

Supporting Information for:

## Ipomoeassin F Binds Sec61 $\alpha$ to Inhibit Protein Translocation

Guanghai Zong,<sup>a,b,†</sup> Zhijian Hu,<sup>a,†</sup> Sarah O’Keefe,<sup>c,#</sup> Dale Tranter,<sup>d,e,#</sup> Michael J. Iannotti,<sup>f,#</sup> Ludivine Baron,<sup>g,h,#</sup> Belinda Hall,<sup>i,#</sup> Katherine Corfield,<sup>i,#</sup> Anja O. Paatero,<sup>d,e,#</sup> Mark J. Henderson,<sup>f,#</sup> Peristera Roboti,<sup>c,#</sup> Jianhong Zhou,<sup>j</sup> Xianwei Sun,<sup>a,k</sup> Mugunthan Govindarajan,<sup>a,l</sup> Jason M. Rohde,<sup>f</sup> Nicolas Blanchard,<sup>m</sup> Rachel Simmonds,<sup>i,\*</sup> James Inglese,<sup>f,\*</sup> Yuchun Du,<sup>j,\*</sup> Caroline Demangel,<sup>g,h,\*</sup> Stephen High,<sup>c,\*</sup> Ville O. Paavilainen,<sup>d,e,\*</sup> and Wei Q. Shi<sup>a,n,\*</sup>

<sup>a</sup> Department of Chemistry and Biochemistry, and <sup>j</sup> Department of Biological Sciences, J. William Fulbright College of Arts & Science, University of Arkansas, Fayetteville, Arkansas, 72701, USA

<sup>b</sup> Department of Chemistry and Biochemistry, University of Maryland, College Park, Maryland 20742, United States

<sup>c</sup> School of Biological Sciences, Faculty of Biology, Medicine and Health, University of Manchester, Manchester, M13 9PT, United Kingdom.

<sup>d</sup> University of Helsinki, HiLIFE, and <sup>e</sup> Institute of Biotechnology, Helsinki, Finland

<sup>f</sup> National Center for Advancing Translational Sciences, National Institutes of Health, Rockville, Maryland 20850, USA.

<sup>g</sup> Institut Pasteur, Immunobiology of Infection Unit, 75015 and <sup>h</sup> INSERM, U1221, 75005 Paris, France

<sup>i</sup> Department of Microbial Sciences, School of Biosciences and Medicine, University of Surrey, Guildford, Surrey GU2 7XH, United Kingdom

<sup>k</sup> Department of Radiology, Baylor College of Medicine, Houston, TX, 77030, USA

<sup>l</sup> Emory Institute for Drug Development, Emory University, 954 Gatewood Road, Atlanta, Georgia, 30329, USA

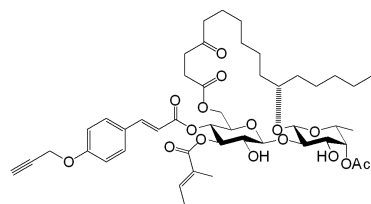
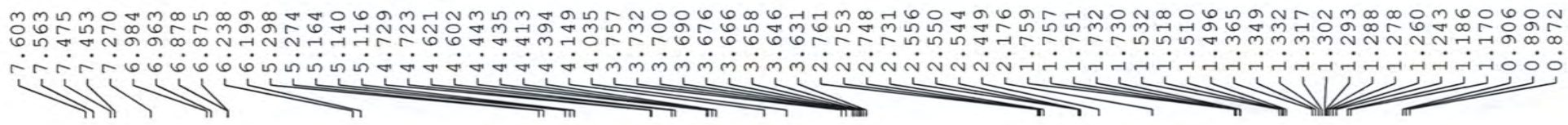
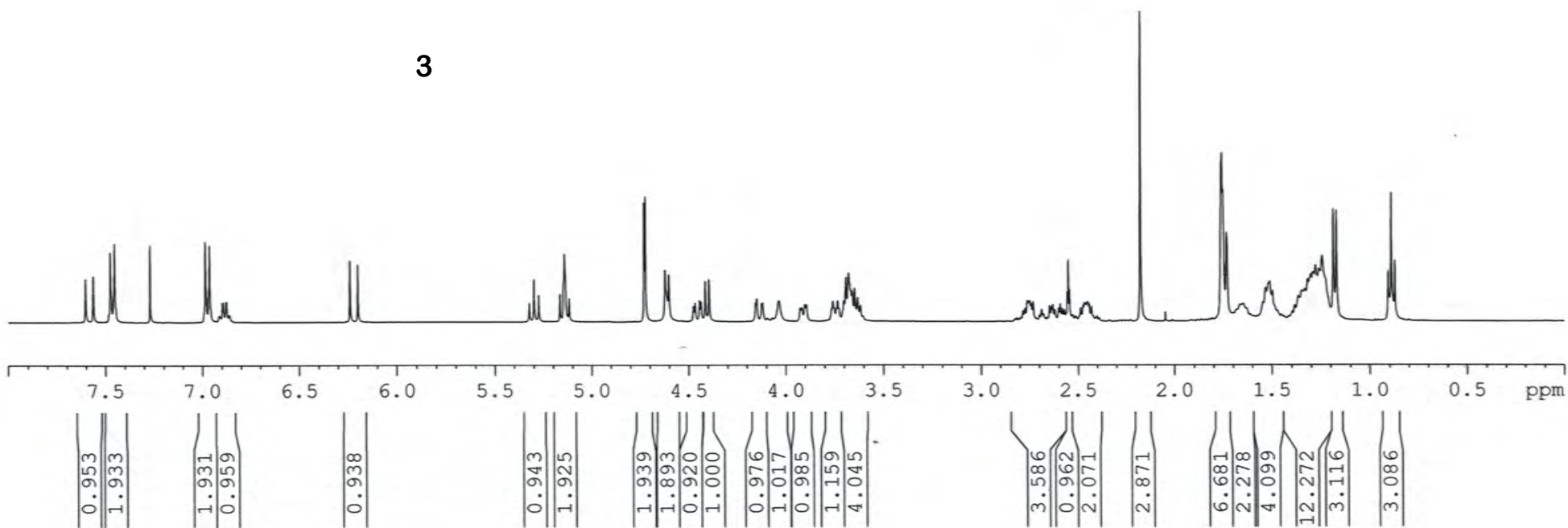
<sup>m</sup> Université de Haute-Alsace, Université de Strasbourg, CNRS, LIMA, UMR 7042, 68000 Mulhouse, France

<sup>n</sup> Department of Chemistry, Ball State University, Muncie, Indiana 47306, USA

† Equal contribution as first-author

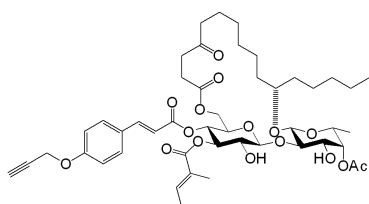
# Equal contribution as second-author

\* Corresponding authors

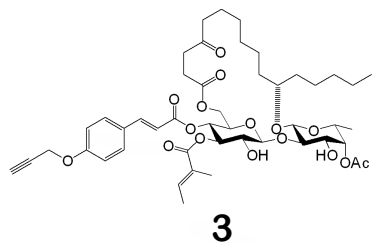
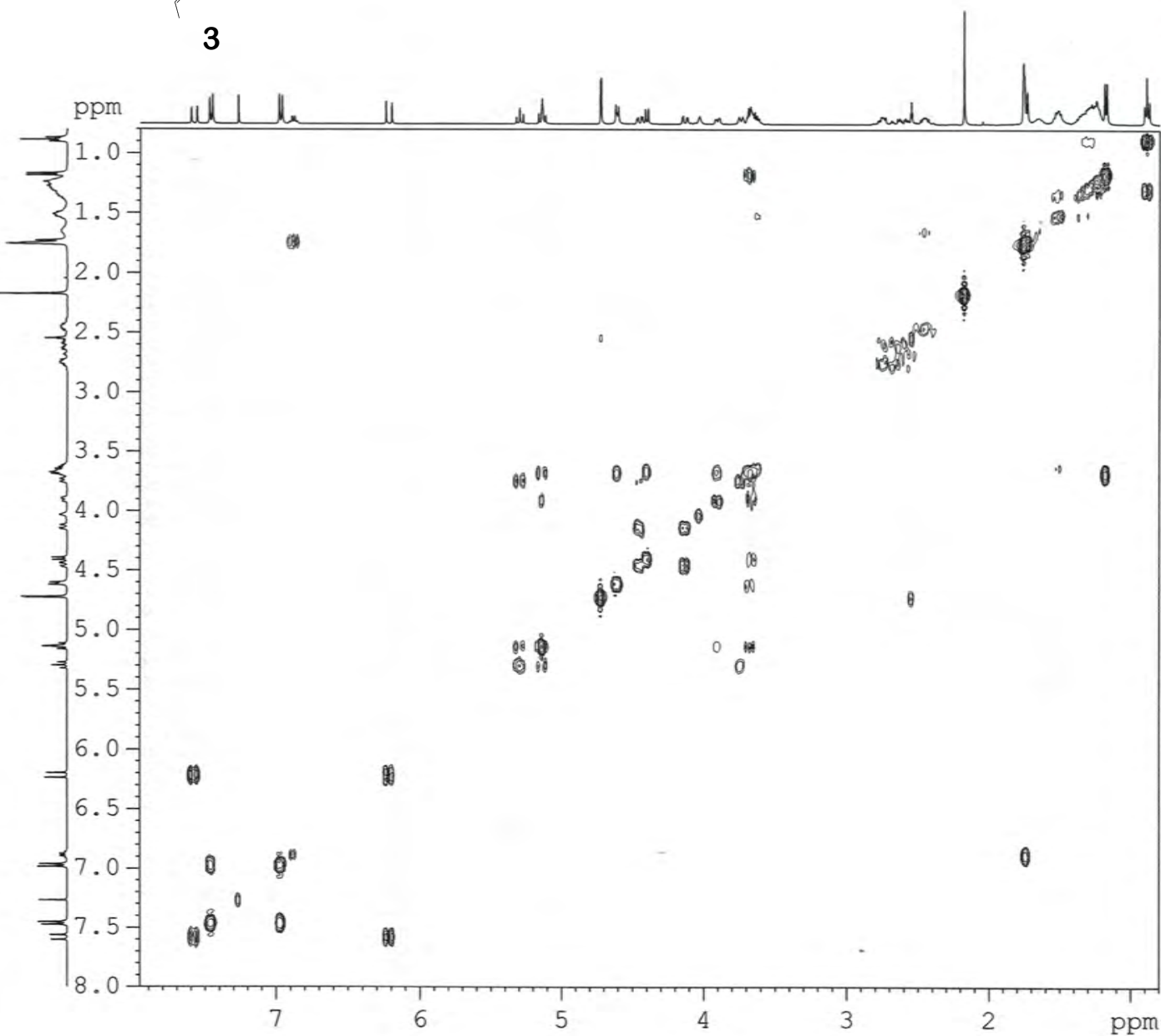
ZGH-*Ipom*-2-91-A-140903 1H in CDCL<sub>3</sub>**3**

ZGH-*Ipom*-2-91-A-140903  $^{13}\text{C}$  in  $\text{CDCl}_3$ 

— 210.023

171.747  
171.686  
168.804  
165.600  
159.413— 145.534  
— 139.730— 129.879  
— 127.535115.195  
114.605105.646  
100.17182.726  
79.71777.898  
77.302  
77.18876.984  
76.666  
75.96875.838  
73.93172.668  
72.573  
72.40368.776  
67.304  
61.76655.770  
41.80337.547  
34.306  
33.06631.874  
29.086  
29.00428.263  
24.646  
24.46523.433  
22.612  
20.90516.304  
14.560**3**

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

ZGH-*Ipom*-2-91-A-140903 COSY

```

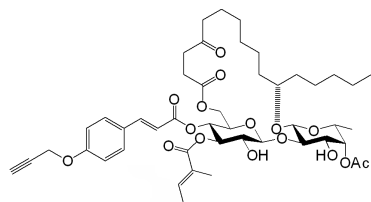
NAME      ZGH-Ipom-2-91-A-140903
EXPNO     2
PROCNO    1
Date_     20140905
Time      23.30
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   cosyppqf
TD         2048
SOLVENT   CDC13
NS         16
DS         8
SWH        5341.880 Hz
FIDRES     2.608340 Hz
AQ         0.1917428 sec
RG         128
DW         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
ND0        1
TD         128
SFO1       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
  
```

**3**ZGH-*Ipom*-2-91-A-140903 HSQC

```

NAME      ZGH-Ipom-2-91-A-140903
EXPNO     4
PROCNO    1
Date_     20140906
Time      7.54
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   hsqcetgps1
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         293.3 K
CNST2     145.0000000
D0         0.000003000 sec
D1         1.500000000 sec
D4         0.00172414 sec
D11        0.030000000 sec
D13        0.000004000 sec
D16        0.000200000 sec
D24        0.001100000 sec
IN0        0.000030000 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

```

```

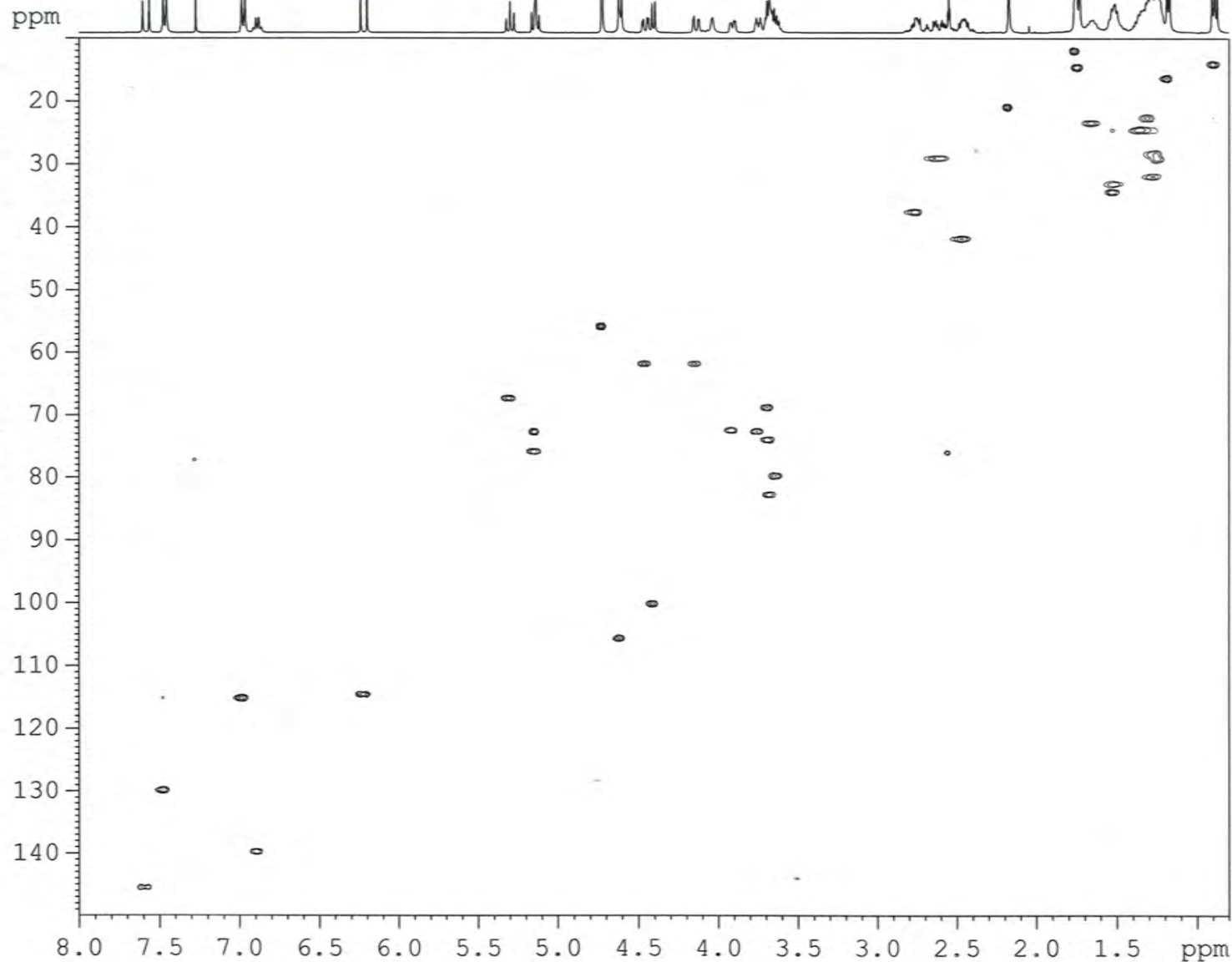
===== CHANNEL f2 =====
CPDPRG2   garp
NUC2      13C
P3        10.00 usec
P4        20.00 usec
PCPD2     75.00 usec
PL2       -2.10 dB
PL12      15.40 dB
PL2W      58.37759399 W
PL12W     1.03811681 W
SFO2      100.6202727 MHz

