

**Supporting Information for:**

**Synergistic Contribution of Tiglate and Cinnamate to**

**Cytotoxicity of Ipomoeassin F**

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## Table of Contents

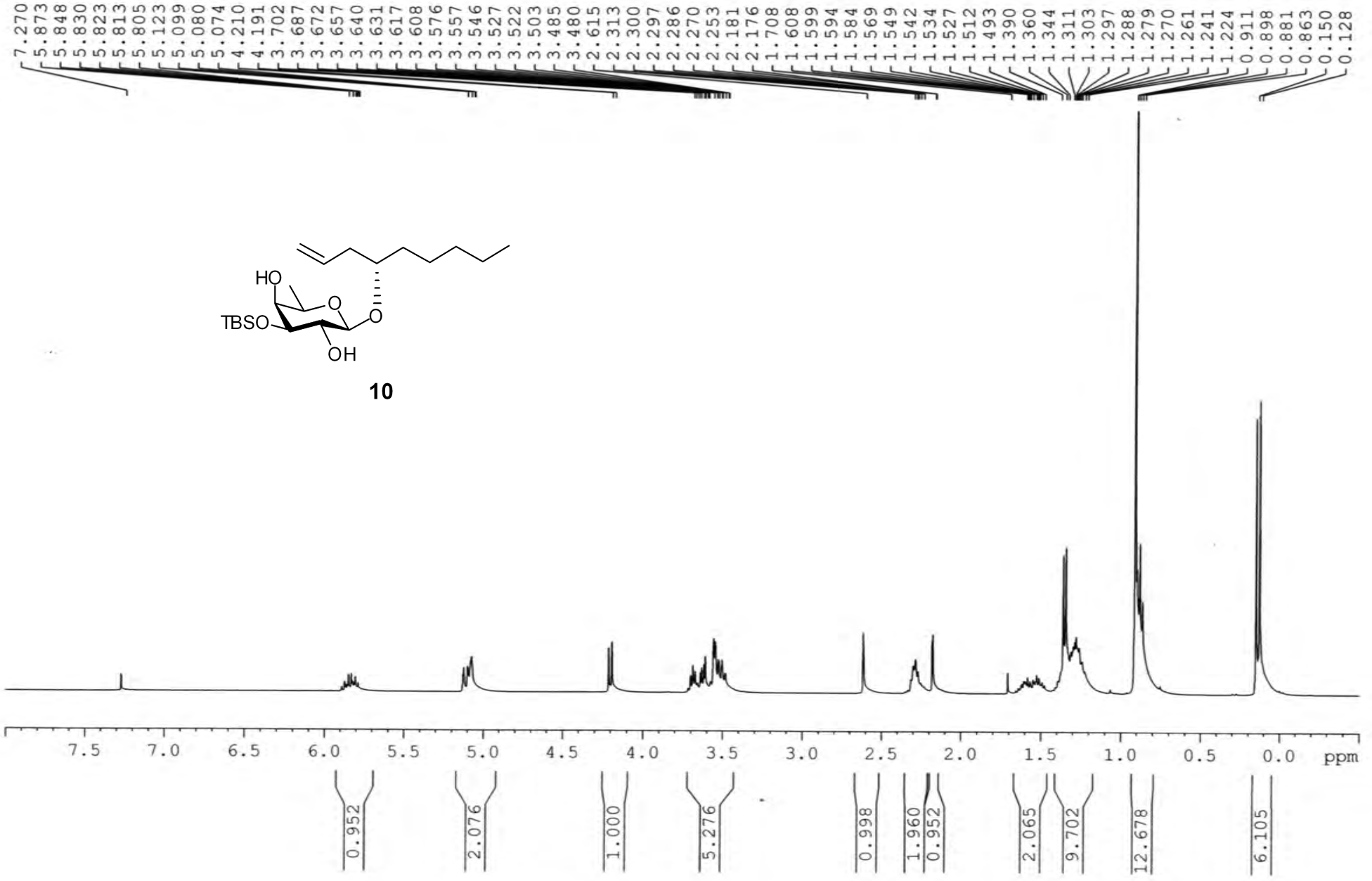
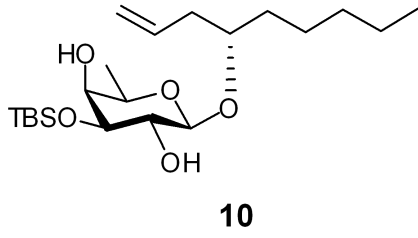
1	<sup>1</sup> H NMR spectrum of compound <b>10</b>	S4
2	<sup>13</sup> C NMR spectrum of compound <b>10</b>	S5
3	COSY NMR spectrum of compound <b>10</b>	S6
4	<sup>1</sup> H NMR spectrum of compound <b>7</b>	S7
5	<sup>13</sup> C NMR spectrum of compound <b>7</b>	S8
6	COSY NMR spectrum of compound <b>7</b>	S9
7	HSQC NMR spectrum of compound <b>7</b>	S10
8	<sup>1</sup> H NMR spectrum of compound <b>14</b>	S11
9	<sup>13</sup> C NMR spectrum of compound <b>14</b>	S12
10	<sup>1</sup> H NMR spectrum of compound <b>15</b>	S13
11	<sup>13</sup> C NMR spectrum of compound <b>15</b>	S14
12	<sup>1</sup> H NMR spectrum of compound <b>8</b>	S15
13	<sup>13</sup> C NMR spectrum of compound <b>8</b>	S16
14	<sup>1</sup> H NMR spectrum of compound <b>6</b>	S17
15	<sup>13</sup> C NMR spectrum of compound <b>6</b>	S18
16	COSY NMR spectrum of compound <b>6</b>	S19
17	HSQC NMR spectrum of compound <b>6</b>	S20
18	HMBC NMR spectrum of compound <b>6</b>	S21-22
19	<sup>1</sup> H NMR spectrum of compound <b>16</b>	S23
20	<sup>13</sup> C NMR spectrum of compound <b>16</b>	S24
21	COSY NMR spectrum of compound <b>16</b>	S25
22	HSQC NMR spectrum of compound <b>16</b>	S26
23	<sup>1</sup> H NMR spectrum of compound <b>17</b>	S27
24	<sup>13</sup> C NMR spectrum of compound <b>17</b>	S28
25	COSY NMR spectrum of compound <b>17</b>	S29

26	HSQC NMR spectrum of compound <b>17</b>	S30
27	<sup>1</sup> H NMR spectrum of compound <b>19</b>	S31
28	<sup>13</sup> C NMR spectrum of compound <b>19</b>	S32
29	COSY NMR spectrum of compound <b>19</b>	S33
30	HSQC NMR spectrum of compound <b>19</b>	S34
31	HMBC NMR spectrum of compound <b>19</b>	S35-36
32	<sup>1</sup> H NMR spectrum of compound <b>4</b>	S37
33	<sup>13</sup> C NMR spectrum of compound <b>4</b>	S38
34	COSY NMR spectrum of compound <b>4</b>	S39
35	HSQC NMR spectrum of compound <b>4</b>	S40
36	<sup>1</sup> H NMR spectrum of compound <b>20</b>	S41
37	<sup>13</sup> C NMR spectrum of compound <b>20</b>	S42
38	COSY NMR spectrum of compound <b>20</b>	S43
39	HSQC NMR spectrum of compound <b>20</b>	S44
40	<sup>1</sup> H NMR spectrum of compound <b>5</b>	S45
41	<sup>13</sup> C NMR spectrum of compound <b>5</b>	S46
42	COSY NMR spectrum of compound <b>5</b>	S47
43	HSQC NMR spectrum of compound <b>5</b>	S48
44	<sup>1</sup> H NMR spectrum of compound <b>5'</b>	S49
45	<sup>13</sup> C NMR spectrum of compound <b>5'</b>	S50
46	COSY NMR spectrum of compound <b>5'</b>	S51
47	HSQC NMR spectrum of compound <b>5'</b>	S52
48	<sup>1</sup> H NMR spectrum of compound <b>21_Method 1</b>	S53
49	<sup>13</sup> C NMR spectrum of compound <b>21_Method 1</b>	S54
50	COSY NMR spectrum of compound <b>21_Method 1</b>	S55

51	HSQC NMR spectrum of compound <b>21</b> _Method 1	S56
52	HMBC NMR spectrum of compound <b>21</b> _Method 1	S57-59
53	<sup>1</sup> H NMR spectrum of compound <b>21</b> _Method 2	S60
54	<sup>13</sup> C NMR spectrum of compound <b>21</b> _Method 2	S61
55	COSY NMR spectrum of compound <b>21</b> _Method 2	S62
56	HSQC NMR spectrum of compound <b>21</b> _Method 2	S63
57	<sup>1</sup> H NMR spectrum of compound <b>Ipomoeassin F</b>	S64
58	<sup>13</sup> C NMR spectrum of compound <b>Ipomoeassin F</b>	S65
59	COSY NMR spectrum of compound <b>Ipomoeassin F</b>	S66
60	HSQC NMR spectrum of compound <b>Ipomoeassin F</b>	S67
61	<sup>1</sup> H NMR spectrum of compound <b>2</b>	S68
62	<sup>13</sup> C NMR spectrum of compound <b>2</b>	S69

63	COSY NMR spectrum of compound <b>2</b>	S70
64	HSQC NMR spectrum of compound <b>2</b>	S71
65	HMBC NMR spectrum of compound <b>2</b>	S72-73
66	HRMS spectrum of compound <b>2</b>	S74
67	<sup>1</sup> H NMR spectrum of compound <b>3</b>	S75
68	<sup>13</sup> C NMR spectrum of compound <b>3</b>	S76
69	COSY NMR spectrum of compound <b>3</b>	S77
70	HSQC NMR spectrum of compound <b>3</b>	S78
71	HMBC NMR spectrum of compound <b>3</b>	S79-80
72	HRMS spectrum of compound <b>3</b>	S81
73	IC <sub>50</sub> curves of ipomoeassin F and analogues <b>1-3</b> against the MCF7 cell line and MDA-MB-231 cell line	S82
74	NCI-60 cell line screen of ipomoeassin F	S83-86

ZGH-*Ipom*-3-22-150910-1H in CDCl<sub>3</sub>

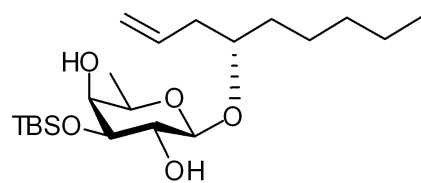
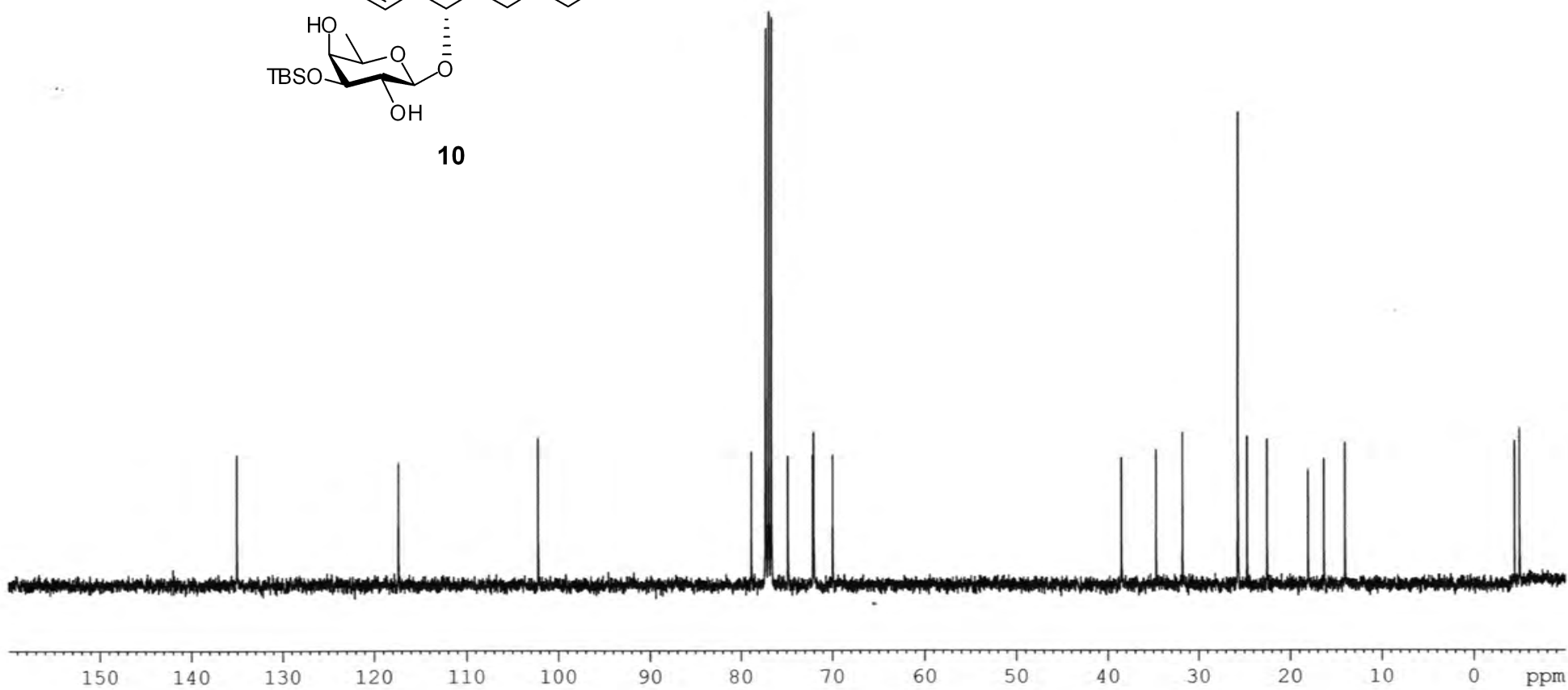


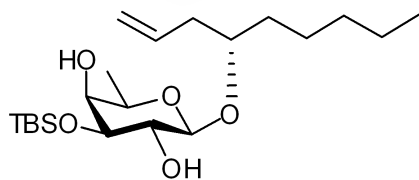
ZGH-*Ipom*-3-22-150910-A 13C in CDCl<sub>3</sub>

— 135.051

— 117.360

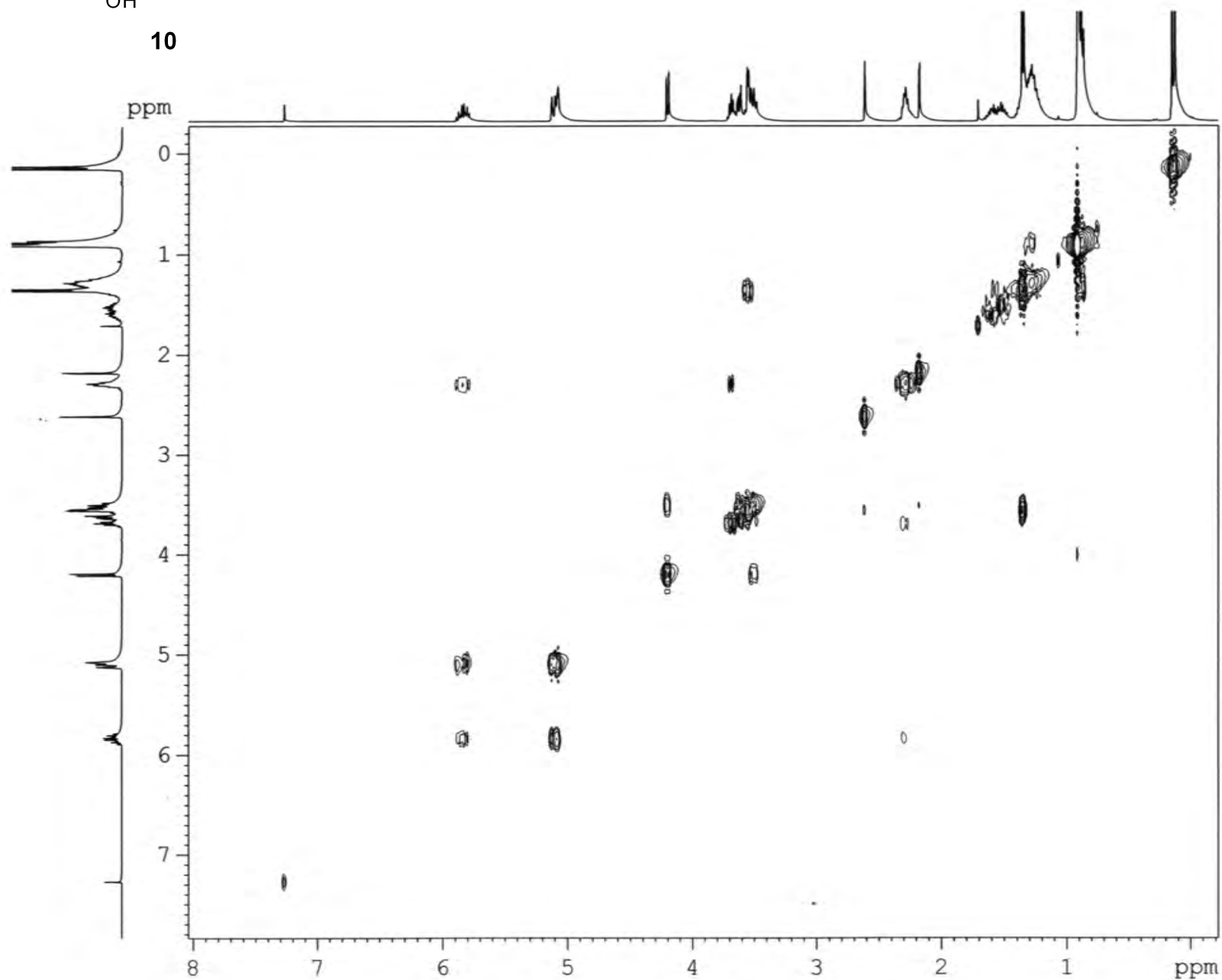
— 102.230

78.859  
77.317  
76.681  
74.854  
72.133  
72.053  
69.984— 38.523  
— 34.706  
— 31.78725.729  
24.712  
22.542  
18.084  
16.353  
14.062— 4.440  
— 4.991**10**



10

## ZGH-Ipom-3-22-150910-A COSY

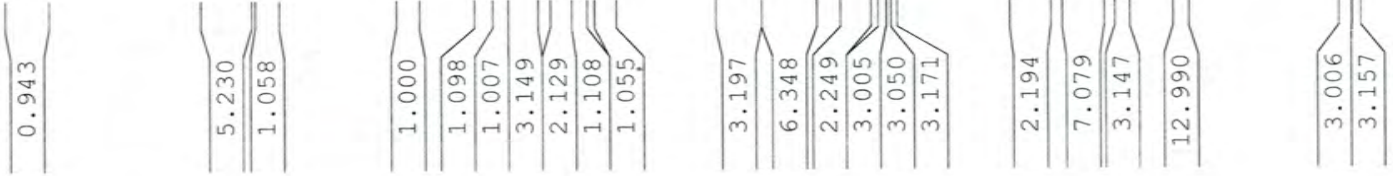
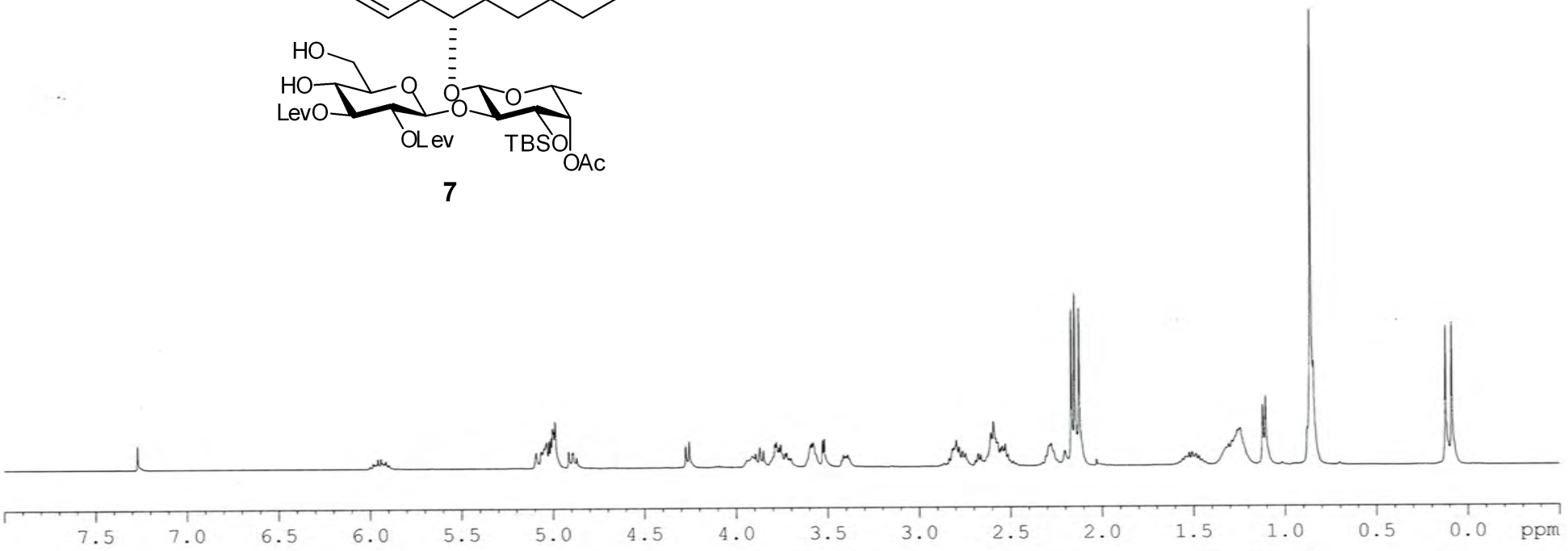
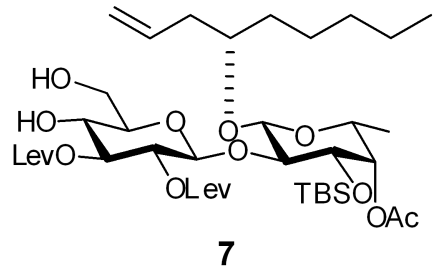


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 PULPROG cosygpgf  
 TD 2048  
 SOLVENT CDCl3  
 NS 4  
 DS 8  
 SWH 5341.880 Hz  
 FIDRES 2.608340 Hz  
 AQ 0.1917428 sec  
 RG 71.8  
 DW 93.600 usec  
 DE 6.50 usec  
 TE 292.6 K  
 DO 0.00000300 sec  
 D1 1.48689198 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 IN0 0.00018720 sec

===== CHANNEL f1 =====  
 NUC1  $^1\text{H}$   
 P0 10.00 usec  
 P1 10.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1324057 MHz

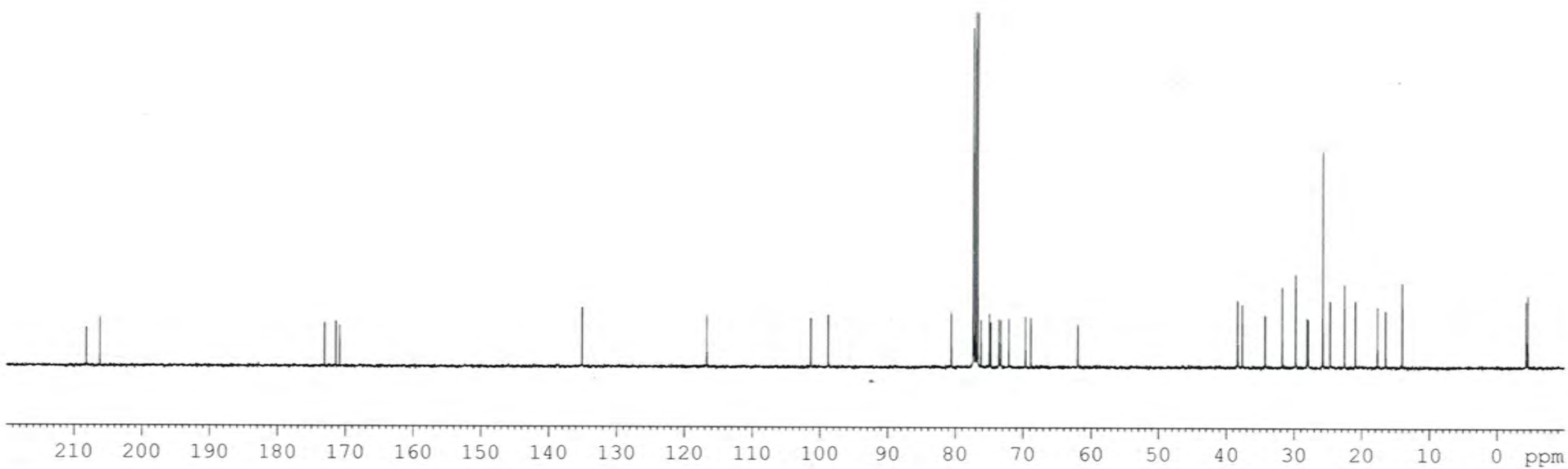
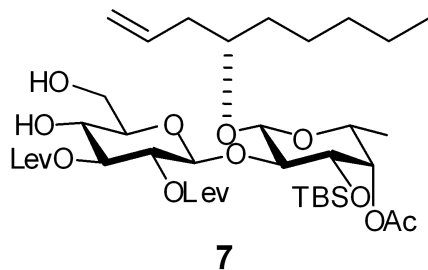
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 FIDRES 70.287903 Hz  
 SW 13.350 ppm  
 PhMODE QF  
 SI 1024  
 SF 400.1300040 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00  
 SI 1024  
 MC2 QF  
 SF 400.1300033 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

ZGH-*Ipom*-2-67-A-140629 1H in CDCl3

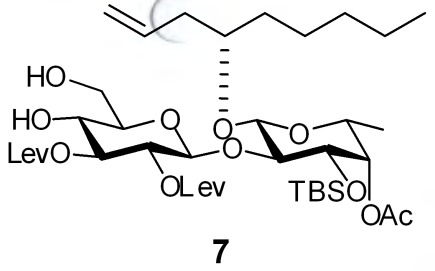


ZGH-Ipom-2-67-A-140629  $^{13}\text{C}$  in  $\text{CDCl}_3$ 

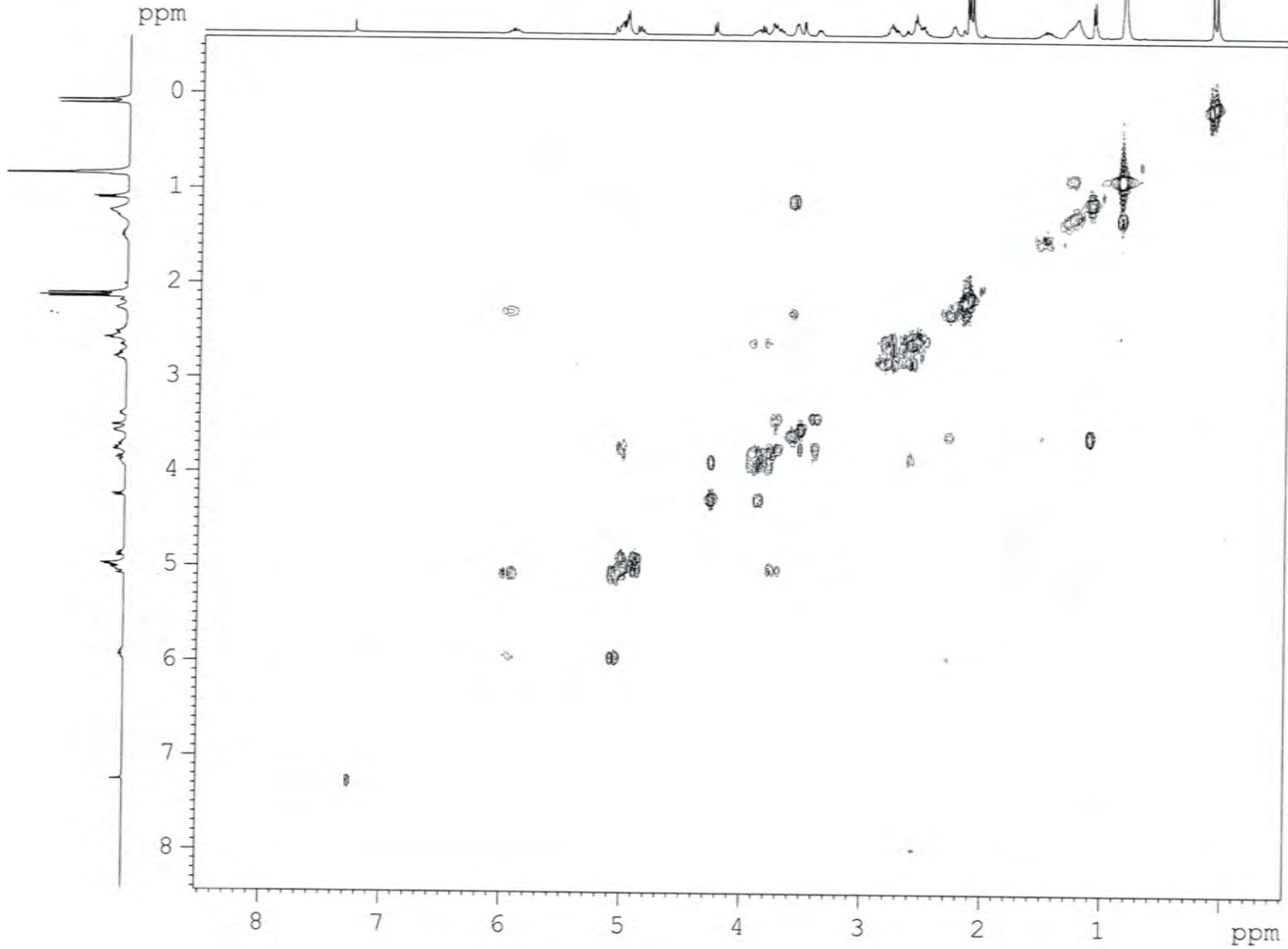
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 77.326  
 77.209  
 77.008  
 76.690  
 76.172  
 74.942  
 74.752  
 73.545  
 73.269  
 72.082  
 69.601  
 68.813  
 61.936  
 38.316  
 38.287  
 37.621  
 34.250  
 31.719  
 29.741  
 28.037  
 27.863  
 25.731  
 24.653  
 22.541  
 20.939  
 17.653  
 16.461  
 14.002  
 -4.358  
 -4.611







ZGH-Ipom-2-67-A-140629 COSY



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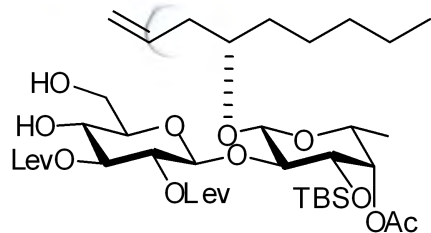
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PULPROG   cosygpgf
TD         2048
SOLVENT   CDC13
NS         4
DS         8
SWH        5341.880 Hz
FIDRES     2.608340 Hz
AQ         0.1917428 sec
RG         50.8
DW         93.600 usec
DE         6.50 usec
TE         292.2 K
D0         0.00000300 sec
D1         1.48689198 sec
D13        0.00000400 sec
D16        0.00020000 sec
INO        0.00018720 sec
    
```

```

===== CHANNEL f1 =====
NUC1      1H
P0         10.00 usec
P1         10.00 usec
PL1        -3.50 dB
PL1W       31.17620277 W
SF01       400.1324057 MHz
    
```

```

===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPZ1       10.00 %
P16        1000.00 usec
ND0        1
TD         128
SF01       400.1324 MHz
FIDRES     41.733440 Hz
SW         13.350 ppm
FnMODE     QF
SI         1024
SF         400.1300040 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
SI         1024
MC2        QF
SF         400.1300033 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
    
```



7

ZGH-*Ipom*-2-67-A-140629 HSQC

```

NAME      ZGH-Ipom-2-67-A-140629
EXPNO     4
PROCNO    1
Date_     20140630
Time      20.15
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   hsqcetgps1
TD         1024
SOLVENT   CDC13
NS         4
DS         16
SWH        5341.880 Hz
FIDRES     5.216680 Hz
AQ         0.0958964 sec
RG         2050
DW         93.600 usec
DE         6.50 usec
TE         293.0 K
CNST2     145.0000000
D0         0.00000300 sec
D1         1.50000000 sec
D4         0.00172414 sec
D11        0.03000000 sec
D13        0.00000400 sec
D16        0.00020000 sec
D24        0.00110000 sec
INO        0.00003000 sec
ZGPTNS

```

```

===== CHANNEL f1 =====
NUC1      1H
P1        10.00 usec
P2        20.00 usec
P28       1000.00 usec
PL1       -3.50 dB
PL1W      31.17620277 W
SFO1      400.1324057 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2   garp
NUC2      13C
P3        10.00 usec
P4        20.00 usec
PCPD2     75.00 usec
PL2       -2.10 dB
PL12      15.40 dB
PL2W      58.37759399 W
PL12W     1.03811681 W
SFO2      100.6202727 MHz

