Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Chemical synthesis and biological evaluation of penta- to octa-saccharide fragments of Vi polysaccharide from *Salmonella typhi*

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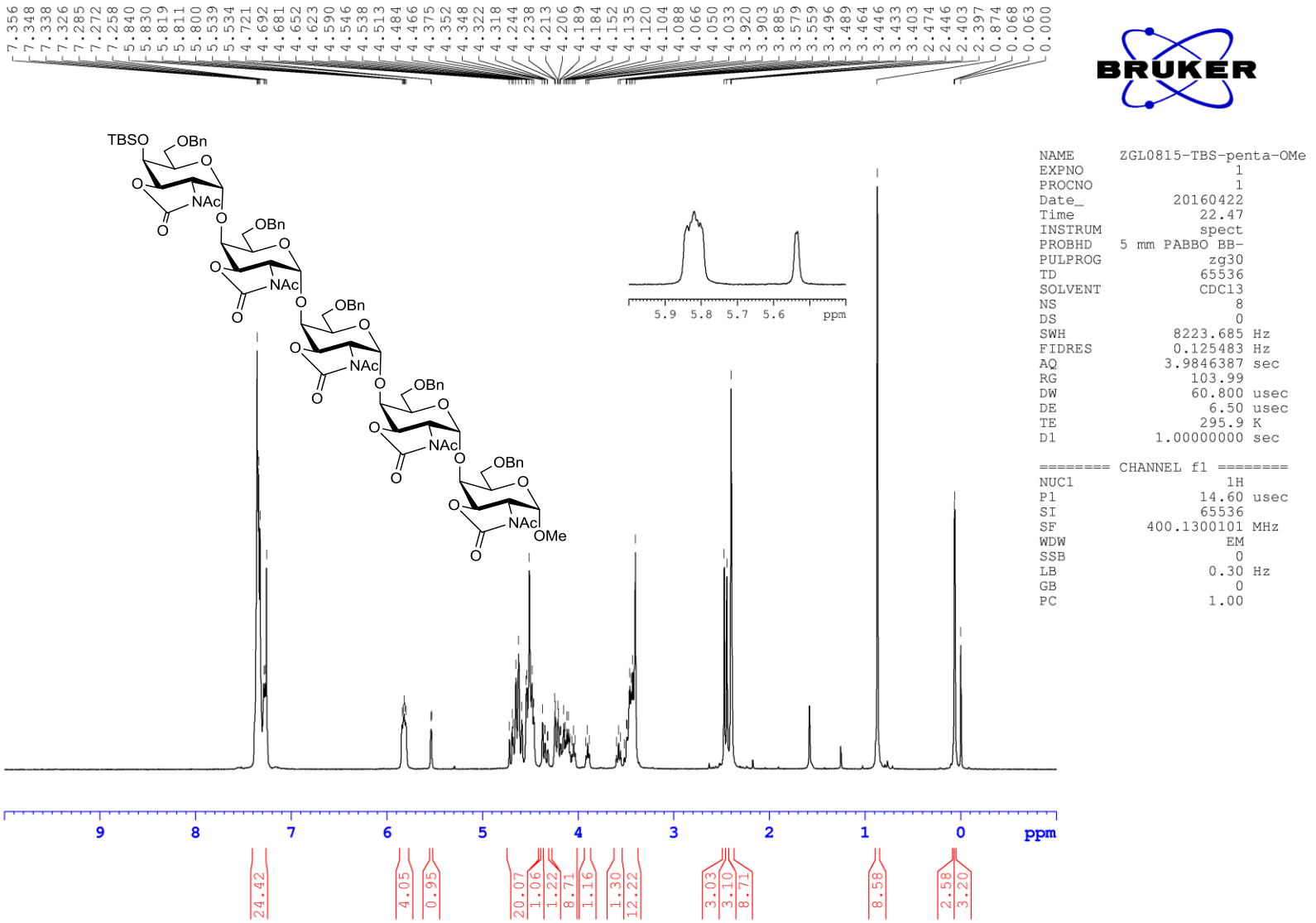
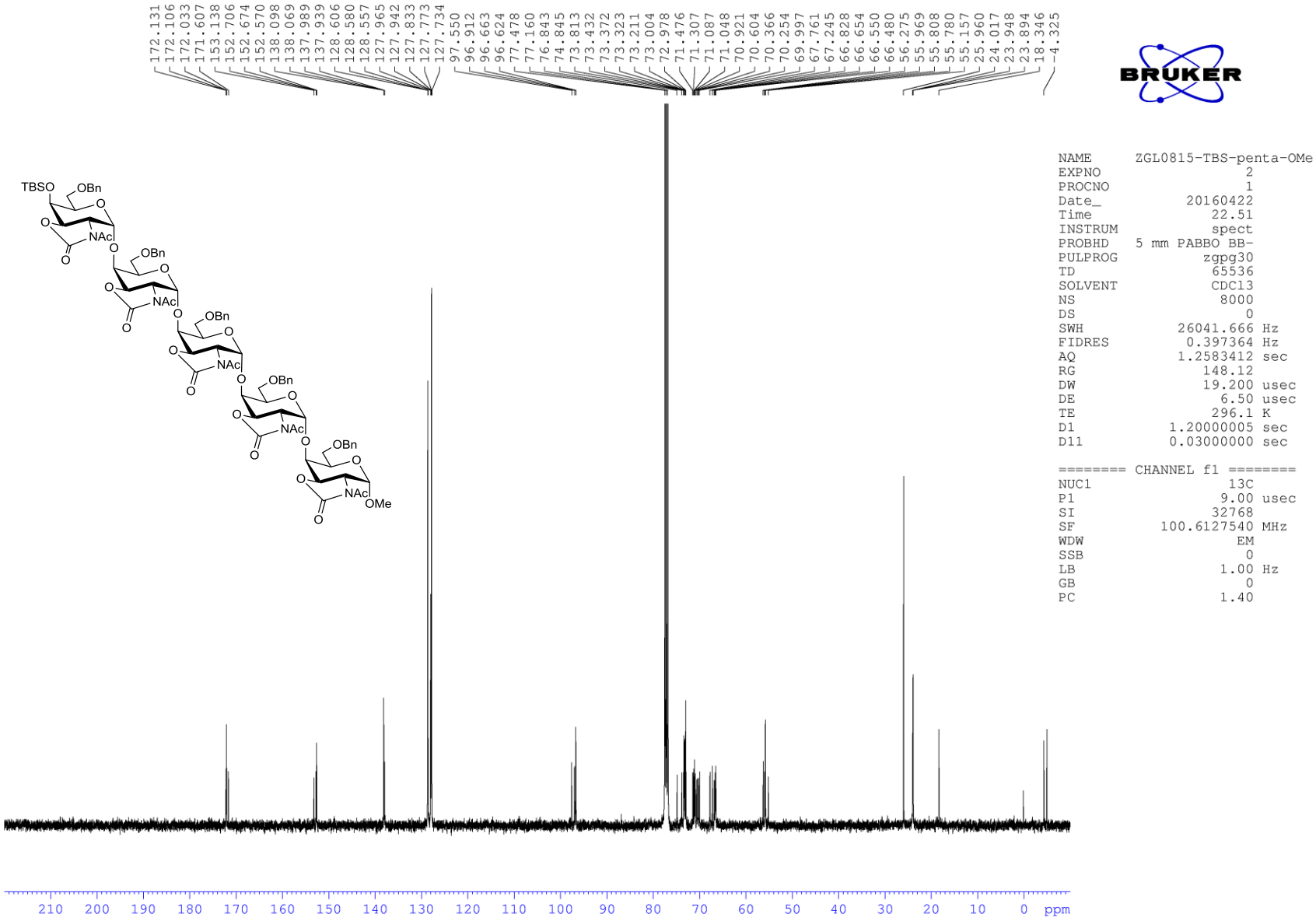
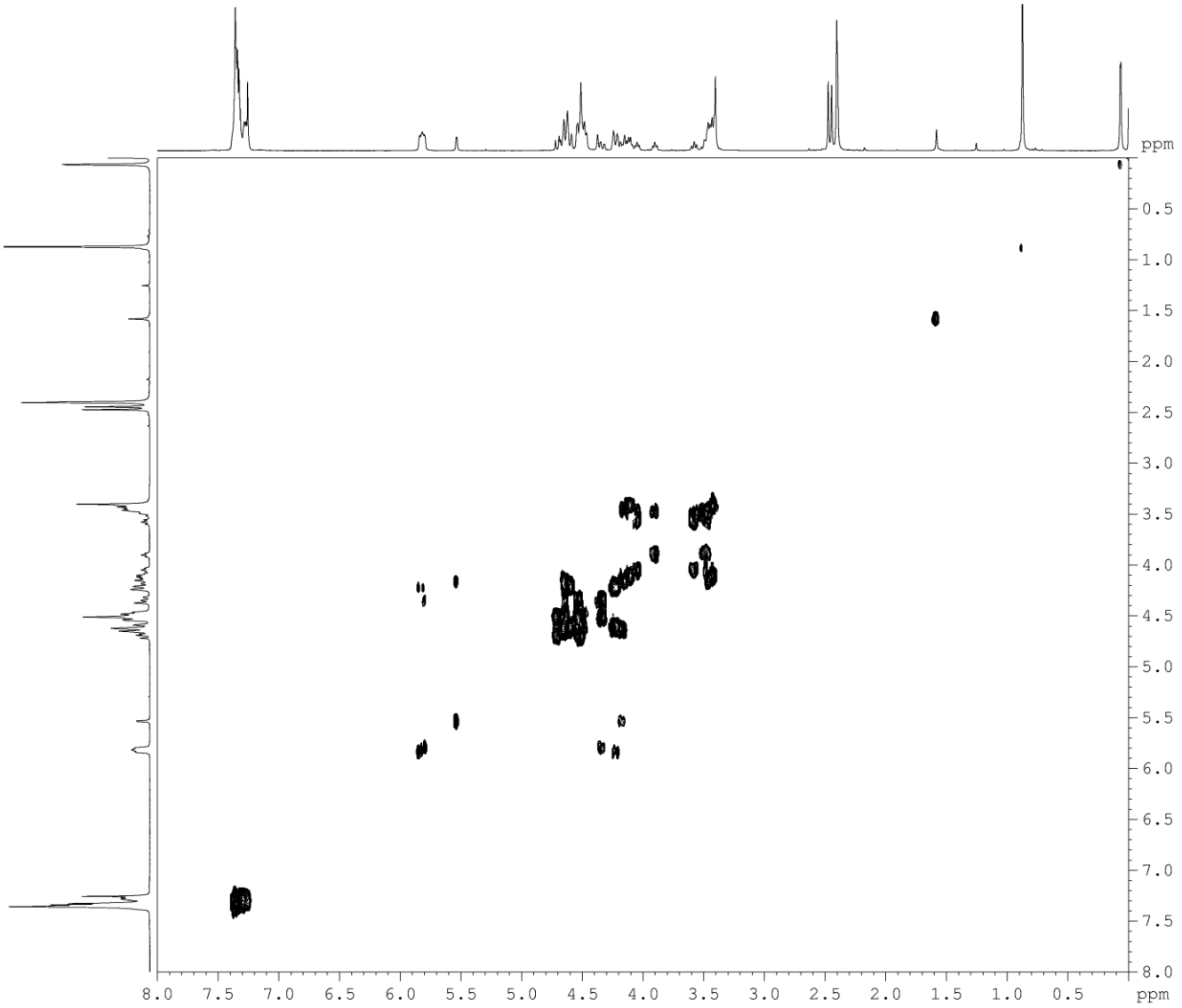


