

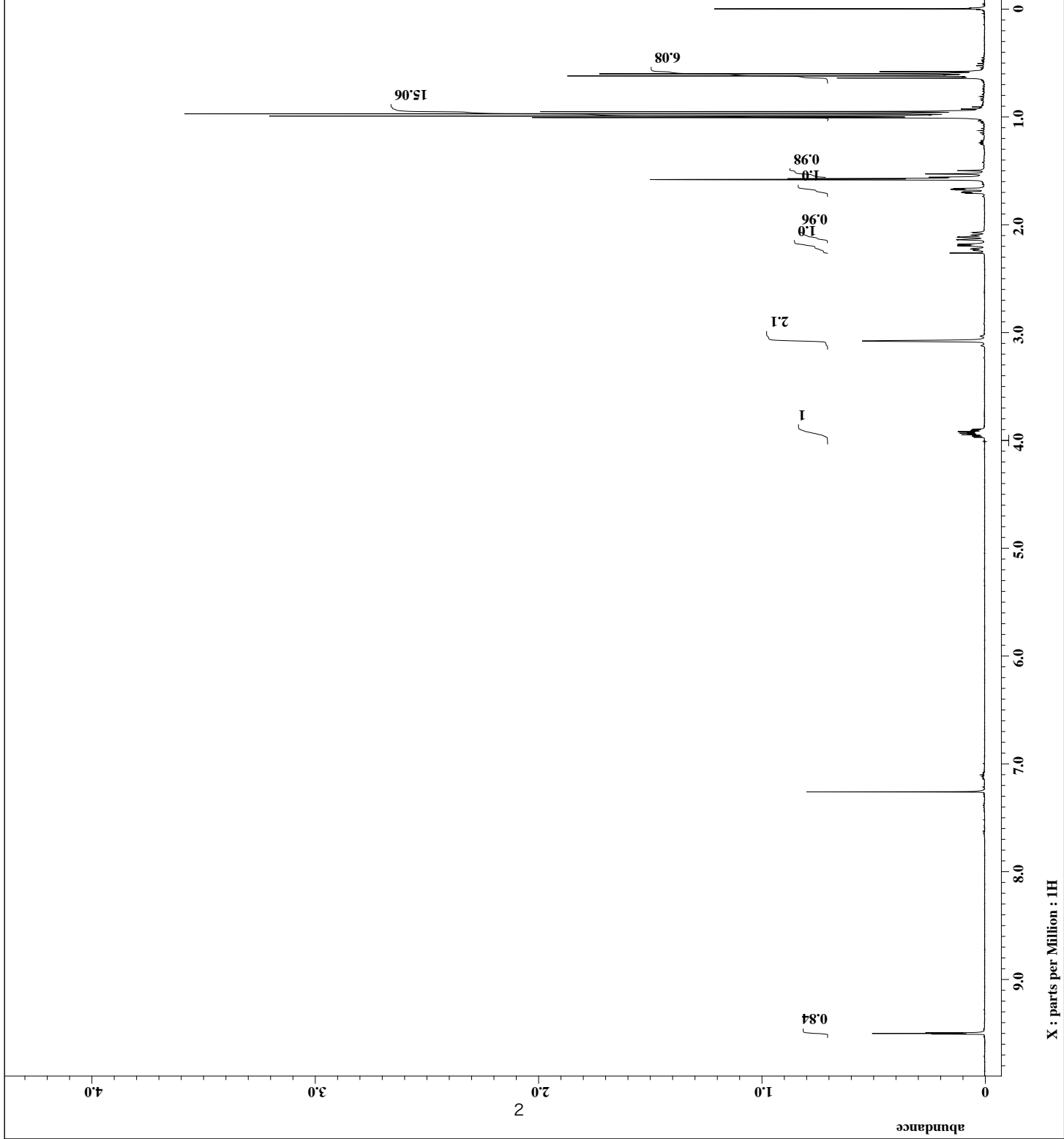
Stereocontrolled Total Synthesis of Fucoxanthin and its Polyene Chain-modified Derivative

Takayuki Kajikawa,^a Satoshi Okumura,^a Takashi Iwashita,^b Daisuke Kosumi,^c Hideki Hashimoto^c and Shigeo Katsumura^{a}*

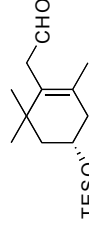
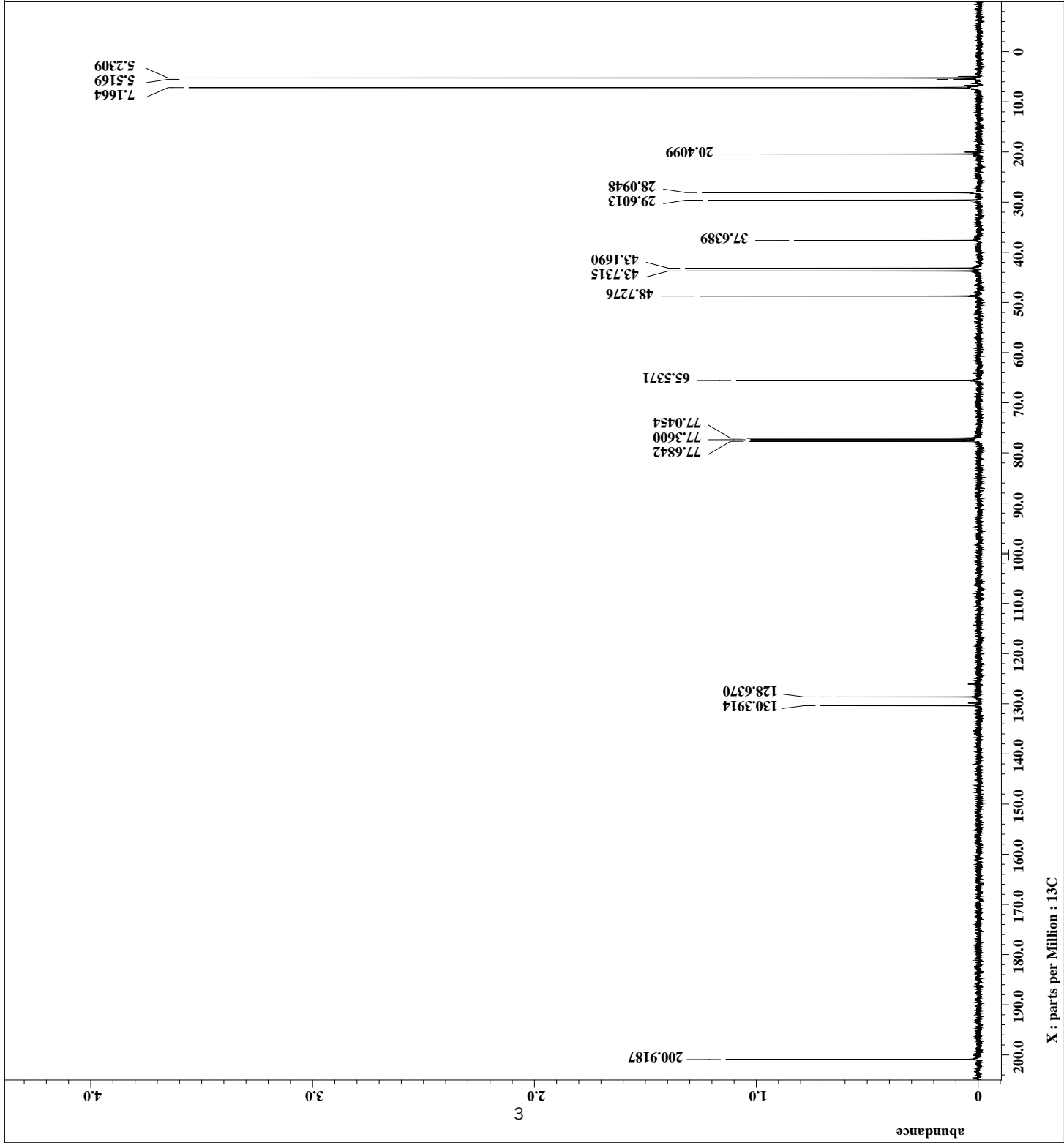
^aDepartment of Chemistry, School of Science and Technology, Kwansei Gakuin University, Gakuen, Sanda, Hyogo 669-1337 ^bSuntory Institute For Bioorganic Research, Wakayamadai, Shimamoto, Mishimagun, Osaka 618-8503 ^cDepartment of Physics and CREST/JST, Graduate School of Science, Osaka City University, Sugimoto, Sumiyoshi-ku, Osaka 558-8585, Japan.

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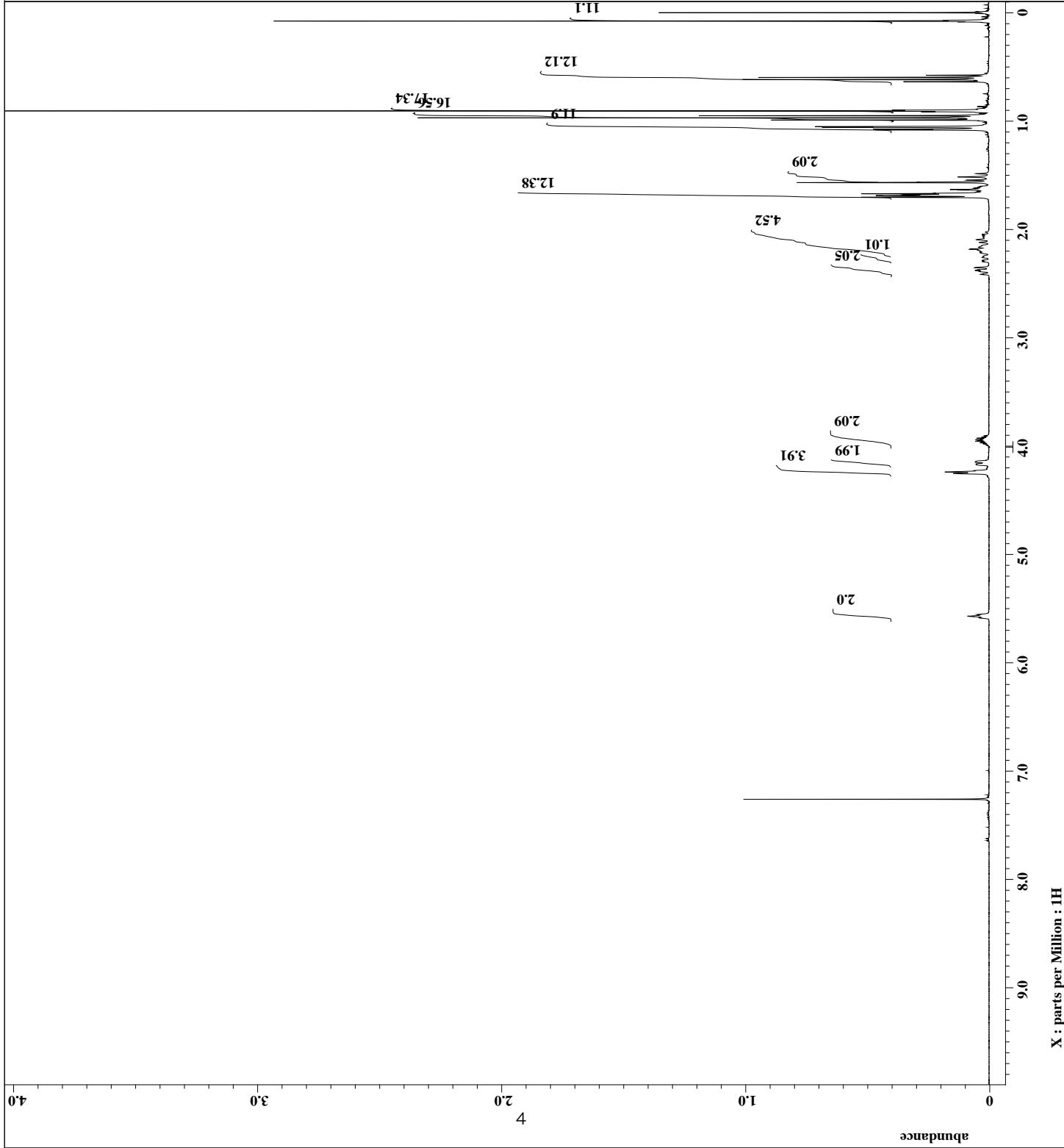
NMR spectra



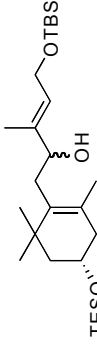
Filename = aldehyde-1H-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 30-JUN-2010 12:14:20
Revision_time = 21-DEC-2010 10:27:17
Current_time = 21-DEC-2010 10:27:58
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 24.5[dC]

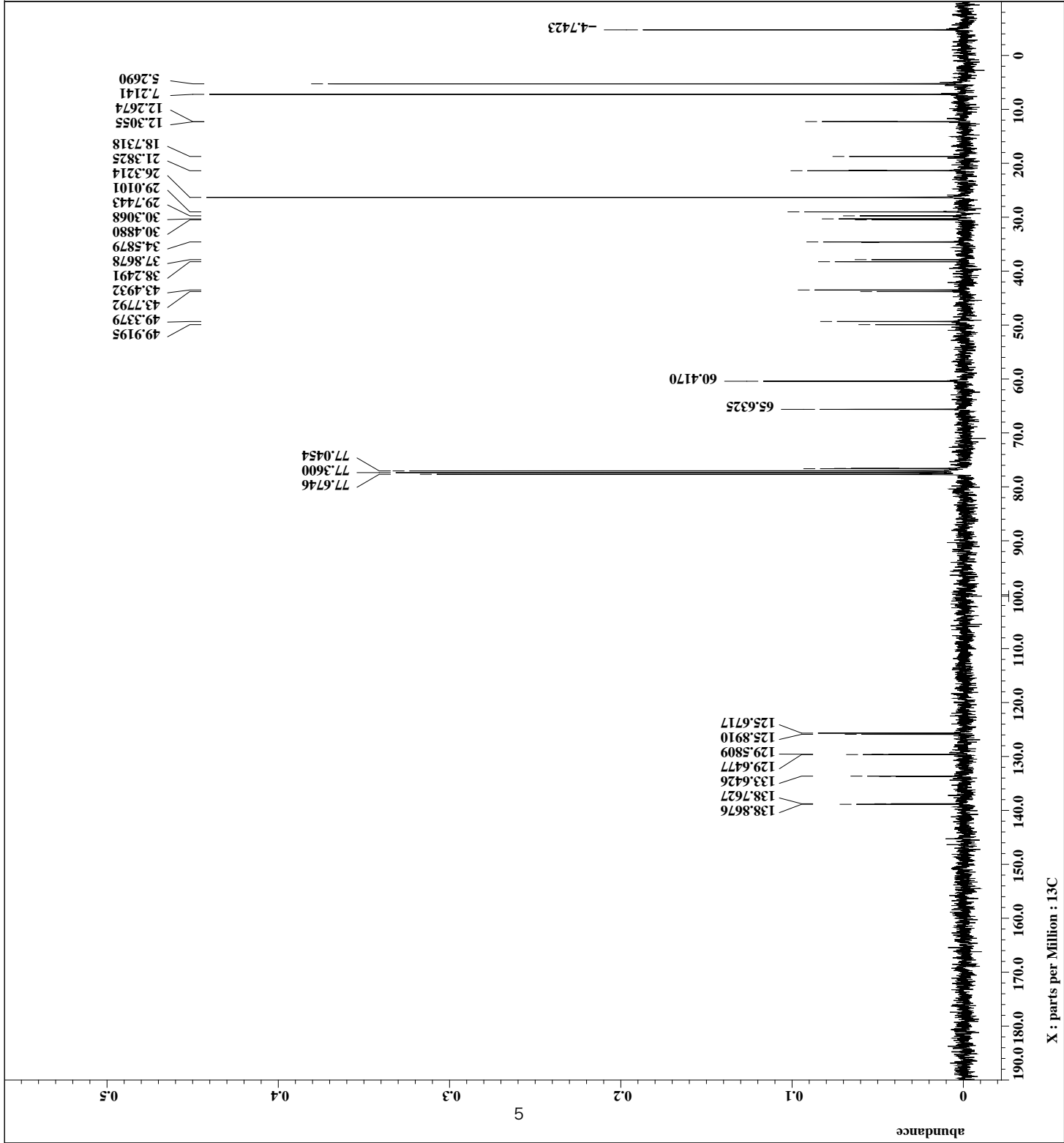


Filename = aldehyde-13C-3.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#476692
Solvent = CHLOROFORM-D
Creation_time = 30-JUN-2010 12:29:51
Revision_time = 21-DEC-2010 09:58:47
Current_time = 21-DEC-2010 09:59:37
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 68
Total_scans = 68
X_90_width = 9.2[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[dB]
X_pulse = 4.6[us]
Irr_atn_dec = 22.2[dB]
Irr_atn_noe = 22.2[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 60
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.8[dC]

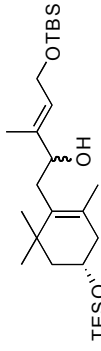


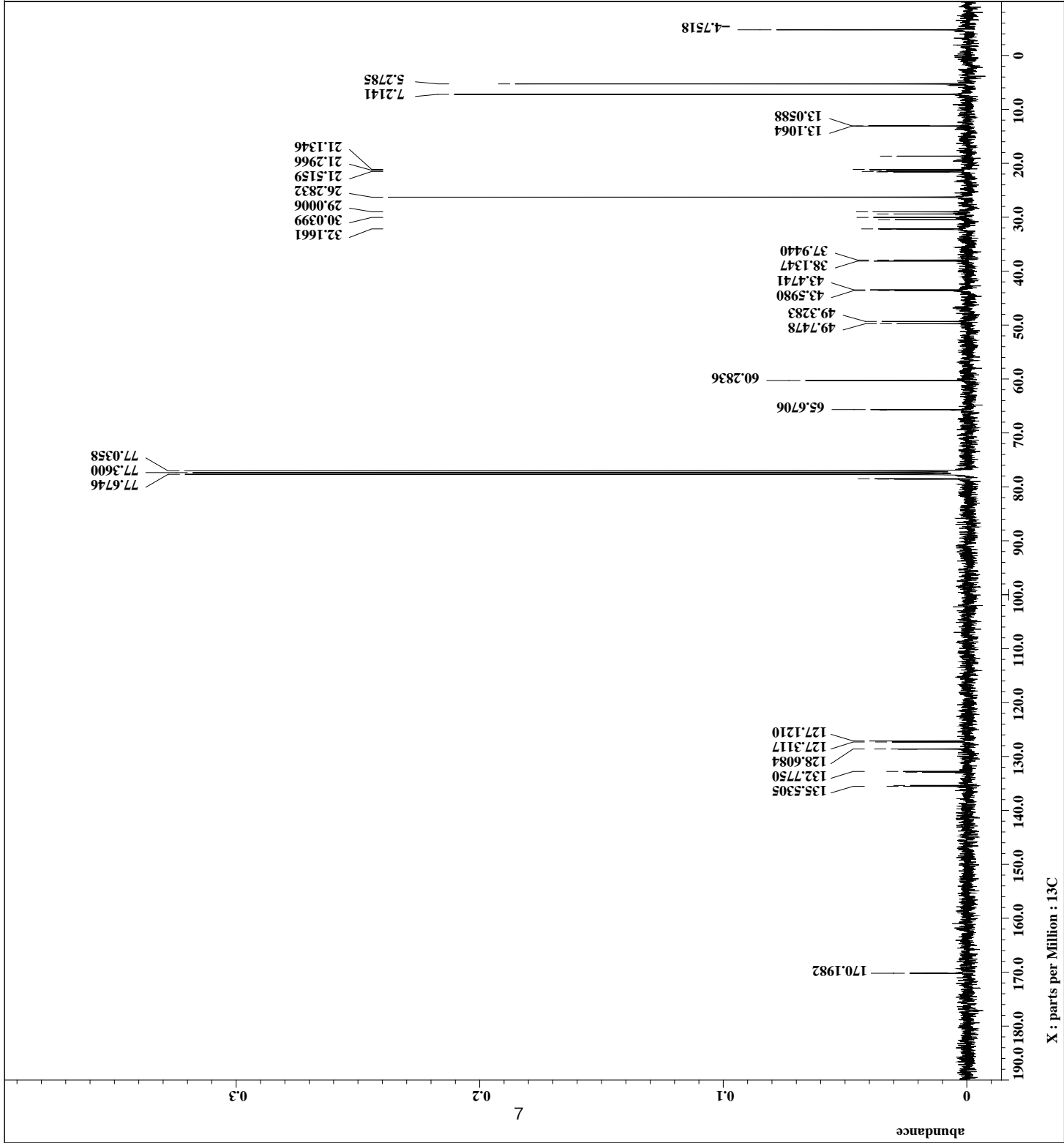
Filename = tes-OH-tbs-1H-6.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 9-JUL-2010 18:24:44
Revision_time = 16-JUL-2011 11:20:21
Current_time = 16-JUL-2011 11:21:48
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 25[dc]



