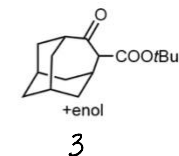


Towards a qualitative understanding of carbonyl reactivity of disubstituted homoadamantane-4-ones.

Supporting information

Contains ^1H , ^{13}C NMR, DEPT-135 and 2d-spectra

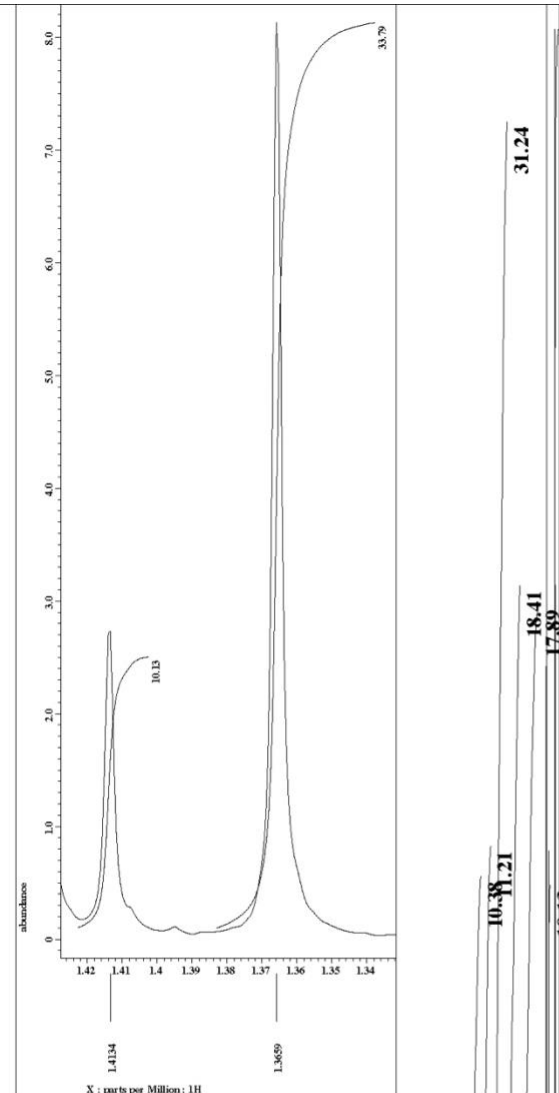


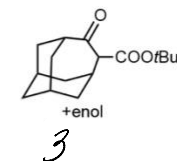
Filename = TIM_1H_175-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_175
 Solvent = DMSO-D6
 Creation_time = 28-DEC-2018 12:42:53
 Revision_time = 13-FEB-2023 12:37:27
 Current_time = 13-FEB-2023 12:37:50

Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 11.9[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 5.95[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 30
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 20.1[dC]



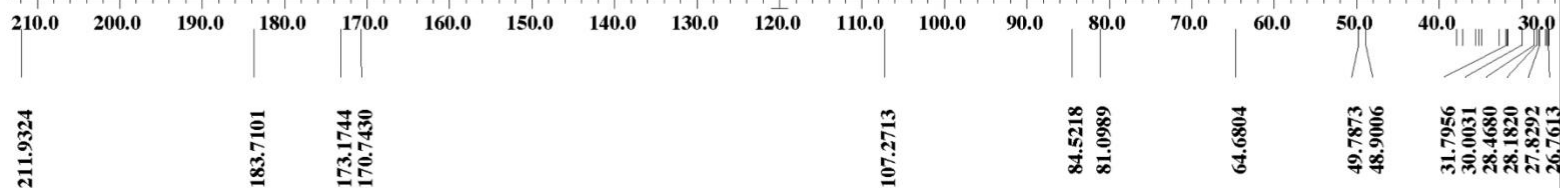
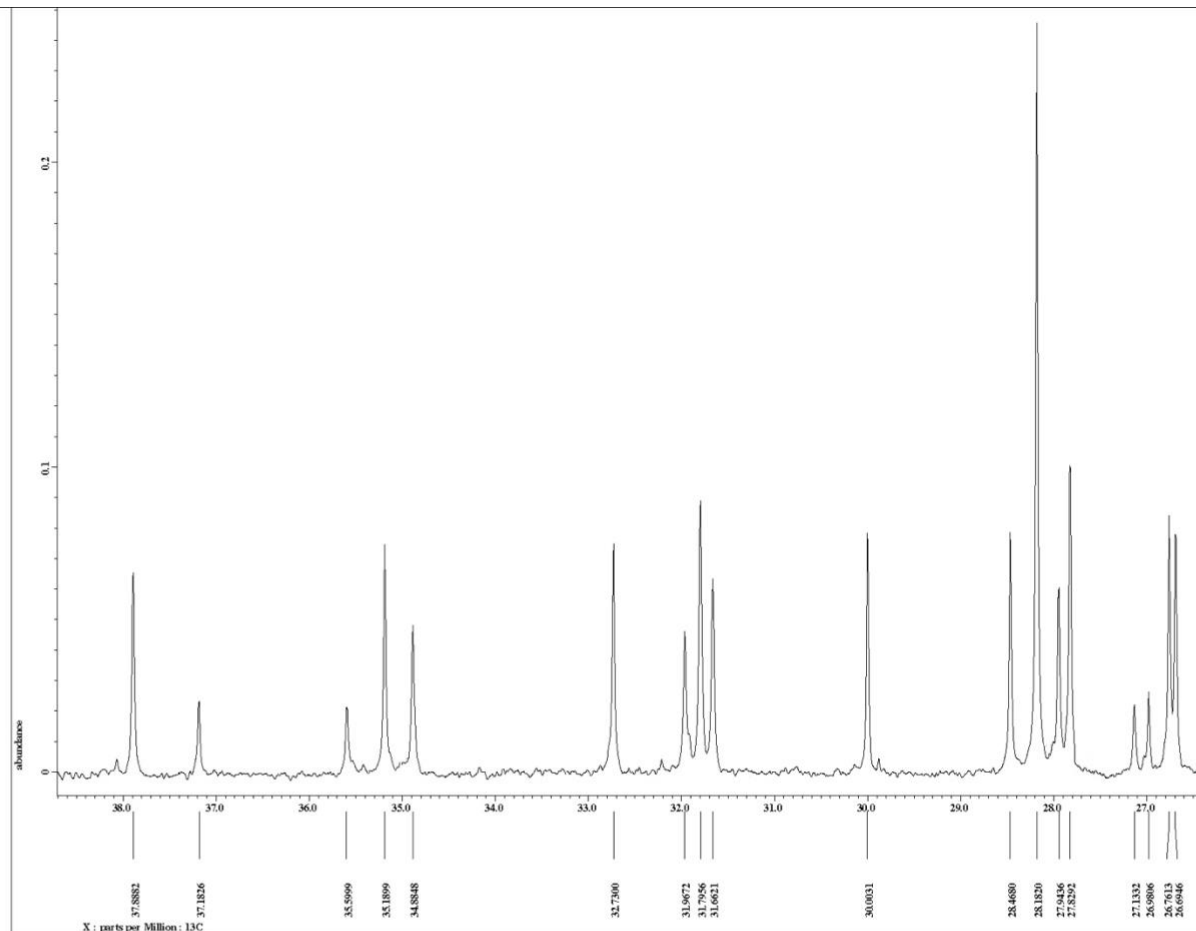


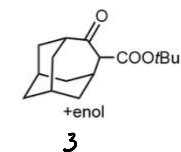
Filename = TIM_13C_175-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_175
 Solvent = DMSO-D6
 Creation_time = 28-DEC-2018 13:10:33
 Revision_time = 13-FEB-2023 12:54:16
 Current_time = 13-FEB-2023 12:54:49

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 491
 Total_scans = 491

X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 44
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 22.7[dc]



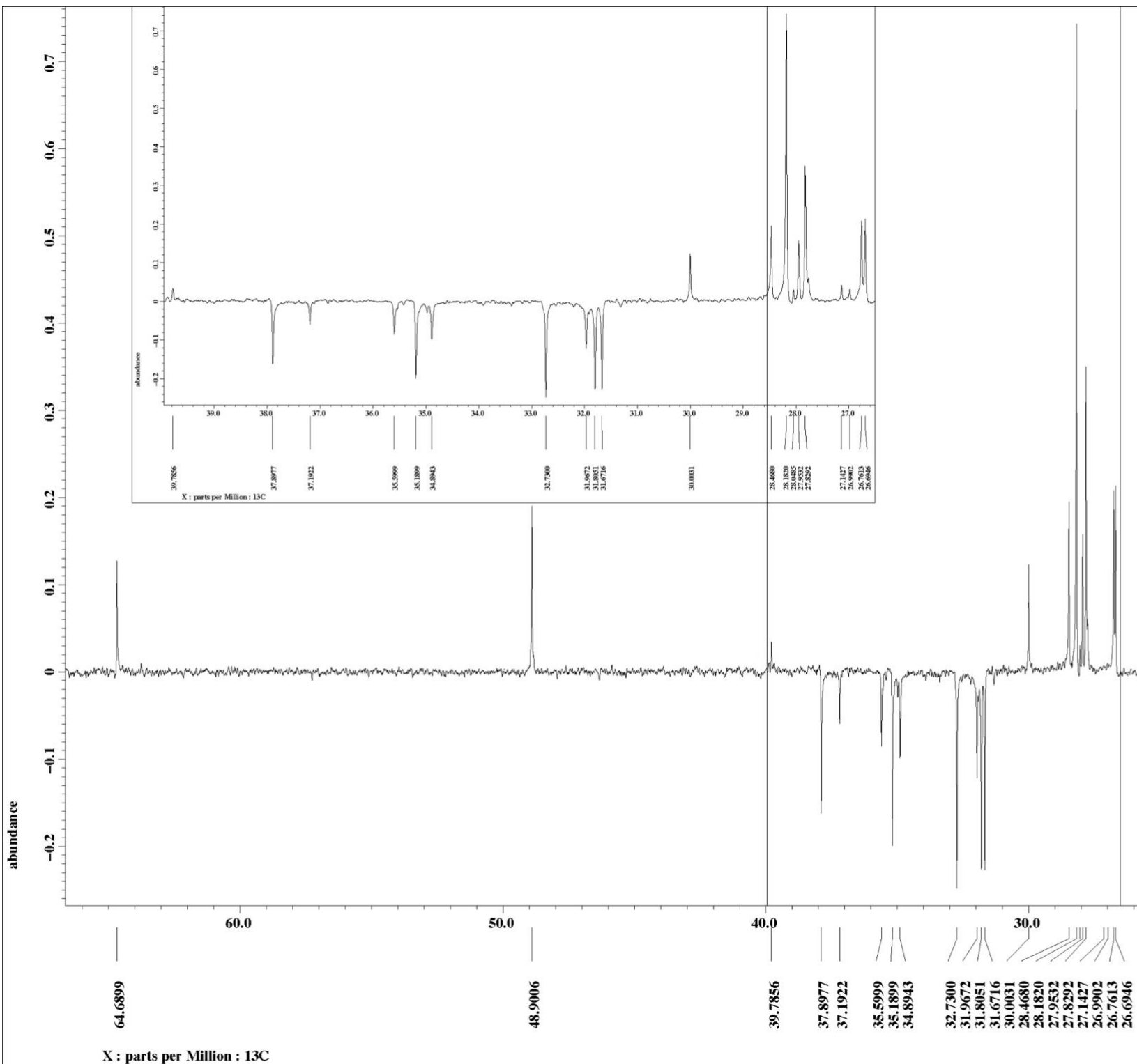
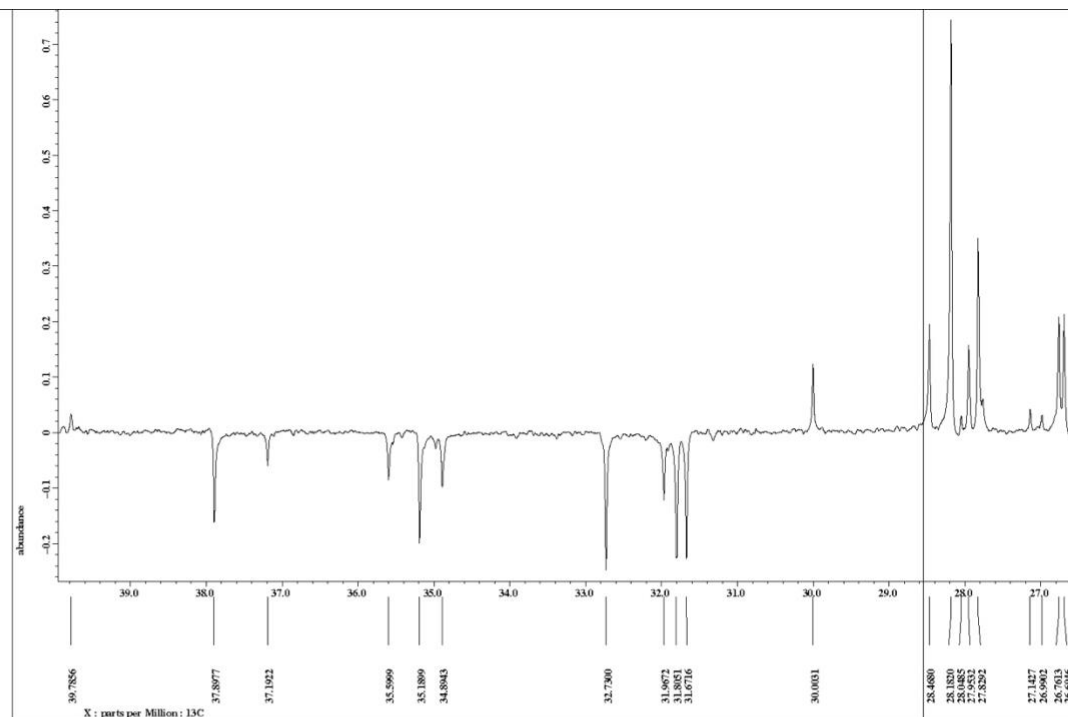


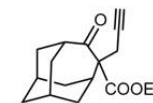
Filename = TIM_DEPT135_175-3.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_175
 Solvent = DMSO-D6
 Creation_time = 28-DEC-2018 13:14:08
 Revision_time = 13-FEB-2023 12:57:15
 Current_time = 13-FEB-2023 12:57:43

Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 64
 Total_scans = 64

X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 22.8[degC]





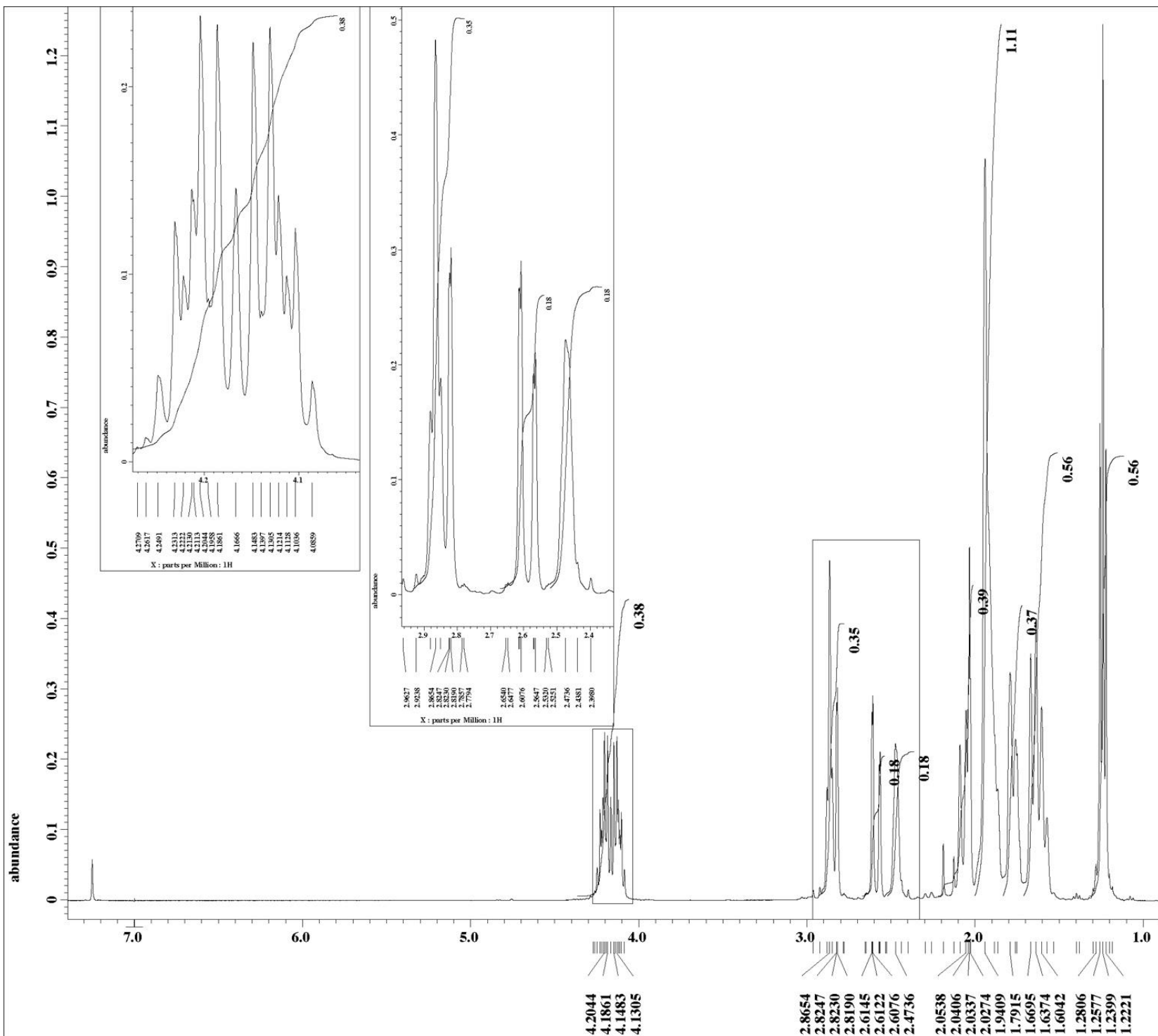
2a

Filename = TIM_1H_245-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM 245
 Solvent = CHLOROFORM-D
 Creation_time = 27-JAN-2020 17:04:02
 Revision_time = 10-FEB-2023 13:10:10
 Current_time = 10-FEB-2023 13:11:07

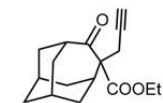
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 5.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3.5[dB]
 X_pulse = 2.75[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 22
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 0[dc]



X : parts per Million : 1H



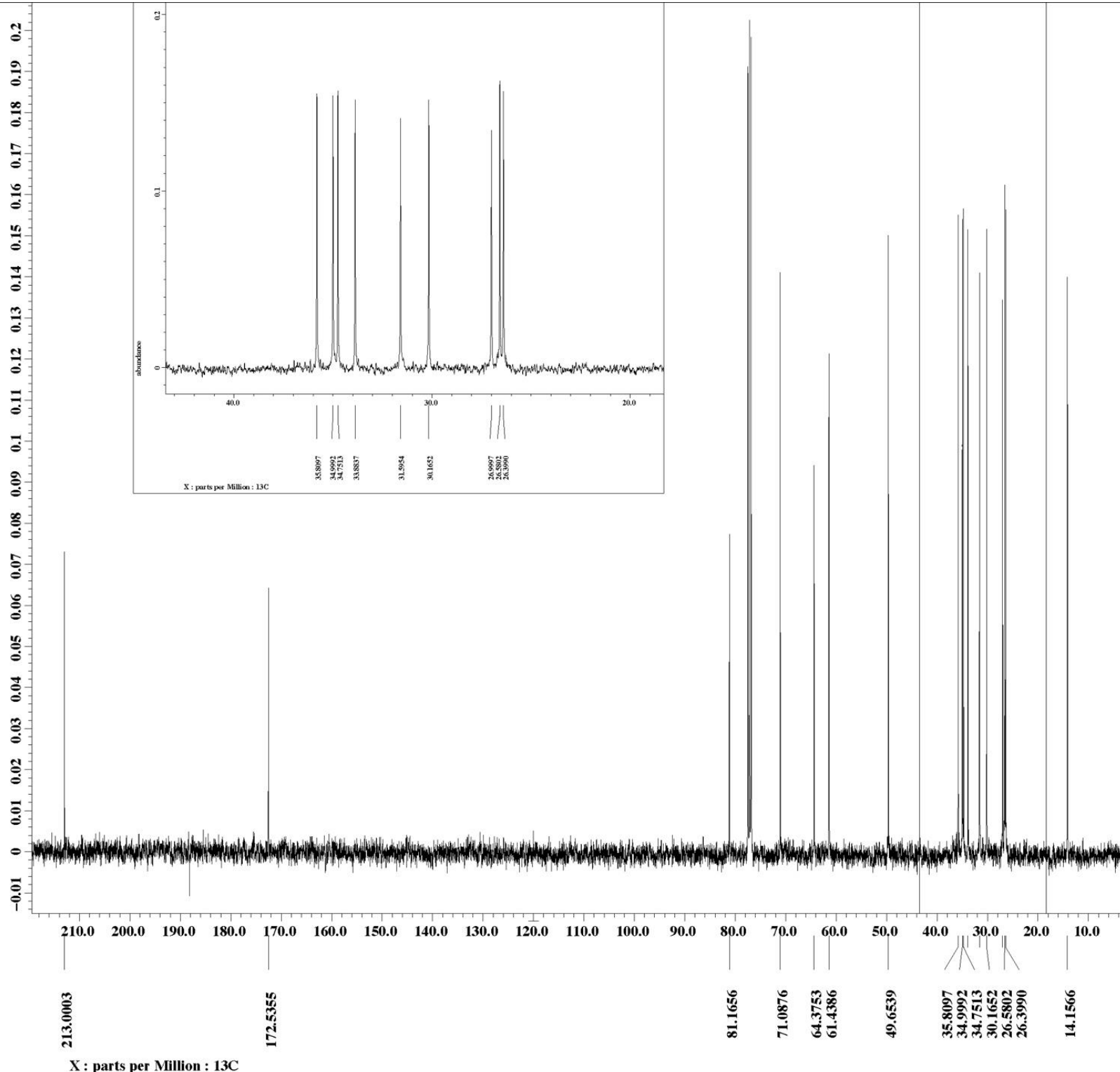
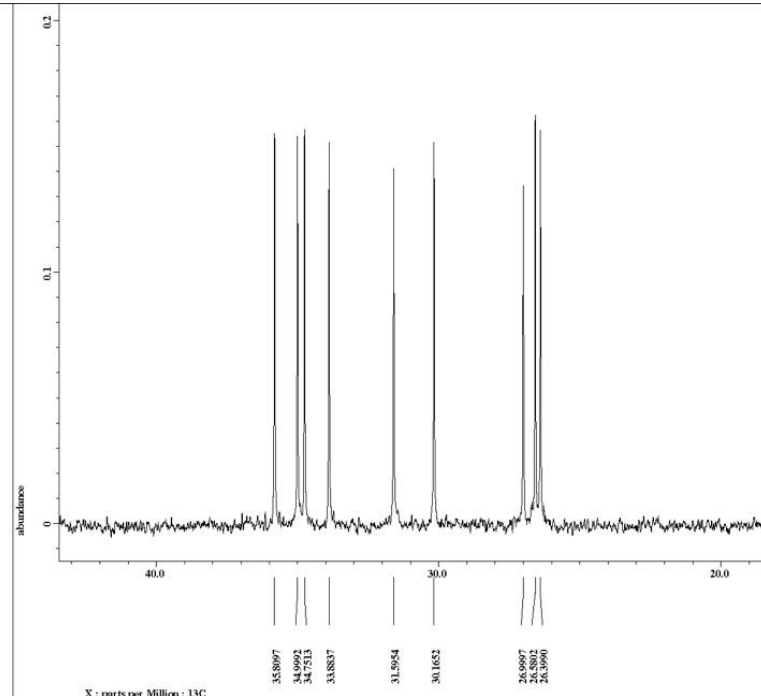
2a

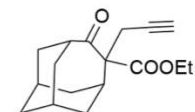
Filename = TIM_13C_245-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_245
 Solvent = CHLOROFORM-D
 Creation_time = 27-JAN-2020 17:29:09
 Revision_time = 10-FEB-2023 13:11:31
 Current_time = 10-FEB-2023 13:11:54

Comment = single pulse decouple
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

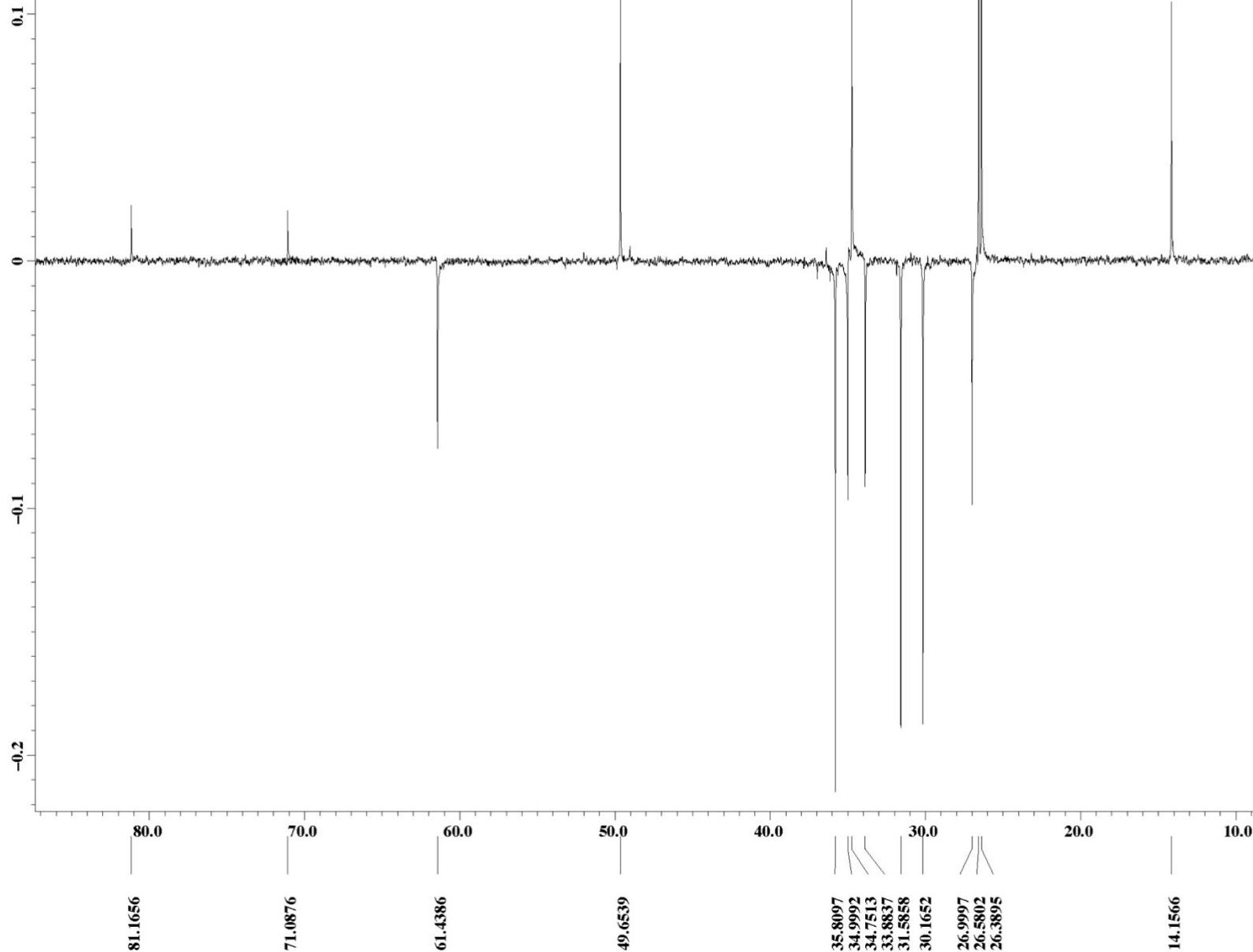
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 448
 Total_scans = 448

X_90_width = 13.87[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 5.2[dB]
 X_pulse = 4.62333333[us]
 Irr_atn_dec = 29.907[dB]
 Irr_atn_noe = 29.907[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 0[dc]





2a



X : parts per Million : 13C

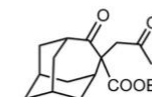
```

Filename      = TIM_DEPT135_245-4.jdf
Author       = delta
Experiment   = dept.ex2
Sample_id    = TIM_245
Solvent      = CHLOROFORM-D
Creation_time = 27-JAN-2020 17:54:23
Revision_time = 10-FEB-2023 13:12:15
Current_time  = 10-FEB-2023 13:12:47

Comment      = DEPT with decoupling
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECX 400
Spectrometer  = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain       = 13C
X_freq         = 100.52530333[MHz]
X_offset       = 120[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          = 489.0
Total_scans    = 489.0

X_acq_time     = 1.04333312[s]
X_atn          = 5.2[dB]
X_pulse        = 13.87[us]
Irr_atn        = 3.5[dB]
Irr_atn_dec    = 29.907[dB]
Irr_noise      = WALTZ
Irr_pulse      = 5.5[us]
Decoupling     = TRUE
Initial_wait   = 1[s]
J_constant     = 140[Hz]
Recvr_gain     = 46
Relaxation_delay = 2[s]
Selection_angle = 135[deg]
Selection_pulse = 8.25[us]
Temp_get       = 0[dC]
  
```



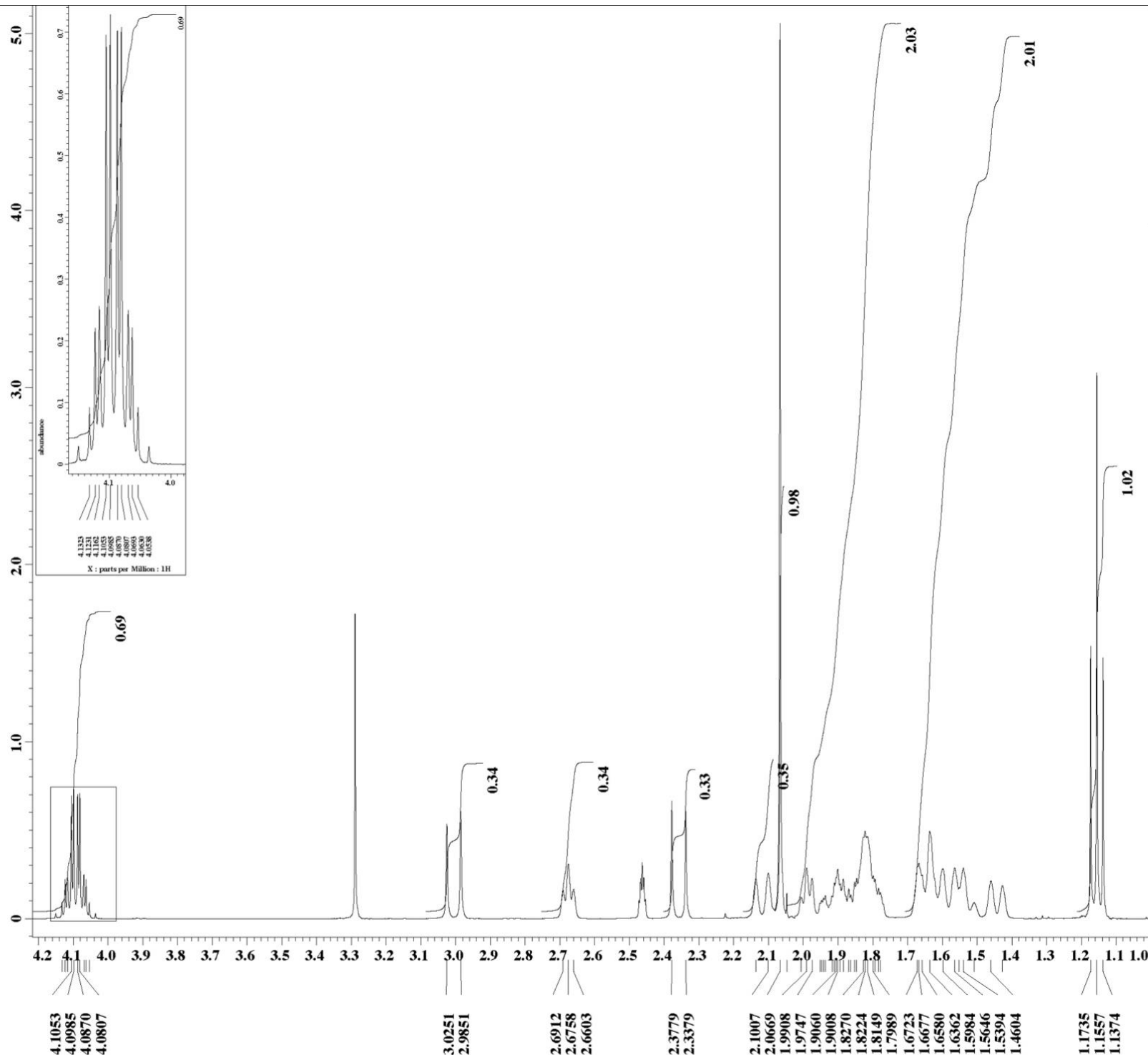
2b

Filename = TIM_1H_253-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_253
 Solvent = DMSO-D6
 Creation_time = 16-MAR-2020 11:31:50
 Revision_time = 10-FEB-2023 15:04:11
 Current_time = 10-FEB-2023 15:05:59

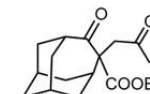
Comment = single pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838 [MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 11.9[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 5.95[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 34
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 0[dc]



X: parts per Million : 1H



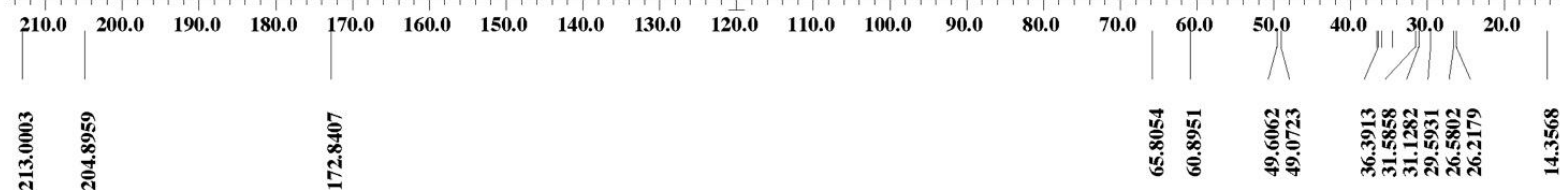
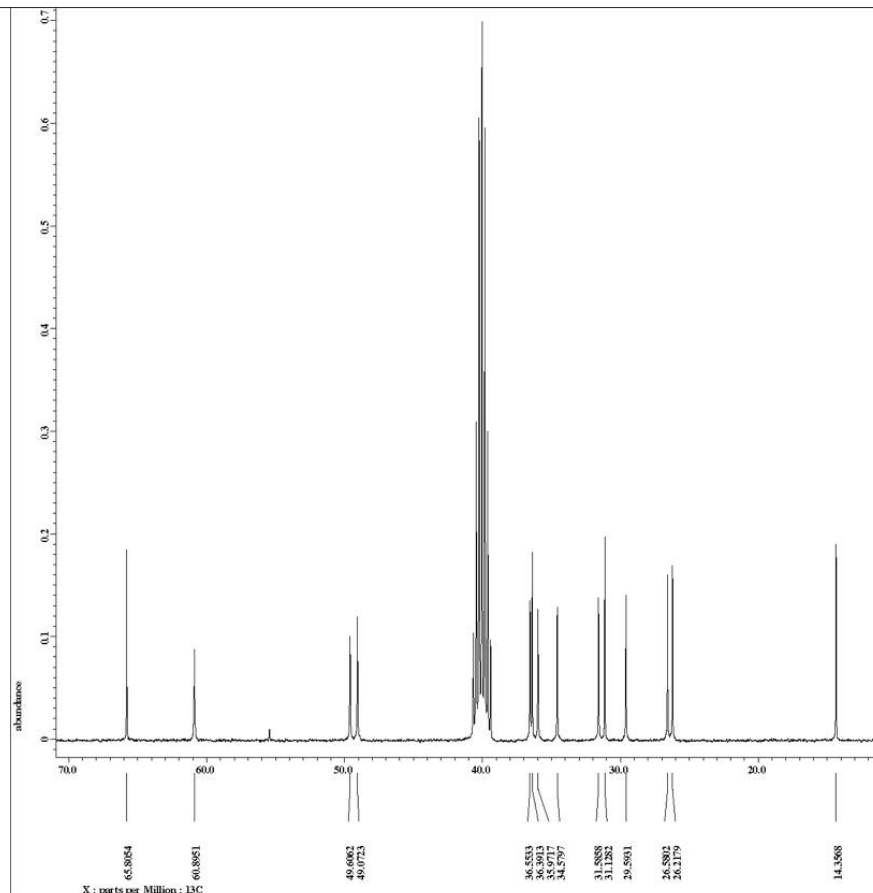
2b

Filename = TIM_13C_253-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_253
 Solvent = DMSO-D6
 Creation_time = 16-MAR-2020 12:41:31
 Revision_time = 10-FEB-2023 15:06:38
 Current_time = 10-FEB-2023 15:08:15

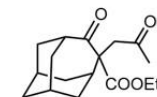
 Comment = single pulse decouple
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1024
 Total_scans = 1024

 X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 0[dc]



X : parts per Million : 13C



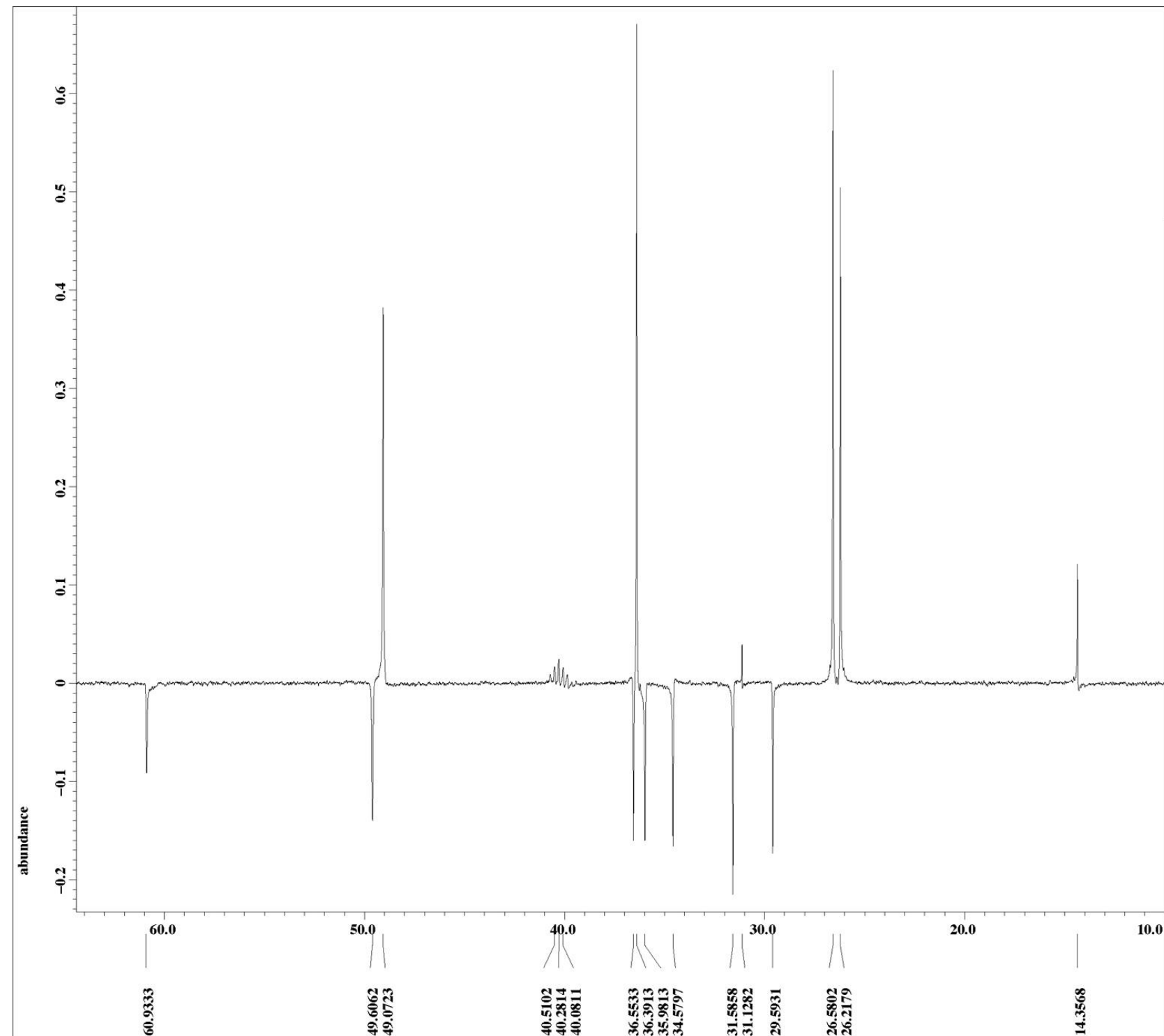
26

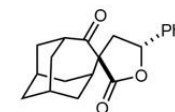
Filename = TIM_DEPT135_253-3.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_253
 Solvent = DMSO-D6
 Creation_time = 16-MAR-2020 13:33:08
 Revision_time = 10-FEB-2023 15:09:09
 Current_time = 10-FEB-2023 15:09:51

Comment = DEPT with decoupling
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1000
 Total_scans = 1000

X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 0[dc]





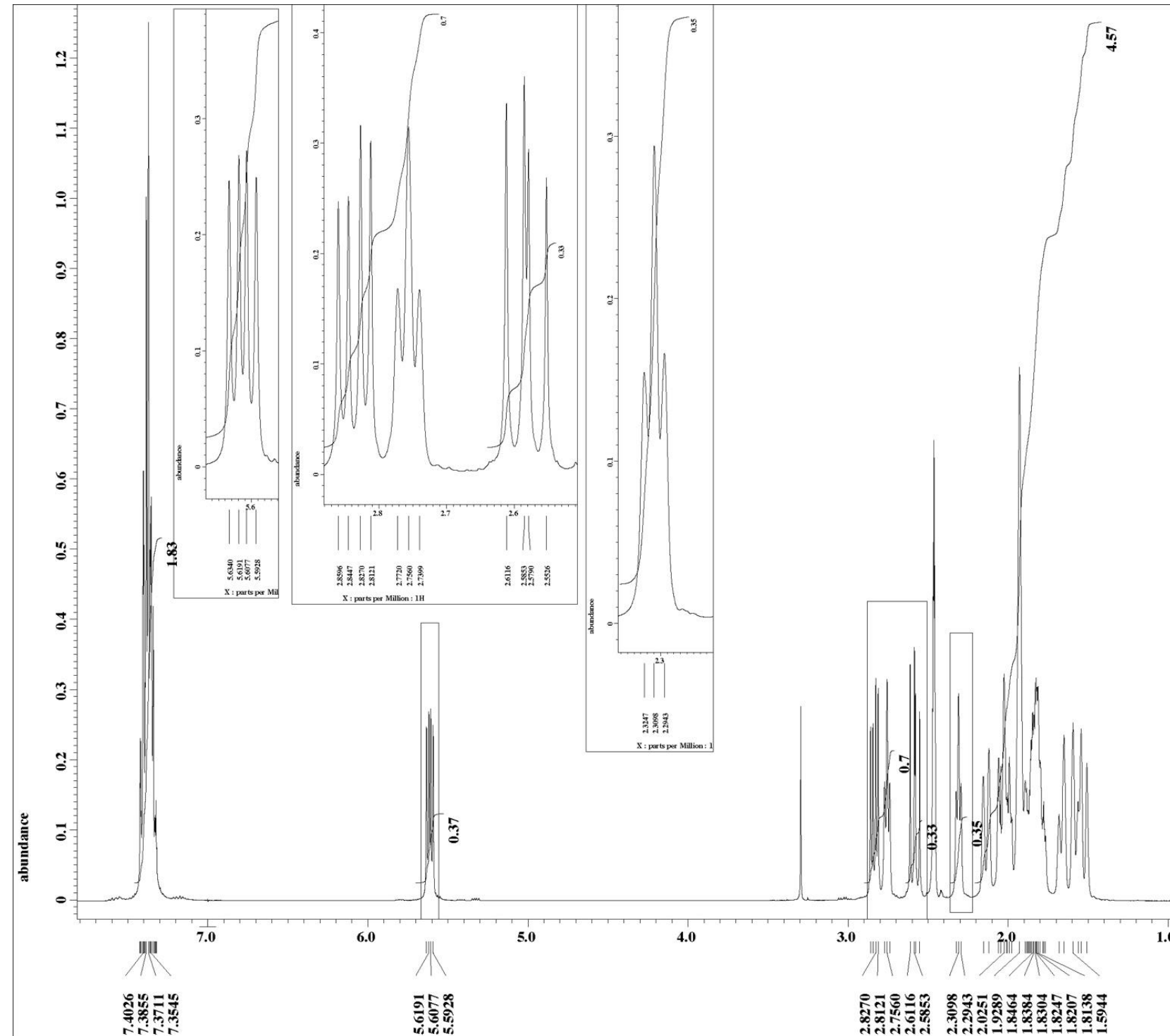
2c

Filename = TIM_1H_Phspirolactone
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_PhspirolactoneNa2
 Solvent = DMSO-D6
 Creation_time = 20-JAN-2022 08:05:11
 Revision_time = 10-FEB-2023 15:36:03
 Current_time = 10-FEB-2023 15:37:33

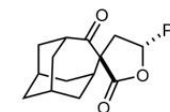
Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 5.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3.5[dB]
 X_pulse = 2.75[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 24
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 0[dc]



X : parts per Million : 1H



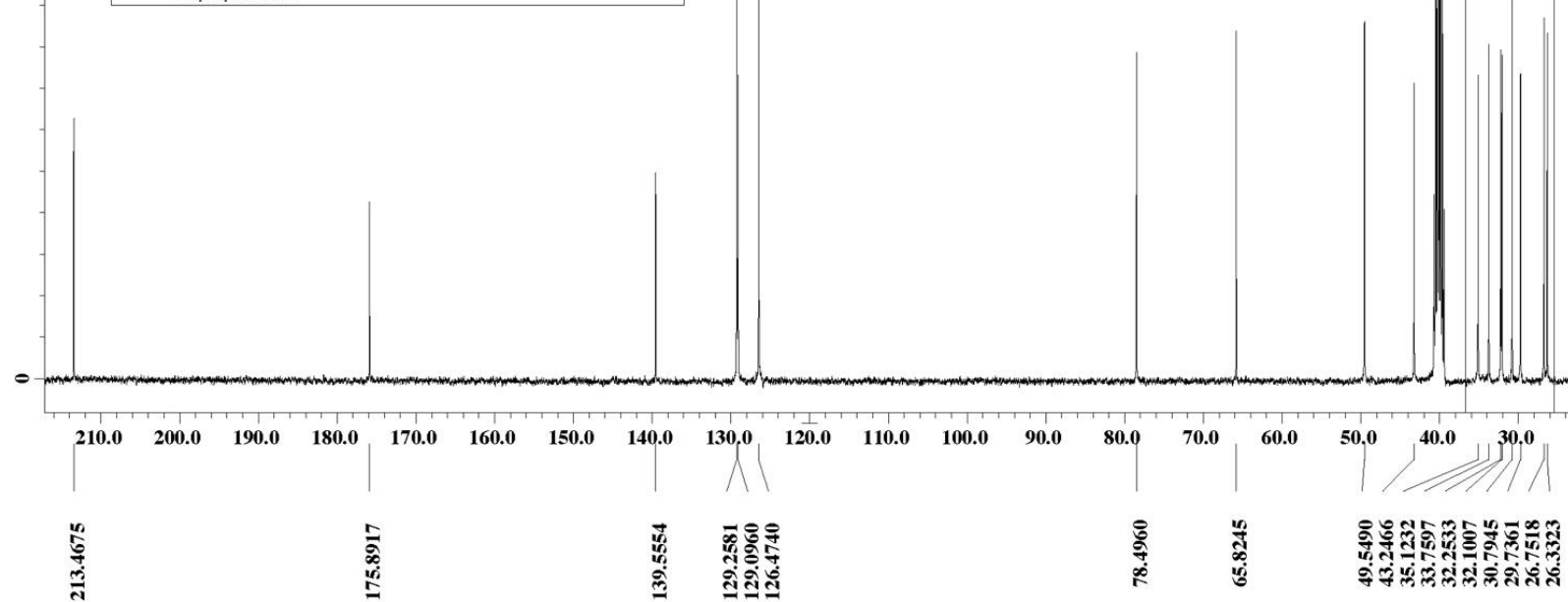
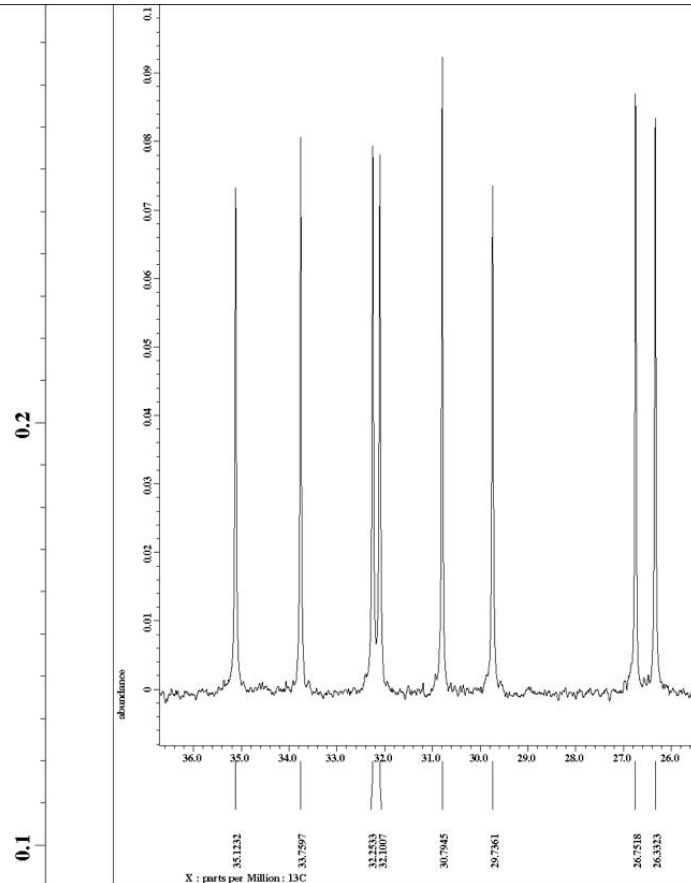
2c

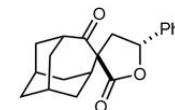
Filename = TIM_13C_Phspirolacton
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_PhspirolactoneNa2
 Solvent = DMSO-D6
 Creation_time = 20-JAN-2022 10:39:56
 Revision_time = 10-FEB-2023 15:37:48
 Current_time = 10-FEB-2023 15:38:20

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 3000
 Total_scans = 3000

X_90_width = 13.87[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 5.2[dB]
 X_pulse = 4.62333333[us]
 Irr_atn_dec = 29.907[dB]
 Irr_atn_noe = 29.907[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 48
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 0[dc]