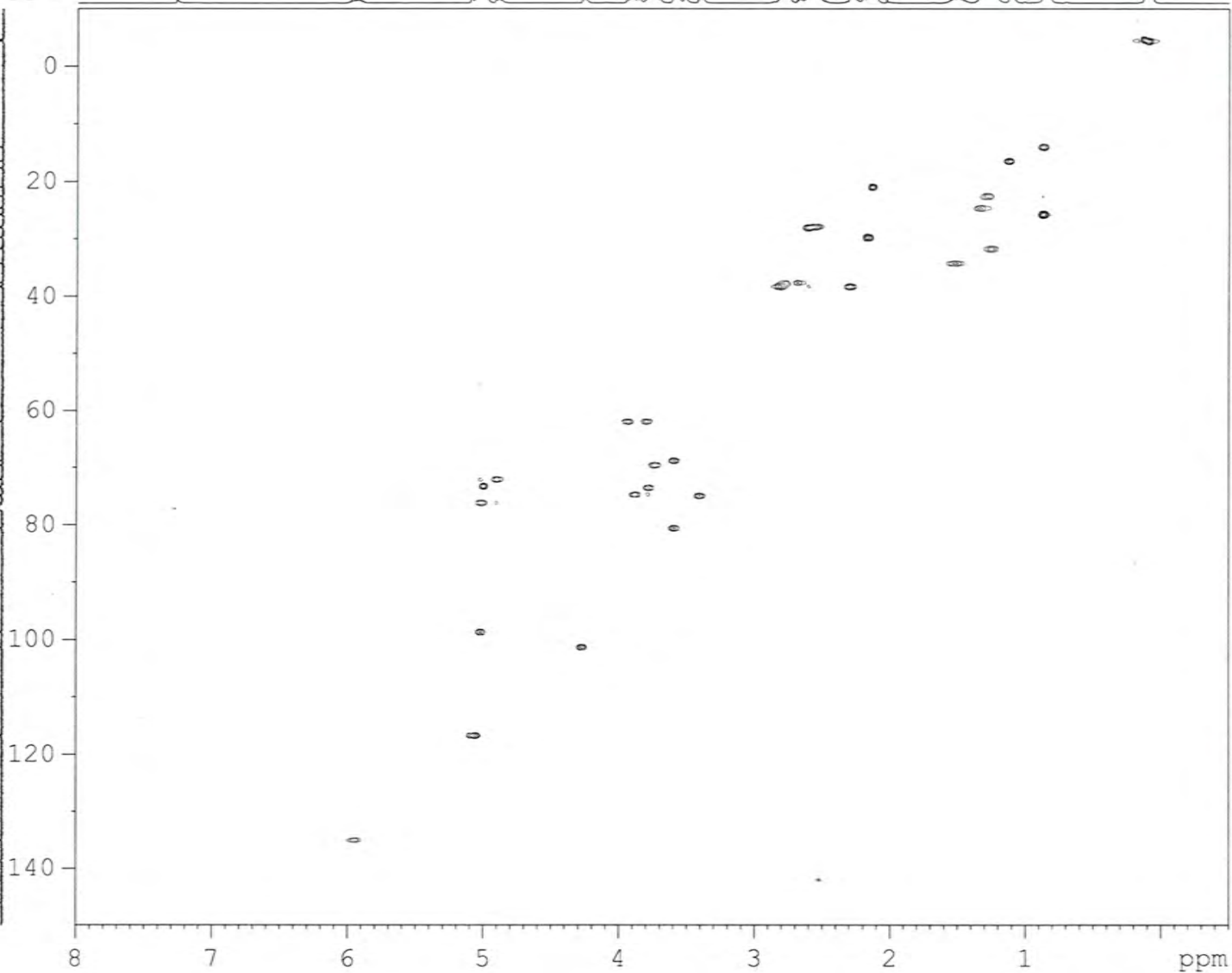
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===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    .SINE.100
GPZ1      80.00
GPZ2      20.10
P16       1000.00 usec
ND0       2
TD         256
SFO1      100.6203 MHz
FIDRES     65.104164 Hz
SW         165.639 ppm
FrMODE    Echo-Antiecho
SI         1024
SF         400.1300000 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.00
SI         1024
MC2       echo-antiecho
SF         100.6127690 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0

```

ppm



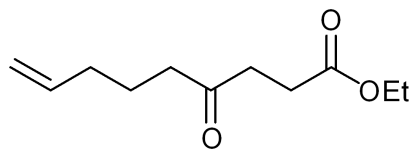
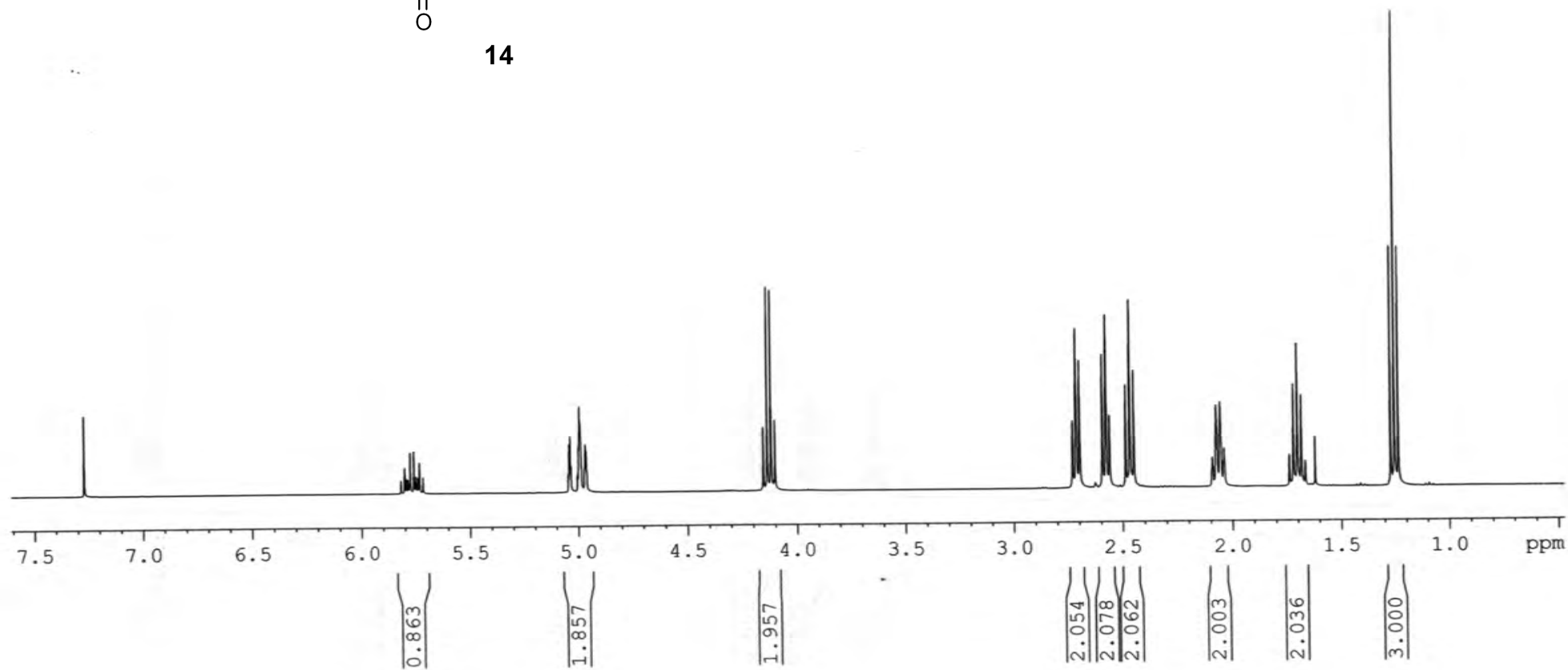
ppm

ZGH-*Ipom*-2-121-A-150310 1H in CDCl<sub>3</sub>

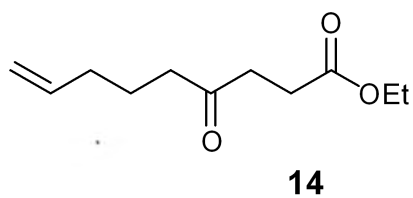
— 7.270

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5.785  
5.776  
5.759  
5.750  
5.742  
5.733  
5.716  
5.046  
5.042  
5.038  
5.034  
5.003  
4.999  
4.994  
4.991  
4.986  
4.971  
4.968  
4.965  
4.963  
4.960  
4.156  
4.138  
4.120  
4.102

2.730  
2.715  
2.698  
2.593  
2.576  
2.561  
2.486  
2.467  
2.449  
2.095  
2.092  
2.089  
2.074  
2.056  
2.042  
2.038  
2.035  
1.739  
1.720  
1.702  
1.684  
1.665  
1.621  
1.272  
1.255  
1.237

**14**

ZGH-Ipom-2-121-A-150310 13C in CDCl3



— 208.857

— 172.804

— 137.908

— 115.233

77.317  
77.201  
76.999  
76.681

— 60.584

— 41.852

— 37.088

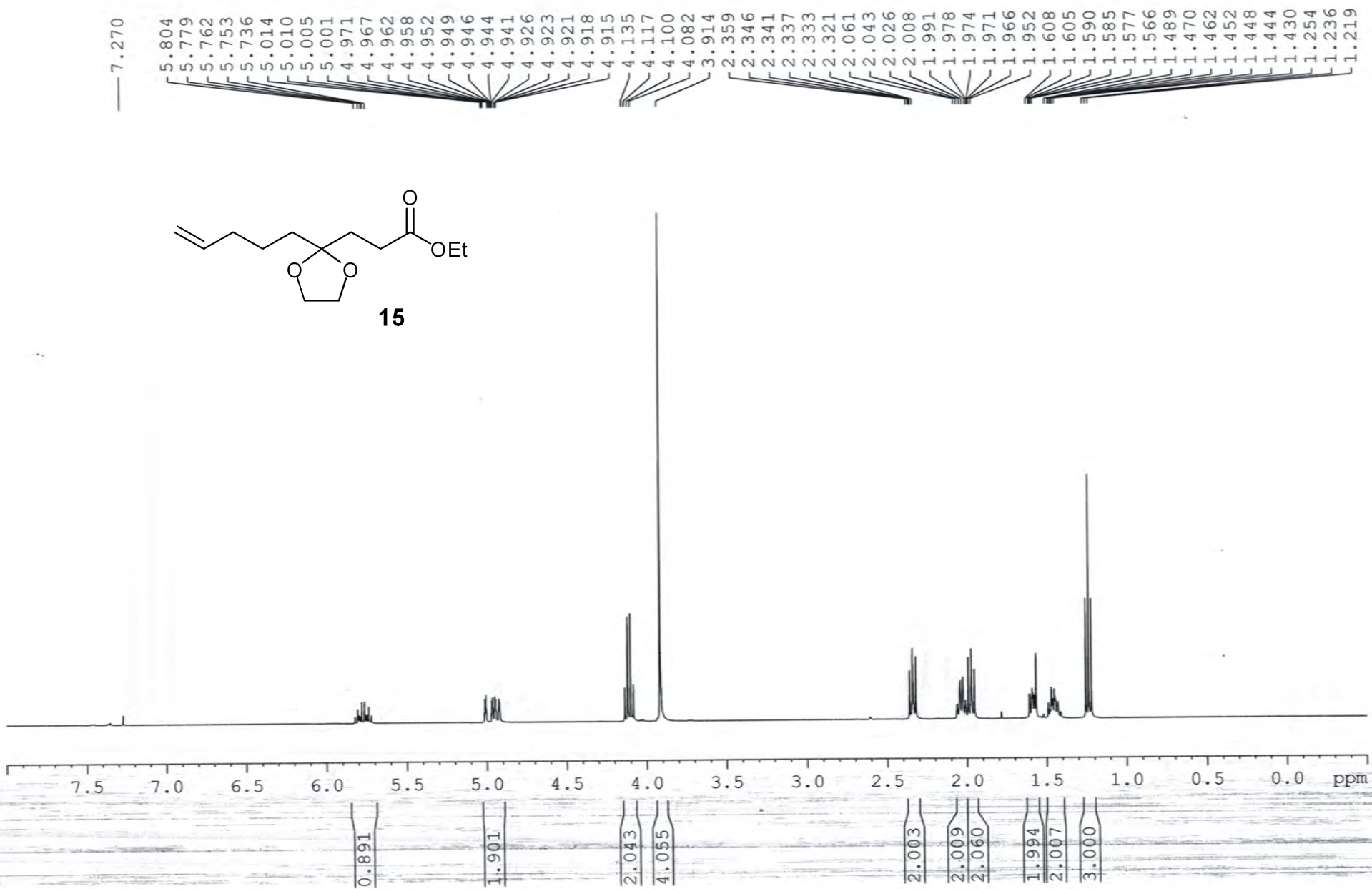
— 33.017

— 27.959

— 22.720

— 14.149

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

ZGH-*Ipom*-2-131-A-150331 1H in CDCl<sub>3</sub>

ZGH-Ipom-2-131-A-150331 13C in CDCl3

— 173.538

— 138.436

— 114.650

— 110.744

77.319  
77.001  
76.683

— 64.981

— 60.229

— 36.721

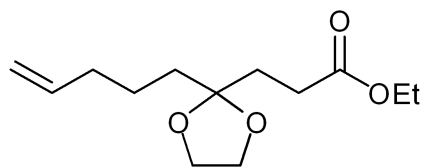
— 33.734

— 32.004

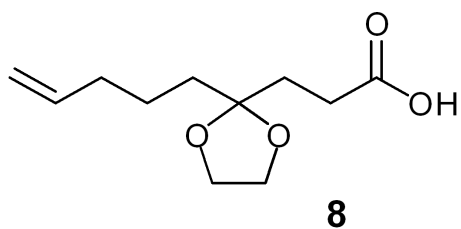
— 28.873

— 22.963

— 14.155

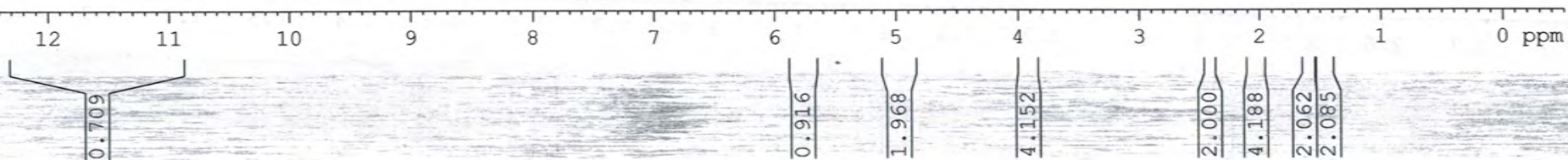
**15**

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

ZGH-*Ipom*-2-132-A-150406 1H in CDCL<sub>3</sub>

— 11.592

7.273  
7.271  
5.835  
5.818  
5.809  
5.801  
5.792  
5.775  
5.766  
5.759  
5.750  
5.733  
5.027  
5.023  
4.984  
4.981  
4.969  
4.967  
4.964  
4.944  
4.941  
4.939  
3.945  
2.431  
2.412  
2.393  
2.078  
2.060  
2.043  
2.025  
2.006  
1.988  
1.629  
1.612  
1.608  
1.598  
1.588  
1.503  
1.484  
1.475  
1.466  
1.444



ZGH-*Ipom*-2-132-A-150406  $^{13}\text{C}$  in  $\text{CDCl}_3$ 

— 179.791

— 138.413

— 114.760

— 110.708

77.316

76.999

76.681

— 65.054

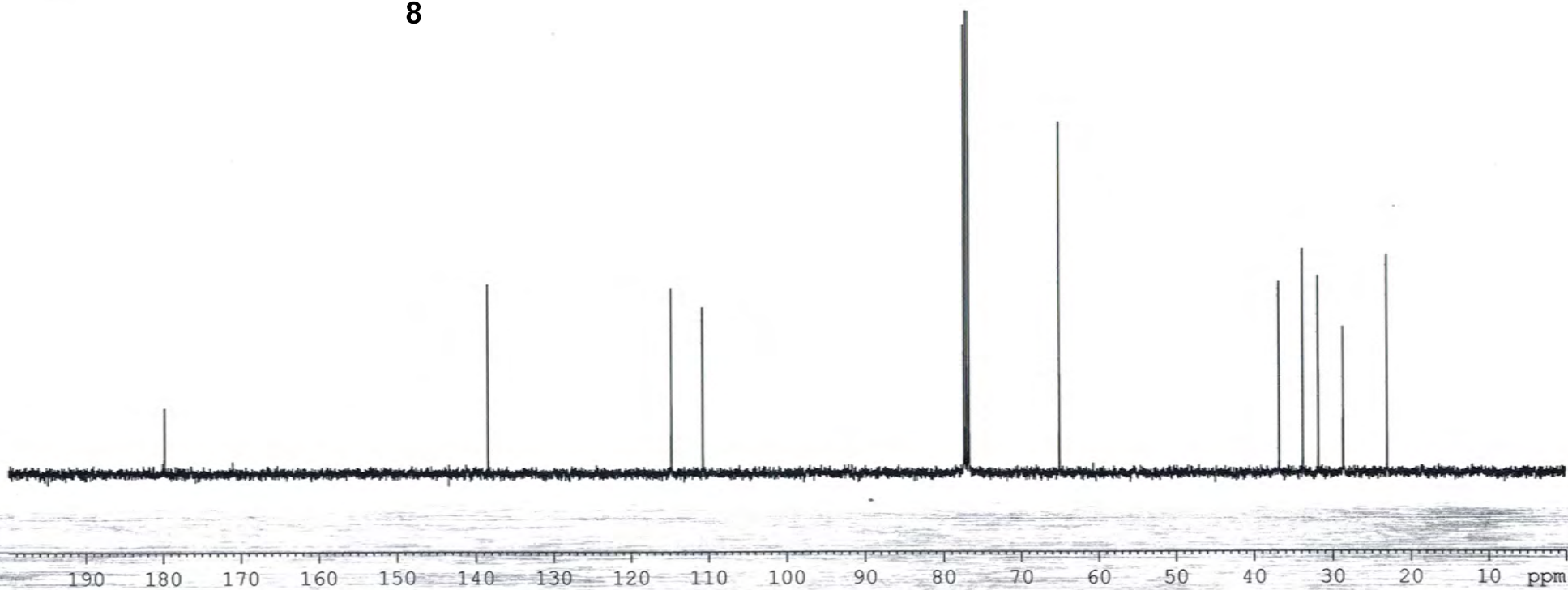
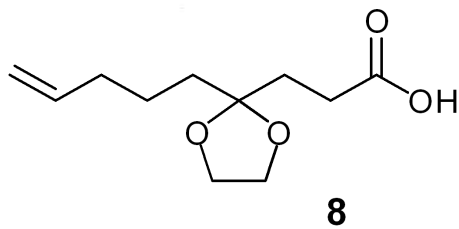
— 36.766

— 33.734

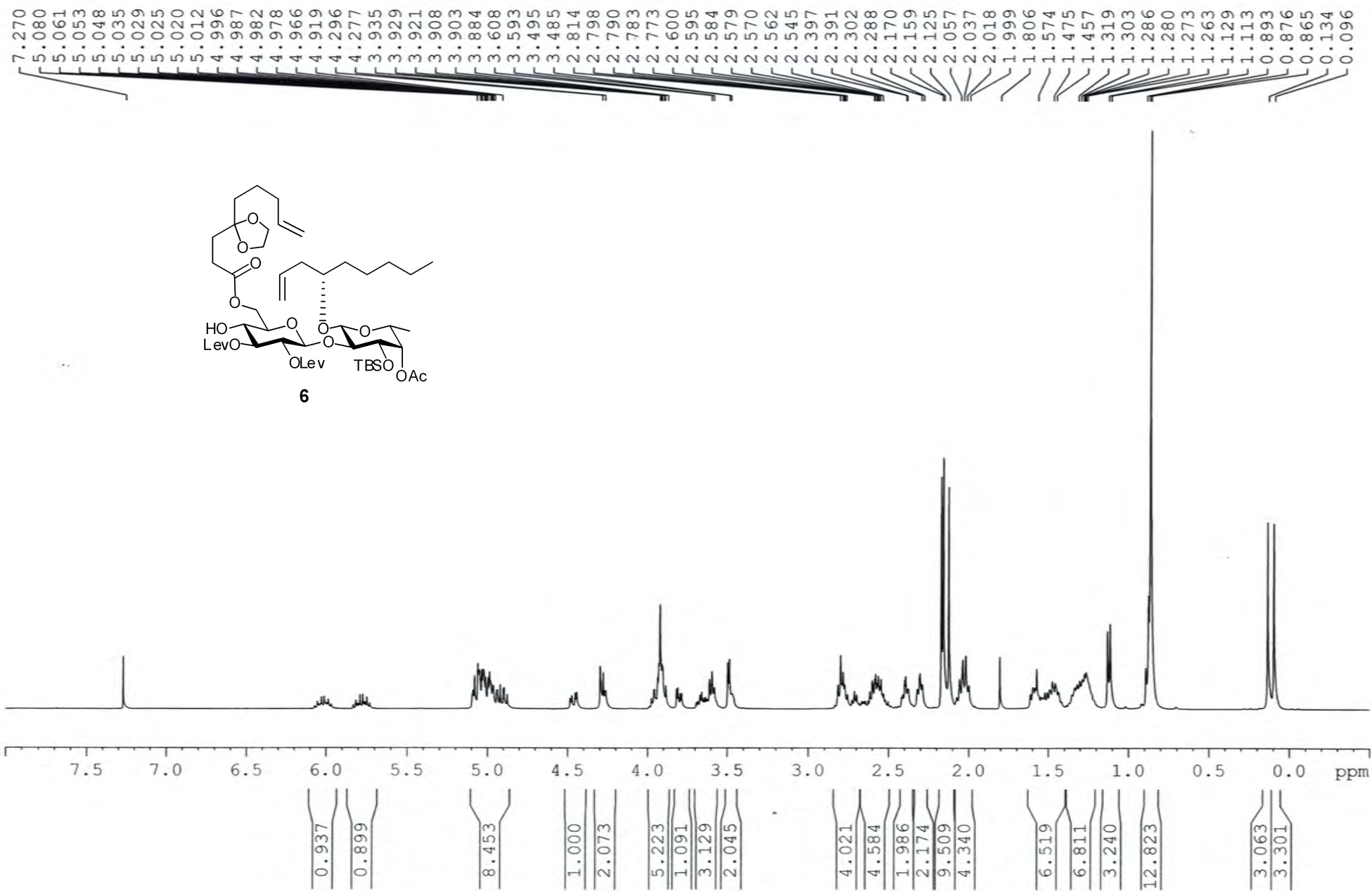
— 31.769

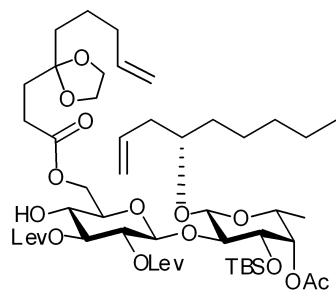
— 28.645

— 23.014



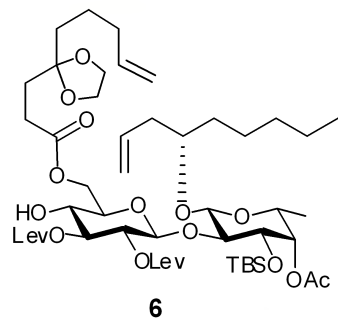


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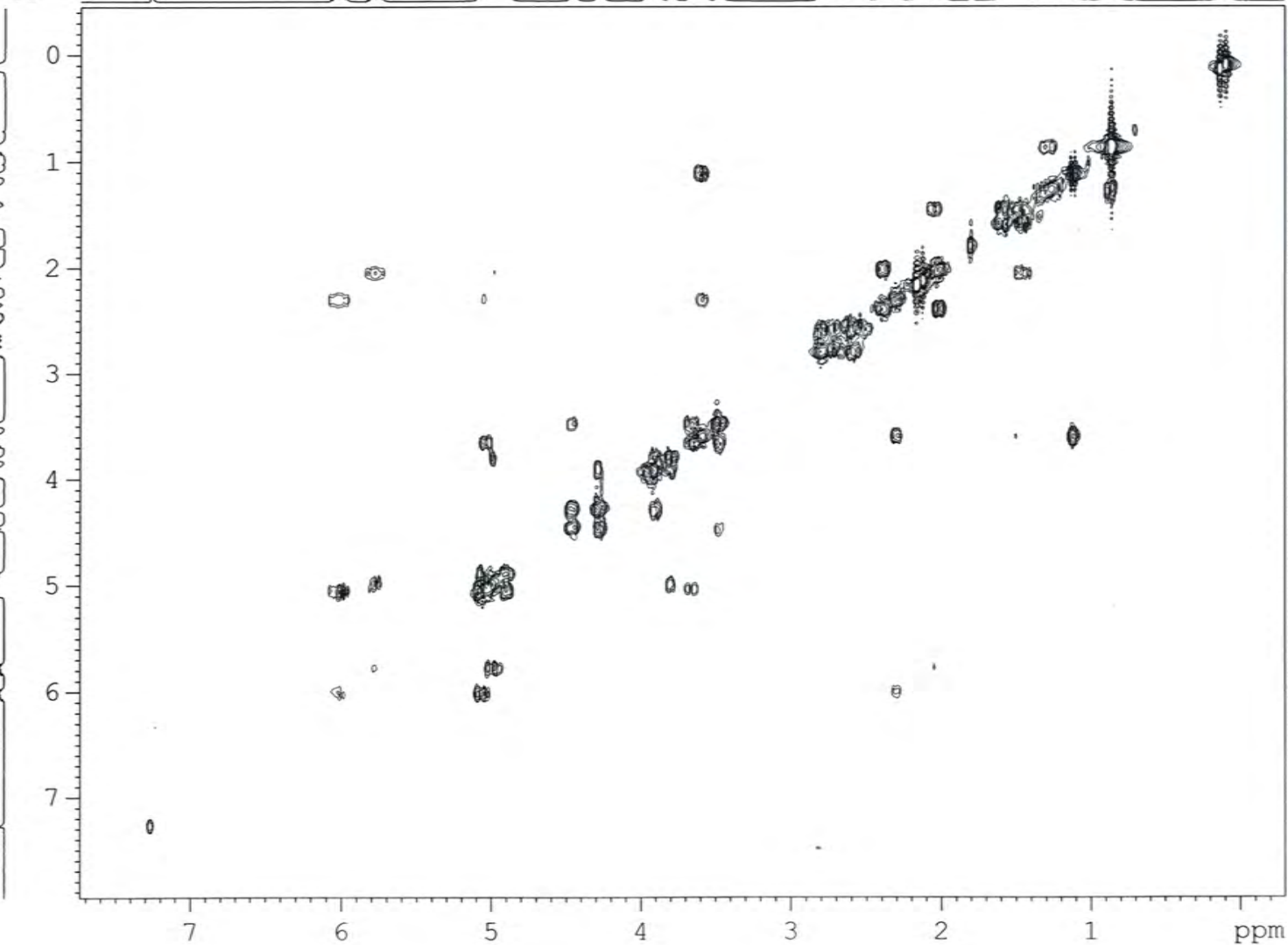
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77.19976.679  
75.388  
74.996  
73.932  
73.552  
73.46972.363  
68.831  
68.723  
65.143  
65.057  
62.89738.481  
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37.696  
36.862  
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31.814  
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28.677  
27.978  
27.84825.819  
24.583  
22.955  
22.575  
20.895  
17.73216.501  
14.027  
-4.455  
-4.492

6

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ZGH-*Ipom*-2-154-A-150407 COSY

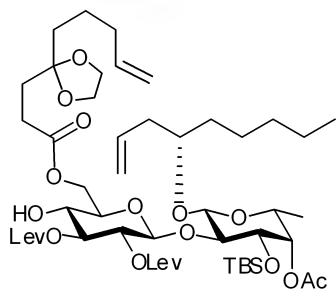
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 TD 2048  
 SOLVENT CDCl3  
 NS 8  
 DS 8  
 SWH 5341.880 Hz  
 FIDRES 2.608340 Hz  
 AQ 0.1917428 sec  
 RG 80.6  
 DW 93.600 usec  
 DE 6.50 usec  
 TE 292.8 K  
 D0 0.0000300 sec  
 D1 1.48689198 sec  
 D13 0.0000400 sec  
 D16 0.00020000 sec  
 IN0 0.00018720 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P0 10.00 usec  
 P1 10.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1324057 MHz

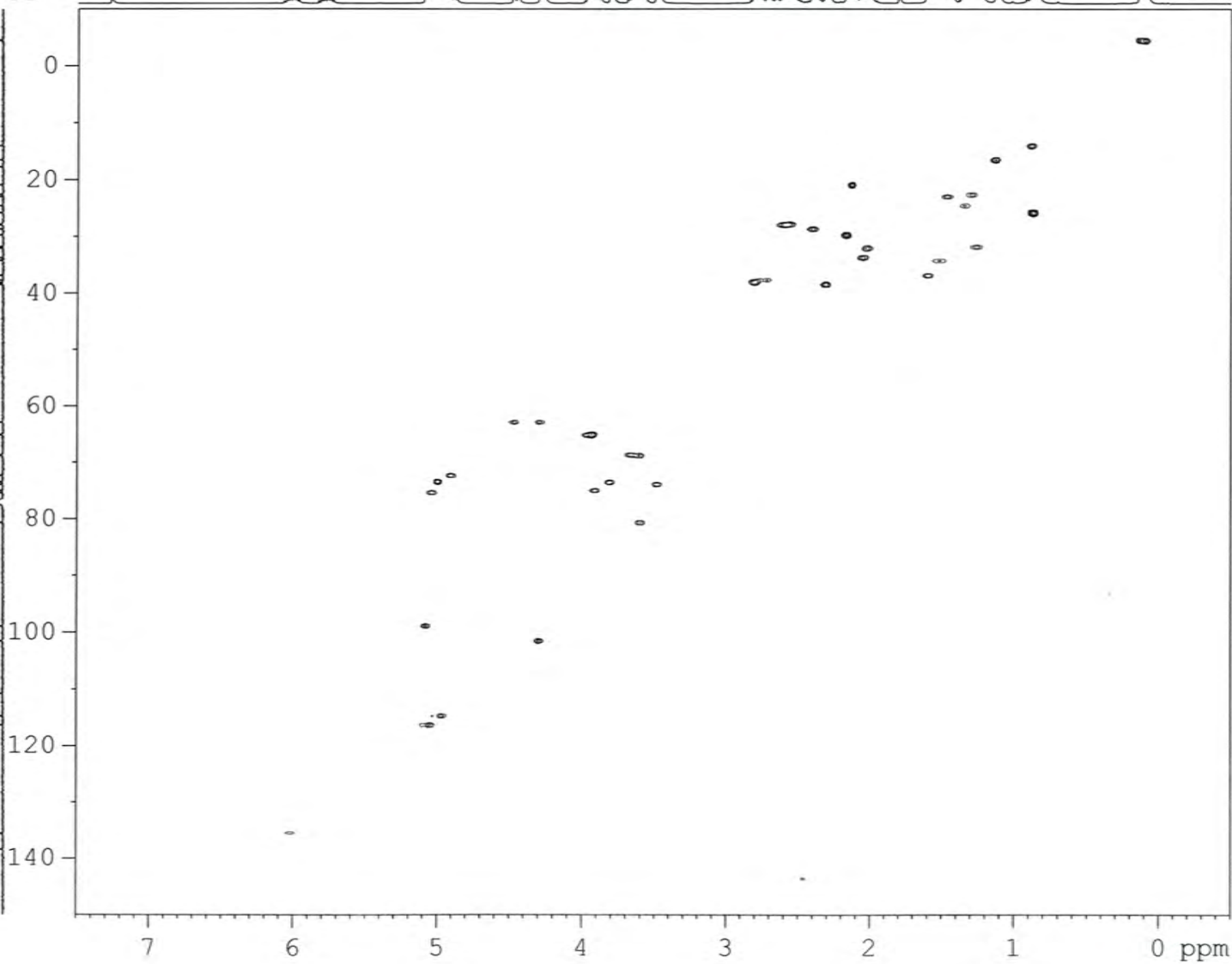
===== GRADIENT CHANNEL =====  
 GPNAM1 SINE.100  
 GPZ1 10.00 %  
 P16 1000.00 usec  
 ND0 1  
 TD 128  
 SFO1 400.1324 MHz  
 FIDRES 41.733440 Hz  
 SW 13.350 ppm  
 FmMODE QF  
 SI 1024  
 SF 400.1300040 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00  
 SI 1024  
 MC2 QF  
 SF 400.1300033 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0



6

## ZGH-Ipom-2-154-A-150407 HSQC

ppm



```

NAME      ZGH-Ipom-2-154-A-150407
EXPNO     4
PROCNO    1
Date_     20150409
Time      2.12
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   hsqcetgpsi
TD         1024
SOLVENT   CDC13
NS         8
DS         16
SWH        5341.880 Hz
FIDRES     5.216680 Hz
AQ         0.0958964 sec
RG         2050
DW         93.600 usec
DE         6.50 usec
TE         292.6 K
CNST2     145.0000000
DO         0.00000300 sec
D1         1.50000000 sec
D4         0.00172414 sec
D11        0.03000000 sec
D13        0.00000400 sec
D16        0.00020000 sec
D24        0.00110000 sec
IN0        0.00003000 sec
ZGPTNS

```

```

===== CHANNEL f1 =====
NUC1      1H
P1         10.00 usec
P2         20.00 usec
P28        1000.00 usec
PL1        -3.50 dB
PL1W       31.17620277 W
SFO1       400.1324057 MHz

```

```

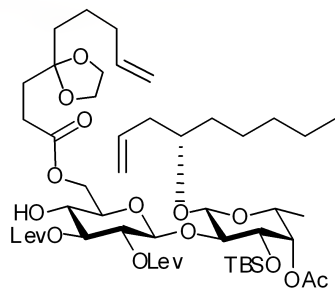
===== CHANNEL f2 =====
CPDPRG2   garp
NUC2      13C
P3         10.00 usec
P4         20.00 usec
PCPD2     75.00 usec
PL2        -2.10 dB
PL12       15.40 dB
PL2W       -58.37759399 W
PL12W      1.03811681 W
SFO2       100.6202727 MHz

```

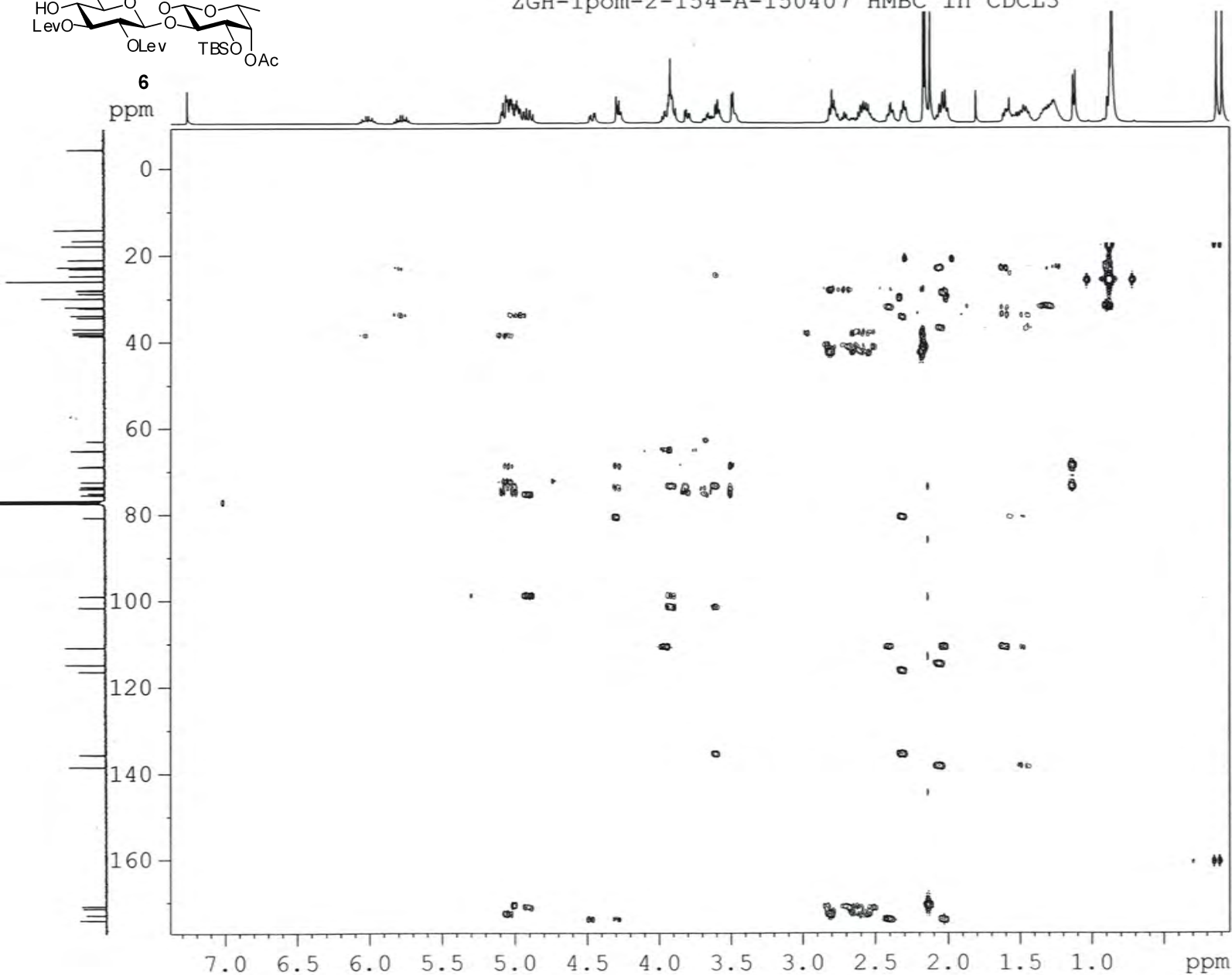
```

===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    SINE.100
GFZ1      80.00 %
GFZ2      20.10 %
P16       1000.00 usec
ND0       2
TD         256
SFO1      100.6203 MHz
FIDRES    65.104164 Hz
SW        165.639 ppm
FnMODE    Echo-Antiecho
S1        1024
SF        400.1300000 MHz
WDW       QSINE
SSB       2
LB         0.00 Hz
GB         0
PC         1.00
SI        1024
MC2       echo-antiecho
SF        100.6127690 MHz
WDW       QSINE
SSB       2
LB         0.00 Hz
GB         0

```



## ZGH-Ipom-2-154-A-150407 HMBC in CDCL3

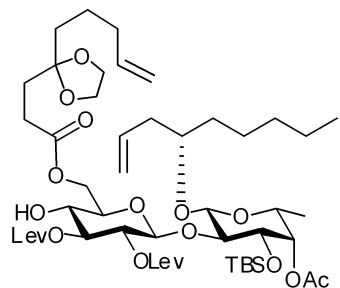


NAME ZGH-Ipom-2-154-A-150407  
 EXPNO 5  
 PROCNO 1  
 Date\_ 20150409  
 Time\_ 3.09  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hmbcgp1pndgf  
 TD 4096  
 SOLVENT CDCL3  
 NS 45  
 DS 16  
 SWH 5208.333 Hz  
 FIDRES 1.271566 Hz  
 AQ 0.3932660 sec  
 RG 2050  
 DW 96.000 usec  
 DE 6.50 usec  
 TE 292.5 K  
 CNST2 145.0000000  
 CNST13 10.0000000  
 D0 0.00000300 sec  
 D1 1.50000000 sec  
 D2 0.00344828 sec  
 D6 0.05000000 sec  
 D16 0.00020000 sec  
 IN0 0.00003010 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 P2 20.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1325208 MHz

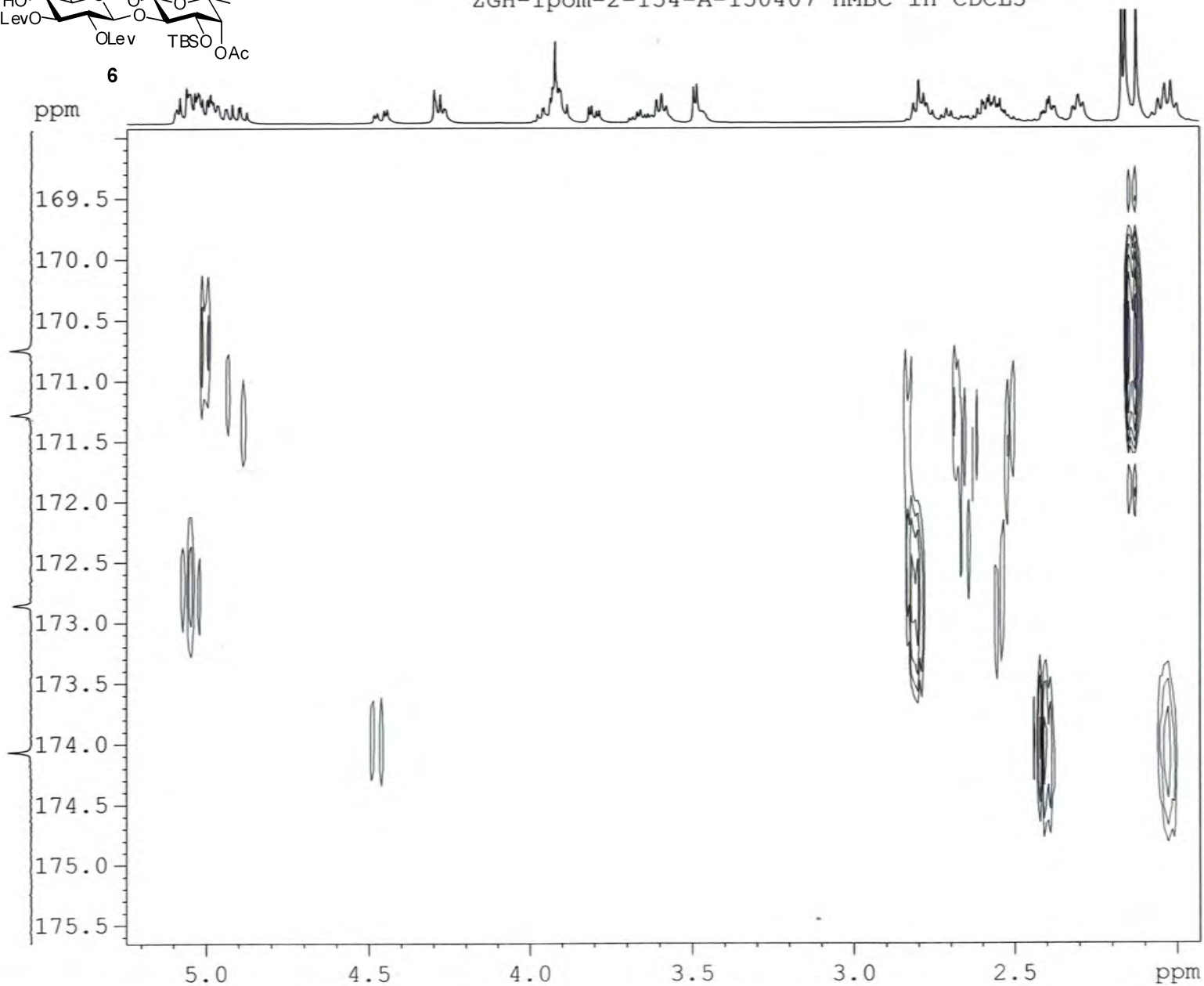
===== CHANNEL f2 =====  
 NUC2 13C  
 P3 10.00 usec  
 PL2 -2.10 dB  
 PL2W 58.37759399 W  
 SFO2 100.6228138 MHz

===== GRADIENT CHANNEL =====  
 GPNAM1 SINE.100  
 GPNAM2 SINE.100  
 GPNAM3 SINE.100  
 GPZ1 50.00 %  
 GPZ2 30.00 %  
 GPZ3 40.10 %  
 P16 1000.00 usec  
 ND0 2  
 TD 128  
 SFO1 100.6228 MHz  
 FIDRES 129.709091 Hz  
 SW 165.000 ppm  
 PnMODE QF  
 SI 2048  
 SF 400.1300000 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 4.00  
 SI 1024  
 MC2 QF  
 SF 100.6127690 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0



6

## ZGH-Ipom-2-154-A-150407 HMBC in CDCL3



```

NAME      ZGH-Ipom-2-154-A-150407
EXPNO     5
PROCNO    1
Date_     20150409
Time      3.09
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   hmbcgp1pndqf
TD         4096
SOLVENT   CDCL3
NS         45
DS         16
SWH        5208.333 Hz
FIDRES     1.271566 Hz
AQ         0.3932660 sec
RG         2050
DW         96.000 usec
DE         6.50 usec
TE         292.5 K
CNST2     145.0000000
CNST13    10.0000000
D0         0.00000300 sec
D1         1.50000000 sec
D2         0.00344828 sec
D6         0.05000000 sec
D16        0.00020000 sec
IN0        0.00003010 sec
  
```

```

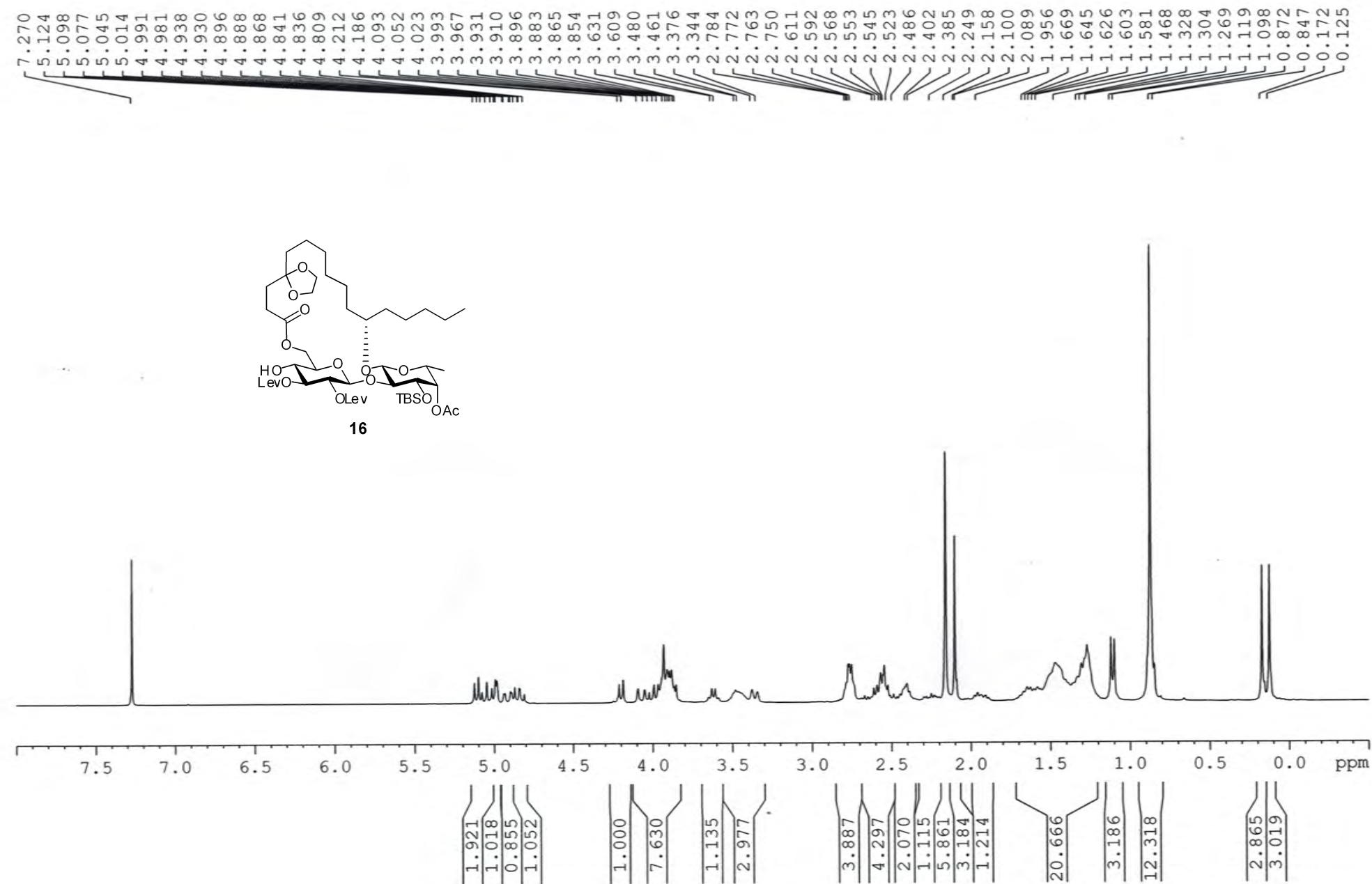
===== CHANNEL f1 =====
NUC1      1H
P1        10.00 usec
P2        20.00 usec
PL1       -3.50 dB
PL1W      31.17620277 W
SFO1      400.1325208 MHz
  
```

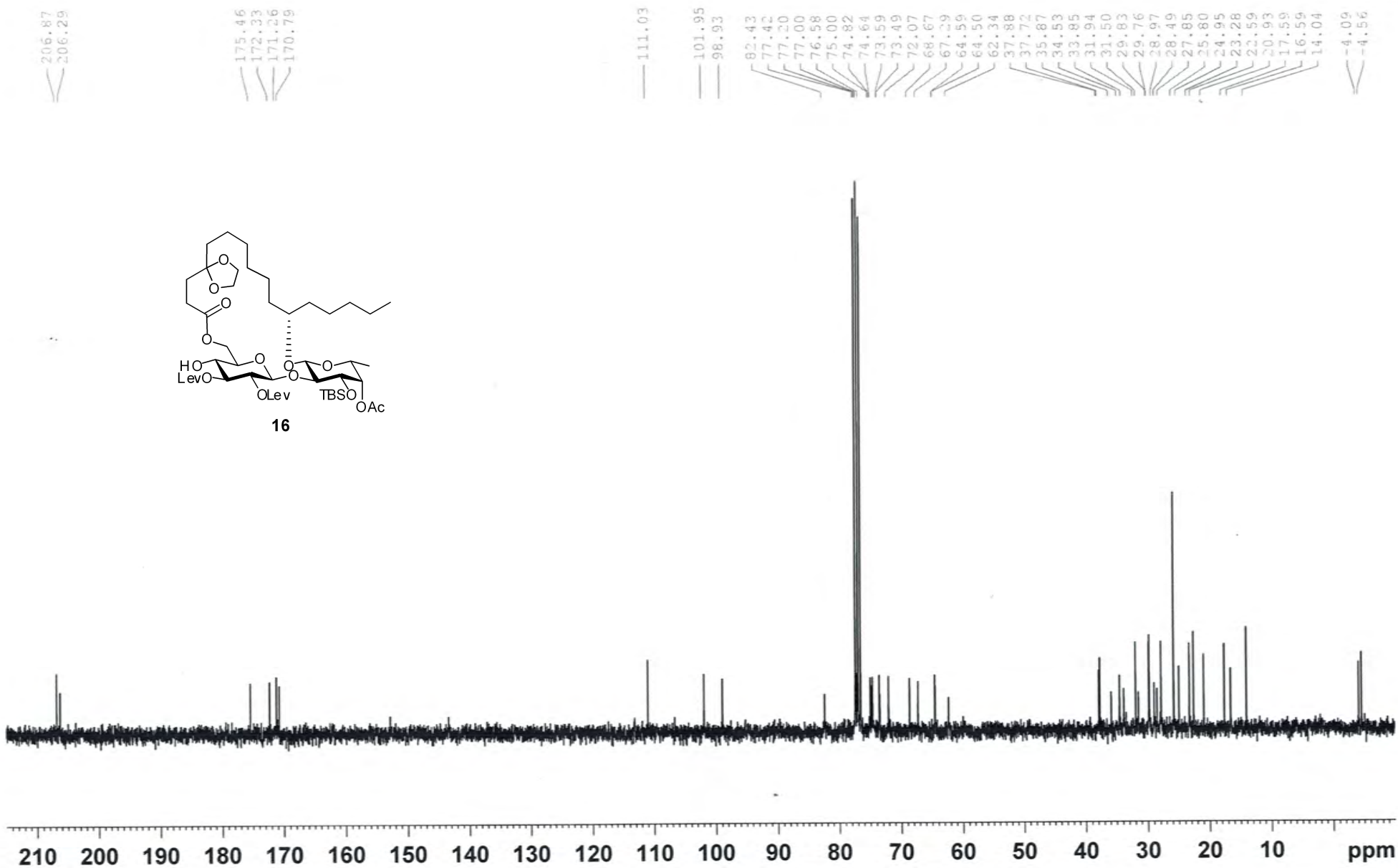
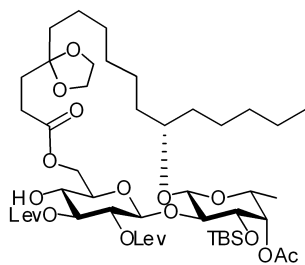
```

===== CHANNEL f2 =====
NUC2      13C
P3        10.00 usec
P2        -2.10 dB
PL2W      58.37759399 W
SFO2      100.6228138 MHz
  
```

```

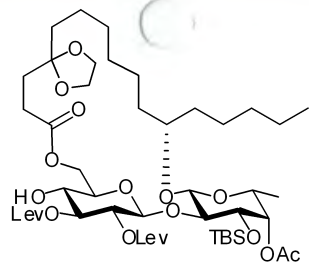
===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    SINE.100
GPNAM3    SINE.100
GPZ1      50.00 %
GPZ2      30.00 %
GPZ3      40.10 %
P16       1000.00 usec
ND0        2
TD         128
SFO1      100.6228 MHz
FIDRES    129.709091 Hz
SW         165.000 ppm
FnMODE    QF
SI         2048
SF         400.1300003 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         4.00
SI         1024
MC2        QF
SF         100.6127690 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
  
```

ZGH-Ipom-2-134-A-151210 (3) in CDCl<sub>3</sub>

ZGH-*Ipom*-2-134-A-151210 (3)  $^{13}\text{C}$ 



## ZGH-Ipom-2-134-A-150122 COSY



16

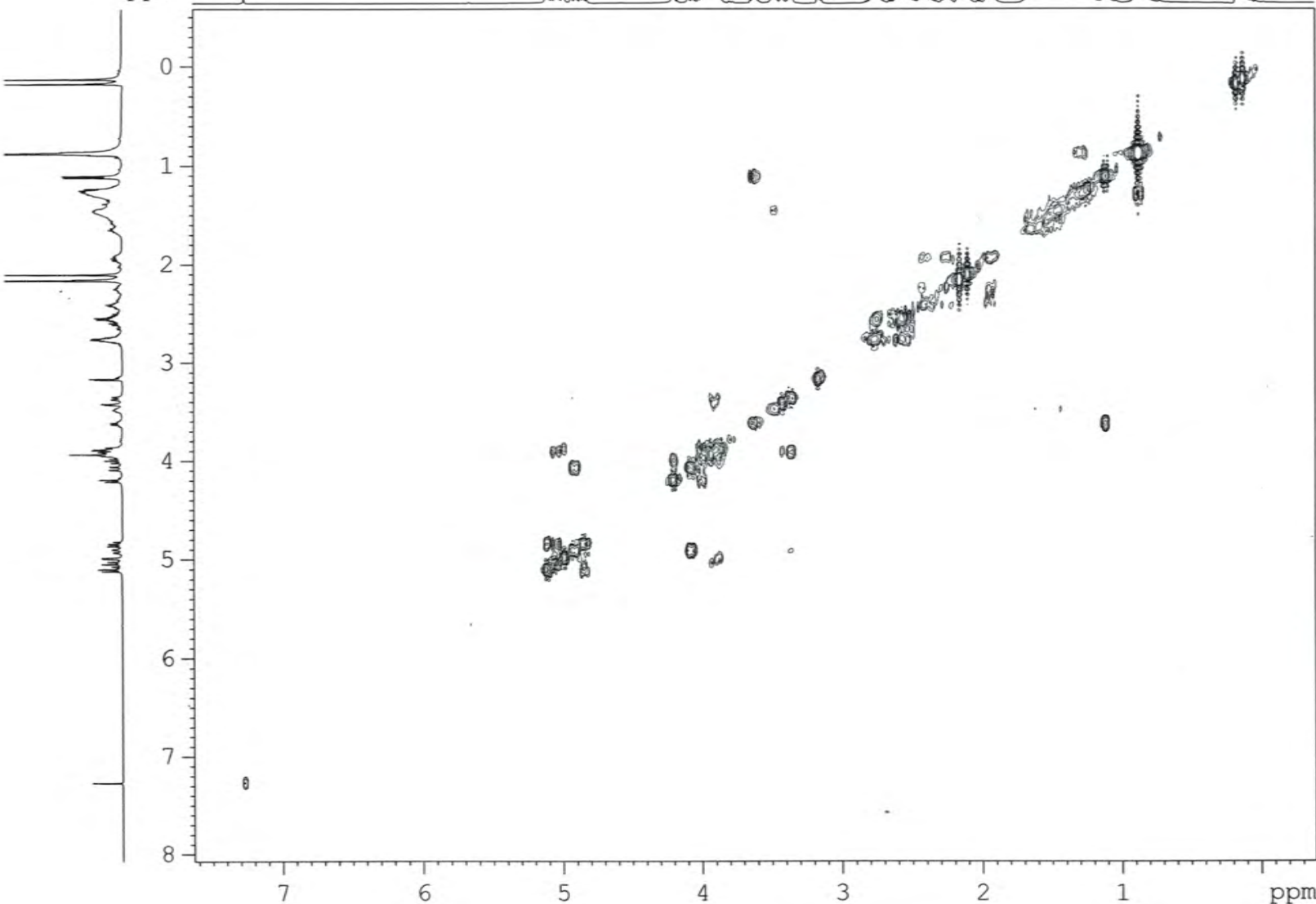
NAME ZGH-Ipom-2-134-A-150122  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20150123  
 Time 19.39  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosygpqf  
 TD 2048  
 SOLVENT CDC13  
 NS 4  
 DS 8  
 SWH 5341.880 Hz  
 FIDRES 2.608340 Hz  
 AQ 0.1917428 sec  
 RG 57  
 DW 93.600 usec  
 DE 6.50 usec  
 TE 292.1 K  
 D0 0.00000300 sec  
 D1 1.48689198 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 IN0 0.00018720 sec

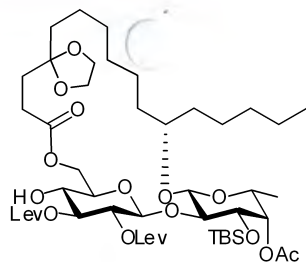
----- CHANNEL f1 -----  
 NUC1 1H  
 P0 10.00 usec  
 P1 10.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1324057 MHz

----- GRADIENT CHANNEL -----  
 GPNAM1 SINE.100  
 GFZ1 10.00 %  
 P16 1000.00 usec  
 ND0 1  
 TD 128  
 SFO1 400.1324 MHz  
 FIDRES 41.733440 Hz  
 SW 13.350 ppm  
 FhMODE QF  
 S1 1024  
 SF 400.1300040 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00  
 S1 1024  
 MC2 QF  
 SF 400.1300033 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

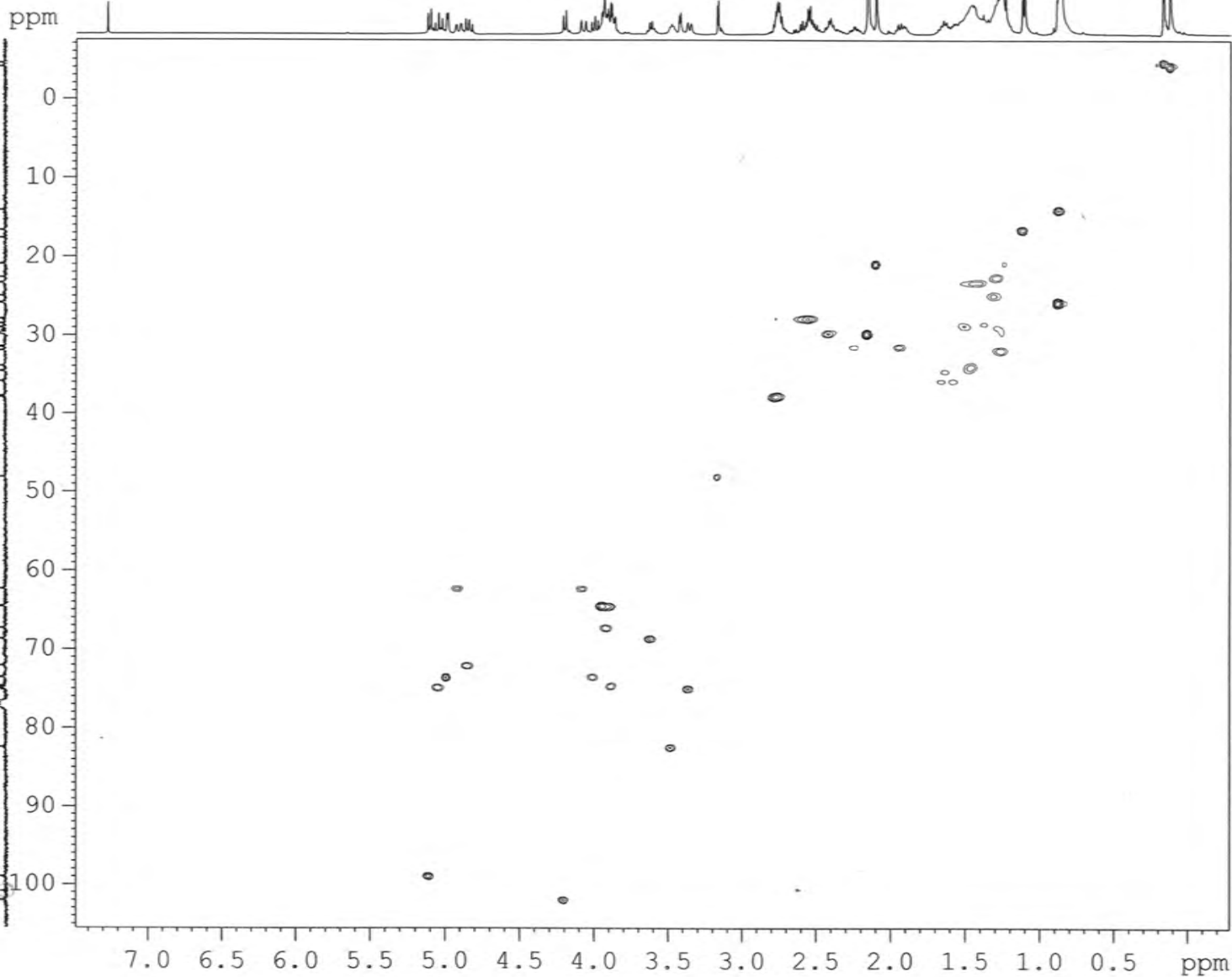
ppm

ppm



ZGH-*Ipom*-2-134-A-150122 HSQC

16



```

NAME      ZGH-Ipom-2-134-A-150122
EXPNO     4
PROCNO    1
Date_     20150123
Time      20.52
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   hsqcetgps1
TD         1024
SOLVENT   CDCl3
NS         4
DS         16
SWH        5341.880 Hz
FIDRES     5.216680 Hz
AQ         0.0958964 sec
RG         2050
DW         93.600 usec
DE         6.50 usec
TE         292.6 K
CNST2     145.0000000
D0         0.00000300 sec
D1         1.50000000 sec
D4         0.00172414 sec
D11        0.03000000 sec
D13        0.00000400 sec
D16        0.00020000 sec
D24        0.00110000 sec
IN0        0.00003000 sec
ZGOPTNS

```

```

===== CHANNEL f1 =====
NUC1       1H
P1         10.00 usec
P2         20.00 usec
P28        1000.00 usec
PL1        -3.50 dB
PL1W       31.17620277 W
SFO1       400.1324057 MHz

```