```

```

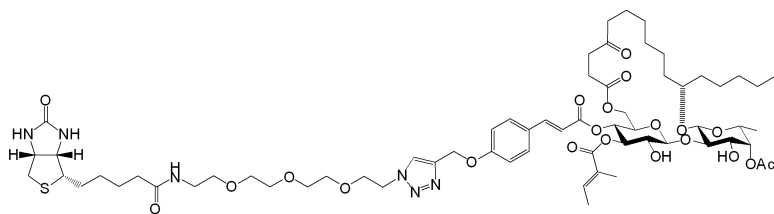
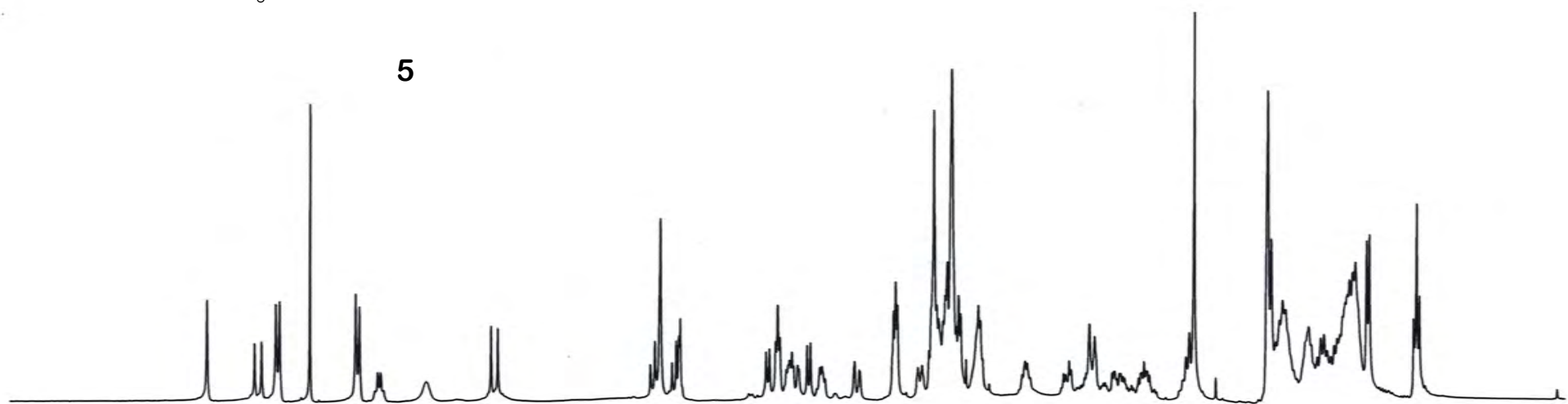
===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    SINE.100
GPZ1      80.00 %
GPZ2      20.10 %
P16       1000.00 usec
ND0       2
TD         256
SFO1      100.6203 MHz
FIDRES    65.104164 Hz
SW        165.639 ppm
FnMODE    Echo-Antiecho
SI         1024
SF        400.1300000 MHz
WDW       QSINE
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*-3-49-160510-A in CDCl<sub>3</sub>

7.861  
7.465  
7.444  
7.270  
7.009  
6.226  
6.186  
5.247  
5.157  
5.141  
5.133  
4.574  
4.562  
3.910  
3.898  
3.886  
3.690  
3.675  
3.658  
3.648  
3.644  
3.621  
3.610  
3.597  
3.572  
3.545  
3.531  
3.519  
3.417  
3.405  
2.772  
2.742  
2.200  
2.174  
1.752  
1.731  
1.683  
1.664  
1.647  
1.514  
1.444  
1.425  
1.350  
1.333  
1.319  
1.303  
1.290  
1.279  
1.262  
1.258  
1.245  
1.180  
1.164  
0.908  
0.891  
0.873

**5**

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

0.96

1.02

1.74

1.78

0.75

0.85

1.69

2.91

1.83

0.93

1.84

2.16

0.95

1.11

0.95

2.81

21.45

2.13

8.83

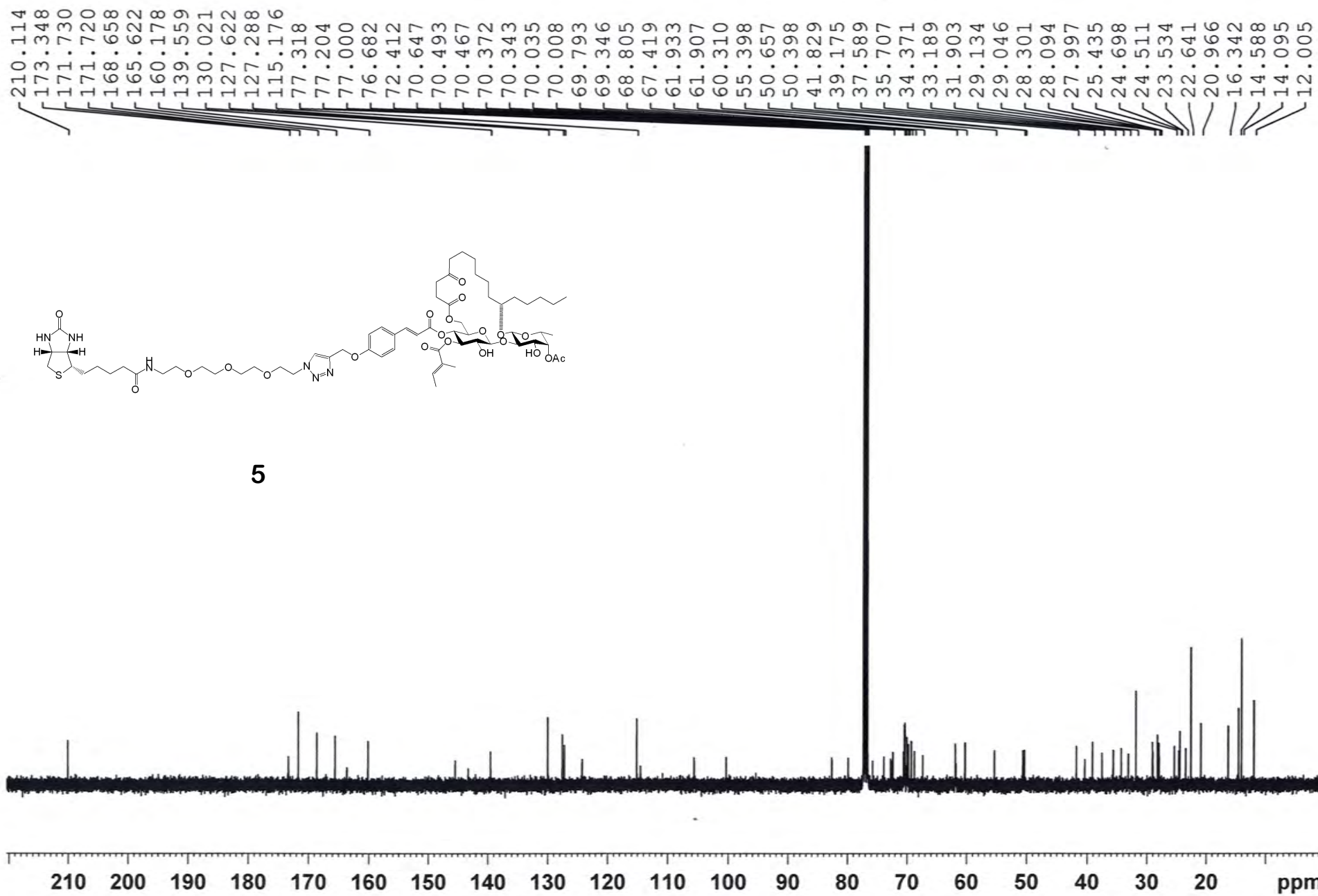
4.97

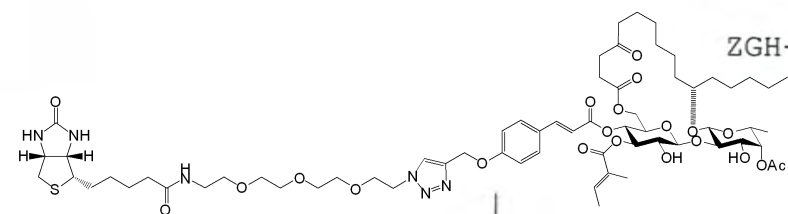
29.84

3.13

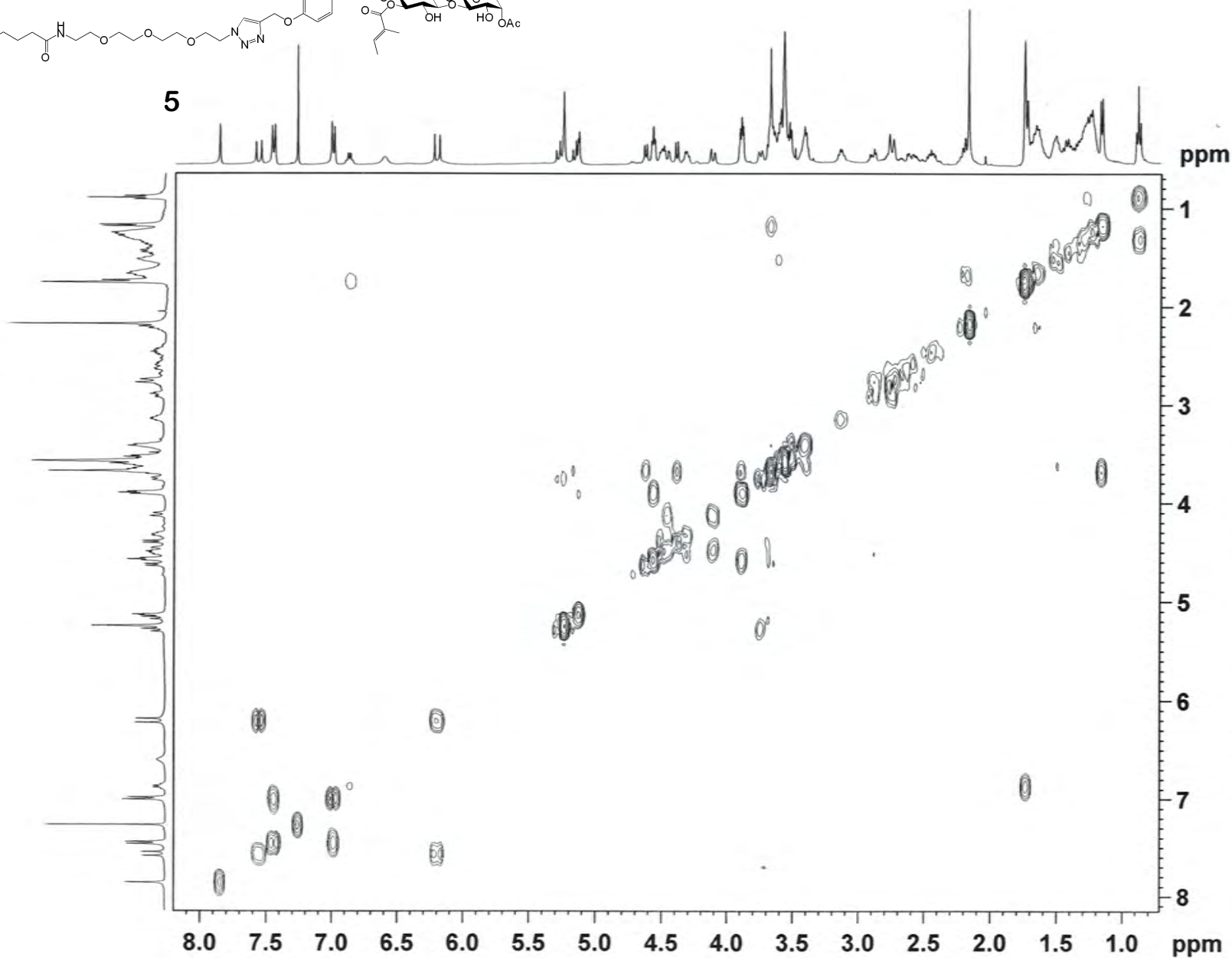
3.00

ZGH-Ipom-3-49-160510-A 13C in CDCl3



ZGH-*Ipom*-3-49-160510-A in CDCL<sub>3</sub>

5



Current Data Parameters  
 NAME ZGH-*Ipom*-3-49-160510-A  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160512  
 Time 1.59  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosygpgf  
 TD 2048  
 SOLVENT CDCL3  
 NS 16  
 DS 8  
 SWH 8012.820 Hz  
 FIDRES 3.912510 Hz  
 AQ 0.1277952 sec  
 RG 322  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 293.9 K  
 DO 0.00000300 sec  
 D1 1.50000000 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 INO 0.00012480 sec

----- CHANNEL f1 -----  
 SF01 400.1520008 MHz  
 NUC1 1H  
 P0 12.50 usec  
 P1 12.50 usec  
 PLW1 20.00000000 W

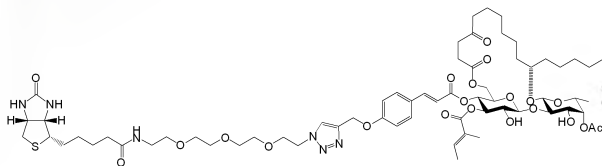
----- GRADIENT CHANNEL -----  
 GPNAM[1] SMSQ10.100  
 GP21 10.00 %  
 P16 1000.00 usec

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

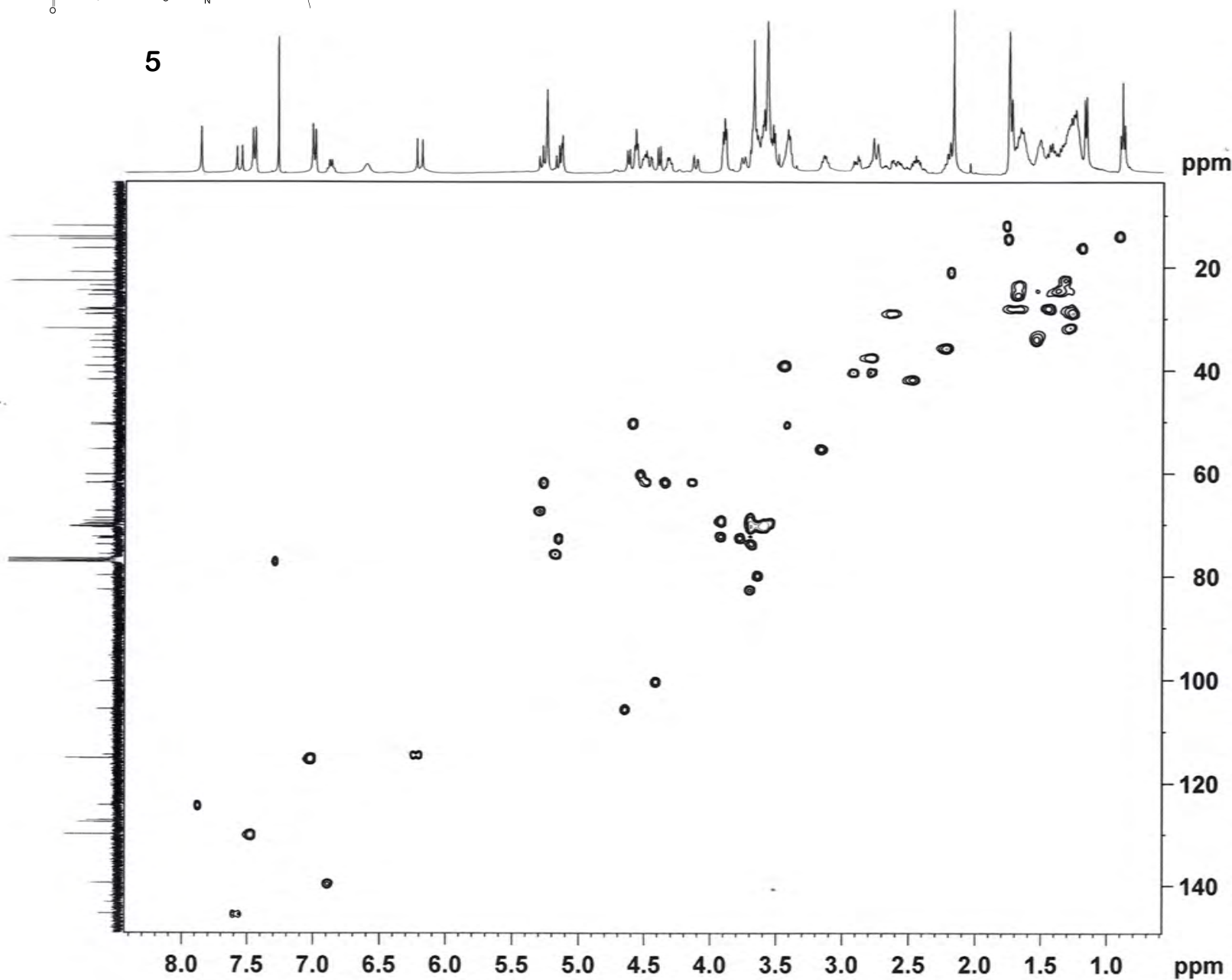
F2 - Processing parameters  
 SI 1024  
 SF 400.1500070 MHz  
 WDW QSINE  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

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



ZGH-Ipom-3-49-160510-A HSQC in CDCl<sub>3</sub>

5



Current Data Parameters  
 NAME ZGH-Ipom-3-49-160510-A  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20160512  
 Time 2.56  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hsqcetpsi  
 TD 1024  
 SOLVENT CDCl<sub>3</sub>  
 NS 16  
 DS 16  
 SWH 5197.505 Hz  
 FIDRES 5.075689 Hz  
 AQ 0.0985088 sec  
 RG 2050  
 DW 96.200 usec  
 DE 6.50 usec  
 TE 293.1 K  
 CNST2 145.0000000  
 D0 0.0000300 sec  
 D1 1.5000000 sec  
 D4 0.00172414 sec  
 D11 0.03000000 sec  
 D16 0.00020000 sec  
 D24 0.00110000 sec  
 IN0 0.00003000 sec  
 ZGOPTNS

----- CHANNEL f1 -----  
 SFO1 400.1524058 MHz  
 NUC1 1H  
 P1 12.50 usec  
 P2 25.00 usec  
 P28 1000.00 usec  
 PLW1 20.00000000 W

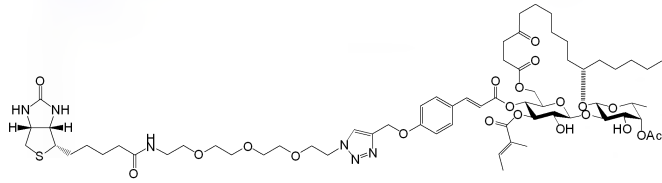
----- CHANNEL f2 -----  
 SFO2 100.6253021 MHz  
 NUC2 13C  
 CPDPRG[2] garp  
 P3 10.00 usec  
 P4 20.00 usec  
 PCPD2 80.00 usec  
 PLW2 65.00000000 W  
 PLW12 1.01559997 W

----- GRADIENT CHANNEL -----  
 GPNAM[1] SMSQ10.100  
 GPNAM[2] SMSQ10.100  
 GPZ1 80.00 %  
 GPZ2 20.10 %  
 P16 1000.00 usec

F1 - Acquisition parameters  
 TD 128  
 SFO1 100.6253 MHz  
 FIDRES 130.208328 Hz  
 SW 165.631 ppm  
 FhMODE Echo-Antiecho

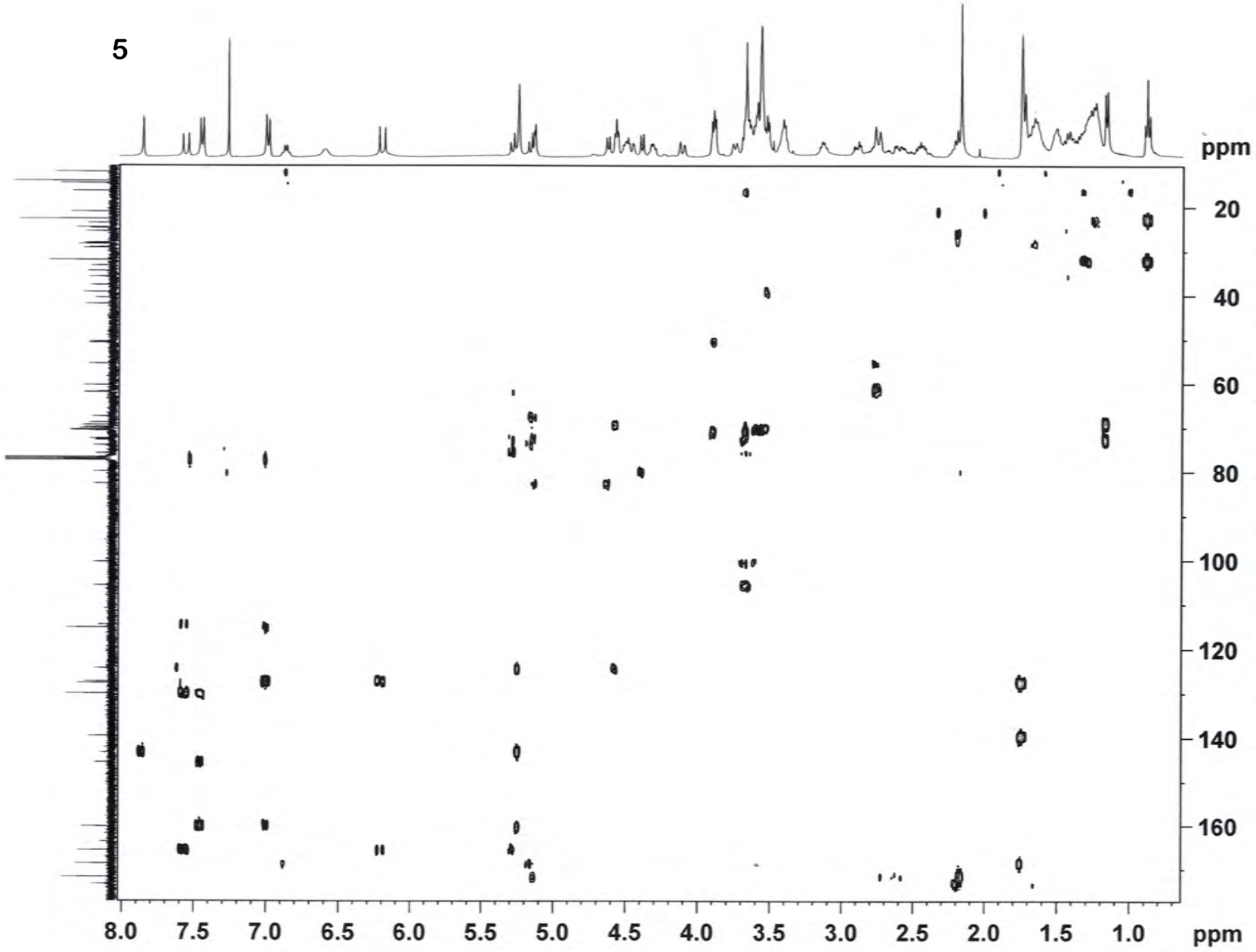
F2 - Processing parameters  
 SI 1024  
 SF 400.1500000 MHz  
 WDW QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0  
 PC 1.40

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



ZGH-*Ipom*-3-49-160510-A HMBC in CDCl<sub>3</sub>

5



Current Data Parameters  
NAME ZGH-*Ipom*-3-49-160510-*f*  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160512  
Time 3.53  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hmcoplrp04f  
TD 4096  
SOLVENT CDCl3  
NS 45  
DS 16  
SWH 5208.333 Hz  
FIDRES 1.271566 Hz  
AQ 0.3932160 sec  
RG 2050  
IN 96.000 usec  
DE 6.50 usec  
TE 293.1 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  
IM0 0.0002240 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  
GPZ1 50.00 %  
GPZ2 30.00 %  
GPZ3 40.10 %  
P16 1000.00 usec

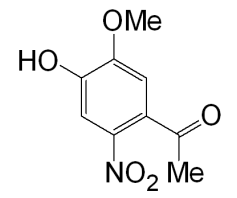
F1 - Acquisition parameters  
TD 128  
SFO1 100.6258 MHz  
FIDRES 174.386154 Hz  
SW 221.826 ppm  
F0MODE QF

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

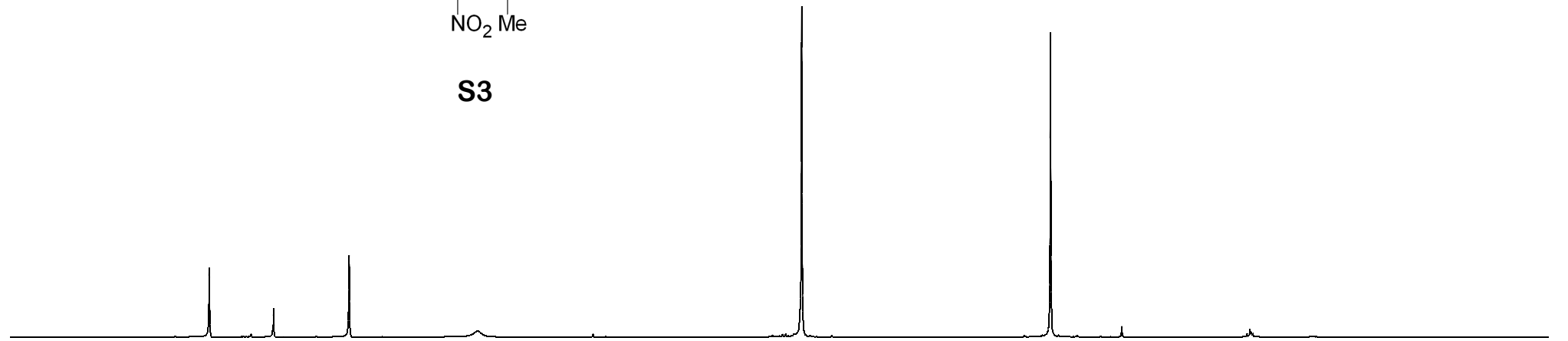
F1 - Processing parameters  
SI 1024  
MC2 QF  
HEW 100.6177921 MHz  
SSB 0  
LB 0 Hz  
GB 0

xws-cl-2018-01-22f 400 H-NMR 400

— 7.666  
— 7.270  
— 6.806  
— 6.015  
— 4.023  
— 2.494



**S3**



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

0.82  
1.00  
0.68  
3.13  
3.27

xws-cl-2018-01-22f in CDCl<sub>3</sub>

—199.832

—150.980

—146.606

—131.862

—110.704

—108.578

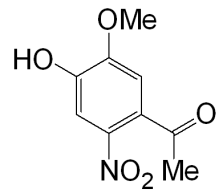
77.316

76.998

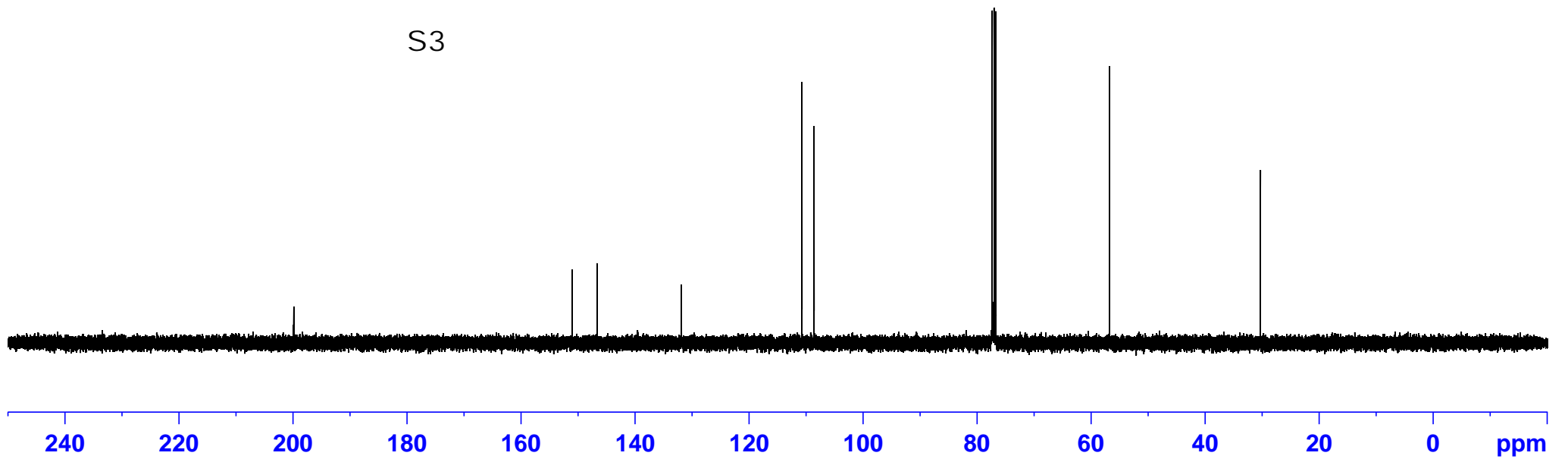
76.681

—56.740

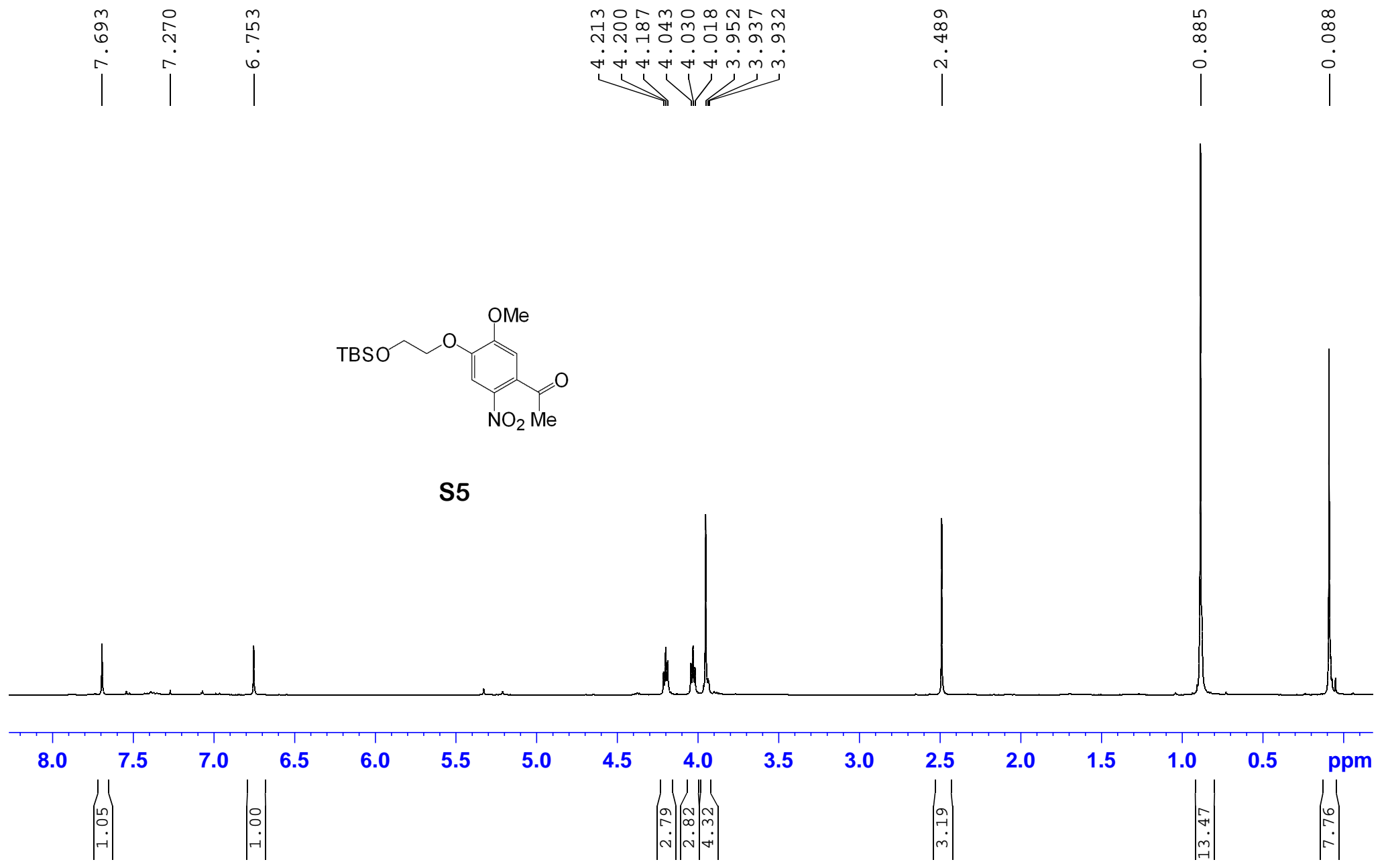
—30.270



S3



xws-cl-2016-10-20c 400 H-NMR 400



xws-cl-2016-10-23a 400 H-NMR 400

8.258  
8.235

7.681

7.356  
7.333

7.114

6.560

6.544

6.528

6.512

4.185

4.172

4.159

4.038

4.025

4.012

3.996

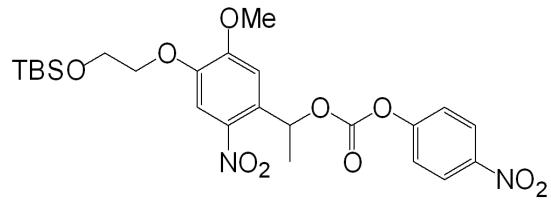
1.783

1.767

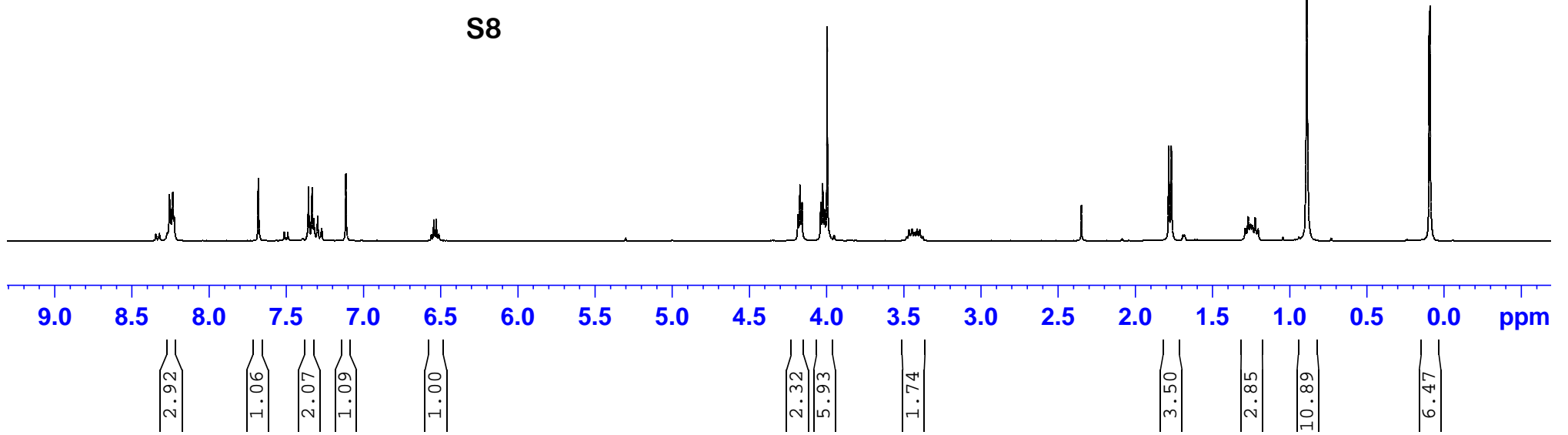
0.889

0.095

0.090



S8



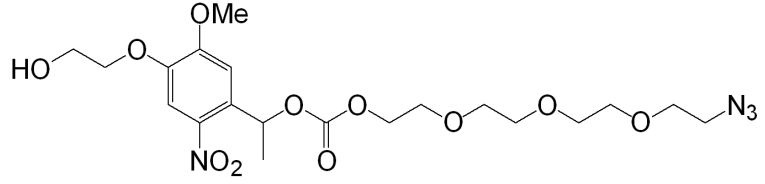




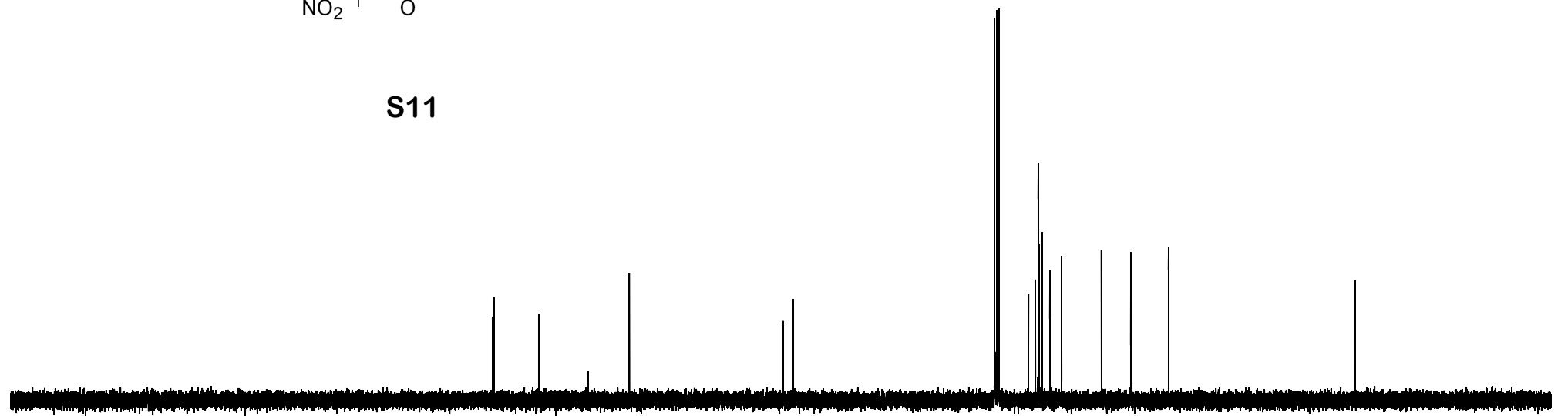


xws-cl-2017-10-17d 13C in CDCl3

154.278  
 154.043  
 147.194  
 139.665  
 133.289  
 109.721  
 108.197  
 77.318  
 77.000  
 76.682  
 72.093  
 71.062  
 70.652  
 70.625  
 70.505  
 70.020  
 68.849  
 67.049  
 60.960  
 56.440  
 50.655  
 22.080

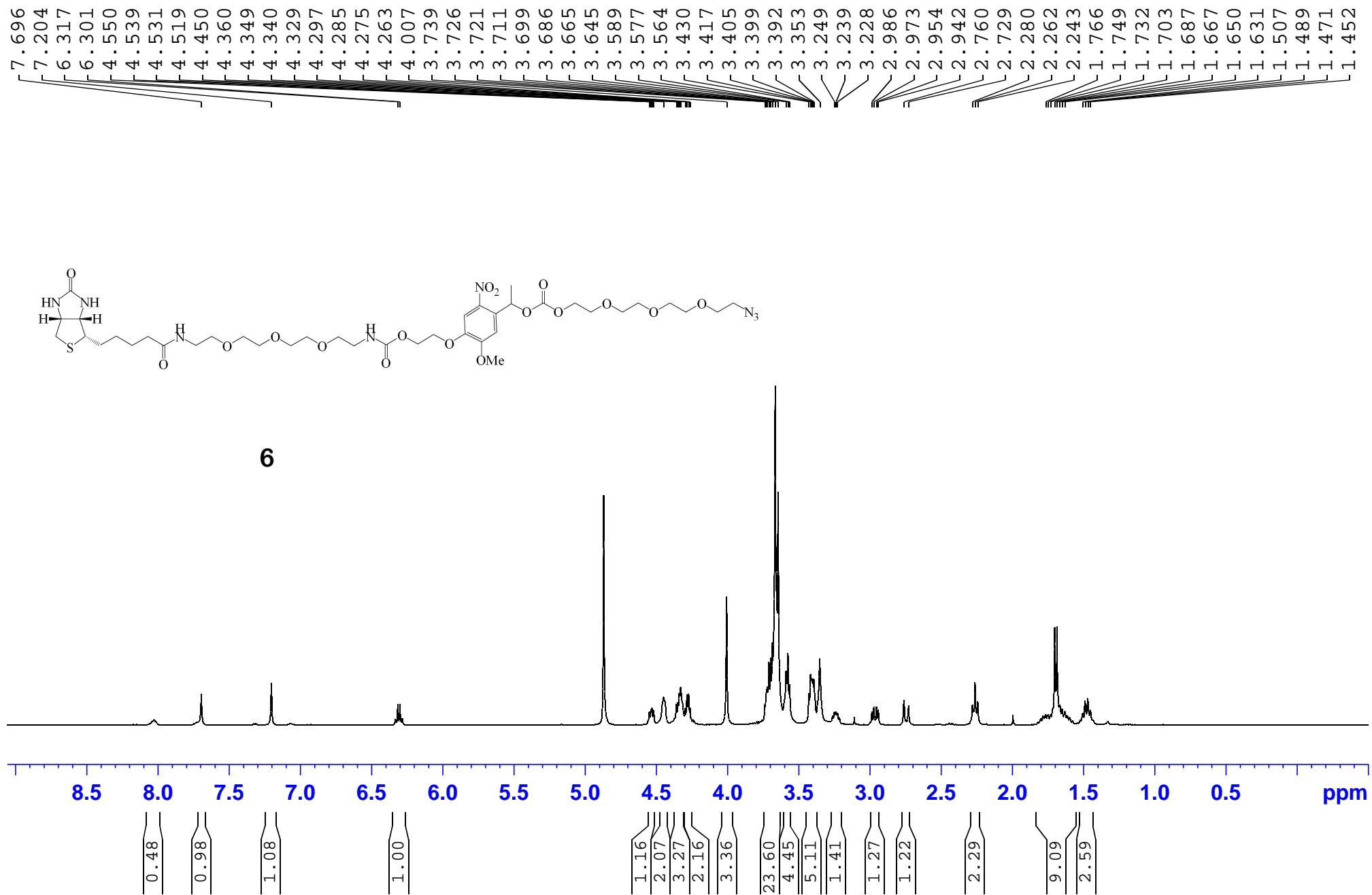


S11

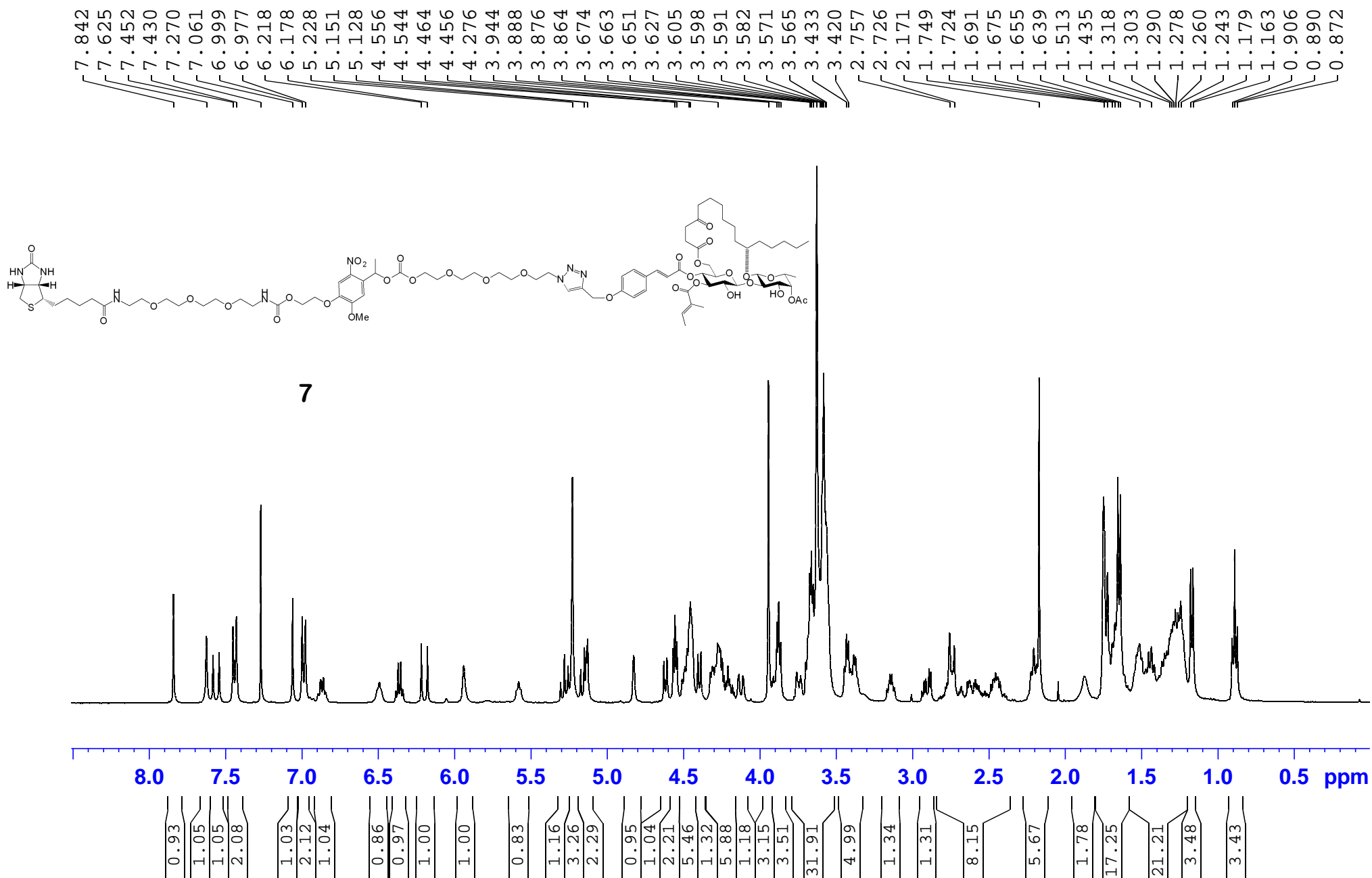


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

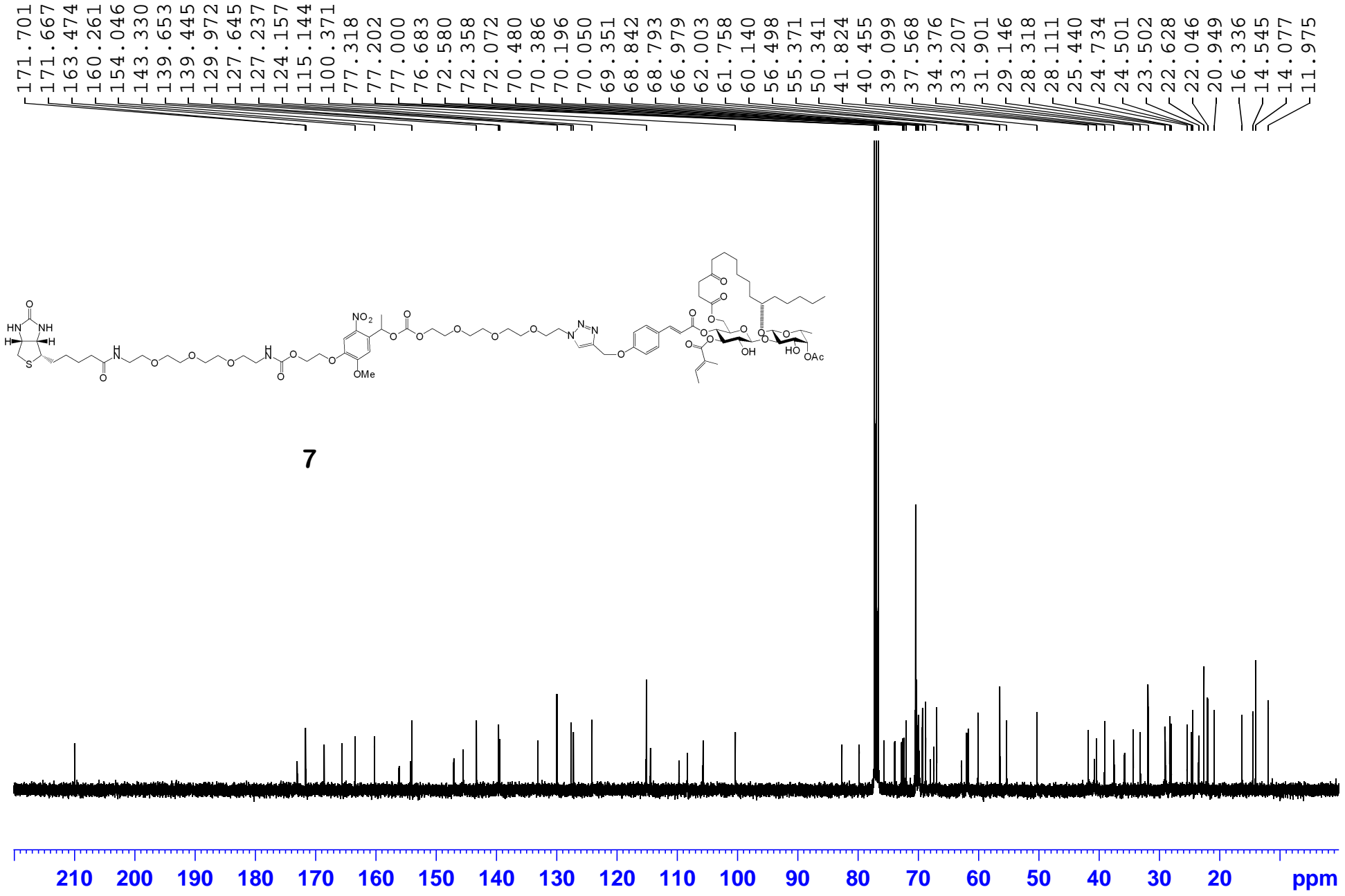
## xws-cl-2017-10-18b 400 H-NMR 400





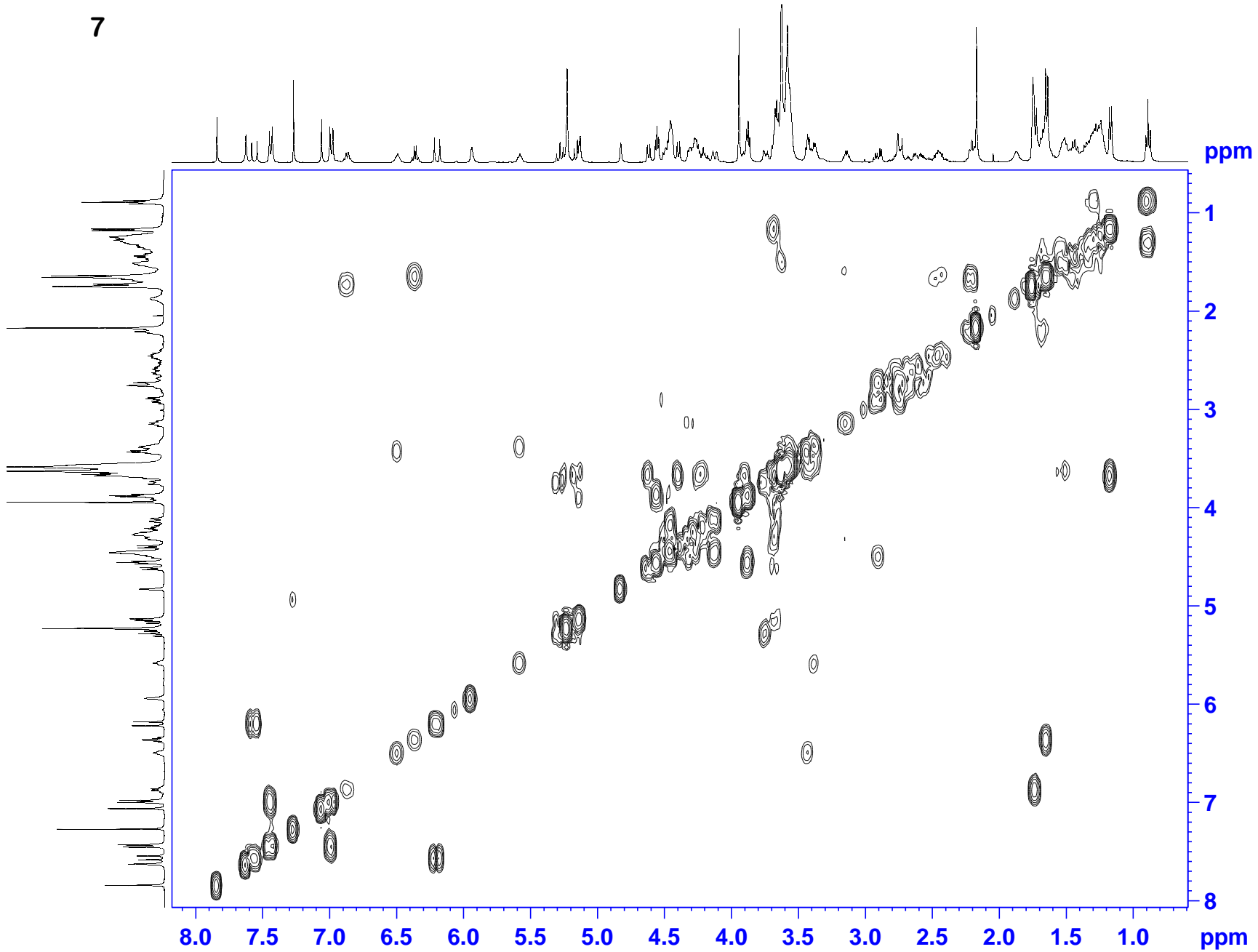
ZGH-Ipom-3-290-171022-A in CDCl<sub>3</sub>

ZGH-Ipom-3-290-171022-A 13C in CDCl3



ZGH-*Ipom*-3-290-171022-A\_2 COSY in CDCL<sub>3</sub>

7



