Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

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

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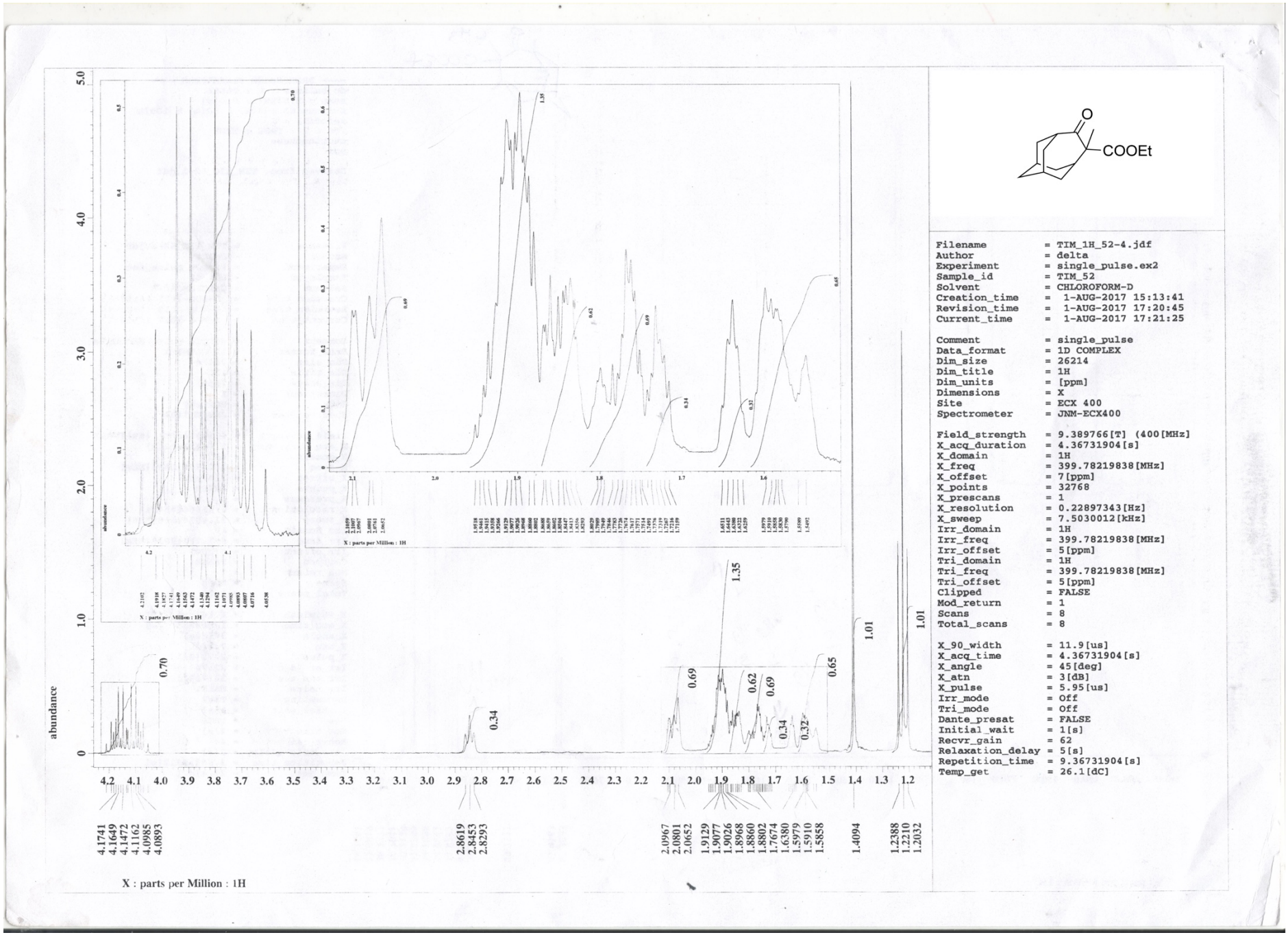
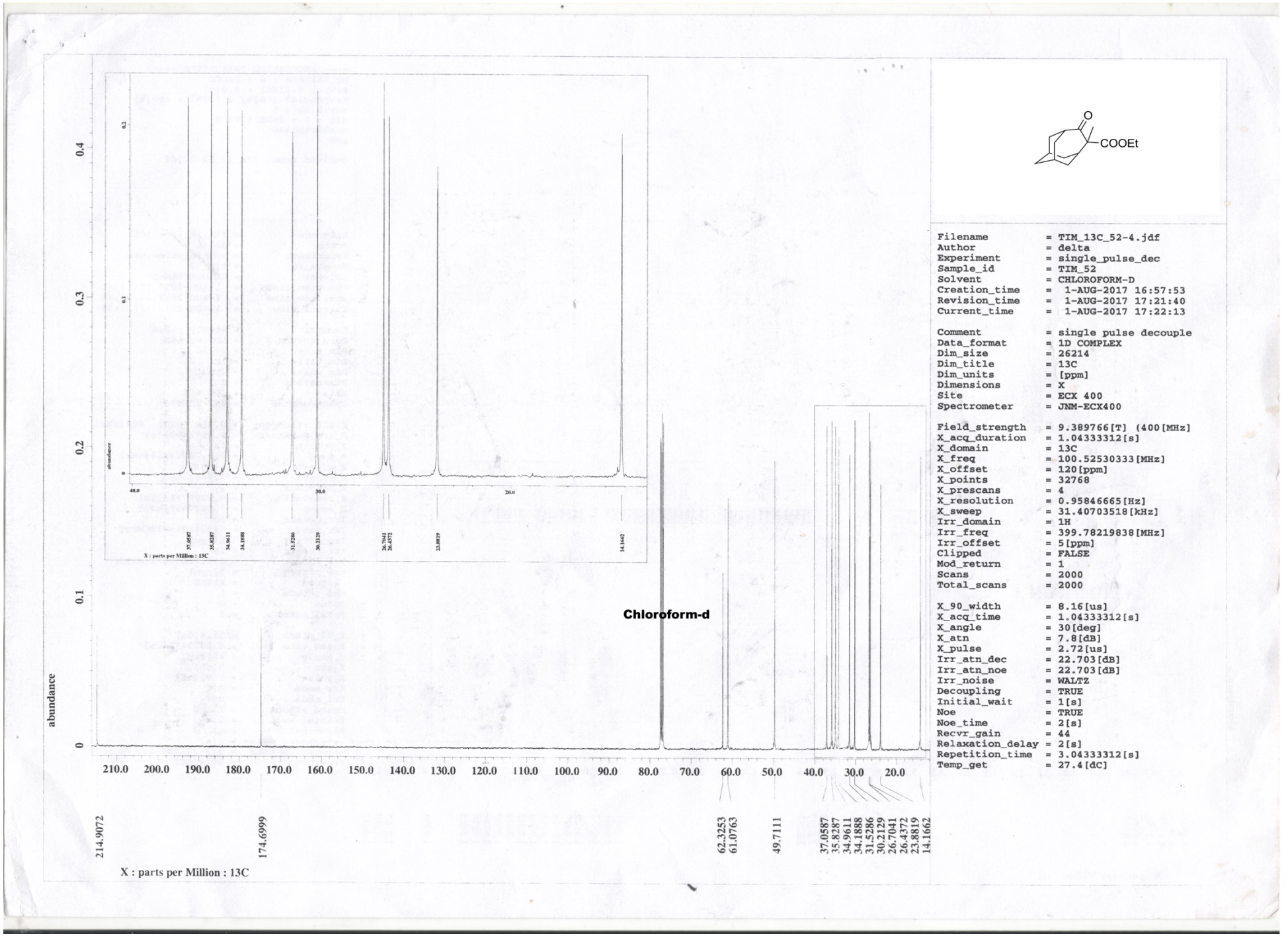
Contains:

copies of ^{1}H, ^{13}C 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.



compound 8 ^{1}H NMR



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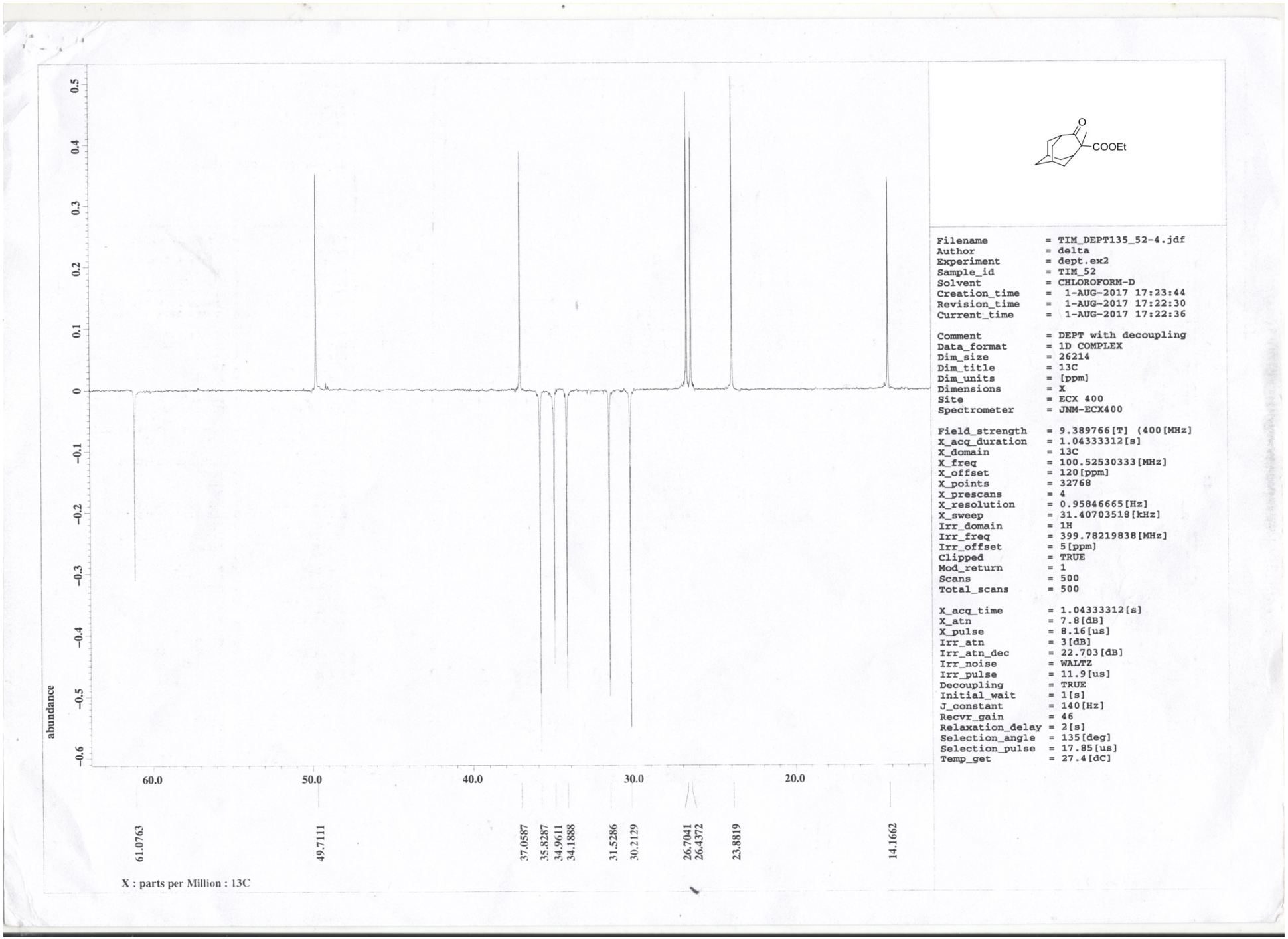
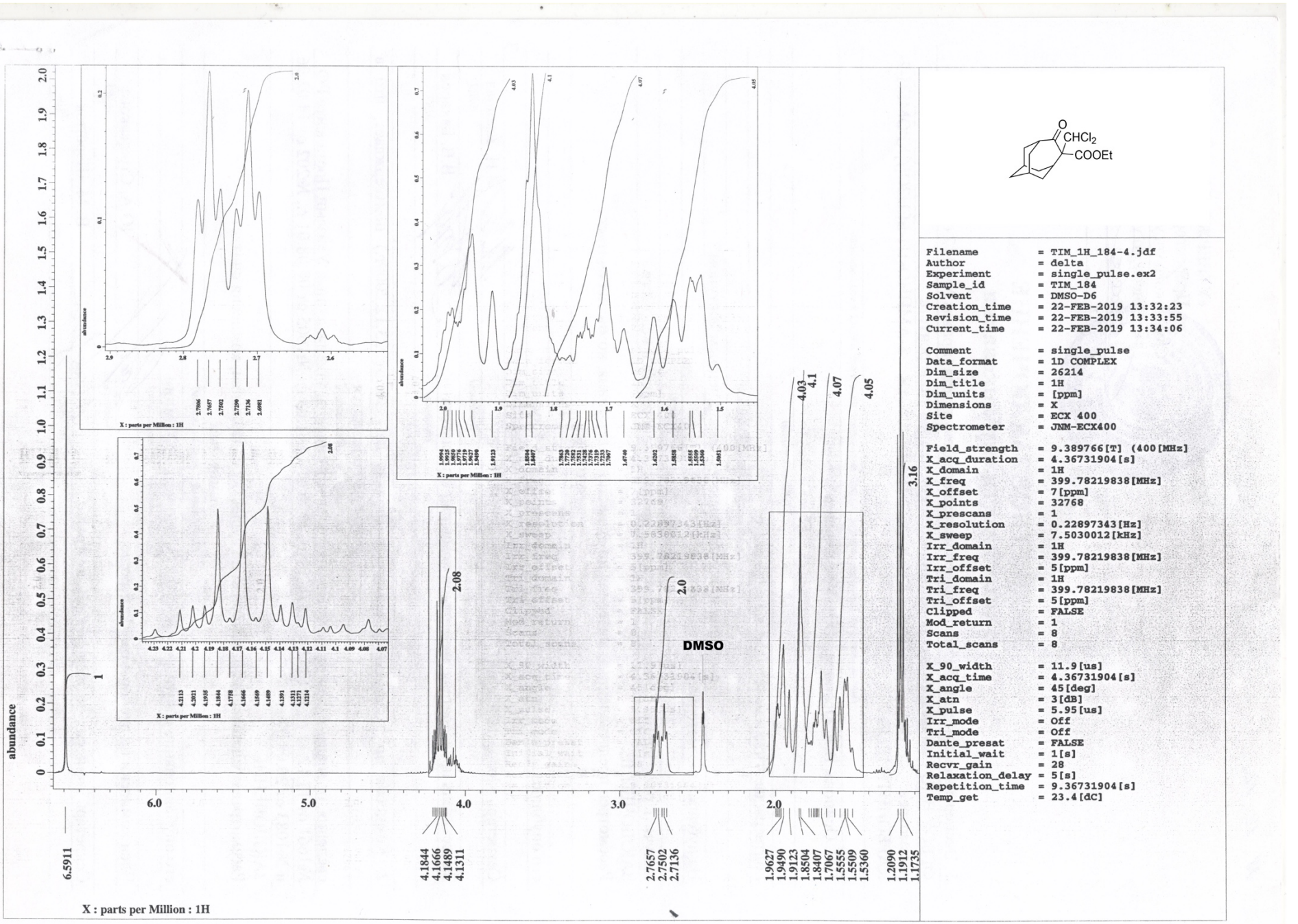


compound 8 DEPT



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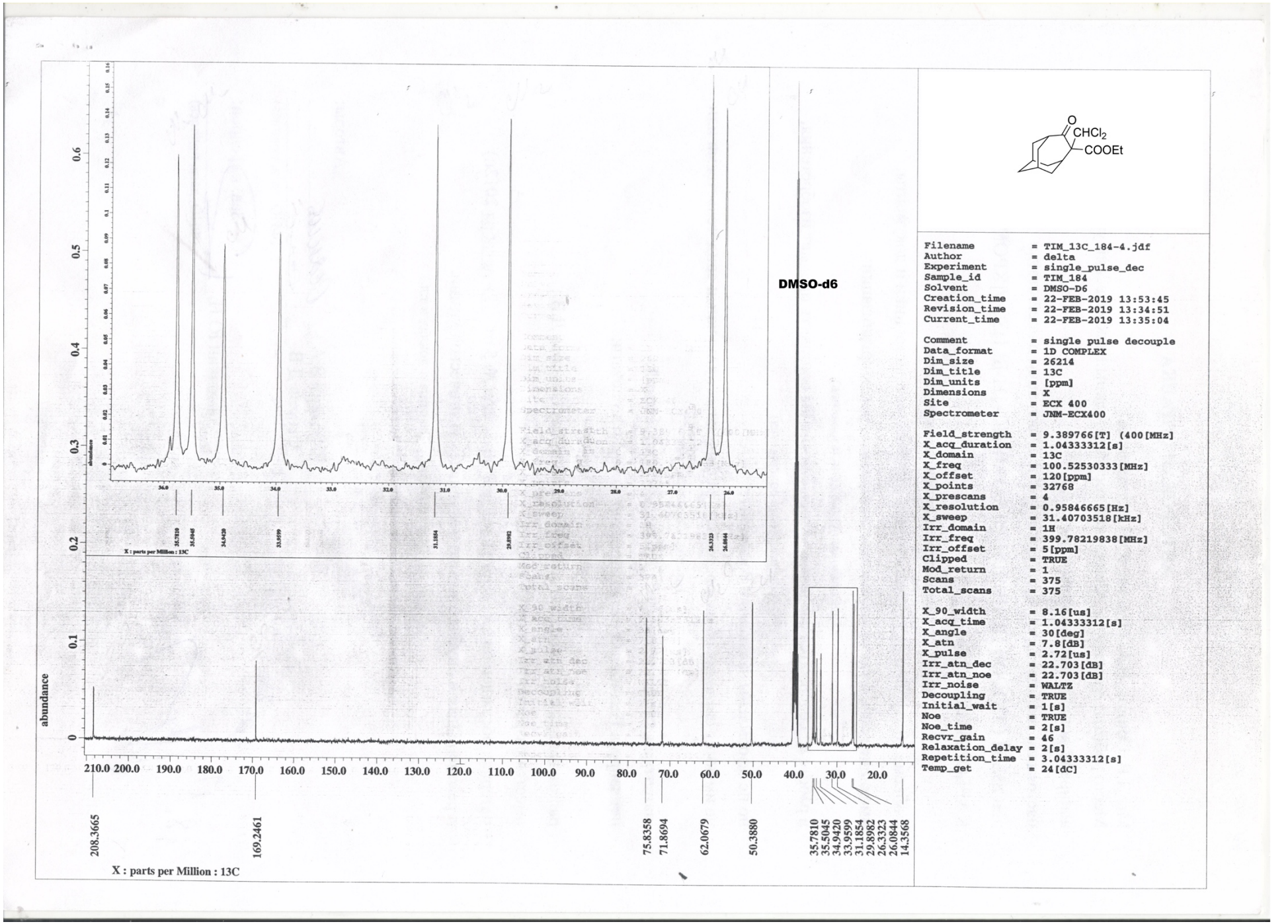
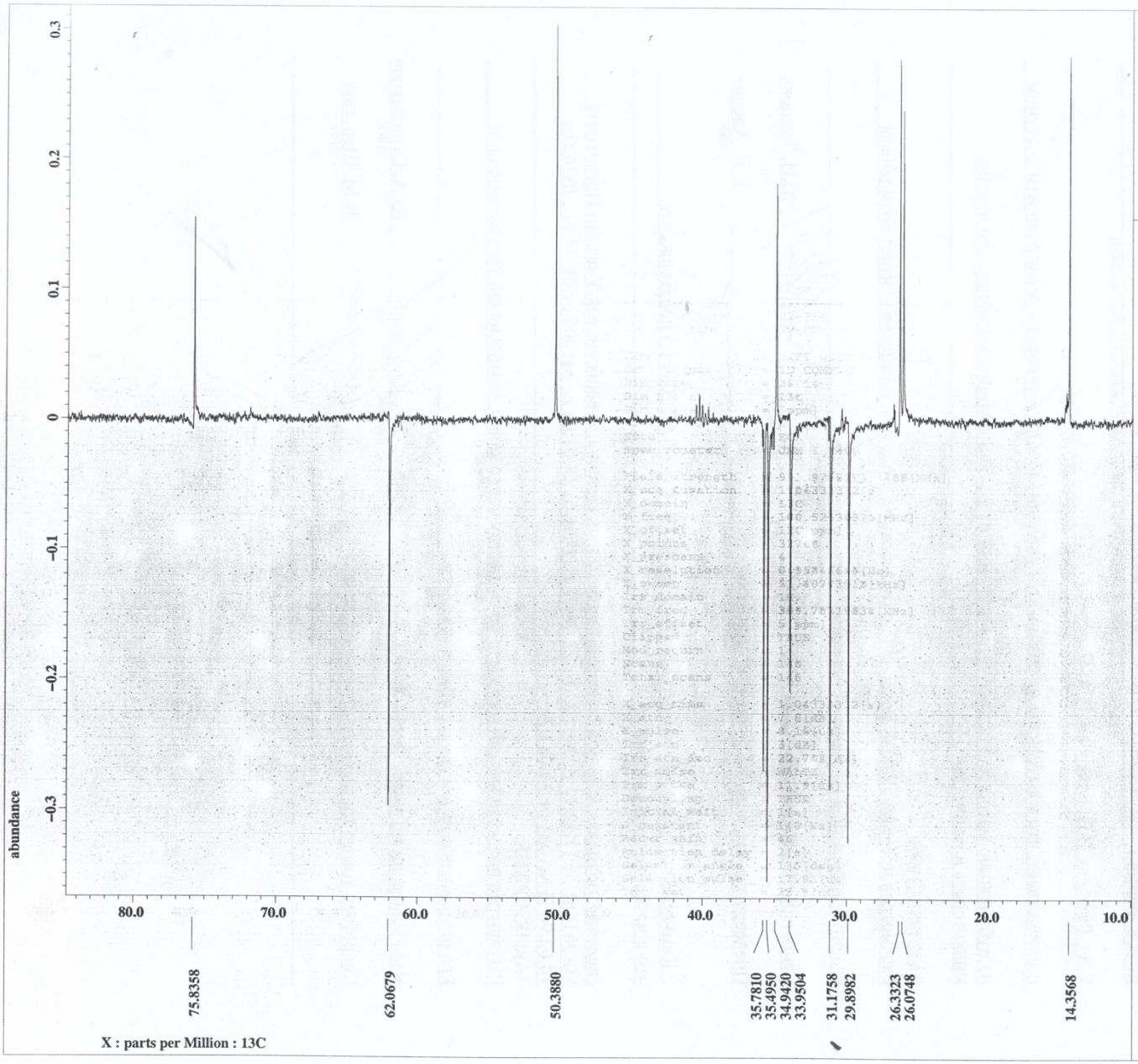
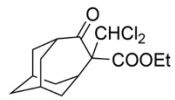


compound 9 ^{13}C NMR





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X_offset	= 120[ppm]
X_points	= 32768
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X_sweep	= 31.40703518[kHz]
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Irr_offset	= 5[ppm]
Clipped	= TRUE
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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
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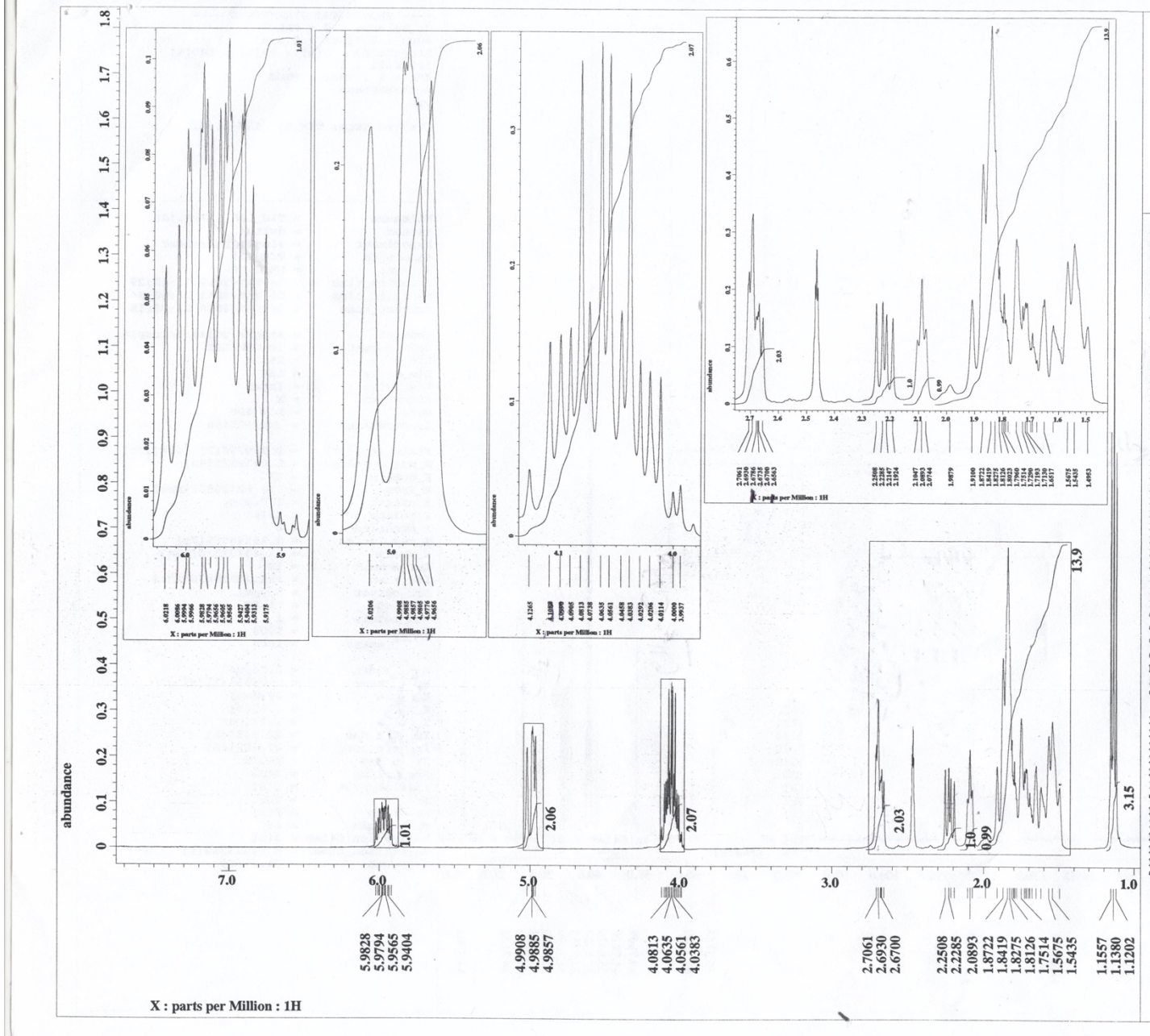
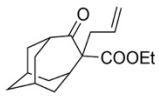
compound 9 DEPT



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Clipped           = FALSE
Mod_return        = 1
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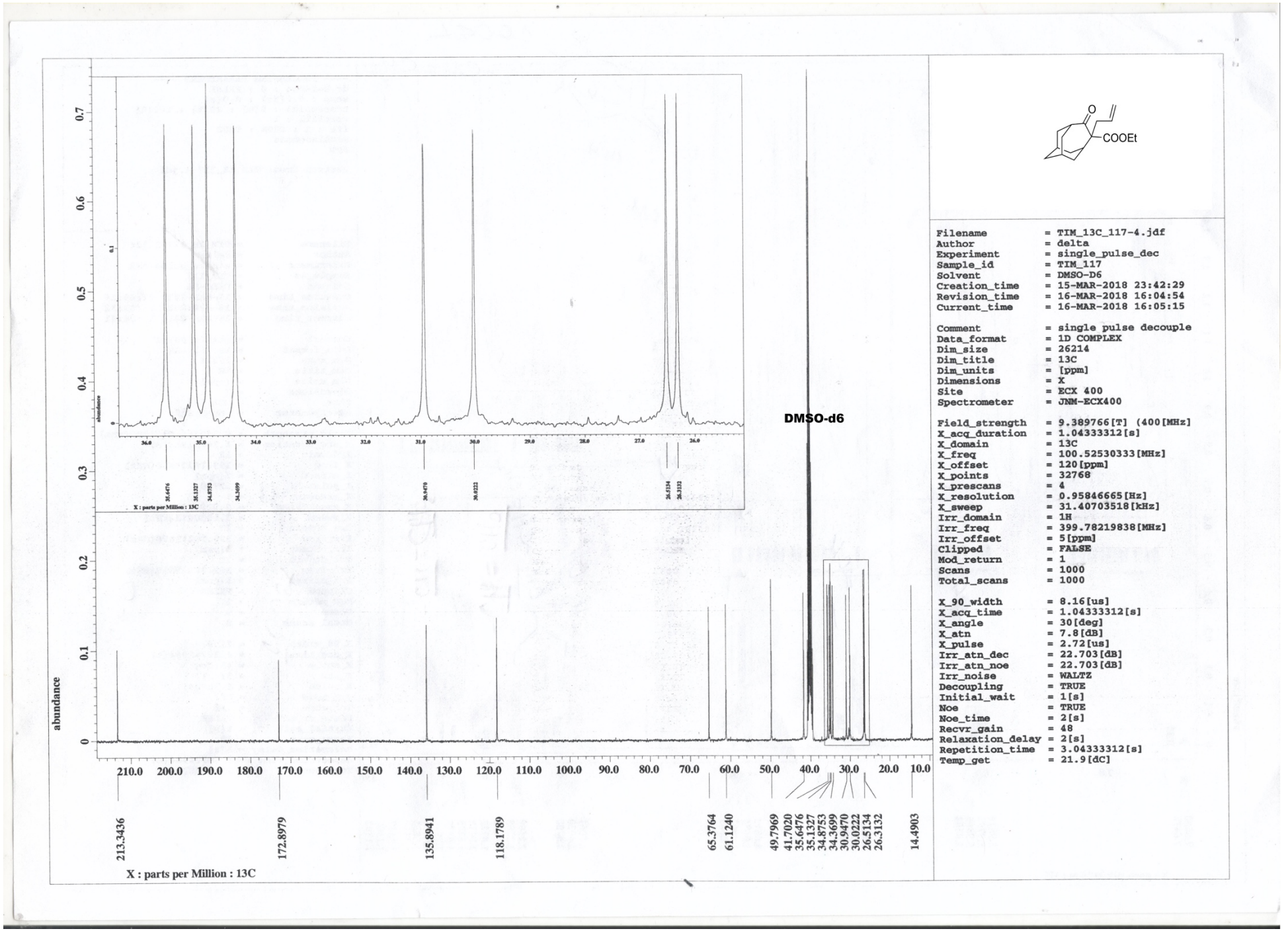
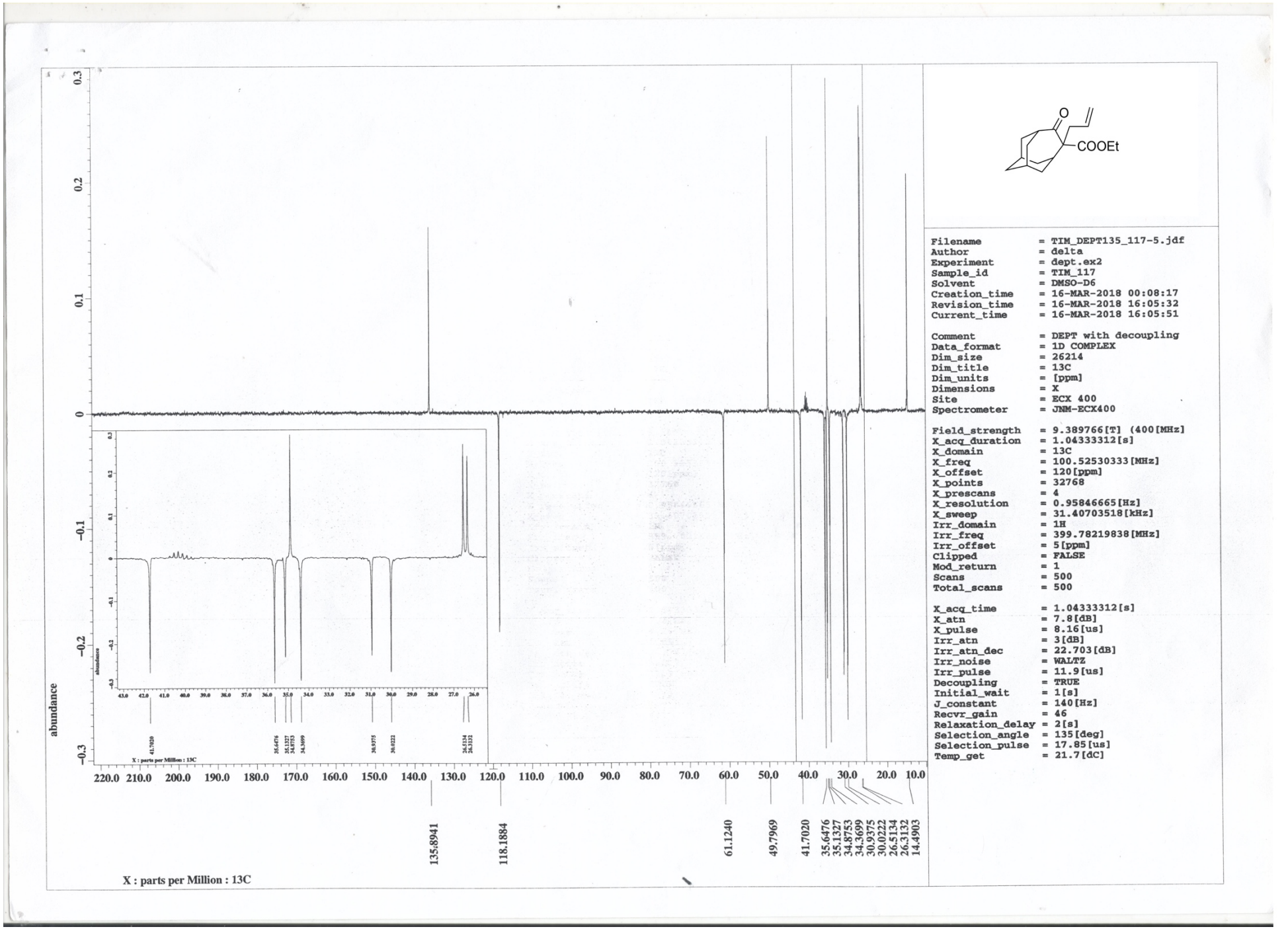
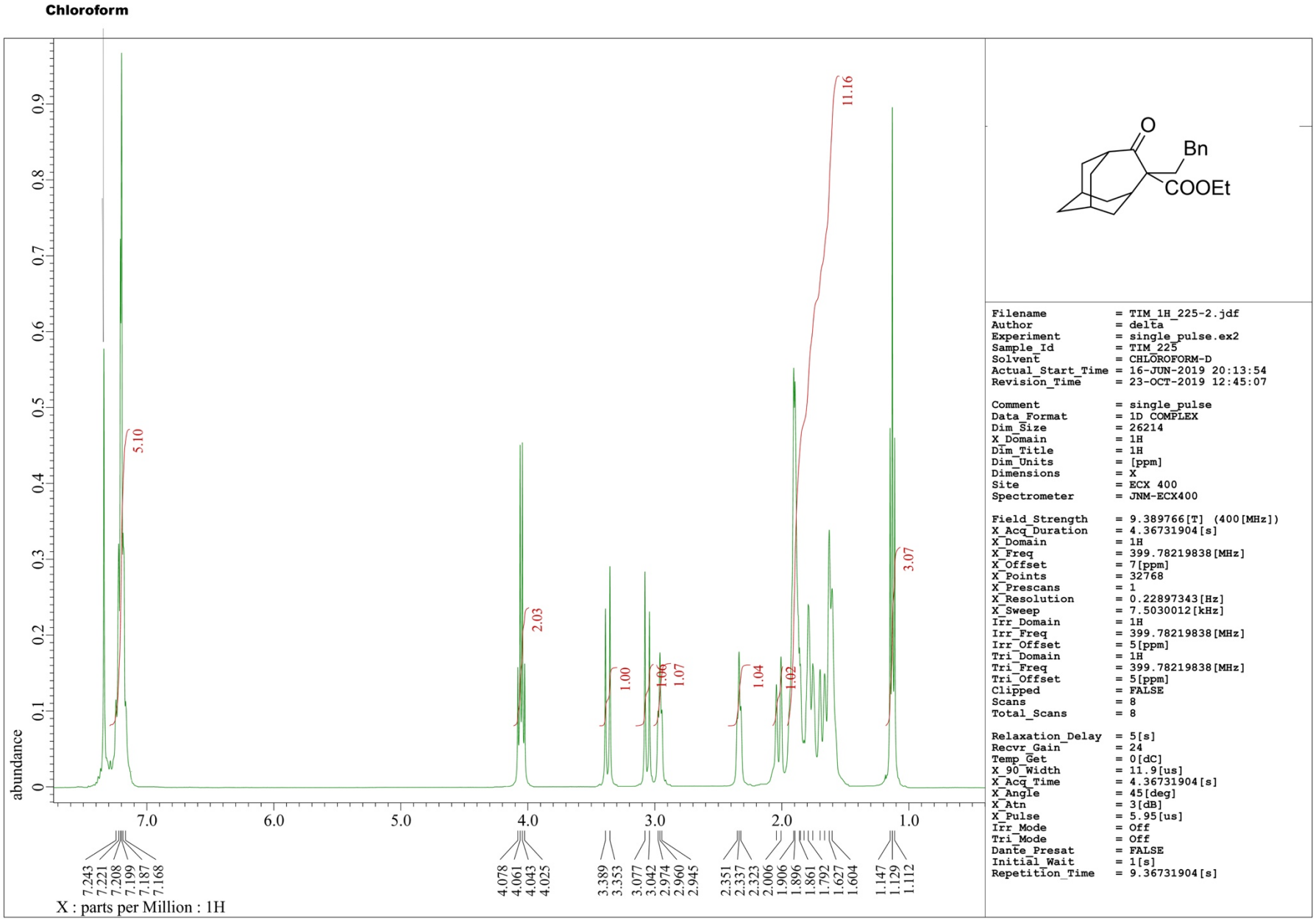
compound 10 ^{1}H NMR



