



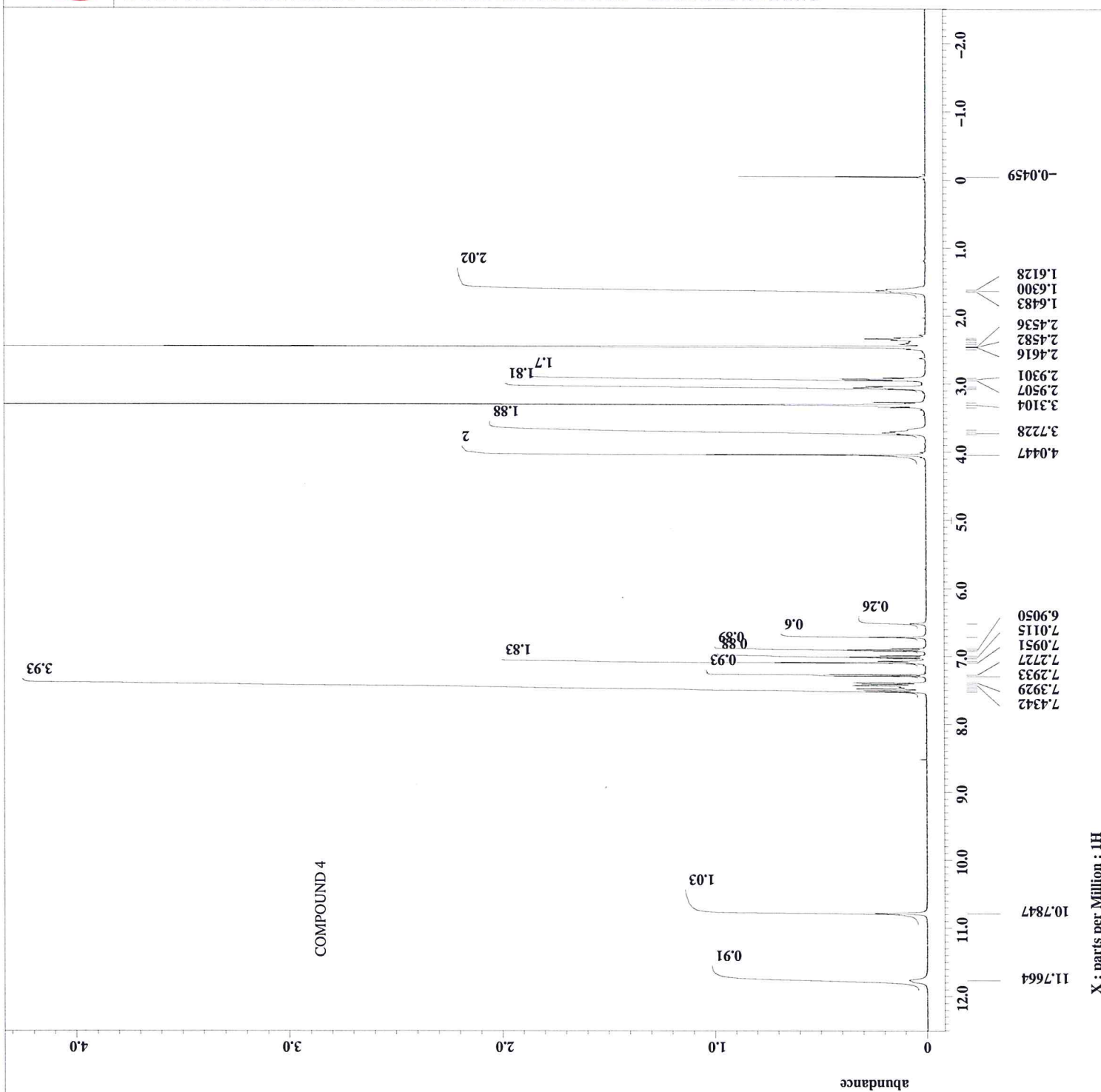
```

Filename = ID-102-45-Org-Bas-Pre
Author = Crider
Experiment = single_pulse.ex2
Sample_id = S#409225
Solvent = DMSO-D6
Creation_time = 7-JUN-2011 11:09:26
Revision_time = 17-MAR-2021 05:50:43
Current_time = 17-MAR-2021 09:50:46

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

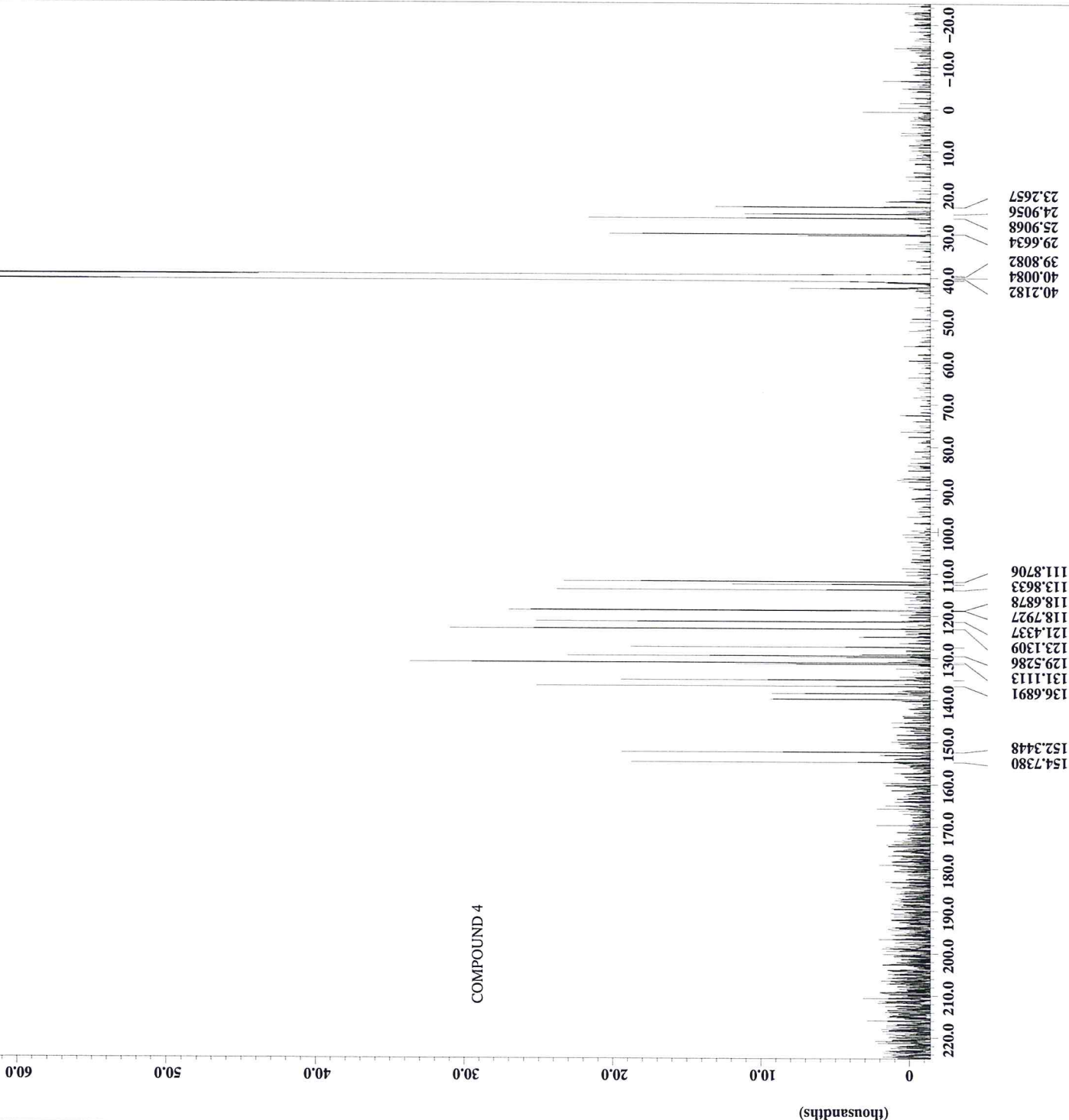
X_90_width = 10.01791 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.008955 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 42
Relaxation_delay = 7.18365952 [s]
Repetition_time = 7.18365952 [s]
Temp_get = 19.3 [dC]
    
```





Filename = ID-102-45-Org-Bas-Pre
Author = Criger
Experiment = single_pulse_dec
Sample_id = S#410454
Solvent = DMSO-D6
Creation_time = 7-JUN-2011 14:25:52
Revision_time = 17-MAR-2021 10:12:39
Current_time = 17-MAR-2021 10:12:43
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[is]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 3859
Total_scans = 3859
X_90_width = 11.9[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 9[db]
X_pulse = 3.96666667[us]
Irr_atn_dec = 27[db]
Irr_atn_noe = 27[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 = 3.04333312[s]
Temp_get = 19.7[dc]

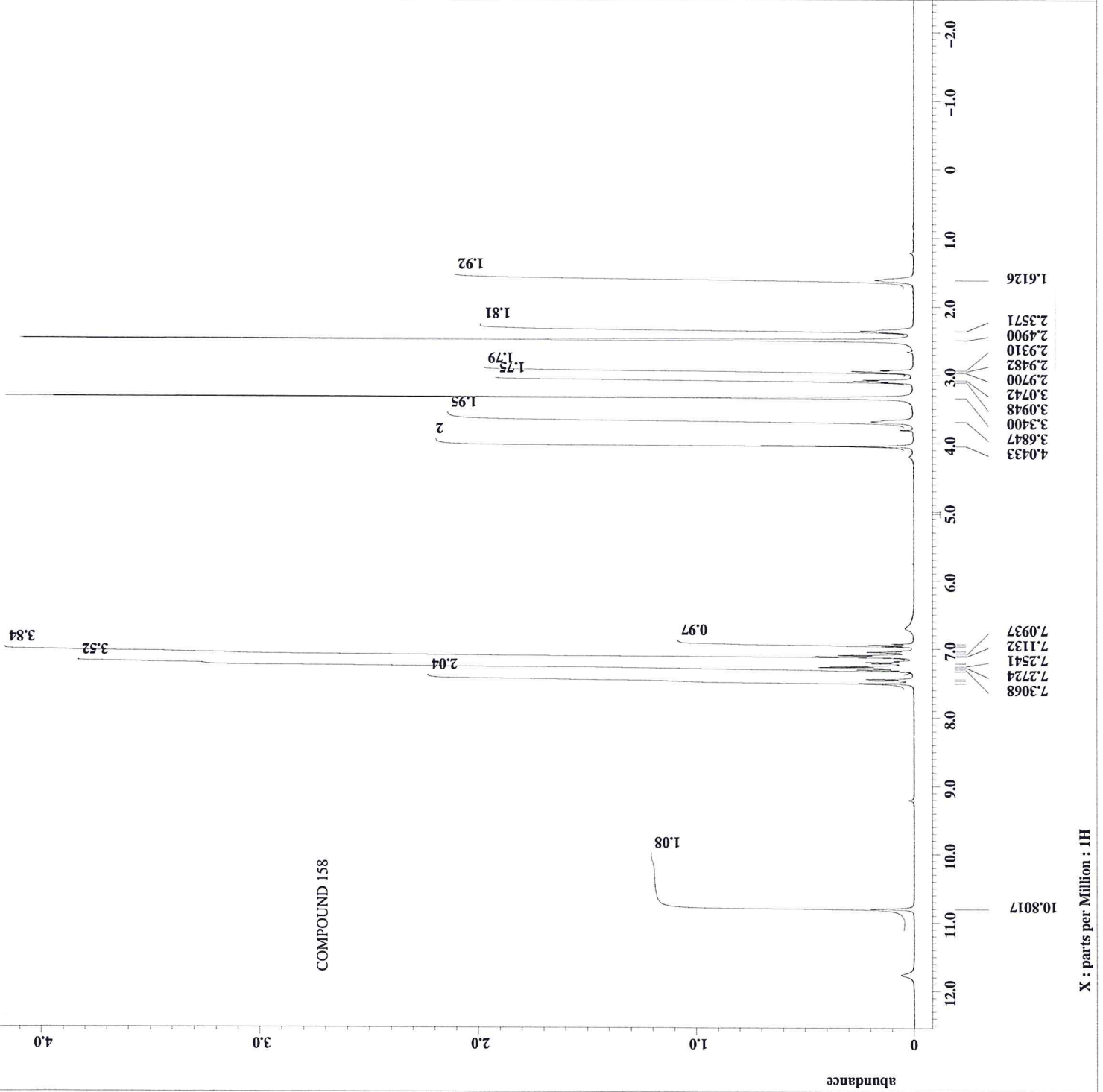
COMPOUND 4



X : parts per Million : 13C



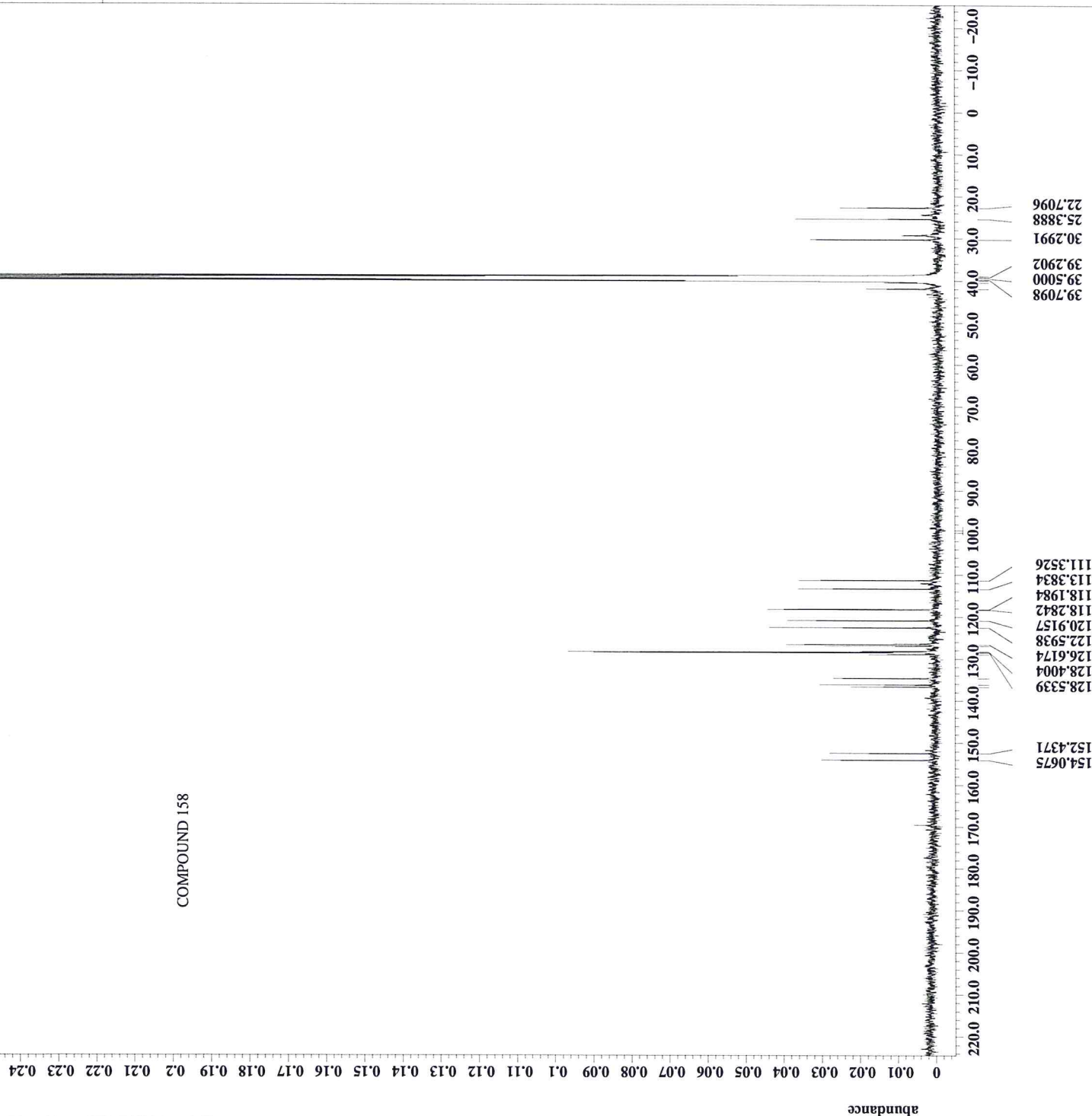
Filename = SM-I-26-1_PROTON-5.jd
Author = Delta
Experiment = single_pulse.exe
Sample_id = SM-I-26-1
Solvent = DMSO-D6
Creation_time = 18-MAY-2016 17:11:50
Revision_time = 11-MAR-2021 08:38:06
Current_time = 11-MAR-2021 08:38:10
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 40
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 20.1 [dC]





Filename = SM-I-26-1-CARBON-5.jd
Author = Delta
Experiment = single_pulse_dec
Sample_id = SM-I-26-1
Solvent = DMSO-D6
Creation_time = 19-MAY-2016 04:45:05
Revision_time = 11-MAR-2021 08:41:15
Current_time = 11-MAR-2021 08:41:19
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = Lppm
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 10240
Total_scans = 10240
X_90_width = 12.84 [us]
X_acq_time = 1.04333312[s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312[s]
Temp_get = 19.6 [dC]

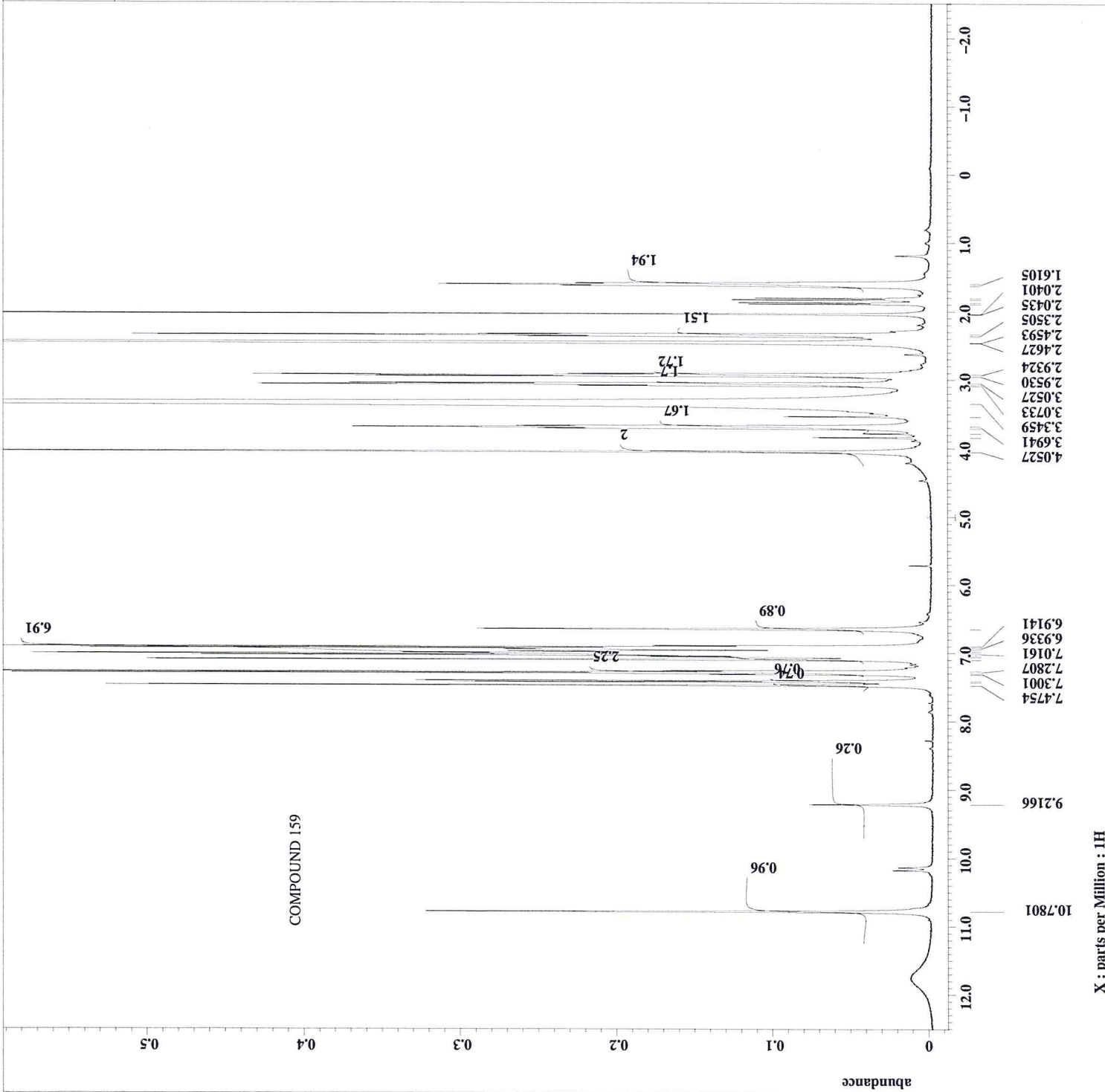
COMPOUND 158



X : parts per Million : 13C



Filename = SM-I-38-F1-3_PROTON-6
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SM-I-38-F1-3
Solvent = DMSO-D6
Creation_time = 31-MAY-2016 17:08:04
Revision_time = 17-MAR-2021 13:56:25
Current_time = 17-MAR-2021 13:56:29
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 36
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 20.5 [dC]

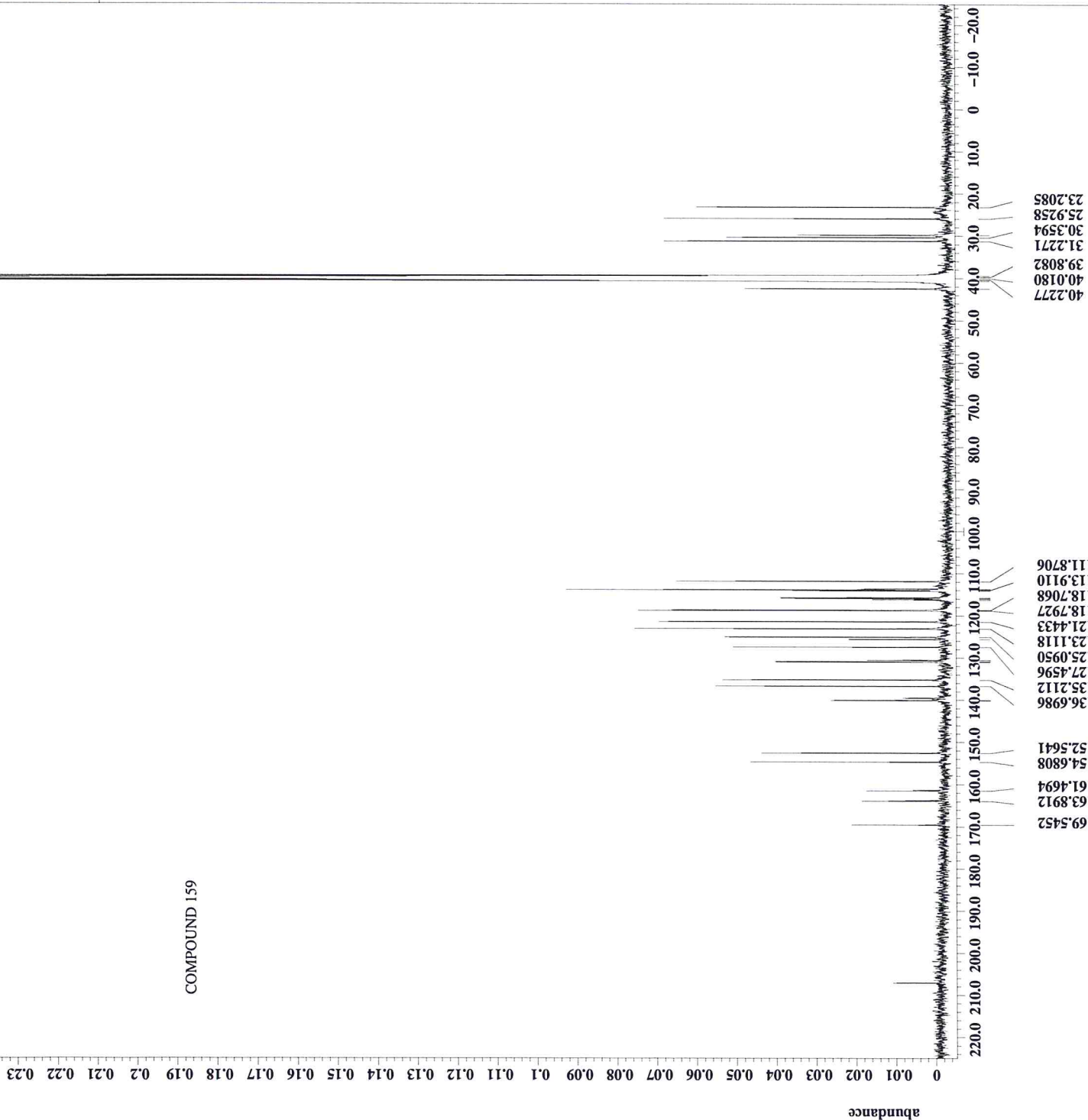


X : parts per Million : 1H



File name = SM-I-38-F1-2_CARBON-6
Author = Delta
Experiment = single_pulse_dec
Sample_id = SM-I-38-F1-2
Solvent = DMSO-D6
Creation time = 14-MAY-2016 03:13:31
Revision time = 10-MAR-2021 16:55:00
Current_time = 10-MAR-2021 16:55:04
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 10240
Total_scans = 10240
X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 20.7 [dC]

COMPOUND 159

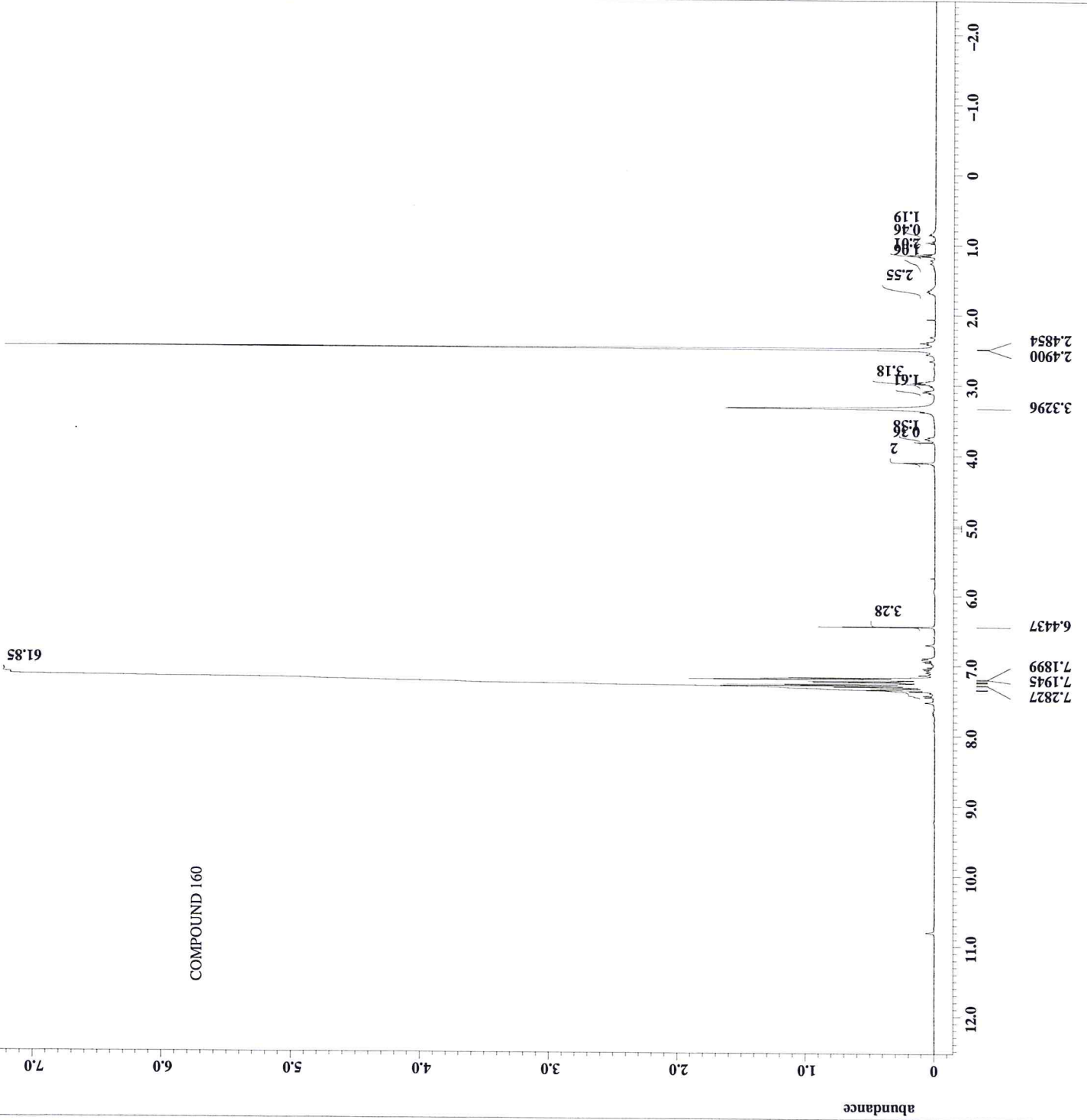


X : parts per Million : 13C

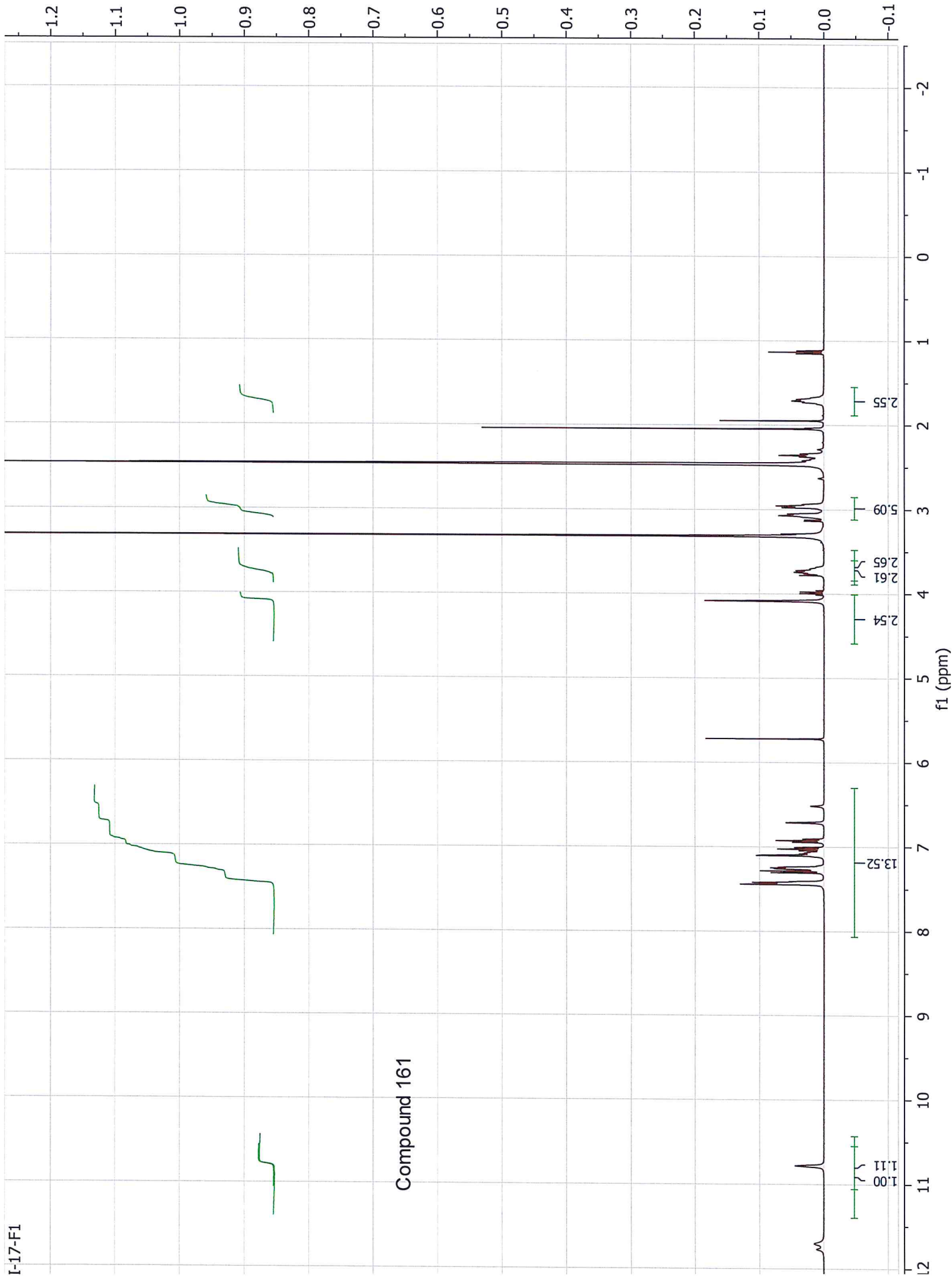


Filename = SM-I-55-F2_PROTON-4.j
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SM-I-55-F2
Solvent = DMSO-D6
Creation_time = 15-MAY-2016 13:04:47
Revision_time = 11-MAR-2021 09:00:53
Current_time = 11-MAR-2021 09:00:57
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [KHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Date_preat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 42
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 19.9 [dC]

COMPOUND 160



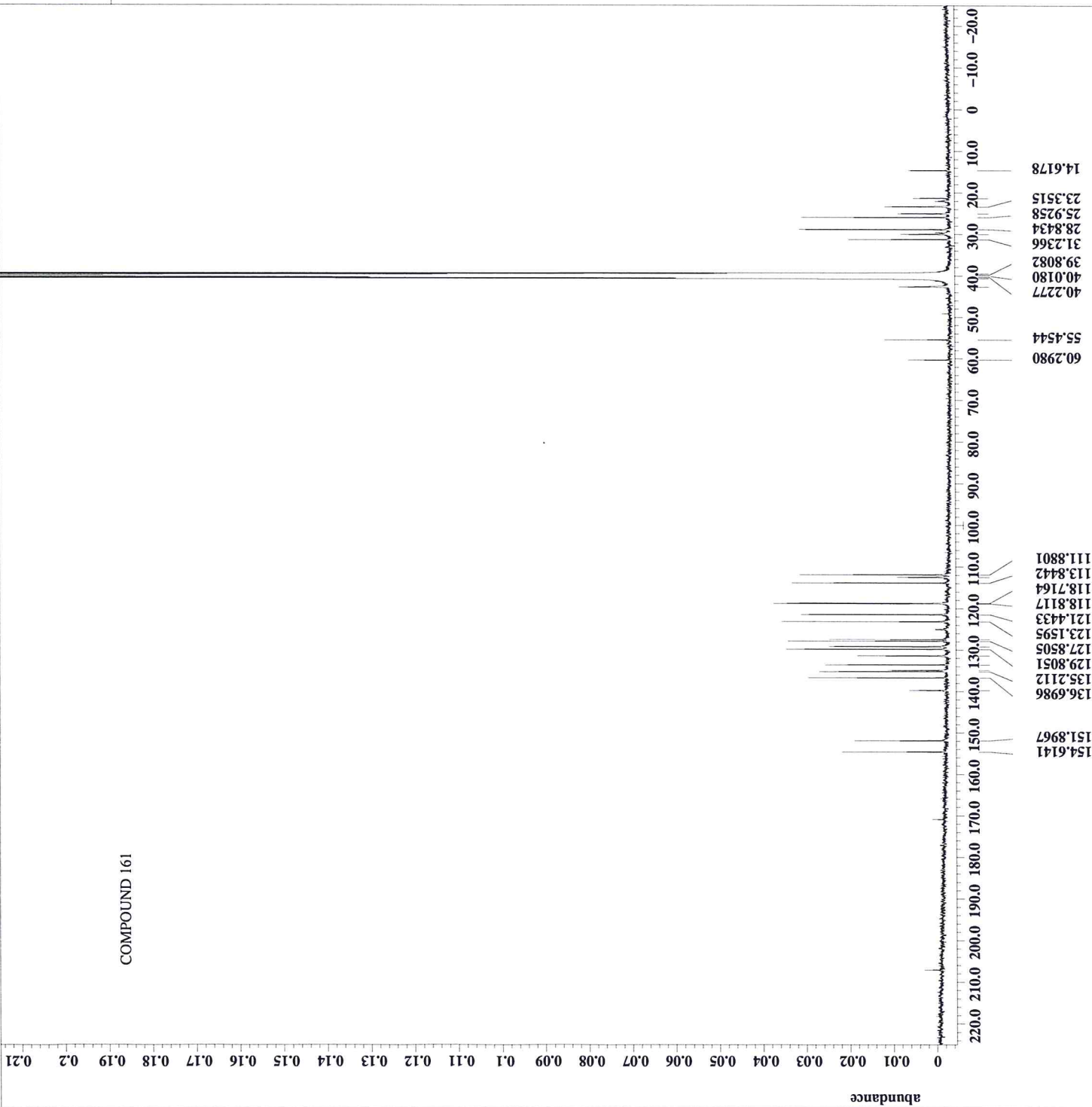
X : parts per Million : 1H



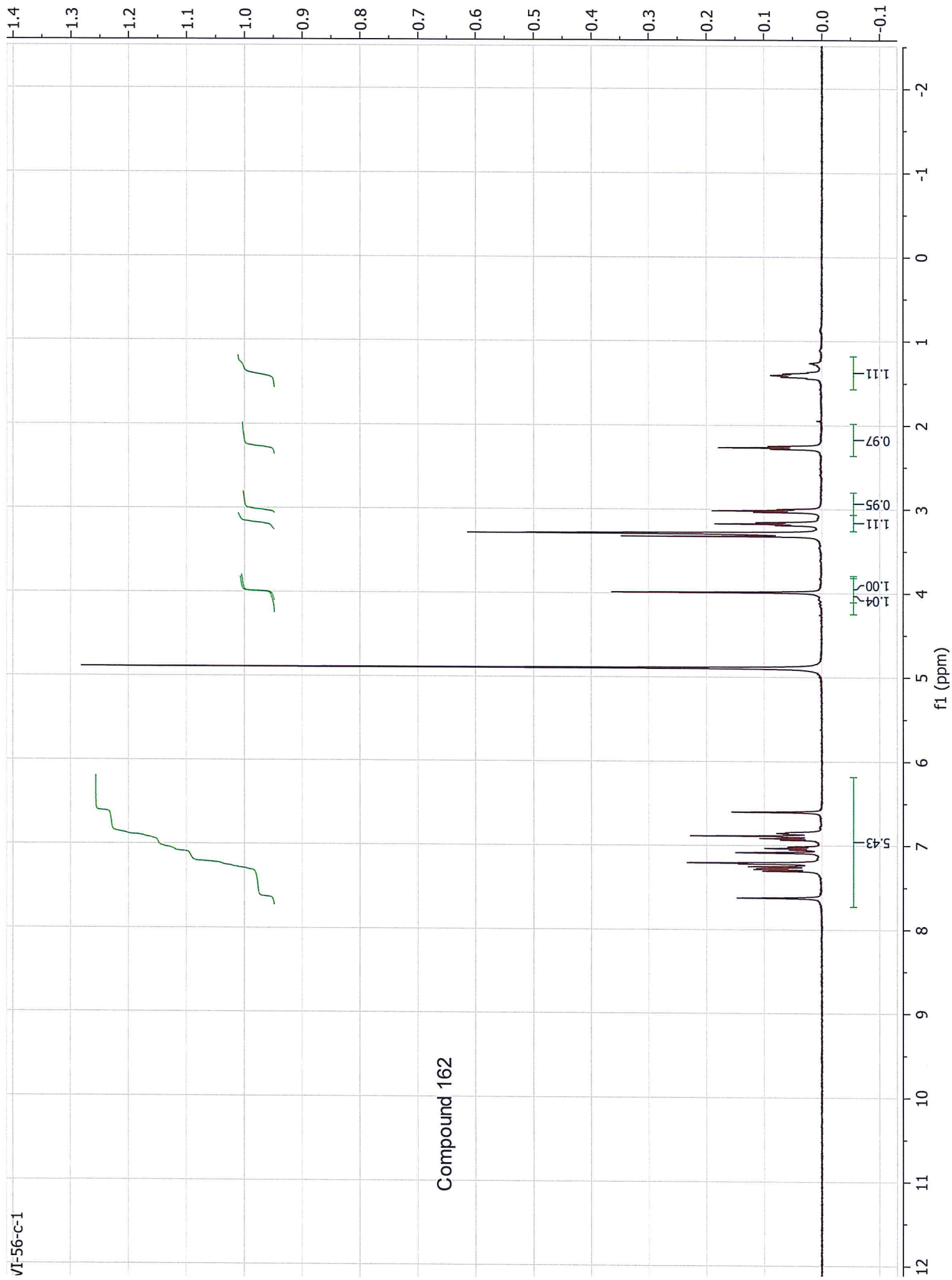


COMPOUND 161

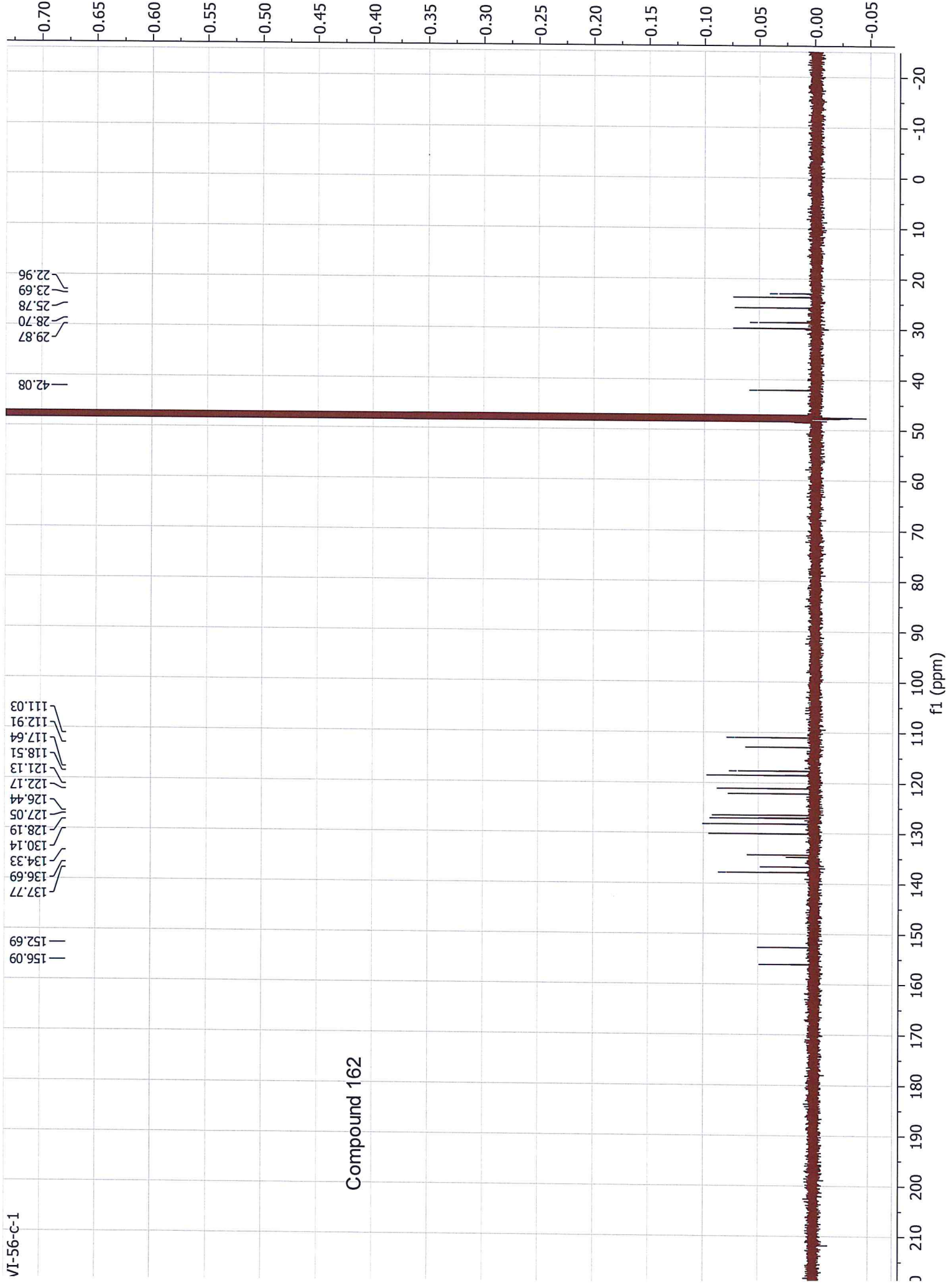
Filename = MM-I-17-F1_CARBON-7.j
Author = Delta
Experiment = single_pulse_dec
Sample_id = MM-I-17-F1
Solvent = DMSO-D6
Creation_time = 25-APR-2016 07:39:46
Revision_time = 10-MAR-2021 11:47:17
Current_time = 10-MAR-2021 11:47:24
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.0433312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 56507.0
Total_scans = 56507.0
X_90_width = 12.84 [us]
X_acq_time = 1.0433312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.0433312 [s]
Temp_get = 20.9 [dC]



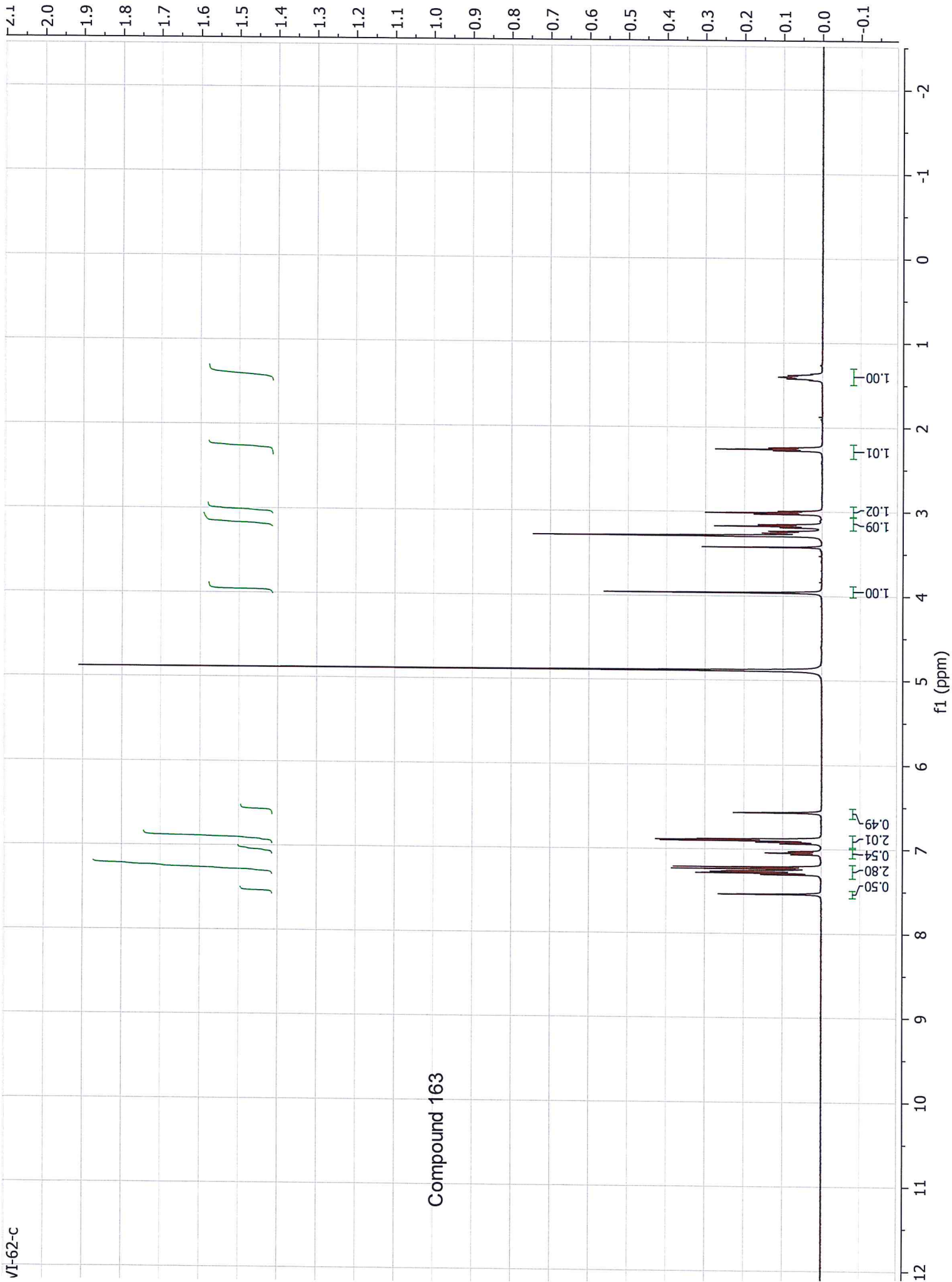
X : parts per Million : 13C



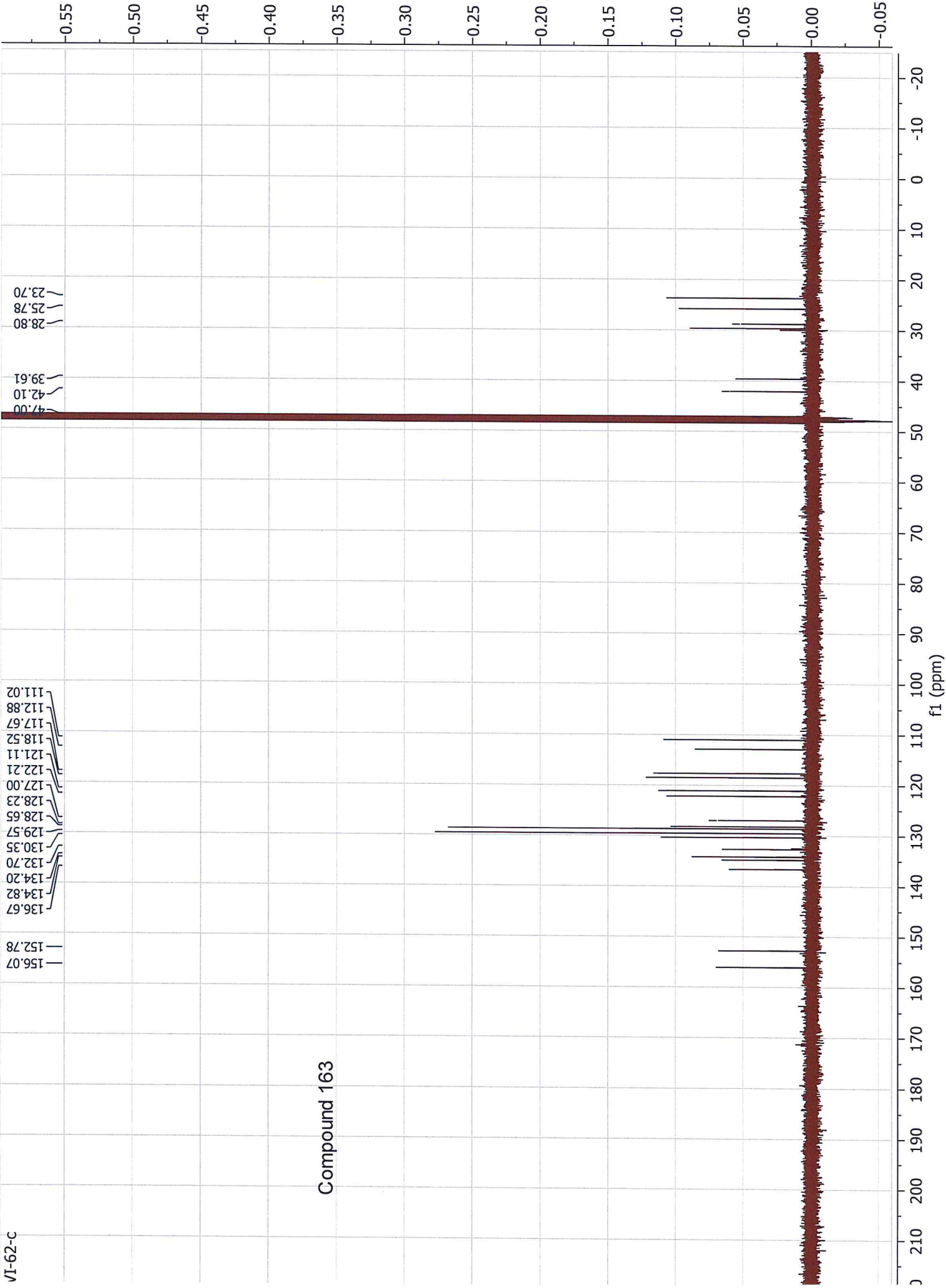
Compound 162



Compound 163



Compound 163





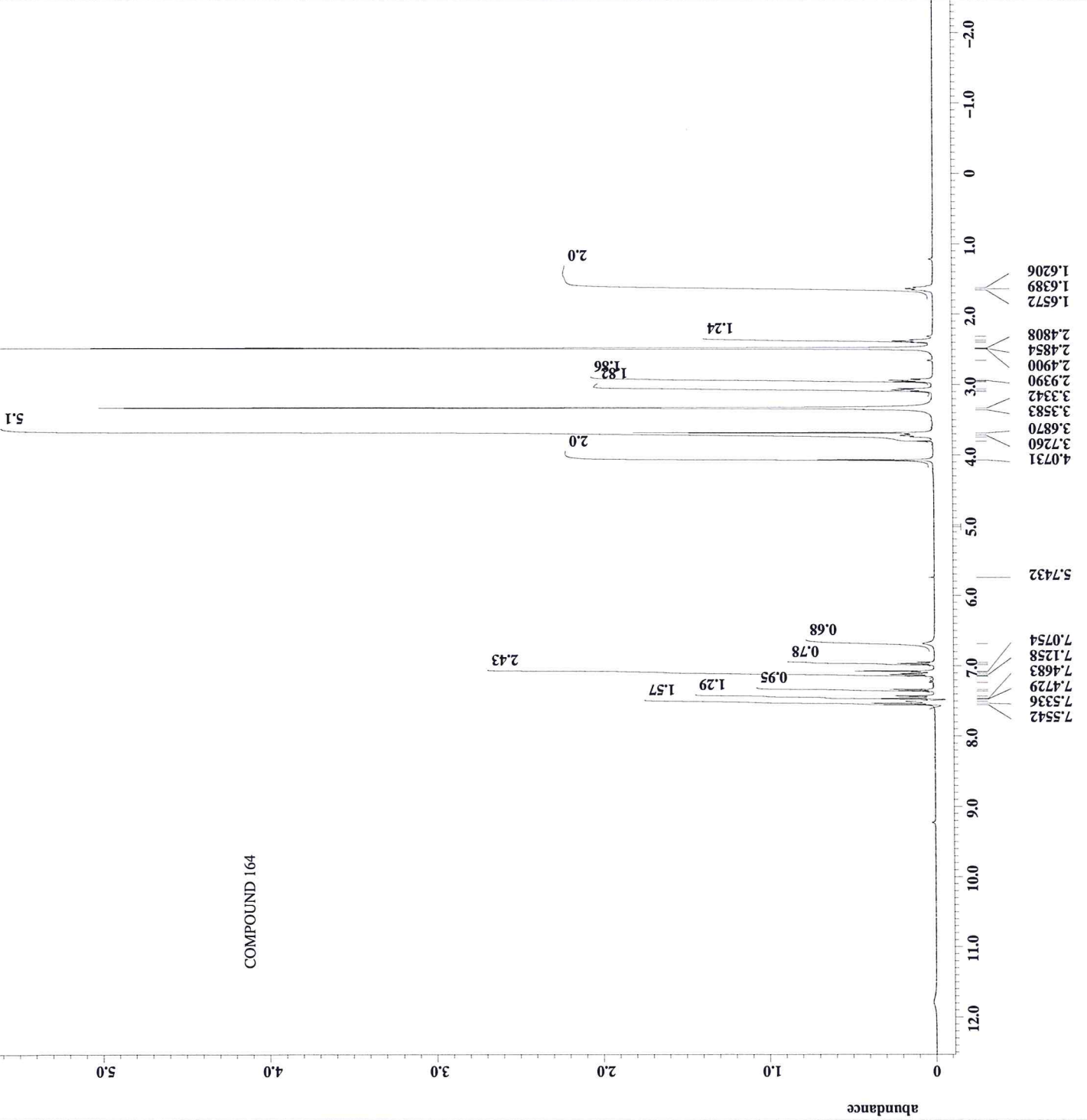
File name = SM-I-60-c-4_PROTON-5.
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SM-I-60-c-4
Solvent = DMSO-D6
Creation_time = 16-MAY-2016 16:41:50
Revision_time = 11-MAR-2021 09:43:03
Current_time = 11-MAR-2021 09:43:07

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 40
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 20.6 [dC]

COMPOUND 164



X : parts per Million : 1H



File name = SM-I-60-c-4_CARBON-5.
Author = Delta
Experiment = single_pulse_dec
Sample_id = SM-I-60-c-4
Solvent = DMSO-D6
Creation_time = 17-MAY-2016 04:15:17
Revision_time = 11-MAR-2021 09:35:24
Current_time = 11-MAR-2021 09:35:28

Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 32768
X_points = 4
X_prescans = 0.95846665[Hz]
X_resolution = 31.40703518[KHz]
X_sweep = 1H
Irr_domain = 399.78219838[MHz]
Irr_freq = 5[ppm]
Irr_offset = FALSE
Clipped = 1
Mod_return = 10240
Total_scans = 10240

X_90_width = 12.84[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 9[dB]
X_pulse = 4.28[us]
Irr_atn_dec = 27[dB]
Irr_atn_noe = 27[dB]
Decoupling = WALTZ
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 3[s]
Recvr_gain = 60
Relaxation_delay = 3[s]
Repetition_time = 4.04333312[s]
Temp_get = 20[dc]

COMPOUND 164

0.24

0.22

0.2

0.18

0.16

0.14

0.12

0.1

0.08

0.06

0.04

0.02

0

abundance

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

40.1293
39.9195
39.7098
39.5000
39.2902
38.8707
32.2251

151.8554
154.1533
137.9159
130.6410
130.6029
129.0583
127.2276
126.9797
121.0683
118.3891
112.7351
109.5410

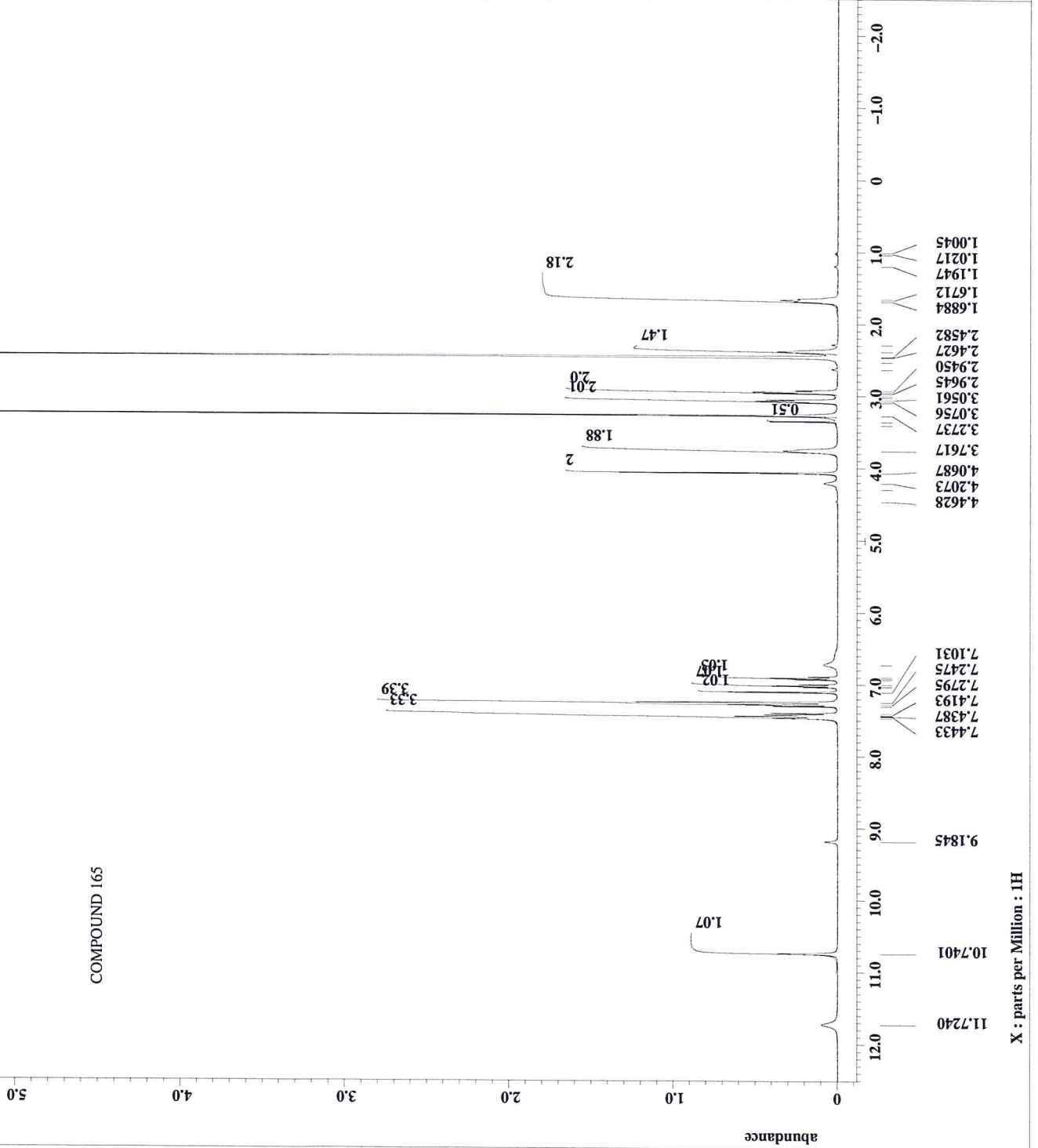
X : parts per Million : 13C



Filename = BN-VI-89-c_PROTON-3.j
Author = Neumann
Experiment = single_pulse.ex2
Sample_id = BN-VI-89-c
Solvent = DMSO-D6
Creation_time = 3-FEB-2016 13:01:18
Revision_time = 10-MAR-2021 11:22:25
Current_time = 10-MAR-2021 11:22:30
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.58[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[dB]
X_pulse = 5.29[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[fs]
Recvr_gain = 42
Relaxation_delay = 4[fs]
Repetition_time = 6.18365952[s]
Temp_get = 30[degC]

