NAZAROV CYCLIZATION OF AN INDOLYL VINYL KETONE PROMOTED BY ACETYL CHLORIDE AND SODIUM IODIDE: FORMAL SYNTHESIS OF BRUCEOLLINE E

Supporting Information

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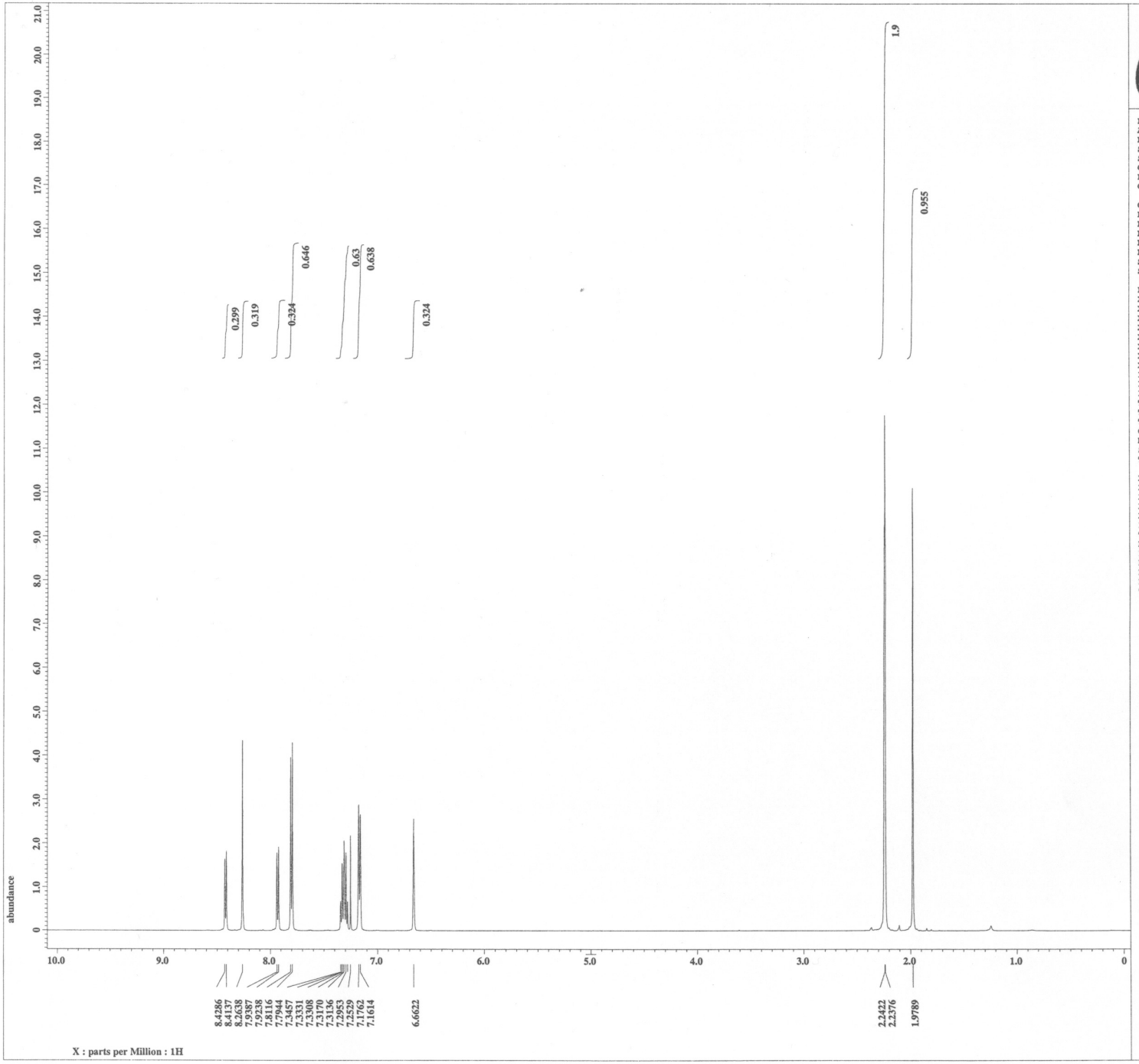



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Experiment = single_pulse.ex2
Sample_id = S#566855
Solvent = CHLOROFORM-D
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Revision_time = 29-JUL-2014 15:50:28
Current_time = 29-JUL-2014 15:51:17

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Dim_title = 1H
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Spectrometer = DELTA2_NMR

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X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 12.6[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.6[dB]
X_pulse = 6.3[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
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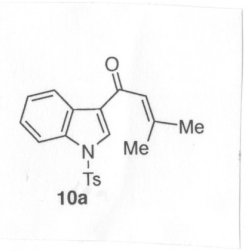
Temp_get = 20.3[dC]



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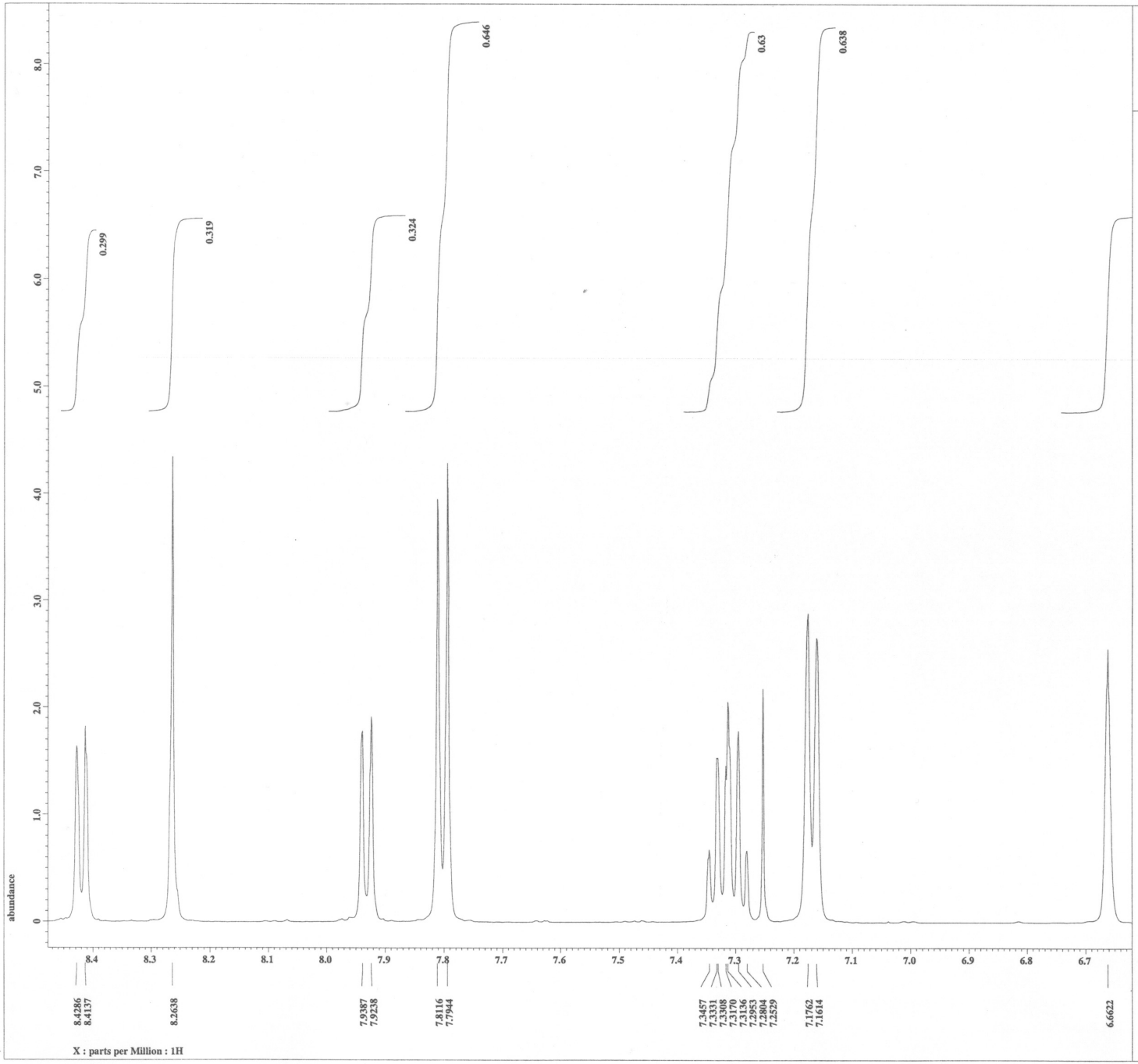



Filename = TA140729-18.jdf
Author = delta
Experiment = single_pulse.ex2
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Revision_time = 29-JUL-2014 15:48:29
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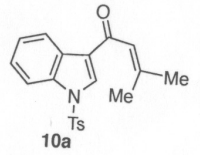
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 12.6[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.6[dB]
X_pulse = 6.3[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 24
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 20.3[dC]



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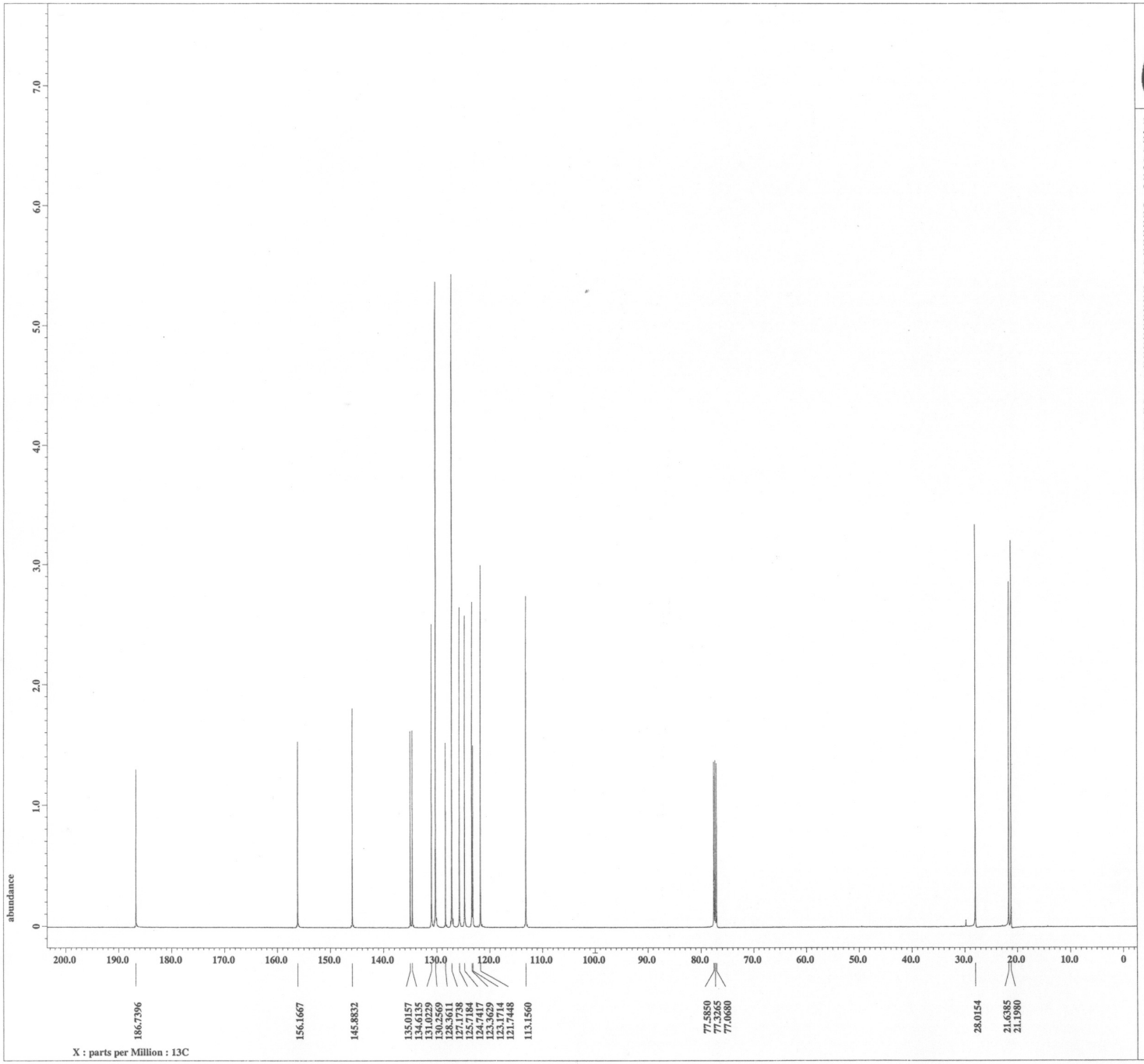
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6.0
5.0
4.0
3.0
2.0
1.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
186.7396
156.1667
145.8832
135.0157
134.6135
131.0229
130.2569
128.3611
127.1738
125.7184
124.7417
123.3629
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113.1560
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77.3265
77.0680
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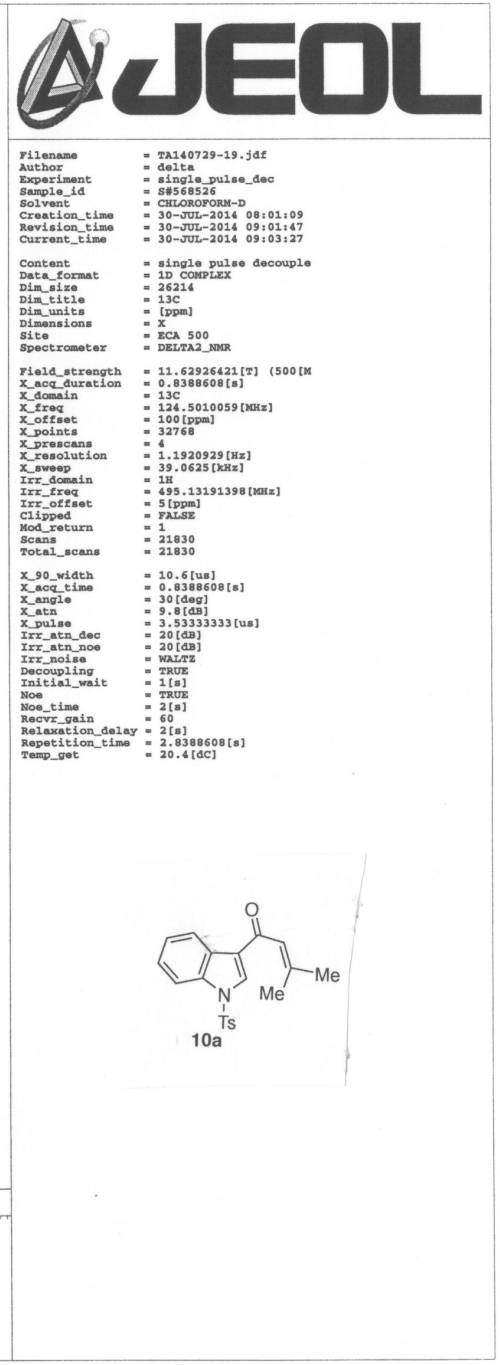
21.6385
21.1980
X : parts per Million : 13C


Filename = TA140729-19.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#568526
Solvent = CHLOROFORM-D
Creation_time = 30-JUL-2014 08:01:09
Revision_time = 30-JUL-2014 09:01:47
Current_time = 30-JUL-2014 09:03:27
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR
Field_strength = 11.62926421[T] (500[M
X_acq_duration = 0.8388608[s]
X_domain = 13C
X_freq = 124.5010059[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.1920929[Hz]
X_sweep = 39.0625[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 21830
Total_scans = 21830
X_90_width = 10.6[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.8[dB]
X_pulse = 3.53333333[us]
Irr_atn_dec = 20[dB]
Irr_atn_noe = 20[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 = 2.8388608[s]
Temp_get = 20.4[dC]

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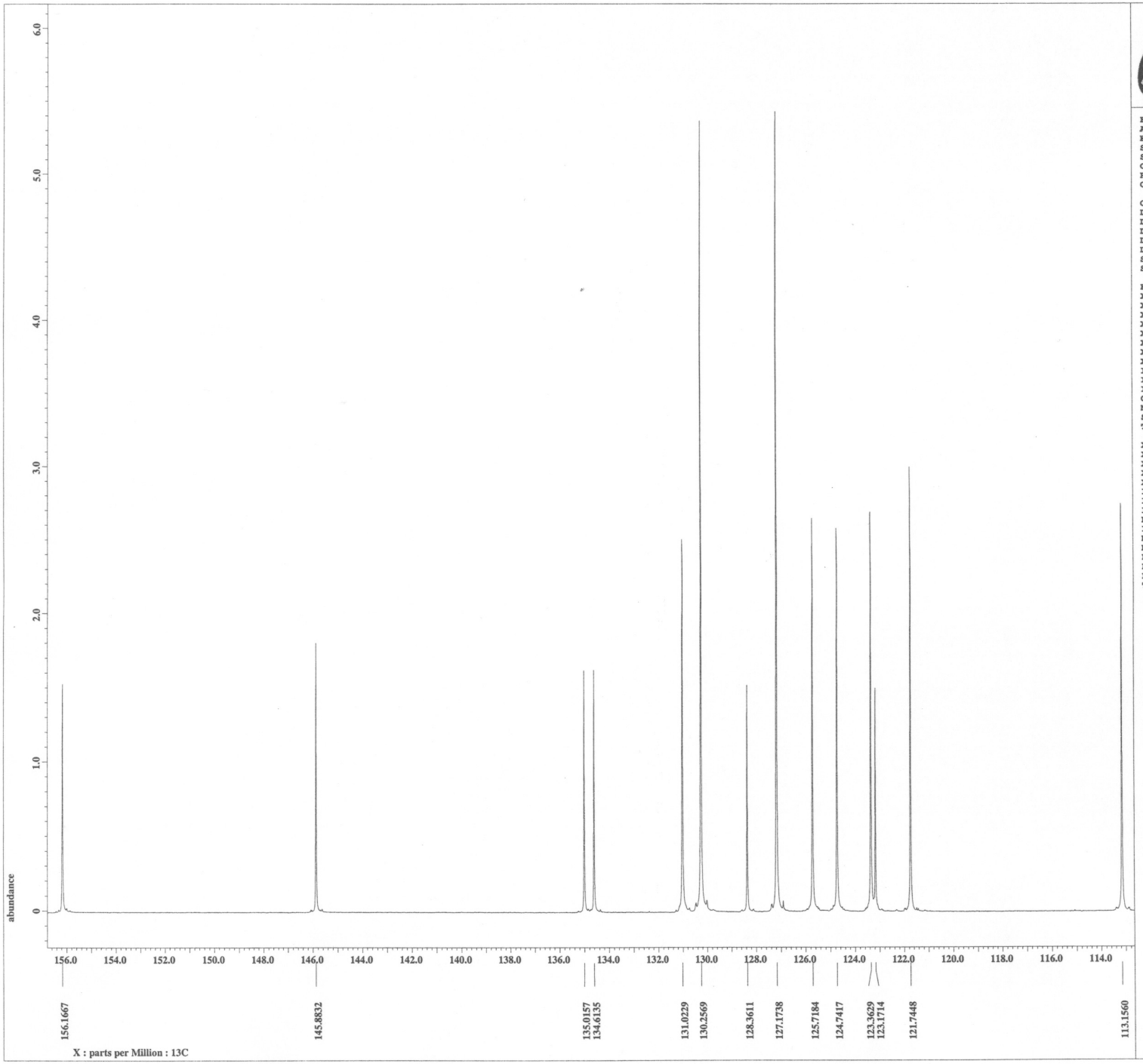

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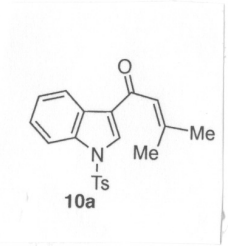
Filename	= TA140729-19.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#568526
Solvent	= CHLOROFORM-D
Creation_time	= 30-JUL-2014 08:01:09
Revision_time	= 30-JUL-2014 09:01:47
Current_time	= 30-JUL-2014 09:02:31
Content	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.62926421[T] (500[M
X_acq_duration	= 0.8388608[s]
X_domain	= 13C
X_freq	= 124.5010059[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.1920929[Hz]
X_sweep	= 39.0625[kHz]
Irr_domain	= 1H
Irr_freq	= 495.13191398[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 21830
Total_scans	= 21830
X_90_width	= 10.6[us]
X_acq_time	= 0.8388608[s]
X_angle	= 30[deg]
X_atn	= 9.8[dB]
X_pulse	= 3.53333333[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[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	= 2.8388608[s]
Temp_get	= 20.4[dC]



