

Supplementary Information

Synthesis of novel Entecavir analogues having 4'-cyano-6"-fluoromethylenecyclopentene skeletons, as an aglycone moiety as highly potent and long-acting anti Hepatitis B virus agent

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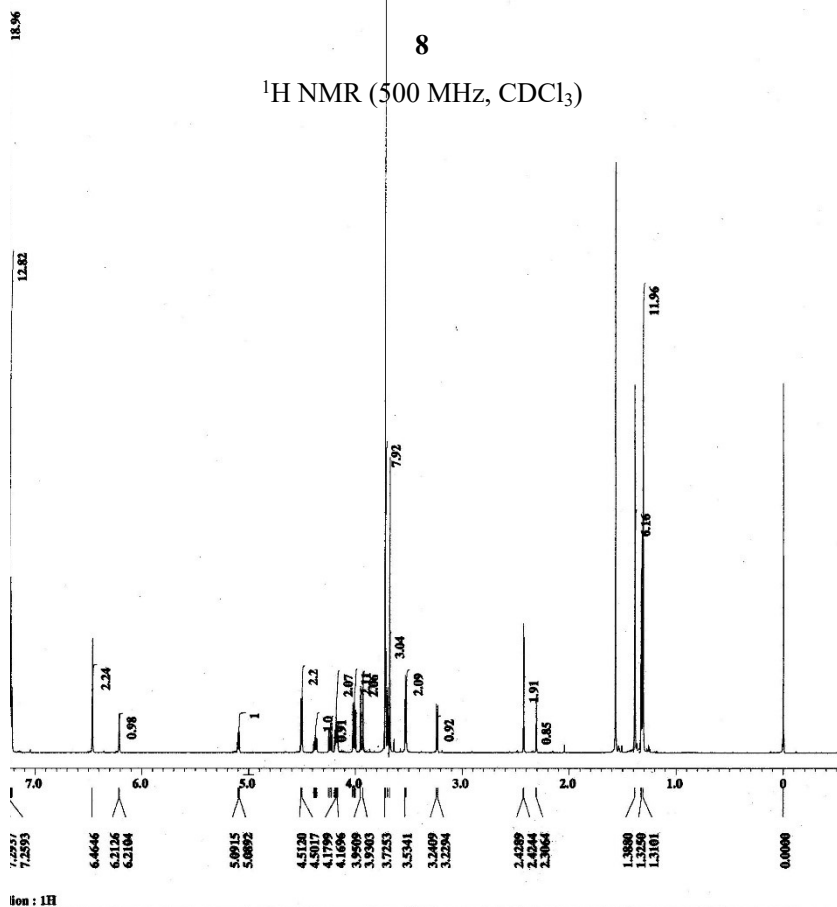
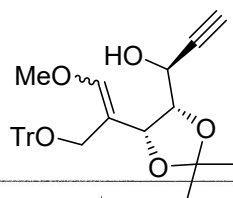
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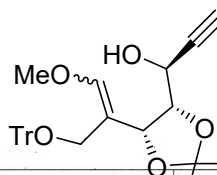
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sweep : 0.2[Hz] : 0.0[s]
 f1 : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46029-re-hplc_PROTON-1.

Filename = KMA46029-re-hplc_PROT
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = KMA46029-re-hplc
 Solvent = CHLOROFORM-D
 Creation_time = 3-OCT-2019 18:00:38
 Revision_time = 3-OCT-2019 18:09:31
 Current_time = 3-OCT-2019 18:09:41

Comment = CDCl3
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 1H
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500

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_resolution = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 12[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 6[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 4[s]
 Repetition_time = 5.74587904[s]
 Temp_get = 21.3[degC]



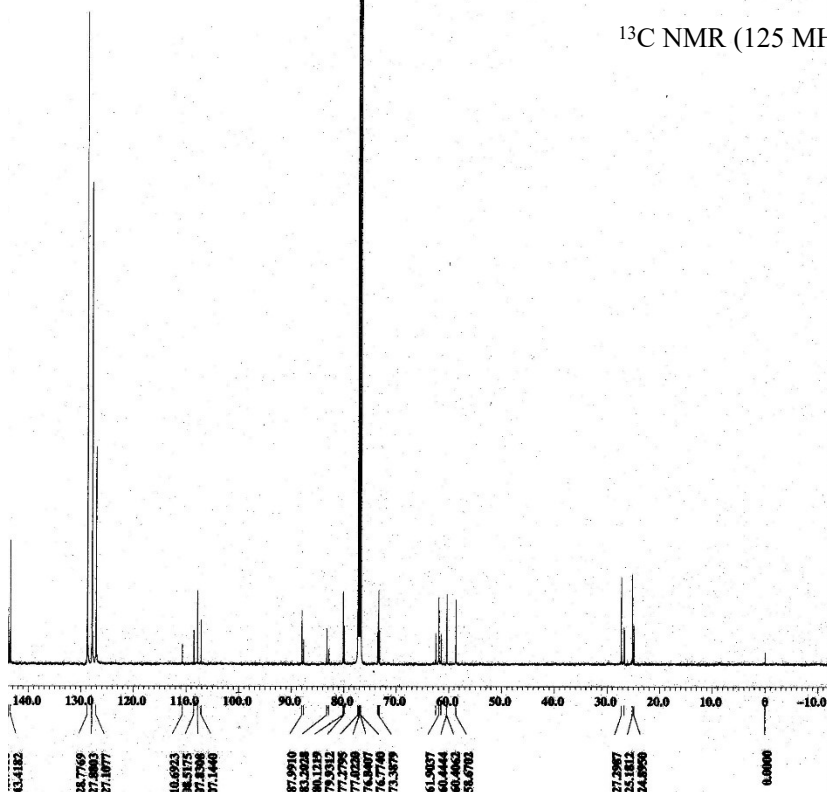
8

¹³C NMR (125 MHz)

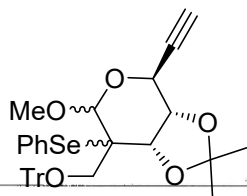
JEOL

----- PROCESSING PARAMETERS -----
 do_balance : 0 : FALSE
 gamma : 13C(101Hz) : 0.0[s]
 t1_rho2 : 0.0[s] : 80[%] : 100[%]
 nu1 : 1
 f2 : 1 : TRUE : TRUE
 machinephase :
 ppm
 Derived from: KMA46029-carbon-1.jdf

Filename = KMA46029-carbon-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = 88733221
 Solvent = CHLOROFORM-D
 Creation_time = 7-JAN-2020 05:48:53
 Revision_time = 7-JAN-2020 07:19:22
 Current_time = 7-JAN-2020 07:20:16
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dia_size = 26214
 Dia_title = 13C
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = 12000
 Total_scans = 12000
 X_90_width = 11.33 [us]
 X_acq_time = 0.83361792[s]
 X_angle = 30 [deg]
 X_atn = 6.6 [dB]
 X_pulse = 3.84333333 [us]
 Irr_atn_dec = 22.192 [dB]
 Irr_atn_noe = 22.192 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Repetition_time = 2.83361792[s]
 Temp_get = 26.2 [C]



13C



9

^1H NMR (500 MHz, CDCl_3)



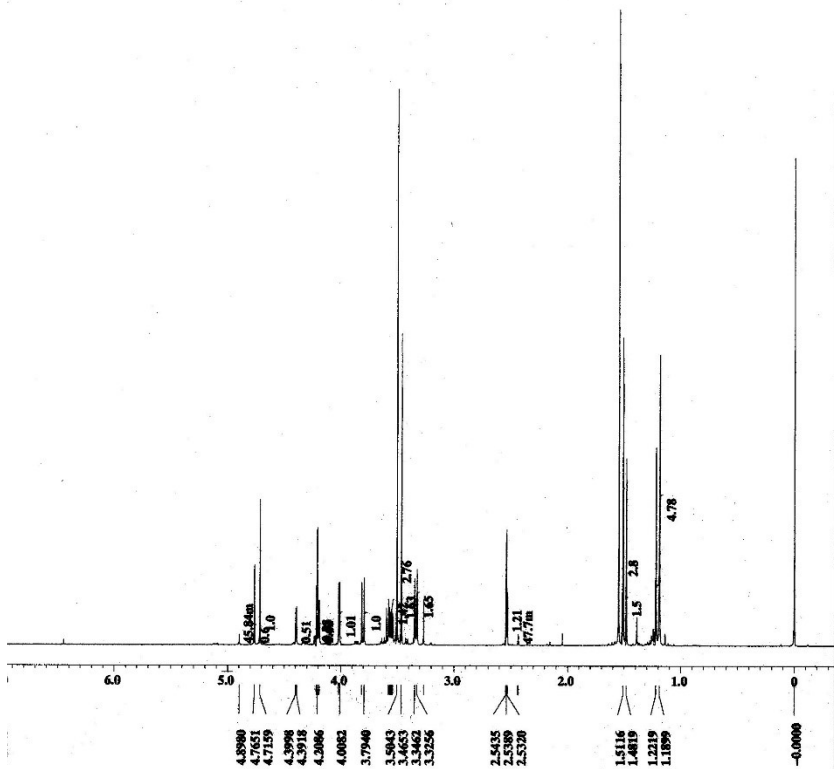
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 do_balance : 0 : FALSE
 exp : 0.2 [Hz] : 0.0 [s]
 f1 : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46139-hp1cCDCL3_PROTON-

Filename = KMA46139-hp1cCDCL3_PR
 Author = delta
 Experiment = single_pulse.exp2
 Sample_id = KMA46139-hp1cCDCL3
 Solvent = CHLOROFORM-D
 Creation_time = 9-OCT-2019 13:33:12
 Revision_time = 9-OCT-2019 13:43:43
 Current_time = 9-OCT-2019 13:44:53

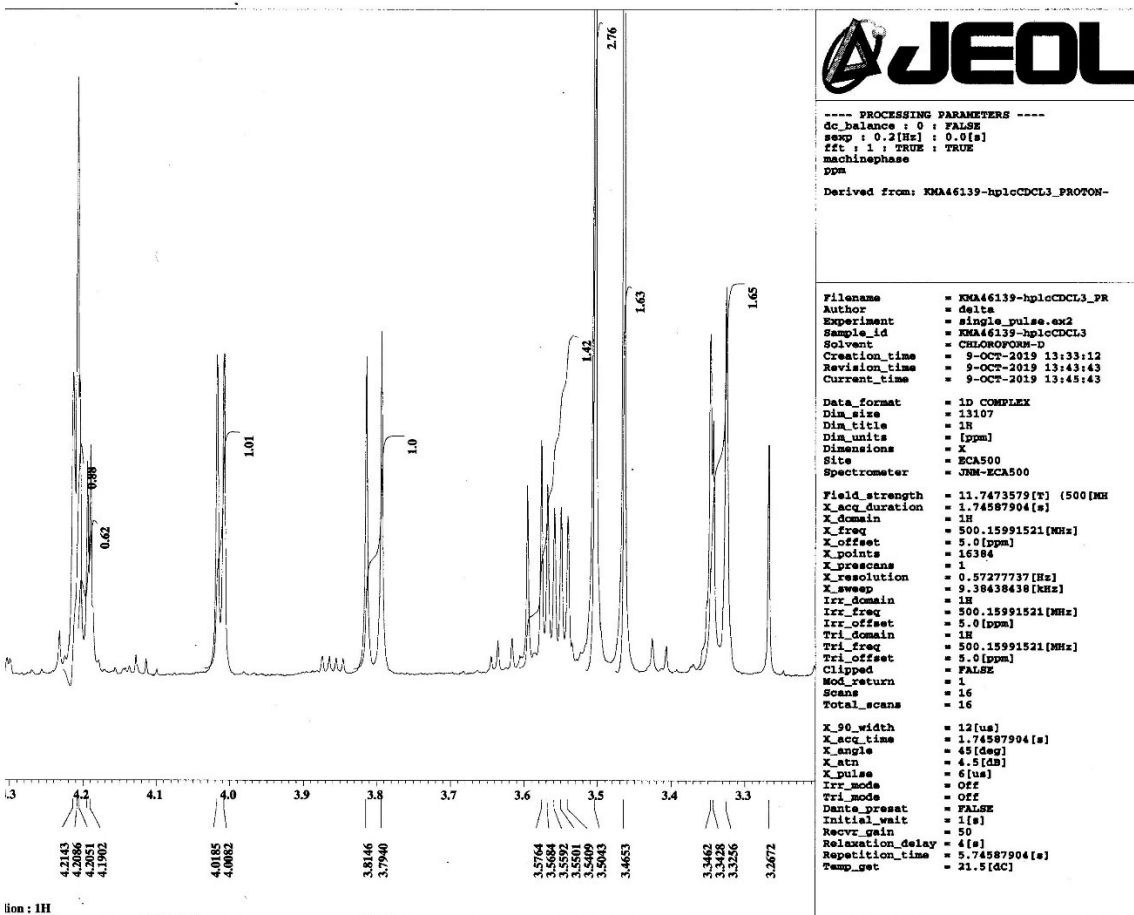
 Data_format = 1D COMPLEX
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 Dia_title = 1H
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500

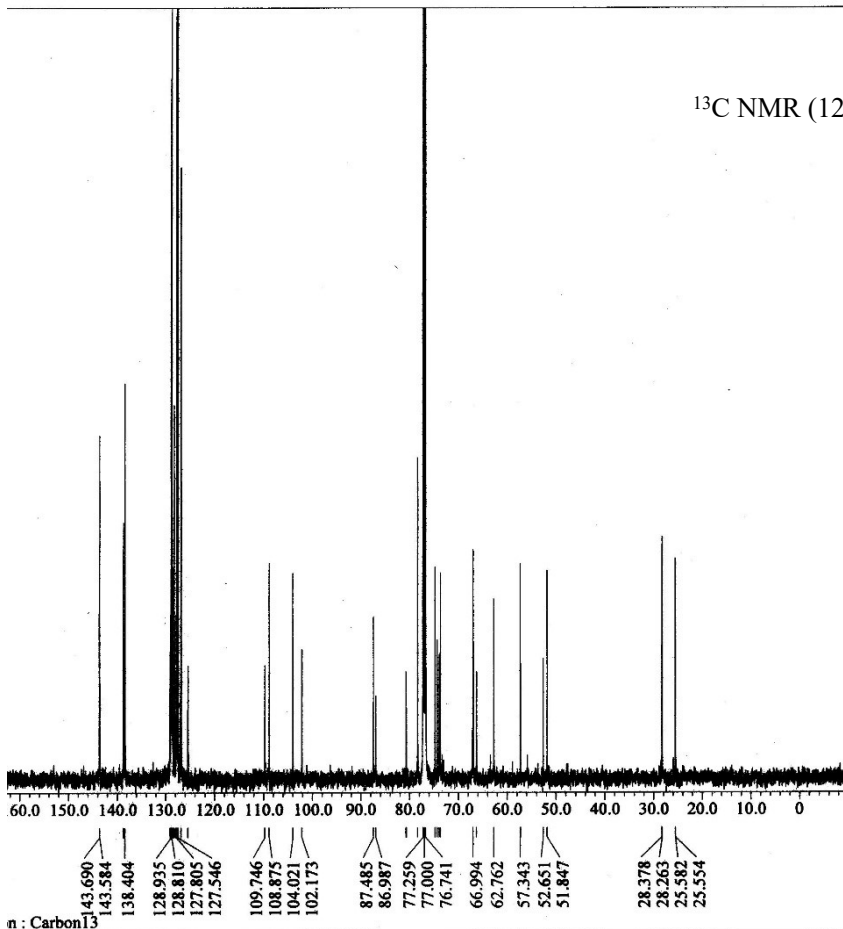
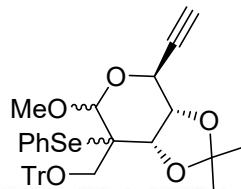
 Field_strength = 11.7473579 [T] (500 [MH]
 X_acq_duration = 1.74587904 [s]
 X_domain = 1H
 X_freq = 500.15991521 [MHz]
 X_offset = 5.0 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.57277737 [Hz]
 X_sweep = 9.38438438 [kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521 [MHz]
 Tri_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

 X_90_width = 12 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_atn = 4.5 [dB]
 X_pulse = 6 [us]
 Irr_mode = Off
 Tri_mode = Off
 Danta_preset = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 50
 Relaxation_delay = 4 [s]
 Repetition_time = 5.74587904 [s]
 Temp_get = 21.5 [dC]



Ion: 1H





9 JEOL RESONANCE ¹³C NMR (125 MHz, CDCl₃) <pre> ===== dc balance(0, FALSE) sexp(2.0[Hz], 0.0[s]) trapenoid(0[Hz], 0[Hz], 80[Hz], 100[Hz]) sarcosyl(1) fft(1, TRUE, TRUE) ppm phase(191.5, 185, 59.37512[Hz]) 以下K由来: XLVI-39_c-1-1.jdf </pre>	
Filename	= XLVI-39_c-1-4.jdf
Author	= delta
Experiment	= single_pulse_dec.jsp
Sample_Id	= XLVI-39
Solvent	= CHLOROFORM-D
Creation_Time	= 26-OCT-2019 18:20:43
Revision_Time	= 2-NOV-2019 19:38:17
Current_Time	= 2-NOV-2019 19:40:05
Comment	= XLVI-39_c
Data_Format	= 1D_COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECK500
Spectrometer	= DELTA2_NMR
Field_Strength	= 11.62926421[T] (500[MHz])
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_Sweep_Clipped	= 31.25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 495.13191398[MHz]
Irr_Offset	= 5[ppm]
Clipped	= TRUE
Scans	= 1000
Total_Scans	= 1000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Gst	= 21.3[degC]
X_90_Width	= 9.2[us]
X_Acq_Time	= 0.8388608[s]
X_Angle	= 30[deg]
X_Atn	= 4.6[dB]
X_Pulse	= 3.06666667[us]
Irr_Atn_Dec	= 21.976[db]
Irr_Atn_Moe	= 21.976[db]
Irr_Moise	= WALTZ
Irr_Width	= 92[us]
Decoupling	= TRUE



```

Filename          = KMA44021_FYOTON-5.j2d
Author            = delta
Experiment        = single_pulse_echo
Sample_id         = KMA44021
Solve            = CXCORPROM-D
Creation_time     = 2-SEP-2019 19:27:22
Revision_time    = 2-SEP-2019 19:43:50
Current_time      = 2-SEP-2019 19:44:11

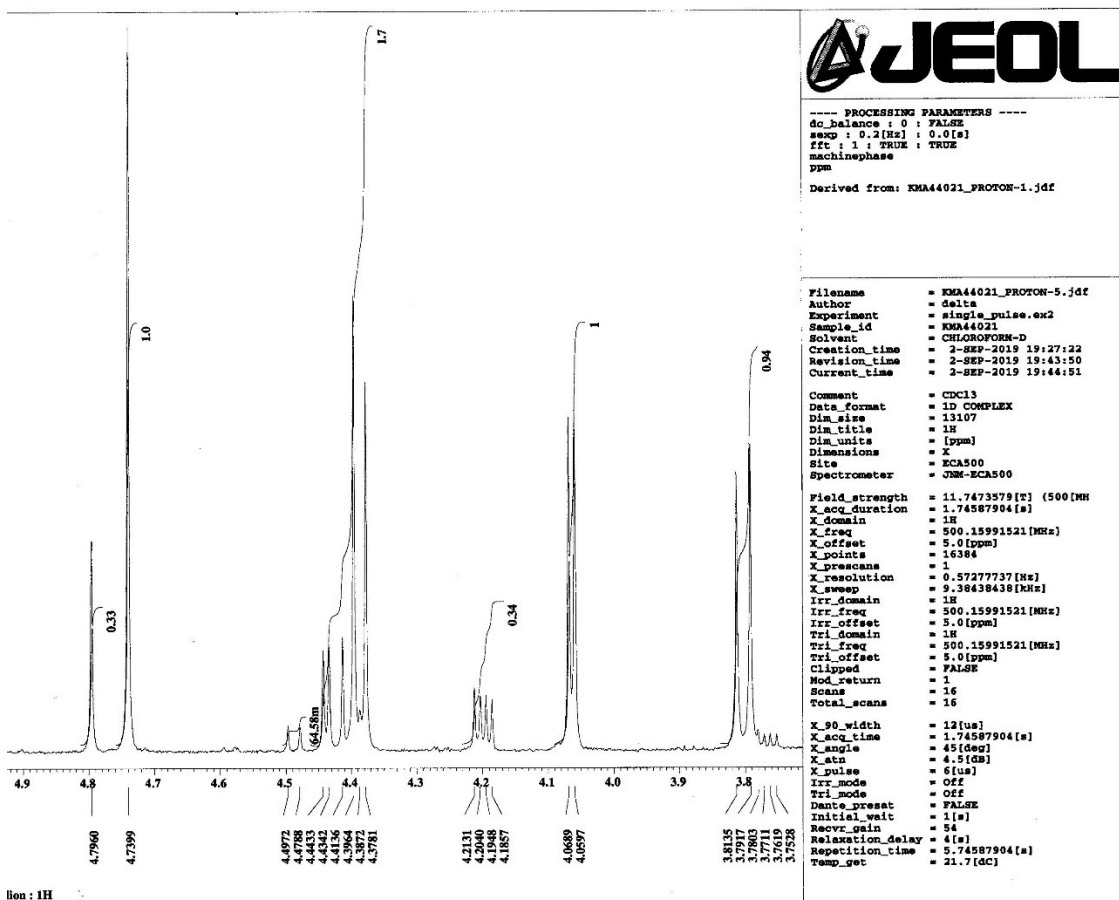
Comment           = CDDC13
Data_format       = 1D COMPLEX
Dis_angle         = 1.74587904[s]
Dis_title         = 1N
Dis_units         = [ppm]
Dimensions        = X
Size              = ECA500
Spectrometer      = JNM-ECA500

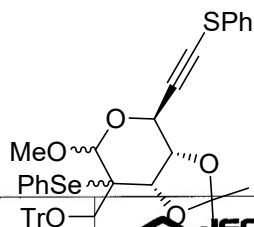
Field_strength    = 11.7437539[T] (500[MH
X_domain          = 1N
X_freq            = 500.159915121[MHz]
X_offset          = 5.0 [ppm]
X_points          = 1284
X_prescans        = 1
X_resolution      = 0.87277737[KHz]
X_sweep           = 38438438[KHz]
Irr_domain        = 1N
Irr_freq          = 500.159915121[MHz]
Irr_offset        = 5.0 [ppm]
Irr_domain2       = 1N
Irr_freq2         = 500.159915121[MHz]
Irr_offset2       = 5.0 [ppm]
Clipped           = FALSE
Mod_return        = 16
Scans             = 16
Total_scans       = 16

X_90_width        = 12[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4.5[dB]
X_pulse           = 6[us]
Irr_mode          = OFF
Irr_pulse         = OFF
Pulse_program     = PRGSE
Initial_wait      = 1[s]
Recov_gain        = 54
Relaxation_delay   = 4[s]
Relaxation_time    = 1.74587904[s]
Temp_get          = 21.7[dc]

