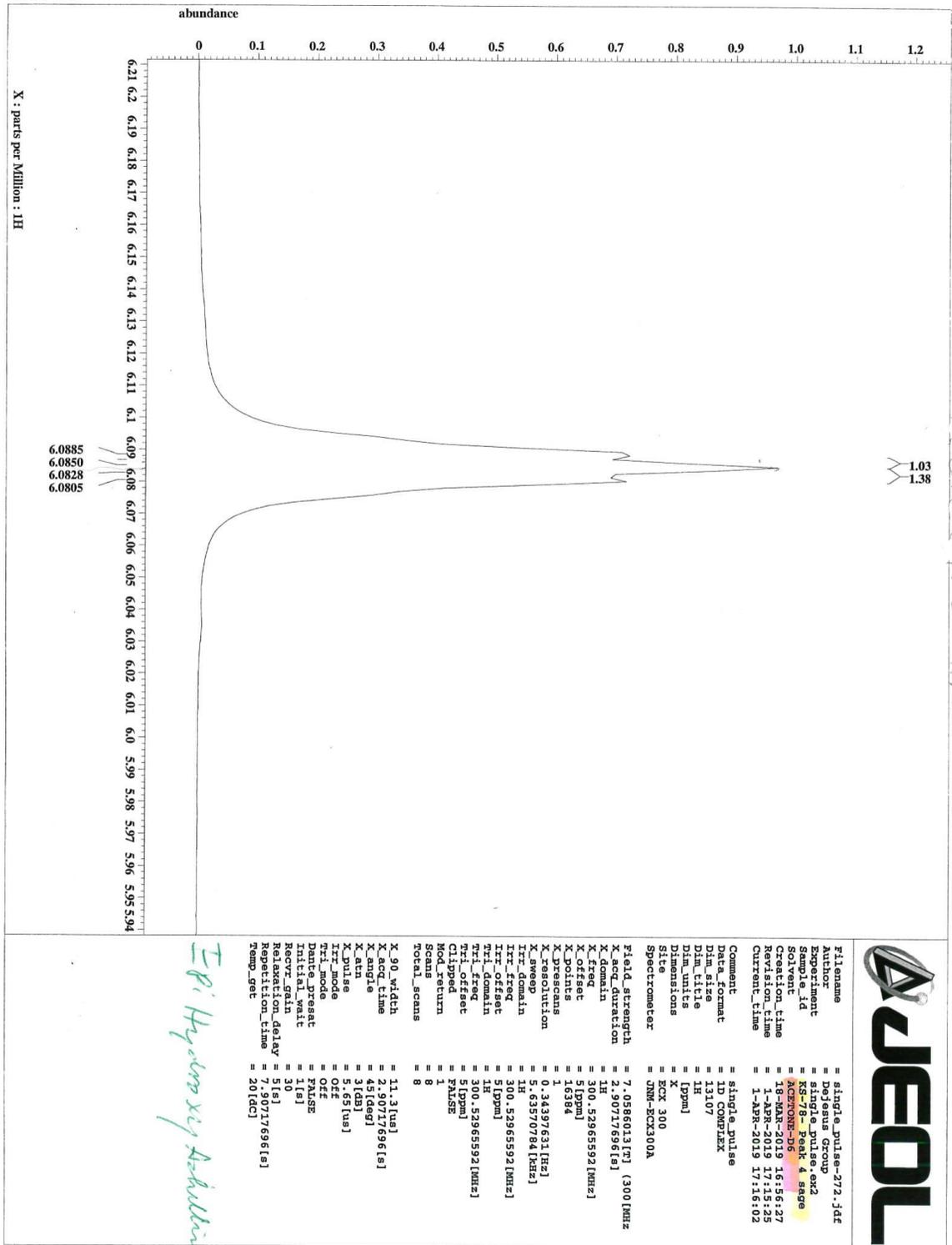
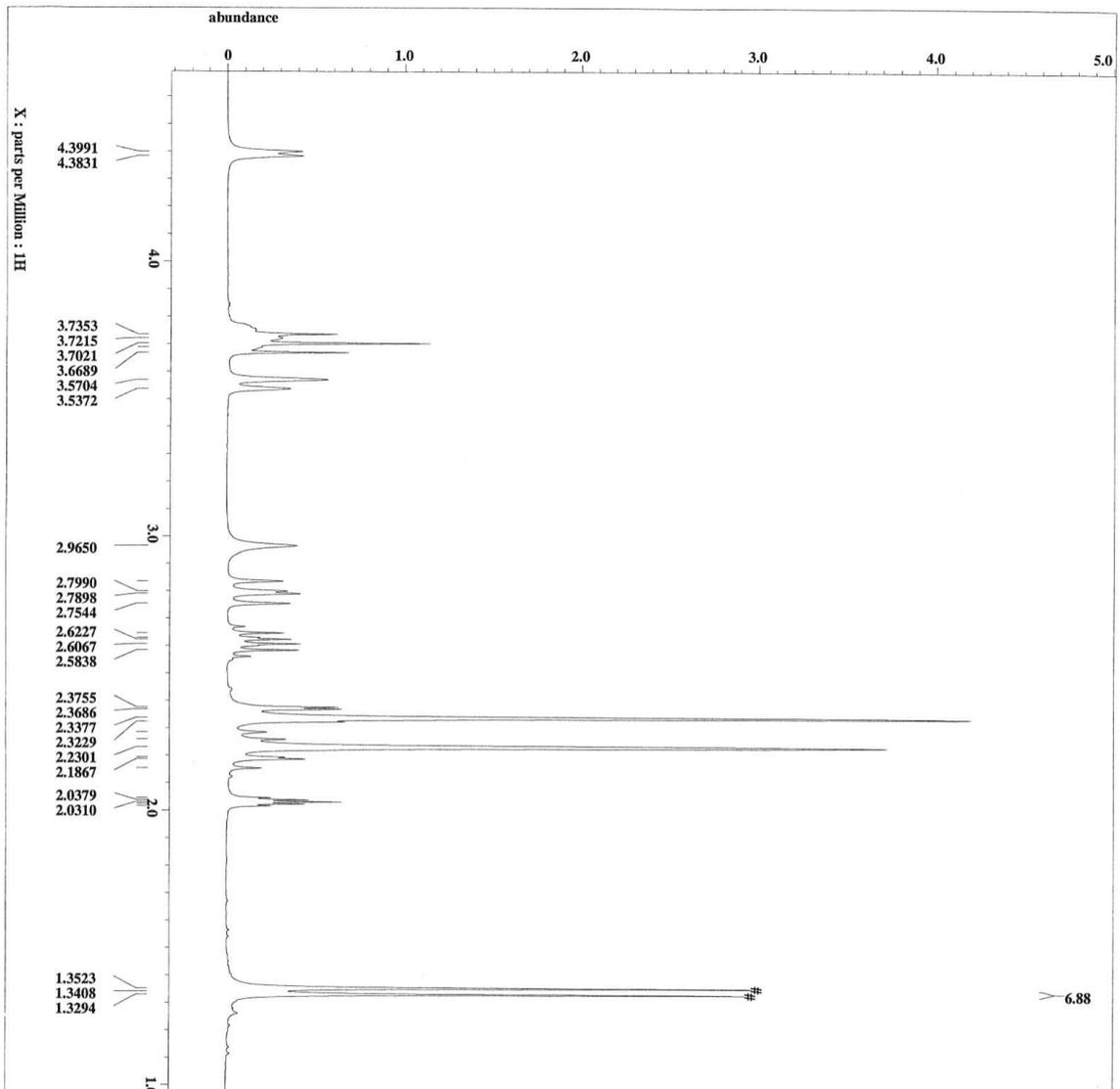


