

Supporting Information

Unexpected transformation of α -substituted 5-oxohomoadamantane-4-carboxylate. Route to 2,4-di and 2,3,4-trisubstituted homoadamantanes.

Ilya M. Tkachenko^{1*}, Polina A. Mankova¹, Victor B. Rybakov², Evgeniy V. Golovin¹, Yuri N. Klimochkin¹

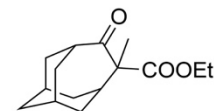
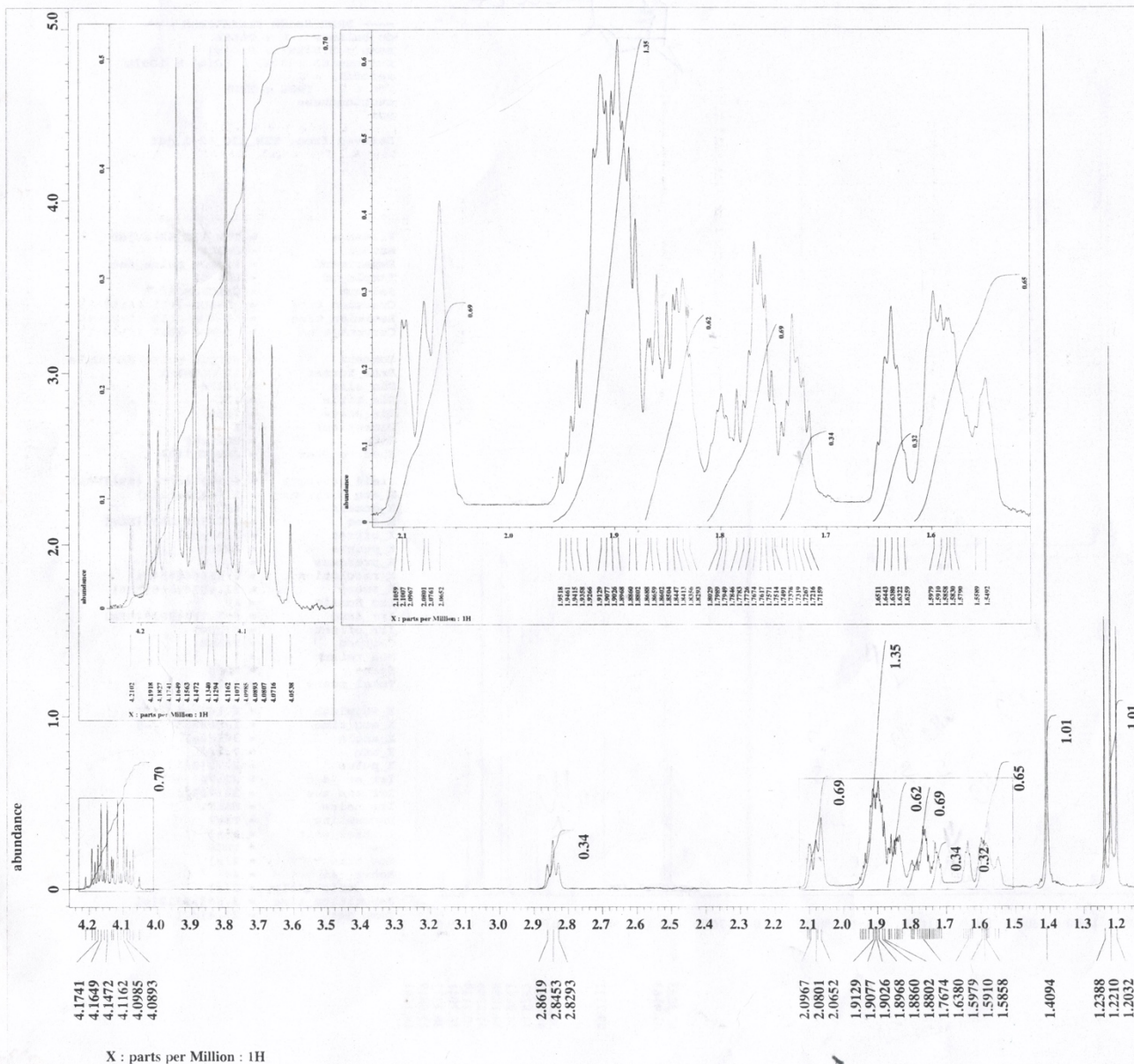
Address: ¹Department of Organic Chemistry, Chemical Technological Faculty, Samara State Technical University, 244 Molodogvardeyskaya st., Samara 443100, Russian Federation. ²Chemistry Department, Faculty of Chemistry, Moscow State University, 1-3 Leninskie gory, Moscow 119991, Russian Federation

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Contains:

copies of ¹H, ¹³C and DEPT NMR spectra of all new compounds, presented in the same order in which they appeared in the experimental part of article; optimization tables for alkylation with ethyl bromoacetate and Michael acceptors.

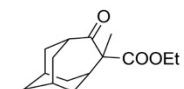
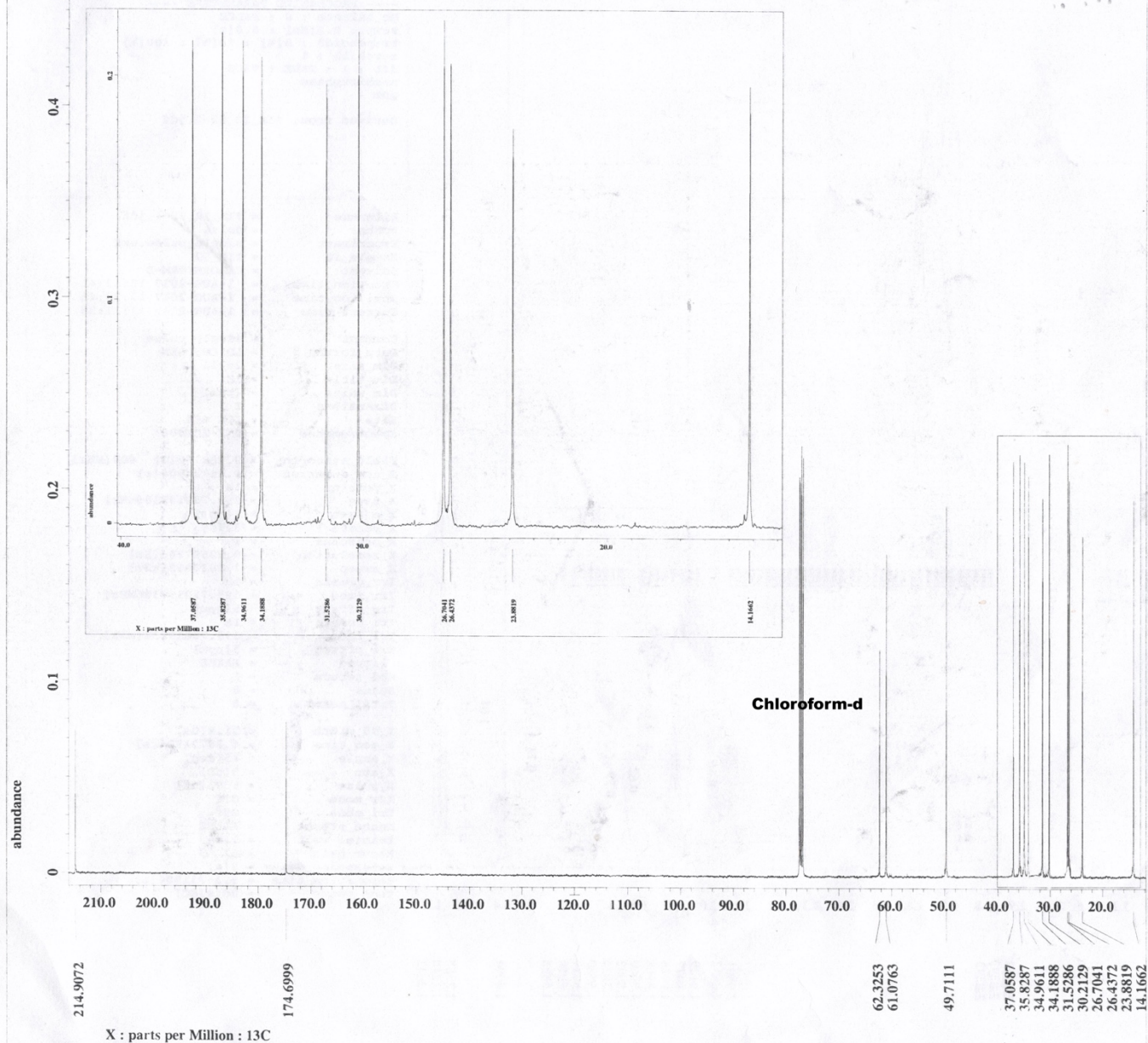


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 X_resolution = 0.22897343[Hz]
 X_sweep = 7.5030012[kHz]
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 Irr_freq = 399.78219838[MHz]
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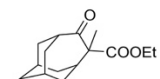
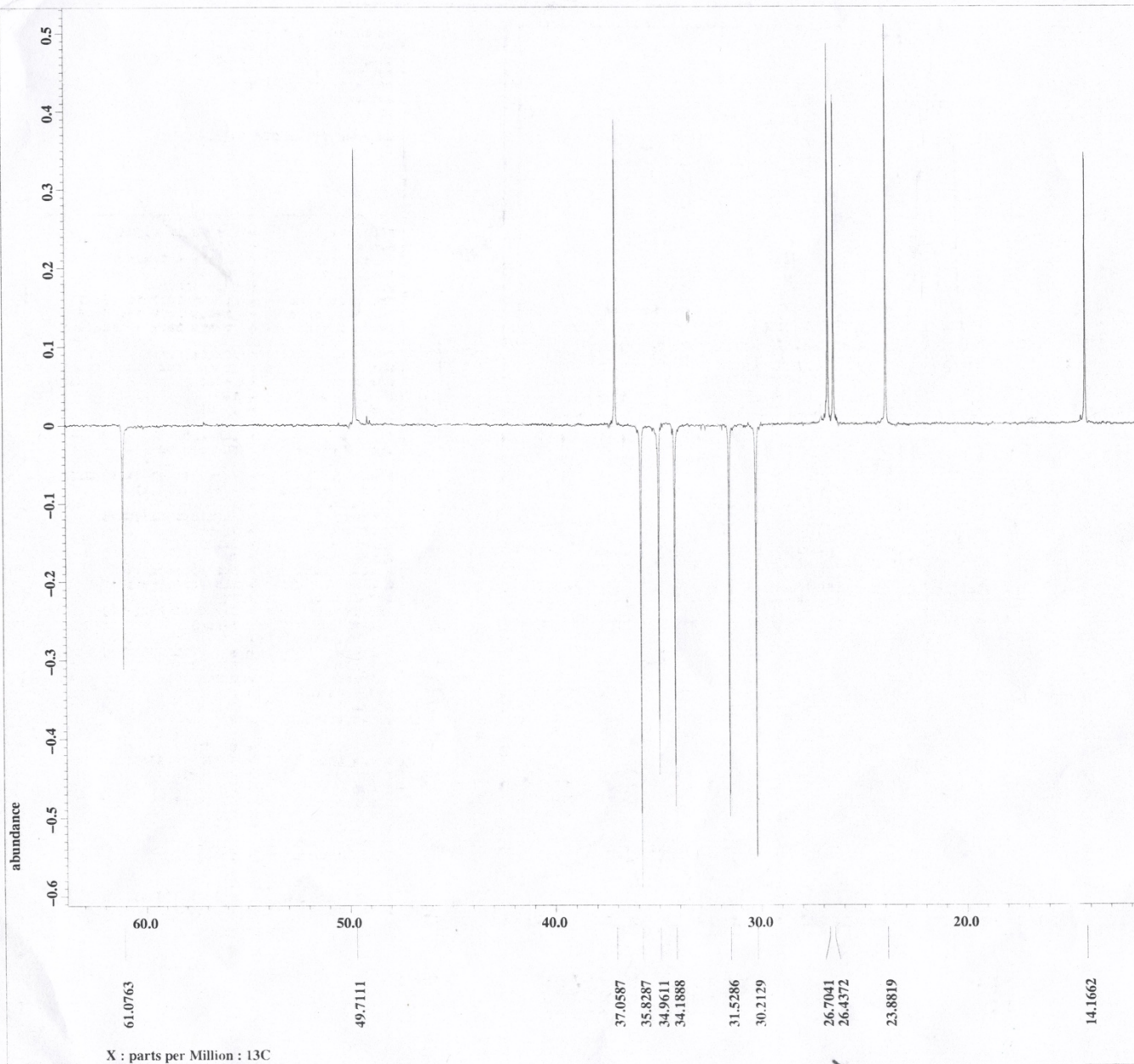


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 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
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 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
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 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
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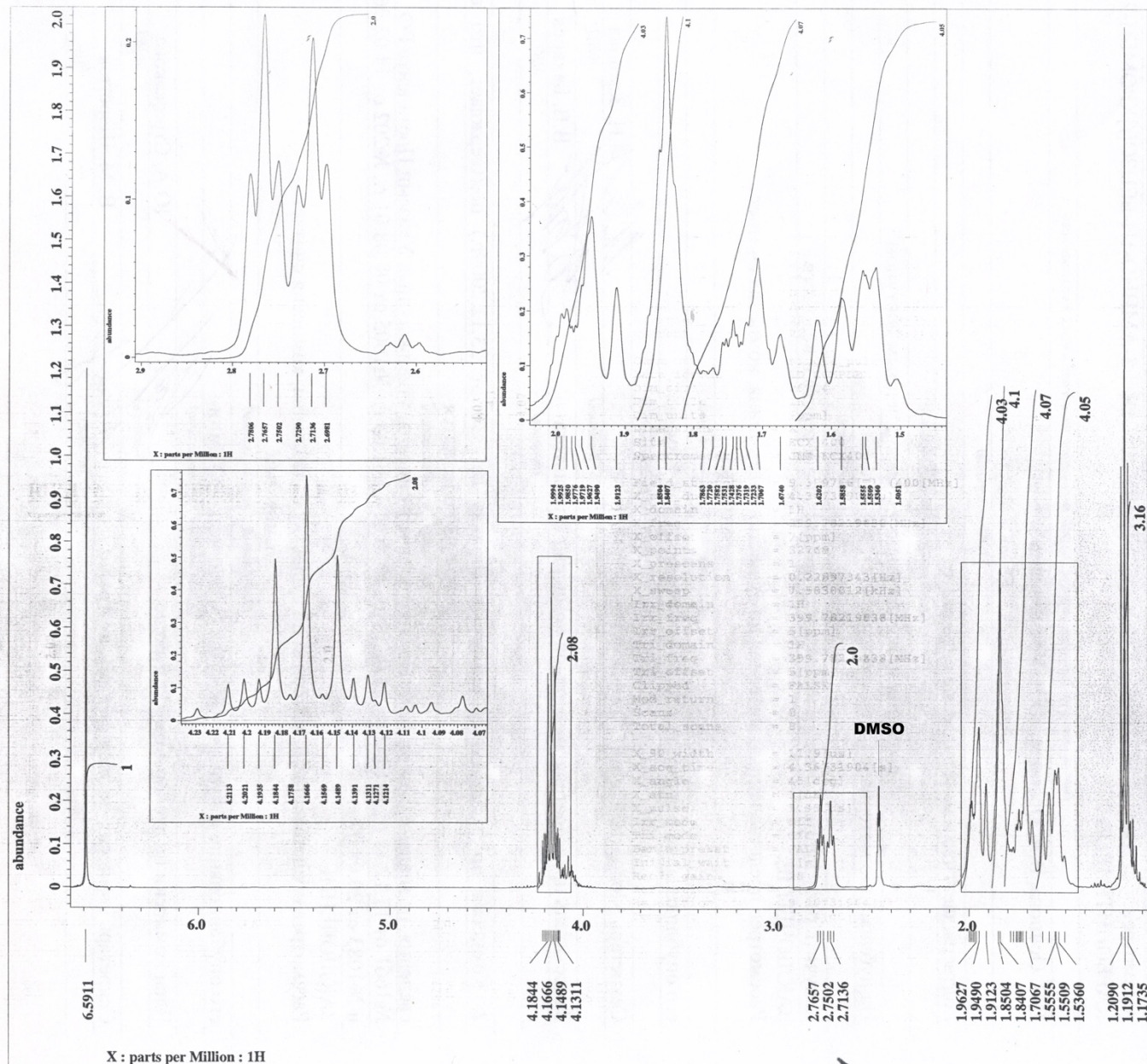
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Spectrometer  = JNM-ECX400

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X_points       = 32768
X_prescans     = 4
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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     = 1.04333312[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]
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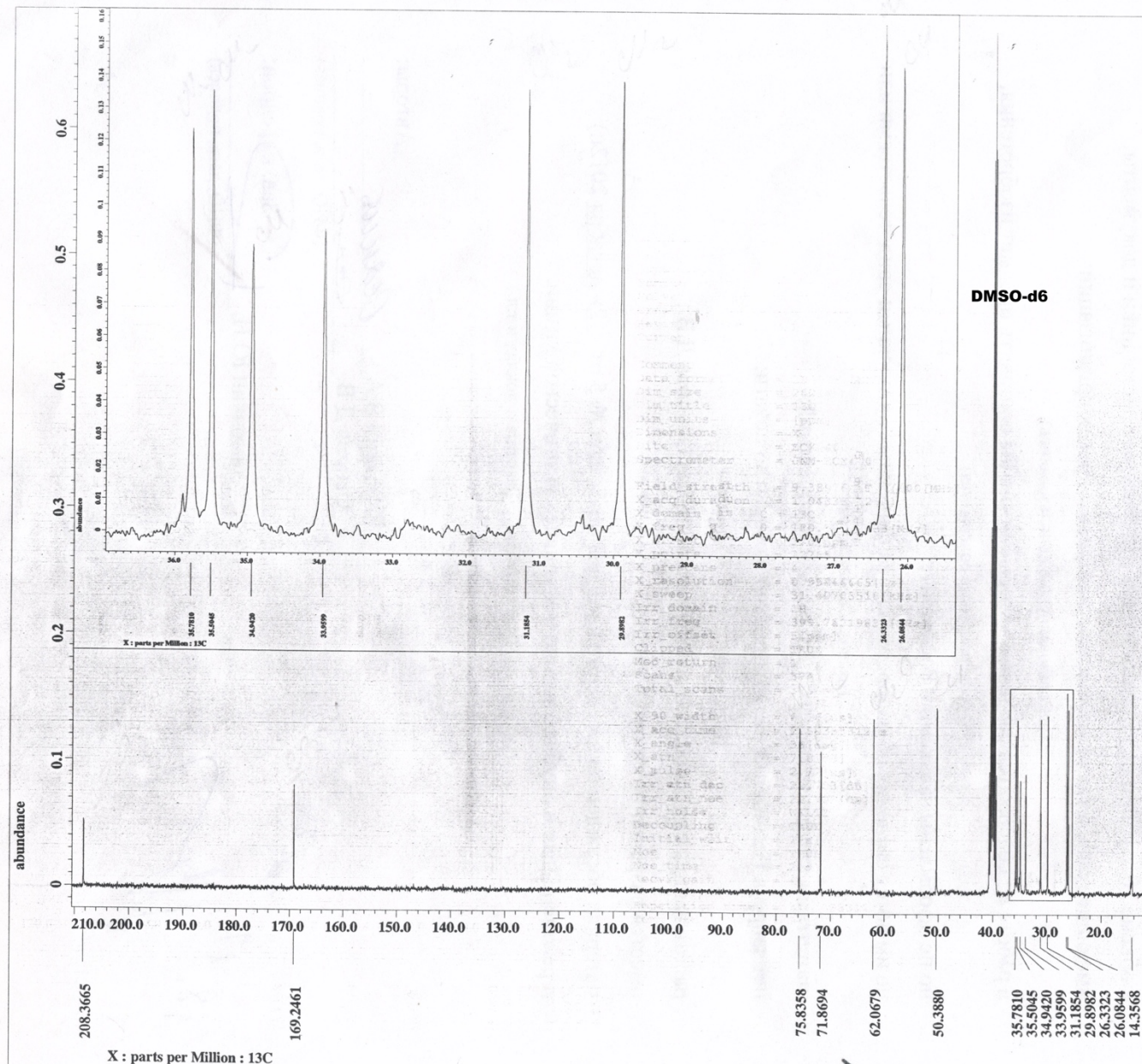



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 Revision_time = 22-FEB-2019 13:33:55
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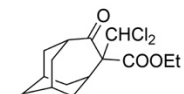
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 Spectrometer = JNM-ECK400

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 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 = 28
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 23.4[dc]



DMSO-d6

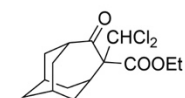
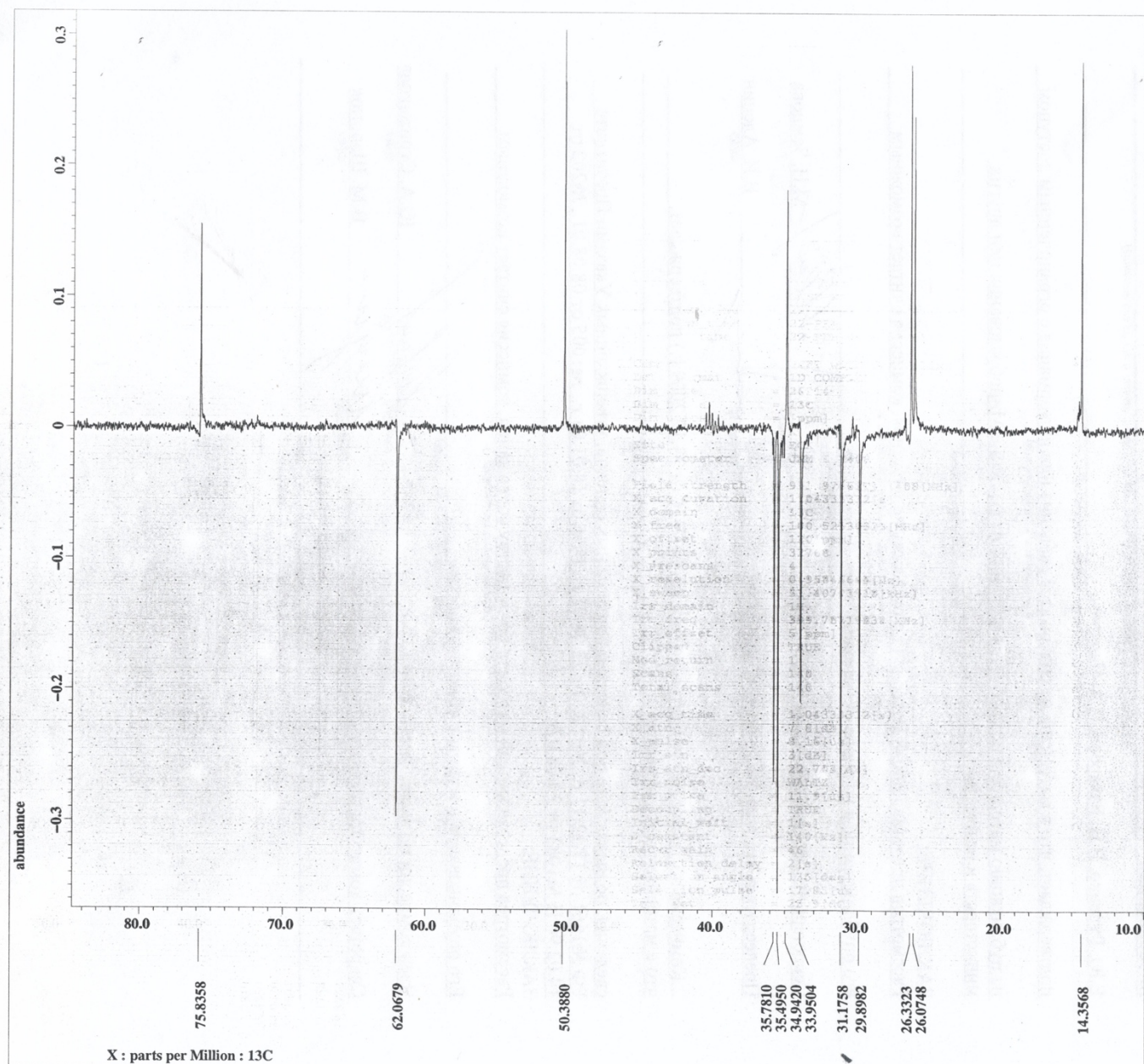


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Revision_time = 22-FEB-2019 13:34:51
Current_time = 22-FEB-2019 13:35:04

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Spectrometer = JNM-ECK400

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X_domain = 13C
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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]
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Mod_return = 1
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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]
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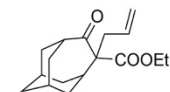
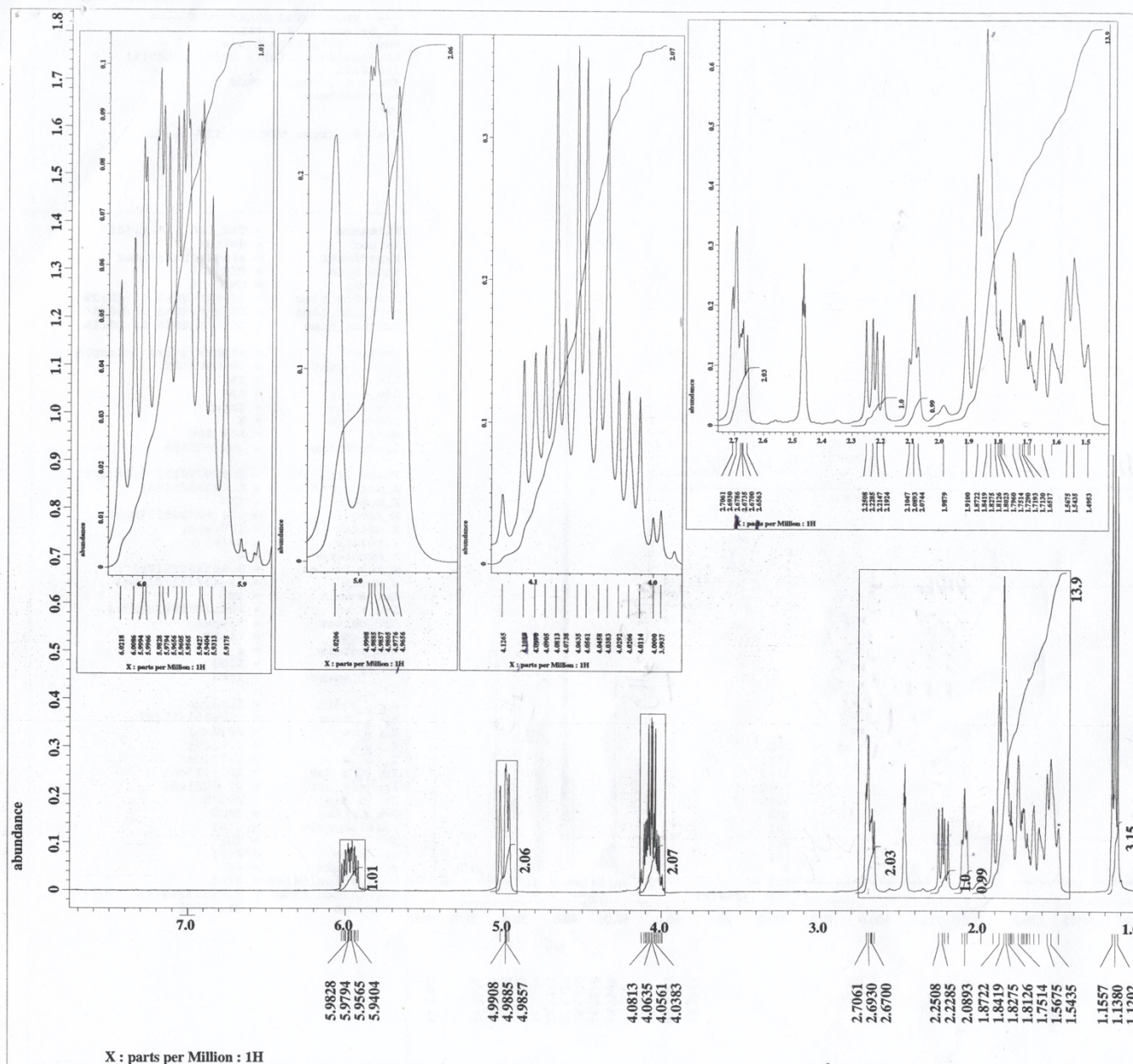


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Current_time = 22-FEB-2019 13:35:21

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Dim_title = 13C
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Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400

Field_strength = 9.389766 [T] (400 [MHz])
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X_freq = 100.5230333 [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 = 140
Total_scans = 140

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 = 23.9 [degC]

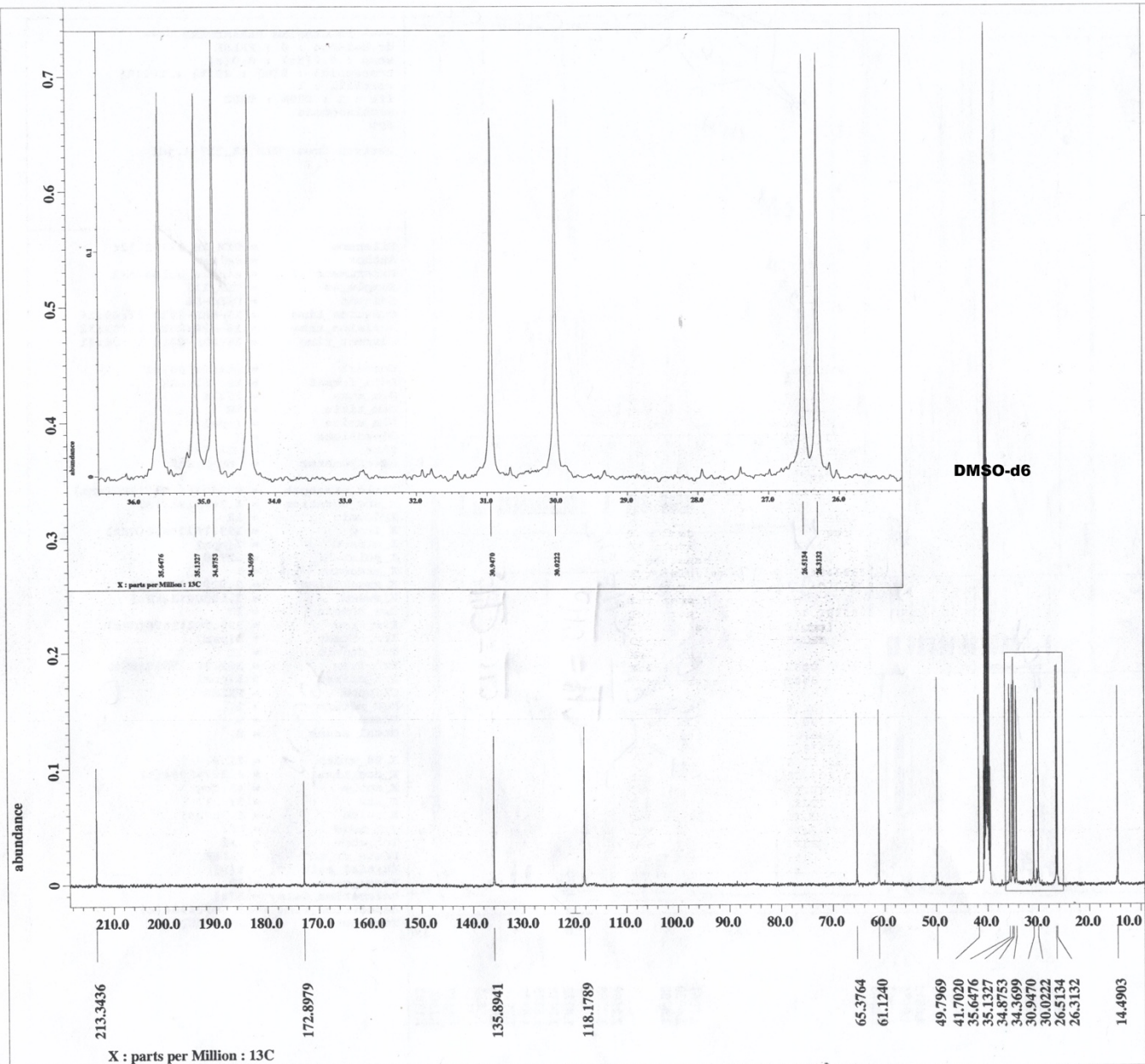


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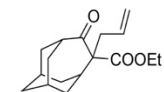
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 X_freq = 399.78219838[MHz]
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 X_prescans = 1
 X_resolution = 0.22897343[Hz]
 X_sweep = 7.5030012[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 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]
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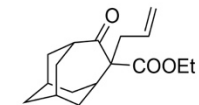
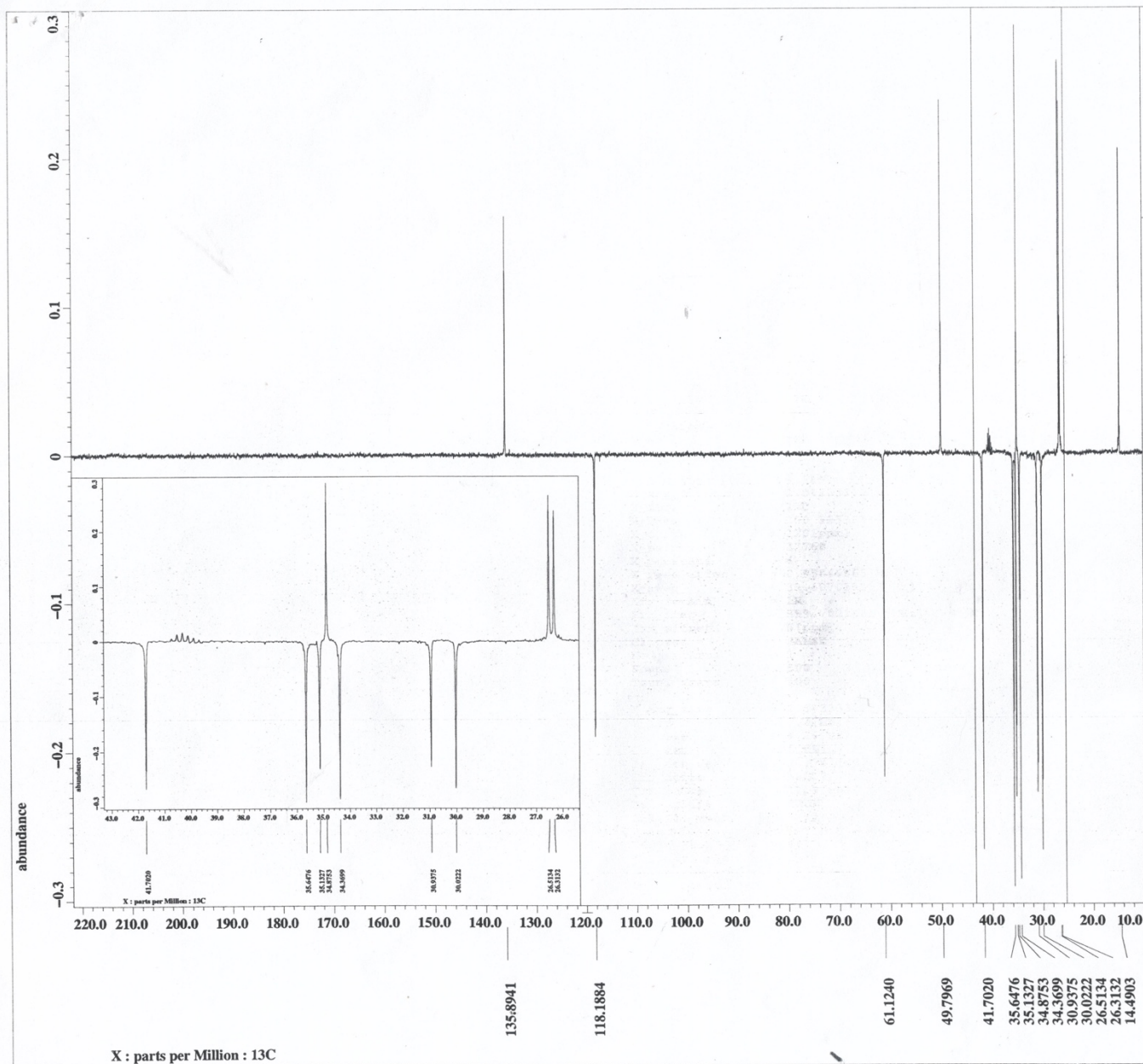
DMSO-d6