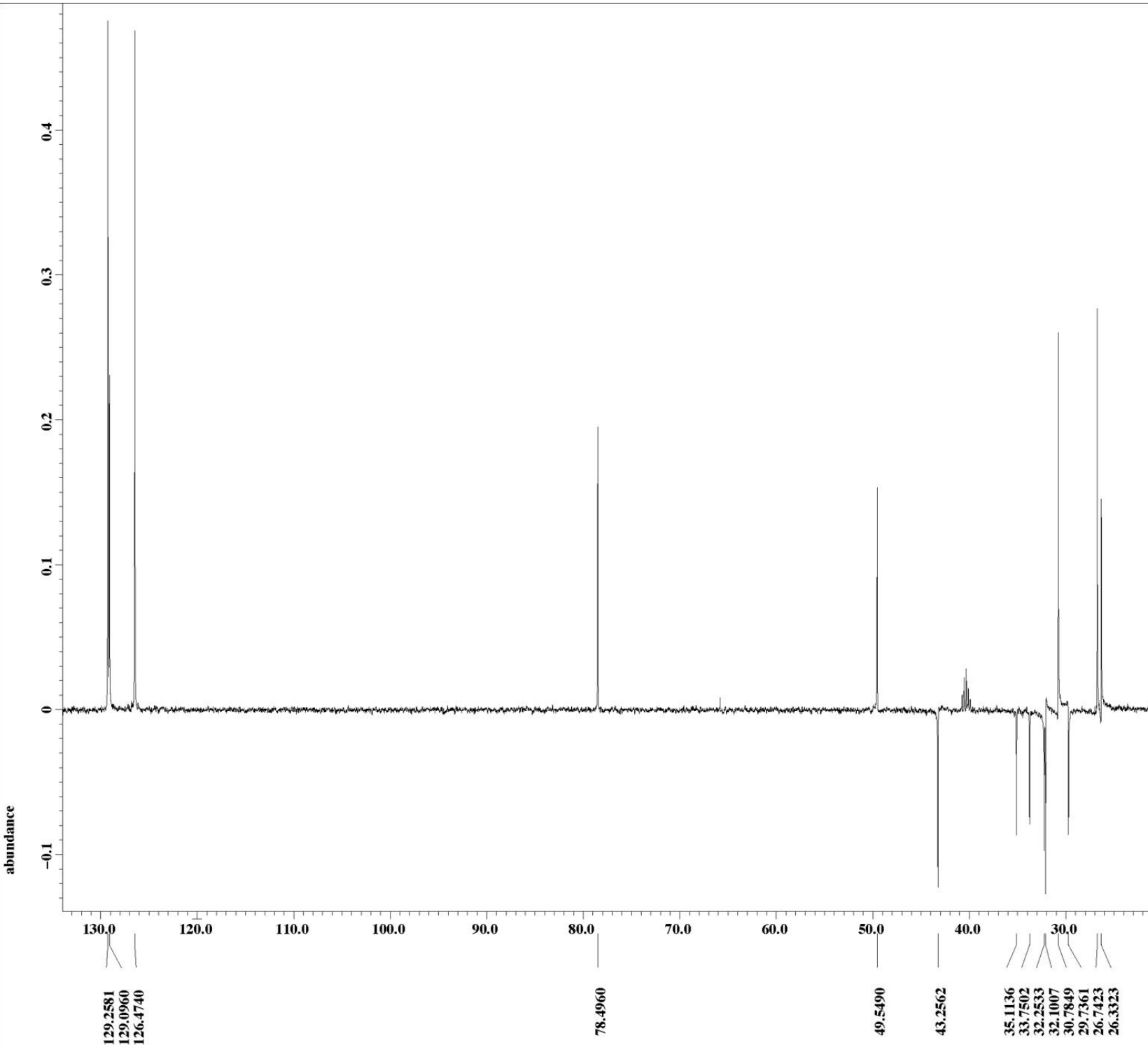
2c

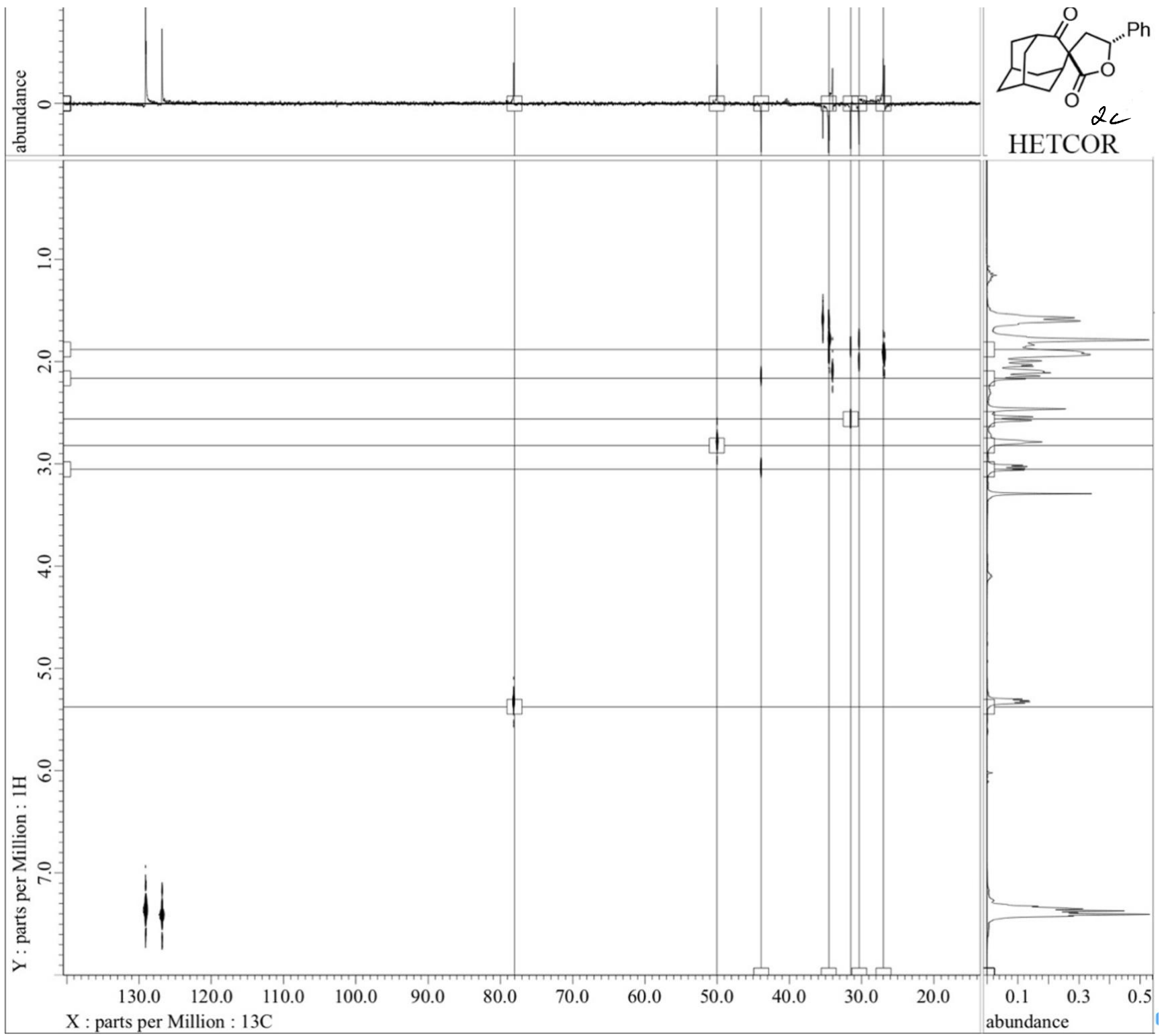
Filename = TIM_DEPT135_Phspirola
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_PhspirolactoneNa2
 Solvent = DMSO-D6
 Creation_time = 20-JAN-2022 11:20:50
 Revision_time = 10-FEB-2023 15:39:02
 Current_time = 10-FEB-2023 15:39:26

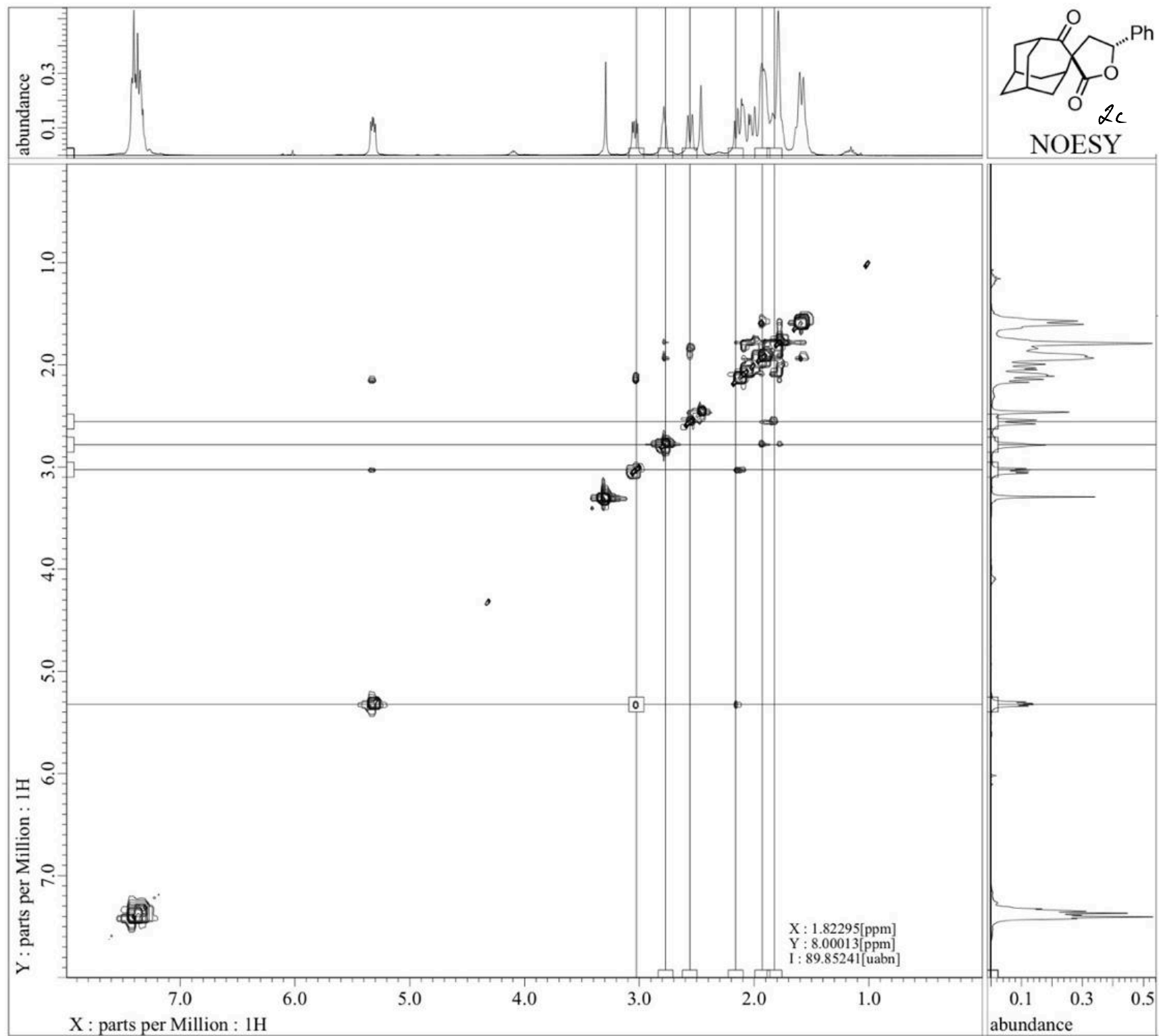
Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

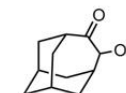
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 786
 Total_scans = 786

X_acq_time = 1.04333312[s]
 X_atn = 5.2[dB]
 X_pulse = 13.87[us]
 Irr_atn = 3.5[dB]
 Irr_atn_dec = 29.907[dB]
 Irr_noise = WALTZ
 Irr_pulse = 5.5[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 8.25[us]
 Temp_get = 0[dc]









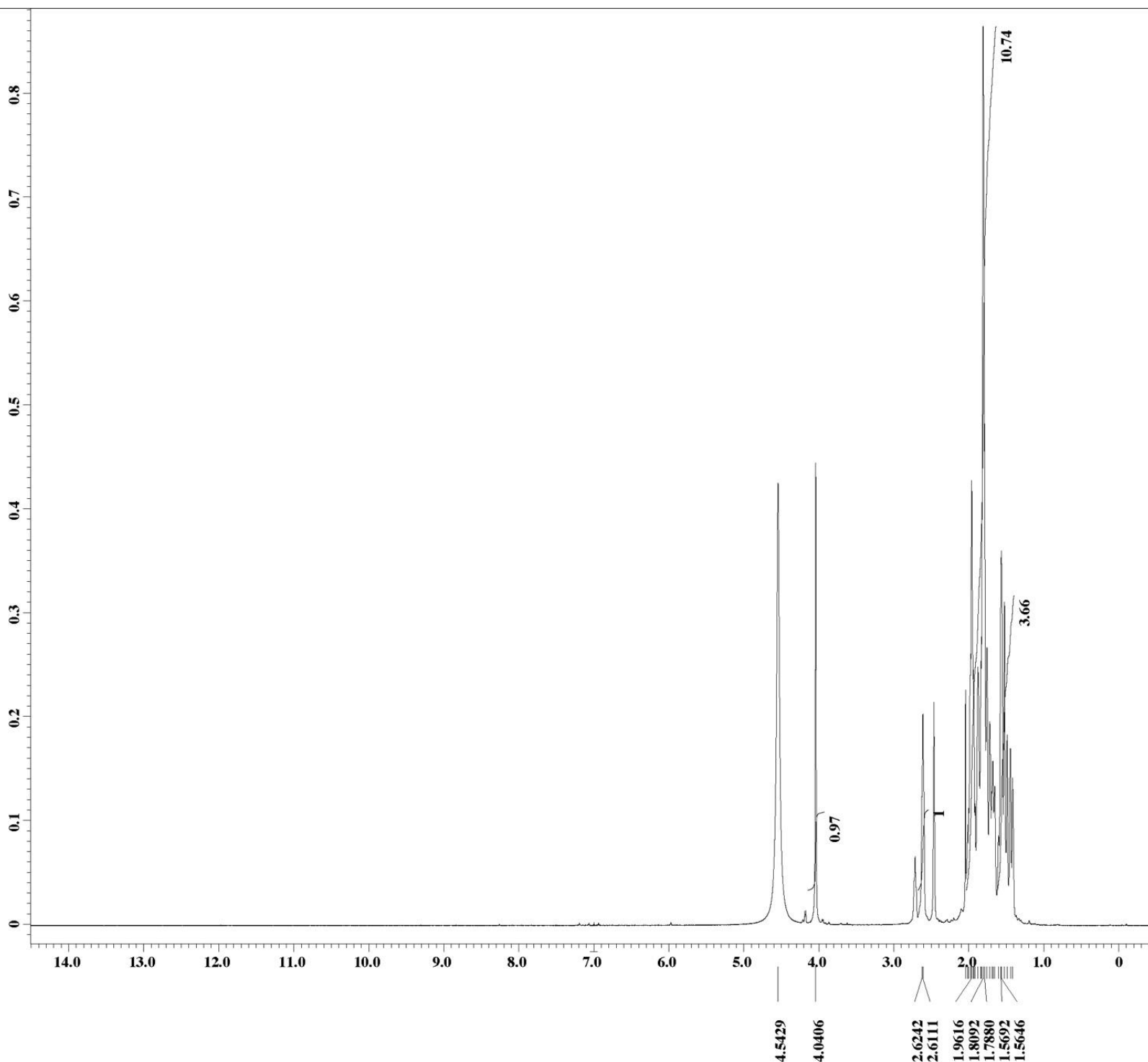
4

Filename = TIM_1H_213-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_213
 Solvent = DMSO-D6
 Creation_time = 14-MAY-2019 08:55:58
 Revision_time = 13-FEB-2023 11:19:39
 Current_time = 13-FEB-2023 11:19:57

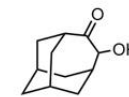
Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 11.9[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 5.95[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 36
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 0[dc]



X : parts per Million : 1H



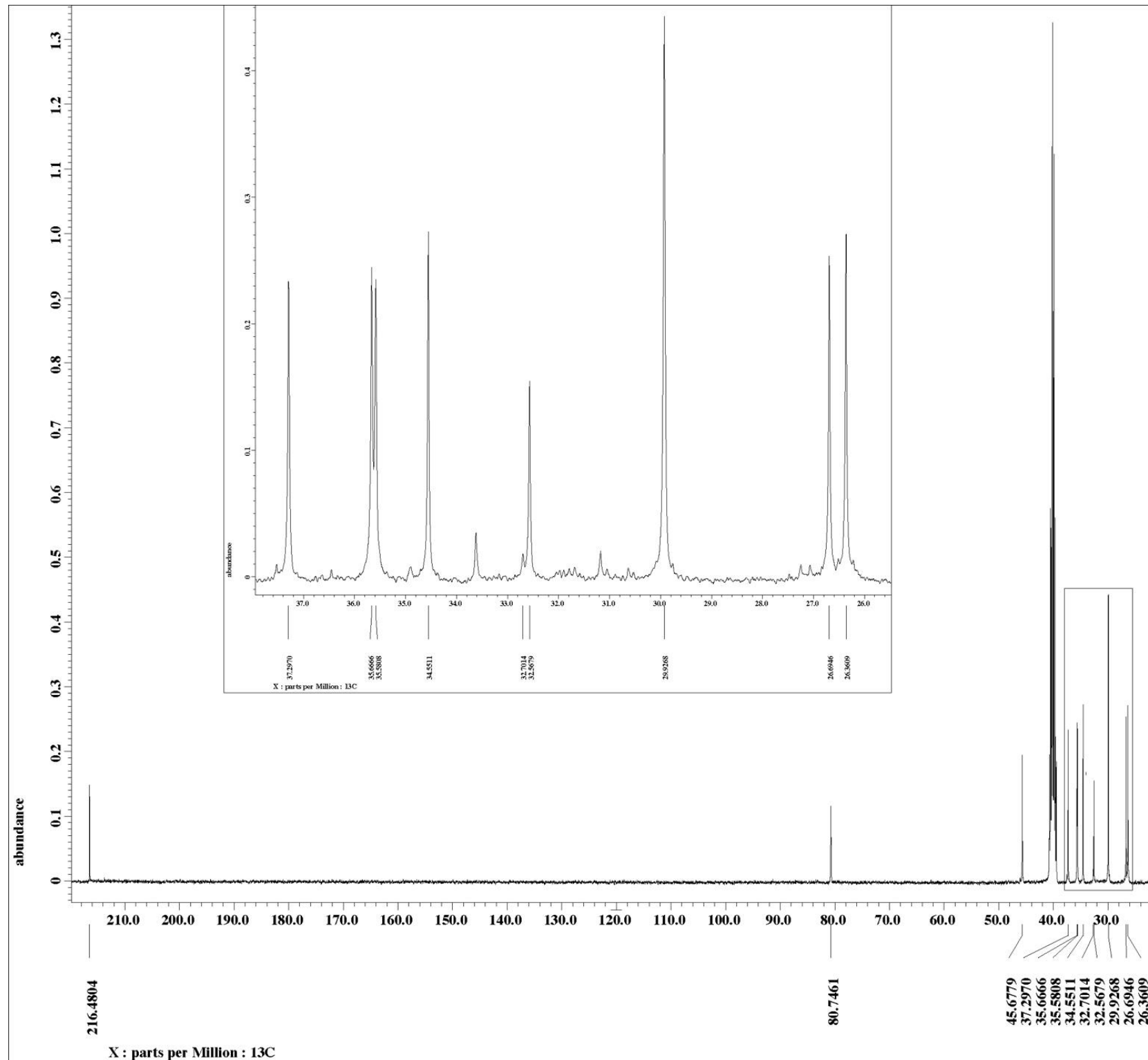
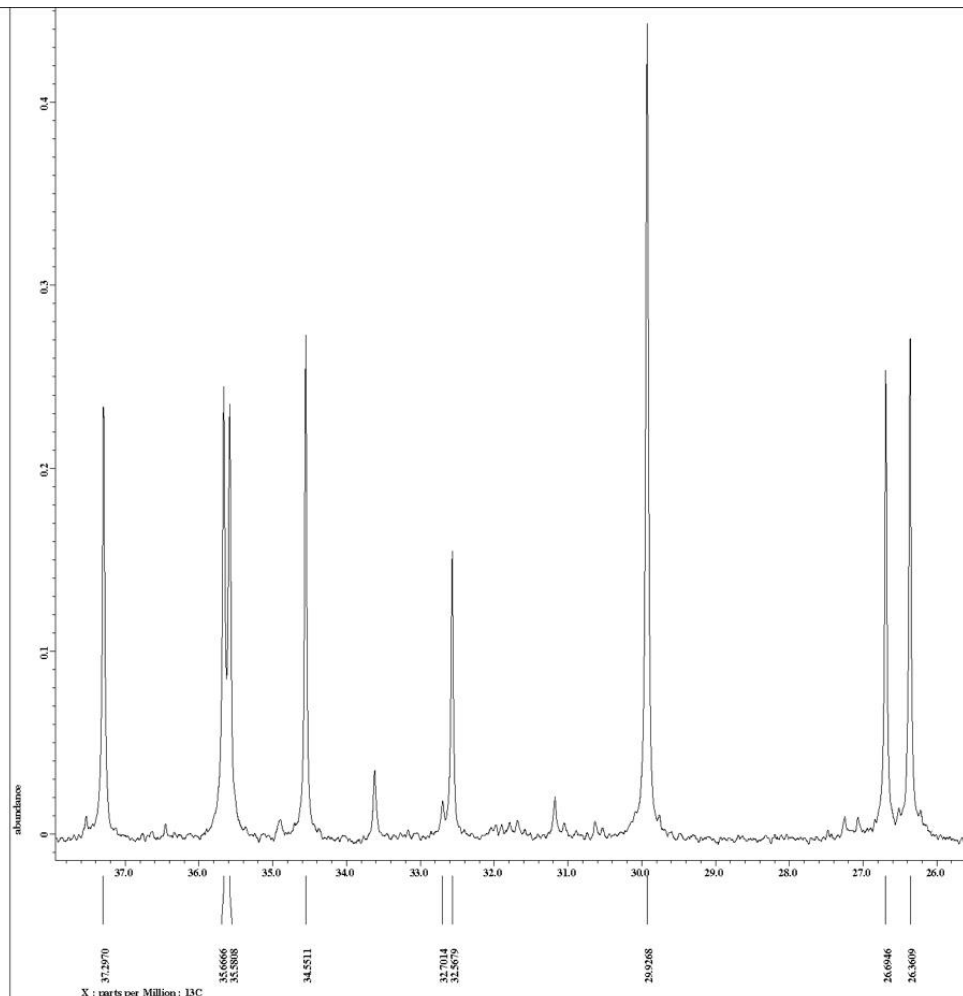
4

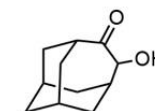
Filename = TIM_13C_213-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_213
 Solvent = DMSO-D6
 Creation_time = 14-MAY-2019 10:38:20
 Revision_time = 13-FEB-2023 11:21:19
 Current_time = 13-FEB-2023 11:21:59

Comment = single pulse decouple
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.0433312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 2000
 Total_scans = 2000

X_90_width = 8.16[us]
 X_acq_time = 1.0433312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 56
 Relaxation_delay = 2[s]
 Repetition_time = 3.0433312[s]
 Temp_get = 0[dc]





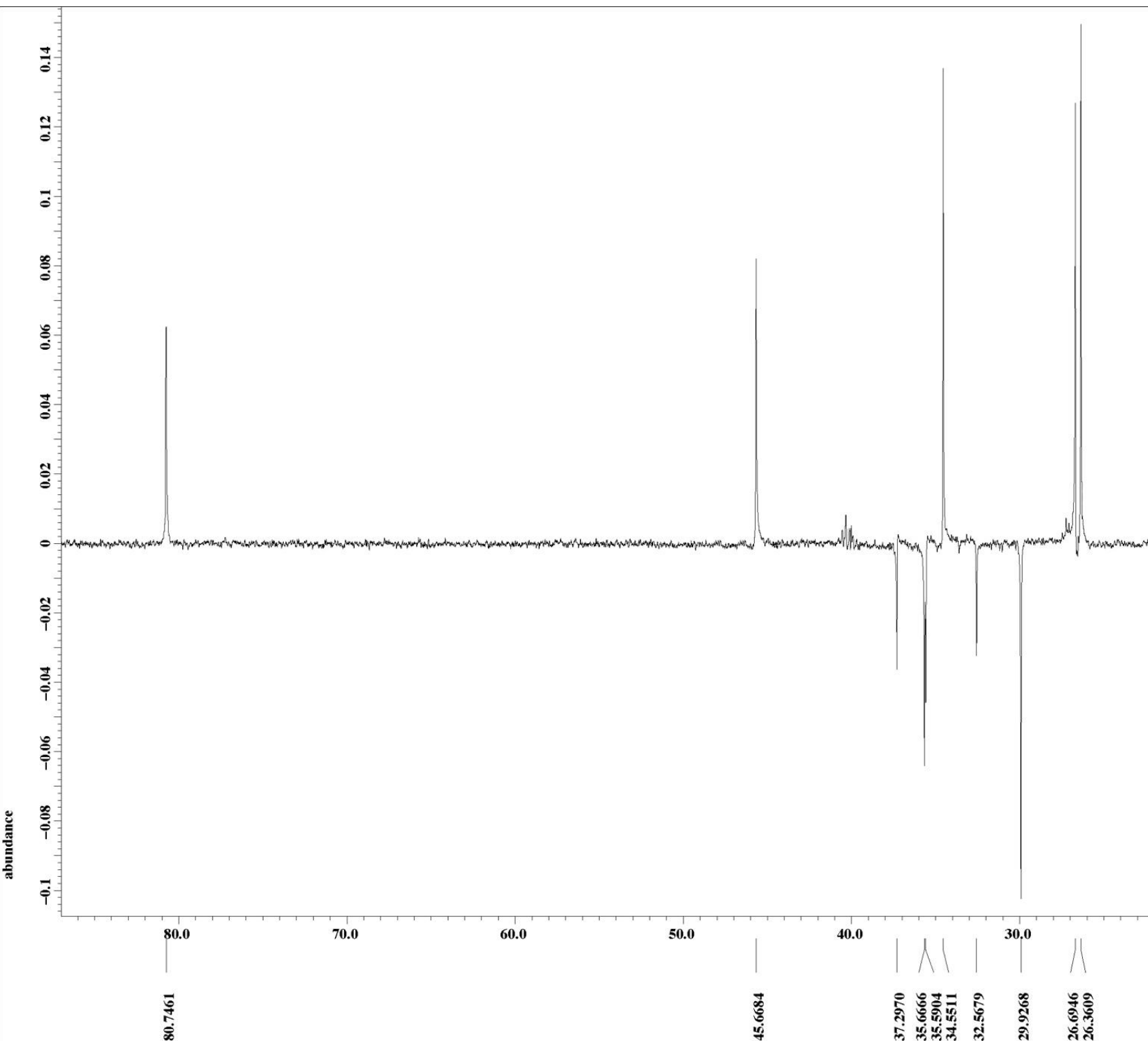
4

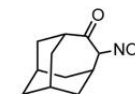
Filename = TIM_DEPT135_213-5.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_213
 Solvent = DMSO-D6
 Creation_time = 14-MAY-2019 11:29:37
 Revision_time = 13-FEB-2023 11:27:12
 Current_time = 13-FEB-2023 11:27:44

Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1000
 Total_scans = 1000

X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 0[dc]





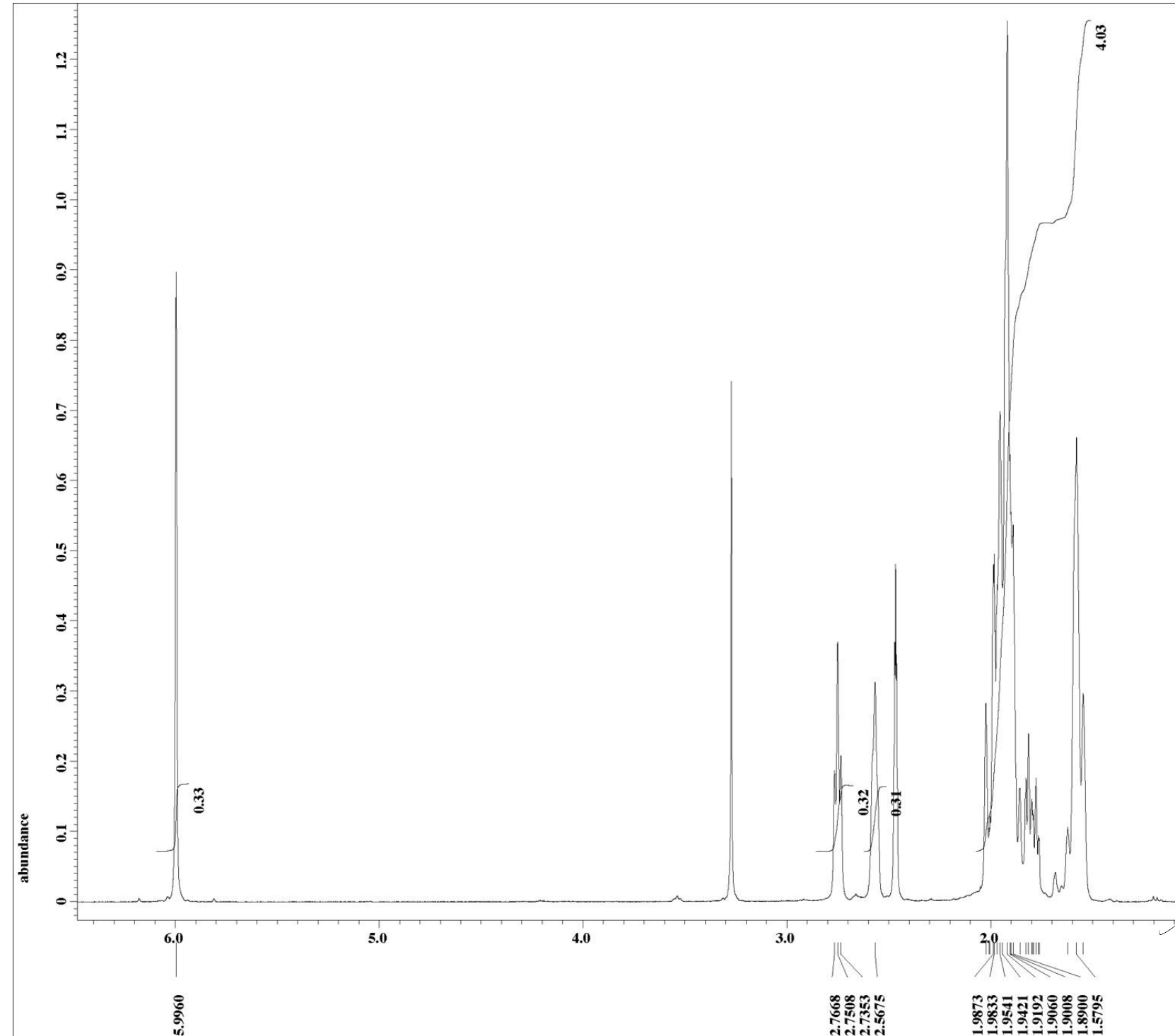
5

Filename = TIM_1H_27-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_27
 Solvent = DMSO-D6
 Creation_time = 17-APR-2017 17:55:02
 Revision_time = 13-FEB-2023 13:05:00
 Current_time = 13-FEB-2023 13:05:22

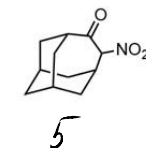
Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 11.9[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 5.95[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 38
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 26.3[dc]



X : parts per Million : 1H

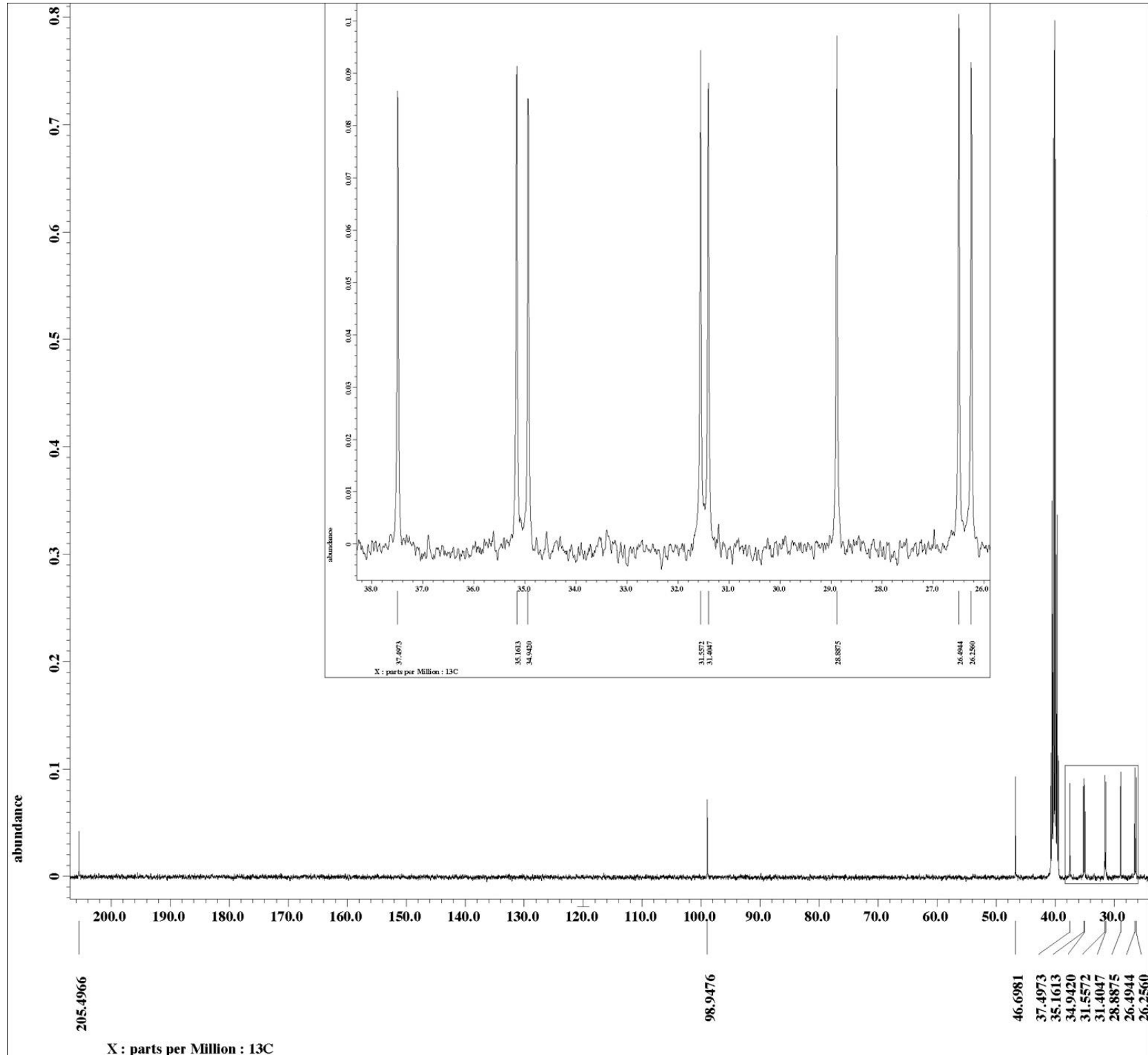
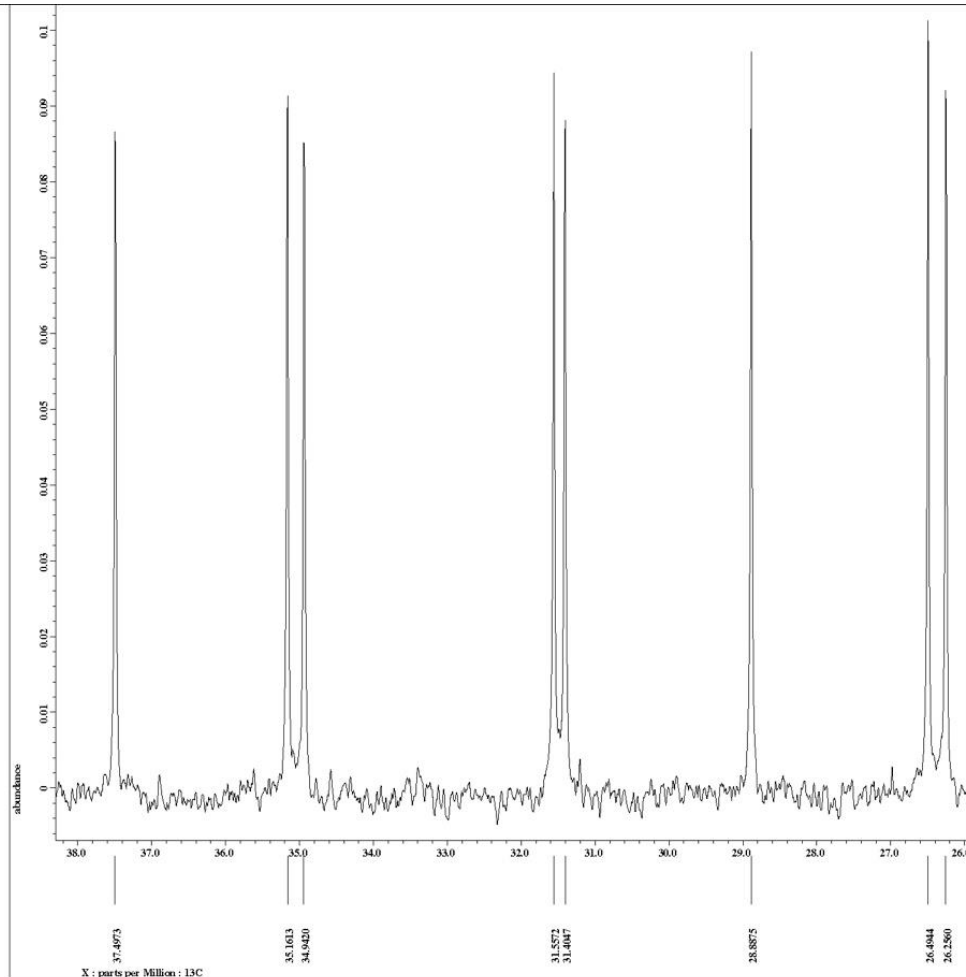


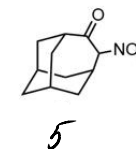
Filename = TIM_13C_27-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_27
 Solvent = DMSO-D6
 Creation_time = 17-APR-2017 18:17:38
 Revision_time = 13-FEB-2023 13:05:47
 Current_time = 13-FEB-2023 13:06:17

Comment = single pulse decouple
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 269
 Total_scans = 269

X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 26.5[dc]



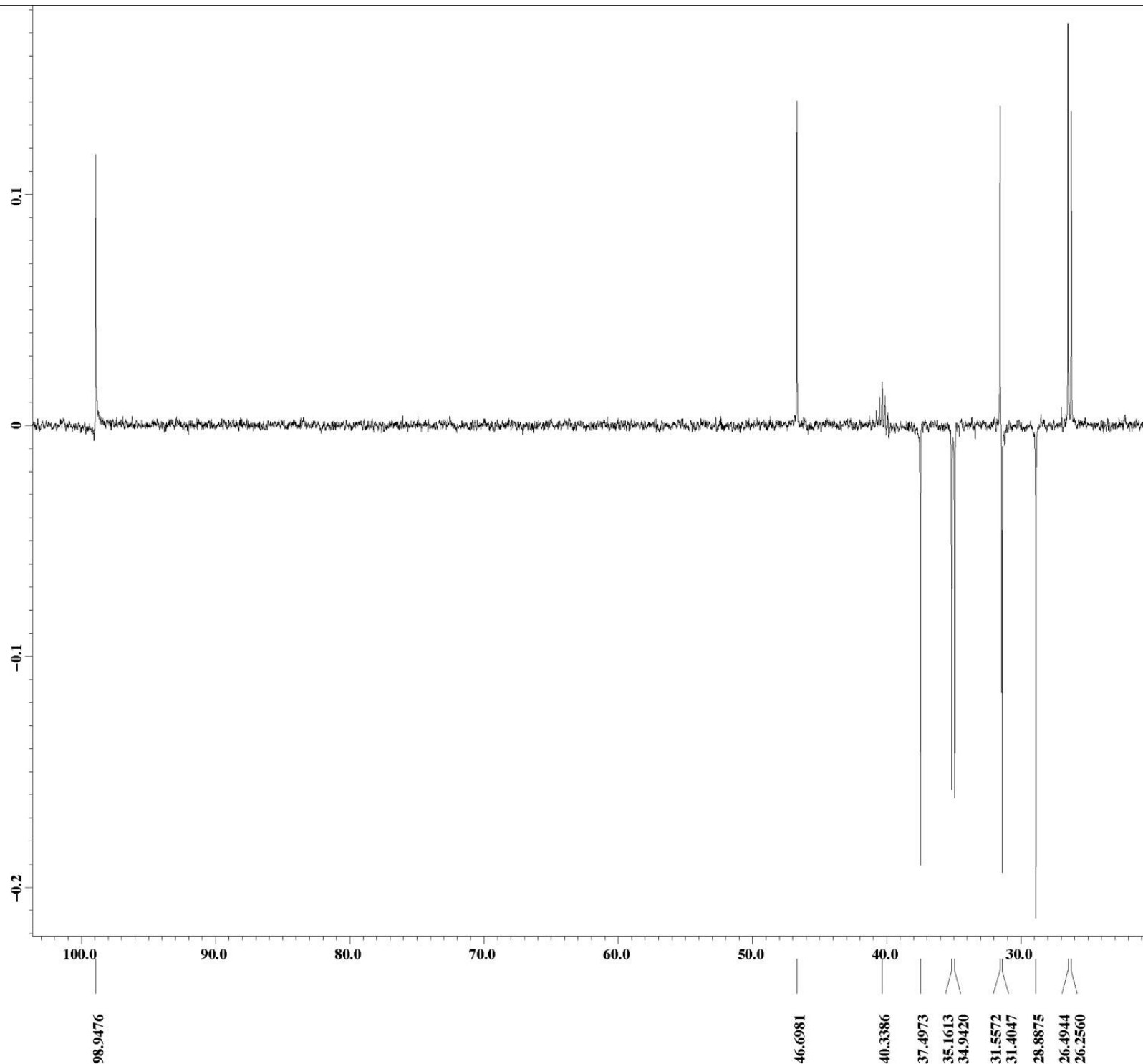


Filename = TIM_DEPT135_27-5.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_27
 Solvent = DMSO-D6
 Creation_time = 17-APR-2017 18:29:20
 Revision_time = 13-FEB-2023 13:06:46
 Current_time = 13-FEB-2023 13:07:06

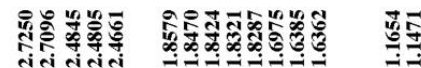
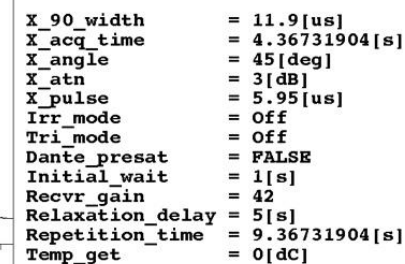
Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 223
 Total_scans = 223

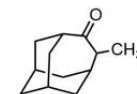
X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 26.4[dC]



X : parts per Million : 13C



X : parts per Million : 1H



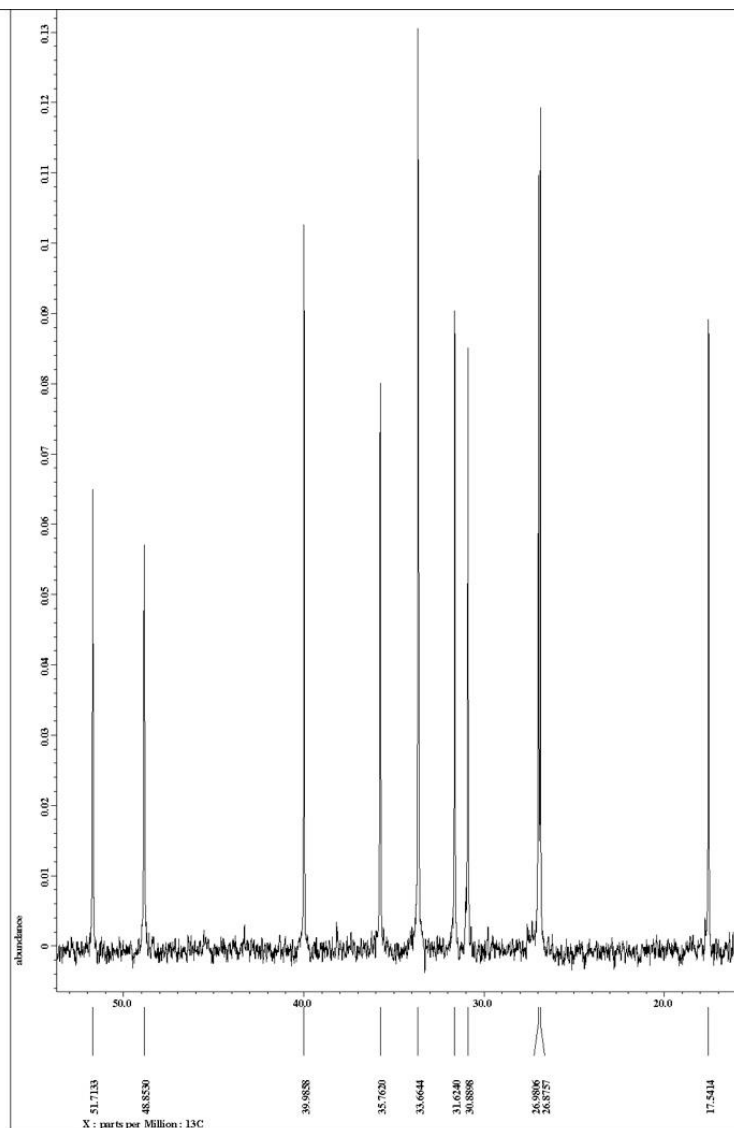
6

Filename = TIM_13C_248-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_248
 Solvent = CHLOROFORM-D
 Creation_time = 3-MAR-2020 09:38:51
 Revision_time = 13-FEB-2023 13:01:47
 Current_time = 13-FEB-2023 13:02:10

 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.0433312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1000
 Total_scans = 1000

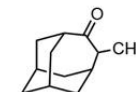
 X_90_width = 8.16[us]
 X_acq_time = 1.0433312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Repetition_time = 3.0433312[s]
 Temp_get = 0[dc]



219.7699

51.7133
48.8530
39.9858
35.7620
33.6644
31.6240
30.8898
26.9806
26.8757
17.5414

X : parts per Million : 13C



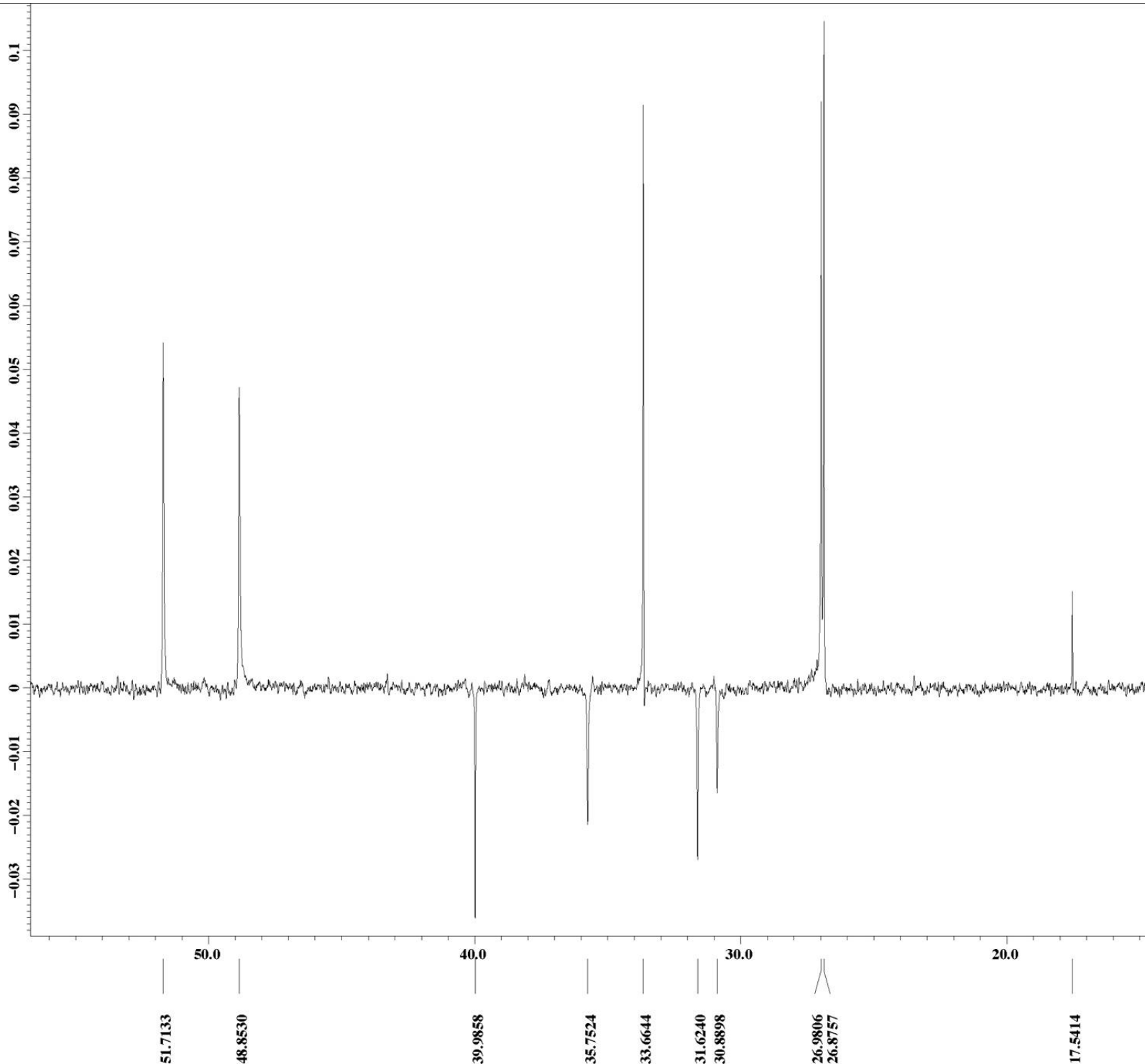
6

Filename = TIM_DEPT135_248-2.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM 248
 Solvent = CHLOROFORM-D
 Creation_time = 3-MAR-2020 10:30:08
 Revision_time = 13-FEB-2023 13:02:16
 Current_time = 13-FEB-2023 13:02:34

 Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1000
 Total_scans = 1000

 X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 0[dc]

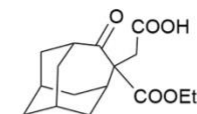


X : parts per Million : 13C



```
X_90_width      = 11.9[us]
X_acq_time      = 4.36731904[s]
X_angle         = 45[deg]
X_atn           = 3[dB]
X_pulse         = 5.95[us]
Irr_mode        = Off
Tri_mode        = Off
Dante_presat    = FALSE
Initial_wait    = 1[s]
Recvr_gain      = 40
Relaxation_delay = 5[s]
Repetition_time = 9.36731904[s]
Temp_get        = 22.7[dC]
```





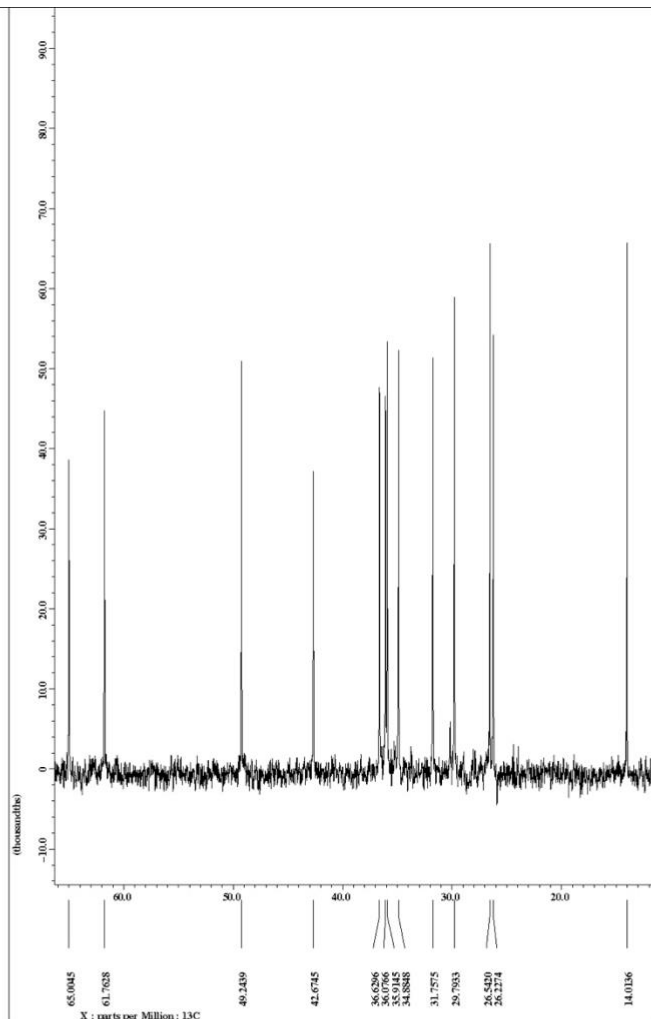
7

Filename = TIM_13C_64-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_64
 Solvent = CHLOROFORM-D
 Creation_time = 25-OCT-2017 16:14:58
 Revision_time = 6-JUN-2023 15:28:44
 Current_time = 6-JUN-2023 15:29:13

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1000
 Total_scans = 1000

X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 23[dc]



214.4782

175.4531
172.5927

65.0045
61.7628

49.2439
42.6745

36.6296
36.0766

35.9145
34.8848

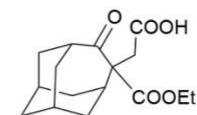
31.7575
29.7933

26.5420
26.2274

14.0136

X : parts per Million : 13C

abundance



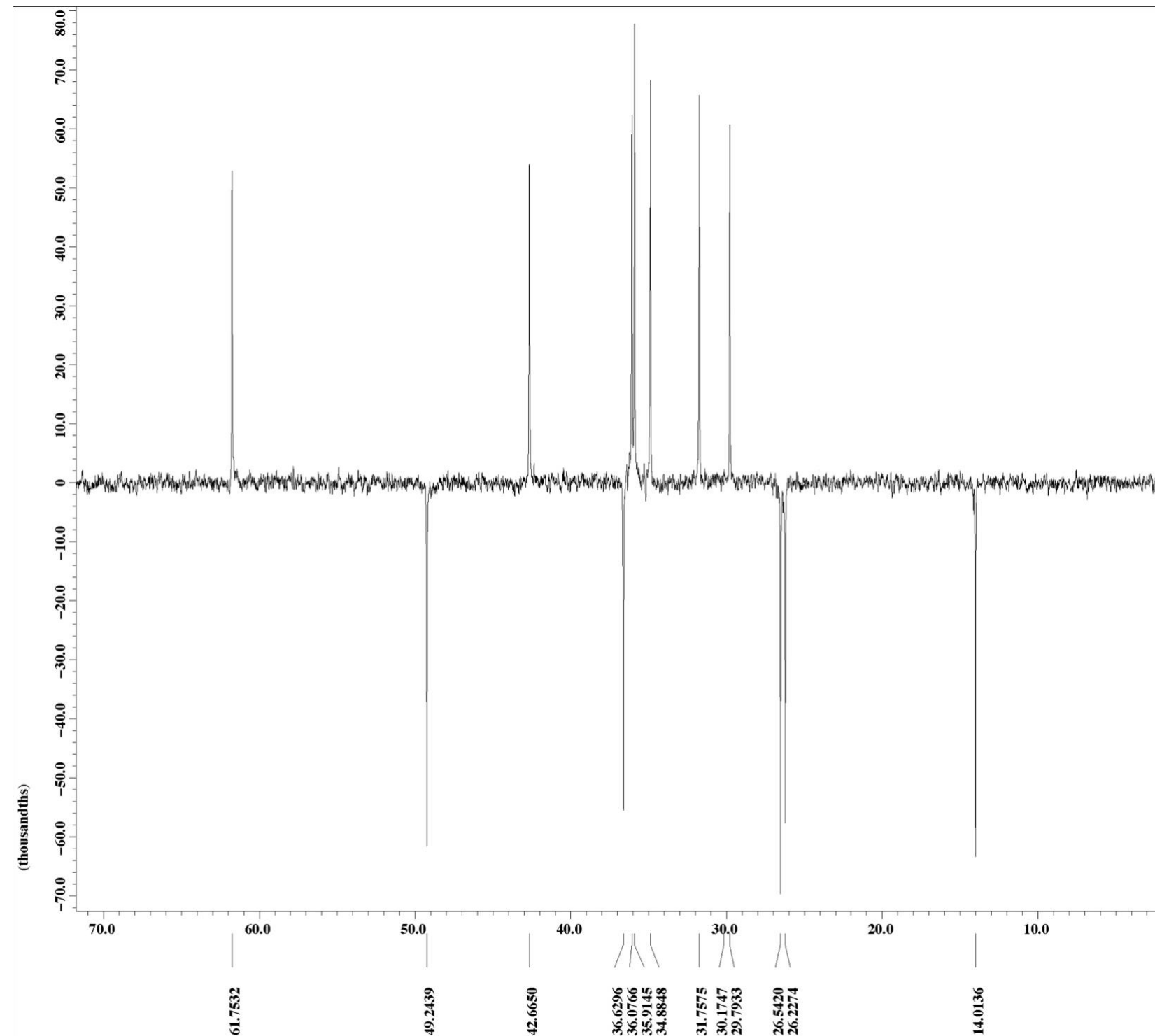
7

Filename = TIM_DEPT135_64-2.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM 64
 Solvent = CHLOROFORM-D
 Creation_time = 25-OCT-2017 16:40:46
 Revision_time = 6-JUN-2023 15:27:38
 Current_time = 6-JUN-2023 15:27:58