7.04

COMPOUND 165



X : parts per Million : 1H



```

Filename = BN-VI-89-c_CARBON-4.j
Author = Neumann
Experiment = single_pulse_dec
Sample_id = BN-VI-89-c
Solvent = DMSO-D6
Creation_time = 3-FER-2016 14:16:46
Revision_time = 10-MAR-2021 11:34:08
Current_time = 10-MAR-2021 11:34:30

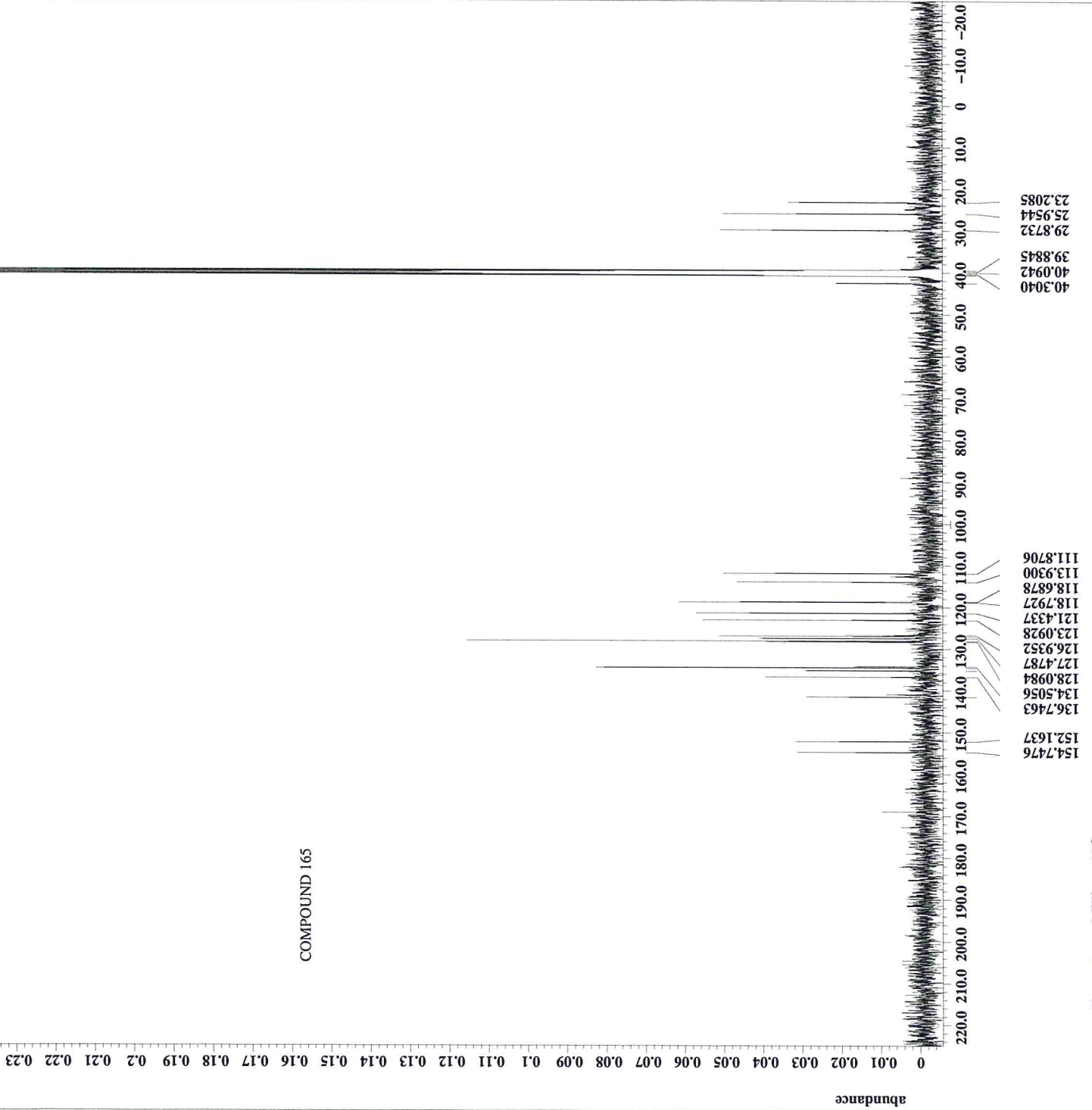
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1452
Total_scans = 1452

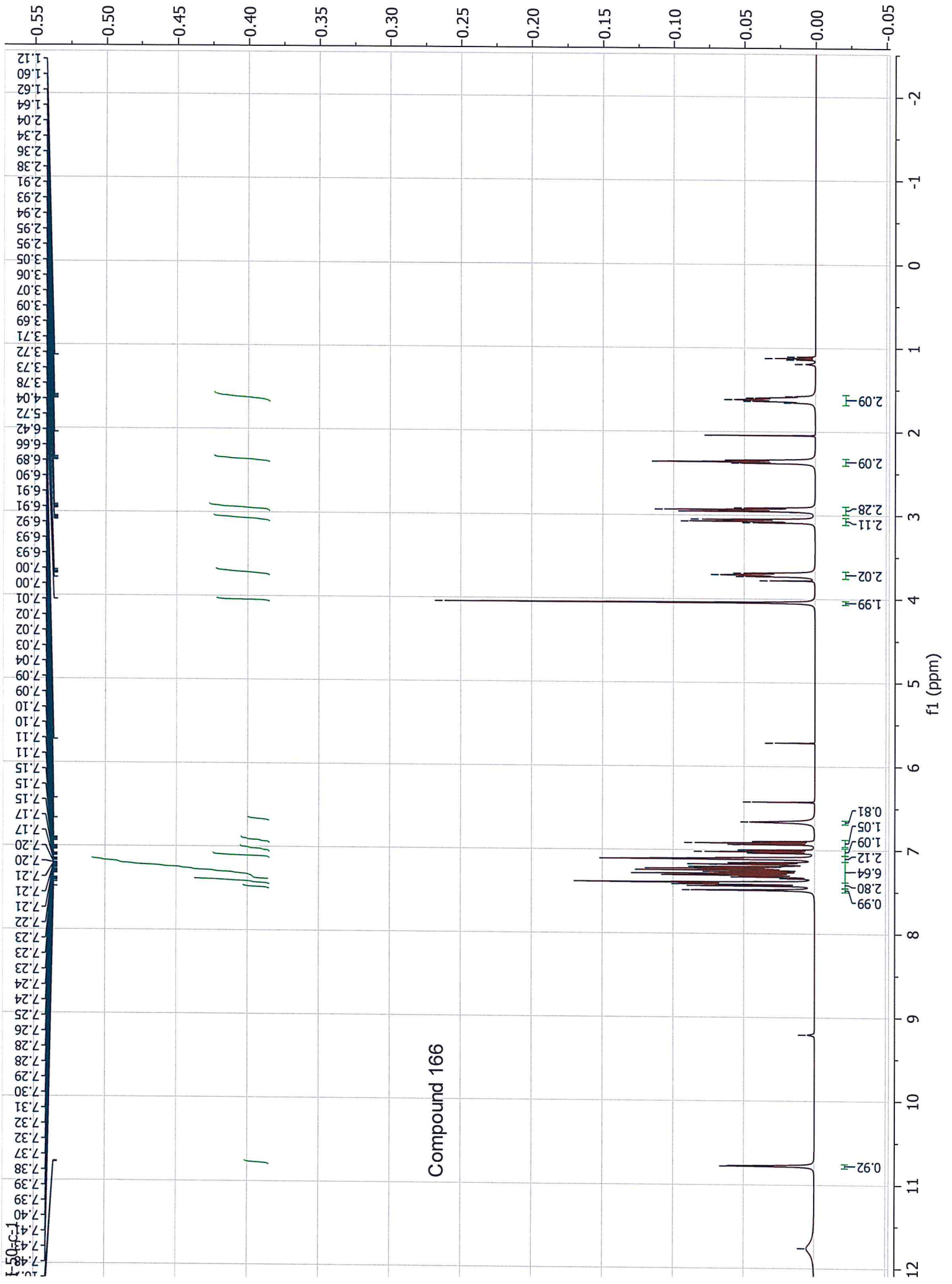
X_90_width = 13.12 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.37333333 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 2 [s]
Recvr_gain = 60
Relaxation_delay = 2 [s]
Repetition_time = 3.04333312 [s]
Temp_get = 30 [DC]

```

COMPOUND 165



X : parts per Million : 13C





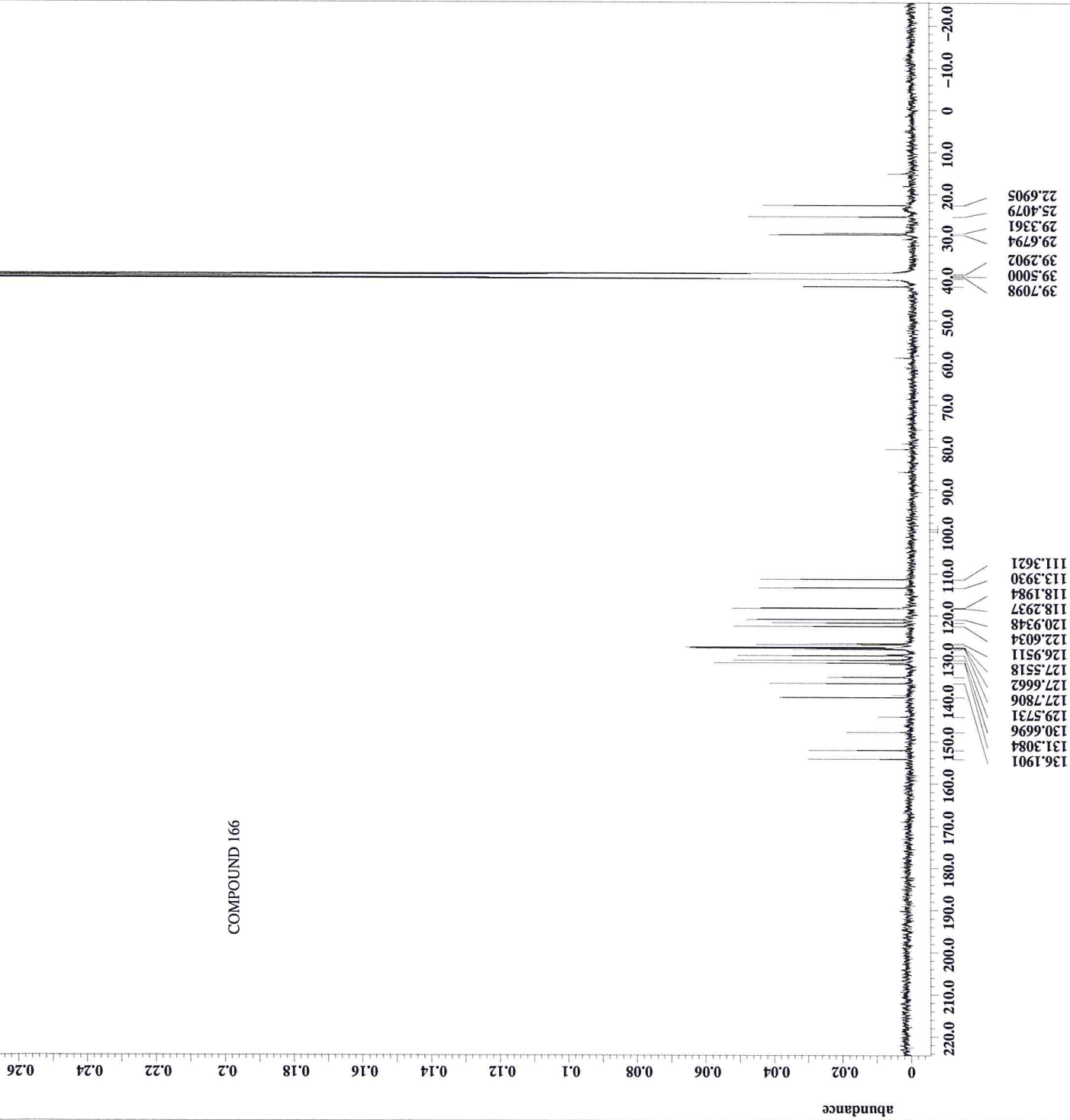
Filename = SW-I-50-C-2_CARBON-5.
Author = Delta
Experiment = single_pulse_dec
Sample_id = SM-I-50-C-2
Solvent = DMSO-D6
Creation_time = 2-JUN-2016 06:11:15
Revision_time = 11-MAR-2021 08:52:15
Current_time = 11-MAR-2021 08:52:20

Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 12000
Total_scans = 12000

X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 20.4 [dC]

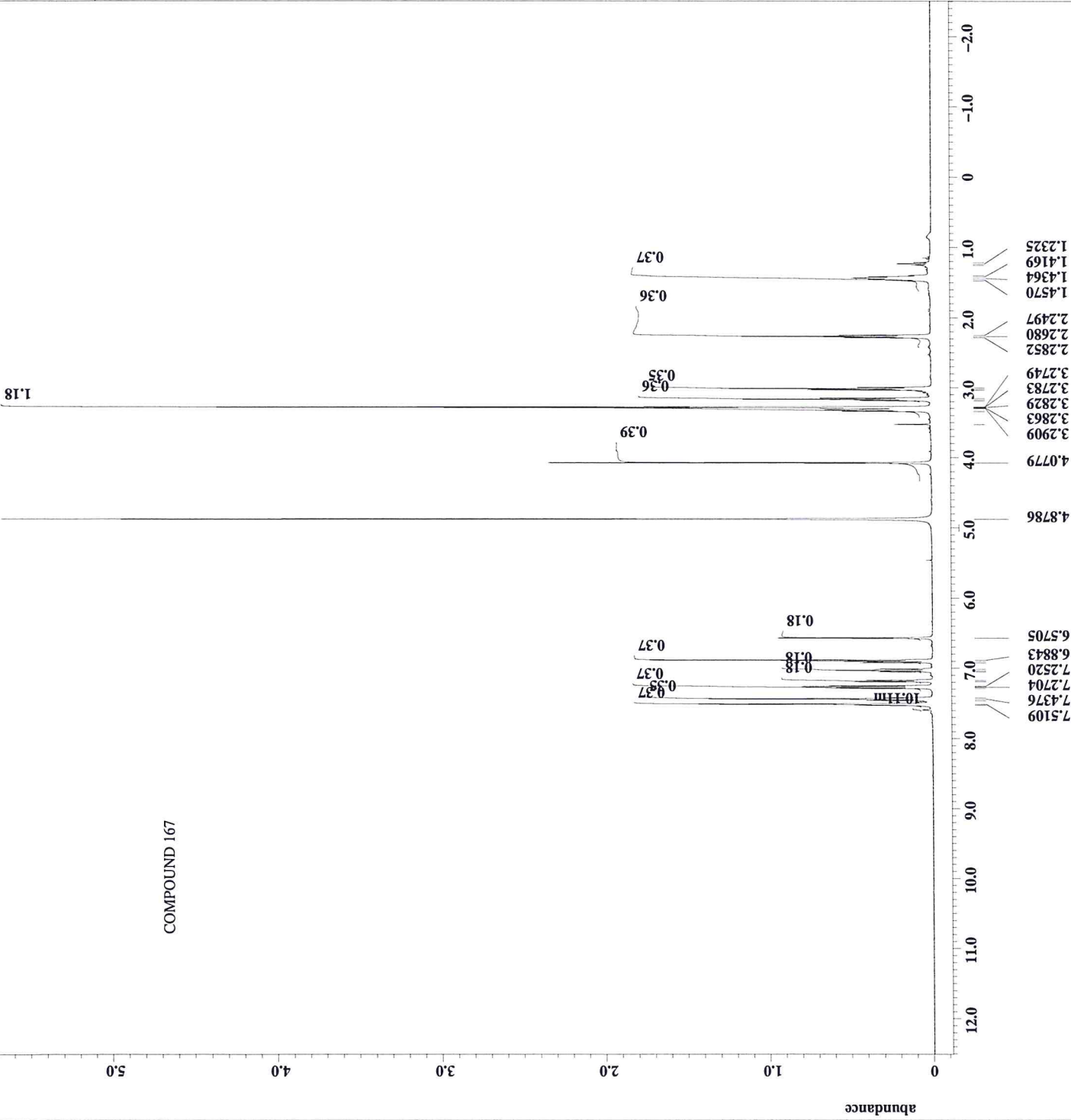
COMPOUND 166



X : parts per Million : 13C



File name = BN-VI-97-C-6-10_PROTO
Author = Delta
Experiment = single_pulse.ex2
Sample_id = BN-VI-97-C-6-10
Solvent = METHANOL-D3
Creation time = 10-JUN-2016 14:50:17
Revision time = 10-MAR-2021 13:22:07
Current_time = 10-MAR-2021 13:22:10
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 44
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 19.7 [degC]



COMPOUND 167

X : parts per Million : 1H



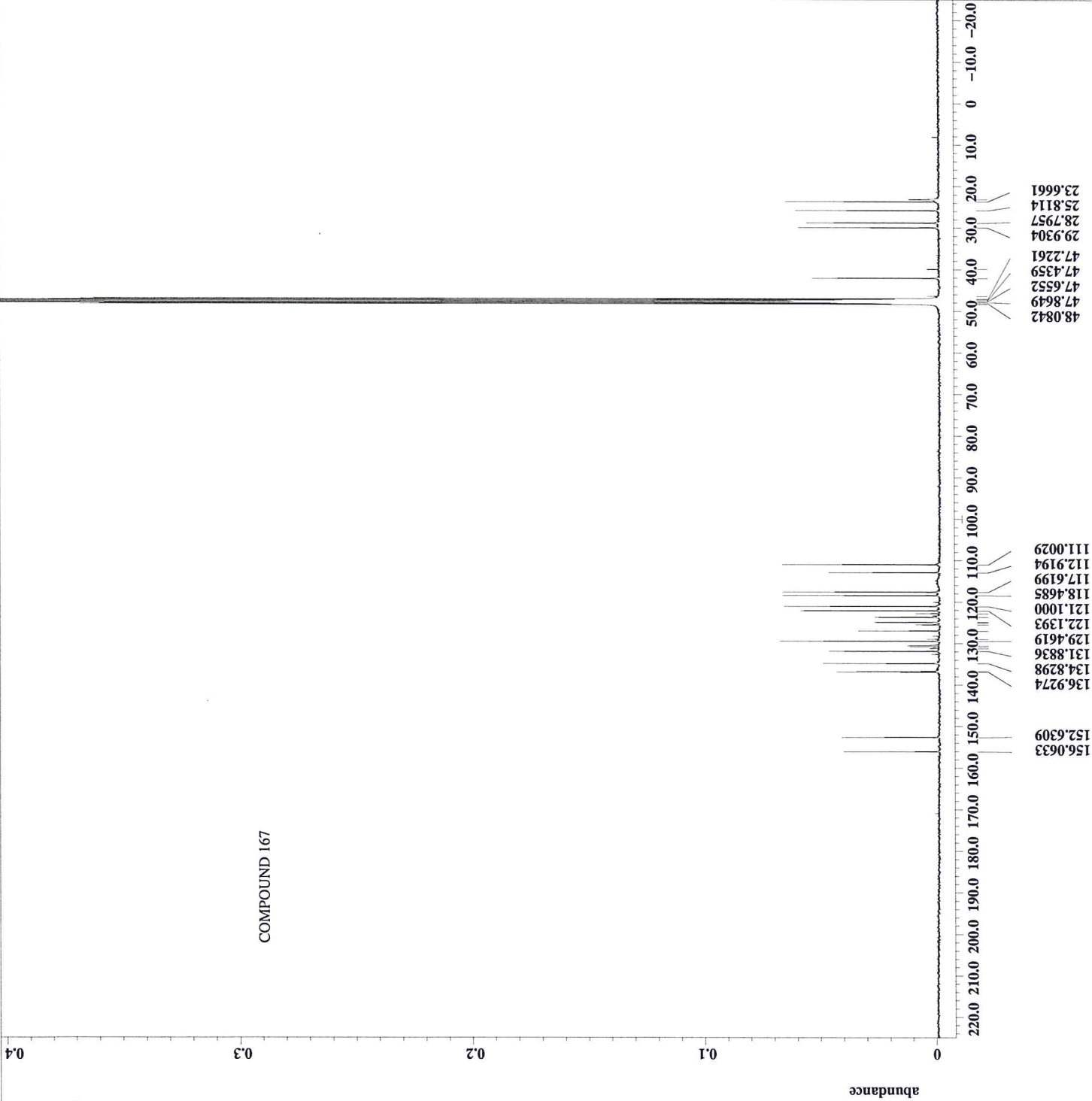
Filename = BN-VI-97-c-6-10_CARBO
Author = Delta
Experiment = single_pulse_dec
Sample_id = BN-VI-97-c-6-10
Solvent = METHANOL-D3
Creation time = 13-JUN-2016 07:37:41
Revision time = 10-MAR-2021 13:23:59
Current_time = 10-MAR-2021 13:24:03

Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 57628
Total_scans = 57628

X_90_width = 12.84[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 9[db]
X_pulse = 4.28[us]
Irr_atn_dec = 27[db]
Irr_atn_noe = 27[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 3[s]
Recvr_gain = 60
Relaxation_delay = 3[s]
Repetition_time = 4.04333312[s]
Temp_get = 20.6[dc]

COMPOUND 167

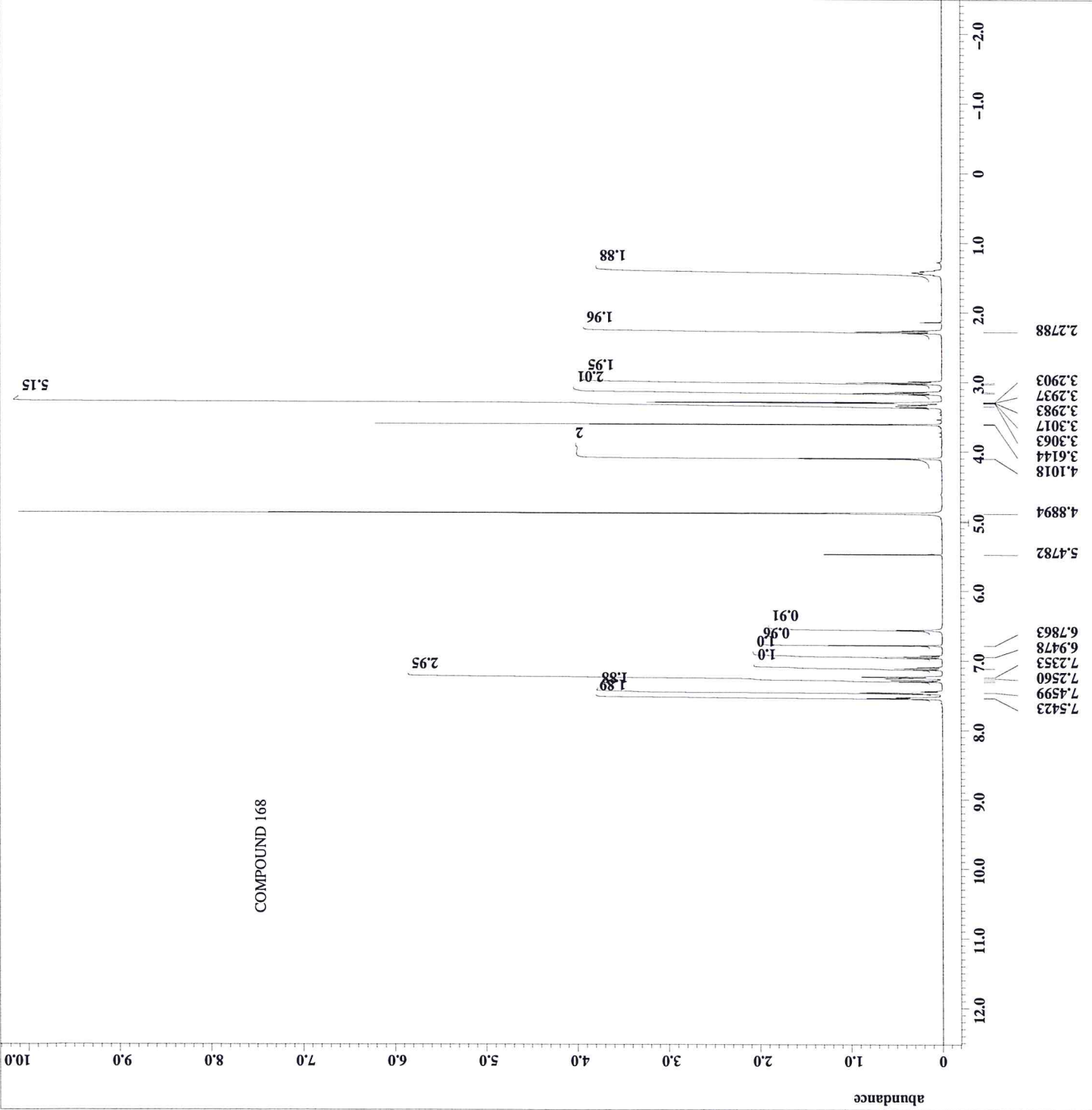


X : parts per Million : 13C



Filename = SM-I-76-F1_PROTON-4.j
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SM-I-76-F1
Solvent = METHANOL-D3
Creation_time = 23-JUN-2016 17:30:41
Revision_time = 11-MAR-2021 09:10:36
Current_time = 11-MAR-2021 09:10:41
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 40
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 20.4 [dC]

COMPOUND 168

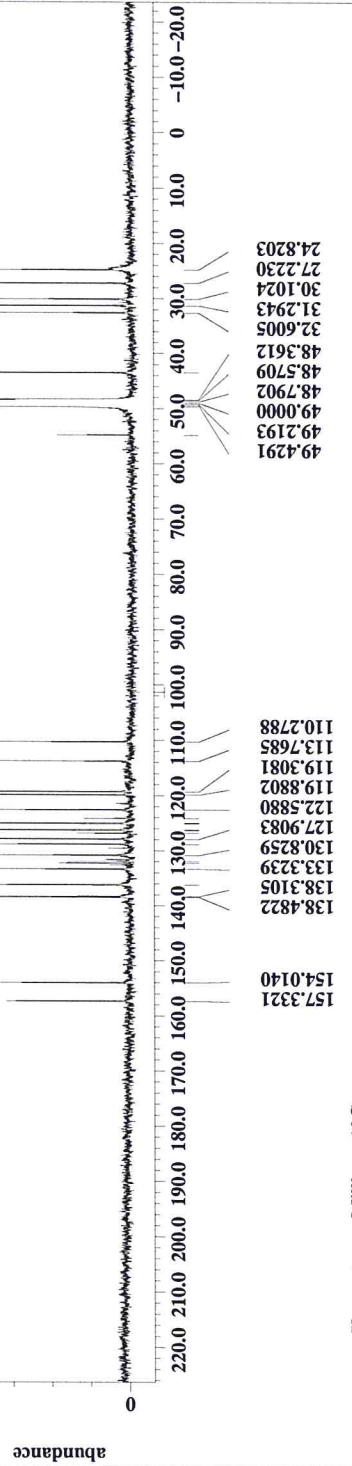


X : parts per Million : 1H



Filename = SM-I-76-F1_CARBON-5.j
Author = Delta
Experiment = single_pulse_dec
Sample_id = SM-I-76-F1
Solvent = METHANOL-D3
Creation_time = 24-JUN-2016 09:14:19
Revision_time = 11-MAR-2021 09:12:40
Current_time = 11-MAR-2021 09:12:45
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 13958
Total_scans = 13958
X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 20.4 [dC]

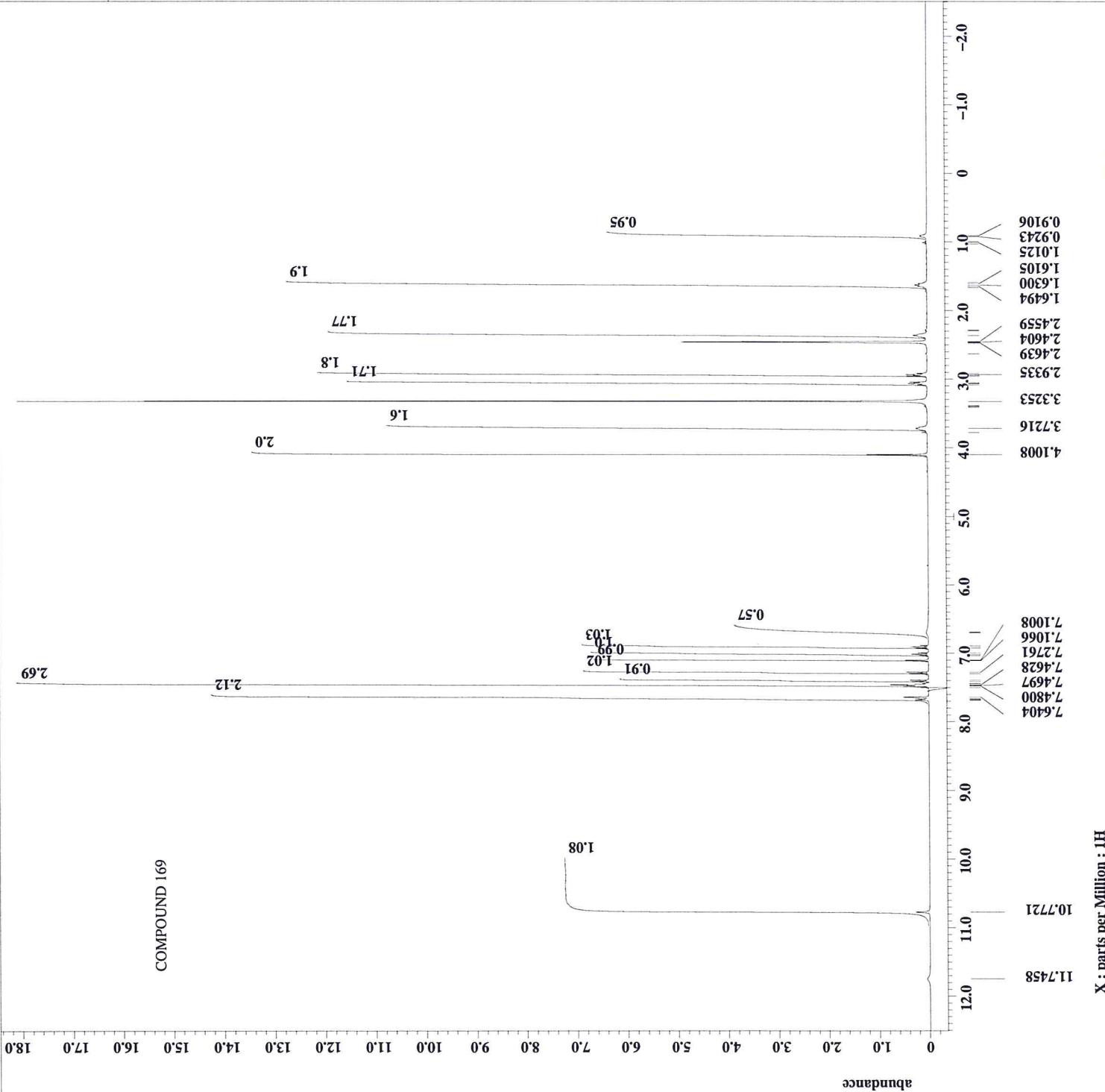
COMPOUND 168



X : parts per Million : 13C



File name = MM-I-63_PROTON-6.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = MM-I-63
Solvent = DMSO-D6
Creation time = 12-OCT-2016 12:14:43
Revision time = 10-MAR-2021 11:54:55
Current_time = 10-MAR-2021 11:54:59
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 38
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 20.1 [dC]





```

Filename = MM-I-63_CARBON-6.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = MM-I-63
Solvent = DMSO-D6
Creation_time = 13-OCT-2016 08:38:32
Revision_time = 10-MAR-2021 11:57:33
Current_time = 10-MAR-2021 11:57:38

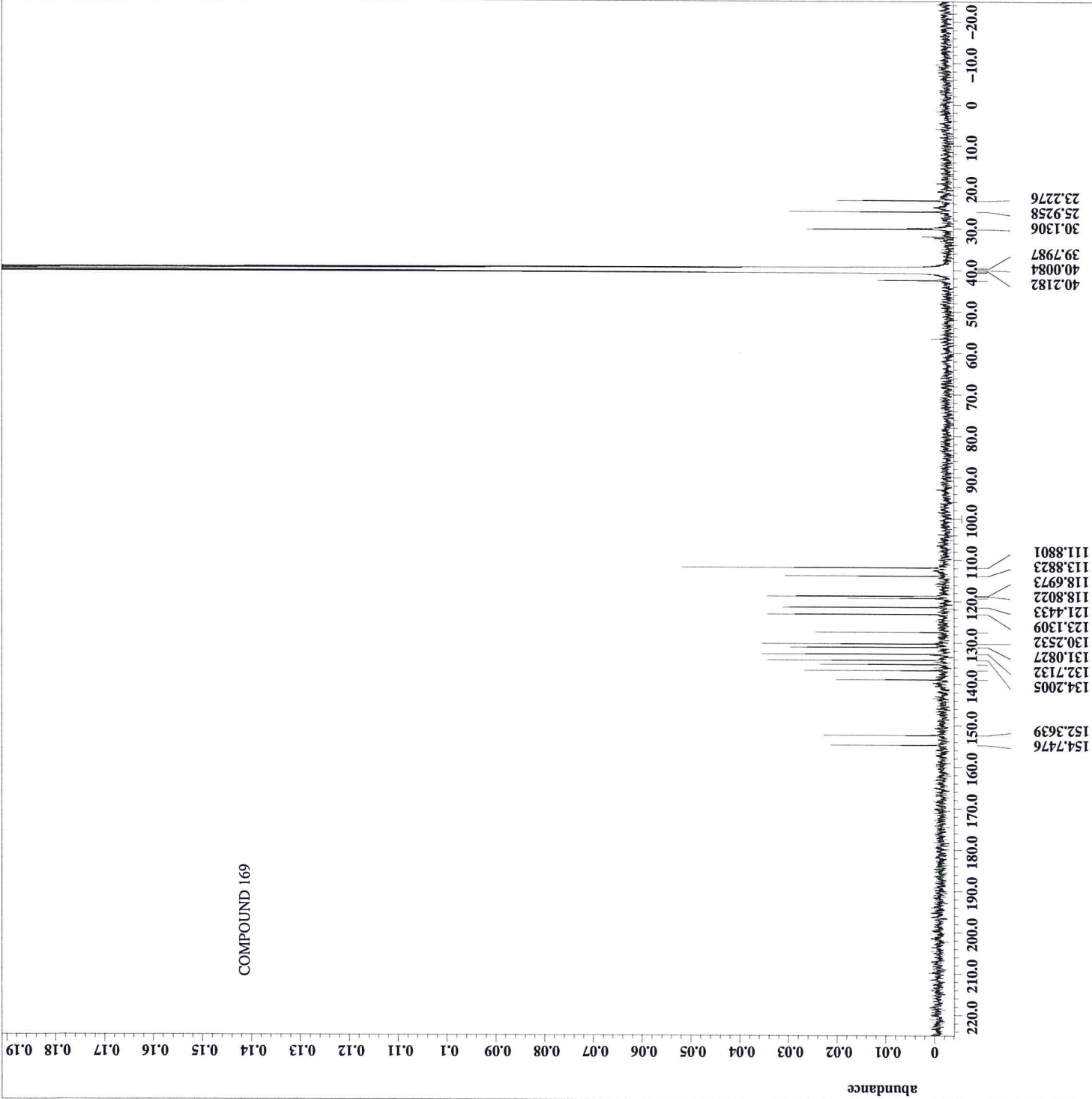
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 13640
Total_scans = 13640

X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Decoupling = WALTZ
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 20.4 [dC]

```

COMPOUND 169



X : parts per Million : 13C



COMPOUND 170

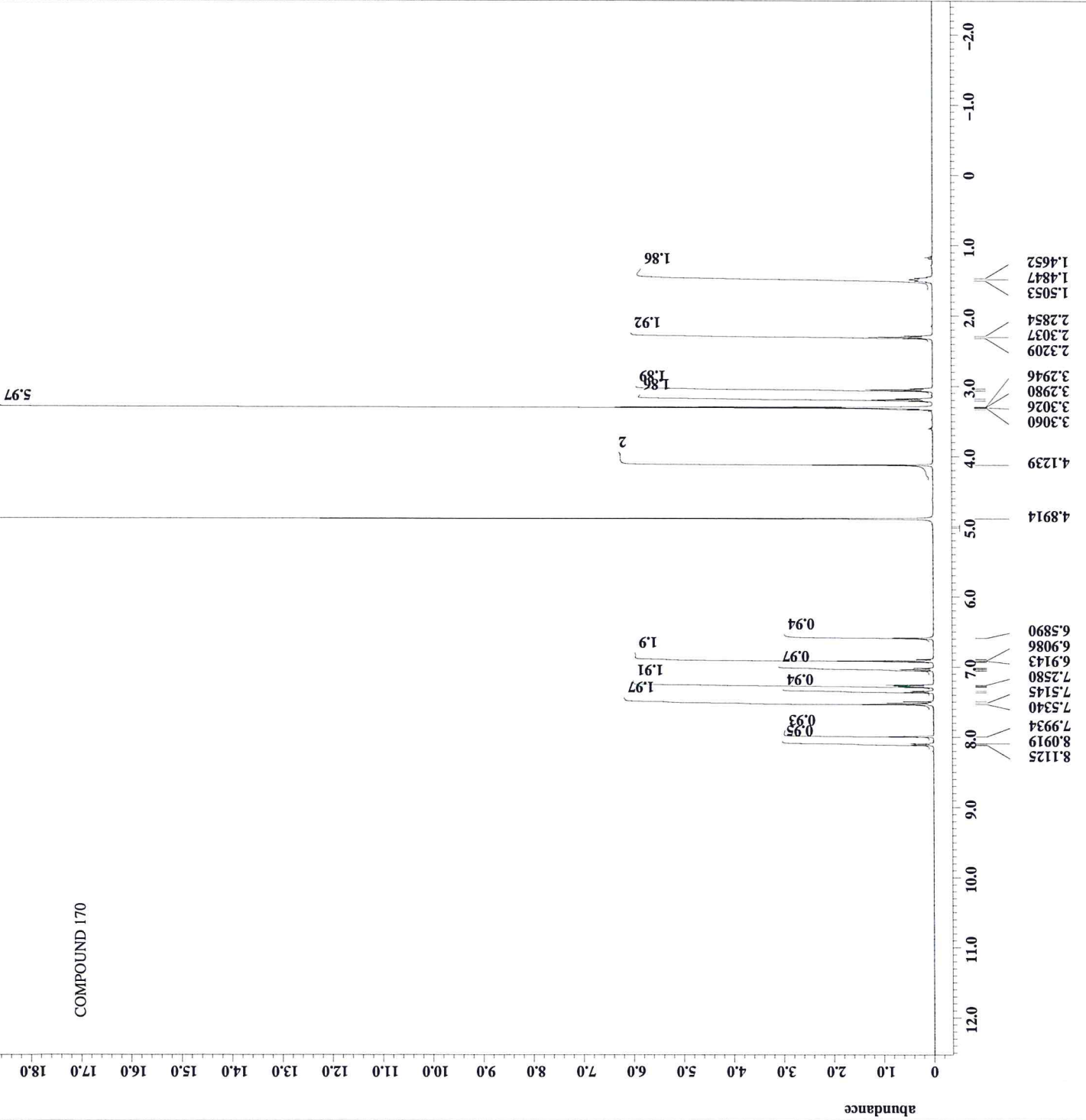
```

File name      = MM-I-43_PROTON-5.jdf
Author        = Delta
Experiment    = single_pulse.ex2
Sample ID     = MM-I-43
Solvent       = METHANOL-D3
Creation time = 21-JUL-2016 10:21:24
Revision time = 10-MAR-2021 13:31:46
Current time  = 10-MAR-2021 13:31:50

Data format   = 1D COMPLEX
Dim size      = 13107
Dim title     = 1H
Dim units     = [ppm]
Dimensions    = X
Site          = ECS 400
Spectrometer  = JNM-ECS400

Field strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain      = 1H
X_freq        = 399.78219838 [MHz]
X_offset      = 5 [ppm]
X_points      = 16384
X_prescans    = 1
X_resolution  = 0.45794685 [Hz]
X_sweep       = 7.5030012 [kHz]
Irr_domain    = 1H
Irr_freq      = 399.78219838 [MHz]
Irr_offset    = 5 [ppm]
Tri_domain    = 1H
Tri_freq      = 399.78219838 [MHz]
Tri_offset    = 5 [ppm]
Clipped       = FALSE
Mod_return    = 1
Total_scans   = 16

X_90_width    = 10.68 [us]
X_acq_time    = 2.18365952 [s]
X_angle       = 45 [deg]
X_atn         = 6 [dB]
X_pulse       = 5.34 [us]
Irr_mode      = Off
Tri_mode      = Off
Dante_presat  = FALSE
Initial_wait  = 1 [s]
Recvr_gain    = 46
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get      = 20 [dC]
  
```

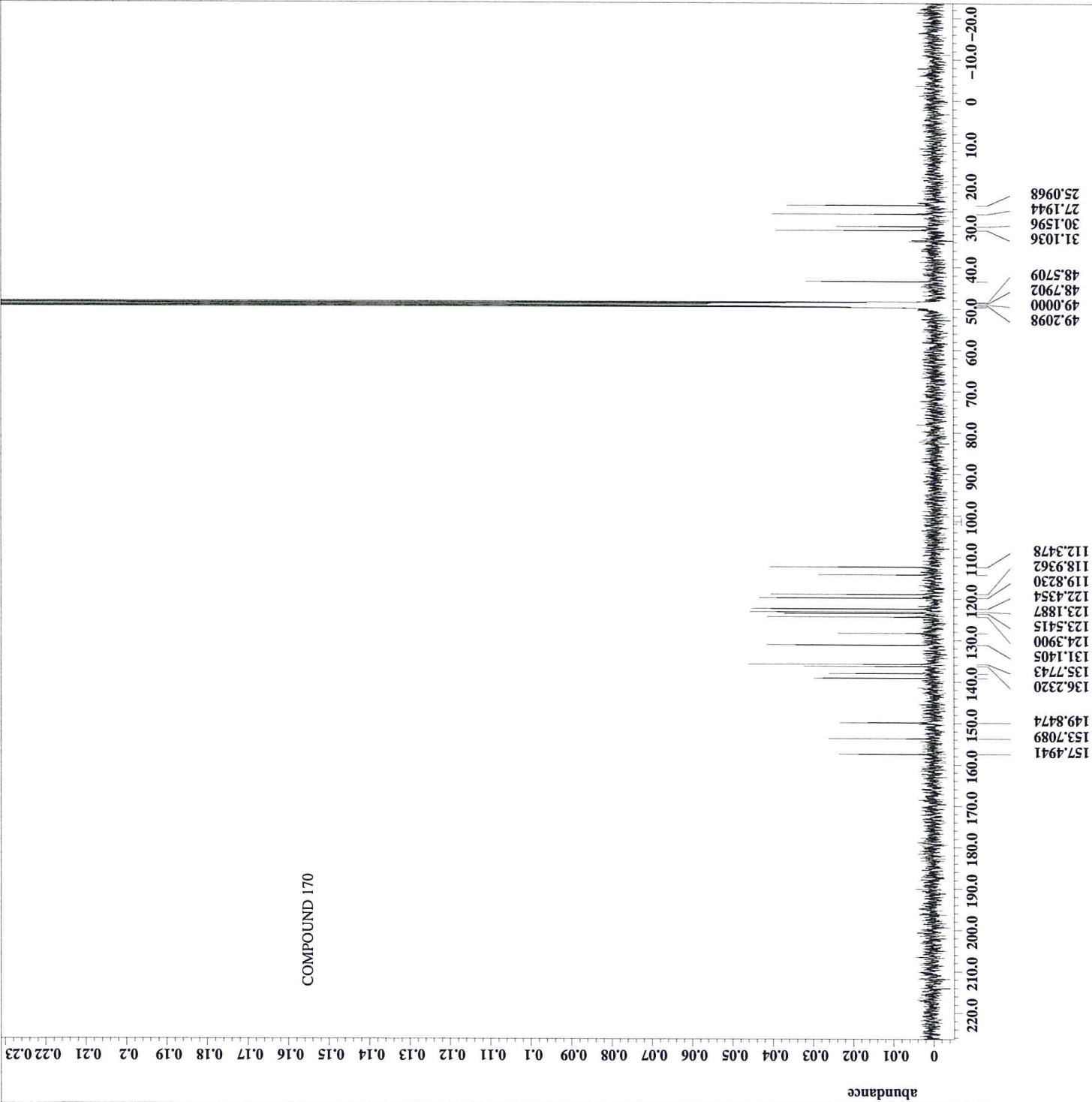


X : parts per Million : 1H

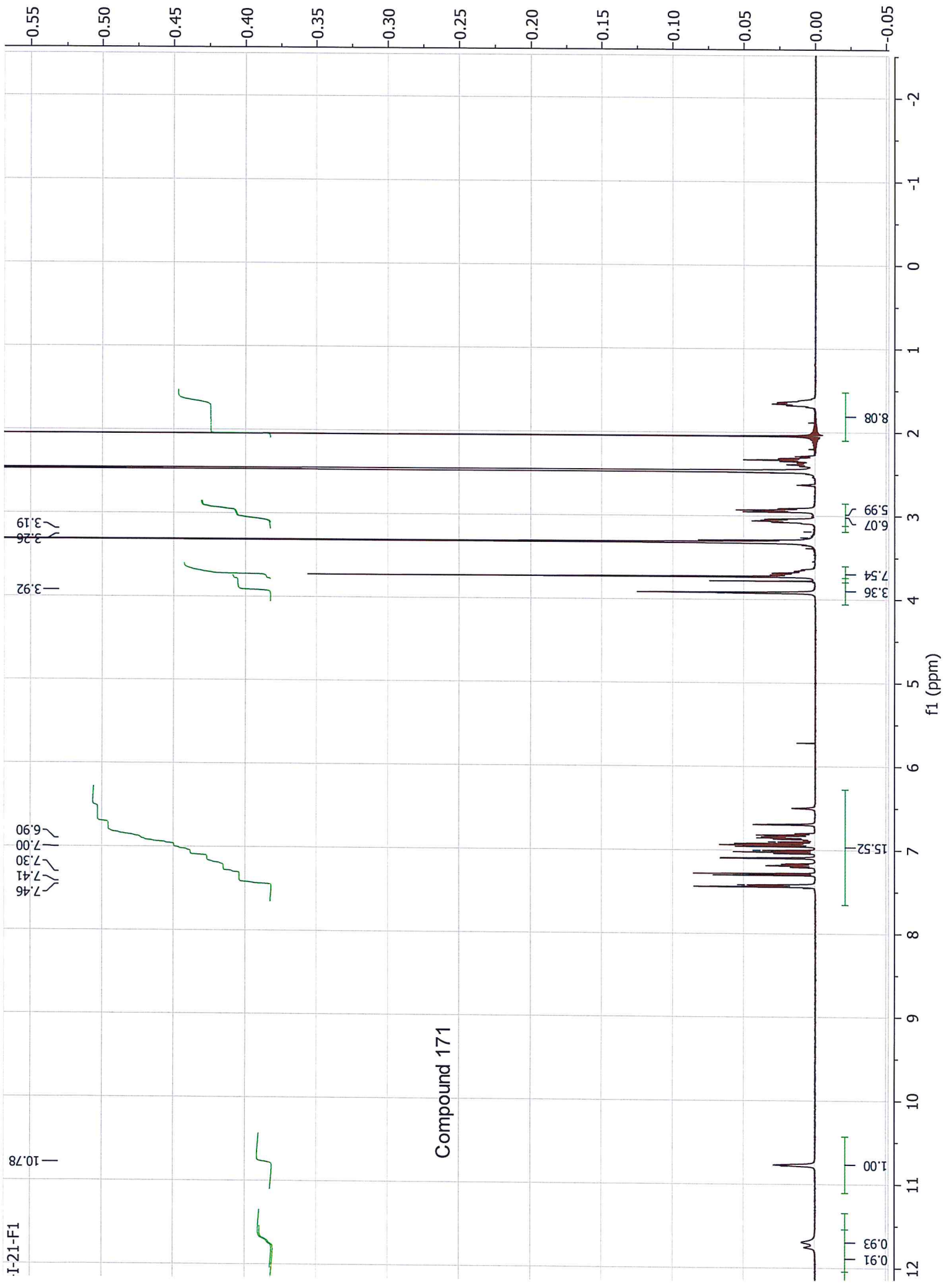


Filename = MM-I-43_CARBON-5.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = MM-I-43
Solvent = METHANOL-D3
Creation_time = 21-JUL-2016 14:41:52
Revision_time = 10-MAR-2021 13:34:22
Current_time = 10-MAR-2021 13:34:26
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 3837
Total_scans = 3837
X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 20.2 [dC]

COMPOUND 170



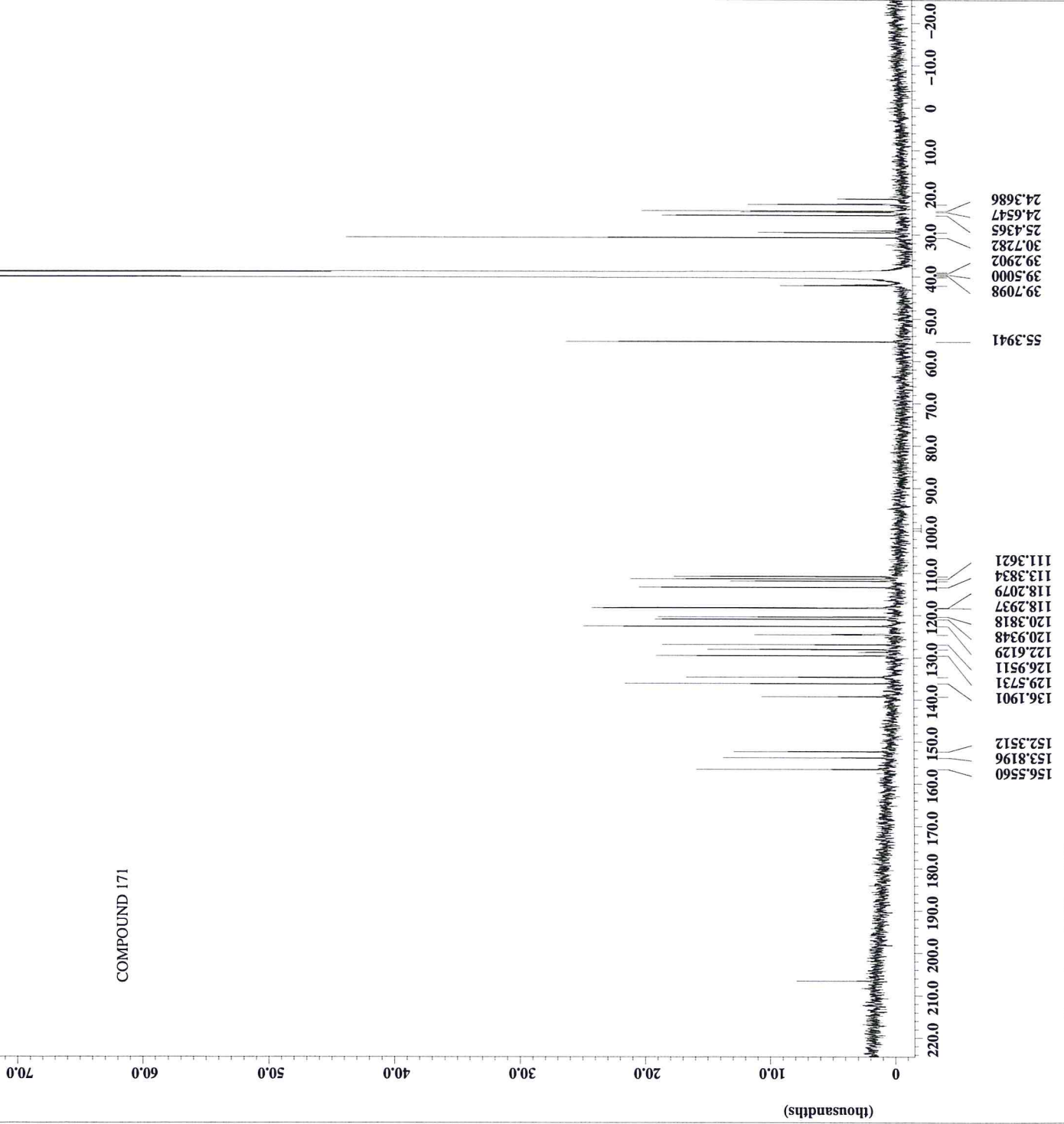
X : parts per Million : 13C





File name = MM-I-21-F1_CARBON-5.j
Author = Delta
Experiment = single_pulse_dec
Sample_id = MM-I-21-F1
Solvent = DMSO-D6
Creation time = 2-MAY-2016 07:35:26
Revision time = 10-MAR-2021 13:38:11
Current_time = 10-MAR-2021 13:38:15
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 57480
Total_scans = 57480
X_90_width = 12.84[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 9[db]
X_pulse = 4.28[us]
Irr_atn_dec = 27[db]
Irr_atn_noe = 27[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 3[s]
Recvr_gain = 60
Relaxation_delay = 3[s]
Repetition_time = 4.04333312[s]
Temp_get = 21.1[degC]

COMPOUND 171



X : parts per Million : 13C



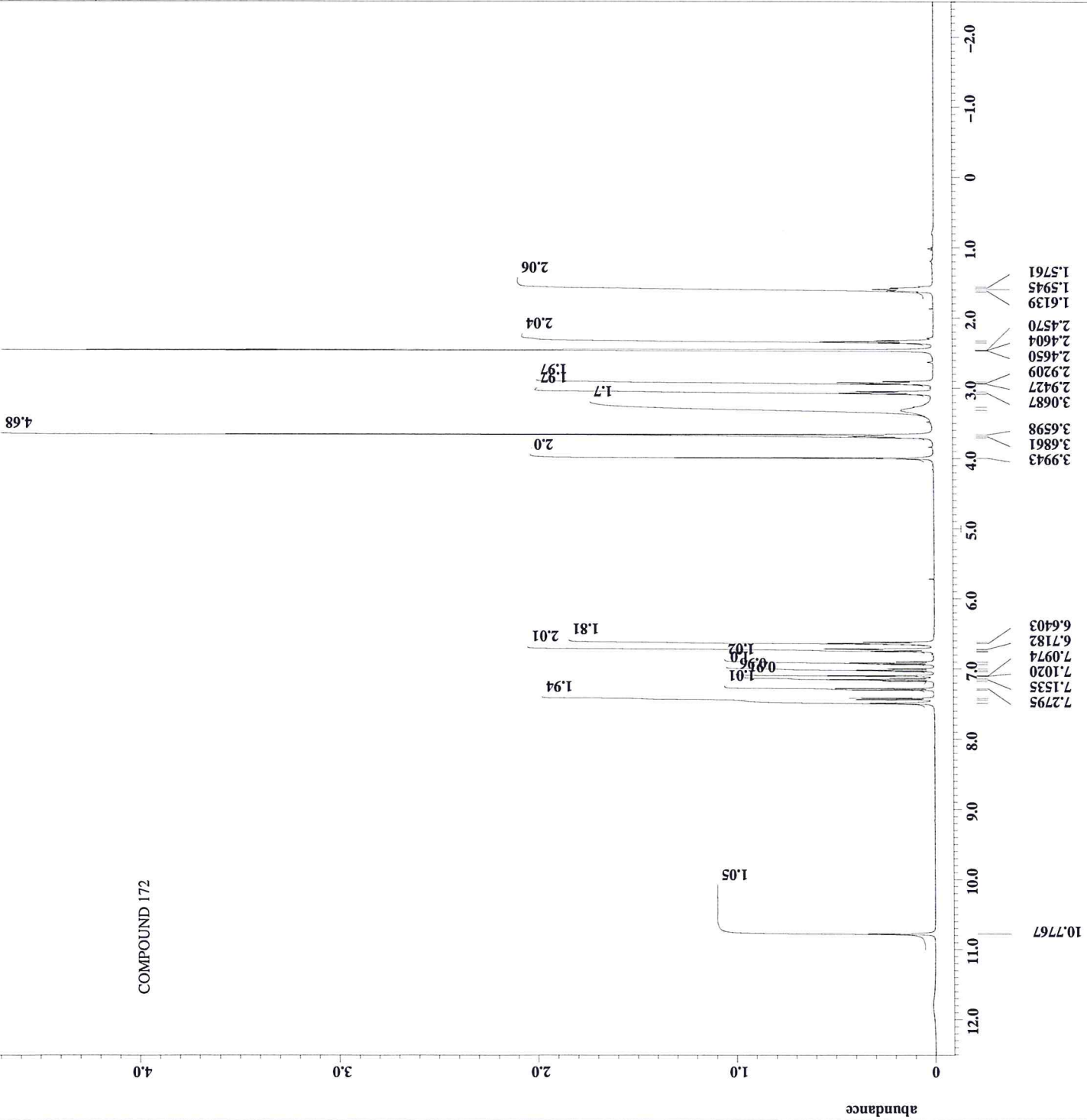
COMPOUND 172

Filename = BN-VI-61-c_PROTON-4.j
Author = Neumann
Experiment = single_pulse.ex2
Sample_id = BN-VI-61-c
Solvent = DMSO-D6
Creation_time = 21-OCT-2015 10:41:08
Revision_time = 10-MAR-2021 11:39:53
Current_time = 10-MAR-2021 11:39:57

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
total_scans = 16

X_90_width = 10.58 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.29 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 38
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
temp_get = 20.2 [degC]

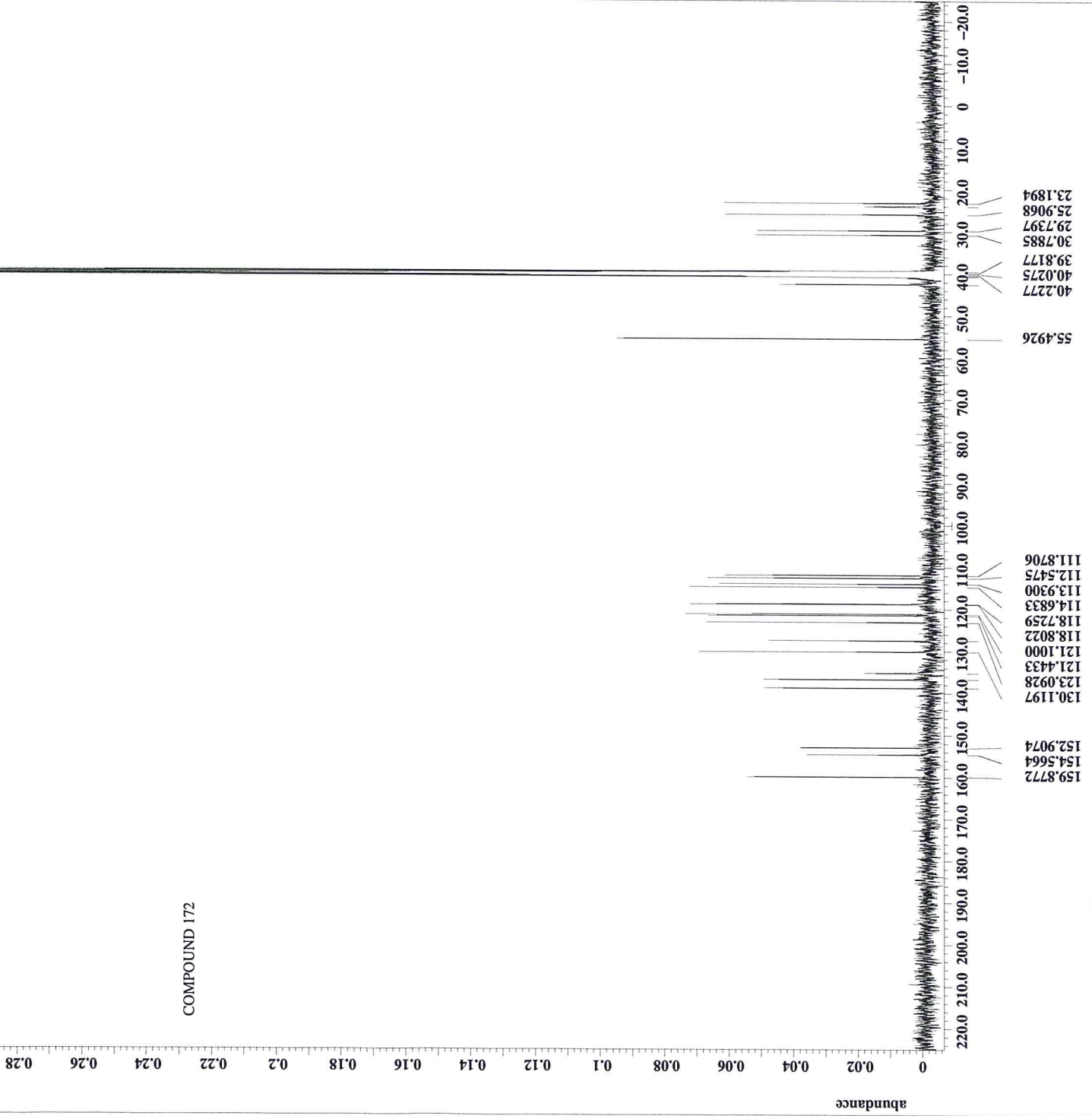


X : parts per Million : 1H



File name = BN-VI-61-C CARBON-4.j
Author = Neumann
Experiment = single_pulse_dec
Sample_id = BN-VI-61-C
Solvent = DMSO-D6
Creation_time = 21-OCT-2015 13:03:14
Revision_time = 10-MAR-2021 11:41:20
Current_time = 10-MAR-2021 11:41:24
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = FALSE
Clipped = FALSE
Mod_return = 1
Scans = 2048
Total_scans = 2048
X_90_width = 13.12 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.37333333 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 20.5 [dC]