```

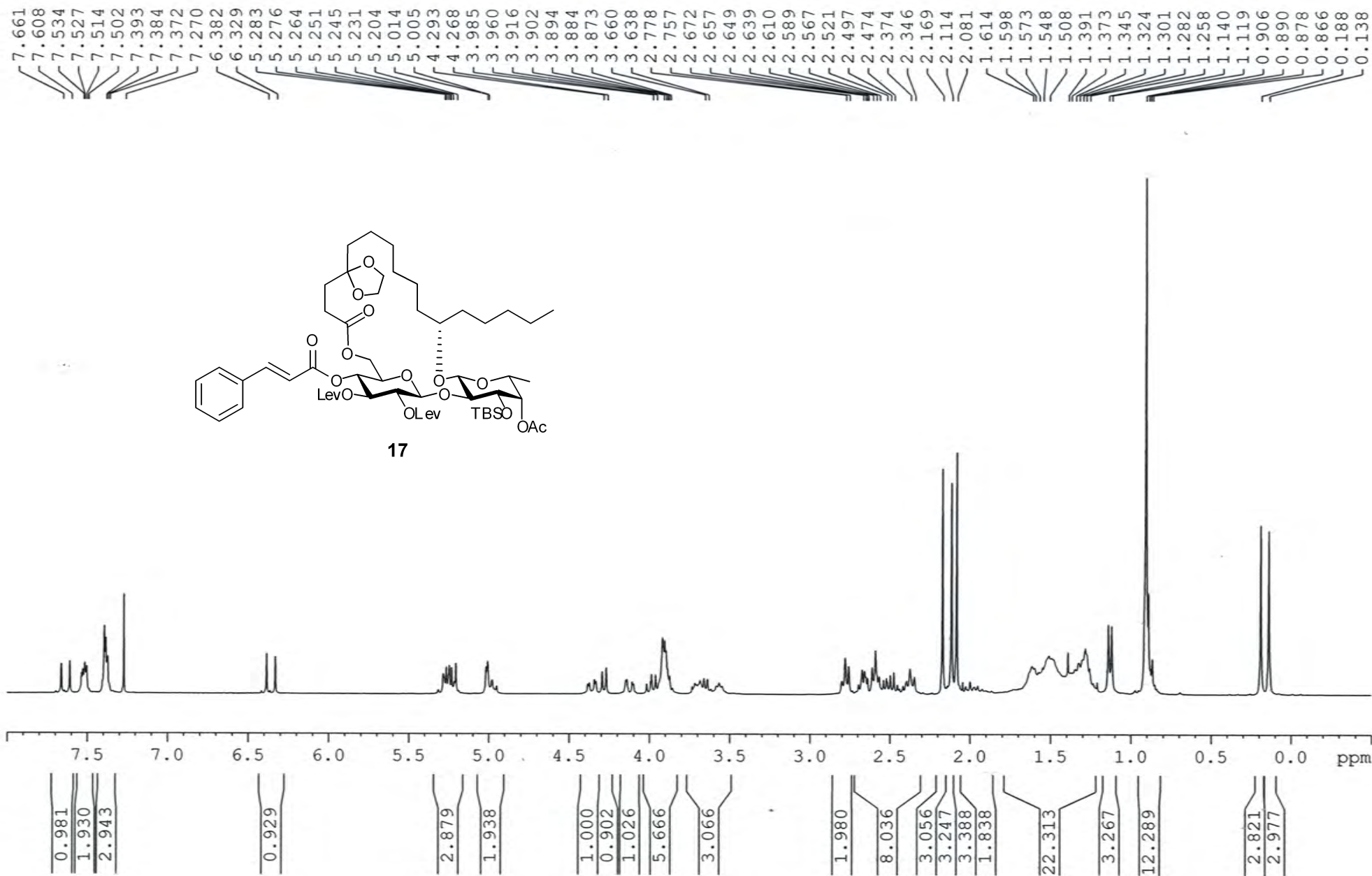
===== CHANNEL f2 =====
CPDPRG2    garp
NUC2       13C
P3         10.00 usec
P4         20.00 usec
PCPD2      75.00 usec
PL2        -2.10 dB
PL12       15.40 dB
PL2W       58.37759399 W
PL12W      1.03811681 W
SFO2       100.6202727 MHz

```

```

===== GRADIENT CHANNEL =====
GNAM1      SINE.100
GNAM2      SINE.100
GPZ1       80.00 %
GPZ2       20.10 %
P16        1000.00 usec
ND0         2
TD          256
SFO1       100.6203 MHz
FIDRES     65.104164 Hz
SW         165.639 ppm
FMODE      Echo-Antiecho
SI         1024
SF         400.1300000 MHz
WDW         QSINE
SSB         2
LB          0.00 Hz
GB          0
PC          1.00
SI         1024
MC2        echo-antiecho
SF         100.6127690 MHz
WDW         QSINE
SSB         2
LB          0.00 Hz
GB          0

```

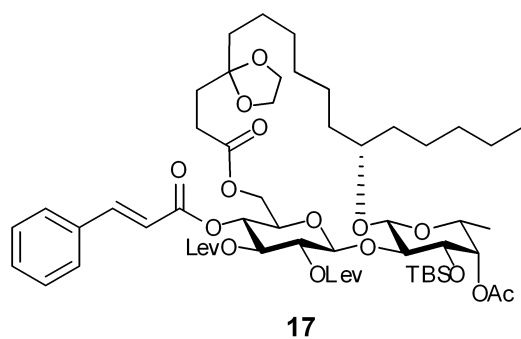
ZGH-*Ipom*-2-136-A-151212 in CDCl<sub>3</sub> (300 MHz)

ZGH-*Ipom*-2-136-A-151212 in CDCl<sub>3</sub> 300 MHz206.24  
206.09172.98  
171.91  
171.16  
170.77  
165.04

146.11

134.06  
130.53  
128.82  
128.26116.70  
111.25

101.44

98.87  
81.9477.42  
77.2077.00  
76.5774.48  
74.0673.59  
73.0172.21  
71.8868.83  
68.4564.52  
61.7237.75  
37.6736.58  
34.5934.34  
33.7232.04  
31.1929.99  
29.8029.57  
28.9528.33  
27.9027.81  
25.8824.84  
24.6424.57  
23.9822.88  
22.6120.89  
17.7516.57  
14.06-4.32  
-4.47

200

180

160

140

120

100

80

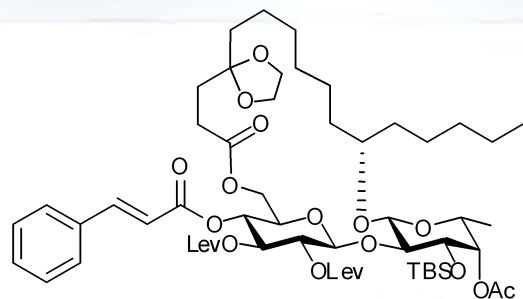
60

40

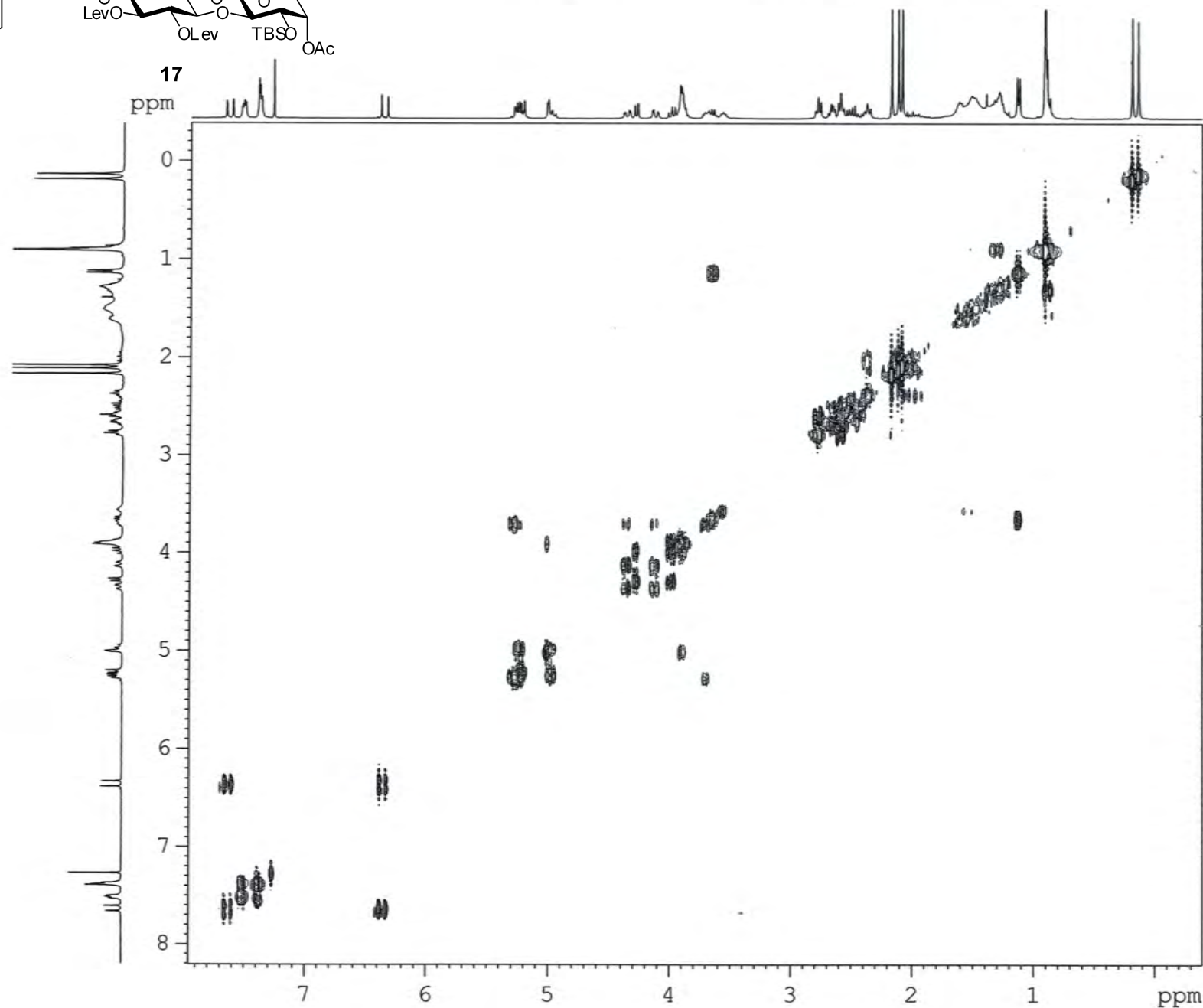
20

0

ppm



## ZGH-Ipom-2-136-A-151212 COSY



```

NAME      ZGH-Ipom-2-136-A-151212
EXPNO     3
PROCNO    1
Date_     20151220
Time      22.45
INSTRUM   spect
PROBHD    5 mm FAPBO BB-
PULPROG   cosyppprqf
TD         4096
SOLVENT   CDC13
NS         16
DS         8
SWH        4816.956 Hz
FIDRES     1.176015 Hz
AQ         0.4252148 sec
RG         128
DW         103.800 usec
DE         6.50 usec
TE         295.0 K
DO         0.00000300 sec
D1         2.00000000 sec
D11        0.03000000 sec
D12        0.00002000 sec
D16        0.00010000 sec
IN0        0.00020785 sec
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P0        12.20 usec
P1        12.20 usec
PL1       -1.00 dB
PL9       51.25 dB
PL1W      13.28156662 W
PL9W      0.00007911 W
SFO1      300.1314102 MHz
  
```

```

===== GRADIENT CHANNEL =====
GPNAM1    SMSQ10.100
GPZ1      20.00 %
P16       1000.00 usec
ND0        1
TD         133
SFO1      300.1314 MHz
FIDRES     36.171562 Hz
SW         16.029 ppm
FrMODE     QF
SI         2048
SF         300.1300043 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
SI         2048
MC2        QF
SF         300.1300000 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
  
```

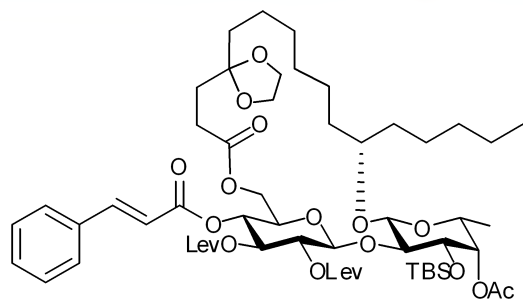
ZGH-*Ipom*-2-136-A-150129 HSQC

NAME ZGH-*Ipom*-2-136-A-150129  
 EXPNO 4  
 PROCNO 1  
 Date\_ 20150201  
 Time\_ 1.38  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hsqcetgpsi  
 TD 1024  
 SOLVENT CDCl3  
 NS 8  
 DS 16  
 SWH 5341.880 Hz  
 FIDRES 5.216680 Hz  
 AQ 0.0958964 sec  
 RG 2050  
 DW 93.600 usec  
 DE 6.50 usec  
 TE 293.2 K  
 CNST2 145.000000  
 D0 0.00000300 sec  
 D1 1.50000000 sec  
 D4 0.00172414 sec  
 D11 0.03000000 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 D24 0.00110000 sec  
 IN0 0.00003000 sec  
 ZGPTNS

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 10.00 usec  
 P2 20.00 usec  
 P28 1000.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1324057 MHz

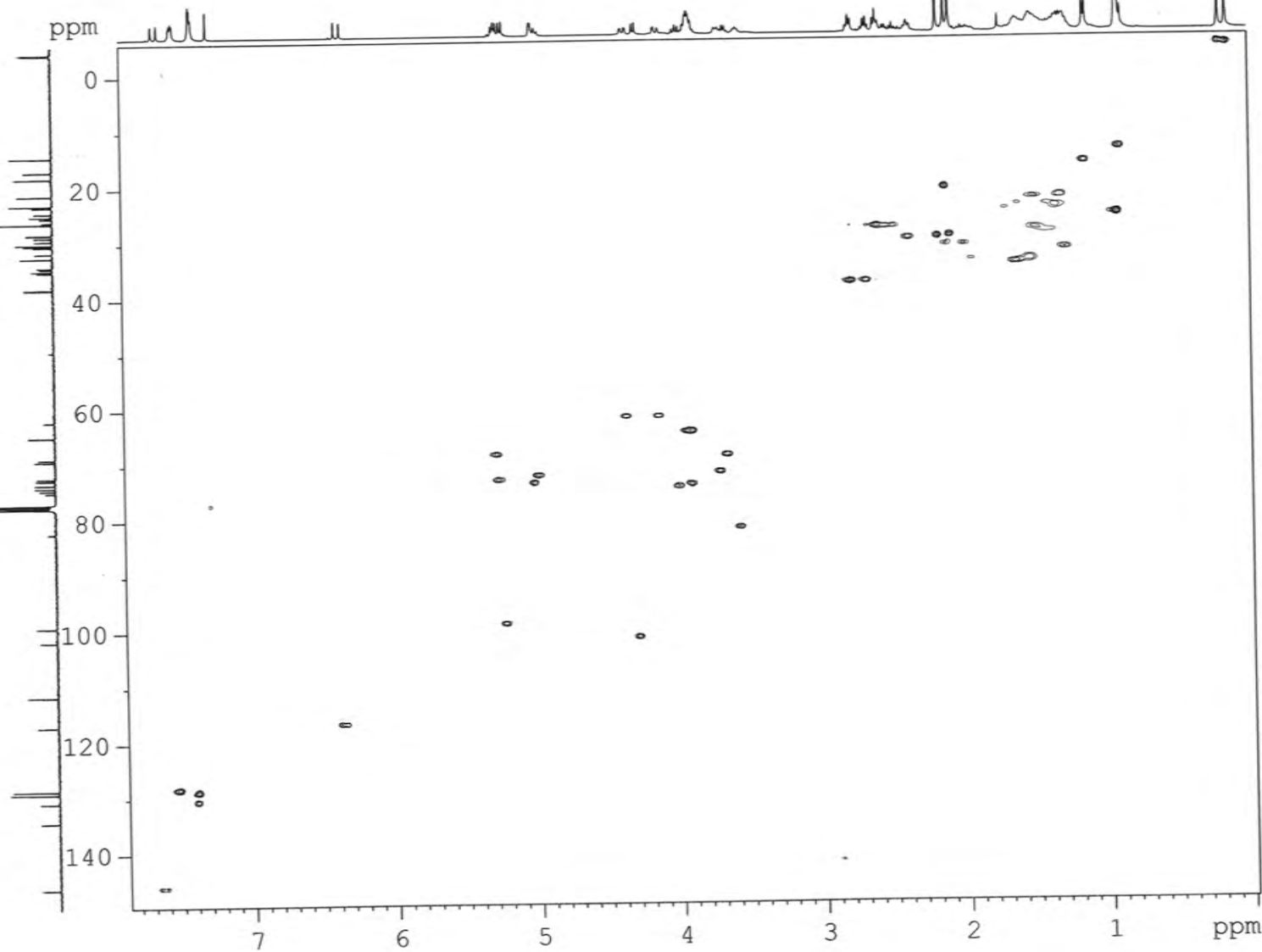
----- CHANNEL f2 -----  
 CPDPRG2 garp  
 NUC2 13C  
 P3 10.00 usec  
 P4 20.00 usec  
 PCPD2 75.00 usec  
 PL2 -2.10 dB  
 PL12 15.40 dB  
 PL2W 58.37759399 W  
 PL12W 1.03811681 W  
 SFO2 100.6202727 MHz

----- GRADIENT CHANNEL -----  
 GPNAM1 SINE.100  
 GPNAM2 SINE.100  
 GPZ1 80.00 %  
 GPZ2 20.10 %  
 P16 1000.00 usec  
 NDO 2  
 TD 256  
 SFO1 100.6203 MHz  
 FIDRES 65.104164 Hz  
 SW 165.639 ppm  
 FhMODE Echo-Antiecho  
 SI 1024  
 SF 400.1300000 MHz  
 WDW QSINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.00  
 SI 1024  
 MC2 echo-antiecho  
 SF 100.6127690 MHz  
 WDW QSINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0

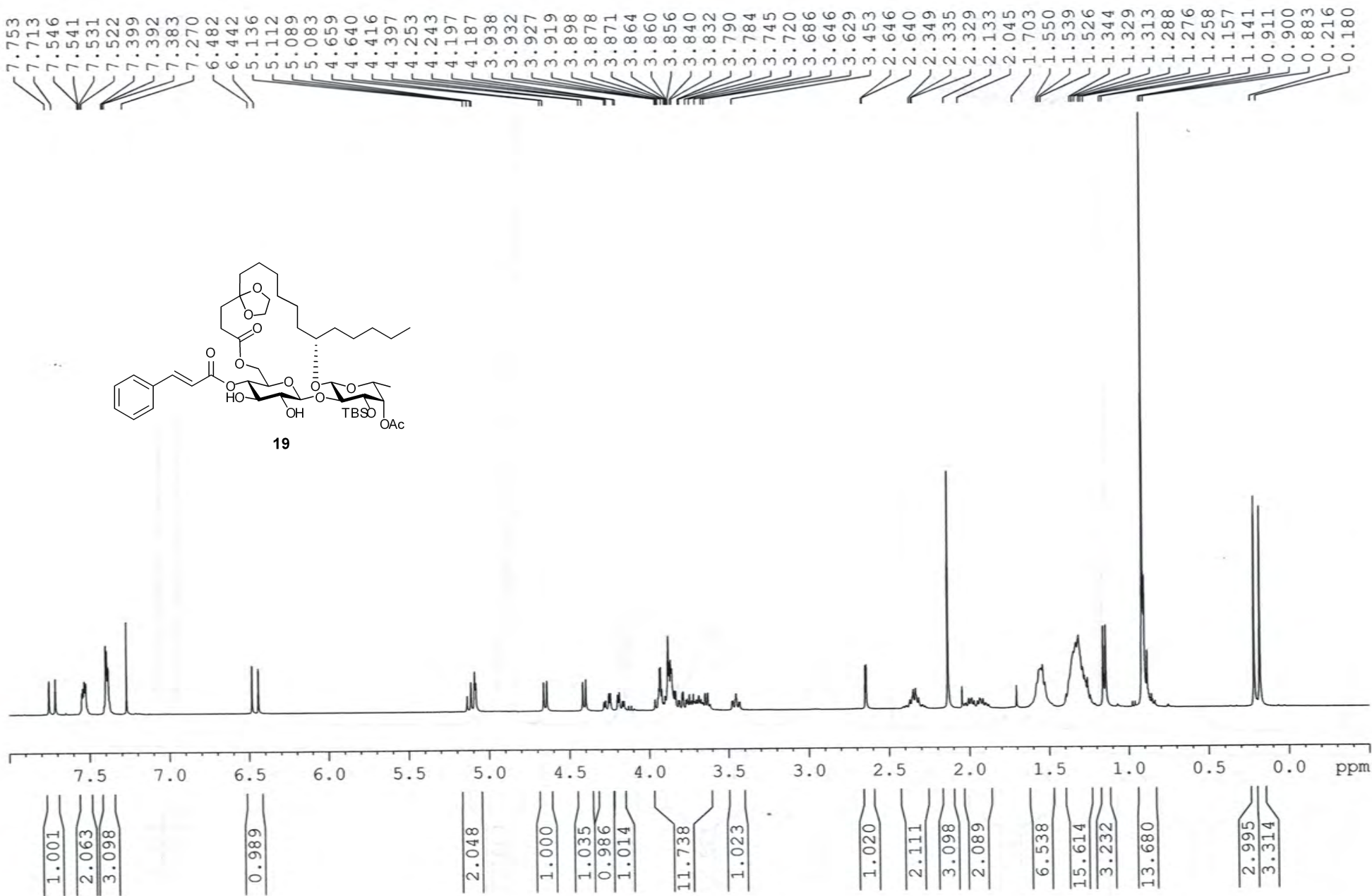


17

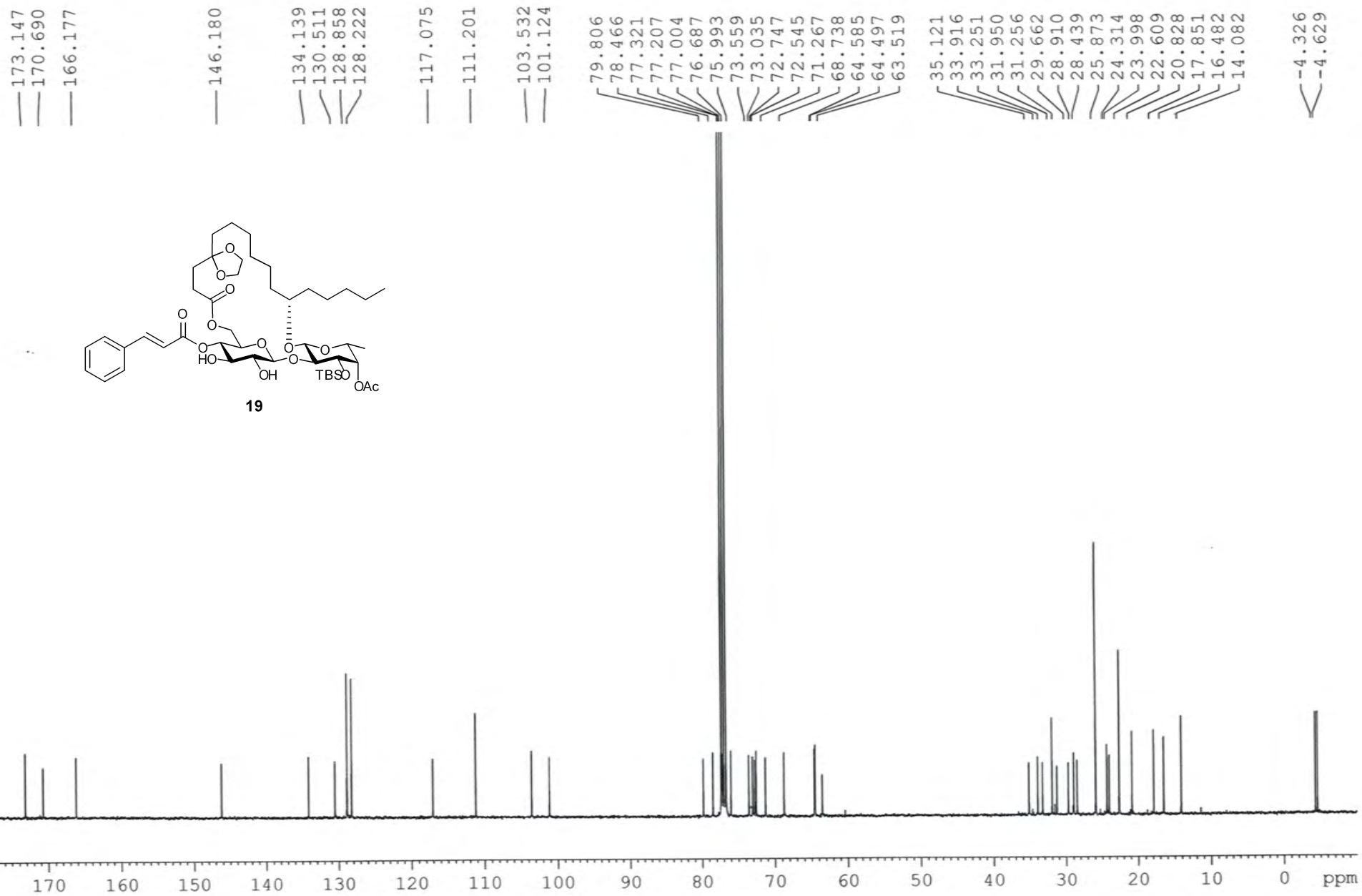
ppm



ppm

ZGH-*Ipom*-2-137-A-150202 1H in CDCl<sub>3</sub>

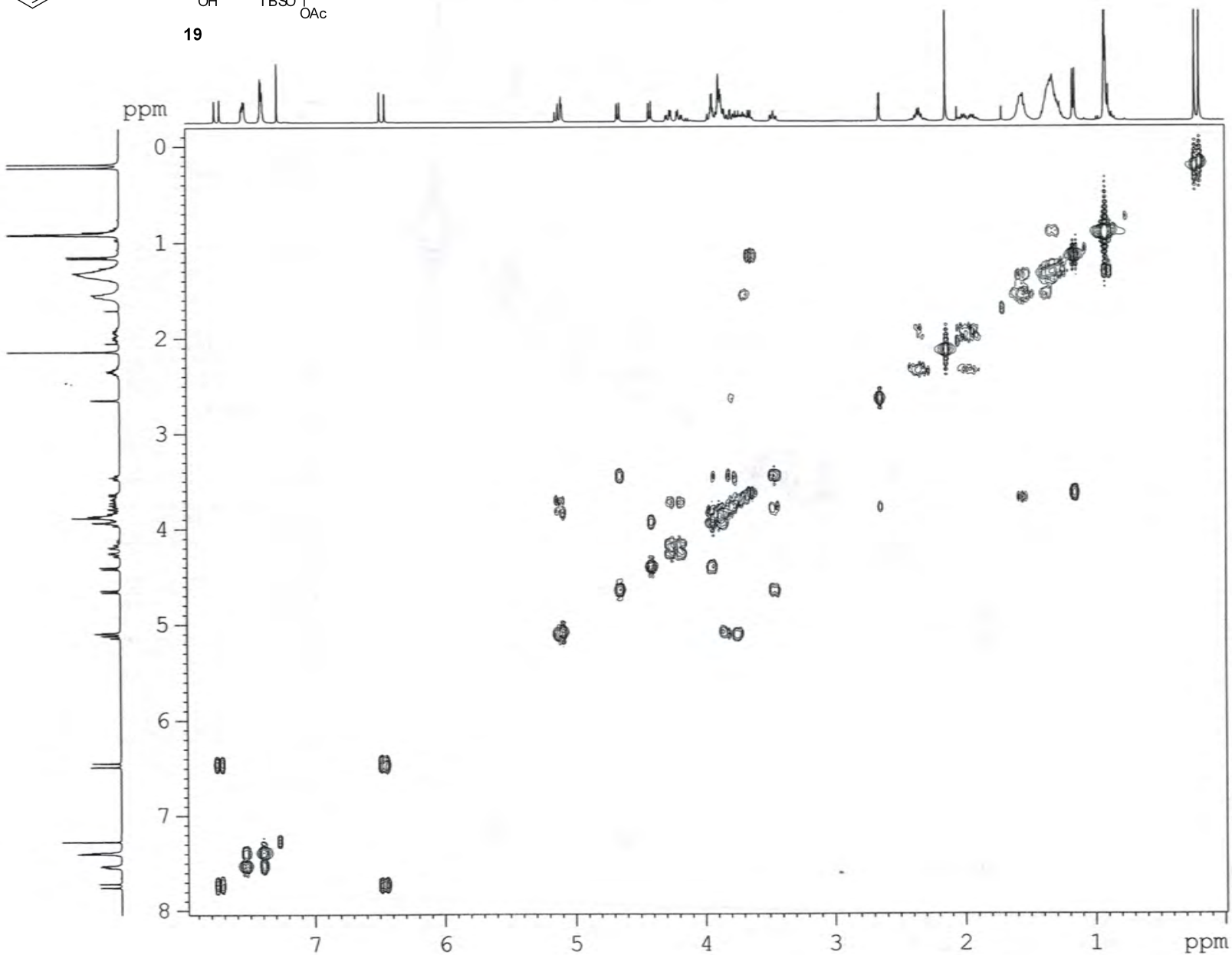
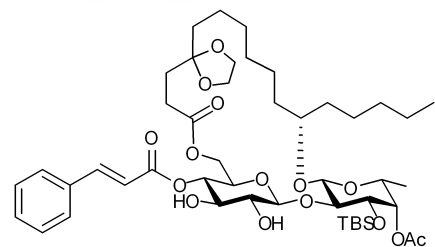
## ZGH-Ipom-2-137-A-150202 13C in CDCl3





ZGH-*Ipom*-2-137-A-150202 COSY

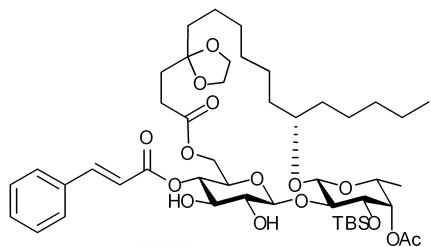
19



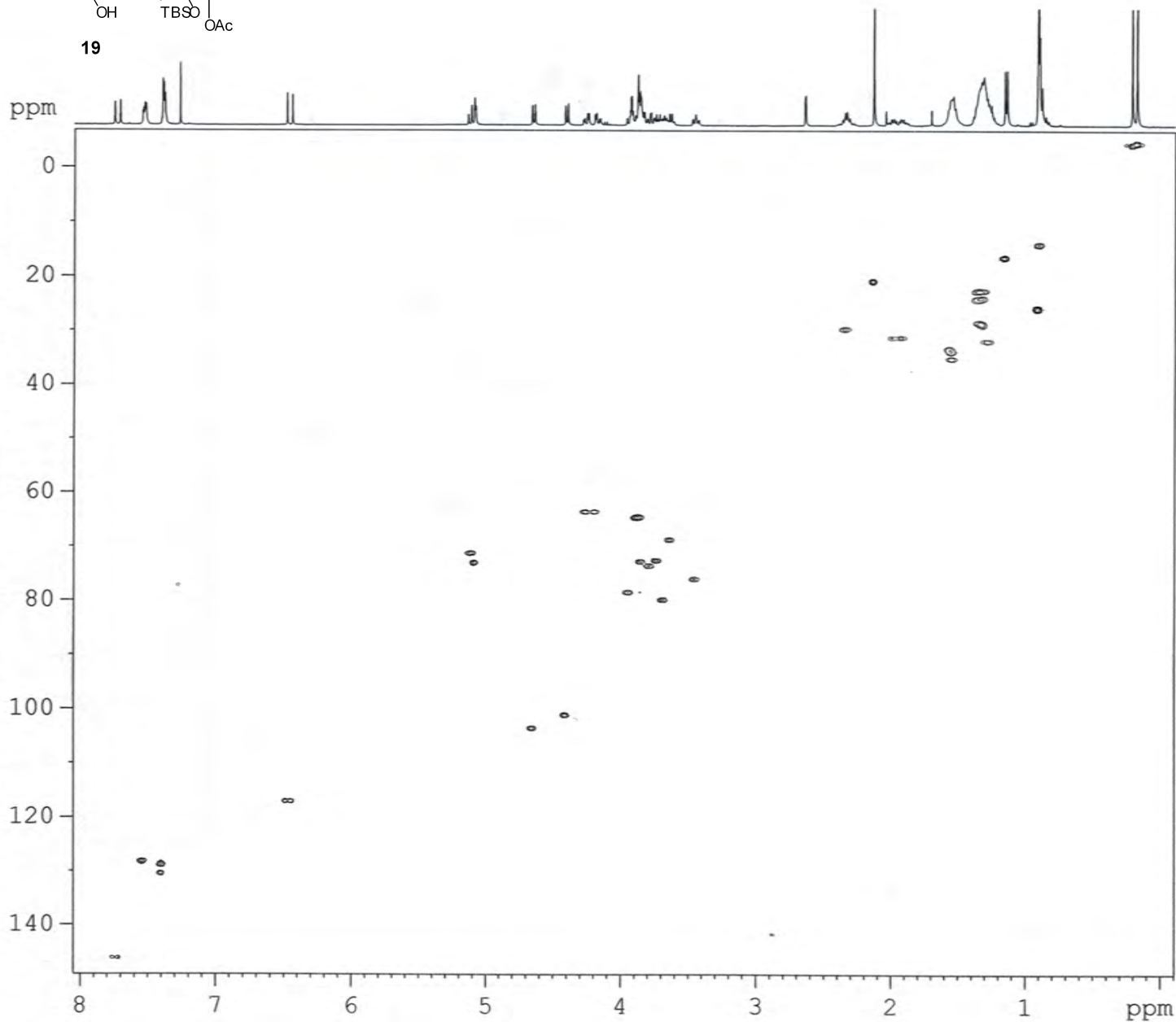
NAME ZGH-*Ipom*-2-137-A-150202  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20150202  
 Time\_ 23.02  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosygpgf  
 TD 2048  
 SOLVENT CDCl3  
 NS 4  
 DS 8  
 SWH 5341.880 Hz  
 FIDRES 2.608340 Hz  
 AQ 0.1917428 sec  
 RG 80.6  
 DW 93.600 usec  
 DE 6.50 usec  
 TE 292.6 K  
 D0 0.00009300 sec  
 D1 1.48689198 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 IN0 0.00018720 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P0 10.00 usec  
 P1 10.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1324057 MHz

===== GRADIENT CHANNEL =====  
 GPNAM1 SINE.100  
 GP21 10.00 %  
 P16 1000.00 usec  
 ND0 1  
 TD 128  
 SFO1 400.1324 MHz  
 FIDRES 41.733440 Hz  
 SW 13.350 ppm  
 FvMODE QF  
 SI 1024  
 SF 400.1300040 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00  
 SI 1024  
 MC2 QF  
 SF 400.1300033 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0



19

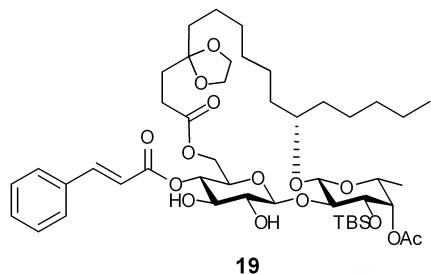
ZGH-*Ipom*-2-137-A-150202 HSQC

NAME ZGH-*Ipom*-2-137-A-150202  
 EXPNO 4  
 PROCNO 1  
 Date\_ 20150203  
 Time\_ 3.56  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hsqcetgpsi  
 TD 1024  
 SOLVENT CDCl3  
 NS 8  
 DS 16  
 SWH 5341.880 Hz  
 FIDRES 5.216680 Hz  
 AQ 0.0958964 sec  
 RG 2050  
 DW 93.600 usec  
 DE 6.50 usec  
 TE 293.5 K  
 CNST2 145.0000000  
 D0 0.00000300 sec  
 D1 1.50000000 sec  
 D4 0.00172414 sec  
 D11 0.03000000 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 D24 0.00110000 sec  
 IN0 0.00003000 sec  
 ZGPTNS

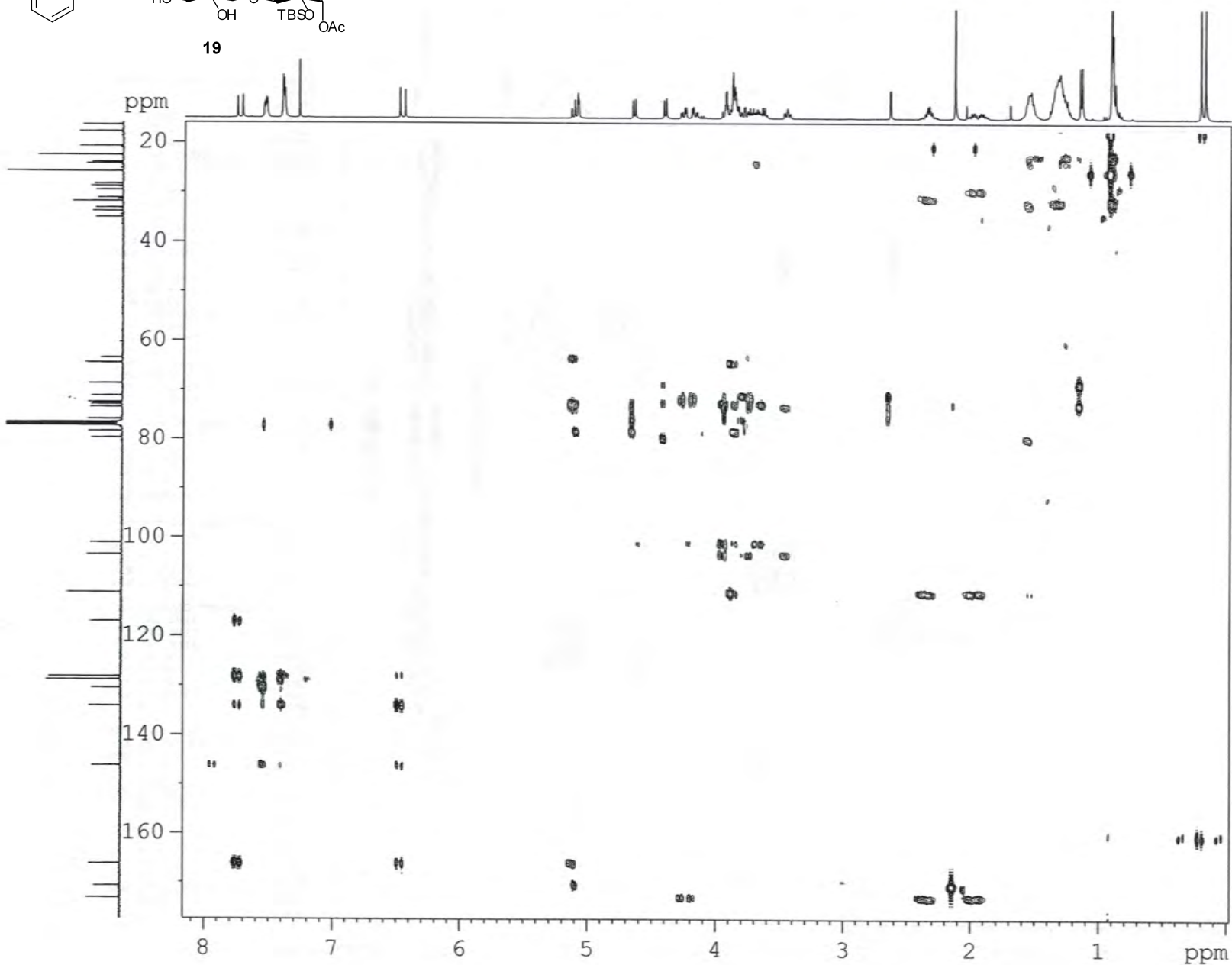
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 P2 20.00 usec  
 P28 1000.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1324057 MHz

===== CHANNEL f2 =====  
 CPDPRG2 garp  
 NUC2 13C  
 P3 10.00 usec  
 P4 20.00 usec  
 PCPD2 75.00 usec  
 PL2 -2.10 dB  
 PL12 15.40 dB  
 PL2W 58.37759399 W  
 PL12W 1.03811681 W  
 SFO2 100.6202727 MHz

===== GRADIENT CHANNEL =====  
 GPNAM1 SINE.100  
 GPNAM2 SINE.100  
 GPZ1 80.00 %  
 GPZ2 20.10 %  
 P16 1000.00 usec  
 ND0 2  
 TD 256  
 SFO1 100.6203 MHz  
 FIDRES 65.104164 Hz  
 SW 165.639 ppm  
 FnmODE Echo-Antiecho  
 SI 1024  
 SF 400.1300000 MHz  
 WDW QSINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.00  
 SI 1024  
 MC2 echo-antiecho  
 SF 100.6127690 MHz  
 WDW QSINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0



ZGH-Ipom-2-137-A-150202 HMBC in CDCL3

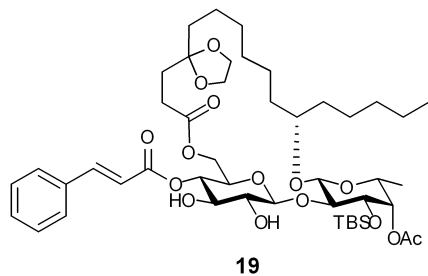
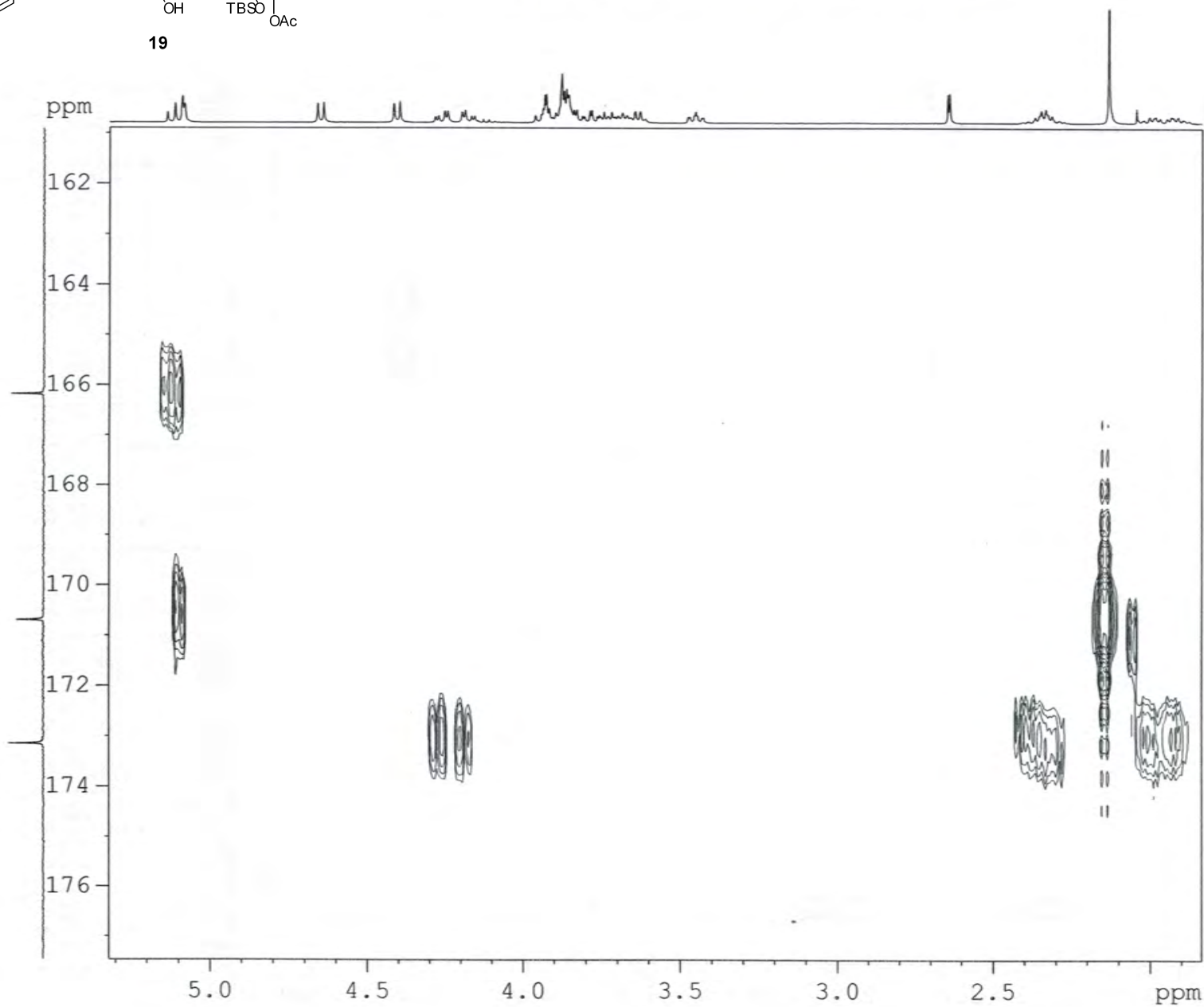


NAME ZGH-Ipom-2-137-A-150202  
 EXPNO 5  
 PROCNO 1  
 Date\_ 20150203  
 Time 4.53  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hmbcgp1pndqf  
 TD 4096  
 SOLVENT CDCL3  
 NS 40  
 DS 16  
 SWH 5208.333 Hz  
 FIDRES 1.271566 Hz  
 AQ 0.3932660 sec  
 RG 2050  
 DW 96.000 usec  
 DE 6.50 usec  
 TE 293.0 K  
 CNST2 145.0000000  
 CNST13 10.0000000  
 D0 0.00000300 sec  
 D1 1.50000000 sec  
 D2 0.00344828 sec  
 D6 0.05000000 sec  
 D16 0.00020000 sec  
 IN0 0.00003010 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 P2 20.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1325208 MHz

===== CHANNEL f2 =====  
 NUC2 13C  
 P3 10.00 usec  
 PL2 -2.10 dB  
 PL2W 58.37759399 W  
 SFO2 100.6228138 MHz

===== GRADIENT CHANNEL =====  
 GPNAM1 SINE.100  
 GPNAM2 SINE.100  
 GPNAM3 SINE.100  
 GPZ1 50.00 %  
 GPZ2 30.00 %  
 GPZ3 40.10 %  
 P16 1000.00 usec  
 ND0 2  
 TD 128  
 SFO1 100.6228 MHz  
 FIDRES 129.709091 Hz  
 SW 165.000 ppm  
 FhMODE QF  
 SI 2048  
 SF 400.1300000 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 4.00  
 SI 1024  
 MC2 QF  
 SF 100.6127690 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

ZGH-*Ipom*-2-137-A-150202 HMBC in CDCl<sub>3</sub>

```

NAME      ZGH-Ipom-2-137-A-150202
EXPNO     5
PROCNO    1
Date_     20150203
Time      4.53
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   hmcgplpndqf
TD         4096
SOLVENT   CDCl3
NS         40
DS         16
SWH       5208.333 Hz
FIDRES    1.271566 Hz
AQ         0.3932660 sec
RG         2050
DW         96.000 usec
DE         6.50 usec
TE         293.0 K
CNST2     145.0000000
CNST13    10.0000000
D0         0.00000300 sec
D1         1.50000000 sec
D2         0.00344828 sec
D6         0.05000000 sec
D16        0.00020000 sec
INO        0.00003010 sec
  
```

