

Supporting Information: np-2010-008015

Malyngamide 3, Cocosamides A and B from the Marine Cyanobacterium

***Lyngbya majuscula* from Cocos Lagoon, Guam**

Sarath P. Gunasekera, Chivas S. Owle, Rana Montaser, Hendrik Luesch and Valerie J. Paul

Smithsonian Marine Station at Ft. Pierce, 701 Seaway Drive, Ft. Pierce, FL 34949, and Department of Medicinal Chemistry, University of Florida, 1600 SW Archer Road, Gainesville, Florida 32610

Contents

	Page #
¹ H NMR (600 MHz, CDCl ₃) spectrum of malyngamide 3 (1)	S 2
¹³ C NMR (150 MHz, CDCl ₃) spectrum of malyngamide 3 (1)	S 3
2D NOESY (600 MHz, CDCl ₃) spectrum of malyngamide 3 (1)	S 4
¹ H NMR (600 MHz, CDCl ₃) spectrum of cocosamide A (2)	S 5
¹³ C NMR (150 MHz, CDCl ₃) spectrum of cocosamide A (2)	S 6
2D NOESY (600 MHz, CDCl ₃) spectrum of cocosamide A (2)	S 7
¹ H NMR (600 MHz, CDCl ₃) spectrum of cocosamide B (3)	S 8
¹³ C NMR (150 MHz, CDCl ₃) spectrum of cocosamide B (3)	S 9
2D NOESY (600 MHz, CDCl ₃) spectrum of cocosamide B (3)	S 10
COSY (600 MHz, CDCl ₃) spectrum of cocosamide B (3)	S 11
HMBC (600 MHz, CDCl ₃) spectrum of cocosamide B (3)	S 12
¹ H NMR (600 MHz, CDCl ₃) spectrum of pitipeptolide A (5)	S 13
2D NOESY (600 MHz, CDCl ₃) spectrum of pitipeptolide A (5)	S 14



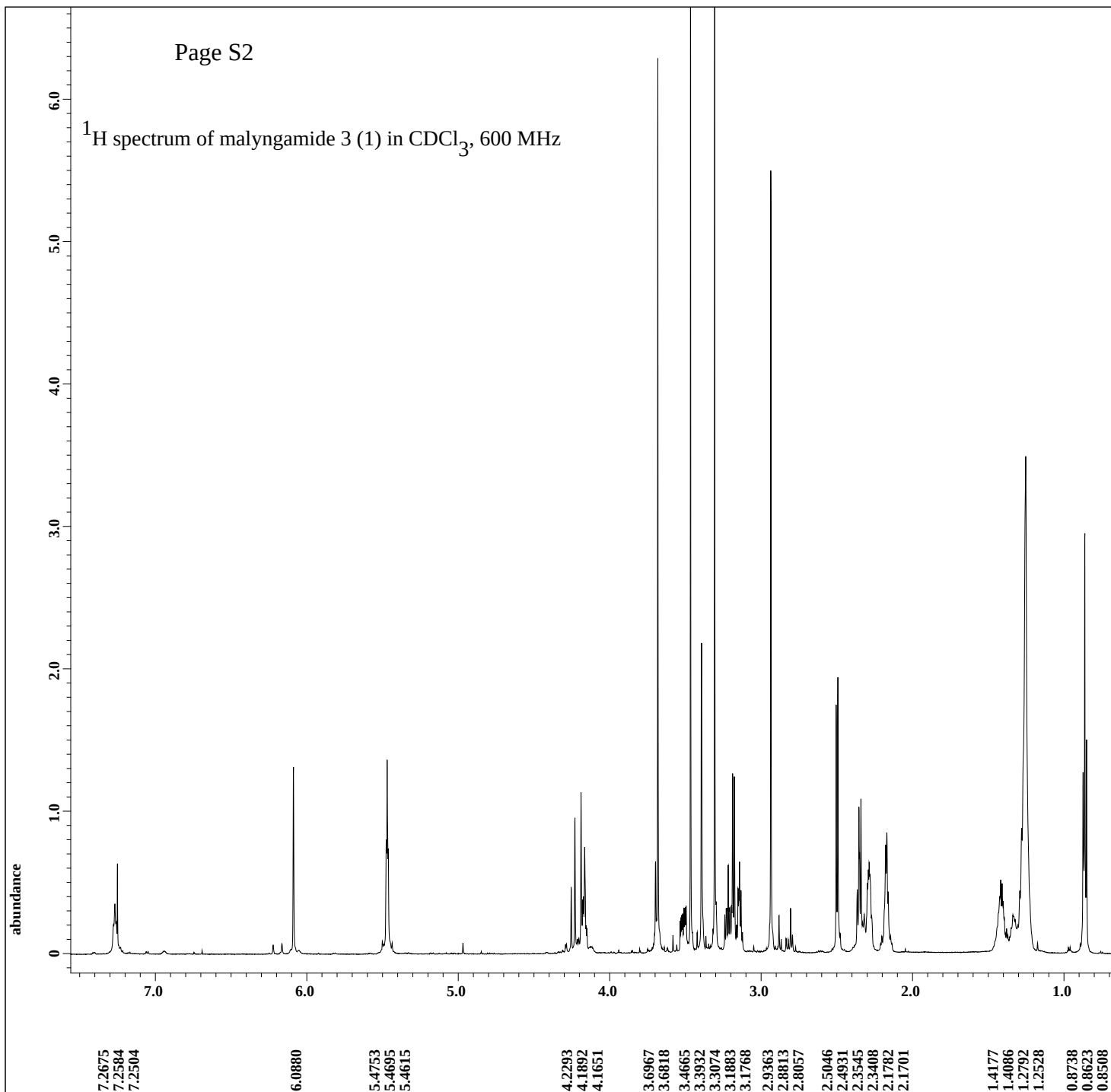
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 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm

Filename = c36-4-cdcl3-single_pu
 Author = Smithsonian
 Experiment = single_pulse.ex2
 Sample_id = c36-4-cdcl3
 Solvent = CHLOROFORM-D
 Creation_time = 10-MAR-2009 09:50:33
 Revision_time = 5-JAN-2011 11:51:29
 Current_time = 5-JAN-2011 11:52:46

Comment = single_pulse
 Data_format = 1D_COMPLEX
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 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = ECA600-AID

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 1.4548992[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.68733284[Hz]
 X_sweep = 11.26126126[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 7.1[us]
 X_acq_time = 1.4548992[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 3.55[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 6.4548992[s]
 Temp_get = 23.2[dc]