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X_prescans = 4
X_resolution = 0.95846665[MHz]
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
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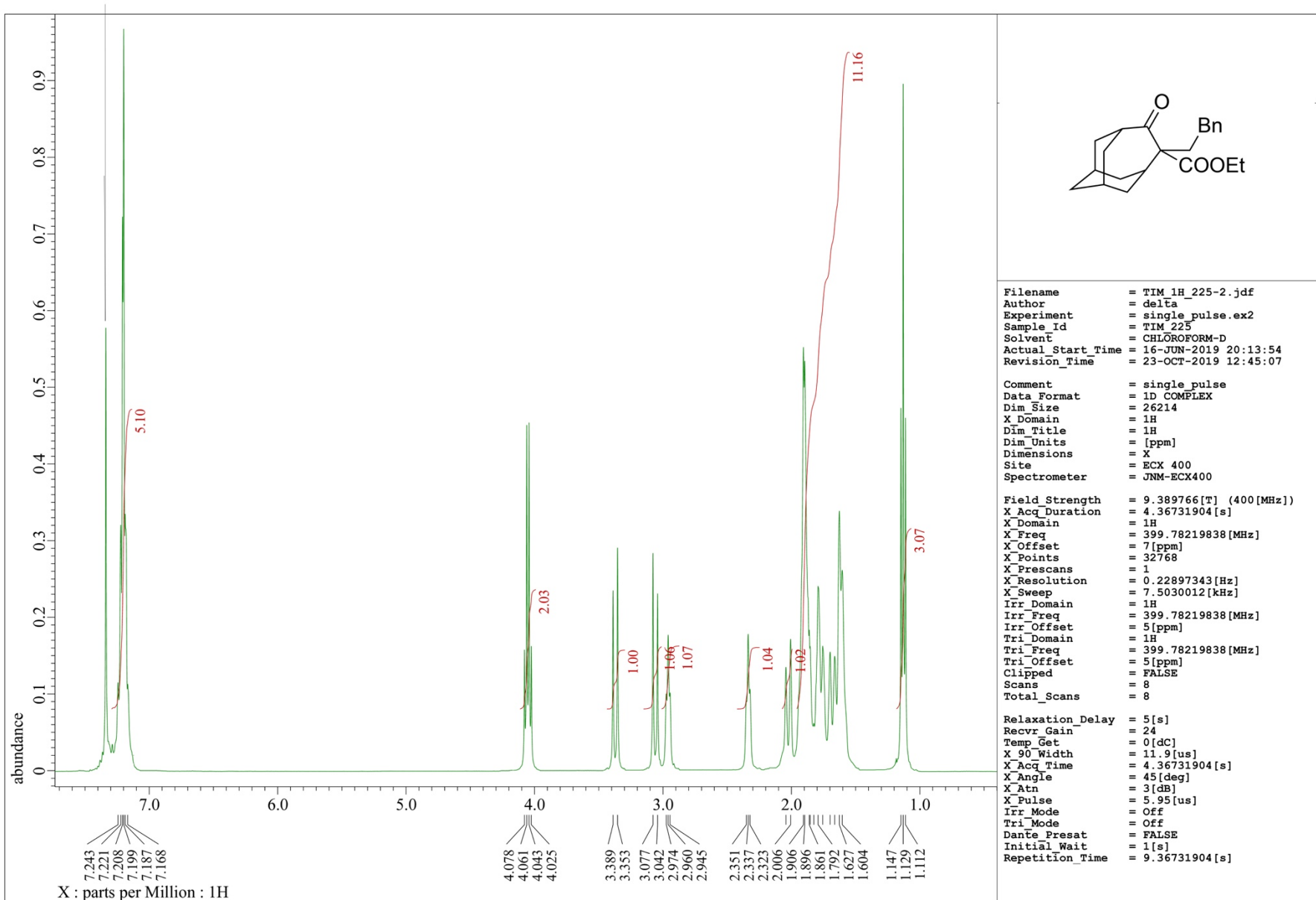
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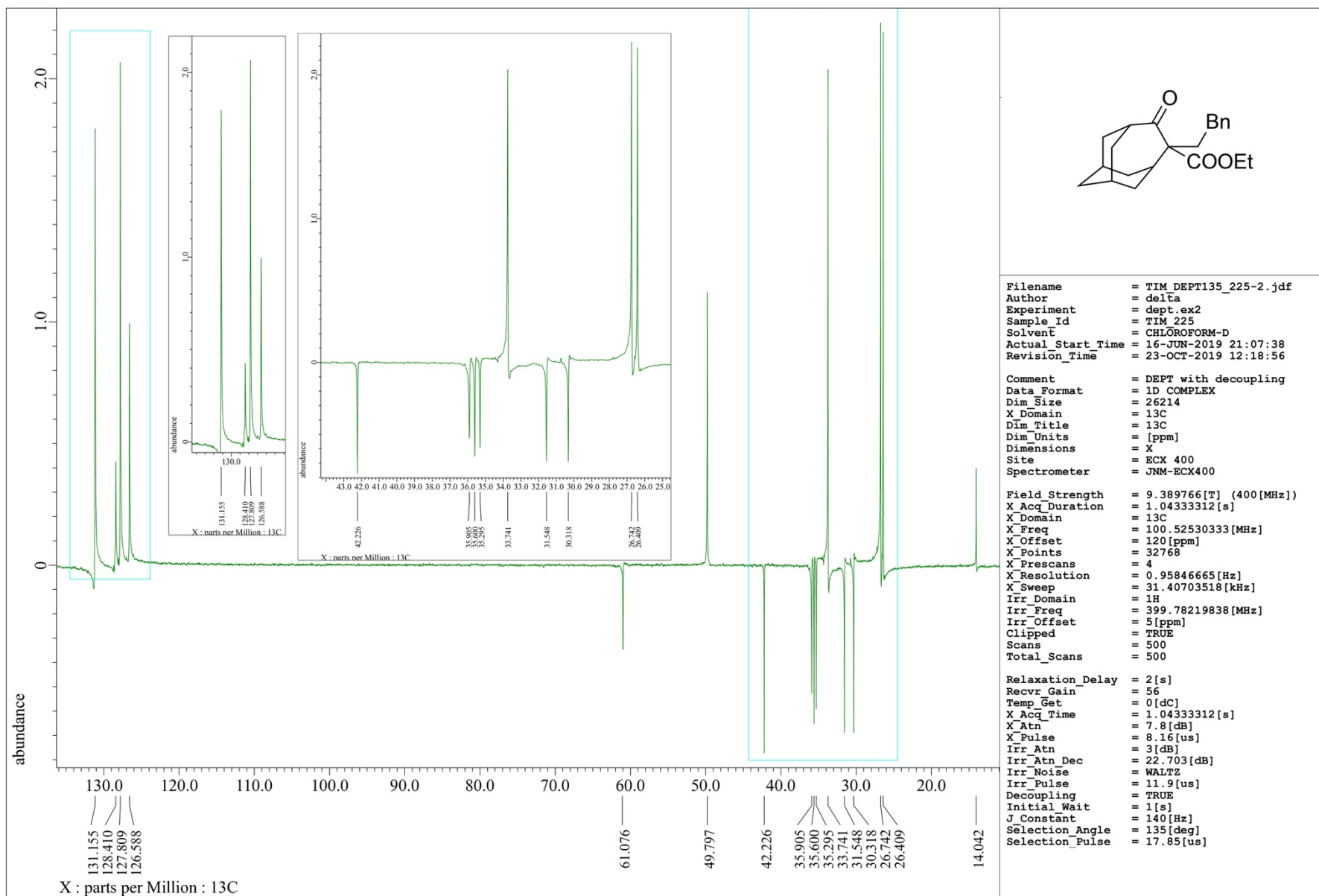
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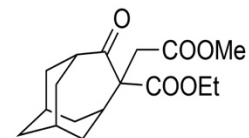
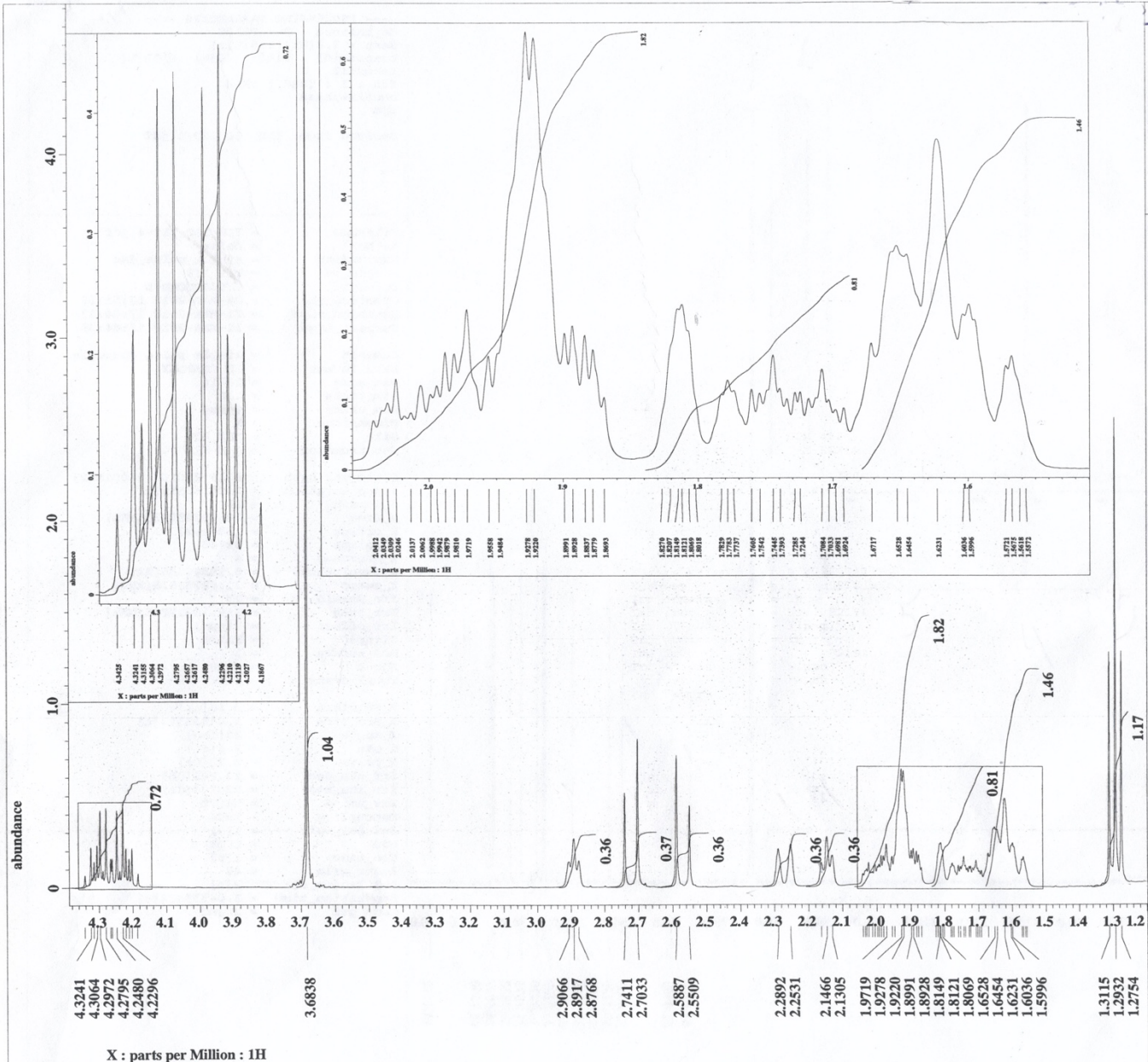
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 X_points = 32768
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 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 500
 Total_scans = 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 = 21.7[dc]

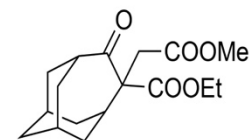
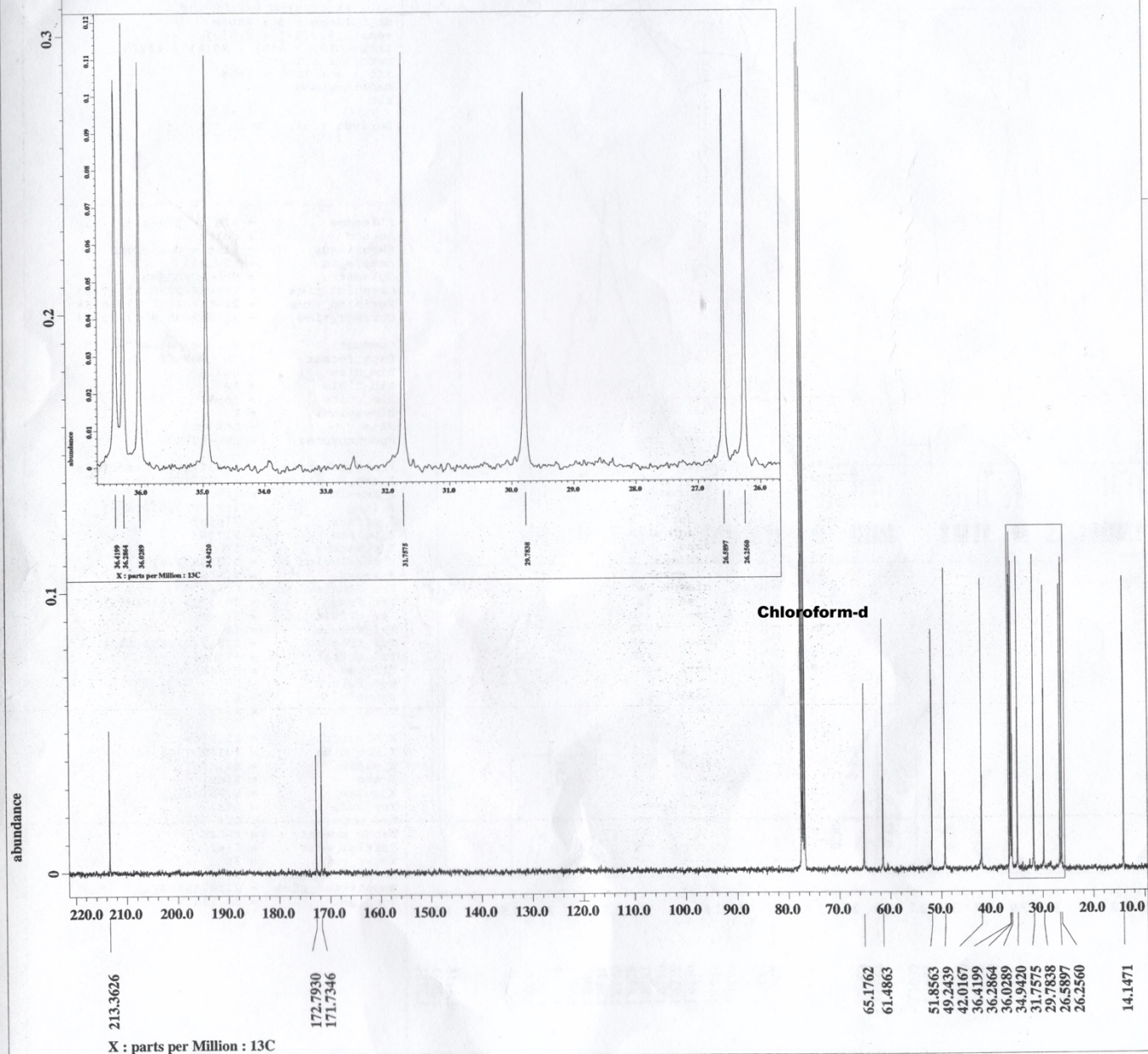
Chloroform







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 Dim_units = [ppm]
 Dimensions = X
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 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
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 Temp_get = 19.7 [dC]

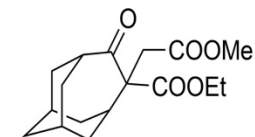
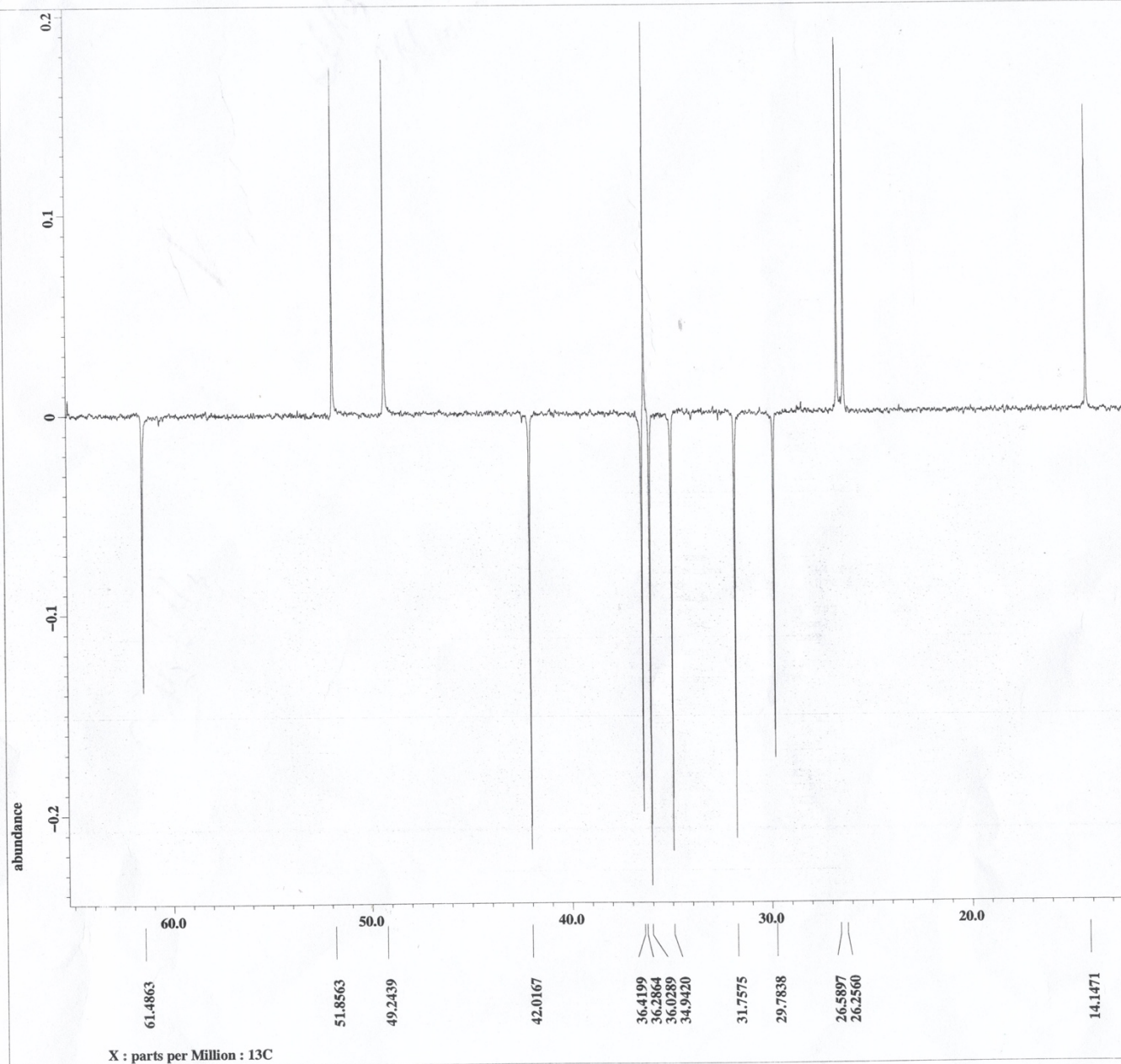


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 Spectrometer = JNM-ECX400

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 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 = 46
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 20[dc]

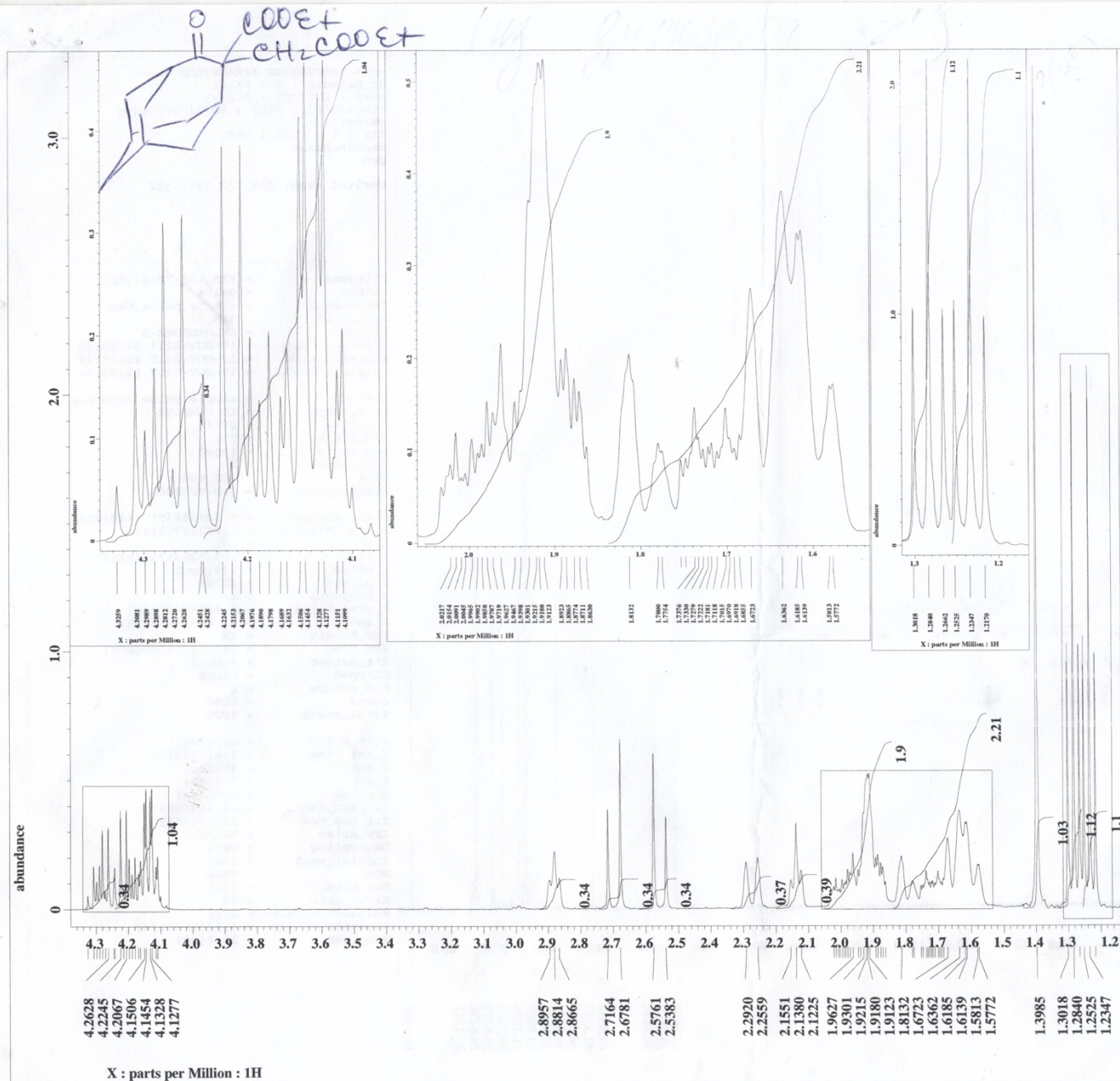


Filename = TIM_DEPT135_119-5.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_119
 Solvent = CHLOROFORM-D
 Creation_time = 20-MAR-2018 13:16:58
 Revision_time = 21-MAR-2018 17:44:54
 Current_time = 21-MAR-2018 17:45:02

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 = 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 = 19.9[dc]



----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sexp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm

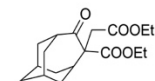
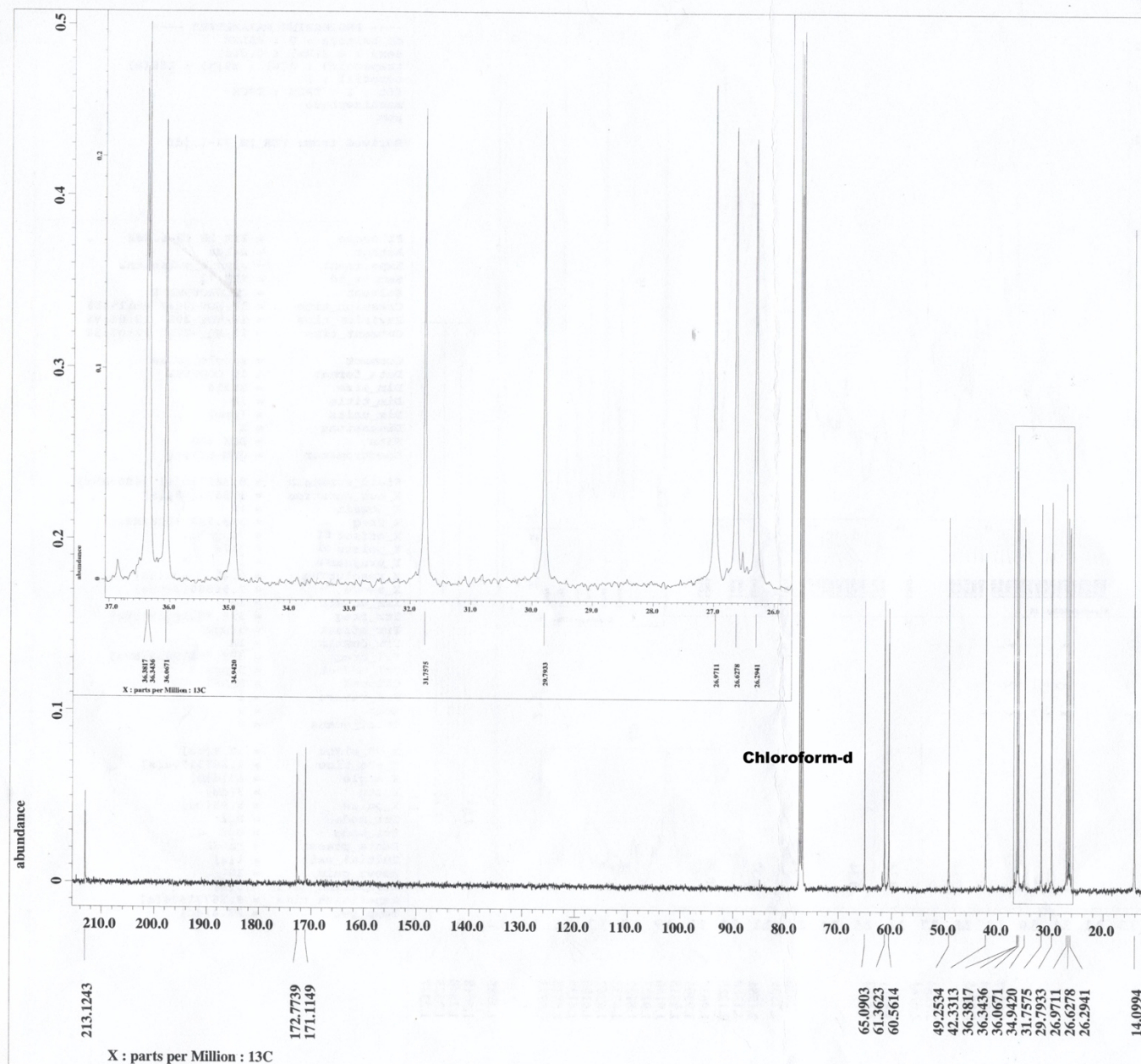
Derived from: TIM_1H_72-1.jdf

Filename = TIM_1H_72-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_72
 Solvent = CHLOROFORM-D
 Creation_time = 17-NOV-2017 05:15:56
 Revision_time = 17-NOV-2017 12:07:06
 Current_time = 17-NOV-2017 12:07:30

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_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 30
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 28.4[dc]

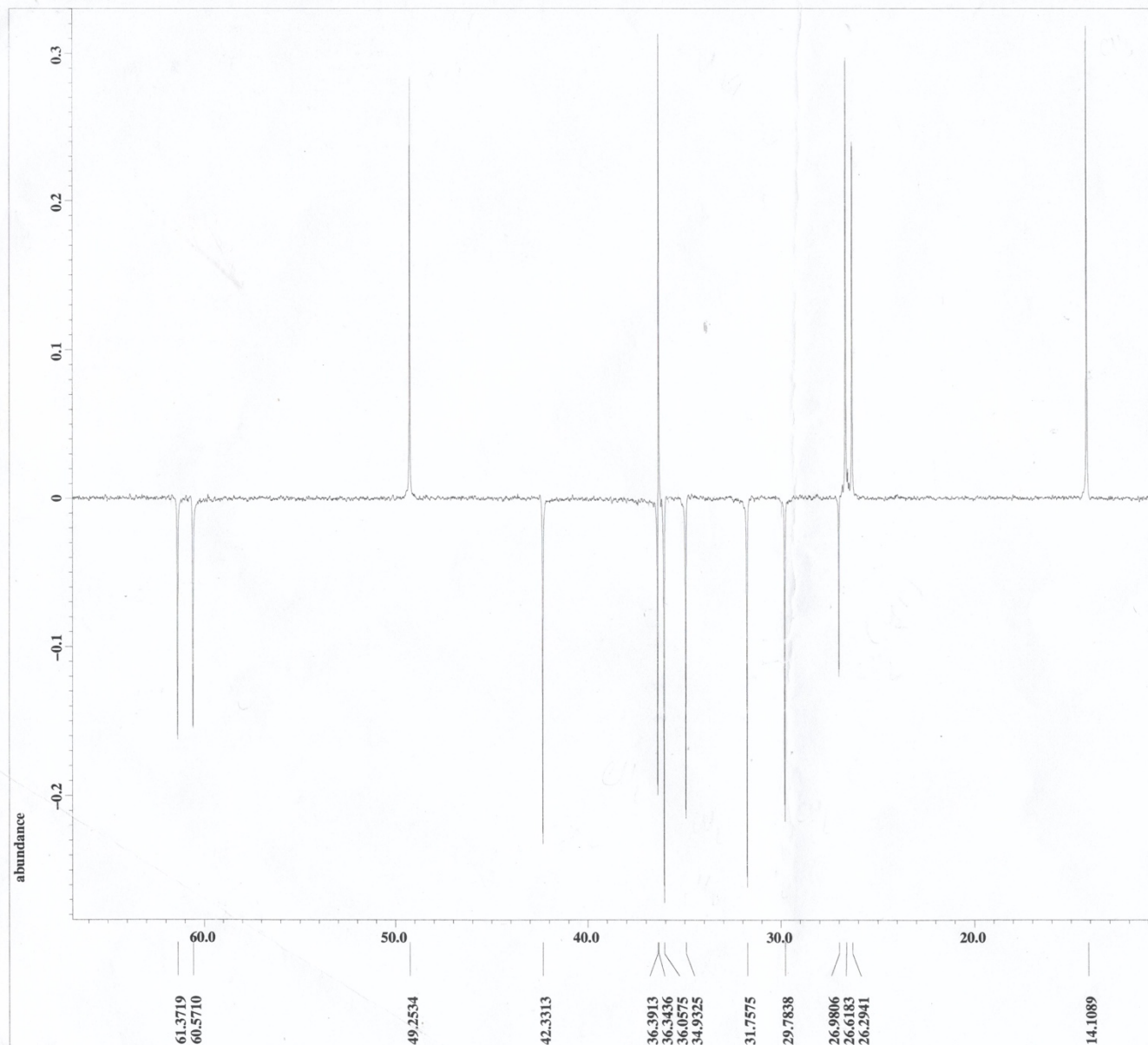


Filename = TIM_13C_72-4.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_72
 Solvent = CHLOROFORM-D
 Creation_time = 17-NOV-2017 06:09:05
 Revision_time = 17-NOV-2017 12:07:39
 Current_time = 17-NOV-2017 12:08:14

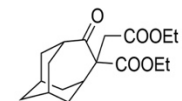
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

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 = 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 = 24.4[dc]



X : parts per Million : 13C

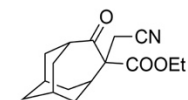
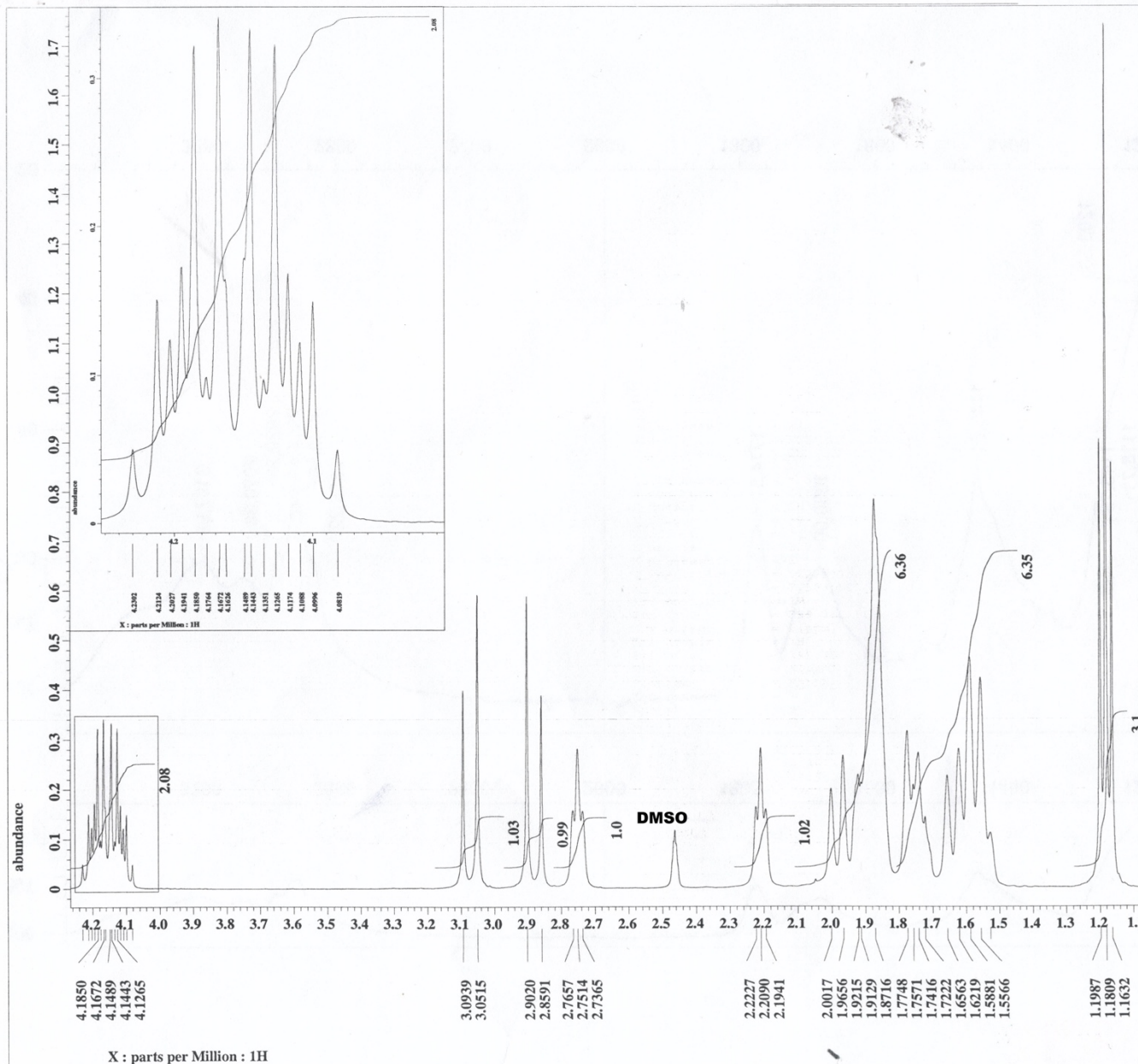


Filename = TIM_DEPT135_72-3.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_72
 Solvent = CHLOROFORM-D
 Creation_time = 17-NOV-2017 06:35:00
 Revision_time = 17-NOV-2017 12:08:23
 Current_time = 17-NOV-2017 12:08:36

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 = 23.8 [dC]