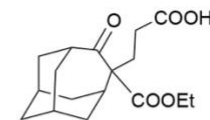
Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 500
 Total_scans = 500

X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 22.9[dc]



X : parts per Million : 13C



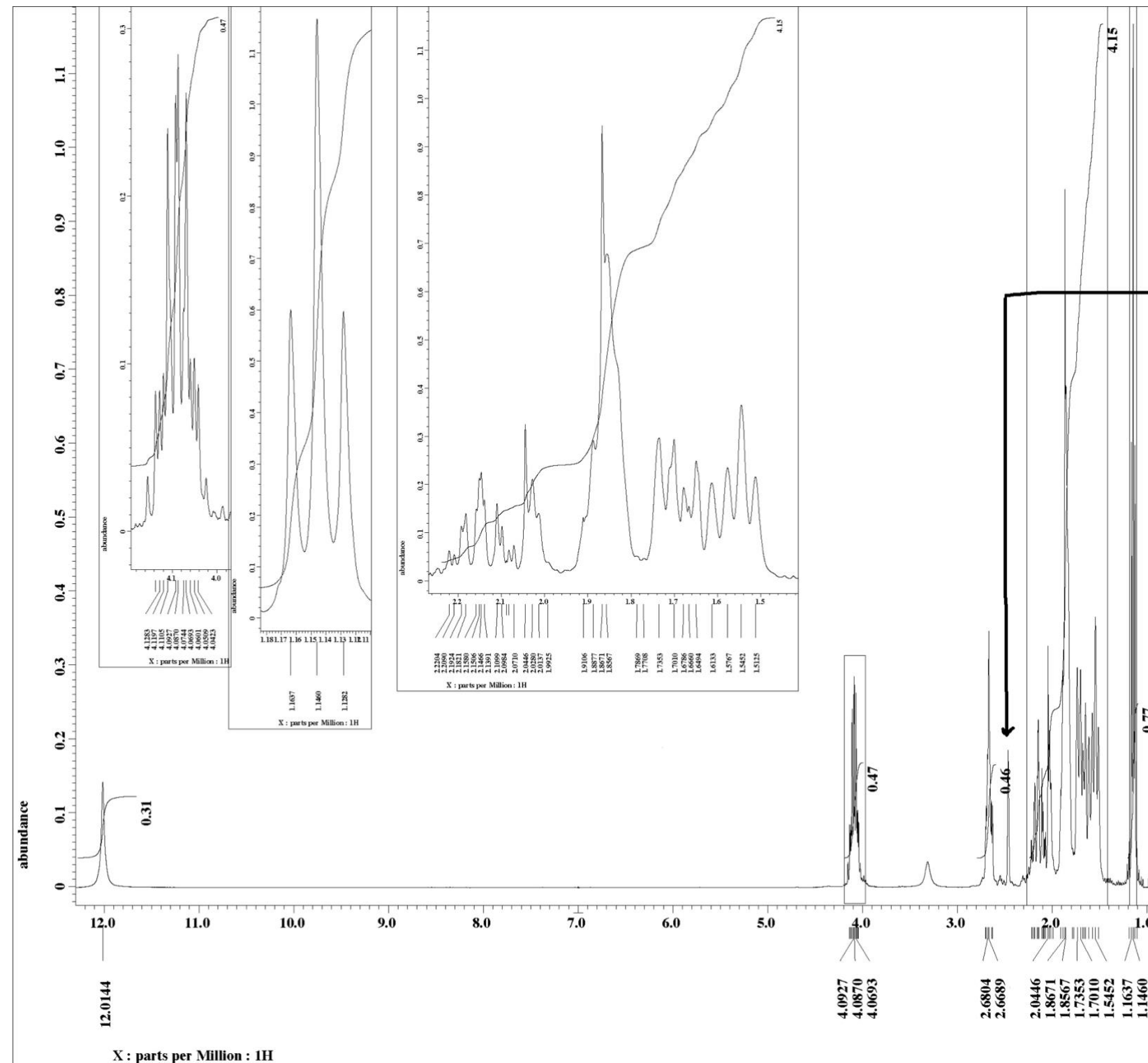
8

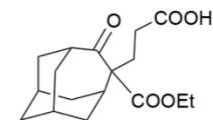
Filename = TIM_1H_240-7.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_240
 Solvent = DMSO-D6
 Creation_time = 17-OCT-2019 13:33:45
 Revision_time = 6-JUN-2023 16:06:47
 Current_time = 6-JUN-2023 16:09:37

Comment = single pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 5.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3.5[dB]
 X_pulse = 2.75[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 22
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 0[dc]





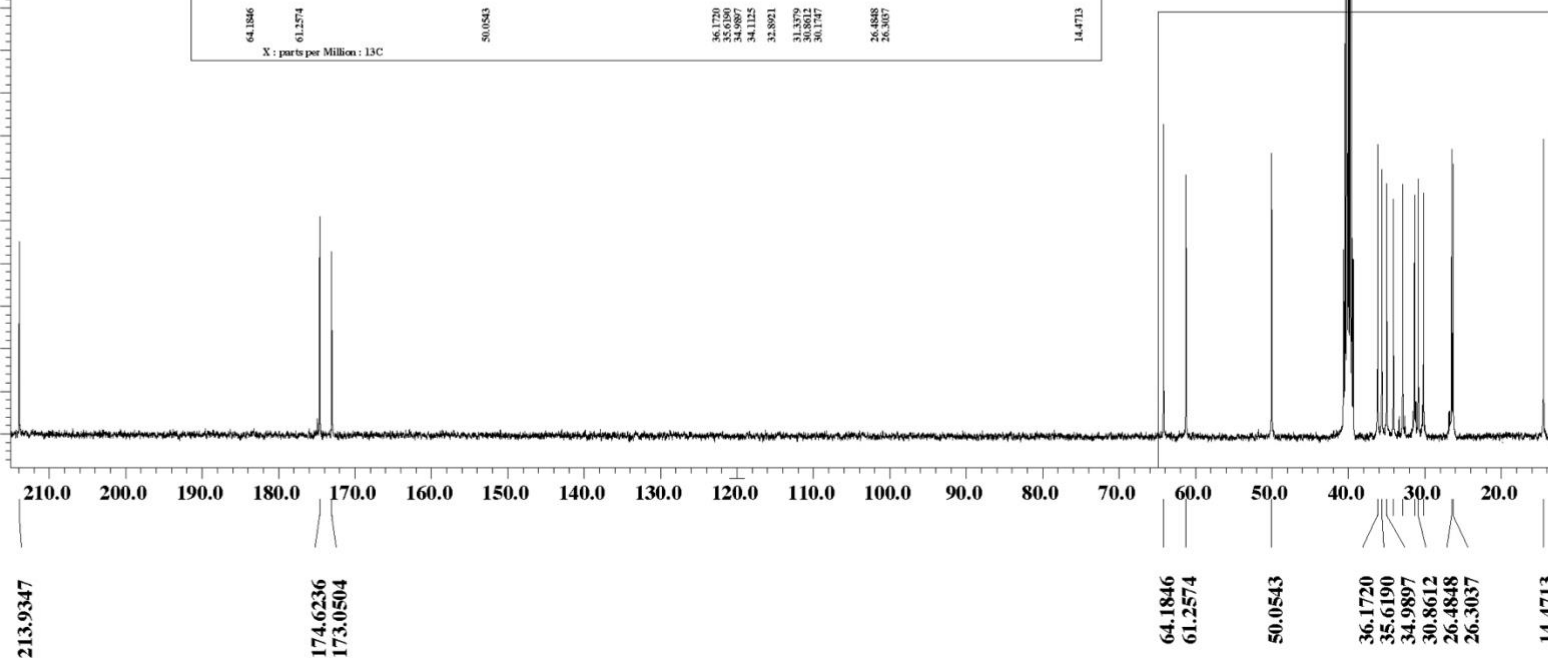
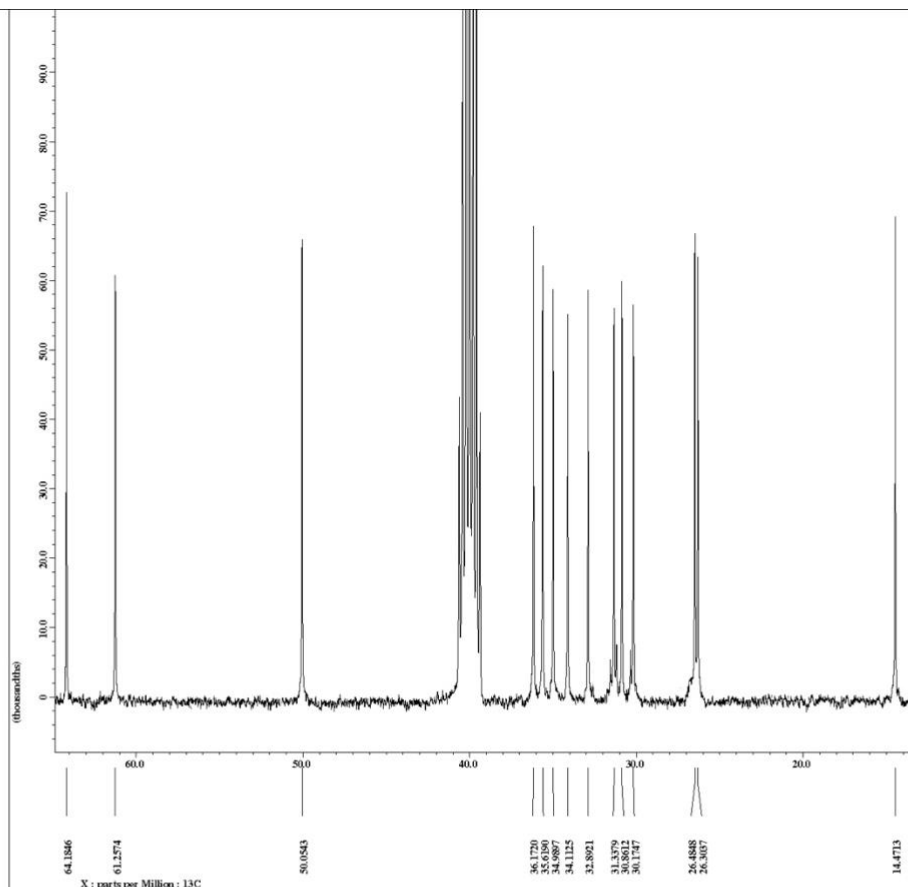
8

Filename = TIM_13C_240-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_240
 Solvent = DMSO-D6
 Creation_time = 17-OCT-2019 16:08:28
 Revision_time = 6-JUN-2023 15:48:54
 Current_time = 6-JUN-2023 15:49:57

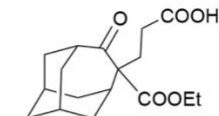
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 3000
 Total_scans = 3000

X_90_width = 13.87[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 5.2[dB]
 X_pulse = 4.62333333[us]
 Irr_atn_dec = 29.907[dB]
 Irr_atn_noe = 29.907[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 48
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 0[dc]



X : parts per Million : 13C



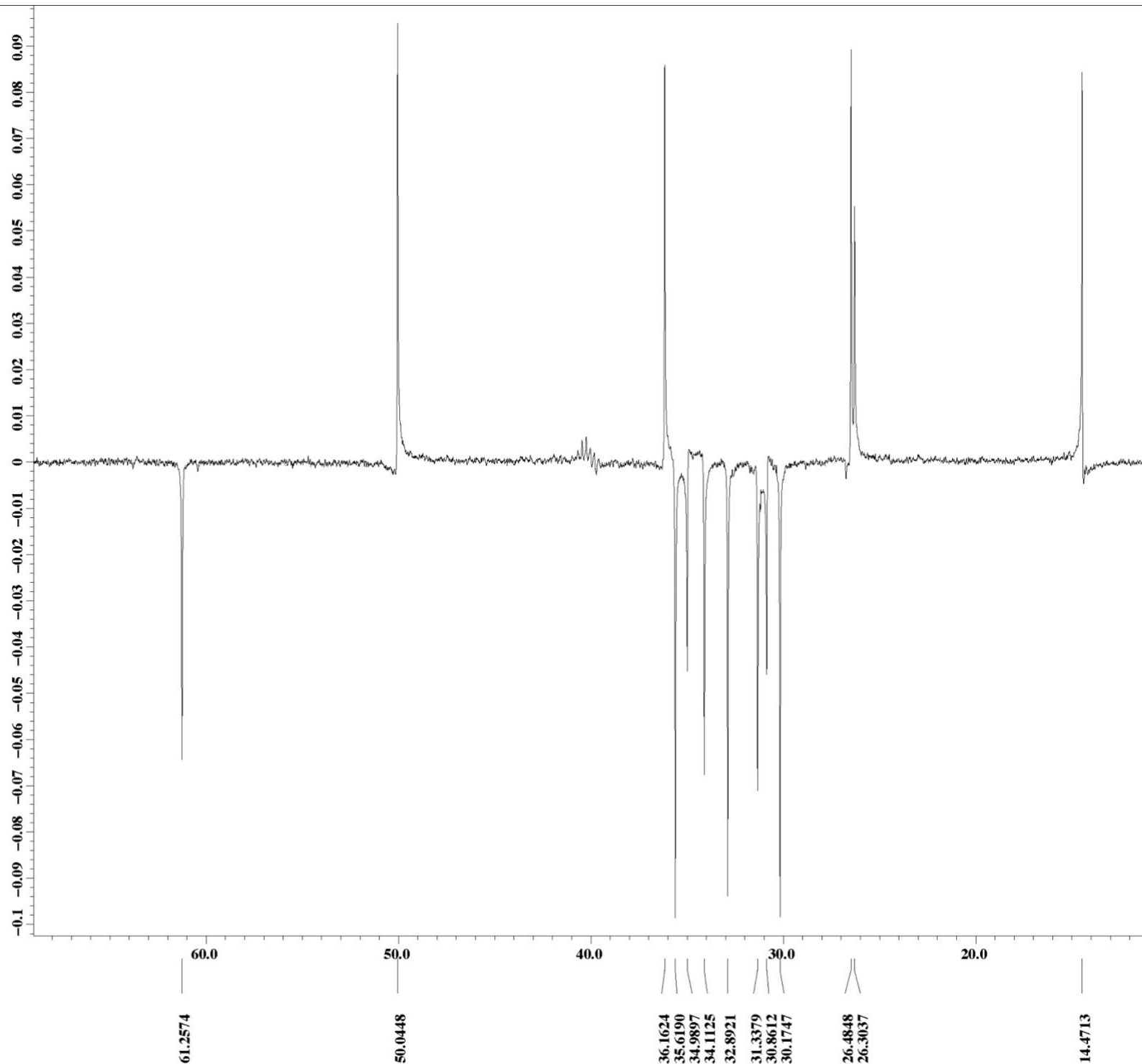
8

Filename = TIM_DEPT135_240-5.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_240
 Solvent = DMSO-D6
 Creation_time = 17-OCT-2019 17:50:42
 Revision_time = 6-JUN-2023 15:50:36
 Current_time = 6-JUN-2023 15:52:46

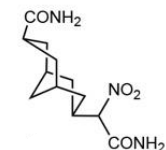
Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 2000
 Total_scans = 2000

X_acq_time = 1.04333312[s]
 X_atn = 5.2[dB]
 X_pulse = 13.87[us]
 Irr_atn = 3.5[dB]
 Irr_atn_dec = 29.907[dB]
 Irr_noise = WALTZ
 Irr_pulse = 5.5[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 8.25[us]
 Temp_get = 0[dC]



X : parts per Million : 13C



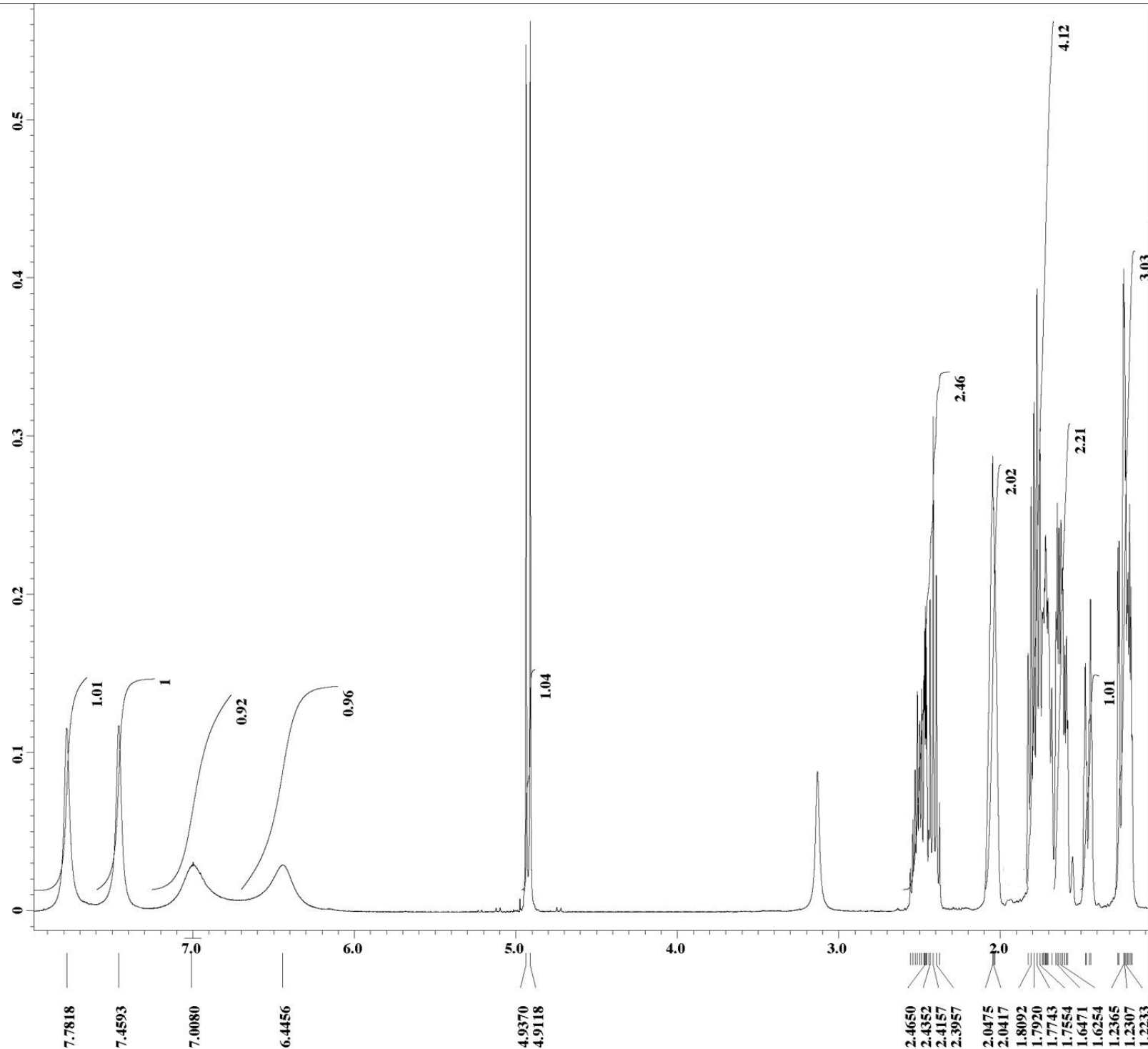
9

Filename = TIM_1H_195_70deg-4.jd
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_195_70deg
 Solvent = DMSO-D6
 Creation_time = 27-MAR-2019 05:22:32
 Revision_time = 16-JAN-2023 11:52:36
 Current_time = 16-JAN-2023 11:53:09

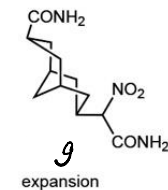
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 11.9[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 5.95[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 30
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 70[dc]



X: parts per Million : 1H

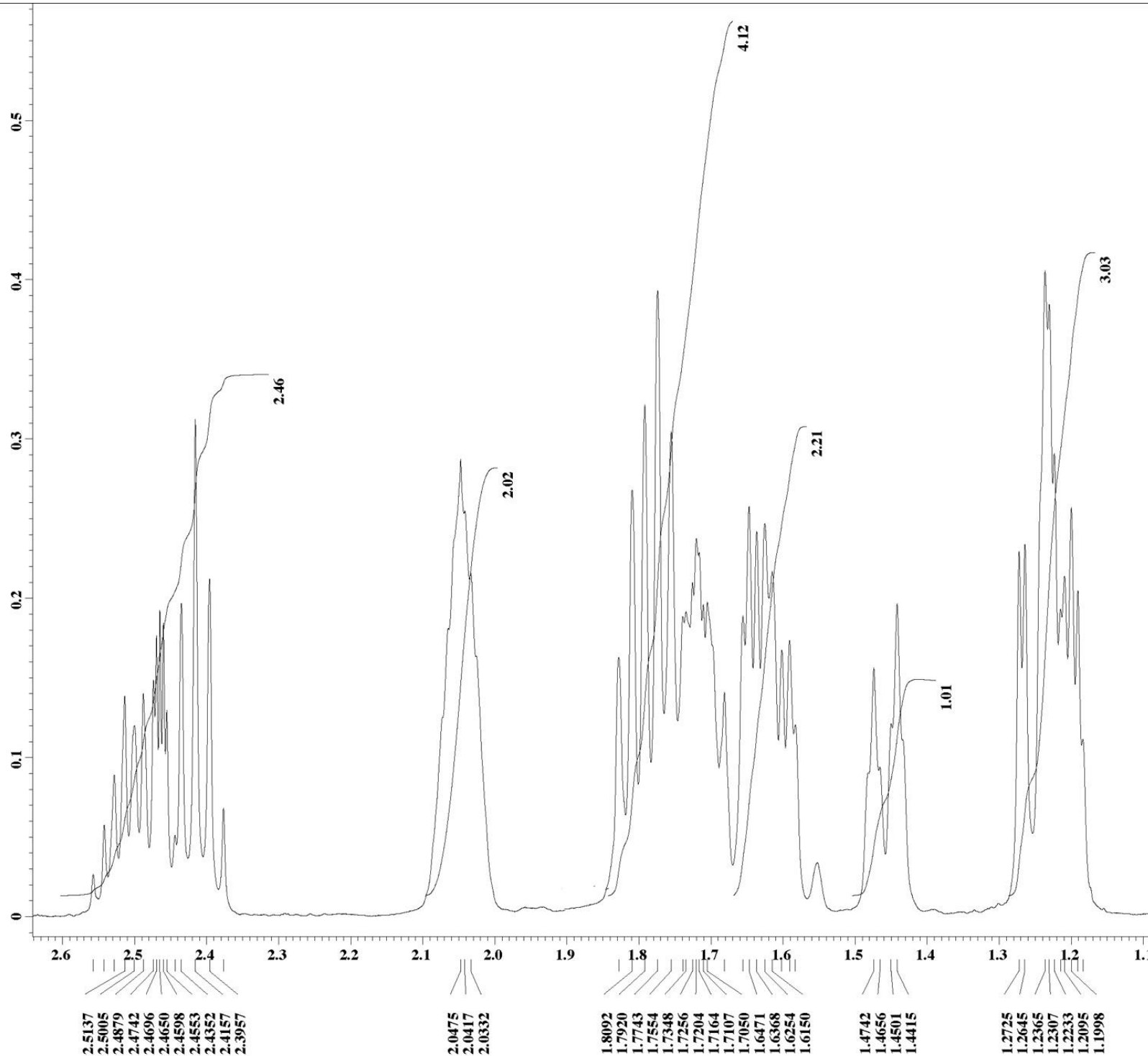


Filename = TIM_1H_195_70deg-4.jd
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_195_70deg
 Solvent = DMSO-D6
 Creation_time = 27-MAR-2019 05:22:32
 Revision_time = 16-JAN-2023 11:52:36
 Current_time = 16-JAN-2023 11:54:03

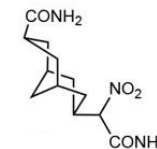
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 11.9[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 5.95[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 30
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 70[dC]



X : parts per Million : 1H



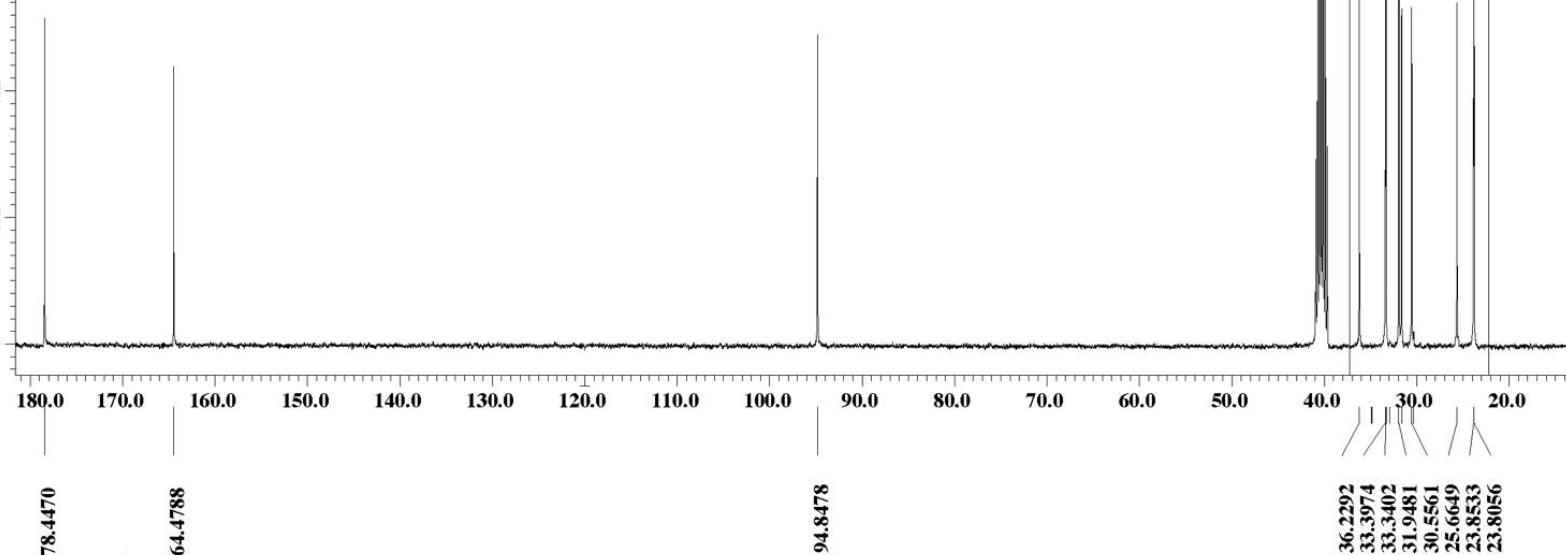
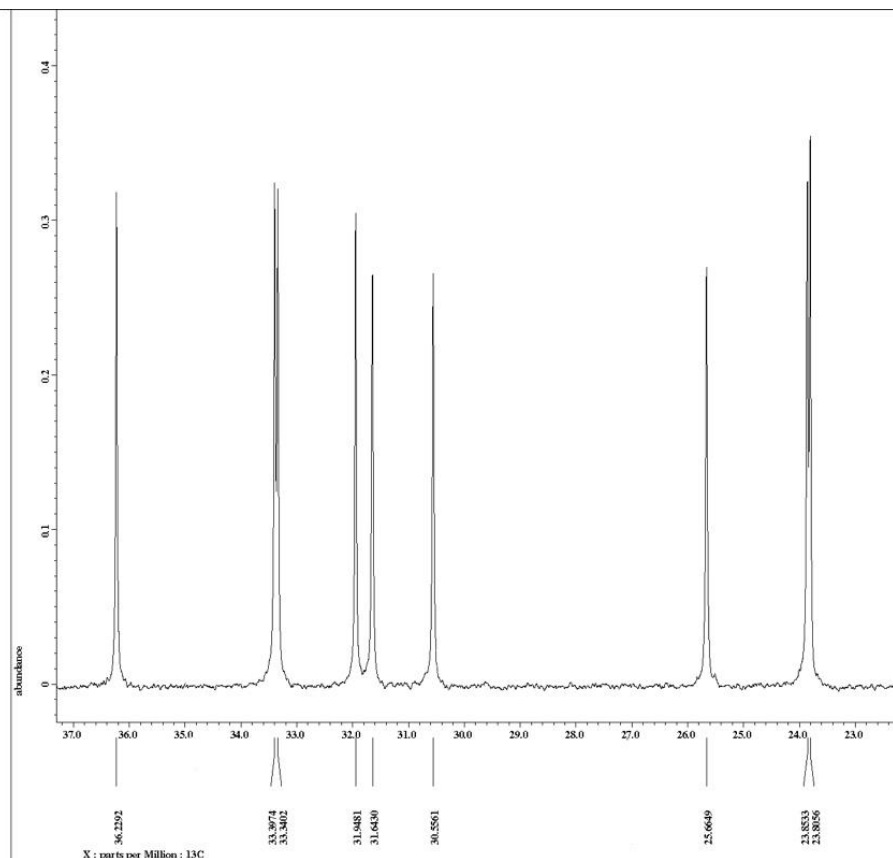
9

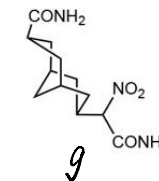
Filename = TIM_13C_195_70deg-3.j
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_195_70deg
 Solvent = DMSO-D6
 Creation_time = 27-MAR-2019 07:06:24
 Revision_time = 16-JAN-2023 11:55:24
 Current_time = 16-JAN-2023 11:56:07

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 2000
 Total_scans = 2000

X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 54
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 70[dc]



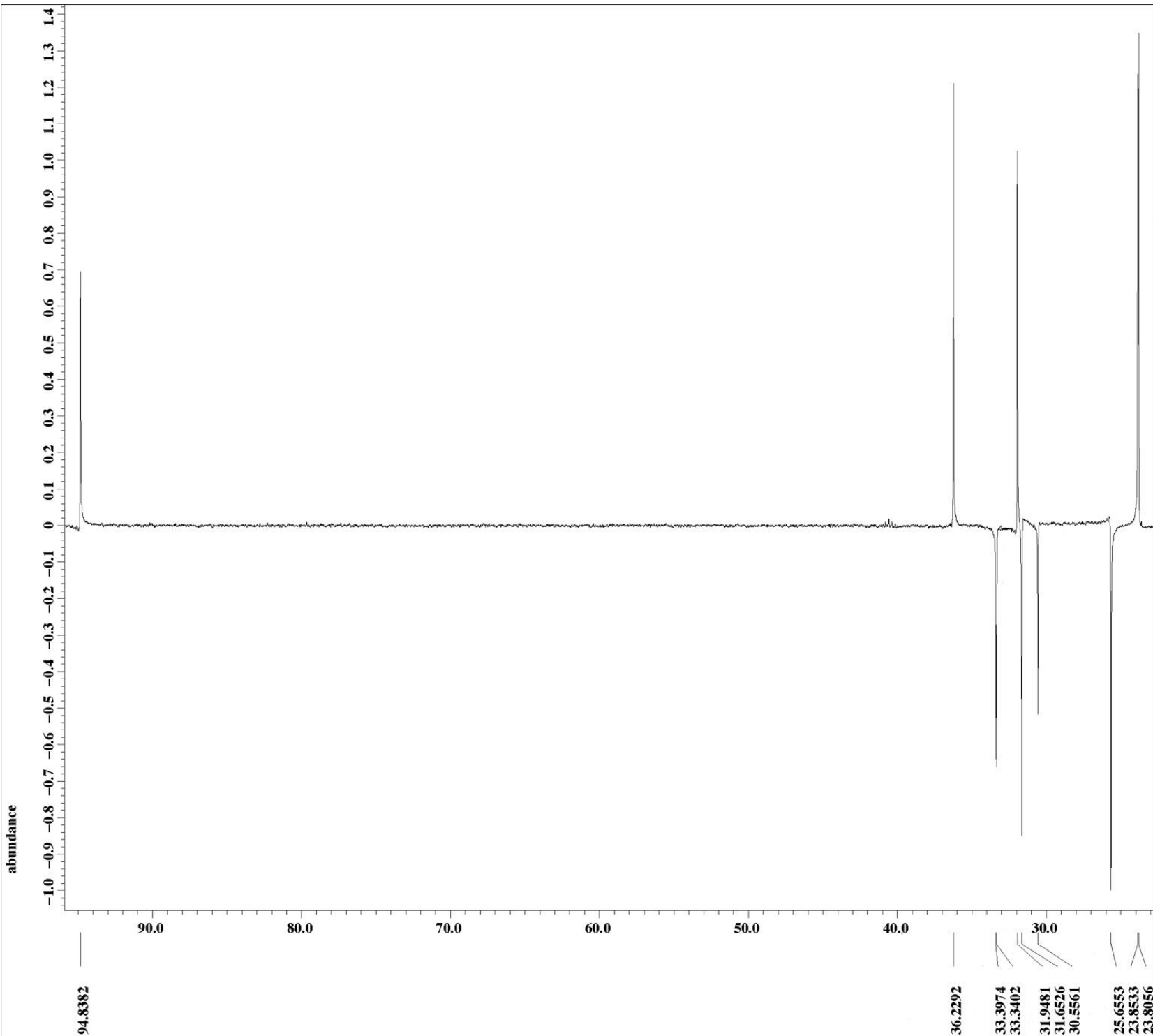


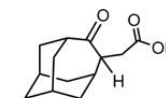
Filename = TIM_DEPT135_195_70deg
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_195_70deg
 Solvent = DMSO-D6
 Creation_time = 27-MAR-2019 07:59:45
 Revision_time = 16-JAN-2023 11:57:26
 Current_time = 16-JAN-2023 11:57:51

Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1000
 Total_scans = 1000

X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 58
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 70[dc]





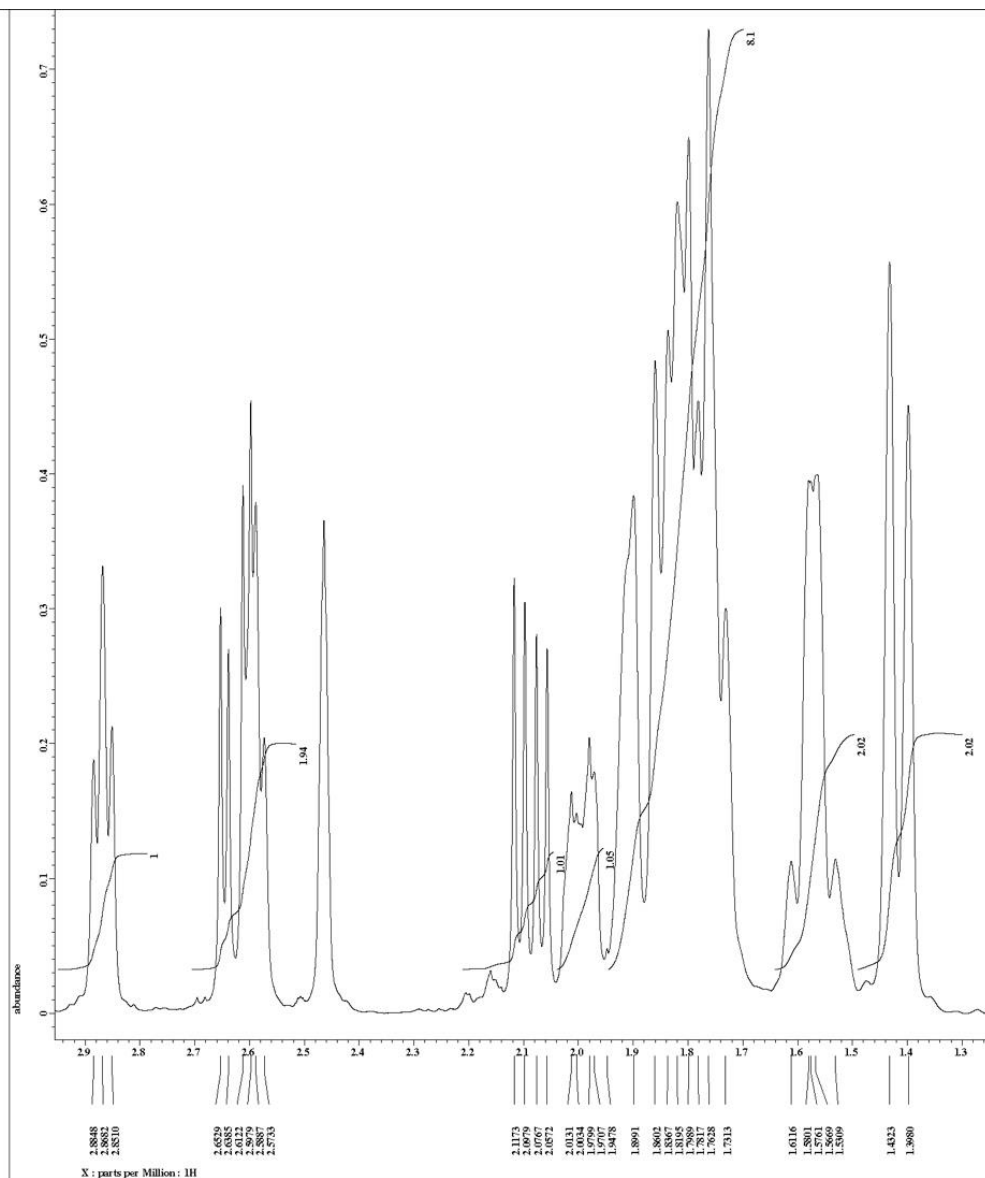
10

Filename = TIM_1H_234-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_234
 Solvent = DMSO-D6
 Creation_time = 20-SEP-2019 08:56:06
 Revision_time = 10-FEB-2023 18:05:41
 Current_time = 10-FEB-2023 18:06:09

Comment = single pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

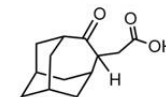
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[Hz]
 X_sweep = 7.5030012[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 5.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3.5[dB]
 X_pulse = 2.75[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 28
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 0[dc]



12.0619
 1.03
 2.8682
 2.6122
 2.5979
 2.5887
 1.8602
 1.8367
 1.8195
 1.7989
 1.7817
 1.7628
 1.4323

X : parts per Million : 1H



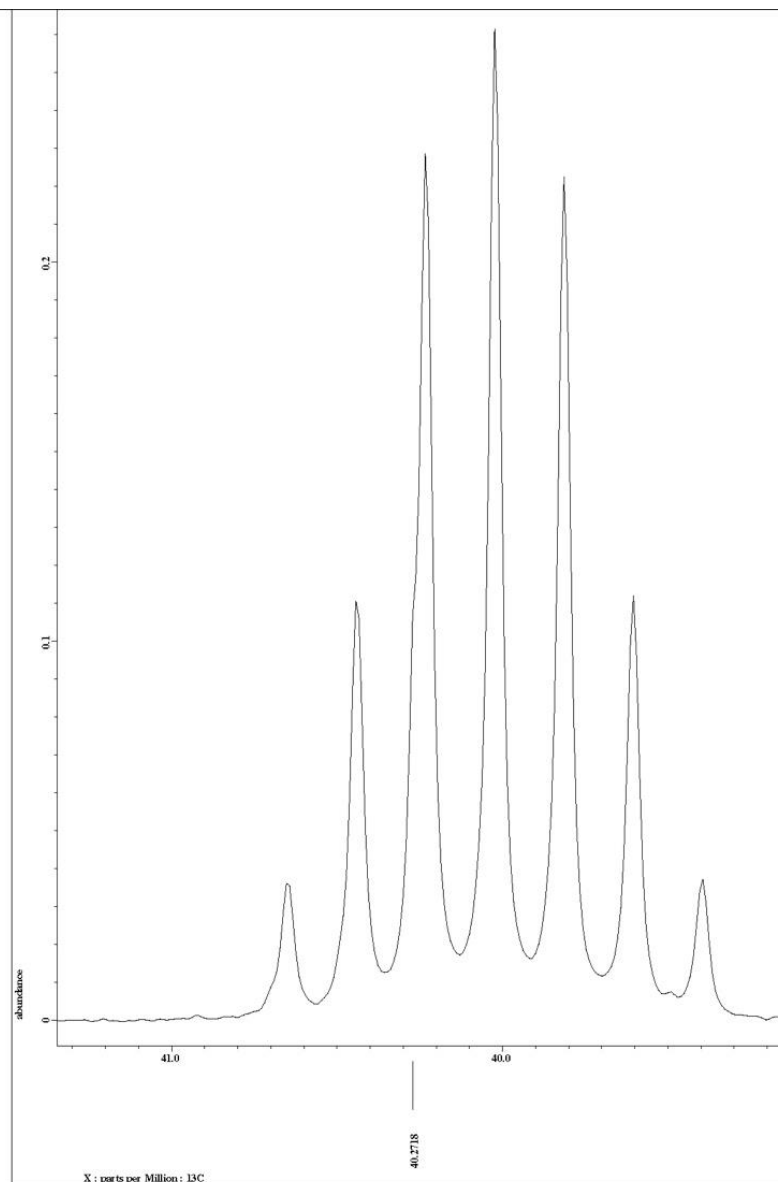
10

Filename = TIM_13C_234-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_234
 Solvent = DMSO-D6
 Creation_time = 20-SEP-2019 11:30:49
 Revision_time = 10-FEB-2023 18:06:55
 Current_time = 10-FEB-2023 18:08:14

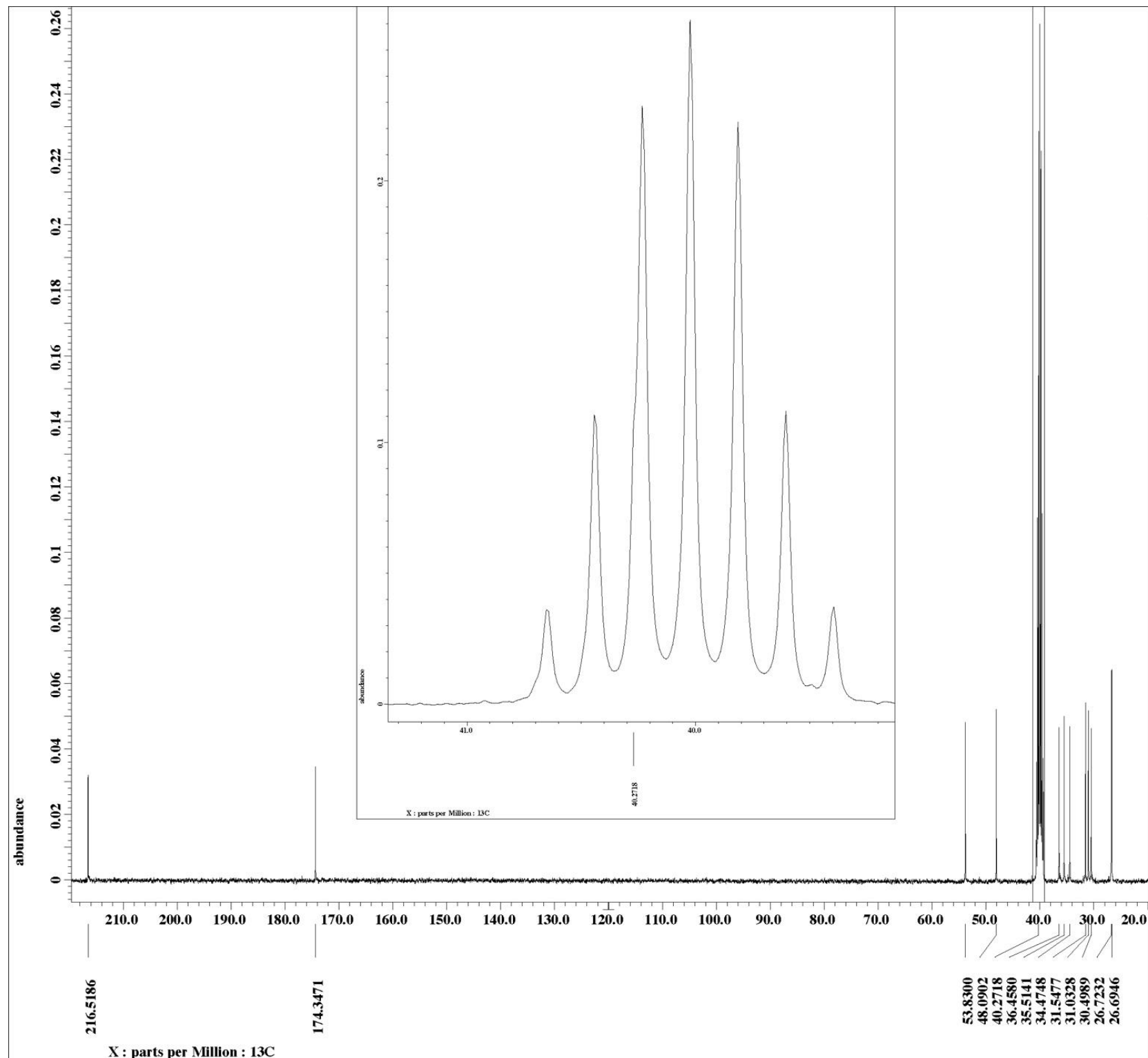
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 3000
 Total_scans = 3000

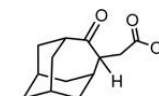
X_90_width = 13.87[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 5.2[dB]
 X_pulse = 4.62333333[us]
 Irr_atn_dec = 29.907[dB]
 Irr_atn_noe = 29.907[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 0[dc]



X : parts per Million : 13C



X : parts per Million : 13C



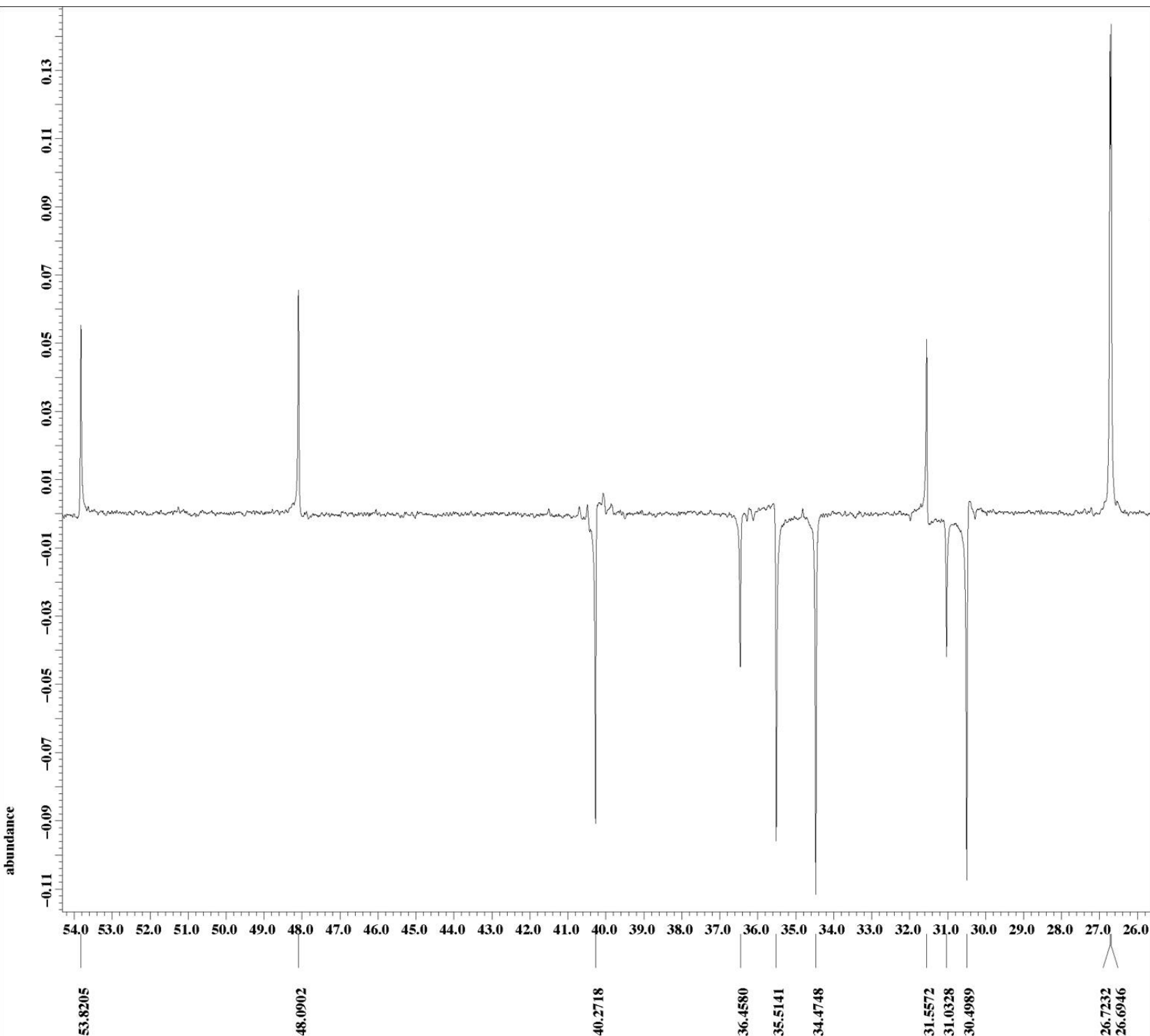
10

Filename = TIM_DEPT135_234-3.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM 234
 Solvent = DMSO-D6
 Creation_time = 20-SEP-2019 13:12:59
 Revision_time = 10-FEB-2023 18:09:23
 Current_time = 10-FEB-2023 18:10:07

Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.0433312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 2000
 Total_scans = 2000

X_acq_time = 1.0433312[s]
 X_atn = 5.2[dB]
 X_pulse = 13.87[us]
 Irr_atn = 3.5[dB]
 Irr_atn_dec = 29.907[dB]
 Irr_noise = WALTZ
 Irr_pulse = 5.5[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 8.25[us]
 Temp_get = 0[dc]





```

Filename      = TIM_1H_270-7.jdf
Author        = delta
Experiment     = single_pulse.ex2
Sample_id     = TIM 270
Solvent       = DMSO-D6
Creation_time  = 6-AUG-2020 19:58:44
Revision_time  = 13-FEB-2023 11:39:13
Current_time   = 13-FEB-2023 11:40:01

```

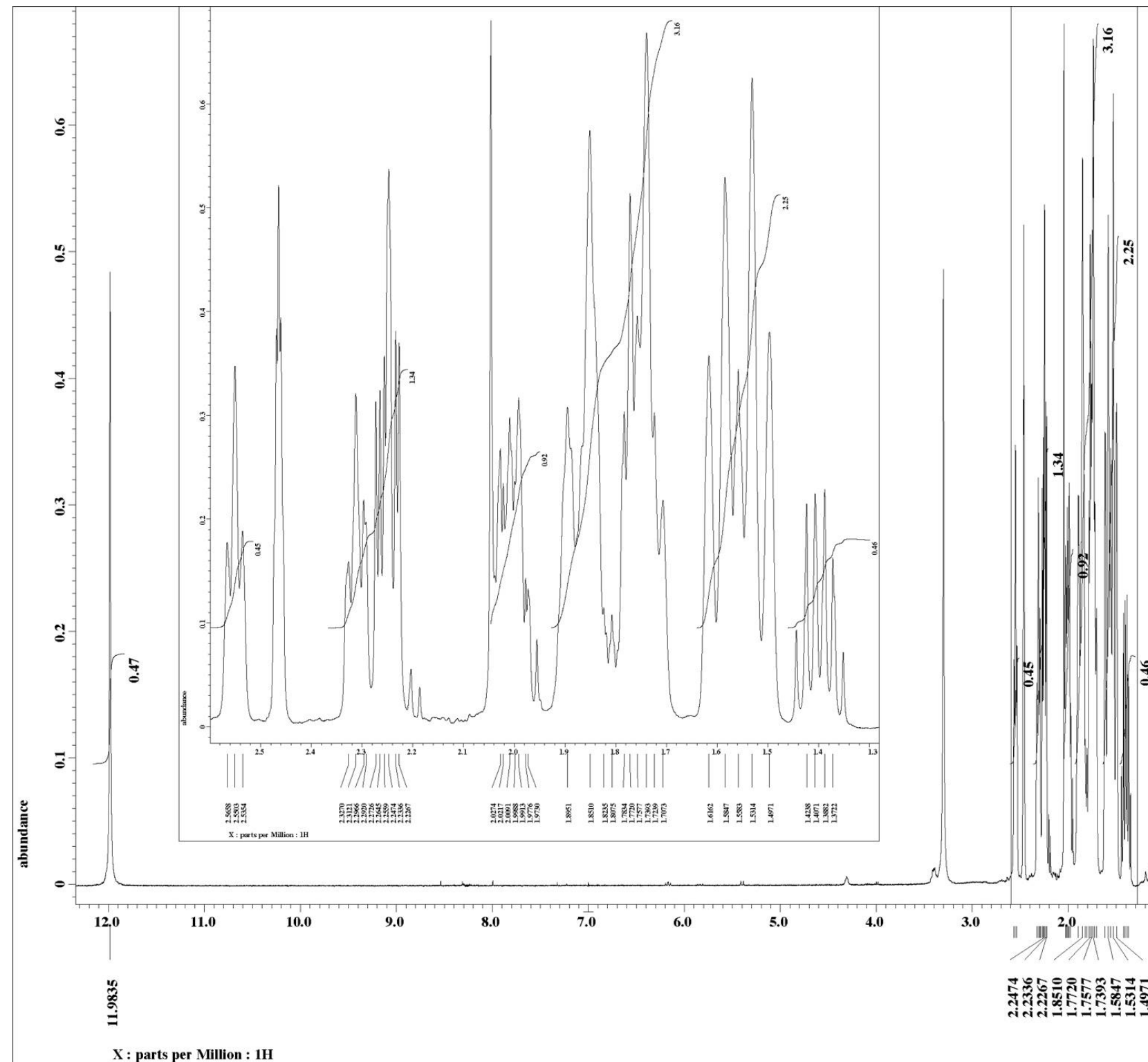
```

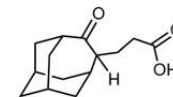
Comment      = single_pulse
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECX 400
Spectrometer = JNM-ECX400

