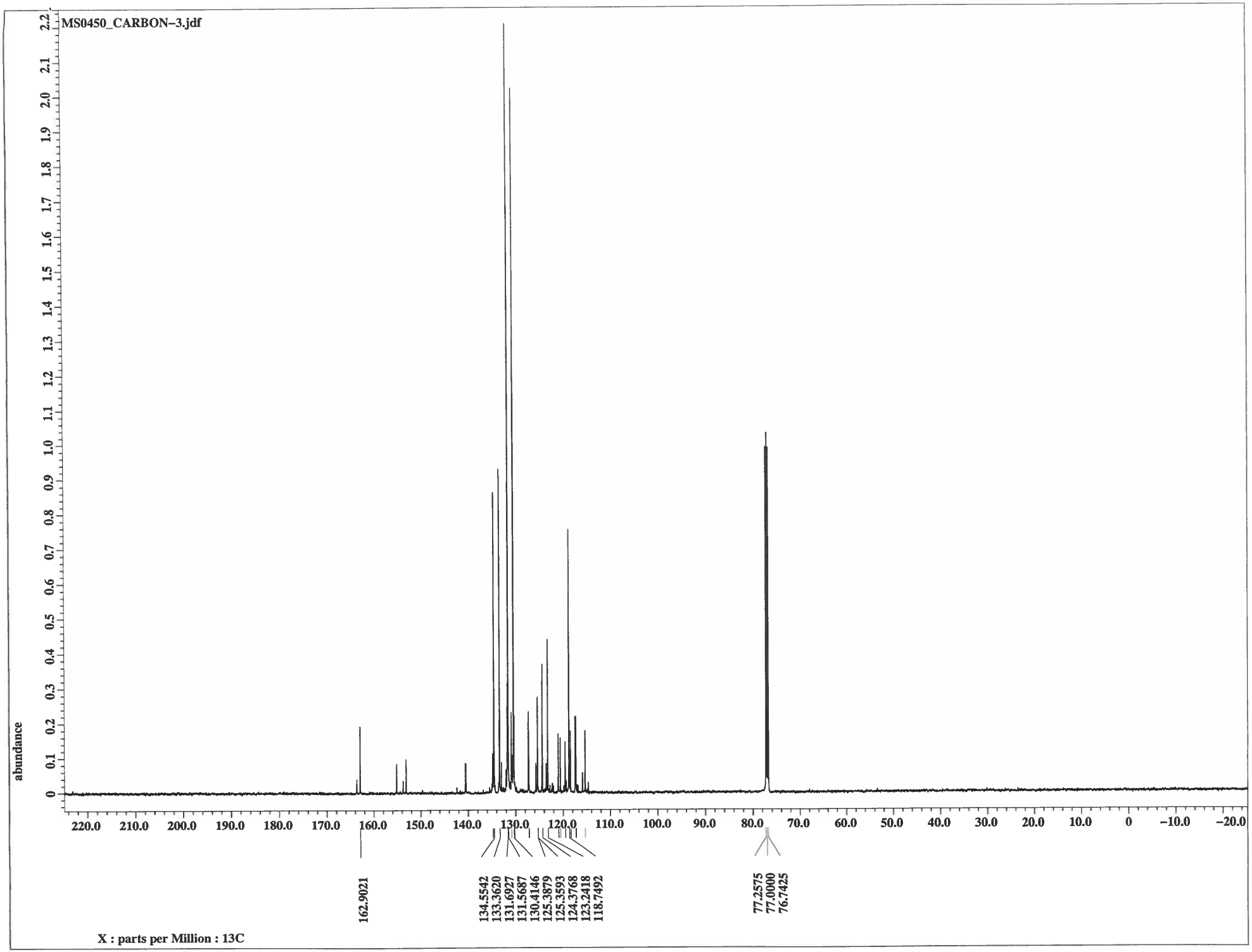
Filename	= MS0886_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0886
Solvent	= CHLOROFORM-D
Creation_time	= 29-NOV-2019 13:40:22
Revision_time	= 29-NOV-2019 13:11:06
Current_time	= 29-NOV-2019 13:11:06
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [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	= 13[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.33333333[us]
Irr_atn_dec	= 21.2[dB]
Irr_atn_noe	= 21.2[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[dC]

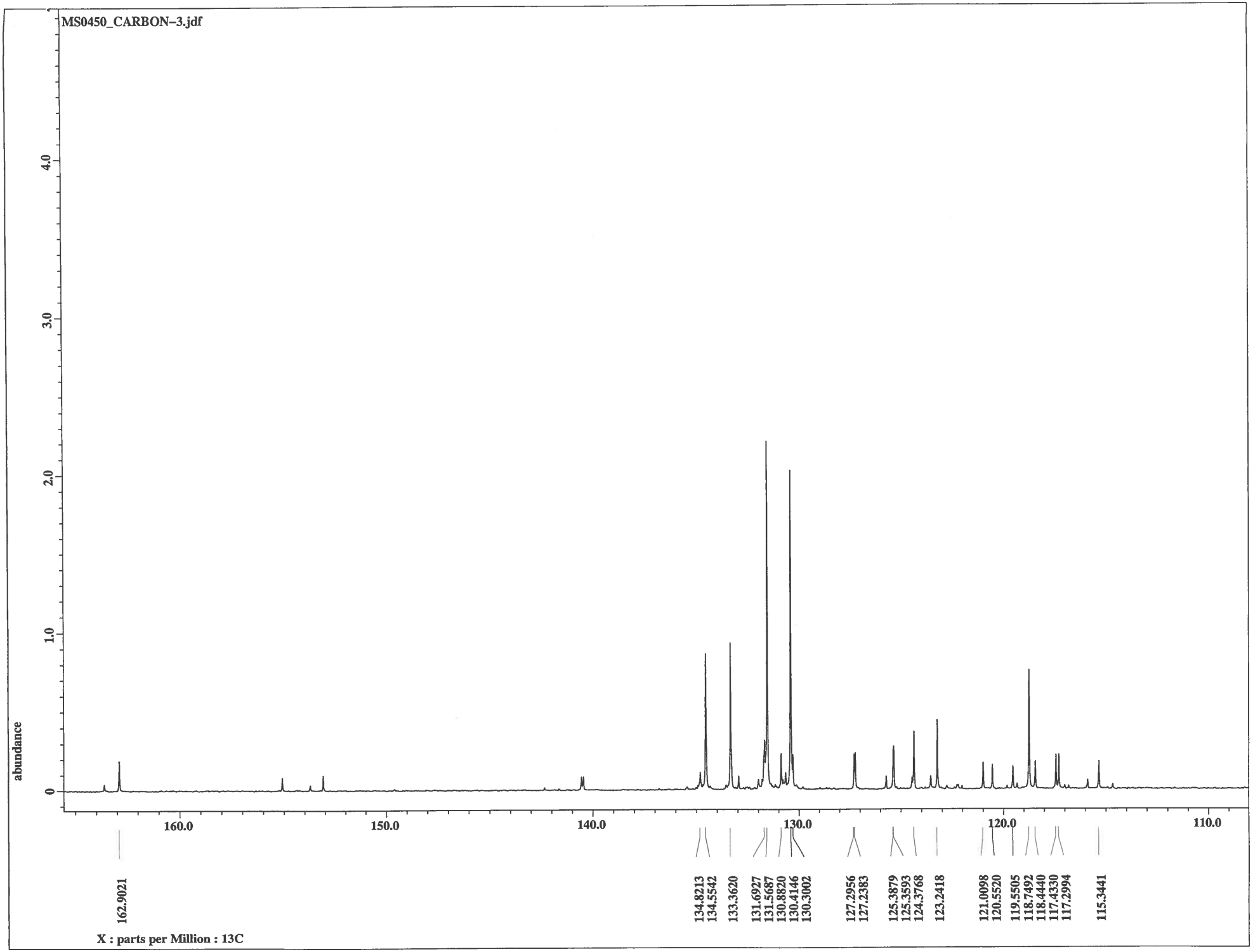

MS0886_CARBON-4.jdf
abundance
3.0
2.0
1.0
0
160.0
150.0
140.0
130.0
120.0
110.0
163.5221
153.6595
134.4588
133.2666
131.4924
130.3288
130.2525
125.6645
124.3864
123.5089
120.9526
120.5043
119.4646
118.3963
115.8400
114.6191
X : parts per Million : 13C

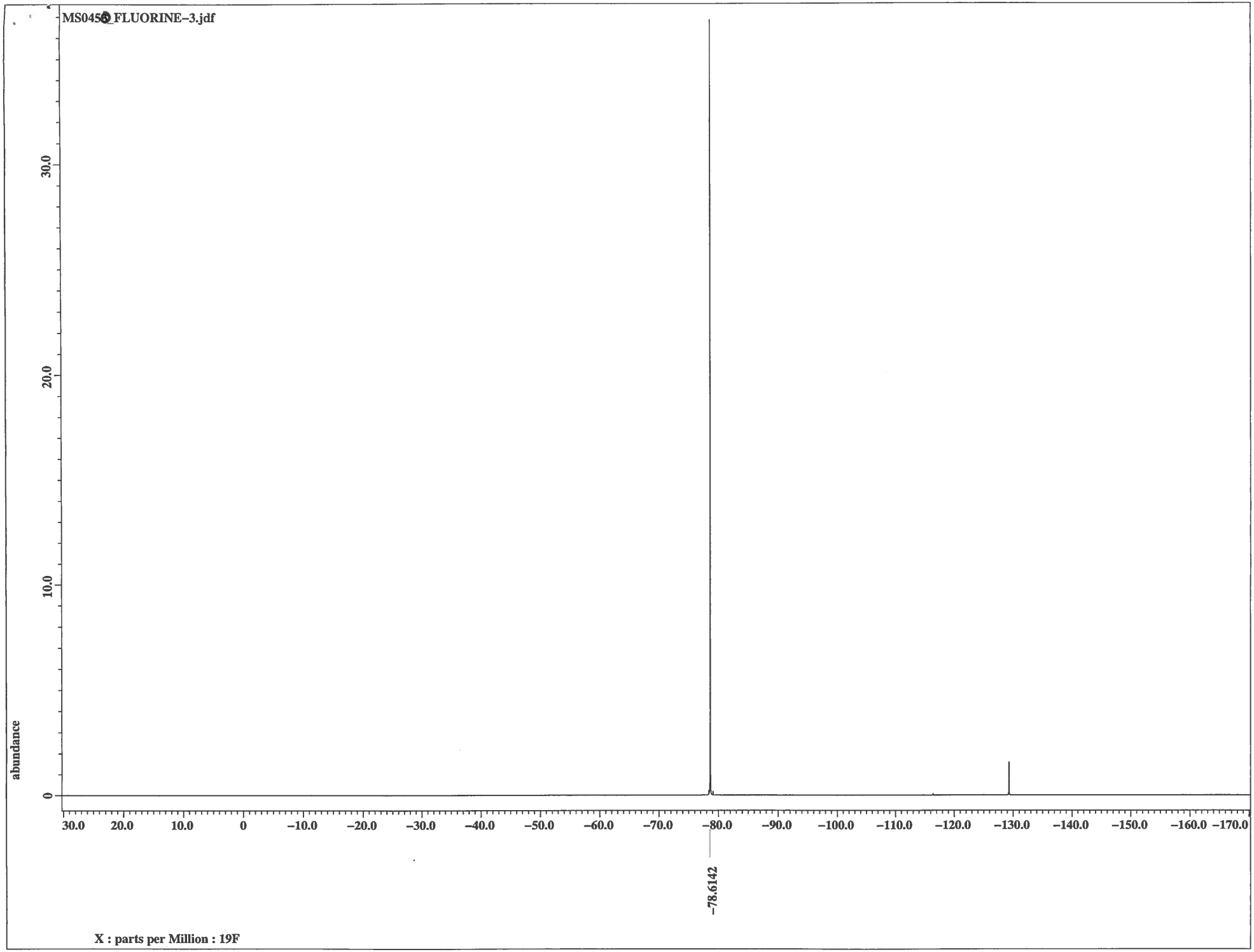

MS0886_FLUORINE-4.jdf
abundance
30.0
20.0
10.0
0
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0 -210.0 -220.0 -230.0 -240.0 -250.0
-78.6010
X : parts per Million : 19F

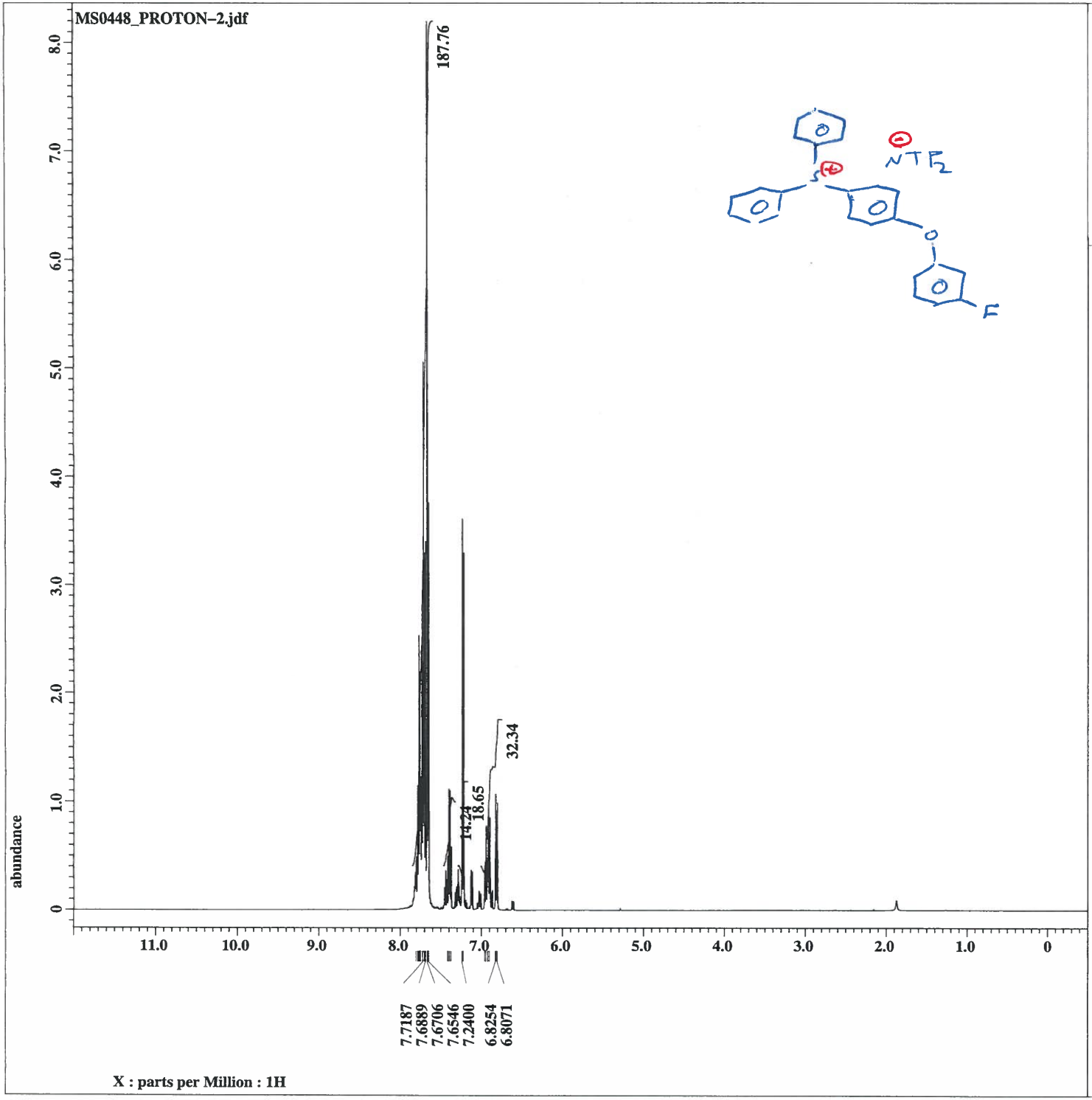

MS0450_PROTON-3.jdf
196.11
79.61
7.7347
7.6912
7.6740
7.6259
7.6191
7.6030
7.1690
abundance
X : parts per Million : 1H


MS0450_PROTON-3.jdf
196.11
79.61
4.06
abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0 25.0
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4
7.7347
7.7301
7.7198
7.6912
7.6809
7.6740
7.6637
7.6603
7.6443
7.6259
7.6191
7.6030
7.3877
7.3717
7.2274
7.2217
7.2160
7.1896
7.1804
7.1759
7.1690
7.1507
7.0659
7.0522
X : parts per Million : 1H

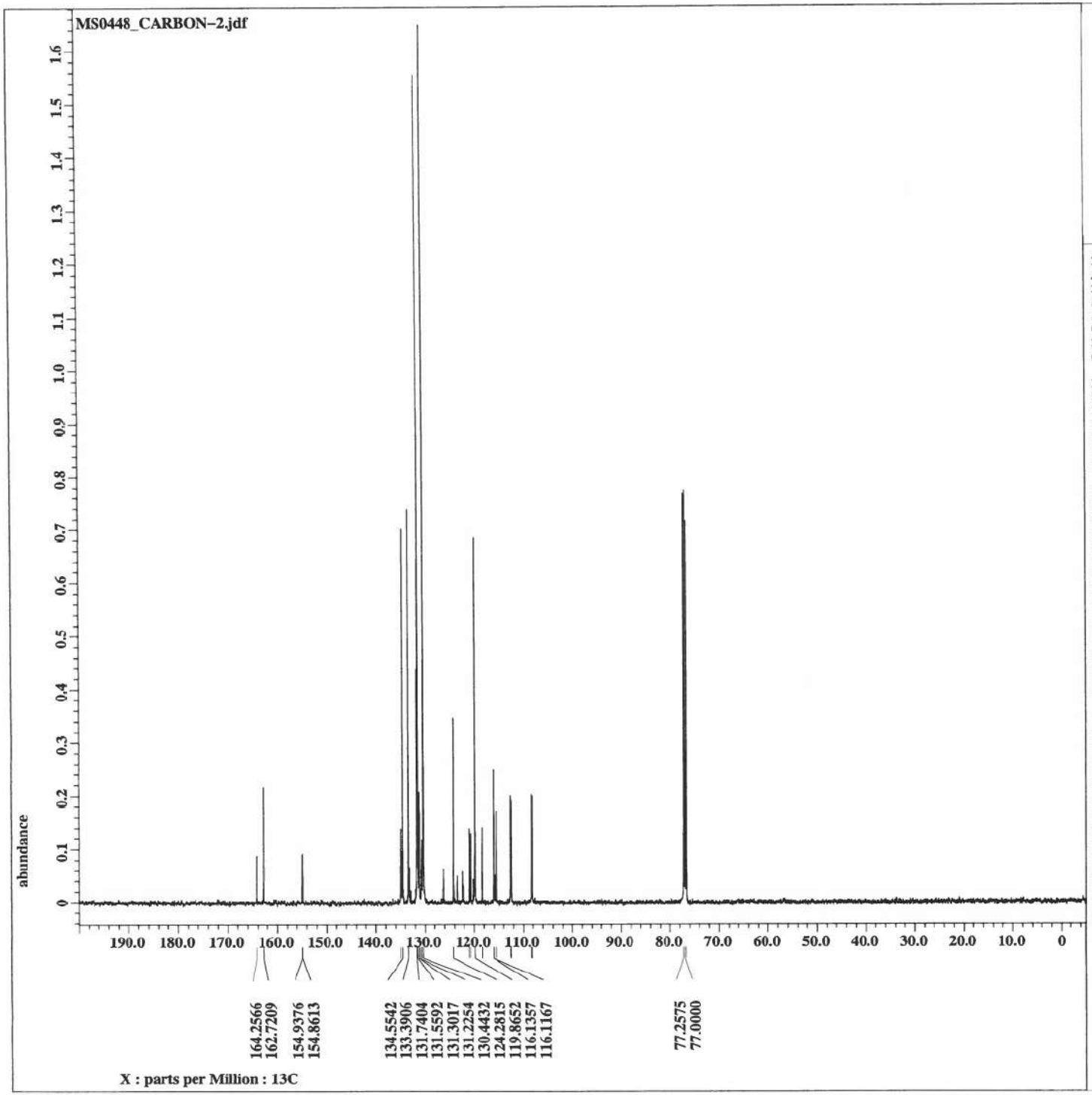

MS0450_CARBON-3.jdf
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2.0
2.1
2.2
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
162.9021
134.5542
133.3620
131.6927
131.5687
130.4146
125.3879
125.3593
124.3768
123.2418
118.7492
77.2575
77.0000
76.7425
X : parts per Million : 13C


MS0450_CARBON-3.jdf
abundance
0
1.0
2.0
3.0
4.0
160.0
150.0
140.0
130.0
120.0
110.0
162.9021
134.8213
134.5542
133.3620
131.6927
131.5687
130.8820
130.4146
130.3002
127.2956
127.2383
125.3879
125.3593
124.3768
123.2418
121.0098
120.5520
119.5505
118.7492
118.4440
117.4330
117.2994
115.3441
X : parts per Million : 13C


MS0450_FLUORINE-3.jdf
30.0
20.0
10.0
0
abundance
30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0
-78.6142
X : parts per Million : 19F

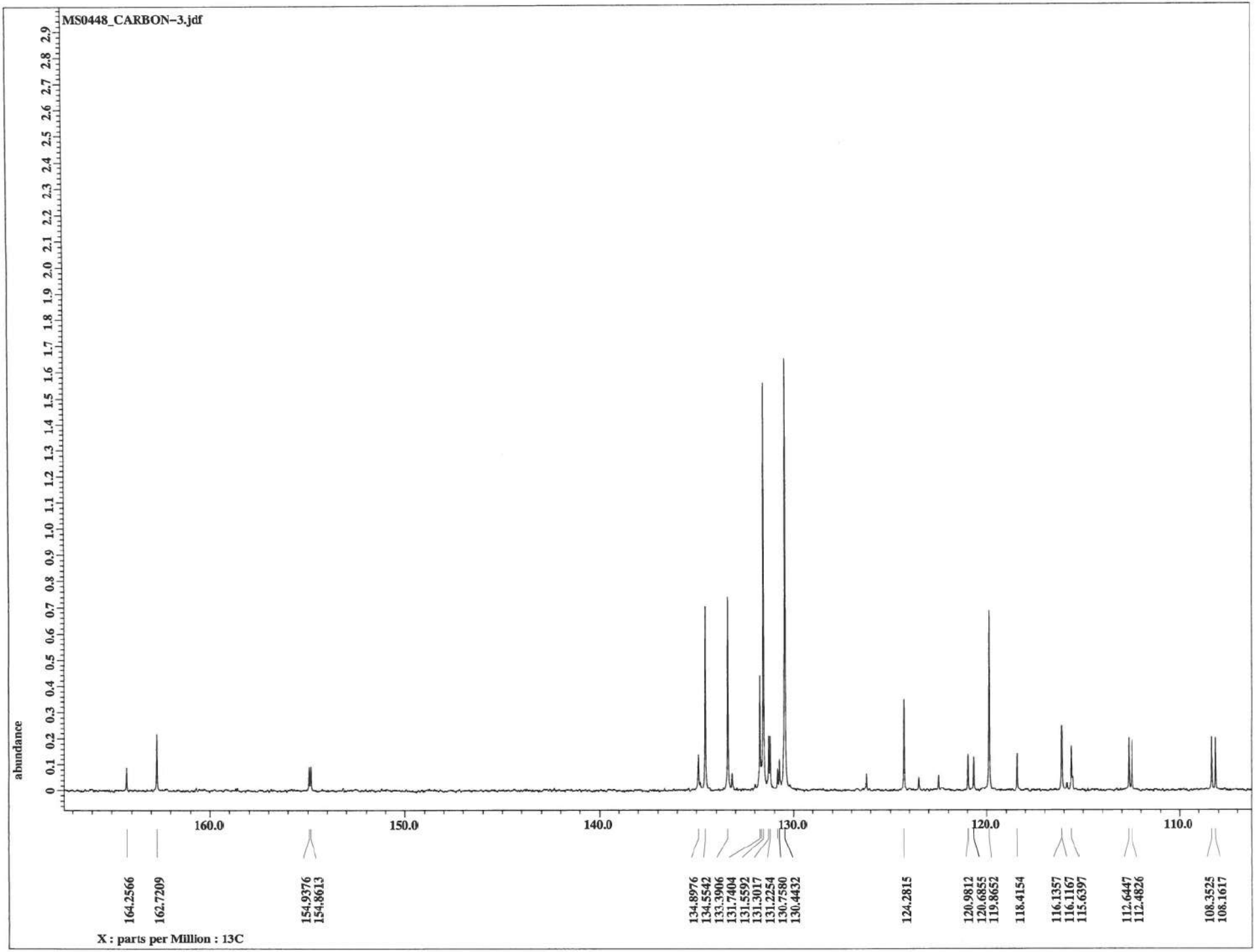


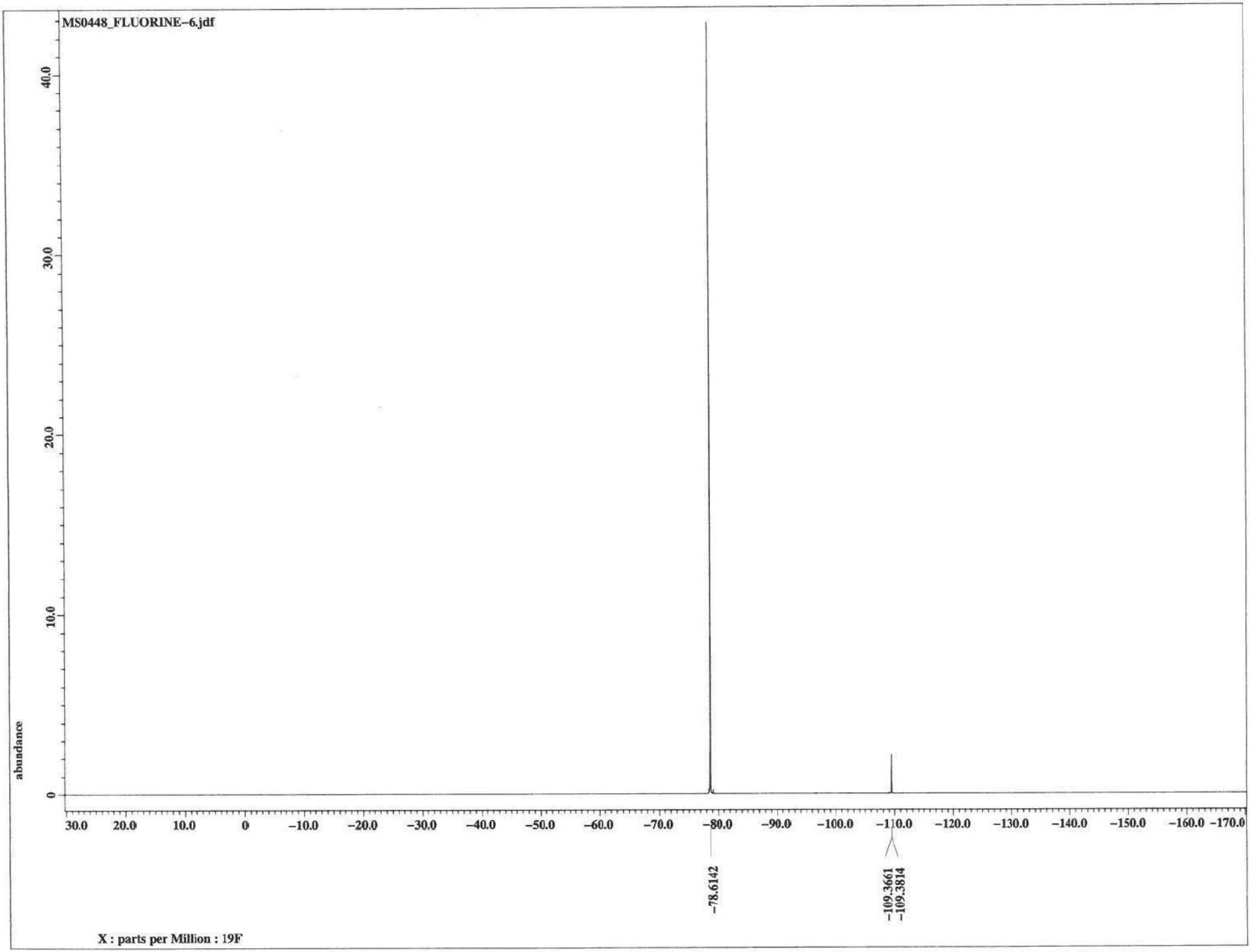
Filename	= MS0448_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0448
Solvent	= CHLOROFORM-D
Creation_time	= 26-NOV-2019 12:41:31
Revision_time	= 26-NOV-2019 12:12:27
Current_time	= 26-NOV-2019 12:12:27
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[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	= 11.3[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 5.65[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	= 19.4[dC]

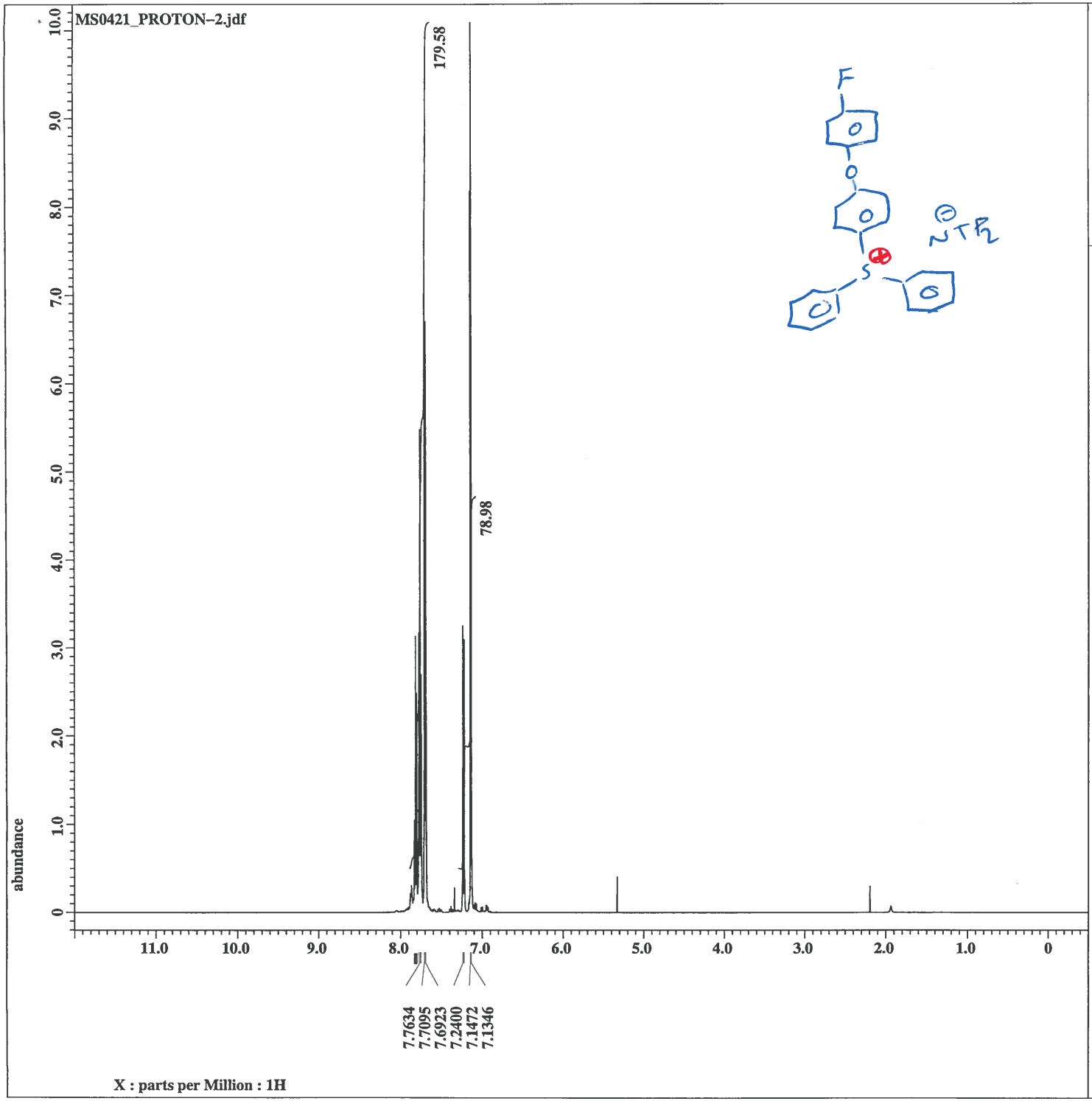


SOUTH ALABAMA JAGUARS

Filename	= MS0448_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0448
Solvent	= CHLOROFORM-D
Creation_time	= 26-NOV-2019 13:01:16
Revision_time	= 26-NOV-2019 12:32:12
Current_time	= 26-NOV-2019 12:32:12
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 400
Total_scans	= 400
X_90_width	= 13[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.33333333[us]
Irr_atn_dec	= 21.2[dB]
Irr_atn_noe	= 21.2[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	= 19.6[dC]

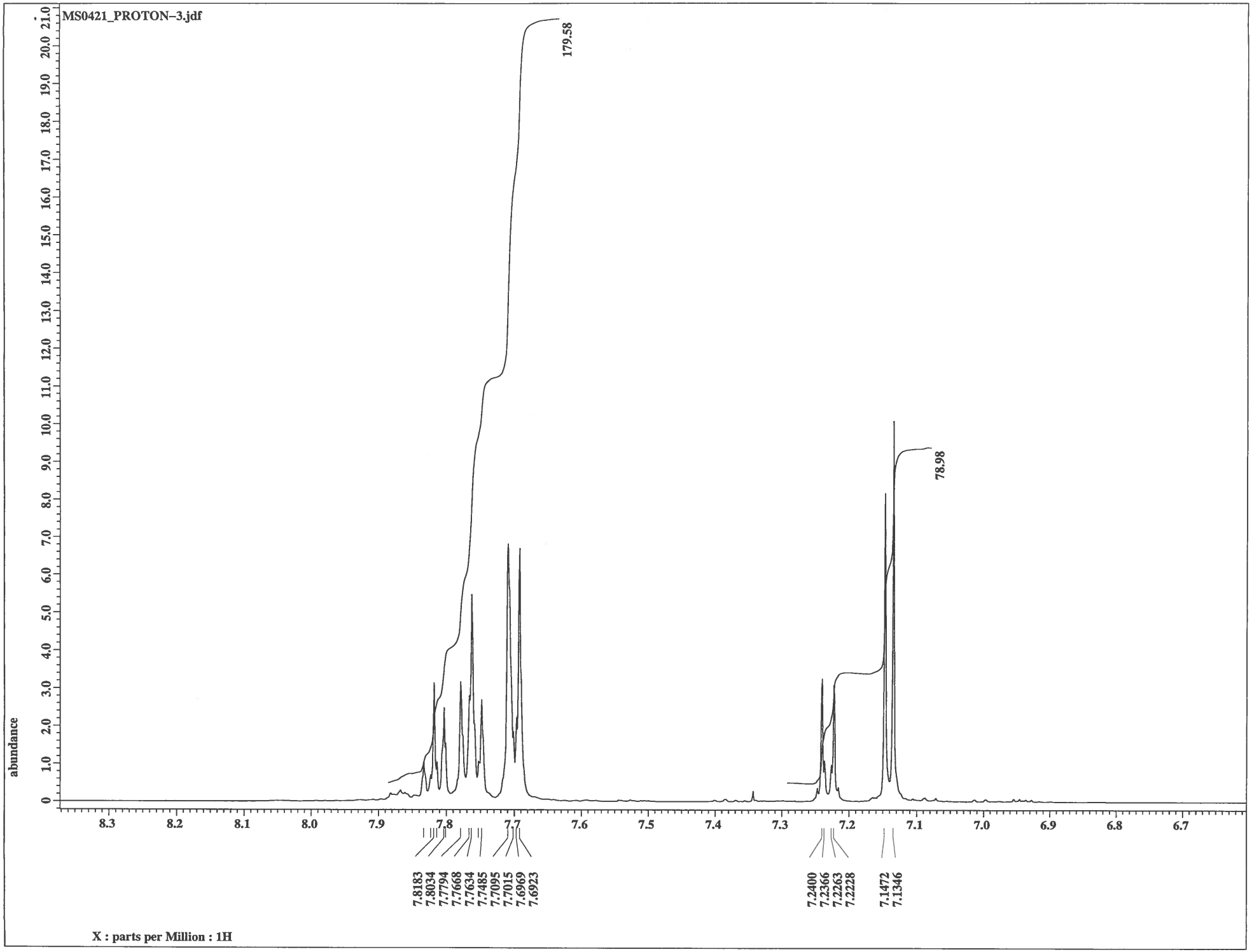

MS0448_CARBON-3.jdf
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3 2.4 2.5 2.6 2.7 2.8 2.9
160.0
150.0
140.0
130.0
120.0
110.0
164.2566
162.7209
154.9376
154.8613
134.8976
134.5542
133.3906
131.7404
131.5592
131.3017
131.2254
130.7580
130.4432
124.2815
120.9812
120.6855
119.8652
118.4154
116.1357
116.1167
115.6397
112.6447
112.4826
108.3525
108.1617
X : parts per Million : 13C

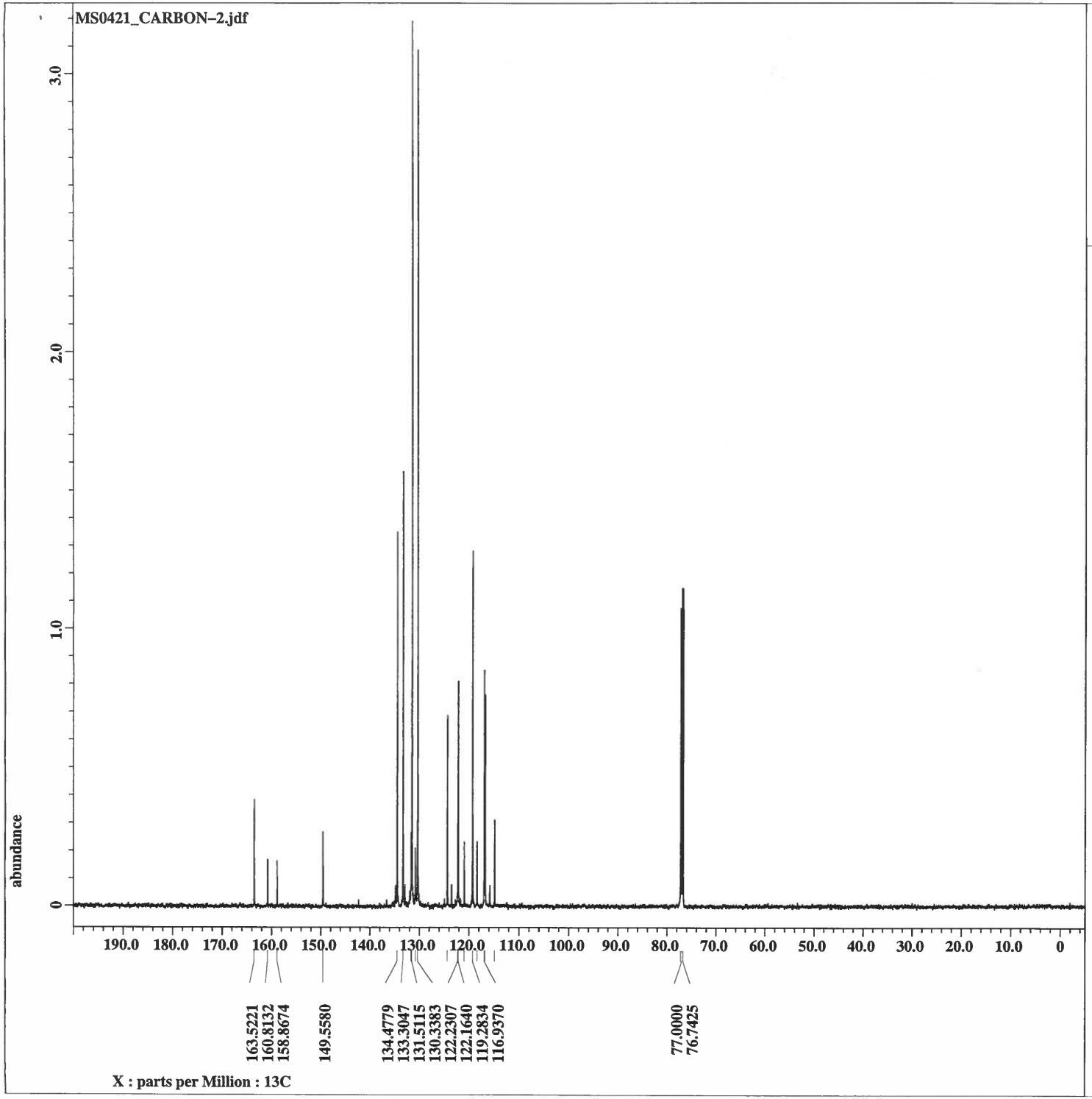

MS0448_FLUORINE-6.jdf
abundance
40.0
30.0
20.0
10.0
0
30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0
-78.6142
-109.3661
-109.3814
X : parts per Million : 19F



