

## Supplementary Information

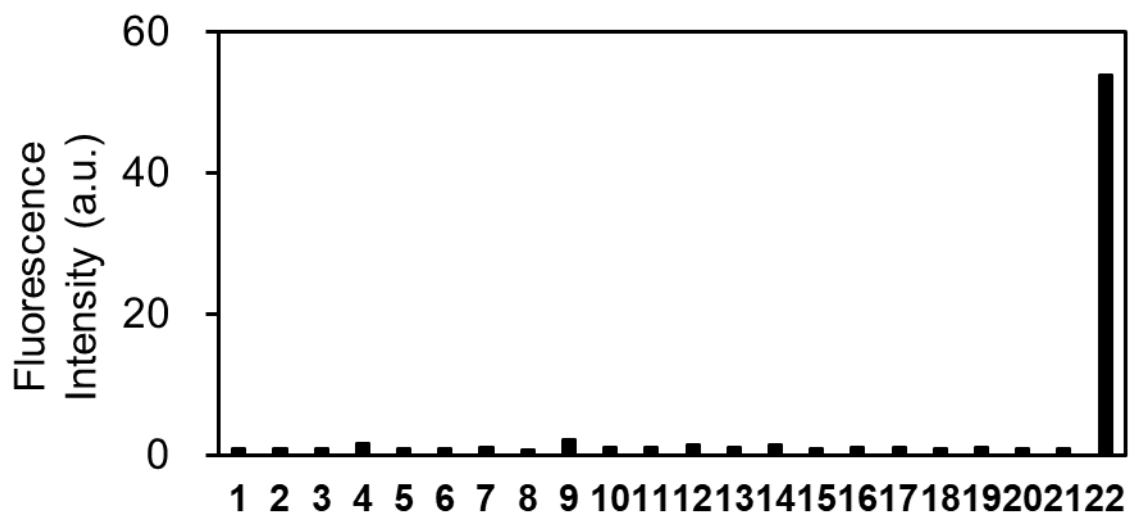
### **A turn-on fluorescent probe containing a $\beta$ -ketoester moiety for the selective detection of intracellular hydrazine**

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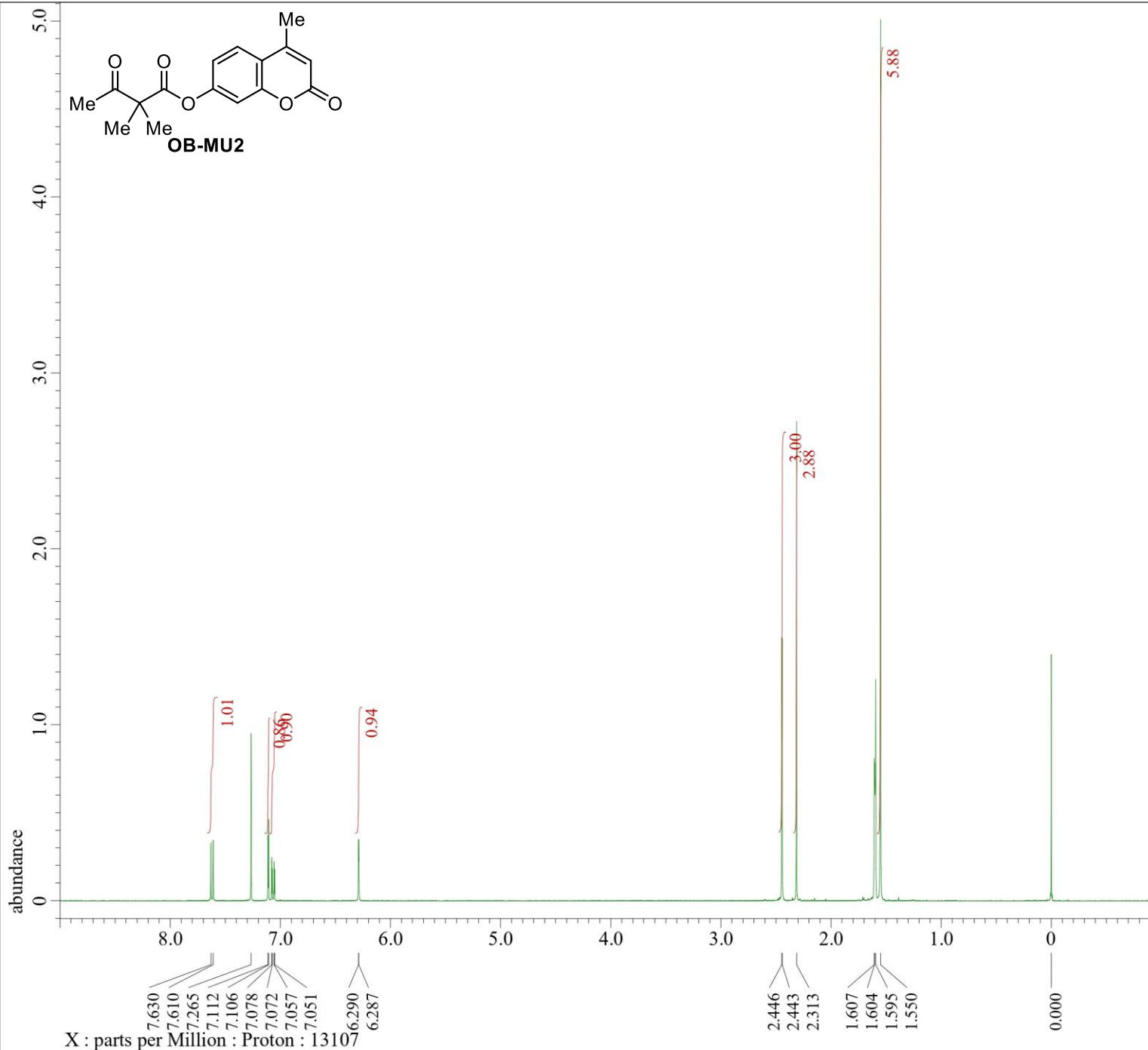
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**Fig. S1.** Fluorescence response of **OB-MU3** (10  $\mu$ M) towards different analytes (200  $\mu$ M) at 25  $^{\circ}$ C, 20 min after addition of analytes in 50 mM HEPES buffer (1% acetonitrile, pH 7.4) ( $\lambda_{\text{ex}}$ : 323 nm,  $\lambda_{\text{em}}$ : 447 nm). Analyte 1: blank, 2: ammonia, 3: hydroxylamine, 4: ethylenediamine, 5:  $\text{S}^{2-}$ , 6: aniline, 7: methylamine, 8: piperidine, 9: *p*-tolylhydrazine, 10: lysine, 11: glycine, 12:  $\text{SO}_3^{2-}$ , 13:  $\text{S}_2\text{O}_3^{2-}$ , 14:  $\text{Cu}^+$ , 15:  $\text{Cu}^{2+}$ , 16:  $\text{Zn}^{2+}$ , 17:  $\text{Fe}^{2+}$ , 18:  $\text{Fe}^{3+}$ , 19:  $\text{Mn}^{2+}$ , 20:  $\text{Ni}^{2+}$ , 21:  $\text{Co}^{2+}$ , 22: hydrazine.



X : parts per Million : Proton : 13107

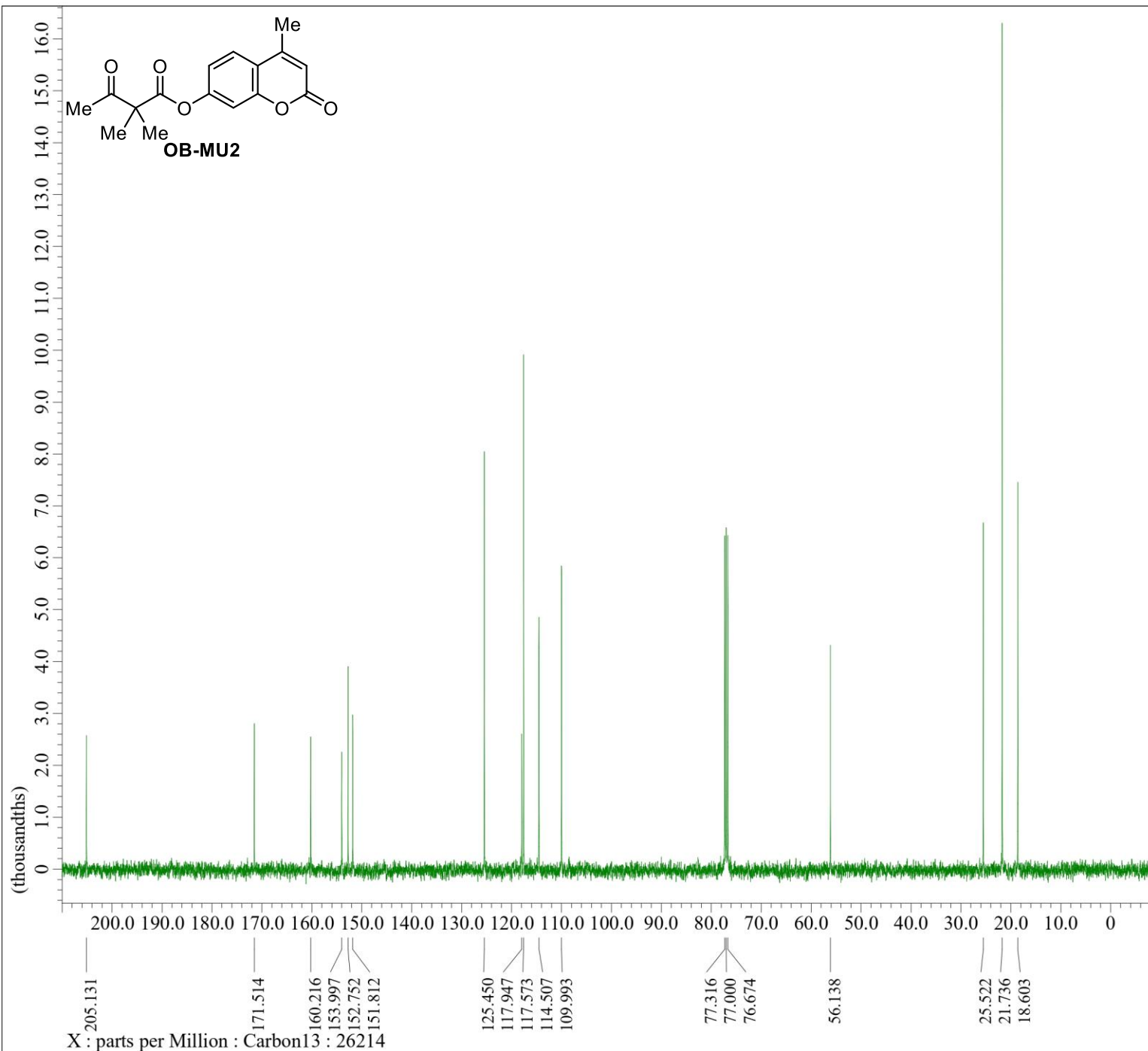
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -0.15555, 1.79469, 72.95895[%] )
```

