

Supporting Information

Synthesis and biological evaluation of novel flexible nucleoside analogues that inhibit flavivirus replication *in vitro*

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Supplemental data:

¹H NMR of compound **1**

¹³C NMR of compound **1**

¹H NMR of compound **2**

¹³C NMR of compound **2**

¹H NMR of compound **1-Ac**

¹³C NMR of compound **1-Ac**

¹H NMR of compound **2-Ac**

¹³C NMR of compound **2-Ac**

¹H NMR of compound **1-MG**

¹³C NMR of compound **1-MG**

³¹P NMR of compound **1-MG**

¹H NMR of compound **2-MG**

¹³C NMR of compound **2-MG**

¹H NMR of compound **1-TP**

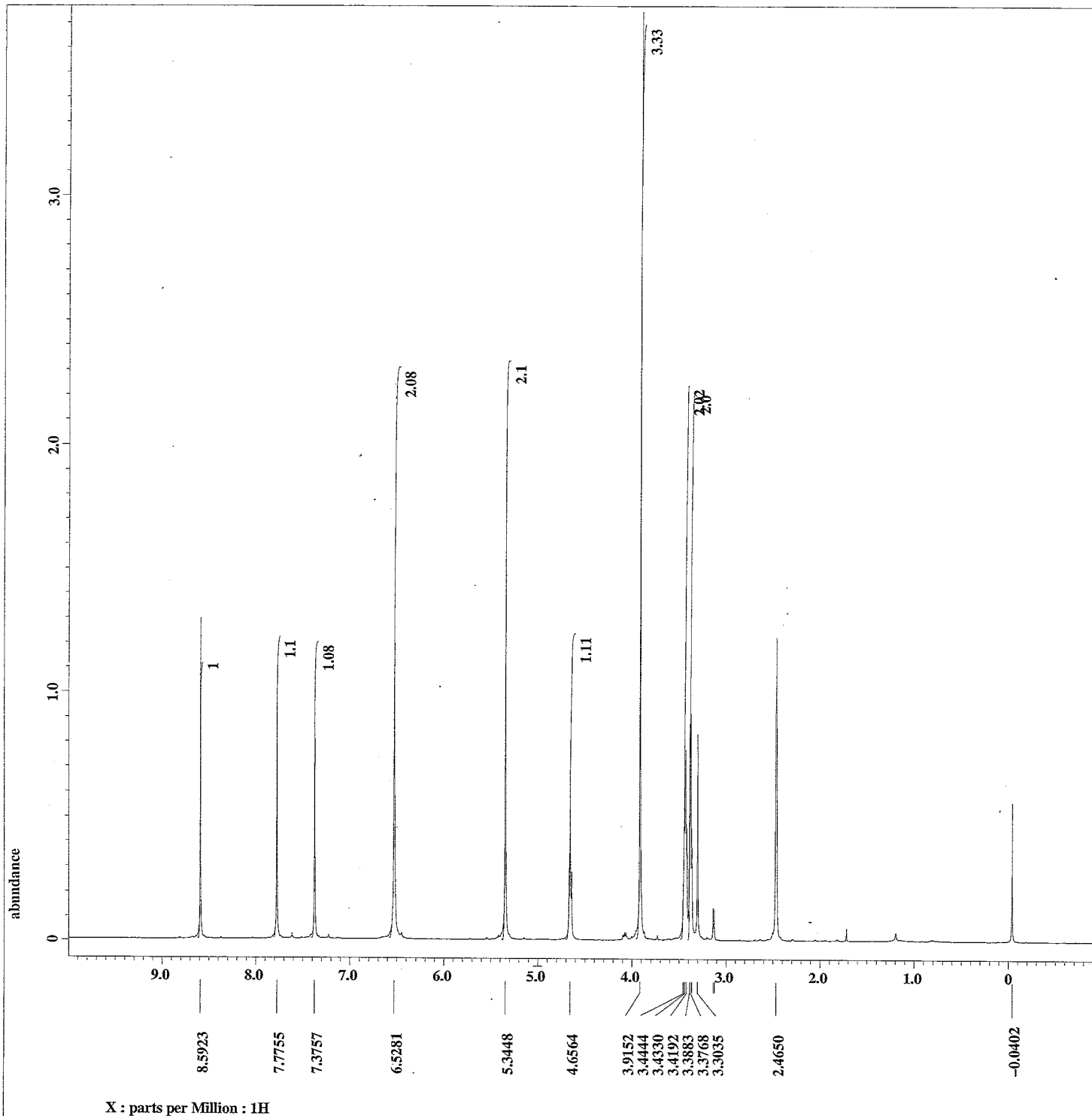
³¹P NMR of compound **1-TP**

¹H NMR of compound **2-TP**

¹³C NMR of compound **1-TP**

³¹P NMR of compound **2-TP**

ESI+ Mass spec of compound **11**

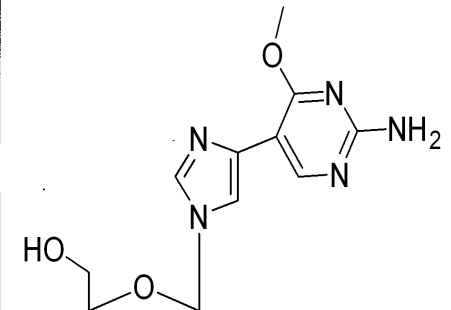


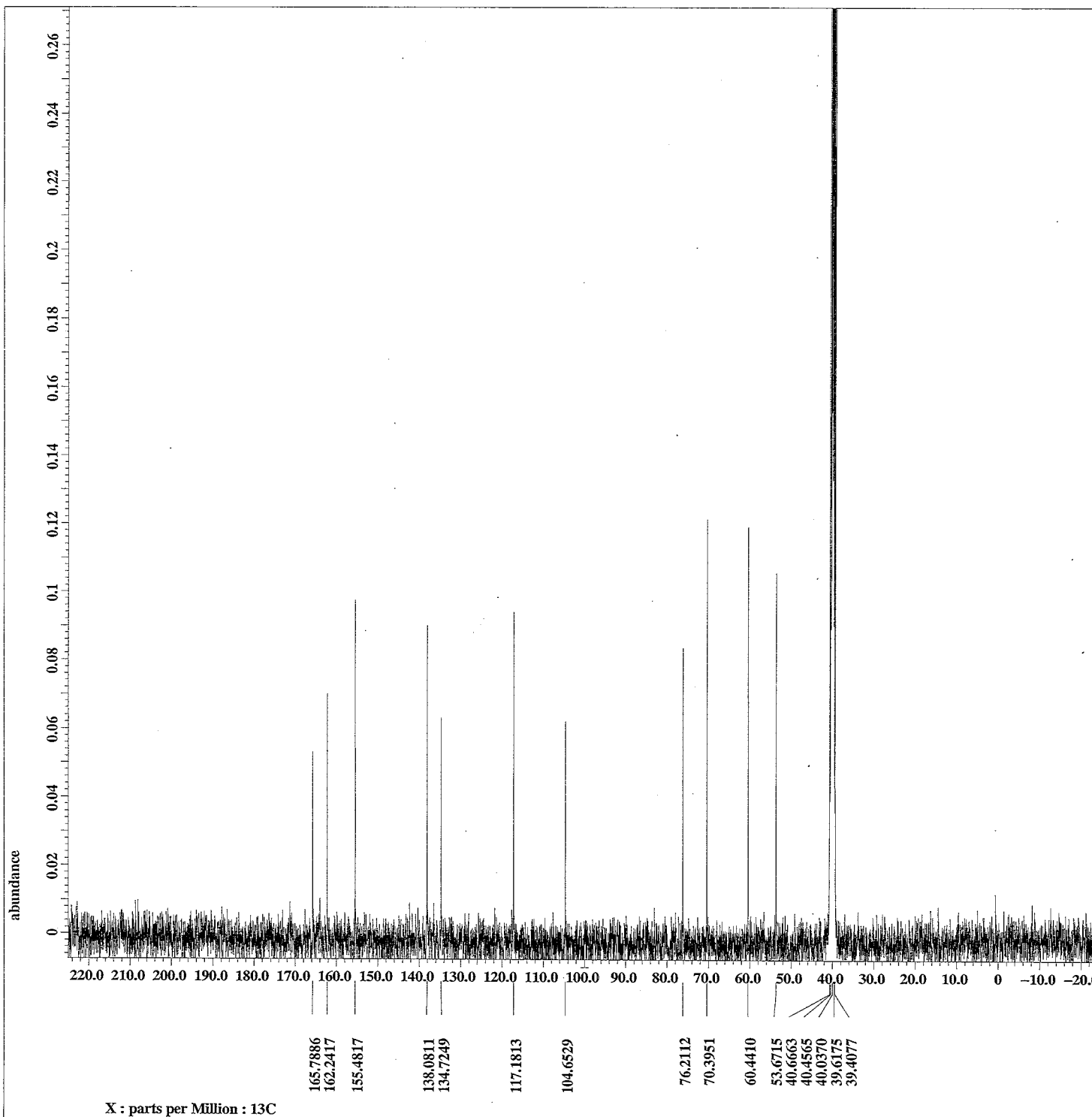
Filename = HP083-4.jdf
Author = Seley
Experiment = single_pulse.ex2
Sample_id = S#405935
Solvent = DMSO-D6
Creation_time = 19-JUN-2020 11:08:22
Revision_time = 19-JUN-2020 11:25:22
Current_time = 19-JUN-2020 11:25:33

Comment = single_pulse
Data_format = 1D_COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 13.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 3[dB]
X_pulse = 6.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
Temp_get = 22.4[dC]