```
Current Data Parameters
NAME      ZGH-Ipom-3-290-171022-A
EXPNO     13
PROCNO    1

F2 - Acquisition Parameters
Date_     20171029
Time      1.19
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   cosyzgpg
TD        6548
SOLVENT   CDCL3
NS        64
DS        8
SWH       8012.820 Hz
FIDRES    3.912510 Hz
AQ        0.1277952 sec
RG        381
DW        62.400 usec
DE        4.50 usec
TE        295.4 K
DQ        0.0000000 sec
D1        1.5000000 sec
D13       0.0000000 sec
D16       0.0000000 sec
IN0       0.00012480 sec

***** CHANNEL f1 *****
SFO1      400.1520008 MHz
NUC1      1H
P0        12.50 usec
P1        12.50 usec
PL1       20.00000000 W

***** GRADIENT CHANNEL *****
GPNAM1)  EMSQ10.100
GP21     10.00 %
P16      1000.00 usec

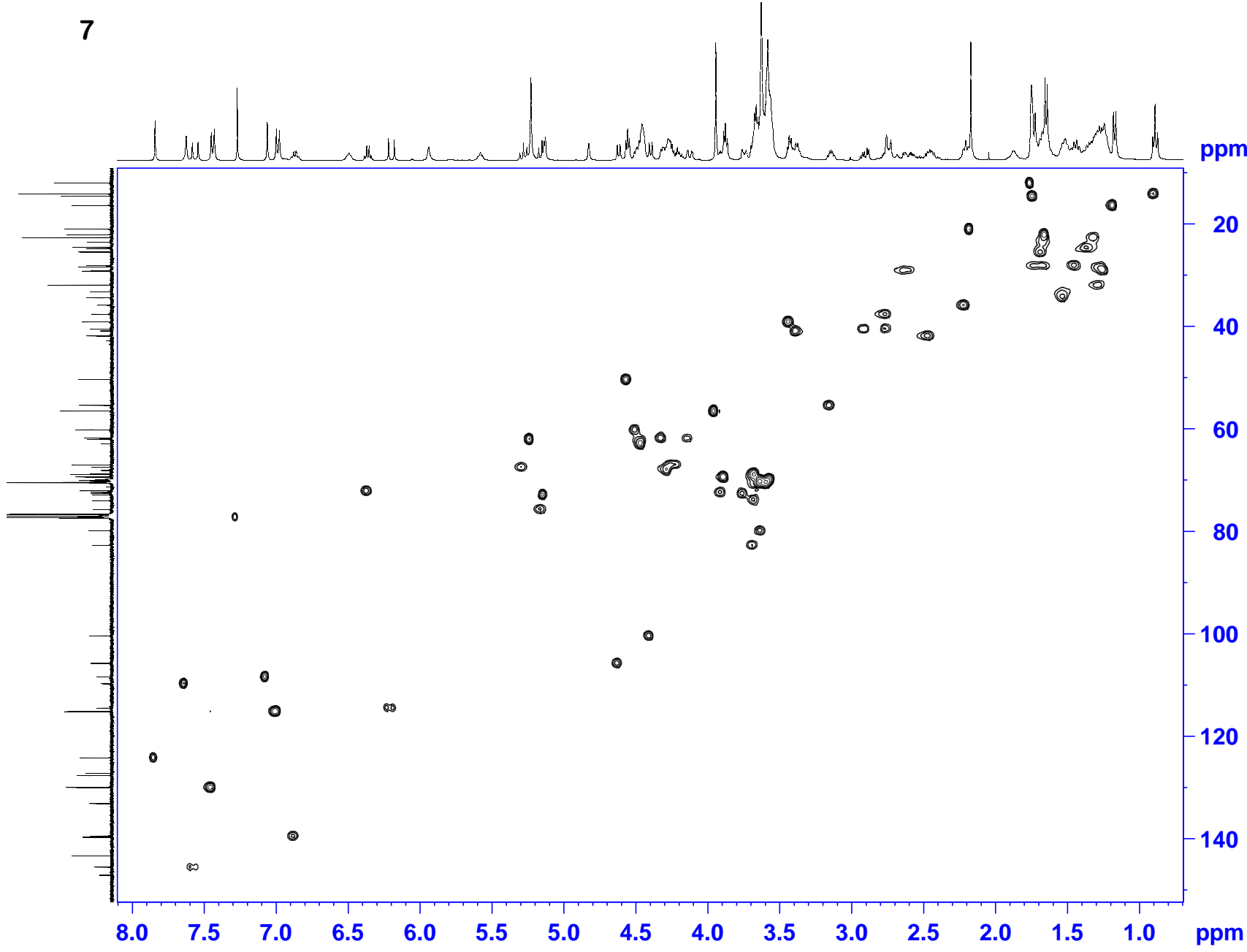
F1 - Acquisition parameters
TD        128
SFO1      400.152 MHz
FIDRES    62.600159 Hz
SW        20.024 ppm
FWDKDE    0

F2 - Processing parameters
SI        1024
SF        400.1500069 MHz
WDW       gauss
SSB       0
LB        0 Hz
GB        0
PC        1.00

F1 - Processing parameters
SI        1024
SF        400.1500054 MHz
WDW       gauss
SSB       0
LB        0 Hz
GB        0
```

ZGH-*Ipom-3-290-171022-A\_2* HSQC in CDCl<sub>3</sub>

7



```

Current Data Parameters
NAME      ZGH-Ipom-3-290-171022-A
EXPNO    14
PROCNO   1

F2 - Acquisition Parameters
Date_    20171029
Time     5.04
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  hsqcetpp4
TD       1024
SOLVENT  CDCl3
NS       16
DS       16
SWH      5197.505 Hz
FIDRES   5.075689 Hz
AQ       0.0985088 sec
RG       2050
DW       96.200 usec
DE       6.50 usec
TE       295.5 K
CMT2     145.000000
DO       0.00000300 sec
D1       1.50000000 sec
D4       0.0017444 sec
D11      0.03000000 sec
D16      0.00020000 sec
D24      0.00110000 sec
IND      0.00001000 sec
ZGPPINS

***** CHANNEL f1 *****
SF01    400.1524058 MHz
NUC1     13C
P1       12.50 usec
P2       25.00 usec
P28      1000.00 usec
PLW1     20.00000000 W

***** CHANNEL f2 *****
SF02    100.6253021 MHz
NUC2     13C
CPRPROG2  gprp
P3       10.00 usec
P4       20.00 usec
PCPD2    80.00 usec
PLW2     65.00000000 W
PLW12    1.01559997 W

***** GRADIENT CHANNEL *****
GPRAM(1) SMSQ10.100
GPRAM(2) SMSQ10.100
GPZ1     80.00 k
GPZ2     20.10 k
P16      1000.00 usec

F1 - Acquisition parameters
TD       128
SF01    100.6253 MHz
FIDRES   130.208328 Hz
SW       165.631 ppm
F2MODE   Echo-Antiecho