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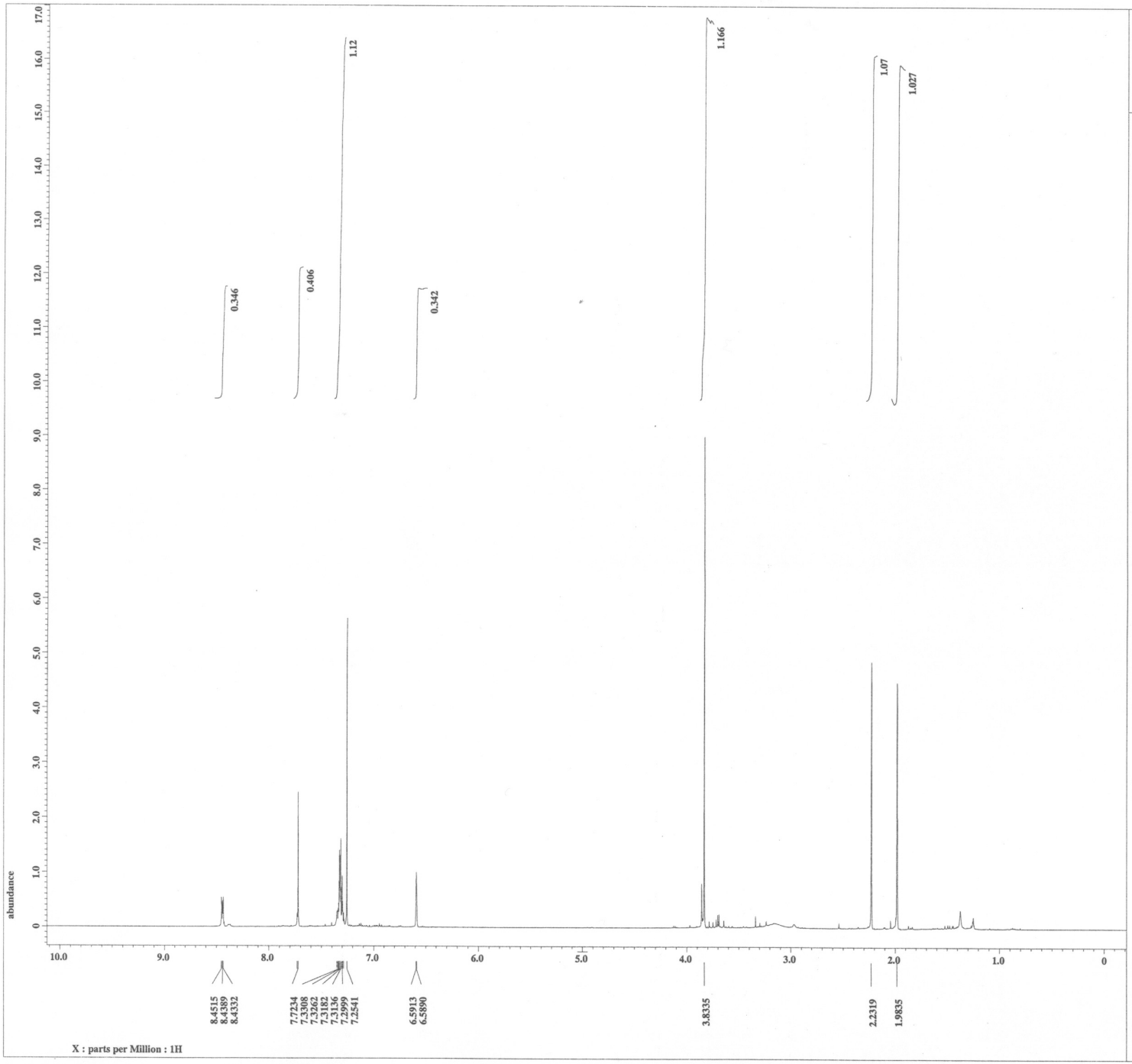



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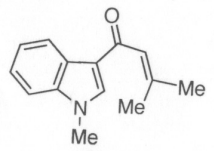
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#317724
Solvent = CHLOROFORM-D
Creation_time = 23-JUL-2014 07:52:25
Revision_time = 23-JUL-2014 08:58:14
Current_time = 23-JUL-2014 08:58:18

Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 12.6[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.6[dB]
X_pulse = 6.3[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 19.6[dC]



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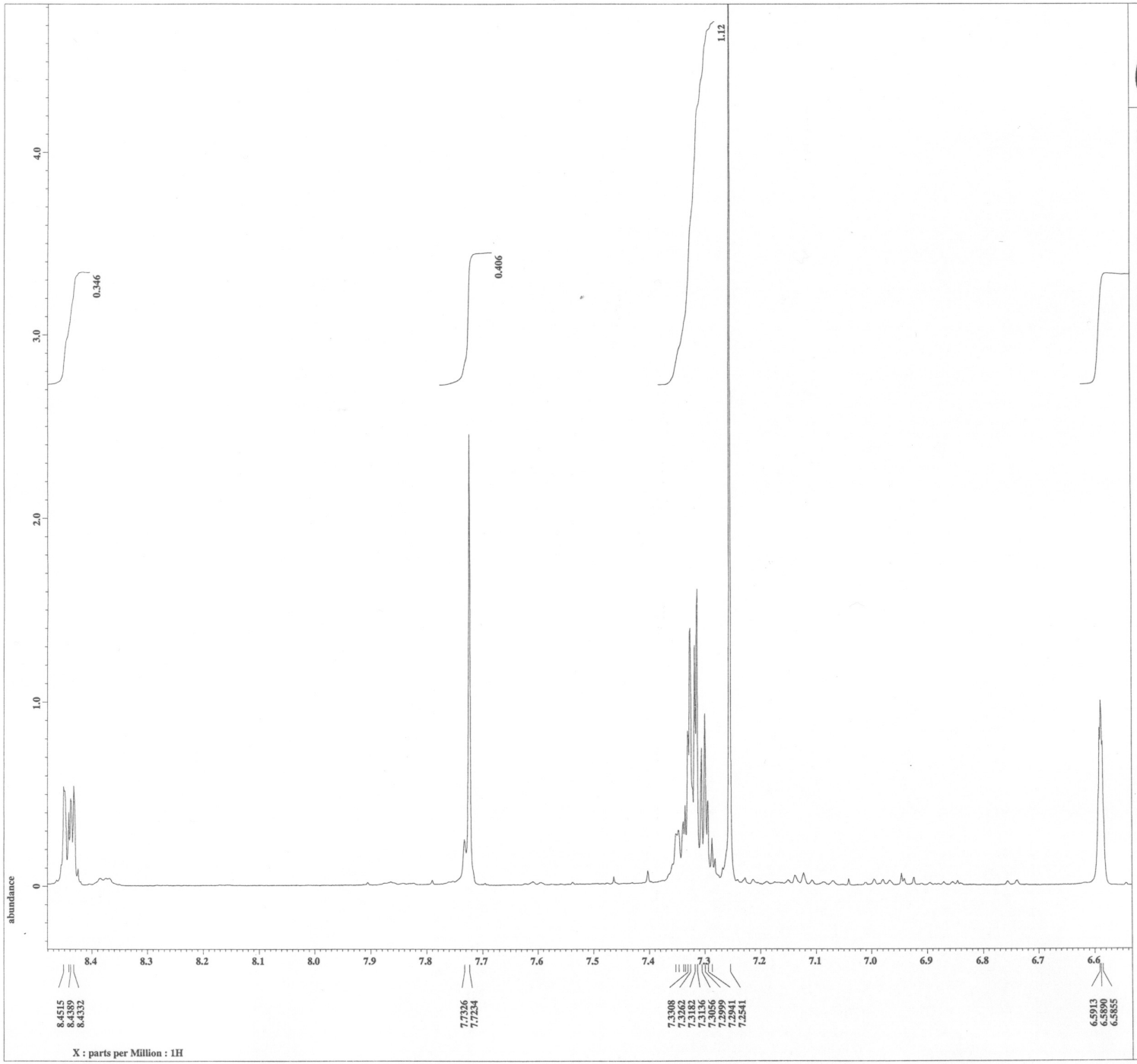
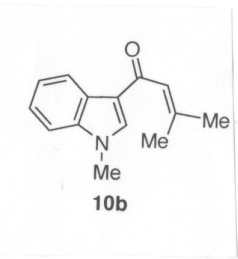


JEOL

Filename	= TA140723-5.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#317724
Solvent	= CHLOROFORM-D
Creation_time	= 23-JUL-2014 07:52:25
Revision_time	= 23-JUL-2014 08:58:32
Current_time	= 23-JUL-2014 08:58:35
Content	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.62926421[T] (500[M
X_acq_duration	= 1.76422912[s]
X_domain	= 1H
X_freq	= 495.13191398[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.5668198[Hz]
X_sweep	= 9.28677563[kHz]
Irr_domain	= 1H
Irr_freq	= 495.13191398[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 495.13191398[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 12.6[us]
X_acq_time	= 1.76422912[s]
X_angle	= 45[deg]
X_atn	= 3.6[dB]
X_pulse	= 6.3[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 42
Relaxation_delay	= 5[s]
Repetition_time	= 6.76422912[s]
Temp_get	= 19.6[dC]



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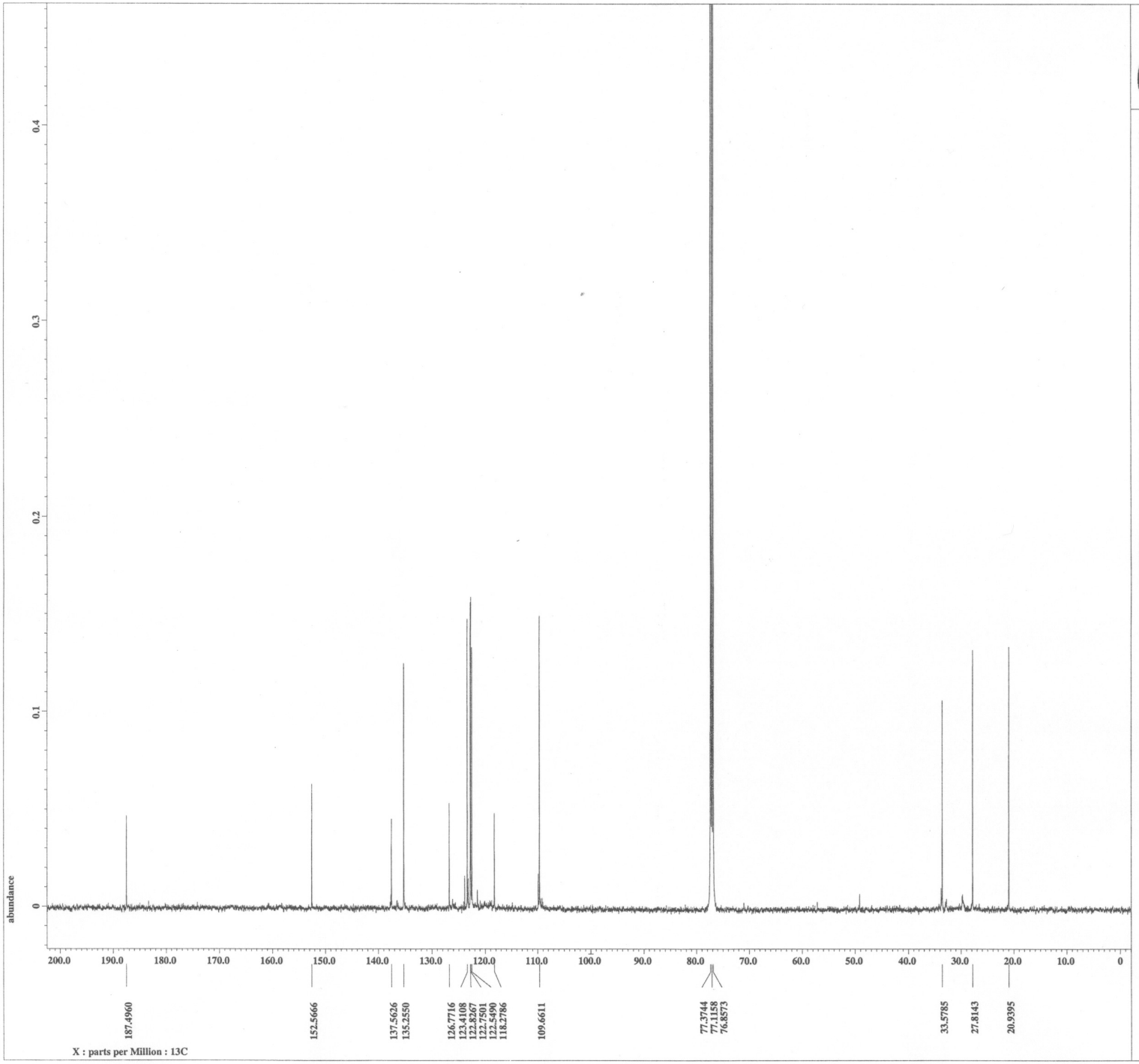

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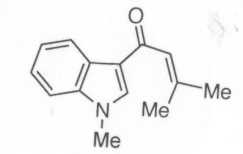
Experiment	= single_pulse_dec
Sample_id	= S#592898
Solvent	= CHLOROFORM-D
Creation_time	= 24-JUL-2014 07:49:57
Revision_time	= 24-JUL-2014 08:51:24
Current_time	= 24-JUL-2014 08:53:09
Content	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.62926421[T] (500[M
X_acq_duration	= 0.8388608[s]
X_domain	= 13C
X_freq	= 124.5010059[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.1920929[Hz]
X_sweep	= 39.0625[kHz]
Irr_domain	= 1H
Irr_freq	= 495.13191398[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 20714
Total_scans	= 20714
X_90_width	= 10.6[us]
X_acq_time	= 0.8388608[s]
X_angle	= 30[deg]
X_atn	= 9.8[dB]
X_pulse	= 3.53333333[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[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	= 2.8388608[s]
Temp_get	= 20.7[dC]



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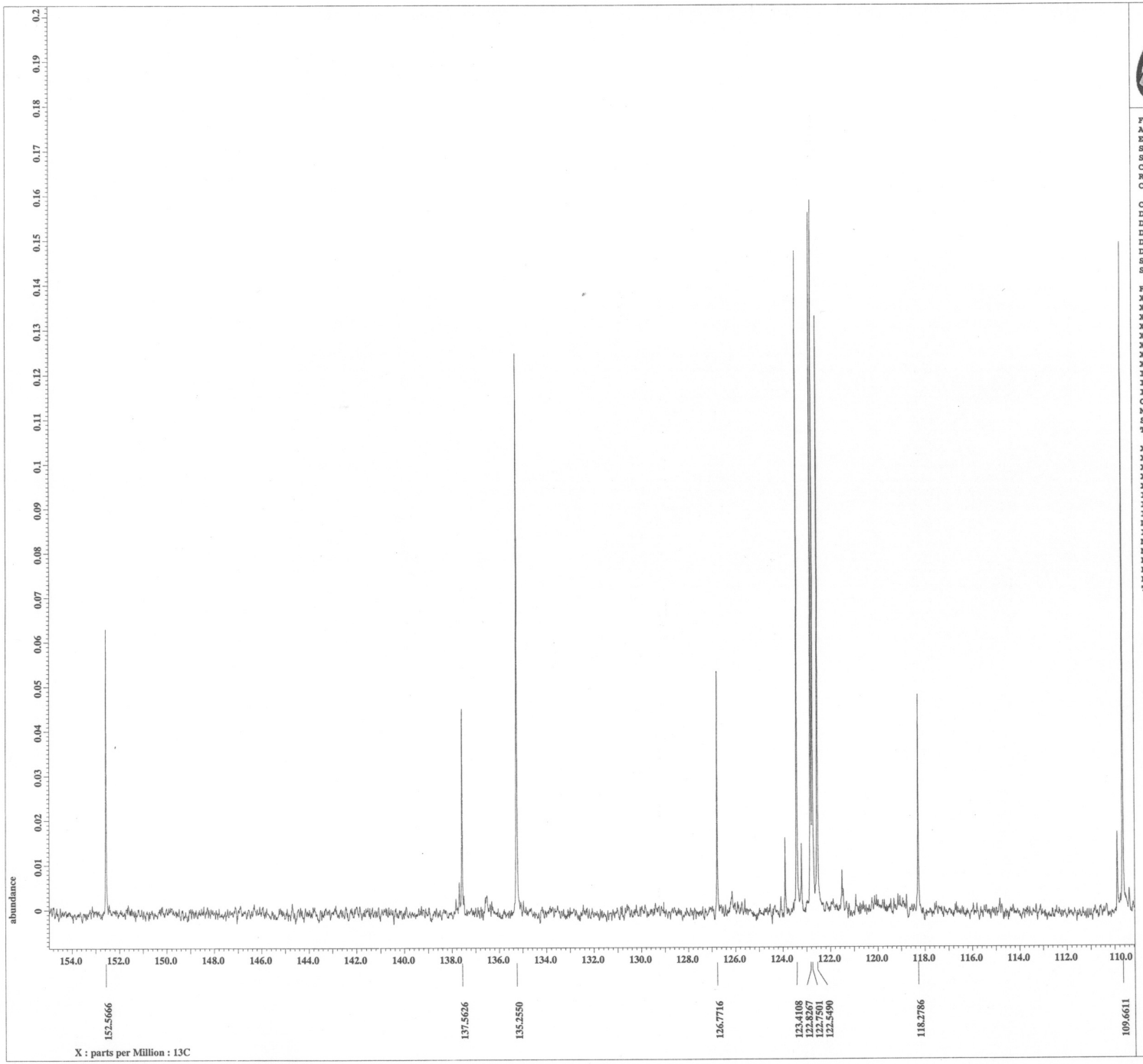
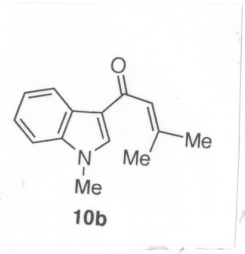


JEOL

Filename	= TA140723-16.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#592898
Solvent	= CHLOROFORM-D
Creation_time	= 24-JUL-2014 07:49:57
Revision_time	= 24-JUL-2014 08:51:24
Current_time	= 24-JUL-2014 08:51:57
Content	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.62926421[T] (500[M
X_acq_duration	= 0.8388608[s]
X_domain	= 13C
X_freq	= 124.5010059[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.1920929[Hz]
X_sweep	= 39.0625[kHz]
Irr_domain	= 1H
Irr_freq	= 495.13191398[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 20714
Total_scans	= 20714
X_90_width	= 10.6[us]
X_acq_time	= 0.8388608[s]
X_angle	= 30[deg]
X_atn	= 9.8[dB]
X_pulse	= 3.53333333[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[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	= 2.8388608[s]
Temp_get	= 20.7[dC]



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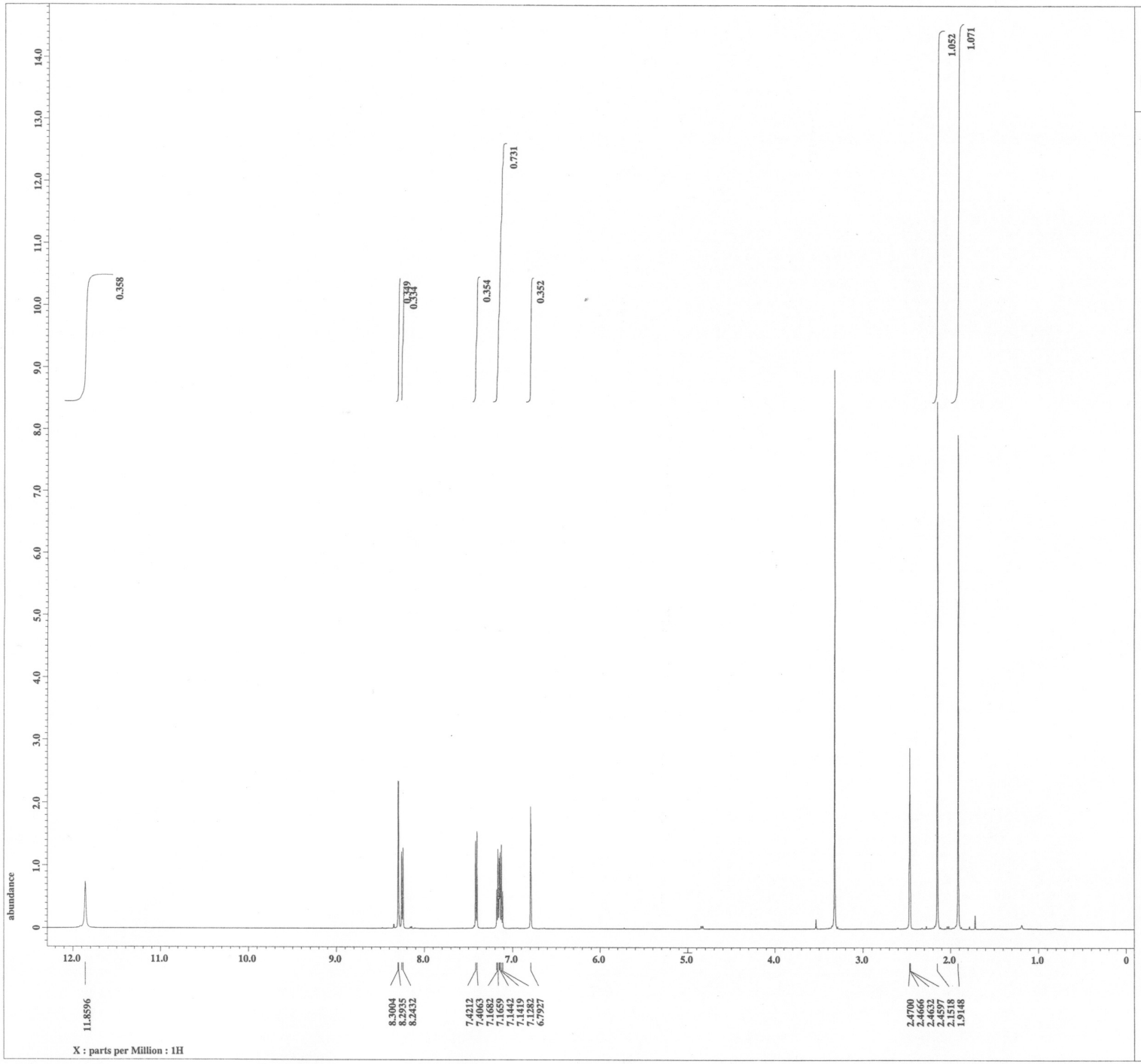
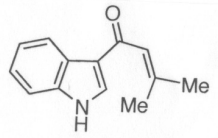