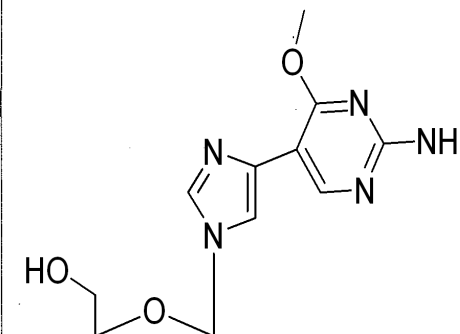
X : parts per Million : 13C

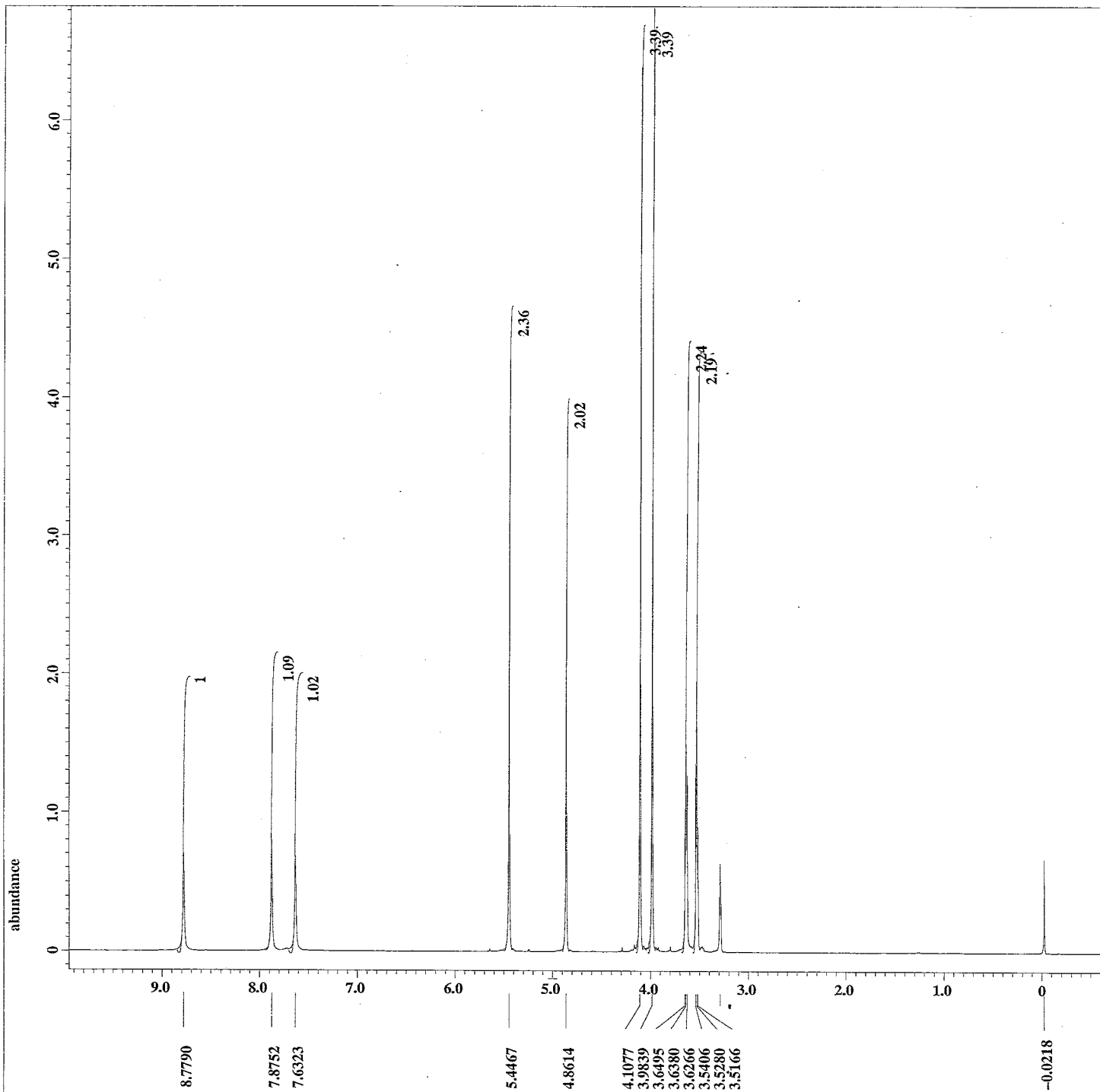
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Filename      = HP083-5.jdf
Author       = Seley
Experiment   = single_pulse_dec
Sample_id    = S#409376
Solvent      = DMSO-D6
Creation_time = 19-JUN-2020 11:35:12
Revision_time = 19-JUN-2020 11:49:07
Current_time  = 19-JUN-2020 11:49:30

Comment      = single pulse decouple
Data_format  = 1D_COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain       = 13C
X_freq         = 100.52530333[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 0.95846665[Hz]
X_sweep        = 31.40703518[kHz]
Irr_domain     = 1H
Irr_freq       = 399.78219838[MHz]
Irr_offset     = 5[ppm]
Clipped        = TRUE
Mod_return     = 1
Scans          = 462
Total_scans    = 462