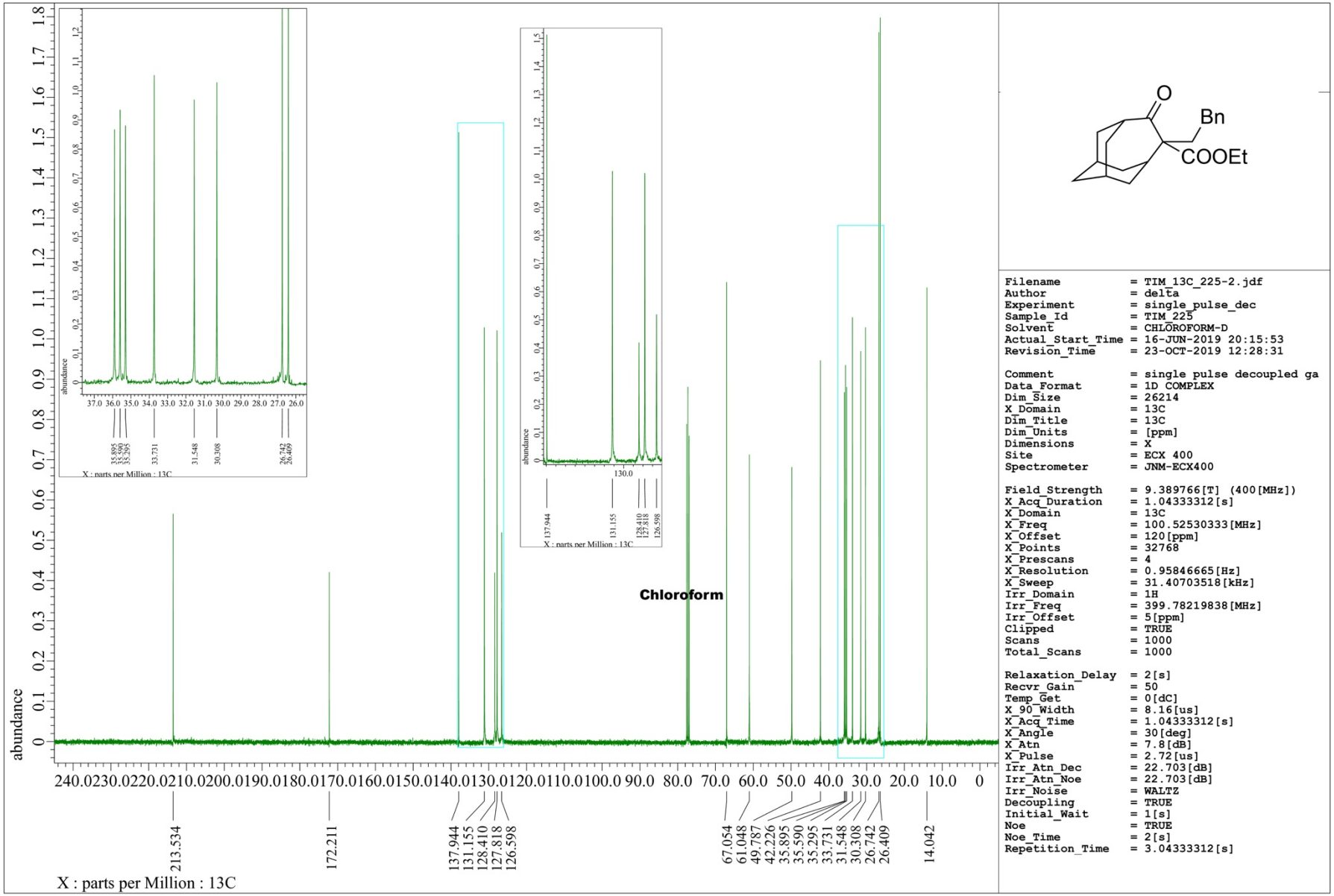
compound 10 ^{13}C NMR



compound 10 DEPT



Compound 11 ^{1}H NMR

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Revision_Time       = 23-OCT-2019 12:28:31

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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             = TRUE
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Total_Scans         = 1000

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 0[dC]
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
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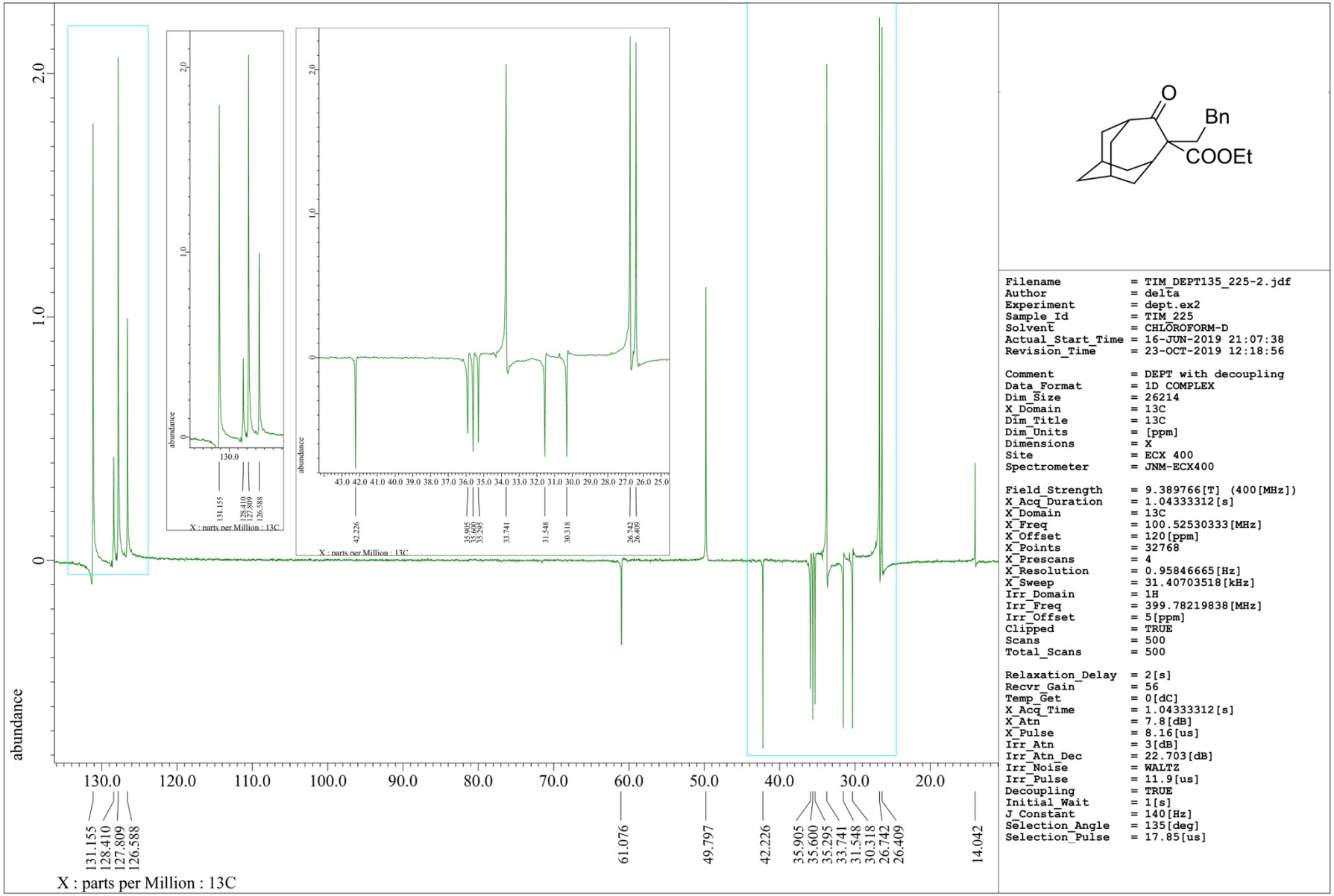
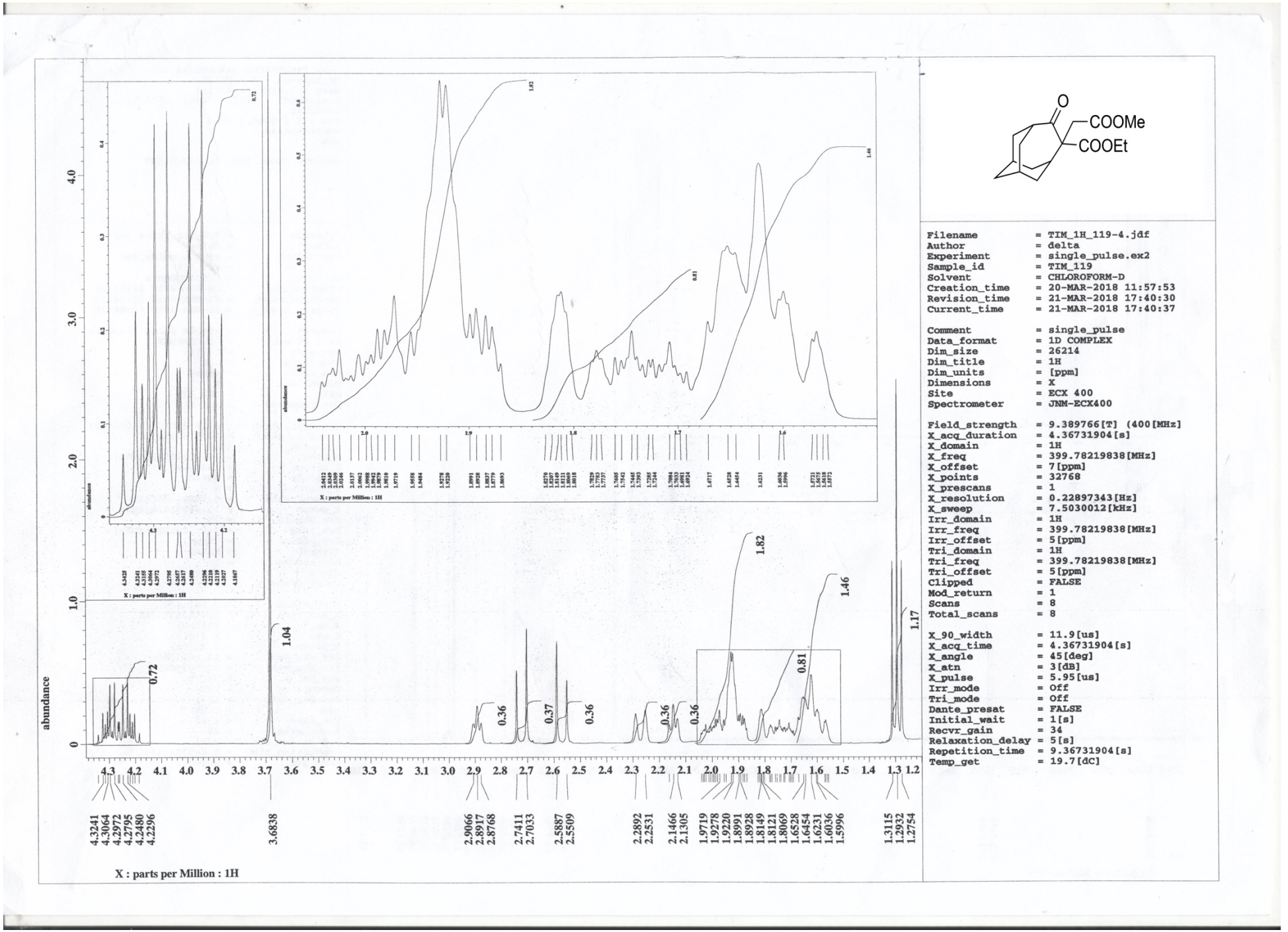
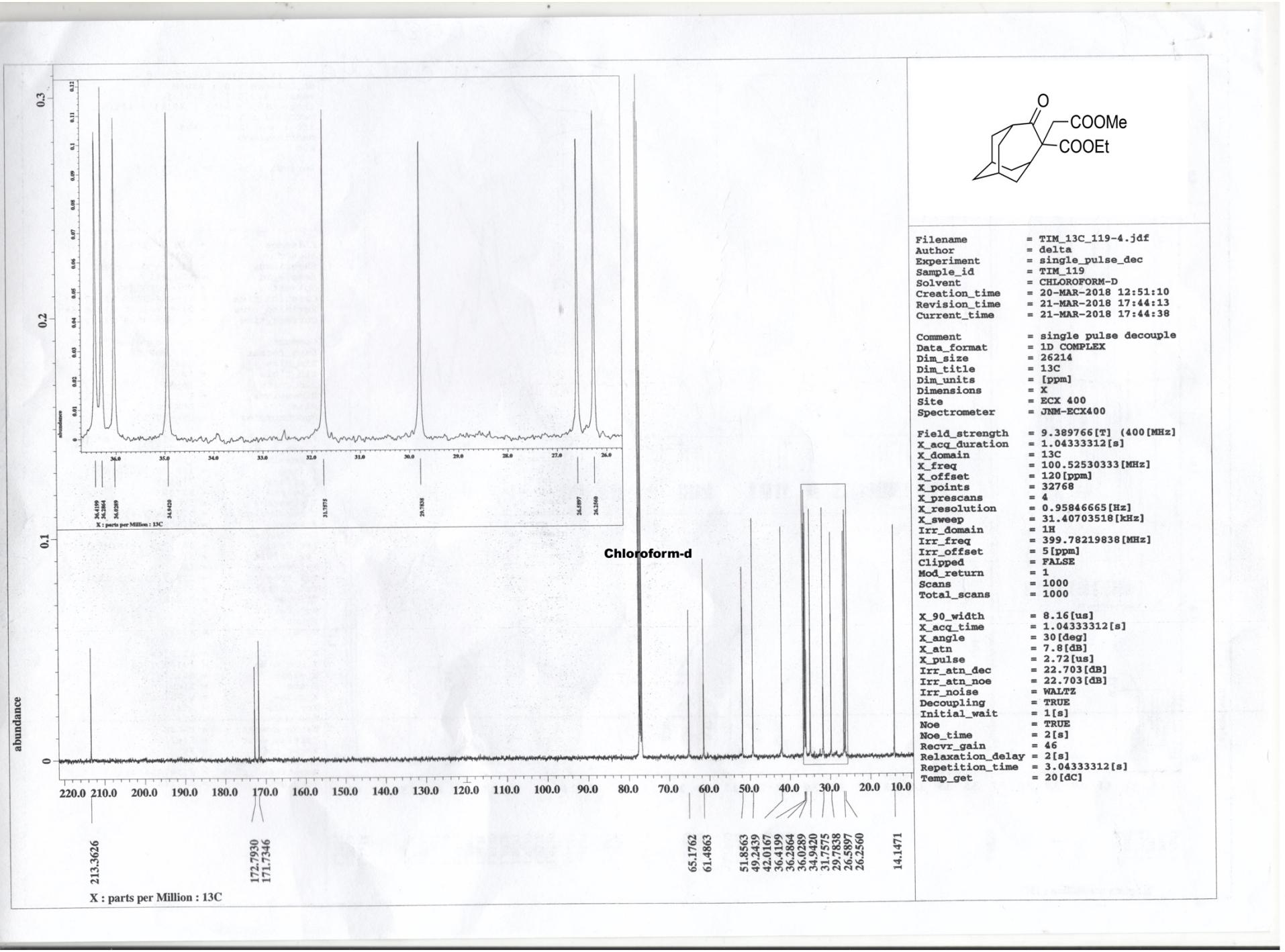
Compound 11 ^{13}C NMR



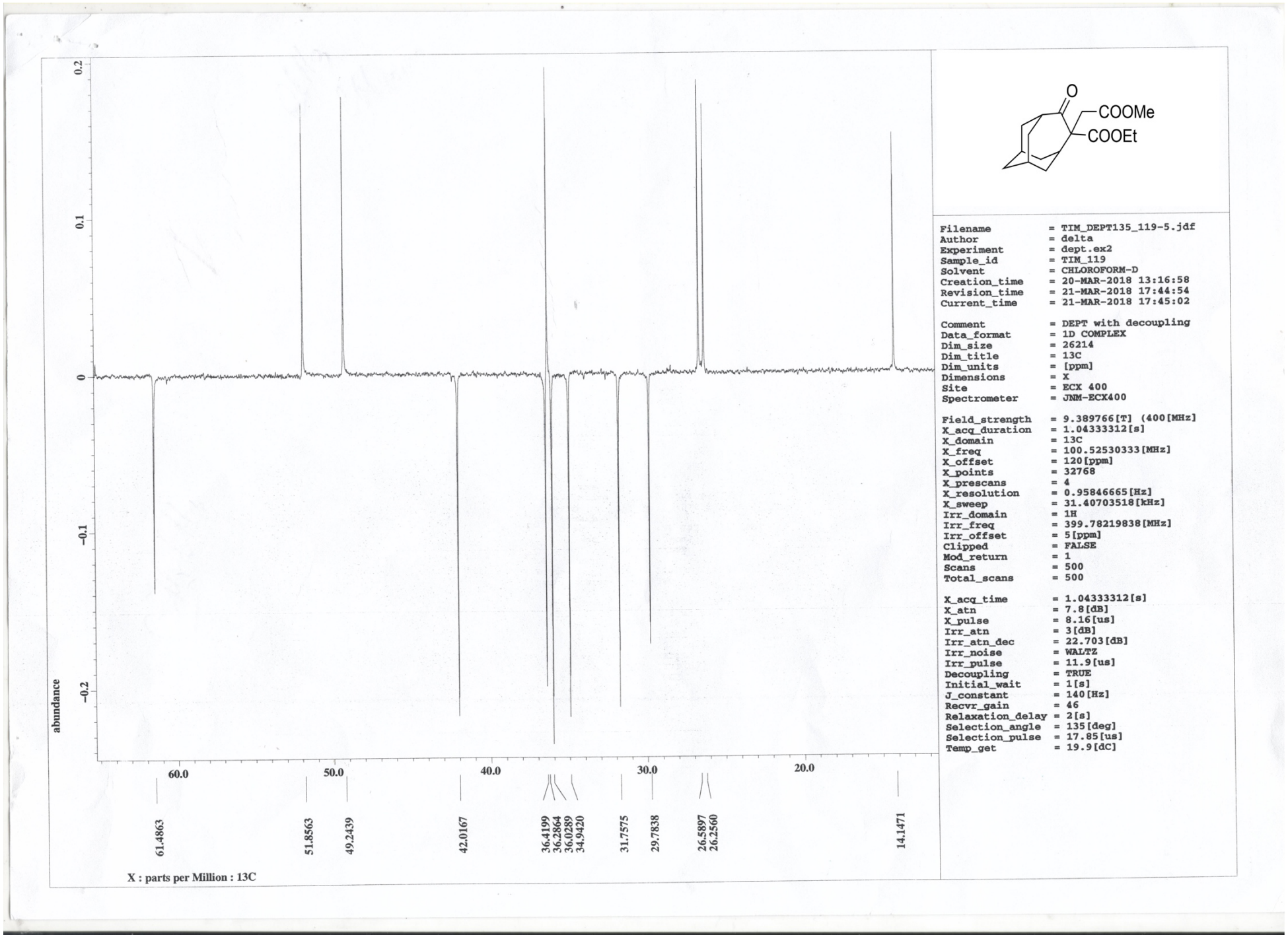
Compound 11 DEPT



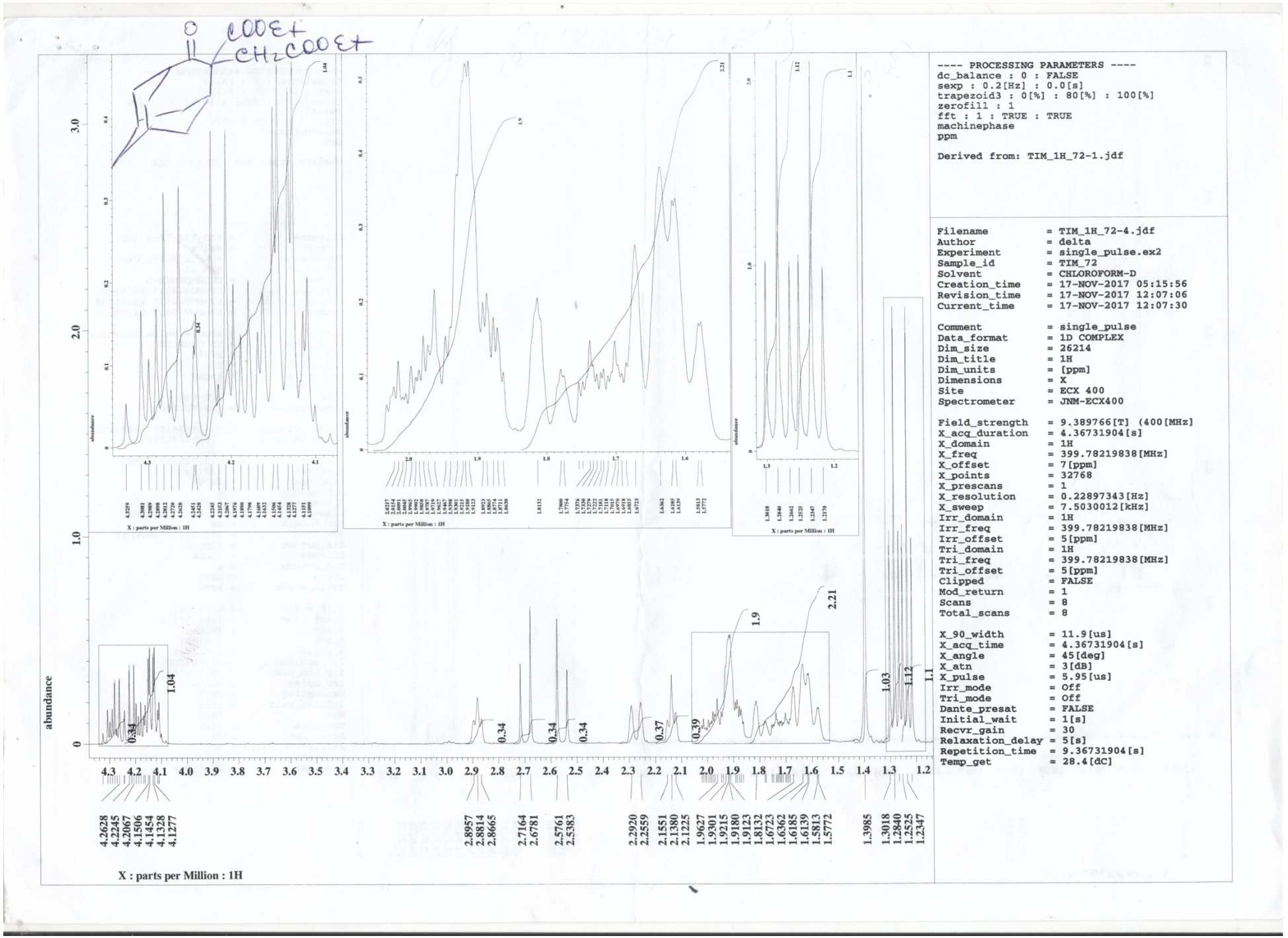
compound 12 ^{1}H NMR



compound 12 ^{13}C NMR



compound 12 DEPT



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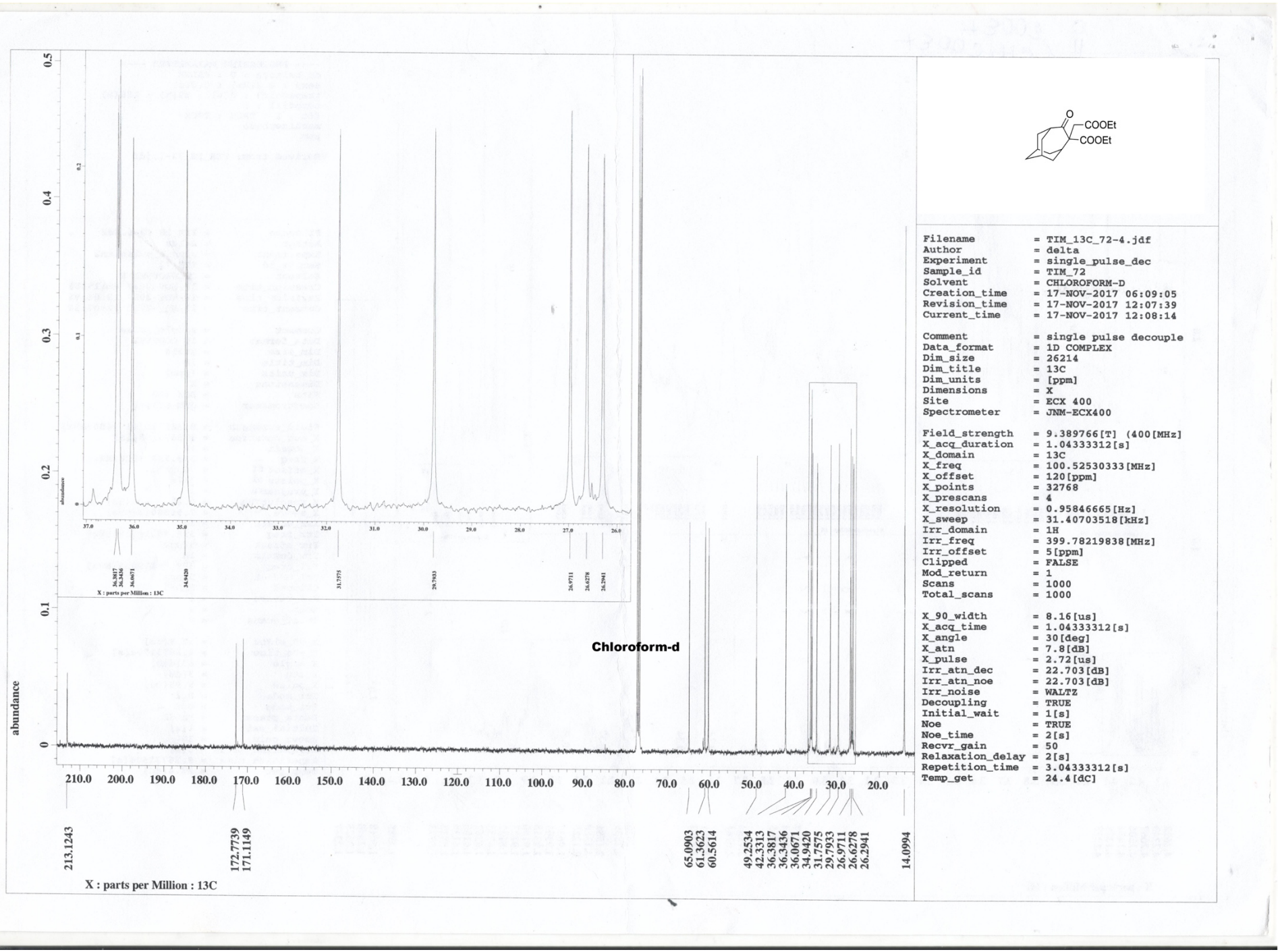
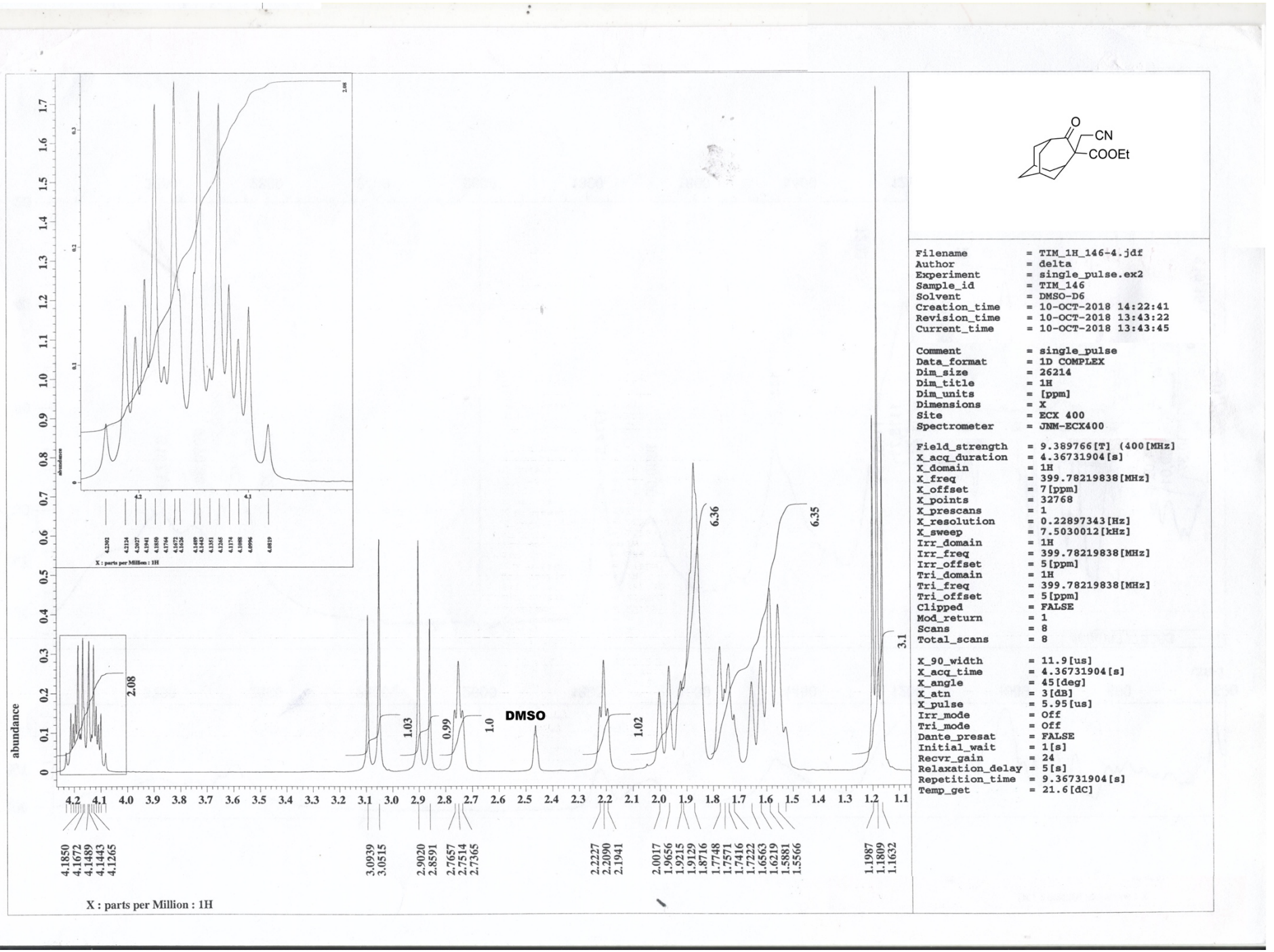
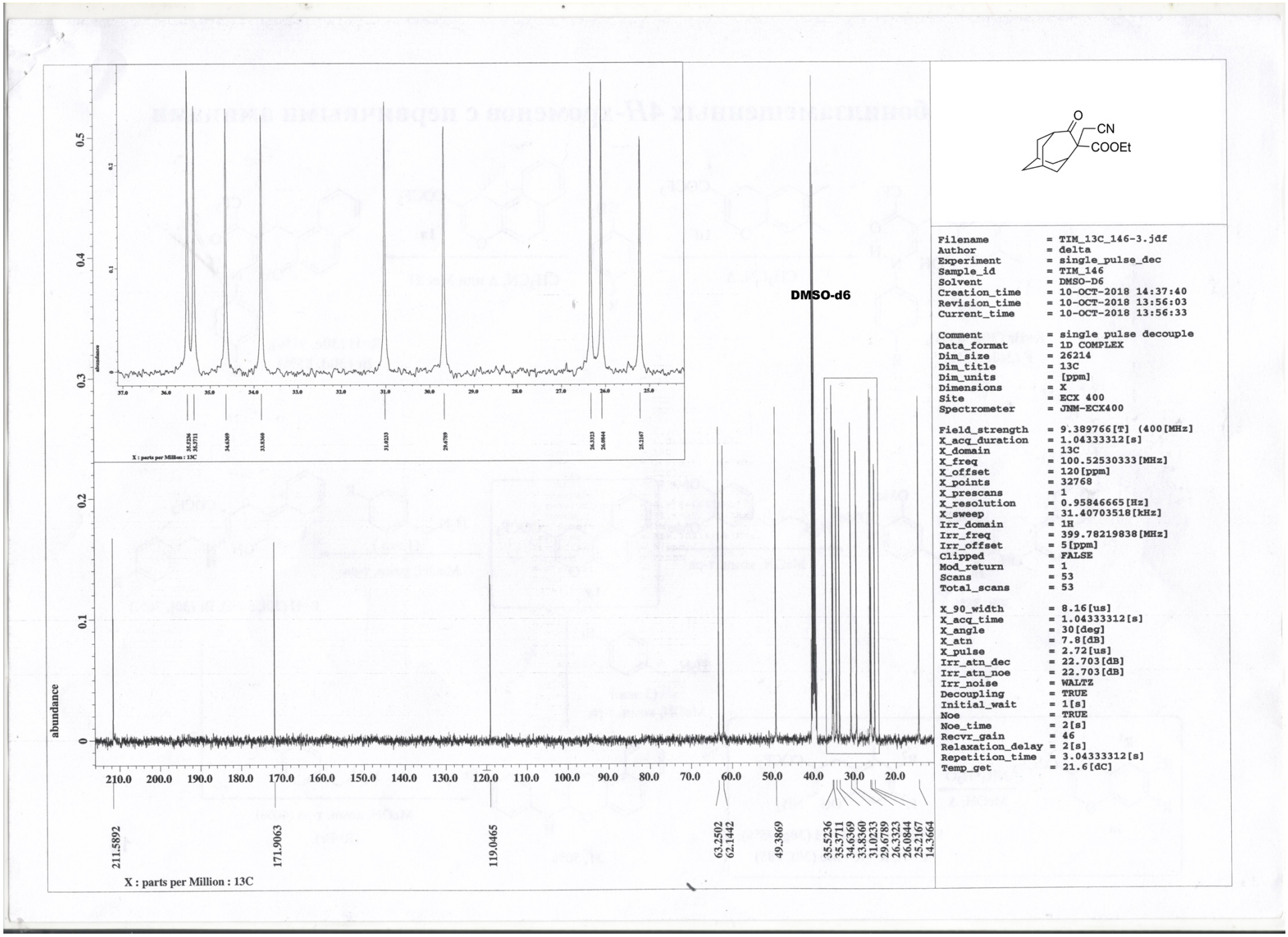