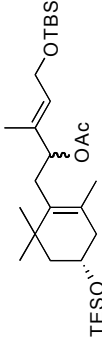


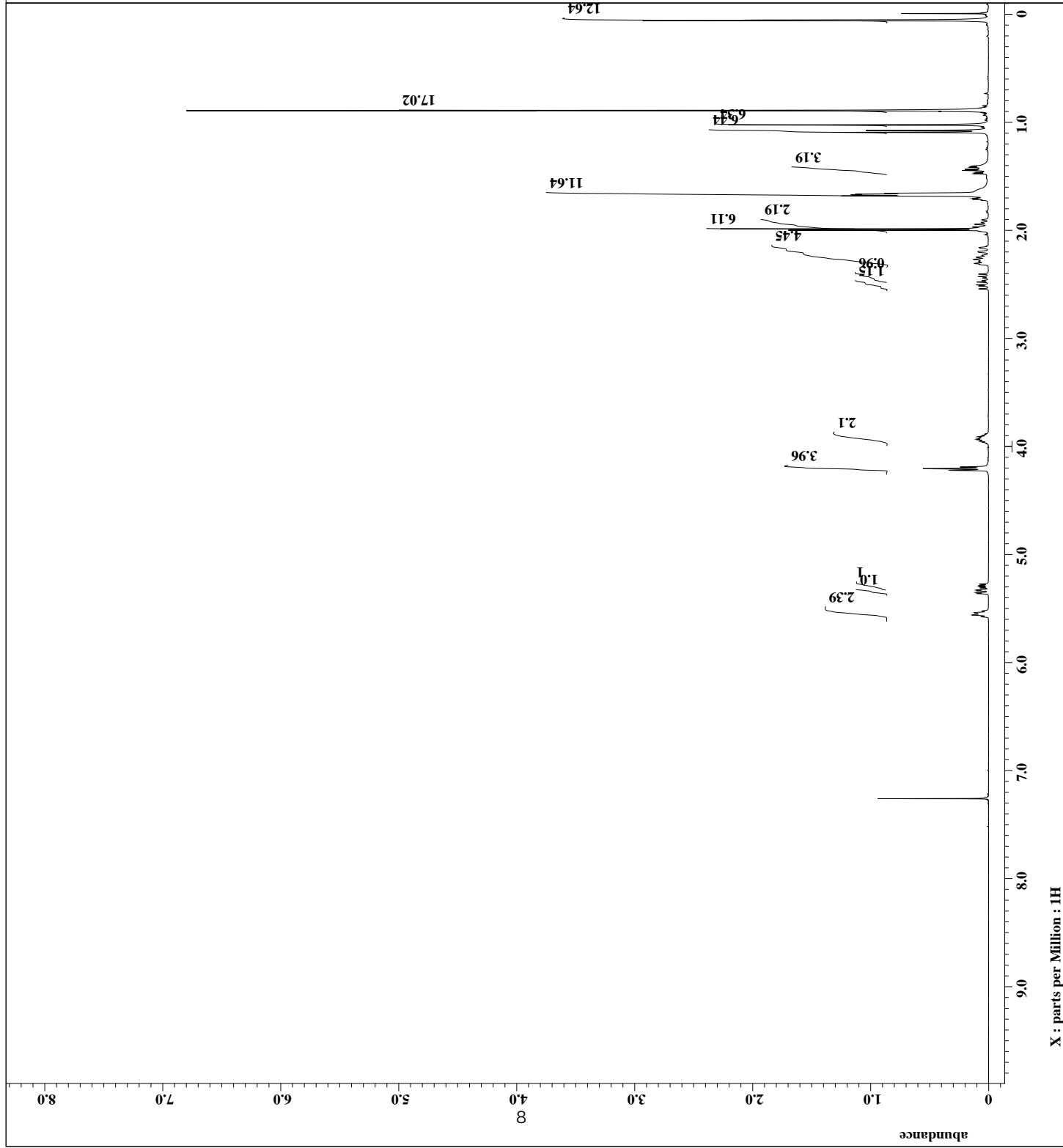
Filename = tes-oh-tbs-13c-3.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#69858
Solvent = CHLOROFORM-D
Creation_time = 9-JUL-2010 18:36:14
Revision_time = 21-DEC-2010 10:00:37
Current_time = 21-DEC-2010 10:01:37
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = x
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
irr_domain = 1H
irr_freq = 399.78219838[MHz]
irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 44
Total_scans = 44
x_90_width = 9.2[us]
x_acq_time = 1.04333312[s]
x_angle = 45[deg]
x_atn = 6.6[dB]
x_pulse = 4.6[us]
irr_atn_dec = 22.2[dB]
irr_atn_noe = 22.2[dB]
irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 25.2[dc]





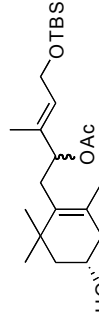
Filename = tes-OAc-tbs-13C-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#348376
Solvent = CHLOROFORM-D
Creation_time = 13-JUL-2010 09:00:07
Revision_time = 16-JUL-2011 11:42:59
Current_time = 16-JUL-2011 11:43:32
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 117
Total_scans = 117
X_90_width = 9.2[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[dB]
X_pulse = 4.6[us]
Irr_atn_dec = 22.2[dB]
Irr_atn_noe = 22.2[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 25.1[degC]

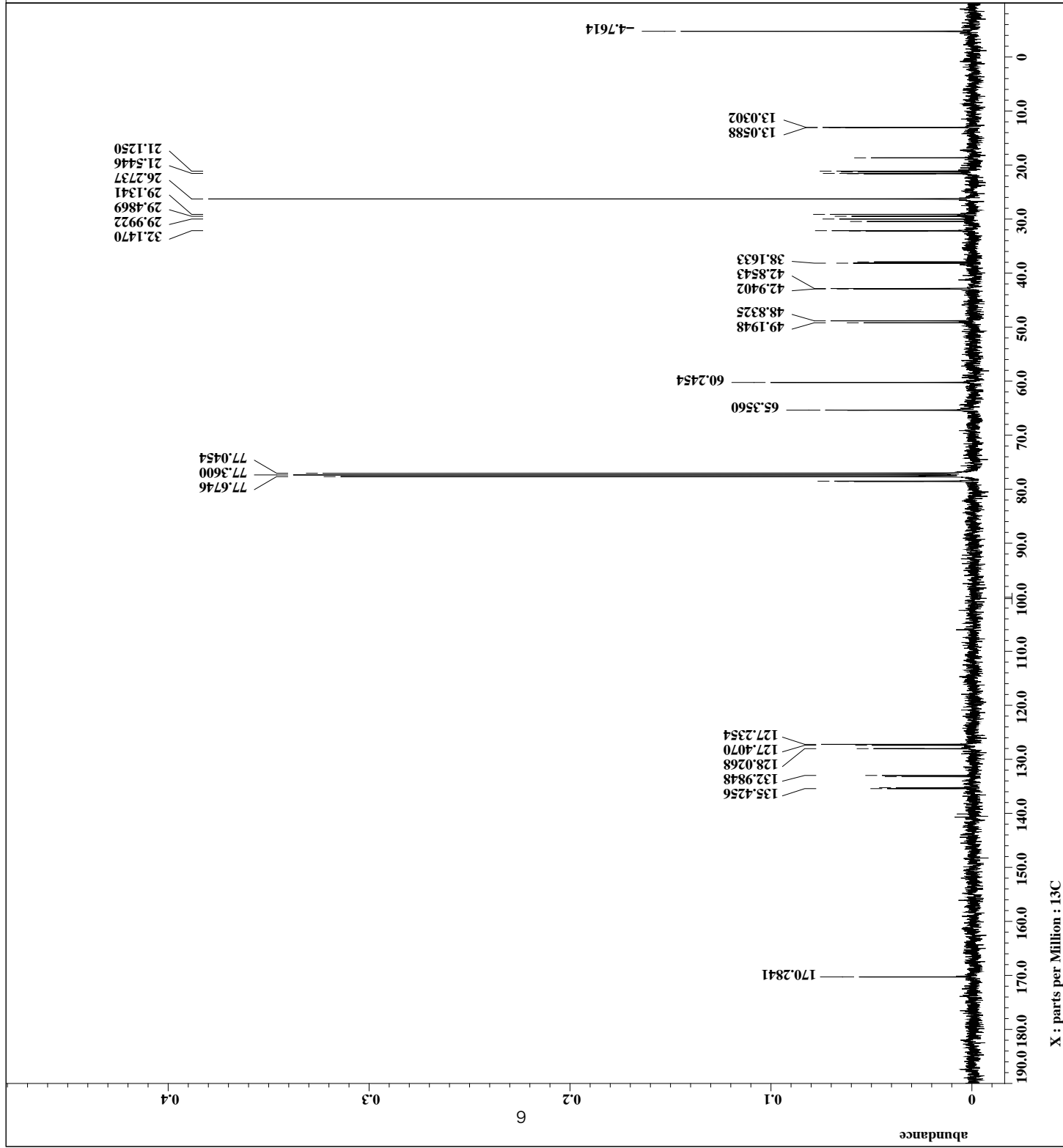




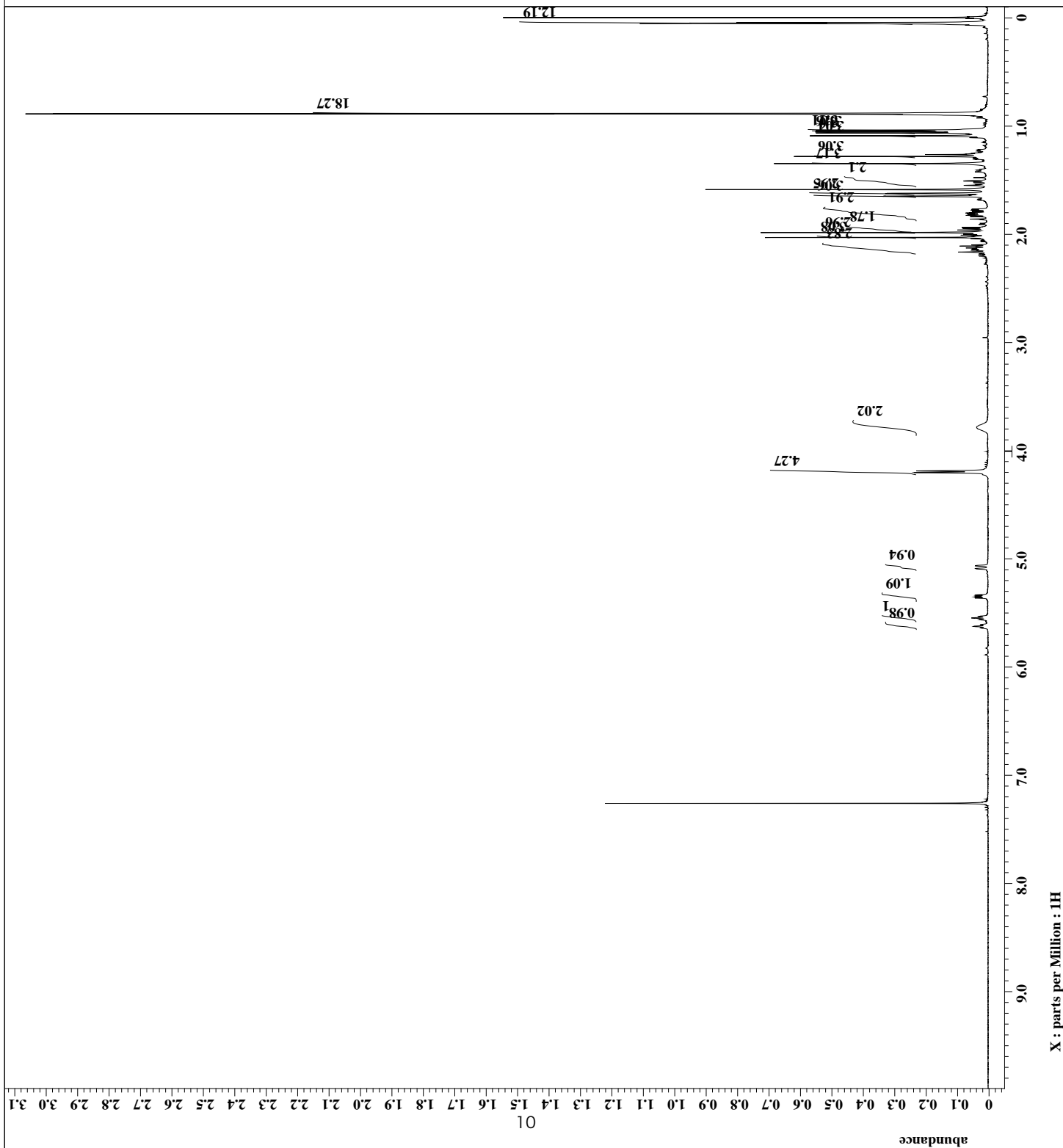
X : parts per Million : 1H

Filename	=	OH-OAc-tbs-1H-3.jdf
Author	=	delta
Experiment	=	single_pulse.ex2
Sample_id	=	1
Solvent	=	CHLOROFORM-D
Creation_time	=	30-JUN-2010 09:51:14
Revision_time	=	16-JUL-2011 11:39:54
Current_time	=	16-JUL-2011 11:40:27
Comment	=	single_pulse
Data format	=	ID COMPLEX
Dim_size	=	13107
Dim_title	=	1H
Dim_units	=	[ppm]
Dimensions	=	x
Site	=	ECX400M
Spectrometer	=	DELTA2_NMR
Field_strength	=	9.389766[T] (400[MHz]
x_acq_duration	=	2.18365952[s]
x_domain	=	1H
x_freq	=	399.78219838[MHz]
x_offset	=	4[ppm]
x_points	=	16384
x_prescans	=	1
x_resolution	=	0.457994685[Hz]
x_sweep	=	7.5030012[kHz]
irr_domain	=	1H
irr_freq	=	399.78219838[MHz]
irr_offset	=	5[ppm]
tri_domain	=	1H
tri_freq	=	399.78219838[MHz]
tri_offset	=	5[ppm]
Clipped	=	FALSE
Mod return	=	1
Scans	=	8
Total_scans	=	8
x_90_width	=	10.5[us]
x_acq_time	=	2.18365952[s]
x_angle	=	45[deg]
x_atn	=	1.4[dB]
x_pulse	=	5.25[us]
irr_mode	=	Off
tri_mode	=	Off
Dante_presat	=	FALSE
Initial_wait	=	1[s]
Recvr_gain	=	34
Relaxation_delay	=	1[s]
Repetition_time	=	3.18365952[s]
Temp get	=	24.4[degC]



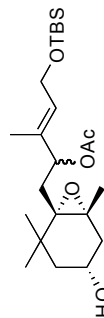


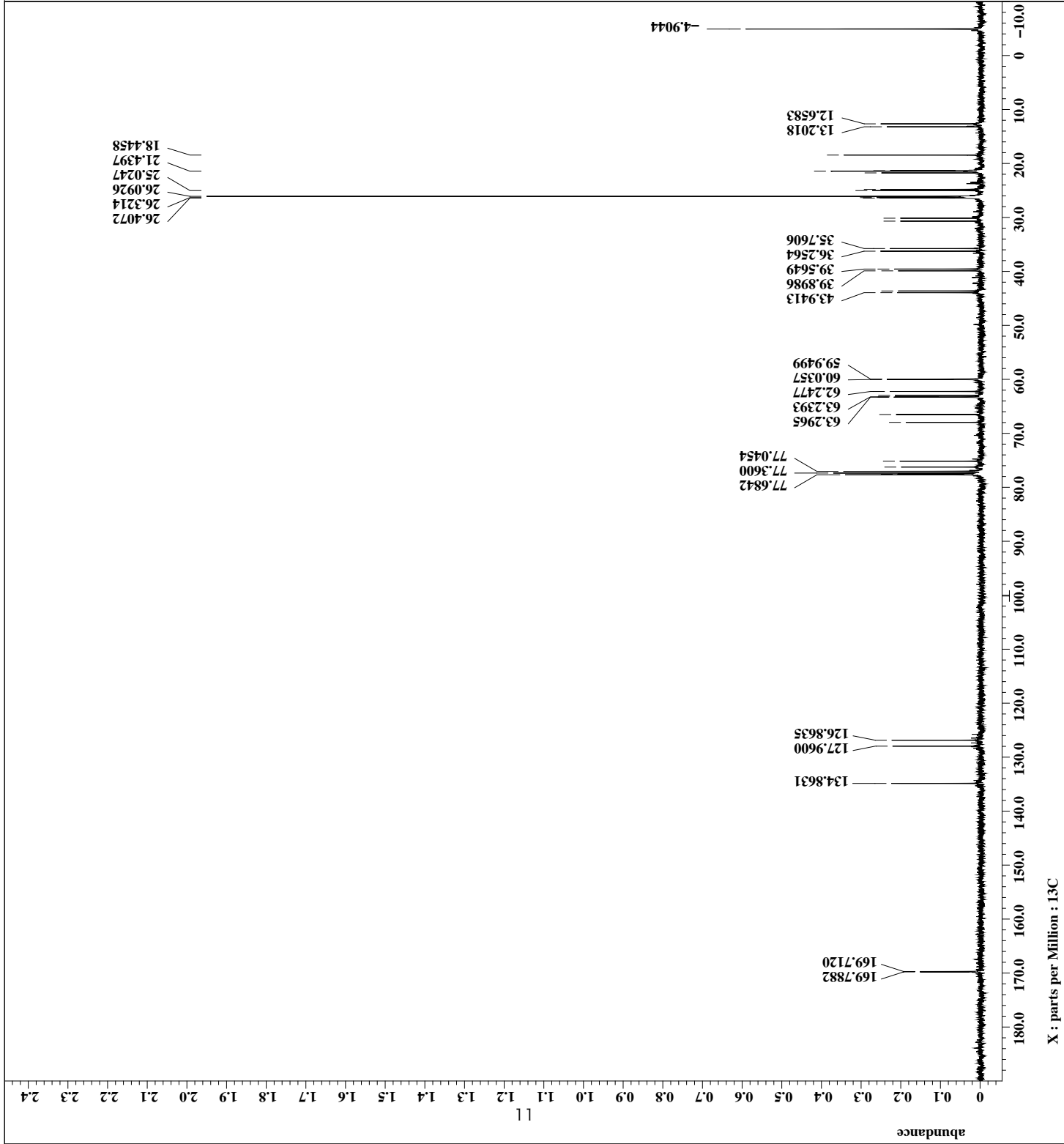
Filename	=	OH-OAC-tbs-13C-3.jdf
Author	=	delta
Experiment	=	single_pulse_dec
Sample_id	=	S#389937
Solvent	=	CHLOROFORM-D
Creation_time	=	30-JUN-2010 10:06:56
Revision_time	=	21-DEC-2010 10:07:56
Current_time	=	21-DEC-2010 10:08:19
Comment	=	single pulse decouple
Data format	=	1D COMPLEX
Dim_size	=	26214
Dim_title	=	13C
Dim_units	=	[ppm]
Dimensions	=	x
Site	=	ECK400M
Spectrometer	=	DELTA2_NMR
Field_strength	=	9.389766[T] (400[MHz]
x_acq_duration	=	1.04333312[s]
x_domain	=	13C
x_freq	=	100.52530333[MHz]
x_offset	=	100[ppm]
x_points	=	32768
x_prescans	=	4
x_resolution	=	0.95846665[Hz]
x_sweep	=	31.40703518[kHz]
irr_domain	=	1H
irr_freq	=	399.78219838[MHz]
irr_offset	=	5[ppm]
Clipped	=	FALSE
Mod return	=	1
Scans	=	84
Total_scans	=	84
x_90_width	=	9.2[us]
x_acq_time	=	1.04333312[s]
x_angle	=	45[deg]
x_atn	=	6.6[dB]
x_pulse	=	4.6[us]
irr_atn_dec	=	22.2[dB]
irr_atn_noe	=	22.2[dB]
irr_noise	=	WALTZ
Decoupling	=	TRUE
Initial_wait	=	1[s]
Noe	=	TRUE
Noe_time	=	5[s]
Recvr_gain	=	50
Relaxation_delay	=	5[s]
Repetition_time	=	6.04333312[s]
Temp_get	=	25[dc]



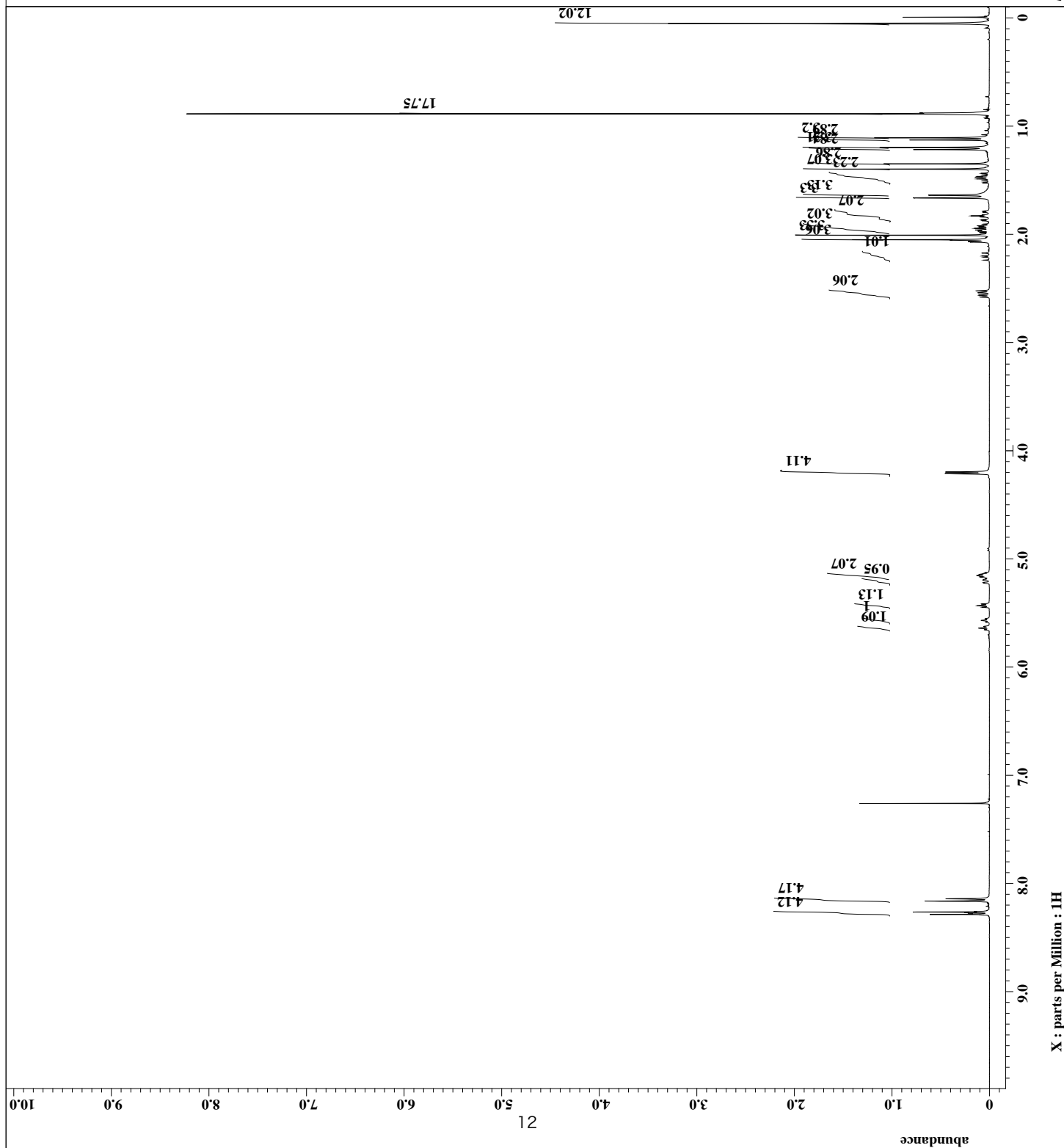
X : parts per Million : 1H

Filename	= OH-epoxide-1H-6.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= 1
Solvent	= CHLOROFORM-D
Creation_time	= 30-JUN-2010 10:19:44
Revision_time	= 16-JUL-2011 11:53:59
Current_time	= 16-JUL-2011 11:54:18
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= x
Site	= ECX400M
Spectrometer	= DELTA2_NMR
Field_strength	= 9.389766[T] (400[MHz]
X_acq_duration	= 2.18365952[s]
X_domain	= 1H
X_freq	= 399.78219838[MHz]
X_offset	= 4[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45794685[Hz]
X_sweep	= 7.5030012[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 10.5[us]
X_acq_time	= 2.18365952[s]
X_angle	= 45[deg]
X_atn	= 1.4[dB]
X_pulse	= 5.25[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 1[s]
Repetition_time	= 3.18365952[s]
Temp_get	= 24.31[$^{\circ}$ C]