COMPOUND 172



X : parts per Million : 13C



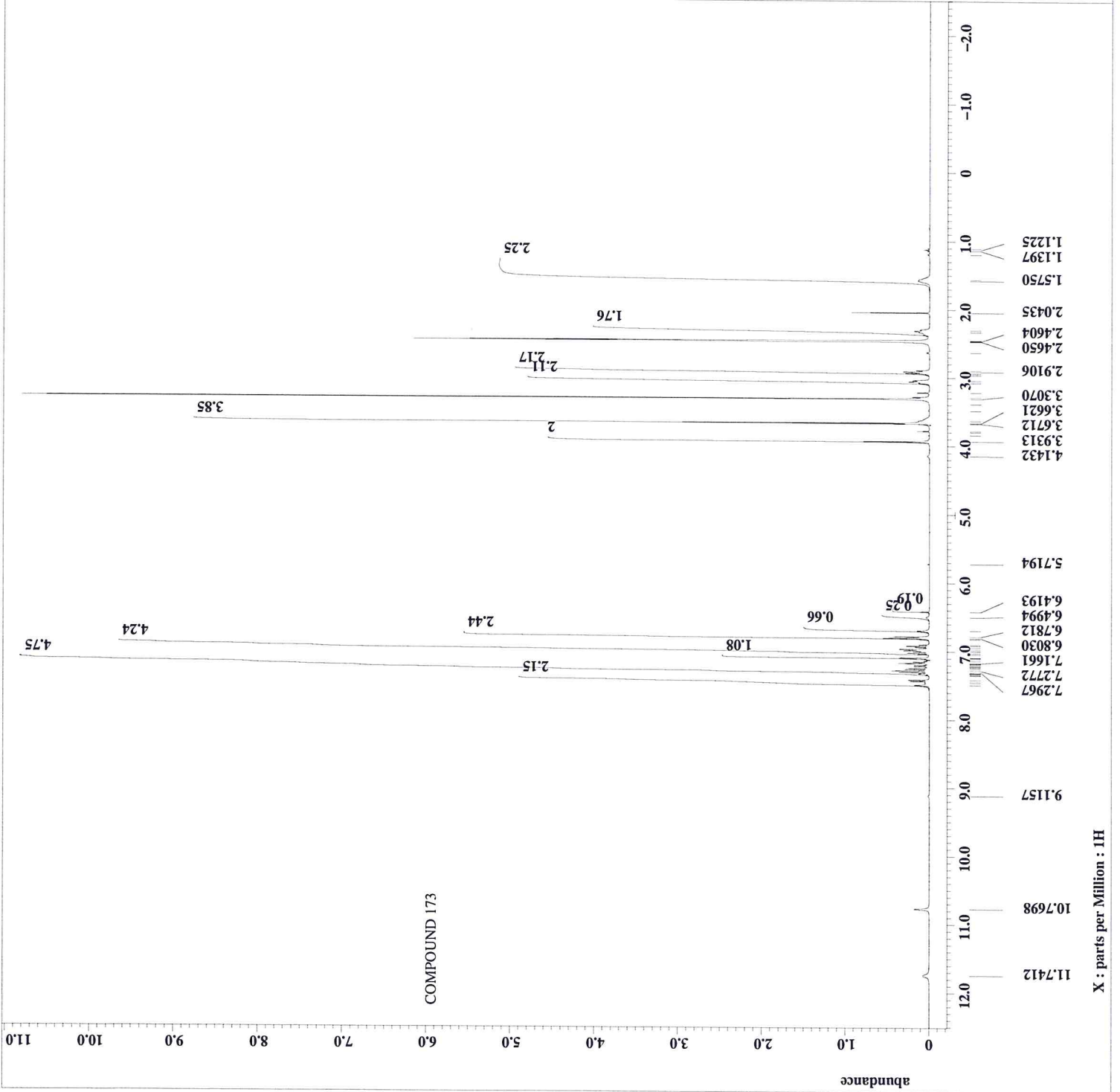
```

Filename = SM-I-29-F1-2_PROTON-6
Author = Deita
Experiment = single_pulse.ex2
Sample_id = SM-I-29-F1-2
Solvent = DMSO-D6
Creation_time = 14-MAY-2016 12:36:49
Revision_time = 17-MAR-2021 13:48:55
Current_time = 17-MAR-2021 13:49:02

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

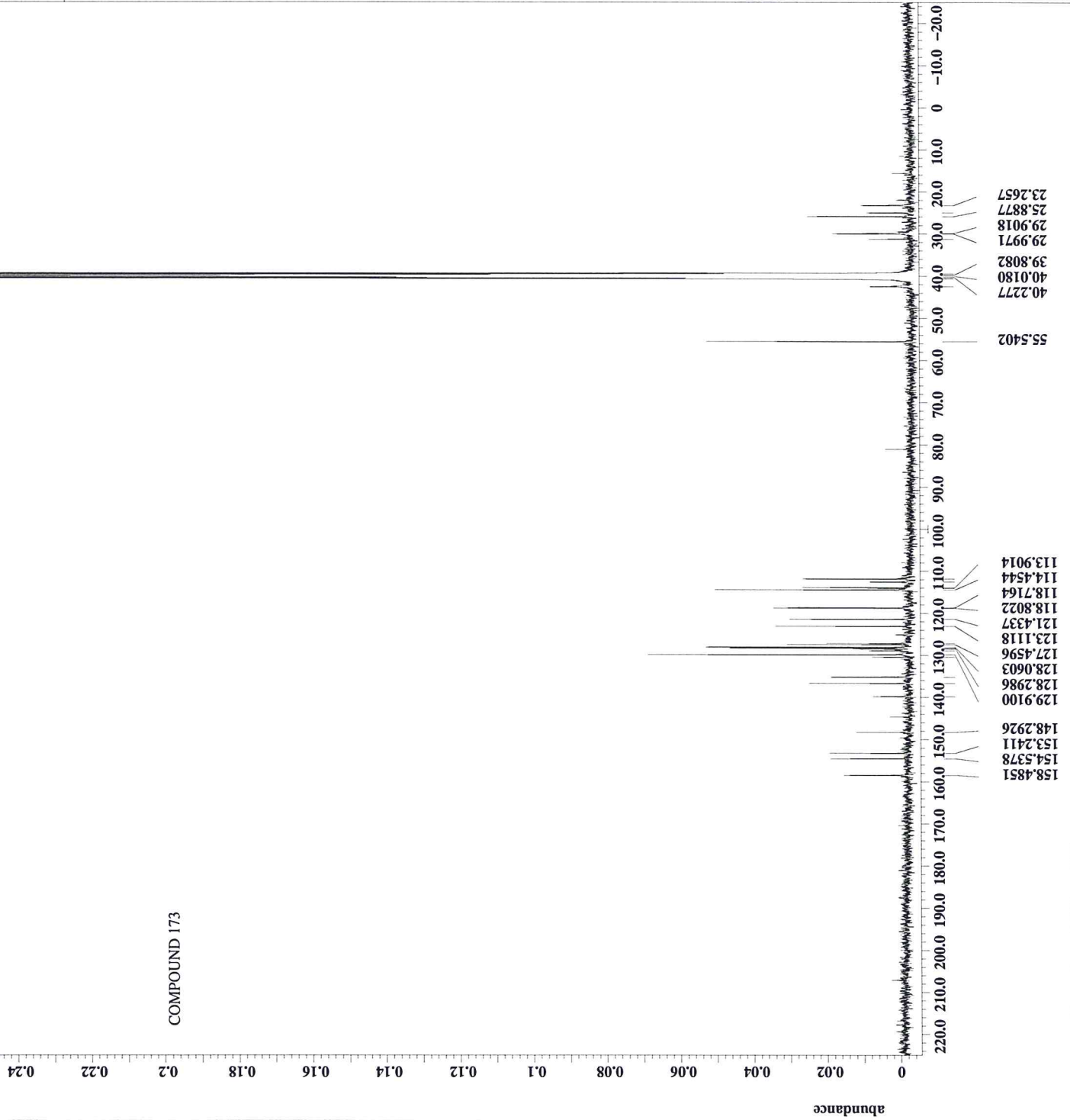
X_90_width = 10.68[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.34[us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 4[s]
Repetition_time = 6.18365952[s]
Temp_get = 20.6[dc]
  
```





File name = SM-I-29-F1-2_CARBON-6
Author = Delta
Experiment = single_pulse_dec
Sample_id = SM-I-29-F1-2
Solvent = DMSO-D6
Creation_time = 15-MAY-2016 00:08:20
Revision_time = 10-MAR-2021 13:47:26
Current_time = 10-MAR-2021 13:47:31
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[MHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 10240
Total_scans = 10240
X_90_width = 12.84[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 9[db]
X_pulse = 4.28[us]
Irr_atn_dec = 27[db]
Irr_atn_noe = 27[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 3[s]
Recvr_gain = 60
Relaxation_delay = 3[s]
Repetition_time = 4.04333312[s]
Temp_get = 19.9[degC]

COMPOUND 173



X : parts per Million : 13C

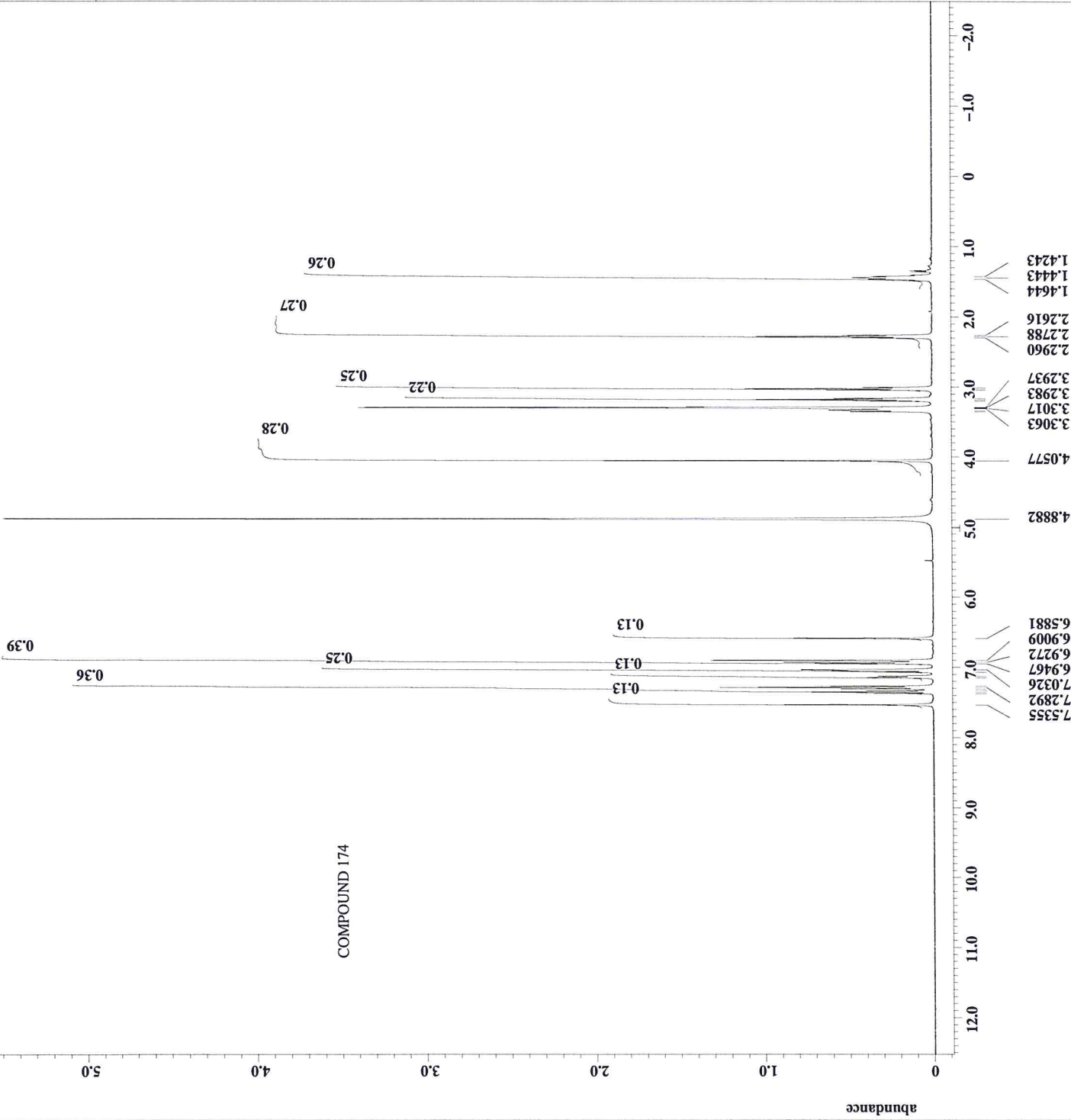


File: MM-I-36_PROTON-4.jdf
Author: Delta
Experiment: single_pulse.ex2
Sample_id: MM-I-36
Solvent: METHANOL-D3
Creation_time: 6-JUL-2016 09:50:38
Revision_time: 11-MAR-2021 10:04:13
Current_time: 11-MAR-2021 10:04:17

Data_format: 1D COMPLEX
Dim_size: 13107
Dim_title: 1H
Dim_units: [ppm]
Dimensions: X
Site: ECS 400
Spectrometer: JNM-ECS400

Field_strength: 9.389766 [T] (400 [MHz])
X_acq_duration: 2.18365952 [s]
X_domain: 1H
X_freq: 399.78219838 [MHz]
X_offset: 5 [ppm]
X_points: 16384
X_prescans: 1
X_resolution: 0.45794685 [Hz]
X_sweep: 7.5030012 [kHz]
Irr_domain: 1H
Irr_freq: 399.78219838 [MHz]
Irr_offset: 5 [ppm]
Tri_domain: 1H
Tri_freq: 399.78219838 [MHz]
Tri_offset: 5 [ppm]
Clipped: FALSE
Mod_return: 1
Scans: 16
Total_scans: 16

X_90_width: 10.68 [us]
X_acq_time: 2.18365952 [s]
X_angle: 45 [deg]
X_atn: 6 [dB]
X_pulse: 5.34 [us]
Irr_mode: Off
Tri_mode: Off
Dante_presat: FALSE
Initial_wait: 1 [s]
Recvr_gain: 44
Relaxation_delay: 4 [s]
Repetition_time: 6.18365952 [s]
Temp_get: 20.8 [dC]



X : parts per Million : 1H



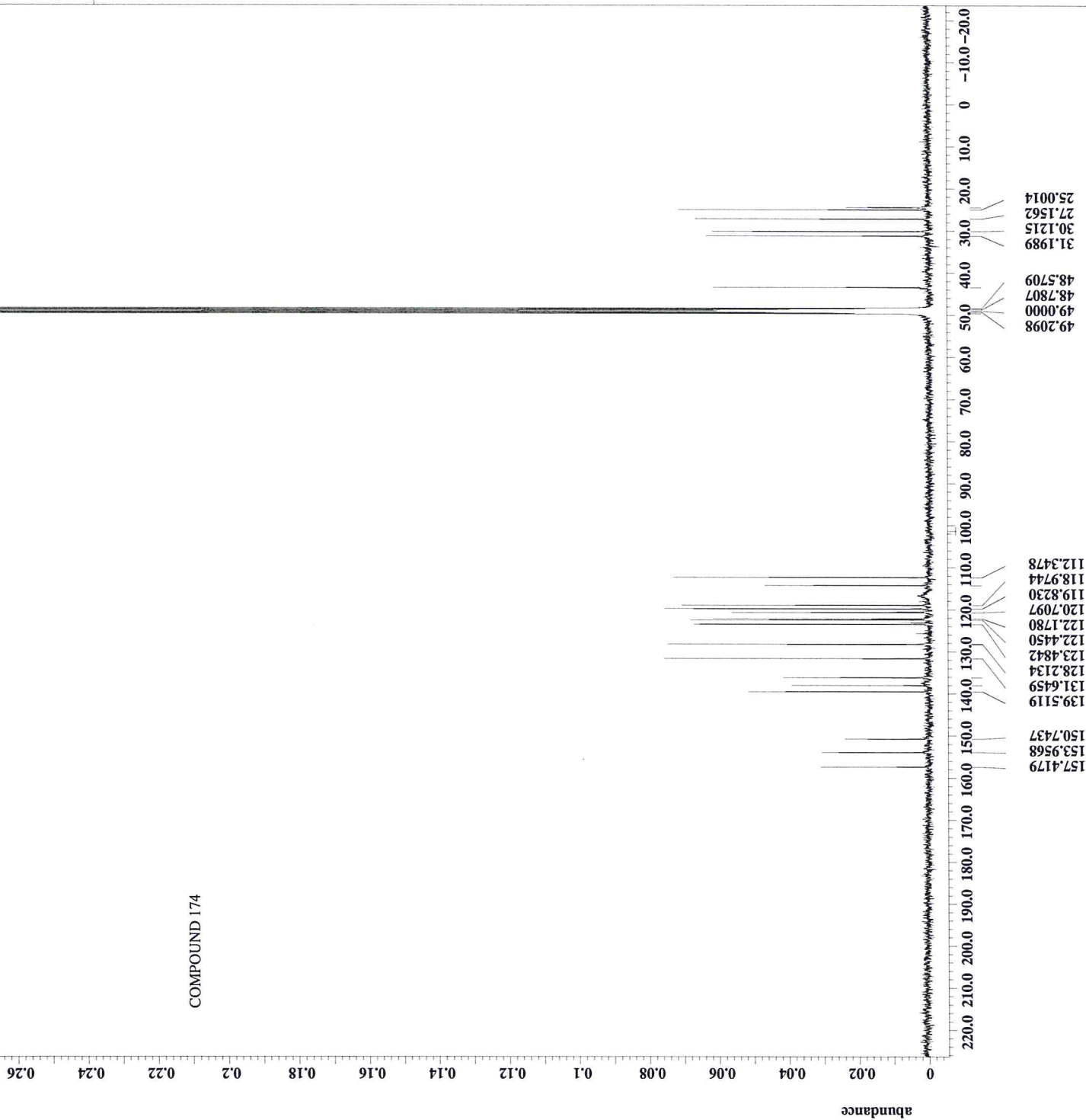
Filename = MM-I-36_CARBON-5.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = MM-I-36
Solvent = METHANOL-D3
Creation time = 7-JUL-2016 08:51:17
Revision time = 11-MAR-2021 10:06:30
Current_time = 11-MAR-2021 10:06:34

Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 14203.0
Total_scans = 14203.0

X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 20.5 [dC]

COMPOUND 174



X : parts per Million : 13C



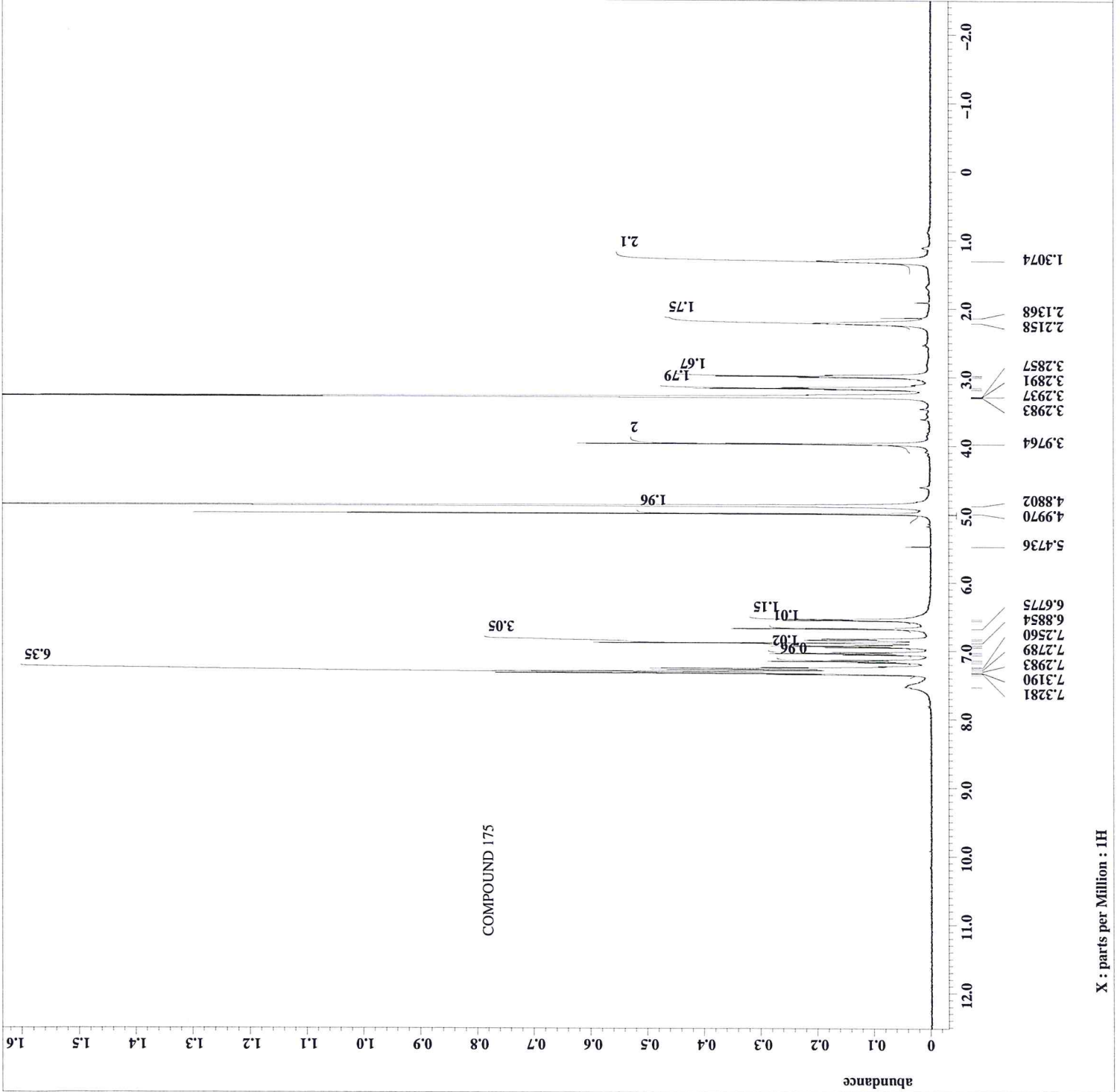
```

= MM-I-53_PROTON-5.jdf
= Delta
= single_pulse.ex2
= MM-I-53
= METHANOL-D3
= 5-AUG-2016 17:53:53
= 17-MAR-2021 14:23:27
= 17-MAR-2021 14:23:30

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

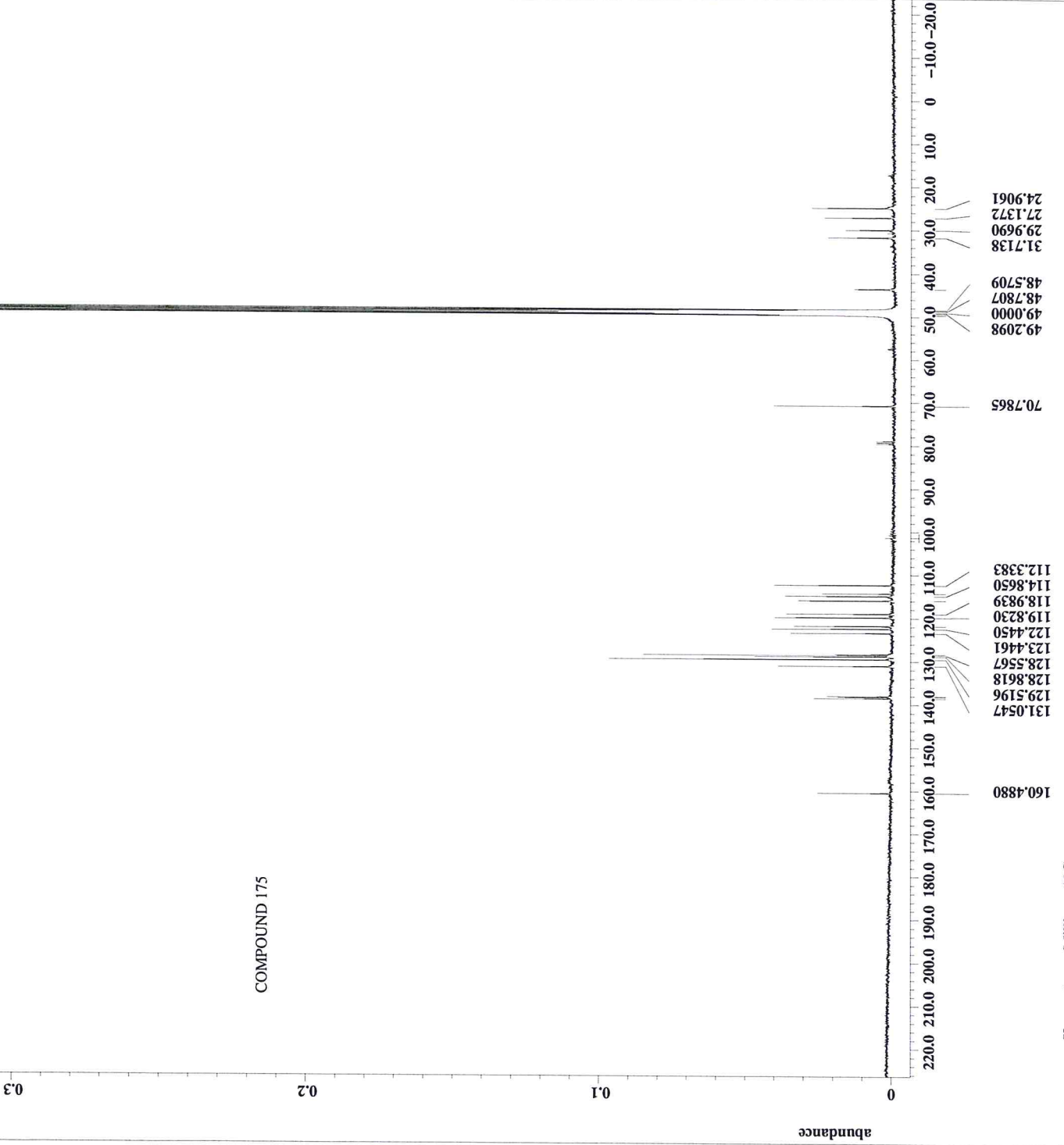
X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 42
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 20.4 [dC]
  
```





Filename = MM-I-53_CARBON-5.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = MM-I-53
Solvent = METHANOL-D3
Creation_time = 8-AUG-2016 07:20:49
Revision_time = 11-MAR-2021 10:19:20
Current_time = 11-MAR-2021 10:19:25
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.0433312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 54685
Total_scans = 54685
X_90_width = 12.84 [us]
X_acq_time = 1.0433312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noise = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.0433312 [s]
Temp_get = 20.5 [dc]

COMPOUND 175



X : parts per Million : 13C

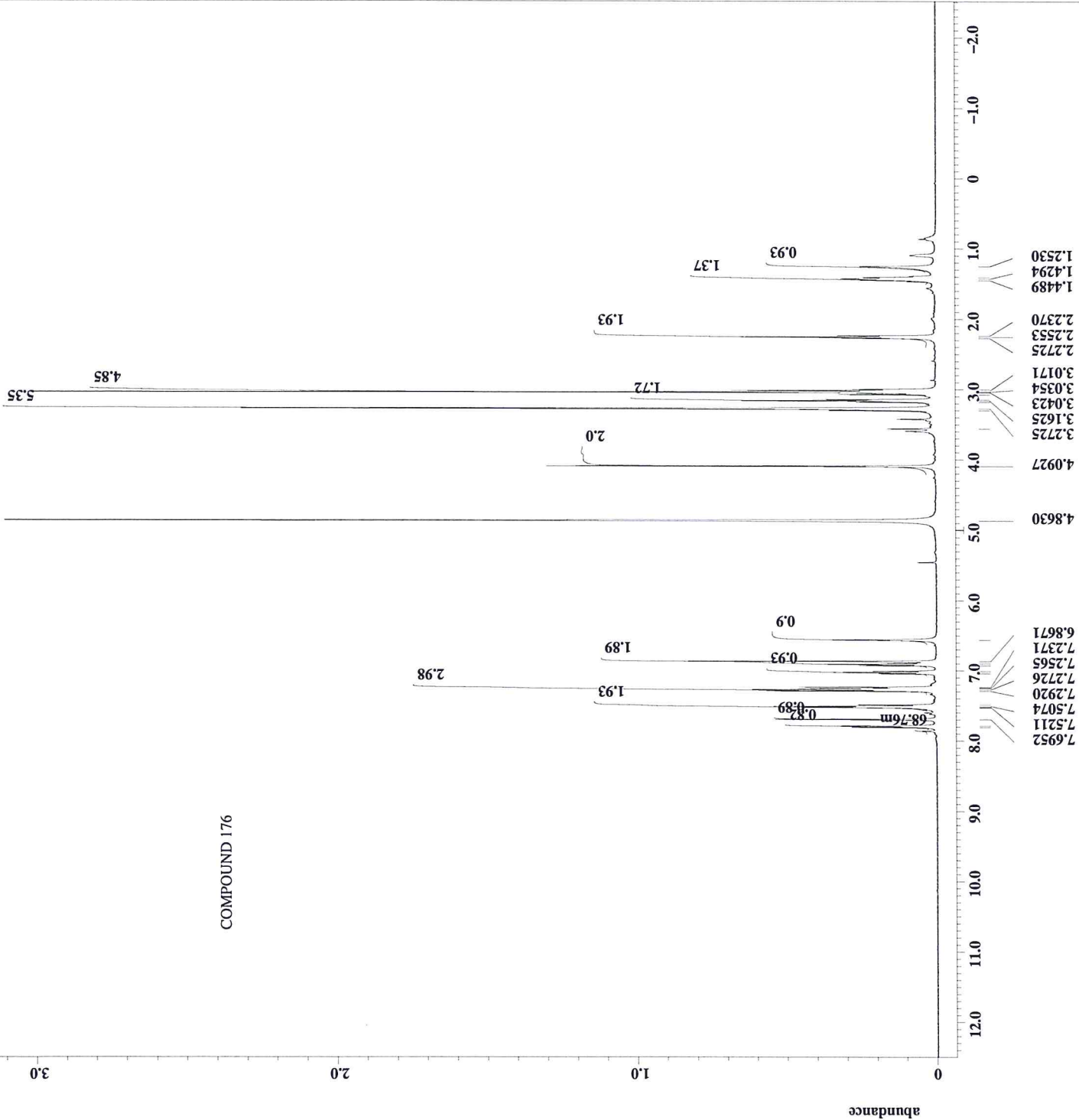


File name = SM-I-92-c_PROTON-4.jd
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SM-I-92-c
Solvent = METHANOL-D3
Creation time = 16-AUG-2016 16:19:57
Revision time = 11-MAR-2021 09:50:01
Current time = 11-MAR-2021 09:50:06

Data format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 10.68[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.34[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 4[s]
Repetition_time = 6.18365952[s]
Temp_get = 19.9[degC]

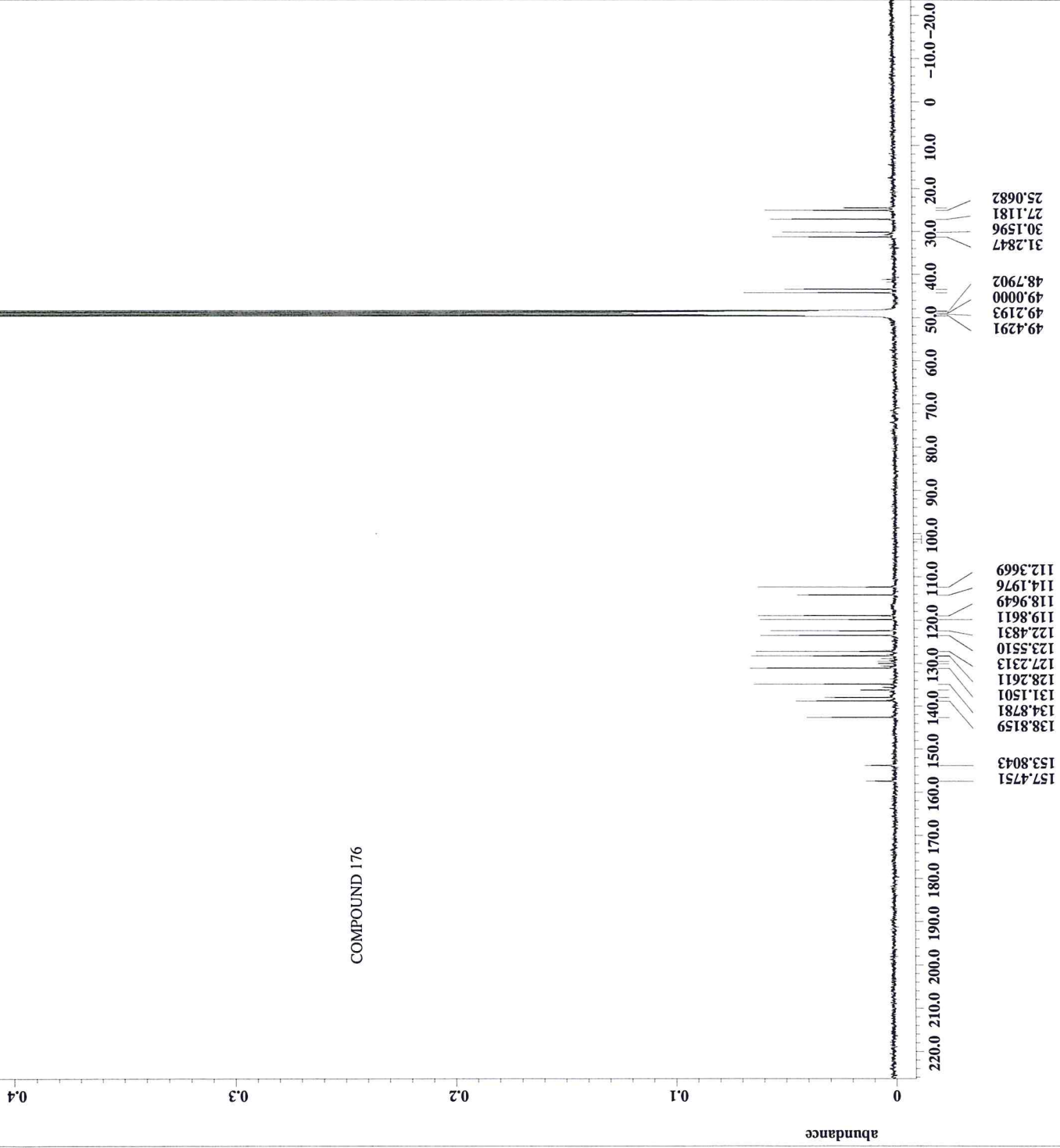


X : parts per Million : 1H



Filename = SW-I-92-C_CARBON-5.jd
Author = Delta
Experiment = single_pulse_dec
Sample_id = SM-I-92-C
Solvent = METHANOL-D3
Creation_time = 17-AUG-2016 08:16:30
Revision_time = 11-MAR-2021 09:52:01
Current_time = 11-MAR-2021 09:52:05
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 14145
Total_scans = 14145
X_90_width = 12.84[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 9[db]
X_pulse = 4.28[us]
Irr_atn_dec = 27[db]
Irr_atn_noe = 27[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 3[s]
Recvr_gain = 60
Relaxation_delay = 3[s]
Repetition_time = 4.04333312[s]
Temp_get = 20[dc]

COMPOUND 176



X : parts per Million : 13C

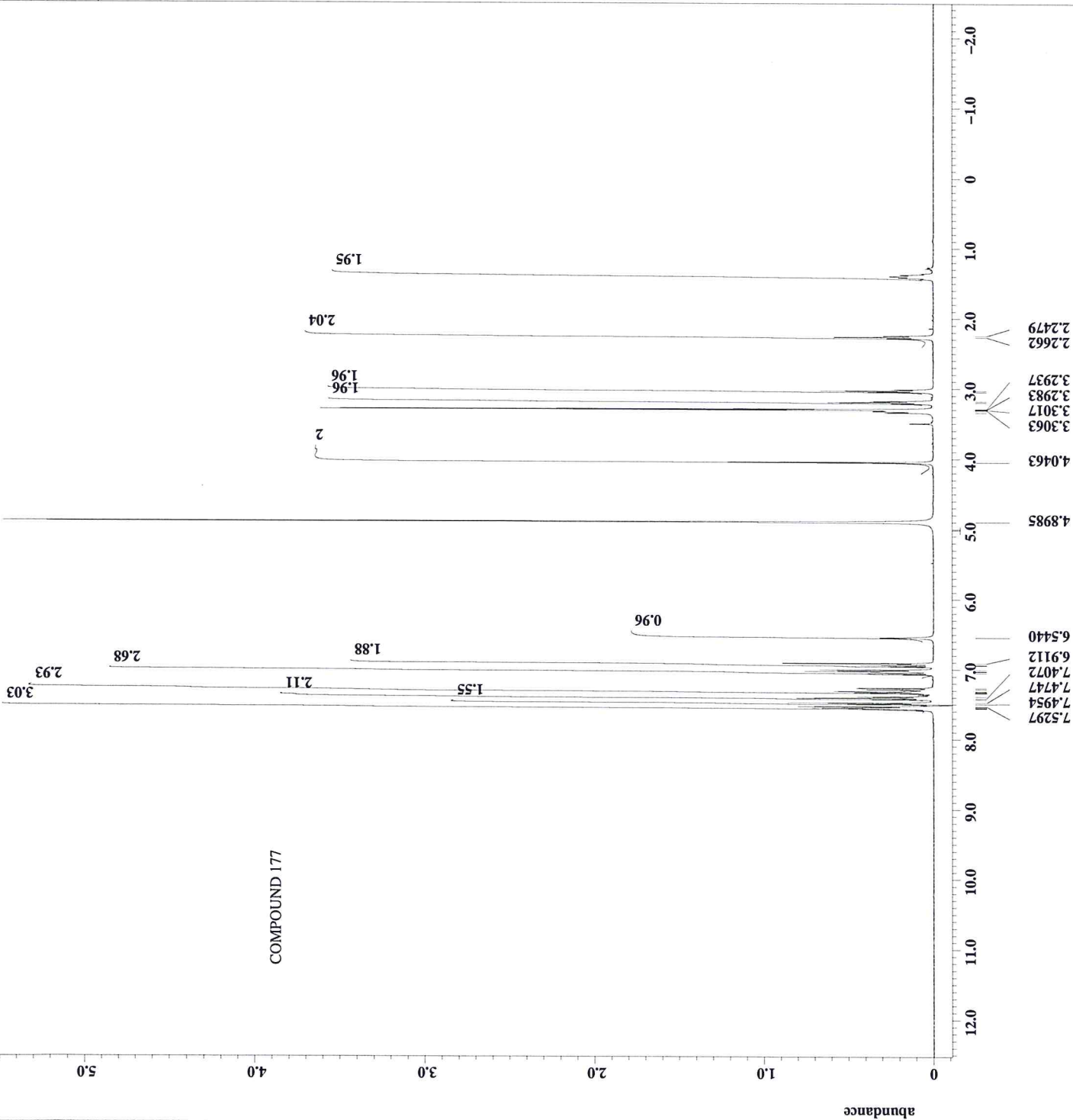


Filename = MM-I-26-F1_PROTON-4.j
Author = Delta
Experiment = single_pulse.ex2
Sample_id = MM-I-26-F1
Solvent = METHANOL-D3
Creation_time = 17-JUN-2016 09:09:08
Revision_time = 11-MAR-2021 10:40:06
Current_time = 11-MAR-2021 10:40:14

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X 400
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 40
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 20 [dC]

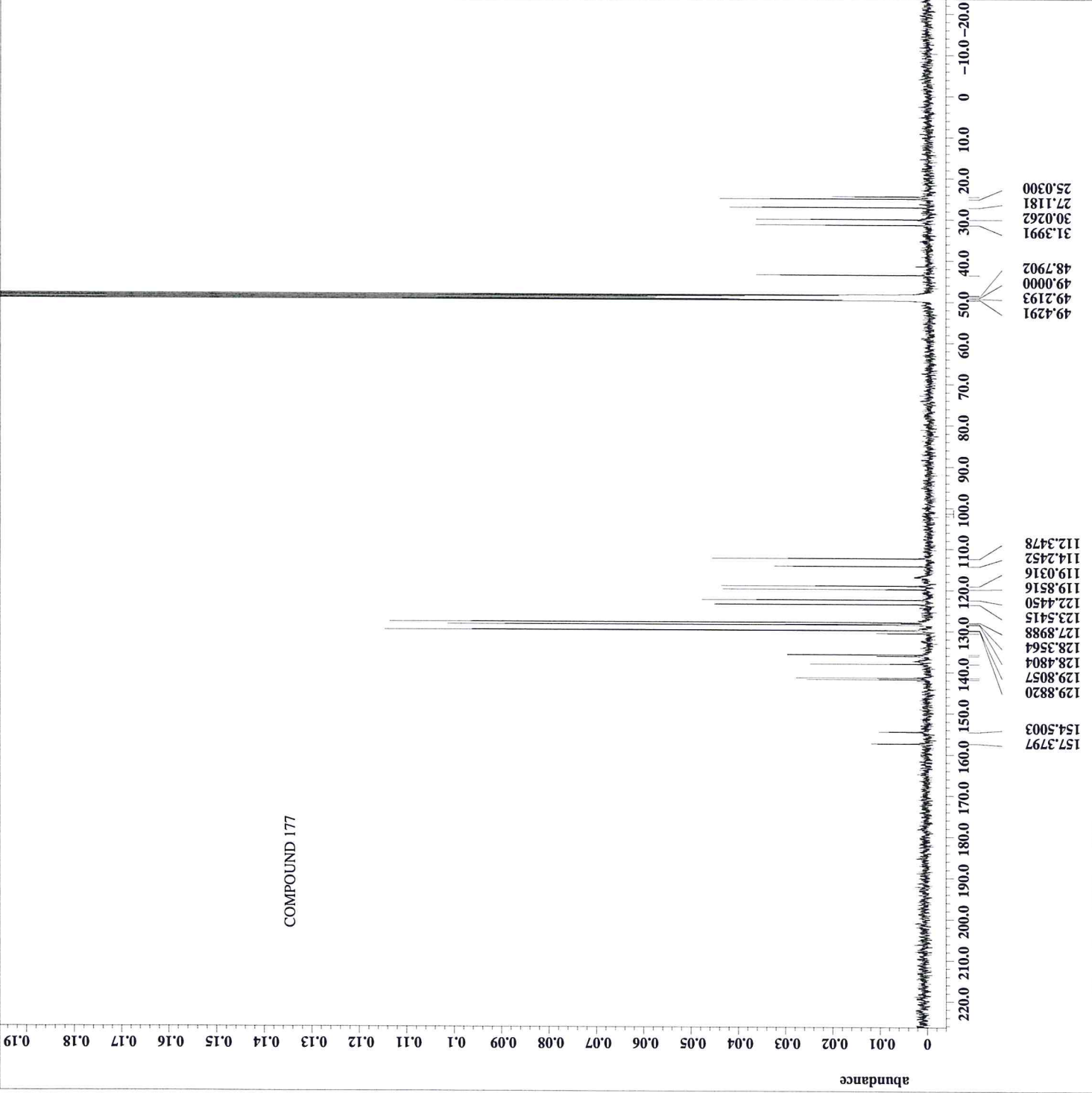


X : parts per Million : 1H



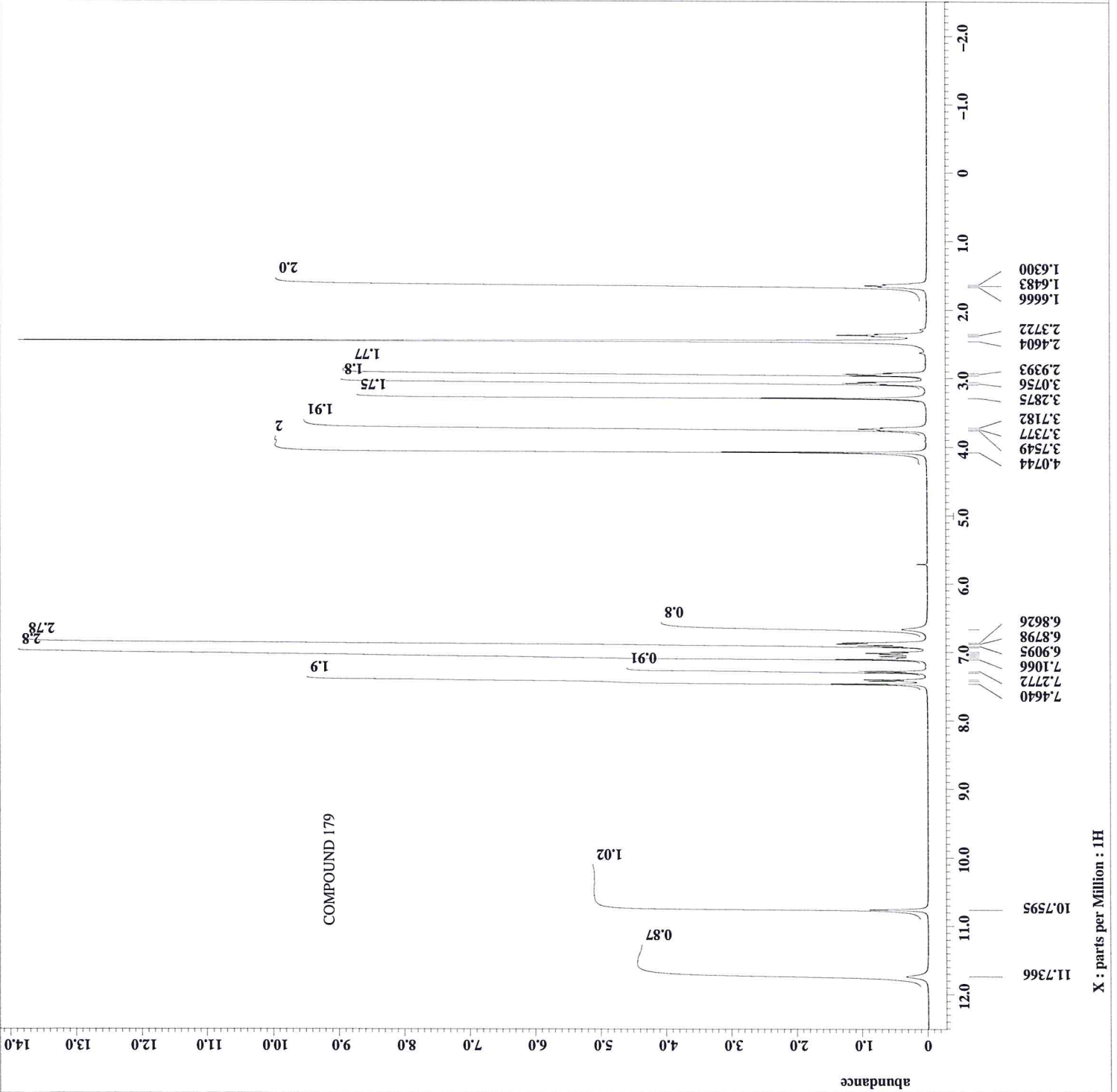
Filename = MM-I-26-F1_CARBON-5.J
Author = Delta
Experiment = single_pulse_dec
Sample_id = MM-I-26-F1
Solvent = METHANOL-D3
Creation_time = 18-JUN-2016 10:42:23
Revision_time = 11-MAR-2021 10:41:55
Current_time = 11-MAR-2021 10:42:00
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [MHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 16000
Total_scans = 16000
X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 20 [dC]

COMPOUND 177





Filename = SM-I-79-4.jdf
Author = mcrider
Experiment = single_pulse.ex2
Sample_id = S#582014
Solvent = DMSO-D6
Creation_time = 18-MAR-2021 12:59:14
Revision_time = 18-MAR-2021 16:21:37
Current_time = 18-MAR-2021 16:21:45
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 13.15 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 6.575 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 50
Relaxation_delay = 5 [s]
Repetition_time = 7.18365952 [s]
Temp_get = 25 [dC]

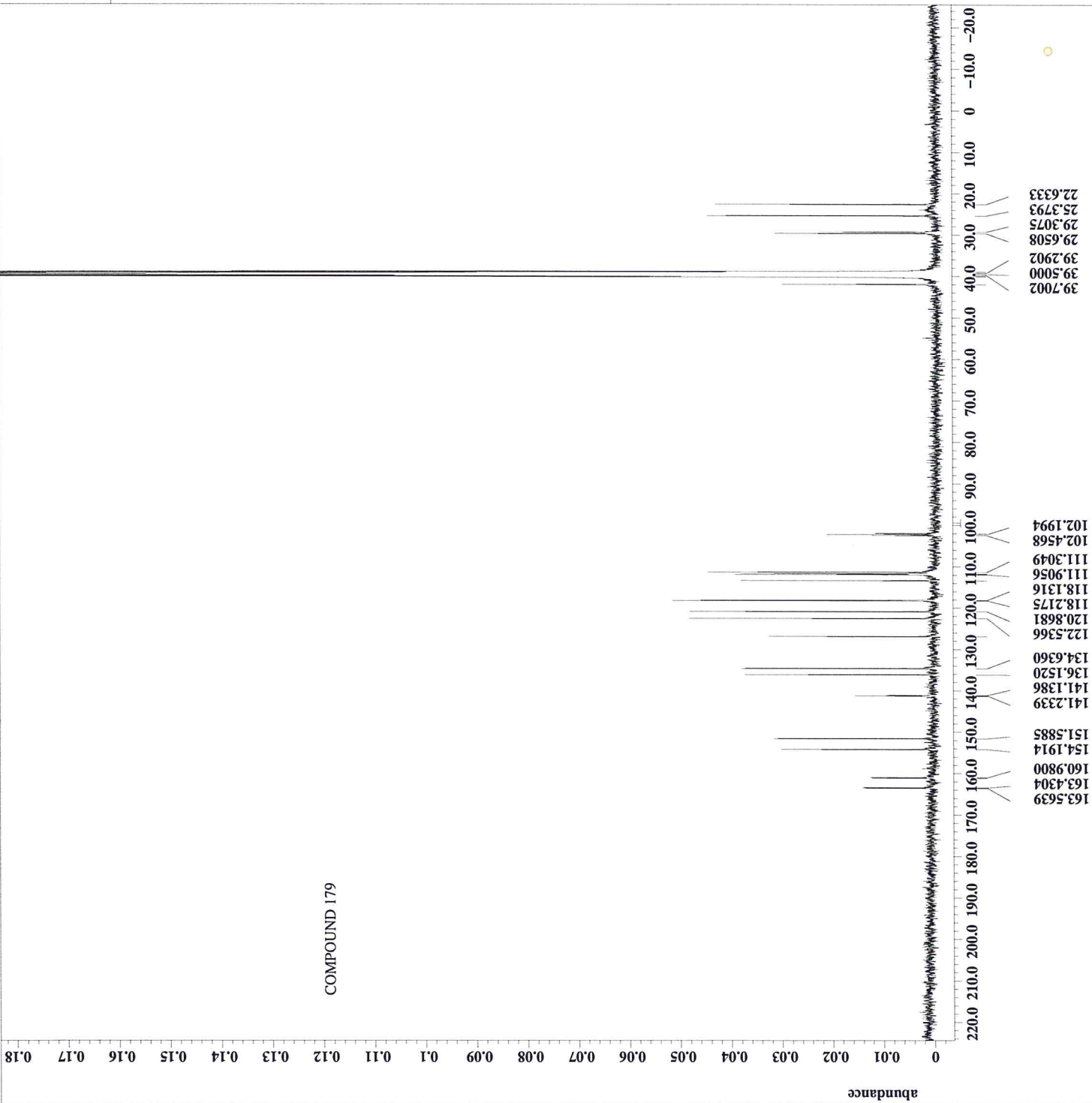


X : parts per Million : 1H



Filename = SM-I-79_CARBON-7.jdf
Author = mcrider
Experiment = single_pulse_dec
Sample_id = SM-I-79
Solvent = DMSO-D6
Creation_time = 19-MAR-2021 01:53:49
Revision_time = 19-MAR-2021 09:14:06
Current_time = 19-MAR-2021 09:15:48
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 15000
Total_scans = 15000
X_90_width = 10.35[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 10.6[db]
X_pulse = 3.45[us]
Irr_atn_dec = 25[db]
Irr_atn_noe = 25[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 58
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 25[dc]

COMPOUND 179



X : parts per Million : 13C

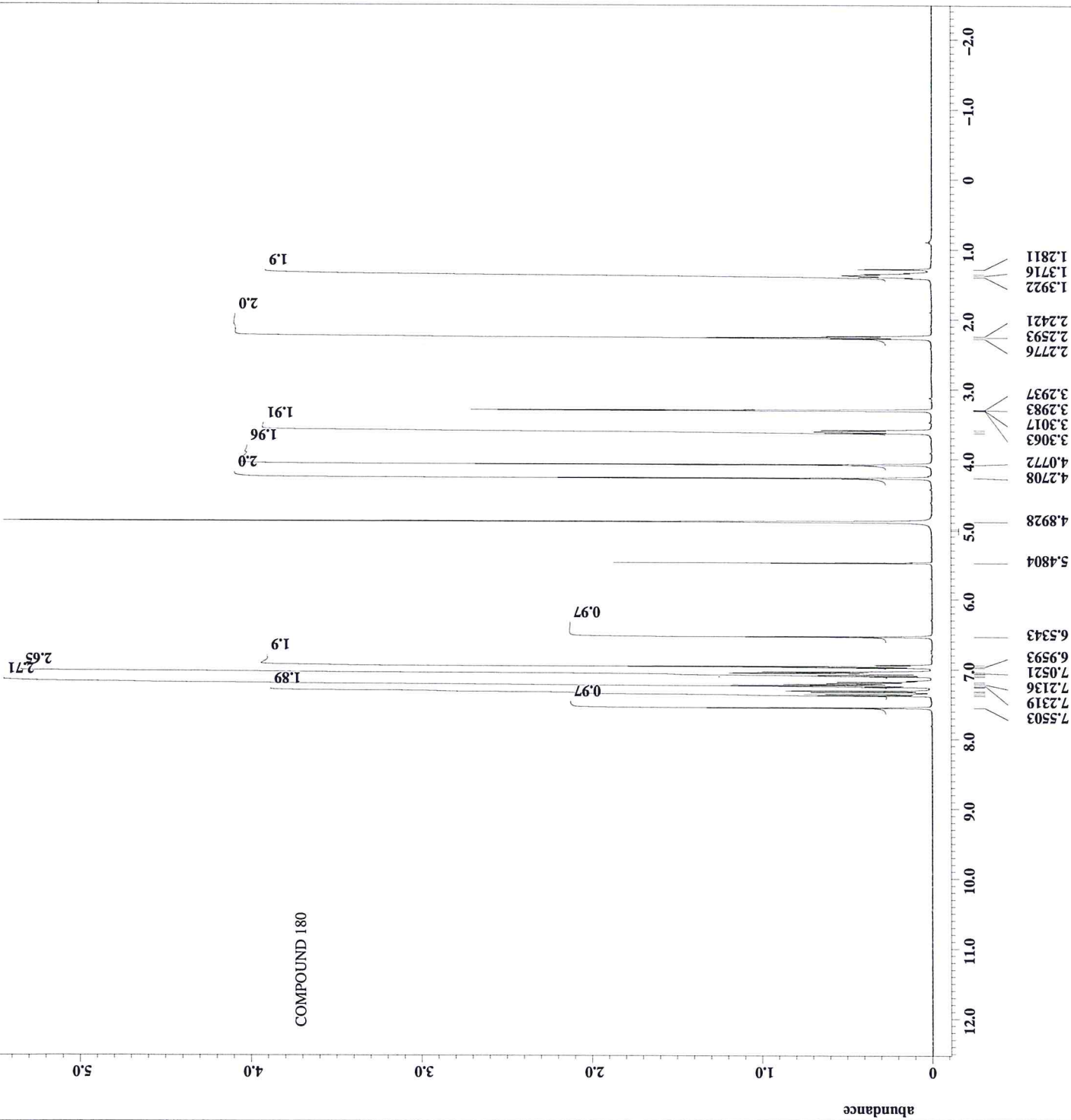


Filename = SK-I-25_PROTON-4.jaf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SK-I-25
Solvent = METHANOL-D3
Creation_time = 21-MAR-2017 09:16:25
Revision_time = 11-MAR-2021 14:22:21
Current_time = 11-MAR-2021 14:22:25

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 44
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 28 [dC]

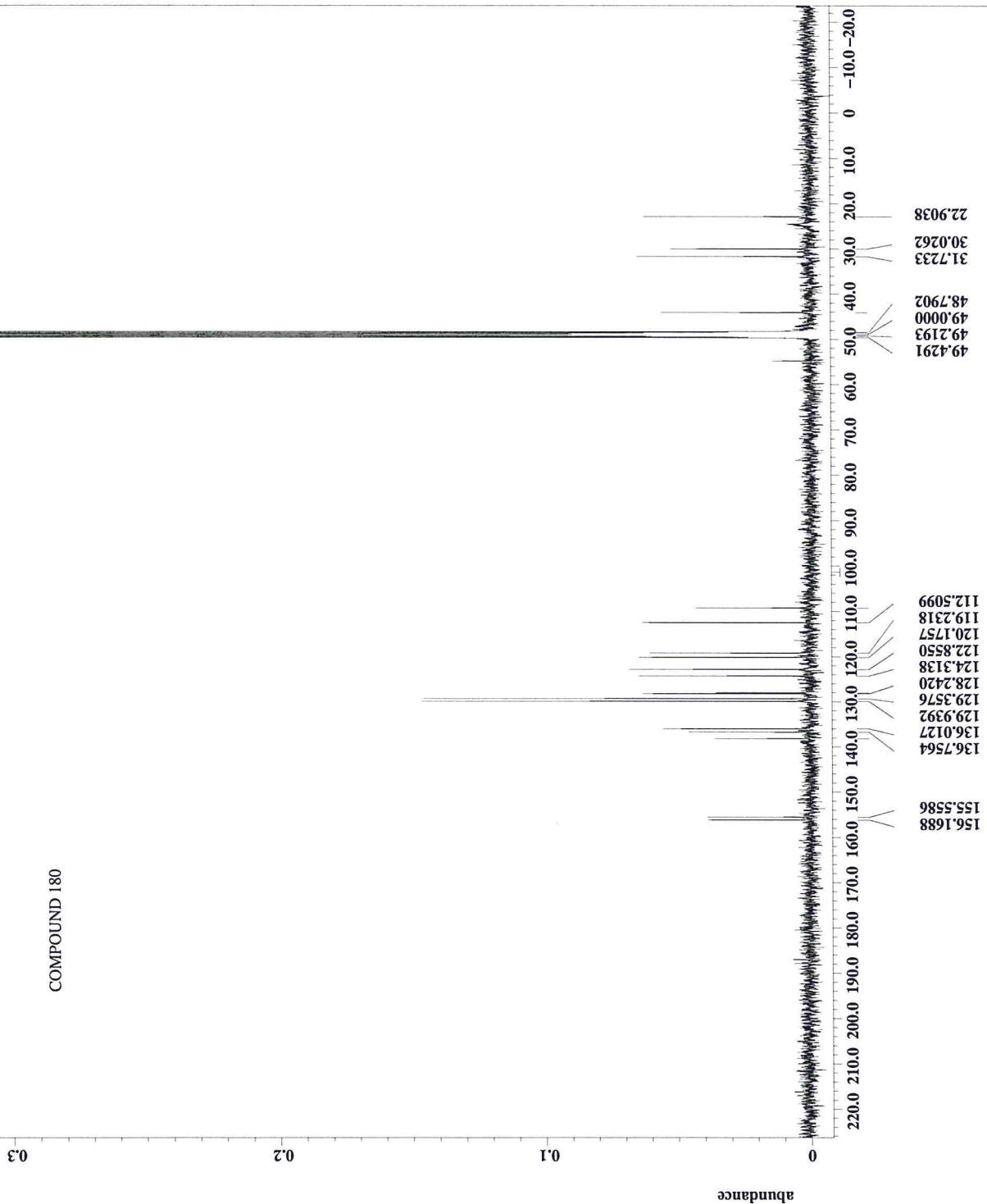


X : parts per Million : 1H



Filename = SK-I-25_CARBON-5.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = SK-I-25
Solvent = METHANOL-D3
Creation_time = 21-MAR-2017 11:02:40
Revision_time = 11-MAR-2021 14:24:33
Current_time = 11-MAR-2021 14:24:37
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 2048
Total_scans = 2048
X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 26.2 [dC]

COMPOUND 180



X : parts per Million : 13C



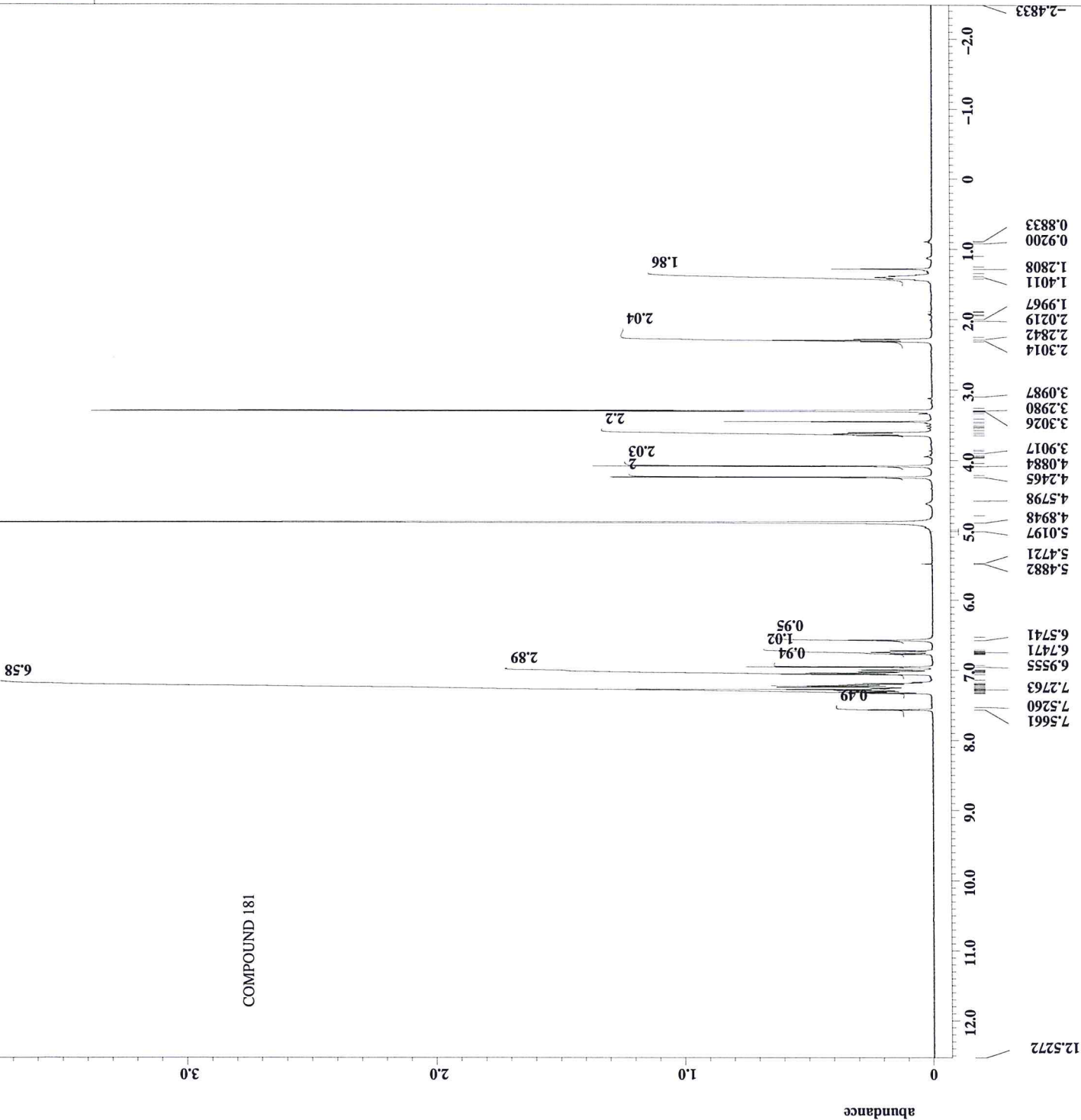
Filename = MM-I-89_PROTON-6.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = MM-I-89
Solvent = METHANOL-D3
Creation_time = 7-APR-2017 12:23:33
Revision_time = 12-MAR-2021 09:30:32
Current_time = 12-MAR-2021 09:30:37

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 44
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 38 [DC]

COMPOUND 181

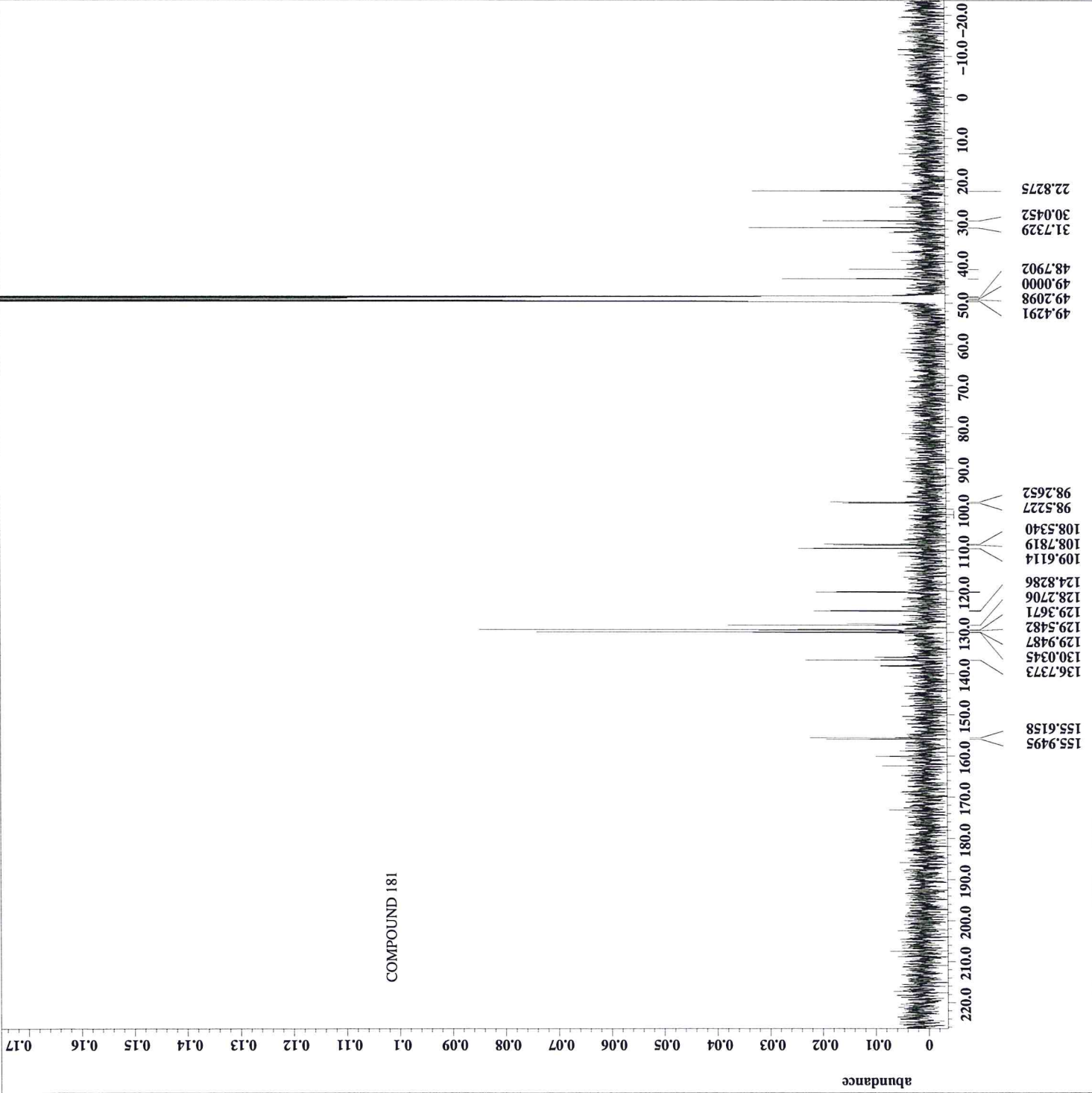


X : parts per Million : 1H



File name = MM-I-89_CARBON-5.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = MM-I-89
Solvent = METHANOL-D3
Creation time = 7-APR-2017 14:35:29
Revision time = 12-MAR-2021 09:33:03
Current_time = 12-MAR-2021 09:33:10
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1929
Total_scans = 1929
X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 38.2 [degC]

