

Biomimetic Synthesis of Iheyamine A from Spirocyclic Oxindoles

Takumi Abe*, Syuhei Satake, and Koji Yamada*

Faculty of Pharmaceutical Sciences, Health Sciences University of Hokkaido,

Ishikari-tobetsu, Hokkaido 0610293, Japan

E-mail: abe-t@hoku-iryu-u.ac.jp

E-mail: kyamada@hoku-iryu-u.ac.jp

SUPPORTING INFORMATION

Contents

| | |
|--|-------|
| 1. Copies of ^1H , ^{13}C NMR spectra----- | S2-23 |
|--|-------|

```

Filename      = yama-16-11-17-13.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = S#625226
Solvent      = CHLOROFORM-D
Creation_time = 17-NOV-2016 17:15:58
Revision_time = 31-JUL-2018 16:21:20
Current_time = 31-JUL-2018 16:21:44
  
```

```

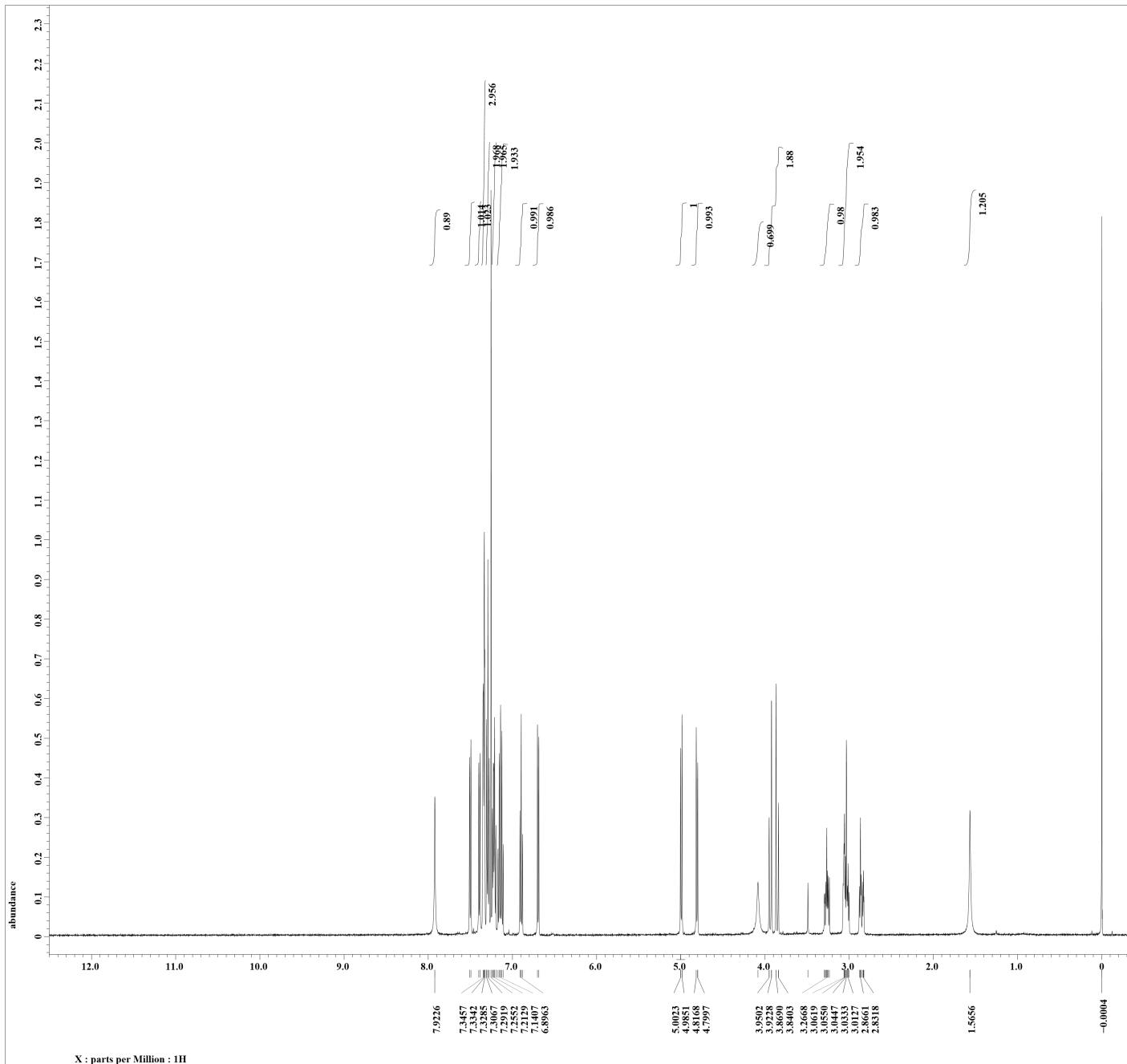
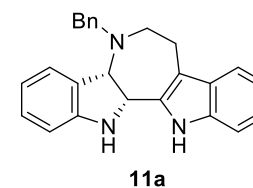
Content       = single_pulse
Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = DELTA2_NMR
  
```

```

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    = 12.7[us]
X_acq_time     = 1.76422912[s]
X_angle        = 45[deg]
X_atn          = 3.6[dB]
X_pulse        = 6.35[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recv_gain      = 44
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get       = 20.5[dc]
  
```



```

Filename      = yama-16-11-17-11.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#626003
Solvent      = CHLOROFORM-D
Creation_time = 18-NOV-2016 07:24:32
Revision_time = 31-JUL-2018 16:17:00
Current_time  = 31-JUL-2018 16:18:05
  
```

```

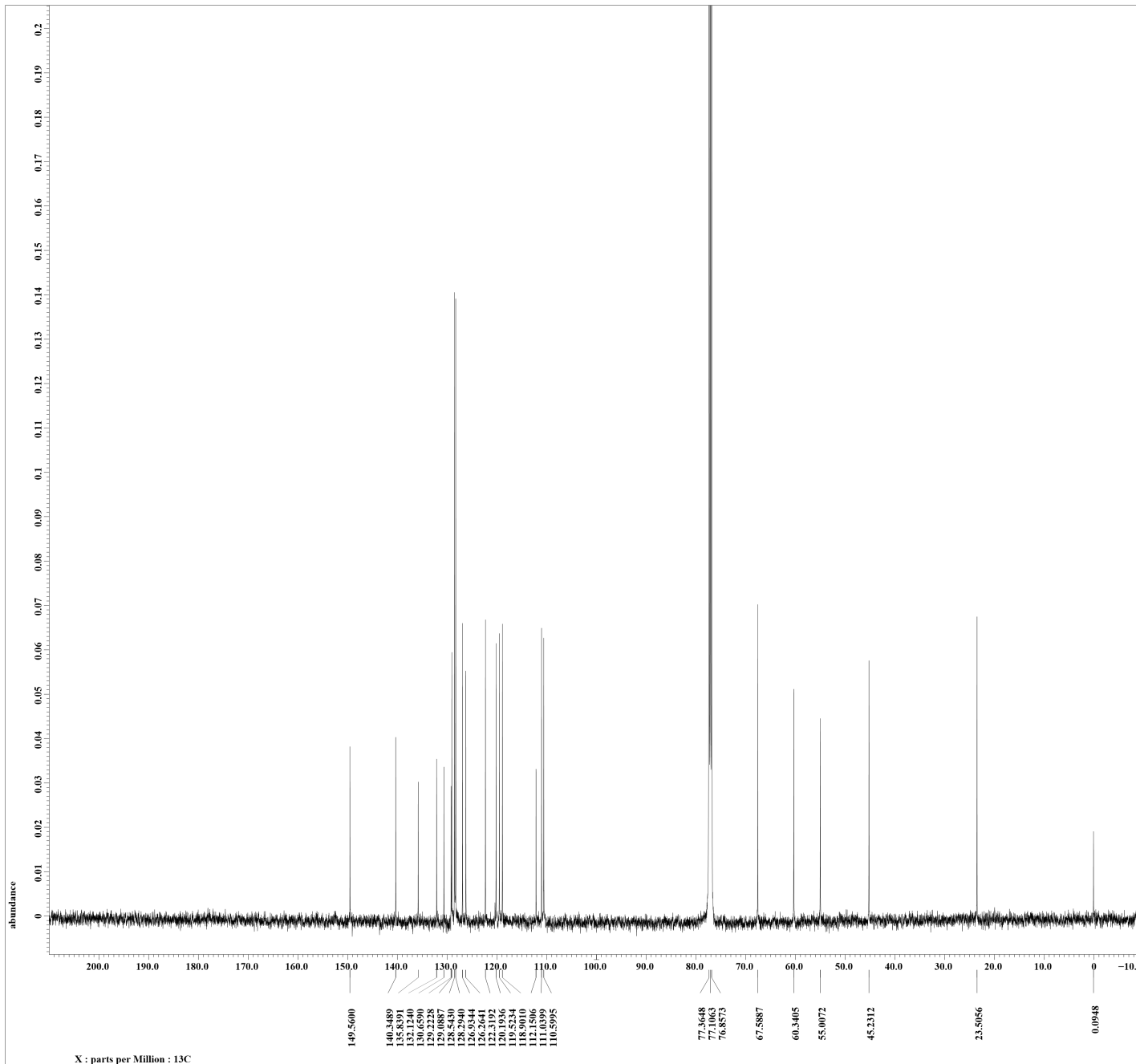
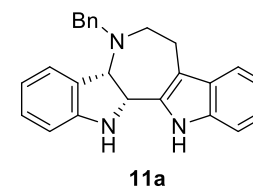
Content      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = DELTA2_NMR
  
```

```

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]
X_domain       = 1H
Irr_freq       = 495.13191398[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 17895
Total_scans    = 17895
  
```

```

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    = 20.8[dB]
Irr_atn_noe    = 20.8[dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 2[s]
RecVc_gain     = 60
Relaxation_delay = 2[s]
Repetition_time = 2.8388608[s]
Temp_get       = 22.4[dc]
  
```

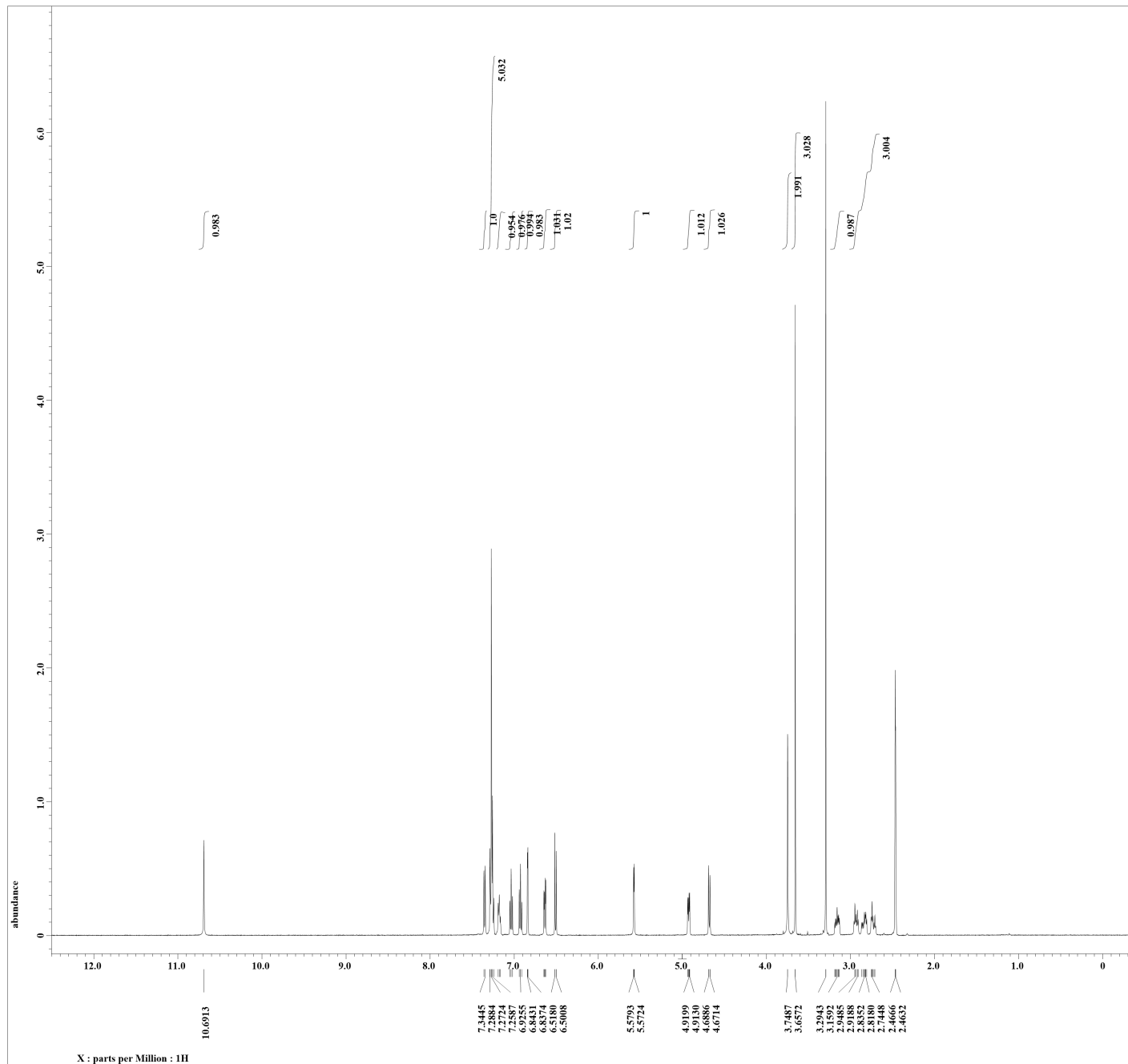
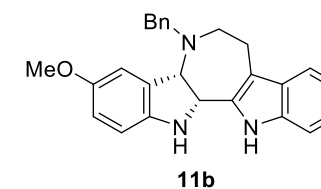