X_90_width    = 7[us]
X_acq_time     = 1.04333312[s]
X_angle        = 30[deg]
X_atn          = 6[dB]
X_pulse        = 2.33333333[us]
Irr_atn_dec    = 21.1[dB]
Irr_atn_noe    = 21.1[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 = 3.04333312[s]
Temp_get       = 22.6[dC]
```





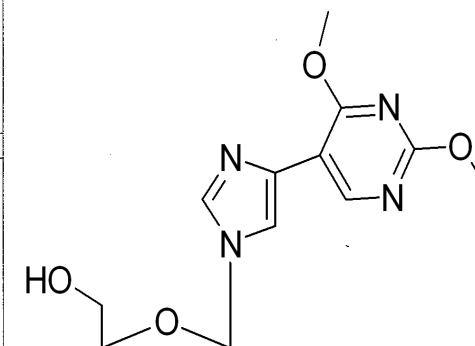
X : parts per Million : 1H

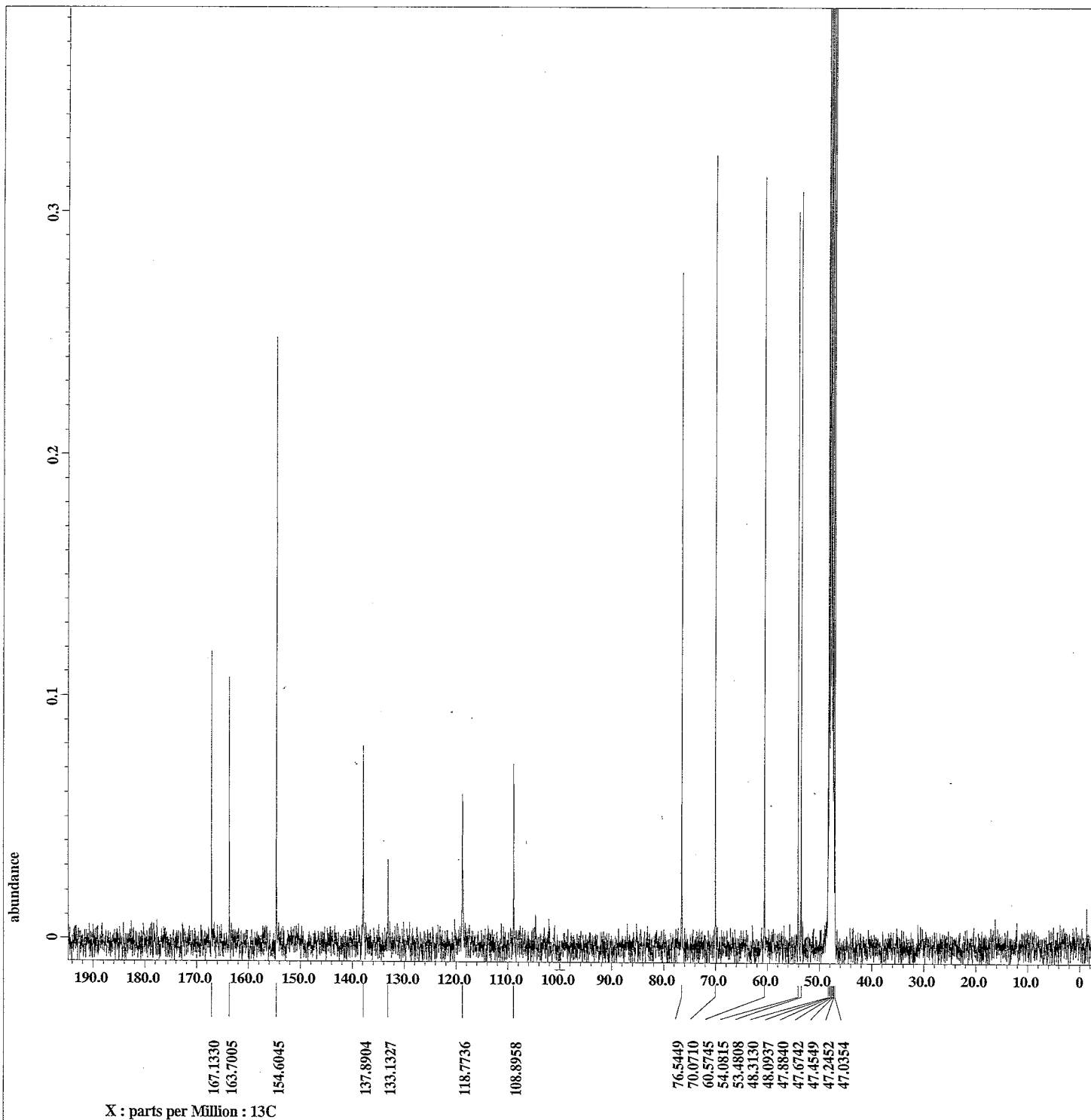
Filename = HP100-3.jdf
Author = Seley
Experiment = single_pulse.ex2
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Solvent = METHANOL-D3
Creation_time = 19-JUN-2020 09:49:45
Revision_time = 19-JUN-2020 10:10:01
Current_time = 19-JUN-2020 10:10:11

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 13.5 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 3 [dB]
X_pulse = 6.75 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 38
Relaxation_delay = 5 [s]
Repetition_time = 7.18365952 [s]
Temp_get = 22.5 [dC]





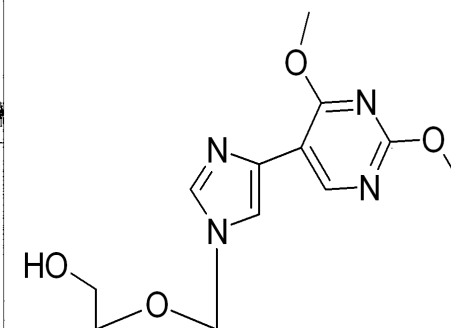
X : parts per Million : 13C

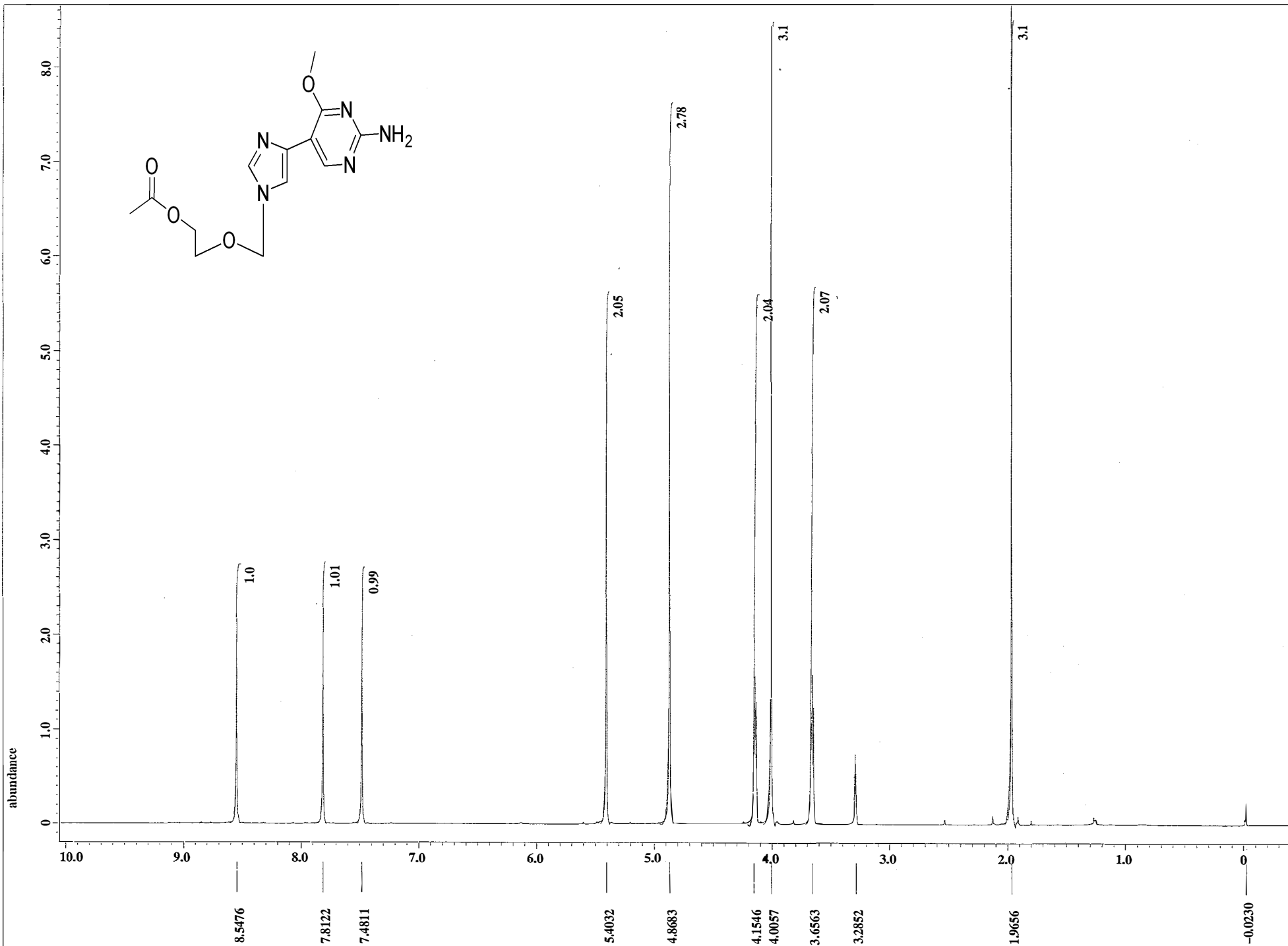
Filename = HP100-4.jdf
Author = Seley
Experiment = single_pulse_dec
Sample_id = S#361903
Solvent = METHANOL-D3
Creation_time = 19-JUN-2020 10:16:06
Revision_time = 19-JUN-2020 10:33:18
Current_time = 19-JUN-2020 10:33:37

Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 462
Total_scans = 462

X_90_width = 7[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 6[db]
X_pulse = 2.33333333[us]
Irr_atn_dec = 21.1[db]
Irr_atn_noe = 21.1[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 = 3.04333312[s]
Temp_get = 22.7[dc]





X : parts per Million : 1H

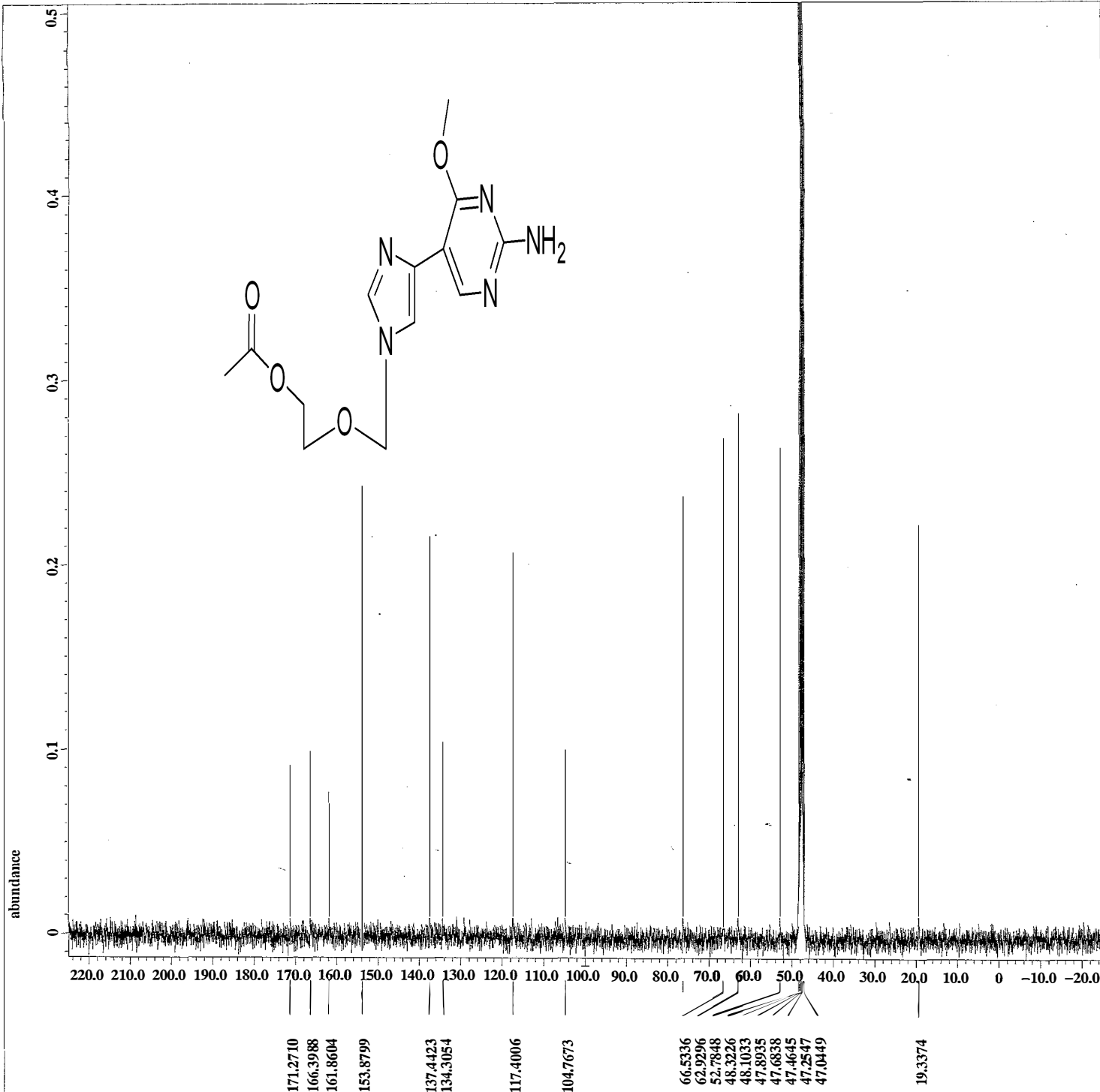


Filename = JET-2-1AC new procedu
Author = Seley
Experiment = single_pulse_dec
Sample_id = S#477284
Solvent = METHANOL-D3