```

```
Field_strength      = 9.389766[T] (400[MHz]
X_acq_duration      = 4.36731904[s]
X_domain            = 1H
X_freq              = 399.78219838[MHz]
X_offset            = 7[ppm]
X_points            = 32768
X_prescans          = 1
X_resolution        = 0.22897343[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      = 11.9[us]
X_acq_time      = 4.36731904[s]
X_angle         = 45[deg]
X_atn           = 3[dB]
X_pulse         = 5.95[us]
Irr_mode        = Off
Tri_mode        = Off
Dante_presat    = FALSE
Initial_wait    = 1[s]
Recvr_gain      = 40
Relaxation_delay = 5[s]
Repetition_time = 9.36731904[s]
Temp_get        = 0[dc]
```





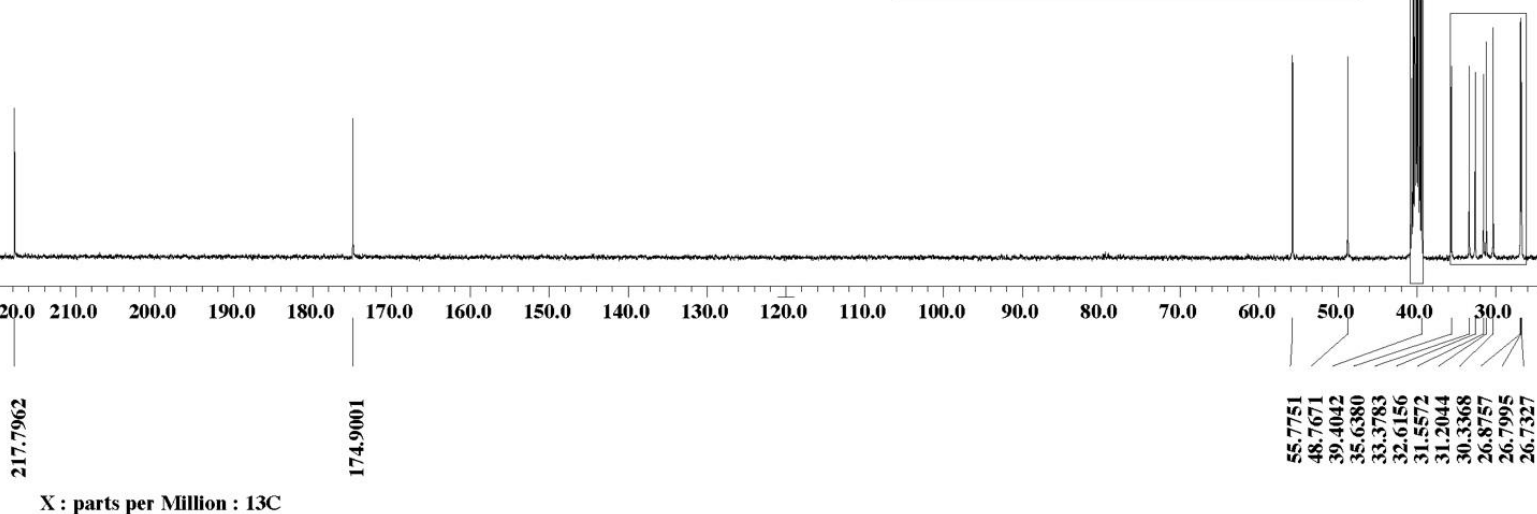
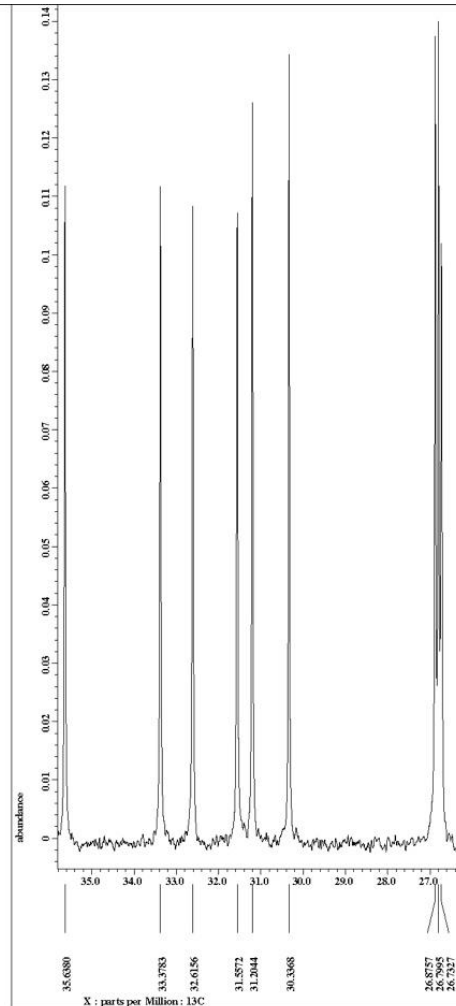
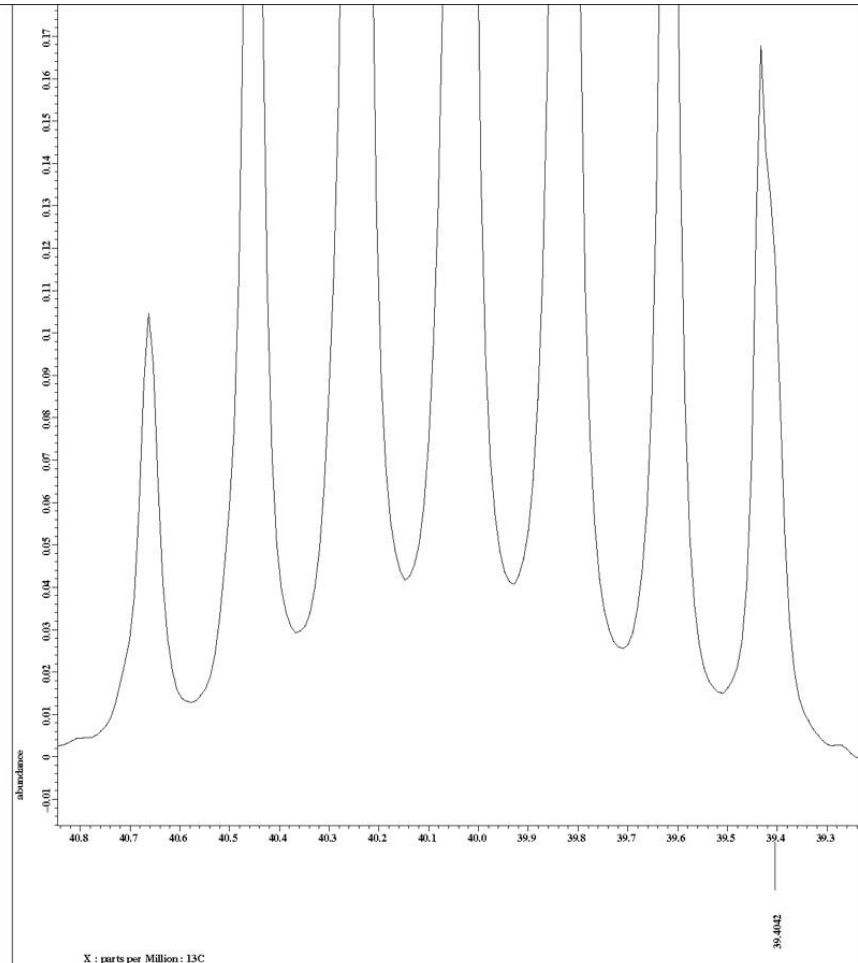
11

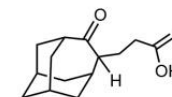
Filename = TIM_13C_270-7.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_270
 Solvent = DMSO-D6
 Creation_time = 6-AUG-2020 20:52:34
 Revision_time = 13-FEB-2023 11:41:45
 Current_time = 13-FEB-2023 11:42:48

Comment = single pulse decouple
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1000
 Total_scans = 1000

X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 48
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 0[dc]





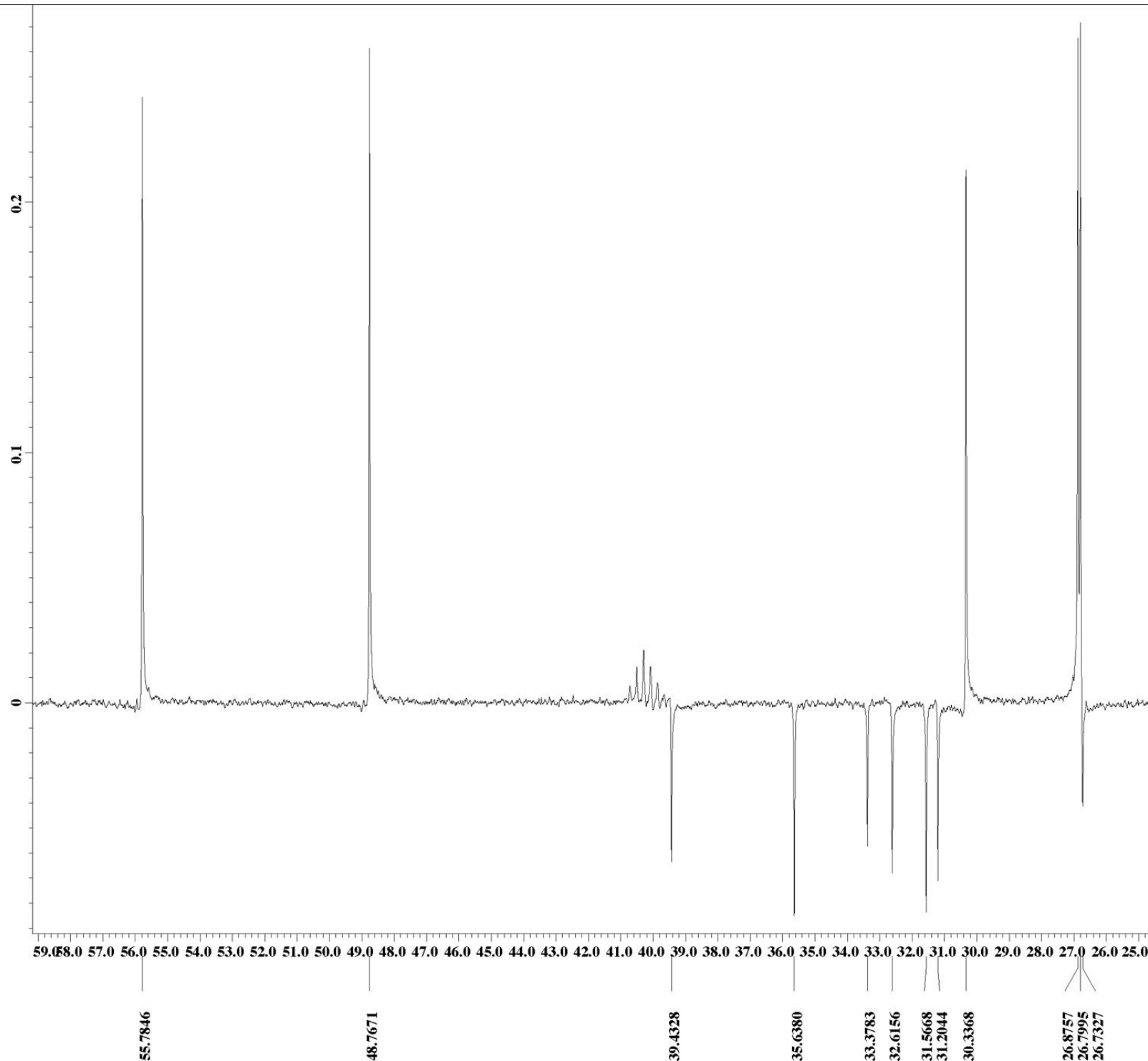
11

Filename = TIM_DEPT135_270-6.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM 270
 Solvent = DMSO-D6
 Creation_time = 6-AUG-2020 21:28:35
 Revision_time = 13-FEB-2023 11:45:08
 Current_time = 13-FEB-2023 11:45:49

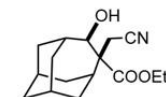
Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.0433312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 700
 Total_scans = 700

X_acq_time = 1.0433312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 48
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 0[dc]



X : parts per Million : 13C



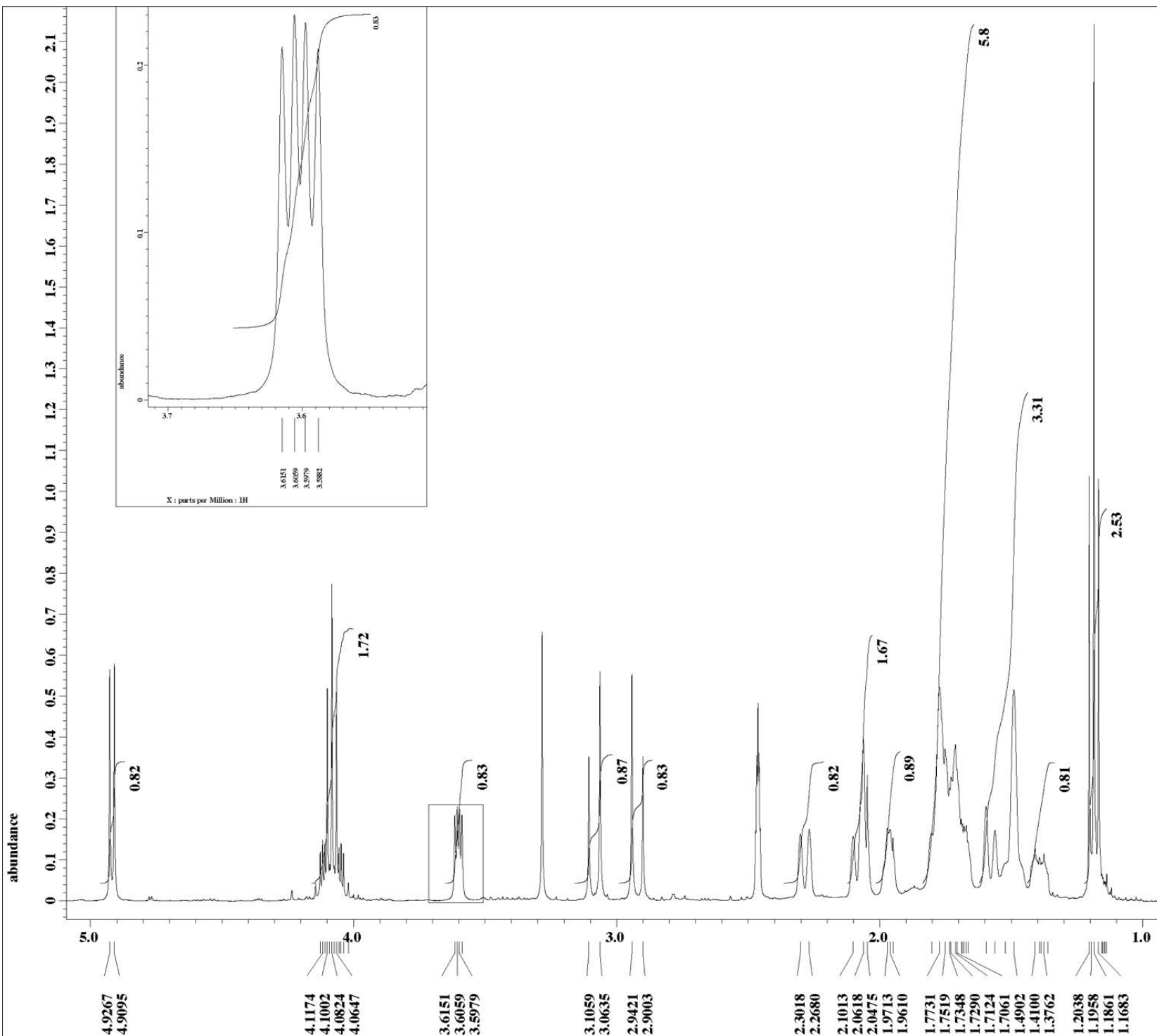
12

Filename = TIM_1H_170-7.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_170
 Solvent = DMSO-D6
 Creation_time = 14-DEC-2018 12:21:04
 Revision_time = 13-FEB-2023 16:56:45
 Current_time = 13-FEB-2023 16:57:38

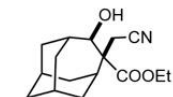
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 11.9[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 5.95[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 34
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 23.5[dc]



X : parts per Million : 1H



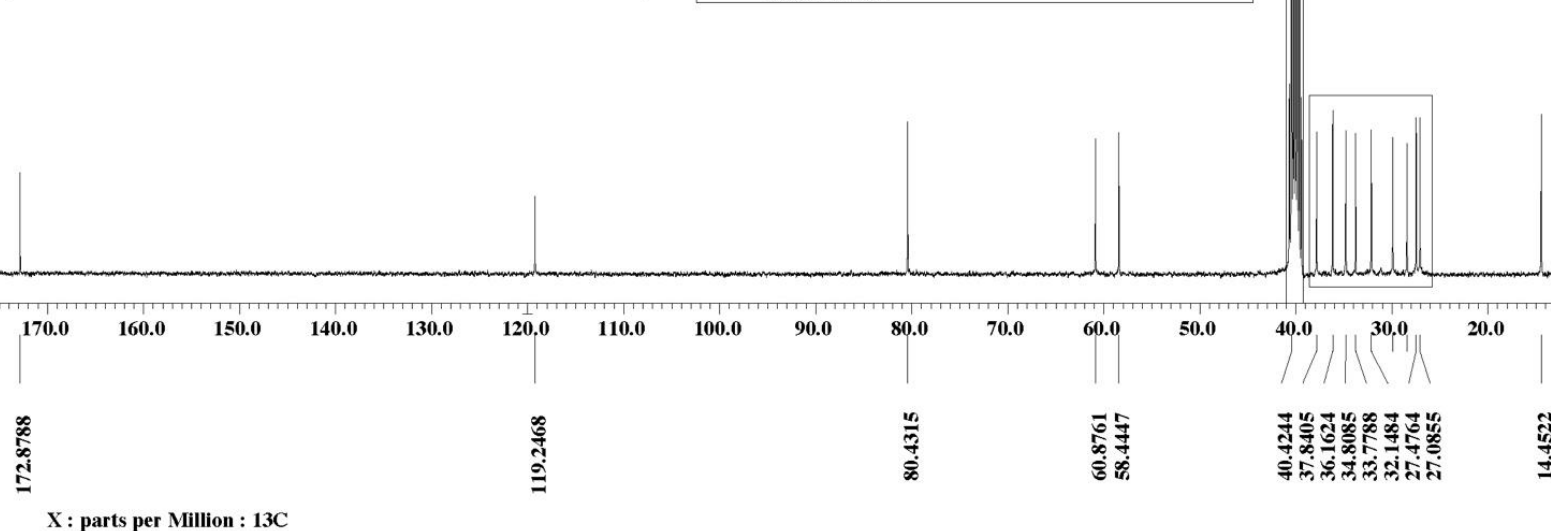
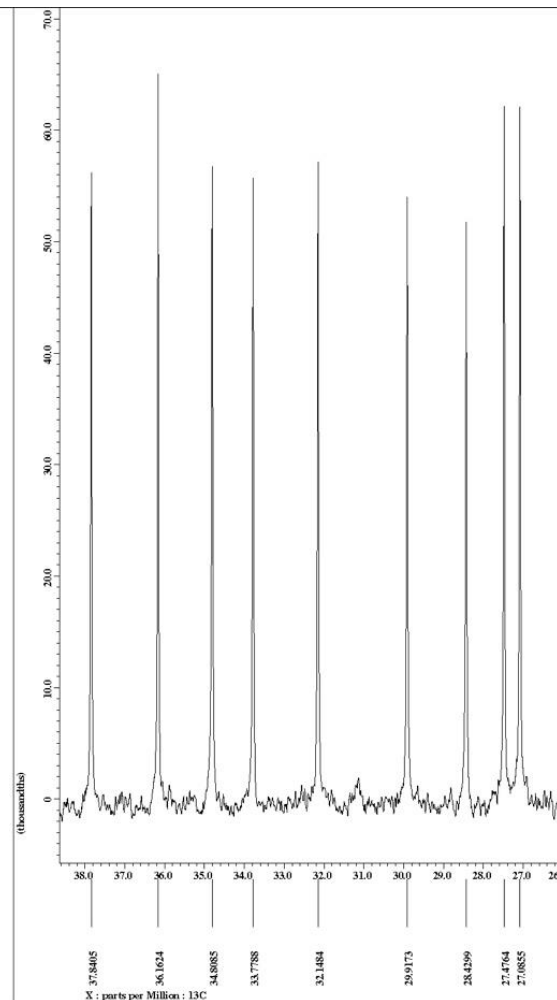
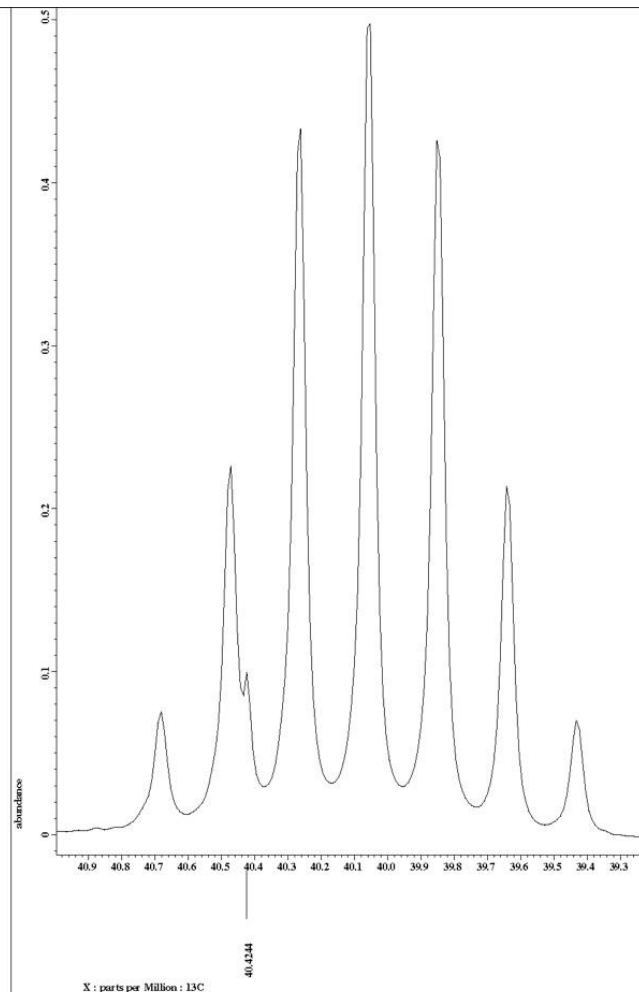
12

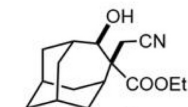
Filename = TIM_13C_170-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_170
 Solvent = DMSO-D6
 Creation_time = 14-DEC-2018 11:51:42
 Revision_time = 13-FEB-2023 16:57:53
 Current_time = 13-FEB-2023 16:58:44

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

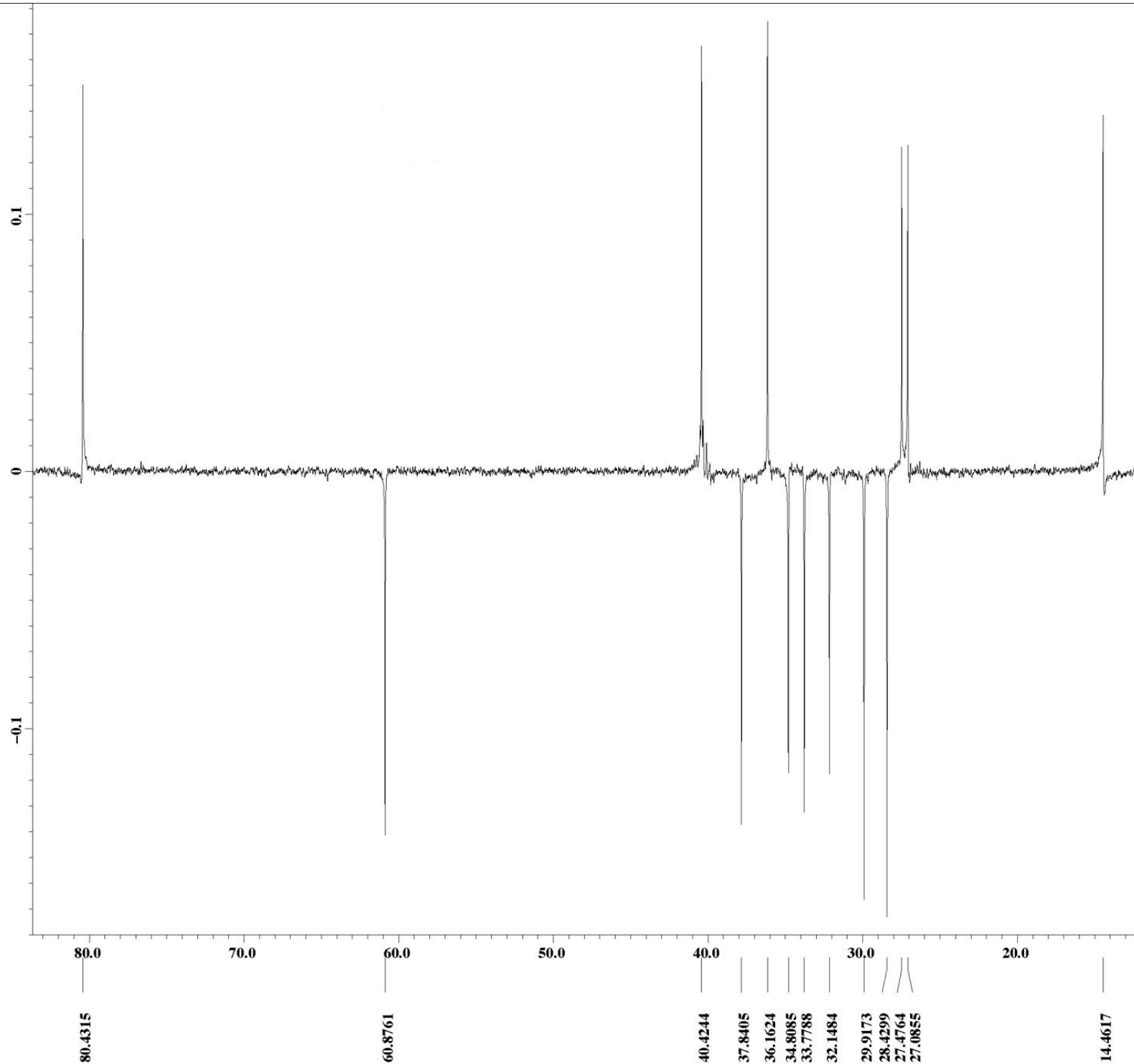
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.0433312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 1000
 Total_scans = 1000

X_90_width = 8.16[us]
 X_acq_time = 1.0433312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 44
 Relaxation_delay = 2[s]
 Repetition_time = 3.0433312[s]
 Temp_get = 23.7[dc]





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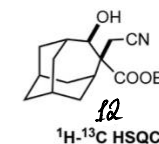
X : parts per Million : ^{13}C

Filename = TIM_DEPT135_170-4.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM 170
 Solvent = DMSO-D6
 Creation_time = 14-DEC-2018 12:17:31
 Revision_time = 13-FEB-2023 16:59:35
 Current_time = 13-FEB-2023 16:59:57

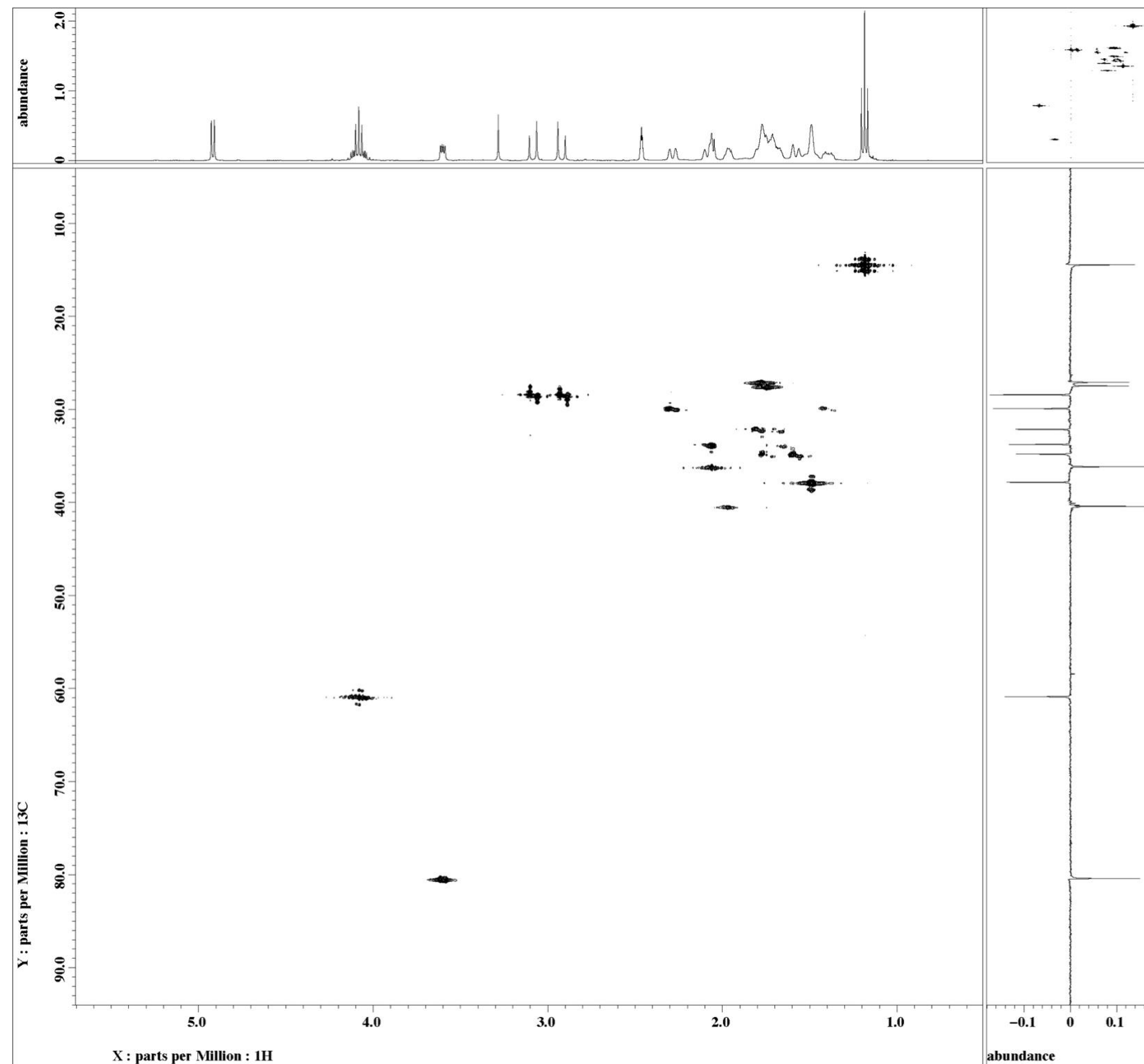
Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

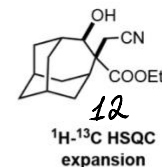
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.0433312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 500
 Total_scans = 500

X_acq_time = 1.0433312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 23.6[degC]

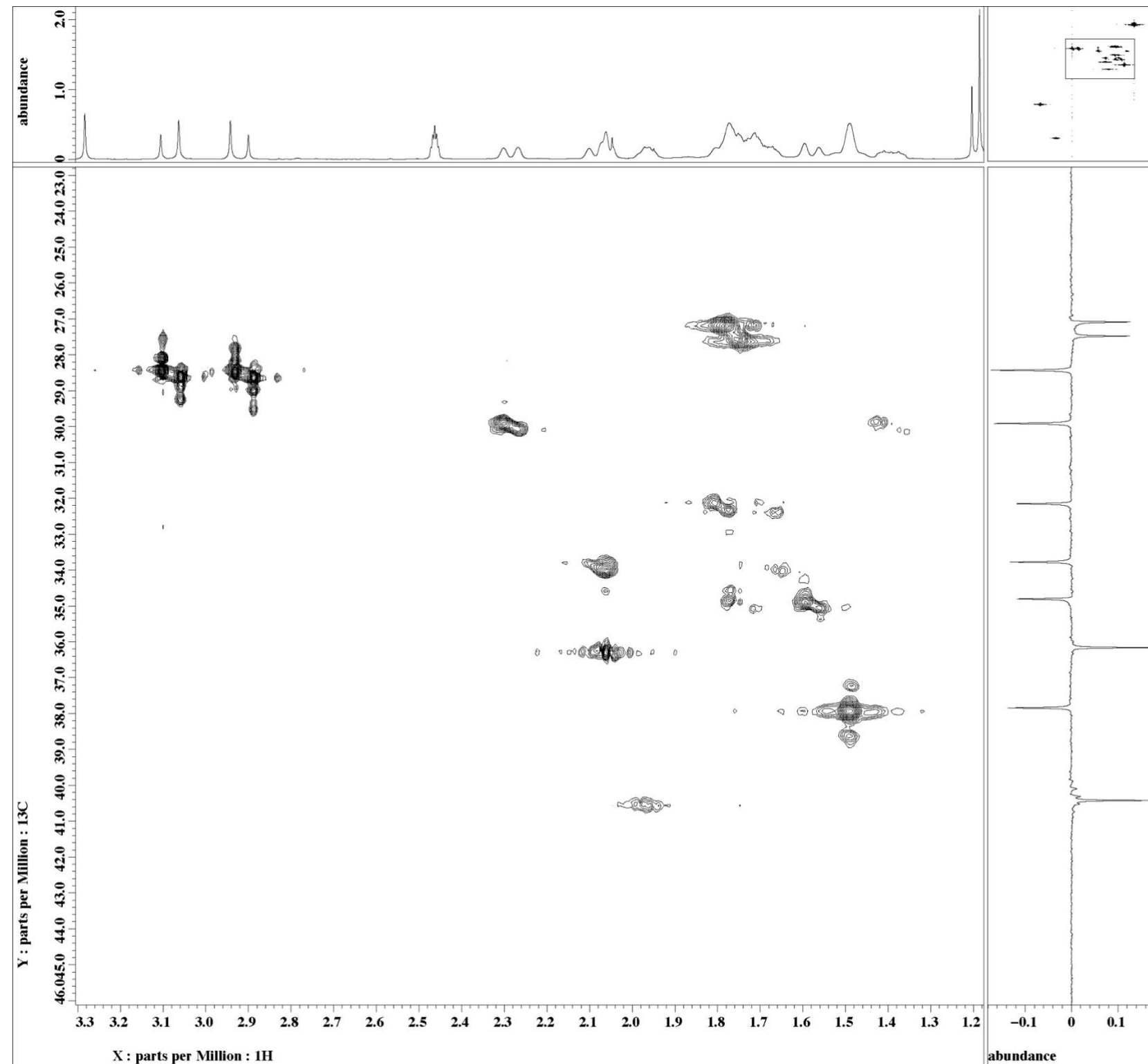


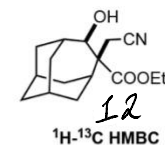
Filename	=	TIM_HMQC_170-4.jdf
Author	=	delta
Experiment	=	hmqc_pfg.ex2
Sample_id	=	TIM_170
Solvent	=	DMSO-D6
Creation_time	=	18-JUN-2019 23:23:43
Revision_time	=	20-APR-2023 18:35:24
Current_time	=	20-APR-2023 18:37:00
Comment	=	gradient enhanced HMQ
Data_format	=	2D REAL REAL
Dim_size	=	819, 1024
Dim_title	=	1H 13C
Dim_units	=	[ppm] [ppm]
Dimensions	=	X Y
Site	=	ECX 400
Spectrometer	=	JNM-ECX400
Field_strength	=	9.389766[T] (400[MHz])
X_acq_duration	=	0.39395328[s]
X_domain	=	1H
X_freq	=	399.78219838[MHz]
X_offset	=	3.1[ppm]
X_points	=	1024
X_prescans	=	4
X_resolution	=	2.53837206[Hz]
X_sweep	=	2.59929299[kHz]
Y_domain	=	13C
Y_freq	=	100.52530333[MHz]
Y_offset	=	49.0[ppm]
Y_points	=	512
Y_prescans	=	0
Y_resolution	=	17.67214079[Hz]
Y_sweep	=	9.04813608[kHz]
Tri_domain	=	1H
Tri_freq	=	399.78219838[MHz]
Tri_offset	=	5[ppm]
Clipped	=	FALSE
Mod_return	=	1
Scans	=	4
Total_scans	=	2048
X_acq_time	=	0.39395328[s]
X_atn	=	3[dB]
X_pulse	=	11.9[us]
Y_acq_time	=	56.58624[ms]
Y_atn	=	7.8[dB]
Y_pulse	=	8.16[us]
Irr_atn_dec	=	32.913[dB]
Irr_noise	=	MPF8
Tri_mode	=	Off
Dante_presat	=	FALSE
Decoupling	=	TRUE
Grad_1	=	1[ms]
Grad_1_amp	=	0.18[T/m]
Grad_2	=	1[ms]
Grad_2_amp	=	0.18[T/m]
Grad_3	=	1[ms]
Grad_3_amp	=	90.54325956[mT/m]
Grad_recover	=	0.1[ms]





Filename	=	TIM_HMQC_170-4.jdf
Author	=	delta
Experiment	=	hmqc_pfg.ex2
Sample_id	=	TIM_170
Solvent	=	DMSO-D6
Creation_time	=	18-JUN-2019 23:23:43
Revision_time	=	20-APR-2023 18:35:24
Current_time	=	20-APR-2023 18:37:25
Comment	=	gradient enhanced HMQC
Data_format	=	2D REAL REAL
Dim_size	=	819, 1024
Dim_title	=	1H 13C
Dim_units	=	[ppm] [ppm]
Dimensions	=	X Y
Site	=	ECX 400
Spectrometer	=	JNM-ECX400
Field_strength	=	9.389766[T] (400[MHz])
X_acq_duration	=	0.39395328[s]
X_domain	=	1H
X_freq	=	399.78219838[MHz]
X_offset	=	3.1[ppm]
X_points	=	1024
X_prescans	=	4
X_resolution	=	2.53837206[Hz]
X_sweep	=	2.59929299[kHz]
Y_domain	=	13C
Y_freq	=	100.52530333[MHz]
Y_offset	=	49.0[ppm]
Y_points	=	512
Y_prescans	=	0
Y_resolution	=	17.67214079[Hz]
Y_sweep	=	9.04813608[kHz]
Tri_domain	=	1H
Tri_freq	=	399.78219838[MHz]
Tri_offset	=	5[ppm]
Clipped	=	FALSE
Mod_return	=	1
Scans	=	4
Total_scans	=	2048
X_acq_time	=	0.39395328[s]
X_atn	=	3[dB]
X_pulse	=	11.9[us]
Y_acq_time	=	56.58624[ms]
Y_atn	=	7.8[dB]
Y_pulse	=	8.16[us]
Irr_atn_dec	=	32.913[dB]
Irr_noise	=	MPF8
Tri_mode	=	Off
Dante_presat	=	FALSE
Decoupling	=	TRUE
Grad_1	=	1[ms]
Grad_1_amp	=	0.18[T/m]
Grad_2	=	1[ms]
Grad_2_amp	=	0.18[T/m]
Grad_3	=	1[ms]
Grad_3_amp	=	90.54325956[mT/m]
Grad_recover	=	0.1[ms]



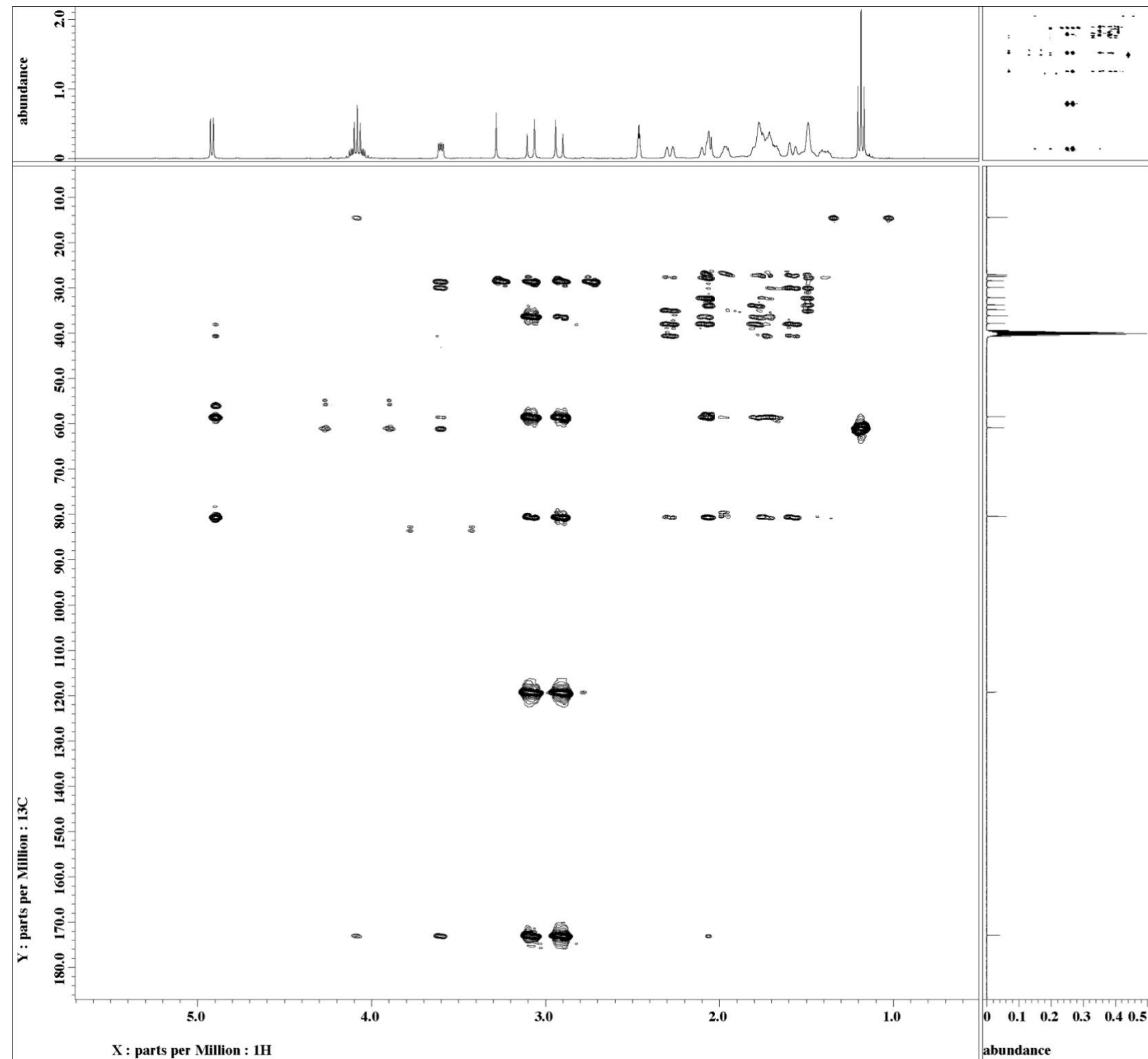


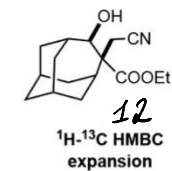
Filename = TIM_HMBC_170-3.jdf
 Author = delta
 Experiment = hmhc_pfg.ex2
 Sample_id = TIM_170
 Solvent = DMSO-D6
 Creation_time = 19-JUN-2019 01:38:45
 Revision_time = 20-APR-2023 18:32:35
 Current_time = 20-APR-2023 18:40:08

Comment = gradient enhanced HMB
 Data_format = 2D REAL REAL
 Dim_size = 819, 1024
 Dim_title = 1H 13C
 Dim_units = [ppm] [ppm]
 Dimensions = X Y
 Site = ECX 400
 Spectrometer = JNM-ECX400

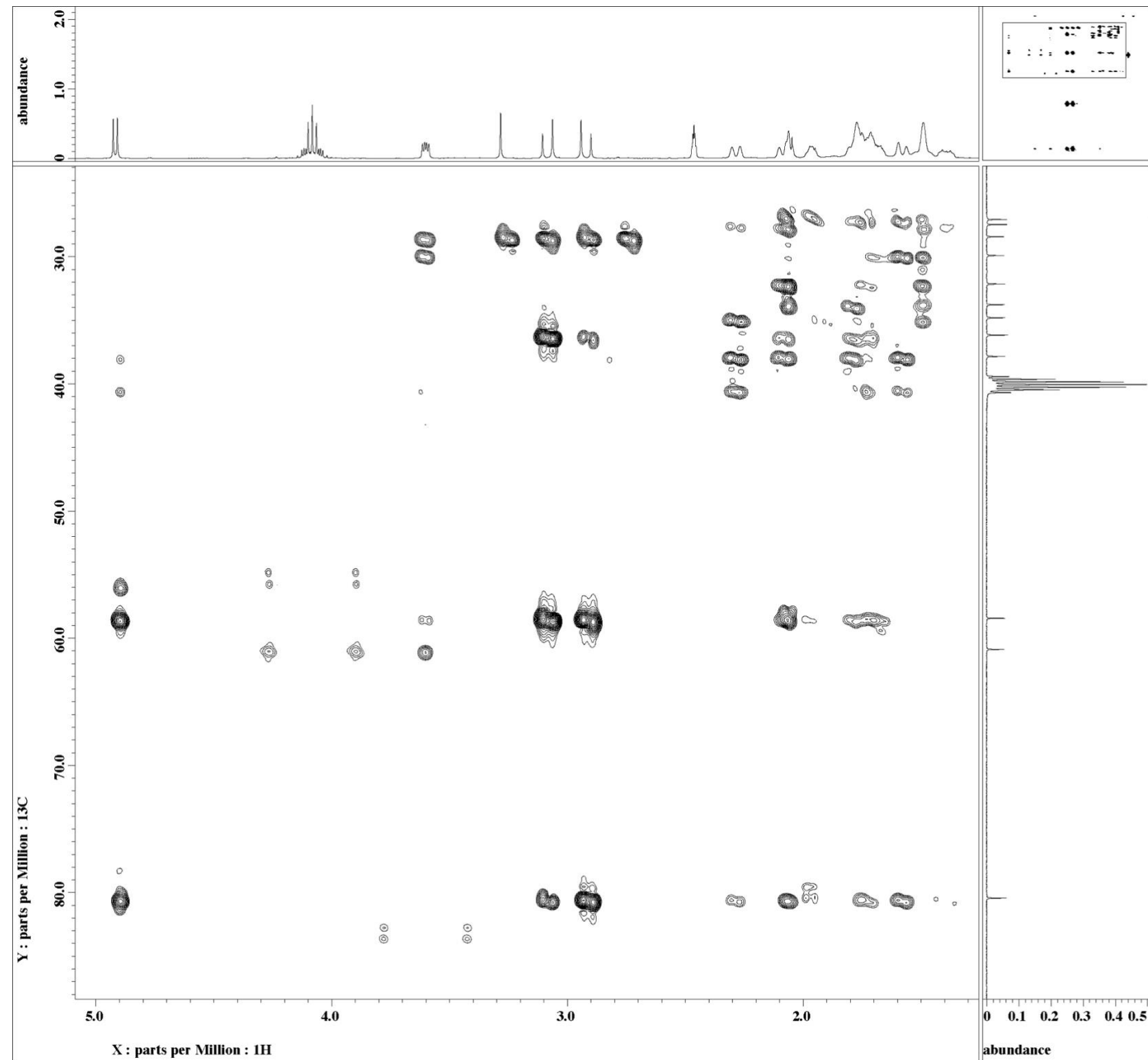
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 0.39395328[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 3.1[ppm]
 X_points = 1024
 X_prescans = 4
 X_resolution = 2.53837206[Hz]
 X_sweep = 2.59929299[kHz]
 Y_domain = 13C
 Y_freq = 100.52530333[MHz]
 Y_offset = 95[ppm]
 Y_points = 512
 Y_prescans = 0
 Y_resolution = 36.14220947[Hz]
 Y_sweep = 18.50481125[kHz]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 4096

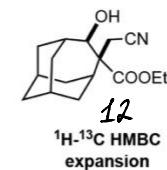
X_acq_time = 0.39395328[s]
 X_atn = 3[dB]
 X_pulse = 11.9[us]
 Y_acq_time = 27.66848[ms]
 Y_atn = 7.8[dB]
 Y_pulse = 8.16[us]
 Tri_mode = Off
 Dante_presat = FALSE
 Delta = 62.5[ms]
 Grad_1 = 1[ms]
 Grad_1_amp = 0.18[T/m]
 Grad_2 = 1[ms]
 Grad_2_amp = 0.18[T/m]
 Grad_3 = 1[ms]
 Grad_3_amp = 90.54325956[mT/m]
 Grad_recover = 0.1[ms]
 Grad_selection = 13C = 1.988:1.98
 Grad_shape = SINE



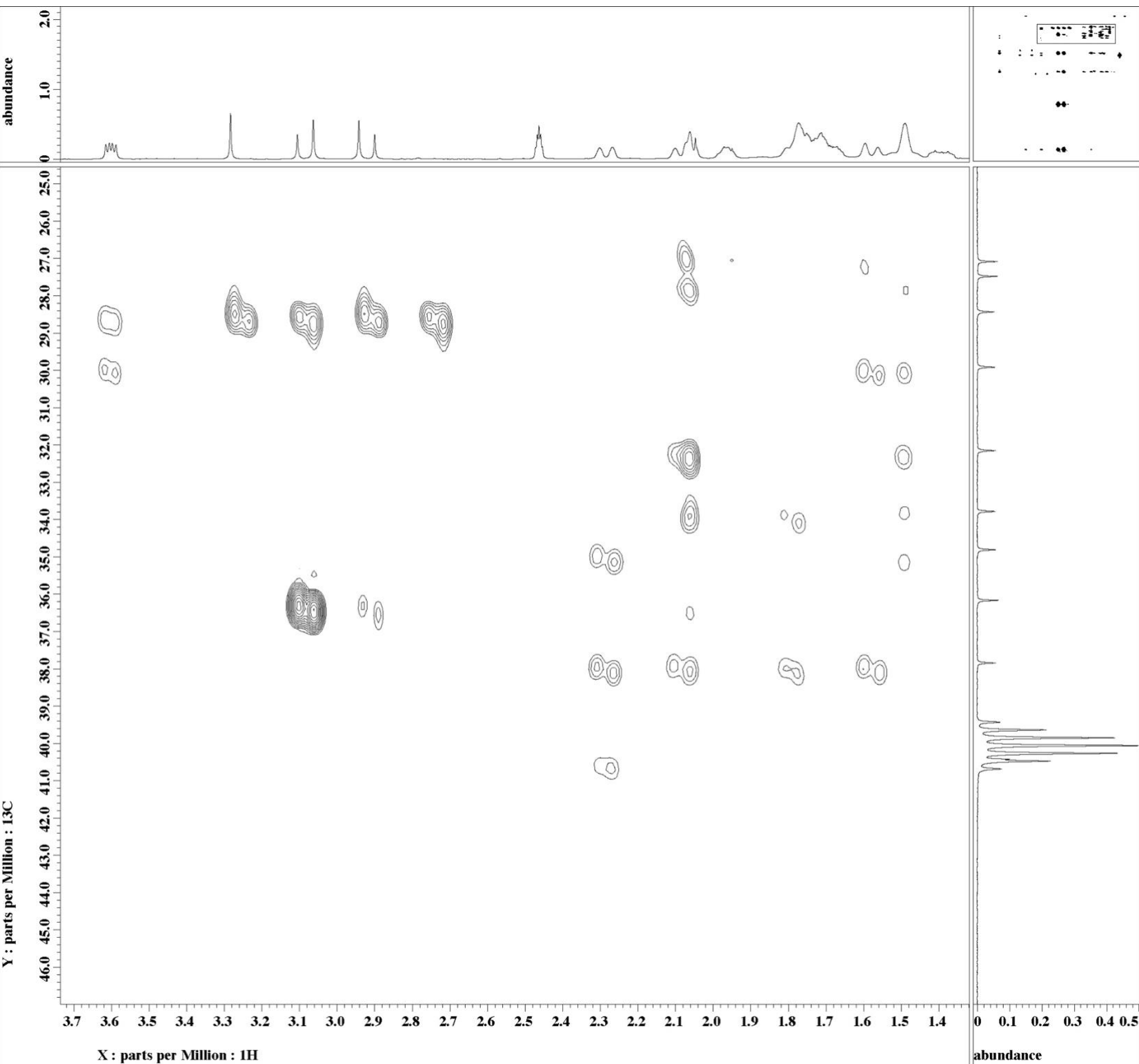
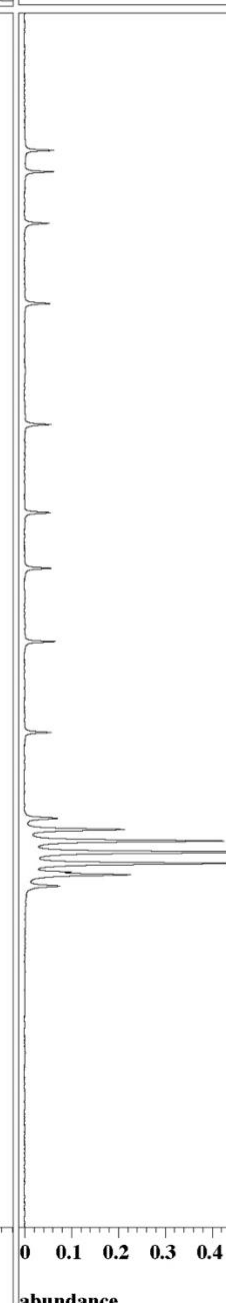
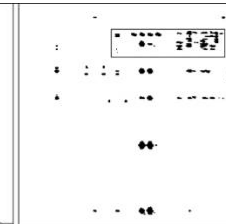