X : parts per Million : 1H



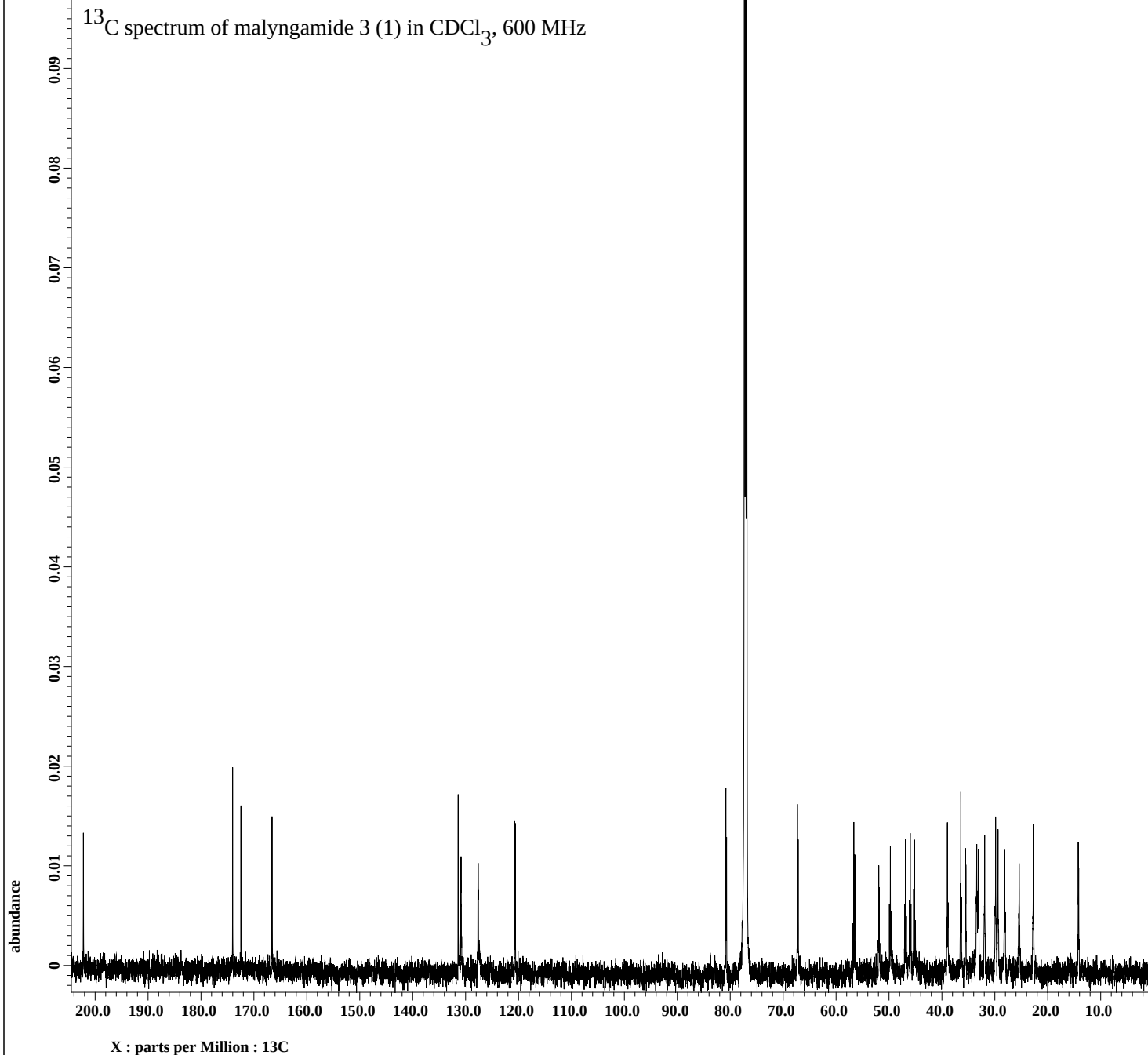
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 secp : 2.0[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm

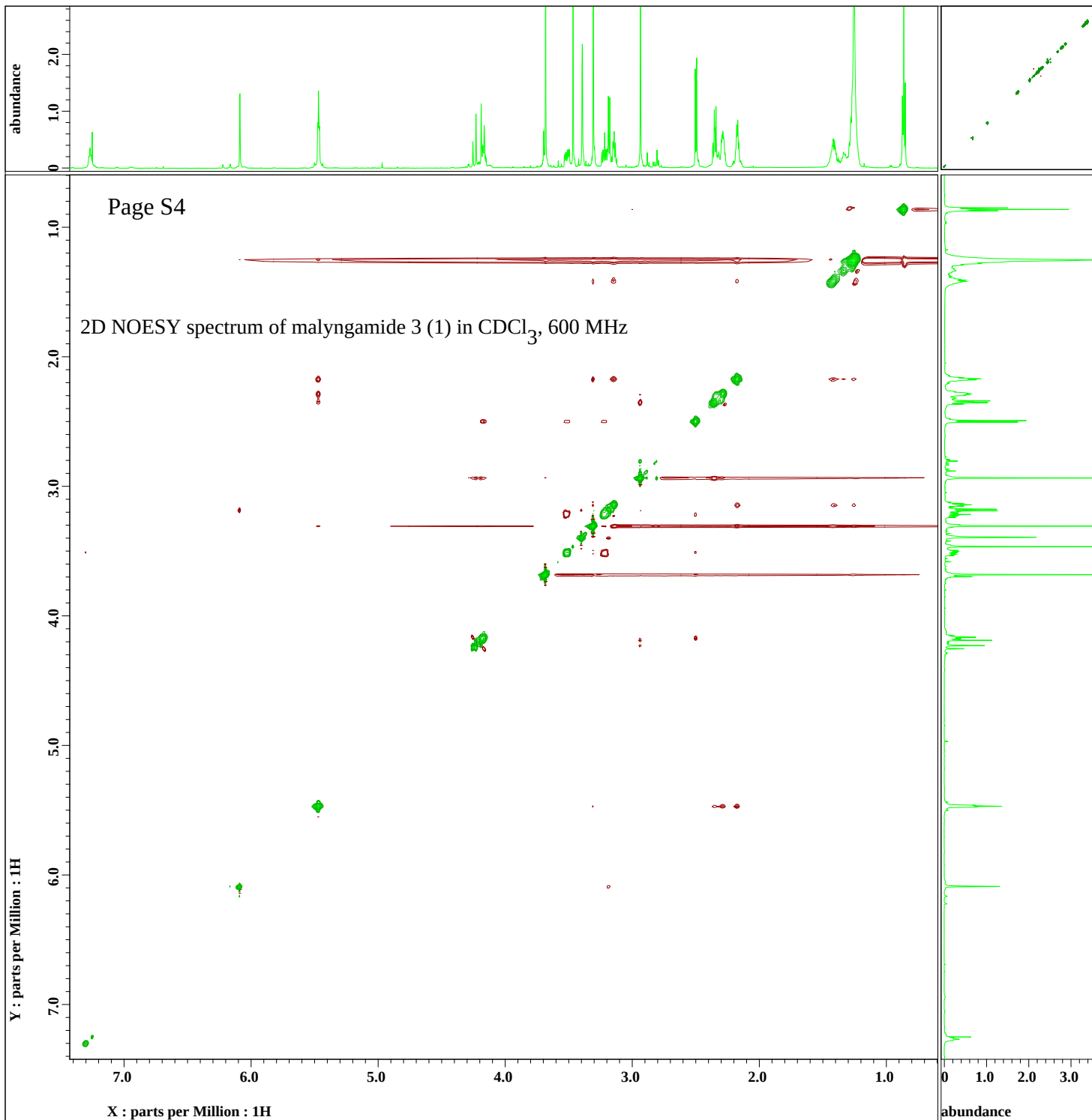
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 Author = Smithsonian
 Experiment = single_pulse_dec
 Sample_id = c36-4-cdcl3
 Solvent = CHLOROFORM-D
 Creation_time = 24-MAR-2009 05:46:48
 Revision_time = 5-JAN-2011 10:05:38
 Current_time = 5-JAN-2011 10:07:04

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = ECA600-AID

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.69206016[s]
 X_domain = 13C
 X_freq = 150.91343039[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.44496109[Hz]
 X_sweep = 47.34848485[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 20000
 Total_scans = 20000

X_90_width = 14.16[us]
 X_acq_time = 0.69206016[s]
 X_angle = 30[deg]
 X_atn = 2[dB]
 X_pulse = 4.72[us]
 Irr_atn_dec = 25[dB]
 Irr_atn_noe = 25[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 = 2.69206016[s]
 Temp_get = 23.8[dc]





```

---- PROCESSING PARAMETERS ----
sexp : 5.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
ppm
machinephase
[transpose]
sexp : 5.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 2
fft : 1 : TRUE : TRUE
ppm
machinephase