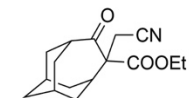
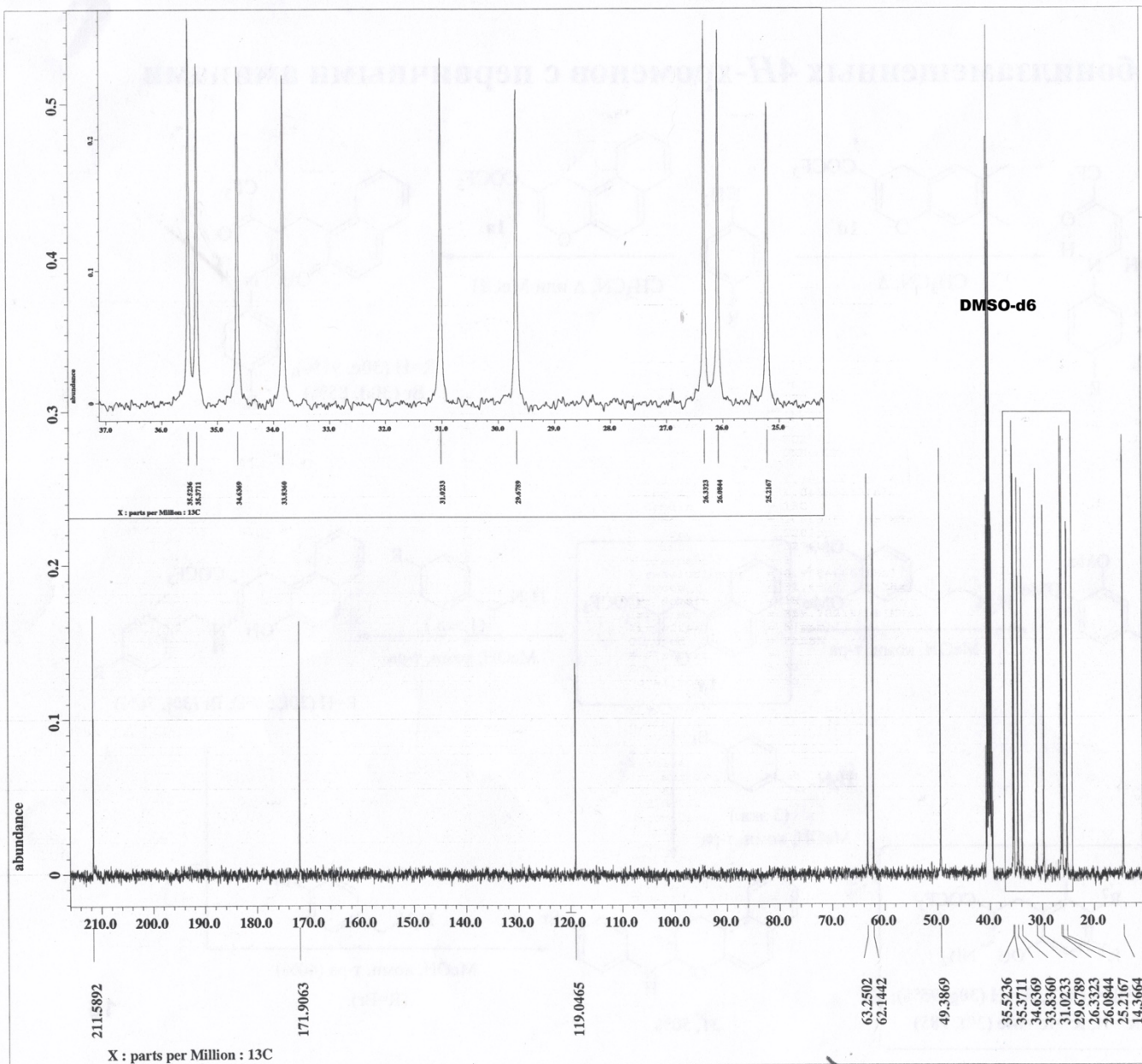


Filename = TIM_1H_146-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_146
 Solvent = DMSO-D6
 Creation_time = 10-OCT-2018 14:22:41
 Revision_time = 10-OCT-2018 13:43:22
 Current_time = 10-OCT-2018 13:43:45

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 = 24
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 21.6[dc]

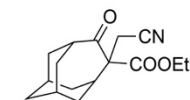
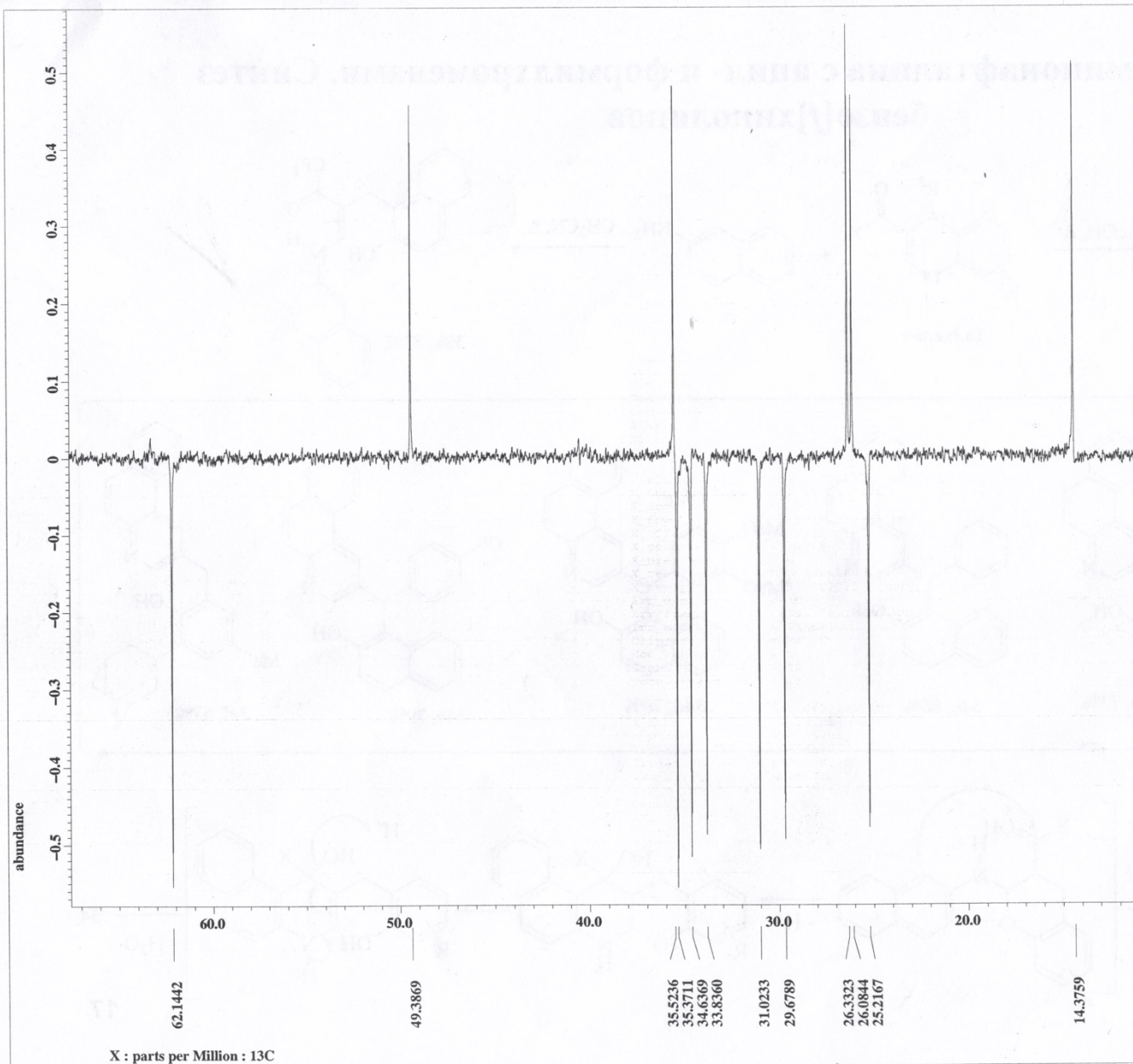


Filename = TIM_13C_146-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_146
 Solvent = DMSO-D6
 Creation_time = 10-OCT-2018 14:37:40
 Revision_time = 10-OCT-2018 13:56:03
 Current_time = 10-OCT-2018 13:56:33

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECK 400
 Spectrometer = JNM-ECK400

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 = 53
 Total_scans = 53

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 = 21.6[dc]

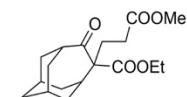
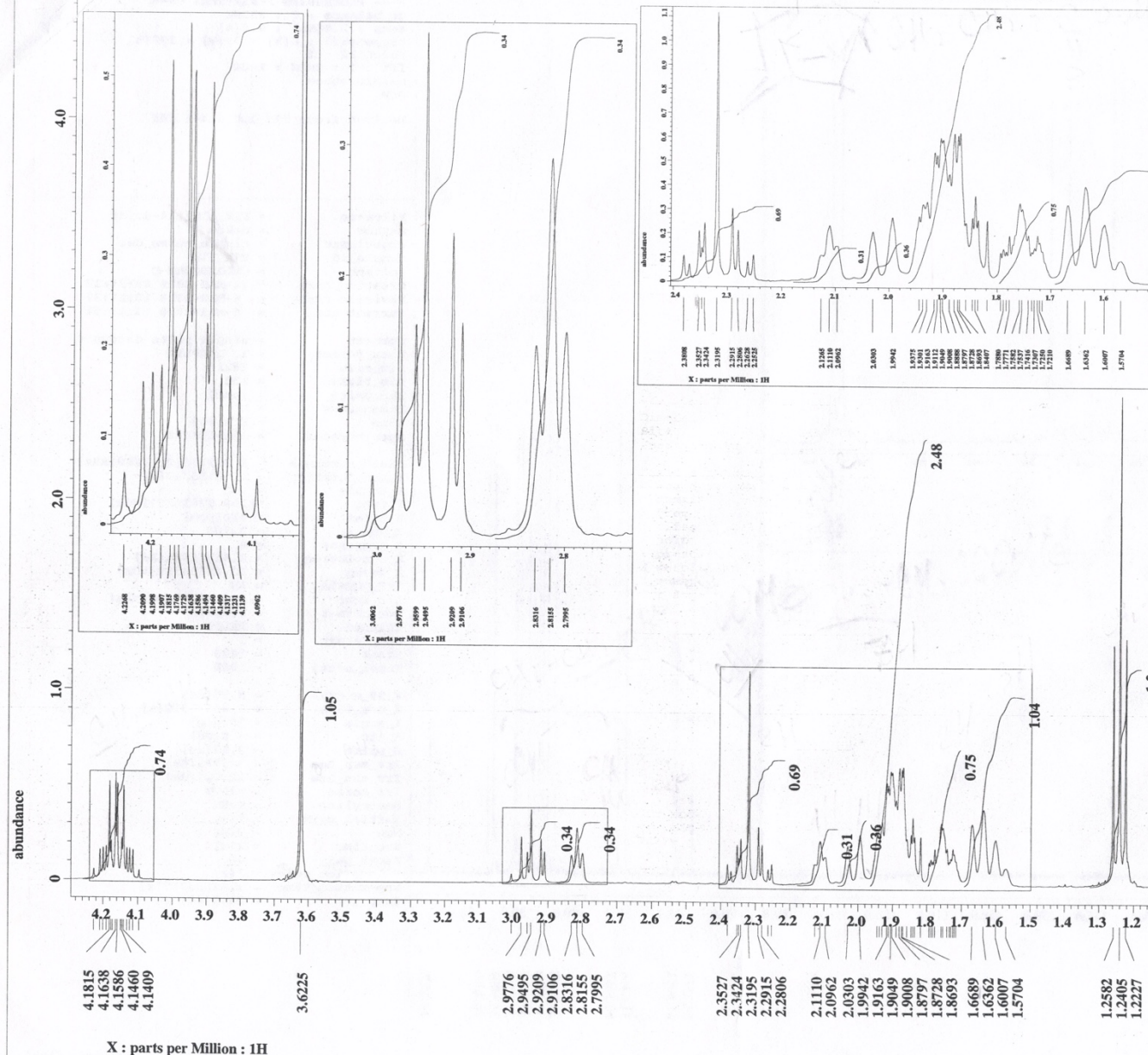


Filename = TIM_DEPT135_146-4.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_146
 Solvent = DMSO-D6
 Creation_time = 10-OCT-2018 14:38:34
 Revision_time = 10-OCT-2018 13:57:10
 Current_time = 10-OCT-2018 13:57:17

Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = ^{13}C
 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 = ^{13}C
 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 = 11
 Total_scans = 11

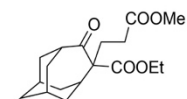
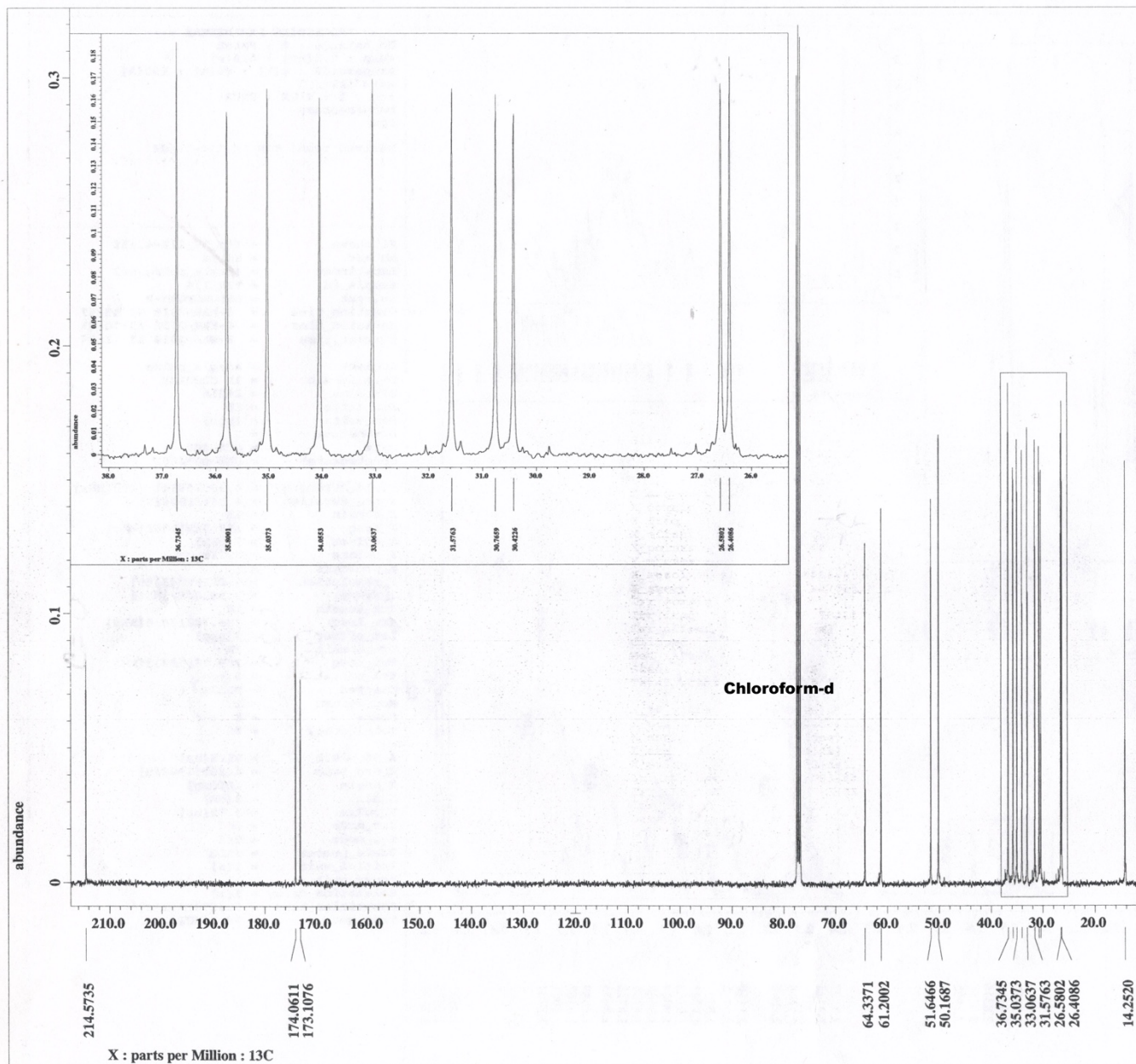
X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]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



Filename = TIM_1H_114-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_114
 Solvent = CHLOROFORM-D
 Creation_time = 6-MAR-2018 08:38:57
 Revision_time = 6-MAR-2018 13:10:45
 Current_time = 6-MAR-2018 13:11:24

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 = 20.3[dc]

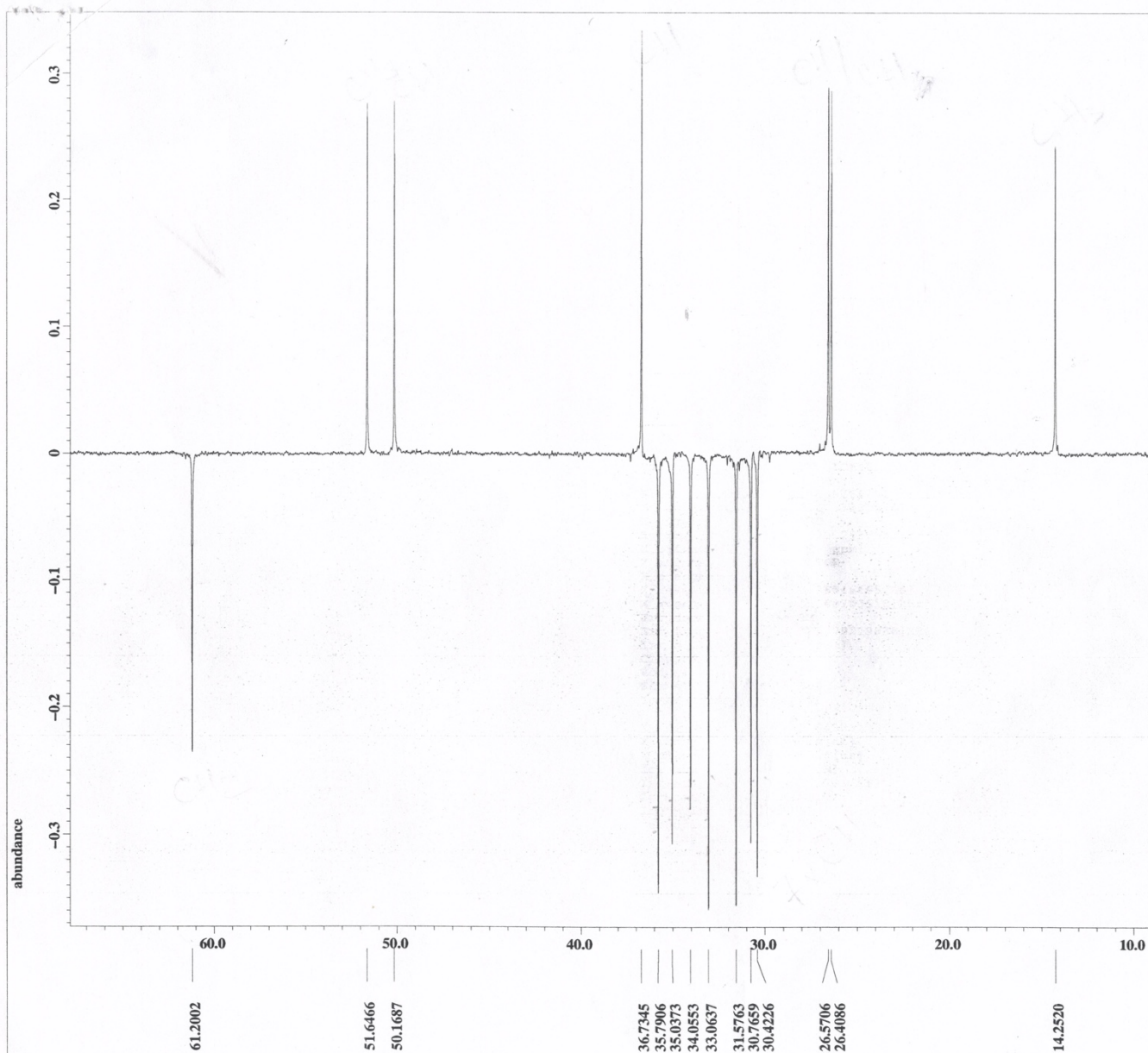


Filename = TIM_13C_114-4.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_114
 Solvent = CHLOROFORM-D
 Creation_time = 6-MAR-2018 09:32:12
 Revision_time = 6-MAR-2018 13:11:37
 Current_time = 6-MAR-2018 13:11:50

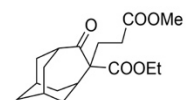
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

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 = 46
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 20.2[dc]



X : parts per Million : 13C

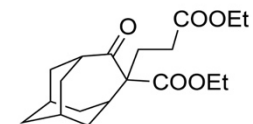
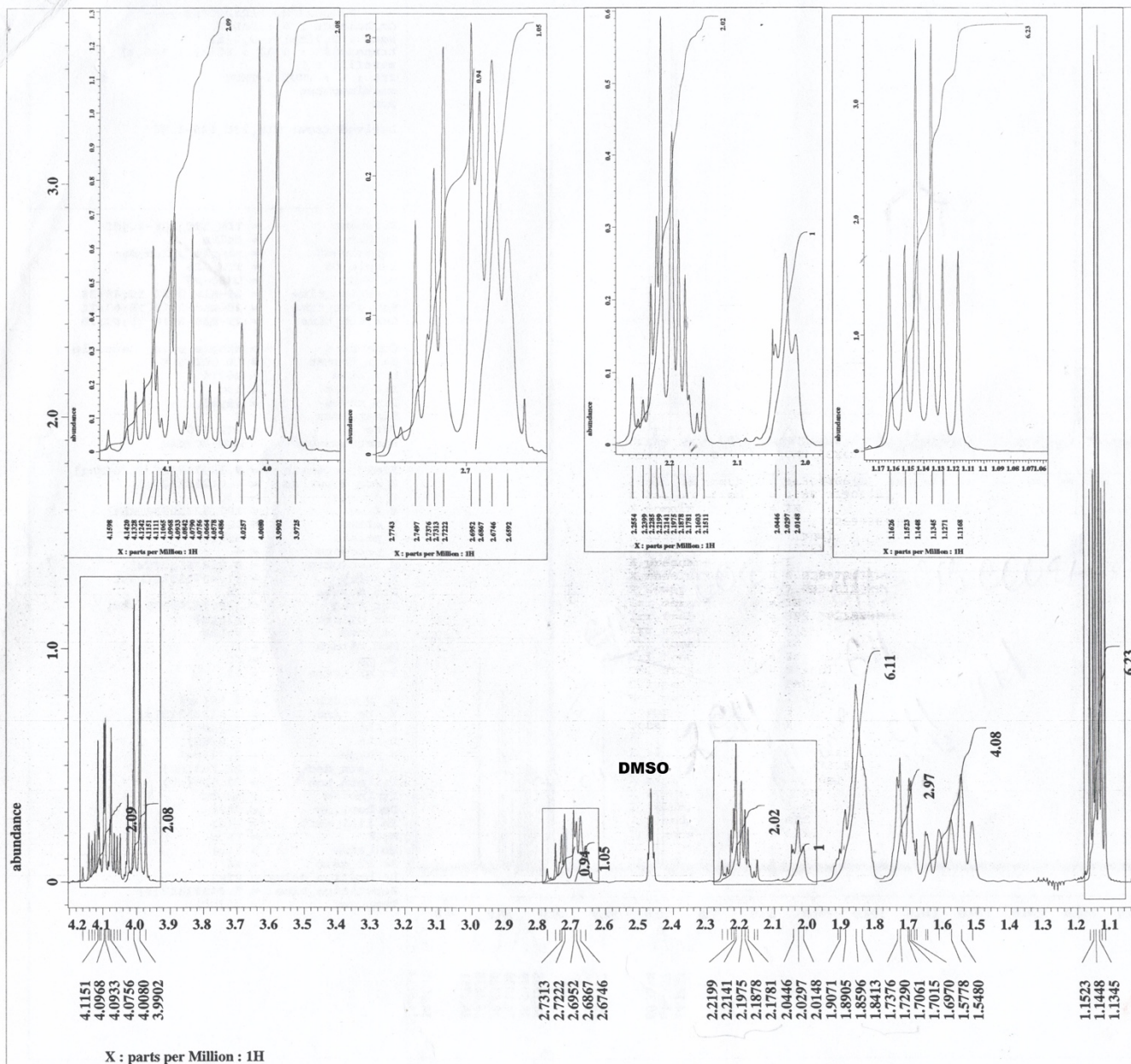


Filename = TIM_DEPT135_114-4.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_114
 Solvent = CHLOROFORM-D
 Creation_time = 6-MAR-2018 09:58:04
 Revision_time = 6-MAR-2018 13:12:00
 Current_time = 6-MAR-2018 13:12:04

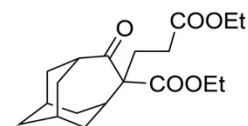
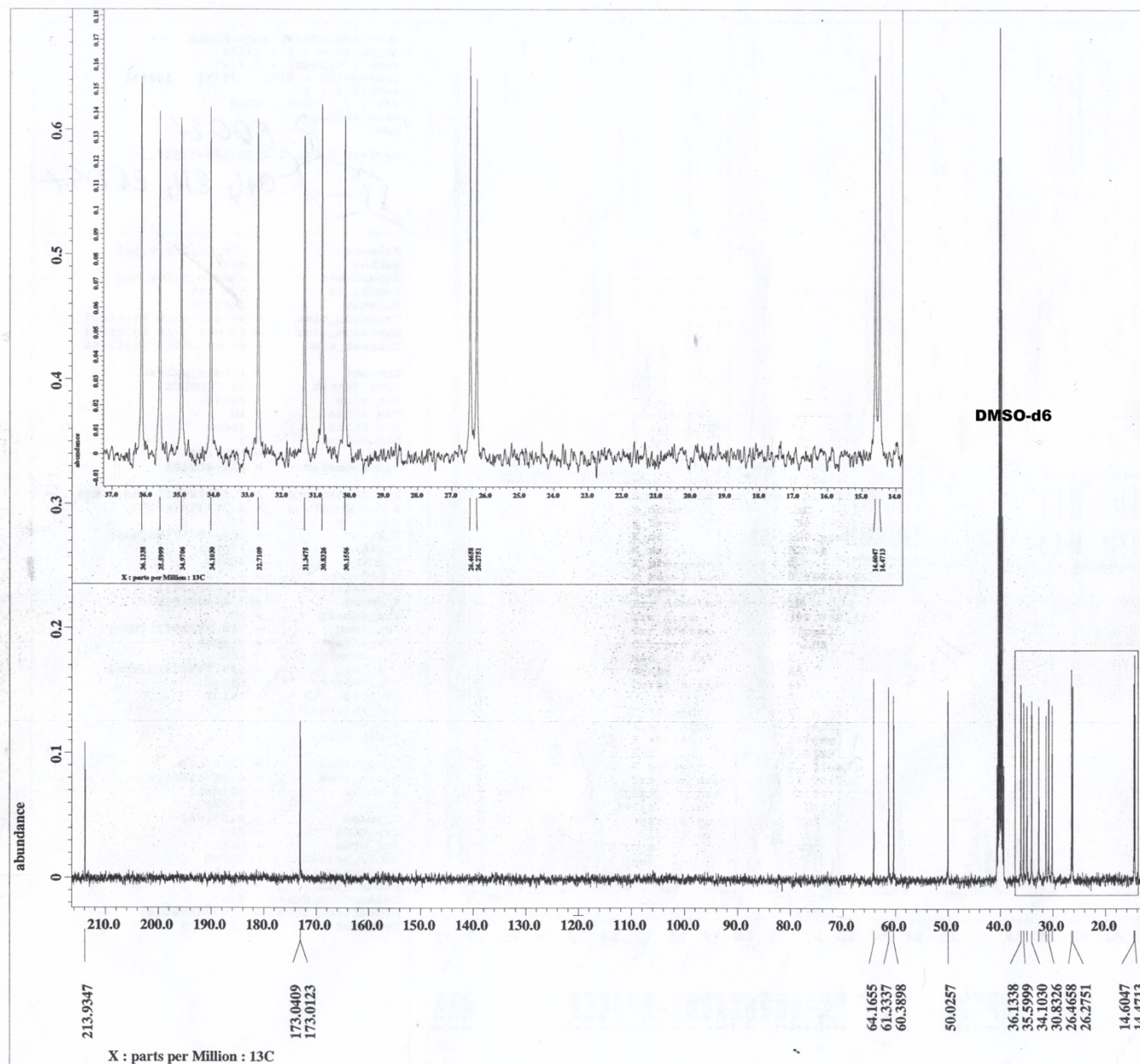
Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

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

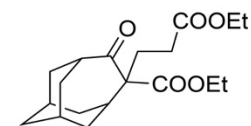
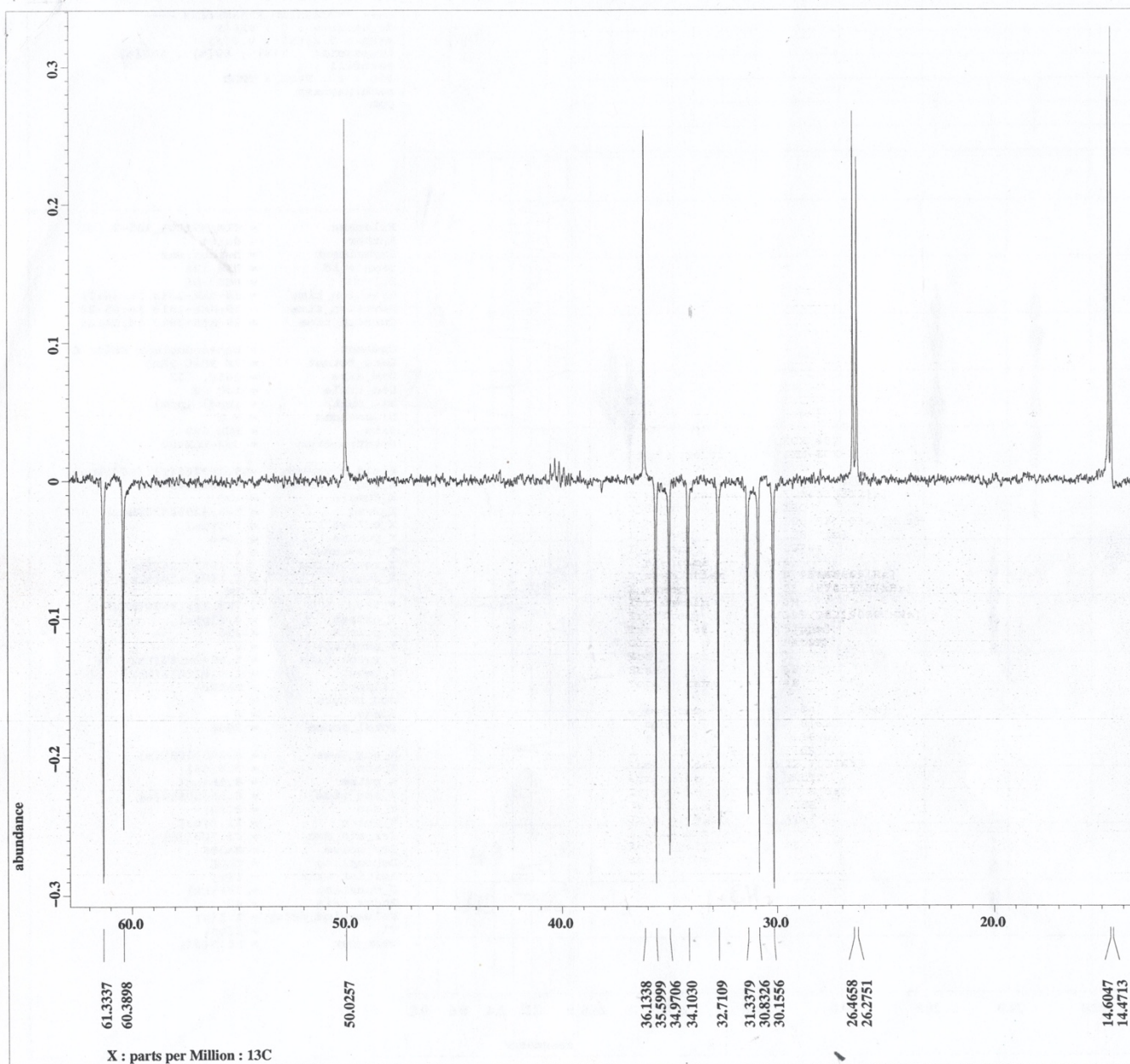
X_acq_time = 1.0433312[s]
 X_atn = 7.8[db]
 X_pulse = 8.16[us]
 Irr_atn = 3[db]
 Irr_atn_dec = 22.703[db]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 20[dc]



Filename = TIM_1H_125-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_125
 Solvent = DMSO-D6
 Creation_time = 29-MAR-2018 15:42:37
 Revision_time = 29-MAR-2018 18:01:23
 Current_time = 29-MAR-2018 18:02:54
 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 = 19.9[dc]



Filename = TIM_13C_125-4.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_125
 Solvent = DMSO-D6
 Creation_time = 29-MAR-2018 15:48:24
 Revision_time = 29-MAR-2018 18:03:11
 Current_time = 29-MAR-2018 18:03:28
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECK400
 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 = 65
 Total_scans = 65
 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 = 20 [dC]

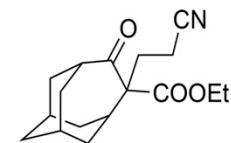
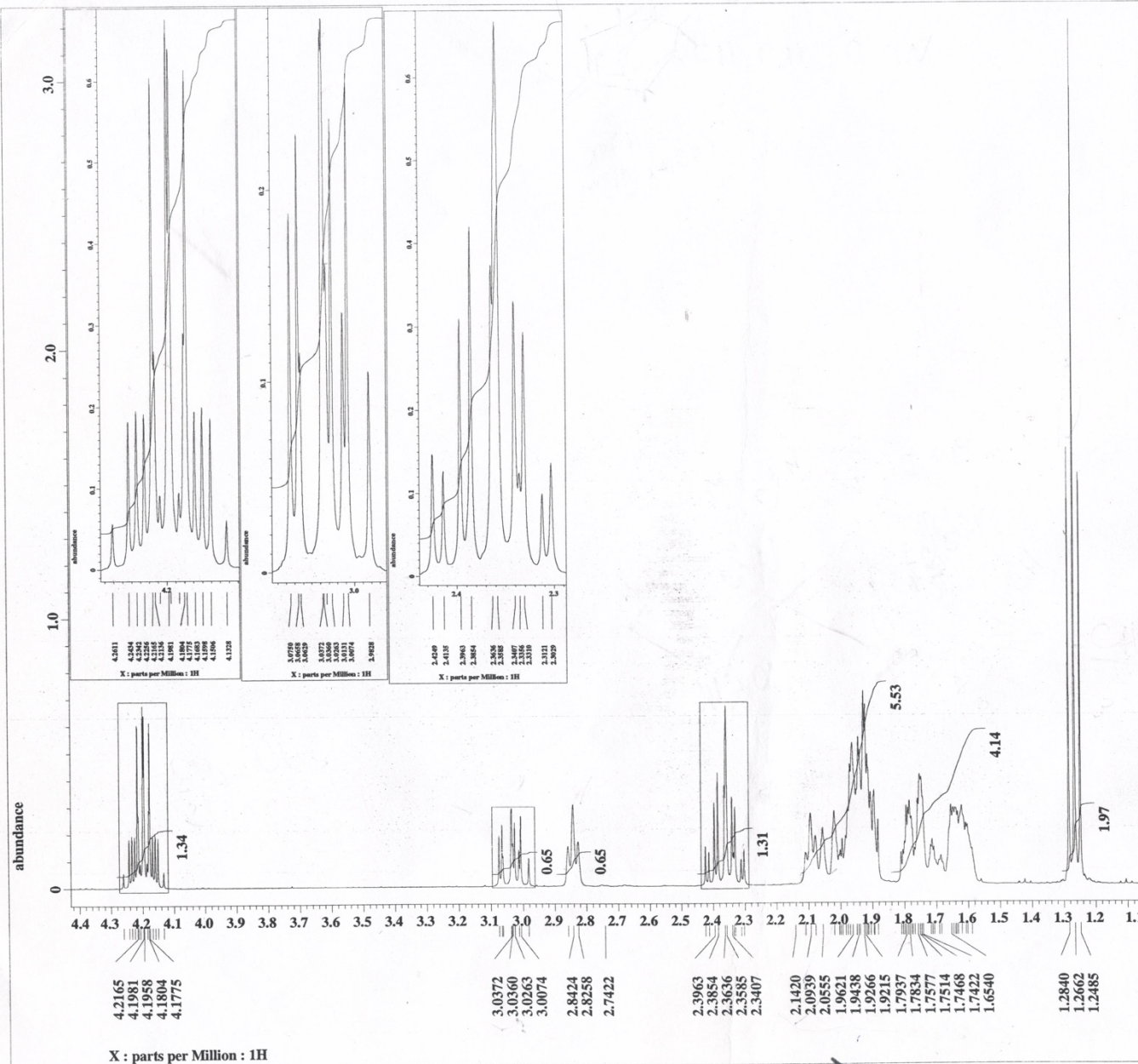


Filename = TIM_DEPT135_125-4.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_125
 Solvent = DMSO-D6
 Creation_time = 29-MAR-2018 15:52:13
 Revision_time = 29-MAR-2018 15:01:26
 Current_time = 29-MAR-2018 18:03:44

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 = 68
 Total_scans = 68

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 = 19.9[dc]