```

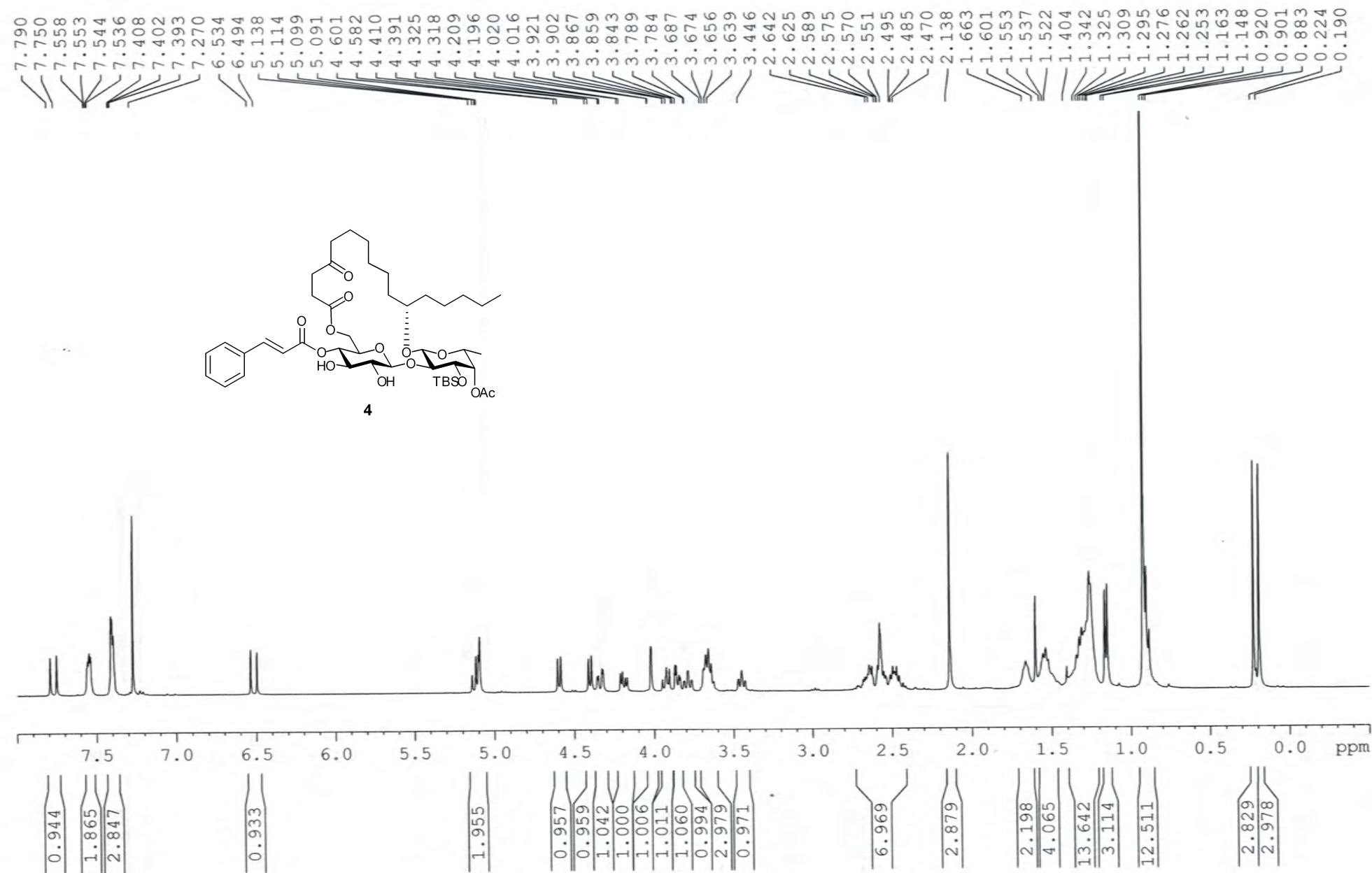
===== CHANNEL f1 =====
NUC1      1H
P1         10.00 usec
P2         20.00 usec
PL1        -3.50 dB
PL1W       31.17620277 W
SFO1       400.1325208 MHz
  
```

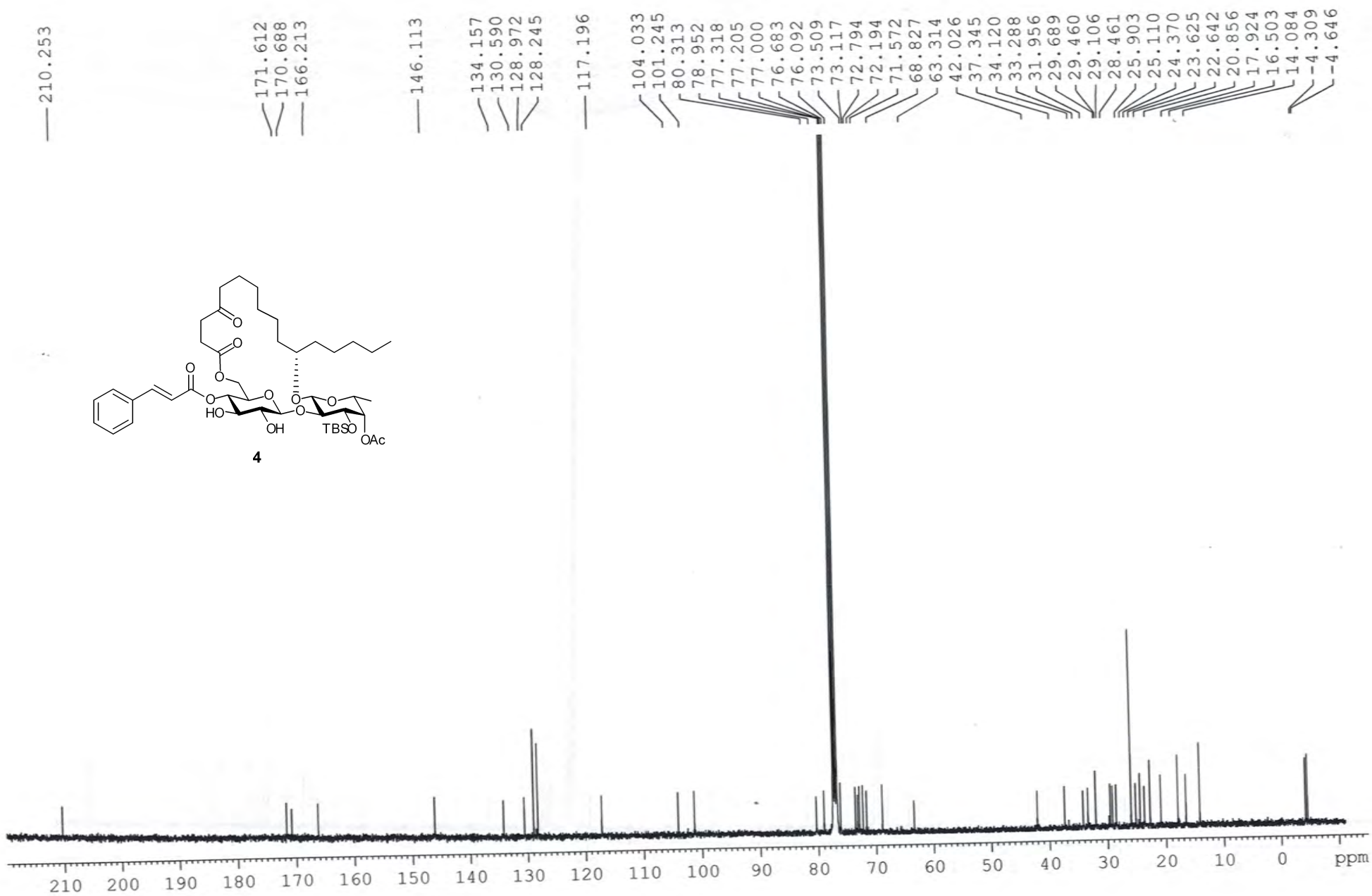
```

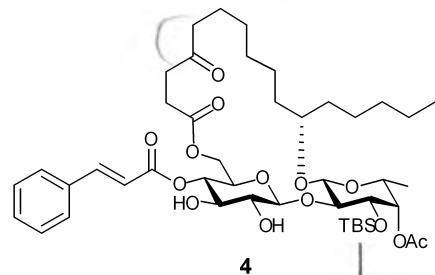
===== CHANNEL f2 =====
NUC2      13C
P3         10.00 usec
P2         -2.10 dB
PL2W       58.37759399 W
SFO2       100.6228138 MHz
  
```

```

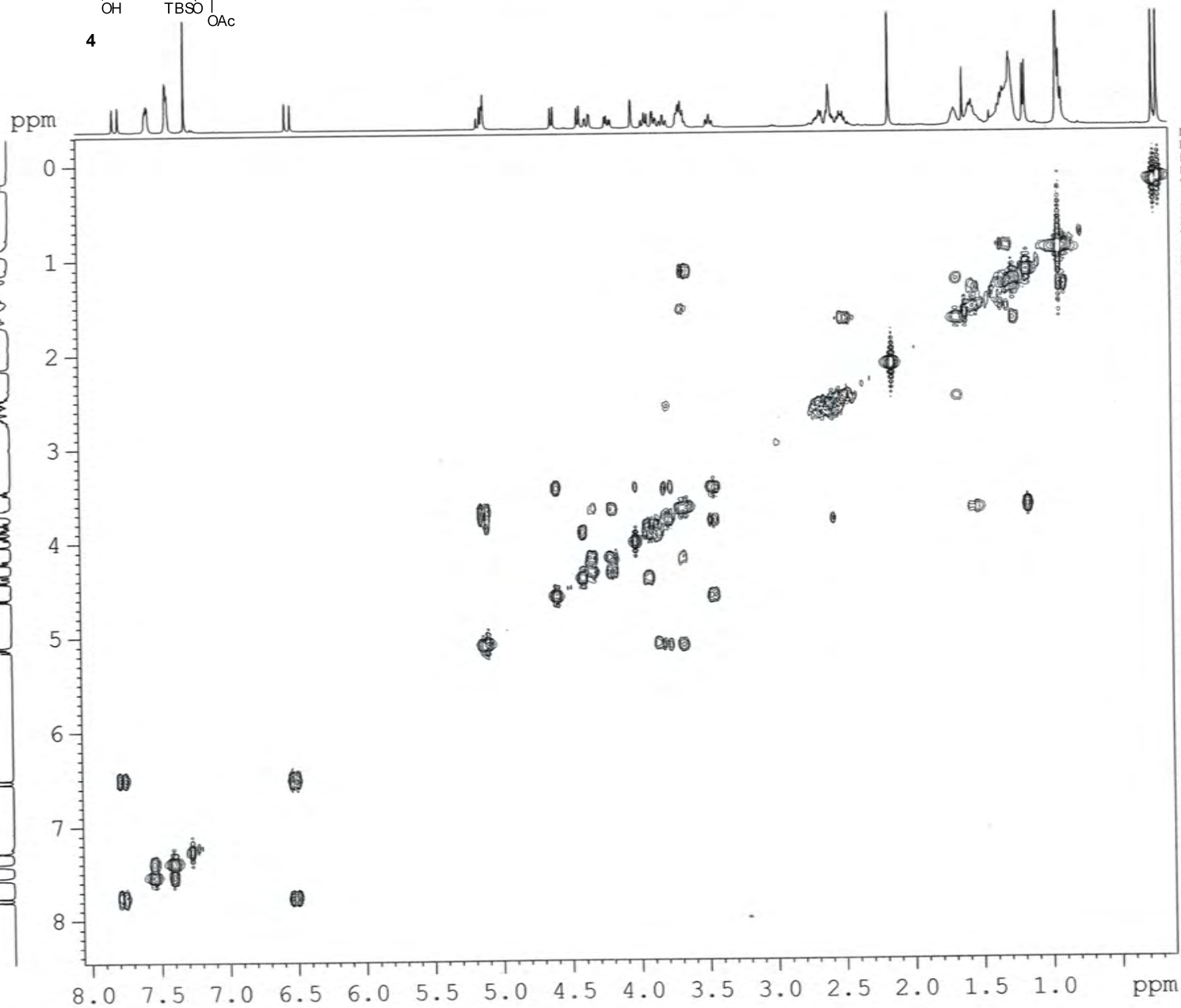
===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    SINE.100
GPNAM3    SINE.100
GPZ1      50.00 %
GPZ2      30.00 %
GPZ3      40.10 %
P16       1000.00 usec
ND0        2
TD         128
SFO1       100.6228 MHz
FIDRES     129.709091 Hz
SW         165.000 ppm
FnMODE     QF
SI         2048
SF         400.1300000 MHz
WDW        SINE
SSB         0
LB         0.00 Hz
GB         0
PC         4.00
SI         1024
MC2        QF
SF         100.6127690 MHz
WDW        SINE
SSB         0
LB         0.00 Hz
GB         0
  
```

ZGH-*Ipom*-2-140-B-150209 1H in CDCl<sub>3</sub>

ZGH-*Ipom*-2-140-B-150209 13C in CDCl<sub>3</sub>



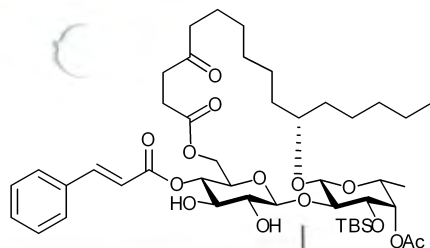
## ZGH-Ipom-2-140-B-150209 COSY



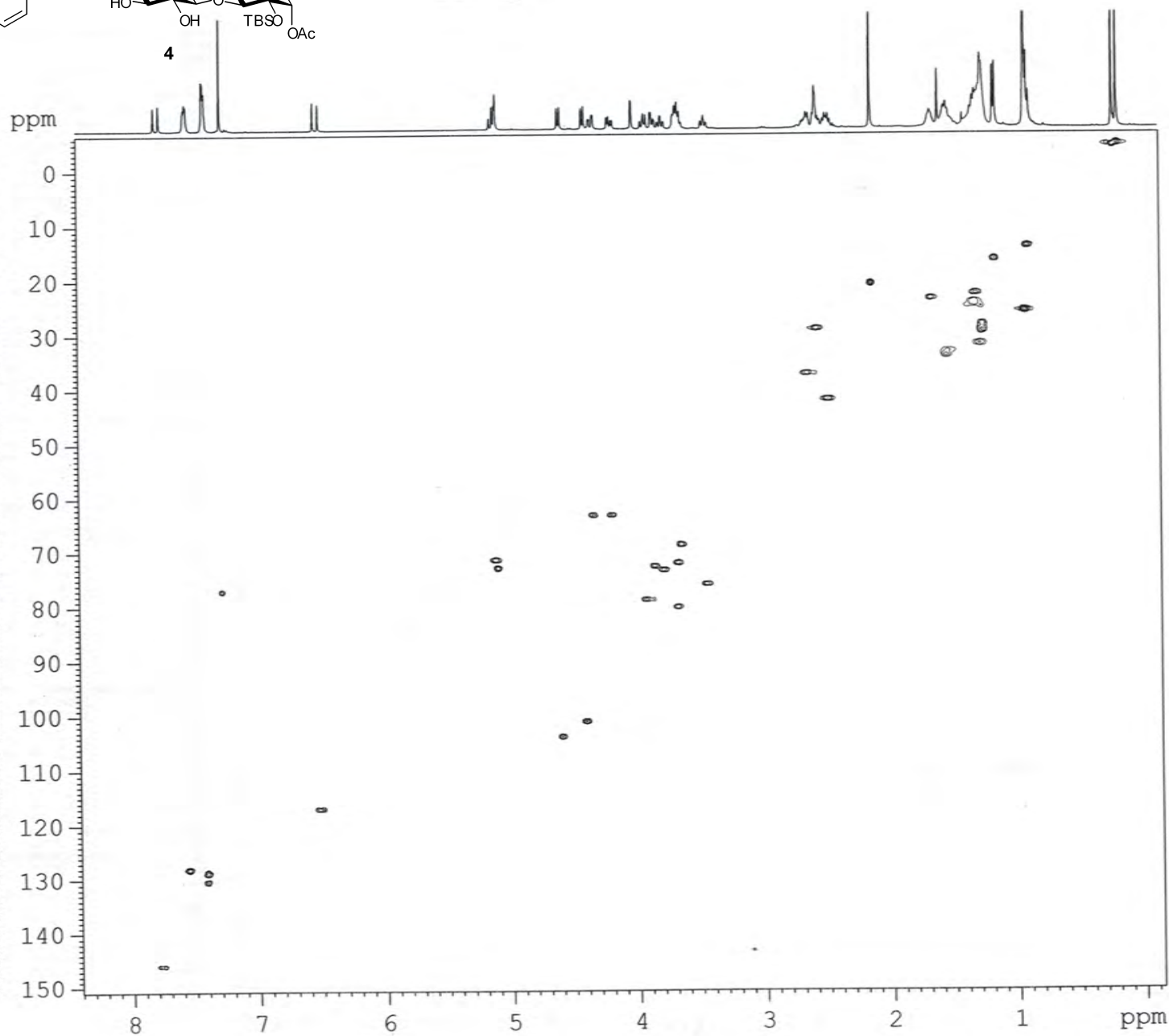
NAME ZGH-Ipom-2-140-B-150209  
 EXPNO 2  
 PROCNO 1  
 Date 20150209  
 Time 22.41  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosygpgf  
 TD 2048  
 SOLVENT CDCl3  
 NS 8  
 DS 8  
 SWH 5341.880 Hz  
 FIDRES 2.608340 Hz  
 AQ 0.1917428 sec  
 RG 287  
 DW 93.600 usec  
 DE 6.50 usec  
 TE 292.3 K  
 D0 0.00000300 sec  
 D1 1.48689198 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 IN0 0.00018720 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P0 10.00 usec  
 P1 10.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1324057 MHz

===== GRADIENT CHANNEL =====  
 GPNAM1 SINE.100  
 GPZ1 10.00 %  
 P16 1000.00 usec  
 NDO 1  
 TD 128  
 SFO1 400.1324 MHz  
 FIDRES 41.733440 Hz  
 SW 13.350 ppm  
 FMODE QF  
 SI 1024  
 SF 400.1300040 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00  
 SI 1024  
 MC2 QF  
 SF 400.1300033 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0



## ZGH-Ipom-2-140-B-150209 HSQC



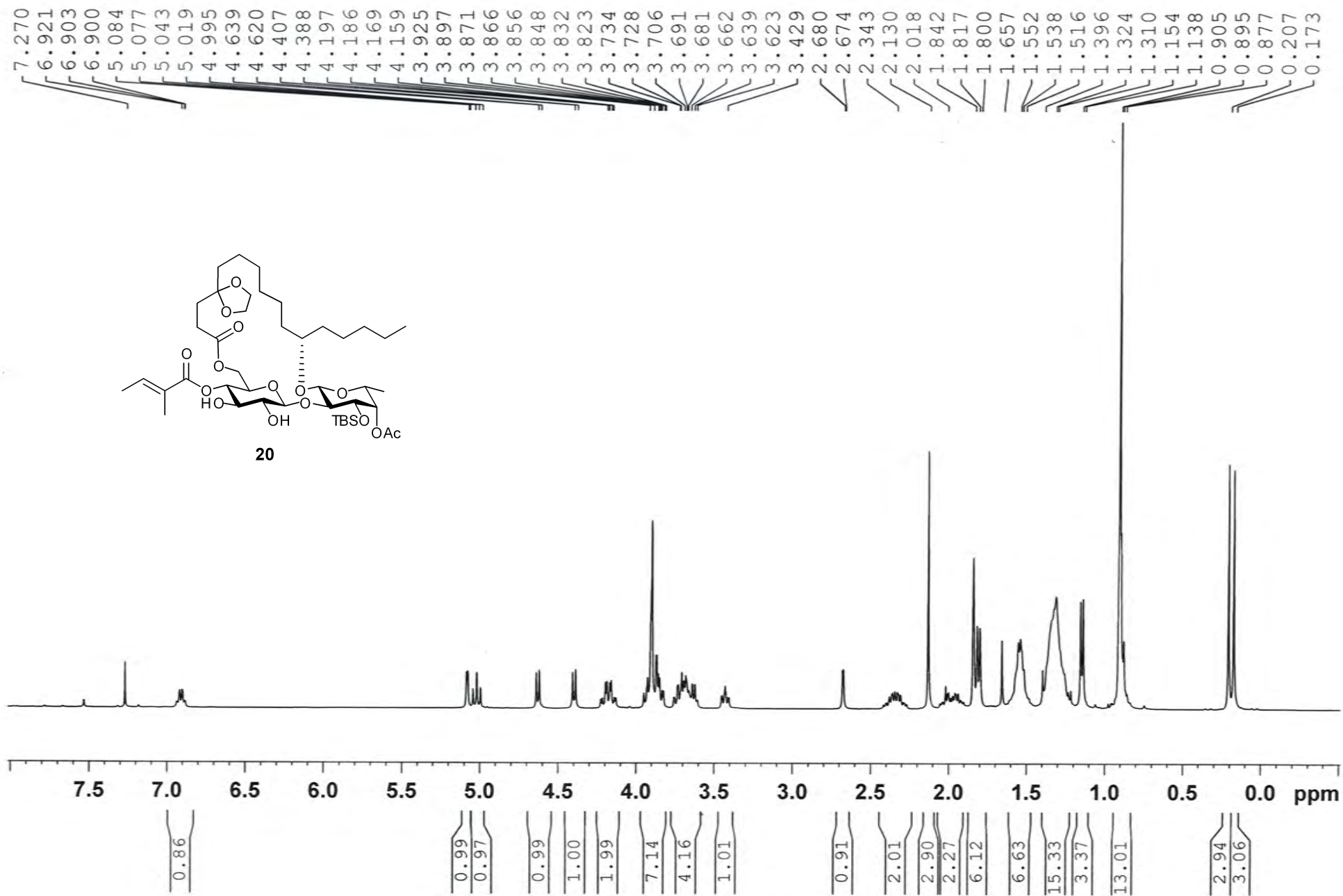
NAME ZGH-Ipom-2-140-B-150209  
 EXPNO 4  
 PROCNO 1  
 Date 20150210  
 Time 6.36  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hsqcetgpsi  
 TD 1024  
 SOLVENT CDCl3  
 NS 8  
 DS 16  
 SWH 5341.880 Hz  
 FIDRES 5.216680 Hz  
 AQ 0.0958964 sec  
 RG 2050  
 DW 93.600 usec  
 DE 6.50 usec  
 TE 293.6 K  
 CNST2 145.000000  
 D0 0.0000300 sec  
 D1 1.5000000 sec  
 D4 0.00172414 sec  
 D11 0.03000000 sec  
 D13 0.0000400 sec  
 D16 0.00020000 sec  
 D24 0.00110000 sec  
 IN0 0.00003000 sec  
 ZGPTNS

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 P2 20.00 usec  
 P28 1000.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1324057 MHz

===== CHANNEL f2 =====  
 CPDPRG2 garp  
 NUC2 13C  
 P3 10.00 usec  
 P4 20.00 usec  
 PCPD2 75.00 usec  
 PL2 -2.10 dB  
 PL12 15.40 dB  
 PL2W 58.37759399 W  
 PL12W 1.03811681 W  
 SFO2 100.6202727 MHz

===== GRADIENT CHANNEL =====  
 GPNAM1 SINE.100  
 GPNAM2 SINE.100  
 GPZ1 80.00 %  
 GPZ2 20.10 %  
 P16 1000.00 usec  
 ND0 2  
 TD 256  
 SFO1 100.6203 MHz  
 FIDRES 65.104164 Hz  
 SW 165.639 ppm  
 FmMODE Echo-Antiecho  
 SI 1024  
 SF 400.1300000 MHz  
 WDW QSINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.00  
 SI 1024  
 MC2 echo-antiecho  
 SF 100.6127690 MHz  
 WDW QSINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0

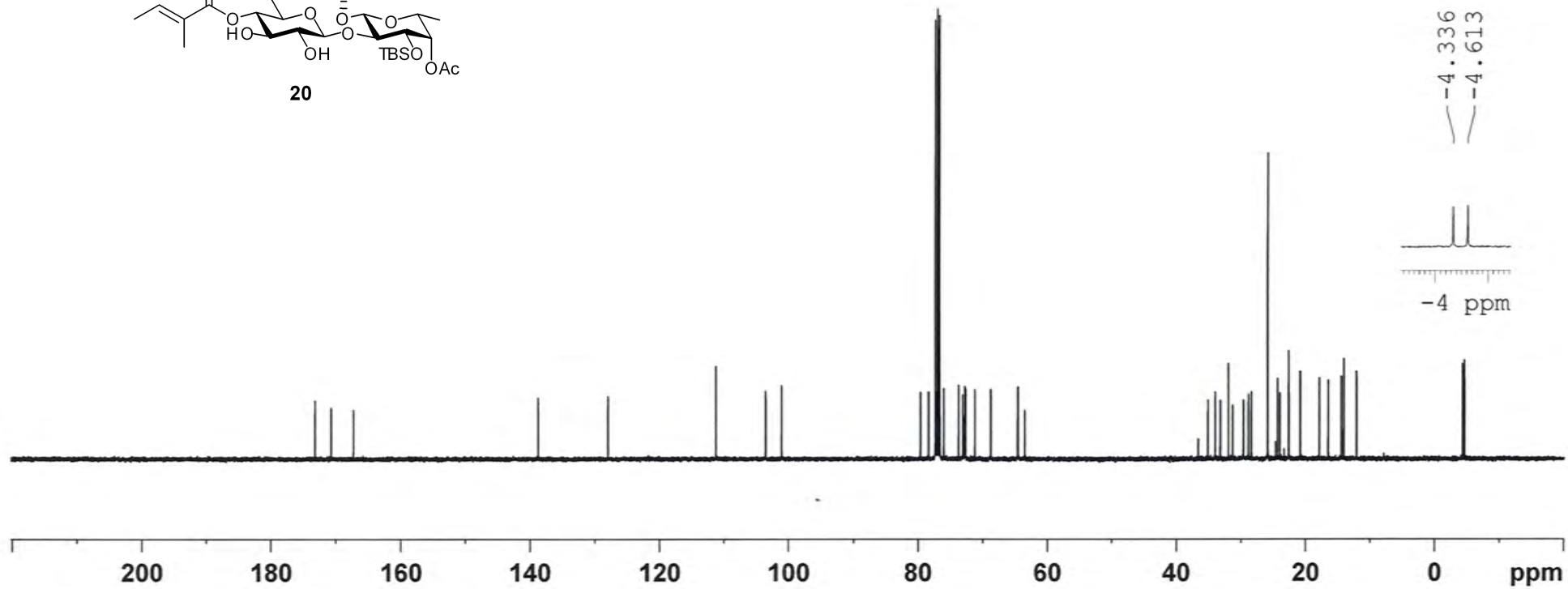
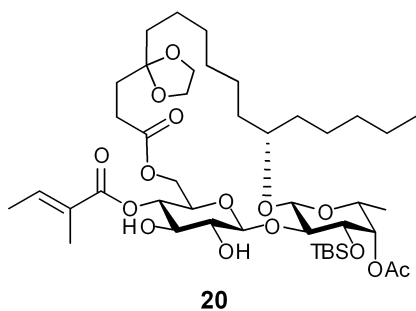


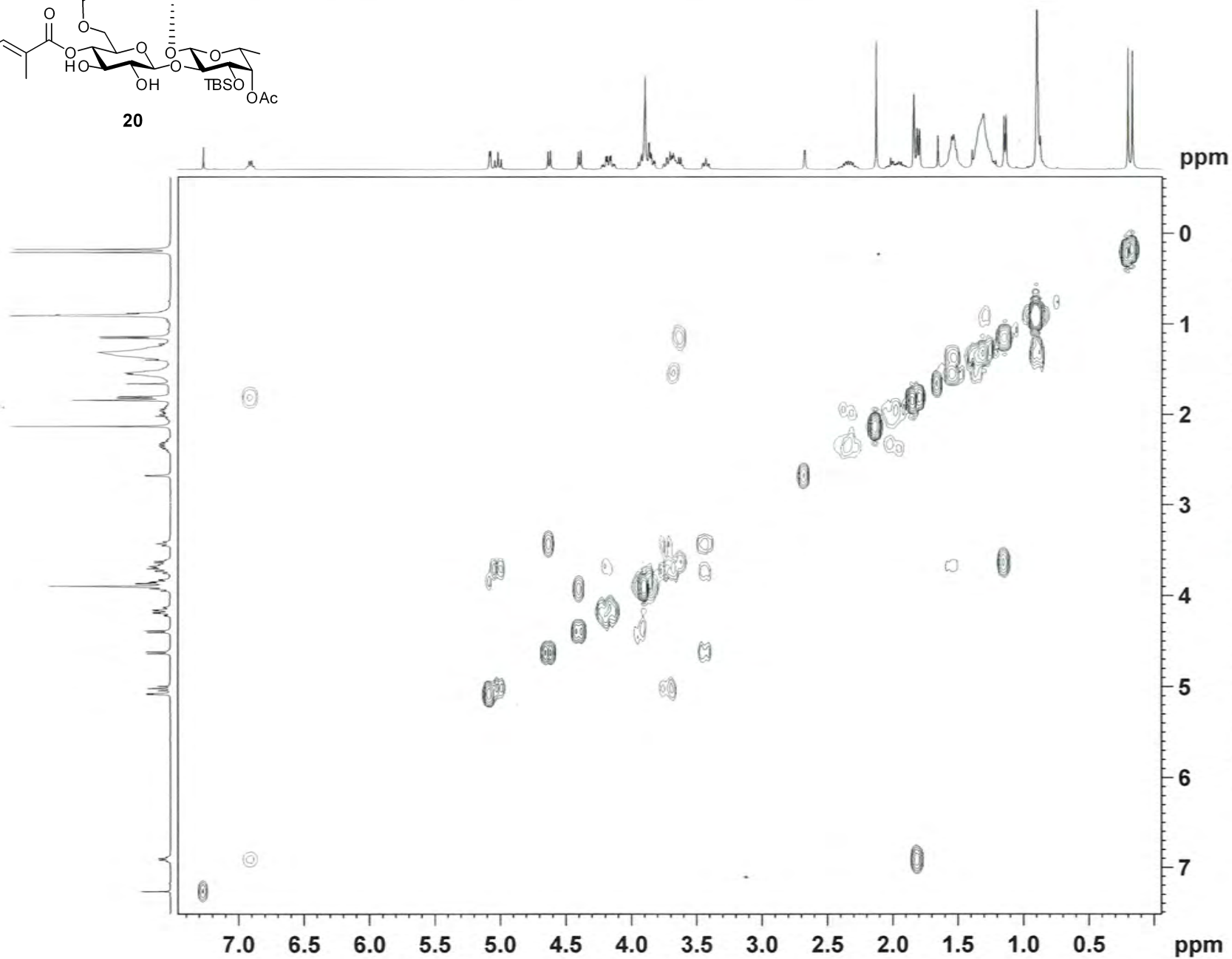
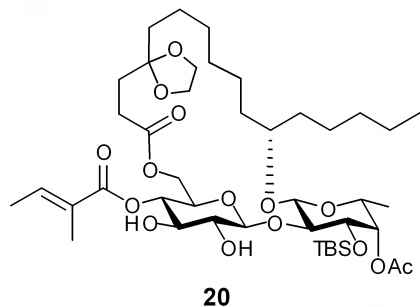
ZGH-*Ipom*-3-159-161101-A in CDCl<sub>3</sub>

ZGH-*Ipom*-3-159-161101-A <sup>13</sup>C in CDCl<sub>3</sub>

173.191  
170.708  
167.286

138.732  
127.967  
111.220  
103.495  
101.032  
79.631  
78.380  
77.317  
77.000  
76.682  
76.023  
73.743  
73.079  
72.785  
72.685  
71.209  
68.751  
64.598  
64.535  
63.480  
35.105  
33.984  
33.203  
31.953  
31.315  
29.628  
28.845  
28.402  
25.876  
24.353  
23.992  
22.624  
22.587  
20.834  
17.853  
16.478  
14.455



ZGH-*Ipom*-3-159-161101-A in CDCl<sub>3</sub>

Current Data Parameters  
 NAME ZGH-*Ipom*-3-159-161101-A  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161102  
 Time\_ 6.08  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosyppf  
 TD 2048  
 SOLVENT CDCl<sub>3</sub>  
 NS 16  
 DS 8  
 SMH 8012.820 Hz  
 FIDRES 3.912510 Hz  
 AQ 0.1277952 sec  
 RG 114  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.8 K  
 DO 0.00000300 sec  
 D1 1.50000000 sec  
 D16 0.00020000 sec  
 INO 0.00012480 sec

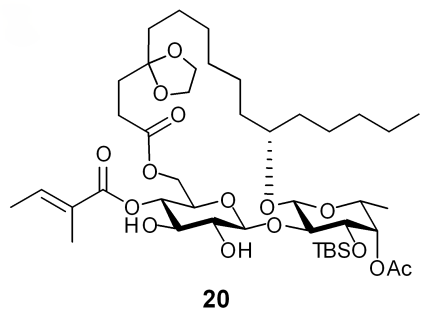
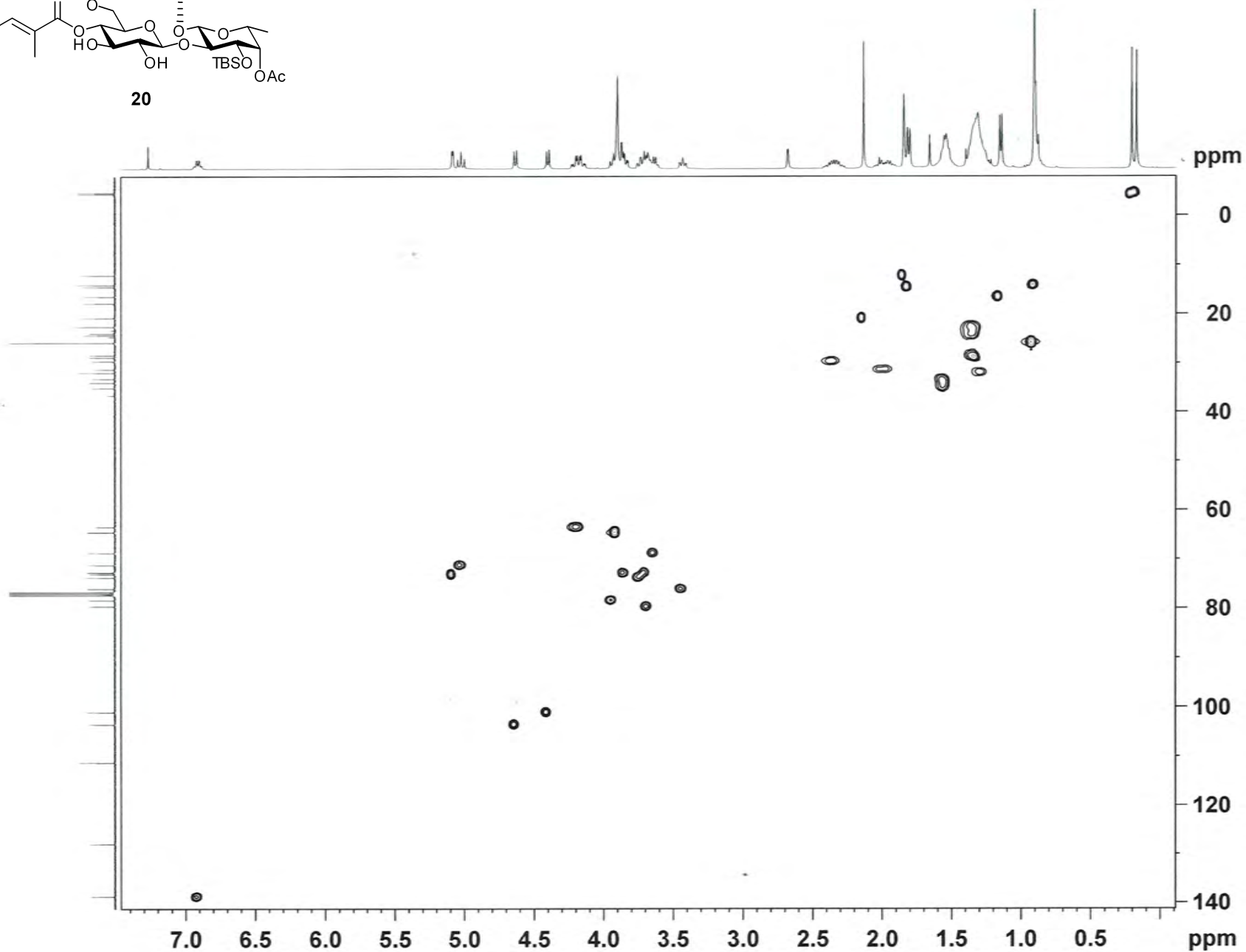
----- CHANNEL f1 -----  
 SF01 400.1520009 MHz  
 NUC1 1H  
 PO 12.50 usec  
 P1 12.50 usec  
 PLM1 20.00000000 W

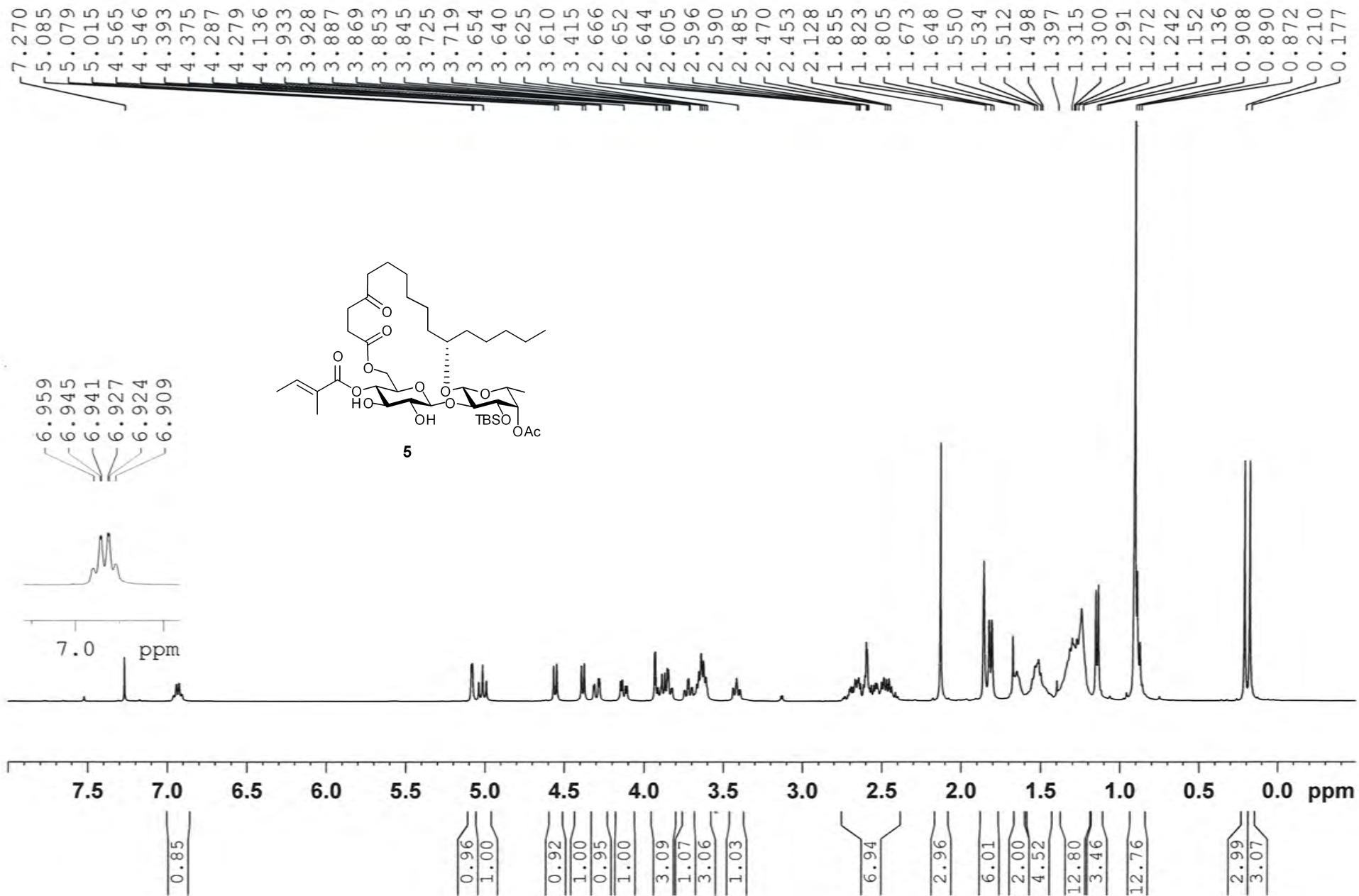
----- GRADIENT CHANNEL -----  
 GPNAM[1] SMSQ10.100  
 GP21 10.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters  
 TD 128  
 SF01 400.152 MHz  
 FIDRES 62.600159 Hz  
 SW 20.024 ppm  
 FxMODE QF

F2 - Processing parameters  
 SI 1024  
 SF 400.1500070 MHz  
 MDW QSINE  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 QF  
 SF 400.1500052 MHz  
 MDW QSINE  
 SSB 0  
 LB 0 Hz  
 GB 0

ZGH-*Ipom*-3-159-161101-A HSQC in CDCl<sub>3</sub>

ZGH-*Ipom*-3-179-170111-A(2) in CDCl<sub>3</sub>

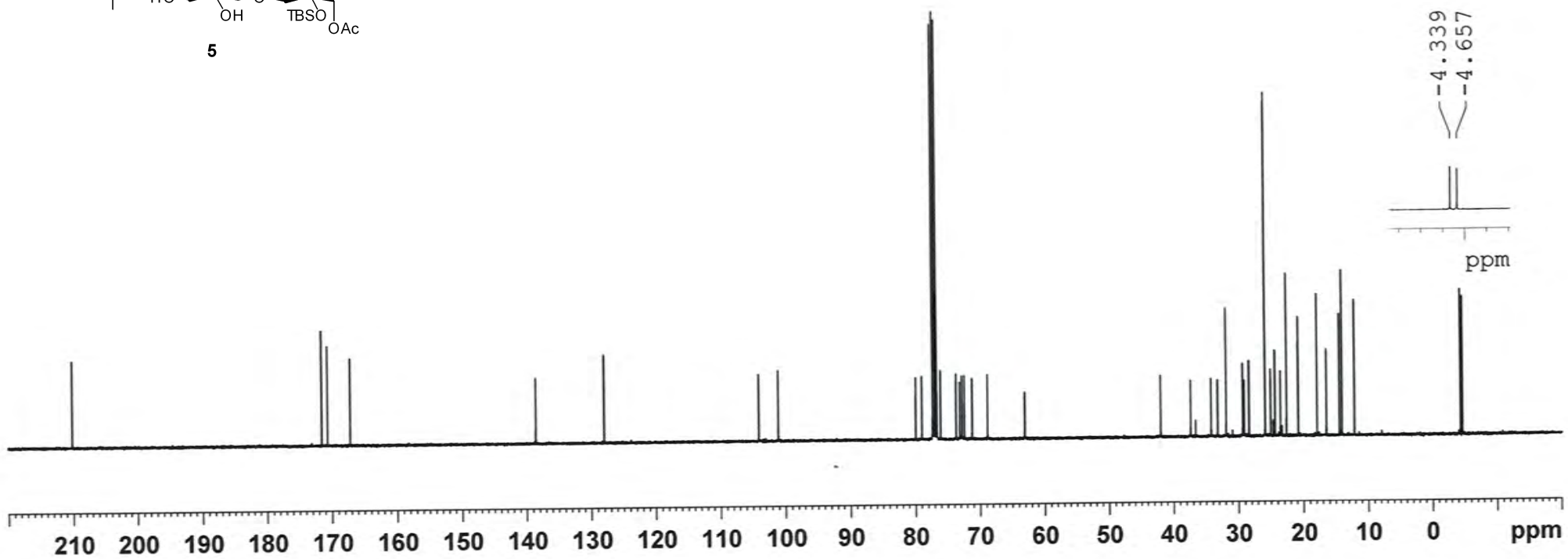
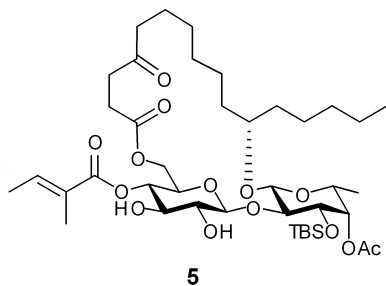
ZGH-Ipom-3-179-170111-A(2) 13C in CDC13

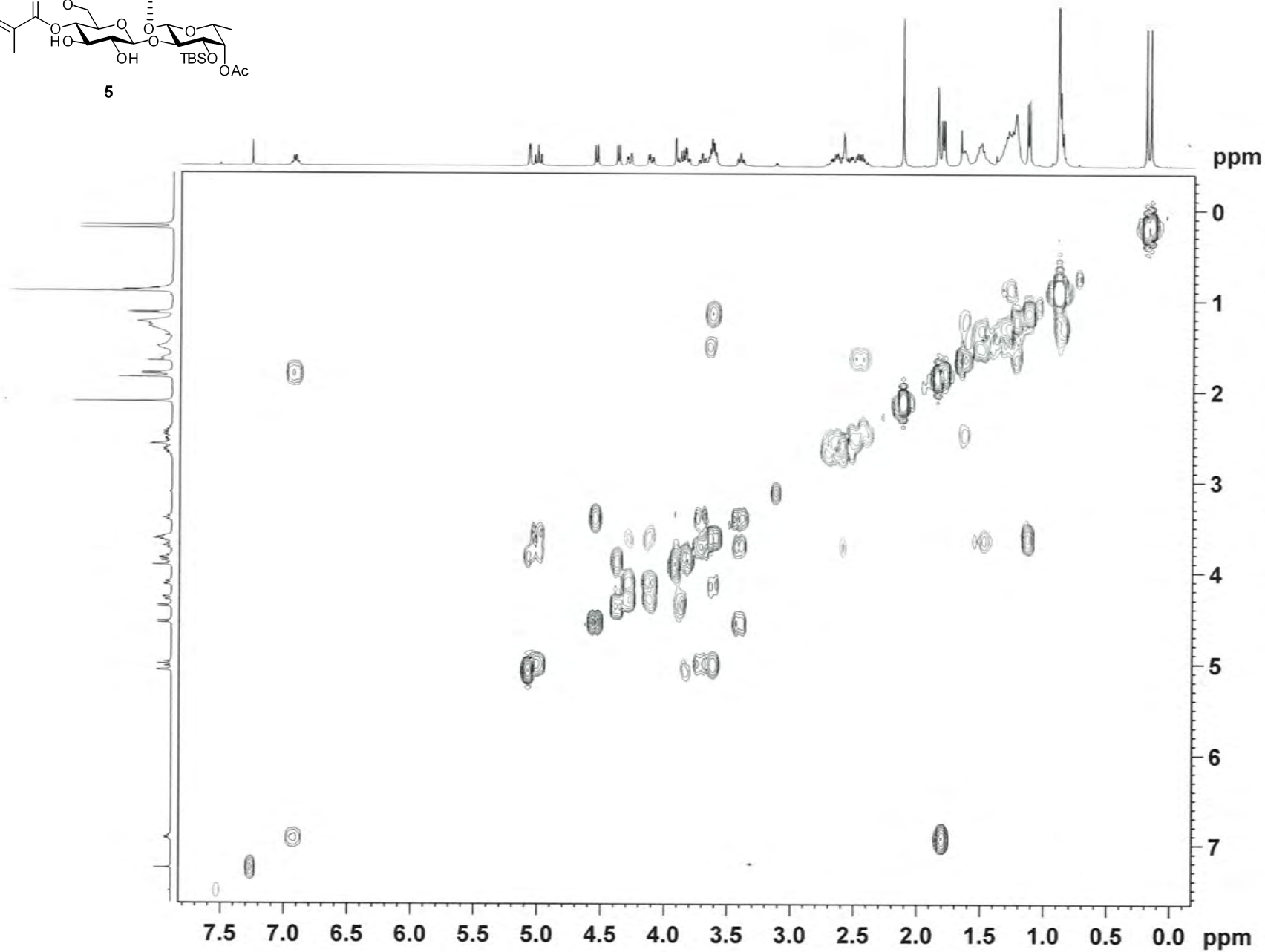
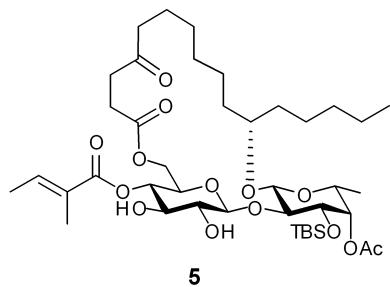
—210.221

 < 171.617  
 < 170.690  
 < 167.221

—138.594

—128.048

 104.116  
 101.114  
 79.943  
 78.990  
 77.318  
 77.000  
 76.683  
 76.083  
 73.672  
 73.118  
 72.789  
 72.391  
 71.213  
 68.819  
 63.079  
 41.990  
 37.377  
 34.200  
 33.219  
 31.923  
 29.358  
 29.114  
 28.380  
 25.894  
 25.045  
 24.385  
 23.554  
 22.633  
 20.821  
 17.900  
 16.467  
 14.446  
 14.056  
 12.128


ZGH-*Ipom*-3-179-170111-A(2) in CDCL<sub>3</sub>

```

Current Data Parameters
NAME      ZGH-Ipom-3-179-170111-A(2)
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20170315
Time     6.34
INSTRUM  spect
PROBHD   5 mm PABBO 90-
PULPROG  zgpg30
TD        32768
SOLVENT  CDCl3
NS        16
DS        8
SFO      400.141800 MHz
FIDRES   0.1277902 sec
AQ        0.1277902 sec
RG         101
SWH       42.400 MHz
DE         4.70 usec
TE        299.6 K
DQ         0.0000000 sec
SFO1     1.5000000 MHz
SFO2     0.0600040 MHz
SFO3     0.0600000 MHz
SFO4     0.0600000 MHz
SFO5     0.0600000 MHz
SFO6     0.0600000 MHz