```
Filename      = 16ATA2-65-2_Proton-1-
Author        = delta
Experiment    = proton_auto.jxp
Sample_Id     = 16ATA2-65-2
Solvent       = CHLOROFORM-D
Actual_Start_Time = 26-JUN-2021 14:57:54
Revision_Time  = 26-JUN-2021 15:03:59
```

```
Comment       = single_pulse
Data_Format   = 1D COMPLEX
Dim_Size      = 13107
X_Domain      = Proton
Dim_Title     = Proton
Dim_Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ400S/L1
```

```
Field Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain       = Proton
X_Freq         = 399.78219838[MHz]
X_Offset       = 5[ppm]
X_Points       = 16384
X_Prescans     = 1
X_Resolution   = 0.45739775[Hz]
X_Sweep        = 7.4940048[kHz]
X_Sweep_Clippped = 5.99520384[kHz]
Irr_Domain     = Proton
Irr_Freq       = 399.78219838[MHz]
Irr_Offset     = 5[ppm]
Tri_Domain     = Proton
Tri_Freq       = 399.78219838[MHz]
Tri_Offset     = 5[ppm]
Blanking       = 2.0[us]
Clipped        = FALSE
Scans          = 8
Total_Scans    = 8
```

```
Relaxation_Delay = 5[s]
Recvr_Gain        = 56
Temp_Get          = 22.8[dC]
X_90_Width       = 6.6[us]
X_Acq_Time        = 2.18628096[s]
X_Angle          = 45[deg]
X_Atn            = 6.5[dB]
X_Pulse          = 3.3[us]
Irr_Mode         = Off
Tri_Mode         = Off
```



```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

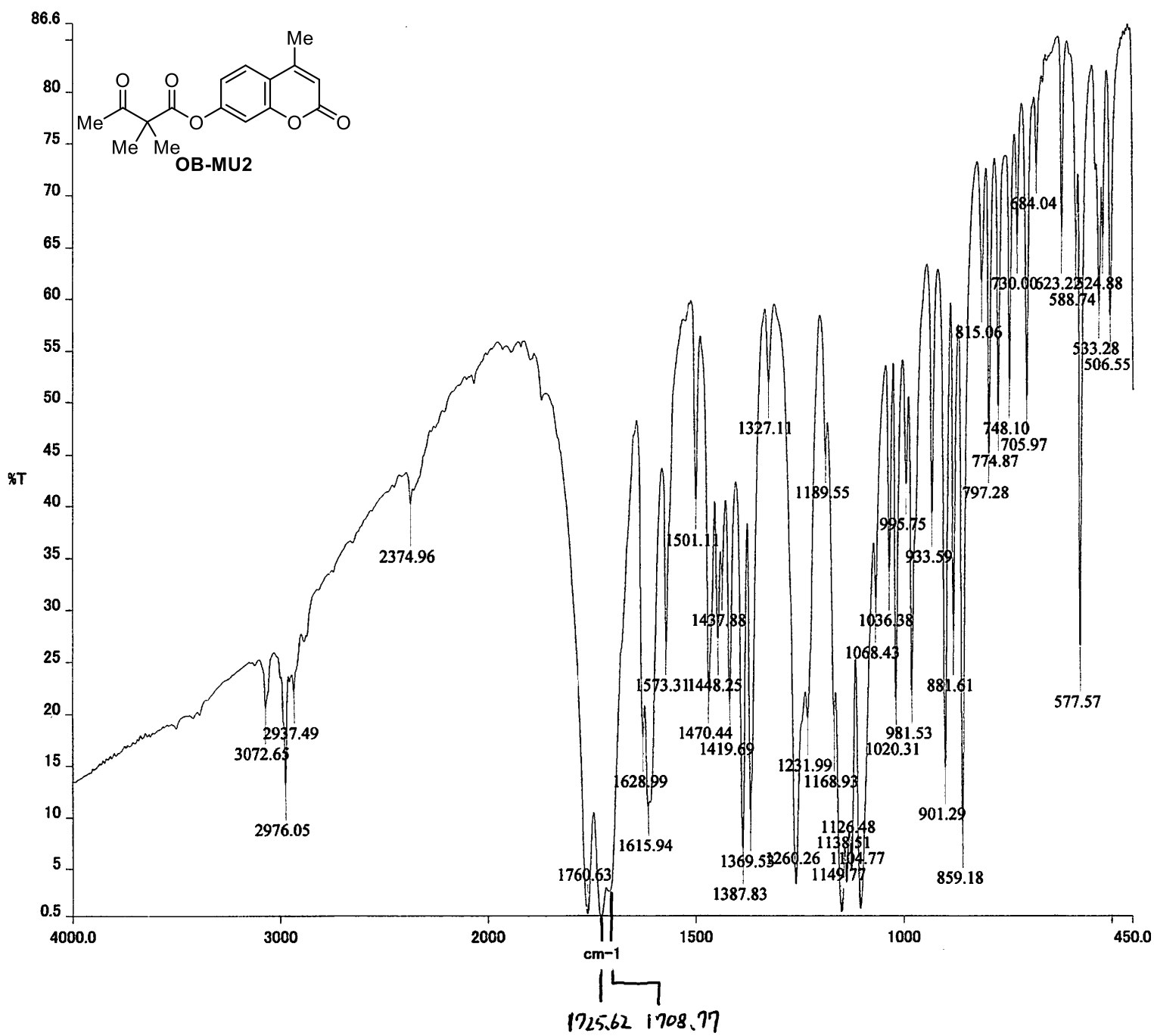
```
Filename = 16ATA2-65-2_Carbon
Author = delta
Experiment = carbon_auto.jxp
Sample_Id = 16ATA2-65-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-JUN-2021 20:22:
Revision_Time = 26-JUN-2021 20:29:
```

```
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
```