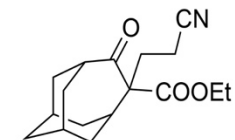
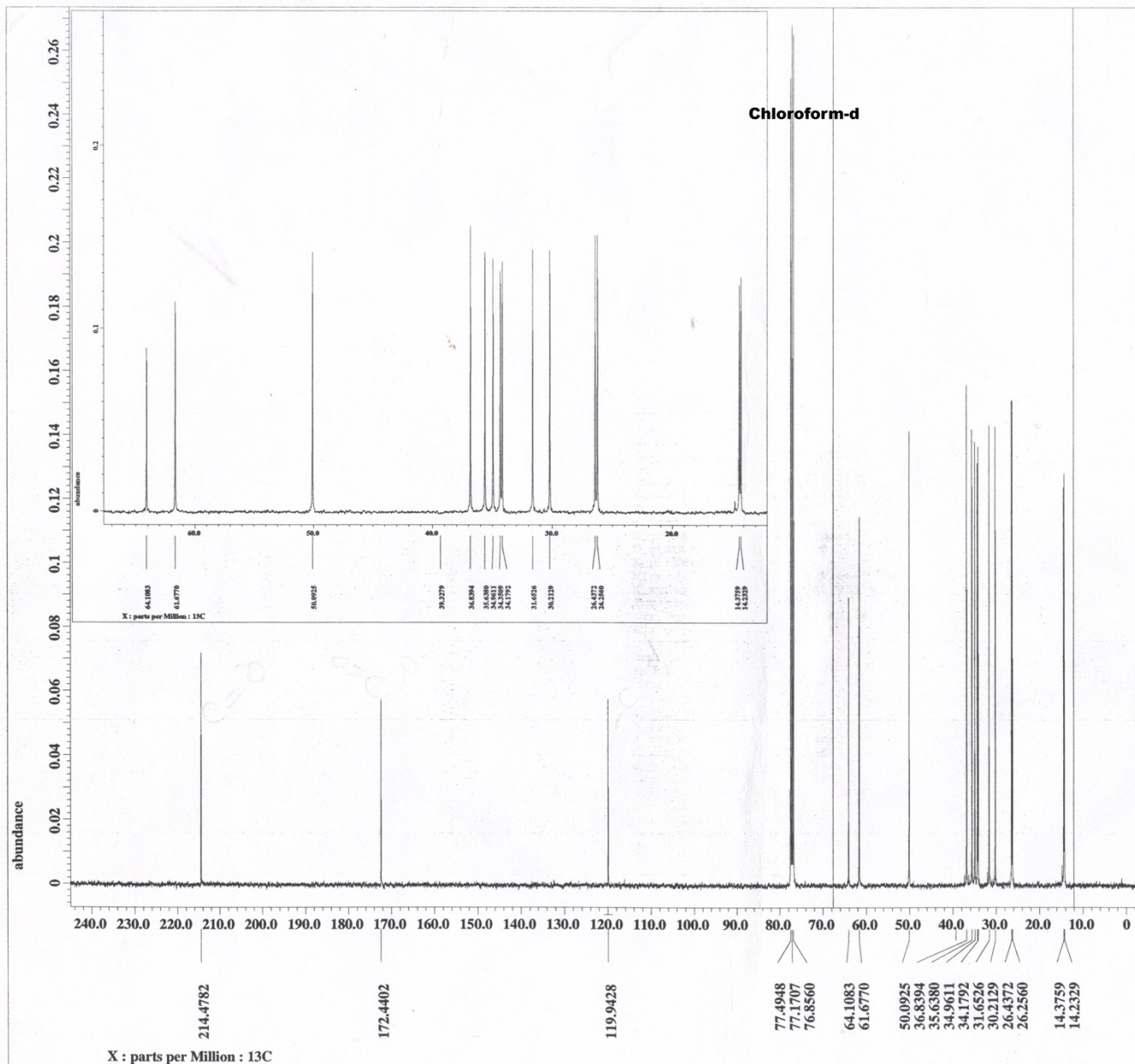


Filename = TIM_1H_106-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_106
 Solvent = CHLOROFORM-D
 Creation_time = 16-FEB-2018 04:37:01
 Revision_time = 16-FEB-2018 10:49:31
 Current_time = 16-FEB-2018 10:51:11

Comment = single pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECK 400
 Spectrometer = JNM-ECK400

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 = 19.7[dc]



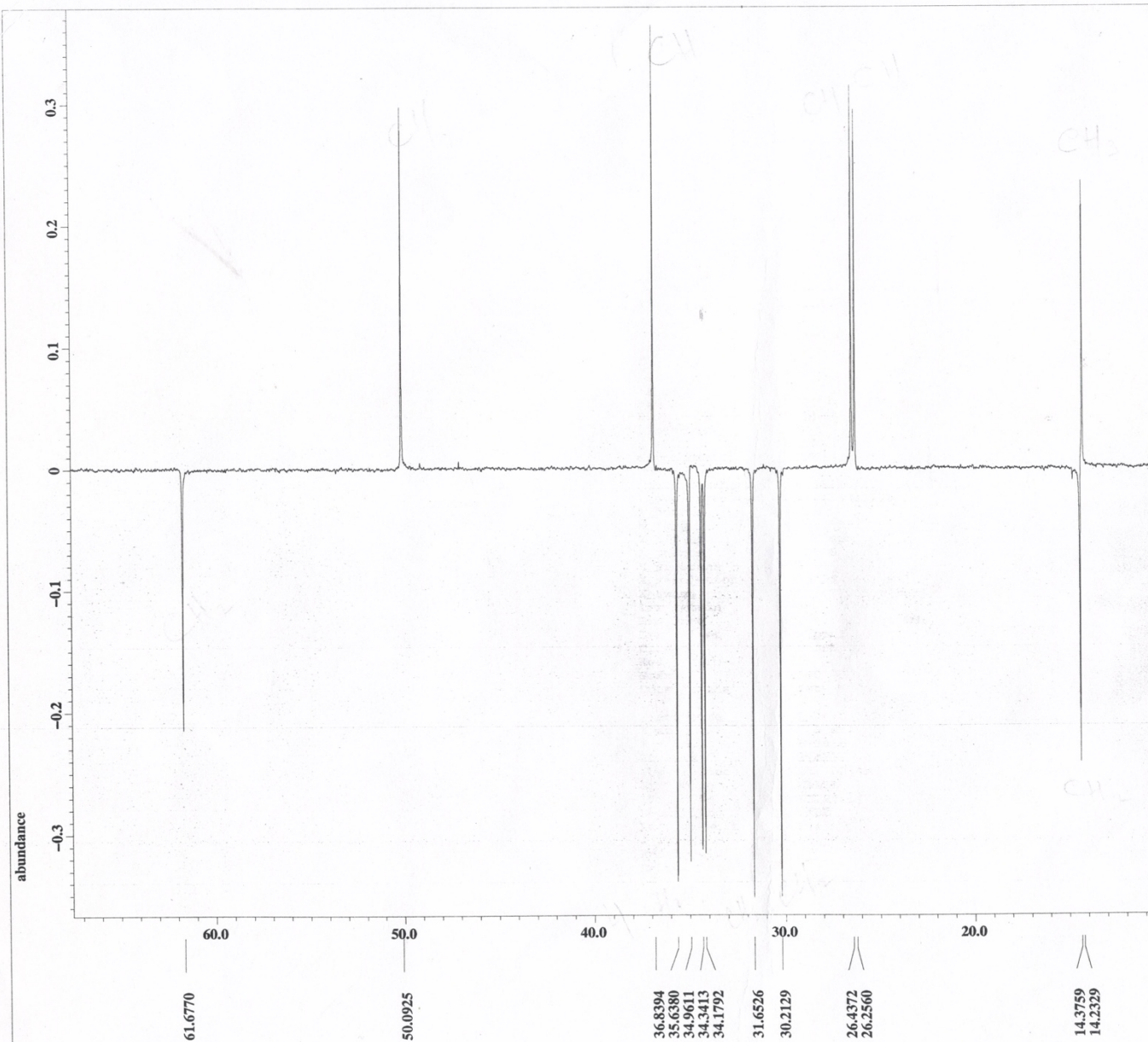
```

Filename      = TIM_13C_106-3.jdf
Author       = delta
Experiment    = single_pulse_dec
Sample_id     = TIM_106
Solvent       = CHLOROFORM-D
Creation_time = 16-FEB-2018 05:31:33
Revision_time = 16-FEB-2018 10:51:35
Current_time  = 16-FEB-2018 10:51:55

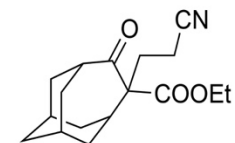
Comment      = single pulse decouple
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECX 400
Spectrometer  = JNM-ECX400

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     = 44
Relaxation_delay = 2 [s]
Repetition_time = 3.04333312 [s]
Temp_get       = 20 [dc]
  
```

X : parts per Million : 13C

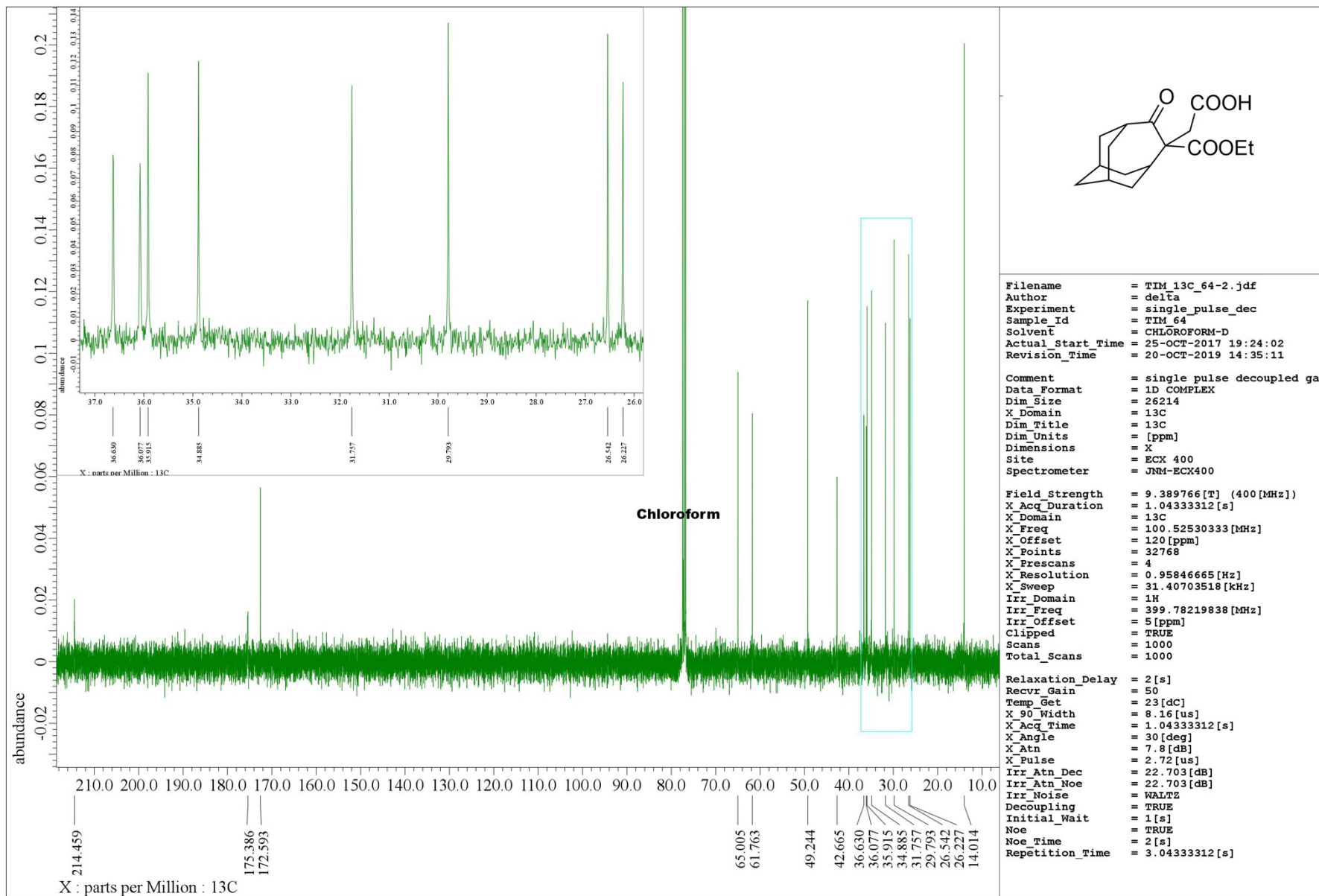


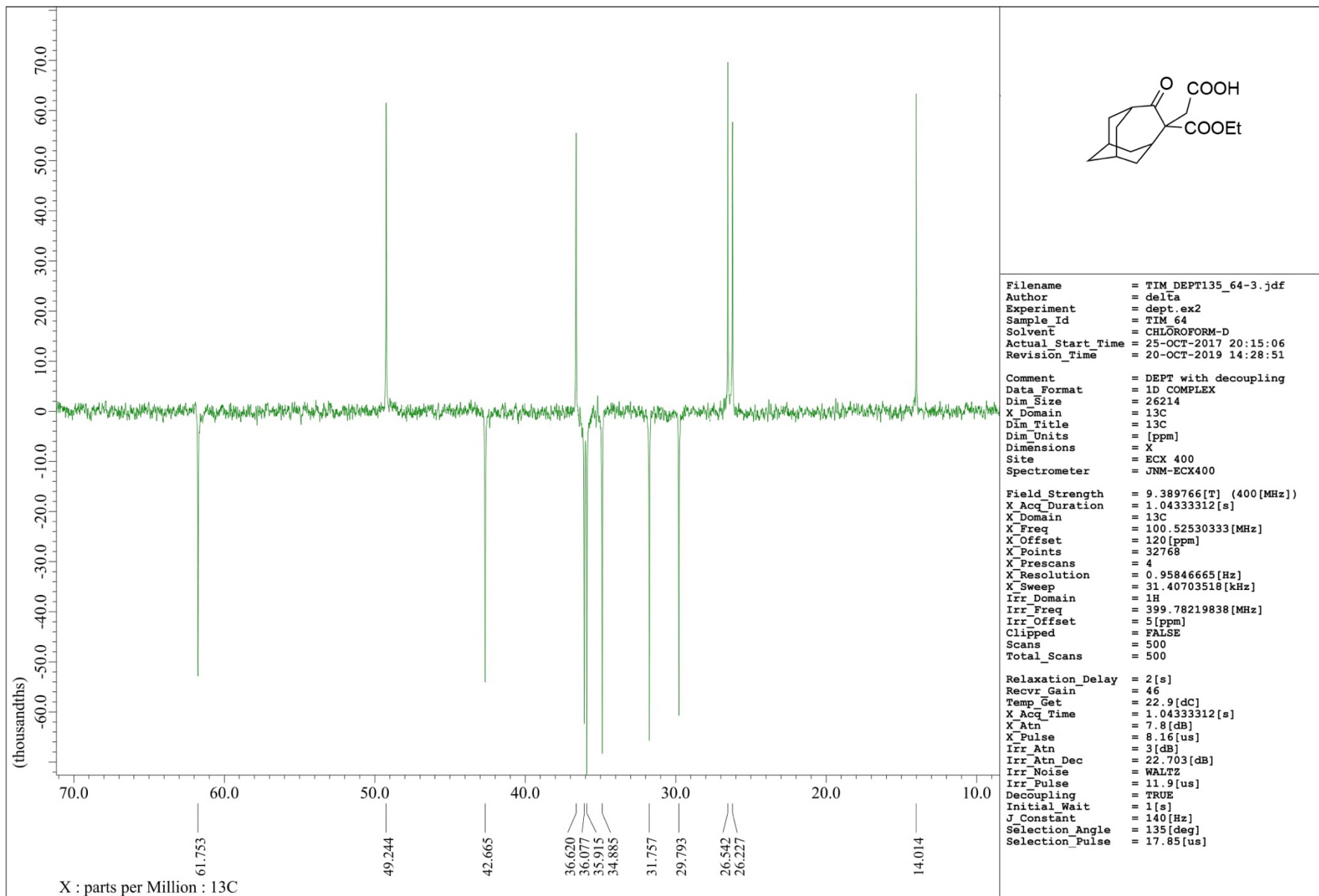
Filename = TIM_DEPT135_106-3.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_106
 Solvent = CHLOROFORM-D
 Creation_time = 16-FEB-2018 05:57:23
 Revision_time = 16-FEB-2018 10:52:15
 Current_time = 16-FEB-2018 10:52:23

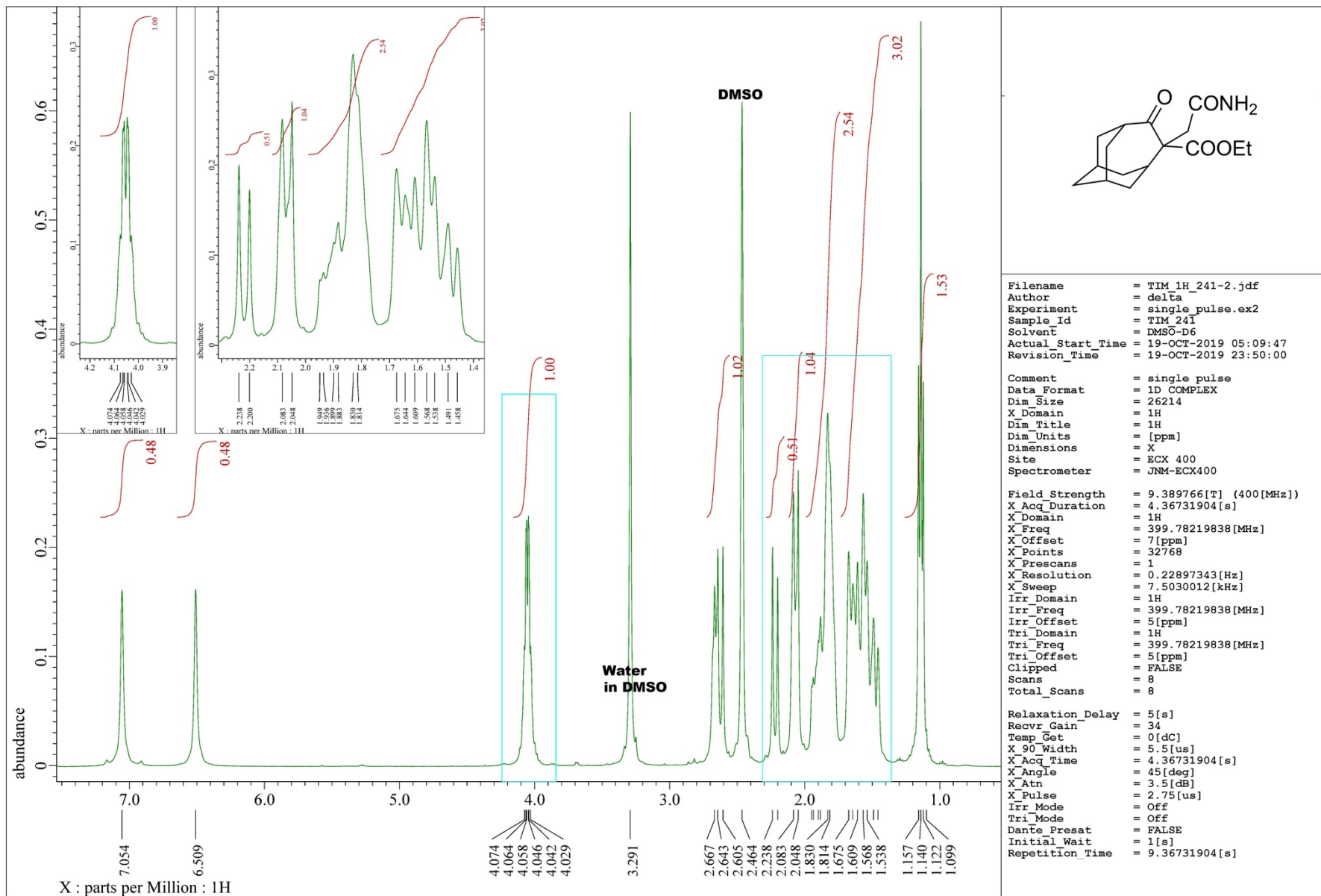
Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECK 400
 Spectrometer = JNM-ECX400

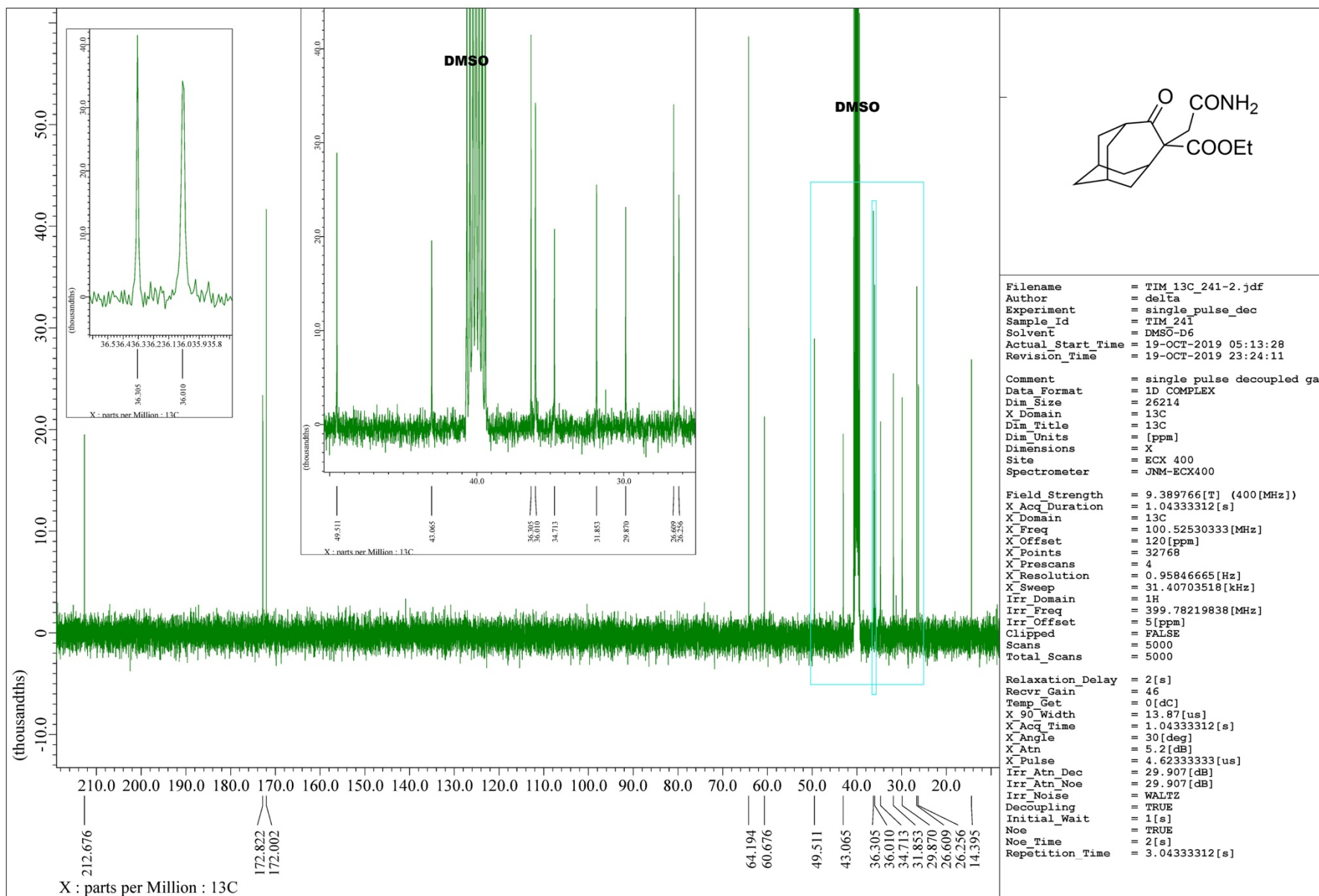
Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 120[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 500
 Total_scans = 500

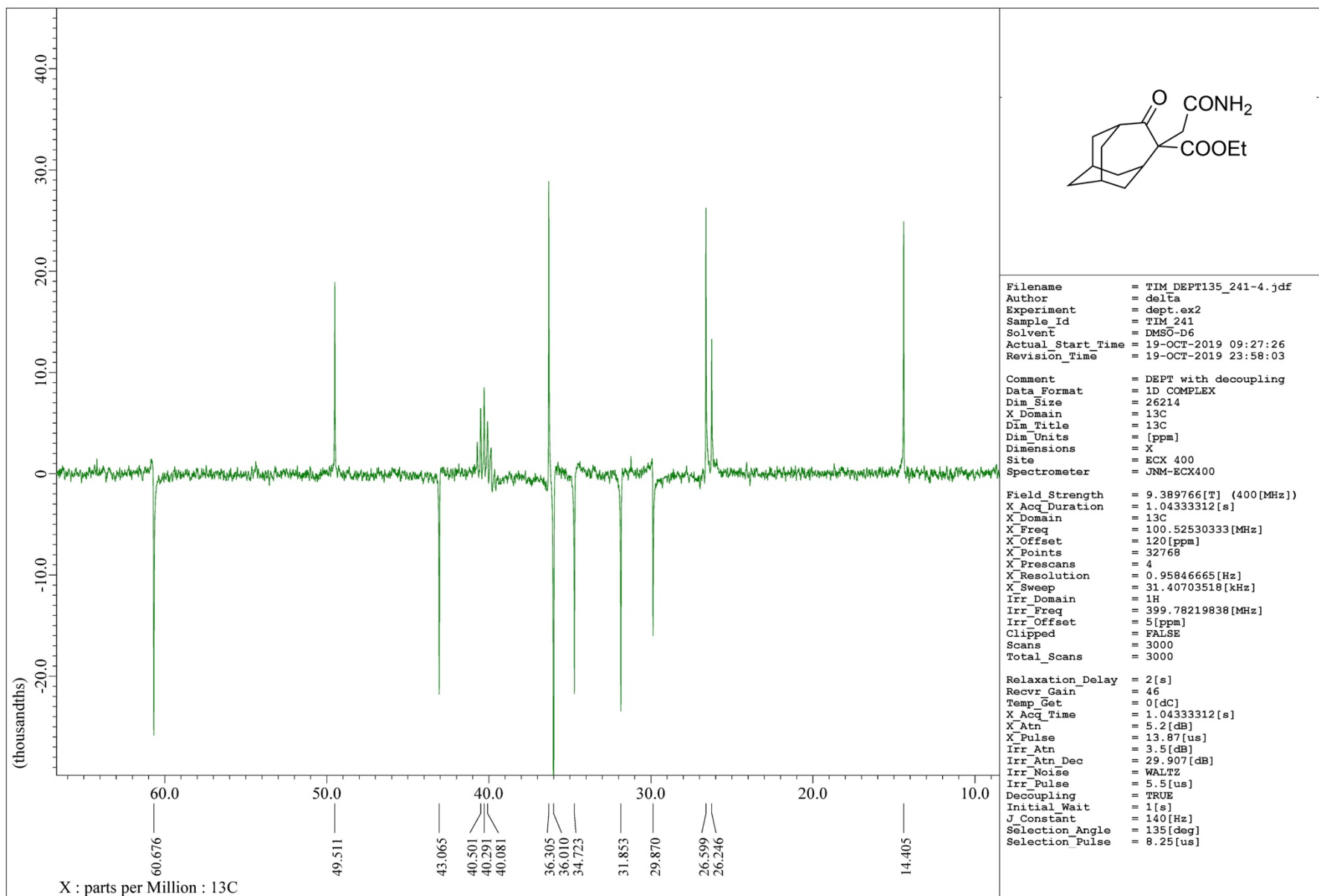
X_acq_time = 1.04333312[s]
 X_atn = 7.8[dB]
 X_pulse = 8.16[us]
 Irr_atn = 3[dB]
 Irr_atn_dec = 22.703[dB]
 Irr_noise = WALTZ
 Irr_pulse = 11.9[us]
 Decoupling = TRUE
 Initial_wait = 1[s]
 J_constant = 140[Hz]
 Recvr_gain = 46
 Relaxation_delay = 2[s]
 Selection_angle = 135[deg]
 Selection_pulse = 17.85[us]
 Temp_get = 19.9[dc]