JEOL

Filename	= TA140721-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#366006
Solvent	= DMSO-D6
Creation_time	= 21-JUL-2014 09:13:13
Revision_time	= 21-JUL-2014 10:16:44
Current_time	= 21-JUL-2014 10:16:51
Content	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.62926421[T] (500[M
X_acq_duration	= 1.76422912[s]
X_domain	= 1H
X_freq	= 495.13191398[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.5668198[Hz]
X_sweep	= 9.286777563[kHz]
Irr_domain	= 1H
Irr_freq	= 495.13191398[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 495.13191398[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 12.6[us]
X_acq_time	= 1.76422912[s]
X_angle	= 45[deg]
X_atn	= 3.6[dB]
X_pulse	= 6.3[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 5[s]
Repetition_time	= 6.76422912[s]
Temp_get	= 20.2[dC]



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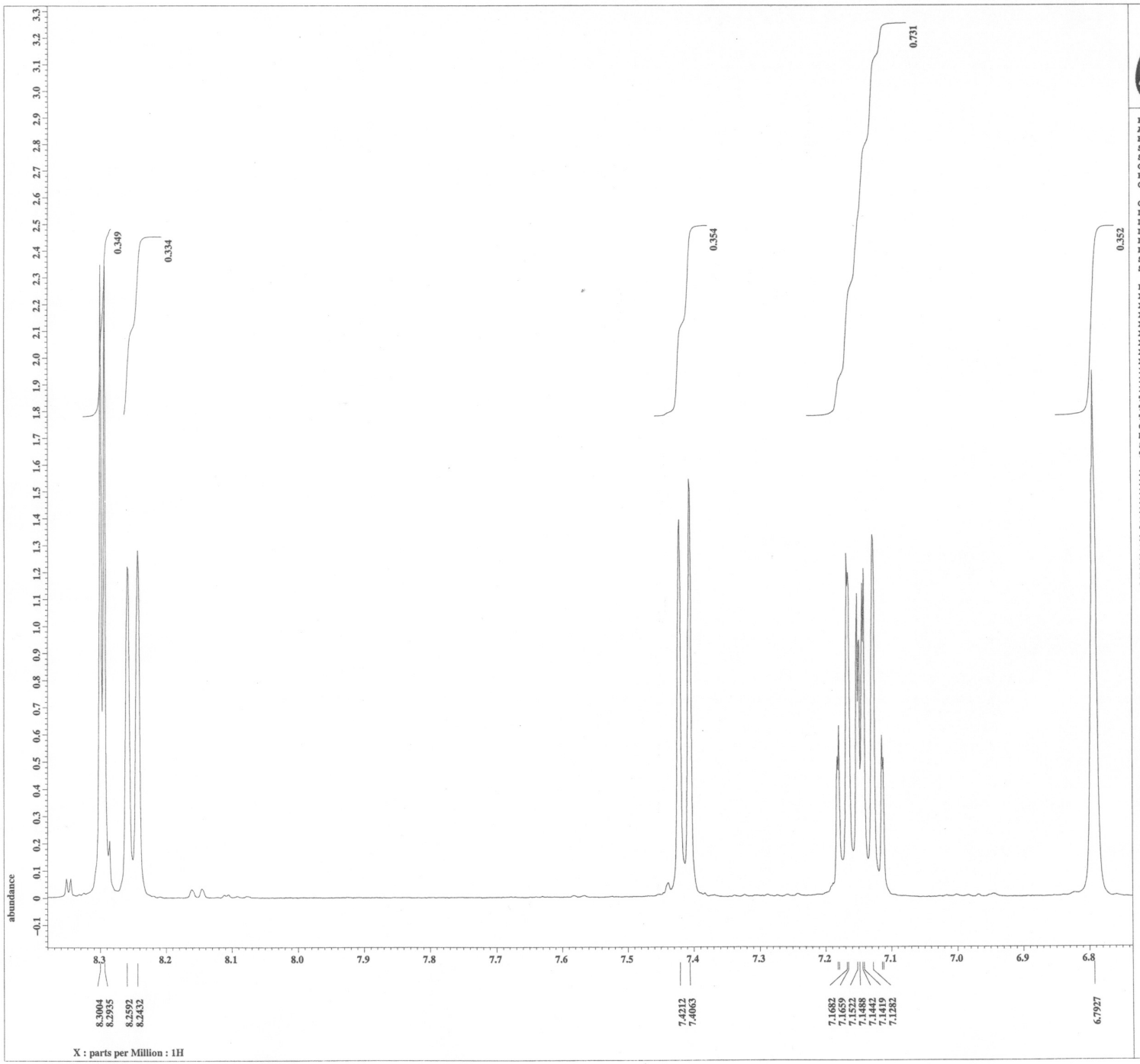
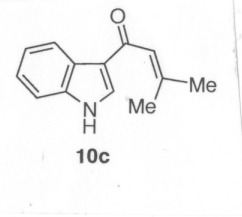


Filename = TA140721-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#366006
Solvent = DMSO-D6
Creation_time = 21-JUL-2014 09:13:13
Revision_time = 21-JUL-2014 10:13:57
Current_time = 21-JUL-2014 10:15:00

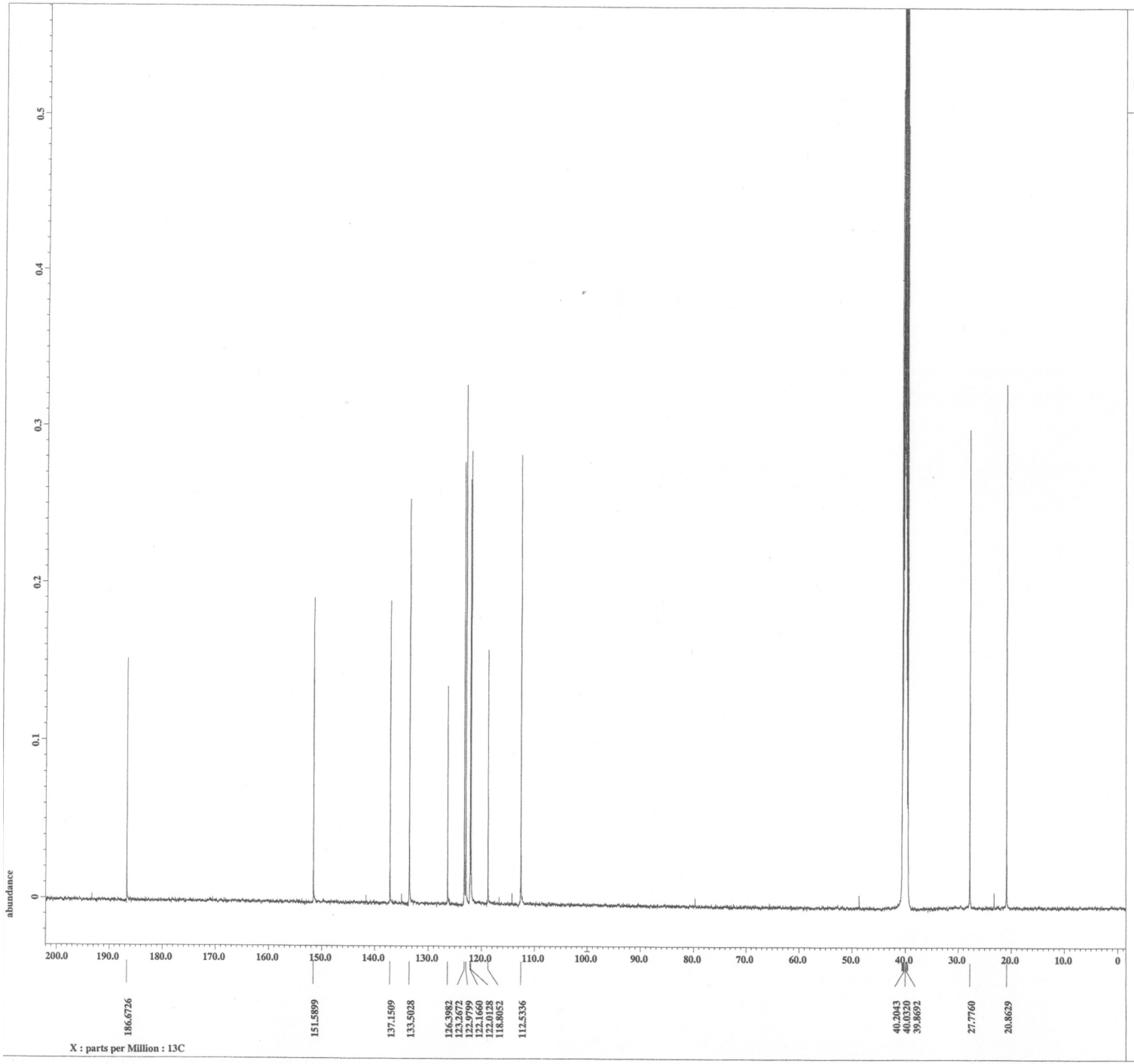
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 12.6[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.6[dB]
X_pulse = 6.3[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 20.2[dC]

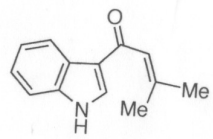


10c

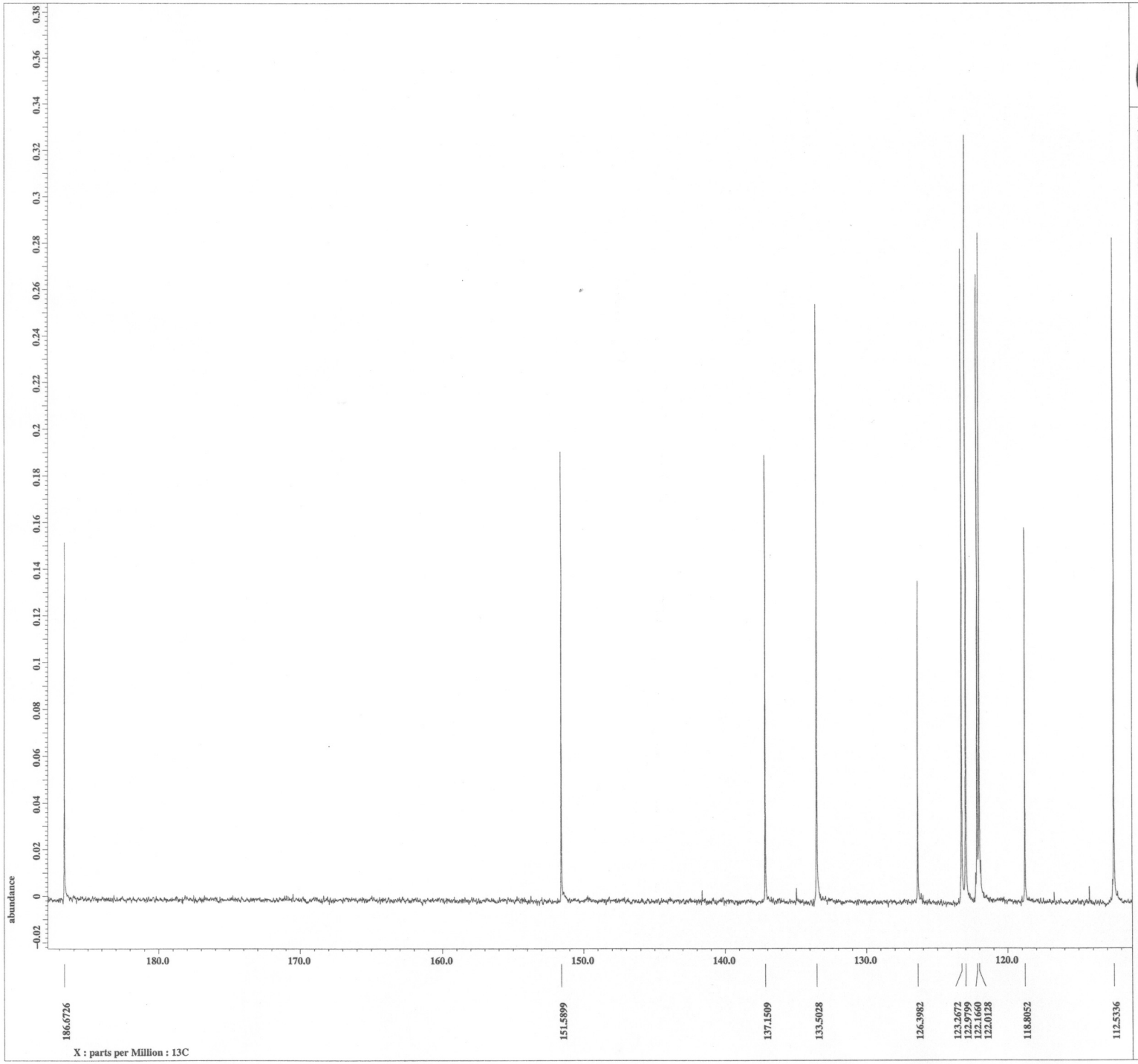


JEOL

Filename	= TA140721-3.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#367482
Solvent	= DMSO-D6
Creation_time	= 22-JUL-2014 08:39:19
Revision_time	= 22-JUL-2014 09:39:18
Current_time	= 22-JUL-2014 09:39:40
Content	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.62926421[T] (500[M
X_acq_duration	= 0.8388608[s]
X_domain	= 13C
X_freq	= 124.5010059[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.1920929[Hz]
X_sweep	= 39.0625[kHz]
Irr_domain	= 1H
Irr_freq	= 495.13191398[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 29688
Total_scans	= 29688
X_90_width	= 10.6[us]
X_acq_time	= 0.8388608[s]
X_angle	= 30[deg]
X_atn	= 9.8[dB]
X_pulse	= 3.53333333[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[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	= 2.8388608[s]
Temp_get	= 21.3[dC]

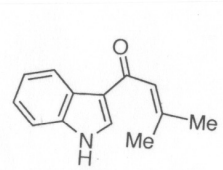


10c

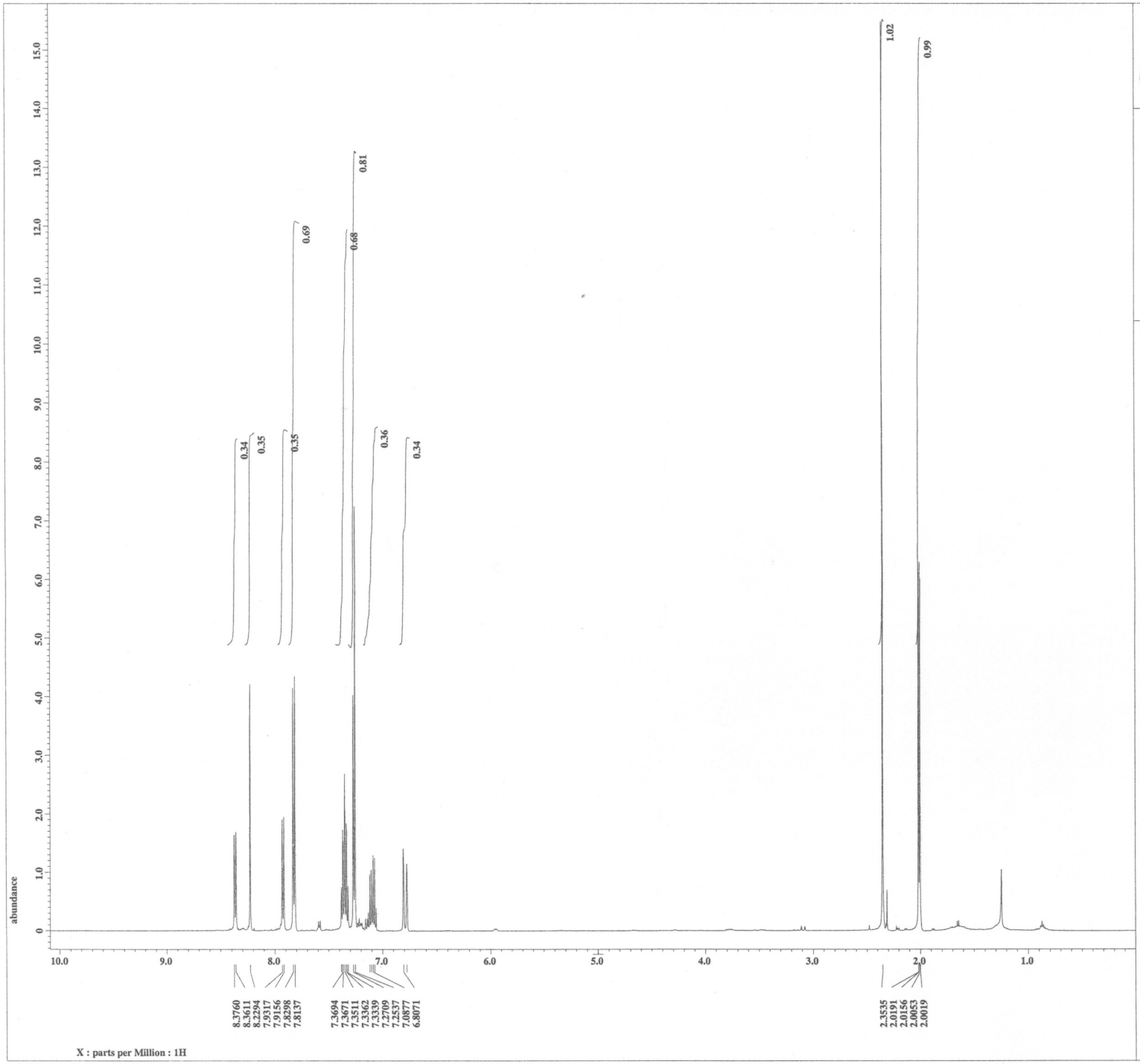




Filename	= TA140721-3.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#367482
Solvent	= DMSO-D6
Creation_time	= 22-JUL-2014 08:39:19
Revision_time	= 22-JUL-2014 09:39:18
Current_time	= 22-JUL-2014 09:42:37
Content	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.62926421[T] (500[M
X_acq_duration	= 0.8388608[s]
X_domain	= 13C
X_freq	= 124.5010059[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.1920929[Hz]
X_sweep	= 39.0625[kHz]
Irr_domain	= 1H
Irr_freq	= 495.13191398[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 29688
Total_scans	= 29688
X_90_width	= 10.6[us]
X_acq_time	= 0.8388608[s]
X_angle	= 30[deg]
X_atn	= 9.8[dB]
X_pulse	= 3.53333333[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[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	= 2.8388608[s]
Temp_get	= 21.3[dC]