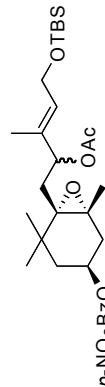


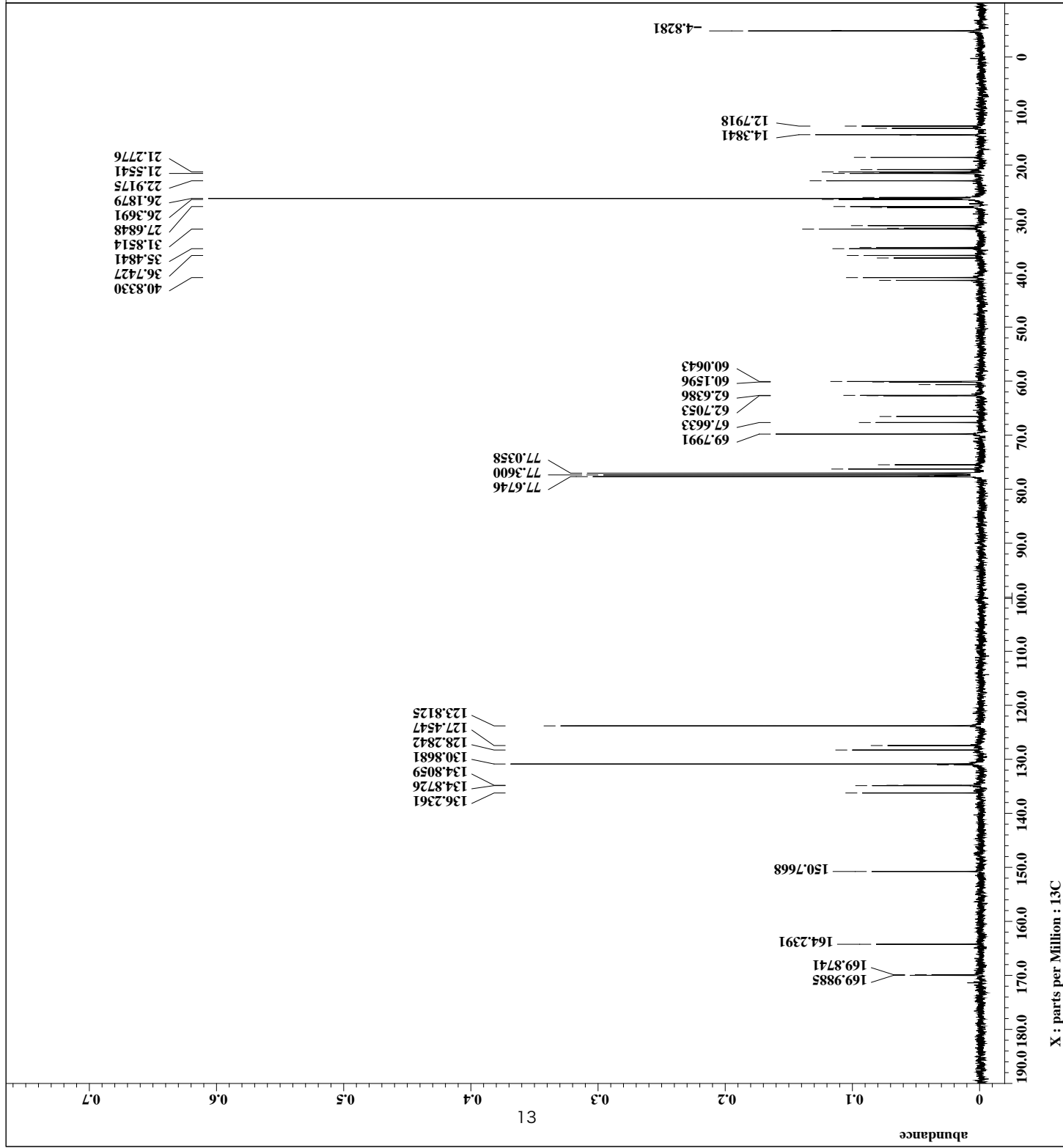


Filename = OH-epoxide-13C-3-jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#408183
Solvent = CHLOROFORM-D
Creation_time = 30-JUN-2010 10:30:41
Revision_time = 21-DEC-2010 10:07:00
Current_time = 21-DEC-2010 10:07:31
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = x
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 22
Total_scans = 22
X_90_width = 9.2[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[dB]
X_pulse = 4.6[us]
Irr_atn_dec = 22.2[dB]
Irr_atn_noe = 22.2[dB]
Irr_noise = WAITZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 25.2[dc]



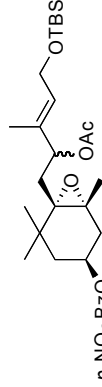
Filename	=	pNO2Bz-OAc-tbs-1H-3-J
Author	=	delta
Experiment	=	single_pulse.ex2
Sample id	=	1
Solvent	=	CHLOROFORM-D
Creation time	=	14-JUL-2010 14:11:30
Revision time	=	16-JUL-2011 12:03:29
Current time	=	16-JUL-2011 12:04:02
Comment	=	single pulse
Data format	=	1D COMPLEX
Dim_size	=	13107
Dim_title	=	1H
Dim_units	=	[ppm]
Dimensions	=	x
Site	=	EXCA400M
Spectrometer	=	DELTA2_NMR
Field_strength	=	9.389766[T] (400[MHz]
X_acq_duration	=	2.18365952[s]
X_domain	=	1H
X_freq	=	399.78219838[MHz]
X_offset	=	4[ppm]
X_points	=	16384
X_prescans	=	1
X_resolution	=	0.45794685[Hz]
X_sweep	=	7.5030012[kHz]
Ir1_domain	=	1H
Ir1_freq	=	399.78219838[MHz]
Ir1_offset	=	5[ppm]
Tr1_domain	=	1H
Tr1_freq	=	399.78219838[MHz]
Tr1_offset	=	5[ppm]
Clipped	=	FALSE
Mod_return	=	1
Scans	=	8
Total_scans	=	8
X_90_width	=	10.5[us]
X_acq_time	=	2.18365952[s]
X_angle	=	45[deg]
X_atn	=	1.4[db]
X_pulse	=	5.25[us]
Ir1_mode	=	Off
Tr1_mode	=	Off
Dante_presat	=	FALSE
Initial_wait	=	1[s]
Recvr_gain	=	34
Relaxation_delay	=	1[s]
Repetition_time	=	3.18365952[s]
Temp_get	=	25.3[deg]

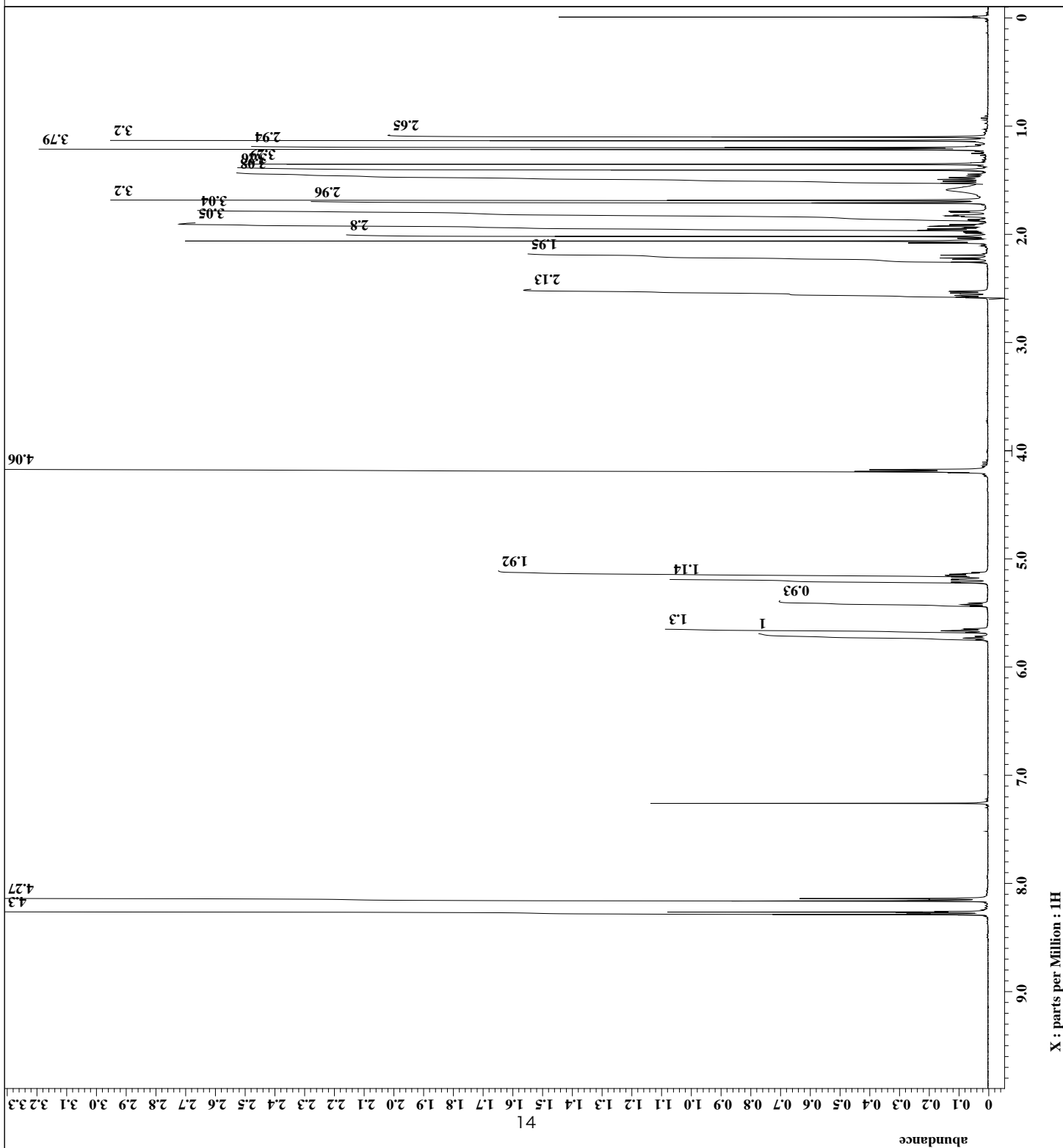




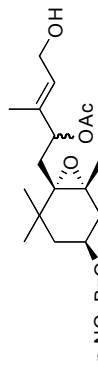
X : parts per Million : 13C

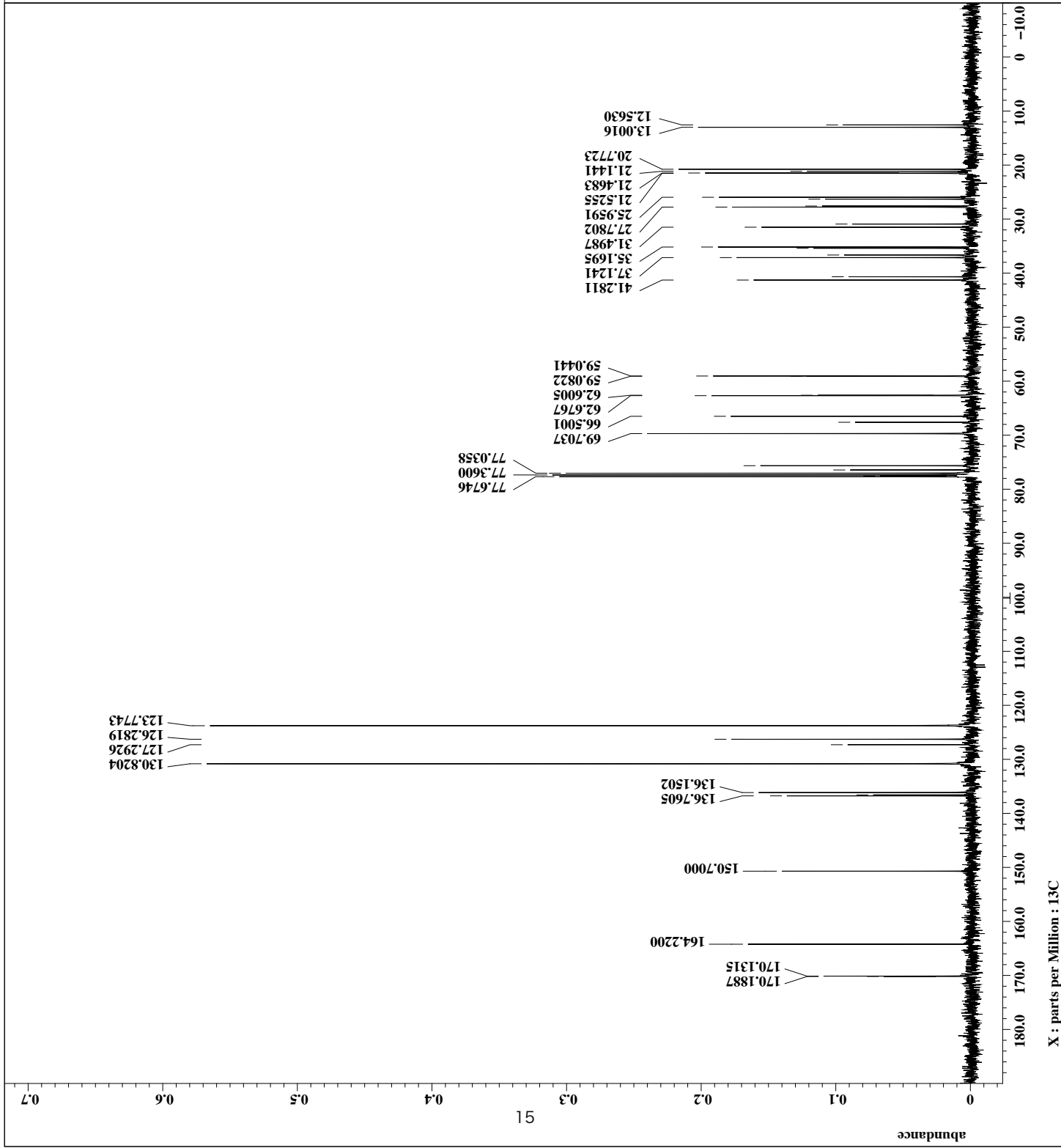
Filename	=	pN02Bz-OAc-tbs-13C-3-
Author	=	data
Experiment	=	single_pulse_dec
Sample_id	=	S#547774
Solvent	=	CHLOROFORM-D
Creation_time	=	14-JUL-2010 14:31:20
Revision_time	=	21-DEC-2010 10:10:54
Current_time	=	21-DEC-2010 10:11:17
Comment	=	single pulse decouple
Data format	=	1D COMPLEX
Dim_size	=	26214
Dim_title	=	13C
Dim_units	=	[ppm]
Dimensions	=	x
Site	=	ECX400M
Spectrometer	=	DELTA2_NMR
Field_strength	=	9.389766[T] (400[MHz]
x_acq_duration	=	1.04333312[s]
x_domain	=	13C
x_freq	=	100.52530333[MHz]
x_offset	=	100[ppm]
x_points	=	32768
x_prescans	=	4
x_resolution	=	0.95846665[Hz]
x_sweep	=	31.40703518[kHz]
irr_domain	=	1H
irr_freq	=	399.78219838[MHz]
irr_offset	=	5[ppm]
Clipped	=	FALSE
Mod return	=	1
Scans	=	111
Total_scans	=	111
x_90_width	=	9.2[us]
x_acq_time	=	1.04333312[s]
x_angle	=	45[deg]
x_atn	=	6.6[dB]
x_pulse	=	4.6[us]
irr_atn_dec	=	22.2[dB]
irr_atn_noe	=	22.2[dB]
irr_noise	=	WALTZ
Decoupling	=	TRUE
Initial_wait	=	1[s]
Noe	=	TRUE
Noe_time	=	5[s]
Recvr_gain	=	50
Relaxation_delay	=	5[s]
Repetition_time	=	6.04333312[s]
Temp get	=	25.3[degC]





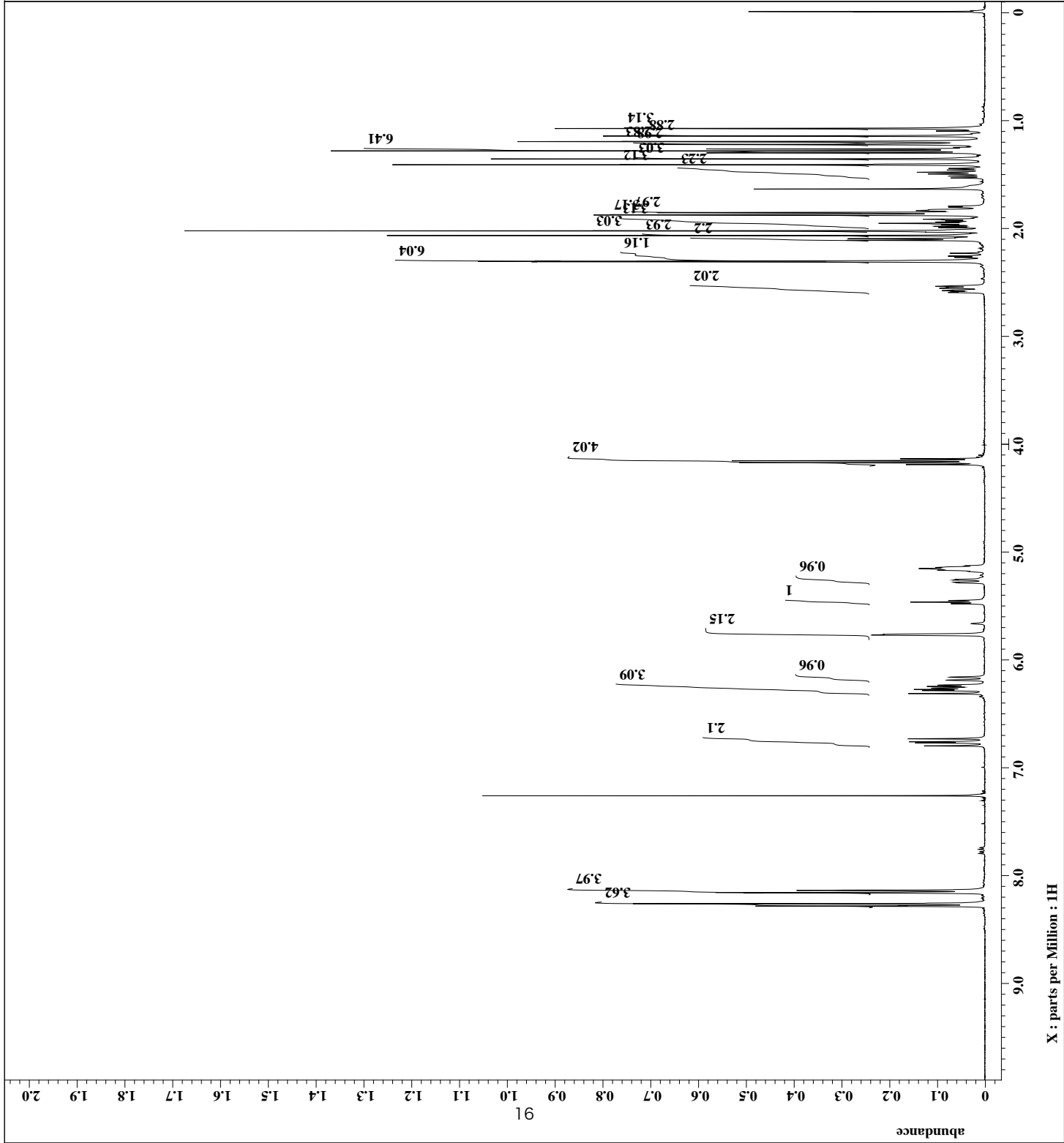
Filename	=	pNO2Bz-OAc-OH-1H-3.jd
Author	=	delta
Experiment	=	single_pulse.ex2
Sample id	=	1
Solvent	=	CHLOROFORM-D
Creation time	=	15-JUL-2010 15:38:03
Revision time	=	16-JUL-2011 12:17:14
Current time	=	16-JUL-2011 12:17:56
Comment	=	single_pulse
Data format	=	1D COMPLEX
Din_size	=	13107
Din_title	=	1H
Din_units	=	[ppm]
Dimensions	=	x
Site	=	EXK400M
Spectrometer	=	DELTA2_NMR
Field_strength	=	9.389766[T] (400[MHz]
X_acq_duration	=	2.18365952[s]
X_domain	=	1H
X_freq	=	399.78219838[MHz]
X_offset	=	4[ppm]
X_points	=	16384
X_prescans	=	1
X_resolution	=	0.45794685[Hz]
X_sweep	=	7.5030012[kHz]
Irr_domain	=	1H
Irr_freq	=	399.78219838[MHz]
Irr_offset	=	5[ppm]
Tri_domain	=	1H
Tri_freq	=	399.78219838[MHz]
Tri_offset	=	5[ppm]
Clipped	=	FALSE
Mod_return	=	1
Scans	=	8
Total_scans	=	8
X_90_width	=	10.5[us]
X_acq_time	=	2.18365952[s]
X_angle	=	45[deg]
X_atn	=	1.4[db]
X_pulse	=	5.225[us]
Irr_mode	=	Off
Tri_mode	=	Off
Dante_presat	=	FALSE
Initial_wait	=	1[s]
Recvr_gain	=	36
Relaxation_delay	=	1[s]
Repetition_time	=	3.18365952[s]
Temp_get	=	25[dc]