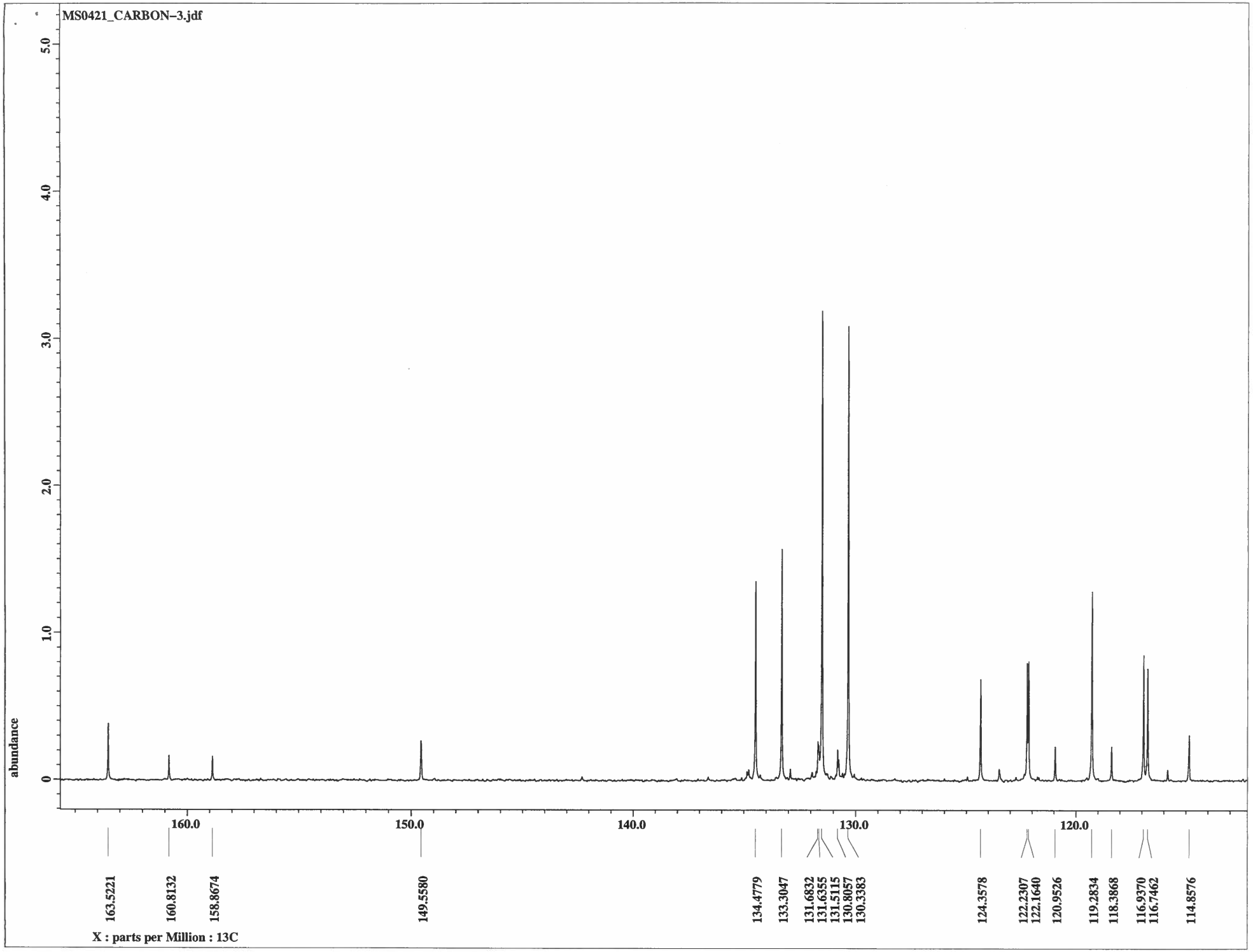
SOUTH ALABAMA JAGUARS

Filename	= MS0421_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0421
Solvent	= CHLOROFORM-D
Changer_sample	= 1
Creation_time	= 18-APR-2018 10:34:59
Revision_time	= 18-APR-2018 10:12:47
Current_time	= 18-APR-2018 10:12:47
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	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 22
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.7[dC]

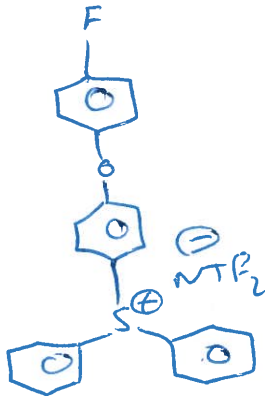

MS0421_PROTON-3.jdf
179.58
78.98
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
7.8183
7.8034
7.7794
7.7668
7.7634
7.7485
7.7095
7.7015
7.6969
7.6923
7.2400
7.2366
7.2263
7.2228
7.1472
7.1346
X : parts per Million : 1H



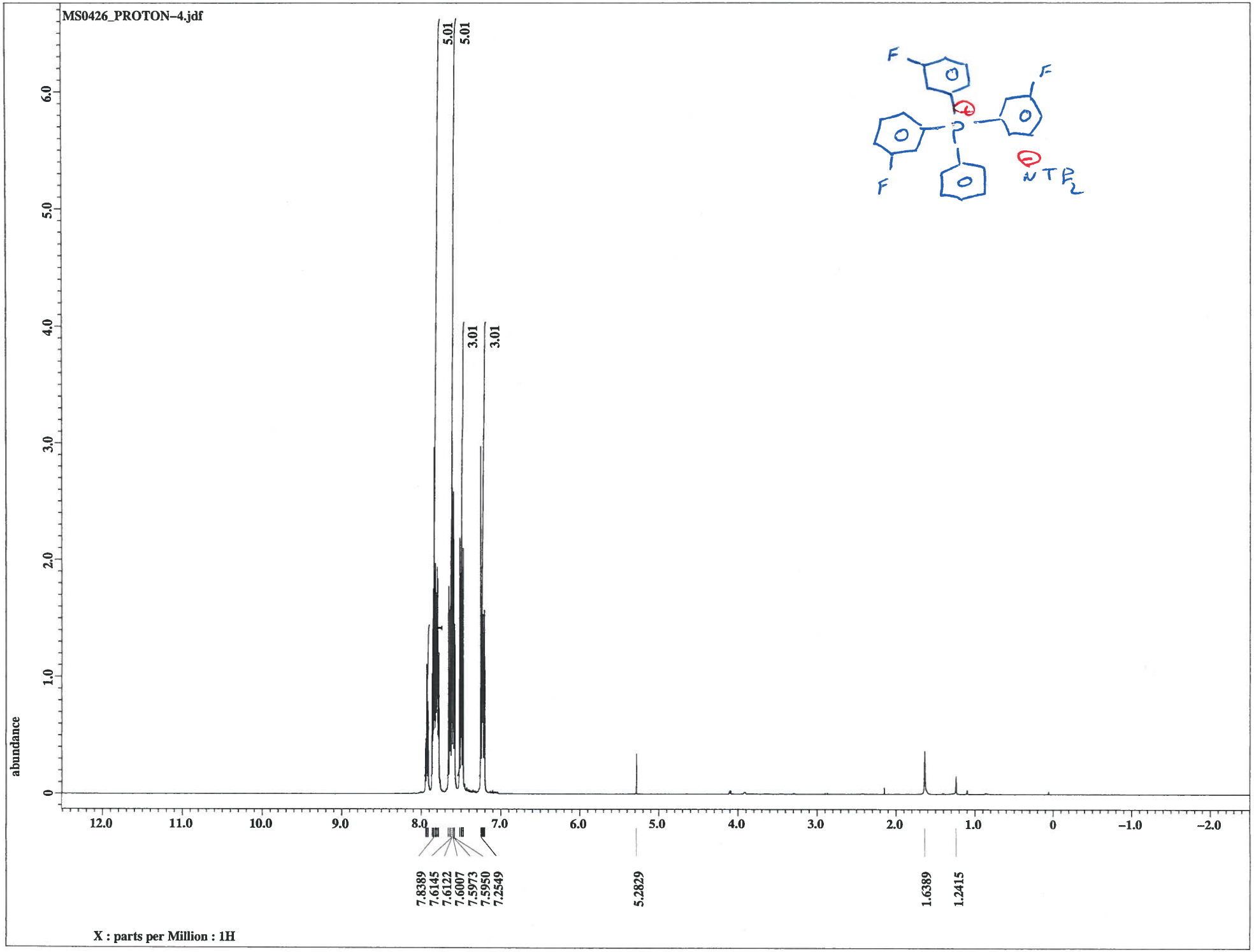
Filename	= MS0421_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0421
Solvent	= CHLOROFORM-D
Changer_sample	= 1
Creation_time	= 18-APR-2018 10:49:35
Revision_time	= 18-APR-2018 10:27:22
Current_time	= 18-APR-2018 10:27:22
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 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	= 256
Total_scans	= 256
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 23.4[dC]

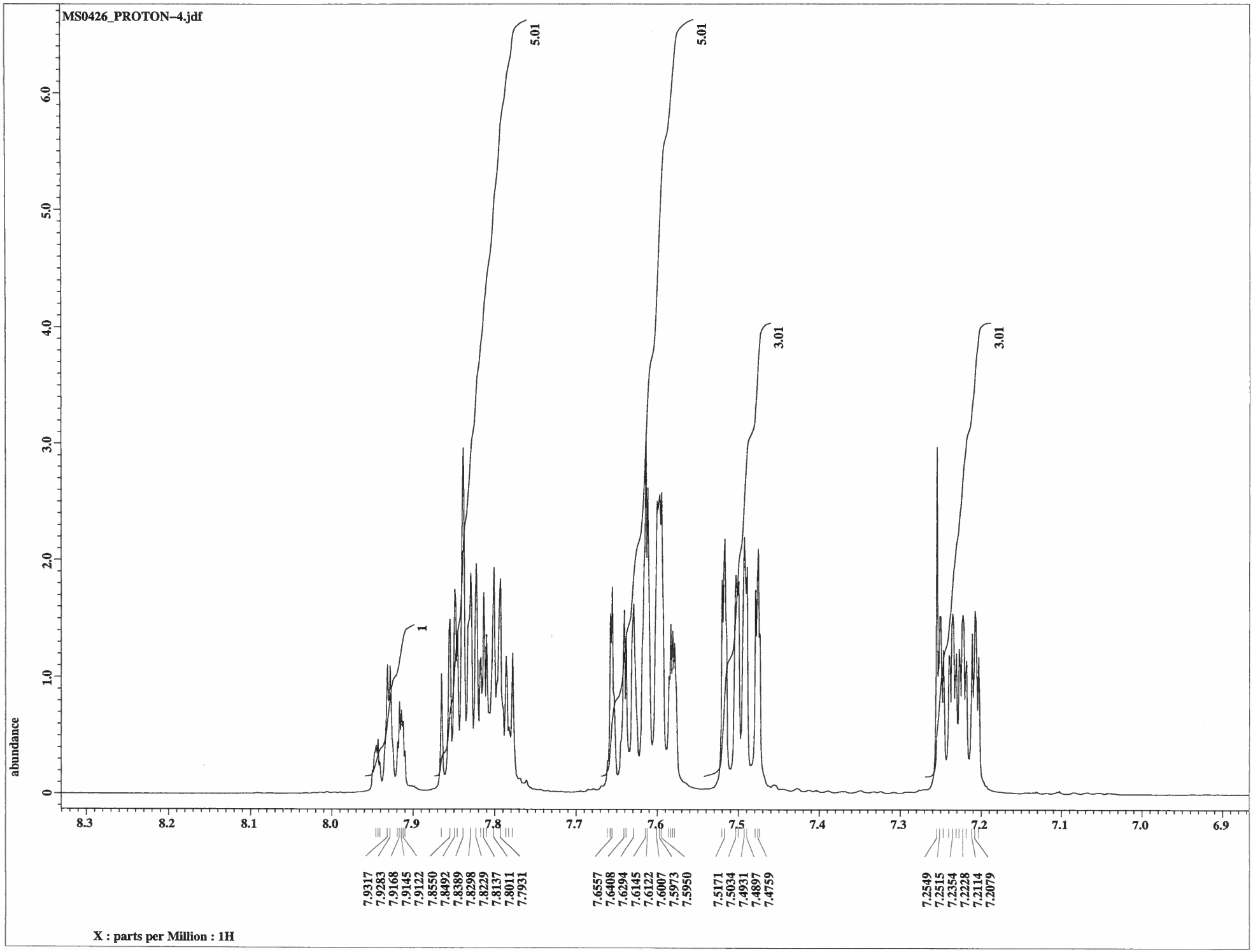

MS0421_CARBON-3.jdf
abundance
5.0
4.0
3.0
2.0
1.0
0
160.0
150.0
140.0
130.0
120.0
163.5221
160.8132
158.8674
149.5580
134.4779
133.3047
131.6832
131.6355
131.5115
130.8057
130.3383
124.3578
122.2307
122.1640
120.9526
119.2834
118.3868
116.9370
116.7462
114.8576
X : parts per Million : 13C

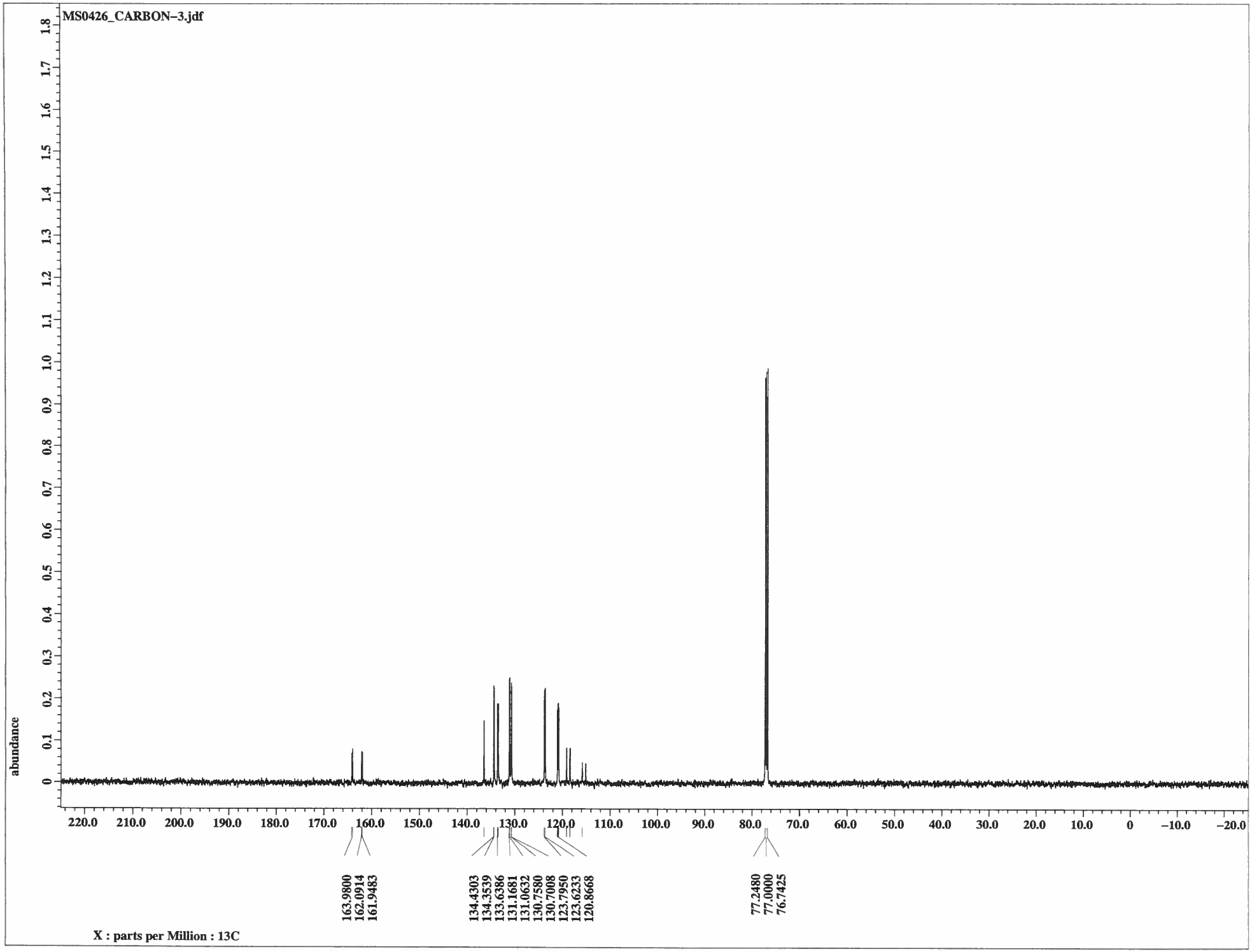
MS0421_FLUORINE-2.jdf

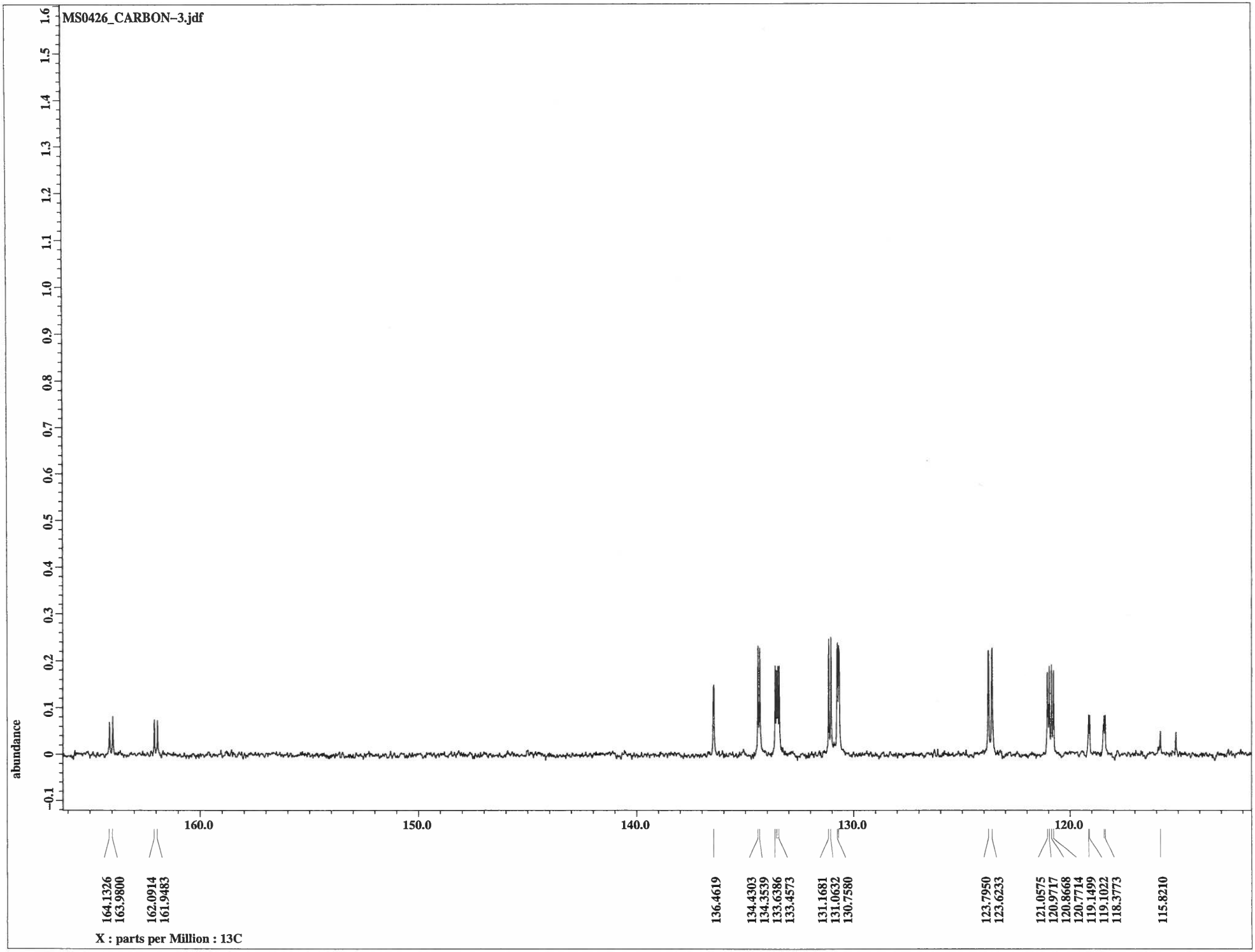


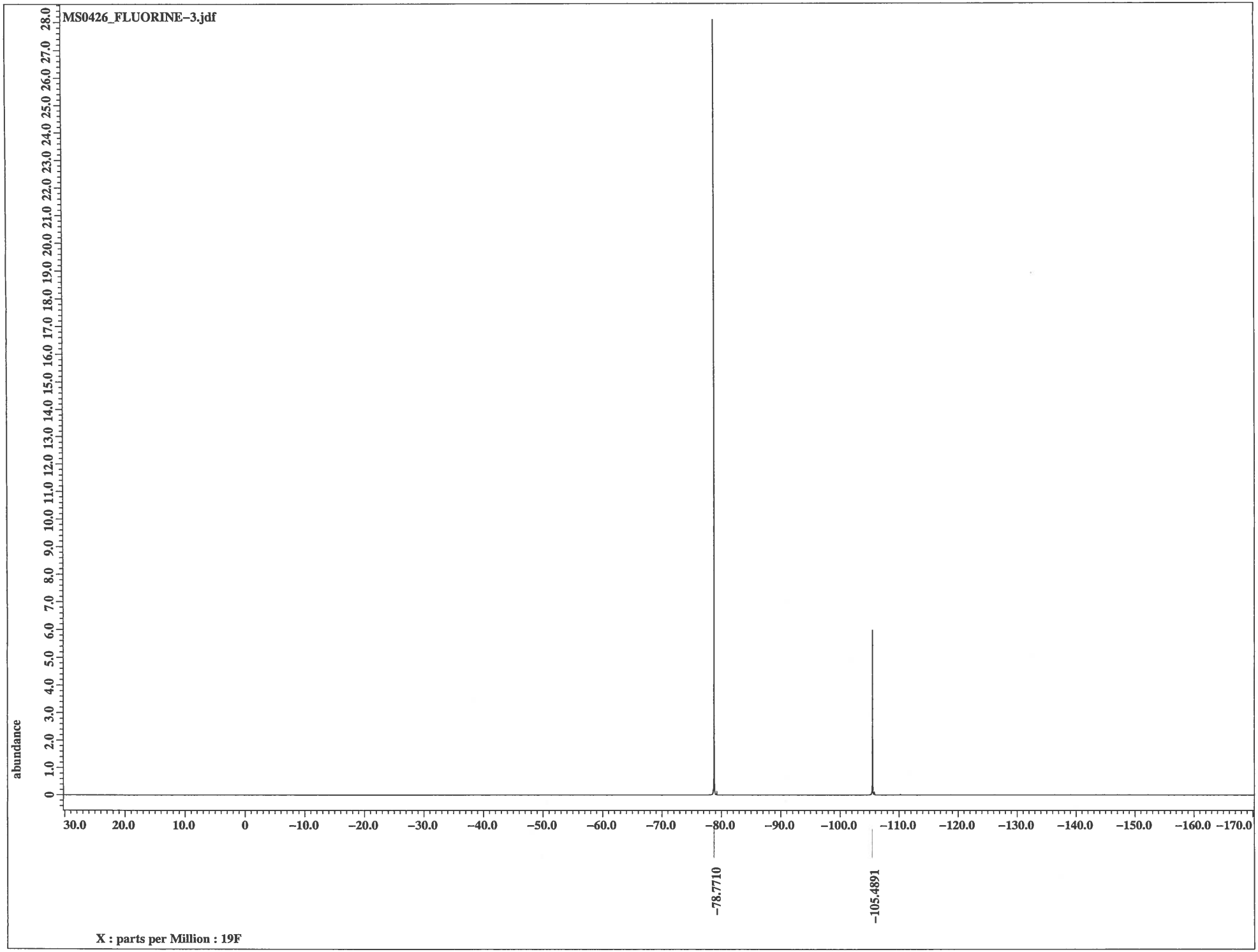
Filename	= MS0421_FLUORINE-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0421
Solvent	= CHLOROFORM-D
Changer_sample	= 1
Creation_time	= 18-APR-2018 10:31:25
Revision_time	= 18-APR-2018 10:09:13
Current_time	= 18-APR-2018 10:09:13
Data_format	= 1D COMPLEX
Dim_size	= 52428
Dim_title	= 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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 32
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.6[dC]

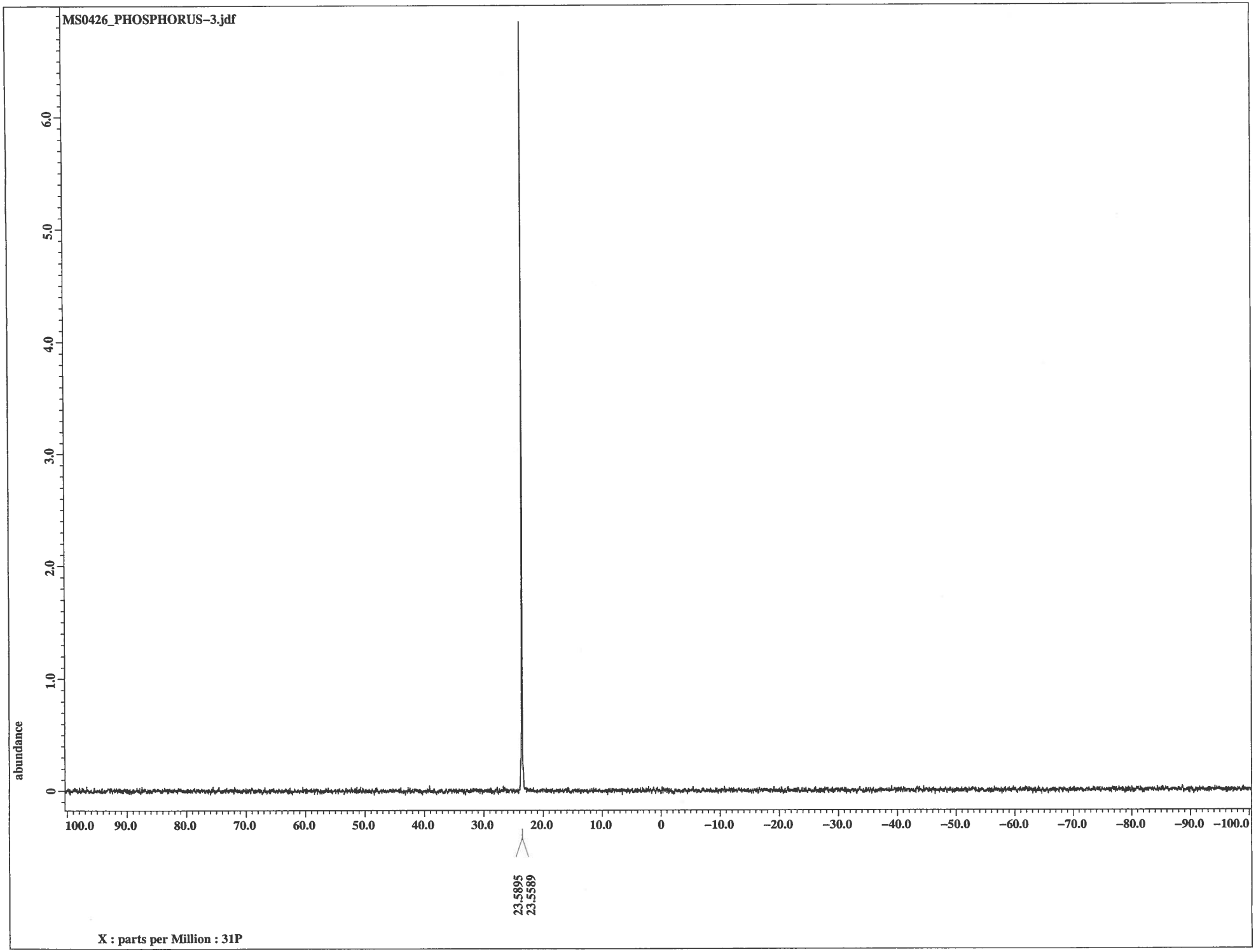

MS0426_PROTON-4.jdf
5.01
5.01
3.01
3.01
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
7.8389
7.6145
7.6122
7.6007
7.5973
7.5950
7.2549
5.2829
1.6389
1.2415
X : parts per Million : 1H

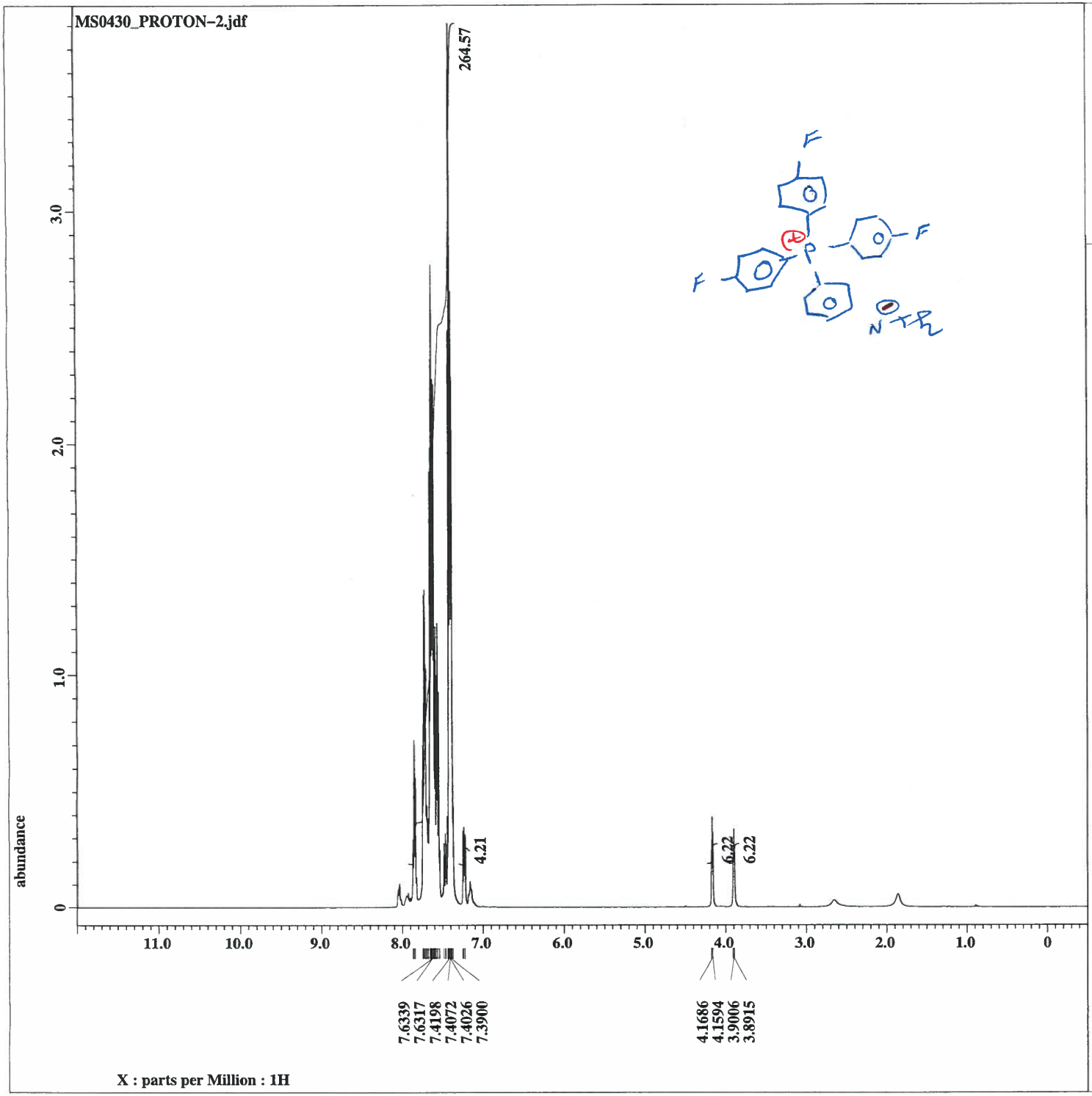

MS0426_PROTON-4.jdf
abundance
X : parts per Million : 1H
5.01
5.01
3.01
3.01
1
7.9317
7.9283
7.9168
7.9145
7.9122
7.8550
7.8492
7.8389
7.8298
7.8229
7.8137
7.8011
7.7931
7.6557
7.6408
7.6294
7.6145
7.6122
7.6007
7.5973
7.5950
7.5171
7.5034
7.4931
7.4897
7.4759
7.2549
7.2515
7.2354
7.2228
7.2114
7.2079


MS0426_CARBON-3.jdf
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
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
163.9800
162.0914
161.9483
134.4303
134.3539
133.6386
131.1681
131.0632
130.7580
130.7008
123.7950
123.6233
120.8668
77.2480
77.0000
76.7425
X : parts per Million : 13C


MS0426_CARBON-3.jdf
abundance
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
160.0
150.0
140.0
130.0
120.0
164.1326
163.9800
162.0914
161.9483
136.4619
134.4303
134.3539
133.6386
133.4573
131.1681
131.0632
130.7580
123.7950
123.6233
121.0575
120.9717
120.8668
120.7714
119.1499
119.1022
118.3773
115.8210
X : parts per Million : 13C

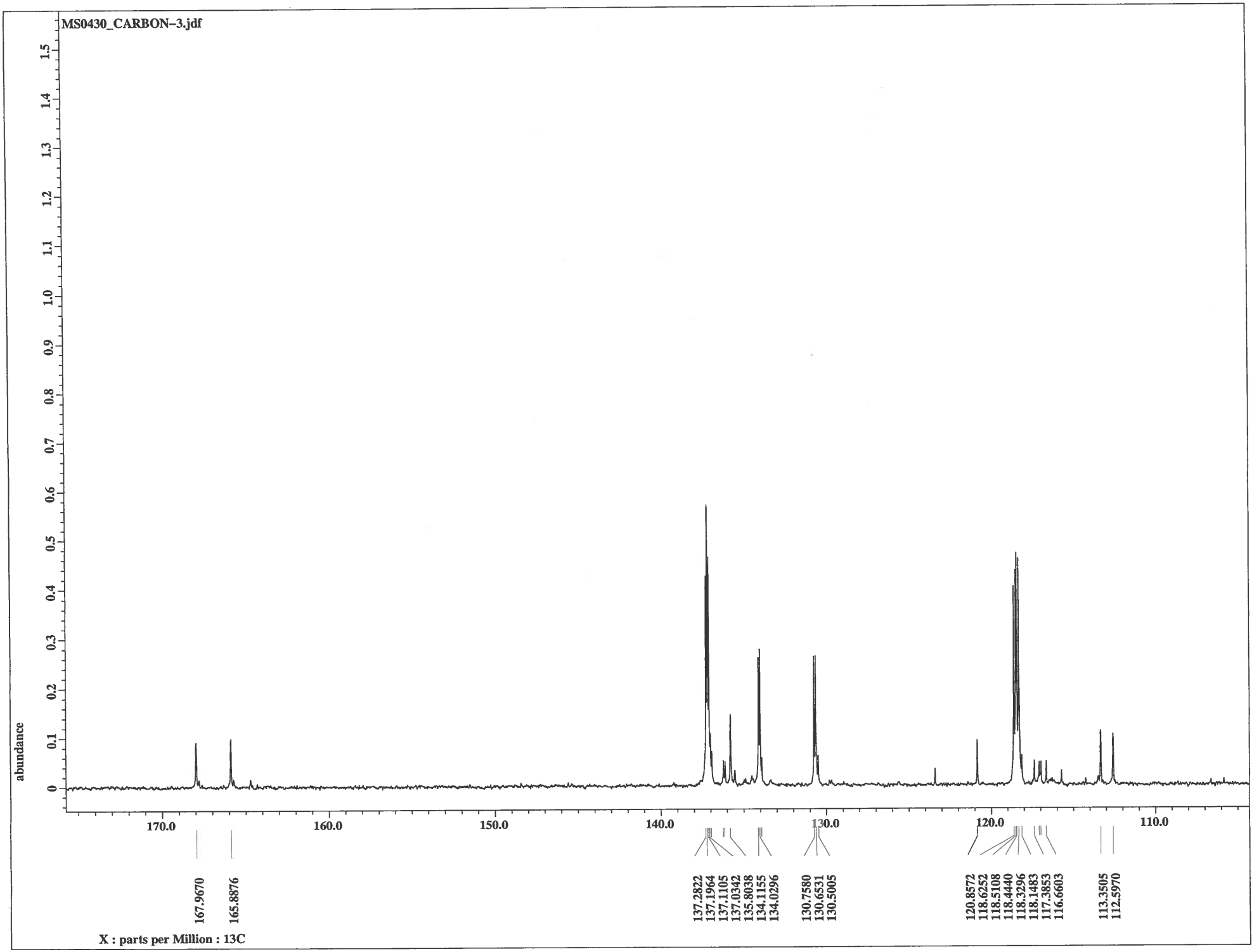

MS0426_FLUORINE-3.jdf
abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0 25.0 26.0 27.0 28.0
30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0
-78.7710
-105.4891
X : parts per Million : 19F