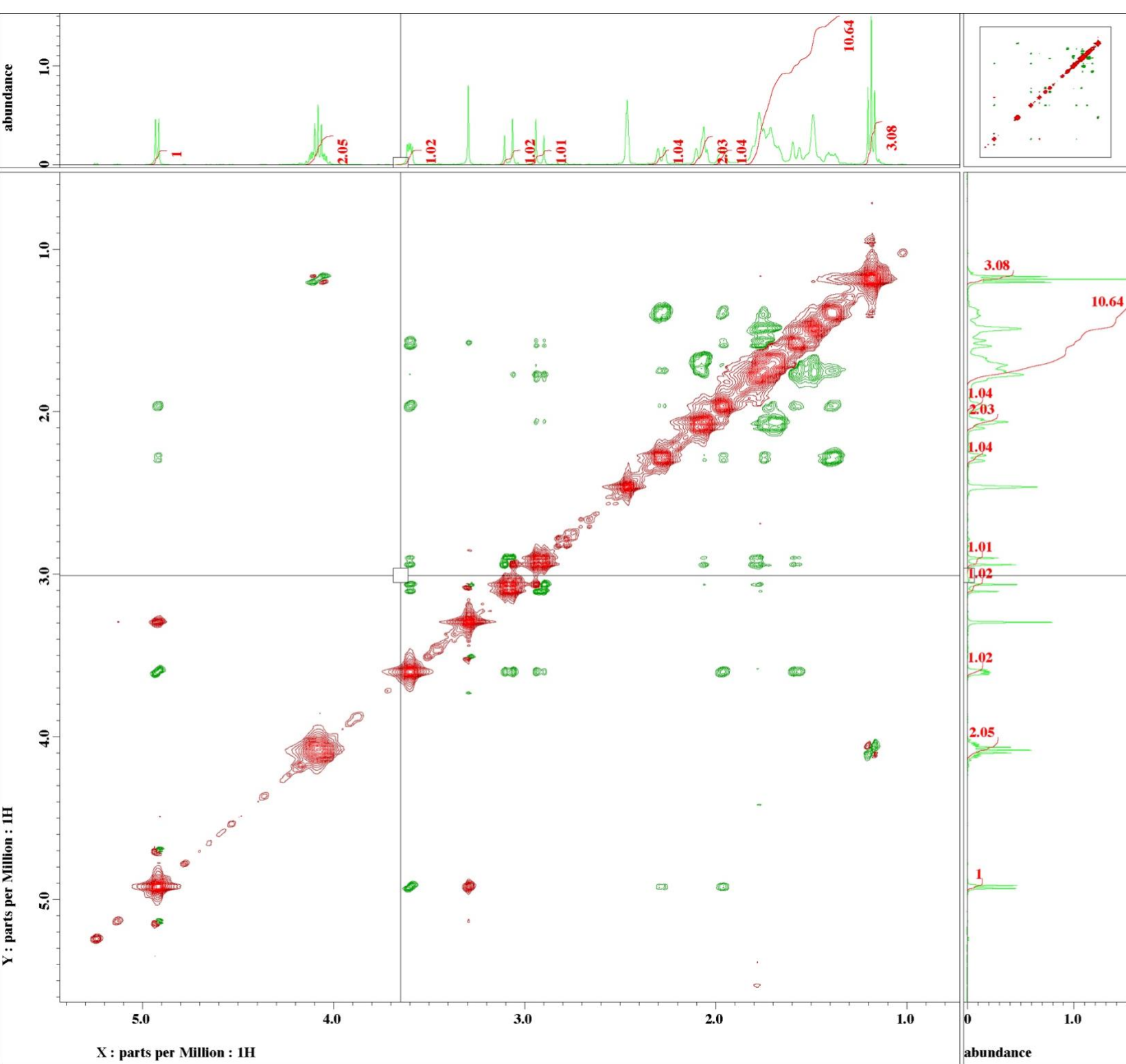
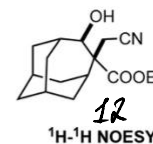
Filename = TIM_HMBC_170-3.jdf
 Author = delta
 Experiment = hmhc_pfg.ex2
 Sample_id = TIM_170
 Solvent = DMSO-D6
 Creation_time = 19-JUN-2019 01:38:45
 Revision_time = 20-APR-2023 18:32:35
 Current_time = 20-APR-2023 18:41:01
 Comment = gradient enhanced HMB
 Data_format = 2D REAL REAL
 Dim_size = 819, 1024
 Dim_title = 1H 13C
 Dim_units = [ppm] [ppm]
 Dimensions = X Y
 Site = ECX 400
 Spectrometer = JNM-ECX400
 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 0.39395328[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 3.1[ppm]
 X_points = 1024
 X_prescans = 4
 X_resolution = 2.53837206[Hz]
 X_sweep = 2.59929299[kHz]
 Y_domain = 13C
 Y_freq = 100.52530333[MHz]
 Y_offset = 95[ppm]
 Y_points = 512
 Y_prescans = 0
 Y_resolution = 36.14220947[Hz]
 Y_sweep = 18.50481125[kHz]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 4096
 X_acq_time = 0.39395328[s]
 X_atn = 3[dB]
 X_pulse = 11.9[us]
 Y_acq_time = 27.66848[ms]
 Y_atn = 7.8[dB]
 Y_pulse = 8.16[us]
 Tri_mode = Off
 Dante_presat = FALSE
 Delta = 62.5[ms]
 Grad_1 = 1[ms]
 Grad_1_amp = 0.18[T/m]
 Grad_2 = 1[ms]
 Grad_2_amp = 0.18[T/m]
 Grad_3 = 1[ms]
 Grad_3_amp = 90.54325956[mT/m]
 Grad_recover = 0.1[ms]
 Grad_selection = 13C = 1.988:1.98
 Grad_shape = SINE



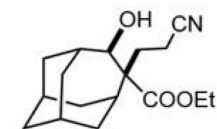


Filename = TIM_HMBC_170-3.jdf
 Author = delta
 Experiment = hmbc_pfg.ex2
 Sample_id = TIM_170
 Solvent = DMSO-D6
 Creation_time = 19-JUN-2019 01:38:45
 Revision_time = 20-APR-2023 18:32:35
 Current_time = 20-APR-2023 18:41:58
 Comment = gradient enhanced HMB
 Data_format = 2D REAL REAL
 Dim_size = 819, 1024
 Dim_title = 1H 13C
 Dim_units = [ppm] [ppm]
 Dimensions = X Y
 Site = ECX 400
 Spectrometer = JNM-ECX400
 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 0.39395328[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 3.1[ppm]
 X_points = 1024
 X_prescans = 4
 X_resolution = 2.53837206[Hz]
 X_sweep = 2.59929299[kHz]
 Y_domain = 13C
 Y_freq = 100.52530333[MHz]
 Y_offset = 95[ppm]
 Y_points = 512
 Y_prescans = 0
 Y_resolution = 36.14220947[Hz]
 Y_sweep = 18.50481125[kHz]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 4096
 X_acq_time = 0.39395328[s]
 X_atn = 3[dB]
 X_pulse = 11.9[us]
 Y_acq_time = 27.66848[ms]
 Y_atn = 7.8[dB]
 Y_pulse = 8.16[us]
 Tri_mode = Off
 Dante_presat = FALSE
 Delta = 62.5[ms]
 Grad_1 = 1[ms]
 Grad_1_amp = 0.18[T/m]
 Grad_2 = 1[ms]
 Grad_2_amp = 0.18[T/m]
 Grad_3 = 1[ms]
 Grad_3_amp = 90.54325956[mT/m]
 Grad_recover = 0.1[ms]
 Grad_selection = 13C = 1.988:1.98
 Grad_shape = SINE





Filename	=	TIM_NOESY_170exx-2.jd
Author	=	delta
Experiment	=	noesy_phase_zqf_
Sample_id	=	TIM_170exx
Solvent	=	DMSO-D6
Creation_time	=	22-APR-2023 00:51:46
Revision_time	=	22-APR-2023 00:24:15
Current_time	=	22-APR-2023 10:34:48
Comment	=	phase sensitive noesy
Data_format	=	2D COMPLEX COMPLEX
Dim_size	=	409, 1024
Dim_title	=	1H 1H
Dim_units	=	[ppm] [ppm]
Dimensions	=	X Y
Site	=	ECX 400
Spectrometer	=	JNM-ECX400
Field_strength	=	9.389766[T] (400[MHz])
X_acq_duration	=	0.17047552[s]
X_domain	=	1H
X_freq	=	399.78219838[MHz]
X_offset	=	3[ppm]
X_points	=	512
X_prescans	=	4
X_resolution	=	5.86594486[Hz]
X_sweep	=	3.00336377[kHz]
Y_domain	=	1H
Y_freq	=	399.78219838[MHz]
Y_offset	=	3[ppm]
Y_points	=	512
Y_prescans	=	0
Y_resolution	=	4.68510123[Hz]
Y_sweep	=	2.39877183[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	=	2048
X_acq_time	=	0.17047552[s]
X_atn	=	3.5[dB]
X_pulse	=	5.5[us]
Y_acq_time	=	0.21344256[s]
Y_pl_correction	=	180.0
Irr_mode	=	Off
Tri_mode	=	Off
Adiabatic_pulse	=	50[ms]
B1_attn	=	43.80211242[dB]
Band_width	=	30[kHz]
Chirp_atn	=	31.19788758[dB]
Chirp_pulse	=	50[ms]
Chirp_shape	=	CHIRP
Chirp_smooth	=	10[%]
Dante_presat	=	FALSE



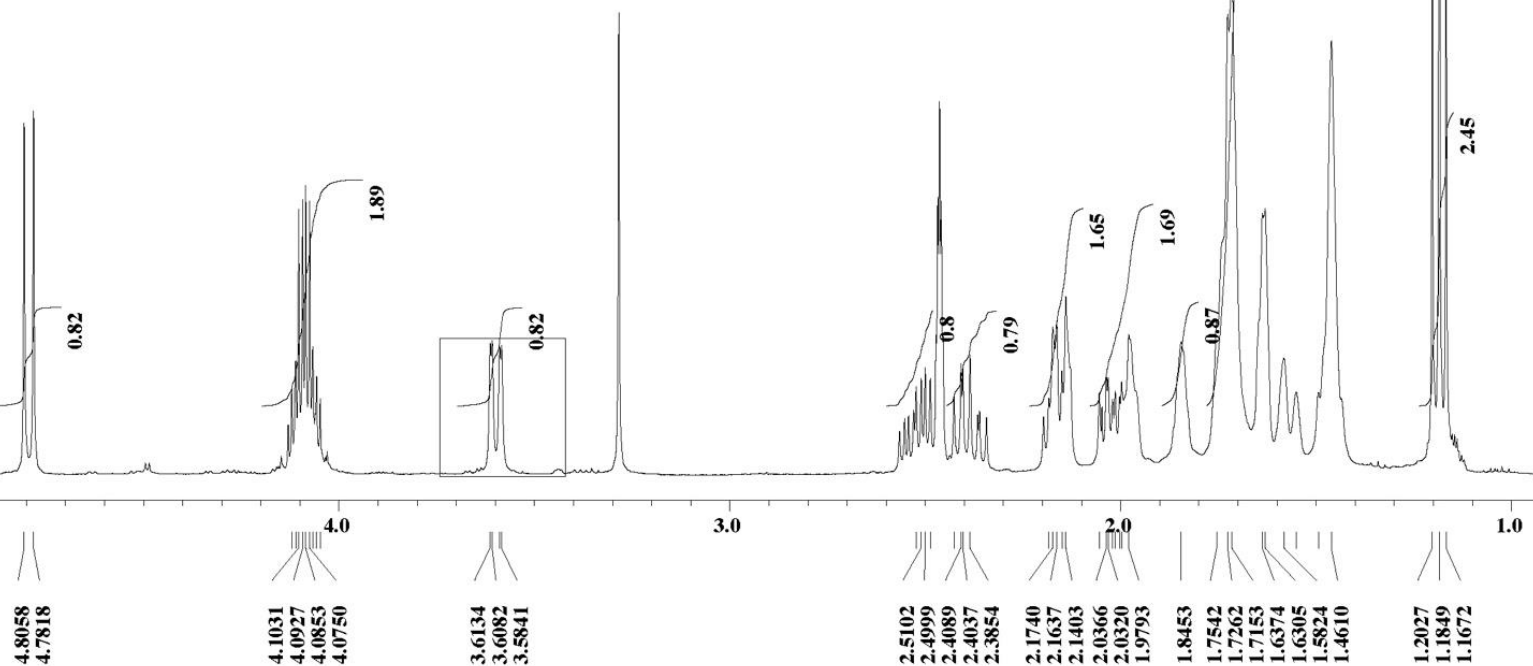
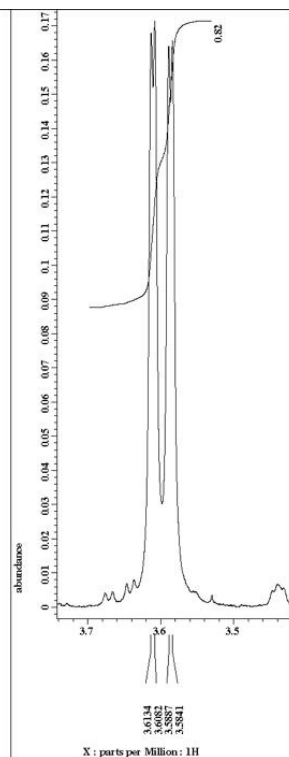
13

Filename = TIM_1H_158-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_158
 Solvent = DMSO-D6
 Creation_time = 17-NOV-2018 06:25:32
 Revision_time = 13-FEB-2023 17:03:42
 Current_time = 13-FEB-2023 17:04:49

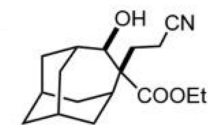
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 11.9[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 5.95[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 34
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 22.6[dc]



X : parts per Million : 1H



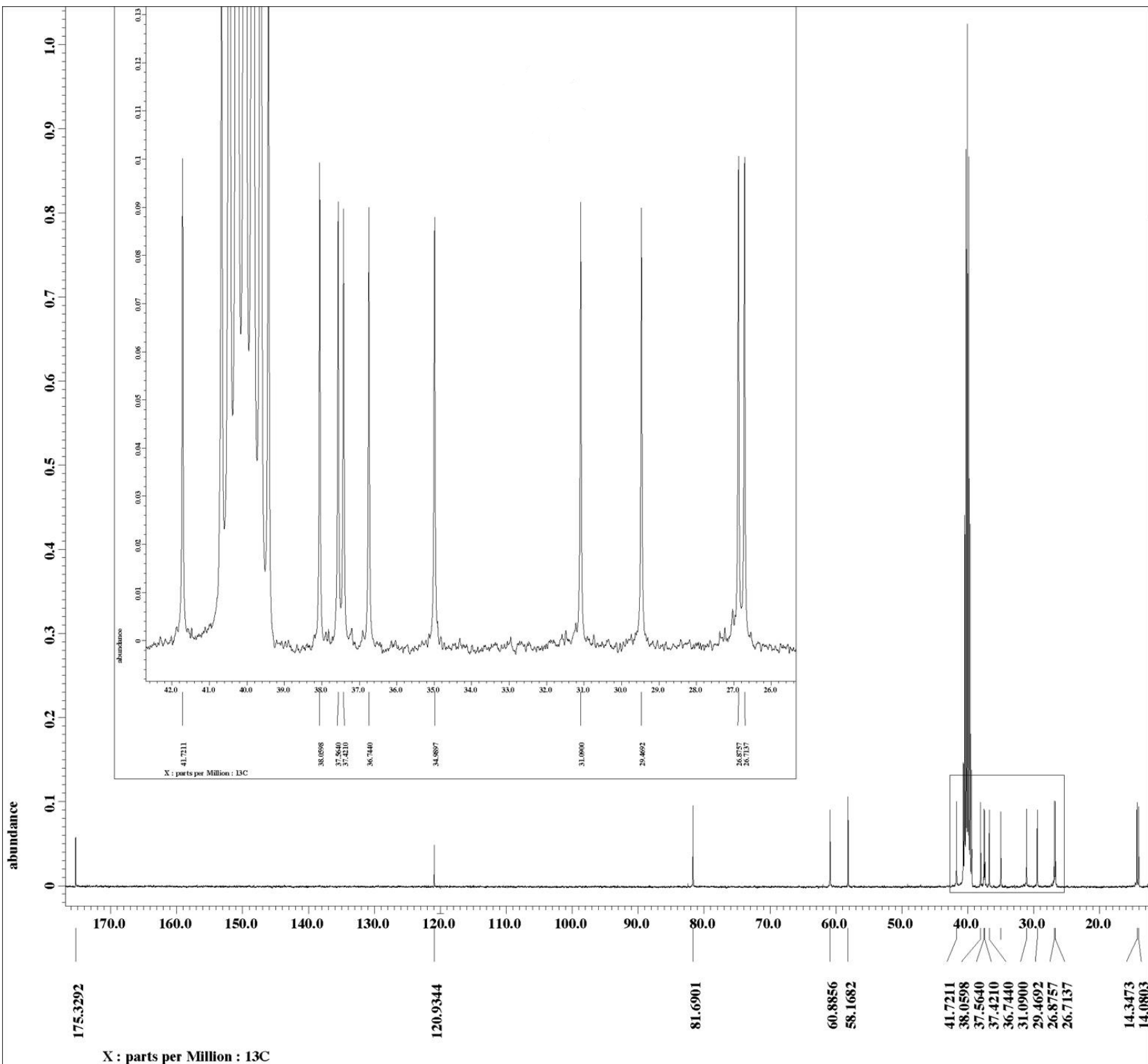
13

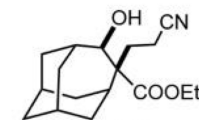
Filename = TIM_13C_158-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_158
 Solvent = DMSO-D6
 Creation_time = 17-NOV-2018 09:00:03
 Revision_time = 13-FEB-2023 17:05:08
 Current_time = 13-FEB-2023 17:05:54

Comment = single pulse decouple
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 3000
 Total_scans = 3000

X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 22.7[dc]





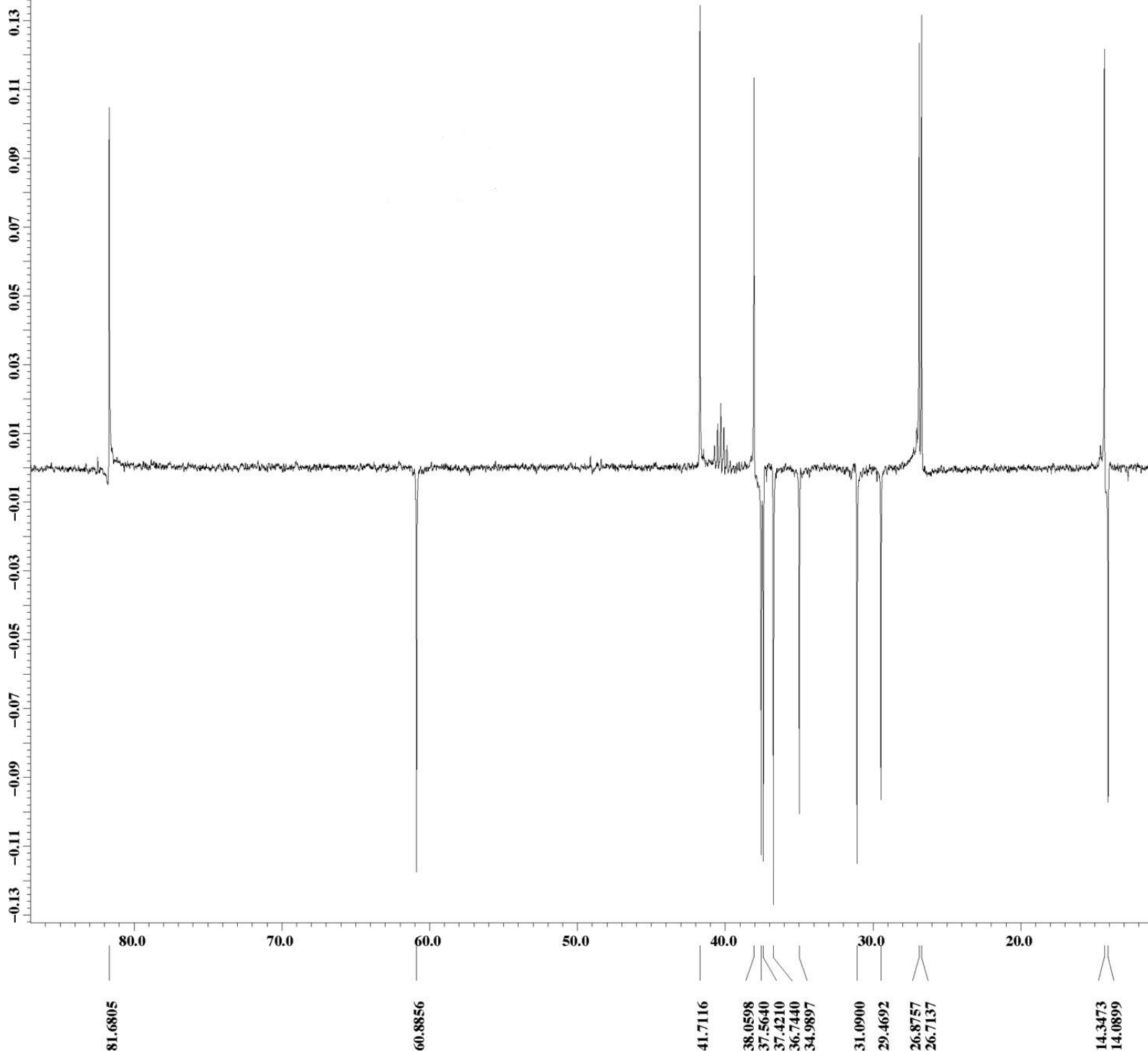
13

Filename = TIM_DEPT135_158-3.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM 158
 Solvent = DMSO-D6
 Creation_time = 17-NOV-2018 09:51:20
 Revision_time = 13-FEB-2023 17:06:08
 Current_time = 13-FEB-2023 17:06:37

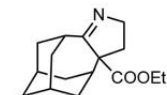
Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1000
 Total_scans = 1000

X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 22.6[degC]



X : parts per Million : 13C



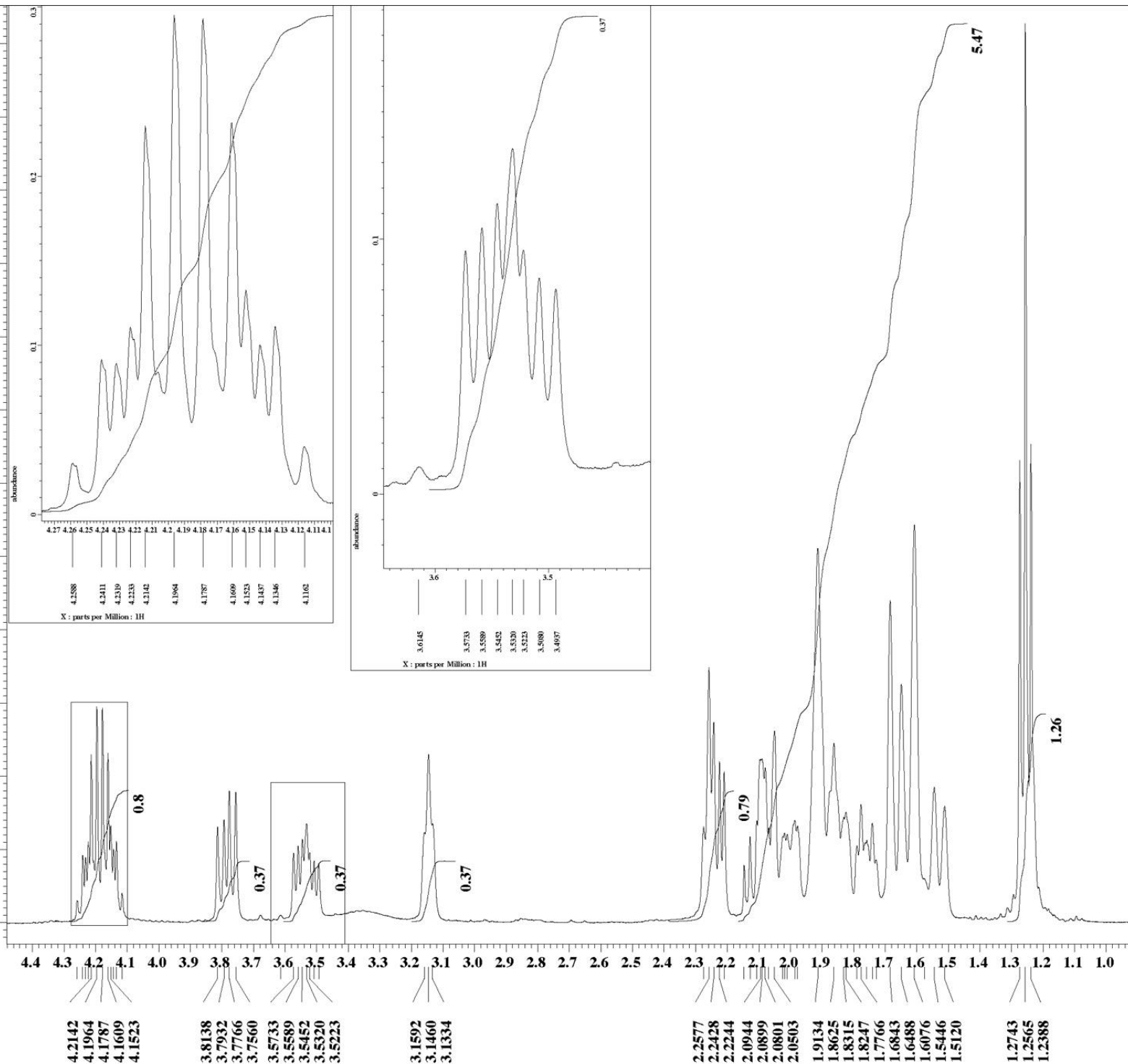
14

Filename = TIM_1H_191-3.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_191
 Solvent = CHLOROFORM-D
 Creation_time = 17-MAR-2019 00:32:02
 Revision_time = 10-FEB-2023 14:58:40
 Current_time = 10-FEB-2023 15:00:05

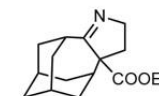
Comment = single pu
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 11.9[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 5.95[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 38
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 23.8[dc]



X : parts per Million : 1H



14

Filename = TIM_13C_191-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_191
 Solvent = CHLOROFORM-D
 Creation_time = 17-MAR-2019 02:16:01
 Revision_time = 10-FEB-2023 15:00:27
 Current_time = 10-FEB-2023 15:00:52

 Comment = single pulse decouple
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 2000
 Total_scans = 2000

 X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 48
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 24.4[dc]

0.3

0.2

0.1

0

abundance

186.0174

174.7476

68.6944

61.0572

56.9097

40.5960

36.7154

35.6190

33.2162

30.1461

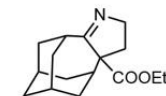
30.0794

27.3334

27.1141

14.2996

X : parts per Million : 13C



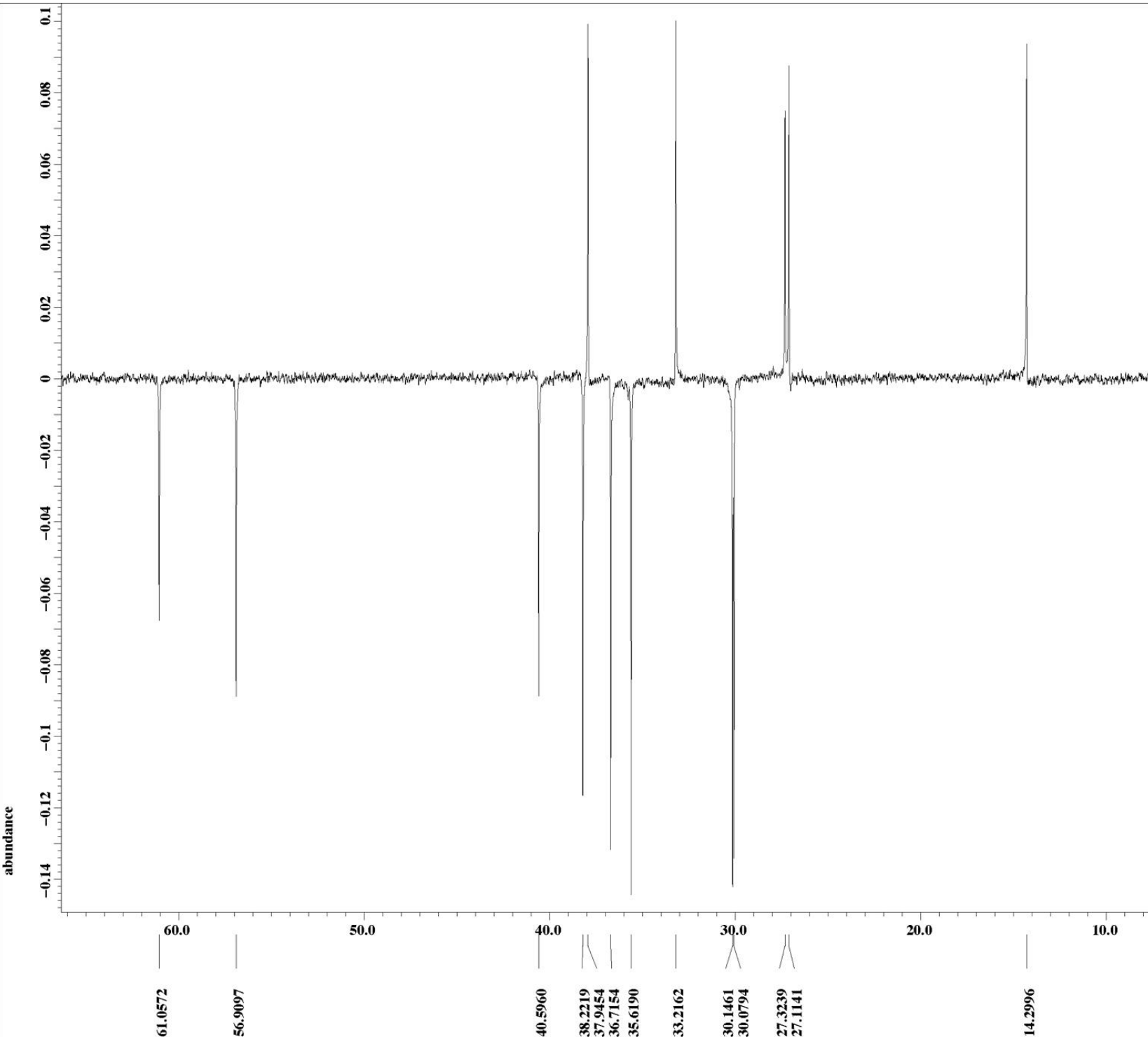
14

Filename = TIM_DEPT135_191-4.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM 191
 Solvent = CHLOROFORM-D
 Creation_time = 17-MAR-2019 03:07:17
 Revision_time = 10-FEB-2023 15:01:07
 Current_time = 10-FEB-2023 15:01:29

Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

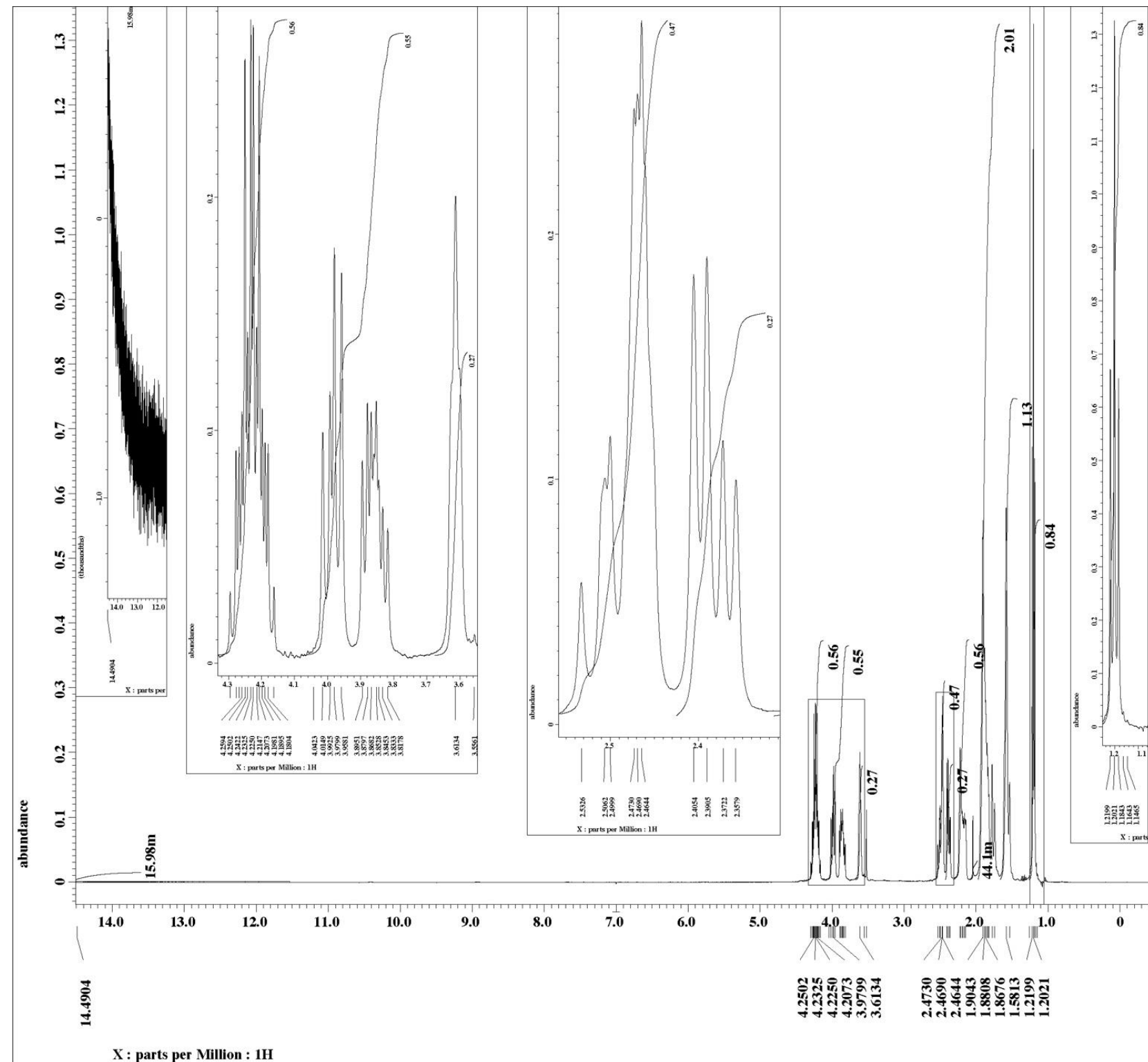
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 1000
 Total_scans = 1000

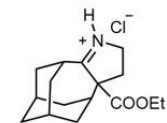
X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 24.2[degC]





```
X_90_width      = 11.9[us]
X_acq_time      = 4.36731904[s]
X_angle         = 45[deg]
X_atn           = 3[dB]
X_pulse         = 5.95[us]
Irr_mode        = Off
Tri_mode        = Off
Dante_presat    = FALSE
Initial_wait    = 1[s]
Recvr_gain      = 34
Relaxation_delay = 5[s]
Repetition_time = 9.36731904[s]
Temp_get        = 0[dc]
```





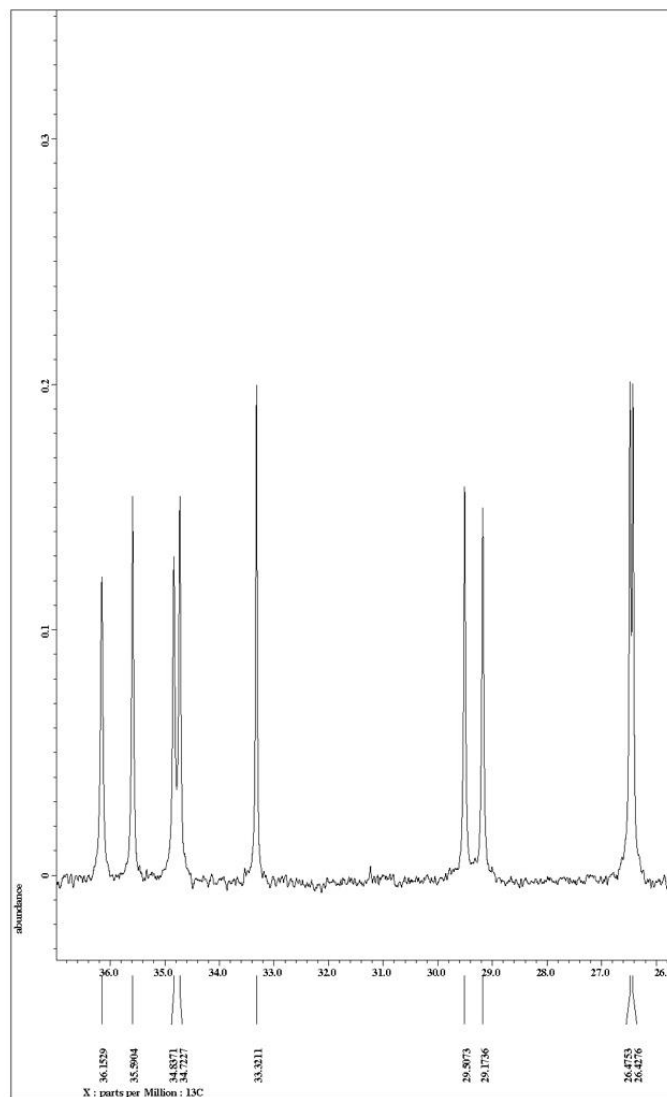
15

Filename = TIM_13C_216-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_216
 Solvent = DMSO-D6
 Creation_time = 22-MAY-2019 23:46:33
 Revision_time = 10-FEB-2023 15:30:58
 Current_time = 10-FEB-2023 15:31:31

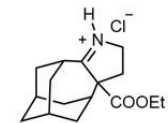
Comment = single pulse decouple
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1000
 Total_scans = 1000

X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 54
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 0[dc]



X : parts per Million : 13C



15

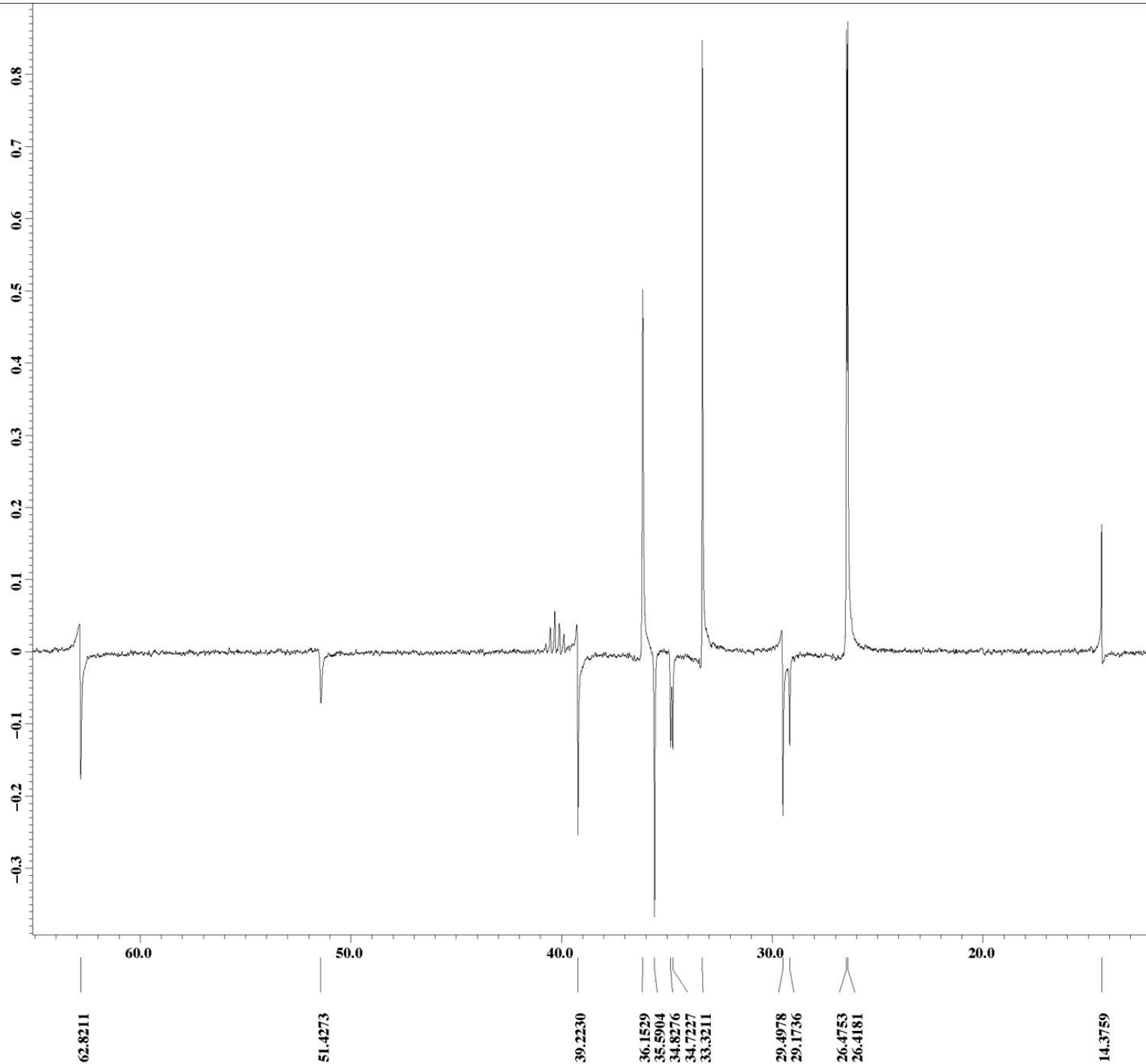
Filename = TIM_DEPT135_216-6.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM 216
 Solvent = DMSO-D6
 Creation_time = 23-MAY-2019 01:03:45
 Revision_time = 10-FEB-2023 15:33:26
 Current_time = 10-FEB-2023 15:33:51

Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1500
 Total_scans = 1500

X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 58
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 0[dc]

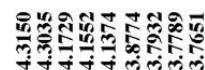
abundance



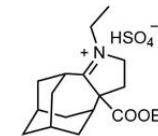
X: parts per Million : 13C



```
X_90_width      = 16.25[us]
X_acq_time      = 4.36731904[s]
X_angle         = 45[deg]
X_atn           = 3[dB]
X_pulse         = 8.125[us]
Irr_mode        = Off
Tri_mode        = Off
Dante_presat    = FALSE
Initial_wait    = 1[s]
Recvr_gain      = 48
Relaxation_delay = 5[s]
Repetition_time = 9.36731904[s]
Temp_get        = 0[dc]
```



X : parts per Million : 1H



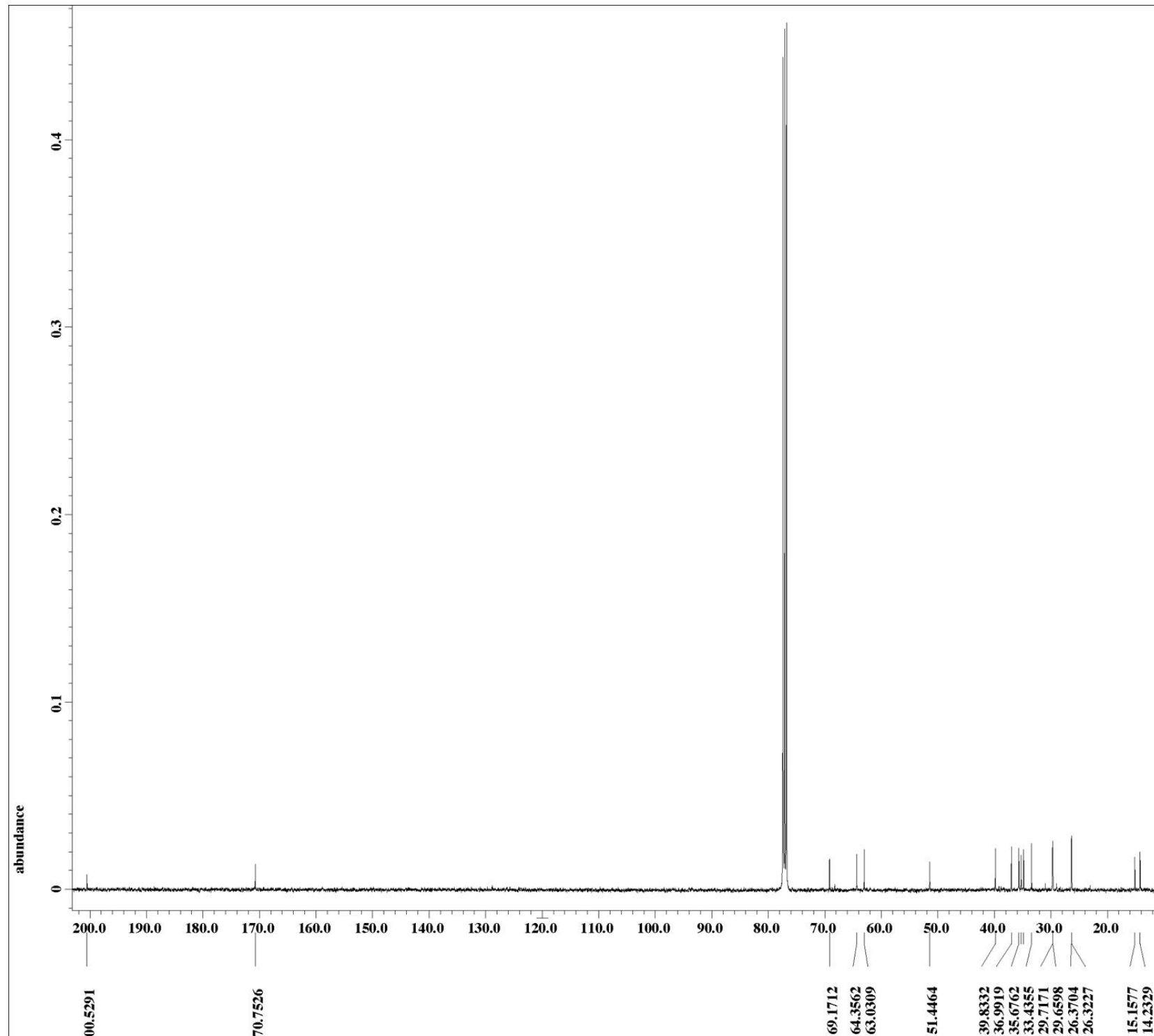
16

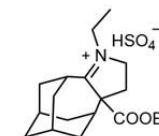
Filename = TIM_13C_59frdihydropy
 Author = delta
 Experiment = single pulse_dec
 Sample_id = TIM_59frdihydropyrrol
 Solvent = CHLOROFORM-D
 Creation_time = 29-MAY-2021 04:01:18
 Revision_time = 18-APR-2023 15:01:32
 Current_time = 18-APR-2023 15:02:14

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.0433312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 3000
 Total_scans = 3000

X_90_width = 8.16[us]
 X_acq_time = 1.0433312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Repetition_time = 3.0433312[s]
 Temp_get = 0[dc]





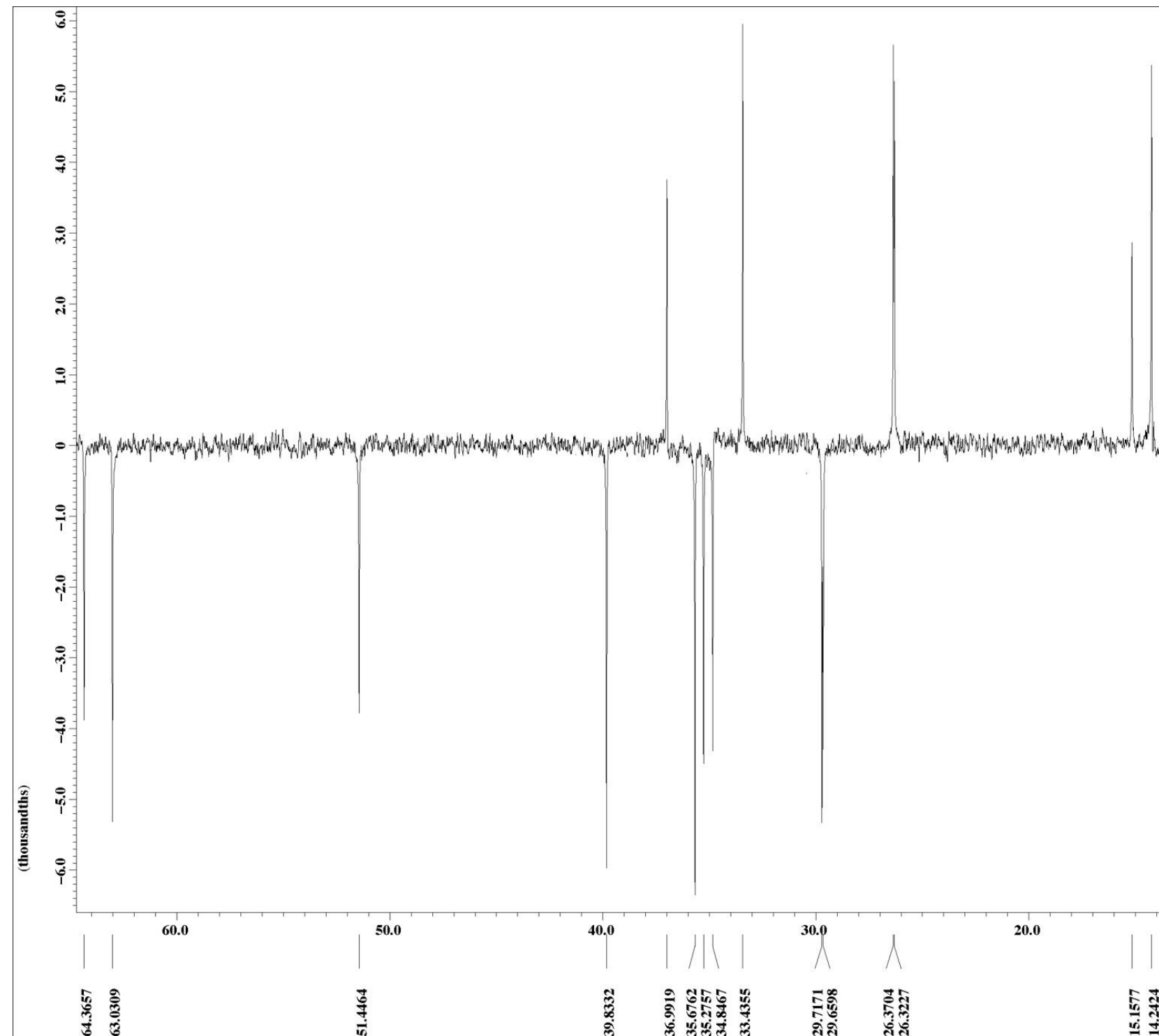
16

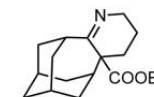
Filename = TIM_DEPT135_59frdihyd
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_59frdihydropyrrol
 Solvent = CHLOROFORM-D
 Creation_time = 29-MAY-2021 05:18:02
 Revision_time = 18-APR-2023 15:02:44
 Current_time = 18-APR-2023 15:04:03

Comment = DEPT with decoupling
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1500
 Total_scans = 1500

X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 16.25[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 30
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 24.375[us]
 Temp_get = 0[dc]