^{1}H NMR spectrum of compound **4**



^{13}C NMR spectrum of compound **4**

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PROBHD    5 mm PABBO BB-
PULPROG             cosygpmfqf
TD                         2048
SOLVENT                   CDCl3
NS                            4
DS                           16
SWH                  5341.880 Hz
FIDRES               2.608340 Hz
AQ                   0.1917428 sec
RG                      183.47
DW                      93.600 usec
DE                       6.50 usec
TE                      296.3 K
D0                   0.00000300 sec
D1                   2.00000000 sec
D13                  0.00000400 sec
D16                  0.00020000 sec
IN0                  0.00018720 sec

======== CHANNEL f1 ========
NUC1                         1H
P1                       14.60 usec
ND0                           1
TD                          128
SFO1                 400.1324 MHz
FIDRES                41.733440 Hz
SW                       13.350 ppm
FnMODE                       QF
SI                         1024
SF                 400.1300007 MHz
WDW                        SINE
SSB                           0
LB                        0.00 Hz
GB                            0
PC                         1.40
SI                         1024
MC2                          QF
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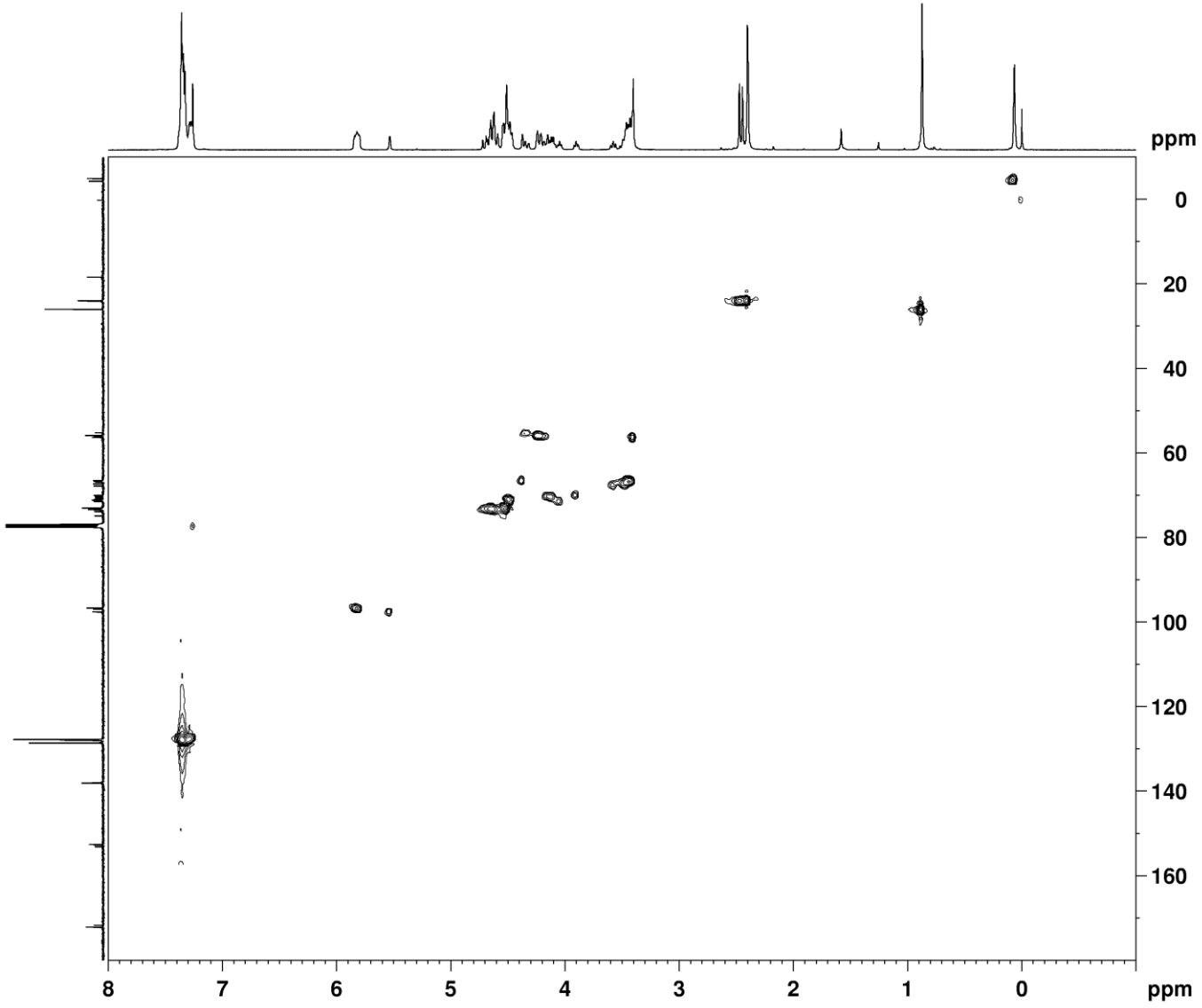
WDW                        SINE
SSB                           0
LB                        0.00 Hz
GB                            0
```

COSY NMR spectrum of compound **4**

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NAME          ZGL0815-TBS-penta-OMe
EXPNO                             4
PROCNO                            1
Date_                      20160423
Time                           4.49
INSTRUM                       spect
PROBHD    5 mm PABBO BB-
PULPROG                   hsqcetgp
TD                            1024
SOLVENT                     CDCl3
NS                                4
DS                               16
SWH                       5341.880 Hz
FIDRES                    5.216680 Hz
AQ                        0.0958964 sec
RG                           183.47
DW                           93.600 usec
DE                            6.50 usec
TE                           295.9 K
CNST2                145.0000000
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D1                    1.50000000 sec
D4                    0.00172414 sec
D11                   0.03000000 sec
D13                   0.00000400 sec
D16                   0.00020000 sec
IN0                   0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                          1H
P1                         14.60 usec
P2                         29.20 usec
P28                      1000.00 usec
ND0                           2
TD                          128
SFO1                  100.6203 MHz
FIDRES                130.208328 Hz
SW                       165.639 ppm
FnMODE            Echo-Antiecho
SI                          1024
SF                  400.1300007 MHz
WDW                       QSINE
SSB                           2
LB                         0.00 Hz
GB                            0
PC                         1.40
SI                          1024
MC2               echo-antiecho
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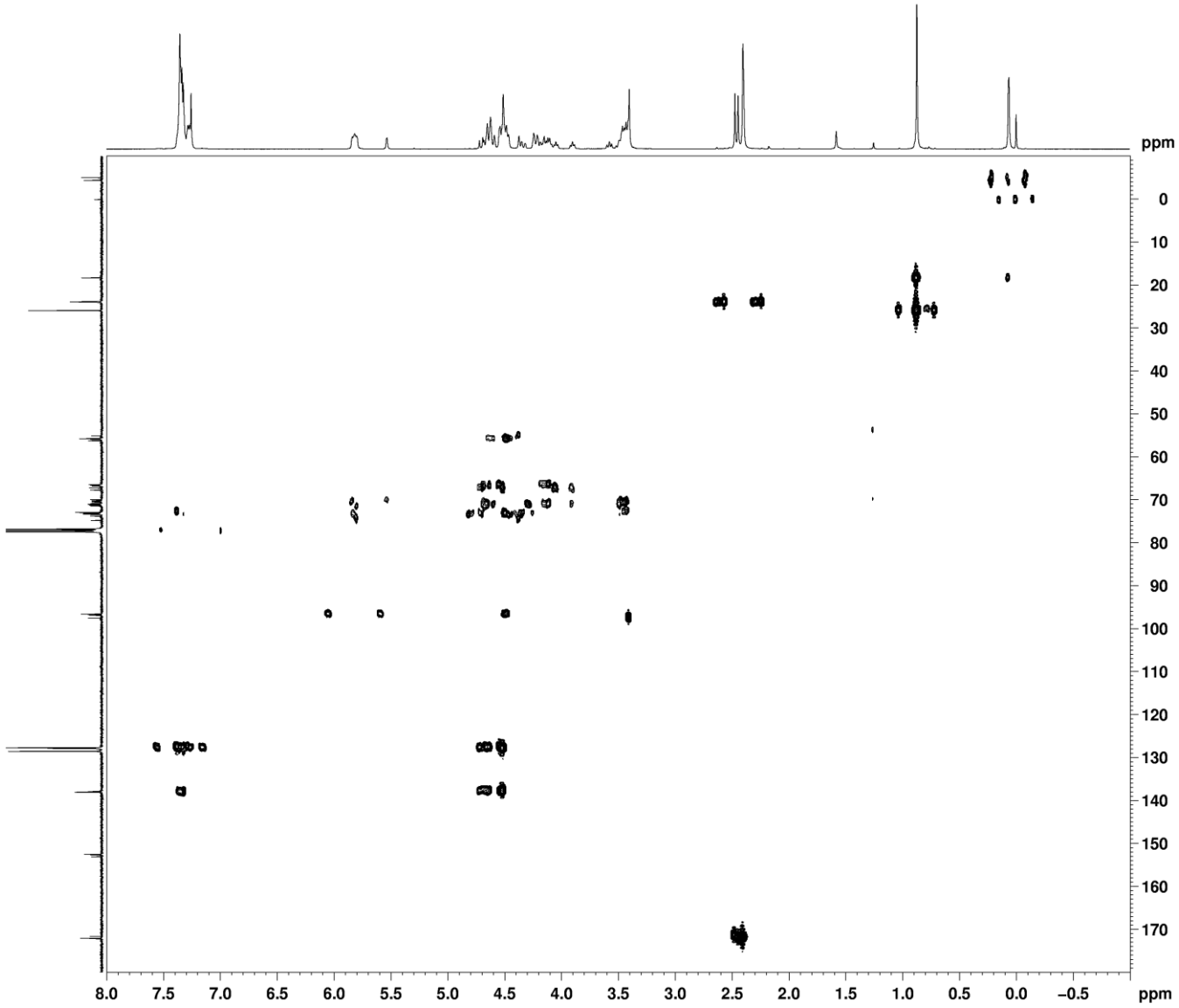
WDW                       QSINE
SSB                           2
LB                         0.00 Hz
GB                            0
```