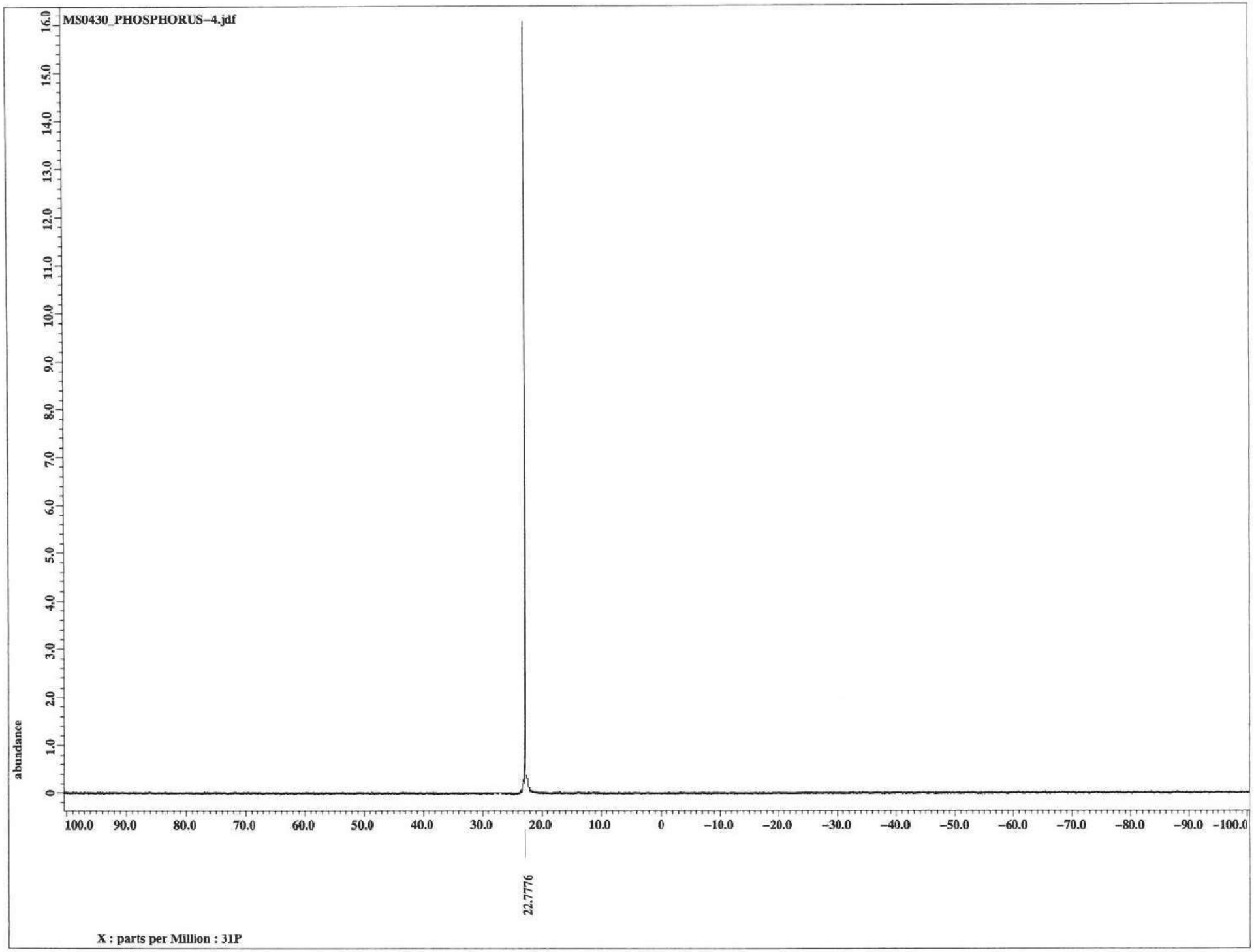

MS0426_PHOSPHORUS-3.jdf
abundance
6.0
5.0
4.0
3.0
2.0
1.0
0
100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0
23.5895
23.5589
X : parts per Million : 31P

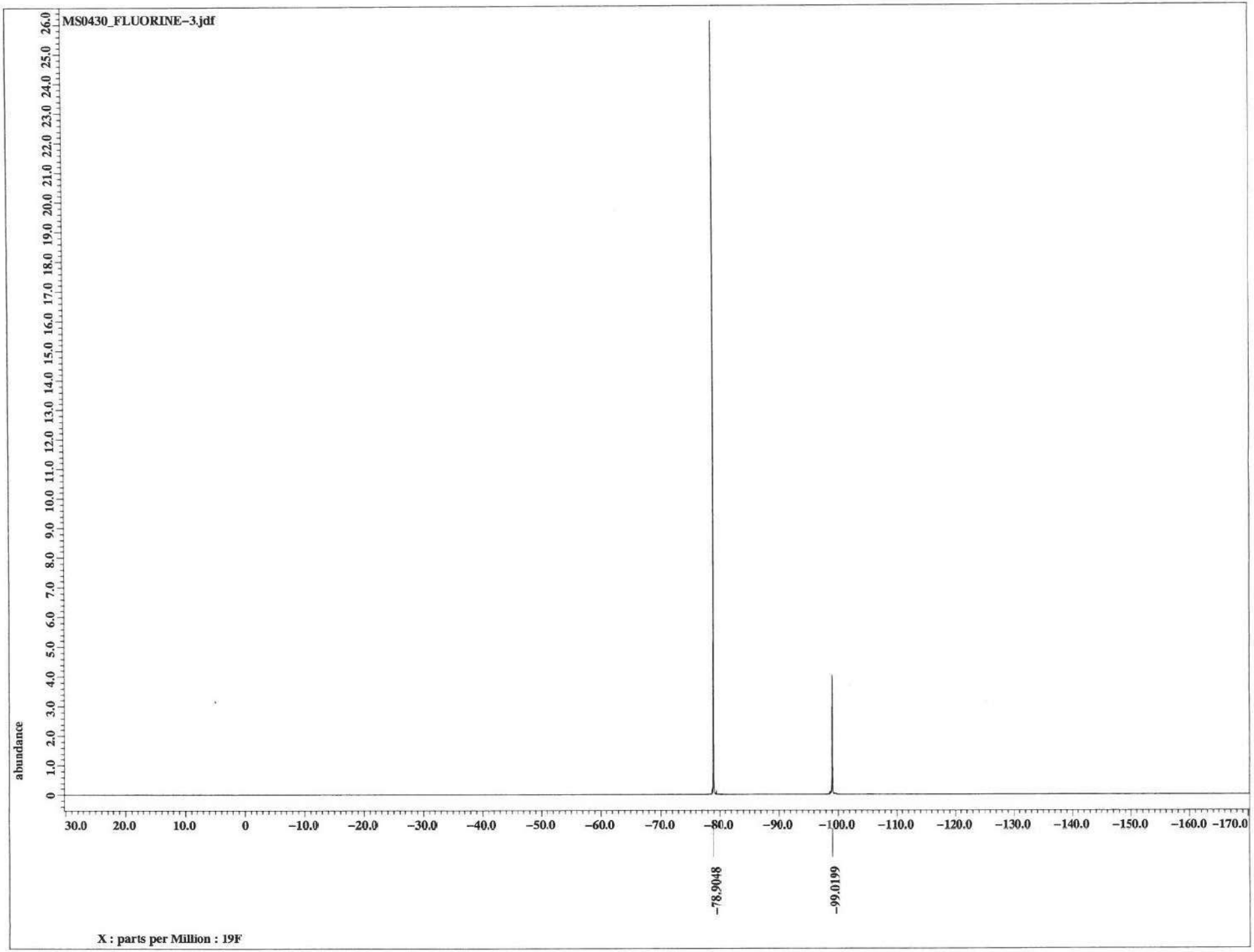


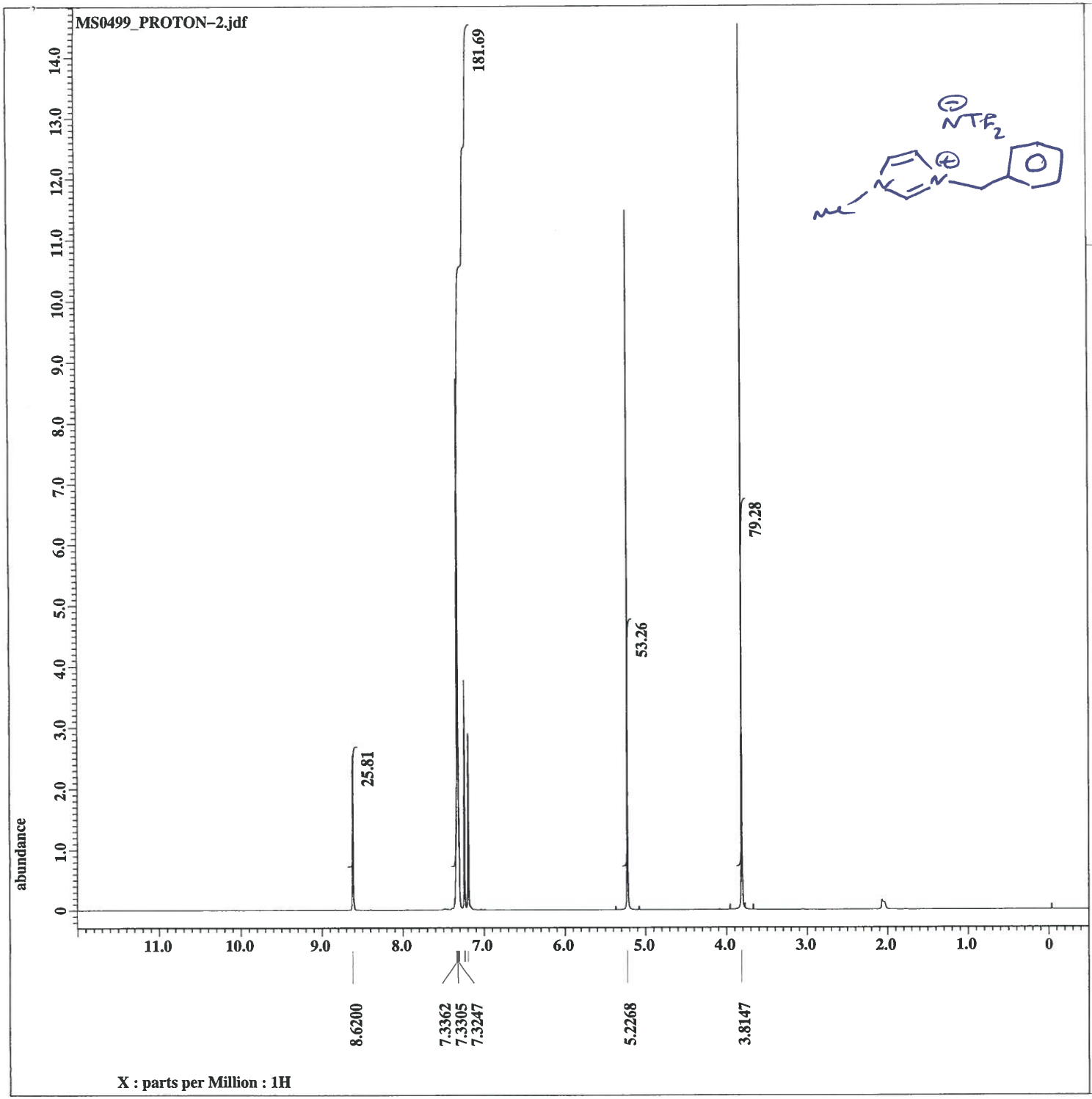
SOUTH ALABAMA JAGUARS

Filename	= MS0430_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0430
Solvent	= CHLOROFORM-D
Creation_time	= 26-NOV-2019 12:03:37
Revision_time	= 26-NOV-2019 11:34:33
Current_time	= 26-NOV-2019 11:34:33
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	= 11.3[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 5.65[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	= 19.1[dC]


MS0430_CARBON-3.jdf
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
170.0
160.0
150.0
140.0
130.0
120.0
110.0
167.9670
165.8876
137.2822
137.1964
137.1105
137.0342
135.8038
134.1155
134.0296
130.7580
130.6531
130.5005
120.8572
118.6252
118.5108
118.4440
118.3296
118.1483
117.3853
116.6603
113.3505
112.5970
X : parts per Million : 13C

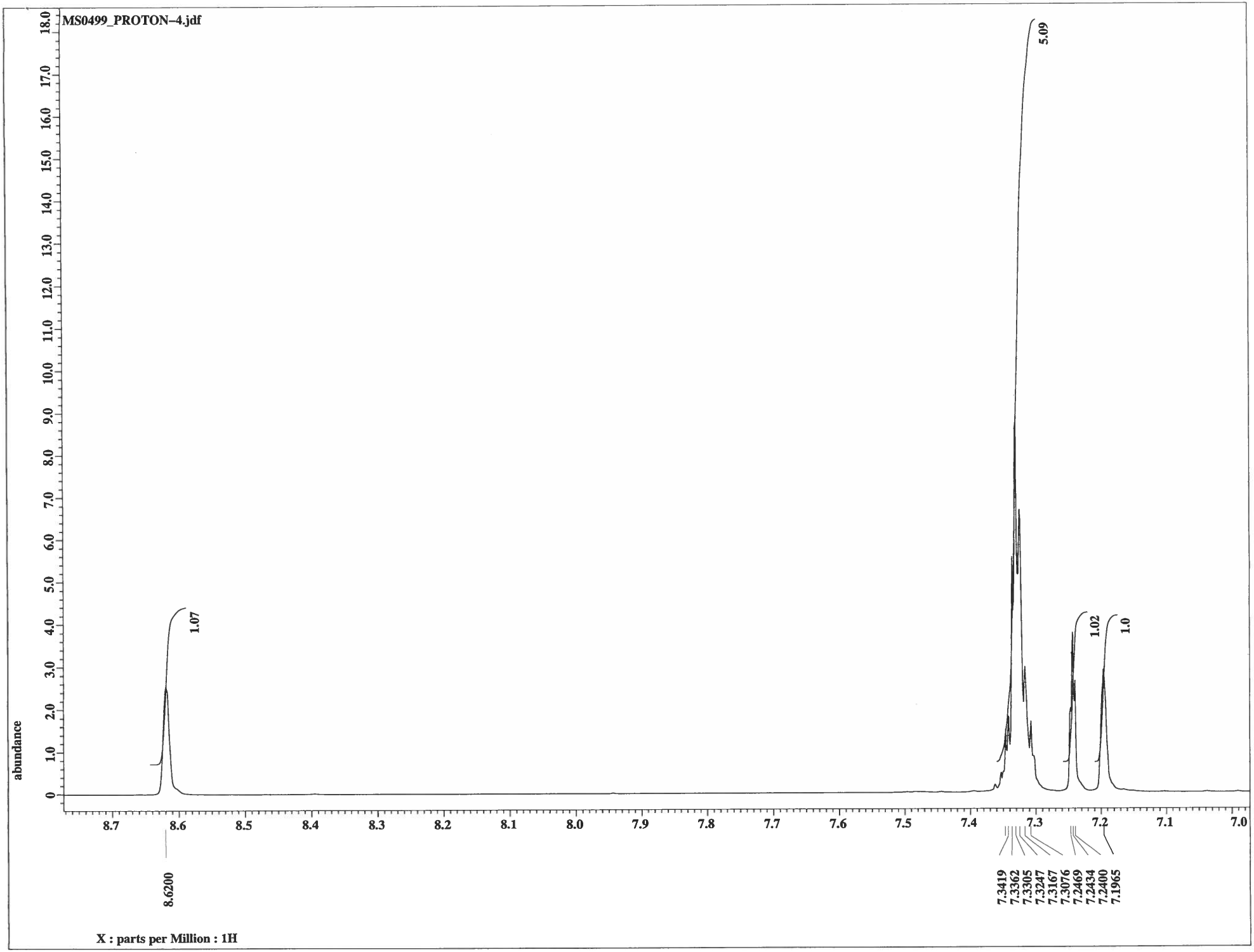

MS0430_PHOSPHORUS-4.jdf
abundance
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0
22.7776
X : parts per Million : 31P

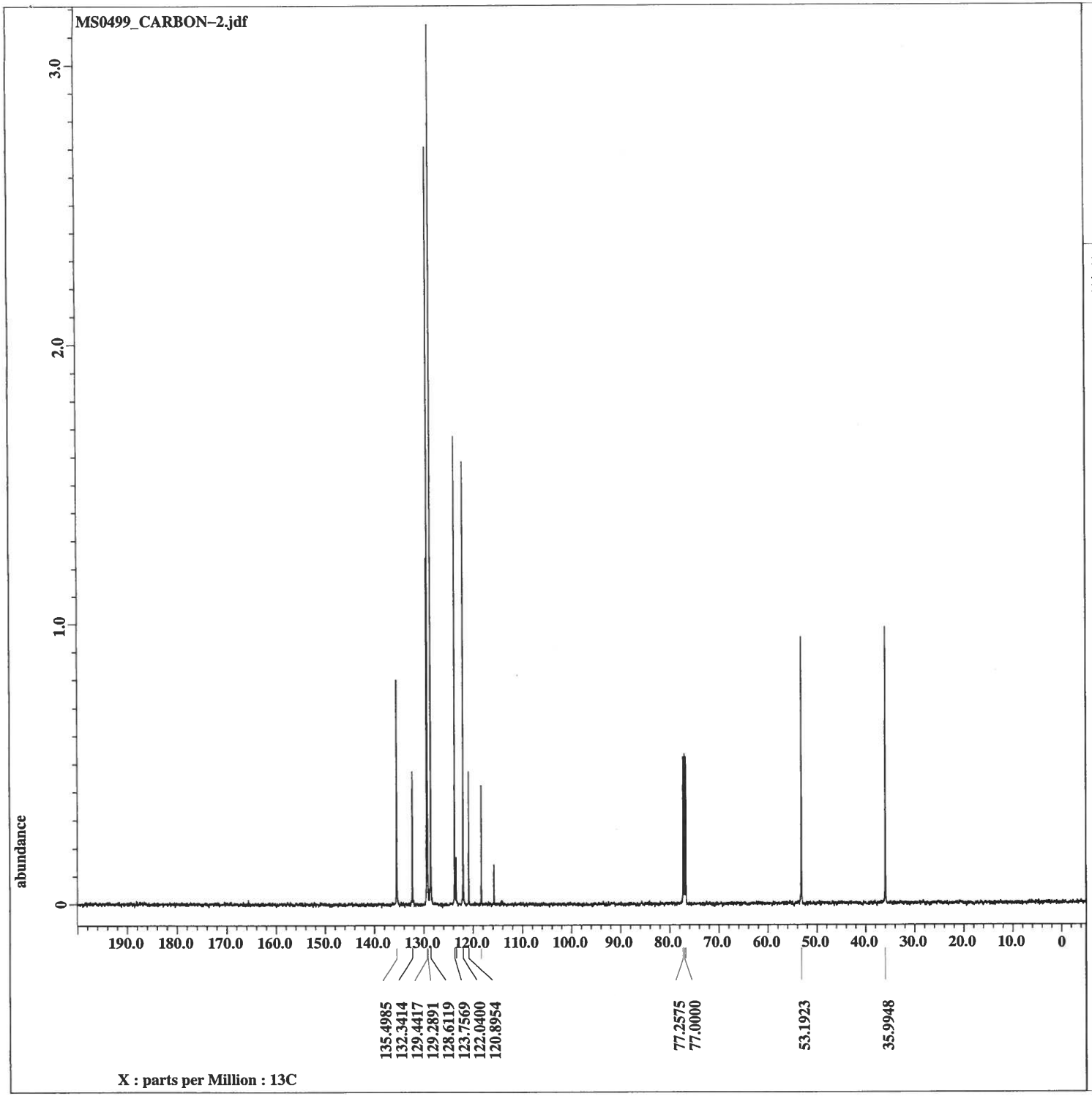

MS0430_FLUORINE-3.jdf
abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0 25.0 26.0
30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0
-78.9048
-99.0199
X : parts per Million : 19F



SOUTH ALABAMA JAGUARS

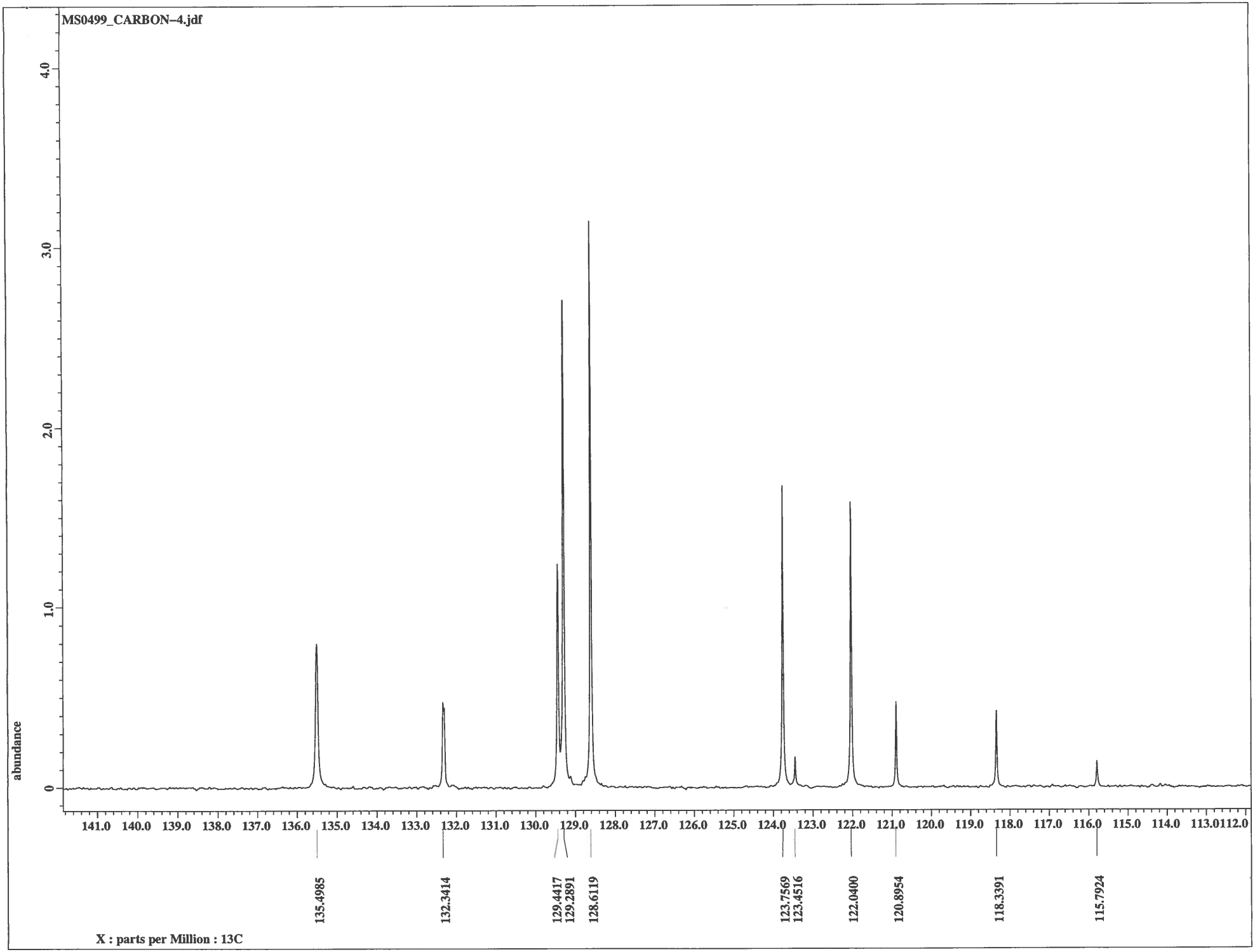
Filename	= MS0499_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0499
Solvent	= CHLOROFORM-D
Changer_sample	= 9
Creation_time	= 12-JUL-2018 18:21:04
Revision_time	= 12-JUL-2018 17:58:39
Current_time	= 12-JUL-2018 17:58:39
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 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	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 24
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.7[dC]

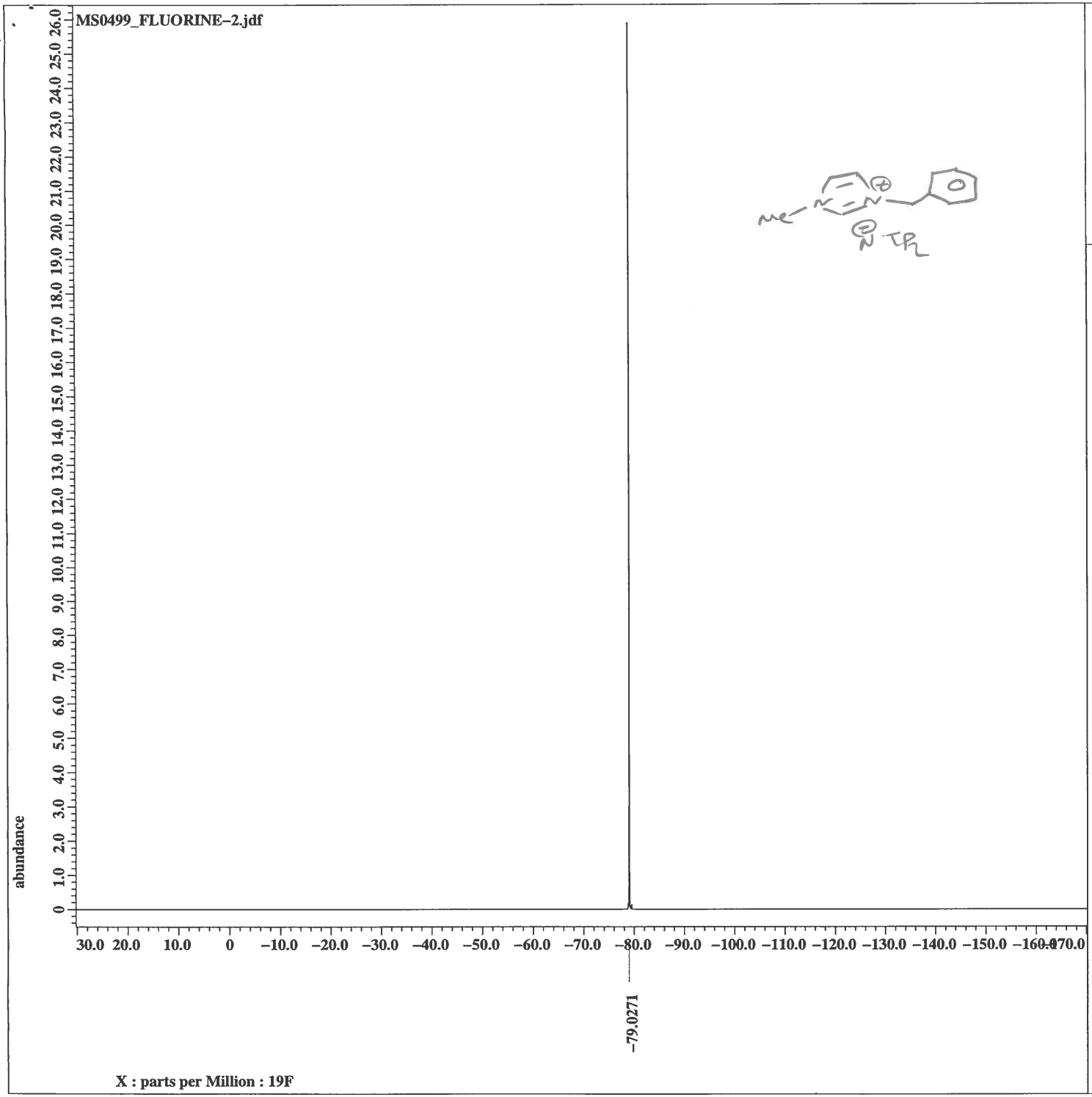

MS0499_PROTON-4.jdf
abundance
X : parts per Million : 1H
1.07
5.09
1.02
1.0
8.6200
7.3419
7.3362
7.3305
7.3247
7.3167
7.3076
7.2469
7.2434
7.2400
7.1965



SOUTH ALABAMA JAGUARS™

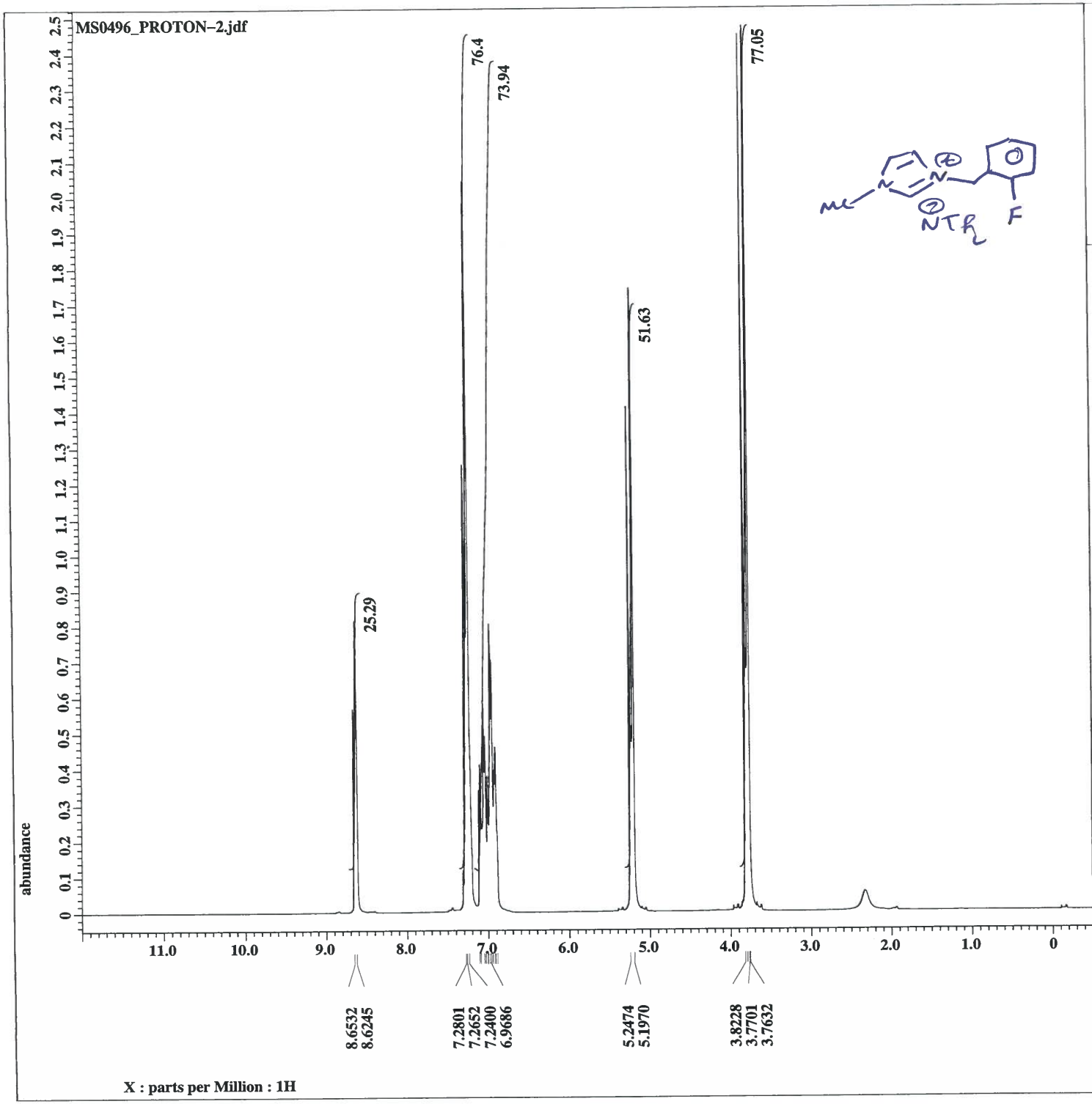
Filename	= MS0499_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0499
Solvent	= CHLOROFORM-D
Changer_sample	= 9
Creation_time	= 12-JUL-2018 18:33:38
Revision_time	= 12-JUL-2018 18:11:15
Current_time	= 12-JUL-2018 18:11:15
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 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	= 256
Total_scans	= 256
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 23.2[dC]


MS0499_CARBON-4.jdf
abundance
4.0
3.0
2.0
1.0
0
141.0 140.0 139.0 138.0 137.0 136.0 135.0 134.0 133.0 132.0 131.0 130.0 129.0 128.0 127.0 126.0 125.0 124.0 123.0 122.0 121.0 120.0 119.0 118.0 117.0 116.0 115.0 114.0 113.0 112.0
135.4985
132.3414
129.4417
129.2891
128.6119
123.7569
123.4516
122.0400
120.8954
118.3391
115.7924
X : parts per Million : 13C



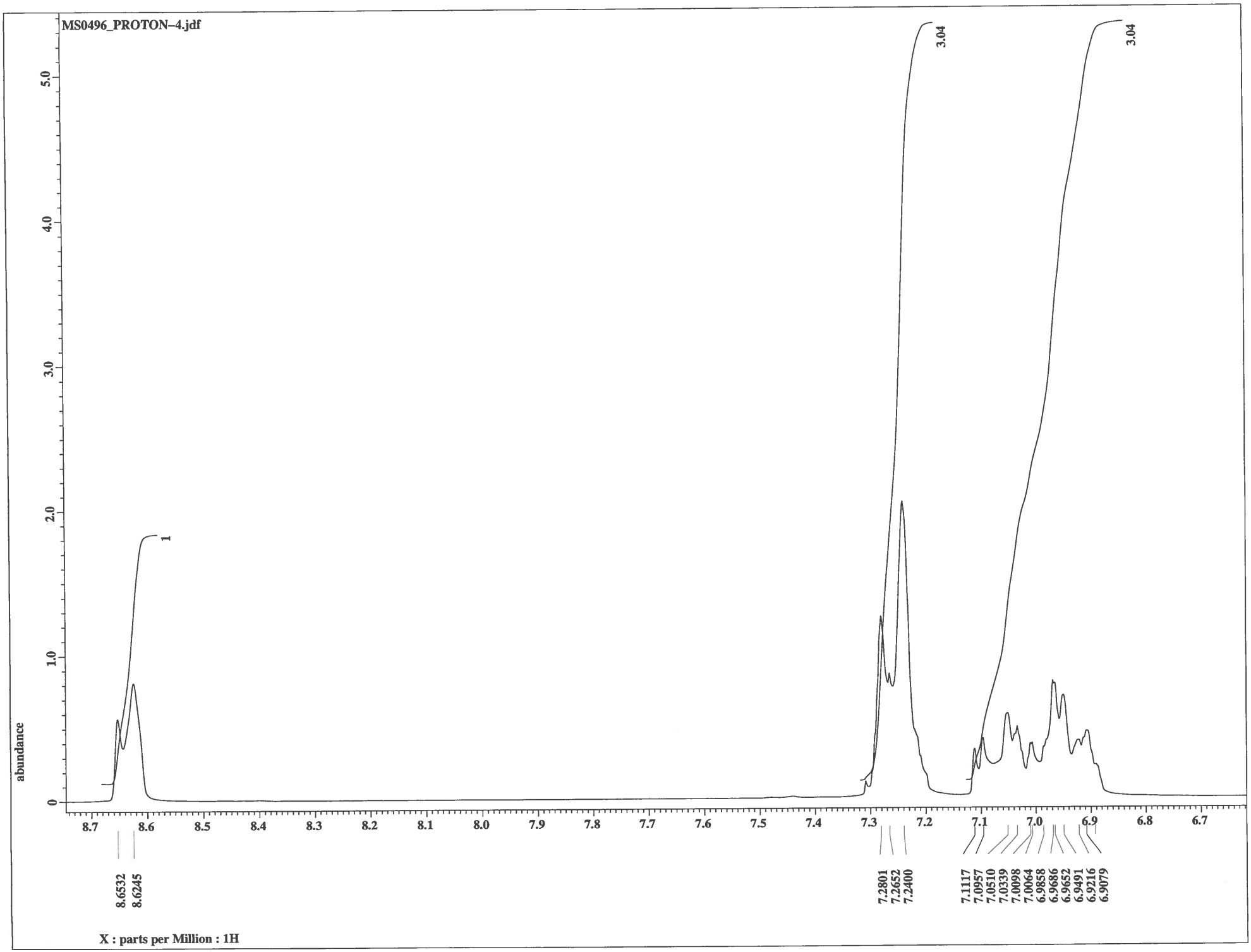
SOUTH ALABAMA JAGUARS

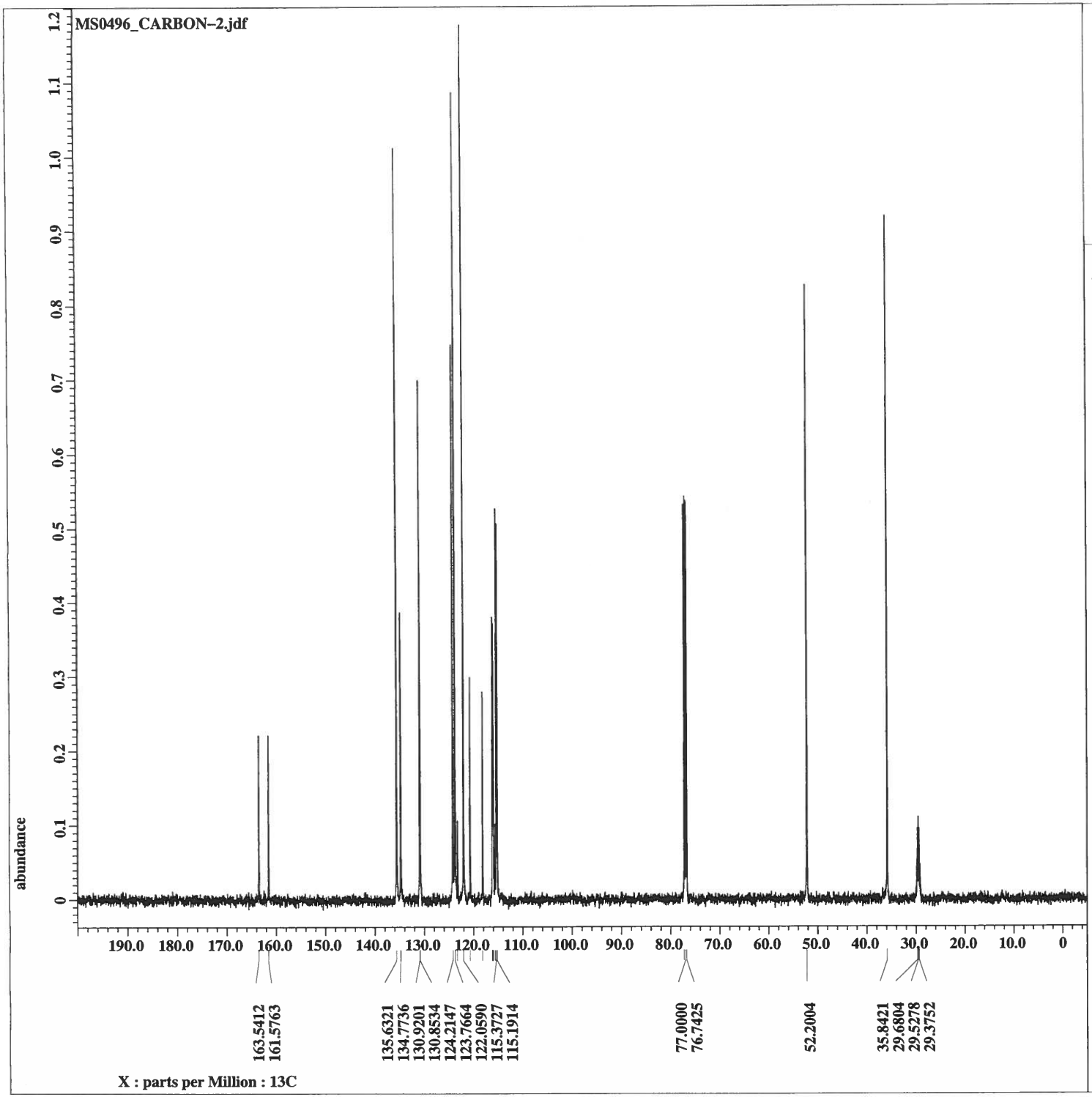
Filename	= MS0499_FLUORINE-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0499
Solvent	= CHLOROFORM-D
Changer_sample	= 9
Creation_time	= 12-JUL-2018 16:38:27
Revision_time	= 12-JUL-2018 16:16:04
Current_time	= 12-JUL-2018 16:16:04
Data_format	= 1D COMPLEX
Dim_size	= 52428
Dim_title	= 19F
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 30
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.5[dC]