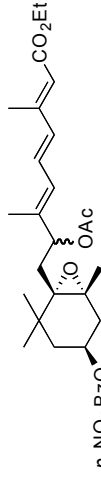


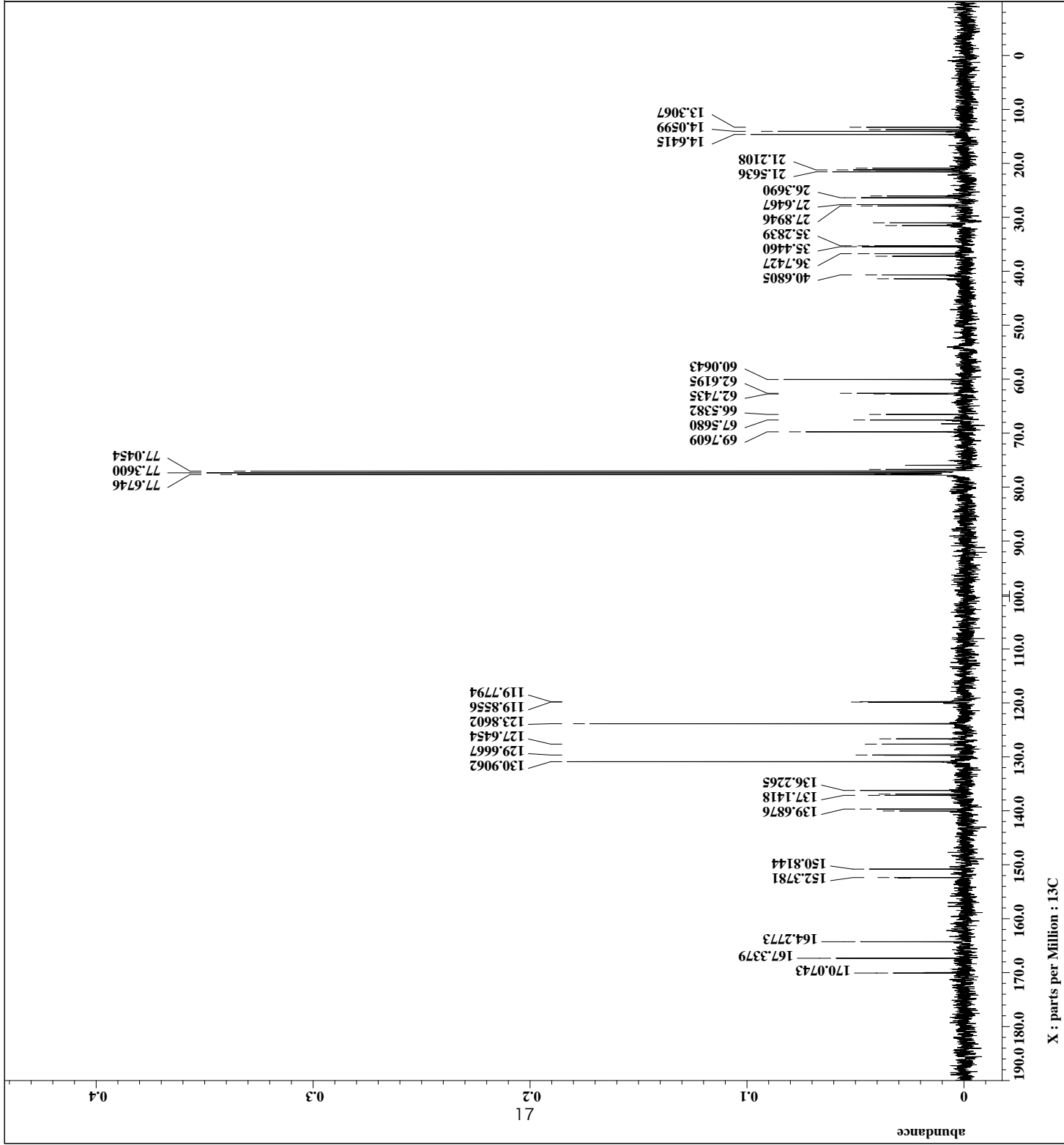
Filename	=	pNO2Ba-OAc-OH-13C-3.3.j
Author	=	delta
Experiment	=	single_pulse_dec
Sample_id	=	S#59344
Solvent	=	CHLOROFORM-D
Creation_time	=	15-JUL-2010 15:50:40
Revision_time	=	21-DEC-2010 10:09:41
Current_time	=	21-DEC-2010 10:10:03
Comment	=	single pulse decouple
Data_format	=	1D COMPLEX
Dim_size	=	26214
Dim_title	=	13C
Dim_units	=	[ppm]
Dimensions	=	x
Site	=	ECX400M
Spectrometer	=	DELTA2_NMR
Field_strength	=	9.399766[T] (400[MHz]
X_acq_duration	=	1.04333312[s]
X_domain	=	13C
X_freq	=	100.52530333[MHz]
X_offset	=	100[ppm]
X_points	=	32768
X_prescans	=	4
X_resolution	=	0.95846665[Hz]
X_sweep	=	31.40703518[kHz]
Ir_r_domain	=	1H
Ir_r_freq	=	399.78219838[MHz]
Ir_r_offset	=	5[ppm]
Clipped	=	FALSE
Mod_return	=	1
Scans	=	45
Total_scans	=	45
X_90_width	=	9.2[us]
X_acq_time	=	1.04333312[s]
X_angle	=	45[deg]
X_atn	=	6.6[dB]
X_pulse	=	4.6[us]
Ir_r_atn_dec	=	22.2[dB]
Ir_r_atn_noe	=	22.2[dB]
Ir_r_noise	=	TRUE
Decoupling	=	WALTZ
Initial_wait	=	1[s]
Noe	=	TRUE
Noe_time	=	5[s]
Recvr_gain	=	50
Relaxation_delay	=	5[s]
Repetition_time	=	6.04333312[s]
Temp_get	=	25.7[degC]



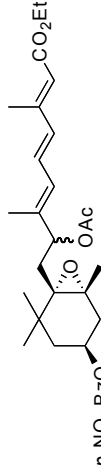


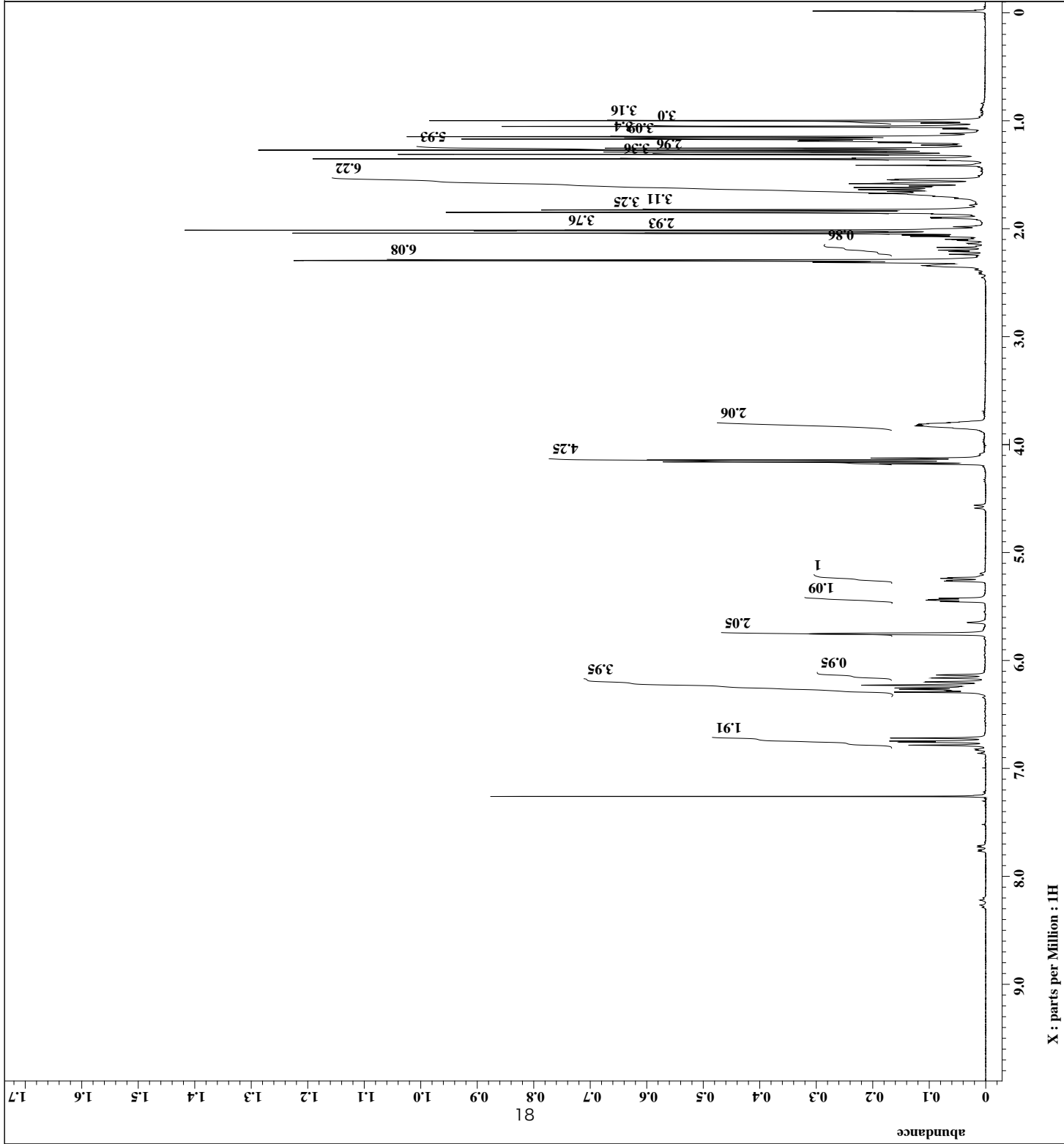
Filename = pNO2Bz-OAc-trieneeste
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 15-JUL-2010 20:12:41
Revision_time = 16-JUL-2011 12:24:57
Current_time = 16-JUL-2011 12:25:12
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 32
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 25.2[dc]



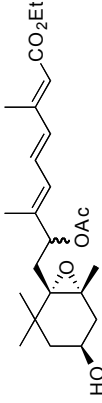


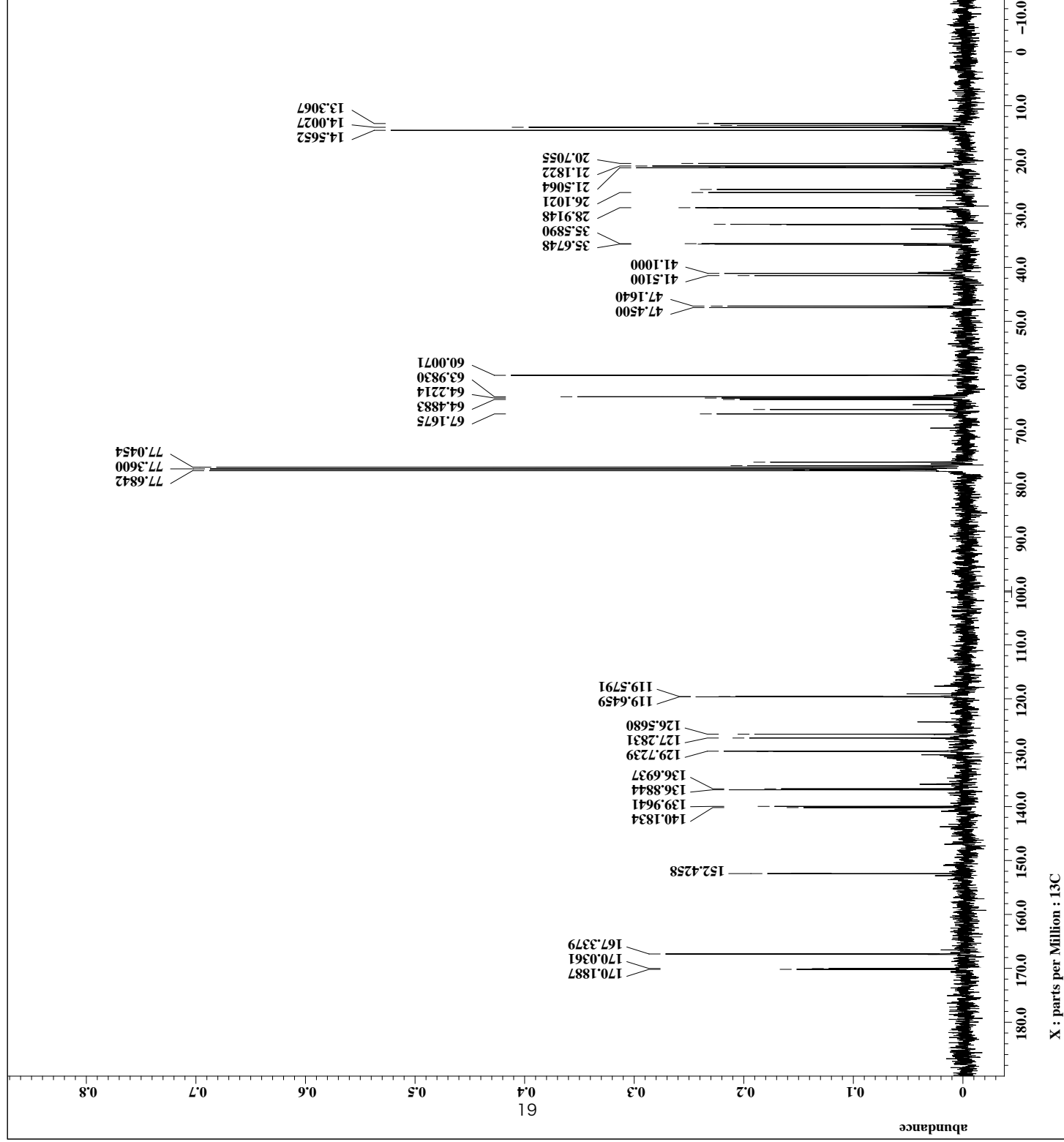
Filename = pNO2Bz-OAc-trieneeste
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#764026
 Solvent = CHLOROFORM-D
 Creation_time = 15-JUL-2010 20:27:09
 Revision_time = 21-DEC-2010 10:11:50
 Current_time = 21-DEC-2010 10:13:28
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = x
 Site = ECX400M
 Spectrometer = DELTA2_NMR
 Field_strength = 9.389766[T] (400[MHz])
 X_acq_duration = 1.04333312[s]
 X_domain = 13C
 X_freq = 100.52530333[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665[Hz]
 X_sweep = 31.40703518[kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 61
 Total_scans = 61
 X_90_width = 9.2[us]
 X_acq_time = 1.04333312[s]
 X_angle = 45[deg]
 X_atn = 6.6[dB]
 X_pulse = 4.6[us]
 Irr_atn_dec = 22.2[dB]
 Irr_atn_noe = 22.2[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 5[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 6.04333312[s]
 Temp_get = 25.8[degC]



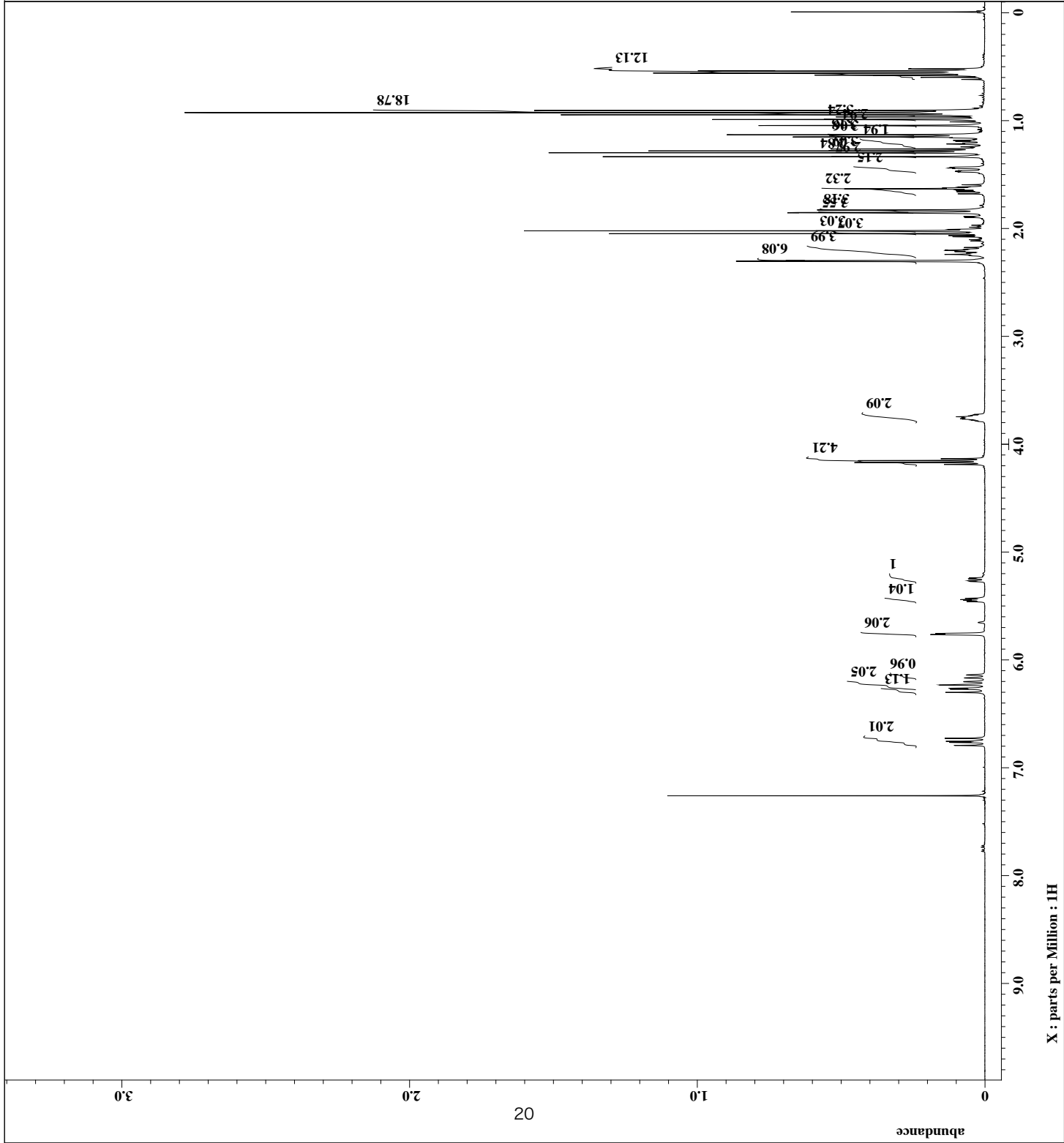


Filename = OH-OAc-trieneester-1H
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 12-JUL-2010 09:22:09
Revision_time = 16-JUL-2011 13:01:33
Current_time = 16-JUL-2011 13:01:53
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 24.8[dC]

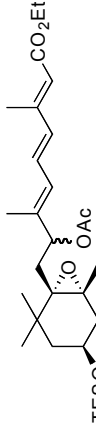


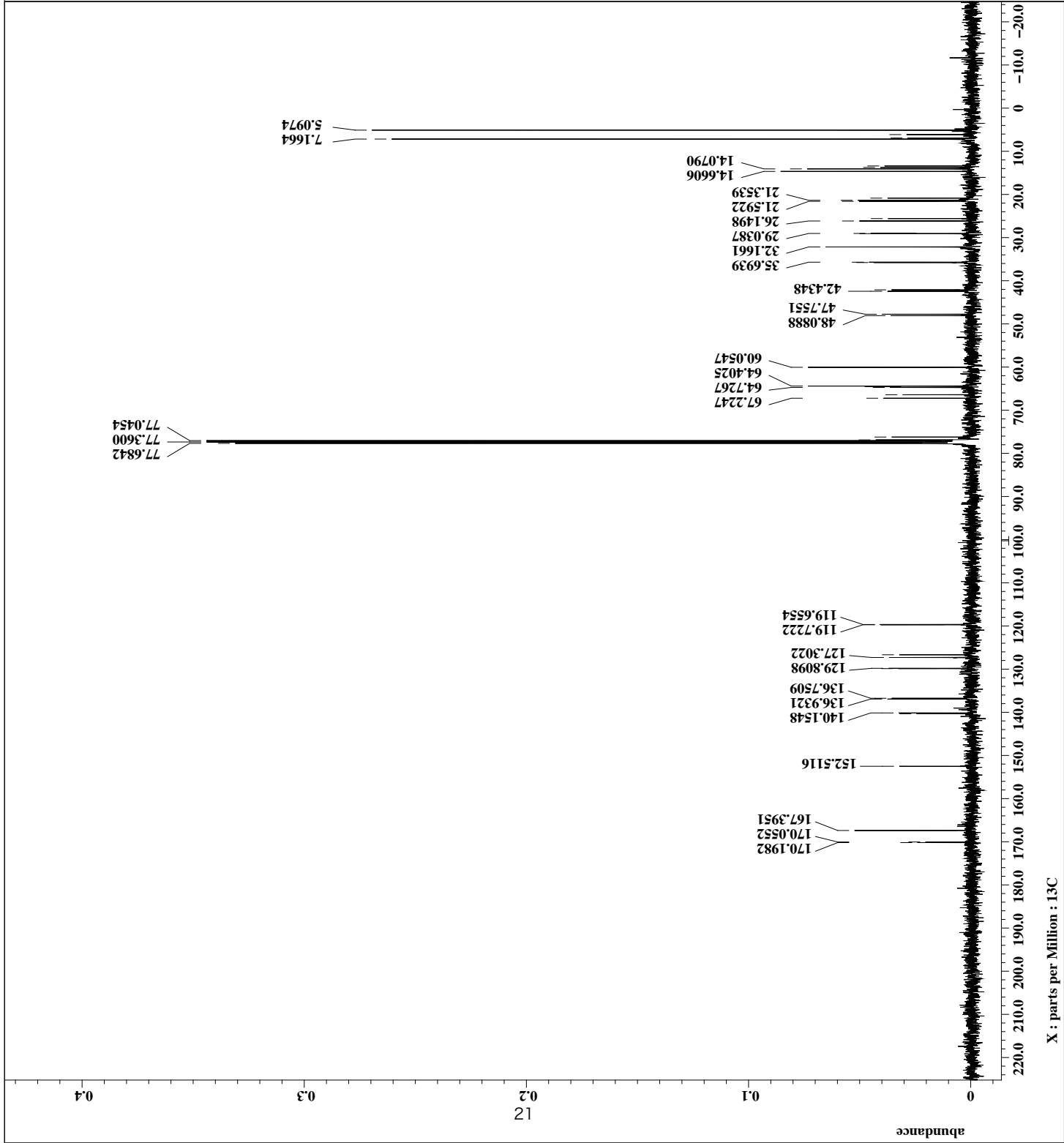


Filename = OH-OAc-trieneester-13
Author = delta
Experiment = single_pulse_dec
Sample_id = S#377349
Solvent = CHLOROFORM-D
Creation_time = 12-JUL-2010 09:40:53
Revision_time = 21-DEC-2010 10:08:40
Current_time = 21-DEC-2010 10:09:07
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = x
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
irr_domain = 1H
irr_freq = 399.78219838[MHz]
irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 43
Total_scans = 43
x_90_width = 9.2[us]
x_acq_time = 1.04333312[s]
x_angle = 45[deg]
x_atn = 6.6[db]
x_pulse = 4.6[us]
irr_atn_dec = 22.2[db]
irr_atn_noe = 22.2[db]
irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 56
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 25.1[dc]