Creation_time = 12-MAY-2020 13:32:11
Revision_time = 12-MAY-2020 13:45:21
Current_time = 12-MAY-2020 13:45:37

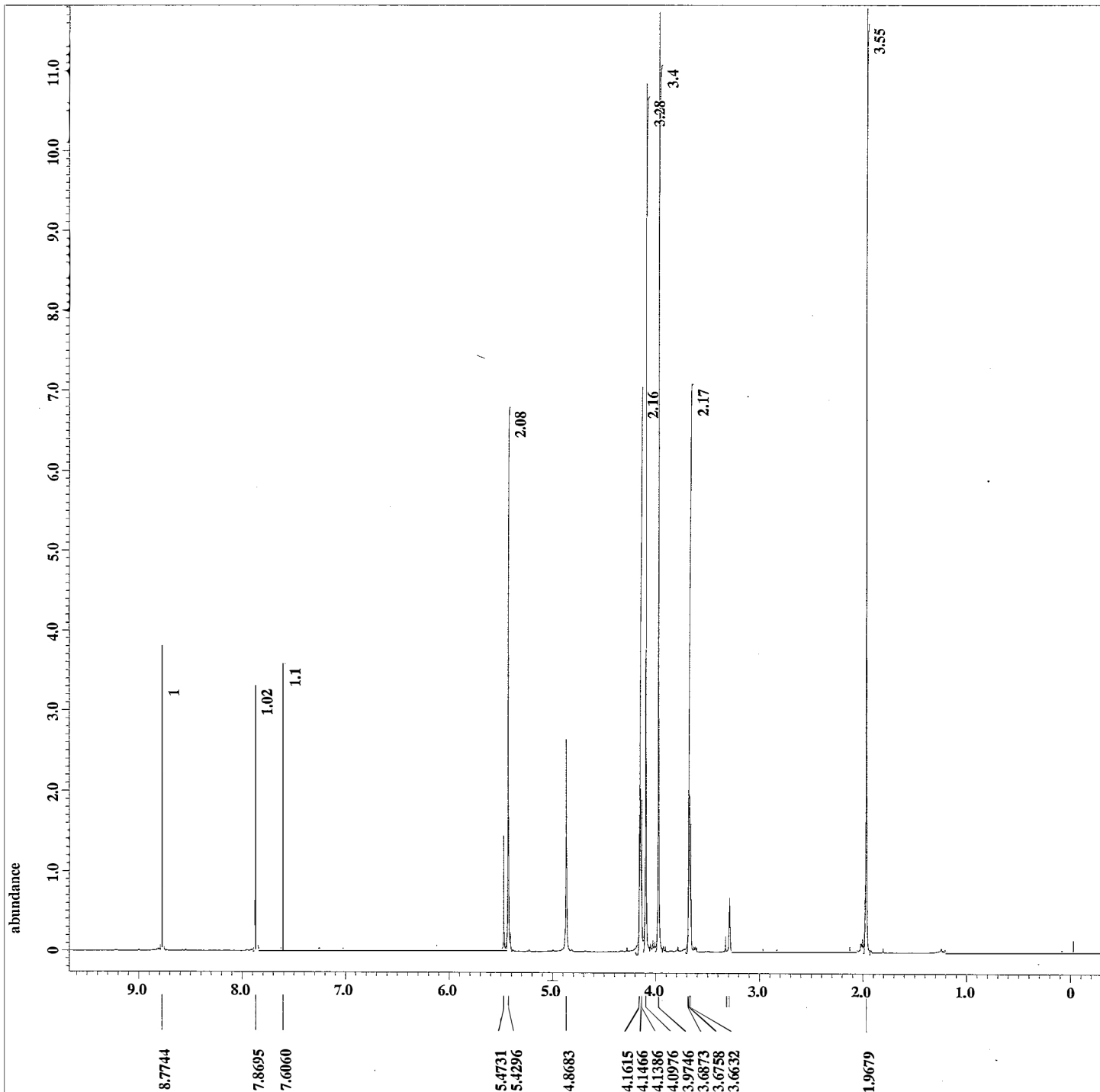
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Dim_size = 26214
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Dimensions = x
Site = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 507
Total_scans = 507

X_90_width = 7 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 6 [dB]
X_pulse = 2.33333333 [us]
Irr_atn_dec = 21.1 [dB]
Irr_atn_noe = 21.1 [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 = 3.04333312 [s]
Temp_get = 21.8 [dC]



X : parts per Million : 13C



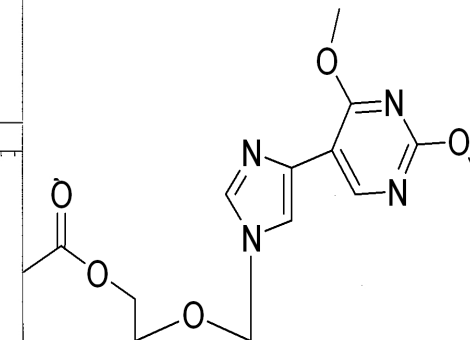
X : parts per Million : 1H

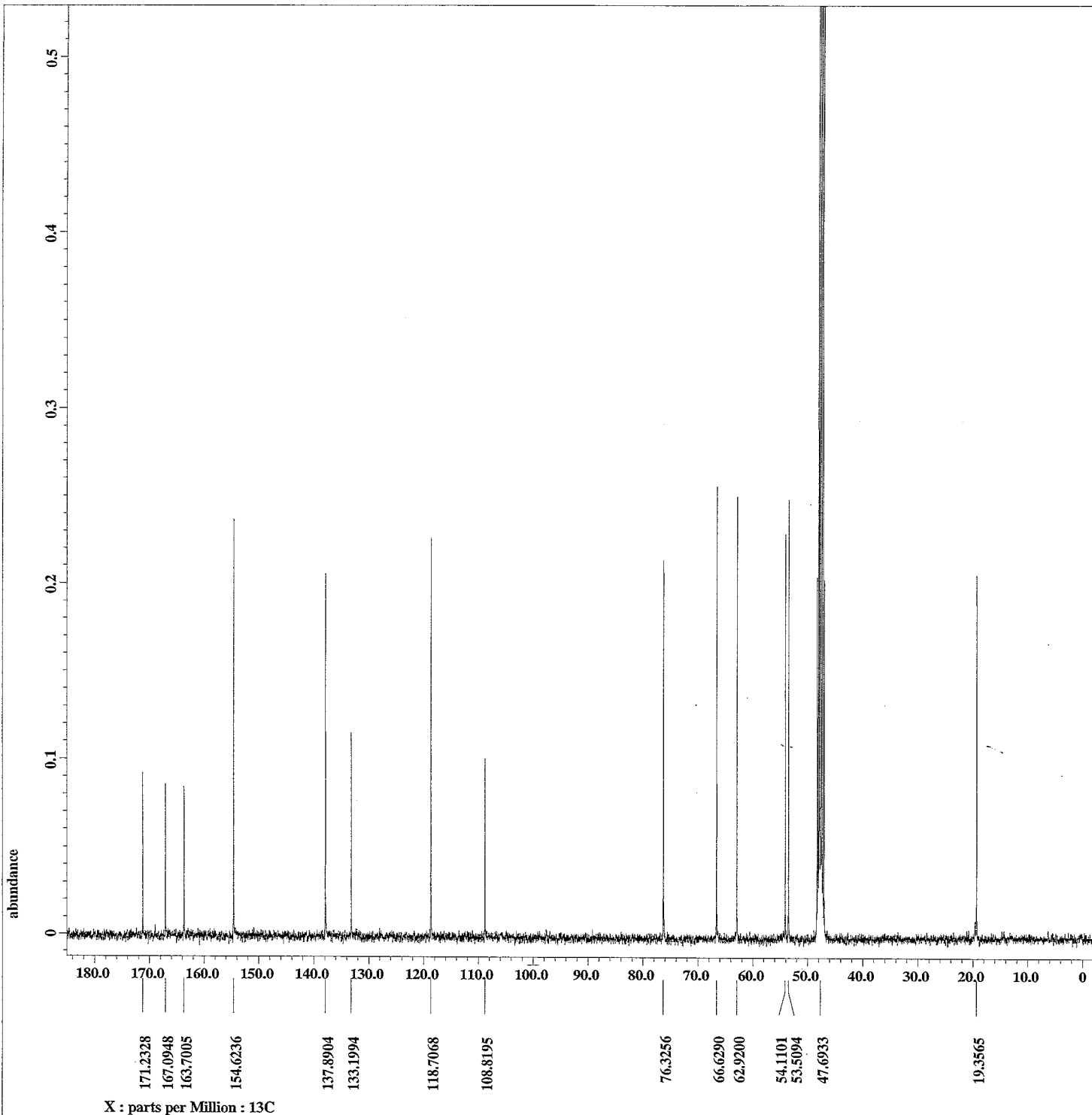
Filename = JET-2Ac-3.jdf
Author = Seley
Experiment = single_pulse.ex2
Sample_id = S#427412
Solvent = METHANOL-D3
Creation_time = 15-MAY-2020 11:43:57
Revision_time = 15-MAY-2020 12:00:55
Current_time = 15-MAY-2020 12:01:21

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 13.5 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 3 [dB]
X_pulse = 6.75 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 36
Relaxation_delay = 5 [s]
Repetition_time = 7.18365952 [s]
Temp_get = 403.6 [dC]



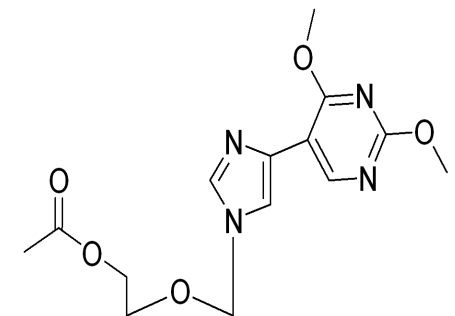


Filename = JET-2Ac-4.jdf
Author = Seley
Experiment = single_pulse_dec
Sample_id = S#430269
Solvent = METHANOL-D3
Creation_time = 15-MAY-2020 12:14:19
Revision_time = 15-MAY-2020 12:28:04
Current_time = 15-MAY-2020 12:28:24

Comment = single pulse decouple
Data_format = 1D_COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 535
Total_scans = 535

X_90_width = 7 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 6 [dB]
X_pulse = 2.33333333 [us]
Irr_atn_dec = 21.1 [dB]