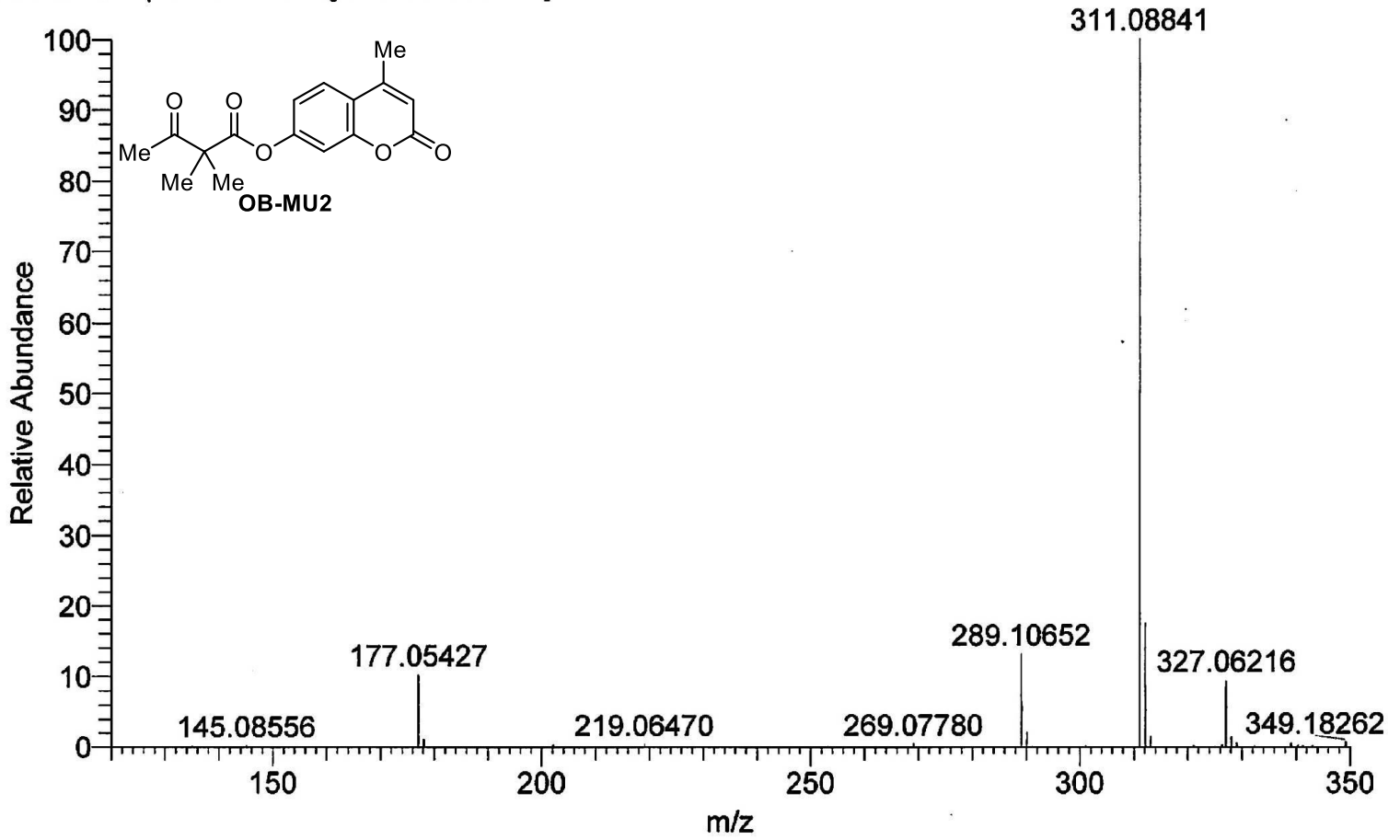
```
Field_Strength = 9.389766[T] (400[M]
X_Acq_Duration = 1.03809024[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clippped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 105
Total_Scans = 105
```

```
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.7[dC]
X_90_Width = 10.5[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8.2[dB]
X_Pulse = 3.5[us]
Irr_Atn_Dec = 31.323[dB]
Irr_Atn_Dec_Calc = 31.323[dB]
Irr_Atn_Dec_Default_Calc = 31.323[dB]
Irr_Atn_No = 31.323[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
```

date: 2022年7月22日



YY18HSH2-2-2 #56-68 RT: 0.30-0.35 AV: 3 SB: 4 1.00-1.11 NL: 4.04E7  
 F: FTMS + p ESI Full ms [100.00-1000.00]



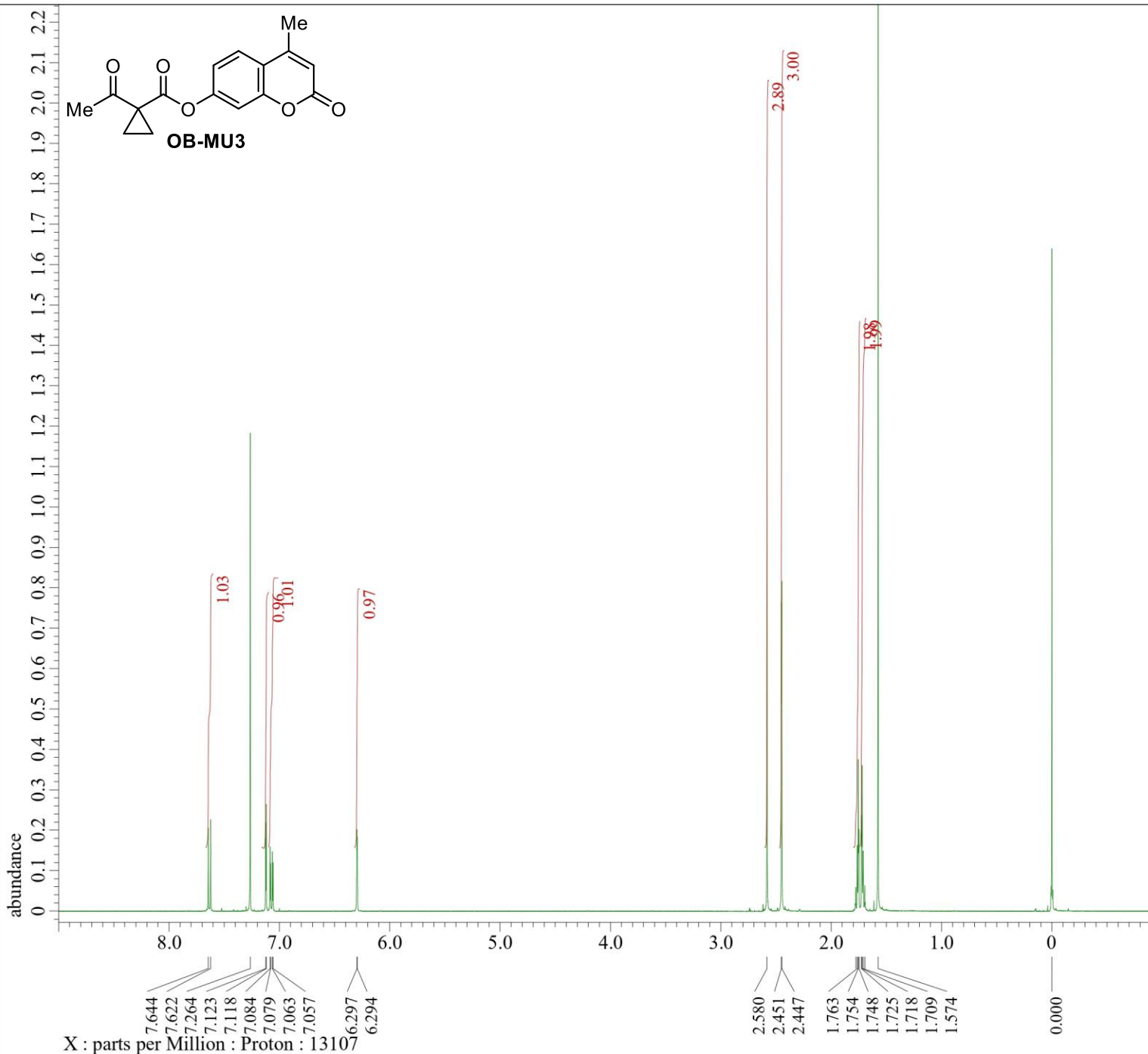
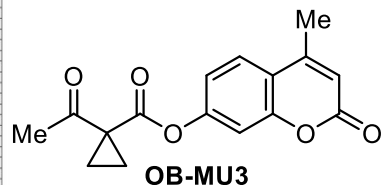
YY18HSH2-2-2#56-68 RT: 0.30-0.35 AV: 3

SB: 4 1.00-1.11

F: FTMS + p ESI Full ms [100.00-1000.00]

m/z= 288.10313-311.78142

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
289.10652	5398060.5	12.91	289.10705	-0.53	C <sub>16</sub> H <sub>17</sub> O <sub>5</sub>
311.08841	41799176.0	100.00	311.08899	-0.59	C <sub>16</sub> H <sub>16</sub> O <sub>5</sub> Na



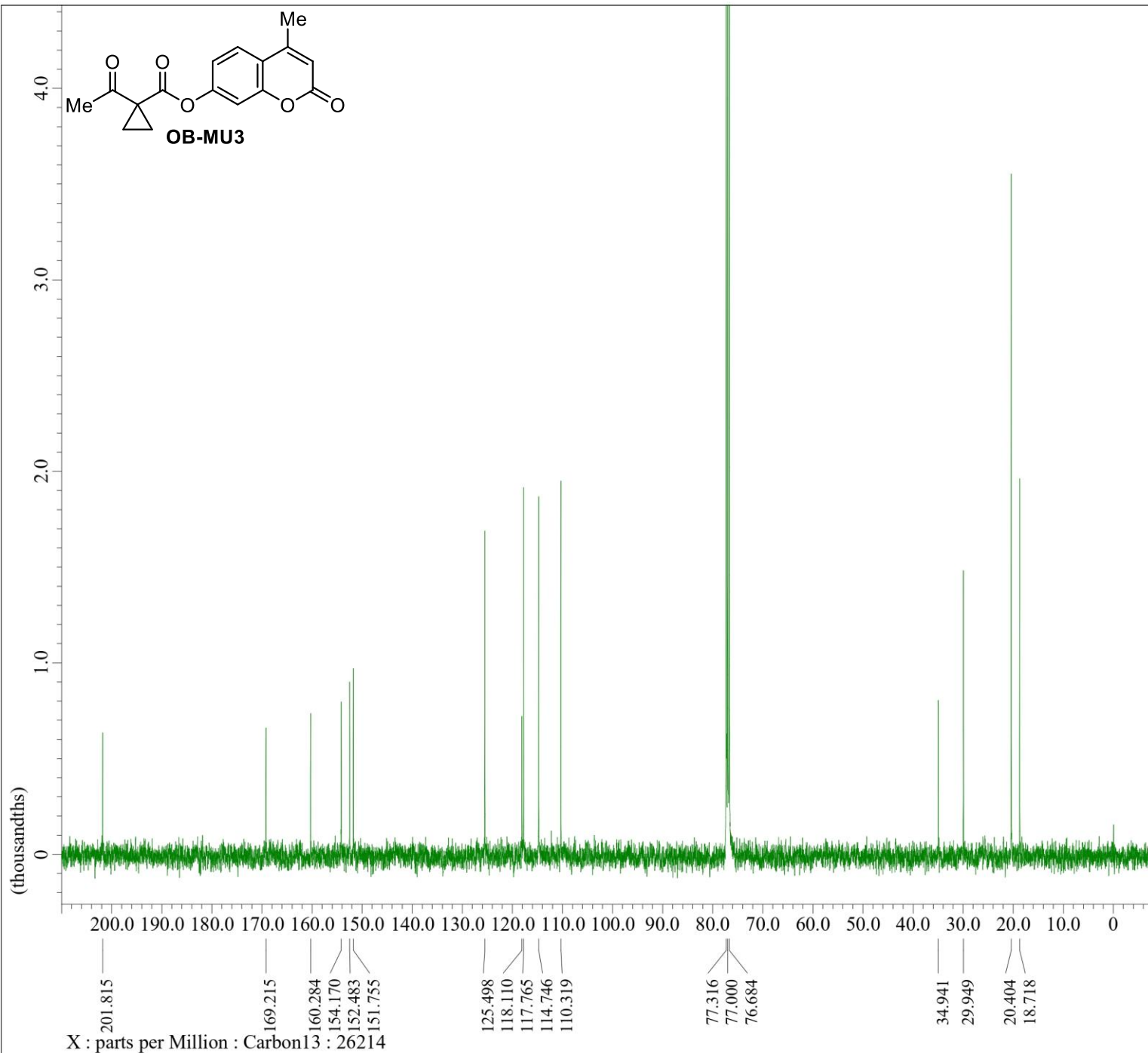
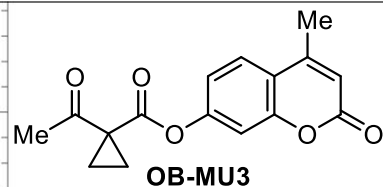
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 2, -5, 72.95895[%] )
```