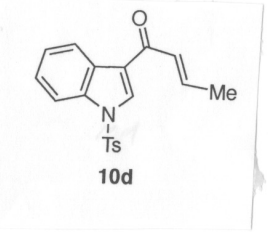
10c



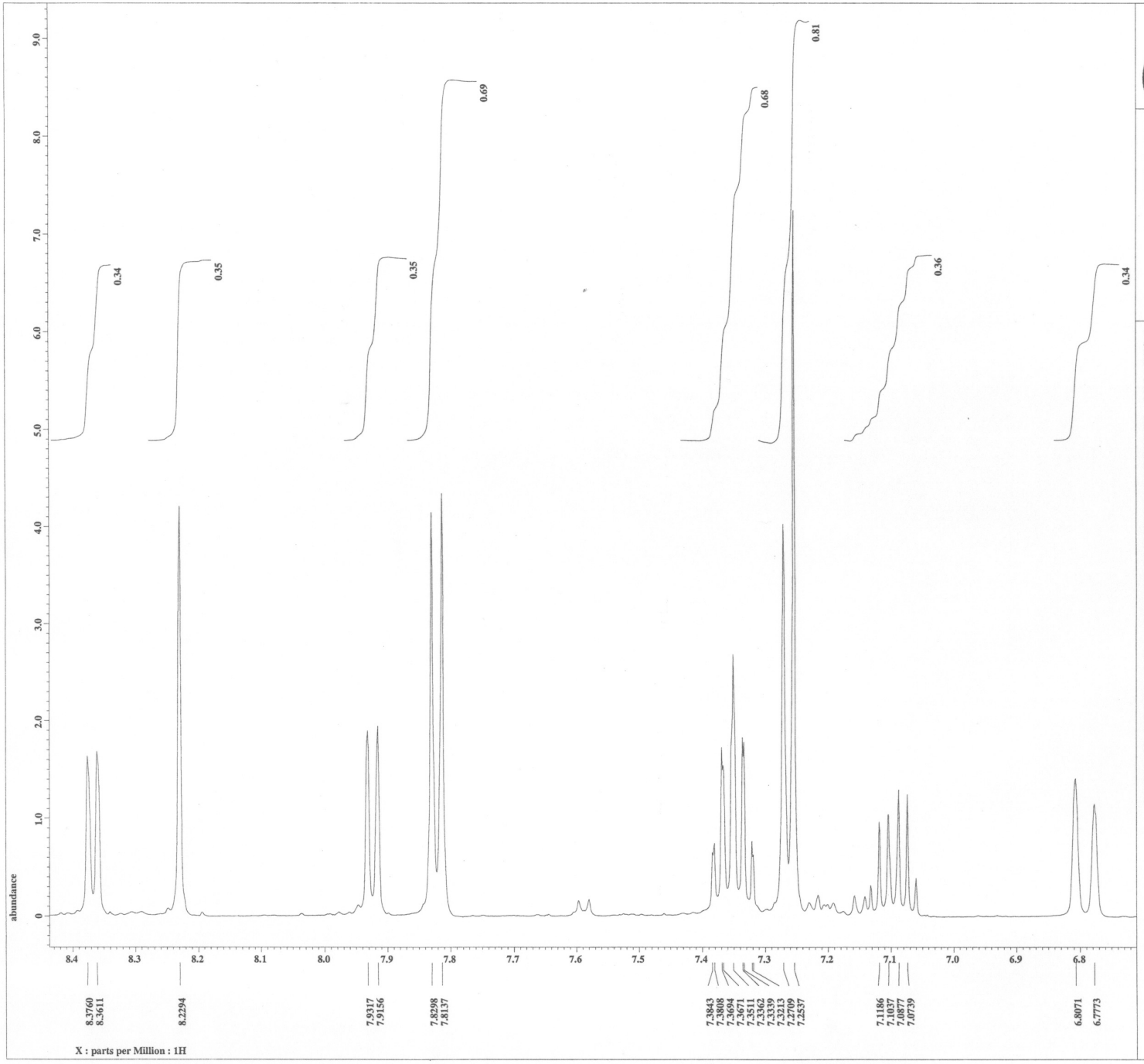
JEOL

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

Derived from: TA140901-3.jdf
```

Filename	= TA140901-6.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#290120
Solvent	= CHLOROFORM-D
Creation_time	= 1-SEP-2014 08:04:24
Revision_time	= 1-SEP-2014 08:07:23
Current_time	= 1-SEP-2014 08:08:20
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 11.9[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 3.4[dB]
X_pulse	= 5.95[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 50
Relaxation_delay	= 5[s]
Repetition_time	= 6.74587904[s]
Temp_get	= 22.2[dC]



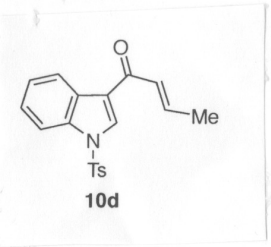
10d



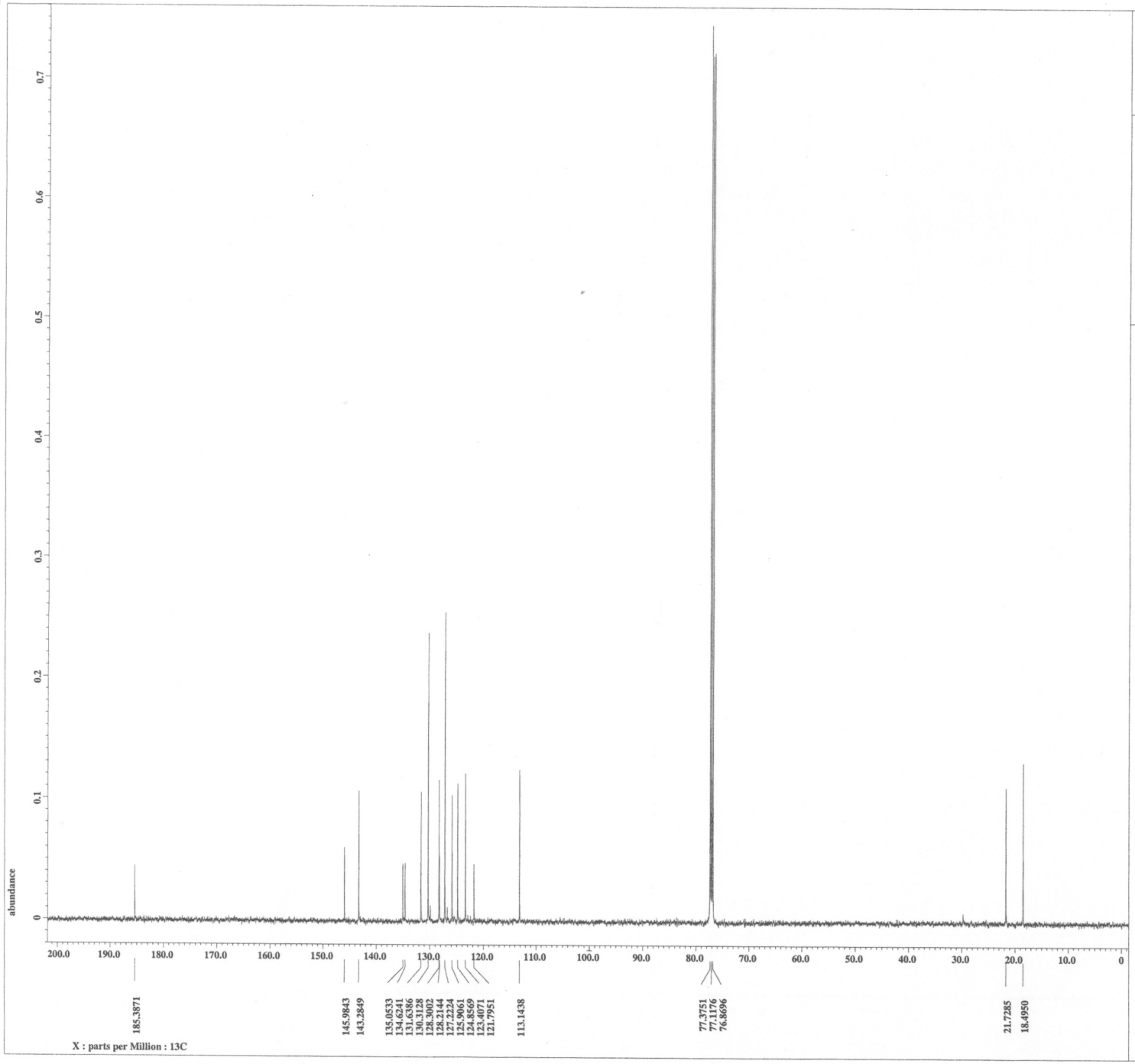


```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA140901-3.jdf
```

Filename	= TA140901-6.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#290120
Solvent	= CHLOROFORM-D
Creation_time	= 1-SEP-2014 08:04:24
Revision_time	= 1-SEP-2014 08:06:24
Current_time	= 1-SEP-2014 08:06:37
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 11.9[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 3.4[dB]
X_pulse	= 5.95[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 50
Relaxation_delay	= 5[s]
Repetition_time	= 6.74587904[s]
Temp_get	= 22.2[dC]



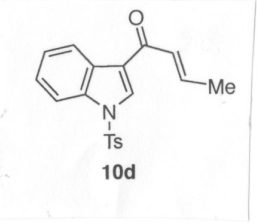
10d



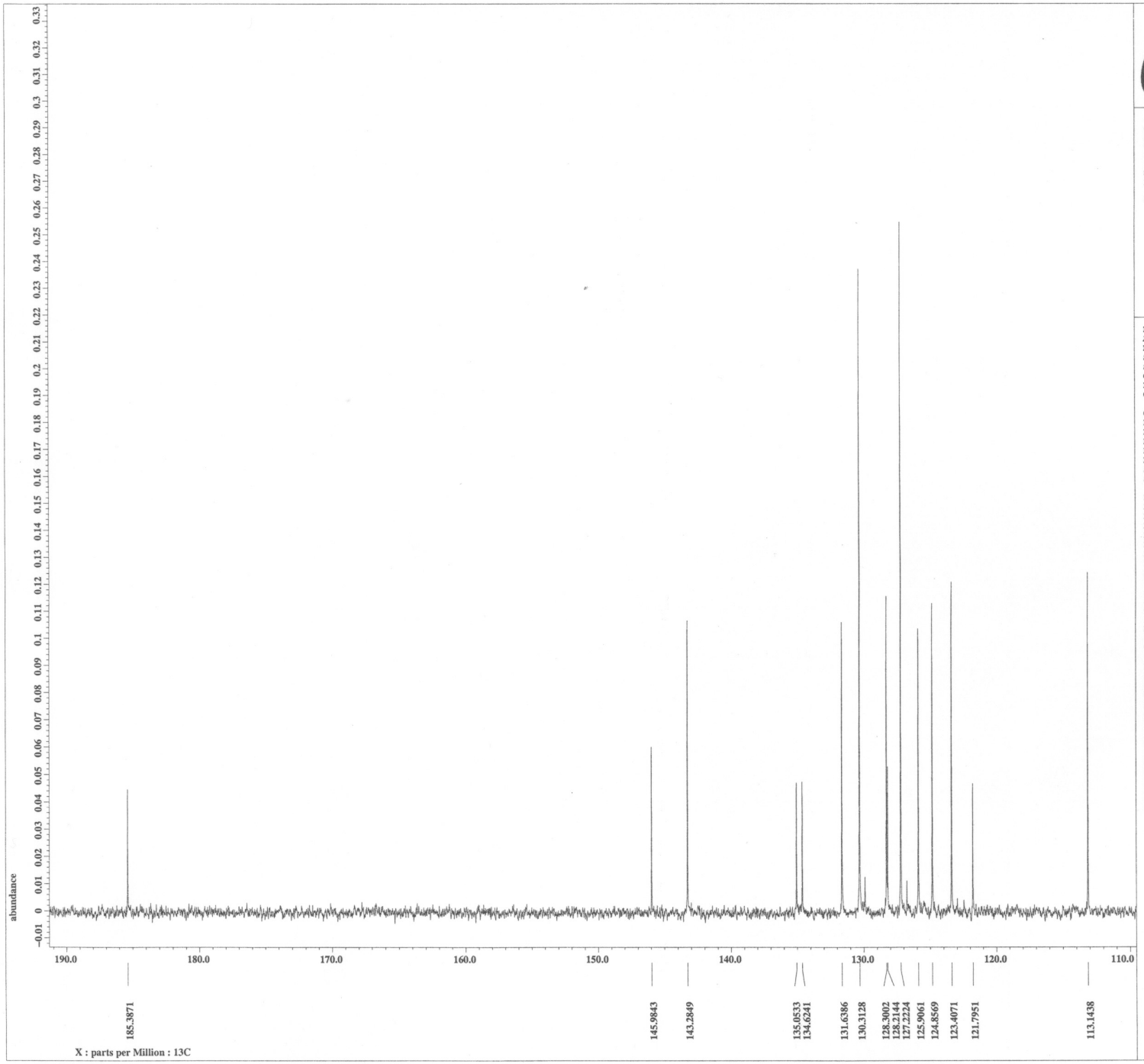


```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA140901_copy-1.jdf
```

```
Filename          = TA140901_copy-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#291315
Solvent           = CHLOROFORM-D
Creation_time     =  1-SEP-2014 09:21:03
Revision_time     =  1-SEP-2014 09:23:19
Current_time      =  1-SEP-2014 09:25:42

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Incomplete_copy   = TRUE
Mod_return        = 1
Scans             = 1594
Total_scans       = 1594

X_90_width        = 10.8[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 5.5[dB]
X_pulse           = 3.6[us]
Irr_atn_dec       = 21.16482[dB]
Irr_atn_noe       = 21.16482[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   = 2.83361792[s]
Temp_get          = 22.9[dC]
```



10d



---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

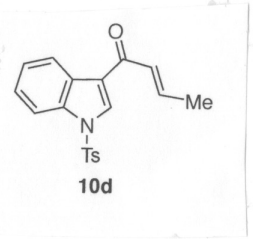
Derived from: TA140901_copy-1.jdf

Filename = TA140901_copy-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#291315
Solvent = CHLOROFORM-D
Creation_time = 1-SEP-2014 09:21:03
Revision_time = 1-SEP-2014 09:23:19
Current_time = 1-SEP-2014 09:24:46

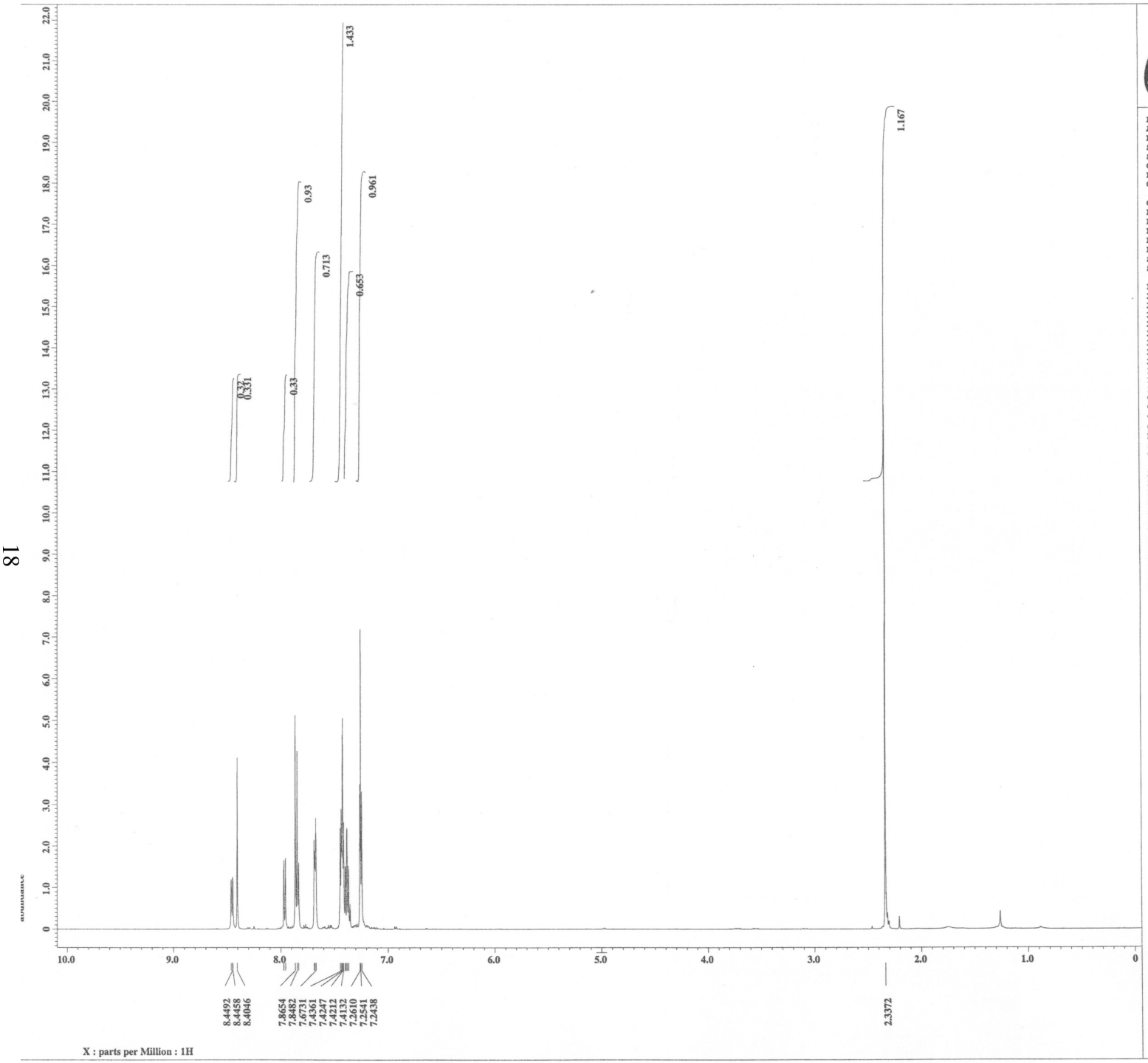
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA500
Spectrometer = DELTA2_NMR

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain = 13C
X_freq = 125.76529768[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.19959034[Hz]
X_sweep = 39.3081761[kHz]
Irr_domain = 1H
Irr_freq = 500.15991521[MHz]
Irr_offset = 5.0[ppm]
Clipped = FALSE
Incomplete_copy = TRUE
Mod_return = 1
Scans = 1594
Total_scans = 1594

X_90_width = 10.8[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 5.5[dB]
X_pulse = 3.6[us]
Irr_atn_dec = 21.16482[dB]
Irr_atn_noe = 21.16482[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 = 2.83361792[s]
Temp_get = 22.9[dC]



10d



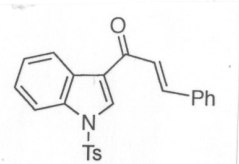


Filename = TA140807-11.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#554233
Solvent = CHLOROFORM-D
Creation_time = 7-AUG-2014 14:23:53
Revision_time = 7-AUG-2014 15:28:53
Current_time = 7-AUG-2014 15:30:27

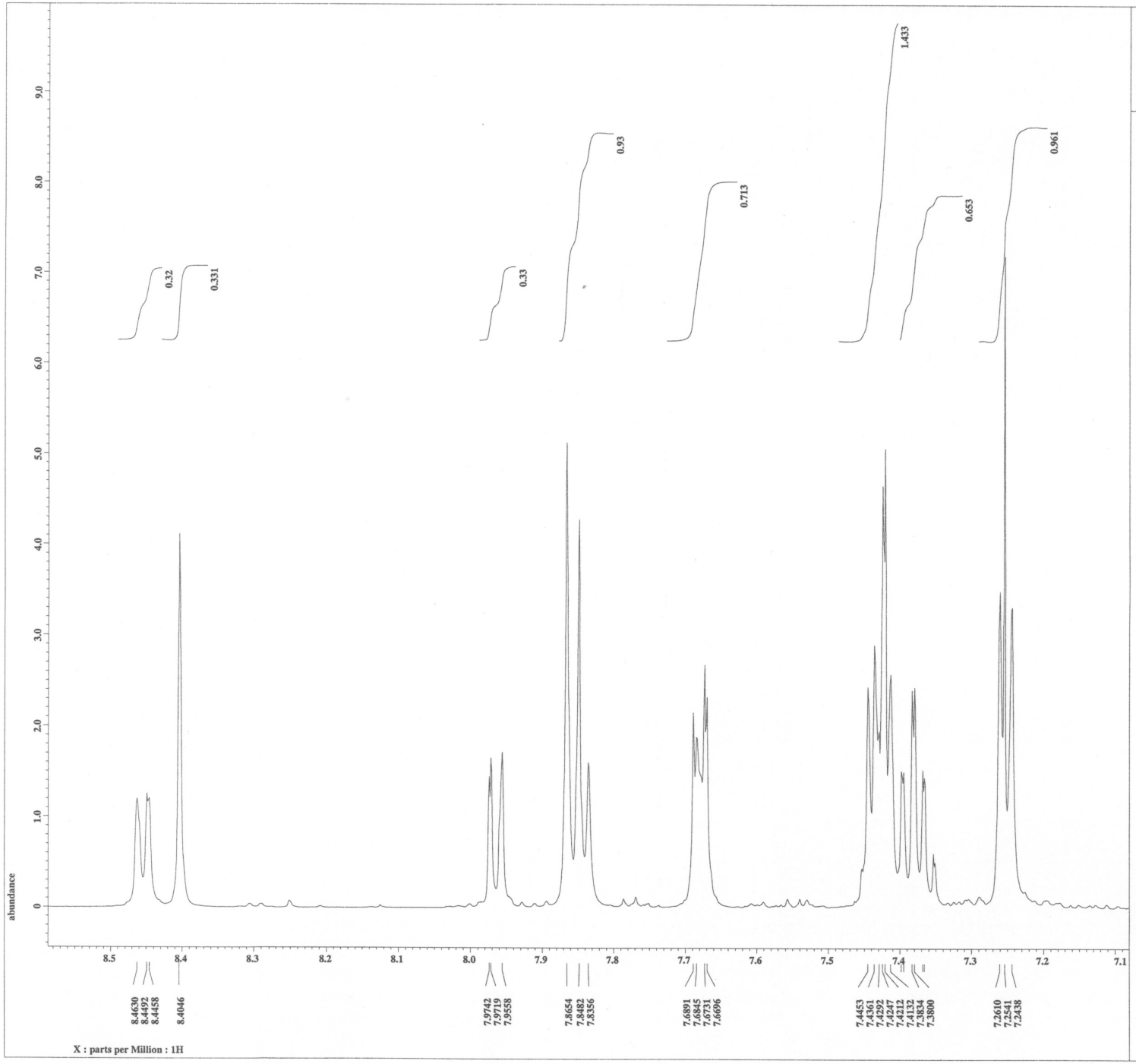
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 12.6[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.6[dB]
X_pulse = 6.3[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 20.6[dC]



10e



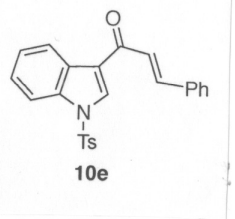
JEOL

Filename = TA140807-11.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#554233
Solvent = CHLOROFORM-D
Creation_time = 7-AUG-2014 14:23:53
Revision_time = 7-AUG-2014 15:30:44
Current_time = 7-AUG-2014 15:30:47

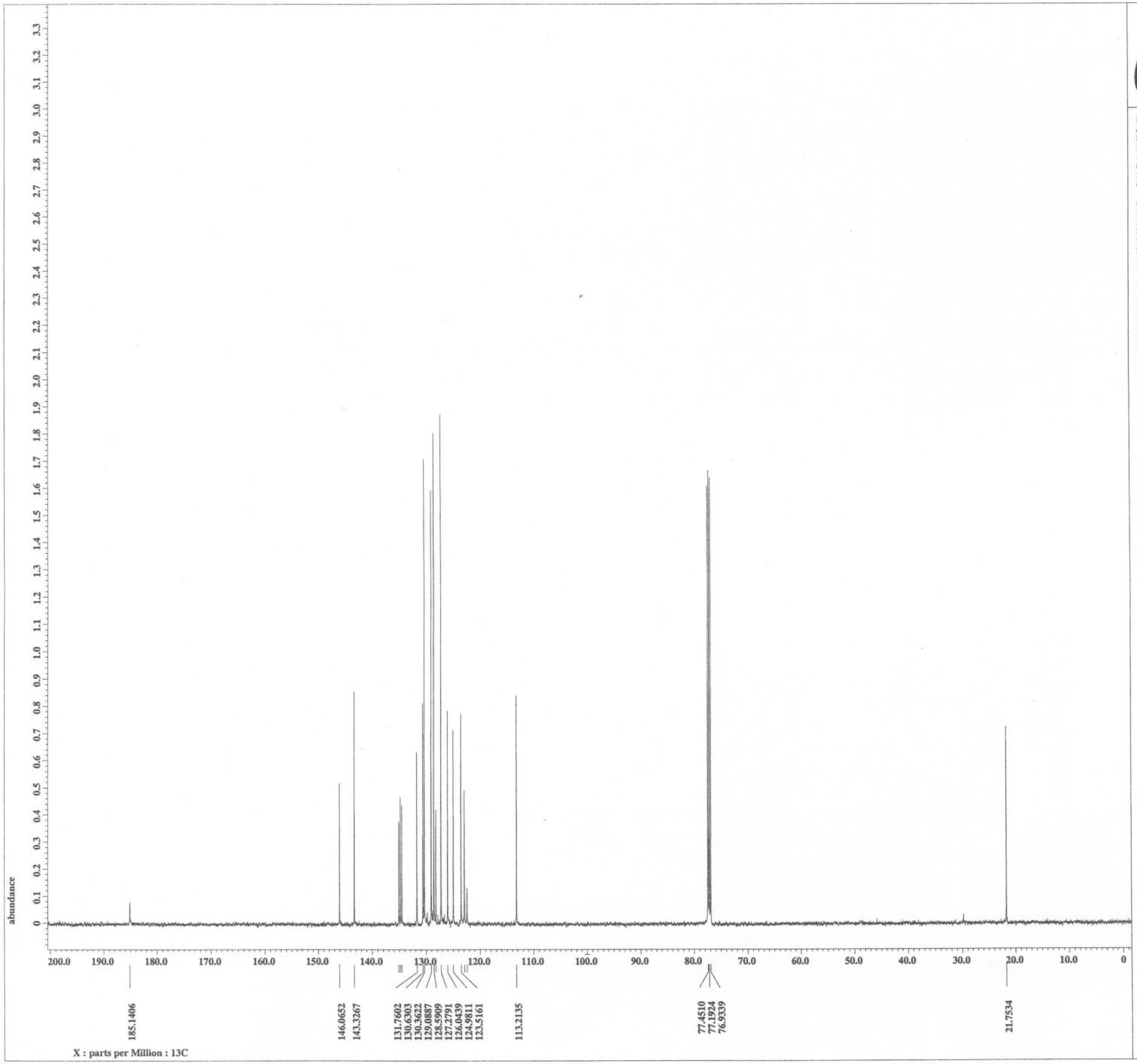
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 12.6[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.6[dB]
X_pulse = 6.3[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 20.6[dC]

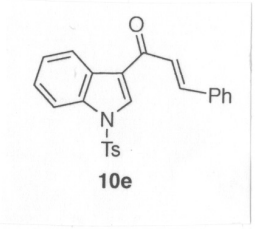


10e

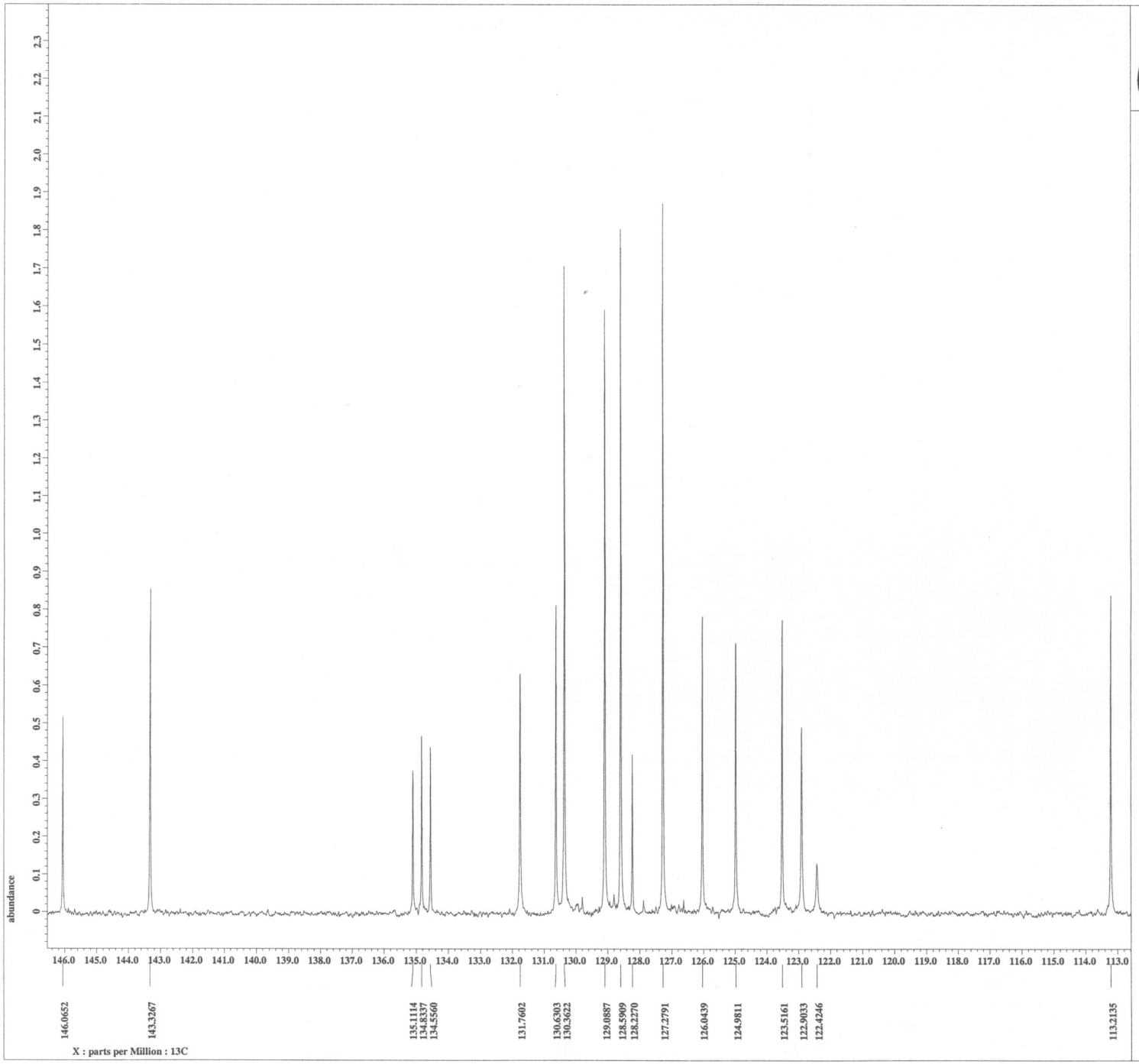


JEOL

