Supporting Information:

Caldoramide, a Modified Pentapeptide from the Marine Cyanobacterium *Caldora penicillata*

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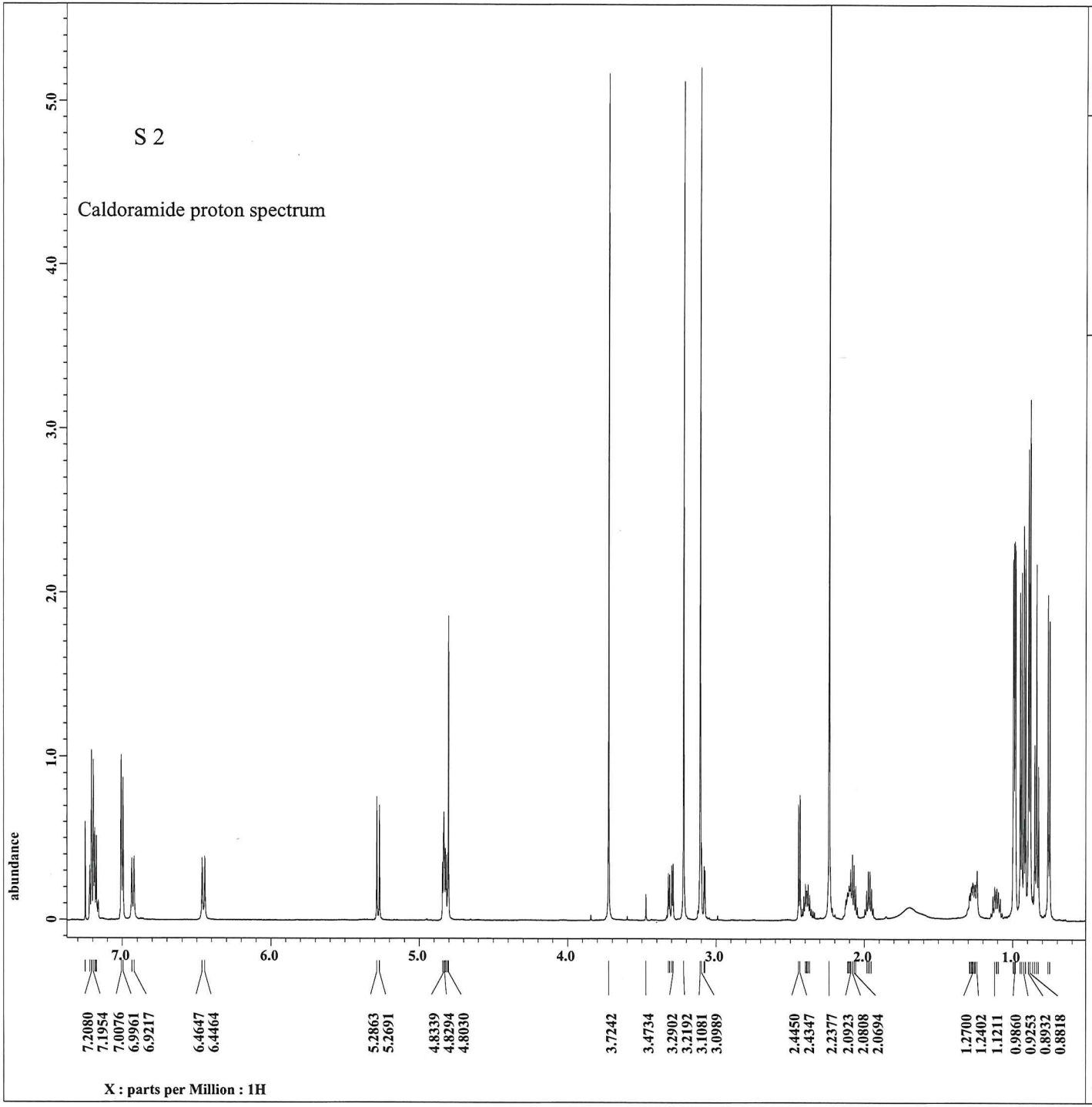
Caldoramide proton spectrum

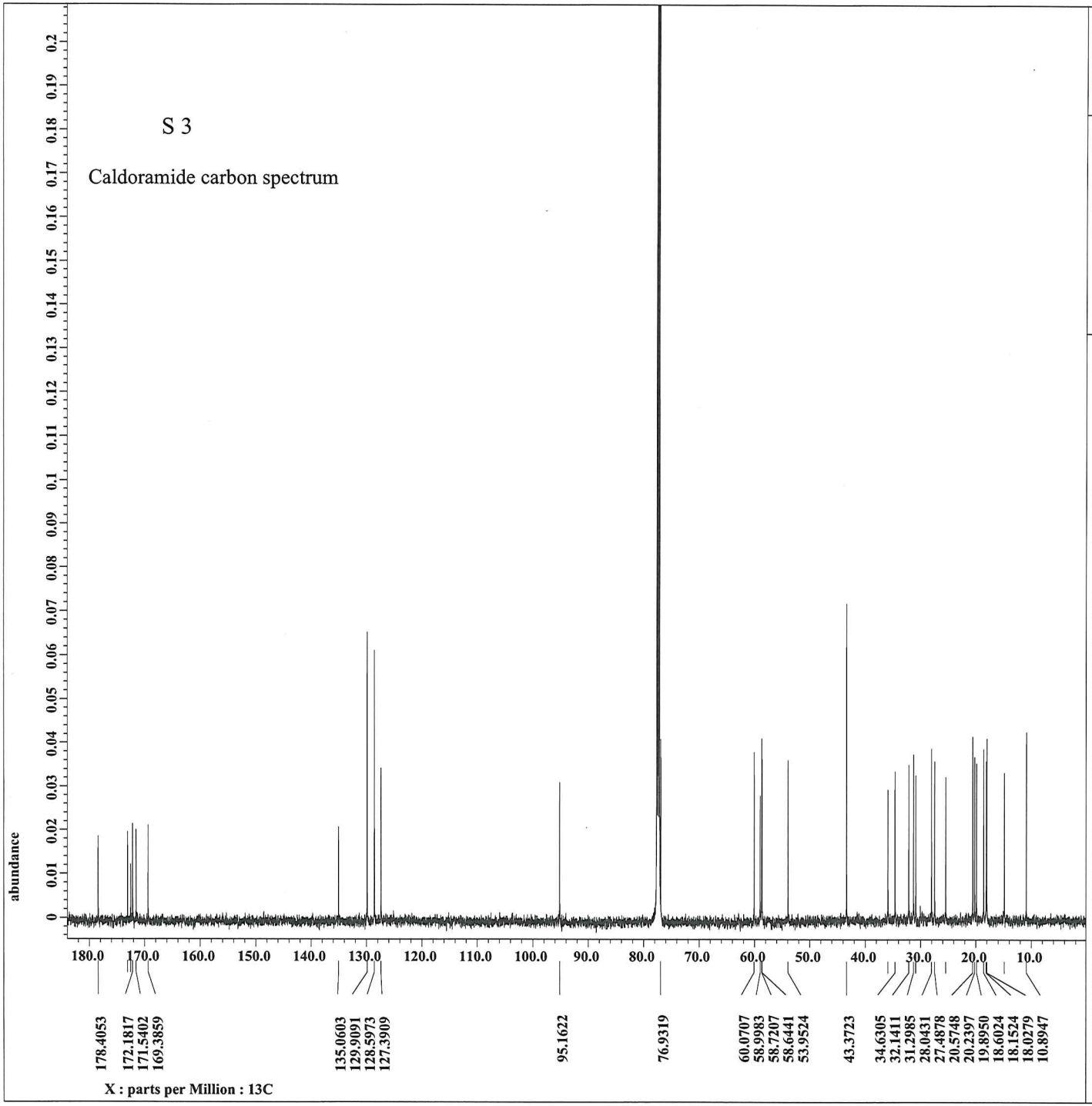


```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
```

Filename	= cg110-3-cdcl3-single_
Author	= Smithsonian
Experiment	= single_pulse.ex2
Sample_id	= cg110-3-cdcl3
Solvent	= CHLOROFORM-D
Creation_time	= 26-JUN-2015 02:59:03
Revision_time	= 29-OCT-2015 12:00:53
Current_time	= 29-OCT-2015 12:01:29
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	= 16
Total_scans	= 16
X_90_width	= 7.5[us]
X_acq_time	= 1.4548992[s]
X_angle	= 45[deg]
X_atn	= 2[dB]
X_pulse	= 3.75[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	= 24.5[dC]