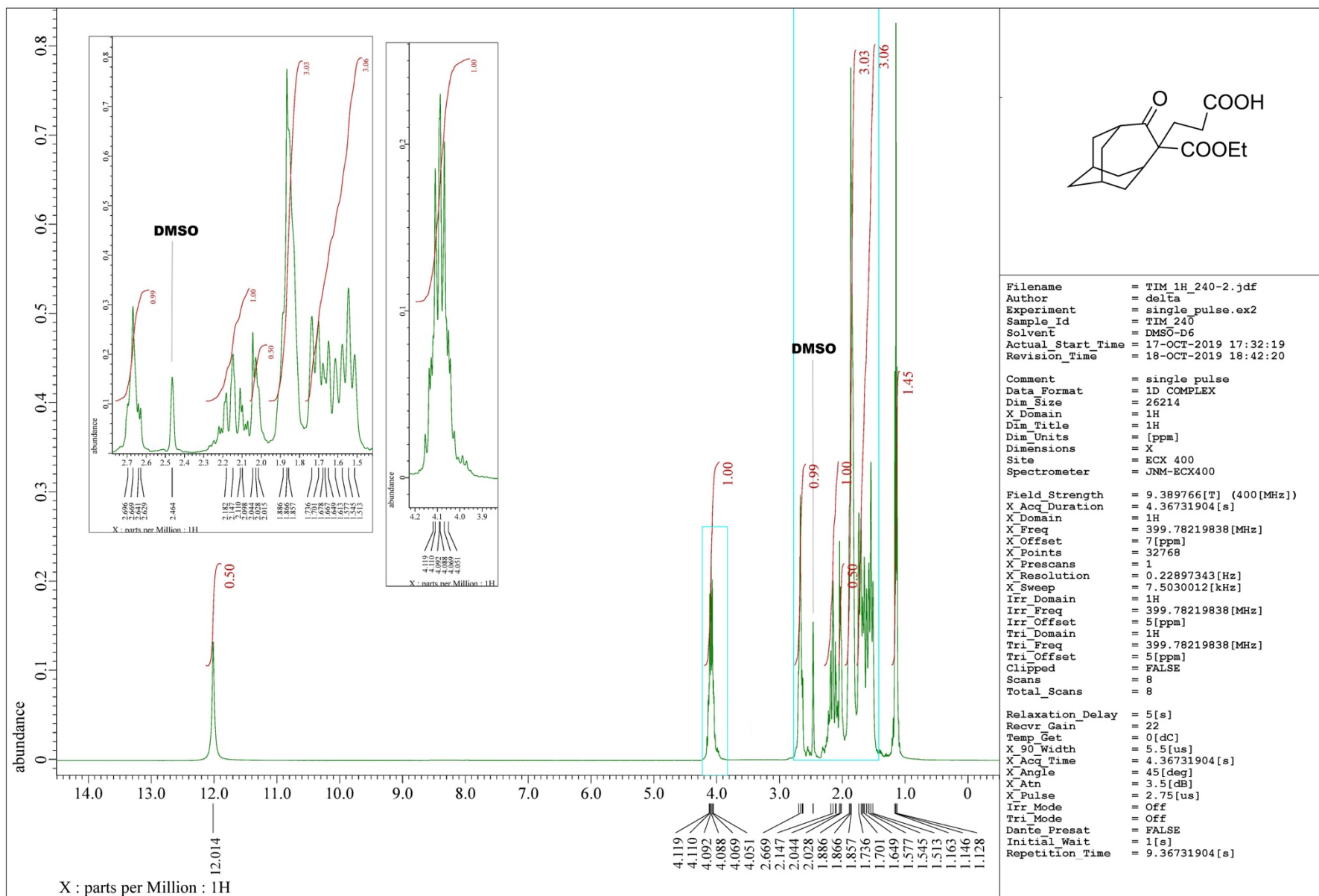


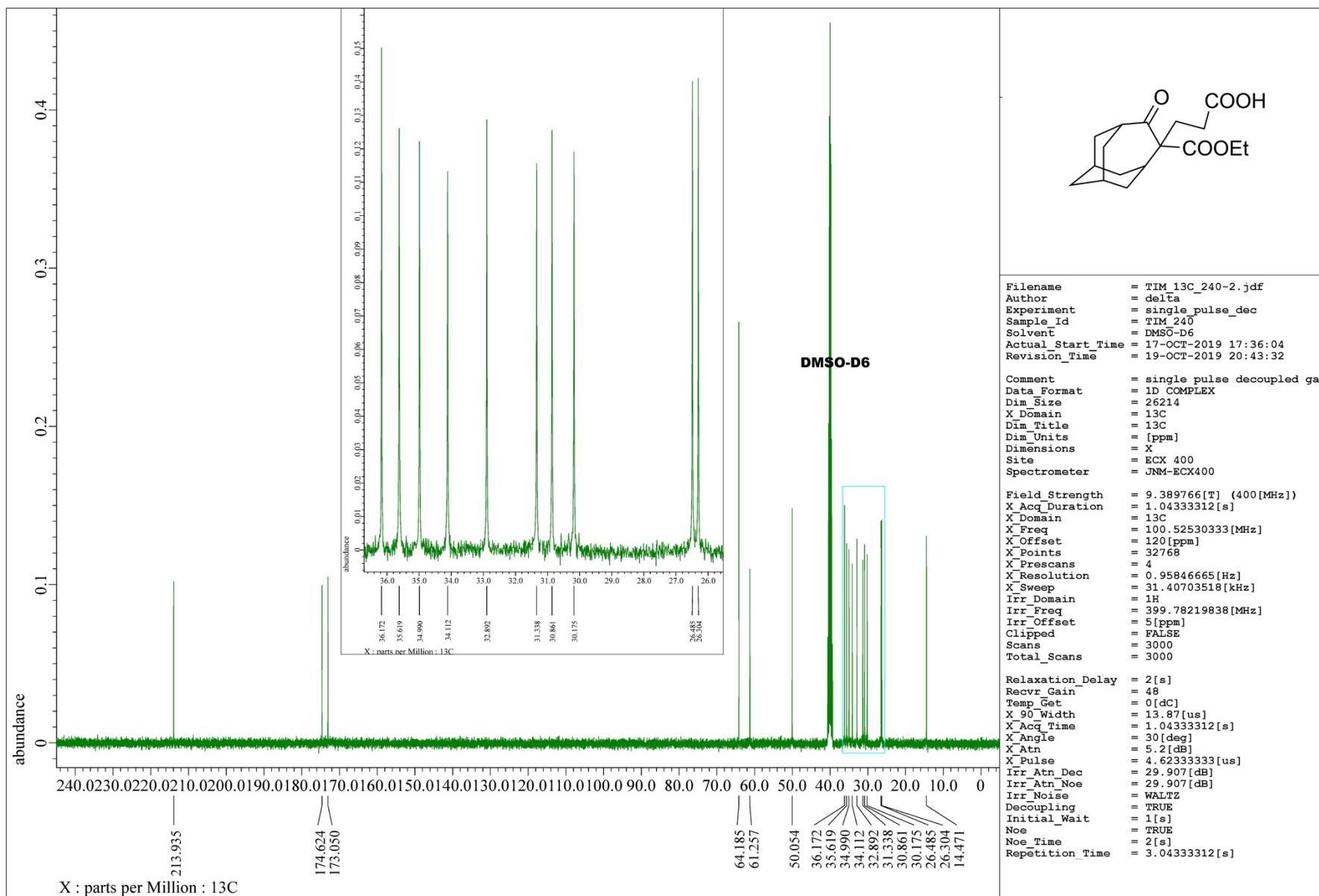


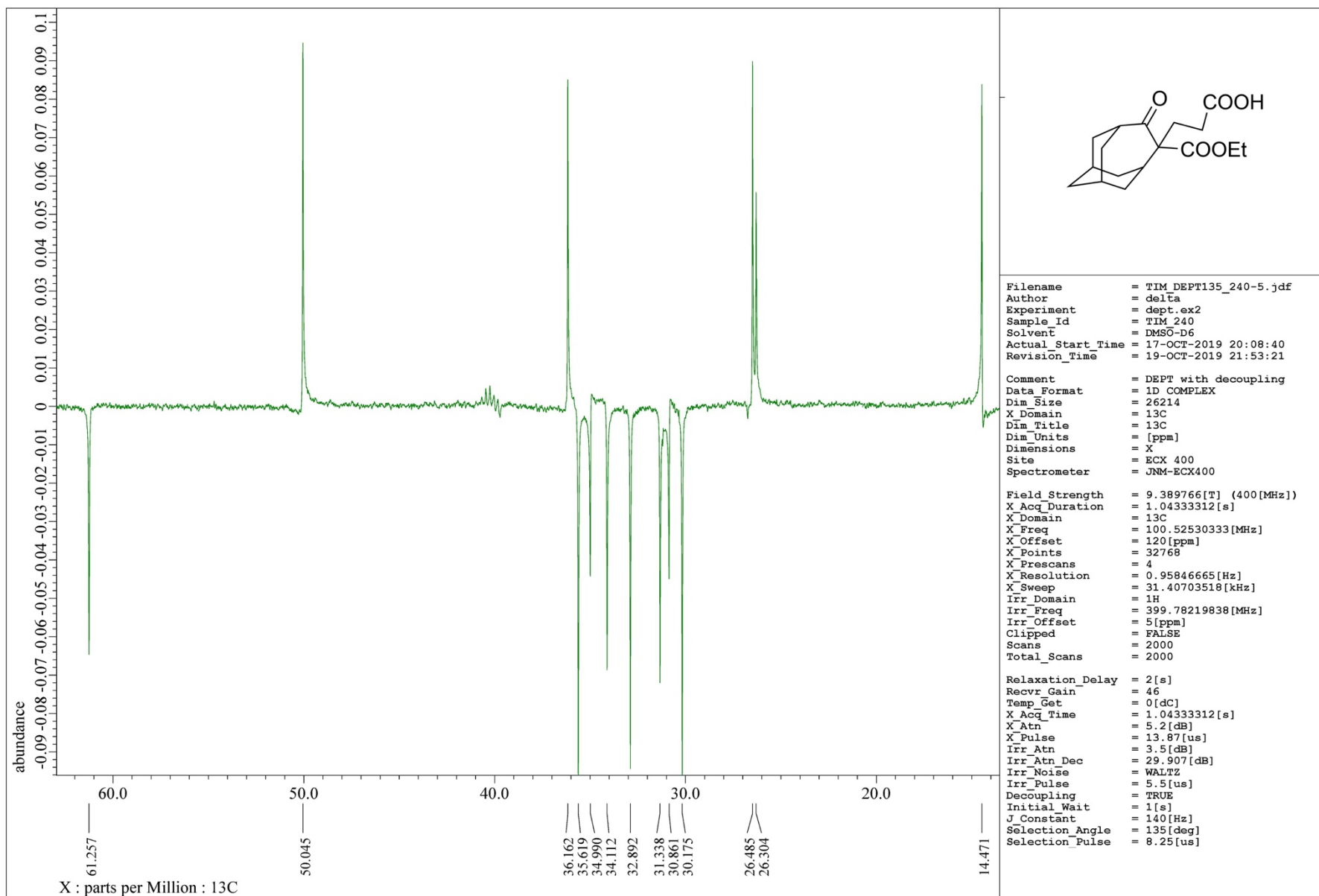


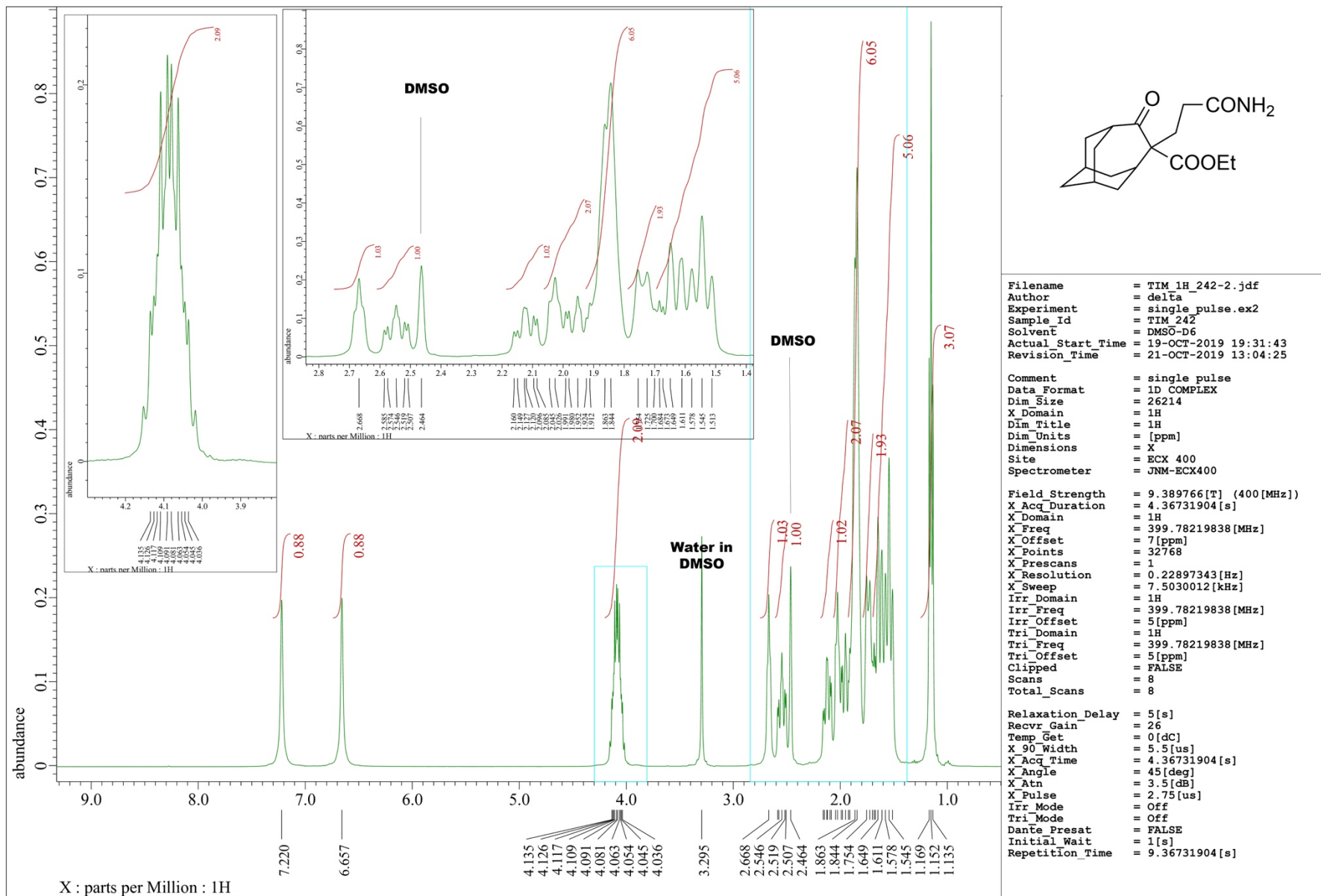


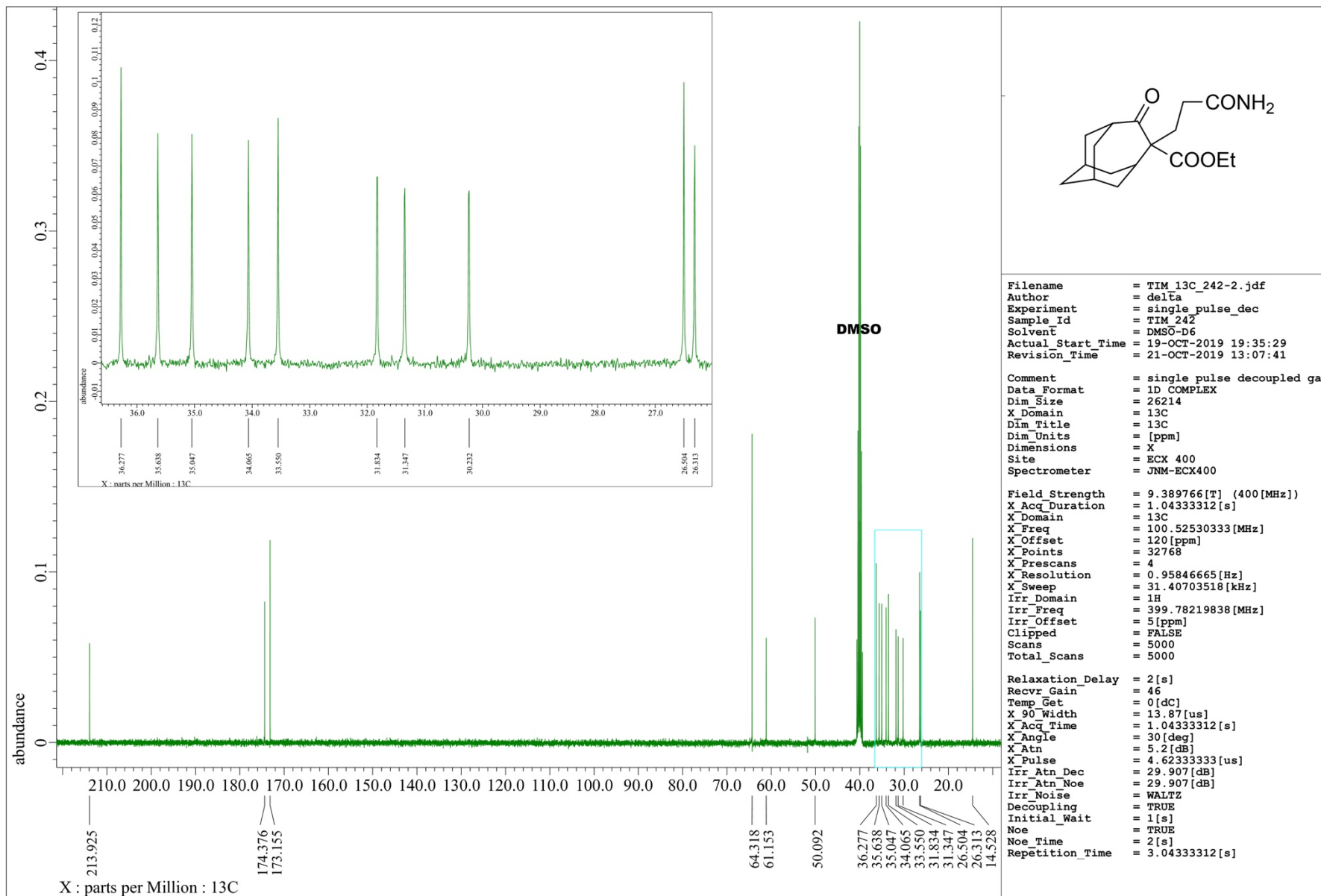


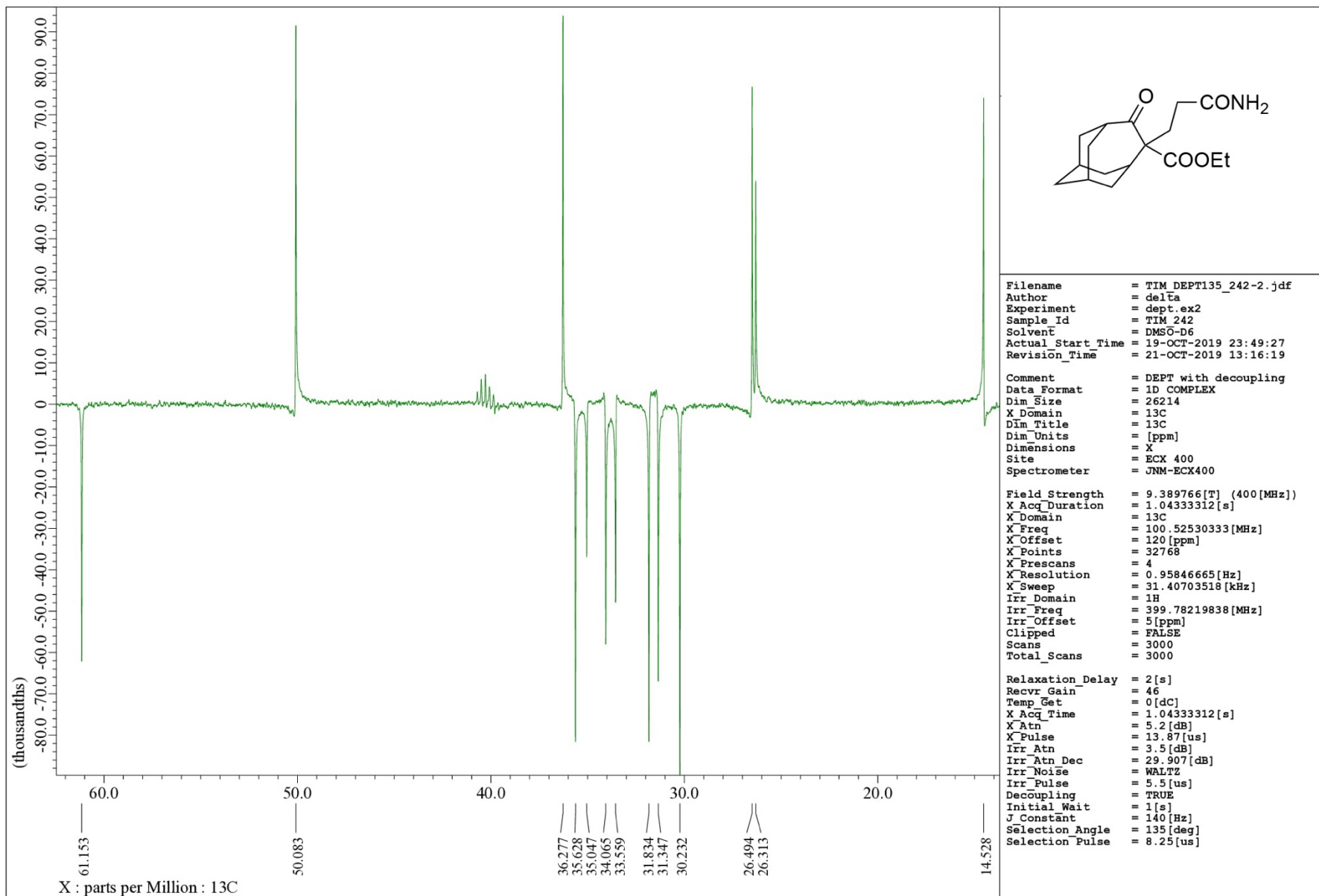


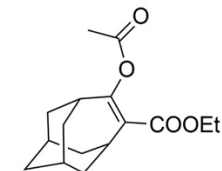
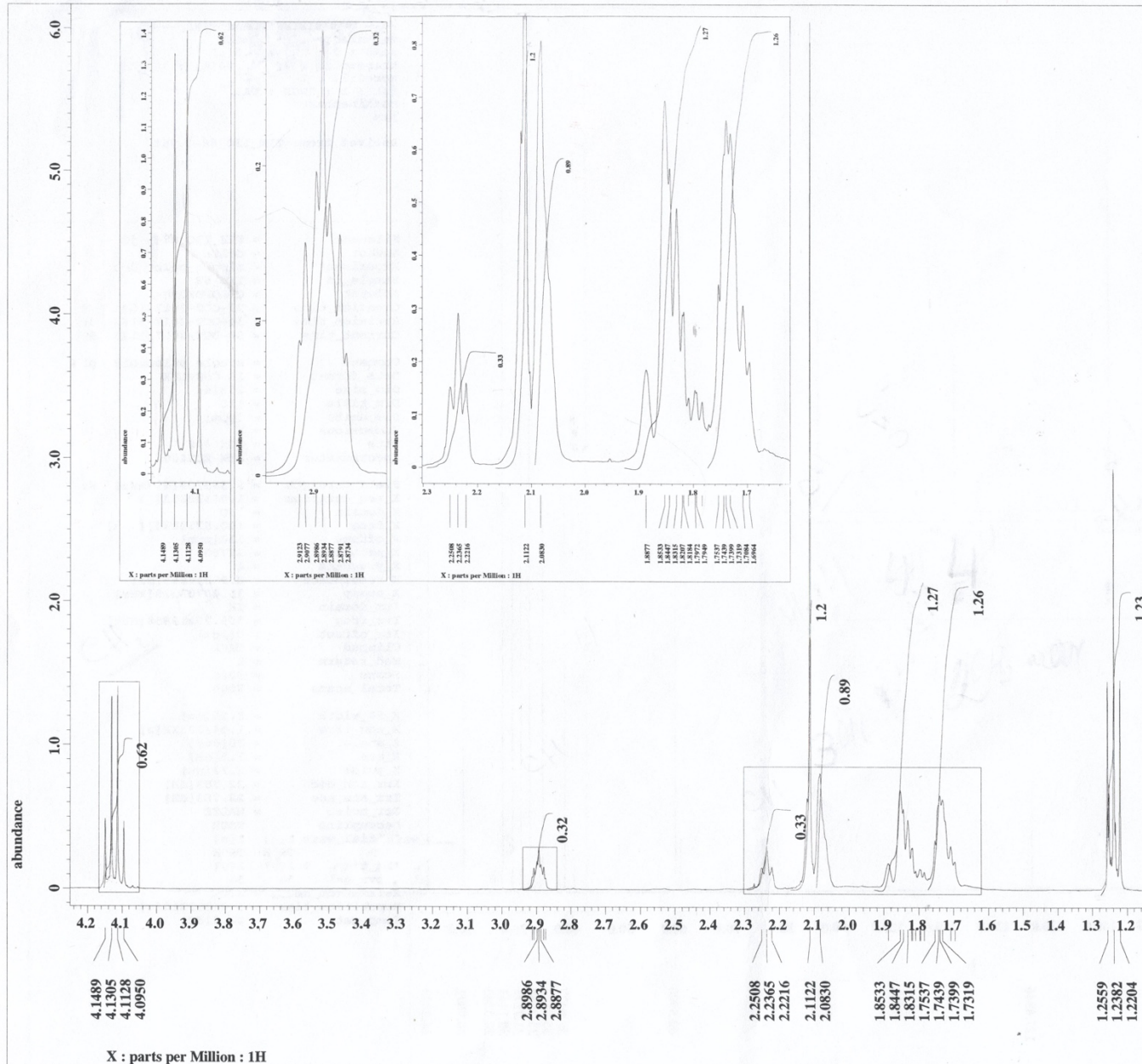










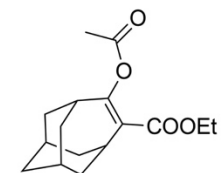
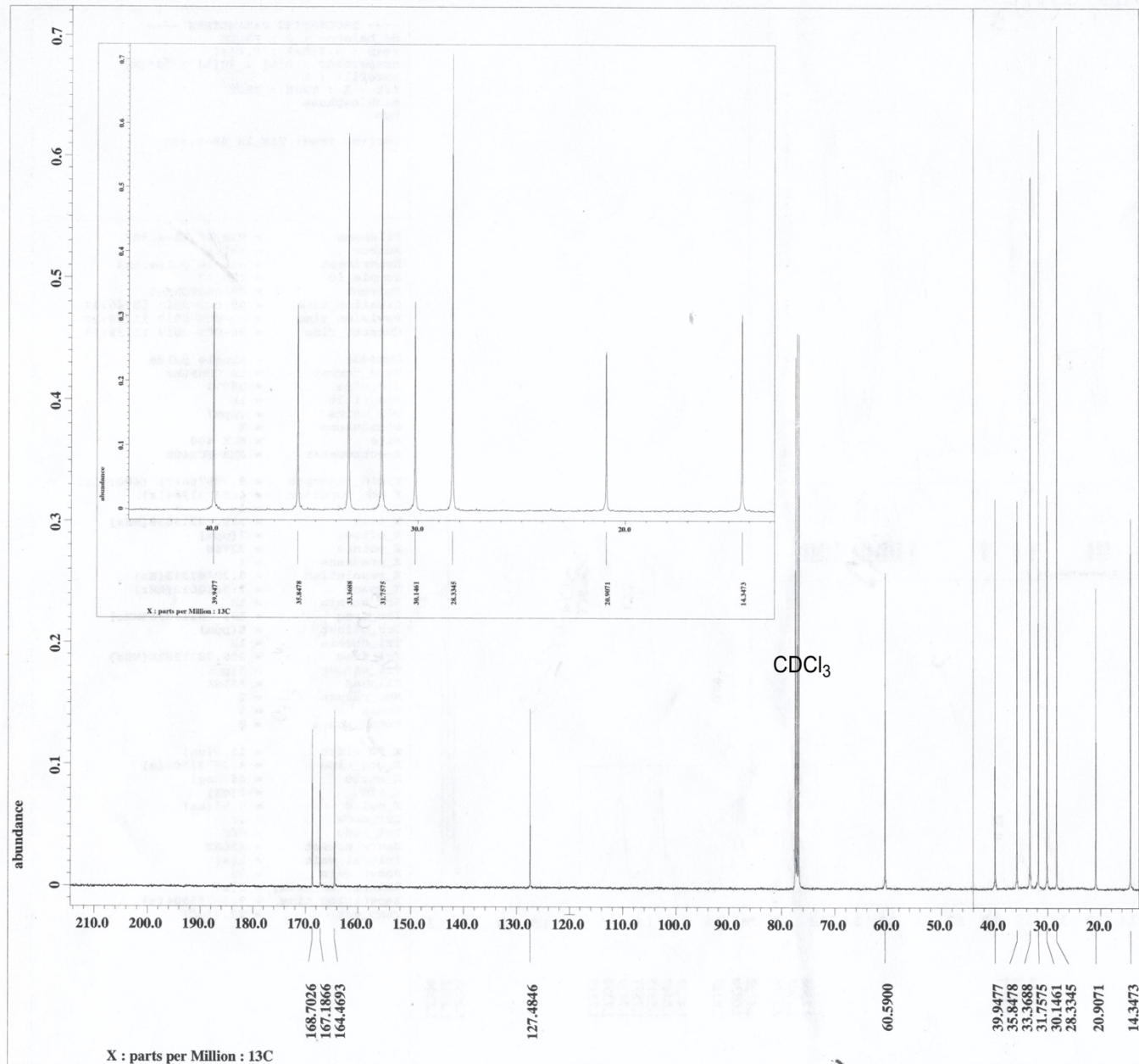


Filename = TIM_1H_68-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_68
 Solvent = CHLOROFORM-D
 Creation_time = 29-OCT-2017 13:40:47
 Revision_time = 30-OCT-2017 11:38:30
 Current_time = 30-OCT-2017 11:39:17

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[kHz]
 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_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 28
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 22.7[dc]



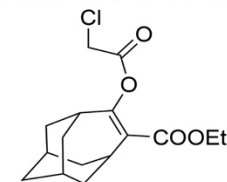
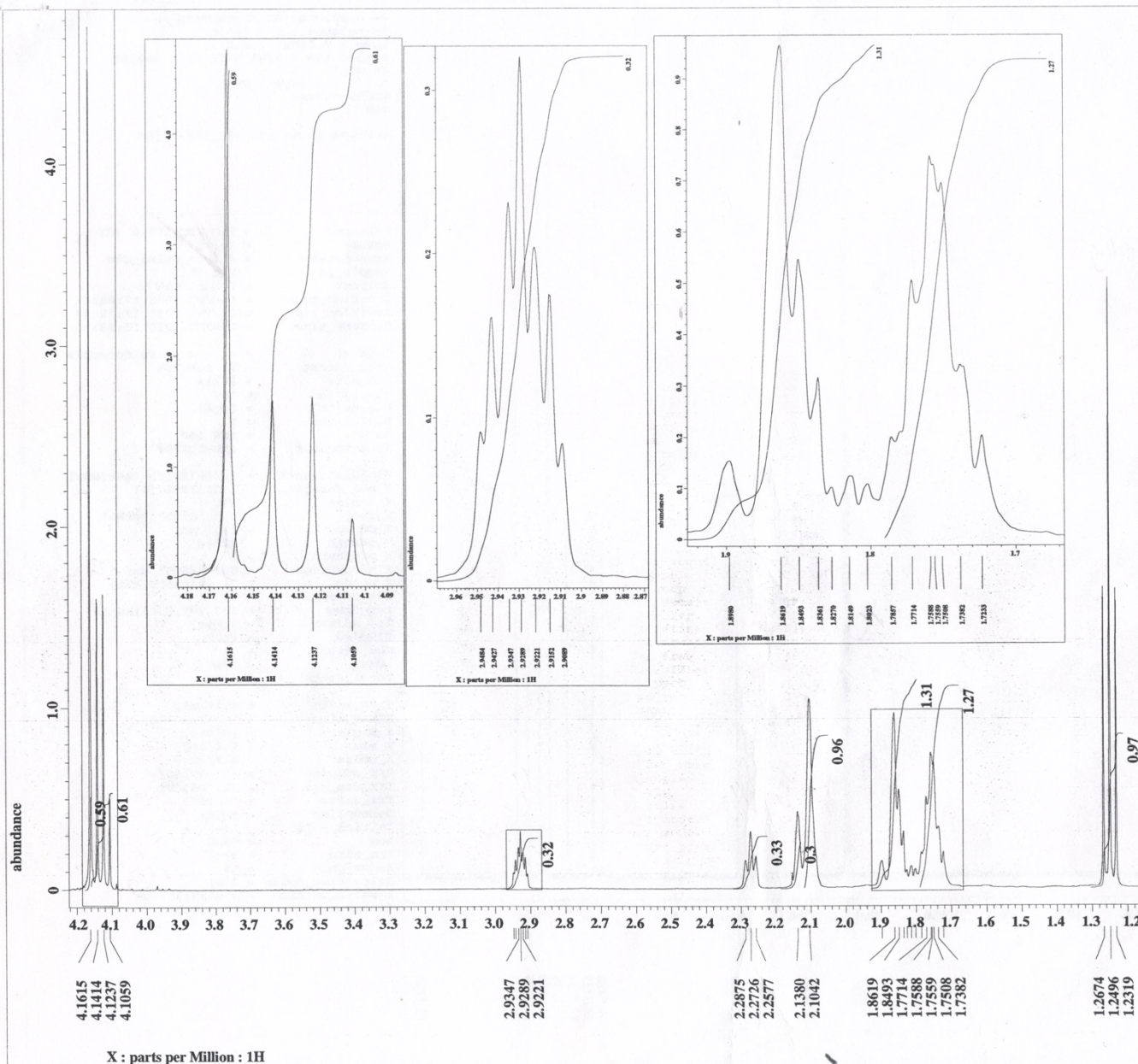
```

Filename      = TIM_13C_68-4.jdf
Author       = delta
Experiment    = single_pulse_dec
Sample_id     = TIM_68
Solvent       = CHLOROFORM-D
Creation_time = 29-OCT-2017 16:15:20
Revision_time = 30-OCT-2017 11:39:36
Current_time  = 30-OCT-2017 11:39:52

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          = 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       = 23.3[dc]
  
```

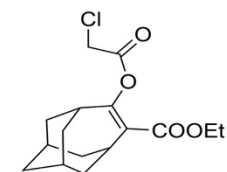
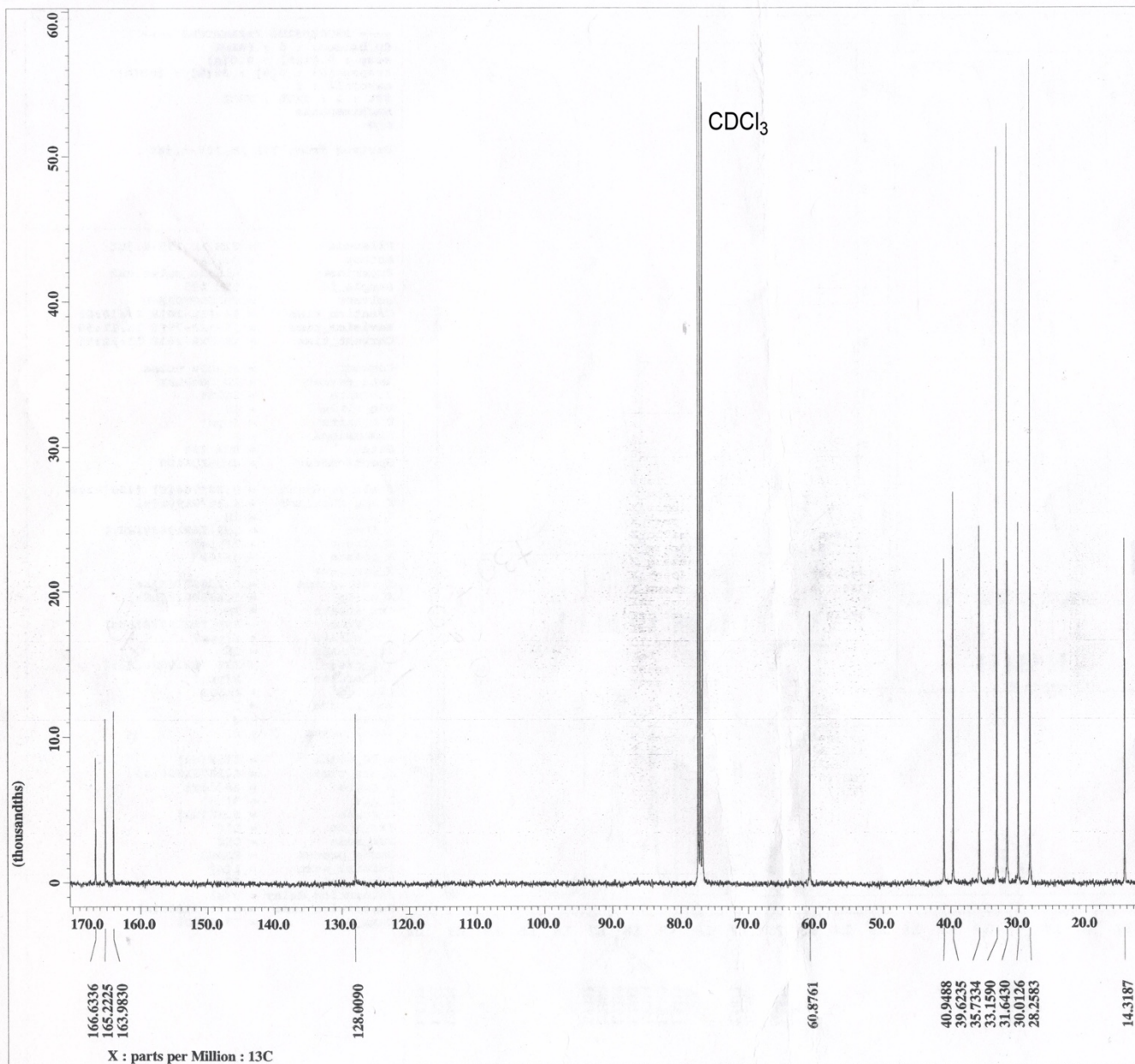



Filename = TIM_1H_105-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_105
 Solvent = CHLOROFORM-D
 Creation_time = 14-FEB-2018 16:10:05
 Revision_time = 15-FEB-2018 13:11:58
 Current_time = 15-FEB-2018 13:12:35

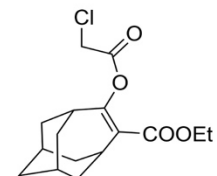
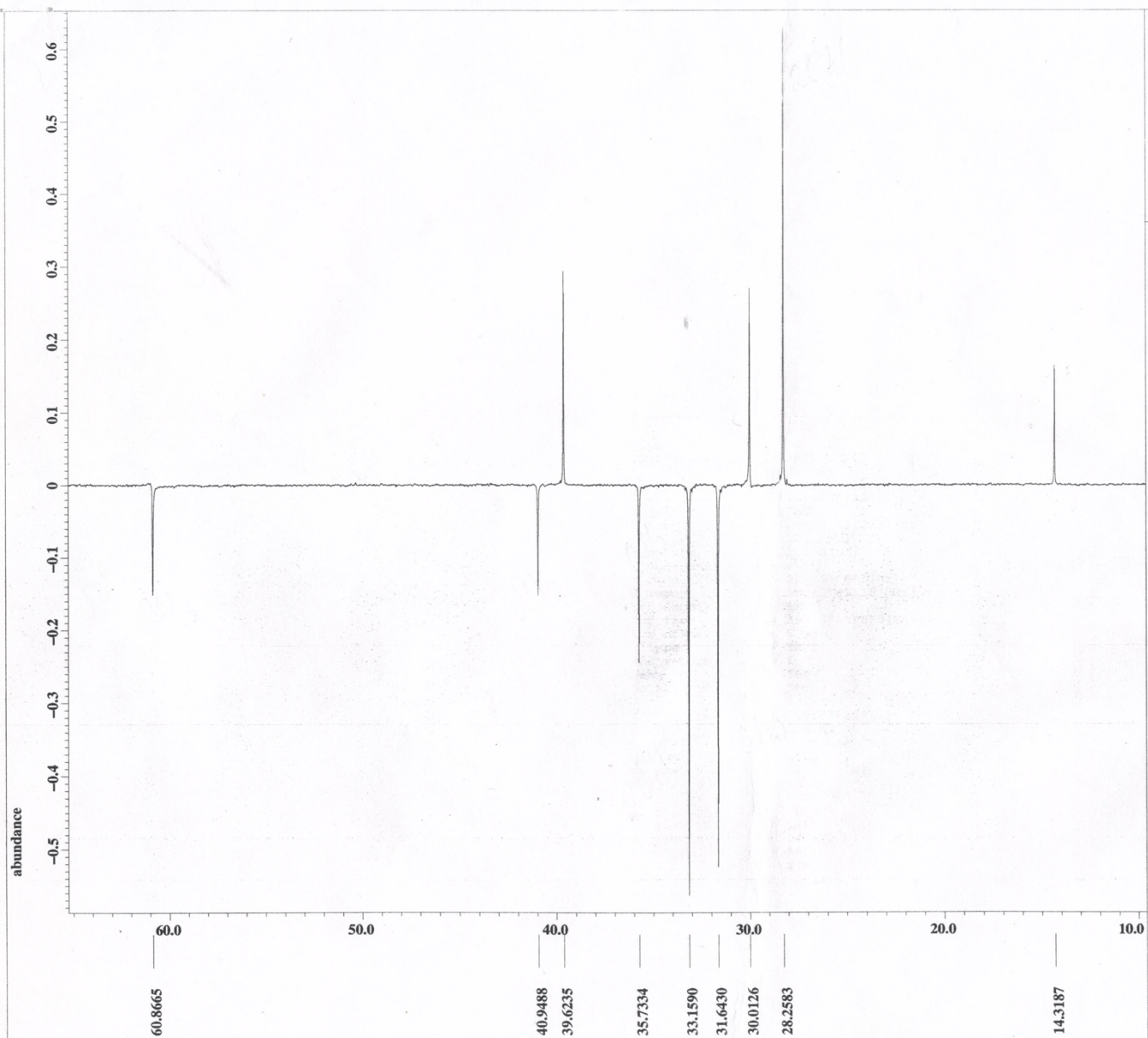
Comment = single pulse
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

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 = 32
 Relaxation_delay = 5 [s]
 Repetition_time = 9.36731904 [s]
 Temp_get = 18.7 [dC]



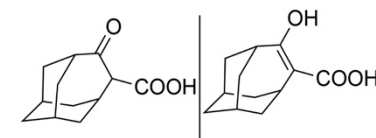
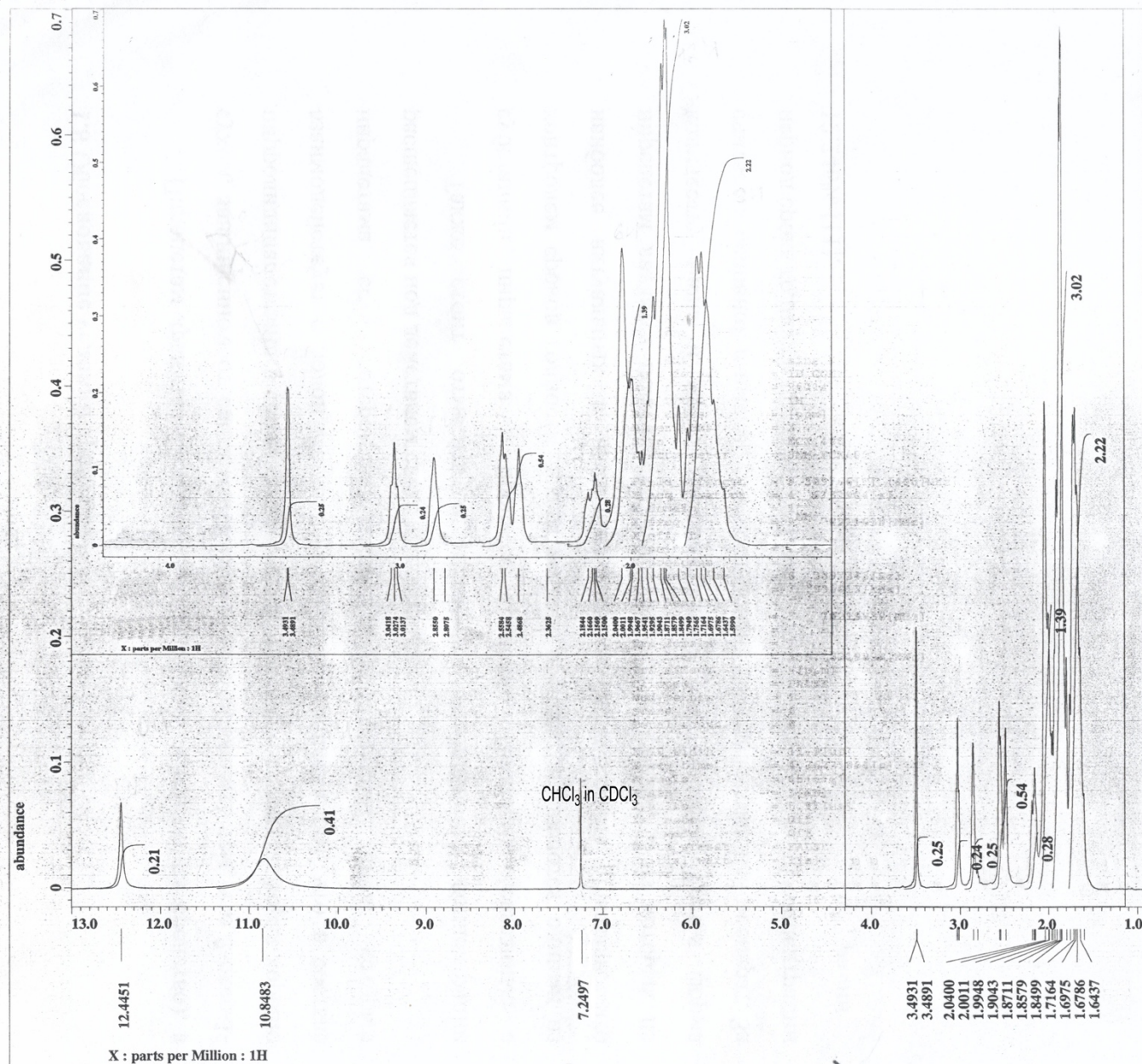
Filename = TIM_13C_105-4.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_105
 Solvent = CHLOROFORM-D
 Creation_time = 14-FEB-2018 17:04:41
 Revision_time = 15-FEB-2018 13:12:48
 Current_time = 15-FEB-2018 13:12:54
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 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 = 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 = 30
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 19.2[dc]