```

```

Filename      = c36-4-cdcl3-noesy pha
Author        = Smithsonian
Experiment    = noesy_phase_pfgz
Sample_id     = c36-4-cdcl3
Solvent       = CHLOROFORM-D
Creation_time  = 13-APR-2009 21:05:44
Revision_time = 5-JAN-2011 10:19:37
Current time  = 5-JAN-2011 10:20:34

```

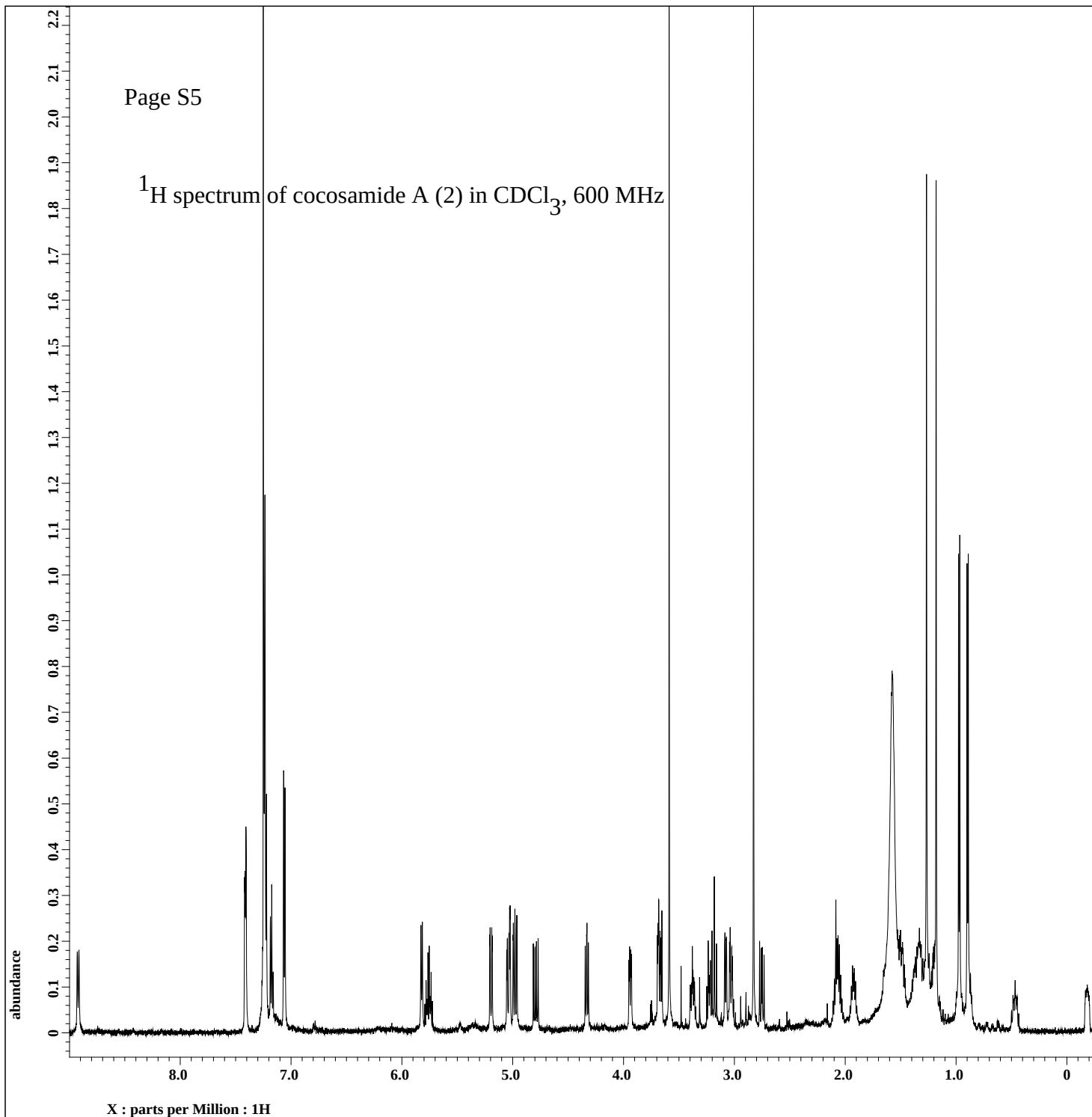
```

Comment      = phase sensitive noesy
Data_format  = 2D COMPLEX COMPLEX
Dim_size     = 819, 512
Dim_title    = 1H 1H
Dim_units    = [ppm] [ppm]
Dimensions   = X Y
Site         = ECA 600
Spectrometer = ECA600-AID

```

```
Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.1994752[s]
X_domain = 1H
X_freq = 600.1723046[MHz]
X_offset = 4.00277[ppm]
X_points = 1024
X_prescans = 4
X_resolution = 5.01315452[Hz]
X_sweep = 5.13347023[kHz]
Y_domain = 1H
Y_freq = 600.1723046[MHz]
Y_offset = 4.00277[ppm]
Y_points = 256
Y_prescans = 0
Y_resolution = 16.03682568[Hz]
Y_sweep = 4.10542737[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 600.1723046[MHz]
Tri_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 16
Total_scans = 4096
```

```
X_acq_time      = 0.1994752[s]
X_atn           = 3[dB]
X_pulse         = 7.1[us]
Y_acq_time      = 62.35648[ms]
Y_p1_correction = 180.0
Irr_mode        = Off
Tri_mode        = Off
Dante_presat     = FALSE
Grad_1          = 1[ms]
```

^1H spectrum of cocosamide A (2) in CDCl_3 , 600 MHz

----- 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

Filename = c36-3-cdcl3-single_pu
Author = Smithsonian
Experiment = single_pulse.ex2
Sample_id = c36-3-cdcl3
Solvent = CHLOROFORM-D
Creation_time = 10-MAR-2009 09:44:53
Revision_time = 9-AUG-2010 10:40:11
Current_time = 9-AUG-2010 10:41:04

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 600
Spectrometer = ECA600-AID

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 1.4548992[s]
X_domain = 1H
X_freq = 600.1723046[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.68733284[Hz]
X_sweep = 11.26126126[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 600.1723046[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 7.1[us]
X_acq_time = 1.4548992[s]
X_angle = 45[deg]
X_atn = 3[dB]
X_pulse = 3.55[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 62
Relaxation_delay = 5[s]
Repetition_time = 6.4548992[s]
Temp_get = 23.2[degC]



```

---- 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
phase : 3 : 0 : 50[%]

```

```

Filename      = c36-3-cdcl3-single_pu
Author       = Smithsonian
Experiment   = single_pulse_dec
Sample_id    = c36-3-cdcl3
Solvent      = CHLOROFORM-D
Creation_time = 2-MAY-2009 11:14:13
Revision_time = 9-AUG-2010 10:47:29
Current_time  = 9-AUG-2010 10:48:16

```

```

Comment      = single pulse decouple
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 600
Spectrometer  = ECA600-AID