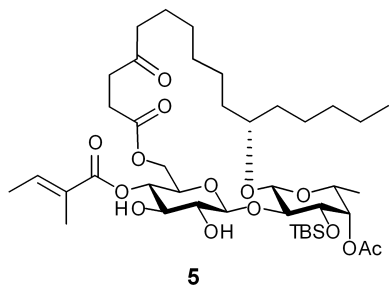
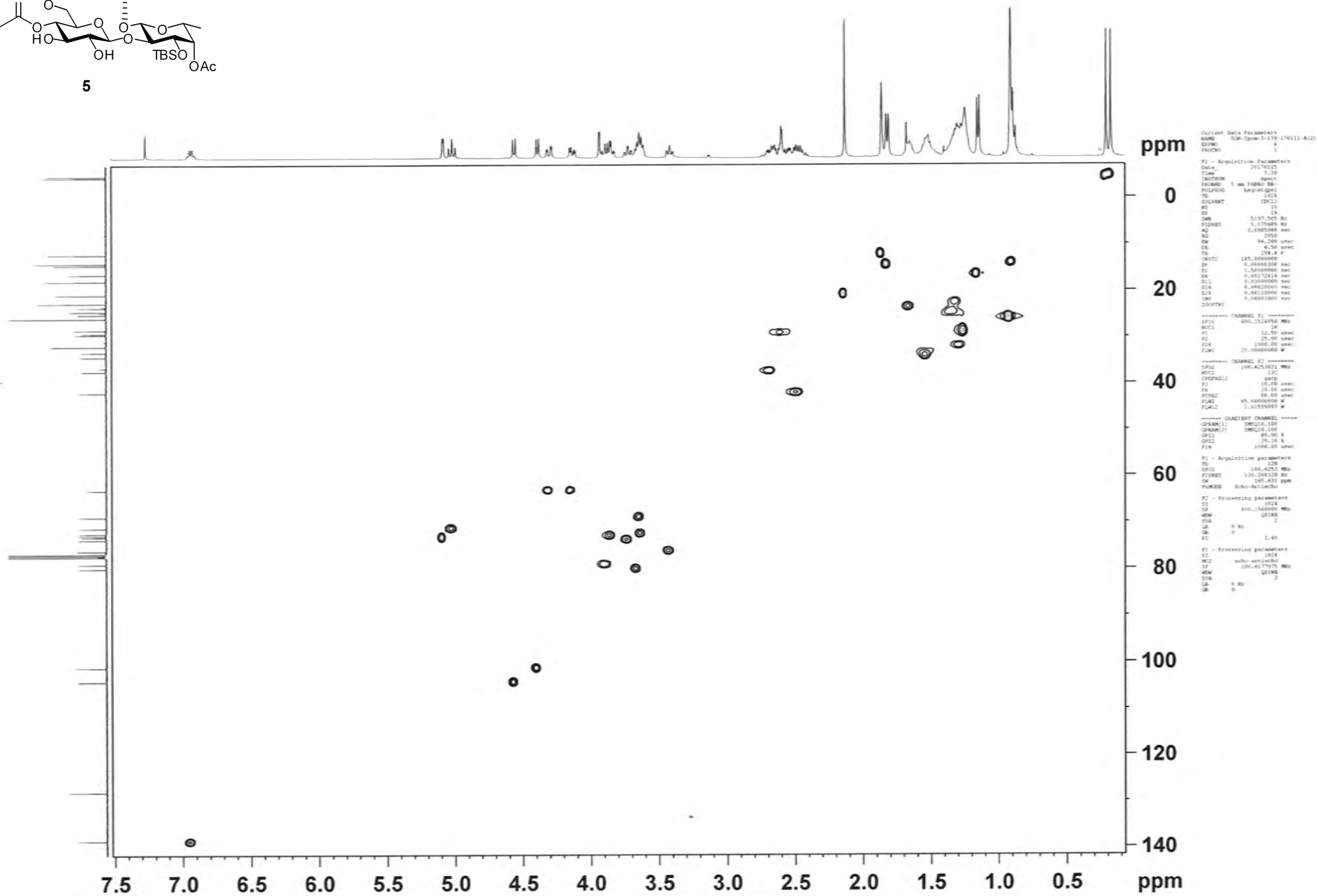
----- CHANNEL f1 -----
SFO1     400.141800 MHz
NUC1     13C
P1        12.00 usec
PL1       0.00 dB
PL12     12.00 usec
PL12     20.0000000 dB

----- GRADIENT CHANNEL -----
GPMAX1   800.00000 MHz
GPI1     10.00 A
P14      1000.00 usec

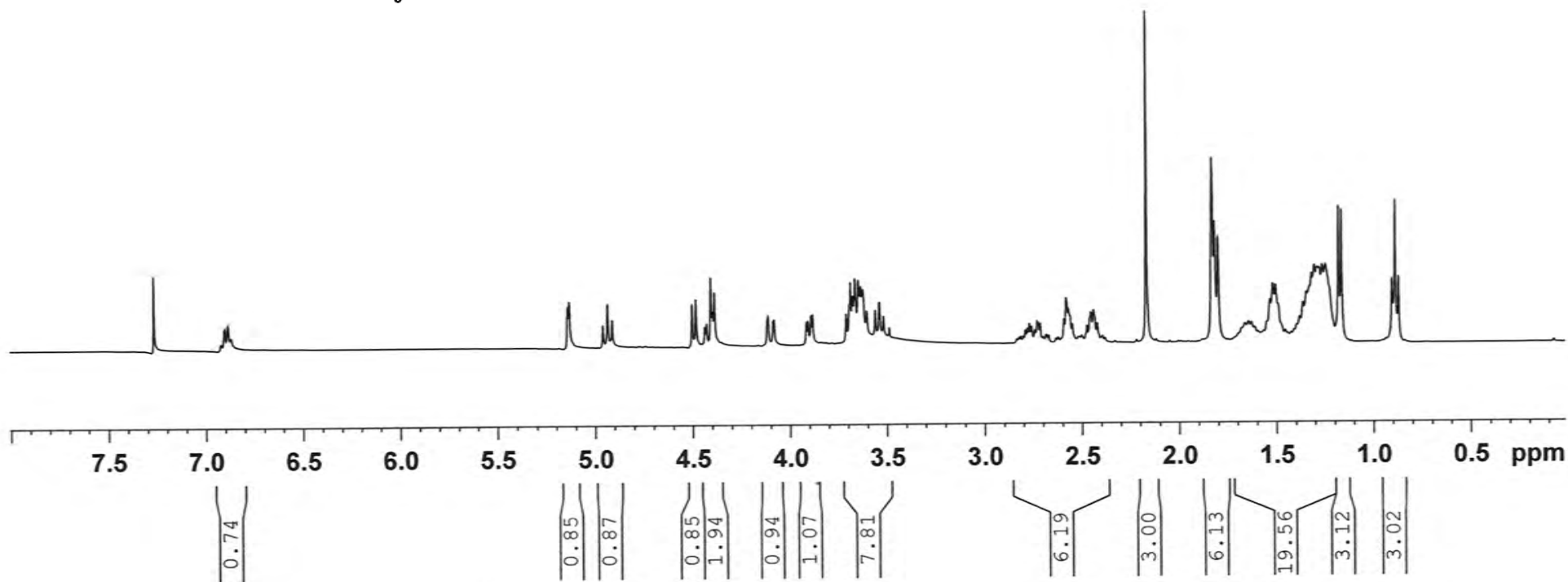
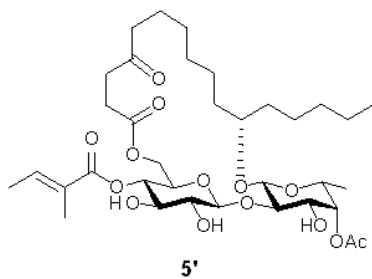
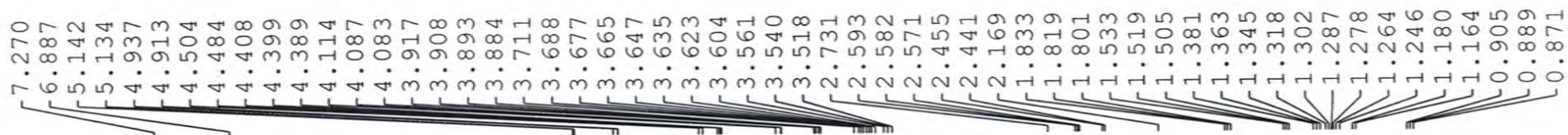
F1 - Acquisition parameters
TD        128
SFO1     400.141800 MHz
FIDRES   42.400159 MHz
SWH       20.004 ppm
FNUC1    13C

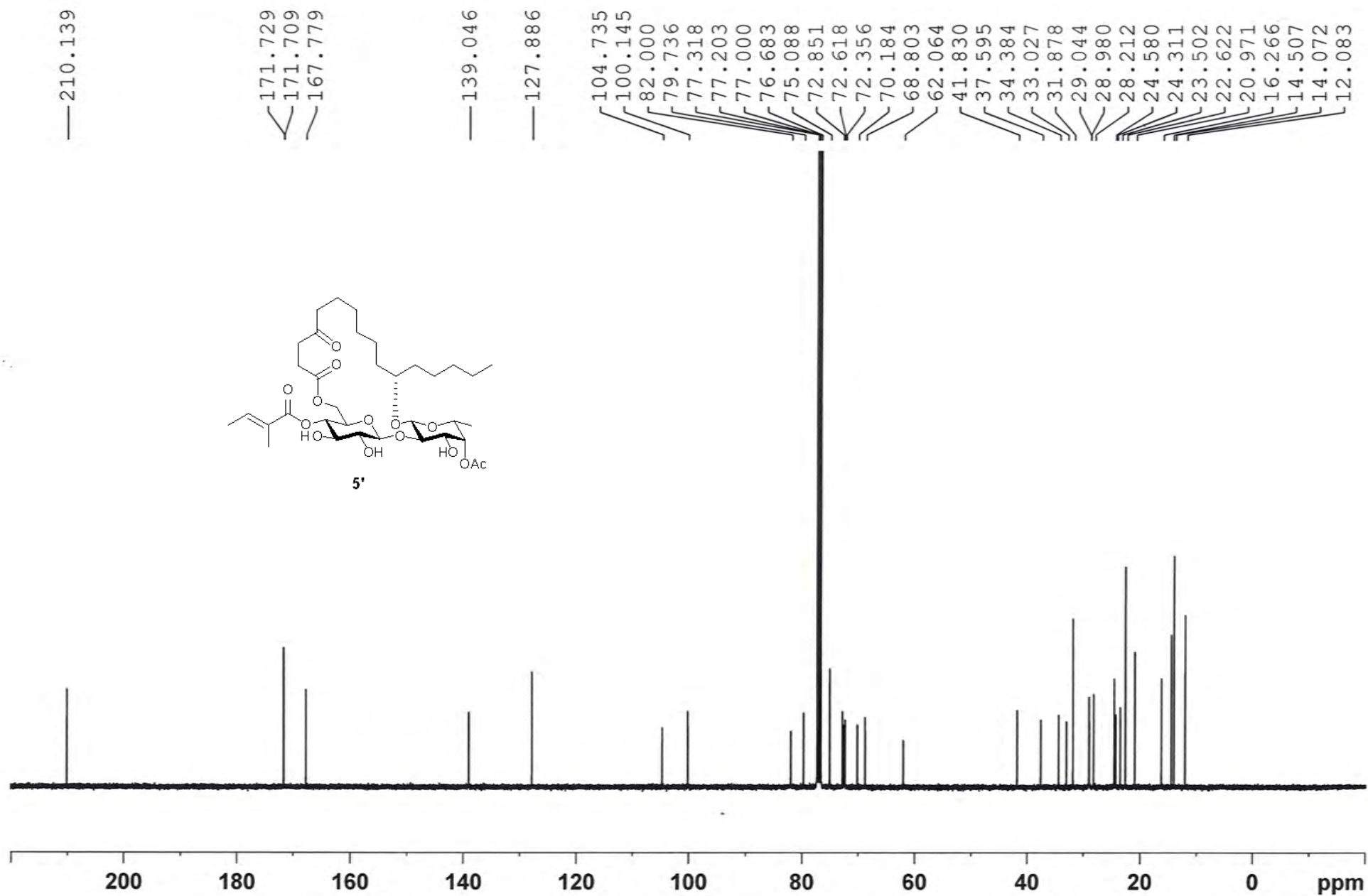
F2 - Processing parameters
SI        1024
SF        400.1400000 MHz
WDW       EM
SSB       0
LB        0 Hz
GB        0
PC        1.00

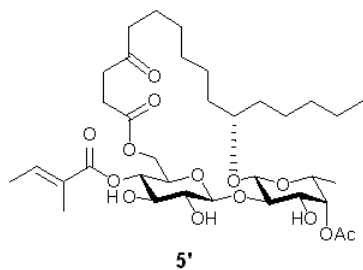
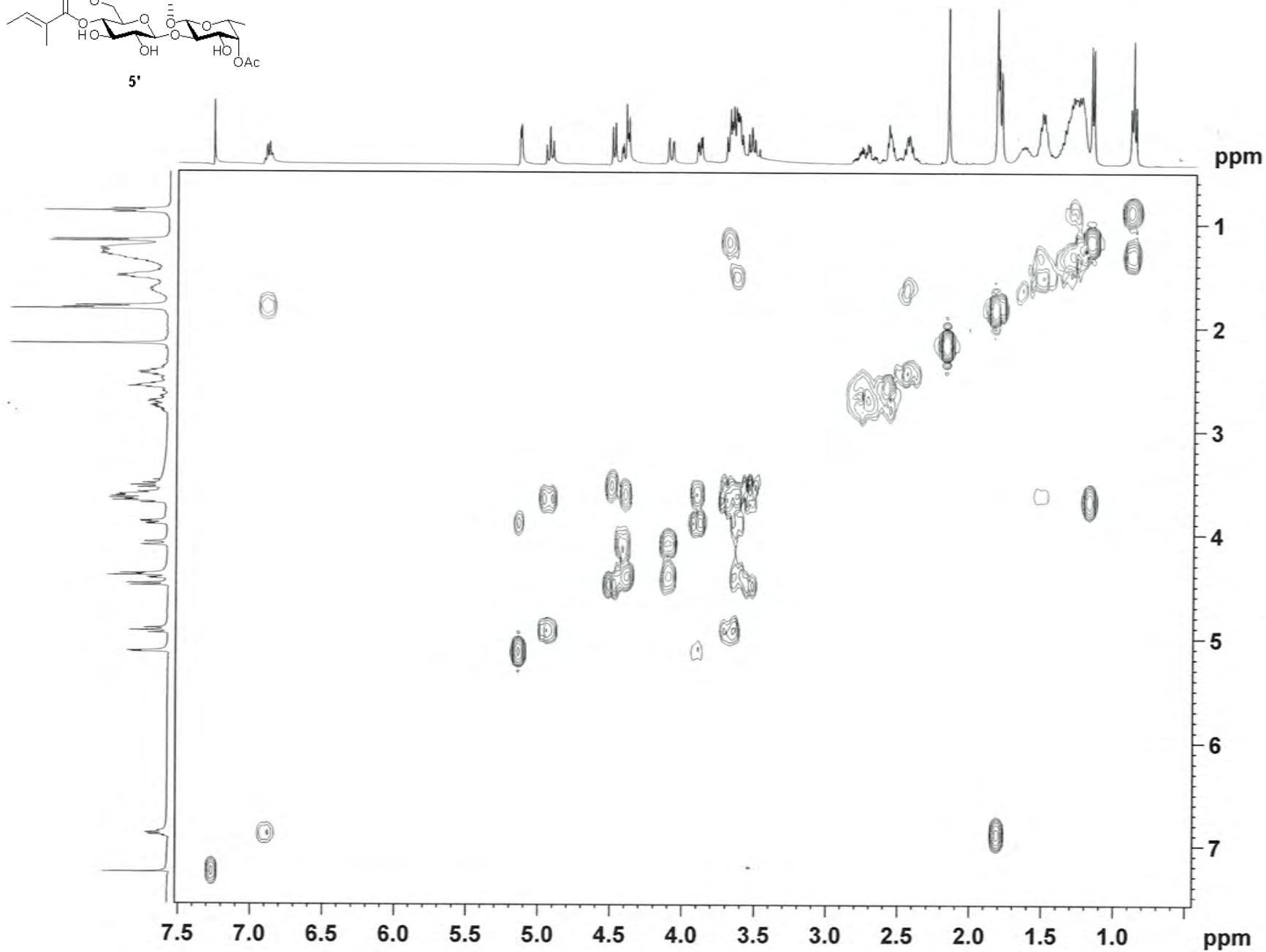
F1 - Processing parameters
SI        1024
SF        400.1400000 MHz
WDW       EM
SSB       0
LB        0 Hz
GB        0
PC        0
  
```

ZGH-*Ipom*-3-179-170111-A(2) HSQC in CDCl<sub>3</sub>



ZGH-*Ipom*-3-179-170111-B in CDCl<sub>3</sub>

ZGH-*Ipom*-3-179-170111-B 13C in CDCl<sub>3</sub>

ZGH-Ipom-3-179-170111-B in CDCl<sub>3</sub>

```

Current Data Parameters
NAME      ZGH-Ipom-3-179-170111-B
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20170527
Time      6.21
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         2048
SOLVENT   CDCl3
NS         24
DS         8
SWH        8012.820 Hz
FIDRES     0.121510 Hz
AQ         0.127192 sec
RG         263
INW        62.400 usec
DE         6.50 usec
TE         295.1 K
D0         0.0000100 sec
D1         1.5000000 sec
D11        0.0000000 sec
D16        0.0002000 sec
D18        0.0012480 sec

----- CHANNEL f1 -----
SFO1      400.150000 MHz
NUC1      1H
P0         12.50 usec
P1         12.50 usec
PL1        20.0000000 dB

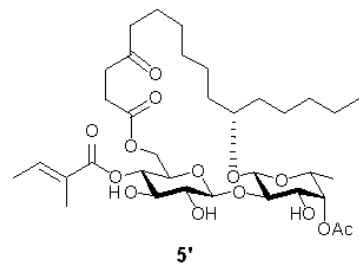
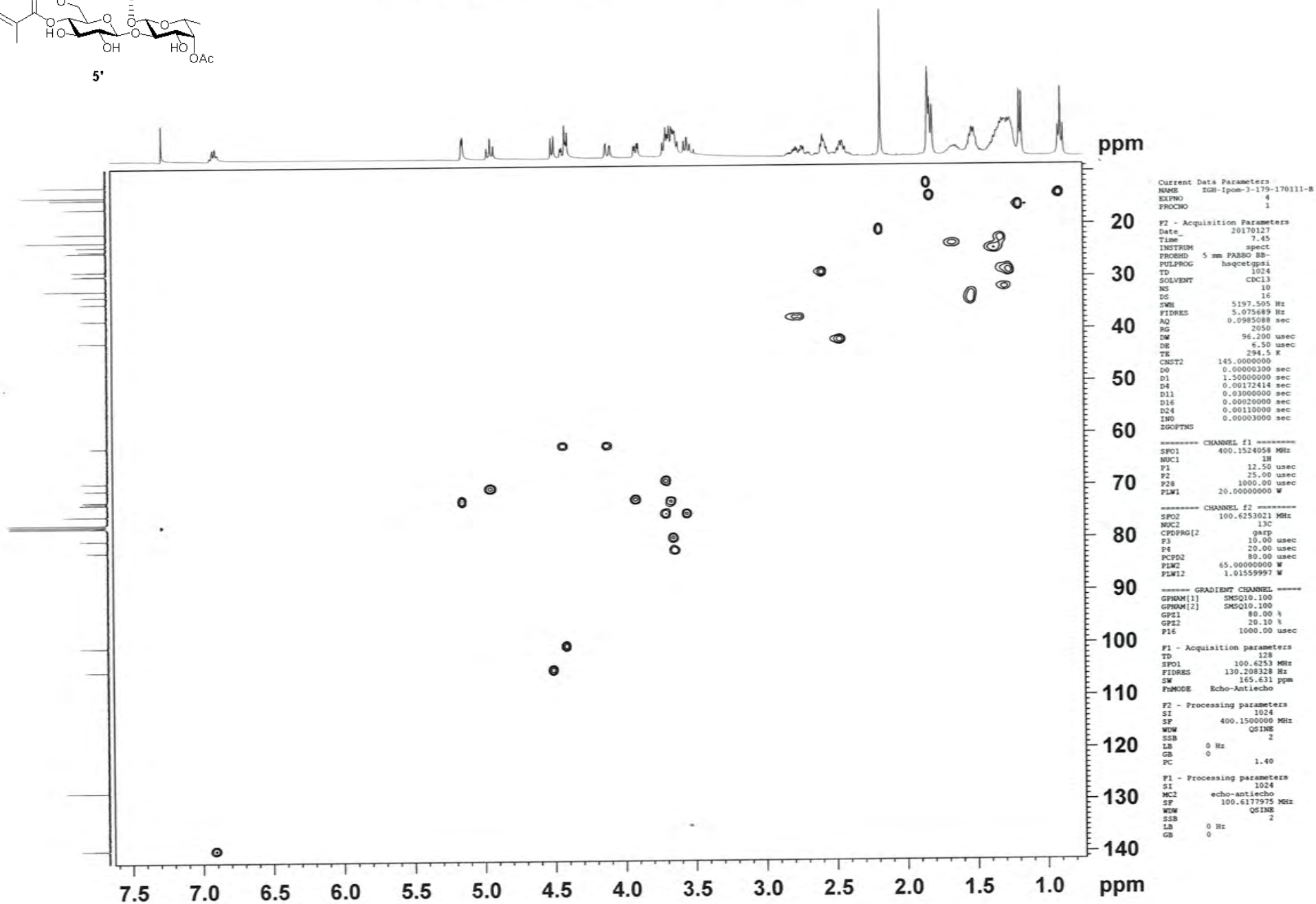
----- GRABENT CHANNEL -----
GRABENT1  SWH20.100
GPR1      10.00 K
P16        1000.00 usec

F1 - Acquisition parameters
TD         327
SFO1      400.151 MHz
FIDRES     62.600159 Hz
SW         20.024 ppm
PULPROG   zgpg30

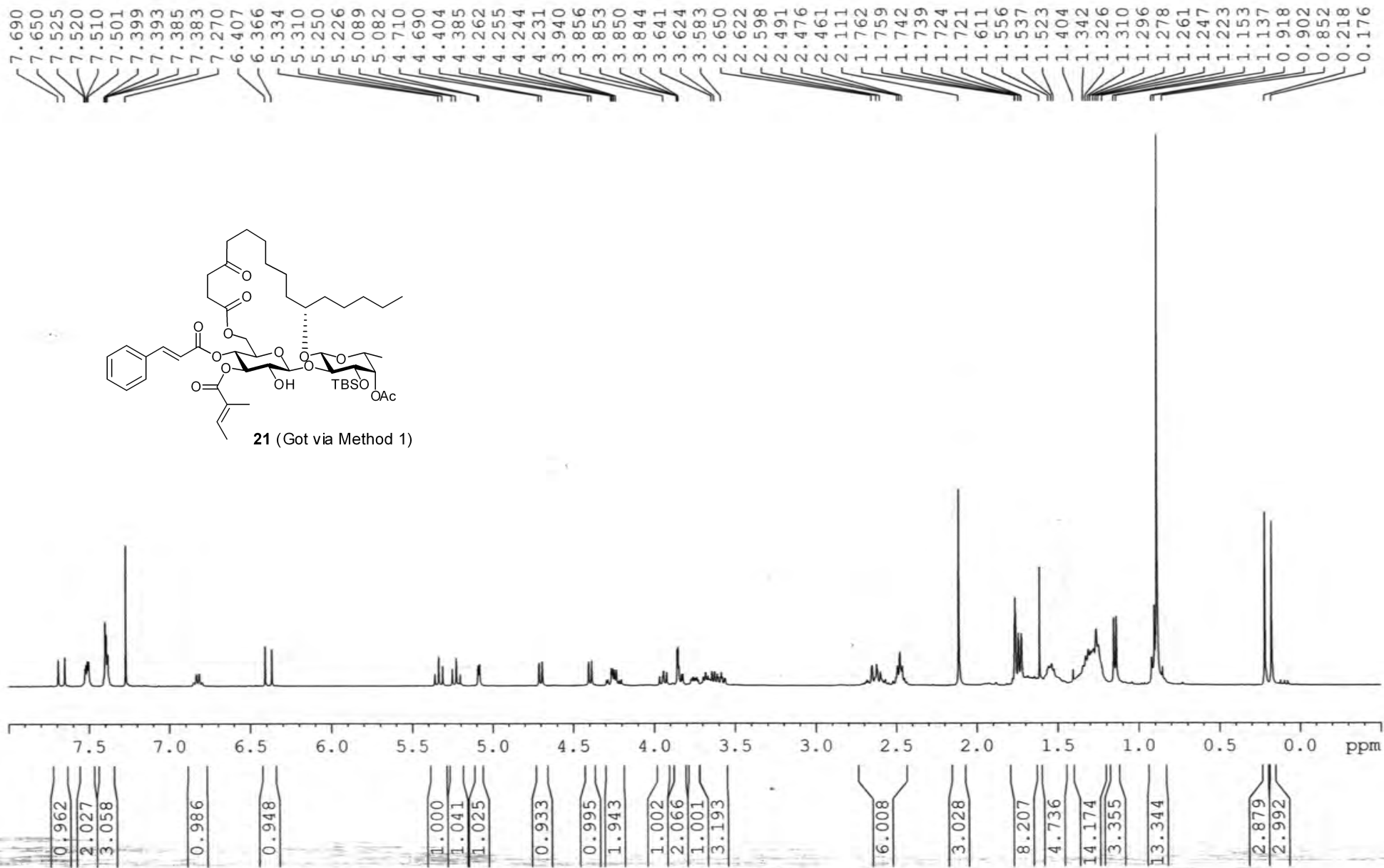
F2 - Processing parameters
SI         1024
SF         400.1500070 MHz
WDW        QMINE
SSB         0
LA         0 Hz
GB         0
PC         1.00

F1 - Processing parameters
SI         1024
SF         400.1500000 MHz
WDW        QMINE
SSB         0
LA         0 Hz
GB         0

```

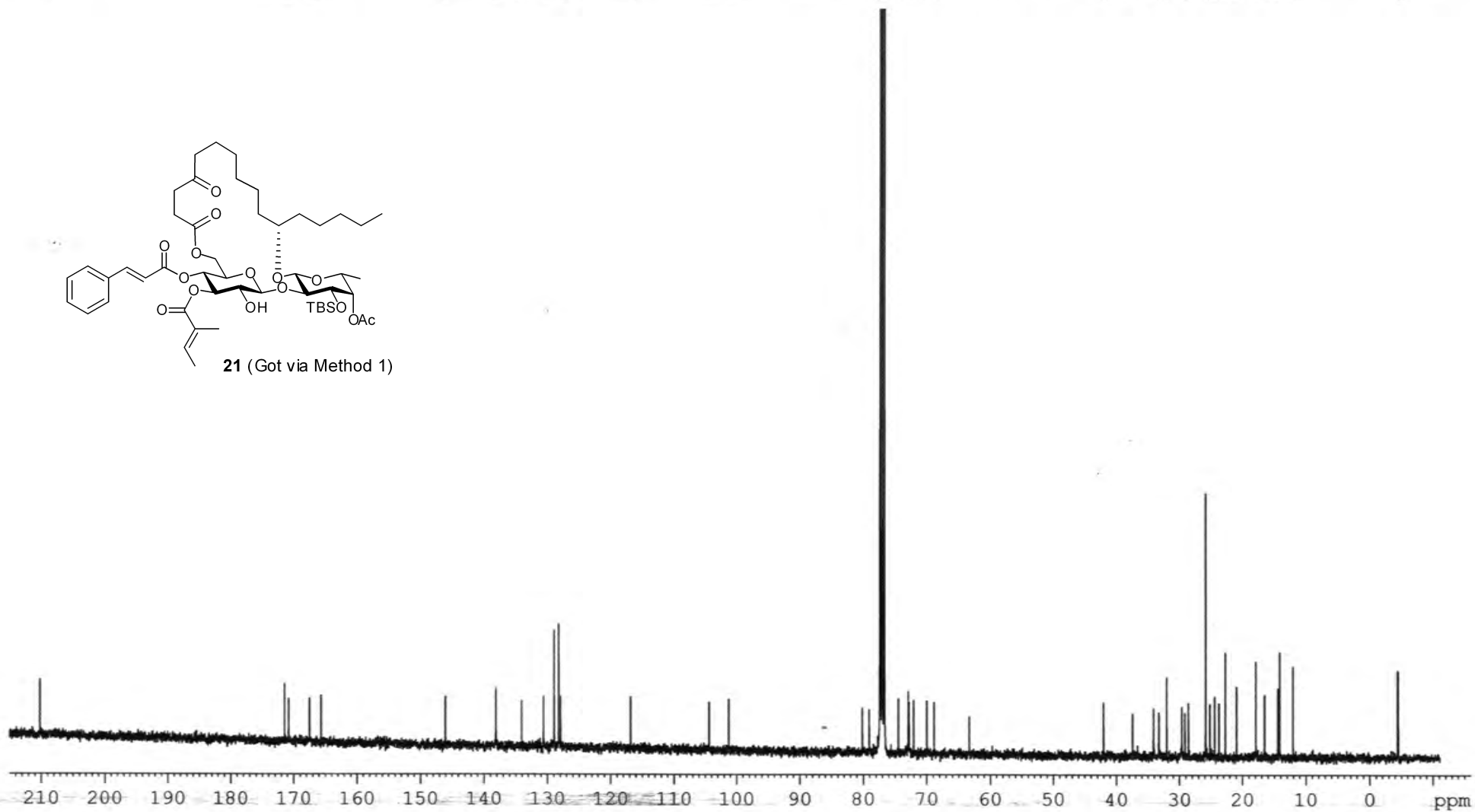
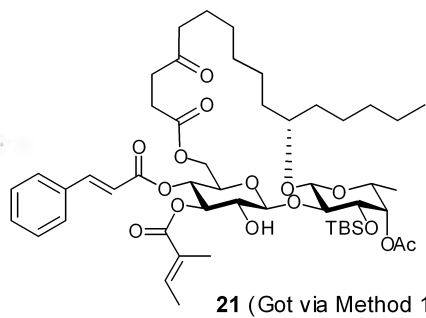
ZGH-Ipom-3-179-170111-B HSQC in CDCl<sub>3</sub>

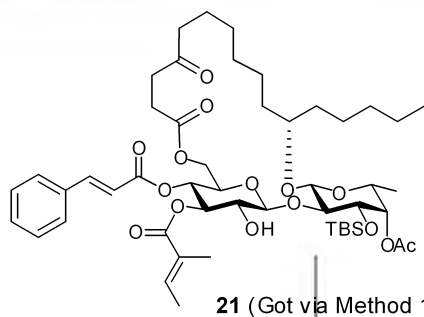
## ZGH-Ipom-2-143-A-150423 1H in CDCL3



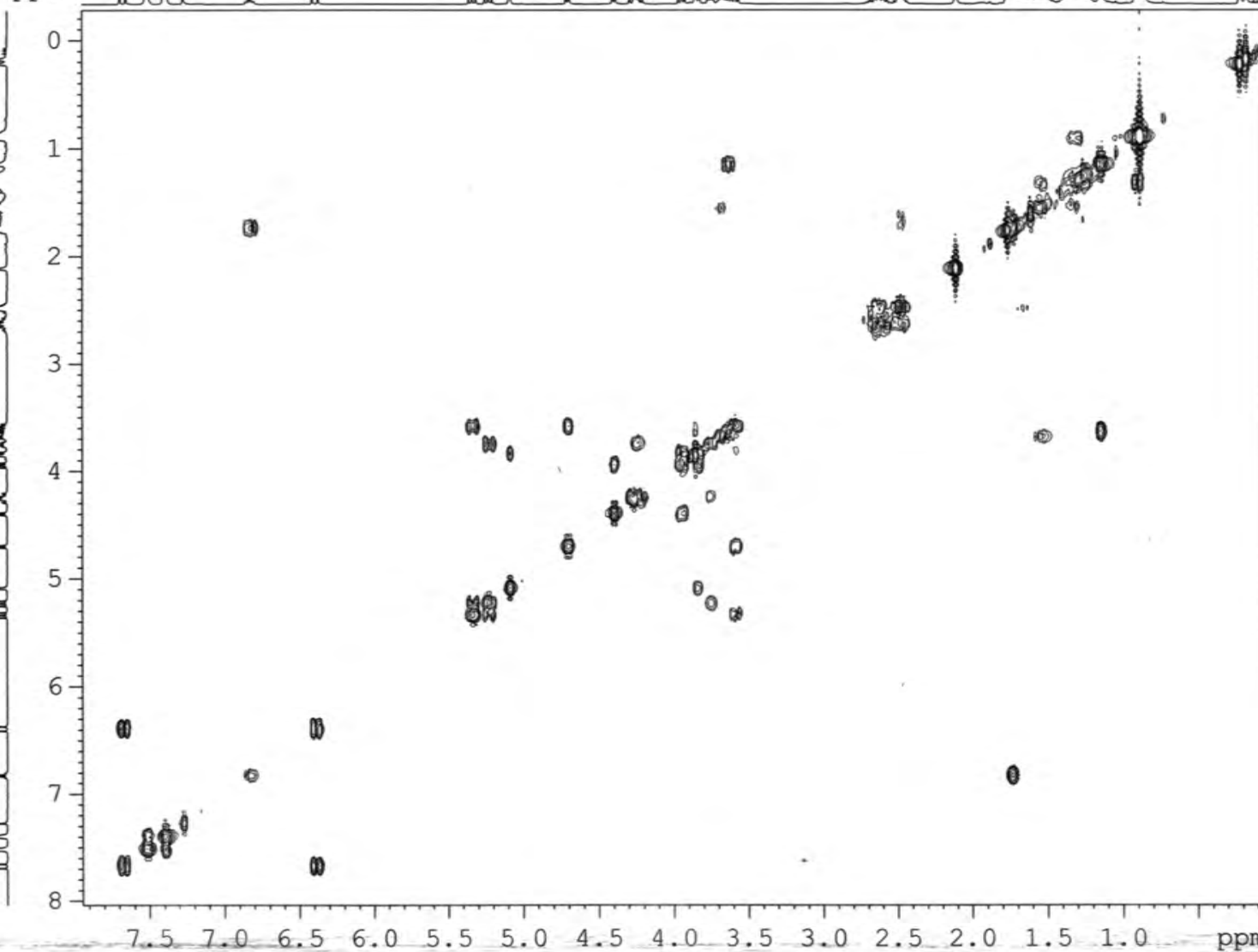
ZGH-*Ipom*-2-143-A-150423 <sup>13</sup>C in CDCl<sub>3</sub>

— 210.137

— 171.446  
— 170.803  
— 167.450  
— 165.633— 146.048  
— 138.107  
— 134.046  
— 130.583  
— 128.915  
— 128.214  
— 127.948  
— 116.824— 104.359  
— 101.196  
80.156  
79.018  
77.317  
77.203  
77.000  
76.683  
74.464  
72.878  
72.768  
72.017  
69.934  
68.820  
63.297  
41.993  
37.430  
34.103  
33.224  
31.973  
29.588  
29.089  
28.566  
25.794  
25.125  
24.354  
23.665  
22.649  
20.888  
17.857  
16.483  
14.366  
14.092  
11.989  
-4.417  
-4.572

ZGH-*Ipom*-2-143-A-150423 COSY

ppm



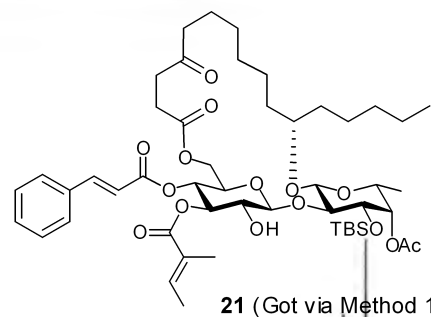
NAME ZGH-*Ipom*-2-143-A-150423  
 EXPNO 2  
 PROCNO 1  
 Date 20150429  
 Time 22.20  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 FULPROG cosygpgf  
 TD 2048  
 SOLVENT CDCl3  
 NS 8  
 DS 8  
 SWH 5341.880 Hz  
 FIDRES 2.608340 Hz  
 AQ 0.1917428 sec  
 RG 203  
 DW 93.600 usec  
 DE 6.50 usec  
 TE 292.2 K  
 D0 0.00000300 sec  
 D1 1.48689198 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 IN0 0.00018720 sec

## ----- CHANNEL f1 -----

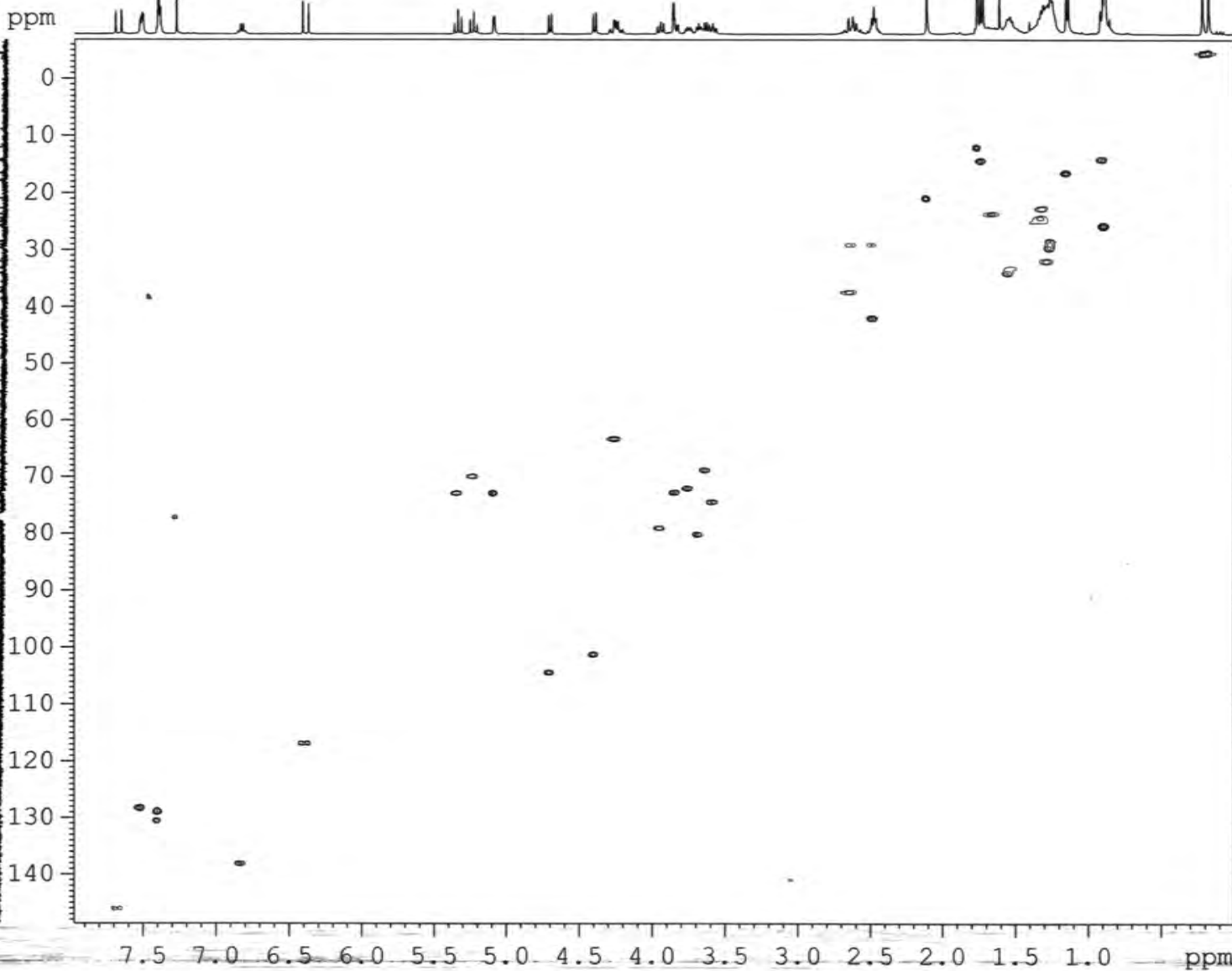
NUC1 1H  
 P0 10.00 usec  
 P1 10.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1324057 MHz

## ----- GRADIENT CHANNEL -----

GPNAME1 SINE.100  
 GPZ1 10.00 usec  
 P16 1000.00 usec  
 ND0 1  
 TD 128  
 SFO1 400.1324 MHz  
 FIDRES 41.733440 Hz  
 SW 13.350 ppm  
 FhMODE QF  
 SI 1024  
 SF 400.1300040 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00  
 SI 1024  
 MC2 QF  
 SF 400.1300033 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0



## ZGH-Ipom-2-143-A-150423 HSQC



NAME ZGH-Ipom-2-143-A-150423  
 EXPNO 4  
 PROCNO 1  
 Date\_ 20150430  
 Time 3.16  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hsqcetgpsi  
 TD 1024  
 SOLVENT CDC13  
 NS 8  
 DS 16  
 SWH 5341.880 Hz  
 FIDRES 5.216680 Hz  
 AQ 0.0958964 sec  
 RG 2050  
 DM 93.600 usec  
 DE 6.50 usec  
 TE 292.8 K  
 CNST2 145.000000  
 D0 0.0000300 sec  
 D1 1.5000000 sec  
 D4 0.00172414 sec  
 D11 0.0300000 sec  
 D13 0.0000400 sec  
 D16 0.0002000 sec  
 D24 0.0011000 sec  
 IN0 0.00003000 sec  
 ZGPTNS

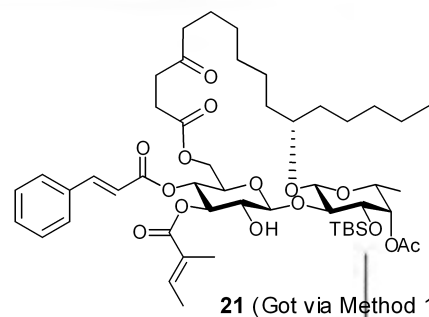
----- CHANNEL f1 -----  
 NUC1 1H  
 P1 10.00 usec  
 P2 20.00 usec  
 P28 1000.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1324057 MHz

----- CHANNEL f2 -----  
 CPDPRG2 garp  
 NUC2 13C  
 F3 10.00 usec  
 F4 20.00 usec  
 FCPD2 75.00 usec  
 PL2 -2.10 dB  
 PL12 15.40 dB  
 PL2W 58.37759399 W  
 PL12W 1.03811681 W  
 SFO2 100.6202727 MHz

----- GRADIENT CHANNEL -----  
 GPNAM1 SINE.100  
 GPNAM2 SINE.100  
 GFZ1 80.00 %  
 GFZ2 20.10 %  
 P16 1000.00 usec  
 ND0 2  
 TD 256  
 SFO1 100.6203 MHz  
 FIDRES 65.104164 Hz  
 SW 165.639 ppm  
 FmMODE Echo-Antiecho  
 SI 1024  
 SF 400.1300000 MHz  
 WDW QSINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.00  
 SI 1024  
 MC2 echo-antiecho  
 SF 100.6127690 MHz  
 WDW QSINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0



## ZGH-Ipom-2-143-A-150423 HMBC in CDCL3



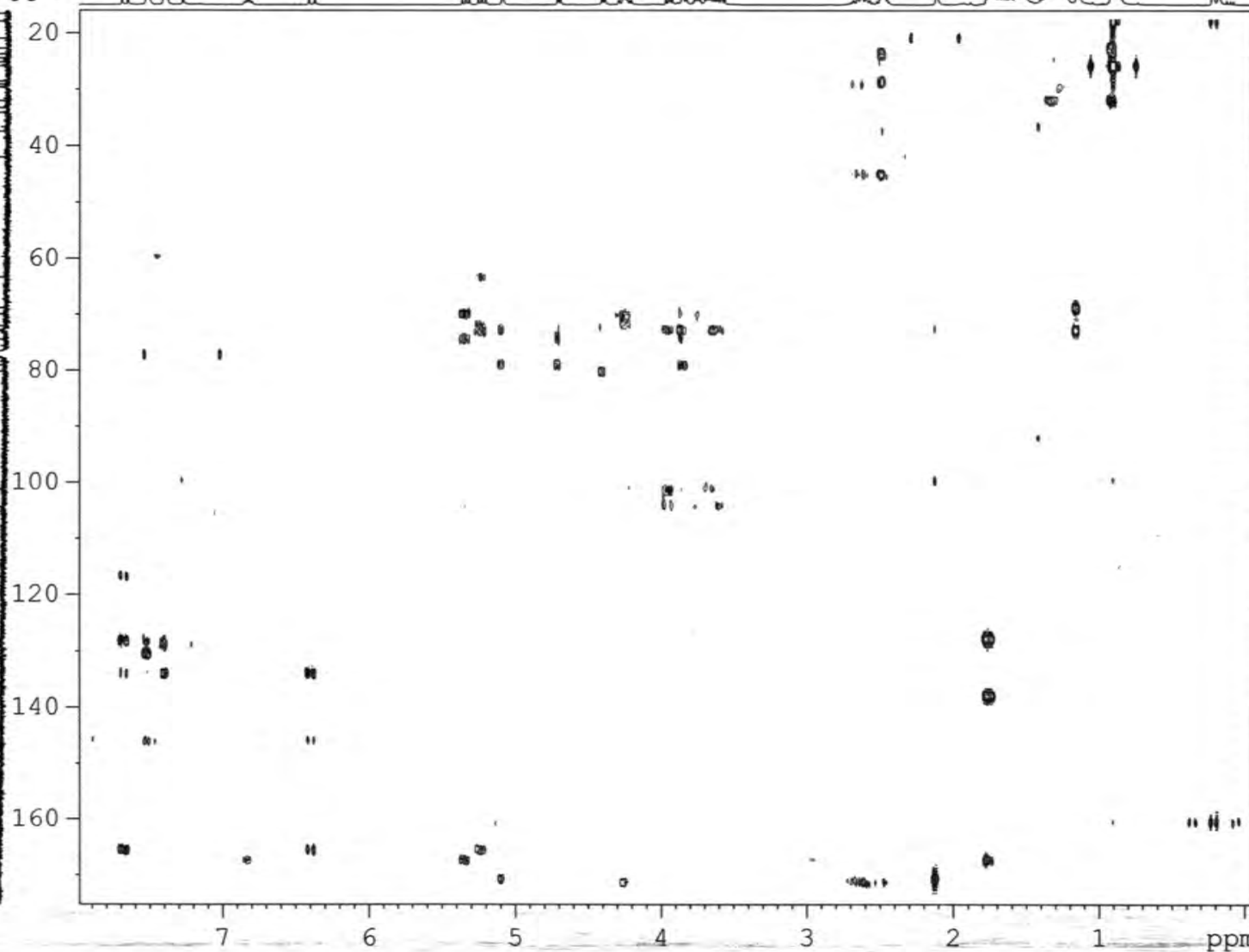
NAME ZGH-Ipom-2-143-A-150423  
 EXPNO 5  
 PROCNO 1  
 Date\_ 20150430  
 Time\_ 4.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hmbcgp1pdqf  
 TD 4096  
 SOLVENT CDCL3  
 NS 35  
 DS 16  
 SWH 5208.333 Hz  
 FIDRES 1.271566 Hz  
 AQ 0.3932660 sec  
 RG 2050  
 DW 96.000 usec  
 DE 6.50 usec  
 TE 292.3 K  
 CNST2 145.0000000  
 CNST13 10.0000000  
 D0 0.00000300 sec  
 D1 1.50000000 sec  
 D2 0.00344828 sec  
 D6 0.05000000 sec  
 D16 0.00020000 sec  
 IN0 0.00003010 sec

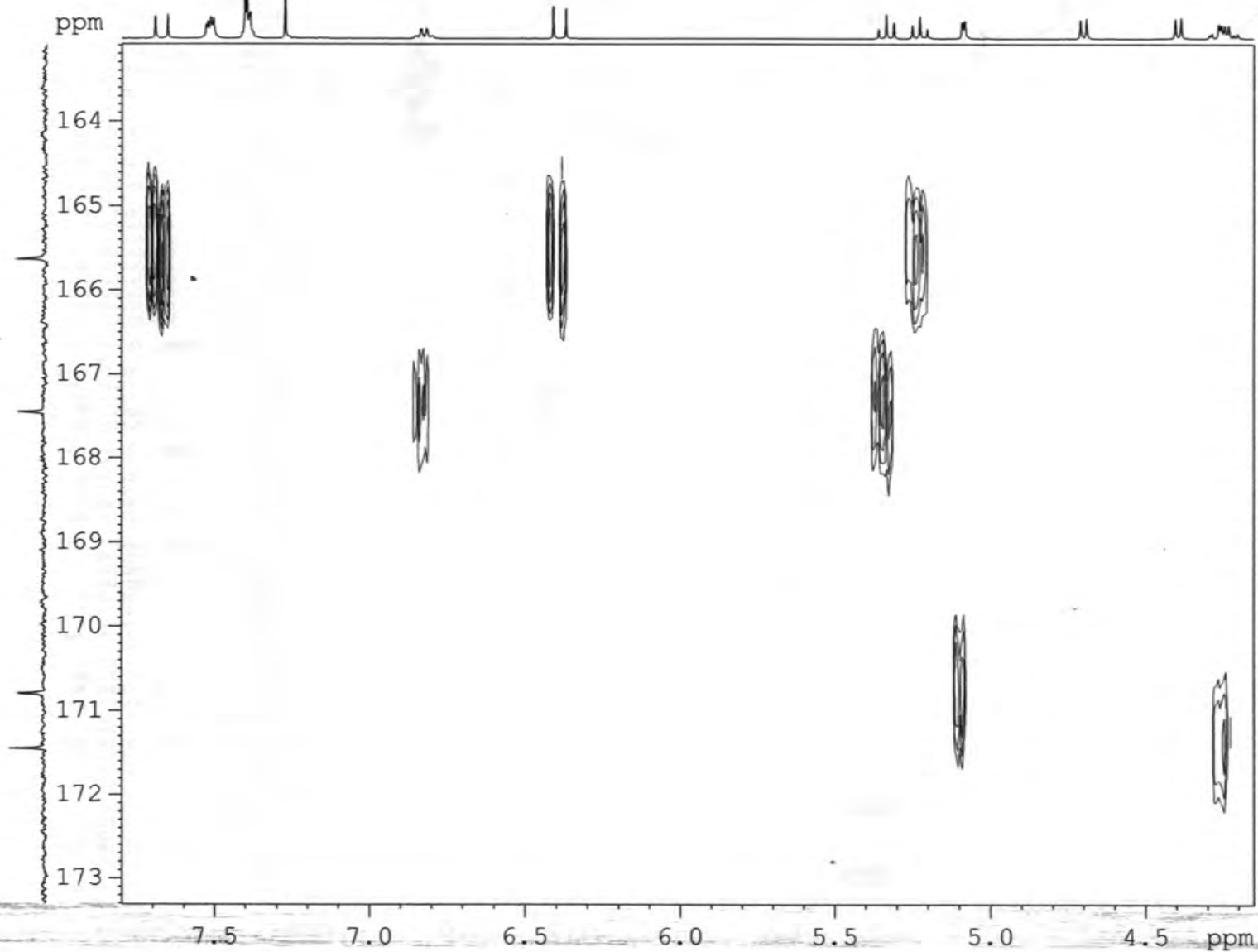
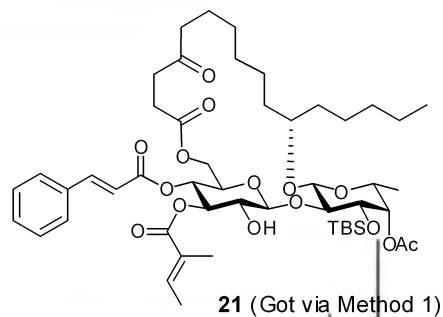
----- CHANNEL f1 -----  
 NUC1 1H  
 P1 10.00 usec  
 P2 20.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1325208 MHz

----- CHANNEL f2 -----  
 NUC2 13C  
 P3 10.00 usec  
 PL2 -2.10 dB  
 PL2W 58.37759399 W  
 SFO2 100.6228138 MHz

----- GRADIENT CHANNEL -----  
 GPNAM1 SINE.100  
 GPNAM2 SINE.100  
 GPNAM3 SINE.100  
 GPZ1 50.00 %  
 GPZ2 30.00 %  
 GPZ3 40.10 %  
 P16 1000.00 usec  
 NDO 2  
 TD 128  
 SFO1 100.6228 MHz  
 FIDRES 129.709091 Hz  
 SW 165.000 ppm  
 FmMODE QF  
 SI 2048  
 SF 400.1300000 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 4.00  
 SI 1024  
 MC2 QF  
 SF 100.6127690 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

ppm



ZGH-*Ipom*-2-143-A-150423 HMBC in CDCl<sub>3</sub>