```



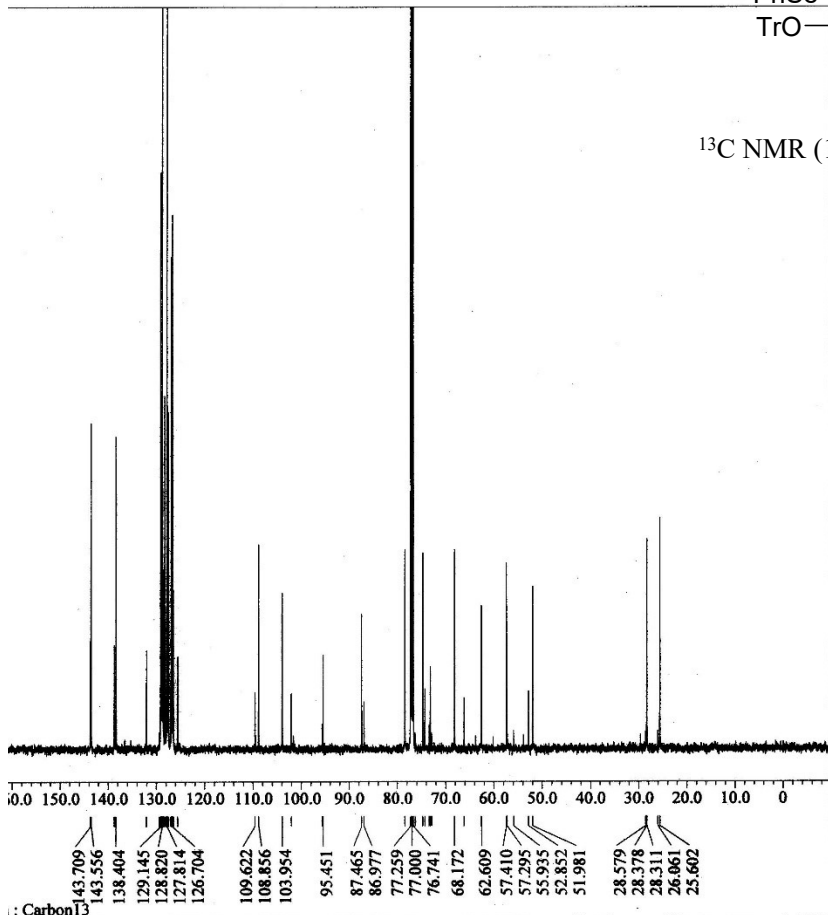




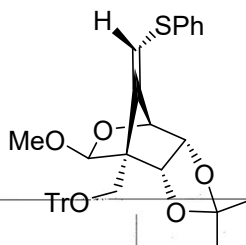
¹³C NMR (101 MHz, CDCl₃)

10
 PROCESSING PARAMETERS ----
 dc balance(0, FALSE)
 smp(2.0[Hz], 0.0[Hz])
 C13P1(101.0[Hz], 100[Hz])
 ffc(1, TRUE, TRUE)
 ppm
 phase(199.25, 200, 59.192[Hz])
 以下K由来: XLVI-21_o-1-1.jdf

Filename = XLVI-21_o-1-1.jdf
 Author = delta
 Experiment = single pulse dec.jxp
 Sample Id = XLVI-21
 Solvent = CHLOROFORM-D
 Creation Time = 2-NOV-2019 19:33:32
 Revision Time = 2-NOV-2019 20:36:21
 Current Time = 2-NOV-2019 20:38:08
 Comment = XLVI-21.c
 Data Format = 1D COMPLEX
 Dia Size = 26214
 Dia Title = Carbon13
 Dia Units = [ppm]
 Dimensions = 1
 Site = JNM-ECS500
 Spectrometer = DELTA2 NMR
 Field Strength = 11.62926421[T] (500[MHz])
 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 Sweep Clipped = 31.25[kHz]
 Irr Domain = Proton
 Irr Freq = 499.13191398[MHz]
 Irr Offset = 5[ppm]
 Clipped = TRUE
 Scans = 1000
 Total Scans = 1000
 Relaxation Delay = 2[s]
 Recvr Gain = 60
 Temp Set = 21.1[deg]
 X 90 Width = 9.2[us]
 X Acq Time = 0.8388608[s]
 X Angle = 30[deg]
 X Atn = 4.6[dB]
 X Pulse = 3.06666667[us]
 Irr Atn Dec = 21.976[dB]
 Irr Atn Noe = 21.976[dB]
 Irr Noise = WALTZ
 Irr Pwidth = 92[us]
 Decoupling = TRUE



: Carbon13

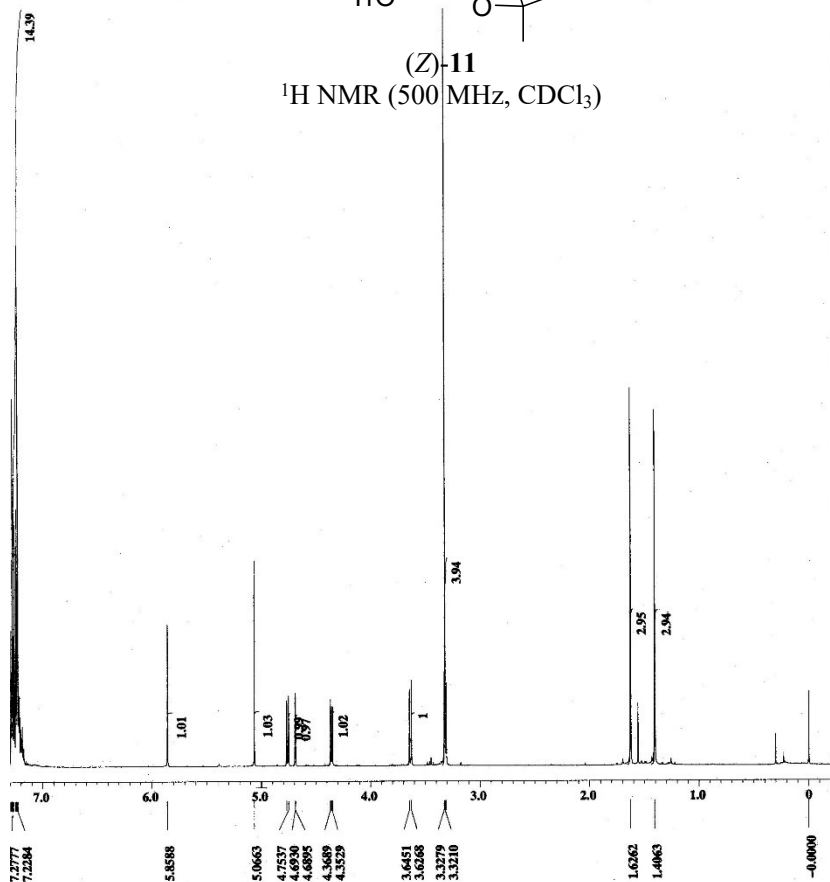


(Z)-11
¹H NMR (500 MHz, CDCl₃)

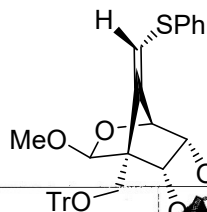


----- PROCESSING PARAMETERS -----
 ds_balance : 0 : FALSE
 sump : 0.2[Hz] : 0.0[s]
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46077-ppp_PROTON-1.jds

Filename = KMA46077-ppp_PROTON-5
 Author = delta
 Experiment = single_pulse.ac2
 Sample_id = KMA46077-ppp
 Solvent = CHLOROFORM-D
 Creation_time = 8-MAR-2020 11:06:38
 Revision_time = 8-MAR-2020 11:14:05
 Current_time = 8-MAR-2020 11:14:25
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 1H
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = 0.5727737 [Hz]
 X_sweep = 9.38438438 [kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521 [MHz]
 Tri_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 6[us]
 Irr_mode = OFF
 Tri_mode = OFF
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 44
 Relaxation_delay = 4[s]
 Repetition_time = 5.74587904[s]
 Temp_get = 23.4[dc]



Mon : 1H

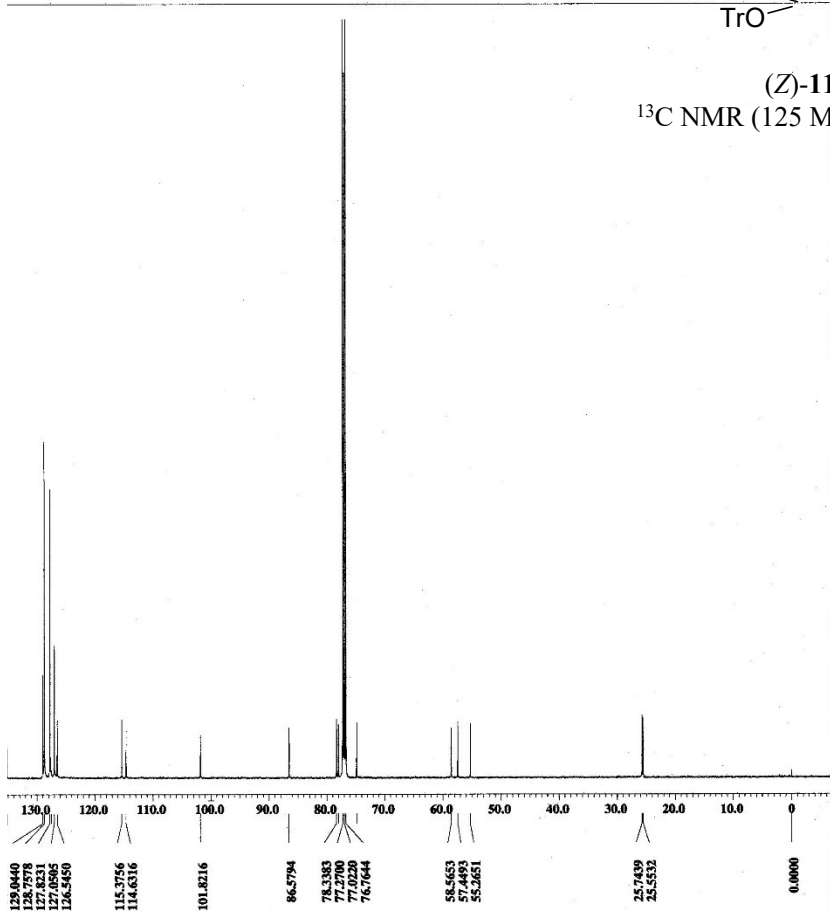


(Z)-11

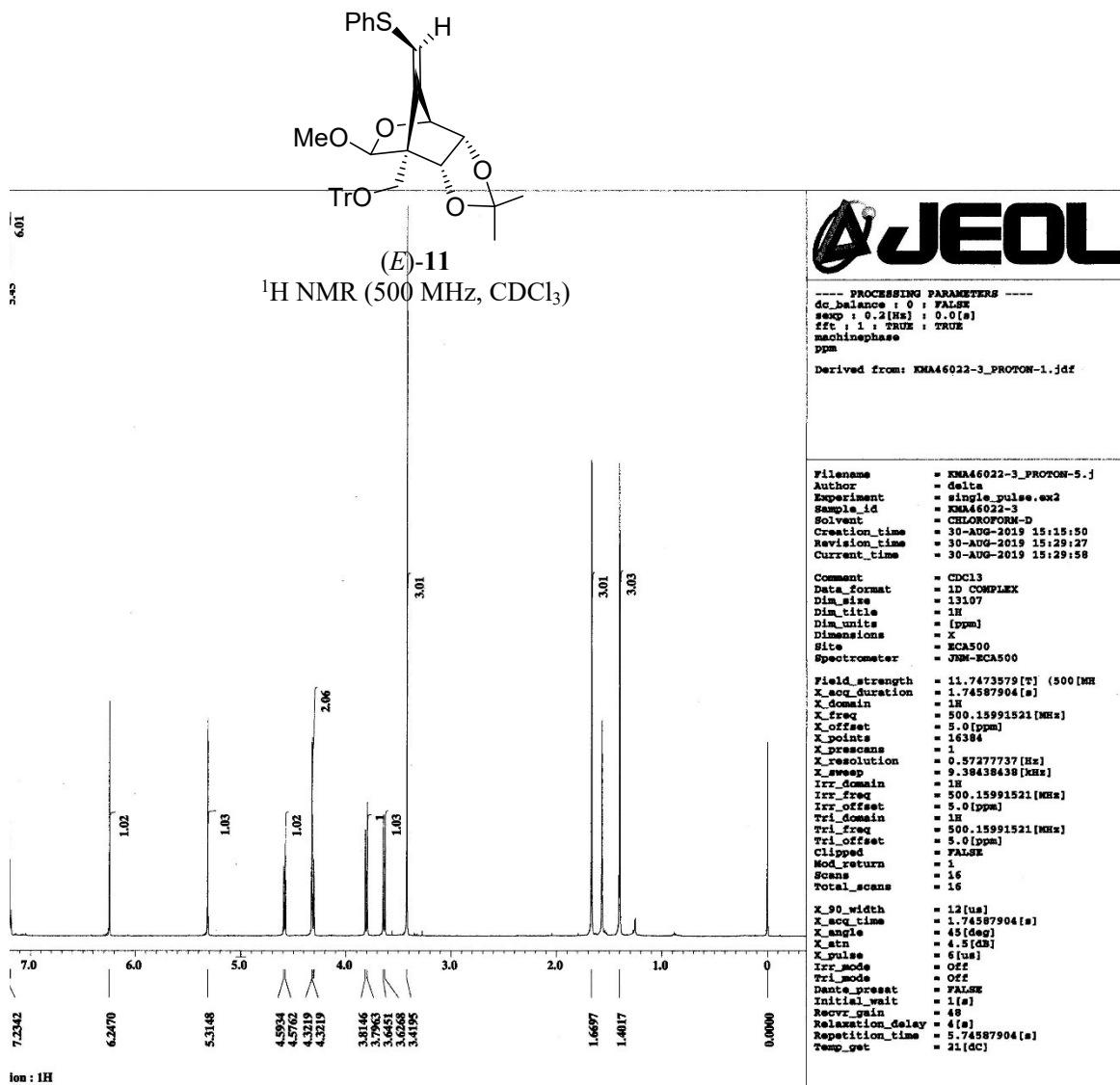
¹³C NMR (125 MHz, CDCl₃)

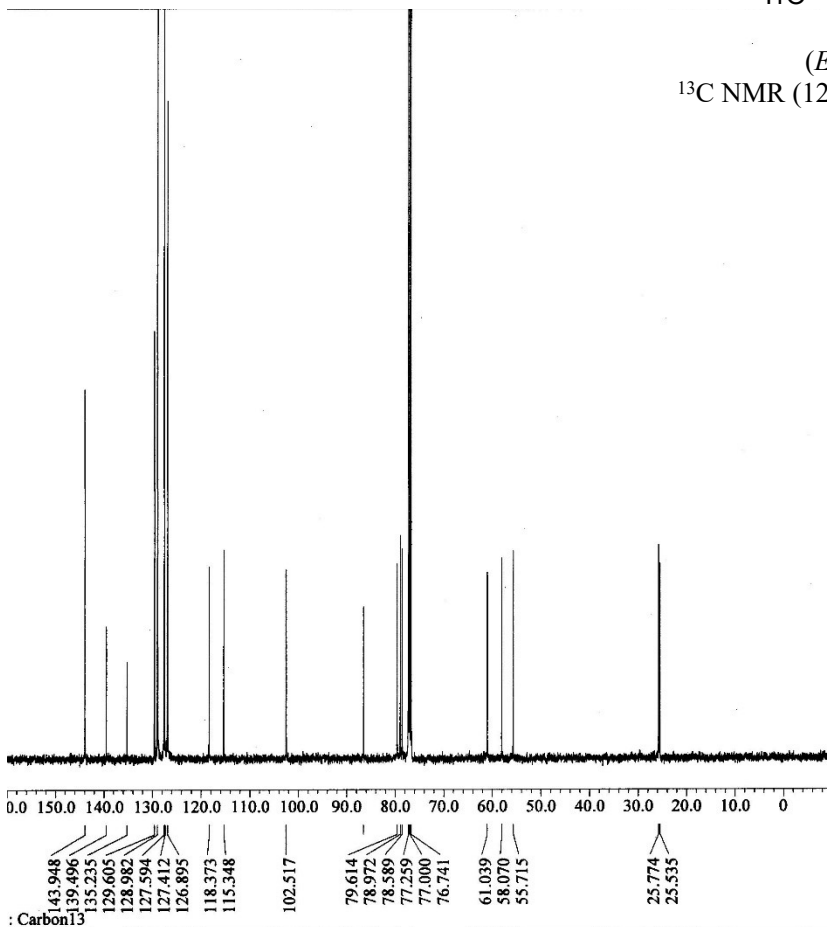
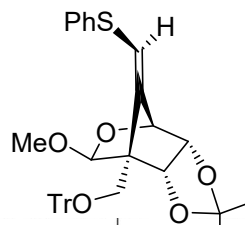
 PROCESSING PARAMETERS
 File: KMA46077-ppp-carbon-3
 Acq: 2.0[Hz] : 0.0[s]
 Trap: 0.0[Hz] : 0.0[s]
 SFO: 1 : 1
 Fft: 1 : TRUE : TRUE
 Machine: phase
 ppm
 Derived from: KMA46077-ppp-carbon-1.jdf

 File: KMA46077-ppp-carbon-3
 Author: Delta
 Experiment: single_pulse_dec
 Sample_id: S8528866
 Solvent: CHLOROFORM-D
 Creation_time: 9-MAR-2020 06:24:49
 Revision_time: 9-MAR-2020 07:45:35
 Current_time: 9-MAR-2020 07:47:09
 Comment: single pulse decouple
 Data_format: 1D COMPLEX
 Dia_size: 26214
 Dia_title: 13C
 Dia_units: [ppm]
 Dimensions: X
 Site: ECA500
 Spectrometer: JNM-ECA500
 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[MHz]
 Irr_domain: 1H
 Irr_freq: 500.15991521[MHz]
 Irr_offset: 5.0[ppm]
 Clipped: FALSE
 Mod_return: 1
 Scans: 20000
 Total_scans: 20000
 X_90_width: 11.53[us]
 X_acq_time: 0.83361792[s]
 X_angle: 30[deg]
 X_atn: 6.6[db]
 X_pulse: 3.84333333[us]
 Irr_atn_dec: 22.192[db]
 Irr_atn_noe: 22.192[db]
 Irr_noise: WALTZ
 Decoupling: TRUE
 Initial_wait: 1[s]
 Noe: TRUE
 Noe_time: 2[s]
 Recvr_gain: 50
 Relaxation_delay: 2[s]
 Repetition_time: 2.83361792[s]
 Temp_get: 24.1[dc]



Non: 13C





(E)-11
¹³C NMR (125 MHz, CDCl₃)

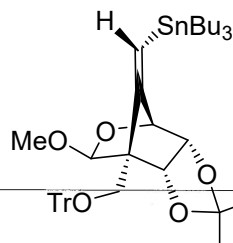
----- PROCESSING PARAMETERS -----
 do_balance(0, FALSE)
 sasp(2.0[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1)
 fft(1, TRUE, TRUE)
 ppm
 phase(231, 220, 38.96921[%])
 以下K由表: XLVI-22-3_c-1-1.jdf

Filename = XLVI-22-3_c-1-4.jdf
 Author = delta
 Experiment = single_pulse_dec.jxp
 Sample_Id = XLVI-22-3
 Solvent = CHLOROFORM-D
 Creation Time = 2-NOV-2019 21:16:59
 Revision Time = 13-NOV-2019 17:10:49
 Current Time = 13-NOV-2019 17:15:21

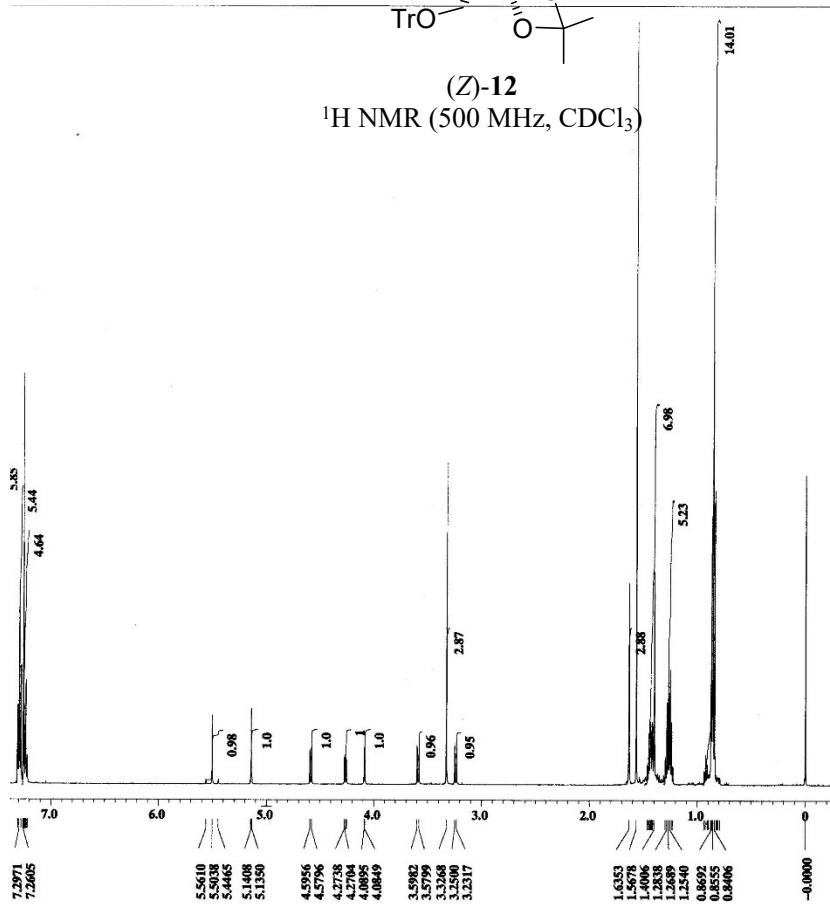
Comment = XLVI-22-3_c
 Data Format = 1D COMPLEX
 Dim_Size = 26214
 Dim_Title = Carbon13
 Dim_Units = [ppm]
 Dimensions = 2
 Site = JNM-ECK500
 Spectrometer = DELTA2_NMR

Field Strength = 11.62926421[T] (500[MHz])
 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_Sweep_Clipped = 31.25[kHz]
 Irr_Domain = Proton
 Irr_Freq = 495.13191398[MHz]
 Irr_Offset = 5[ppm]
 Clipped = TRUE
 Scans = 512
 Total_Scans = 512

Relaxation_Delay = 2[s]
 Recvr_Gain = 60
 Temp_Set = 21.2[deg]
 X_90_Width = 9.2[us]
 X_Acq_Time = 0.8388608[s]
 X_Angle = 30[deg]
 X_Atn = 4.6[dB]
 X_Pulse = 9.06666667[us]
 Irr_Atn_Dec = 21.976[dB]
 Irr_Atn_Noe = 21.976[dB]
 Irr_Noise = WALTZ
 Irr_Pwidth = 92[us]
 Decoupling = TRUE