```
Filename      = 16ATA3-44-pure3_Proto
Author        = delta
Experiment    = proton_auto.jxp
Sample_Id     = 16ATA3-44-pure3
Solvent       = CHLOROFORM-D
Actual_Start_Time = 23-JUN-2022 12:25:47
Revision_Time  = 23-JUN-2022 13:43:50
```

```
Comment       = single_pulse
Data_Format   = 1D COMPLEX
Dim_Size      = 13107
X_Domain      = Proton
Dim_Title     = Proton
Dim_Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ400S/L1
```

```
Field Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain       = Proton
X_Freq         = 399.78219838[MHz]
X_Offset       = 5 [ppm]
X_Points       = 16384
X_Prescans     = 1
X_Resolution   = 0.45739775 [Hz]
X_Sweep        = 7.4940048 [kHz]
X_Sweep_Clippped = 5.99520384 [kHz]
Irr_Domain     = Proton
Irr_Freq       = 399.78219838[MHz]
Irr_Offset     = 5 [ppm]
Tri_Domain     = Proton
Tri_Freq       = 399.78219838[MHz]
Tri_Offset     = 5 [ppm]
Blanking       = 2.0 [us]
Clipped        = FALSE
Scans          = 8
Total_Scans    = 8
```

```
Relaxation_Delay = 5 [s]
Recvr_Gain       = 56
Temp_Get         = 22 [dC]
X_90_Width       = 6.6 [us]
X_Acq_Time       = 2.18628096 [s]
X_Angle          = 45 [deg]
X_Atn            = 6.5 [dB]
X_Pulse          = 3.3 [us]
Irr_Mode         = Off
Tri_Mode         = Off
```



```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE )
machinephase
ppm
```

```
Filename = 16ATA3-44-pure_Car
Author = delta
Experiment = carbon_auto.jxp
Sample_Id = 16ATA3-44-pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-JUN-2022 21:02:
Revision_Time = 25-JUN-2022 11:33:
```

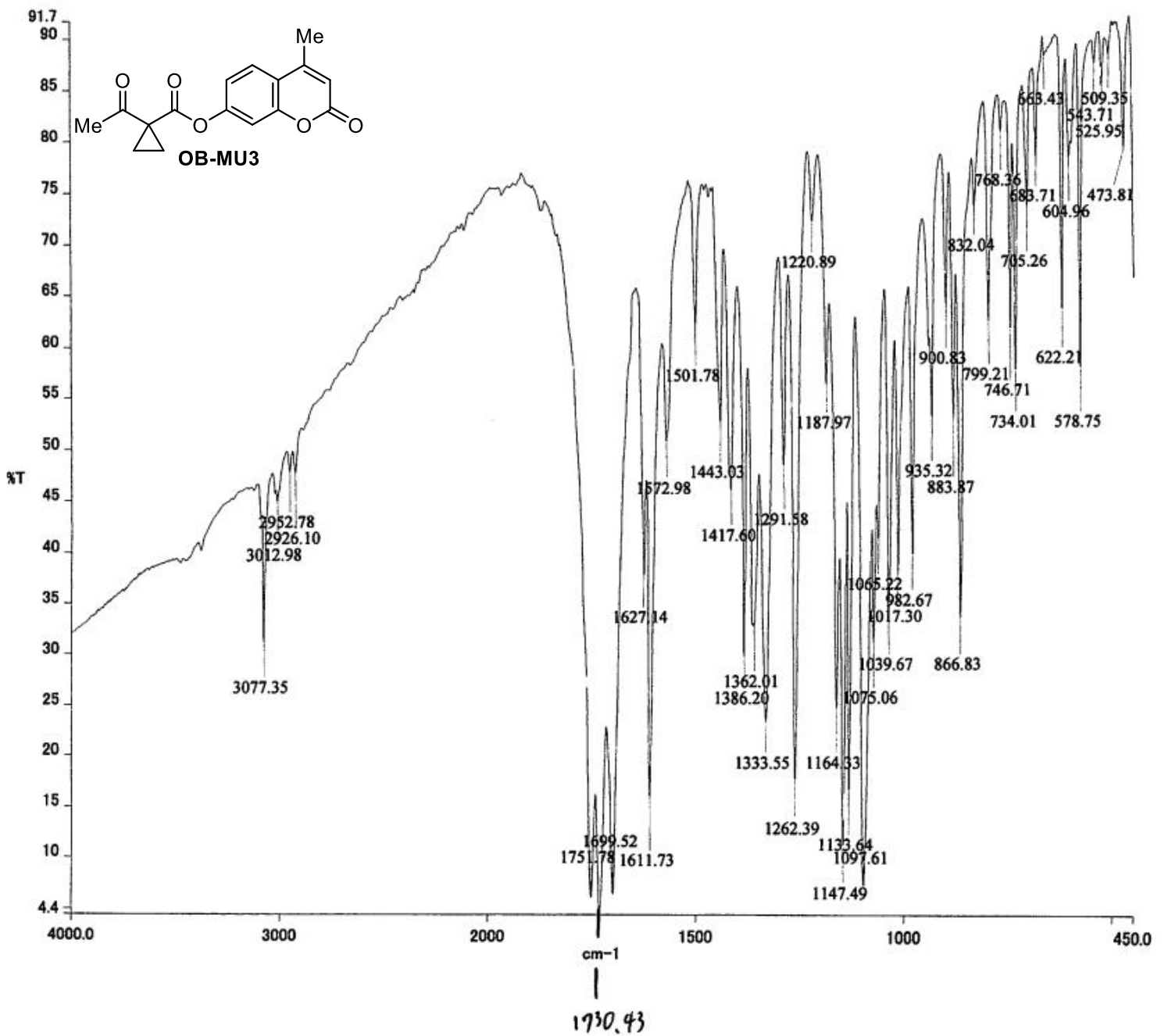
```
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
```