SOUTH ALABAMA JAGUARS

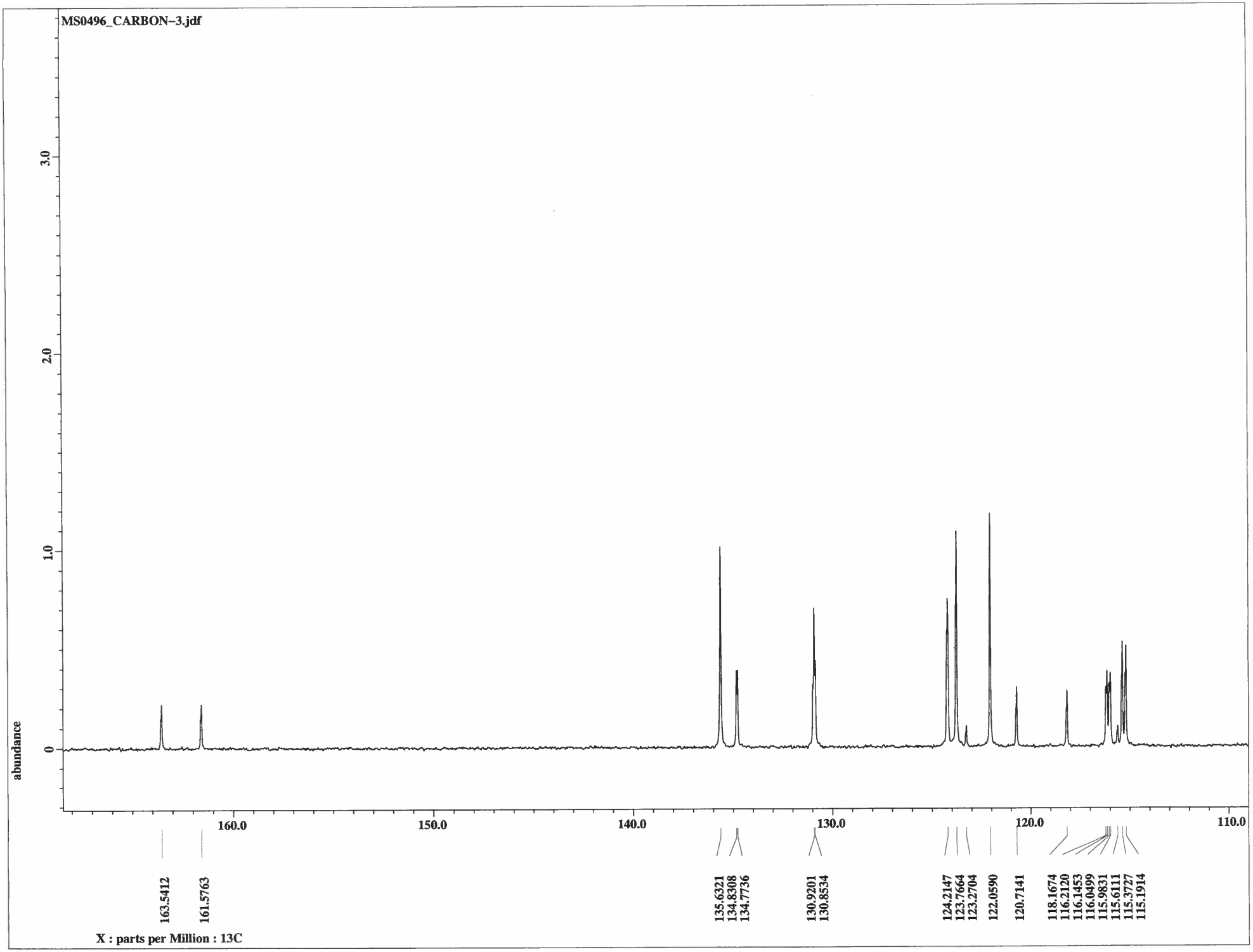
Filename	= MS0496_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0496
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 12-JUL-2018 17:39:41
Revision_time	= 12-JUL-2018 17:17:17
Current_time	= 12-JUL-2018 17:17:17
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 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	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
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]

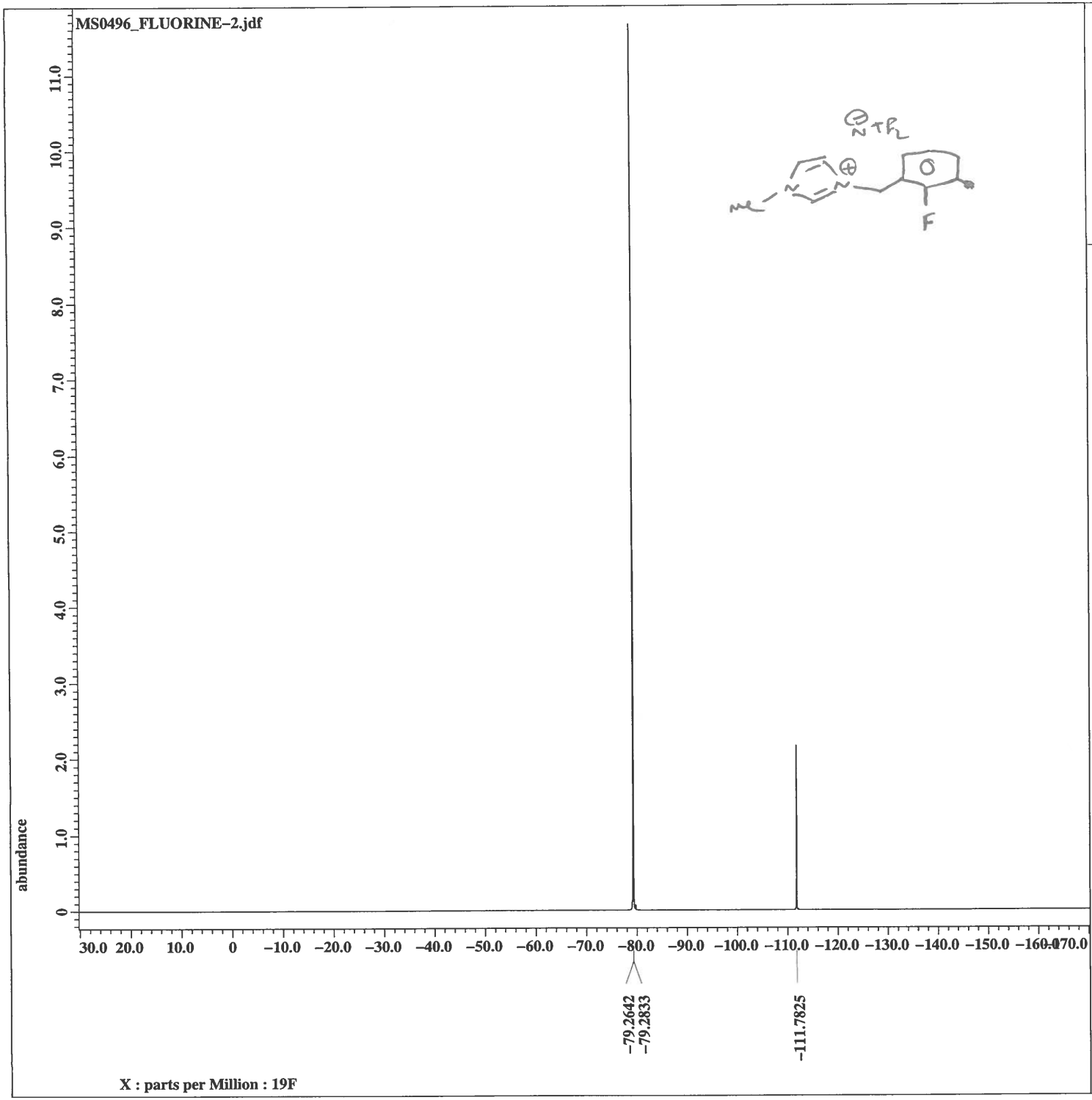

MS0496_PROTON-4.jdf
abundance
0
1.0
2.0
3.0
4.0
5.0
1
3.04
3.04
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
8.6532
8.6245
7.2801
7.2652
7.2400
7.1117
7.0957
7.0510
7.0339
7.0098
7.0064
6.9858
6.9686
6.9652
6.9491
6.9216
6.9079
X : parts per Million : 1H



SOUTH ALABAMA JAGUARS

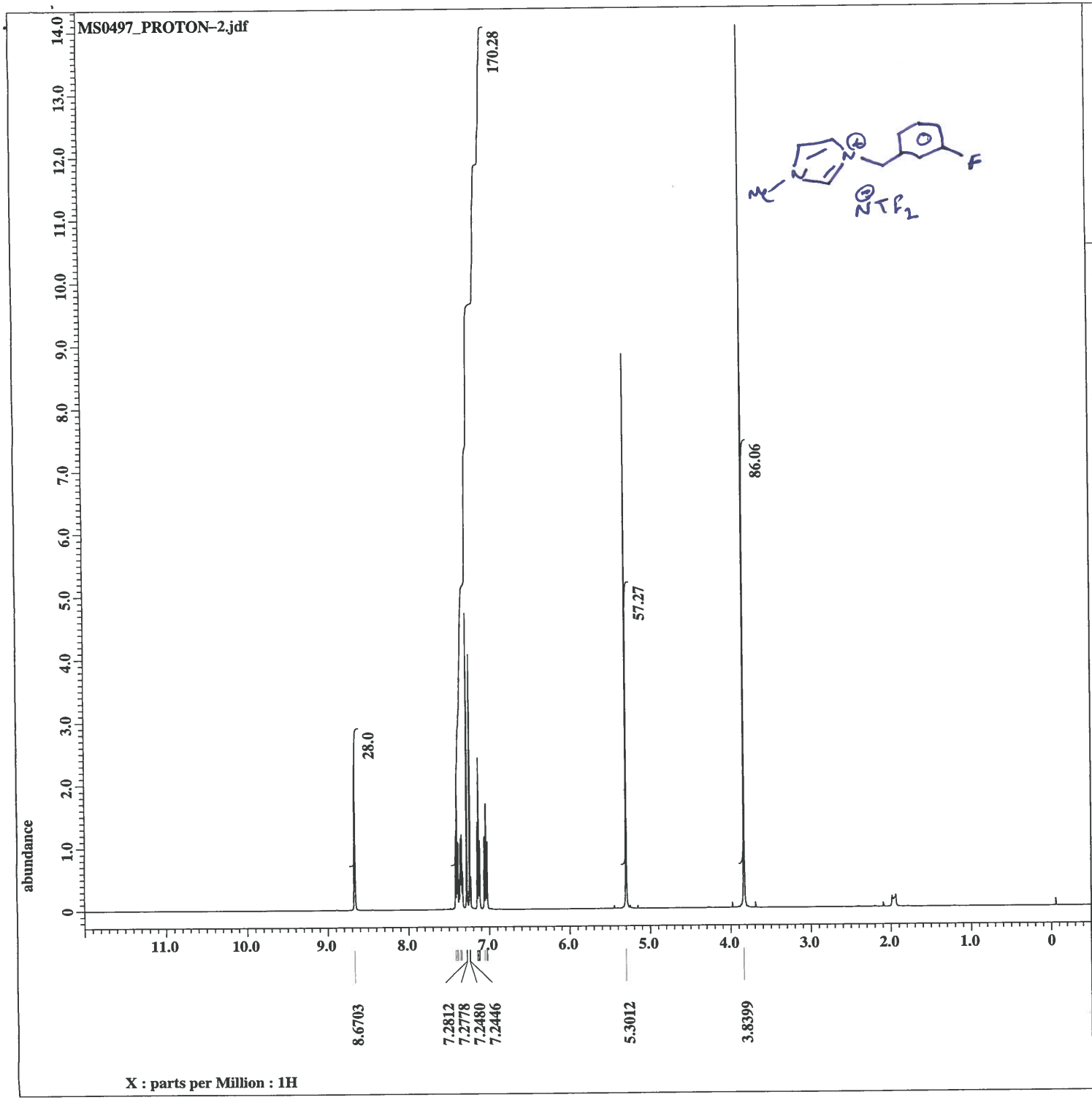
Filename	= MS0496_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0496
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 12-JUL-2018 17:54:02
Revision_time	= 12-JUL-2018 17:31:38
Current_time	= 12-JUL-2018 17:31:38
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 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	= 256
Total_scans	= 256
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 23[dC]


MS0496_CARBON-3.jdf
abundance
3.0
2.0
1.0
0
160.0
150.0
140.0
130.0
120.0
110.0
163.5412
161.5763
135.6321
134.8308
134.7736
130.9201
130.8534
124.2147
123.7664
123.2704
122.0590
120.7141
118.1674
116.2120
116.1453
116.0499
115.9831
115.6111
115.3727
115.1914
X : parts per Million : 13C



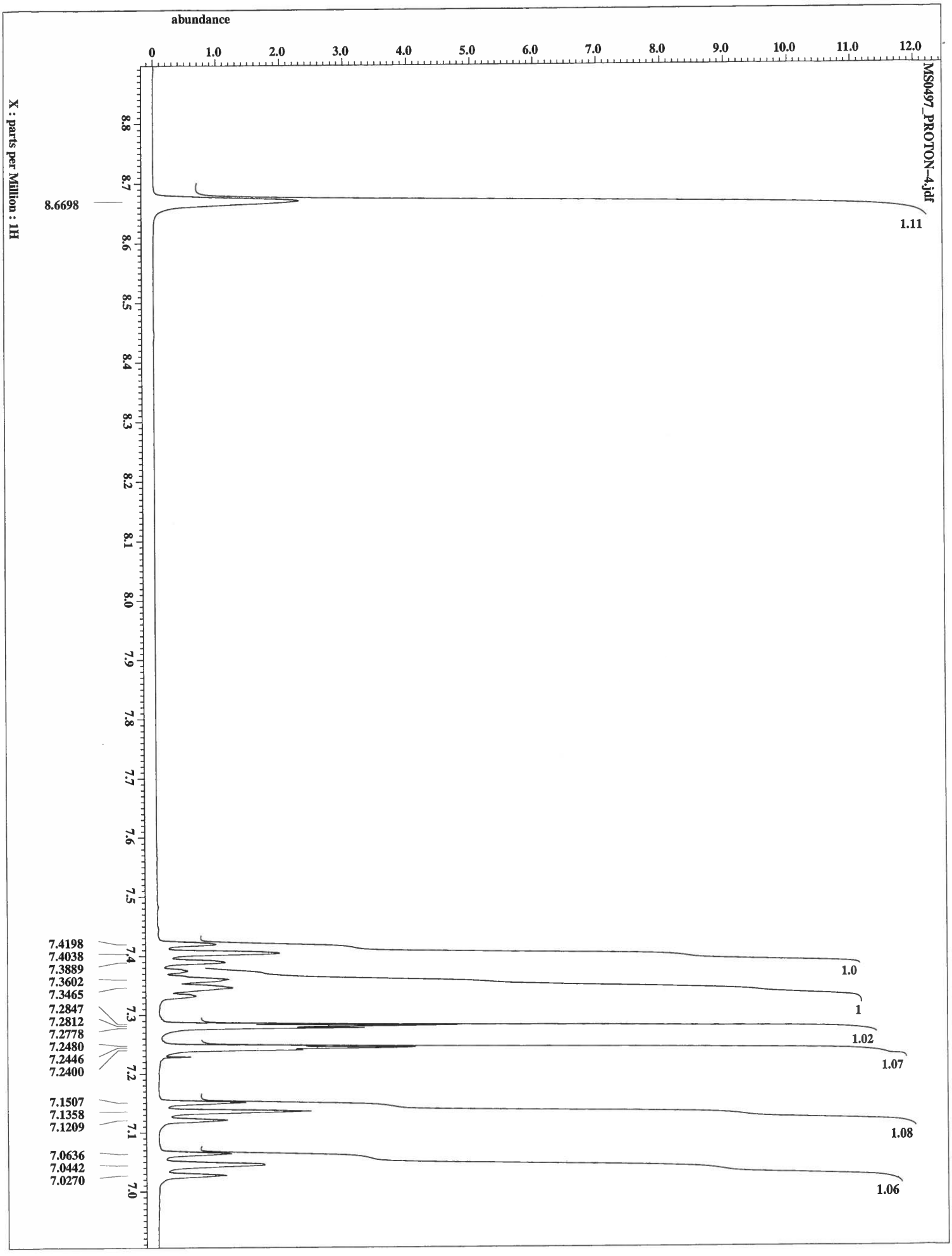
SOUTH ALABAMA JAGUARS

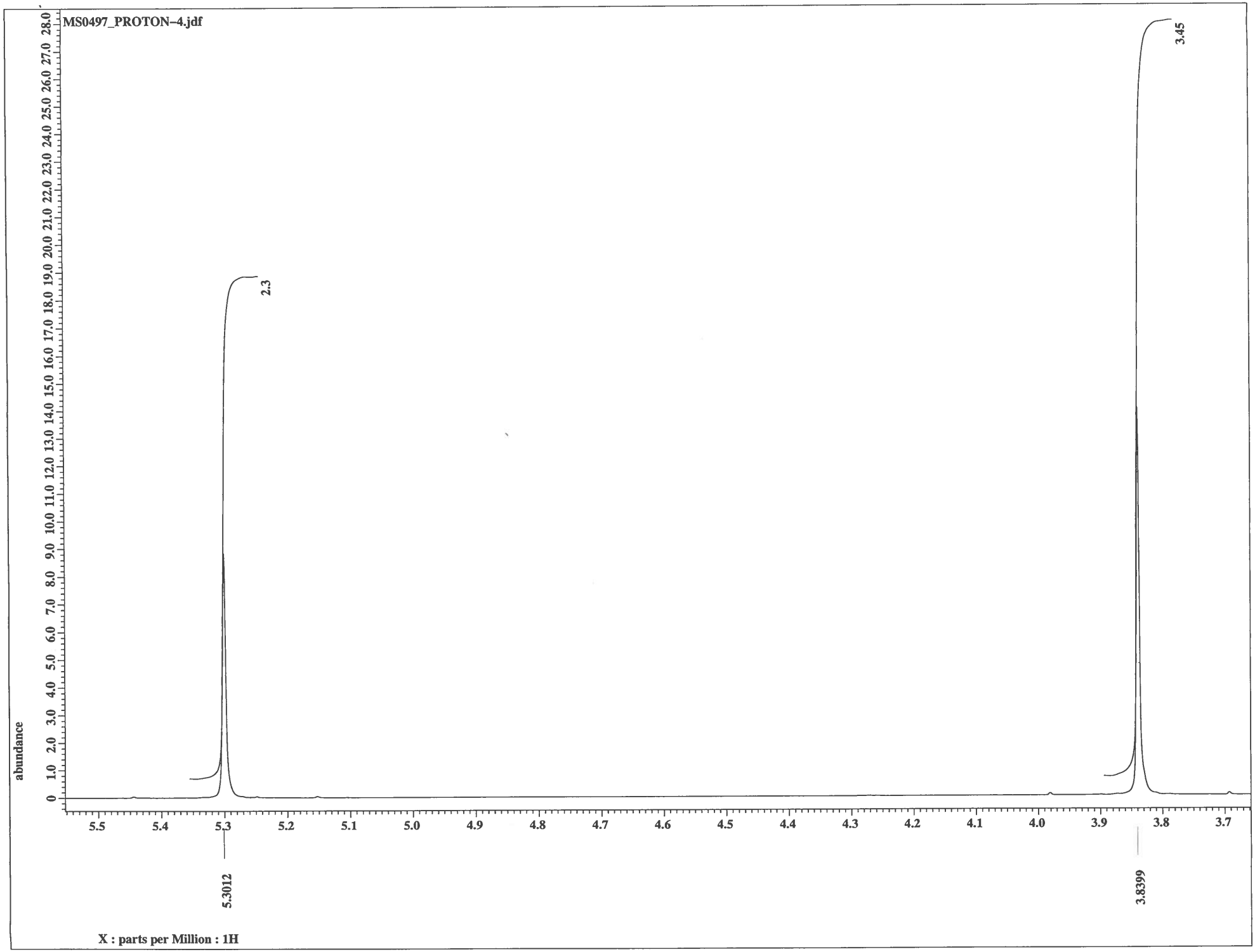
Filename	= MS0496_FLUORINE-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0496
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 12-JUL-2018 16:18:09
Revision_time	= 12-JUL-2018 15:55:46
Current_time	= 12-JUL-2018 15:55:46
Data_format	= 1D COMPLEX
Dim_size	= 52428
Dim_title	= 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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 26
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.5[dC]

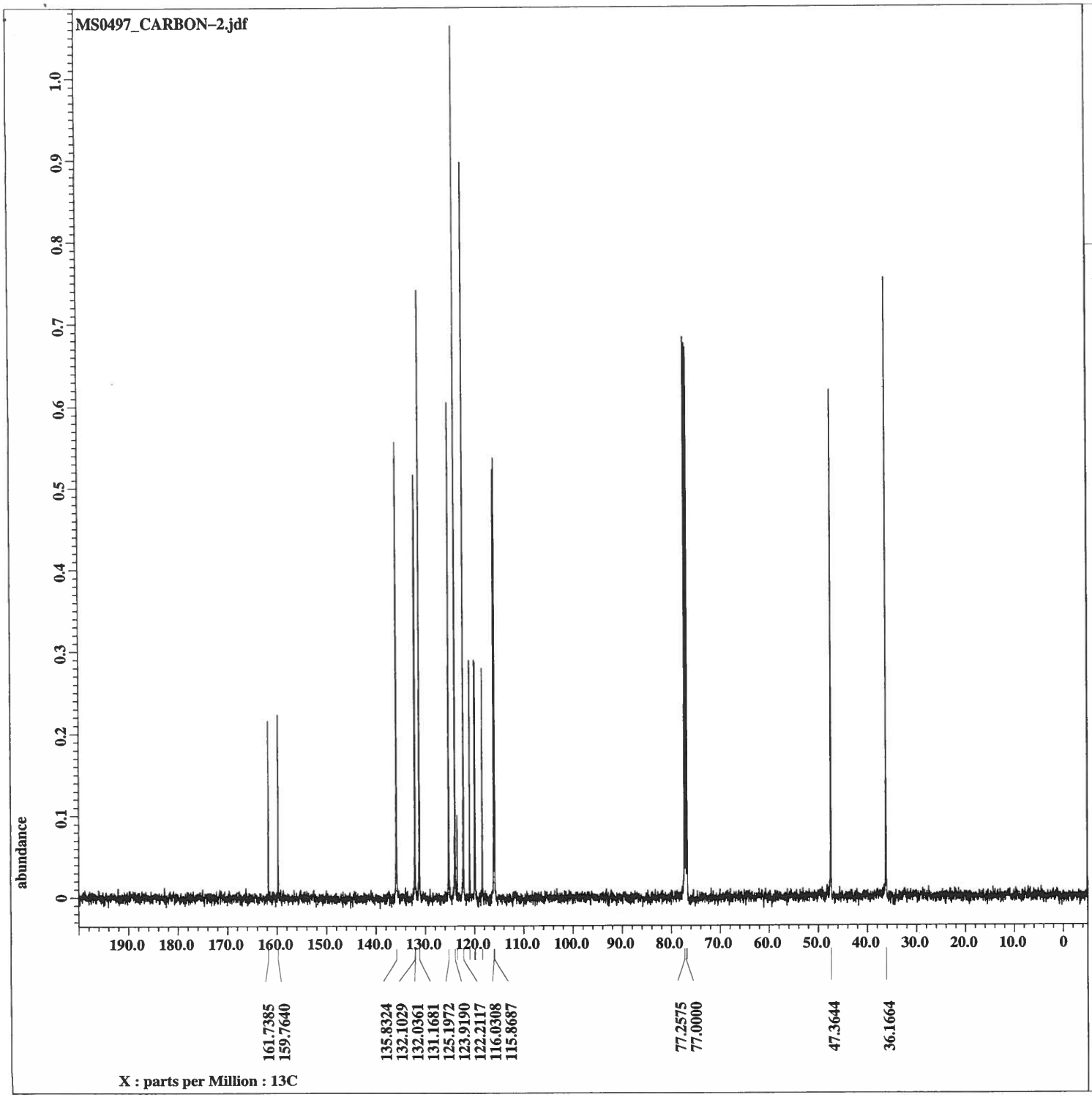


SOUTH ALABAMA JAGUARS

Filename	= MS0497_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0497
Solvent	= CHLOROFORM-D
Changer_sample	= 7
Creation_time	= 12-JUL-2018 18:01:19
Revision_time	= 12-JUL-2018 17:38:55
Current_time	= 12-JUL-2018 17:38:55
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	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
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]

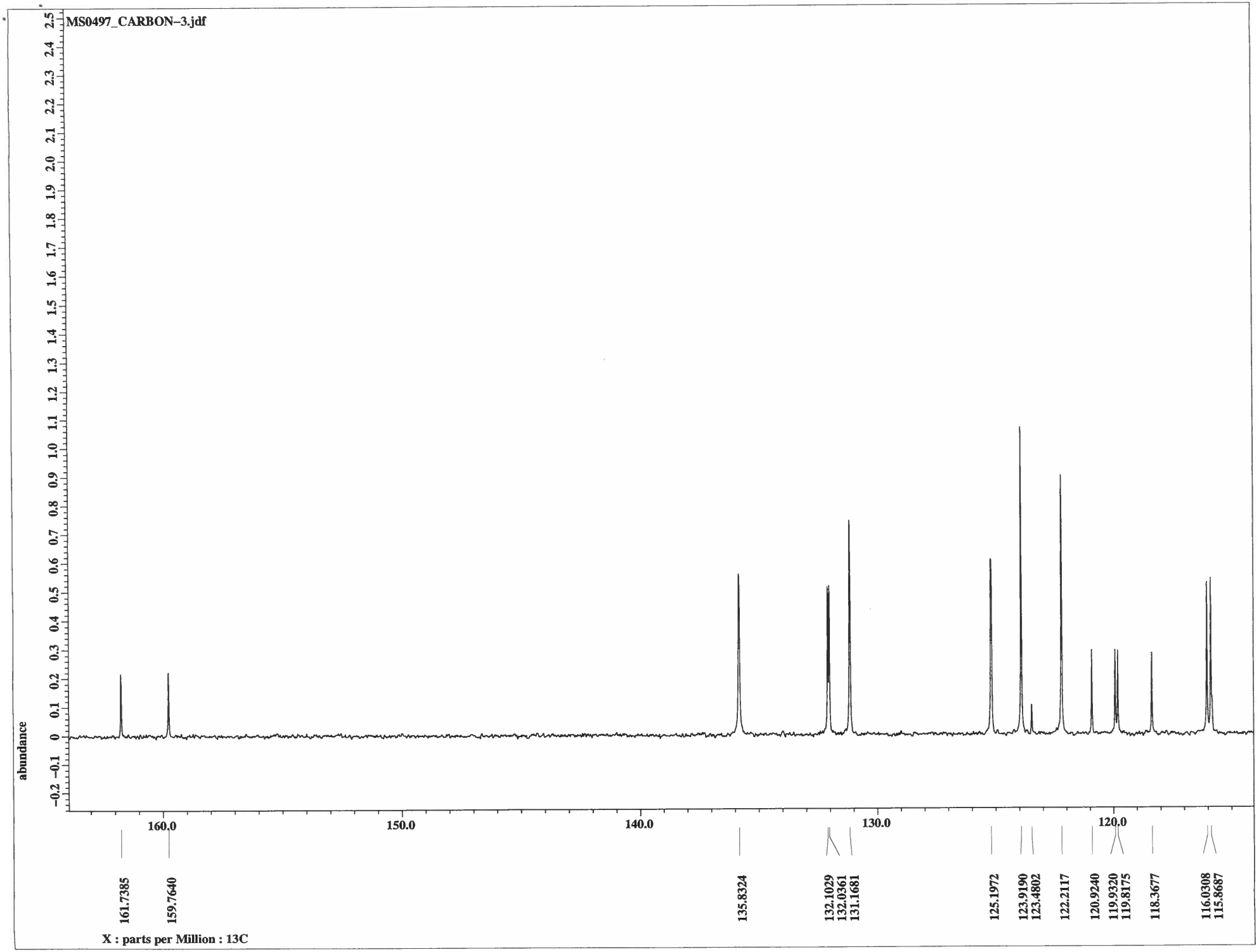

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
MS0497_PROTON-4.jdf
X : parts per Million : 1H
8.6698
1.11
7.4198
7.4038
7.3889
7.3602
7.3465
7.2847
7.2812
7.2778
7.2480
7.2446
7.2400
7.1507
7.1358
7.1209
7.0636
7.0442
7.0270
1.0
1
1.02
1.07
1.08
1.06

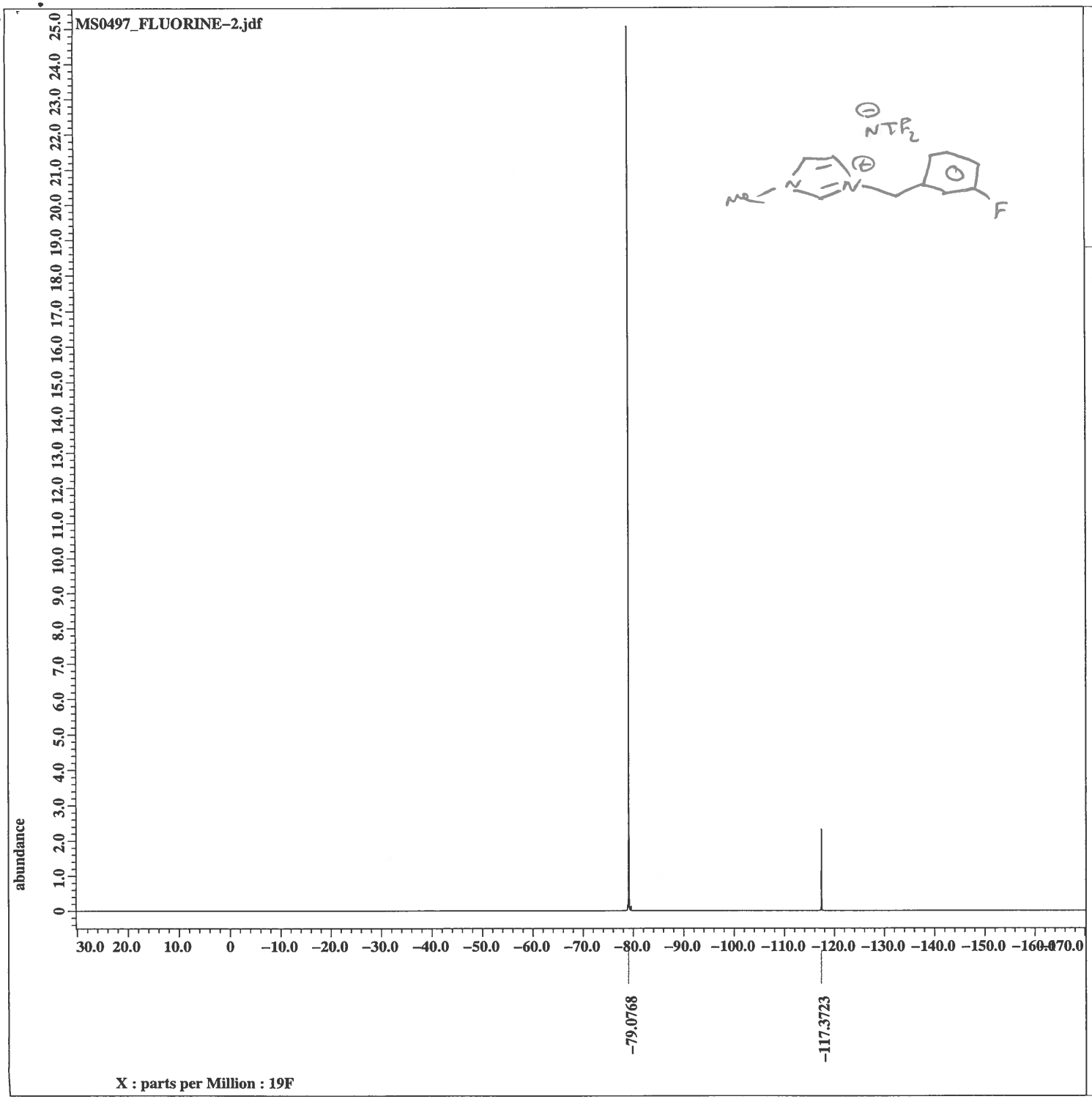

MS0497_PROTON-4.jdf
abundance
2.3
3.45
5.3012
3.8399
X : parts per Million : 1H



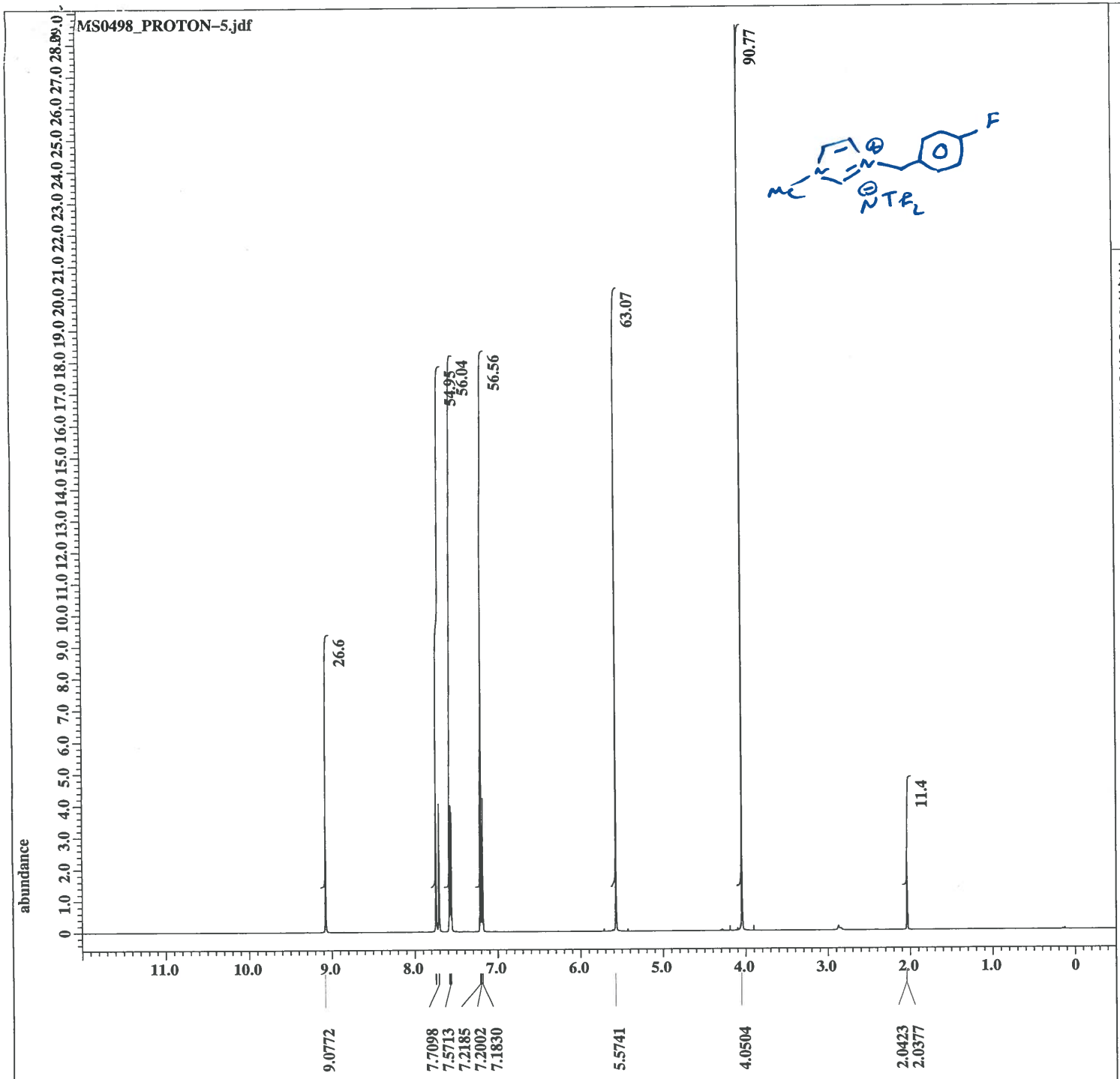
SOUTH ALABAMA JAGUARS

Filename	= MS0497_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0497
Solvent	= CHLOROFORM-D
Changer_sample	= 7
Creation_time	= 12-JUL-2018 18:13:54
Revision_time	= 12-JUL-2018 17:51:29
Current_time	= 12-JUL-2018 17:51:29
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	= 256
Total_scans	= 256
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 23.1[dC]


MS0497_CARBON-3.jdf
abundance
-0.2 -0.1 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
160.0
150.0
140.0
130.0
120.0
161.7385
159.7640
135.8324
132.1029
132.0361
131.1681
125.1972
123.9190
123.4802
122.2117
120.9240
119.9320
119.8175
118.3677
116.0308
115.8687
X : parts per Million : 13C