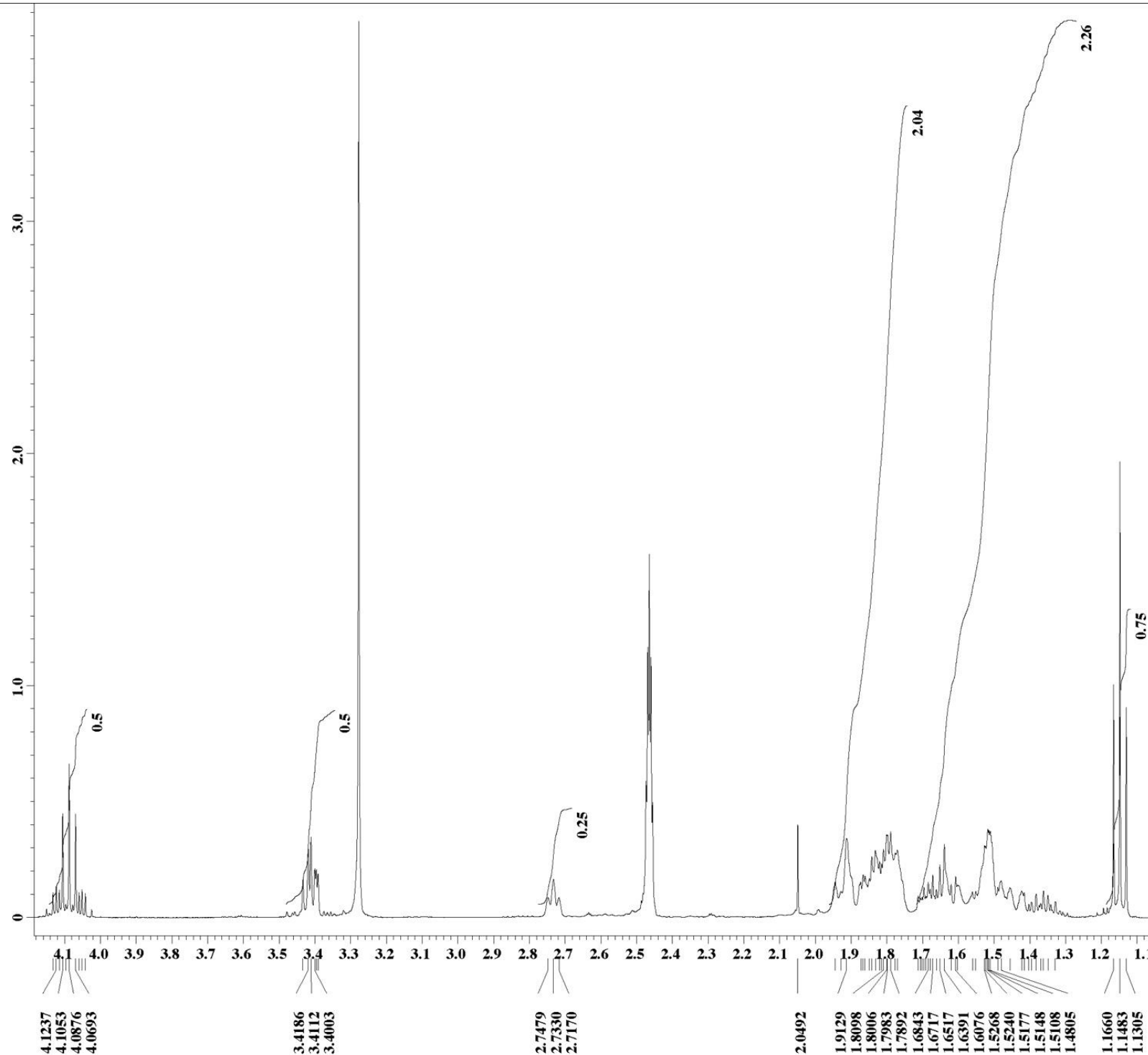
17

Filename = TIM_1H_acrCNadductH2N
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_acrCNadductH2Nidi
 Solvent = DMSO-D6
 Creation_time = 29-JUN-2021 15:49:28
 Revision_time = 10-FEB-2023 17:54:04
 Current_time = 10-FEB-2023 17:55:02

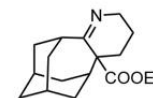
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 16.25[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 8.125[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 44
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 0[dc]



X : parts per Million : 1H



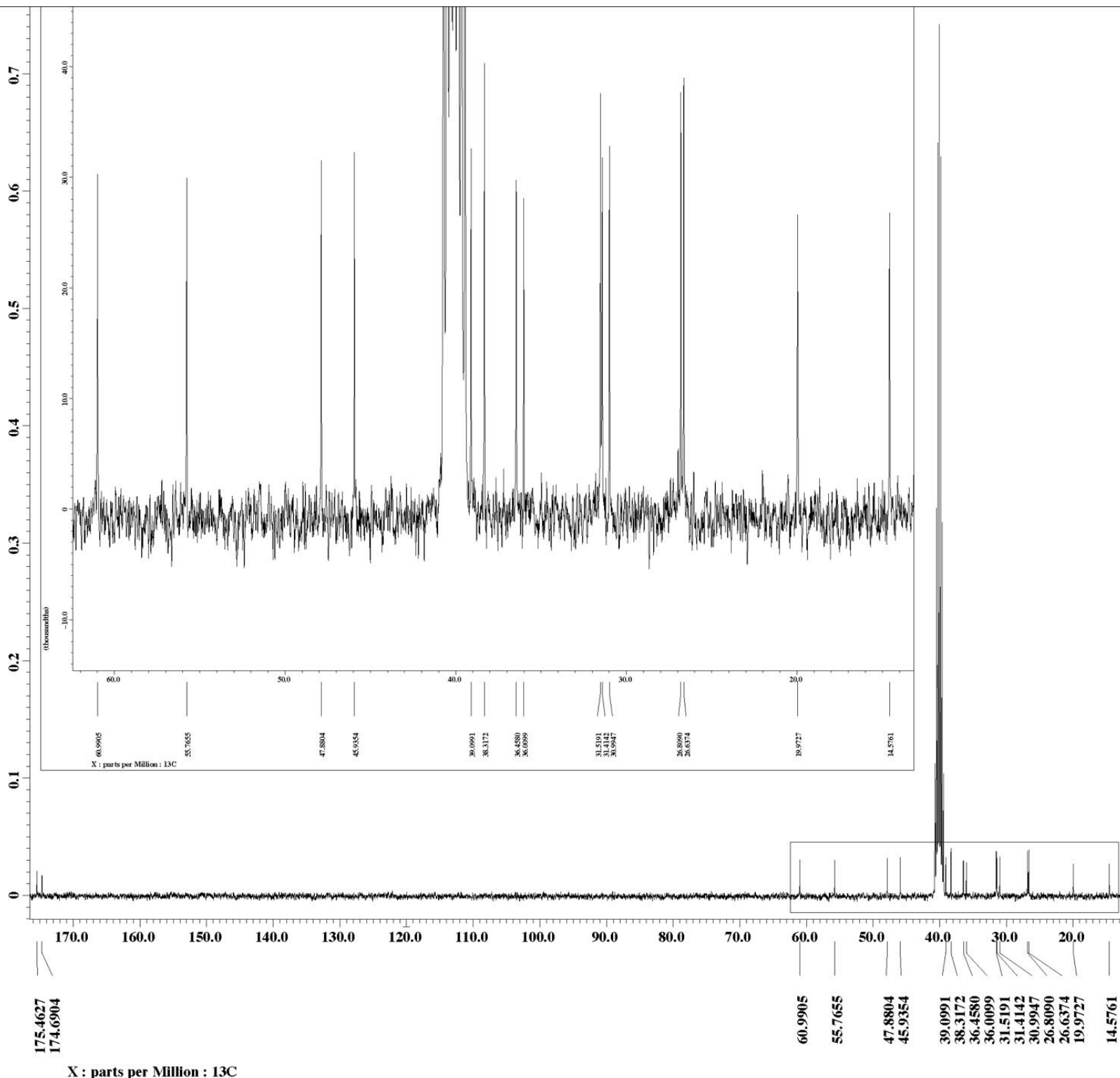
17

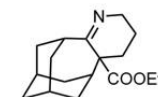
Filename = TIM_13C_acrCNadductH2
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_acrCNadductH2Nidi
 Solvent = DMSO-D6
 Creation_time = 29-JUN-2021 16:10:04
 Revision_time = 18-APR-2023 15:53:53
 Current_time = 18-APR-2023 15:56:38

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 356
 Total_scans = 356

X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 0[dc]





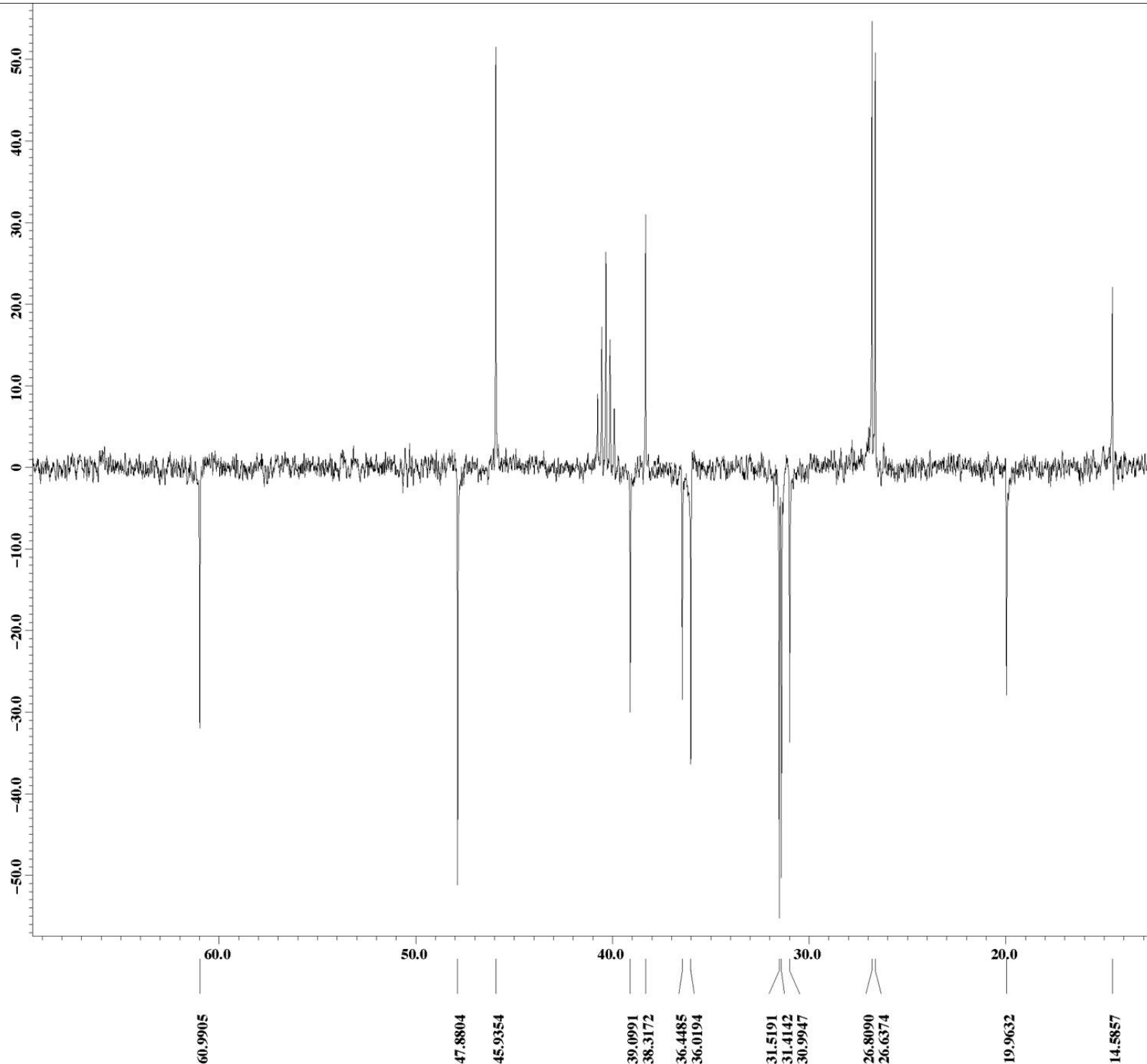
17

Filename = TIM_DEPT135_acrCNaddu
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_acrCNadductH2Nidi
 Solvent = DMSO-D6
 Creation_time = 29-JUN-2021 21:12:05
 Revision_time = 18-APR-2023 15:56:53
 Current_time = 18-APR-2023 15:57:11

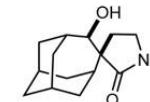
Comment = DEPT with decoupling
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 500
 Total_scans = 500

X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 16.25[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 24.375[us]
 Temp_get = 0[dc]



X : parts per Million : 13C



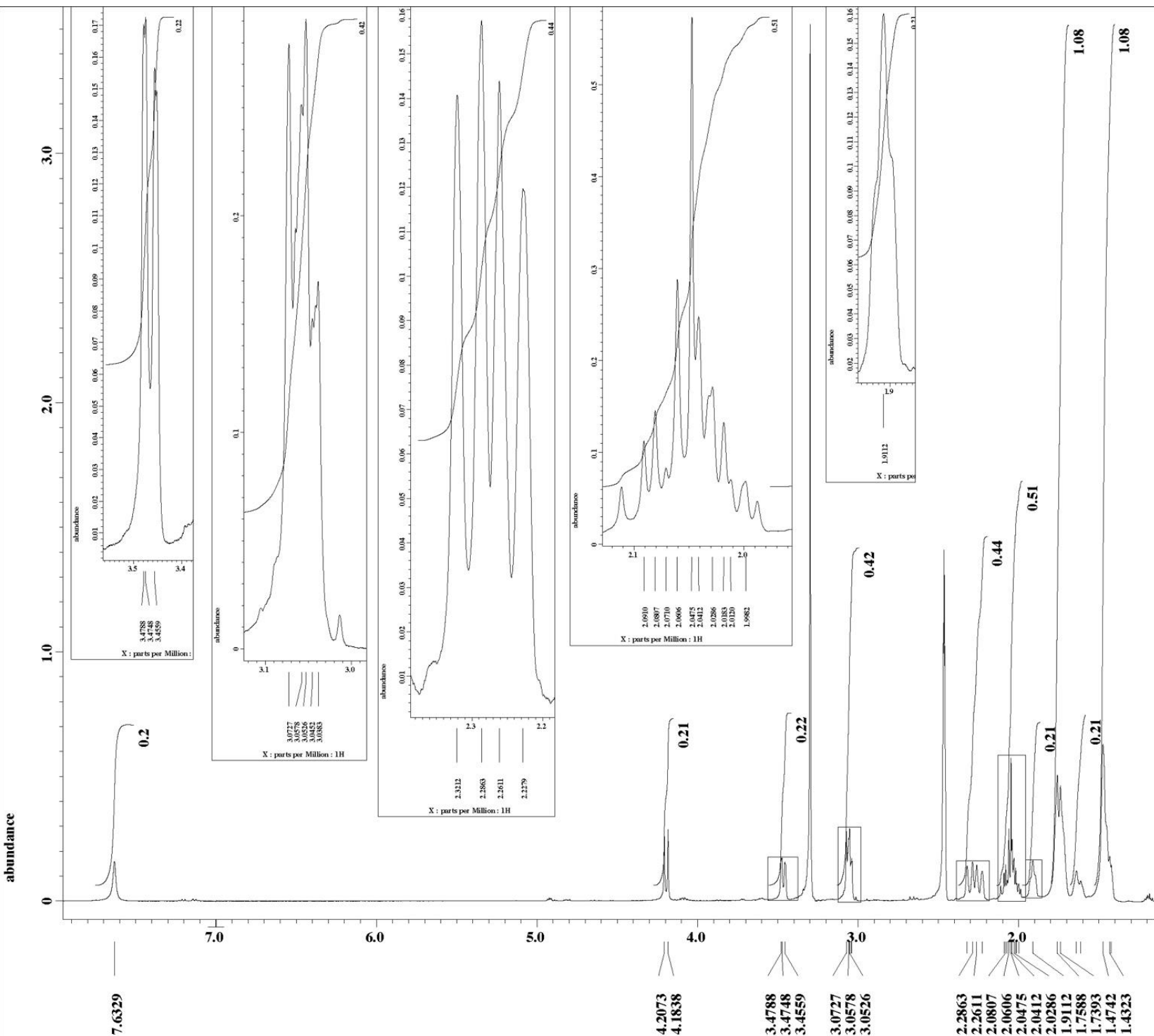
18

Filename = TIM_1H_OHAcetonitrile
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_OHAcetonitrileH2N
 Solvent = DMSO-D6
 Creation_time = 4-JUN-2021 11:08:26
 Revision_time = 10-FEB-2023 14:12:48
 Current_time = 10-FEB-2023 14:15:44

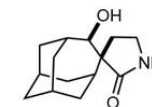
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 16.25[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 8.125[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 40
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 0[dc]



X : parts per Million : 1H



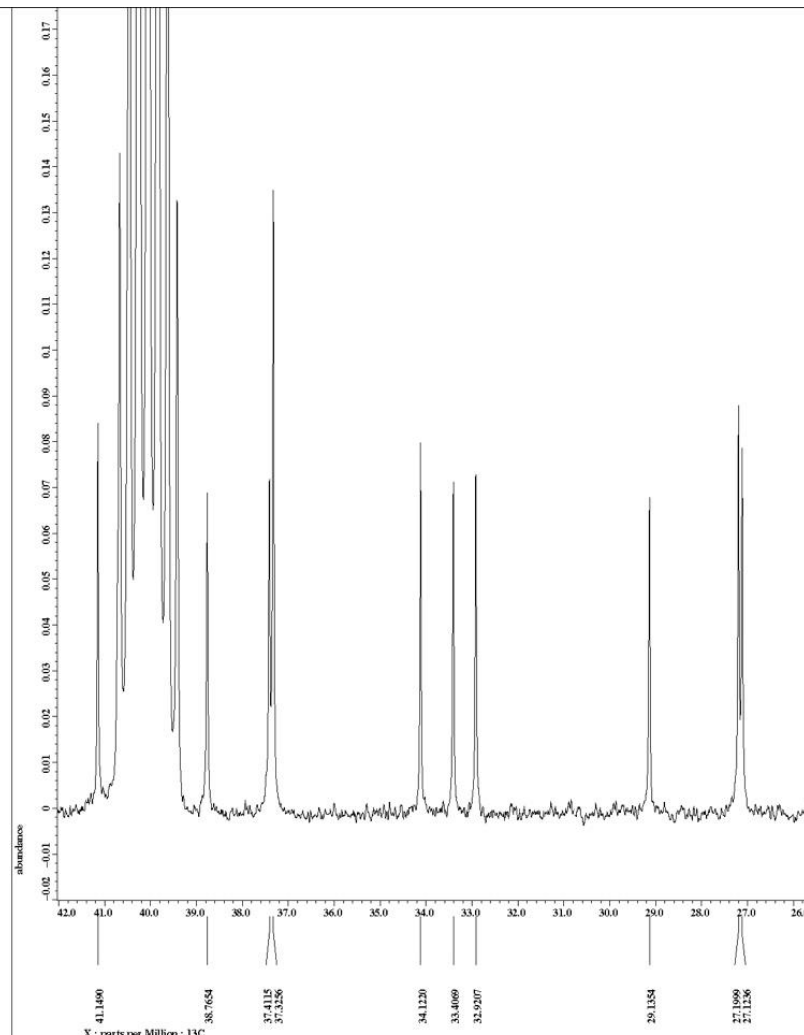
18

Filename = TIM_13C_OHAcetonitril
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_OHAcetonitrileH2N
 Solvent = DMSO-D6
 Creation_time = 4-JUN-2021 12:01:43
 Revision_time = 10-FEB-2023 14:45:32
 Current_time = 10-FEB-2023 14:46:58

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1000
 Total_scans = 1000

X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 0[dc]



81.9475

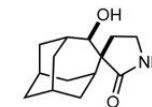
56.4997

41.1490
38.7654
37.4115
37.3256
34.1220
33.4069
32.9207
27.1999
27.1236

X : parts per Million : 13C

179.7056

abundance



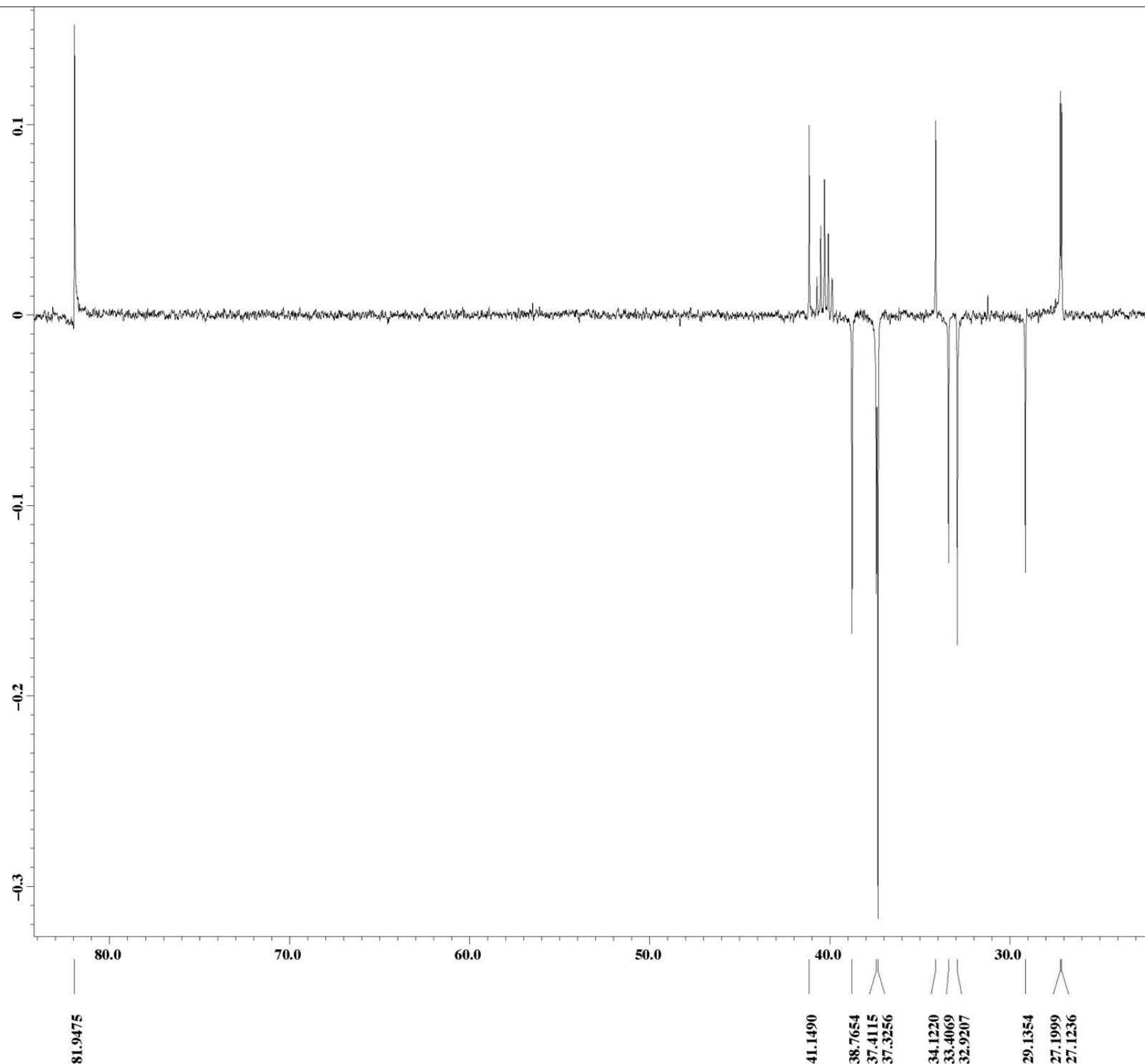
18

Filename = TIM_DEPT135_OHAcetoni
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_OHAcetonitrileH2N
 Solvent = DMSO-D6
 Creation_time = 4-JUN-2021 12:24:06
 Revision_time = 10-FEB-2023 14:46:29
 Current_time = 10-FEB-2023 14:49:15

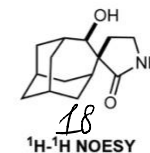
 Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 432
 Total_scans = 432

 X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 16.25[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 24.375[us]
 Temp_get = 0[dc]



X : parts per Million : 13C

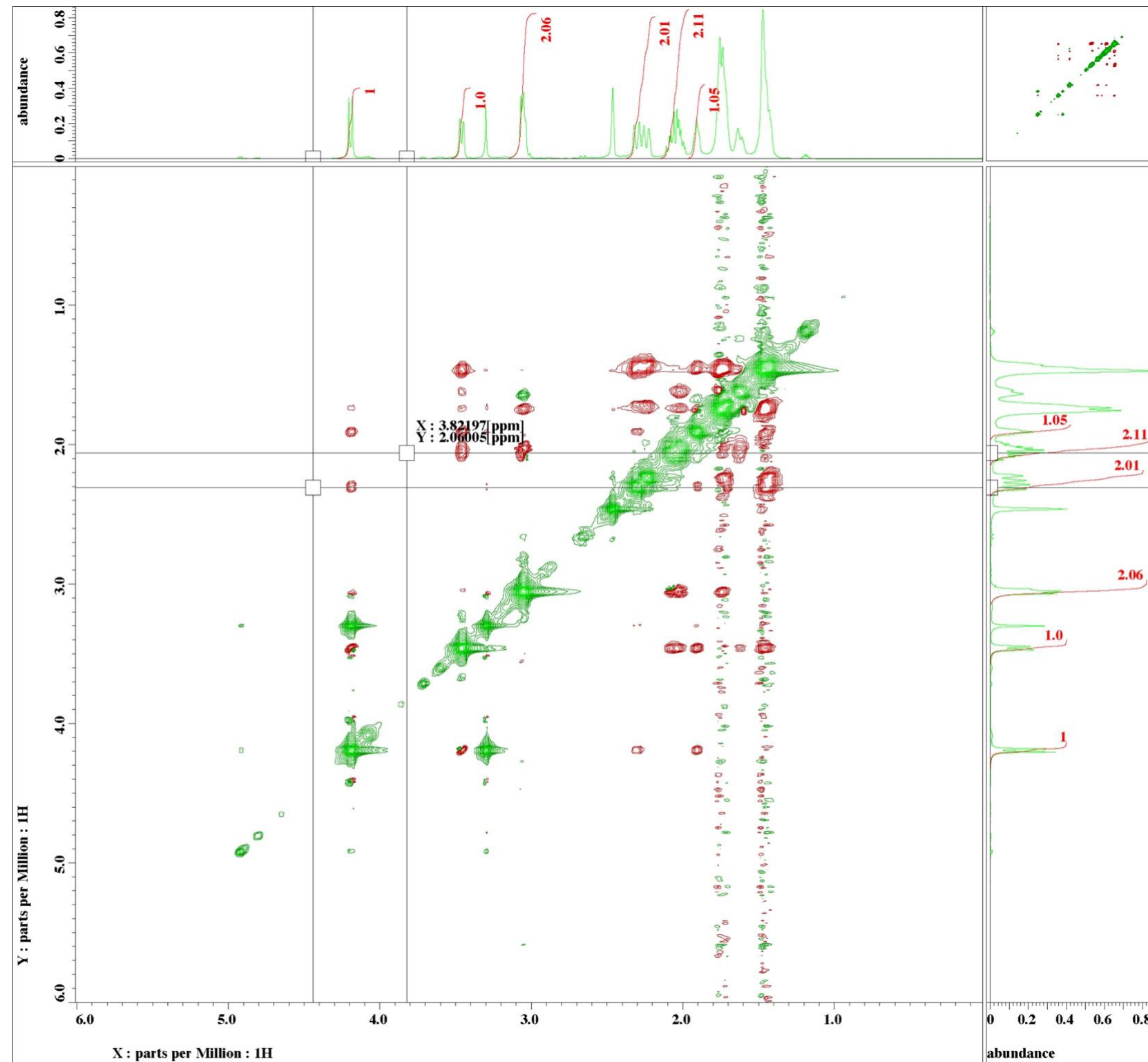


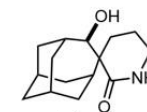
Filename = TIM_NOESY_170-2.jdf
 Author = delta
 Experiment = noesy_phase_zqf_
 Sample_id = TIM_170
 Solvent = DMSO-D6
 Creation_time = 21-APR-2023 15:33:19
 Revision_time = 21-APR-2023 18:20:27
 Current_time = 22-APR-2023 10:38:22

Comment = phase sensitive noesy
 Data_format = 2D COMPLEX COMPLEX
 Dim_size = 409, 1024
 Dim_title = 1H 1H
 Dim_units = [ppm] [ppm]
 Dimensions = X Y
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 0.17047552[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 3[ppm]
 X_points = 512
 X_prescans = 4
 X_resolution = 5.86594486[Hz]
 X_sweep = 3.00336377[kHz]
 Y_domain = 1H
 Y_freq = 399.78219838[MHz]
 Y_offset = 3[ppm]
 Y_points = 512
 Y_prescans = 0
 Y_resolution = 4.68510123[Hz]
 Y_sweep = 2.39877183[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 = 2048

X_acq_time = 0.17047552[s]
 X_atn = 3.5[dB]
 X_pulse = 5.5[us]
 Y_acq_time = 0.21344256[s]
 Y_pl_correction = 180.0
 Irr_mode = Off
 Tri_mode = Off
 Adiabatic_pulse = 50[ms]
 B1_attn = 43.80211242[dB]
 Band_width = 30[kHz]
 Chirp_atn = 31.19788758[dB]
 Chirp_pulse = 50[ms]
 Chirp_shape = CHIRP
 Chirp_smooth = 10[%]
 Dante_presat = FALSE





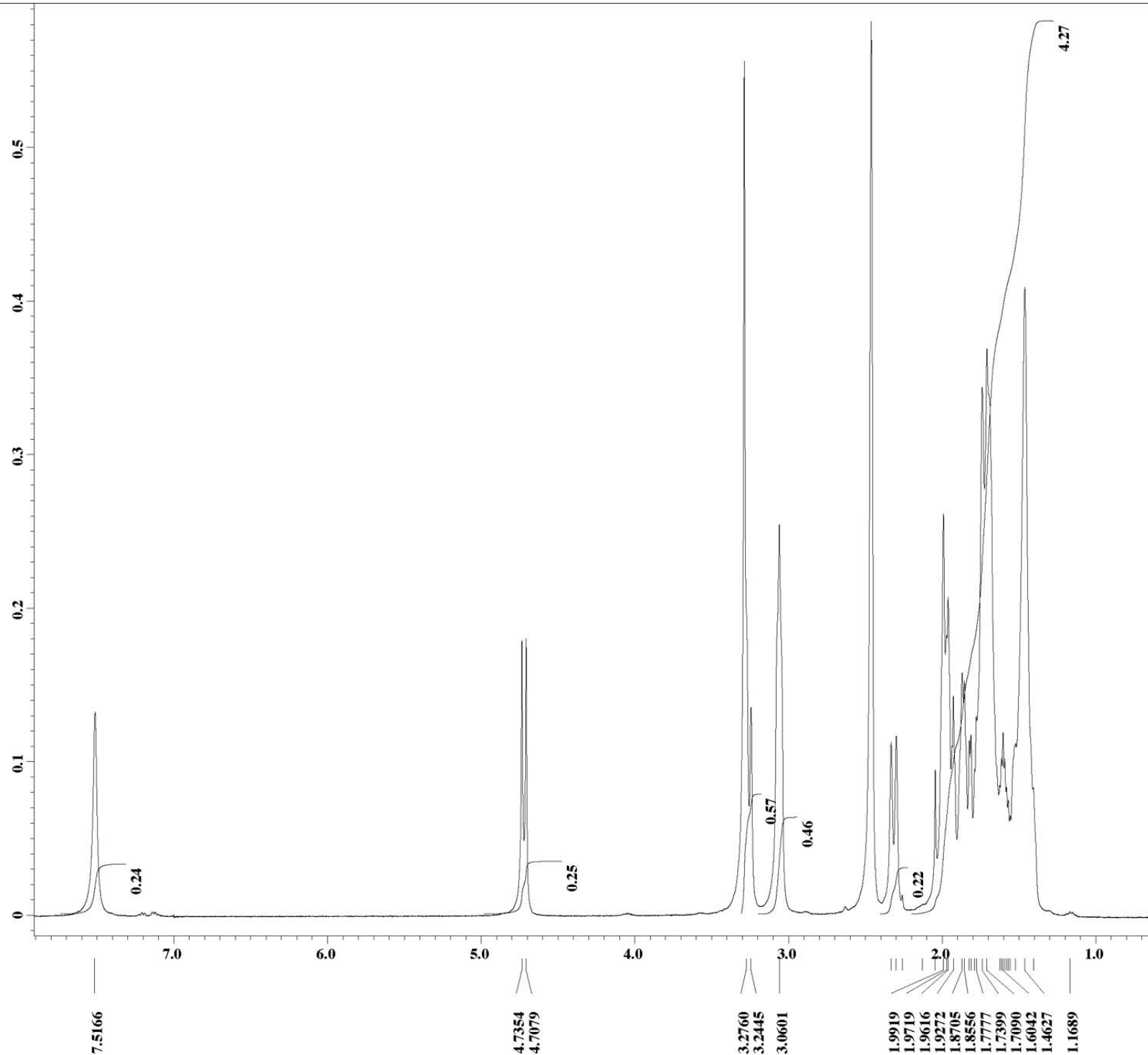
19

Filename = TIM_1H_OHhAd(CO2Et) (C)
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_OHhAd(CO2Et) (CH2)
 Solvent = DMSO-D6
 Creation_time = 1-JUN-2021 05:18:07
 Revision_time = 10-FEB-2023 13:55:13
 Current_time = 10-FEB-2023 13:56:53

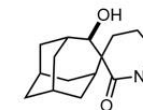
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 16.25[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 8.125[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 36
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 0[dc]



X : parts per Million : 1H



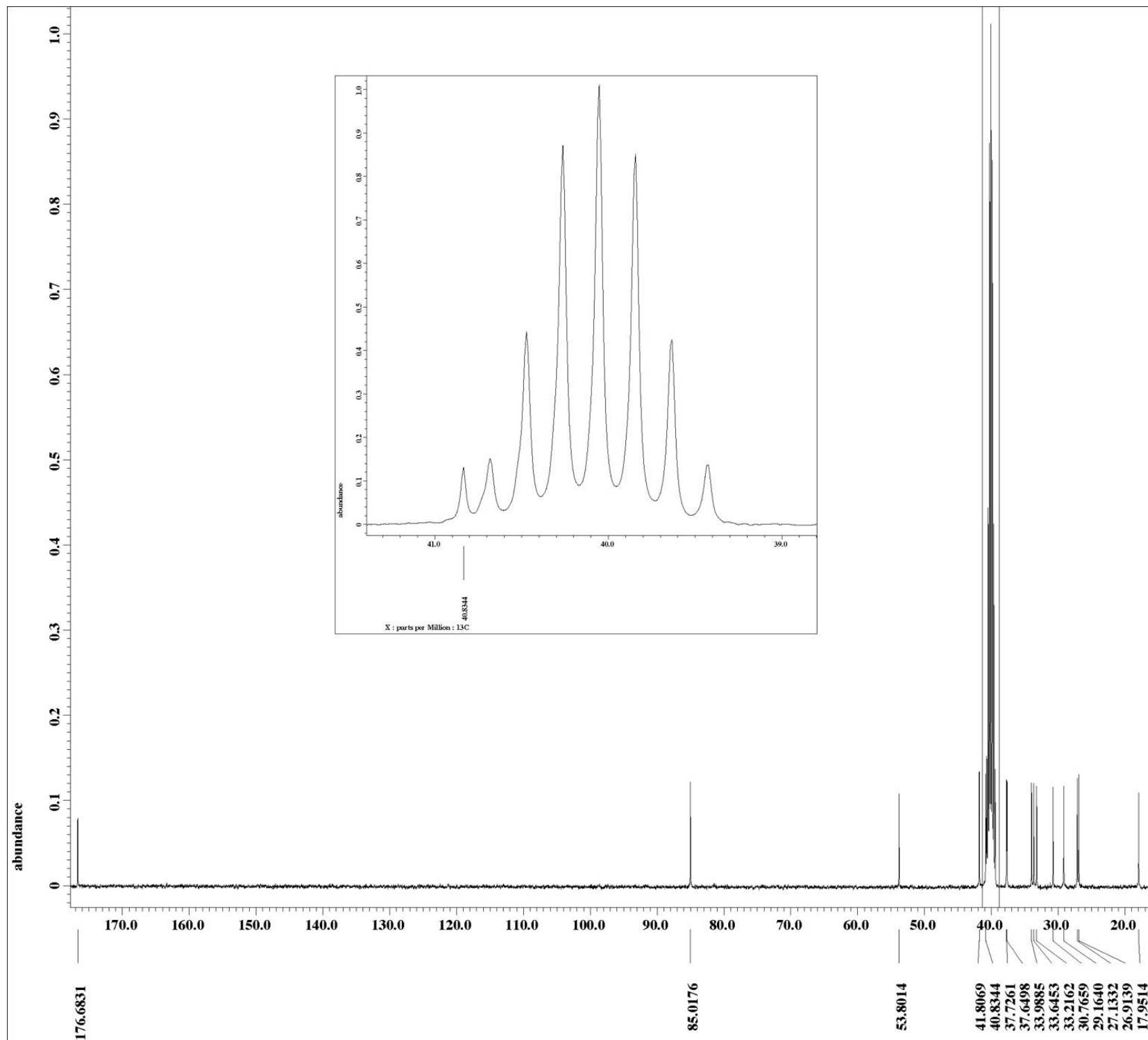
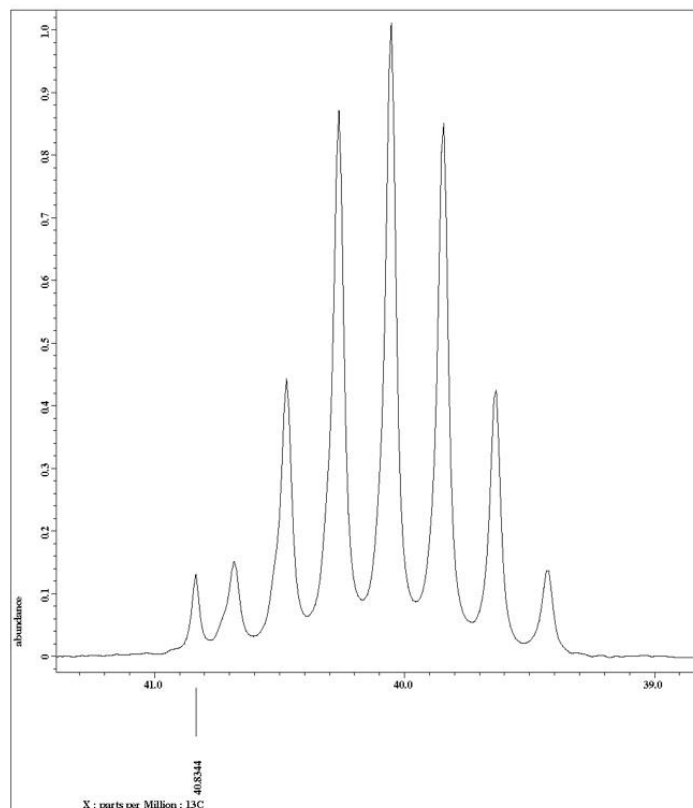
19

Filename = TIM_13C_OHhAd(CO2Et) (
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_OHhAd(CO2Et) (CH2)
 Solvent = DMSO-D6
 Creation_time = 1-JUN-2021 06:11:30
 Revision_time = 10-FEB-2023 13:57:43
 Current_time = 10-FEB-2023 13:59:54

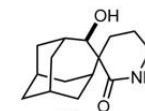
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766 [T] (400 [MHz])
 X_acq_duration = 1.04333312 [s]
 X_domain = 13C
 X_freq = 100.52530333 [MHz]
 X_offset = 120 [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 = 1000
 Total_scans = 1000

X_90_width = 8.16 [us]
 X_acq_time = 1.04333312 [s]
 X_angle = 30 [deg]
 X_atn = 7.8 [dB]
 X_pulse = 2.72 [us]
 Irr_atn_dec = 22.703 [dB]
 Irr_atn_noe = 22.703 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 52
 Relaxation_delay = 2 [s]
 Repetition_time = 3.04333312 [s]
 Temp_get = 0 [dC]



X : parts per Million : 13C



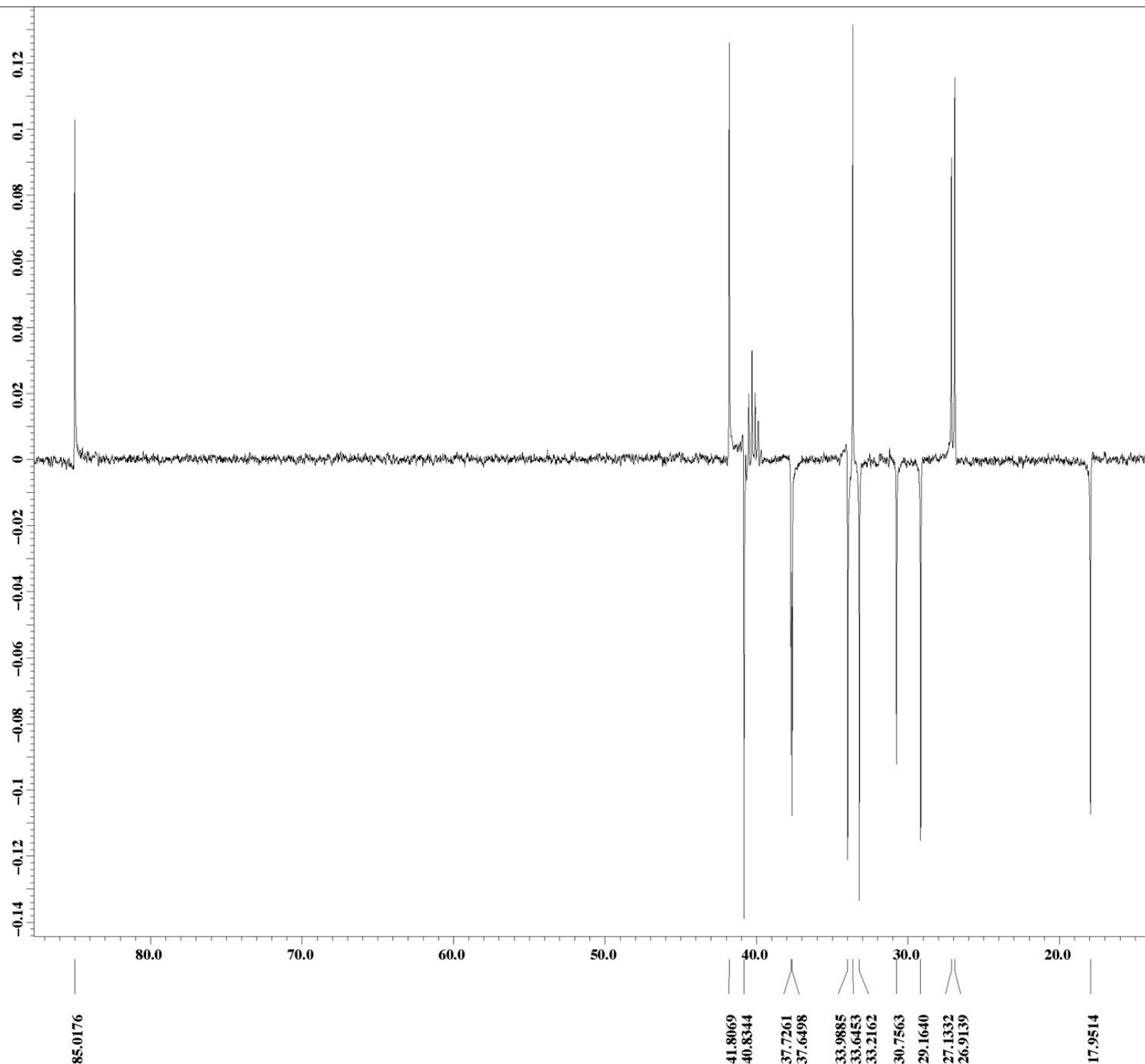
19

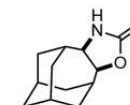
Filename = TIM_DEPT135_OHhAd(CO2
Author = delta
Experiment = dept.ex2
Sample_id = TIM_OHhAd(CO2Et)(CH2)
Solvent = DMSO-D6
Creation_time = 1-JUN-2021 06:37:19
Revision_time = 10-FEB-2023 14:01:44
Current_time = 10-FEB-2023 14:02:39

Comment = DEPT with decoupling
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.0433312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 120[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 = 500
Total_scans = 500

X_acq_time = 1.0433312[s]
X_atn = 7.8[dB]
X_pulse = 8.16[us]
Irr_atn = 3[dB]
Irr_atn_dec = 22.703[dB]
Irr_noise = WALTZ
Irr_pulse = 16.25[us]
Decoupling = TRUE
Initial_wait = 1[s]
J_constant = 140[Hz]
Recvr_gain = 46
Relaxation_delay = 2[s]
Selection_angle = 135[deg]
Selection_pulse = 24.375[us]
Temp_get = 0[dc]





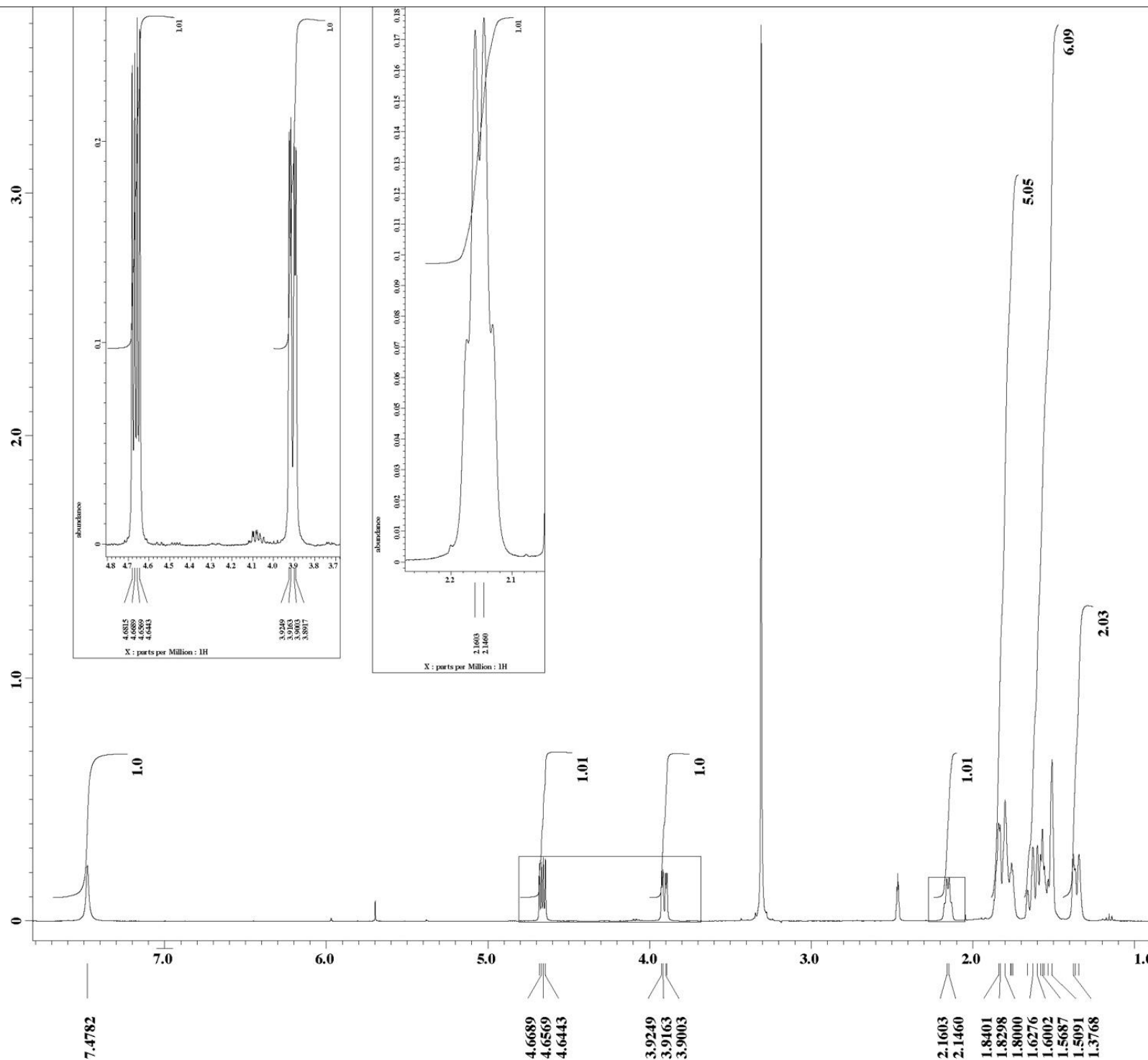
20

Filename = TIM_1H_204-6.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_204
 Solvent = DMSO-D6
 Creation_time = 12-APR-2019 23:47:35
 Revision_time = 13-FEB-2023 13:20:22
 Current_time = 13-FEB-2023 13:21:17

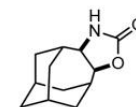
Comment = single pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 11.9[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 5.95[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 30
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 28.9[dc]



X : parts per Million : 1H



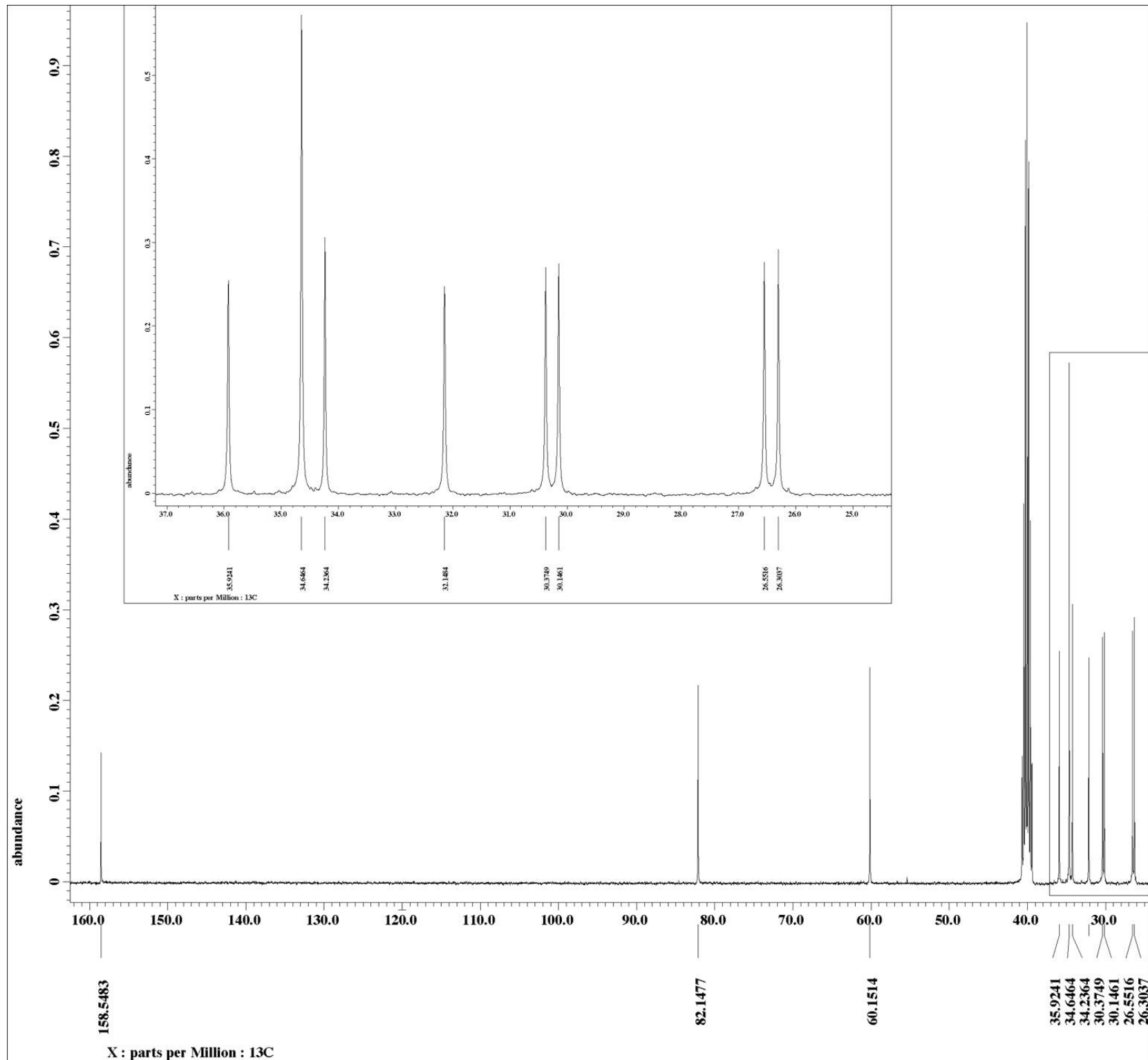
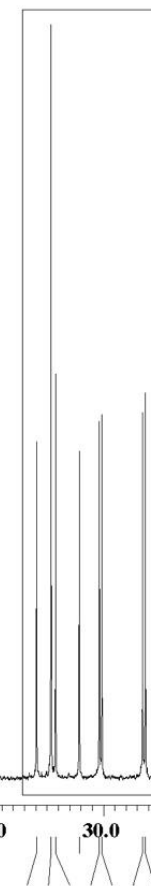
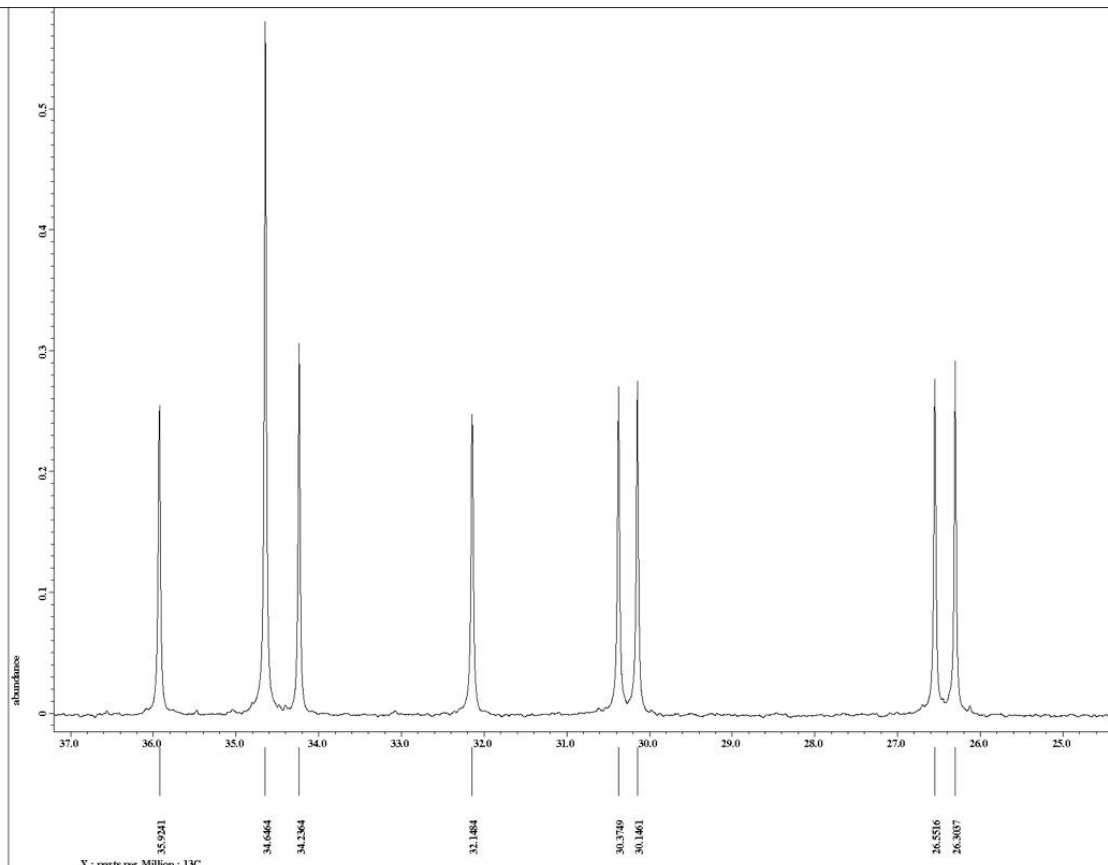
20