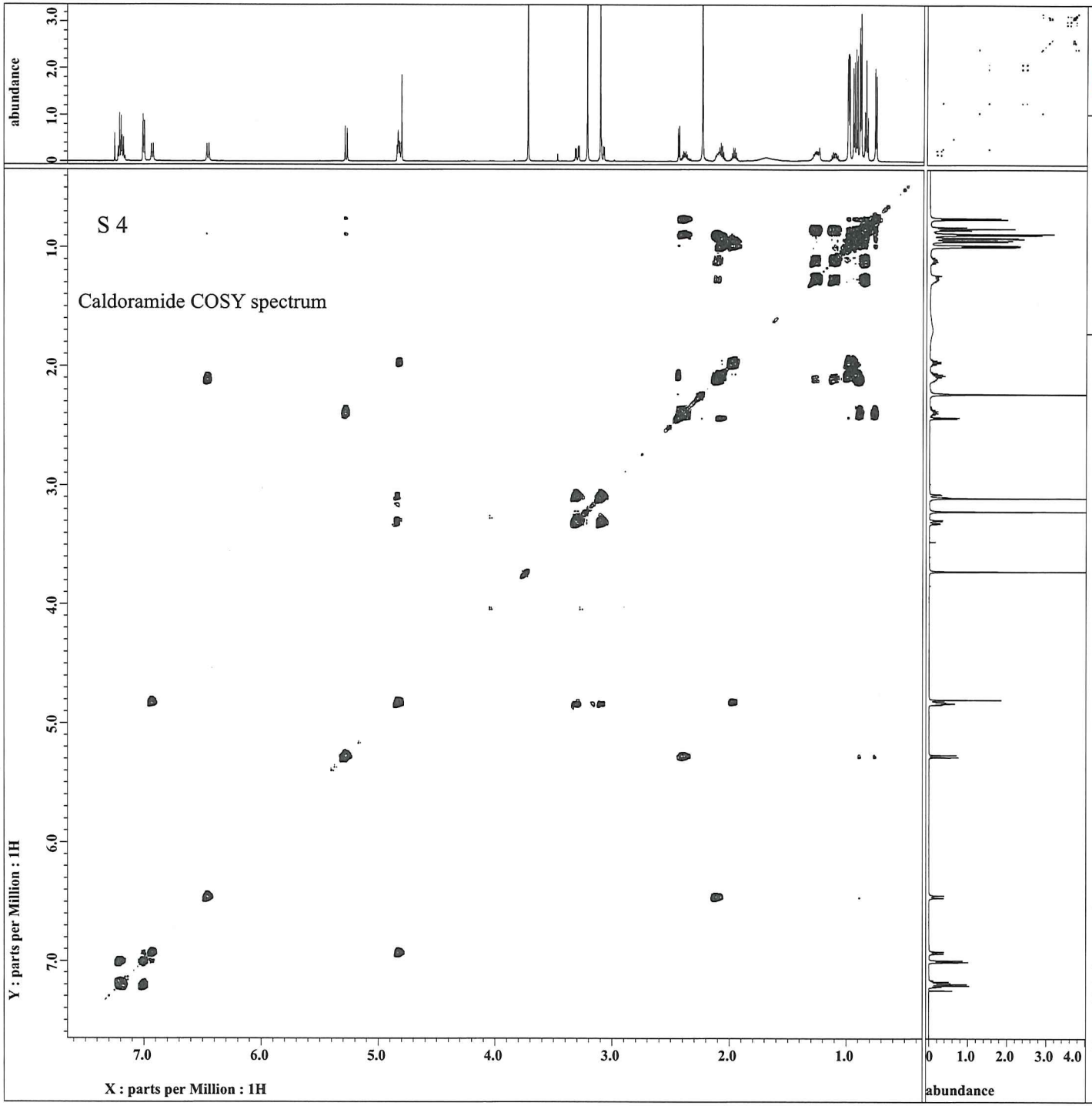
S 3

Caldoramide carbon spectrum



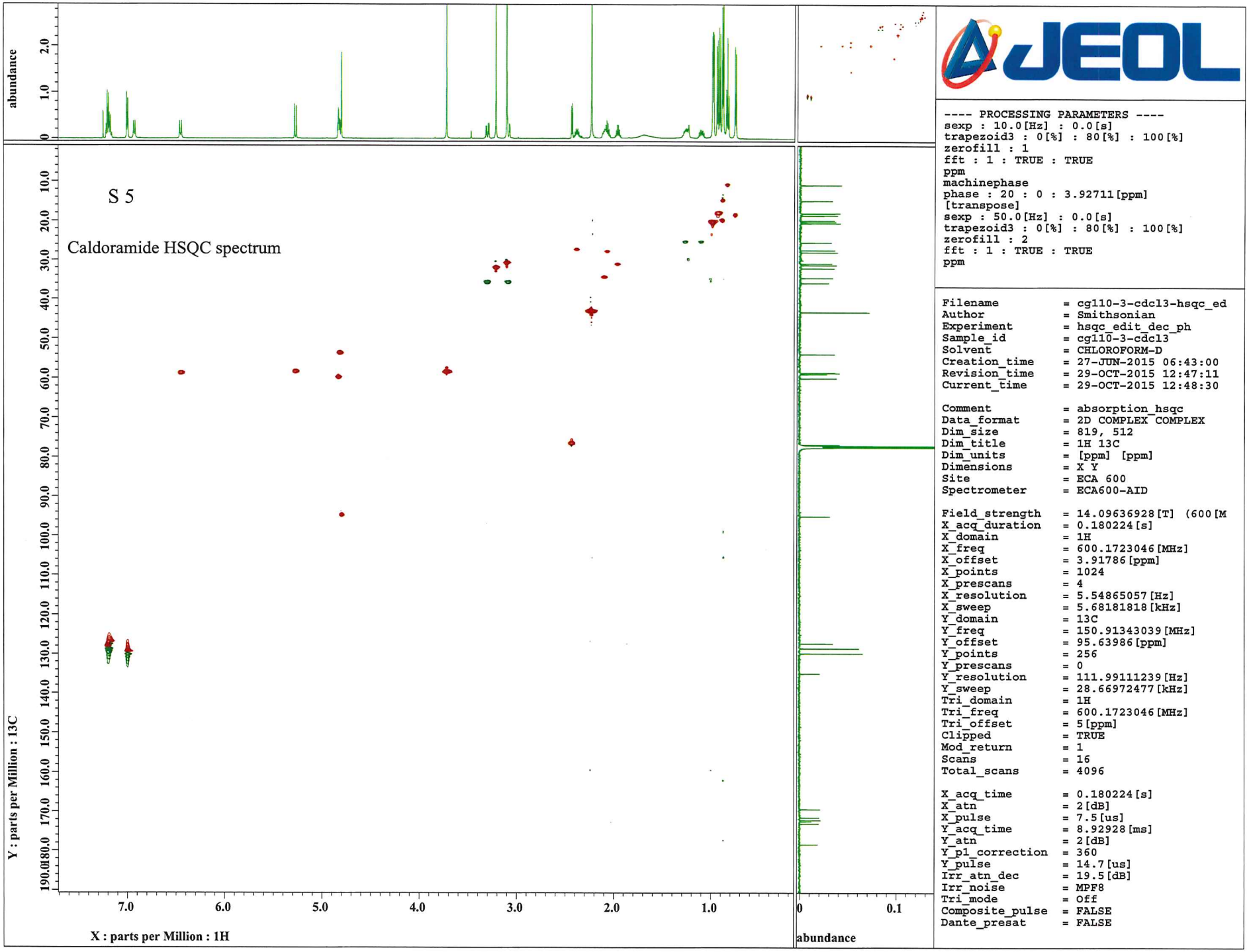
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
```

Filename	= cg110-3-cdcl3-single_
Author	= Smithsonian
Experiment	= single_pulse_dec
Sample_id	= cg110-3-cdcl3
Solvent	= CHLOROFORM-D
Creation_time	= 26-JUN-2015 17:58:15
Revision_time	= 29-OCT-2015 11:50:18
Current_time	= 29-OCT-2015 11:50:52
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	= 14.7[us]
X_acq_time	= 0.69206016[s]
X_angle	= 30[deg]
X_atn	= 2[dB]
X_pulse	= 4.9[us]
Irr_atn_dec	= 24[dB]
Irr_atn_noe	= 24[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	= 24.6[dC]



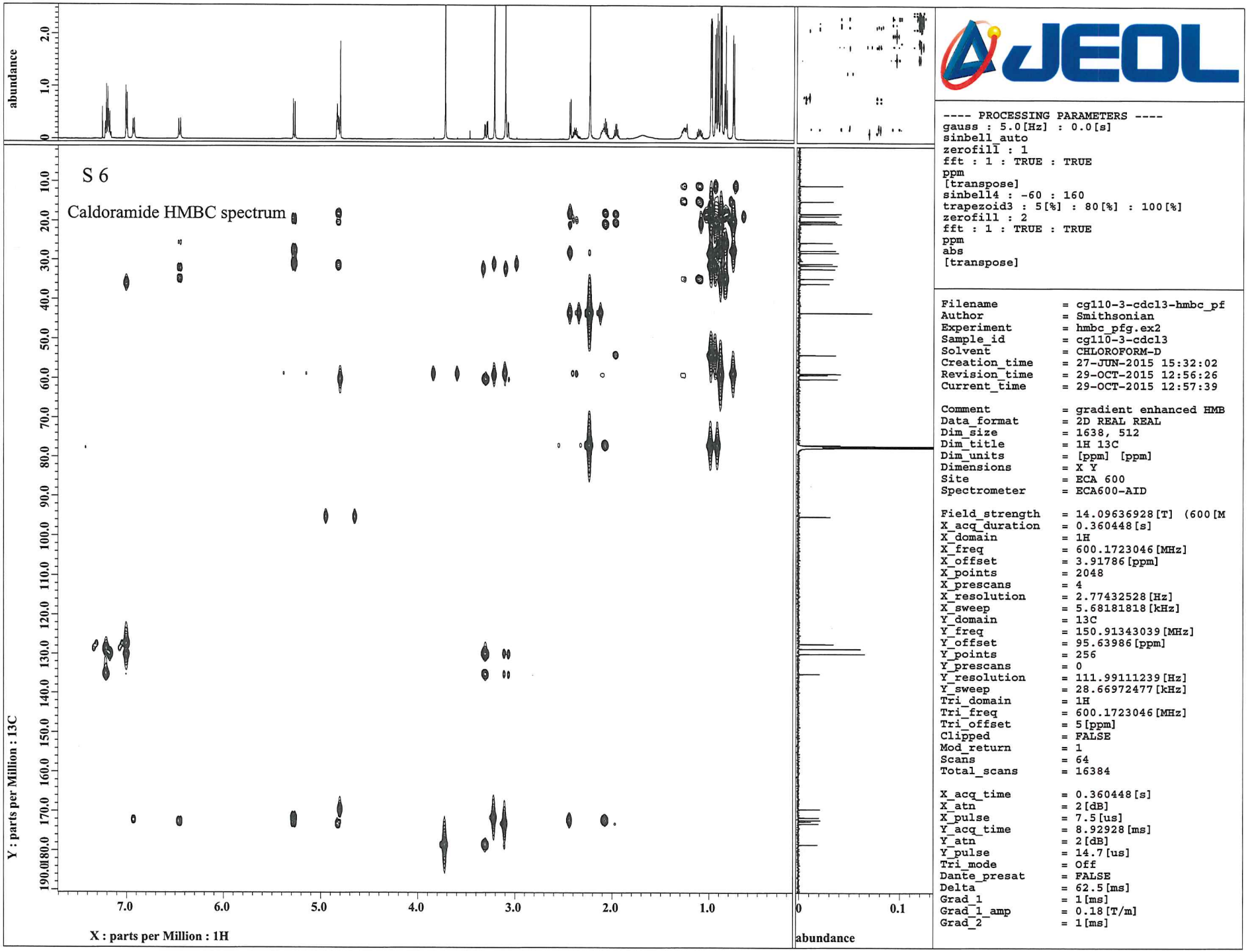

```
---- PROCESSING PARAMETERS ----
sinbell_auto