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

F1 - Processing parameters
SI       1024
MC2     echo-antiecho
SF       100.6177975 MHz
WDW      QUINE
SSB      2
LB       0 Hz
GB       0
  
```

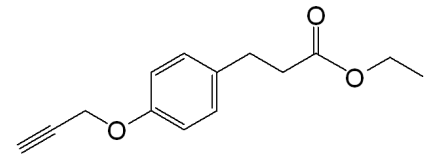
ZGH-*Ipom*-3-218-170605-A in CDCl<sub>3</sub>

7.270  
7.153  
7.131  
6.921  
6.916  
6.900

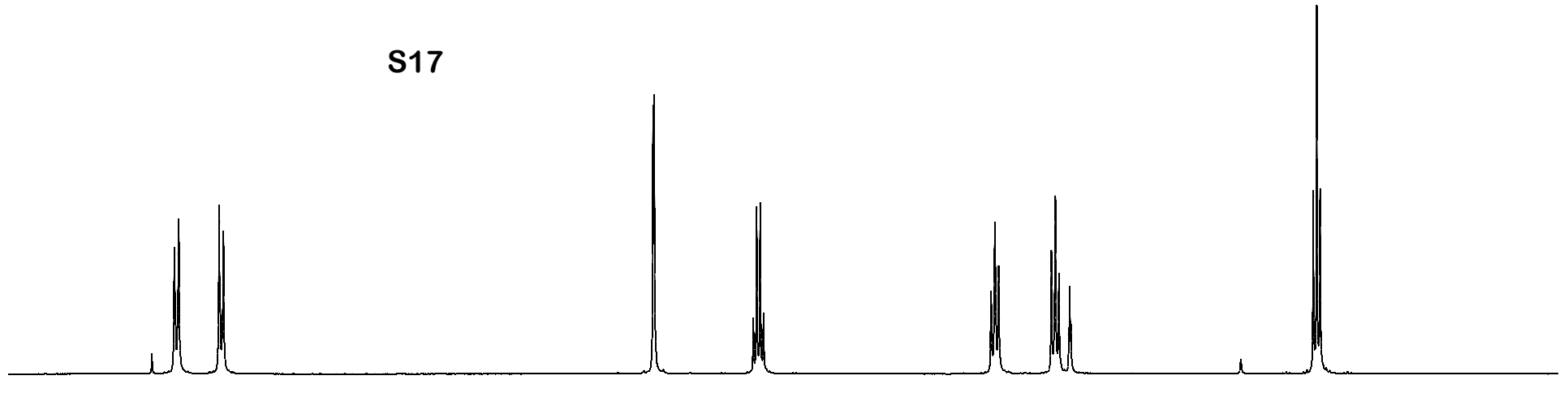
4.675  
4.669  
4.157  
4.139  
4.121  
4.103

2.925  
2.906  
2.886  
2.613  
2.593  
2.574  
2.524  
2.518  
2.512

1.258  
1.240  
1.222



S17



7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

1.99  
1.96

2.18

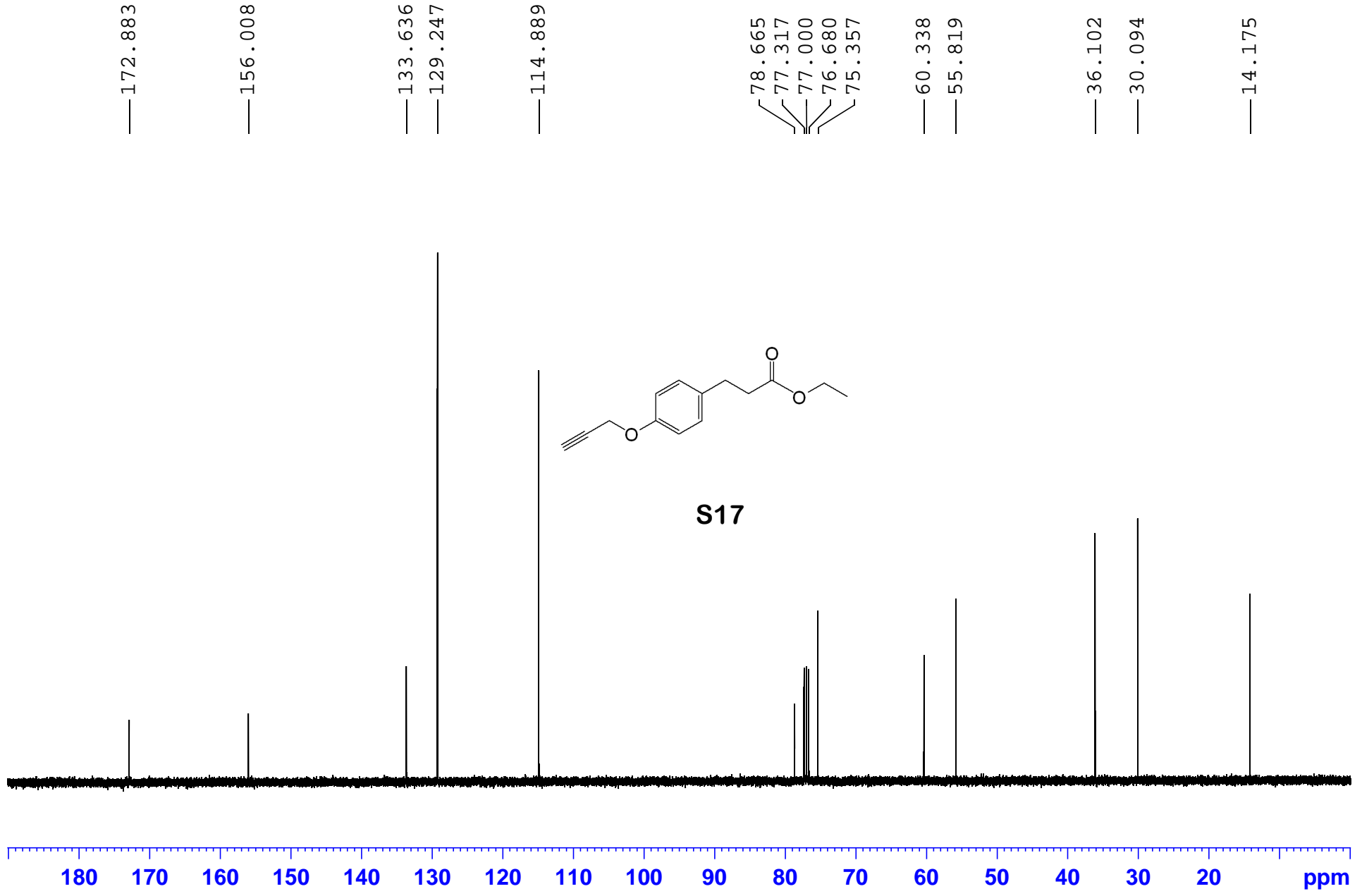
2.02

2.27  
2.21  
0.70

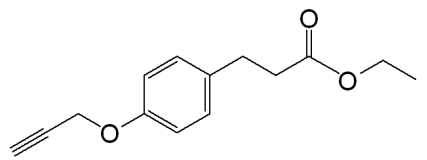
3.00



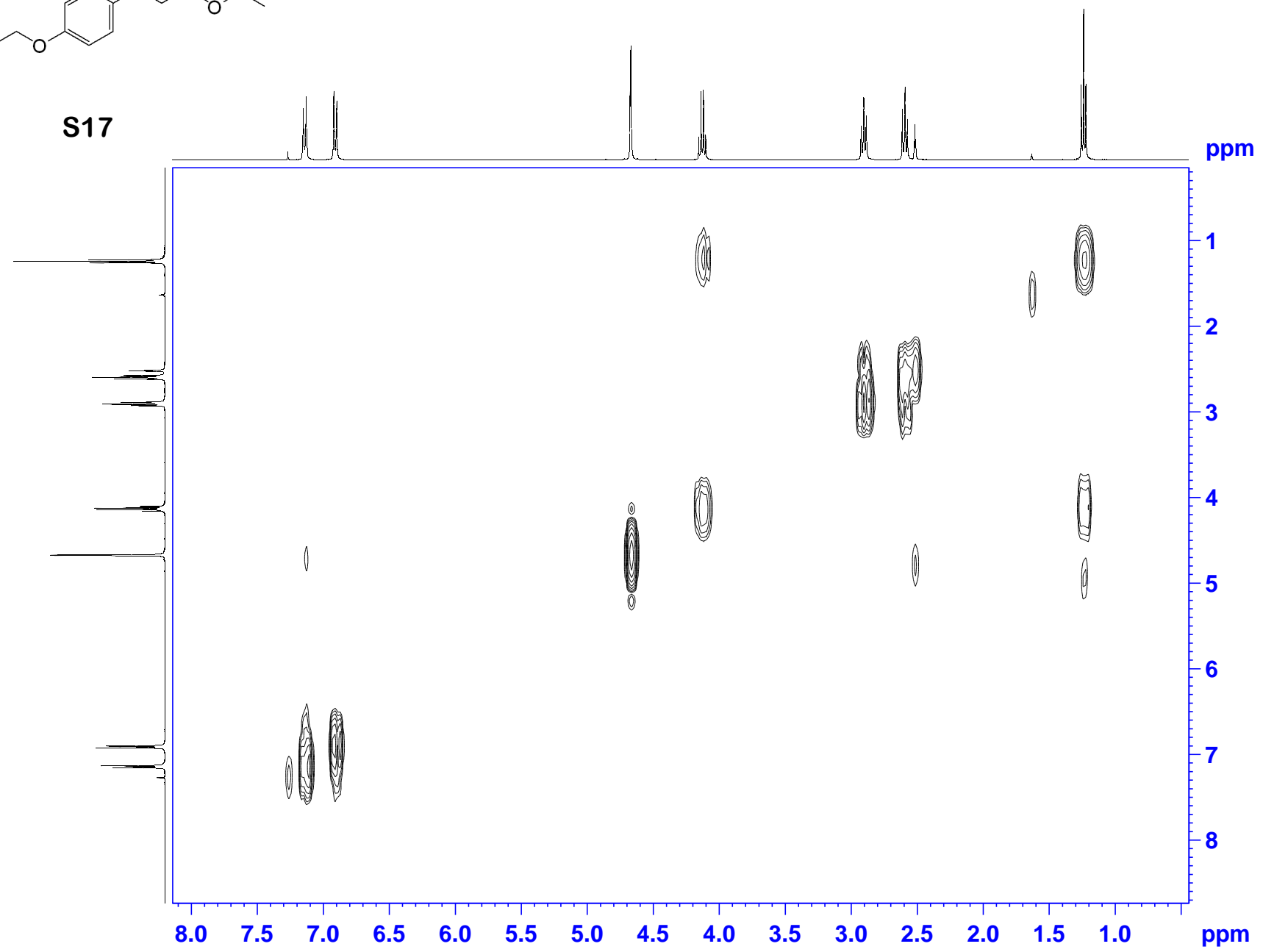
ZGH-Ipom-3-218-170605-A 13C in CDCl3



ZGH-Ipom-3-218-170605-A in CDCL3



S17



Current Data Parameters  
NAME ZGH-Ipom-3-218-170605-A  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170607  
Time 17.18  
INSTRUM spect  
PROBHD 5 mm PABBO HS-  
PULPROG cosygpgf  
TD 2048  
SOLVENT CDCL3  
NS 16  
DS 8  
SWH 8012.820 Hz  
FIDRES 3.912510 Hz  
AQ 0.1277352 sec  
RG 90.5  
DW 62.400 usec  
DE 6.50 usec  
TE 294.9 K  
D0 0.0000000 sec  
D1 1.5000000 sec  
D13 0.0000400 sec  
D16 0.0000000 sec  
IND 0.00012480 sec

===== CHANNEL f1 =====  
SFO1 400.152008 MHz  
NUC1 1H  
PO 12.50 usec  
PL 12.50 usec  
PLW1 20.0000000 W

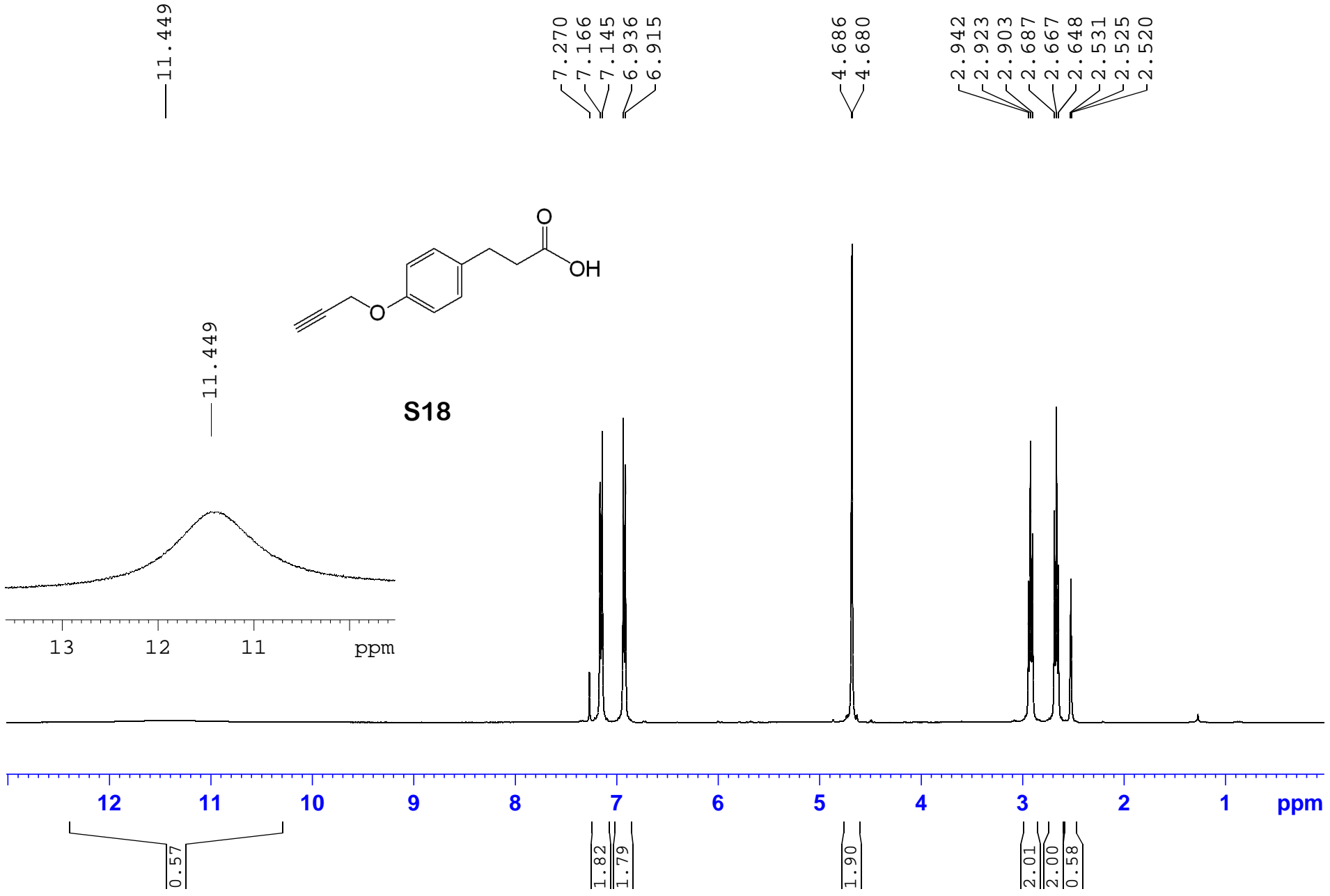
===== GRADIENT CHANNEL =====  
GPNAM[1] SMSQ10.100  
GPZ1 10.00 %  
PL6 1000.00 usec

F1 - Acquisition parameters  
TD 47  
SFO1 400.152 MHz  
FIDRES 170.48550 Hz  
SW 20.024 ppm  
PnMODE QF

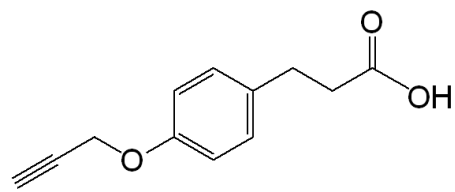
F2 - Processing parameters  
SI 1024  
SF 400.1500070 MHz  
WDW QSINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

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

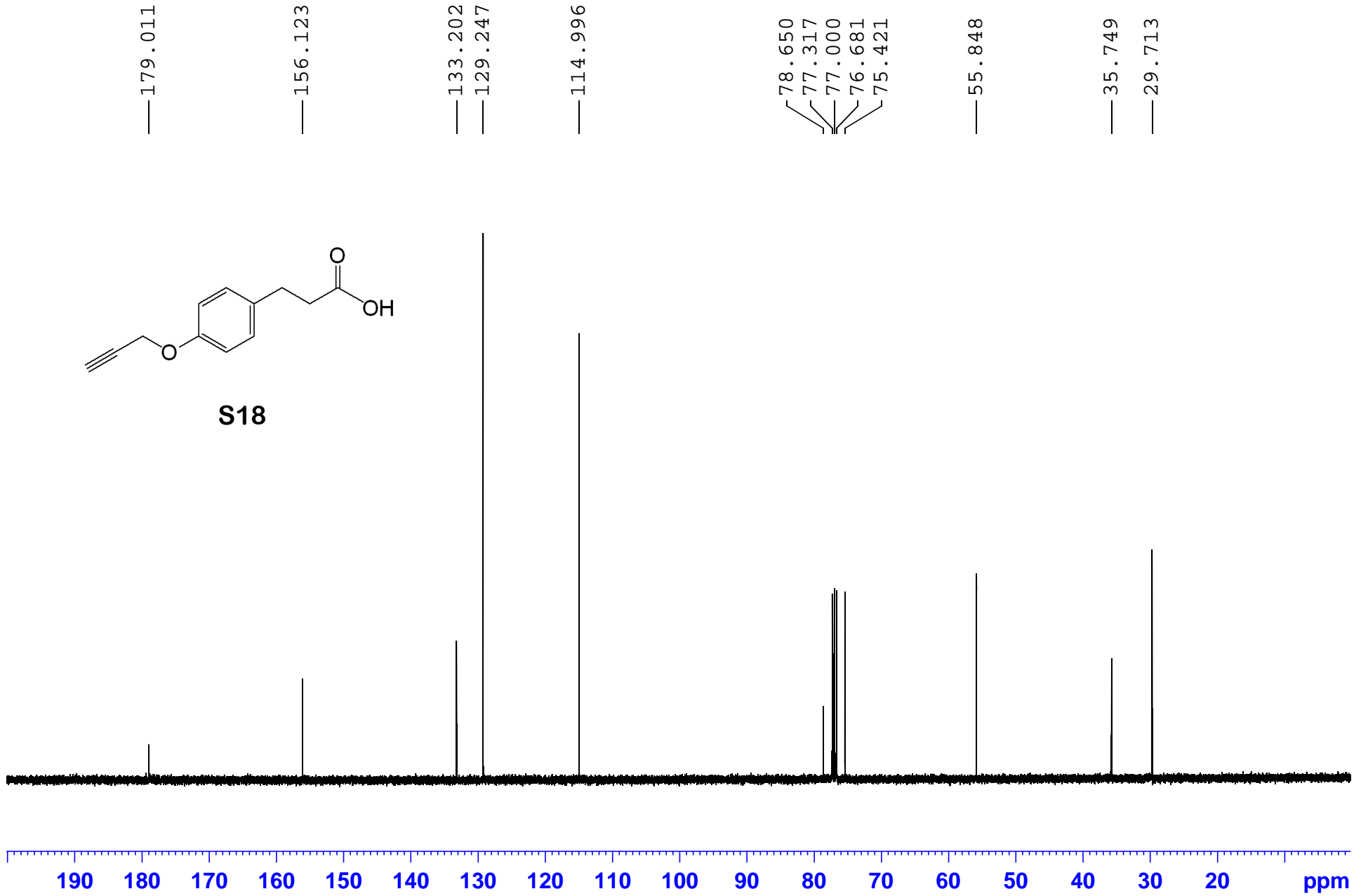
ZGH-*Ipom*-3-220-170607-A in CDCl<sub>3</sub>

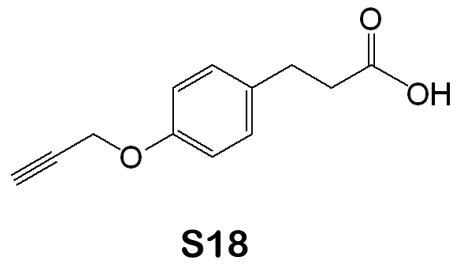


ZGH-*Ipom*-3-220-170607-A 13C in CDCl<sub>3</sub>

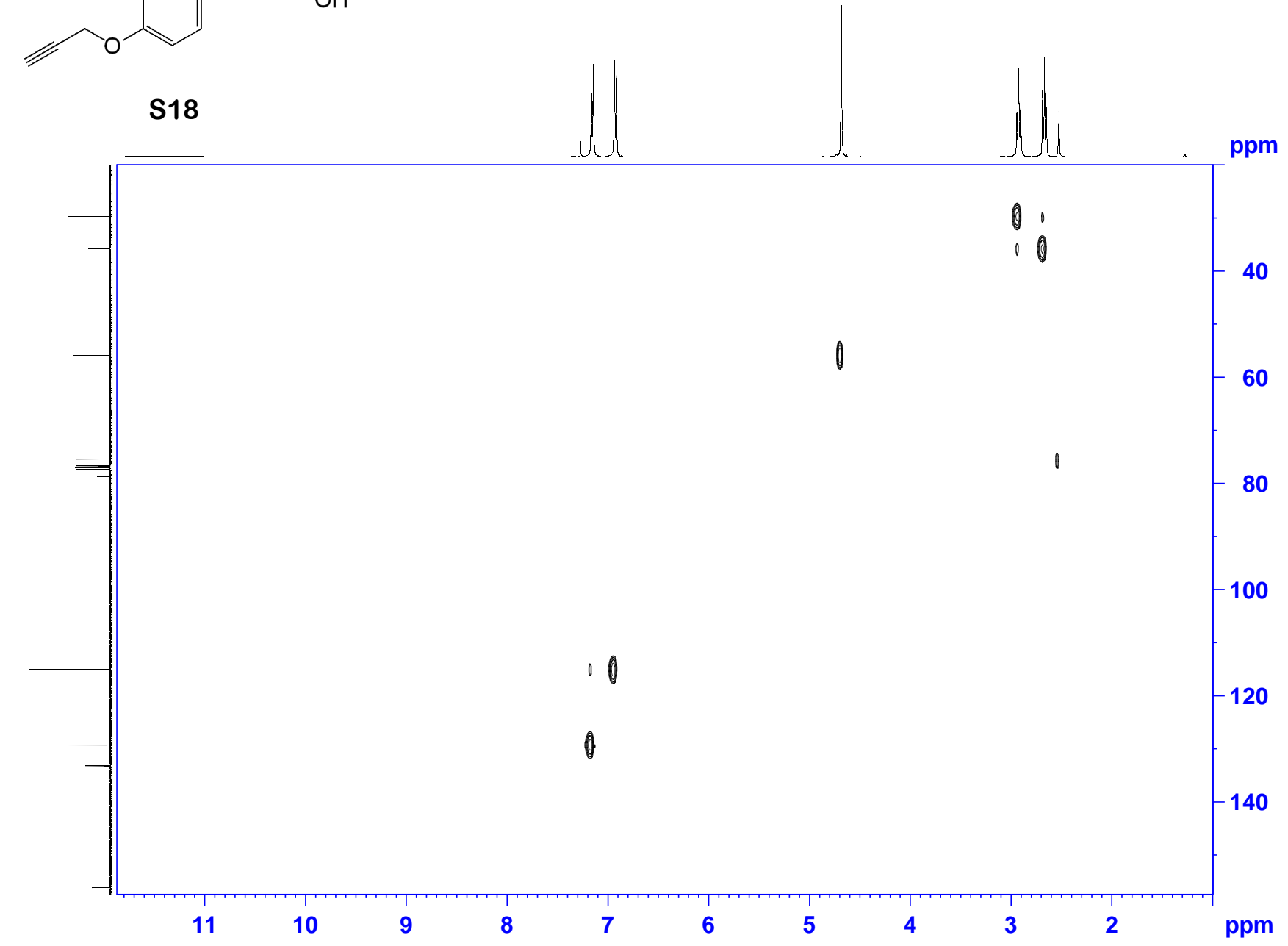


S18





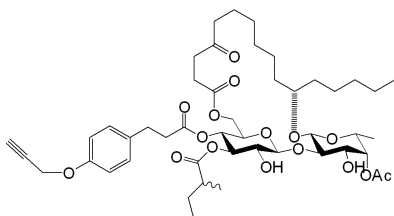
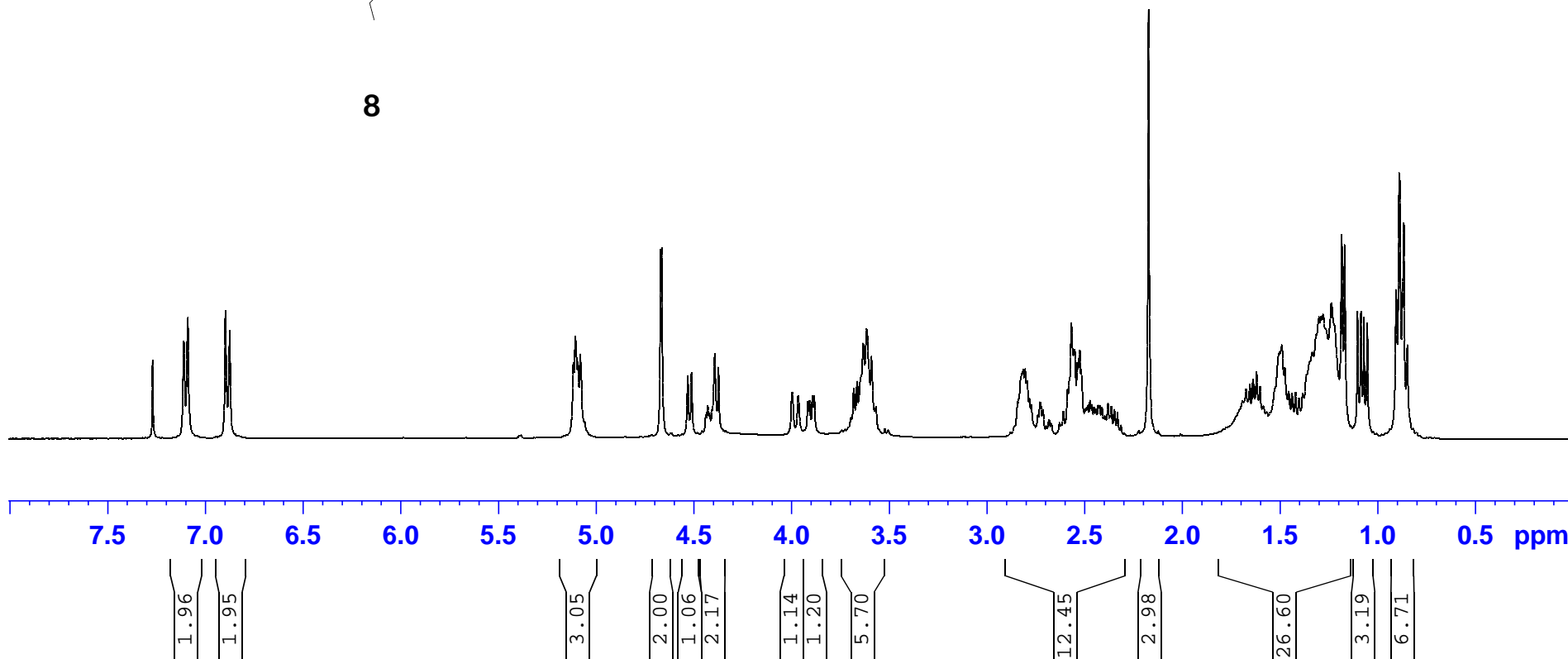
ZGH-Ipom-3-220-170607-A HSQC in CDCl3



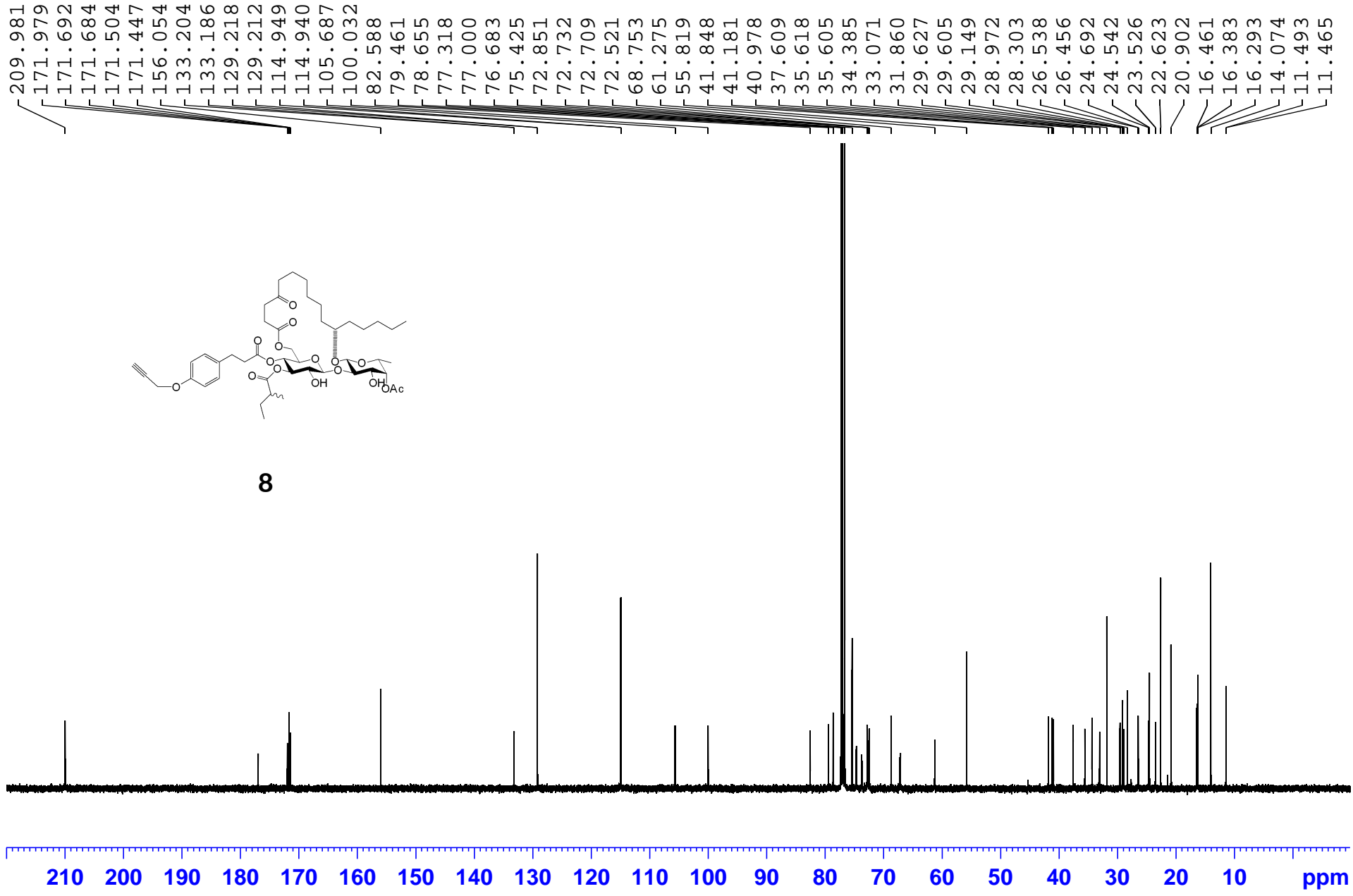
```
Current Data Parameters
NAME      ZGH-Ipom-3-220-170607-A
EXPNO    4
PROCNO   1
F2 - Acquisition Parameters
Date_    20170608
Time     21.38
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  huqzgpgui
TD        1524
SOLVENT  CDCl3
NS        8
DS        16
SHE       5197.505 Hz
FIDRES   5.975689 Hz
AQ        0.098558 sec
RG         2050
SW         96.200 usec
DE         6.50 usec
TE         295.4 K
CONST2   148.000000 sec
D0         0.0000000 sec
D1         1.8000000 sec
D4         0.0017244 sec
D11        0.0300000 sec
D16        0.0000000 sec
D24        0.0011000 sec
D30        0.0000000 sec
ZDZPTNS
----- CHANNEL f1 -----
SFO1     400.1524558 MHz
NUC1      1H
P1         12.50 usec
P2         25.00 usec
P3         1000.00 usec
PLW1      20.00000000 W
----- CHANNEL f2 -----
SFO2     100.6257021 MHz
NUC2      13C
CQPCPRG2  gmpf
P1         15.00 usec
P4         20.00 usec
PCPD2     80.00 usec
PLW2      65.00000000 W
PLW12     1.01559997 W
----- GRADIENT CHANNEL -----
GRAN1[1]  SNG10.100
GRAN1[2]  SNG10.100
GP21      80.00 %
GP22      20.10 %
P16       1000.00 usec
F1 - Acquisition parameters
TD         1524
SFO1      400.1524558 MHz
FIDRES    5.975689 Hz
SW         96.200 usec
PRWDOR    Echo-Antiecho
F2 - Processing parameters
SI         1024
SF         400.1524558 MHz
WDW        USINE
SSB         2
LB          0 Hz
GB          0
PC          1.40
F1 - Processing parameters
SI         1024
