ASYMMETRIC SYNTHESIS OF β-LACTAMS BY INTRAMOLECULAR CONJUGATE ADDITION OF SERINE AND CYSTEINE DERIVATIVES VIA MEMORY OF CHIRALITY

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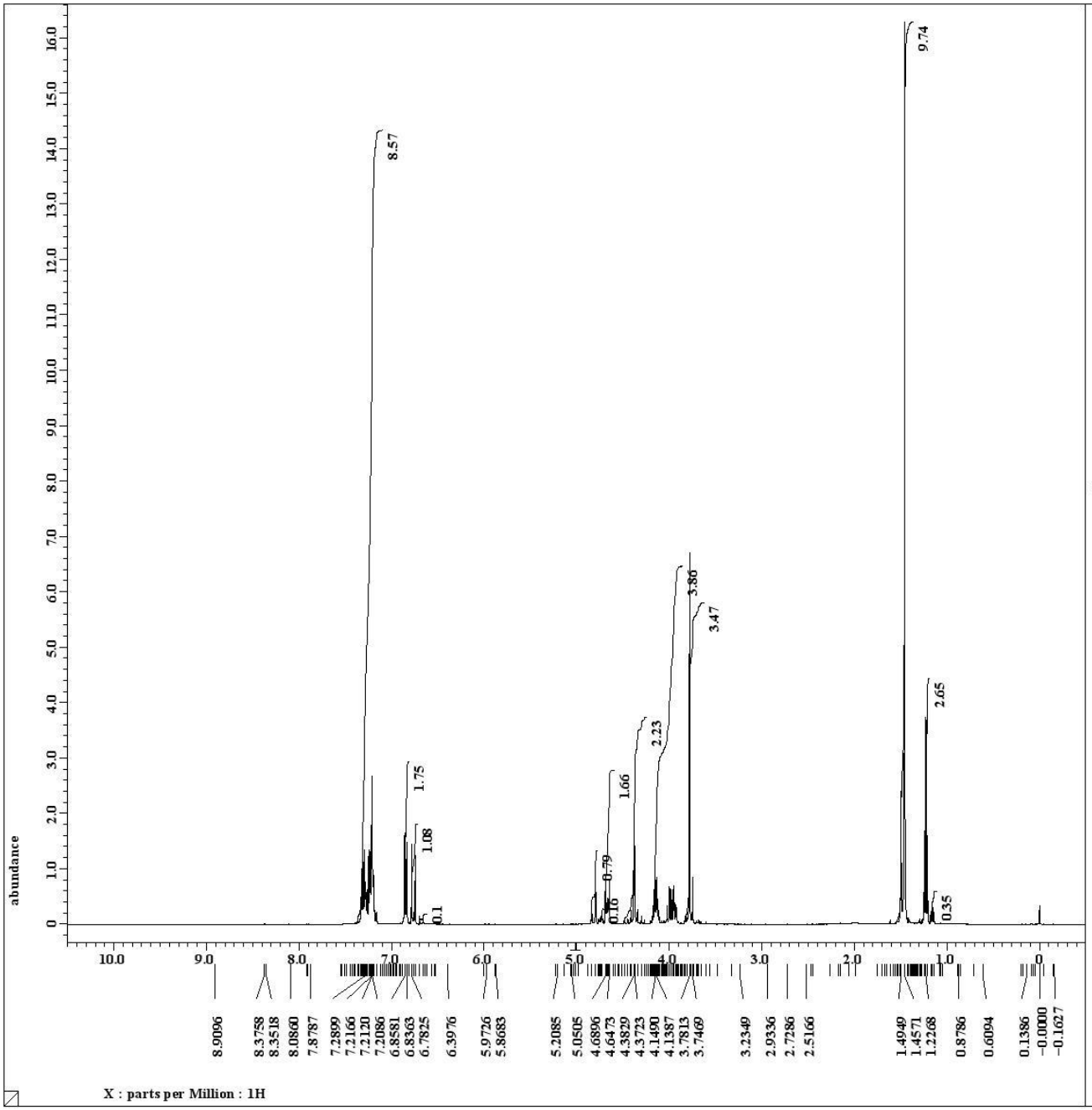
Supporting Information

Table of Contents

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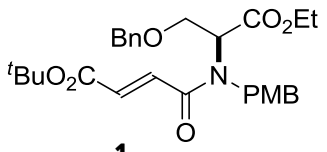
Filename          = RM1188-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 21-OCT-2014 14:08:09
Revision_time     = 21-OCT-2014 23:03:19
Current_time      = 21-OCT-2014 23:03:25

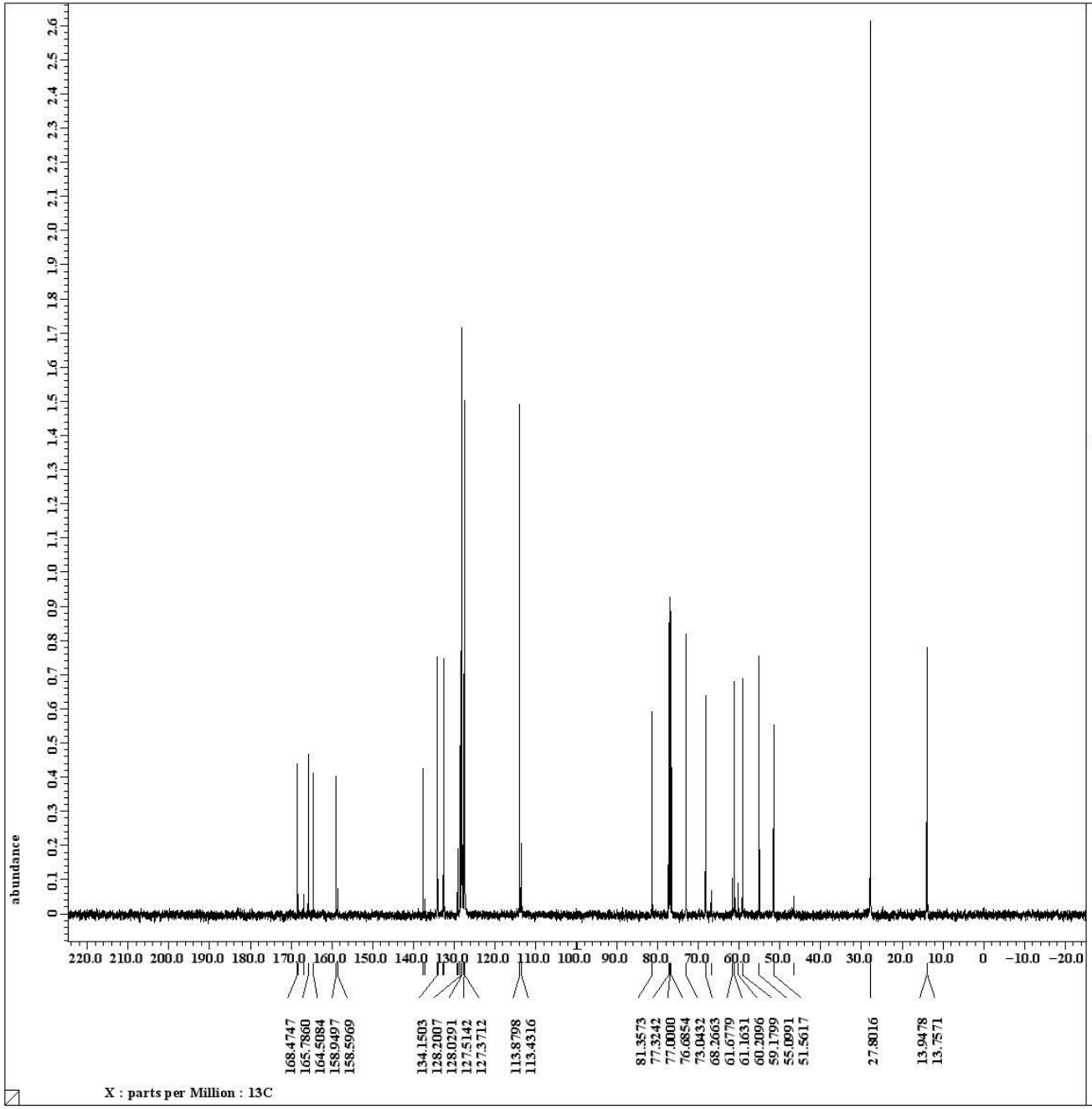
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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

X_90_width        = 11.14[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 0.3[dB]
X_pulse           = 5.57[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 22
Relaxation_delay  = 5[s]
Repetition_time   = 7.18365952[s]
Temp_get          = 18.4[dC]
```



1

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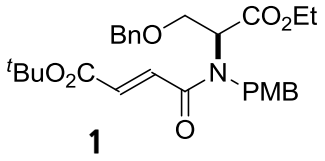
Filename          = RM1188-13C-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 21-OCT-2014 14:15:18
Revision_time     = 21-OCT-2014 22:49:19
Current_time      = 21-OCT-2014 22:49:29

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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             = 100
Total_scans       = 100

X_90_width        = 10.54[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.51333333[us]
Irr_atn_dec       = 20.58[dB]
Irr_atn_noe       = 20.58[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 18.8[dC]
```



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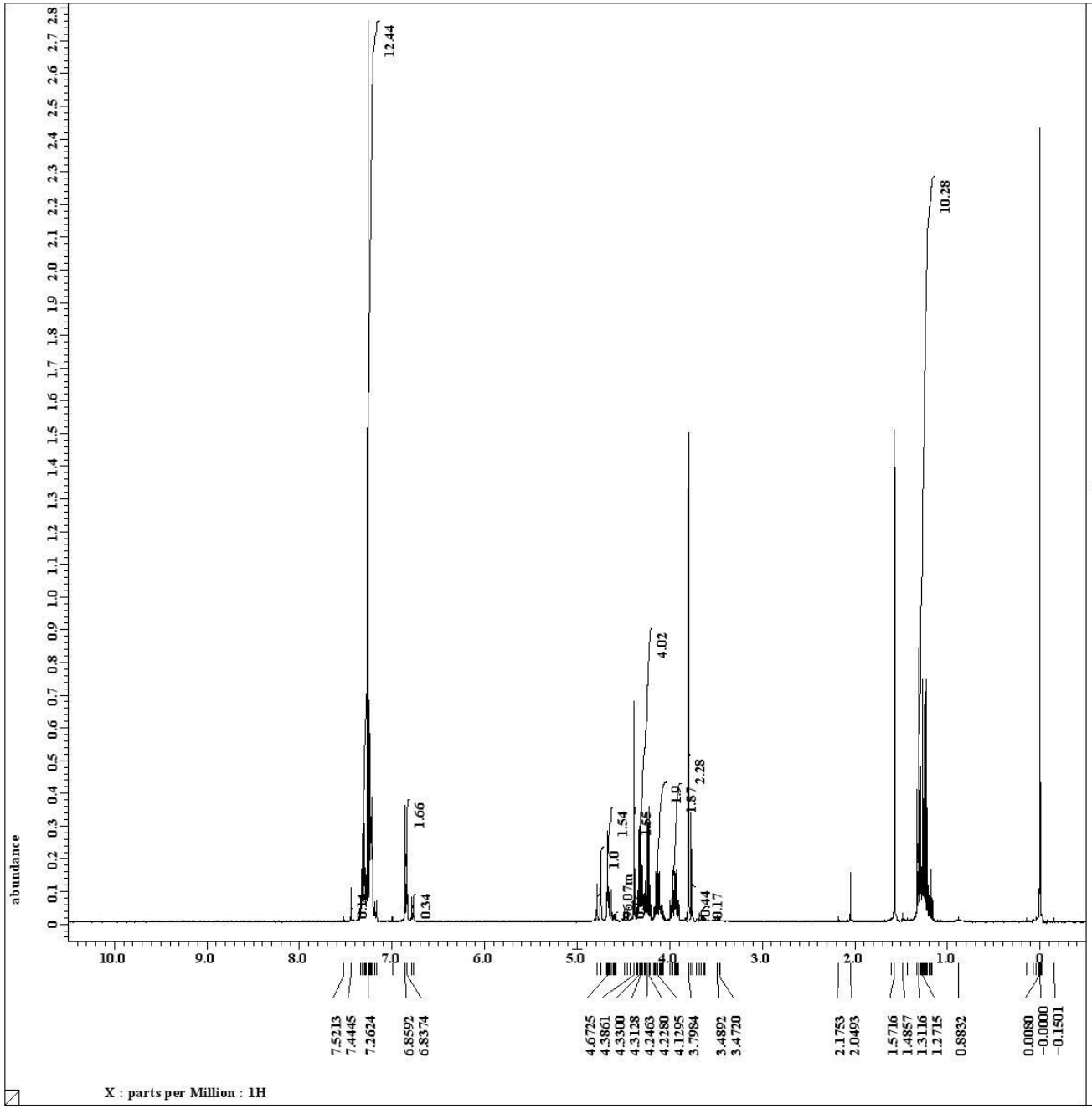


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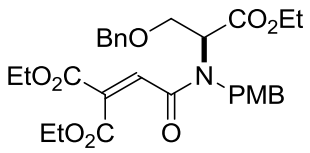
Filename          = RM401-column-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#749352
Solvent           = CHLOROFORM-D
Creation_time     =  7-APR-2012 13:32:23
Revision_time     = 21-OCT-2014 15:30:37
Current_time      = 21-OCT-2014 15:30:52

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.45794685[Hz]
X_sweep           = 7.5030012[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.78219838[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 10[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 0.3[dB]
X_pulse           = 5[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 7.18365952[s]
Temp_get          = 18.3[dC]
```



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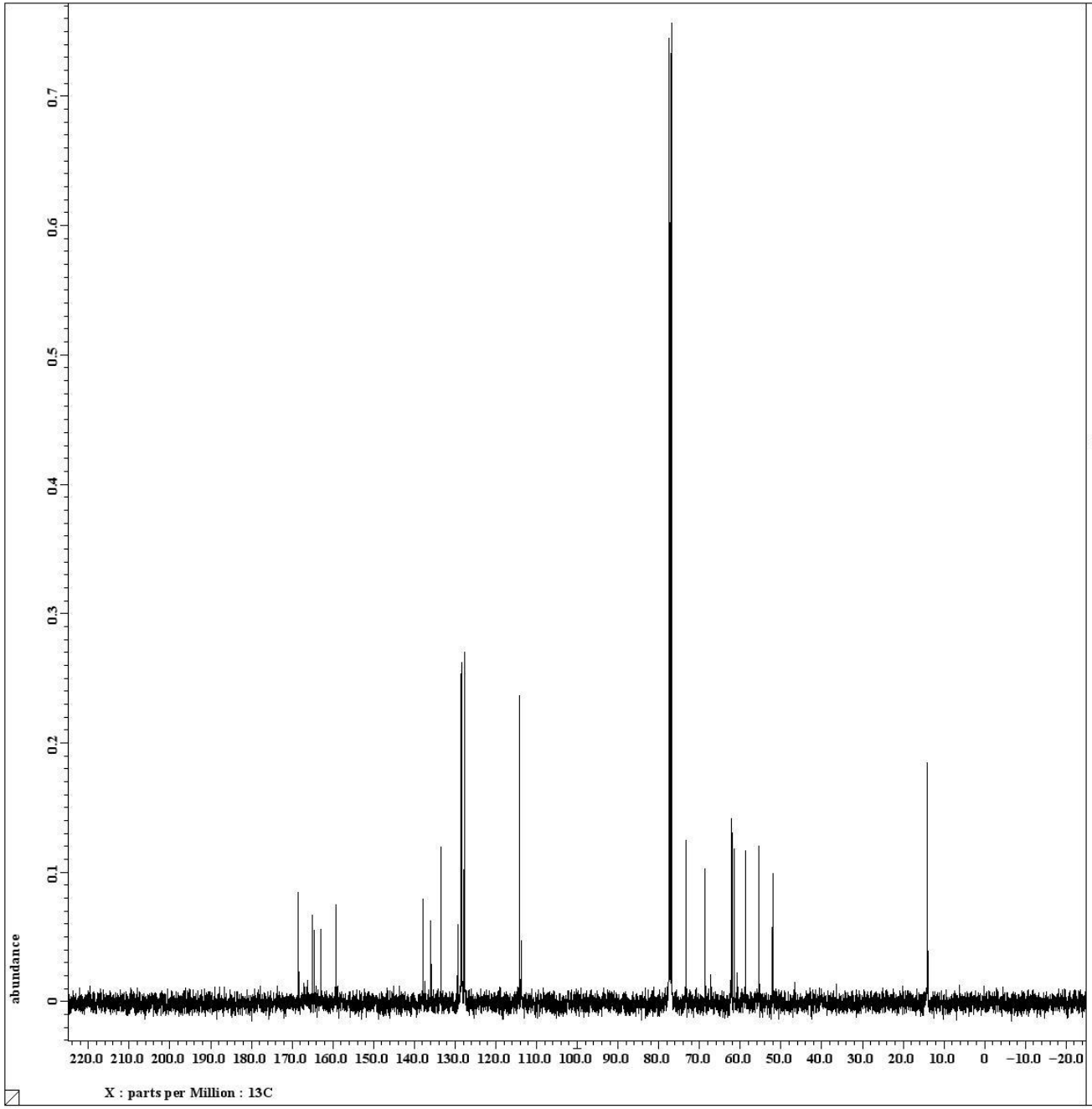


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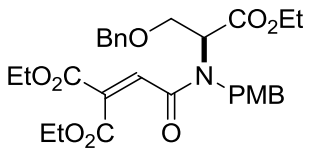
Filename          = RM439-13C-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = a
Solvent           = CHLOROFORM-D
Creation_time     =  3-FEB-2013 10:38:44
Revision_time     =  2-OCT-2015 21:50:03
Current_time      =  2-OCT-2015 21:53:39

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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             = 179
Total_scans       = 179

X_90_width        = 10.2[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.4[us]
Irr_atn_dec       = 20.8[dB]
Irr_atn_noe       = 20.8[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          = 19[dC]
```