Filename = tes-OAC-trieneester-1
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 16-JUL-2010 13:15:06
Revision_time = 16-JUL-2011 13:08:41
Current_time = 16-JUL-2011 13:09:04
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 24.7[dc]





tes-OAc-trieneester-1

File name =

Author = delta

Experiment = single_pulse_dec

Sample_id = S#513665

Solvent = CHLOROFORM-D

Creation_time = 16-JUL-2010 13:34:56

Revision_time = 21-DEC-2010 10:22:44

Current_time = 21-DEC-2010 10:23:20

Comment = single pulse decouple

Data_format = 1D COMPLEX

Dim_size = 26214

Dim_title = 13C

Dim_units = [ppm]

Dimensions = X

Site = ECX400M

Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])

X_acq_duration = 1.04333312[s]

X_domain = 13C

X_freq = 100.52530333[MHz]

X_offset = 100[ppm]

X_points = 32768

X_prescans = 4

X_resolution = 0.95846665[Hz]

X_sweep = 31.40703518[kHz]

Irr_domain = 1H

Irr_freq = 399.78219838[MHz]

Irr_offset = 5[ppm]

Clipped = FALSE

Mod_return = 1

Scans = 116.0

Total_scans = 116.0

X_90_width = 9.2[us]

X_acq_time = 1.04333312[s]

X_angle = 45[deg]

X_atn = 6.6[dB]

X_pulse = 4.6[us]

Irr_atn_dec = 22.2[dB]

Irr_atn_noe = 22.2[dB]

Irr_noise = WALTZ

Decoupling = TRUE

Initial_wait = 1[s]

Noe = TRUE

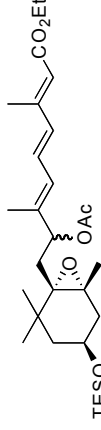
Noe_time = 5[s]

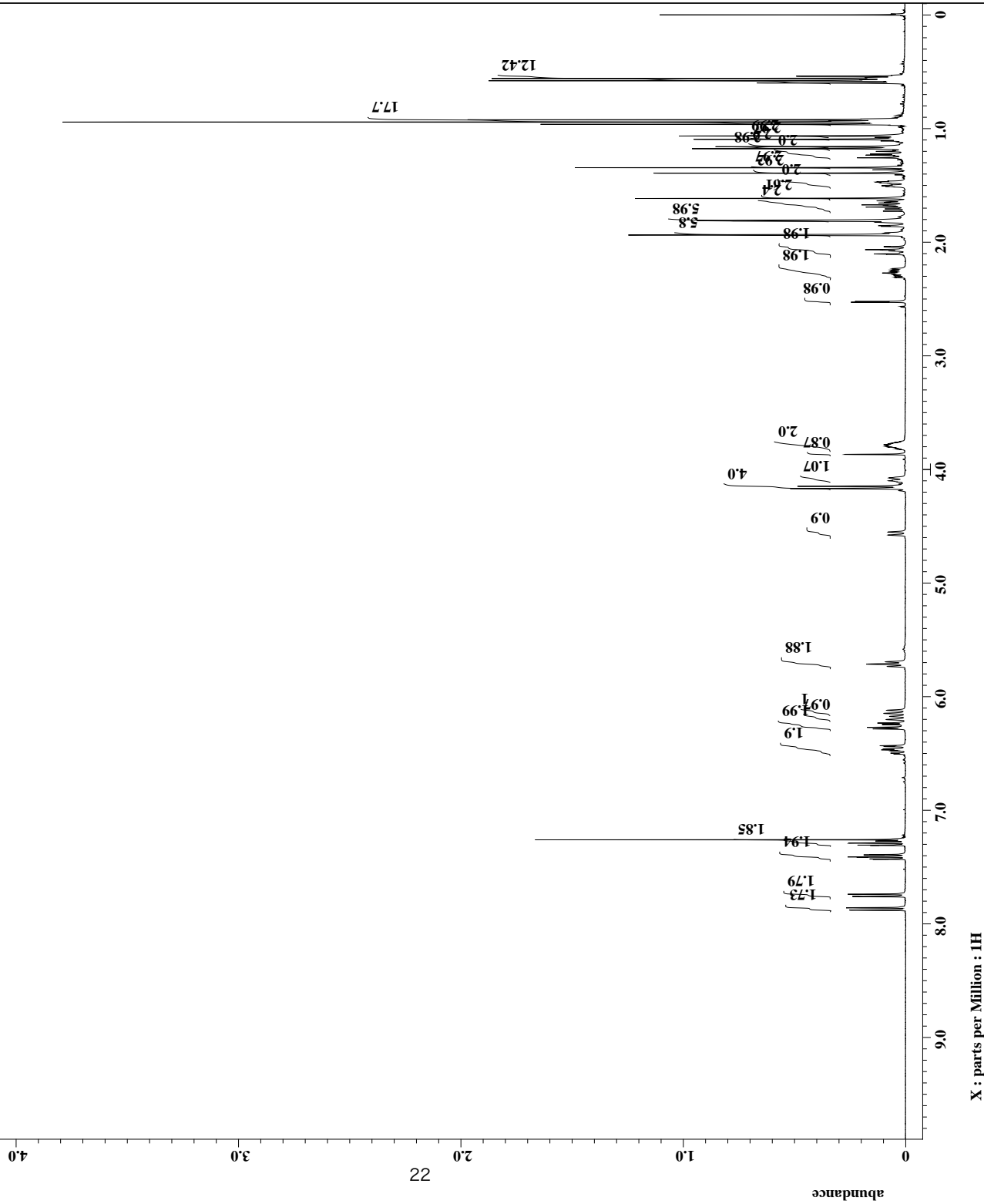
Recvr_gain = 50

Relaxation_delay = 5[s]

Repetition_time = 6.04333312[s]

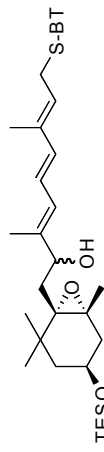
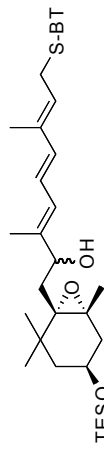
Temp_get = 24.8[degC]

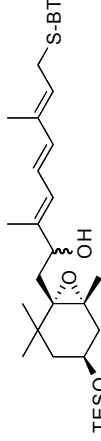
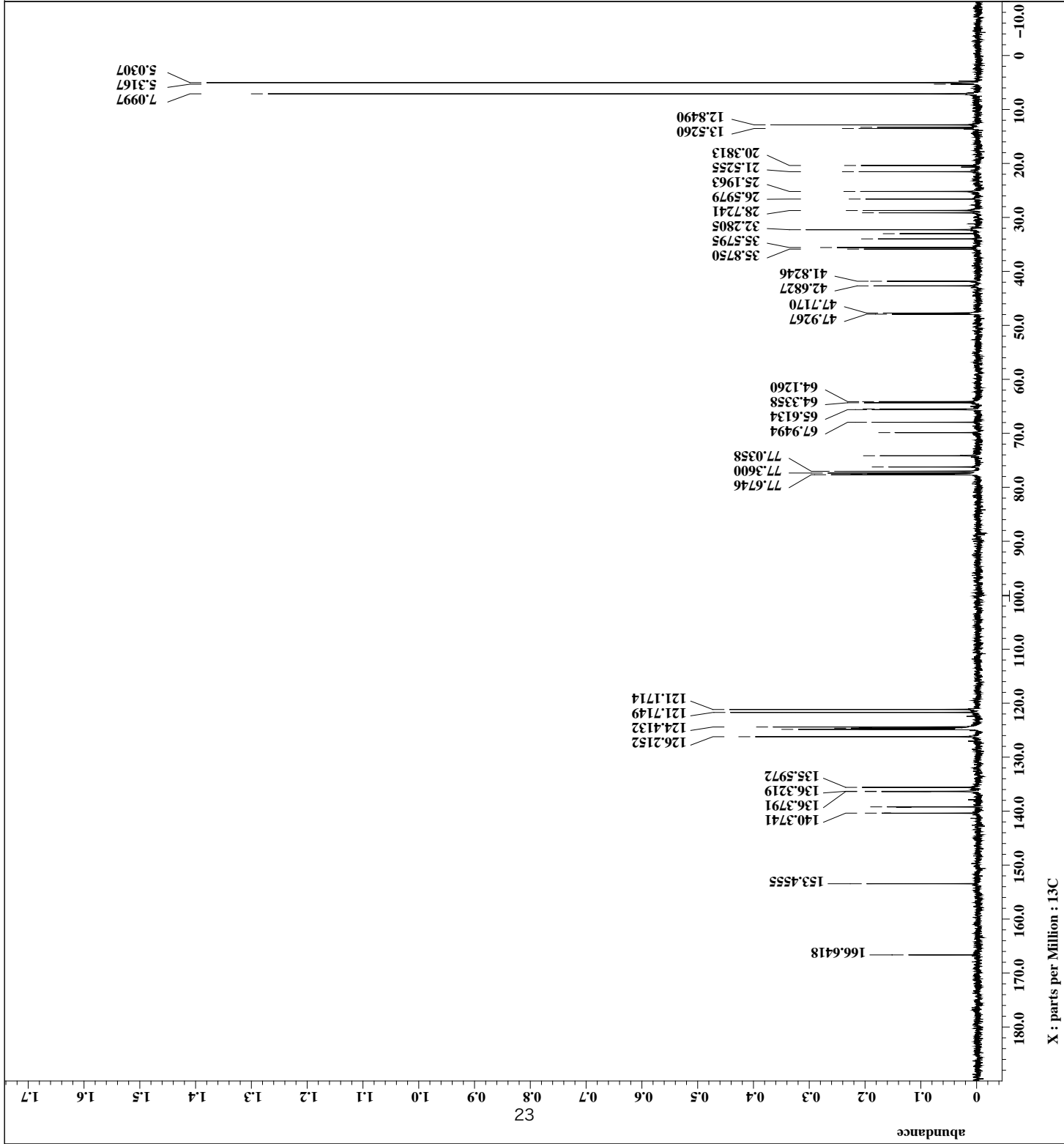




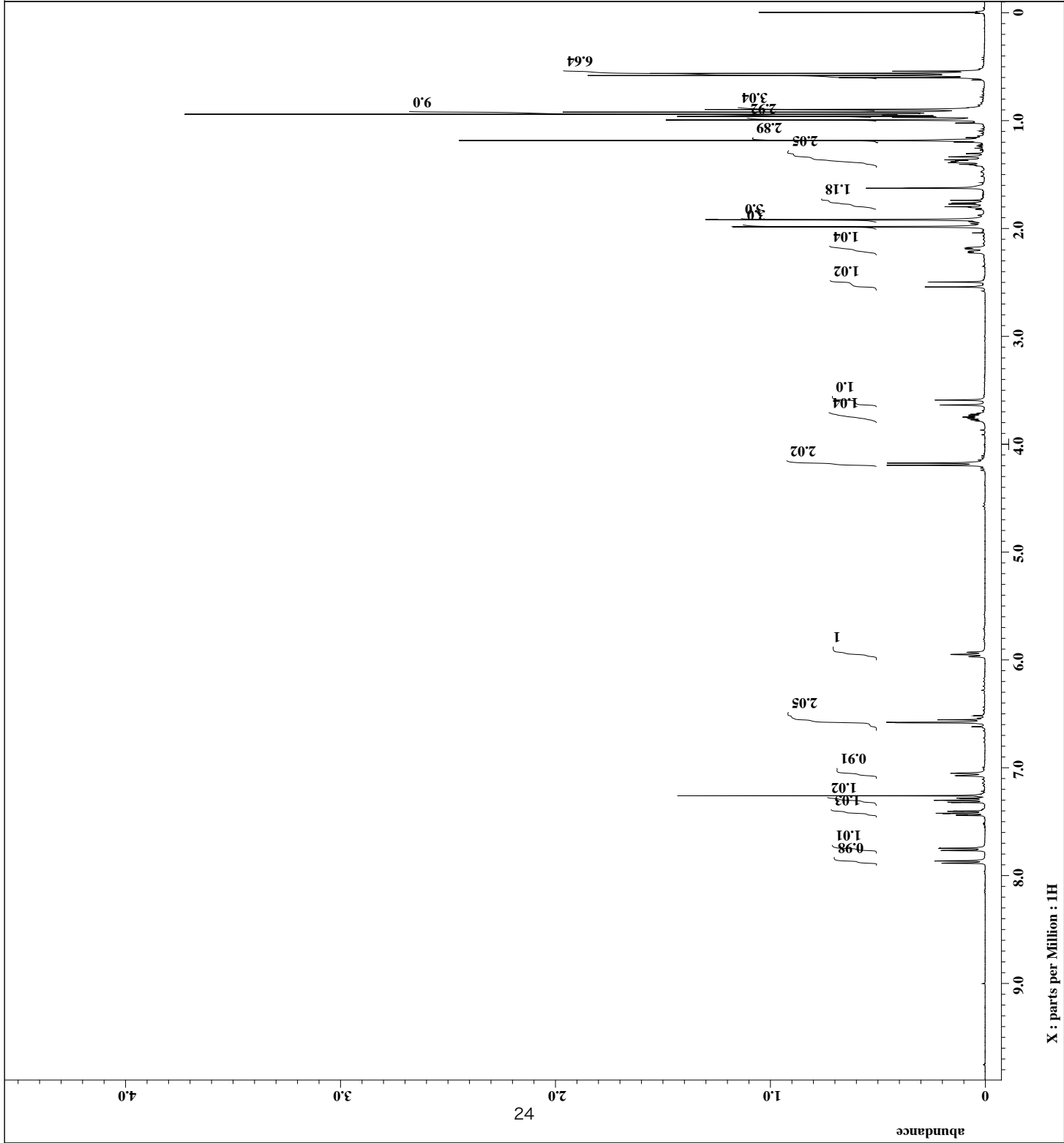
X : parts per Million : 1H

Filename	=	tes-OH-sulfide-1H-3-J
Author	=	delta
Experiment	=	single_pulse.ex2
Sample id	=	1
Solvent	=	CHLOROFORM-D
Creation time	=	16-JUL-2010 19:17:26
Revision_time	=	16-JUL-2011 13:20:03
Current_time	=	16-JUL-2011 13:20:27
Comment	=	single pulse
Data format	=	1D COMPLEX
Dim_Size	=	13107
Dim_title	=	1H
Dim_units	=	[ppm]
Dimensions	=	x
Site	=	ECX400M
Spectrometer	=	DELTA2_NMR
Field_strength	=	9.389766[T] (400[MHz]
x_acq_duration	=	2.18365952[s]
x_domain	=	1H
x_freq	=	399.78219838[MHz]
x_offset	=	4[ppm]
x_points	=	16384
x_prescans	=	1
x_resolution	=	0.45794685[Hz]
x_sweep	=	7.5030012[kHz]
irr_domain	=	1H
irr_freq	=	399.78219838[MHz]
irr_offset	=	5[ppm]
tri_domain	=	1H
tri_freq	=	399.78219838[MHz]
tri_offset	=	5[ppm]
Clipped	=	FALSE
Mod return	=	1
Scans	=	8
Total_scans	=	8
x_90_width	=	10.5[us]
x_acq_time	=	2.18365952[s]
x_angle	=	45[deg]
x_atn	=	1.4[db]
x_pulse	=	5.25[us]
irr_mode	=	Off
tri_mode	=	Off
Dante_preset	=	FALSE
Initial_wait	=	1[s]
Recvr_gain	=	34
Relaxation_delay	=	1[s]
Repetition_time	=	3.18365952[s]
Temp get	=	25.2[°C]

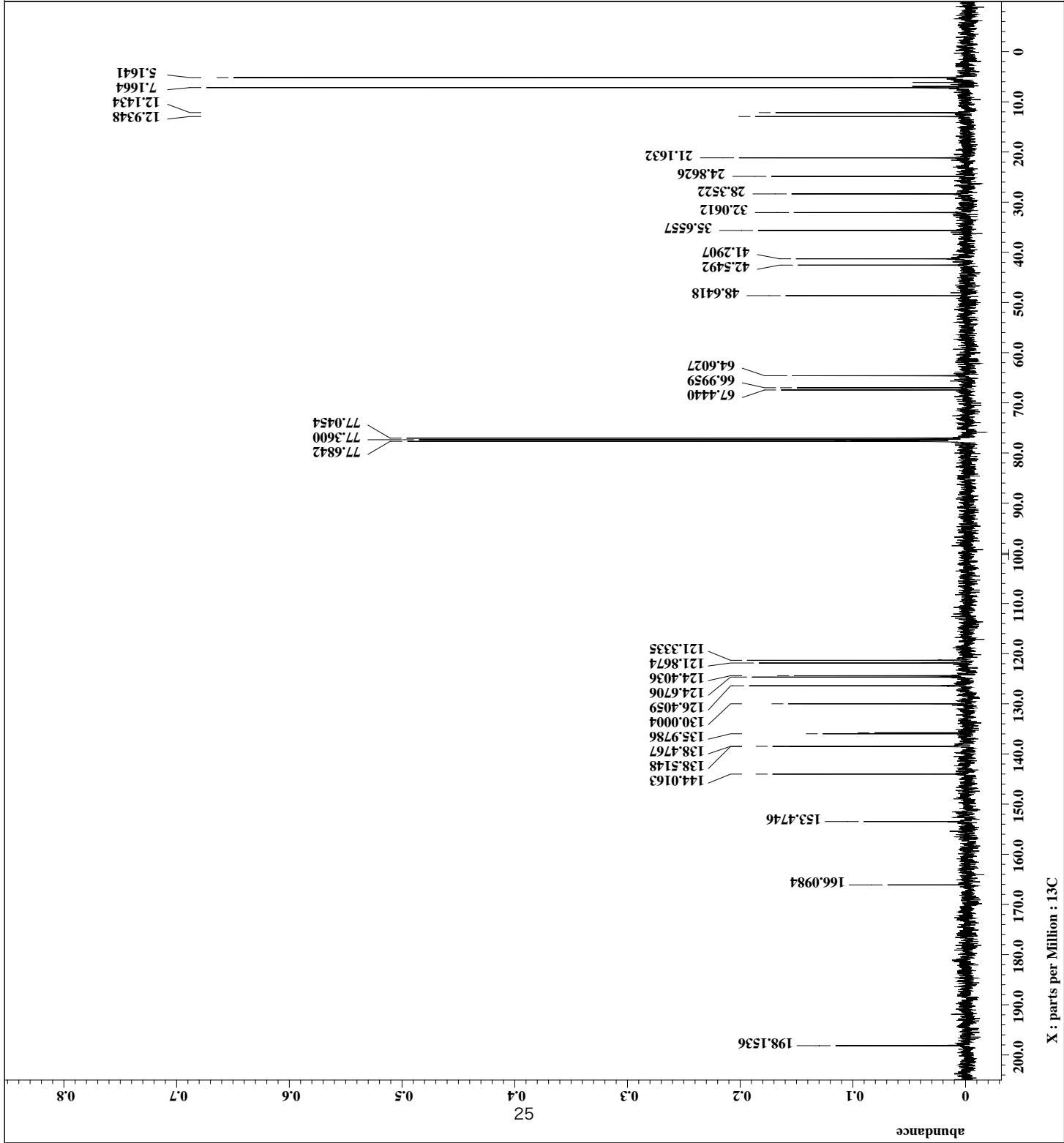




Filename = tes-OH-sulfide-13C-3.
Author = delta
Experiment = single_pulse_dec
Sample_id = S#734976
Solvent = CHLOROFORM-D
Creation_time = 16-JUL-2010 19:37:19
Revision_time = 21-DEC-2010 10:24:06
Current_time = 21-DEC-2010 10:24:32
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = x
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 42
Total_scans = 42
X_90_width = 9.2[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[dB]
X_pulse = 4.6[us]
Irr_atn_dec = 22.2[dB]
Irr_atn_noe = 22.2[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 52
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 25.5[dC]



Filename = tes-ketone-sulfide-1H
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 17-JUL-2010 16:19:03
Revision_time = 16-JUL-2011 13:24:26
Current_time = 16-JUL-2011 13:24:51
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 24.5[dC]



tes-ketone-sulfide-13

File name = tes-ketone-sulfide-13

Author = delta

Experiment = single_pulse_dec

Sample_id = S#623950

Solvent = CHLOROFORM-D

Creation_time = 17-JUL-2010 16:32:38

Revision_time = 21-DEC-2010 10:17:49

Current_time = 21-DEC-2010 10:18:18

Comment = single pulse decouple

Data_format = 1D COMPLEX

Dim_size = 26214

Dim_title = 13C

Dim_units = [ppm]

Dimensions = X

Site = ECX400M

Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])

X_acq_duration = 1.04333312[s]

X_domain = 13C

X_freq = 100.52530333[MHz]

X_offset = 100[ppm]

X_points = 32768

X_prescans = 4

X_resolution = 0.95846665[Hz]