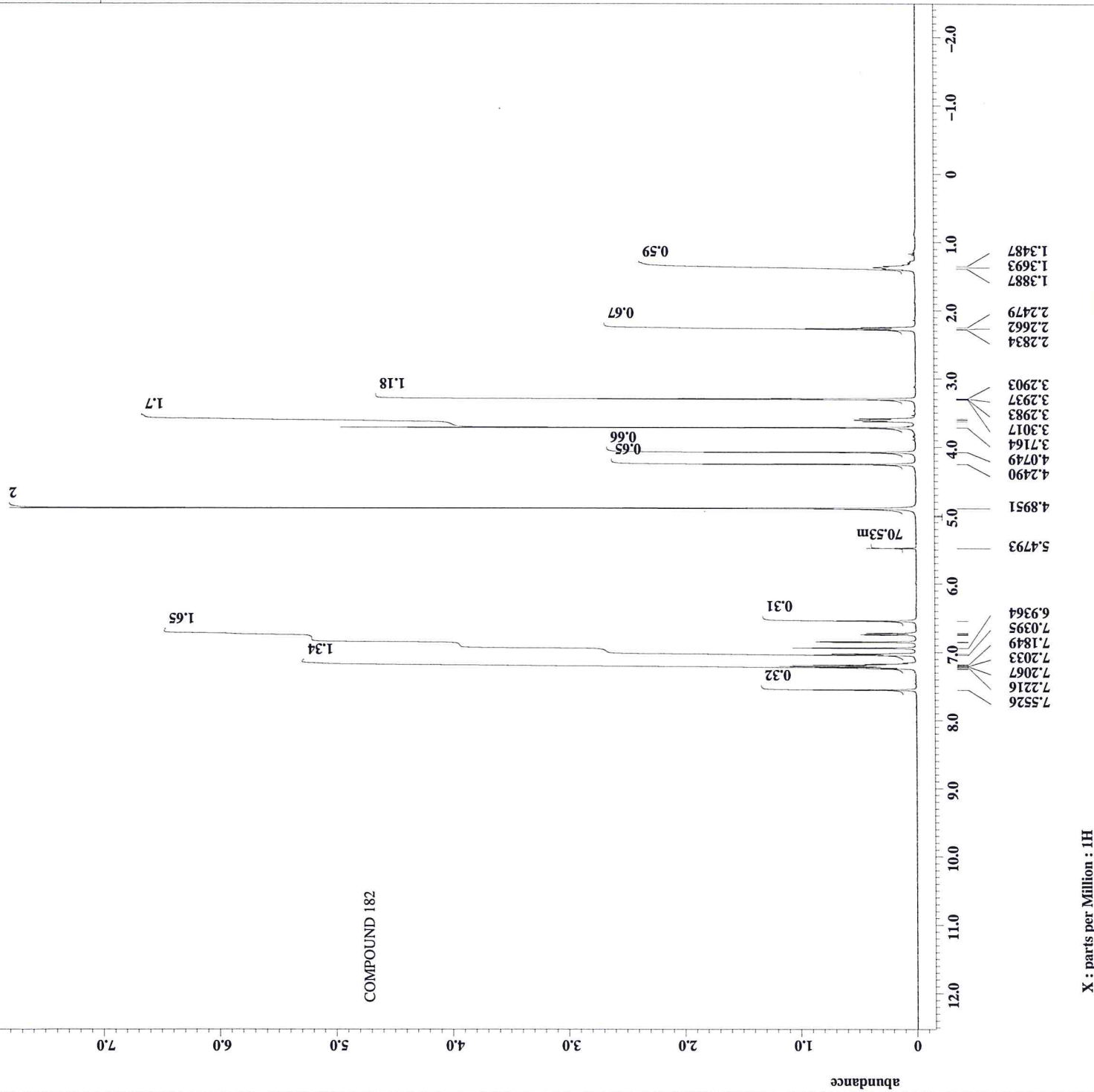
COMPOUND 181



X : parts per Million : 13C



Filename = SK-I-53_PROTON-6.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SK-I-53
Solvent = METHANOL-D3
Creation_time = 1-JUN-2017 10:31:01
Revision_time = 12-MAR-2021 11:28:10
Current_time = 12-MAR-2021 11:28:14
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 16
X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 44
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 460.0 [dC]





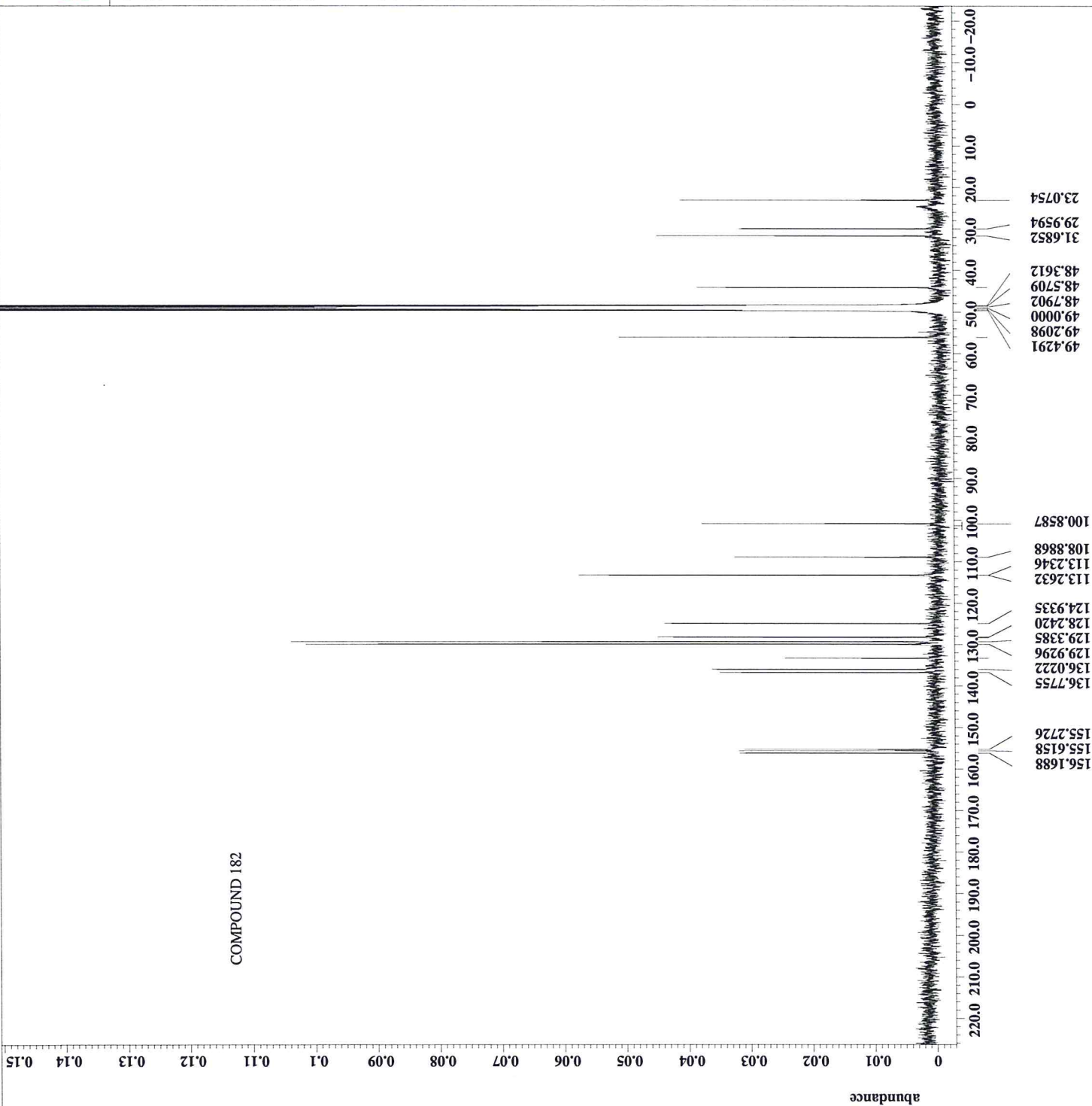
File name = SK-I-53_CARBON-8.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = SK-I-53
Solvent = METHANOL-D3
Creation_time = 15-JUN-2017 04:26:29
Revision_time = 12-MAR-2021 11:30:29
Current_time = 12-MAR-2021 11:30:33

Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = EGS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 12000

X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 460.0 [dC]

COMPOUND 182

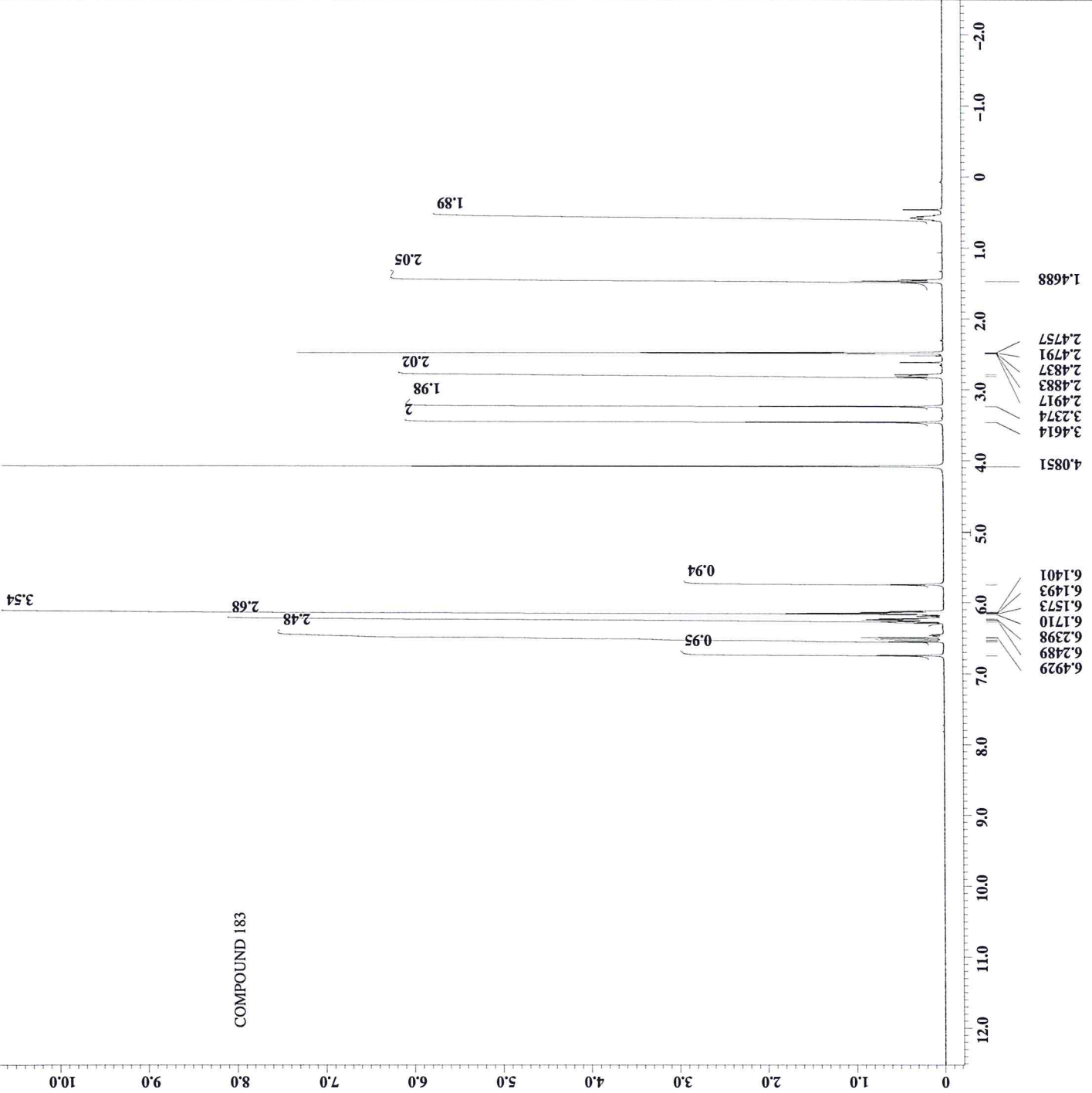


X : parts per Million : 13C



Filename = SK-I-16_PROTON-7.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SK-I-16
Solvent = DMSO-D6
Creation_time = 12-APR-2018 14:59:41
Revision_time = 11-MAR-2021 14:39:20
Current_time = 11-MAR-2021 14:39:24
Date_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = EGS 400
Spectrometer = UNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 16
X_90_width = 10.65 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.325 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 46
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 18.7 [dC]

COMPOUND 183



X : parts per Million : 1H



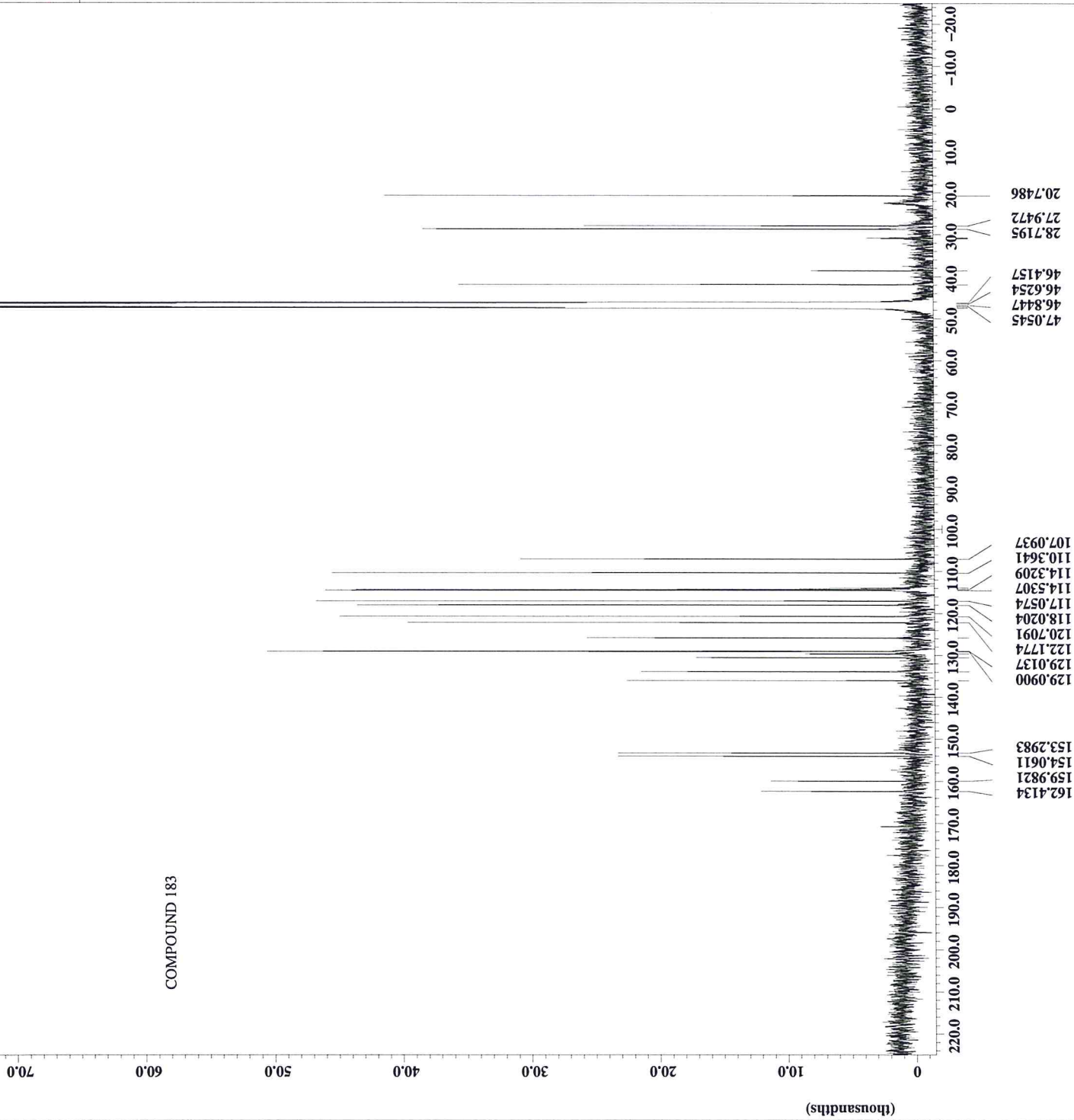
Filename = SK-I-16_CARBON-8.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = SK-I-16
Solvent = DMSO-D6
Creation_time = 13-APR-2018 07:56:38
Revision_time = 11-MAR-2021 14:41:23
Current_time = 11-MAR-2021 14:41:27

Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 20000

X_90_width = 13.22 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.40666667 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 19 [dC]

COMPOUND 183

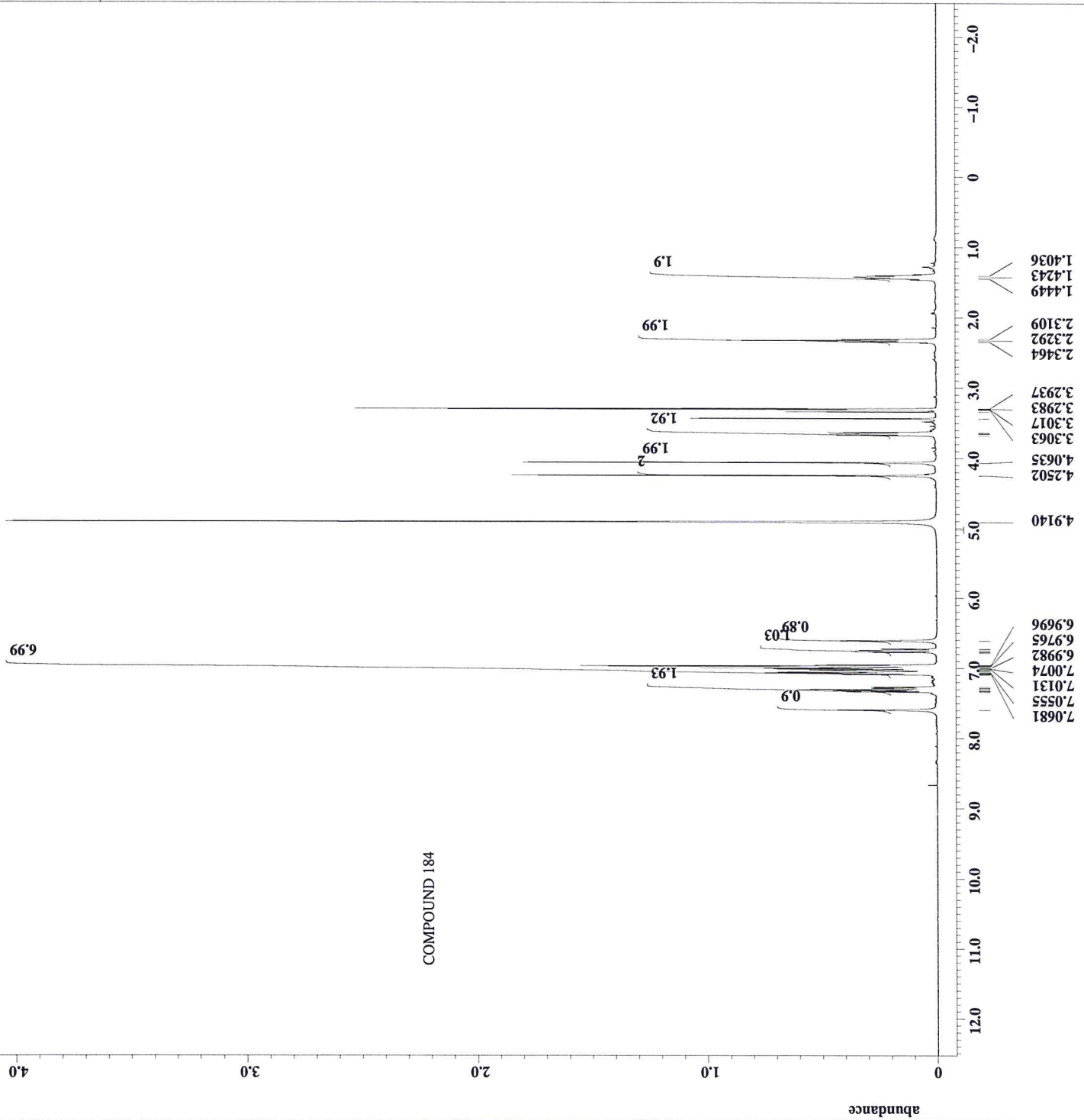


X : parts per Million : 13C



File: SK-I-91_PROTON-7.jdf
Author: Delta
Experiment: single_pulse.ex2
Sample ID: SK-I-91
Solvent: METHANOL-D3
Creation time: 13-APR-2018 16:08:12
Revision time: 12-MAR-2021 11:33:39
Current time: 12-MAR-2021 11:33:43
Data format: 1D COMPLEX
Dim size: 13107
Dim title: 1H
Dim units: [ppm]
Dimensions: X
Site: ECS 400
Spectrometer: JNM-ECS400
Field strength: 9.389766 [T] (400 [MHz])
X_acq_duration: 2.18365952 [s]
X_domain: 1H
X_freq: 399.78219838 [MHz]
X_offset: 5 [ppm]
X_points: 16384
X_prescans: 1
X_resolution: 0.45794685 [Hz]
X_sweep: 7.5030012 [kHz]
Irr_domain: 1H
Irr_freq: 399.78219838 [MHz]
Irr_offset: 5 [ppm]
Tri_domain: 1H
Tri_freq: 399.78219838 [MHz]
Tri_offset: 5 [ppm]
Clipped: FALSE
Mod_return: 1
Scans: 16
Total_scans: 16
X_90_width: 10.65 [us]
X_acq_time: 2.18365952 [s]
X_angle: 45 [deg]
X_atn: 6 [dB]
X_pulse: 5.325 [us]
Irr_mode: Off
Tri_mode: Off
Dante_presat: FALSE
Initial_wait: 1 [s]
Recvr_gain: 40
Relaxation_delay: 4 [s]
Repetition_time: 6.18365952 [s]
Temp_get: 18.7 [dC]

COMPOUND 184

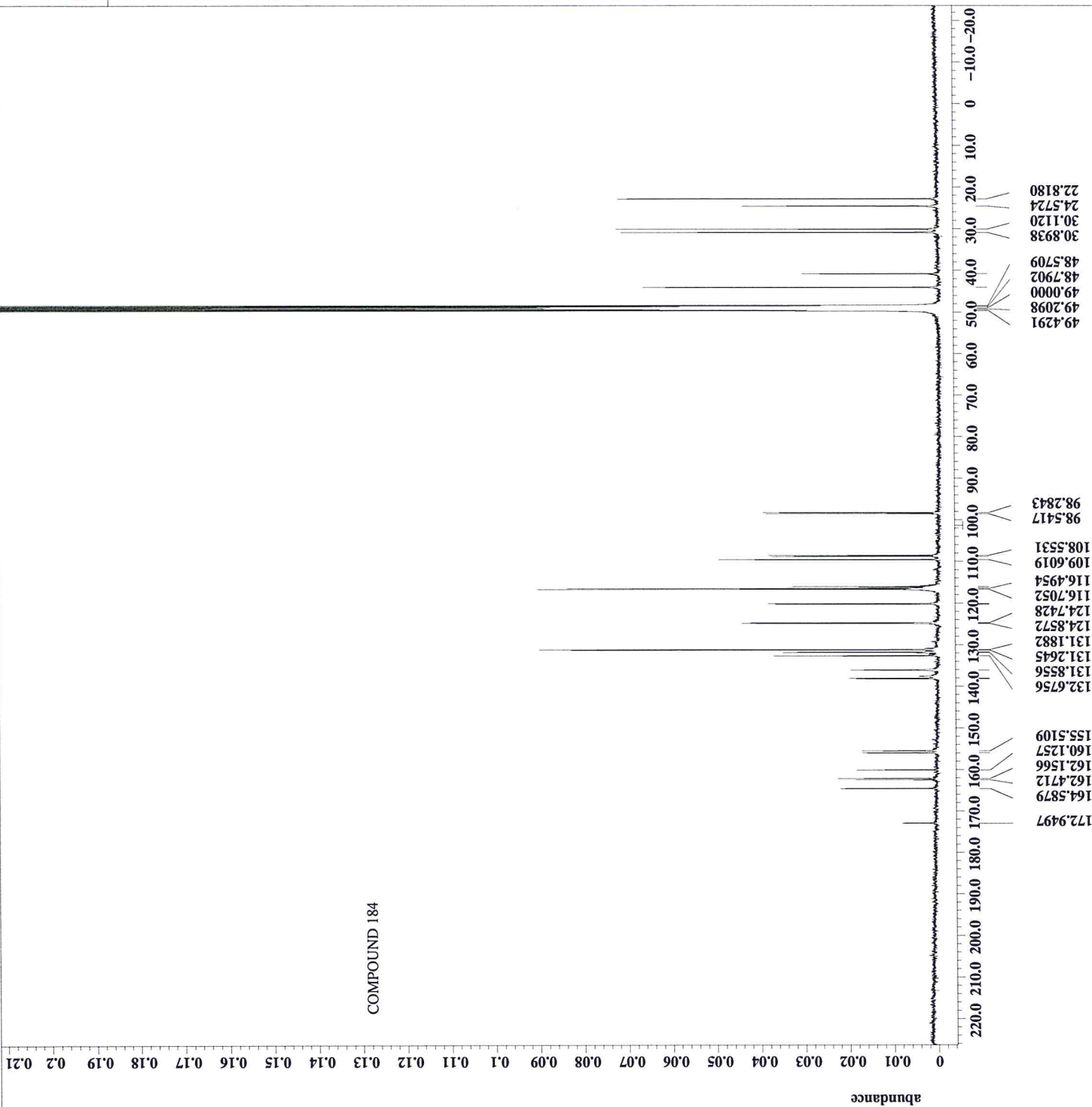


X : parts per Million : 1H



File name = SK-I-91_CARBON-8.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = SK-I-91
Solvent = METHANOL-D3
Creation_time = 16-APR-2018 08:14:13
Revision_time = 12-MAR-2021 11:36:01
Current_time = 12-MAR-2021 11:36:05
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 75793
Total_scans = 75793
X_90_width = 13.22 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.40666667 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 19.3 [dC]

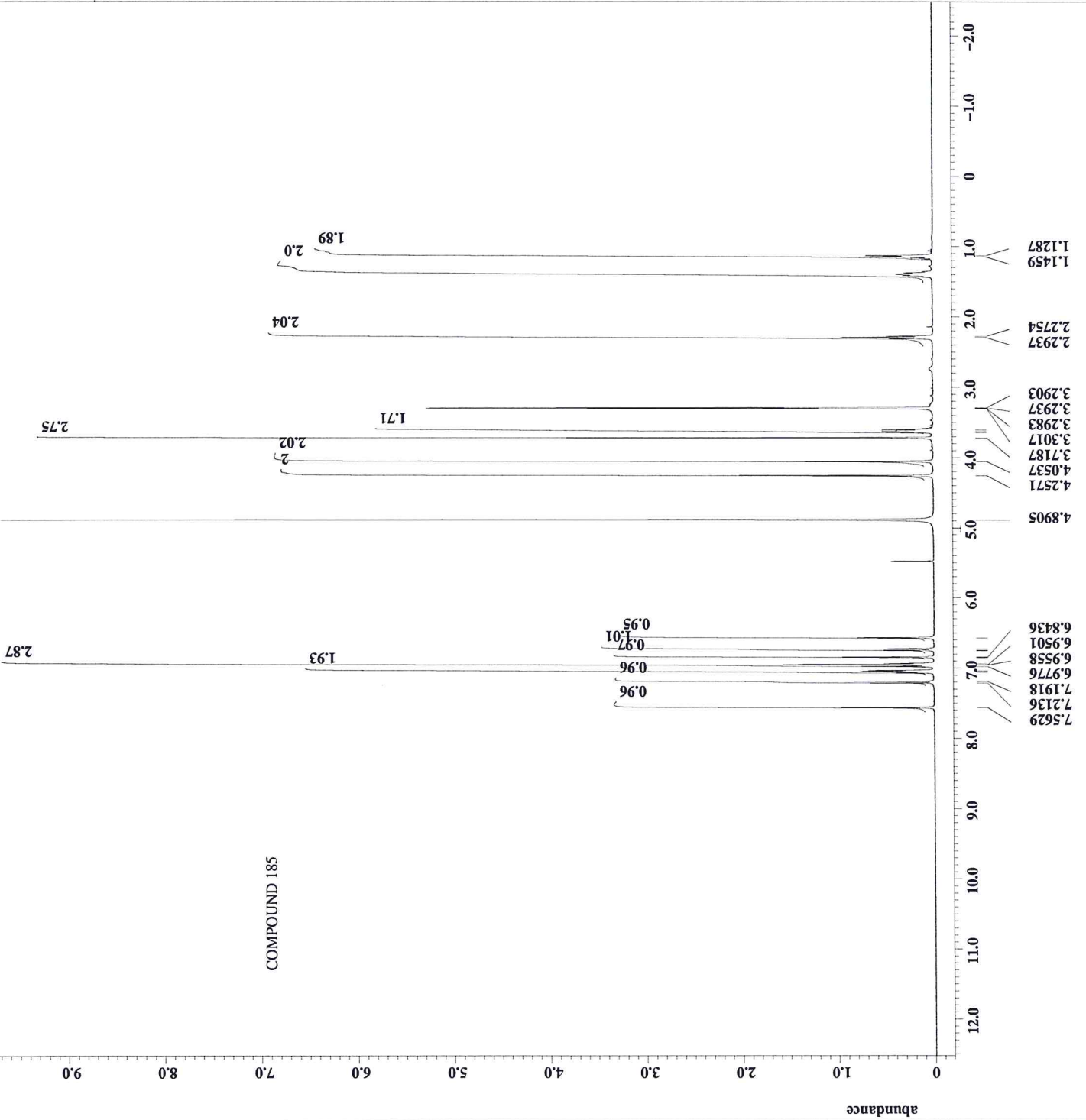
COMPOUND 184



X : parts per Million : 13C



File name = SK-I-55_PROTON-4.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SK-I-55
Solvent = METHANOL-D3
Creation_time = 2-JUN-2017 10:19:19
Revision_time = 12-MAR-2021 11:21:27
Current_time = 12-MAR-2021 11:21:31
Data_format = 1D_COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
total_scans = 16
X_90_width = 10.68[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.34[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 48
Relaxation_delay = 4[s]
Repetition_time = 6.18365952[s]
temp_get = 460.0[dc]

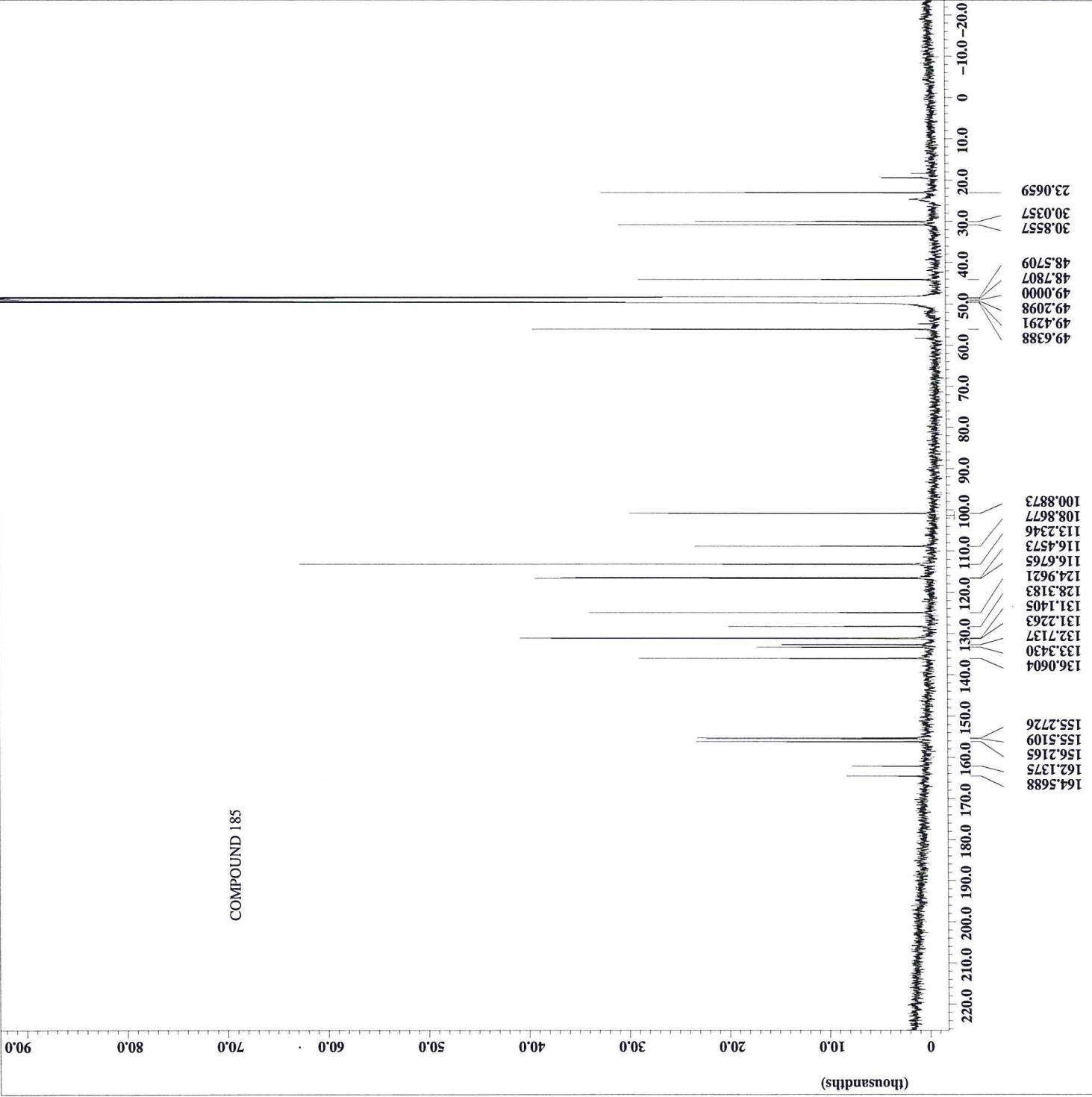


X : parts per Million : 1H



File name = SK-I-55_weekend_CARBO
Author = Delta
Experiment = single_pulse_dec
Sample_id = SK-I-55_weekend
Solvent = METHANOL-D3
Creation time = 12-JUN-2017 08:21:07
Revision time = 12-MAR-2021 11:23:36
Current_time = 12-MAR-2021 11:23:40
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 72275
X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 460.0 [dC]

COMPOUND 185

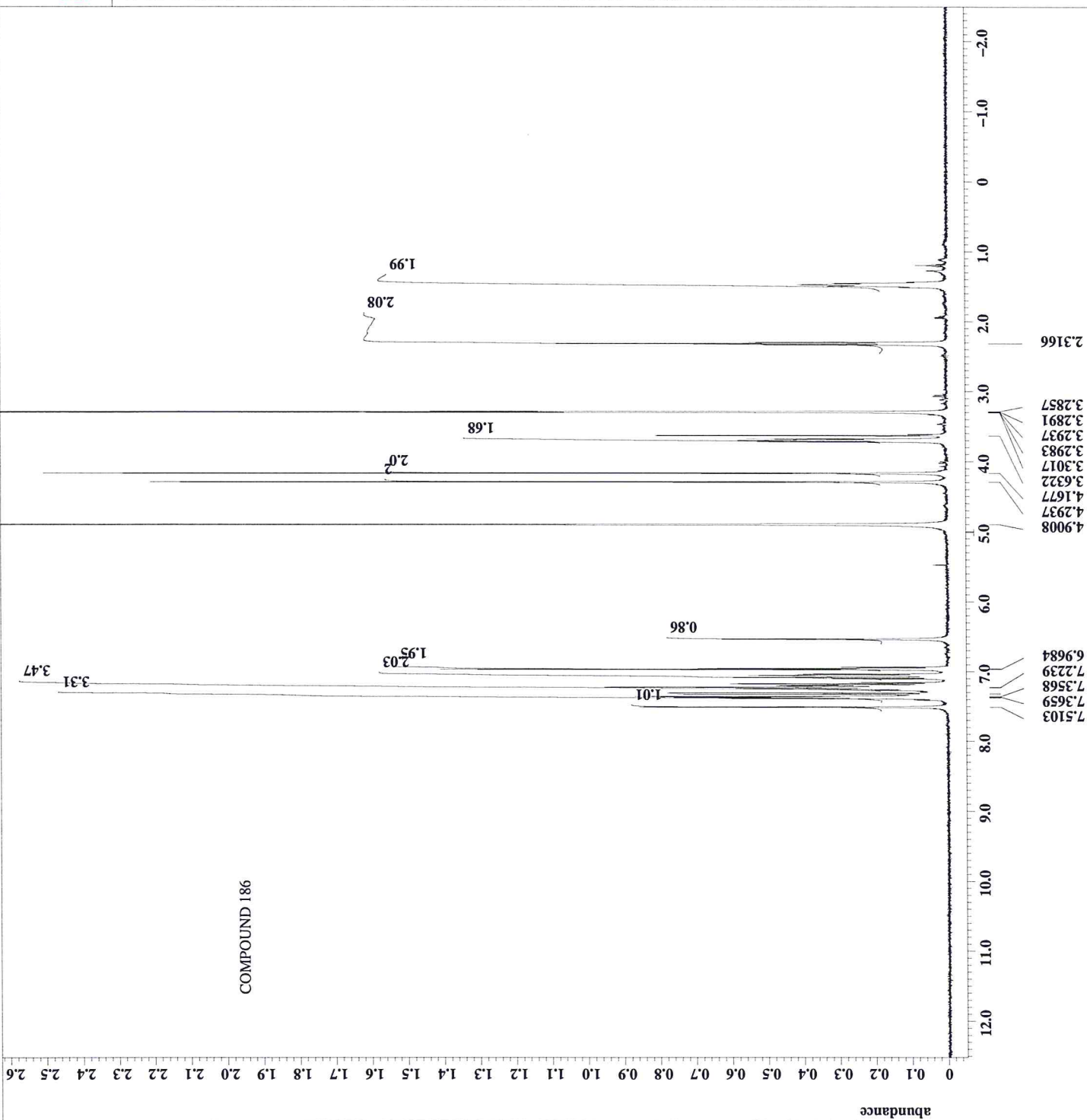


X : parts per Million : 13C



Filename = KS-I-15-C_PROTON-7.jd
Author = Delta
Experiment = single_pulse.ex2
Sample_id = KS-I-15-C
Solvent = METHANOL-D3
Creation_time = 14-FEB-2019 13:23:52
Revision_time = 11-MAR-2021 11:04:33
Current_time = 11-MAR-2021 11:04:37
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4
X_90_width = 11.365 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.6825 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 46
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 18 [DC]

COMPOUND 186

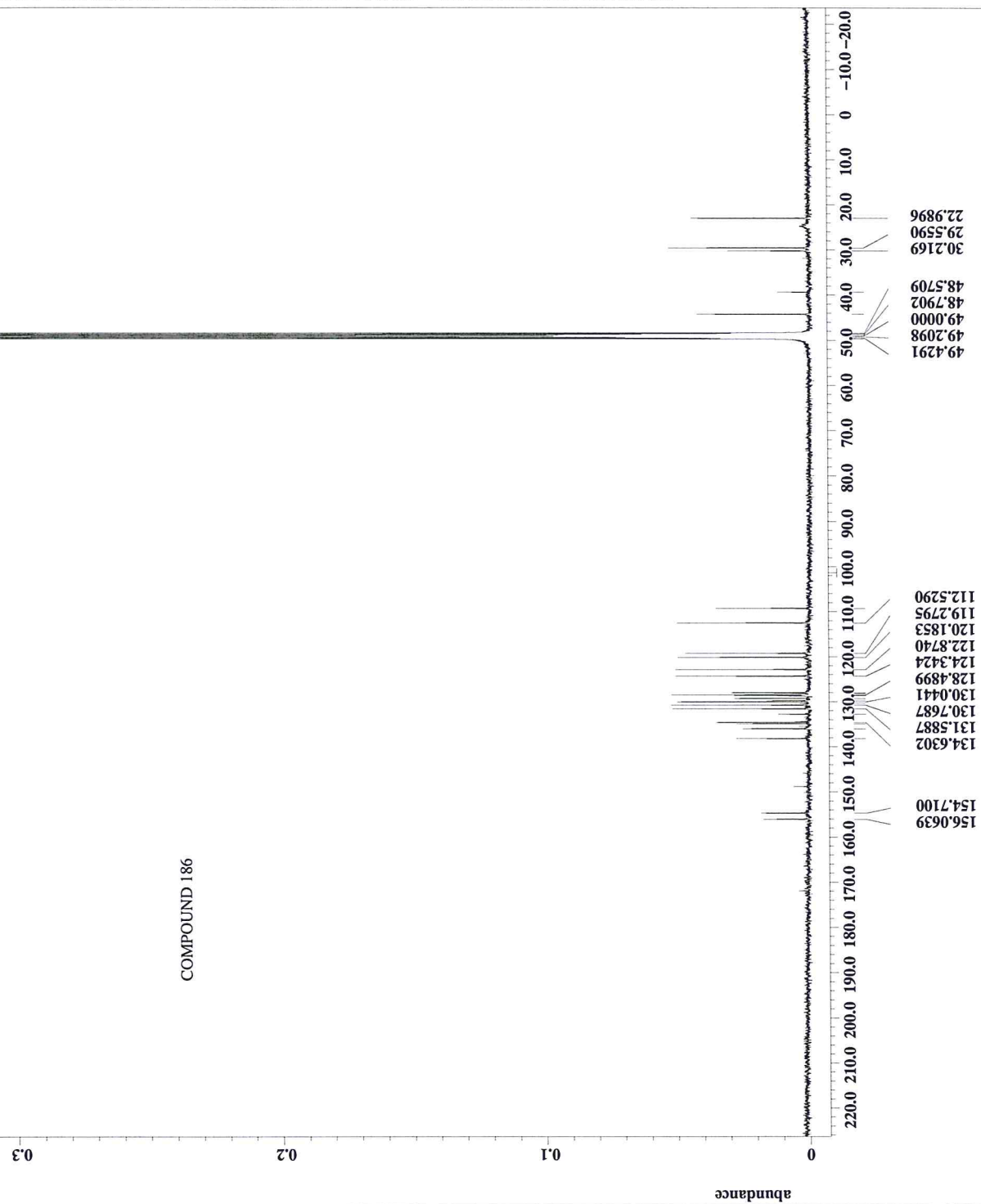


X : parts per Million : 1H



Filename = KS-I-15-C_Long_CARBON
Author = Delta
Experiment = single_pulse_dec
Sample_id = KS-I-15-C_Long
Solvent = METHANOL-D3
Creation_time = 15-FEB-2019 07:15:49
Revision_time = 11-MAR-2021 11:07:15
Current_time = 11-MAR-2021 11:07:18
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 14483
Total_scans = 14483
X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.46666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WAITZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 58
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 17.8 [dC]

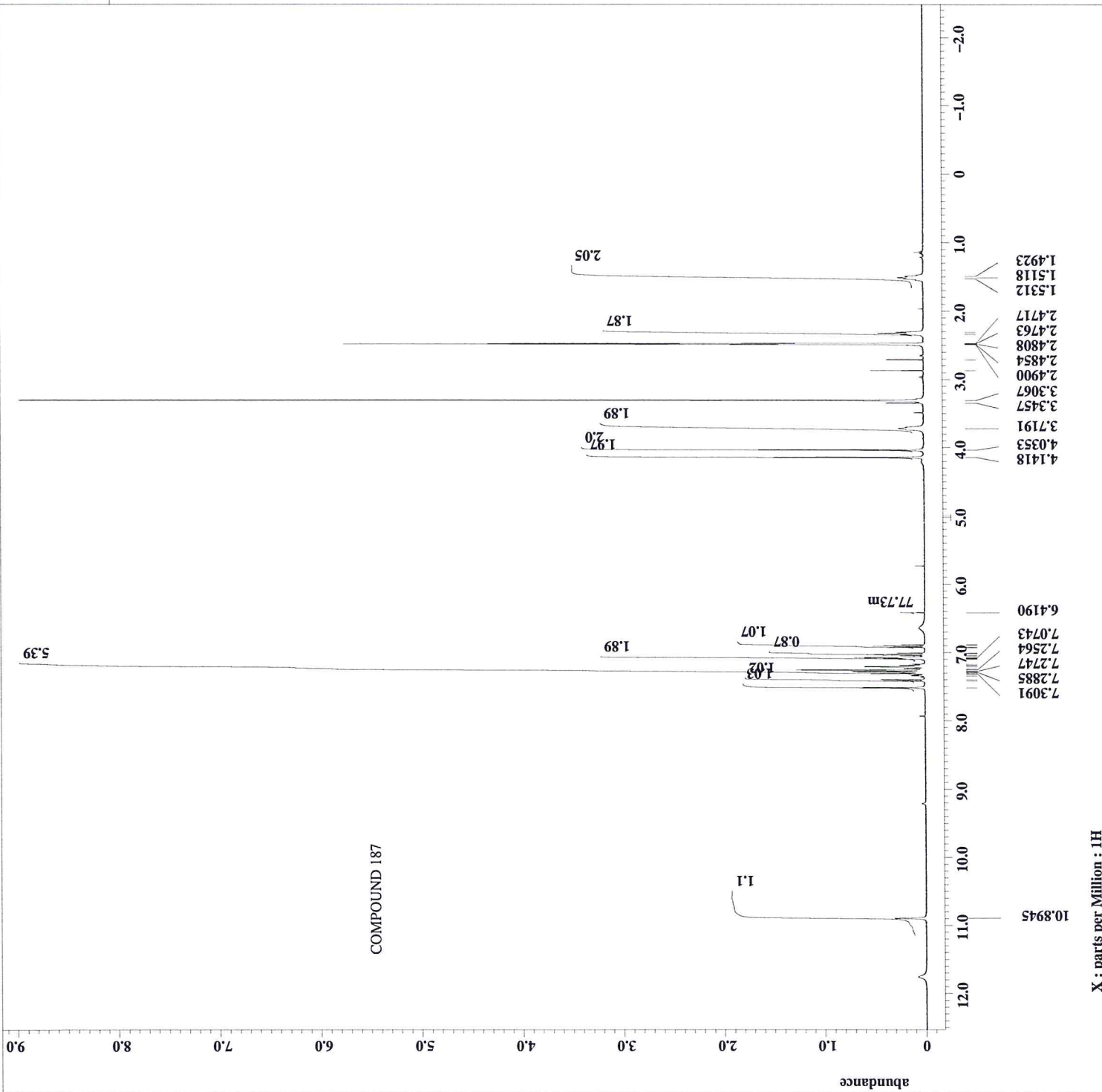
COMPOUND 186



X : parts per Million : 13C



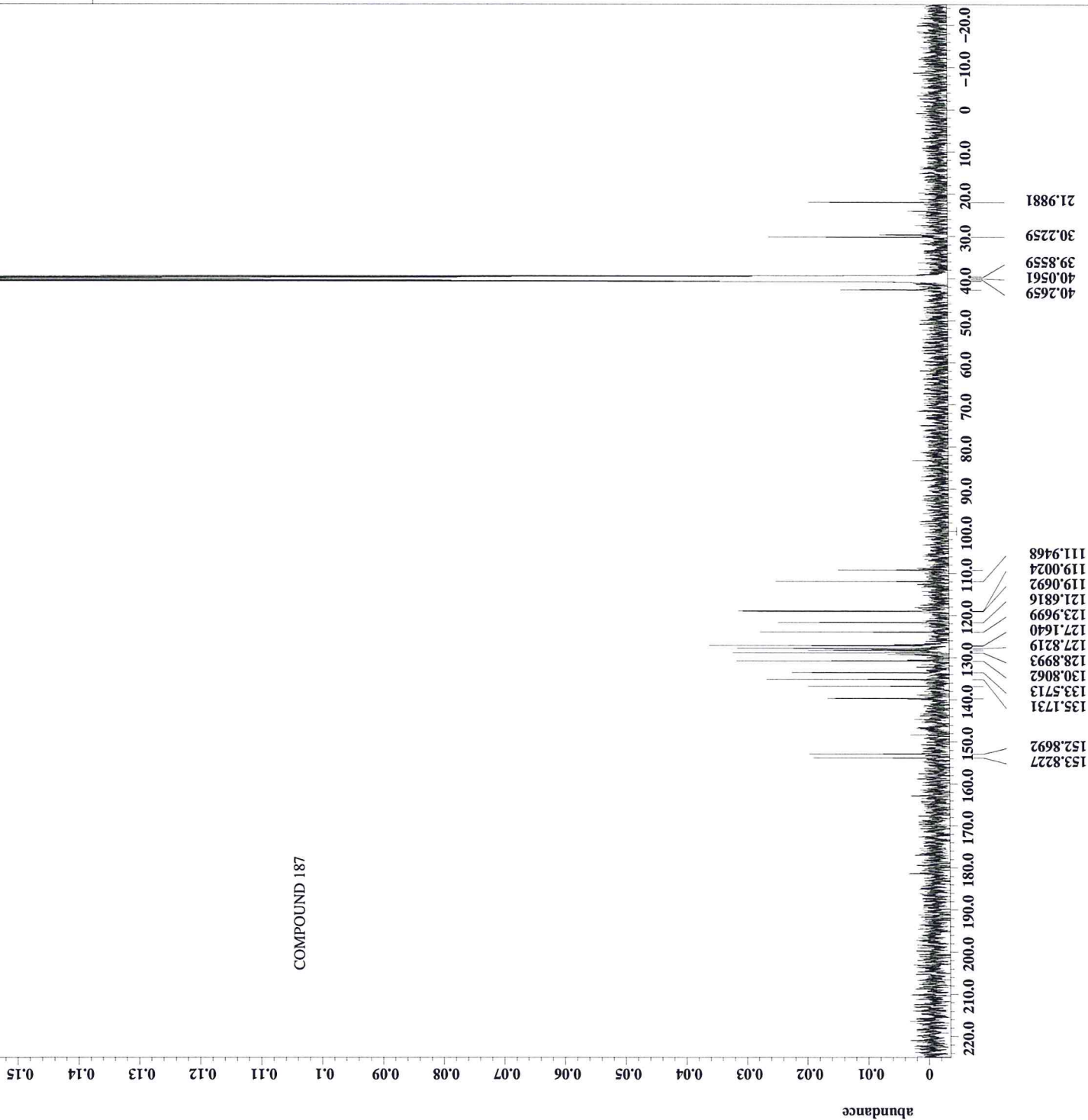
Filename = KS-I-8-C_PROTON-5.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = KS-I-8-C
Solvent = DMSO-D6
Creation_time = 5-FEB-2019 12:03:30
Revision_time = 11-MAR-2021 11:13:18
Current_time = 11-MAR-2021 11:13:22
Date_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4
X_90_width = 11.365 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.6825 [us]
Irr_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 44
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 25 [dC]





Filename = KS-I-8-C_CARBON-7.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = KS-I-8-C
Solvent = DMSO-D6
Creation_time = 5-FER-2019 14:38:58
Revision_time = 11-MAR-2021 11:17:22
Current_time = 11-MAR-2021 11:17:26
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 2952
Total_scans = 2952
X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.46666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 2 [s]
Recvr_gain = 58
Relaxation_delay = 2 [s]
Repetition_time = 3.04333312 [s]
Temp_get = 25 [dC]

COMPOUND 187



X : parts per Million : 13C



```

Filename = KS-I-57-C_PROTON-5.jd
Author = Delta
Experiment = single_pulse.ex2
Sample_id = KS-I-57-C
Solvent = DMSO-D6
Creation_time = 21-JUL-2019 11:06:26
Revision_time = 15-MAR-2021 15:47:50
Current_time = 15-MAR-2021 15:47:55

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

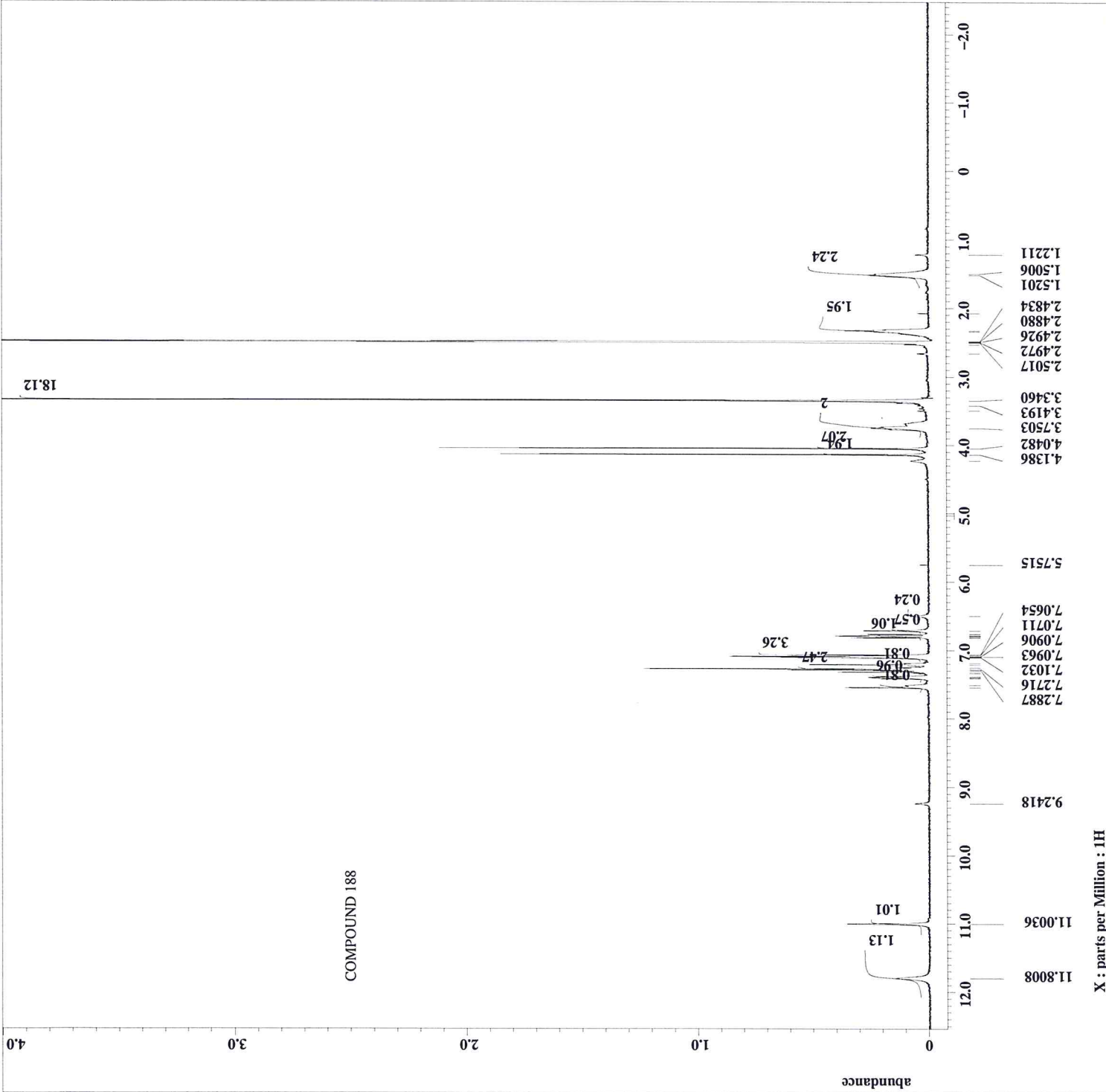
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4

X_90_width = 11.365[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[dB]
X_pulse = 5.6825[us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Recvr_gain = 46
Relaxation_delay = 4[s]
Repetition_time = 6.18365952[s]
Temp_get = 19.2[dc]

```

18.12

COMPOUND 188



X : parts per Million : 1H



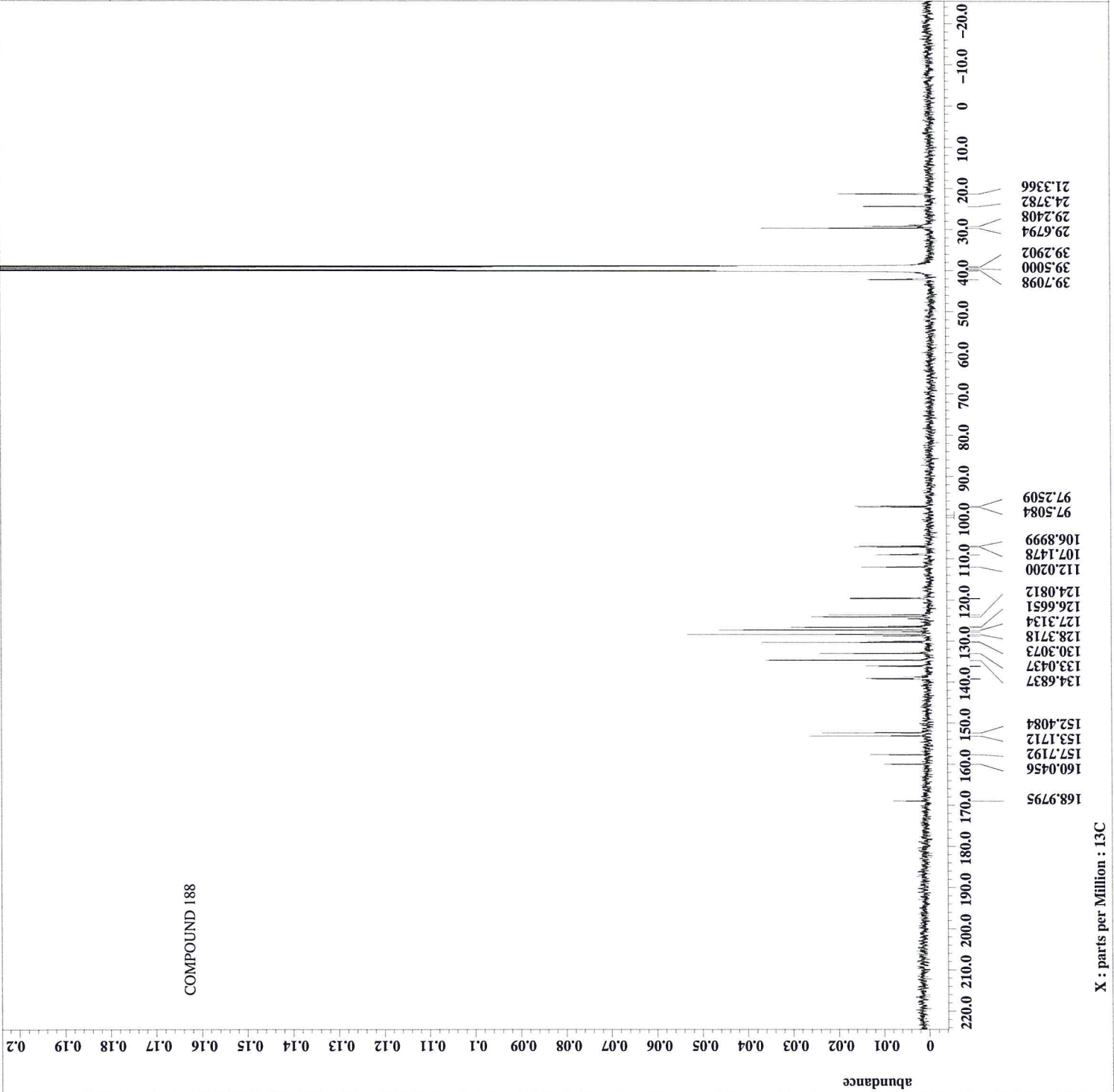
File name = KS-I-57-C-CARBON-5.jd
Author = Delta
Experiment = single_pulse_dec
Sample_id = KS-I-57-C
Solvent = DMSO-D6
Creation time = 22-JUL-2019 09:00:51
Revision time = 15-MAR-2021 15:52:55
Current time = 15-MAR-2021 15:52:59

Data format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 25848
Total_scans = 25848

X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.46666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [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 = 3.04333312 [s]
Temp_get = 20.6 [dC]

COMPOUND 188



X : parts per Million : 13C



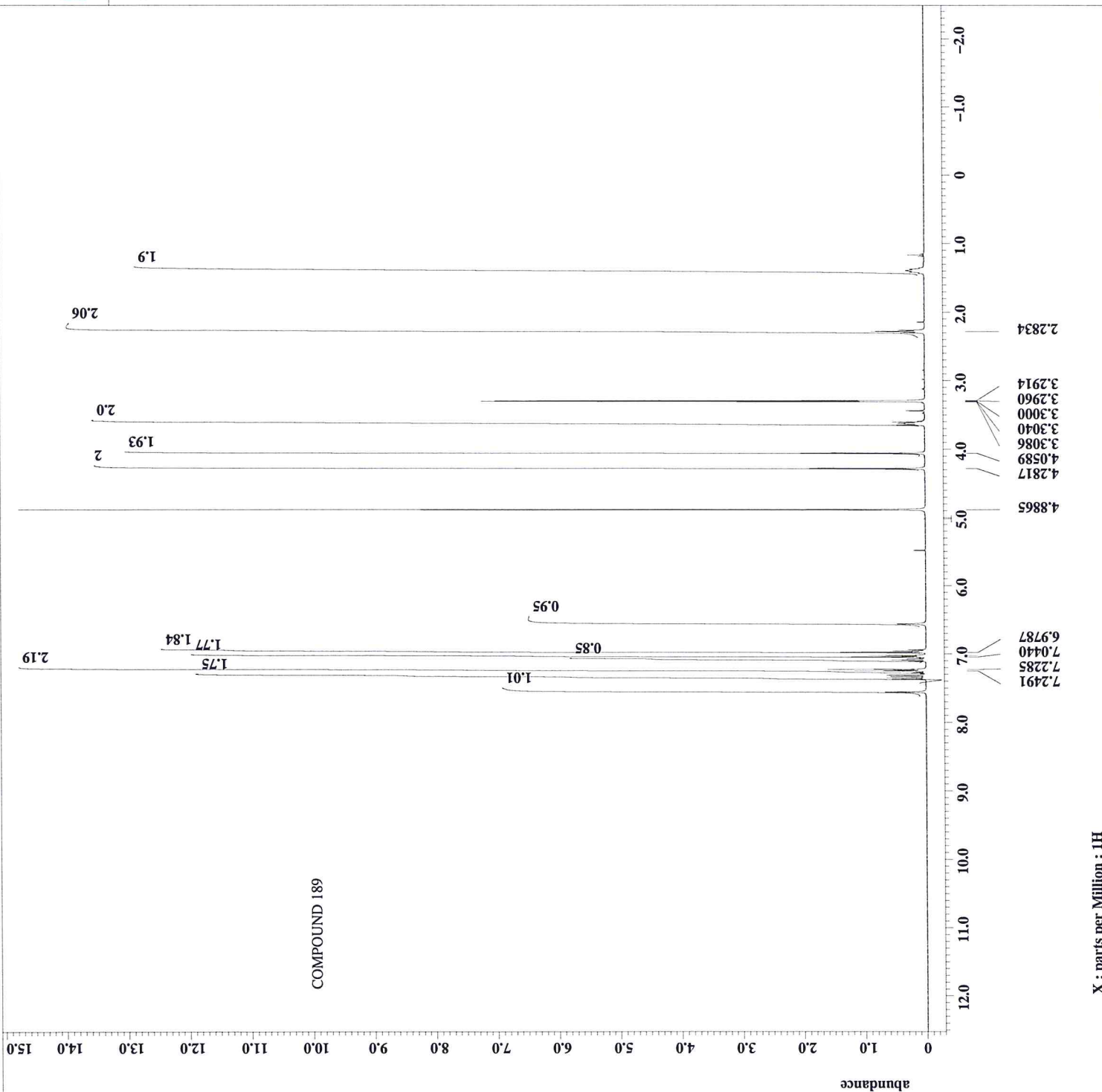
```

Filename = SK-I-22_PROTON-4.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SK-I-22
Solvent = METHANOL-D3
Creation_time = 8-MAR-2017 09:49:02
Revision_time = 11-MAR-2021 14:31:12
Current_time = 11-MAR-2021 14:31:16

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 48
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 460.0 [dC]
  