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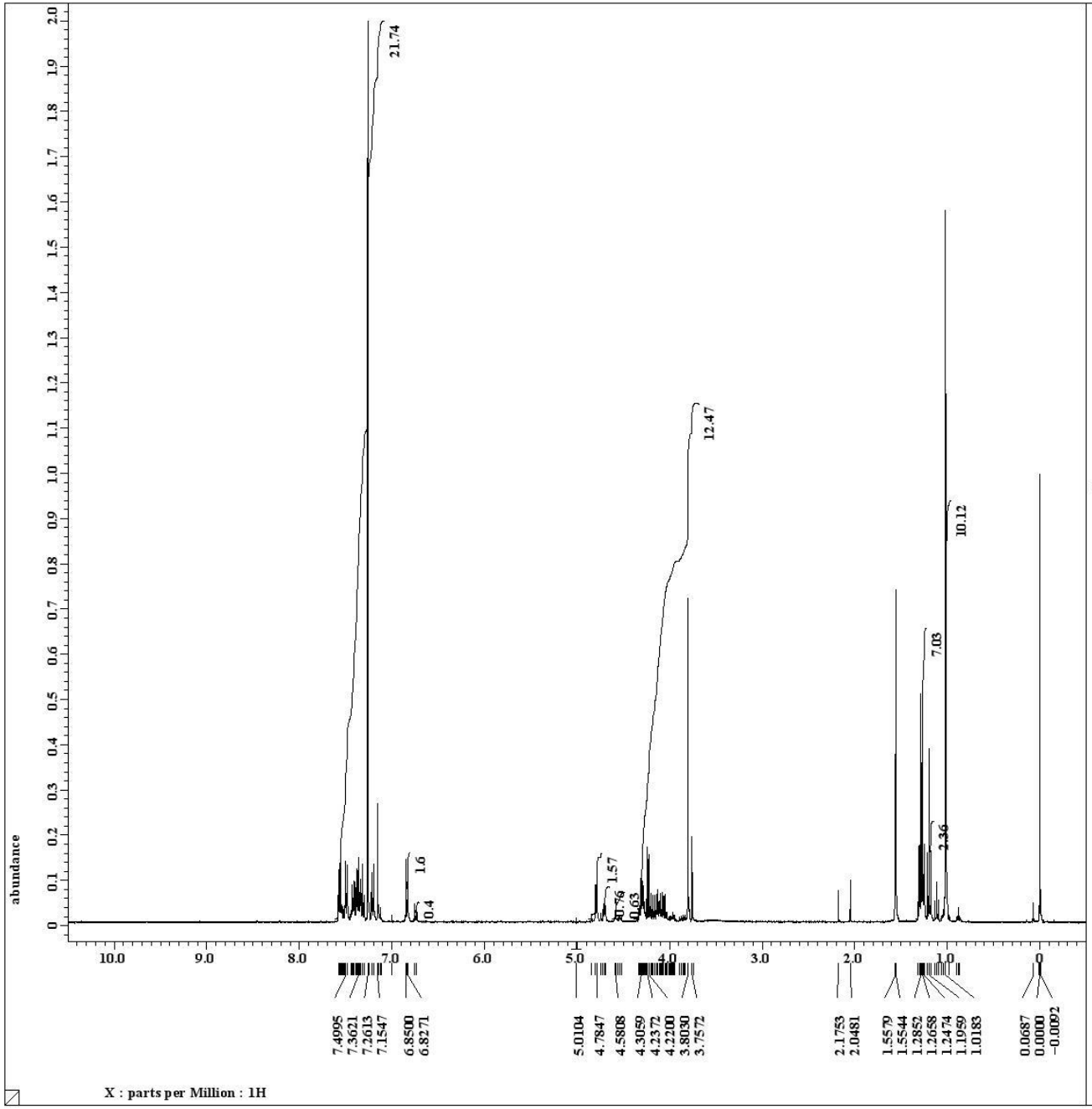


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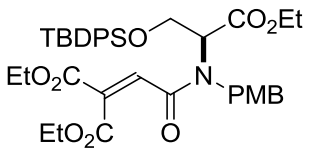
Filename          = RM346-recycle-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#734600
Solvent           = CHLOROFORM-D
Creation_time     = 31-JAN-2012 13:16:19
Revision_time     = 21-OCT-2014 15:43:38
Current_time      = 21-OCT-2014 15:43:51

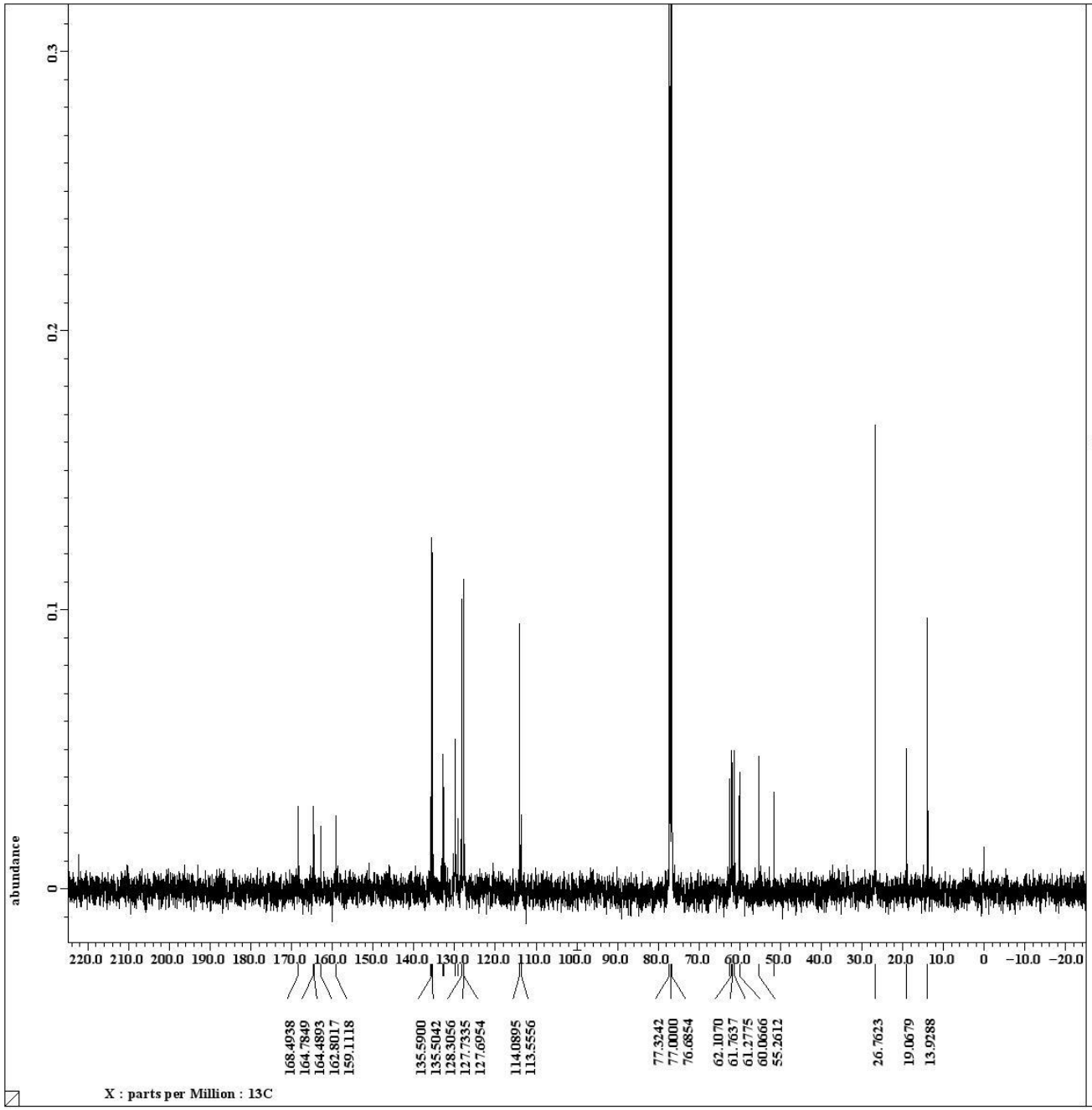
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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

X_90_width        = 10[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 0.3[dB]
X_pulse           = 5[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 7.18365952[s]
Temp_get          = 19.2[dC]
```



6

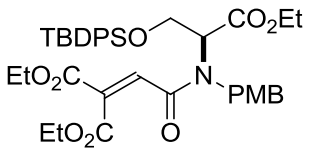



```
Filename          = TBDPSprecusor-13C-6.j
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = a
Solvent           = CHLOROFORM-D
Creation_time     = 26-FEB-2013 08:11:28
Revision_time     = 21-OCT-2014 15:45:21
Current_time      = 21-OCT-2014 15:45:27

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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             = 502.0
Total_scans       = 502.0

X_90_width        = 10.2[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.4[us]
Irr_atn_dec       = 20.8[dB]
Irr_atn_noe       = 20.8[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 18.5[dC]
```



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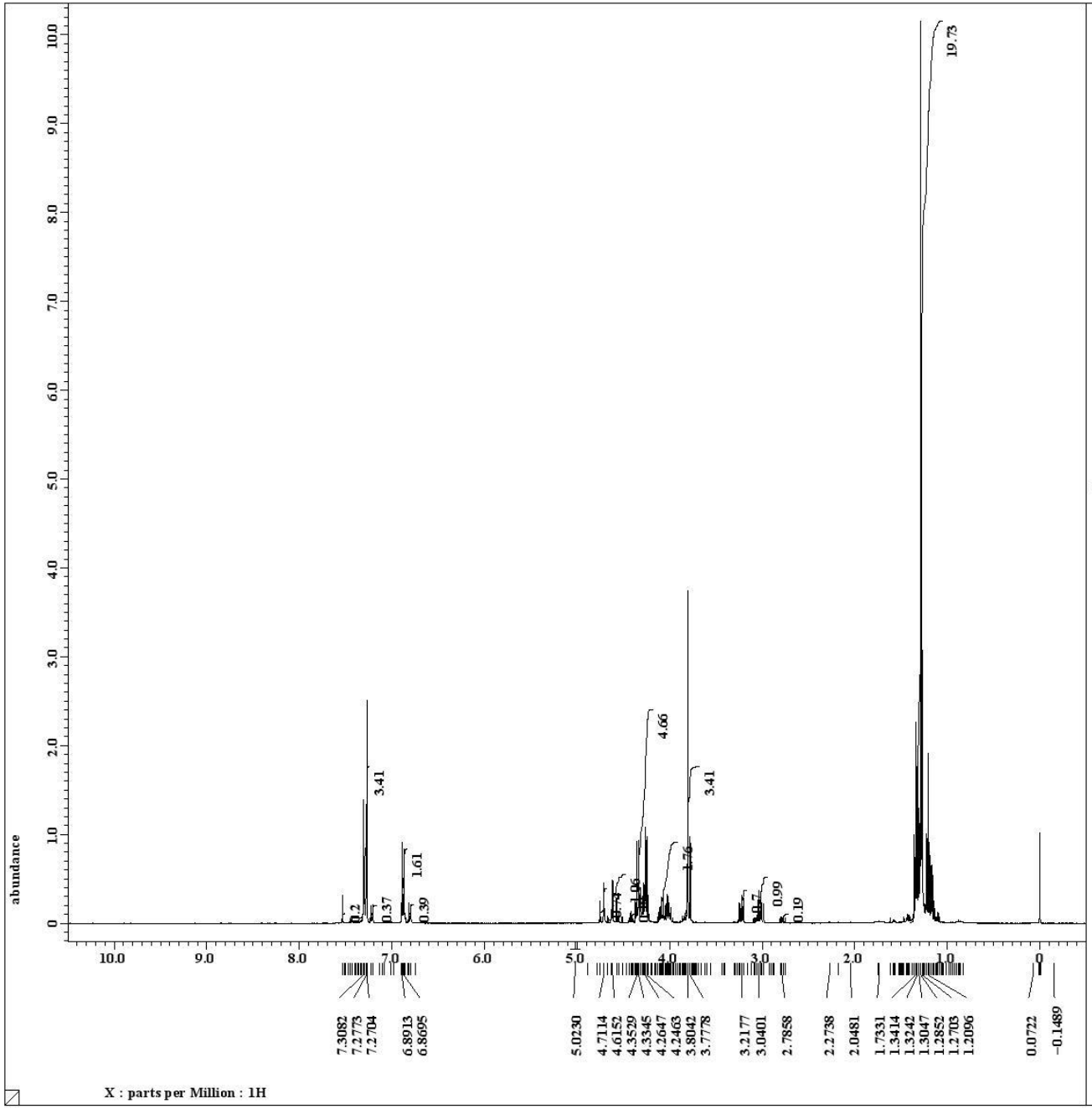
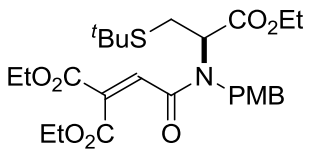


Filename	= RM641-20130222-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#533973
Solvent	= CHLOROFORM-D
Creation_time	= 22-FEB-2013 07:30:21
Revision_time	= 21-OCT-2014 16:05:19
Current_time	= 21-OCT-2014 16:05:35
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
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	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45794685[Hz]
X_sweep	= 7.5030012[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 10.75[us]
X_acq_time	= 2.18365952[s]
X_angle	= 45[deg]
X_atn	= 0.3[dB]
X_pulse	= 5.375[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 32
Relaxation_delay	= 5[s]
Repetition_time	= 7.18365952[s]
Temp_get	= 18.6[dC]



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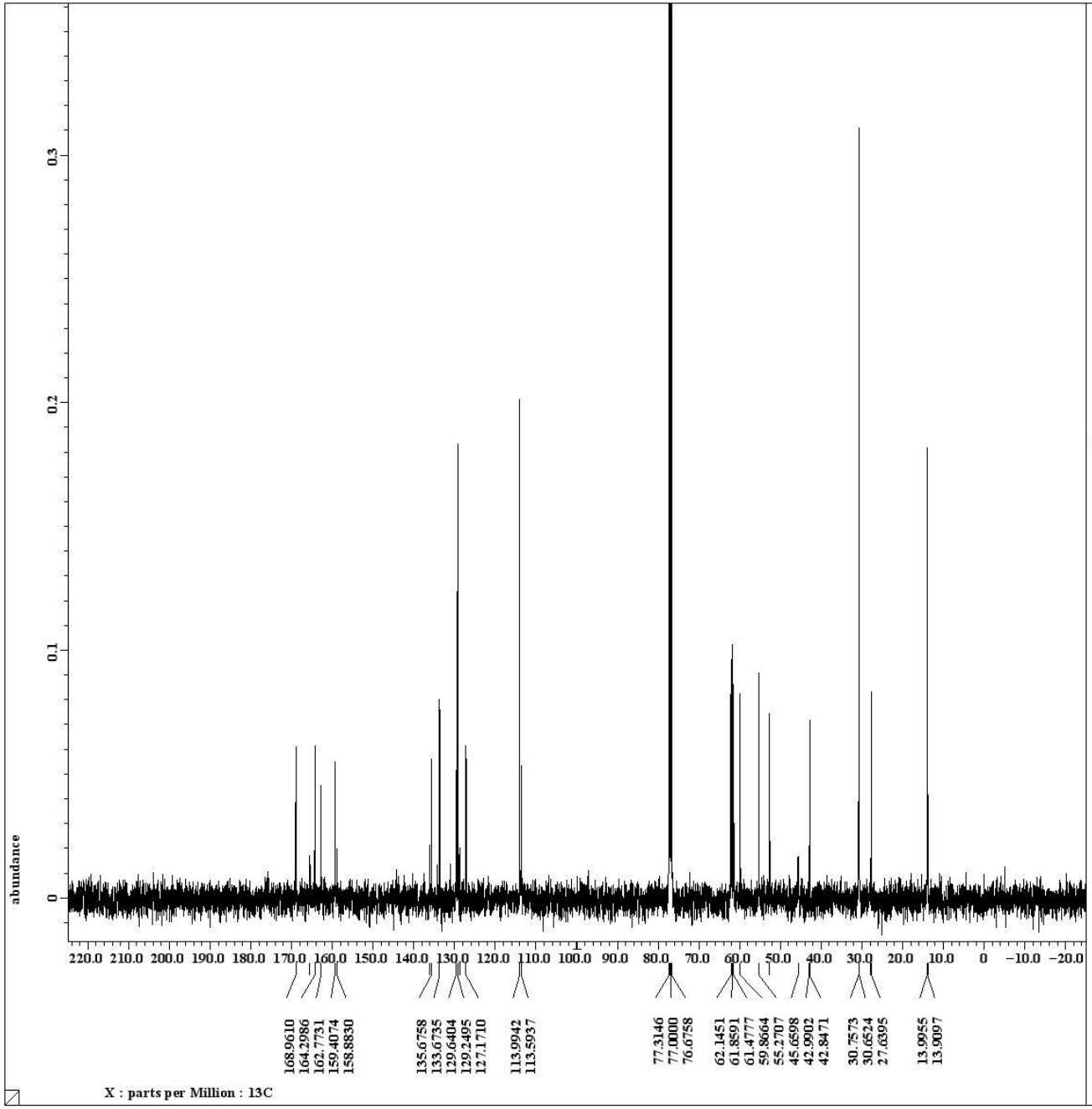


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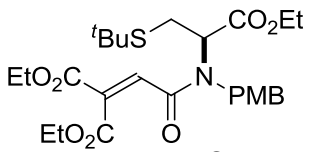
Filename          = RM641-13C-5.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#535772
Solvent           = CHLOROFORM-D
Creation_time     = 22-FEB-2013 07:43:02
Revision_time     = 21-OCT-2014 16:07:31
Current_time      = 21-OCT-2014 16:07:45

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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             = 202
Total_scans       = 202

X_90_width        = 10.2[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.4[us]
Irr_atn_dec       = 20.8[dB]
Irr_atn_noe       = 20.8[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          = 19.1[dC]
```