Filename = yama-18-07-31-2-4.jdf
 Author = delta
 Experiment = single pulse.ex2
 Sample_id = S#671161
 Solvent = DMSO-d6
 Creation_time = 31-JUL-2018 17:42:35
 Revision_time = 31-JUL-2018 18:49:42
 Current_time = 31-JUL-2018 18:52:15

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 = 12.63[us]
 X_acq_time = 1.76422912[s]
 X_angle = 45[deg]
 X_atn = 3.3[dB]
 X_pulse = 6.315[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvc_gain = 44
 Relaxation_delay = 5[s]
 Repetition_time = 6.76422912[s]
 Temp_get = 23.1[dc]



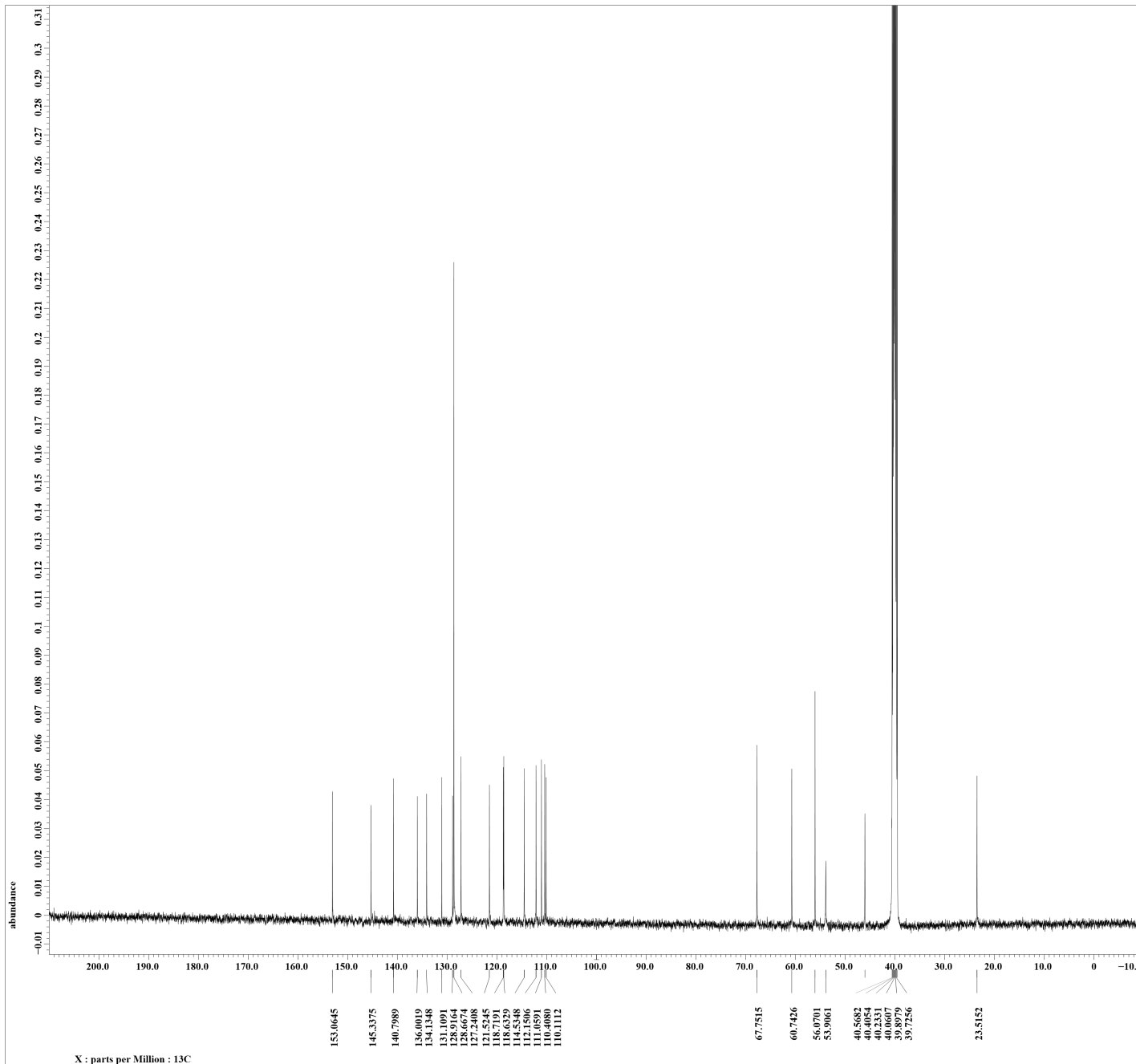
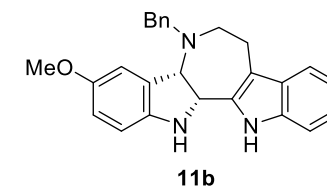


Filename = yama-18-07-31-2-6.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#673769
Solvent = DMSC-D6
Creation_time = 1-AUG-2018 07:50:15
Revision_time = 1-AUG-2018 08:50:41
Current_time = 1-AUG-2018 08:51:59

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 = TRUE
Mod_return = 1
Scans = 17841
Total_scans = 17841

X_90_width = 10.83[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.5[db]
X_pulse = 3.61[us]
Irr_atn_dec = 20.548[db]
Irr_atn_noe = 20.548[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
RecVc_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.8388608[s]
Temp_get = 24.9[dc]



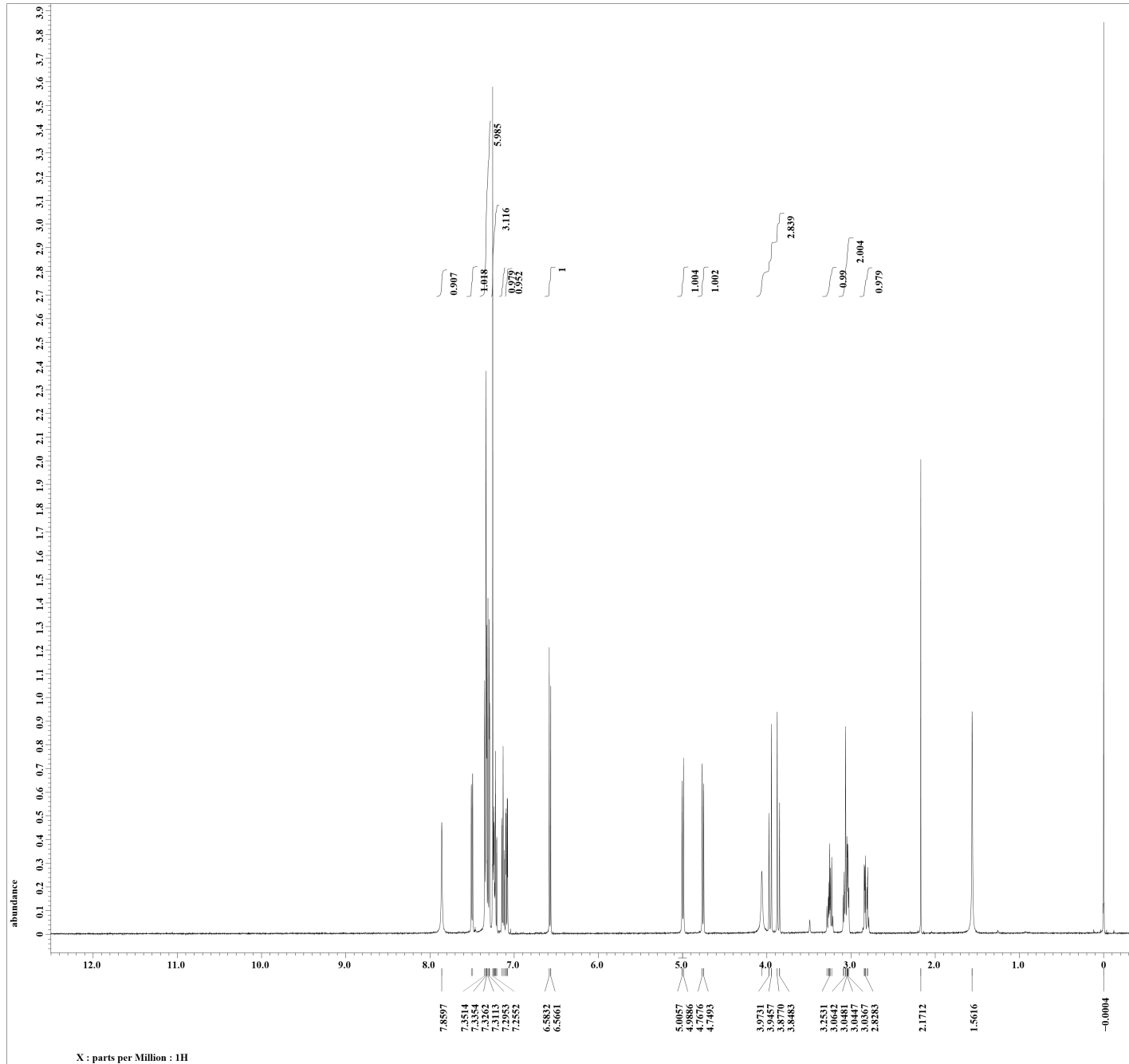
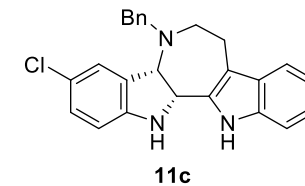


Filename = SS-18-07-06-01-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#495808
Solvent = CHLOROFORM-D
Creation_time = 6-JUL-2018 13:01:07
Revision_time = 6-JUL-2018 18:58:50
Current_Time = 6-JUL-2018 19:01:46

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]
F1_domain = 1H
F1_freq = 495.13191398 [MHz]
F1_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 = 12.63 [us]
X_acq_time = 1.76422912 [s]
X_angle = 45 [deg]
X_atn = 3.3 [dB]
X_pulse = 6.315 [us]
F1_mode = Off
Tri_mode = Off
DANTE_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 46
Relaxation_delay = 5 [s]
Repetition_time = 6.76422912 [s]
Temp_get = 23.4 [dC]