6.4 Hydroxyachillin NMR Spectra





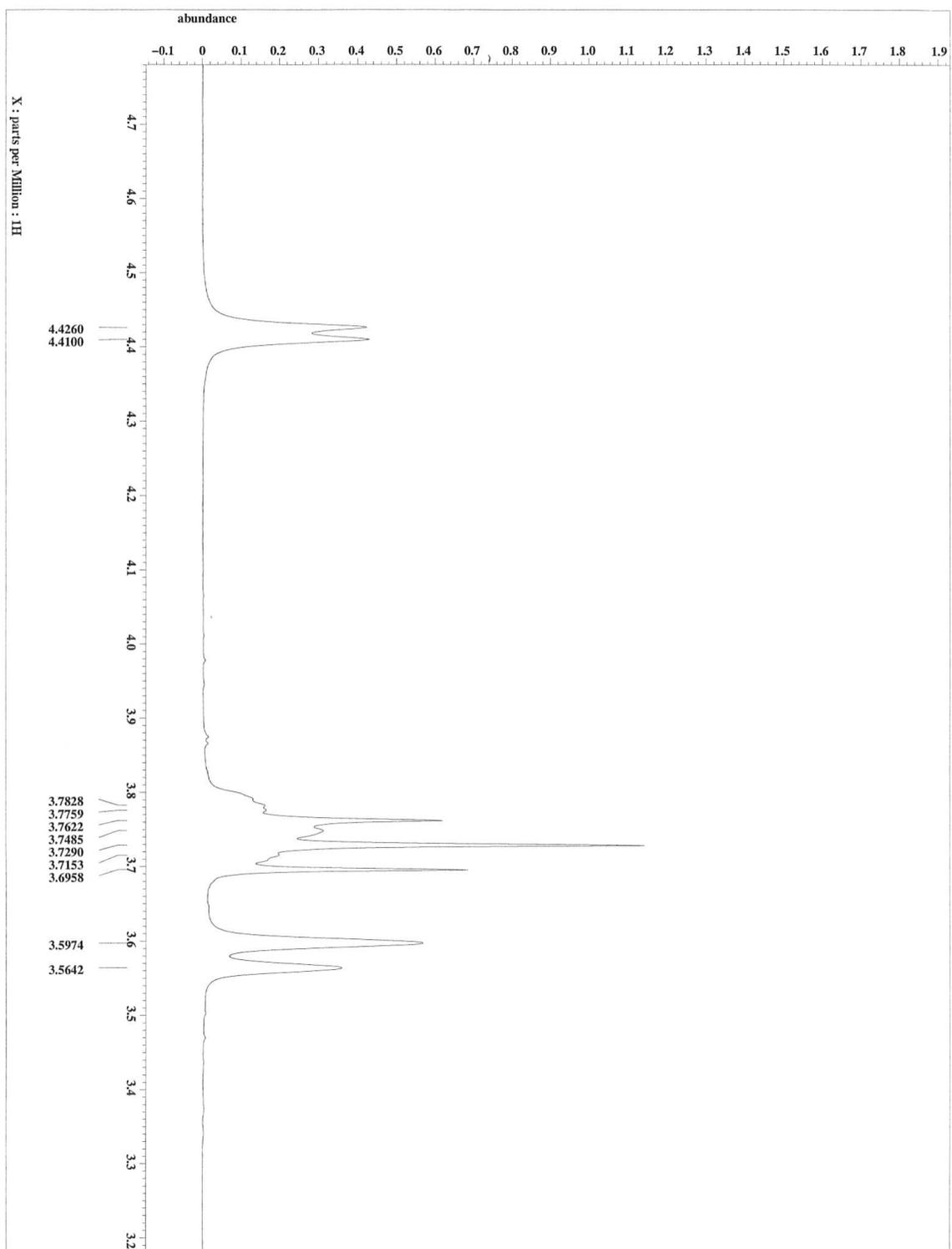
```

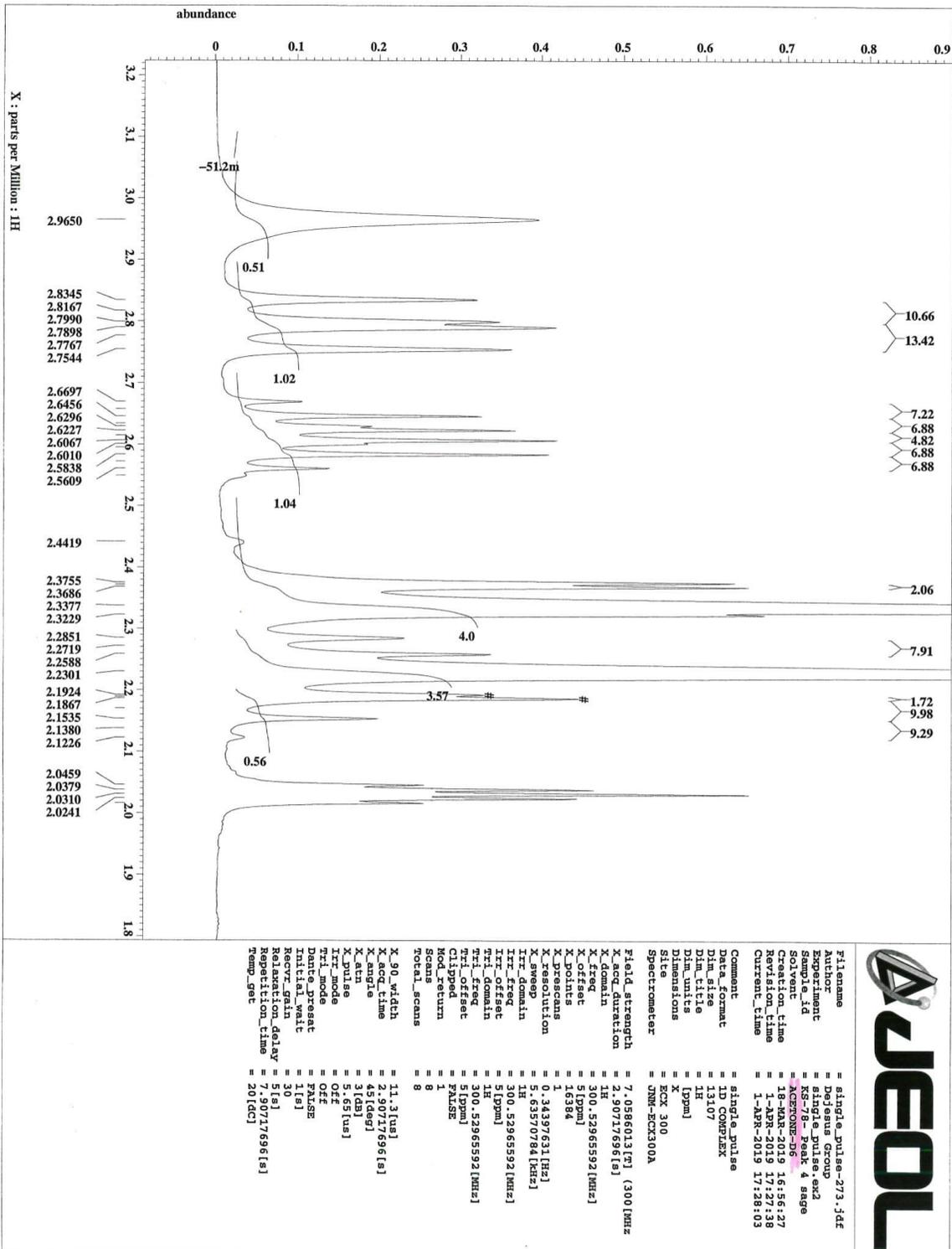
Filename = single_pulse-272.fdf
Author = Dejeus Group
Experiment = single_pulse.ex2
Sample_id = KS-78-Resk_4_sage
Create_time = 16-Nov-2019 16:56:27
Revision_time = 1-Apr-2019 17:15:25
Current_time = 1-Apr-2019 17:15:30

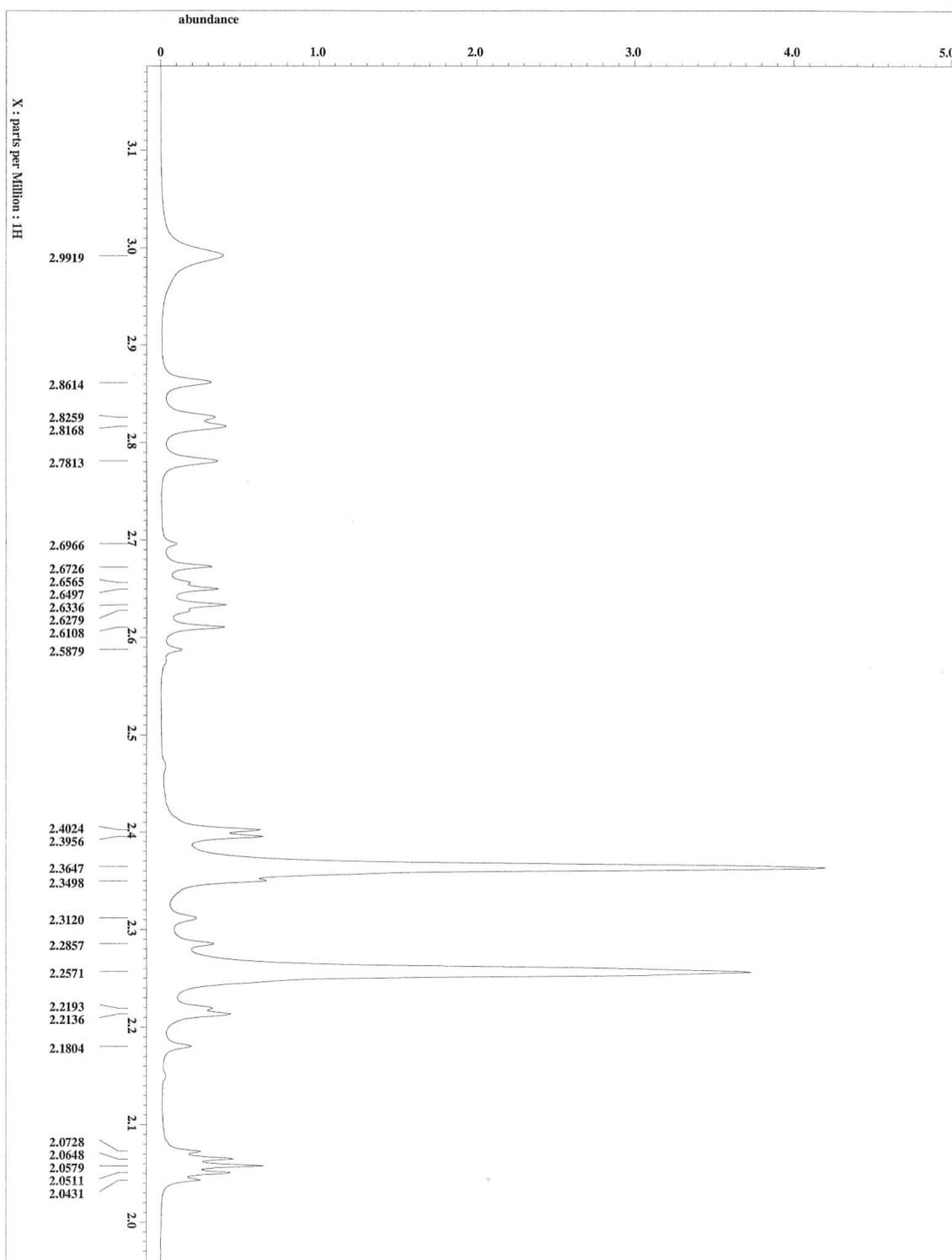
Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 13107
Dim_title = 1H
Dimensions = X [ppm]
Site = ECK 300
Spectrometer = JNM-ECX300A

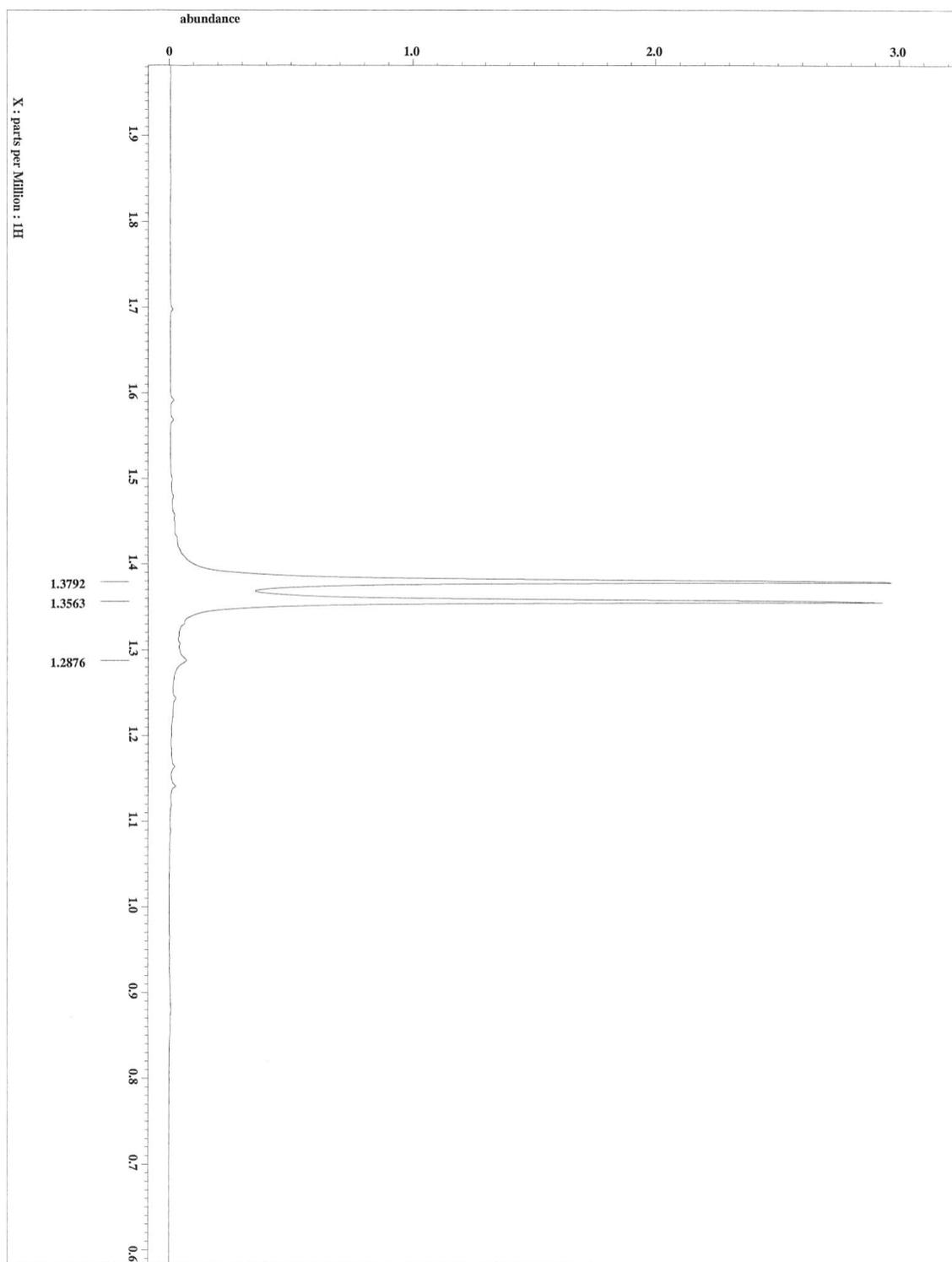
Field_strength = 7.0586013171 (300) [MHz]
X_acq_duration = 2.90717696 [s]