```

```

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.69206016[s]
X_domain       = 13C
X_freq         = 150.91343039[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.44496109[Hz]
X_sweep        = 47.34848485[kHz]
Irr_domain     = 1H
Irr_freq       = 600.1723046[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 24000
Total_scans    = 24000

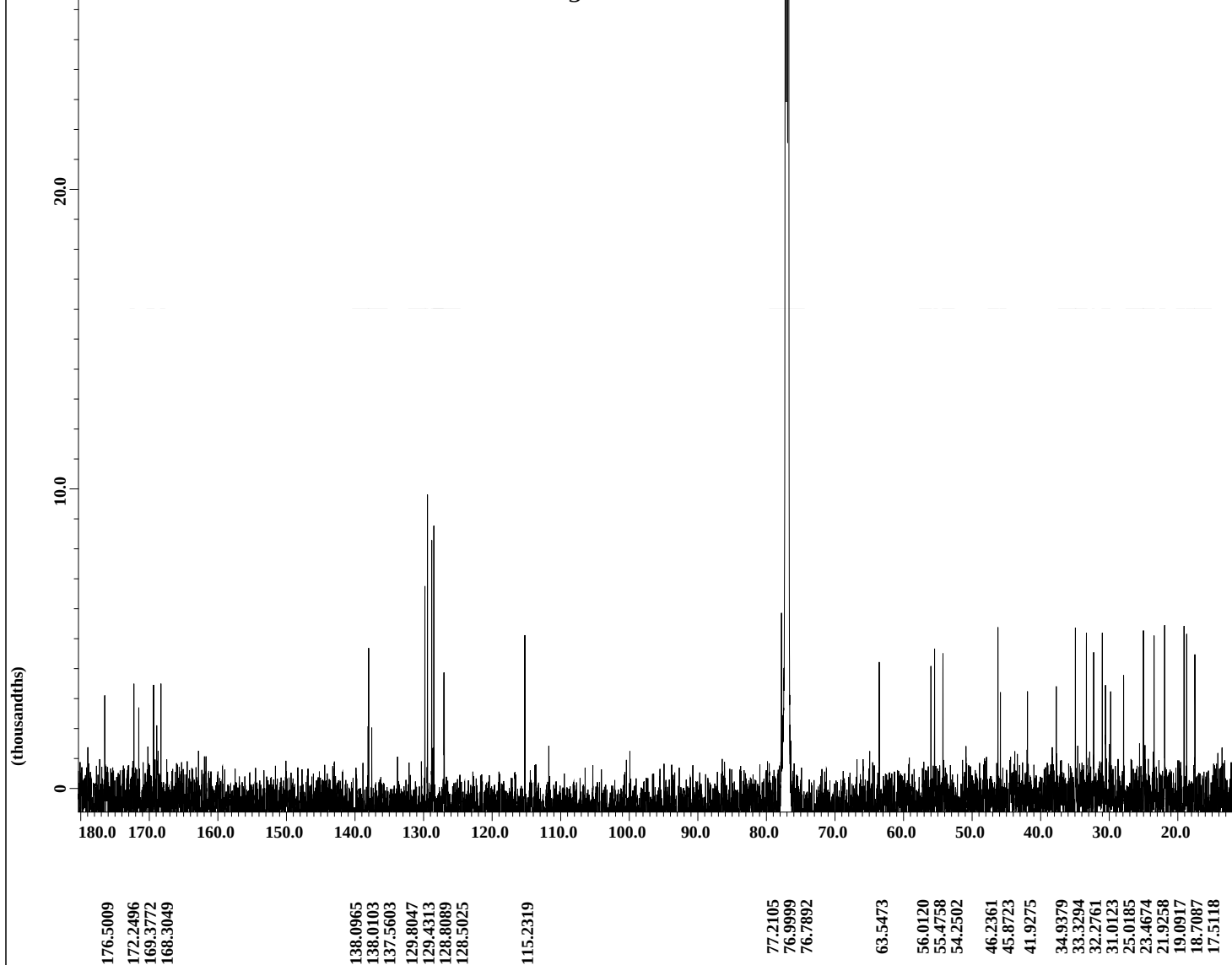
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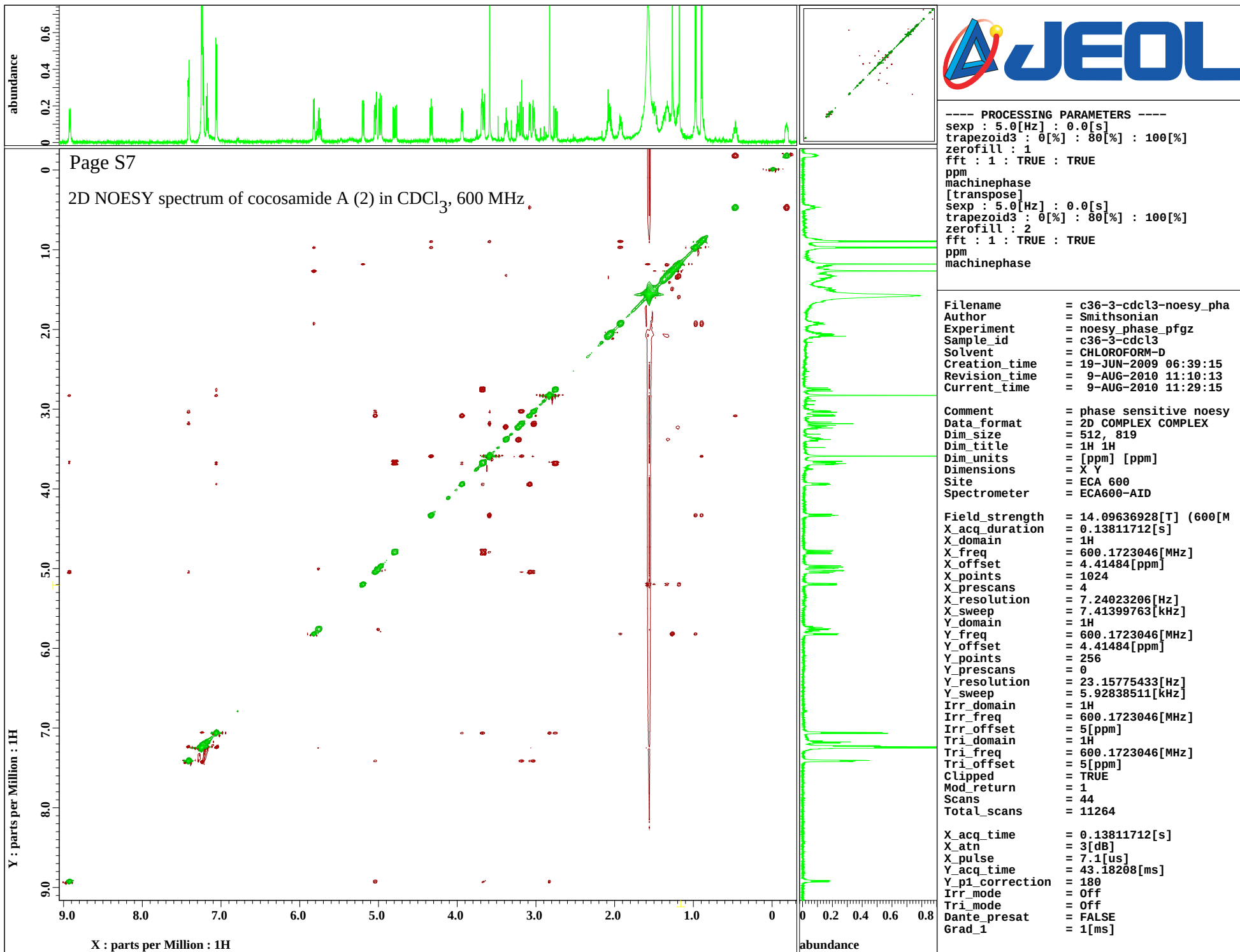
X_90_width     = 14.16[us]
X_acq_time      = 0.69206016[s]
X_angle        = 30[deg]
X_atn          = 2[dB]
X_pulse        = 4.72[us]
Irr_atn_dec    = 25[dB]
Irr_atn_noe    = 25[dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 2[s]
Recvr_gain     = 60
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Temp_get       = 23.7[dc]