X : parts per Million : 1H

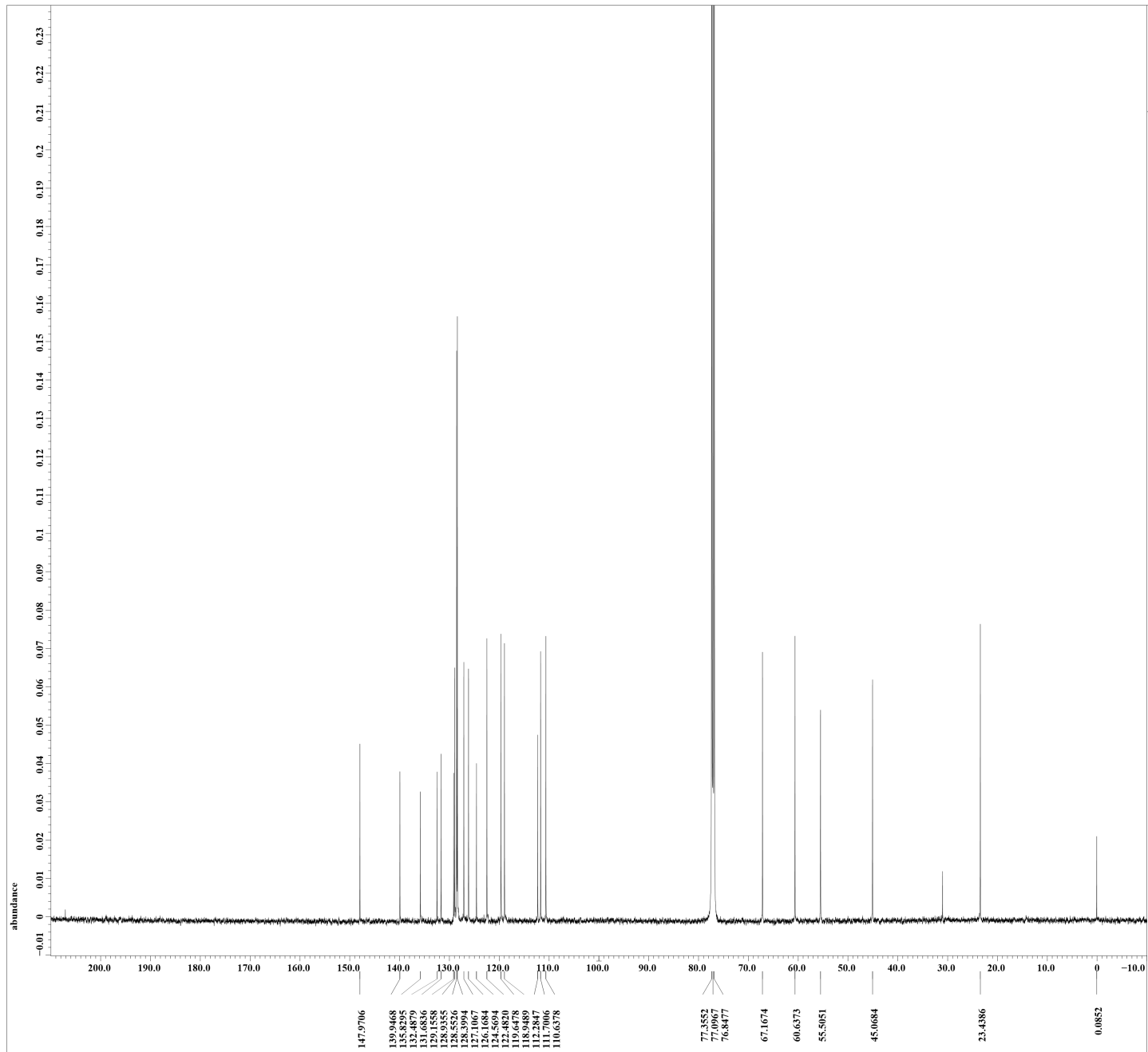
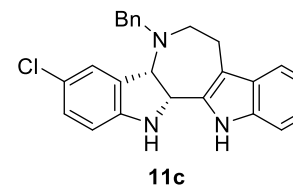


Filename = SS-18-07-06-01-7.jdf
Author = delta
Experiment = single pulse dec
Sample_id = S#682593
Solvent = CHLOROFORM-D
Creation_time = 9-JUL-2018 06:59:28
Revision_time = 9-JUL-2018 07:49:26
Current_Time = 9-JUL-2018 07:50:05

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 = TRUE
Mod_return = 1
Scans = 77099
Total_scans = 77099

X_90_width = 10.83[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.5[dB]
X_pulse = 3.61[us]
Irr_atn_dec = 20.548[dB]
Irr_atn_noe = 20.548[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 = 24.6[dc]



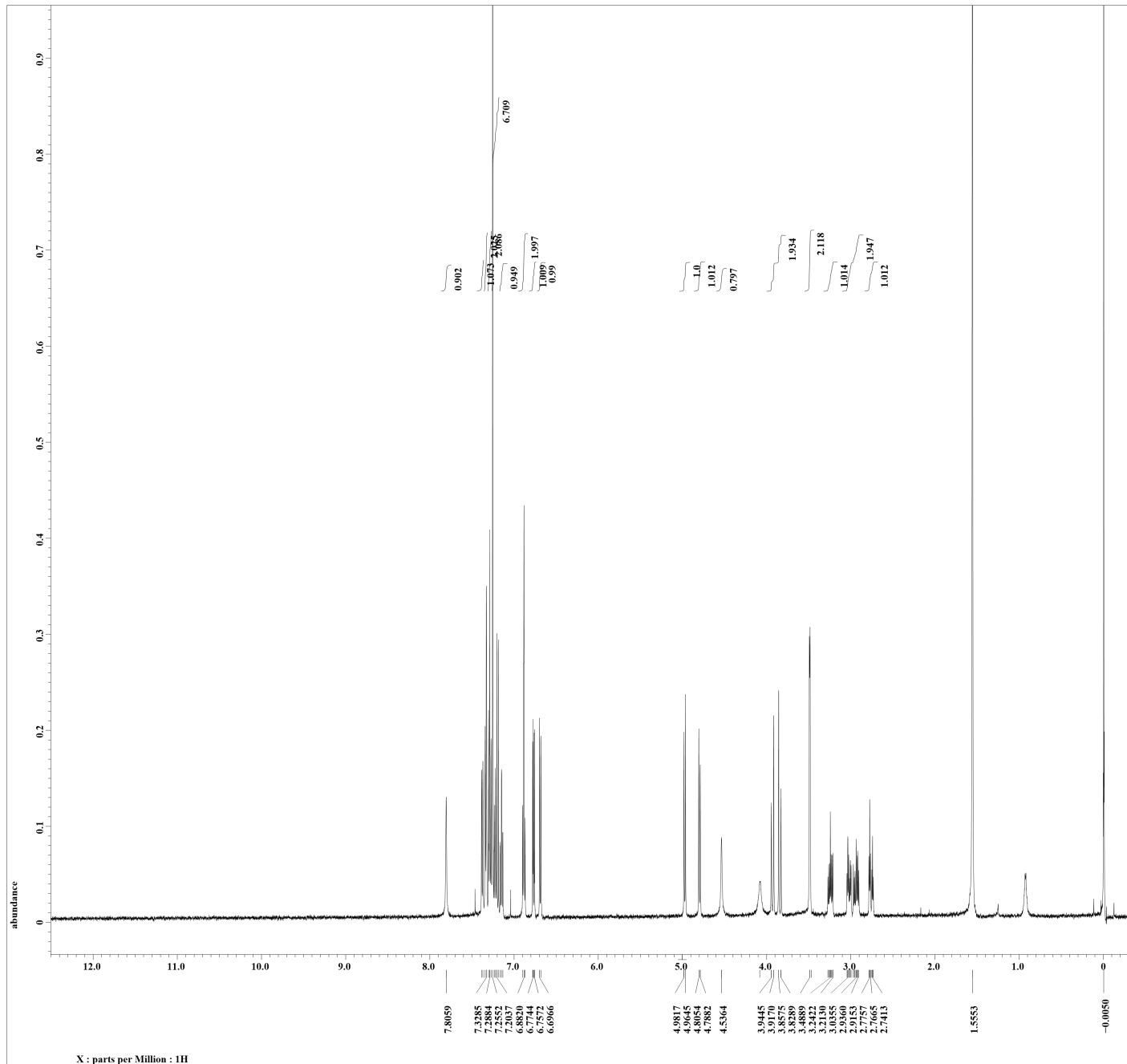
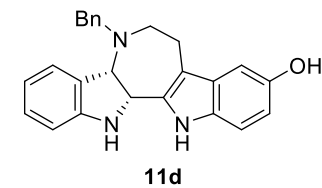


Filename = SS-18-07-12-04-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#679487
Solvent = CHLOROFORM-D
Creation_time = 12-JUL-2018 18:06:17
Revision_time = 12-JUL-2018 18:58:15
Current_time = 12-JUL-2018 18:59:14

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]
IR_domain = 1H
IR_freq = 495.13191398[MHz]
IR_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 = 12.63[us]
X_acq_time = 1.76422912[s]
X_angle = 45[deg]
X_atn = 3.3[dB]
X_atn = 3.3[dB]
X_pulse = 6.315[us]
IR_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 46
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get = 23.6[dc]



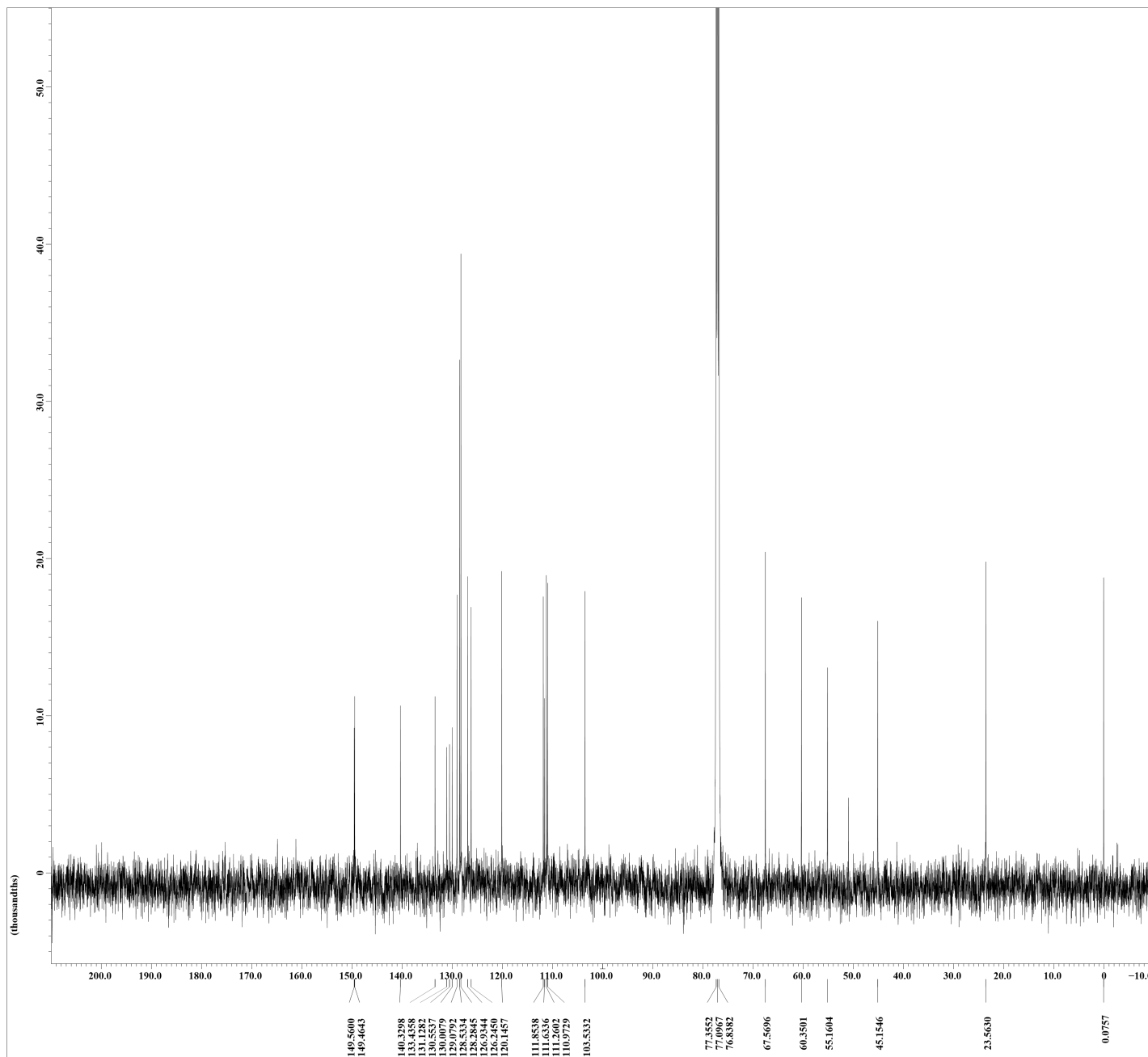
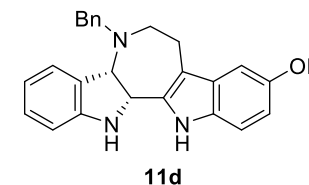
```

Filename      = SS-18-07-12-04-5.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = #680823
Solvent      = CHLOROFORM-D
Creation_time = 13-JUL-2018 06:58:30
Revision_time = 13-JUL-2018 07:50:48
Current_Time = 13-JUL-2018 07:51:07

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]
IRF_domain     = 1H
IRF_freq       = 499.13191398[MHz]
IRF_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16291
Total_scans    = 16291

X_90_width    = 10.83[us]
X_acq_time    = 0.8388608[s]
X_angle       = 30[deg]
X_atn         = 9.5[dB]
X_pulse       = 3.61[us]
IRF_atn_dec   = 20.548[dB]
IRF_atn_noe   = 20.548[dB]
IRF_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      = 24.3[dC]
  