Filename = TIM_DEPT135_105-3.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_105
 Solvent = CHLOROFORM-D
 Creation_time = 14-FEB-2018 17:30:29
 Revision_time = 15-FEB-2018 13:13:00
 Current_time = 15-FEB-2018 13:13:03

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 = TRUE
 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 = 19.3[degC]

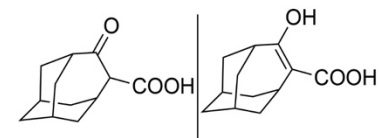
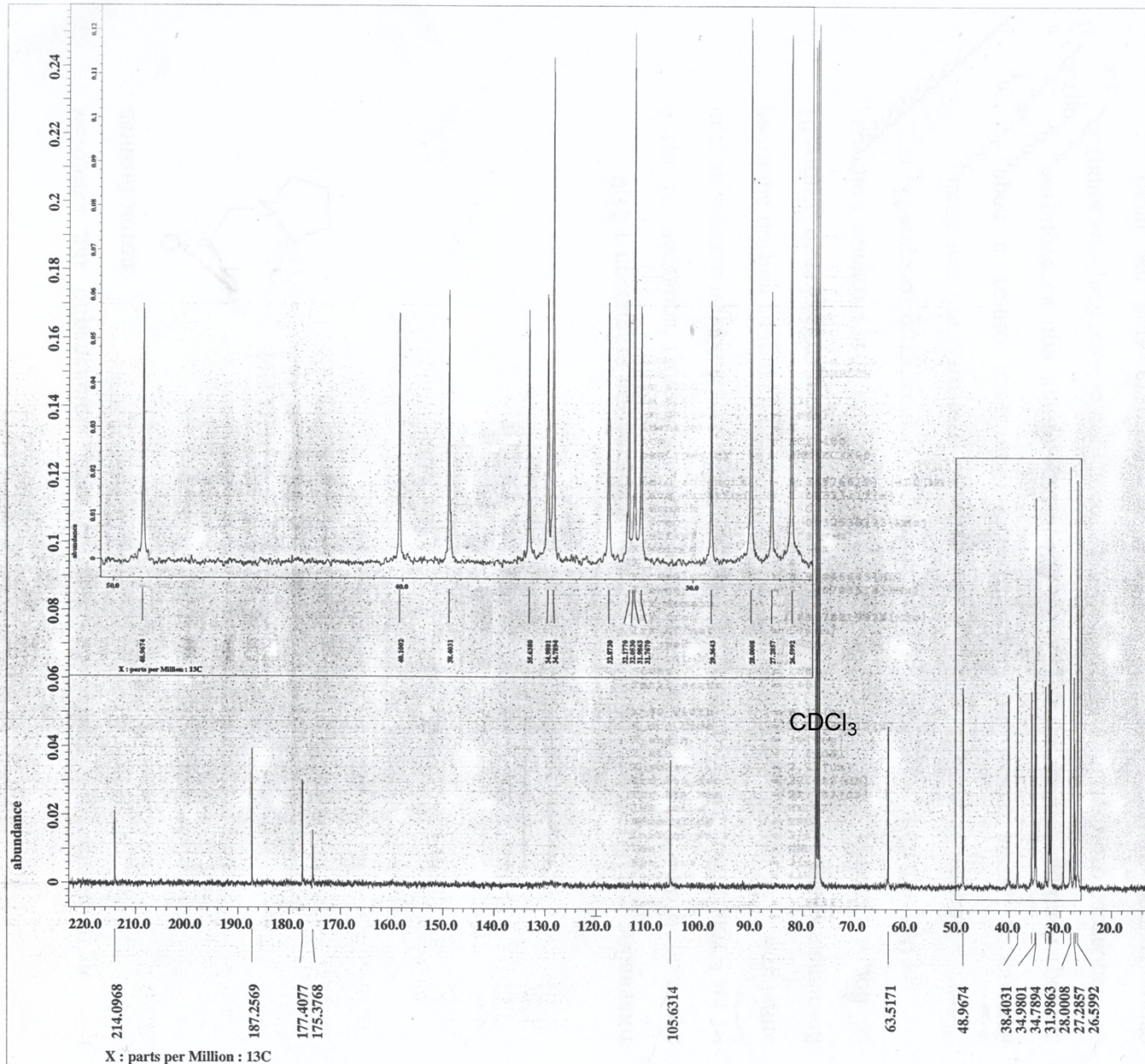


Filename = TIM_1H_173-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_173
 Solvent = CHLOROFORM-D
 Creation_time = 21-DEC-2018 16:38:28
 Revision_time = 24-DEC-2018 10:23:55
 Current_time = 24-DEC-2018 10:24:16

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 = 22.1[dc]

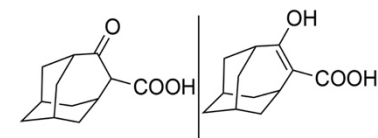
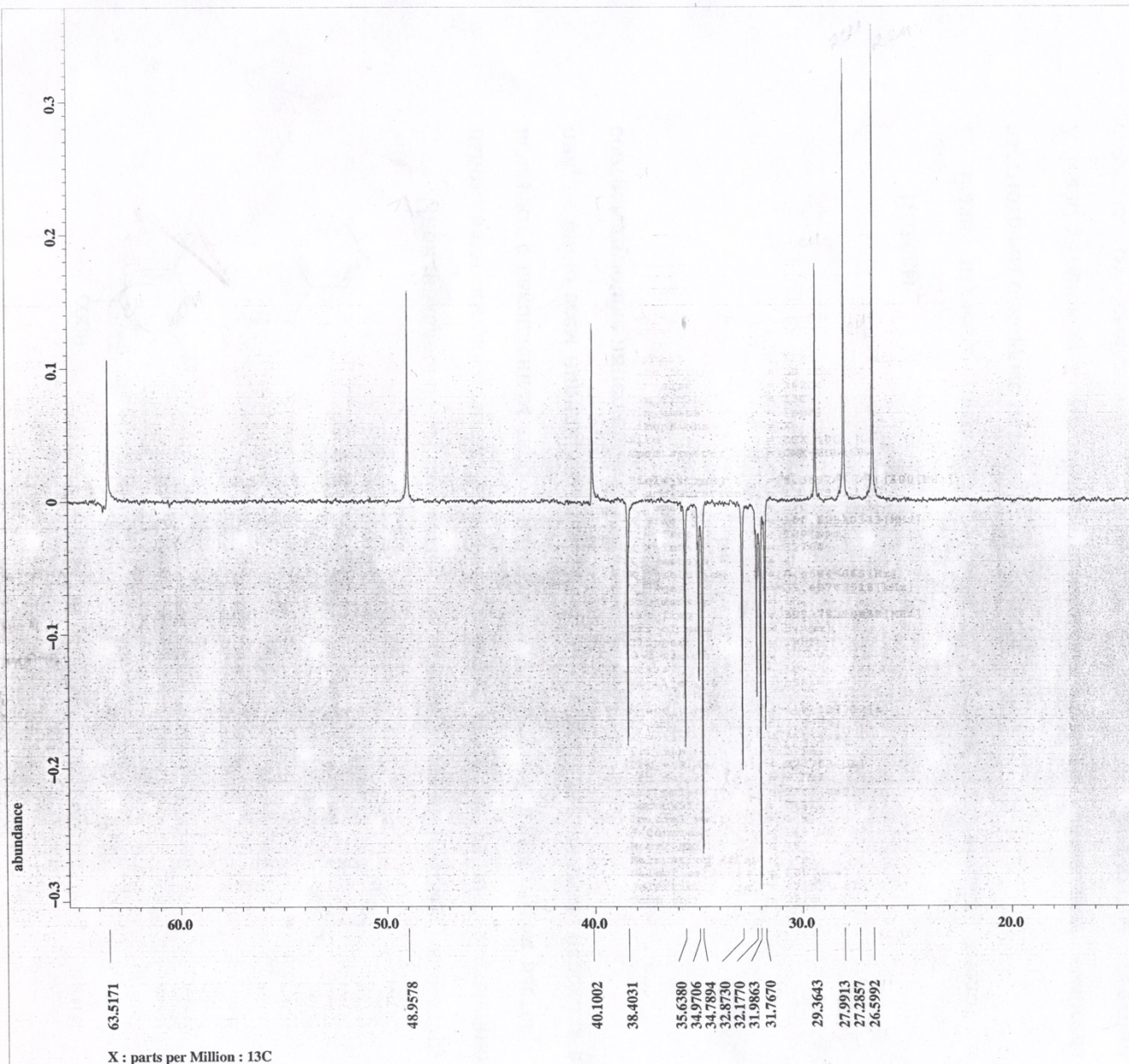


Filename = TIM_13C_173-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_173
 Solvent = CHLOROFORM-D
 Creation_time = 21-DEC-2018 17:32:03
 Revision_time = 24-DEC-2018 10:24:42
 Current_time = 24-DEC-2018 10:24:59

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 = 1.04333312[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 = 44
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 22.3[dc]

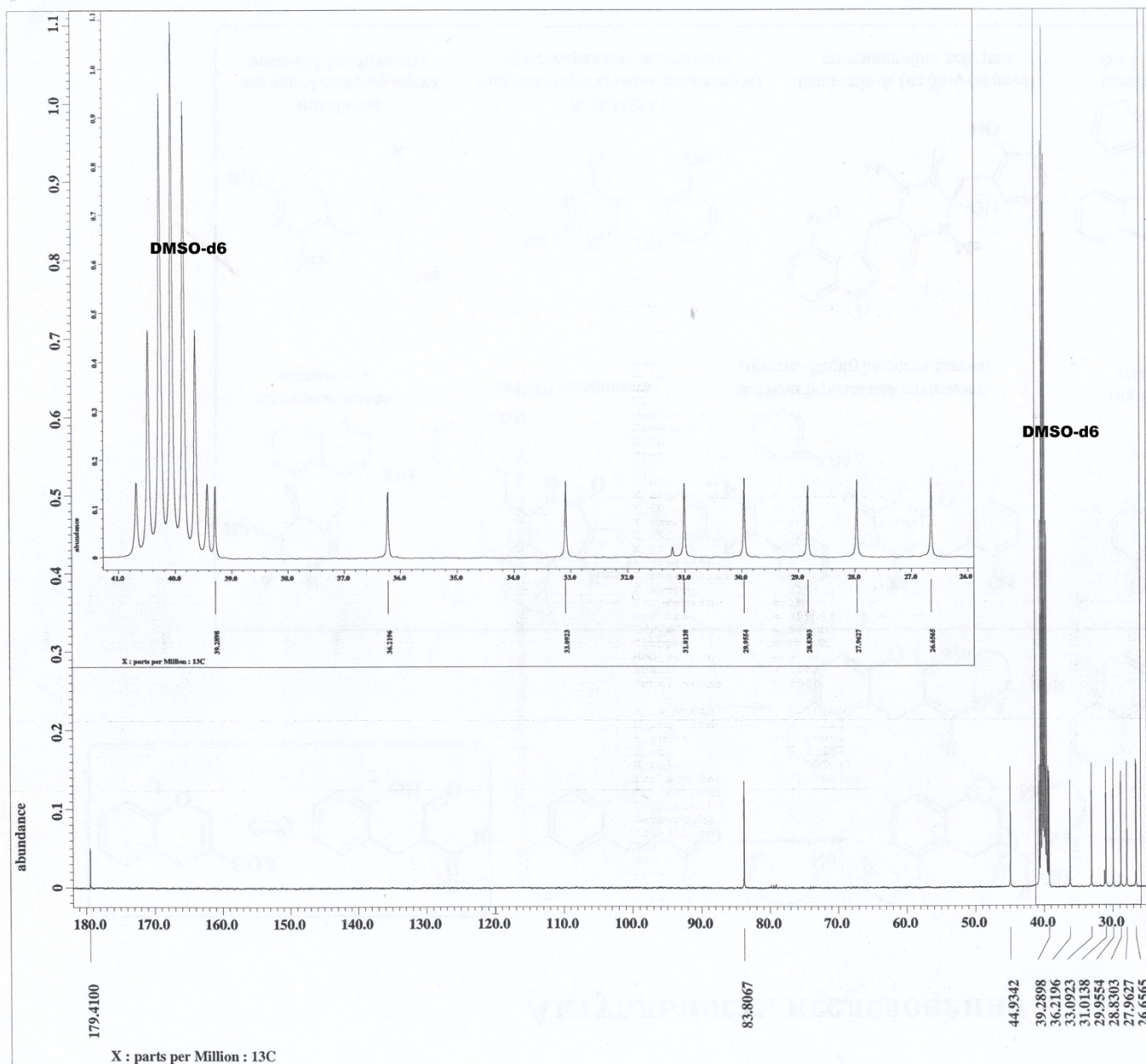


Filename = TIM_DEPT135_173-4.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_173
 Solvent = CHLOROFORM-D
 Creation_time = 21-DEC-2018 17:57:50
 Revision_time = 24-DEC-2018 10:25:24
 Current_time = 24-DEC-2018 10:25:34

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 = TRUE
 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[dc]

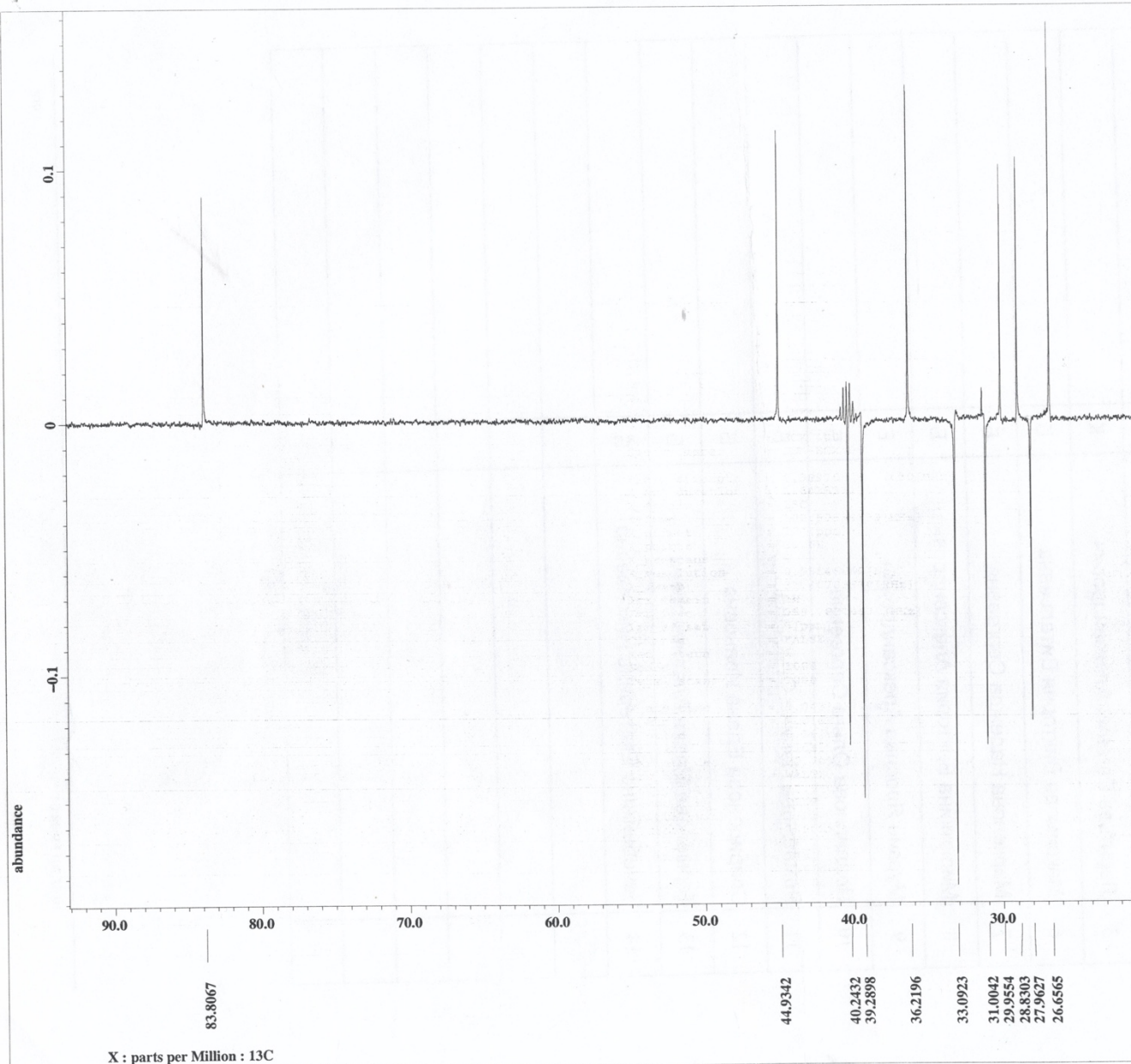


Filename = TIM_13C_152-4.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_152
 Solvent = DMSO-D6
 Creation_time = 21-OCT-2018 20:30:50
 Revision_time = 23-OCT-2018 15:39:05
 Current_time = 23-OCT-2018 15:39:18

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 = 23.3[dc]

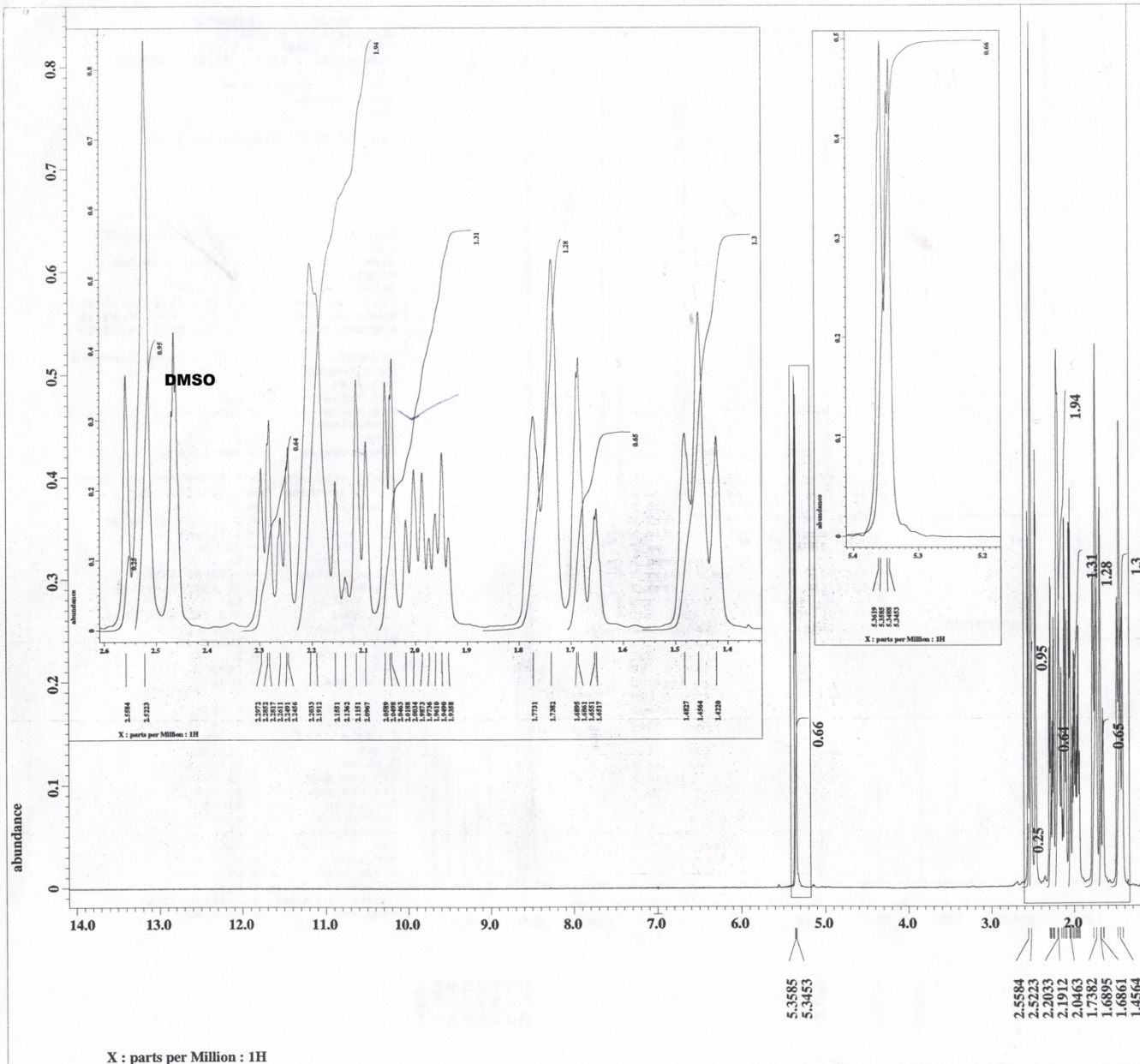


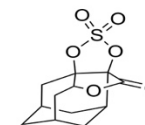
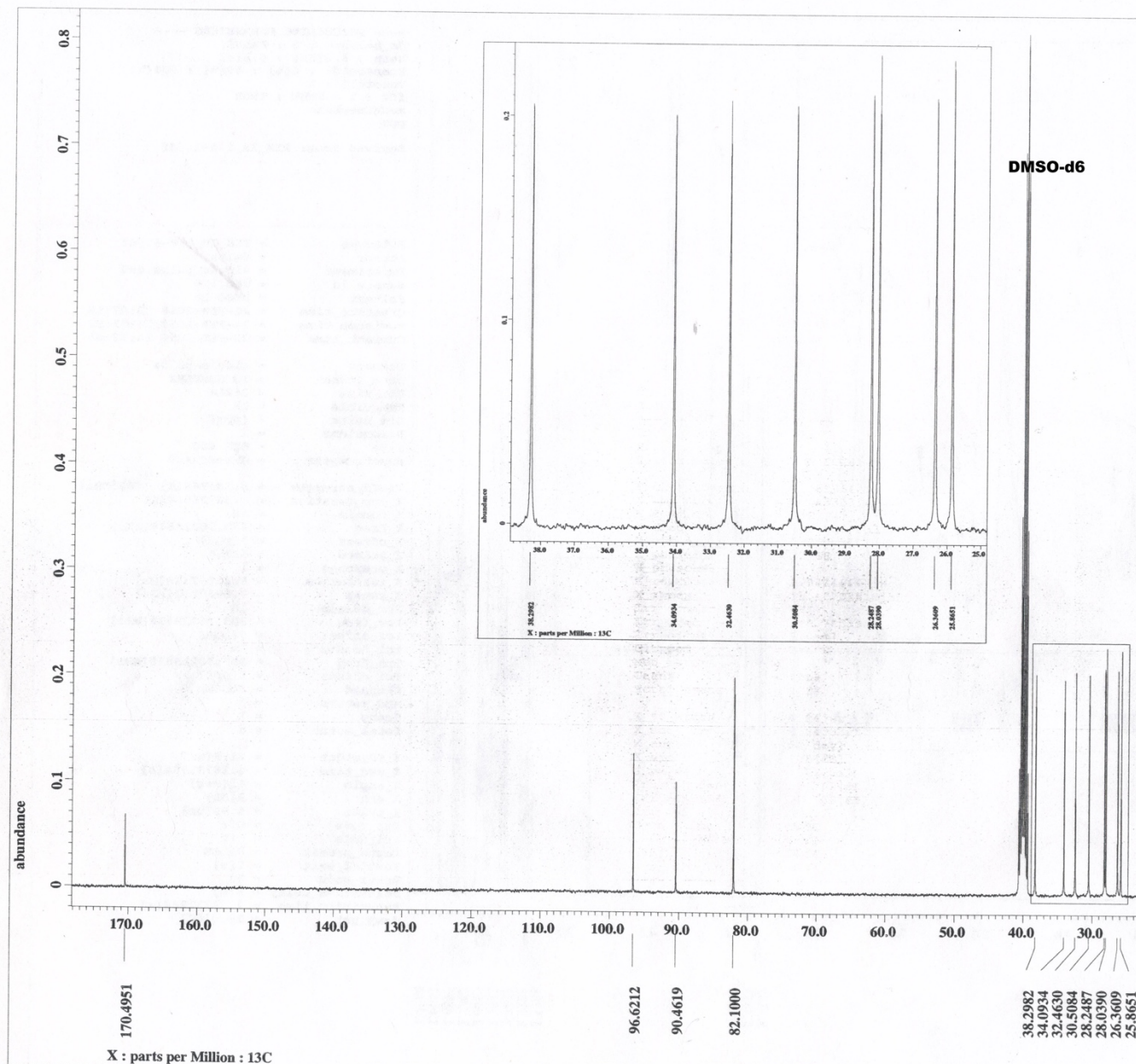
Filename = TIM_DEPT135_152-5.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_152
 Solvent = DMSO-D6
 Creation_time = 21-OCT-2018 21:22:07
 Revision_time = 23-OCT-2018 15:39:29
 Current_time = 23-OCT-2018 15:39:34

 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 = 23.2[degC]



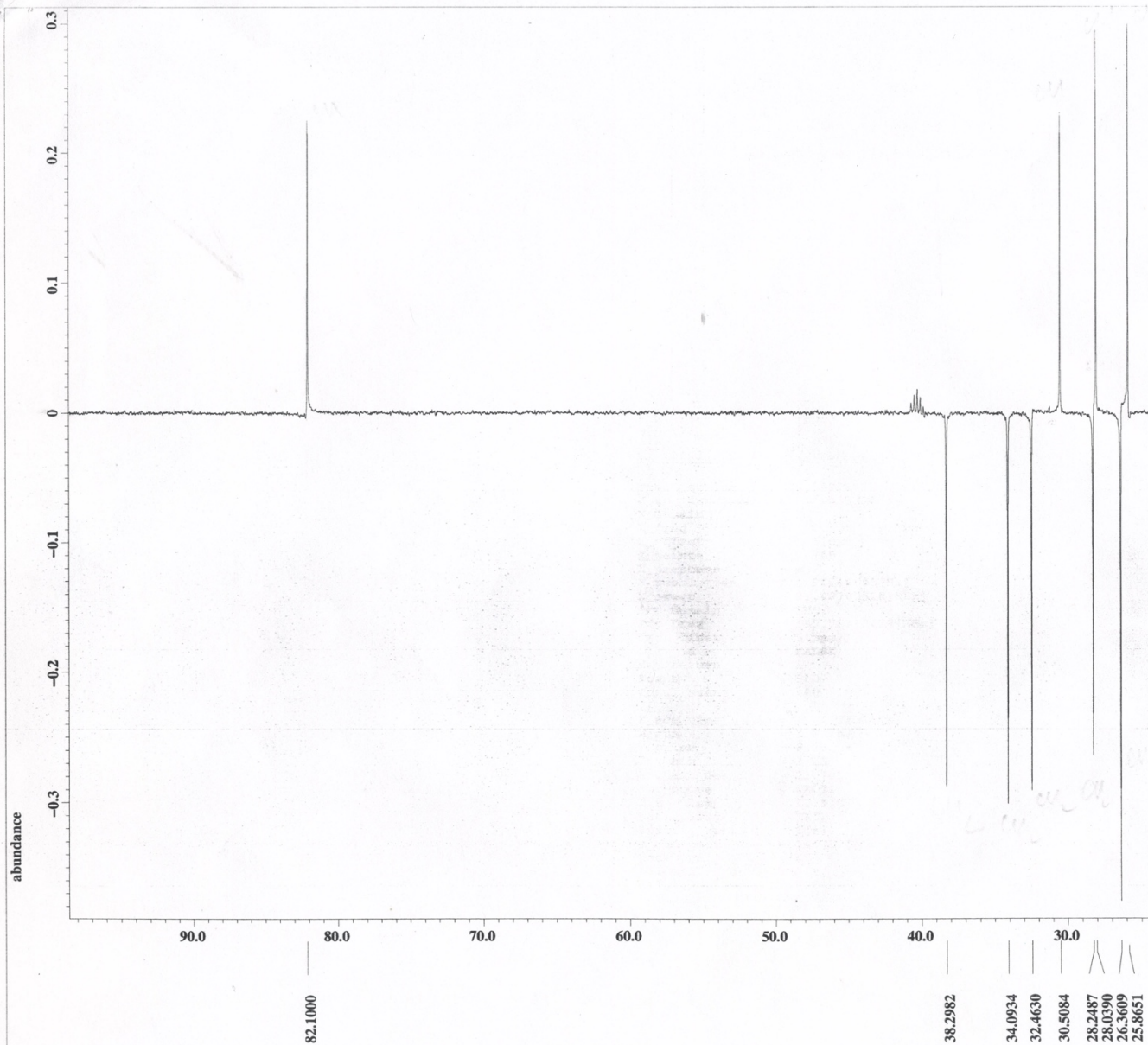


Filename = TIM_13C_110-4.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_110
 Solvent = DMSO-D6
 Creation_time = 21-FEB-2018 14:01:41
 Revision_time = 22-FEB-2018 14:32:35
 Current_time = 22-FEB-2018 14:32:59

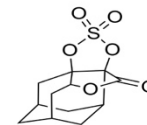
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 400
 Spectrometer = JNM-ECX400

Field_strength = 9.389766[T] (400 [MHz])
 X_acq_duration = 1.04333312[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 = 19.3 [dc]



X : parts per Million : 13C

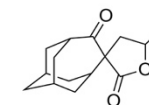
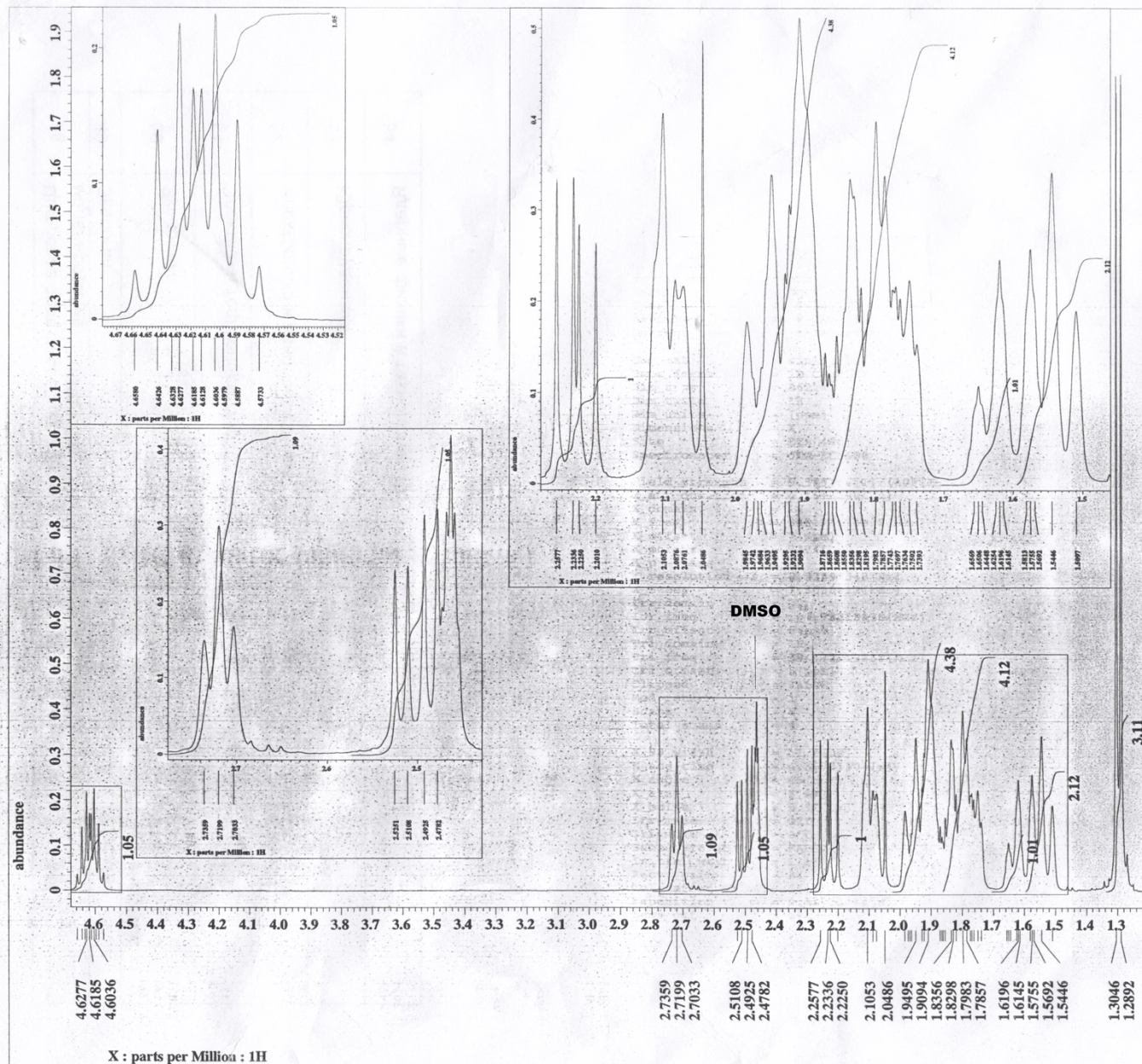


Filename = TIM_DEPT135_110-4.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_110
 Solvent = DMSO-D6
 Creation_time = 21-FEB-2018 14:27:28
 Revision_time = 22-FEB-2018 14:33:11
 Current_time = 22-FEB-2018 14:33:20

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 = 19.1[dC]

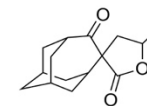
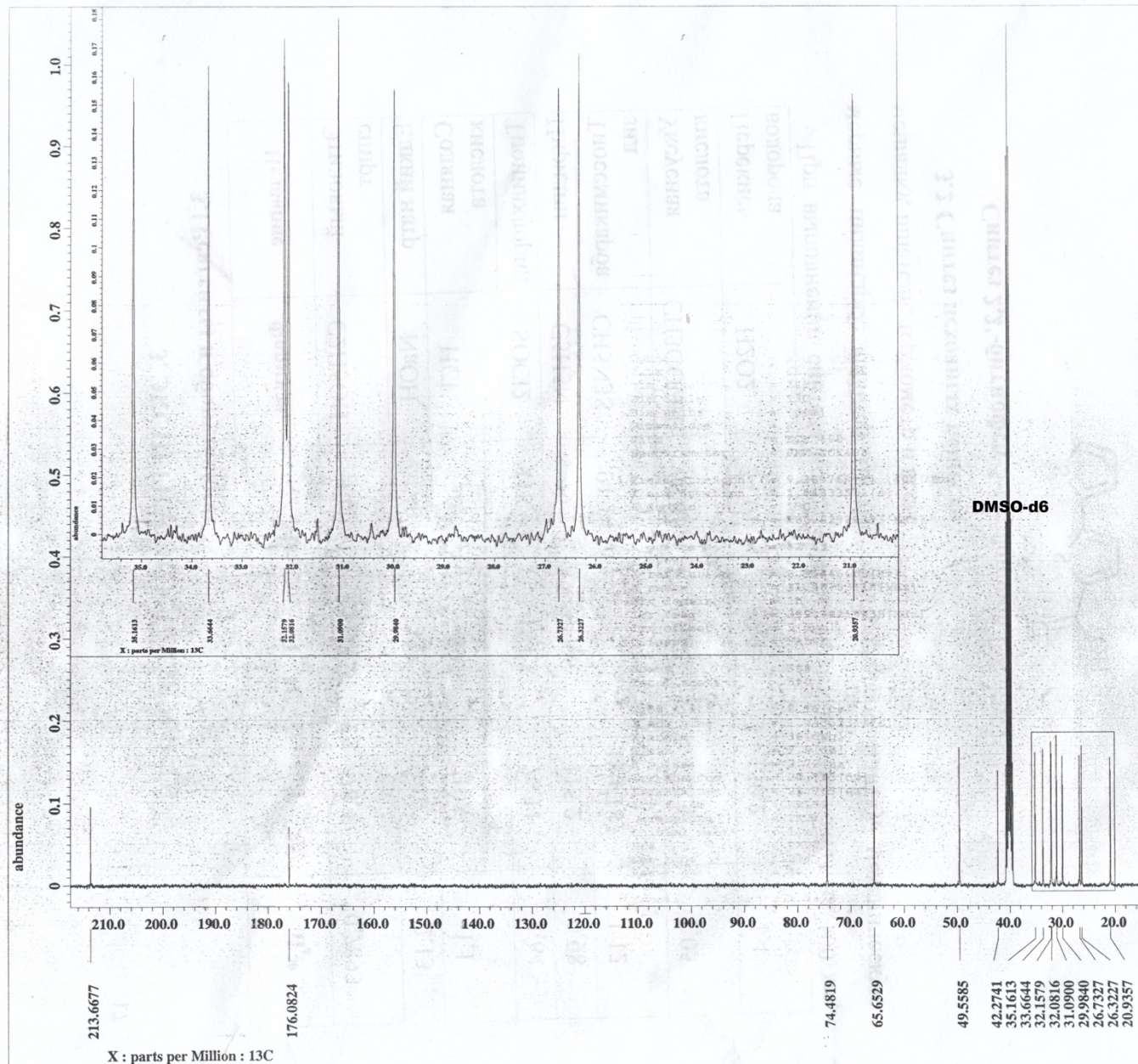