fft : 1 : TRUE : TRUE
ppm
[transpose]
zerofill : 4
sinbell_auto
fft : 1 : TRUE : TRUE
ppm
abs
thresh : 2[%] : 1
symmetrize : Cosy : 24
[transpose]
```

Filename	= cg110-3-cdcl3-dqf_cos
Author	= Smithsonian
Experiment	= dqf_cosy_pfg.ex2
Sample_id	= cg110-3-cdcl3
Solvent	= CHLOROFORM-D
Creation_time	= 26-JUN-2015 18:36:08
Revision_time	= 29-OCT-2015 11:58:13
Current_time	= 29-OCT-2015 11:59:42
Comment	= gradient absolute val
Data_format	= 2D REAL REAL
Dim_size	= 1024, 1024
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	= 0.2333696[s]
X_domain	= 1H
X_freq	= 600.1723046[MHz]
X_offset	= 3.99617[ppm]
X_points	= 1280
X_prescans	= 4
X_resolution	= 4.28504827[Hz]
X_sweep	= 5.48486178[kHz]
Y_domain	= 1H
Y_freq	= 600.1723046[MHz]
Y_offset	= 3.99617[ppm]
Y_points	= 256
Y_prescans	= 0
Y_resolution	= 17.13868901[Hz]
Y_sweep	= 4.38750439[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	= 4
Total_scans	= 1024
X_acq_time	= 0.2333696[s]
X_atn	= 2[dB]
X_pulse	= 7.5[us]
Y_acq_time	= 58.34752[ms]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Grad_1	= 1[ms]
Grad_1_amp	= 60[mT/m]



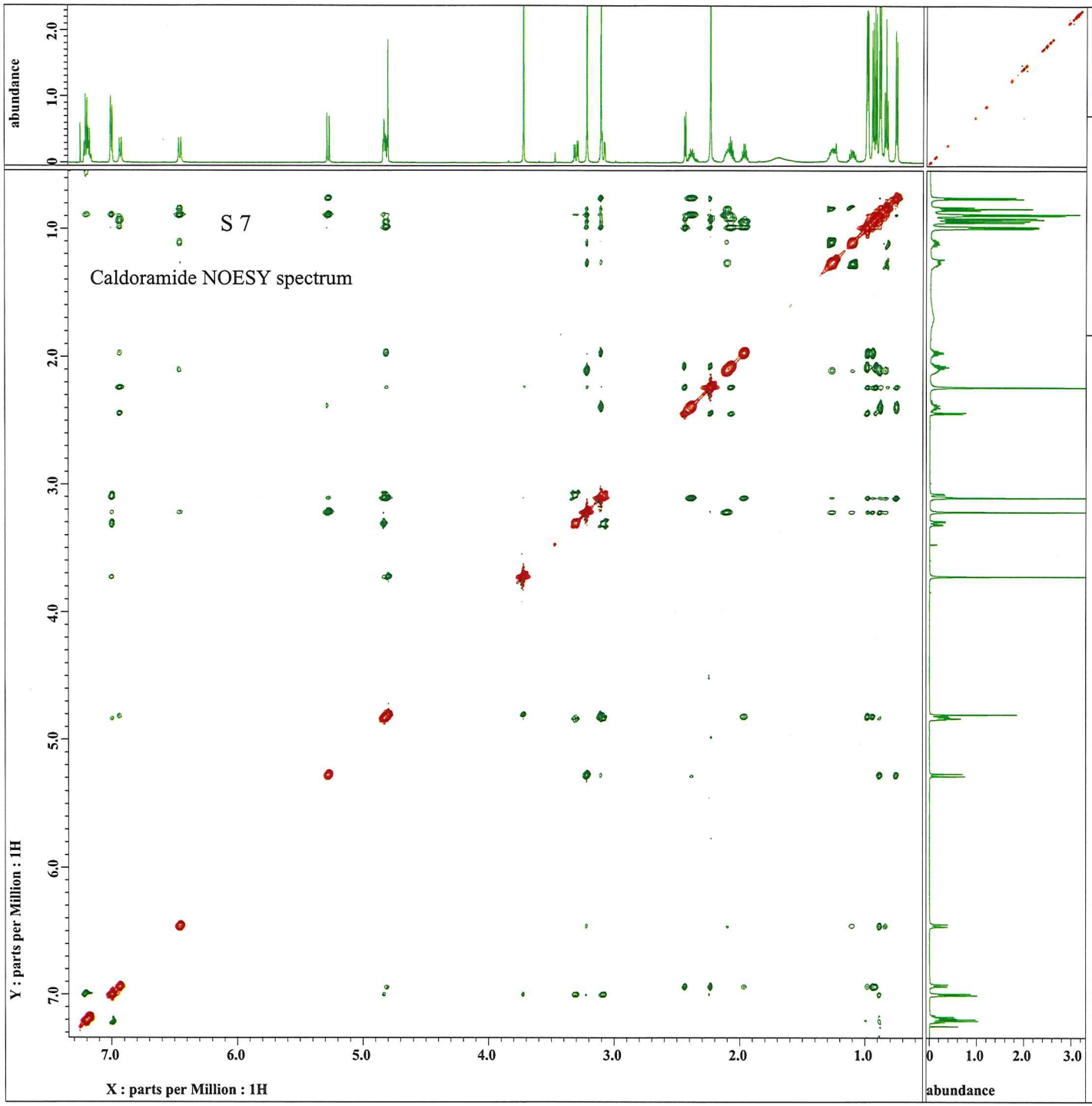

```
---- PROCESSING PARAMETERS ----
sexp : 10.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
ppm
machinephase
phase : 20 : 0 : 3.92711[ppm]
[transpose]
sexp : 50.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 2
fft : 1 : TRUE : TRUE
ppm
```

Filename	= cg110-3-cdcl3-hsqc_ed
Author	= Smithsonian
Experiment	= hsqc_edit_dec_ph
Sample_id	= cg110-3-cdcl3
Solvent	= CHLOROFORM-D
Creation_time	= 27-JUN-2015 06:43:00
Revision_time	= 29-OCT-2015 12:47:11