```





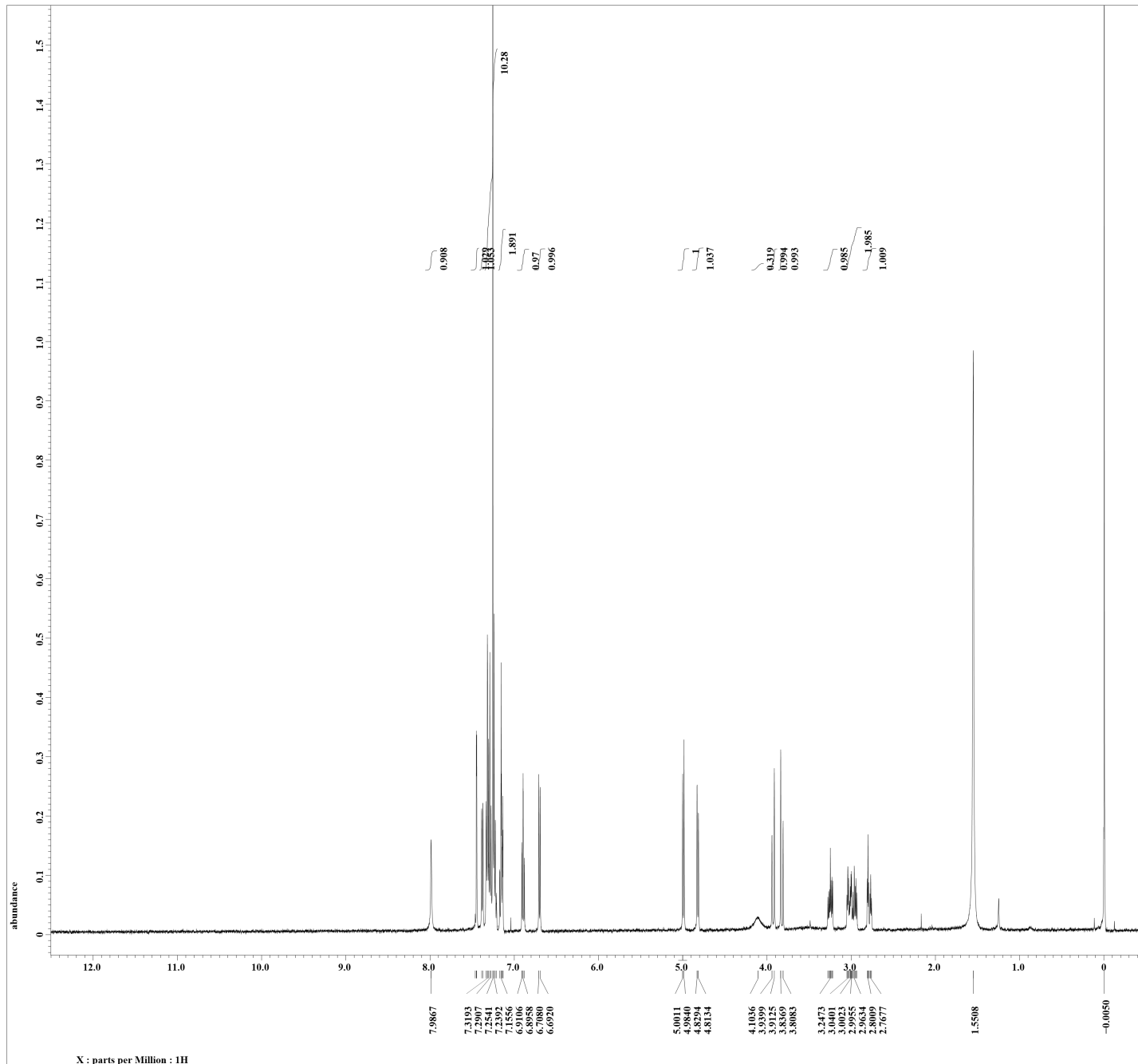
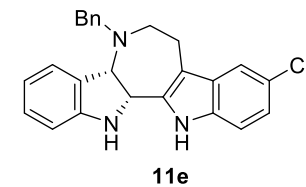
```

Filename      = SS-18-07-10-03-4.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = S#468067
Solvent      = CHLOROFORM-D
Creation time = 10-JUL-2018 12:14:08
Revision time = 10-JUL-2018 15:13:29
Current_Time = 10-JUL-2018 15:14:53

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]
F1r_domain    = 1H
F1r_freq      = 495.13191398 [MHz]
F1r_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    = 12.63 [us]
X_acq_time    = 1.76422912 [s]
X_angle       = 45 [deg]
X_atn         = 3.3 [dB]
X_pulse       = 6.315 [us]
F1r_mode      = Off
Tri_mode      = Off
DanTe_preset = FALSE
Initial_wait  = 1 [s]
Recvr_gain    = 48
Relaxation_delay = 5 [s]
Repetition_time = 6.76422912 [s]
Temp_get     = 23.4 [dC]
  
```



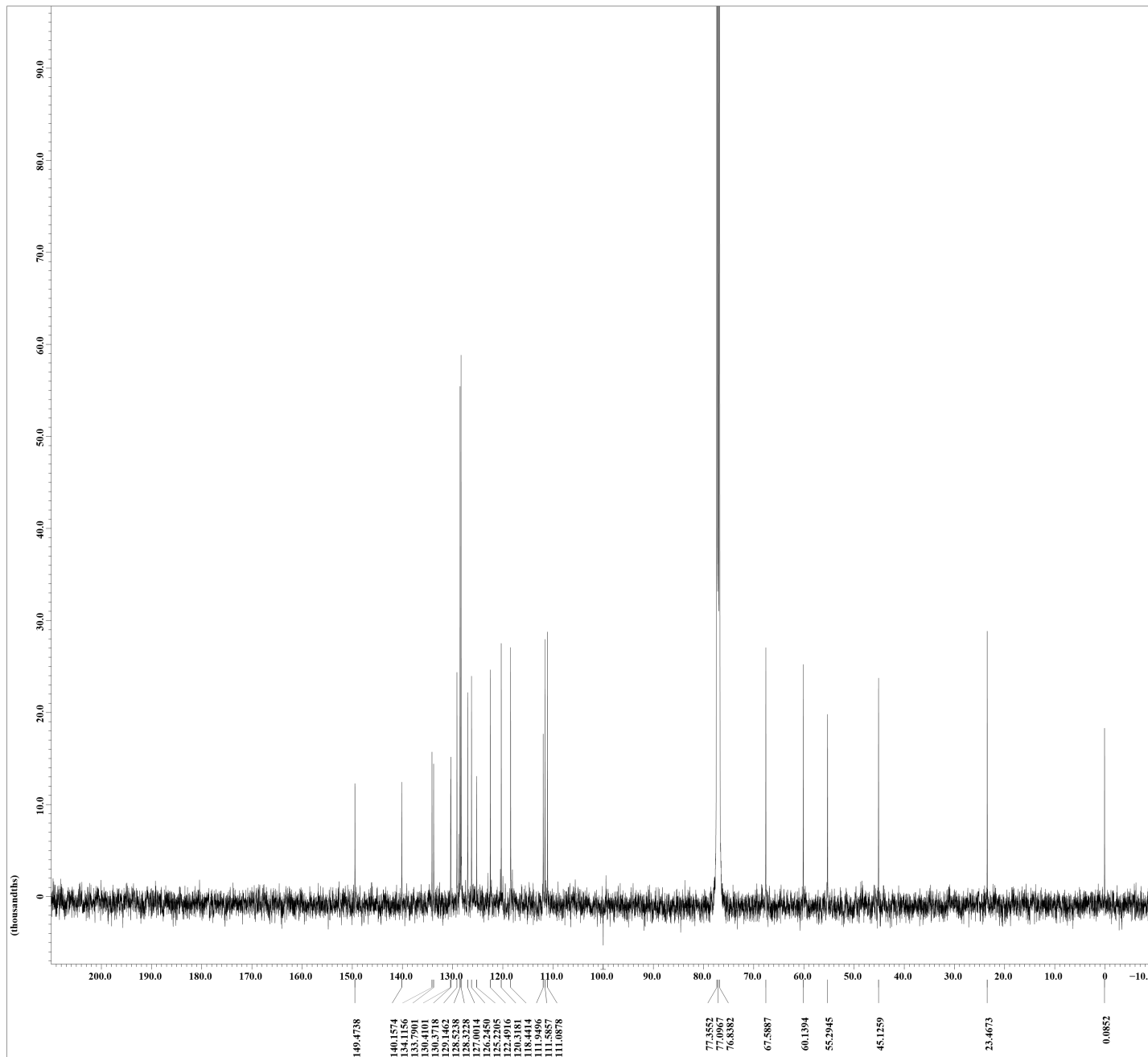
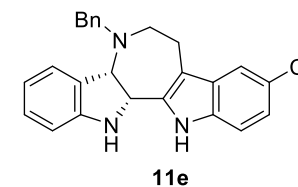
X : parts per Million : 1H

Filename = SS-18-07-10-03-6.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#657465
 Solvent = CHLOROFORM-D
 Creation_time = 11-JUL-2018 06:58:51
 Revision_time = 11-JUL-2018 07:49:14
 Current_Time = 11-JUL-2018 07:49:40

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 = 17075
 Total_scans = 17075

X_90_width = 10.83 [us]
 X_acq_time = 0.8388608 [s]
 X_angle = 30 [deg]
 X_atn = 9.5 [dB]
 X_pulse = 3.61 [us]
 Irr_atn_dec = 20.548 [dB]
 Irr_atn_noe = 20.548 [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 = 24.8 [dC]

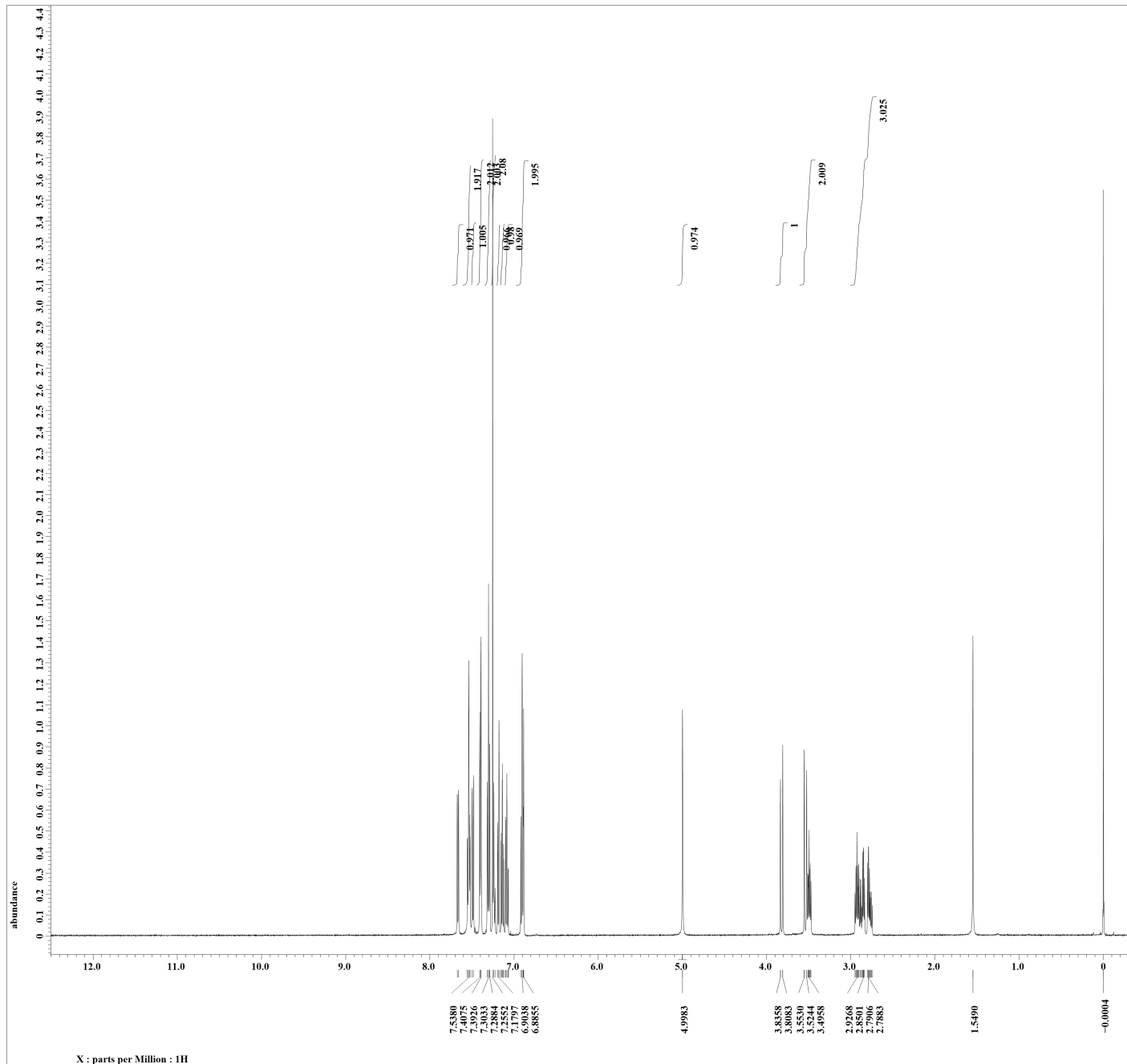
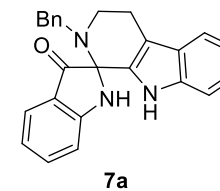