X_domain = 1H
X_freq = 300.52965592 [MHz]
X_gain = 16384
X_points = 1
X_prescans = 1
X_resolution = 0.34397631 [Hz]
X_sweep = 5.63570784 [MHz]
Irr_domain = 1H
Irr_freq = 300.52965592 [MHz]
Irr_offset = 5 [ppm]
Irr_offset_min = 300.52965592 [MHz]
Irr_offset_max = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 8

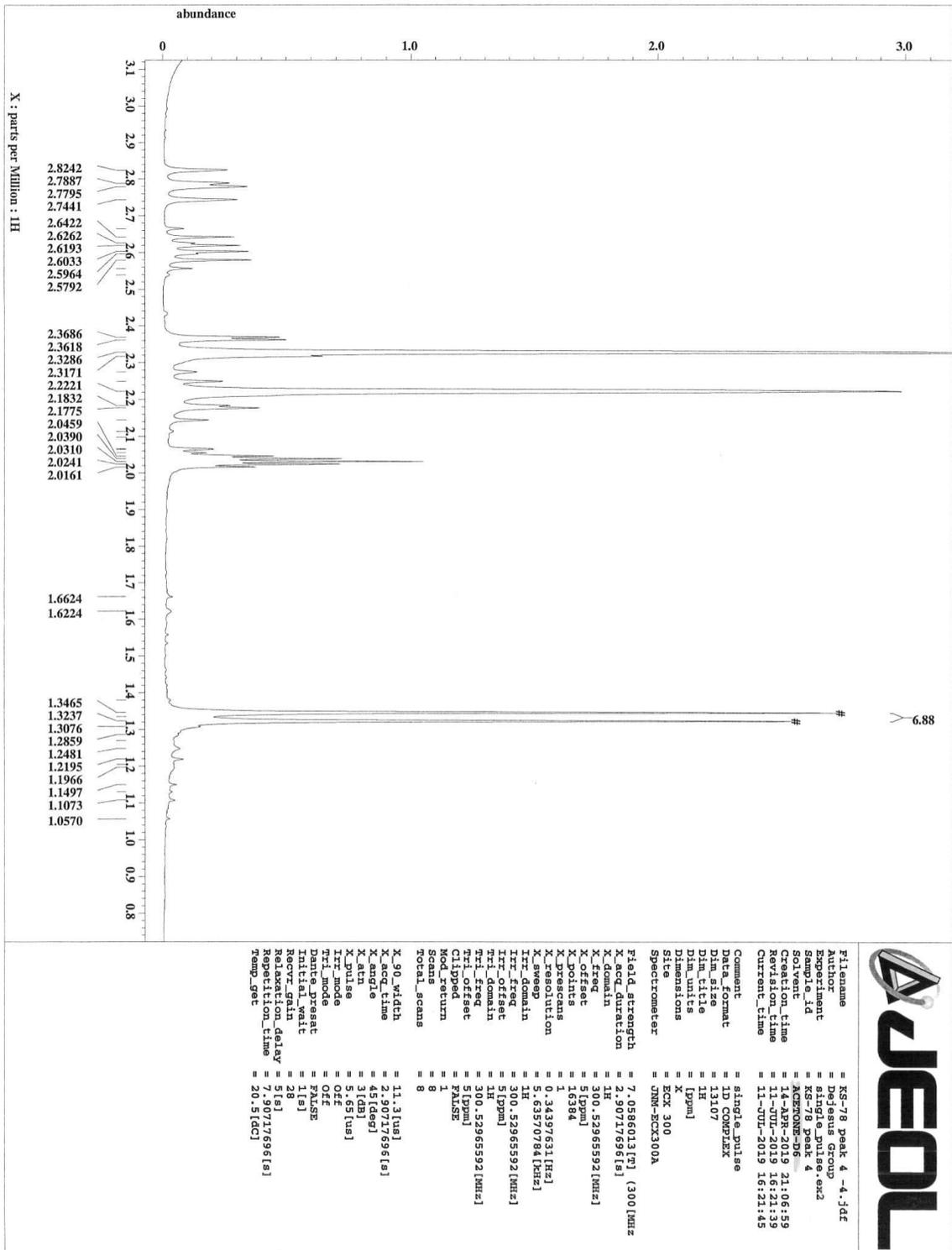
X_90_width = 11.31 [us]
X_acq_time = 2.90717696 [s]
X_angle = 45 [deg]
X_atn = 3 [db]
X_pulse = 5.65 [us]
Irr_mode = Off
Irr_mode_min = Off
Irr_mode_max = Off
Data_presat = FALSE
Initial_wait = 1 [s]
Relaxation_delay = 5 [s]
Repetition_time = 7.90717696 [s]
Temp_get = 20 [dc]
    
```