HSQC NMR spectrum of compound **4**



BRUKER

NAME	ZGL0815-TBS-penta-OM
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PROCNO	1
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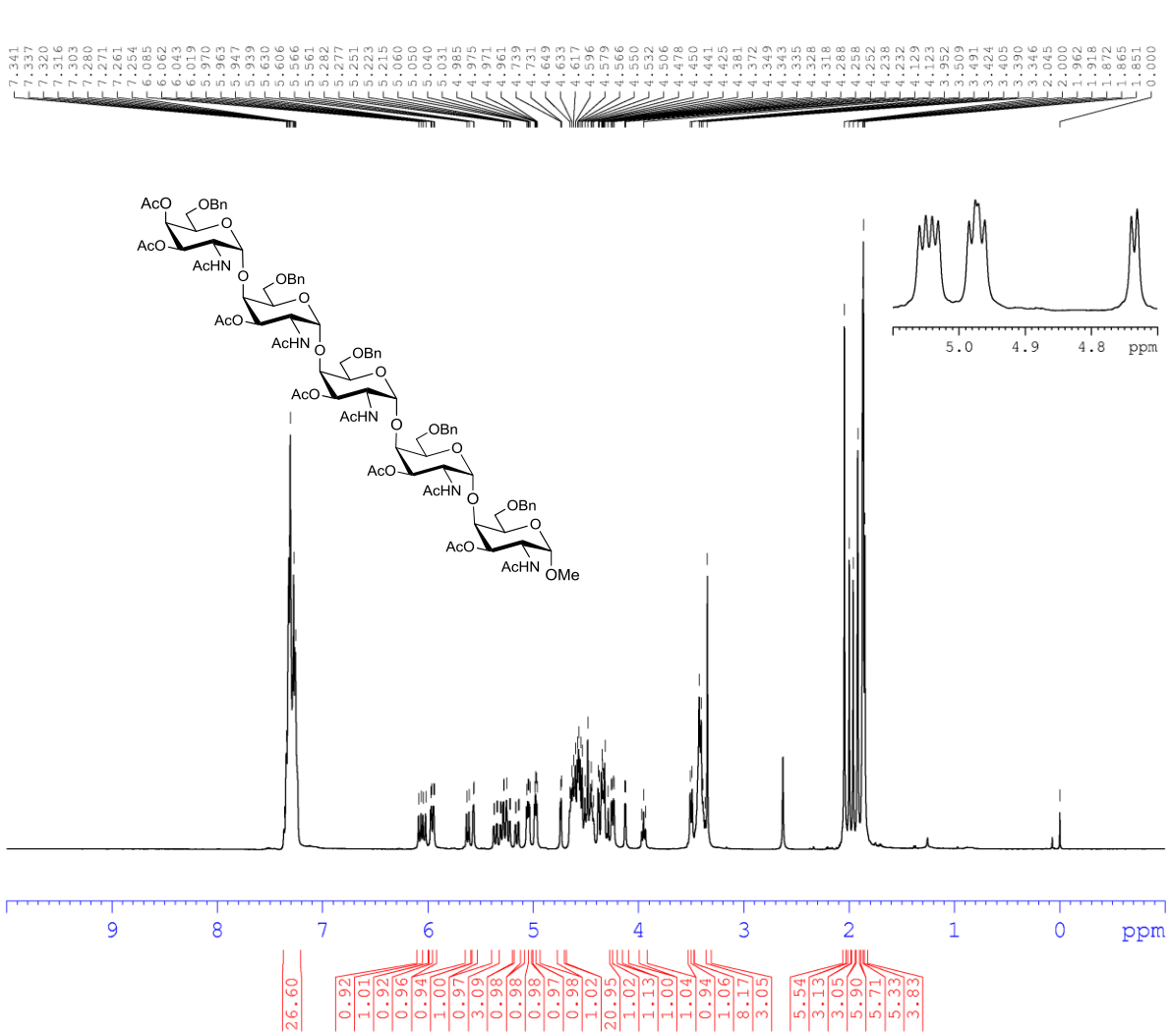
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	hmbcgpndqf
TD	4096
SOLVENT	CDCl3
NS	32
DS	16
SWH	5330.490 Hz
FIDRES	1.301389 Hz
AQ	0.3842548 sec
RG	183.47
DW	93.800 usec
DE	6.50 usec
TE	295.9 K
CNST13	8.0000000
D0	0.00000300 sec
D1	1.50000000 sec
D6	0.06250000 sec
D16	0.00020000 sec
IN0	0.00002235 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	14.60 usec
P2	29.20 usec
ND0	2
TD	128
SFO1	100.6228 MHz
FIDRES	174.592422 Hz
SW	222.095 ppm
FnMODE	QF
SI	1024