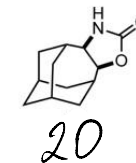
Filename = TIM_13C_204-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_204
 Solvent = DMSO-D6
 Creation_time = 13-APR-2019 01:31:34
 Revision_time = 13-FEB-2023 13:16:17
 Current_time = 13-FEB-2023 13:16:56

Comment = single pulse decouple
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 2000
 Total_scans = 2000

X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 28.9[dc]



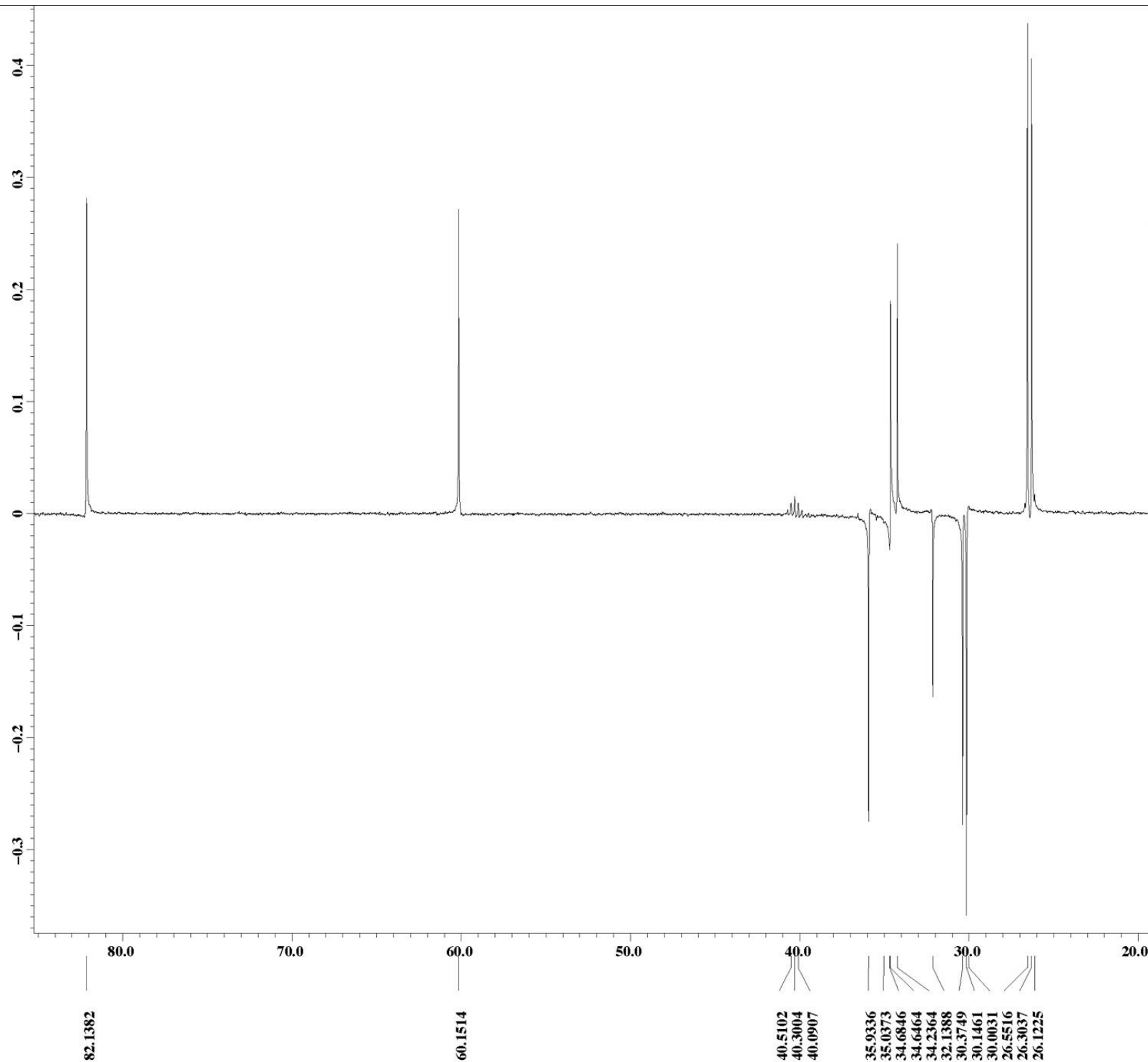


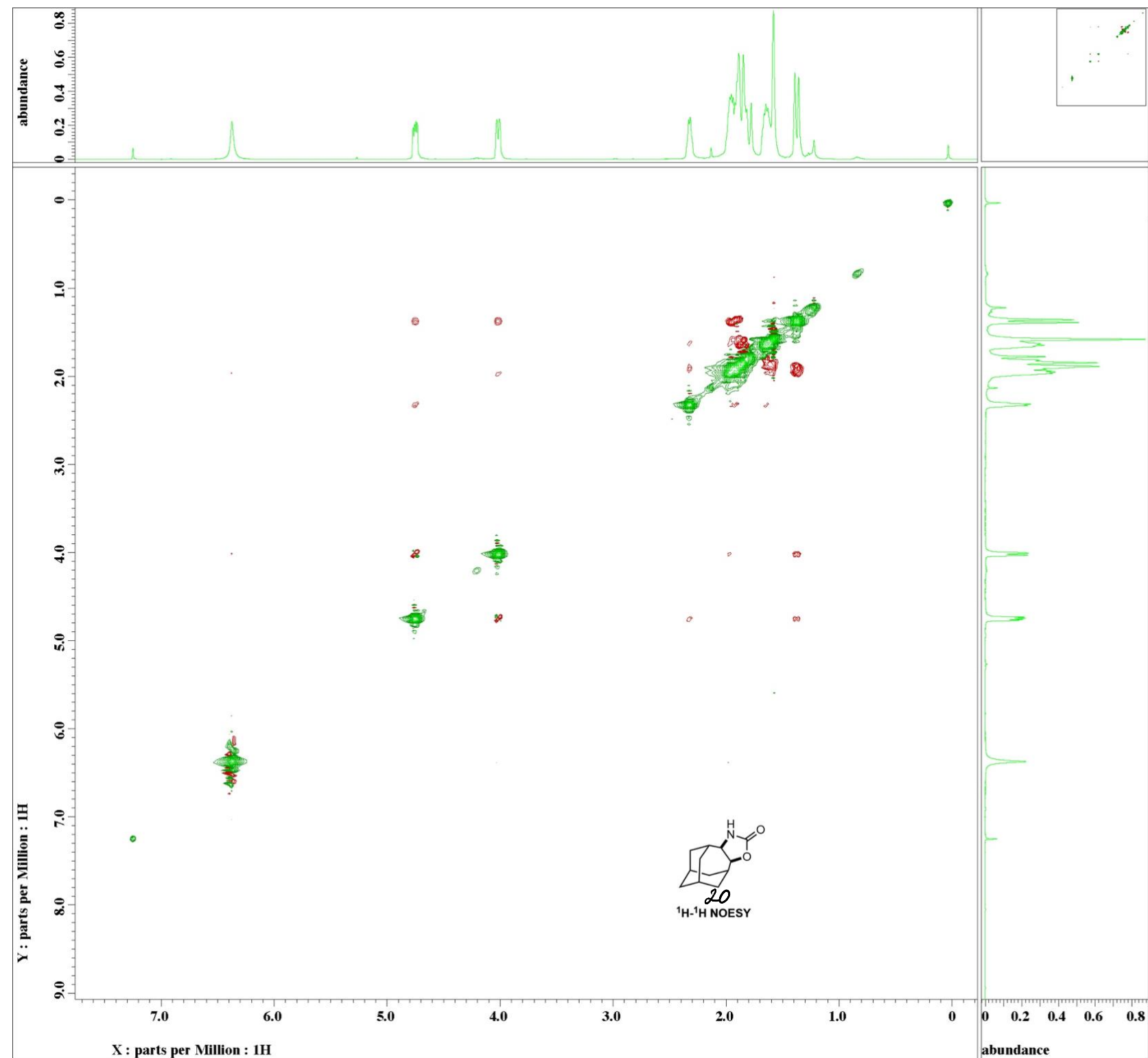
Filename = TIM_DEPT135_204-2.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM 204
 Solvent = DMSO-D6
 Creation_time = 13-APR-2019 02:22:52
 Revision_time = 13-FEB-2023 13:21:25
 Current_time = 13-FEB-2023 13:21:44

Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1000
 Total_scans = 1000

X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 30.3[degC]





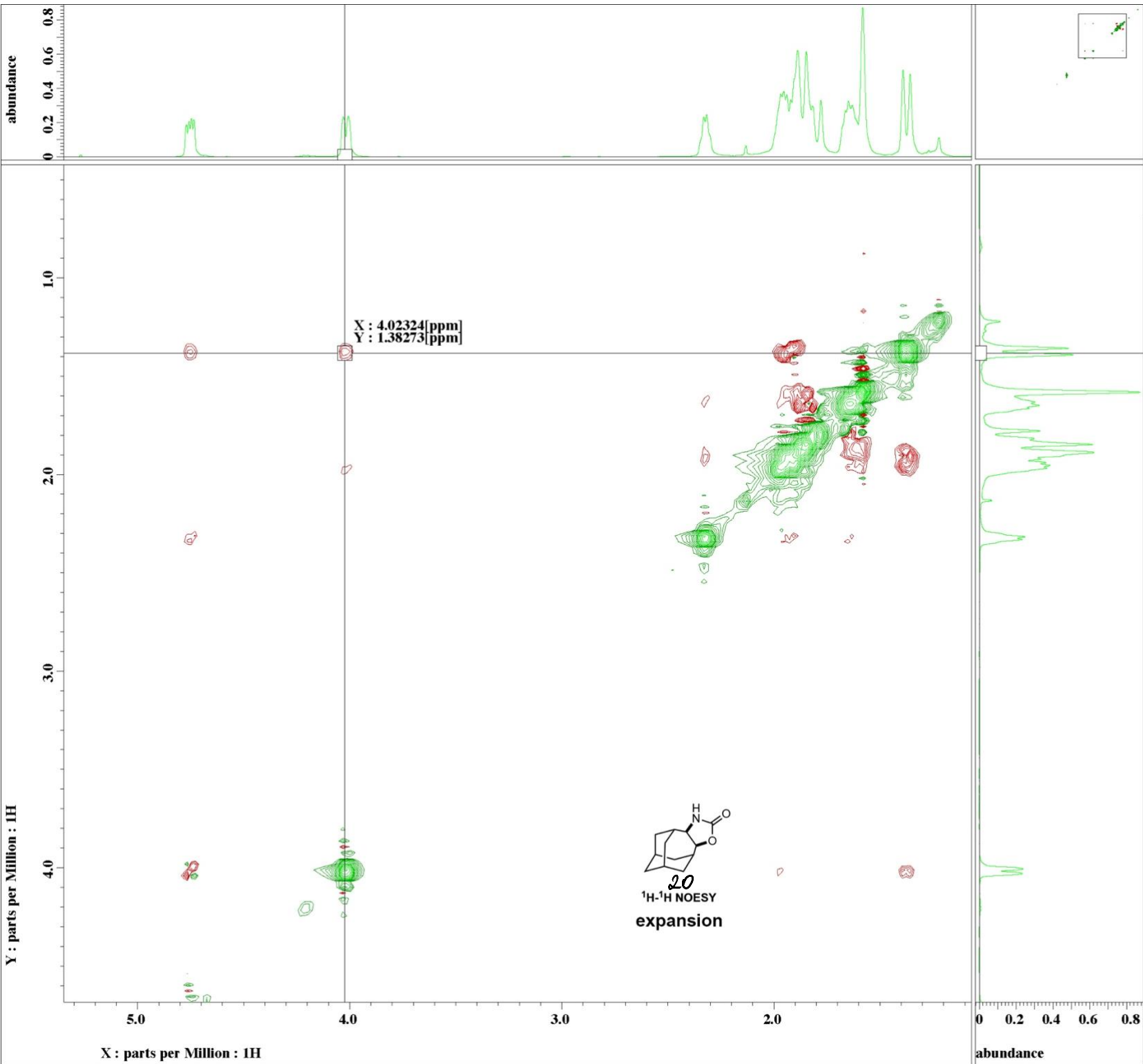
----- PROCESSING PARAMETERS -----
sexp : 5.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
ppm
machinephase
[transpose]
sexp : 5.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 2
fft : 1 : TRUE : TRUE
ppm
machinephase

Filename = TIM_NOESY_204-2.jdf
Author = delta
Experiment = noesy_phase_zqf_
Sample_id = TIM_204
Solvent = CHLOROFORM-D
Creation_time = 25-JUN-2019 07:49:17
Revision_time = 19-APR-2023 17:44:38
Current_time = 19-APR-2023 17:47:06

Comment = phase sensitive noesy
Data_format = 2D COMPLEX COMPLEX
Dim_size = 819, 512
Dim_title = 1H 1H
Dim_units = [ppm] [ppm]
Dimensions = X Y
Site = ECX 400
Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 0.13656064[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 7 [ppm]
X_points = 1024
X_prescans = 4
X_resolution = 7.3227542 [Hz]
X_sweep = 7.4985003 [kHz]
Y_domain = 1H
Y_freq = 399.78219838 [MHz]
Y_offset = 7 [ppm]
Y_points = 256
Y_prescans = 0
Y_resolution = 23.42719204 [Hz]
Y_sweep = 5.99736116 [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 = 2048

X_acq_time = 0.13656064[s]
X_atn = 3 [dB]
X_pulse = 11.9 [us]
Y_acq_time = 42.68544 [ms]
Y_pl_correction = 180
Irr_mode = Off
Tri_mode = Off
Adiabatic_pulse = 50 [ms]
Bi_attn = 43.80211242 [dB]
Band_width = 30 [kHz]
Chirp_atn = 31.19788758 [dB]
Chirp_pulse = 50 [ms]
Chirp_shape = CHIRP
Chirp_smooth = 10 [%]
Dante_presat = FALSE



----- PROCESSING PARAMETERS -----

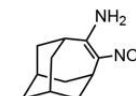
sexp : 5.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
ppm
machinephase
[transpose]
sexp : 5.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 2
fft : 1 : TRUE : TRUE
ppm
machinephase

Filename = TIM_NOESY_204-2.jdf
Author = delta
Experiment = noesy_phase_zqf_
Sample_id = TIM_204
Solvent = CHLOROFORM-D
Creation_time = 25-JUN-2019 07:49:17
Revision_time = 19-APR-2023 17:44:38
Current_time = 19-APR-2023 17:48:10

Comment = phase sensitive noesy
Data_format = 2D COMPLEX COMPLEX
Dim_size = 819, 512
Dim_title = 1H 1H
Dim_units = [ppm] [ppm]
Dimensions = X Y
Site = ECX 400
Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 0.13656064[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 7[ppm]
X_points = 1024
X_prescans = 4
X_resolution = 7.3227542[Hz]
X_sweep = 7.4985003[kHz]
Y_domain = 1H
Y_freq = 399.78219838[MHz]
Y_offset = 7[ppm]
Y_points = 256
Y_prescans = 0
Y_resolution = 23.42719204[Hz]
Y_sweep = 5.99736116[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 = 2048

X_acq_time = 0.13656064[s]
X_atn = 3[dB]
X_pulse = 11.9[us]
Y_acq_time = 42.68544[ms]
Y_pl_correction = 180
Irr_mode = Off
Tri_mode = Off
Adiabatic_pulse = 50[ms]
Bi_attn = 43.80211242[dB]
Band_width = 30[kHz]
Chirp_atn = 31.19788758[dB]
Chirp_pulse = 50[ms]
Chirp_shape = CHIRP
Chirp_smooth = 10[%]
Dante_presat = FALSE



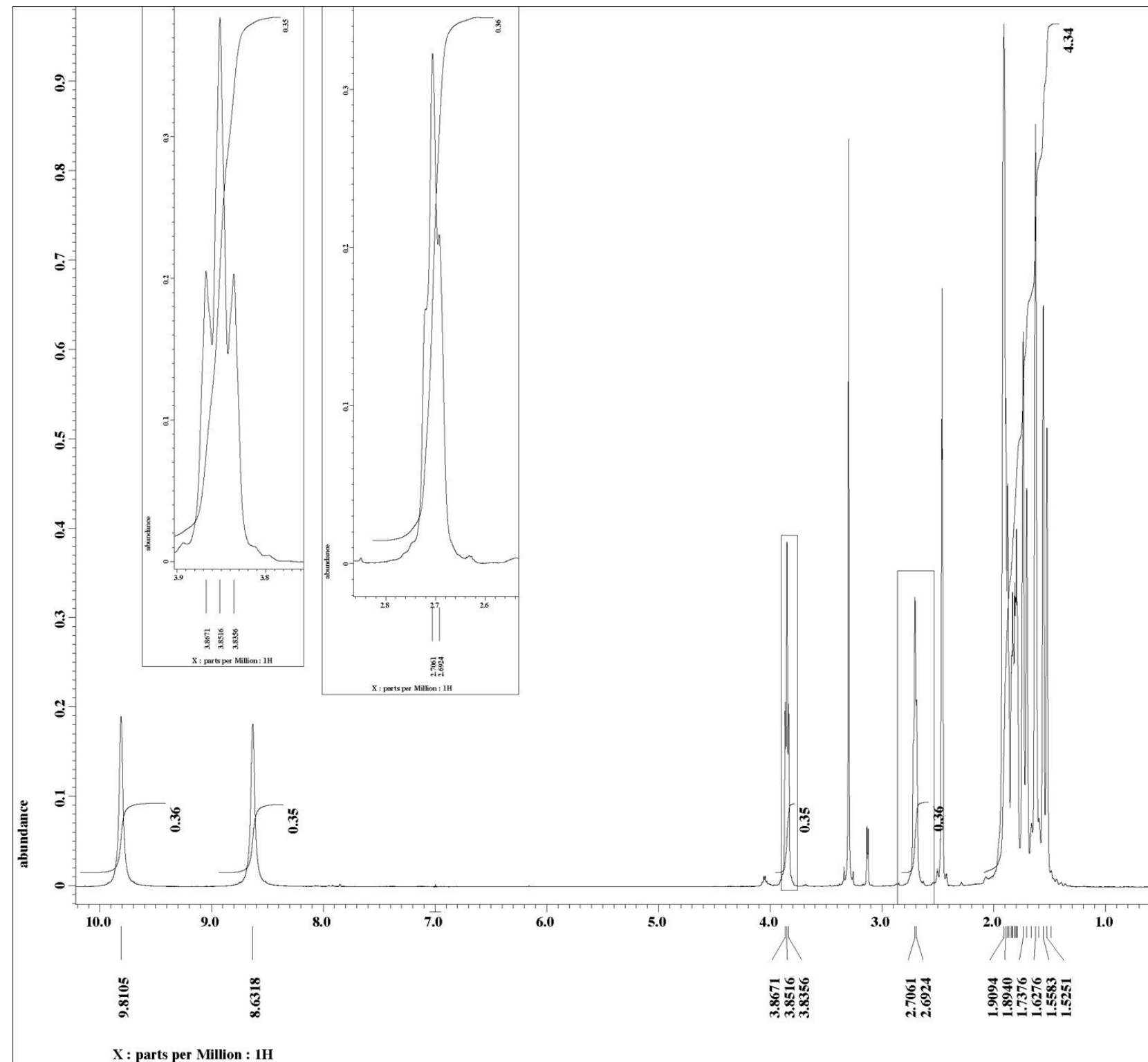
21

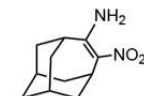
Filename = TIM_1H_nitroKE_leucar
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_nitroKE_leucart
 Solvent = DMSO-D6
 Creation_time = 30-NOV-2021 14:14:44
 Revision_time = 10-FEB-2023 12:05:59
 Current_time = 10-FEB-2023 12:06:18

Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 5.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3.5[dB]
 X_pulse = 2.75[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 24
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 0[dc]





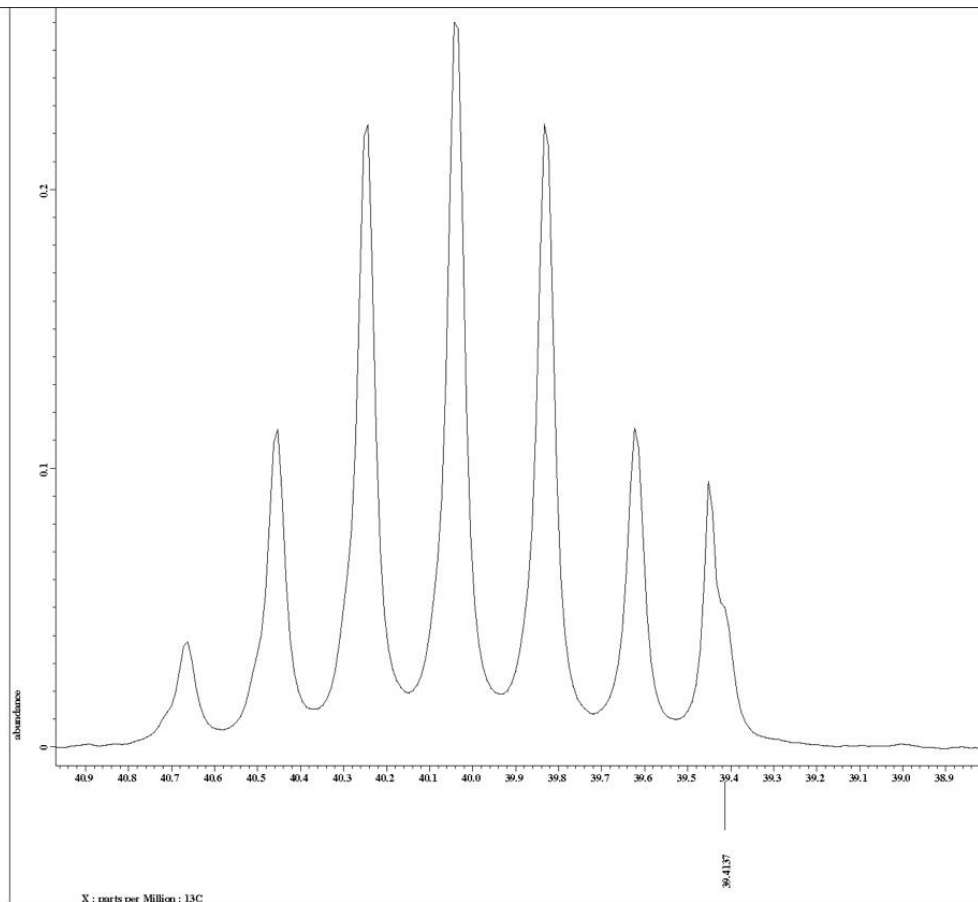
21

Filename = TIM_13C_nitroKEleucar
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_nitroKEleucart
 Solvent = DMSO-D6
 Creation_time = 27-NOV-2021 08:36:50
 Revision_time = 10-FEB-2023 12:37:01
 Current_time = 10-FEB-2023 12:37:28

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

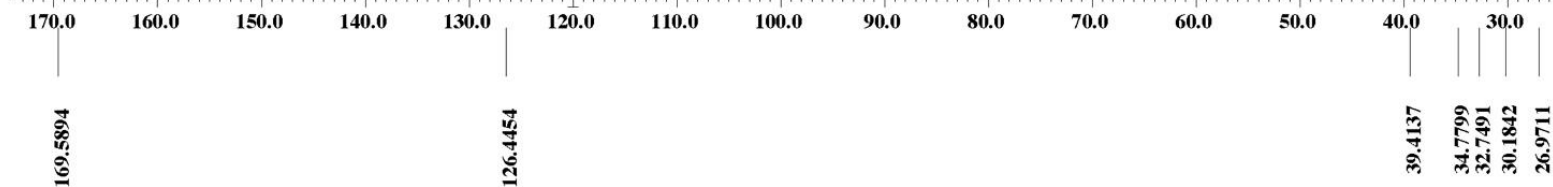
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.0433312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 3000
 Total_scans = 3000

X_90_width = 13.87[us]
 X_acq_time = 1.0433312[s]
 X_angle = 30[deg]
 X_atn = 5.2[dB]
 X_pulse = 4.62333333[us]
 Irr_atn_dec = 29.907[dB]
 Irr_atn_noe = 29.907[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Repetition_time = 3.0433312[s]
 Temp_get = 0[dc]

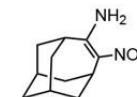


X : parts per Million : 13C

abundance



X : parts per Million : 13C



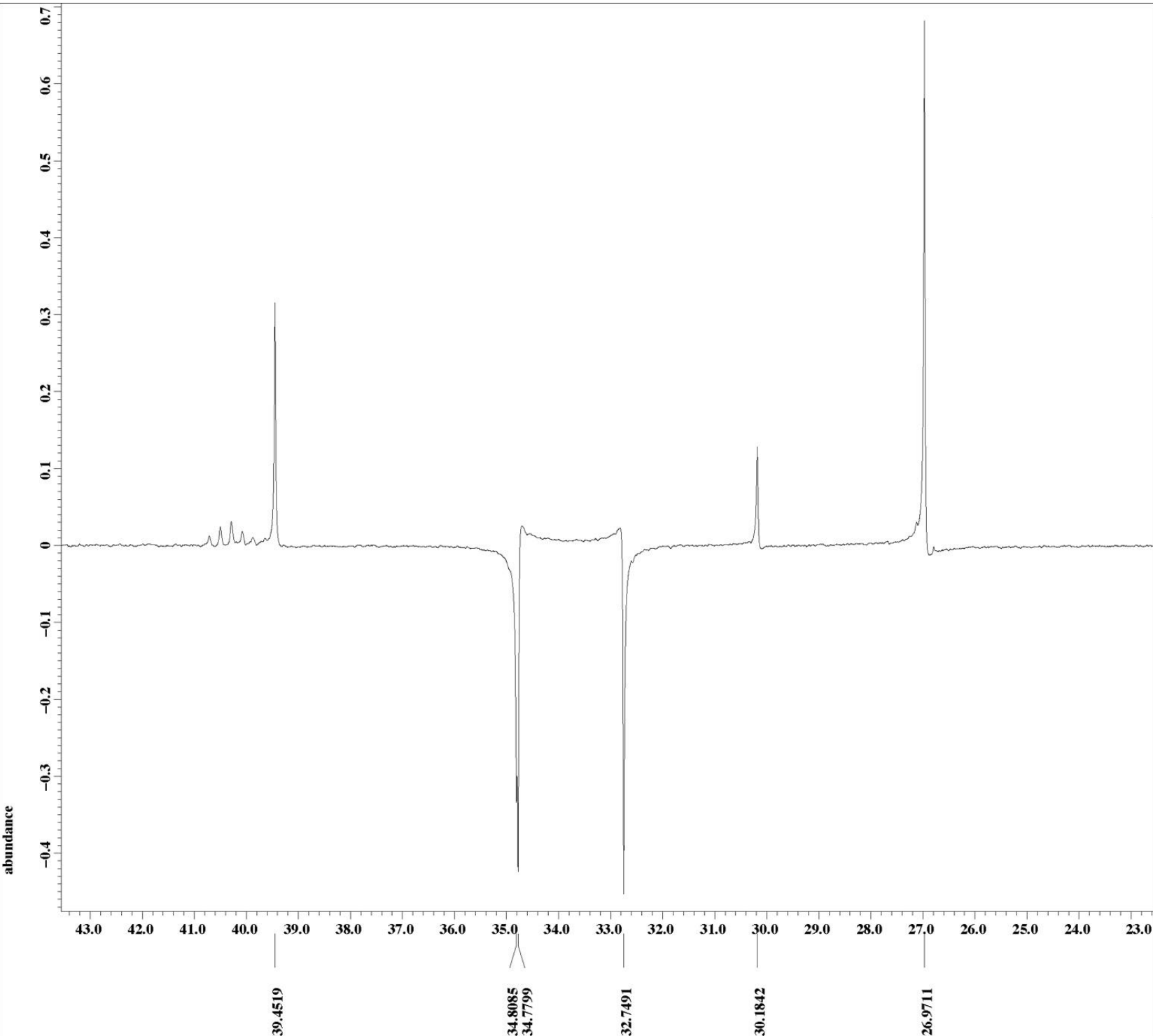
21

Filename = TIM_DEPT135_nitroKELe
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_nitroKELeucart
 Solvent = DMSO-D6
 Creation_time = 27-NOV-2021 09:54:02
 Revision_time = 10-FEB-2023 12:39:22
 Current_time = 10-FEB-2023 12:39:46

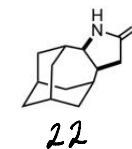
Comment = DEPT with decoupling
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1500
 Total_scans = 1500

X_acq_time = 1.04333312[s]
 X_atn = 5.2[dB]
 X_pulse = 13.87[us]
 Irr_atn = 3.5[dB]
 Irr_atn_dec = 29.907[dB]
 Irr_noise = WALTZ
 Irr_pulse = 5.5[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 8.25[us]
 Temp_get = 0[dc]



X : parts per Million : 13C

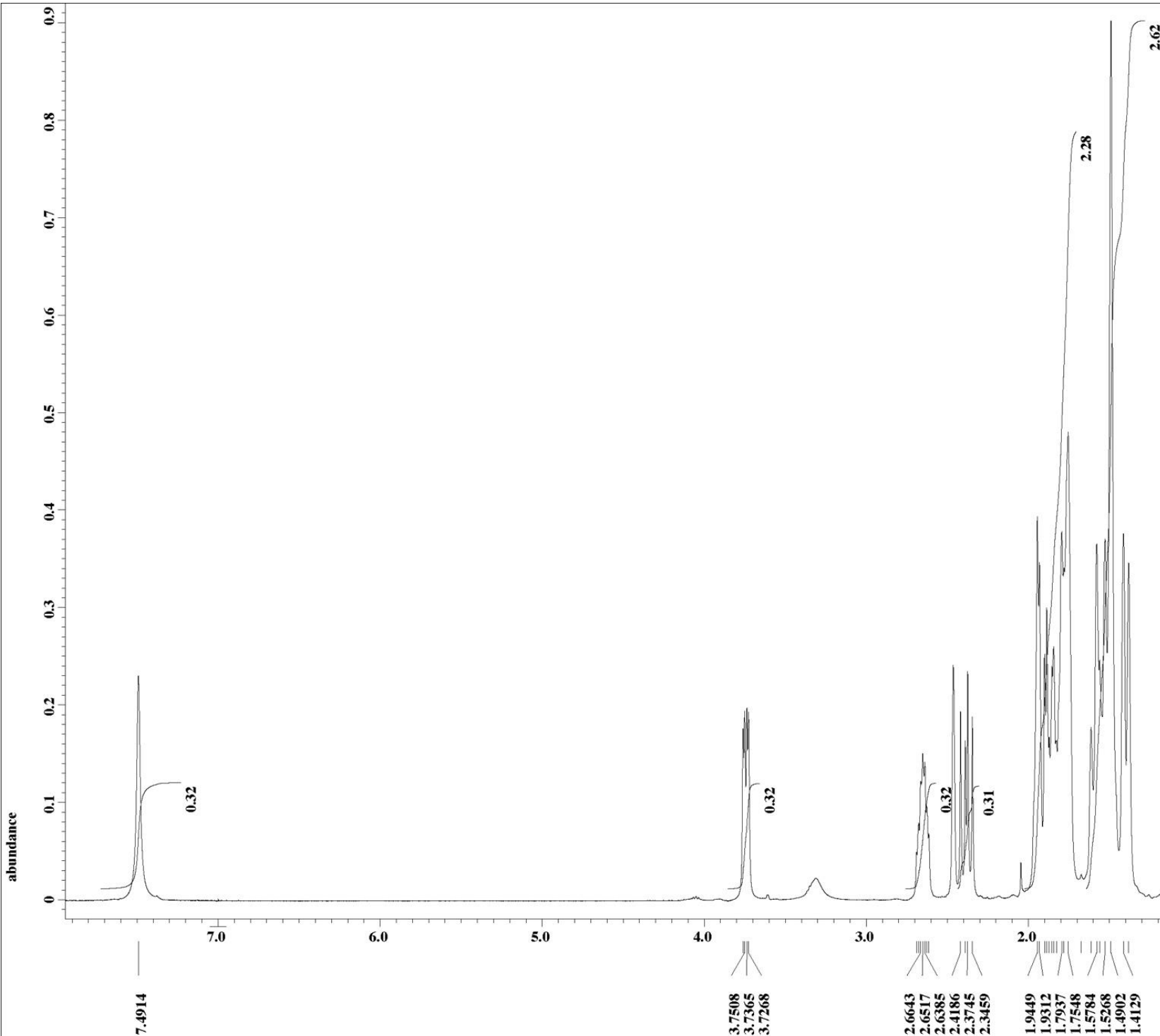


Filename = TIM_1H_147-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_147
 Solvent = DMSO-D6
 Creation_time = 10-OCT-2018 14:27:52
 Revision_time = 18-APR-2023 19:11:59
 Current_time = 18-APR-2023 19:12:21

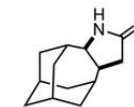
Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 11.9[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 5.95[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 30
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 21.6[degC]



X : parts per Million : 1H



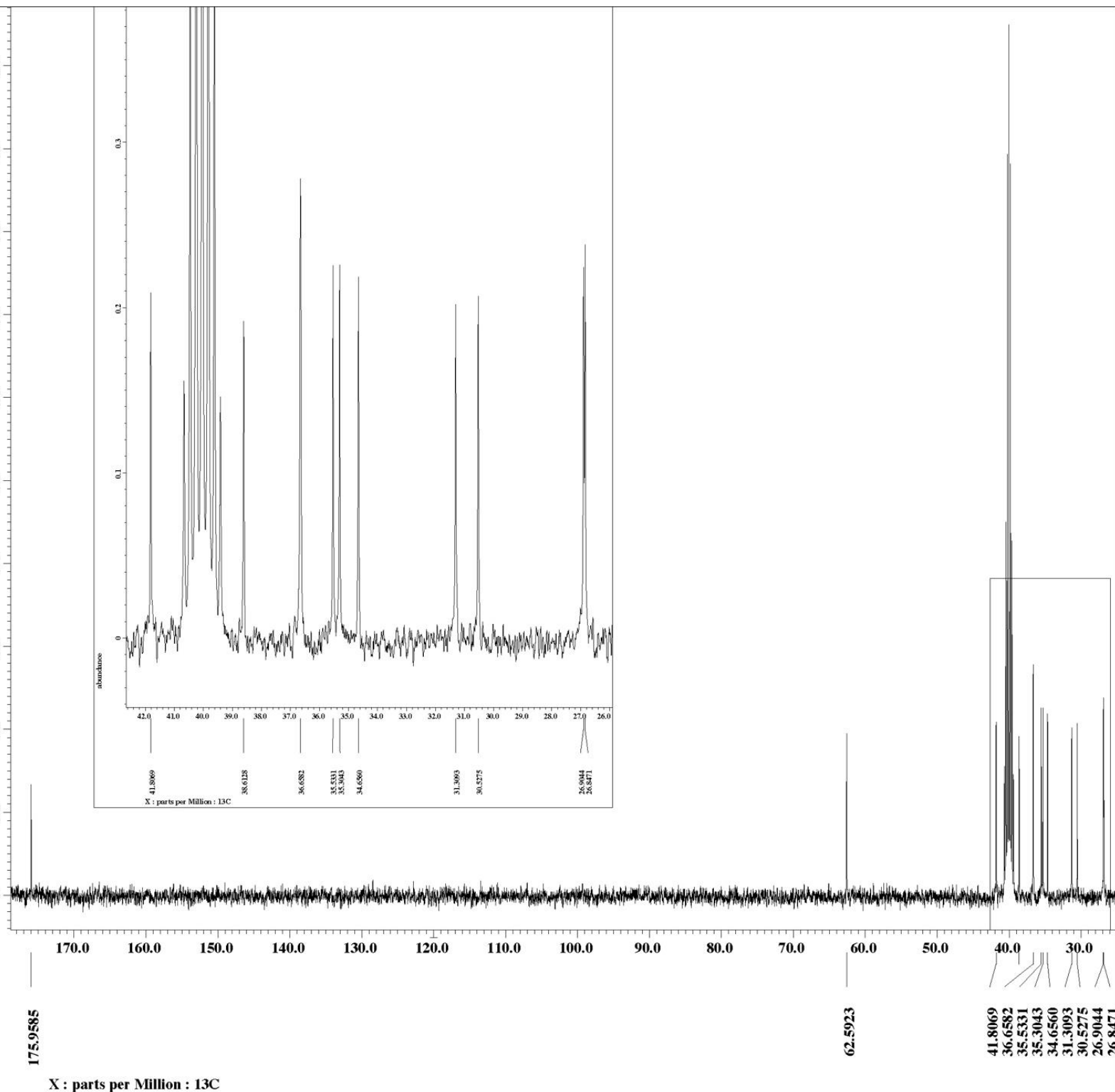
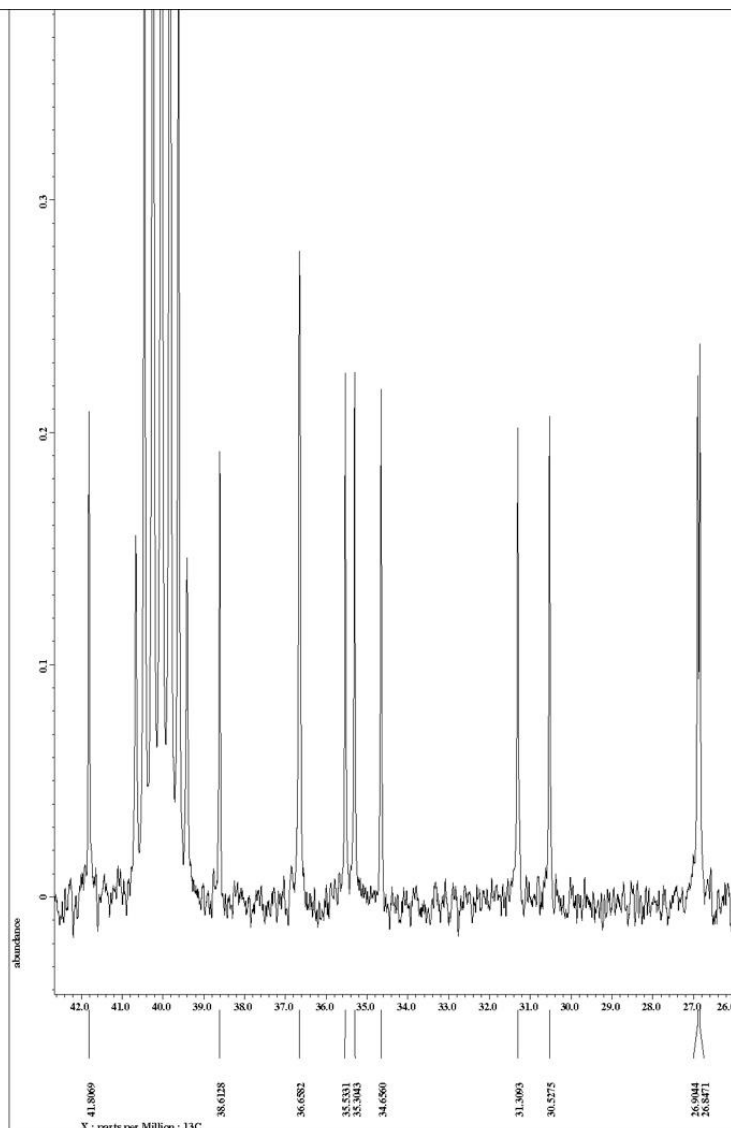
22

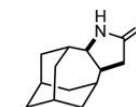
Filename = TIM_13C_147-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_147
 Solvent = DMSO-D6
 Creation_time = 10-OCT-2018 14:29:20
 Revision_time = 18-APR-2023 19:12:34
 Current_time = 18-APR-2023 19:14:28

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[ppm]
 X_points = 32768
 X_prescans = 1
 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 = 21
 Total_scans = 21

X_90_width = 8.16[us]
 X_acq_time = 1.04333312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 21.6[degC]





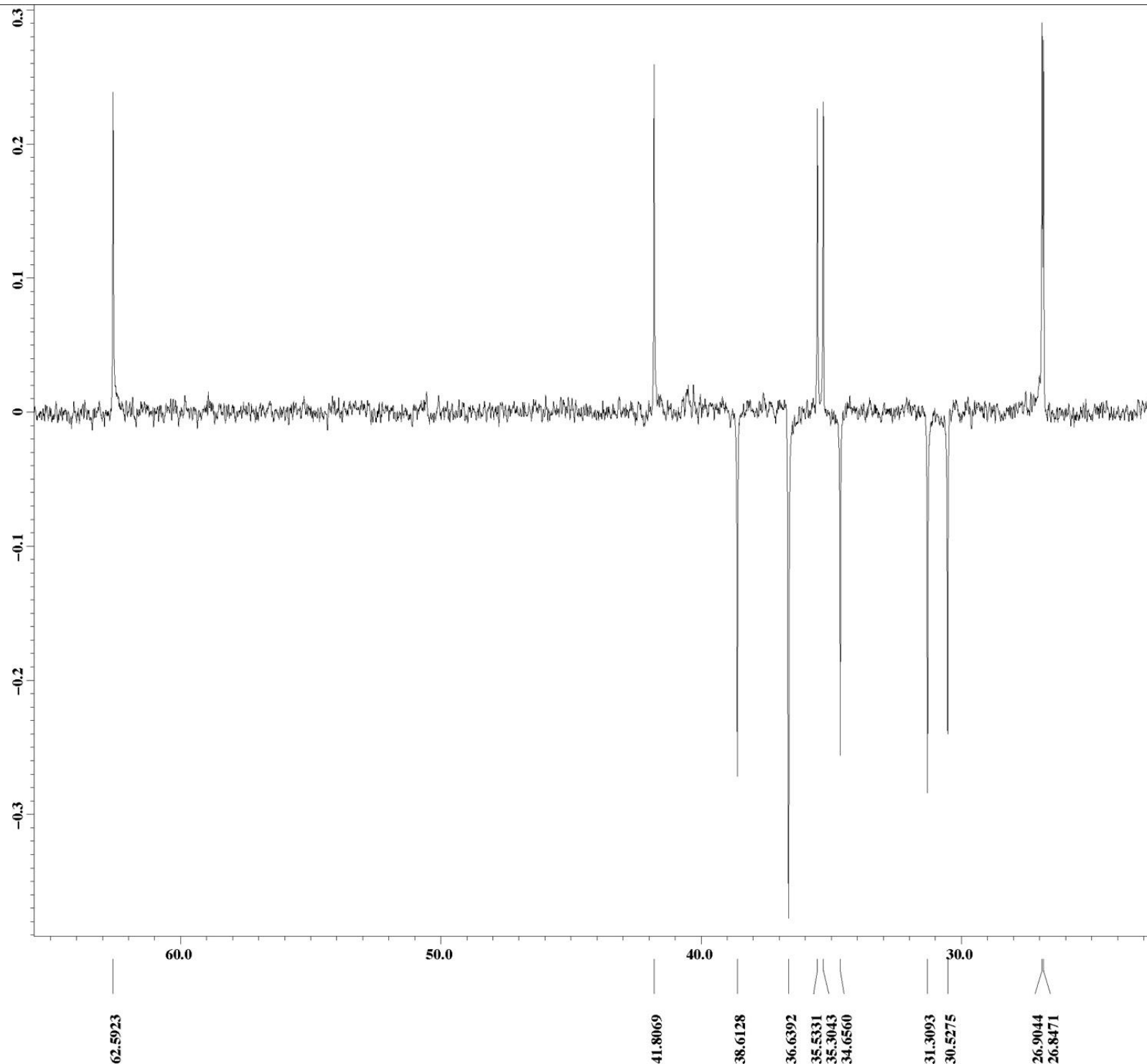
22

Filename = TIM_DEPT135_147-4.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM 147
 Solvent = DMSO-D6
 Creation_time = 10-OCT-2018 14:30:18
 Revision_time = 18-APR-2023 19:13:12
 Current_time = 18-APR-2023 19:13:59

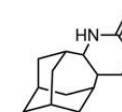
Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 12
 Total_scans = 12

X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 21.6[dC]



X : parts per Million : 13C



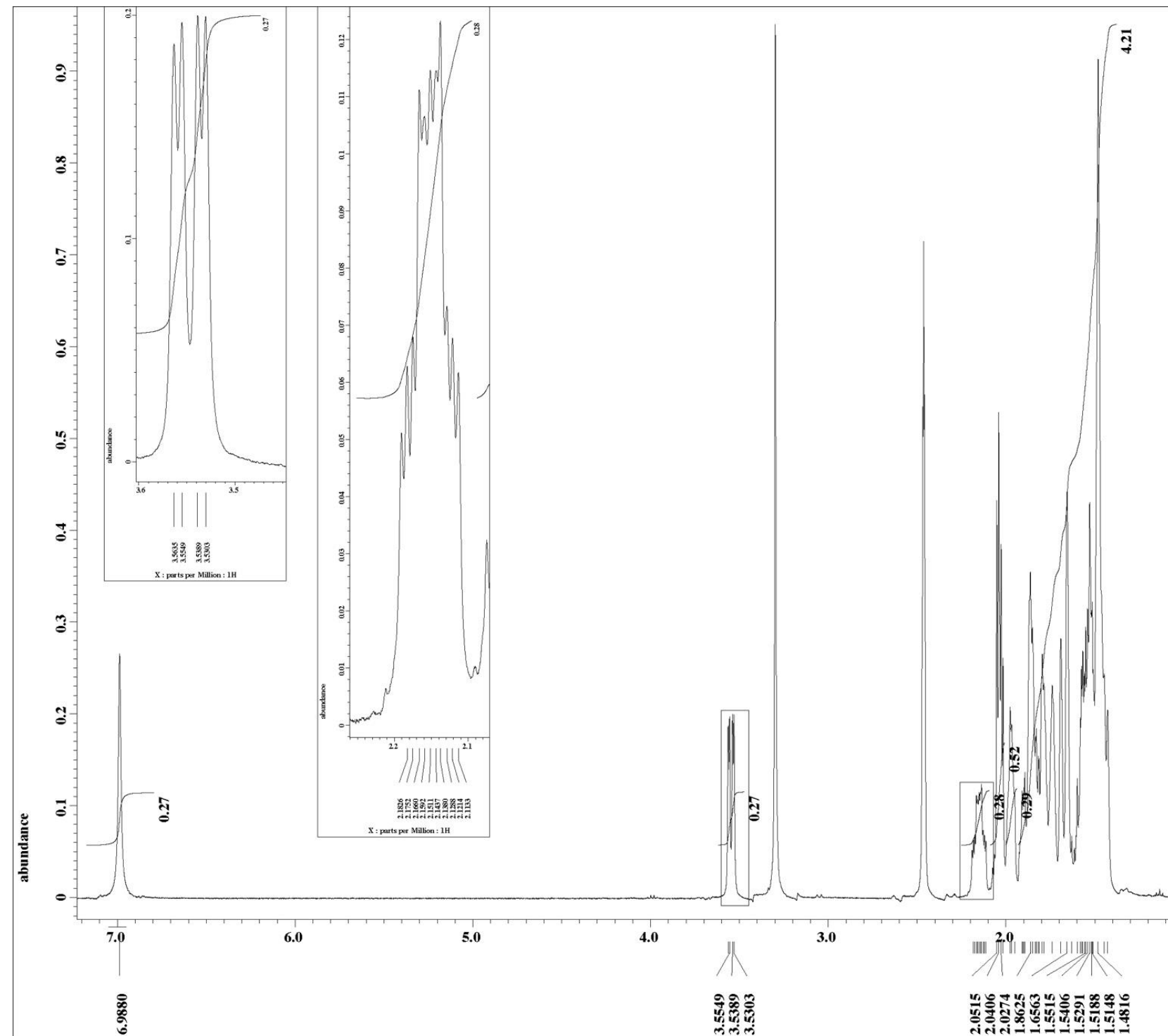
23

Filename = TIM_1H_209-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_209
 Solvent = DMSO-D6
 Creation_time = 30-APR-2019 19:00:16
 Revision_time = 10-FEB-2023 14:51:28
 Current_time = 10-FEB-2023 14:52:56

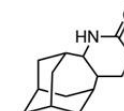
Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 11.9[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 5.95[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 42
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 21.8[dc]



X : parts per Million : 1H



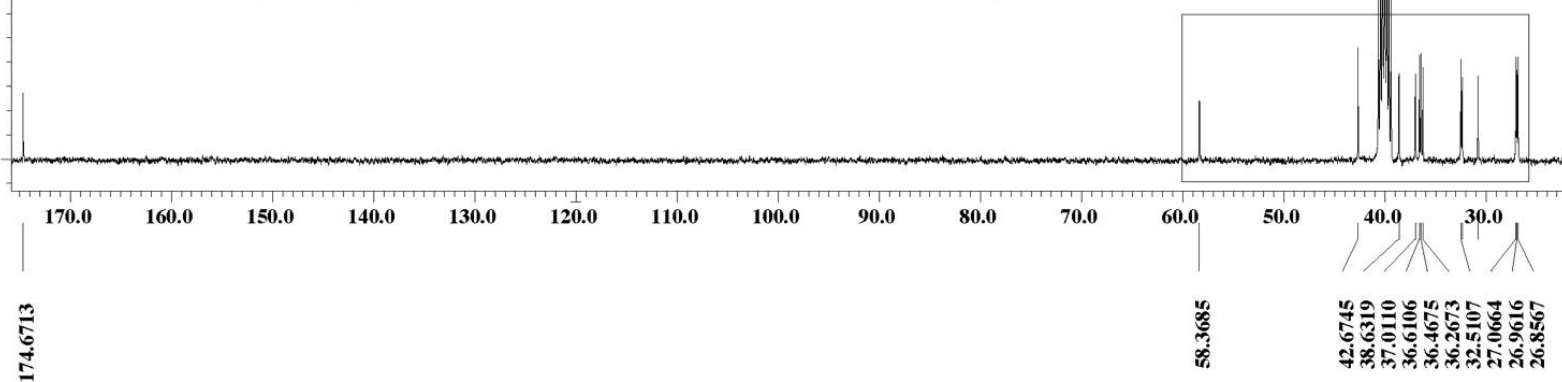
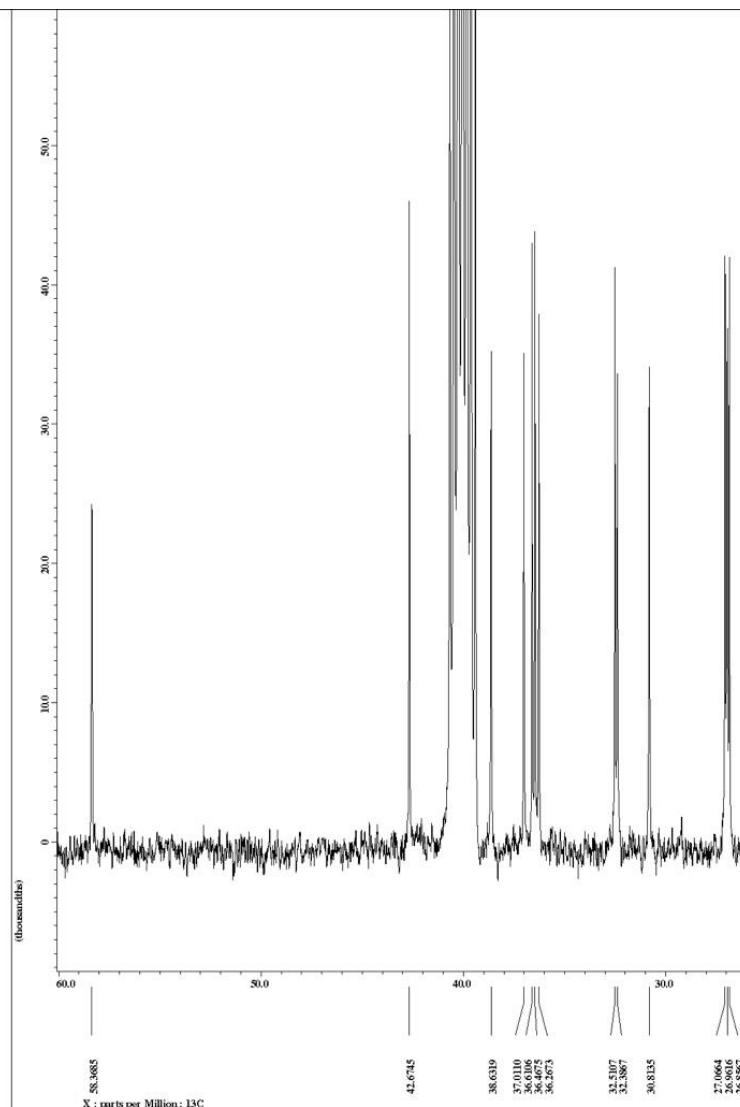
23