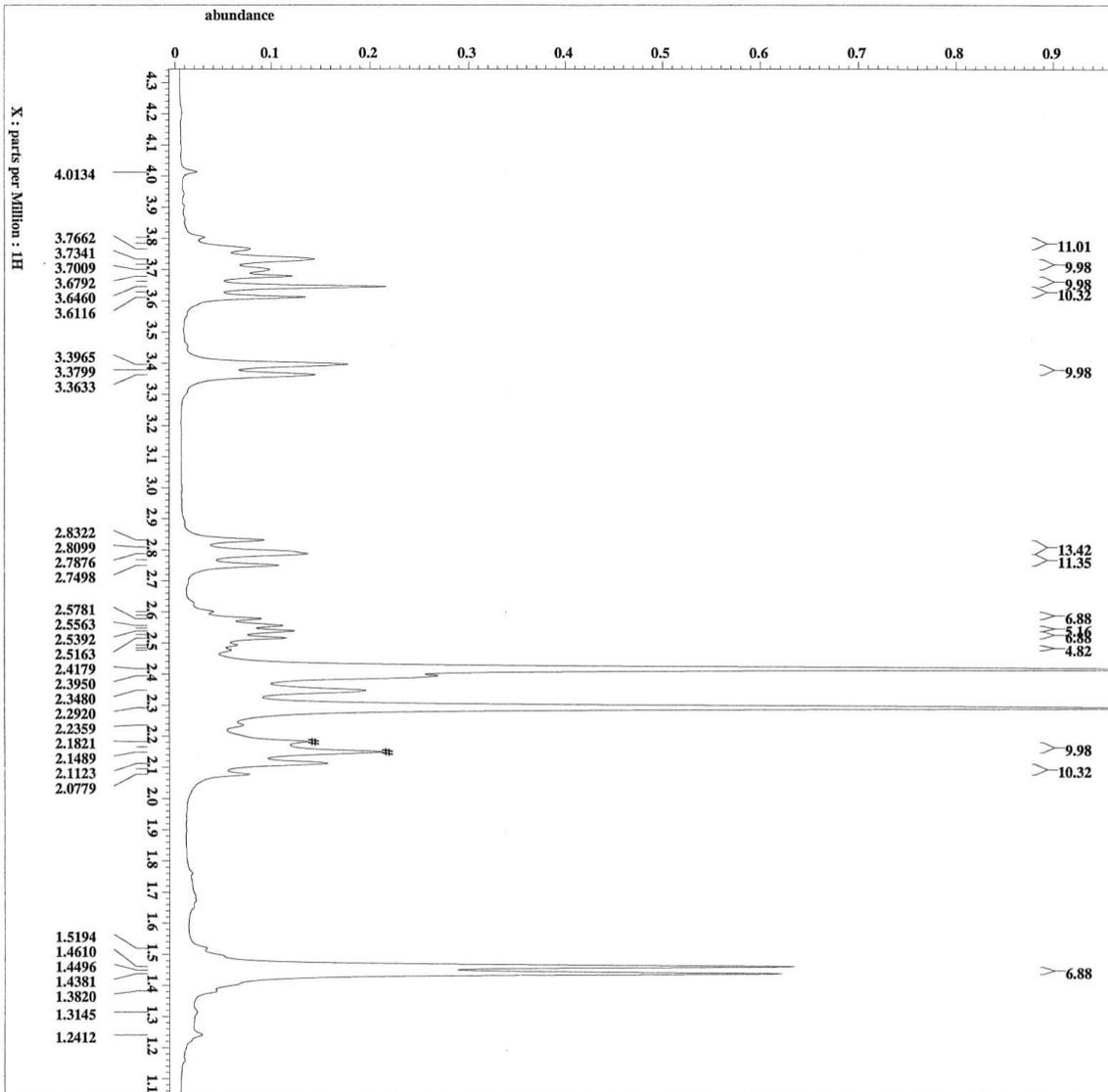










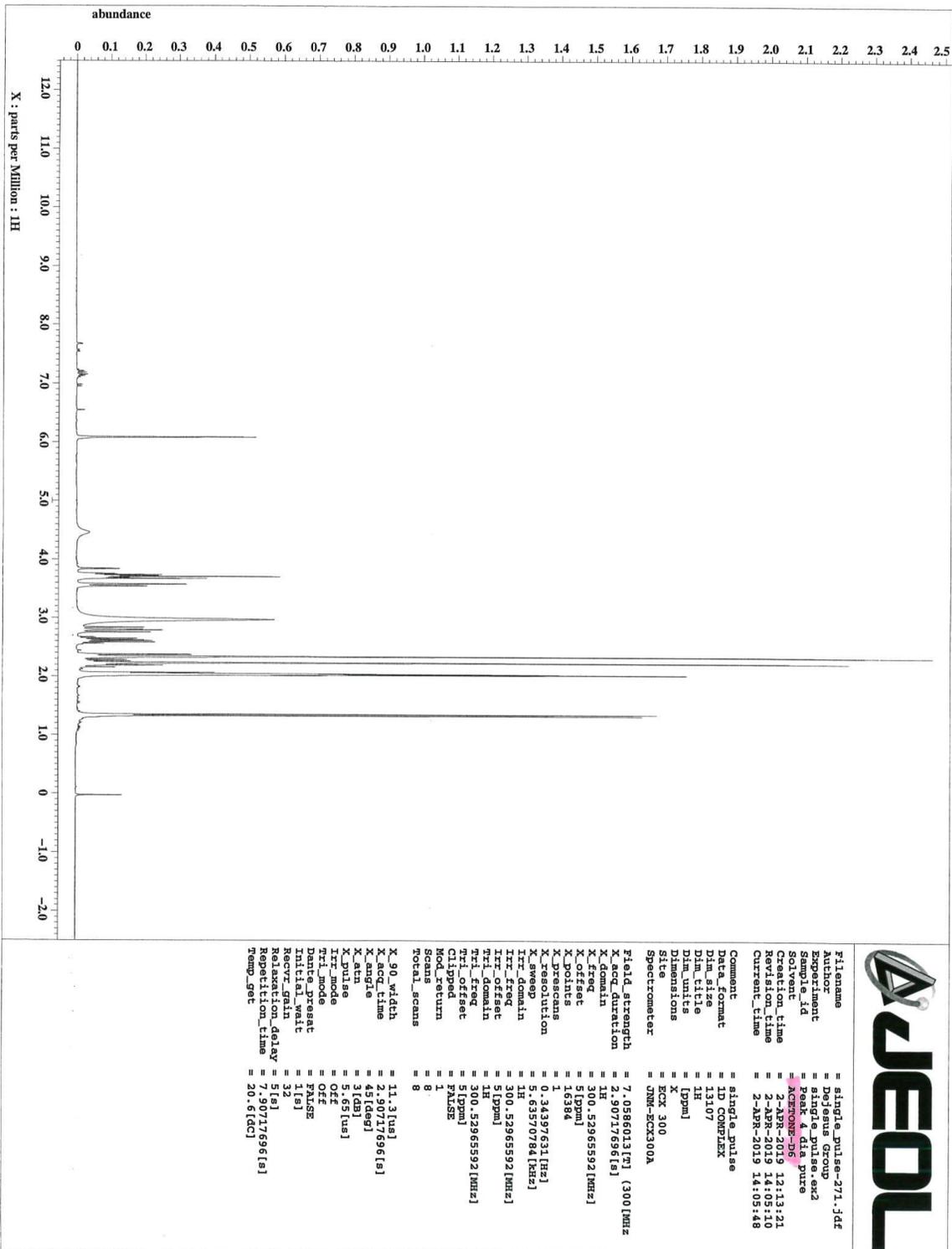


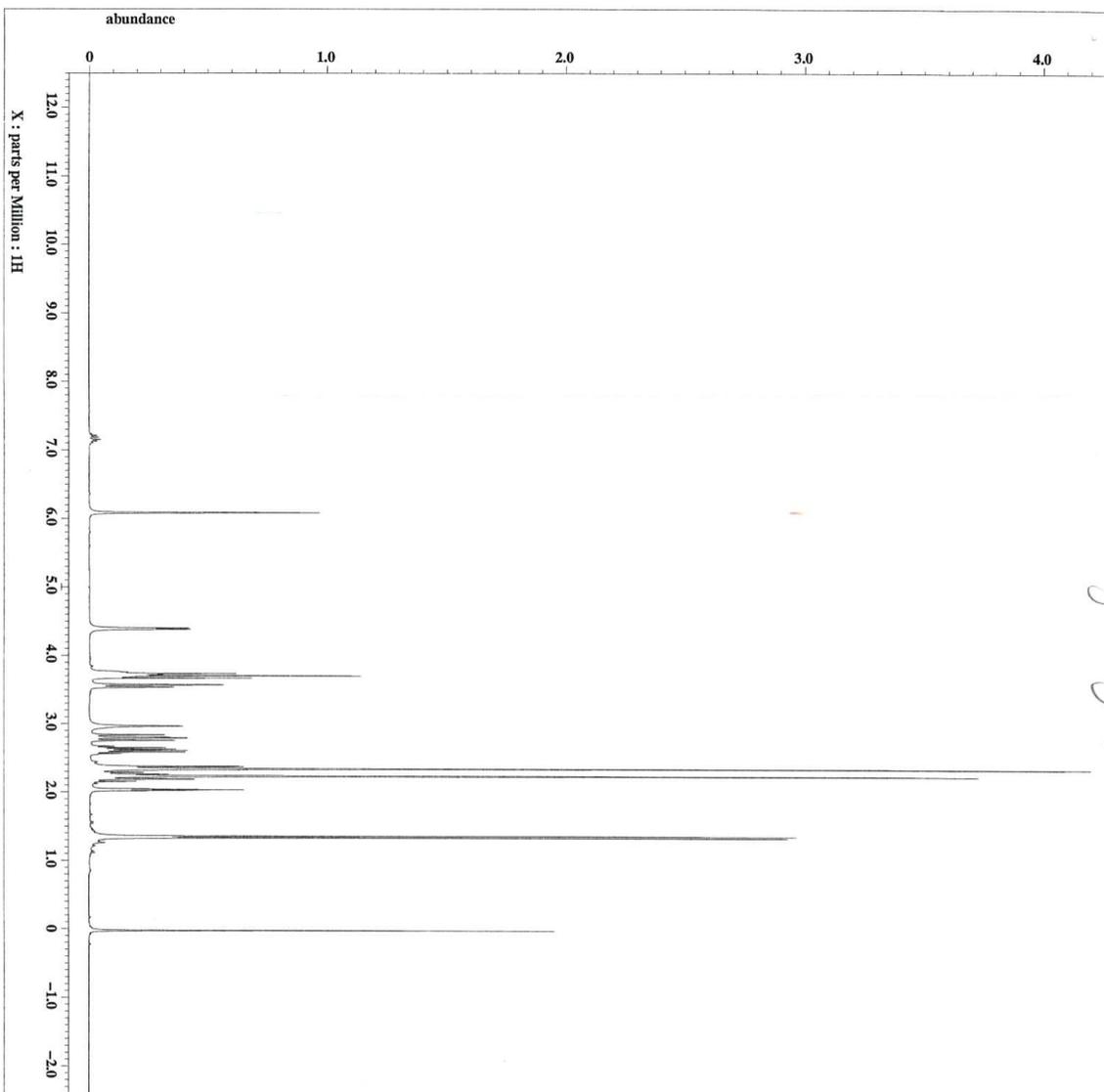
JEOL

```

=====
Filename          = KS-I-23 peak 4 pure-4
Author           = 
Experiment       = 
Sample id       = 
Solvent         = CHLOROFORM-D
Creation time   = 12-Oct-2018 21:06:06
Revision time  = 1-Apr-2019 17:01:14
Current time    = 1-Apr-2019 17:01:26
=====
Comment          = KS-I-23 peak 4 pure
Data format     = COMPMASK
Date_          = 13/07
Dim units      = [ppm]
Dimensions     = X
Site           = ECTX 300
Spectrometer   = JNM-ECTX300A
Field strength = 7.0566013(F1) (300) [MHz]
Acq_resolution = 2.9717696 [Hz]
X_domain       = 1H
X_freq         = 300.52965592 [MHz]
X_offset      = 5 [ppm]
X_points      = 16384
X_procscans   = 1
X_sweep       = 0.34397631 [Hz]
X_resolution  = 5.63570784 [kHz]
X_domain      = 300.52965592 [MHz]
X_offset      = 5 [ppm]
X_domain      = 1H
X_freq        = 300.52965592 [MHz]
X_offset      = 5 [ppm]
Clipped       = FALSE
Mod_return    = 1
Mod_scan      = 64
Mod_return    = 64
X_90_width    = 11.3 [us]
X_acq_time    = 2.90717696 [s]
X_angle       = 45 [deg]
X_atn         = 3 [dB]
X_pulse       = 5.65 [us]
X_mode        = OF
X_datapoint   = PULSE
Initial wait  = 1 [s]
Recvr_gain    = 40
Relaxation_delay = 5 [s]
Repetition_time = 7.90717696 [s]
Temp_get      = 20.4 [dC]
=====
    
```