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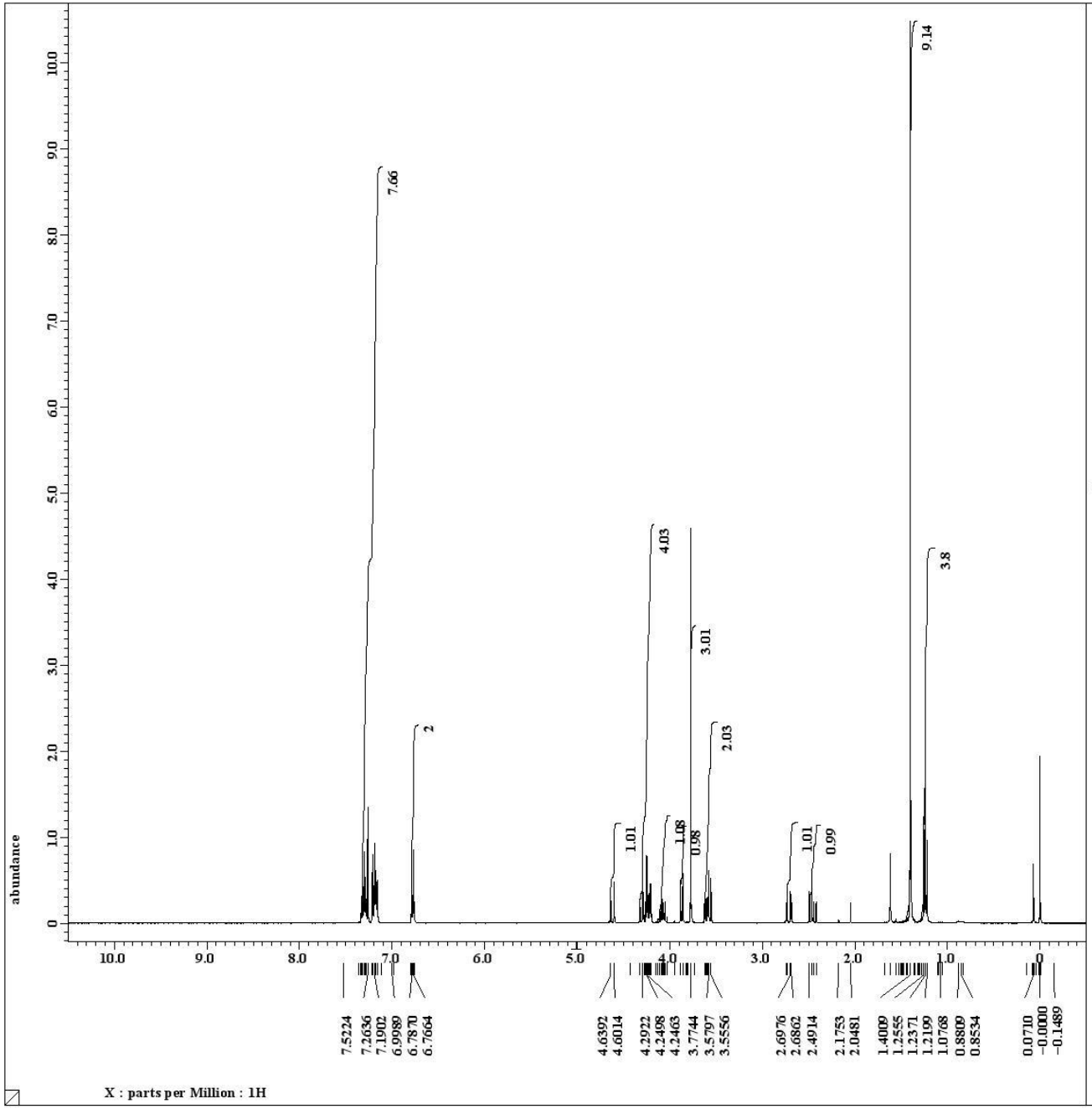


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Filename          = RM139-HPLC1st-1-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#419199
Solvent           = CHLOROFORM-D
Creation_time     =  1-JUN-2011 04:51:05
Revision_time     = 21-OCT-2014 17:19:47
Current_time      = 21-OCT-2014 17:19:54

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.45794685[Hz]
X_sweep           = 7.5030012[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.78219838[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 10[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 0.3[dB]
X_pulse           = 5[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 36
Relaxation_delay  = 5[s]
Repetition_time   = 7.18365952[s]
Temp_get          = 19.1[dC]
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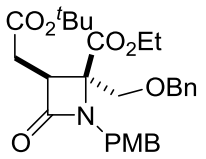
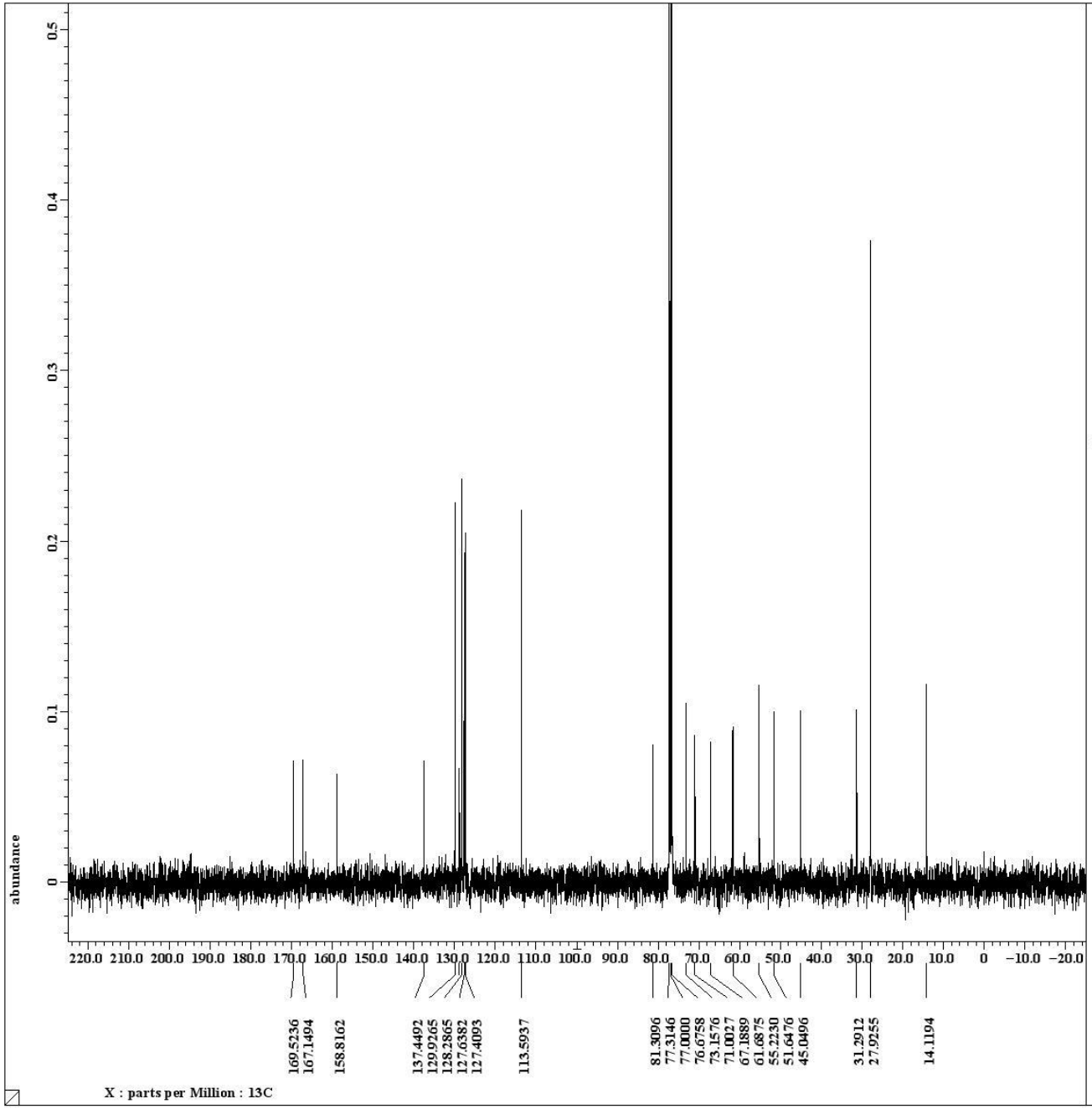


2a

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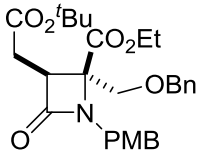
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = a
Solvent           = CHLOROFORM-D
Creation_time     = 27-FEB-2013 03:49:20
Revision_time     = 21-OCT-2014 17:23:56
Current_time      = 21-OCT-2014 17:24:08

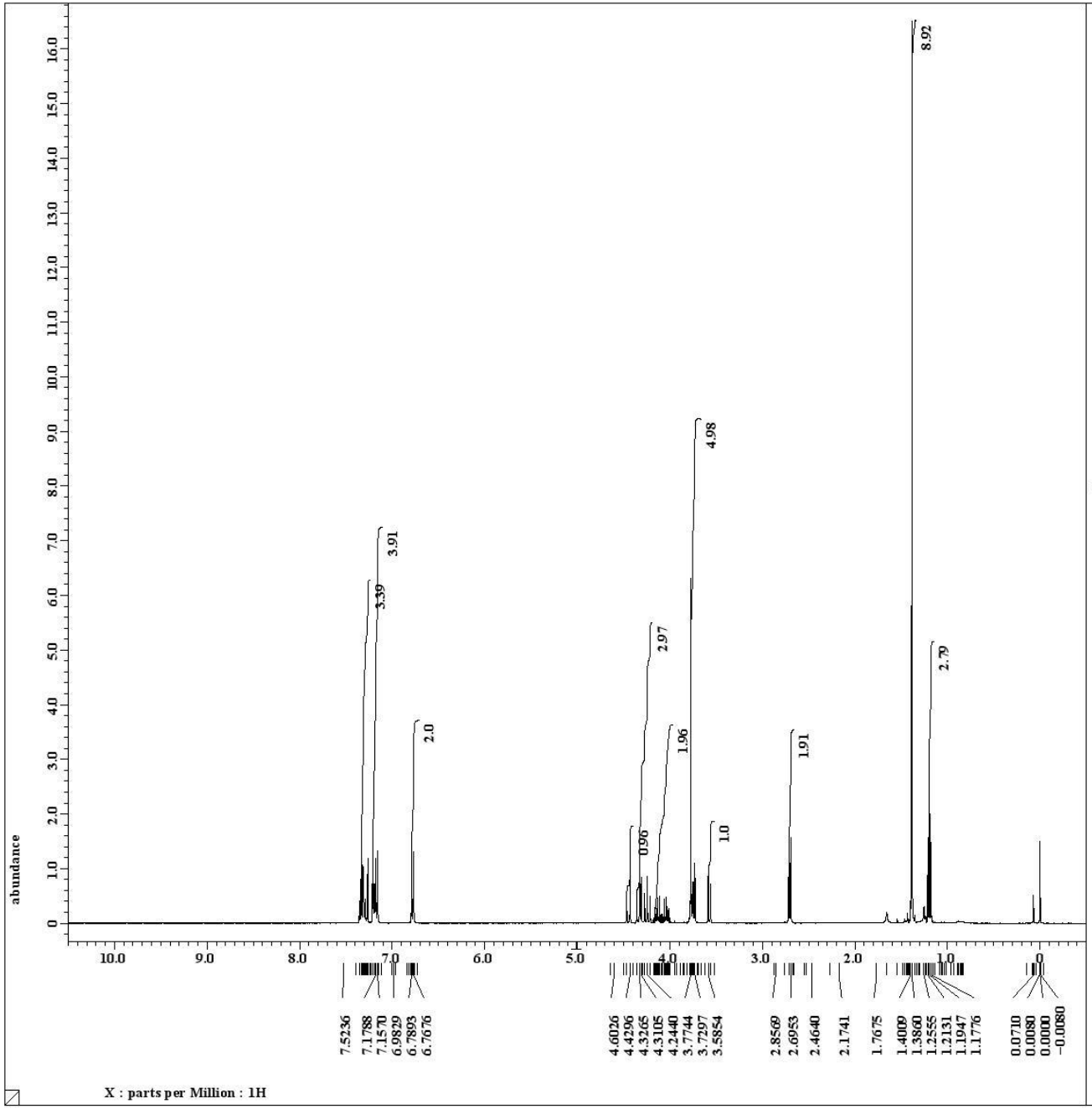
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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             = 145
Total_scans       = 145

X_90_width        = 10.2[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.4[us]
Irr_atn_dec       = 20.8[dB]
Irr_atn_noe       = 20.8[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 18.6[dC]
```



2a

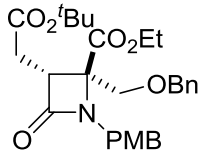



```
Filename          = RH60-HPLC3-20130227-4
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = a
Solvent           = CHLOROFORM-D
Creation_time     = 27-FEB-2013 03:57:18
Revision_time     = 21-OCT-2014 17:27:42
Current_time      = 21-OCT-2014 17:27:47

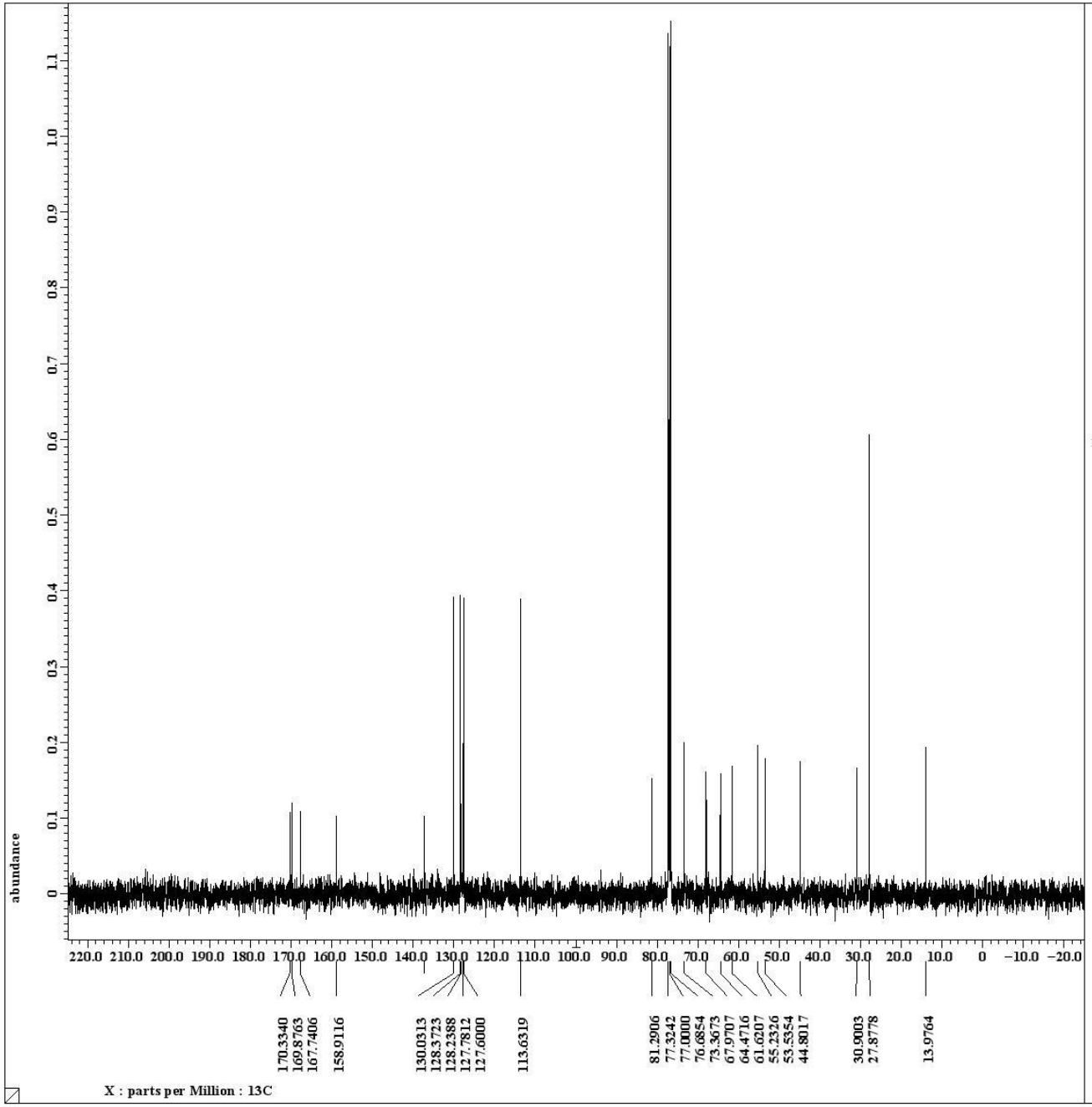
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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