Irr_atn_noe = 21.1 [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 = 3.04333312 [s]
Temp_get = 404.1 [dC]



X : parts per Million : 13C

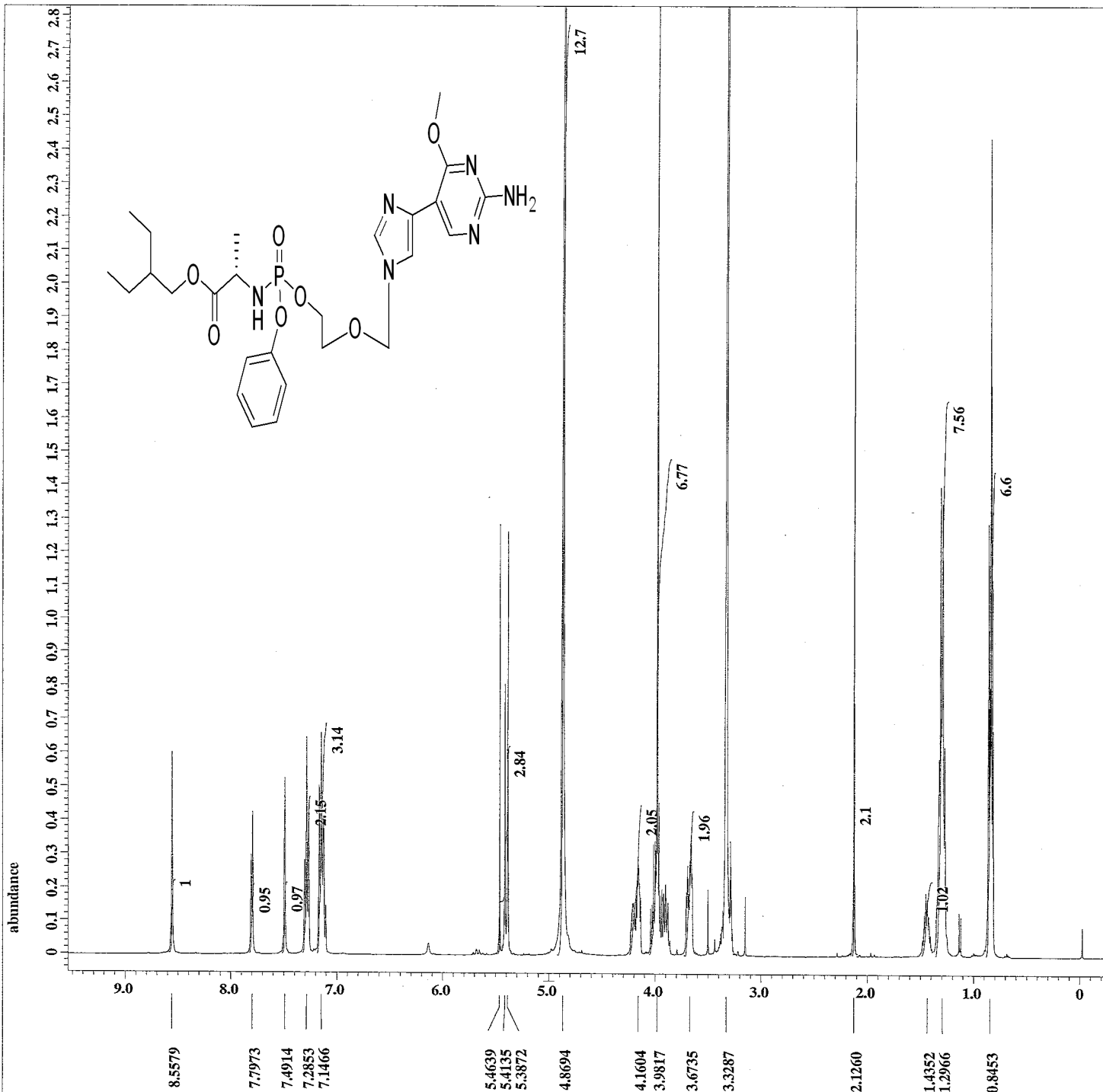


Filename = JET-2-023 1-MG-3.jdf
Author = Seley
Experiment = single_pulse.ex2
Sample_id = S#611604
Solvent = METHANOL-D3
Creation_time = 23-APR-2020 16:51:38
Revision_time = 23-APR-2020 17:08:57
Current_time = 23-APR-2020 17:09:16

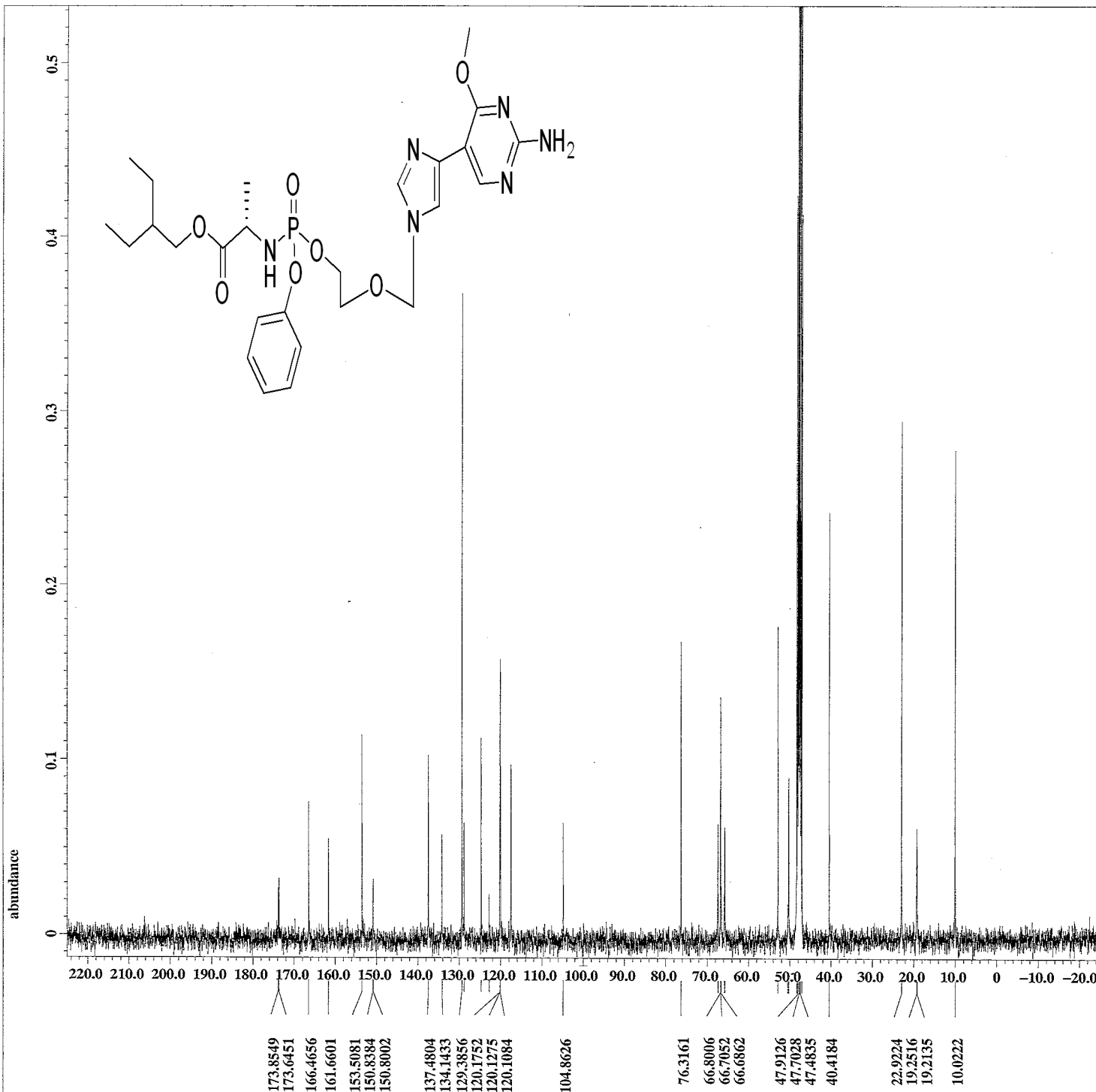
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Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766 [T] (400 [MHZ])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHZ]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHZ]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHZ]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 24
Total_scans = 24

X_90_width = 13.5 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 3 [dB]
X_pulse = 6.75 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 30
Relaxation_delay = 5 [s]
Repetition_time = 7.18365952 [s]
Temp_get = 21.9 [dC]



X : parts per Million : 1H



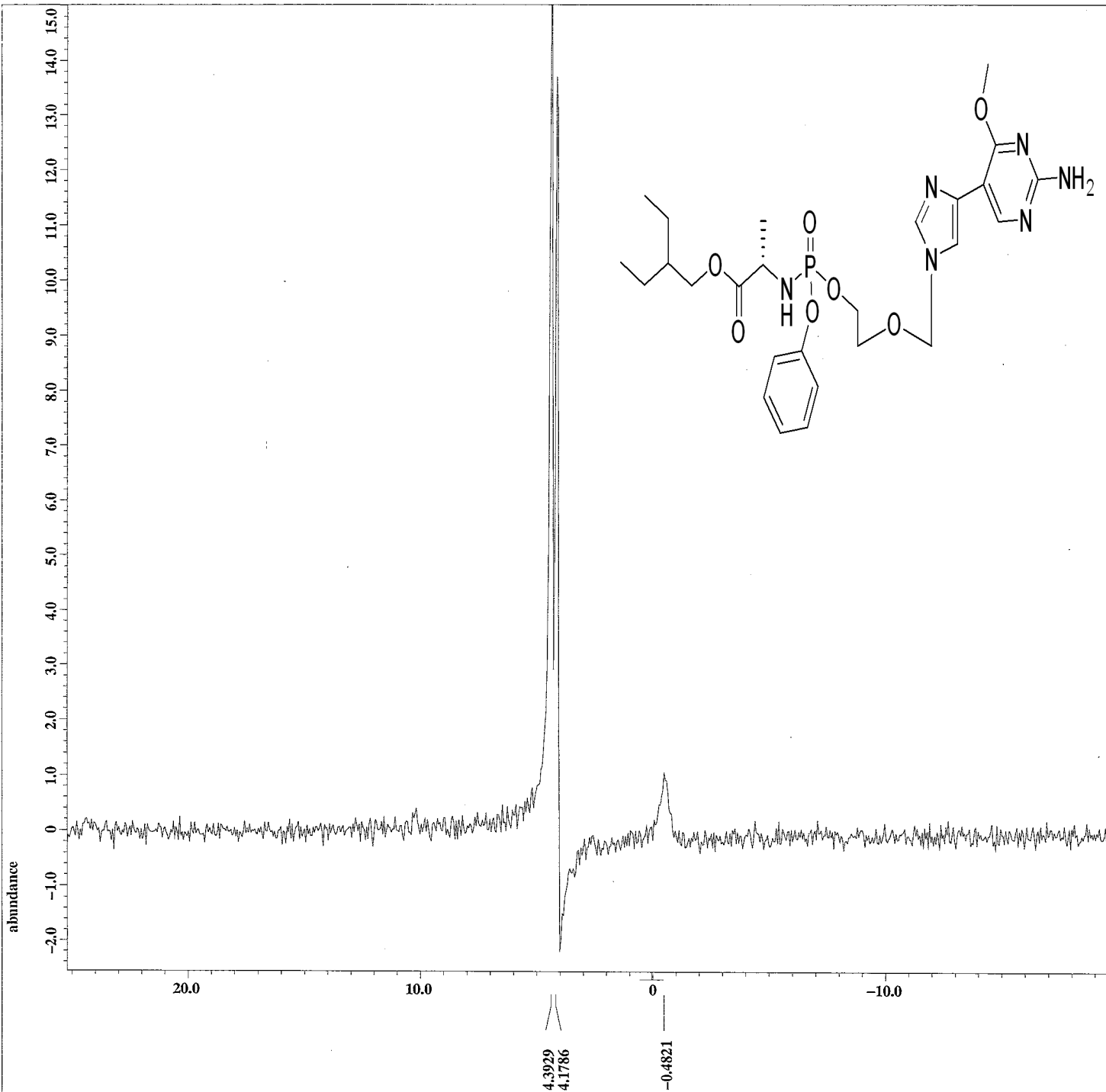
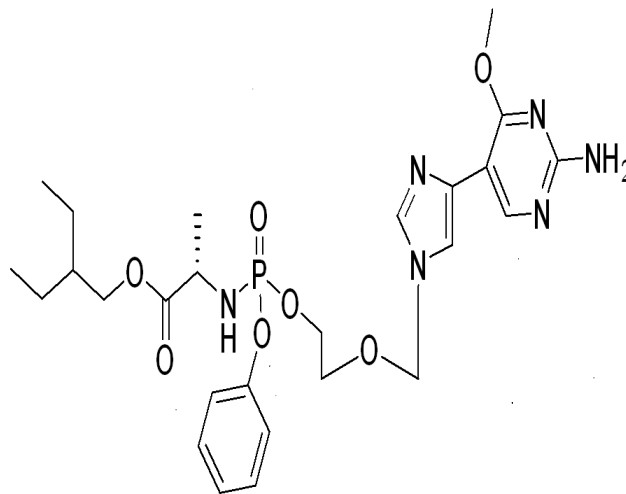
Filename = JET-1-MG-3.jdf
Author = Seley
Experiment = single_pulse_dec
Sample_id = S#411547
Solvent = METHANOL-D3
Creation_time = 25-JUN-2020 11:36:59
Revision_time = 25-JUN-2020 11:53:32
Current_time = 25-JUN-2020 11:54:23

Comment = single pulse decouple
Data_format = 1D_COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 428
Total_scans = 428

X_90_width = 7 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 6 [dB]
X_pulse = 2.33333333 [us]
Irr_atn_dec = 21.1 [dB]
Irr_atn_noe = 21.1 [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 = 3.04333312 [s]
Temp_get = 22.7 [dC]