Filename = TIM_1H_176-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_176
 Solvent = DMSO-D6
 Creation_time = 9-JAN-2019 12:31:11
 Revision_time = 9-JAN-2019 11:52:17
 Current_time = 9-JAN-2019 11:53:08

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 = 25.2[dc]

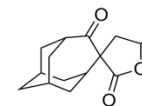
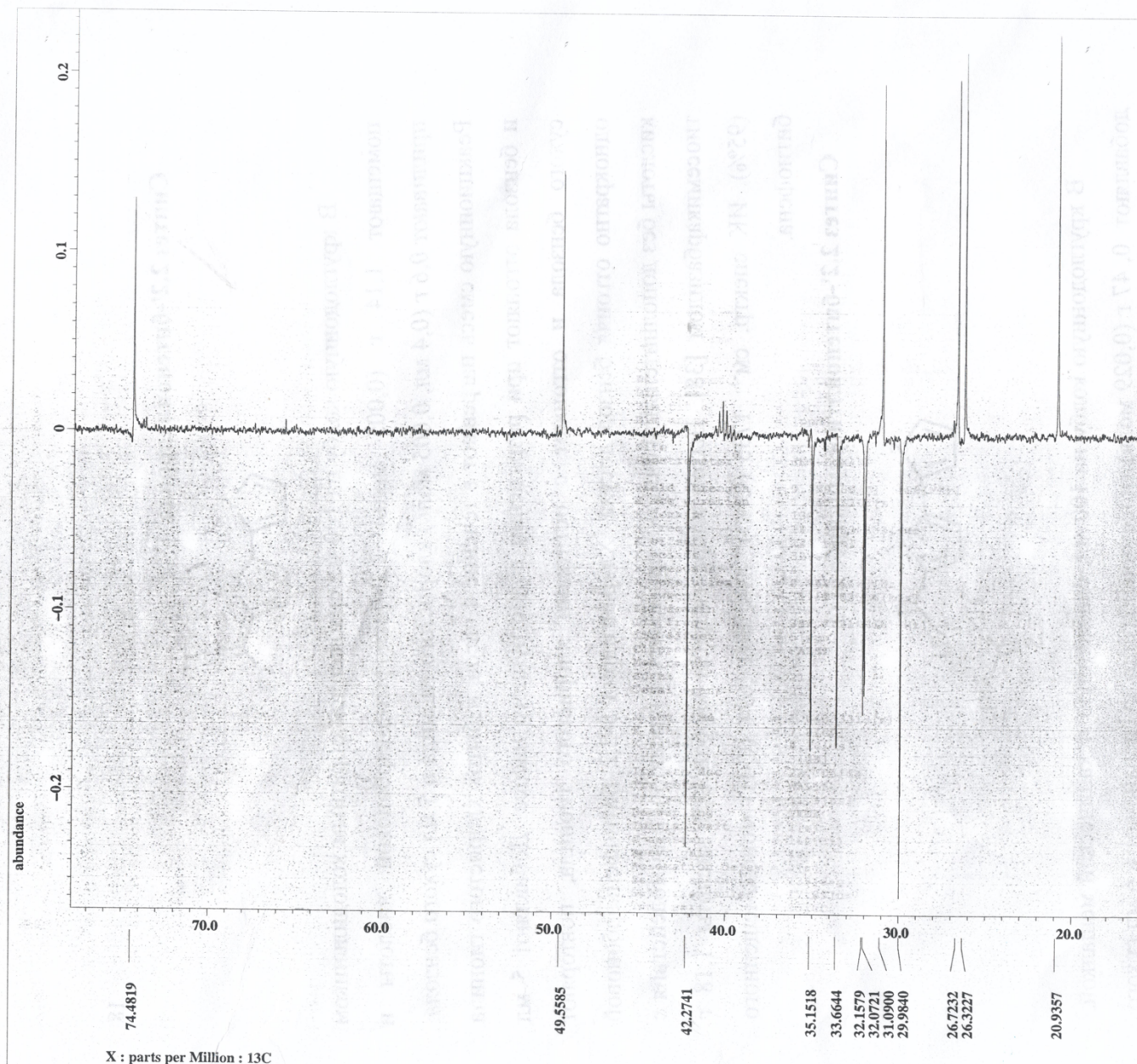


Filename = TIM_13C_176-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_176
 Solvent = DMSO-D6
 Creation_time = 9-JAN-2019 13:03:27
 Revision_time = 9-JAN-2019 12:33:43
 Current_time = 9-JAN-2019 12:34:00

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 = 590
 Total_scans = 590

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 = 25.2[dC]

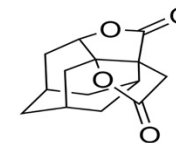
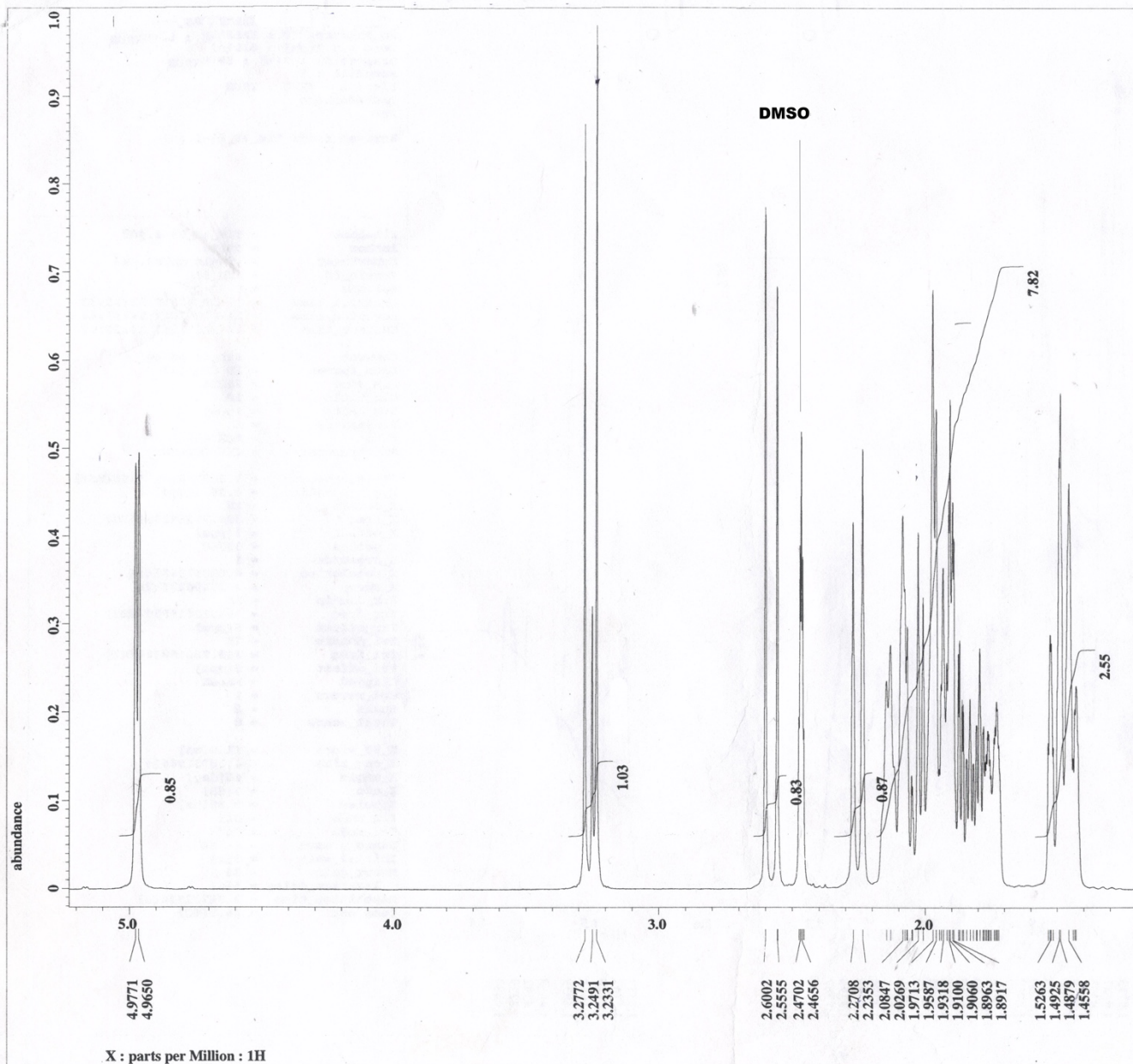


Filename = TIM_DEPT135_176-4.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_176
 Solvent = DMSO-D6
 Creation_time = 9-JAN-2019 13:14:50
 Revision_time = 9-JAN-2019 12:34:13
 Current_time = 9-JAN-2019 12:35:19

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 = 217
 Total_scans = 217

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 = 25[dc]

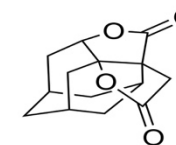
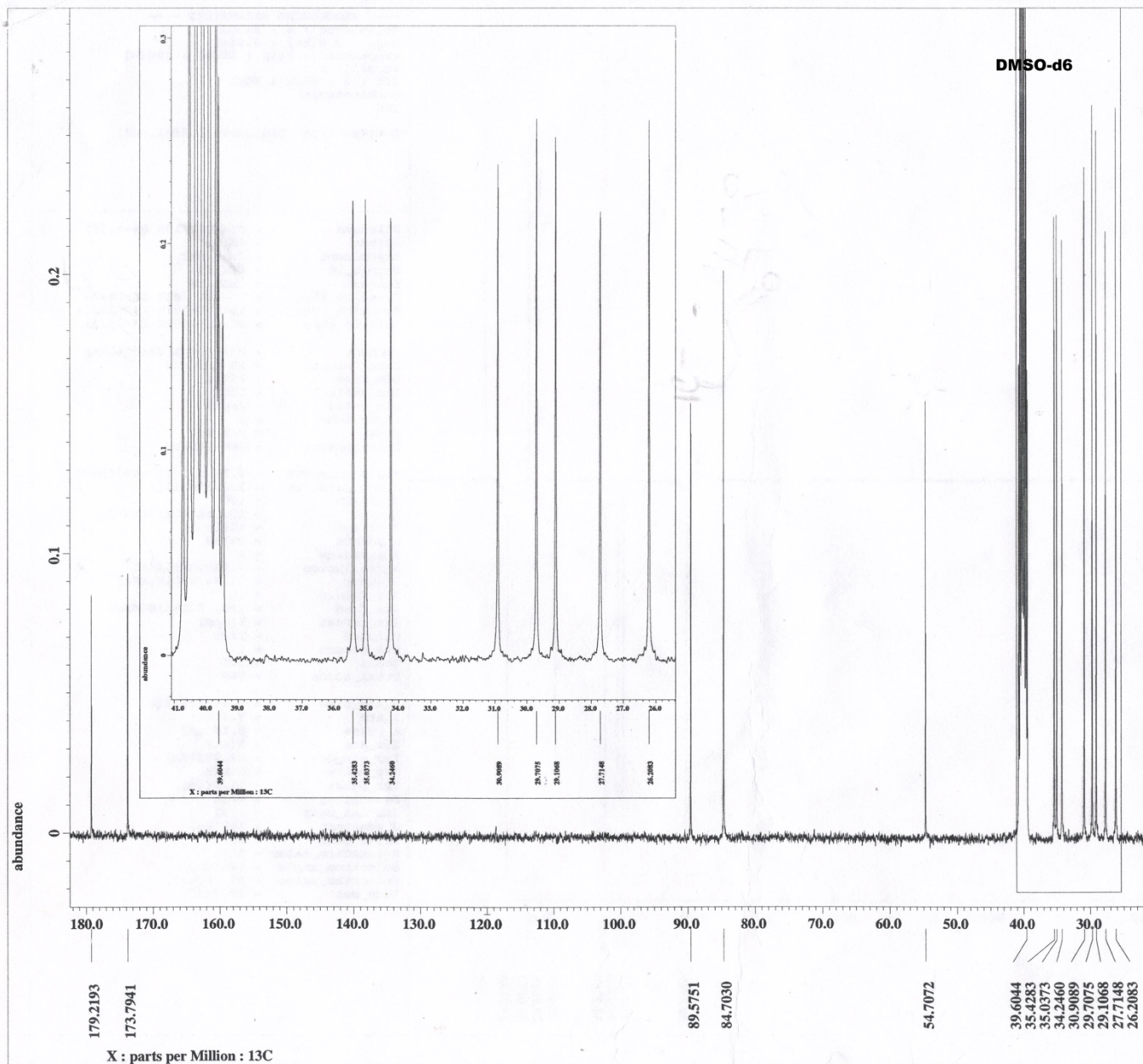


Filename = TIM_1H_89-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_89
 Solvent = DMSO-D6
 Creation_time = 13-DEC-2017 23:15:33
 Revision_time = 14-DEC-2017 14:37:43
 Current_time = 14-DEC-2017 14:37:56

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 = 34
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 29.5[dc]

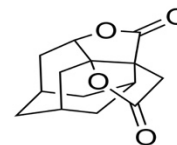
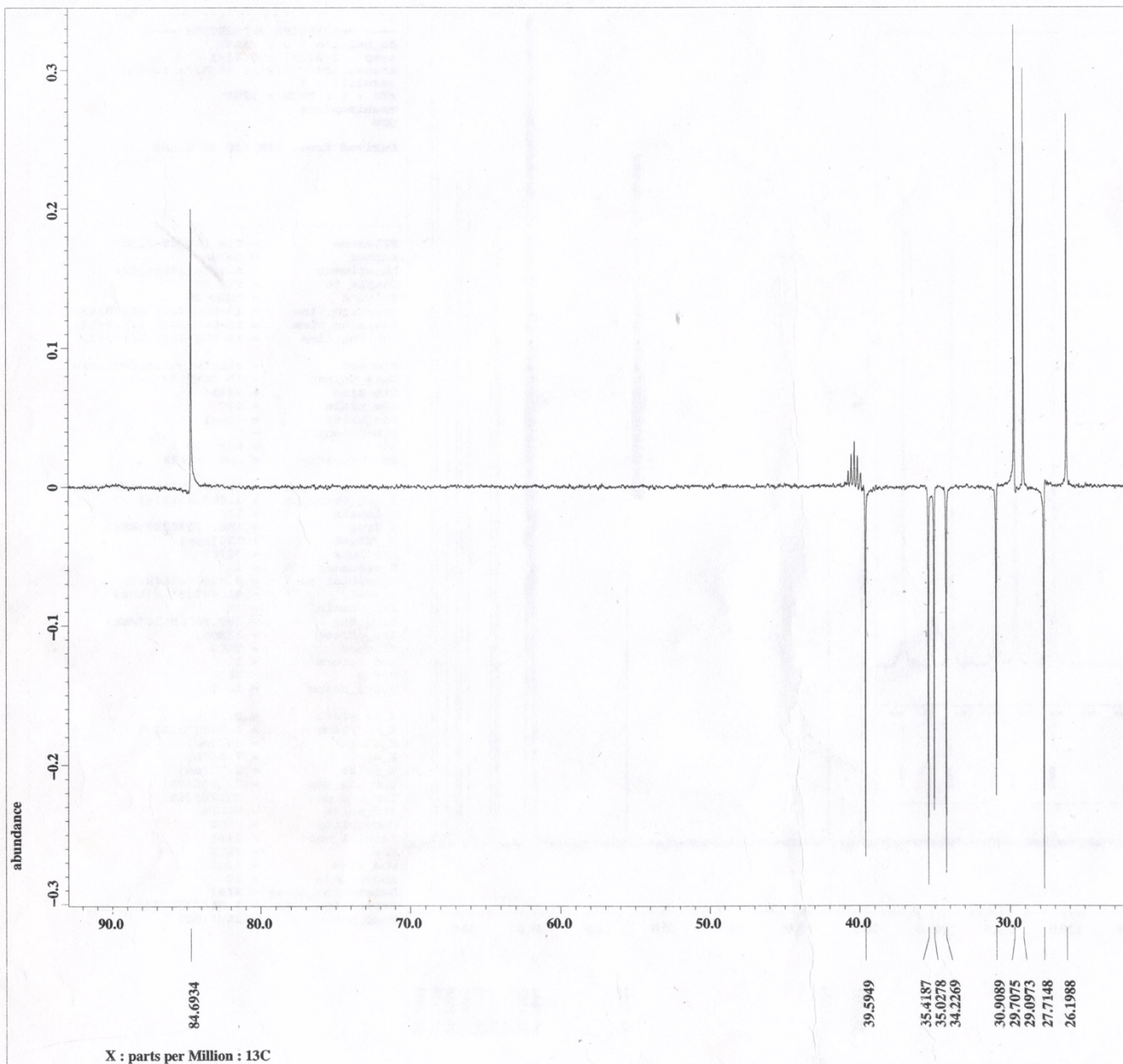


Filename = TIM_13C_89-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_89
 Solvent = DMSO-D6
 Creation_time = 14-DEC-2017 00:08:42
 Revision_time = 14-DEC-2017 14:38:58
 Current_time = 14-DEC-2017 14:39:33

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 = 26.3[dc]



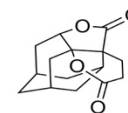
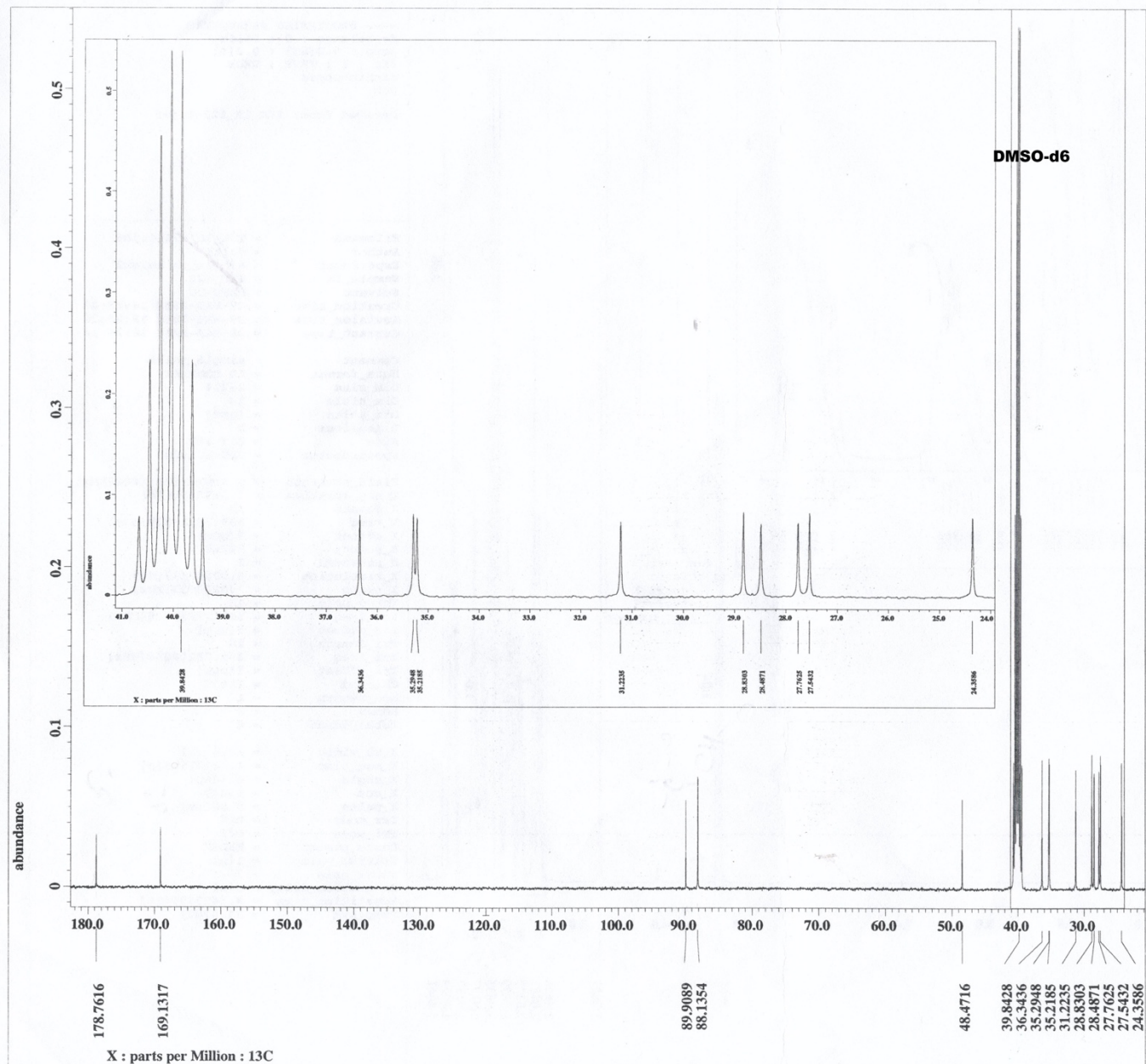
```

Filename      = TIM_DEPT135_89-3.jdf
Author        = delta
Experiment    = dept.ex2
Sample_id     = TIM_89
Solvent       = DMSO-D6
Creation_time  = 14-DEC-2017 00:34:31
Revision_time  = 14-DEC-2017 14:40:10
Current_time   = 14-DEC-2017 14:40:21

Comment       = DEPT with decoupling
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECK 400
Spectrometer   = JNM-ECK400

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          = 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       = 25.7[dc]
  
```

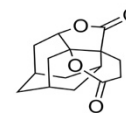
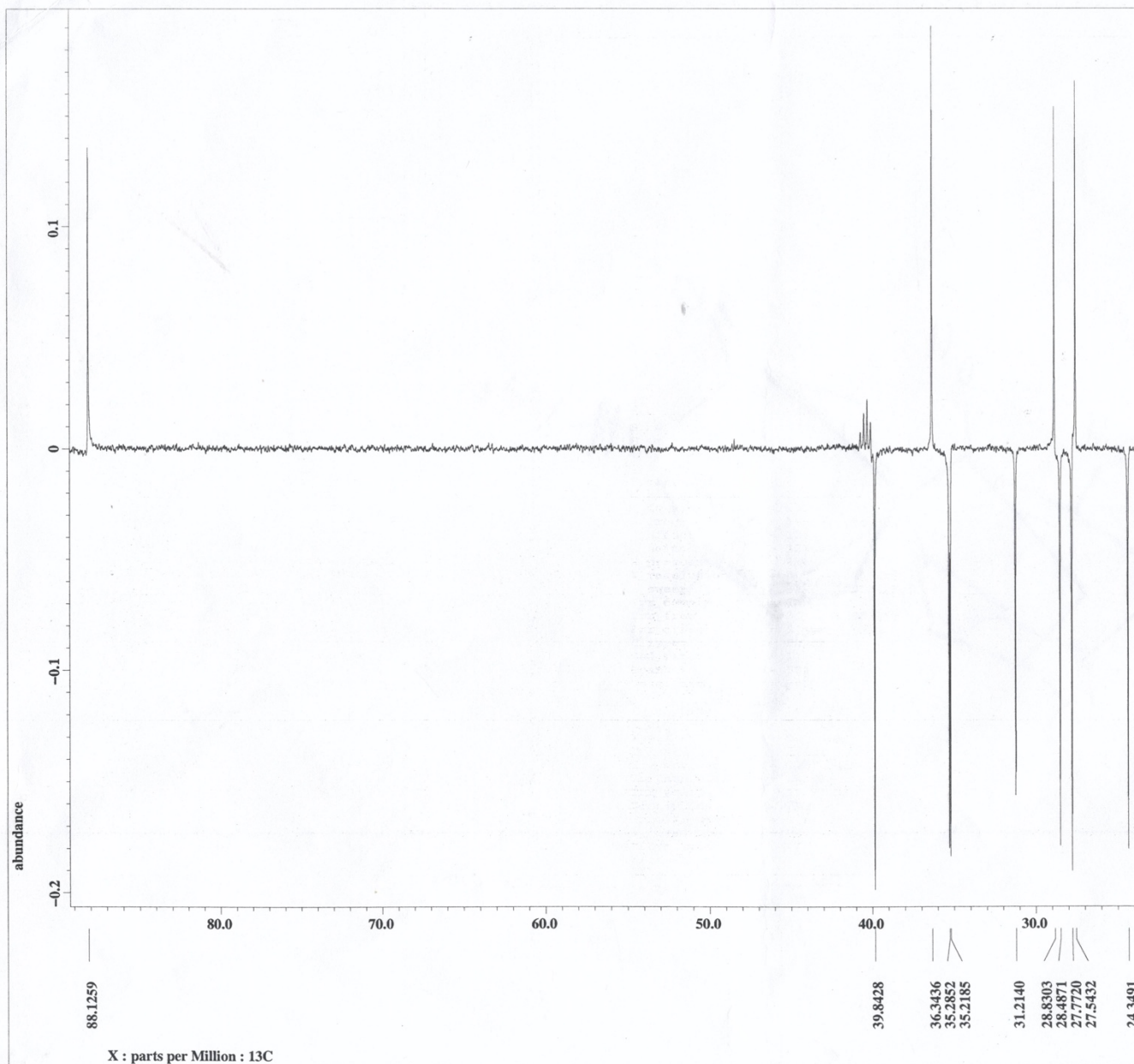



Filename = TIM_13C_122-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_122
 Solvent = DMSO-D6
 Creation_time = 27-MAR-2018 17:41:40
 Revision_time = 28-MAR-2018 18:27:34
 Current_time = 28-MAR-2018 18:28:05

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 = 1.04333312[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 = 44
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 21.2[dc]

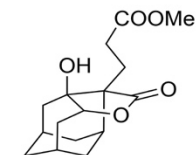
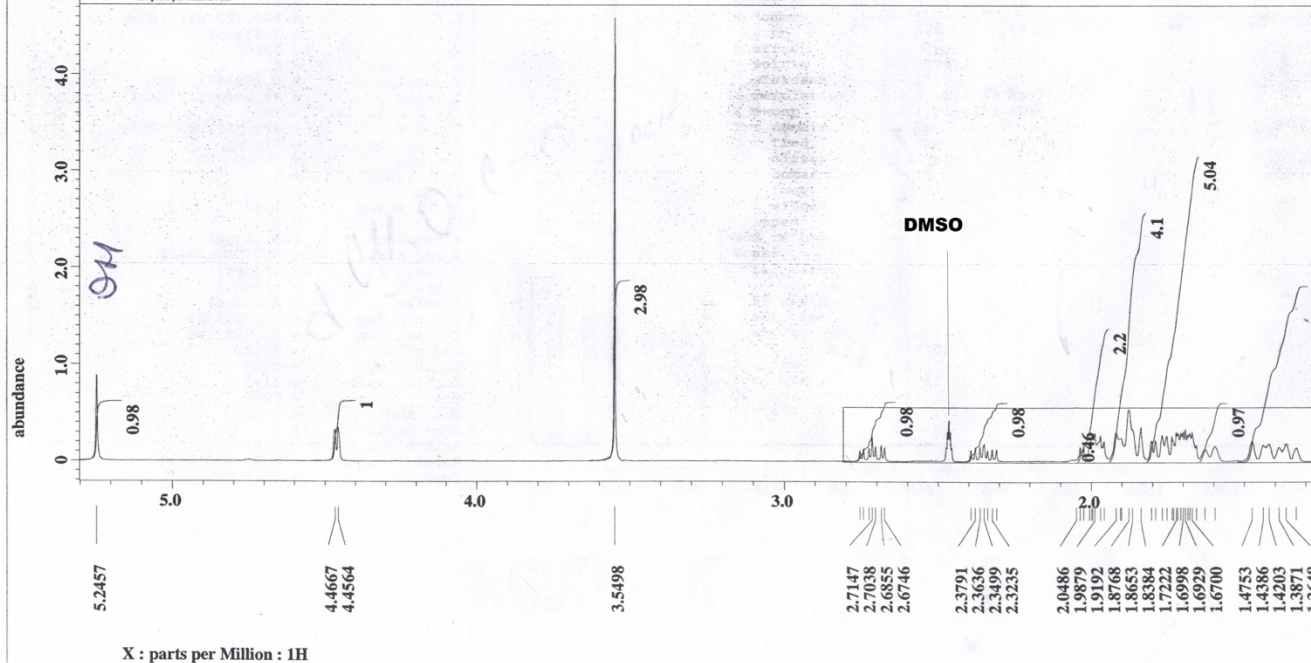


Filename = TIM_DEPT135_122-4.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_122
 Solvent = DMSO-D6
 Creation_time = 27-MAR-2018 18:07:28
 Revision_time = 28-MAR-2018 18:26:56
 Current_time = 28-MAR-2018 18:28:11

Comment = DEPT with decoupling
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECU 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 = 20.4[degC]



```

Filename      = TIM_1H_116-4.jdf
Author        = delta
Experiment     = single_pulse.ex2
Sample_id     = TIM_116
Solvent       = DMSO-D6
Creation_time  = 13-MAR-2018 04:00:15
Revision_time  = 13-MAR-2018 12:08:28
Current_time   = 13-MAR-2018 12:08:59

```

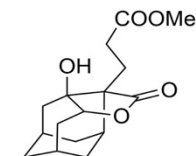
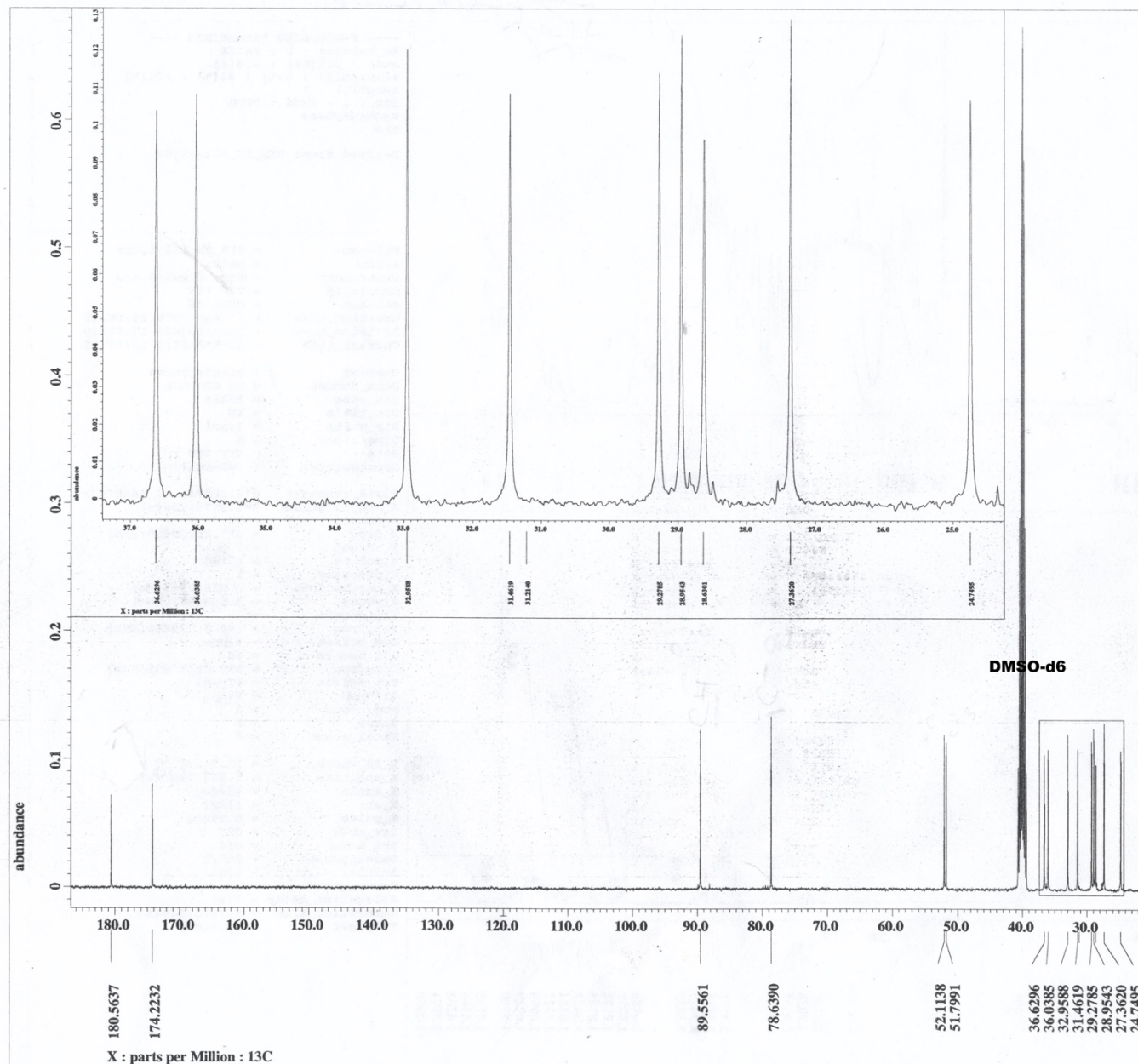
```

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      = 32
Relaxation_delay = 5[s]
Repetition_time = 9.36731904[s]
Temp_get        = 20.9[degC]
```

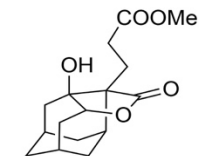
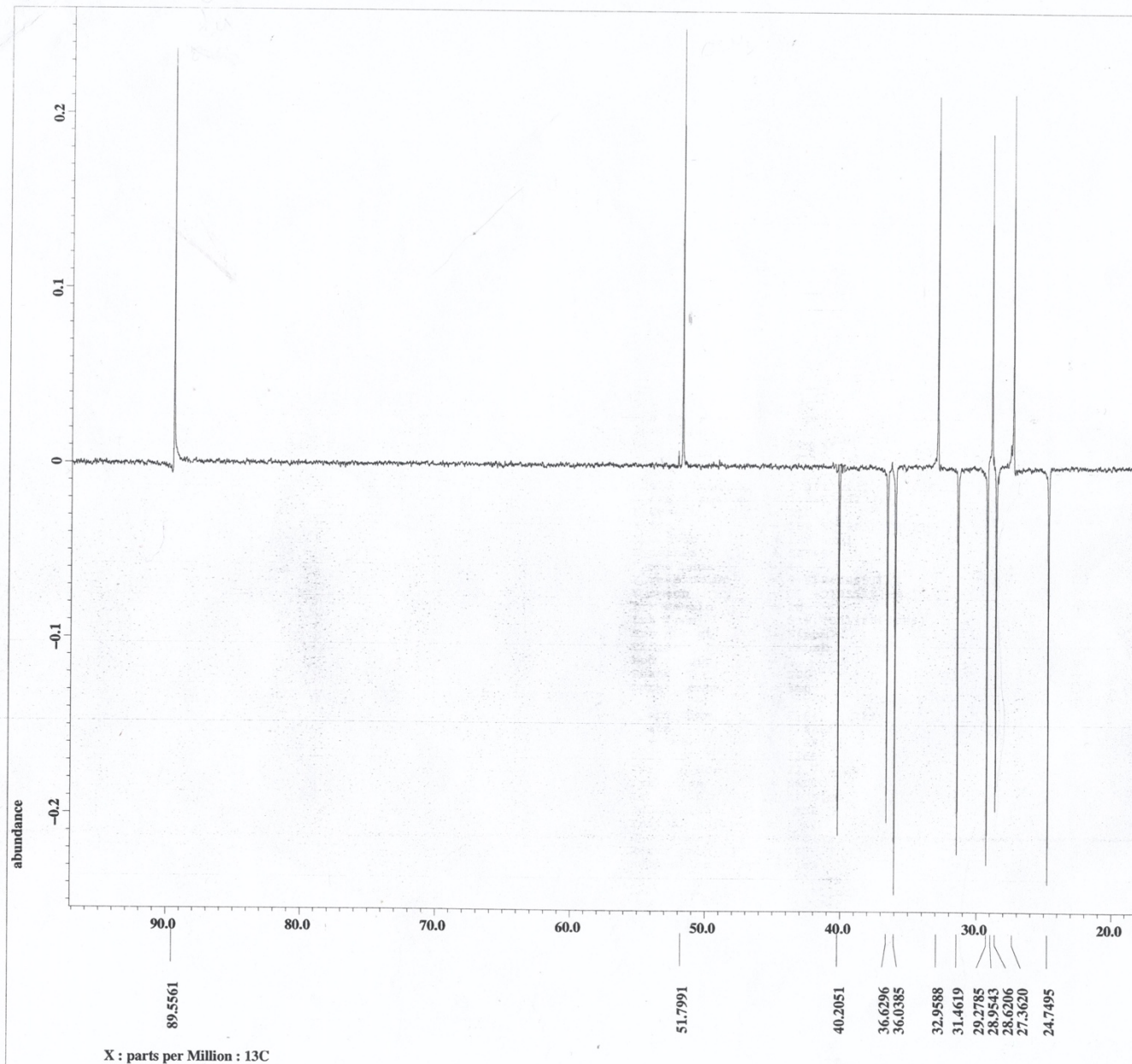