MC2        echo-antiecho
SF         100.6177776 MHz
WDW        USINE
SSB         2
LB          0 Hz
GB          0
```

ZGH-*Ipom*-3-222-170610-A<sub>2</sub> in CDCl<sub>3</sub>

7.270  
7.111  
7.091  
6.897  
6.876  
5.116  
5.107  
5.093  
5.081  
4.670  
4.664  
4.531  
4.511  
4.393  
4.374  
3.681  
3.665  
3.634  
3.616  
3.591  
2.814  
2.804  
2.794  
2.587  
2.568  
2.551  
2.538  
2.531  
2.524  
2.518  
2.173  
1.673  
1.654  
1.638  
1.620  
1.602  
1.503  
1.490  
1.475  
1.456  
1.335  
1.315  
1.299  
1.290  
1.279  
1.236  
1.184  
1.168  
1.103  
1.085  
1.070  
1.053  
0.905  
0.889  
0.866  
0.848

**8**

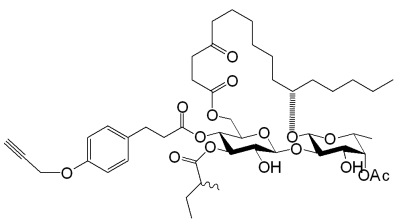
ZGH-*Ipom*-3-222-170610-A\_2 <sup>13</sup>C in CDCl<sub>3</sub>



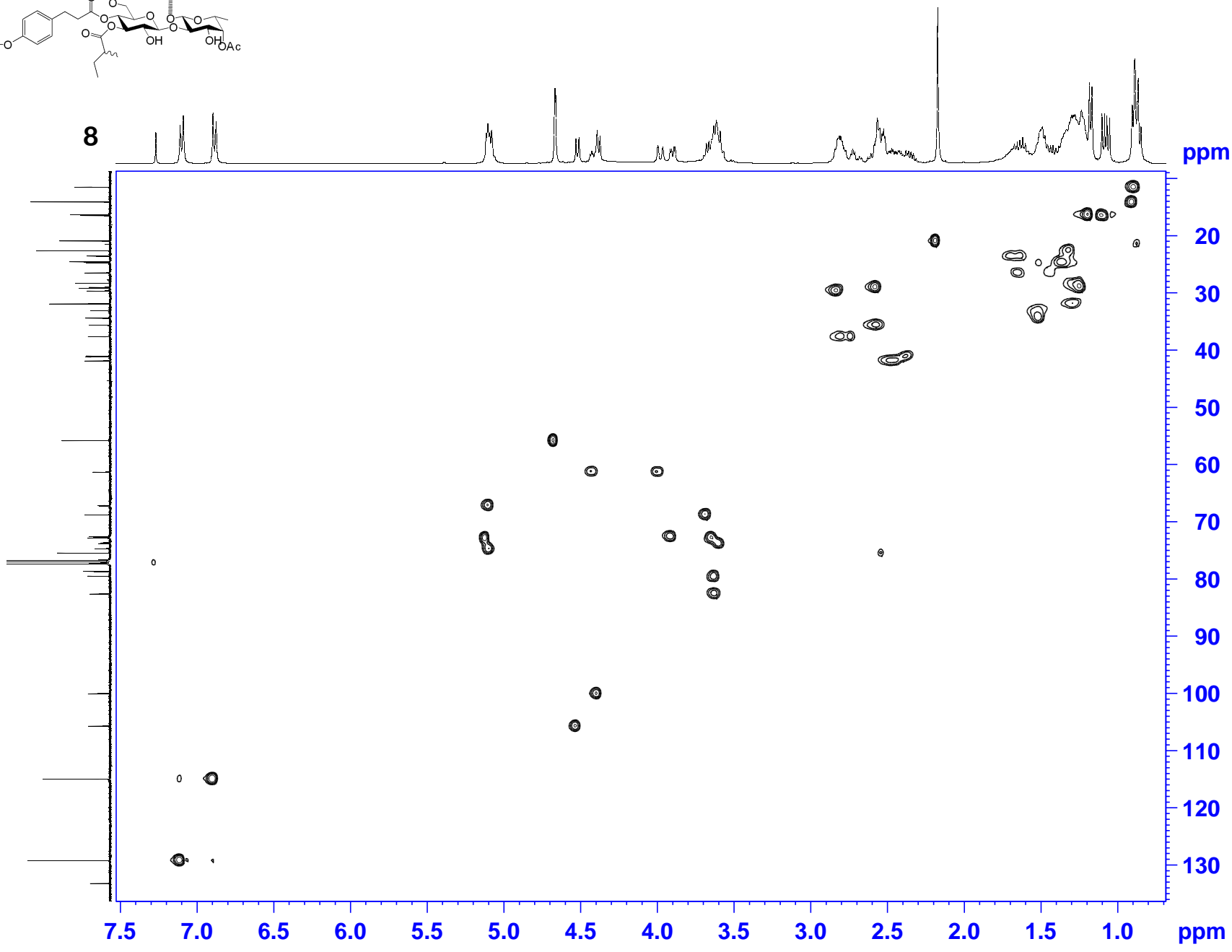




ZGH-*Ipom-3-222-170610-A\_2* HSQC in CDCl<sub>3</sub>



8



Current Data Parameters  
NAME zgh-*ipom-3-222-170610-A\_2*  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170610  
Time 9.09  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hsqcetppa  
TD 3274  
SOLVENT CDCl<sub>3</sub>  
NS 8  
DS 16  
SWH 5197.505 Hz  
FIDRES 5.075689 Hz  
AQ 0.0985088 sec  
RG 2050  
DW 96.200 usec  
DE 6.50 usec  
TE 295.0 K  
CMT2 145.000000 sec  
D0 0.00000000 sec  
D1 1.50000000 sec  
D4 0.00172414 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00110000 sec  
INO 0.00003000 sec  
ZGPPPM

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
SFO1 400.1524058 MHz  
NUC1 1H  
P1 12.50 usec  
P2 25.00 usec  
P28 1000.00 usec  
PL181 20.00000000 W

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
SFO2 100.6253021 MHz  
NUC2 13C  
CPCPRG2 gmpg  
P3 10.00 usec  
P4 20.00 usec  
PCPD2 80.00 usec  
PLW2 65.00000000 W  
PLW12 1.0155997 W

\*\*\*\*\* GRADIENT CHANNEL \*\*\*\*\*  
GRNAM[1] SMSQ10.100  
GRNAM[2] SMSQ10.100  
GFZ1 80.00 %  
GFZ2 20.10 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 328  
SFO1 100.6253 MHz  
FIDRES 130.208528 Hz  
SW 165.631 ppm  
PRMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 400.1500000 MHz  
WDW Q8INE  
SSB 2  
LR 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
WC2 echo-antiecho  
SF 100.6177975 MHz  
WDW Q8INE  
SSB 2  
LR 0 Hz  
GB 0

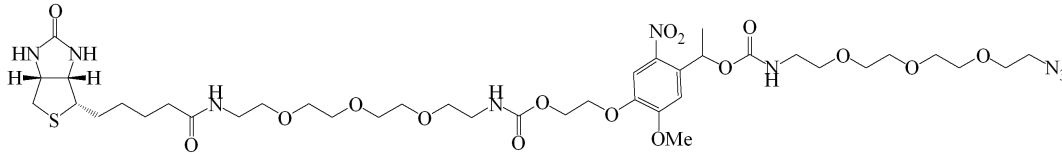




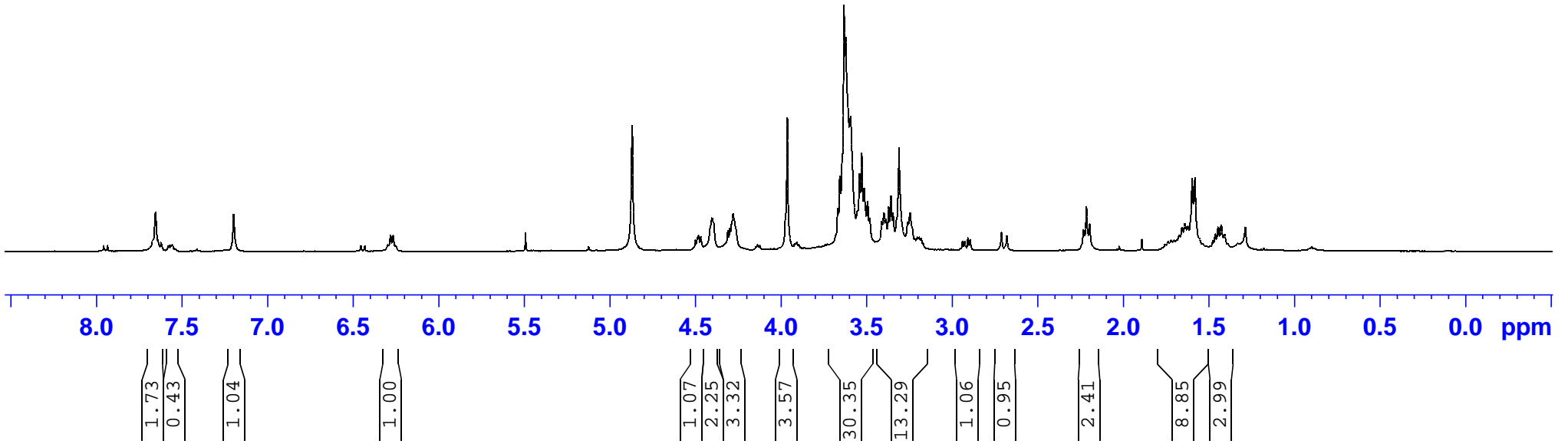


xws-cl-2018-01-29ggg 400 H-NMR 400

7.655  
7.198  
6.281  
6.265  
4.870  
4.500  
4.481  
4.469  
4.403  
4.310  
4.299  
4.290  
4.279  
3.963  
3.668  
3.656  
3.631  
3.621  
3.593  
3.541  
3.528  
3.514  
3.495  
3.481  
3.411  
3.399  
3.387  
3.371  
3.357  
3.345  
3.314  
3.310  
3.306  
3.302  
3.259  
3.246  
2.939  
2.926  
2.907  
2.894  
2.712  
2.680  
2.233  
2.215  
2.197  
1.737  
1.721  
1.704  
1.673  
1.656  
1.640  
1.623  
1.597  
1.582  
1.477  
1.462  
1.445  
1.427  
1.408

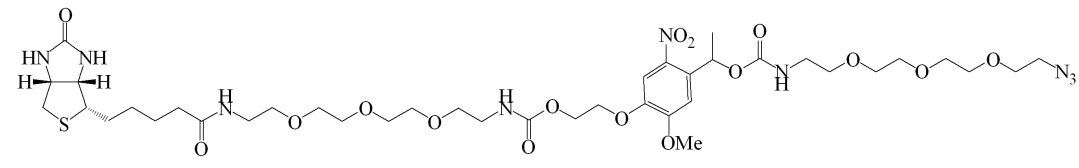


S24

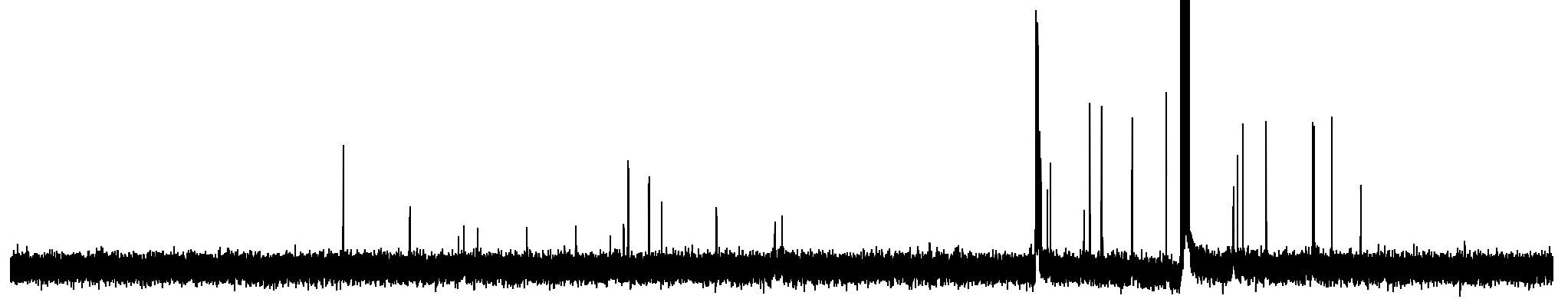


xws-cl-2018-01-29ggg in CDCl3

- 176.119
- 166.040
- 157.923
- 155.783
- 148.399
- 140.978
- 133.785
- 133.758
- 133.119
- 133.018
- 130.037
- 129.915
- 128.012
- 119.746
- 110.916
- 109.835
- 71.507
- 71.460
- 71.415
- 71.232
- 71.199
- 71.118
- 70.997
- 70.749
- 69.735
- 69.307
- 64.223
- 63.336
- 61.617
- 57.039
- 56.976
- 51.807
- 49.637
- 49.425
- 49.212
- 48.999
- 48.786
- 48.573
- 48.360
- 41.744
- 41.624
- 41.050
- 40.273
- 36.724
- 29.726
- 29.492

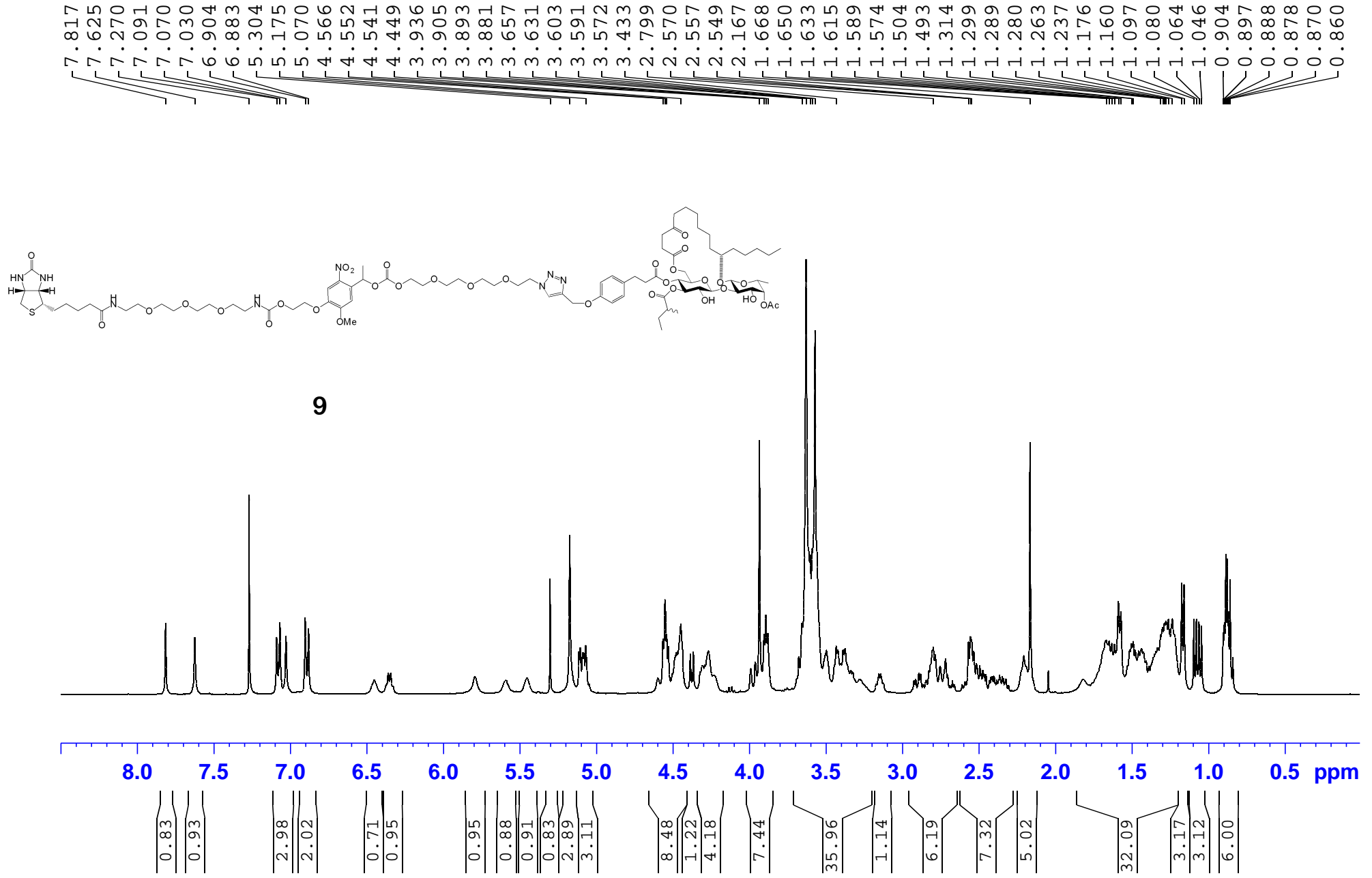


S24

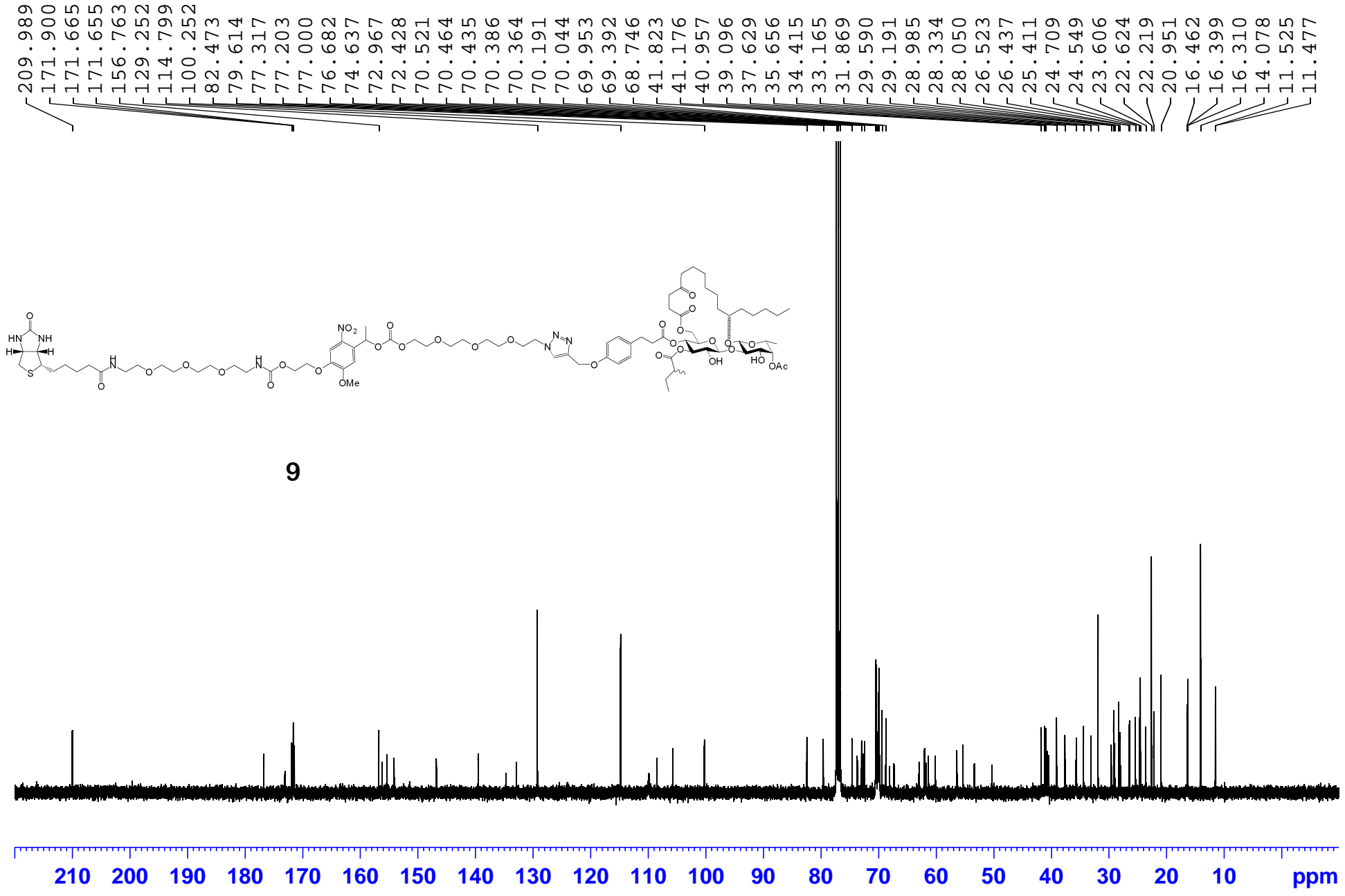


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

ZGH-Ipom-4-26-180201-A in CDCl3



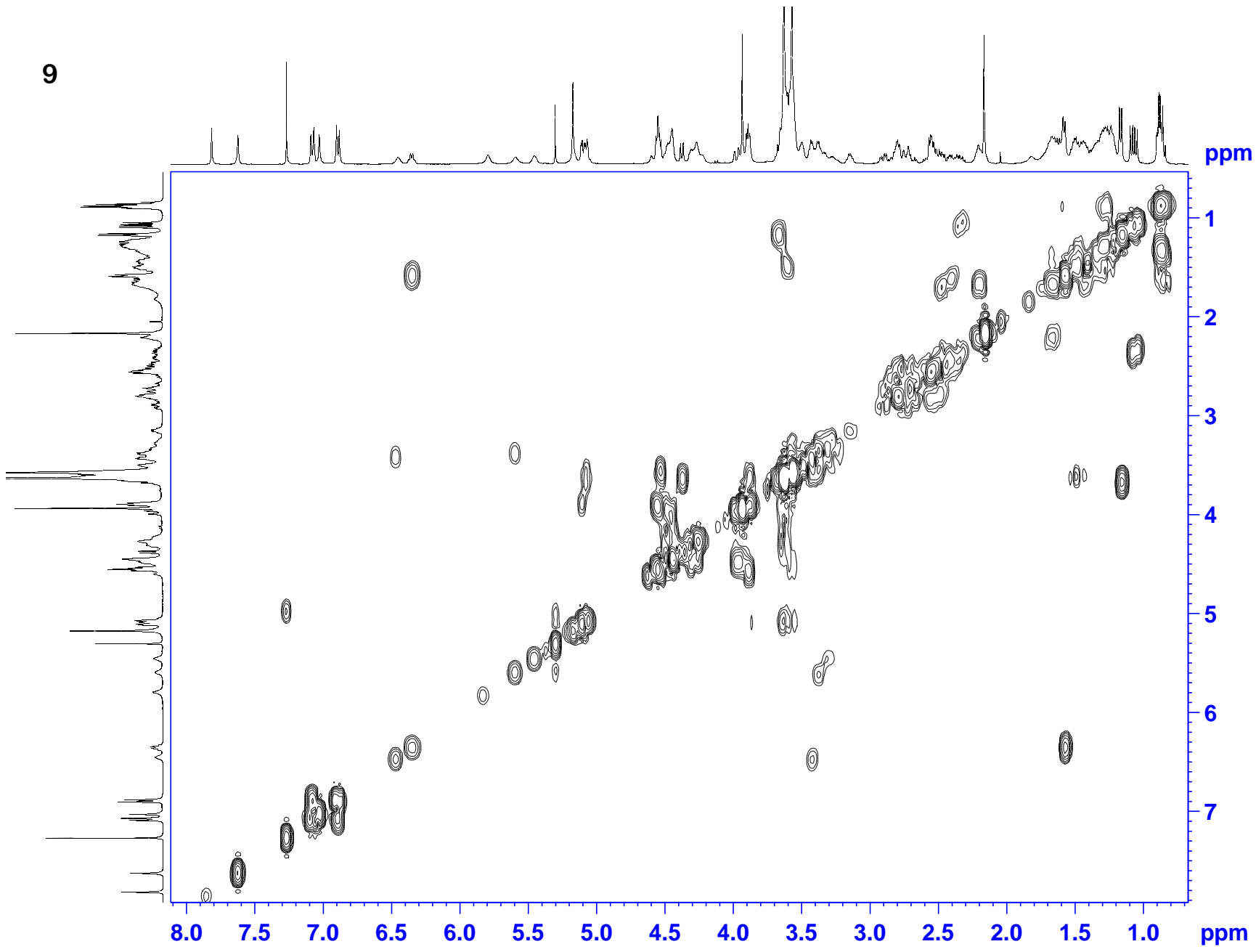
ZGH-Ipom-4-26-180201-A 13C in CDCl3





ZGH-*Ipom*-4-26-180201-A in CDCL<sub>3</sub>

9