X : parts per Million : 13C



X : parts per Million : 31P

Filename = JET-1MG Phosphorous-3
Author = Seley
Experiment = single_pulse.ex2
Sample_id = S#429200
Solvent = METHANOL-D3
Creation_time = 25-JUN-2020 11:45:02
Revision_time = 25-JUN-2020 11:58:42
Current_time = 25-JUN-2020 11:59:04

Comment = single_pulse
Data_format = 1D_COMPLEX
Dim_size = 13107
Dim_title = 31P
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 0.11534336[s]
X_domain = 31P
X_freq = 161.83469309[MHz]
X_offset = 0[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 8.66976651[Hz]
X_sweep = 142.04545455[kHz]
Irr_domain = 31P
Irr_freq = 161.83469309[MHz]
Irr_offset = 5[ppm]
Tri_domain = 31P
Tri_freq = 161.83469309[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 16.2[us]
X_acq_time = 0.11534336[s]
X_angle = 45[deg]
X_atn = 3[dB]
X_pulse = 8.1[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 56
Relaxation_delay = 5[s]
Repetition_time = 5.11534336[s]
Temp_get = 22.5[degC]

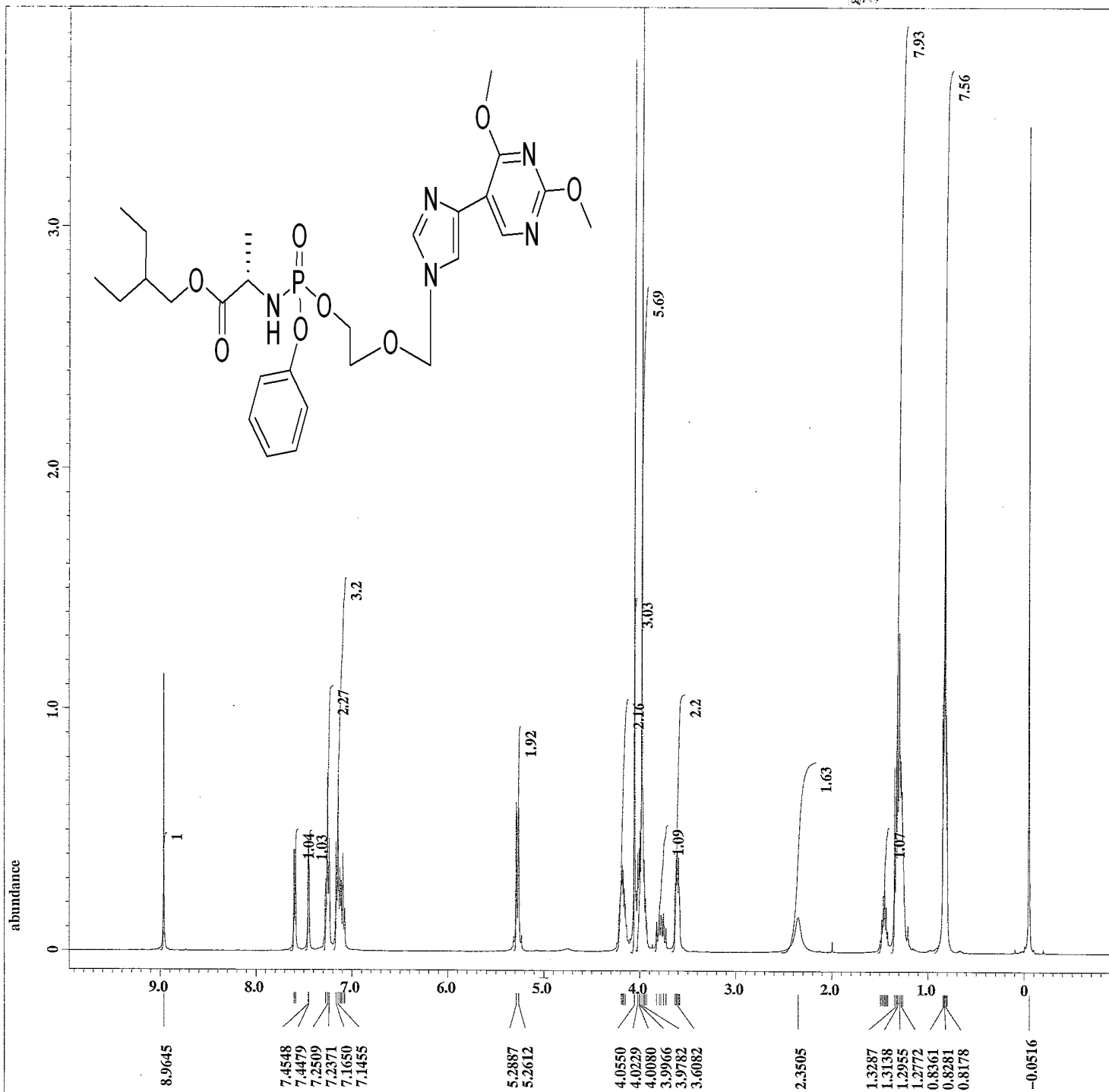


Filename = JET-2MG-3.jdf
Author = Seley
Experiment = single_pulse.ex2
Sample_id = S#446794
Solvent = CHLOROFORM-D
Creation_time = 1-JUN-2020 12:16:33
Revision_time = 1-JUN-2020 12:45:55
Current_time = 1-JUN-2020 12:46:08

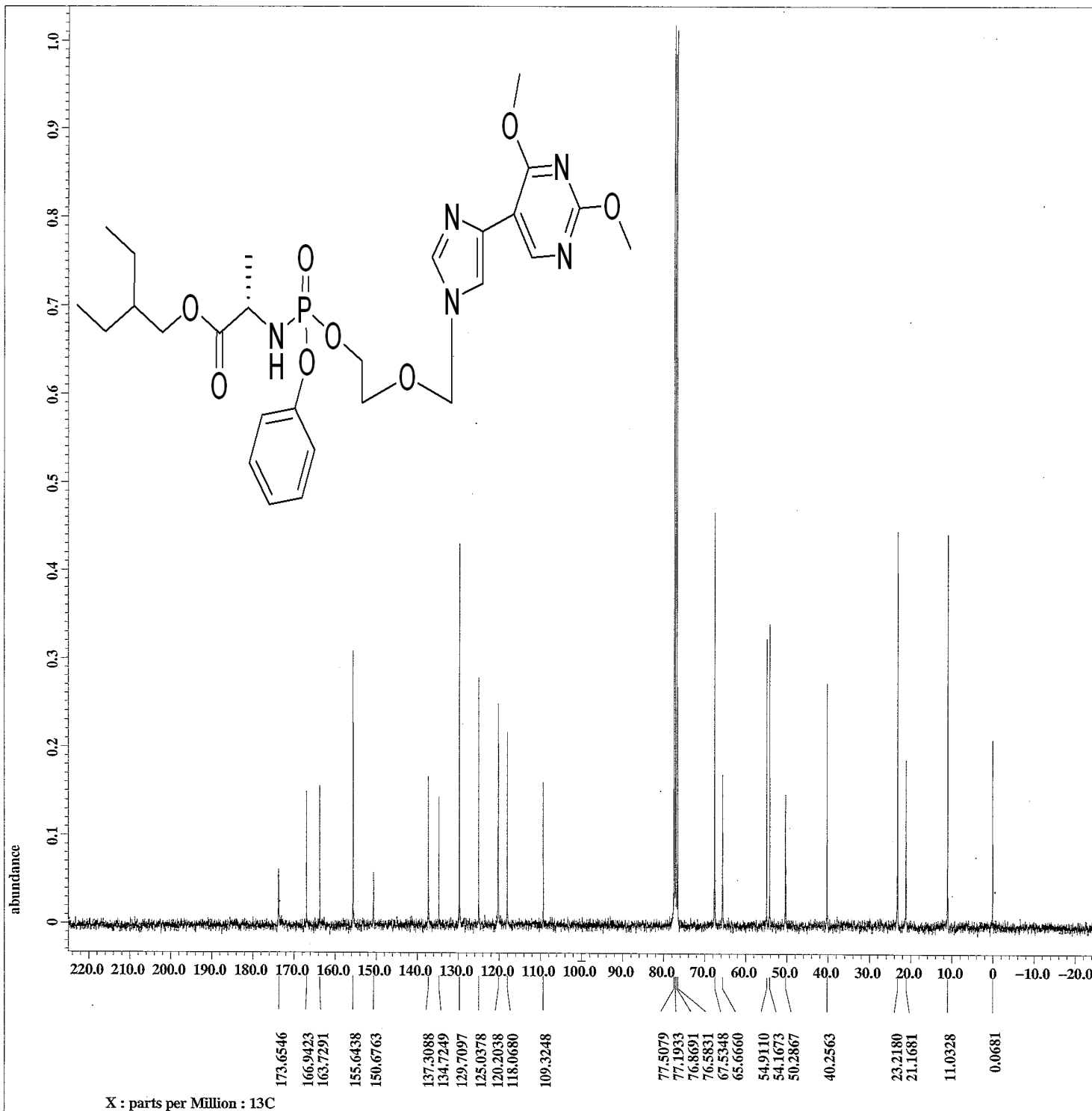
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 13.5 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 3 [dB]
X_pulse = 6.75 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 32
Relaxation_delay = 5 [s]
Repetition_time = 7.18365952 [s]
Temp_get = 19.6 [dC]



X : parts per Million : 1H



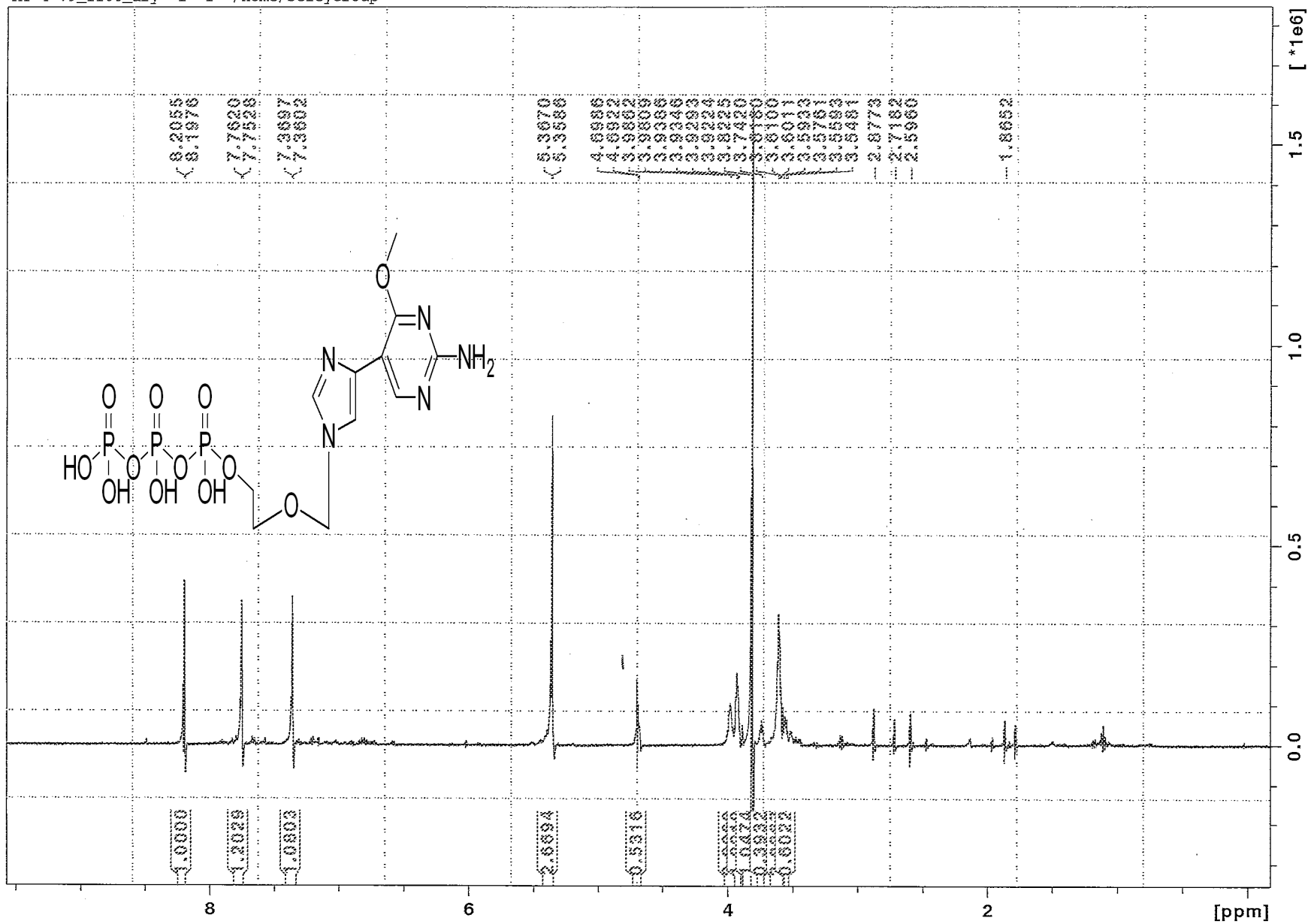
Filename = JET-2MG-4.jdf
Author = Seley
Experiment = single_pulse_dec
Sample_id = S#449657
Solvent = CHLOROFORM-D
Creation_time = 1-JUN-2020 12:46:21