Filename = TIM_13C_209-3.jdf
 Author = delta
 Experiment = single pulse_dec
 Sample_id = TIM_209
 Solvent = DMSO-D6
 Creation_time = 30-APR-2019 19:59:45
 Revision_time = 10-FEB-2023 14:53:20
 Current_time = 10-FEB-2023 14:54:29

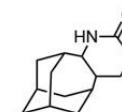
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.0433312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 459
 Total_scans = 459

X_90_width = 8.16[us]
 X_acq_time = 1.0433312[s]
 X_angle = 30[deg]
 X_atn = 7.8[dB]
 X_pulse = 2.72[us]
 Irr_atn_dec = 22.703[dB]
 Irr_atn_noe = 22.703[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 44
 Relaxation_delay = 2[s]
 Repetition_time = 3.0433312[s]
 Temp_get = 22[dc]



X : parts per Million : 13C



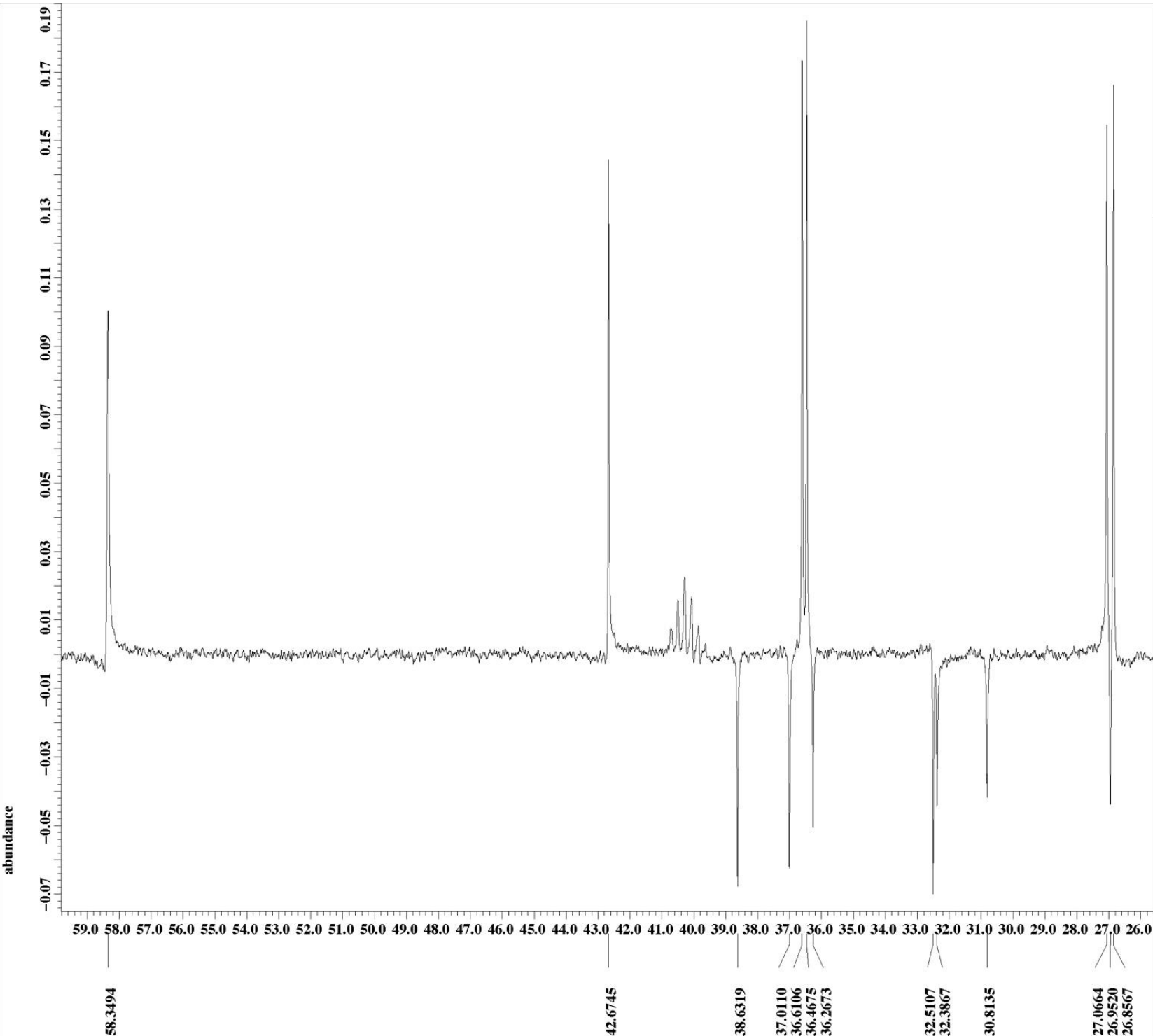
23

Filename = TIM_DEPT135_209-3.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM 209
 Solvent = DMSO-D6
 Creation_time = 30-APR-2019 20:51:28
 Revision_time = 10-FEB-2023 14:54:44
 Current_time = 10-FEB-2023 14:55:02

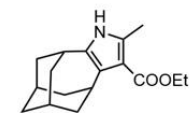
Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 1000
 Total_scans = 1000

X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 22.1[degC]



X : parts per Million : 13C



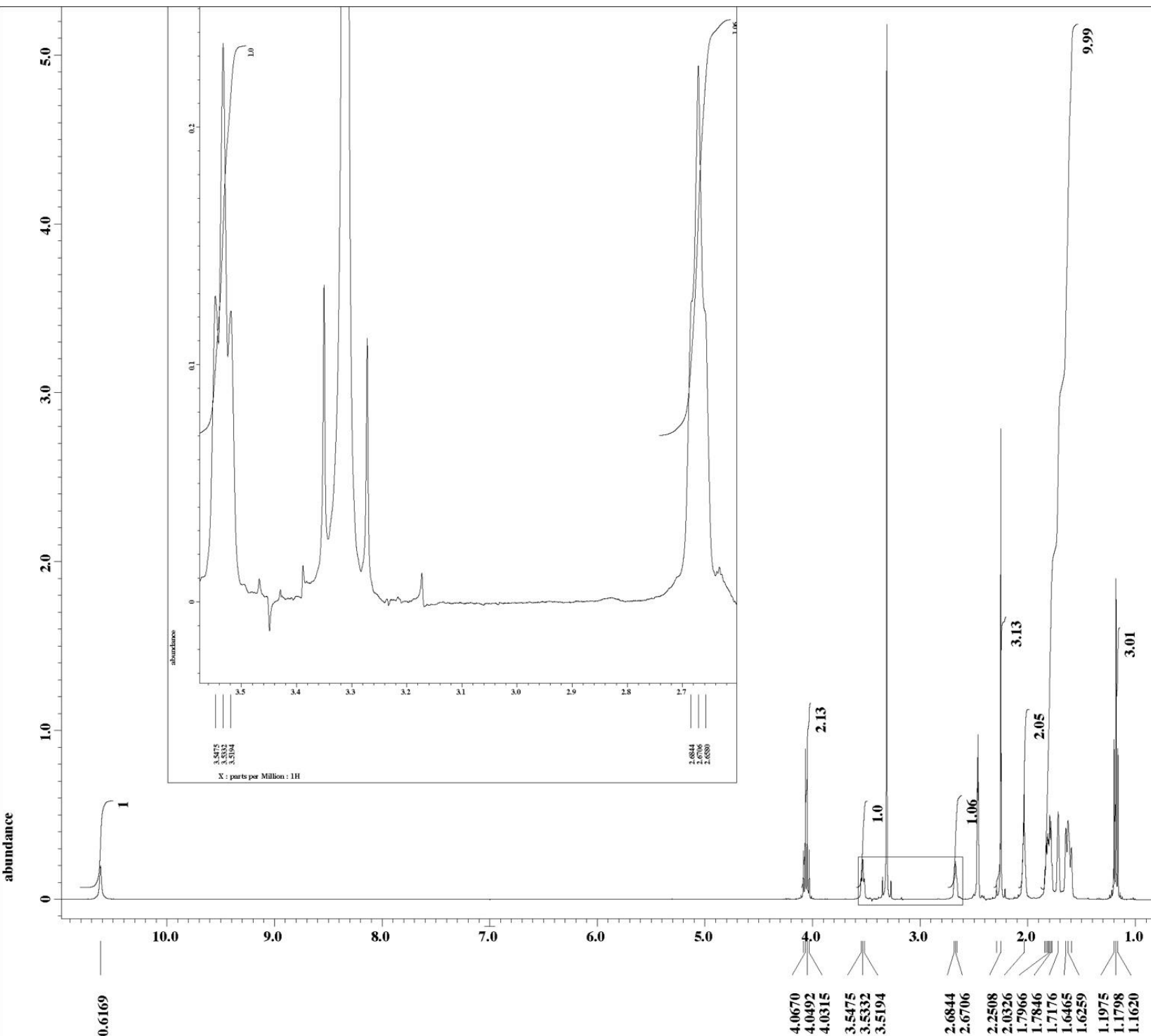
24

Filename = TIM_1H_homoadonacetone
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM homoadonacetoneCO
 Solvent = DMSO-D6
 Creation_time = 17-JUL-2022 08:00:07
 Revision_time = 15-DEC-2022 14:04:29
 Current_time = 15-DEC-2022 14:05:02

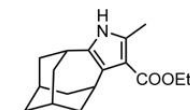
Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 5.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3.5[dB]
 X_pulse = 2.75[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 30
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 0[dc]



X : parts per Million : 1H



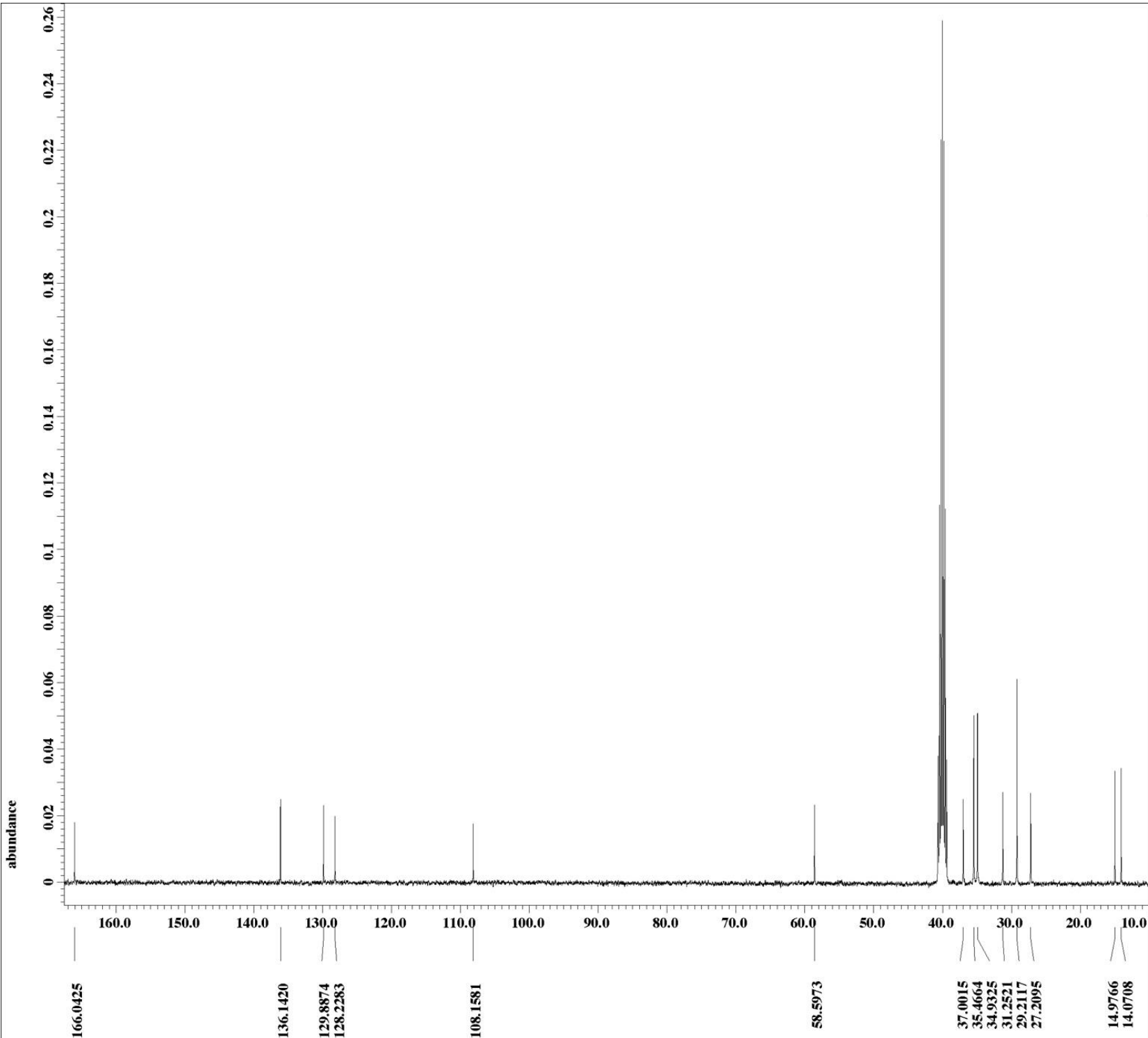
24

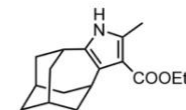
Filename = TIM_13C_homoadonaceto
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM homoadonacetoneCO
 Solvent = DMSO-D6
 Creation_time = 17-JUL-2022 11:23:49
 Revision_time = 15-DEC-2022 14:06:42
 Current_time = 15-DEC-2022 14:08:05

Comment = single_pulse_decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.0433312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 4000
 Total_scans = 4000

X_90_width = 13.87[us]
 X_acq_time = 1.0433312[s]
 X_angle = 30[deg]
 X_atn = 5.2[dB]
 X_pulse = 4.62333333[us]
 Irr_atn_dec = 29.907[dB]
 Irr_atn_noe = 29.907[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 48
 Relaxation_delay = 2[s]
 Repetition_time = 3.0433312[s]
 Temp_get = 0[dc]





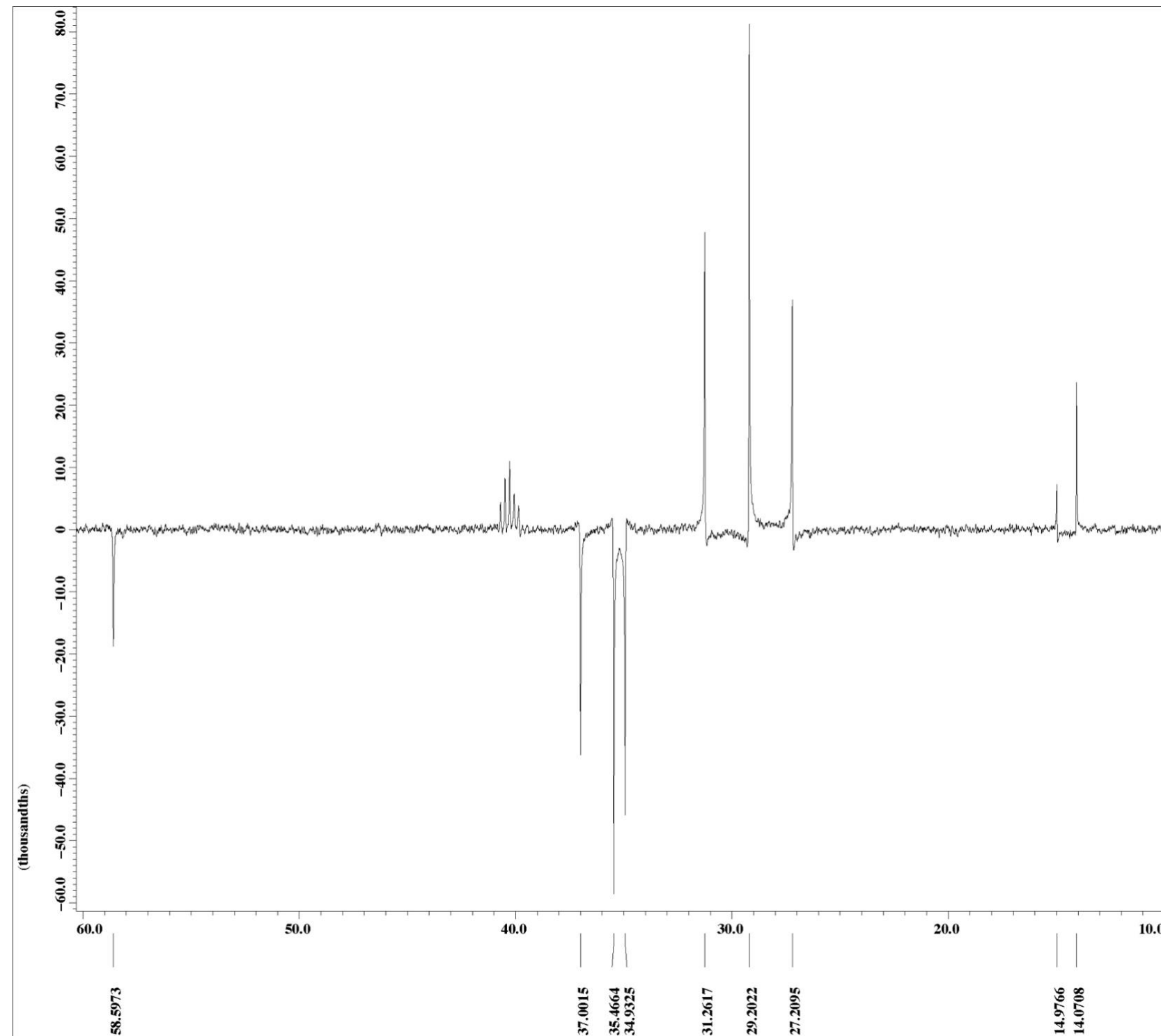
24

Filename = TIM_DEPT135_homoadona
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_homoadonacetoneCO
 Solvent = DMSO-D6
 Creation_time = 17-JUL-2022 13:05:57
 Revision_time = 15-DEC-2022 14:06:58
 Current_time = 15-DEC-2022 14:07:39

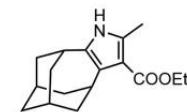
Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 2000
 Total_scans = 2000

X_acq_time = 1.04333312[s]
 X_atn = 5.2[dB]
 X_pulse = 13.87[us]
 Irr_atn = 3.5[dB]
 Irr_atn_dec = 29.907[dB]
 Irr_noise = WALTZ
 Irr_pulse = 5.5[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 8.25[us]
 Temp_get = 0[dc]



X : parts per Million : 13C



24

¹H-¹⁵N HMBC

Y : parts per Million : 15N

Filename = TIM_15NHMBC_homoAdace
Author = delta
Experiment = hmbc_pfg.ex2
Sample_id = TIM_homoAdacetoneCOOE
Solvent = DMSO-D6
Creation_time = 9-AUG-2022 19:59:41
Revision_time = 15-DEC-2022 14:09:26
Current_time = 15-DEC-2022 14:10:49

Comment = gradient enhanced HMB
Data_format = 2D REAL REAL
Dim_size = 819, 512
Dim_title = 1H 15N
Dim_units = [ppm] [ppm]
Dimensions = X Y
Site = ECX 400
Spectrometer = JNM-ECX400

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 0.20283392 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5.84 [ppm]
X_points = 1024
X_prescans = 4
X_resolution = 4.93014186 [Hz]
X_sweep = 5.04846527 [kHz]
Y_domain = 15N
Y_freq = 40.50976341 [MHz]
Y_offset = 0 [ppm]
Y_points = 256
Y_prescans = 0
Y_resolution = 94.99635214 [Hz]
Y_sweep = 24.31906615 [kHz]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4
Total_scans = 1024

X_acq_time = 0.20283392 [s]
X_atn = 3.5 [dB]
X_pulse = 5.5 [us]
Y_acq_time = 10.52672 [ms]
Y_atn = 4.5 [dB]
Y_pulse = 26.5 [us]
Tri_mode = Off
Dante_presat = FALSE
Delta = 62.5 [ms]
Grad_1 = 1 [ms]
Grad_1_amp = 0.18 [T/m]
Grad_2 = 1 [ms]
Grad_2_amp = 0.18 [T/m]
Grad_3 = 1 [ms]
Grad_3_amp = 36.48895196 [mT/m]
Grad_recover = 0.1 [ms]
Grad_selection = 15N = 4.933:4.93
Grad_shape = SINE

(thousandths)

X : parts per Million : 1H

-200.0

-100.0

0

100.0

200.0

300.0

10.0

9.0

8.0

7.0

6.0

5.0

4.0

3.0

2.0

1.0

1.0

2.0

3.0

4.0

5.0

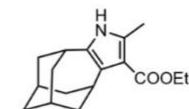
6.0

7.0

8.0

9.0

10.0



24

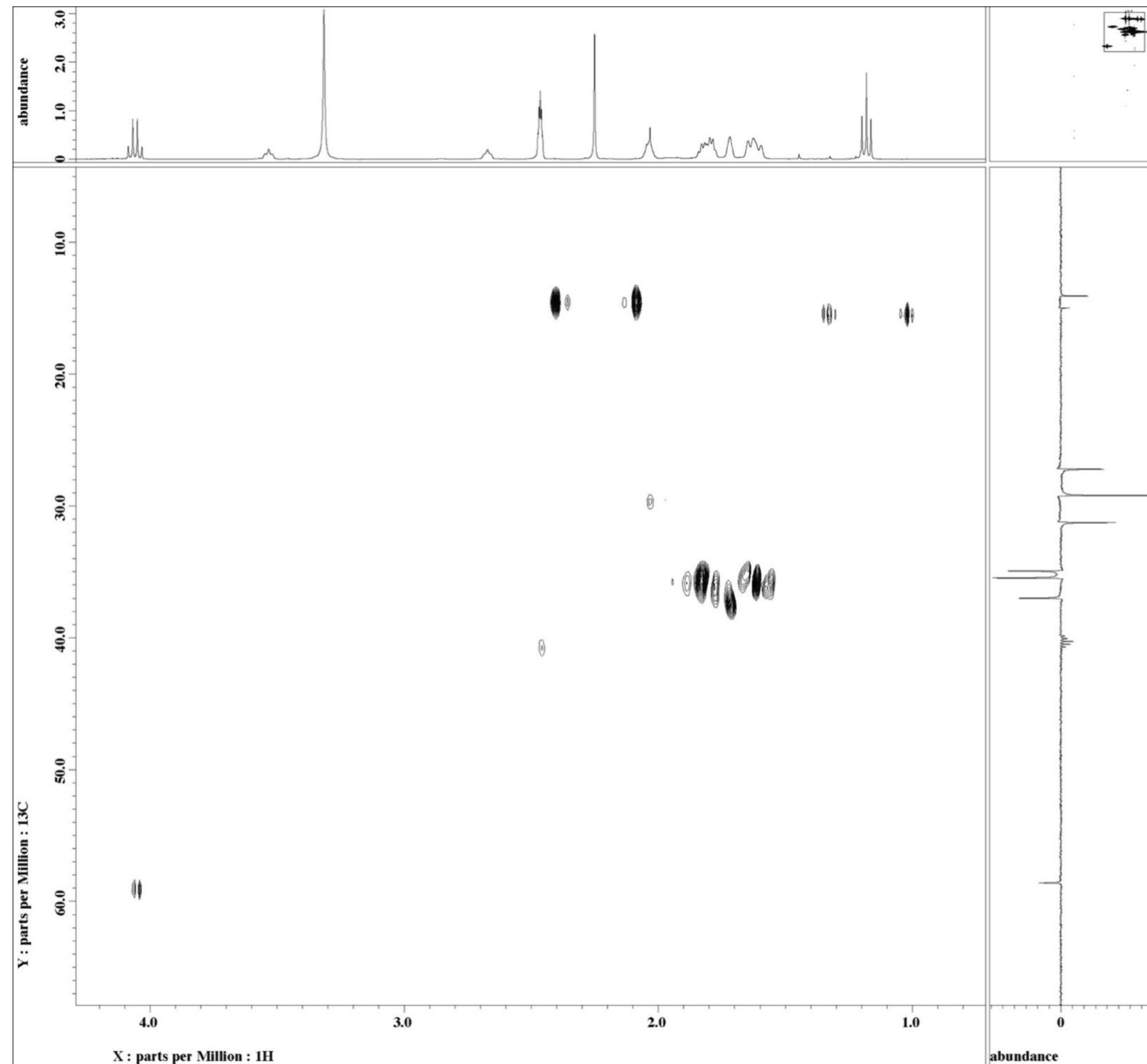
¹H-¹³C HMQC

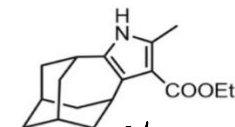
Filename = TIM_HMQC_homoAdacetone
 Author = delta
 Experiment = hmqc_pfg.ex2
 Sample_id = TIM_homoAdacetoneCOOE
 Solvent = DMSO-D6
 Creation_time = 9-AUG-2022 18:23:53
 Revision_time = 19-APR-2023 17:06:03
 Current_time = 19-APR-2023 17:18:19

Comment = gradient enhanced HMQC
 Data_format = 2D REAL REAL
 Dim_size = 1638, 556
 Dim_title = 1H 13C
 Dim_units = [ppm] [ppm]
 Dimensions = X Y
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 0.27312128[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 2048
 X_prescans = 4
 X_resolution = 3.6613771[Hz]
 X_sweep = 7.4985003[kHz]
 Y_domain = 13C
 Y_freq = 100.52530333[MHz]
 Y_offset = 120[ppm]
 Y_points = 278
 Y_prescans = 0
 Y_resolution = 90.47088285[Hz]
 Y_sweep = 25.15090543[kHz]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 4
 Total_scans = 1112

X_acq_time = 0.27312128[s]
 X_atn = 3.5[dB]
 X_pulse = 5.5[us]
 Y_acq_time = 20.35712[ms]
 Y_atn = 5.2[dB]
 Y_pulse = 13.87[us]
 Irr_atn_dec = 25.705[dB]
 Irr_noise = MPP8
 Tri_mode = Off
 Dante_presat = FALSE
 Decoupling = TRUE
 Grad_1 = 1[ms]
 Grad_1_amp = 0.18[T/m]
 Grad_2 = 1[ms]
 Grad_2_amp = 0.18[T/m]
 Grad_3 = 1[ms]
 Grad_3_amp = 90.54325956[mT/m]
 Grad_recover = 0.1[ms]





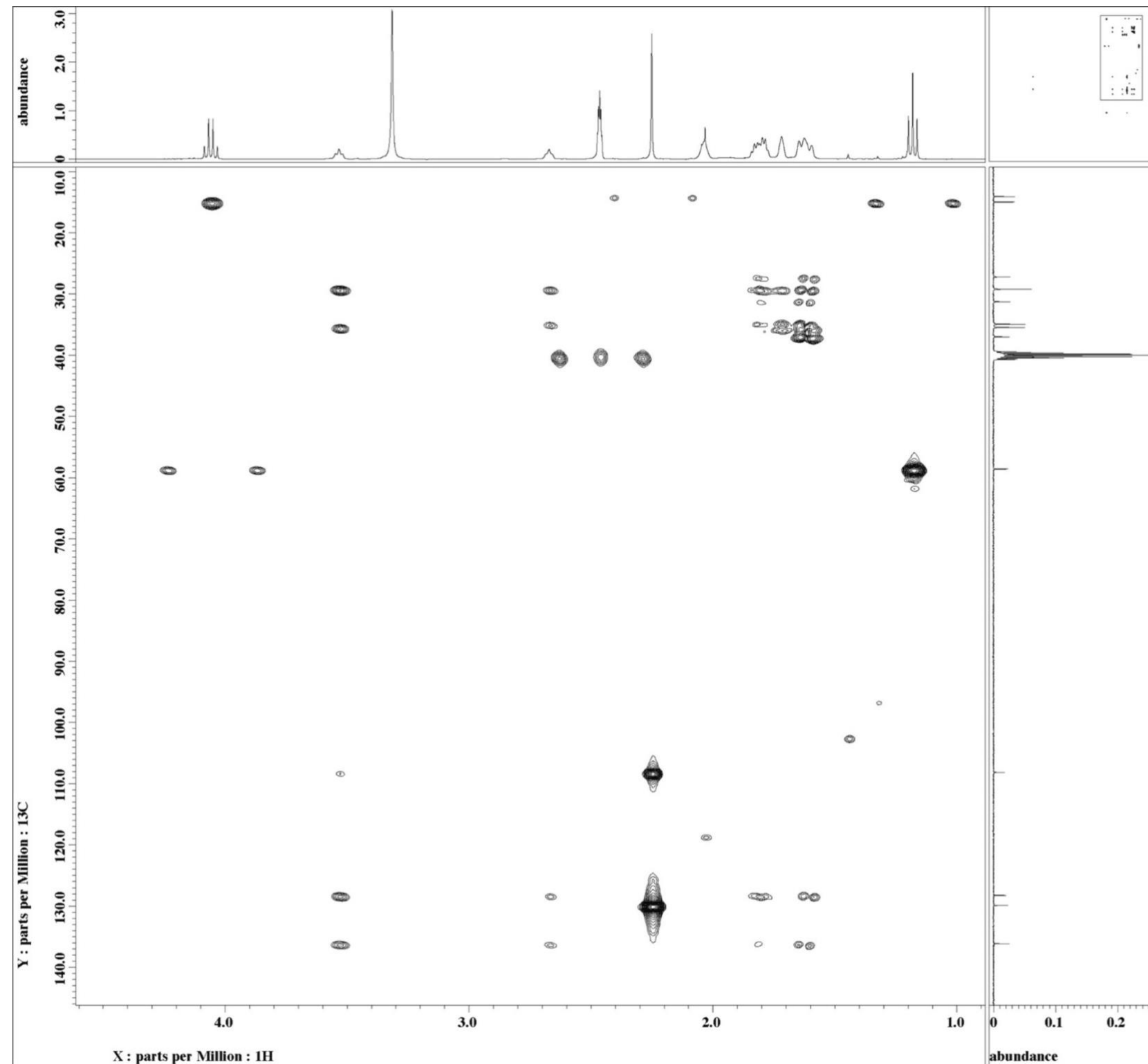
24
¹H-¹³C HMQC
 expansion

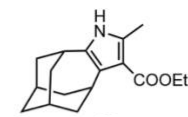
Filename = TIM_HMBC_homoAdaceton
 Author = delta
 Experiment = hmbc_pfg.ex2
 Sample_id = TIM_homoAdacetonCOOE
 Solvent = DMSO-D6
 Creation_time = 9-AUG-2022 19:27:15
 Revision_time = 19-APR-2023 17:18:53
 Current_time = 19-APR-2023 17:20:46

Comment = gradient enhanced HMB
 Data_format = 2D REAL REAL
 Dim_size = 1638, 1024
 Dim_title = 1H 13C
 Dim_units = [ppm] [ppm]
 Dimensions = X Y
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766 [T] (400 [MHz])
 X_acq_duration = 0.27312128 [s]
 X_domain = 1H
 X_freq = 399.78219838 [MHz]
 X_offset = 7 [ppm]
 X_points = 2048
 X_prescans = 4
 X_resolution = 3.6613771 [Hz]
 X_sweep = 7.4985003 [kHz]
 Y_domain = 13C
 Y_freq = 100.52530333 [MHz]
 Y_offset = 120 [ppm]
 Y_points = 512
 Y_prescans = 0
 Y_resolution = 49.12286217 [Hz]
 Y_sweep = 25.15090543 [kHz]
 Tri_domain = 1H
 Tri_freq = 399.78219838 [MHz]
 Tri_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 4
 Total_scans = 2048

X_acq_time = 0.27312128 [s]
 X_atn = 3.5 [dB]
 X_pulse = 5.5 [us]
 Y_acq_time = 20.35712 [ms]
 Y_atn = 5.2 [dB]
 Y_pulse = 13.87 [us]
 Tri_mode = Off
 Dante_presat = FALSE
 Delta = 62.5 [ms]
 Grad_1 = 1 [ms]
 Grad_1_amp = 0.18 [T/m]
 Grad_2 = 1 [ms]
 Grad_2_amp = 0.18 [T/m]
 Grad_3 = 1 [ms]
 Grad_3_amp = 90.54325956 [mT/m]
 Grad_recover = 0.1 [ms]
 Grad_selection = 13C = 1.988:1.98
 Grad_shape = SINE





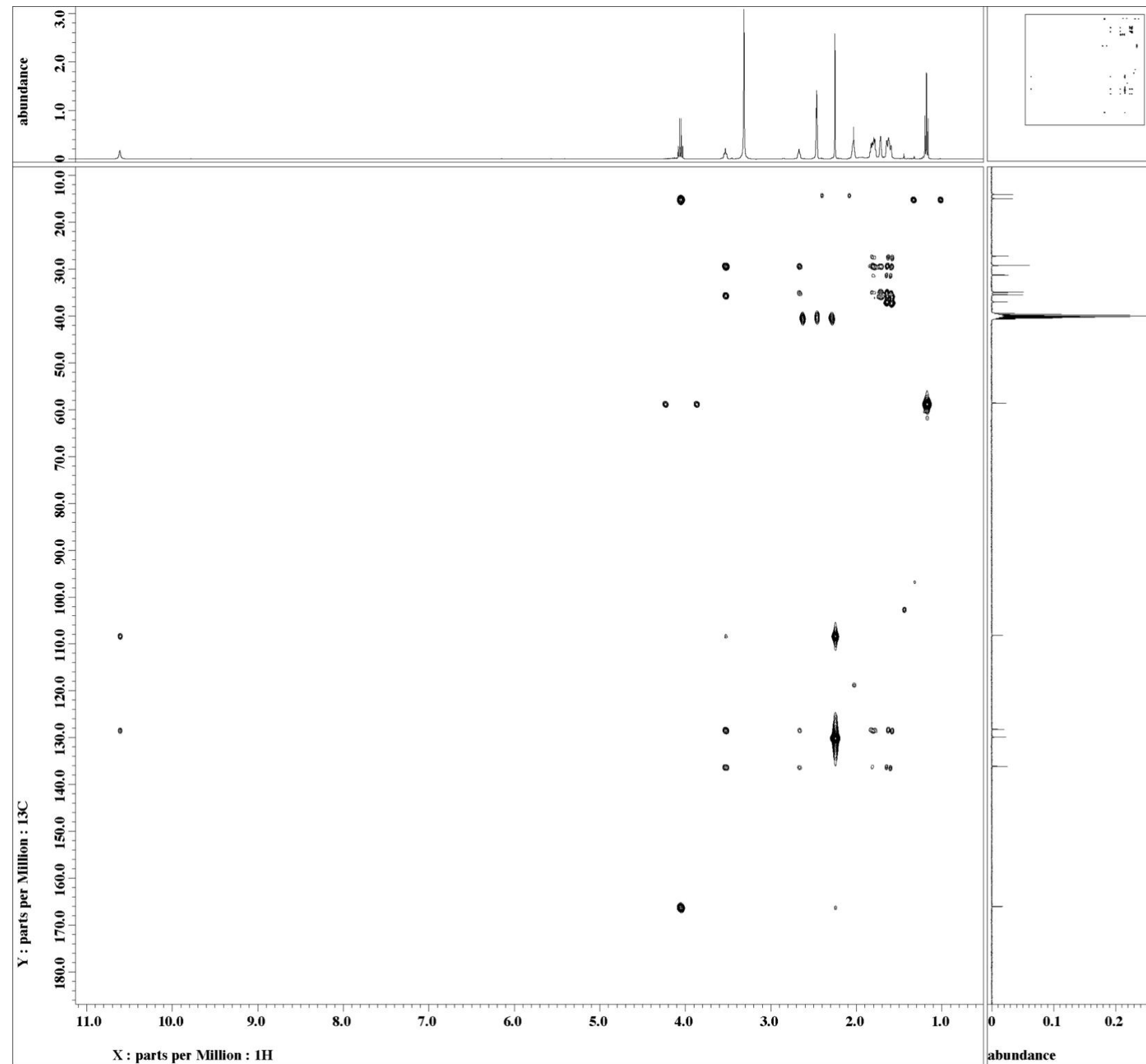
24
¹³C-¹H HMBC

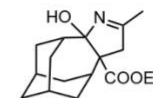
Filename = TIM_HMBC_homoAdacetone
 Author = delta
 Experiment = hmbc_pfg.ex2
 Sample_id = TIM_homoAdacetoneCOOE
 Solvent = DMSO-D6
 Creation_time = 9-AUG-2022 19:27:15
 Revision_time = 19-APR-2023 17:18:53
 Current_time = 19-APR-2023 17:37:15

Comment = gradient enhanced HMB
 Data_format = 2D REAL REAL
 Dim_size = 1638, 1024
 Dim_title = 1H 13C
 Dim_units = [ppm] [ppm]
 Dimensions = X Y
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 0.27312128[s]
 X_domain = 1H
 X_freq = 399.78219838 [MHz]
 X_offset = 7 [ppm]
 X_points = 2048
 X_prescans = 4
 X_resolution = 3.6613771 [Hz]
 X_sweep = 7.4985003 [kHz]
 Y_domain = 13C
 Y_freq = 100.52530333 [MHz]
 Y_offset = 120 [ppm]
 Y_points = 512
 Y_prescans = 0
 Y_resolution = 49.12286217 [Hz]
 Y_sweep = 25.15090543 [kHz]
 Tri_domain = 1H
 Tri_freq = 399.78219838 [MHz]
 Tri_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 4
 Total_scans = 2048

X_acq_time = 0.27312128[s]
 X_atn = 3.5 [dB]
 X_pulse = 5.5 [us]
 Y_acq_time = 20.35712 [ms]
 Y_atn = 5.2 [dB]
 Y_pulse = 13.87 [us]
 Tri_mode = Off
 Dante_presat = FALSE
 Delta = 62.5 [ms]
 Grad_1 = 1 [ms]
 Grad_1_amp = 0.18 [T/m]
 Grad_2 = 1 [ms]
 Grad_2_amp = 0.18 [T/m]
 Grad_3 = 1 [ms]
 Grad_3_amp = 90.54325956 [mT/m]
 Grad_recover = 0.1 [ms]
 Grad_selection = 13C = 1.988:1.98
 Grad_shape = SINE





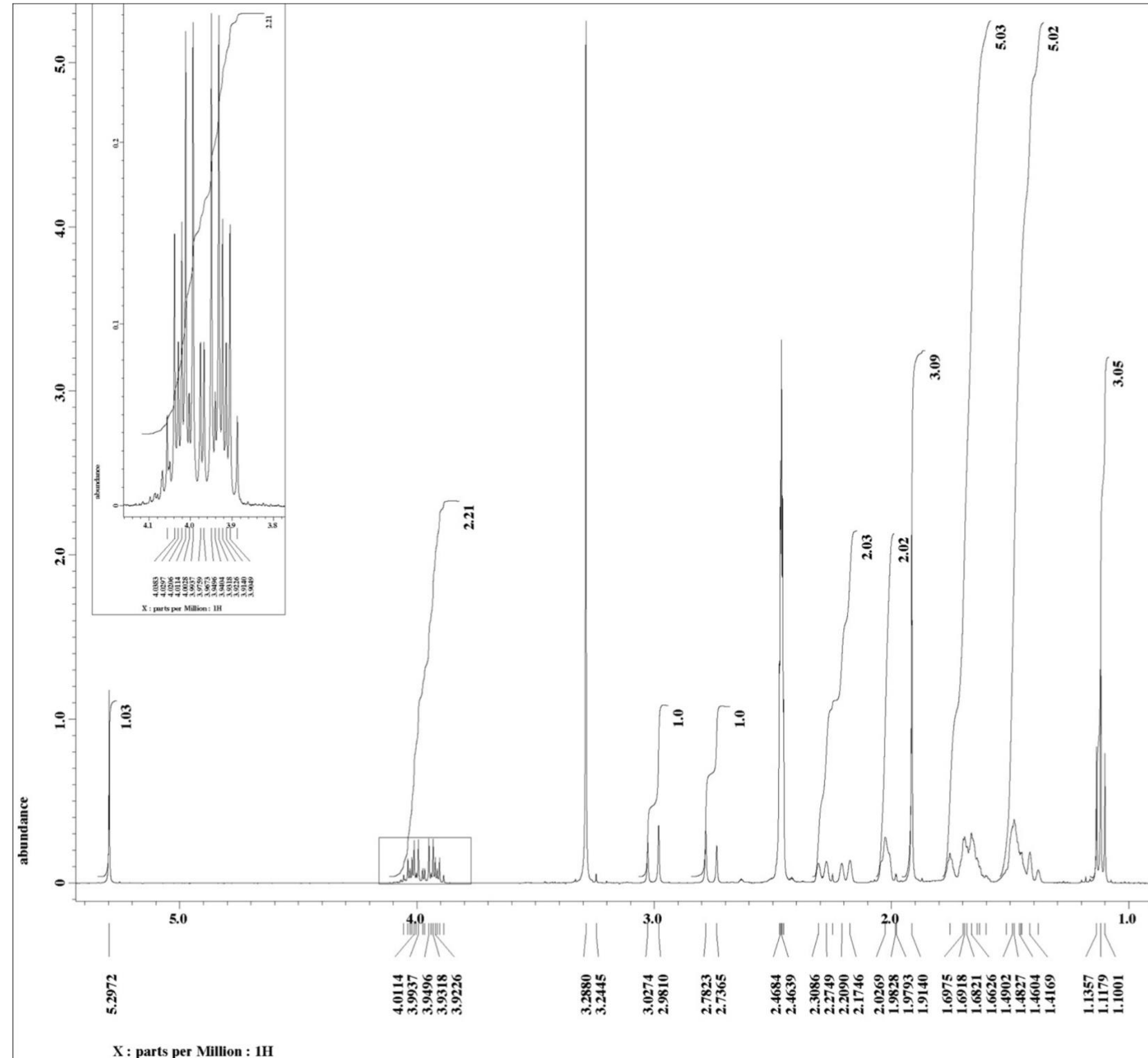
25

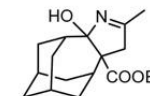
Filename = TIM_1H_acetonylNH3-4.
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_acetonylNH3
 Solvent = DMSO-D6
 Creation_time = 12-SEP-2022 19:06:17
 Revision_time = 15-DEC-2022 14:17:11
 Current_time = 15-DEC-2022 14:18:11

Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 4.36731904[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 32768
 X_prescans = 1
 X_resolution = 0.22897343[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 = 5.5[us]
 X_acq_time = 4.36731904[s]
 X_angle = 45[deg]
 X_atn = 3.5[dB]
 X_pulse = 2.75[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 38
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 0[degC]





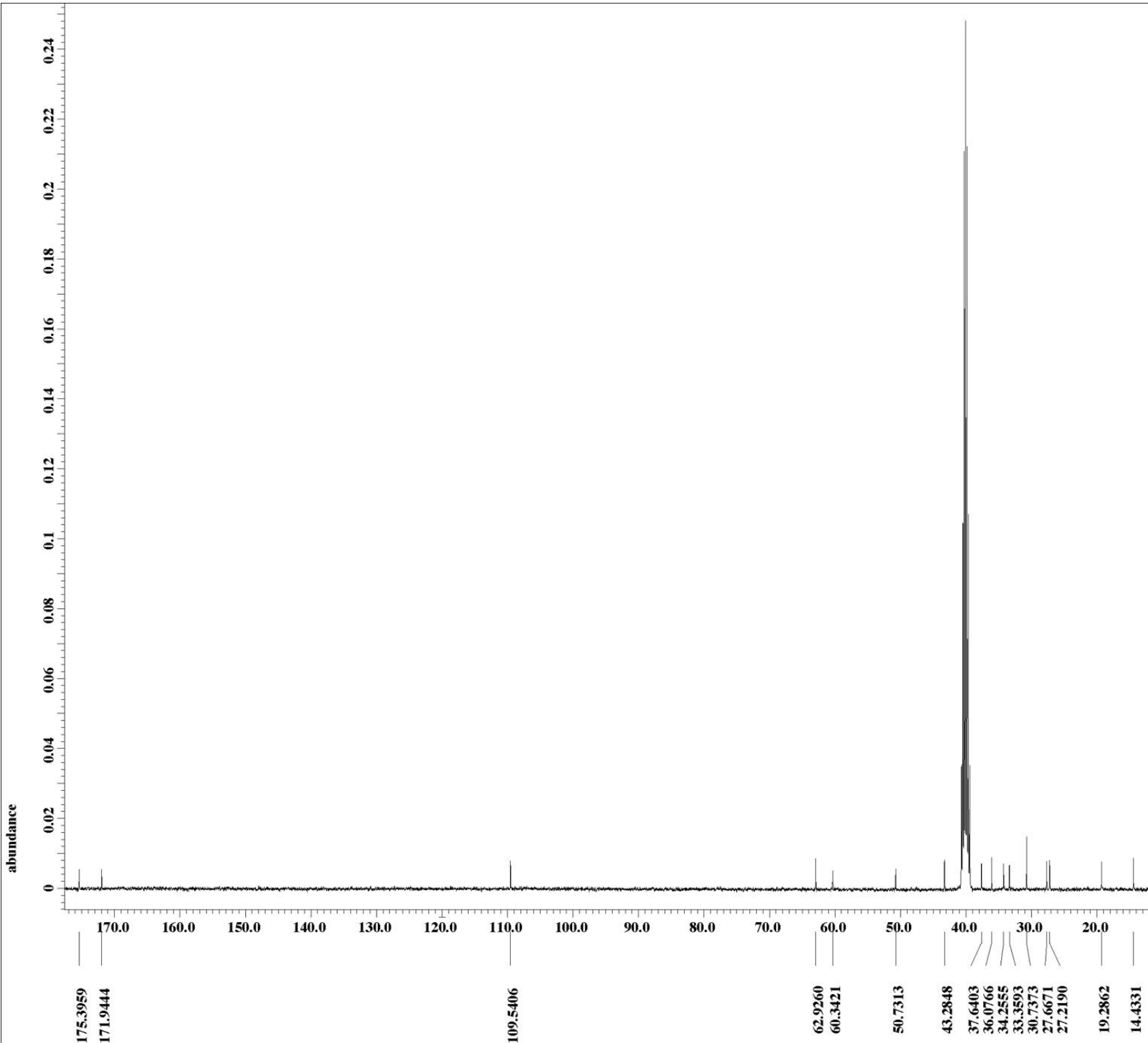
25

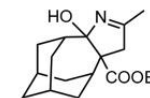
Filename = TIM_13C_acetonylNH3-6
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_acetonylNH3
 Solvent = DMSO-D6
 Creation_time = 13-SEP-2022 17:13:04
 Revision_time = 15-DEC-2022 14:19:10
 Current_time = 15-DEC-2022 14:20:29

Comment = single pulse decouple
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.0433312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[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 = 5000
 Total_scans = 5000

X_90_width = 13.87[us]
 X_acq_time = 1.0433312[s]
 X_angle = 30[deg]
 X_atn = 5.2[dB]
 X_pulse = 4.62333333[us]
 Irr_atn_dec = 29.907[dB]
 Irr_atn_noe = 29.907[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Repetition_time = 3.0433312[s]
 Temp_get = 0[dc]





25

10.0

0

-10.0

60.0

50.0

40.0

30.0

20.0

10.0

60.3421

50.7408

43.2943

37.6498

36.0862

34.2555

33.3593

30.7468

27.6671

27.2285

19.2862

14.4331

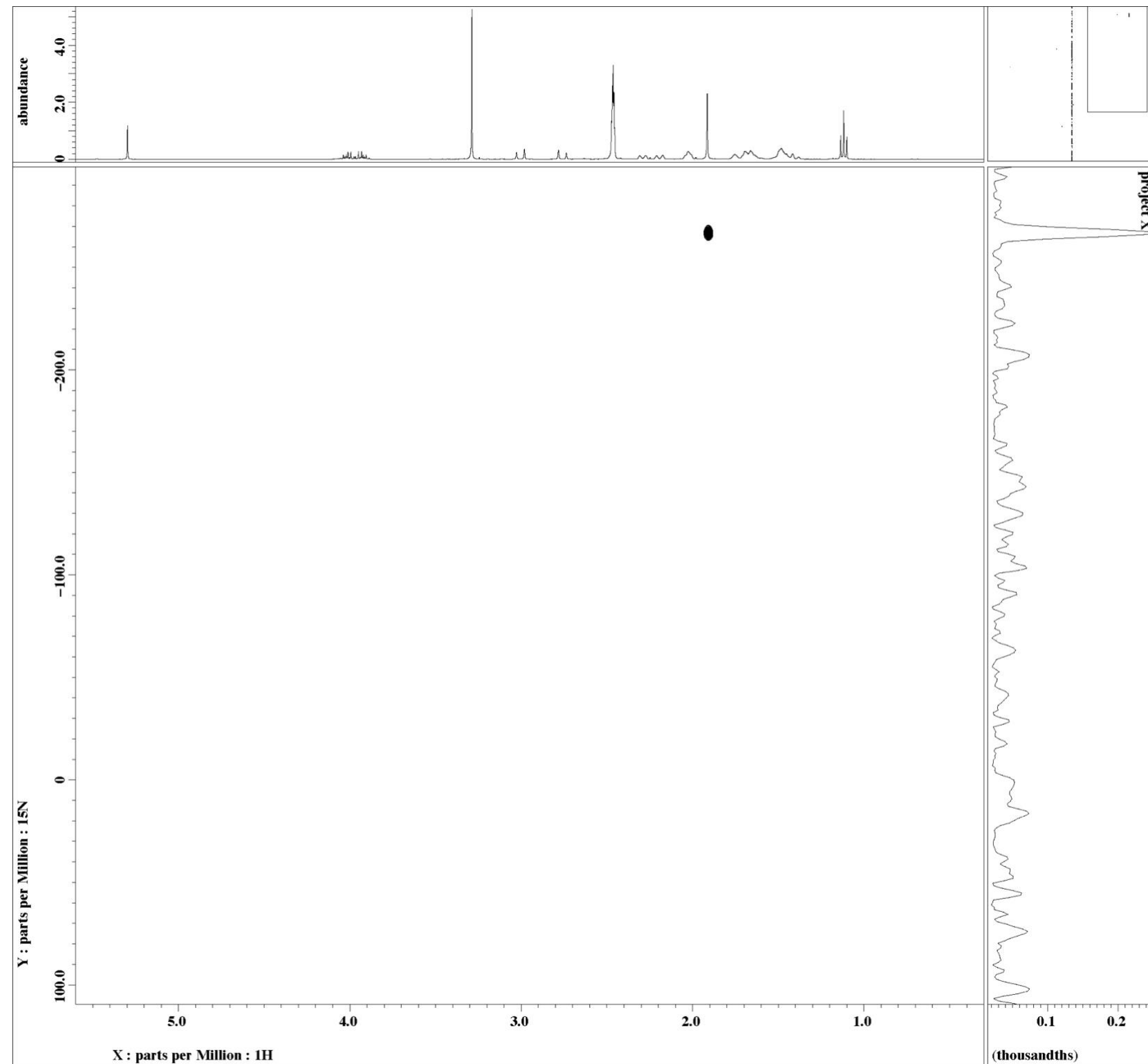
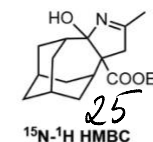
X : parts per Million : 13C

Filename = TIM_DEPT135_acetonylN
Author = delta
Experiment = dept.ex2
Sample_id = TIM_acetonylNH3
Solvent = DMSO-D6
Creation_time = 14-SEP-2022 20:45:49
Revision_time = 15-DEC-2022 14:19:36
Current_time = 15-DEC-2022 14:19:59

Comment = DEPT with decoupling
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 120[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 = 2000
Total_scans = 2000

X_acq_time = 1.04333312[s]
X_atn = 5.2[dB]
X_pulse = 13.87[us]
Irr_atn = 3.5[dB]
Irr_atn_dec = 29.907[dB]
Irr_noise = WALTZ
Irr_pulse = 5.5[us]
Decoupling = TRUE
Initial_wait = 1[s]
J_constant = 140[Hz]
Recvr_gain = 46
Relaxation_delay = 2[s]
Selection_angle = 135[deg]
Selection_pulse = 8.25[us]
Temp_get = 0[dc]



Filename = TIM_15NHMBC_acetonylN
 Author = delta
 Experiment = hmbc_pfg.ex2
 Sample_id = TIM_acetonylNH3
 Solvent = DMSO-D6
 Creation_time = 16-SEP-2022 13:31:17
 Revision_time = 19-APR-2023 17:38:26
 Current_time = 19-APR-2023 17:40:00

Comment = gradient enhanced HMB
 Data_format = 2D REAL REAL
 Dim_size = 1638, 512
 Dim_title = 1H 15N
 Dim_units = [ppm] [ppm]
 Dimensions = X Y
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 0.27312128[s]
 X_domain = 1H
 X_freq = 399.78219838[MHz]
 X_offset = 7[ppm]
 X_points = 2048
 X_prescans = 4
 X_resolution = 3.6613771[Hz]
 X_sweep = 7.4985003[kHz]
 Y_domain = 15N
 Y_freq = 40.50976341[MHz]
 Y_offset = 0[ppm]
 Y_points = 256
 Y_prescans = 0
 Y_resolution = 94.99635214[Hz]
 Y_sweep = 24.31906615[kHz]
 Tri_domain = 1H
 Tri_freq = 399.78219838[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 2048

X_acq_time = 0.27312128[s]
 X_atn = 3.5[dB]
 X_pulse = 5.5[us]
 Y_acq_time = 10.52672[ms]
 Y_atn = 4.5[dB]
 Y_pulse = 26.5[us]
 Tri_mode = Off
 Dante_presat = FALSE
 Delta = 62.5[ms]
 Grad_1 = 1[ms]
 Grad_1_amp = 0.18[T/m]
 Grad_2 = 1[ms]
 Grad_2_amp = 0.18[T/m]
 Grad_3 = 1[ms]
 Grad_3_amp = 36.48895196[mT/m]
 Grad_recover = 0.1[ms]
 Grad_selection = 15N = 4.933:4.93
 Grad_shape = SINE