```
Filename          = TA140807_copy-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#556105
Solvent           = CHLOROFORM-D
Creation_time     =  7-AUG-2014 15:06:35
Revision_time     =  7-AUG-2014 16:14:37
Current_time      =  7-AUG-2014 16:15:19

Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Incomplete_copy   = TRUE
Mod_return        = 1
Scans             = 853.0
Total_scans       = 853.0

X_90_width        = 10.6[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.8[dB]
X_pulse           = 3.53333333[us]
Irr_atn_dec       = 20[dB]
Irr_atn_noe       = 20[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   = 2.8388608[s]
Temp_get          = 21.1[dC]
```

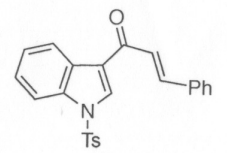


10e

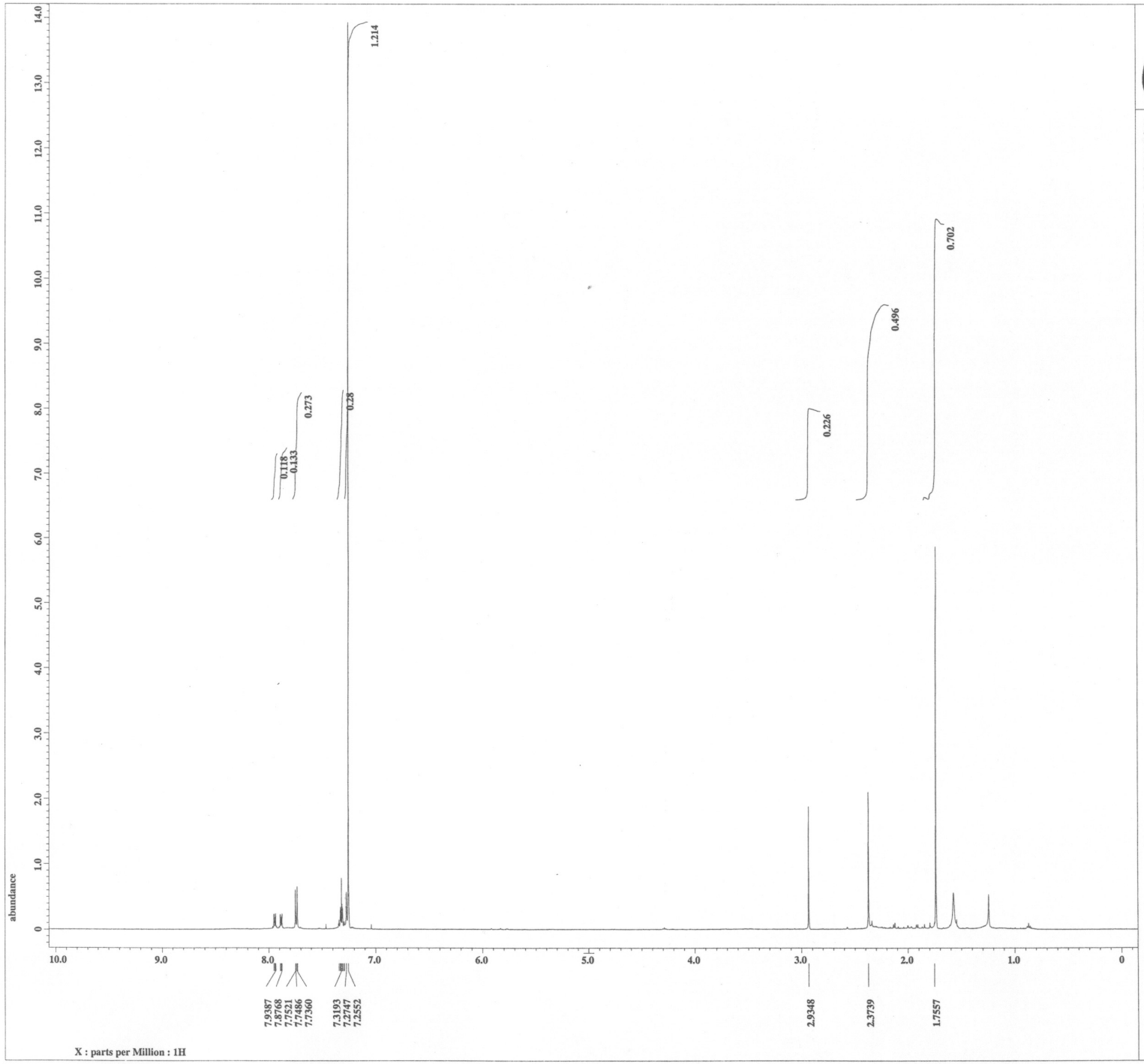


JEOL

Filename	= TA140807_copy-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#556105
Solvent	= CHLOROFORM-D
Creation_time	= 7-AUG-2014 15:06:35
Revision_time	= 7-AUG-2014 16:14:37
Current_time	= 7-AUG-2014 16:15:43
Content	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.62926421[T] (500[M
X_acq_duration	= 0.8388608[s]
X_domain	= 13C
X_freq	= 124.5010059[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.1920929[Hz]
X_sweep	= 39.0625[kHz]
Irr_domain	= 1H
Irr_freq	= 495.13191398[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Incomplete_copy	= TRUE
Mod_return	= 1
Scans	= 853.0
Total_scans	= 853.0
X_90_width	= 10.6[us]
X_acq_time	= 0.8388608[s]
X_angle	= 30[deg]
X_atn	= 9.8[dB]
X_pulse	= 3.53333333[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[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	= 2.8388608[s]
Temp_get	= 21.1[dC]

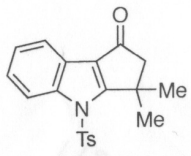


10e

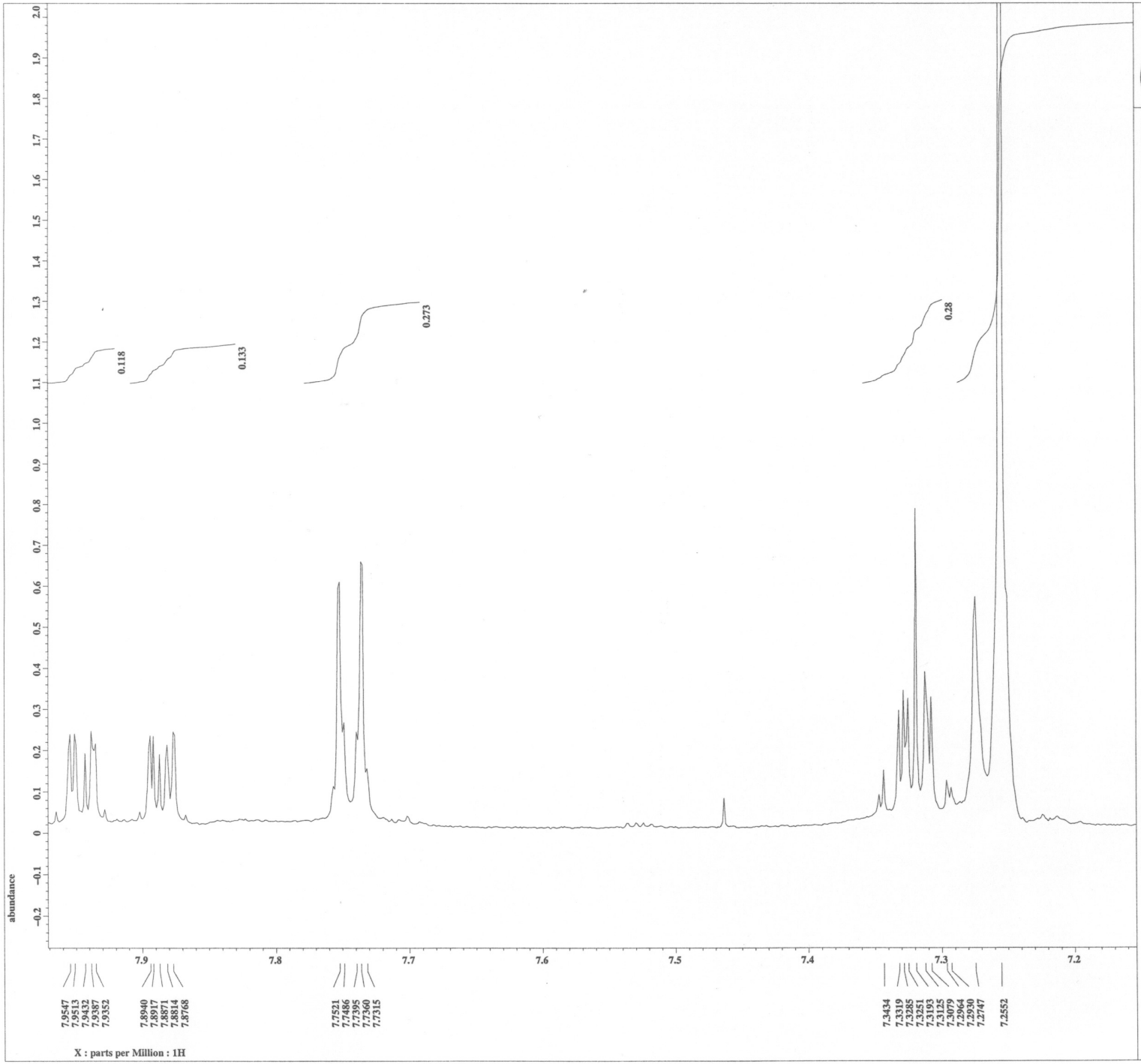


JEOL

```
Filename          = TA140709-13.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#564339
Solvent           = CHLOROFORM-D
Creation_time     =  9-JUL-2014 14:45:43
Revision_time     =  9-JUL-2014 15:48:46
Current_time      =  9-JUL-2014 15:49:02