Revision_time = 1-JUN-2020 13:00:13
Current_time = 1-JUN-2020 13:00:16

Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECK 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.0433312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 528
Total_scans = 528

X_90_width = 7 [us]
X_acq_time = 1.0433312 [s]
X_angle = 30 [deg]
X_atn = 6 [dB]
X_pulse = 2.33333333 [us]
Irr_atn_dec = 21.1 [dB]
Irr_atn_noe = 21.1 [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 = 3.0433312 [s]
Temp_get = 19.8 [dC]

MY-4-79_1108_dry 1 1 /home/SeleyGroup



H₂O

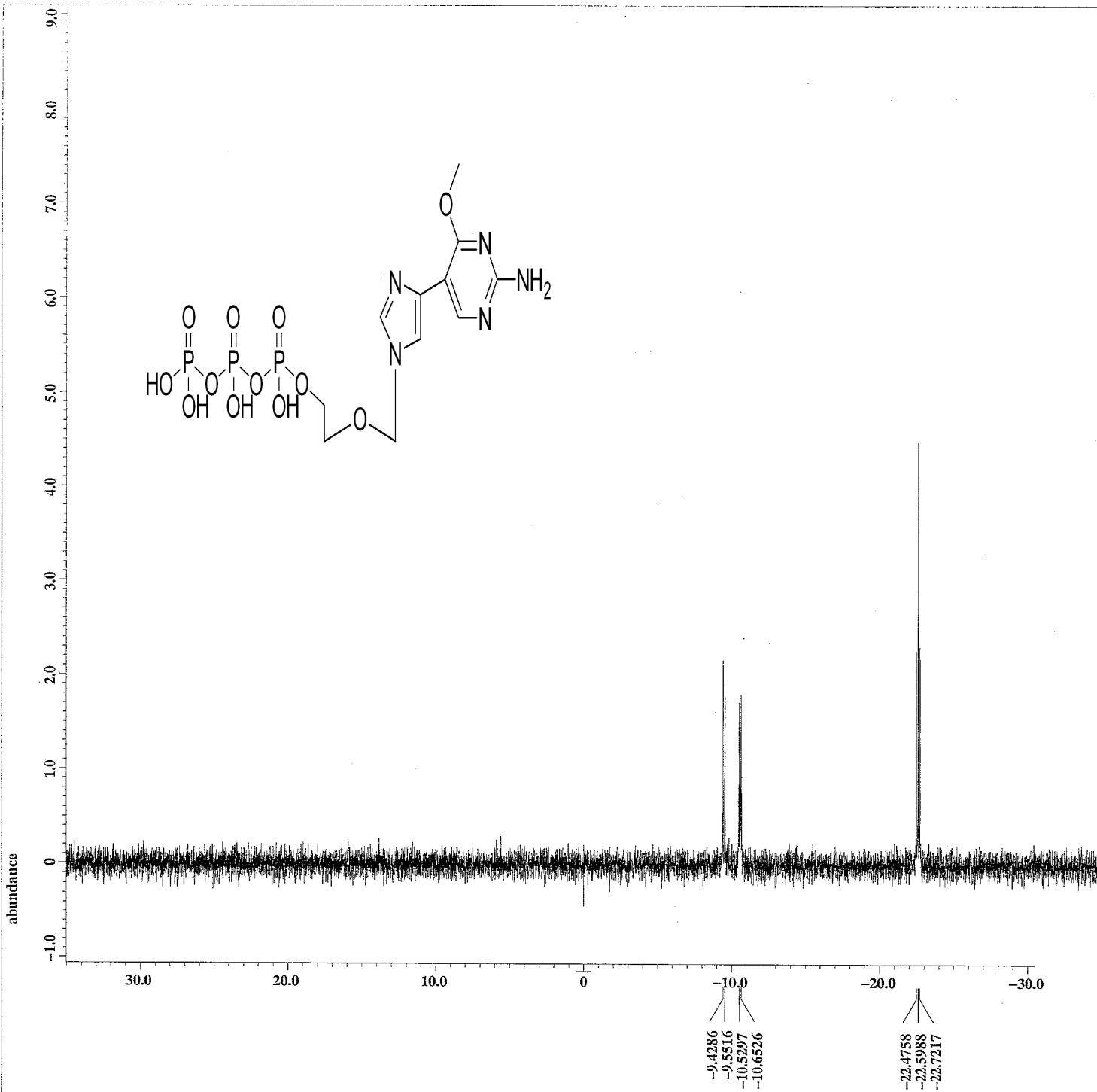


Filename = MY-1-219.2-ttw4 -2.jd
Author = Seley
Experiment = single_pulse.ex2
Sample_id = S#385127
Solvent = D2O
Creation_time = 19-DEC-2016 10:57:55
Revision_time = 19-DEC-2016 10:46:49
Current_time = 19-DEC-2016 10:46:58

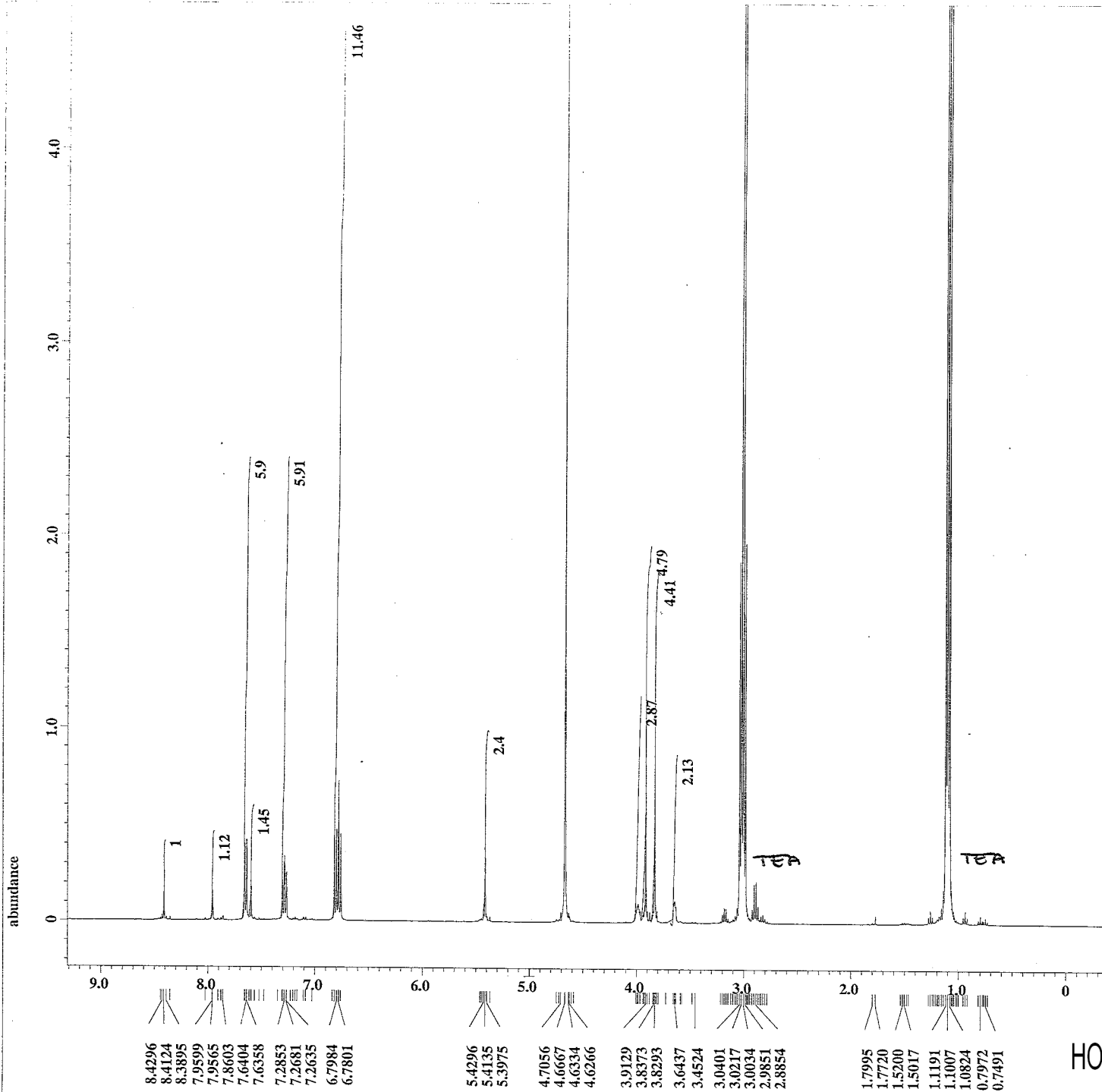
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 31P
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.15605504[s]
X_domain = 31P
X_freq = 161.83469309[MHz]
X_offset = 0[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.86501072[Hz]
X_sweep = 14.1723356[kHz]
Irr_domain = 31P
Irr_freq = 161.83469309[MHz]
Irr_offset = 5[ppm]
Tri_domain = 31P
Tri_freq = 161.83469309[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 32
Total_scans = 32

X_90_width = 16.2[us]
X_acq_time = 1.15605504[s]
X_angle = 45[deg]
X_atn = 3[dB]
X_pulse = 8.1[us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Recvr_gain = 68
Relaxation_delay = 5[s]
Repetition_time = 6.15605504[s]
Temp_get = 22.3[degC]



X : parts per Million : 31P



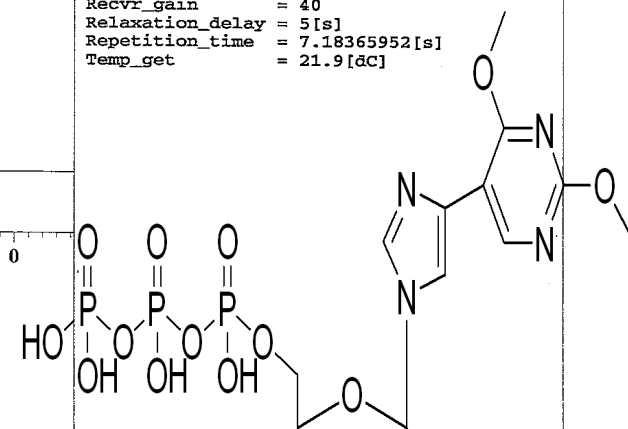
Filename = MY-4-003_lyoph_0327-3
Author = Seley
Experiment = single_pulse.ex2
Sample_id = S#467455
Solvent = D2O