SF	400.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	100.6127690 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

HMBC NMR spectrum of compound **4**

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NAME       ZGL0818-5-Ac-penta-OMe
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PROCNO                  1
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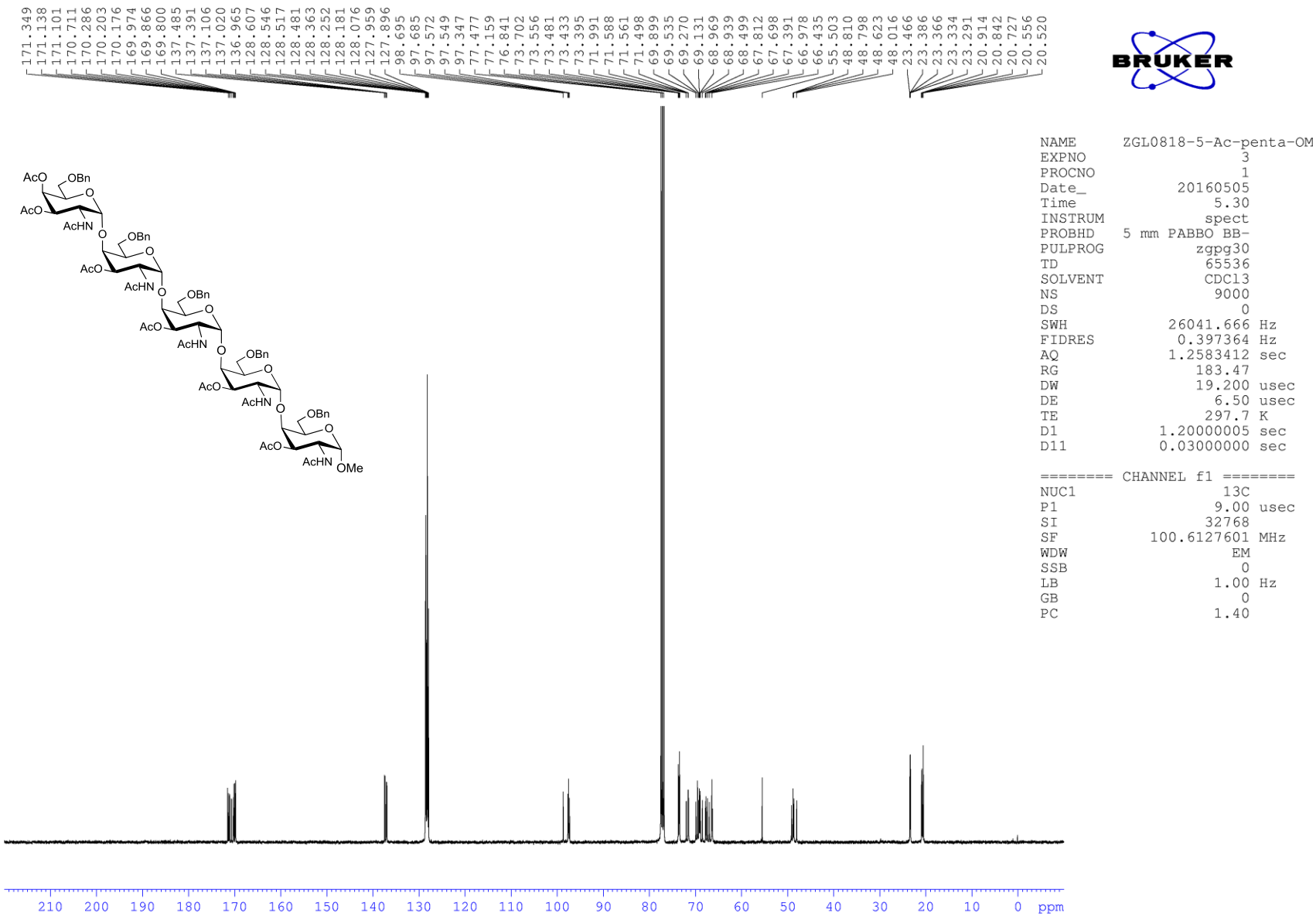
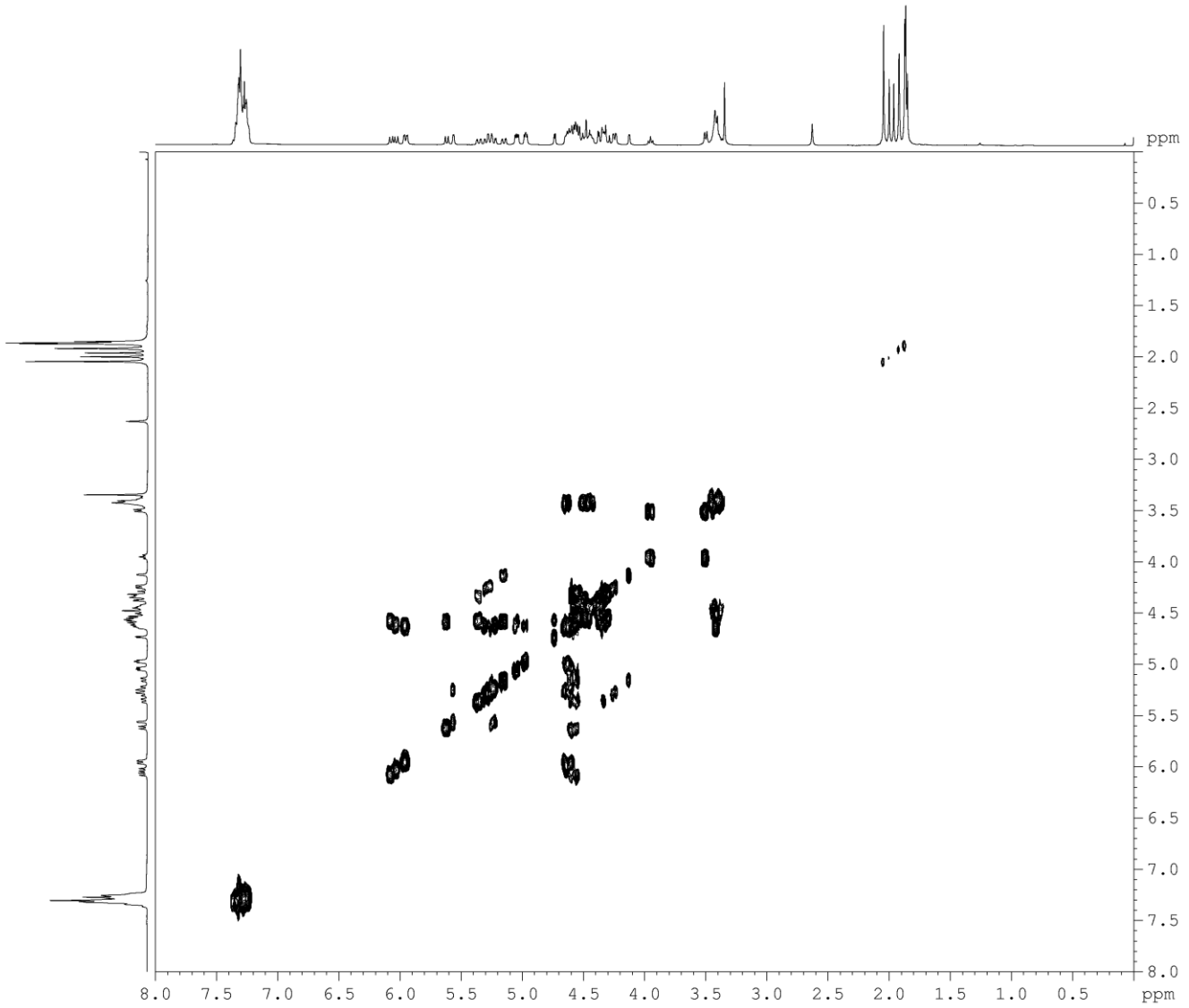
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                  58.05
DW                 60.800 usec
DE                  6.50 usec
TE                 296.3 K
D1             1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.60 usec
SI                  65536
SF           400.1300050 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