Current_time	= 29-OCT-2015 12:48:30
Comment	= absorption_hsqc
Data_format	= 2D COMPLEX COMPLEX
Dim_size	= 819, 512
Dim_title	= 1H 13C
Dim_units	= [ppm] [ppm]
Dimensions	= X Y
Site	= ECA 600
Spectrometer	= ECA600-AID
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 0.180224[s]
X_domain	= 1H
X_freq	= 600.1723046[MHz]
X_offset	= 3.91786[ppm]
X_points	= 1024
X_prescans	= 4
X_resolution	= 5.54865057[Hz]
X_sweep	= 5.68181818[kHz]
Y_domain	= 13C
Y_freq	= 150.91343039[MHz]
Y_offset	= 95.63986[ppm]
Y_points	= 256
Y_prescans	= 0
Y_resolution	= 111.99111239[Hz]
Y_sweep	= 28.66972477[kHz]
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	= 0.180224[s]
X_atn	= 2[dB]
X_pulse	= 7.5[us]
Y_acq_time	= 8.92928[ms]
Y_atn	= 2[dB]
Y_pl_correction	= 360
Y_pulse	= 14.7[us]
Irr_atn_dec	= 19.5[dB]
Irr_noise	= MPF8
Tri_mode	= Off
Composite_pulse	= FALSE
Dante_presat	= FALSE




```
---- PROCESSING PARAMETERS ----
gauss : 5.0[Hz] : 0.0[s]
sinbell_auto
zerofill : 1
fft : 1 : TRUE : TRUE
ppm
[transpose]
sinbell4 : -60 : 160
trapezoid3 : 5[%] : 80[%] : 100[%]
zerofill : 2
fft : 1 : TRUE : TRUE
ppm
abs
[transpose]
```

Filename	= cg110-3-cdcl3-hmbc_pf
Author	= Smithsonian
Experiment	= hmbc_pfg.ex2
Sample_id	= cg110-3-cdcl3
Solvent	= CHLOROFORM-D
Creation_time	= 27-JUN-2015 15:32:02
Revision_time	= 29-OCT-2015 12:56:26
Current_time	= 29-OCT-2015 12:57:39
Comment	= gradient enhanced HMB
Data_format	= 2D REAL REAL
Dim_size	= 1638, 512
Dim_title	= 1H 13C
Dim_units	= [ppm] [ppm]
Dimensions	= X Y
Site	= ECA 600
Spectrometer	= ECA600-AID
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 0.360448[s]