Abilim - 04
Original Peak 4





hydroxyanthranilic

COSY HMR, CPMR



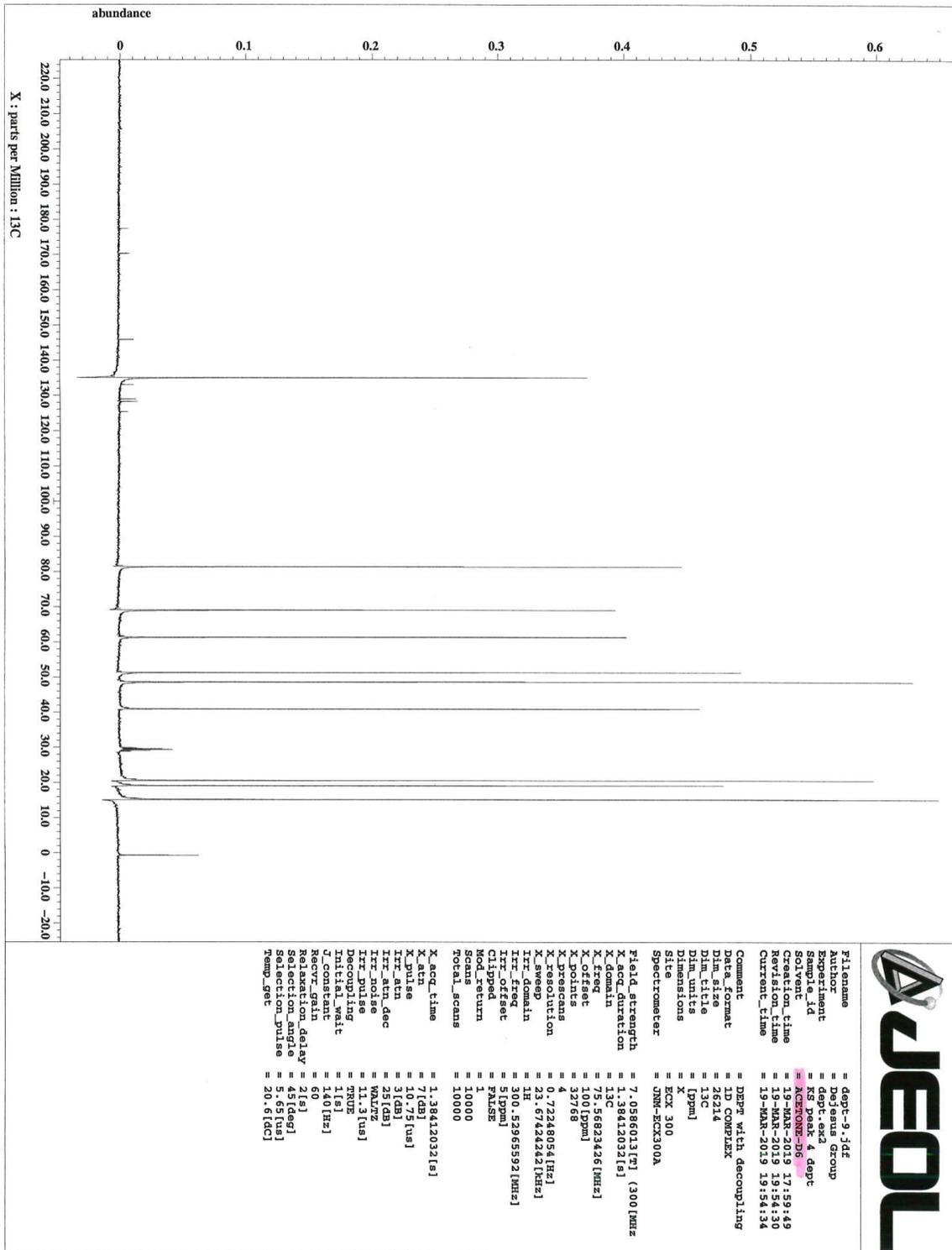
```

Filename = single_pulse-258.fid
Experiment =
Subexperiment =
Sample id =
Solvent = ACERONE-D6
Creation time = 18-MAR-2019 16:56:27
Revision time = 18-MAR-2019 18:49:33
Current time = 18-MAR-2019 18:50:40

Comment =
Data format = single_pulse
Dim size = 1D3272MK
Dim 1 size = 13107
Dim 1 title =
Dim 1 units = [ppm]
Dimensions = X
Site = ECK 300
Spectrometer = JNM-ECK300A

Field strength = 7.059613 [G] (300 MHz)
X_resolution = 2.9717696 [G]
X_domain = 1H
X_freq = 300.5296592 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.34397631 [Hz]
X_sweep = 5.63570784 [kHz]
X_time = 300.5296592 [MHz]
F1_f1_freq = 300.5296592 [MHz]
F1_domain = 1H
F1_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 8

X_90_width = 11.3 [us]
X_acq_time = 2.90717696 [s]
X_angle = 45 [deg]
X_atn = 3 [dB]
X_pulse = 5.85 [us]
X_mode = OF2
X_phase = 0 [deg]
Pulse program = FALSP
Recovery delay = 30 [s]
Relaxation delay = 5 [s]
Repetition time = 7.90717696 [s]
Temp_get = 20 [C]
    
```