```

^{13}C spectrum of cocosamide A (2) in CDCl_3 , 150 MHz



X : parts per Million : 13C





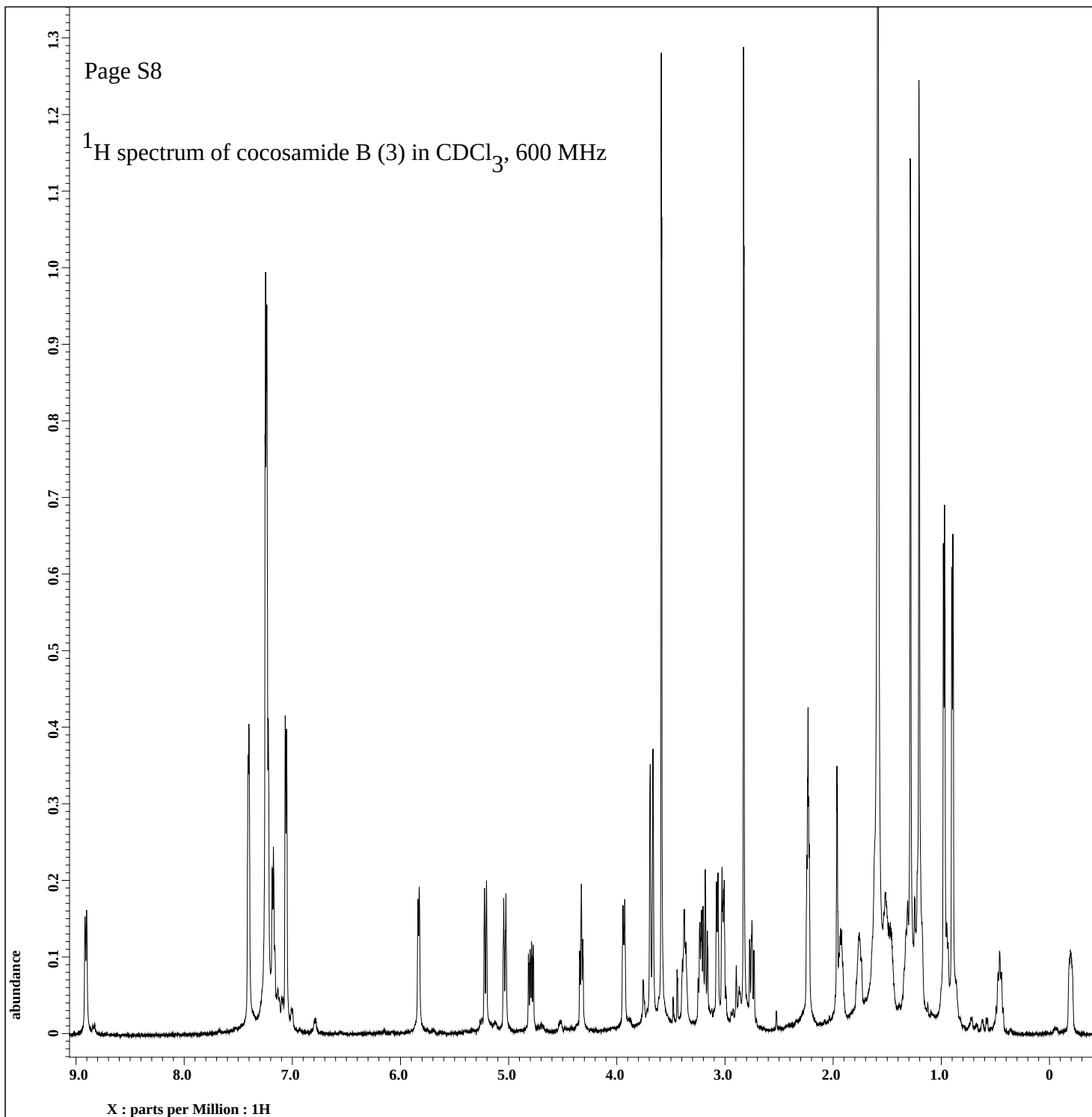
----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
sext : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Filename = c48-6-cdcl3-single_pu
Author = Smithsonian
Experiment = single_pulse.ex2
Sample_id = c48-6-cdcl3
Solvent = CHLOROFORM-D
Creation_time = 7-APR-2009 11:26:18
Revision_time = 9-AUG-2010 11:44:44
Current_time = 9-AUG-2010 11:46:36

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA 600
Spectrometer = ECA600-AID

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 1.4548992[s]
X_domain = 1H
X_freq = 600.1723046[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.68733284[Hz]
X_sweep = 11.26126126[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 600.1723046[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 7.1[us]
X_acq_time = 1.4548992[s]
X_angle = 45[deg]
X_atn = 3[dB]
X_pulse = 3.55[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 48
Relaxation_delay = 5[s]
Repetition_time = 6.4548992[s]
Temp_get = 22.7[degC]





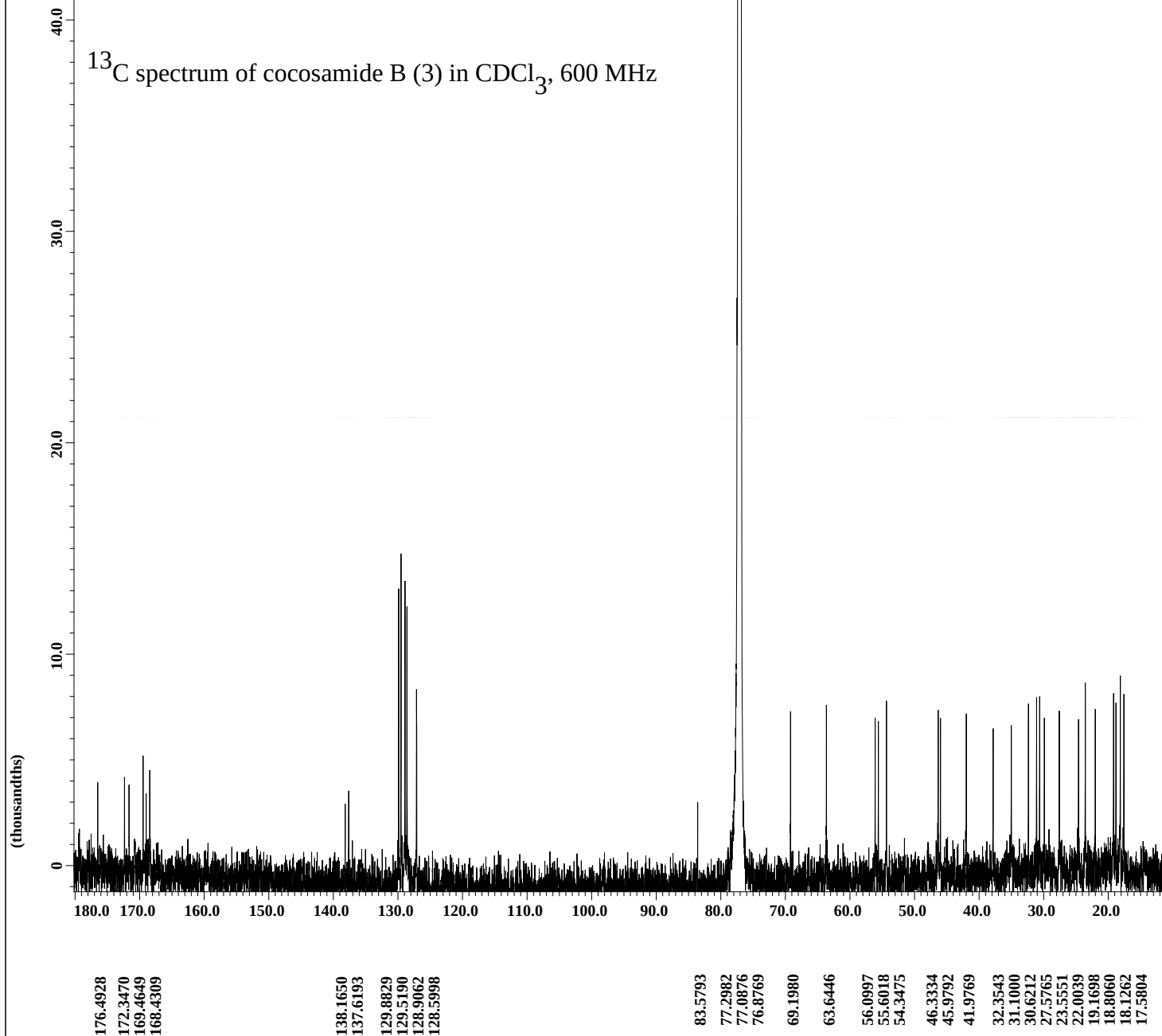
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 secp : 2.0[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm

Filename = c48-6-cdcl3-single_pu
 Author = Smithsonian
 Experiment = single_pulse_dec
 Sample_id = c48-6-cdcl3
 Solvent = CHLOROFORM-D
 Creation_time = 8-APR-2009 08:39:09
 Revision_time = 9-AUG-2010 11:52:28
 Current_time = 9-AUG-2010 11:53:16

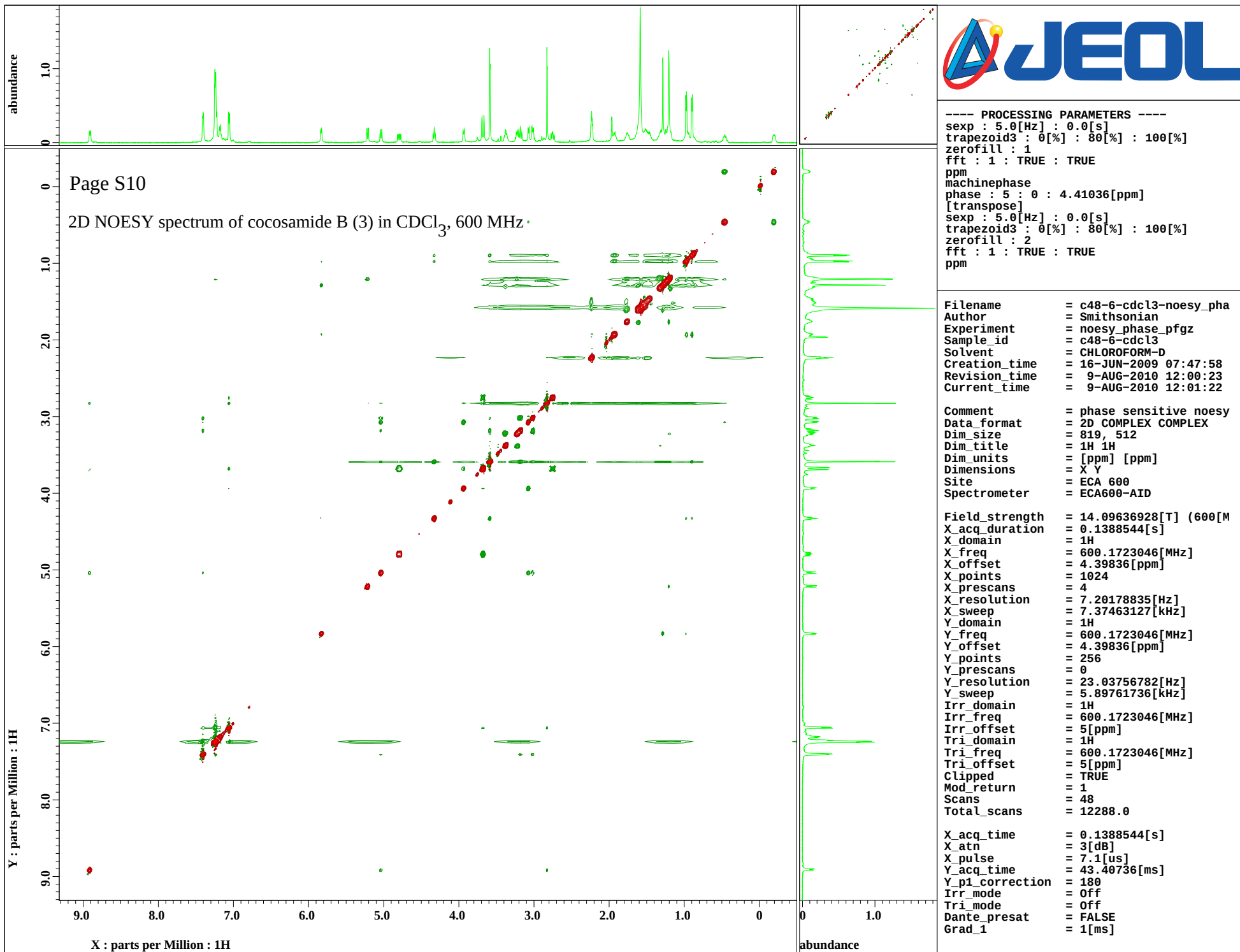
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = ECA600-AID

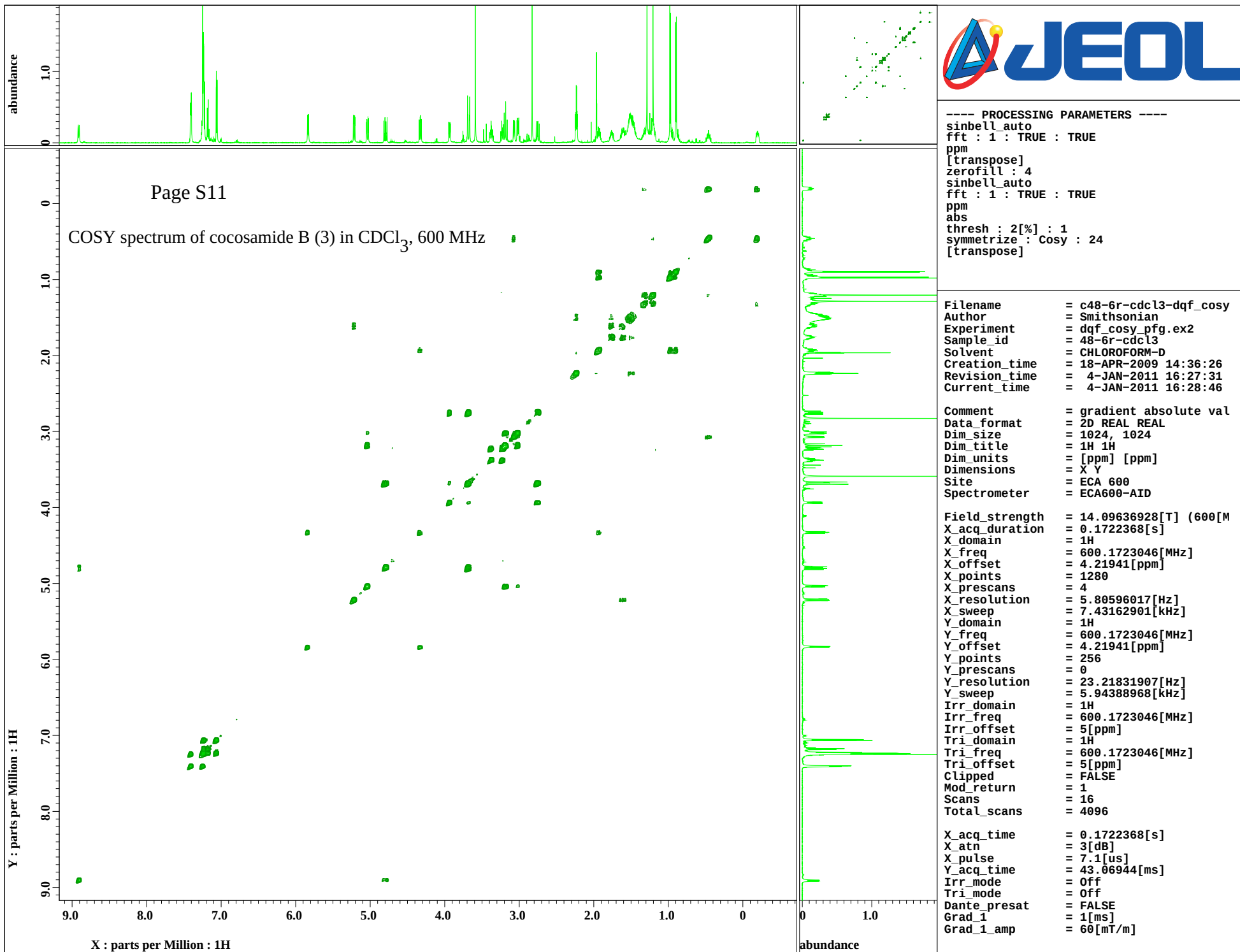
Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 0.69206016[s]
 X_domain = 13C
 X_freq = 150.91343039[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.44496109[Hz]
 X_sweep = 47.34848485[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 21000
 Total_scans = 21000