Creation_time = 27-MAR-2018 12:03:00
Revision_time = 27-MAR-2018 13:04:29
Current_time = 27-MAR-2018 13:04:56

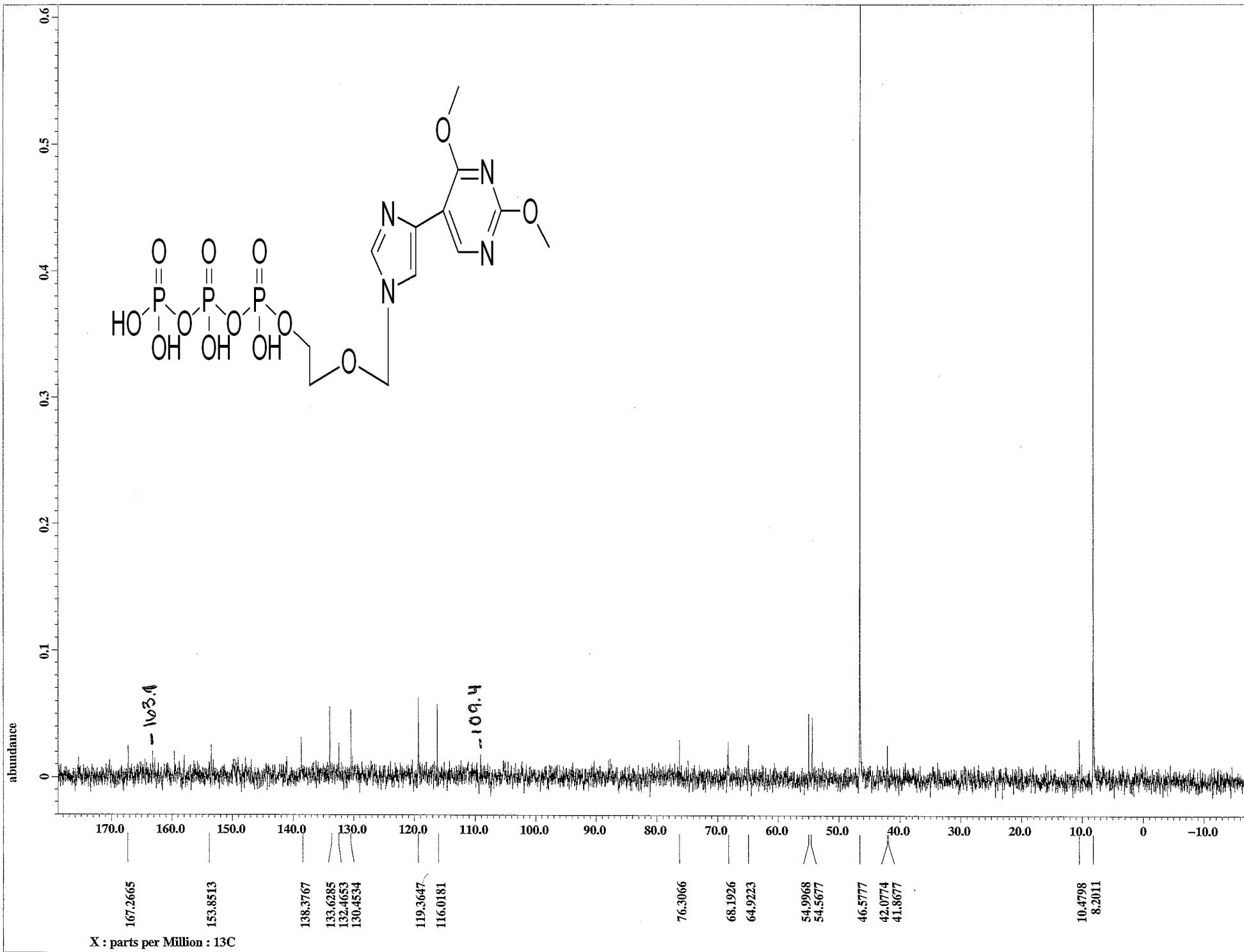
Comment = single_pulse
Data_format = 1D_COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = DELTA2_NMR

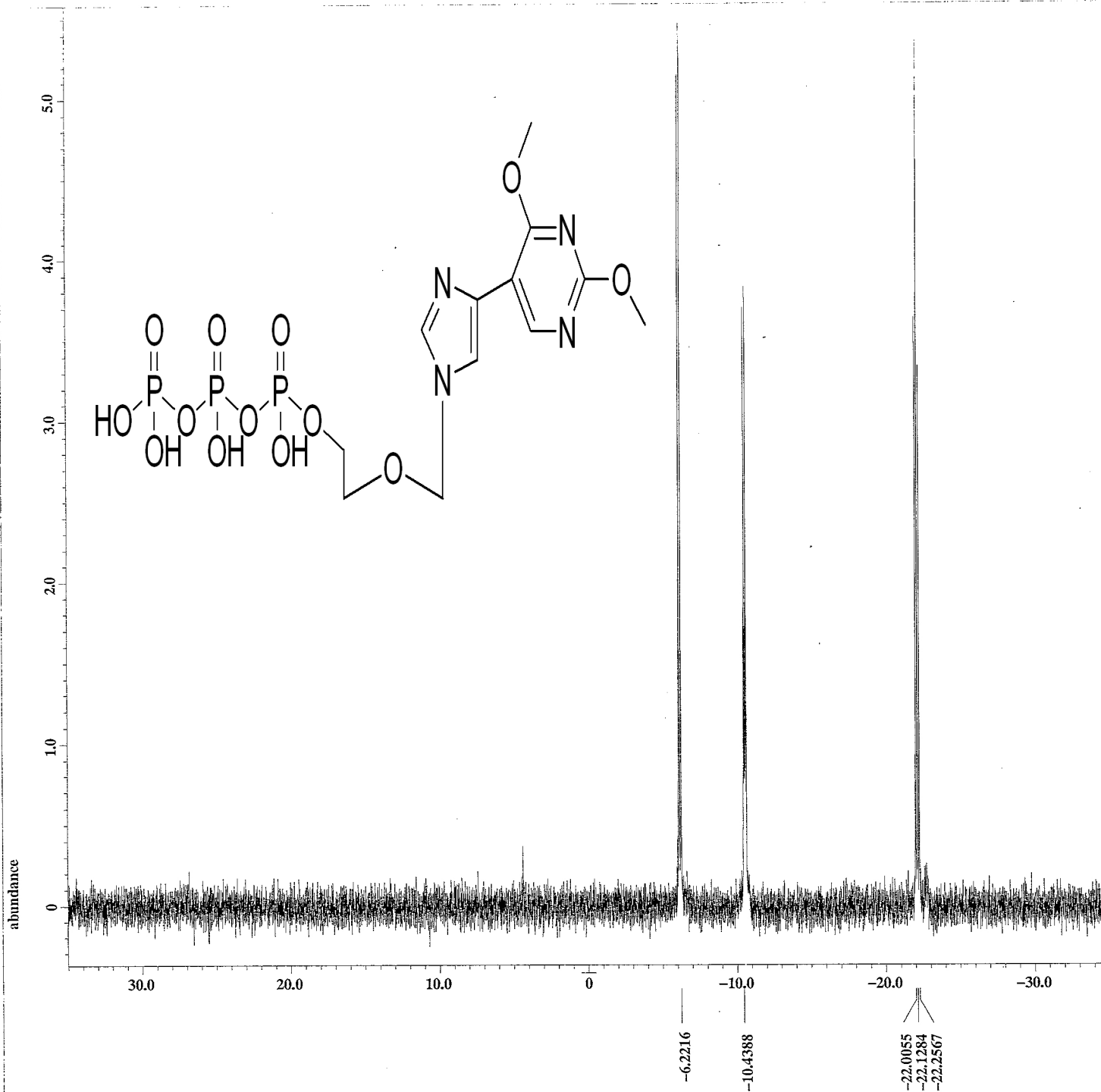
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 13.5 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 3 [dB]
X_pulse = 6.75 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 40
Relaxation_delay = 5 [s]
Repetition_time = 7.18365952 [s]
Temp_get = 21.9 [dC]

X : parts per Million : 1H







Filename = MY-3-034.PHOS-3.jdf
Author = Seley
Experiment = single_pulse.ex2
Sample_id = S#588947
Solvent = D2O
Creation_time = 18-JUL-2017 16:24:04
Revision_time = 18-JUL-2017 16:27:15
Current_time = 18-JUL-2017 16:27:24

Comment = single_pulse
Data_format = 1D_COMPLEX
Dim_size = 13107
Dim_title = 31P
Dim_units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.15605504[s]
X_domain = 31P
X_freq = 161.83469309[MHz]
X_offset = 0[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.86501072[Hz]
X_sweep = 14.1723356[kHz]
Irr_domain = 31P
Irr_freq = 161.83469309[MHz]
Irr_offset = 5[ppm]
Tri_domain = 31P
Tri_freq = 161.83469309[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 32
Total_scans = 32

X_90_width = 16.2[us]
X_acq_time = 1.15605504[s]
X_angle = 45[deg]
X_atn = 3[dB]
X_pulse = 8.1[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 66
Relaxation_delay = 5[s]
Repetition_time = 6.15605504[s]
Temp_get = 22.5[degC]

Generic Display Report

Analysis Info

Analysis Name D:\Data\Seley\Joy\JET-2-boronic ester suzuki00.d
Method Seley_ESI_Pos_Generic.m
Sample Name .ACh
Comment

Acquisition Date 5/19/2020 2:24:56 PM

Operator ADM
Instrument amaZon speed