Filename = yama-18-07-04-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#569783
 Solvent = CHLOROFORM-D
 Creation_time = 4-JUL-2018 15:04:43
 Revision_time = 4-JUL-2018 15:54:48
 Current_Time = 4-JUL-2018 15:57:15

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]
 IR_domain = 1H
 IR_freq = 495.13191398[MHz]
 IR_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 = 12.63[us]
 X_acq_time = 1.76422912[s]
 X_angle = 45[deg]
 X_atn = 3.3[dB]
 X_pulse = 6.315[us]
 IR_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recv_gain = 46
 Relaxation_delay = 5[s]
 Repetition_time = 6.76422912[s]
 Temp_get = 23.7[dc]



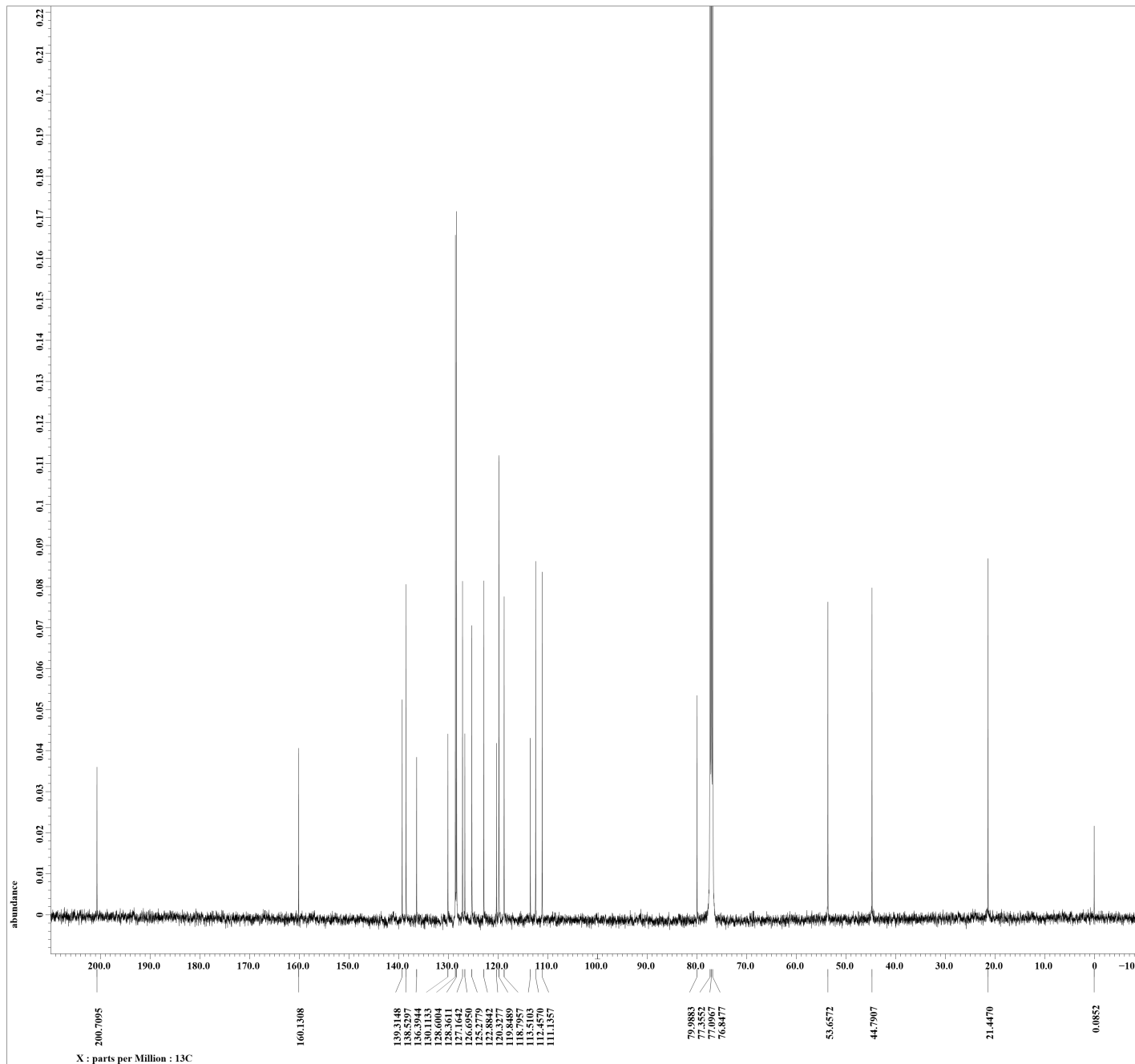
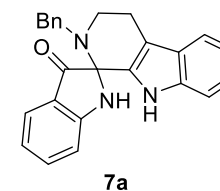
```

Filename      = yama-18-07-04-6.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#571682
Solvent      = CHLOROFORM-D
Creation_time = 5-JUL-2018 07:11:34
Revision_time = 5-JUL-2018 07:59:26
Current_Time = 5-JUL-2018 07:59:52

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]
IRF_domain     = 1H
IRF_freq       = 499.13191398[MHz]
IRF_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 20386
Total_scans    = 20386

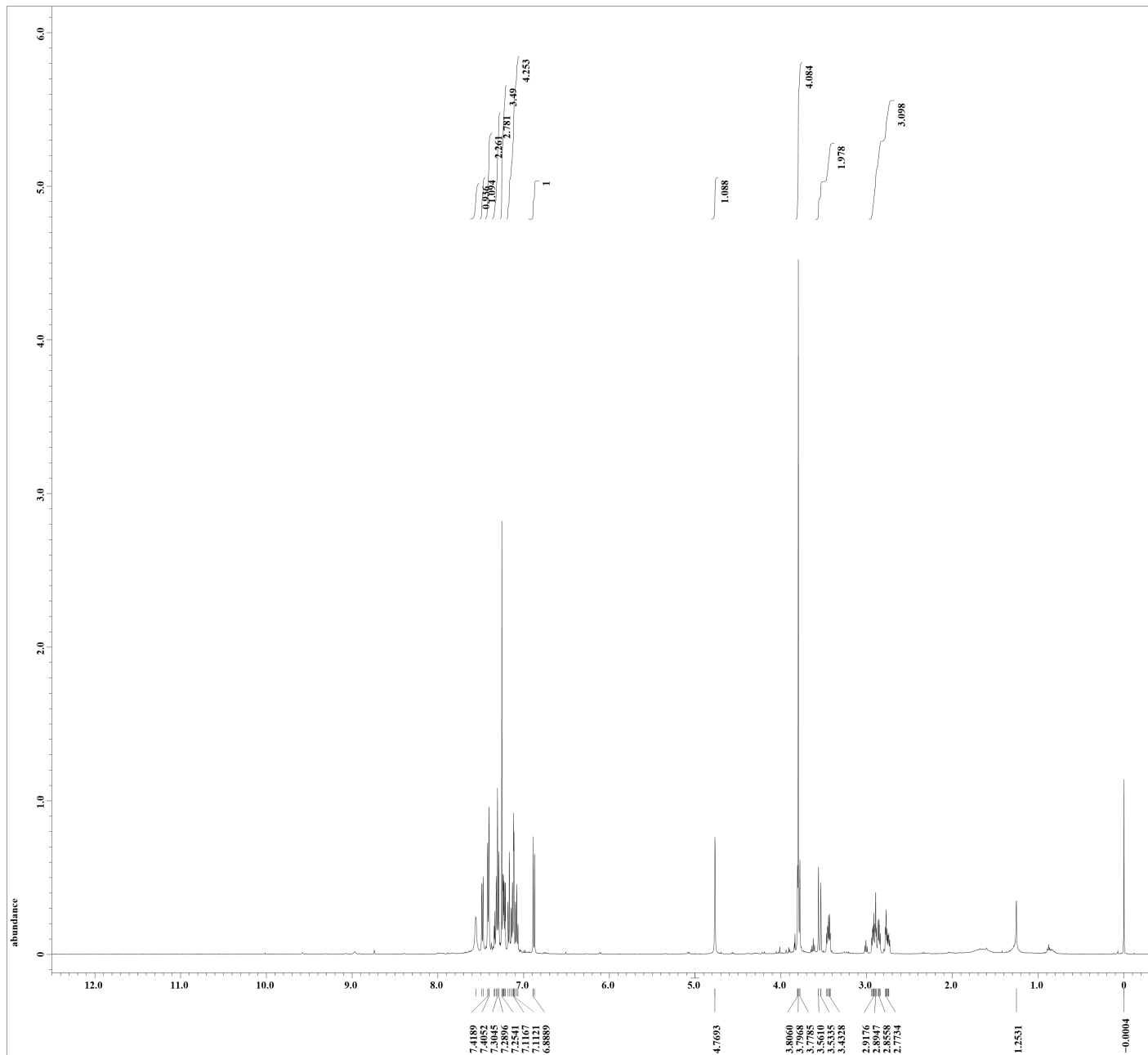
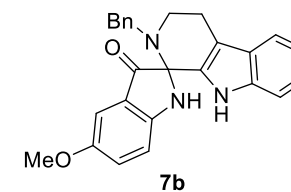
X_90_width    = 10.83[us]
X_acq_time    = 0.8388608[s]
X_angle       = 30[deg]
X_atn         = 9.5[dB]
X_pulse       = 3.61[us]
IRF_atn_dec   = 20.548[dB]
IRF_atn_noe   = 20.548[dB]
IRF_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 2[s]
Recvr_gain    = 60
Relaxation_delay = 2[s]
Repetition_time = 2.8388608[s]
Temp_get      = 24.8[dc]
  
```



Filename = yama-17-09-26-5.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#331488
 Solvent = CHLOROFORM-D
 Creation_time = 26-SEP-2017 09:11:02
 Revision_time = 26-SEP-2017 09:20:58
 Current_Time = 26-SEP-2017 09:21:30

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]
 IR_domain = 1H
 IR_freq = 495.13191398[MHz]
 IR_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 495.13191398[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 32
 Total_scans = 32

X_90_width = 12.63[us]
 X_acq_time = 1.76422912[s]
 X_angle = 45[deg]
 X_atn = 3.3[dB]
 X_pulse = 6.315[us]
 IR_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 = 21.7[dc]