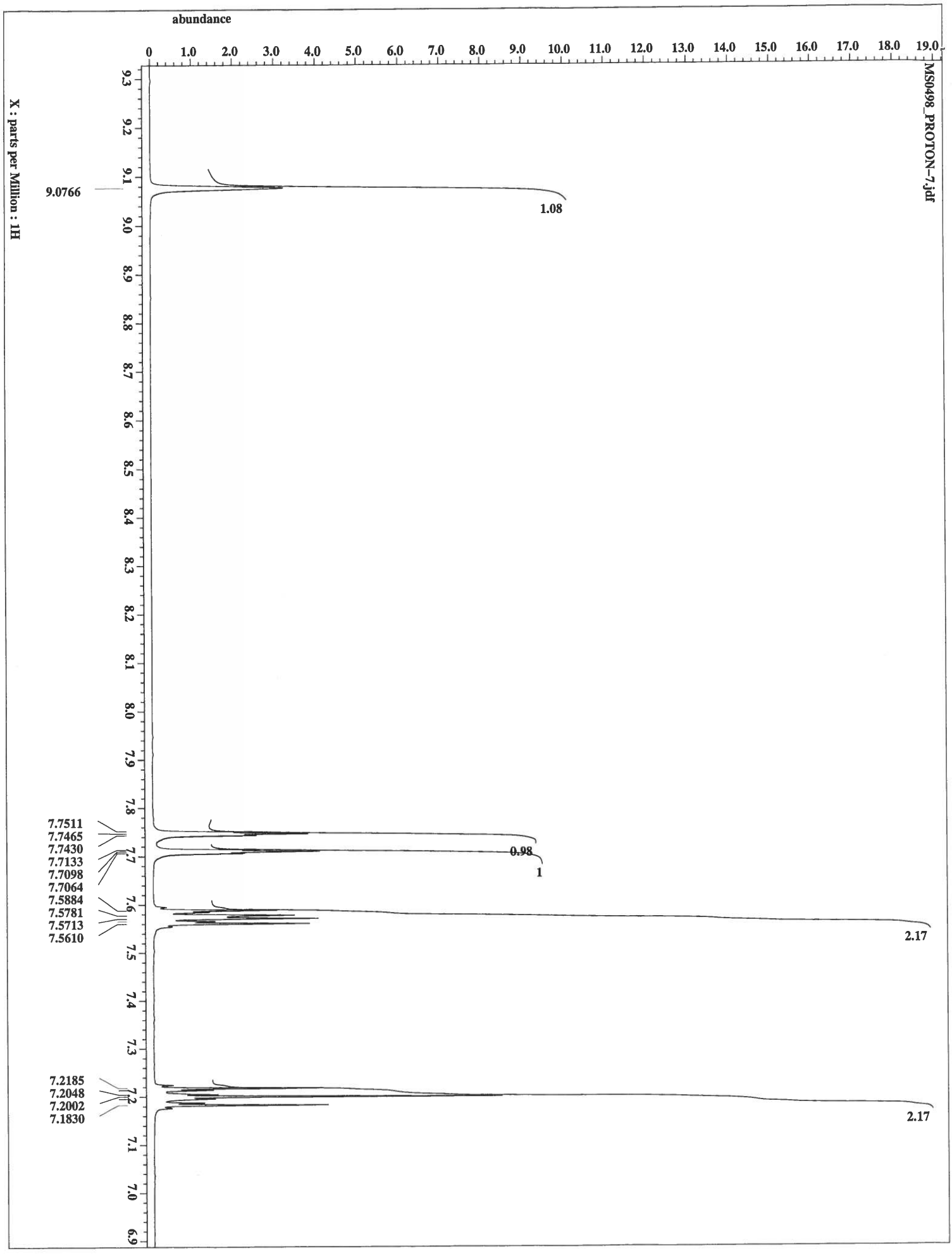


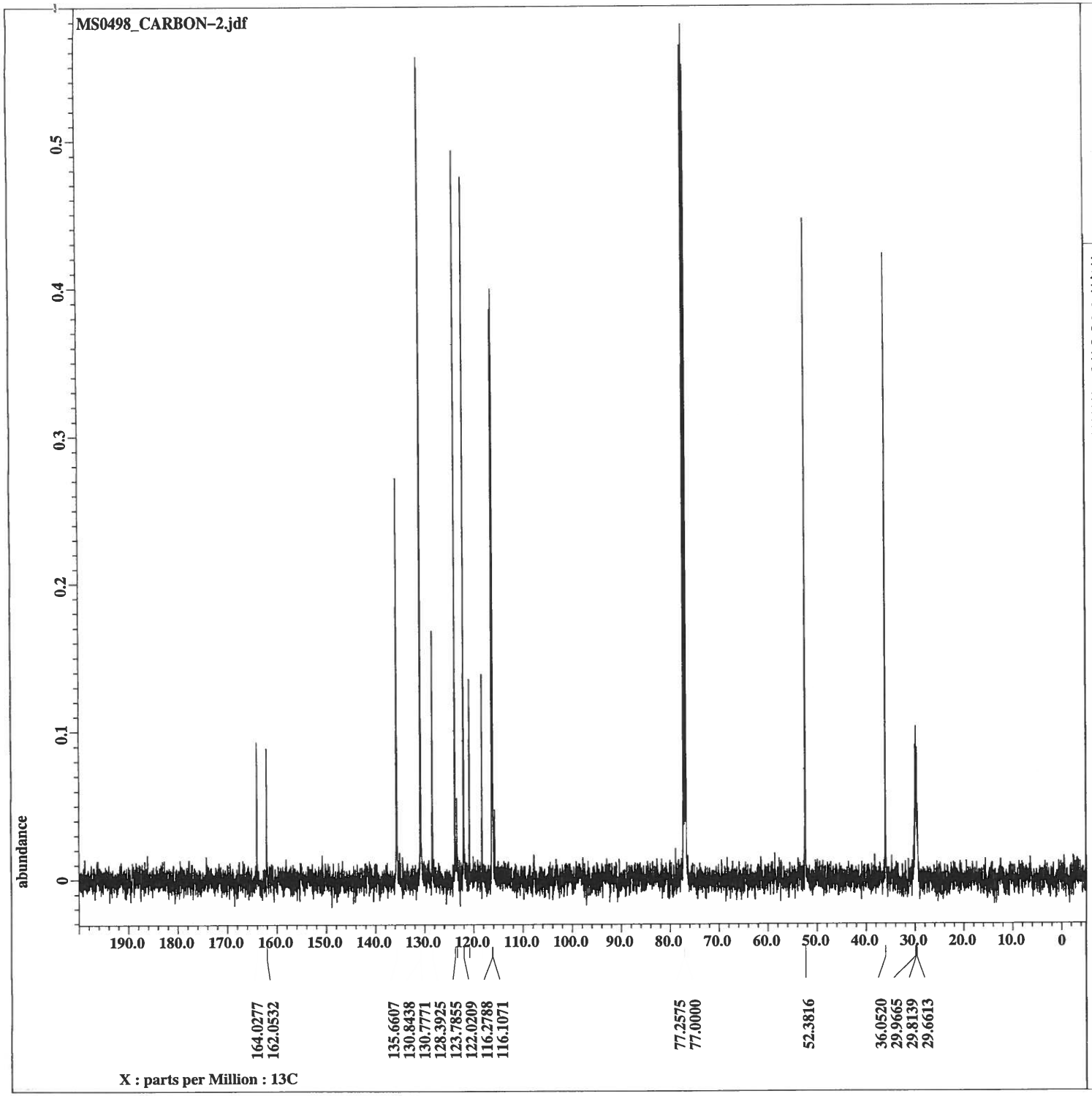
Filename	= MS0497_FLUORINE-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0497
Solvent	= CHLOROFORM-D
Changer_sample	= 7
Creation_time	= 12-JUL-2018 16:25:02
Revision_time	= 12-JUL-2018 16:02:38
Current_time	= 12-JUL-2018 16:02:38
Data_format	= 1D COMPLEX
Dim_size	= 52428
Dim_title	= 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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 30
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.4[dC]



SOUTH ALABAMA JAGUARS

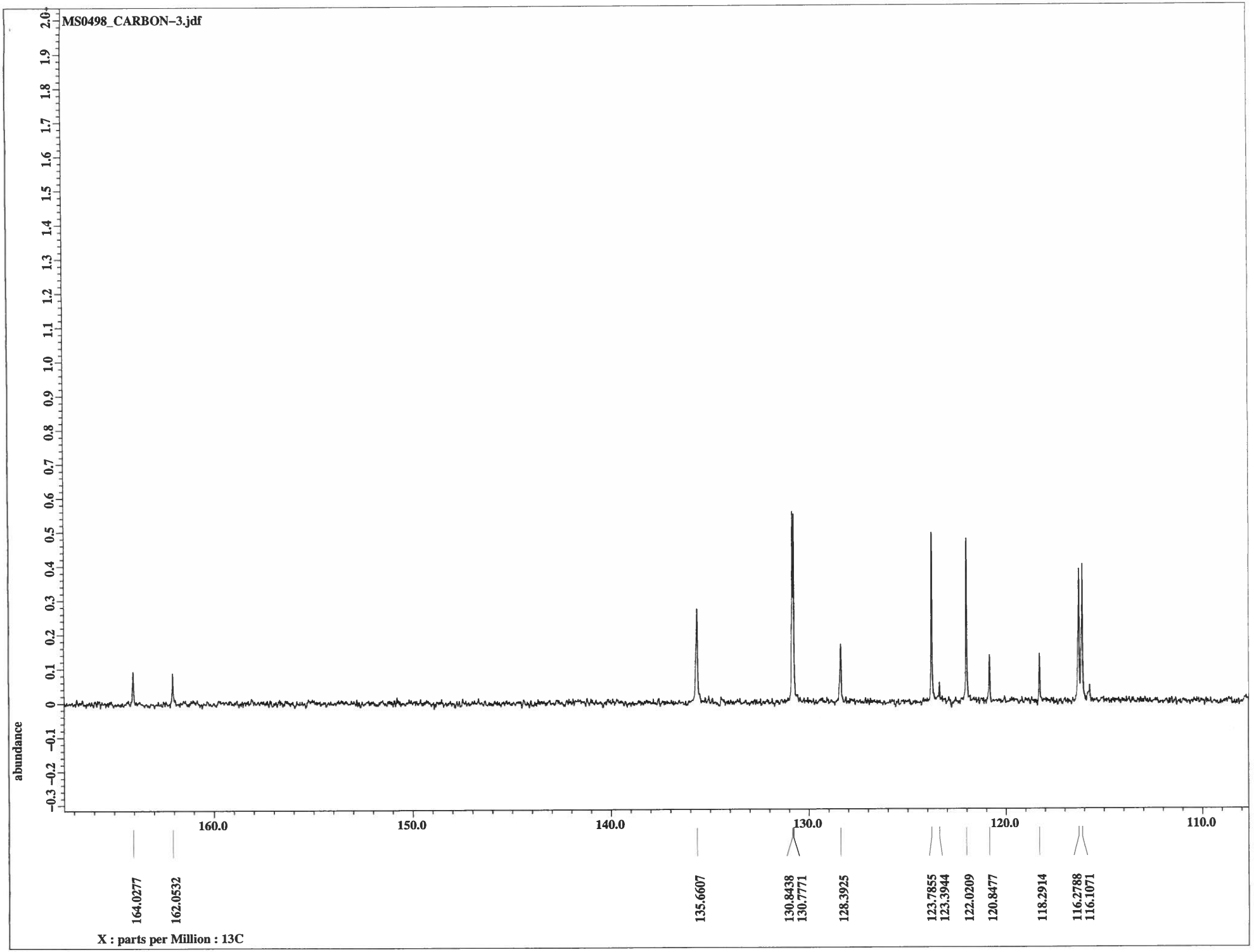
Filename	= MS0498_PROTON-5.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0498
Solvent	= ACETONE-D6
Changer_sample	= 8
Creation_time	= 13-JUL-2018 09:18:13
Revision_time	= 13-JUL-2018 08:55:45
Current_time	= 13-JUL-2018 08:55:45
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 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	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 34
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.5[dC]

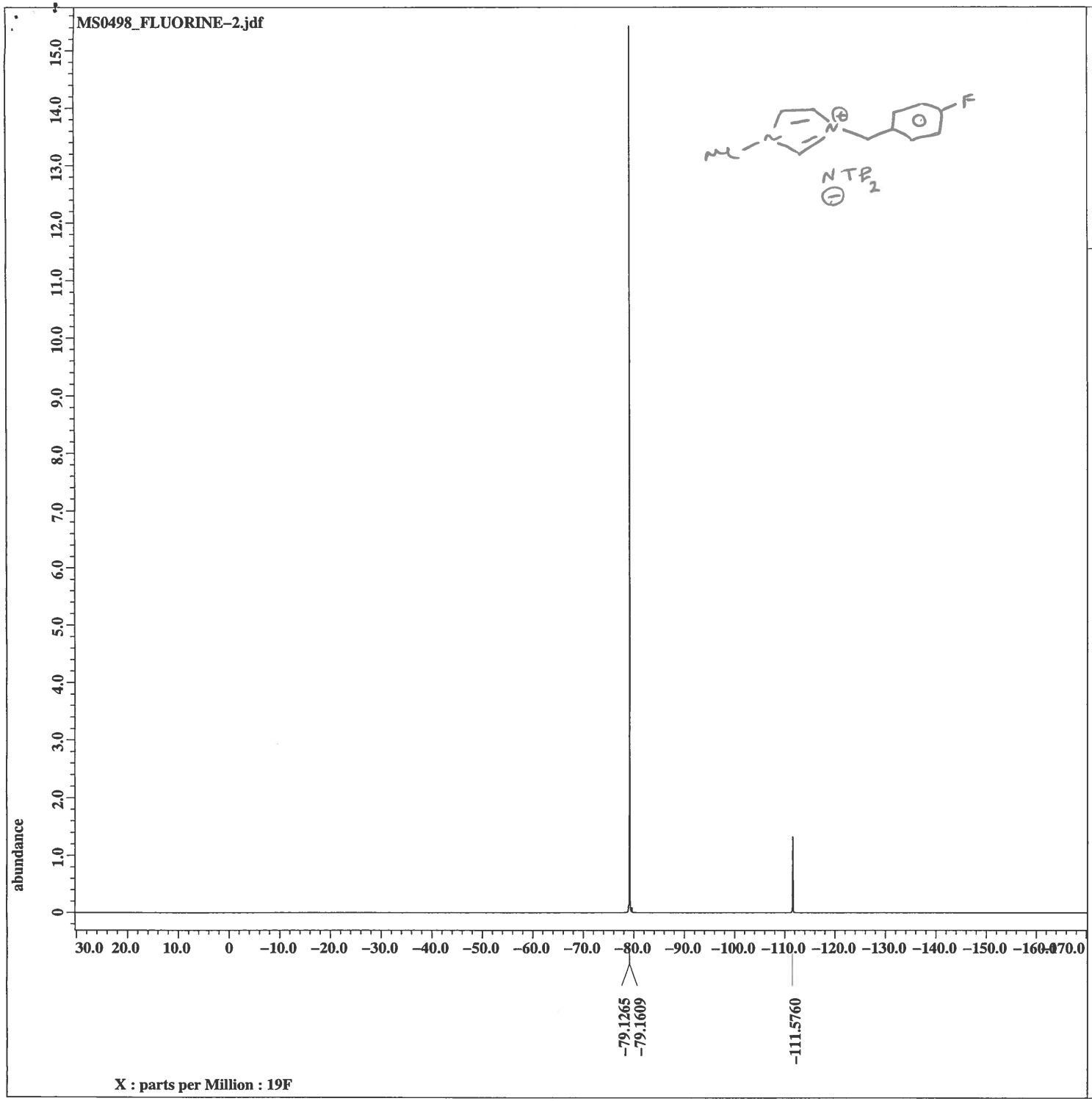

abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0
MS0498_PROTON-7.jdf
X : parts per Million : 1H
9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
9.0766
1.08
7.7511
7.7465
7.7430
7.7133
7.7098
7.7064
7.5884
7.5781
7.5713
7.5610
0.98
1
2.17
7.2185
7.2048
7.2002
7.1830
2.17



SOUTH ALABAMA JAGUARS

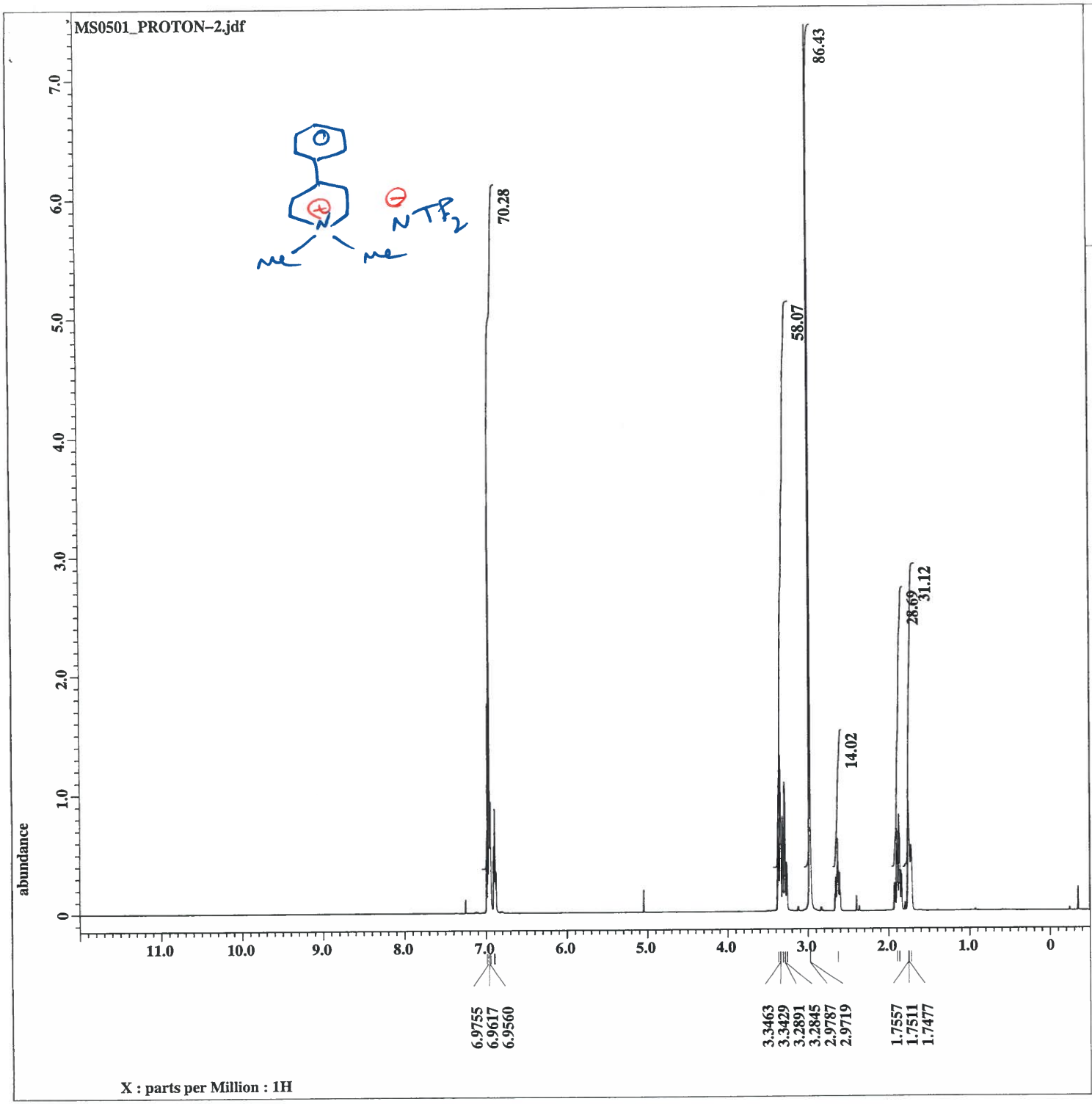
Filename	= MS0498_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0498
Solvent	= CHLOROFORM-D
Changer_sample	= 8
Creation_time	= 12-JUL-2018 17:31:59
Revision_time	= 12-JUL-2018 17:09:35
Current_time	= 12-JUL-2018 17:09:35
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
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	= 128
Total_scans	= 128
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 23[dC]


MS0498_CARBON-3.jdf
abundance
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
160.0
150.0
140.0
130.0
120.0
110.0
164.0277
162.0532
135.6607
130.8438
130.7771
128.3925
123.7855
123.3944
122.0209
120.8477
118.2914
116.2788
116.1071
X : parts per Million : 13C



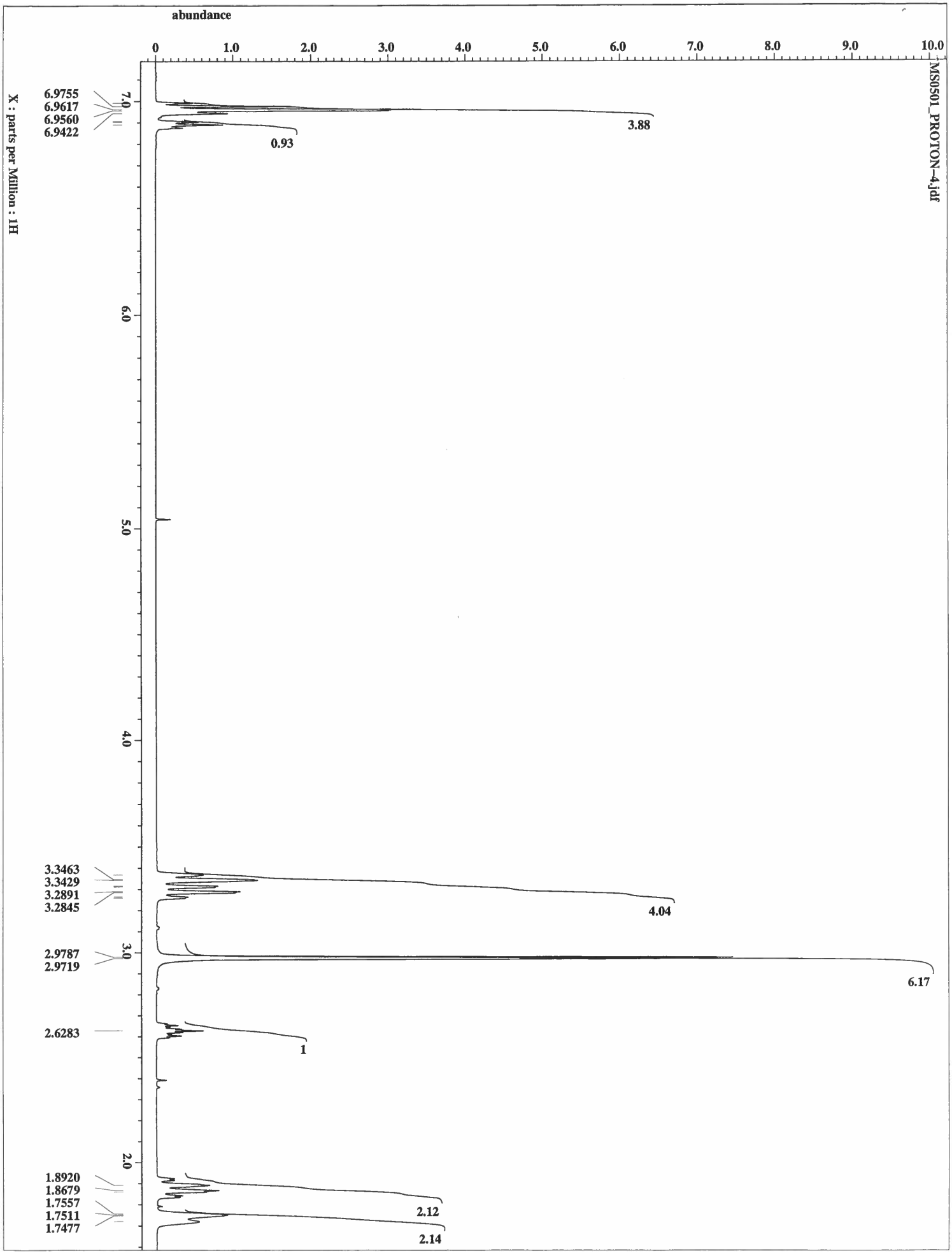
SOUTH ALABAMA JAGUARS

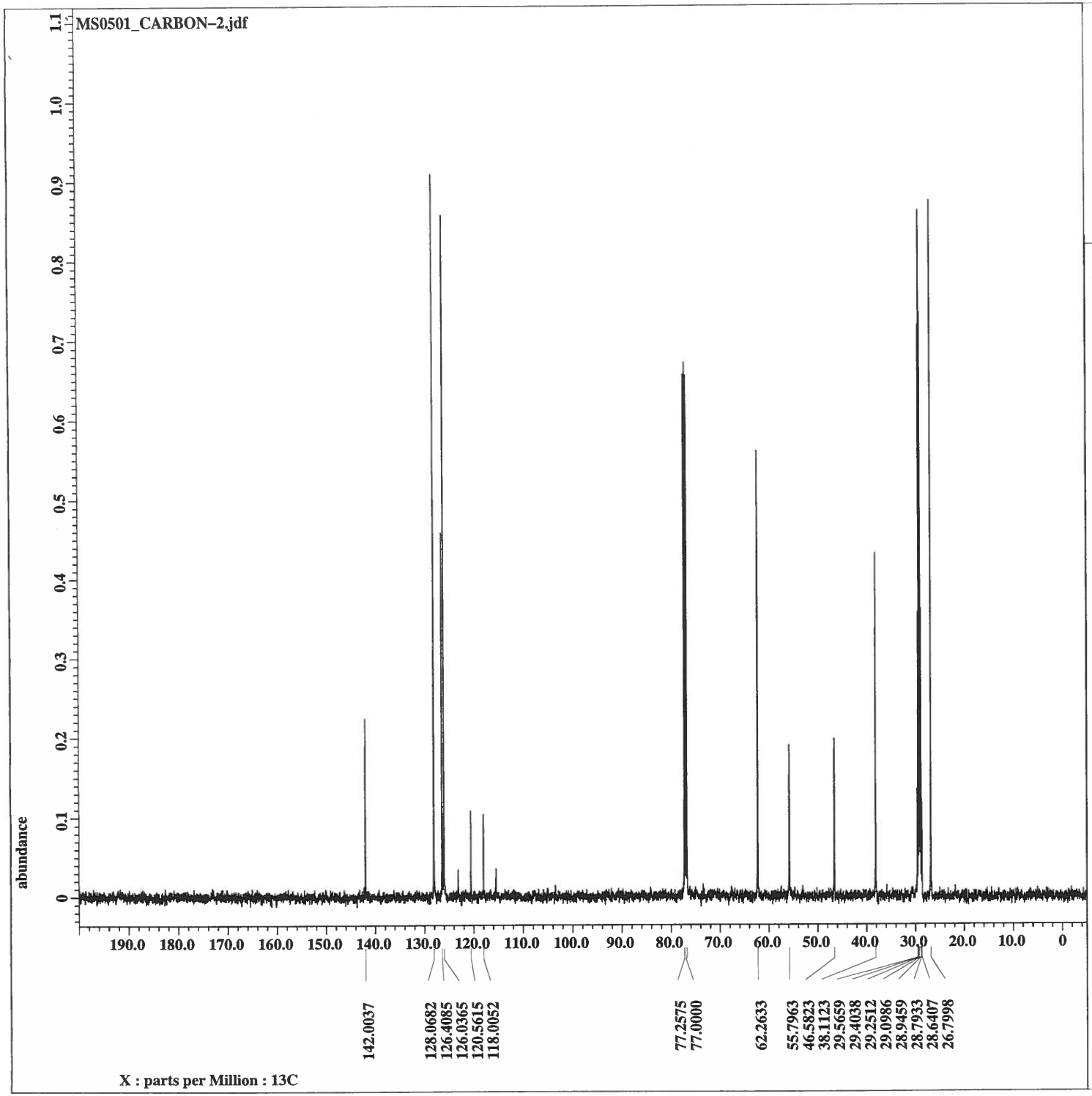
Filename	= MS0498_FLUORINE-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0498
Solvent	= CHLOROFORM-D
Changer_sample	= 8
Creation_time	= 12-JUL-2018 16:31:45
Revision_time	= 12-JUL-2018 16:09:22
Current_time	= 12-JUL-2018 16:09:23
Data_format	= 1D COMPLEX
Dim_size	= 52428
Dim_title	= 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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.4[dC]



SOUTH ALABAMA JAGUARS

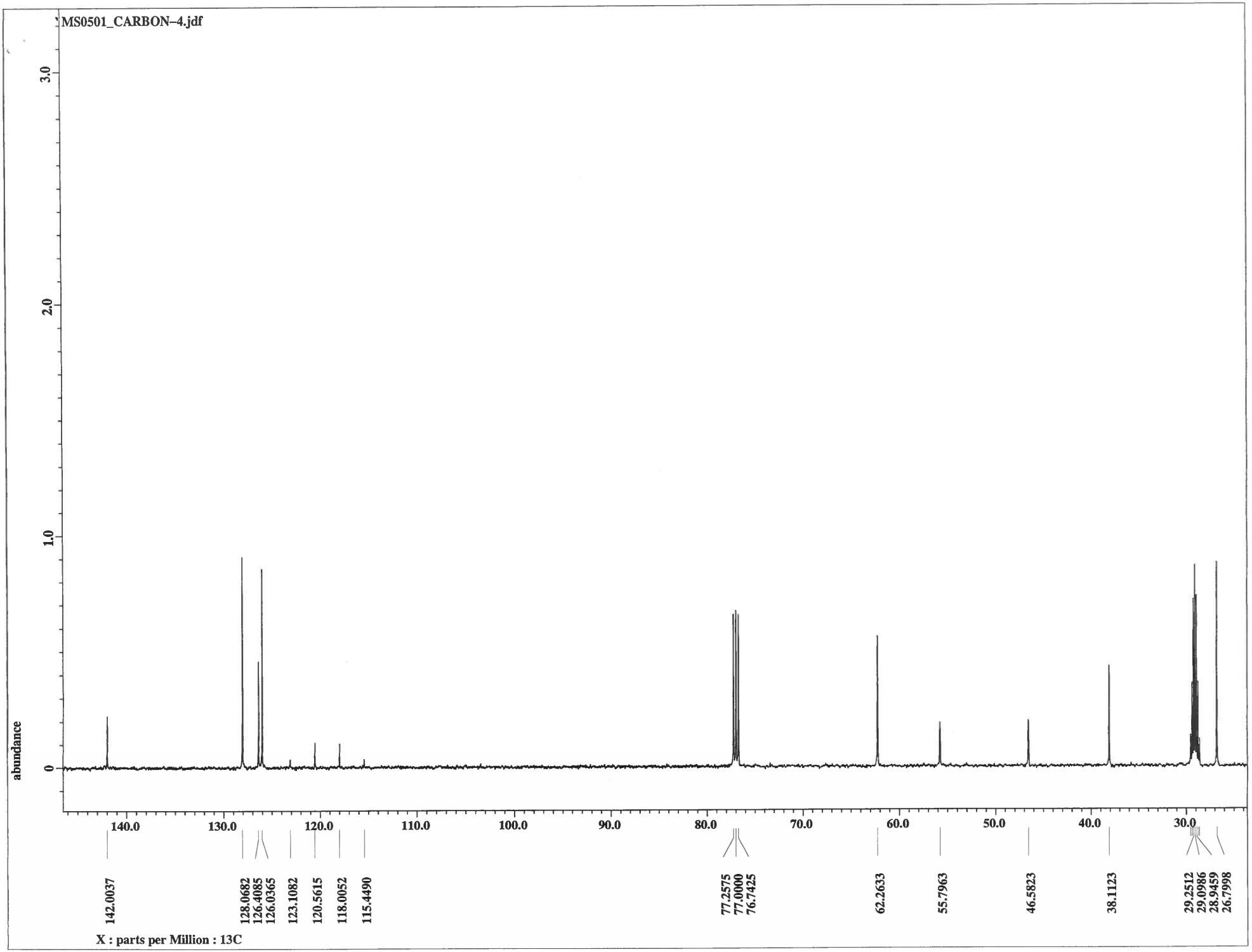
Filename	= MS0501_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0501
Solvent	= CHLOROFORM-D
Changer_sample	= 11
Creation_time	= 5-JUL-2018 16:43:37
Revision_time	= 5-JUL-2018 16:20:08
Current_time	= 5-JUL-2018 16:20:08
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 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	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 30
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.7[dC]

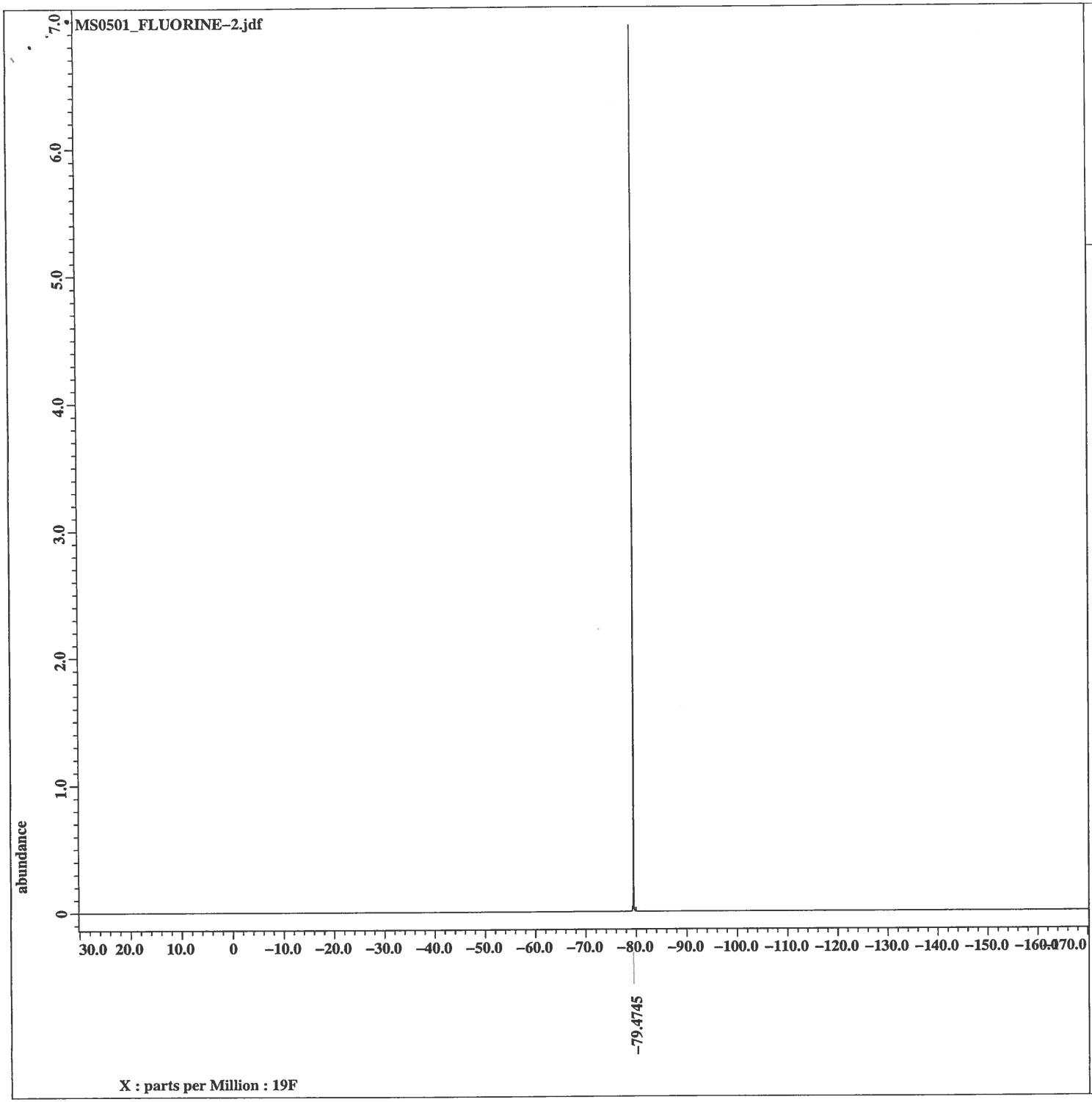

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
MS0501_PROTON-4.jdf
X : parts per Million : 1H
6.9755
6.9617
6.9560
6.9422
3.88
0.93
3.3463
3.3429
3.2891
3.2845
4.04
2.9787
2.9719
6.17
2.6283
1
1.8920
1.8679
1.7557
1.7511
1.7477
2.12
2.14



SOUTH ALABAMA JAGUARS

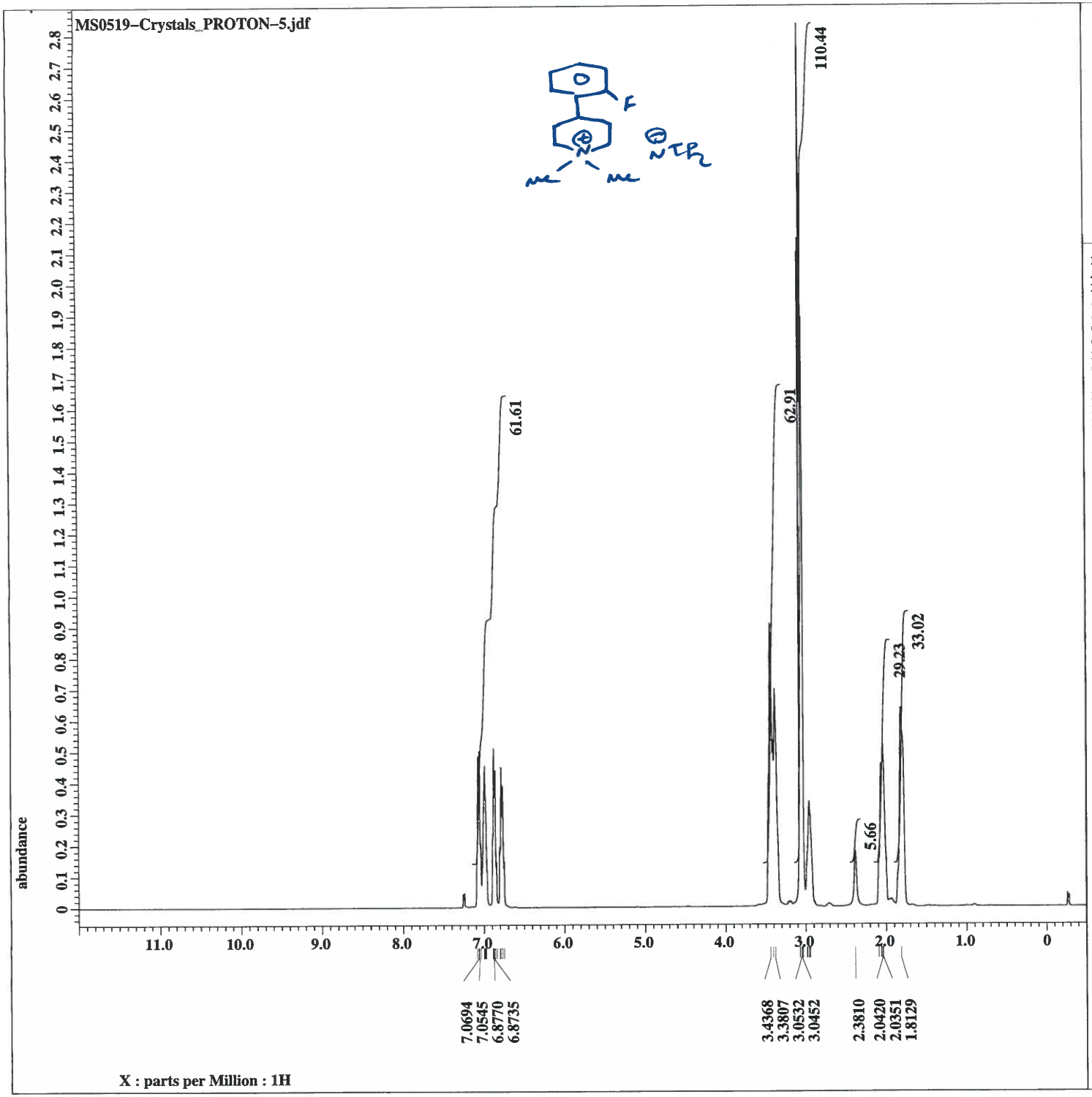
Filename	= MS0501_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0501
Solvent	= CHLOROFORM-D
Changer_sample	= 11
Creation_time	= 5-JUL-2018 16:57:55
Revision_time	= 5-JUL-2018 16:34:26
Current_time	= 5-JUL-2018 16:34:26
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 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	= 256
Total_scans	= 256
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 23.2[dC]


MS0501_CARBON-4.jdf
abundance
3.0
2.0
1.0
0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
142.0037
128.0682
126.4085
126.0365
123.1082
120.5615
118.0052
115.4490
77.2575
77.0000
76.7425
62.2633
55.7963
46.5823
38.1123
29.2512
29.0986
28.9459
26.7998
X : parts per Million : 13C