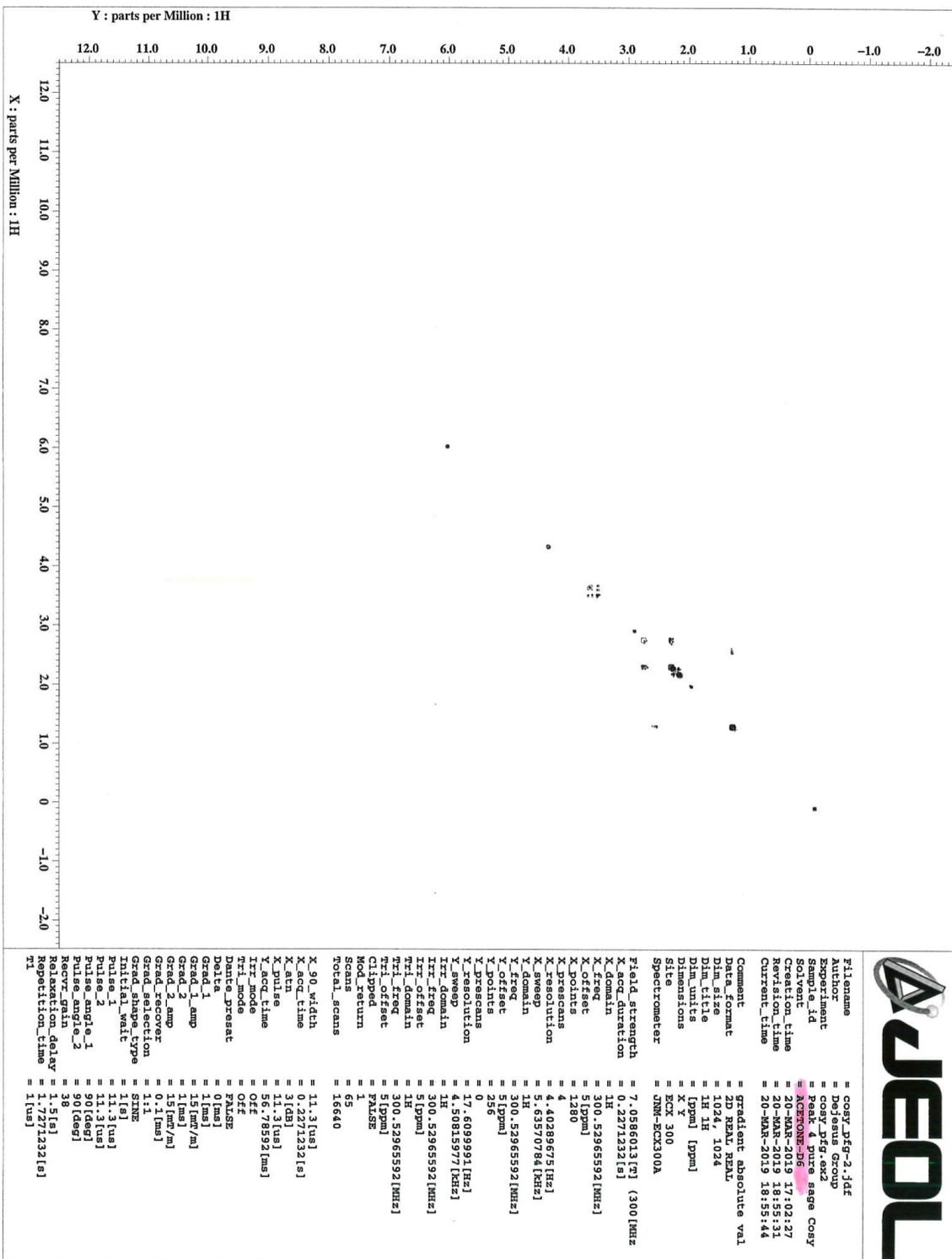
```

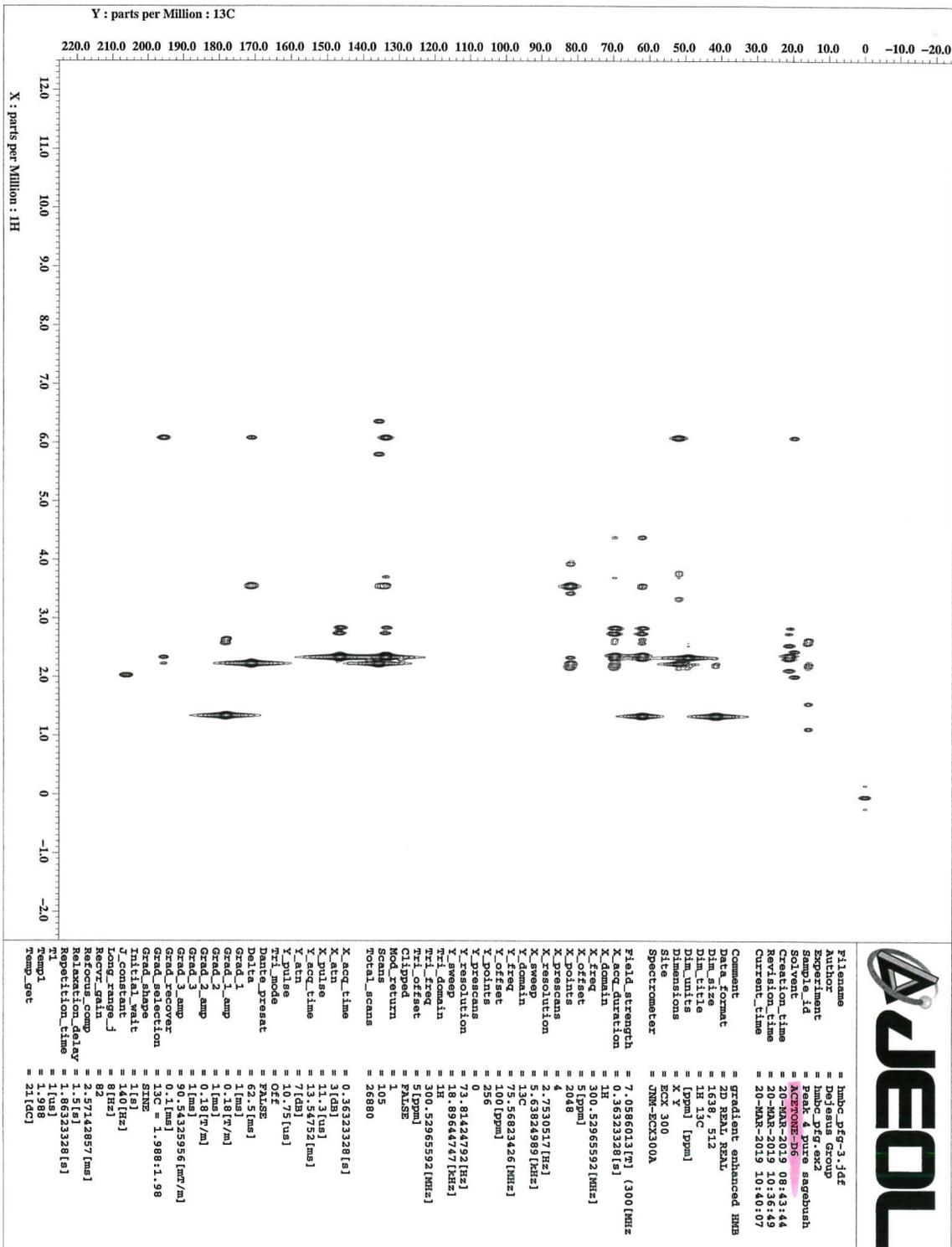
PlaneName      = dept-9_1d4
Author          = Desjeans_Group
Experiment      = dept.ex2
Sample_ID      = KS_peak_4_dept
Solvent        = ACETONE-D6
Creation_time   = 19-MAR-2019 17:59:49
Revision_time  = 19-MAR-2019 19:54:30
Current_time   = 19-MAR-2019 19:54:34

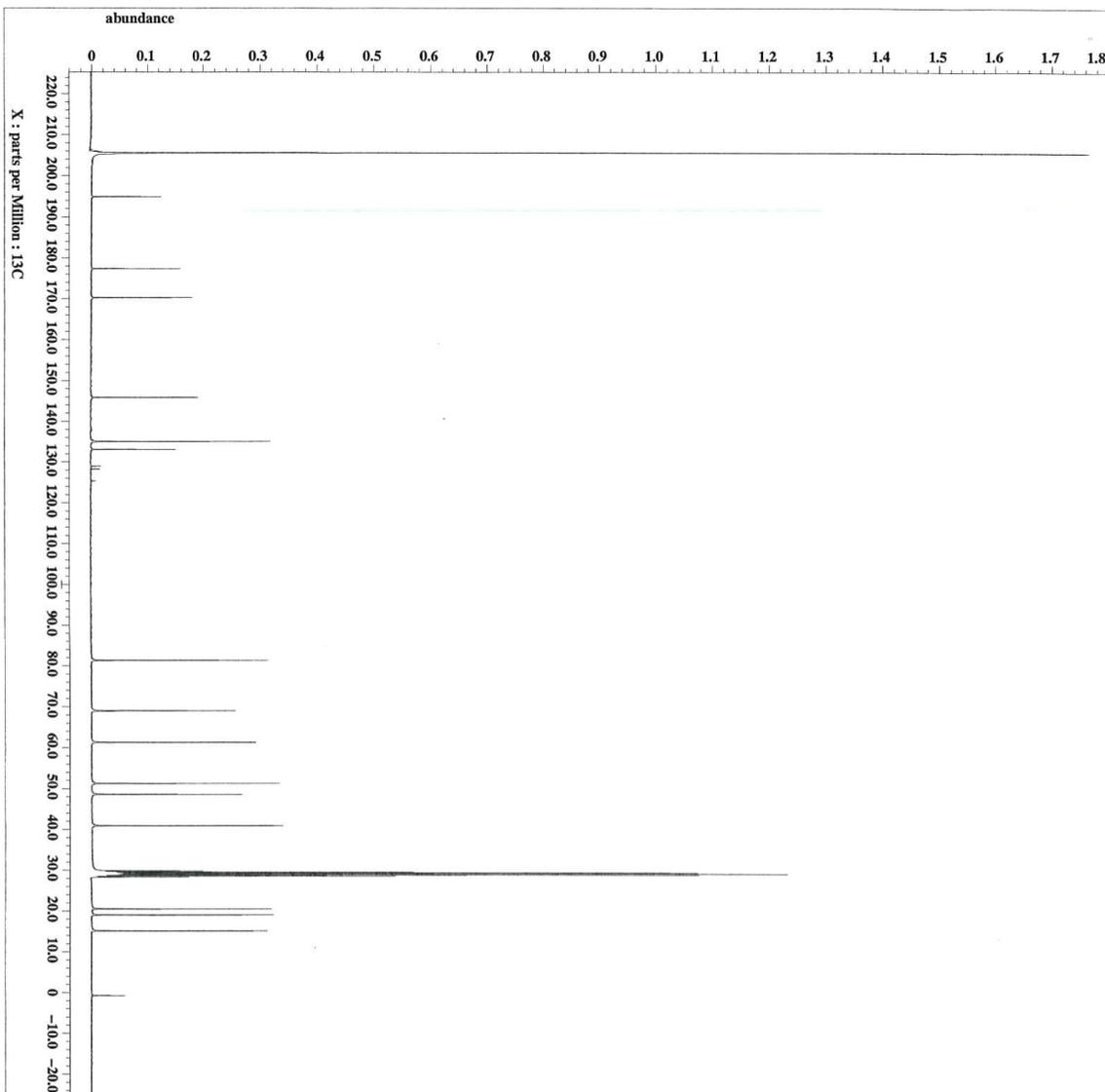
Comment
Data format    = ID COMPLEX
Dim_size       = 26214
Dim_title      = 13C
Dim_units      = [ppm]
Dimensions     = X
Site           = ECK 300
Spectrometer   = JNM-ECA300A

Field_strength = 7.0586013 [T] (300 MHz)
X.acq_duration = 1.38412032 [s]
X.domain       = 13C
X.freq         = 75.56823426 [MHz]
X.offset       = 100 [ppm]
X.points       = 32768
X.ppscan      = 4
X.resolution   = 7.2248954 [Hz]
X.sfs          = 27.6742424 [kHz]
X.tau          = 18
X.ir_domain    = 300.5296592 [kHz]
X.ir_freq      = 51 [ppm]
X.ir_offset    = FALSE
Mod_return     = 1
Scans          = 10000
Total_scans    = 10000

X.acq_time     = 1.38412032 [s]
X.atn          = 7 [db]
X.pulse        = 10.75 [us]
X.ref          = 3 [db]
X.ir_atn       = 25 [db]
X.ir_atn_dec   = WALTZ
X.ir_noise     = 11.3 [us]
X.pulse_prog   = WALTZ
X.ref_prog     = 1 [s]
X.ref_offset   = 140 [Hz]
J.constant     = 60
Recvr_gain     = Relaxation_delay = 2 [s]
Selection_angle = 5.65 [deg]
Selection_pulse = 5.65 [us]
Temp_get       = 20.6 [degC]
    
```