X : parts per Million : 1H

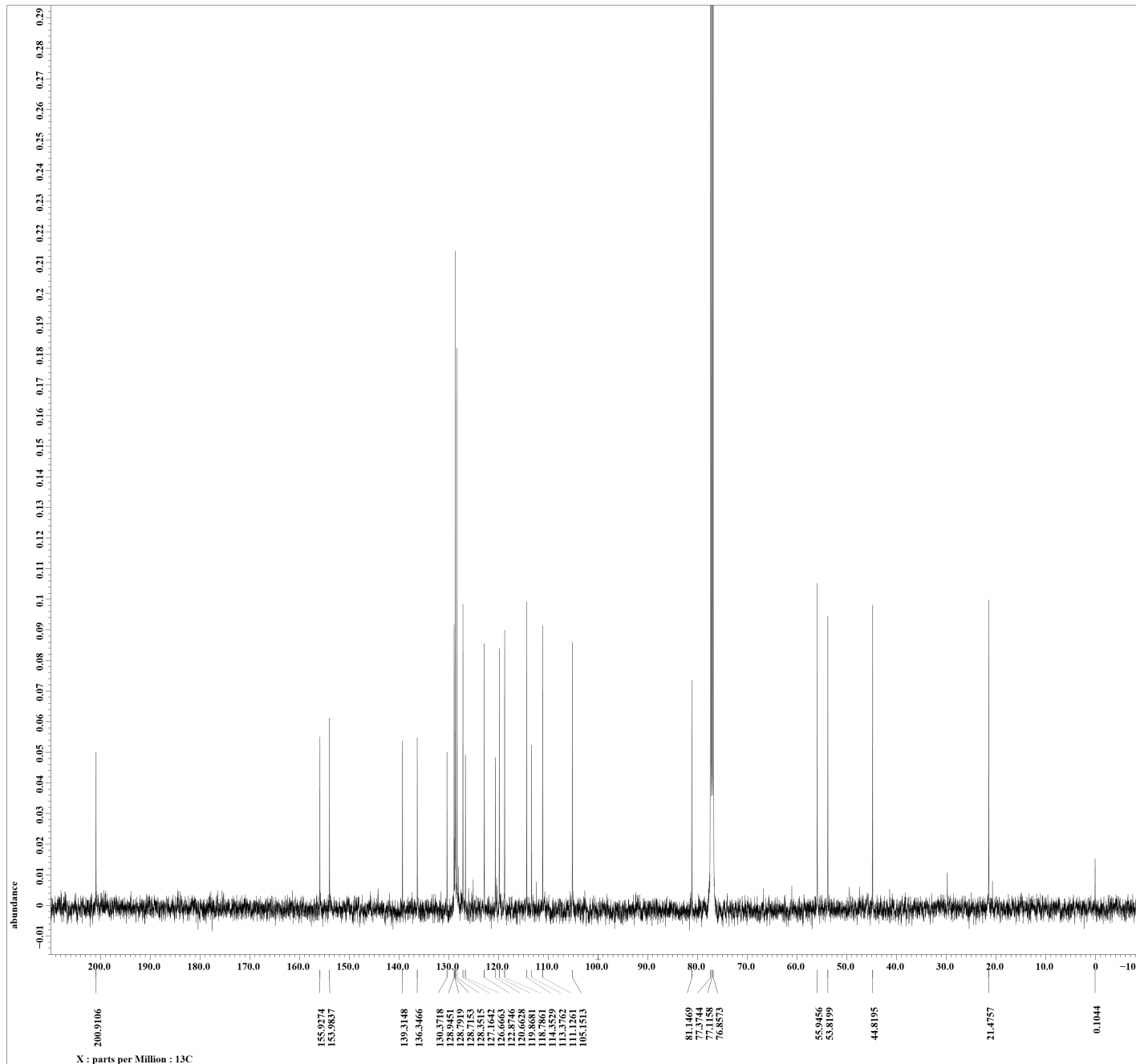
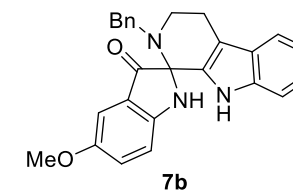
```

Filename      = yama-17-09-26-8.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#334906
Solvent      = CHLOROFORM-D
Creation_time = 26-SEP-2017 11:39:33
Revision_time = 26-SEP-2017 11:48:18
Current_Time = 26-SEP-2017 11:49:11

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]
IRF_domain    = 1H
IRF_freq       = 499.13191398[MHz]
IRF_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 3098
Total_scans    = 3098

X_90_width    = 10.83[us]
X_acq_time     = 0.8388608[s]
X_angle        = 30[deg]
X_atn          = 9.5[dB]
X_pulse        = 3.61[us]
IRF_atn_dec    = 20.548[dB]
IRF_atn_noe   = 20.548[dB]
IRF_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       = 21.8[dc]
  
```



```

Filename      = yama-18-07-10-4.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = S#634968
Solvent      = CHLOROFORM-D
Creation_time = 3-JUL-2018 04:37:55
Revision_time = 2-AUG-2018 08:41:21
Current_Time = 2-AUG-2018 08:42:17
  
```

```

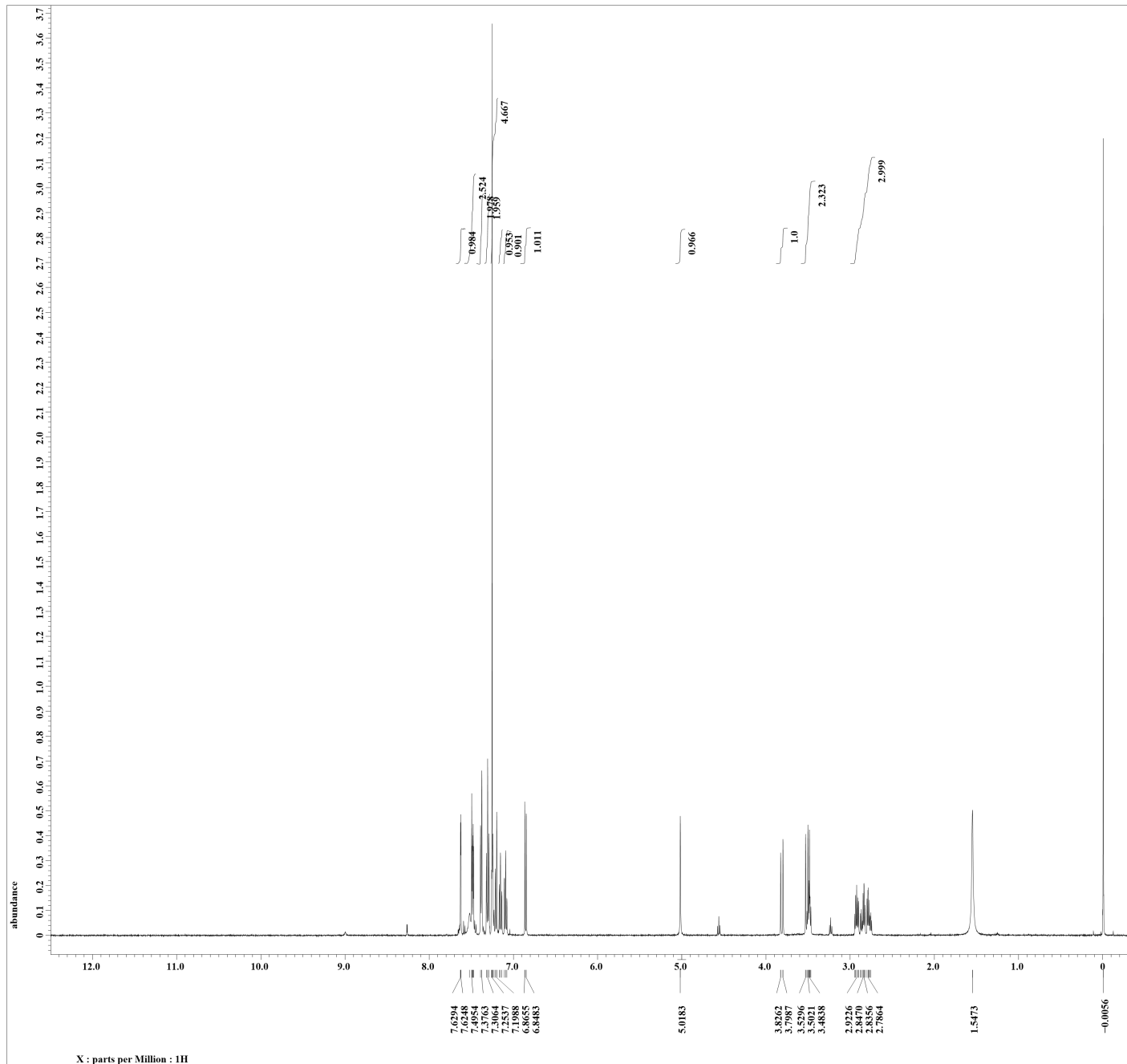
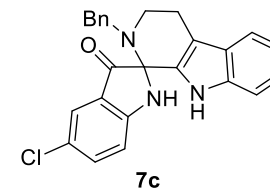
Content      = single_pulse
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA500
Spectrometer = DELTA2_NMR
  
```

```

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]
IRF_domain    = 1H
IRF_freq      = 500.15991521[MHz]
IRF_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    = 12.39[us]
X_acq_time     = 1.74587904[s]
X_angle       = 45[deg]
X_atn         = 3.4[dB]
X_pulse       = 6.195[us]
IRF_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      = 21.9[dc]
  
```



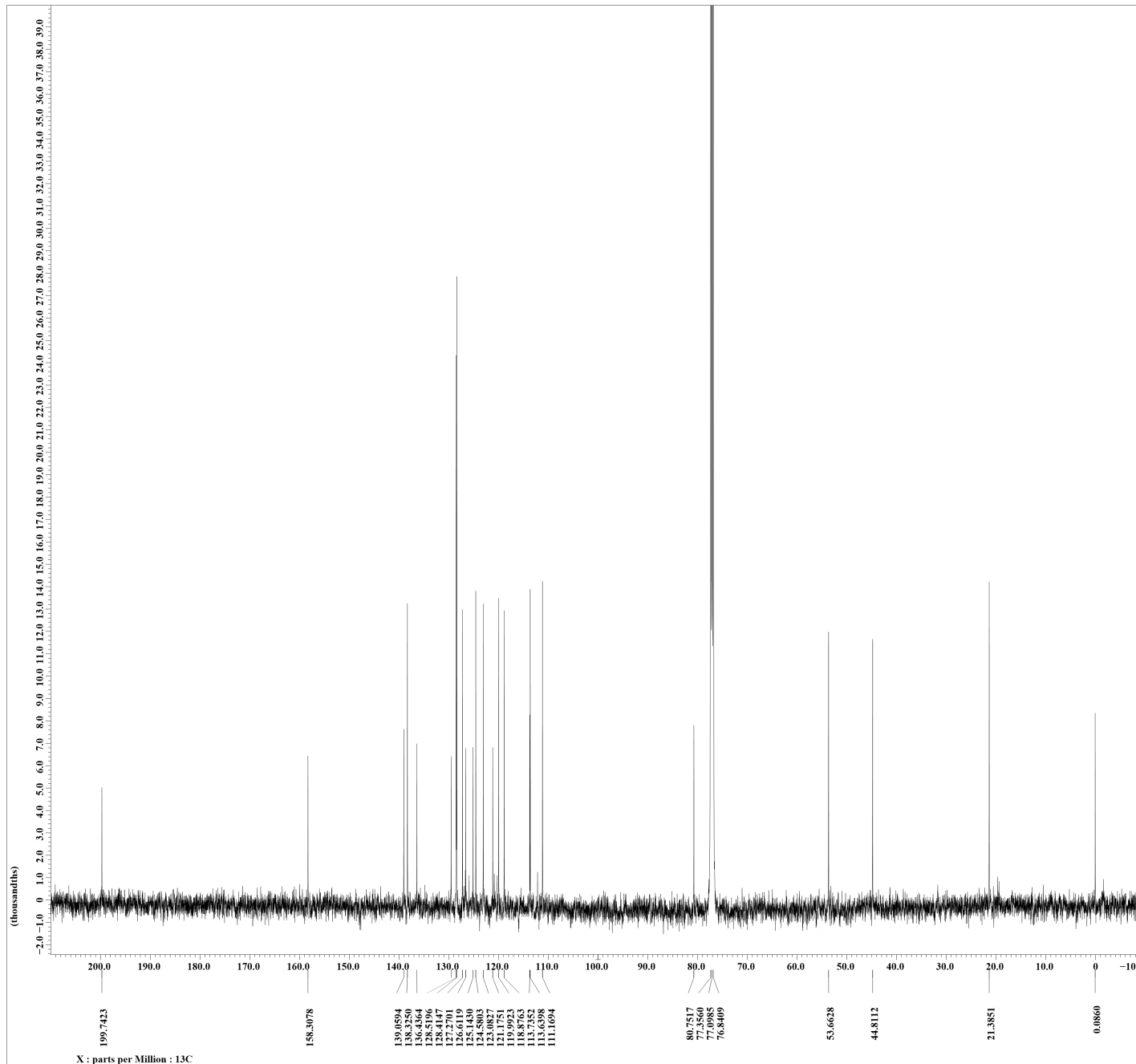
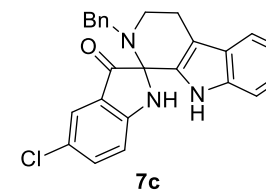
```

Filename      = yama-18-07-10-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#638276
Solvent      = CHLOROFORM-D
Creation_time = 3-JUL-2018 18:12:21
Revision_time = 15-JUL-2018 12:51:40
Current_Time = 15-JUL-2018 12:52:16

Content      = 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
Mod_return     = 1
Scans          = 17138
Total_scans    = 17138

X_90_width    = 11.43[us]
X_acq_time    = 0.83361792[s]
X_angle       = 30[deg]
X_atn         = 5.3[dB]
X_pulse       = 3.81[us]
Irr_atn_dec   = 20.81[dB]
Irr_atn_noe   = 20.81[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 = 2.83361792[s]
Temp_get      = 23.1[dc]
  