```

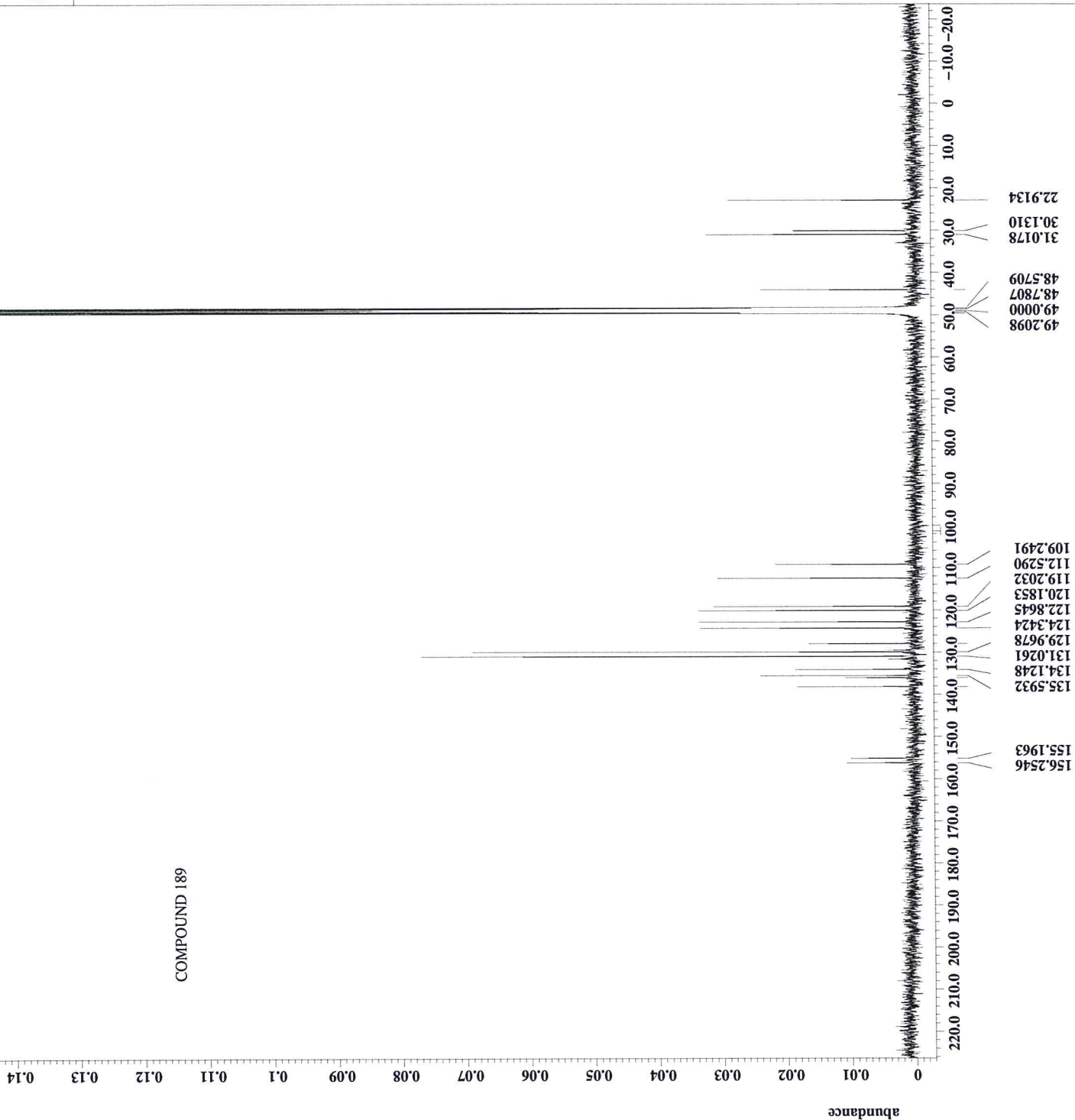


X : parts per Million : 1H



File name = SK-I-22_CARBON-8-jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = SK-I-22
Solvent = METHANOL-D3
Creation time = 22-MAR-2017 02:30:26
Revision time = 11-MAR-2021 14:33:31
Current time = 11-MAR-2021 14:33:37
Data format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95946665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 14000
Total_scans = 14000
X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 27.6 [dC]

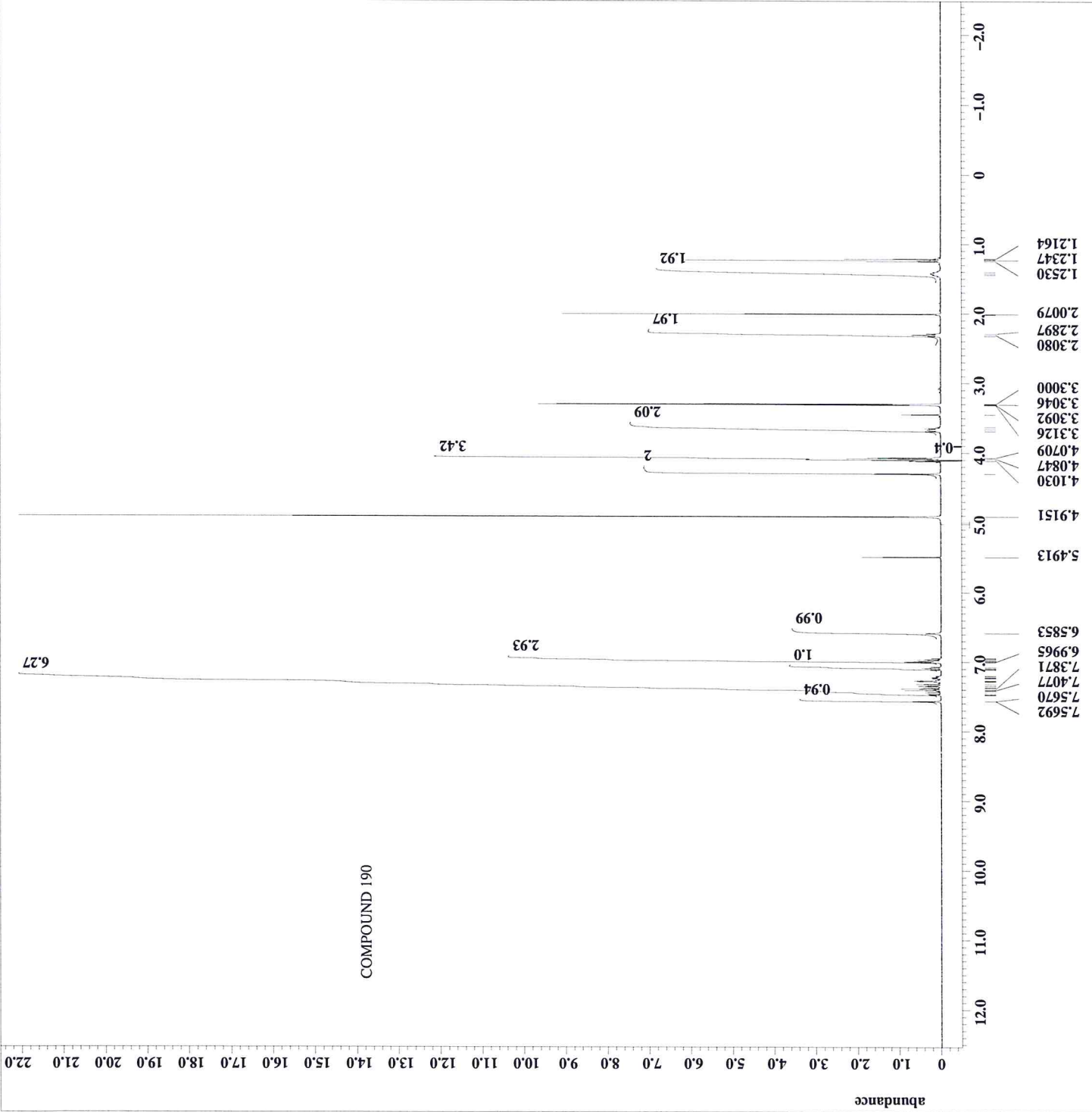
COMPOUND 189



X : parts per Million : 13C



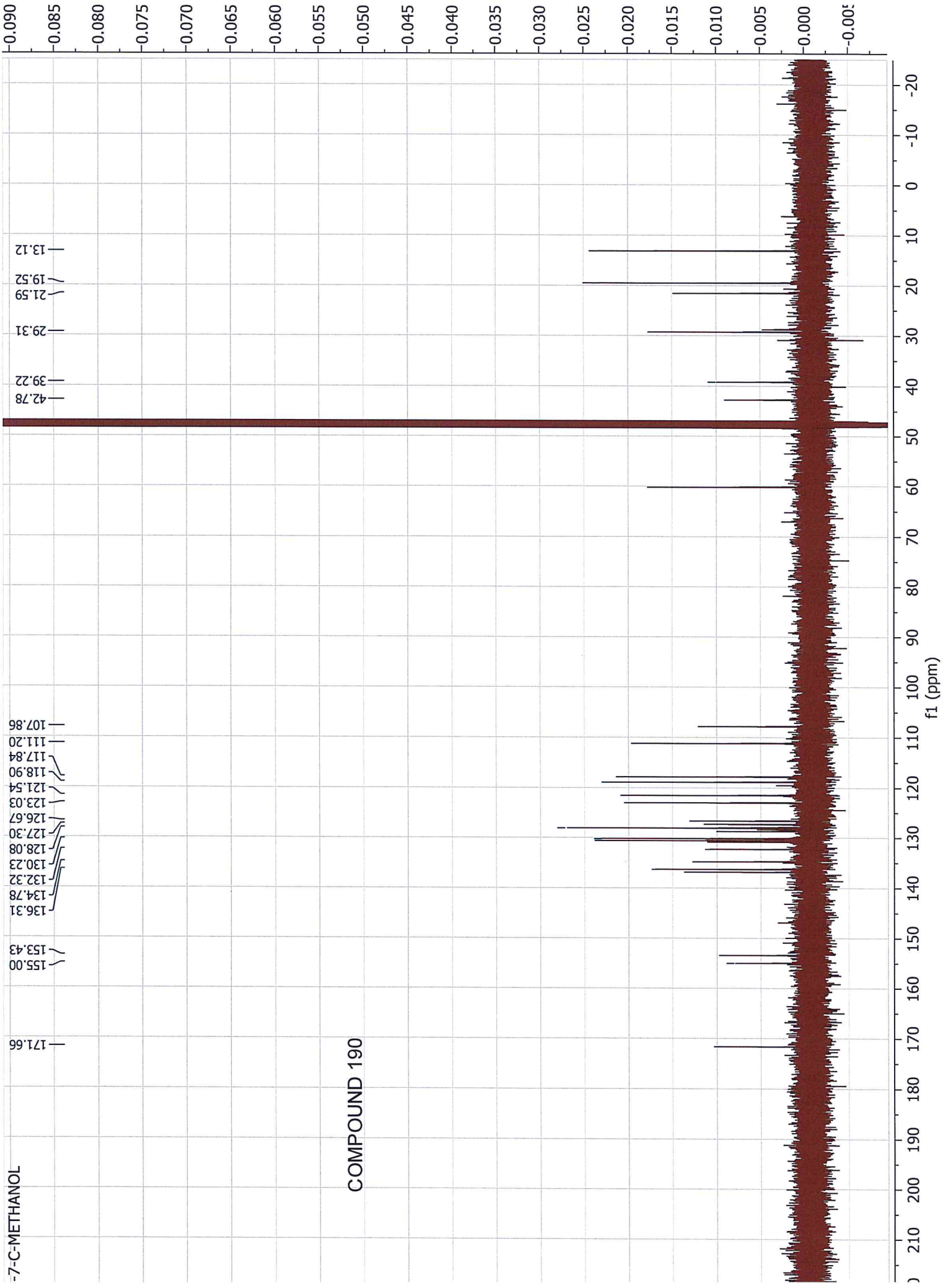
Filename = RF-I-7-C_METHANOL_PRO
Author = Delta
Experiment = single_pulse.ex2
Sample_id = RF-I-7-C
Solvent = METHANOL-D3
Creation_time = 13-FEB-2019 09:32:51
Revision_time = 17-MAR-2021 14:14:50
Current_time = 17-MAR-2021 14:15:06
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4
X_90_width = 11.365 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.6825 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 48
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 17.2 [dC]



X : parts per Million : 1H

-7-C-METHANOL

COMPOUND 190





```

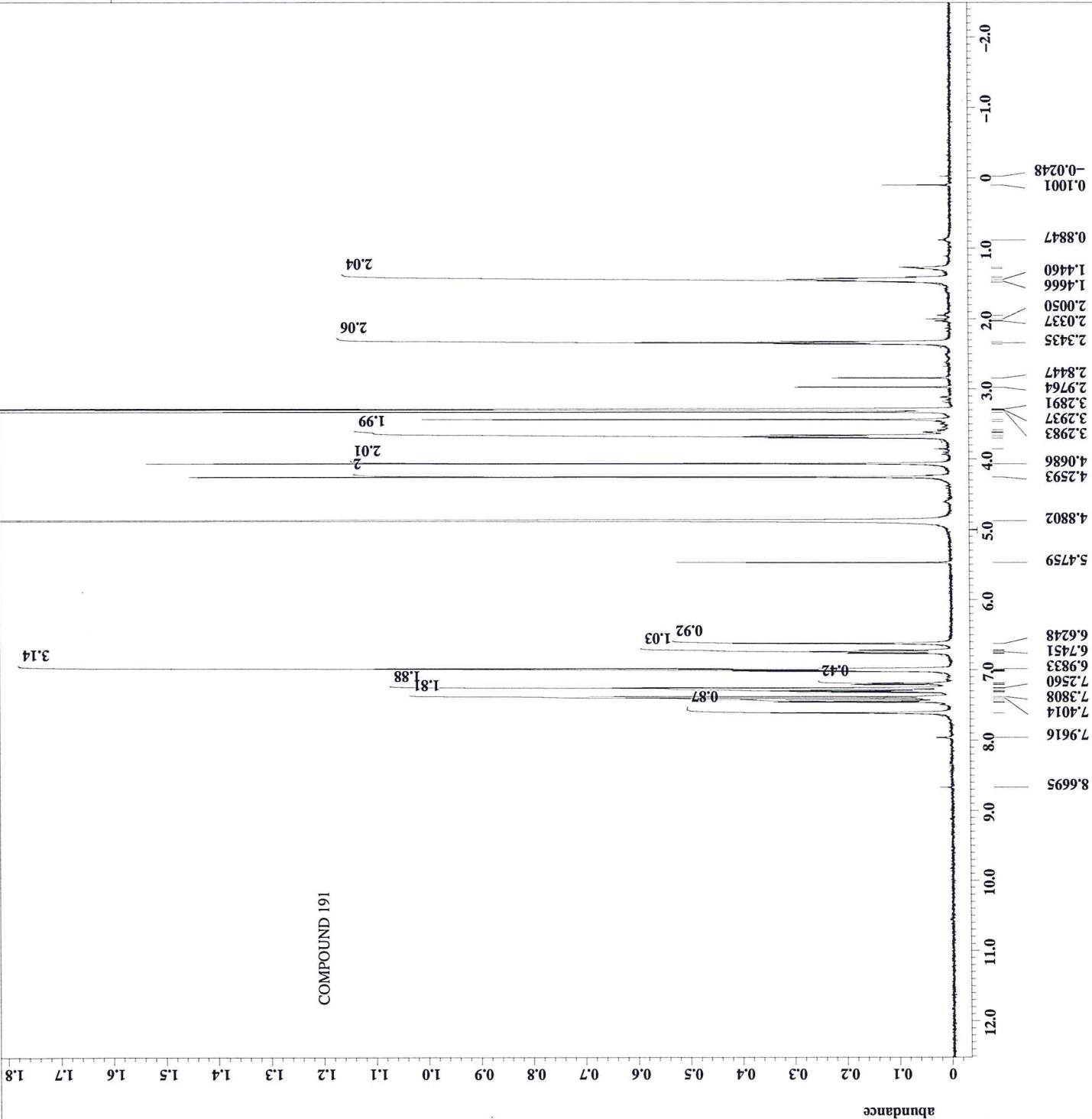
File      = RF-I-28_II_MeOH_PROTO
Author    = Delta
Experiment = single_pulse.ex2
Sample_id = RF-I-28_II_MeOH
Solvent   = METHANOL-D3
Creation_time = 5-JUL-2019 16:12:14
Revision_time = 12-MAR-2021 09:40:25
Current_time = 12-MAR-2021 09:40:29

Data_format = 1D COMPLEX
Dim_size    = 13107
Dim_title   = 1H
Dim_units   = [ppm]
Dimensions  = X
Site        = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain       = 1H
X_freq         = 399.78219838 [MHz]
X_offset       = 5 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.45794685 [Hz]
X_sweep        = 7.5030012 [kHz]
Irr_domain     = 1H
Irr_freq       = 399.78219838 [MHz]
Irr_offset     = 5 [ppm]
Tri_domain     = 1H
Tri_freq       = 399.78219838 [MHz]
Tri_offset     = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width    = 11.365 [us]
X_acq_time    = 2.18365952 [s]
X_angle       = 45 [deg]
X_atn         = 6 [dB]
X_pulse       = 5.6825 [us]
Irr_mode      = Off
Tri_mode      = Off
Dante_presat  = FALSE
Initial_wait  = 1 [s]
Recvr_gain    = 46
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get      = 20.3 [C]
  
```

COMPOUND 191



X : parts per Million : 1H



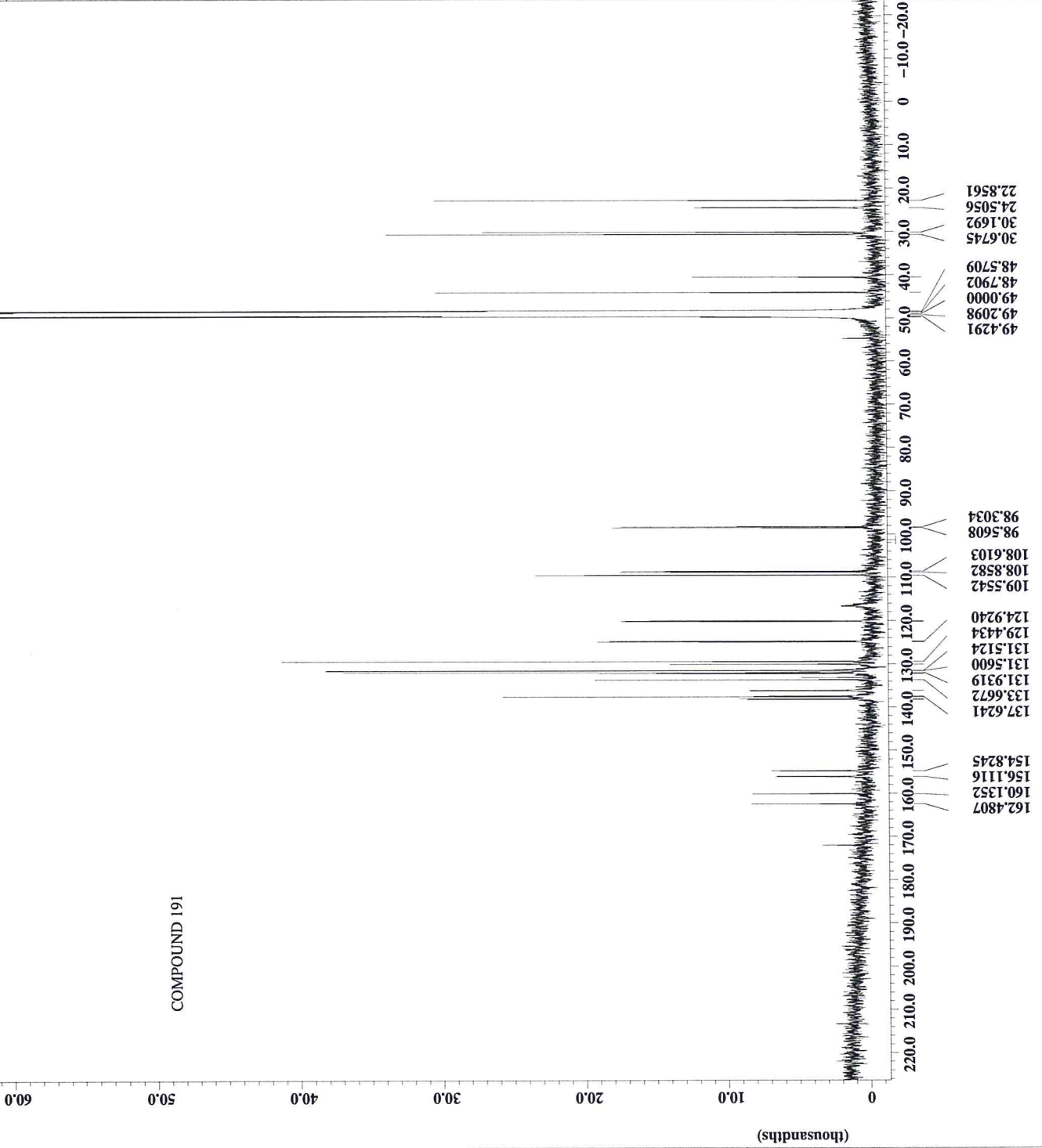
Filename = RF-I-28_II_MeOH_CARBO
Author = Delta
Experiment = single_pulse_dec
Sample_id = RF-I-28_II_MeOH
Solvent = METHANOL-D3
Creation_time = 7-JUL-2019 14:19:20
Revision_time = 12-MAR-2021 09:43:18
Current_time = 12-MAR-2021 09:43:22

Data_format = 1D_COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 41024
Total_scans = 41024

X_90_width = 10.4[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 9[db]
X_pulse = 3.46666667[us]
Irr_atn_dec = 24.2[db]
Irr_atn_noe = 24.2[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 3[s]
Recvr_gain = 58
Relaxation_delay = 3[s]
Repetition_time = 4.04333312[s]
Temp_get = 20.8[degC]

COMPOUND 191



X : parts per Million : 13C



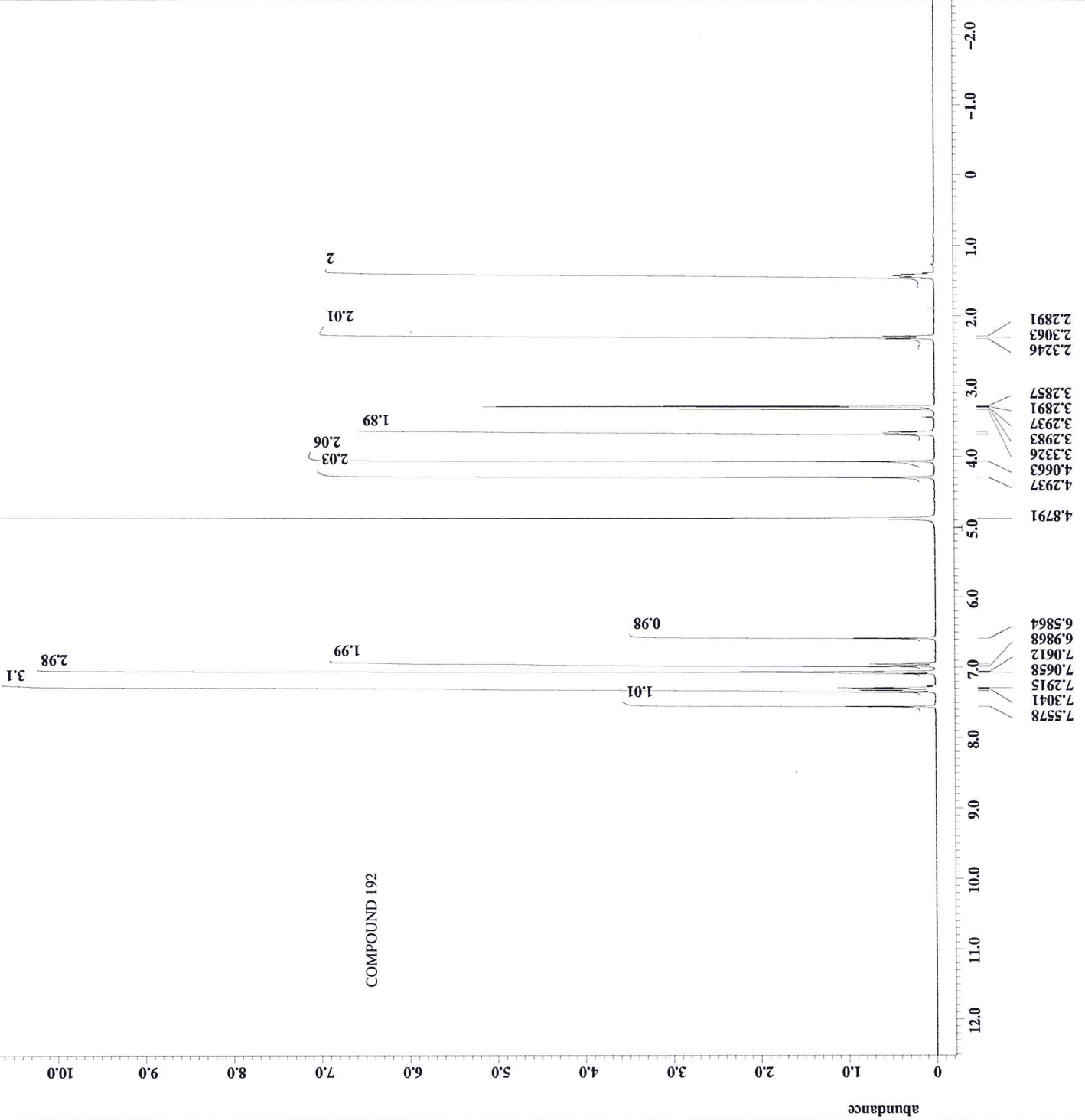
```

Filename = RF-I-39-MeOH_PROTON-4
Author = Delta
Experiment = single_pulse.ex2
Sample_id = RF-I-39-MeOH
Solvent = METHANOL-D3
Creation_time = 23-JUL-2019 20:21:35
Revision_time = 17-MAR-2021 13:24:06
Current_time = 17-MAR-2021 13:24:09

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 8

X_90_width = 11.365 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.6825 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 46
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 20.4 [dC]
  
```





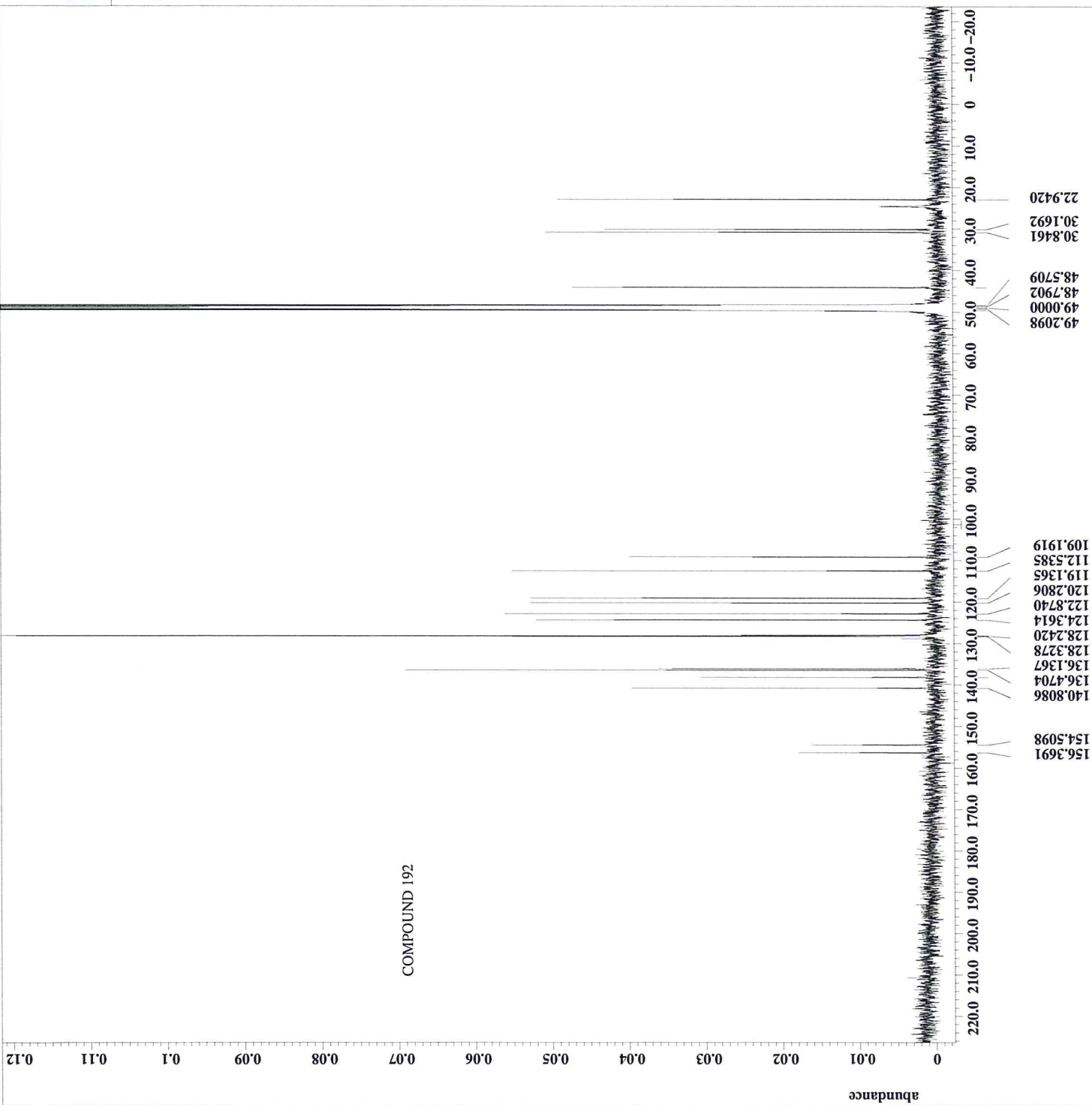
Filename = RF-I-39-MeOH-CARBON-5
Author = Delta
Experiment = single_pulse_dec
Sample_id = RF-I-39-MeOH
Solvent = METHANOL-D3
Creation_time = 24-JUL-2019 08:35:20
Revision_time = 17-MAR-2021 13:26:52
Current_time = 17-MAR-2021 13:26:56

Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 10850
Total_scans = 10850

X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.46666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 58
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 19.6 [dC]

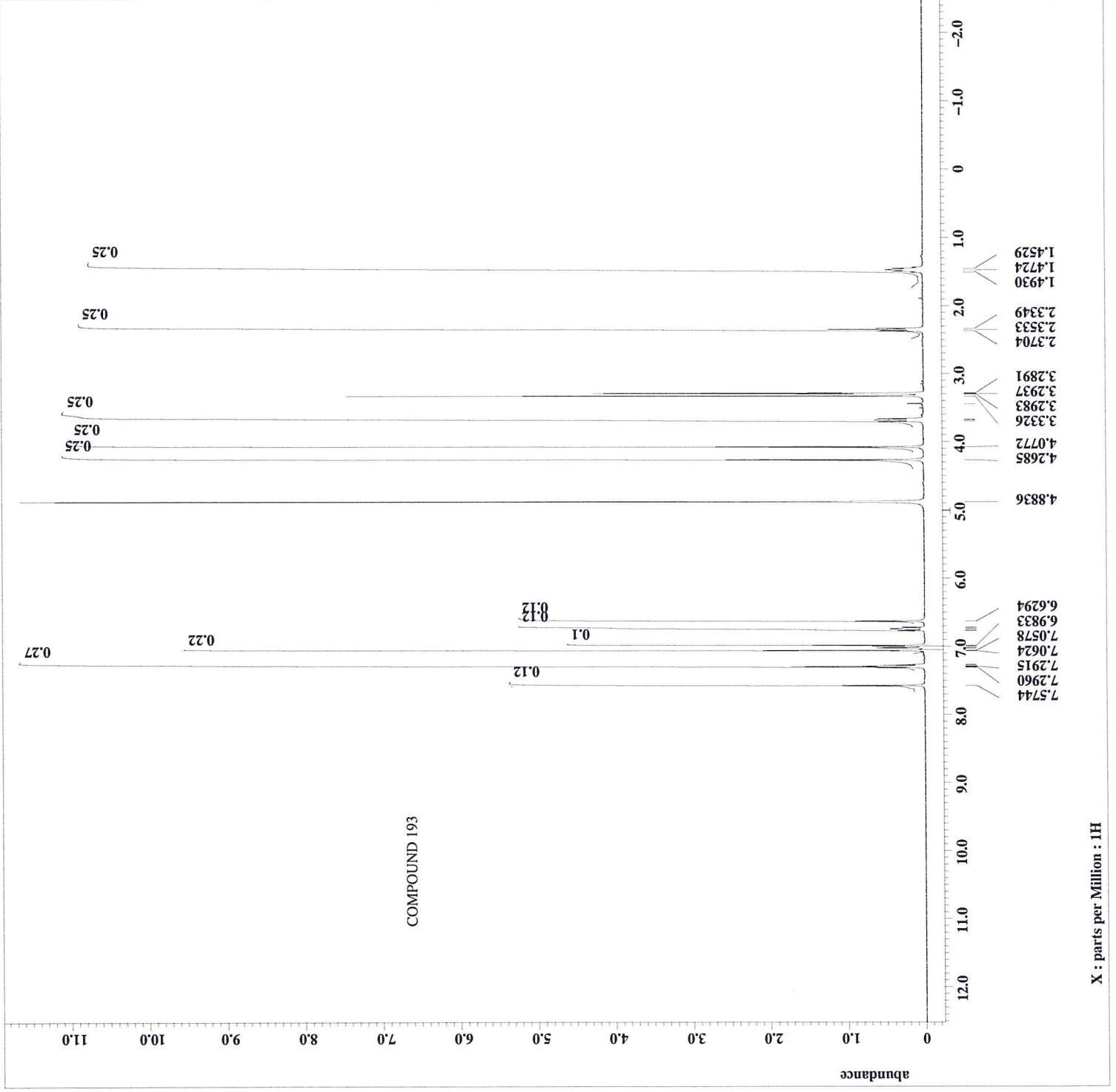
COMPOUND 192



X : parts per Million : 13C



Filename = RF-I-38_MEOH_PROTON-5
Author = Delta
Experiment = single_pulse.ex2
Sample_id = RF-I-38_MEOH
Solvent = METHANOL-D3
Creation_time = 22-JUL-2019 16:53:08
Revision_time = 17-MAR-2021 13:14:06
Current_time = 17-MAR-2021 13:14:10
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.365 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.6825 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 46
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 20 [dc]

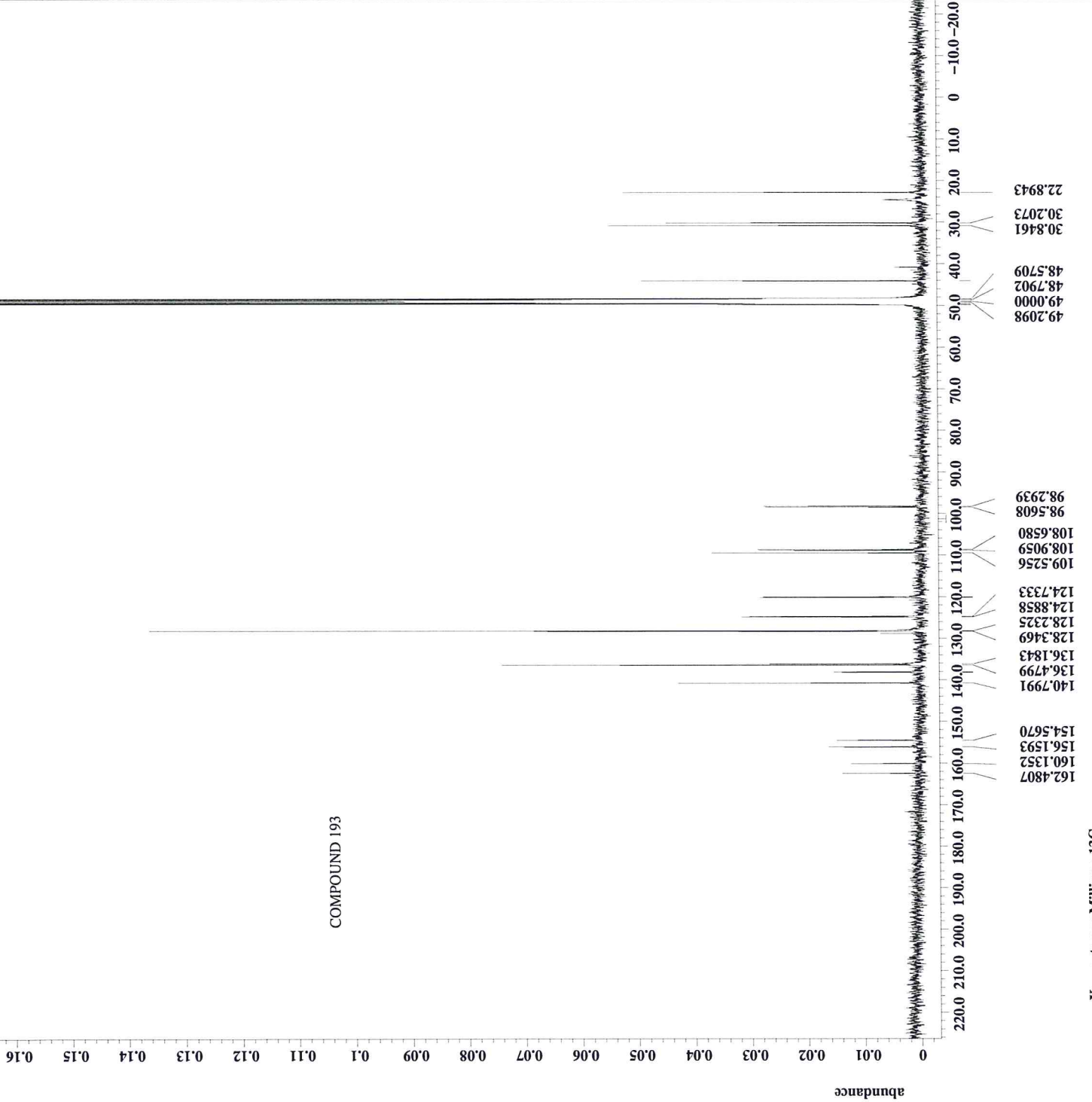


X : parts per Million : 1H



Filename = RF-I-38_MEOH_CARBON-5
Author = Delta
Experiment = single_pulse_dec
Sample_id = RF-I-38_MEOH
Solvent = METHANOL-D3
Creation_time = 23-JUL-2019 07:03:23
Revision_time = 17-MAR-2021 13:10:38
Current_time = 17-MAR-2021 13:10:42
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 12579
Total_scans = 12579
X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.46666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 3 [s]
Recvr_gain = 58
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 19.8 [dC]

COMPOUND 193



X : parts per Million : 13C



Filename = MM-I-83_PROTON-5.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = MM-I-83
Solvent = METHANOL-D3
Creation_time = 24-JAN-2017 17:13:17
Revision_time = 15-MAR-2021 14:58:40
Current_time = 15-MAR-2021 14:58:44

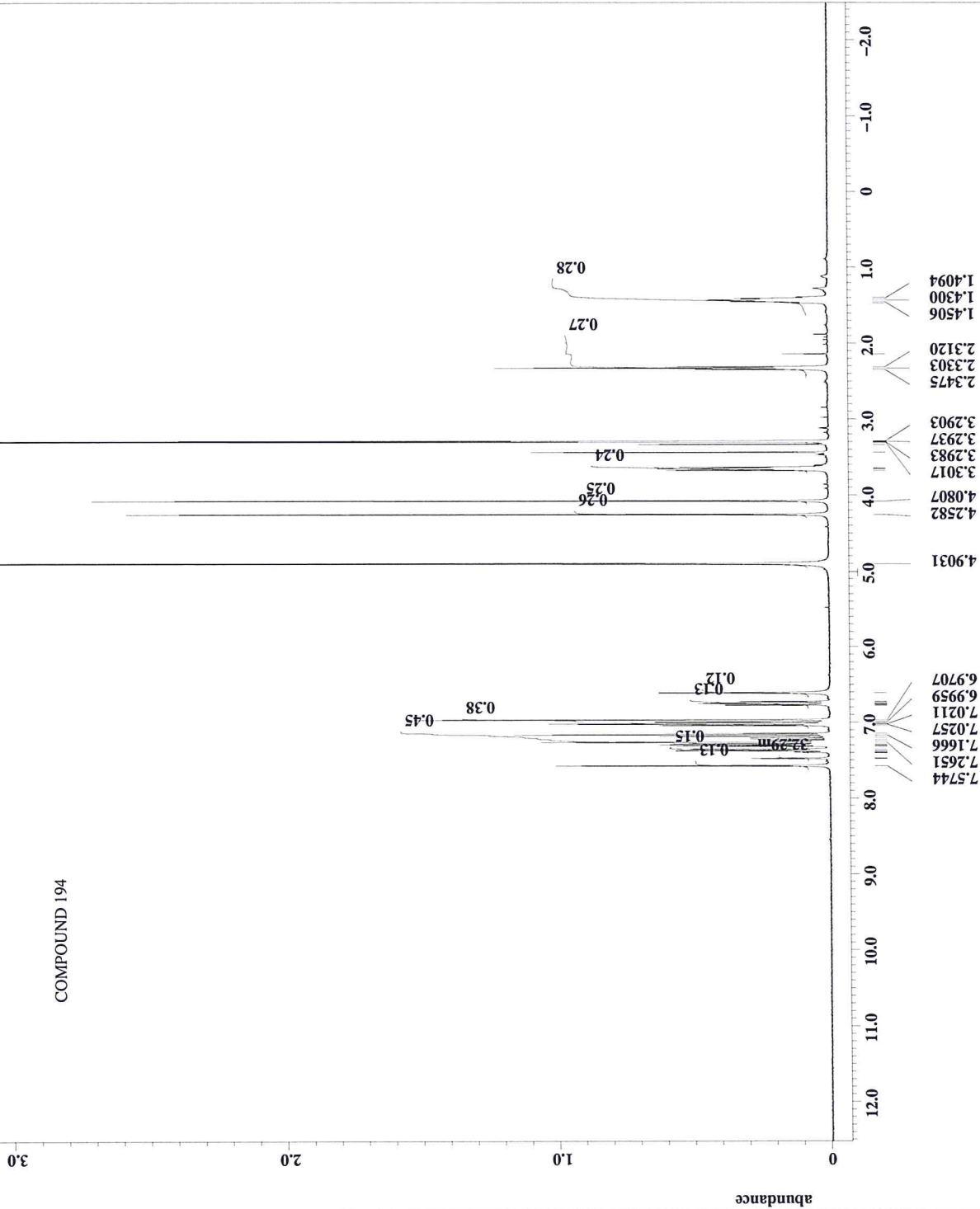
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 16

X_90_width = 10.68[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.34[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 46
Relaxation_delay = 4[s]
Repetition_time = 6.18365952[s]
Temp_get = 18.3[degC]

COMPOUND 194

78.22

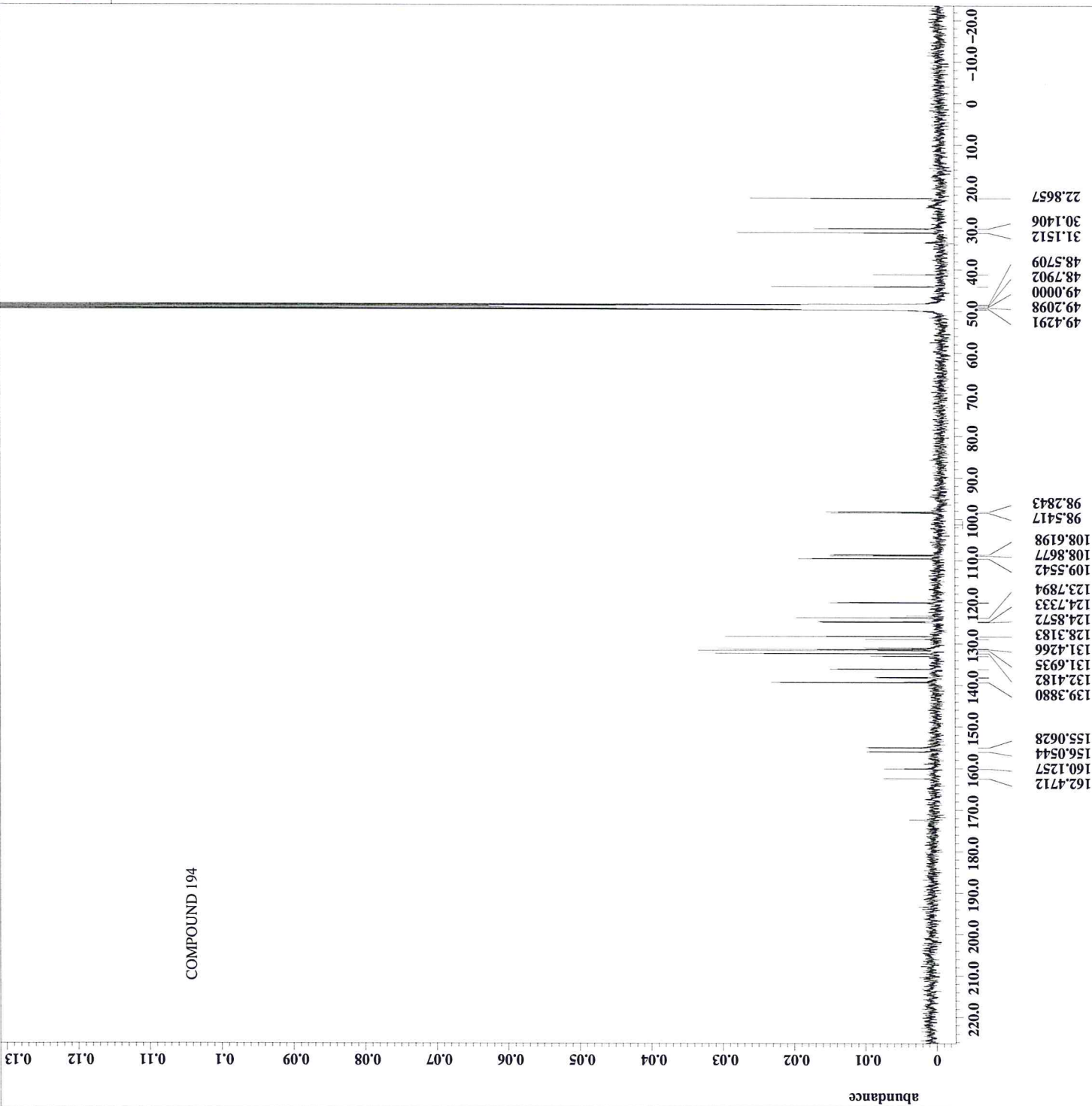


X : parts per Million : 1H



File name = MM-I-83_CARBON-5.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = MM-I-83
Solvent = METHANOL-D3
Creation time = 25-JAN-2017 06:46:12
Revision time = 15-MAR-2021 15:00:44
Current_time = 15-MAR-2021 15:00:48
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = TRUE
Clipped = TRUE
Mod_return = 1
Total_scans = 16000
X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 2 [s]
Recvr_gain = 58
Relaxation_delay = 2 [s]
Repetition_time = 3.04333312 [s]
Temp_get = 15.5 [dC]

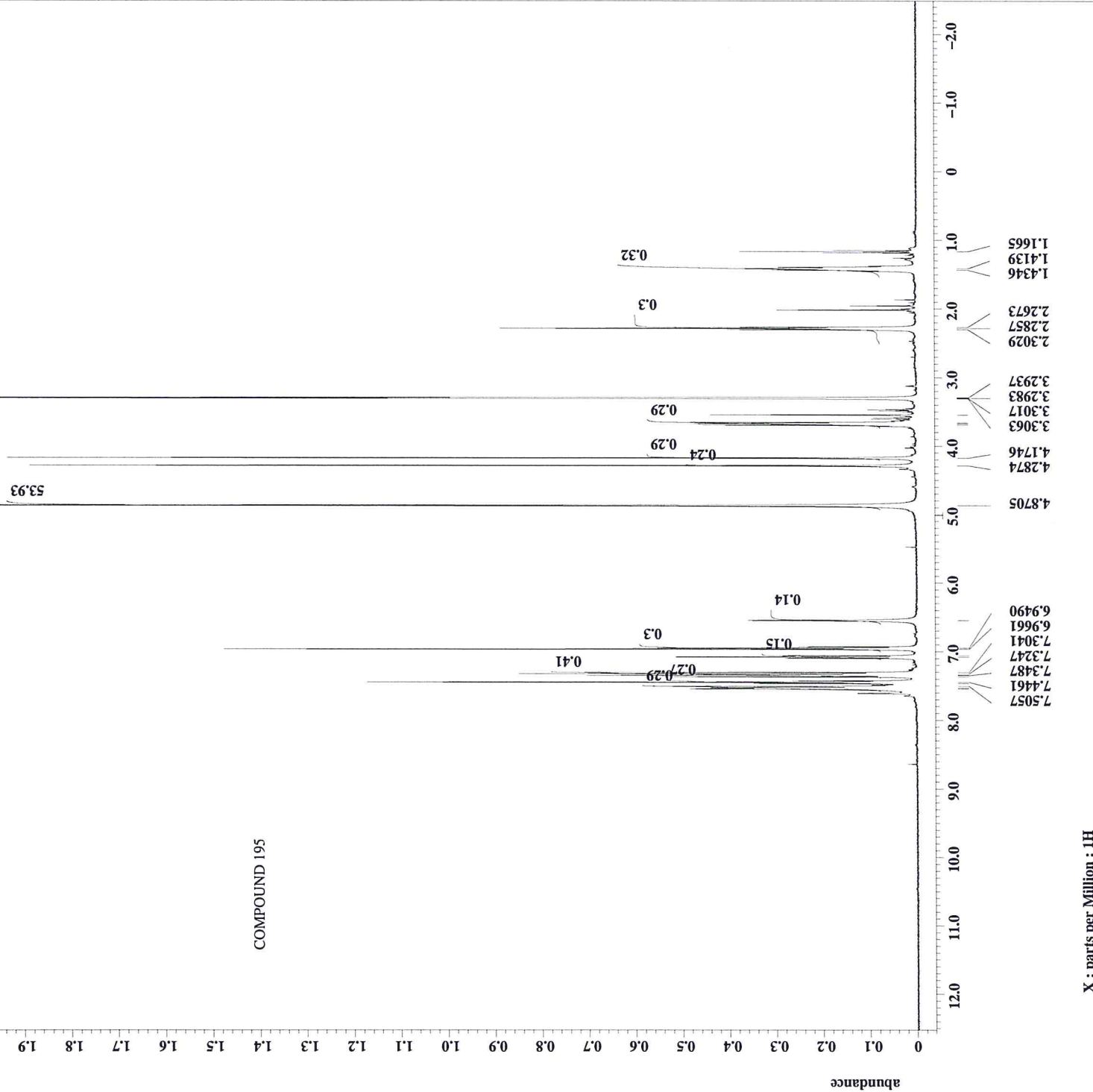
COMPOUND 194



X : parts per Million : 13C



= MM-I-66_PROTON-4.jdf
 = Delta
 = single_pulse.ex2
 = MM-I-66
 = METHANOL-D3
 = 9-NOV-2016 17:19:35
 = 11-MAR-2021 10:54:15
 = 11-MAR-2021 10:54:19
 = 1D COMPLEX
 = 13107
 = 1H
 = [ppm]
 = X
 = ECS 400
 = JNM-ECS400
 = 9.389766[T] (400[MHz])
 = 2.18365952[s]
 = 1H
 = 399.78219838[MHz]
 = 5[ppm]
 = 16384
 = 1
 = 0.45794685[Hz]
 = 7.5030012[kHz]
 = 1H
 = 399.78219838[MHz]
 = 5[ppm]
 = 1H
 = 399.78219838[MHz]
 = 5[ppm]
 = FALSE
 = 1
 = 16
 = 16
 = 10.68[us]
 = 2.18365952[s]
 = 45[deg]
 = 6[db]
 = 5.34[us]
 = Off
 = Off
 = FALSE
 = 1[s]
 = 44
 = 4[us]
 = 6.18365952[s]
 = 22[dc]

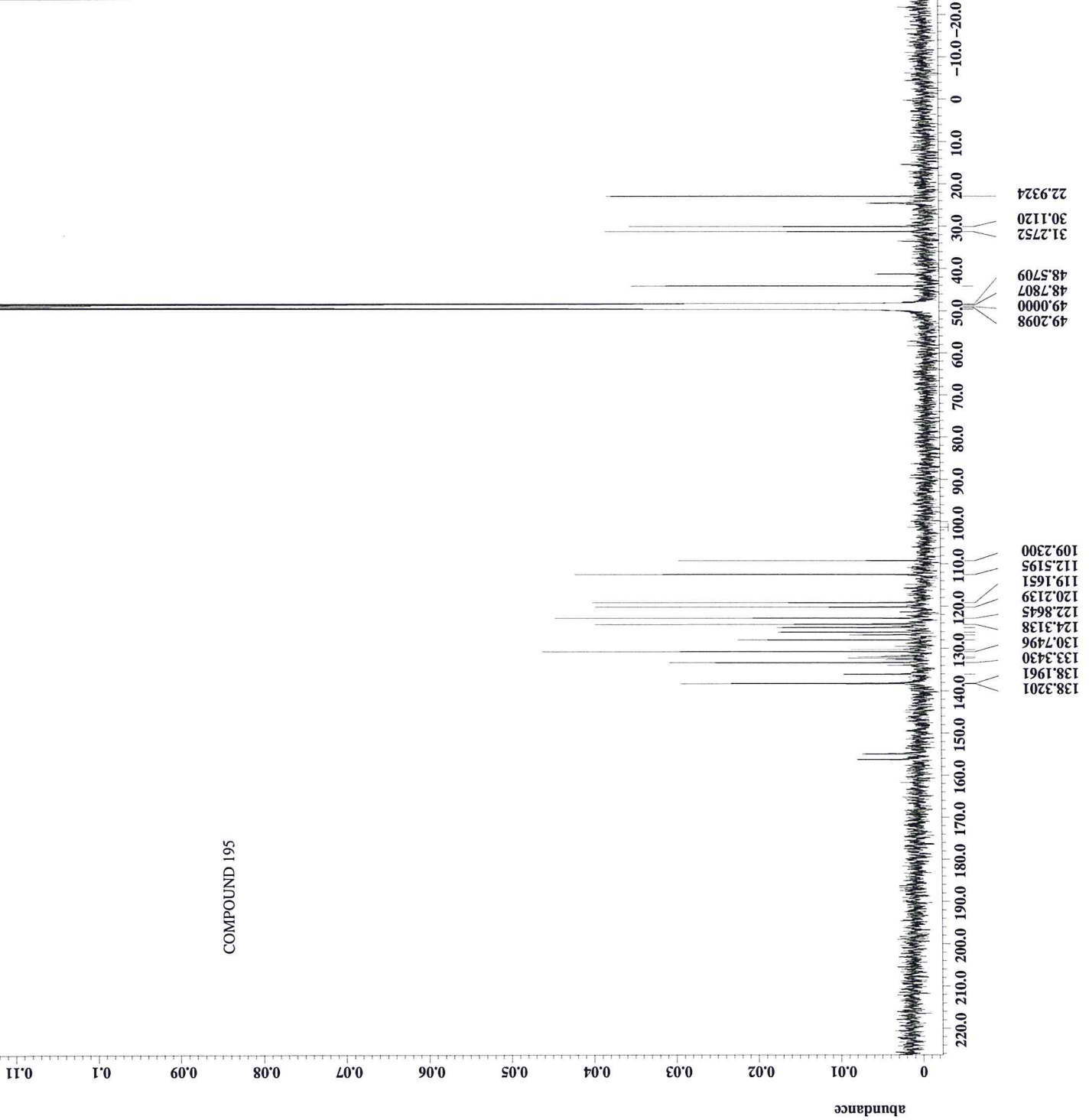


X : parts per Million : 1H



Filename = MM-I-66_CARBON-6.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = MM-I-66
Solvent = METHANOL-D3
Creation_time = 10-NOV-2016 07:36:19
Revision_time = 11-MAR-2021 10:57:06
Current_time = 11-MAR-2021 10:57:10
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = TRUE
Clipped = TRUE
Mod_return = 1
Scans = 12683
Total_scans = 12683
X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 22 [dC]

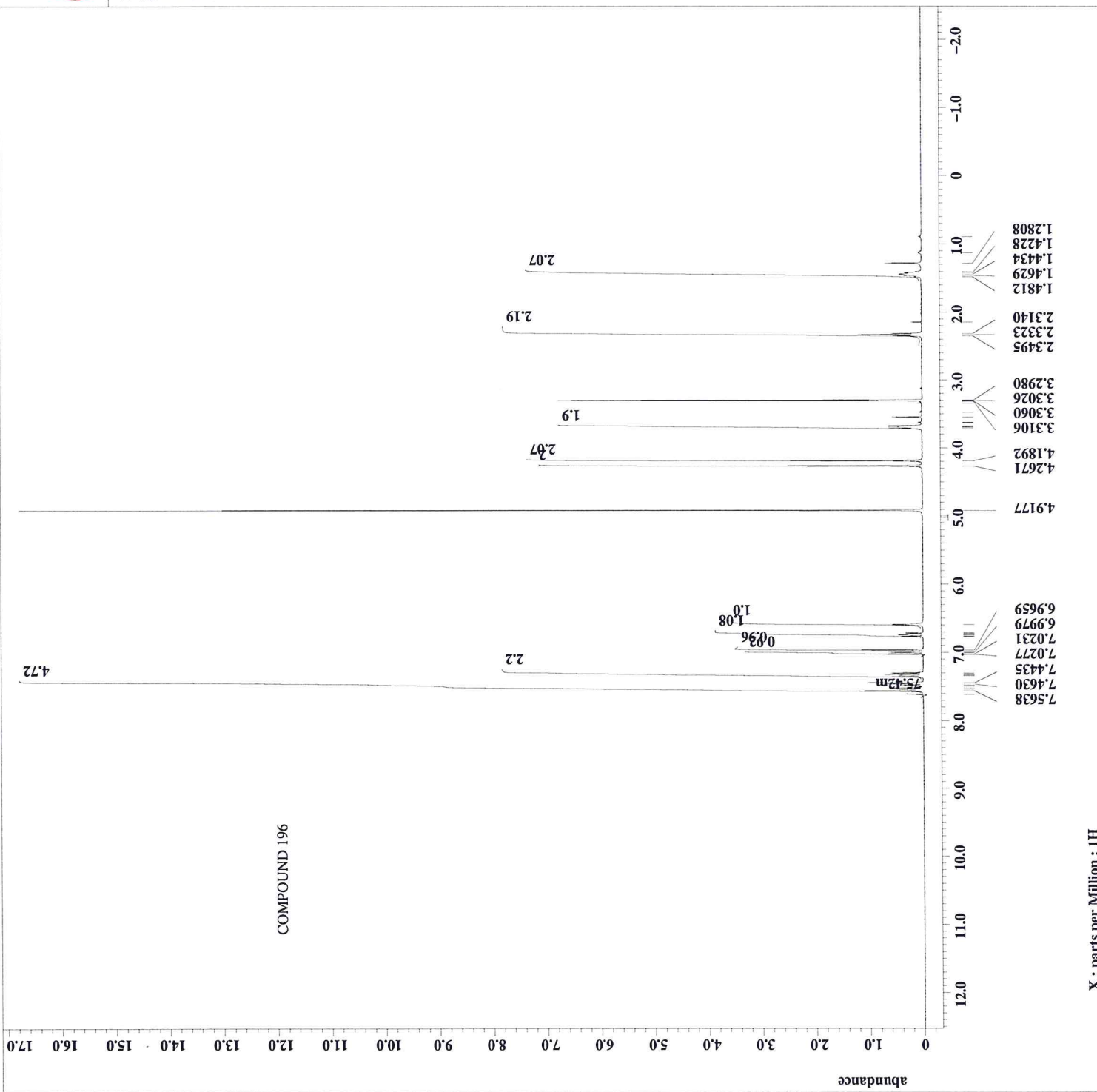
COMPOUND 195



X : parts per Million : 13C



Filename = MM-I-87_PROTON-5.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = MM-I-87
Solvent = METHANOL-D3
Creation_time = 16-FEB-2017 17:24:42
Revision_time = 15-MAR-2021 15:27:16
Current_time = 15-MAR-2021 15:27:18
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.68 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.34 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 46
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 17.1 [dC]