^{1}H NMR spectrum of compound **5**



^{13}C NMR spectrum of compound **5**




```
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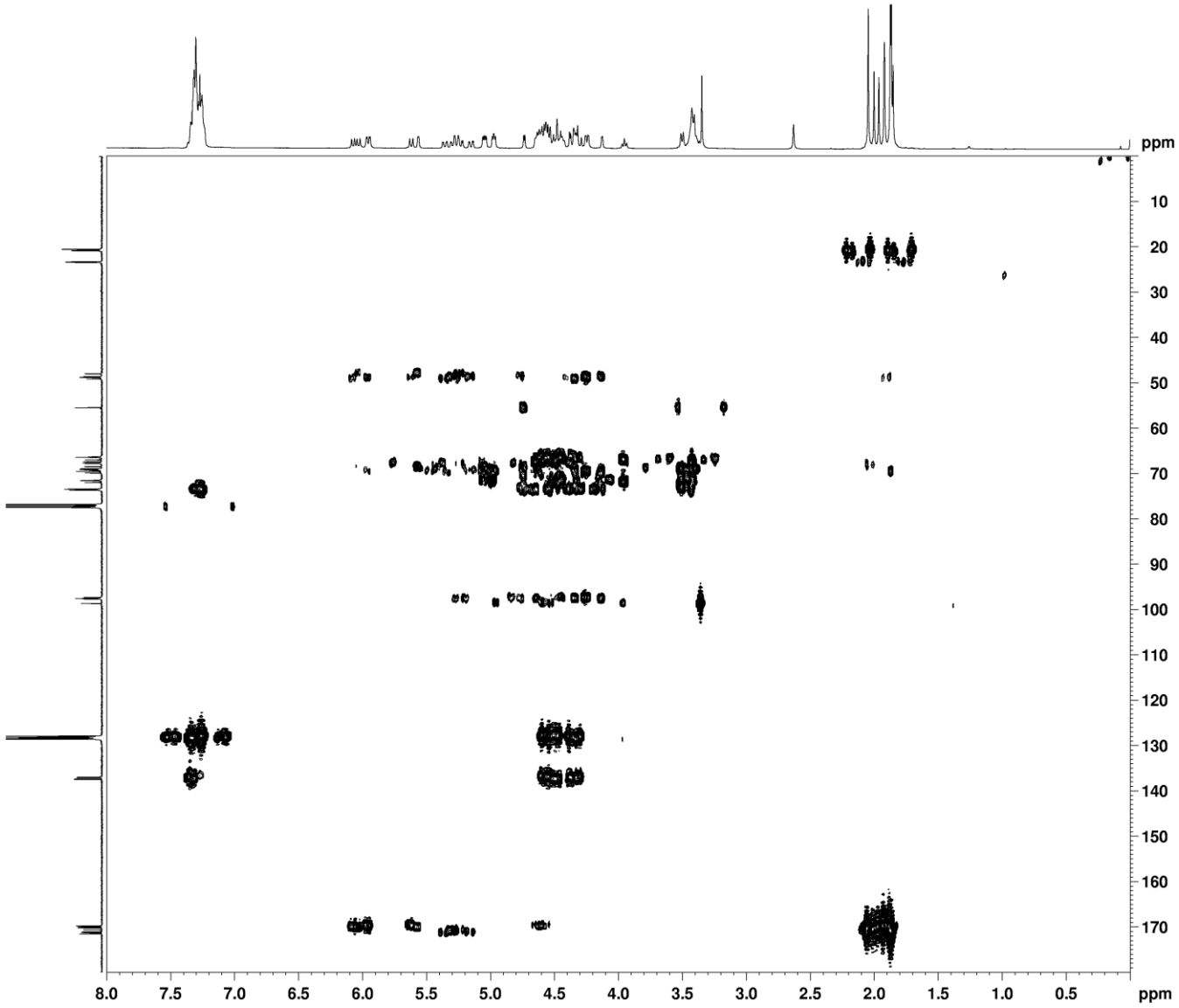
PROCNO                         1
Date_                   20160504
Time                       22.52
INSTRUM                    spect
PROBHD   5 mm PABBO BB-
PULPROG              cosygpmfqf
TD                          2048
SOLVENT                    CDCl3
NS                             4
DS                            16
SWH                     5341.880 Hz
FIDRES                  2.608340 Hz
AQ                      0.1917428 sec
RG                         183.47
DW                         93.600 usec
DE                          6.50 usec
TE                         296.3 K
D0                      0.00000300 sec
D1                      2.00000000 sec
D13                     0.00000400 sec
D16                     0.00020000 sec
IN0                     0.00018720 sec

======== CHANNEL f1 ========
NUC1                          1H
P1                         14.60 usec
ND0                            1
TD                           128
SFO1                    400.1324 MHz
FIDRES                  41.733440 Hz
SW                         13.350 ppm
FnMODE                        QF
SI                           1024
SF                    400.1300021 MHz
WDW                         SINE
SSB                            0
LB                          0.00 Hz
GB                             0
PC                          1.40
SI                           1024
MC2                           QF
SF                    400.1299999 MHz
WDW                         SINE
SSB                            0
LB                          0.00 Hz
GB                             0
```