```
Current Data Parameters
NAME      ZGH-Ipom-4-26-180201-A
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20180205
Time      21.33
INSTRUM   spect
PROBHD    5 mm PABBO BH-
PULPROG   cosygpgf
TD        2048
SOLVENT   CDCL3
NS        20
DS        8
SWH       8012.800 Hz
FIDRES    3.912510 Hz
AQ        0.1277952 sec
RG        287
DW        62.400 usec
DE        6.50 usec
TE        295.2 K
DO        0.0000300 sec
D1        1.5000000 sec
D13       0.0000400 sec
D16       0.0000000 sec
IN        0.00012480 sec

===== CHANNEL f1 =====
SFO1      400.1520008 MHz
NUC1      1H
P0        12.50 usec
P1        12.50 usec
PLW1      20.00000000 W

===== GRADIENT CHANNEL =====
GPRAM[1]  SMO10.100
CZ1       10.00 t
P16       1000.00 usec

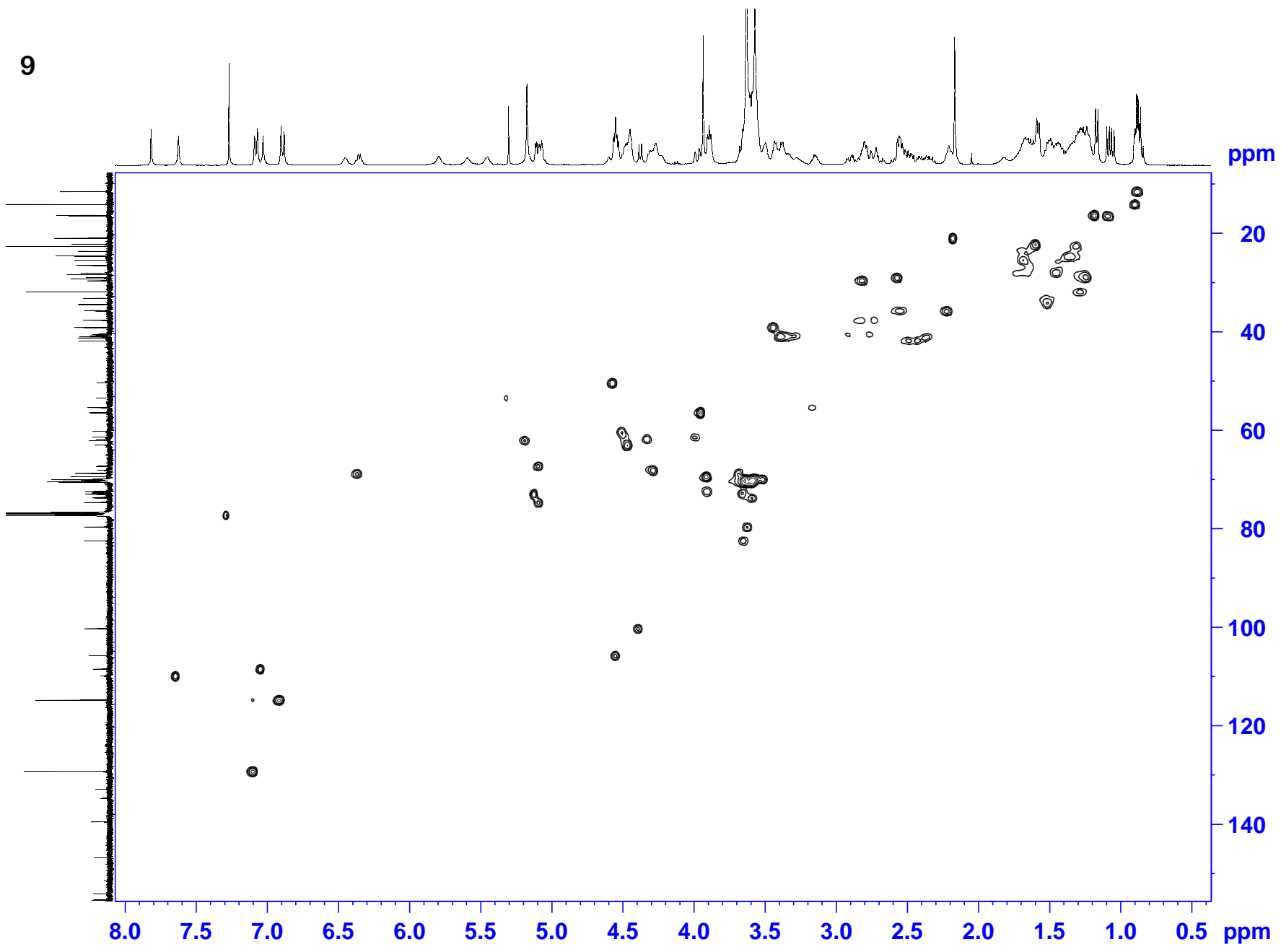
F1 - Acquisition parameters
TD        128
SFO1      400.152 MHz
FIDRES    62.600159 Hz
SW        20.024 ppm
F1MODE    QF

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

F1 - Processing parameters
SI        1024
MC2       QF
SF        400.1500052 MHz
WDW       QUINE
SSB       0
LB        0 Hz
GB        0
```

ZGH-Ipom-4-26-180201-A HSQC in CDCl3

9



```

Current Data Parameters
NAME      ZGH-Ipom-4-26-180201-A
EXPNO    4
PROCNO   1

P2 - Acquisition Parameters
Date_    20180205
Time     22:44
INSTRUM  spect
PROBHD   5 mm PABBO MM-
PULPROG  zgpg30q1
TD       1024
SOLVENT  CDCl3
NS       12
DS       16
SWH      5197.505 Hz
FIDRES   5.376589 Hz
AQ       0.0985888 sec
RG       250
WDW      96.200 usec
SSB      4.50 usec
TE       295.2 K
CHRG2    145.0000000
DO       0.0000000 usec
DI       1.5000000 usec
DE       0.00172414 usec
DIL      0.0300000 usec
DIA      0.0000000 usec
SZA      0.0010000 usec
INJ      0.0000000 usec
SFOPTN3

----- CHANNEL f1 -----
NUC1     400.1544088 MHz
P1       12.50 usec
P2       25.00 usec
P3       1500.00 usec
PLM1     20.00000000 M

----- CHANNEL f2 -----
NUC2     100.6131211 MHz
P3       10.00 usec
P4       80.00 usec
PCPD2    80.00 usec
PLM2     1.01599997 M

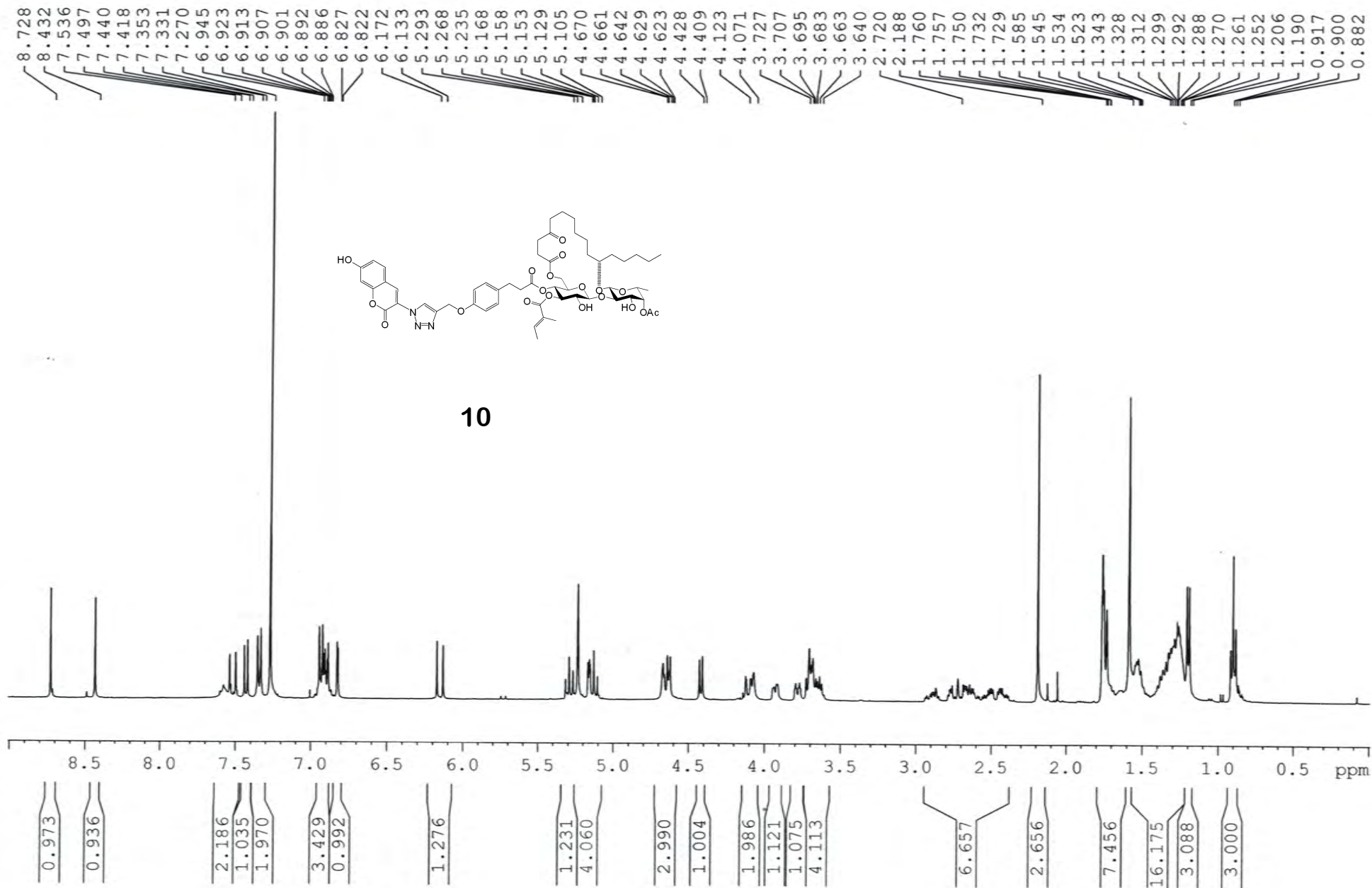
----- GRABBER CHANNEL -----
GRABM(1) SMO210.100
GRABM(2) SMO210.100
GRF1     80.10 Hz
GRF2     20.10 Hz
P14      1000.00 usec