Content           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 495.13191398[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.6[us]
X_acq_time        = 1.76422912[s]
X_angle           = 45[deg]
X_atn             = 3.6[dB]
X_pulse           = 6.3[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
Relaxation_delay  = 5[s]
Repetition_time   = 6.76422912[s]
Temp_get          = 20.1[dC]
```

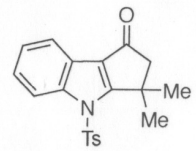


11a

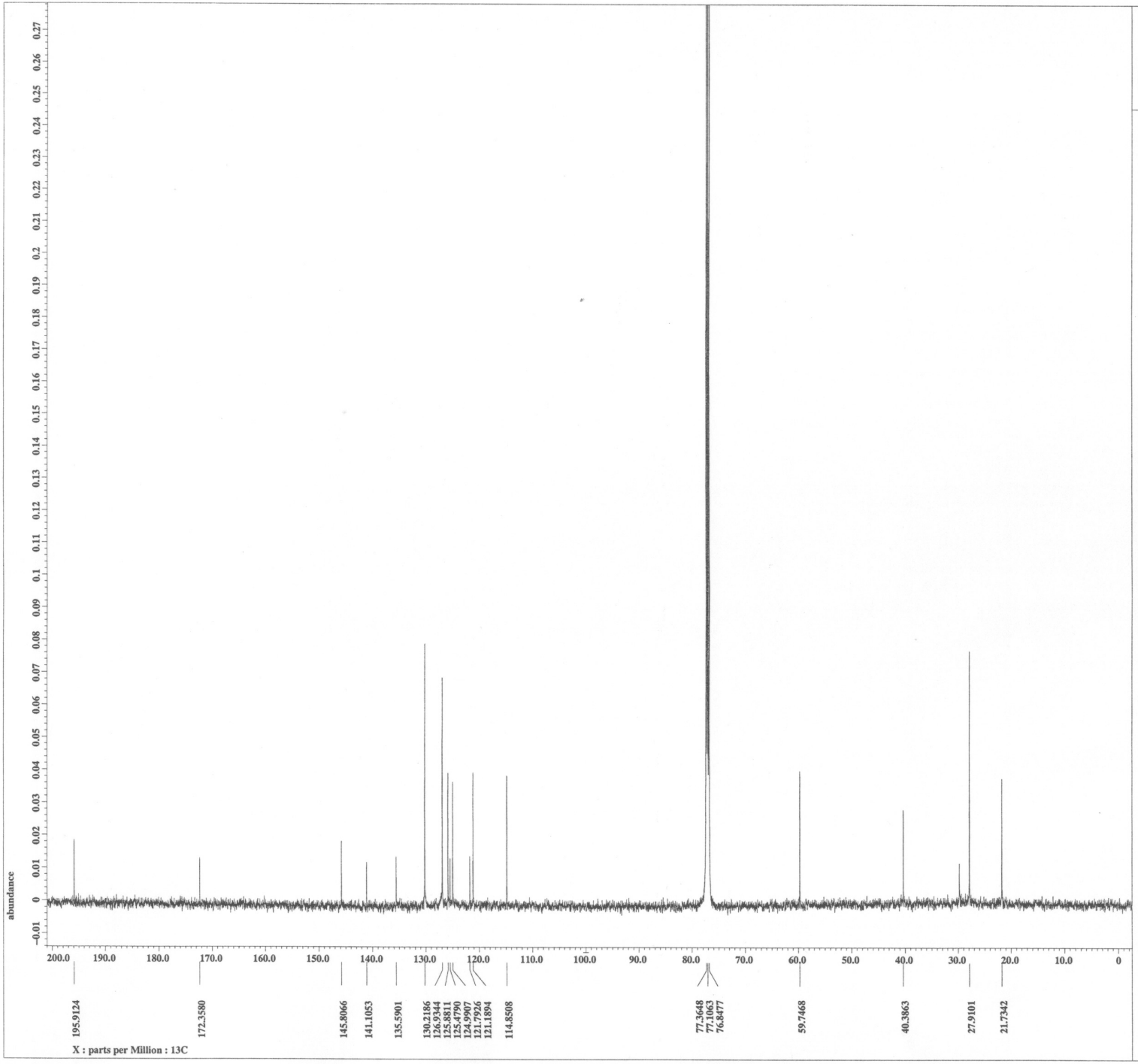


JEOL

Filename	= TA140709-13.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#564339
Solvent	= CHLOROFORM-D
Creation_time	= 9-JUL-2014 14:45:43
Revision_time	= 9-JUL-2014 15:47:47
Current_time	= 9-JUL-2014 15:47:50
Content	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.62926421[T] (500[M
X_acq_duration	= 1.76422912[s]
X_domain	= 1H
X_freq	= 495.13191398[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.5668198[Hz]
X_sweep	= 9.28677563[kHz]
Irr_domain	= 1H
Irr_freq	= 495.13191398[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 495.13191398[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 12.6[us]
X_acq_time	= 1.76422912[s]
X_angle	= 45[deg]
X_atn	= 3.6[dB]
X_pulse	= 6.3[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 44
Relaxation_delay	= 5[s]
Repetition_time	= 6.76422912[s]
Temp_get	= 20.1[dC]

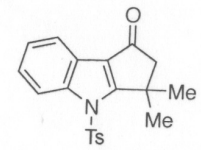


11a

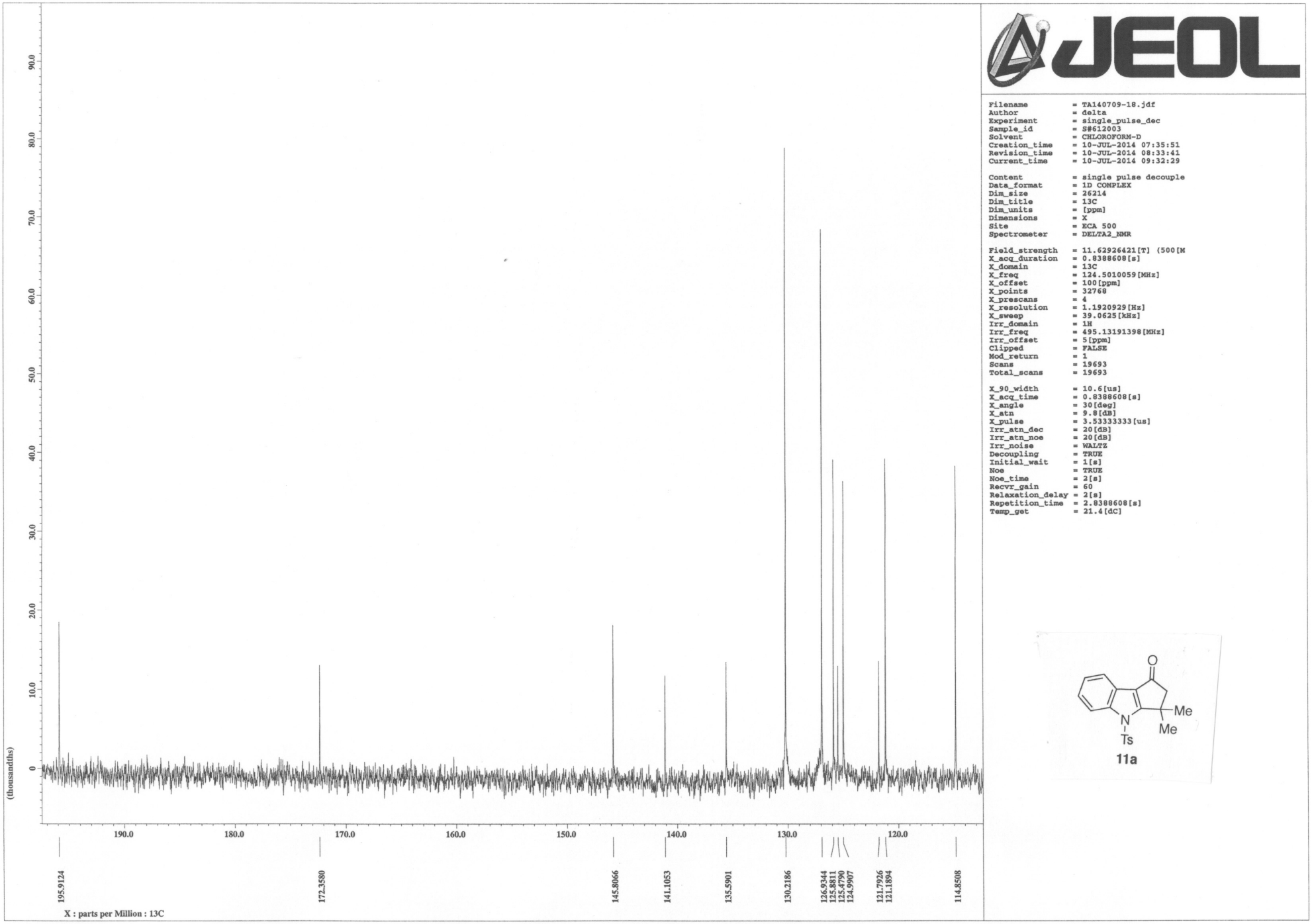


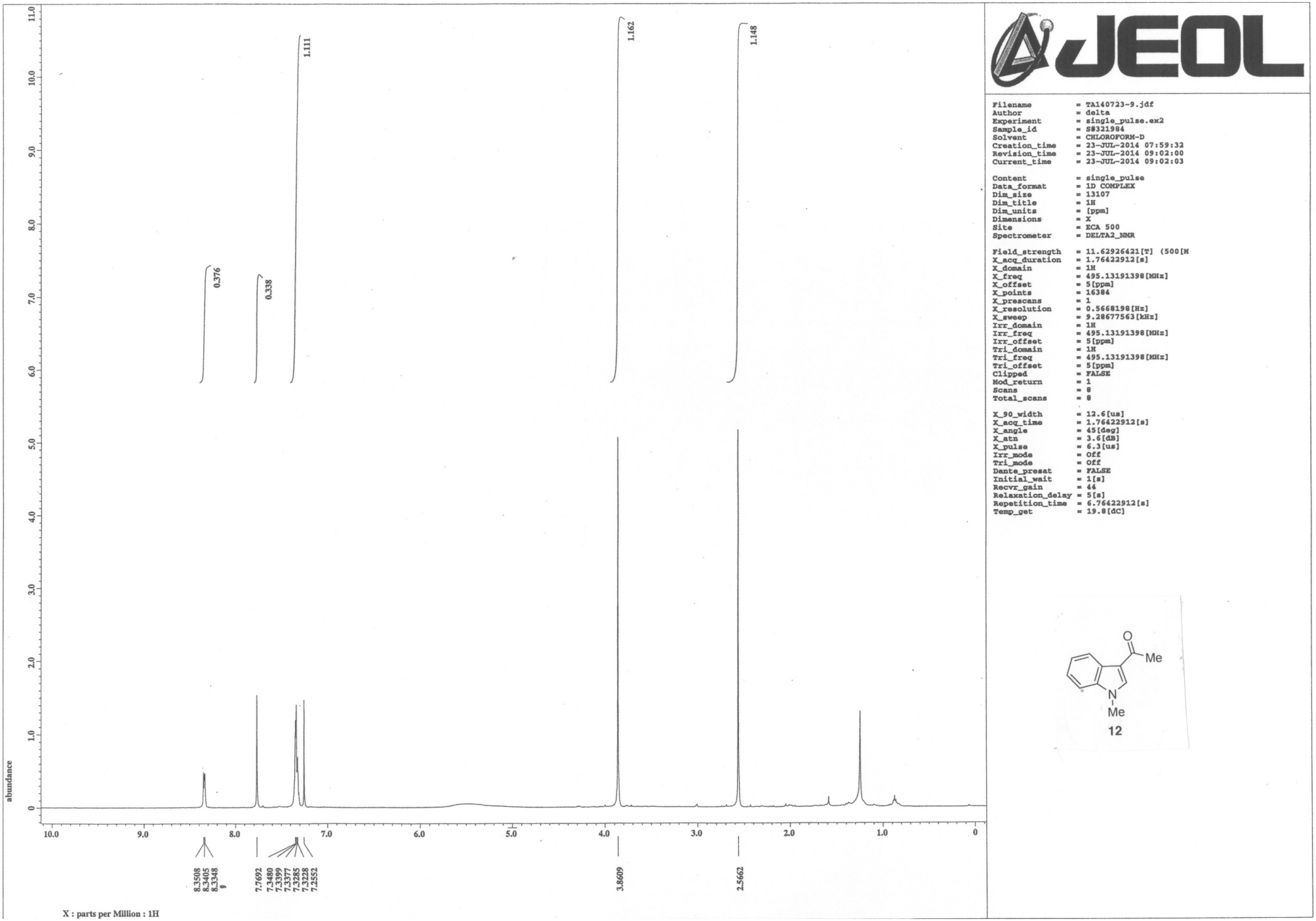
JEOL

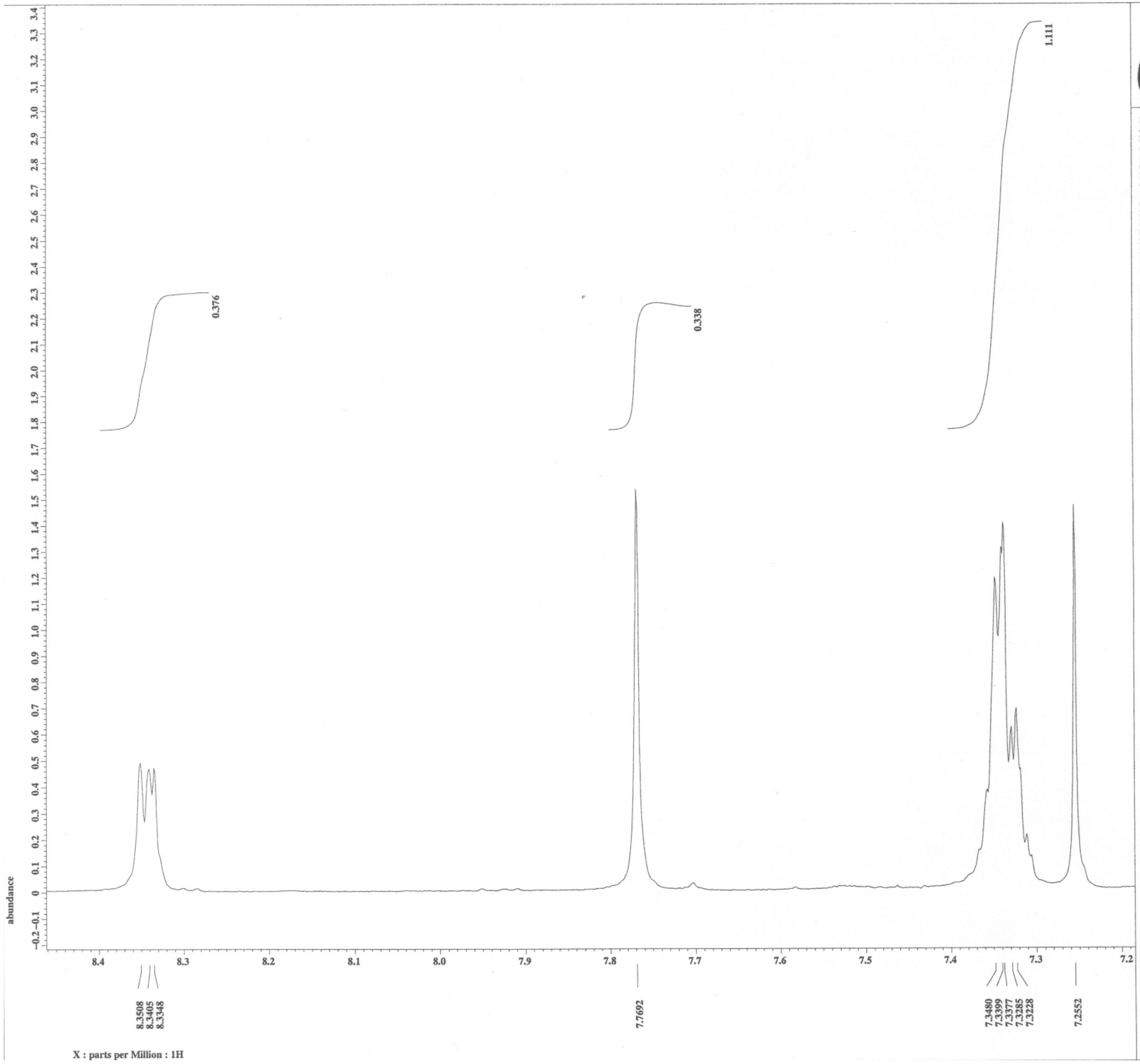
Filename	= TA140709-20.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#612003
Solvent	= CHLOROFORM-D
Creation_time	= 10-JUL-2014 07:35:51
Revision_time	= 10-JUL-2014 09:38:36
Current_time	= 10-JUL-2014 09:38:43
Content	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.62926421[T] (500[M
X_acq_duration	= 0.8388608[s]
X_domain	= 13C
X_freq	= 124.5010059[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.1920929[Hz]
X_sweep	= 39.0625[kHz]
Irr_domain	= 1H
Irr_freq	= 495.13191398[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 19693
Total_scans	= 19693
X_90_width	= 10.6[us]
X_acq_time	= 0.8388608[s]
X_angle	= 30[deg]
X_atn	= 9.8[dB]
X_pulse	= 3.53333333[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[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	= 2.8388608[s]
Temp_get	= 21.4[dC]



11a

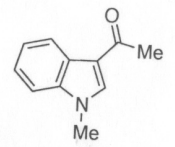

JEOL
Filename = TA140709-18.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#612003
Solvent = CHLOROFORM-D
Creation_time = 10-JUL-2014 07:35:51
Revision_time = 10-JUL-2014 08:33:41
Current_time = 10-JUL-2014 09:32:29
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR
Field_strength = 11.62926421[T] (500[M
X_acq_duration = 0.8388608[s]
X_domain = 13C
X_freq = 124.5010059[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.1920929[Hz]
X_sweep = 39.0625[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 19693
Total_scans = 19693
X_90_width = 10.6[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.8[dB]
X_pulse = 3.53333333[us]
Irr_atn_dec = 20[dB]
Irr_atn_noe = 20[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 = 2.8388608[s]
Temp_get = 21.4[dC]
(thousandths)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
195.9124
172.3580
145.8066
141.1053
135.5901
130.2186
126.9344
125.8811
125.4790
124.9907
121.7926
121.1894
114.8508
X : parts per Million : 13C
O
Me
Me
N
Ts
11a


JEOL
Filename = TA140723-9.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#321984
Solvent = CHLOROFORM-D
Creation_time = 23-JUL-2014 07:59:32
Revision_time = 23-JUL-2014 09:02:00
Current_time = 23-JUL-2014 09:02:03
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR
Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 12.6[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.6[dB]
X_pulse = 6.3[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 19.8[dC]
0.376
0.338
1.111
1.162
1.148
abundance
8.3508
8.3405
8.3348
7.7692
7.3480
7.3399
7.3377
7.3285
7.3228
7.2552
3.8609
2.5662
X : parts per Million : 1H
O
Me
N
Me
12

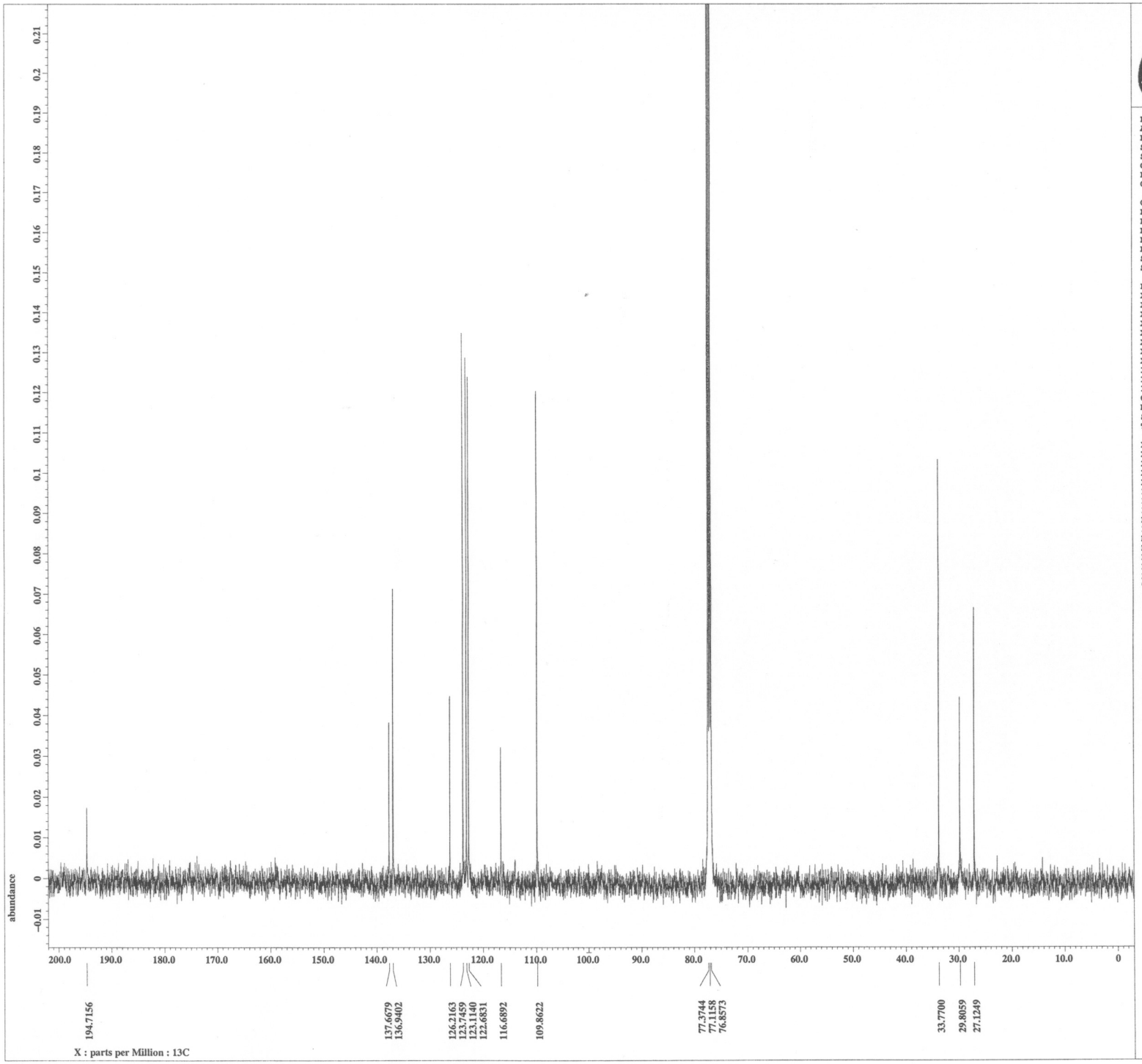




```
Filename          = TA140723-9.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#321984
Solvent           = CHLOROFORM-D
Creation_time     = 23-JUL-2014 07:59:32
Revision_time     = 23-JUL-2014 09:02:39
Current_time      = 23-JUL-2014 09:02:41