```
Field_Strength = 9.389766[T] (400[M]
X_Acq_Duration = 1.03809024[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5.0[us]
Clipped = FALSE
Scans = 513
Total_Scans = 513
```

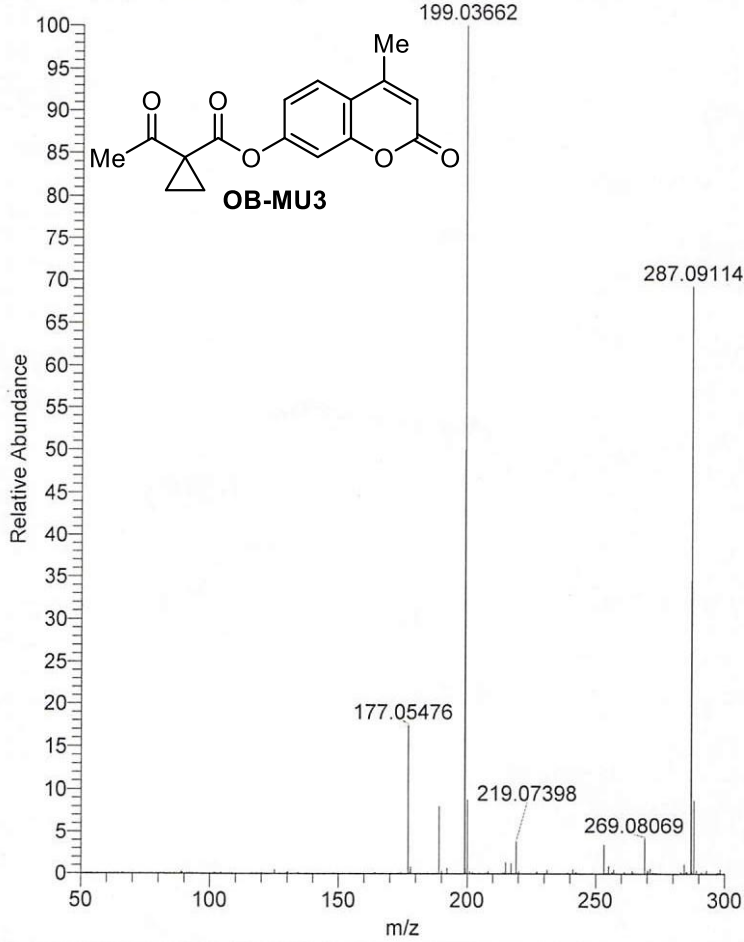
```
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 23[dc]
X_90_Width = 10.5[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8.2[dB]
X_Pulse = 3.5[us]
Irr_Atn_Dec = 31.323[dB]
Irr_Atn_Dec_Calc = 31.323[dB]
Irr_Atn_Dec_Default_Calc = 31.323[dB]
Irr_Atn_No = 31.323[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
```



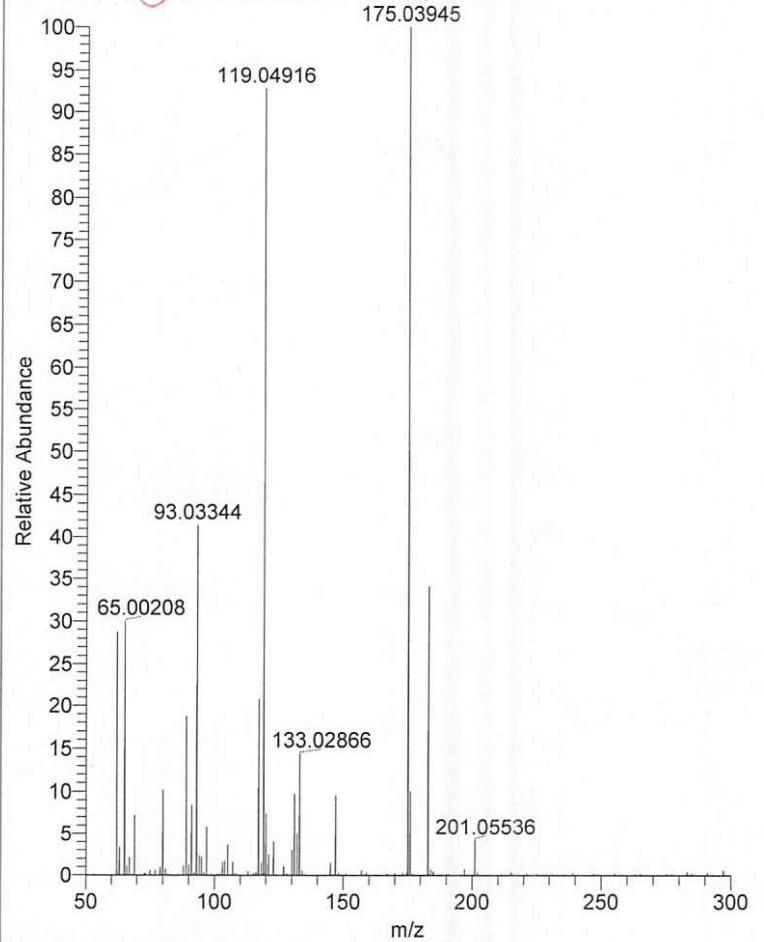
date: 2022年7月22日



YY16ATA3-93-3 #27-32 RT: 0.62-0.70 AV: 3 SB: 3 0.40-0.52 NL: 1.55E5  
 T: FTMS {1,1} + p ESI Full ms [50.00-300.00]



YY16ATA3-93-3 #38-40 RT: 0.84-0.88 AV: 2 SB: 3 0.40-0.52 NL: 8.93E5  
 T: FTMS {1,2} - p ESI Full ms [50.00-300.00]

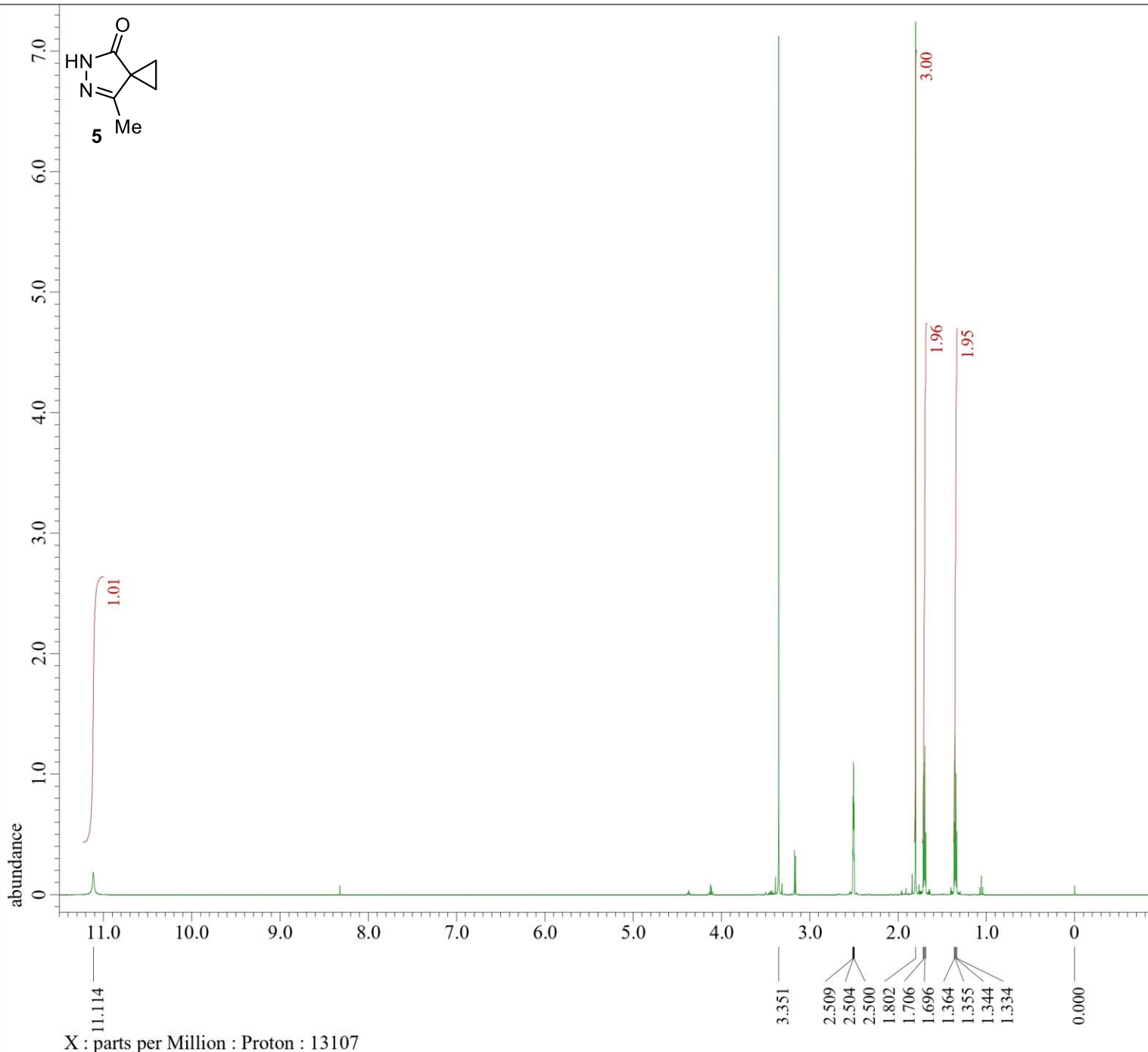


YY16ATA3-93-3#27-31 RT: 0.62-0.70 AV: 3  
 SB: 3 0.40-0.52  
 T: FTMS {1,1} + p ESI Full ms [50.00-300.00]  
 m/z= 164.39929-209.45230

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Compositi
177.05476	27282.1	17.24	177.05462	0.81	C <sub>10</sub> H <sub>9</sub> O <sub>3</sub>
199.03662	158289.8	100.00	199.03657	0.26	C <sub>10</sub> H <sub>8</sub> O <sub>3</sub> Na

YY16ATA3-93-3#38-40 RT: 0.84-0.88 AV: 2  
 SB: 3 0.40-0.52  
 T: FTMS {1,2} - p ESI Full ms [50.00-300.00]  
 m/z= 170.01352-180.76481

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Compositi
175.03945	906152.4	100.00	175.04007	-3.50	C <sub>10</sub> H <sub>7</sub> O <sub>3</sub>



---- PROCESSING PARAMETERS ----  
sexp( 0.2[Hz], 0.0[s] )  
trapezoid( 0[%], 0[%], 80[%], 100[%] )  
zerofill( 1, TRUE )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm

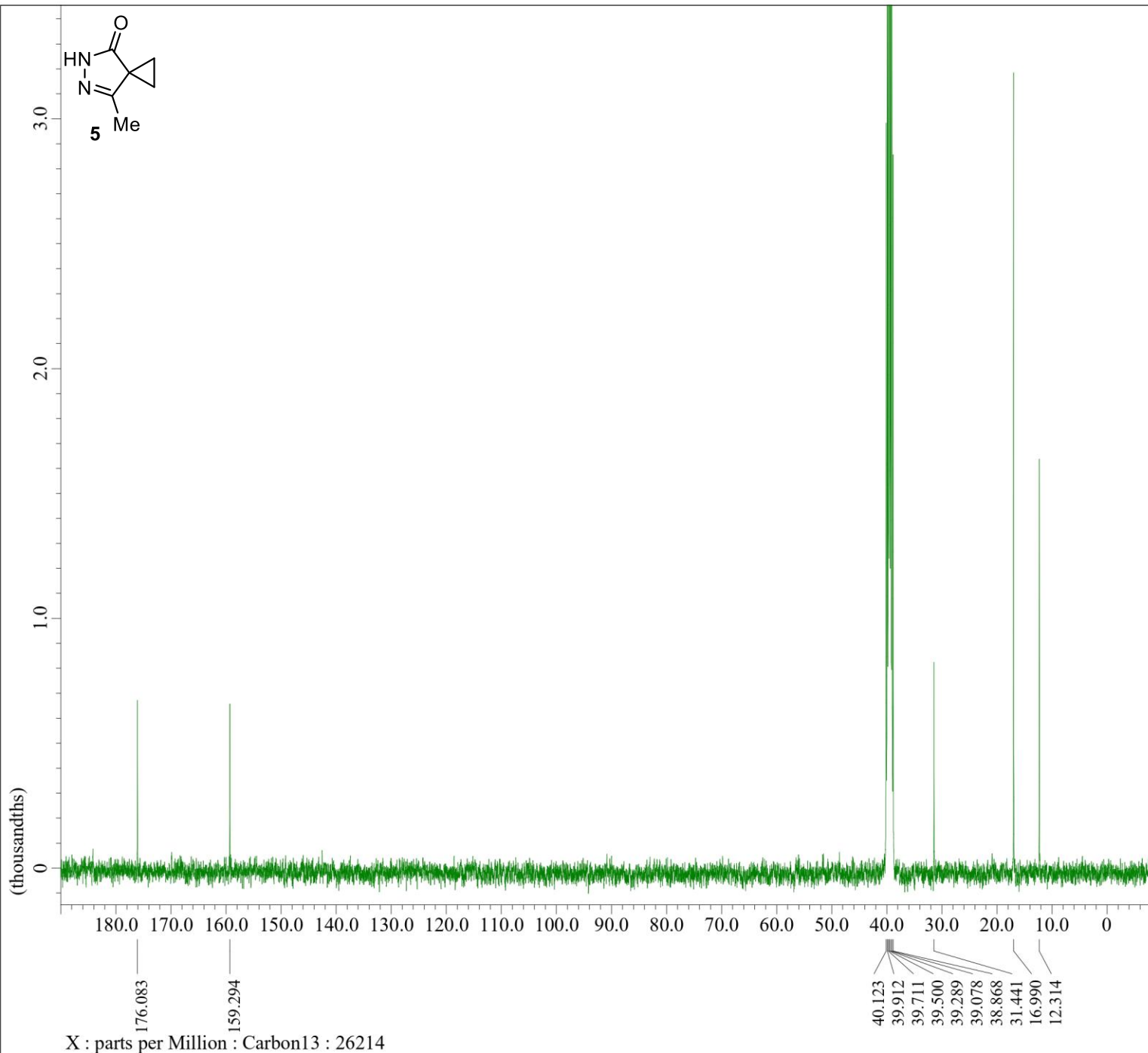
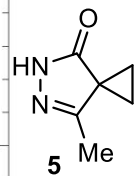
以下に由来: 16ATA3-50-3\_Proton-1-1.jdf

Filename = 16ATA3-50-3\_Proton-1-  
Author = delta  
Experiment = proton\_auto.jxp  
Sample\_Id = 16ATA3-50-3  
Solvent = DMSO-D6  
Actual\_Start\_Time = 6-MAR-2022 19:33:53  
Revision\_Time = 19-NOV-2024 19:52:10

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
X\_Domain = Proton  
Dim\_Title = Proton  
Dim\_Units = [ppm]  
Dimensions = X  
Spectrometer = JNM-ECZ400S/L1

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18628096[s]  
X\_Domain = Proton  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45739775[Hz]  
X\_Sweep = 7.4940048[kHz]  
X\_Sweep\_Clipped = 5.99520384[kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = Proton  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Blanking = 2.0[us]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 56  
Temp\_Get = 19.4[dc]  
X\_90\_Width = 6.6[us]  
X\_Acq\_Time = 2.18628096[s]  
X\_Angle = 45[deg]  
X\_Atn = 6.5[dB]  
X\_Pulse = 3.3[us]  
Irr\_Mode = Off  
Tri\_Mode = Off