```

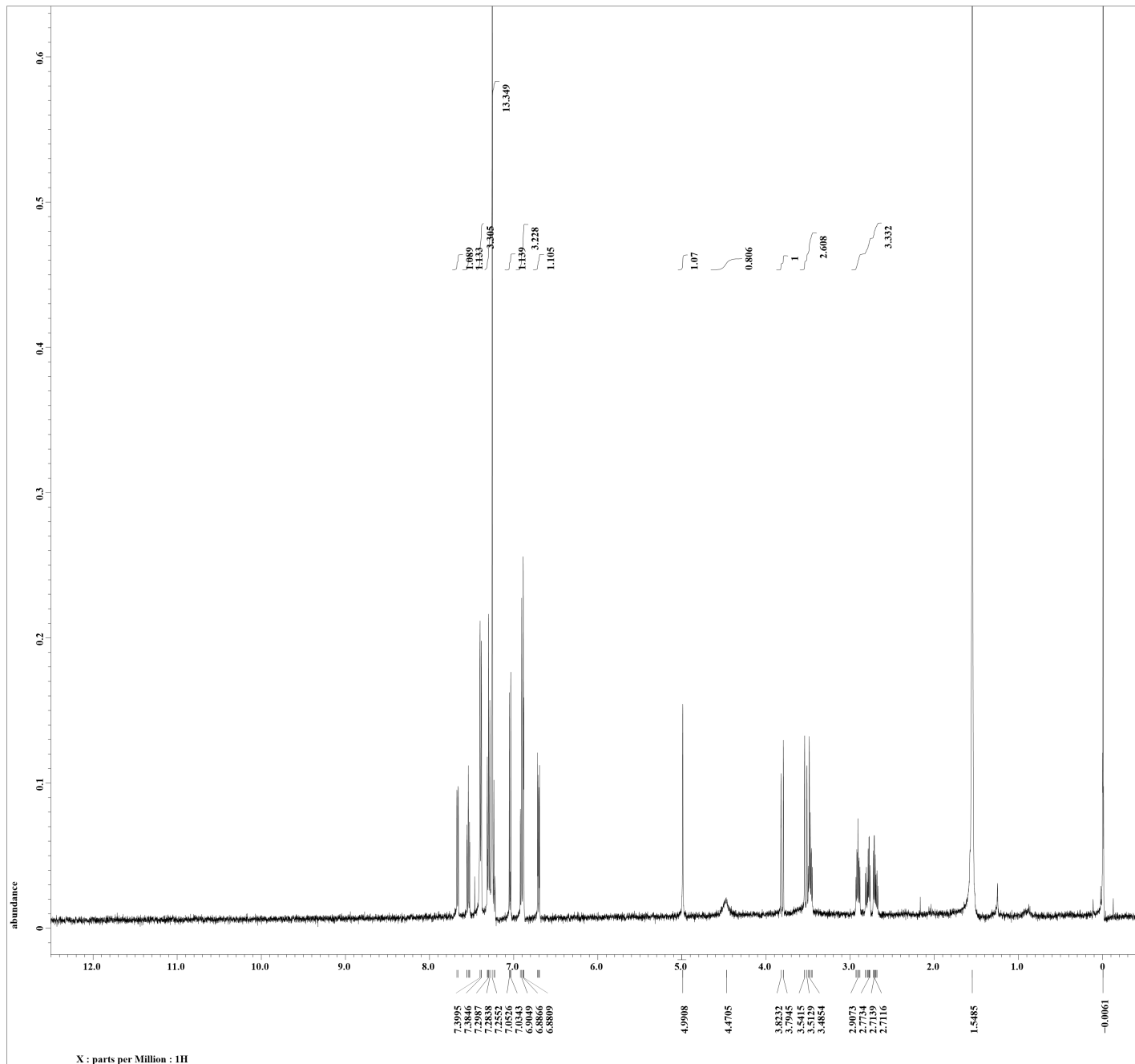
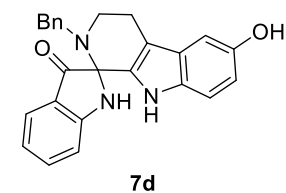


Filename = SS-18-07-15-02-13.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#379614
 Solvent = CHLOROFORM-D
 Creation_time = 17-JUL-2018 09:45:32
 Revision_time = 17-JUL-2018 10:42:06
 Current_time = 17-JUL-2018 10:42:43

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]
 IFR_domain = 1H
 IFR_freq = 495.13191398[MHz]
 IFR_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 = 12.63[us]
 X_acq_time = 1.76422912[s]
 X_angle = 45[deg]
 X_atn = 3.3[dB]
 X_pulse = 6.315[us]
 IFR_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 48
 Relaxation_delay = 5[s]
 Repetition_time = 6.76422912[s]
 Temp_get = 23.1[dC]



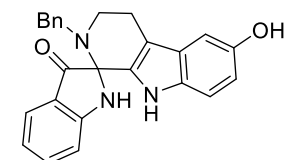


Filename = SS-18-07-25-01-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#674109
Solvent = CHLOROFORM-D
Creation_time = 26-JUL-2018 07:53:05
Revision_time = 26-JUL-2018 08:43:58
Current_time = 26-JUL-2018 08:44:55

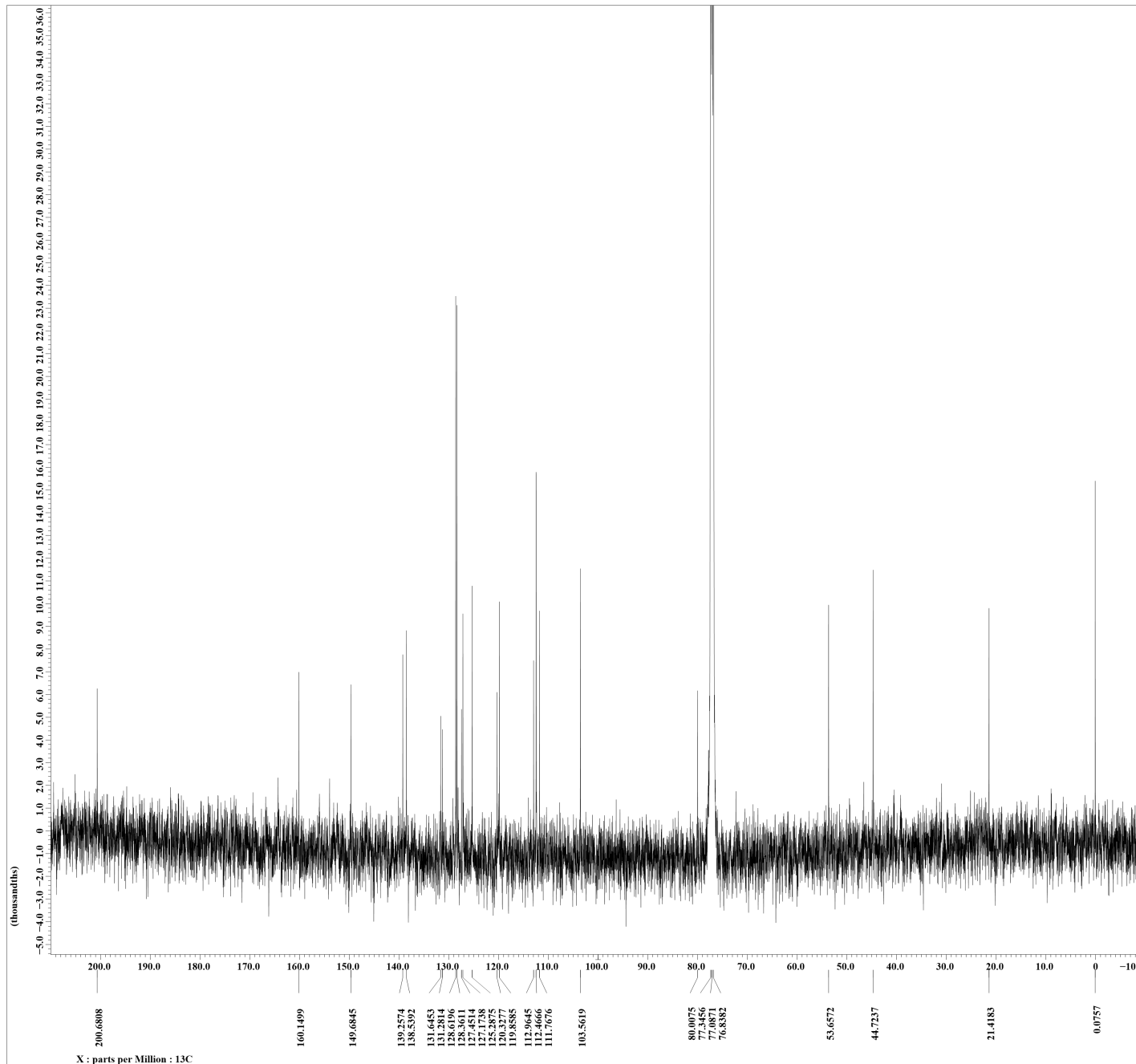
Content = single_pulse_decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

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]
IRF_domain = 1H
IRF_freq = 499.13191398[MHz]
IRF_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 17633
Total_scans = 17633

X_90_width = 10.83[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.5[dB]
X_pulse = 3.61[us]
IRF_atn_dec = 20.548[dB]
IRF_atn_noe = 20.548[dB]
IRF_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 = 24.7[dc]



7d



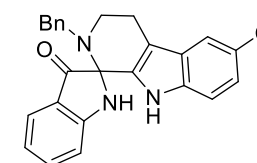


Filename = SS-18-07-13-01-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#411021
 Solvent = CHLOROFORM-D
 Creation_time = 13-JUL-2018 10:38:28
 Revision_time = 13-JUL-2018 11:31:06
 Current_Time = 13-JUL-2018 11:36:39

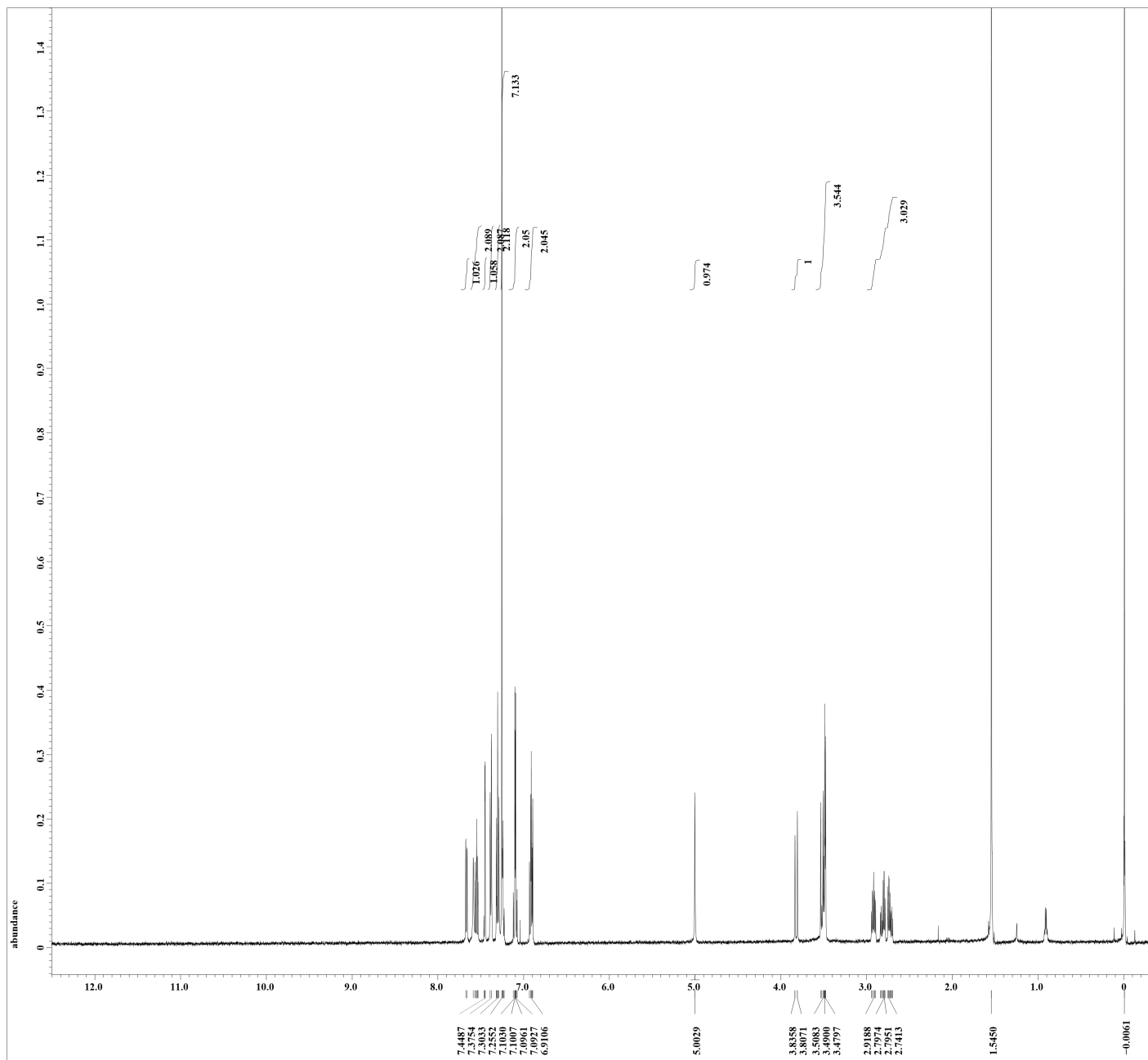
Content = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = DELTA2_NMR