compound 13 ^{13}C NMR

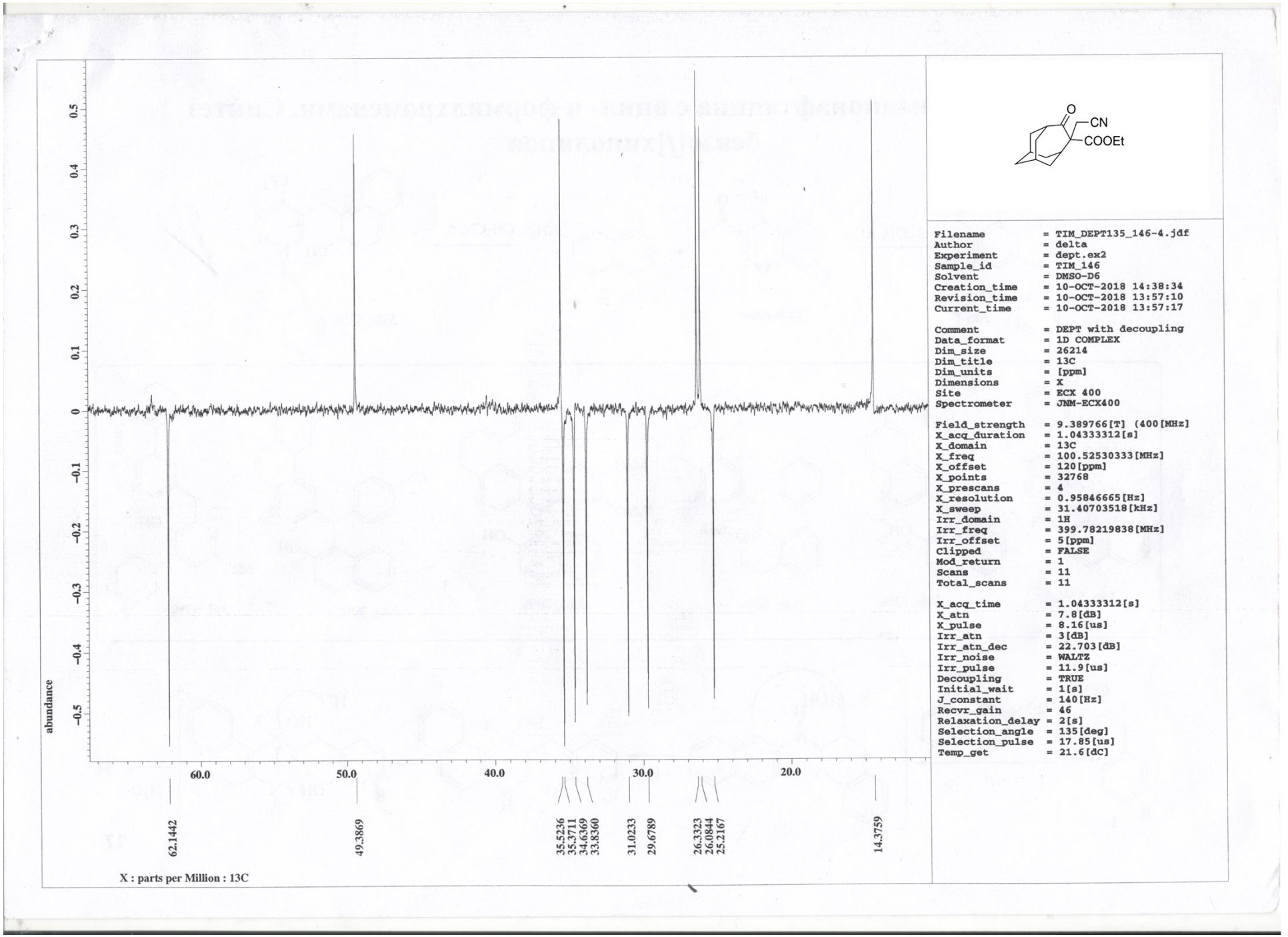
compound 13 DEPT



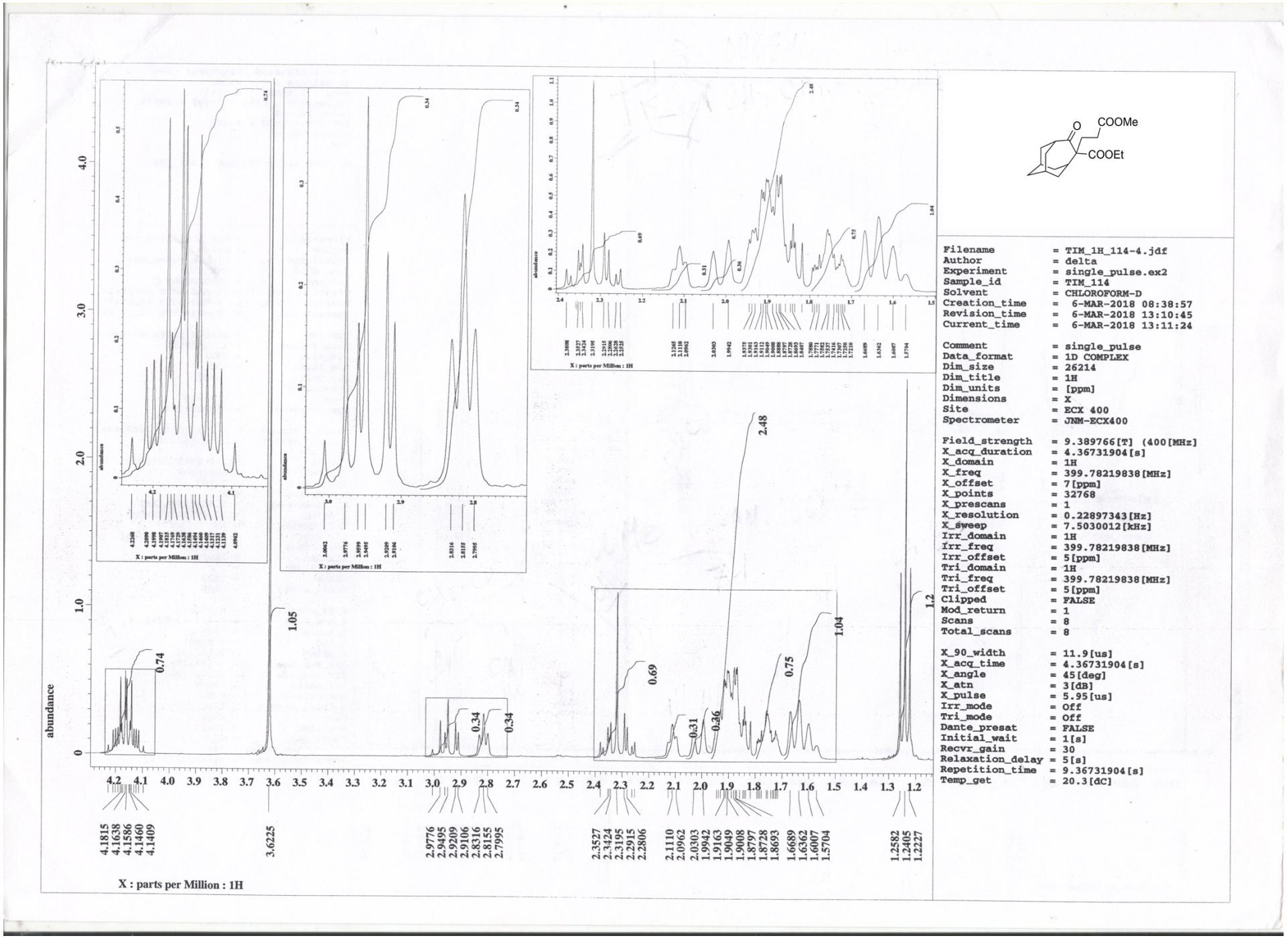
compound 14 ^{1}H NMR



compound 14 ^{13}C NMR



compound 14 DEPT



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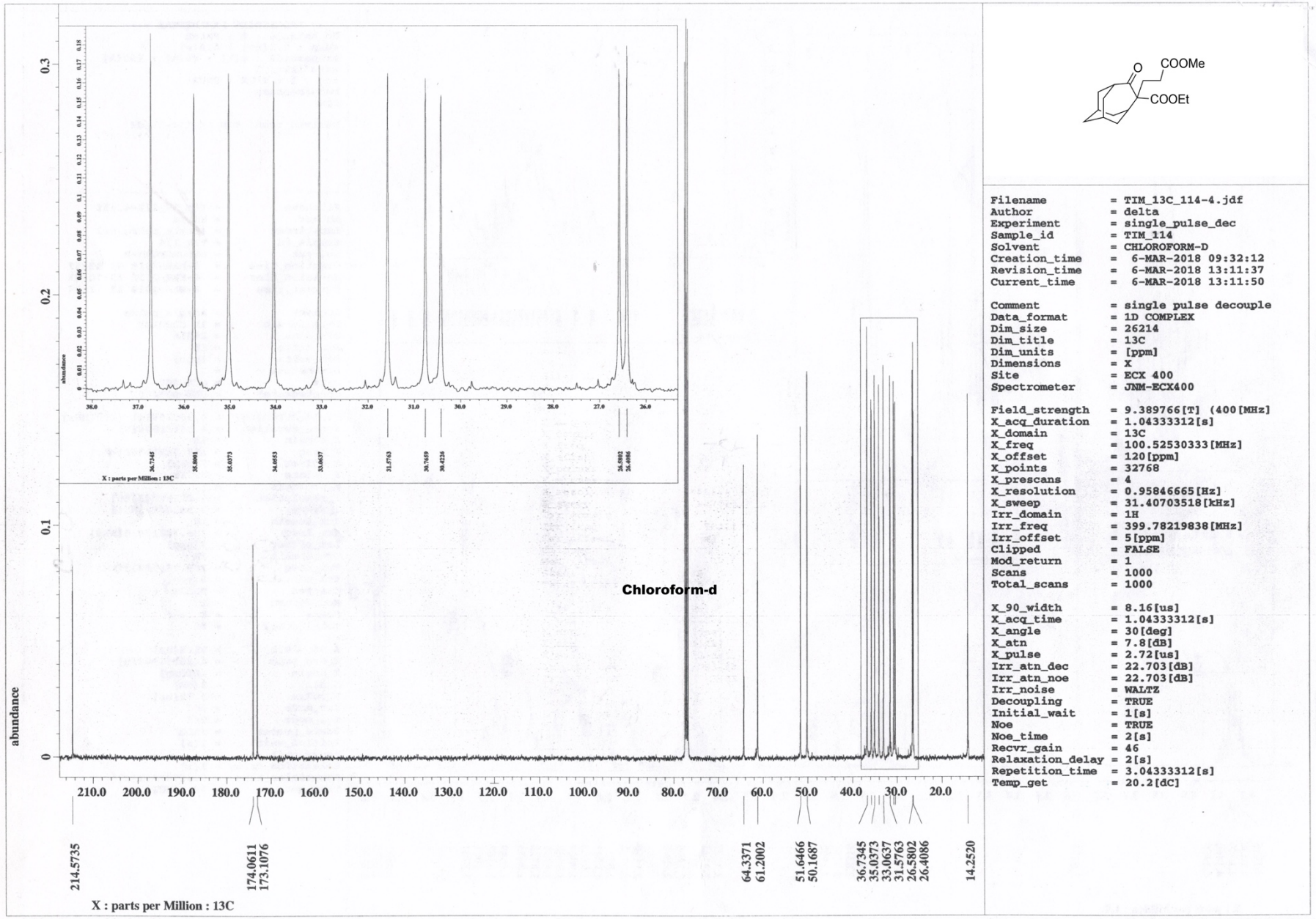

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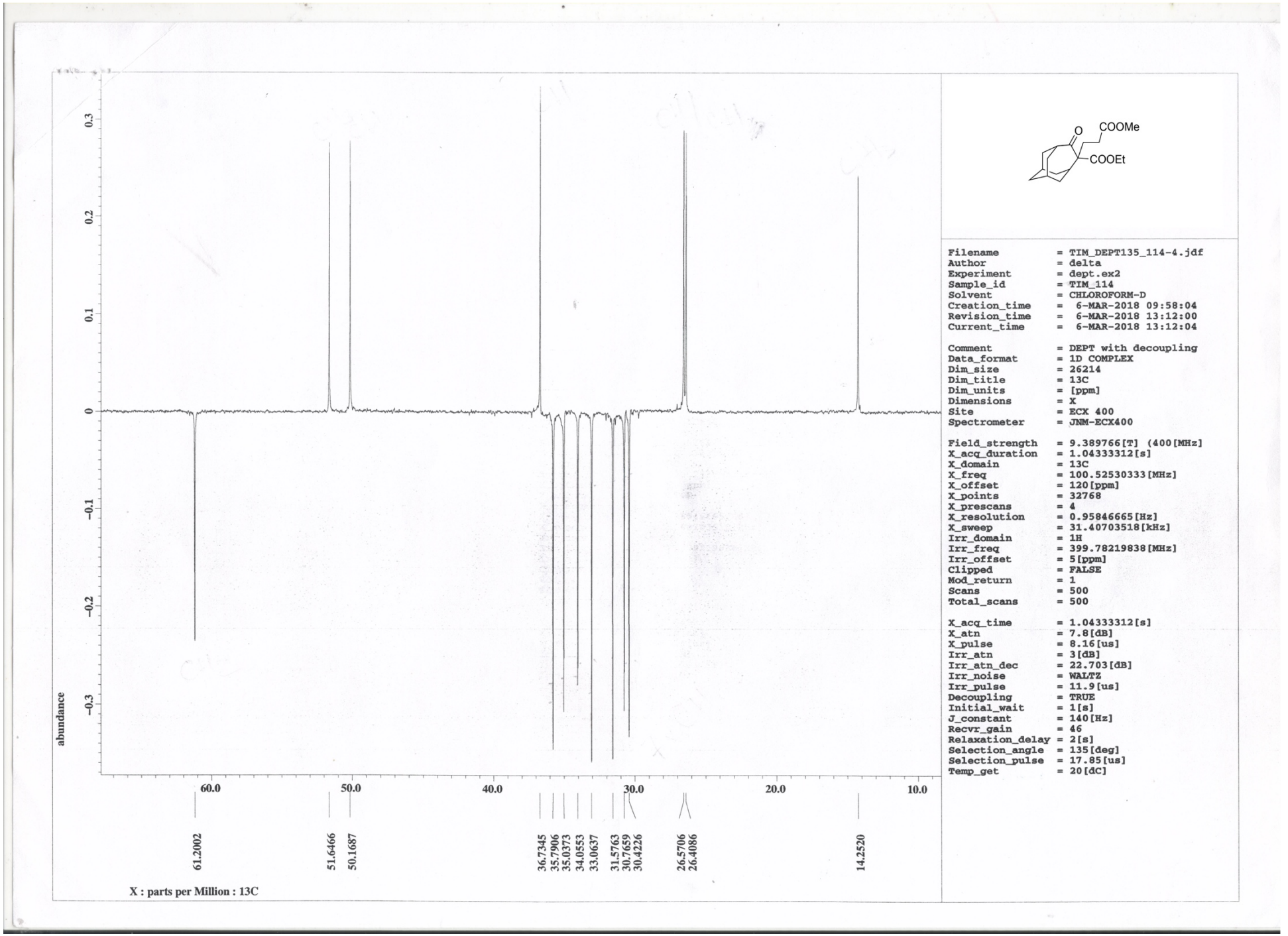

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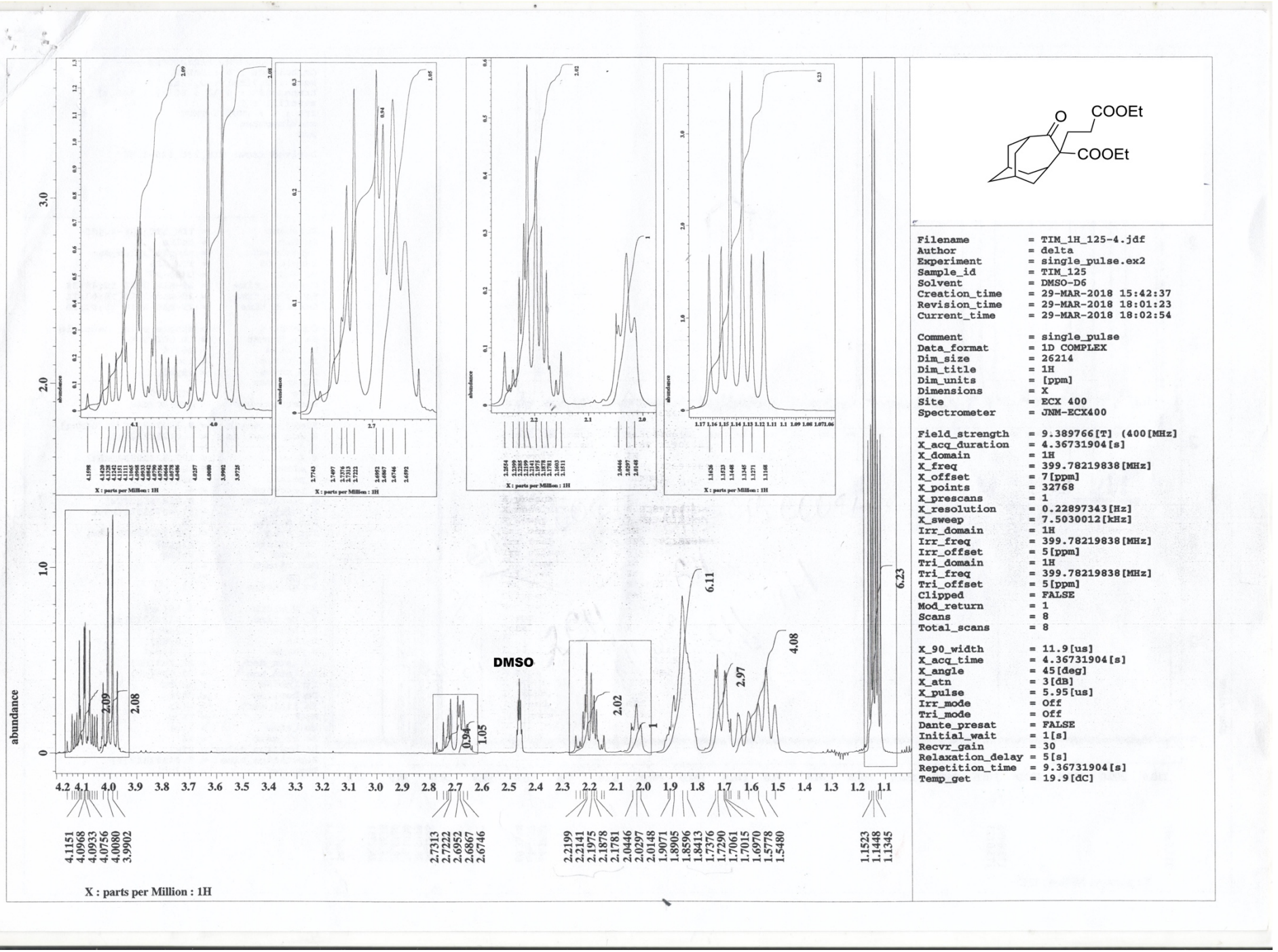

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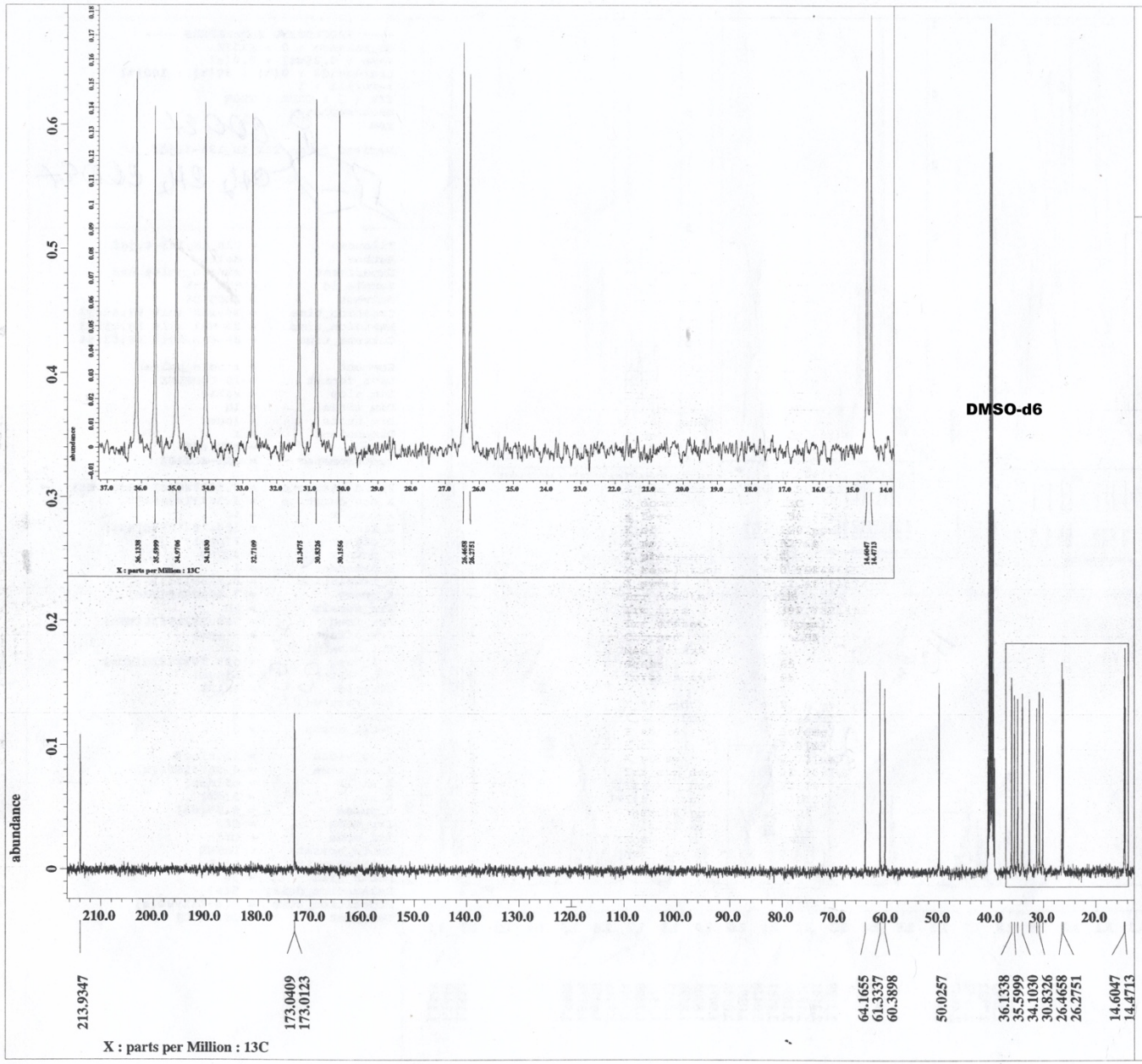

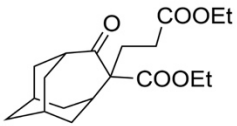


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X_sweep           = 31.40703518[kHz]
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X_pulse           = 2.72[us]
Irr_atn_dec       = 22.703[dB]
Irr_atn_noe       = 22.703[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
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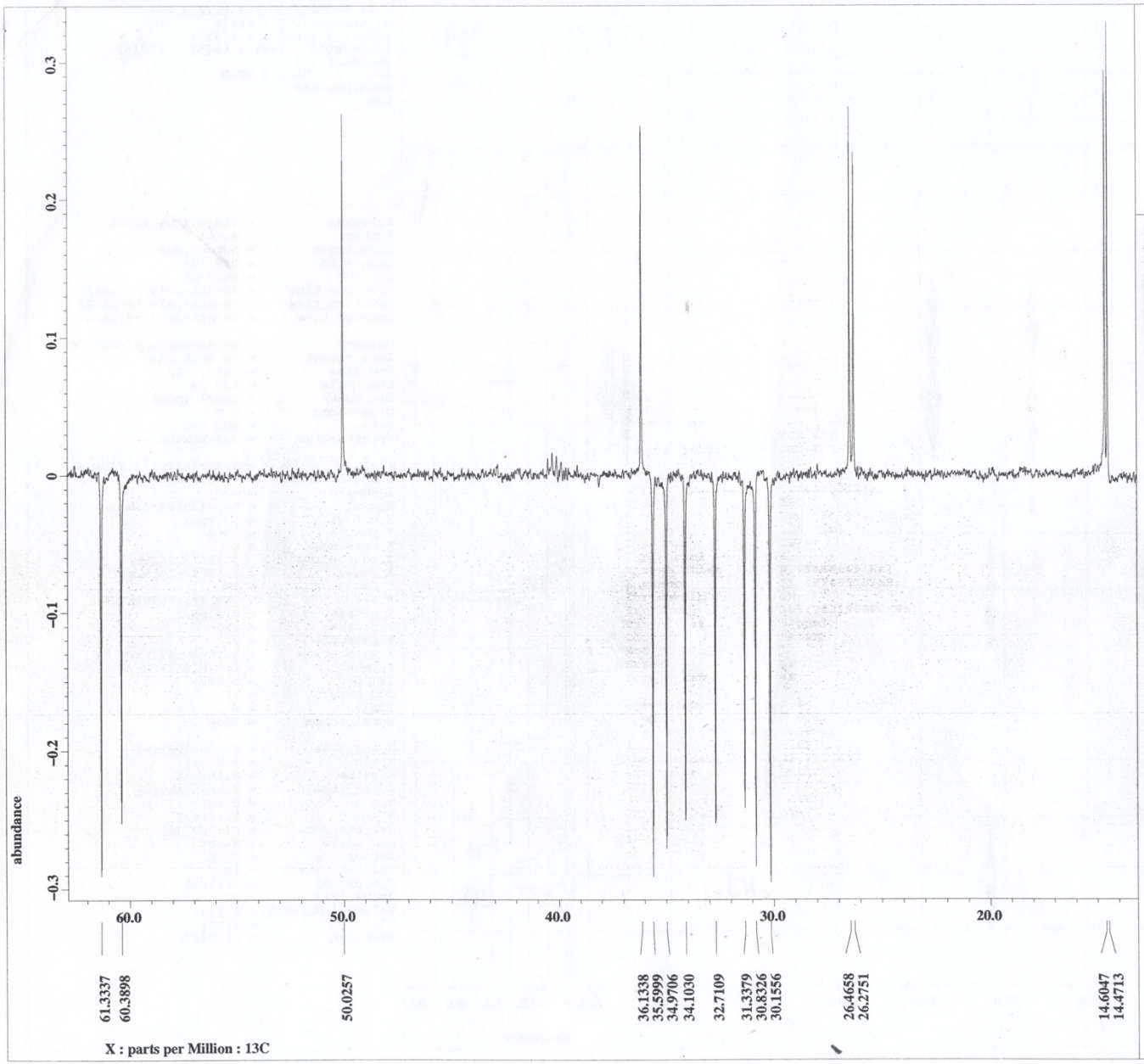
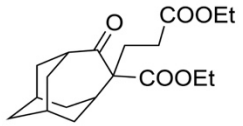
compound 16 ^{13}C NMR



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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

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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
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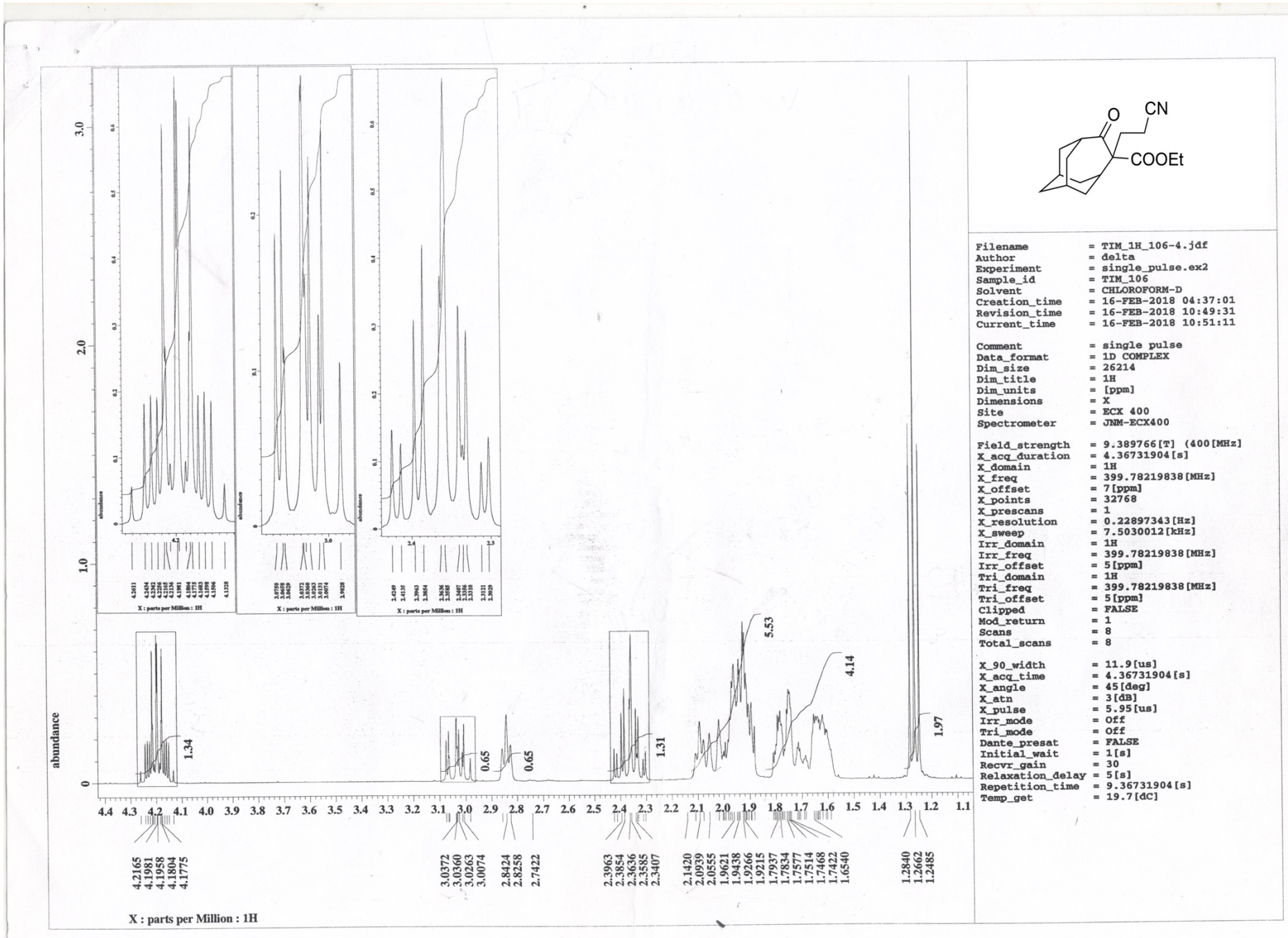
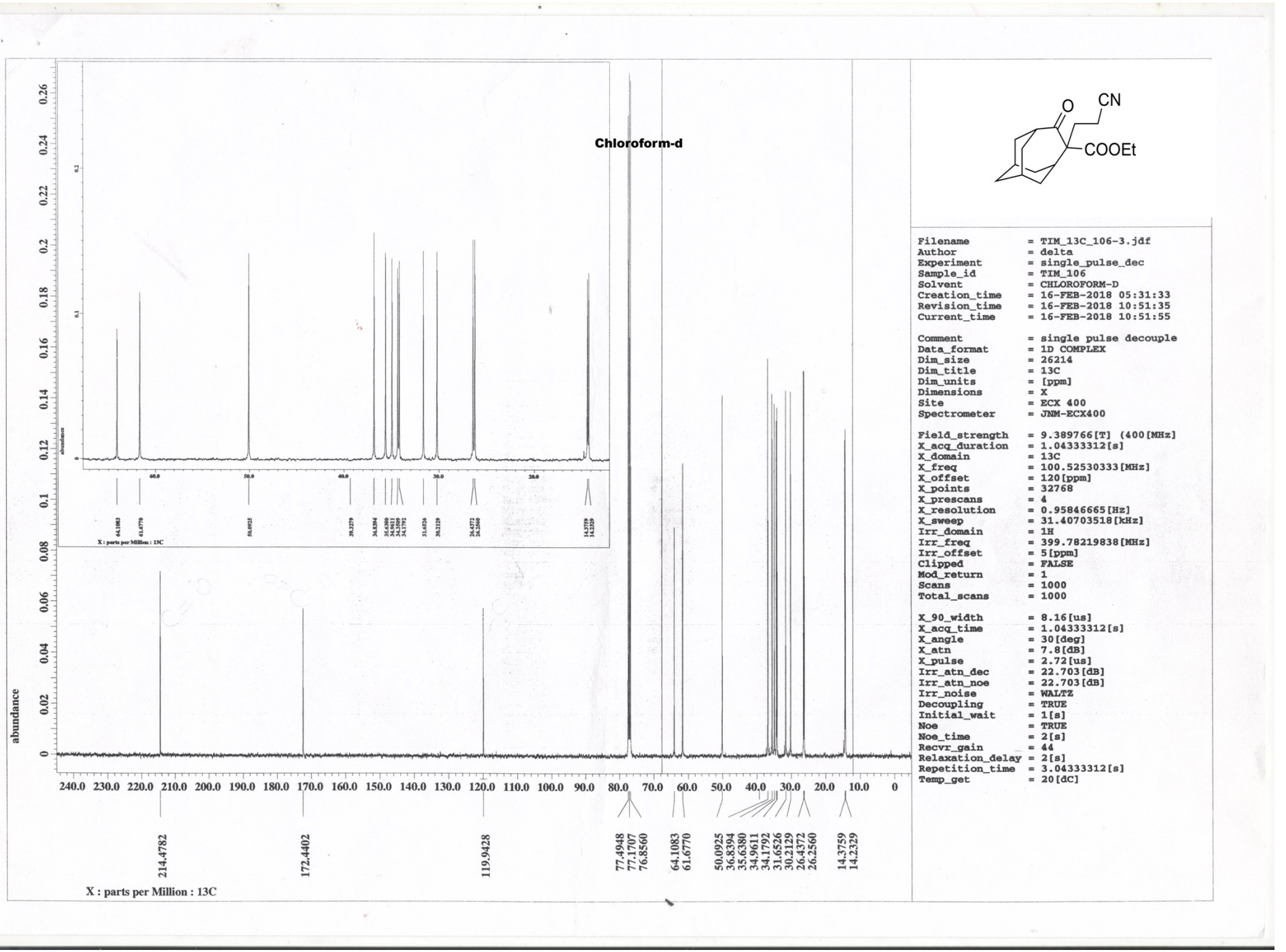
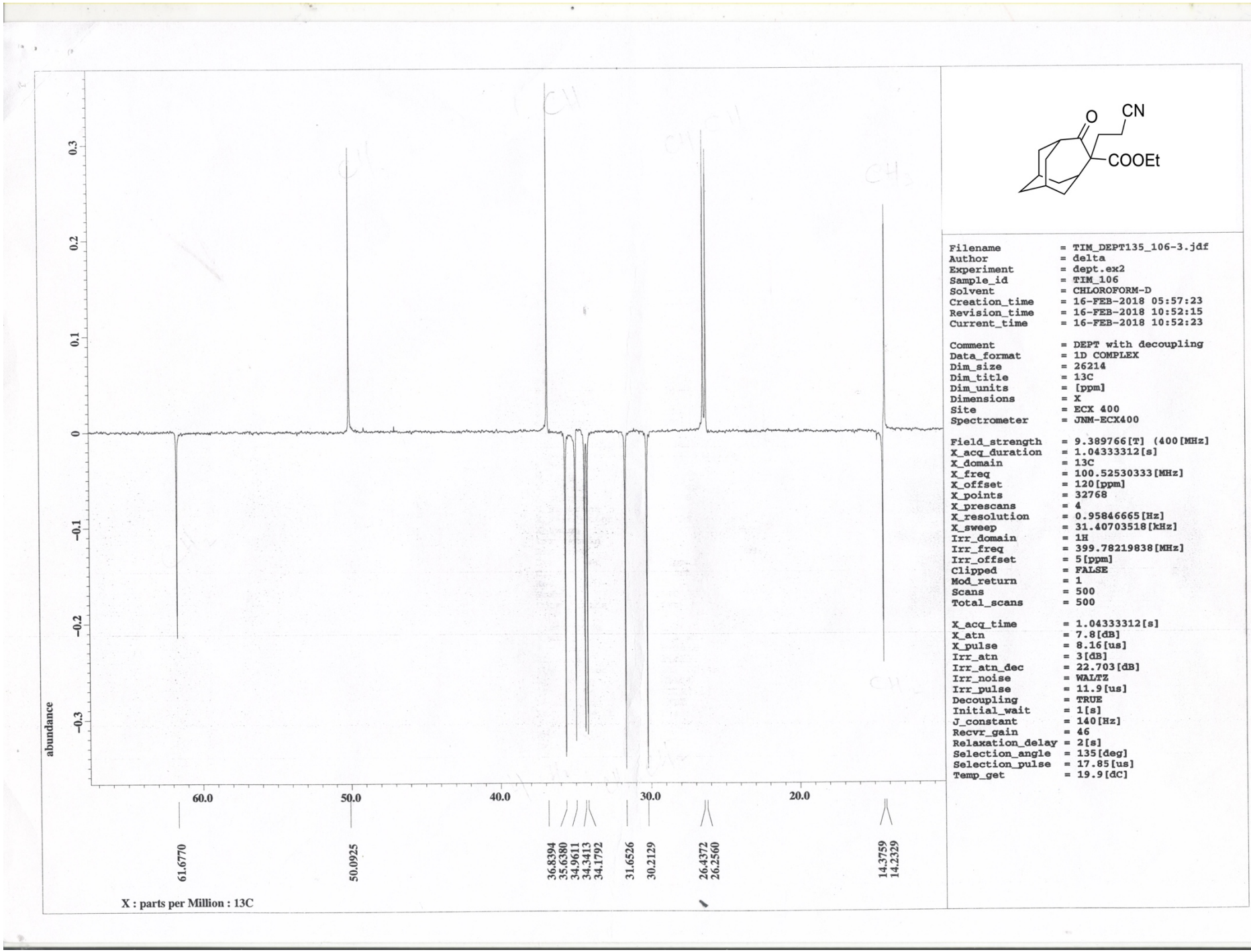
compound 16 DEPT