X_90_width        = 10.75[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 0.3[dB]
X_pulse           = 5.375[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 34
Relaxation_delay  = 5[s]
Repetition_time   = 7.18365952[s]
Temp_get          = 18.2[dC]
```



2b

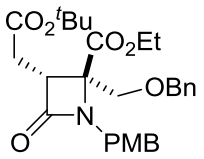



```
Filename          = RM60-HPLC3-13C-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = a
Solvent           = CHLOROFORM-D
Creation_time     = 27-FEB-2013 04:02:53
Revision_time     = 21-OCT-2014 17:28:55
Current_time      = 21-OCT-2014 17:29:03

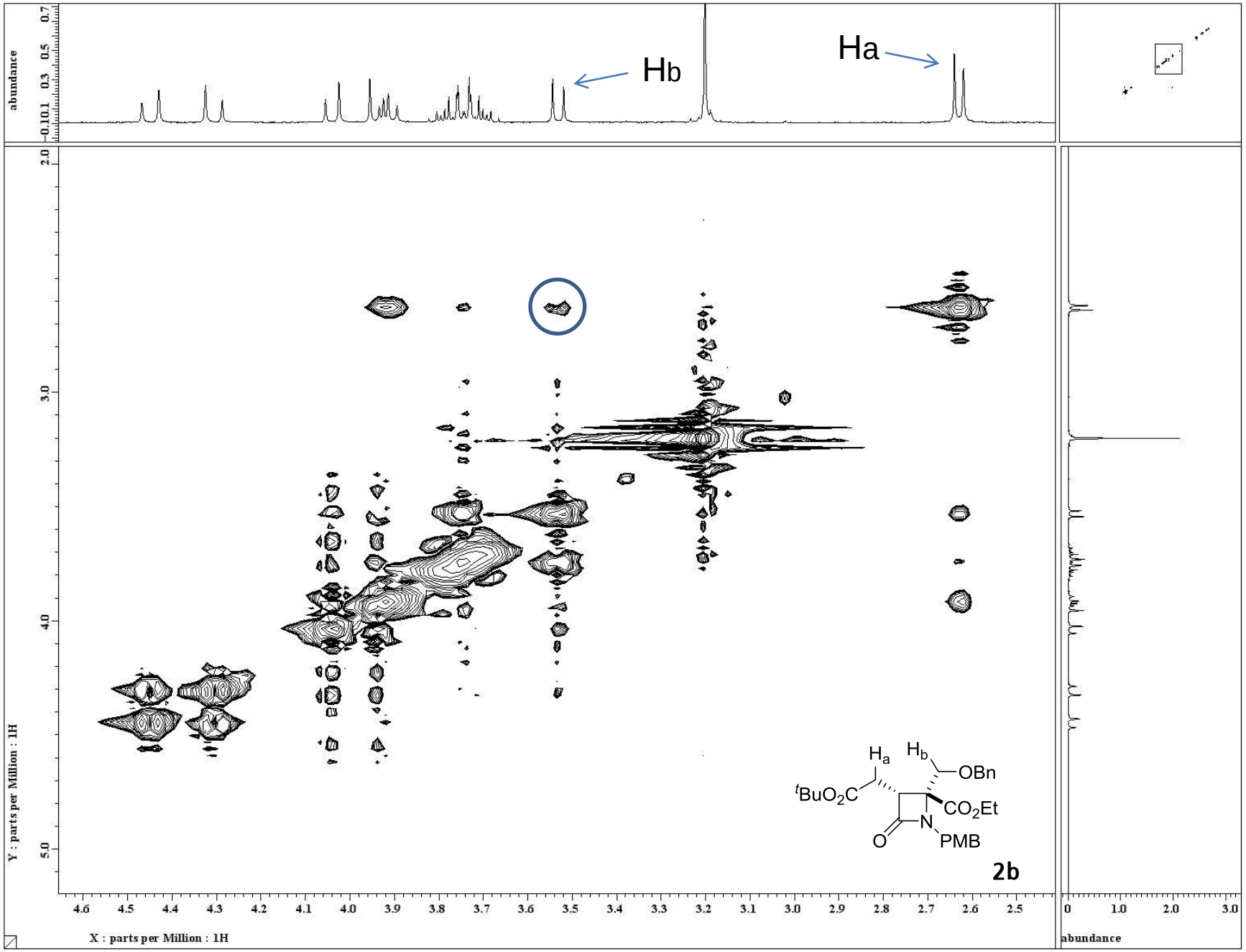
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

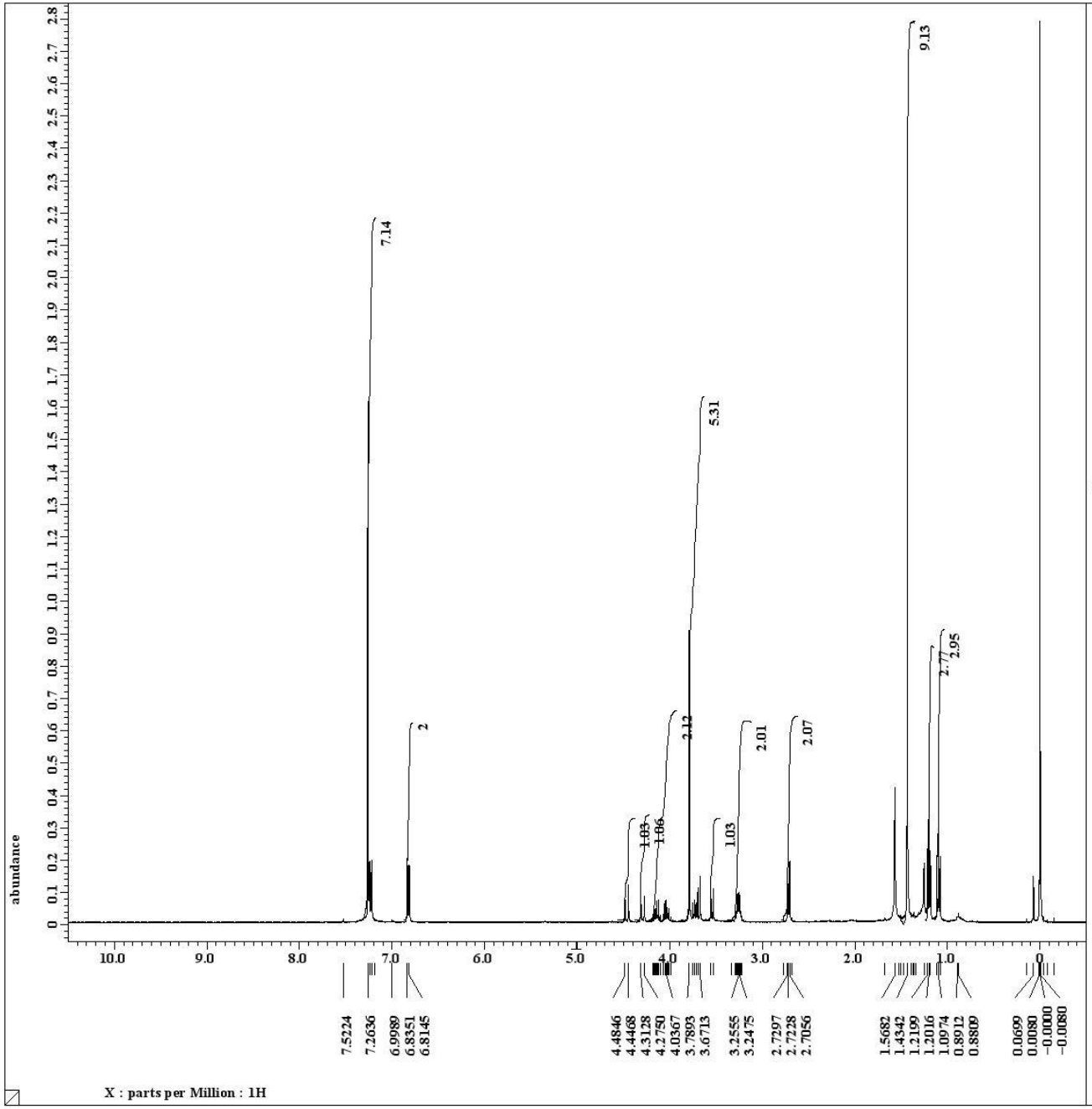
Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 67
Total_scans       = 67

X_90_width        = 10.2[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.4[us]
Irr_atn_dec       = 20.8[dB]
Irr_atn_noe       = 20.8[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 18.3[dC]
```



2b


Hb
Ha
abundance
Y : parts per Million : 1H
X : parts per Million : 1H
abundance
Ha
Hb
OBn
tBuO2C
CO2Et
N
PMB
O
2b

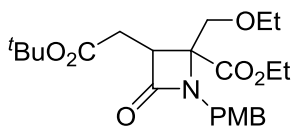



```
Filename          = RM55-HPLC4-6.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#770533
Solvent           = CHLOROFORM-D
Creation_time     = 24-FEB-2011 14:47:46
Revision_time     = 23-OCT-2014 08:45:51
Current_time      = 23-OCT-2014 08:46:03

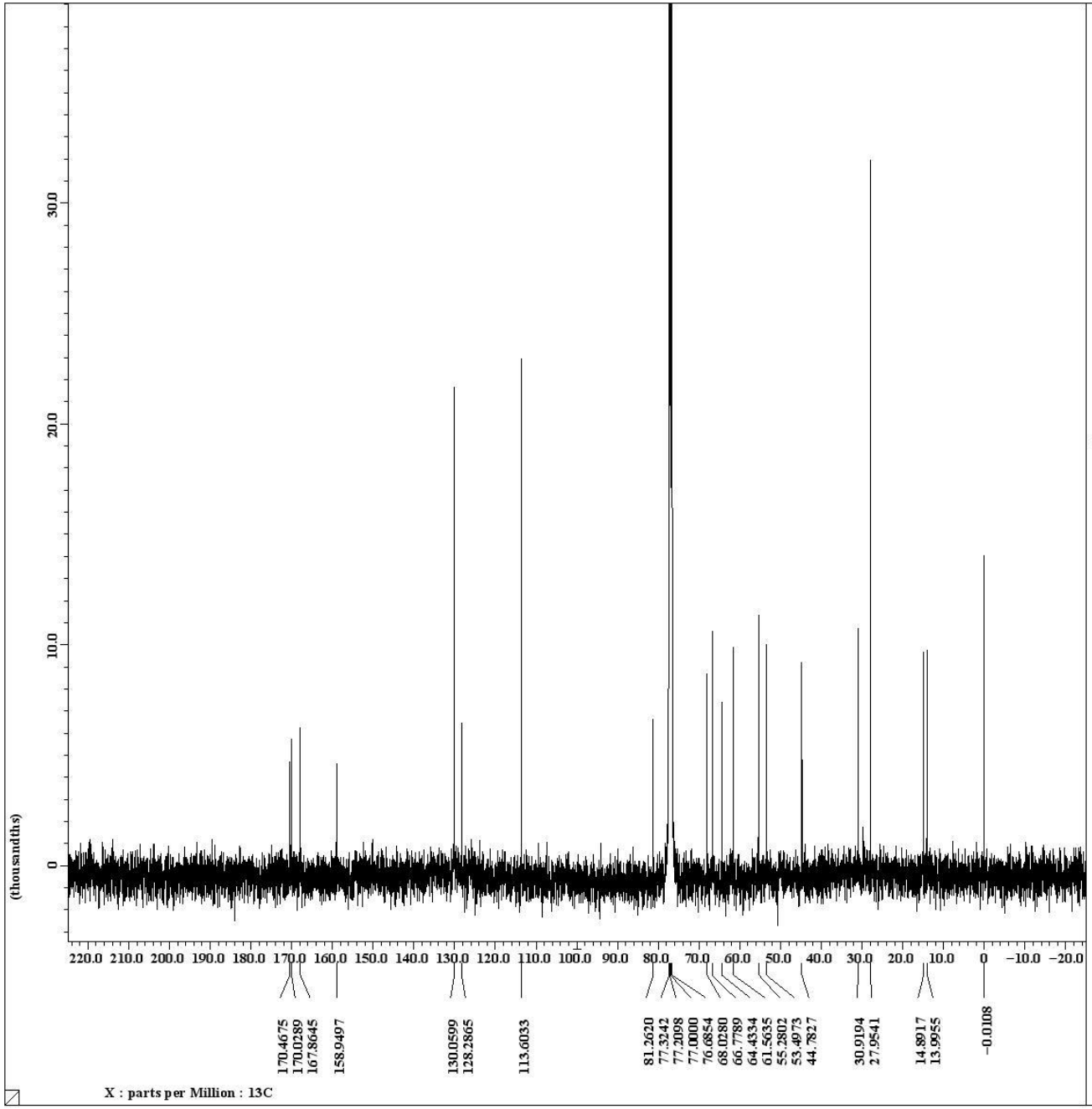
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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

X_90_width        = 10[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 0.3[dB]
X_pulse           = 5[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 7.18365952[s]
Temp_get          = 18.3[dC]
```



3

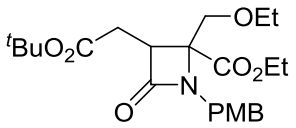



```
Filename          = RM55-HPLC4-13C-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     = 23-OCT-2014 00:45:57
Revision_time     = 23-OCT-2014 08:49:08
Current_time      = 23-OCT-2014 08:49:14

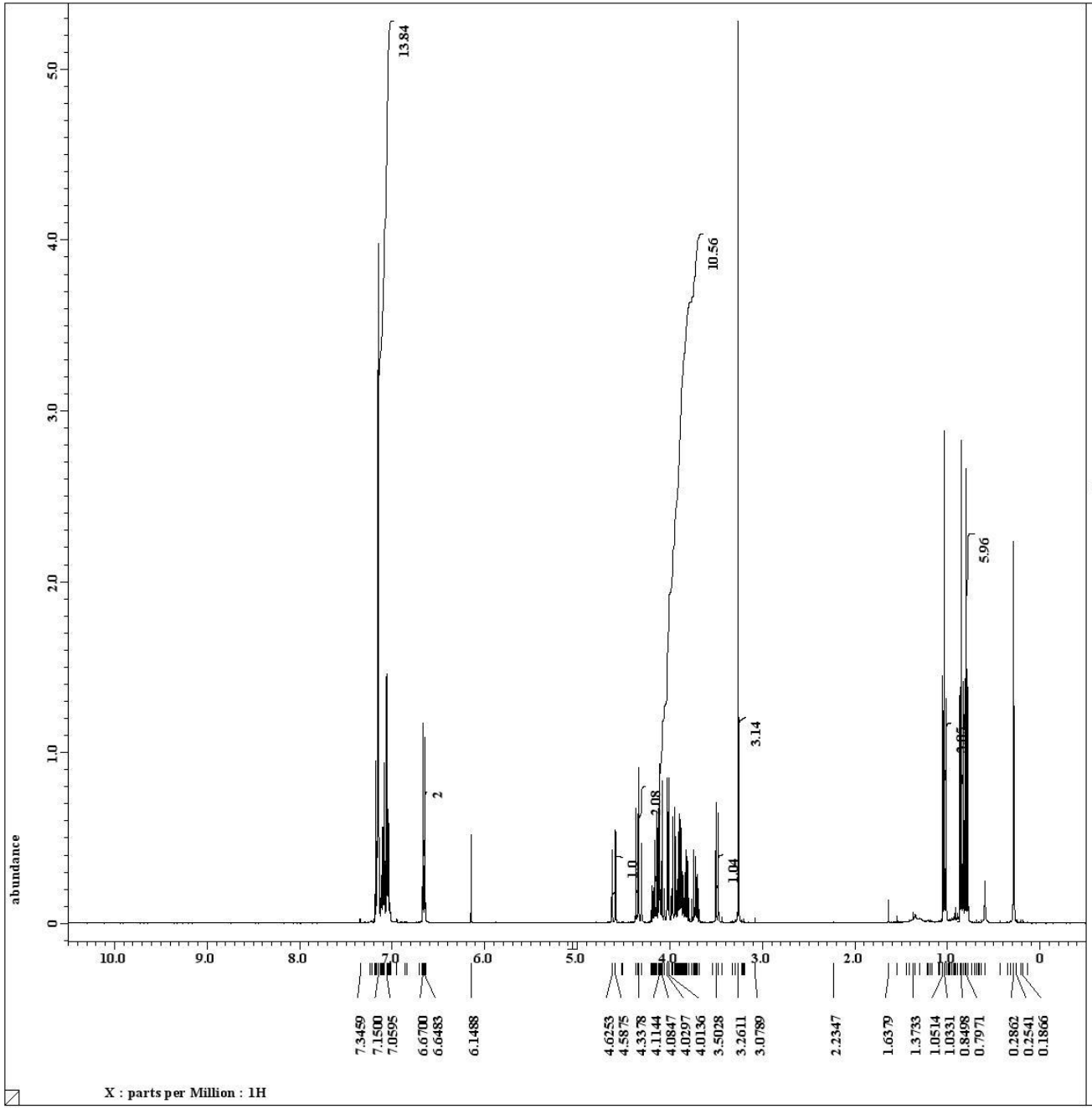
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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             = 10400
Total_scans       = 10400