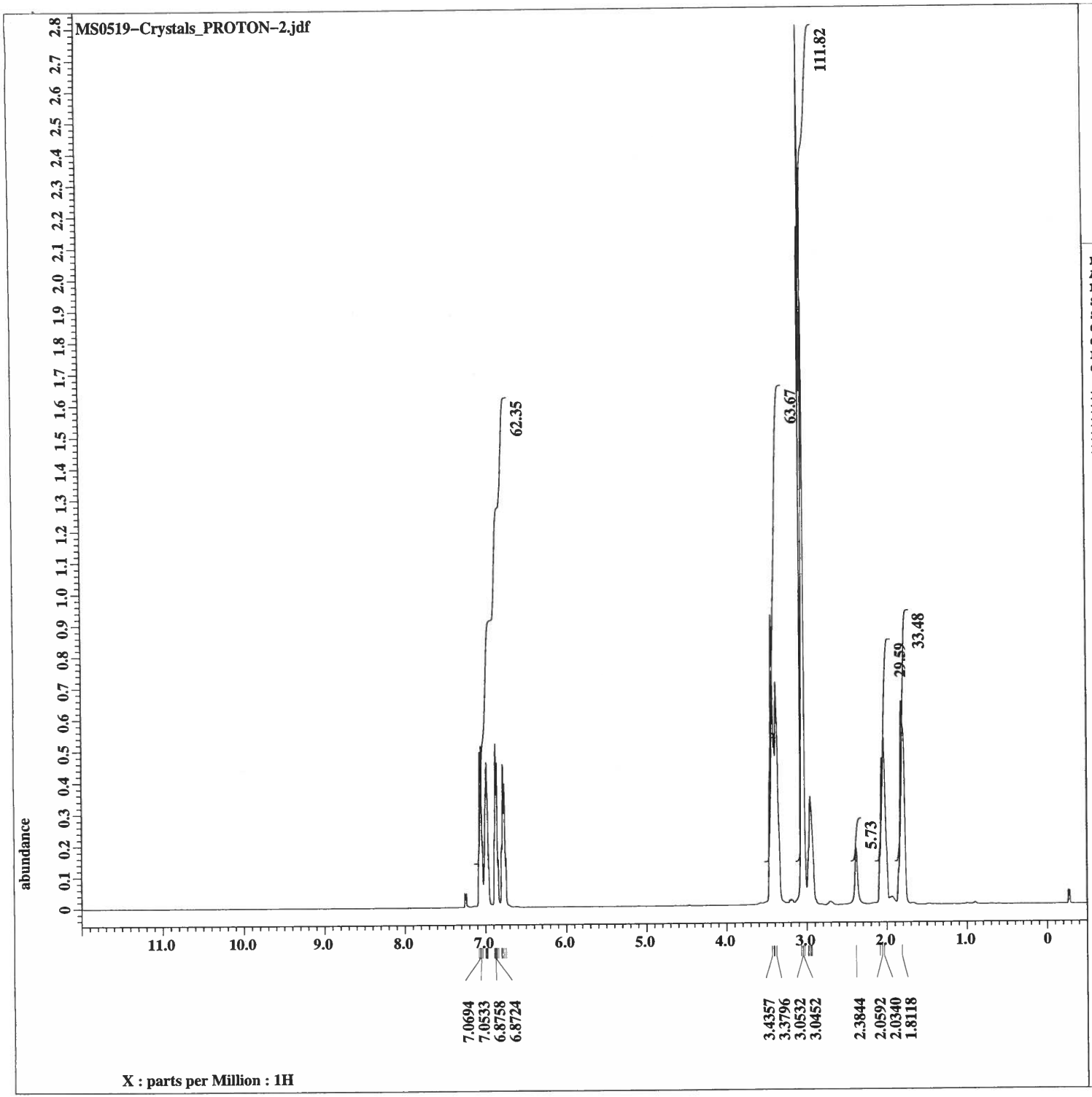
SOUTH ALABAMA JAGUARS

Filename	= MS0501_FLUORINE-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0501
Solvent	= CHLOROFORM-D
Changer_sample	= 11
Creation_time	= 5-JUL-2018 17:00:44
Revision_time	= 5-JUL-2018 16:37:16
Current_time	= 5-JUL-2018 16:37:16
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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 38
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.8[dC]

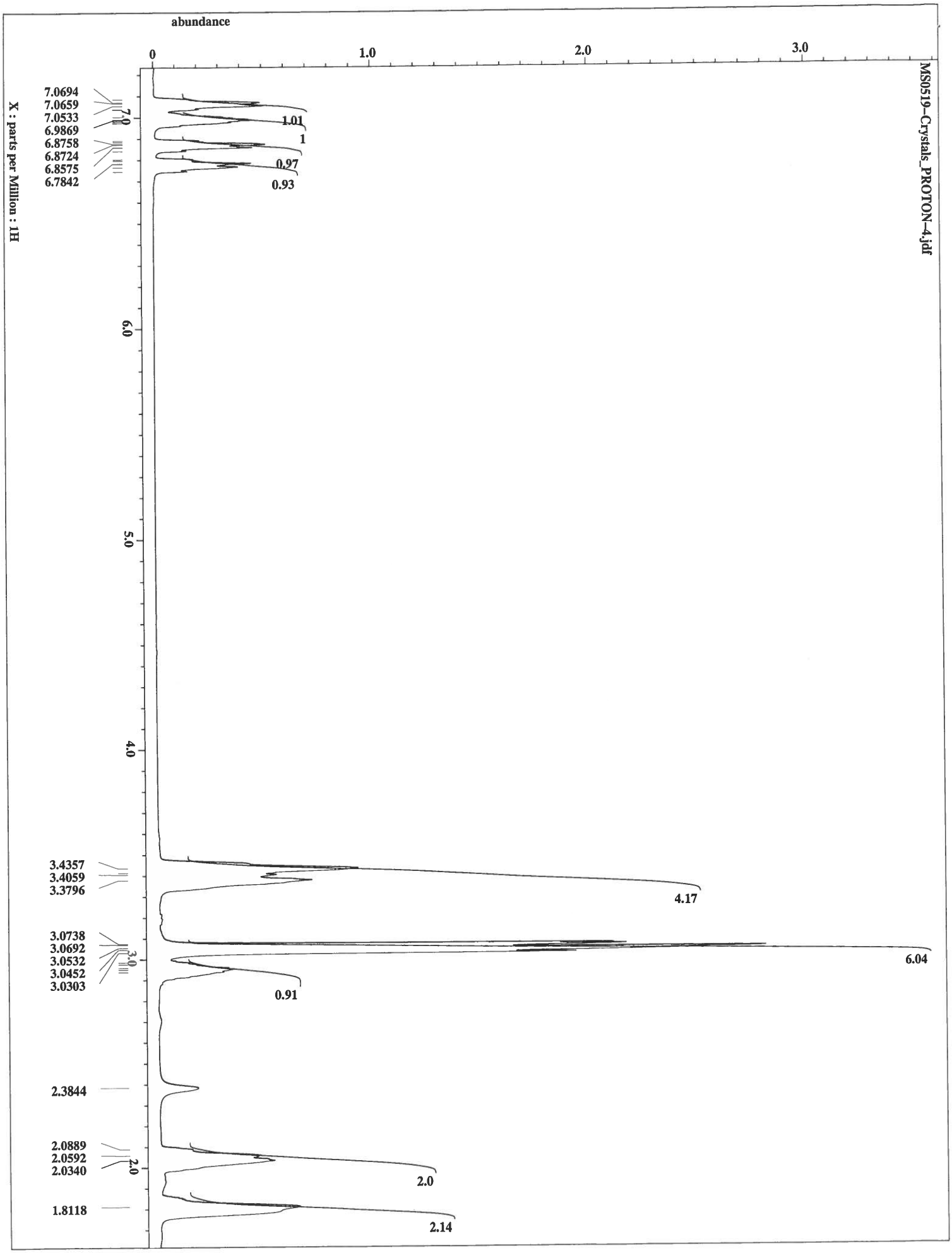


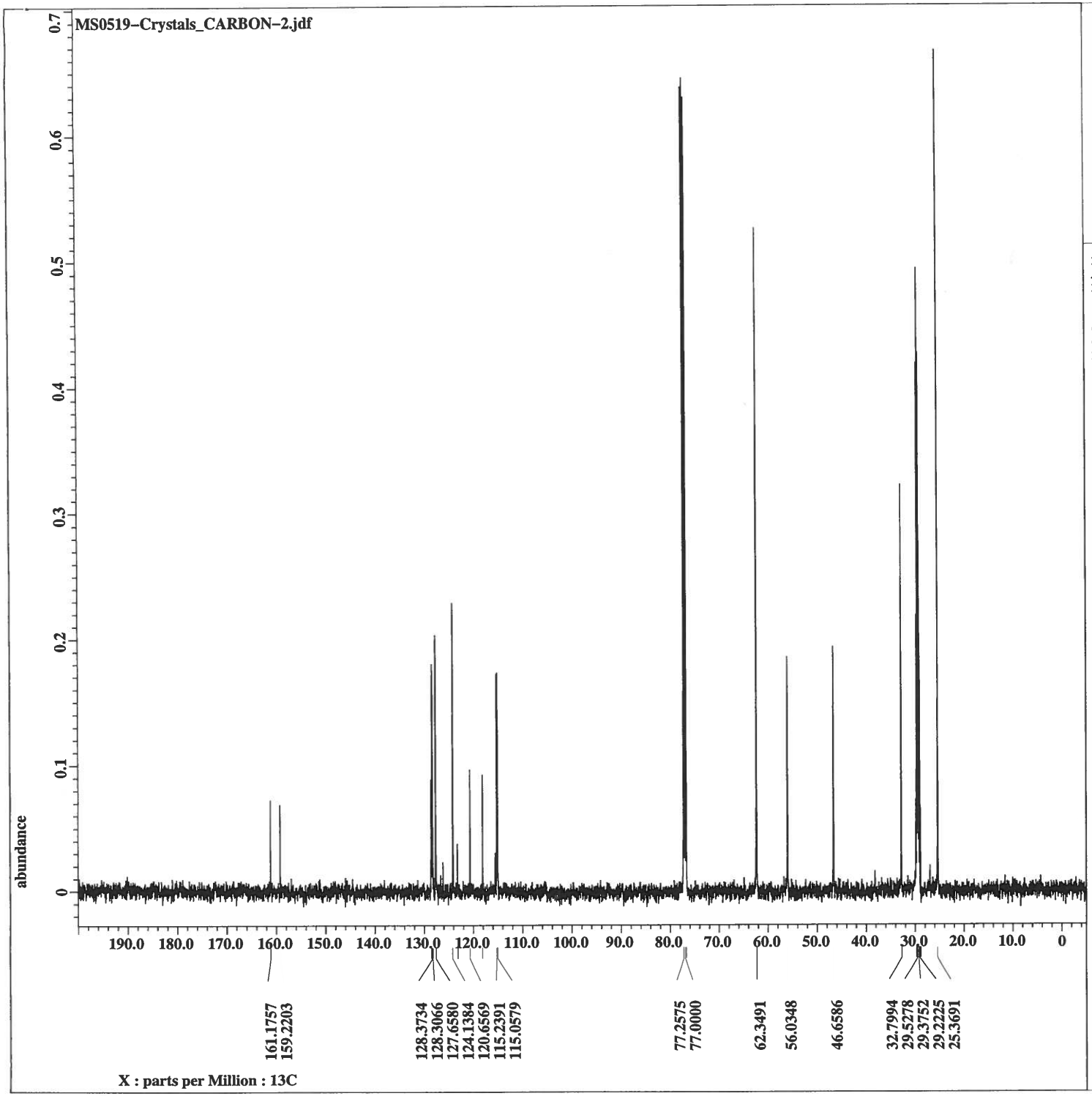
SOUTH ALABAMA JAGUARS

Filename	= MS0519-Crystals_PROTO
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0519-Crystals
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 25-JUL-2018 09:12:03
Revision_time	= 25-JUL-2018 08:48:40
Current_time	= 25-JUL-2018 08:48:40
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	= 50
Total_scans	= 50
X_90_width	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 30
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.4[dC]



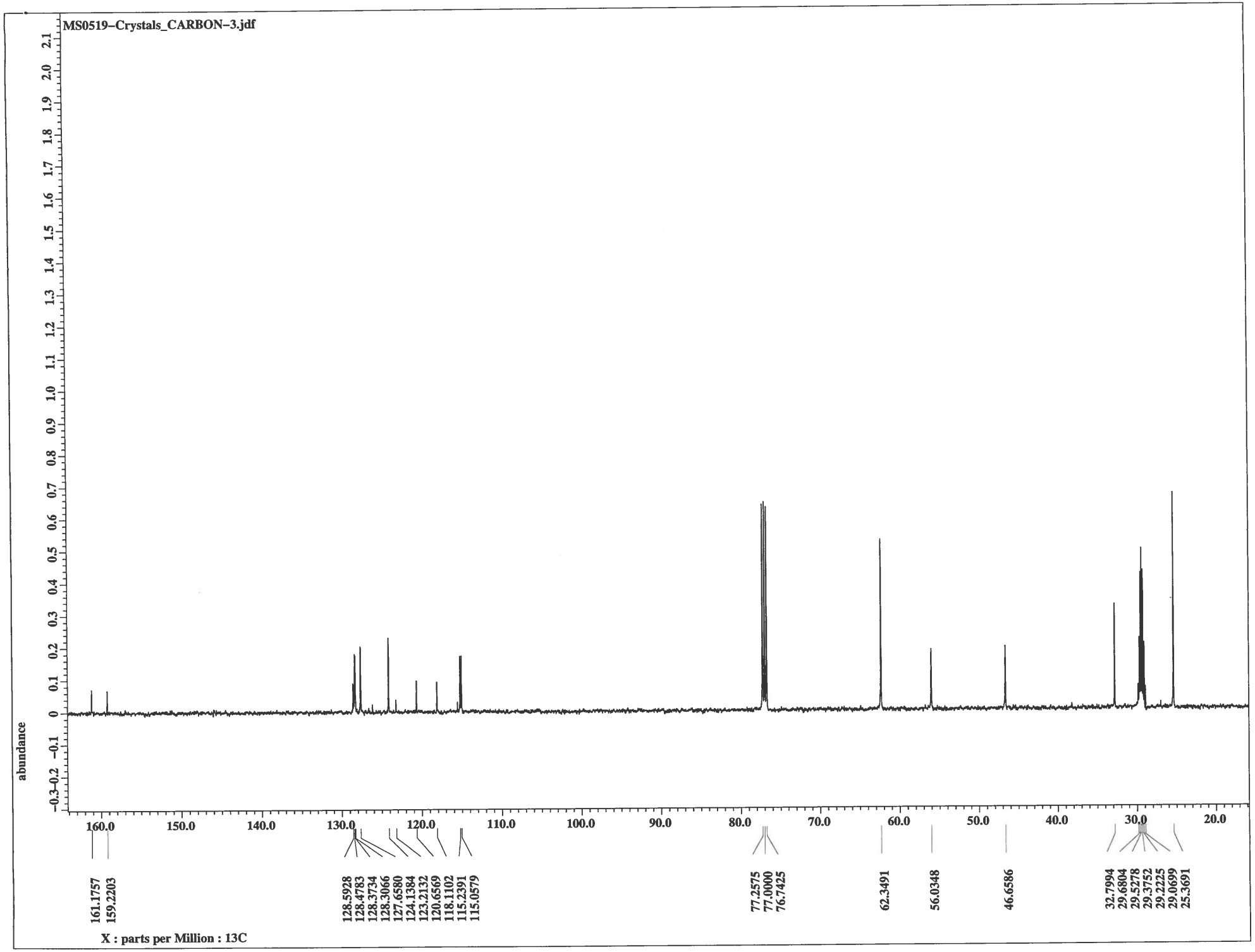
Filename	= MS0519-Crystals_PROTO
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0519-Crystals
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 25-JUL-2018 08:46:11
Revision_time	= 25-JUL-2018 08:22:50
Current_time	= 25-JUL-2018 08:22:50
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 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	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
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[dC]

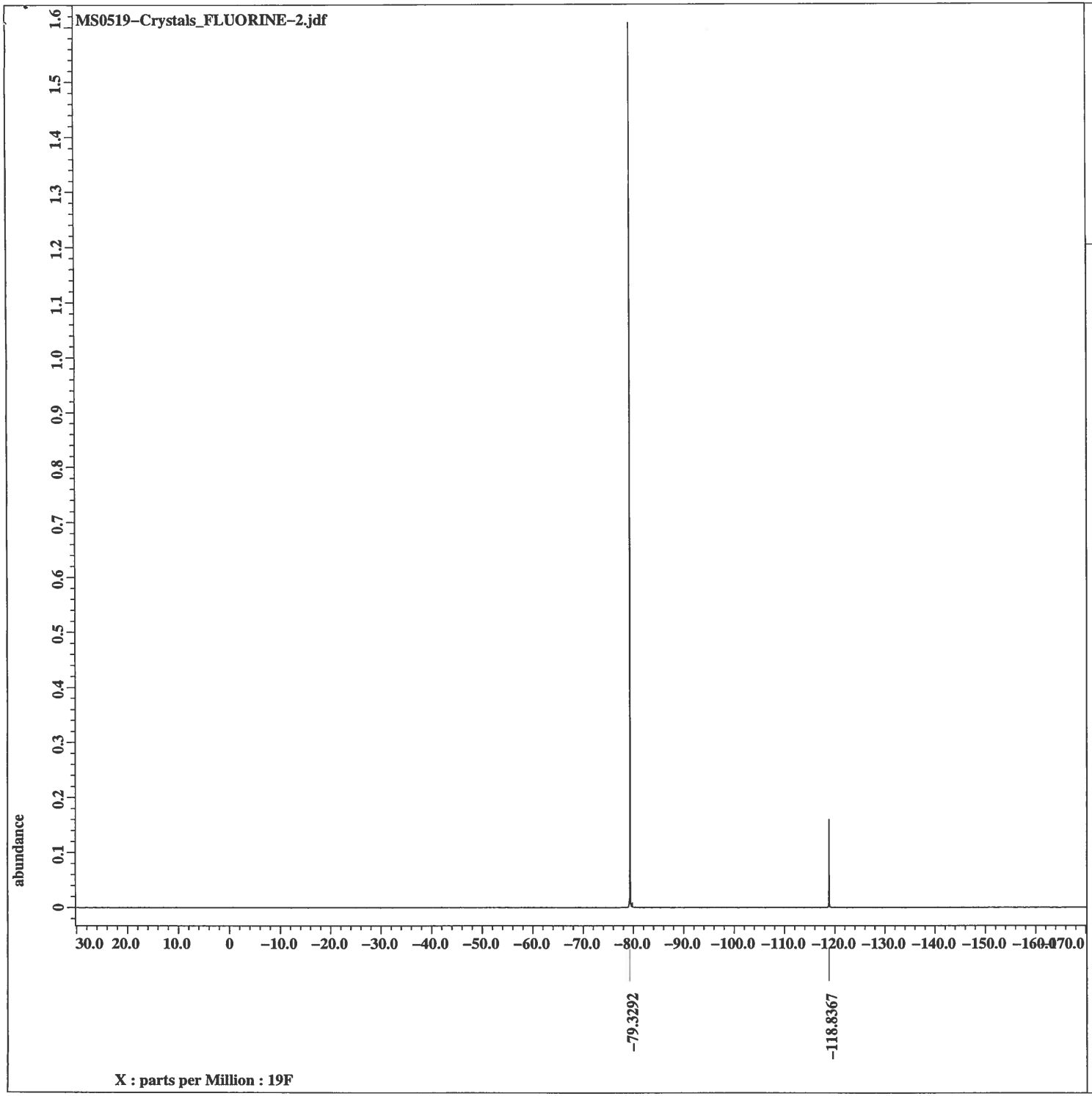

abundance
0
1.0
2.0
3.0
MS0519-Crystals_PROTON-4.jdf
X : parts per Million : 1H
7.0694
7.0659
7.0533
6.9869
6.8758
6.8724
6.8575
6.7842
7.0
1.01
1
0.97
0.93
6.0
5.0
4.0
3.4357
3.4059
3.3796
4.17
3.0738
3.0692
3.0532
3.0452
3.0303
3.0
6.04
0.91
2.3844
2.0889
2.0592
2.0340
2.0
2.0
1.8118
2.14



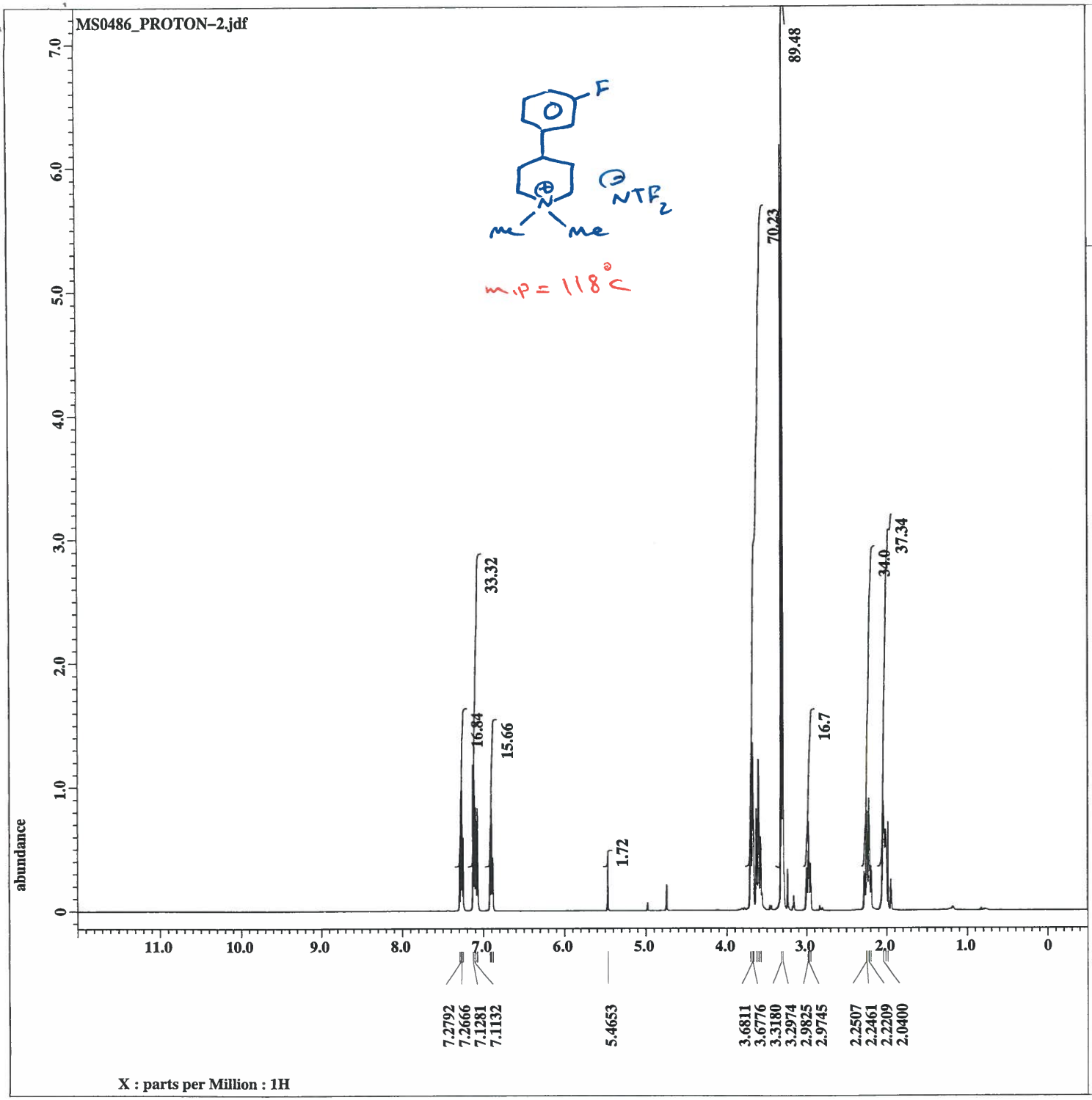
SOUTH ALABAMA JAGUARS

Filename	= MS0519-Crystals_CARBO
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0519-Crystals
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 25-JUL-2018 09:02:33
Revision_time	= 25-JUL-2018 08:39:11
Current_time	= 25-JUL-2018 08:39:11
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	= 300
Total_scans	= 300
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 22.5[dC]


MS0519–Crystals_CARBON–3.jdf
abundance
161.1757
159.2203
128.5928
128.4783
128.3734
128.3066
127.6580
124.1384
123.2132
120.6569
118.1102
115.2391
115.0579
77.2575
77.0000
76.7425
62.3491
56.0348
46.6586
32.7994
29.6804
29.5278
29.3752
29.2225
29.0699
25.3691
X : parts per Million : 13C

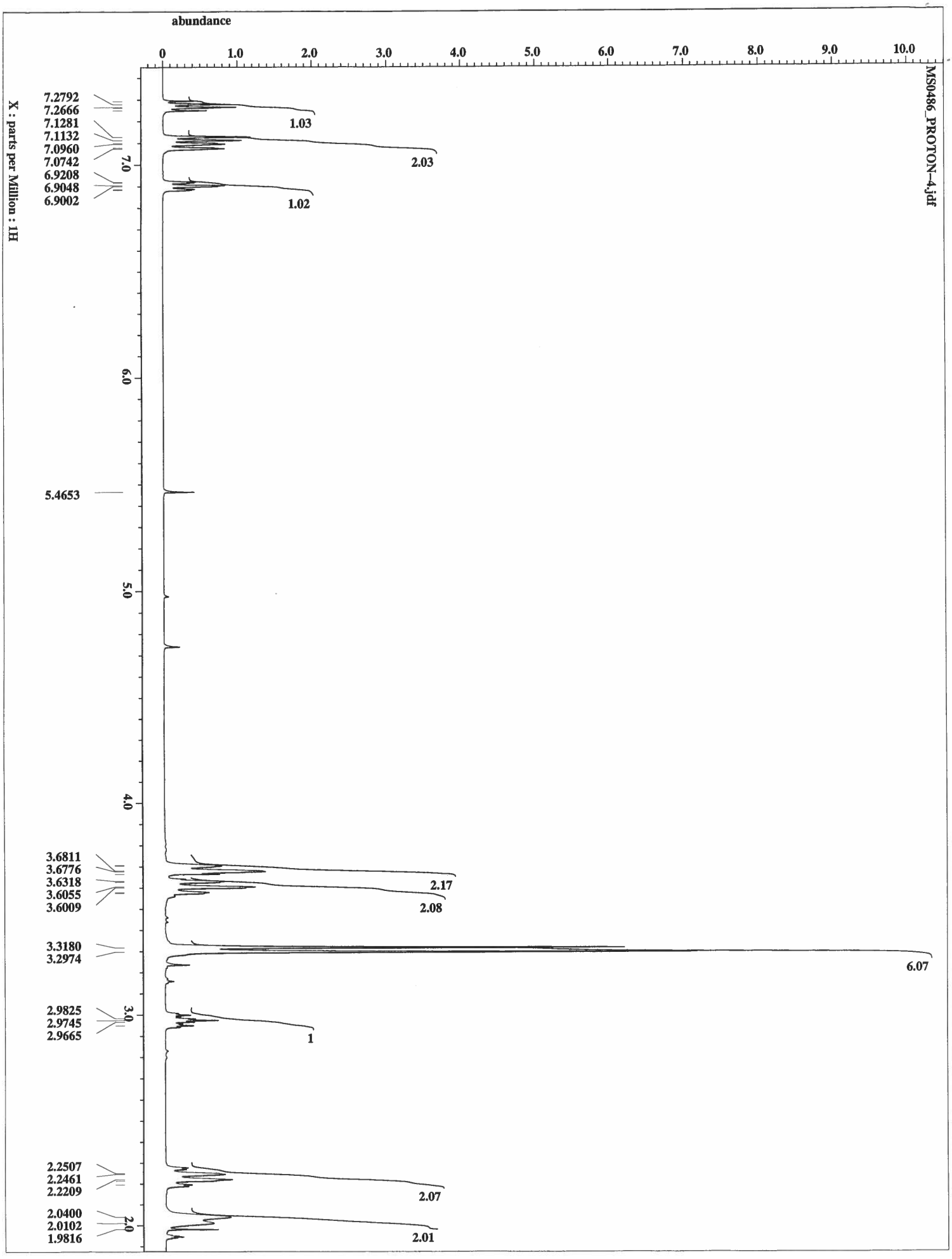


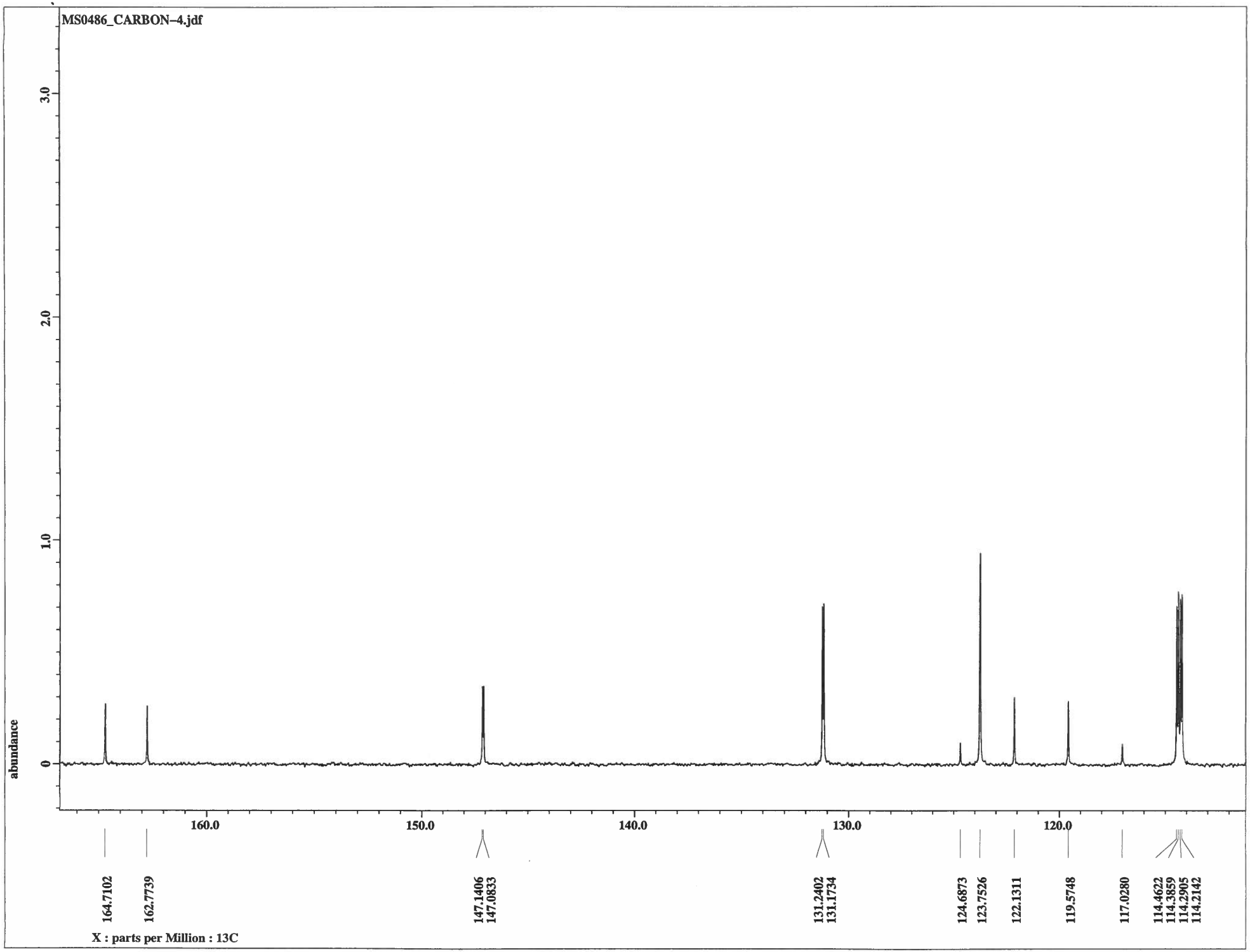
Filename	= MS0519-Crystals_FLUOR
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0519-Crystals
Solvent	= CHLOROFORM-D
Changer_sample	= 6
Creation_time	= 25-JUL-2018 09:05:38
Revision_time	= 25-JUL-2018 08:42:15
Current_time	= 25-JUL-2018 08:42:15
Data_format	= 1D COMPLEX
Dim_size	= 52428
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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.4[dC]

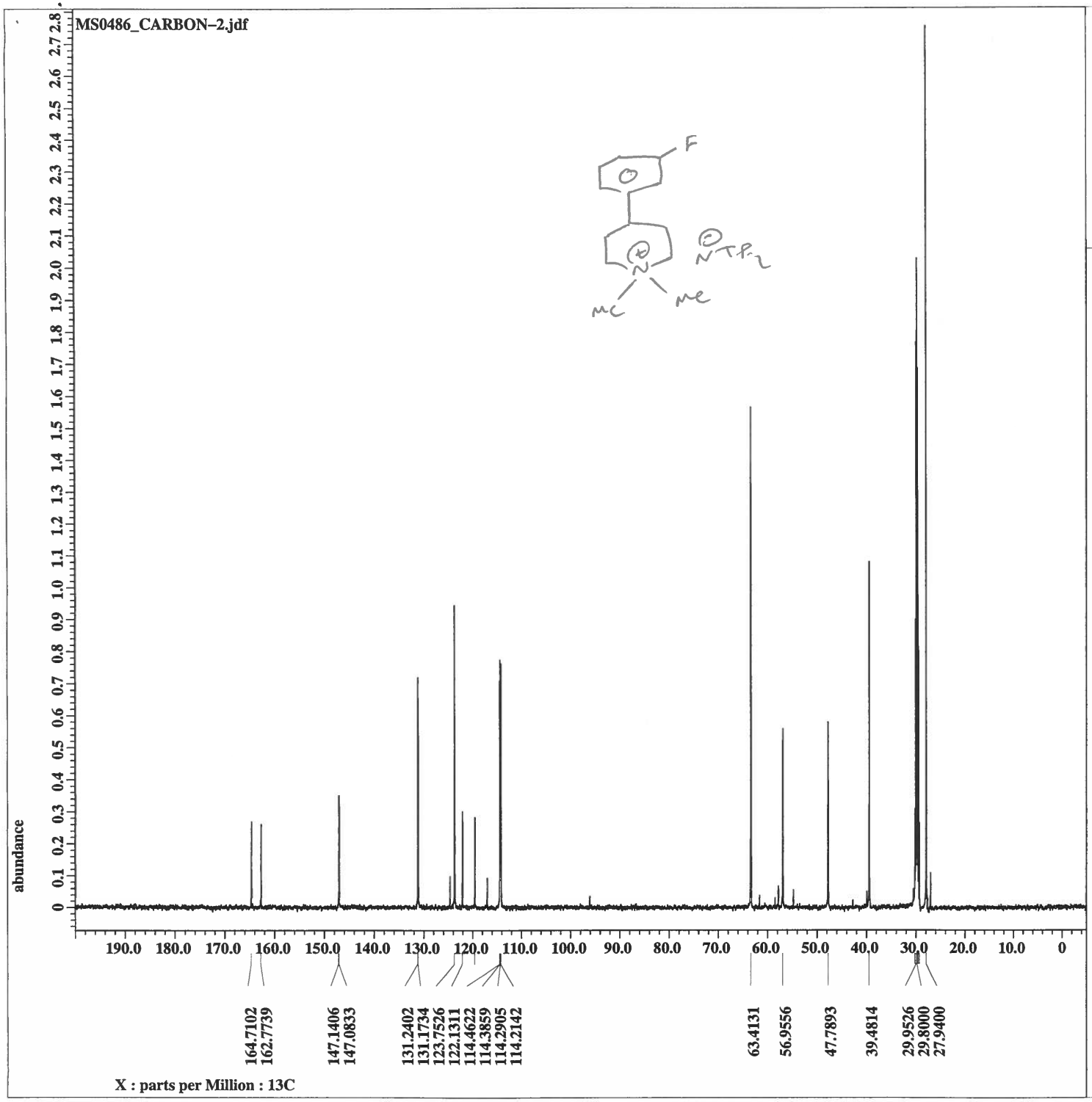


SOUTH ALABAMA JAGUARS

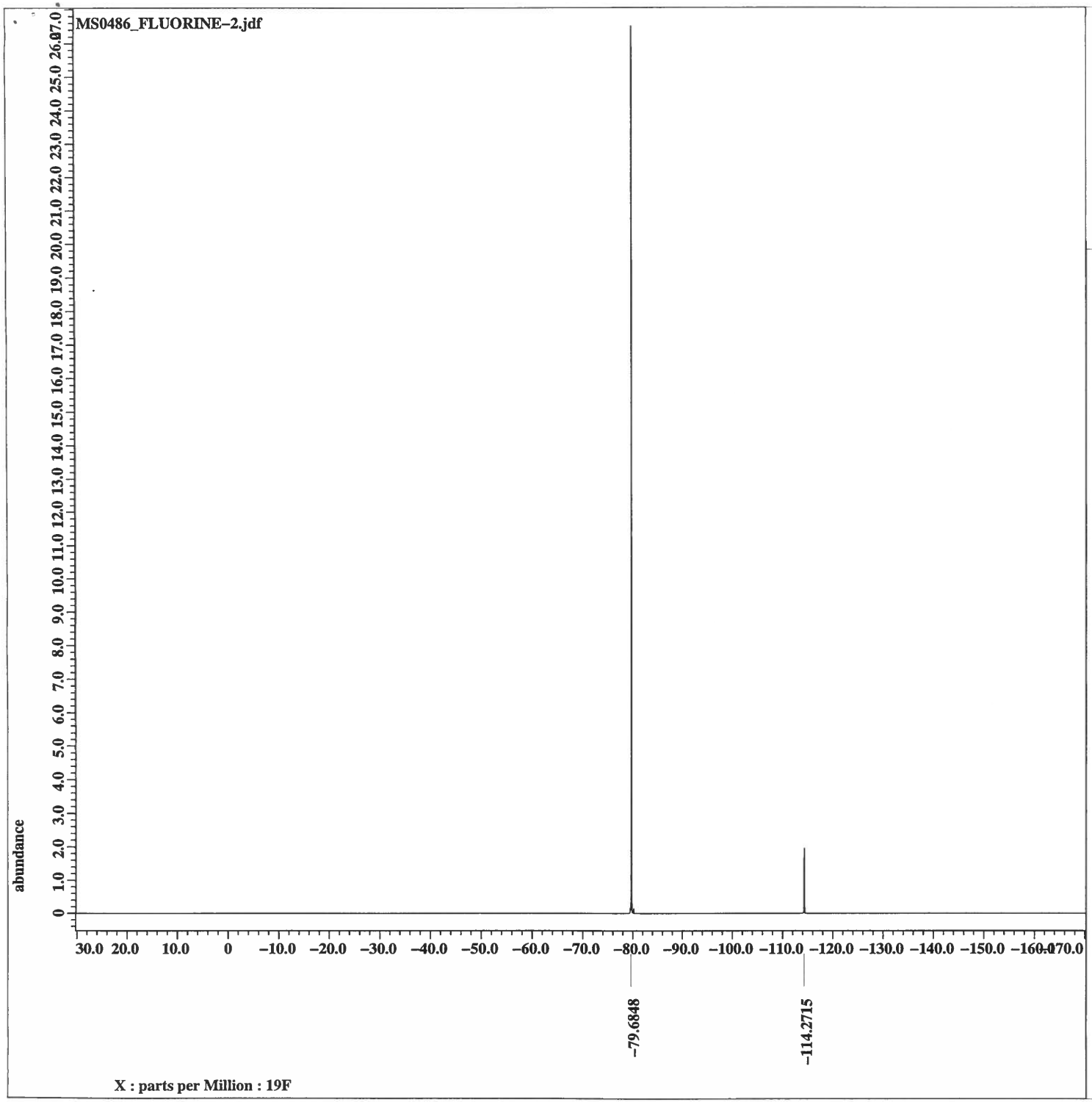
Filename	= MS0486_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0486
Solvent	= ACETONE-D6
Changer_sample	= 11
Creation_time	= 27-JUN-2018 10:42:54
Revision_time	= 27-JUN-2018 10:20:02
Current_time	= 27-JUN-2018 10:20:02
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 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	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 22
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 22.3[dC]


abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
MS0486_PROTON-4.jdf
X : parts per Million : 1H
7.2792
7.2666
7.1281
7.1132
7.0960
7.0742
6.9208
6.9048
6.9002
1.03
2.03
1.02
5.4653
3.6811
3.6776
3.6318
3.6055
3.6009
2.17
2.08
3.3180
3.2974
6.07
2.9825
2.9745
2.9665
1
2.2507
2.2461
2.2209
2.07
2.0400
2.0102
1.9816
2.01


MS0486_CARBON-4.jdf
abundance
3.0
2.0
1.0
0
160.0
150.0
140.0
130.0
120.0
164.7102
162.7739
147.1406
147.0833
131.2402
131.1734
124.6873
123.7526
122.1311
119.5748
117.0280
114.4622
114.3859
114.2905
114.2142
X : parts per Million : 13C