(Z)-12
¹H NMR (500 MHz, CDCl₃)



```

----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
sweep : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: KMA46024-1_PROTON-1.jdf

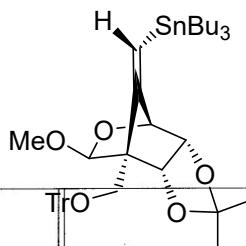
Filename      = KMA46024-1_PROTON-5.j
Author        = delta
Experiment    = single_pulse.ex2
Sample_id     = KMA46024-1
Solvent       = CHLOROFORM-D
Creation_time  = 11-SEP-2019 09:46:01
Revision_time = 11-SEP-2019 09:55:25
Current_time  = 11-SEP-2019 09:55:53

Comment       = CDCl3
Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA500
Spectrometer  = JNM-ECA500

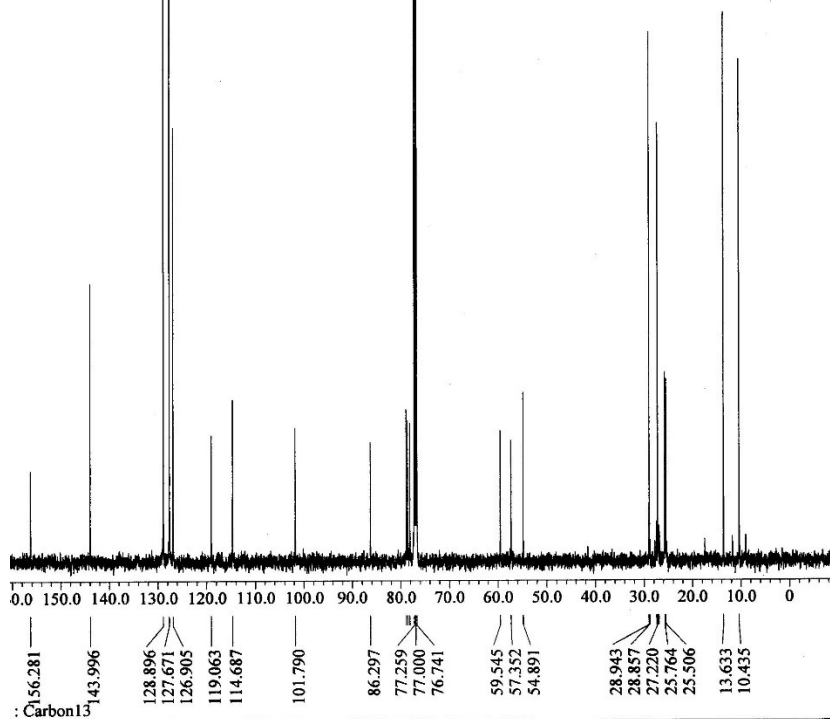
Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 12[us]
X_acq_time     = 1.74587904[s]
X_angle        = 45[deg]
X_atn          = 4.5[db]
X_pulse        = 6[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_preset   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 50
Relaxation_delay = 4[s]
Repetition_time = 5.74587904[s]
Temp_get       = 21.2[dc]
  
```

on: 1H

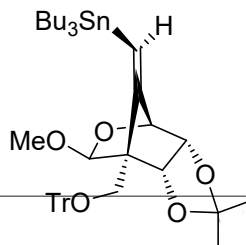


^{13}C NMR (125 MHz,
 CDCl_3)



----- PROCESSING PARAMETERS -----
 do_balance(0, FALSE)
 samp(2.0[Hz], 0.0[s])
 trapexoid(0[Hz], 0[Hz], 80[Hz], 100[Hz])
 zerofill(1)
 fft(1, TRUE, TRUE)
 ppm
 phase(187, 190, 59.00889[Hz])
 以下に由来: XLVI-24-1_c-1-1.jdf

Filename = XLVI-24-1_c-1-1.jdf
 Author = delta
 Experiment = single_pulse_dec.jsp
 Sample Id = XLVI-24-1
 Solvent = CHLOROFORM-D
 Creation Time = 29-OCT-2019 21:34:16
 Revision Time = 2-NOV-2019 19:57:36
 Current Time = 2-NOV-2019 19:58:11
 Comment = XLVI-24-1_c
 Data Format = 1D COMPLEX
 Dim Size = 26214
 Dim Title = Carbon13
 Dim Units = [ppm]
 Dimensions = 1
 Site = JNM-ECK500
 Spectrometer = DELTA2_NMR
 Field Strength = 11.62926421[T] (500[MHz])
 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_Sweep_Clipped = 31.25[kHz]
 Irr_Domain = Proton
 Irr_Freq = 495.13191398[MHz]
 Irr_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 512
 Total_Scans = 512
 Relaxation_Delay = 2[s]
 Recvr_Gain = 60
 Temp_Get = 21.3[degC]
 X_90_Width = 9.2[us]
 X_Acq_Time = 0.8388608[s]
 X_Angle = 30[deg]
 X_Atn = 4.6[dB]
 X_Pulse = 3.06666667[us]
 Irr_Atn_Dec = 21.976[dB]
 Irr_Atn_Noise = 21.976[dB]
 Irr_Noise = WALTZ
 Irr_Pwidth = 92[us]
 Decoupling = TRUE

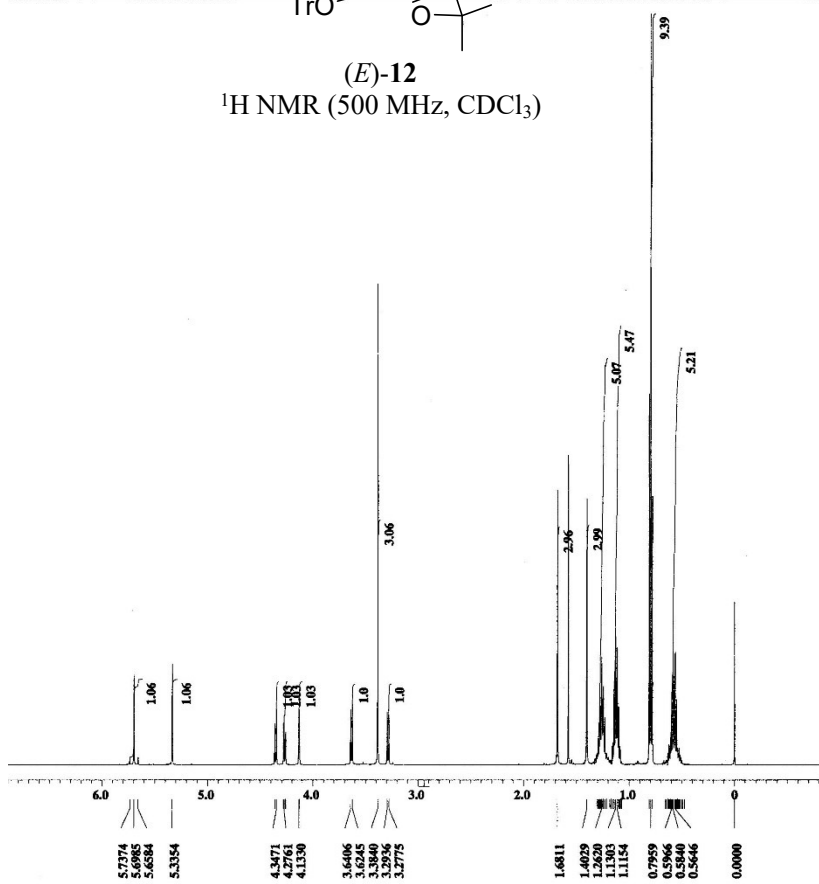


(E)-12
 ^1H NMR (500 MHz, CDCl_3)

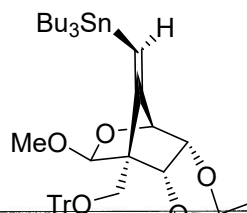


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 0.2 [Hz] : 0.0 [s]
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46024-2_PROTON-1.jdf

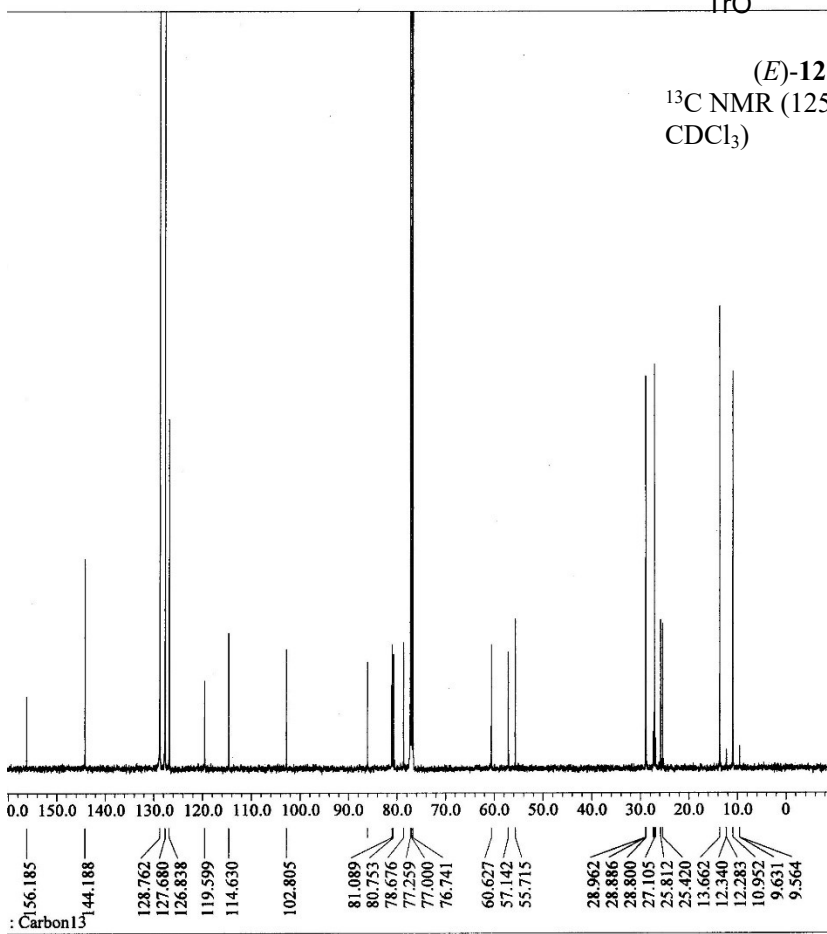
Filename = KMA46024-2_PROTON-5.j
 Author = dehta
 Experiment = siptle_pulse.ex2
 Sample_id = KMA46024-2
 Solvent = CHLOROFORM-D
 Creation_time = 11-SEP-2019 09:59:39
 Revision_time = 11-SEP-2019 09:11:59
 Current_time = 11-SEP-2019 09:12:24
 Comment = CDCl3
 Data_format = 1D COMPLEX
 Dim_size = 13,07
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECP500
 Spectrometer = JNM-ECA500
 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 = 0.97277737 [Hz]
 X_sweep = 9.38438438 [kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521 [MHz]
 Tri_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_atn = 4.5 [dB]
 X_pulse = 6 [us]
 Irr_mode = Off
 Tri_mode = Off
 Dants_presat = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 40
 Relaxation_delay = 4 [s]
 Repetition_time = 5.74587904 [s]
 Temp_get = 21.3 [dC]



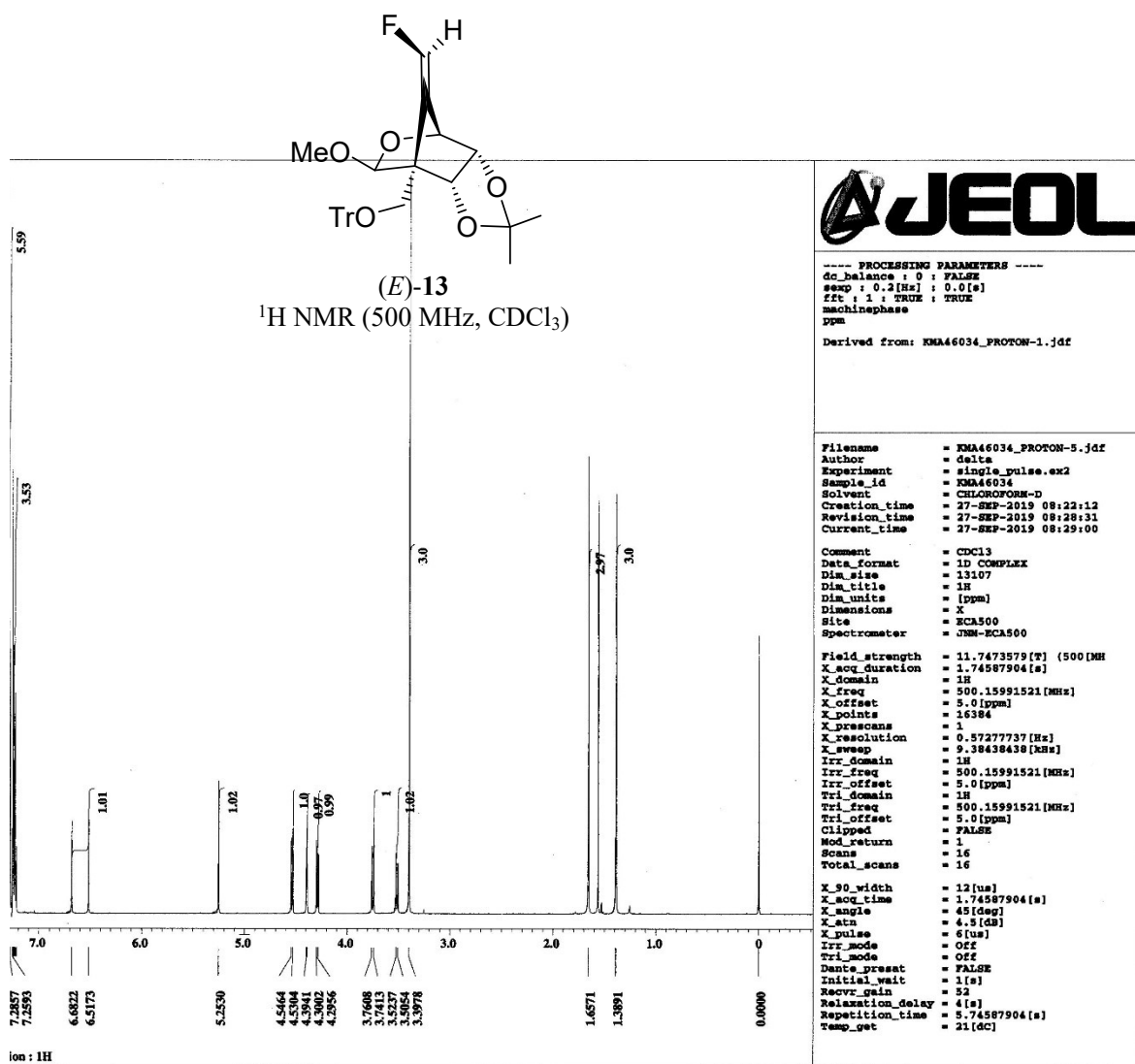
Ion: 1H

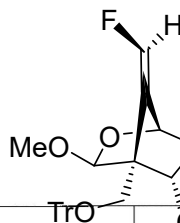


(E)-12
 ^{13}C NMR (125 MHz)
 CDCl_3



PROCESSING PARAMETERS	
do balance	(0, FALSE)
exp	(2.0[Hz], 0.0[s])
trapezoid	(0[%], 0[%], 80[%], 100[%])
zerofill	(1)
fft	(1, TRUE, TRUE)
ppm	Phase(184.25, 190, 59.00889[%])
以下に由来: XLVI-24-2_c-1-1.jdf	
Filename	= XLVI-24-2_c-1-1.jdf
Author	= delta
Experiment	= single_pulse_dec.jpg
Sample Id	= XLVI-24-2
Solvent	= CHLOROFORM-D
Creation Time	= 29-OCT-2019 22:22:59
Revision Time	= 2-NOV-2019 20:50:24
Current Time	= 2-NOV-2019 20:52:25
Comment	= XLVI-24-2_c
Data Format	= 1D COMPLEX
Dim Size	= 26214
Dim Title	= Carbon13
Dim Units	= [ppm]
Dimensions	= X
Site	= JNM-ECP500
Spectrometer	= DELTA2_NMR
Field Strength	= 11.62926421[T] (500[MHz])
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 Sweep Clipped	= 31.25[kHz]
Irr Domain	= Proton
Irr Freq	= 495.13191398[MHz]
Irr Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1000
Total Scans	= 1000
Relaxation Delay	= 2[s]
Recvr Gain	= 60
Temp Get	= 21.7[°C]
X 90 Width	= 9.2[us]
X Acq Time	= 0.8388608[s]
X Angle	= 30[deg]
X Atn	= 4.6[dB]
X Pulse	= 3.06666667[us]
Irr Atn Dec	= 21.976[dB]
Irr Atn Noe	= 21.976[dB]
Irr Noise	= WALTZ
Irr Pwidth	= 92[us]
Decoupling	= TRUE



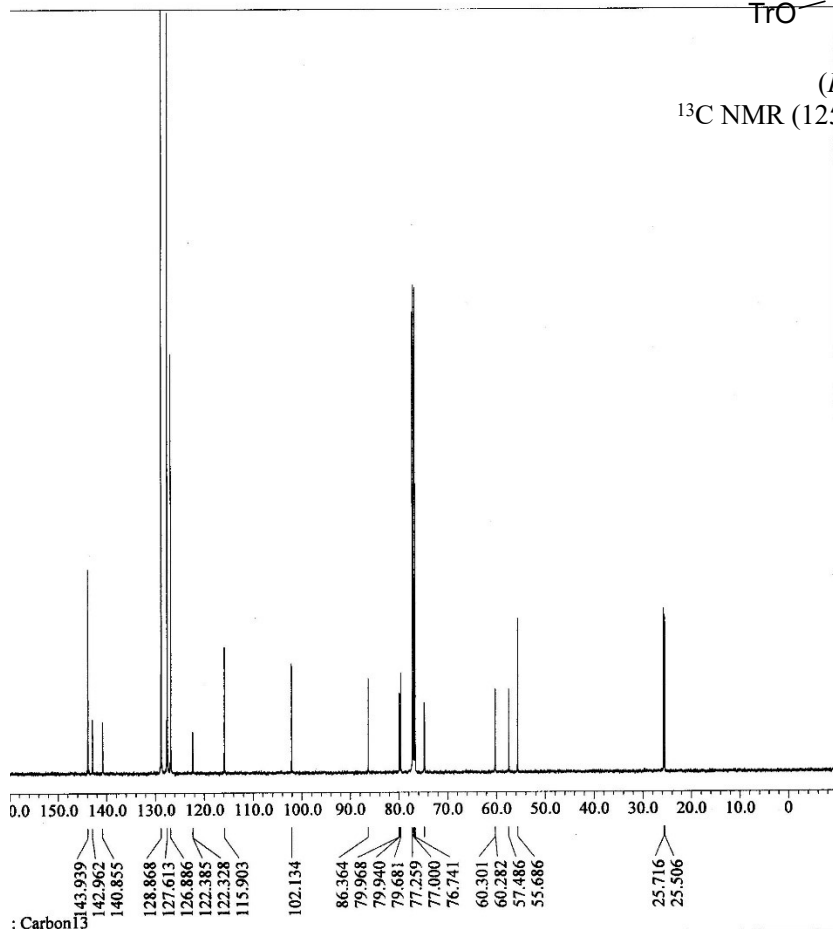


JEOL
RESONANCE

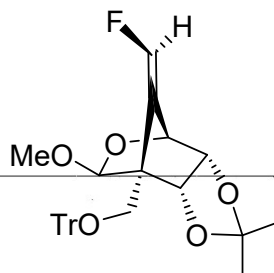
¹³C NMR (125

 deconvolve (0, 2, 2, 2)
 samp(2.0[Hz], 0.0[Hz])
 trapezoid(0[Hz], 0[Hz], 80[Hz], 100[Hz])
 zerofill(1)
 fft(1, TRUE, TRUE)
 ppm
 phase(231.25, 205.0, 38.96921[Hz])
 以下に由来: XLVI-34_c-1-1.jdf

Filename = XLVI-34_c-1-4.jdf
 Author = delta
 Experiment = single_pulse_dec.jxp
 Sample_Id = XLVI-34
 Solvent = CHLOROFORM-D
 Creation Time = 18-NOV-2019 18:55:35
 Revision Time = 18-NOV-2019 14:17:13
 Current Time = 18-NOV-2019 14:17:57
 Comment = XLVI-34_c
 Data Format = 1D COMPLEX
 Dim Size = 26214
 Dim Title = Carbon13
 Dim Units = [ppm]
 Dimensions = X
 Site = JNM-ECX500
 Spectrometer = DELTA2 NMR
 Field Strength = 11.62926421[T] (500[MHz])
 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_Sweep_Clipped = 31.25[kHz]
 Irr_Domain = Proton
 Irr_Freq = 499.13191398[MHz]
 Irr_Offset = 5[ppm]
 Clipped = TRUE
 Scans = 1000
 Total_Scans = 1000
 Relaxation_Delay = 2[s]
 Recvr_Gain = 60
 Temp_Get = 21.7[dC]
 X_90_Width = 9.2[us]
 X_Acq_Time = 0.8388608[s]
 X_Angle = 30[deg]
 X_Atn = 4.6[dB]
 X_Pulse = 3.06666667[us]
 Irr_Atn_Dec = 21.976[dB]
 Irr_Atn_Noise = 21.976[dB]
 Irr_Noise = WALTZ
 Irr_Fwidth = 92[us]
 Decoupling = TRUE



: Carbon13



(E)-13
¹⁹F NMR (470 MHz, CDCl₃)



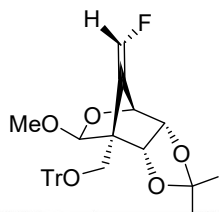
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA47088-19F-1.jdf

Filename = KMA47088-19F-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S857660
 Solvent = CHLOROFORM-D
 Creation_time = 22-JAN-2021 18:20:31
 Revision_time = 22-JAN-2021 18:24:40
 Current_time = 22-JAN-2021 18:25:30
 Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[MHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 64
 Total_scans = 64
 X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 46
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_get = 22.7[degC]

0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0

-136.1120
 -136.2688

ion : 19F

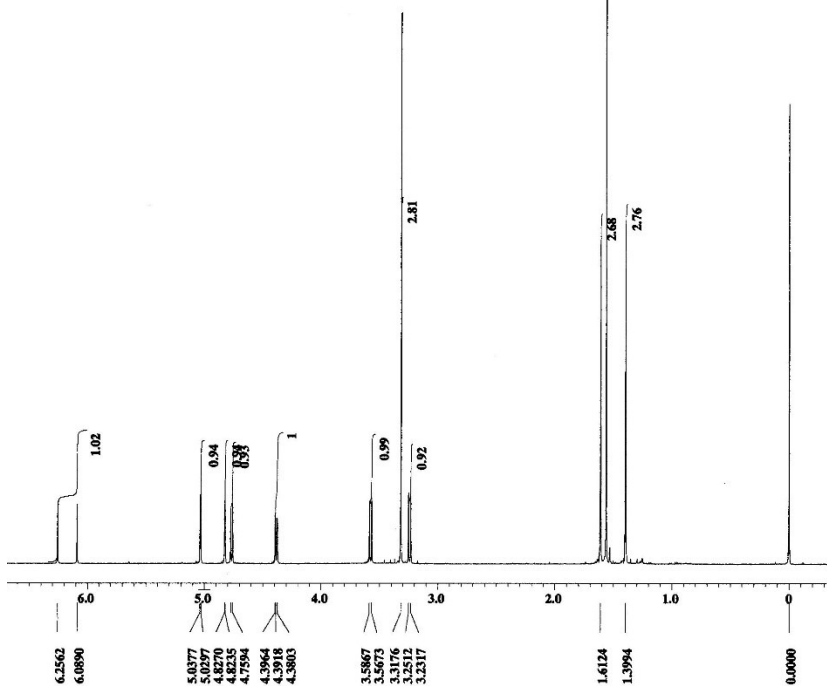


(Z)-13
¹H NMR (500 MHz, CDCl₃)

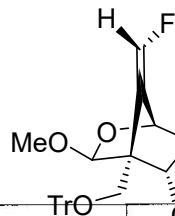


----- PROCESSING PARAMETERS -----
 ac_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46026_PROTON-1.jdf