X_90_width        = 10.54[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.51333333[us]
Irr_atn_dec       = 20.58[dB]
Irr_atn_noe       = 20.58[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          = 19[dC]
```



3

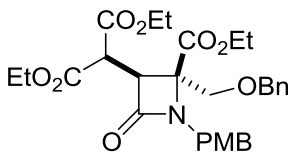



```
Filename          = RM442-mae-benzene-201
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#397326
Solvent           = BENZENE-D6
Creation_time     = 21-JUN-2012 11:04:04
Revision_time     = 21-OCT-2014 16:45:16
Current_time      = 21-OCT-2014 16:45:24

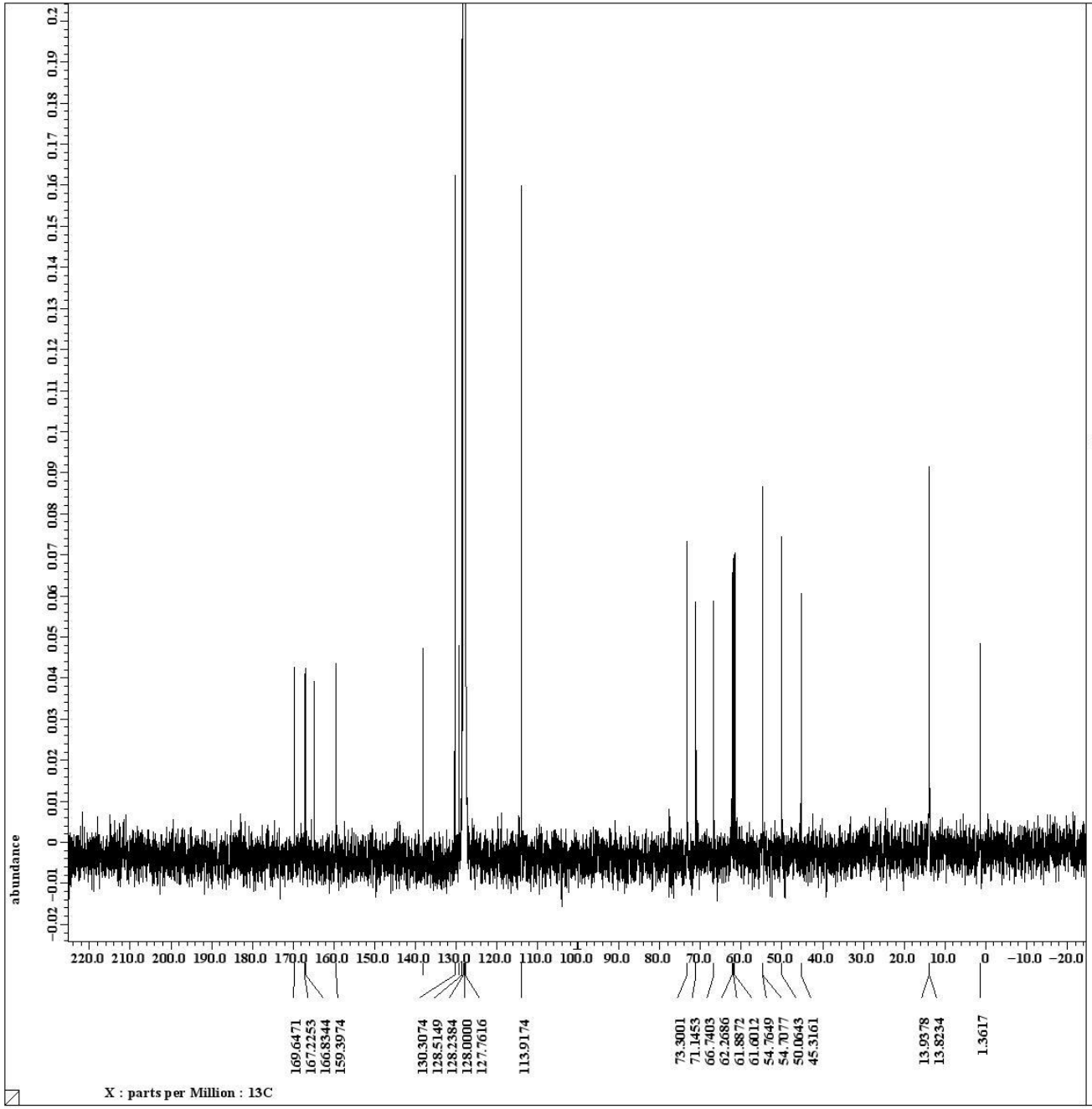
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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

X_90_width        = 10.75[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 0.3[dB]
X_pulse           = 5.375[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 7.18365952[s]
Temp_get          = 18.9[dC]
```



5a

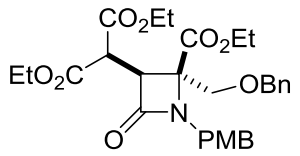



```
Filename          = RM442-mae-benzene-13C
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#400284
Solvent           = BENZENE-D6
Creation_time     = 21-JUN-2012 11:21:52
Revision_time     = 21-OCT-2014 16:48:11
Current_time      = 21-OCT-2014 16:48:22

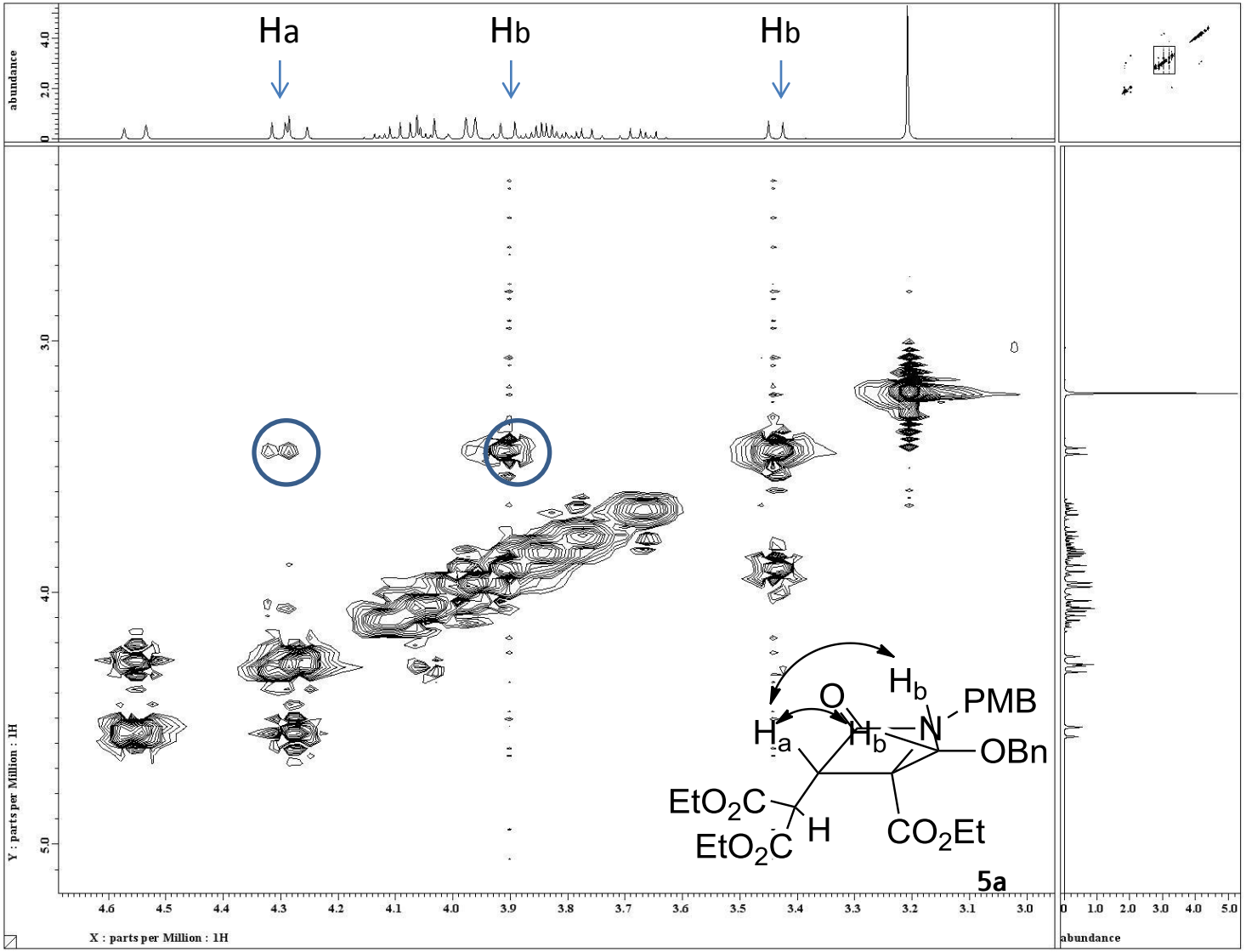
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

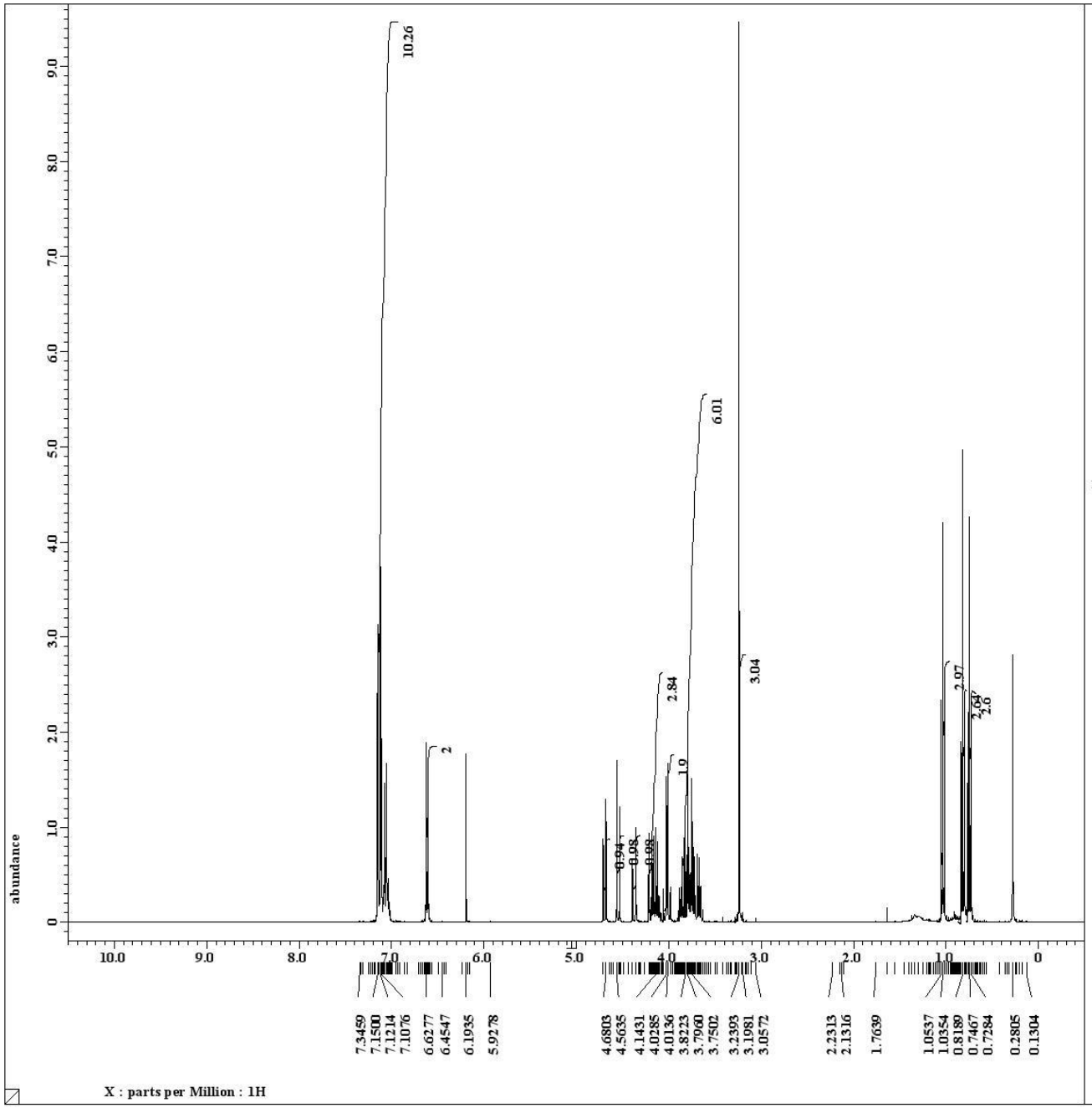
Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 256
Total_scans       = 256

X_90_width        = 10.2[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.4[us]
Irr_atn_dec       = 20.8[dB]
Irr_atn_noe       = 20.8[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          = 19.2[dC]
```



5a


Ha
Hb
Hb
abundance
Y : parts per Million : 1H
X : parts per Million : 1H
abundance
Hb
O
PMB
Ha
Hb
N
OBn
EtO2C
H
CO2Et
EtO2C
5a

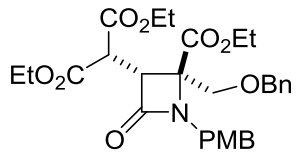



```
Filename          = RM442-ushiro-benzened
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#612486
Solvent           = BENZENE-D6
Creation_time     = 18-JUN-2012 17:02:33
Revision_time     = 21-OCT-2014 16:51:00
Current_time      = 21-OCT-2014 16:51:04

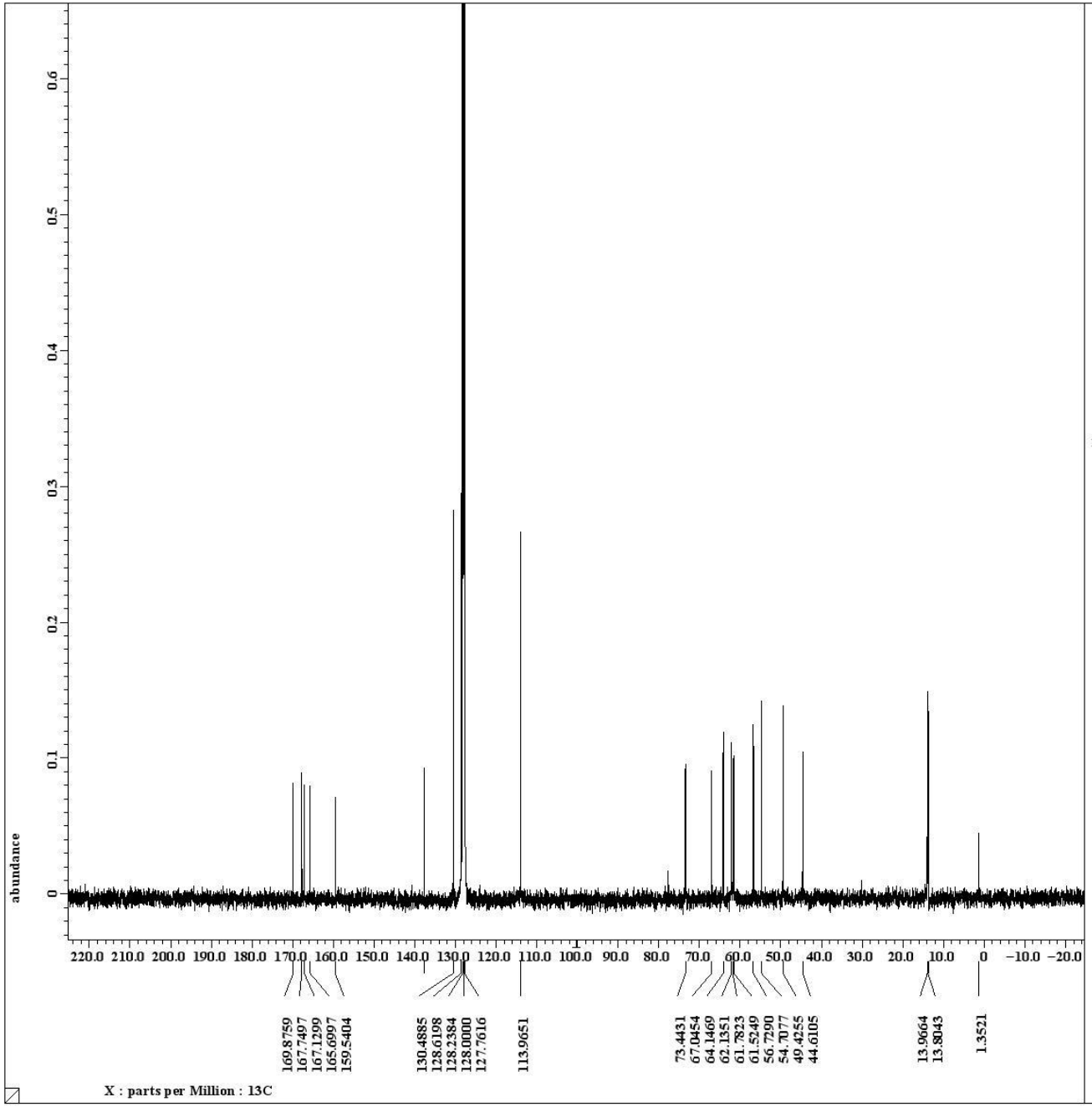
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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