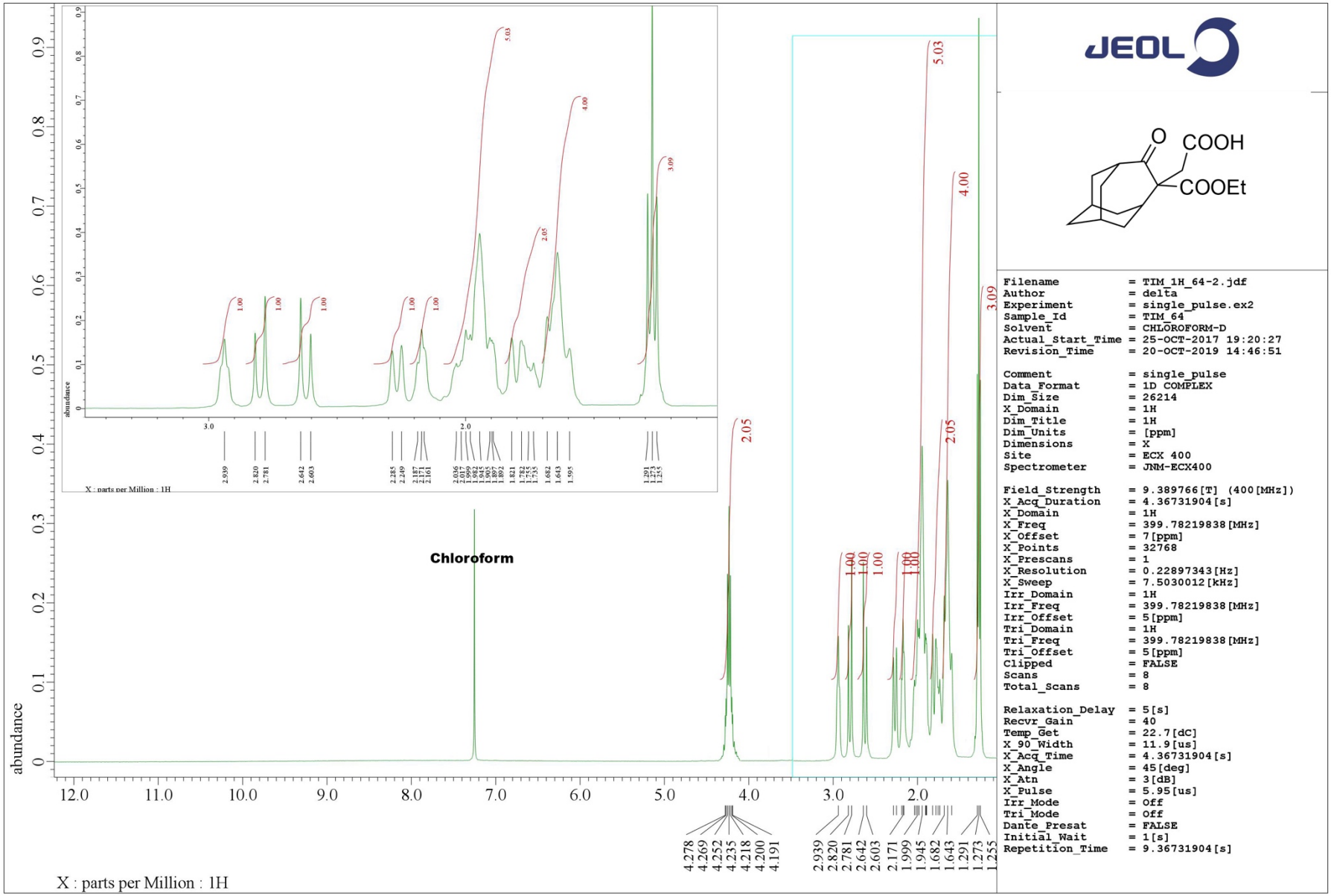
compound 17 ^{1}H NMR



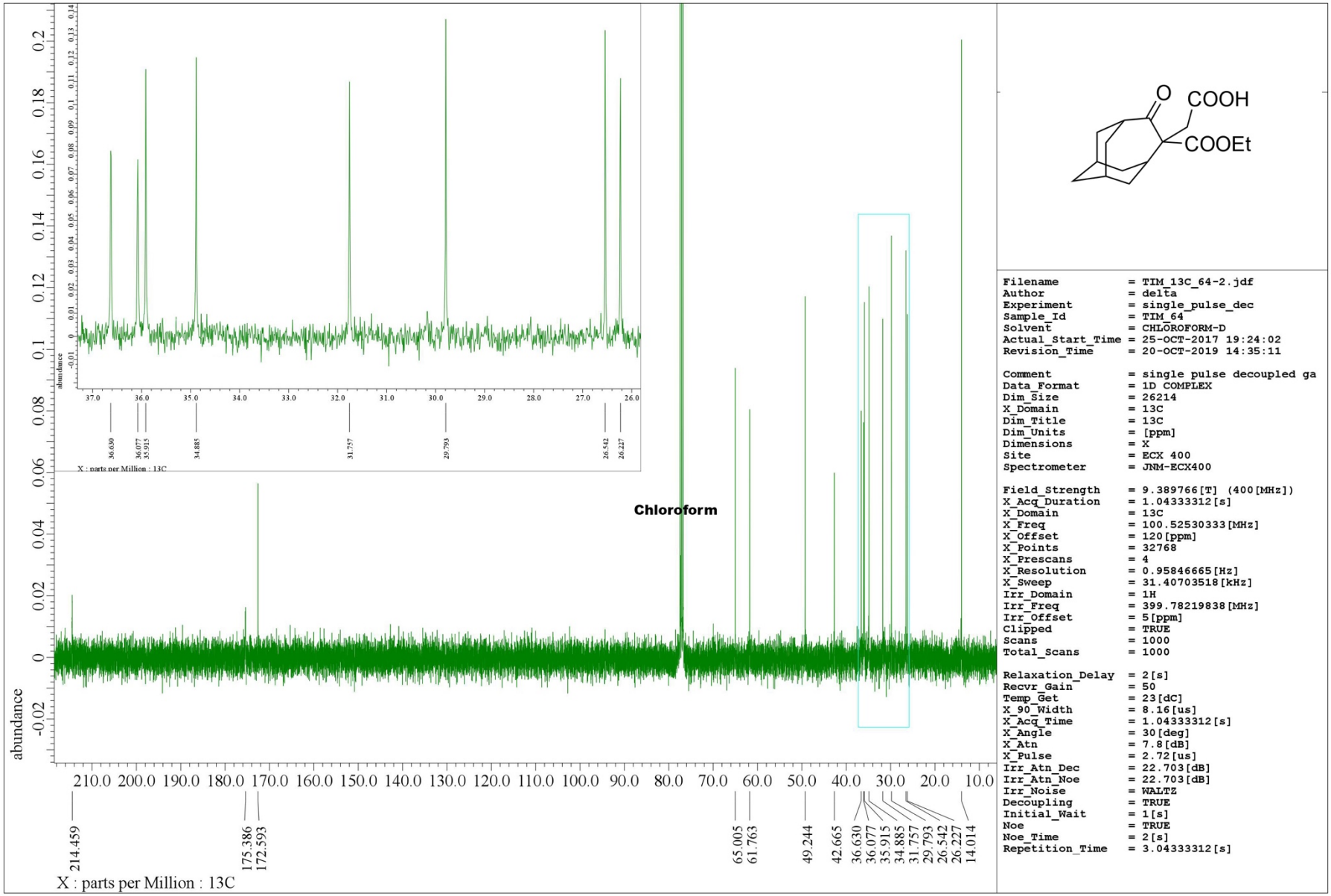
compound 17 ^{13}C NMR



compound 17 DEPT



Compound 18 ^{1}H NMR



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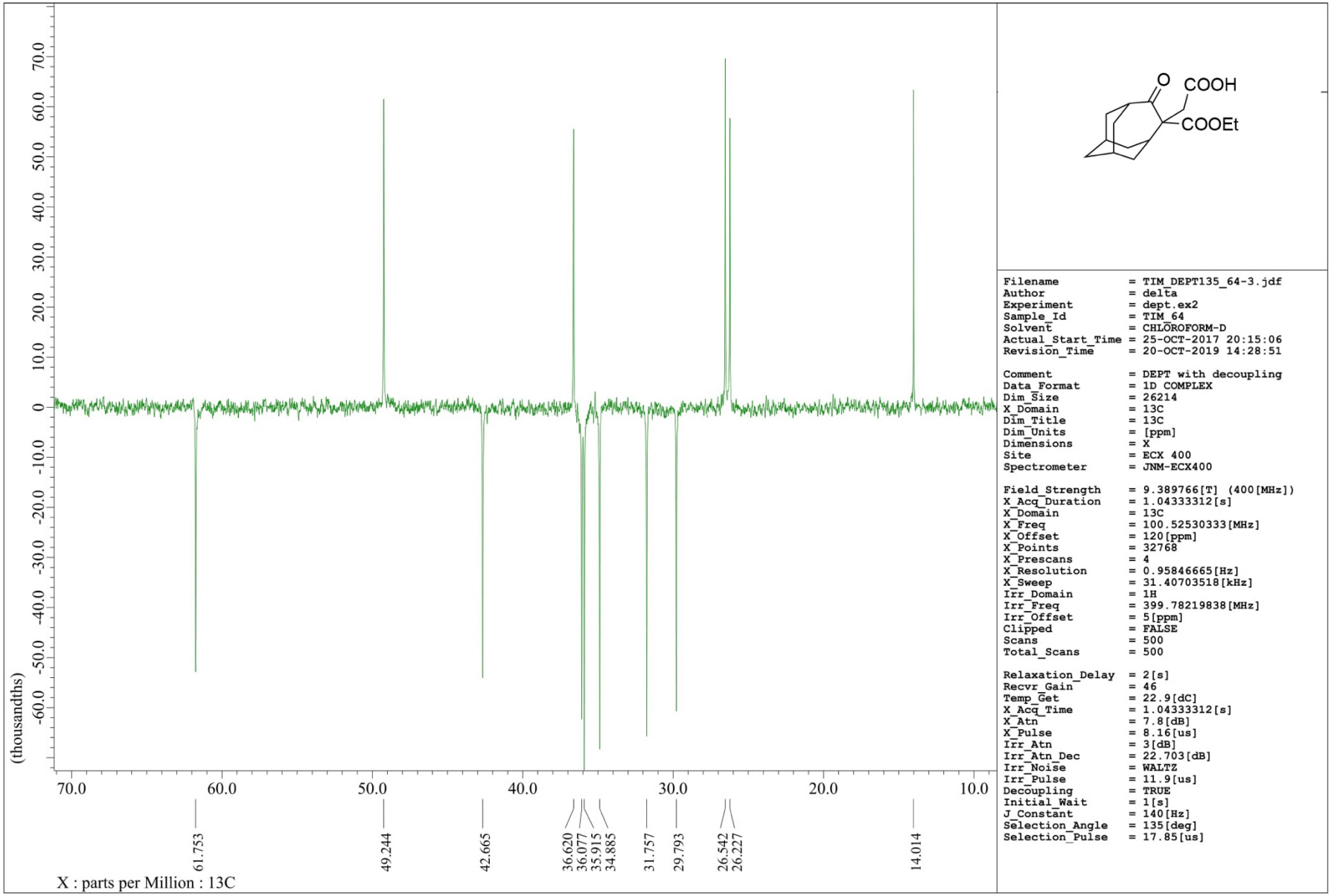
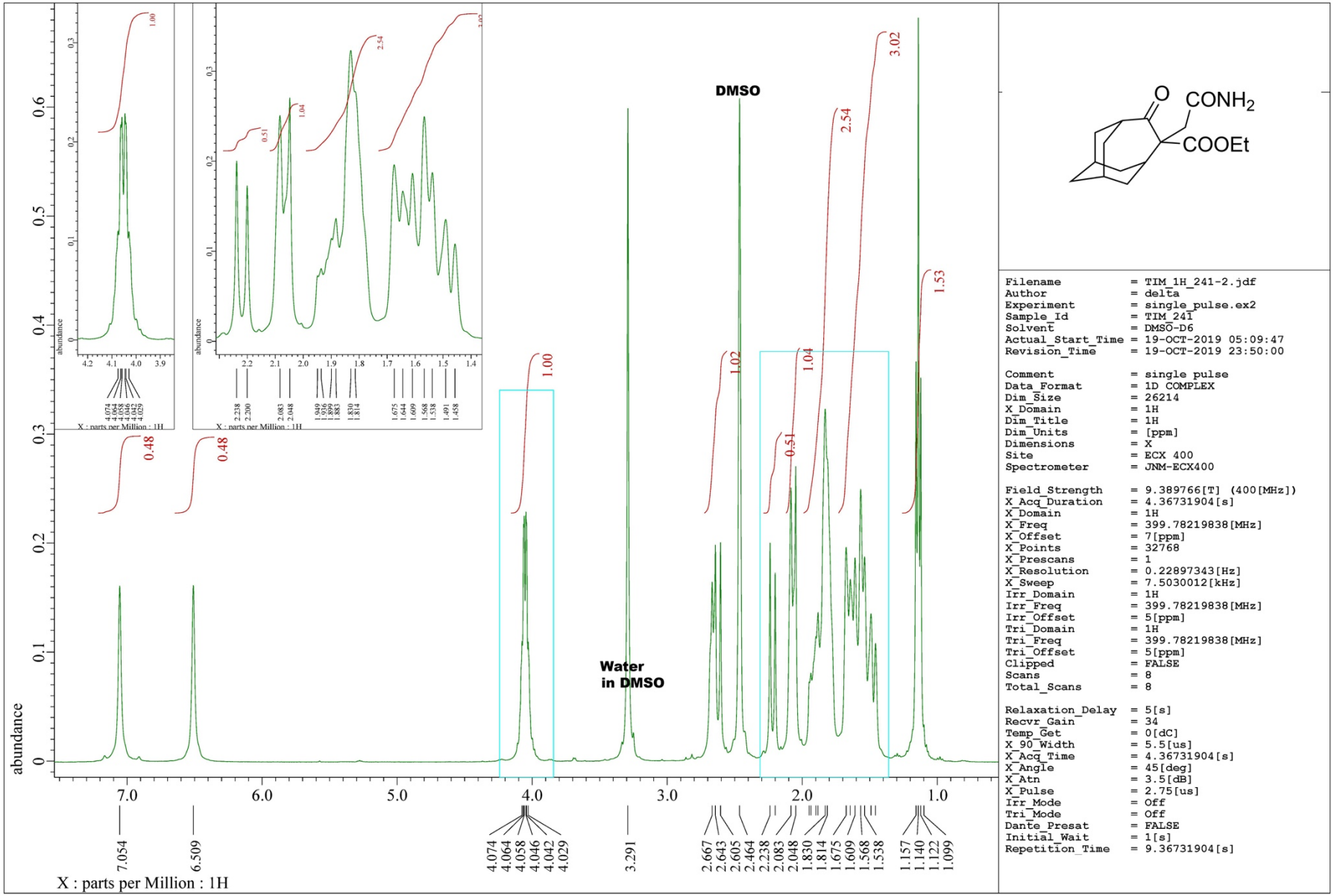
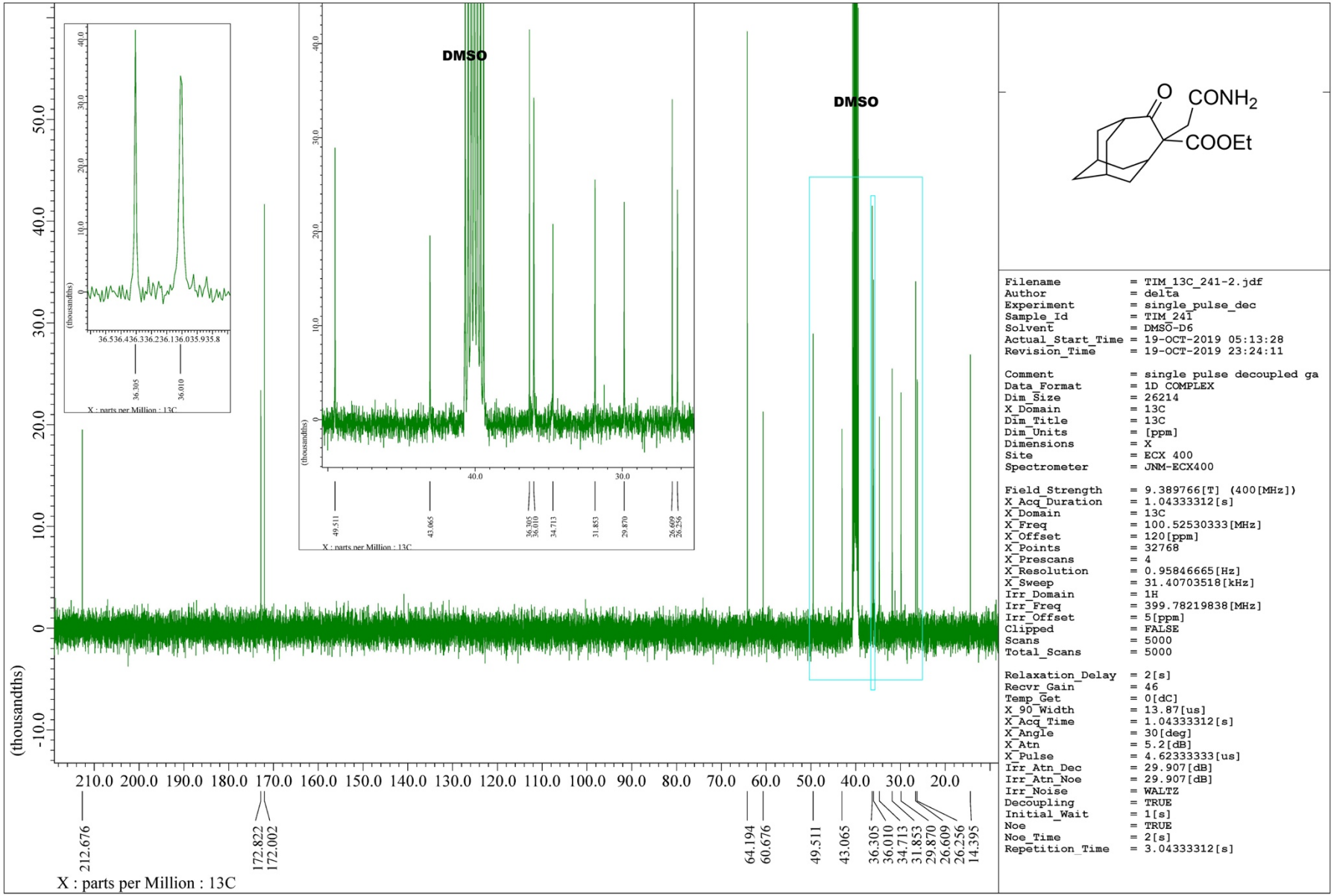


Compound 18 DEPT

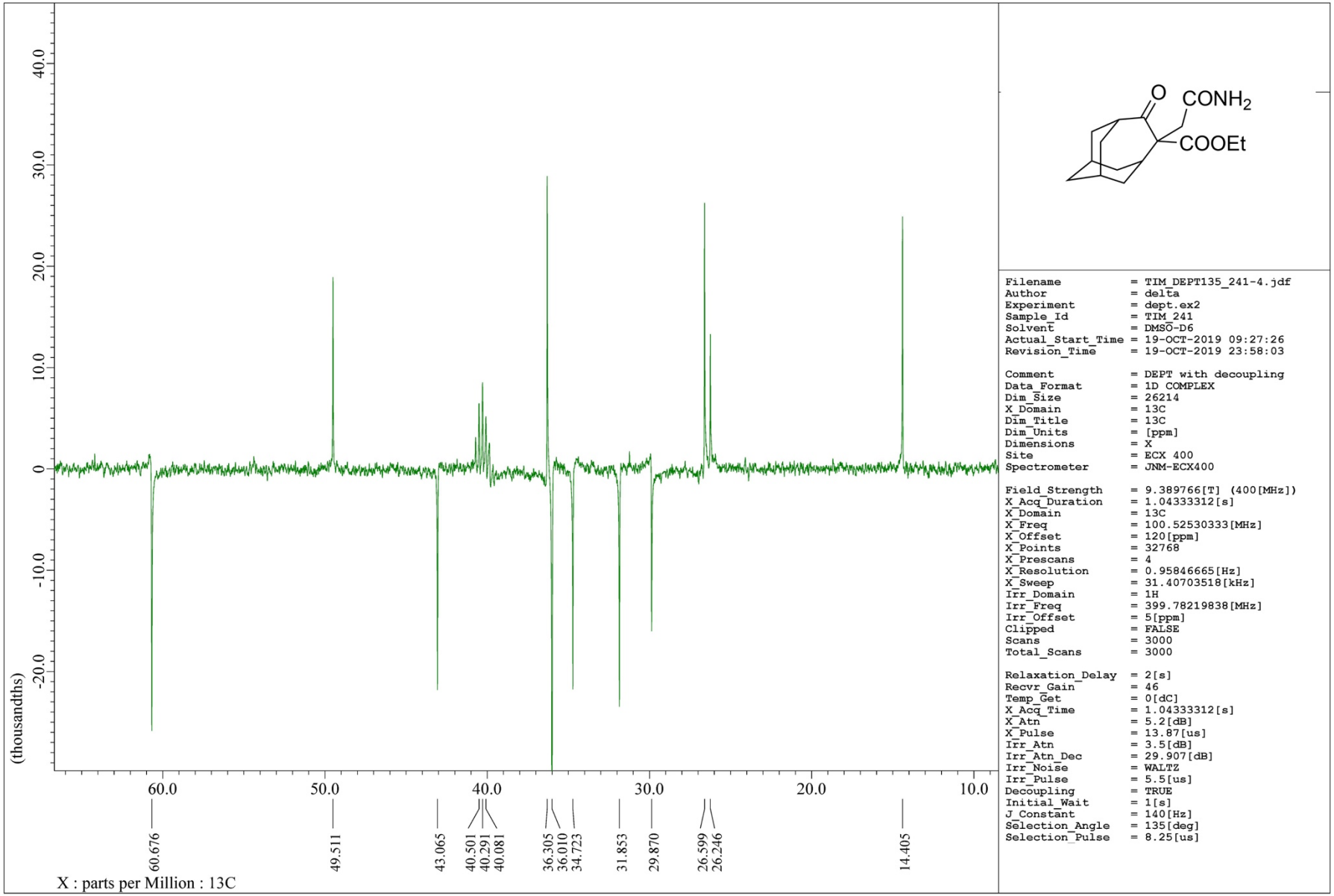



```
Filename            = TIM_1H_241-2.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = TIM_241
Solvent             = DMSO-D6
Actual_Start_Time   = 19-OCT-2019 05:09:47
Revision_Time       = 19-OCT-2019 23:50:00

Comment             = single pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 1H
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
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 34
Temp_Get            = 0[dC]
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]
Repetition_Time     = 9.36731904[s]
```

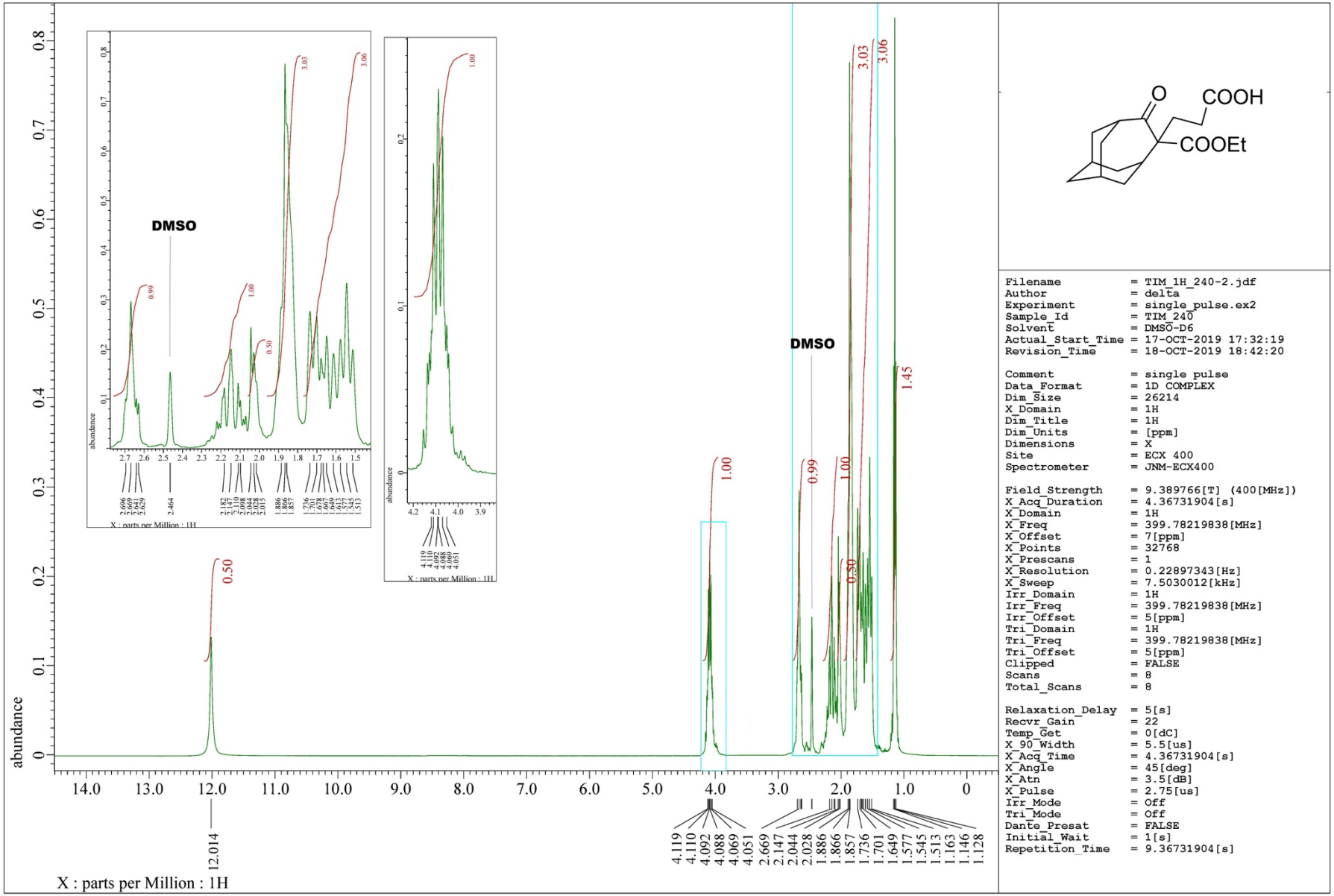
Compound 39 ^{1}H NMR



Compound 19 ^{13}C NMR

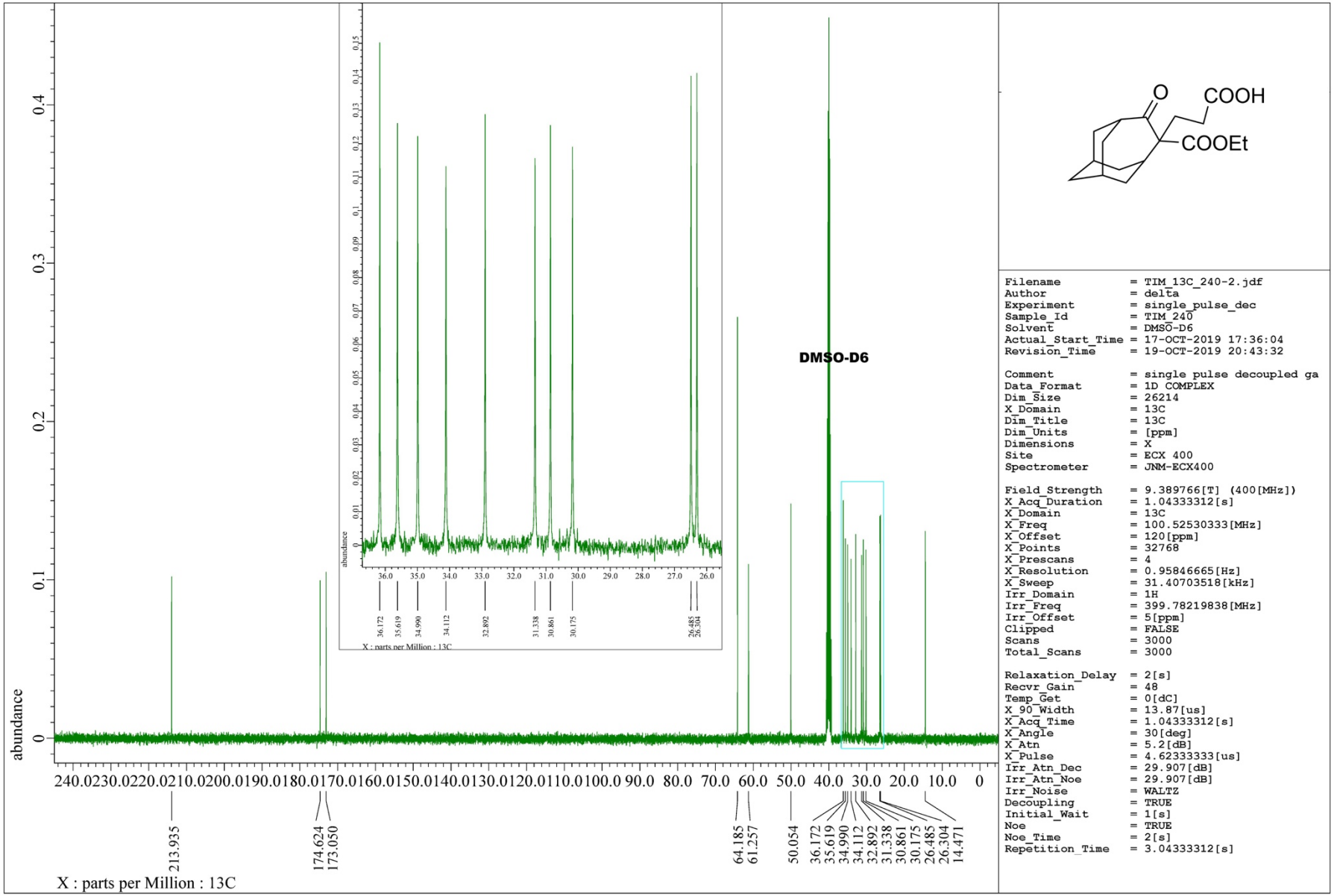


Compound 19 DEPT

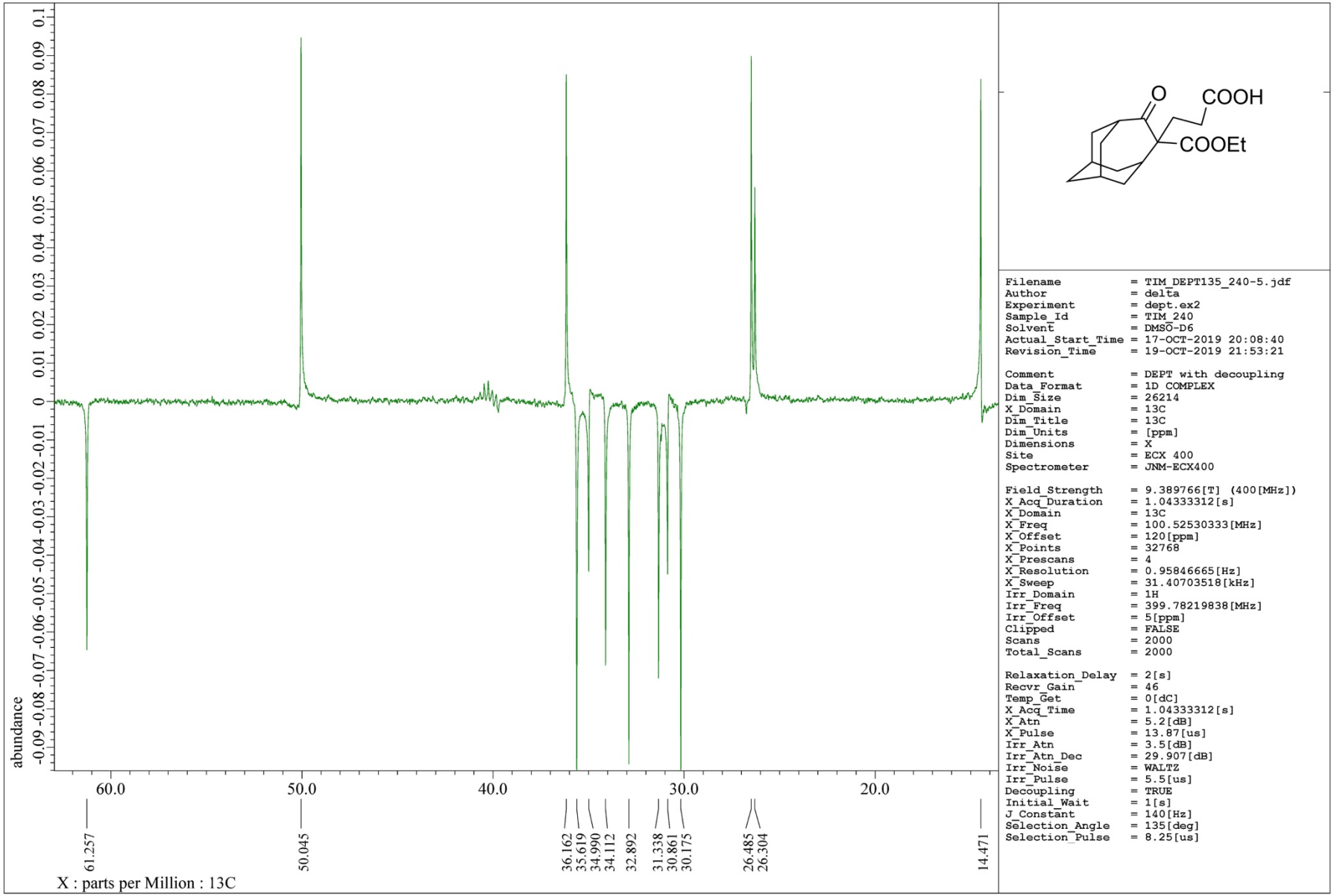



```
Filename            = TIM_1H_240-2.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = TIM_240
Solvent             = DMSO-D6
Actual_Start_Time   = 17-OCT-2019 17:32:19
Revision_Time       = 18-OCT-2019 18:42:20

Comment             = single pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 1H
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
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 22
Temp_Get            = 0[dC]
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]
Repetition_Time     = 9.36731904[s]
```