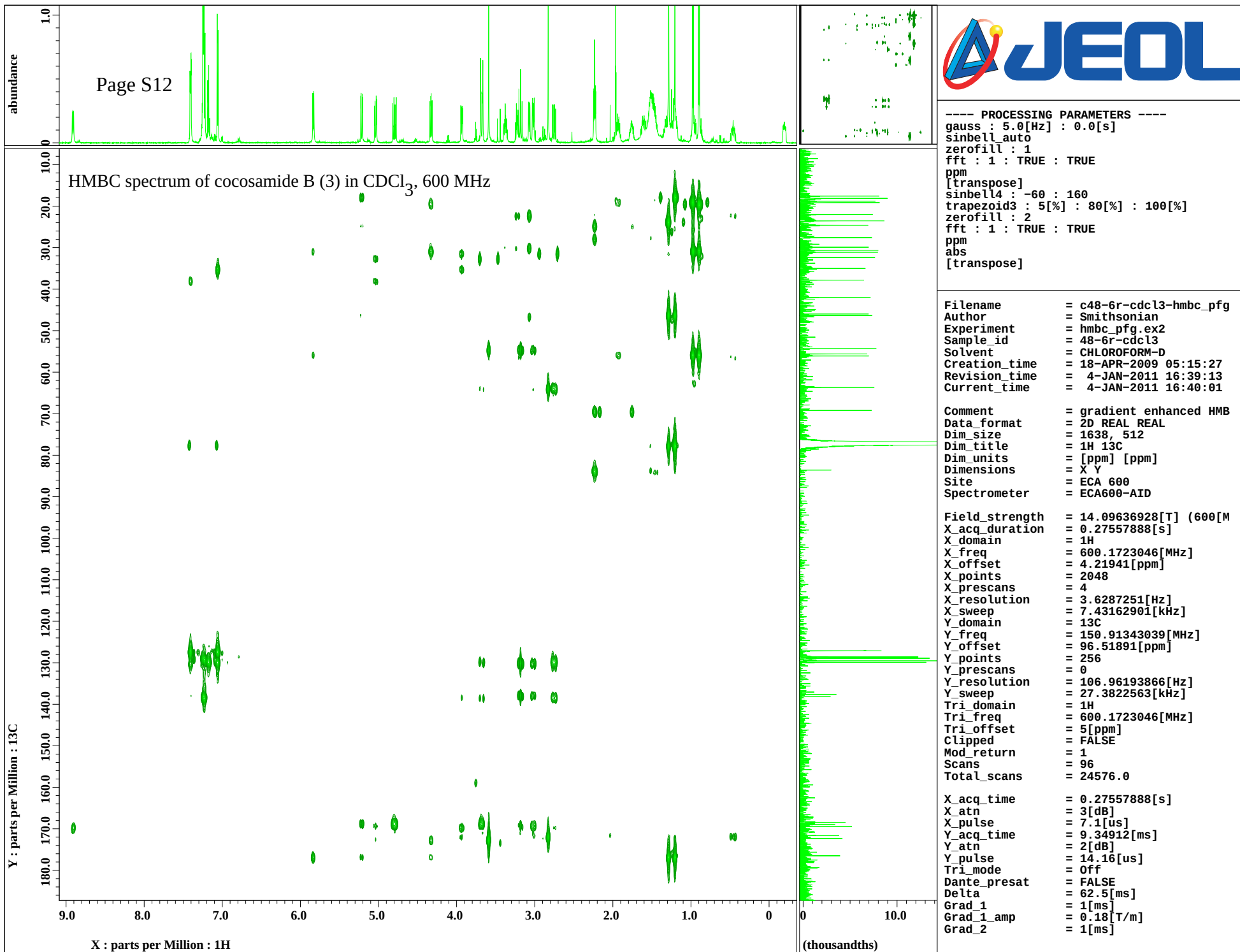
X_90_width = 14.16[us]
 X_acq_time = 0.69206016[s]
 X_angle = 30[deg]
 X_atn = 2[dB]
 X_pulse = 4.72[us]
 Irr_atn_dec = 25[dB]
 Irr_atn_noe = 25[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 60
 Relaxation_delay = 2[s]
 Repetition_time = 2.69206016[s]
 Temp_get = 23.3[dc]