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]
 IIR_domain = 1H
 IIR_freq = 495.13191398[MHz]
 IIR_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 = 12.63[us]
 X_acq_time = 1.76422912[s]
 X_angle = 45[deg]
 X_atn = 3.3[dB]
 X_pulse = 6.315[us]
 IIR_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 48
 Relaxation_delay = 5[s]
 Repetition_time = 6.76422912[s]
 Temp_get = 23.7[dc]



7e



X : parts per Million : 1H

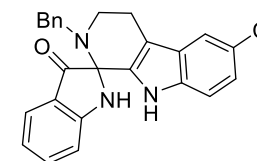


Filename = SS-18-07-13-01-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#657893
Solvent = CHLOROFORM-D
Creation_time = 15-JUL-2018 07:38:49
Revision_time = 15-JUL-2018 08:30:13
Current_Time = 15-JUL-2018 08:30:54

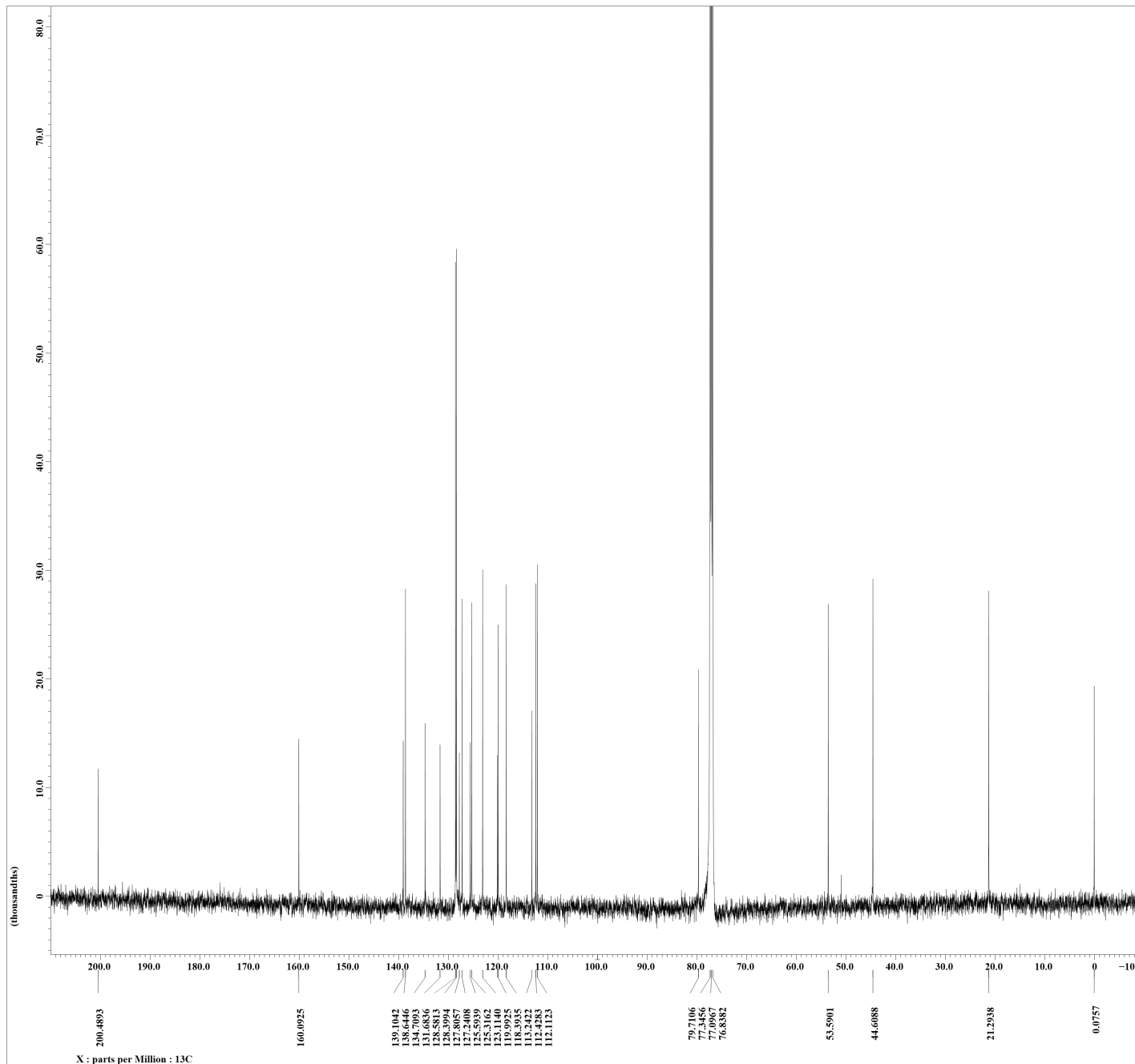
Content = single_pulse_decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 500
Spectrometer = DELTA2_NMR

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]
IR_domain = 1H
IR_freq = 495.13191398[MHz]
IR_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 48352
Total_scans = 48352

X_90_width = 10.83[us]
X_acq_time = 0.8388608[s]
X_angle = 30[deg]
X_atn = 9.5[dB]
X_pulse = 3.61[us]
IR_atn_dec = 20.548[dB]
IR_atn_noe = 20.548[dB]
IR_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 = 24.7[dc]



7e



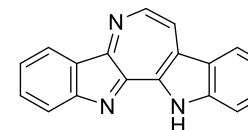
```

Filename      = yama-18-03-15-4-4.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = S#658498
Solvent      = CHLOROFORM-D
Creation_time = 15-MAR-2018 17:50:10
Revision_time = 15-MAR-2018 18:20:57
Current_Time = 15-MAR-2018 18:21:44

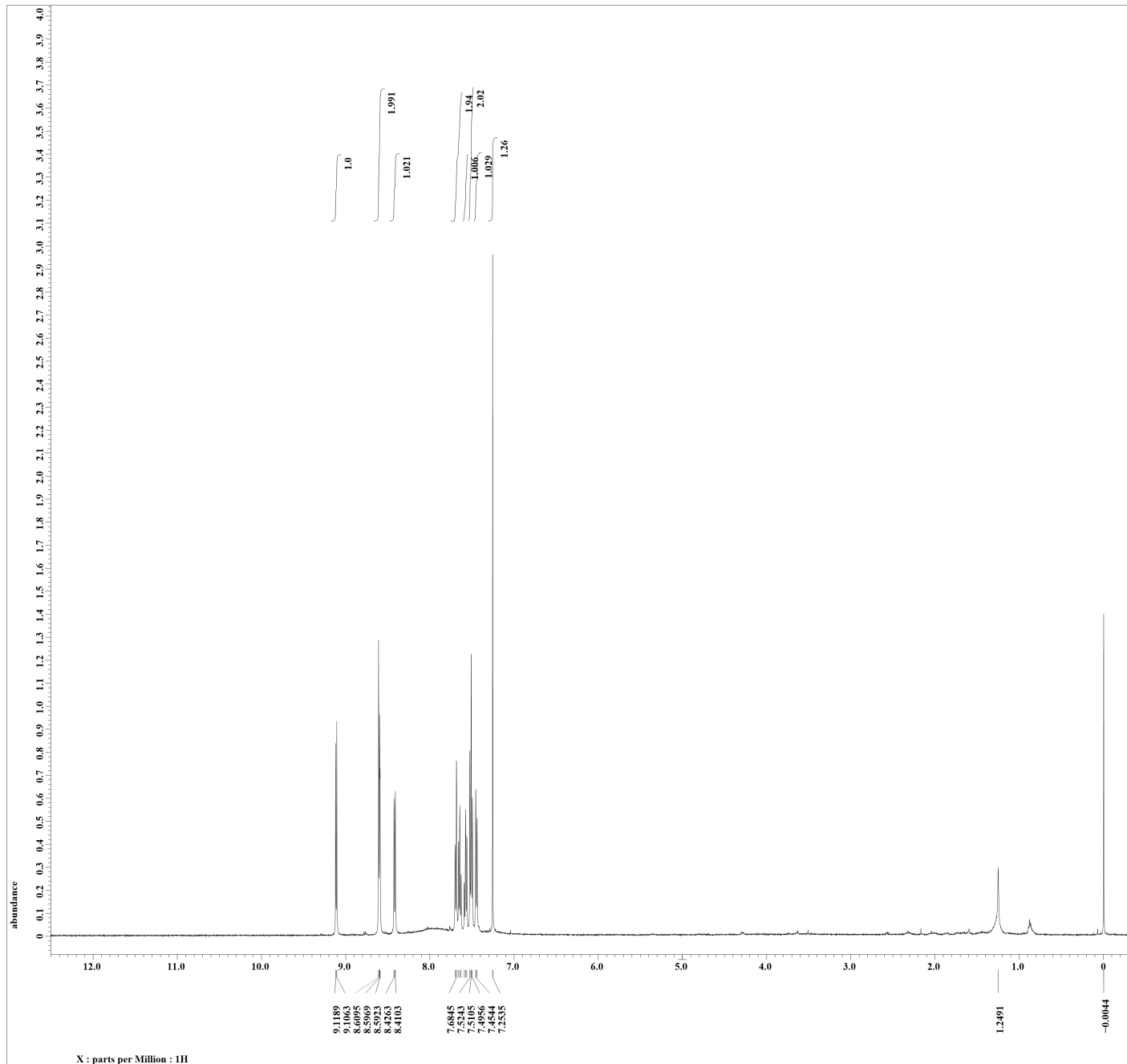
Content      = single_pulse
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = DELTA2_NMR

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]
IRF_domain    = 1H
IRF_freq      = 495.13191398[MHz]
IRF_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    = 12.63[us]
X_acq_time    = 1.76422912[s]
X_angle       = 45[deg]
X_atn         = 3.3[dB]
X_pulse       = 6.315[us]
IRF_mode      = Off
Tri_mode      = Off
Dante_presat  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 46
Relaxation_delay = 5[s]
Repetition_time = 6.76422912[s]
Temp_get      = 23.7[dc]
  
```



17



```

Filename      = yama-18-03-15-4-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#658826
Solvent      = CHLOROFORM-D
Creation_time = 16-MAR-2018 07:01:28
Revision_time = 16-MAR-2018 07:34:35
Current_Time = 16-MAR-2018 07:35:19
  
```

```

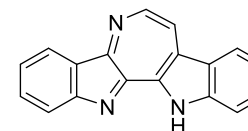
Content      = single_pulse_decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = DELTA2_NMR
  
```

```

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]
IRF_domain     = 1H
IRF_freq       = 499.13191398[MHz]
IRF_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16697
Total_scans    = 16697
  
```

```

X_90_width    = 10.83[us]
X_acq_time     = 0.8388608[s]
X_angle        = 30[deg]
X_atn          = 9.5[dB]
X_pulse        = 3.61[us]
IRF_atn_dec    = 20.548[dB]
IRF_atn_noe    = 20.548[dB]
IRF_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       = 24.1[dC]
  
```



17