```

NAME      ZGH-Ipom-2-143-A-150423
EXPNO     5
PROCNO    1
Date_     20150430
Time      4.13
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   hmbcgp1pndqf
TD         4096
SOLVENT   CDCl3
NS         35
DS         16
SWH       5208.333 Hz
FIDRES    1.271566 Hz
AQ        0.3932660 sec
RG         2050
DW        96.000 usec
DE         6.50 usec
TE        292.3 K
CNST2     145.0000000
CNST13    10.0000000
D0         0.00000300 sec
D1         1.50000000 sec
D2         0.00344828 sec
D6         0.05000000 sec
D16        0.00020000 sec
INO        0.00003010 sec

----- CHANNEL f1 -----
NUC1      1H
P1        10.00 usec
P2        20.00 usec
PL1       -3.50 dB
PL1W      31.17620277 W
SFO1      400.1325208 MHz

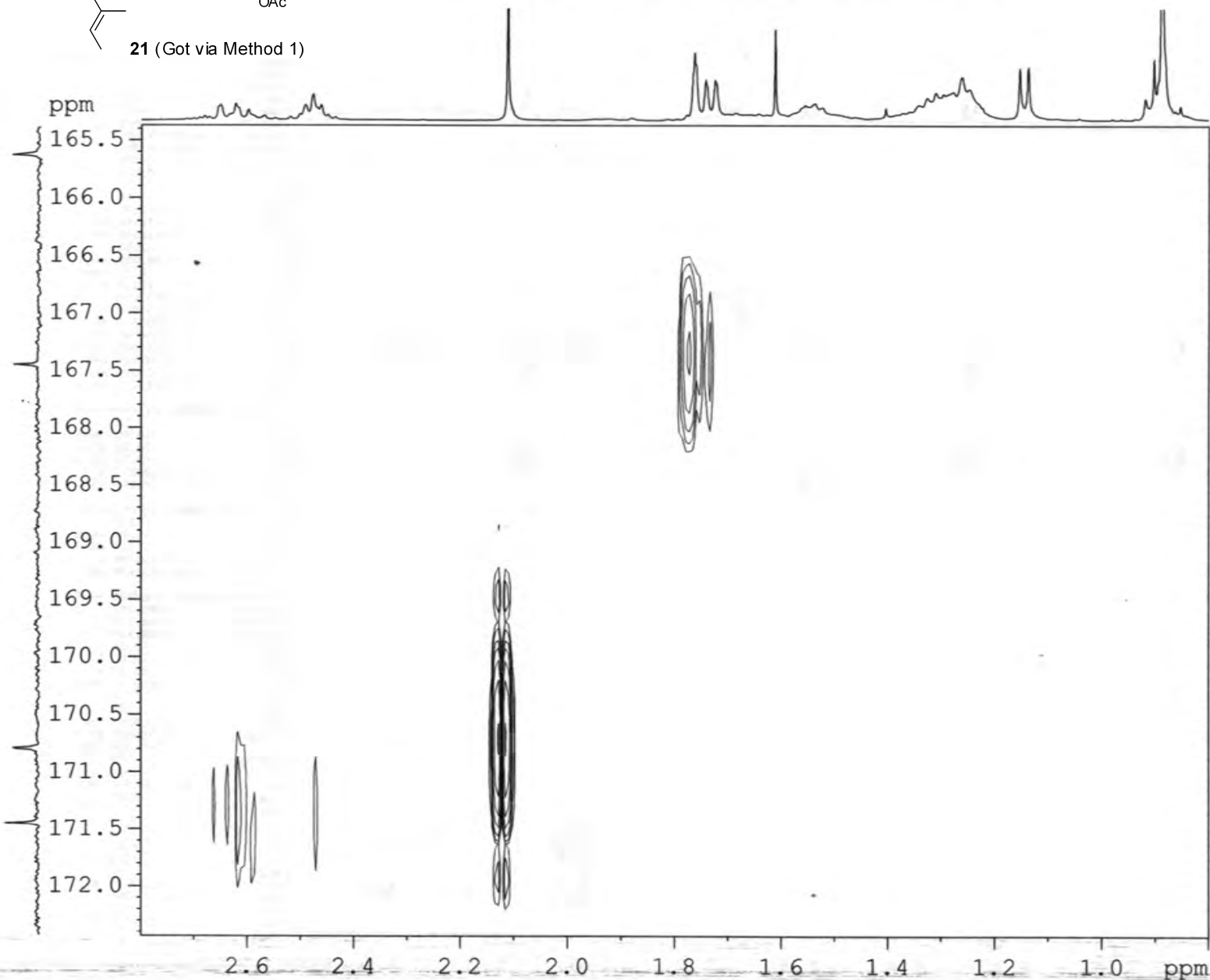
----- CHANNEL f2 -----
NUC2      13C
P3        10.00 usec
PL2       -2.10 dB
PL2W      58.37759399 W
SFO2      100.6228138 MHz

----- GRADIENT CHANNEL -----
GPNAM1    SINE.100
GPNAM2    SINE.100
GPNAM3    SINE.100
GP21      50.00 %
GP22      30.00 %
GP23      40.10 %
P16       1000.00 usec
ND0        2
TD         128
SFO1      100.6228 MHz
FIDRES    129.709091 Hz
SW        165.000 ppm
FnMODE    QF
SI         2048
SF        400.1300000 MHz
WDW       SINE
SSB        0
LB         0.00 Hz
GB         0
PC         4.00
SI         1024
MC2       QF
SF        100.6127690 MHz
WDW       SINE
SSB        0
LB         0.00 Hz
GB         0

```

ZGH-*Ipom*-2-143-A-150423 HMBC in CDCl<sub>3</sub>

21 (Got via Method 1)

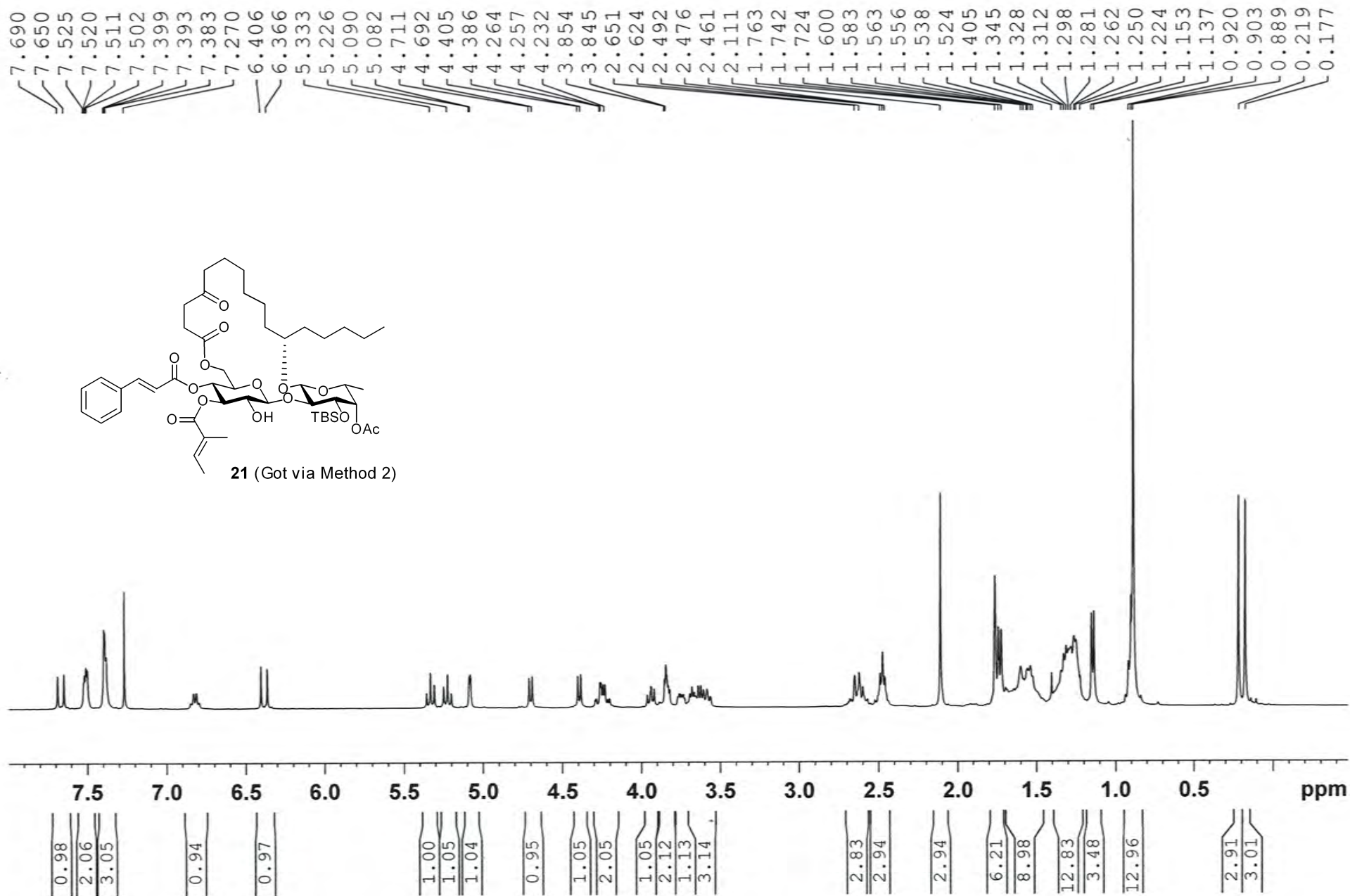


NAME ZGH-*Ipom*-2-143-A-150423  
 EXPNO 5  
 PROCNO 1  
 Date 20150430  
 Time 4.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hmcgplpndqf  
 TD 4096  
 SOLVENT CDCl<sub>3</sub>  
 NS 35  
 DS 16  
 SWH 5208.333 Hz  
 FIDRES 1.271566 Hz  
 AQ 0.3932660 sec  
 RG 2050  
 DW 96.000 usec  
 DE 6.50 usec  
 TE 292.3 K  
 CNST2 145.000000  
 CNST13 10.000000  
 D0 0.00000300 sec  
 D1 1.50000000 sec  
 D2 0.00344828 sec  
 D6 0.05000000 sec  
 D16 0.00020000 sec  
 INO 0.00003010 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 P2 20.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1325208 MHz

===== CHANNEL f2 =====  
 NUC2 13C  
 P3 10.00 usec  
 PL2 -2.10 dB  
 PL2W 58.37759399 W  
 SFO2 100.6228138 MHz

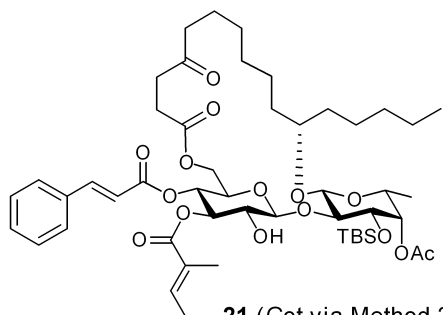
===== GRADIENT CHANNEL =====  
 GPNAM1 SINE.100  
 GPNAM2 SINE.100  
 GPNAM3 SINE.100  
 GPZ1 50.00 %  
 GPZ2 30.00 %  
 GPZ3 40.10 %  
 P16 1000.00 usec  
 ND0 2  
 TD 128  
 SFO1 100.6228 MHz  
 FIDRES 129.709091 Hz  
 SW 165.000 ppm  
 FMODE QF  
 SI 2048  
 SF 400.1300000 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 4.00  
 SI 1024  
 MC2 QF  
 SF 100.6127690 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

ZGH-*Ipom*-3-192-170205-A in CDCl<sub>3</sub>

ZGH-*Ipom*-3-192-170205-A <sup>13</sup>C in CDCl<sub>3</sub>

— 210.119

171.462  
170.794  
167.456  
165.627  
146.026  
138.086  
134.073  
130.579  
128.918  
128.218  
127.929  
116.853  
104.375  
101.199  
80.110  
79.039  
77.318  
77.203  
77.000  
76.683  
74.448  
72.928  
72.788  
72.055  
69.924  
68.832  
63.282  
41.980  
37.407  
36.618  
34.102  
33.231  
31.978  
29.551  
29.091  
28.538  
25.805  
25.128  
24.667  
24.374  
23.665  
22.649  
20.882  
17.867  
16.486  
14.361  
14.087  
11.987  
-4.411  
-4.567



200

180

160

140

120

100

80

60

40

20

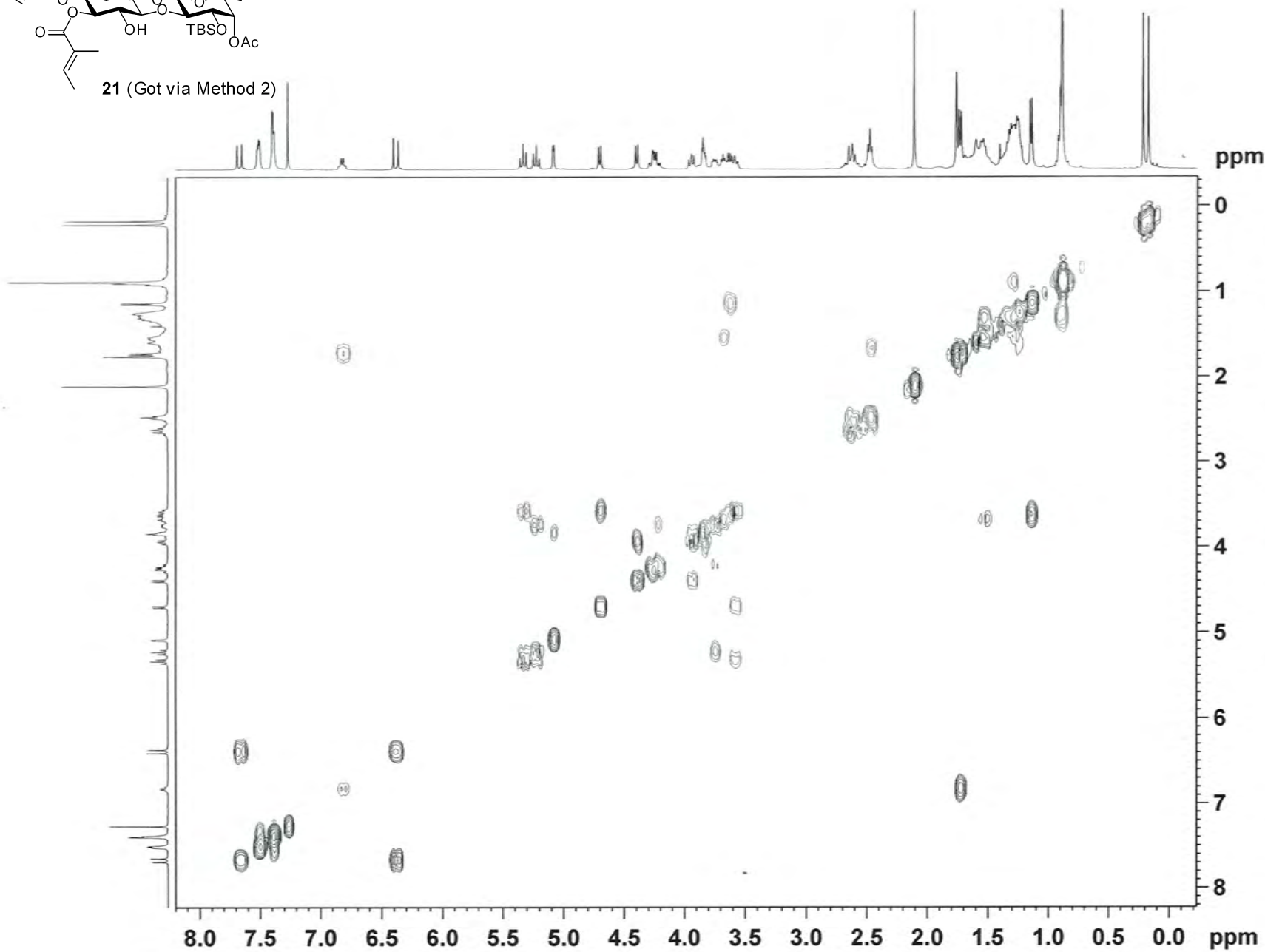
0

-20

ppm

ZGH-*Ipom*-3-192-170205-A in CDCL<sub>3</sub>

21 (Got via Method 2)



Current Data Parameters  
 NAME ZGH-*Ipom*-3-192-170205-A  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170206  
 Time 7:02  
 INSTRUM spect  
 PROBHD 5 mm PABBO 5H-1  
 PULPROG zgpg30  
 TD 2048  
 SOLVENT CDCl3  
 NS 24  
 DS 8  
 SWH 8032.800 Hz  
 FIDRES 3.912510 Hz  
 AQ 0.1277552 sec  
 RG 406  
 DM 62.400 usec  
 DE 6.50 usec  
 TE 294.8 K  
 D0 0.0000300 sec  
 D1 1.5000000 sec  
 D12 0.0000400 sec  
 D14 0.0000000 sec  
 IM0 0.00012480 sec

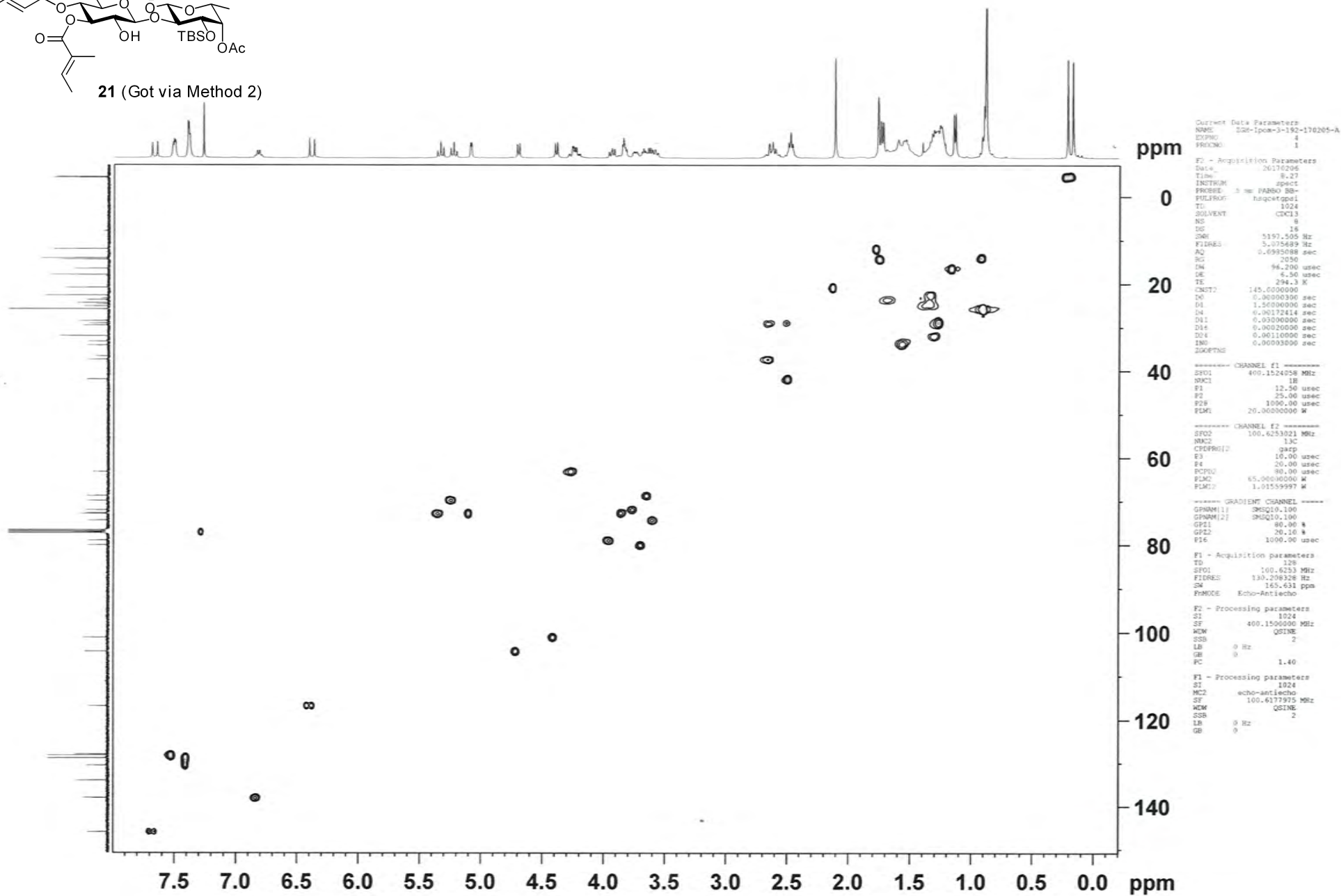
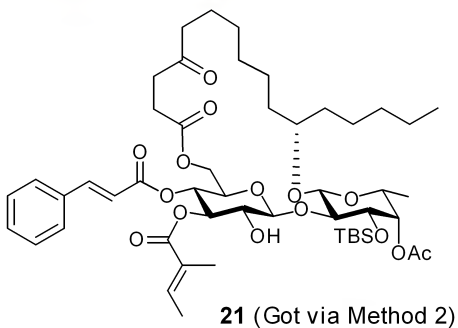
----- CHANNEL f1 -----  
 SF01 400.1520008 MHz  
 NUC1 1H  
 P1 12.50 usec  
 PL1 20.0000000 W

----- GRADIENT CHANNEL -----  
 GPM111 SW010.100  
 GP1 10.00 %  
 P11 1000.00 usec

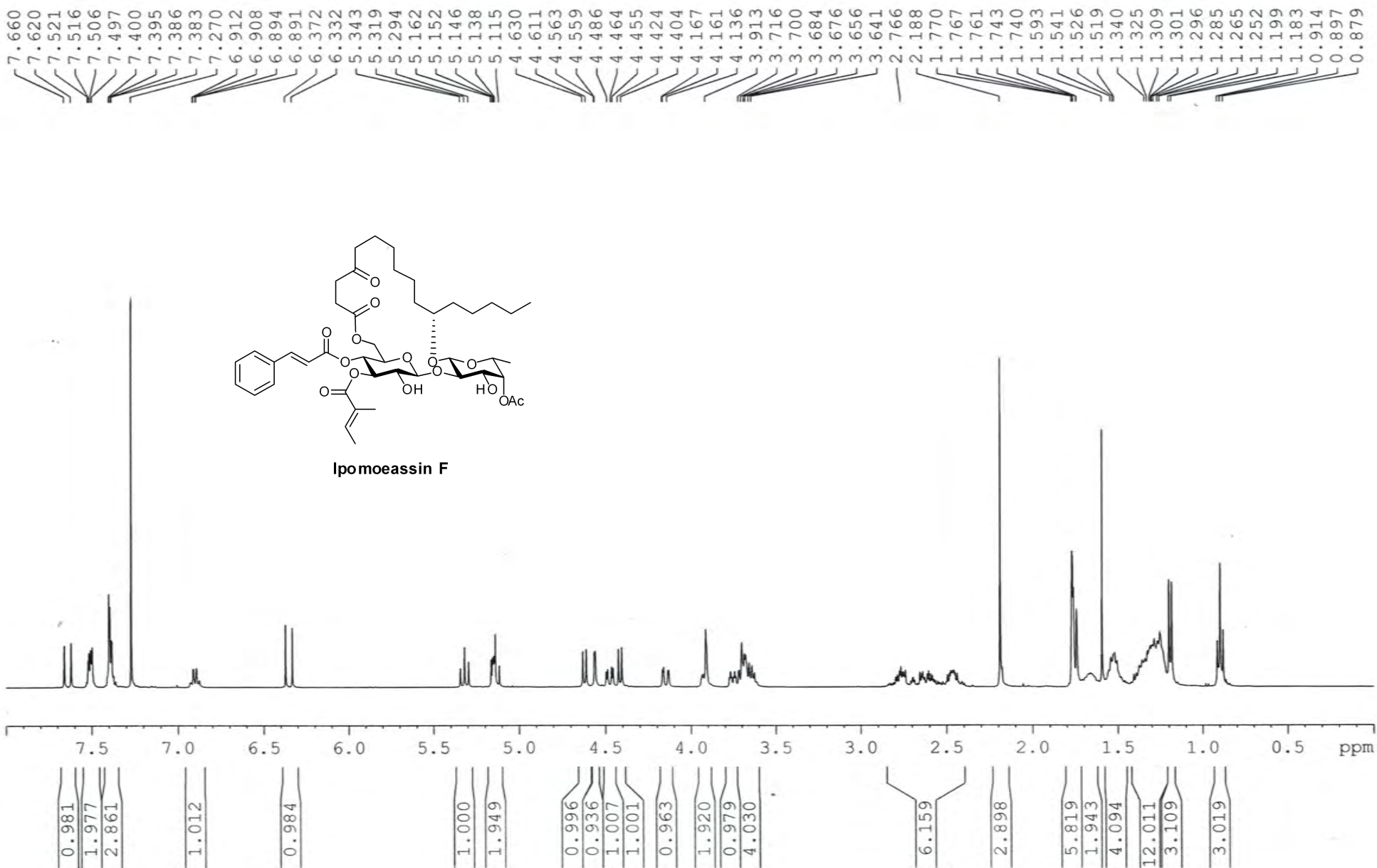
F1 - Acquisition parameters  
 TS 128  
 SF01 400.152 MHz  
 FIDRES 62.600159 Hz  
 SW 20.024 ppm  
 FWHM 0F

F2 - Processing parameters  
 SI 3274  
 SF 400.1500070 MHz  
 NEM QFTM2  
 SSB 0  
 LB 0 Hz  
 GB 0  
 ZC 1.00

F1 - Processing parameters  
 SI 3274  
 SF 400.1500052 MHz  
 NEM QFTM2  
 SSB 0  
 LB 0 Hz  
 GB 0

ZGH-*Ipom*-3-192-170205-A HSQC in CDCl<sub>3</sub>

## ZGH-Ipom-2-165-A-150509 1H in CDCL3



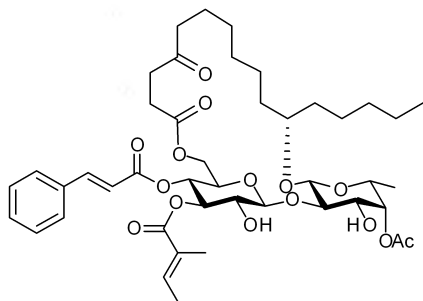


ZGH-*Ipom-2-165-A-150509*  $^{13}\text{C}$  in  $\text{CDCl}_3$ 

— 210.003

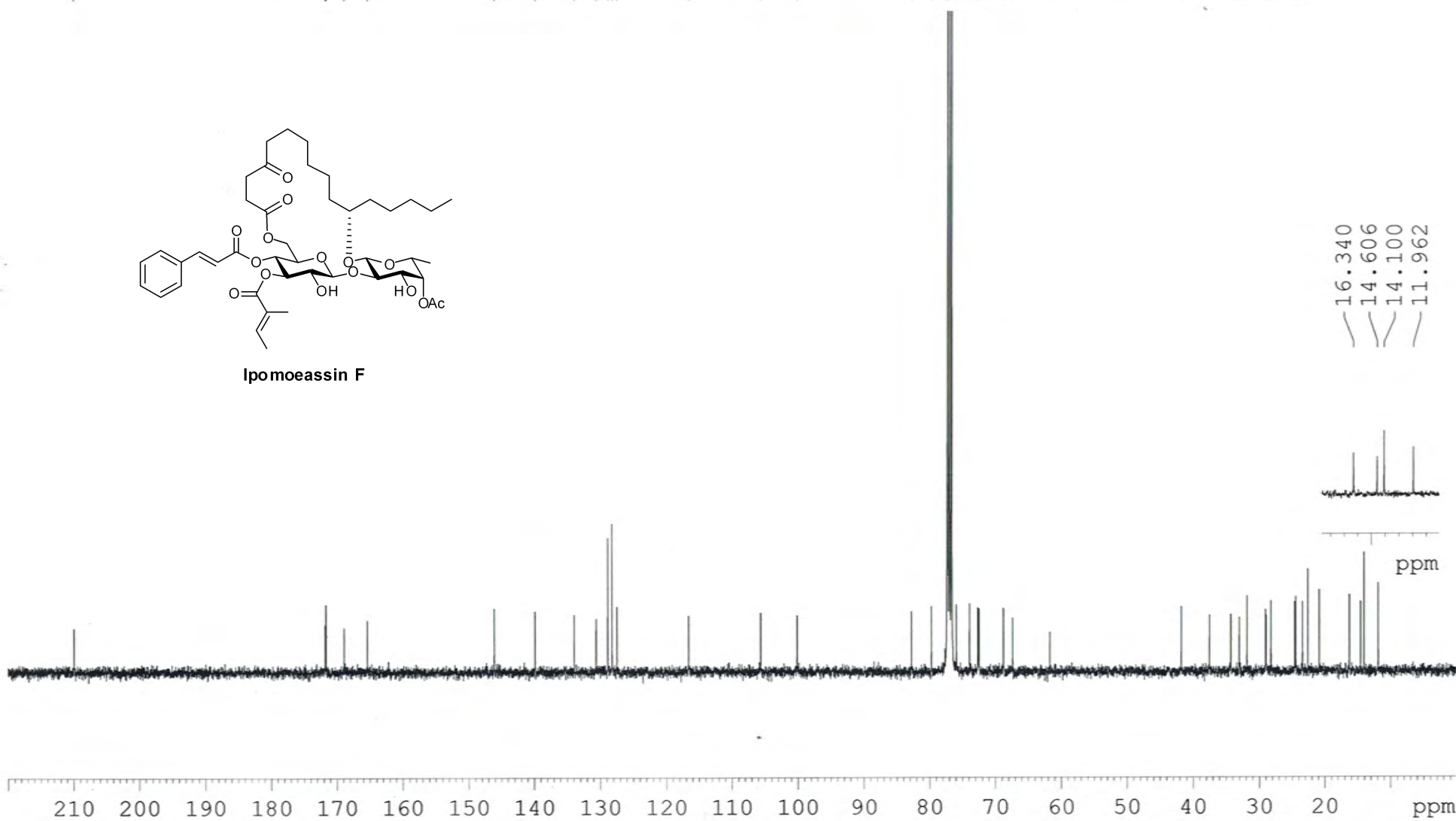
171.815  
171.713  
168.907  
165.416

146.164  
139.897  
133.972  
130.647  
128.893  
128.266  
127.526  
116.666  
105.670  
100.169  
82.804  
79.753  
77.711  
77.314  
77.200  
76.996  
76.678  
75.953  
73.954  
72.696  
72.602  
72.503  
68.818  
67.411  
61.757  
41.848  
37.581  
34.339  
33.083  
31.908  
29.116  
29.031  
28.294  
24.664  
24.504  
23.468  
22.649  
20.941

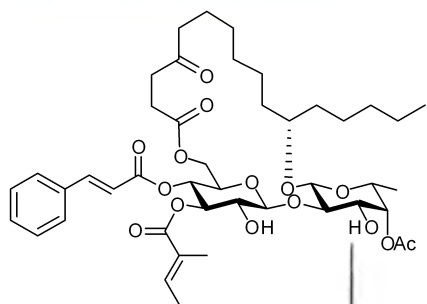


Ipomoeassin F

16.340  
14.606  
14.100  
11.962



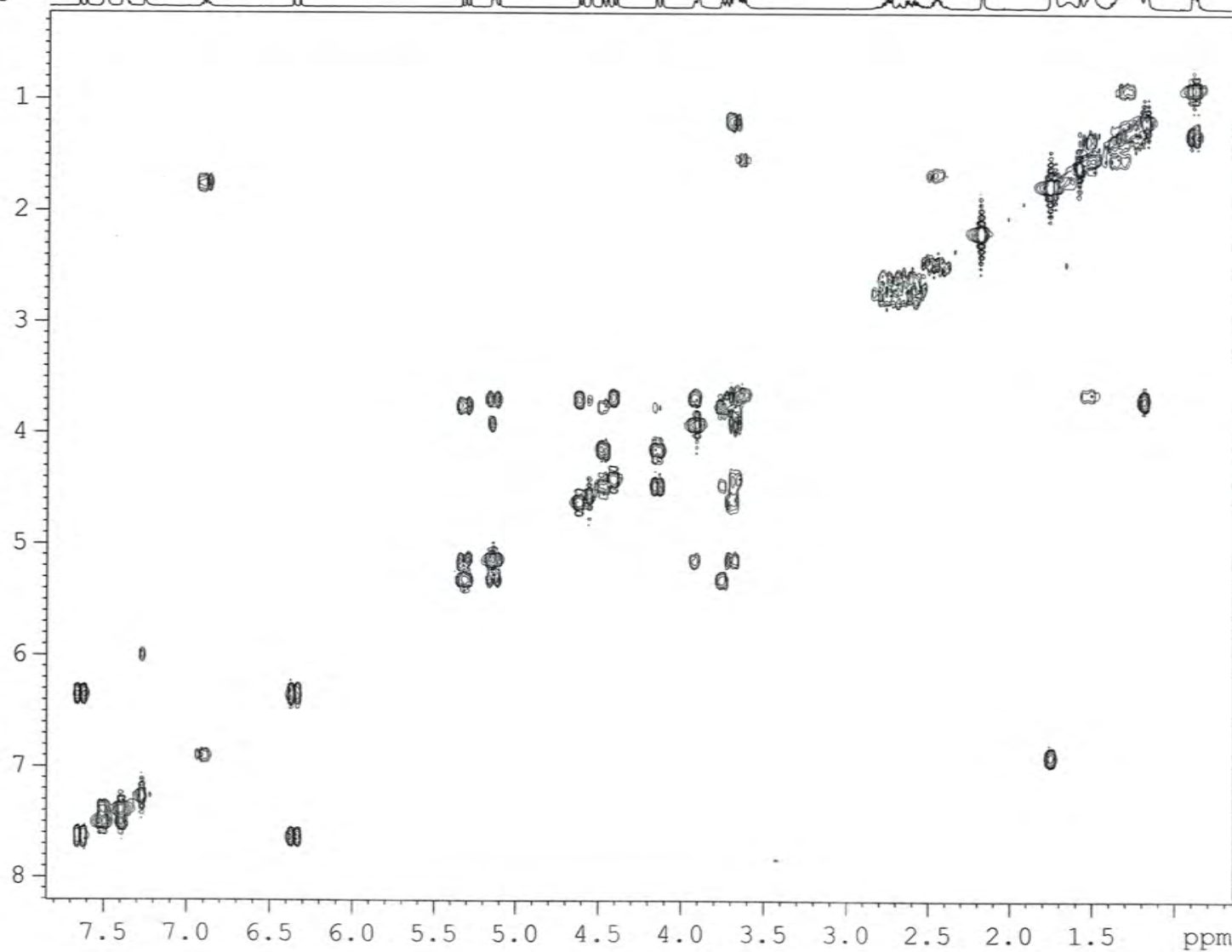
## ZGH-Ipom-2-165-A-150509 COSY

Ipomoeassin F  
ppm

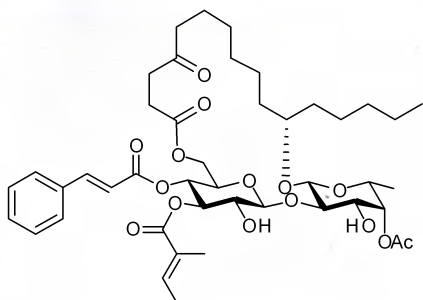
NAME ZGH-Ipom-2-165-A-150509  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20150511  
 Time 1.14  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosygpgf  
 TD 2048  
 SOLVENT CDC13  
 NS 16  
 DS 8  
 SWH 5341.880 Hz  
 FIDRES 2.608340 Hz  
 AQ 0.1917428 sec  
 RG 512  
 DW 93.600 usec  
 DE 6.50 usec  
 TE 292.4 K  
 D0 0.00000300 sec  
 D1 1.48689198 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 IN0 0.00018720 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P0 10.00 usec  
 P1 10.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1324057 MHz

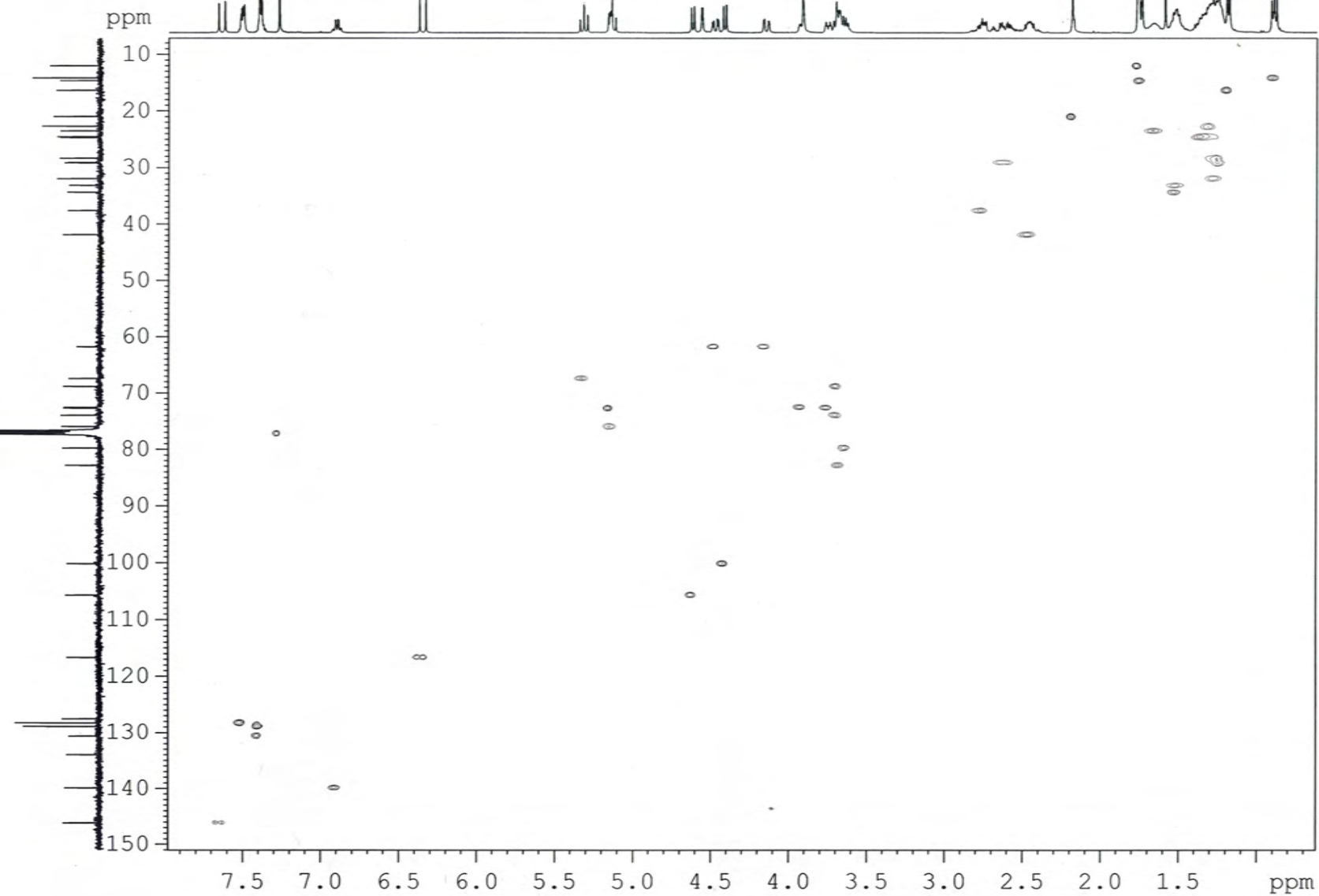
===== GRADIENT CHANNEL =====  
 GPNAM1 SINE.100  
 GPZ1 10.00 %  
 P16 1000.00 usec  
 ND0 1  
 TD 128  
 SFO1 400.1324 MHz  
 FIDRES 41.733440 Hz  
 SW 13.350 ppm  
 PhMODE QF  
 SI 1024  
 SF 400.1300040 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00  
 SI 1024  
 MC2 QF  
 SF 400.1300033 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0



## ZGH-Ipom-2-165-A-150509 HSQC



Ipomoeassin F



```

Current Data Parameters
NAME      ZGH-Ipom-2-165-A-150509
EXPNO    3
PROCNO   1

F2 - Acquisition Parameters
Date_    20150311
Time     2.12
INSTRUM  spect
PROBHD   5 mm ZABBO BB-
PULPROG  hsqcetgpg1
TD        1024
SOLVENT  CDCl3
NS        16
DS        16
SWH       5341.480 Hz
FIDRES    5.216480 Hz
AQ        0.0958464 sec
RG        2050
DSW       93.600 usec
DE        6.50 usec
TE        292.2 K
CONST2   145.000000
D0        0.0000300 sec
D1        1.5000000 sec
D4        0.00172414 sec
D11       0.0300000 sec
D13       0.0000400 sec
D16       0.0002000 sec
D24       0.0011000 sec
IN0       0.0000300 sec
ZOGPINS

----- CHANNEL f1 -----
NUC1      1H
P1        10.00 usec
PC        20.00 usec
P28       1000.00 usec
PL1       -3.50 dB
PL1W      31.17620277 M
SFO1      400.1324057 MHz

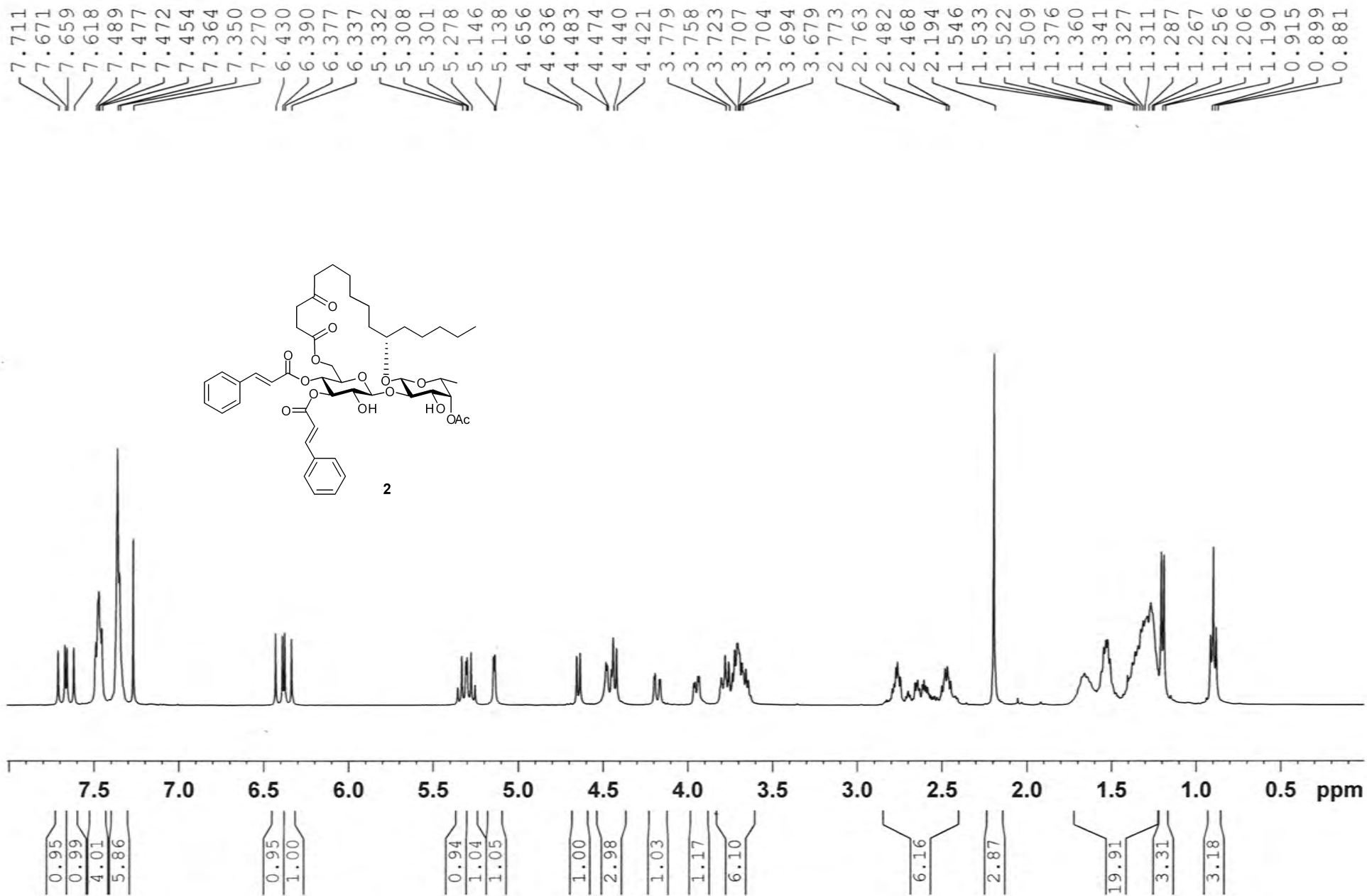
----- CHANNEL f2 -----
CPOPRG2   gspc
NUC2      13C
P3         10.00 usec
P4         20.00 usec
PCPE2     75.00 usec
PL2       -2.10 dB
PL12      35.40 dB
PL2W      58.37759399 M
PL12W     1.03811481 M
SFO2      100.6203277 MHz