X : parts per Million : 13C

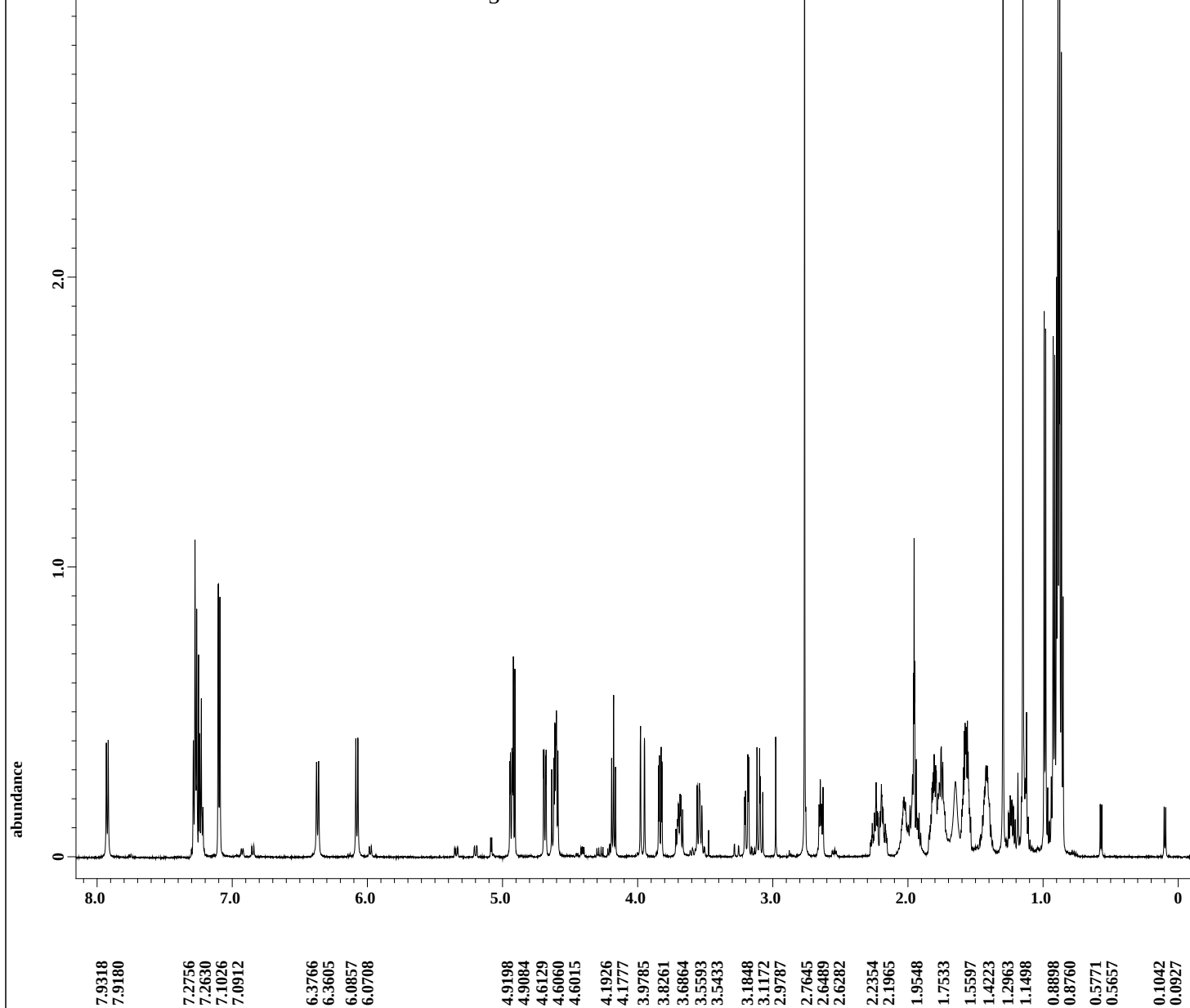








^1H spectrum of pitipeptolide A (5) in CDCl_3 , 600 MHz



X : parts per Million : 1H

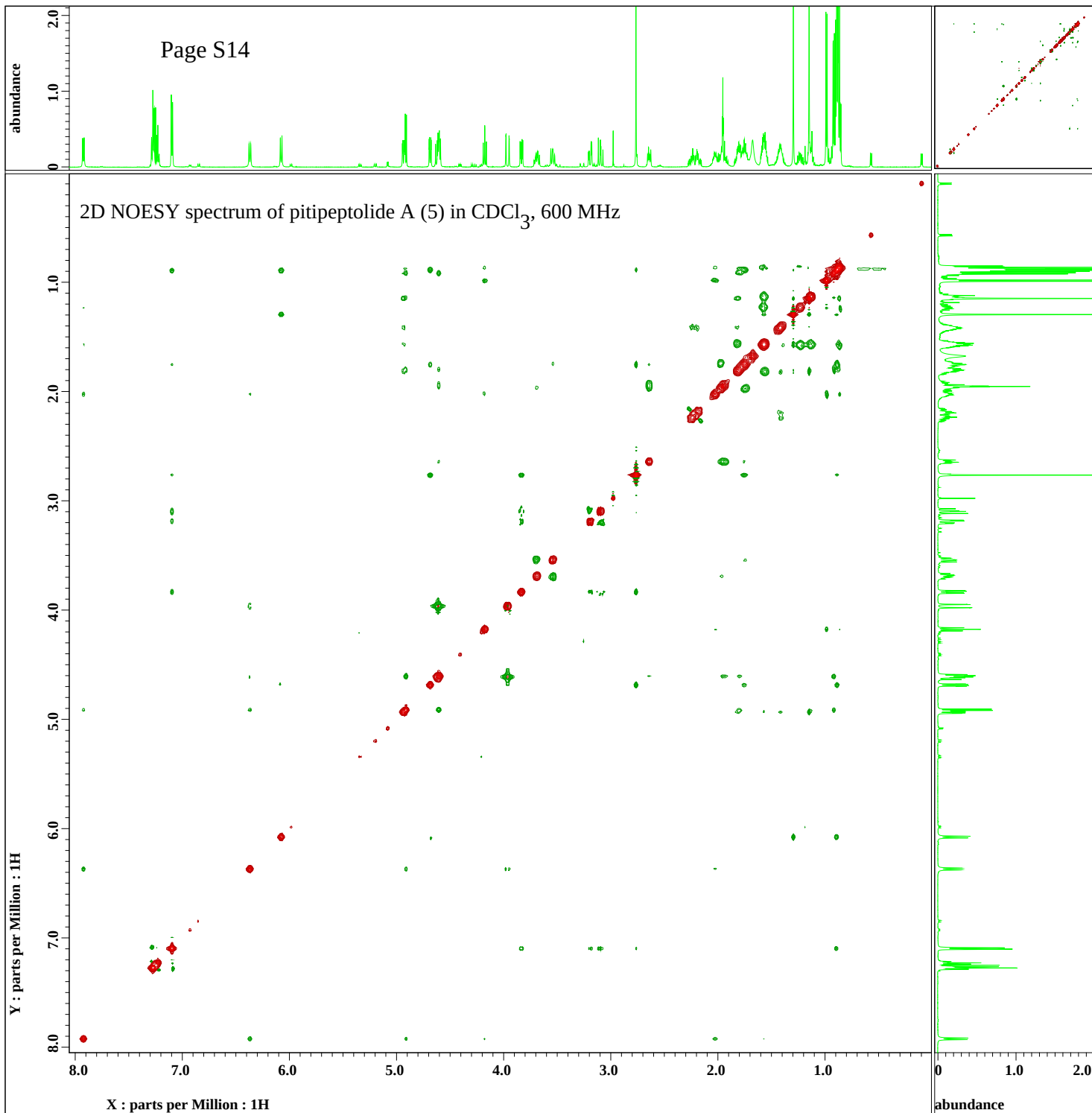
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 secp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm

Filename = pitipeptolide-A-cdcl3
 Author = Smithsonian
 Experiment = single_pulse.ex2
 Sample_id = pitipeptolide-A-cdcl3
 Solvent = CHLOROFORM-D
 Creation_time = 28-JUL-2010 16:51:50
 Revision_time = 5-JAN-2011 12:05:50
 Current_time = 5-JAN-2011 12:07:14

Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = ECA600-AID

Field_strength = 14.09636928[T] (600[M]
 X_acq_duration = 1.4548992[s]
 X_domain = 1H
 X_freq = 600.1723046[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.68733284[Hz]
 X_sweep = 11.26126126[kHz]
 Irr_domain = 1H
 Irr_freq = 600.1723046[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 600.1723046[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 7.31[us]
 X_acq_time = 1.4548992[s]
 X_angle = 45[deg]
 X_atn = 3[dB]
 X_pulse = 3.655[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 54
 Relaxation_delay = 5[s]
 Repetition_time = 6.4548992[s]
 Temp_get = 22[dc]



----- 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

Filename = pitipeptolide A-cdcl3
Author = Smithsonian
Experiment = noesy_phase_pfgz
Sample_id = pitipeptolide A-cdcl3
Solvent = CHLOROFORM-D
Creation_time = 30-JUN-2010 15:05:32
Revision_time = 5-JAN-2011 09:19:00
Current_time = 5-JAN-2011 09:19:44

Comment = phase sensitive noesy
Data_format = 2D COMPLEX COMPLEX
Dim_size = 819, 512
Dim_title = 1H 1H
Dim_units = [ppm] [ppm]
Dimensions = X Y
Site = ECA 600
Spectrometer = ECA600-AID

Field_strength = 14.09636928[T] (600[M]
X_acq_duration = 0.16932864[s]
X_domain = 1H
X_freq = 600.1723046[MHz]
X_offset = 4.02106[ppm]
X_points = 1024
X_prescans = 4
X_resolution = 5.9056755[Hz]
X_sweep = 6.04741171[kHz]
Y_domain = 1H
Y_freq = 600.1723046[MHz]
Y_offset = 4.02106[ppm]
Y_points = 256
Y_prescans = 0
Y_resolution = 18.8926775[Hz]
Y_sweep = 4.83652544[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 600.1723046[MHz]
Tri_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 12
Total_scans = 3072

X_acq_time = 0.16932864[s]
X_atn = 3[dB]
X_pulse = 7.31[us]
Y_acq_time = 52.93056[ms]
Y_p1_correction = 180
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Grad_1 = 1[ms]