Filename = KMA46026_PROTON-5.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = KMA46026
 Solvent = CHLOROFORM-D
 Creation_time = 18-SEP-2019 08:02:50
 Revision_time = 18-SEP-2019 08:08:54
 Current_time = 18-SEP-2019 08:09:24
 Comment = CDCl3
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = 9.38438430 [kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 6[us]
 Irr_mode = OFF
 Tri_mode = OFF
 Dents_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 56
 Relaxation_delay = 4[s]
 Repetition_time = 5.74587904[s]
 Temp_set = 20.8[degC]



on : 1H



(Z)-13

^{13}C NMR (125 MHz, CDCl₃)

JEOL
RESONANCE

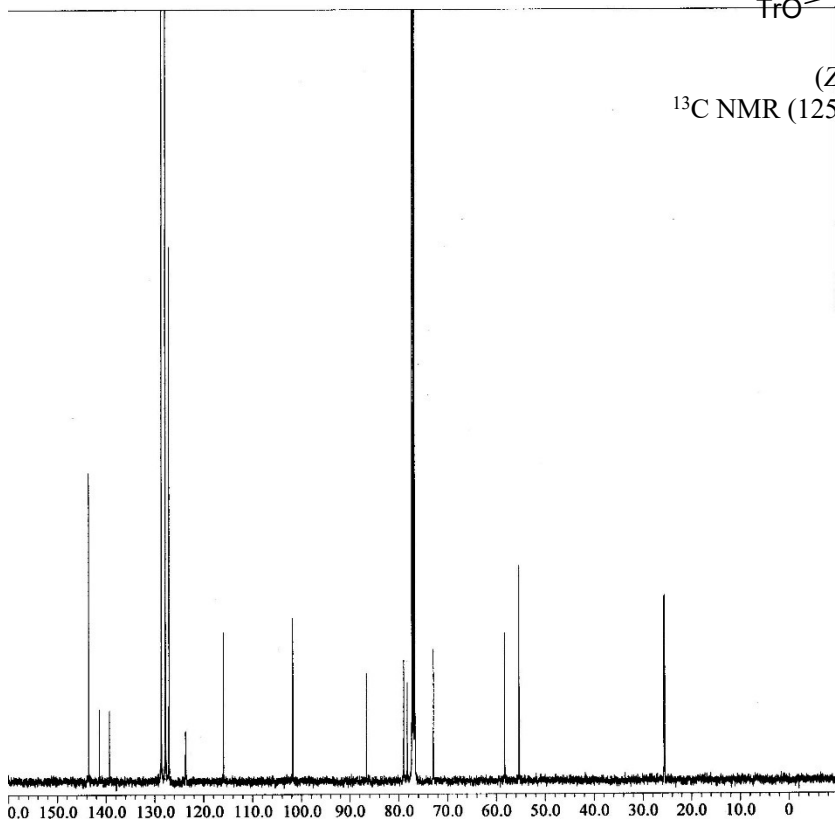
 dc balance(0, FALSE)
 acq(2.0[Hz], 0.0[s])
 trapezoid(0[Hz], 0[Hz], 80[Hz], 100[Hz])
 zerofill(1)
 fft(1, TRUE, TRUE)
 ppm
 phase(189, 200, 59.192[Hz])
 以下に由来: XLVI-26_c-1-1.jdf

Filename = XLVI-26_c-1-4.jdf
 Author = delta
 Experiment = single_pulse_dec.jpg
 Sample_Id = XLVI-26
 Solvent = CHLOROFORM-D
 Creation_Time = 25-OCT-2019 21:26:39
 Revision_Time = 2-NOV-2019 19:28:33
 Current_Time = 2-NOV-2019 19:29:37

Comment = XLVI-26_c
 Data_Format = 1D_COMPLEX
 Dim_Size = 26214
 Dim_Title = Carbon13
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECS500
 Spectrometer = DELTA2_NMR

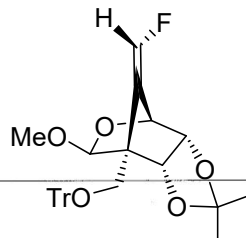
Field_Strength = 11.62926421[T] (500[MHz])
 X_Acq_Duration = 0.8388608[s]
 X_Domain = 13C
 X_Freq = 124.5010059[MHz]
 X_Offset = 100[ppm]
 X_Points = 32768
 X_Prescans = 4
 X_Resolution = 1.1920929[Hz]
 X_Sweep = 39.0625[kHz]
 X_Sweep_Clipped = 31.25[kHz]
 Irr_Domain = Proton
 Irr_Freq = 495.13191398[MHz]
 Irr_Offset = 5[ppm]
 Clipped = TRUE
 Scans = 2000
 Total_Scans = 2000

Relaxation_Delay = 2[s]
 Recvr_Gain = 58
 Temp_Get = 21[deg]
 X_90_Width = 9.2[us]
 X_Acq_Time = 0.8388608[s]
 X_Angle = 30[deg]
 X_Atn = 4.6[db]
 X_Pulse = 3.06666667[us]
 Irr_Atn_Dec = 21.976[db]
 Irr_Atn_Moe = 21.976[db]
 Irr_Moise = WALTZ
 Irr_Pwidth = 92[us]
 Decoupling = TRUE



43.575
 141.372
 139.295
 128.686
 127.853
 127.115
 123.716
 123.621
 115.970
 101.780
 86.642
 79.020
 78.302
 77.259
 77.000
 76.741
 72.892
 58.319
 55.370
 55.341
 55.303
 25.678
 25.525

: Carbon13

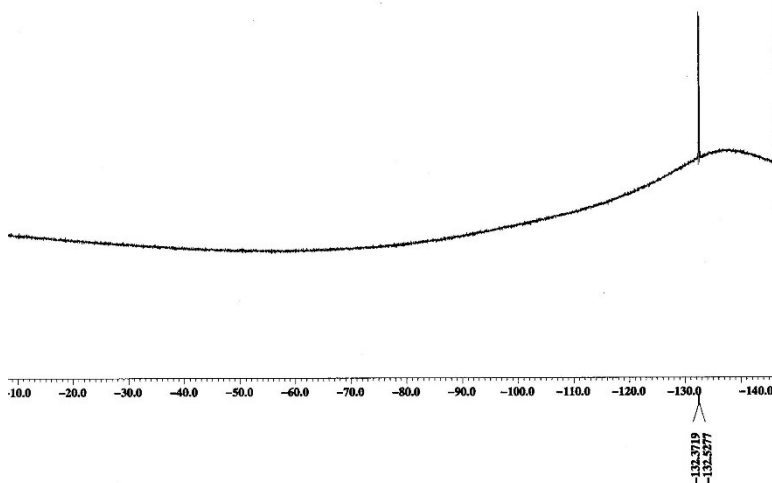


(Z)-13
¹⁹F NMR (470 MHz, CDCl₃)

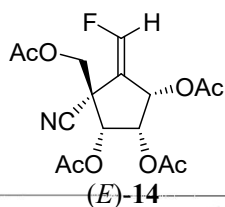


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sump : 0.2[Hz] : 0.0[Hz]
 trapenoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46016-19F-1.jdf

Filename = KMA46016-19F-4.jdf
 Author = Delta
 Experiment = single_pulse.ex2
 Sample_id = S8569945
 Solvent = CHLOROFORM-D
 Creation_time = 13-MAR-2021 15:51:13
 Revision_time = 13-MAR-2021 15:58:15
 Current_time = 13-MAR-2021 15:58:36
 Comment = single_pulse
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 19F
 Dia_units = [ppm]
 Dimensions = 1
 Site = ECA500
 Spectrometer = JNM-ECA500
 Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_pscans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[Hz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 64
 Total_scans = 64
 X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_sec = 22.6[degC]



Non: 19F

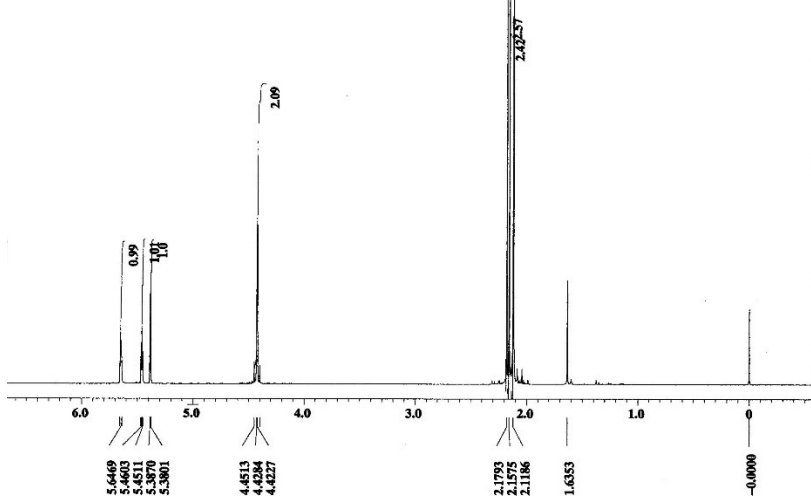


¹H NMR (500 MHz, CDCl₃)

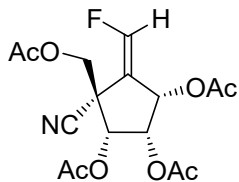


----- PROCESSING PARAMETERS -----
 do_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 sft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46037-pp_PROTON-1.jdf

Filename = KMA46037-pp_PROTON-5.
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = KMA46037-pp
 Solvent = CHLOROFORM-D
 Creation_time = 17-OCT-2019 17:38:04
 Revision_time = 17-OCT-2019 17:43:43
 Current_time = 17-OCT-2019 17:44:12
 Comment = CDCl3
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4.5[db]
 X_pulse = 6[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 initial_wait = 1[s]
 Recvr_gain = 48
 Relaxation_delay = 4[s]
 Repetition_time = 5.74587904[s]
 Temp_set = 21.6[degC]



1H



(E)-14

^{13}C NMR (125 MHz, CDCl_3)



```

---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
ppm
phase( 187.38406, 224.06905, 59.00889[%] )
phase( 0, 0, 0.91939[%] )
reference( 77.12541[ppm], 77[ppm] )
以下に由来: XLVI-37_c-1-1.jdf
  
```

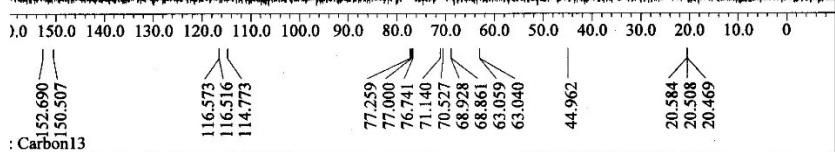
```

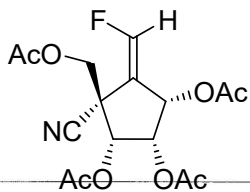
Filename      = XLVI-37_c-1-1.jdf
Author        = Delta
Experiment     = single_pulse_dec.jxp
Sample Id     = XLVI-37
Solvent       = CHLOROFORM-D
Creation Time  = 18-NOV-2019 16:55:05
Revision Time  = 19-NOV-2019 17:10:45
Current Time   = 19-NOV-2019 17:13:38

Comment       = XLVI-37_c
Data Format    = 1D COMPLEX
Dim Size      = 26214
Dim Title     = Carbon13
Dim Units     = [ppm]
Dimensions    = X
Site          = JNM-ECK500
Spectrometer  = DELTA2_NMR

Field Strength = 11.62926421[T] (500[MHz])
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_Sweep Clipped = 31.25[kHz]
Irr_Domain     = Proton
Irr_Freq       = 495.13191398[MHz]
Irr_Offset     = 5[ppm]
Clipped        = FALSE
Scans          = 1000
Total Scans    = 1000

Relaxation_Delay = 2[s]
Recvr Gain       = 60
Temp Set         = 21.2[dc]
X_90 Width      = 9.2[us]
X_Acq Time       = 0.8388608[s]
X_Angle         = 30[deg]
X_Atn           = 4.6[db]
X_Pulse         = 3.06666667[us]
Irr_Atn Dec     = 21.976[db]
Irr_Atn Noe     = 21.976[db]
Irr_Mode        = WALTZ
Irr_Pwidth      = 92[us]
Decoupling      = TRUE
  
```





(E)-14
 ^{19}F NMR (470 MHz, CDCl_3)



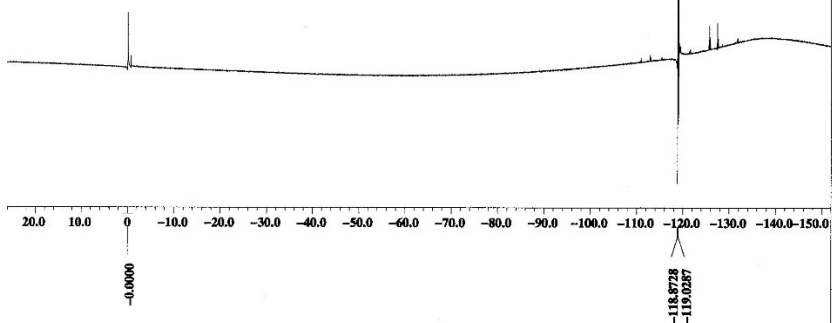
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinaphase
 ppm
 Derived from: KMA14092-19F-1.jdf

Filename = KMA14092-19F-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#495689
 Solvent = CHLOROFORM-D
 Creation_time = 7-FEB-2021 13:49:37
 Revision_time = 15-AUG-2021 10:48:52
 Current_time = 15-AUG-2021 10:48:58

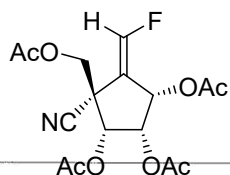
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[kHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 60
 Total_scans = 60

X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 46
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_get = 23.4[degC]



30 : 19F



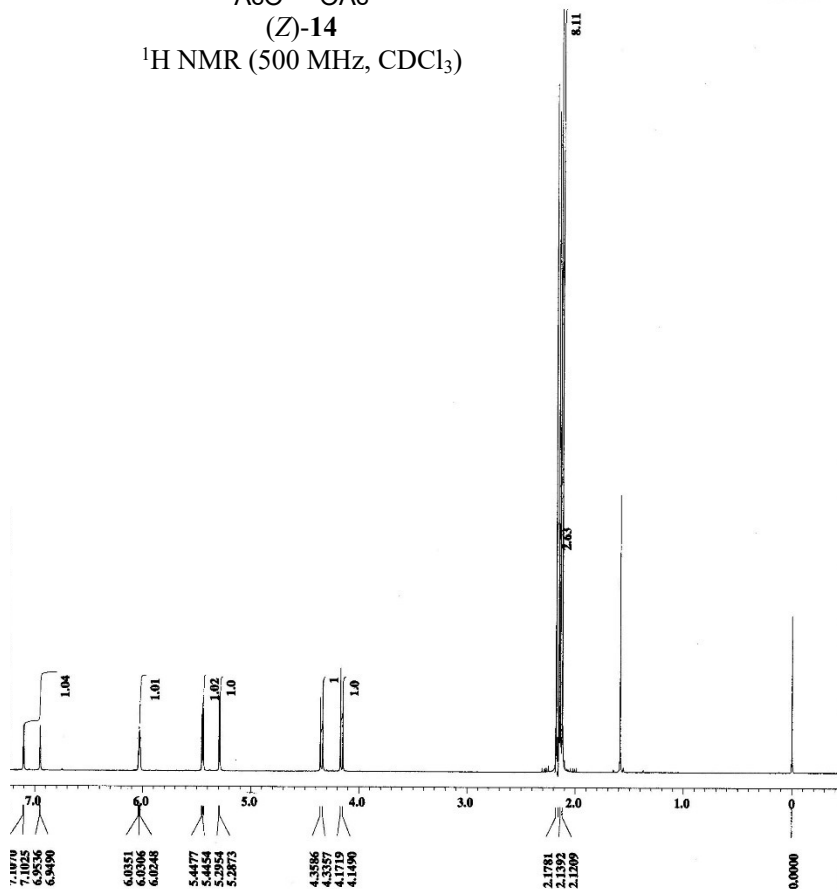
(Z)-14

¹H NMR (500 MHz, CDCl₃)

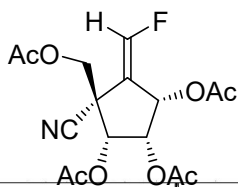


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 expm : 0.2[Hz] : 0.0[s]
 ffr : 1 : TRUE : TRUE
 machinephase :
 ppm
 Derived from: KMA16041-2CDC13_PROTON-1.j

Filename = KMA16041-2CDC13_PROTO
 Author = Delta
 Experiment = single_pulse.ex2
 Sample_id = KMA16041-2CDC13
 Solvent = CHLOROFORM-D
 Creation_time = 30-OCT-2019 08:10:39
 Revision_time = 30-OCT-2019 08:18:04
 Current_time = 30-OCT-2019 08:18:12
 Data_format = 1D COMPLEX
 Dm_name = 13107
 Dm_title = 1H
 Dm_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4.5[db]
 X_pulse = 6[us]
 Irr_mode = Off
 Tri_mode = Off
 Danta_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 54
 Relaxation_delay = 4[s]
 Repetition_time = 5.74587904[s]
 Temp_set = 21.6[dc]



Million : 1H



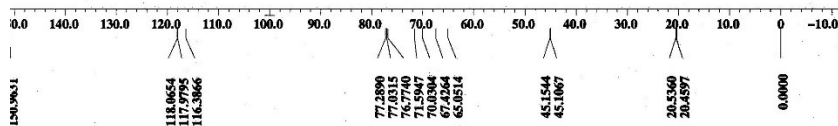
(Z)-14

¹³C NMR (125 MHz, CDCl₃)

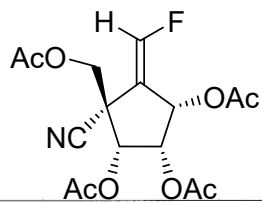
JEOL

----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sump : 2.0 [Hz] : 0.0 [s]
 trapasoid3 : 0 [%] : 80 [%] : 100 [%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46041-carbon-1.jdf

Filename = KMA46041-carbon-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S8538095
 Solvent = CHLOROFORM-D
 Creation_time = 3-JAN-2020 03:33:16
 Revision_time = 3-JAN-2020 11:30:50
 Current_time = 3-JAN-2020 11:32:00
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dia_size = 26216
 Dia_title = 13C
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = TRUE
 Mod_return = 1
 Scans = 16000
 Total_scans = 16000
 X_90_width = 11.53 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 6.6 [dB]
 X_pulse = 3.84333333 [us]
 Irr_atn_dec = 22.192 [dB]
 Irr_atn_noe = 22.192 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 34
 Relaxation_delay = 2 [s]
 Repetition_time = 2.83361792 [s]
 Temp_get = 24.6 [dC]



ion : 13C



(Z)-14

¹⁹F NMR (470 MHz, CDCl₃)



----- PROCESSING PARAMETERS -----
 ds_balance : 0 : FALSE
 seqp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46041-19F-1.jdf

Filename = KMA46041-19F-3.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S8398102
 Solvent = CHLOROFORM-D
 Creation_time = 11-JAN-2020 11:08:50
 Revision_time = 11-JAN-2020 11:13:26
 Current_time = 11-JAN-2020 11:13:55

Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dia_size = 13107
 Dia_title = 19F
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500

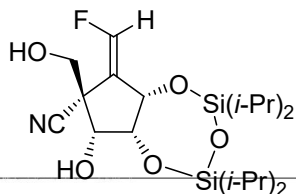
Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[KHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 64
 Total_scans = 64

X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[GB]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_get = 25.9[DC]

-10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0

-118.1609
 -118.3425

on: 19F



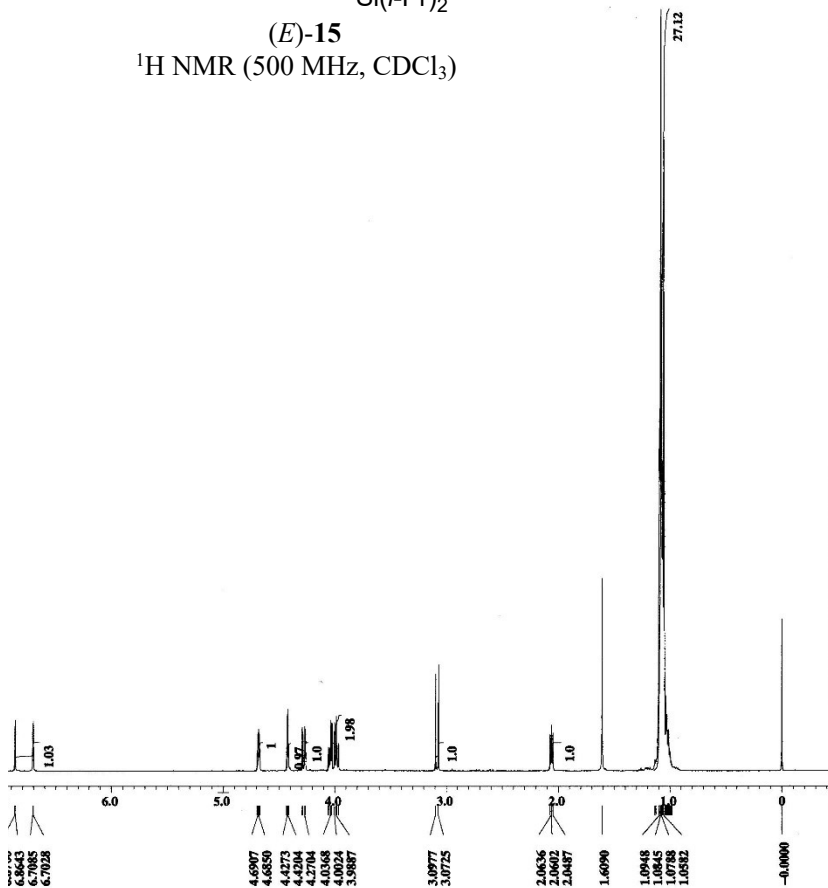
(E)-15

¹H NMR (500 MHz, CDCl₃)

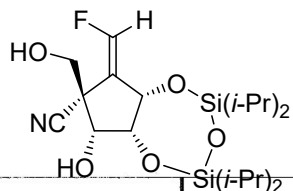


----- PROCESSING PARAMETERS -----
 ds_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 ffc : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46044_PROTON-1.jdf

Filename = KMA46044_PROTON-5.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = KMA46044
 Solvent = CHLOROFORM-D
 Creation_time = 1-NOV-2019 07:59:34
 Revision_time = 1-NOV-2019 08:06:42
 Current_time = 1-NOV-2019 08:07:26
 Comment = CDCl3
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 1H
 Dia_units = [ppm]
 Dimensions = 2
 Site = ECA500
 Spectrometer = JNM-ECA500
 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]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4.5[db]
 X_pulse = 6[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 48
 Relaxation_delay = 4[s]
 Repetition_time = 5.74587904[s]
 Temp_get = 21.8[dc]



on : 1H



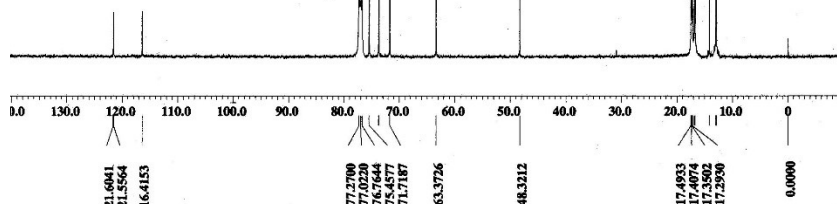
(E)-15

¹³C NMR (125 MHz, CDCl₃)

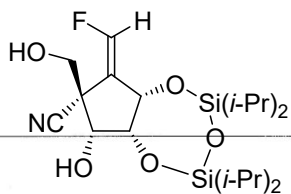


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 2.0[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46044-carbon-1.jdf