X_90_width        = 10.75[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 0.3[dB]
X_pulse           = 5.375[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.18365952[s]
Temp_get          = 19.7[dC]
```



5b

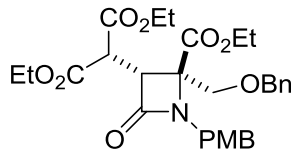



```
Filename          = RM442-ushiro-benzene-
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#617060
Solvent           = BENZENE-D6
Creation_time     = 18-JUN-2012 17:22:03
Revision_time     = 21-OCT-2014 16:52:44
Current_time      = 21-OCT-2014 16:53:08

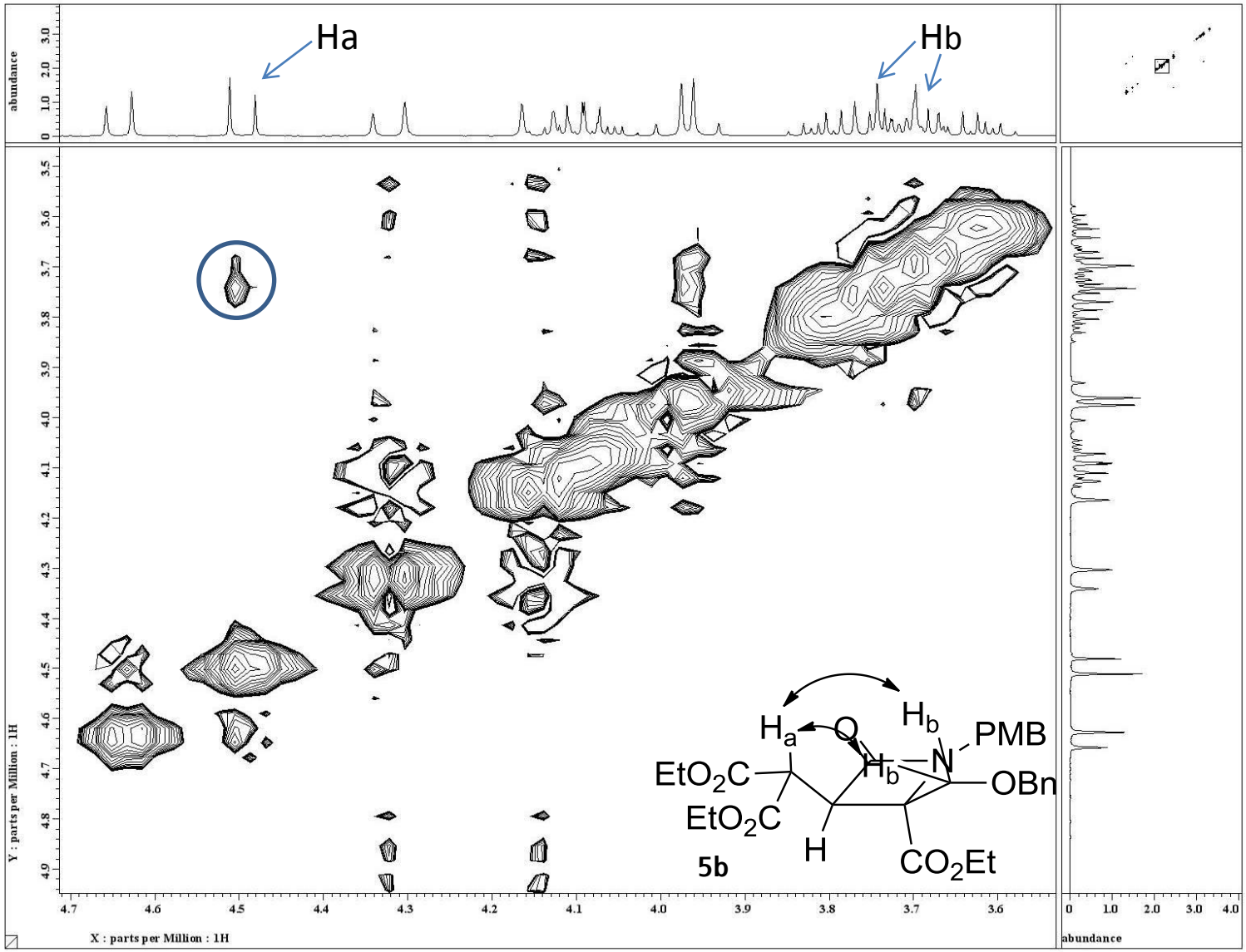
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

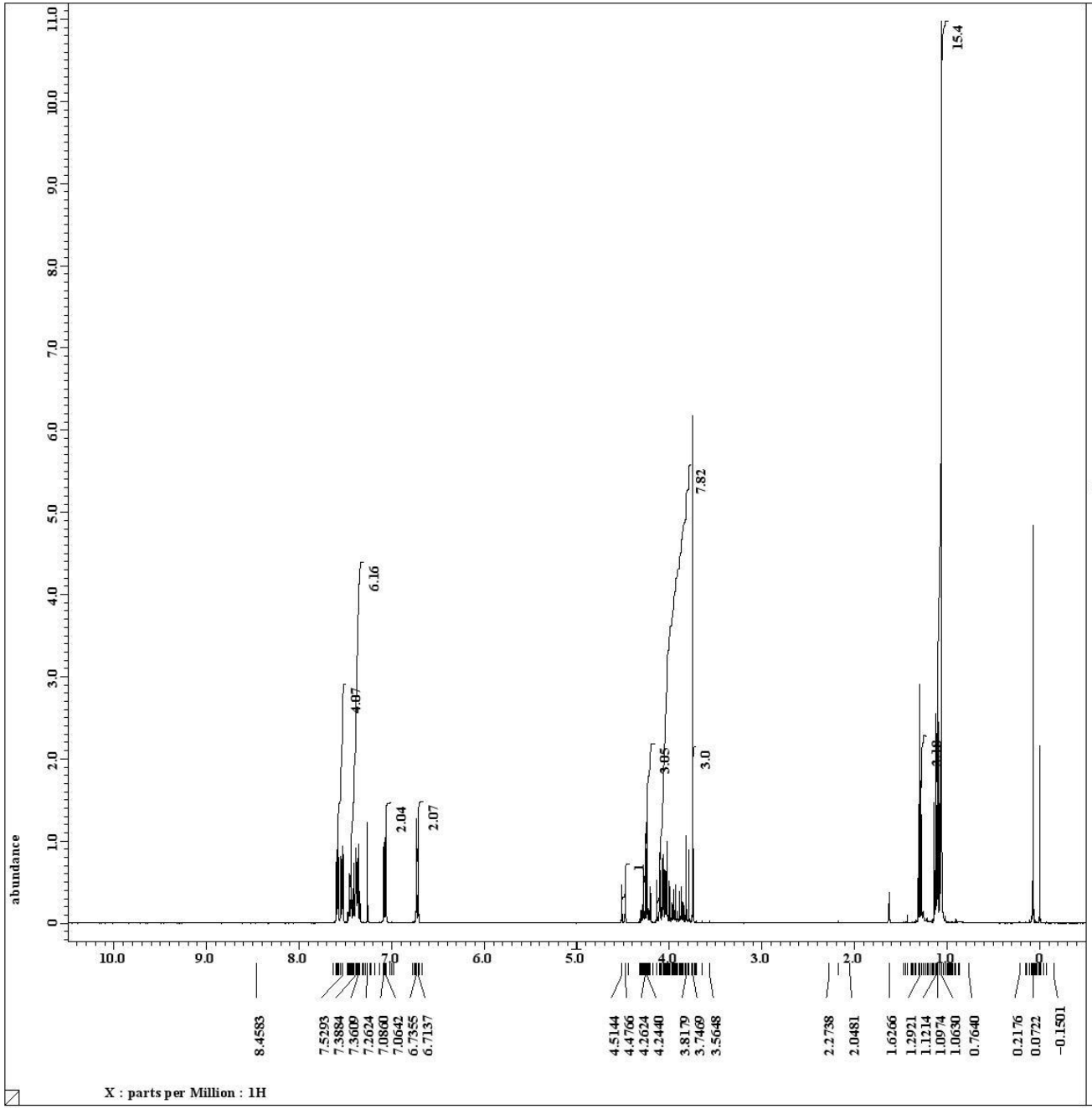
Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 256
Total_scans       = 256

X_90_width        = 10.2[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.4[us]
Irr_atn_dec       = 20.8[dB]
Irr_atn_noe       = 20.8[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          = 19.9[dC]
```



5b


Ha
Hb
abundance
Y : parts per Million : 1H
X : parts per Million : 1H
abundance
Ha
O
Hb
PMB
N
Hb
EtO2C
OBn
EtO2C
H
CO2Et
5b

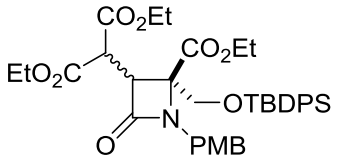



```
Filename          = RM363-mae-20121221-4.
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#589968
Solvent           = CHLOROFORM-D
Creation_time     = 21-DEC-2012 09:09:31
Revision_time     = 21-OCT-2014 17:32:22
Current_time      = 21-OCT-2014 17:32:28

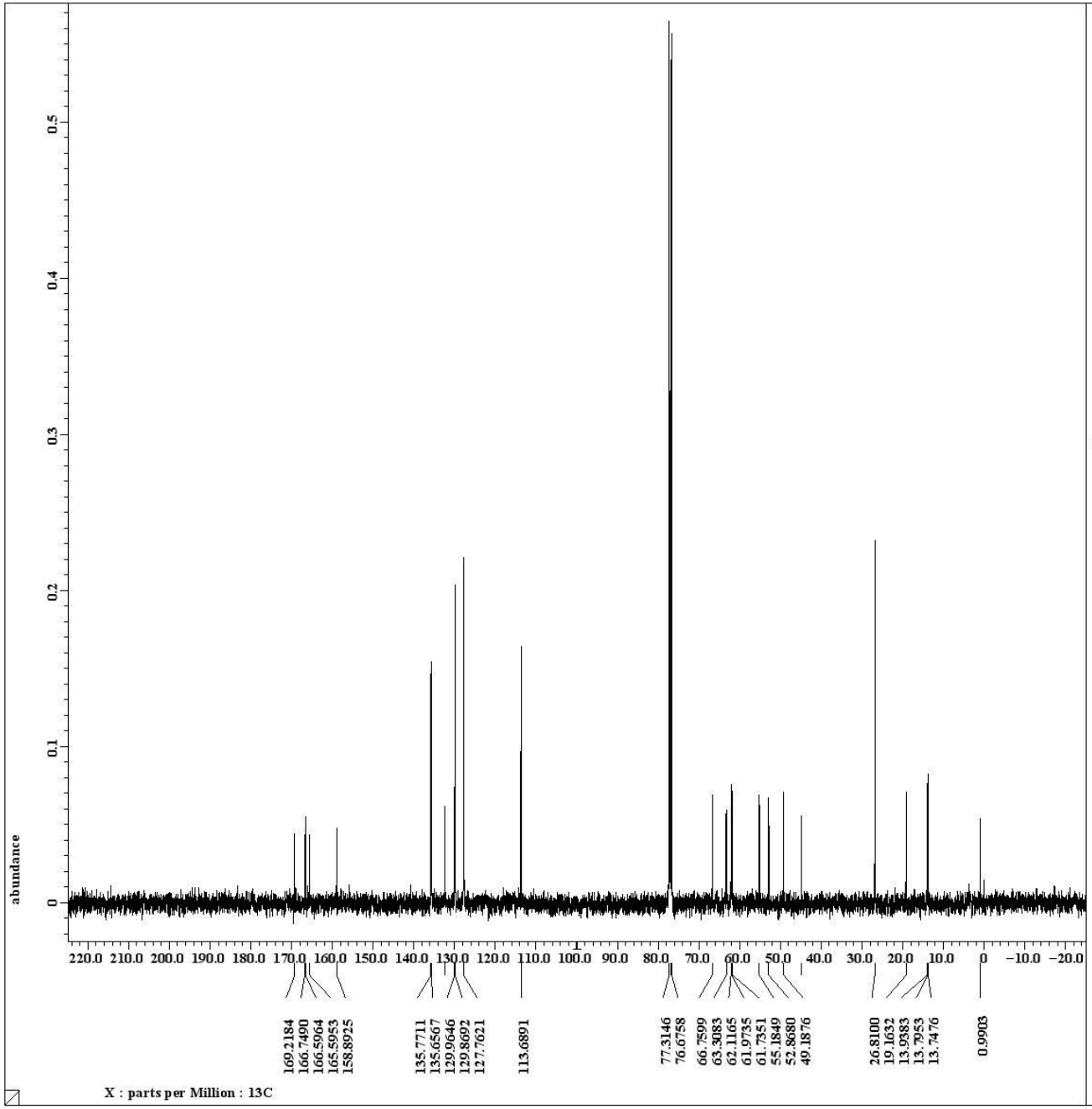
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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

X_90_width        = 10.75[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 0.3[dB]
X_pulse           = 5.375[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 34
Relaxation_delay  = 5[s]
Repetition_time   = 7.18365952[s]
Temp_get          = 17.3[dC]
```



One diastereomer of **7**

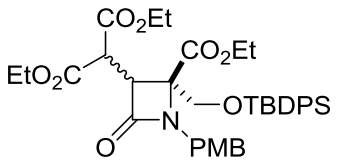



```
Filename          = RM363-mae-13C-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#591444
Solvent           = CHLOROFORM-D
Creation_time     = 21-DEC-2012 09:19:38
Revision_time     = 21-OCT-2014 17:34:41
Current_time      = 21-OCT-2014 17:34:50