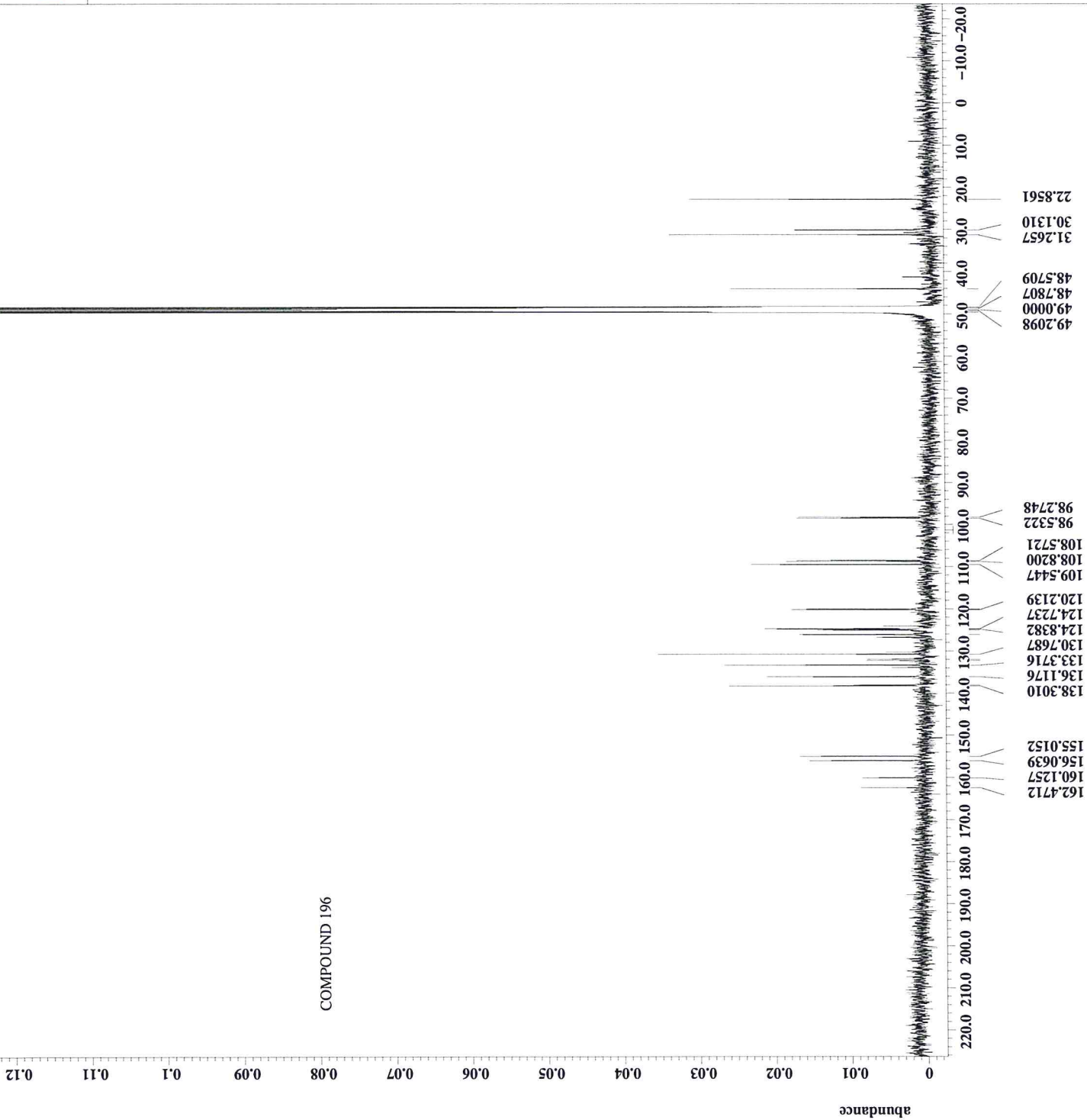


X : parts per Million : 1H



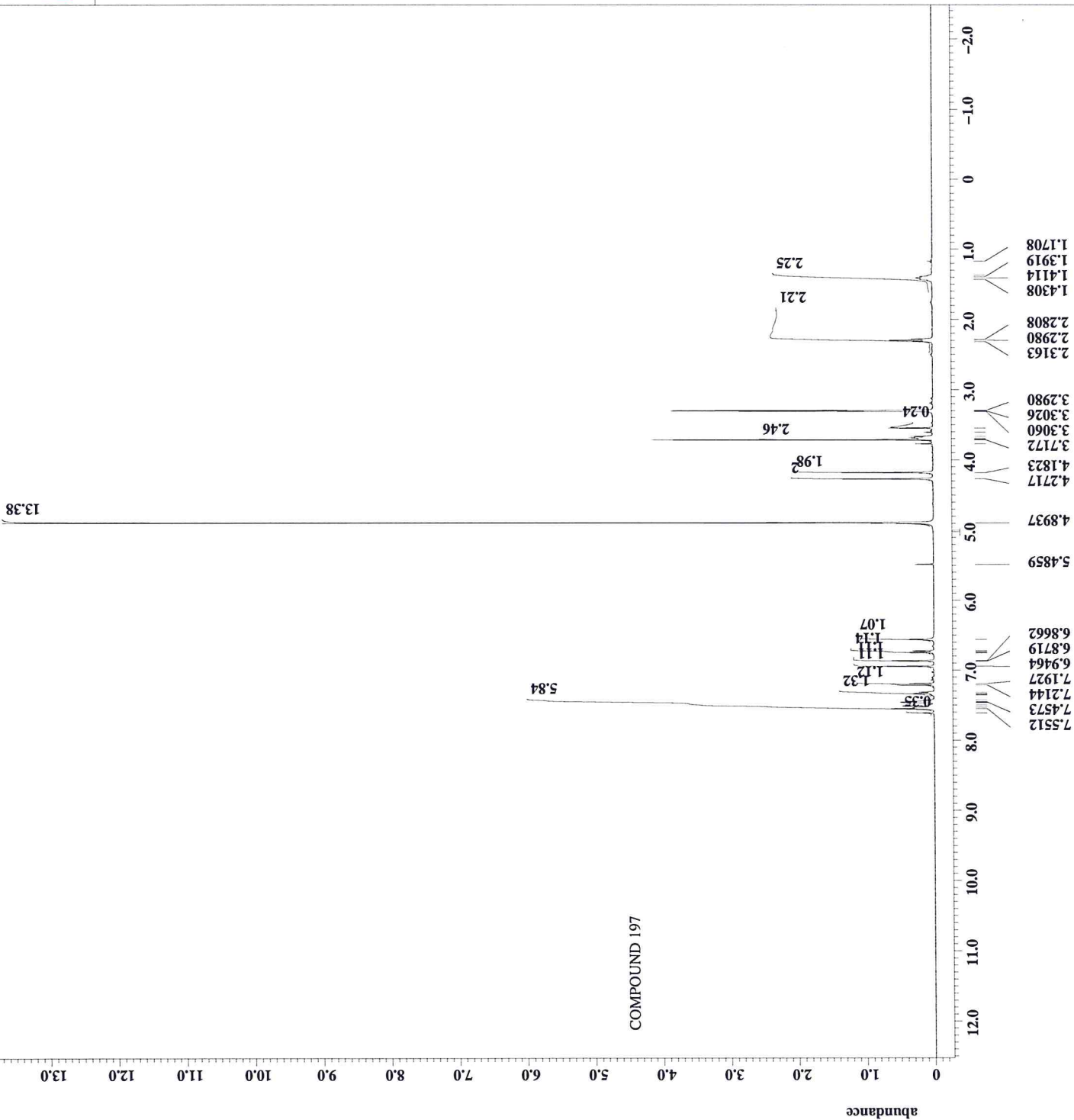
Filename = MM-I-87_CARBON-5.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = MM-I-87
Solvent = METHANOL-D3
Creation_time = 17-FEB-2017 05:17:17
Revision_time = 15-MAR-2021 15:29:37
Current_time = 15-MAR-2021 15:29:31
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 14000
X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 19.2 [dC]

COMPOUND 196





Filename = SK-I-57_PROTON-5.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SK-I-57
Solvent = METHANOL-D3
Creation_time = 6-JUN-2017 12:10:18
Revision_time = 12-MAR-2021 10:51:13
Current_time = 12-MAR-2021 10:51:30
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.68[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.34[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 46
Relaxation_delay = 4[s]
Repetition_time = 6.18365952[s]
Temp_get = 460.0[dc]

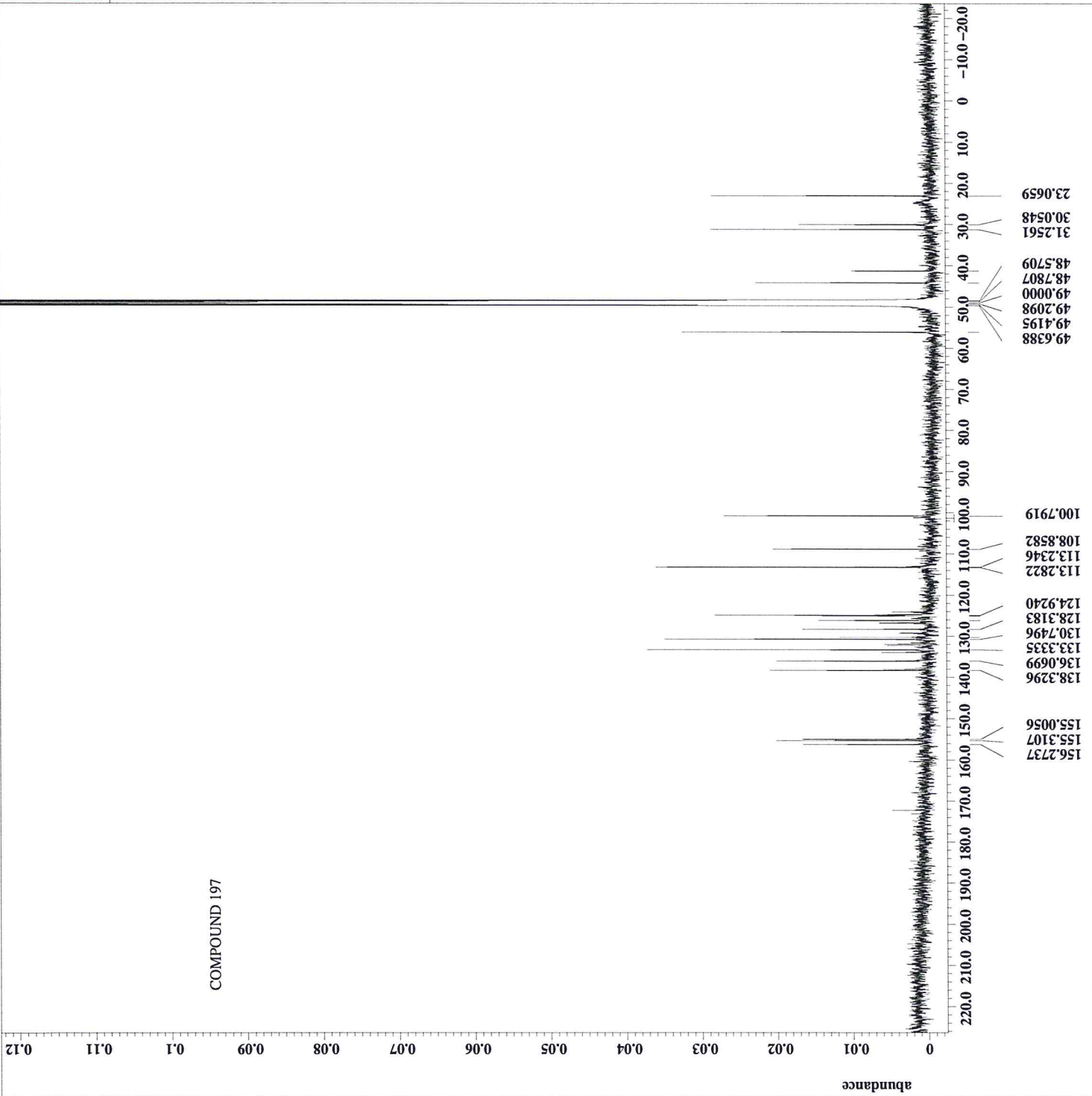


X : parts per Million : 1H



File name = SK-I-57-overnight_CAR
Author = Delta
Experiment = single_pulse_dec
Sample_id = SK-I-57-overnight
Solvent = METHANOL-D3
Creation_time = 9-JUN-2017 07:54:55
Revision_time = 12-MAR-2021 09:59:10
Current_time = 12-MAR-2021 09:59:15
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 18845
X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 460.0 [dC]

COMPOUND 197



X : parts per Million : 13C



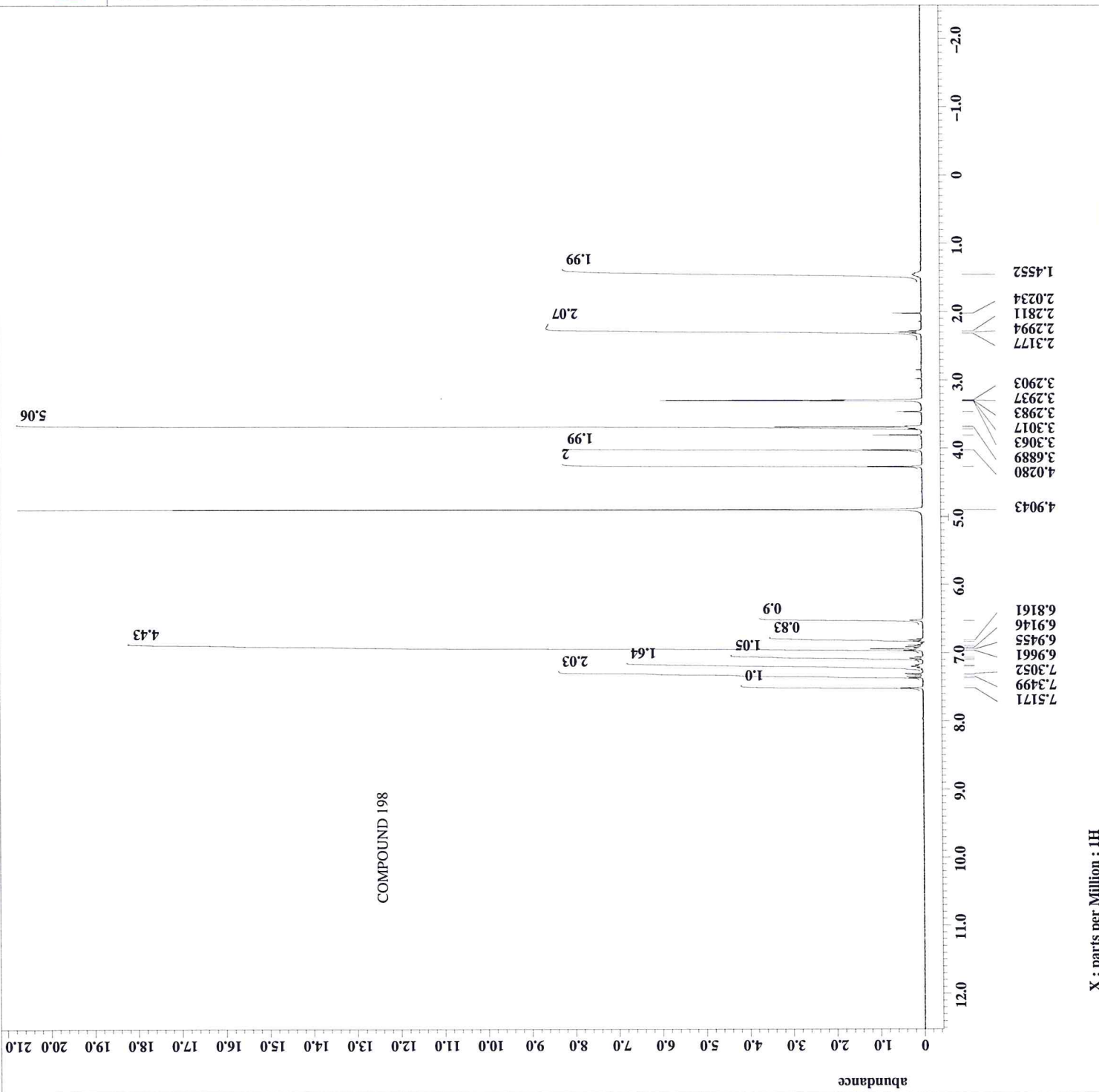
```

Filename = RF-I-16-METHANOL_PROT
Author = Delta
Experiment = single_pulse.ex2
Sample_id = RF-I-16-METHANOL
Solvent = METHANOL-D3
Creation_time = 20-FEB-2019 15:36:46
Revision_time = 17-MAR-2021 11:24:17
Current_time = 17-MAR-2021 11:24:22

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = EGS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4

X_90_width = 11.365 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.6825 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 50
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 17.6 [dC]
  
```

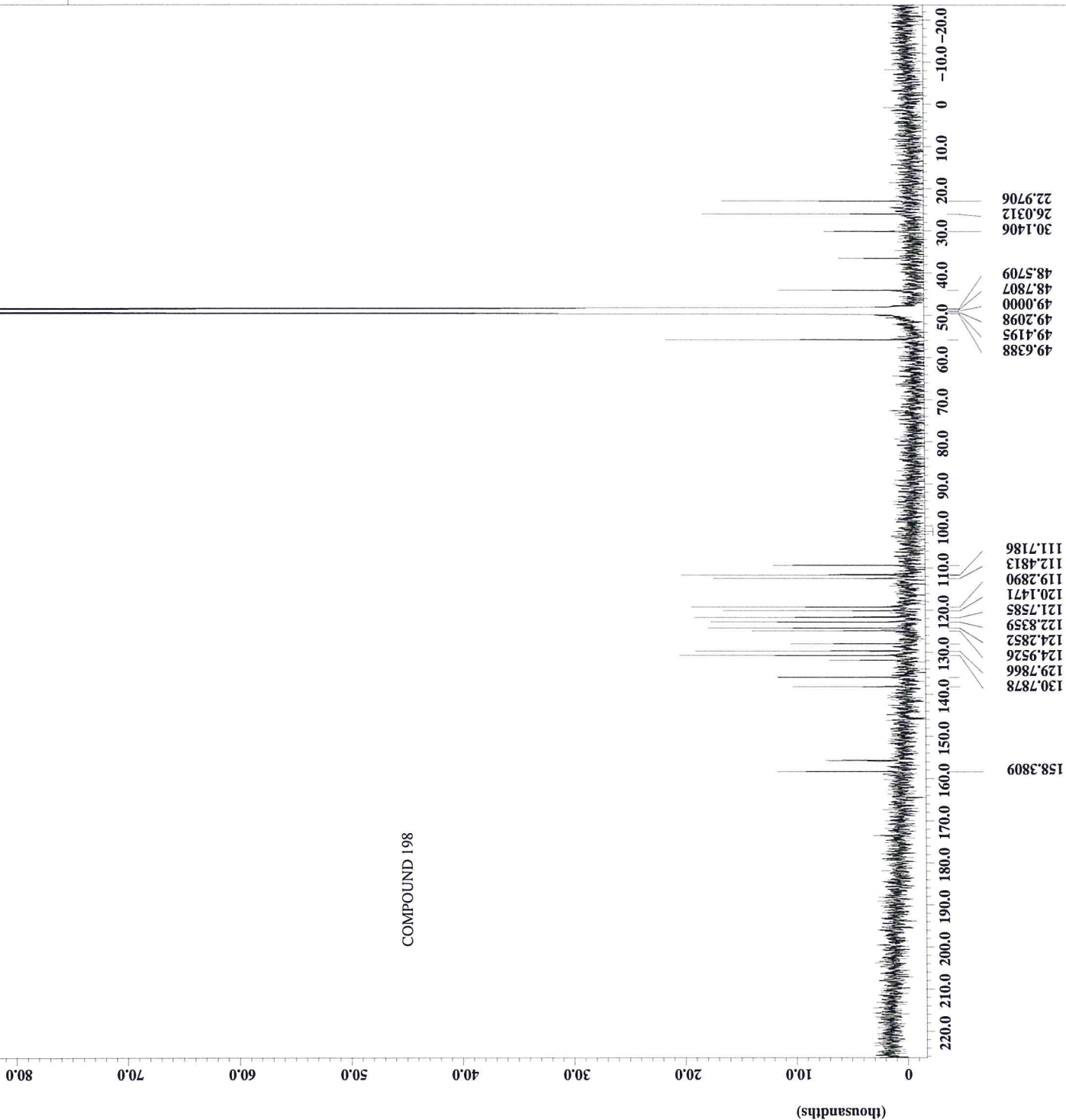


X : parts per Million : 1H



Filename = RF-I-16-METHANOL_CARB
Author = Delta
Experiment = single_pulse_dec
Sample_id = RF-I-16-METHANOL
Solvent = METHANOL-D3
Creation_time = 21-FEB-2019 07:42:09
Revision_time = 17-MAR-2021 11:27:06
Current_time = 17-MAR-2021 11:27:15
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [kHz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = FALSE
Clipped = FALSE
Mod_return = 1
Scans = 14275
Total_scans = 14275
X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.465666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 58
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 17.9 [dc]

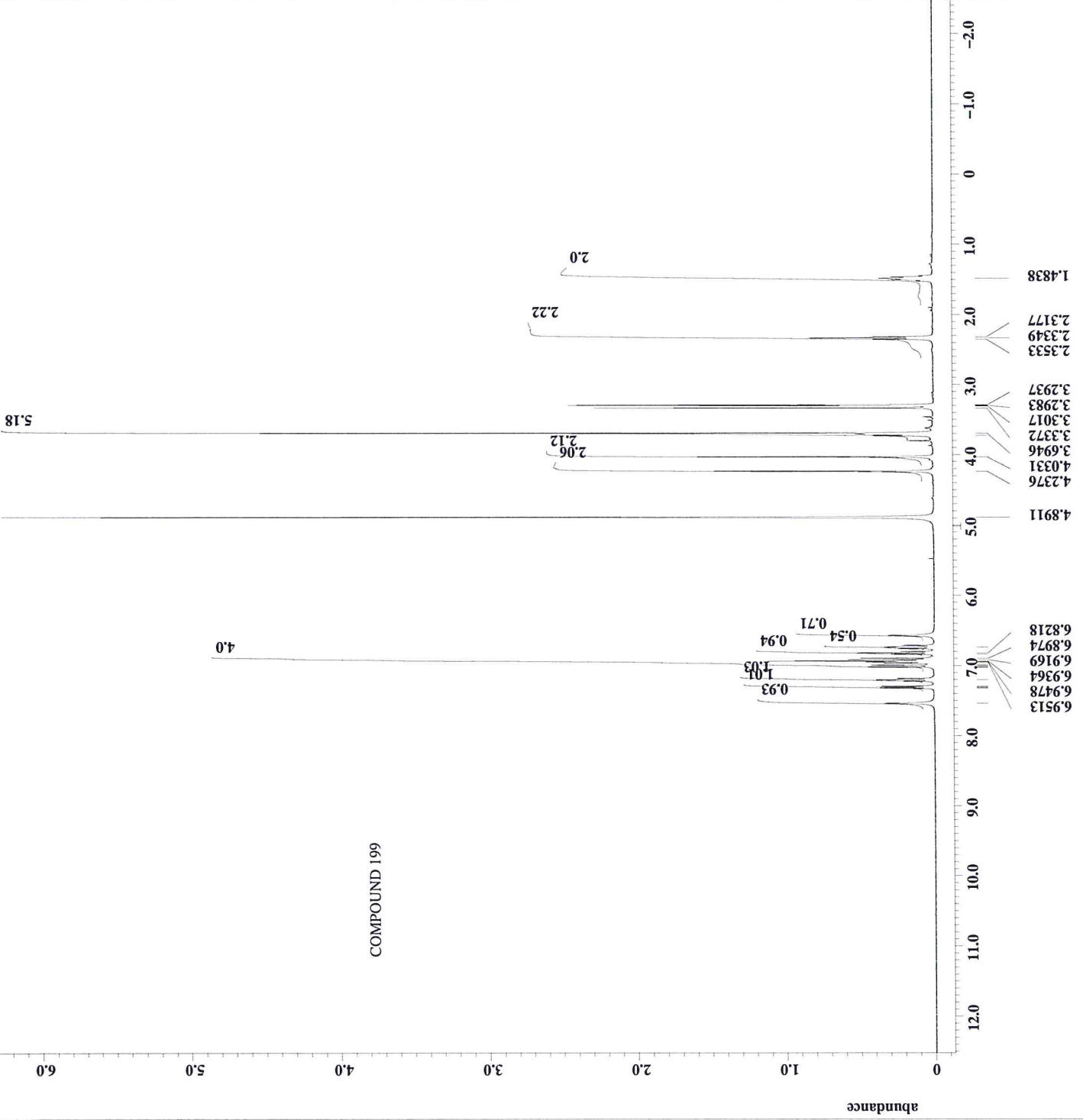
COMPOUND 198



X : parts per Million : 13C



Filename = RF-I-34-METHANOL_PROT
Author = Delta
Experiment = single_pulse.ex2
Sample_id = RF-I-34-METHANOL
Solvent = METHANOL-D3
Creation_time = 1-JUL-2019 15:17:28
Revision_time = 17-MAR-2021 13:07:43
Current_time = 17-MAR-2021 13:07:47
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.365 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.6825 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 42
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 19.9 [dC]

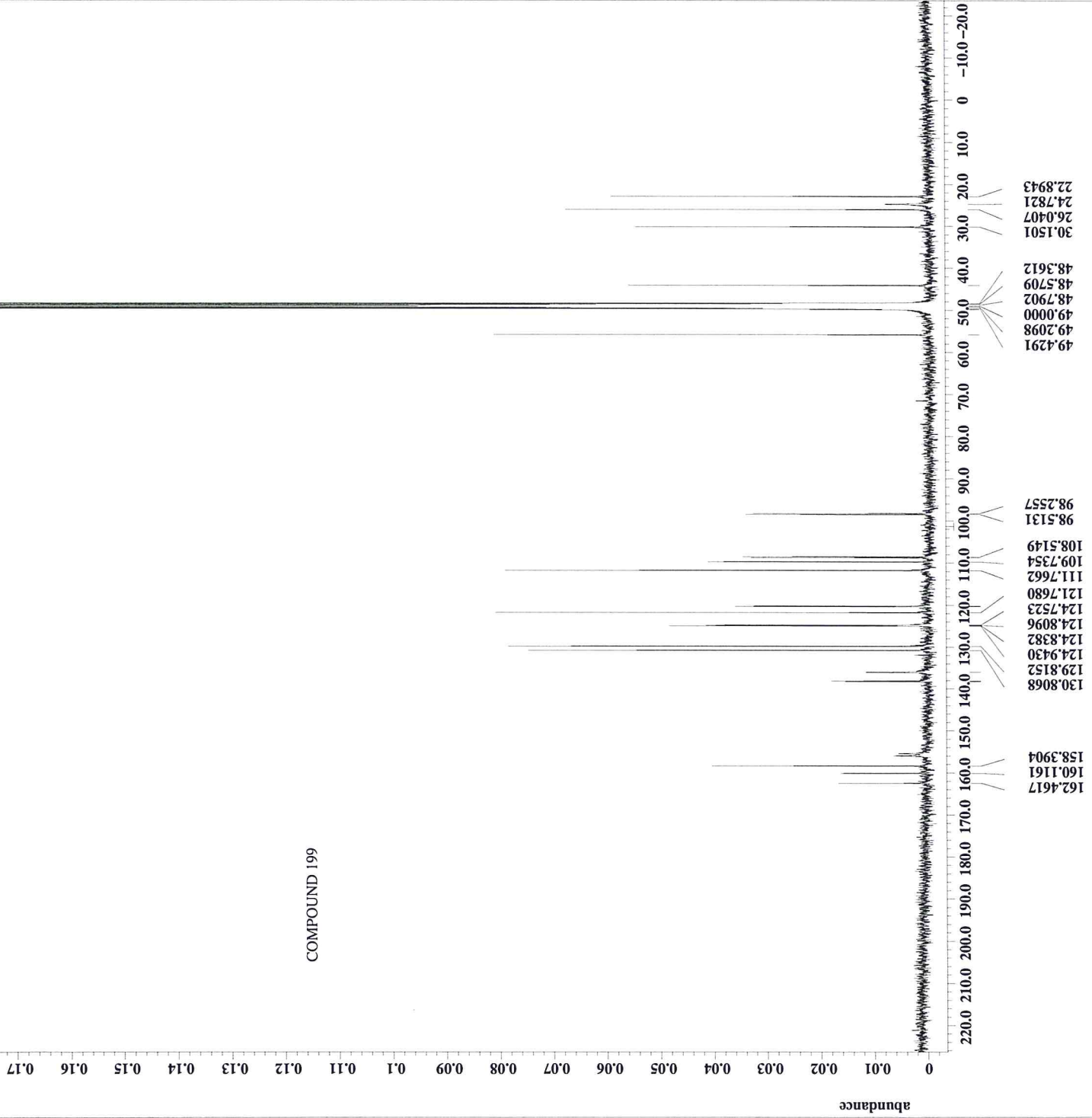


X : parts per Million : 1H



Filename = RF-I-34-METHANOL_CARB
Author = Delta
Experiment = single_pulse_dec
Sample_id = RF-I-34-METHANOL
Solvent = METHANOL-D3
Creation_time = 2-JUL-2019 06:33:57
Revision_time = 17-MAR-2021 13:16:54
Current_time = 17-MAR-2021 13:16:56
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [KHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 13573
Total_scans = 13573
X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.46666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 3 [s]
Recvr_gain = 58
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 20.2 [dC]

COMPOUND 199



X : parts per Million : 13C



```

Filename = RE-I-23-METHANOL_PROT
Author = Delta
Experiment = single_pulse.ex2
Sample_id = RE-I-23-METHANOL
Solvent = METHANOL-D3
Creation_time = 7-MAR-2019 15:45:47
Revision_time = 17-MAR-2021 11:32:13
Current_time = 17-MAR-2021 11:32:17

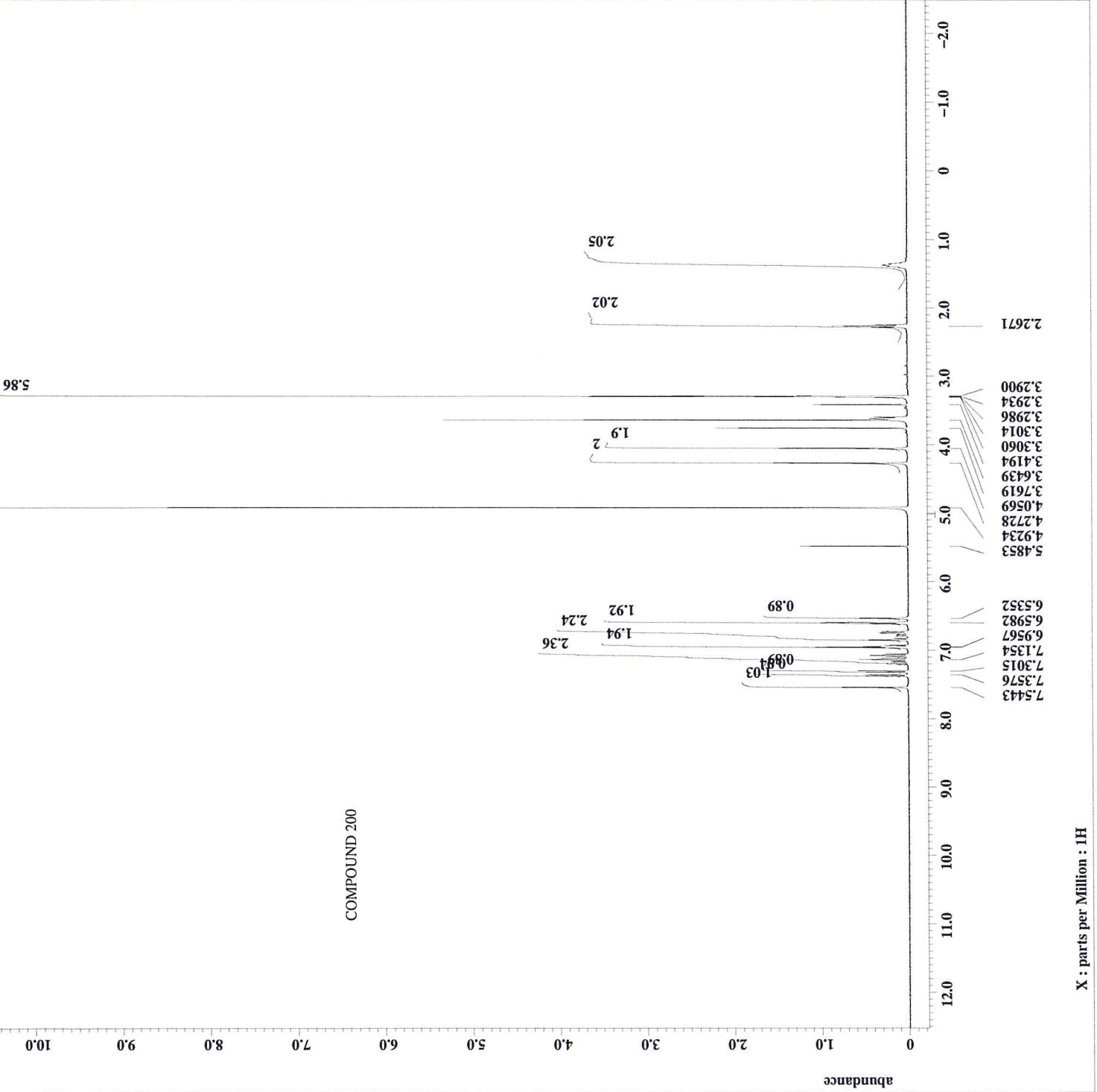
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = UNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 4

X_90_width = 11.365[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.6825[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 46
Relaxation_delay = 4[s]
Repetition_time = 6.18365952[s]
Temp_get = 15.7[dc]
  
```

5.86

COMPOUND 200

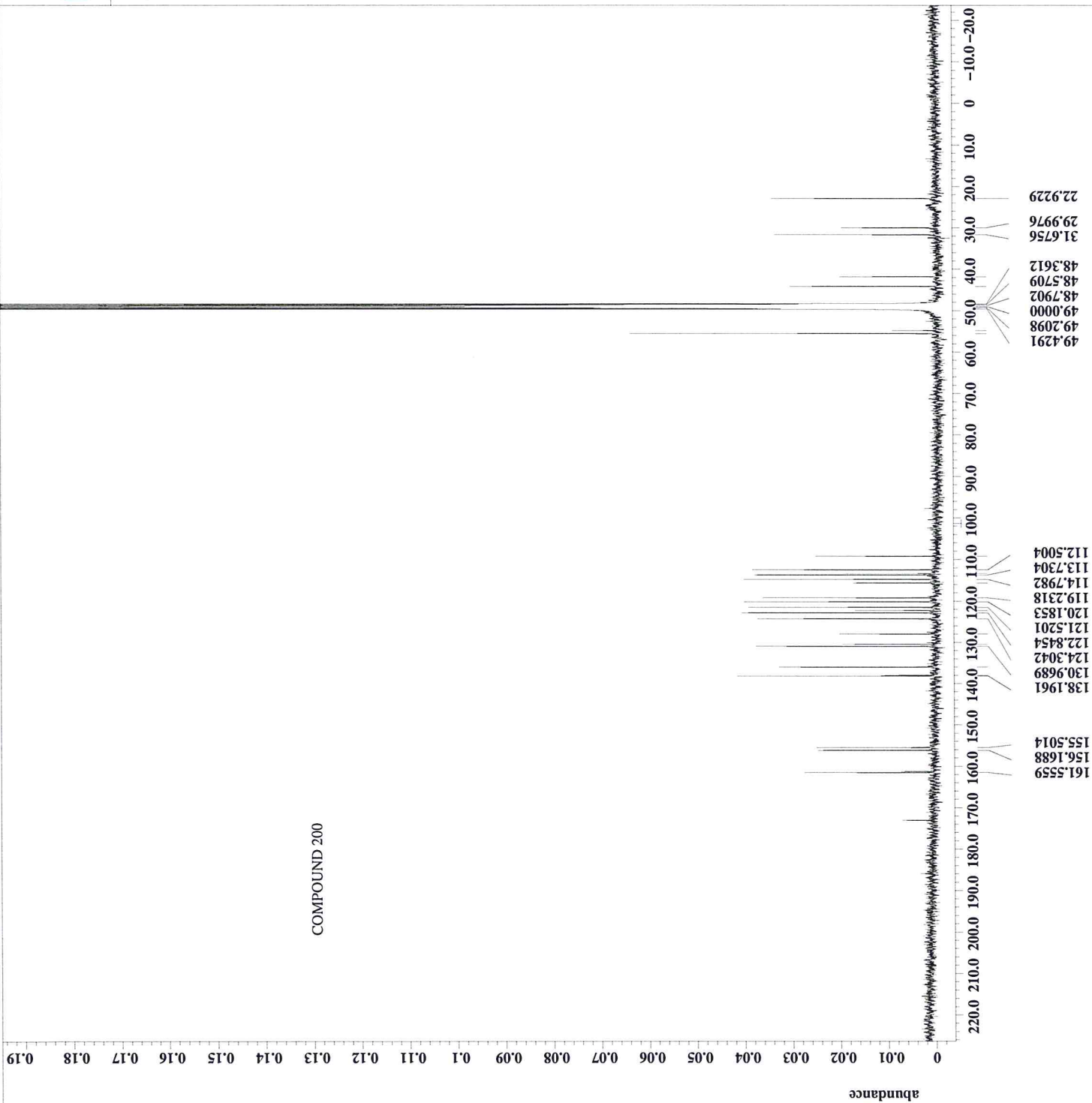


X : parts per Million : 1H



Filename = RE-I-23-METHANOL_CARB
Author = Delta
Experiment = single_pulse_dec
Sample_id = RF-I-23-METHANOL
Solvent = METHANOL-D3
Creation_time = 8-MAR-2019 07:46:23
Revision_time = 17-MAR-2021 11:34:16
Current_time = 17-MAR-2021 11:34:19
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = TRUE
Clipped = TRUE
Mod_return = 1
Scans = 14201
Total_scans = 14201
X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.46666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 58
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 16.6 [dC]

COMPOUND 200



X : parts per Million : 13C



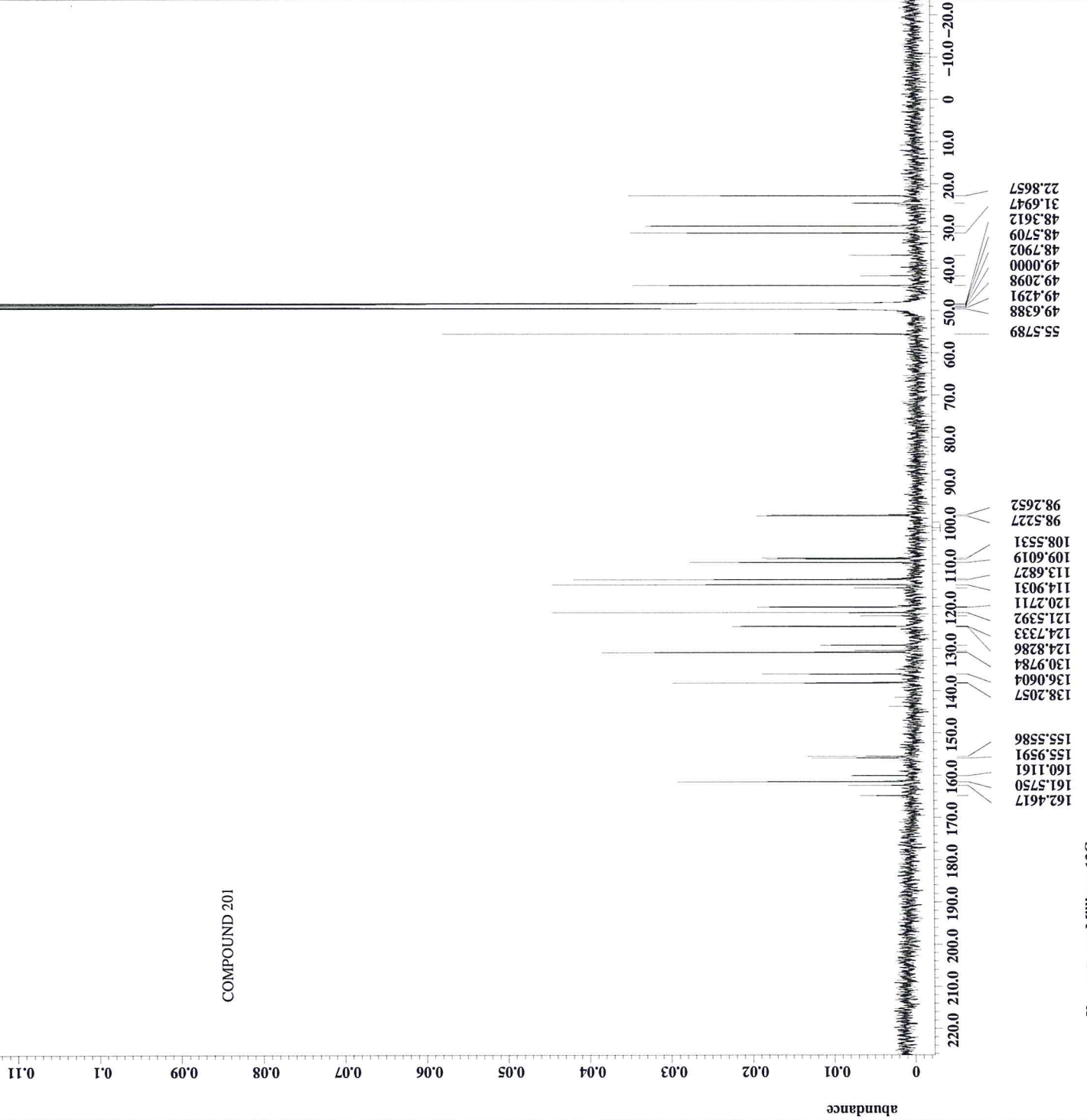
Filename = RF-I-31_METHANOL_CARB
Author = Delta
Experiment = single_pulse_dec
Sample_id = RF-I-31_METHANOL
Solvent = METHANOL-D3
Creation_time = 15-JUN-2019 06:56:42
Revision_time = 17-MAR-2021 11:37:24
Current_time = 17-MAR-2021 11:37:28

Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = FALSE
Clipped = FALSE
Mod_return = 1
Scans = 14540
Total_scans = 14540

X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.46666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 56
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 20 [dC]

COMPOUND 201



X : parts per Million : 13C

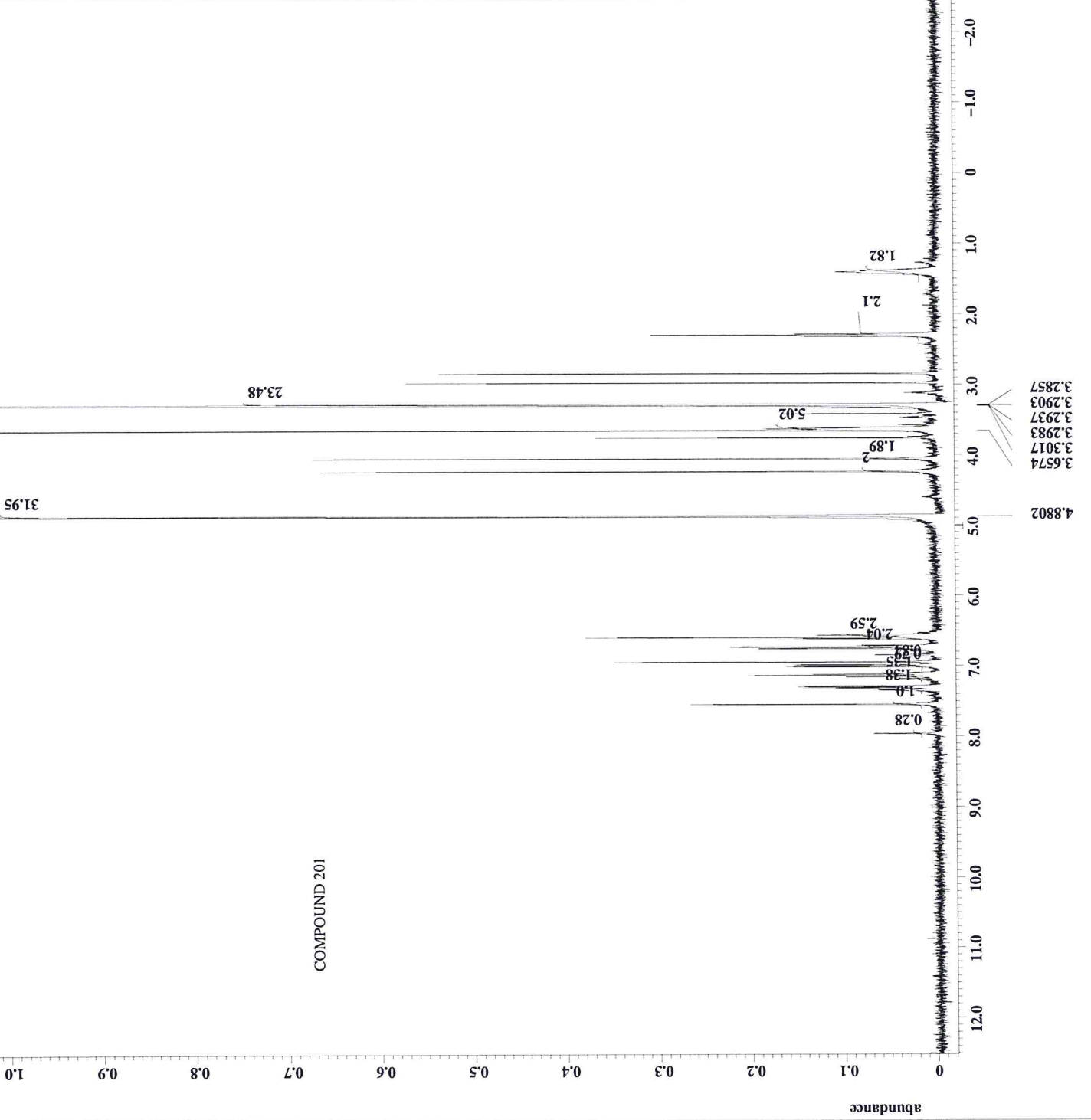


Filename = RF-I-31_METHANOL_II_P
Author = Delta
Experiment = single_pulse.ex2
Sample_id = RF-I-31_METHANOL_II
Solvent = METHANOL-D3
Creation_time = 17-JUN-2019 11:57:29
Revision_time = 17-MAR-2021 11:42:58
Current_time = 17-MAR-2021 11:43:02
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.3665 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.6825 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 50
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 19.7 [DC]

31.95

23.48

COMPOUND 201

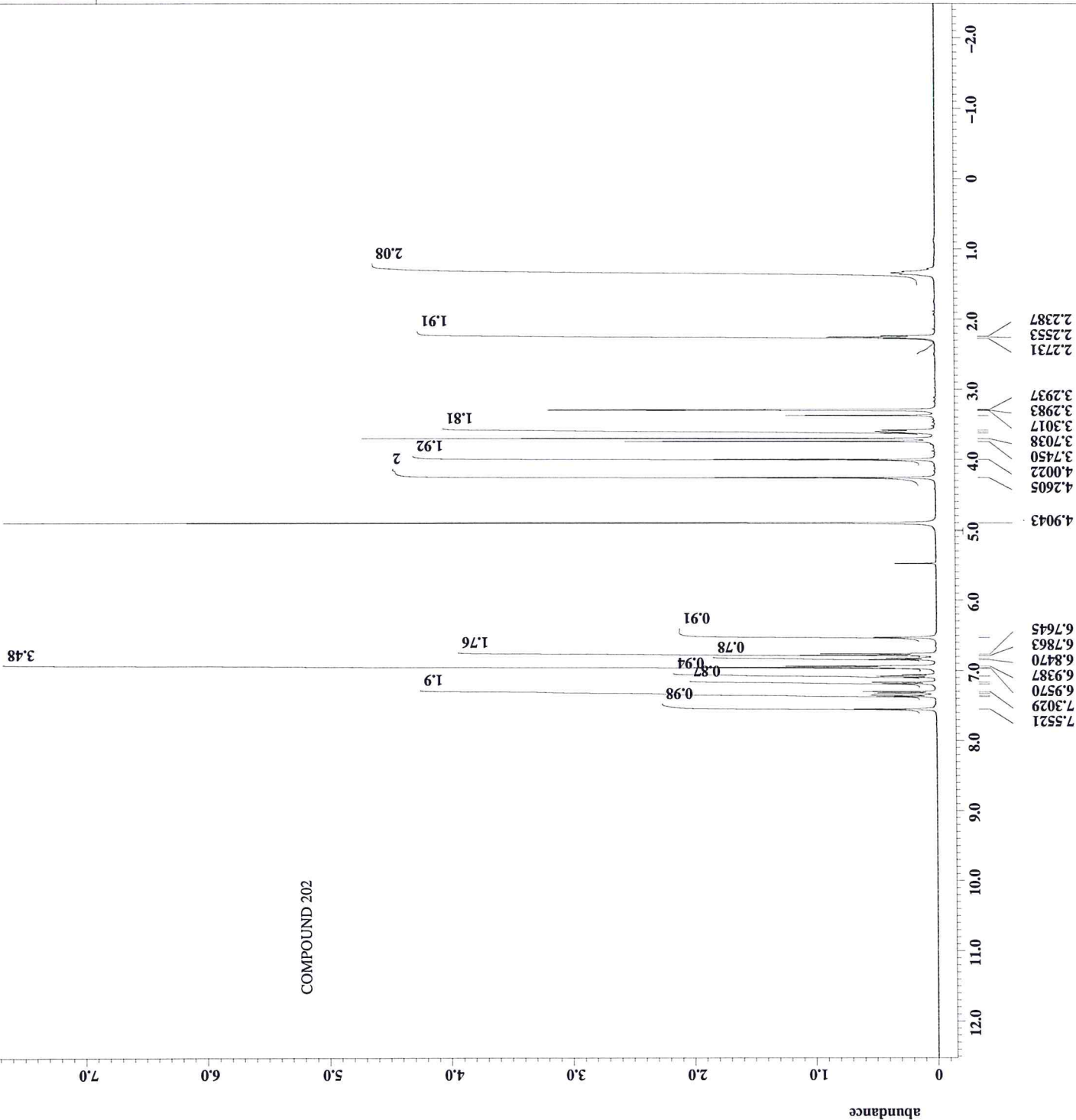


X : parts per Million : 1H



Filename = SK-I-23_PROTON-7.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SK-I-23
Solvent = METHANOL-D3
Creation_time = 15-MAR-2017 10:04:47
Revision_time = 11-MAR-2021 14:59:05
Current_time = 11-MAR-2021 14:59:13
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.68[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.54[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 46
Relaxation_delay = 4[fs]
Repetition_time = 6.18365952[s]
Temp_get = 460.0[dc]

COMPOUND 202



X : parts per Million : 1H



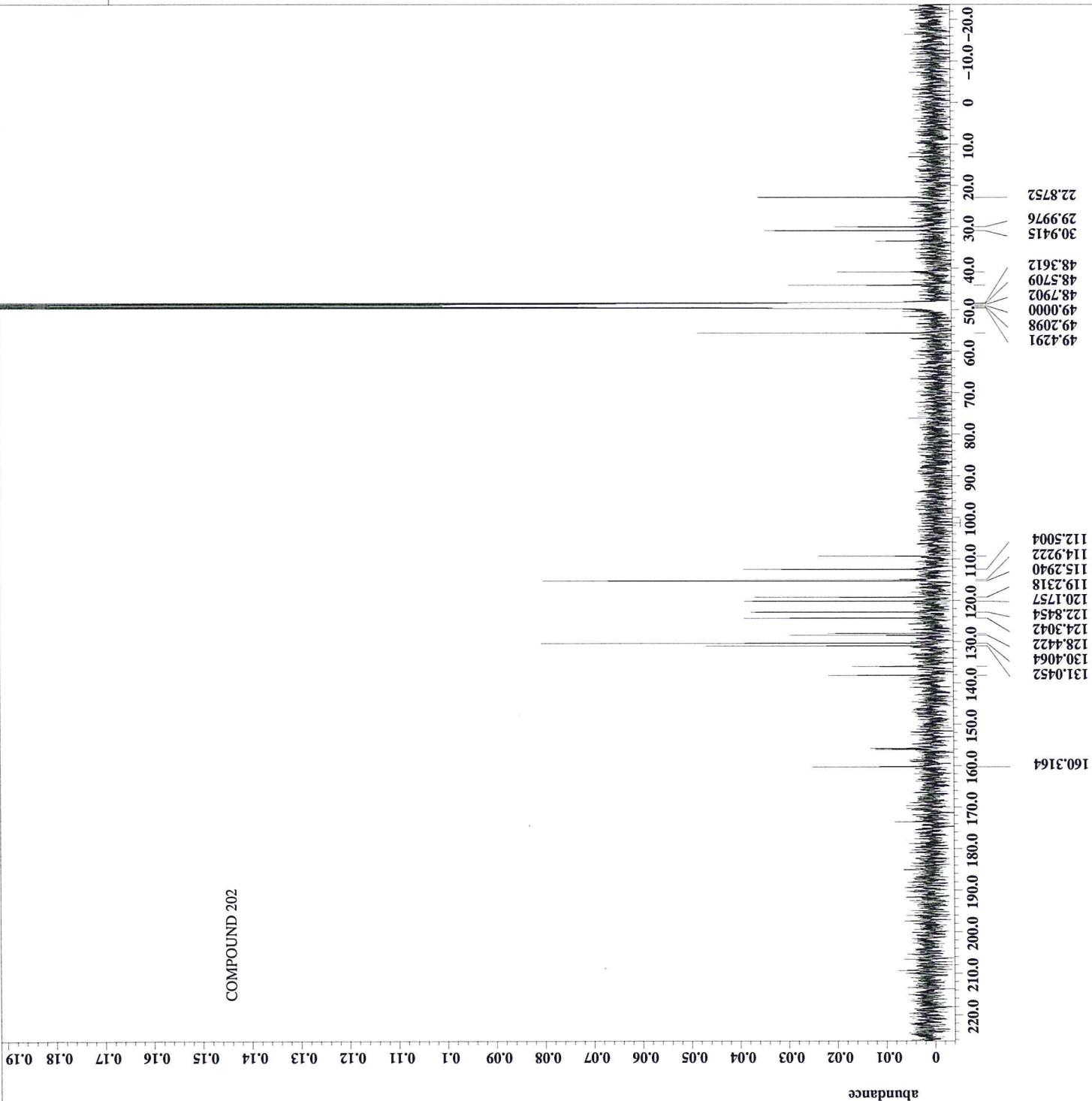
File name = SK-I-23_CARBON-8.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = SK-I-23
Solvent = METHANOL-D3
Creation time = 15-MAR-2017 13:36:20
Revision time = 11-MAR-2021 15:01:36
Current time = 11-MAR-2021 15:01:42

Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 2048
Total_scans = 2048

X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 460.0 [dC]

COMPOUND 202



X : parts per Million : 13C

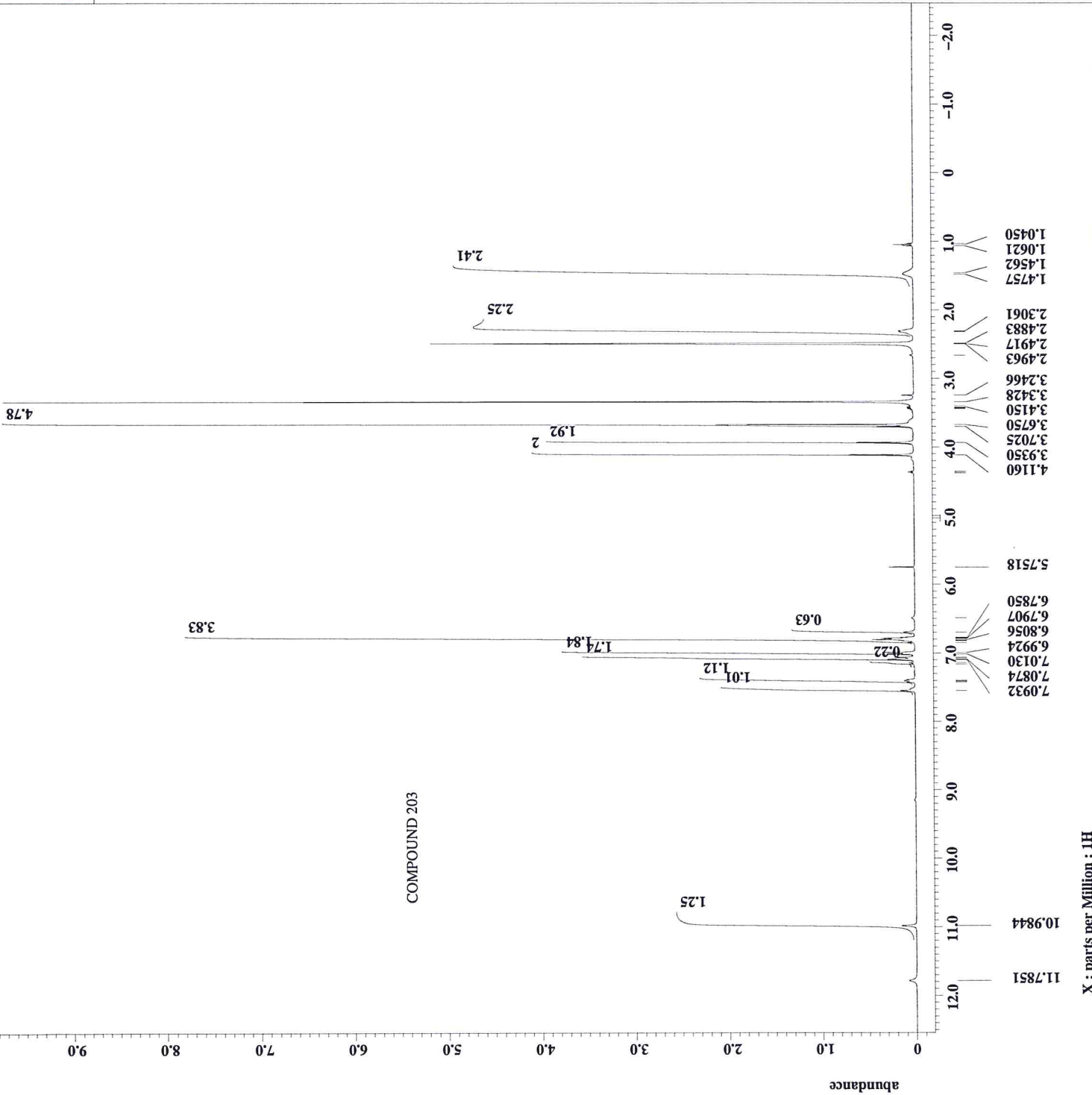


Filename = SK-I-105_PROTON-5-jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SK-I-105
Solvent = DMSO-D6
Creation_time = 23-OCT-2017 09:14:44
Revision_time = 12-MAR-2021 11:42:48
Current_time = 12-MAR-2021 11:42:52

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = EGS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
total_scans = 16

X_90_width = 10.65 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.325 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 40
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
temp_get = 19.81 [dC]

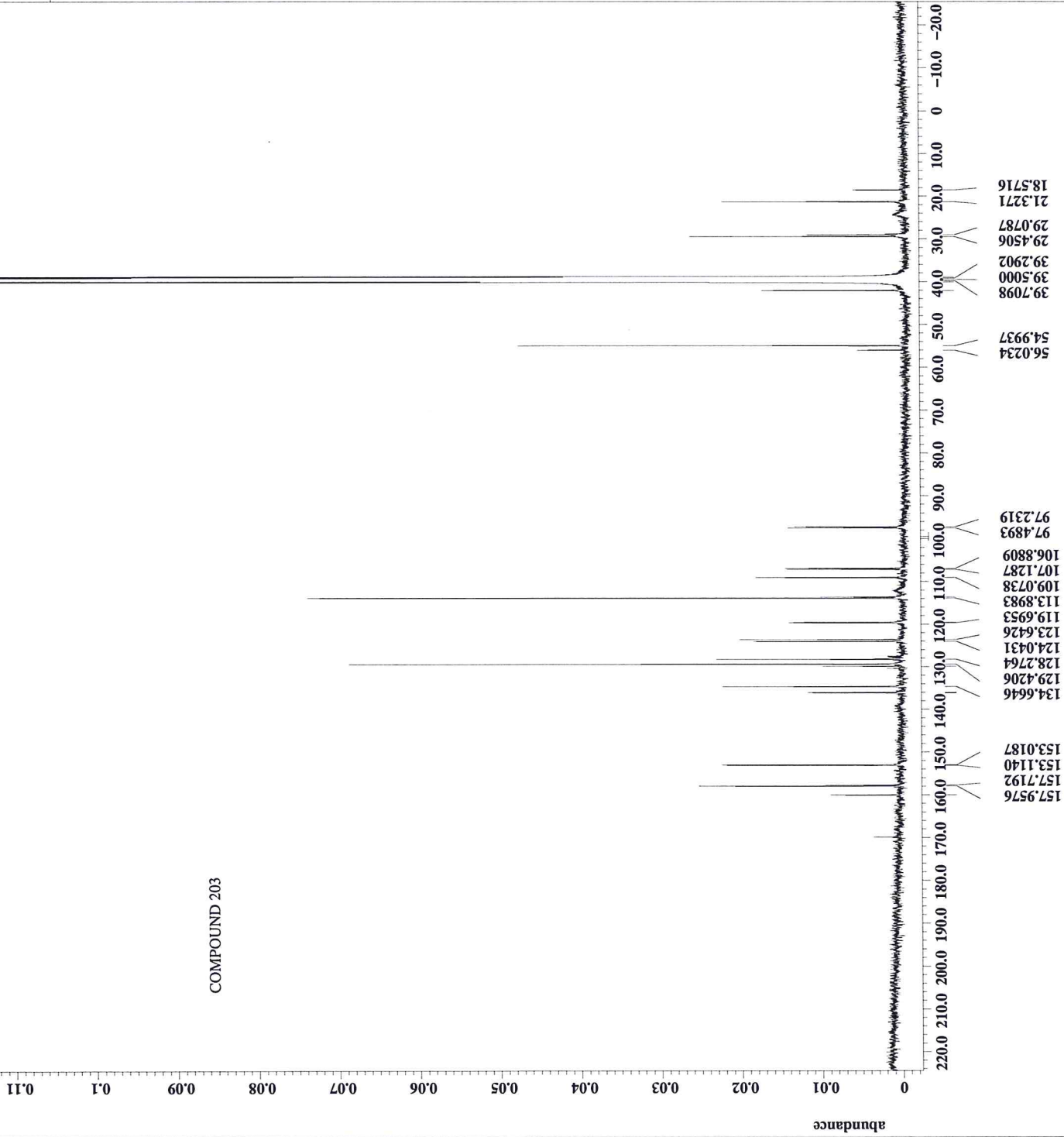


X : parts per Million : 1H



Filename = SK-I-105_CARBON-5.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = SK-I-105
Solvent = DMSO-D6
Creation_time = 30-OCT-2017 06:23:23
Revision_time = 12-MAR-2021 11:45:52
Current_time = 12-MAR-2021 11:45:57
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 74299
Total_scans = 74299
X_90_width = 13.22 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.40666667 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 20.4 [dC]

COMPOUND 203

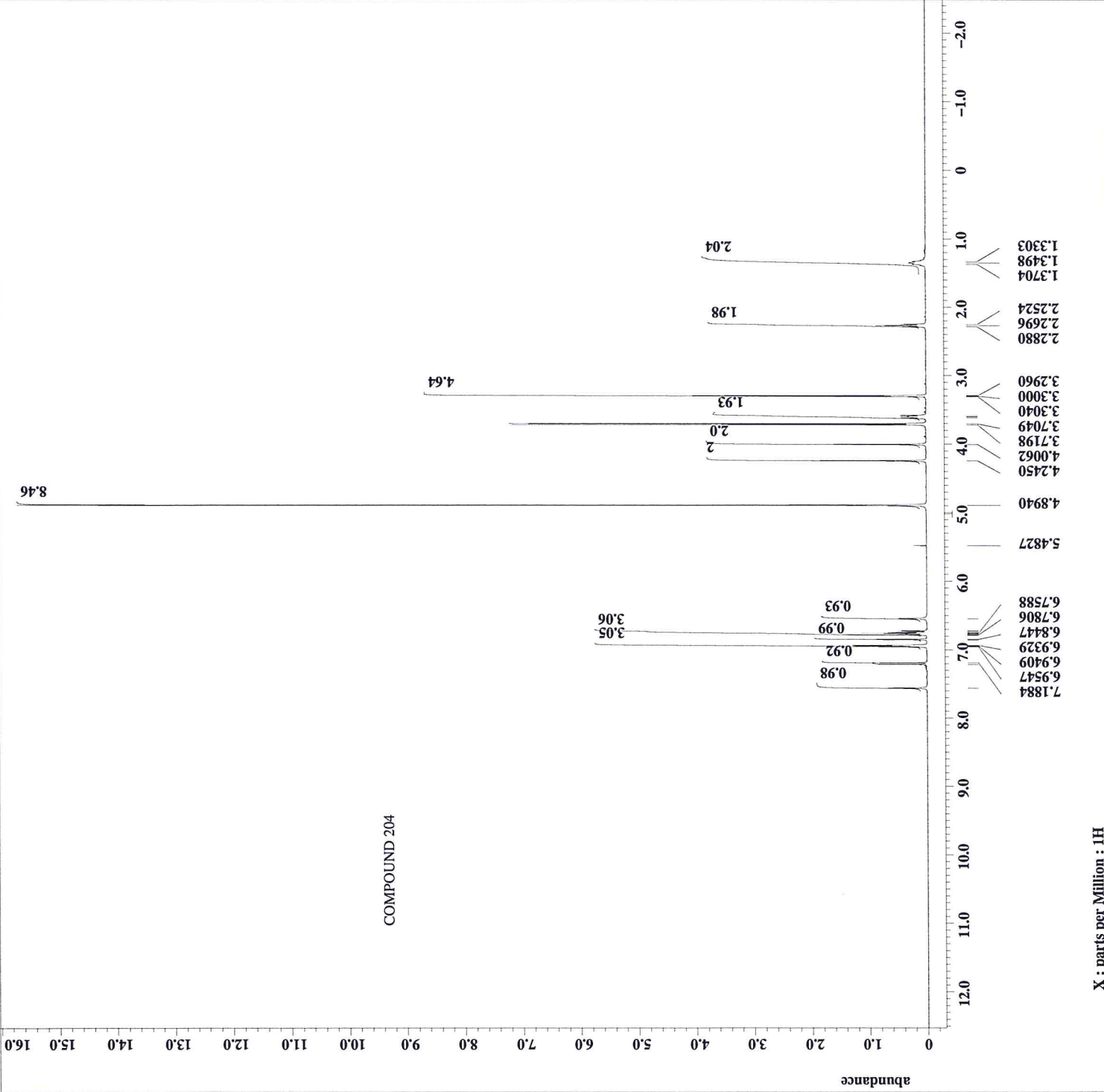


X : parts per Million : 13C



```

= SK-I-56_PROTON-5.jdf
= Delta
= single_pulse.ex2
= SK-I-56
= METHANOL-D3
= 6-JUN-2017 11:59:34
= 12-MAR-2021 11:08:41
= 12-MAR-2021 11:08:45
= 1D COMPLEX
= 13107
= 1H
= [ppm]
= X
= ECS 400
= JNM-ECS400
= 9.389766[T] (400 [MHZ]
= 2.18365952[s]
= 1H
= 399.78219838 [MHZ]
= 5 [ppm]
= 16384
= 1
= 0.45794685 [Hz]
= 7.5030012 [kHz]
= 1H
= 399.78219838 [MHZ]
= 5 [ppm]
= 1H
= 399.78219838 [MHZ]
= 5 [ppm]
= FALSE
= 1
= 16
= 10.68 [us]
= 2.18365952 [s]
= 45 [deg]
= 6 [dB]
= 5.34 [us]
= Off
= Off
= FALSE
= 1 [s]
= 44
= 4 [s]
= 6.18365952 [s]
= 460.0 [dC]
  