Filename = KMA46044-carbon-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S8846045
 Solvent = CHLOROFORM-D
 Creation_time = 2-JAN-2020 14:47:39
 Revision_time = 2-JAN-2020 14:49:03
 Current_time = 2-JAN-2020 14:49:36
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dia_size = 26214
 Dia_title = 13C
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = TRUE
 Mod_return = 1
 Scans = 30000
 Total_scans = 30000
 X_90_width = 11.53[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 6.6[db]
 X_pulse = 3.84333333[us]
 Irr_atn_dec = 22.192[db]
 Irr_atn_noe = 22.192[db]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 28
 Relaxation_delay = 2[s]
 Repetition_time = 2.83361792[s]
 Temp_get = 25.2[degC]



ion : 13C



(E)-15

^{19}F NMR (470 MHz, CDCl_3)



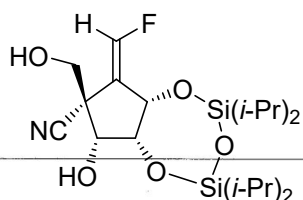
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA47101-19F-1.jdf

Filename = KMA47101-19F-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S8401011
 Solvent = CHLOROFORM-D
 Creation_time = 19-FEB-2021 11:10:13
 Revision_time = 19-FEB-2021 11:17:28
 Current_time = 19-FEB-2021 11:18:17
 Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[MHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 64
 Total_scans = 64
 X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 5.85[us]
 Irr_mode = OFF
 Tri_mode = OFF
 Danta_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_set = 23.3[degC]

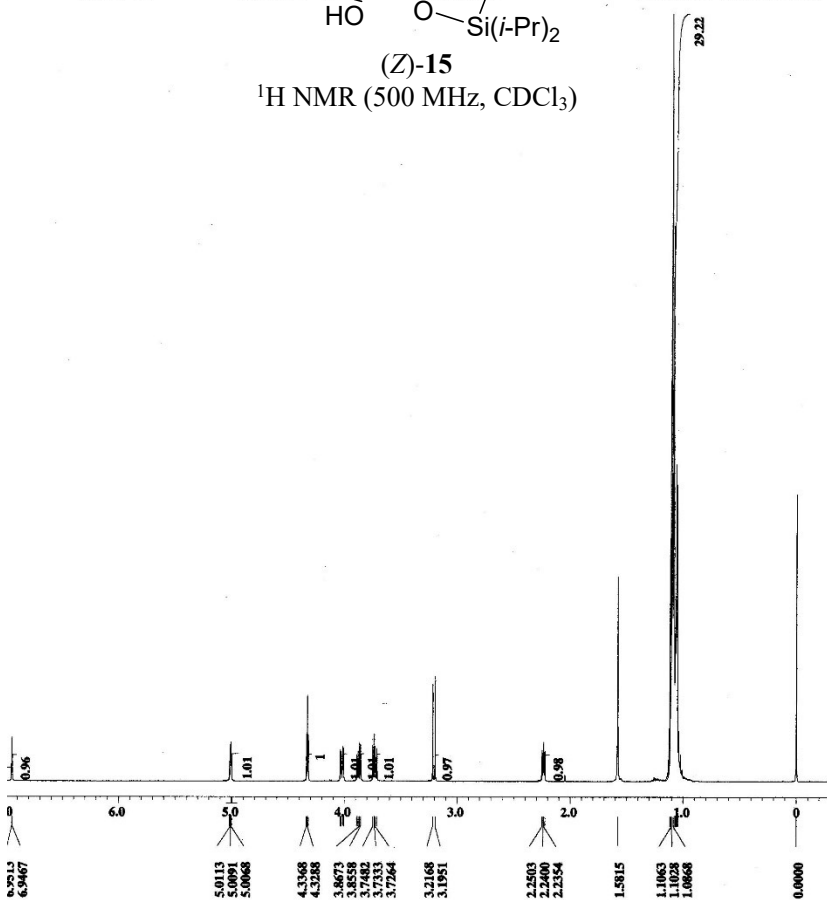
-10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0

-130.4078
-130.5948

Non : 19F



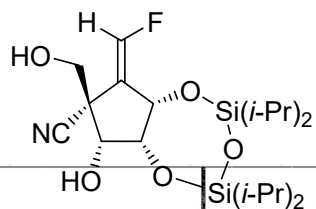
(Z)-15
¹H NMR (500 MHz, CDCl₃)



----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 f1 : 1 : TRUE : TRUE
 machinephase :
 ppm
 Derived from: KMA46047_PROTON-1.jdf

Filename = KMA46047_PROTON-5.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = KMA46047
 Solvent = CHLOROFORM-D
 Creation_time = 9-NOV-2019 09:23:17
 Revision_time = 9-NOV-2019 09:29:15
 Current_time = 9-NOV-2019 09:29:27
 Comment =
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 1H
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 6[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 4[s]
 Repetition_time = 5.74587904[s]
 Temp_get = 22.7[degC]

on: 1H

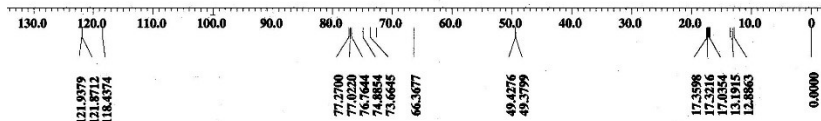


(Z)-15
¹³C NMR (125 MHz, CDCl₃)

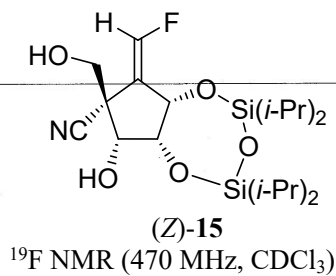


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 samp : 2.0[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 f1t : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46047-carbon-1.jdf

Filename = KMA46047-carbon-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S8711874
 Solvent = CHLOROFORM-D
 Creation_time = 28-DEC-2019 08:23:45
 Revision_time = 28-DEC-2019 08:43:03
 Current_time = 28-DEC-2019 08:44:02
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = TRUE
 Mod_return = 1
 Scans = 16000
 Total_scans = 16000
 X_90_width = 11.53[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 6.6[db]
 X_pulse = 3.84333333[us]
 Irr_atn_dec = 22.192[db]
 Irr_atn_noe = 22.192[db]
 Irr_noise = NAUTZ
 Decoupling = TRUE
 Initial_walt = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 28
 Relaxation_delay = 2[s]
 Repetition_time = 2.83361792[s]
 Temp_get = 23.7[dc]

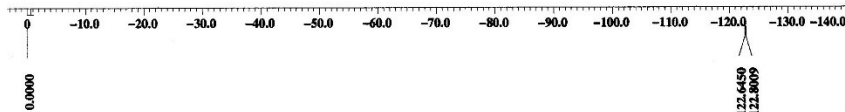


ion : 13C

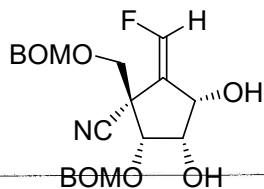


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sump : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46047-19F-1.jdf

Filename = KMA46047-19F-4.jdf
 Author = Delta
 Experiment = single_pulse.ex2
 Sample_id = S#661658
 Solvent = CHLOROFORM-D
 Creation_time = 15-MAR-2021 18:23:57
 Revision_time = 15-MAR-2021 18:30:41
 Current_time = 15-MAR-2021 18:31:01
 Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 19F
 Dim_units = [ppm]
 Dimensions = 2
 Site = ECA500
 Spectrometer = JNM-ECA500
 Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[MHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 64
 Total_scans = 64
 X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_get = 21[deg]



Million : 19F

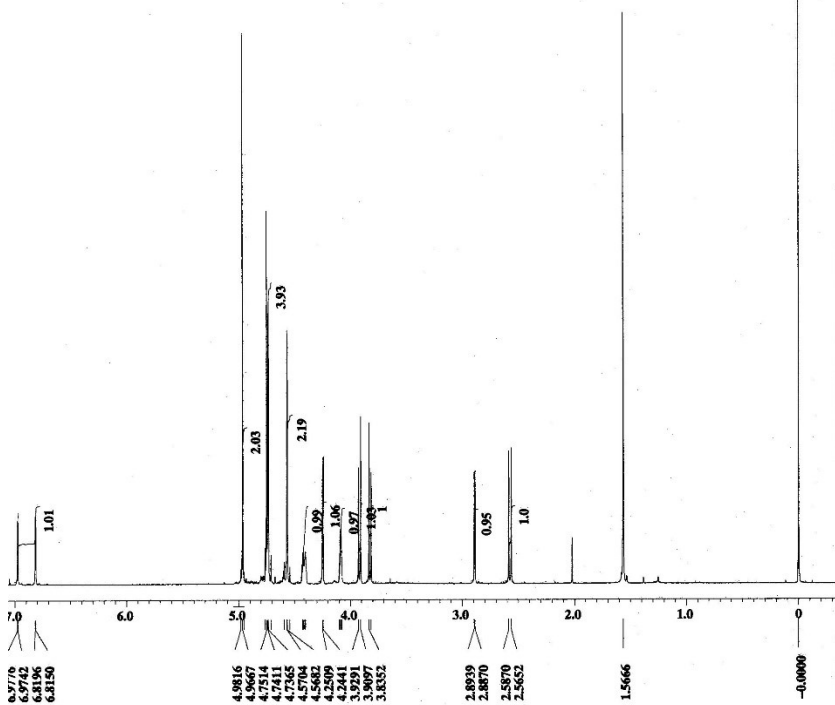


(E)-16
¹H NMR (500 MHz, CDCl₃)

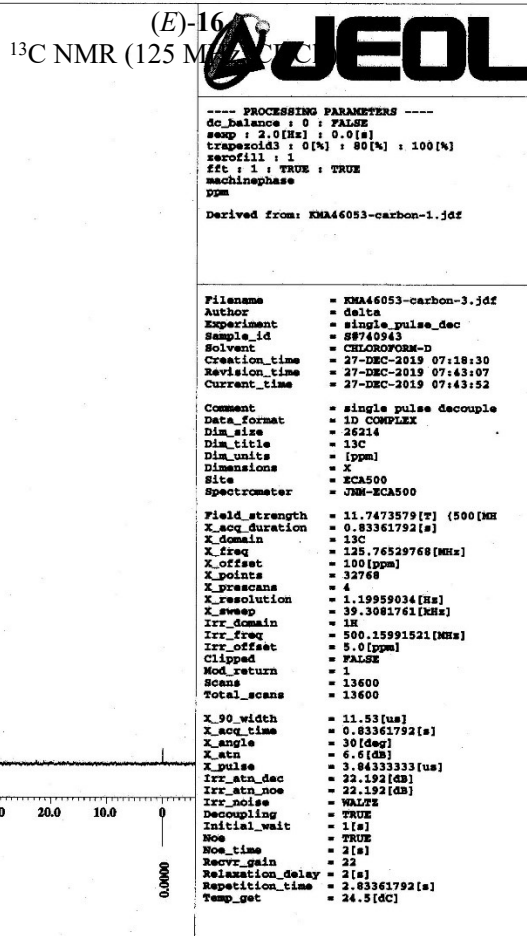
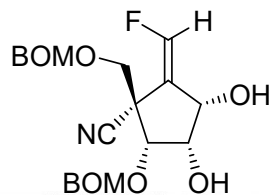


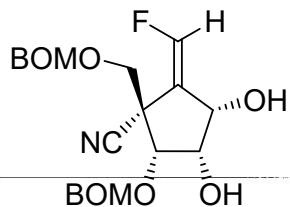
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: kma46053PP_PROTON-1.jdf

Filename = kma46053PP_PROTON-5.j
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = kma46053PP
 Solvent = CHLOROFORM-D
 Creation_time = 22-NOV-2019 07:43:39
 Revision_time = 22-NOV-2019 07:51:31
 Current_time = 22-NOV-2019 07:52:12
 Comment = cdcL3
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 1H
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = 9.39438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4.5[db]
 X_pulse = 6[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 56
 Relaxation_delay = 4[s]
 Repetition_time = 5.74587904[s]
 Temp_get = 23.2[degC]



ion: 1H





BOMO OH
(E)-16
¹⁹F NMR (470 MHz, CDCl₃)



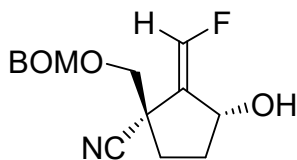
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sump : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA47108-19F-1.jdf

Filename = KMA47108-19F-3.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S865982P
 Solvent = CHLOROFORM-D
 Creation_time = 11-MAR-2021 18:21:05
 Revision_time = 11-MAR-2021 18:27:55
 Current_time = 11-MAR-2021 18:28:08
 Comment = single_pulse
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 19F
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[kHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 64
 Total_scans = 64
 X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_get = 21.3[degC]

-10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0

-128.6087
-128.7626

on : 19F



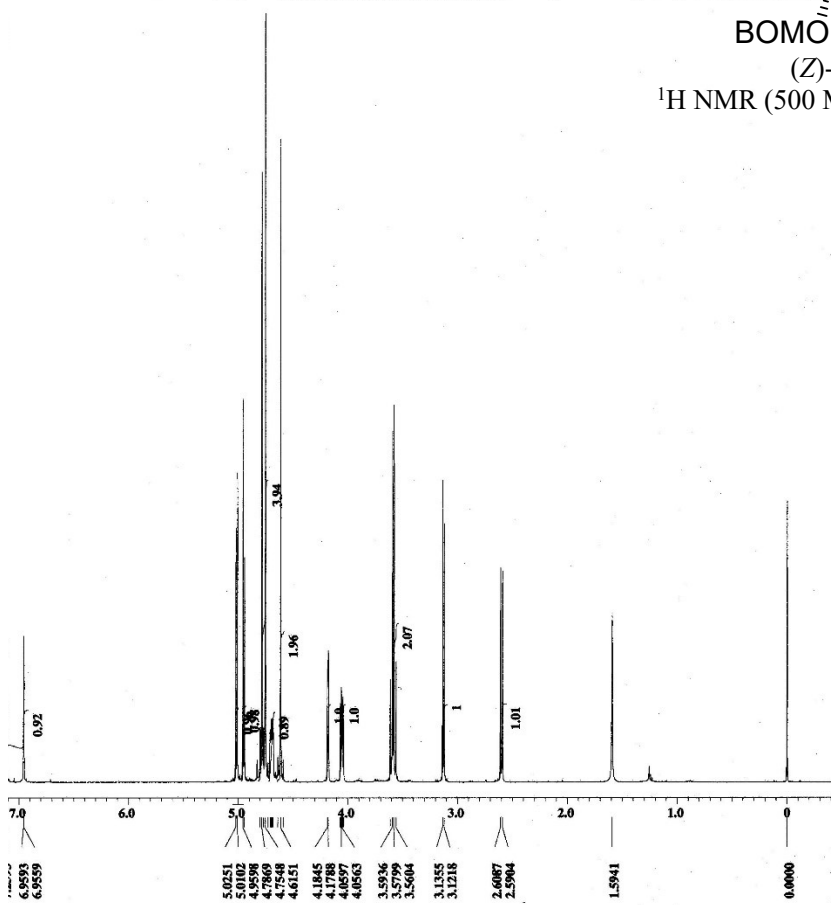
BOMO
(Z)-1

JEOL

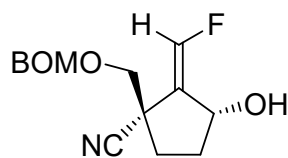
¹H NMR (500 MHz, CDCl₃)

dc balance : 0 : FALSE
 smp : 0.2 [Hz] : 0.0 [s]
 f1 : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46058-p_PROTON-1.jdf

Filename = KMA46058-p_PROTON-5.j
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = KMA46058-p
 Solvent = CHLOROFORM-D
 Creation_time = 17-DEC-2019 07:40:02
 Revision_time = 17-DEC-2019 07:51:43
 Current_time = 17-DEC-2019 07:52:28
 Comment = CDC13
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = 9.39438438 [kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521 [MHz]
 Tri_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_atn = 4.5 [dB]
 X_pulse = 6 [us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 50
 Relaxation_delay = 4 [s]
 Repetition_time = 5.74587904 [s]
 Temp_get = 22.1 [dC]



on : 1H



BOMO
(Z)-

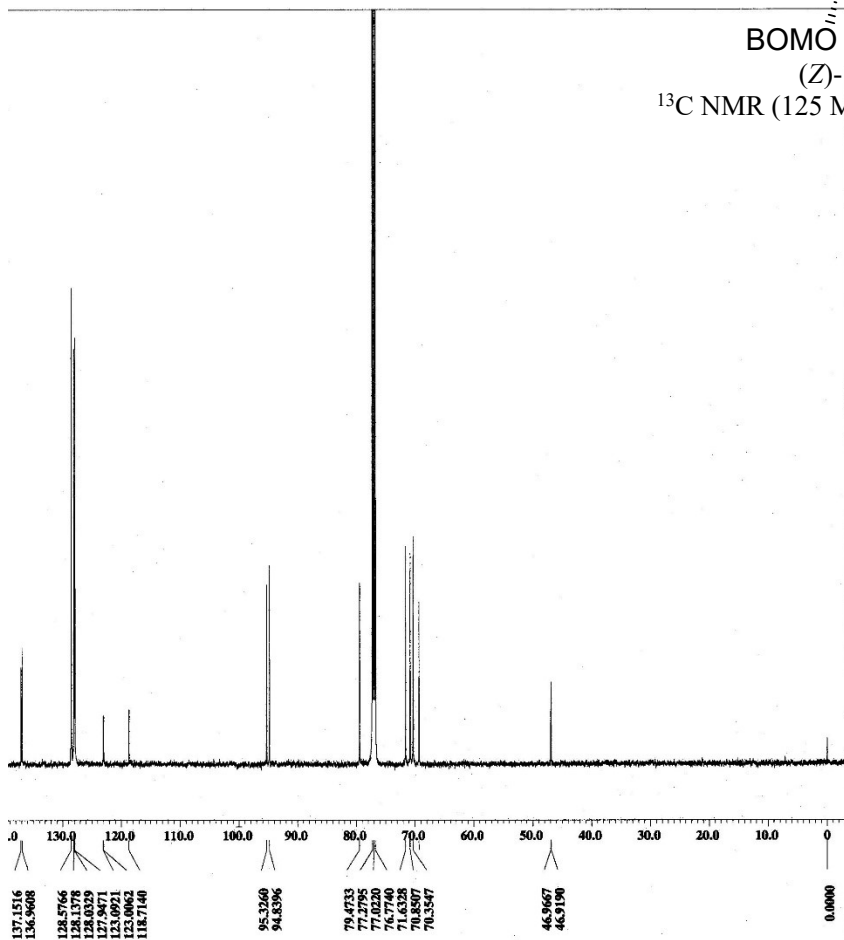
JEOL

¹³C NMR (125 MHz, CDCl₃)

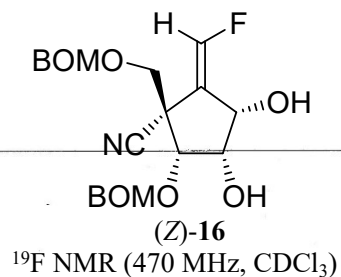
----- PROCESSING PARAMETERS -----
 ac_balance : 0 : FALSE
 smp : 2.0[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 ift : 1 : TRUE : TRUE
 machinephase
 ppm

Derived from: KMA46058-carbon-1.jdf

Filename = KMA46058-carbon-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S8728447
 Solvent = CHLOROFORM-D
 Creation_time = 25-DEC-2019 05:41:20
 Revision_time = 25-DEC-2019 07:26:31
 Current_time = 25-DEC-2019 07:27:17
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dia_size = 26214
 Dia_title = 13C
 Dia_units = [ppm]
 Dimensions = 2
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = TRUE
 Mod_return = 1
 Scans = 12000
 Total_scans = 12000
 X_90_width = 11.53[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 6.6[db]
 X_pulse = 3.84333333[us]
 Irr_atn_dec = 22.192[db]
 Irr_atn_noe = 22.192[db]
 Irr_pulse = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 50
 Relaxation_delay = 2[s]
 Repetition_time = 2.83361792[s]
 Temp_get = 25.7[degC]



on: 13C



¹⁹F NMR (470 MHz, CDCl₃)



----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 samp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 sft : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA16058-19F-1.jdf

Filename = KMA16058-19F-3.jdf
 Author = delta
 Experiment = single_pulse.exe2
 Sample_id = 8840382
 Solvent = CHLOROFORM-D
 Creation_time = 11-JAN-2020 11:17:37
 Revision_time = 11-JAN-2020 11:22:47
 Current_time = 11-JAN-2020 11:23:00

Comment = single_pulse
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 19F
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500

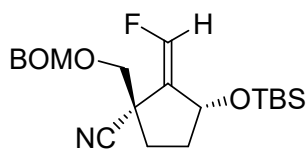
Field_strength = 11.7473579[T] (500[MH]
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_ppscaus = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[kHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 64
 Total_scans = 64

X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_get = 25.6[degC]

0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0

0.625

Mon : 19F



BOMO OH
(E)-17
¹H NMR (500 MHz, CDCl₃)



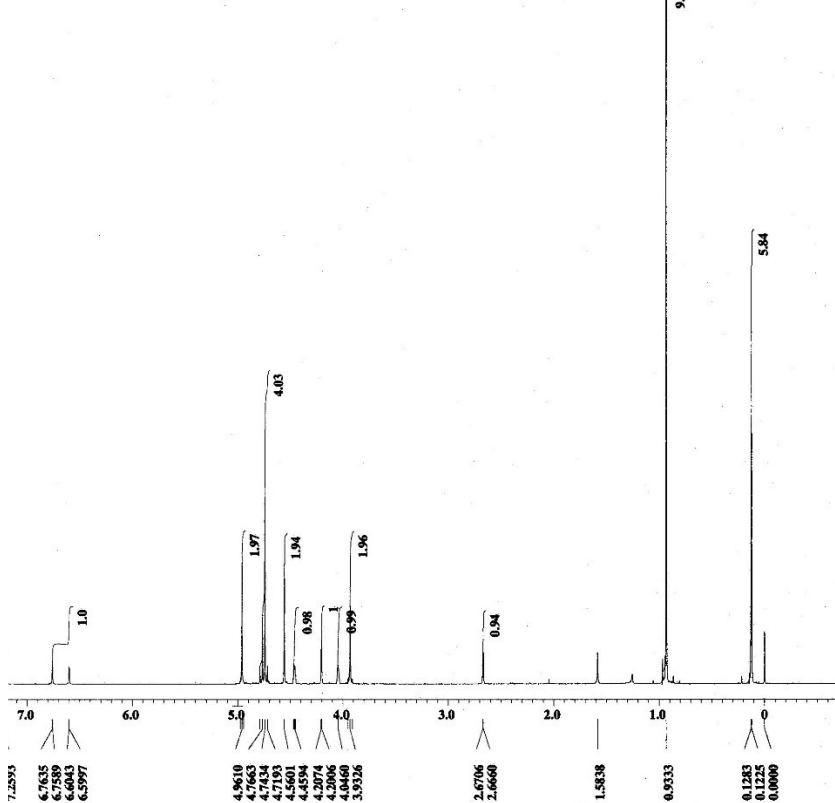
----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
sweep : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE
machinphase
ppm
Derived from: KMA46054pylc_PROTON-1.jdf

Filename = KMA46054pylc_PROTON-5
Author = Delta
Experiment = single_pulse.ex2
Sample_id = KMA46054pylc
Solvent = CHLOROFORM-D
Creation_time = 3-DEC-2019 18:22:56
Revision_time = 3-DEC-2019 18:35:25
Current_time = 3-DEC-2019 18:35:41