X_domain	= 1H
X_freq	= 600.1723046[MHz]
X_offset	= 3.91786[ppm]
X_points	= 2048
X_prescans	= 4
X_resolution	= 2.77432528[Hz]
X_sweep	= 5.68181818[kHz]
Y_domain	= 13C
Y_freq	= 150.91343039[MHz]
Y_offset	= 95.63986[ppm]
Y_points	= 256
Y_prescans	= 0
Y_resolution	= 111.99111239[Hz]
Y_sweep	= 28.66972477[kHz]
Tri_domain	= 1H
Tri_freq	= 600.1723046[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 64
Total_scans	= 16384
X_acq_time	= 0.360448[s]
X_atn	= 2[dB]
X_pulse	= 7.5[us]
Y_acq_time	= 8.92928[ms]
Y_atn	= 2[dB]
Y_pulse	= 14.7[us]
Tri_mode	= Off
Dante_presat	= FALSE
Delta	= 62.5[ms]
Grad_1	= 1[ms]
Grad_1_amp	= 0.18[T/m]
Grad_2	= 1[ms]




```
---- 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	= cg110-3a-noesy_phase_
Author	= Smithsonian
Experiment	= noesy_phase_pfgz
Sample_id	= cg110-3a
Solvent	= CHLOROFORM-D
Creation_time	= 8-JUL-2015 13:18:38
Revision_time	= 29-OCT-2015 13:03:20
Current_time	= 29-OCT-2015 13:04:22
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	= 0.20037632[s]
X_domain	= 1H
X_freq	= 600.1723046[MHz]
X_offset	= 3.93305[ppm]
X_points	= 1024
X_prescans	= 4
X_resolution	= 4.99060967[Hz]
X_sweep	= 5.1103843[kHz]
Y_domain	= 1H
Y_freq	= 600.1723046[MHz]
Y_offset	= 3.93305[ppm]
Y_points	= 256
Y_prescans	= 0
Y_resolution	= 15.9660345[Hz]
Y_sweep	= 4.08730483[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	= 32
Total_scans	= 8192
X_acq_time	= 0.20037632[s]
X_atn	= 2[dB]
X_pulse	= 7.5[us]
Y_acq_time	= 62.63296[ms]
Y_p1_correction	= 180
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Grad_1	= 1[ms]