X_sweep = 31.40703518[kHz]

Irr_domain = 1H

Irr_freq = 399.78219838[MHz]

Irr_offset = 5[ppm]

Clipped = FALSE

Mod_return = 1

Scans = 48

Total_scans = 48

X_90_width = 9.2[us]

X_acq_time = 1.04333312[s]

X_angle = 45[deg]

X_atn = 6.6[dB]

X_pulse = 4.6[us]

Irr_atn_dec = 22.2[dB]

Irr_atn_noe = 22.2[dB]

Irr_noise = WALTZ

Decoupling = TRUE

Initial_wait = 1[s]

Noe = TRUE

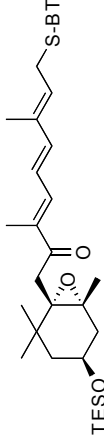
Noe_time = 5[s]

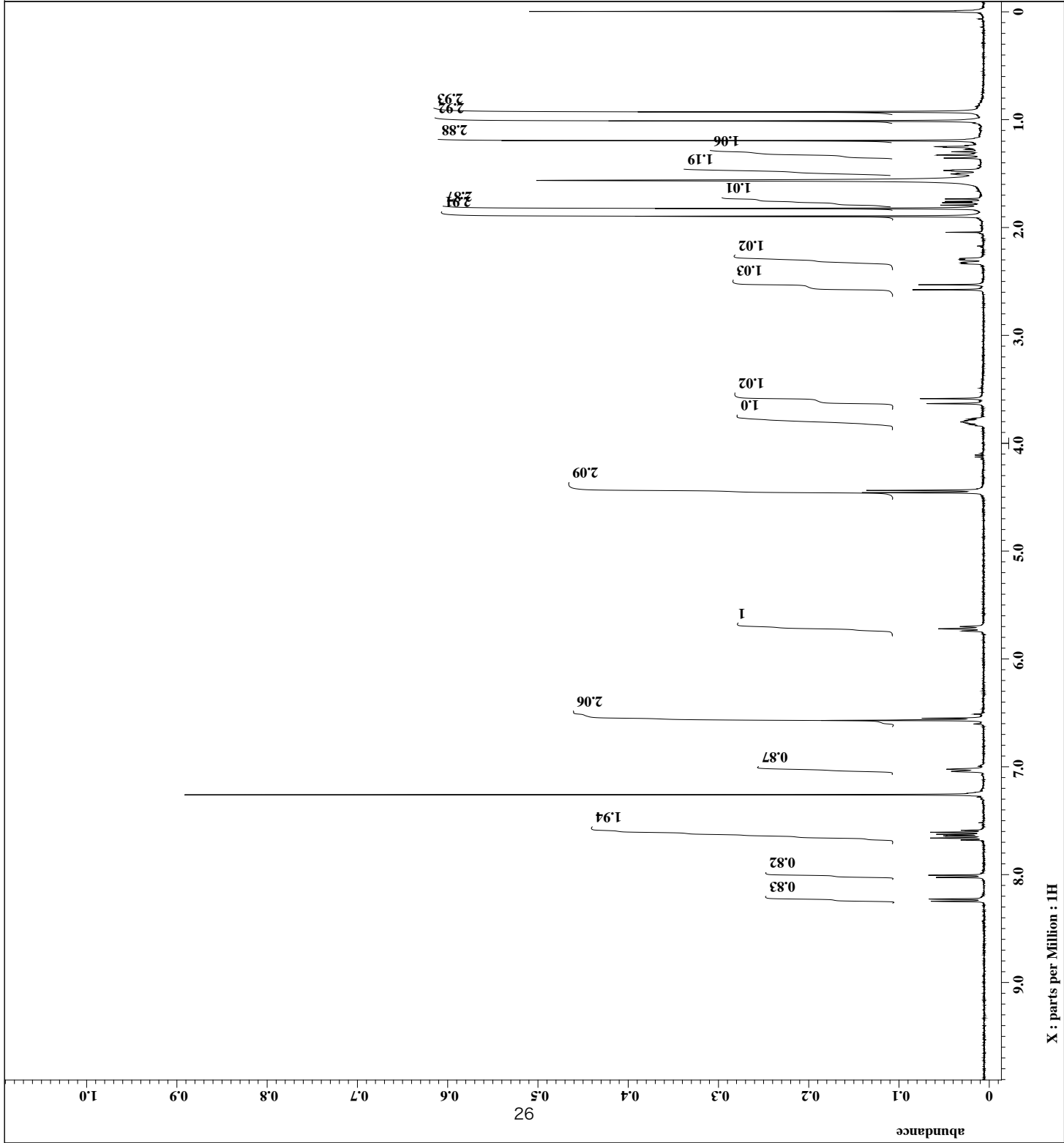
Recvr_gain = 54

Relaxation_delay = 5[s]

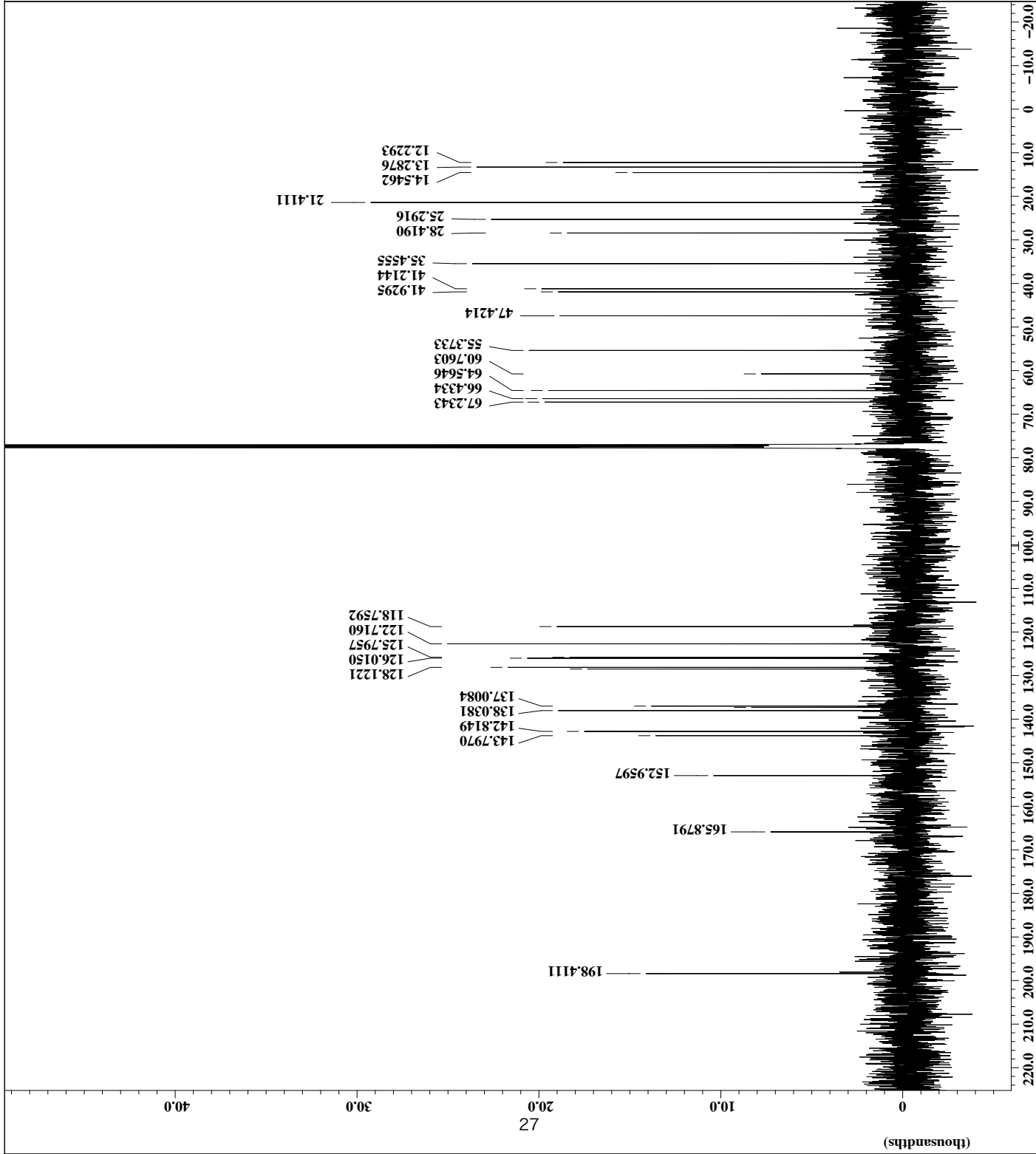
Repetition_time = 6.04333312[s]

Temp_get = 24.7[degC]

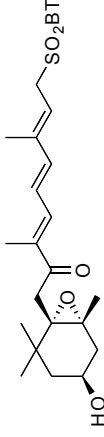


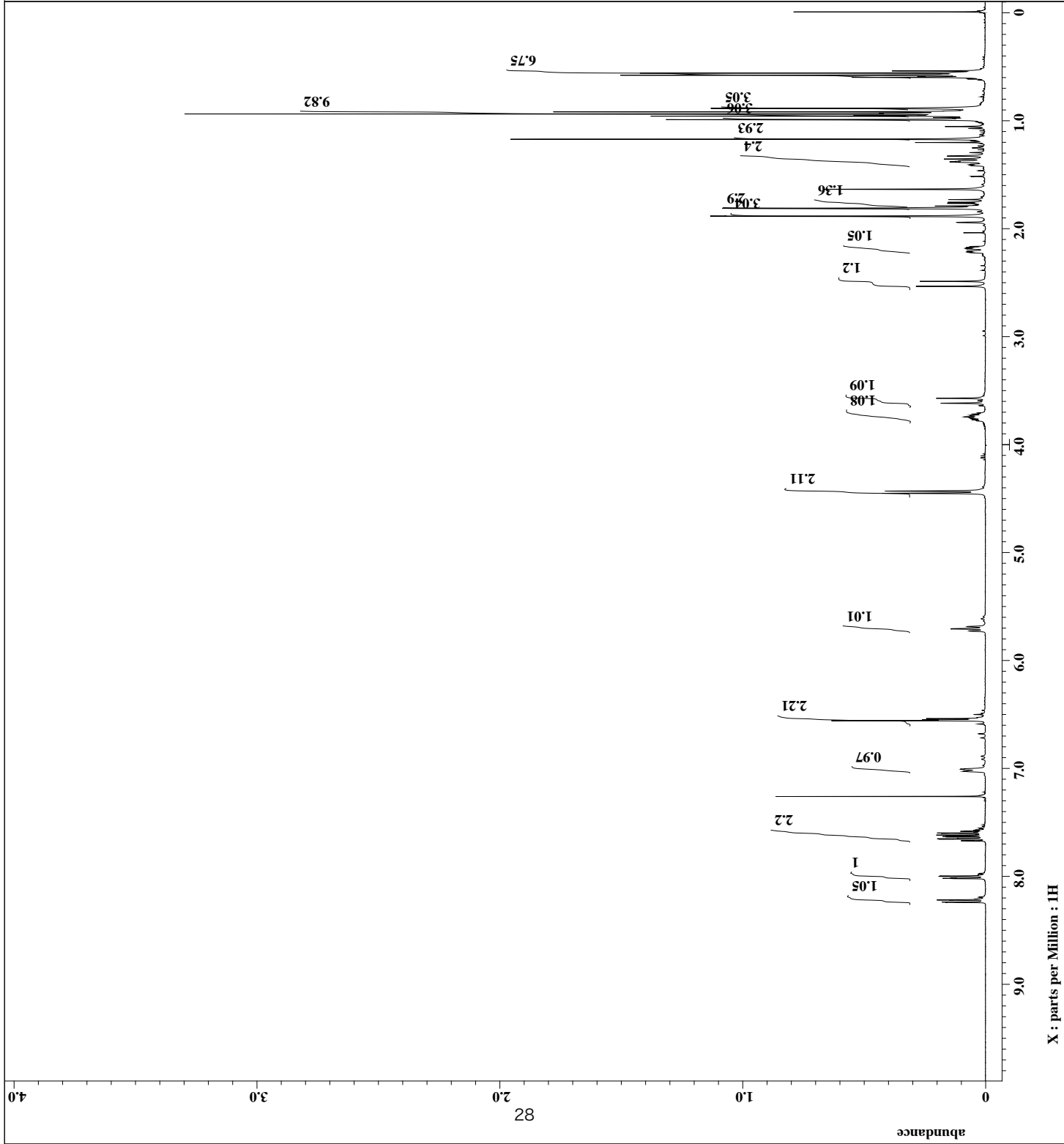


Filename = OH-ketone-sulfone-1H-
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 15-APR-2011 14:08:16
Revision_time = 16-JUL-2011 13:39:20
Current_time = 16-JUL-2011 13:39:49
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 9.4[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 0.7[dB]
X_pulse = 4.7[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 21.9[degC]

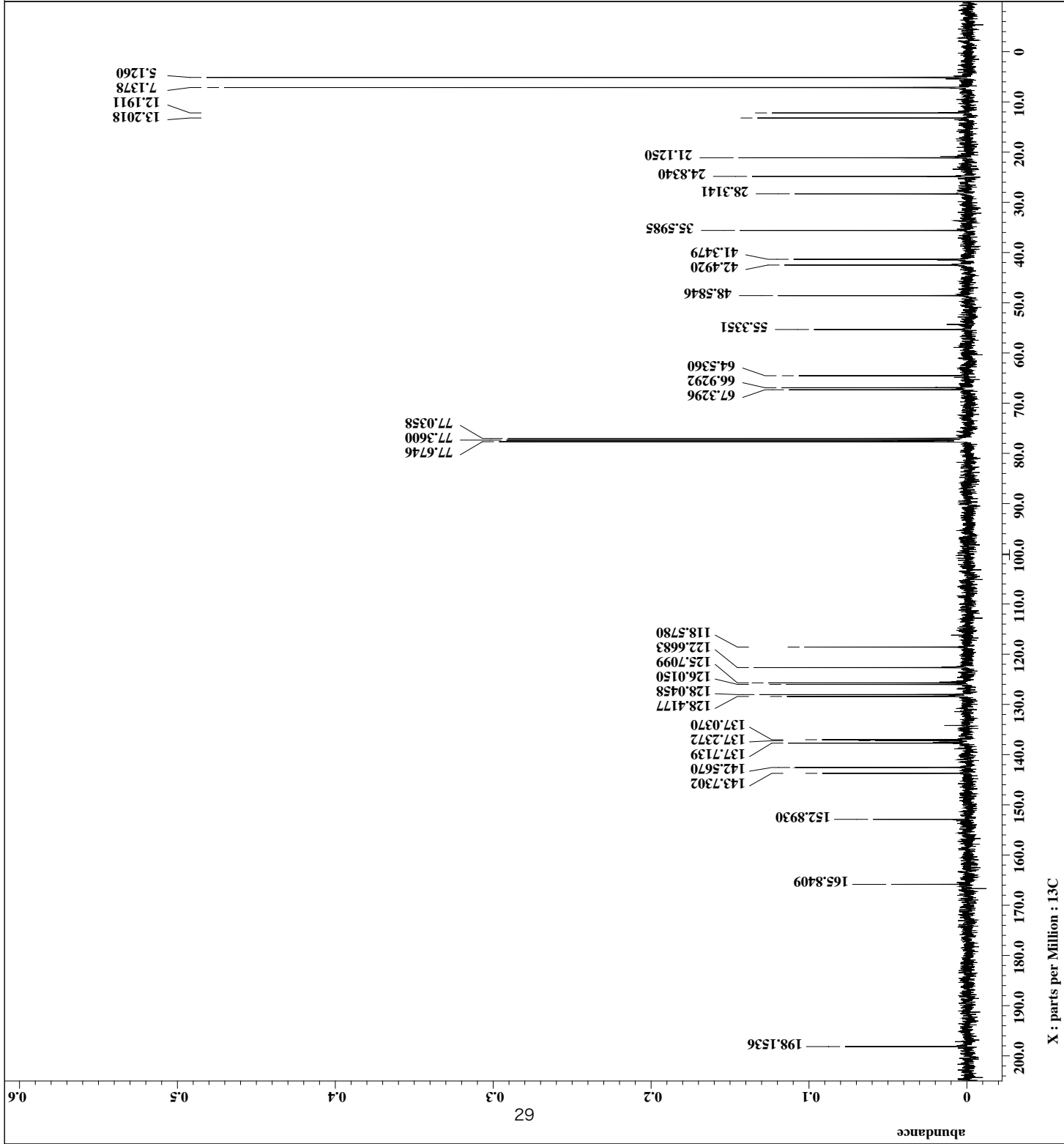


Filename = OH-ketone-sulfone-13C
Author = Delta
Experiment = single_pulse_dec
Sample_id = S#649286
Solvent = CHLOROFORM-D
Creation_time = 15-APR-2011 17:26:19
Revision_time = 16-JUL-2011 13:46:44
Current_time = 16-JUL-2011 13:48:10
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 379
Total_scans = 379
X_90_width = 9.2[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[db]
X_pulse = 4.6[us]
Irr_atn_dec = 22.5[db]
Irr_atn_noe = 22.5[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 22[dc]





Filename = tes-ketone-sulfone-1H
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 24-JUL-2010 14:48:10
Revision_time = 16-JUL-2011 13:27:57
Current_time = 16-JUL-2011 13:28:18
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 32
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 24.1[degC]



tes-ketone-sulfone-13

File name = tes-ketone-sulfone-13

Author = delta

Experiment = single_pulse_dec

Sample_id = S#570229

Solvent = CHLOROFORM-D

Creation_time = 24-JUL-2010 15:02:55

Revision_time = 21-DEC-2010 10:15:49

Current_time = 21-DEC-2010 10:16:23

Comment = single pulse decouple

Data_format = 1D COMPLEX

Dim_size = 26214

Dim_title = 13C

Dim_units = [ppm]

Dimensions = X

Site = ECX400M

Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])

X_acq_duration = 1.04333312[s]

X_domain = 13C

X_freq = 100.52530333[MHz]

X_offset = 100[ppm]

X_points = 32768

X_prescans = 4

X_resolution = 0.95846665[Hz]

X_sweep = 31.40703518[kHz]

Irr_domain = 1H

Irr_freq = 399.78219838[MHz]

Irr_offset = 5[ppm]

Clipped = FALSE

Mod_return = 1

Scans = 59

Total_scans = 59

X_90_width = 9.2[us]

X_acq_time = 1.04333312[s]

X_angle = 45[deg]

X_atn = 6.6[dB]

X_pulse = 4.6[us]

Irr_atn_dec = 22.2[dB]

Irr_atn_noe = 22.2[dB]

Irr_noise = WALTZ

Decoupling = TRUE

Initial_wait = 1[s]

Noe = TRUE

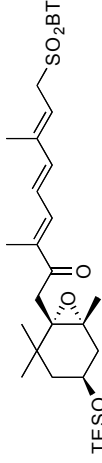
Noe_time = 5[s]

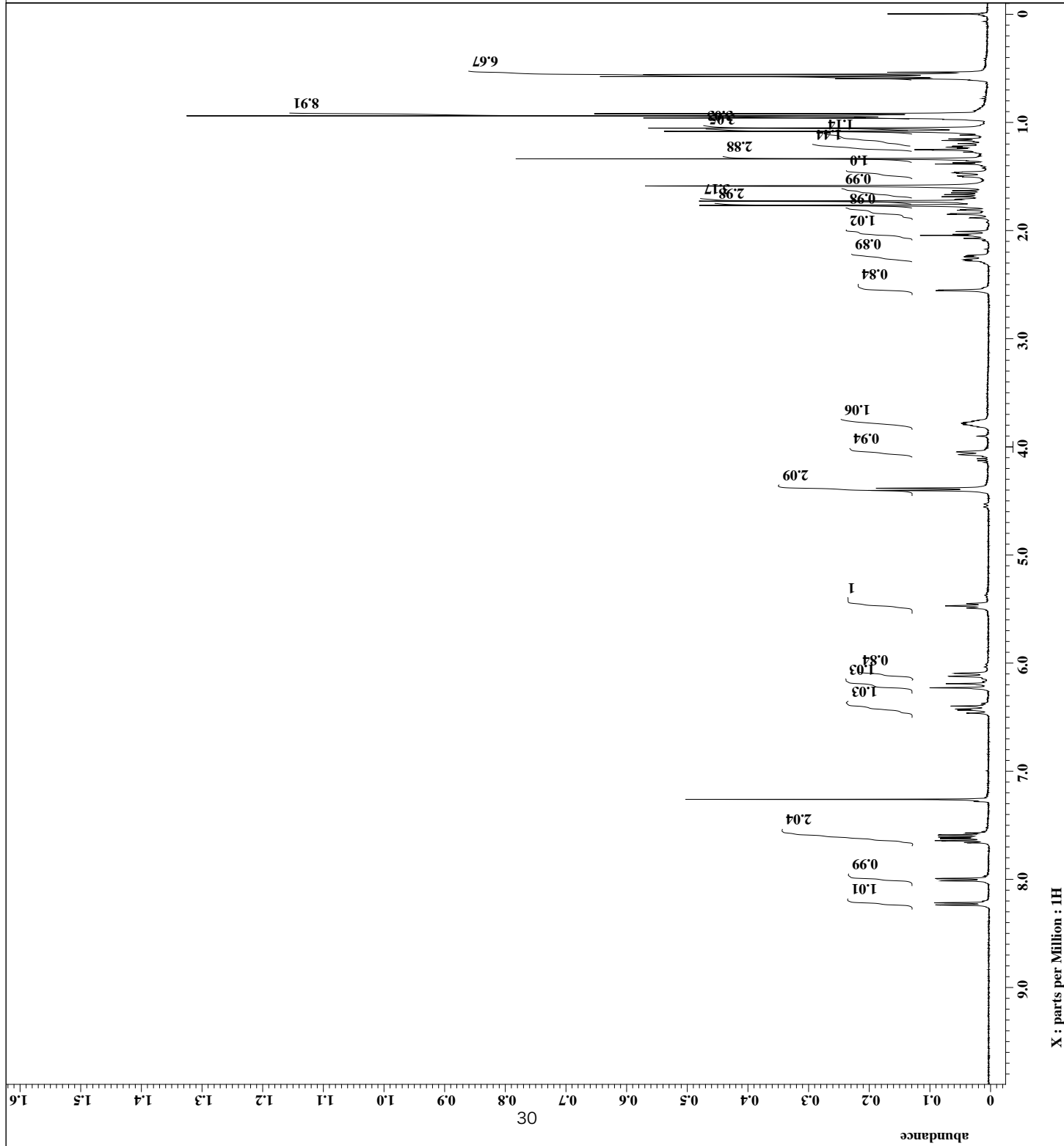
Recvr_gain = 50

Relaxation_delay = 5[s]