```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

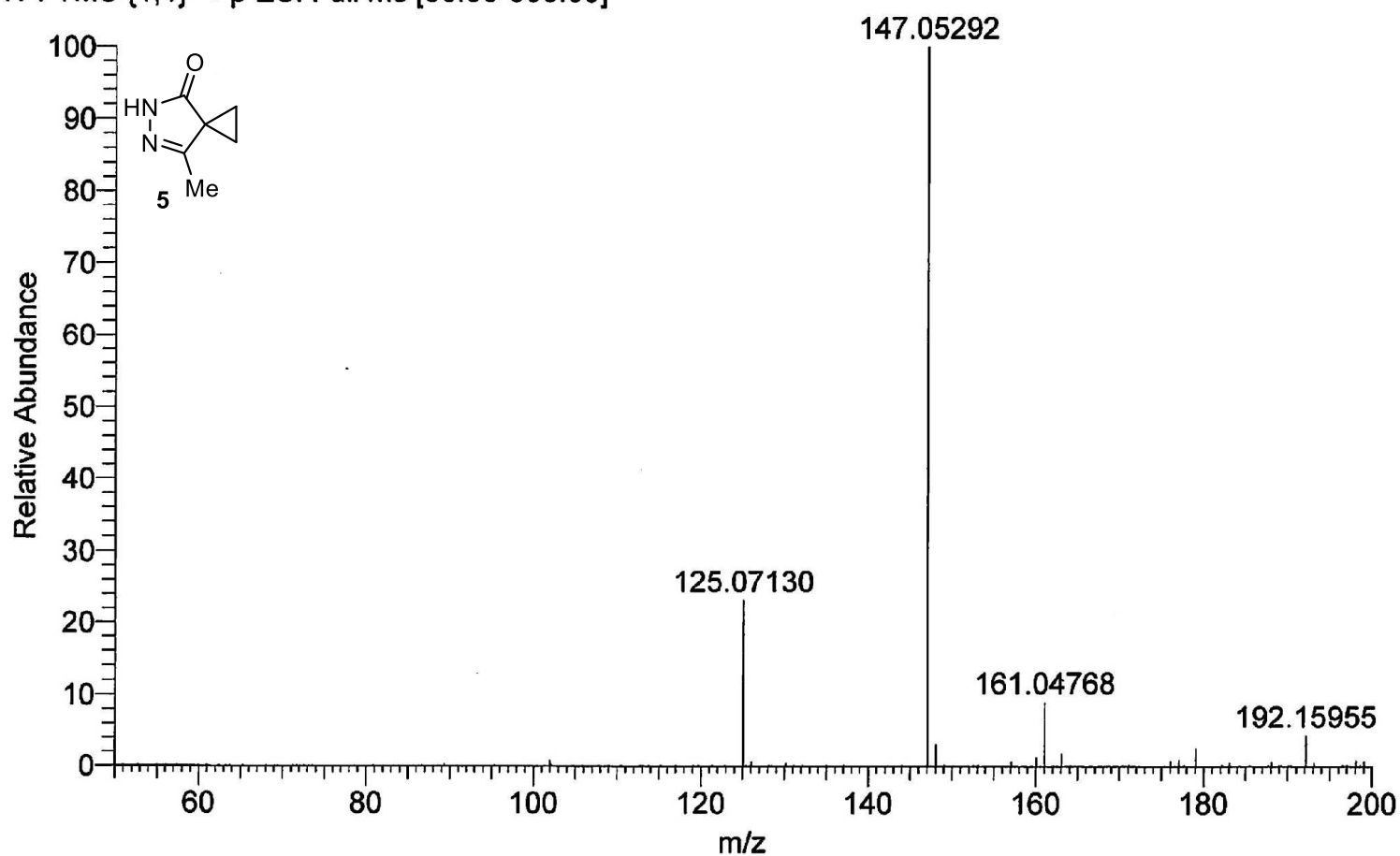
```
Filename      = 16ATA3-50-3-13C_Ca
Author       = delta
Experiment   = carbon_auto.jxp
Sample_Id    = 16ATA3-50-3-13C
Solvent      = DMSO-D6
Actual_Start_Time = 6-MAR-2022 20:59:
Revision_Time  = 7-MAR-2022 18:53:
```

```
Comment      = single pulse decou
Data_Format  = 1D COMPLEX
Dim_Size     = 26214
X_Domain    = Carbon13
Dim_Title    = Carbon13
Dim_Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ400S/L1
```

```
Field Strength = 9.389766[T] (400[M]
X_Acq_Duration = 1.03809024[s]
X_Domain       = Carbon13
X_Freq         = 100.52530333[MHz]
X_Offset       = 100[ppm]
X_Points       = 32768
X_Prescans     = 4
X_Resolution   = 0.96330739[Hz]
X_Sweep        = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain     = Proton
Irr_Freq       = 399.78219838[MHz]
Irr_Offset     = 5[ppm]
Blanking       = 5.0[us]
Clipped        = FALSE
Scans          = 1024
Total_Scans    = 1024
```

```
Relaxation_Delay = 2[s]
Recvr_Gain       = 50
Temp_Get         = 19.7[dC]
X_90_Width      = 10.5[us]
X_Acq_Time       = 1.03809024[s]
X_Angle         = 30[deg]
X_Atn           = 8.2[dB]
X_Pulse         = 3.5[us]
Irr_Atn_Dec     = 31.323[dB]
Irr_Atn_Dec_Calc = 31.323[dB]
Irr_Atn_Dec_Default_Calc = 31.323[dB]
Irr_Atn_No     = 31.323[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
```