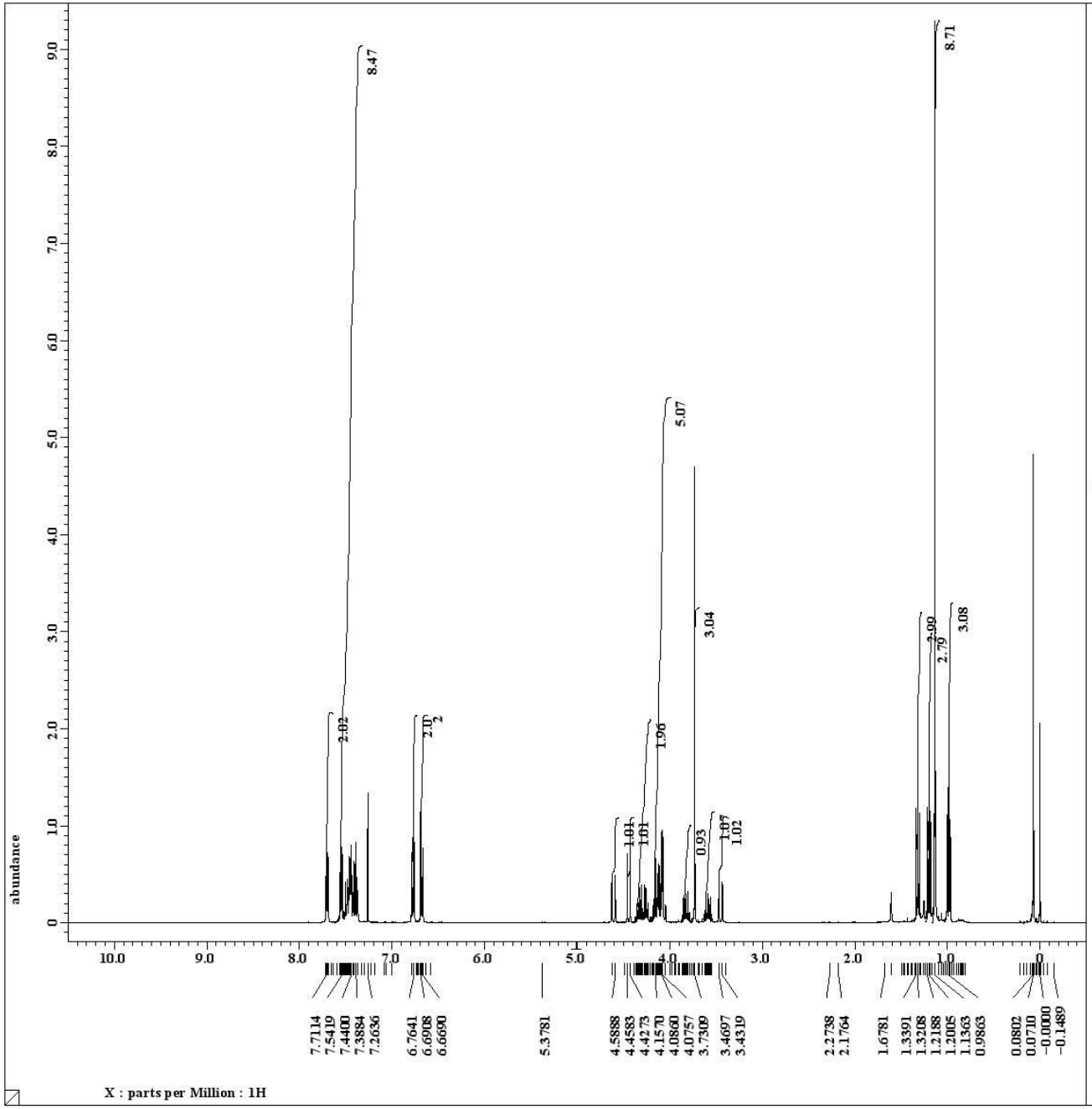
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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             = 148
Total_scans       = 148

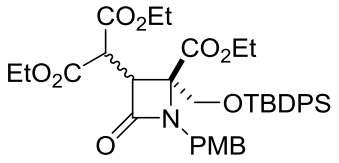
X_90_width        = 10[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.33333333[us]
Irr_atn_dec       = 20.8[dB]
Irr_atn_noe       = 20.8[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 54
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 17.9[dC]
```



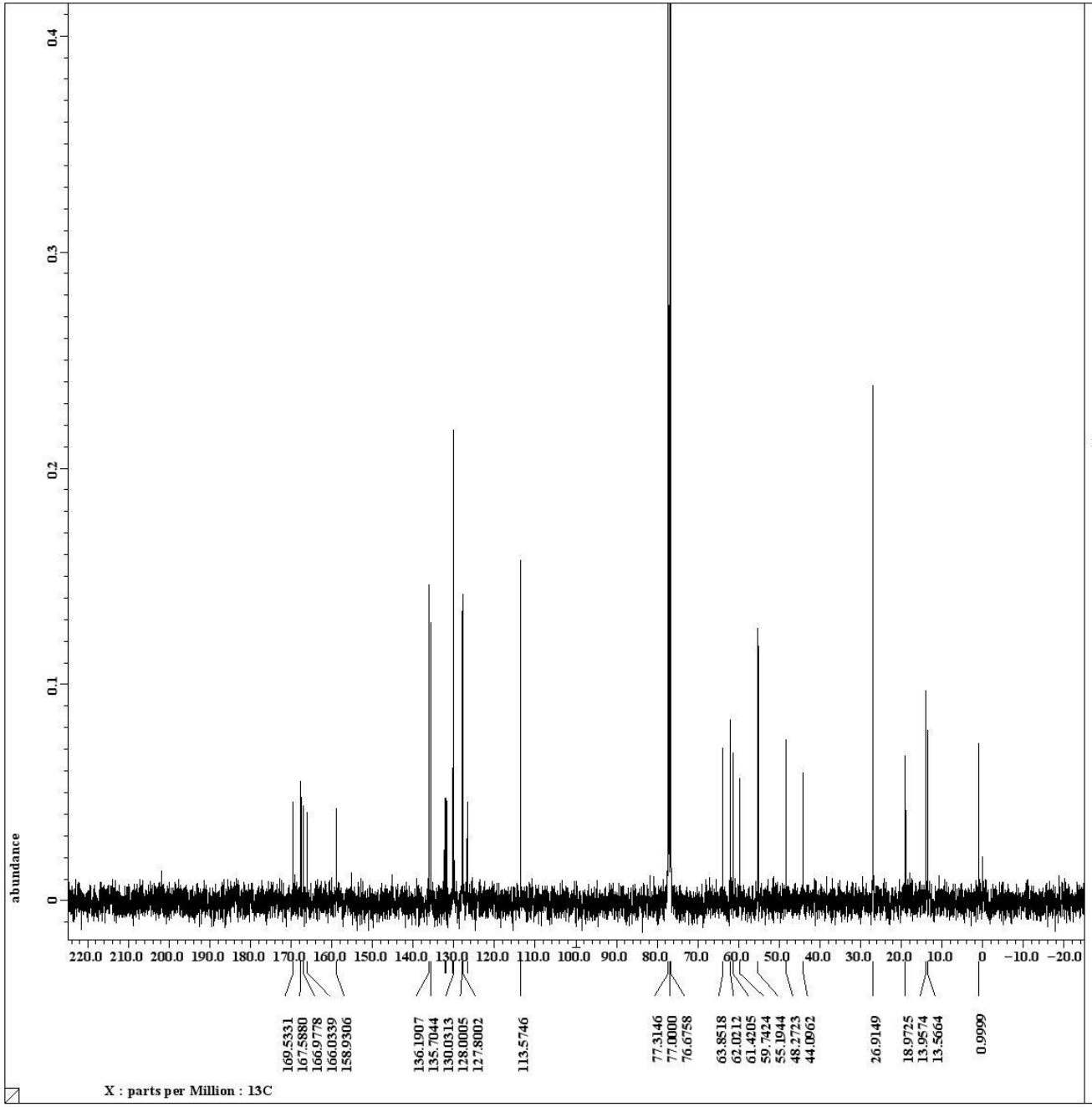
One diastereomer of **7**



Filename	= RM363-ushiro-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= a
Solvent	= CHLOROFORM-D
Creation_time	= 3-FEB-2013 11:13:53
Revision_time	= 21-OCT-2014 17:39:32
Current_time	= 21-OCT-2014 17:39:36
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
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	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45794685[Hz]
X_sweep	= 7.5030012[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 10.75[us]
X_acq_time	= 2.18365952[s]
X_angle	= 45[deg]
X_atn	= 0.3[dB]
X_pulse	= 5.375[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 5[s]
Repetition_time	= 7.18365952[s]
Temp_get	= 17.8[dC]



The other diastereomer of **7**

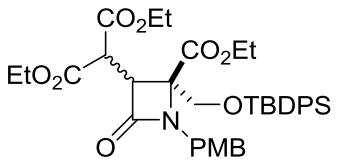



```
Filename          = RM363-13C-ushiro-4.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = a
Solvent           = CHLOROFORM-D
Creation_time     =  3-FEB-2013 11:27:35
Revision_time     = 21-OCT-2014 17:40:36
Current_time      = 21-OCT-2014 17:40:49

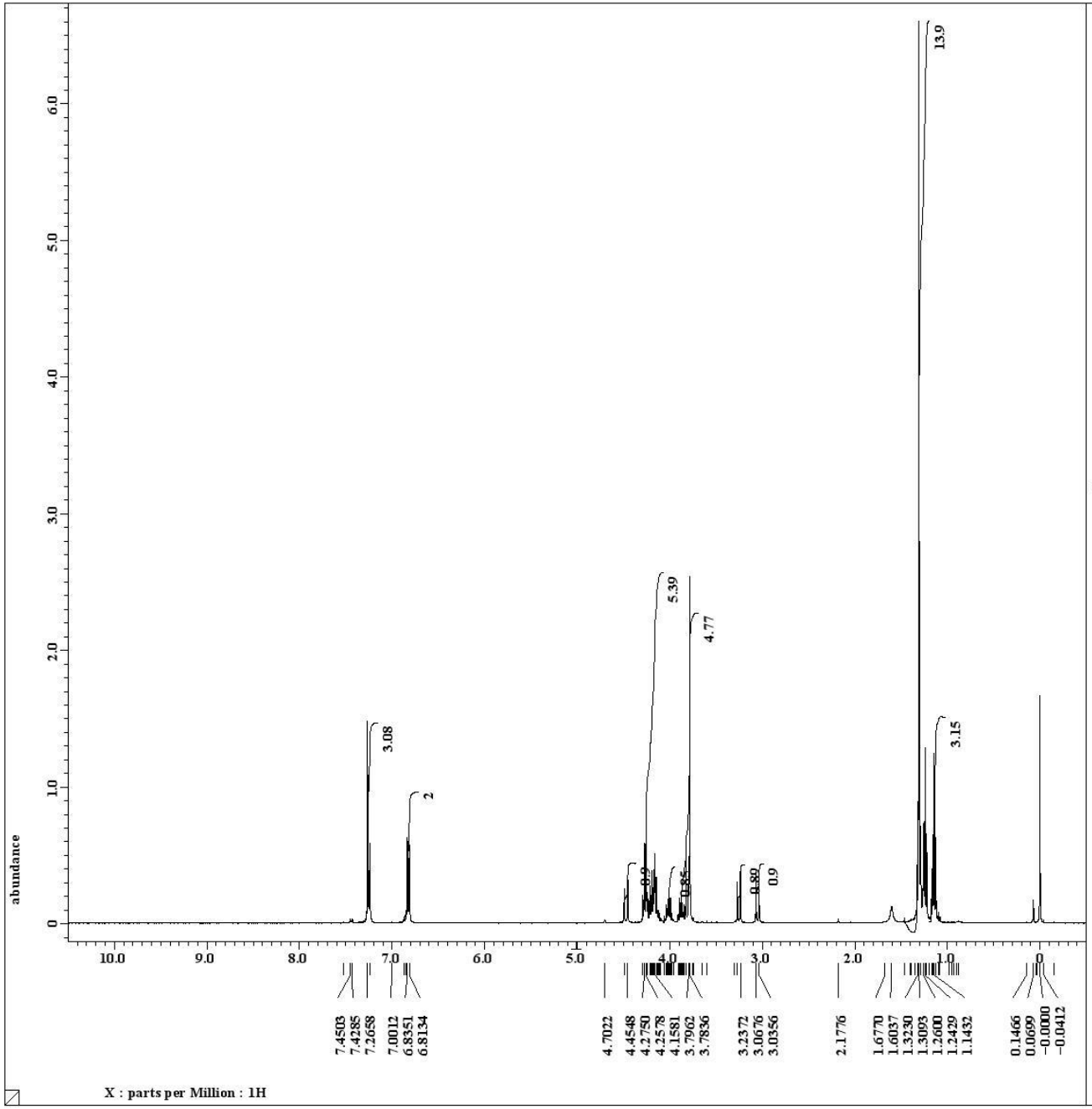
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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             = 211
Total_scans       = 211

X_90_width        = 10.2[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.4[us]
Irr_atn_dec       = 20.8[dB]
Irr_atn_noe       = 20.8[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 18.6[dC]
```



The other diastereomer of **7**

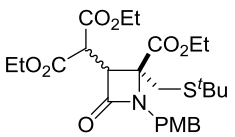



```
Filename          = RM645-PTLC1-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#650839
Solvent           = CHLOROFORM-D
Creation_time     = 23-DEC-2012 10:50:53
Revision_time     = 21-OCT-2014 18:26:38
Current_time      = 21-OCT-2014 18:26:43

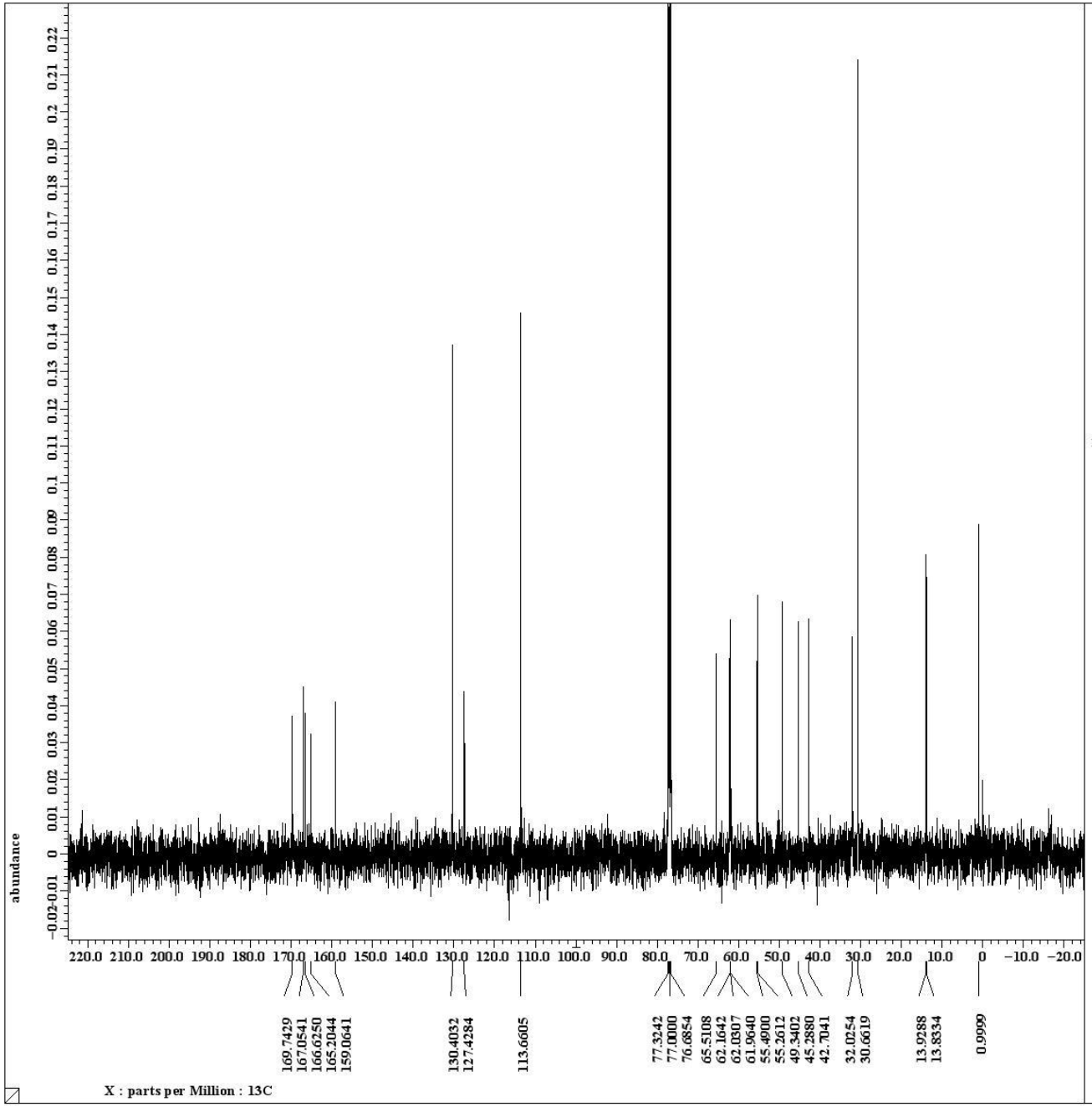
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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

X_90_width        = 10.75[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 0.3[dB]
X_pulse           = 5.375[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.18365952[s]
Temp_get          = 17.8[dC]
```



One diastereomer of **9**

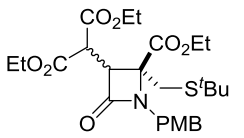



```
Filename          = RM645-PTLC1-13C-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#656746
Solvent           = CHLOROFORM-D
Creation_time     = 26-DEC-2012 11:11:10
Revision_time     = 21-OCT-2014 18:27:26
Current_time      = 21-OCT-2014 18:27:32