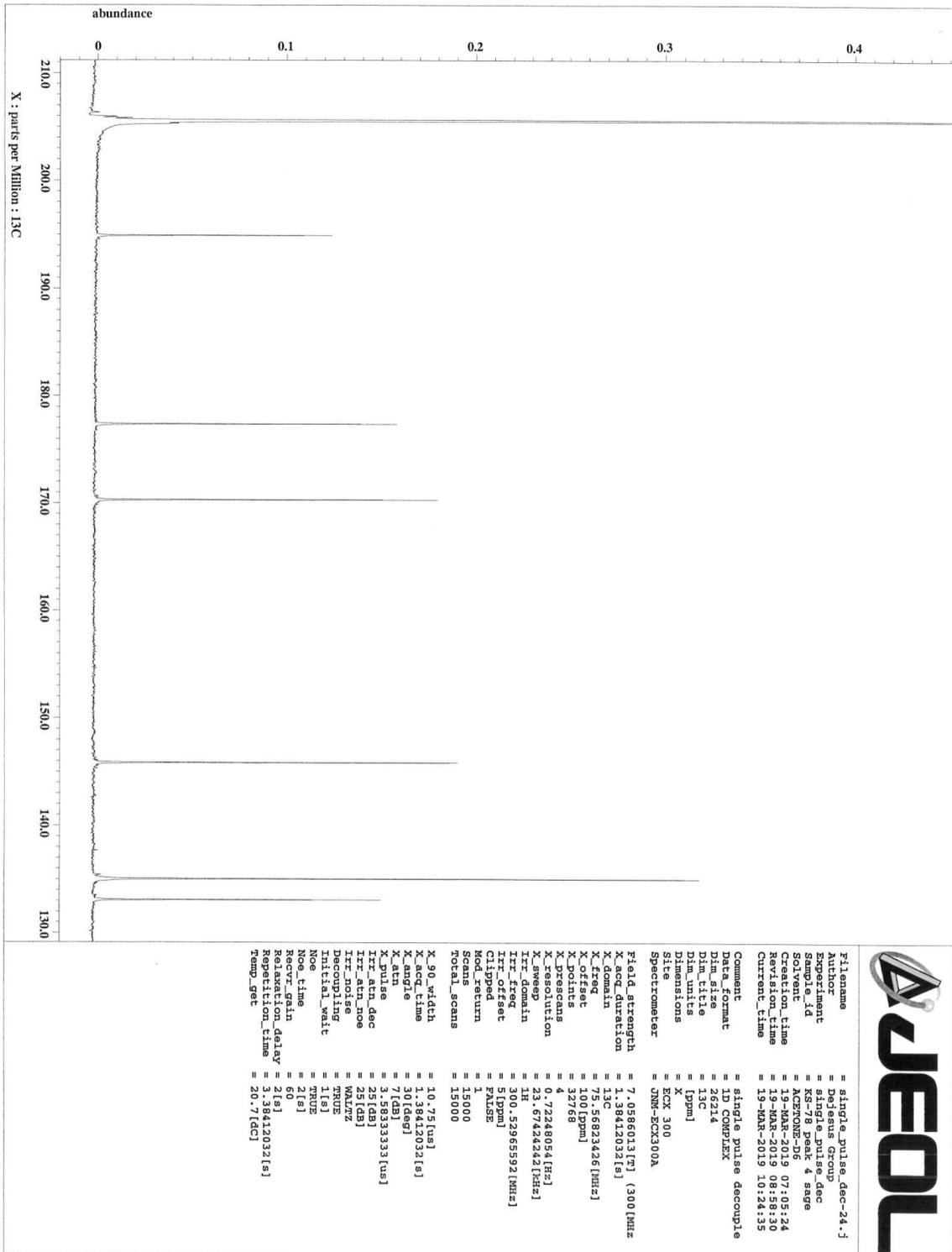
```

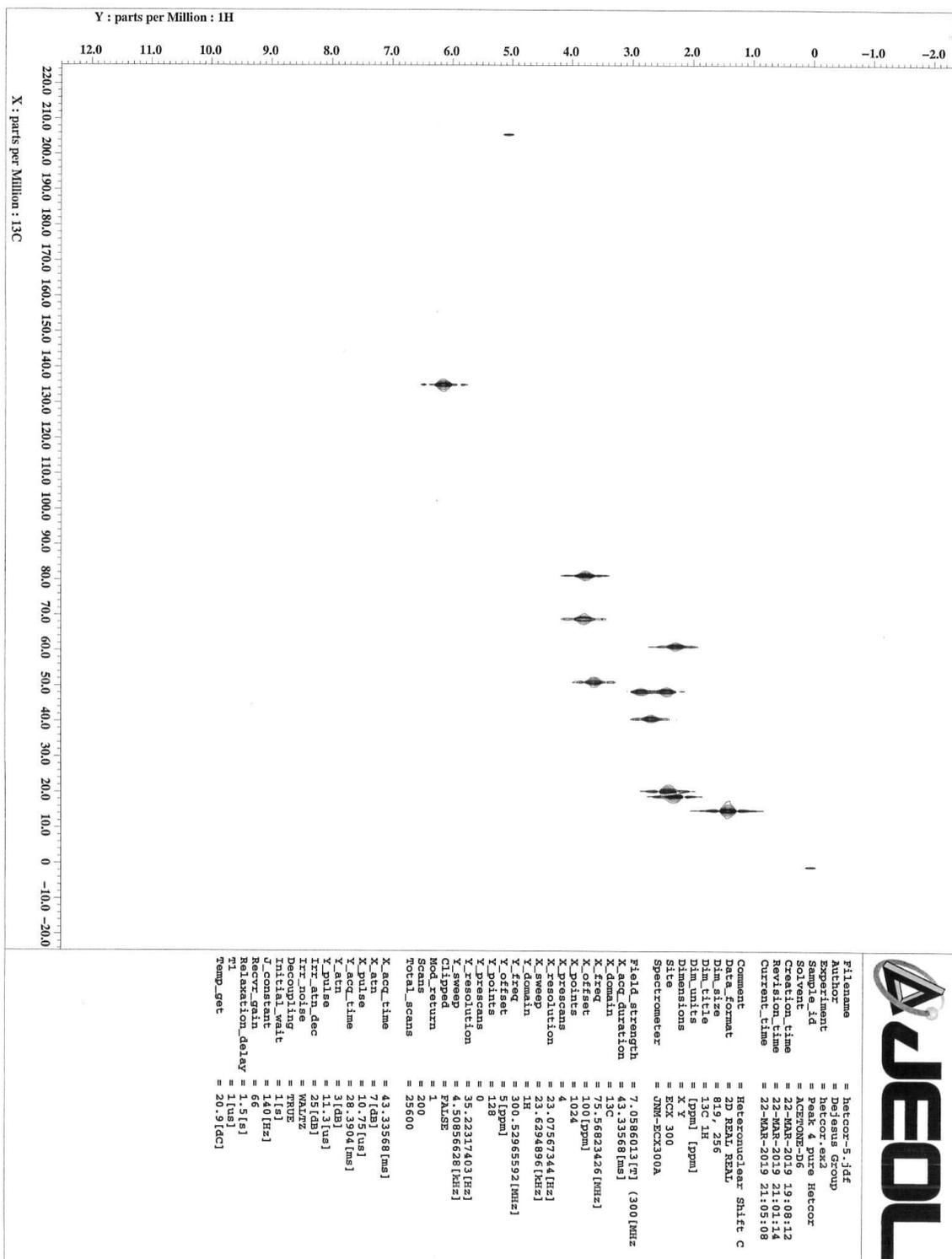
Filename = single_pulse_dec-24.f
Experiment Group =
Experiment =
Sample ID = KS-78 Peak 4 sage
Solvent = ACETONE-D6
Creation_time = 19-MAR-2019 07:05:24
Revision_time = 19-MAR-2019 08:58:30
Current_time = 19-MAR-2019 10:24:01

Comment = single pulse decouple
Data Format = 1D COMPLEX
Dim Size = 26214
Dim Title = 13C
Dim Units = [ppm]
Dimensions = X
Site = ECK 300
Spectrometer = JNM-ECK300A

P1/d_strength = 7.05866013 [s] (300 MHz)
X_acq_duration = 1.3841302 [s]
X_domain = 13C
X_freq = 75.56823426 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 7.2248054 [Hz]
X_res_domain = 22.6742424 [kHz]
X_res_freq = 12
X_res_offset = 300.5296592 [MHz]
Clipped = FALSE
Mod_return = 1
Scans = 15000
Total_scans = 15000

X_90_width = 10.75 [us]
X_acq_time = 1.3841302 [s]
X_angle = 30 [deg]
X_atn = 7 [dB]
X_pulse = 3.5833333 [us]
Irr_atn_dec = 25 [dB]
Irr_atn_noe = 25 [dB]
Irr_atn_p1 = 25 [dB]
Irr_atn_p2 = 25 [dB]
Irr_atn_p3 = 25 [dB]
Irr_atn_p4 = 25 [dB]
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 21 [s]
Noe_time = 60
Recvr_gain = 21 [s]
Relaxation_delay = 2 [s]
Repetition_time = 3.3841302 [s]
Temp_get = 20.7 [deg]
    
```