P1 - Acquisition parameters
TD       218
FIDRES   100.62328 MHz
FIDRES2  110.108520 Hz
SM       145.611 ppm
PROMODE  Echo-Antiecho

P2 - Processing parameters
SI       1024
SF       400.1500000 MHz
WDW      Q5INE
SSB      0 Hz
LB       2
GB       0
PC       1.40

P1 - Processing parameters
SI       1024
MC2      echo-antiecho
SF       100.6177976 MHz
WDW      Q5INE
SSB      0 Hz
LB       2
GB       0

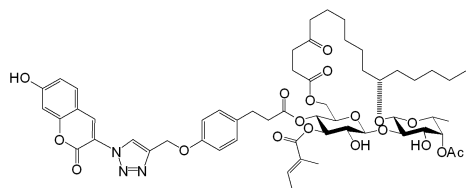
```

ZGH-*Ipom*-3-28-150929-A(3) 1H in CDCl<sub>3</sub>

ZGH-*Ipom-3-28-150929-A(3')* <sup>13</sup>C in CDCl<sub>3</sub>

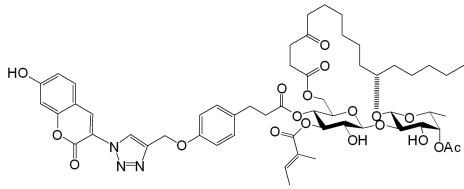
— 210.211

172.711  
171.917  
169.133  
165.706  
161.342  
160.172  
156.181  
154.565  
145.739  
140.168  
134.161  
130.211  
129.957  
127.489  
127.143  
124.238  
119.651  
114.948  
114.635  
114.165  
111.019  
105.882  
103.215  
100.283  
83.151  
79.885  
77.713  
77.319  
77.200  
77.000  
76.682  
76.213  
73.989  
72.724  
72.555  
68.839  
66.947  
61.784  
61.673  
41.811  
37.722  
34.435  
33.251  
31.896  
29.690  
29.201  
29.165  
28.365  
24.763  
24.567  
23.616  
22.647  
20.947  
16.338  
14.642  
14.103  
11.970

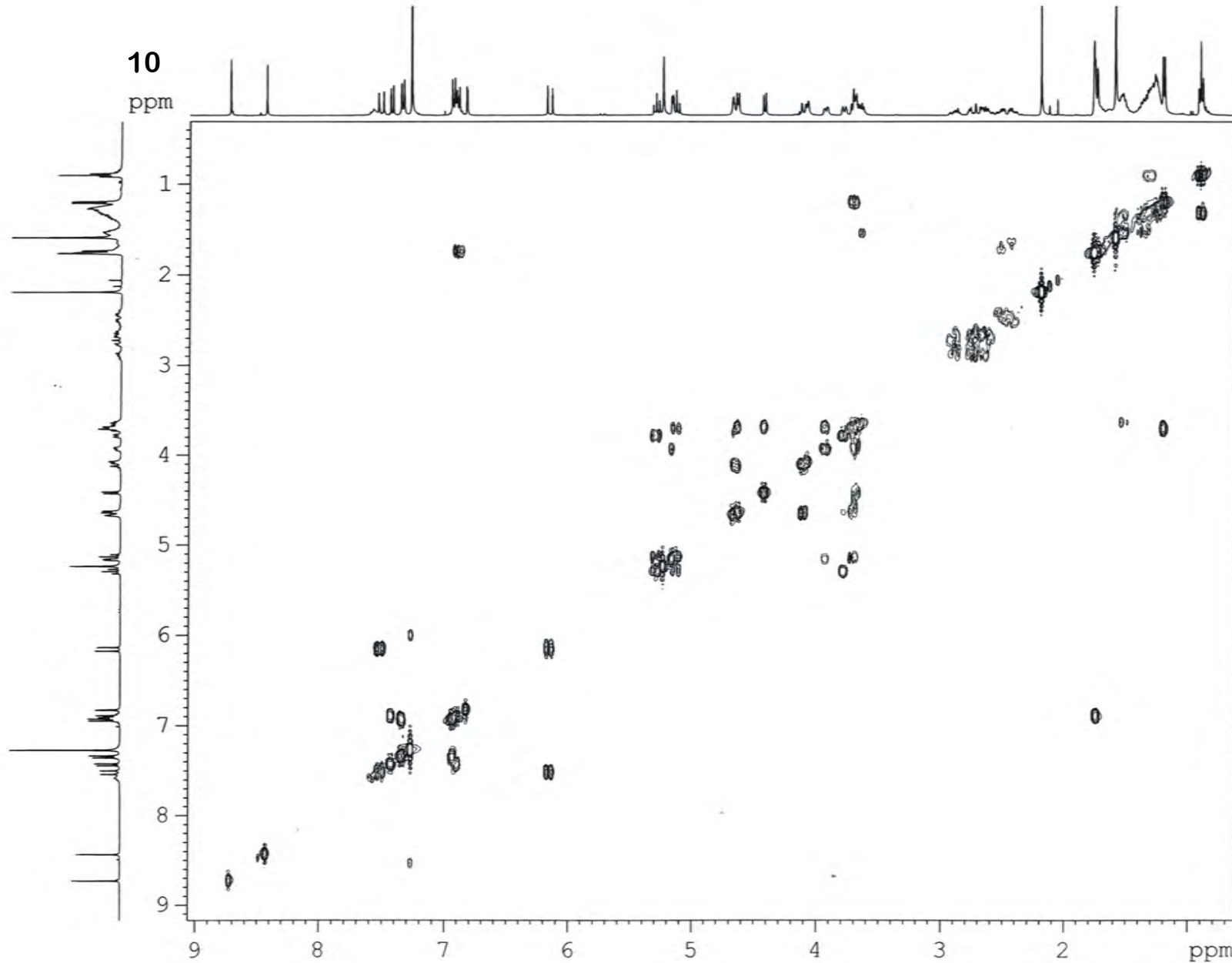


10

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



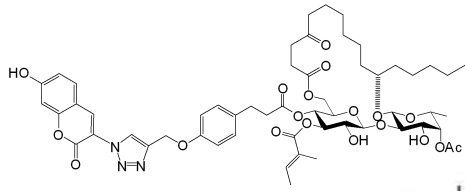
ZGH-Ipom-3-28-150929-A(3) COSY

10  
ppm

NAME ZGH-Ipom-3-28-150929-A(3)  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20151003  
 Time\_ 1.07  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosygppf  
 TD 2048  
 SOLVENT CDCl3  
 NS 16  
 DS 8  
 SWH 5341.880 Hz  
 FIDRES 2.608340 Hz  
 RG 1440  
 AQ 0.1917428 sec  
 DW 93.600 usec  
 DE 6.50 usec  
 TE 292.7 K  
 DO 0.00000300 sec  
 D1 1.48689198 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 INO 0.00018720 sec

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

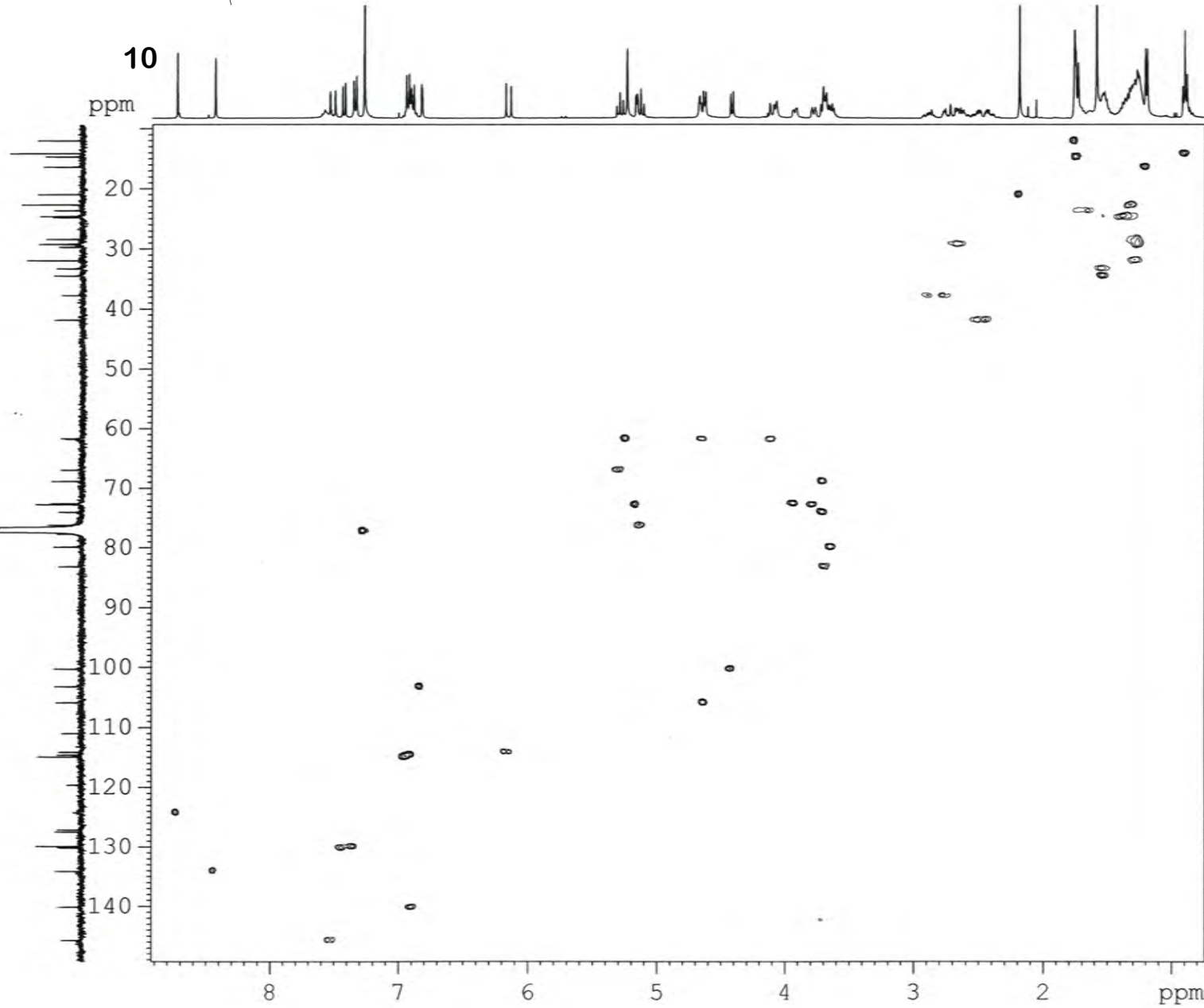
----- GRADIENT CHANNEL -----  
 GPNAMI SINE.100  
 GPZ1 10.00 %  
 P16 1000.00 usec  
 NDO 1  
 TD 128  
 SFO1 400.1324 MHz  
 FIDRES 41.733440 Hz  
 SW 13.350 ppm  
 FMODE QF  
 SI 1024  
 SF 400.1300040 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00  
 SI 1024  
 MC2 QF  
 SF 400.1300033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



ZGH-Ipom-3-28-150929-A(3) HSQC

10

ppm



```

NAME      ZGH-Ipom-3-28-150929-A(3)
EXPNO     3
PROCNO    1
Date_     20151003
Time      2.06
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   hsqcetgpsi
TD         1024
SOLVENT   CDCl3
NS         16
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     145.0000000
D0         0.000003000 sec
D1         1.500000000 sec
D4         0.00172414 sec
D11        0.030000000 sec
D13        0.000004000 sec
D16        0.000200000 sec
D24        0.001100000 sec
INO        0.000030000 sec
    
```

```

===== 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
    
```

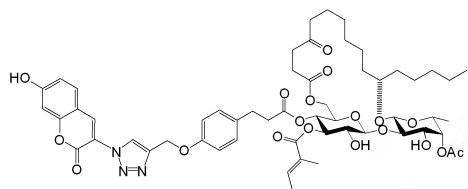
```

===== 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
    
```

```

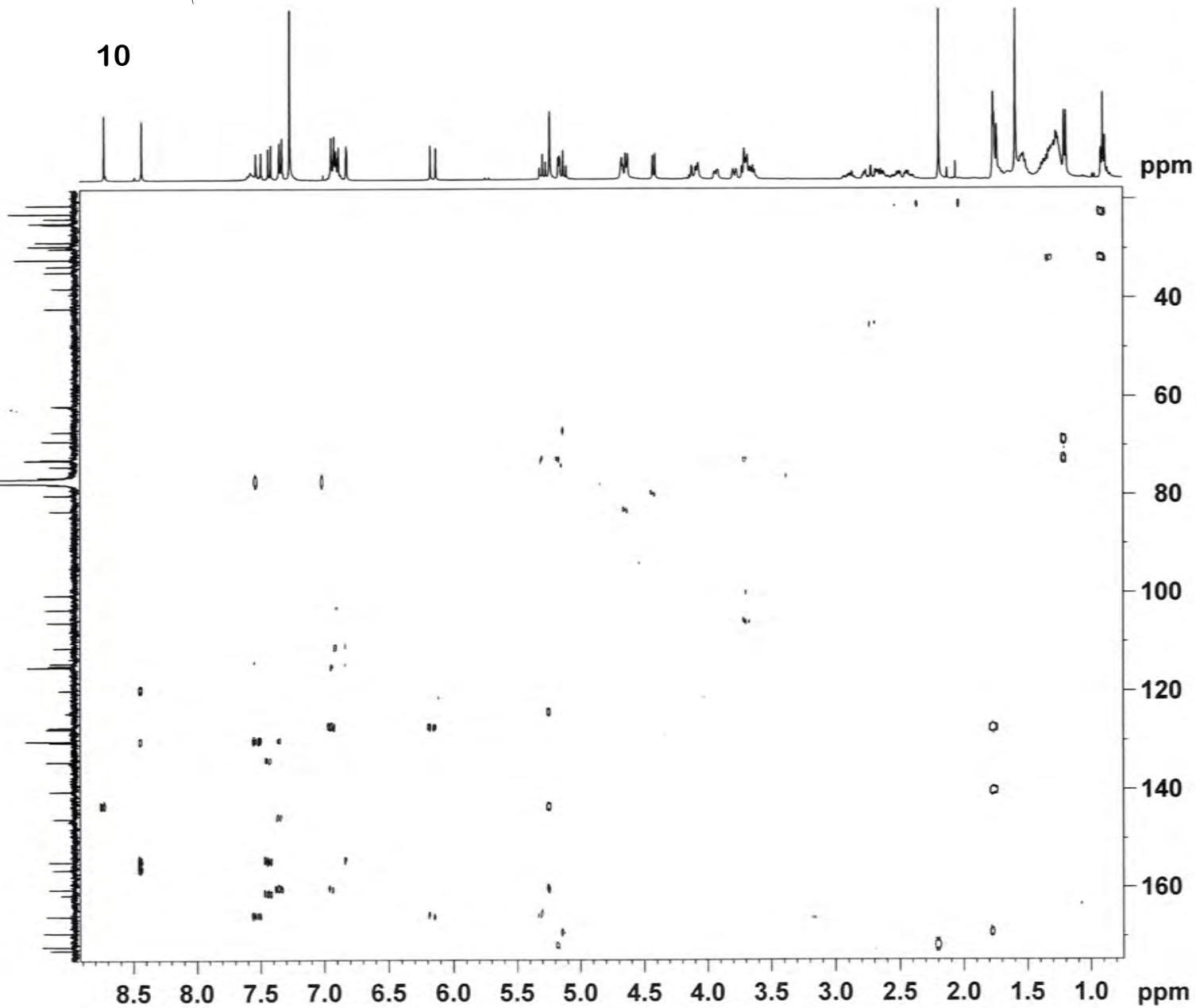
===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    SINE.100
GPZ1      80.00 %
GPZ2      20.10 %
P16       1000.00 usec
ND0        2
TD         256
SFO1       100.6203 MHz
FIDRES    65.104164 Hz
SW         165.639 ppm
FnMODE    Echo-Antiecho
SI         1024
SF         400.1300000 MHz
WDW        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
    