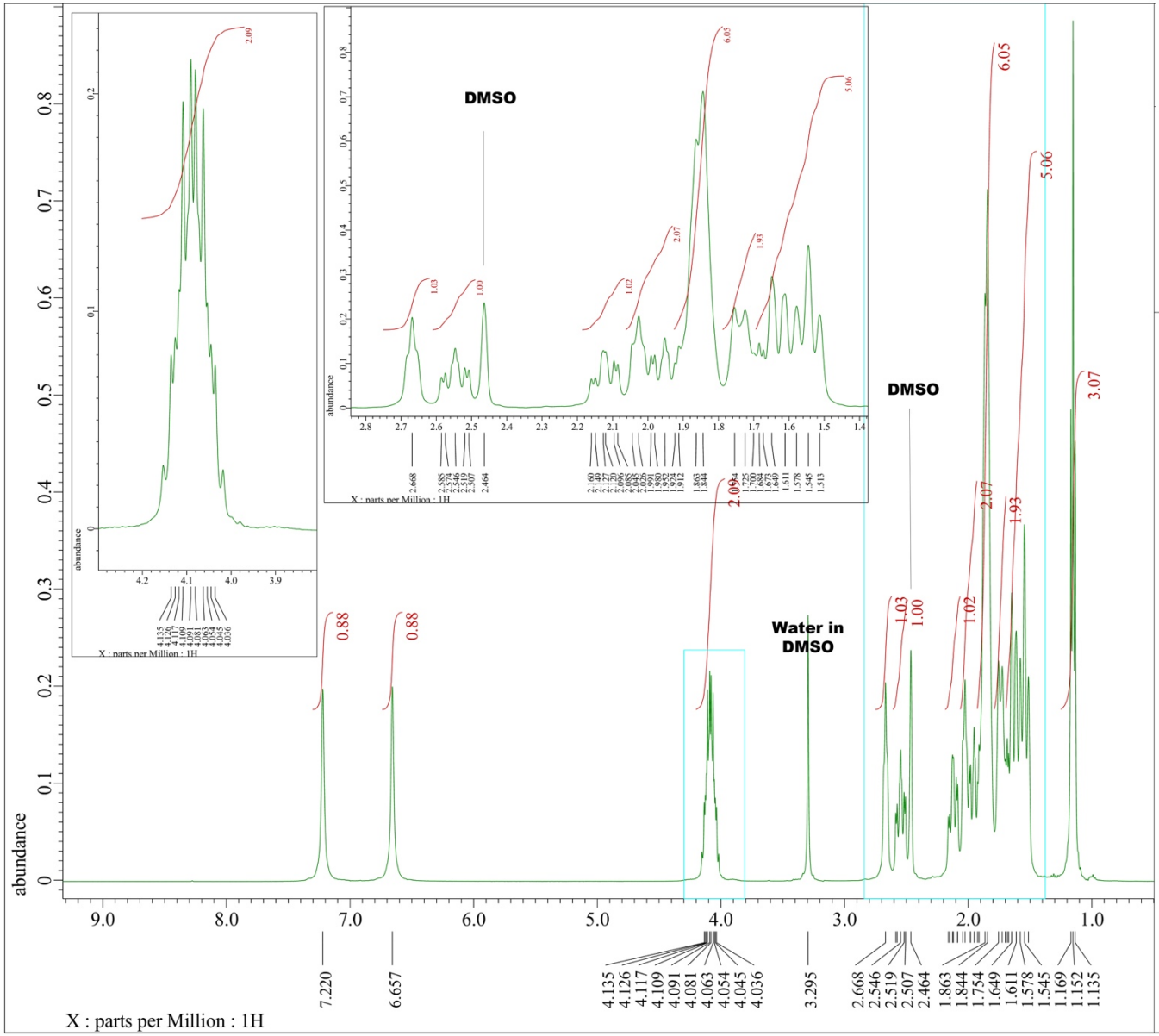
Compound 20 ^{1}H NMR

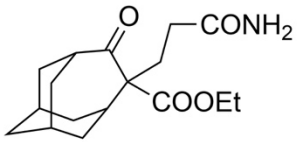


Compound 20 ^{13}C NMR



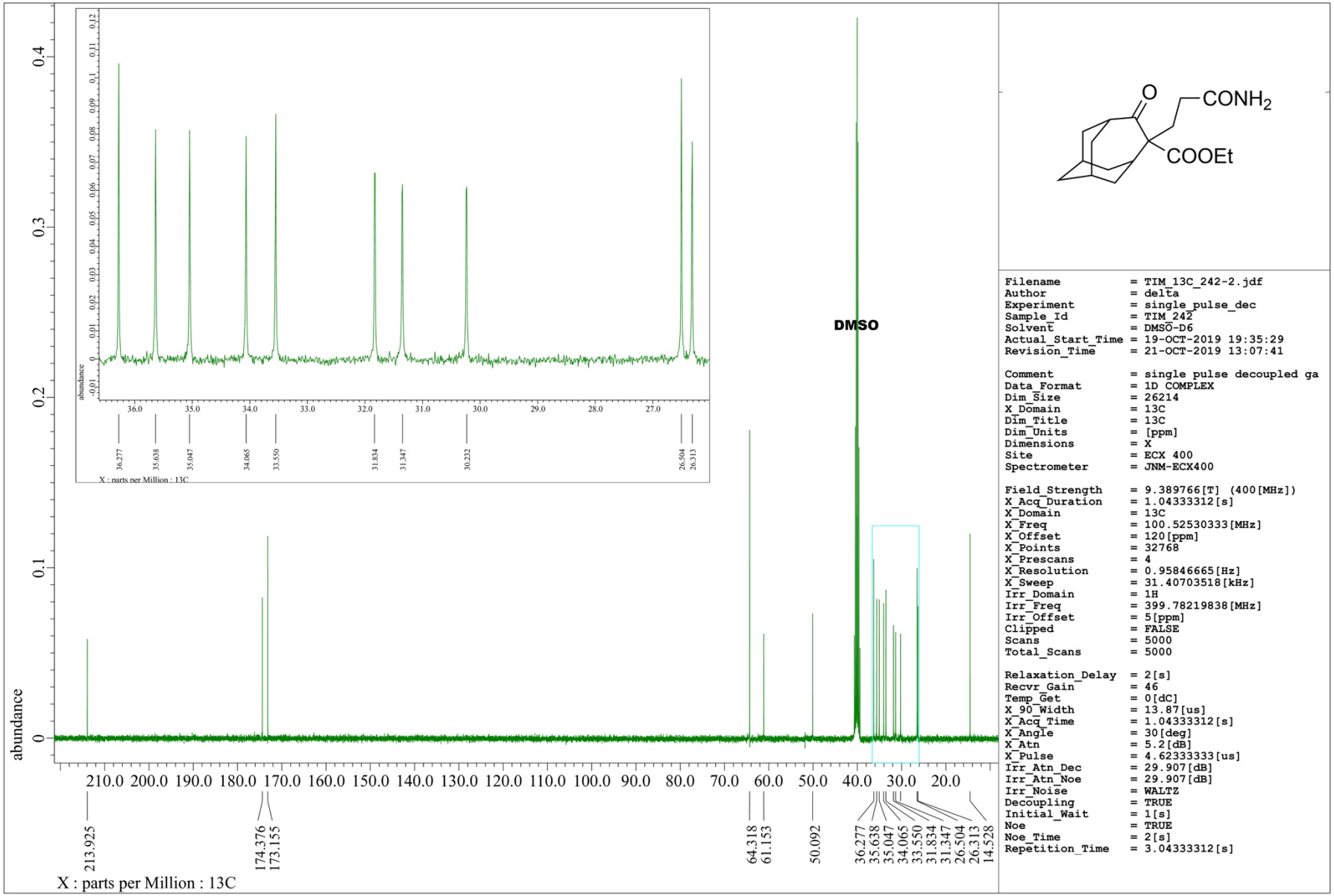
Compound 20 DEPT



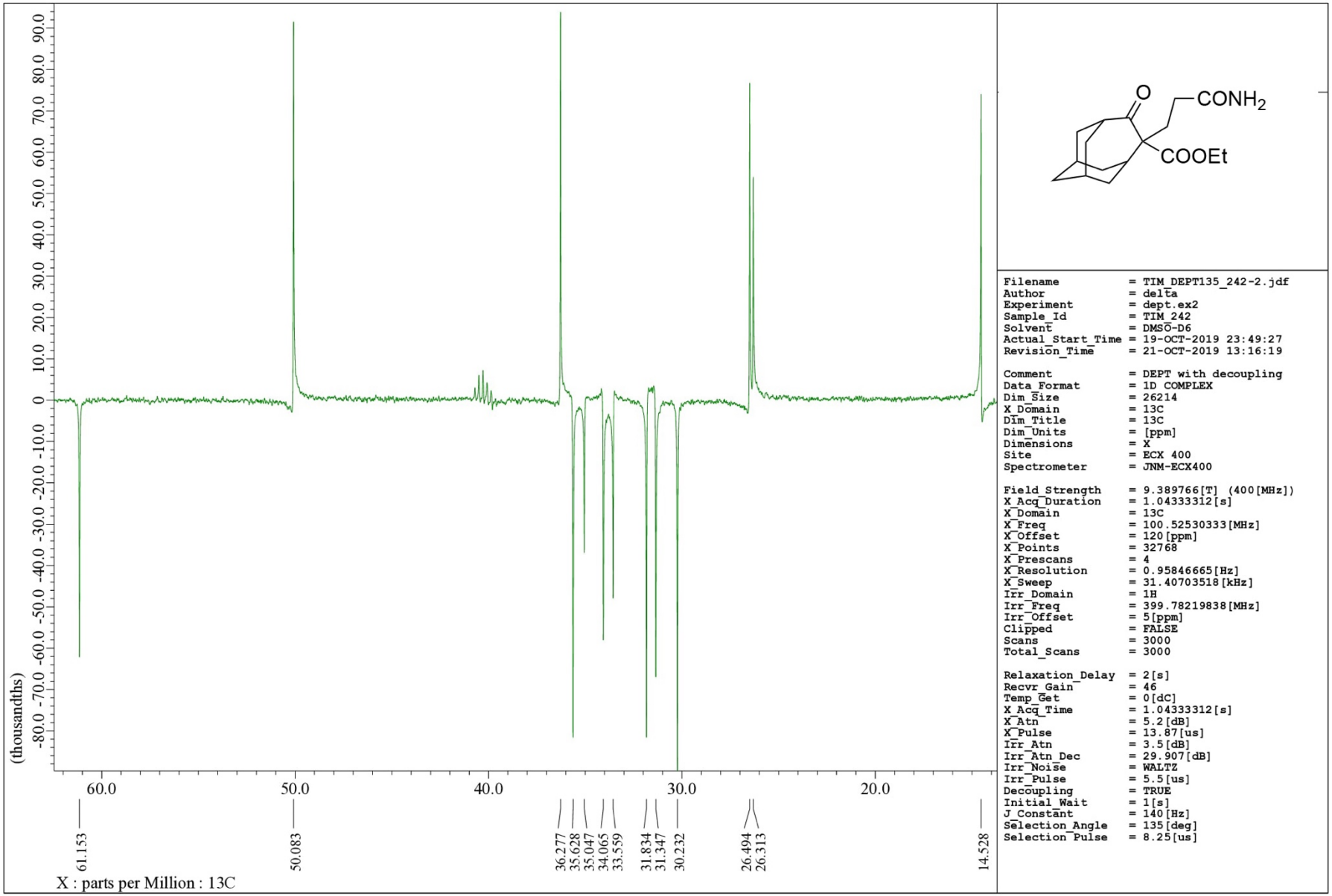



```
Filename            = TIM_1H_242-2.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = TIM_242
Solvent             = DMSO-D6
Actual_Start_Time   = 19-OCT-2019 19:31:43
Revision_Time       = 21-OCT-2019 13:04:25

Comment             = single pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 1H
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
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 26
Temp_Get            = 0[dC]
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]
Repetition_Time     = 9.36731904[s]
```

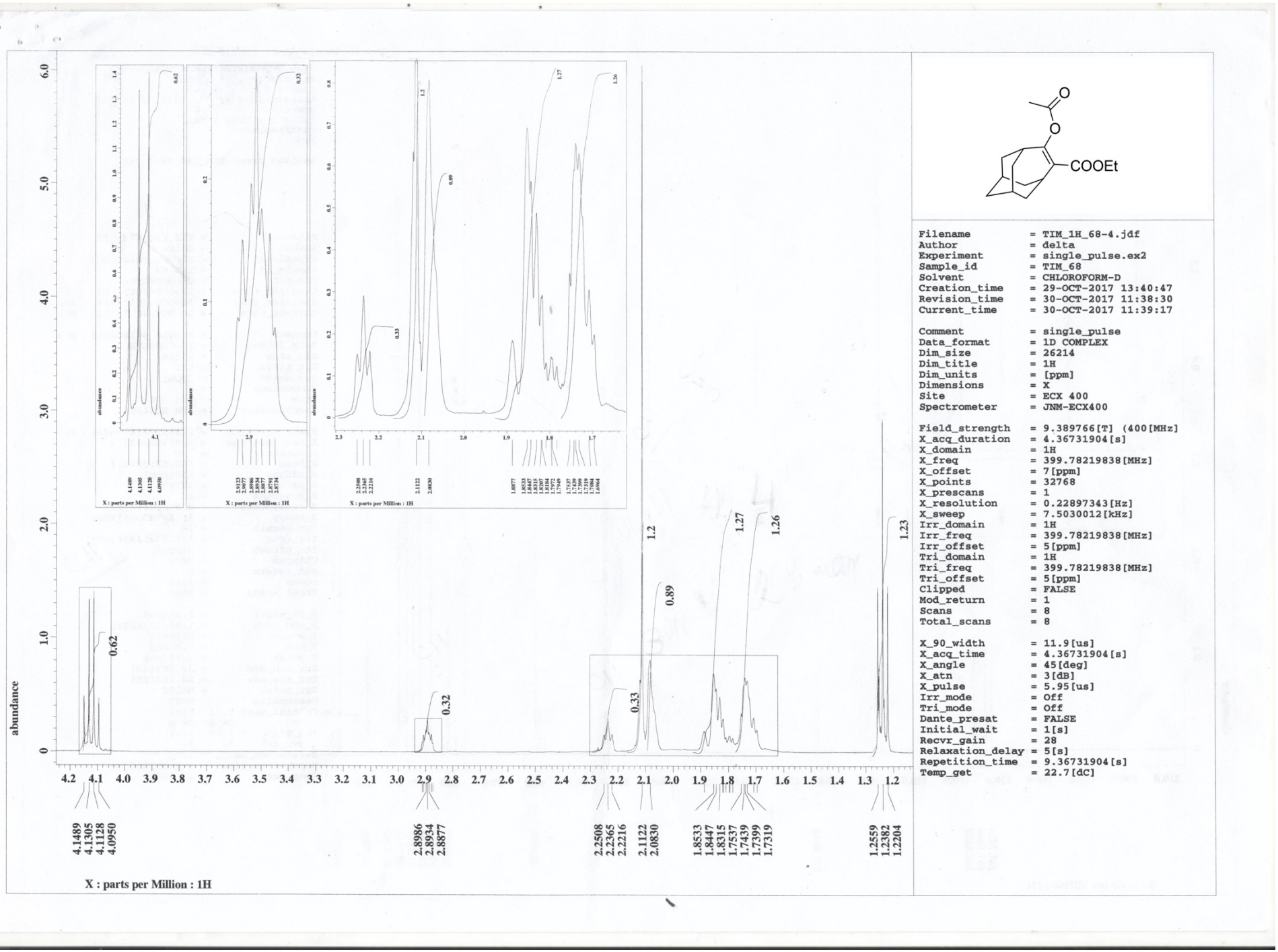
Compound 21 ^{1}H NMR



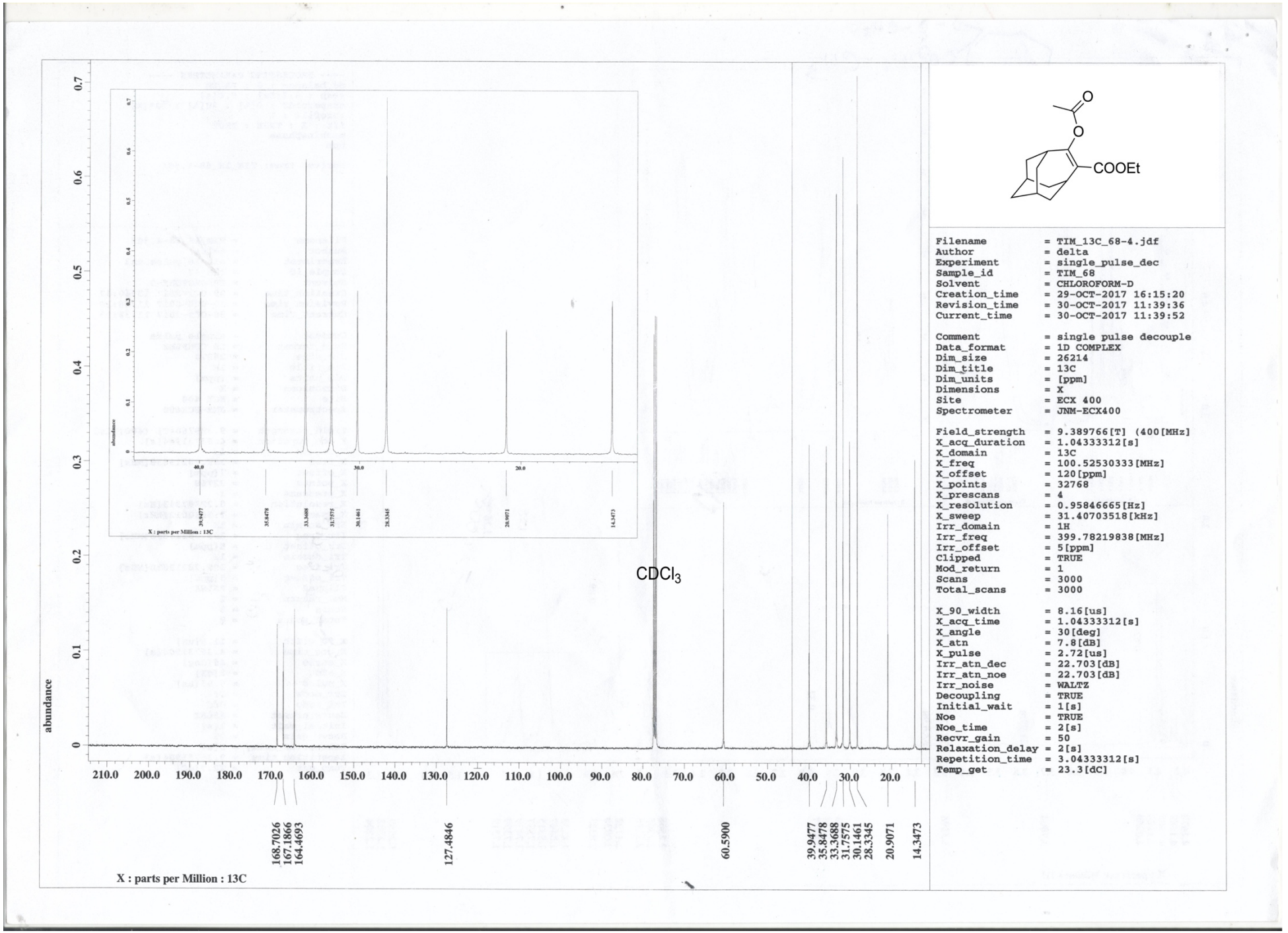
Compound 21 ^{13}C NMR



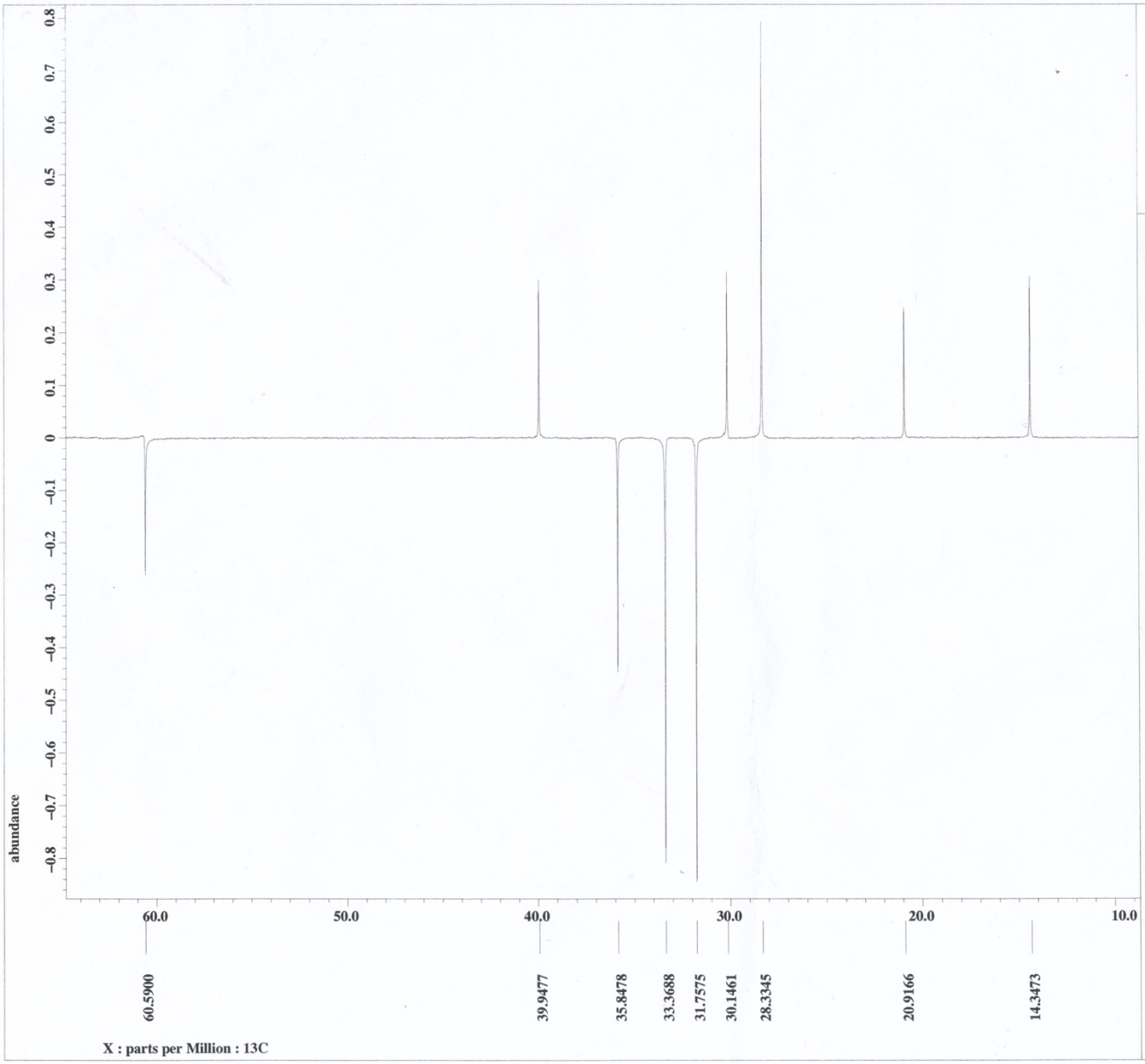
Compound 21 DEPT

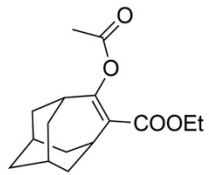


compound 22 ^{1}H NMR



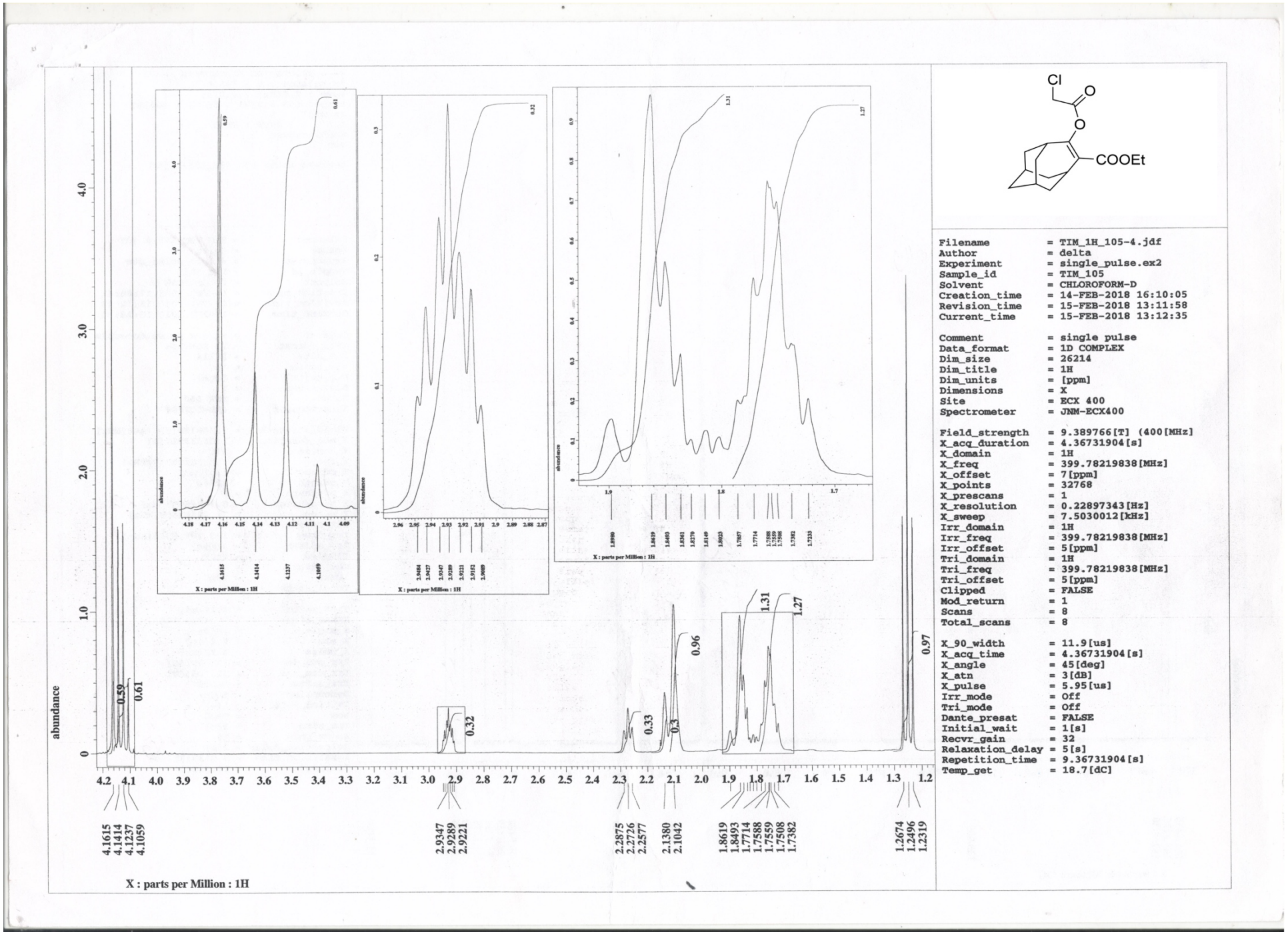
compound 22 ^{13}C NMR



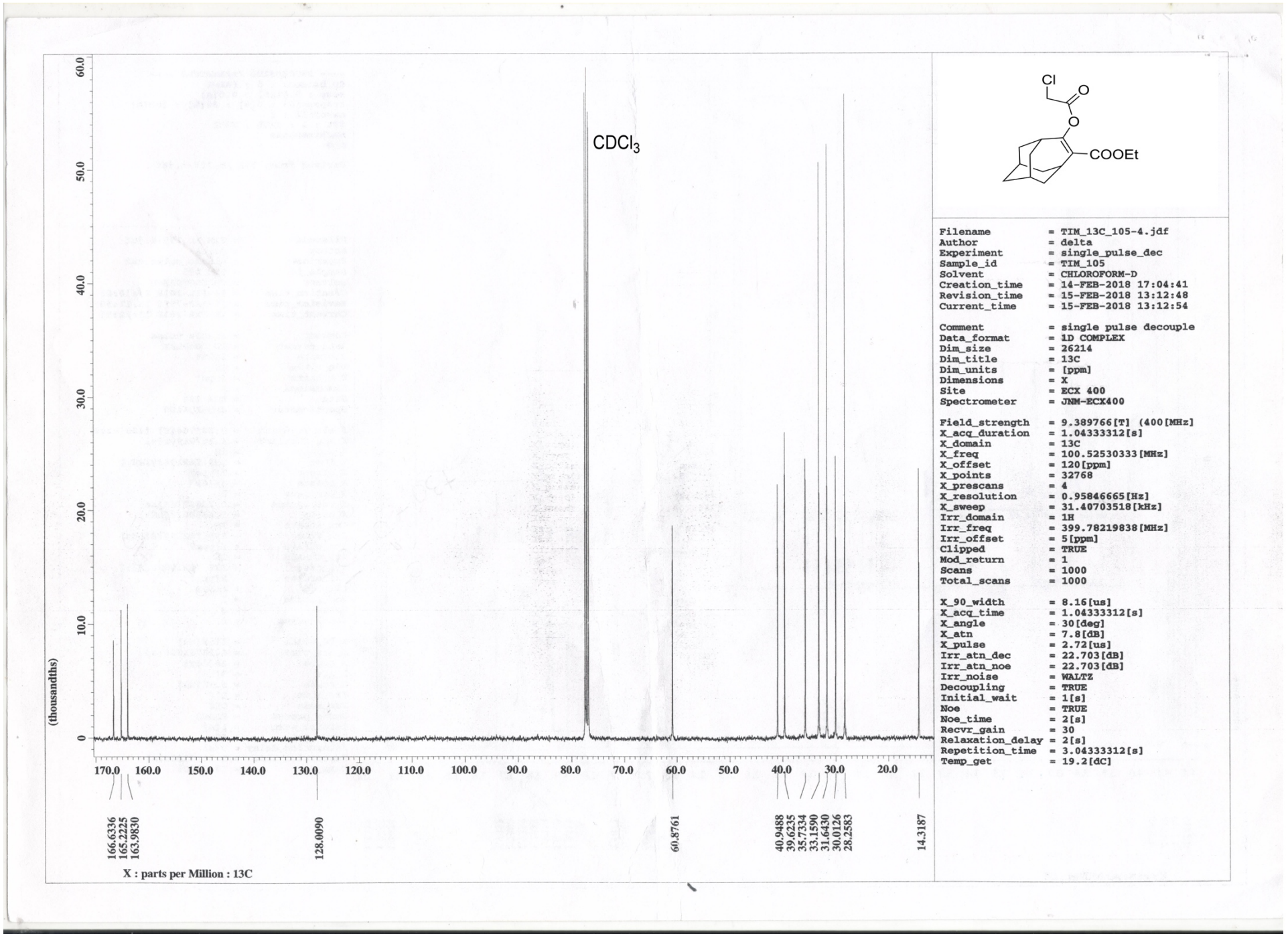



```
Filename          = TIM_DEPT135_68-4.jdf
Author            = delta
Experiment        = dept.ex2
Sample_id         = TIM_68
Solvent           = CHLOROFORM-D
Creation_time     = 29-OCT-2017 17:06:37
Revision_time     = 30-OCT-2017 11:40:04
Current_time      = 30-OCT-2017 11:40:06

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             = 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[dC]
```