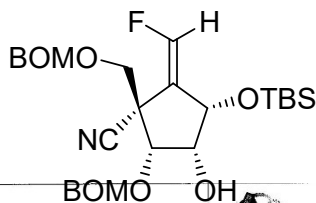
Comment = CDCl₃
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA500
Spectrometer = JNM-ECA500

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]
Irr_domain = 1H
Irr_freq = 500.15991521 [MHz]
Irr_offset = 5.0 [ppm]
Tri_domain = 1H
Tri_freq = 500.15991521 [MHz]
Tri_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16

X_90_width = 12 [us]
X_acq_time = 1.74587904 [s]
X_angle = 45 [deg]
X_atn = 4.5 [dB]
X_pulse = 6 [us]
Irr_mode = OFF
Tri_mode = OFF
Dante_preset = FALSE
Initil_wait = 1 [s]
Recvr_gain = 46
Relaxation_delay = 4 [s]
Repetition_time = 5.74587904 [s]
Temp_get = 21.2 [C]



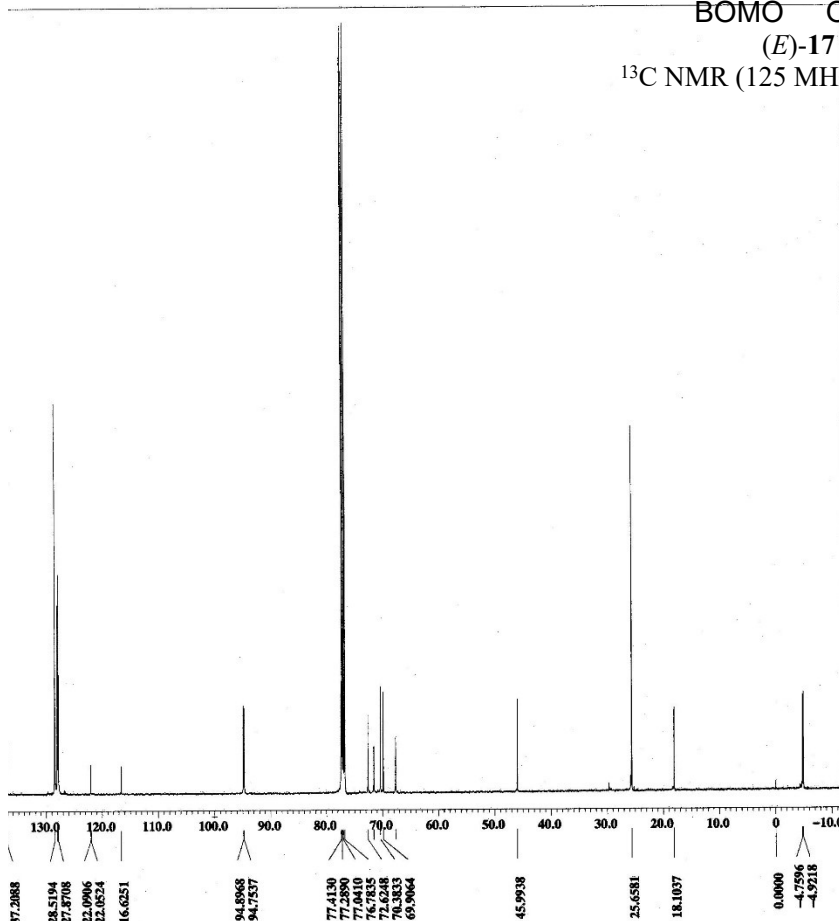
ion : 1H⁺



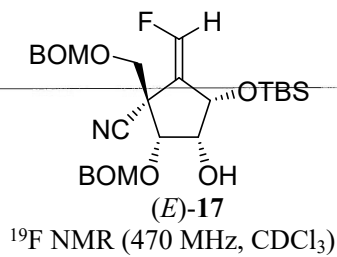
(E)-17
¹³C NMR (125 MHz, CDCl₃)

----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 2.0 [Hz] : 0.0 [s]
 trapezoid3 : 0 [%] : 80 [%] : 100 [%]
 zerofill : 1
 ift : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46054-carbon-1.jdf

Filename = KMA46054-carbon-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = 88724129
 Solvent = CHLOROFORM-D
 Creation_time = 26-DEC-2019 07:09:03
 Revision_time = 26-DEC-2019 07:52:13
 Current_time = 26-DEC-2019 07:52:40
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Data_size = 26214
 Data_title = 13C
 Data_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 [MHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 14000
 Total_scans = 14000
 X_90_width = 11.53 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 6.6 [dB]
 X_pulse = 3.84333333 [us]
 Irr_atn_dec = 22.192 [dB]
 Irr_atn_noe = 22.192 [dB]
 Irr_noise = WALTE
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 26
 Relaxation_delay = 2 [s]
 Repetition_time = 2.83361792 [s]
 Temp_get = 24.2 [deg]



Don : 13C



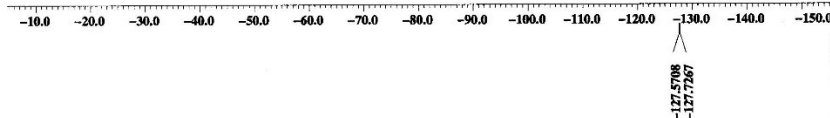
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 sarofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA47121-19F-1.jdf

Filename = KMA47121-19F-3.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = 88719109
 Solvent = CHLOROFORM-D
 Creation_time = 10-MAR-2021 20:01:41
 Revision_time = 10-MAR-2021 20:08:12
 Current_time = 10-MAR-2021 20:08:27

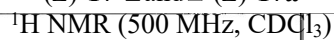
 Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500

 Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 69.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[MHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 64
 Total_scans = 64

 X_90_width = 11.7[us]
 X_acq_time = 69.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 46
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_get = 21[degC]



on : 19F

¹H NMR (500 MHz, CDCl₃)¹H NMR (500 MHz, CDCl₃)

```

----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
semp : 0.2[Hx] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: KMA45063_PROTON-1.jdf

```

```

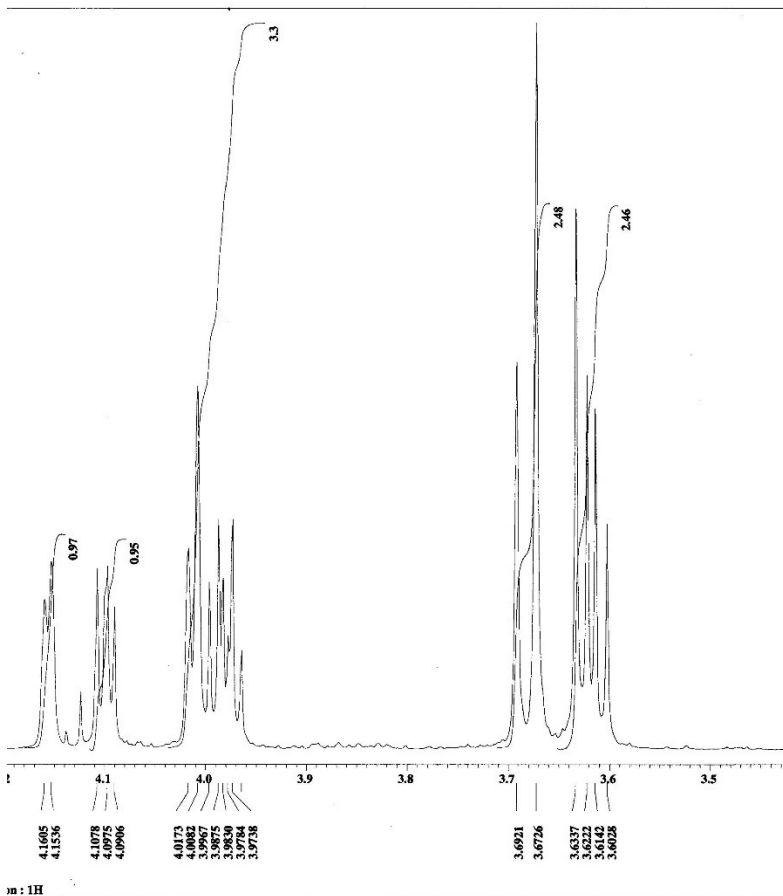
Filename      = JMA46063_PROTON-5.jzd
Author        =
Experiment    =
Sample_id     =
Solve         =
Creation_time  = 30-DEC-2019 12:48:26
Revision_time = 30-DEC-2019 13:02:27
Current_time  = 30-DEC-2019 13:02:59

Comment       =
Data_format   = ID CDD13
Dia_size      = 13.107
Dia_units     =
Dimensions    = X
Size          = ECA500
Spectrometer  = JNM-ECA500

Field_strength = 1.7453759 [T] (500 [MH
X_domain      = 1H
X_freq        = 500.15991521 [MHz]
X_offset      = 5.0 [ppm]
X_pulses      = 1384
X_prescans    = 1
X_resolution  = 0.52727737 [Hz]
X_sweep       = 9.38438438 [kHz]
Irr_domain    = 500.15991521 [MHz]
Irr_offset    = 5.0 [ppm]
Irr_domain    = 500.15991521 [MHz]
Irr_freq      = 500.15991521 [MHz]
Irr_offset    = 5.0 [ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 16
Total_scans   = 16

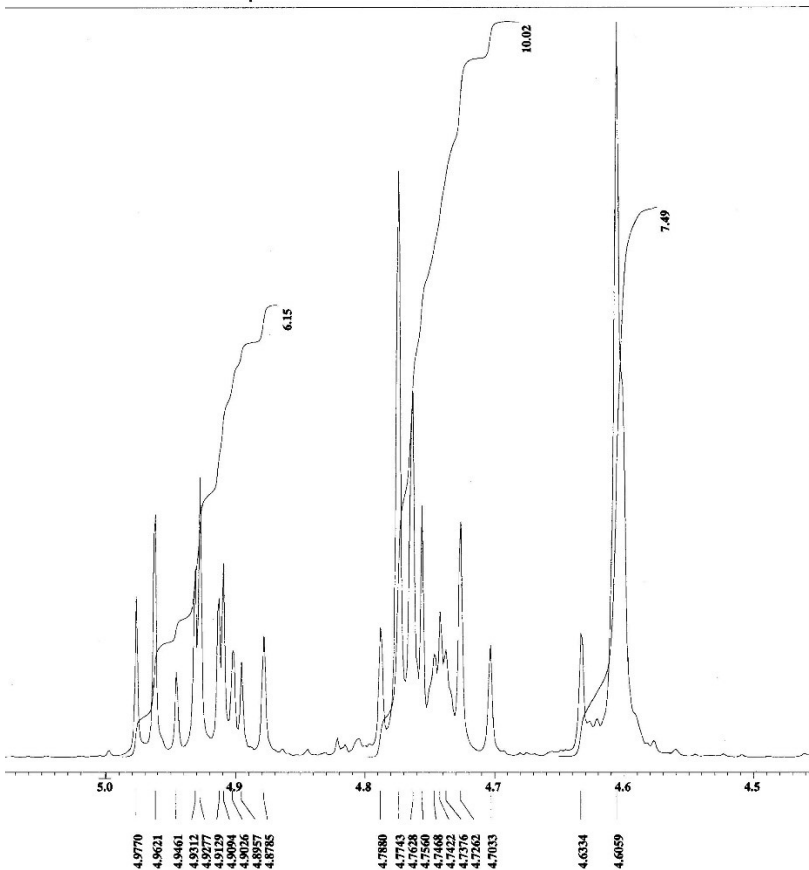
X_90_width    = 12 [us]
X_acq_time    = 1.74587904 [s]
X_angle       = 45 [deg]
X_atn         = 45 [dB]
X_pulse       = 1 [us]
Irr_mode      = off
Irr_mode      = off
Irr_mode      = FALSE
Initial_wait  = 1 [s]
Recvr_gain    = 38
Relaxation_delay = 4 [s]
Relaxation_time = 1.74587904 [s]
Temp_get      = 32.34 [dC]

```



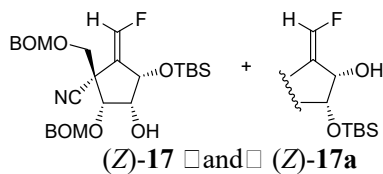
----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sump : 0.2[Hz] : 0.0[s]
 ffr : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA46063_PROTON-1.jdf

Filename = KMA46063_PROTON-5.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = KMA46063
 Solvent = CHLOROFORM-D
 Creation_time = 30-DEC-2019 12:48:26
 Revision_time = 30-DEC-2019 13:02:27
 Current_time = 30-DEC-2019 13:04:00
 Comment = CDCl3
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 1H
 Dia_units = [ppm]
 Dimensions = 2
 Site = ECA500
 Spectrometer = JNM-ECA500
 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]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 6[us]
 Irr_mode = Off
 Tri_mode = Off
 Dance_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 38
 Relaxation_delay = 4[s]
 Repetition_time = 5.74587904[s]
 Temp_get = 24.3[dc]



----- PROCESSING PARAMETERS ----- dc_balance : 0 : FALSE sump : 0.2[Hz] : 0.0[s] sft : 1 : TRUE : TRUE machinephase ppm Derived from: KMA46063_PROTON-1.jdf	
Filename	= KMA46063_PROTON-5.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= KMA46063
Solvent	= CHLOROFORM-D
Creation_time	= 30-DEC-2019 12:48:26
Revision_time	= 30-DEC-2019 13:02:27
Current_time	= 30-DEC-2019 13:03:36
Comment	= CDC13
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA500
Spectrometer	= JNM-ECA500
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	= 16394
X_prescans	= 1
X_resolution	= 0.57277737[Hz]
X_sweep	= 0.38438439[MHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 12[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4.5[dB]
X_pulse	= 6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_preset	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 38
Relaxation_delay	= 4[s]
Repetition_time	= 5.74587904[s]
Temp_get	= 24.3[degC]

1H NMR : 1H

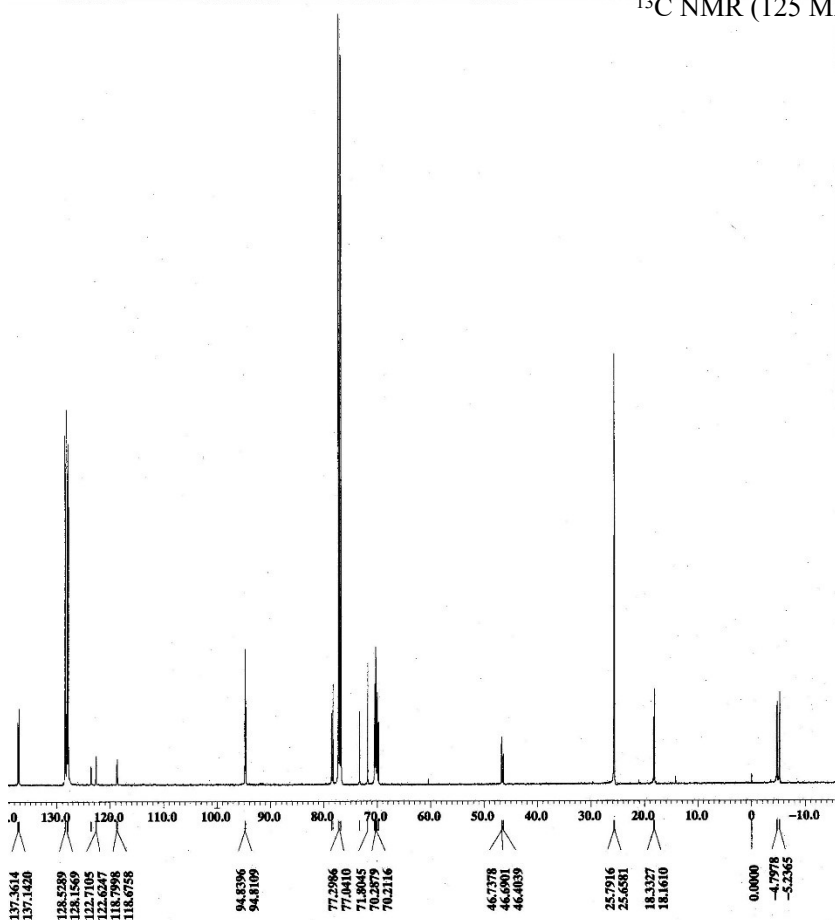


¹³C NMR (125 MHz, CDCl₃)

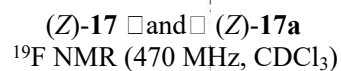
JEOL

----- PROCESSING PARAMETERS -----
 dc balance : 0 : FALSE
 smp : 2.0[Hz] : 0.0[s]
 trapzoid3 : 0[%] : 80[%] : 100[%]
 secfill : 1
 fft : 1 : TRUE : TRUE
 machinephase :
 ppm
 Derived from: KMA46063-carbon-1.jdf

Filename = KMA46063-carbon-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = 88541942
 Solvent = CHLOROFORM-D
 Creation_time = 31-DEC-2019 09:59:04
 Revision_time = 31-DEC-2019 10:24:31
 Current_time = 31-DEC-2019 10:25:09
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Data_size = 26214
 Data_title = 13C
 Data_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = TRUE
 Mod_return = 1
 Scans = 24000
 Total_scans = 24000
 X_90_width = 11.53[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 6.6[db]
 X_pulse = 3.84333333[us]
 Irr_atn_dec = 22.192[db]
 Irr_atn_poe = 22.192[db]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 30
 Relaxation_delay = 2[s]
 Repetition_time = 2.83361792[s]
 Temp_get = 24.6[dc]

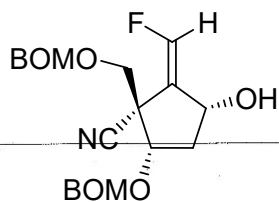


on: 13C



Derived from: KMA46063-CFC13-1.jdf

```
X_90_width      = 11.7[us]
X_acq_time      = 68.15744[ms]
X_angle         = 45[deg]
X_atn           = 4.5[db]
X_pulse         = 5.85[us]
Irr_mode        = Off
Tri_mode        = Off
Dante_presat    = FALSE
Initial_wait    = 1[s]
Recvr_gain      = 50
Relaxation_delay = 5[s]
Repetition_time = 5.06815744[s]
Temp_get        = 20.7[°C]
```

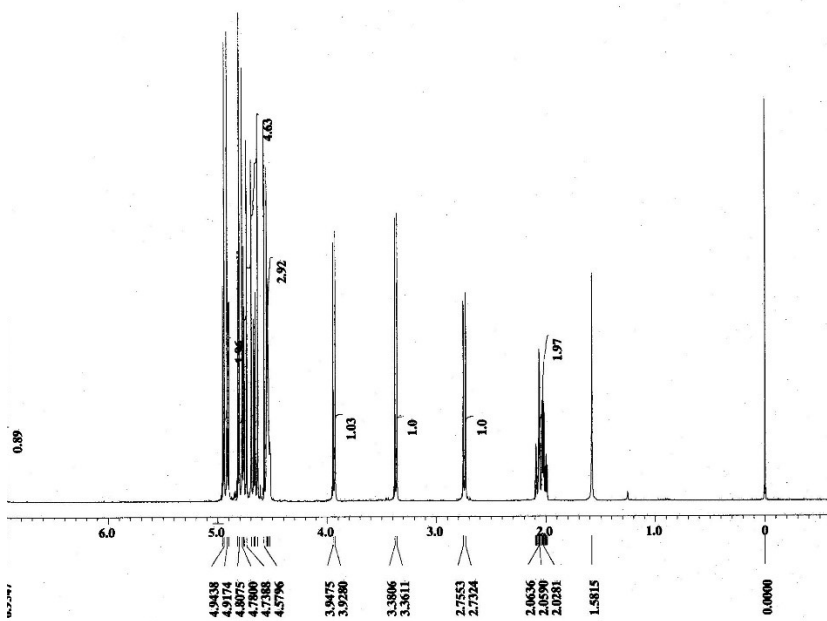


(E)-18
¹H NMR (500 MHz, CDCl₃)

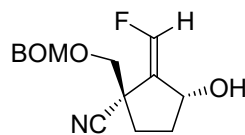
JEOL

--- PROCESSING PARAMETERS ---
 balance : 0 : FALSE
 exp : 0.2 [Hz] : 0.0 [s]
 f1 : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46057_PROTON-1.jdf

Filename = KMA46057_PROTON-5.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = KMA46057
 Solvent = CHLOROFORM-D
 Creation_time = 16-DEC-2019 07:50:07
 Revision_time = 16-DEC-2019 08:04:51
 Current_time = 16-DEC-2019 08:05:14
 Comment = CDCl3
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521 [MHz]
 Tri_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12 [us]
 X_acq_time = 1.74587904 [s]
 X_angle = 45 [deg]
 X_atn = 4.5 [dB]
 X_pulse = 6 [us]
 Irr_mode = Off
 Tri_mode = Off
 Data_preset = FALCK
 Initial_wait = 1 [s]
 Recvr_gain = 50
 Relaxation_delay = 4 [s]
 Repetition_time = 5.74587904 [s]
 Temp_get = 21.9 [dc]



ion: 1H



BOMO

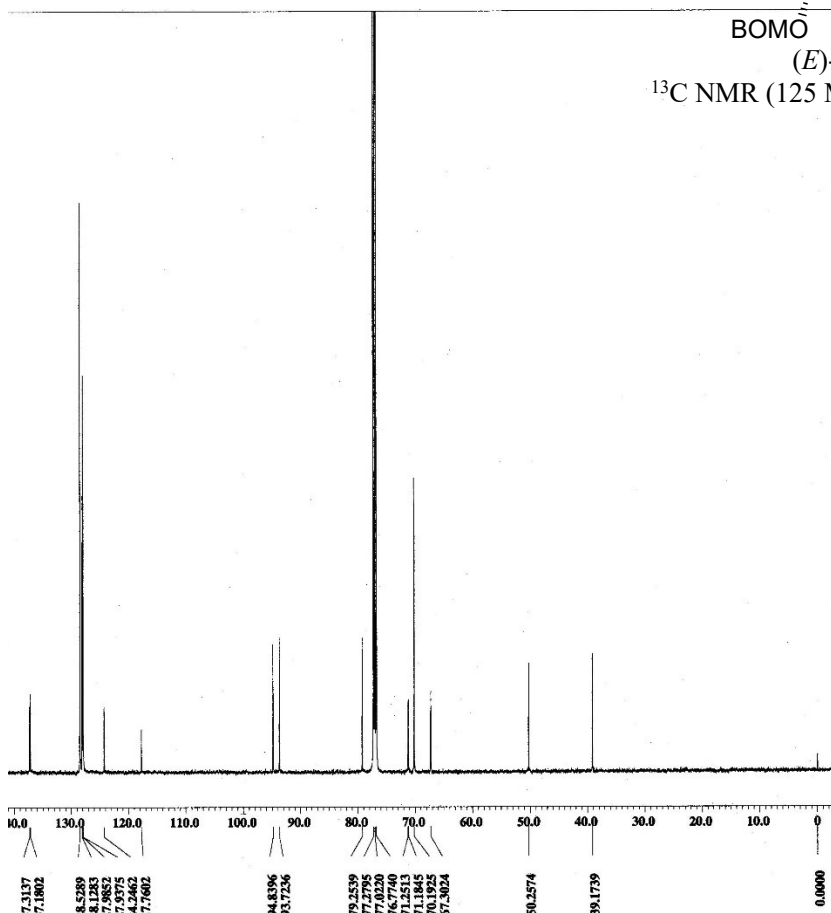
(E)-

¹³C NMR (125 MHz, CDCl₃)