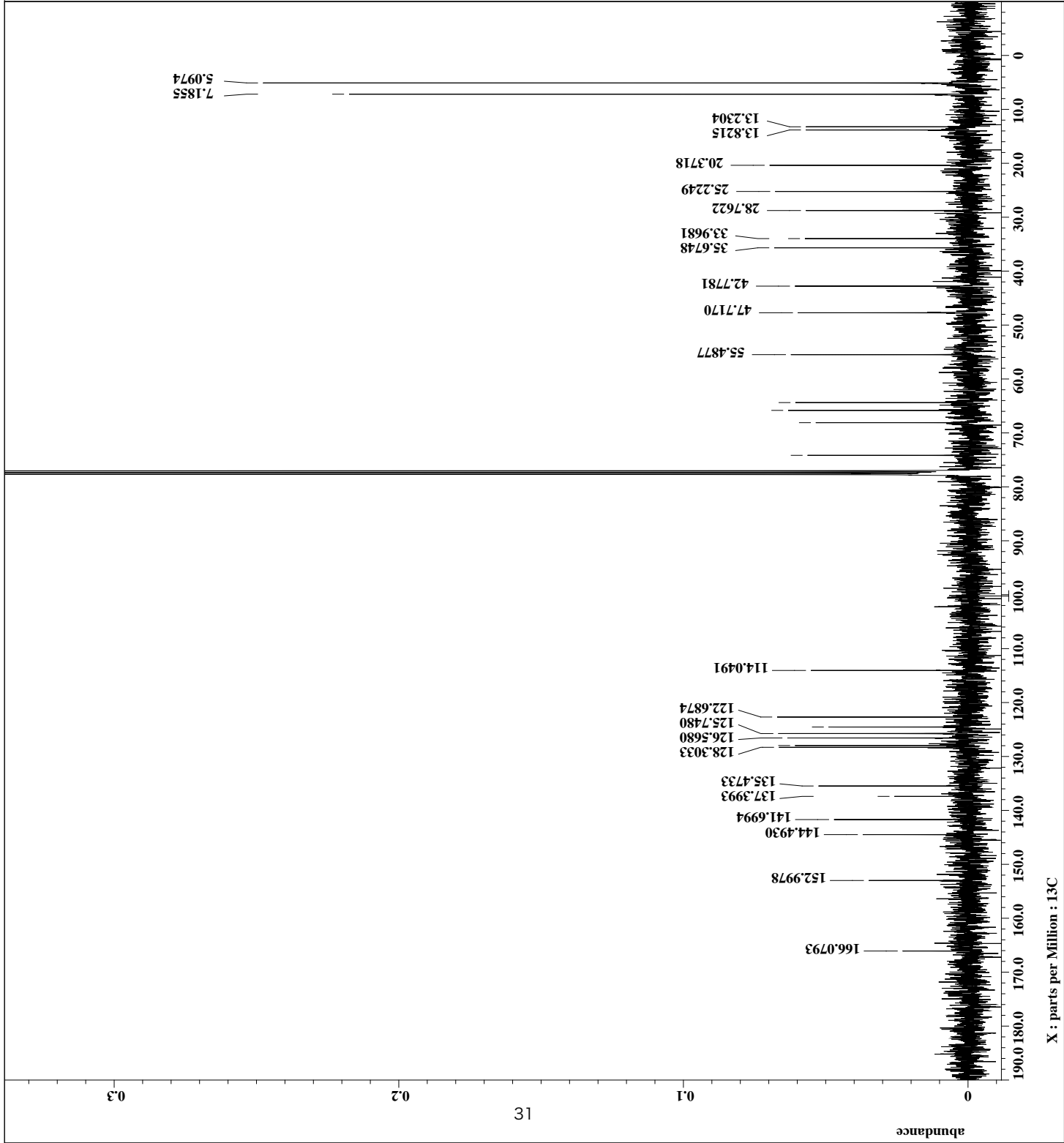
Repetition_time = 6.04333312[s]

Temp_get = 24.5[degC]

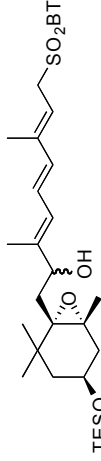


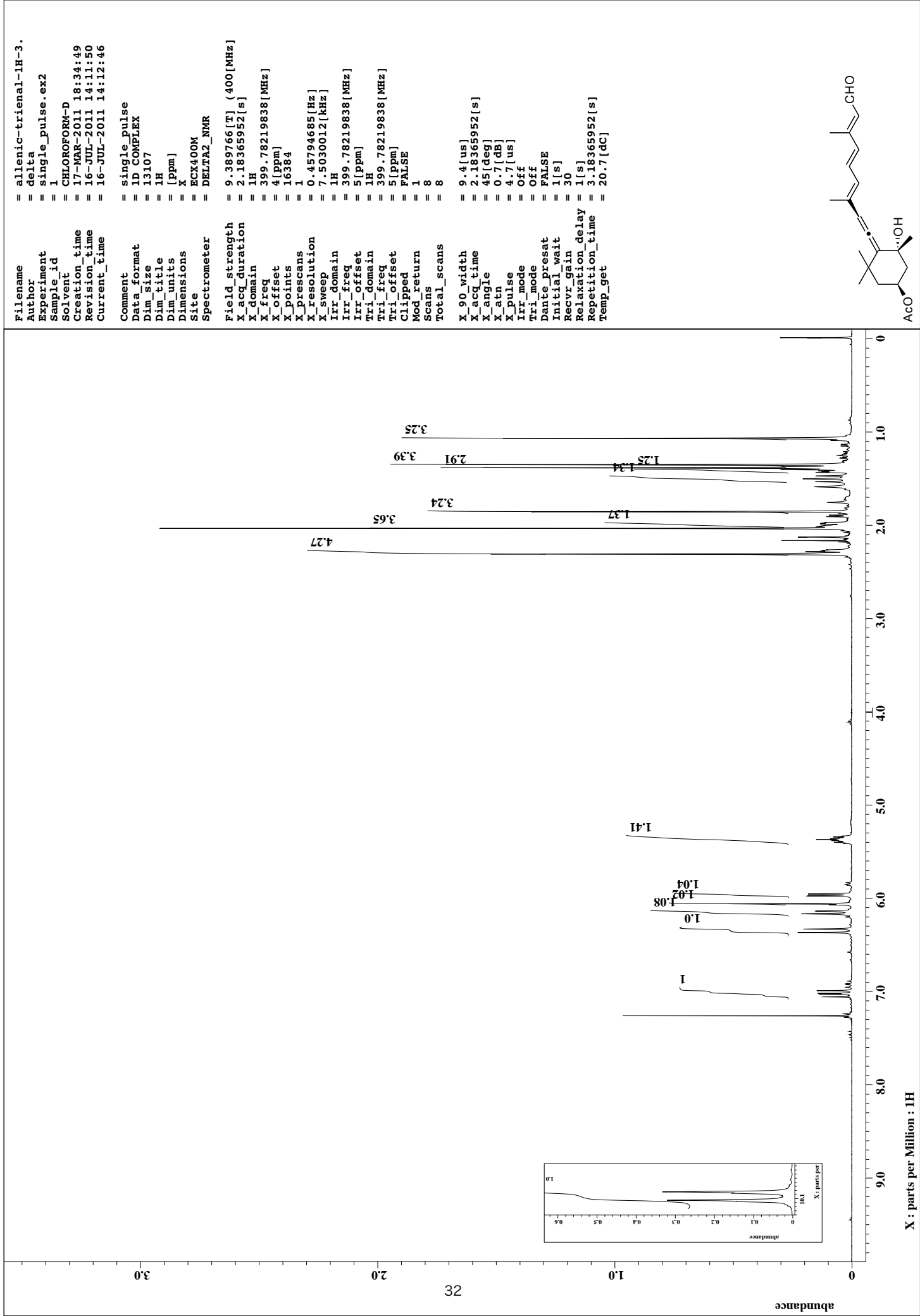


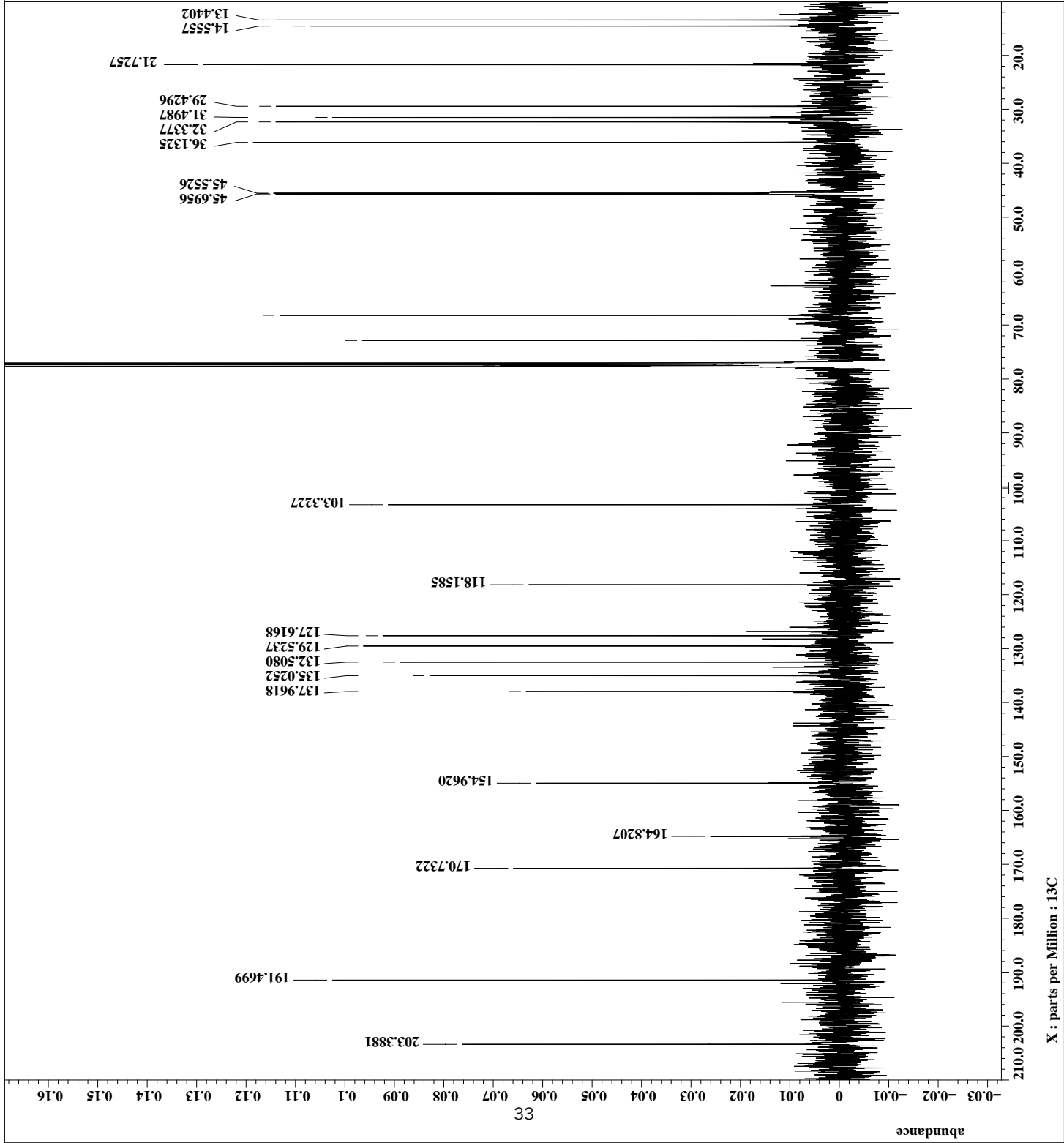
Filename	=	tes-OH-sulfone-lh-3.3.j
Author	=	delta
Experiment	=	single_pulse.ex2
Sample id	=	1
Solvent	=	CHLOROFORM-D
Creation time	=	4-JUN-2011 15:50:03
Revision time	=	16-JUL-2011 13:43:57
Current_time	=	16-JUL-2011 13:44:22
Comment	=	single pulse
Data format	=	1D COMPLEX
Dim_size	=	13107
Dim_title	=	1H
Dim_units	=	[ppm]
Dimensions	=	x
Site	=	EXC400M
Spectrometer	=	DELTA2_NMR
Field_strength	=	9.389766[T] (400[MHz]
X_acq_duration	=	2.18365952[s]
X_domain	=	1H
X_freq	=	399.78219838[MHz]
X_offset	=	4[ppm]
X_points	=	16384
X_prescans	=	1
X_resolution	=	0.45794685[Hz]
X_sweep	=	7.5030012[kHz]
Irr_domain	=	1H
Irr_freq	=	399.78219838[MHz]
Irr_offset	=	5[ppm]
Tri_domain	=	1H
Tri_freq	=	399.78219838[MHz]
Tri_offset	=	5[ppm]
Clipped	=	FALSE
Mod_return	=	1
Scans	=	8
Total_scans	=	8
X_90_width	=	9.4[us]
X_acq_time	=	2.18365952[s]
X_angle	=	45[deg]
X_atn	=	0.7[dB]
X_pulse	=	4.7[us]
Irr_mode	=	Off
Tri_mode	=	Off
Dante_presat	=	FALSE
Initial_wait	=	1[s]
Recvr_gain	=	36
Relaxation_delay	=	1[s]
Repetition_time	=	3.18365952[s]
Temp_get	=	21.9[AC]



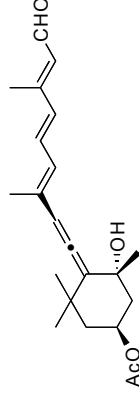
Filename = tes-OH-sulfone-13C-3.
Author = delta
Experiment = single_pulse_dec
Sample_id = S#62607
Solvent = CHLOROFORM-D
Creation_time = 4-JUN-2011 16:16:47
Revision_time = 16-JUL-2011 13:45:20
Current_time = 16-JUL-2011 13:45:59
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 110
Total_scans = 110
X_90_width = 9.2[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[dB]
X_pulse = 4.6[us]
Irr_atn_dec = 22.5[dB]
Irr_atn_noe = 22.5[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 56
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 22.2[degC]

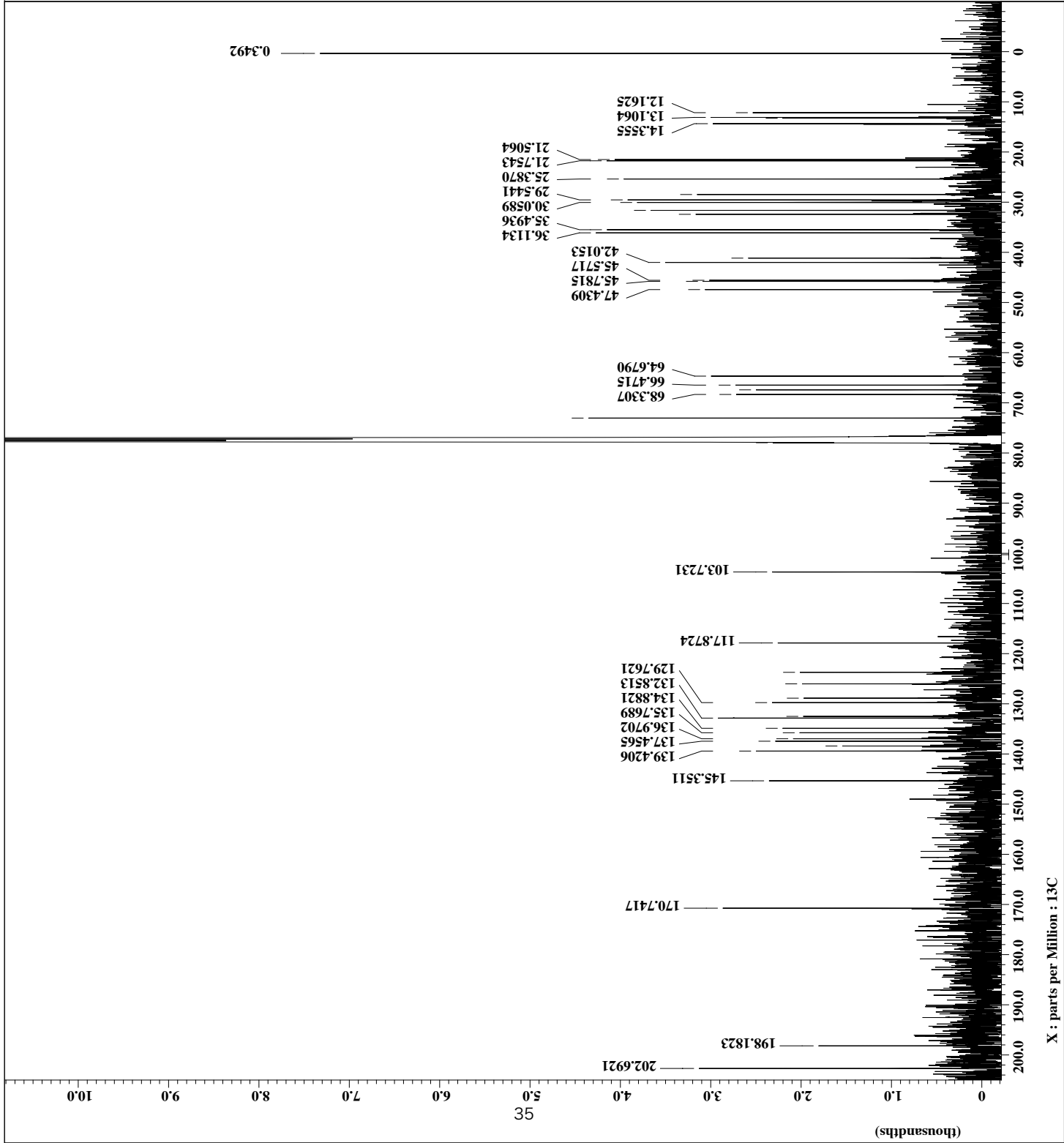




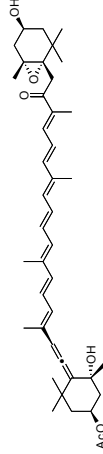


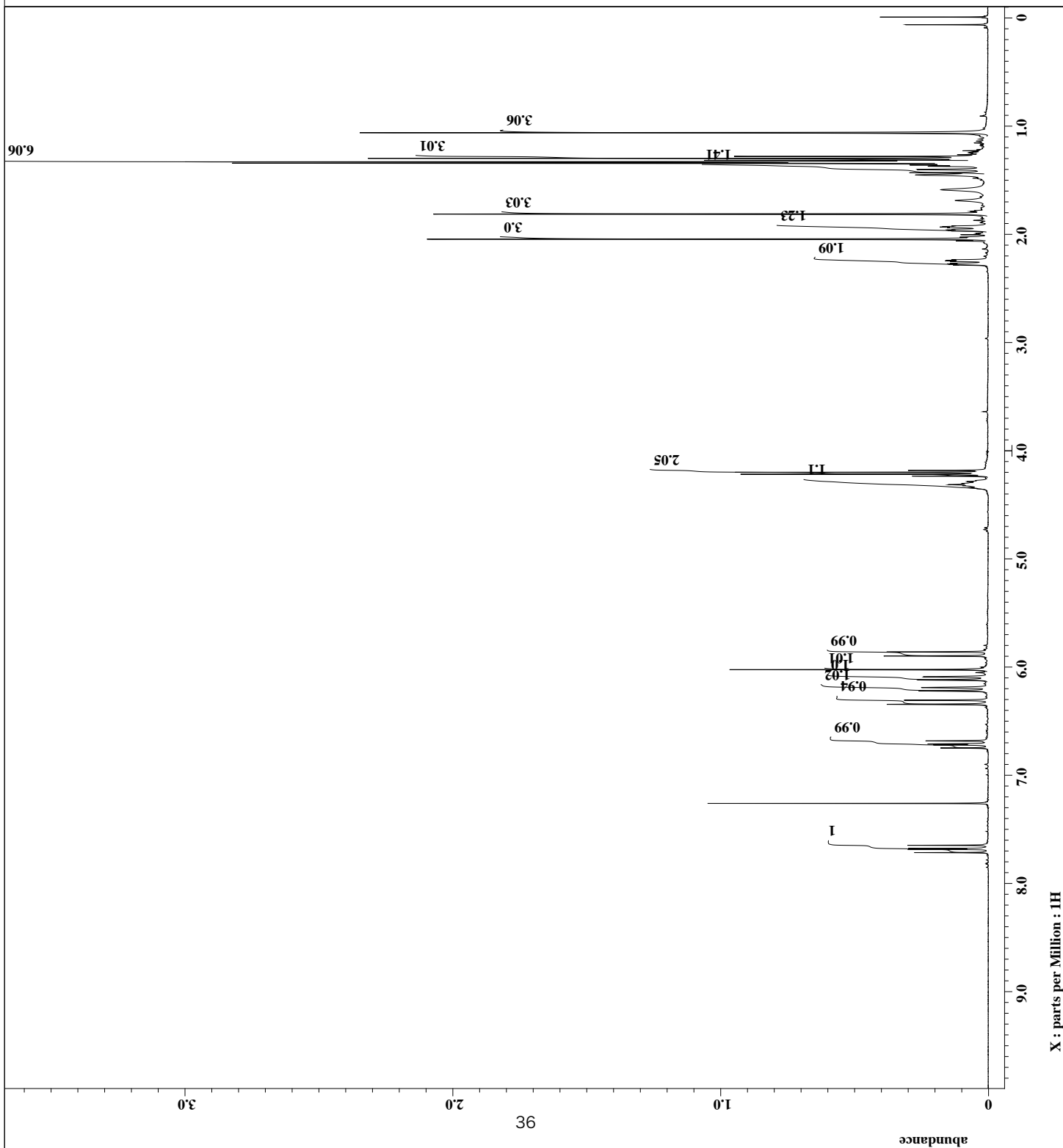
Filename = allenic-trienal-13C-3
Author = delta
Experiment = single_pulse_dec
Sample_id = S#714568
Solvent = CHLOROFORM-D
Creation_time = 17-MAR-2011 18:50:54
Revision_time = 16-JUL-2011 14:17:17
Current_time = 16-JUL-2011 14:17:53
Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 123
Total_scans = 123
X_90_width = 9.2[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[db]
X_pulse = 4.6[us]
Irr_atn_dec = 22.5[db]
Irr_atn_noe = 22.5[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 56
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 20.7[dc]