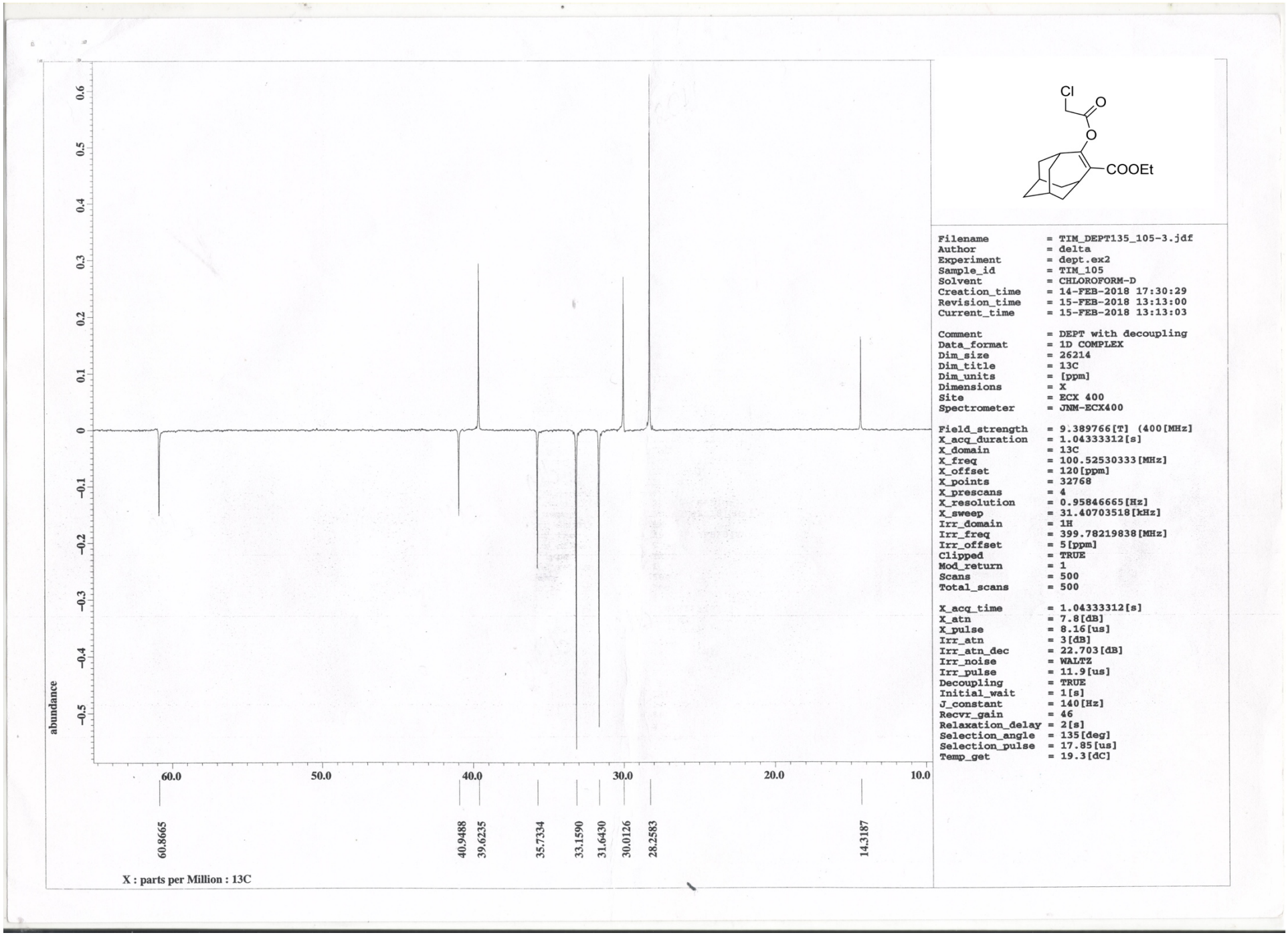
compound 22 DEPT



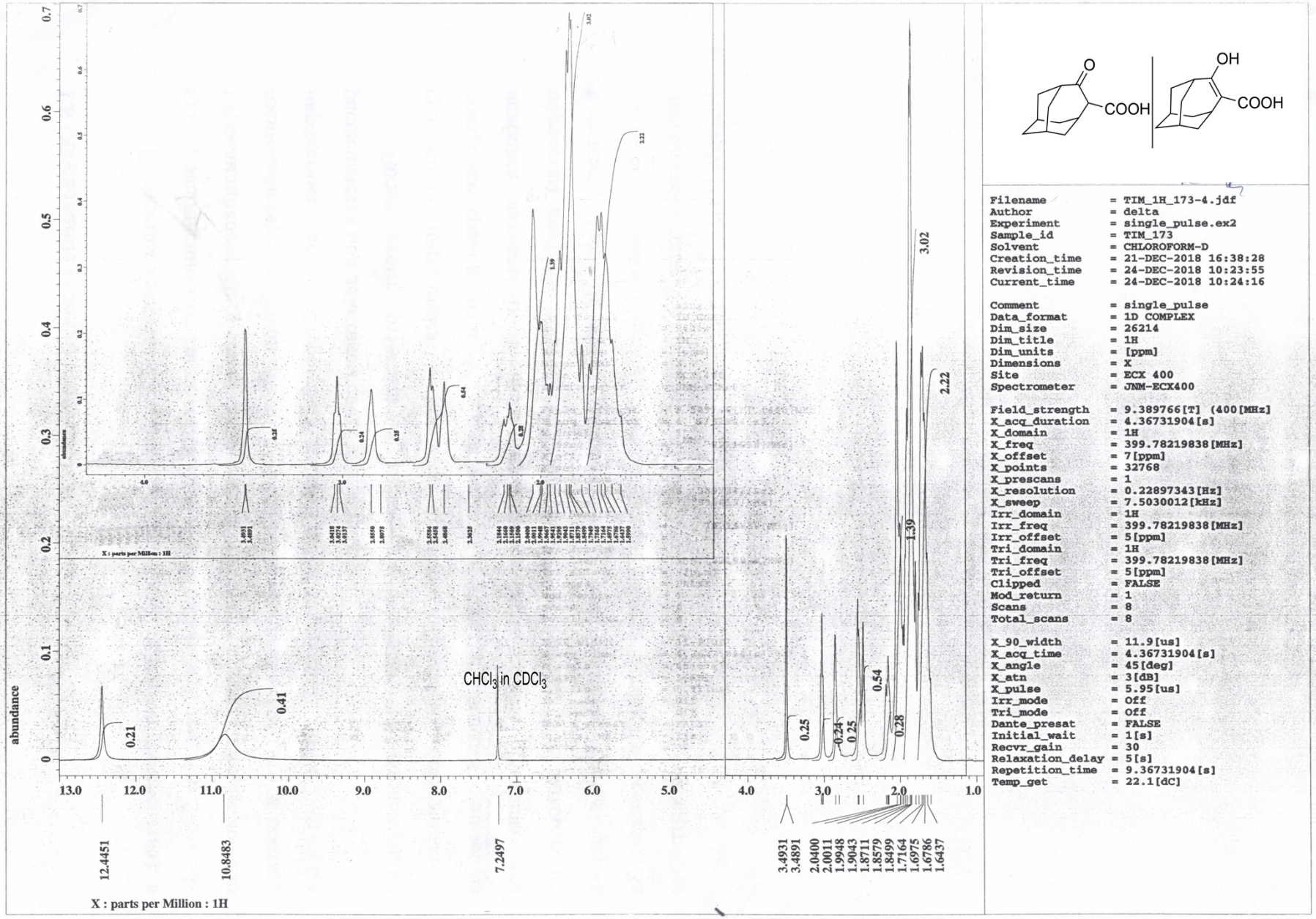
compound 23 ^{1}H NMR



compound 23 ^{13}C NMR

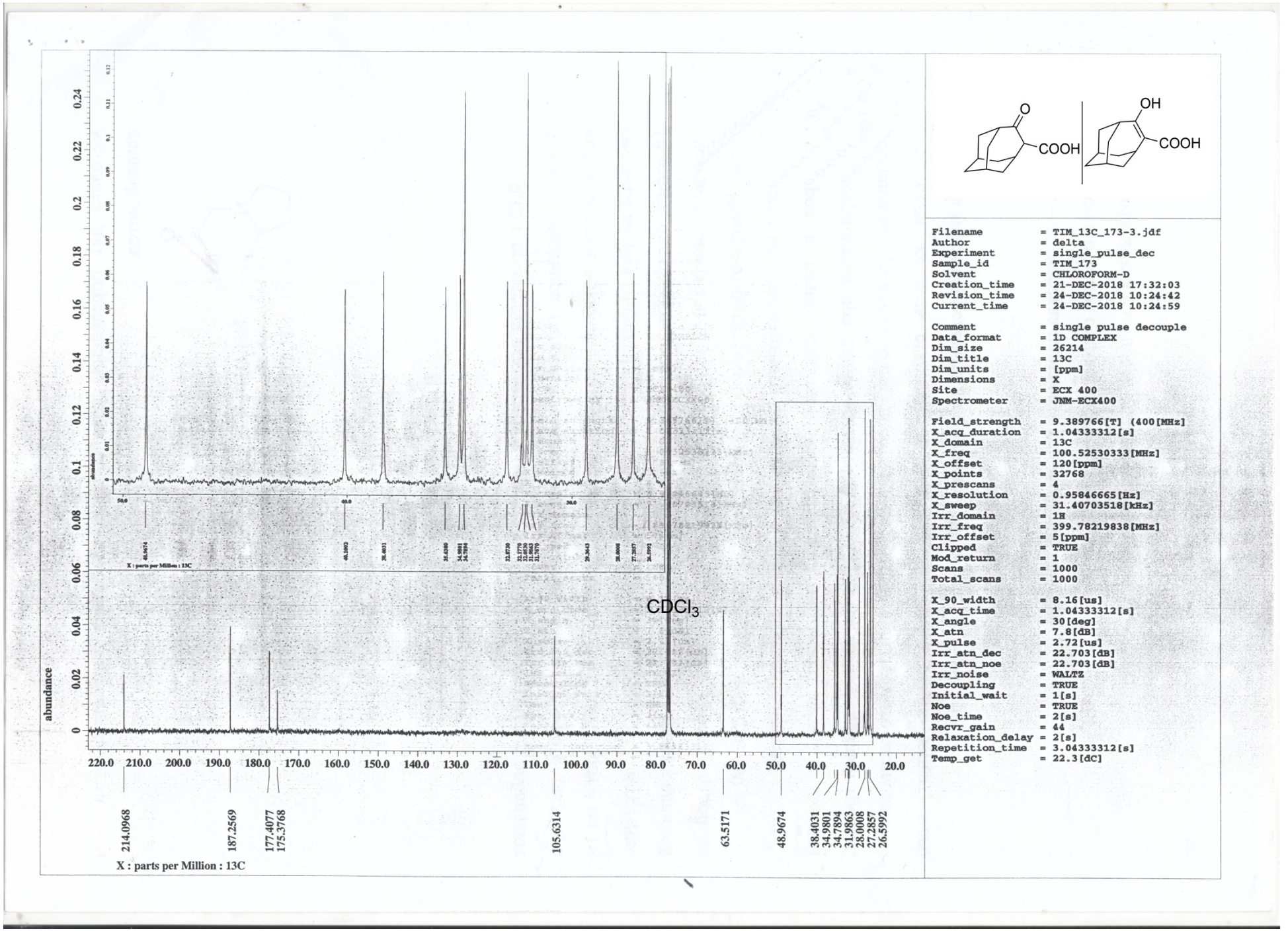


compound 23 DEPT

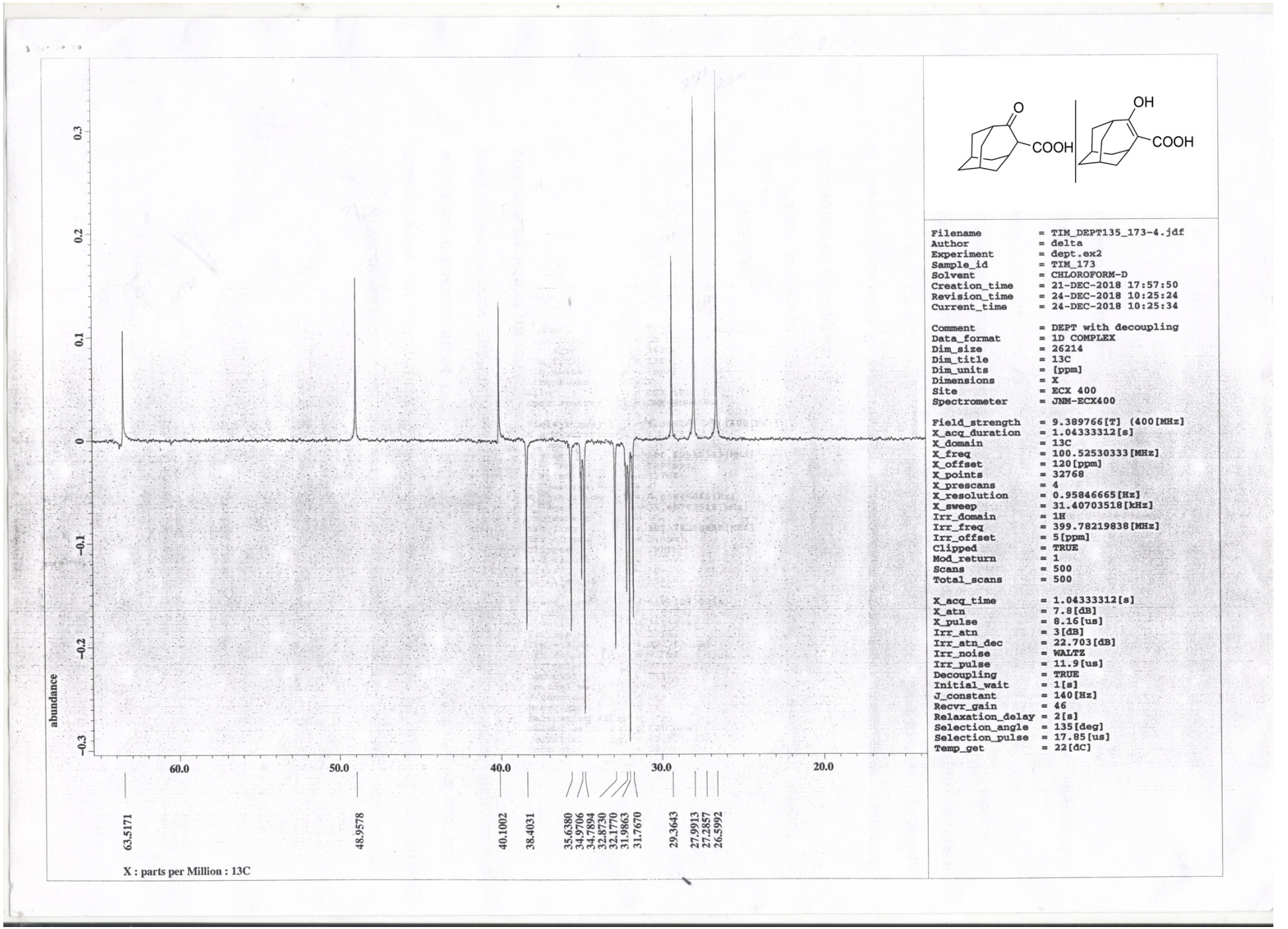



```
Filename          = TIM_1H_173-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = TIM_173
Solvent           = CHLOROFORM-D
Creation_time     = 21-DEC-2018 16:38:28
Revision_time     = 24-DEC-2018 10:23:55
Current_time      = 24-DEC-2018 10:24:16

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]
```

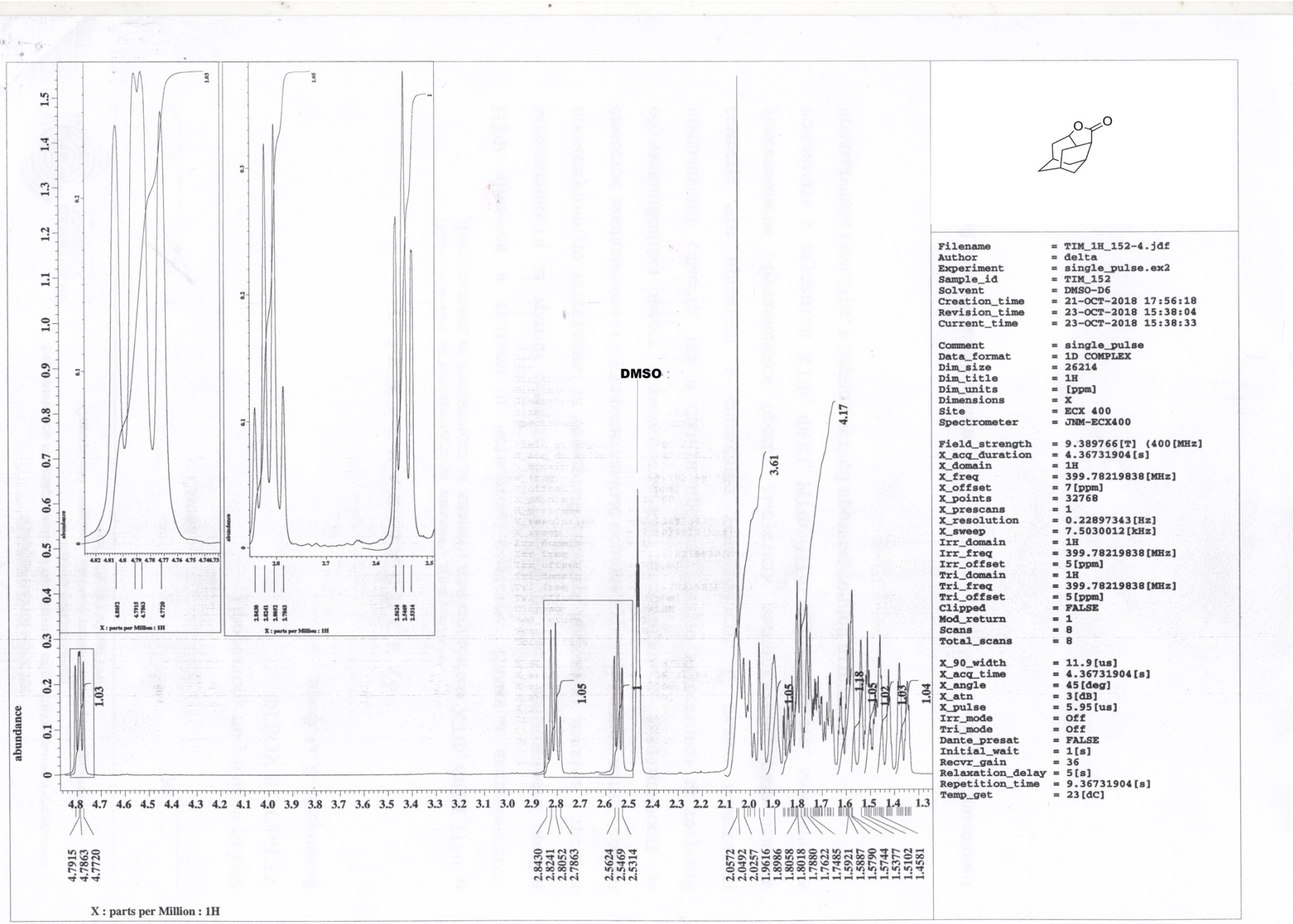
compound 24 ^{1}H NMR



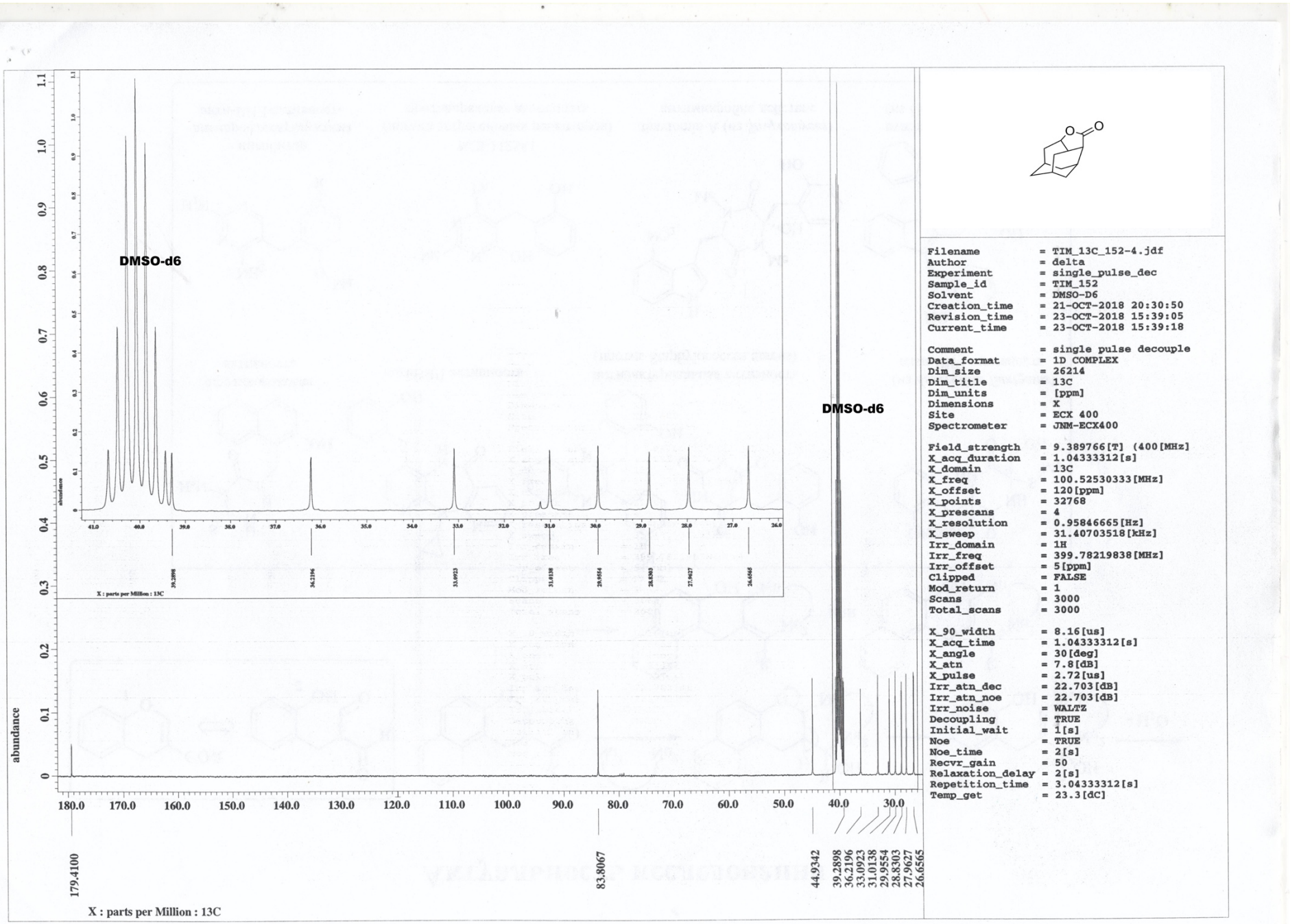
compound 24 ^{13}C NMR



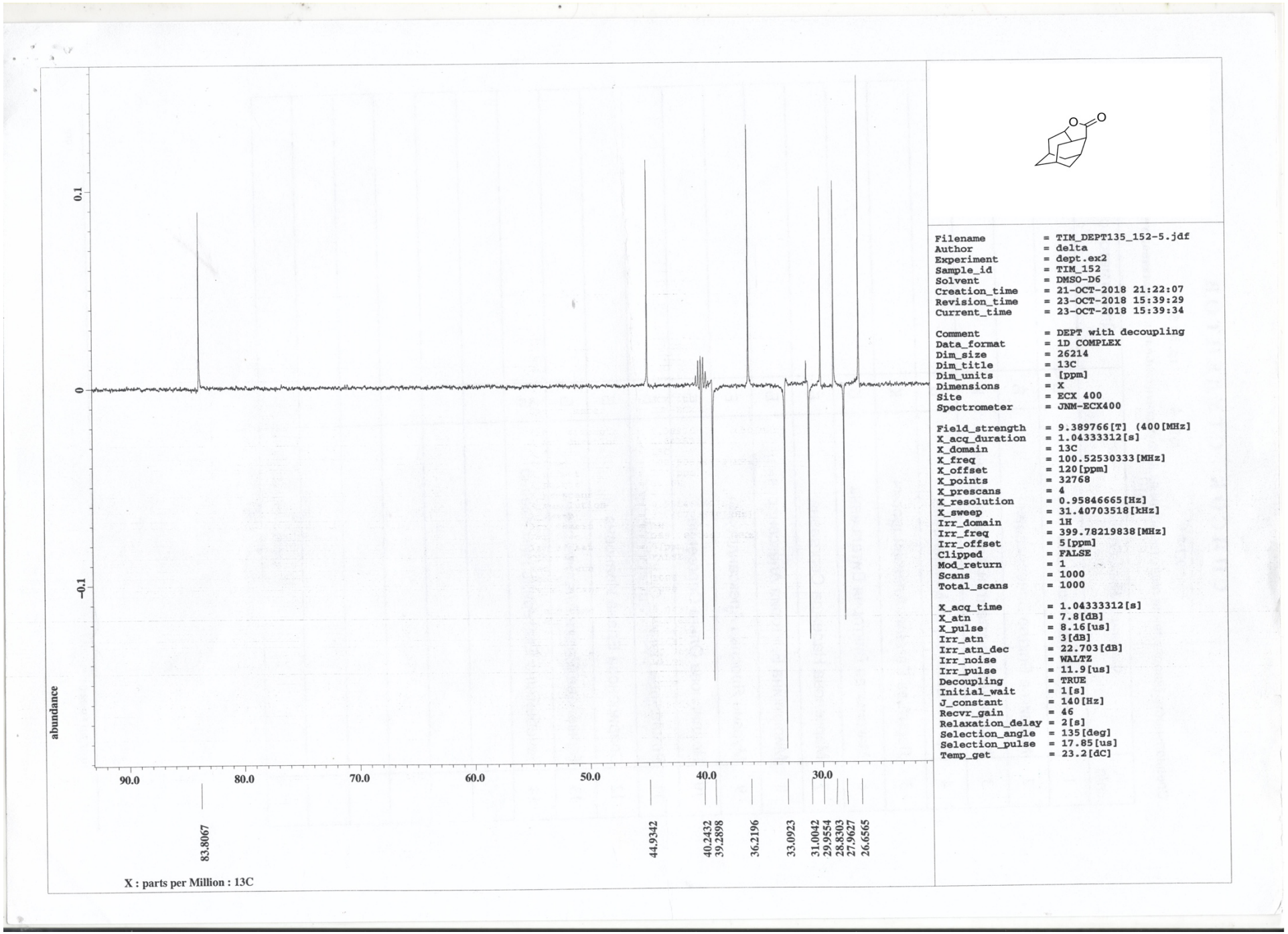
compound 24 DEPT



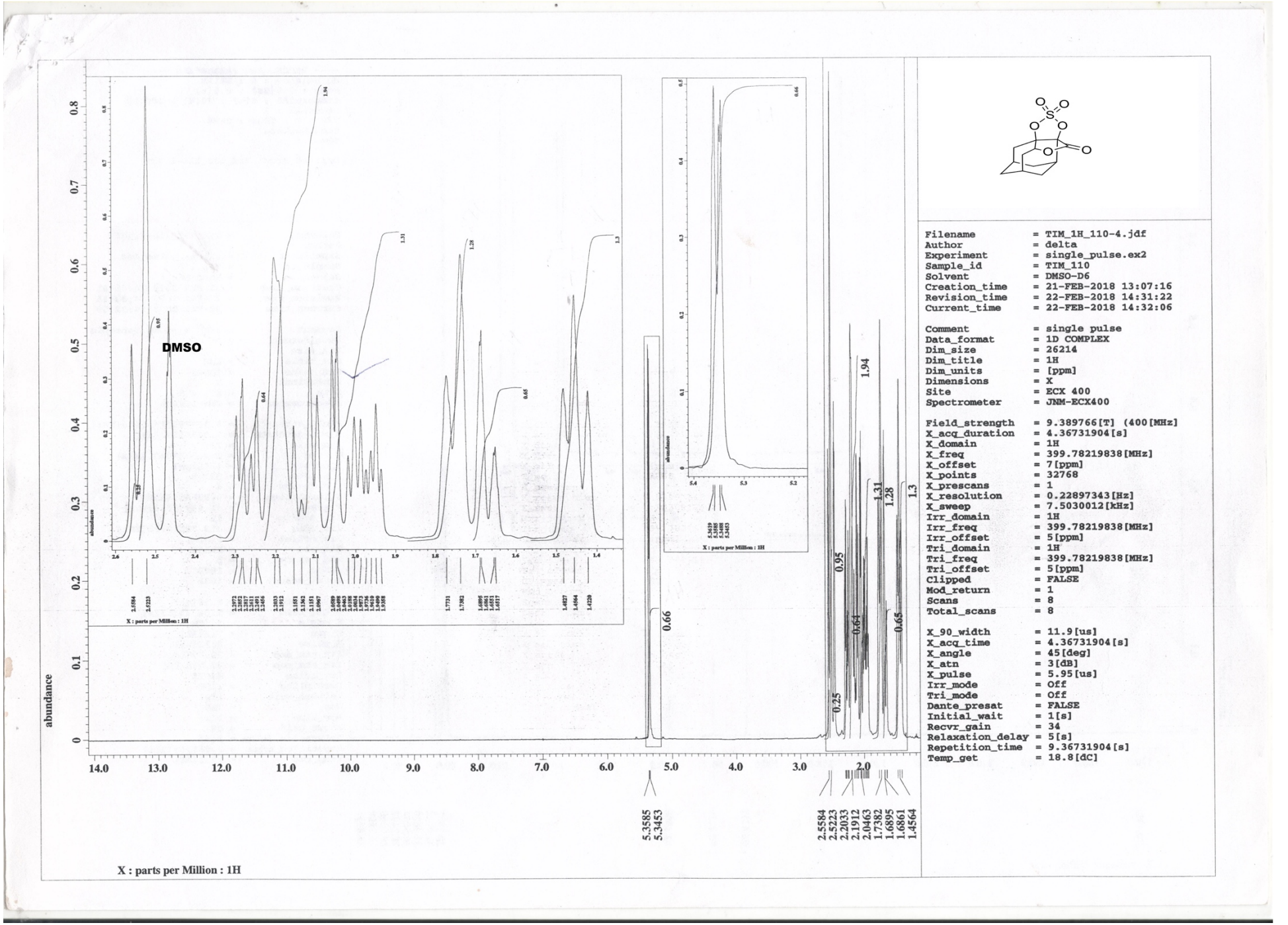
compound 25 ^{1}H NMR



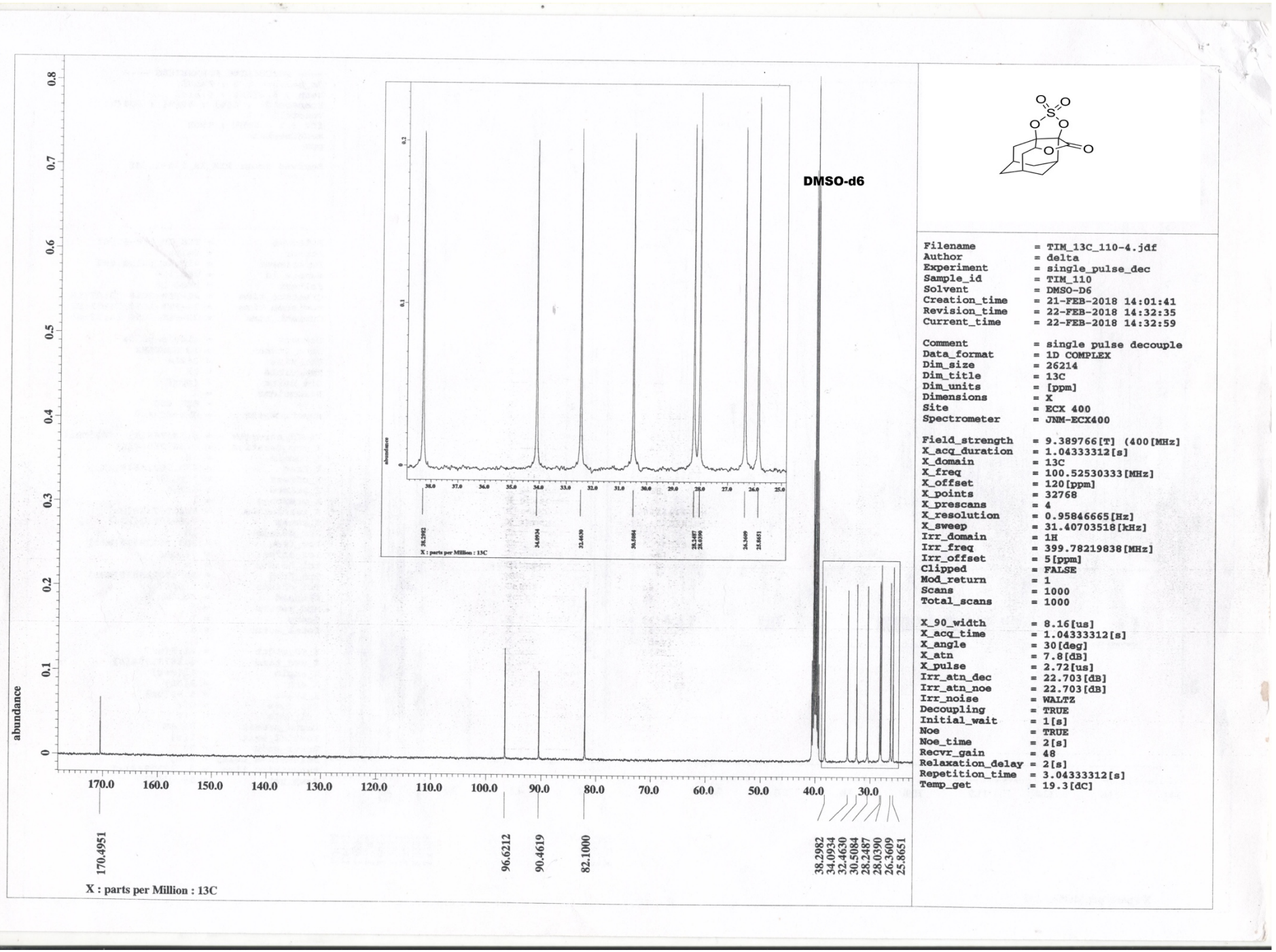
compound 25 ^{13}C NMR



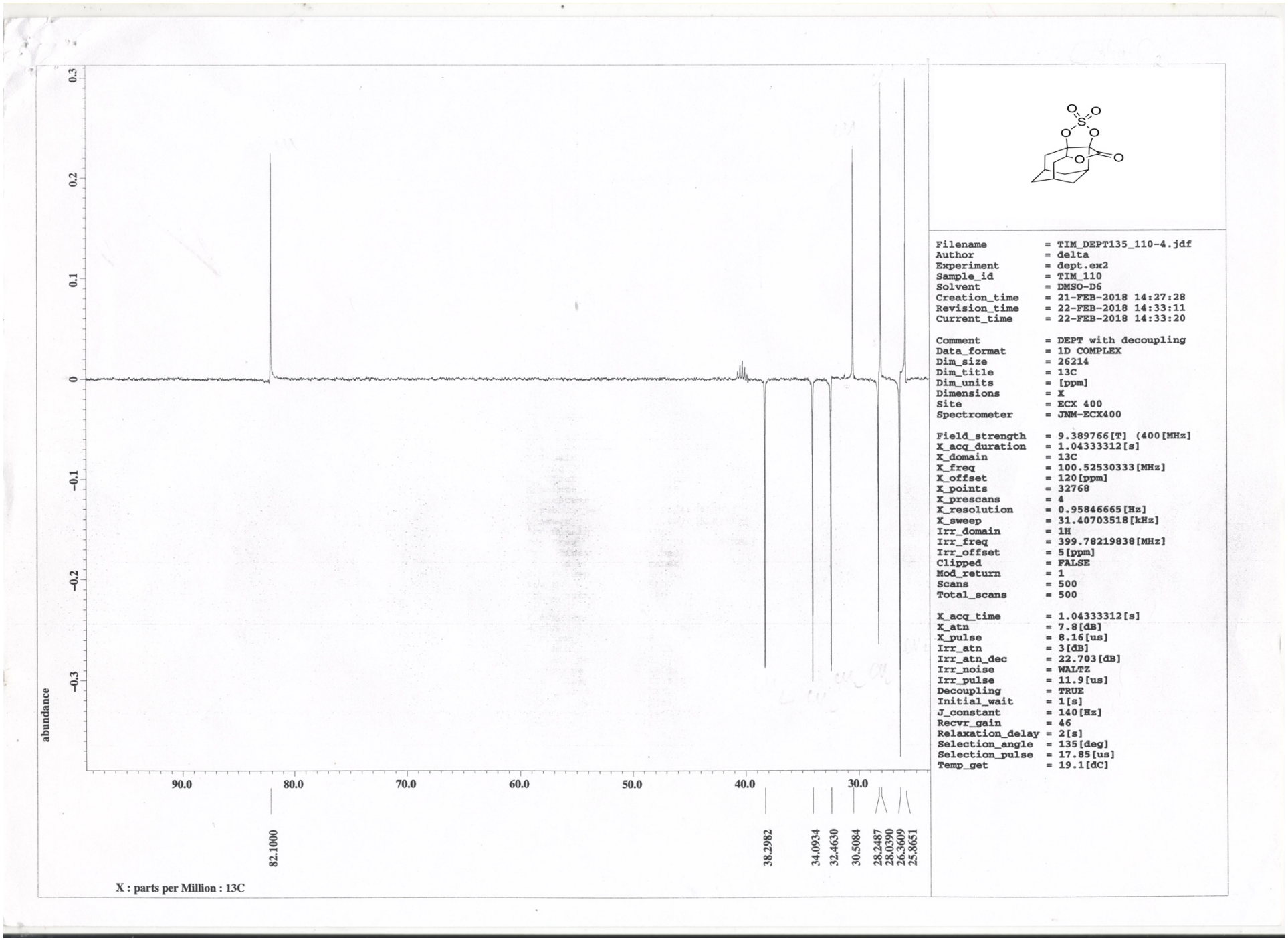
compound 25 DEPT



compound 26 ^{1}H NMR

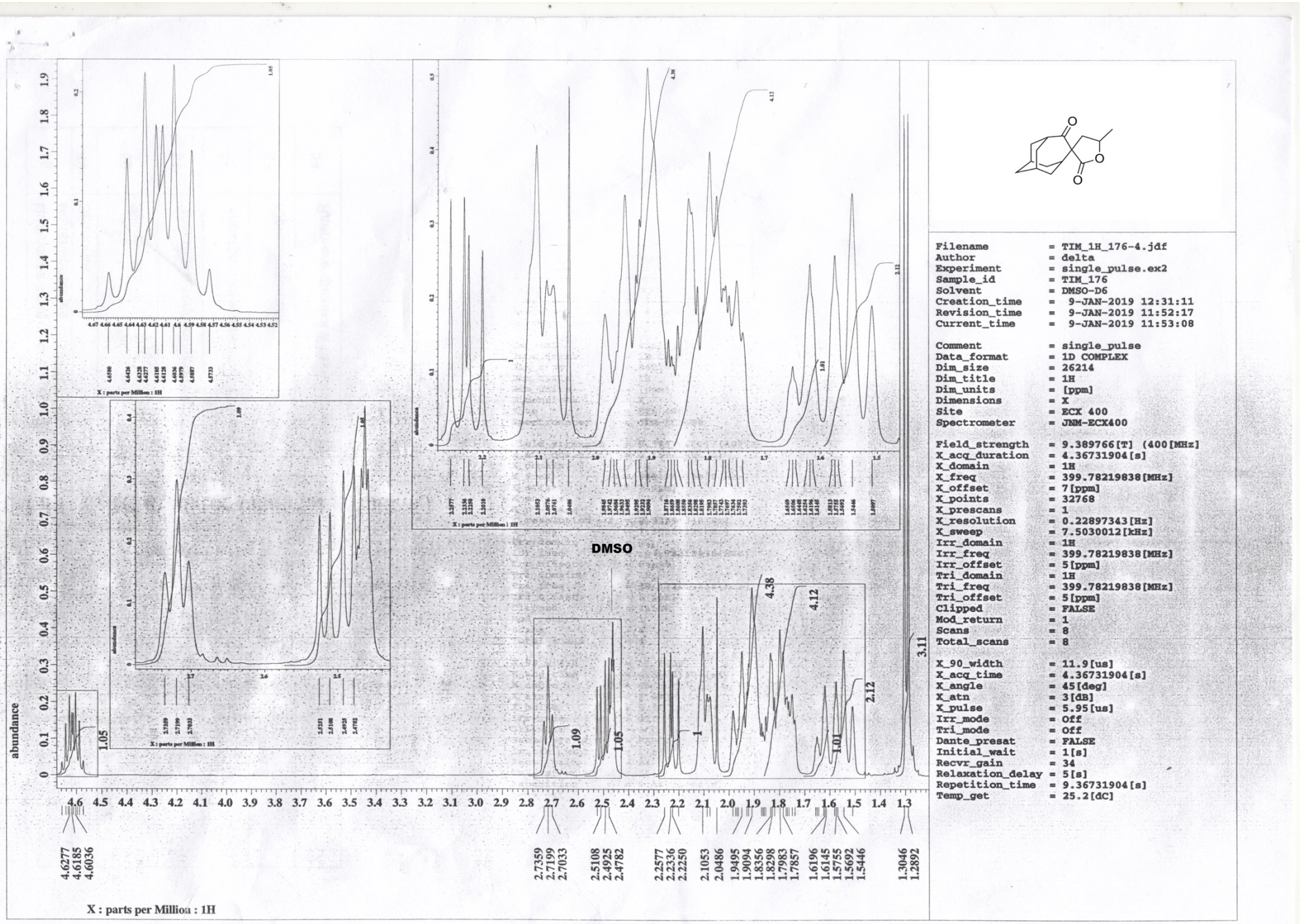


compound 26 ^{13}C NMR

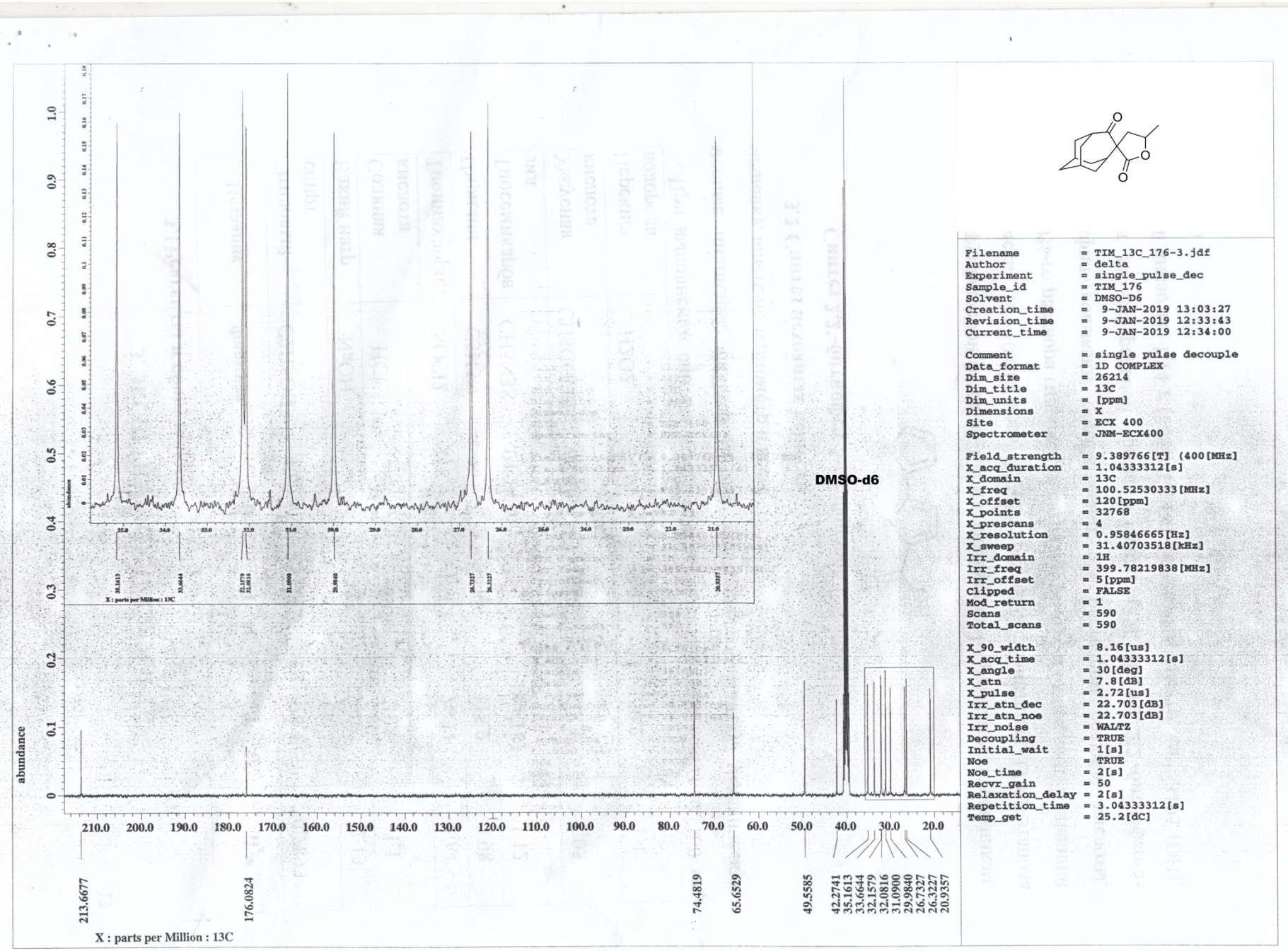



```
Filename          = TIM_DEPT135_110-4.jdf
Author            = delta
Experiment        = dept.ex2
Sample_id         = TIM_110
Solvent           = DMSO-D6
Creation_time     = 21-FEB-2018 14:27:28
Revision_time     = 22-FEB-2018 14:33:11
Current_time      = 22-FEB-2018 14:33:20

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]
```