COSY NMR spectrum of compound **5**




```
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PROCNO                            1
Date_                      20160505
Time                           5.47
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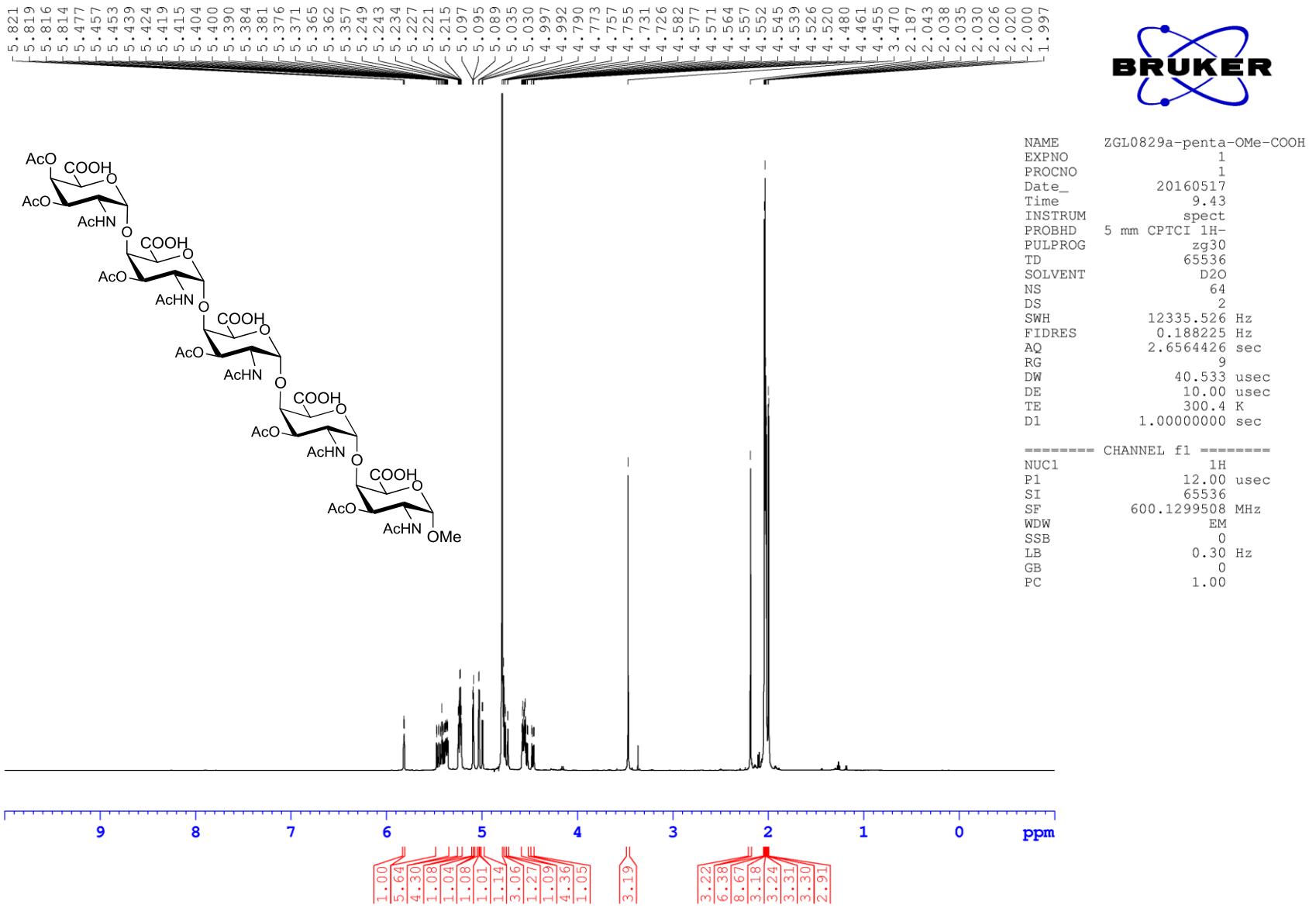
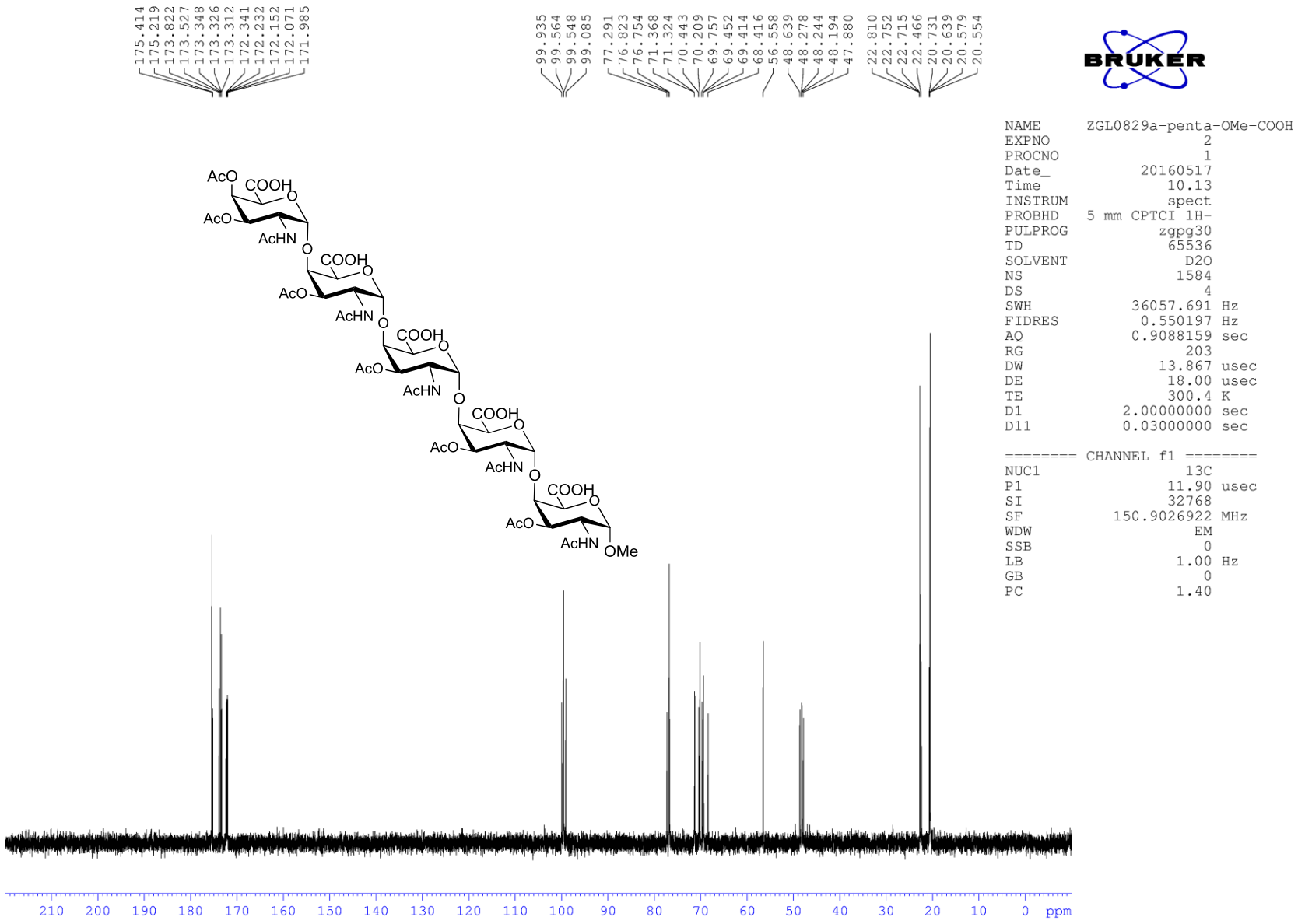
PULPROG              hmbcgpndqf
TD                             4096
SOLVENT                     CDCl3
NS                               32
DS                               16
SWH                      5330.490 Hz
FIDRES                   1.301389 Hz
AQ                       0.3842548 sec
RG                          183.47
DW                          93.800 usec
DE                            6.50 usec
TE                           296.3 K
CNST13                    8.0000000
D0                        0.00000300 sec
D1                        1.50000000 sec
D6                        0.06250000 sec
D16                       0.00020000 sec
IN0                       0.00002235 sec

======== CHANNEL f1 ========
NUC1                            1H
P1                           14.60 usec
P2                           29.20 usec
ND0                              2
TD                             128
SFO1                    100.6228 MHz
FIDRES                  174.592422 Hz
SW                       222.095 ppm
FnMODE                          QF
SI                            1024
SF                    400.1300000 MHz
WDW                           SINE
SSB                              0
LB                            0.00 Hz
GB                               0
PC                            1.40
SI                            1024
MC2                             QF
SF                    100.6127690 MHz
WDW                           SINE
SSB                              0
LB                            0.00 Hz
GB                               0
```