YY16ATA3-93-2\_221107164145 #35-37 RT: 0.80-0.85 AV: 2 SB: 3 0.40-0.52 NL: 1.84E4  
T: FTMS {1,1} + p ESI Full ms [50.00-300.00]



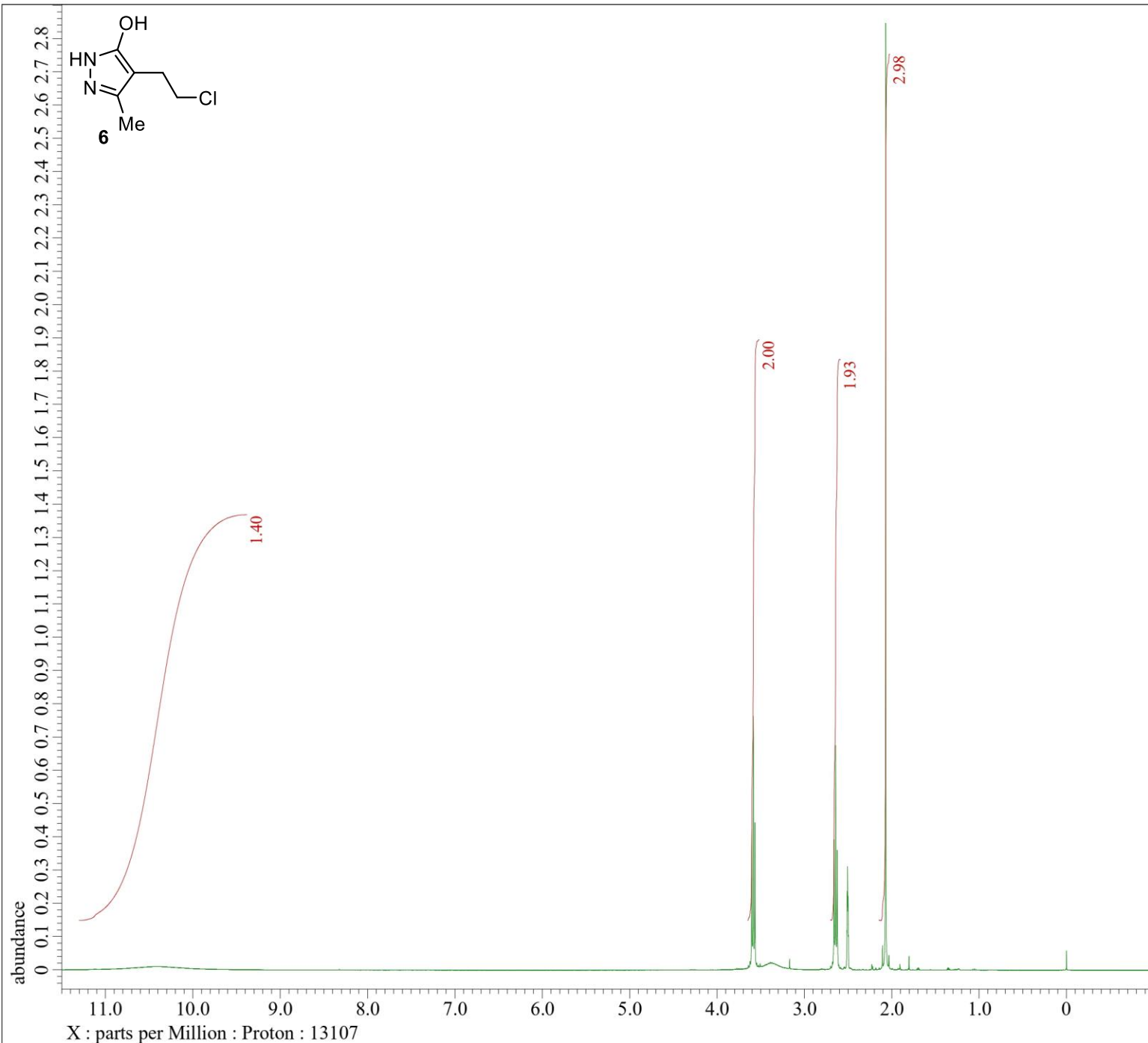
YY16ATA3-93-2\_221107164145#35-37 RT: 0.80-0.85 AV: 2

SB: 3 0.40-0.52

T: FTMS {1,1} + p ESI Full ms [50.00-300.00]

m/z= 122.50831-150.16611

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
125.07130	4260.8	22.88	125.07094	2.91	C <sub>6</sub> H <sub>9</sub> ON <sub>2</sub>
147.05292	18624.5	100.00	147.05288	0.25	C <sub>6</sub> H <sub>8</sub> ON <sub>2</sub> Na



```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
  
```

```

Filename      = 16ATA3-50-4_Proton-1-
Author        = delta
Experiment    = proton_auto.jxp
Sample_Id     = 16ATA3-50-4
Solvent       = DMSO-D6
Actual_Start_Time = 6-MAR-2022 19:39:32
Revision_Time  = 6-MAR-2022 20:23:37
  
```

```

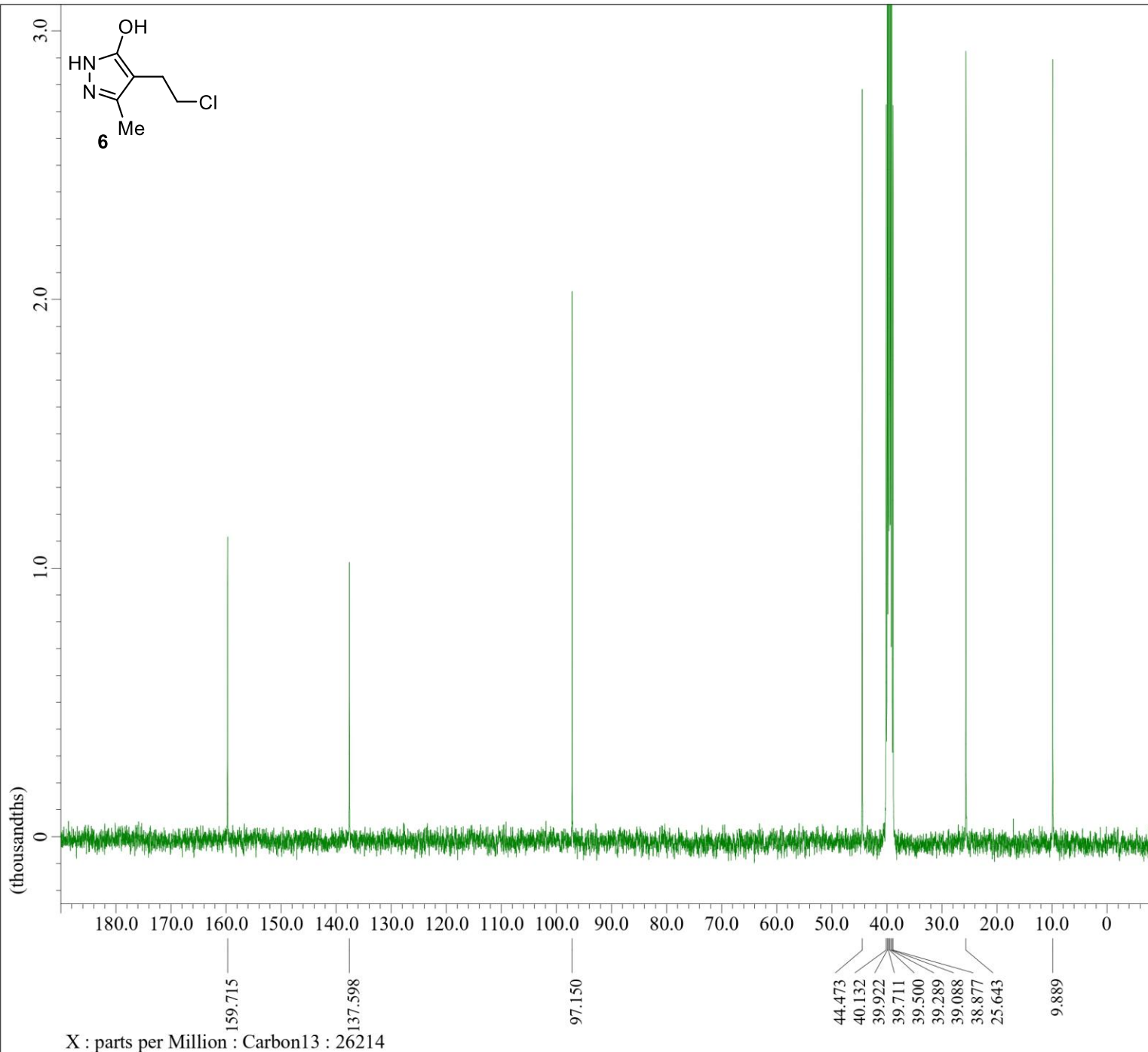
Comment       = single_pulse
Data_Format   = 1D COMPLEX
Dim_Size      = 13107
X_Domain      = Proton
Dim_Title     = Proton
Dim_Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ400S/L1
  