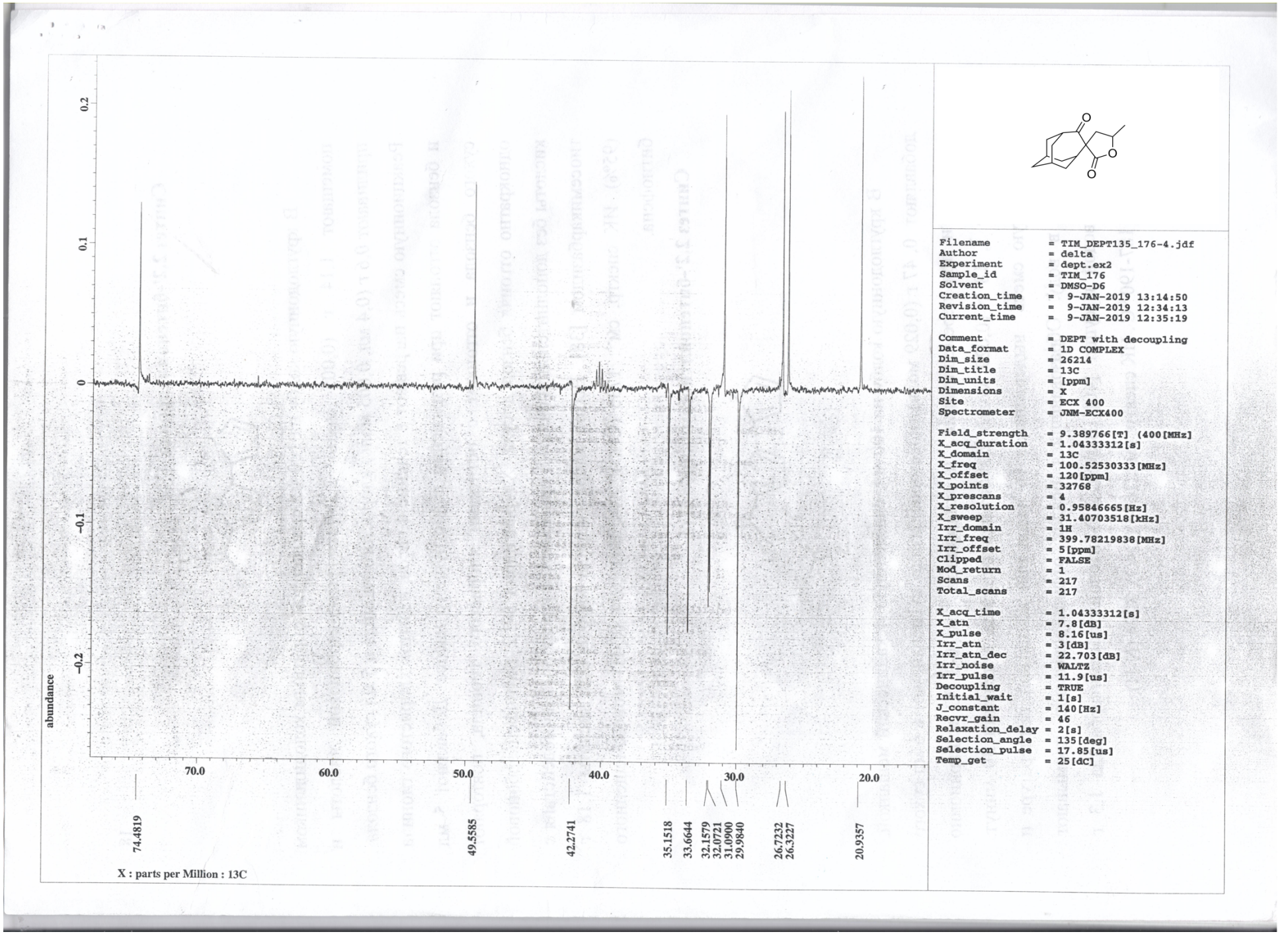
compound 24 DEPT



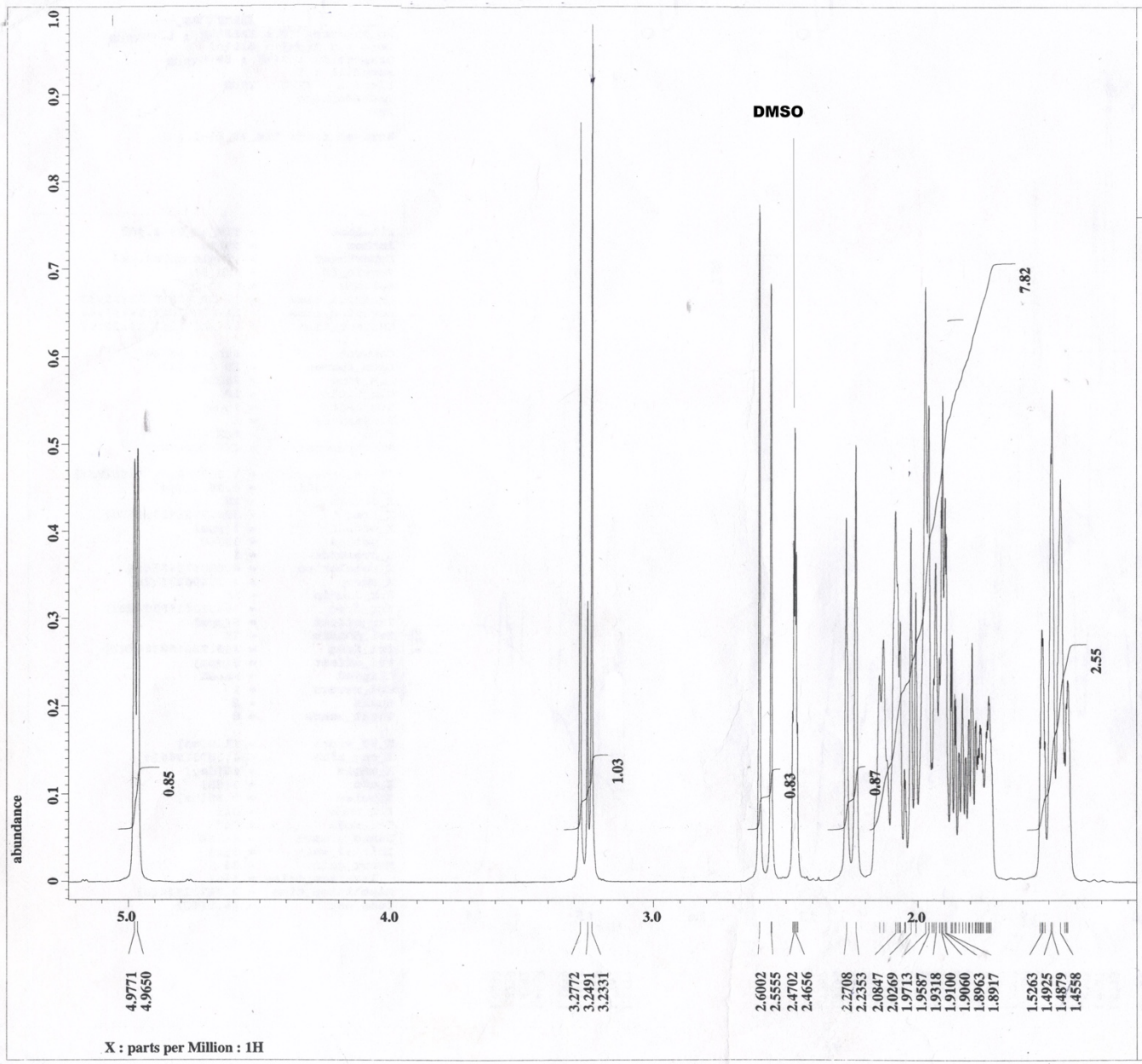
compound 25 ^{1}H NMR

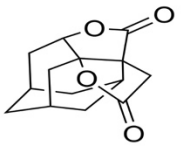


compound 27 ^{13}C NMR



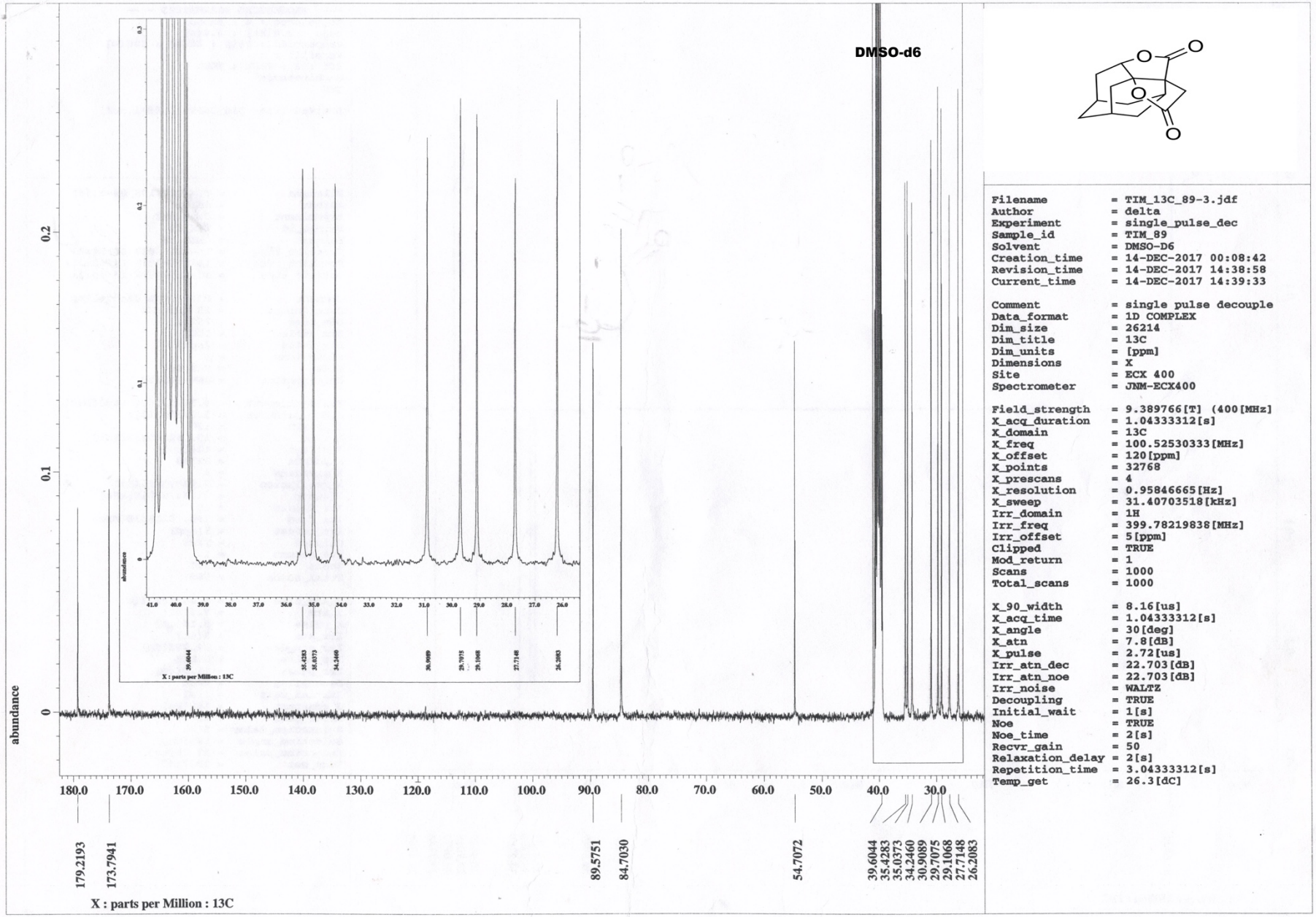
compound 27 DEPT



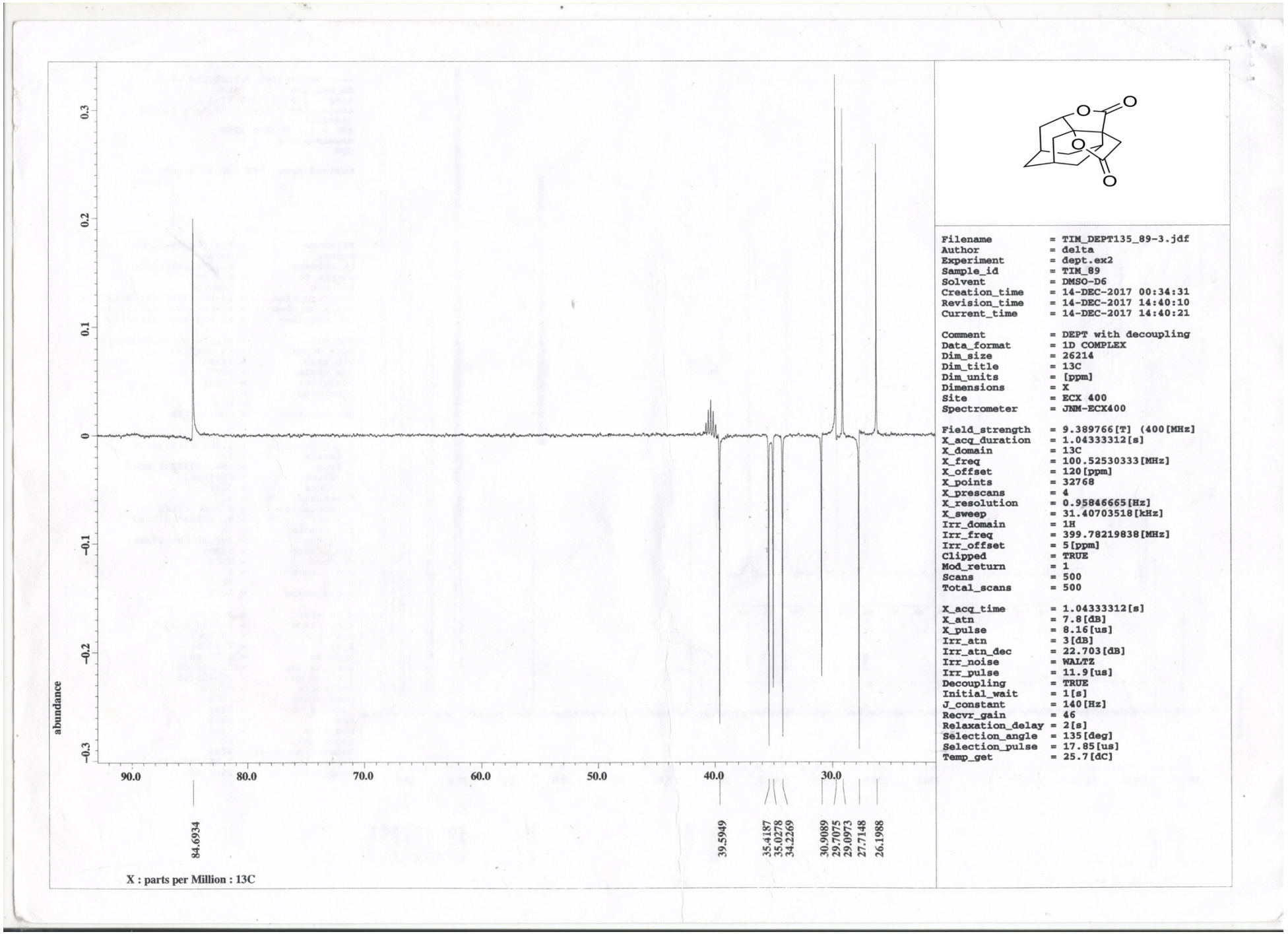


```
Filename          = TIM_1H_89-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = TIM_89
Solvent           = DMSO-D6
Creation_time     = 13-DEC-2017 23:15:33
Revision_time     = 14-DEC-2017 14:37:43
Current_time      = 14-DEC-2017 14:37:56

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]
```

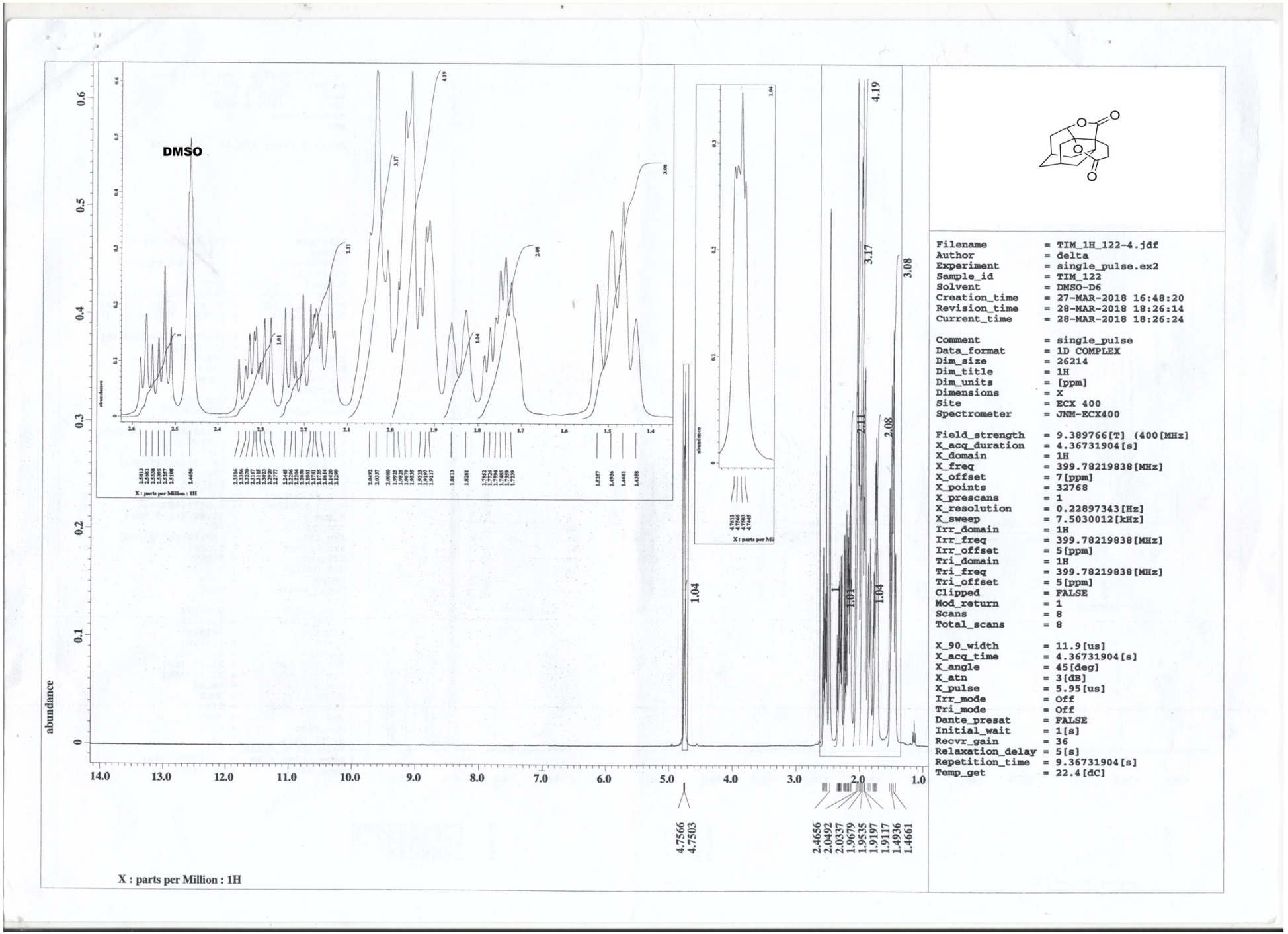
compound 28 ^{1}H NMR



compound.28 ^{13}C NMR

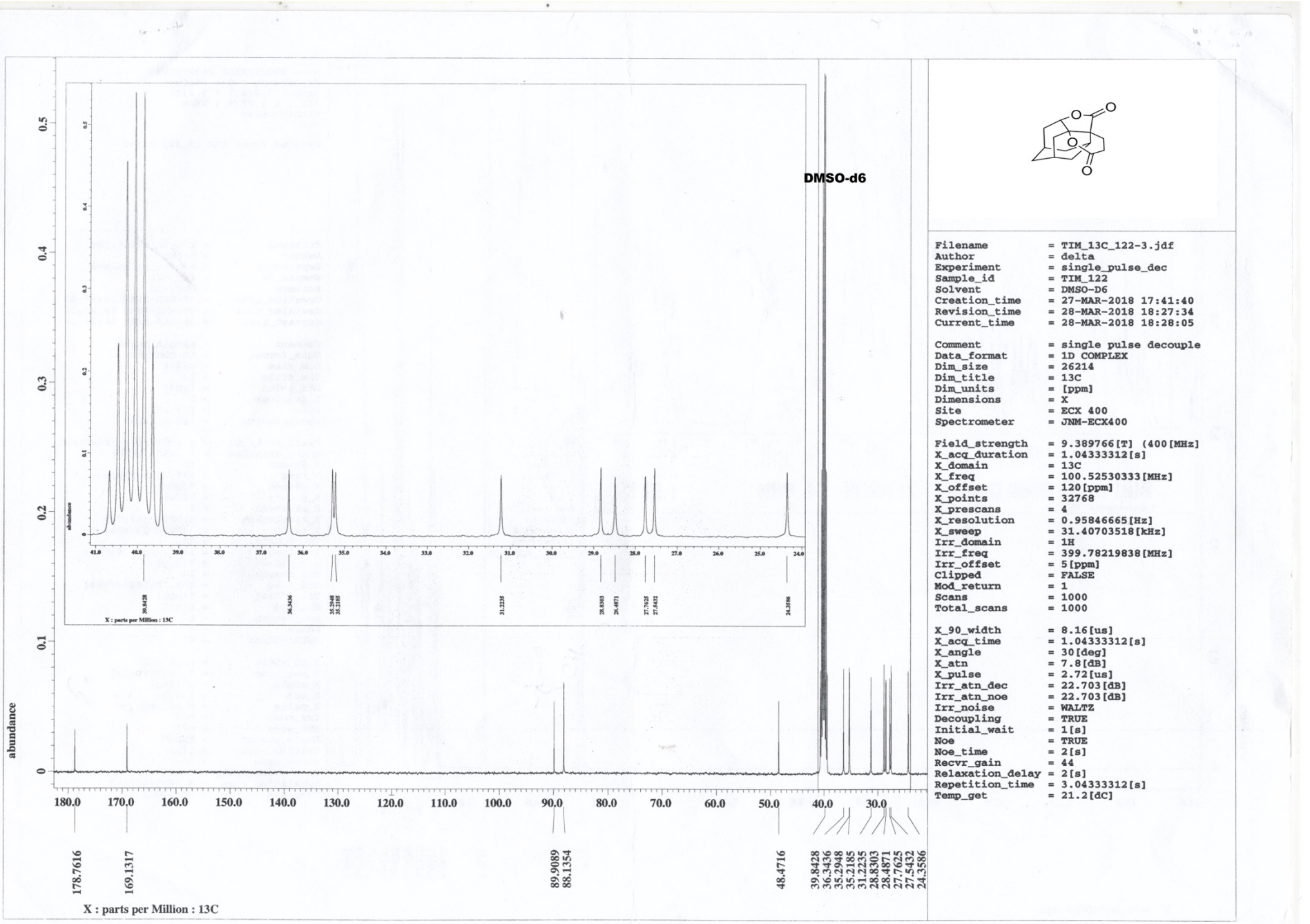


compound 28 DEPT

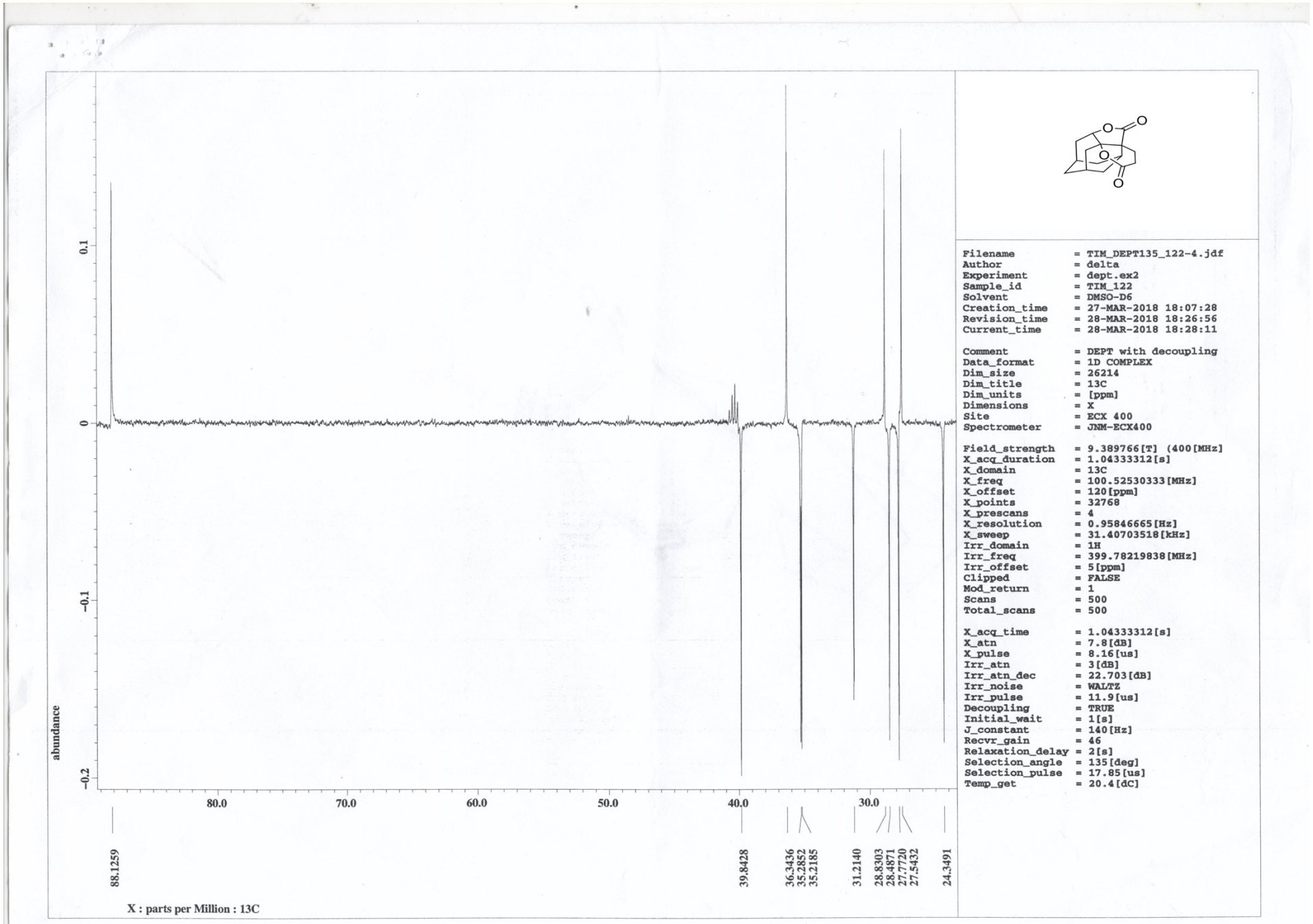



```
Filename          = TIM_1H_122-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = TIM_122
Solvent           = DMSO-D6
Creation_time     = 27-MAR-2018 16:48:20
Revision_time     = 28-MAR-2018 18:26:14
Current_time      = 28-MAR-2018 18:26:24

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        = 36
Relaxation_delay  = 5[s]
Repetition_time   = 9.36731904[s]
Temp_get          = 22.4[dC]
```