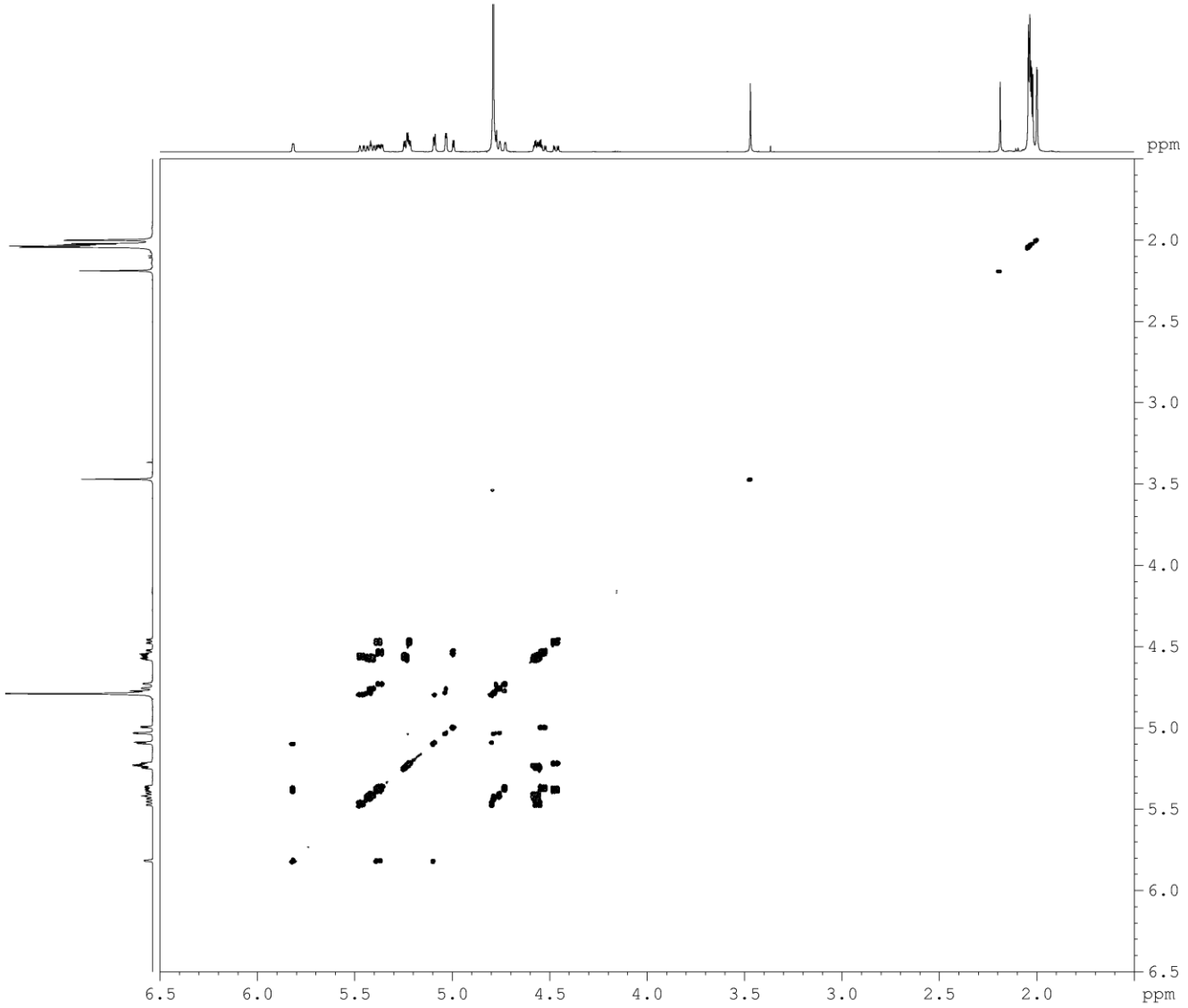
HMBC NMR spectrum of compound **5**



^{1}H NMR spectrum of compound **6**



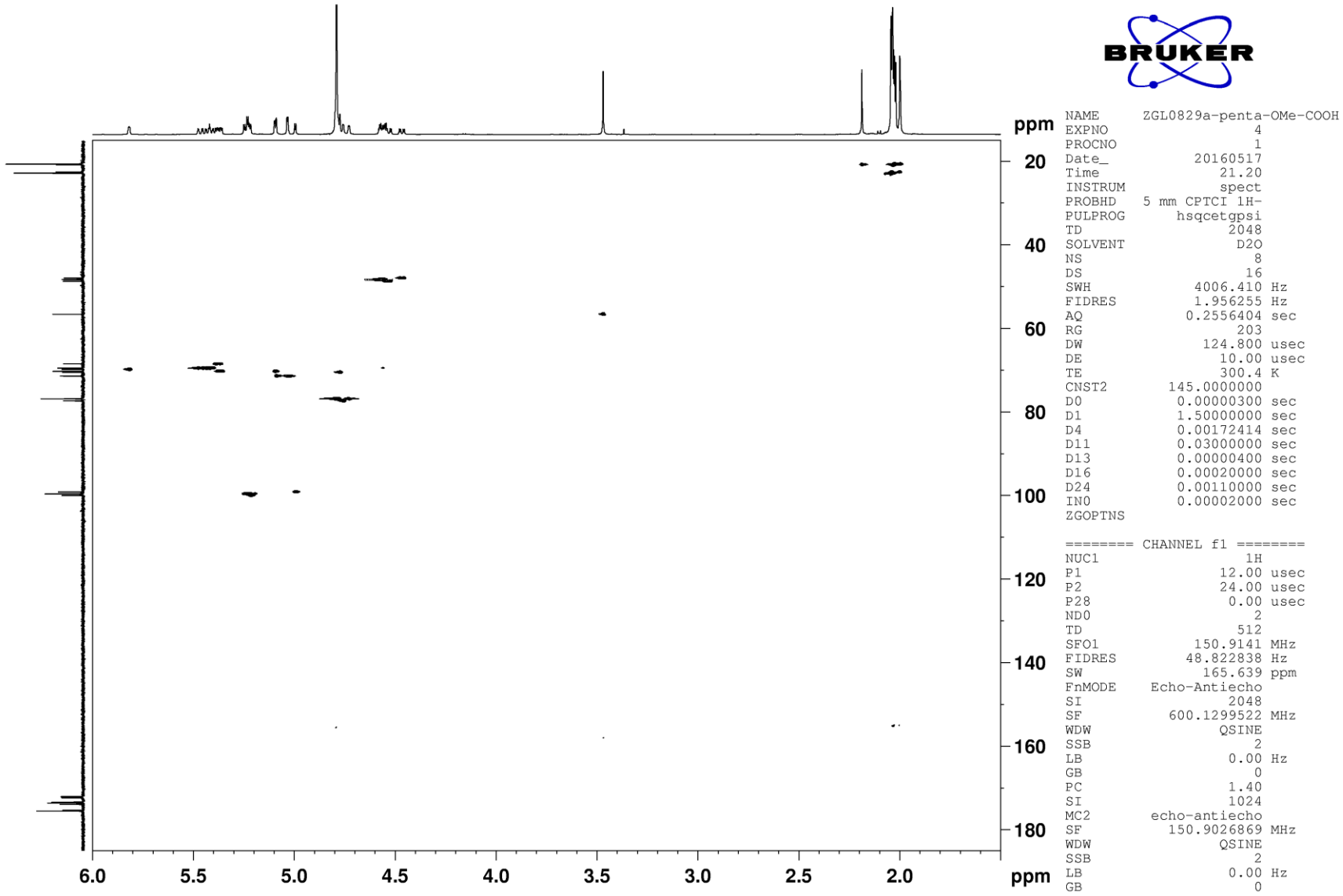
^{13}C NMR spectrum of compound **6**




```
NAME        ZGL0829a-penta-OMe-COOH
EXPNO                             3
PROCNO                            1
Date_                      20160517
Time                          14.30
INSTRUM                       spect
PROBHD    5 mm CPTCI 1H-
PULPROG           cosygpmfqf
TD                             2048
SOLVENT                         D2O
NS                                8
DS                                8
SWH                    4006.410 Hz
FIDRES                 1.956255 Hz
AQ                     0.2556404 sec
RG                              203
DW                       124.800 usec
DE                        10.00 usec
TE                         300.4 K
D0                     0.00000300 sec
D1                     2.00000000 sec
D13                    0.00000400 sec
D16                    0.00020000 sec
IN0                    0.00024960 sec

======== CHANNEL f1 ========
NUC1                            1H
P1                        13.10 usec
ND0                               1
TD                              512
SFO1                   600.1321 MHz
FIDRES                 7.825062 Hz
SW                        6.676 ppm
FnMODE                         QF
SI                             2048
SF                   600.1299504 MHz
WDW                          SINE
SSB                             0
LB                         0.00 Hz
GB                              0
PC                           1.40
SI                           1024
MC2                            QF
SF                   600.1299485 MHz
WDW                          SINE
SSB                             0
LB                         0.00 Hz
GB                              0
```