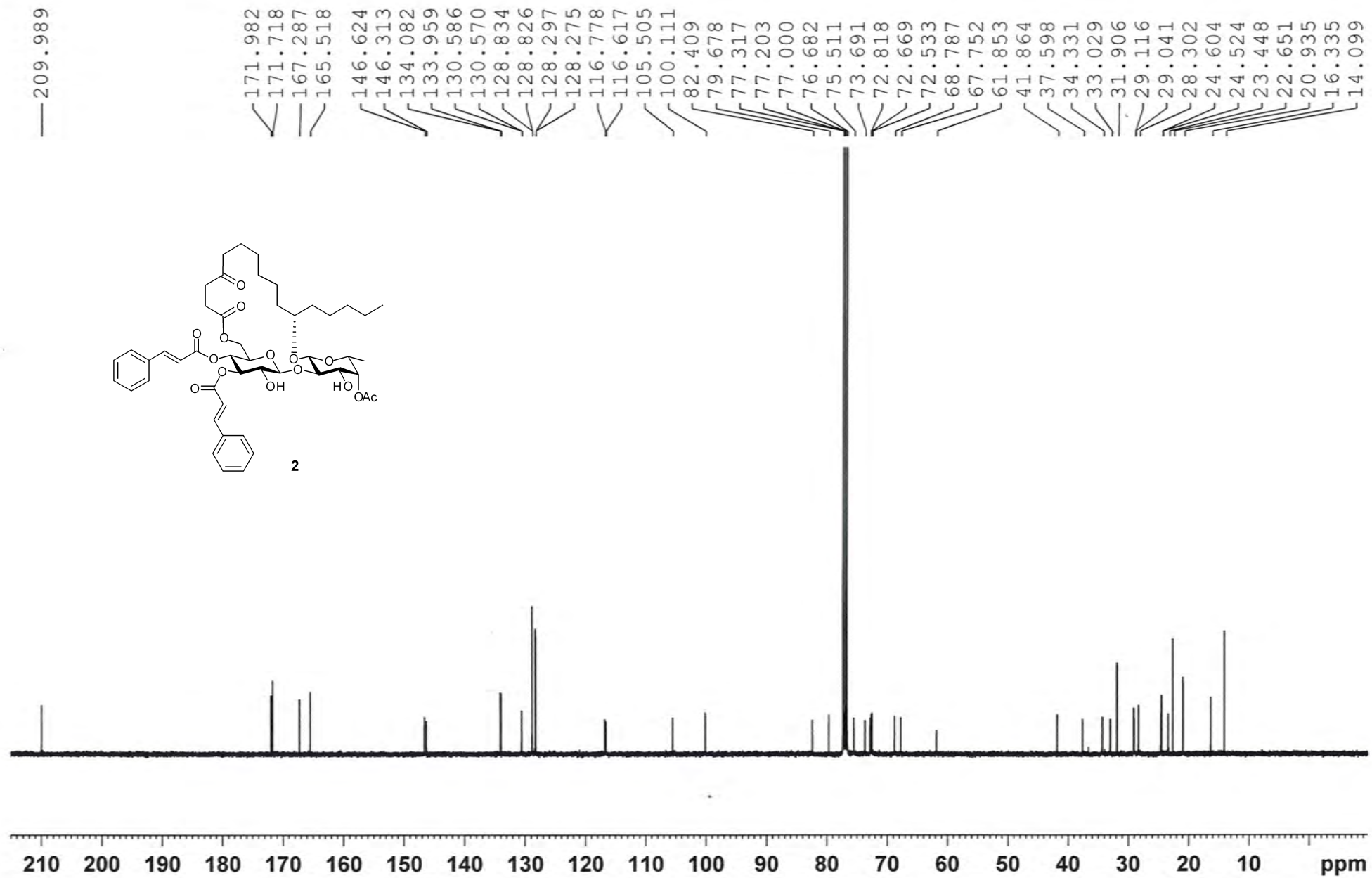
----- GRADIENT CHANNEL -----
GNAM[1]   SINE.100
GNAM[2]   SINE.100
GP21      80.00 %
GP22      20.10 %
P16       1000.00 usec

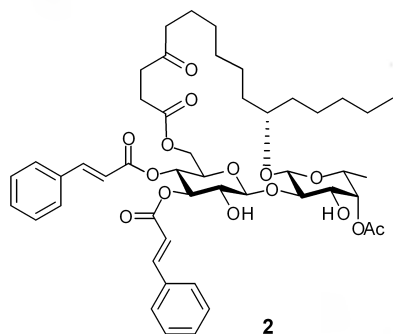
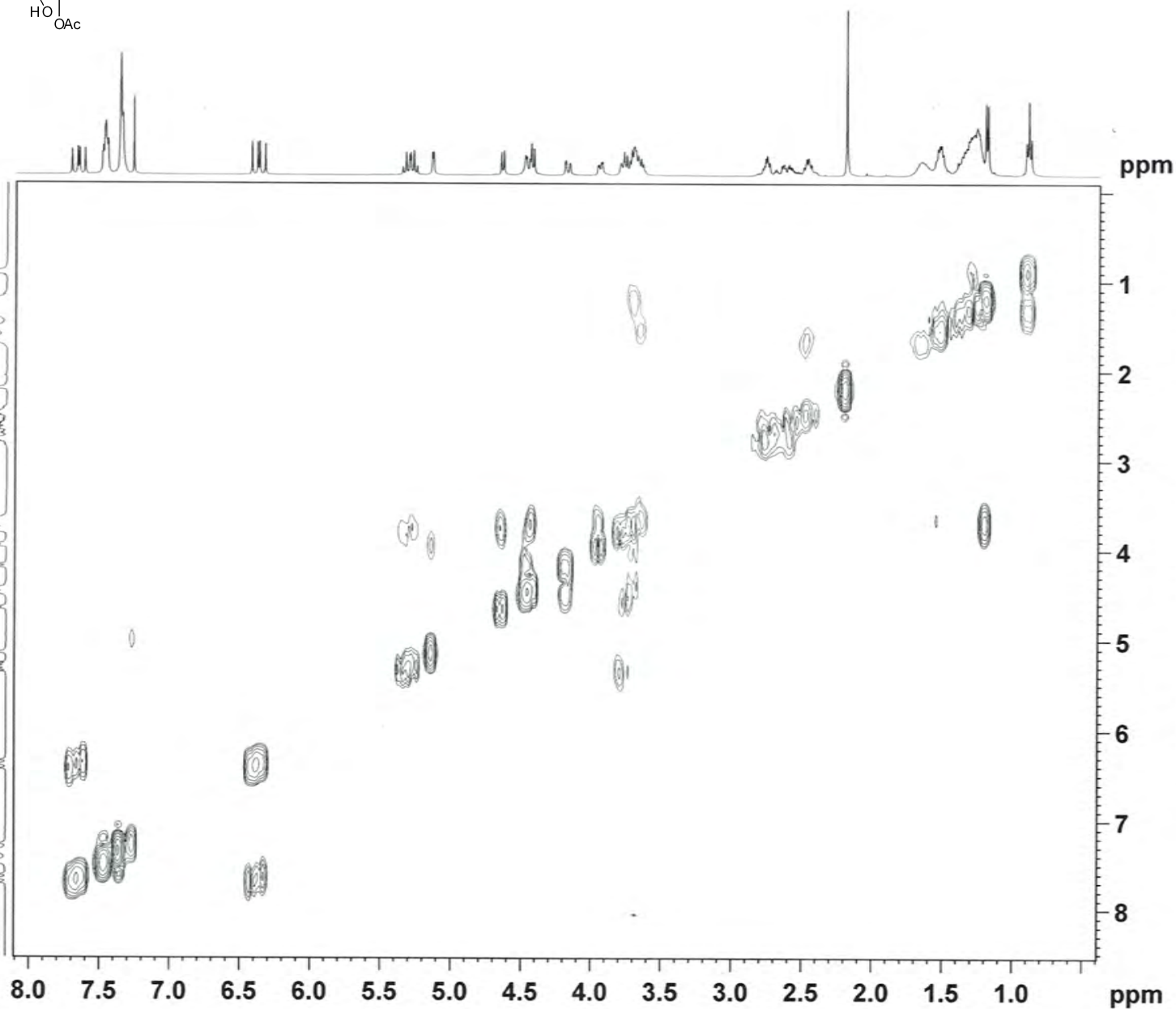
F1 - Acquisition parameters
TD         256
SFO1      100.6203 MHz
FIDRES     65.104164 Hz
SW         165.639 ppm
PRMODE     Echo-Antiecho

F2 - Processing parameters
SI         1024
SF         400.1300000 MHz
WDW        QSINE
SSB        2
LB         0 Hz
GB         0
PC         1.00

F1 - Processing parameters
SI         1024
WC2        echo-antiecho
SF         100.6127690 MHz
WDW        QSINE
SSB        2
LB         0 Hz
GB         0
  
```

ZGH-*Ipom*-3-161-161104-A in CDCl<sub>3</sub>

ZGH-*Ipom*-3-161-161104-A 13C in CDCl<sub>3</sub>

ZGH-Ipom-3-161-161104-A in CDCl<sub>3</sub>

Current Data Parameters  
 NAME ZGH-Ipom-3-161-161104-A  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161107  
 Time 22.38  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosyypqf  
 TD 2048  
 SOLVENT CDCl3  
 NS 32  
 DS 8  
 SWH 8012.820 Hz  
 FIDRES 3.912510 Hz  
 AQ 0.1277952 sec  
 RG 362  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 293.0 K  
 D0 0.0000300 sec  
 D1 1.5000000 sec  
 D13 0.0000400 sec  
 D16 0.0002000 sec  
 INO 0.00012489 sec

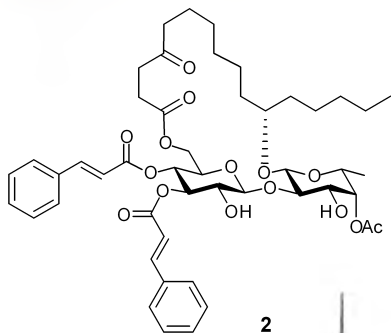
----- CHANNEL f1 -----  
 SFO1 400.1520008 MHz  
 NUCL1 1H  
 P0 12.50 usec  
 P1 12.50 usec  
 PLM1 20.0000000 W

----- GRADIENT CHANNEL -----  
 GPRAM[1] 250010.100  
 GR1 10.00 A  
 P16 1000.00 usec

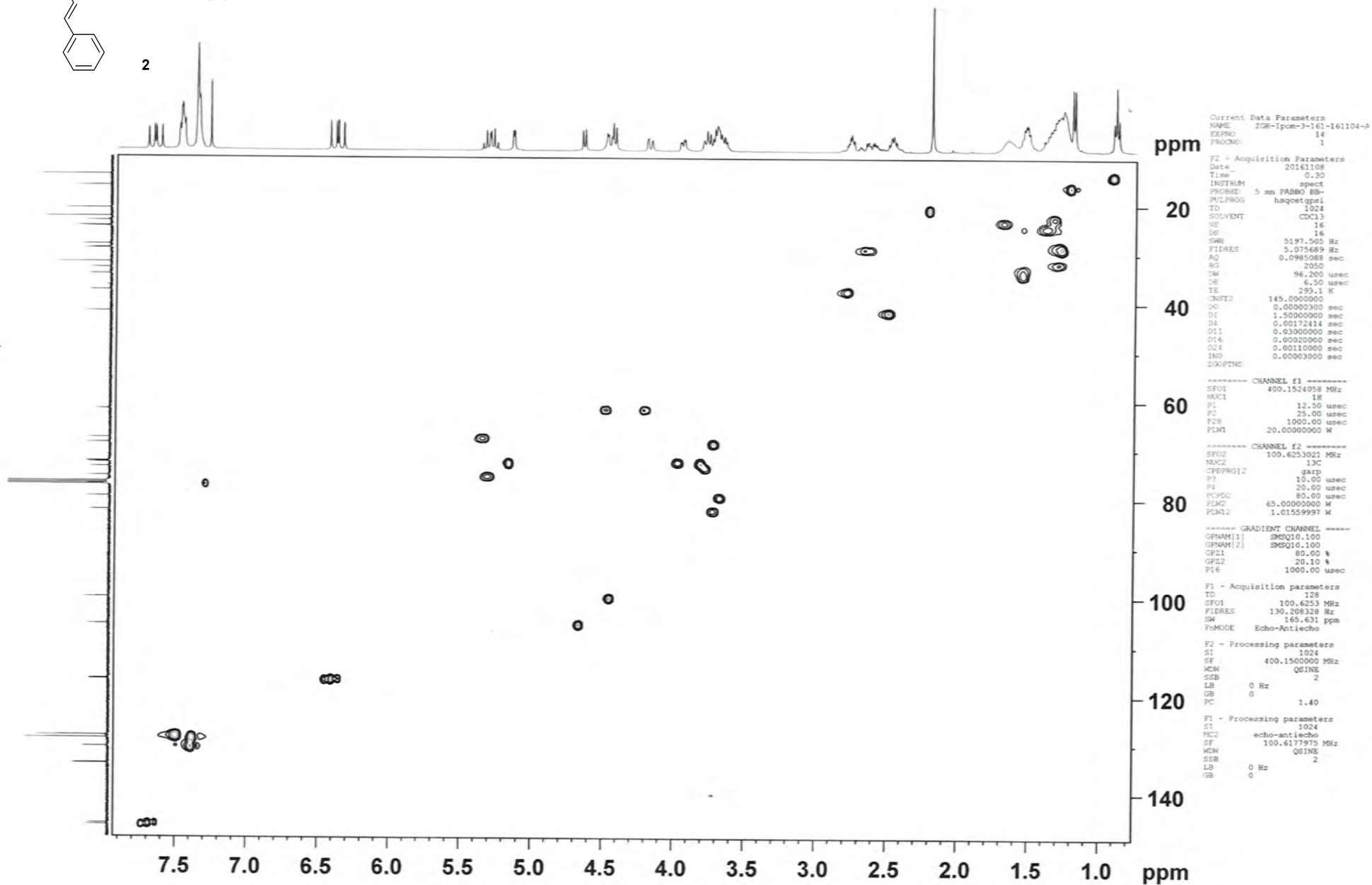
F1 - Acquisition parameters  
 TD 128  
 SFO1 400.152 MHz  
 FIDRES 62.600159 Hz  
 SW 20.024 ppm  
 FWHDE QF

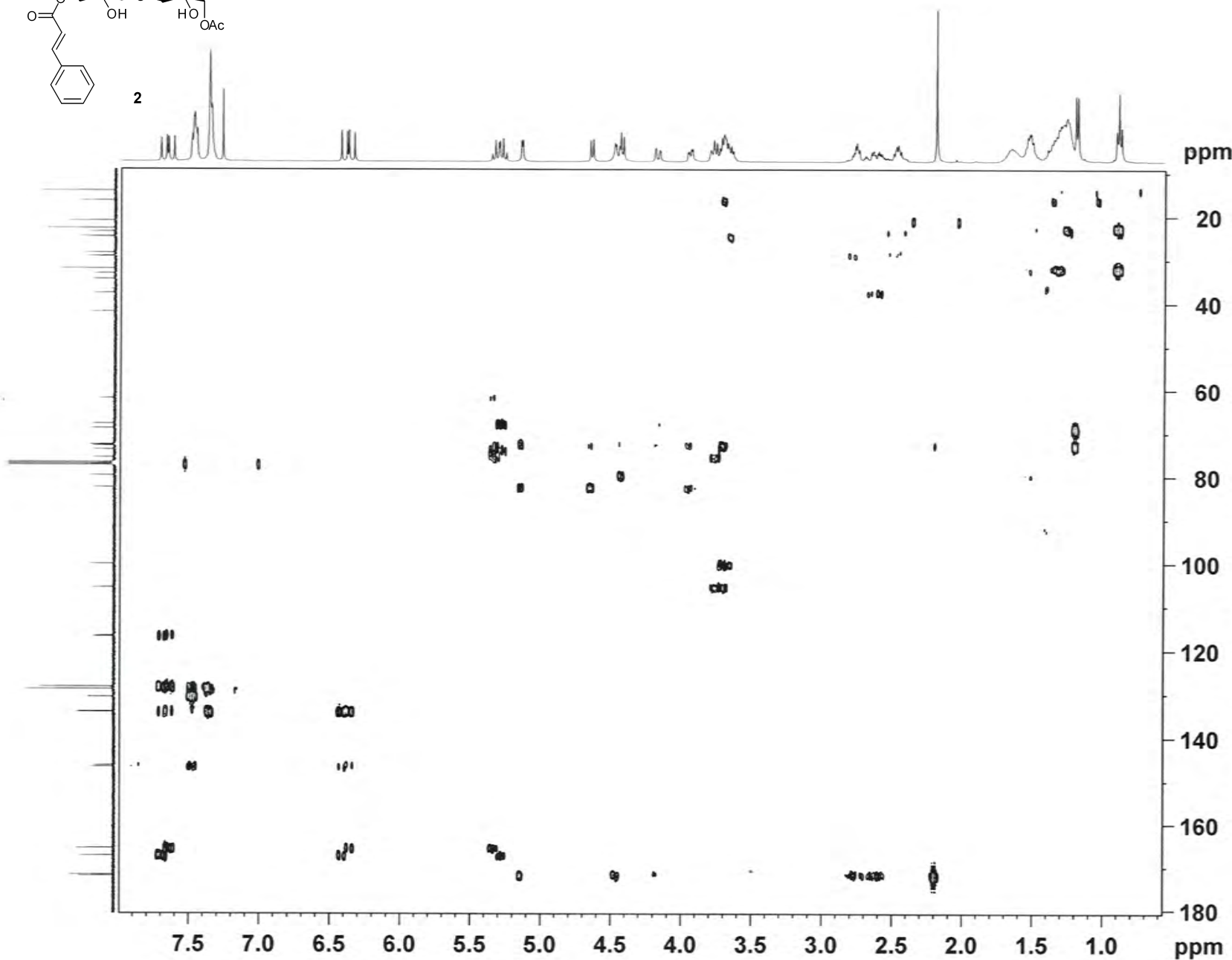
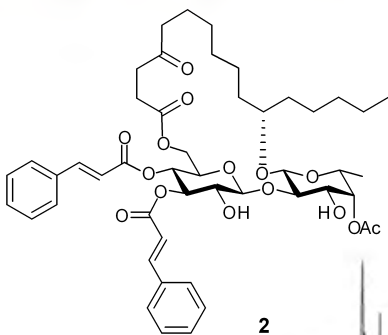
F2 - Processing parameters  
 SI 1024  
 SF 400.1500070 MHz  
 HEM QSINE  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 QF  
 SF 400.1500052 MHz  
 HEM QSINE  
 SSB 0  
 LB 0 Hz  
 GB 0



ZGH-Ipom-3-161-161104-A HSQC in CDC13



ZGH-*Ipom*-3-161-161104-A HMBC in CDCl<sub>3</sub>

Current Data Parameters  
 NAME ZGH-*Ipom*-3-161-161104-A  
 EXPNO 15  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161108  
 Time 1.29  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hmhbcplpndgdf  
 TD 4096  
 SOLVENT CDCl3  
 NS 100  
 DS 16  
 SMH 5208.333 Hz  
 FIDRES 1.271566 Hz  
 AQ 0.3932160 sec  
 RG 2050  
 DW 96.000 usec  
 DE 6.50 usec  
 TE 293.2 K  
 CNST2 145.0000000  
 CNST13 10.0000000  
 DO 0.00000300 sec  
 D1 1.50000000 sec  
 D2 0.00344828 sec  
 D6 0.05000000 sec  
 D16 0.00020000 sec  
 INO 0.00002240 sec

----- CHANNEL f1 -----  
 SFO1 400.1516006 MHz  
 NUC1 1H  
 P1 12.50 usec  
 P2 25.00 usec  
 PLM1 20.00000000 W

----- CHANNEL f2 -----  
 SFO2 100.6258470 MHz  
 NUC2 13C  
 P3 10.00 usec  
 PLM2 65.00000000 W

----- GRADIENT CHANNEL -----  
 GPNAM[1] SINE.100  
 GPNAM[2] SINE.100  
 GPNAM[3] SINE.100  
 GP21 50.00 u  
 GP22 30.00 u  
 GP23 40.10 u  
 P16 1000.00 usec

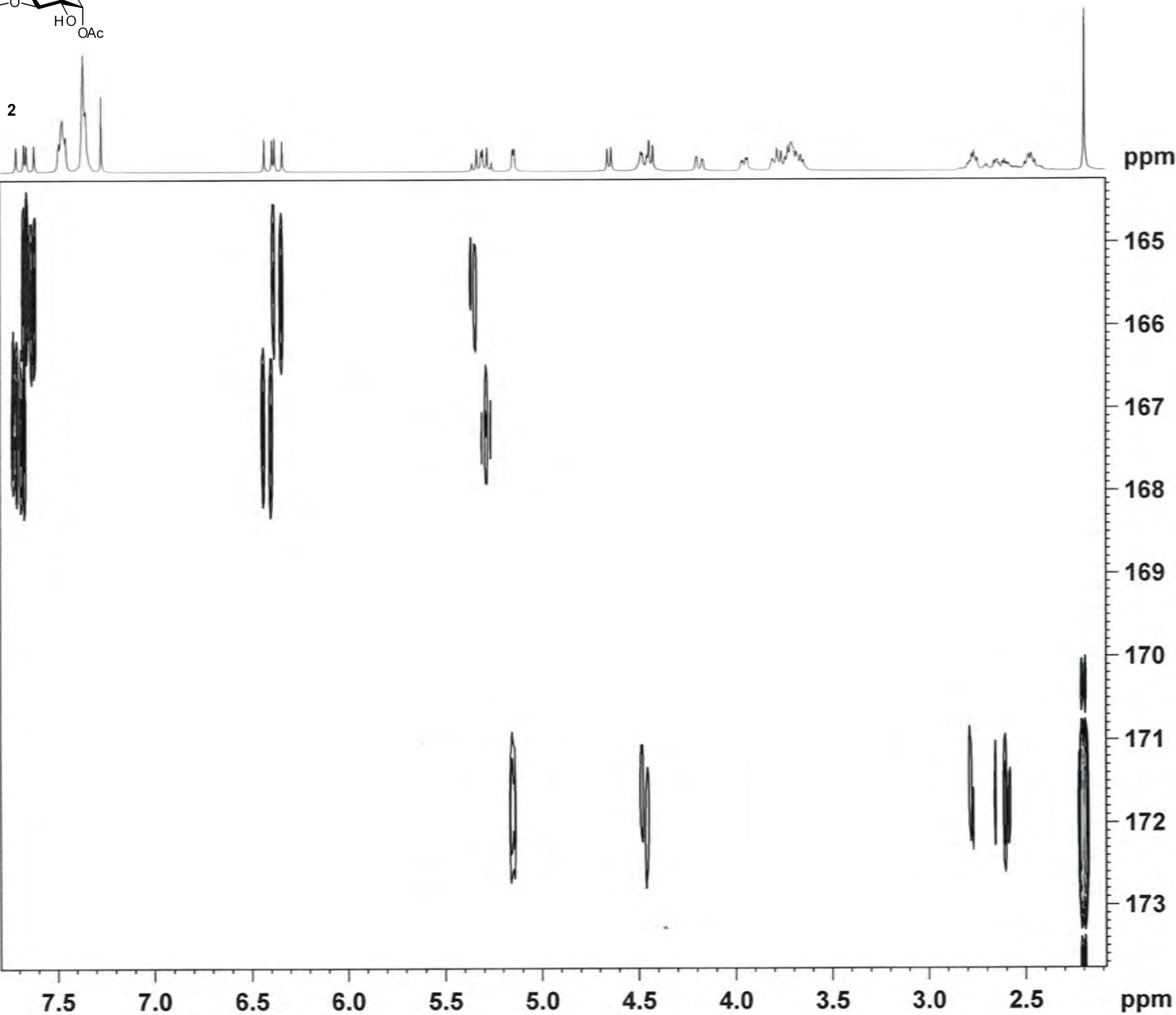
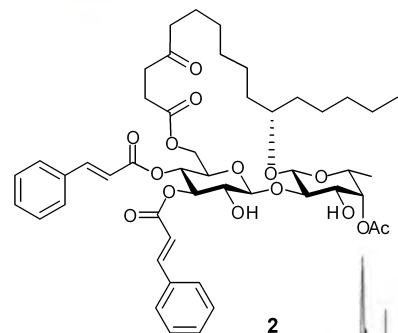
F1 - Acquisition parameters  
 TD 328  
 SFO1 100.6258 MHz  
 FIDRES 174.386154 Hz  
 SW 221.826 ppm  
 FMODE QF

F2 - Processing parameters  
 SI 2048  
 SF 400.1500046 MHz  
 WDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 4.00

F1 - Processing parameters  
 SI 1024  
 MC2 QF  
 SF 100.6177921 MHz  
 WDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0



## ZGH-Ipom-3-161-161104-A HMBC in CDCl3



Current Data Parameters  
 NAME ZGH-Ipom-3-161-161104-A  
 EXPNO 15  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161108  
 Time 1.29  
 INSTRUM spect  
 PROBRD 5 mm PARBO BB-  
 PULPROG hmbcqp1pndqf  
 TD 4096  
 SOLVENT CDCl3  
 NS 100  
 DS 16  
 SWH 5208.333 Hz  
 FIDRES 1.271566 Hz  
 AQ 0.3932160 sec  
 RG 2050  
 DW 96.000 usec  
 DE 6.50 usec  
 TE 293.2 K  
 CNST2 145.0000000  
 CNST13 10.0000000  
 D0 0.0000300 sec  
 D1 1.50000000 sec  
 D2 0.00344828 sec  
 D4 0.05000000 sec  
 D16 0.00020000 sec  
 IN0 0.00002240 sec

----- CHANNEL f1 -----  
 SF01 400.1516006 MHz  
 NUC1 1H  
 P1 12.50 usec  
 P2 25.00 usec  
 PLW1 20.00000000 W

----- CHANNEL f2 -----  
 SF02 100.6258470 MHz  
 NUC2 13C  
 P3 10.00 usec  
 PLW2 65.00000000 W

----- GRADIENT CHANNEL -----  
 GPNAM[1] SINE.100  
 GPNAM[2] SINE.100  
 GPNAM[3] SINE.100  
 GP21 50.00 %  
 GP22 30.00 %  
 GP23 40.10 %  
 P16 1000.00 usec

F1 - Acquisition parameters  
 TD 128  
 SF01 100.6258 MHz  
 FIDRES 174.386154 Hz  
 SW 221.826 ppm  
 FbMODE QF

F2 - Processing parameters  
 SI 2048  
 SF 400.1500046 MHz  
 MDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 4.00

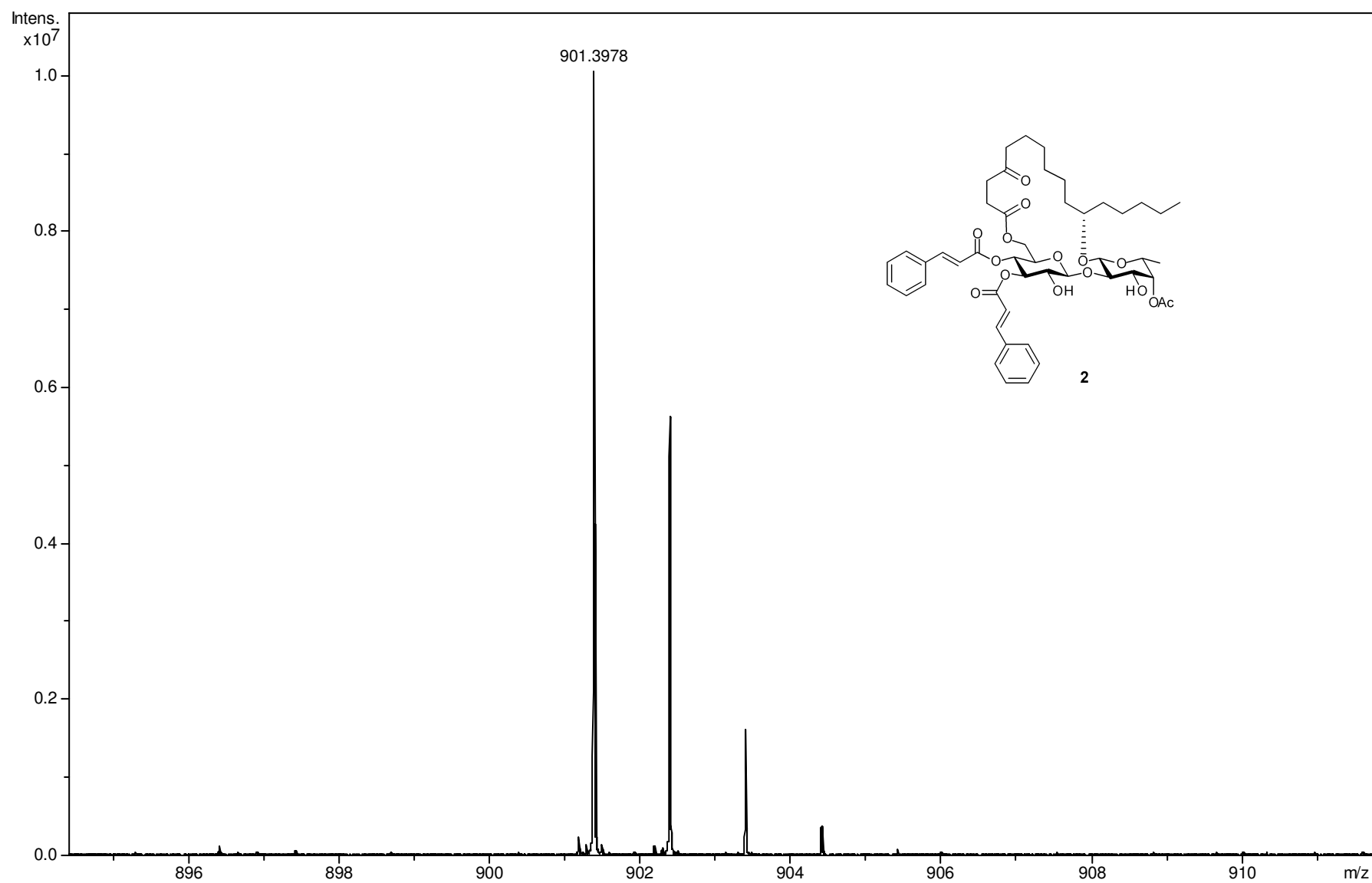
F1 - Processing parameters  
 SI 1024  
 MC2 QF  
 SF 100.6177921 MHz  
 MDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0

## Arkansas Statewide Mass Spectrometry Facility

## ESI-FTMS Mass Spectrum

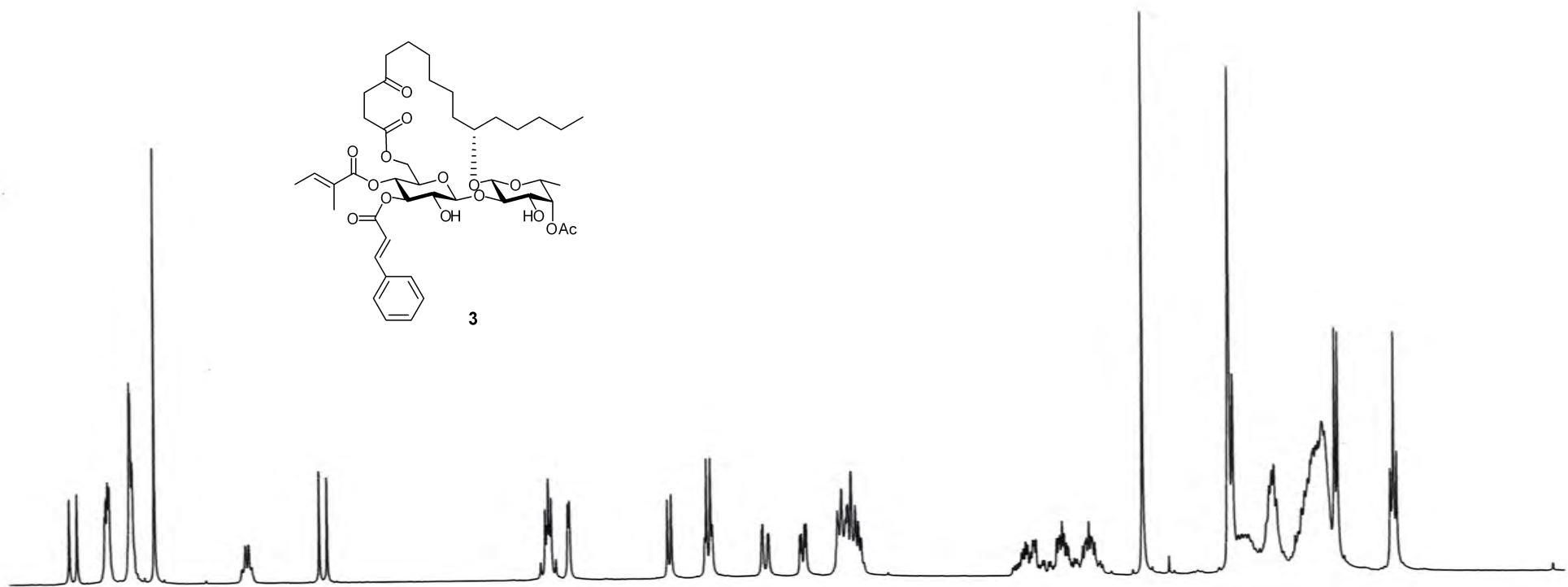
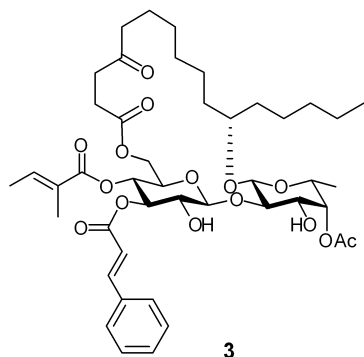
Sample Name: ZIF-50  
Sample id#: 918  
Instrument: Bruker ApexII-FTMS

2/8/2017



ZGH-Ipom-3-189-170120-A\_4 in CDCl<sub>3</sub>

7.707  
7.667  
7.524  
7.519  
7.510  
7.501  
7.397  
7.392  
7.384  
7.270  
6.423  
6.383  
5.260  
5.251  
5.244  
5.236  
5.229  
5.143  
5.135  
4.635  
4.616  
4.434  
4.414  
3.919  
3.758  
3.736  
3.716  
3.709  
3.705  
3.687  
3.666  
3.650  
2.604  
2.467  
2.190  
1.745  
1.725  
1.538  
1.525  
1.513  
1.500  
1.371  
1.355  
1.338  
1.324  
1.308  
1.295  
1.285  
1.267  
1.262  
1.251  
1.201  
1.185  
0.911  
0.895  
0.877



0.93  
1.89  
2.70

0.88  
0.93

1.89  
0.98

1.00  
1.93

1.16  
1.14

5.02

5.83

2.70

12.38

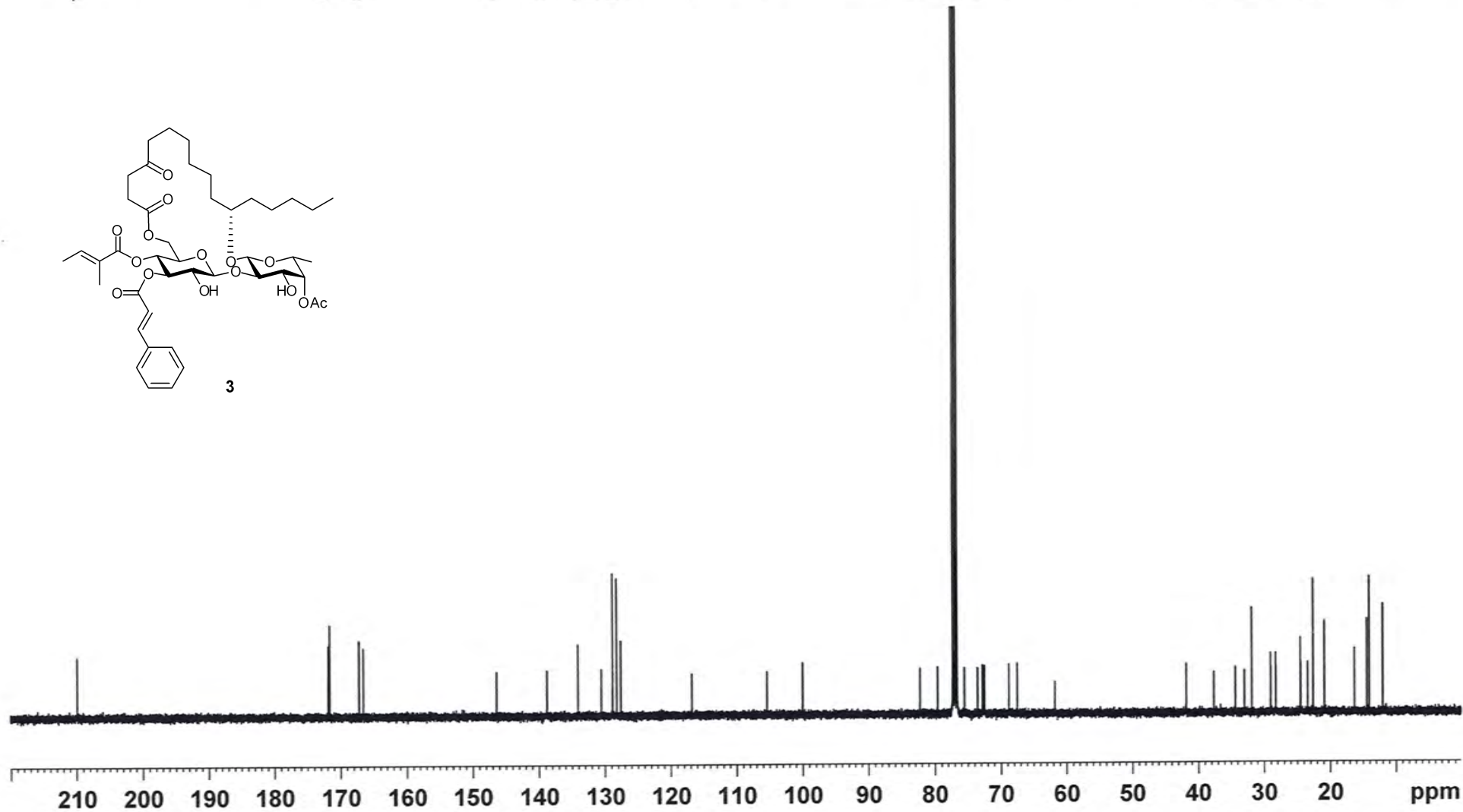
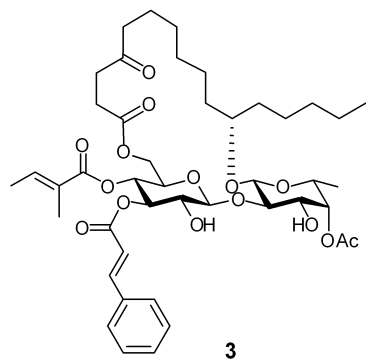
12.05

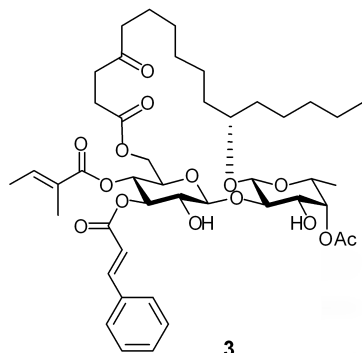
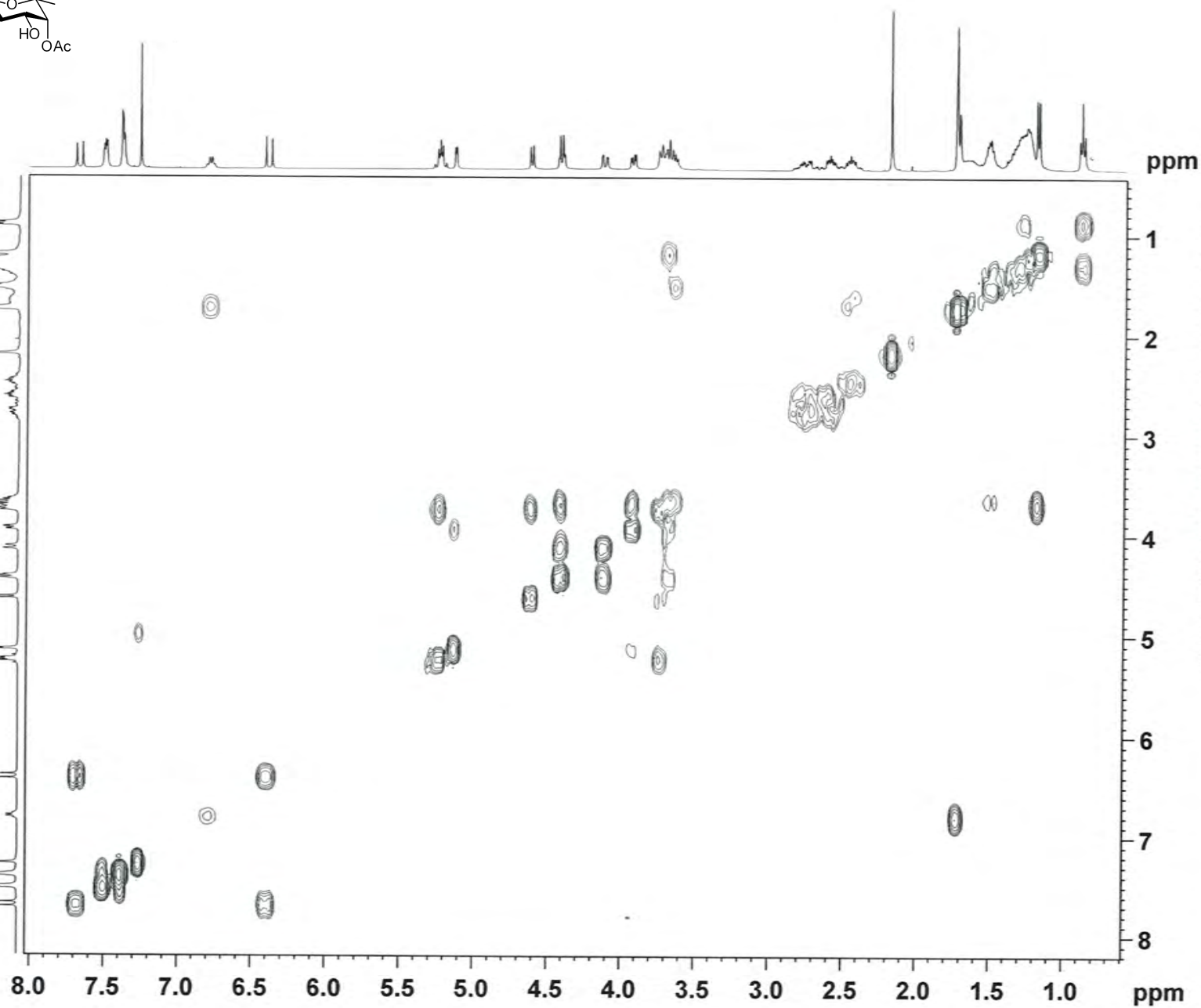
3.05

3.02

ZGH-Ipom-3-189-170120-A\_4 <sup>13</sup>C in CDCl<sub>3</sub>

— 209.974

171.940  
171.720  
167.261  
166.617146.467  
138.856  
134.131  
130.599  
128.894  
128.279  
127.669  
— 116.851  
105.442  
100.069  
82.305  
79.634  
77.317  
77.203  
77.000  
76.682  
75.574  
73.576  
72.833  
72.795  
72.524  
68.824  
67.551  
61.804  
41.851  
37.654  
34.378  
33.011  
31.894  
29.072  
29.037  
28.276  
24.565  
24.500  
23.441  
22.642  
20.926

ZGH-*Ipom*-3-189-170120-A\_4 in CDCl<sub>3</sub>

```

Current Data Parameters
NAME  ZGH-Ipom-3-189-170120-A_4
EXPNO  1
PROCNO  1

F2 - Acquisition Parameters
Date_  20170201
Time   22.15
INSTRUM spect
PROBHD 3 mm F4000 BBO
PULPROG zgpg30
TD      65536
SOLVENT CDCl3
NS      32
DS      4
SWH     8012.820 Hz
FIDRES  3.92210 Hz
AQ      0.1277982 sec
RG       424
DQ      62.400 usec
DE      6.50 usec
TE      294.0 K
DC      0.00000300 sec
DI      1.50000000 sec
D13     0.0000440 sec
D14     0.0002000 sec
IND     0.0001240 sec

----- CHANNEL f1 -----
SFO1   400.1520008 MHz
NUC1    1H
P1      12.50 usec
PL1     0.00000000 W
F1W1    20.00000000 W

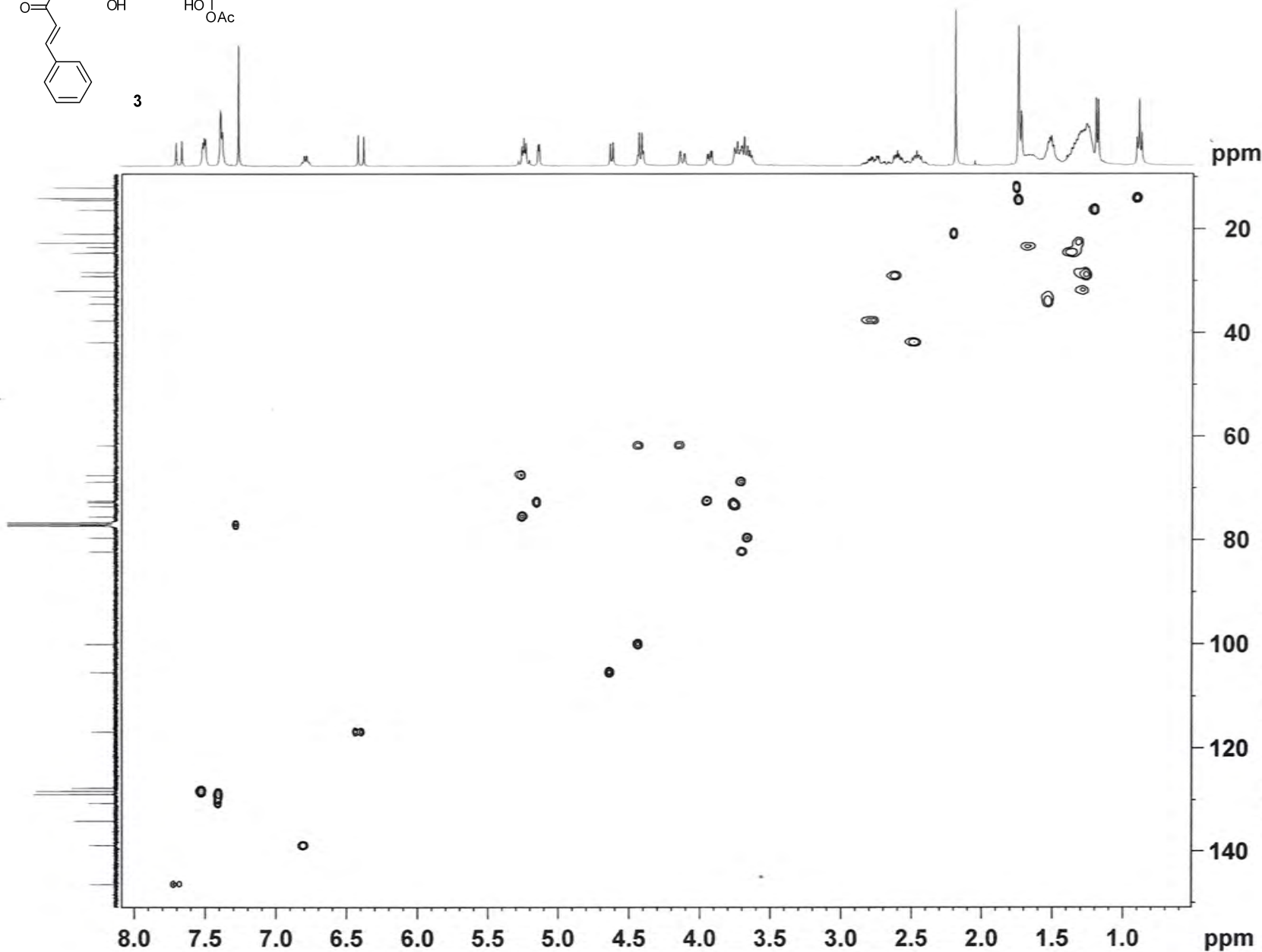
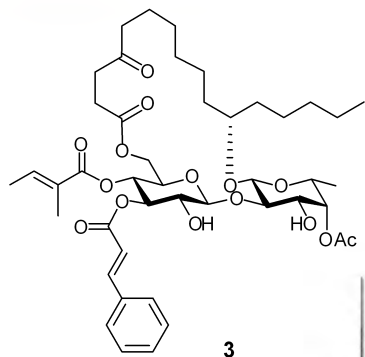
----- GRADIENT CHANNEL -----
GPM1[1] SMOG10.100
GR1     10.00 usec
PL1     1000.00 usec

F1 - Acquisition parameters
TD      65536
SFO1   400.1520008 MHz
FIDRES  42.4001519 Hz
DQ      62.4001519 usec
P1W1    20.00000000 W
P1MODE  QF

F2 - Processing parameters
SI      1024
SF      400.1500070 MHz
SFR     0
GB      0 Hz
GBW     0
PC      1.00