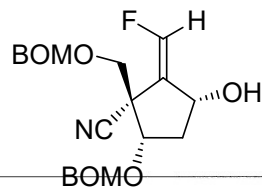
JEOL

----- PROCESSING PARAMETERS -----
 dq_balance : 0 : FALSE
 sump : 2.0 [Hz] : 0.0 [s]
 trapezoid3 : 0 [Hz] : 80 [Hz] : 100 [%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA-46057-carbon-1.jdf

Filename = KMA-46057-carbon-3.jd
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S8718516
 Solvent = CHLOROFORM-D
 Creation_time = 24-DEC-2019 05:24:51
 Revision_time = 24-DEC-2019 07:35:41
 Current_time = 24-DEC-2019 07:36:52
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dia_size = 26214
 Dia_title = 13C
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = TRUE
 Mod_return = 1
 Scans = 12000
 Total_scans = 12000
 X_90_width = 11.53 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 6.6 [dB]
 X_pulse = 5.84333333 [us]
 Irr_atn_dec = 22.192 [dB]
 Irr_atn_noe = 22.192 [dB]
 Irr_noise = WALTE
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 50
 Relaxation_delay = 2 [s]
 Repetition_time = 2.83361792 [s]
 Temp_get = 24.6 [dC]



ion : 13C

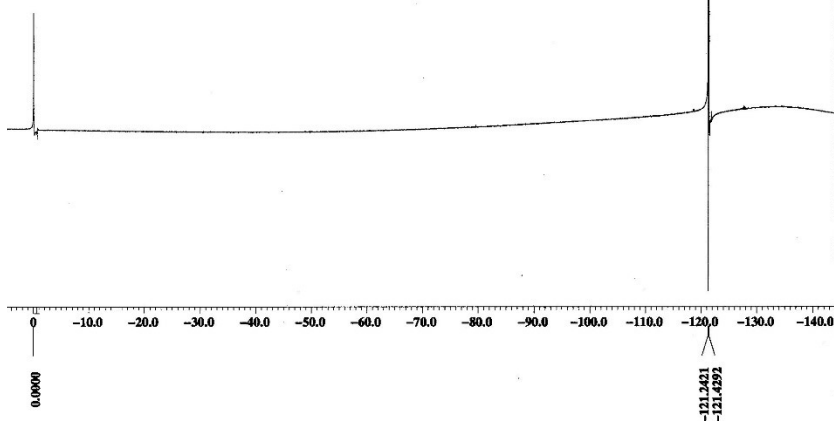


(E)-18
¹⁹F NMR (470 MHz, CDCl₃)



----- PROCESSING PARAMETERS -----
 gc_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA47126-2-19F-1.jdf

Filename = KMA47126-2-19F-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S8310808
 Solvent = CHLOROFORM-D
 Creation_time = 17-MAR-2021 08:39:09
 Revision_time = 17-MAR-2021 08:46:07
 Current_time = 17-MAR-2021 08:46:22
 Comment = single_pulse
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 19F
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[kHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 64
 Total_scans = 64
 X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[deg]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_get = 21.5[degC]



ion : 19F



JEOL



```

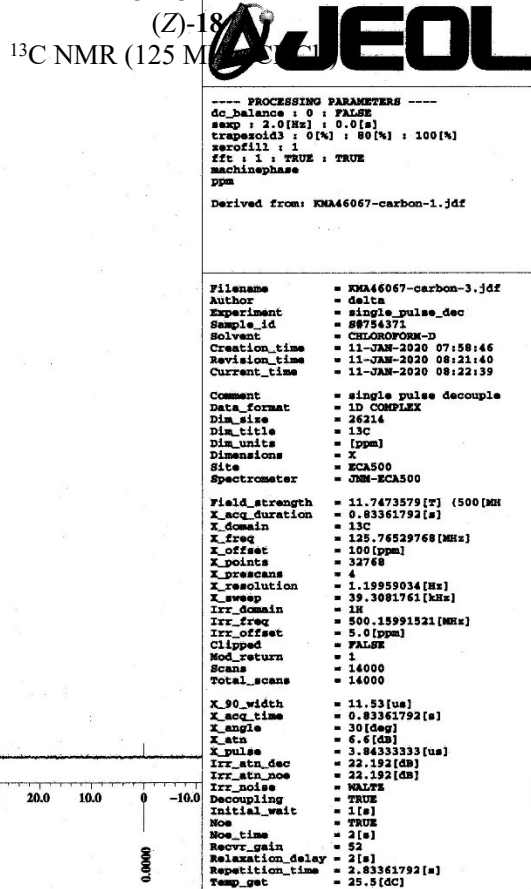
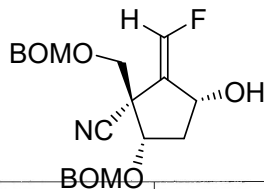
Filename      = DMS46067p_PROTON-5.1d
Author        = delta
Experiment    = single_pulse_wx2
Sample_id     = DMS46067p
Solvent       = CDCl3
Creation_time = 10-JAN-2020 18:46:58
Revision_time = 10-JAN-2020 18:55:22
Current_time  = 10-JAN-2020 18:56:02

Comment
Data_format   = 1D COMPLEX
Sol_id        = 1107
Dir_title     = 1H
Dim_units     = [ppm]
Dimensions    = 2
Site          = XCA500
Spectrometer  = QNP-XCA500

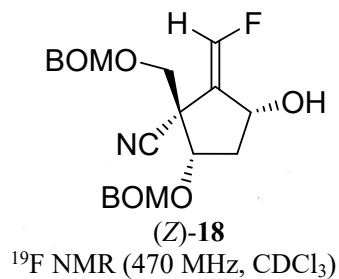
Field_strength = 11.7473579[T] (500[MH
X_domain      = 1.74587904[s]
X_freq        = 500.15991521[MHz]
X_offset      = 5.0 [ppm]
X_points      = 1
X_prescans    = 1
X_resolution  = 0.58277737 [Hz]
X_sweep       = 3.38438438 [kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521[MHz]
Irr_offset    = 5.0 [ppm]
Tri_domain    = 1H
Tri_freq      = 500.15991521[MHz]
Tri_offset    = 5.0 [ppm]
Clipped       = FALSE
Mod_return    = 16
Scans         = 16
Total_scans   = 16

X_90_width    = 12[us]
X_acq_time    = 1.74587904[s]
X_angle       = 45[deg]
X_atn         = 4.5[dB]
X_pulse       = 5[us]
Irr_mode      = Off
Tri_mode      = Off
X_presat      = TRUE
Initial_wait  = 1[s]
Recvr_gain    = 46
Relaxation_delay = 4[s]
X_90_offset   = 1.74587904[s]
Temp_get      = 24.9[degC]

```

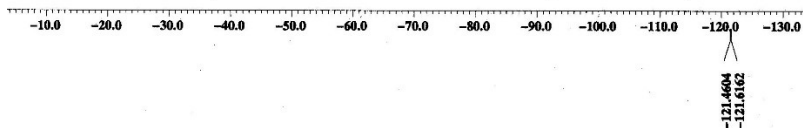


ion : 13C

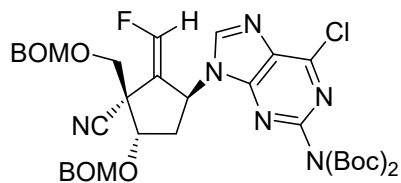


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sexp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: XMA46067-19F-1.jdf

Filename = XMA46067-19F-3.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = 08409084
 Solvent = CHLOROFORM-D
 Creation_time = 11-JAN-2020 11:27:39
 Revision_time = 11-JAN-2020 11:30:22
 Current_time = 11-JAN-2020 11:30:49
 Comment = single_pulse
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 19F
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[MHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 64
 Total_scans = 64
 X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Danta_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 46
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_get = 25.6[deg]



on : 19F

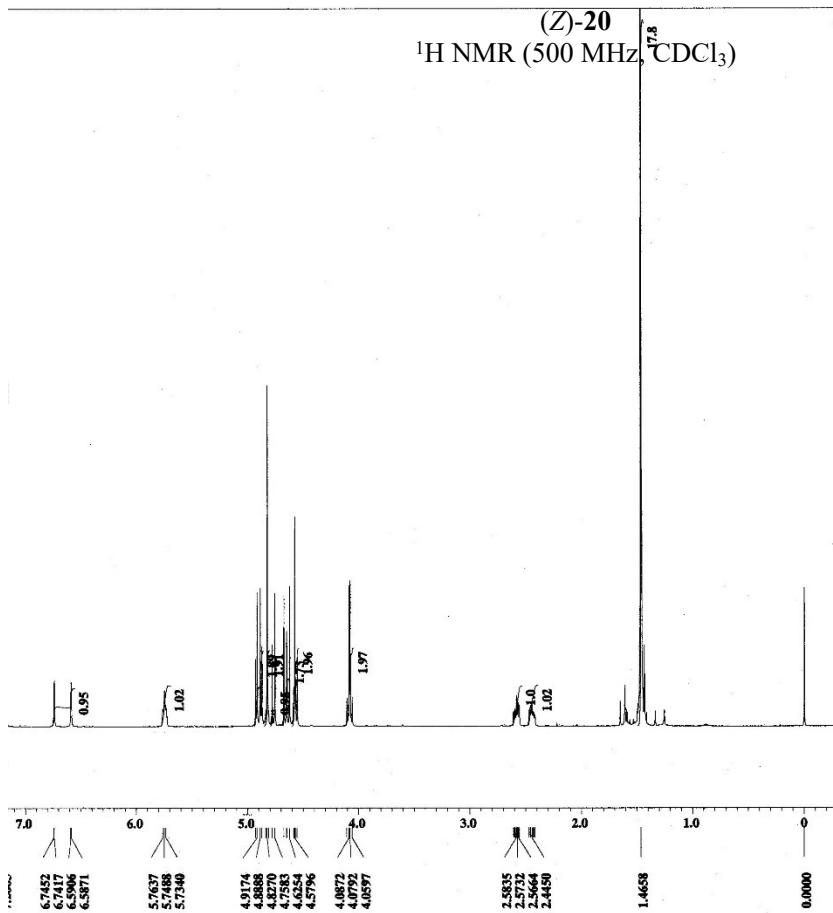


(Z)-20
¹H NMR (500 MHz, CDCl₃)

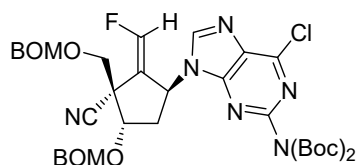


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 f1t : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA46064_PROTON-1.jdf

Filename = KMA46064_PROTON-5.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = KMA46064
 Solvent = CHLOROFORM-D
 Creation_time = 28-DEC-2019 15:15:59
 Revision_time = 30-DEC-2019 15:11:22
 Current_time = 30-DEC-2019 15:11:57
 Comment = CDCl3
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 1H
 Dia_units = [ppm]
 Dimensions = X
 Site = ECAS00
 Spectrometer = JNM-ECAS00
 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[MHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4.5[db]
 X_pulse = 6[us]
 Irr_mode = OFF
 Tri_mode = OFF
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 48
 Relaxation_delay = 4[s]
 Repetition_time = 5.74587904[s]
 Temp_get = 24.5[degC]



on: 1H

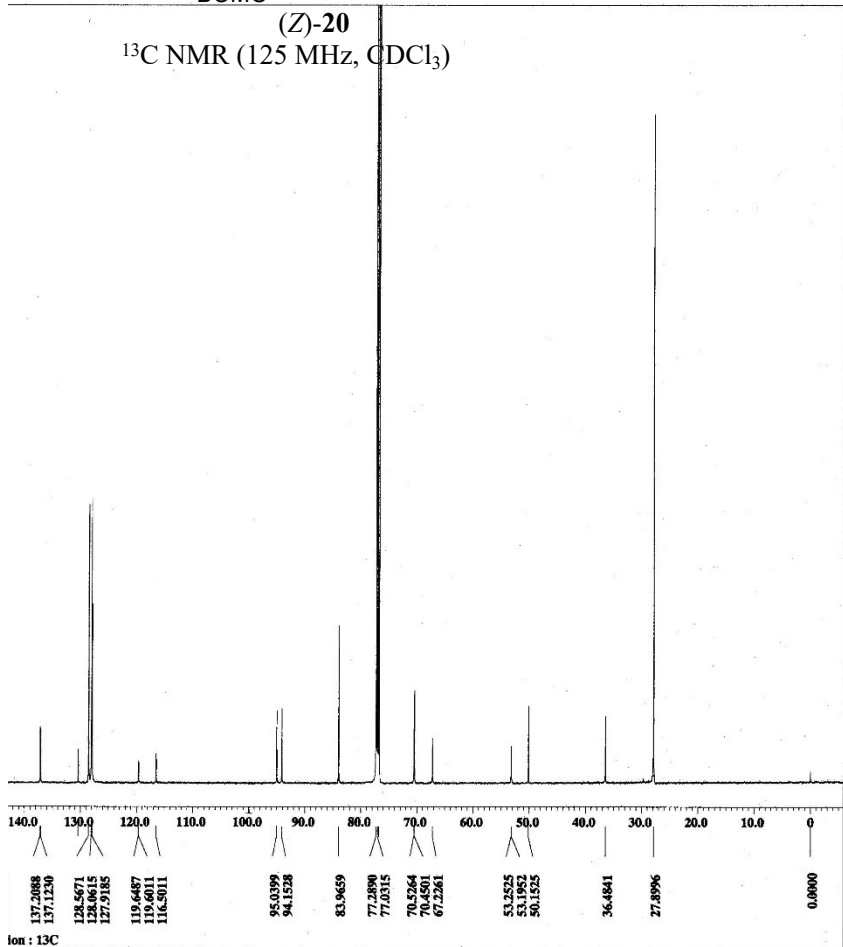


(Z)-20
 ^{13}C NMR (125 MHz, CDCl_3)

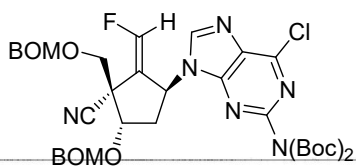


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 2.0[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 serofill : 1
 fft : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA46064-carbon-1.jdf

Filename = KMA46064-carbon-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S8508793
 Solvent = CHLOROFORM-D
 Creation_time = 30-DEC-2019 09:02:23
 Revision_time = 30-DEC-2019 09:45:08
 Current_time = 30-DEC-2019 09:47:08
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dia_size = 26214
 Dia_title = 13C
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = TRUE
 Mod_return = 1
 Scans = 24000
 Total_scans = 24000
 X_90_width = 11.83[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 6.6[db]
 X_pulse = 3.84333333[us]
 Irr_atn_dec = 22.192[db]
 Irr_atn_noe = 22.192[db]
 Irr_noise = WALZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 26
 Relaxation_delay = 2[s]
 Repetition_time = 2.83361792[s]
 Temp_get = 25.3[degC]



ion : 13C

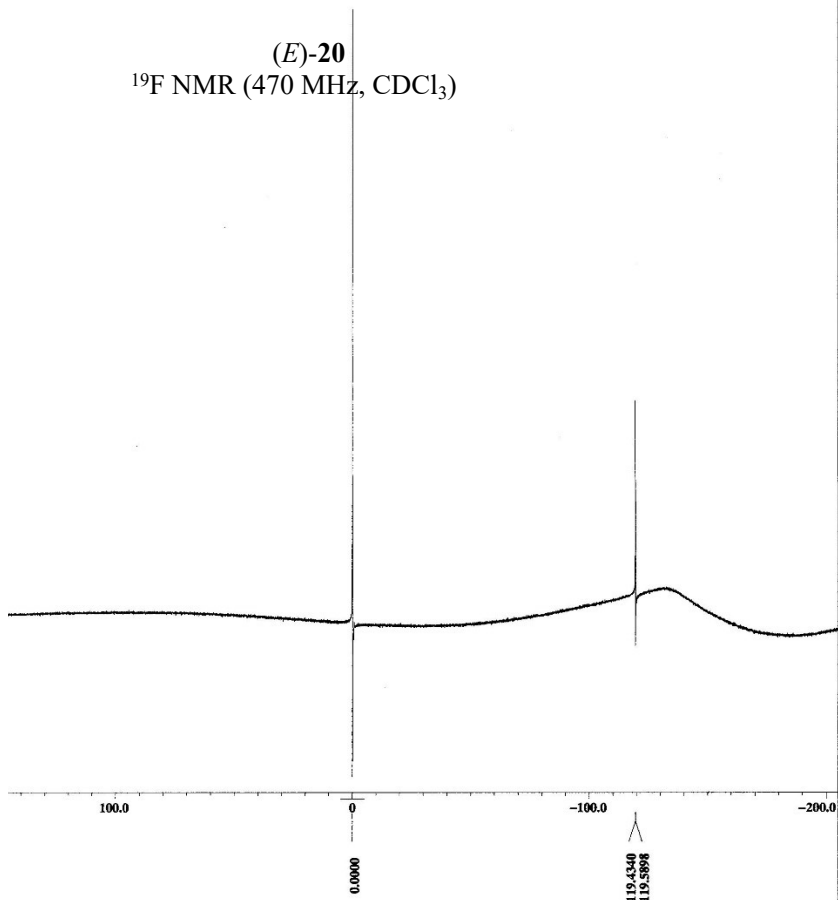


(E)-20
 ^{19}F NMR (470 MHz, CDCl_3)

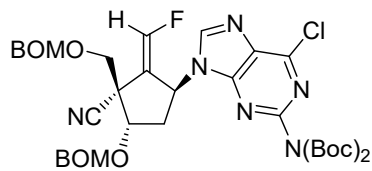


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 sump : 0.2[Hz] : 0.0[s]
 trapxoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: KMA46064-19F-1.jdf

Filename = KMA46064-19F-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S8630384
 Solvent = CHLOROFORM-D
 Creation_time = 18-JAN-2021 17:30:30
 Revision_time = 15-AUG-2021 11:46:21
 Current_time = 15-AUG-2021 11:46:27
 Comment = single_pulse
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 19F
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[KHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[db]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_get = 23[dc]



on: 19F



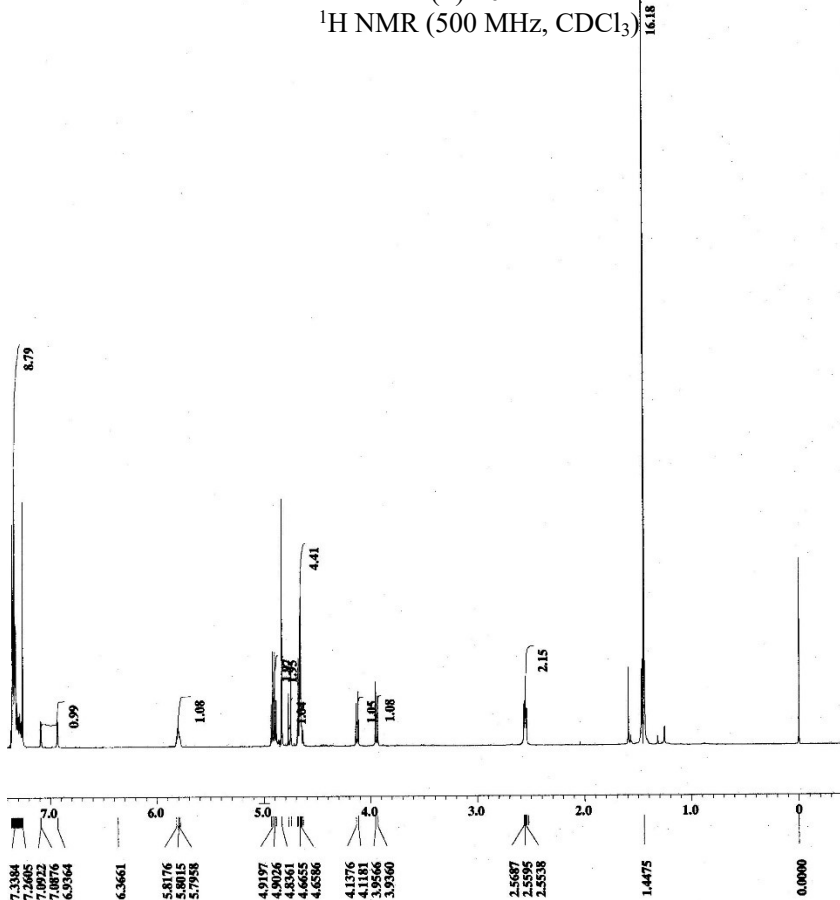
(Z)-20

¹H NMR (500 MHz, CDCl₃)

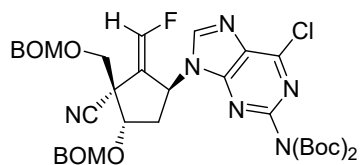


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 f1 : 1 : TRUE : TRUE
 machinephase :
 ppm
 Derived from: KMA46068_PROTON-1.jdf

Filename = KMA46068_PROTON-5.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = KMA46068
 Solvent = CHLOROFORM-D
 Creation_time = 16-JAN-2020 19:56:34
 Revision_time = 16-JAN-2020 20:04:19
 Current_time = 16-JAN-2020 20:04:55
 Comment =
 Data_format = CDCl3
 Data_size = 1D COMPLEX
 Data_title = 13107
 Data_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 6[us]
 Irr_mode = Off
 Tri_mode = Off
 Data_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 48
 Relaxation_delay = 4[s]
 Repetition_time = 5.74587904[s]
 Temp_set = 24.7[deg]



ion: 1H

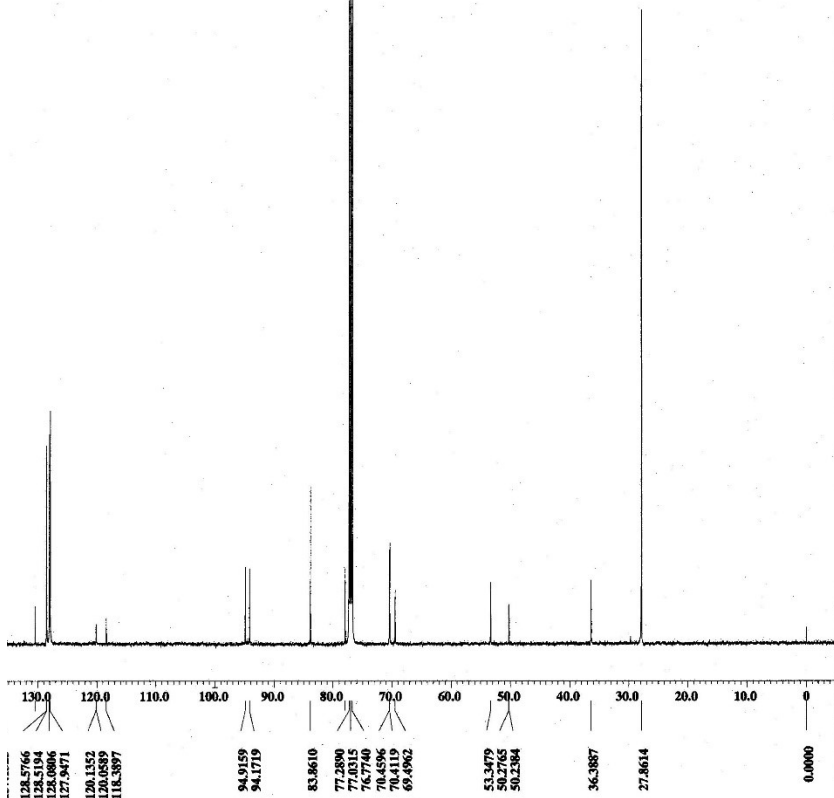


(Z)-20
¹³C NMR (125 MHz, CDCl₃)