Content           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 495.13191398[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.6[us]
X_acq_time        = 1.76422912[s]
X_angle           = 45[deg]
X_atn             = 3.6[dB]
X_pulse           = 6.3[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
Relaxation_delay  = 5[s]
Repetition_time   = 6.76422912[s]
Temp_get          = 19.8[dC]
```

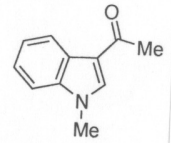


12

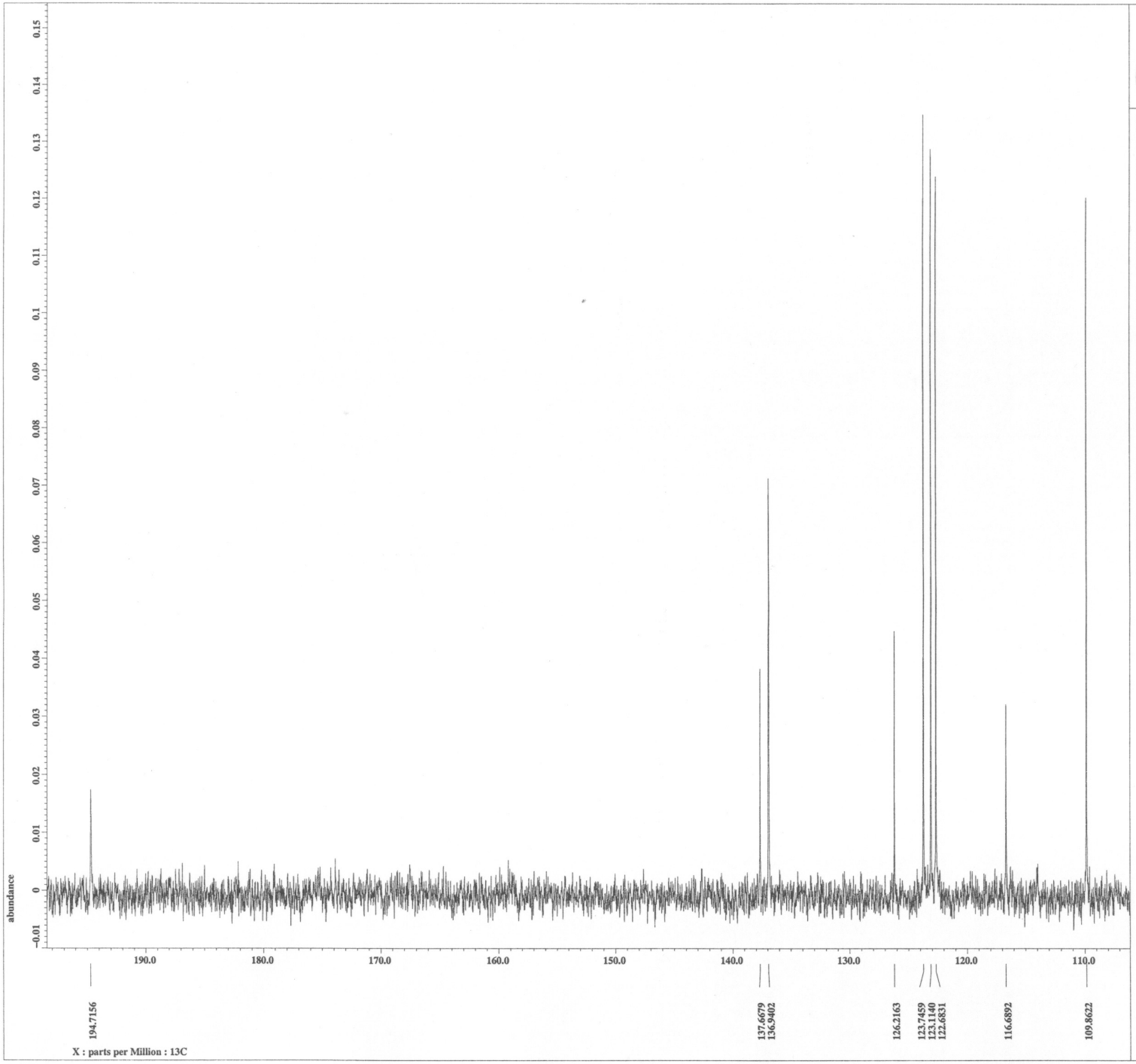


JEOL

```
Filename          = TA140723-12.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#324976
Solvent           = CHLOROFORM-D
Creation_time     = 23-JUL-2014 11:24:01
Revision_time     = 23-JUL-2014 12:24:11
Current_time      = 23-JUL-2014 12:25:13

Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 4238
Total_scans       = 4238

X_90_width        = 10.6[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.8[dB]
X_pulse           = 3.53333333[us]
Irr_atn_dec       = 20[dB]
Irr_atn_noe       = 20[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   = 2.8388608[s]
Temp_get          = 20.4[dC]
```



12



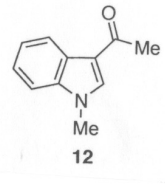
JEOL

Filename = TA140723-12.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#324976
Solvent = CHLOROFORM-D
Creation_time = 23-JUL-2014 11:24:01
Revision_time = 23-JUL-2014 12:24:11
Current_time = 23-JUL-2014 12:24:23

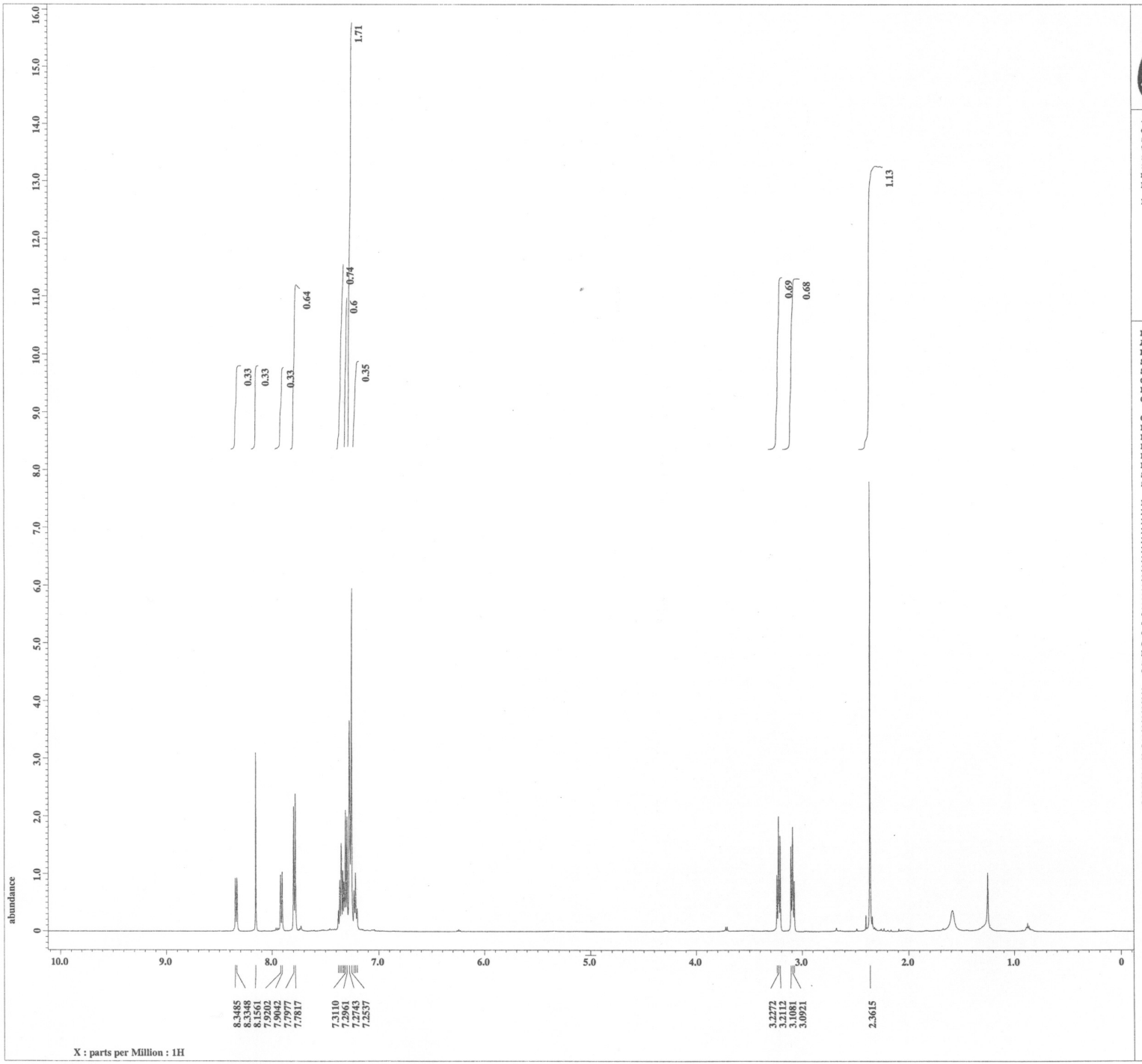
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 0.8388608[s]
X_domain = 13C
X_freq = 124.5010059[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.1920929[Hz]
X_sweep = 39.0625[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 4238
Total_scans = 4238

X_90_width = 10.6[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.8[dB]
X_pulse = 3.53333333[us]
Irr_atn_dec = 20[dB]
Irr_atn_noe = 20[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 = 2.8388608[s]
Temp_get = 20.4[dC]



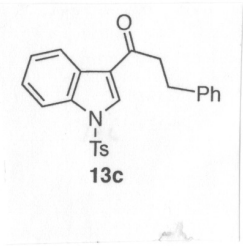
12



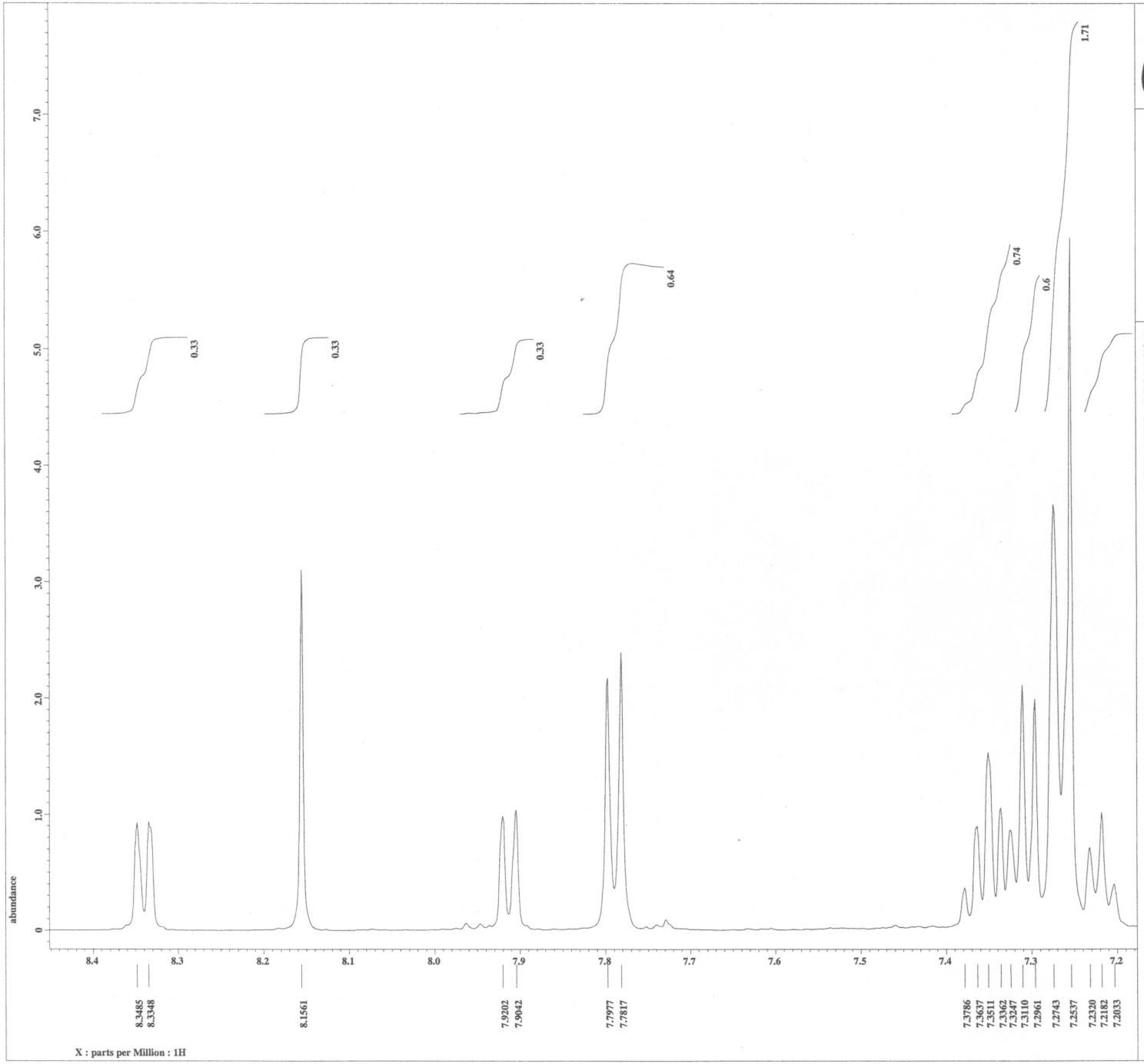
JEOL

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

Derived from: TA140815-2.jdf
```

```
Filename          = TA140815-5.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#449926
Solvent           = CHLOROFORM-D
Creation_time     = 15-AUG-2014 12:34:17
Revision_time     = 15-AUG-2014 12:36:07
Current_time      = 15-AUG-2014 12:36:08

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 13[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 3.4[dB]
X_pulse           = 6.5[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 48
Relaxation_delay  = 5[s]
Repetition_time   = 6.74587904[s]
Temp_get          = 22.1[dC]
```



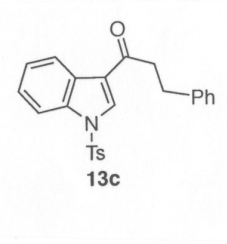
13c



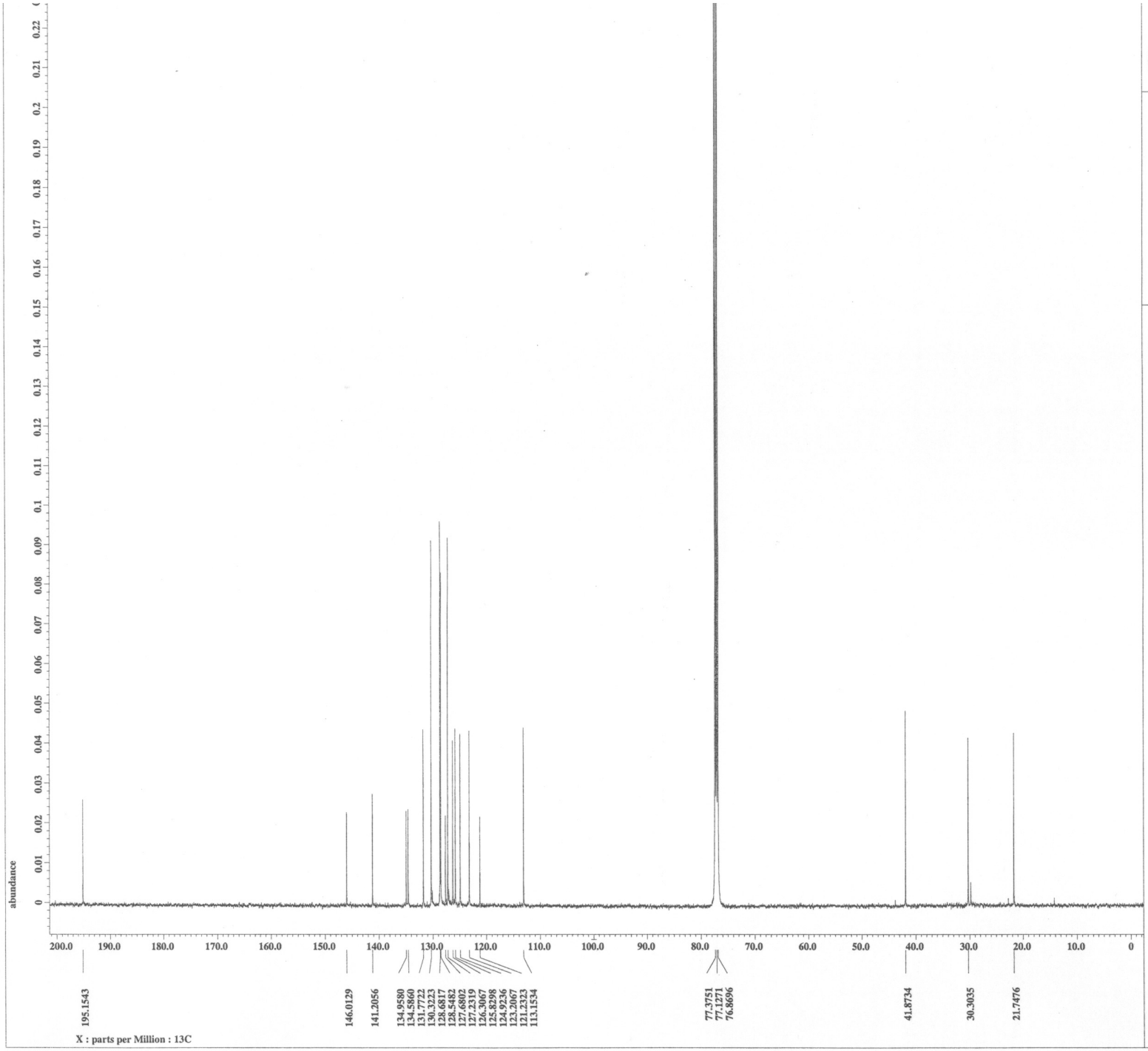


```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA140815-2.jdf
```

Filename	= TA140815-5.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#449926
Solvent	= CHLOROFORM-D
Creation_time	= 15-AUG-2014 12:34:17
Revision_time	= 15-AUG-2014 12:34:12
Current_time	= 15-AUG-2014 12:34:30
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 13[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 3.4[dB]
X_pulse	= 6.5[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 48
Relaxation_delay	= 5[s]
Repetition_time	= 6.74587904[s]
Temp_get	= 22.1[dC]



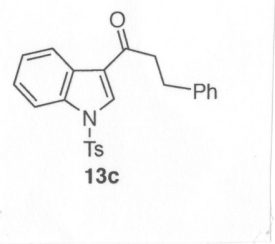
13c



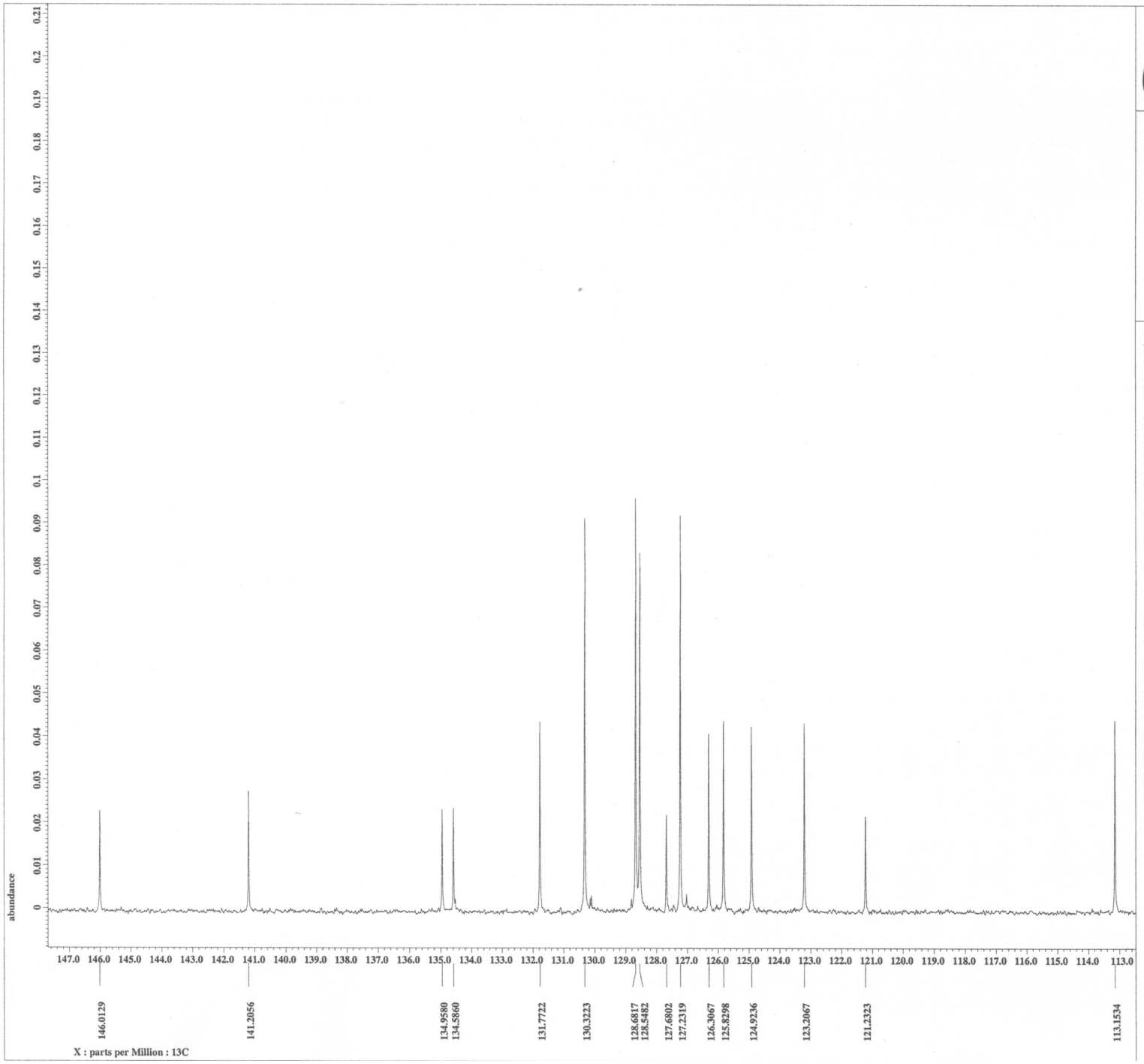


```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA140815-9.jdf
```

```
Filename            = TA140815-11.jdf
Author              = delta
Experiment          = single_pulse_dec
Sample_id           = S#524690
Solvent             = CHLOROFORM-D
Creation_time       = 18-AUG-2014 07:15:53
Revision_time       = 18-AUG-2014 07:14:43
Current_time        = 18-AUG-2014 07:17:09

Comment             = single pulse decouple
Data_format         = 1D COMPLEX
Dim_size            = 26214
Dim_title           = 13C
Dim_units           = [ppm]
Dimensions          = X
Site                = ECA500
Spectrometer        = DELTA2_NMR

Field_strength      = 11.7473579[T] (500[MH
X_acq_duration      = 0.83361792[s]
X_domain            = 13C
X_freq              = 125.76529768[MHz]
X_offset            = 100[ppm]
X_points            = 32768
X_prescans          = 4
X_resolution        = 1.19959034[Hz]
X_sweep             = 39.3081761[kHz]
Irr_domain          = 1H
Irr_freq            = 500.15991521[MHz]
Irr_offset          = 5.0[ppm]
Clipped             = TRUE
Mod_return          = 1
Scans               = 82115.0
Total_scans         = 82115.0

X_90_width          = 14[us]
X_acq_time          = 0.83361792[s]
X_angle             = 30[deg]
X_atn               = 5.5[dB]
X_pulse             = 4.66666667[us]
Irr_atn_dec         = 20.39689[dB]
Irr_atn_noe         = 20.39689[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     = 2.83361792[s]
Temp_get            = 22.9[dC]
```