F1 - Processing parameters
SI      1024
SF      400.1500070 MHz
SFR     0
GB      0 Hz
GBW     0
PC      1.00

```

ZGH-*Ipom*-3-189-170120-A\_4 HSQC in CDCl<sub>3</sub>

Current Data Parameters  
 NAME ZGH-*Ipom*-3-189-170120-A\_4  
 EXPNO 14  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170202  
 Time 0.28  
 INSTRUM spect  
 PROBRD 5 mm PABBO BB-  
 PULPROG hsqcetpp1  
 TD 1024  
 SOLVENT CDCl3  
 NS 16  
 DS 16  
 SWH 5197.305 Hz  
 FIDRES 5.075689 Hz  
 AQ 0.0985068 sec  
 RG 2050  
 SW 36.200 usec  
 DE 6.50 usec  
 TE 294.4 K  
 CNST2 145.0000000  
 DO 0.0000300 sec  
 D1 1.5000000 sec  
 D4 0.0017414 sec  
 D11 0.0300000 sec  
 D16 0.0002000 sec  
 D24 0.0011000 sec  
 INO 0.0003000 sec  
 ZGPPINS

----- CHANNEL f1 -----  
 SF01 400.1524058 MHz  
 NUC1 1H  
 P1 12.50 usec  
 P2 25.00 usec  
 P28 1000.00 usec  
 PLM1 20.0000000 W

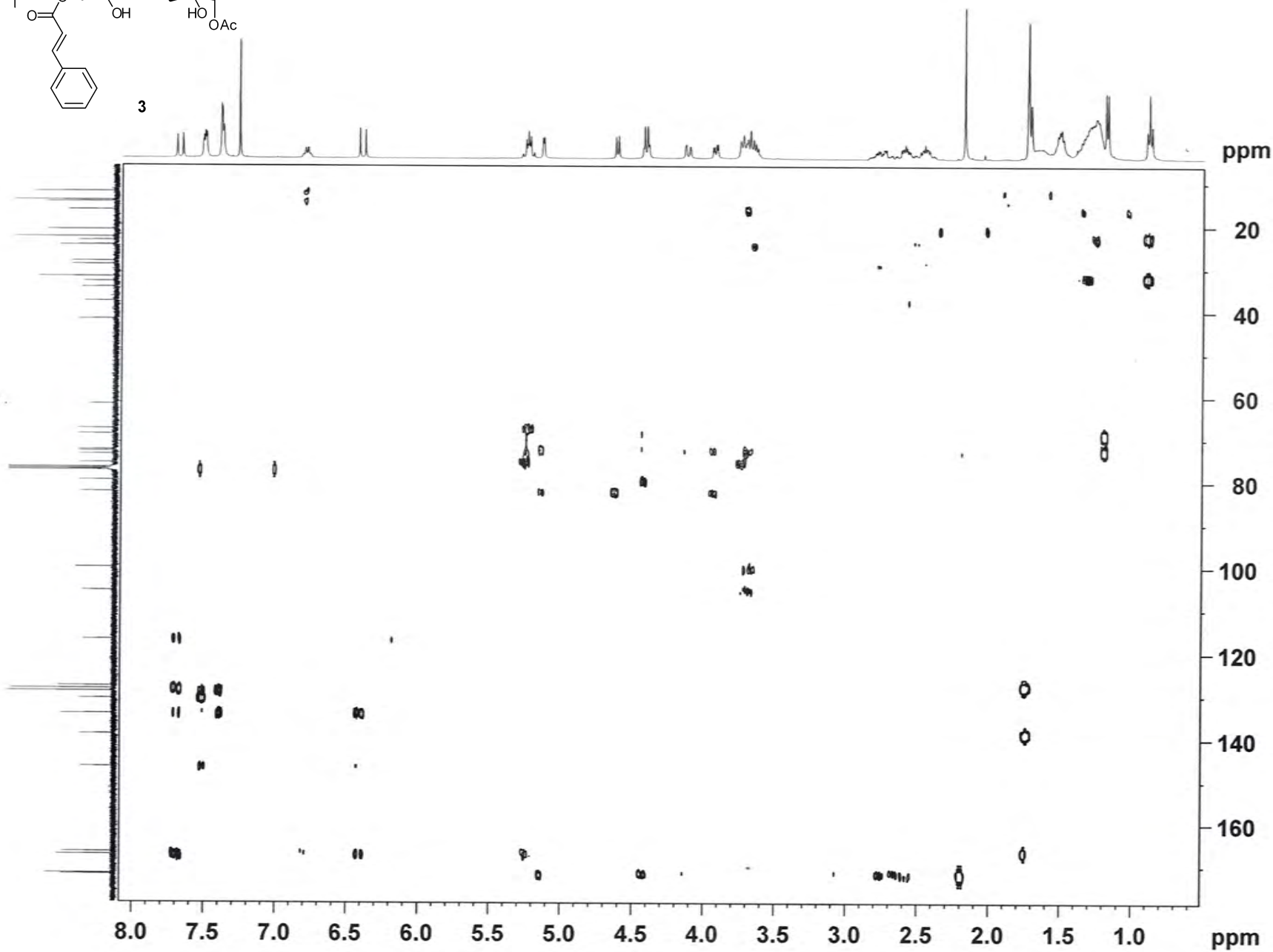
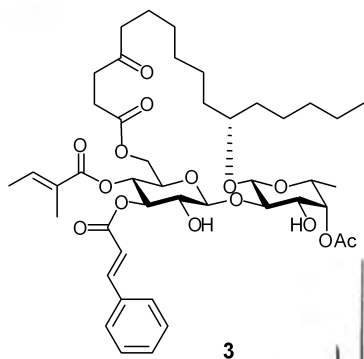
----- CHANNEL f2 -----  
 SF02 100.6230011 MHz  
 NUC2 13C  
 CPDPRG2 garp  
 P3 10.00 usec  
 P4 20.00 usec  
 PCPD2 80.00 usec  
 PLM2 65.0000000 W  
 PLM2 1.01559997 W

----- GRADIENT CHANNEL -----  
 GPRAM[1] RMS[1]0.100  
 GPRAM[2] RMS[2]0.100  
 GPZ1 80.00 %  
 GPZ2 20.10 %  
 P16 1000.00 usec

F1 - Acquisition parameters  
 TD 128  
 SF01 100.6233 MHz  
 FIDRES 130.208328 Hz  
 SN 165.631 ppm  
 PRMODE Echo-Antiecho

F2 - Processing parameters  
 SI 1024  
 SF 400.1500000 MHz  
 WDM QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0  
 PC 1.40

F1 - Processing parameters  
 SI 1024  
 MC2 echo-antiecho  
 SF 100.6177975 MHz  
 WDM QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0

ZGH-Ipom-3-189-170120-A\_4 HMBC in CDCl<sub>3</sub>

Current Data Parameters  
 NAME ZGH-Ipom-3-189-170120-A\_4  
 EXPNO 15  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170207  
 Time 11:26  
 INSTRUM spect  
 PROBHD 5 mm HAD301 SB-  
 PULPROG zgpg30  
 ID 46W  
 SOLVENT CDCl<sub>3</sub>  
 NS 80  
 DS 16  
 SWH 5208.333 Hz  
 FIDRES 1.711564 Hz  
 AQ 6.194160 sec  
 RG 2050  
 SW 94.000 usec  
 LE 6.50 usec  
 TE 304.2 K  
 CHFT2 243.000000  
 CHFT1 16.000000  
 SFO 0.0000000 sec  
 SF 1.5000000 sec  
 SC 0.0044828 sec  
 SE 0.0000000 sec  
 SSK 0.0002000 sec  
 SMC 0.0000249 sec

----- CHANNEL f1 -----  
 SFO1 400.1516000 MHz  
 MCT1 30  
 FE 12.50 usec  
 PD 25.00 usec  
 PLAC 20.0000000 W

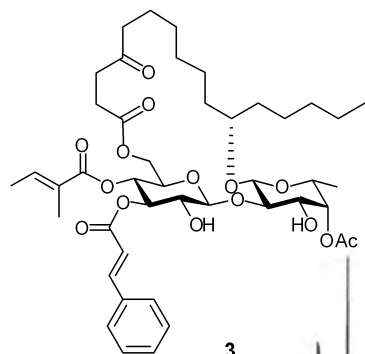
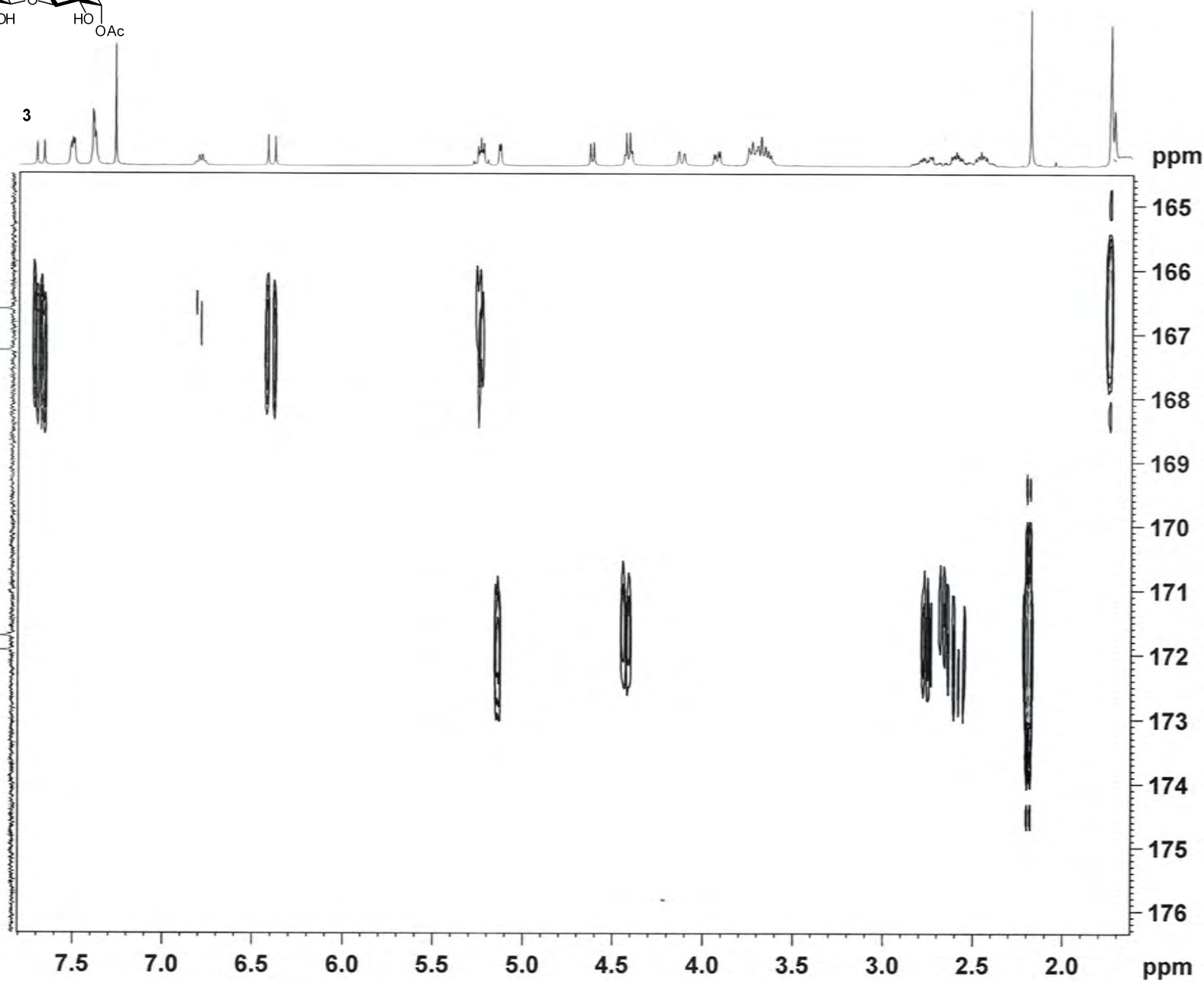
----- CHANNEL f2 -----  
 SFO2 100.6284670 MHz  
 MCT2 30  
 FE 10.00 usec  
 PLAC 65.0000000 W

----- GRADIENT CHANNEL -----  
 GPRAM11 SINE 100  
 GPRAM12 SINE 100  
 GPRAM13 SINE 100  
 GPC1 50.00 V  
 GPC2 30.00 V  
 GPC3 80.10 V  
 FIC 1000.00 usec

F1 - Acquisition parameters  
 ID 128  
 SFO1 100.6284670 MHz  
 FIDRES 174.186154 Hz  
 SW 721.816 ppm  
 FUNDOS QF

F1 - Processing parameters  
 SI 32768  
 SF 400.1500046 MHz  
 NCV 0  
 SSB 0 SINE  
 GB 0 Hz  
 PC 4.00

F2 - Processing parameters  
 SI 1624  
 MCT2 QF  
 SF 100.6177921 MHz  
 NCV 0  
 SSB 0 SINE  
 GB 0 Hz

ZGH-*Ipom*-3-189-170120-A\_4 HMBC in CDCl<sub>3</sub>

Current Data Parameters  
NAME ZGH-*Ipom*-3-189-170120-A\_4  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170205  
Time 1.14  
INSTRUM spect  
PROBHD 5 mm F400 BBO  
PULPROG hmcpgpmodf  
TD 4096  
SOLVENT CDCl<sub>3</sub>  
NS 80  
DS 16  
SWH 5008.313 Hz  
FIDRES 1.271364 Hz  
AQ 0.1932140 sec  
RG 2050  
SW 96.000 usec  
SE 4.50 usec  
TE 294.2 K  
CRO22 145.000000  
CRO23 10.000000  
CO 0.0000000 sec  
C1 1.5000000 sec  
C2 0.00344823 sec  
C3 0.0000000 sec  
C4 0.0000000 sec  
C5 0.0000000 sec  
C6 0.0000000 sec  
C7 0.0000000 sec  
C8 0.0000000 sec  
C9 0.0000000 sec  
C10 0.0000000 sec  
C11 0.0000000 sec  
C12 0.0000000 sec  
C13 0.0000000 sec  
C14 0.0000000 sec  
C15 0.0000000 sec  
C16 0.0000000 sec  
C17 0.0000000 sec  
C18 0.0000000 sec  
C19 0.0000000 sec  
C20 0.0000000 sec  
C21 0.0000000 sec  
C22 0.0000000 sec  
C23 0.0000000 sec  
C24 0.0000000 sec  
C25 0.0000000 sec  
C26 0.0000000 sec  
C27 0.0000000 sec  
C28 0.0000000 sec  
C29 0.0000000 sec  
C30 0.0000000 sec  
C31 0.0000000 sec  
C32 0.0000000 sec  
C33 0.0000000 sec  
C34 0.0000000 sec  
C35 0.0000000 sec  
C36 0.0000000 sec  
C37 0.0000000 sec  
C38 0.0000000 sec  
C39 0.0000000 sec  
C40 0.0000000 sec  
C41 0.0000000 sec  
C42 0.0000000 sec  
C43 0.0000000 sec  
C44 0.0000000 sec  
C45 0.0000000 sec  
C46 0.0000000 sec  
C47 0.0000000 sec  
C48 0.0000000 sec  
C49 0.0000000 sec  
C50 0.0000000 sec  
C51 0.0000000 sec  
C52 0.0000000 sec  
C53 0.0000000 sec  
C54 0.0000000 sec  
C55 0.0000000 sec  
C56 0.0000000 sec  
C57 0.0000000 sec  
C58 0.0000000 sec  
C59 0.0000000 sec  
C60 0.0000000 sec  
C61 0.0000000 sec  
C62 0.0000000 sec  
C63 0.0000000 sec  
C64 0.0000000 sec  
C65 0.0000000 sec  
C66 0.0000000 sec  
C67 0.0000000 sec  
C68 0.0000000 sec  
C69 0.0000000 sec  
C70 0.0000000 sec  
C71 0.0000000 sec  
C72 0.0000000 sec  
C73 0.0000000 sec  
C74 0.0000000 sec  
C75 0.0000000 sec  
C76 0.0000000 sec  
C77 0.0000000 sec  
C78 0.0000000 sec  
C79 0.0000000 sec  
C80 0.0000000 sec  
C81 0.0000000 sec  
C82 0.0000000 sec  
C83 0.0000000 sec  
C84 0.0000000 sec  
C85 0.0000000 sec  
C86 0.0000000 sec  
C87 0.0000000 sec  
C88 0.0000000 sec  
C89 0.0000000 sec  
C90 0.0000000 sec  
C91 0.0000000 sec  
C92 0.0000000 sec  
C93 0.0000000 sec  
C94 0.0000000 sec  
C95 0.0000000 sec  
C96 0.0000000 sec  
C97 0.0000000 sec  
C98 0.0000000 sec  
C99 0.0000000 sec  
C100 0.0000000 sec

----- CHANNEL f1 -----  
SFO2 400.1514000 MHz  
NUC1 13C  
P1 12.50 usec  
P2 25.00 usec  
PLA0 20.00000000 W  
----- CHANNEL f2 -----  
SFO2 100.6254170 MHz  
NUC1 13C  
P1 10.00 usec  
PLA0 45.00000000 W

----- GRADIENT CHANNEL -----  
GPRAM[1] SINE 100  
GPRAM[2] SINE 100  
GPRAM[3] SINE 100  
GPI1 50.00 V  
GPI2 30.00 V  
GPI3 80.00 V  
PI4 1000.00 usec

F1 - Acquisition parameters  
TD 128  
SFO1 100.6174000 MHz  
FIDRES 174.286154 Hz  
SW 221.820 ppm  
F0MODE QF

F2 - Processing parameters  
SI 2048  
SF 400.1500040 MHz  
WDW SINE  
SSB 0 Hz  
LB 0 Hz  
GB 0  
PC 4.00

F1 - Processing parameters  
SI 1024  
SF 100.6173400 MHz  
WDW SINE  
SSB 0 Hz  
LB 0 Hz  
GB 0

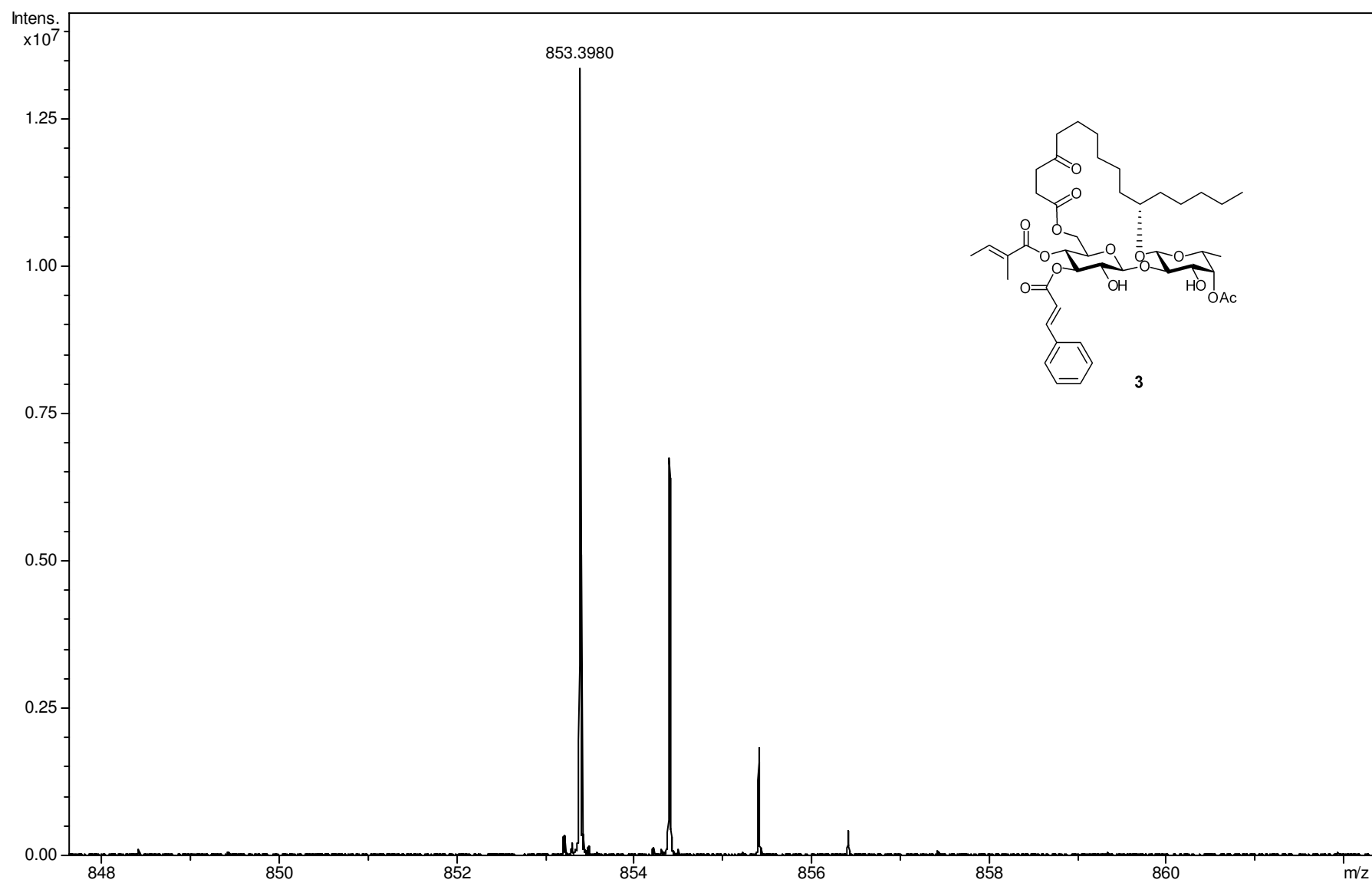


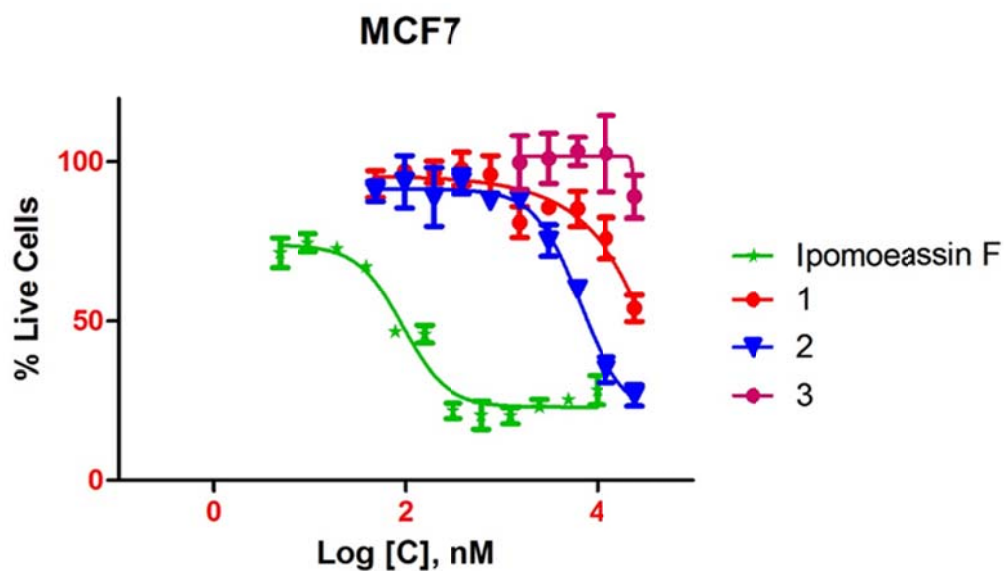
## Arkansas Statewide Mass Spectrometry Facility

## ESI-FTMS Mass Spectrum

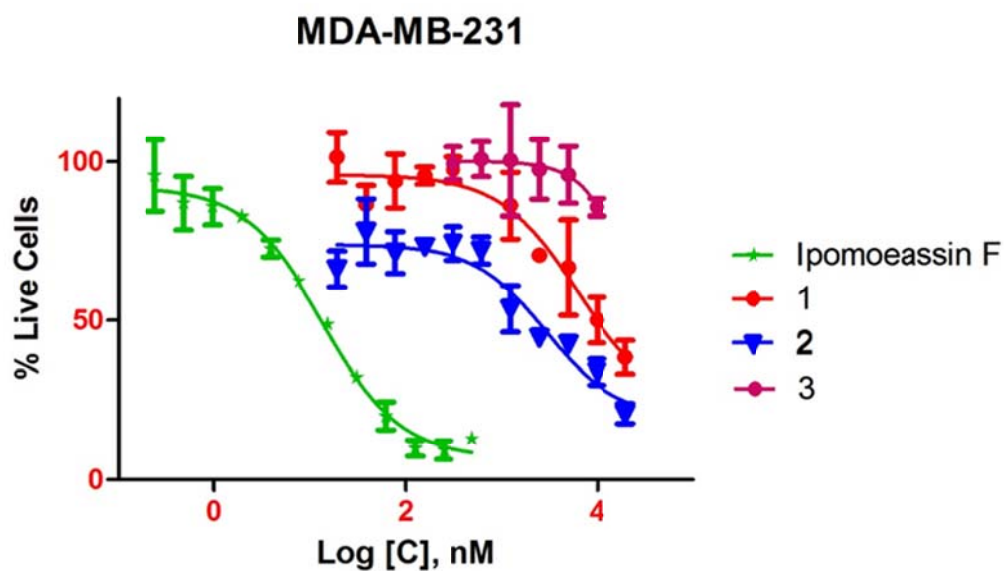
Sample Name: ZIF-54  
Sample id#: 921  
Instrument: Bruker ApexII-FTMS

2/8/2017

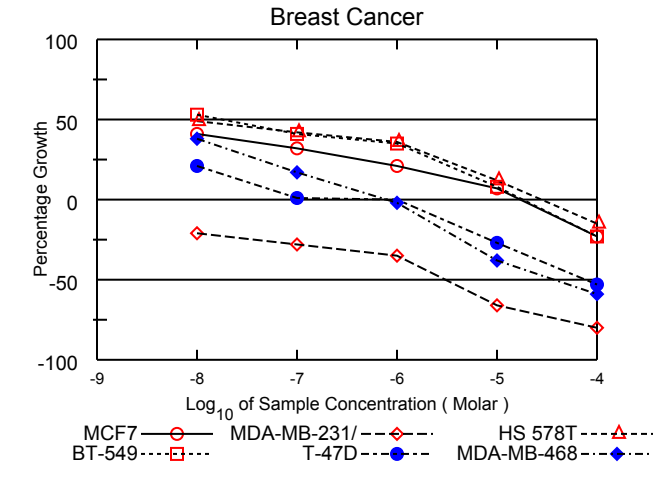
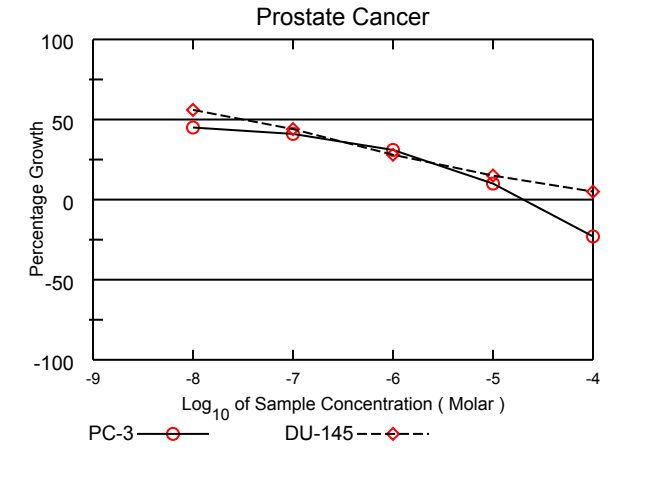
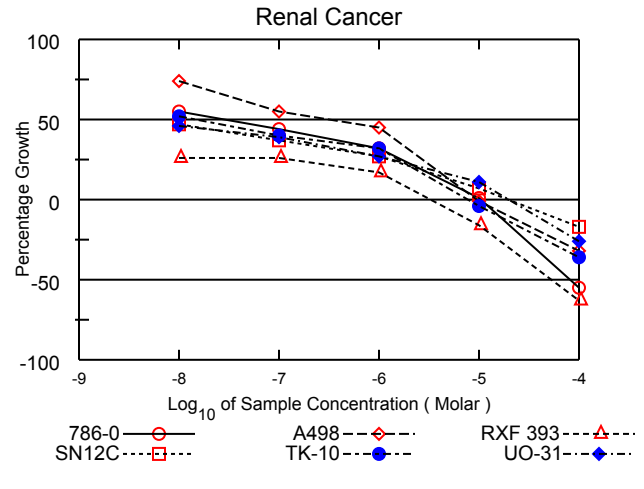
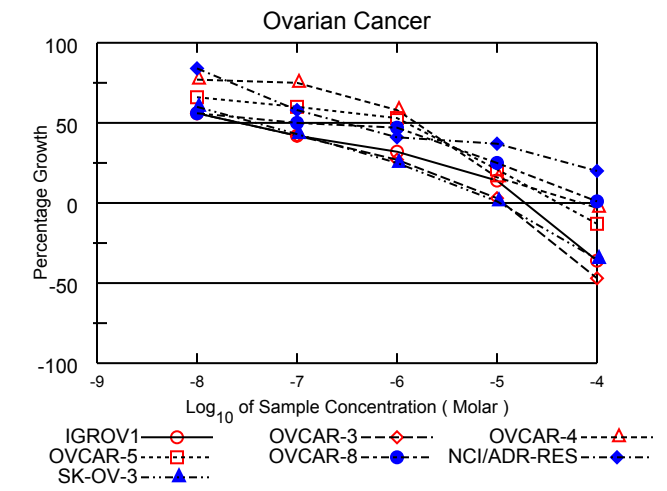
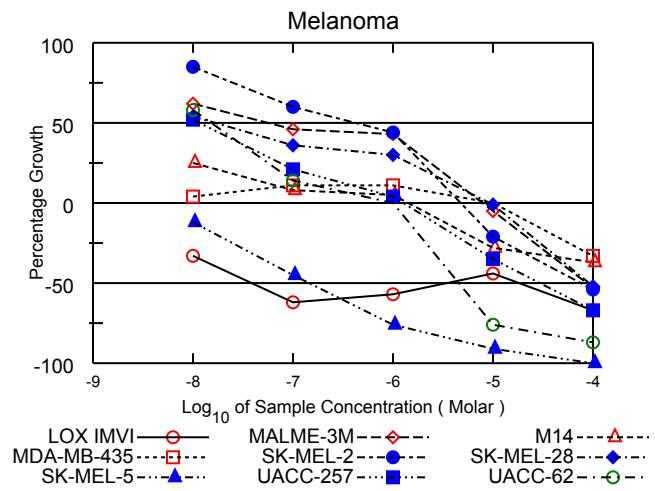
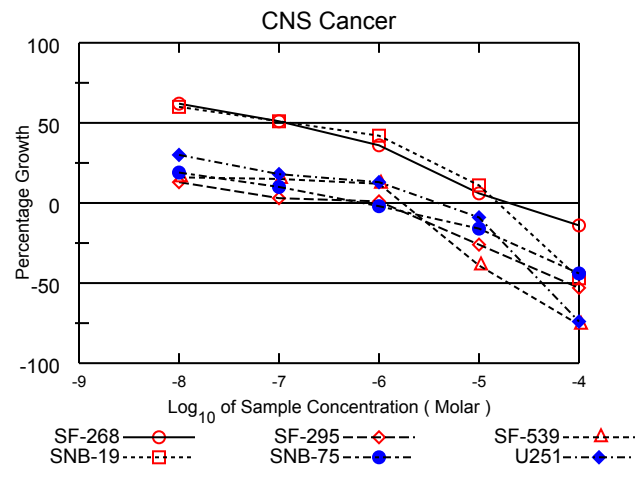
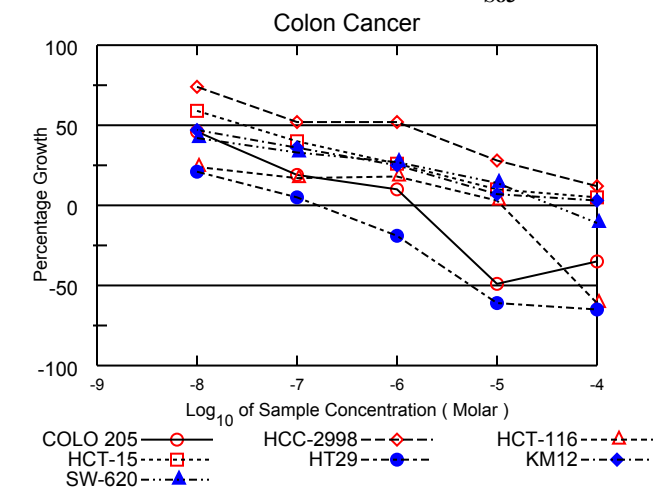
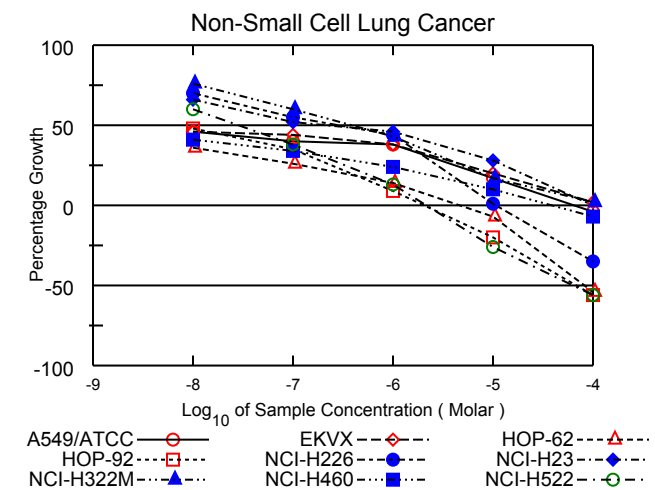
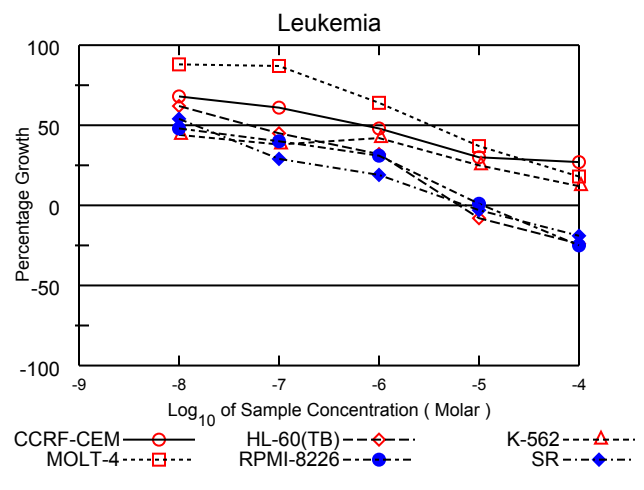




**Figure S1.** IC<sub>50</sub> curves of ipomoeassin F and analogues 1–3 against the MCF7 cell line.



**Figure S2.** IC<sub>50</sub> curves of ipomoeassin F and analogues 1–3 against the MDA-MB-231 cell line.



# National Cancer Institute Developmental Therapeutics Program In-Vitro Testing Results

S84

NSC : D - 791000 / 1	Experiment ID : 1610RS07	Test Type : 08	Units : Molar
Report Date : January 17, 2017	Test Date : October 31, 2016	QNS :	MC :
COMI : ZIF	Stain Reagent : SRB Dual-Pass Related	SSPL : 1A0E	

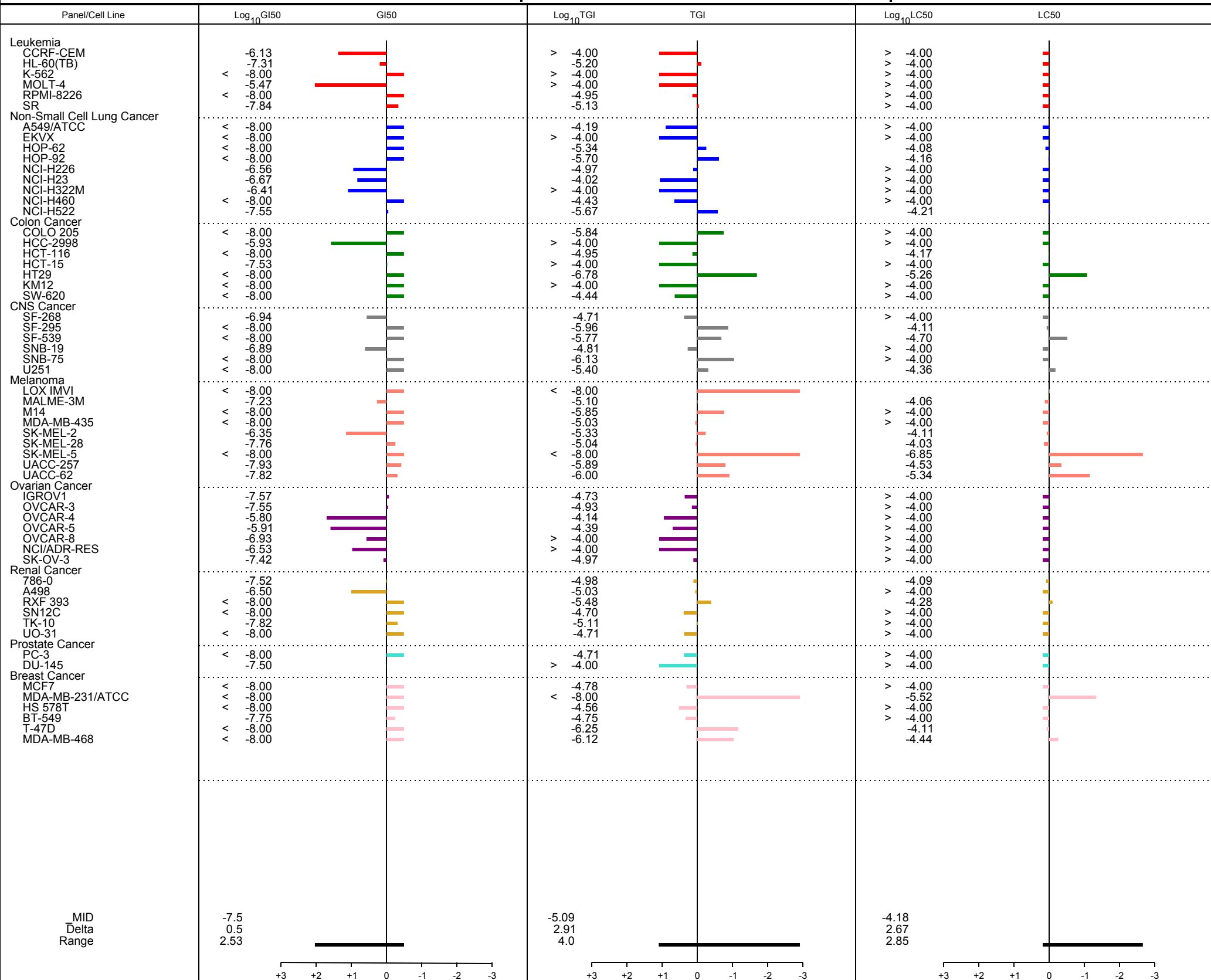
Panel/Cell Line	Log10 Concentration												GI50	TGI	LC50
	Time Zero	Ctrl	-8.0	-7.0	Mean Optical Densities			Percent Growth							
				-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0				
<b>Leukemia</b>															
CCRF-CEM	0.382	1.605	1.218	1.127	0.974	0.747	0.712	68	61	48	30	27	7.41E-7	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.809	2.804	2.048	1.699	1.442	0.746	0.616	62	45	32	-8	-24	4.90E-8	6.33E-6	> 1.00E-4
K-562	0.228	2.065	1.032	0.919	0.992	0.693	0.451	44	38	42	25	12	< 1.00E-8	> 1.00E-4	> 1.00E-4
MOLT-4	0.563	1.986	1.814	1.803	1.480	1.095	0.825	88	87	64	37	18	3.42E-6	> 1.00E-4	> 1.00E-4
RPMI-8226	0.926	2.465	1.669	1.538	1.408	0.948	0.695	48	40	31	1	-25	< 1.00E-8	1.13E-5	> 1.00E-4
SR	0.568	2.300	1.503	1.073	0.905	0.552	0.460	54	29	19	-3	-19	1.44E-8	7.42E-6	> 1.00E-4
<b>Non-Small Cell Lung Cancer</b>															
A549/ATCC	0.470	2.114	1.228	1.129	1.095	0.744	0.452	46	40	38	17	-4	< 1.00E-8	6.50E-5	> 1.00E-4
EKVX	0.853	2.545	1.637	1.598	1.489	1.195	0.881	46	44	38	20	2	< 1.00E-8	> 1.00E-4	> 1.00E-4
HOP-62	0.945	2.009	1.328	1.225	1.091	0.878	0.439	36	26	14	-7	-54	< 1.00E-8	4.55E-6	8.37E-5
HOP-92	1.002	1.608	1.292	1.211	1.055	0.798	0.444	48	35	9	-20	-56	< 1.00E-8	1.99E-6	6.90E-5
NCI-H226	0.768	1.416	1.220	1.123	1.053	0.776	0.498	70	55	44	1	-35	2.76E-7	1.08E-5	> 1.00E-4
NCI-H23	0.648	2.191	1.666	1.448	1.361	1.082	0.644	66	52	46	28	.	2.13E-7	9.52E-5	> 1.00E-4
NCI-H322M	0.967	2.266	1.951	1.743	1.529	1.187	0.992	76	60	43	17	2	3.91E-7	> 1.00E-4	> 1.00E-4
NCI-H460	0.183	2.001	0.933	0.804	0.617	0.360	0.170	41	34	24	10	-7	< 1.00E-8	3.71E-5	> 1.00E-4
NCI-H522	0.922	2.101	1.629	1.367	1.073	0.684	0.404	60	38	13	-26	-56	2.79E-8	2.14E-6	6.23E-5
<b>Colon Cancer</b>															
COLO 205	0.580	1.848	1.159	0.815	0.703	0.293	0.375	46	19	10	-49	-35	< 1.00E-8	1.46E-6	> 1.00E-4
HCC-2998	0.864	2.919	2.378	1.931	1.927	1.442	1.117	74	52	52	28	12	1.18E-6	> 1.00E-4	> 1.00E-4
HCT-116	0.252	2.206	0.718	0.580	0.606	0.319	0.098	24	17	18	3	-61	< 1.00E-8	1.13E-5	6.69E-5
HCT-15	0.330	2.340	1.515	1.137	0.857	0.541	0.430	59	40	26	10	5	2.98E-8	> 1.00E-4	> 1.00E-4
HT29	0.228	1.403	0.479	0.292	0.184	0.089	0.080	21	5	-19	-61	-65	< 1.00E-8	1.66E-7	5.46E-6
KM12	0.566	2.933	1.681	1.414	1.166	0.737	0.638	47	36	25	7	3	< 1.00E-8	> 1.00E-4	> 1.00E-4
SW-620	0.254	1.812	0.913	0.771	0.676	0.474	0.226	42	33	27	14	-11	< 1.00E-8	3.60E-5	> 1.00E-4
<b>CNS Cancer</b>															
SF-268	0.752	2.388	1.767	1.585	1.342	0.848	0.645	62	51	36	6	-14	1.15E-7	1.95E-5	> 1.00E-4
SF-295	0.611	3.049	0.923	0.691	0.636	0.452	0.287	13	3	1	-26	-53	< 1.00E-8	1.09E-6	7.72E-5
SF-539	1.194	3.061	1.490	1.481	1.411	0.728	0.290	16	15	12	-39	-76	< 1.00E-8	1.69E-6	1.99E-5
SNB-19	0.265	1.129	0.781	0.705	0.631	0.358	0.141	60	51	42	11	-47	1.29E-7	1.54E-5	> 1.00E-4
SNB-75	0.941	1.836	1.111	1.033	0.927	0.792	0.528	19	10	-2	-16	-44	< 1.00E-8	7.40E-7	> 1.00E-4
U251	0.495	2.137	0.985	0.798	0.710	0.452	0.131	30	18	13	-9	-74	< 1.00E-8	3.99E-6	4.34E-5
<b>Melanoma</b>															
LOX IMVI	0.462	2.918	0.311	0.178	0.201	0.261	0.152	-33	-62	-57	-44	-67	< 1.00E-8	< 1.00E-8	.
MALME-3M	0.588	1.077	0.890	0.816	0.799	0.561	0.277	62	46	43	-5	-53	5.87E-8	8.01E-6	8.71E-5
M14	0.406	1.633	0.713	0.503	0.468	0.291	0.257	25	8	5	-28	-37	< 1.00E-8	1.42E-6	> 1.00E-4
MDA-MB-435	0.495	2.355	0.571	0.699	0.693	0.494	0.332	4	11	11	.	-33	< 1.00E-8	9.38E-6	> 1.00E-4
SK-MEL-2	1.000	2.081	1.915	1.654	1.479	0.787	0.463	85	60	44	-21	-54	4.45E-7	4.73E-6	7.68E-5
SK-MEL-28	0.560	1.705	1.183	0.975	0.906	0.553	0.271	54	36	30	-1	-52	1.75E-8	9.13E-6	9.29E-5
SK-MEL-5	0.727	2.668	0.642	0.398	0.174	0.066	-0.057	-12	-45	-76	-91	-100	< 1.00E-8	< 1.00E-8	1.43E-7
UACC-257	1.025	2.071	1.572	1.249	1.072	0.663	0.340	52	21	4	-35	-67	1.19E-8	1.30E-6	2.92E-5
UACC-62	0.899	2.944	2.088	1.190	0.902	0.220	0.118	58	14	.	-76	-87	1.53E-8	1.00E-6	4.60E-6
<b>Ovarian Cancer</b>															
IGROV1	0.532	1.904	1.303	1.103	0.969	0.718	0.340	56	42	32	14	-36	2.67E-8	1.88E-5	> 1.00E-4
OVCAR-3	0.441	1.533	1.058	0.902	0.737	0.479	0.233	56	42	27	3	-47	2.83E-8	1.17E-5	> 1.00E-4
OVCAR-4	0.705	1.587	1.388	1.369	1.220	0.848	0.687	77	75	58	16	-3	1.58E-6	7.30E-5	> 1.00E-4
OVCAR-5	0.733	2.240	1.734	1.631	1.530	1.044	0.638	66	60	53	21	-13	1.23E-6	4.11E-5	> 1.00E-4
OVCAR-8	0.522	2.262	1.491	1.396	1.343	0.961	0.546	56	50	47	25	1	1.17E-7	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.647	2.426	2.150	1.677	1.381	1.300	1.009	84	58	41	37	20	2.97E-7	> 1.00E-4	> 1.00E-4
SK-OV-3	1.104	2.045	1.664	1.511	1.342	1.113	0.716	60	43	25	1	-35	3.84E-8	1.06E-5	> 1.00E-4
<b>Renal Cancer</b>															
786-0	0.636	2.295	1.552	1.371	1.167	0.659	0.284	55	44	32	1	-55	3.01E-8	1.06E-5	8.05E-5
A498	1.153	1.933	1.727	1.586	1.501	1.138	0.782	74	55	45	-1	-32	3.15E-7	9.35E-6	> 1.00E-4
RXF 393	0.641	1.315	0.819	0.814	0.755	0.542	0.235	26	26	17	-16	-63	< 1.00E-8	3.32E-6	5.25E-5
SN12C	0.522	2.270	1.339	1.171	0.993	0.648	0.436	47	37	27	7	-17	< 1.00E-8	2.01E-5	> 1.00E-4
TK-10	1.429	2.523	2.000	1.870	1.774	1.375	0.915	52	40	32	-4	-36	1.52E-8	7.82E-6	> 1.00E-4
UO-31	0.508	1.896	1.152	1.045	0.888	0.656	0.375	46	39	27	11	-26	< 1.00E-8	1.95E-5	> 1.00E-4
<b>Prostate Cancer</b>															
PC-3	0.588	1.724	1.098	1.049	0.938	0.698	0.452	45	41	31	10	-23	< 1.00E-8	1.97E-5	> 1.00E-4
DU-145	0.346	1.749	1.133	0.964	0.746	0.553	0.412	56	44	28	15	5	3.19E-8	> 1.00E-4	> 1.00E-4
<b>Breast Cancer</b>															
MCF7	0.360	2.157	1.098	0.934	0.740	0.481	0.276	41	32	21	7	-23	< 1.00E-8	1.67E-5	> 1.00E-4
MDA-MB-231/ATCC	0.573	1.352	0.453	0.412	0.371	0.195	0.114	-21	-28	-35	-66	-80	< 1.00E-8	< 1.00E-8	3.01E-6
HS 578T	1.105	2.160	1.623	1.551	1.486	1.232	0.936	49	42	36	12	-15	< 1.00E-8	2.75E-5	> 1.00E-4
BT-549	1.113	2.143	1.661	1.532	1.470	1.193	0.852	53	41	35	8	-23	1.79E-8	1.77E-5	> 1.00E-4
T-47D	0.851	1.514	0.990	0.859	0.848	0.618	0.401	21	1	.	-27	-53	< 1.00E-8	5.57E-7	7.71E-5
MDA-MB-468	0.913	2.031	1.334	1.100	0.892	0.563	0.372	38	17	-2	-38	-59	< 1.00E-8	7.52E-7	3.60E-5

Mean Graphs

Report Date :January 17, 2017

Test Date :October 31, 2016

585



Dose Response Curves

Report Date: January 17, 2017

Test Date: October 31, 2016

586

All Cell Lines