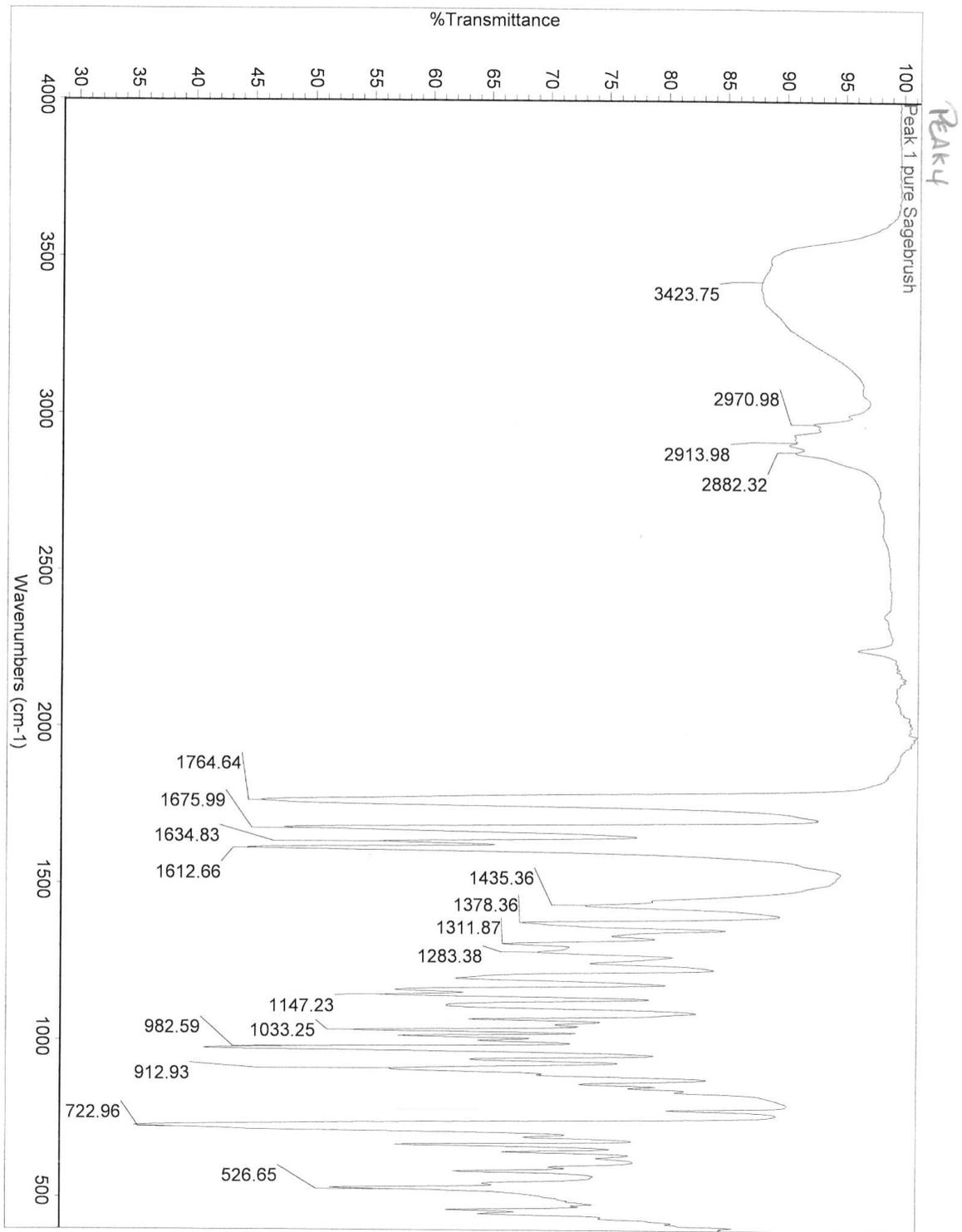


```

Filename      = hetcor-5.jdt
Experiment    = hetcor
Sample Id     = Peak 4 pure Hetcor
Solvent       = ACETONE-D6
Creation time = 22-MAR-2019 19:08:12
Revision time = 22-MAR-2019 21:01:14
Current time  = 22-MAR-2019 21:05:08

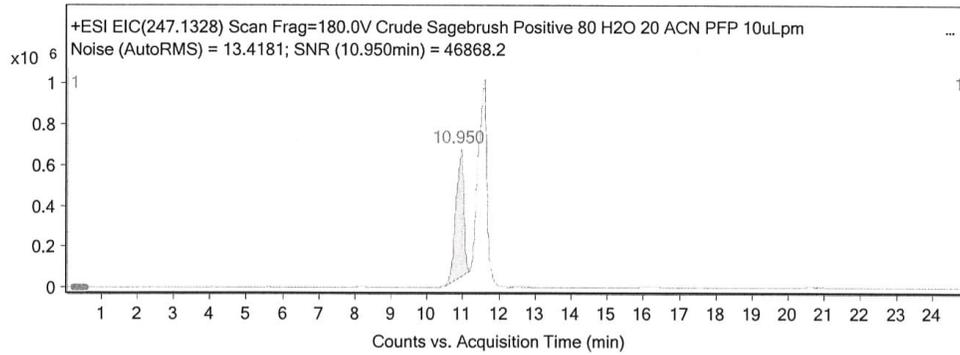
Comment
DataFormat   = Heteroqc1dat Shift C
Dim.size     = 20 256
Dim.title    = 13C 1H
Dim.units    = [ppm] [ppm]
Dimensions   = X Y
Site         = ECK 300
Spectrometer = JNM-ECK300A

F2.f4.strength = 7.0566013 [Hz] (300 MHz)
X.acq.dwelltime = 43.33568 [ms]
X.domain        = 13C
X.freq         = 75.56823426 [MHz]
X.offset       = 100 [ppm]
X.points       = 1024
X.prescans     = 4
X.resolution   = 23.07567344 [Hz]
X.sweep        = 23.6294896 [kHz]
Y.freq         = 300.52965592 [MHz]
Y.offset       = 51 [ppm]
Y.points       = 128
Y.prescans     = 0
Y.resolution   = 35.22317403 [Hz]
X.sweep        = 4.50856628 [kHz]
Clipped       = FALSE
Nuc1          = 13C
Nuc2          = 13C
Total_scans   = 200
X.acq.time    = 43.33568 [ms]
X.atn         = 7 [dB]
X.pulse       = 10.75 [us]
X.acq.time    = 28.3904 [ms]
Y.atn         = 1 [dB]
Y.pulse       = 143 [us]
Irr.atn.dec   = 25 [dB]
Irr_noise     = WALTZ
Decoupling    = PRNU
Initial_wait  = 1 [s]
V.constant    = 140 [Hz]
Recvr_gain    = 66
Relaxation_delay = 1.5 [s]
Temp_get      = 20.9 [degC]
    
```



Qualitative Analysis Report

Fragmentor Voltage 180 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal to Noise
1	10.486	10.95	11.181	628882	9481329	100	46868.2

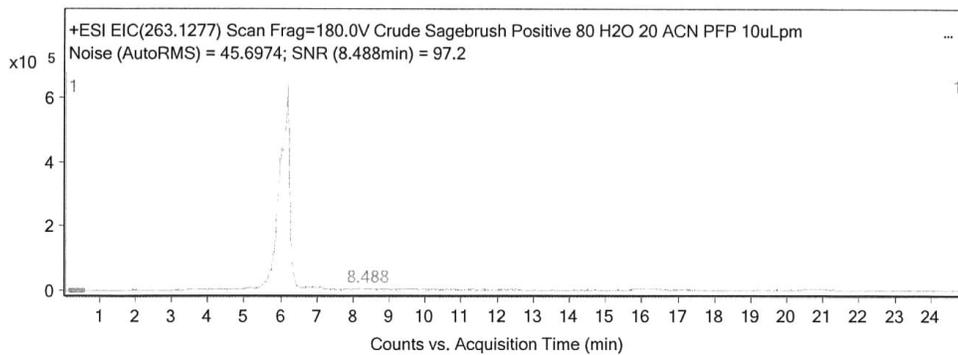
Noise Measurements

Noise Type	Signal Definition	Noise Multiplier	Noise Value
Auto-RMS	Height	1	13.4180994033813

Noise Regions

Start	End
.232366667	.582366667

Fragmentor Voltage 180 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal to Noise
1	8.466	8.488	8.51	4443	3909	100	97.2



Agilent Technologies

Calculated 247.13347