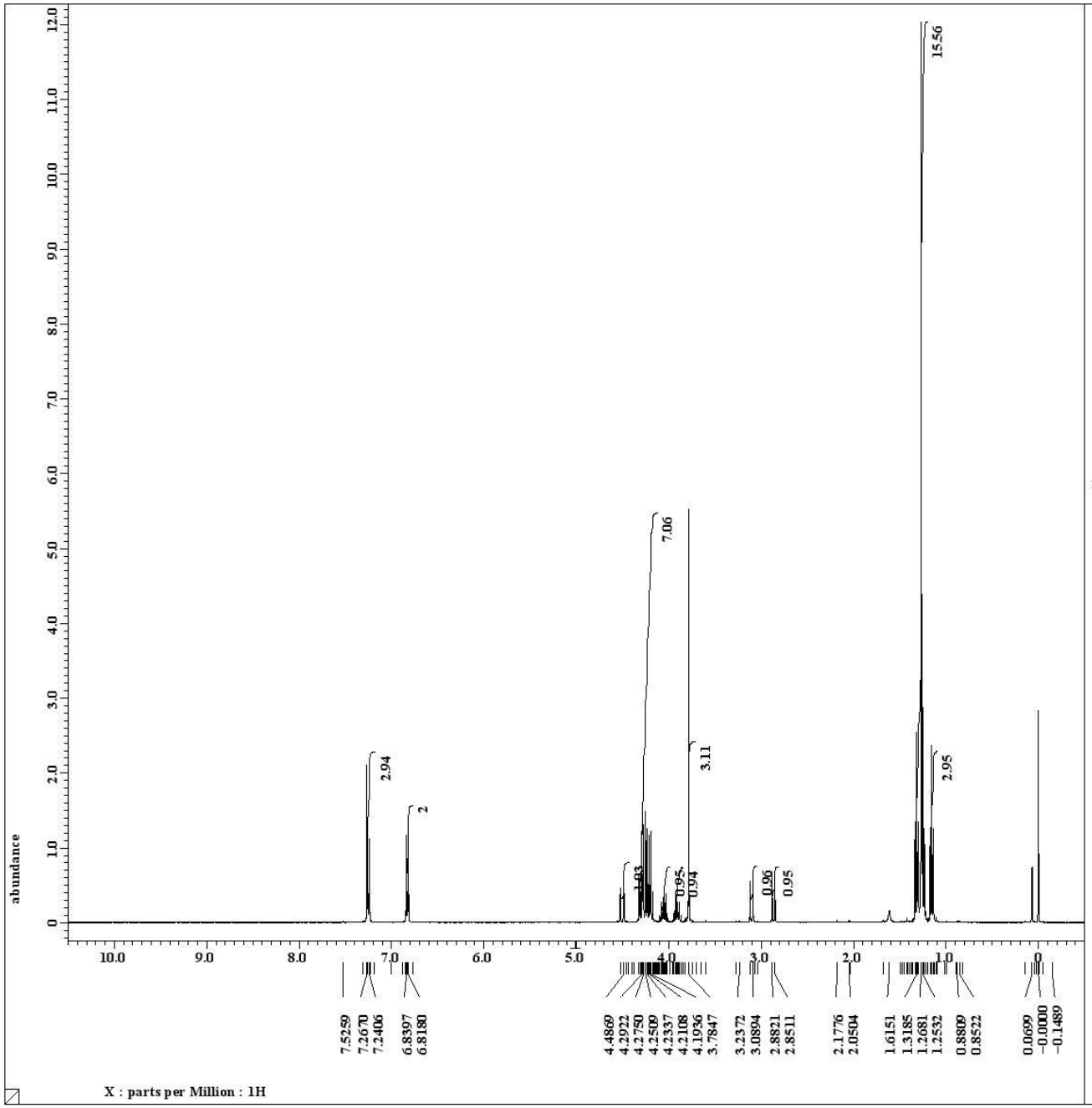
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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             = 208
Total_scans       = 208

X_90_width        = 10[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.33333333[us]
Irr_atn_dec       = 20.8[dB]
Irr_atn_noe       = 20.8[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          = 18.9[dC]
```



One diastereomer of **9**

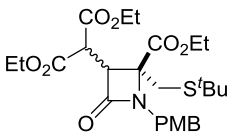



```
Filename          = RM645-PTLC2-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#653663
Solvent           = CHLOROFORM-D
Creation_time     = 23-DEC-2012 10:55:48
Revision_time     = 21-OCT-2014 18:32:08
Current_time      = 21-OCT-2014 18:32:12

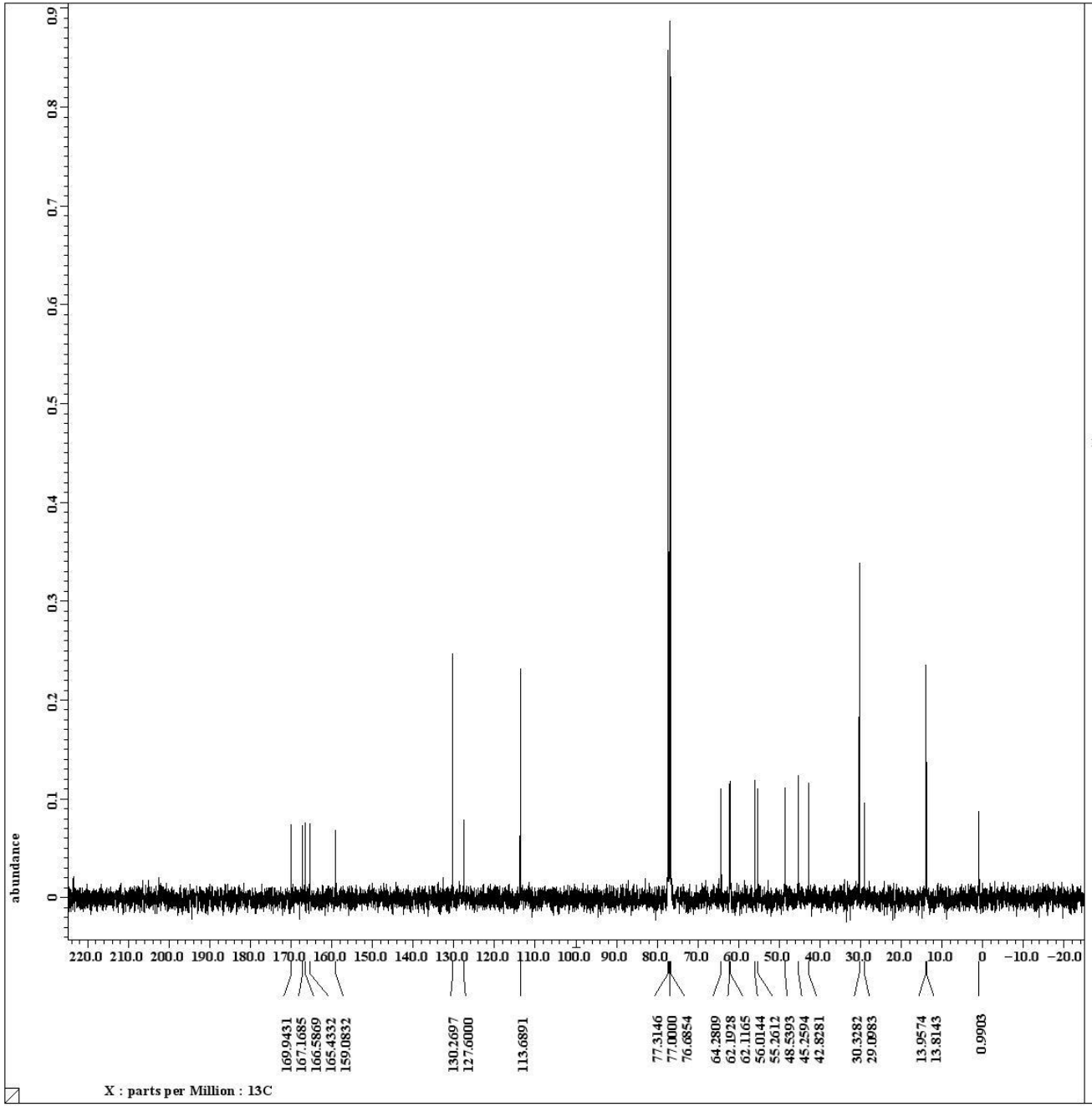
Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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

X_90_width        = 10.75[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 0.3[dB]
X_pulse           = 5.375[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.18365952[s]
Temp_get          = 17.4[dC]
```



The other diastereomer of **9**

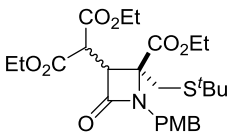



```
Filename          = RM645-PTLC2-13C-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = a
Solvent           = CHLOROFORM-D
Creation_time     = 26-DEC-2012 14:35:02
Revision_time     = 21-OCT-2014 18:29:32
Current_time      = 21-OCT-2014 18:29:38

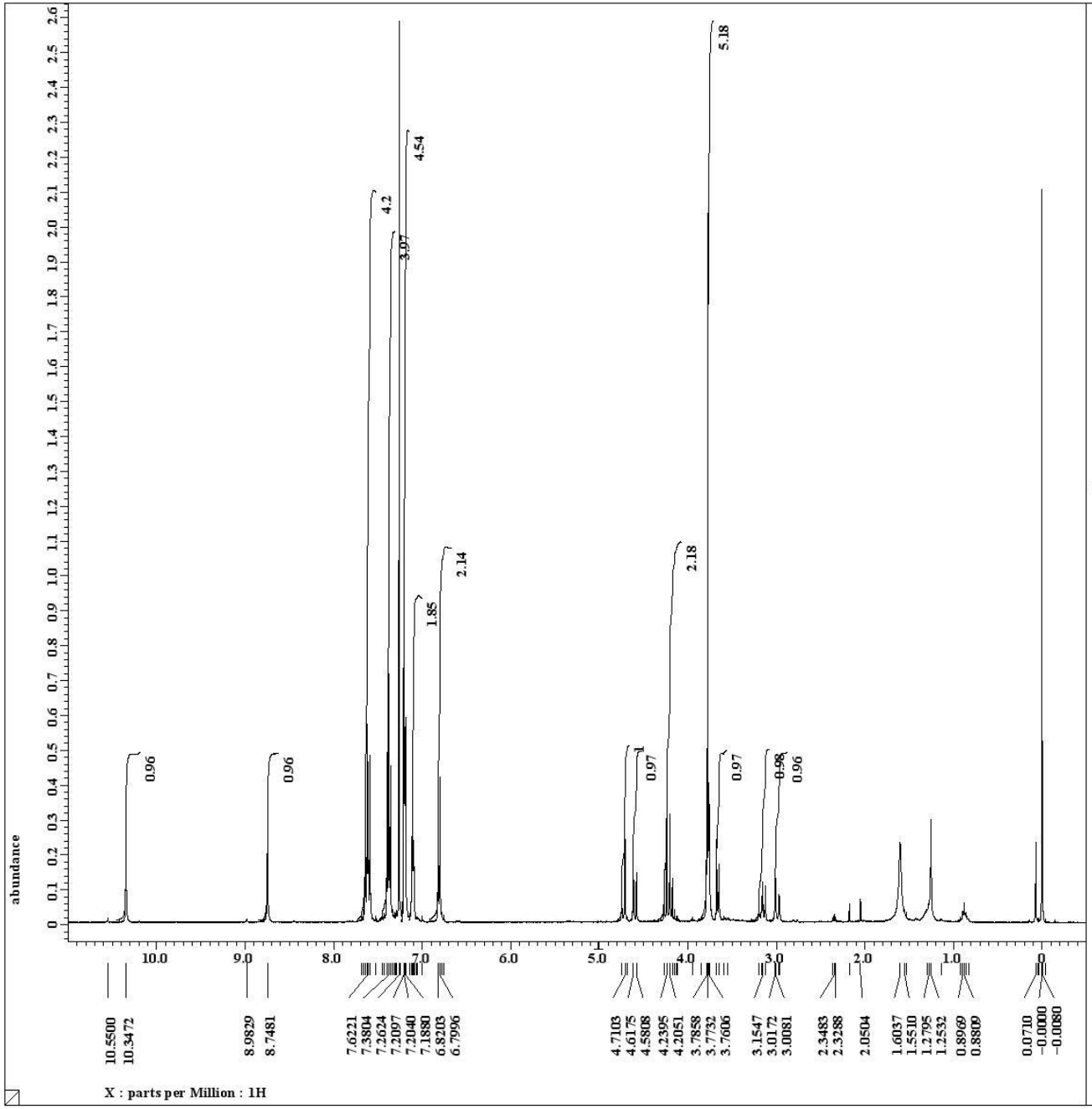
Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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             = 105
Total_scans       = 105

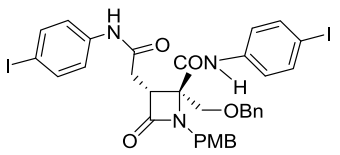
X_90_width        = 10[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.33333333[us]
Irr_atn_dec       = 20.8[dB]
Irr_atn_noe       = 20.8[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 19.3[dC]
```



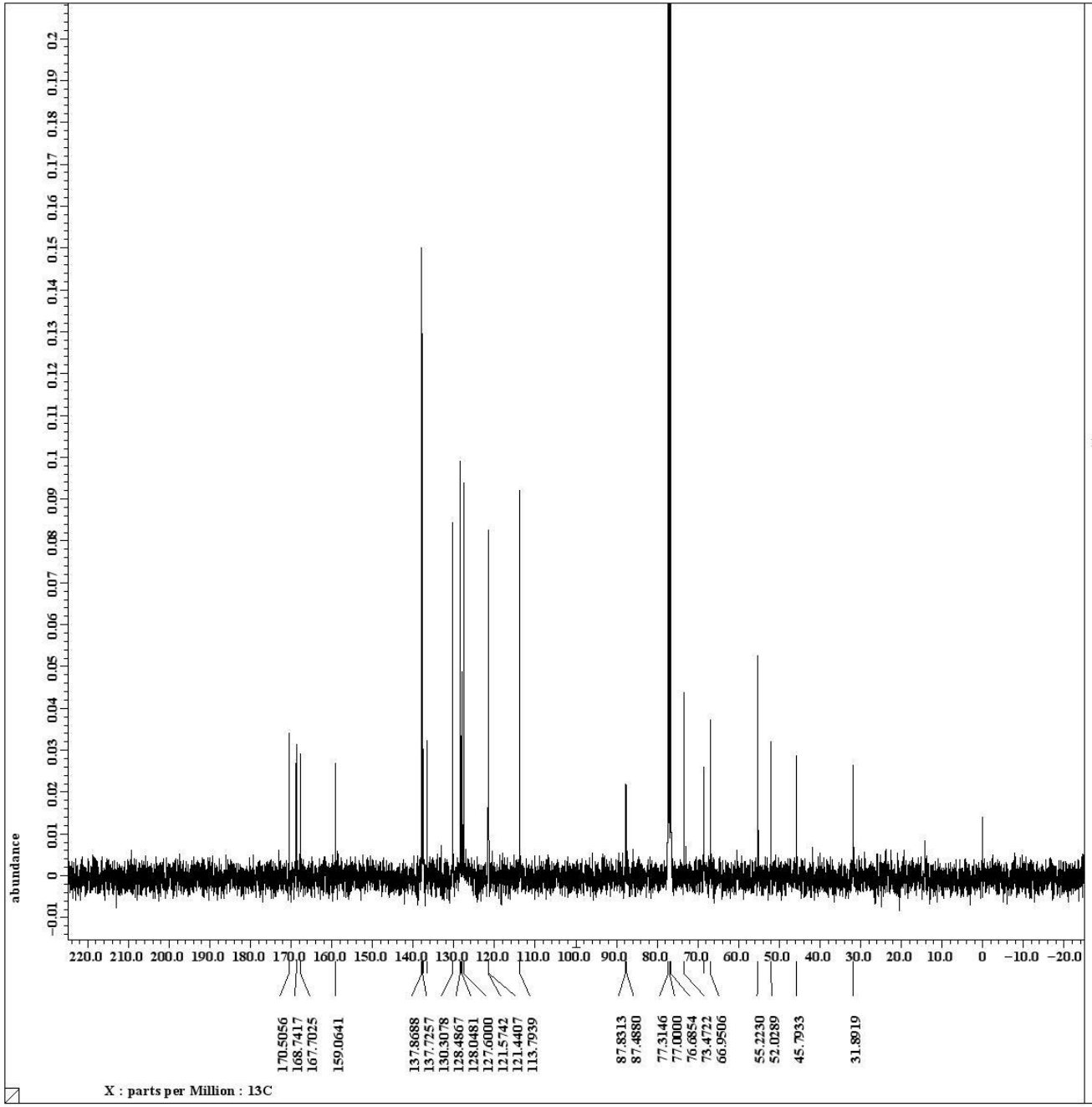
The other diastereomer of **9**



Filename	= RM409-PTLC-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#591168
Solvent	= CHLOROFORM-D
Creation_time	= 19-APR-2012 09:08:16
Revision_time	= 21-OCT-2014 18:05:32
Current_time	= 21-OCT-2014 18:05:38
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
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	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45794685[Hz]
X_sweep	= 7.5030012[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 10[us]
X_acq_time	= 2.18365952[s]
X_angle	= 45[deg]
X_atn	= 0.3[dB]
X_pulse	= 5[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 5[s]
Repetition_time	= 7.18365952[s]
Temp_get	= 17[dC]



10

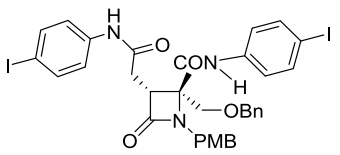



```
Filename          = RM754-13C-shita-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#723796
Solvent           = CHLOROFORM-D
Creation_time     = 11-MAR-2013 12:58:55
Revision_time     = 21-OCT-2014 21:07:48
Current_time      = 21-OCT-2014 21:07:57

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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             = 339
Total_scans       = 339

X_90_width        = 10.2[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.8[dB]
X_pulse           = 3.4[us]
Irr_atn_dec       = 20.8[dB]
Irr_atn_noe       = 20.8[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 54
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 19[dc]
```



10