```

8 7 6 5 4 3 2 ppm



ZGH-Ipom-3-28-150929-A(3) HMBC in CDCL3

10



```

NAME      ZGH-Ipom-3-28-150929-A(3)
EXPNO     4
PROCNO    1
Date_     20151003
Time      4.00
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   hmbcgp1pndqf
TD         4096
SOLVENT   CDC13
NS         120
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         0.0000300 sec
D1         1.5000000 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         400.1300000 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
  
```

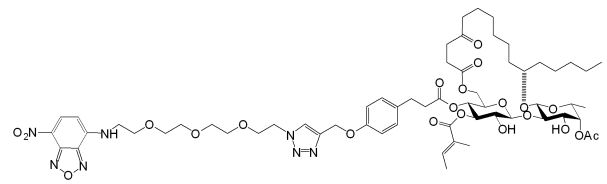




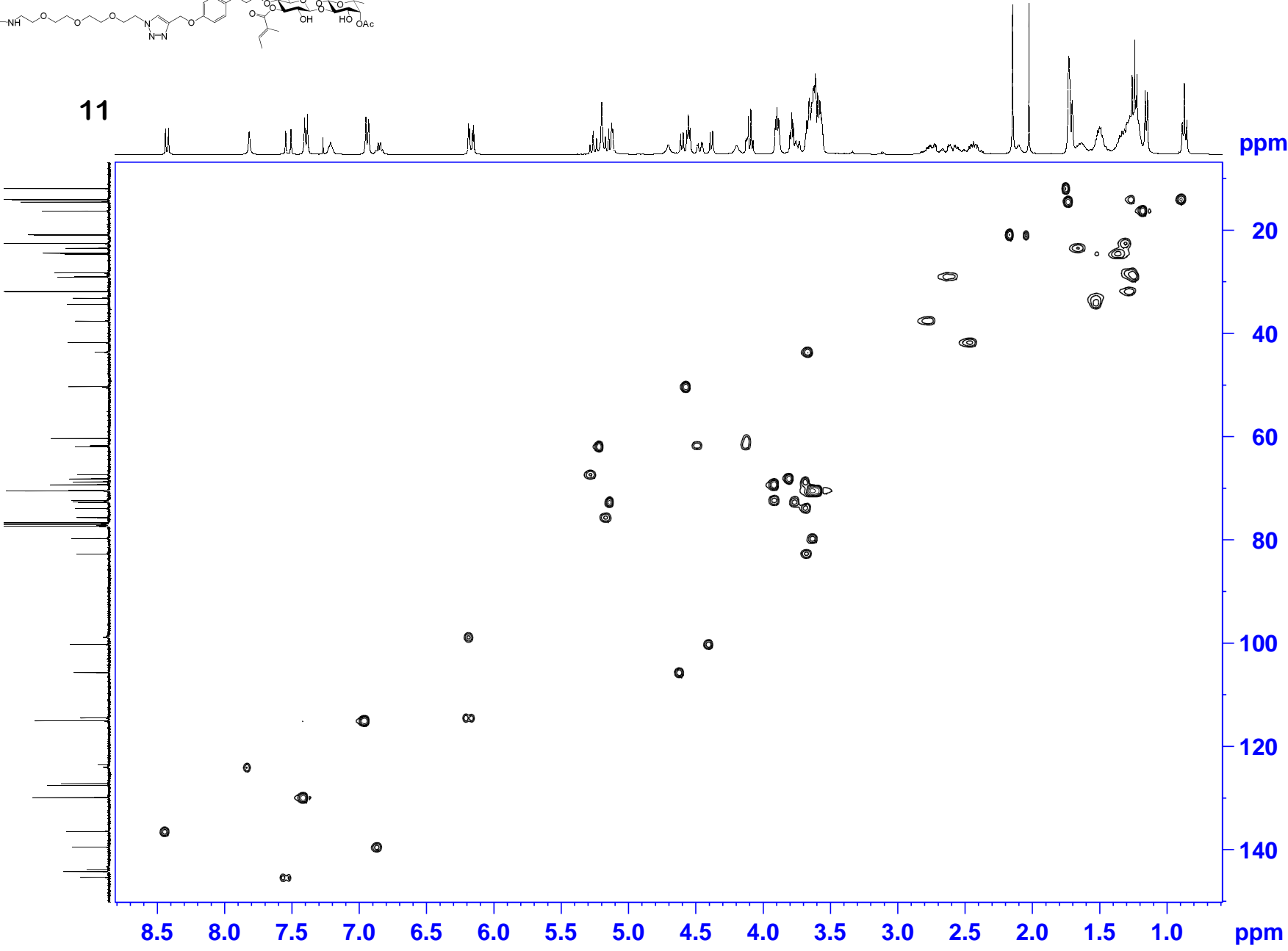




ZGH-*Ipom*-3-231-170705-A HSQC in CDCl<sub>3</sub>



11



Current Data Parameters  
 NAME ZGH-*Ipom*-3-231-170705-A  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170705  
 Time 22.56  
 INSTRUM spect  
 PROBD0 5 mm PABBO BB-  
 PULPROG hsqcetgpr1  
 TD 1024  
 SOLVENT cdcl3  
 NS 16  
 DS 16  
 SWH 5197.505 Hz  
 FIDRES 0.07869 Hz  
 AQ 0.0945088 sec  
 RG 2048  
 DM 96.200 usec  
 DE 6.50 usec  
 TE 298.2 K  
 CMT2 145.000000 sec  
 DO 0.0000000 sec  
 D1 1.0000000 sec  
 D4 0.0017414 sec  
 D11 0.0300000 sec  
 D16 0.0000000 sec  
 D24 0.0011000 sec  
 IM0 0.0000000 sec  
 ZGPPNS

----- CHANNEL f1 -----  
 SFO1 400.1524058 MHz  
 NUC1 1H  
 P1 12.50 usec  
 P2 25.00 usec  
 P2B 1000.00 usec  
 PLW1 20.0000000 W

----- CHANNEL f2 -----  
 SFO2 100.6253021 MHz  
 NUC2 13C  
 CHDPRO2  
 P1 10.00 usec  
 P2 20.00 usec  
 P2B 80.00 usec  
 PLW2 65.0000000 W  
 PLW12 1.0151997 W

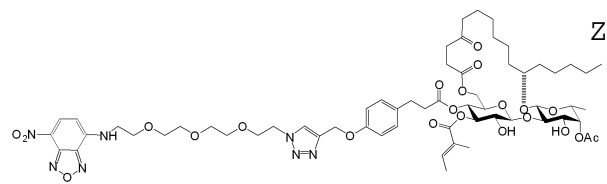
----- GRADIENT CHANNEL -----  
 GRAM[1] SMSG10.100  
 GRAM[2] SMSG10.100  
 GP21 80.00 %  
 GP22 20.10 %  
 P16 1000.00 usec

F1 - Acquisition parameters  
 TS 128  
 SFO1 100.6253 MHz  
 FIDRES 130.226298 Hz  
 SW 145.631 ppm  
 FREQDE Echo-anticho

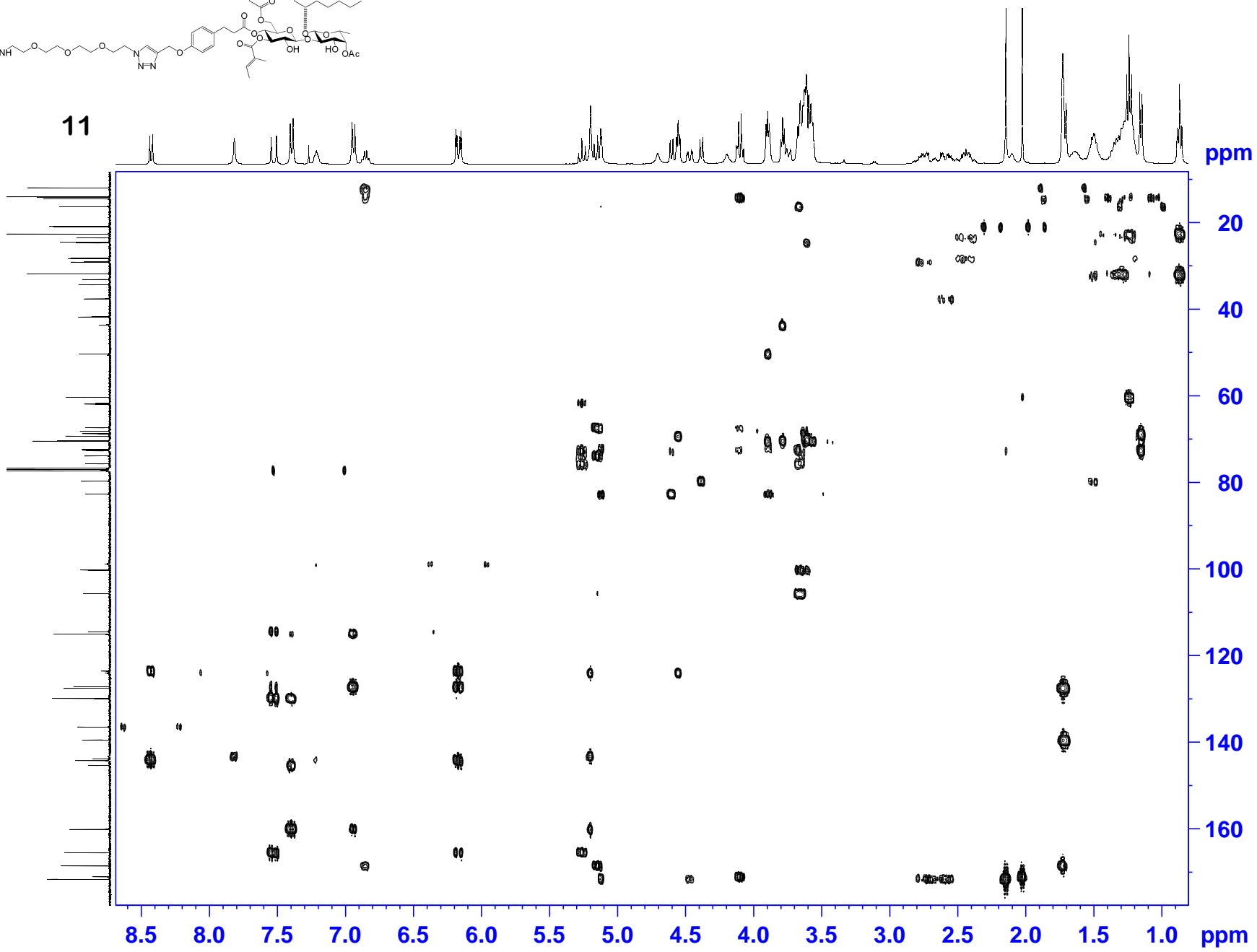
F2 - Processing parameters  
 SI 1024  
 SF 400.1500000 MHz  
 WDW QUINE  
 SSB 2  
 LB 0 Hz  
 GB 0  
 PC 1.40

F1 - Processing parameters  
 SI 1024  
 MC2 echo-anticho  
 SF 100.6177976 MHz  
 WDW QUINE  
 SSB 2  
 LB 0 Hz  
 GB 0

ZGH-*Ipom*-3-231-170705-A HMBC in CDCl<sub>3</sub>



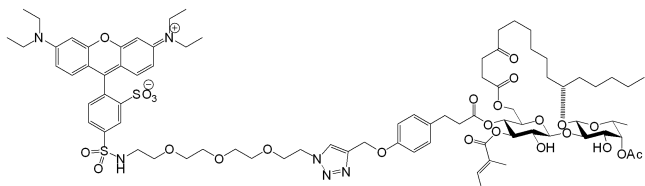
11



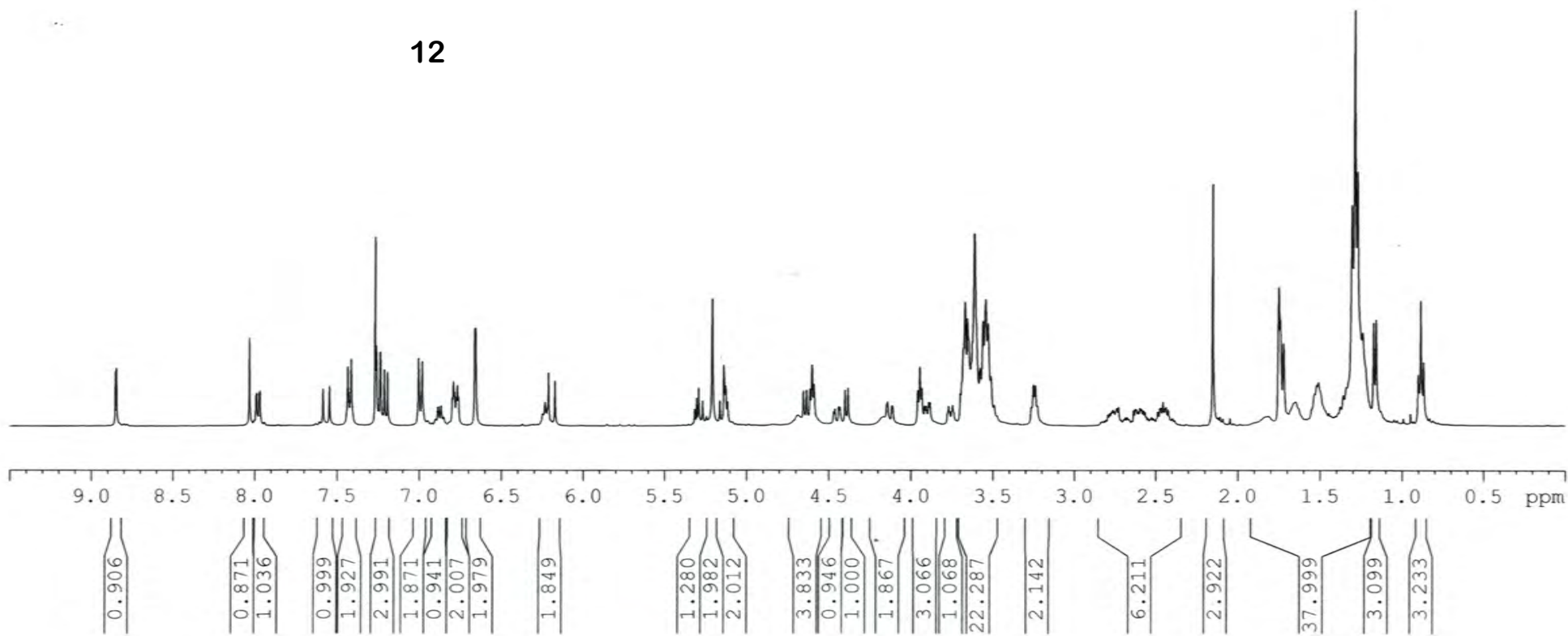
```
Current Data Parameters
NAME      ZGH-Ipom-3-231-170705-A
EXPNO    5
PROCNO   1
F2 - Acquisition Parameters
Date_    20170707
Time     0.16
INSTRUM  spect
PROBHD   5 mm PABBO 1H-
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        40
DS        4
SWH       5208.133 Hz
FIDRES   1.771566 Hz
AQ        0.3932100 sec
RG         99.500
DE        6.500 umsec
TE        298.2 K
CQF21    145.000000
CQF23    10.000000
DD        0.0000000 sec
DQ        0.0000000 sec
DE        0.0000000 sec
DSB       0.0000000 sec
SFO       0.0002240 sec
***** CHANNEL f1 *****
NUC1      13C
P1         12.00 umsec
PL1        20.0000000 W
***** CHANNEL f2 *****
NUC2      13C
P2         10.00 umsec
PL2        65.0000000 W
***** GRABY1 CHANNEL *****
CPGRAM1  1
CPGRAM2  1
CPGRAM3  1
CPGRAM4  1
CPGRAM5  1
CPGRAM6  1
CPGRAM7  1
CPGRAM8  1
CPGRAM9  1
CPGRAM10 1
CPGRAM11 1
CPGRAM12 1
CPGRAM13 1
CPGRAM14 1
CPGRAM15 1
CPGRAM16 1
CPGRAM17 1
CPGRAM18 1
CPGRAM19 1
CPGRAM20 1
CPGRAM21 1
CPGRAM22 1
CPGRAM23 1
CPGRAM24 1
CPGRAM25 1
CPGRAM26 1
CPGRAM27 1
CPGRAM28 1
CPGRAM29 1
CPGRAM30 1
CPGRAM31 1
CPGRAM32 1
CPGRAM33 1
CPGRAM34 1
CPGRAM35 1
CPGRAM36 1
CPGRAM37 1
CPGRAM38 1
CPGRAM39 1
CPGRAM40 1
CPGRAM41 1
CPGRAM42 1
CPGRAM43 1
CPGRAM44 1
CPGRAM45 1
CPGRAM46 1
CPGRAM47 1
CPGRAM48 1
CPGRAM49 1
CPGRAM50 1
CPGRAM51 1
CPGRAM52 1
CPGRAM53 1
CPGRAM54 1
CPGRAM55 1
CPGRAM56 1
CPGRAM57 1
CPGRAM58 1
CPGRAM59 1
CPGRAM60 1
CPGRAM61 1
CPGRAM62 1
CPGRAM63 1
CPGRAM64 1
CPGRAM65 1
CPGRAM66 1
CPGRAM67 1
CPGRAM68 1
CPGRAM69 1
CPGRAM70 1
CPGRAM71 1
CPGRAM72 1
CPGRAM73 1
CPGRAM74 1
CPGRAM75 1
CPGRAM76 1
CPGRAM77 1
CPGRAM78 1
CPGRAM79 1
CPGRAM80 1
CPGRAM81 1
CPGRAM82 1
CPGRAM83 1
CPGRAM84 1
CPGRAM85 1
CPGRAM86 1
CPGRAM87 1
CPGRAM88 1
CPGRAM89 1
CPGRAM90 1
CPGRAM91 1
CPGRAM92 1
CPGRAM93 1
CPGRAM94 1
CPGRAM95 1
CPGRAM96 1
CPGRAM97 1
CPGRAM98 1
CPGRAM99 1
CPGRAM100 1
***** Acquisition parameters *****
TD        65536
SFO       100.617921 MHz
FIDRES   174.366154 Hz
AQ        0.3932100 sec
RG         99.500
DE        6.500 umsec
TE        298.2 K
SOLVENT  CDCl3
***** Processing parameters *****
SI         32768
SF        100.617921 MHz
WDW       EM
SSB       0
LB        0 Hz
GB        0
PC         4.00
***** Processing parameters *****
SI         32768
SF        100.617921 MHz
WDW       EM
SSB       0
LB        0 Hz
GB        0
PC         4.00
```

ZGH-*Ipom*-3-29-151006-A(2) 1H in CDCl<sub>3</sub>

8.852  
8.847  
8.034  
7.969  
7.586  
7.547  
7.436  
7.414  
7.270  
7.263  
7.239  
7.237  
7.214  
7.194  
7.005  
6.984  
6.793  
6.786  
6.769  
6.663  
6.657  
6.213  
6.173  
5.291  
5.208  
5.138  
5.127  
4.655  
4.636  
4.615  
4.602  
4.590  
4.402  
4.383  
3.958  
3.946  
3.934  
3.698  
3.679  
3.669  
3.655  
3.648  
3.625  
3.612  
3.578  
3.559  
3.543  
3.529  
3.512  
3.253  
3.240  
2.153  
1.751  
1.749  
1.741  
1.723  
1.521  
1.510  
1.342  
1.306  
1.289  
1.271  
1.239  
1.174  
1.158  
0.902  
0.868

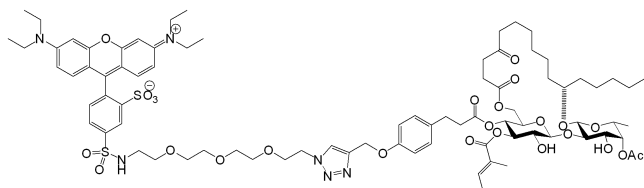


12



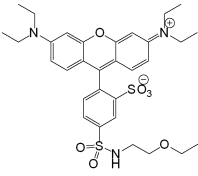
ZGH-*Ipom*-3-29-151006-A(2)  $^{13}\text{C}$  in  $\text{CDCl}_3$ 

210.098  
171.693  
171.657  
165.725  
160.451  
159.018  
157.862  
155.484  
148.418  
145.795  
143.024  
141.988  
139.768  
133.621  
133.403  
129.978  
129.663  
127.575  
127.203  
126.985  
124.859  
115.265  
114.337  
114.173  
113.474  
105.579  
100.369  
95.603  
82.630  
79.933  
77.324  
77.209  
77.007  
76.689  
76.062  
73.946  
72.753  
72.496  
72.439  
70.425  
70.397  
70.277  
69.440  
69.373  
68.808  
67.370  
61.891  
50.287  
45.815  
43.213  
41.822  
37.602  
34.364  
33.189  
31.908  
29.106  
29.032  
28.289  
24.653  
24.500  
23.499  
22.636  
20.945  
16.360  
14.605  
14.091  
12.570  
11.983

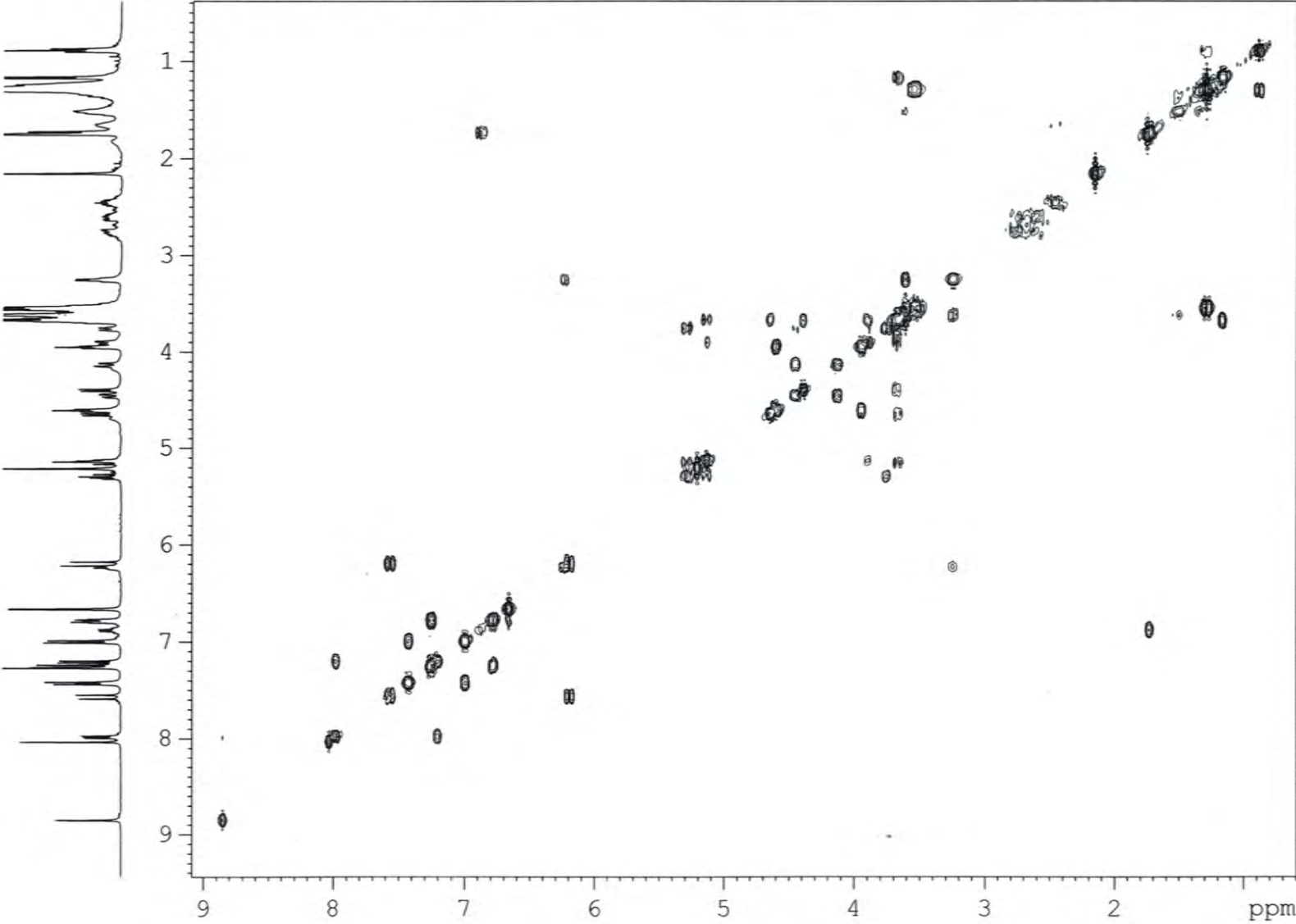


12

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



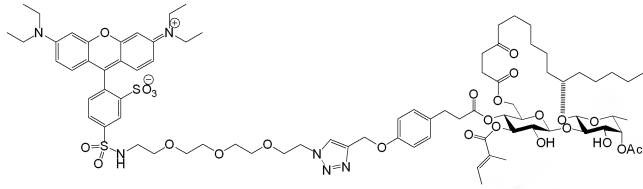
ZGH-Ipom-3-29-151006-A(2) COSY

12  
ppm

NAME ZGH-Ipom-3-29-151006-A(2)  
 EXPNO 2  
 PROCNO 1  
 Date 20151012  
 Time 22.53  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosyppqf  
 TD 2048  
 SOLVENT CDC13  
 NS 8  
 DS 8  
 SWH 5341.880 Hz  
 FIDRES 2.608340 Hz  
 AQ 0.1917428 sec  
 RG 256  
 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

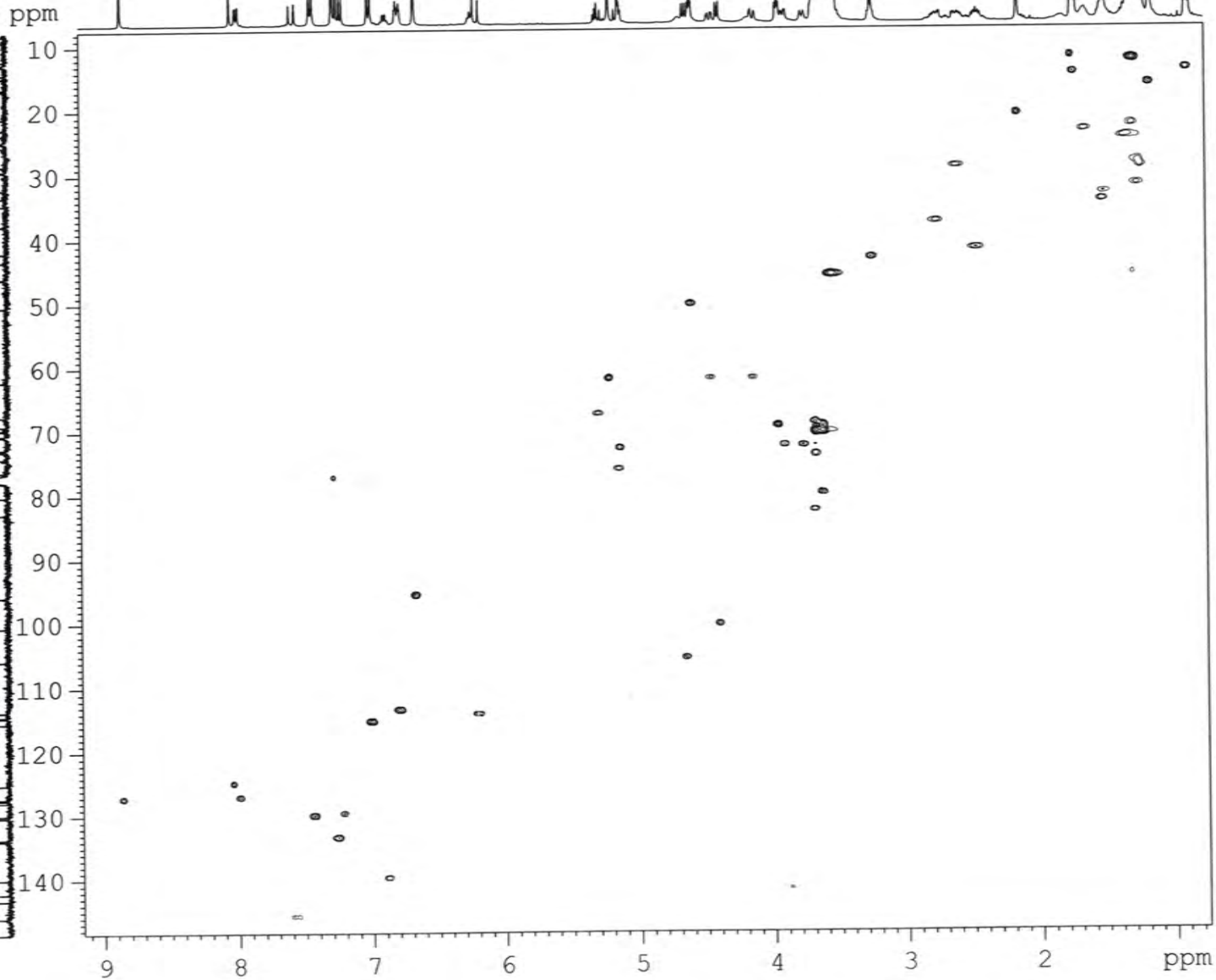
===== CHANNEL f1 =====  
 NUC1 1H  
 P0 10.00 usec  
 P1 10.00 usec  
 PL1 -3.50 dB  
 PL1W 31.17620277 W  
 SFO1 400.1324057 MHz

===== GRADIENT CHANNEL =====  
 GPNAM1 SINE.100  
 GP21 10.00 %  
 P16 1000.00 usec  
 NDO 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



ZGH-Ipom-3-29-151006-A(2) HSQC

12



NAME ZGH-Ipom-3-29-151006-A(2)  
 EXPNO 4  
 PROCNO 1  
 Date\_ 20151013  
 Time\_ 5.53  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hsqcetgpsi  
 TD 1024  
 SOLVENT\_ CDCl3  
 NS 16  
 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 293.4 K  
 CNST2 145.000000  
 D0 0.0000300 sec  
 D1 1.5000000 sec  
 D4 0.00172414 sec  
 D11 0.03000000 sec  
 D13 0.00004000 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  
 FCPD2 75.00 usec  
 FL2 -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  
 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