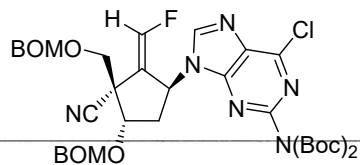
JEOL

----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 2.0[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA46068-carbon-1.jdf

Filename = KMA46068-carbon-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S8752614
 Solvent = CHLOROFORM-D
 Creation_time = 17-JAN-2020 07:17:53
 Revision_time = 17-JAN-2020 07:41:27
 Current_time = 17-JAN-2020 07:42:19
 Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 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 = 13200
 Total_scans = 13200
 X_90_width = 11.53[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 6.6[db]
 X_pulse = 3.84333333[us]
 Irr_atn_dec = 22.192[db]
 Irr_atn_pce = 22.192[db]
 Irr_noise = FALSE
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 2[s]
 Recvr_gain = 52
 Relaxation_delay = 2[s]
 Repetition_time = 2.83361792[s]
 Temp_get = 25[degC]



on: 13C

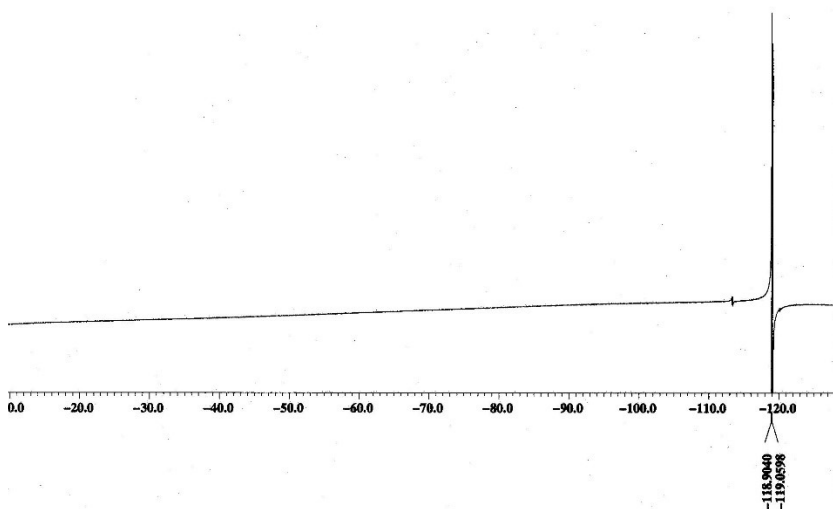


(Z)-20
 ^{19}F NMR (470 MHz, CDCl_3)

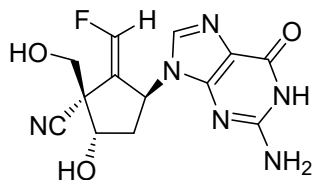


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA46068-19F-1.jdf

Filename = KMA46068-19F-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S8301079
 Solvent = CHLOROFORM-D
 Creation_time = 21-JAN-2020 08:30:30
 Revision_time = 21-JAN-2020 08:32:52
 Current_time = 21-JAN-2020 08:33:16
 Comment = single_pulse
 Data_format = 1D COMPLEX
 Dia_size = 13107
 Dia_title = 19F
 Dia_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[kHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 84
 Total_scans = 84
 X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[db]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 46
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_get = 23.5[dc]



on: 19F



(E)-6

¹H NMR (500 MHz, DMSO-*d*₆)

JEOL

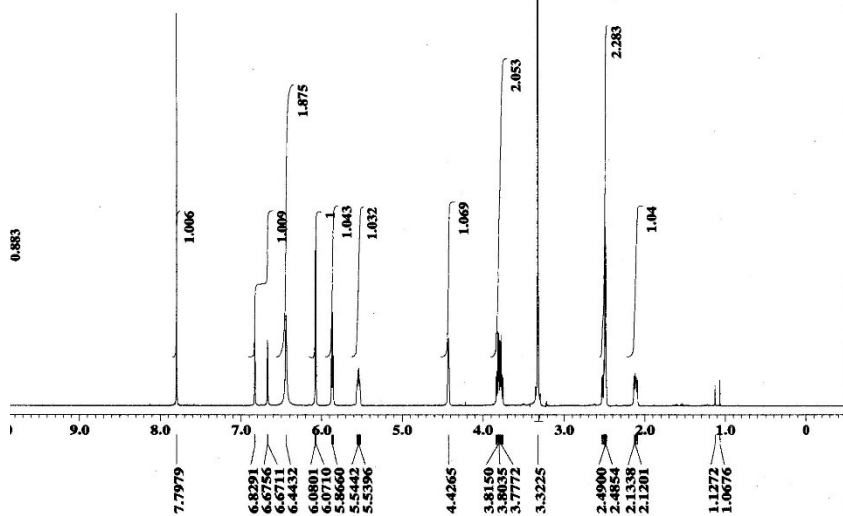
```

----- ACQUISITION PARAMETERS -----
Derived from: KMA-XLIII-99_h.1
File Name      = KMA-XLIII-99_h.4
Author        = Delta
Sample ID     = KMA-XLIII-99
Content       = KMA-XLIII-99_h
Creation Date  = 4-JUL-2016 14:57:05

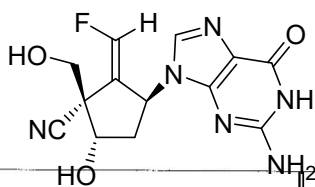
Revision Date  = 5-JUL-2016 18:56:38
Spec Site     = ECA 500

Spec Type     = DELTA2_NMR
Data Format    = 1D COMPLEX
Dimensions    = 2
Dim Title     = 1H
Dim Size      = 13107
Dim Units     = [ppm]
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]
Irr_domain    = 1H
Irr_freq      = 500.15991521[MHz]
Irr_offset    = 5.0[ppm]
Tri_domain    = 1H
Tri_freq      = 500.15991521[MHz]
Tri_offset    = 5.0[ppm]
Mod_return    = 1
Scans         = 8
Total_scans   = 8

X_90_width    = 12.7[us]
X_acq_time     = 1.74587904[s]
X_angle       = 45[deg]
X_atn         = 4.1[dB]
X_pulse       = 6.35[us]
Irr_mode      = Off
Tri_mode      = Off
Dants_preset  = FALSE
Initial_wait   = 1[s]
Relaxation_delay = 3[s]
Repetition_time = 6.74587904[s]
Experiment     = single_pulse.ex2
Recvr_gain     = 54
Solvent        = DMSO-D6
  
```



τ Million : 1H



(E)-6
 ^{13}C NMR (125 MHz, DMSO- d_6)



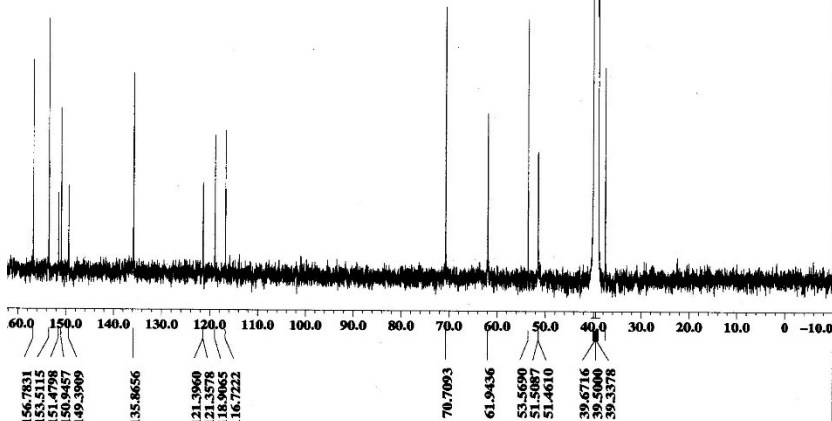
```

----- ACQUISITION PARAMETERS -----
Derived from: KMA-XLIII-99.c.1
File Name      = KMA-XLIII-99.c.4
Author        = delta
Sample ID     = KMA-XLIII-99
Contest       = KMA-XLIII-99.c
Creation Date  = 4-JUL-2016 22:52:35

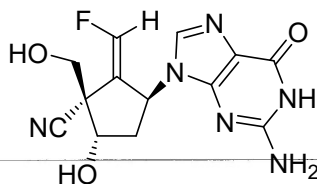
Revision Date  = 11-JUL-2016 12:26:08
Spec Site     = ECA 500

Spec Type     = DELTA2_NMR
Data Format    = 1D COMPLEX
Dimensions    = X
Dim Title     = 13C
Dim Size      = 26214
Dim Units     = [ppm]
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]
Mod_return    = 1
Scans         = 10000
Total_scans   = 10000

X_90_width    = 11.4[us]
X_acq_time     = 0.83361792[s]
X_angle       = 30[deg]
X_atn         = 6.8[db]
X_pulse       = 3.8[us]
Irr_atn_dec   = 21.3[db]
Irr_atn_noe   = 21.3[db]
Irr_pulse     = WALTZ
Decoupling     = TRUE
Initial_wait   = 1[s]
Noe            = TRUE
Noe_time       = 2[s]
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Experiment     = single_pulse_dec
Recvr_gain     = 60
Solvent        = DMSO-D6
  
```



Million : 13C

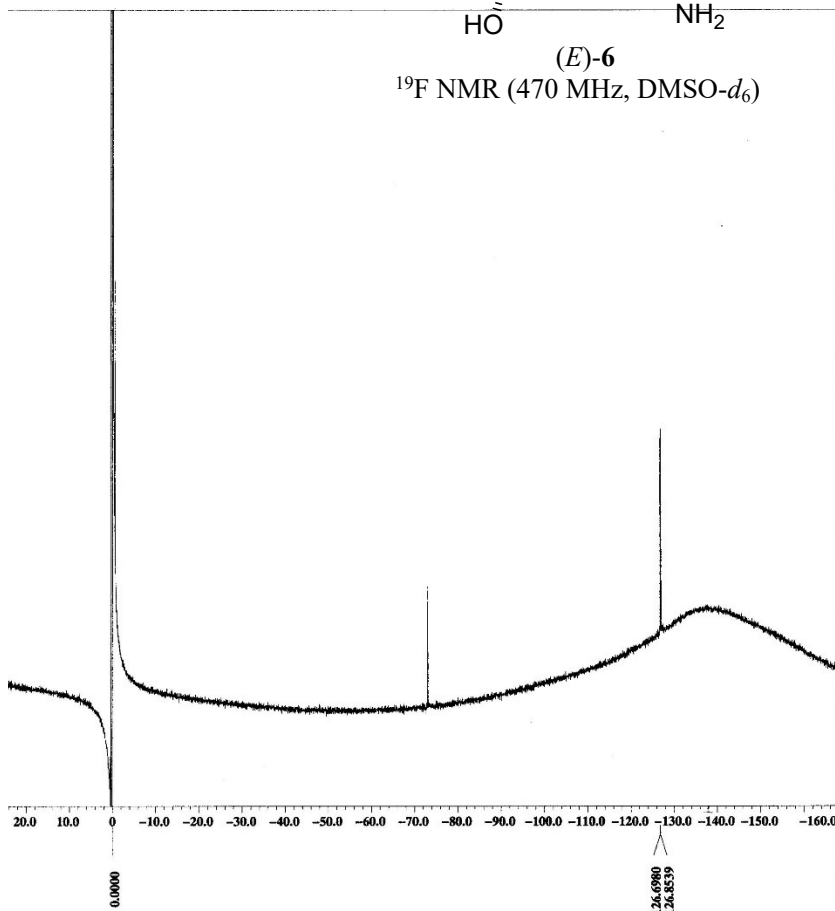


(E)-6
¹⁹F NMR (470 MHz, DMSO-*d*₆)

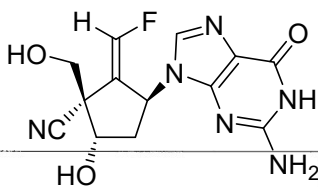


----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 secp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill1 : 1
 fft : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA46083-19F_copy-1.jdf

Filename = KMA46083-19F_copy-4.j
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S865421
 Solvent = DMSO-D6
 Creation_time = 10-MAR-2020 17:07:13
 Revision_time = 15-AUG-2021 12:48:04
 Current_time = 15-AUG-2021 12:48:42
 Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[kHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Incomplete_copy = TRUE
 Mod_return = 1
 Scans = 14
 Total_scans = 14
 X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[db]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_set = 22.9[degC]



on : 19F



(Z)-6
¹H NMR (500 MHz, DMSO-d₆)

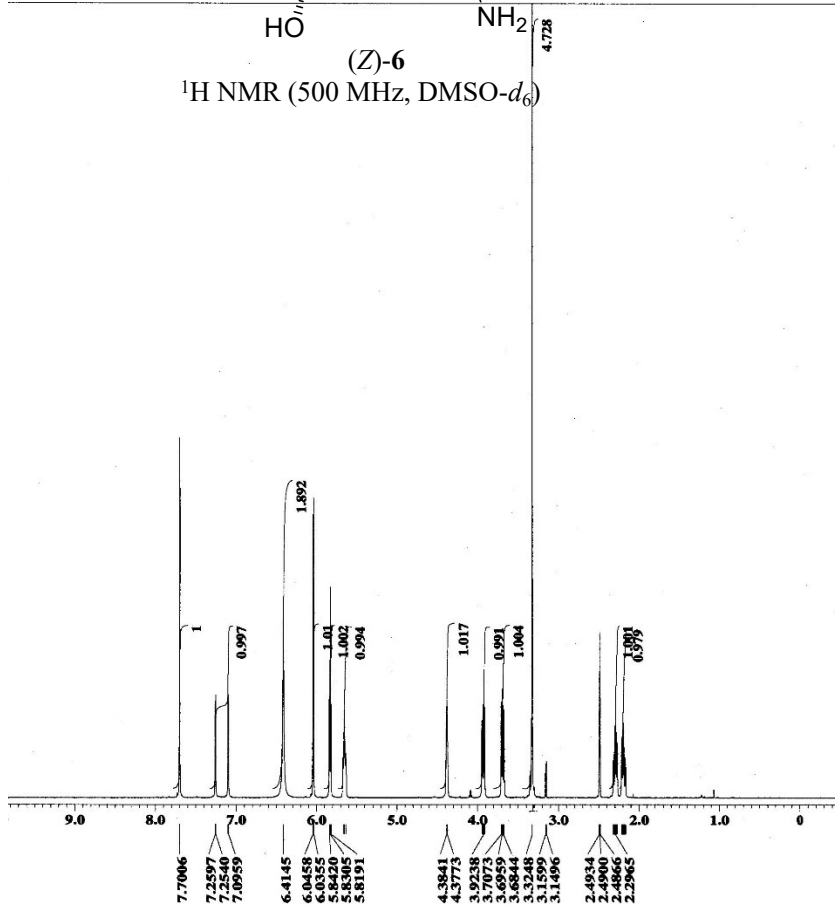
JEOL

```

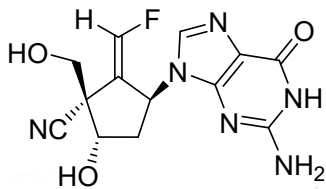
----- ACQUISITION PARAMETERS -----
Derived from: KMA-XLIII-150.h.1
File Name      = KMA-XLIII-150.h.4
Author         = delta
Sample ID      = KMA-XLIII-150
Contest        = KMA-XLIII-150.h
Creation Date   = 13-SEP-2016 17:00:41
Revision Date  = 16-SEP-2016 10:18:01
Spec Site      = RCA 500

Spec Type      = DELTA2_NMR
Data Format     = 1D COMPLEX
Dimensions     = 1H
Dim Title      = 1H
Dim Size       = 13107
Dim Units      = [ppm]
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]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width     = 12.7[us]
X_acq_time      = 1.74587904[s]
X_angle         = 45[deg]
X_atn           = 4.1[dB]
X_pulse         = 6.35[us]
Irr_mode        = Off
Tri_mode        = Off
Dante_preset    = FALSE
Initial_wait    = 1[s]
Relaxation_delay = 5[s]
Repetition_time = 6.74587904[s]
Experiment      = single_pulse.ex2
Recvr_gain      = 50
Solvent         = DMSO-D6
  
```



r Million : 1H



(Z)-6

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

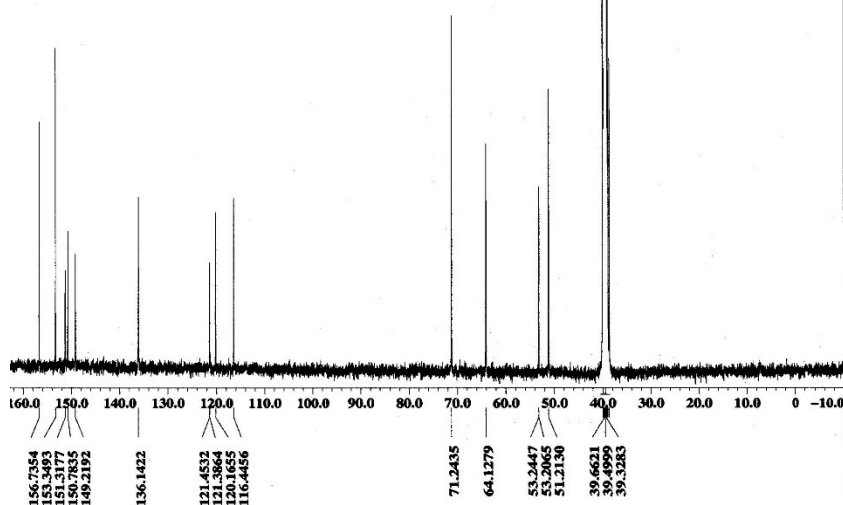
JEOL

```

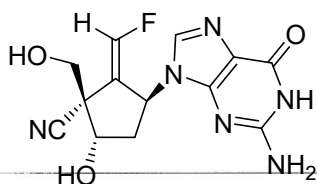
----- ACQUISITION PARAMETERS -----
Derived from: KMA-XLIII-150_c.1
File Name      = KMA-XLIII-150_c.3
Author        = Delta
Sample ID     = KMA-XLIII-150
Content       = KMA-XLIII-150_c
Creation Date  = 14-SEP-2016 04:04:14
Revision Date = 16-SEP-2016 10:22:19
Spec Site     = ECA 500

Spec Type     = DELTA2_NMR
Data Format    = 1D_COMPLEX
Dimensions    = X
Dim Title     = 13C
Dim Size      = 26214
Dim Units     = [ppm]
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      = 500.13991521 [MHz]
Irr_offset    = 5.0 [ppm]
Mod_return    = 1
Scans         = 14000
Total_scans   = 14000

X_90_width    = 11.4 [us]
X_acq_time    = 0.83361792 [s]
X_angle       = 30 [deg]
X_atn         = 6.8 [dB]
X_pulse       = 3.8 [us]
Irr_atn_dec   = 21.3 [dB]
Irr_atn_noe   = 21.3 [dB]
Irr_noise     = WALTE
Decoupling    = TRUE
Initial_wait  = 1 [s]
Noe           = TRUE
Noe_time      = 2 [s]
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Experiment    = single_pulse_dec
Recvr_gain    = 60
Solvent       = DMSO-D6
  
```



r Million : 13C



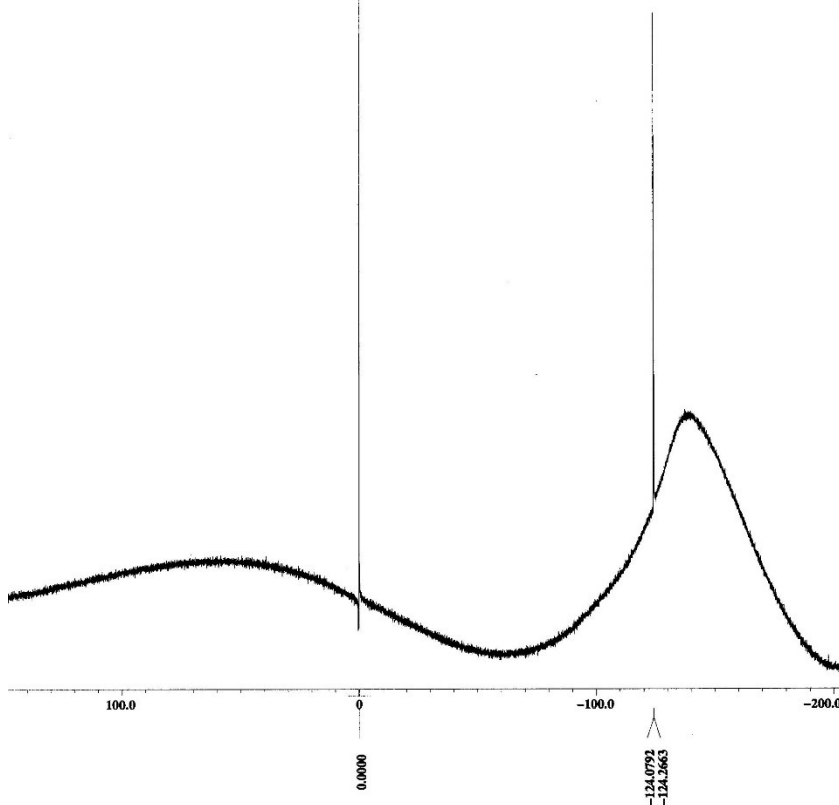
(Z)-6

^{19}F NMR (470 MHz, $\text{DMSO-}d_6$)



----- PROCESSING PARAMETERS -----
 dc_balance : 0 : FALSE
 smp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinphase
 ppm
 Derived from: KMA43150-19-F-1.jdf

Filename = KMA43150-19-F-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#454305
 Solvent = DMSO-D6
 Creation_time = 15-AUG-2021 12:30:23
 Revision_time = 15-AUG-2021 12:44:44
 Current_time = 15-AUG-2021 12:44:53
 Comment = single_pulse
 Data_format = 2D COMPLEX
 Dim_size = 13107
 Dim_title = 19F
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA500
 Spectrometer = JNM-ECA500
 Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 68.15744[ms]
 X_domain = 19F
 X_freq = 470.62046084[MHz]
 X_offset = 0[ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 14.67191256[Hz]
 X_sweep = 240.38461538[kHz]
 Irr_domain = 19F
 Irr_freq = 470.62046084[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 19F
 Tri_freq = 470.62046084[MHz]
 Tri_offset = 5[ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 60
 Total_scans = 60
 X_90_width = 11.7[us]
 X_acq_time = 68.15744[ms]
 X_angle = 45[deg]
 X_atn = 4.5[dB]
 X_pulse = 5.85[us]
 Irr_mode = Off
 Tri_mode = Off
 Danta_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 5.06815744[s]
 Temp_get = 20.8[dc]

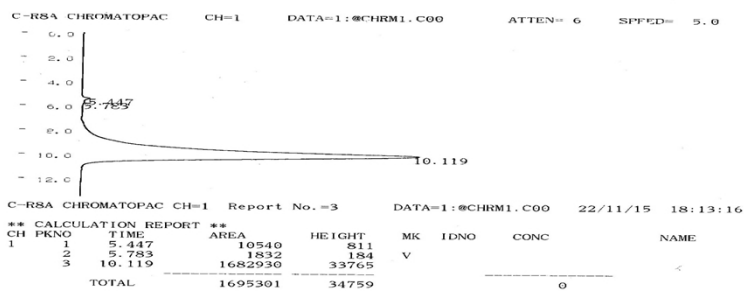


ion : 19F

HPLC traces of biological assay samples (*E*)- and (*Z*)-6

Method: 20% MeOH in H_2O (contained 0.5% of AcOH); 10 mL/mn.

For (*E*)-6; R_t = 10.1 min. Area; 99.3%.



For (Z)-6; $R_t = 11.2$ min. Area; 98.3%.