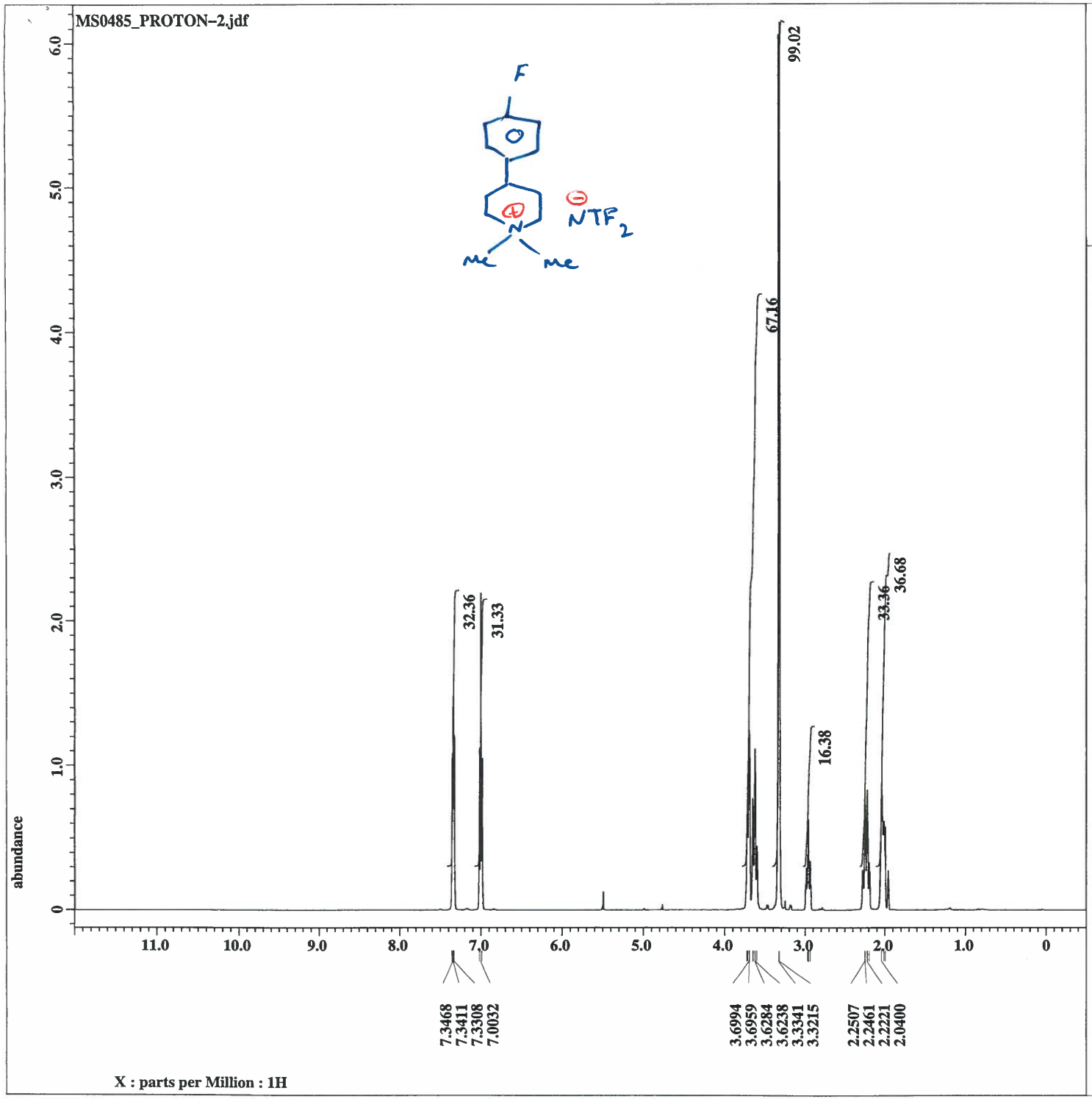


Filename	= MS0486_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0486
Solvent	= ACETONE-D6
Changer_sample	= 11
Creation_time	= 27-JUN-2018 10:57:27
Revision_time	= 27-JUN-2018 10:34:33
Current_time	= 27-JUN-2018 10:34:33
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 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	= 256
Total_scans	= 256
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 22.8[dC]



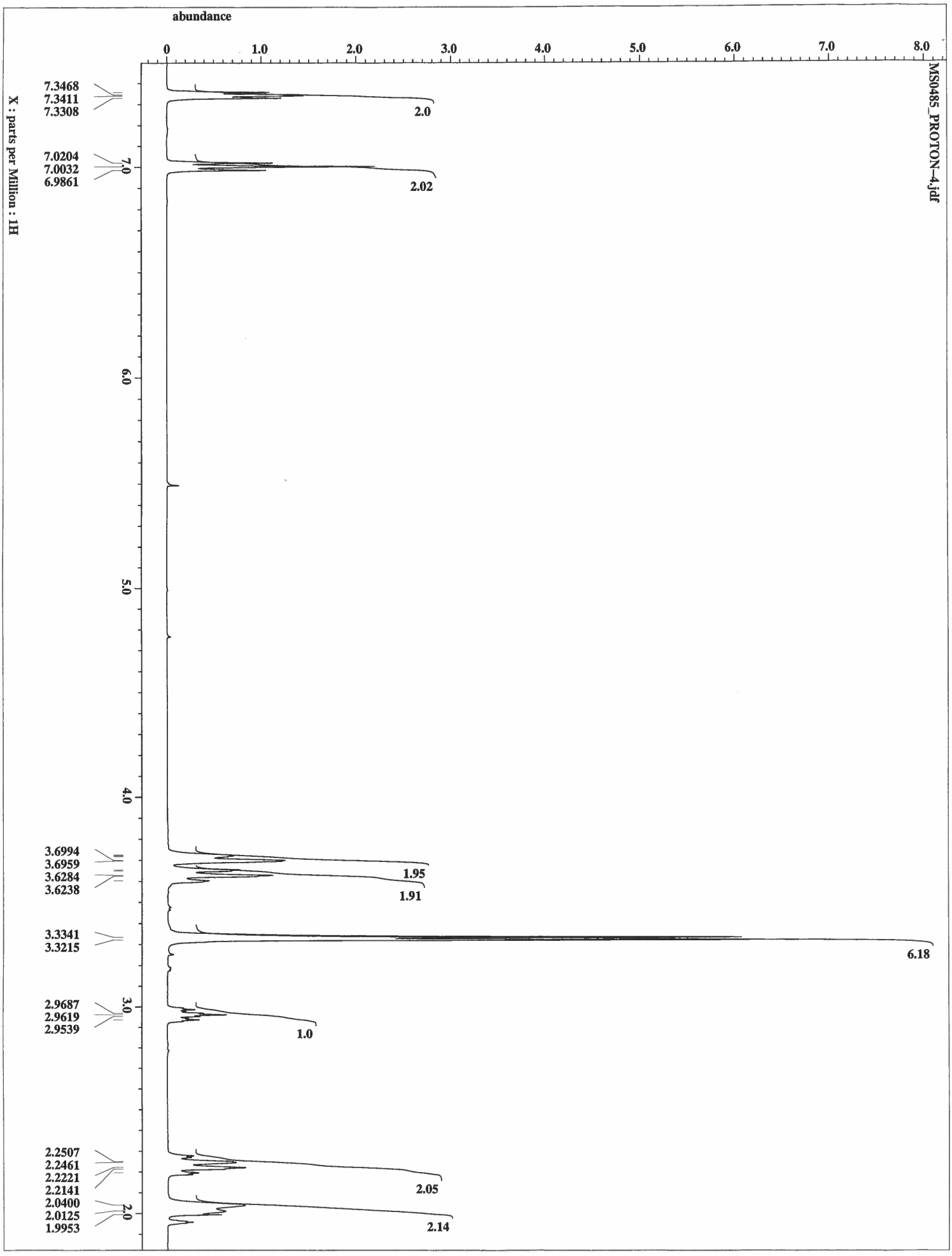
SOUTH ALABAMA JAGUARS

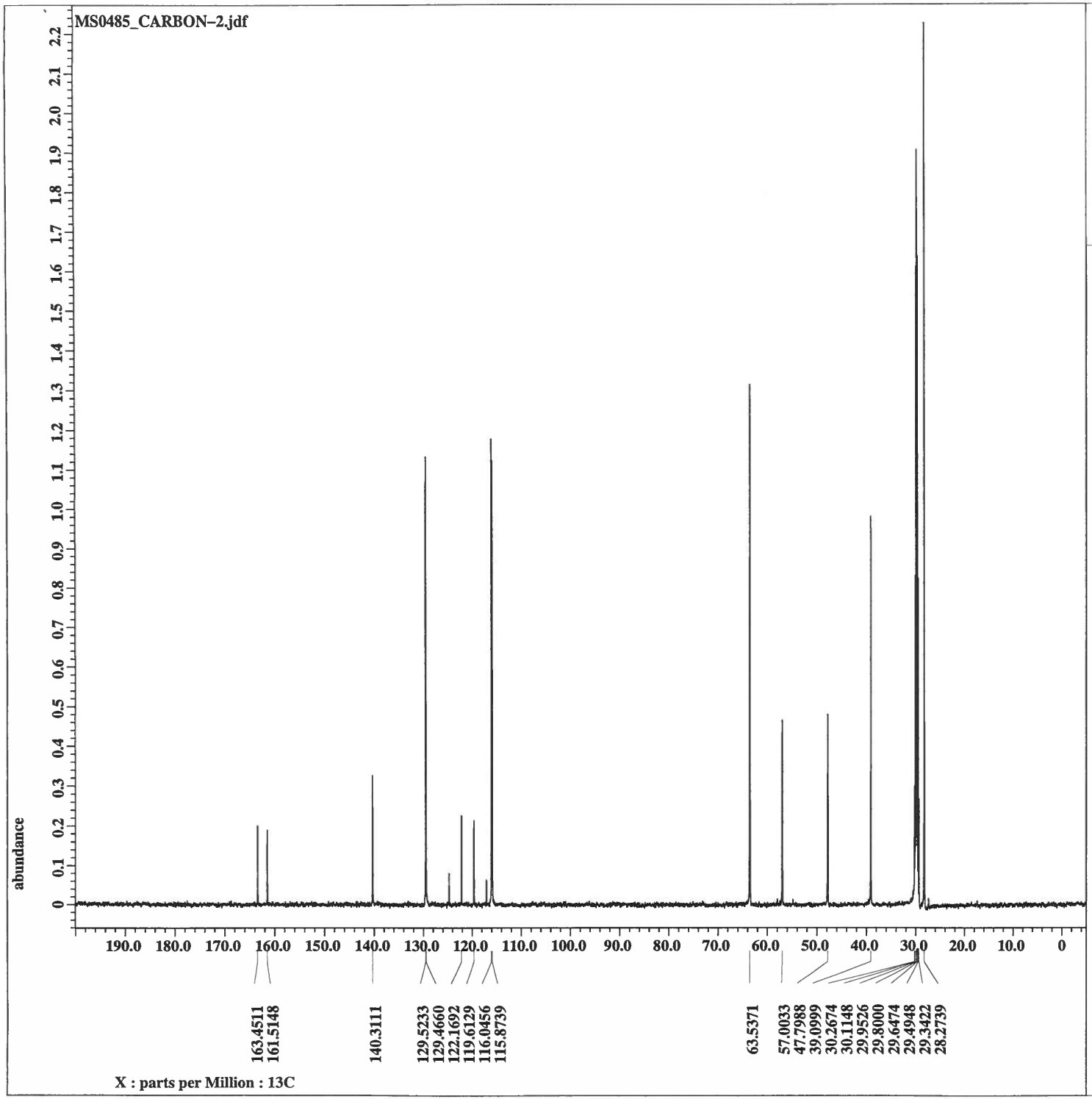
Filename	= MS0486_FLUORINE-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0486
Solvent	= ACETONE-D6
Changer_sample	= 11
Creation_time	= 27-JUN-2018 10:39:16
Revision_time	= 27-JUN-2018 10:16:23
Current_time	= 27-JUN-2018 10:16:24
Data_format	= 1D COMPLEX
Dim_size	= 52428
Dim_title	= 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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 30
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.3[dC]



SOUTH ALABAMA JAGUARS

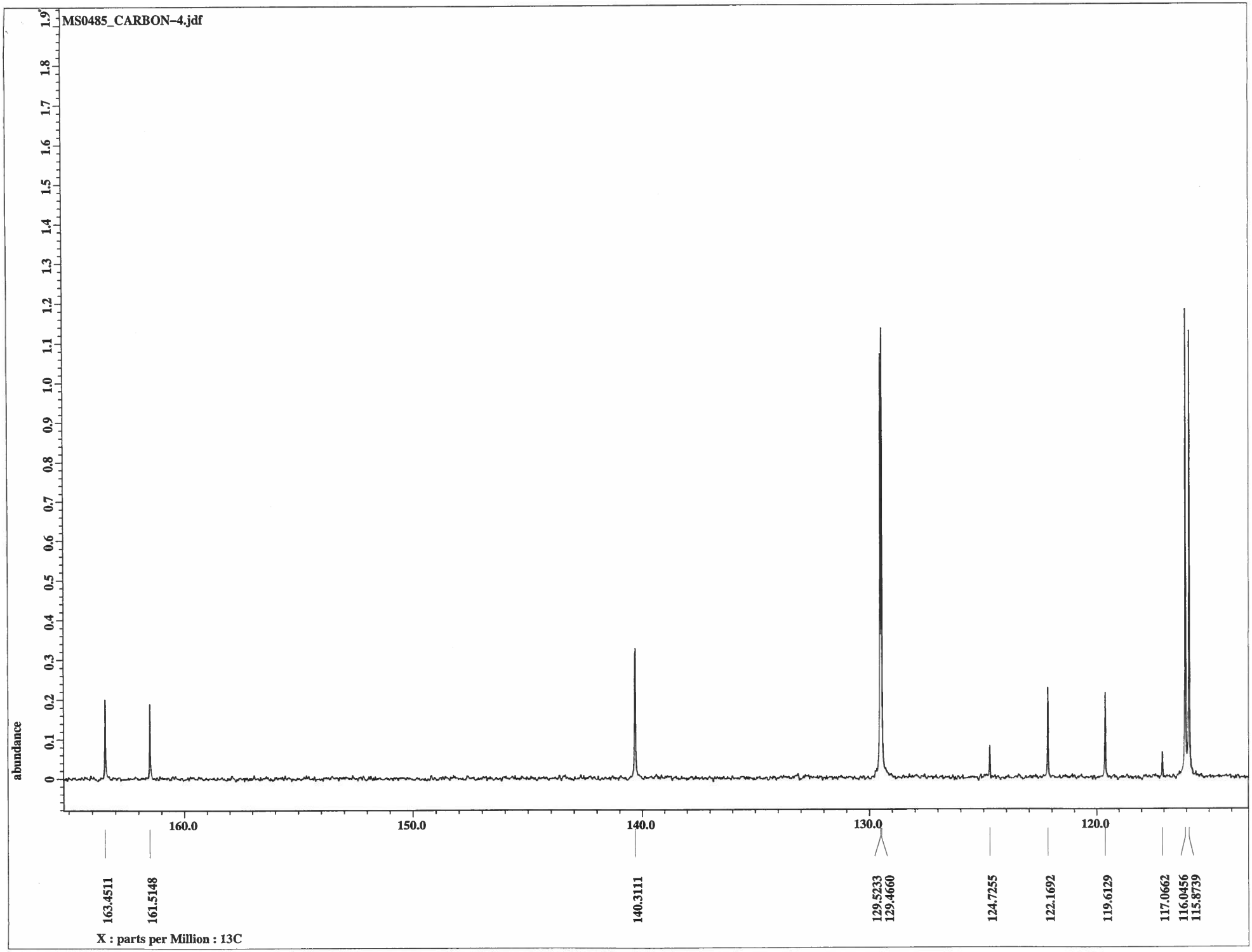
Filename	= MS0485_PROTON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0485
Solvent	= ACETONE-D6
Changer_sample	= 12
Creation_time	= 27-JUN-2018 11:38:17
Revision_time	= 27-JUN-2018 11:15:23
Current_time	= 27-JUN-2018 11:15:23
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
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	= 12.4[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.2[us]
Irr_mode	= Off
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]

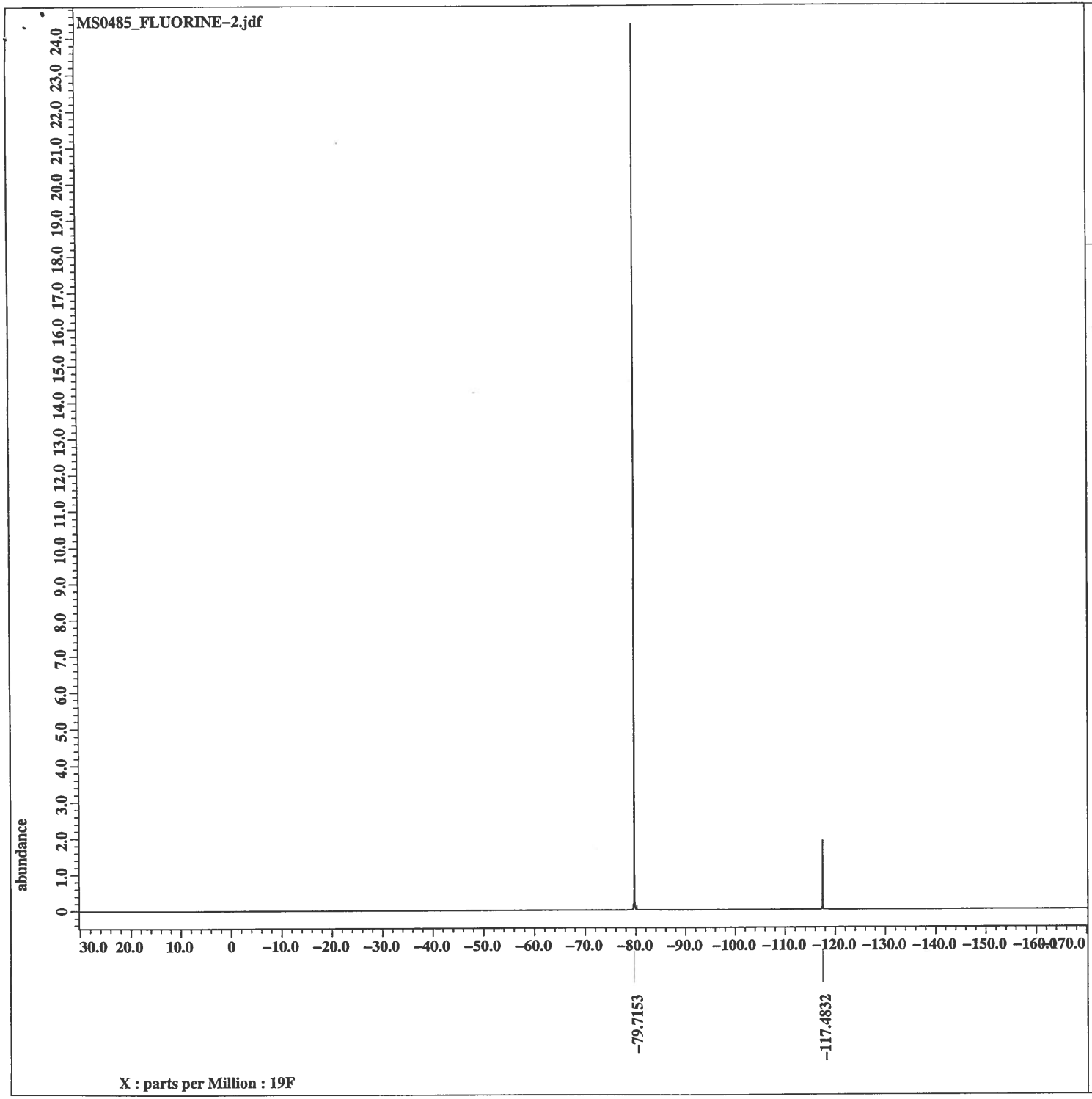

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
MS0485_PROTON-4.jdf
X : parts per Million : 1H
7.3468
7.3411
7.3308
2.0
7.0204
7.0032
6.9861
2.02
7.0
6.0
5.0
4.0
3.6994
3.6959
3.6284
3.6238
1.95
1.91
3.3341
3.3215
6.18
2.9687
2.9619
2.9539
1.0
3.0
2.2507
2.2461
2.2221
2.2141
2.05
2.0400
2.0125
1.9953
2.14
2.0



SOUTH ALABAMA JAGUARS

Filename	= MS0485_CARBON-2.jdf
Author	= Jim Davis
Experiment	= single_pulse_dec
Sample_id	= MS0485
Solvent	= ACETONE-D6
Changer_sample	= 12
Creation_time	= 27-JUN-2018 11:59:25
Revision_time	= 27-JUN-2018 11:36:31
Current_time	= 27-JUN-2018 11:36:31
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 400
Total_scans	= 400
X_90_width	= 13.2[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 6[dB]
X_pulse	= 4.4[us]
Irr_atn_dec	= 20.7[dB]
Irr_atn_noe	= 20.7[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 22.9[dC]


MS0485_CARBON-4.jdf
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
160.0
150.0
140.0
130.0
120.0
163.4511
161.5148
140.3111
129.5233
129.4660
124.7255
122.1692
119.6129
117.0662
116.0456
115.8739
X : parts per Million : 13C



SOUTH ALABAMA JAGUARS

Filename	= MS0485_FLUORINE-2.jdf
Author	= Jim Davis
Experiment	= single_pulse.ex2
Sample_id	= MS0485
Solvent	= ACETONE-D6
Changer_sample	= 12
Creation_time	= 27-JUN-2018 11:34:58
Revision_time	= 27-JUN-2018 11:12:05
Current_time	= 27-JUN-2018 11:12:05
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	= 13.1[us]
X_acq_time	= 0.55574528[s]
X_angle	= 45[deg]
X_atn	= 2.5[dB]
X_pulse	= 6.55[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 34
Relaxation_delay	= 4[s]
Repetition_time	= 4.55574528[s]
Temp_get	= 22.3[dC]

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait **. . . .**

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) JD_POP_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: JD_POP_0m

Bond precision: C-C = 0.0046 A Wavelength=1.54178

Cell: a=18.1884(8) b=9.1975(4) c=18.6788(7)
alpha=90 beta=90 gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	3124.7(2)	3124.7(2)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C30 H24 O P, C2 F6 N O4 S2	C30 H24 O P, C2 F6 N O4 S2
Sum formula	C32 H24 F6 N O5 P S2	C32 H24 F6 N O5 P S2
Mr	711.61	711.61
Dx,g cm-3	1.513	1.513
Z	4	4
Mu (mm-1)	2.739	2.739
F000	1456.0	1456.0
F000'	1464.89	
h,k,lmax	23,11,23	23,11,23
Nref	6873[3547]	5537
Tmin,Tmax	0.663,0.826	0.535,0.754
Tmin'	0.536	

Correction method= # Reported T Limits: Tmin=0.535 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 1.56/0.81 Theta(max)= 80.721

R(reflections)= 0.0303(5354) wR2(reflections)= 0.0813(5537)

S = 1.092 Npar= 561

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ..... 6.24 Note
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0046 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 10 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 5 Note
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 61 %

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 30 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 30 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 2 11.74 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 3 3.25 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O4B ..C3 2.87 Ang.
x,y,z = 1_555 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 532 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 33 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 7 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
14 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

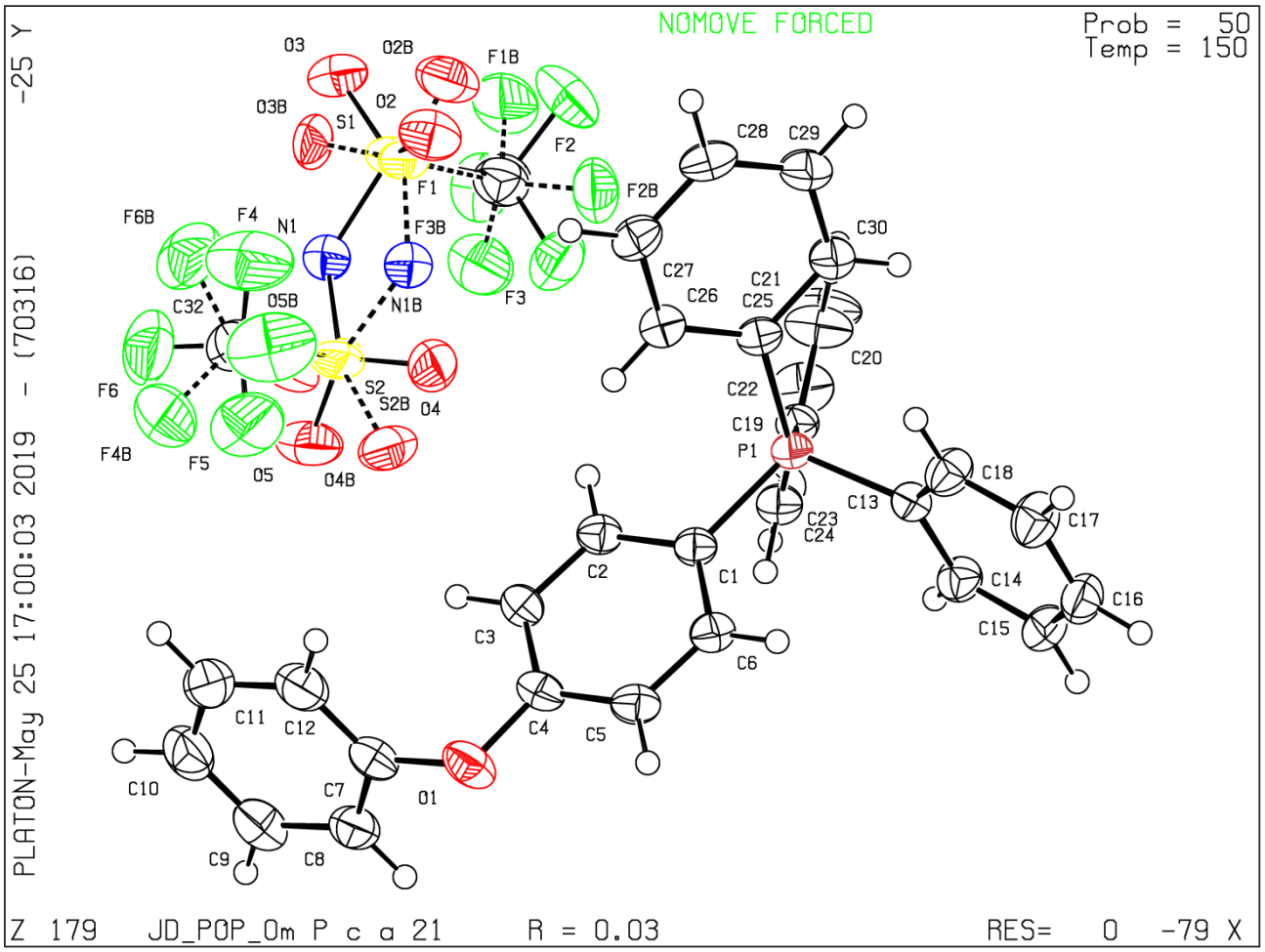
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 03/05/2019; check.def file version of 29/04/2019

Datablock JD_POP_0m - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait .....

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) JD_POP_MF_0m_5

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No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: JD_POP_MF_0m_5

Bond precision: C-C = 0.0040 A Wavelength=0.71073
Cell: a=18.0534(13) b=19.0695(14) c=20.2712(15)
alpha=90 beta=114.239(3) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	6363.5(8)	6363.5(8)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C30 H23 F O P, C2 F6 N O4 S2	C30 H23 F O P, C2 F6 N O4 S2
Sum formula	C32 H23 F7 N O5 P S2	C32 H23 F7 N O5 P S2
Mr	729.60	729.60
Dx,g cm-3	1.523	1.523
Z	8	8
Mu (mm-1)	0.302	0.302
F000	2976.0	2976.0
F000'	2980.76	
h,k,lmax	26,28,29	26,28,29
Nref	21348	20359
Tmin,Tmax	0.871,0.962	0.400,0.746
Tmin'	0.865	

Correction method= # Reported T Limits: Tmin=0.400
Tmax=0.746 AbsCorr = MULTI-SCAN
Data completeness= 0.954 Theta(max)= 31.592
R(reflections)= 0.0534(11965) wR2(reflections)= 0.1450(20359)
S = 1.021 Npar= 1152

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 10 Note

```
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         58 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          7 Note
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Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         68 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         45 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records          3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F1B      --C5       .        6.1 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C61 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C62 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S3         Constrained at        0.5 Check
And 14 other PLAT300 Alerts

PLAT300_ALERT_4_G Atom Site Occupancy of S4         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F9         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F10        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F11        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F12        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F13        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F14        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O7         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O8         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O9         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O10        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C63        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C64        Constrained at        0.5 Check

PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )          3% Note
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  2  )          3% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
And 2 other PLAT302 Alerts

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       100% Note

PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  4          7.50 Check
And 2 other PLAT304 Alerts

PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  5          4.80 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  6          2.70 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact  O12B     ..C6              2.90 Ang.
                                                    x,y,z  =      1_555 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         45 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       786 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       1245 Note
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 0 0 1)         Est.d BASF       0.16 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          3 Note
```

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  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
  4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 39 ALERT level G = General information/check it is not something unexpected

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  8 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
 28 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should

normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

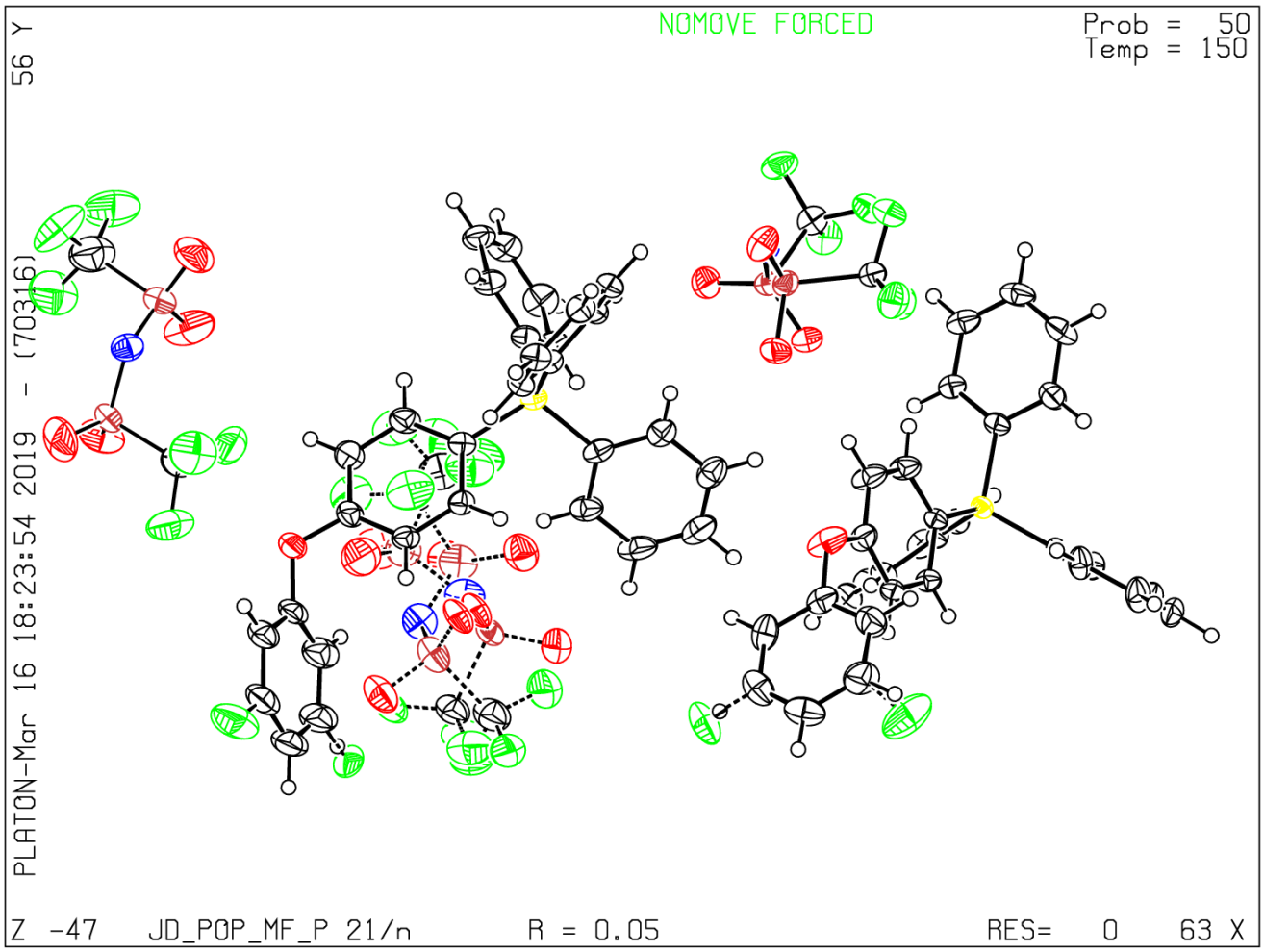
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 18/02/2019; check.def file version of 18/02/2019

Datablock JD_POP_MF_0m_5 - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . . . . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) JD_POP_OF_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: JD_POP_OF_0m

Bond precision: C-C = 0.0026 A Wavelength=0.71073
Cell: a=18.0015(14) b=18.7263(15) c=18.8837(16)
alpha=90 beta=90 gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	6365.7(9)	6365.7(9)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C30 H23 F O P, C2 F6 N O4 S2	C30 H23 F O P, C2 F6 N O4 S2
Sum formula	C32 H23 F7 N O5 P S2	C32 H23 F7 N O5 P S2
Mr	729.60	729.60
Dx,g cm-3	1.523	1.523
Z	8	8
Mu (mm-1)	0.301	0.301
F000	2976.0	2976.0
F000'	2980.76	
h,k,lmax	27,28,29	27,28,29
Nref	12223	12152
Tmin,Tmax	0.855,0.939	0.689,0.747
Tmin'	0.855	

Correction method= # Reported T Limits: Tmin=0.689
Tmax=0.747 AbsCorr = MULTI-SCAN
Data completeness= 0.994 Theta(max)= 33.230
R(reflections)= 0.0579(8861) wR2(reflections)= 0.1854(12152)
S = 1.046 Npar= 579

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT430_ALERT_2_B Short Inter D...A Contact O1 ..O1 . 2.76 Ang.
1-x,-y,1-z = 5_656 Check

Alert level C

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -2.090 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 30 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 30 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for F1 --C2 . 6.4 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 3% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 2 12.68 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 3 2.32 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O5B ..C16 2.95 Ang.
1/2+x,y,1/2-z = 6_656 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 513 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 67 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 9 Info

---

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0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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6 ALERT type 3 Indicator that the structure quality may be low
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1 ALERT type 5 Informative message, check

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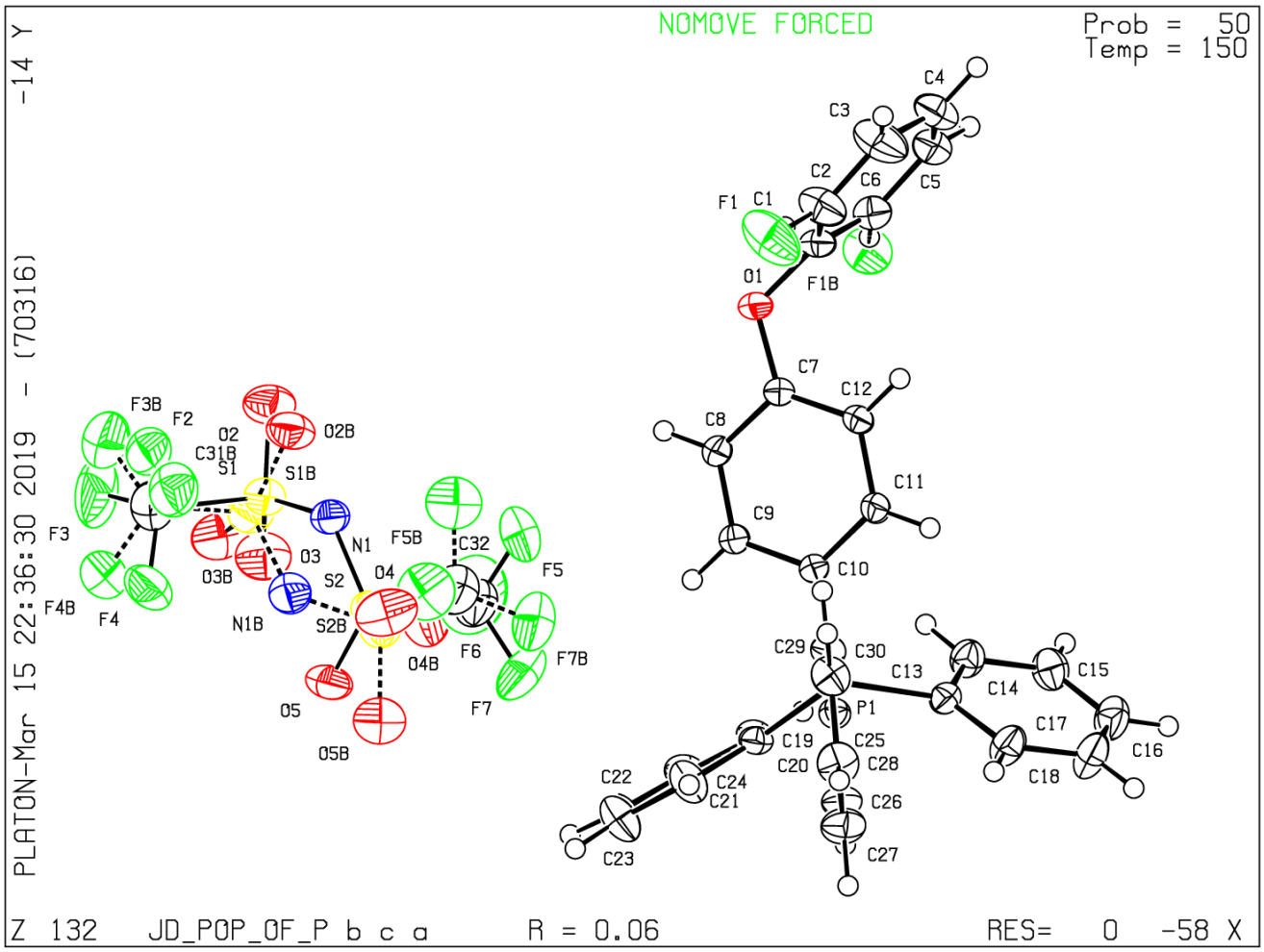
PLATON version of 18/02/2019; check.def file version of 18/02/2019

Datablock JD_POP_OF_0m - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait .....