```



X : parts per Million : 1H



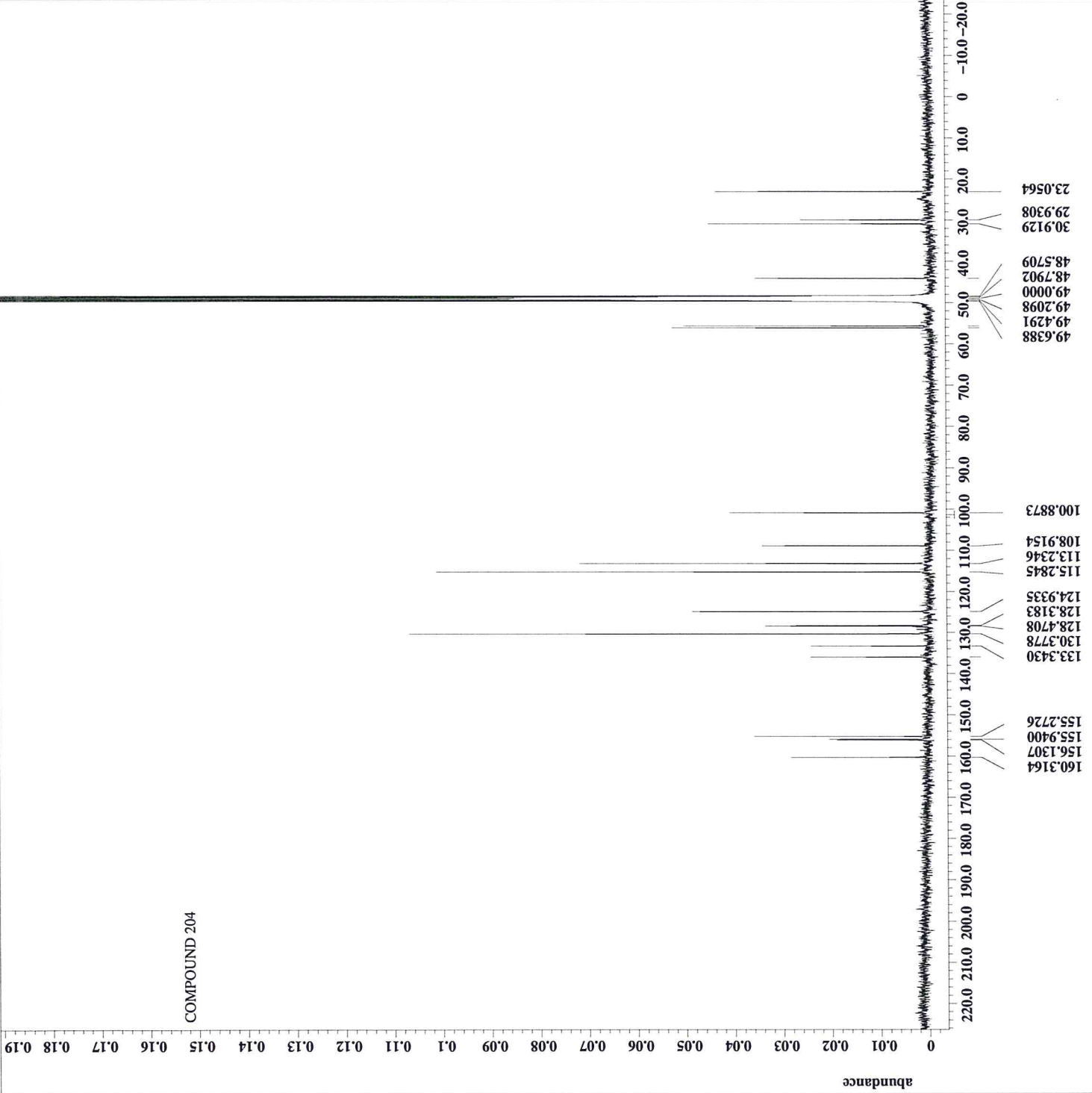
File name = SK-I-56_CARBON-5.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = SK-I-56
Solvent = METHANOL-D3
Creation time = 7-JUN-2017 07:53:15
Revision time = 12-MAR-2021 11:11:11
Current time = 12-MAR-2021 11:11:16

Data format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 18500
Total_scans = 18500

X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 460.0 [dC]

COMPOUND 204



X : parts per Million : 13C



Filename = KS-I-59-C1_PROTON-6.j
 Author = Delta
 Experiment = single_pulse.ex2
 Sample_id = KS-I-59-C1
 Solvent = DMSO-D6
 Creation_time = 2-AUG-2019 14:02:28
 Revision_time = 11-MAR-2021 14:13:10
 Current_time = 11-MAR-2021 14:13:14

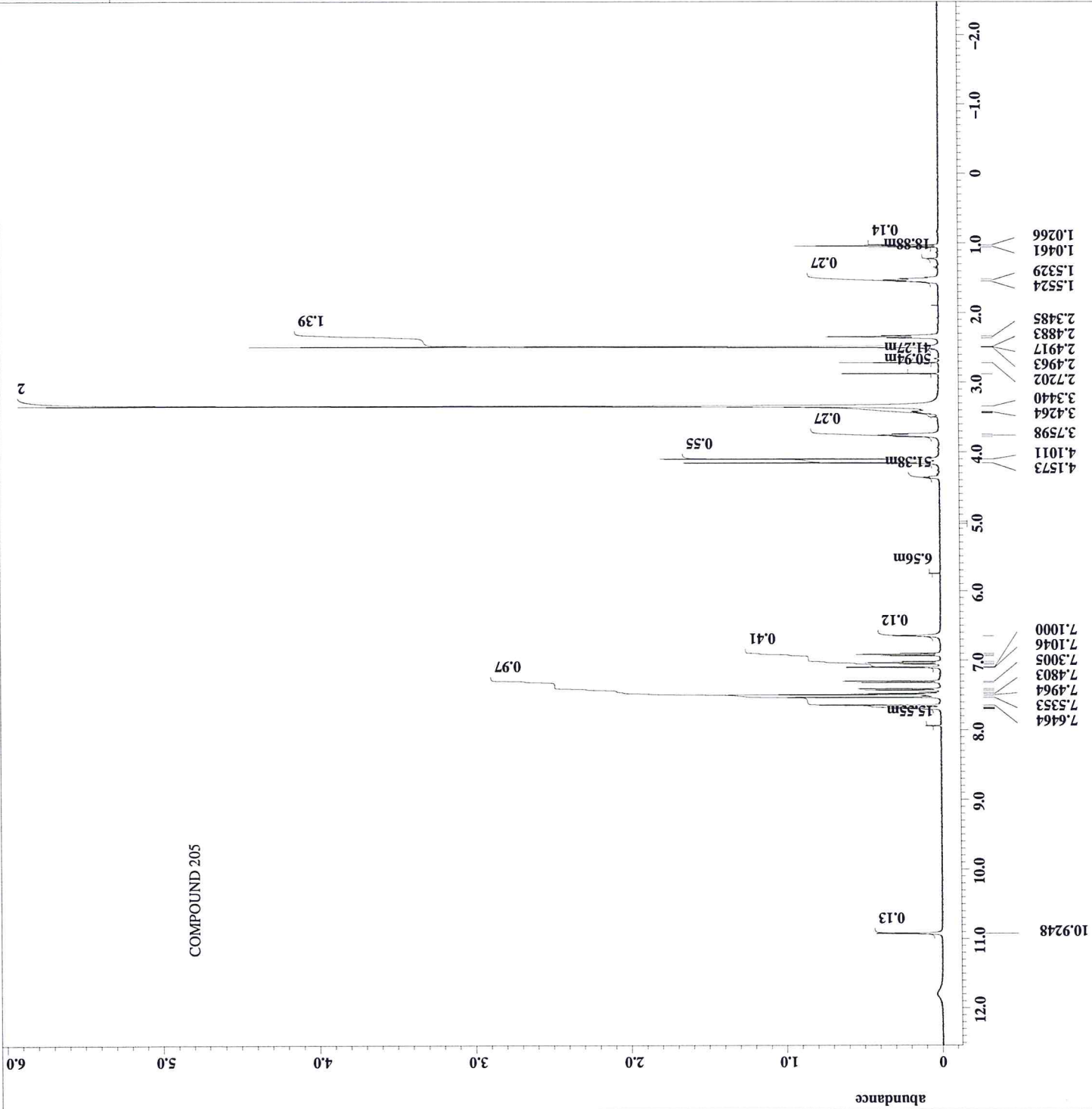
Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECS 400
 Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
 X_acq_duration = 2.18365952[s]
 X_domain = 1H
 X_freq = 399.78219838 [MHz]
 X_offset = 5 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.45794685 [Hz]
 X_sweep = 7.5030012 [kHz]

Irr_domain = 1H
 Irr_freq = 399.78219838 [MHz]
 Irr_offset = 5 [ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838 [MHz]
 Tri_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 4
 Total_scans = 4

X_90_width = 11.365 [us]
 X_acq_time = 2.18365952 [s]
 X_angle = 45 [deg]
 X_atn = 6 [dB]
 X_pulse = 5.6825 [us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 44
 Relaxation_delay = 4 [s]
 Repetition_time = 6.18365952 [s]
 Temp_get = 20.2 [degC]

COMPOUND 205



X : parts per Million : 1H



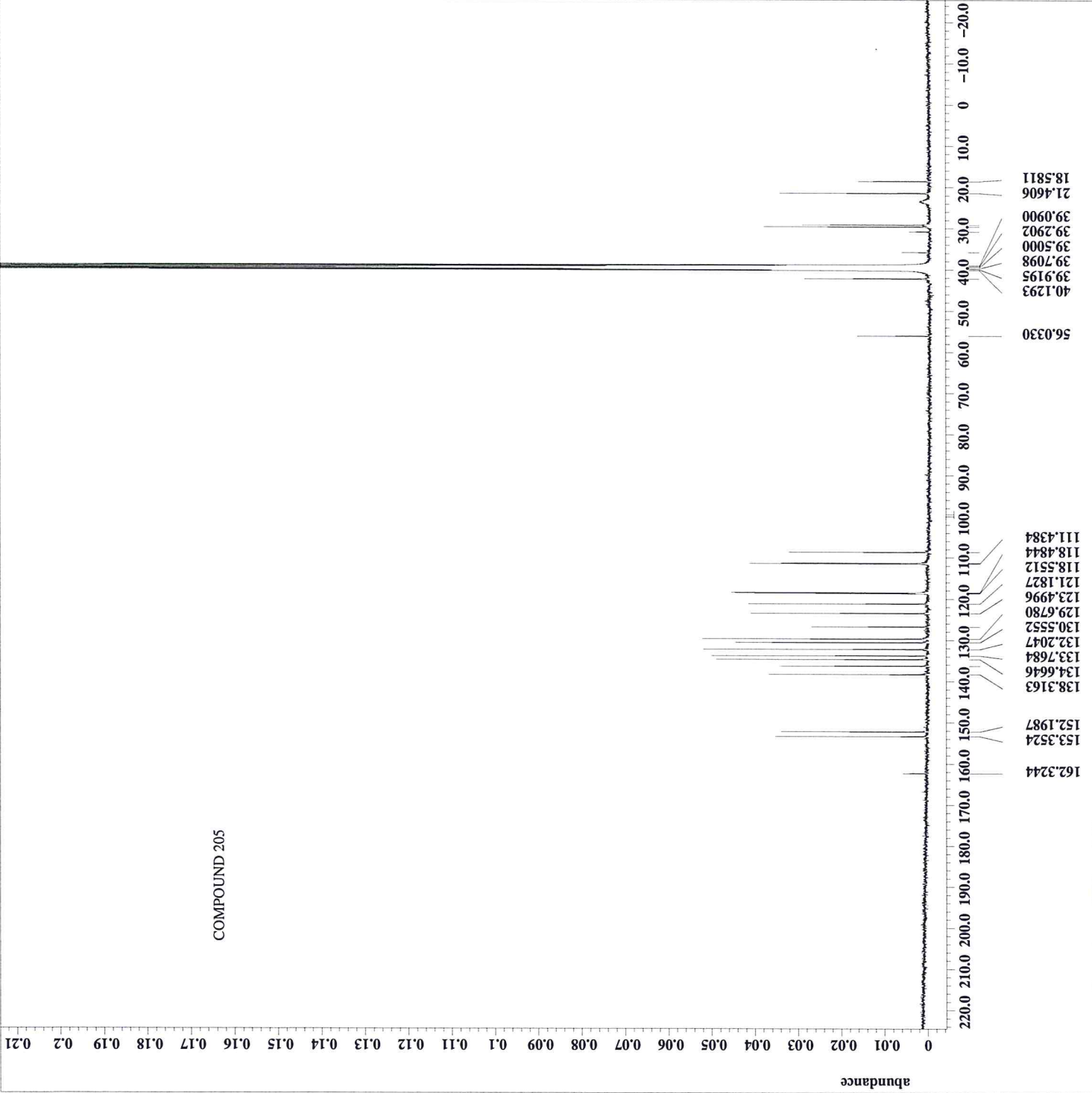
File: KS-I-59-C1_CARBON-5.j
Author: Delta
Experiment: single_pulse_dec
Sample_id: KS-I-59-C1
Solvent: DMSO-D6
Creation_time: 4-AUG-2019 20:10:04
Revision_time: 11-MAR-2021 14:15:07
Current_time: 11-MAR-2021 14:15:11

Data_format: 1D COMPLEX
Dim_size: 26214
Dim_title: 13C
Dim_units: [ppm]
Dimensions: X
Site: ECS 400
Spectrometer: JNM-ECS400

Field_strength: 9.389766 [T] (400 [MHz])
X_acq_duration: 1.04333312 [s]
X_domain: 13C
X_freq: 100.52530333 [MHz]
X_offset: 100 [ppm]
X_points: 32768
X_prescans: 4
X_resolution: 0.95846665 [Hz]
X_sweep: 31.40703518 [kHz]
Irr_domain: 1H
Irr_freq: 399.78219838 [MHz]
Irr_offset: 5 [ppm]
Clipped: FALSE
Mod_return: 1
Scans: 64000
Total_scans: 64000

X_90_width: 10.4 [us]
X_acq_time: 1.04333312 [s]
X_angle: 30 [deg]
X_atn: 9 [dB]
X_pulse: 3.46666667 [us]
Irr_atn_dec: 24.2 [dB]
Irr_atn_noe: 24.2 [dB]
Decoupling: WALTZ
Initial_wait: 1 [s]
Noe: TRUE
Noe_time: 2 [s]
Recvr_gain: 58
Relaxation_delay: 2 [s]
Repetition_time: 3.04333312 [s]
Temp_get: 21 [dC]

COMPOUND 205



X : parts per Million : 13C

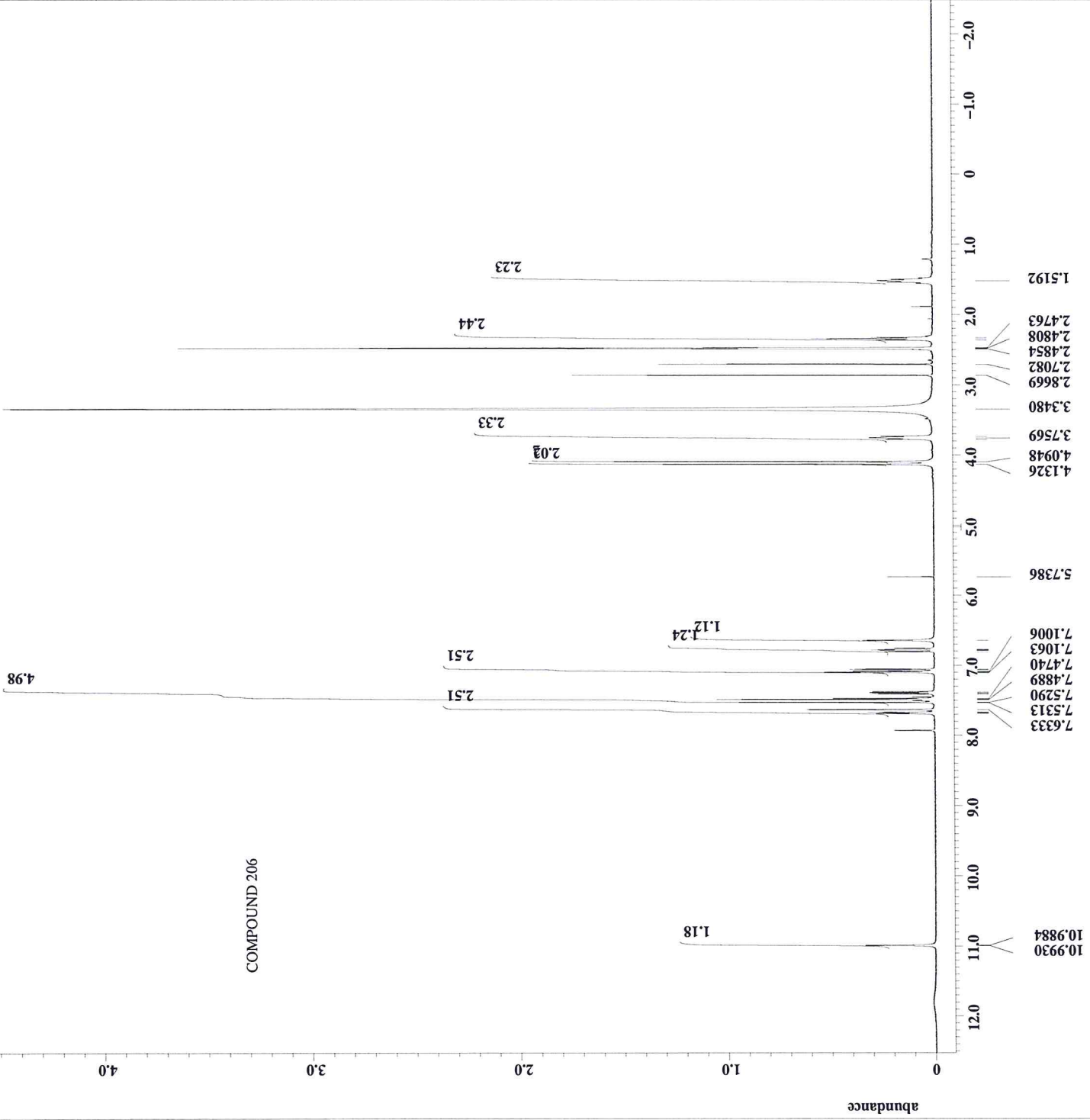


File name = KS-I-61-C_PROTON-4.jd
Author = Delta
Experiment = single_pulse.ex2
Sample_id = KS-I-61-C
Solvent = DMSO-D6
Creation time = 15-AUG-2019 14:29:28
Revision time = 15-MAR-2021 15:39:56
Current time = 15-MAR-2021 15:39:59

Data format = 1D COMPLEX
Dim size = 13107
Dim title = 1H
Dim units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4

X_90_width = 11.365 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [db]
X_pulse = 5.6825 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 40
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 19.5 [degC]

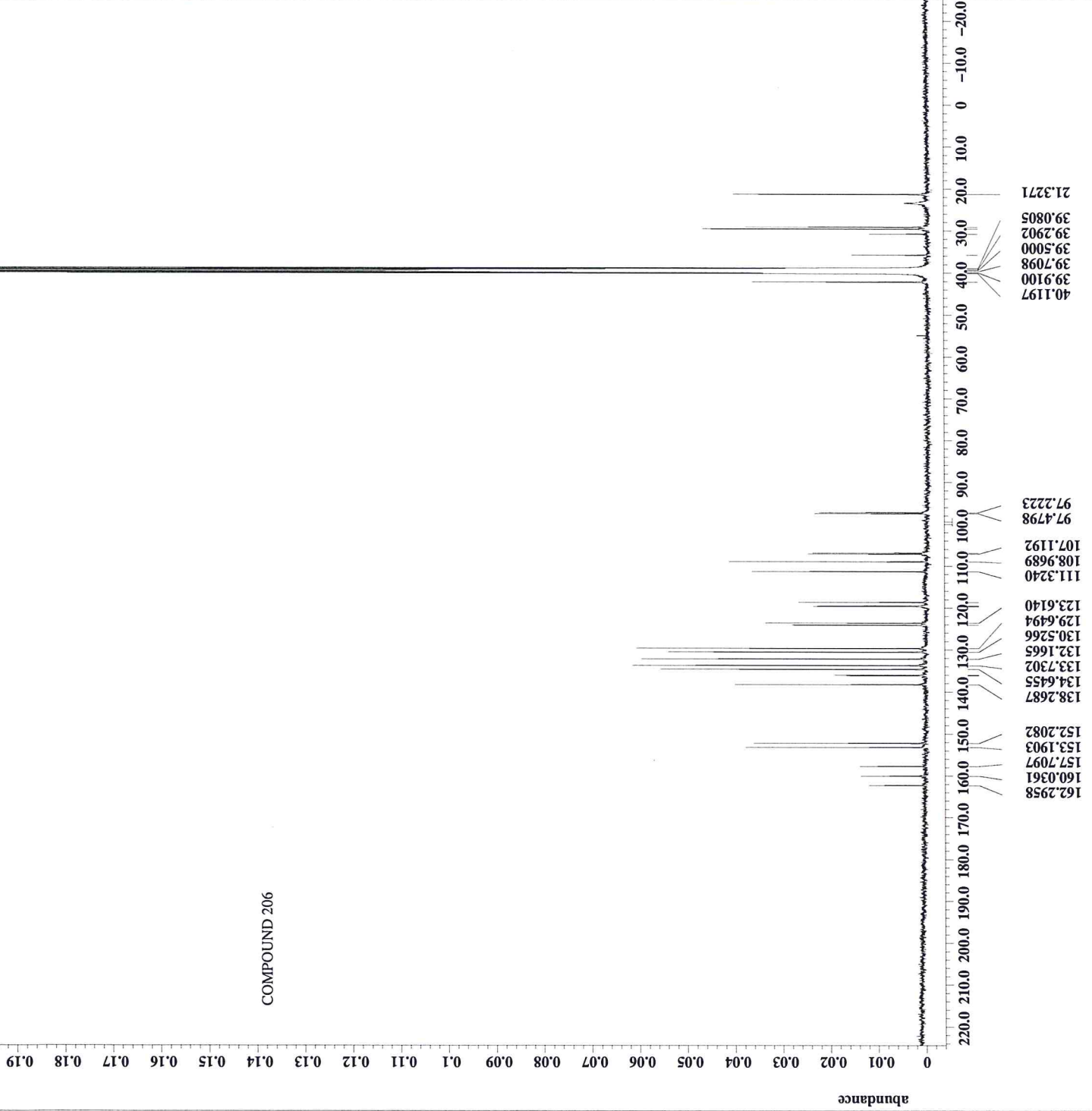


X : parts per Million : 1H

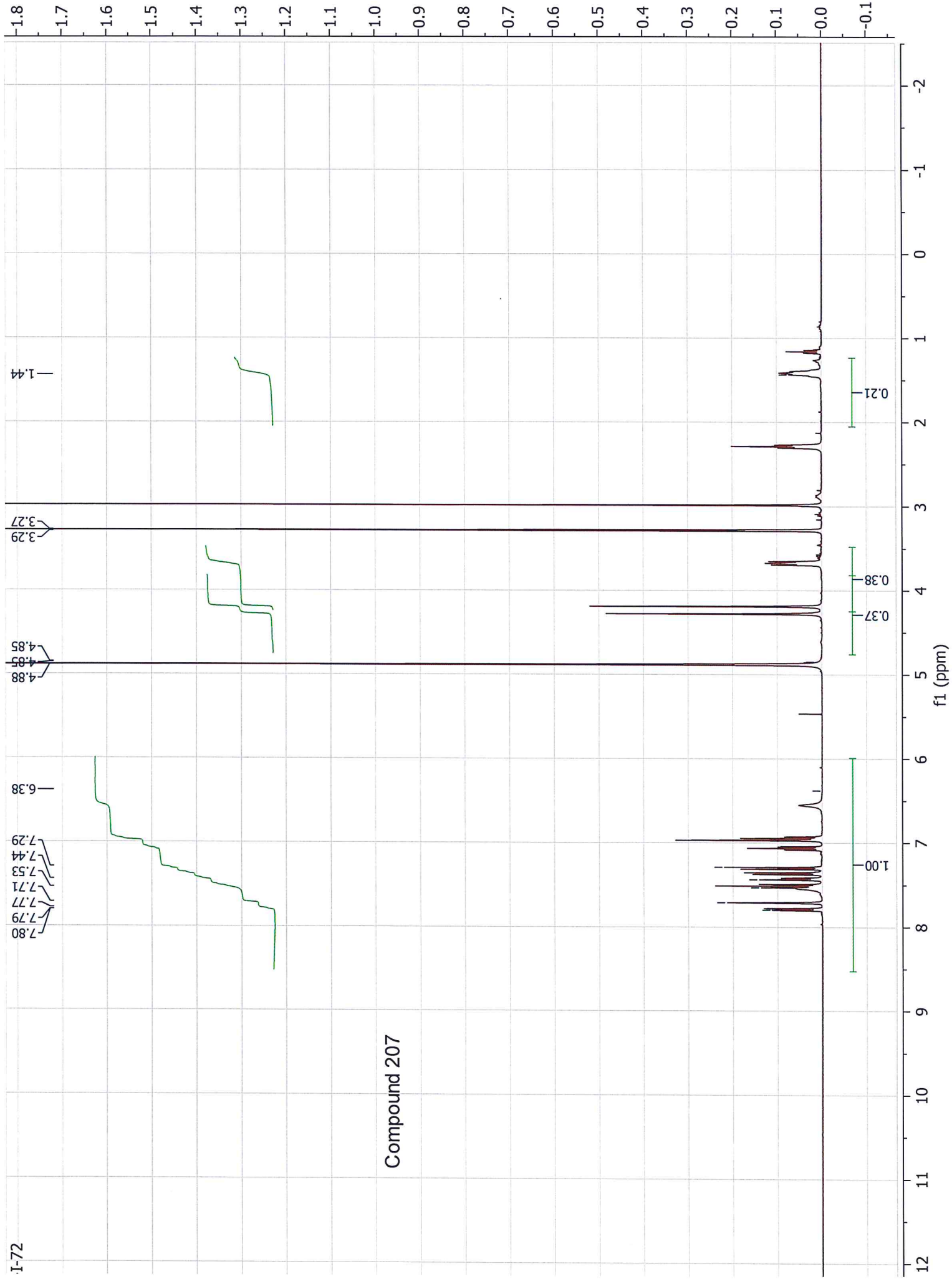


Filename = KS-I-61-C_L_CARBON-5.
Author = Delta
Experiment = single_pulse_dec
Sample_id = KS-I-61-C_L
Solvent = DMSO-D6
Creation_time = 18-AUG-2019 08:06:46
Revision_time = 24-MAR-2021 13:32:10
Current_time = 24-MAR-2021 13:32:23
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 48918
Total_scans = 48918
X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.45666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 2 [s]
Recvr_gain = 58
Relaxation_delay = 2 [s]
Repetition_time = 3.04333312 [s]
Temp_get = 25 [dC]

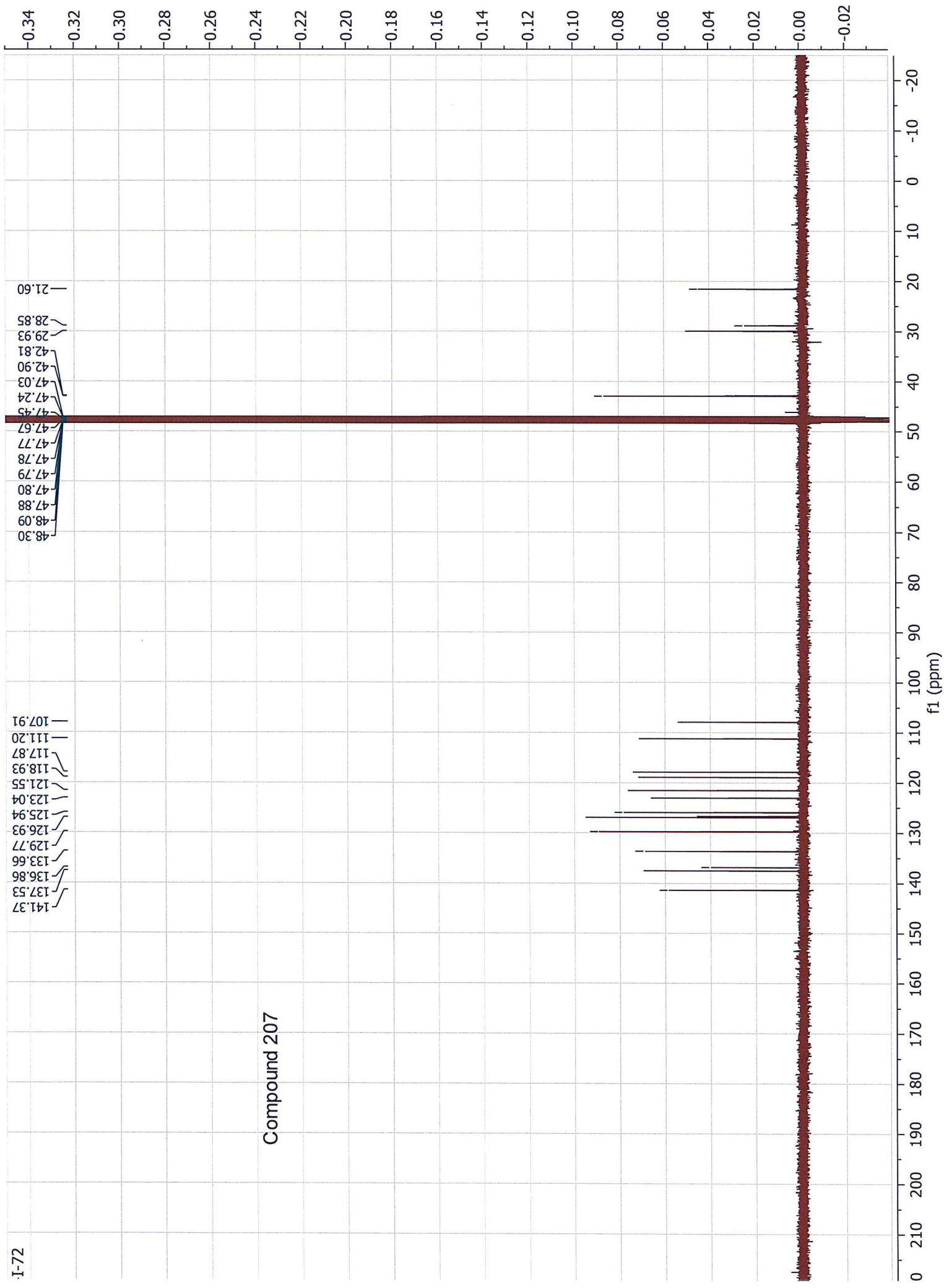
COMPOUND 206



X : parts per Million : 13C



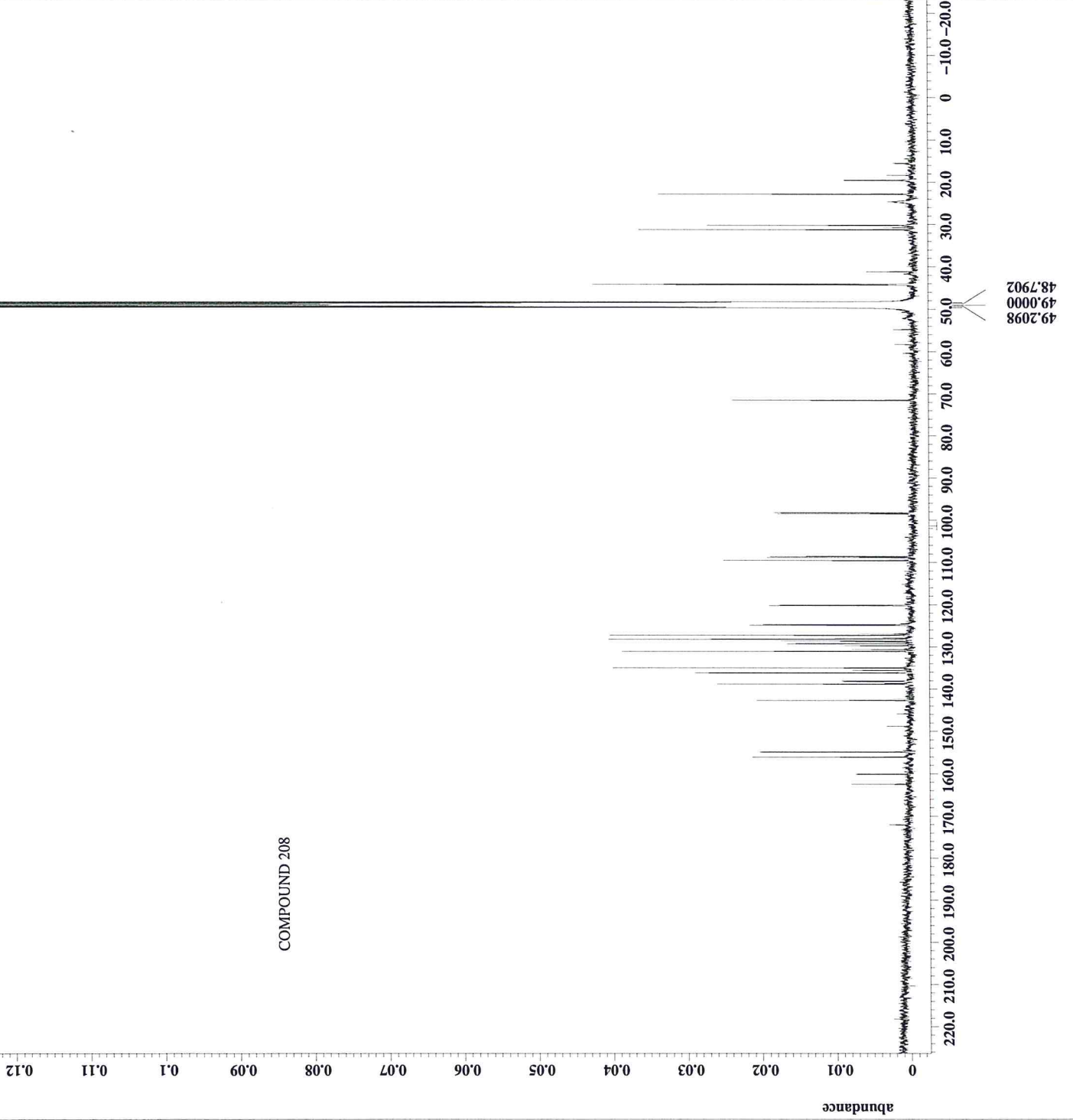
Compound 207





Filename = KS-I-50-C_M_CARBON-4.
Author = Delta
Experiment = single_pulse_dec
Sample_id = KS-I-50-C_M
Solvent = METHANOL-D3
Creation_time = 24-JUN-2019 07:10:59
Revision_time = 18-MAR-2021 08:56:24
Current_time = 18-MAR-2021 08:56:28
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 50749
Total_scans = 50749
X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.45666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 2 [s]
Recvr_gain = 58
Relaxation_delay = 2 [s]
Repetition_time = 3.04333312 [s]
Temp_get = 19.4 [dC]

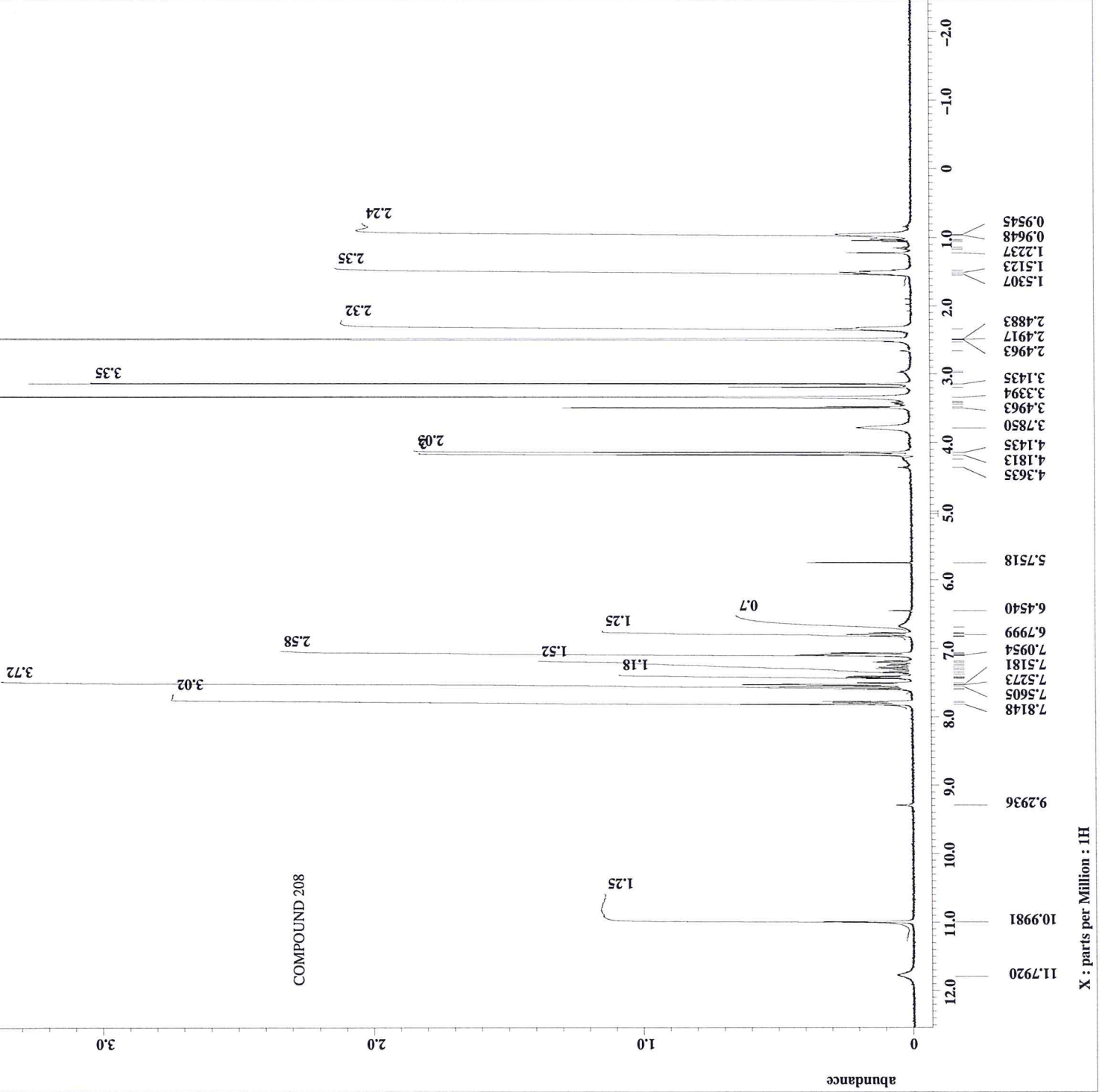
COMPOUND 208



X : parts per Million : 13C



Filename = KS-I-50-C1_PROTON-5.j
Author = Delta
Experiment = single_pulse.ex2
Sample_id = KS-I-50-C1
Solvent = DMSO-D6
Creation_time = 20-JUN-2019 15:07:08
Revision_time = 18-MAR-2021 08:50:52
Current_time = 18-MAR-2021 08:50:59
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4
X_90_width = 11.365 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.6825 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 46
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 19.2 [dC]





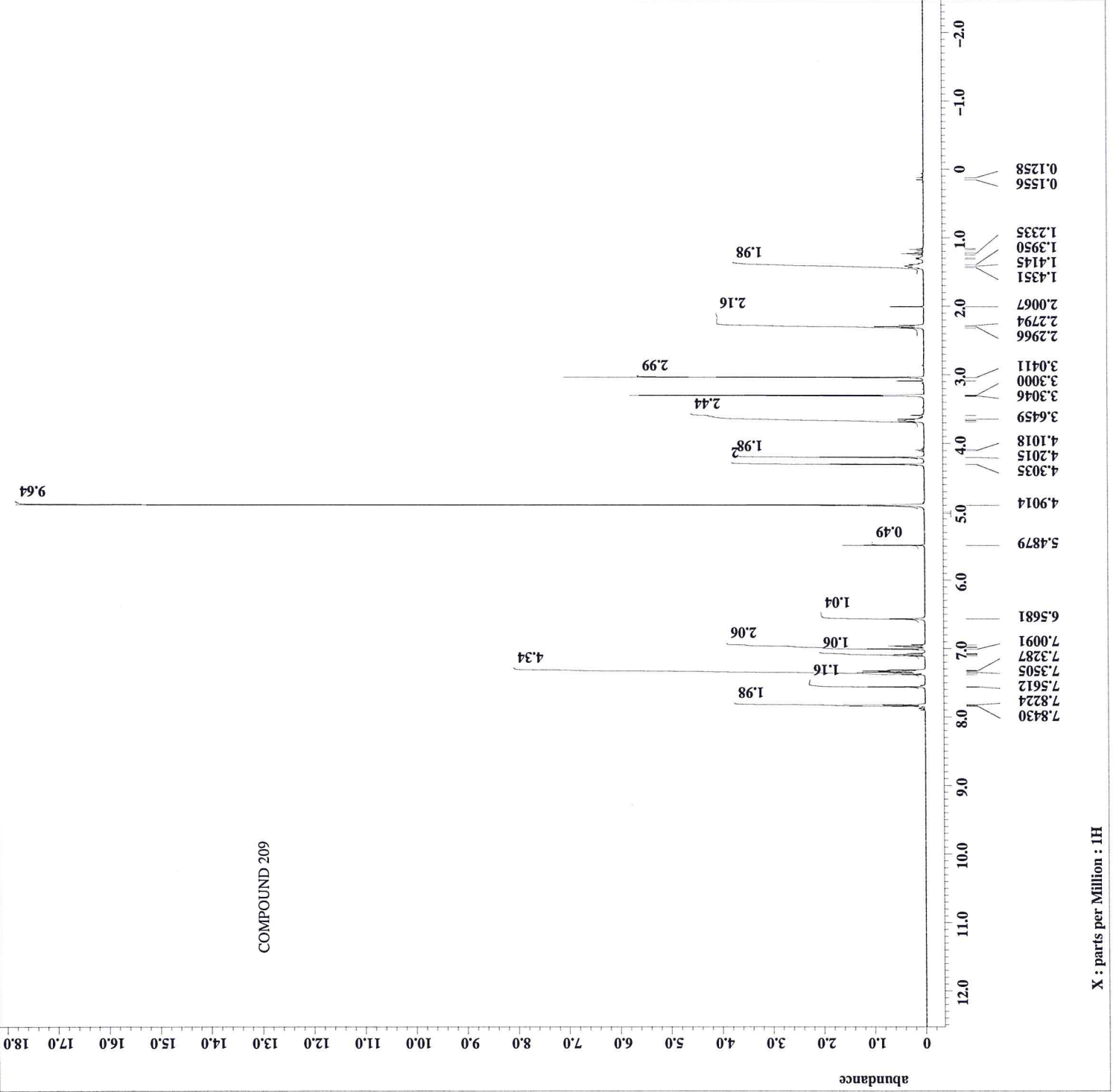
```

Filename = KS-I-27-C_PROTON-5.jd
Author = Delta
Experiment = single_pulse.ex2
Sample_id = KS-I-27-C
Solvent = METHANOL-D3
Creation_time = 13-MAR-2019 11:02:45
Revision_time = 11-MAR-2021 11:35:28
Current_time = 11-MAR-2021 11:35:32

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4

X_90_width = 11.365[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.6825[us]
Irr_mode = Off
Tri_mode = Off
Danta_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 46
Relaxation_delay = 4[s]
Repetition_time = 6.18365952[s]
Temp_get = 18.9[dc]
  
```



X : parts per Million : 1H



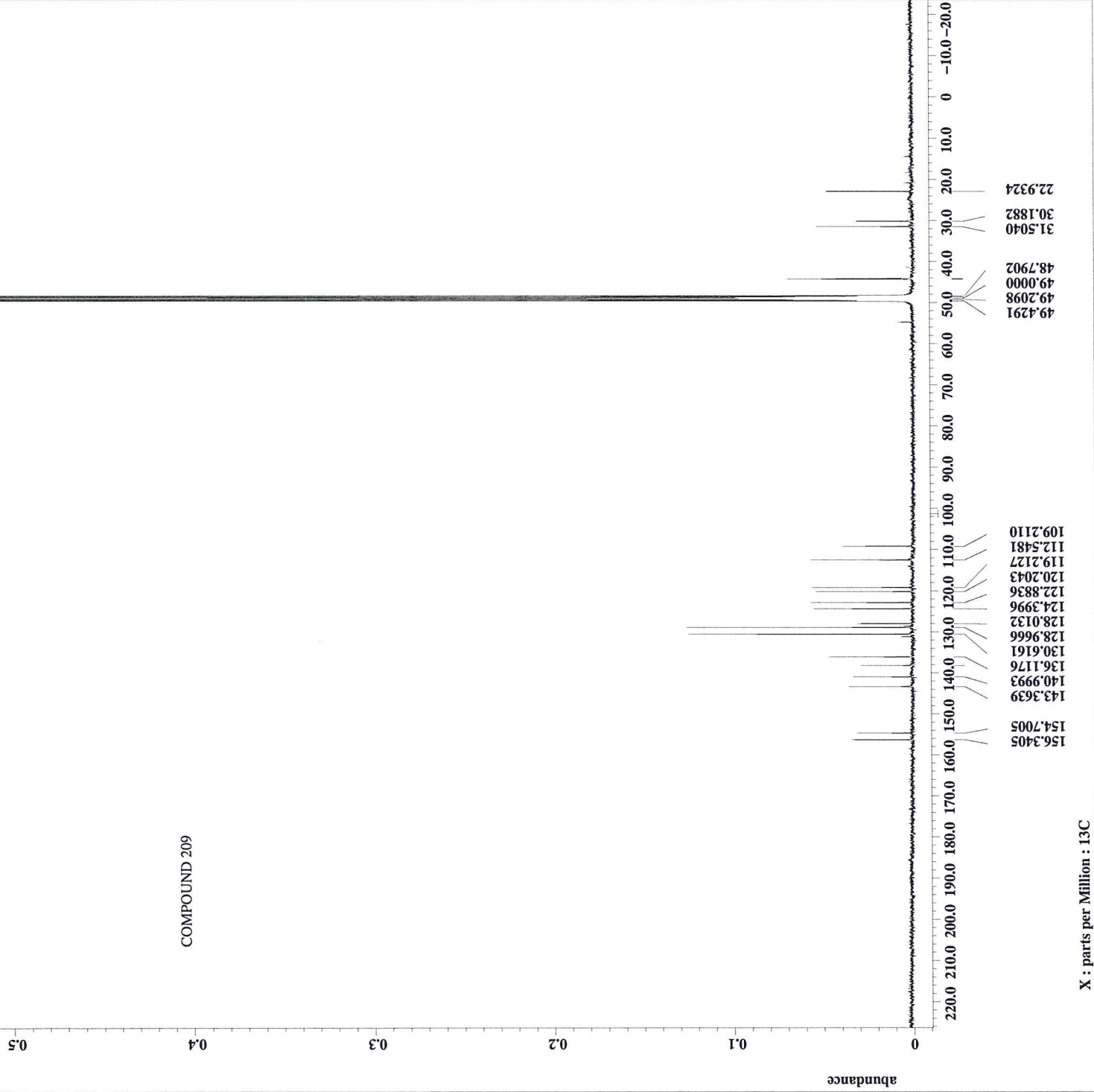
File: KS-I-27-C_CARBON-5.jd
Author: Delta
Experiment: single_pulse_dec
Sample ID: KS-I-27-C
Solvent: METHANOL-D3
Creation time: 14-MAR-2019 03:39:20
Revision time: 11-MAR-2021 11:30:30
Current time: 11-MAR-2021 11:30:39

Data format: 1D COMPLEX
Dim size: 26214
Dim title: 13C
Dim units: [ppm]
Dimensions: X
Site: ECS 400
Spectrometer: JNM-ECS400

Field strength: 9.389766 [T] (400 [MHz])
X_acq_duration: 1.04333312 [s]
X_domain: 13C
X_freq: 100.52530333 [MHz]
X_offset: 100 [ppm]
X_points: 32768
X_prescans: 4
X_resolution: 0.95846665 [Hz]
X_sweep: 31.40703518 [kHz]
Irr_domain: 1H
Irr_freq: 399.78219838 [MHz]
Irr_offset: 5 [ppm]
Clipped: FALSE
Mod_return: 1
Scans: 16000
Total_scans: 16000

X_90_width: 10.4 [us]
X_acq_time: 1.04333312 [s]
X_angle: 30 [deg]
X_atn: 9 [dB]
X_pulse: 3.46666667 [us]
Irr_atn_dec: 24.2 [dB]
Irr_atn_noe: 24.2 [dB]
Decoupling: WALTZ
Initial_wait: 1 [s]
Noe: TRUE
Noe_time: 2 [s]
Recvr_gain: 60
Relaxation_delay: 2 [s]
Repetition_time: 3.04333312 [s]
Temp_get: 20.4 [dC]

COMPOUND 209



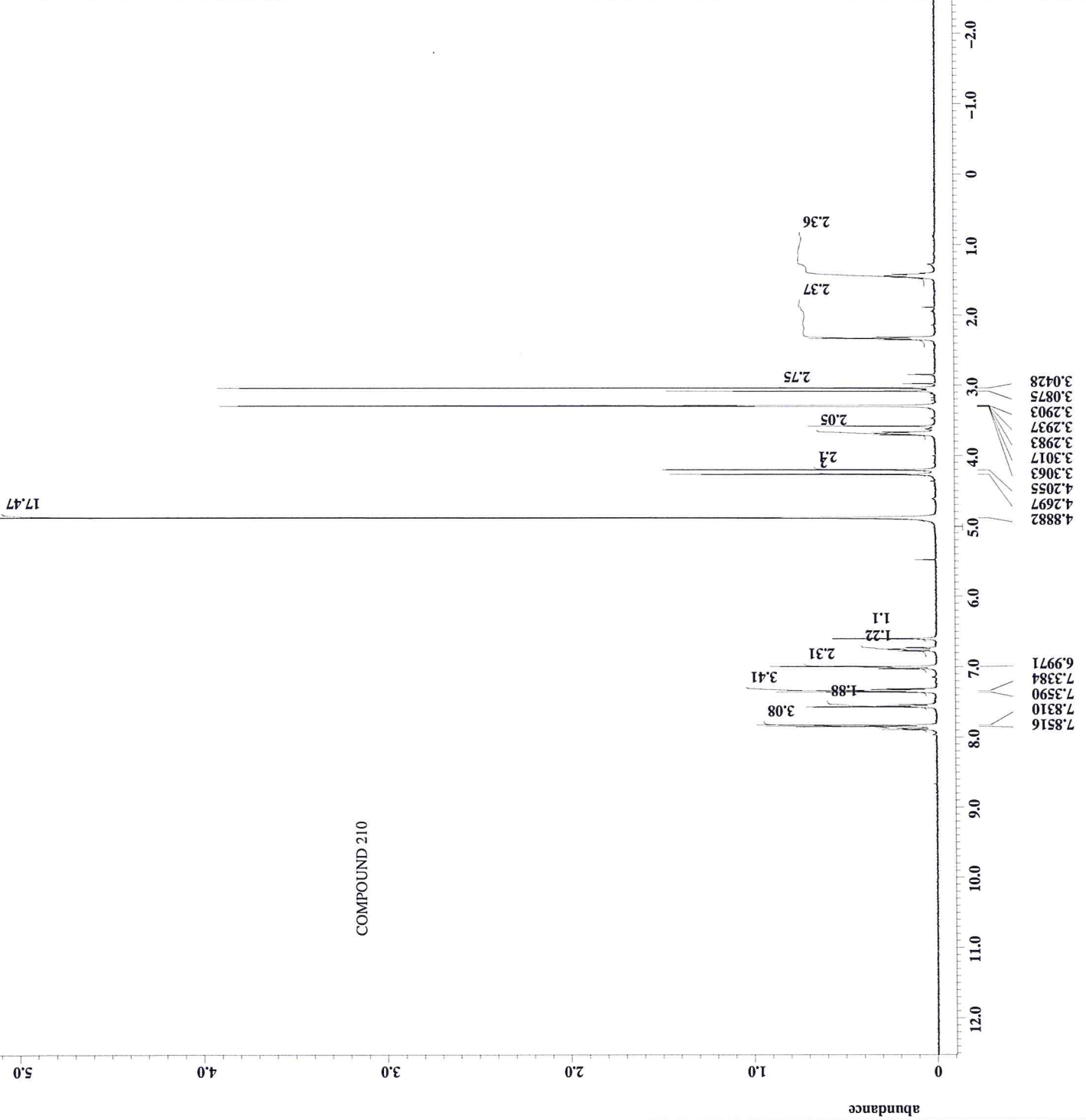
X : parts per Million : 13C



Filename = KS-I-48-C1_PROTON-4.j
Author = Delta
Experiment = single_pulse.ex2
Sample_id = KS-I-48-C1
Solvent = METHANOL-D3
Creation_time = 25-JUN-2019 14:44:02
Revision_time = 16-MAR-2021 10:50:16
Current_time = 16-MAR-2021 10:50:32
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 4
X_90_width = 11.365[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.6825[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 46
Relaxation_delay = 4[s]
Repetition_time = 6.18365952[s]
Temp_get = 19.6[degC]

17.47

COMPOUND 210

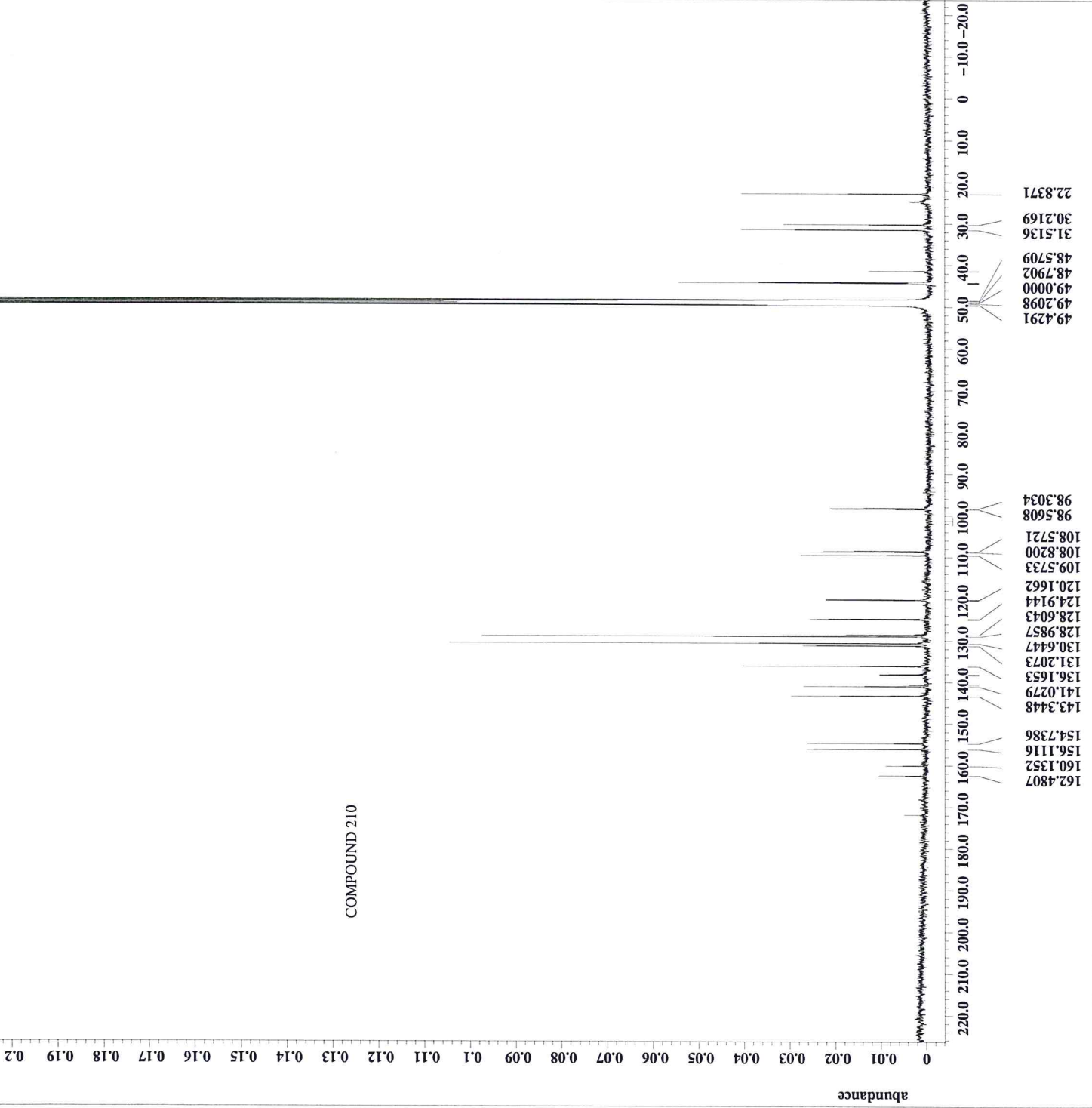


X : parts per Million : 1H



Filename = KS-I-48-C1_CARBON-5.j
Author = Delta
Experiment = single_pulse_dec
Sample_id = KS-I-48-C1
Solvent = METHANOL-D3
Creation_time = 1-JUL-2019 06:05:52
Revision_time = 16-MAR-2021 10:52:35
Current_time = 16-MAR-2021 10:52:57
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_resolution = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 42560
Total_scans = 42560
X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.46666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 2 [s]
Recvr_gain = 60
Relaxation_delay = 2 [s]
Repetition_time = 3.04333312 [s]
Temp_get = 20 [dC]

COMPOUND 210

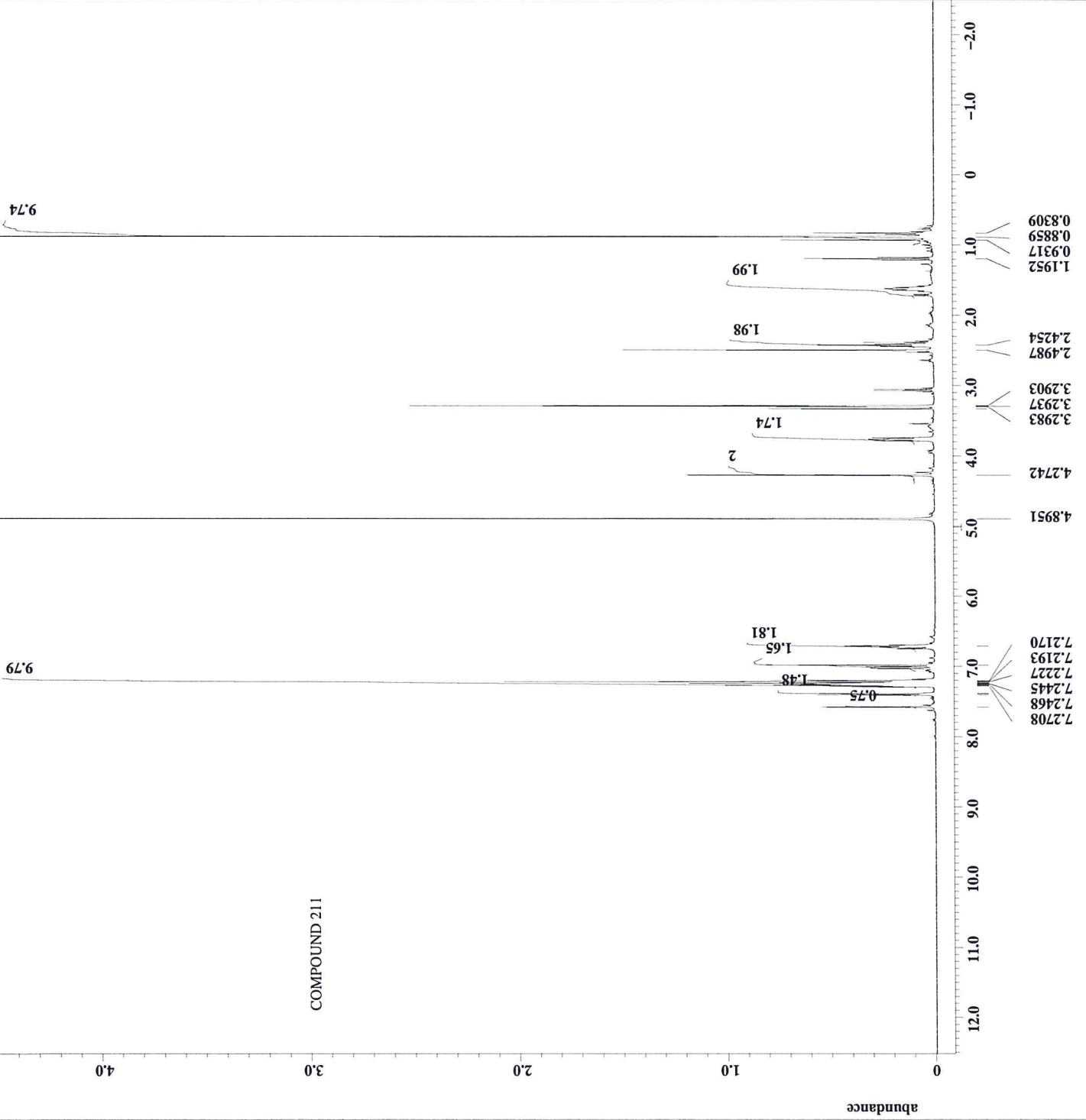


X : parts per Million : 13C



Filename = SK-I-119_PROTON-7.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SK-I-119
Solvent = METHANOL-D3
Creation_time = 17-APR-2018 18:09:25
Revision_time = 18-MAR-2021 08:30:13
Current_time = 18-MAR-2021 08:30:17
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.65[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[dB]
X_pulse = 5.325[us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 4[s]
Repetition_time = 6.18365952[s]
Temp_get = 18.8[degC]