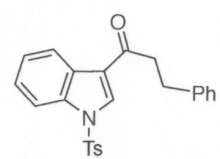
13c



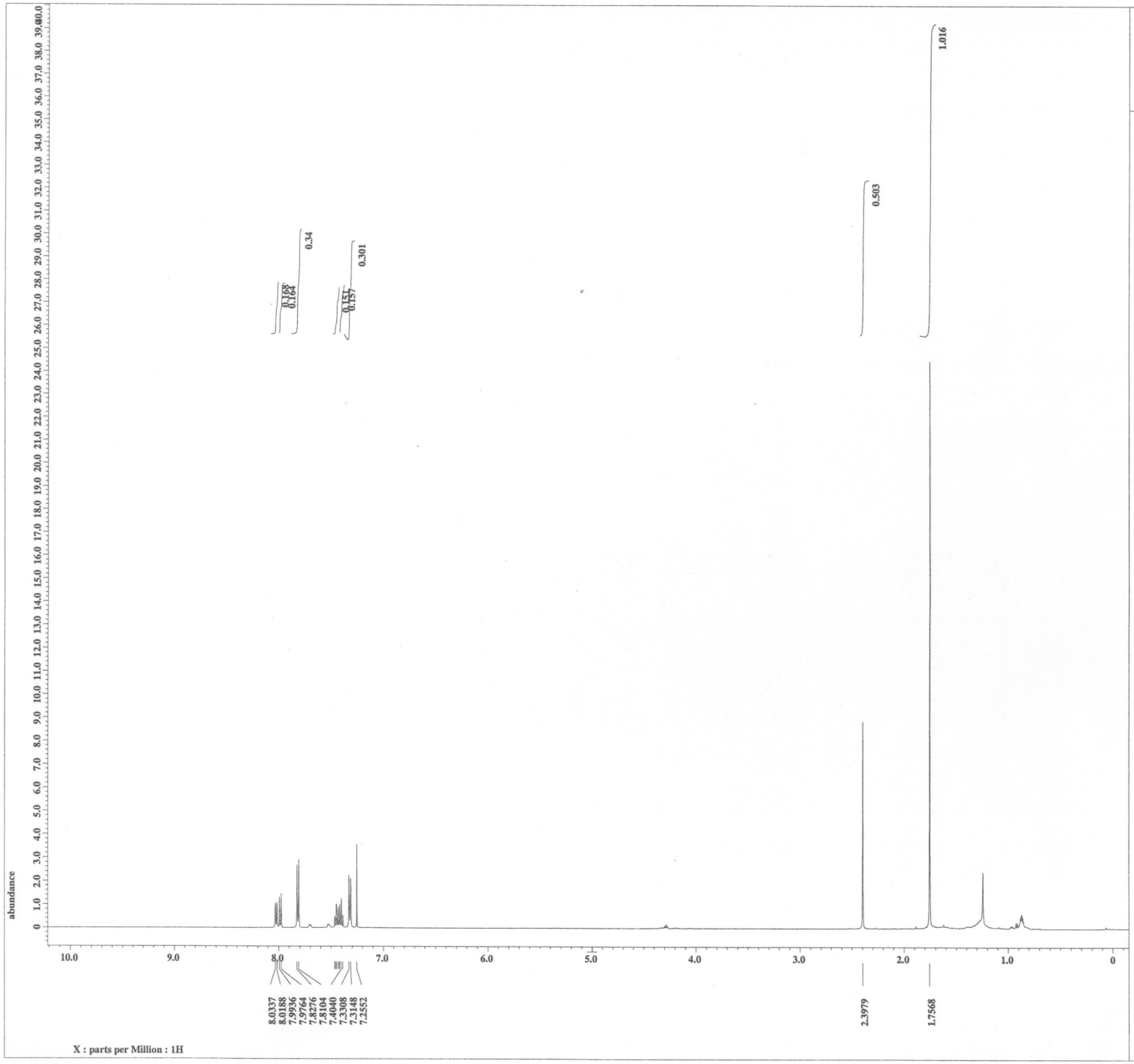
JEOL

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: TA140815-9.jdf.
```

```
Filename          = TA140815-11.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#524690
Solvent           = CHLOROFORM-D
Creation_time     = 18-AUG-2014 07:15:53
Revision_time     = 18-AUG-2014 07:14:43
Current_time      = 18-AUG-2014 07:14:56

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 82115.0
Total_scans       = 82115.0

X_90_width        = 14[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 5.5[dB]
X_pulse           = 4.66666667[us]
Irr_atn_dec       = 20.39689[dB]
Irr_atn_noe       = 20.39689[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   = 2.83361792[s]
Temp_get          = 22.9[dC]
```



13c



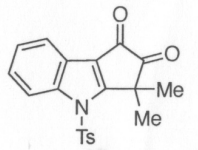


Filename = TA140725-5.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#534867
Solvent = CHLOROFORM-D
Creation_time = 25-JUL-2014 13:53:45
Revision_time = 25-JUL-2014 14:57:54
Current_time = 25-JUL-2014 14:57:58

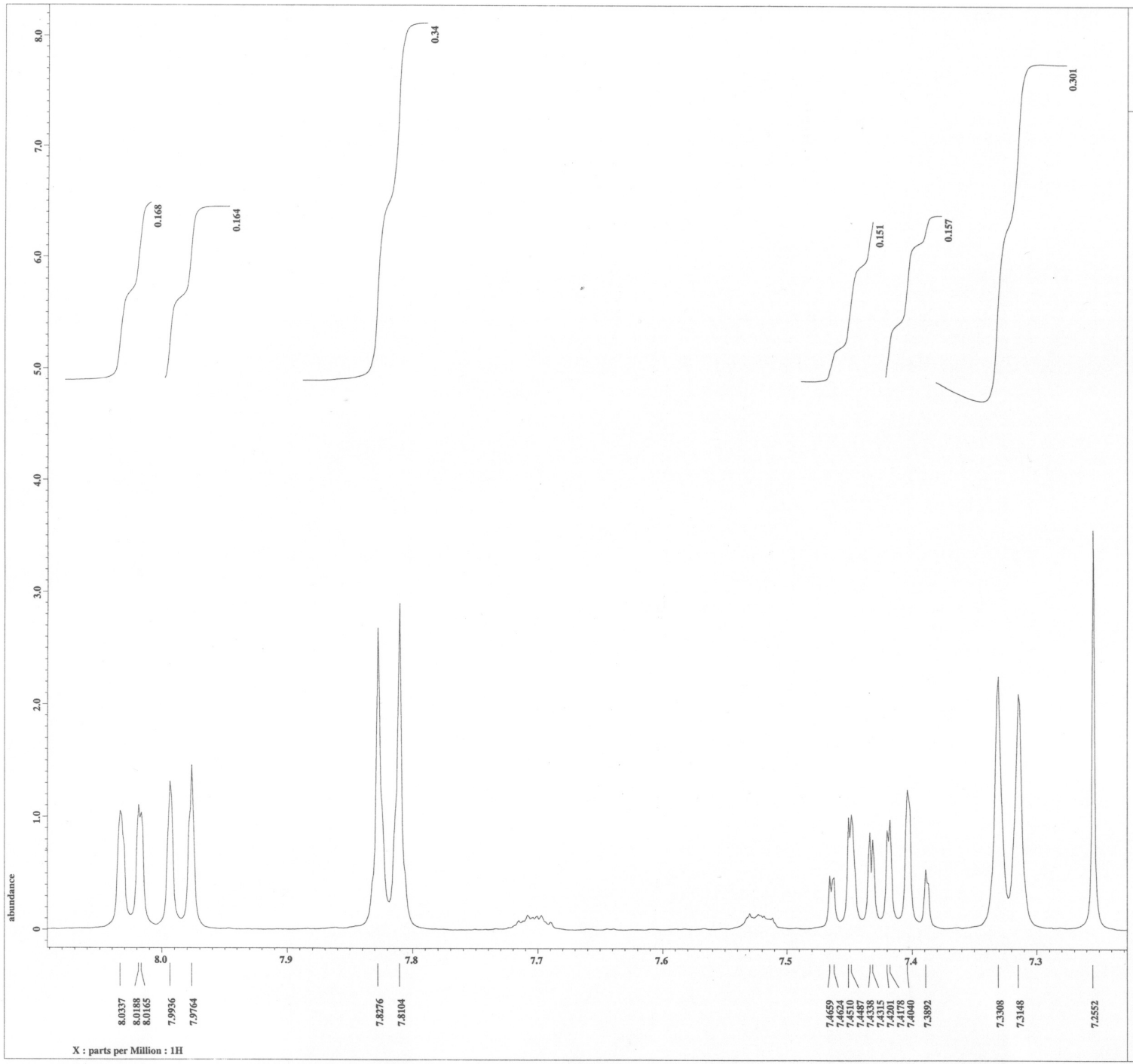
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 1.76422912[s]
X_domain = 1H
X_freq = 495.13191398[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.5668198[Hz]
X_sweep = 9.28677563[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 495.13191398[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 12.6[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.6[dB]
X_pulse = 6.3[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 20.5[dC]

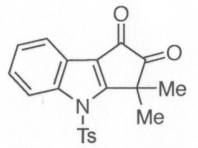


18

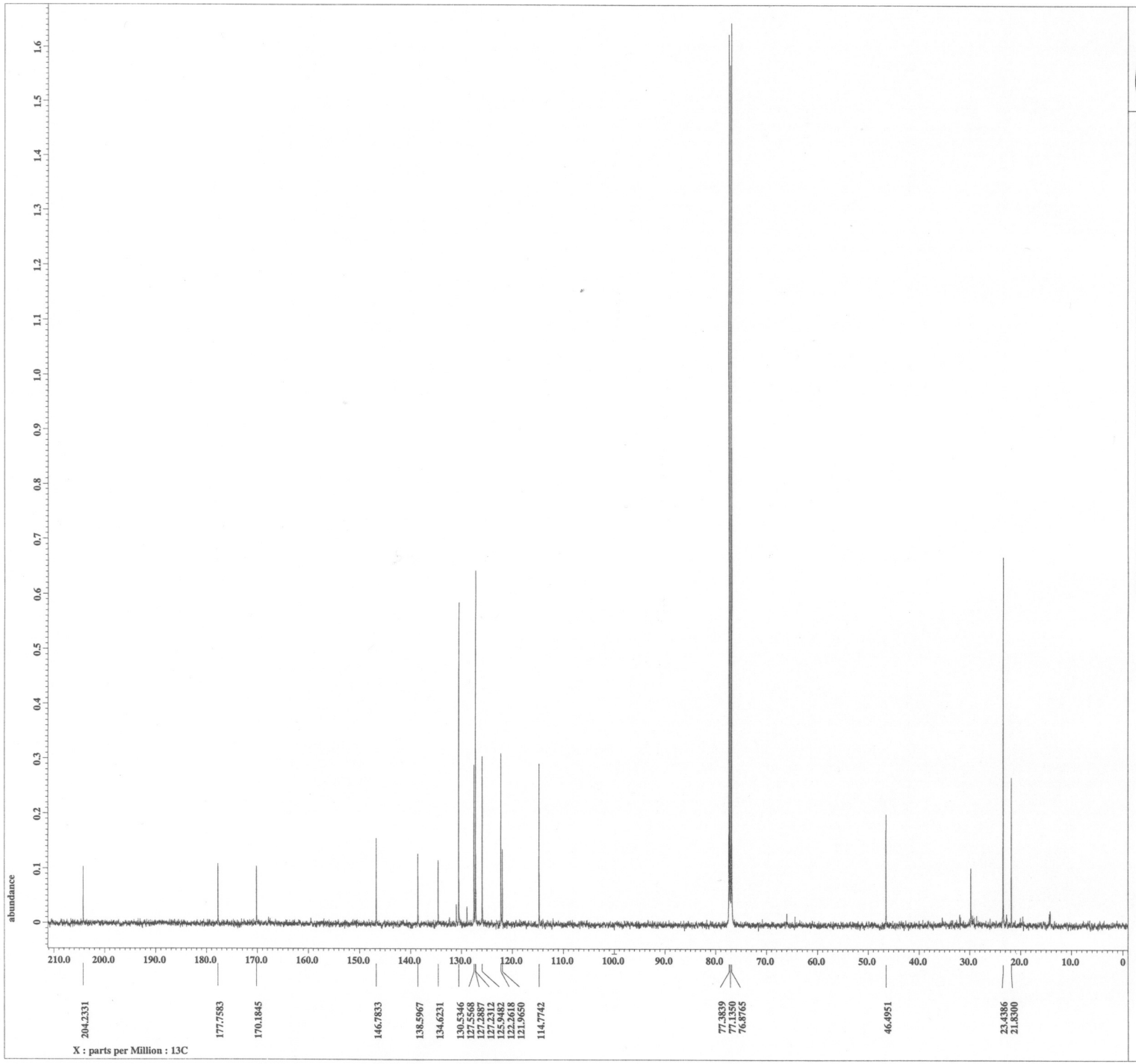


JEOL

```
Filename          = TA140725-5.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#534867
Solvent           = CHLOROFORM-D
Creation_time     = 25-JUL-2014 13:53:45
Revision_time     = 25-JUL-2014 14:54:42
Current_time      = 25-JUL-2014 14:54:46

Content           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 1.76422912[s]
X_domain          = 1H
X_freq            = 495.13191398[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.5668198[Hz]
X_sweep           = 9.28677563[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 495.13191398[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.6[us]
X_acq_time        = 1.76422912[s]
X_angle           = 45[deg]
X_atn             = 3.6[dB]
X_pulse           = 6.3[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 6.76422912[s]
Temp_get          = 20.5[dC]
```



18

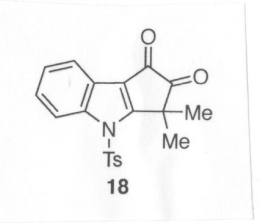


Filename = TA140725-8.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#295648
Solvent = CHLOROFORM-D
Creation_time = 28-JUL-2014 08:14:25
Revision_time = 28-JUL-2014 09:14:46
Current_time = 28-JUL-2014 09:17:02

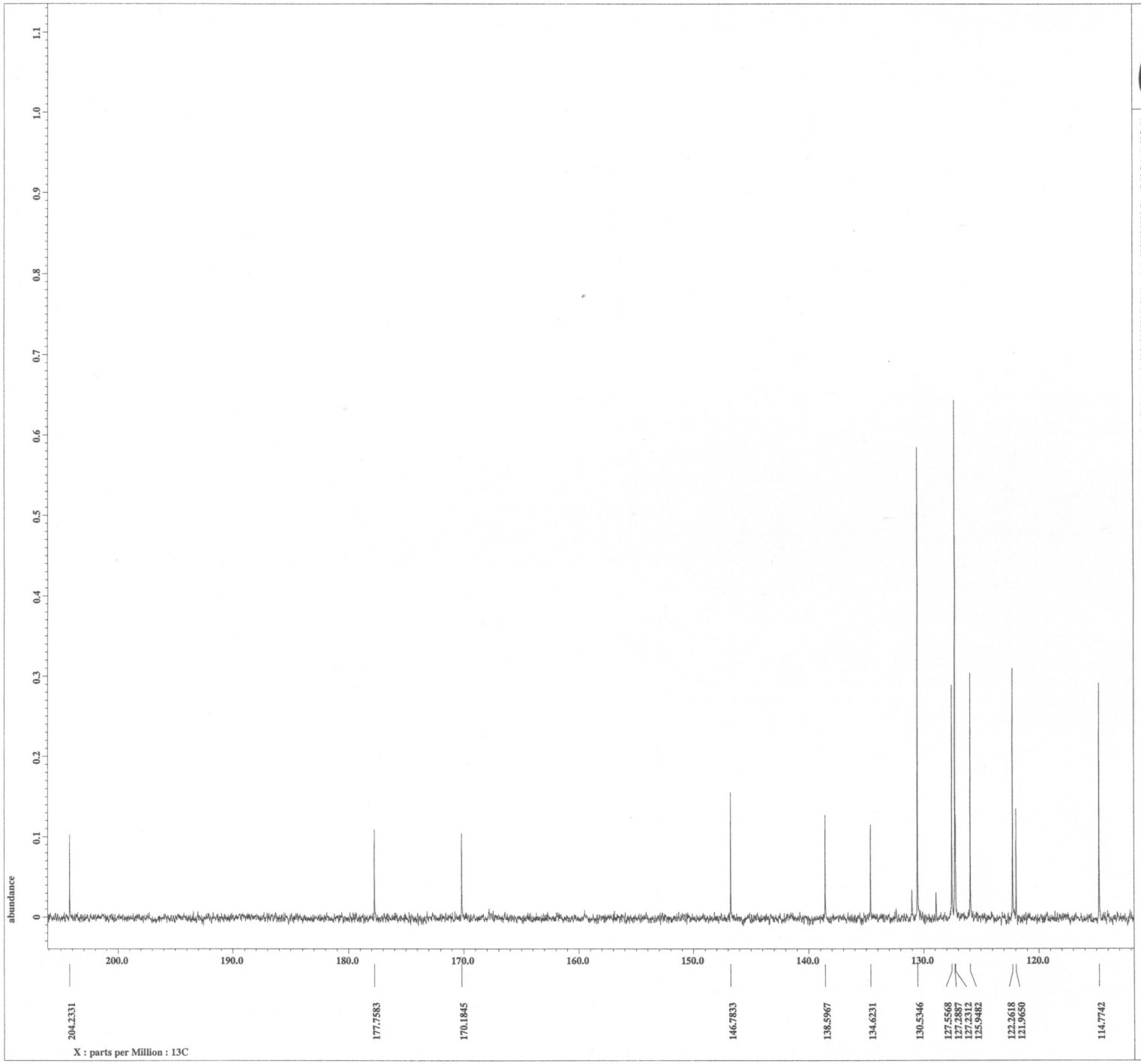
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

Field_strength = 11.62926421[T] (500[M
X_acq_duration = 0.8388608[s]
X_domain = 13C
X_freq = 124.5010059[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.1920929[Hz]
X_sweep = 39.0625[kHz]
Irr_domain = 1H
Irr_freq = 495.13191398[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1274
Total_scans = 1274

X_90_width = 10.6[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.8[dB]
X_pulse = 3.53333333[us]
Irr_atn_dec = 20[dB]
Irr_atn_noe = 20[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 = 2.8388608[s]
Temp_get = 21.3[dC]

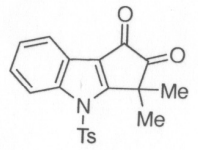


18



JEOL

```
Filename          = TA140725-8.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#295648
Solvent           = CHLOROFORM-D
Creation_time     = 28-JUL-2014 08:14:25
Revision_time     = 28-JUL-2014 09:14:46
Current_time      = 28-JUL-2014 09:16:06

Content           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.62926421[T] (500[M
X_acq_duration    = 0.8388608[s]
X_domain          = 13C
X_freq            = 124.5010059[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.1920929[Hz]
X_sweep           = 39.0625[kHz]
Irr_domain        = 1H
Irr_freq          = 495.13191398[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1274
Total_scans       = 1274

X_90_width        = 10.6[us]
X_acq_time        = 0.8388608[s]
X_angle           = 30[deg]
X_atn             = 9.8[dB]
X_pulse           = 3.53333333[us]
Irr_atn_dec       = 20[dB]
Irr_atn_noe       = 20[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   = 2.8388608[s]
Temp_get          = 21.3[dC]
```



18