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) JD_POP_PF_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Structure factor report

Datablock: JD_POP_PF_0m

Bond precision: C-C = 0.0024 A Wavelength=0.71073

Cell: a=9.5981(8) b=13.6324(11) c=22.2398(18)
alpha=102.938(3) beta=92.159(3) gamma=109.211(3)

Temperature: 150 K

	Calculated	Reported
Volume	2658.5(4)	2658.5(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H19 F P, C2 F6 N O4 S2	C24 H19 F P, C2 F6 N O4 S2
Sum formula	C26 H19 F7 N O4 P S2	C26 H19 F7 N O4 P S2
Mr	637.50	637.51
Dx,g cm-3	1.593	1.593
Z	4	4
Mu (mm-1)	0.345	0.345
F000	1296.0	1296.0
F000'	1298.27	
h,k,lmax	13,19,32	13,19,32
Nref	17132	16986
Tmin,Tmax	0.921,0.973	0.694,0.746
Tmin'	0.921	

Correction method= # Reported T Limits: Tmin=0.694
Tmax=0.746 AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 31.139

R(reflections)= 0.0440(12700) wR2(reflections)= 0.1276(16986)

S = 1.035 Npar= 1073

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT214_ALERT_2_C Atom C51B (Anion/Solvent) ADP max/min Ratio 4.3 oblate
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.746 Check

```
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          6 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         36 Report
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         76 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         60 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.003 Degree
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records          3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F2       --C28      .        5.1 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    S3       --C51      .        6.2 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         4% Note
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  2  )         4% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       100% Note
And 3 other PLAT302 Alerts

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       100% Note

PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  3         14.25 Check
And 3 other PLAT304 Alerts

PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  4         13.05 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  5          0.75 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  6          1.95 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact  O3       ..C39             3.01 Ang.
                                             x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F1C      ..C3              2.93 Ang.
                                           -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F5B      ..C39             2.89 Ang.
                                          2-x,2-y,1-z  =      2_776 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1B      ..C11             2.82 Ang.
                                          1-x,1-y,1-z  =      2_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1B      ..C12             2.90 Ang.
                                          1-x,1-y,1-z  =      2_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2B      ..C9              2.91 Ang.
                                          2-x,1-y,1-z  =      2_766 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O5B      ..C47             2.85 Ang.
                                            1+x,y,z  =      1_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O6B      ..C26             2.89 Ang.
                                           1-x,1-y,-z  =      2_665 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      1242 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       103 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         12 Info
```

```
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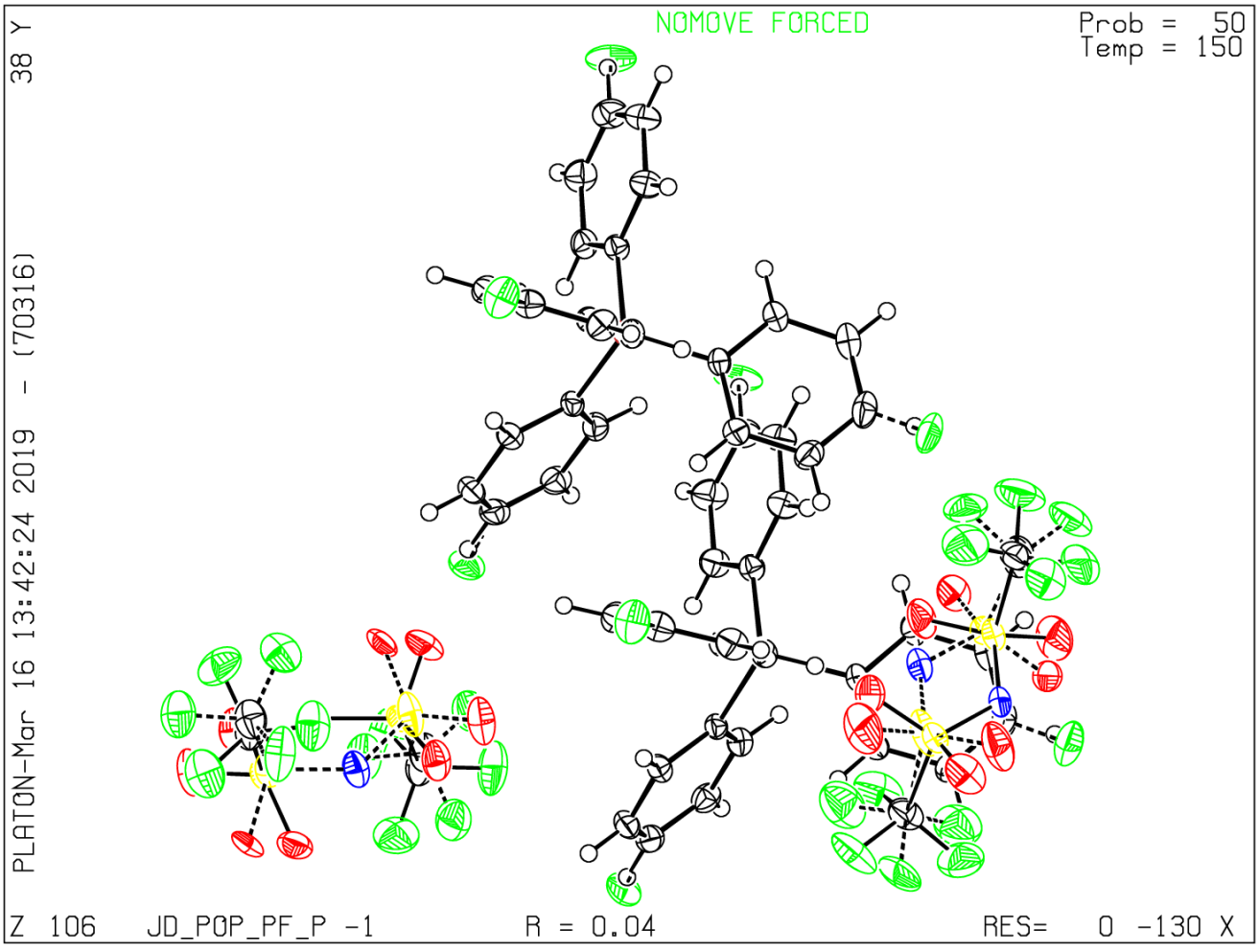
PLATON version of 18/02/2019; check.def file version of 18/02/2019

Datablock JD_POP_PF_0m - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC

Test a new CIF entry

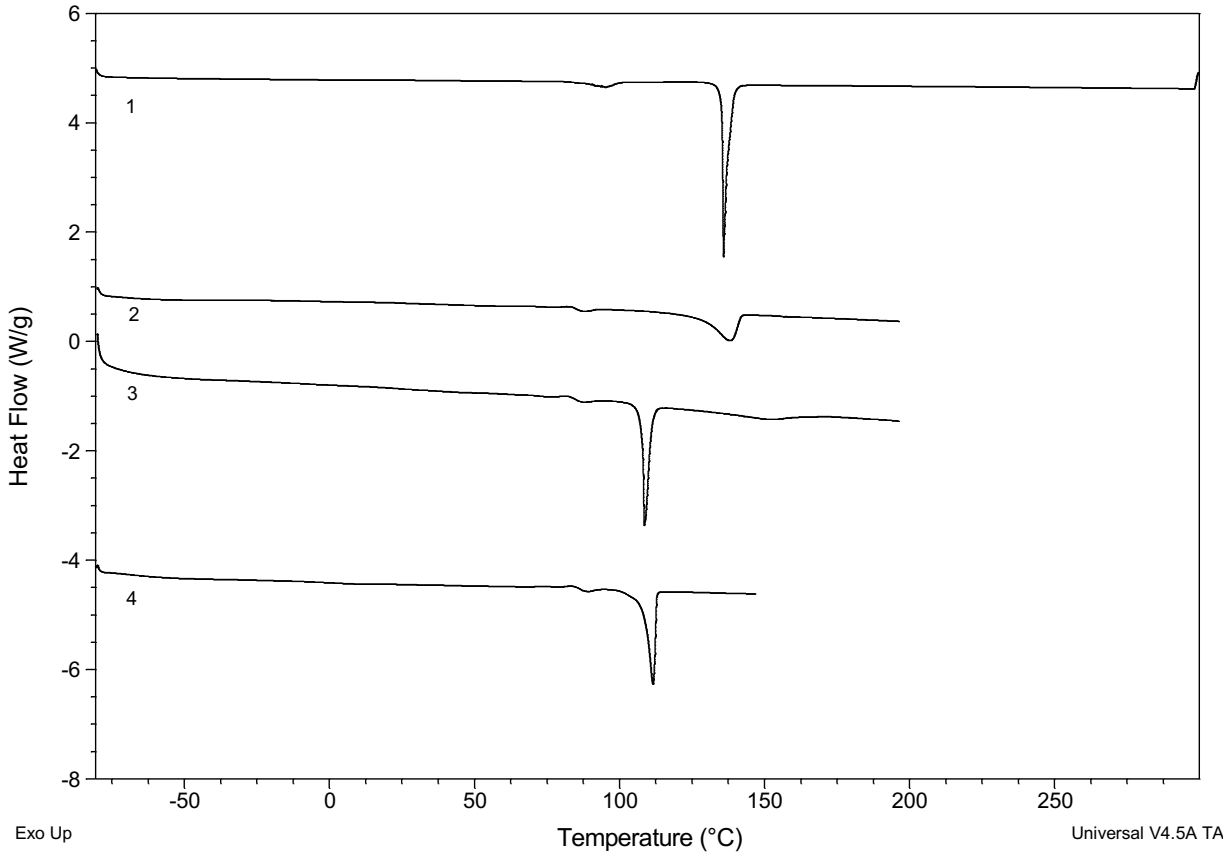


Figure S1: Representative DSC scans for compounds **1**-**4**.

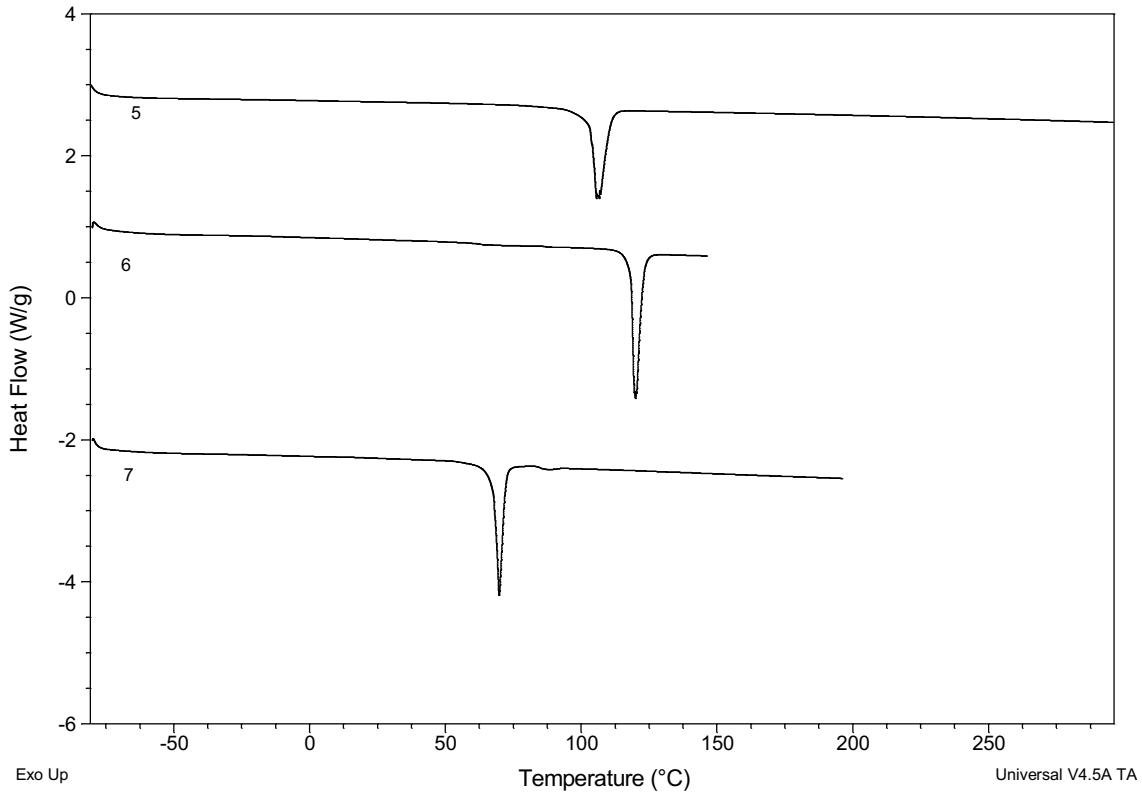


Figure S2: Representative DSC scans for compounds **5**-**7**.

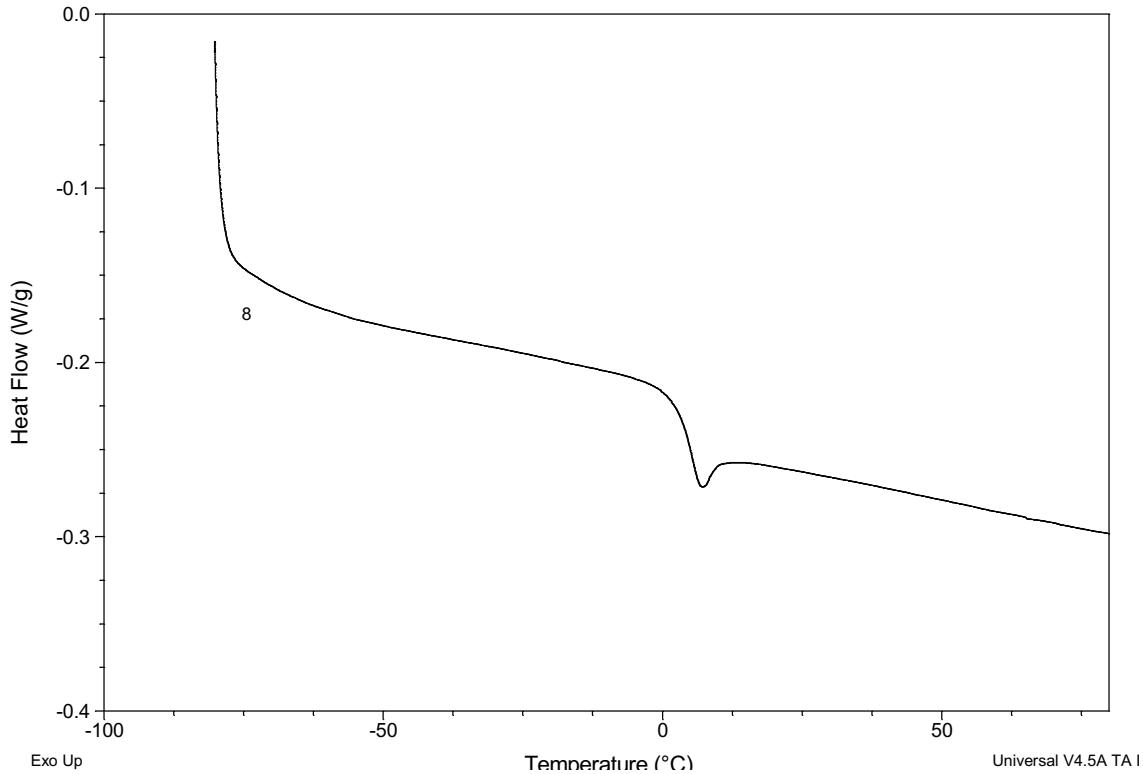


Figure S3: Representative DSC scan for compound **8**, which exhibits a weak glass transition.

,

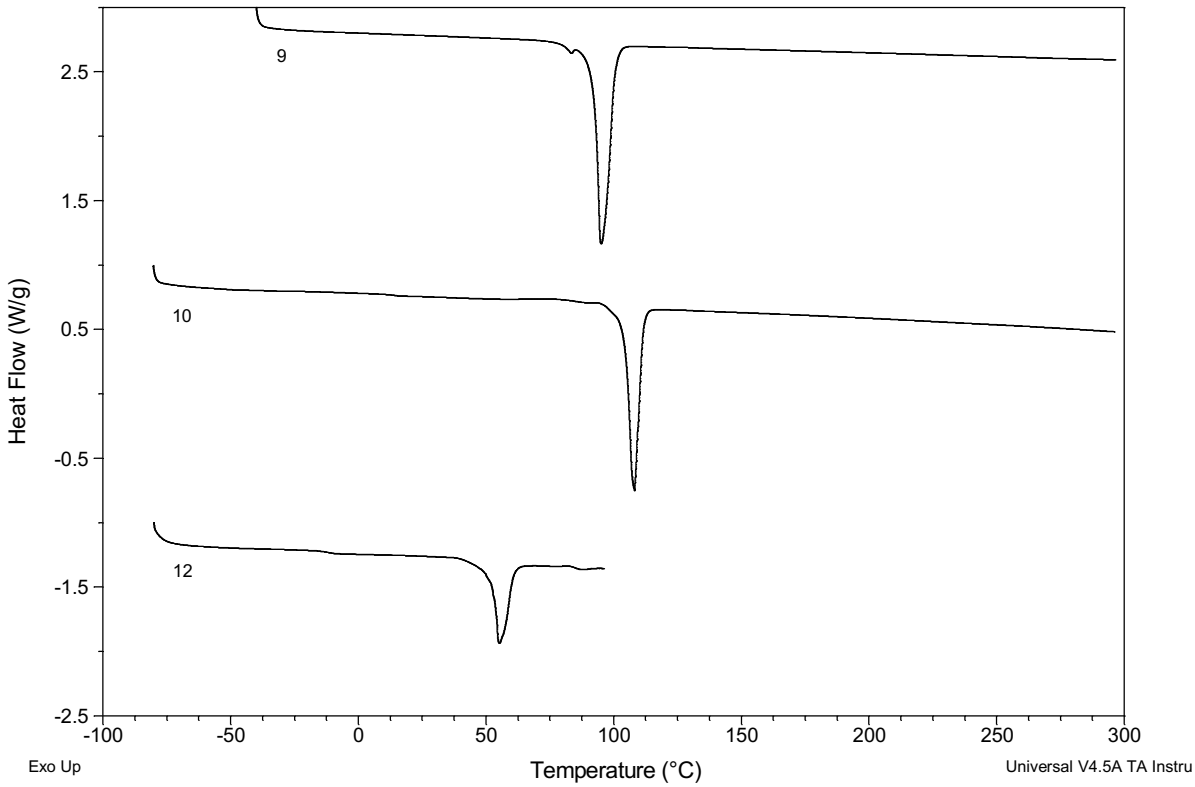


Figure S4: Representative DSC scans for compounds **9,10** and **12**.

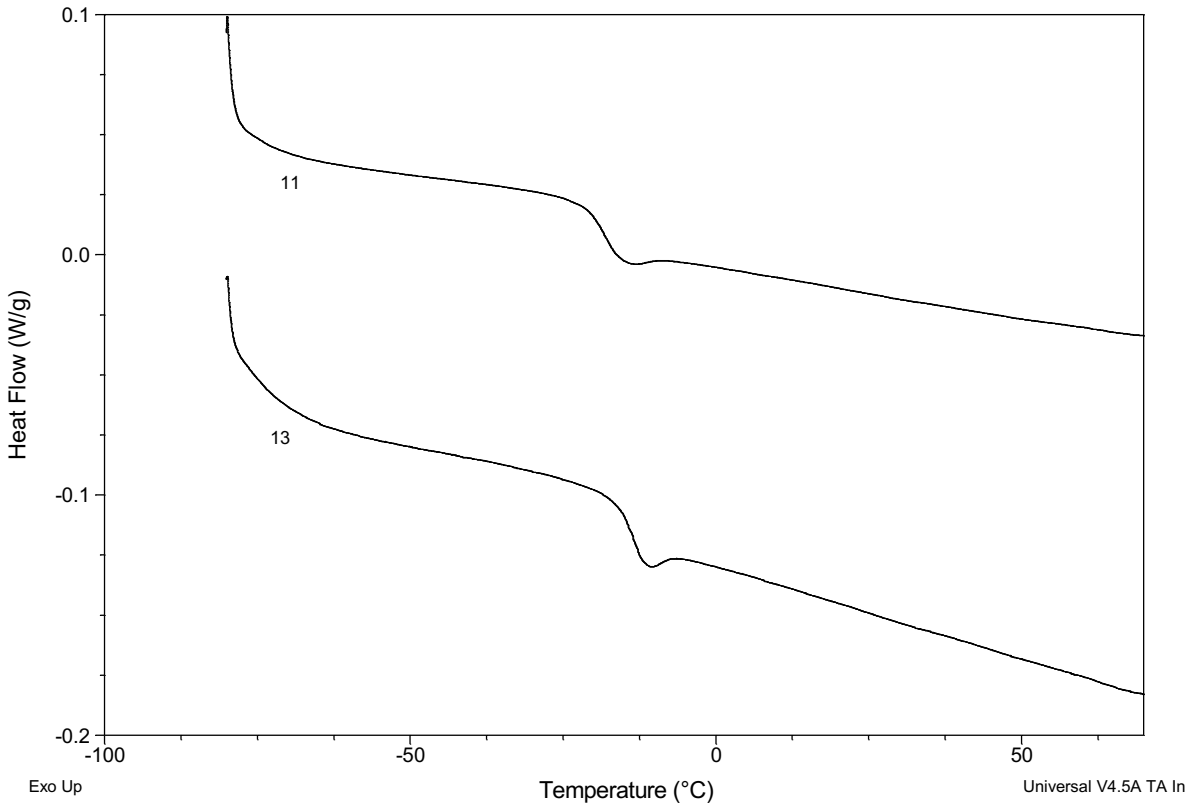


Figure S5: Representative DSC scans for compounds **11** and **13**, which exhibit weak glass transitions.

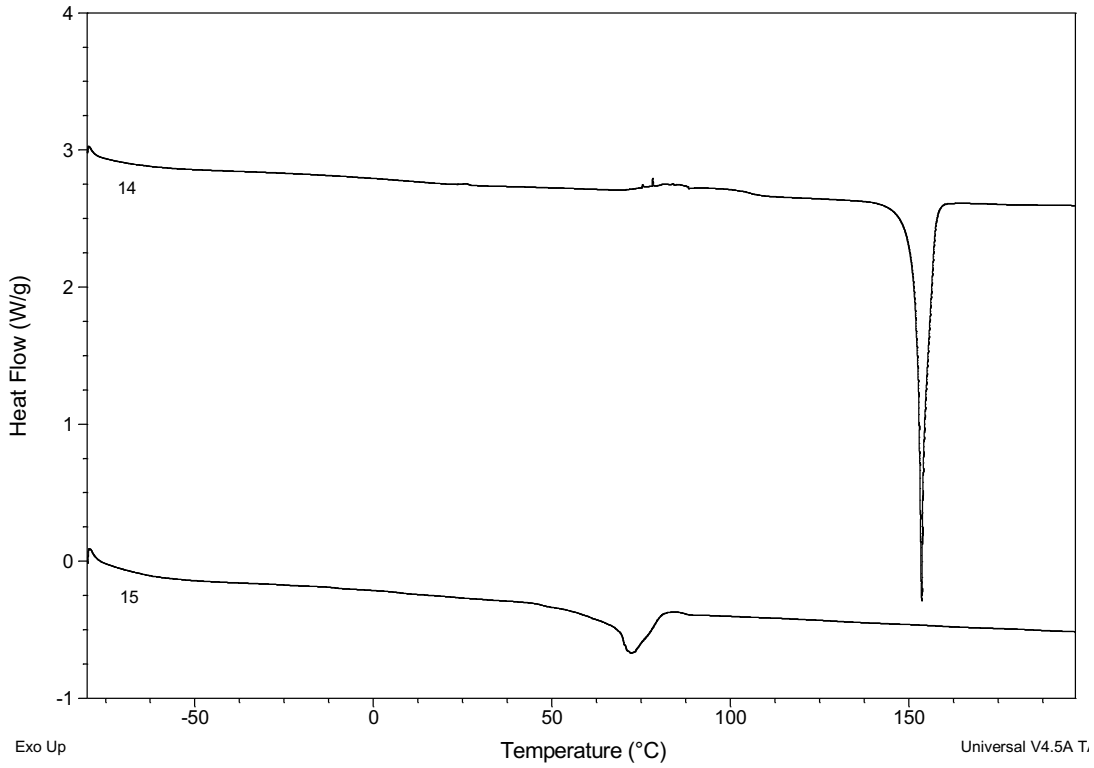


Figure S6: Representative DSC scans for compounds **14** and **15**.

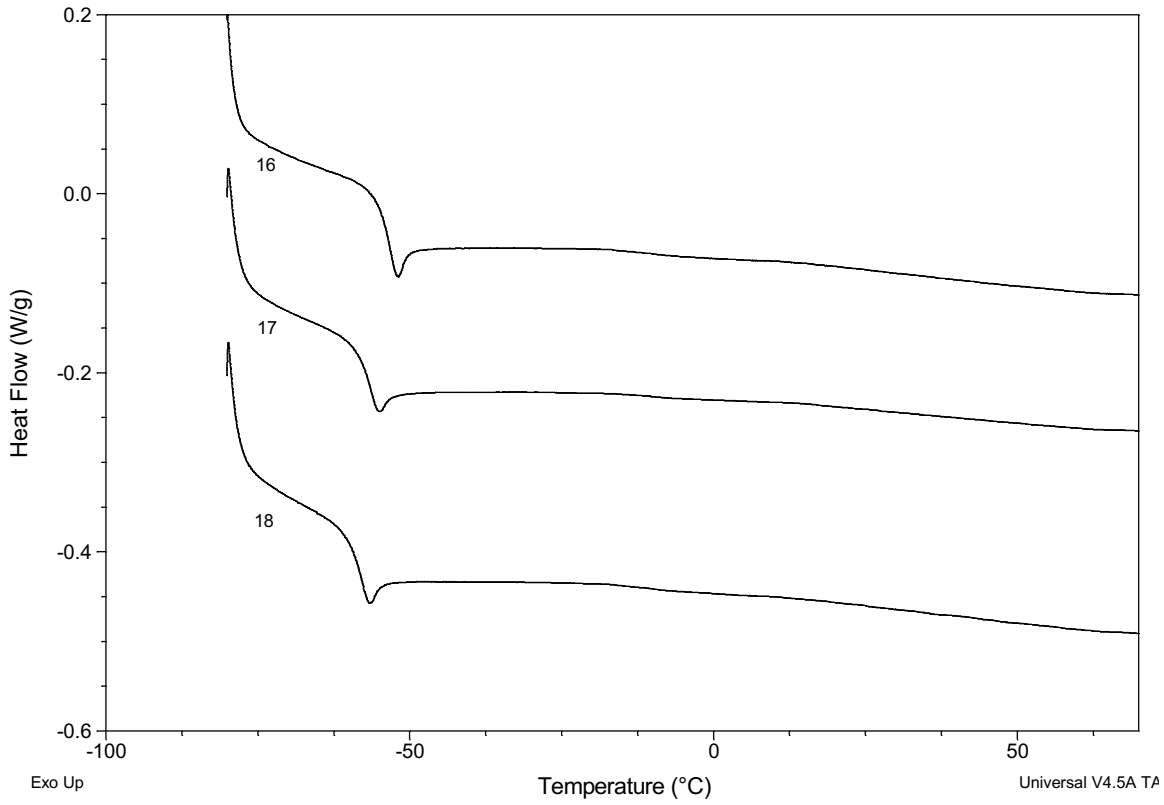


Figure S7: Representative DSC scans for compounds **16-18**. and **13**, which exhibit weak glass transitions.

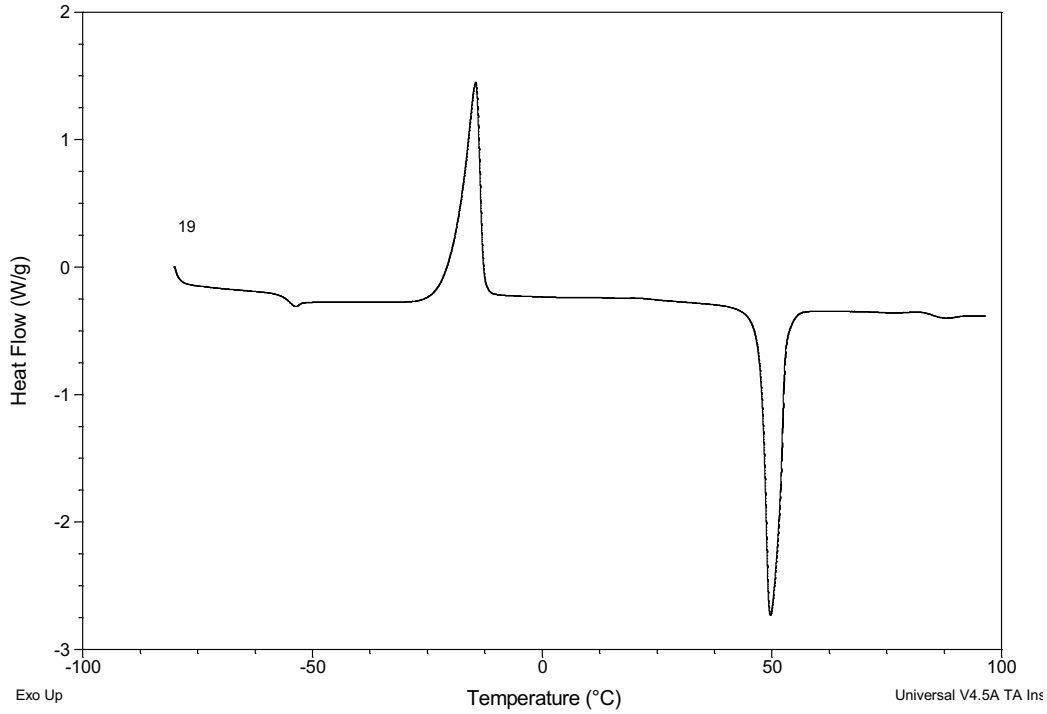


Figure S8: Representative DSC scan for compound **19**.

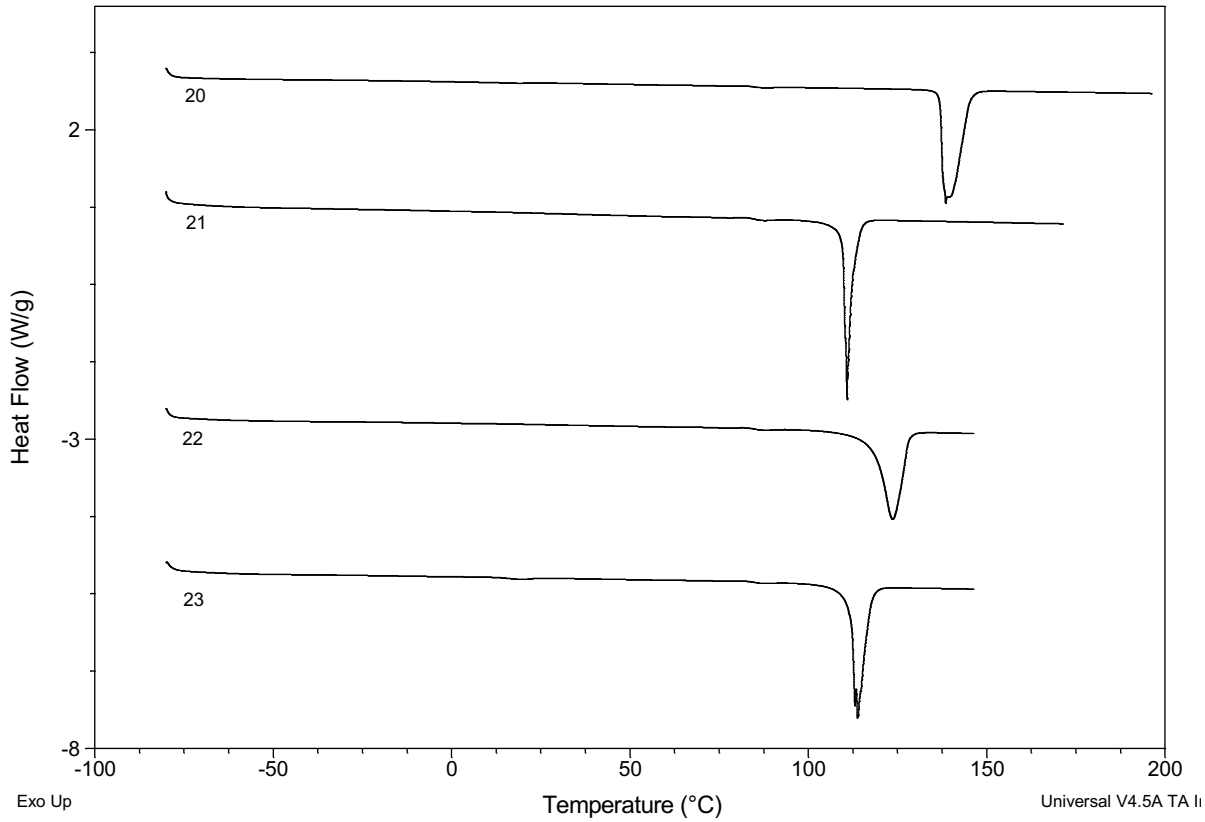


Figure S9: Representative DSC scans for compounds **20**-**23**.

Details of the Single Crystal X-Ray Diffraction Data Collection

CRYSTAL GROWTH:
Crystals of the salts were grown by slow evaporation from solutions in methanol. The crystals were collected by decantation, dried in vacuo, and transferred into a glass vial for storage.

SAMPLE PREPARATION:
Single crystals were taken out of the vial by either spatula (for dry samples) or via pasteur pipette (for crystals in mother liquor) and immersed in a few drops of Fomblin oil (a perfluoroether). Crystals were separated from each other with a MiTeGen micromesh mount (on a magnetic snap on mount), cut to size when required using triangular tipped a carpet cutting razor blade, and picked up on a MiTeGen micromesh mount from the Fomblin oil (using as little oil as possible). The MiTeGen micromesh mount on the magnetic snap on mount was transferred into the cold stream of the diffractometer and flash cooled.

INSTRUMENTATION:	Bruker AXS D8 Quest CMOS diffractometer
RADIATION:	Triumph curved graphite crystal
SOFTWARE PACKAGES:	Apex3 v2018.1-0 (Bruker, 2018)
	SAINT V8.38A (Bruker, 2016)
	SHELXS-97 (Sheldrick, 2008)
DATA COLLECTION:	omega and phi scans

Software and Refinement Methods

DATA COLLECTION:	Apex3 v2018.1-0 (Bruker, 2018)
CELL REFINEMENT:	SAINT V8.38A (Bruker, 2016)
DATA REDUCTION:	SAINT V8.38A (Bruker, 2016)
STRUCTURE SOLUTION:	SHELXS-97 (Sheldrick, 2008)

Special Details of Restraints and Methods

Cation 5, $P(Ph)_3$-p-POP^+

_reflns_special_details
;
Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

_reflns_Friedel_fraction is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences. Completness statistics refer to single and composite reflections containing twin component 1 only.
;

_computing_data_collection 'Apex3 v2018.7-2 (Bruker, 2017)'
_computing_cell_refinement 'SAINT V8.38A (Bruker, 2016)'

_computing_data_reduction 'SAINT V8.38A (Bruker, 2016)'
_computing_structure_solution 'SHELXS-97 (Sheldrick, 2008)'
_computing_structure_refinement
;
SHELXL-2018/3 (Sheldrick, 2015, 2018),
SHELXLE Rev946 (H\"ubschle et al., 2011)
;
_computing_molecular_graphics ?
_computing_publication_material ?
_refine_special_details
;
Refined as a 2-component inversion twin.

The anion is disordered by a pseudo-mirror operation. The two disordered moieties were restrained to have similar geometries. Uij components of ADPs for disordered atoms closer to each other than 2.0 Angstrom were restrained to be similar. Subject to these conditions the occupancy ratio refined to 0.783(3) to 0.217(3).

Cation 6, P(Ph)$_3$-*p*-(*o*-F-POP)$^+$

_reflns_special_details
;
Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

_reflns_Friedel_fraction is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.
;

_computing_data_collection 'Apex3 v2018.1-0 (Bruker, 2018)'
_computing_cell_refinement 'SAINT V8.38A (Bruker, 2016)'
_computing_data_reduction 'SAINT V8.38A (Bruker, 2016)'
_computing_structure_solution 'SHELXS-97 (Sheldrick, 2008)'
_computing_structure_refinement
;
SHELXL-2018/3 (Sheldrick, 2015, 2018),
SHELXLE Rev946 (H\"ubschle et al., 2011)
;
_computing_molecular_graphics ?
_computing_publication_material ?
_refine_special_details
;
The fluorine atom of the fluorophenyl group is disordered over the two ortho positions. The occupancy ratio refined to 0.683(4) to 0.683(4). The anion is disordered over two orientations, with indication of additional disorder which was not sufficiently defined for unambiguous refinement. The two disordered moieties were restrained to have similar geometries. Uij components of ADPs for disordered atoms closer to each other than 2.0 Angstrom were restrained to be similar. Subject to these conditions the occupancy ratio refined to 0.8456(13) to 0.1544(13).

NOTE: The refined structure for this compound had a B-level alert for an O-O contact between the cations. This is due to the dipole-dipole interaction between the C-O bonds of neighboring cations, which overcomes the expected O-O repulsion and the alert regarded as a false alarm.

Cation 7, $P(Ph)_3$-*p*-(*m*-F-POP)$^+$

```
_reflns_special_details
;
 _reflns_Friedel_fraction is defined as the number of unique  Friedel pairs measured divided by
the number that would be  possible theoretically, ignoring centric projections and  systematic
absences. Completness statistics refer to single and  composite reflections containing twin
component 1 only.
;

_computing_data_collection        'Apex3 v2018.1-0 (Bruker, 2018)'
_computing_cell_refinement        'SAINT V8.38A (Bruker, 2016)'
_computing_data_reduction         'SAINT V8.38A (Bruker, 2016)'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 2008)'
_computing_structure_refinement
;
SHELXL-2018/3 (Sheldrick, 2015, 2018),
SHELXLE Rev946 (H\"ubschle et al., 2011)
;
_computing_molecular_graphics     ?
_computing_publication_material   ?
_refine_special_details
;
```

The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell_Now, with the two components being related by a 180 degree rotation around the real a-axis. The two components were integrated using Saint and corrected for absorption using twinabs, resulting in the following statistics:

15502 data (4686 unique) involve domain 1 only, mean I/sigma 23.1
15148 data (4609 unique) involve domain 2 only, mean I/sigma 11.5
75199 data (19329 unique) involve 2 domains, mean I/sigma 14.4
  19 data (19 unique) involve 3 domains, mean I/sigma 11.7

The exact twin matrix identified by the integration program was found to be:

 1.00019 0.00032 0.00040
-0.00035 -1.00000 0.00029
-0.92160 -0.00042 -1.00019

The structure was solved using direct methods with only the non-overlapping reflections of component 1. The structure was refined using the hklf 5 routine with all reflections of component 1 (including the overlapping ones), resulting in a BASF value of 0.1967(6).

The Rint value given is for all reflections and is based on agreement between observed single and composite intensities and those calculated from refined unique intensities and twin fractions (TWINABS (Sheldrick, 2012)).

In bothy cations, the fluorine atom of the fluorophenyl group is disordered over the two meta positions. The C-F distances in the cations were restrained to be similar. Subject to these conditions the occupancy ratio refined to 0.835(6) to 0.165(6) in the cation of P1, and to 0.833(5) to 0.167(5) in the cation of P2.

Two anions are located on inversion centers and are disordered around these. Of these, one is in addition disordered over two alternative positions not related by inversion. The three disordered moieties were restrained to have similar geometries as the one not disordered anion in a general position. Uij components of ADPs for disordered atoms closer to each other than 2.0 Angstrom were restrained to be similar. Subject to these conditions the occupancy rates for the molecule of N3 and N3B refined to two times 0.3200(12) and two times 0.1800(12).
;

Cation 4, $P(Ph)_3$-*p*-F-POP^+

_reflns_special_details
;
Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

_reflns_Friedel_fraction is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.
;

_computing_data_collection 'Apex3 v2018.1-0 (Bruker, 2018)'
_computing_cell_refinement 'SAINT V8.38A (Bruker, 2016)'
_computing_data_reduction 'SAINT V8.38A (Bruker, 2016)'
_computing_structure_solution 'SHELXS-97 (Sheldrick, 2008)'
_computing_structure_refinement
;
SHELXL-2018/3 (Sheldrick, 2015, 2018),
SHELXLE Rev946 (H\"ubschle et al., 2011)
;
_computing_molecular_graphics ?
_computing_publication_material ?
_refine_special_details
;
In both p-F-Ph-PPh3 cations the fluorine atom is disordered over all four possible para positions. All C-F bond lengths in the cations were restrained to be similar. The total occupancy was each constrained to one fluorine. Subject to these conditions the occupancy rates for the F atoms refined to 0.493(3), 0.080(3), 0.175(3) and 0.251(3) for the cation of P1, and to 0.497(3), 0.079(3), 0.248(3) and 0.176(3) for the cation of P2.

The two anions are disordered over each two orientations. The four disordered moieties were restrained to have similar geometries. Uij components of ADPs for disordered atoms closer to each other than 2.0 Angstrom were restrained to be similar. Subject to these conditions the occupancy ratio refined to 0.9503(12) to 0.0497(12) for the molecule of N1, and to 0.8698(16) to 0.1302(16) for the molecule of N2.
;