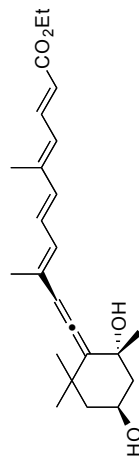


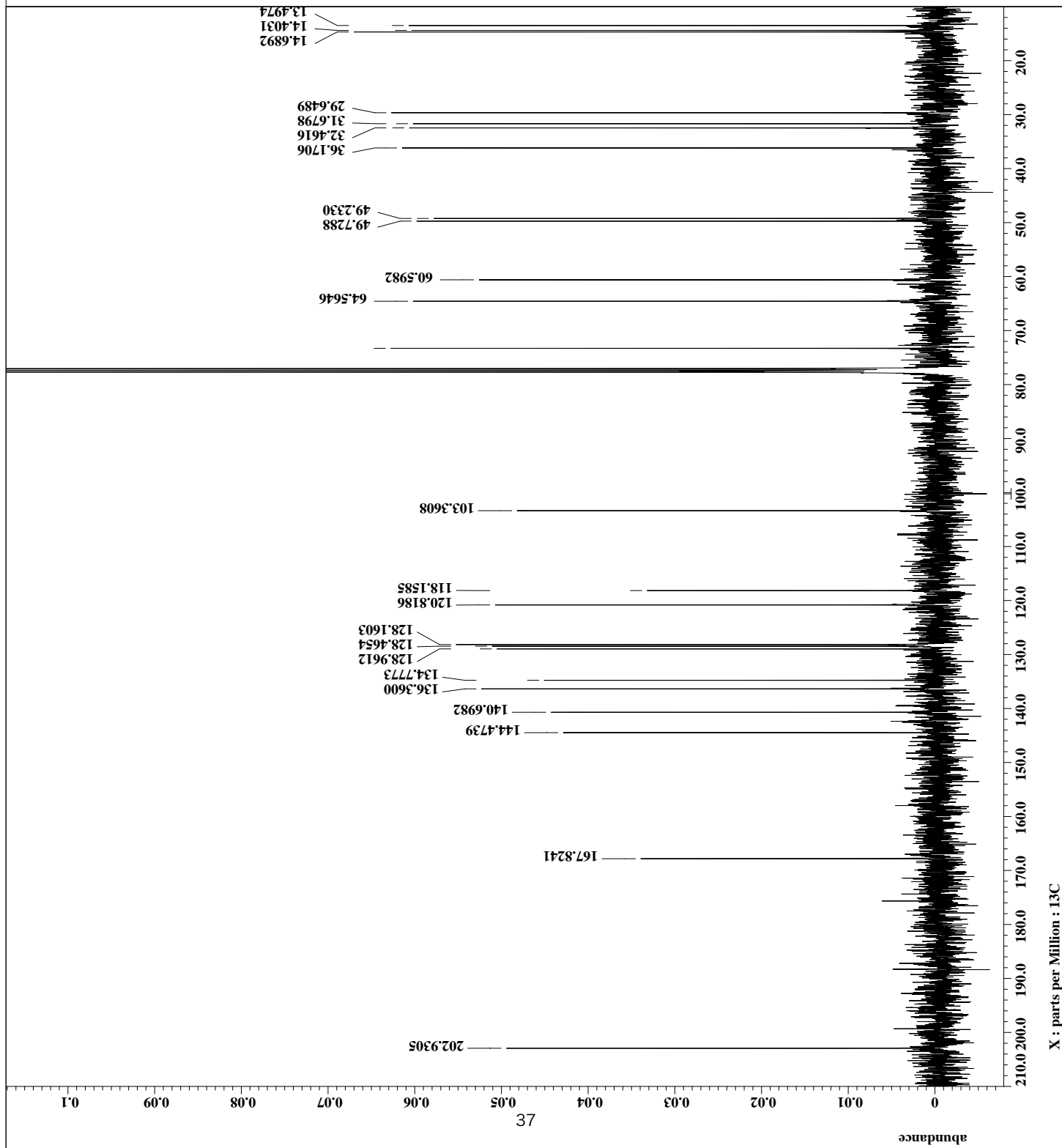
Filename = C40-fucooxanthin-13C-j
Author = delta
Experiment = single_pulse_dec
Sample_id = S#795509
Solvent = CHLOROFORM-D
Creation_time = 11-SEP-2010 09:06:48
Revision_time = 21-DEC-2010 10:03:21
Current_time = 21-DEC-2010 10:04:54
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = x
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 6546
Total_scans = 6546
X_90_width = 9.2[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[db]
X_pulse = 4.6[us]
Irr_atn_dec = 22.5[db]
Irr_atn_noe = 22.5[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 25.4[dc]



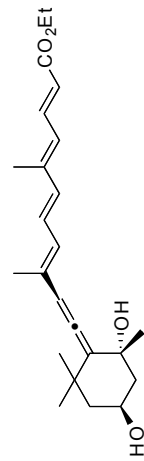


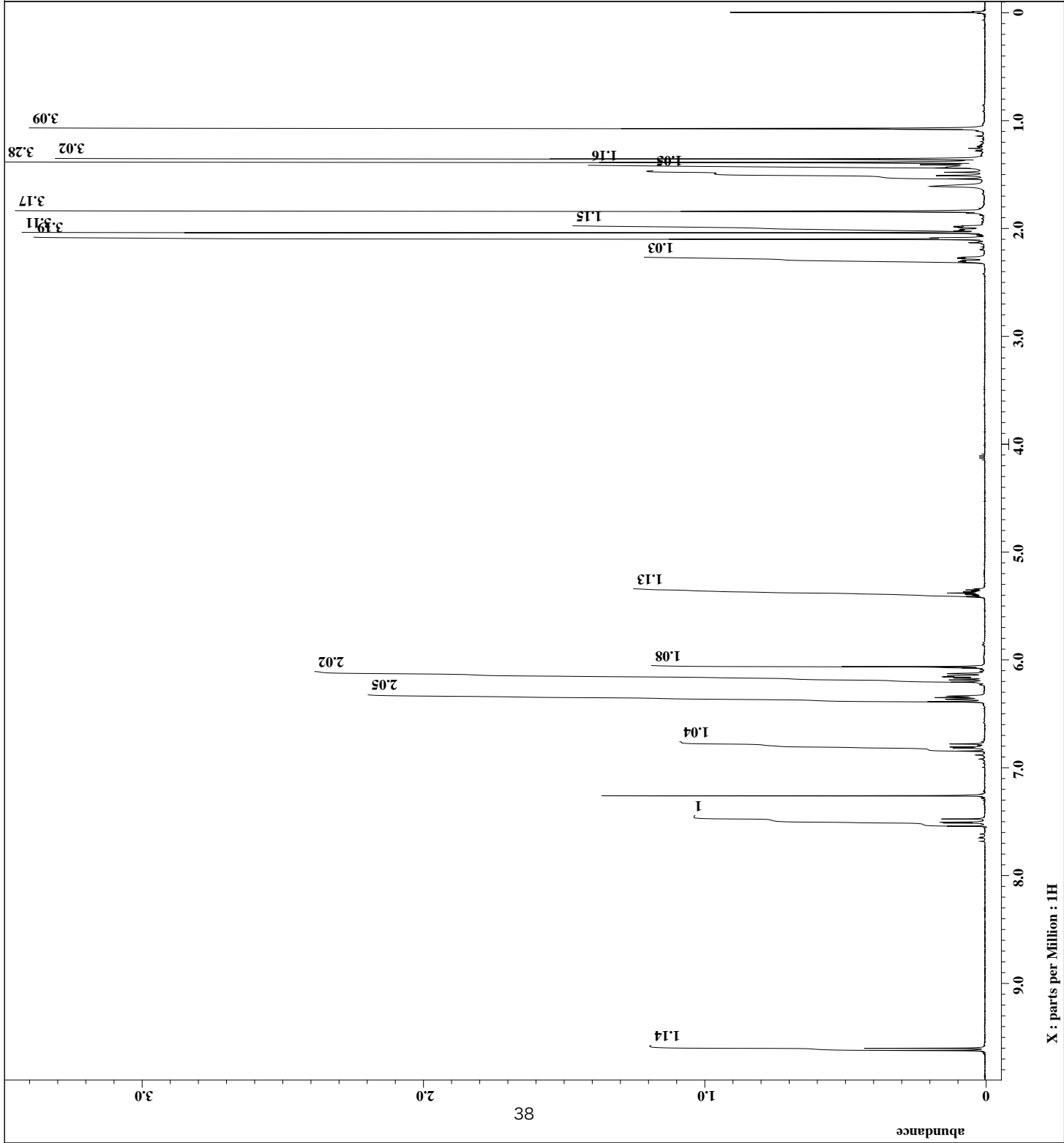
Filename	=	allenic-tetraene-este
Author	=	delta
Experiment	=	single_pulse.ex2
Sample id	=	1
Solvent	=	CHLOROFORM-D
Creation time	=	23-MAR-2011 14:20:25
Revision time	=	16-JUL-2011 13:58:06
Current time	=	16-JUL-2011 13:59:19
Comment	=	single_pulse
Data format	=	1D COMPLEX
Dim_size	=	13107
Dim_title	=	1H
Dim_units	=	[ppm]
Dimensions	=	x
Site	=	ECKA00M
Spectrometer	=	DELTA2_NMR
Field_strength	=	9.389766[T] (400[MHz]
X_acq_duration	=	2.18365952[s]
X_domain	=	1H
X_freq	=	399.78219838[MHz]
X_offset	=	4[ppm]
X_points	=	16384
X_prescans	=	1
X_resolution	=	0.45794685[Hz]
X_sweep	=	7.5030012[kHz]
Irr_domain	=	1H
Irr_freq	=	399.78219838[MHz]
Irr_offset	=	5[ppm]
Tri_domain	=	1H
Tri_freq	=	399.78219838[MHz]
Tri_offset	=	5[ppm]
Clipped	=	FALSE
Mod_return	=	1
Scans	=	8
Total_scans	=	8
X_90_width	=	9.4[us]
X_acq_time	=	2.18365952[s]
X_angle	=	45[deg]
X_atn	=	0.7[dB]
X_pulse	=	4.7[us]
Irr_mode	=	Off
Tri_mode	=	Off
Dante_presat	=	FALSE
Initial_wait	=	1[s]
Recvr_gain	=	34
Relaxation_delay	=	1[s]
Repetition_time	=	3.18365952[s]
Temp_get	=	20.6[dc]



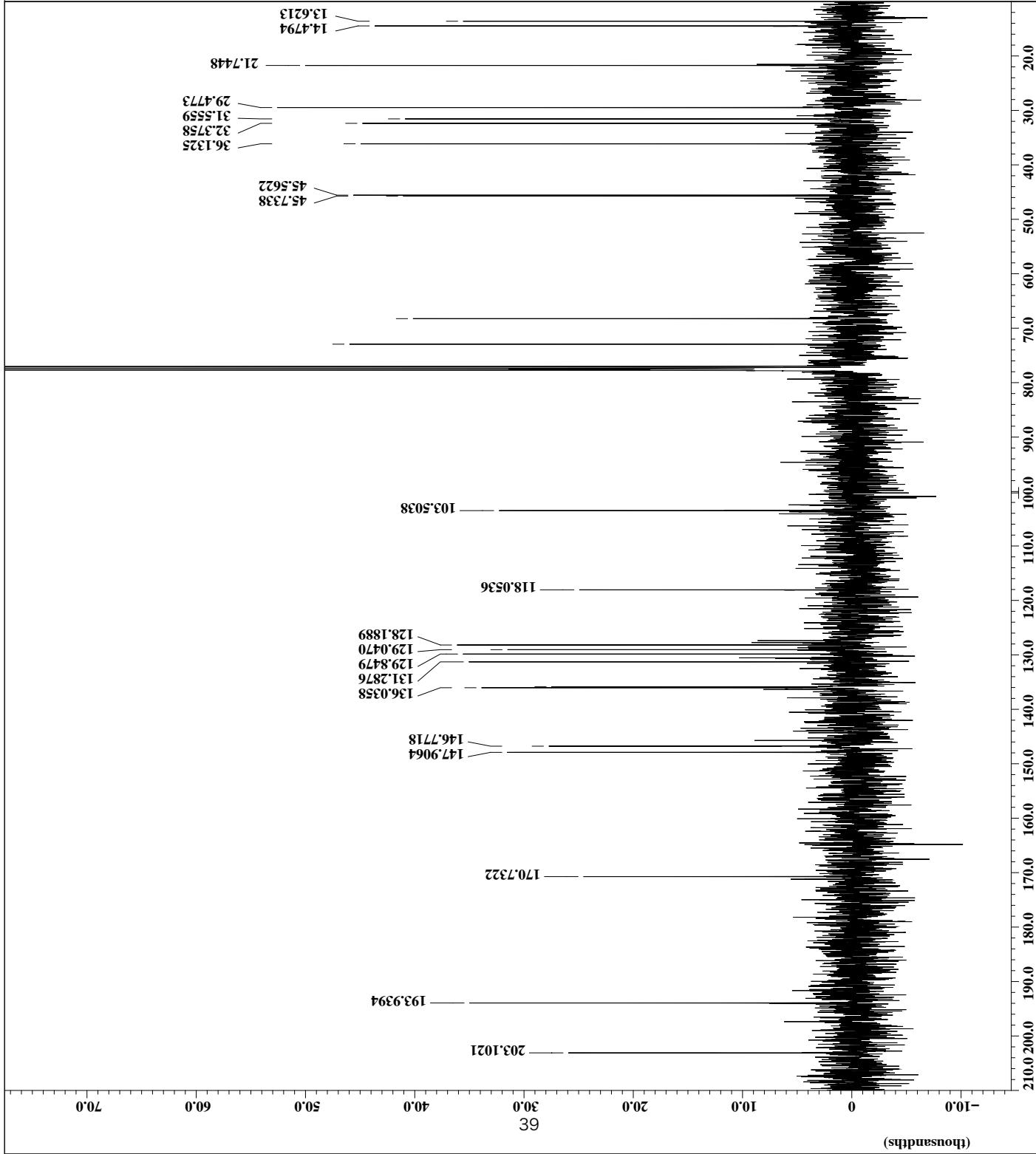


Filename	=	allenlic-tetraene-este
Author	=	delta
Experiment	=	single_pulse_dec
Sample_id	=	S#561878
Solvent	=	CHLOROFORM-D
Creation_time	=	23-MAR-2011 14:41:51
Revision_time	=	16-JUL-2011 14:19:27
Current_time	=	16-JUL-2011 14:20:11
Comment	=	single pulse decouple
Data format	=	1D COMPLEX
Dim_size	=	26214
Dim_title	=	13C
Dim_units	=	[ppm]
Dimensions	=	x
Site	=	EXCA400M
Spectrometer	=	DELTA2_NMR
Field_strength	=	9.389766[T] (400[MHz]
X_acq_duration	=	1.043333312[s]
X_domain	=	13C
X_freq	=	100.52530333[MHz]
X_offset	=	100[ppm]
X_points	=	32768
X_prescans	=	4
X_resolution	=	0.9584665[Hz]
X_sweep	=	31.40703518[kHz]
Y_domain	=	1H
Y_freq	=	399.78219838[MHz]
Y_offset	=	5[ppm]
Clipped	=	FALSE
Mod_return	=	1
Scans	=	183
Total_scans	=	183
X_90_width	=	9.2[us]
X_acq_time	=	1.043333312[s]
X_angle	=	45[deg]
X_atn	=	6.6[db]
X_pulse	=	4.6[us]
X_atn_dec	=	22.5[db]
Irr_atn_noe	=	22.5[db]
Irr_noise	=	WALTZ
Decoupling	=	TRUE
Initial_wait	=	1[s]
Noe	=	TRUE
Noe_time	=	5[s]
Recvr_gain	=	50
Relaxation_delay	=	5[s]
Repetition_time	=	6.043333312[s]
Temp_get	=	21.4[degC]

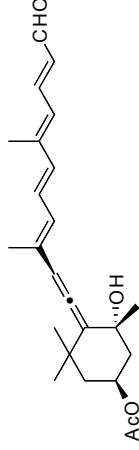




Filename = allenic-tetraenal-1H-
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 5-APR-2011 19:14:42
Revision_time = 16-JUL-2011 14:04:13
Current_time = 16-JUL-2011 14:07:21
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 9.4[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 0.7[dB]
X_pulse = 4.7[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 22.2[degC]

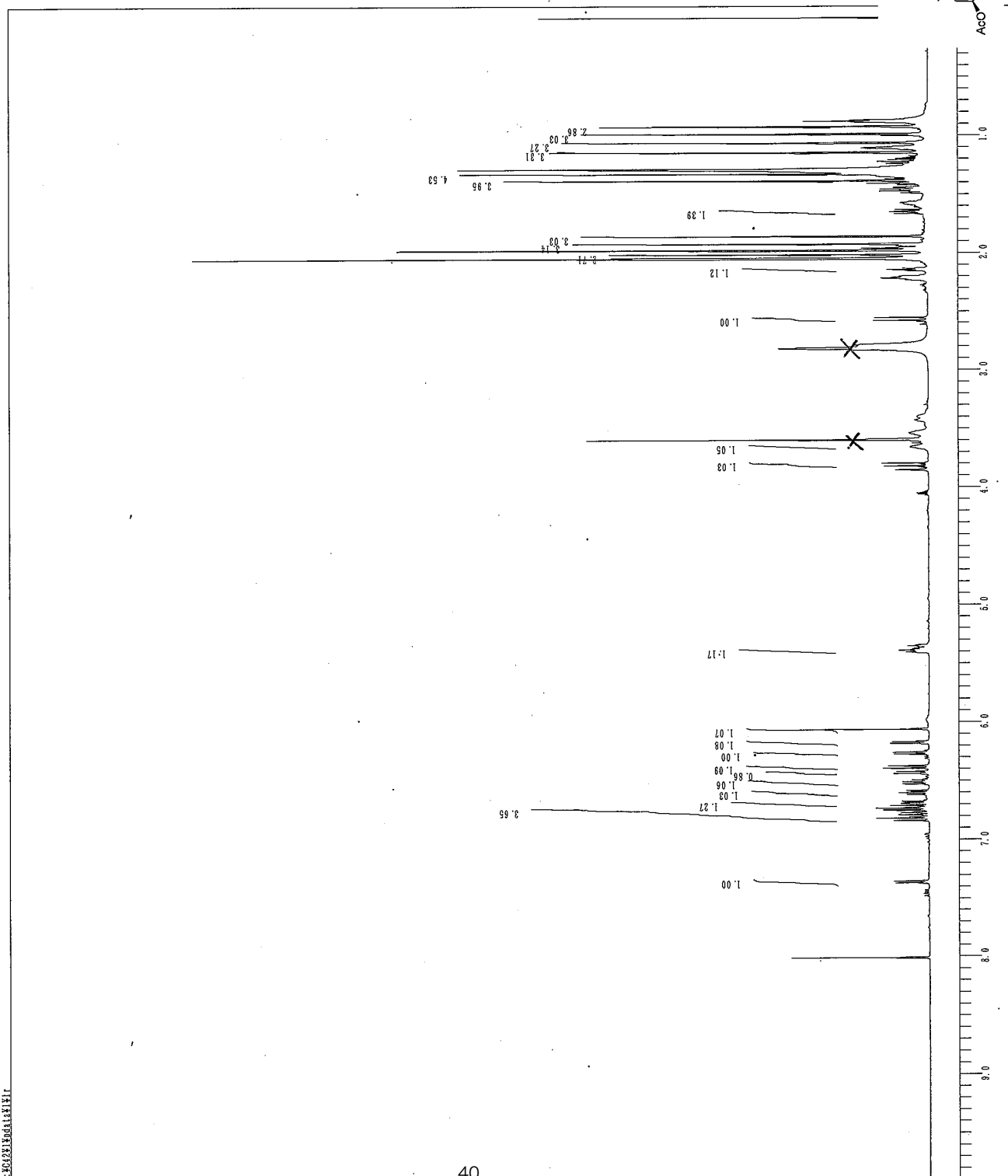


Filename = allenic-tetraenal-13C
Author = delta
Experiment = single_pulse_dec
Sample_id = S#627606
Solvent = CHLOROFORM-D
Creation_time = 5-APR-2011 16:24:01
Revision_time = 16-JUL-2011 14:18:25
Current_time = 16-JUL-2011 14:18:58
Comment = single pulse decouple
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = x
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz])
x_acq_duration = 1.04333312[s]
x_domain = 13C
x_freq = 100.52530333[MHz]
x_offset = 100[ppm]
x_points = 32768
x_prescans = 4
x_resolution = 0.95846665[Hz]
x_sweep = 31.40703518[kHz]
irr_domain = 1H
irr_freq = 399.78219838[MHz]
irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 115.0
Total_scans = 115.0
x_90_width = 9.2[us]
x_acq_time = 1.04333312[s]
x_angle = 45[deg]
x_atn = 6.6[db]
x_pulse = 4.6[us]
irr_atn_dec = 22.5[db]
irr_atn_noe = 22.5[db]
irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 22.7[dc]



F:\VC42\1\pdat\2\1\1\1

IR	FIRST=750.16 L/L
COUNT	11:18:59.02 -750 WASH116.DMS-750
BATH	NH
EXAMIN	1230
EXTEND	750.13 MHz
OBSERV	3.32 KHz
ORIGIN	27.6 Hz
PROBHD	5 mm
FRQNUC	11281.16 Hz
SCANS	2.9088 sec
AQTIME	2.0000 sec
PULP	9.75 msec
FWHM	
TRENG	
SLOPE	Acetone 27.4 C
SLVNT	
EXREF	12.19 DDM
DF	0.40 Hz
RGAIN	64



DFILE COMNT DATIM OBNUC EXMOD OBFRQ OBSET OBFIN POINT FREQU SCANS ACQTM PD PWI IRNUC CTEMP SLYNT EXREF BF RGAIN