```

```

Field Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain       = Proton
X_Freq         = 399.78219838[MHz]
X_Offset       = 5 [ppm]
X_Points       = 16384
X_Prescans     = 1
X_Resolution   = 0.45739775 [Hz]
X_Sweep        = 7.4940048 [kHz]
X_Sweep_Clippped = 5.99520384 [kHz]
Irr_Domain     = Proton
Irr_Freq       = 399.78219838[MHz]
Irr_Offset     = 5 [ppm]
Tri_Domain     = Proton
Tri_Freq       = 399.78219838[MHz]
Tri_Offset     = 5 [ppm]
Blanking       = 2.0 [us]
Clipped        = FALSE
Scans          = 8
Total_Scans    = 8
  
```

```

Relaxation_Delay = 5 [s]
Recvr_Gain       = 46
Temp_Get         = 19.5 [dC]
X_90_Width       = 6.6 [us]
X_Acq_Time       = 2.18628096[s]
X_Angle          = 45 [deg]
X_Atn            = 6.5 [dB]
X_Pulse          = 3.3 [us]
Irr_Mode         = Off
Tri_Mode         = Off
  
```



```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -2, 0, 50[%] )
```

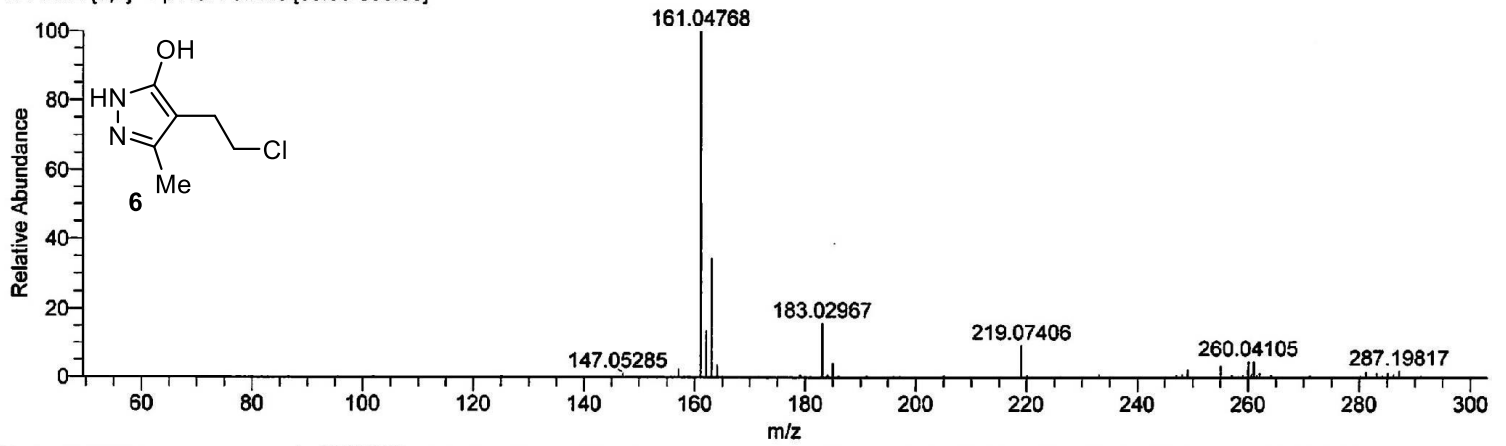
```
Filename      = 16ATA3-50-4-13C_Ca
Author       = delta
Experiment   = carbon_auto.jxp
Sample_Id    = 16ATA3-50-4-13C
Solvent      = DMSO-D6
Actual_Start_Time = 6-MAR-2022 21:55:
Revision_Time   = 7-MAR-2022 18:54:
```

```
Comment      = single pulse decou
Data_Format  = 1D COMPLEX
Dim_Size     = 26214
X_Domain    = Carbon13
Dim_Title    = Carbon13
Dim_Units   = [ppm]
Dimensions  = X
Spectrometer = JNM-ECZ400S/L1
```

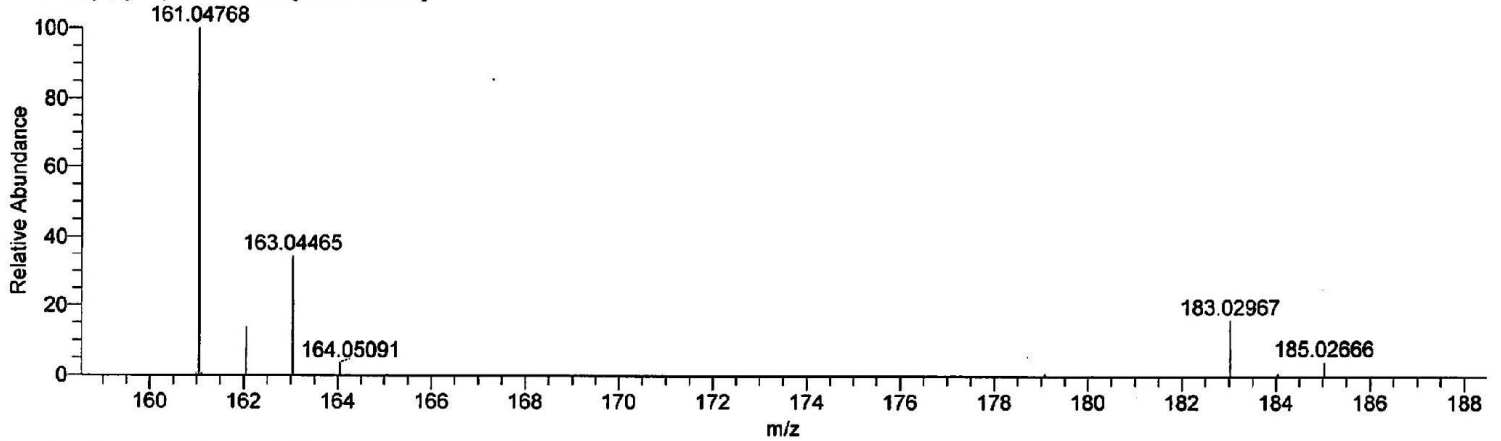
```
Field Strength = 9.389766[T] (400[M]
X_Acq_Duration = 1.03809024[s]
X_Domain       = Carbon13
X_Freq         = 100.52530333[MHz]
X_Offset       = 100[ppm]
X_Points       = 32768
X_Prescans     = 4
X_Resolution   = 0.96330739[Hz]
X_Sweep        = 31.56565657[kHz]
X_Sweep_Clip   = 25.25252525[kHz]
Irr_Domain     = Proton
Irr_Freq       = 399.78219838[MHz]
Irr_Offset     = 5[ppm]
Blanking       = 5.0[us]
Clipped        = FALSE
Scans          = 1024
Total_Scans    = 1024
```

```
Relaxation_Delay = 2[s]
Recvr_Gain       = 50
Temp_Get         = 19.8[dC]
X_90_Width      = 10.5[us]
X_Acq_Time      = 1.03809024[s]
X_Angle         = 30[deg]
X_Atn           = 8.2[dB]
X_Pulse         = 3.5[us]
Irr_Atn_Dec     = 31.323[dB]
Irr_Atn_Dec_Calc = 31.323[dB]
Irr_Atn_Dec_Default_Calc = 31.323[dB]
Irr_Atn_No     = 31.323[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
```

YY16ATA3-93-3-2#35-37 RT: 0.78-0.83 AV: 2 SB: 3 0.41-0.52 NL: 6.72E4  
T: FTMS {1,1} + p ESI Full ms [50.00-300.00]



YY16ATA3-93-3-2#35-37 RT: 0.78-0.83 AV: 2 SB: 3 0.41-0.52 NL: 6.72E4  
T: FTMS {1,1} + p ESI Full ms [50.00-300.00]



YY16ATA3-93-3-2#35-37 RT: 0.78-0.83 AV: 2  
SB: 3 0.41-0.52  
T: FTMS {1,1} + p ESI Full ms [50.00-300.00]  
m/z= 158.54604-188.46439

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
161.04768	68974.2	100.00	161.04762	0.38	C <sub>6</sub> H <sub>10</sub> ON <sub>2</sub> Cl
163.04465	23587.0	34.20	163.04467	-0.08	C <sub>6</sub> H <sub>10</sub> ON <sub>2</sub> <sup>37</sup> Cl

YY16ATA3-93-3-2#35-37 RT: 0.78-0.83 AV: 2  
SB: 3 0.41-0.52  
T: FTMS {1,1} + p ESI Full ms [50.00-300.00]  
m/z= 182.62485-185.30855

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
183.02967	10720.1	100.00	183.02956	0.60	C <sub>6</sub> H <sub>9</sub> ON <sub>2</sub> Cl Na
185.02666	2779.6	25.93	185.02661	0.25	C <sub>6</sub> H <sub>9</sub> ON <sub>2</sub> <sup>37</sup> Cl Na