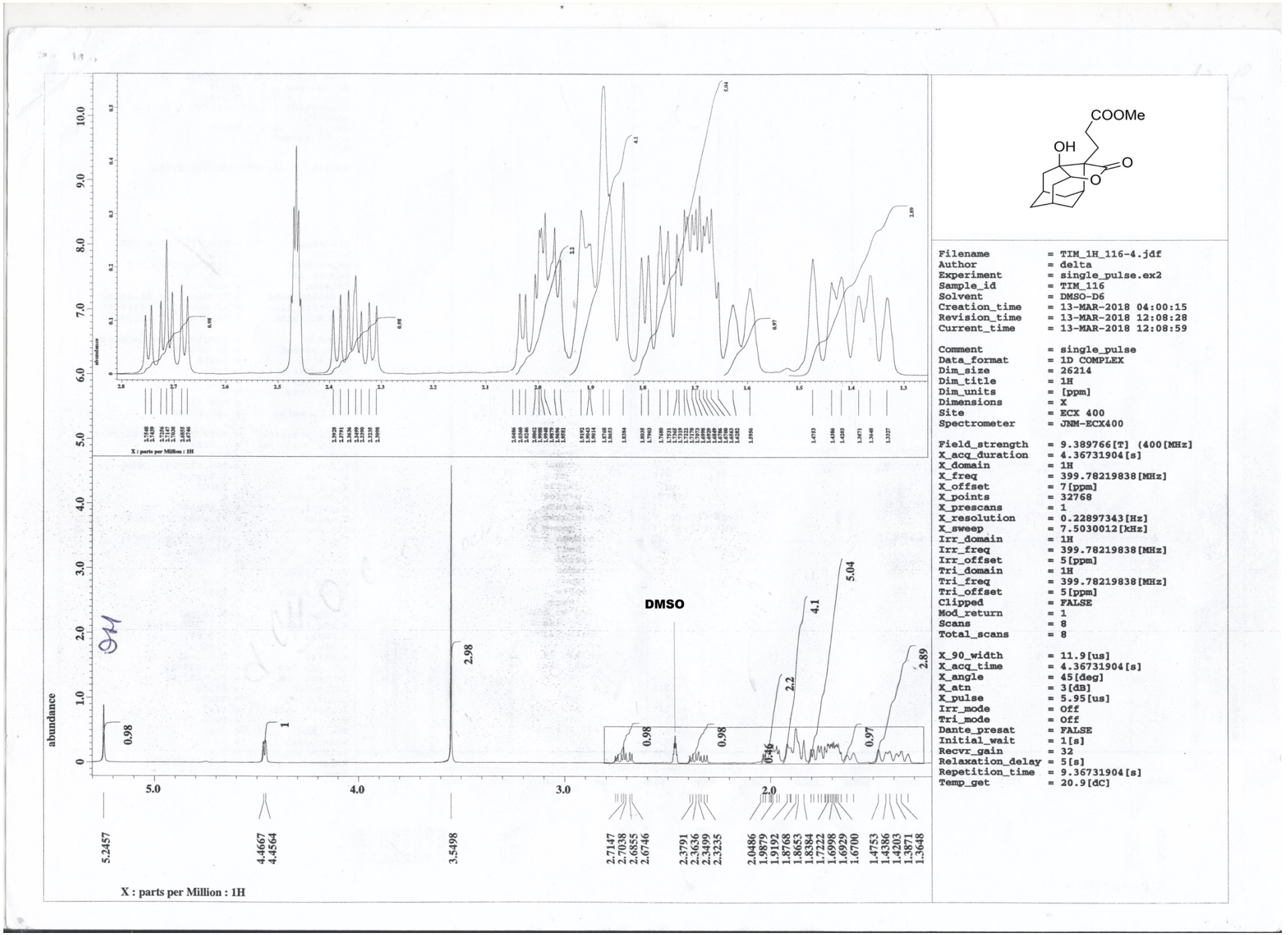
compound 29 ^{1}H NMR



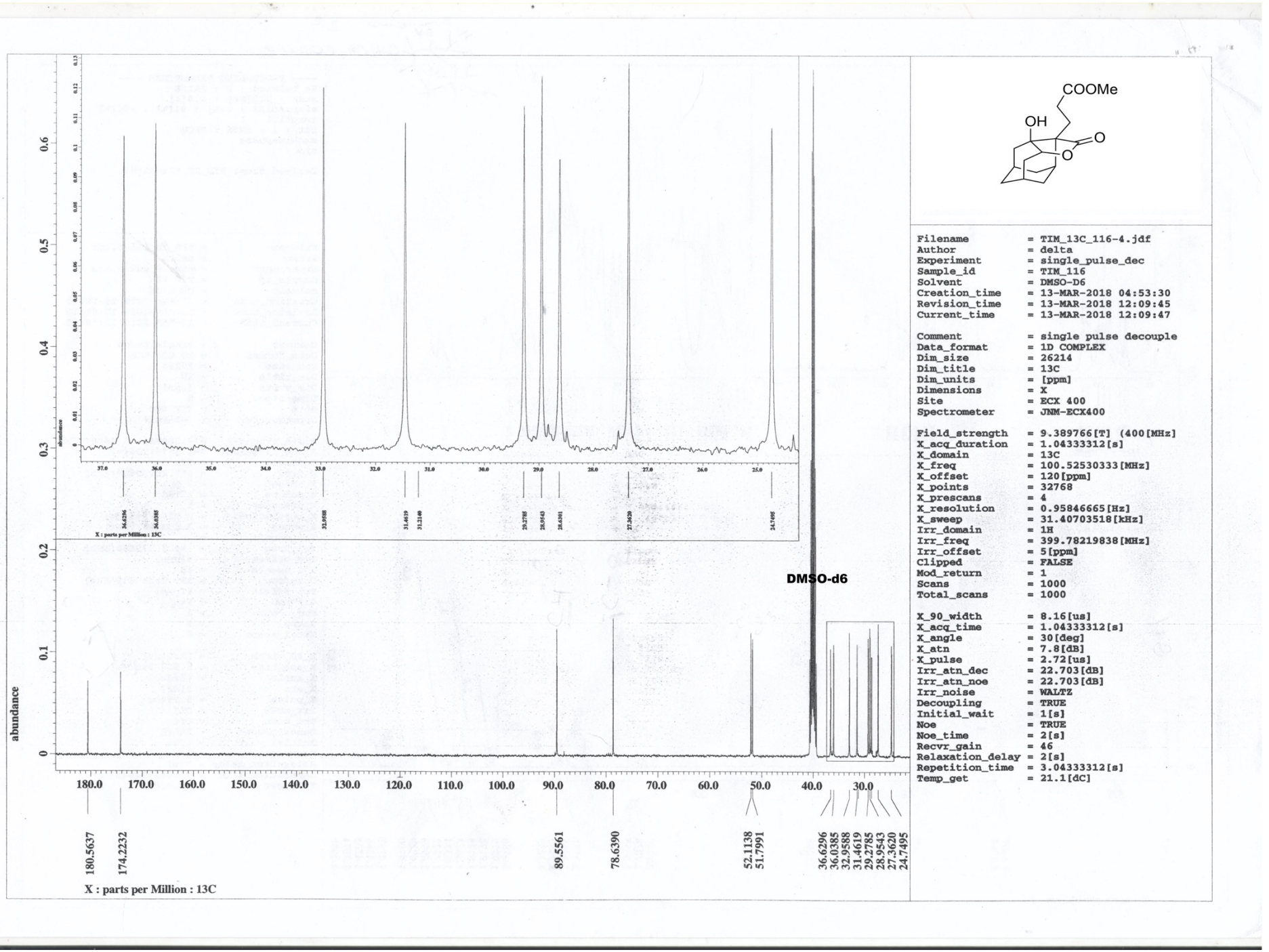
compound 29 ^{13}C NMR



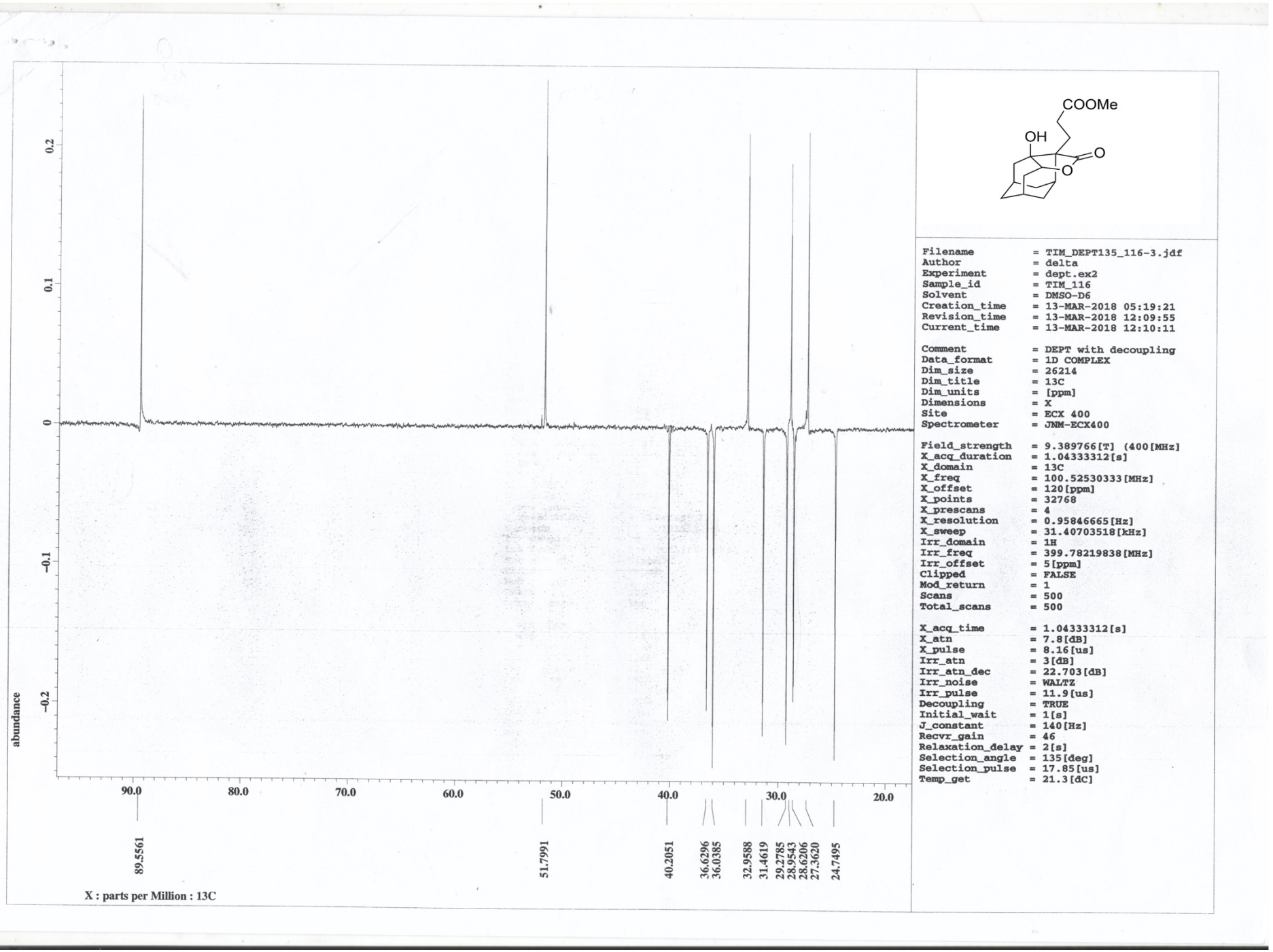
compound 29 DEPT



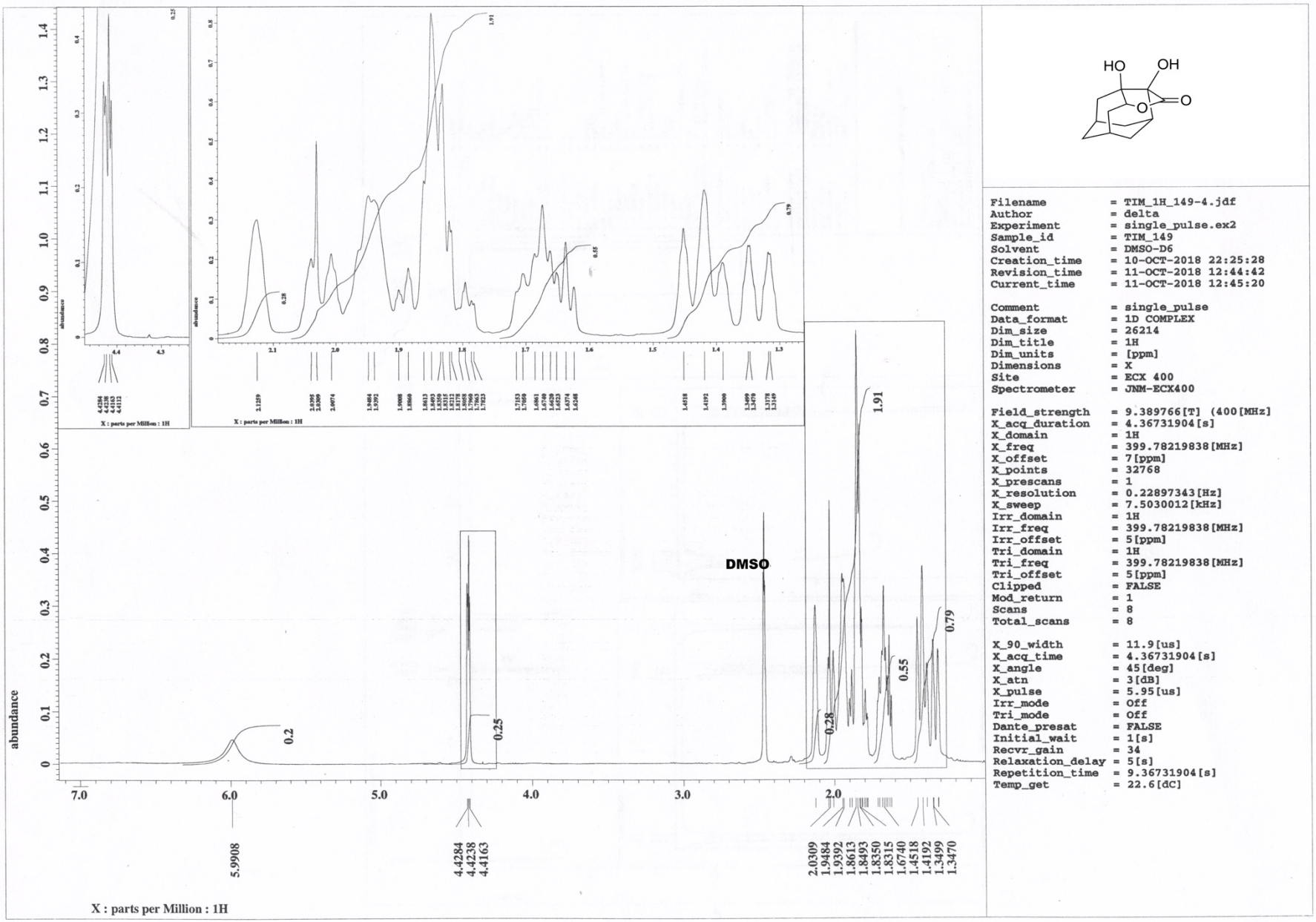
compound 30 ^{1}H NMR



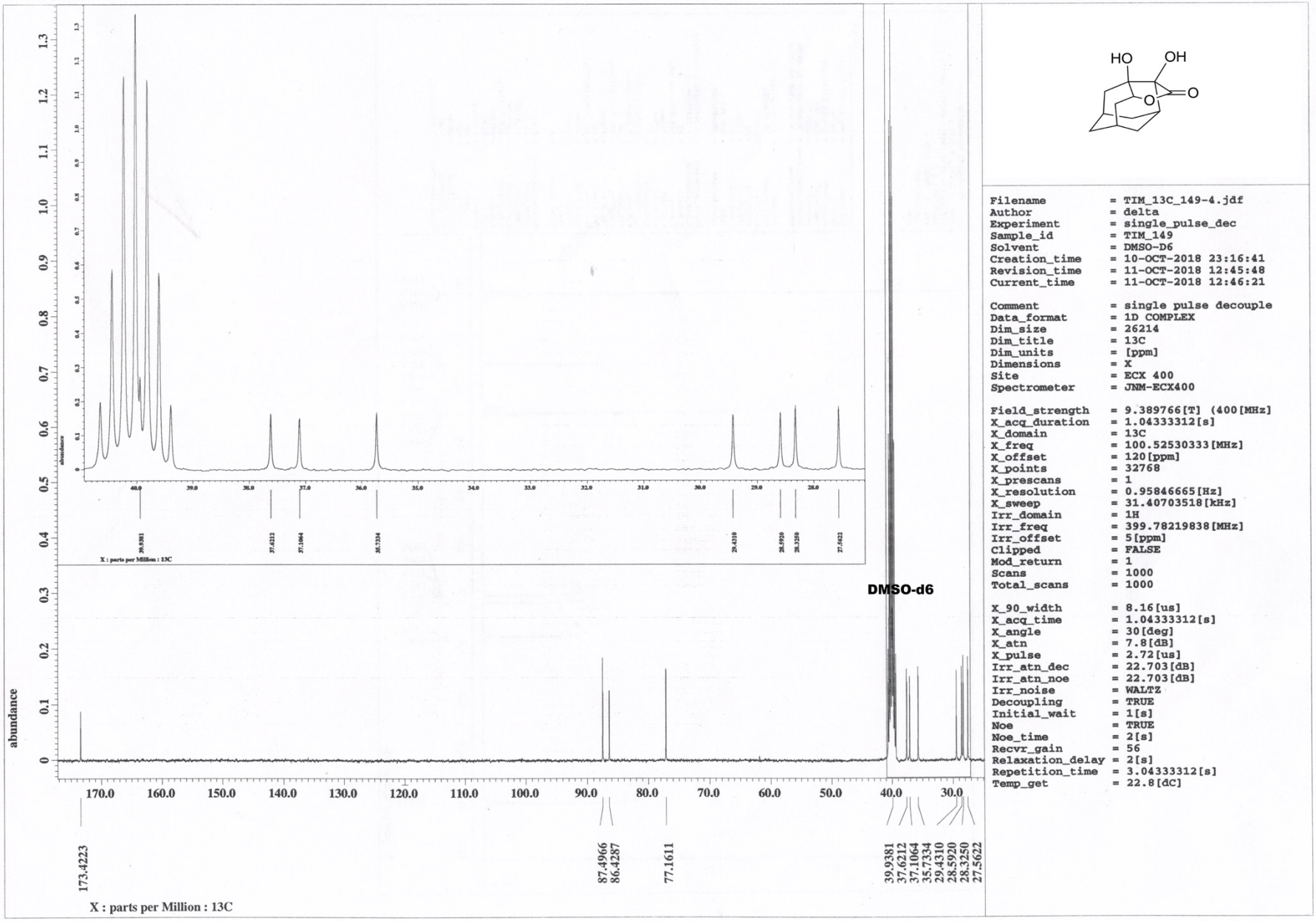
compound 30 ^{13}C NMR



compound 30 DEPT



compound 31 ^{1}H NMR



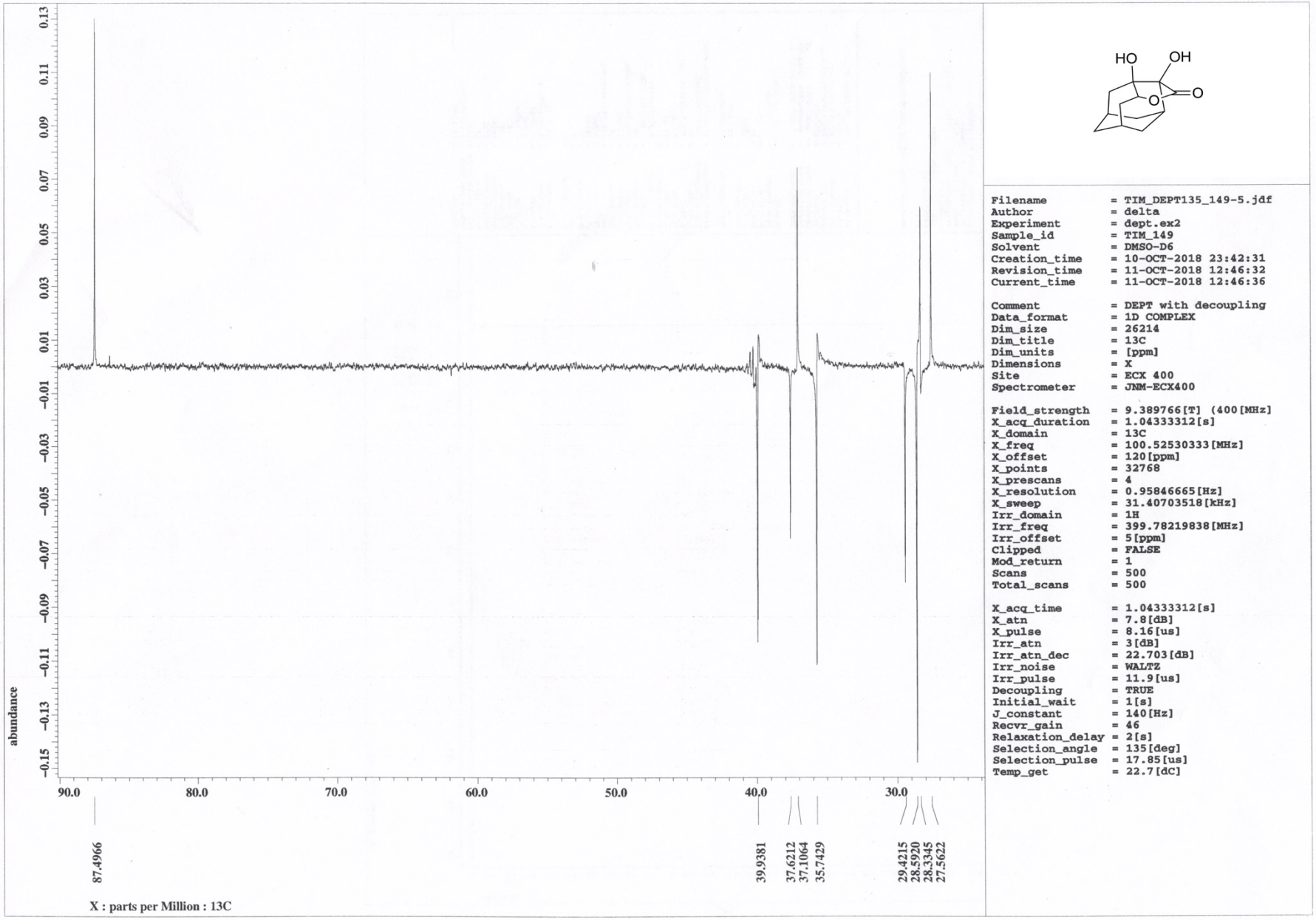
Filename = TIM_13C_149-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = TIM_149
Solvent = DMSO-D6
Creation_time = 10-OCT-2018 23:16:41
Revision_time = 11-OCT-2018 12:45:48
Current_time = 11-OCT-2018 12:46:21

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

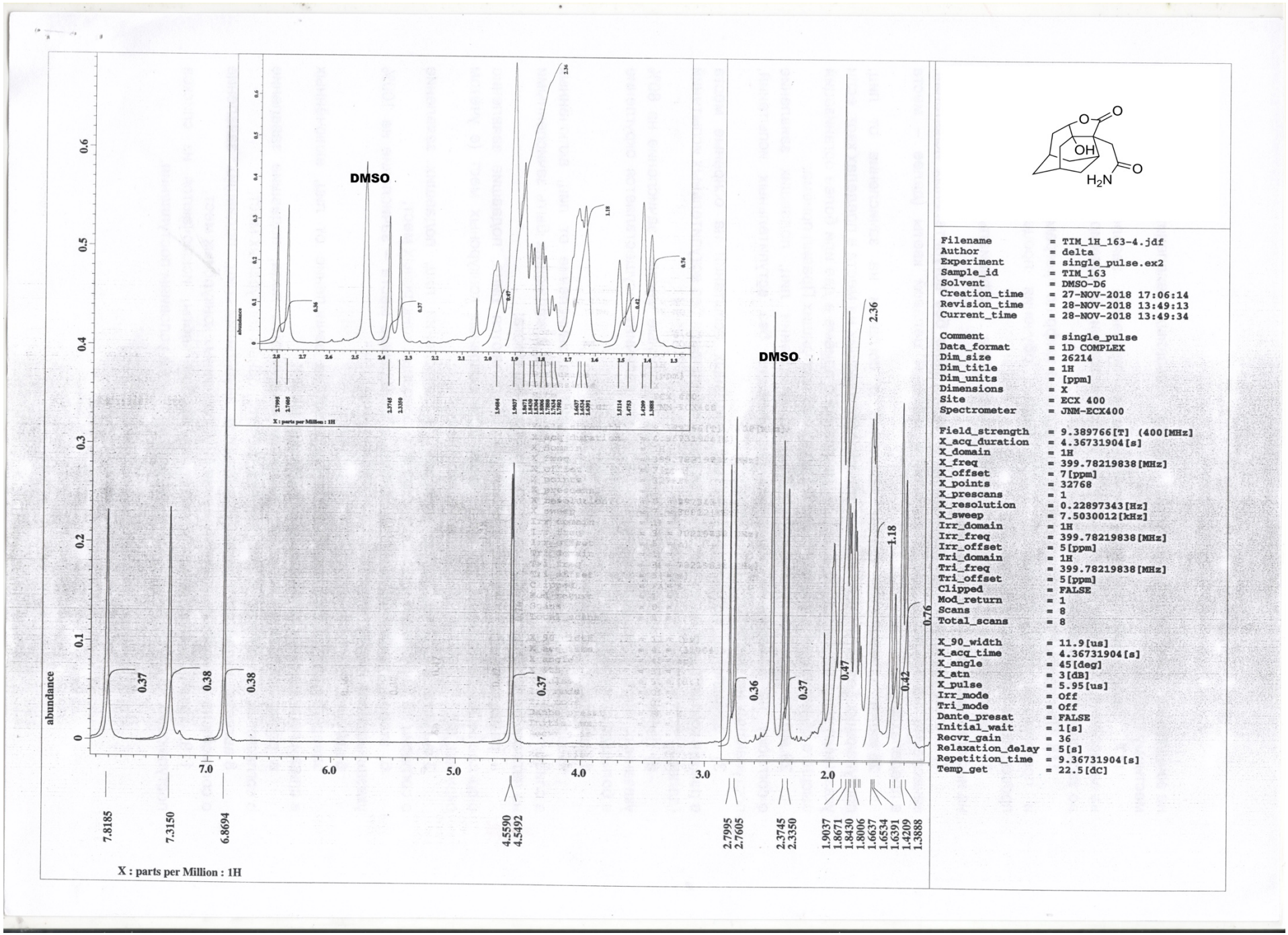
X_90_width = 8.16[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 2.72[us]
Irr_atn_dec = 22.703[dB]
Irr_atn_noe = 22.703[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 56
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 22.8[dC]

compound 31 ^{13}C NMR

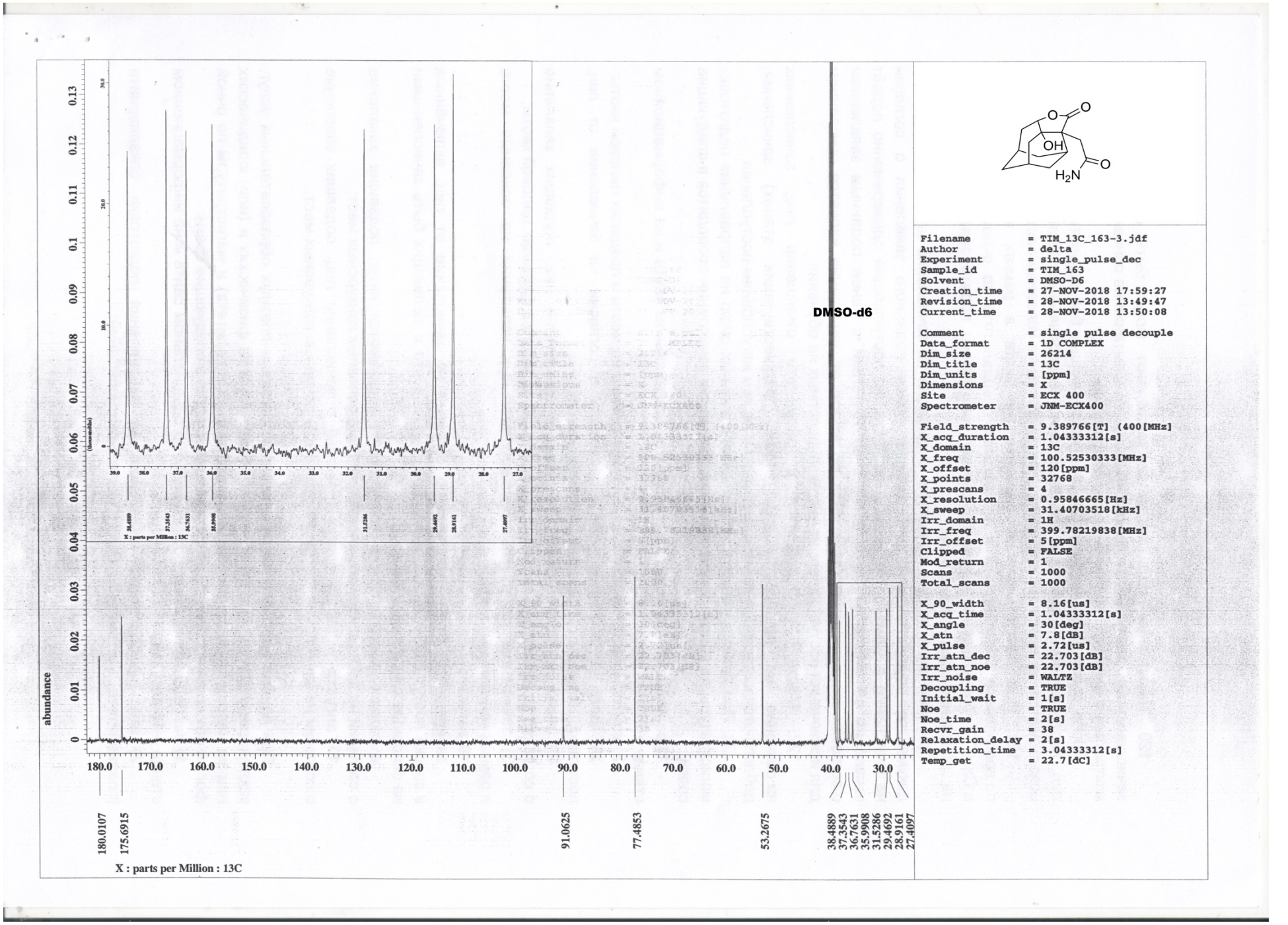



```
Filename          = TIM_DEPT135_149-5.jdf
Author            = delta
Experiment        = dept.ex2
Sample_id         = TIM_149
Solvent           = DMSO-D6
Creation_time     = 10-OCT-2018 23:42:31
Revision_time     = 11-OCT-2018 12:46:32
Current_time      = 11-OCT-2018 12:46:36

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[dC]
```

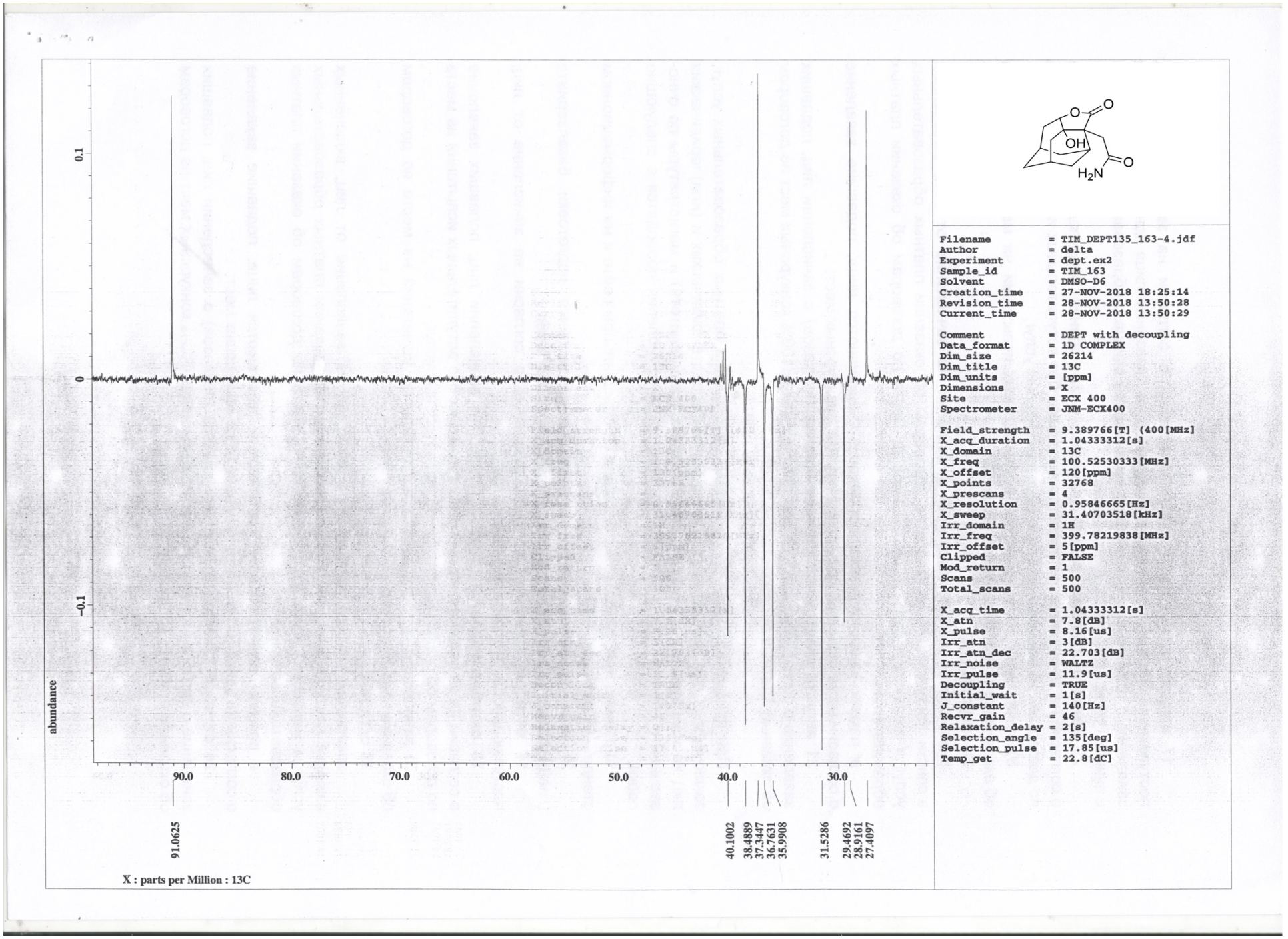
compound 31 DEPT



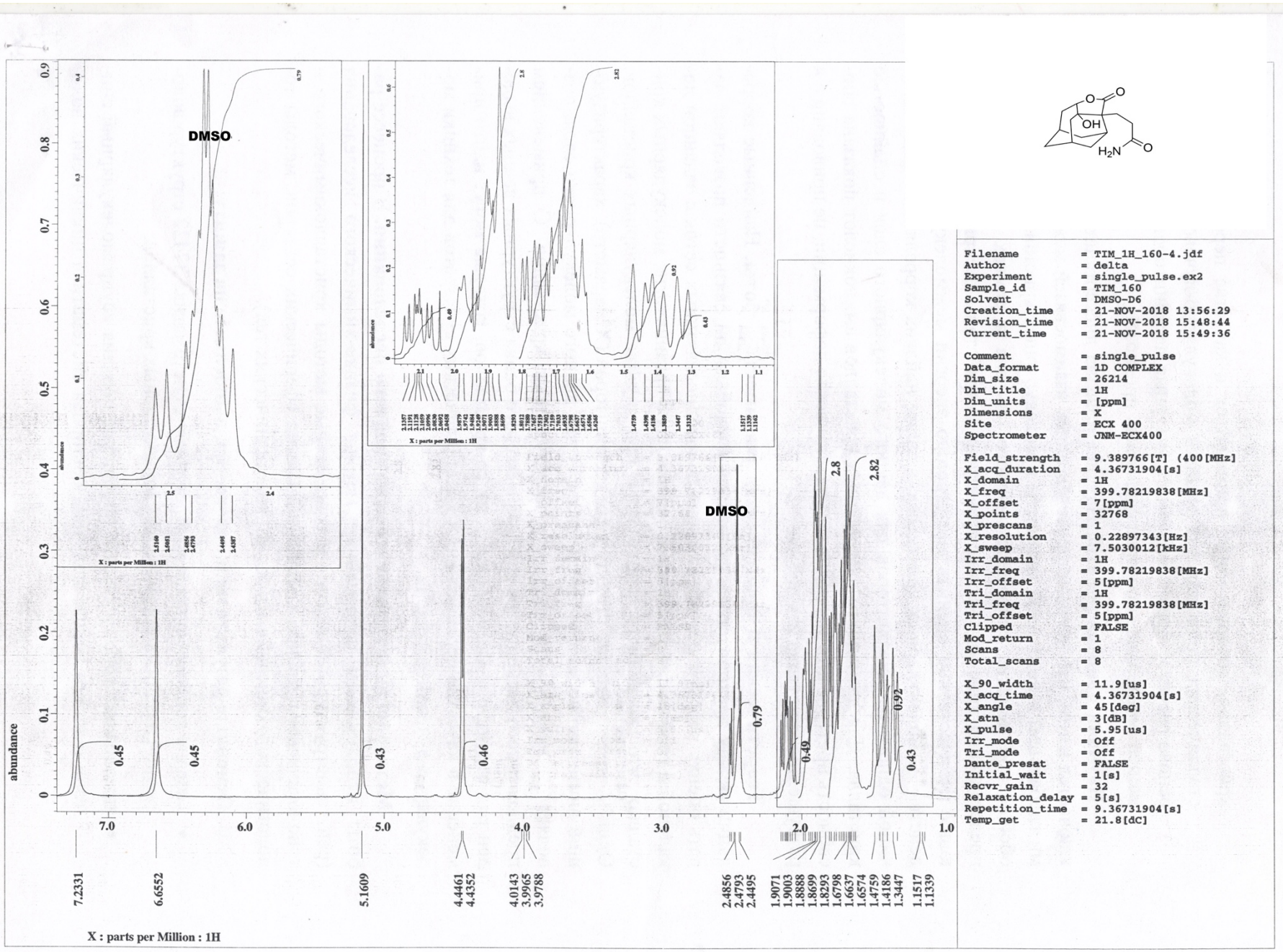
compound 32 ^{1}H NMR



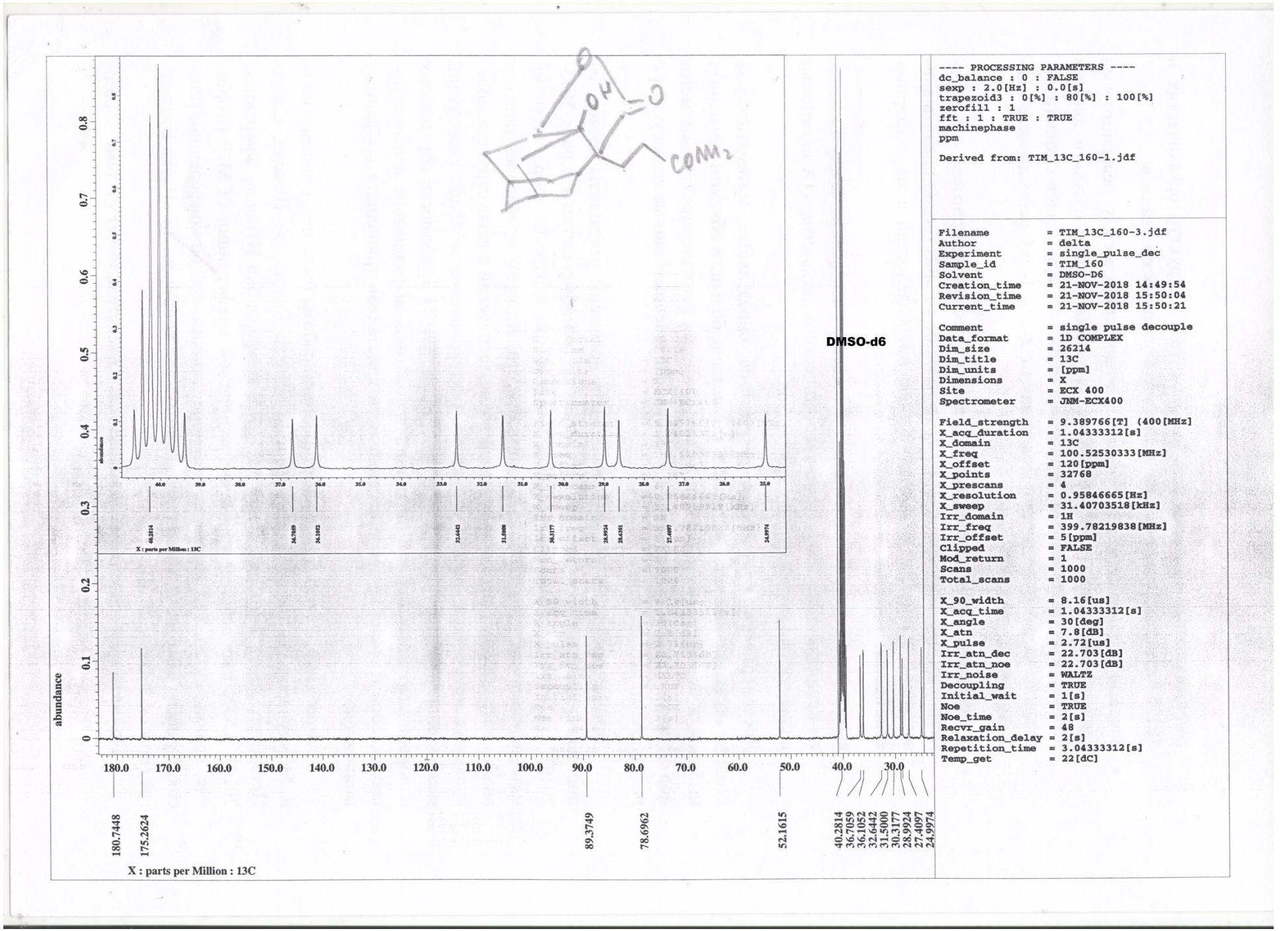
compound 32 ^{13}C NMR



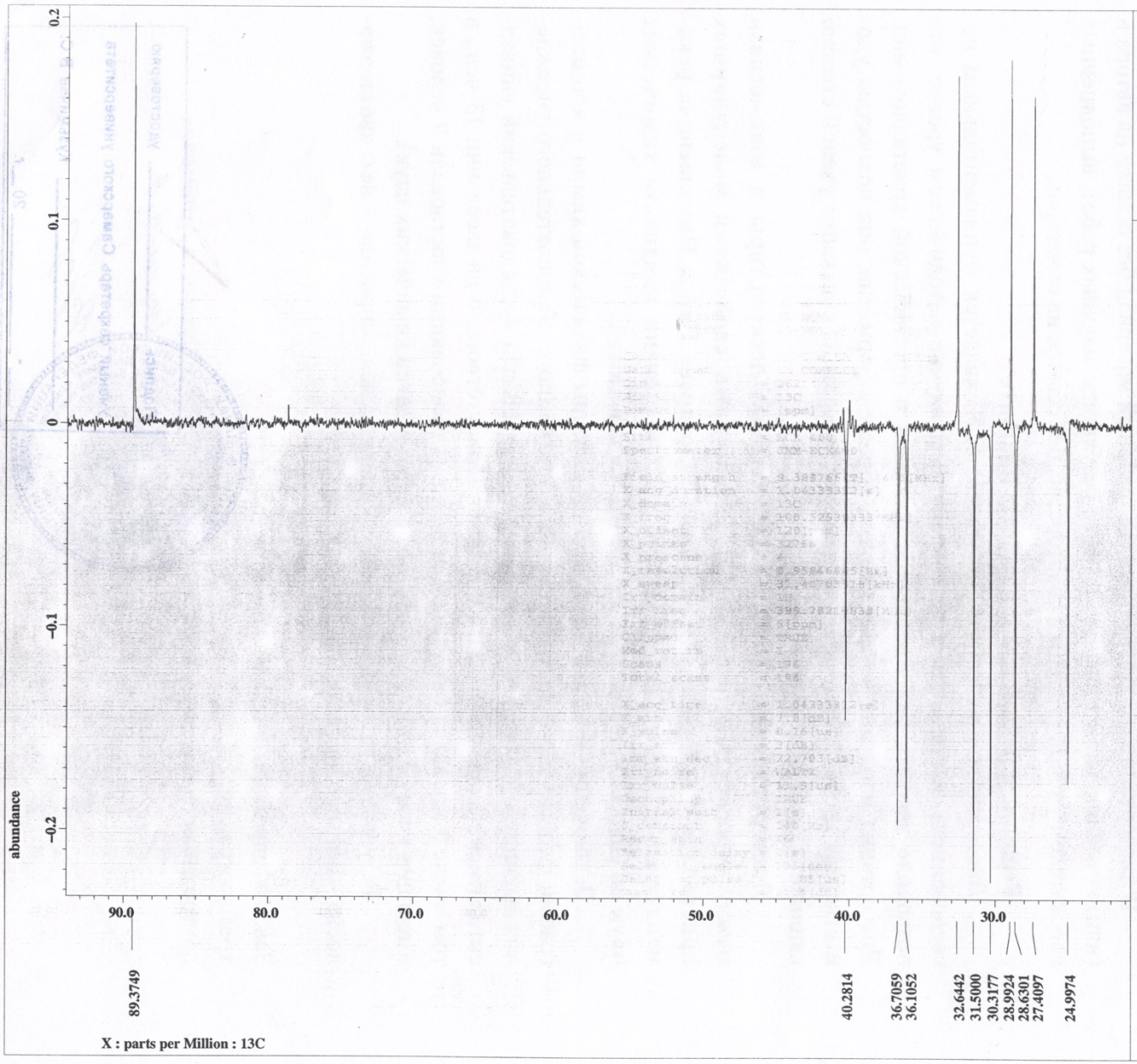
compound 32 DEPT

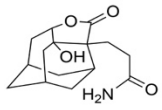


compound 33 ^{1}H NMR



compound 33 ^{13}C NMR





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	= 9.389766[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	= 196
Total_scans	= 196
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	= 21.9[dC]

compound 33 DEPT

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_2O	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 K_2CO_3, with stirring. [Time; yield, %]

Solvent/t, ºC / Michael acceptor	Acetonitrile, 25 ºC	Acetonitrile, 50 ºC	Acetone, 25 ºC	Acetone, 50 ºC	DMF, 25 ºC	DMF, 50 ºC	DMF, 80 ºC	Acetone, 50 ºC, 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%