Filename = TIM_13C_116-4.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_116
 Solvent = DMSO-D6
 Creation_time = 13-MAR-2018 04:53:30
 Revision_time = 13-MAR-2018 12:09:45
 Current_time = 13-MAR-2018 12:09:47

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECK 400
 Spectrometer = JNM-ECK400

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 = 46
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 21.1[dC]

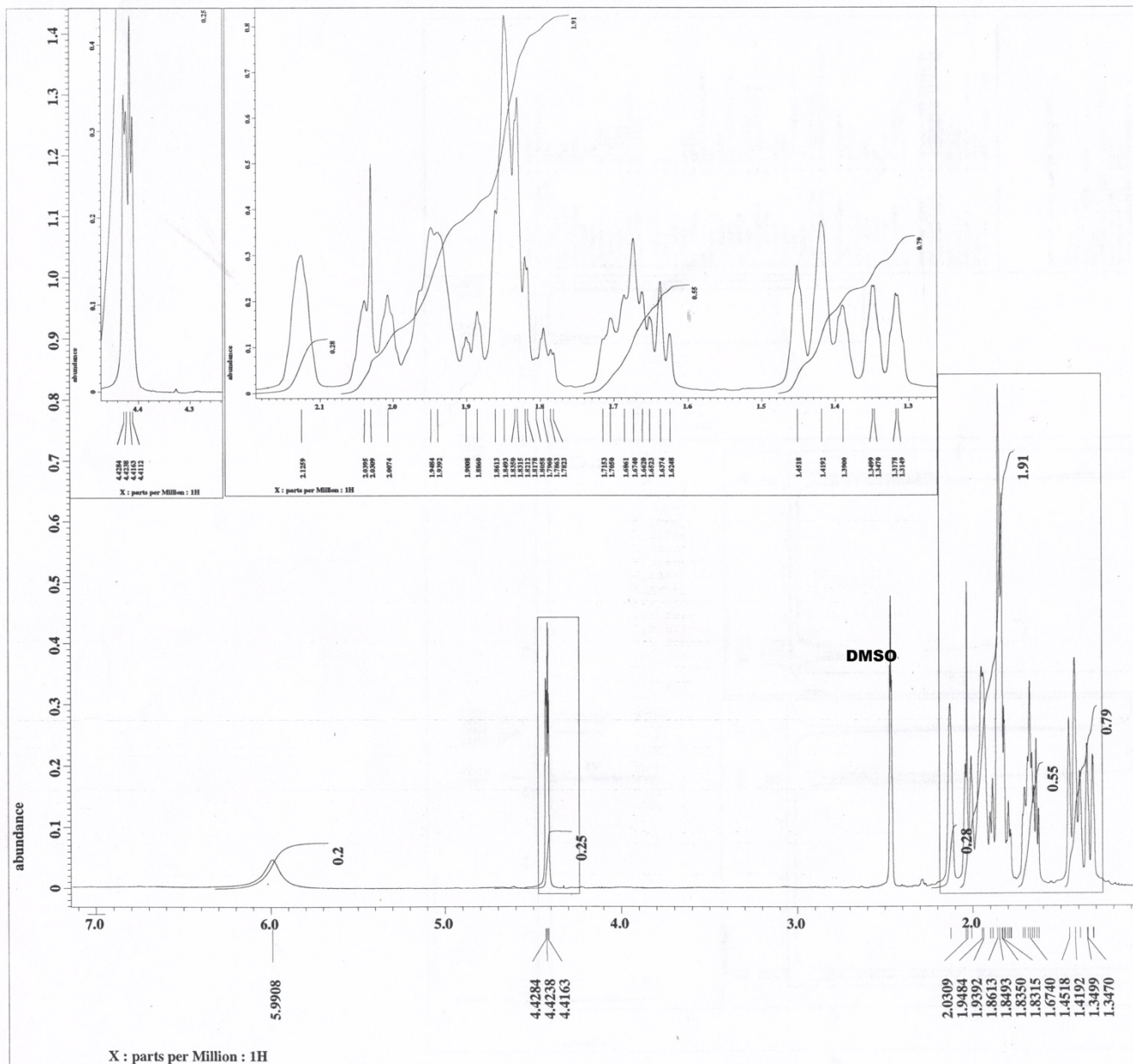


Filename = TIM_DEPT135_116-3.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_116
 Solvent = DMSO-D6
 Creation_time = 13-MAR-2018 05:19:21
 Revision_time = 13-MAR-2018 12:09:55
 Current_time = 13-MAR-2018 12:10:11

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 = 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 = 21.3[degC]

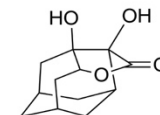
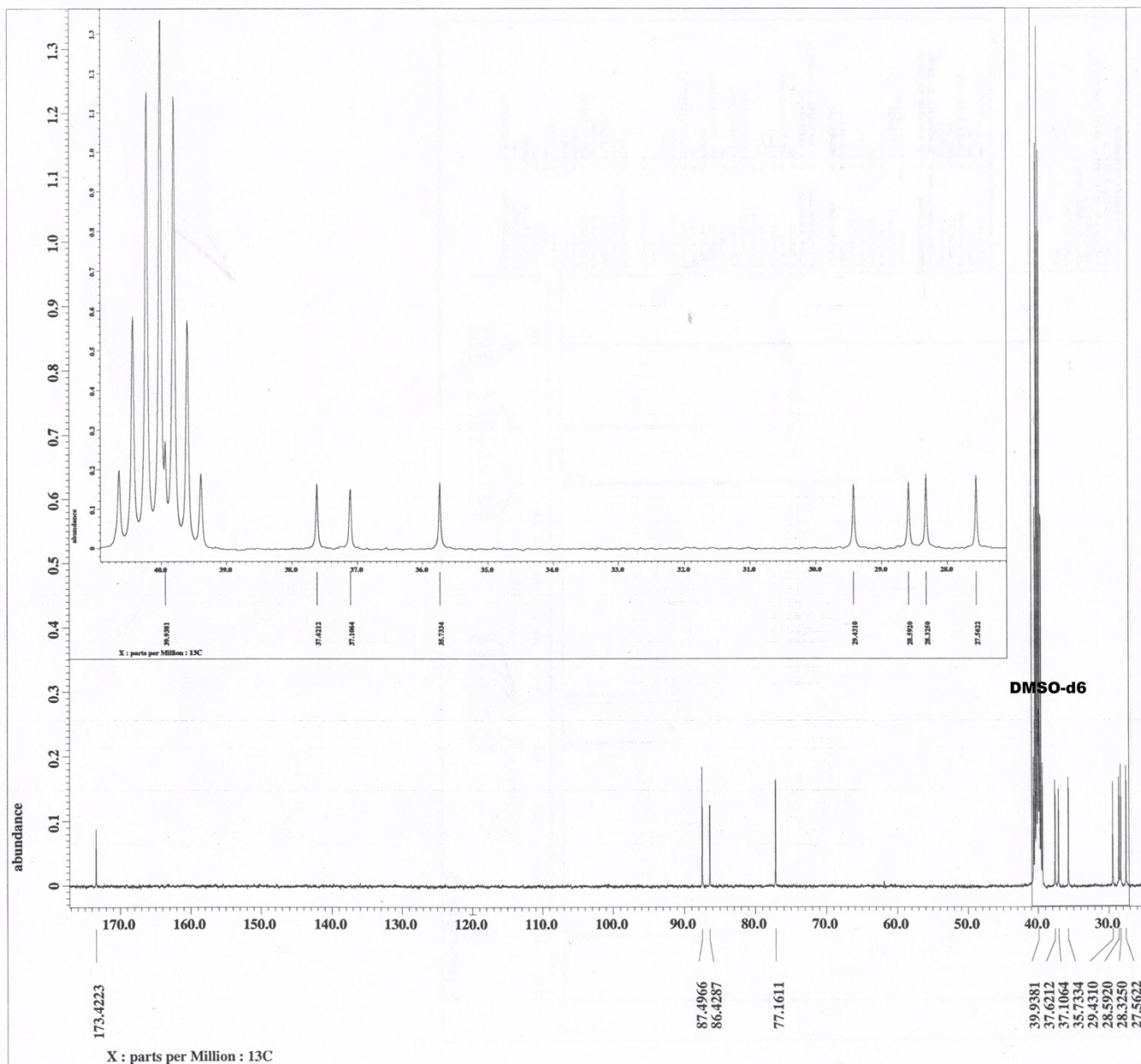


Filename = TIM_1H_149-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_149
 Solvent = DMSO-D6
 Creation_time = 10-OCT-2018 22:25:28
 Revision_time = 11-OCT-2018 12:44:42
 Current_time = 11-OCT-2018 12:45:20

Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 26214
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECK 400
 Spectrometer = JNM-ECK400

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[degC]

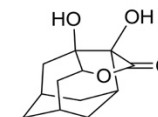
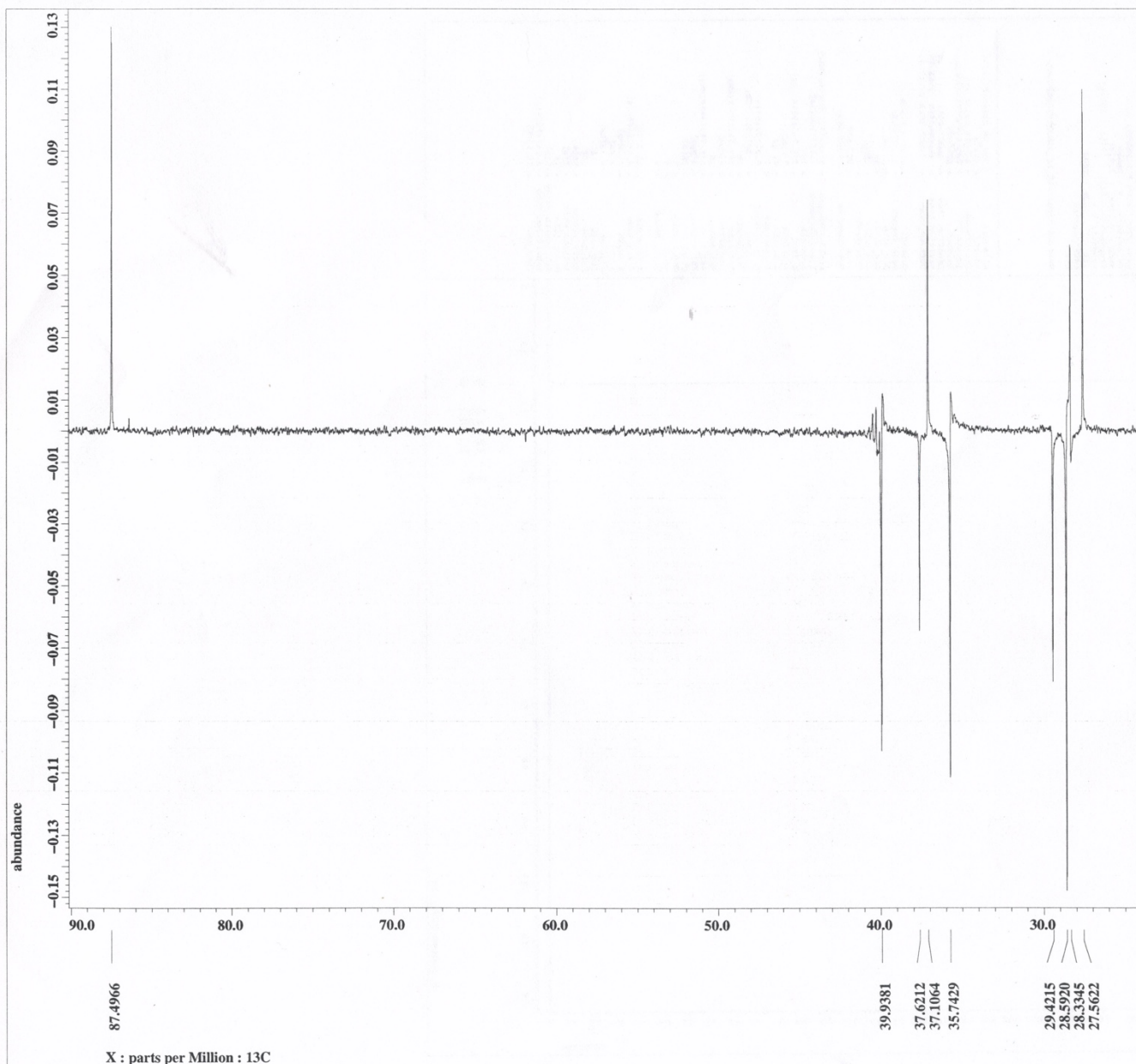


Filename = TIM_13C_149-4.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_149
 Solvent = DMSO-D6
 Creation_time = 10-OCT-2018 23:16:41
 Revision_time = 11-OCT-2018 12:45:48
 Current_time = 11-OCT-2018 12:46:21

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 = 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]
 K_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 = 3.04333312 [s]
 Temp_get = 22.8 [dC]

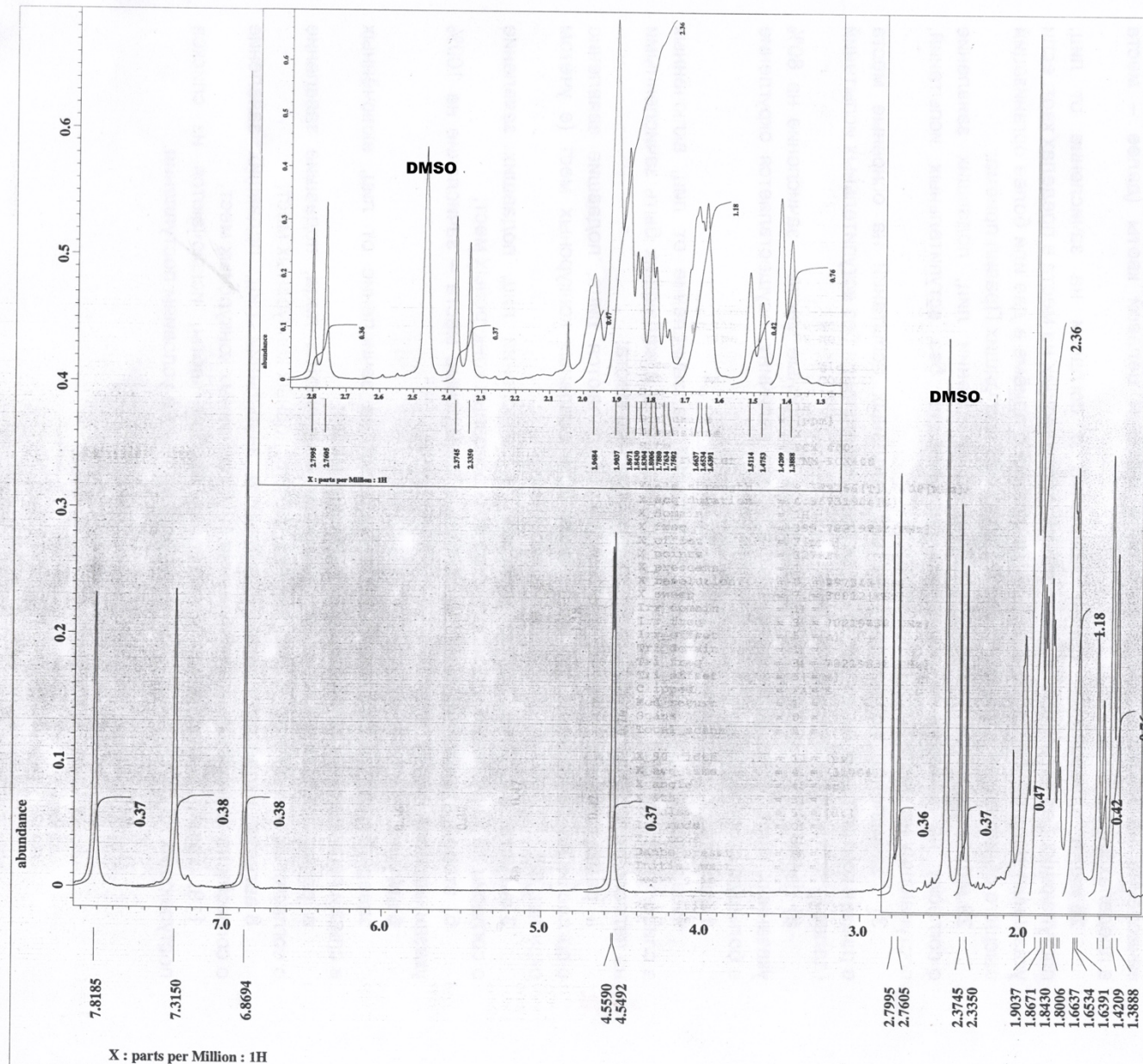


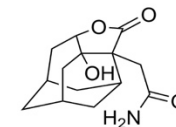
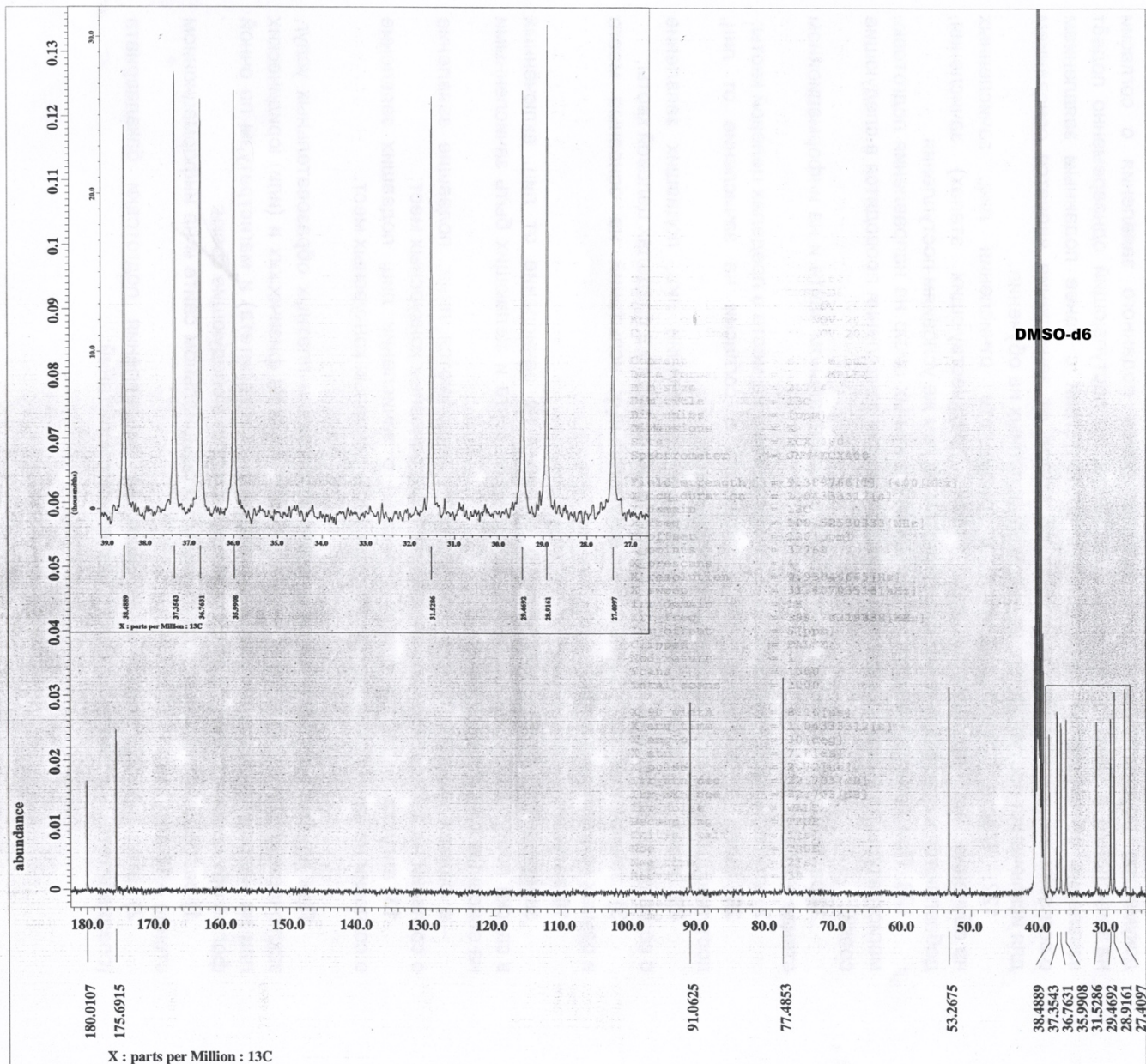
Filename = TIM_DEPT135_149-5.jdf
 Author = delta
 Experiment = dept.ex2
 Sample_id = TIM_149
 Solvent = DMSO-D6
 Creation_time = 10-OCT-2018 23:42:31
 Revision_time = 11-OCT-2018 12:46:32
 Current_time = 11-OCT-2018 12:46:36

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 = 22.7[degC]





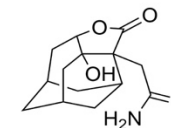
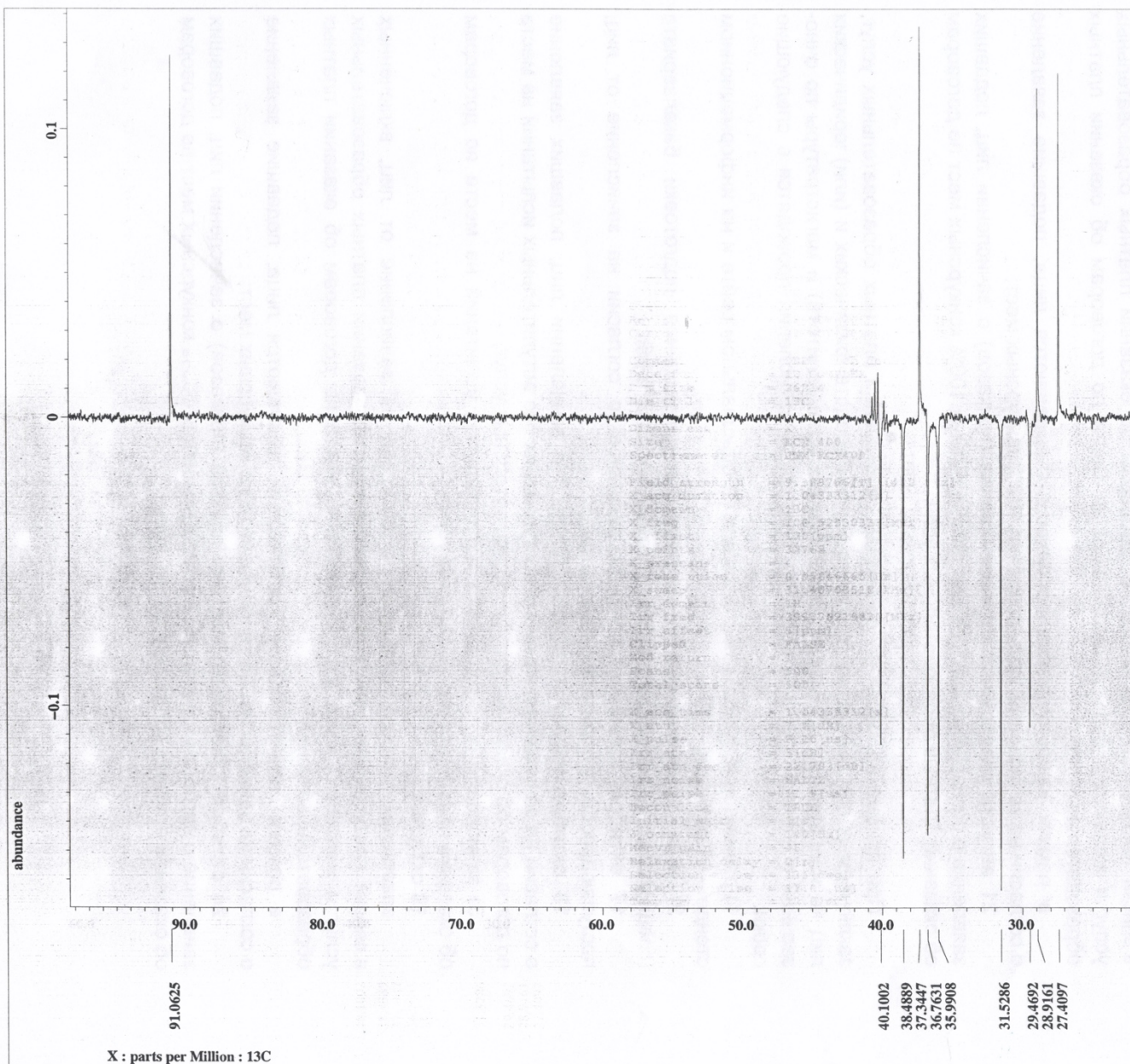
DMSO-d6

Filename = TIM_13C_163-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = TIM_163
 Solvent = DMSO-D6
 Creation_time = 27-NOV-2018 17:59:27
 Revision_time = 28-NOV-2018 13:49:47
 Current_time = 28-NOV-2018 13:50:08

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 = 38
 Relaxation_delay = 2[s]
 Repetition_time = 3.04333312[s]
 Temp_get = 22.7[dc]

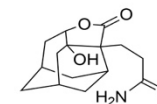
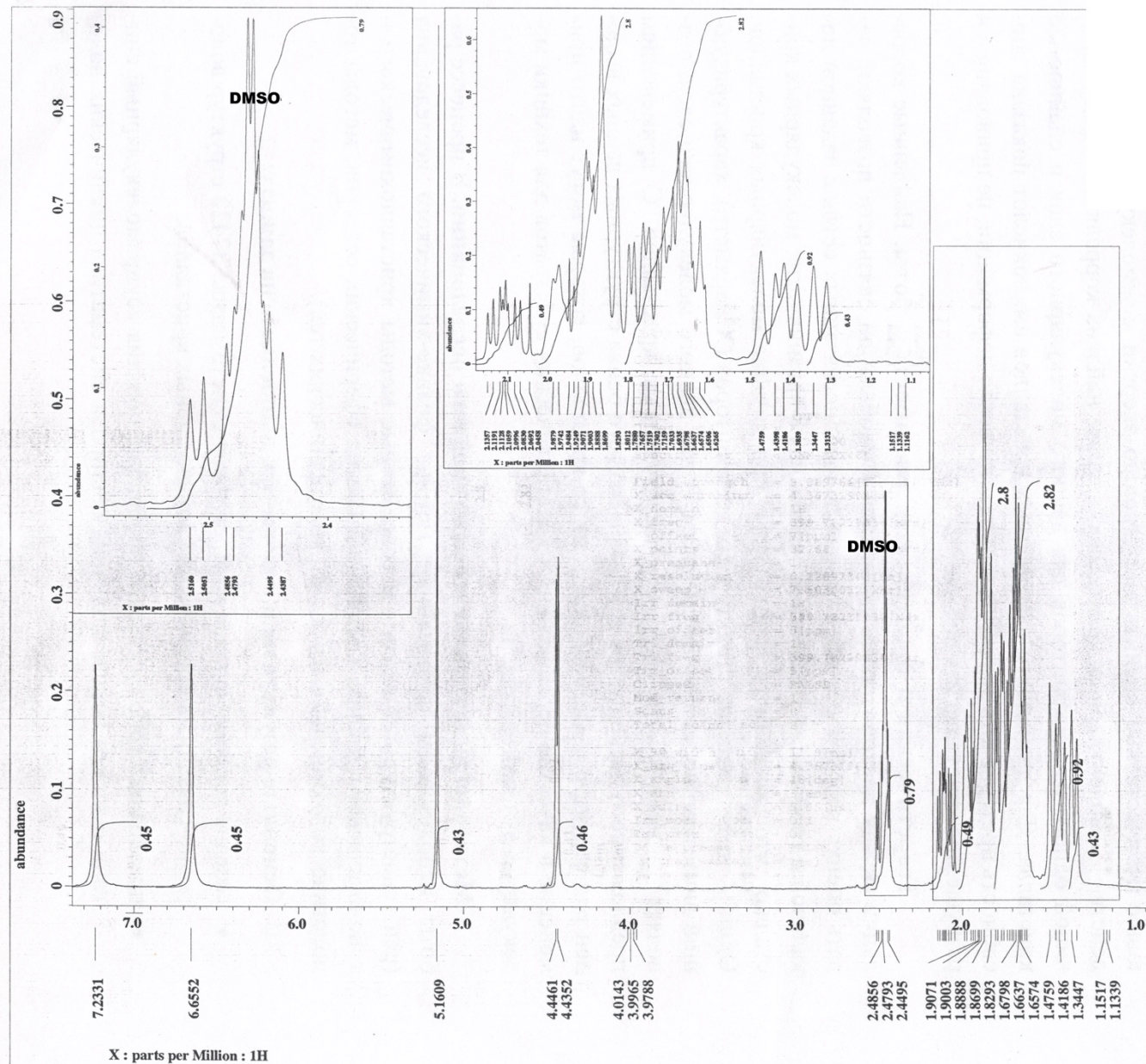


Filename = TIM_DEPT135_163-4.jdf
Author = delta
Experiment = dept.ex2
Sample_id = TIM_163
Solvent = DMSO-D6
Creation_time = 27-NOV-2018 18:25:14
Revision_time = 28-NOV-2018 13:50:28
Current_time = 28-NOV-2018 13:50:29

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 = 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 = 22.8[degC]

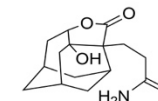
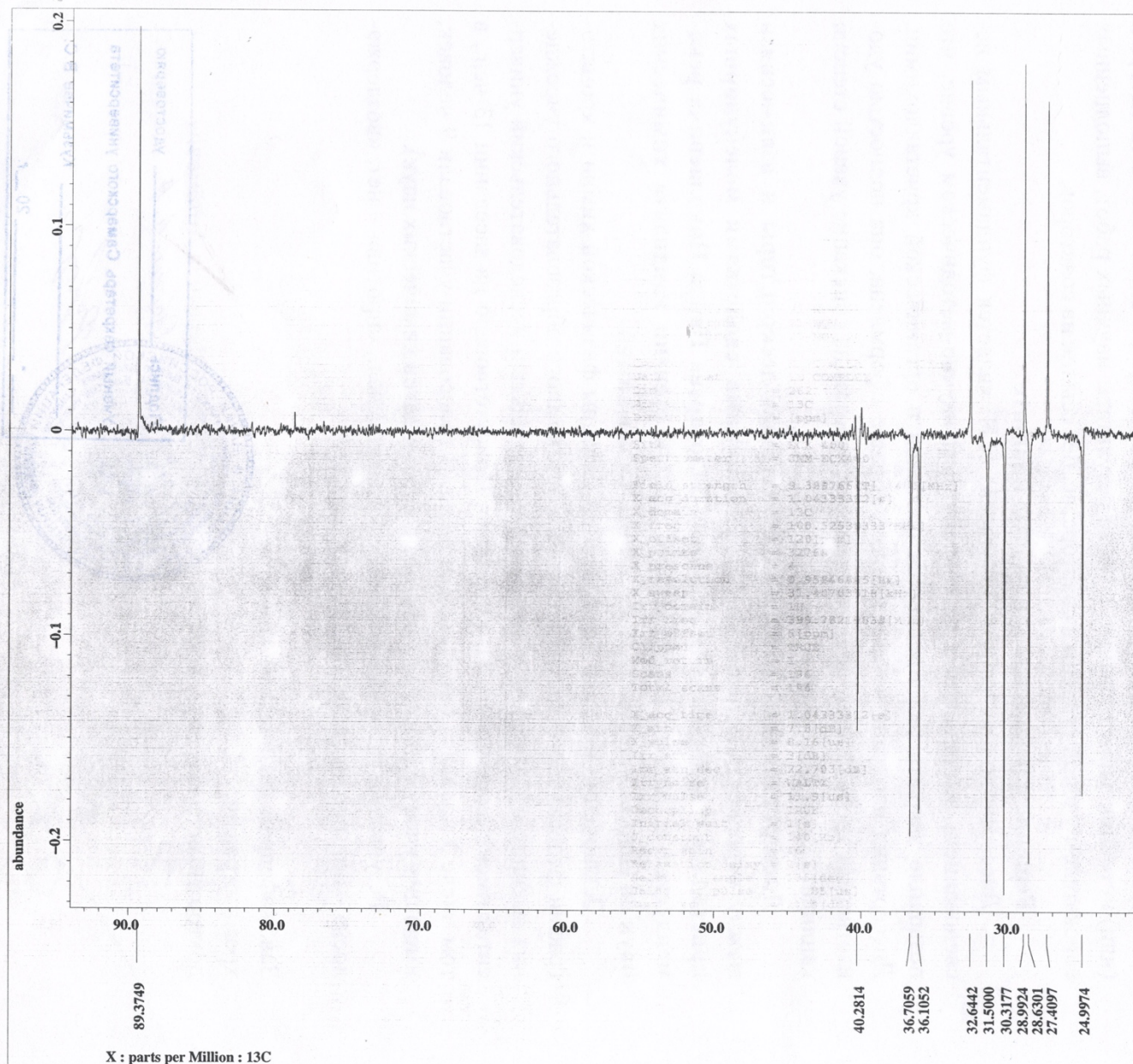


Filename = TIM_1H_160-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = TIM_160
 Solvent = DMSO-D6
 Creation_time = 21-NOV-2018 13:56:29
 Revision_time = 21-NOV-2018 15:48:44
 Current_time = 21-NOV-2018 15:49:36

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_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 32
 Relaxation_delay = 5[s]
 Repetition_time = 9.36731904[s]
 Temp_get = 21.8[dc]



Filename = TIM_DEPT135_160-5.jdf
Author = delta
Experiment = dept.ex2
Sample_id = TIM_160
Solvent = DMSO-D6
Creation_time = 21-NOV-2018 15:00:14
Revision_time = 21-NOV-2018 15:49:57
Current_time = 21-NOV-2018 15:50:25

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 = 9.399766 [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 = 196
Total_scans = 196

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 = 21.9 [degC]

Optimisation of key syntheses.

Optimization table 1 for alkylation with ethyl bromoacetate: 0.5 g of ketoester **1**, 1.1 eq of ethyl bromoacetate (0.26 ml), 1.1 eq (0.93 g) of sodium hydride 60% in oil. Stirring for 24 h in screw top vessel under argon. To prevent product contamination, commercial sodium hydride was washed with hexane before use.

Solvent/time	Et ₂ O	THF	Dioxane
Yield, %	72	84	84

Optimization table 2 for Michael reaction conditions: 0.5 g of ketoester **1**, 5 eq of Michael acceptor, 2.5 eq (0.73 g) of K₂CO₃, with stirring. [Time; yield, %]

Solvent/t, °C Michael acceptor	Acetonitrile , 25 °C	Acetonitrile, 50 °C	Acetone, 25 °C	Acetone, 50 °C	DMF, 25 °C	DMF, 50 °C	DMF, 80 °C	Acetone, 50 °C, with sonication
Acrylonitrile	84 h; 20%	84 h; 43%	84 h; 34%	84 h; 60%	84 h; 32%	84 h; 68%	84 h; 53%	>60 h; 72%
Methylacrylate	84 h; 28%	84 h; 73%	84 h; 32%	84 h; 68%	84 h; 40%	84 h; 70%	84 h; 68%	>60 h; 78%