COMPOUND 211

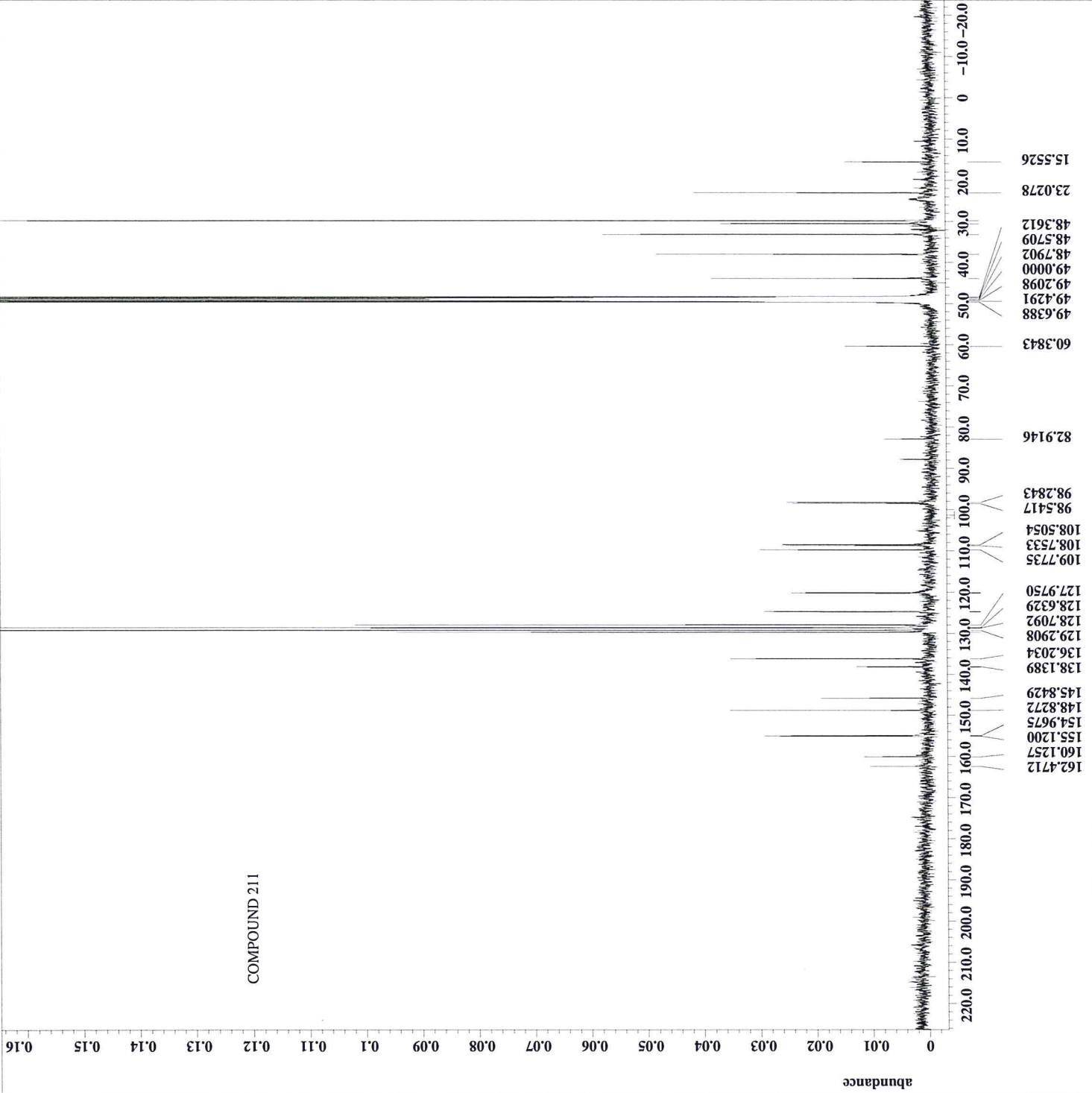


X : parts per Million : 1H



File name = SK-I-119_CARBON-5.jdf
Author = Delta
Experiment = single_pulse_dec
Sample_id = SK-I-119
Solvent = METHANOL-D3
Creation time = 18-APR-2018 06:01:05
Revision time = 15-MAR-2021 14:51:27
Current time = 15-MAR-2021 14:51:31
Data format = 1D COMPLEX
Dim size = 26214
Dim title = 13C
Dim units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 14000
Total_scans = 14000
X_90_width = 13.22 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.40666667 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 19.9 [dC]

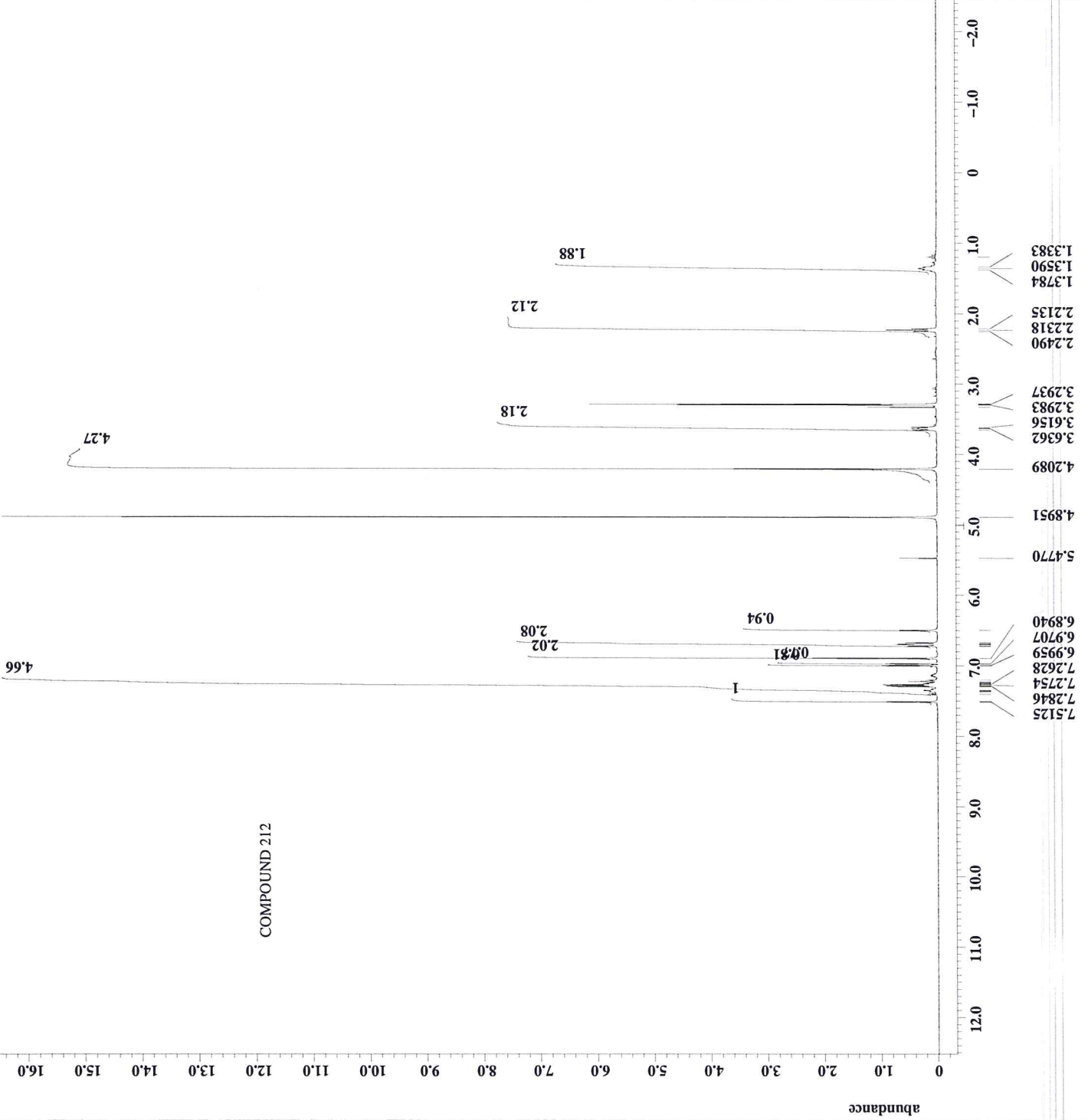
COMPOUND 211



X : parts per Million : 13C



Filename = SK-I-124_PROTON-5.jdf
Author = Delta
Experiment = single_pulse.ex2
Sample_id = SK-I-124
Solvent = METHANOL-D3
Creation_time = 20-APR-2018 14:41:28
Revision_time = 15-MAR-2021 14:29:23
Current_time = 15-MAR-2021 14:29:28
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.65 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.325 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 46
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 18.5 [dC]



X : parts per Million : 1H



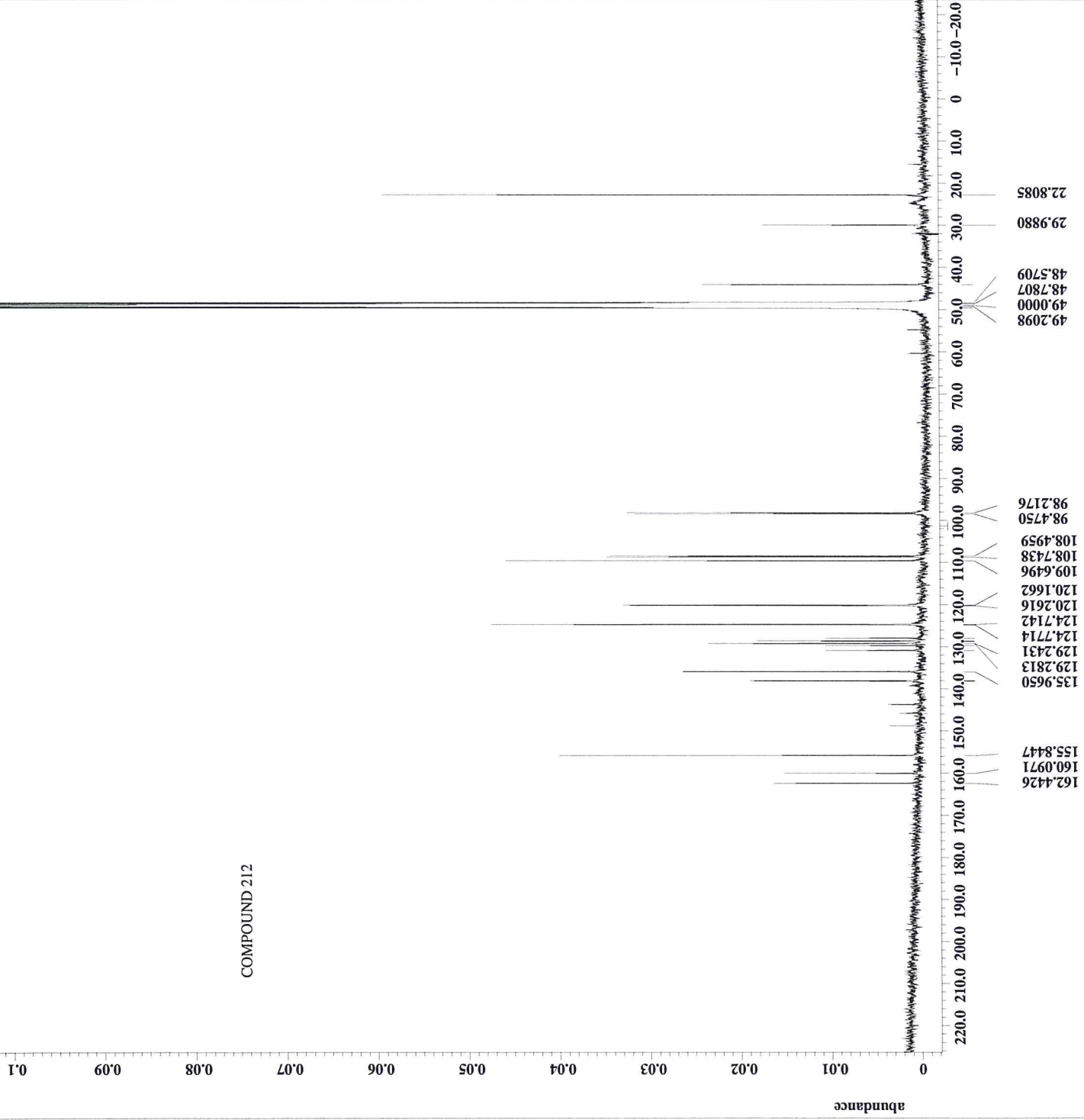
File: SK-I-124_CARBON-5.jdf
Author: Delta
Experiment: single_pulse_dec
Sample_id: SK-I-124
Solvent: METHANOL-D3
Creation_time: 23-APR-2018 08:35:05
Revision_time: 15-MAR-2021 14:34:28
Current_time: 15-MAR-2021 14:34:37

Data_format: 1D COMPLEX
Dim_size: 26214
Dim_title: 13C
Dim_units: [ppm]
Dimensions: X
Site: ECS 400
Spectrometer: JNM-ECS400

Field_strength: 9.389766 [T] (400 [MHz])
X_acq_duration: 1.04333312 [s]
X_domain: 13C
X_freq: 100.52530333 [MHz]
X_offset: 100 [ppm]
X_points: 32768
X_prescans: 4
X_resolution: 0.95846665 [Hz]
X_sweep: 31.40703518 [kHz]
Irr_domain: 1H
Irr_freq: 399.78219838 [MHz]
Irr_offset: 5 [ppm]
Clipped: TRUE
Mod_return: 1
Scans: 77883
Total_scans: 77883

X_90_width: 13.22 [us]
X_acq_time: 1.04333312 [s]
X_angle: 30 [deg]
X_atn: 9 [dB]
X_pulse: 4.40666667 [us]
Irr_atn_dec: 27 [dB]
Irr_atn_noe: 27 [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: 3.04333312 [s]
Temp_get: 19.9 [DC]

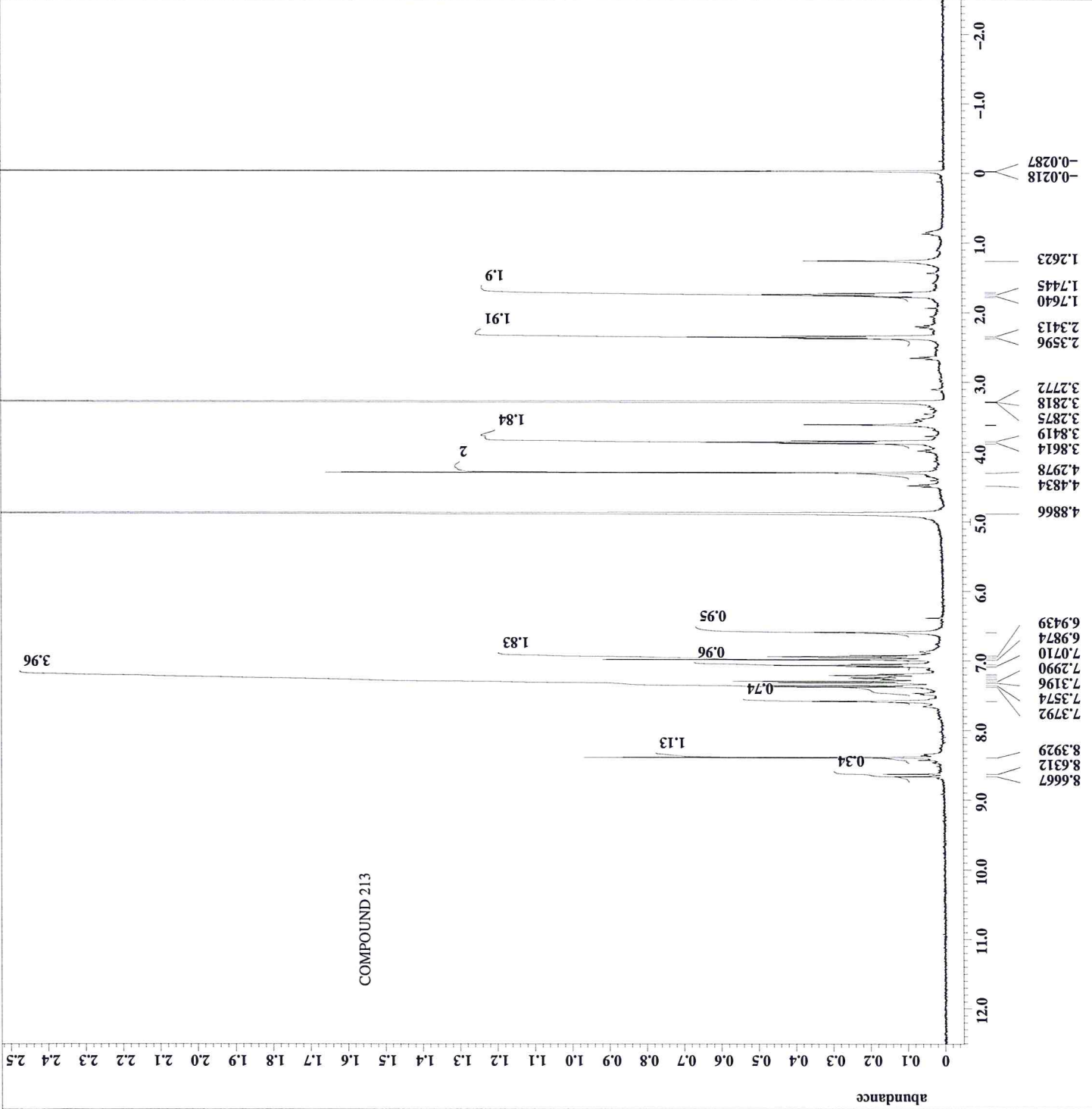
COMPOUND 212



X : parts per Million : 13C



File name = BN-VII-128-4.jdf
Author = mcrider
Experiment = single_pulse.ex2
Sample_id = S#341562
Solvent = METHANOL-D3
Creation_time = 19-MAR-2021 06:18:30
Revision_time = 19-MAR-2021 09:45:10
Current_time = 19-MAR-2021 09:45:14
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 13.15[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[dB]
X_pulse = 6.575[us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
Temp_get = 18.5[dc]

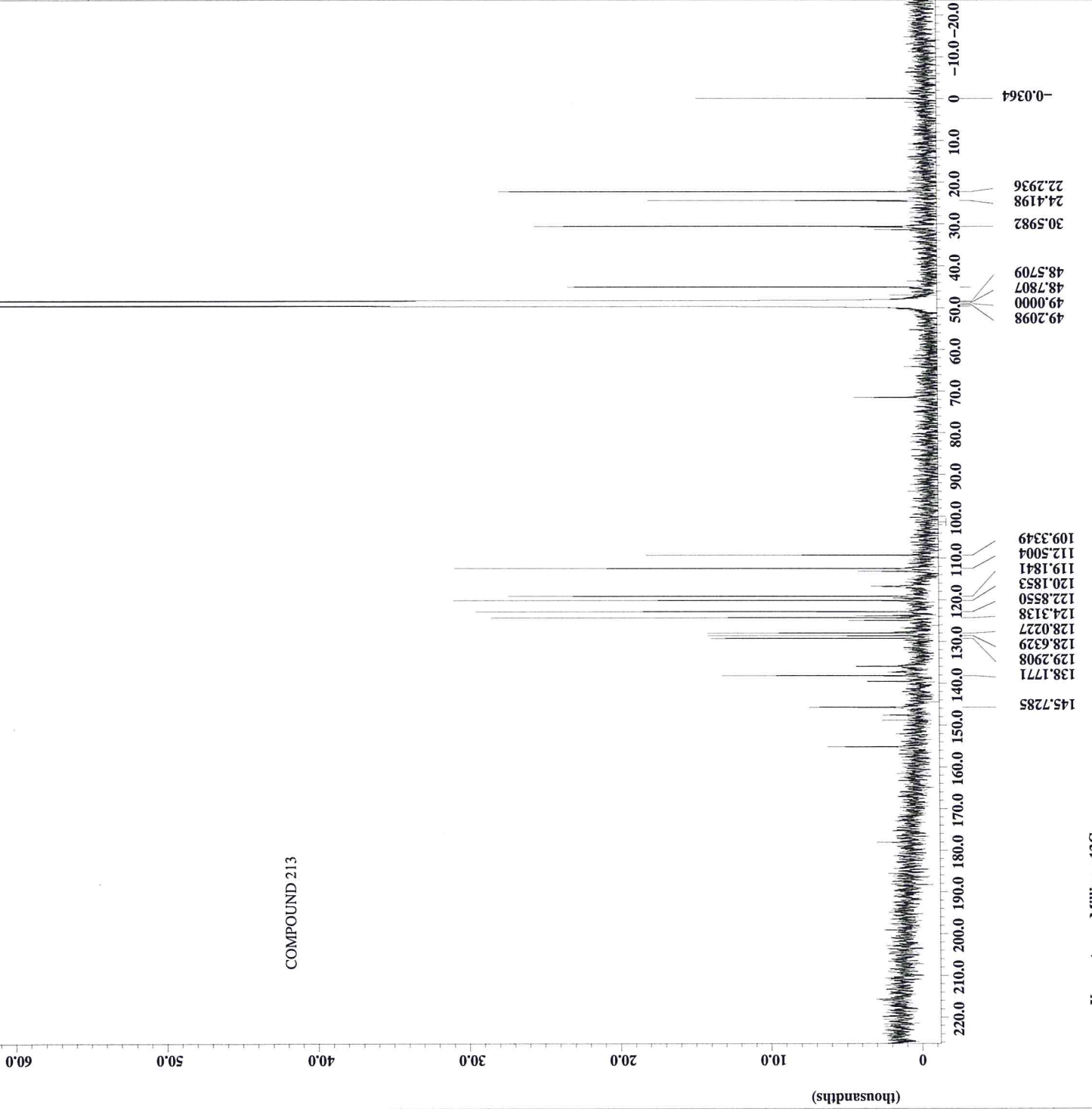


X : parts per Million : 1H



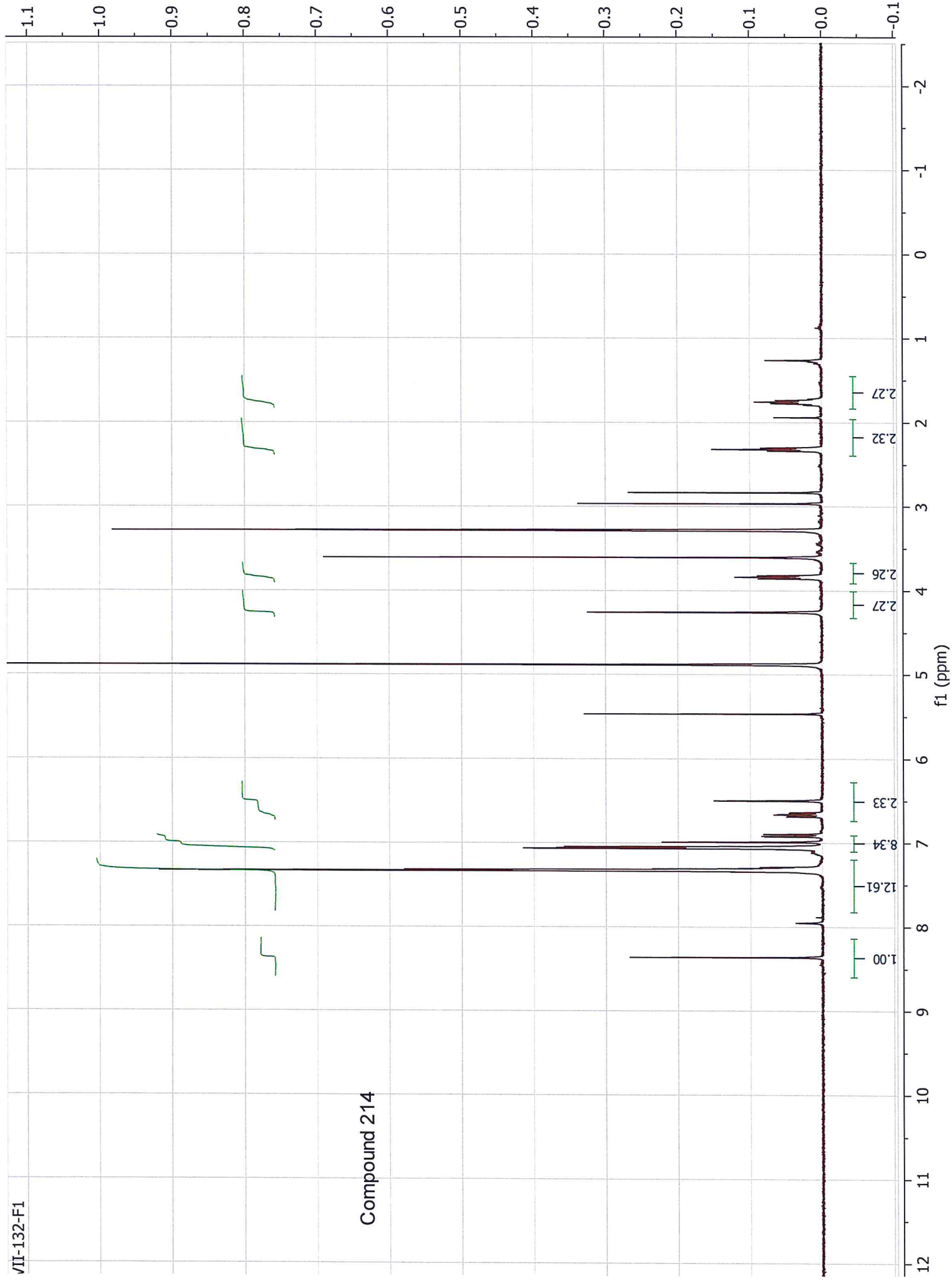
Filename = EN-VII-128-2_CARBON-5
Author = mcrider
Experiment = single_pulse_dec
Sample_id = BN-VII-128-2
Solvent = METHANOL-D3
Creation_time = 20-MAR-2021 20:54:04
Revision_time = 22-MAR-2021 08:14:30
Current_time = 22-MAR-2021 08:14:41
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 40000
Total_scans = 40000
X_90_width = 10.35 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 10.6 [dB]
X_pulse = 3.45 [us]
Irr_atn_dec = 25 [dB]
Irr_atn_noe = 25 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_wait = 2 [s]
Recvr_gain = 60
Relaxation_delay = 2 [s]
Repetition_time = 3.04333312 [s]
Temp_get = 18.3 [dC]

COMPOUND 213

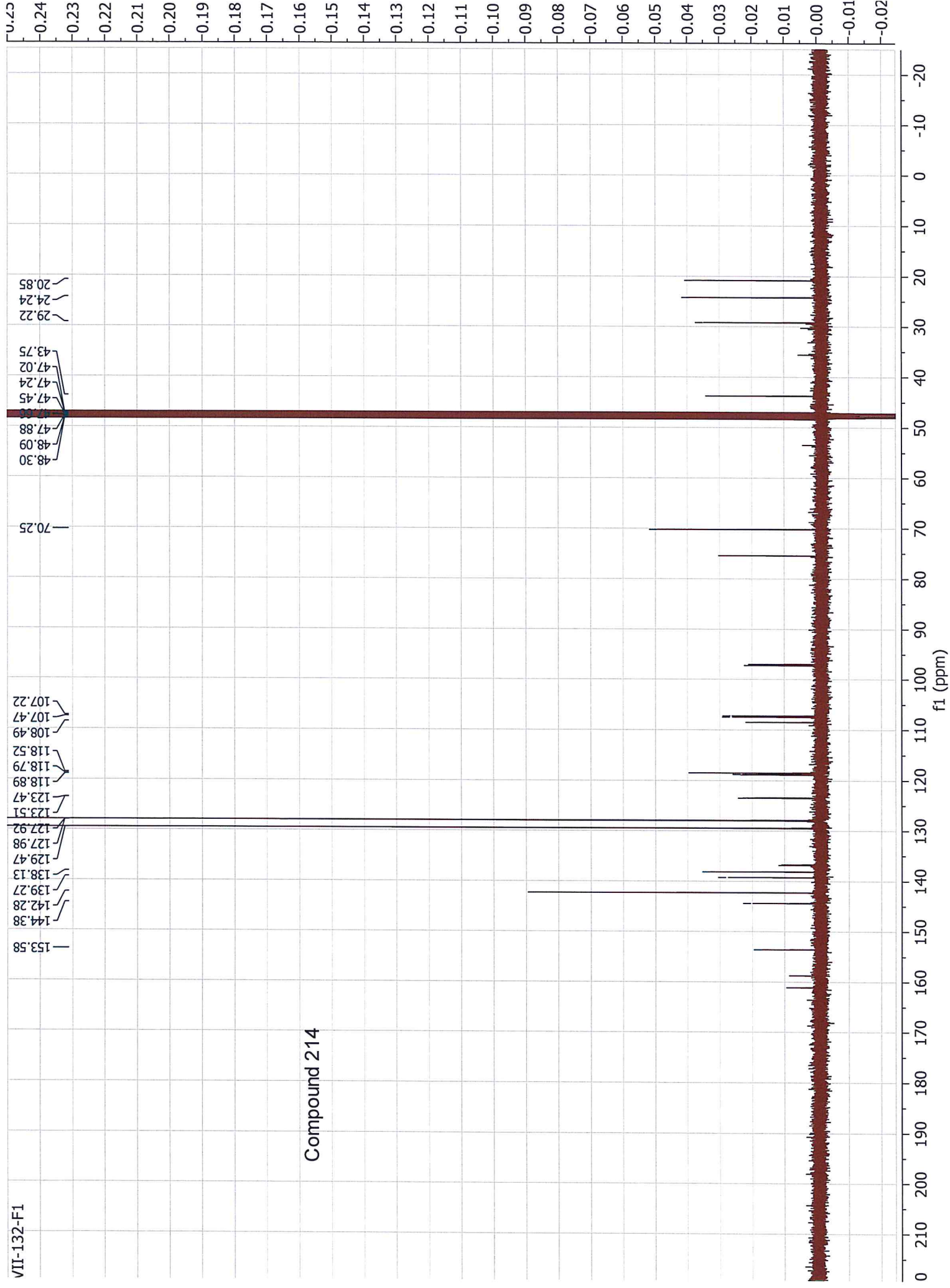


X : parts per Million : 13C

Compound 214



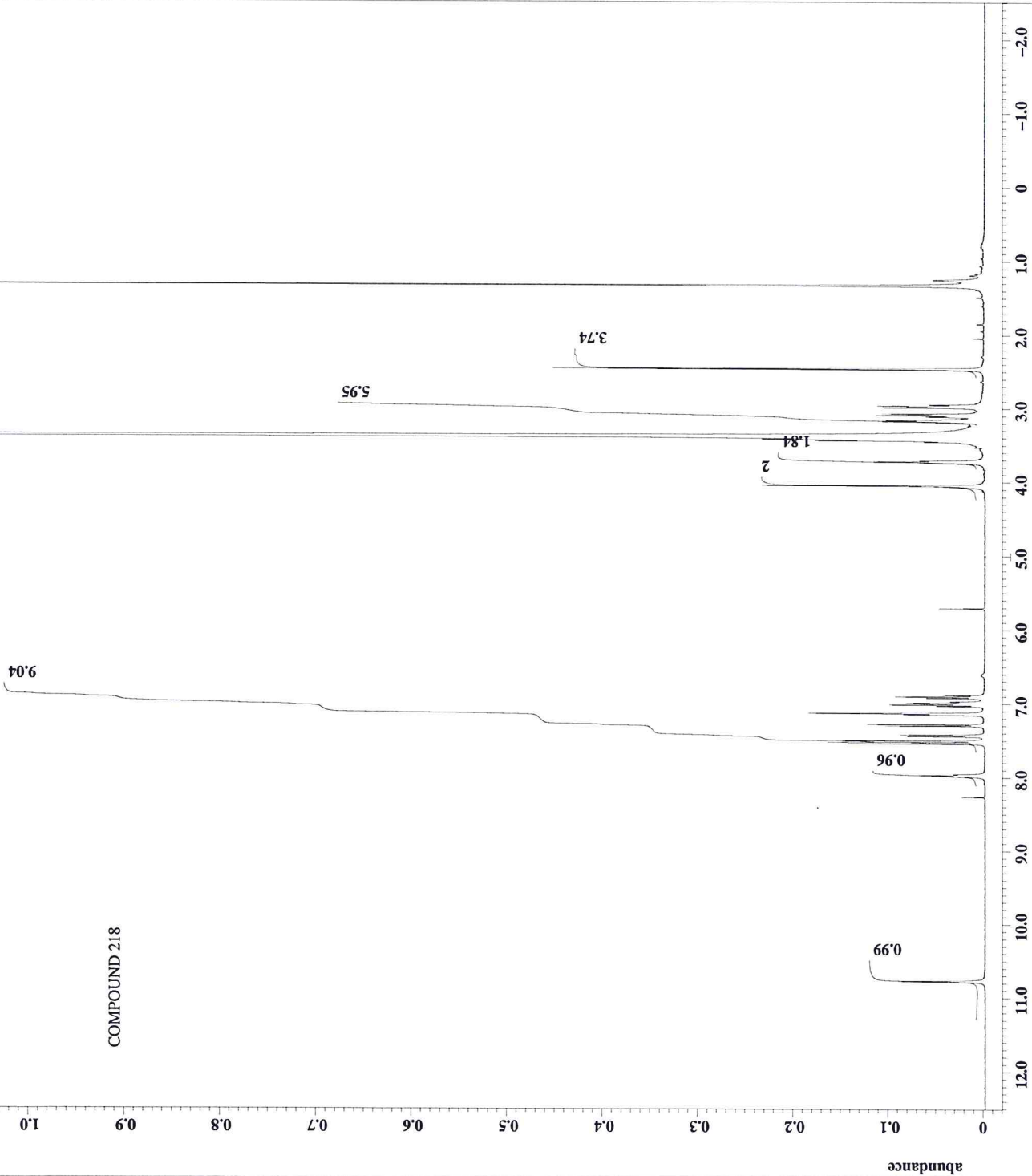
Compound 214





COMPOUND 218

Filename = BN-VI-34-F1_PROTON-3.
Author = Neumann
Experiment = single_pulse.ex2
Sample_id = BN-VI-34-F1
Solvent = DMSO-D6
Creation_time = 31-AUG-2015 08:14:21
Revision_time = 10-MAR-2021 10:50:25
Current_time = 10-MAR-2021 10:50:32
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.58[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.29[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 32
Relaxation_delay = 4[s]
Repetition_time = 6.18365952[s]
Temp_get = 20.4[degC]

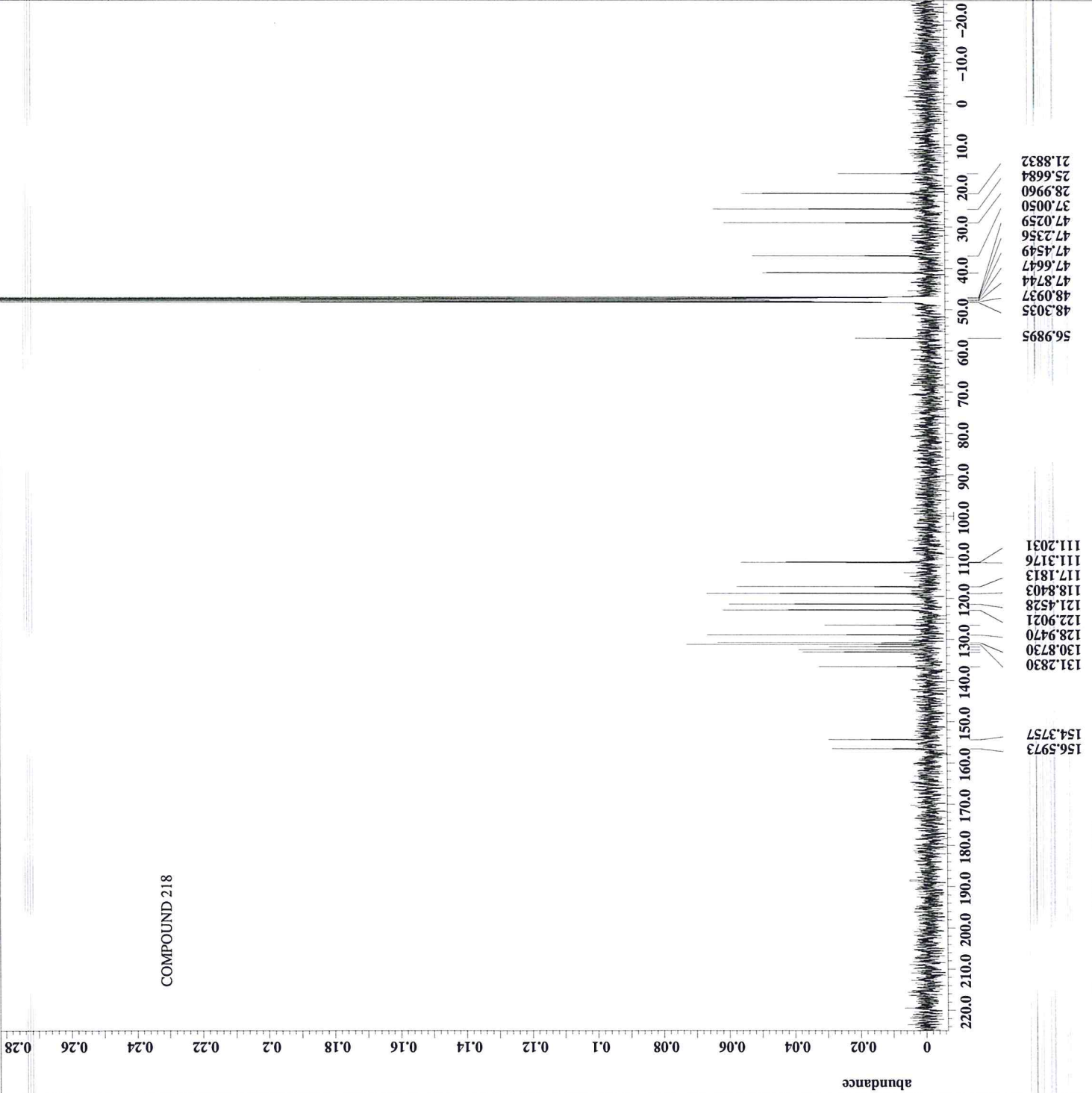


X : parts per Million : 1H



File name = BN-VI-32-c-2_CARBON-3
Author = Neumann
Experiment = single_pulse_dec
Sample_id = BN-VI-32-c-2
Solvent = METHANOL-D3
Creation_time = 4-AUG-2015 16:20:23
Revision_time = 10-MAR-2021 10:22:44
Current_time = 10-MAR-2021 10:23:34
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1345
Total_scans = 1345
X_90_width = 12.36 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.12 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 3 [s]
Recvr_gain = 60
Relaxation_delay = 3 [s]
Repetition_time = 4.04333312 [s]
Temp_get = 20.6 [dC]

COMPOUND 218



X : parts per Million : 13C



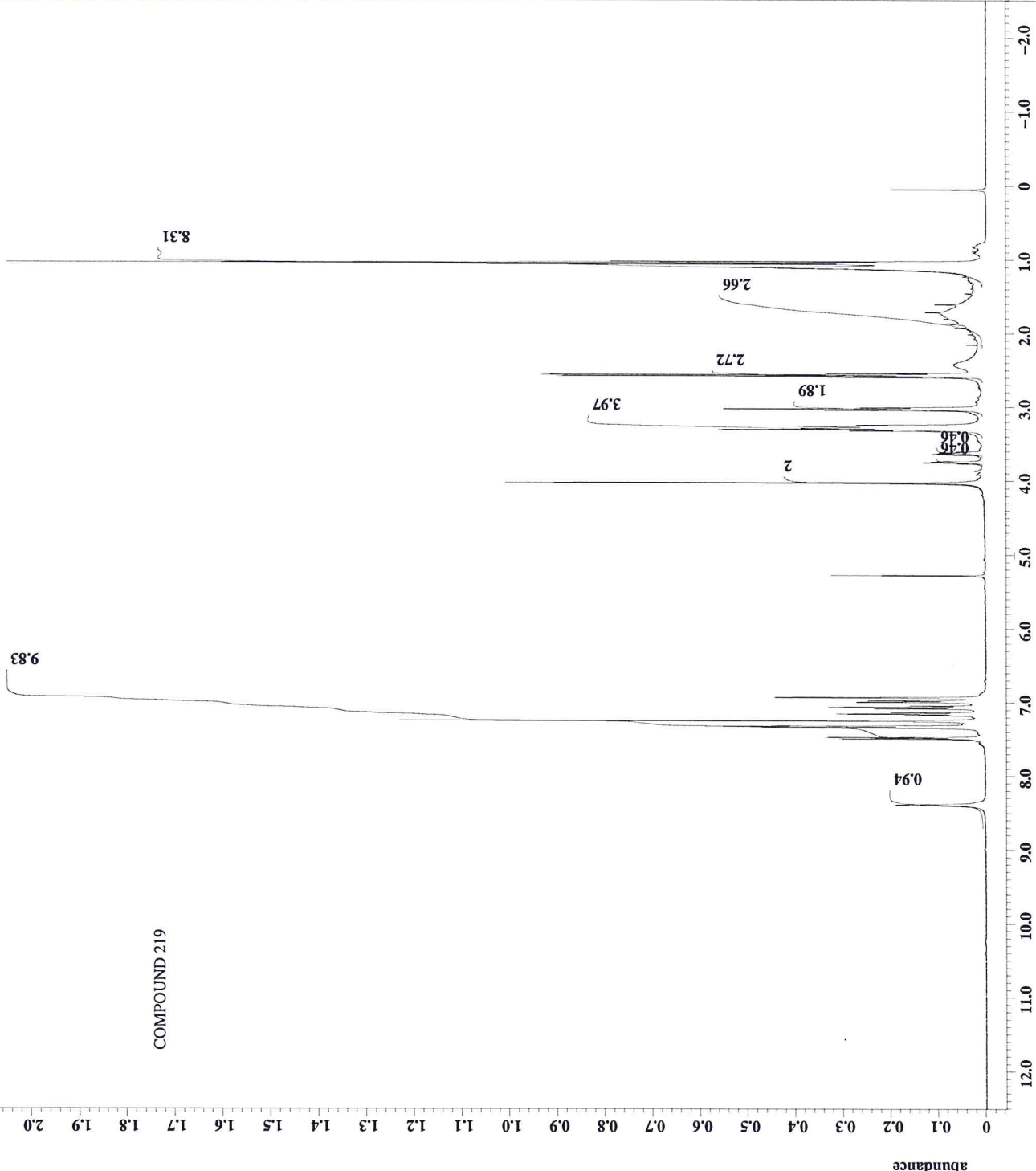
COMPOUND 219

Filename = BN-VI-26-c_PROTON-3.j
Author = Neumann
Experiment = single_pulse.ex2
Sample_id = BN-VI-26-c
Solvent = CHLOROFORM-D
Creation_time = 23-JUL-2015 13:15:39
Revision_time = 10-MAR-2021 11:01:57
Current_time = 10-MAR-2021 11:02:01

Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 10.16[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.08[us]
Irr_mode = Off
Tri_mode = Off
Pante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 4[s]
Repetition_time = 6.18365952[s]
Temp_get = 20.3[dc]



X : parts per Million : 1H



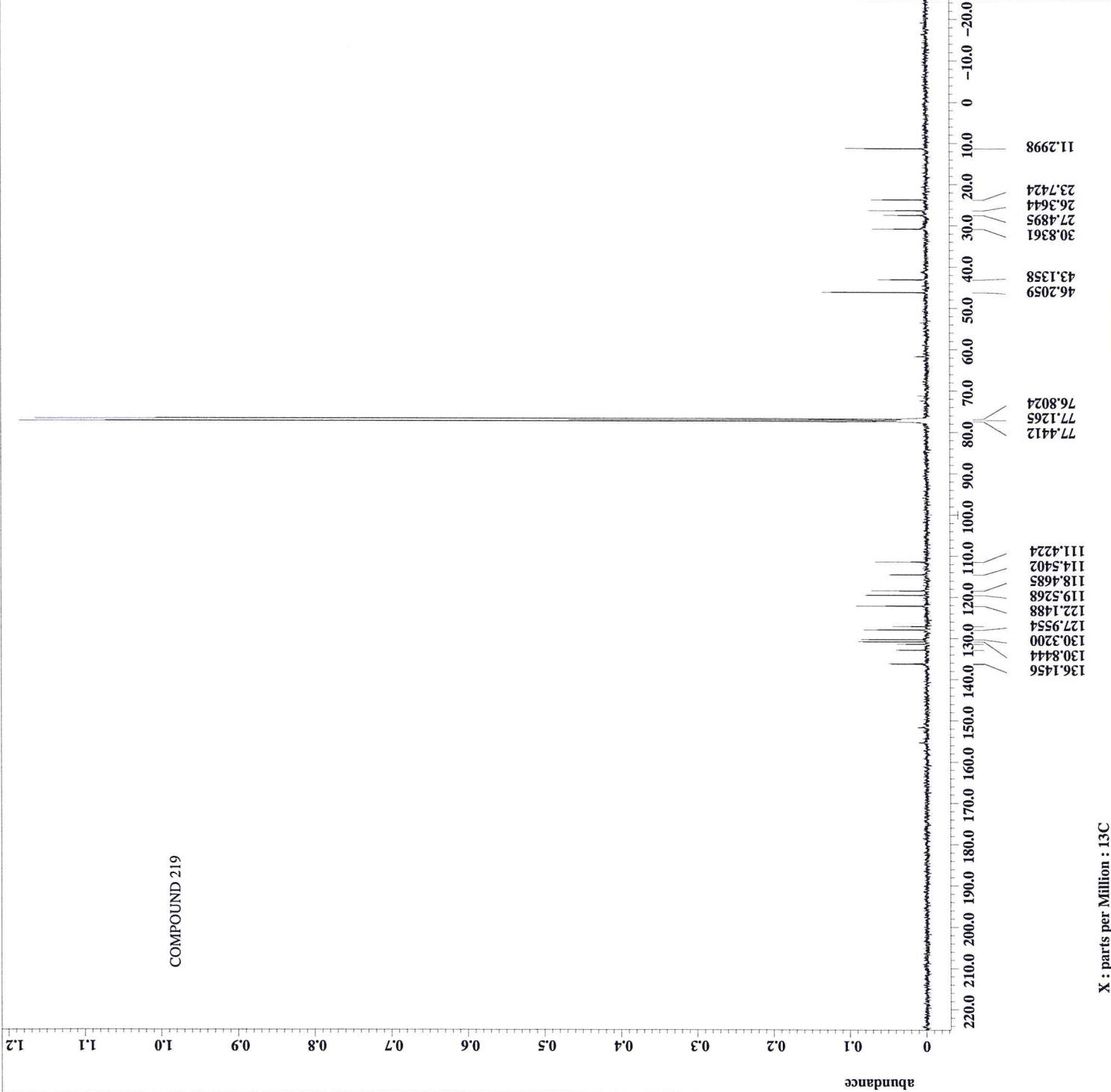
COMPOUND 219

Filename = BN-VI-26-C_CARBON-4.j
Author = Neumann
Experiment = single_pulse_dec
Sample_id = BN-VI-26-c
Solvent = CHLOROFORM-D
Creation_time = 23-JUL-2015 14:59:09
Revision_time = 10-MAR-2021 11:03:03
Current_time = 10-MAR-2021 11:03:23

Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

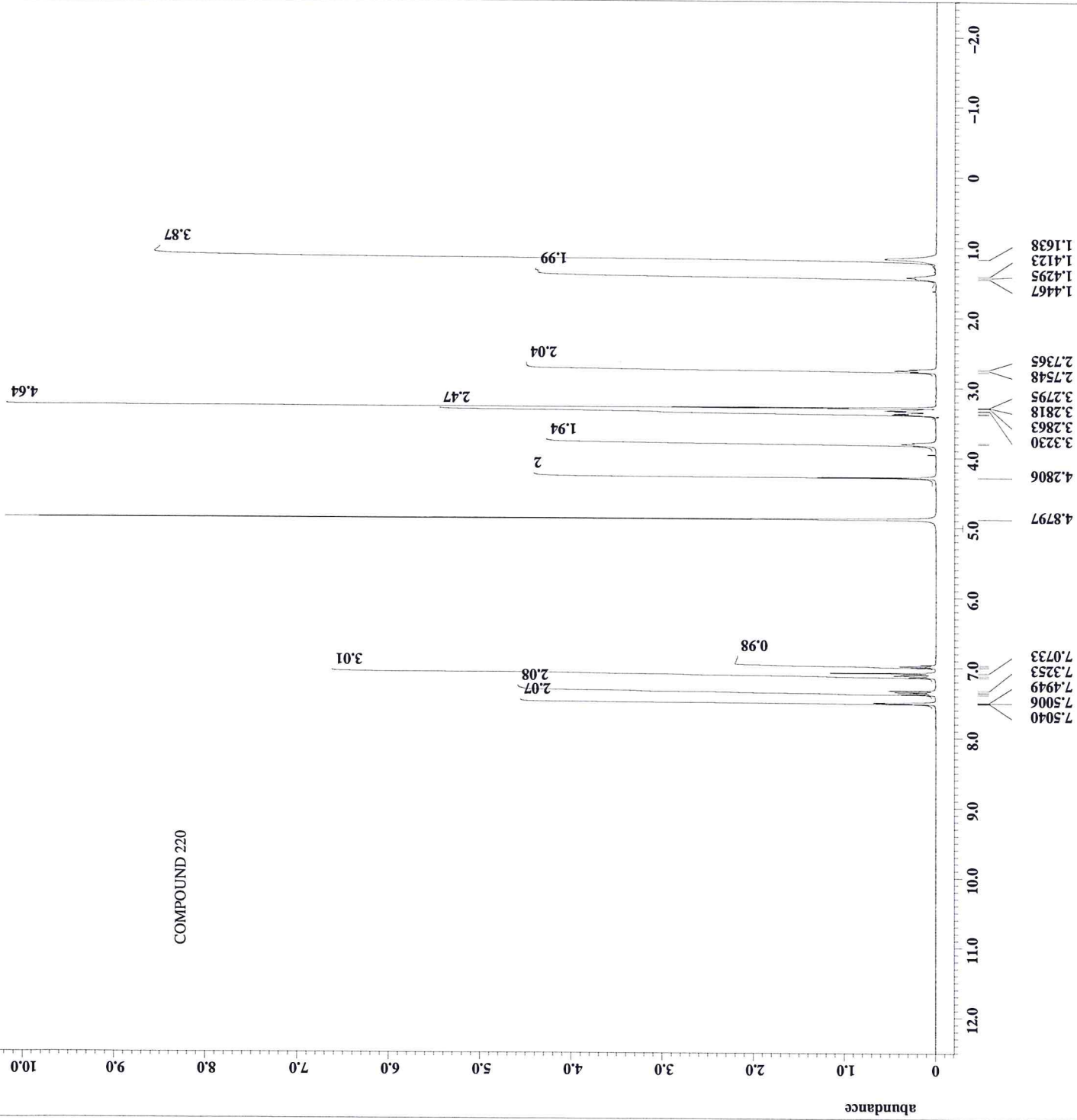
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 1201
Total_scans = 1201

X_90_width = 12.36 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.12 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Decoupling = WALTZ
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 4 [s]
Recvr_gain = 60
Relaxation_delay = 4 [s]
Repetition_time = 5.04333312 [s]
Temp_get = 20.5 [dC]





Filename = BN-VI-27B-C_PROTON-4.
Author = Neumann
Experiment = single_pulse.ex2
Sample_id = BN-VI-27B-C
Solvent = METHANOL-D3
Creation_time = 29-JUL-2015 10:37:21
Revision_time = 10-MAR-2021 11:08:16
Current_time = 10-MAR-2021 11:08:21
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 10.16 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.08 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 42
Relaxation_delay = 4 [s]
Repetition_time = 6.18365952 [s]
Temp_get = 19.9 [dC]

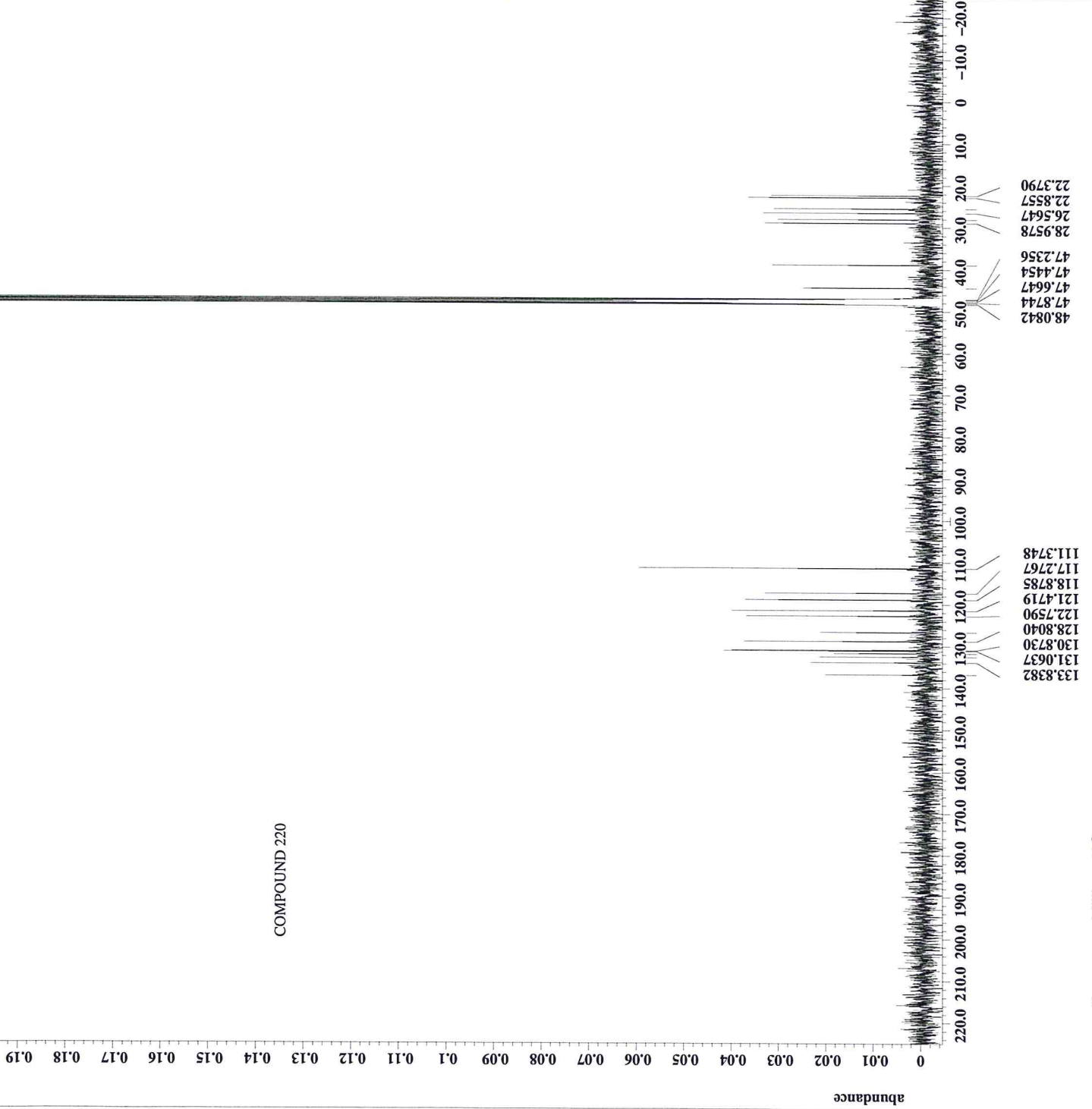


X : parts per Million : 1H



Filename = BN-VI-27B-c CARBON-4.
Author = Neumann
Experiment = single_pulse_dec
Sample_id = BN-VI-27B-C
Solvent = METHANOL-D3
Creation_time = 29-JUL-2015 13:31:38
Revision_time = 10-MAR-2021 11:10:12
Current_time = 10-MAR-2021 11:10:24
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 32768
X_points = 4
X_prescans = 0.95846665[Hz]
X_resolution = 31.40703518[KHz]
X_sweep = 1K
Irr_domain = 399.78219838[MHz]
Irr_freq = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 2048
Total_scans = 2048
X_90_width = 12.36[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 9[db]
X_pulse = 4.12[us]
Irr_atn_dec = 27[db]
Irr_atn_noe = 27[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 4[s]
Recvr_gain = 60
Relaxation_delay = 4[s]
Repetition_time = 5.04333312[s]
Temp_get = 20.2[dc]

COMPOUND 220



X : parts per Million : 13C



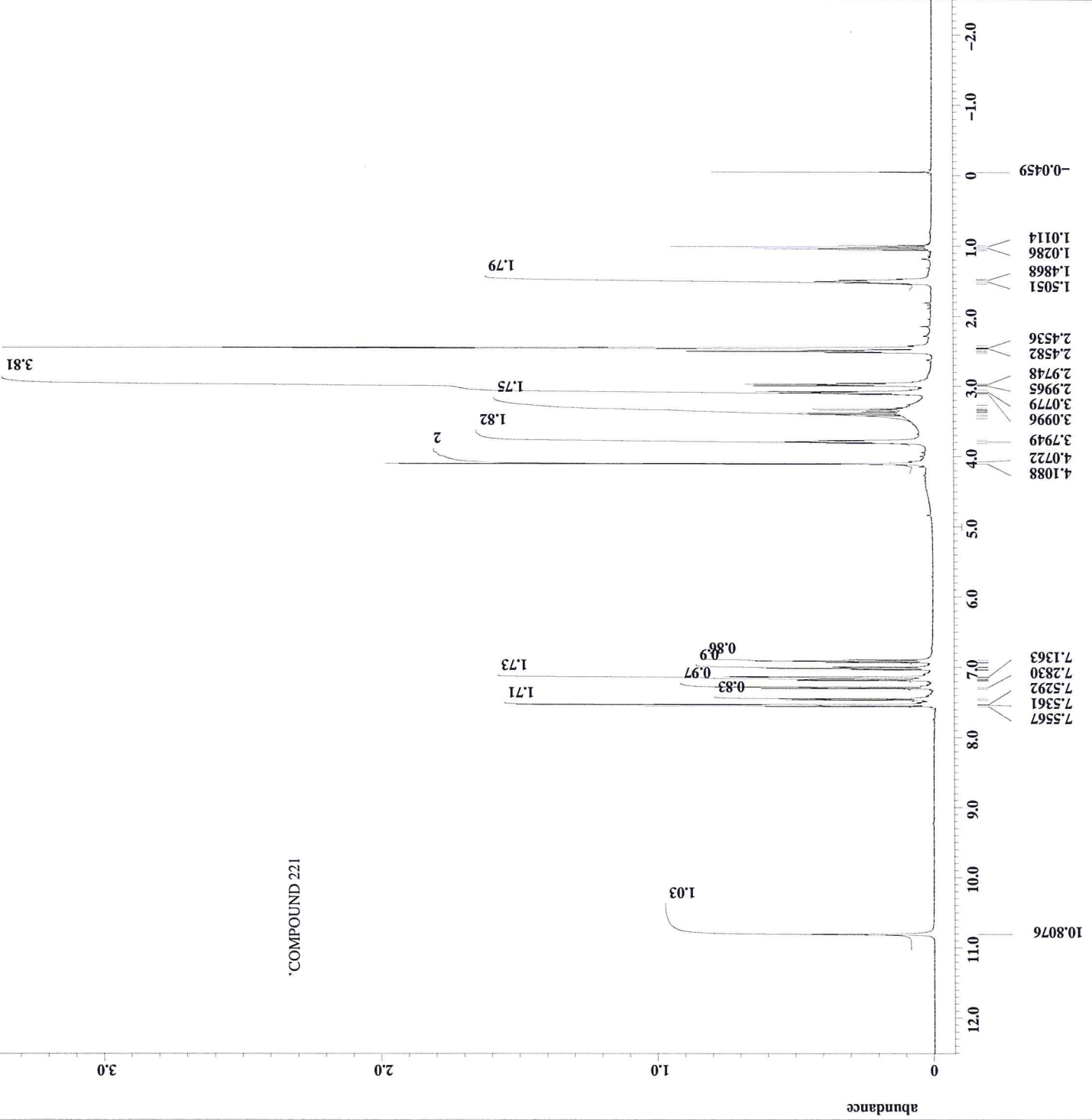
File: ID-102-37-B-5.jdf
Author: Crider
Experiment: single_pulse.ex2
Sample_id: S#730831
Solvent: DMSO-D6
Creation_time: 8-JUN-2011 20:05:30
Revision_time: 17-MAR-2021 09:46:04
Current_time: 17-MAR-2021 09:46:09

Comment: single_pulse
Data_format: 1D COMPLEX
Dim_size: 13107
Dim_title: 1H
Dim_units: [ppm]
Dimensions: X
Site: ECS 400
Spectrometer: JNM-ECS400

Field_strength: 9.389766[T] (400 [MHz])
X_acq_duration: 2.18365952[s]
X_domain: 1H
X_freq: 399.78219838 [MHz]
X_offset: 5 [ppm]
X_points: 16384
X_prescans: 1
X_resolution: 0.45794685 [Hz]
X_sweep: 7.5030012 [kHz]
Irr_domain: 1H
Irr_freq: 399.78219838 [MHz]
Irr_offset: 5 [ppm]
Tri_domain: 1H
Tri_freq: 399.78219838 [MHz]
Tri_offset: 5 [ppm]
Clipped: FALSE
Mod_return: 1
Scans: 8
Total_scans: 8

X_90_width: 10.01791 [us]
X_acq_time: 2.18365952 [s]
X_angle: 45 [deg]
X_atn: 6 [dB]
X_pulse: 5.008955 [us]
Irr_mode: Off
Tri_mode: Off
Dante_preset: FALSE
Initial_wait: 1 [s]
Recvr_gain: 38
Relaxation_delay: 5 [s]
Repetition_time: 7.18365952 [s]
Temp_get: 20.1 [dC]

'COMPOUND 221

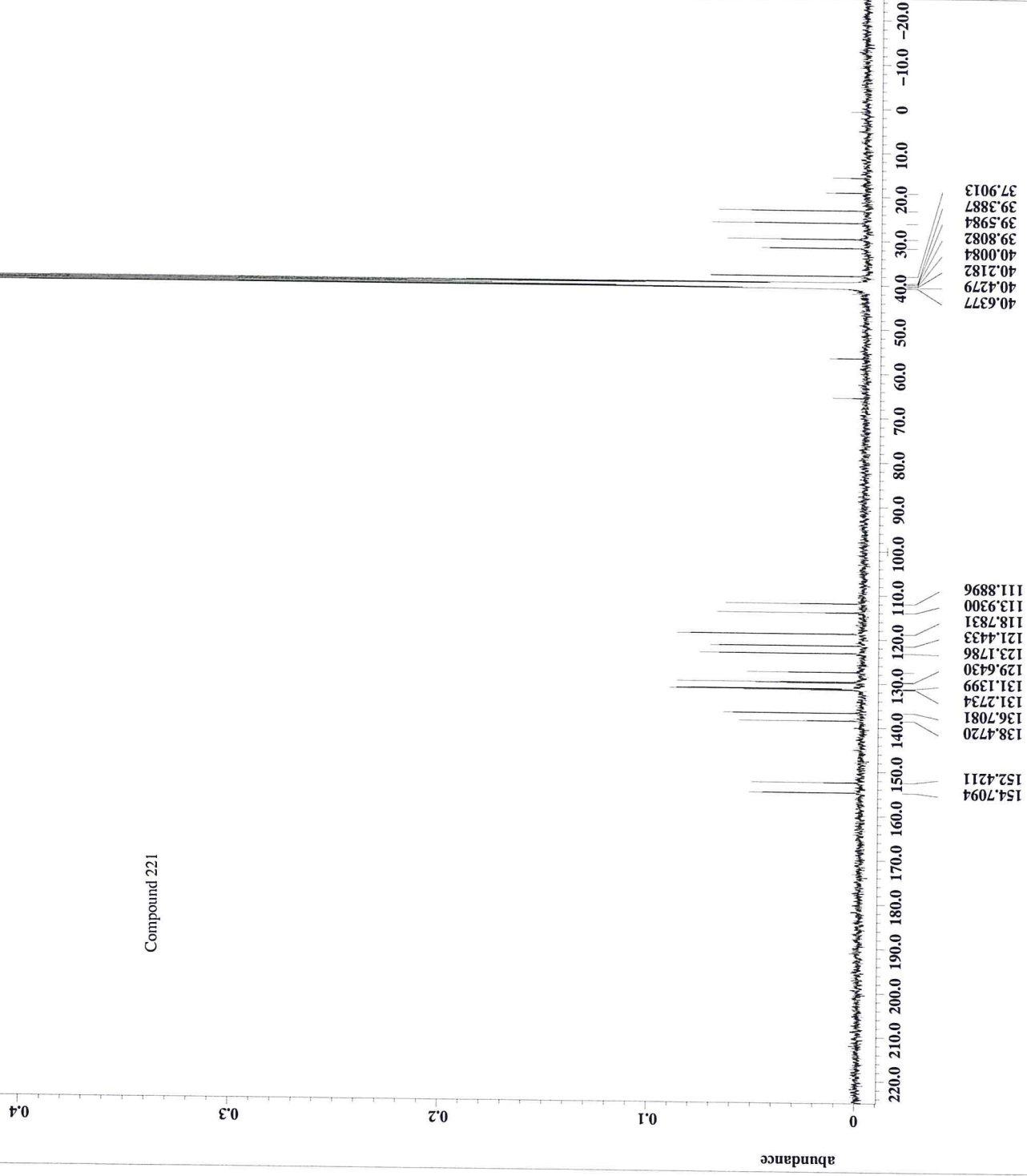


X : parts per Million : 1H



File = ID-102-37-B-5.jdf
Author = Crider
Experiment = single_pulse_dec
Sample_id = S#383557
Solvent = DMSO-D6
Creation_time = 9-JUN-2011 13:53:10
Revision_time = 17-MAR-2021 09:39:12
Current_time = 17-MAR-2021 09:39:16
Comment = single pulse decouple
Data_format = 1D_COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4096
Total_scans = 4096
X_90_width = 11.9 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.96666667 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [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 = 3.04333312 [s]
Temp_get = 19.7 [dC]

Compound 221



X : parts per Million : 13C