COSY NMR spectrum of compound **6**




```
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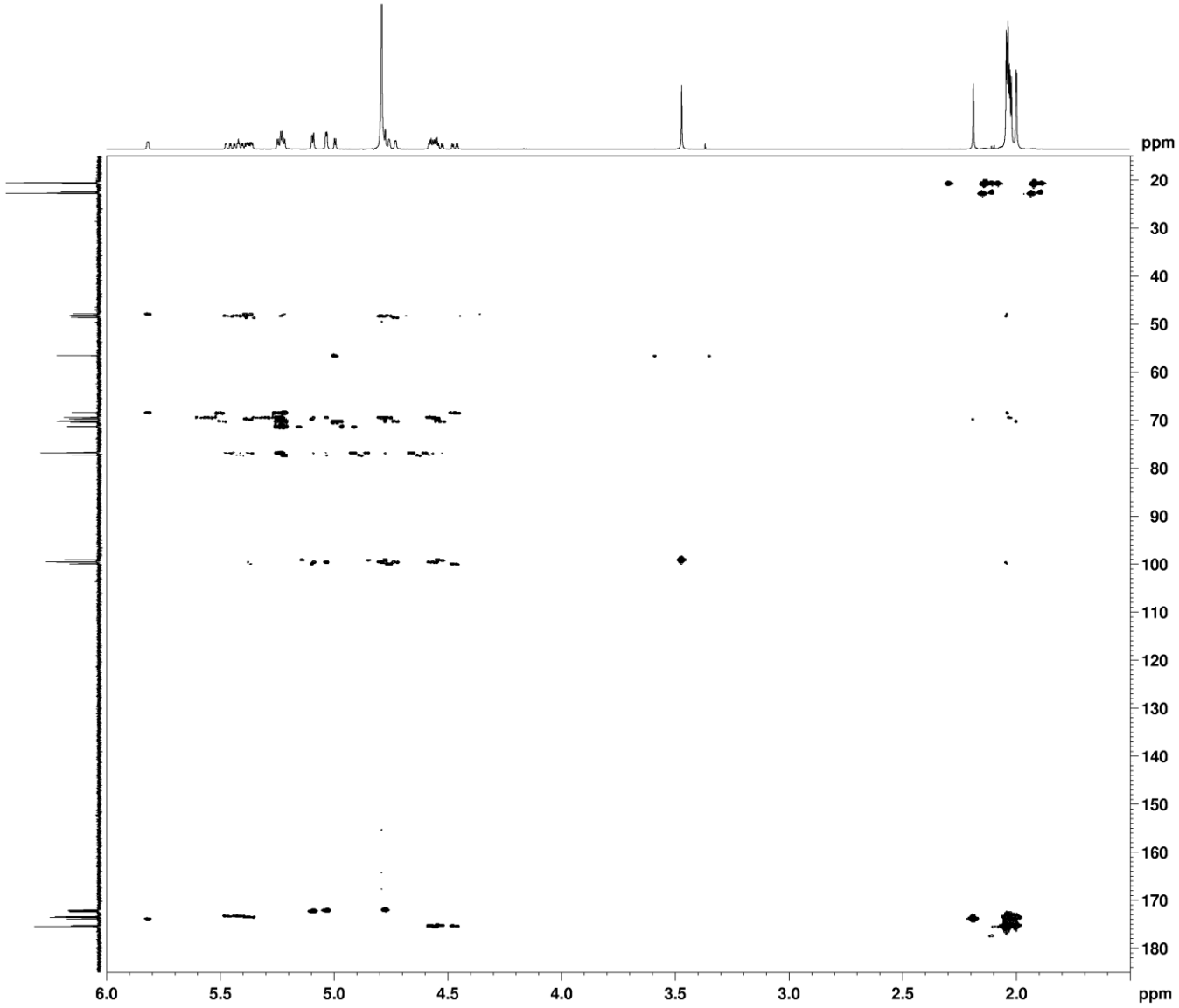
Date_                      20160517
Time                          21.20
INSTRUM                       spect
PROBHD     5 mm CPTCI 1H-
PULPROG            hsqcetgpsi
TD                            2048
SOLVENT                        D2O
NS                               8
DS                              16
SWH                      4006.410 Hz
FIDRES                   1.956255 Hz
AQ                       0.2556404 sec
RG                             203
DW                         124.800 usec
DE                          10.00 usec
TE                           300.4 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                      0.00002000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                            1H
P1                          12.00 usec
P2                          24.00 usec
P28                          0.00 usec
ND0                             2
TD                            512
SFO1                   150.9141 MHz
FIDRES                  48.822838 Hz
SW                        165.639 ppm
FnMODE           Echo-Antiecho
SI                            2048
SF                   600.1299522 MHz
WDW                         QSINE
SSB                             2
LB                           0.00 Hz
GB                              0
PC                           1.40
SI                           1024
MC2                echo-antiecho
SF                   150.9026869 MHz
WDW                         QSINE
SSB                             2
LB                           0.00 Hz
GB                              0
```

HSQC NMR spectrum of compound **6**

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PROCNO                          1
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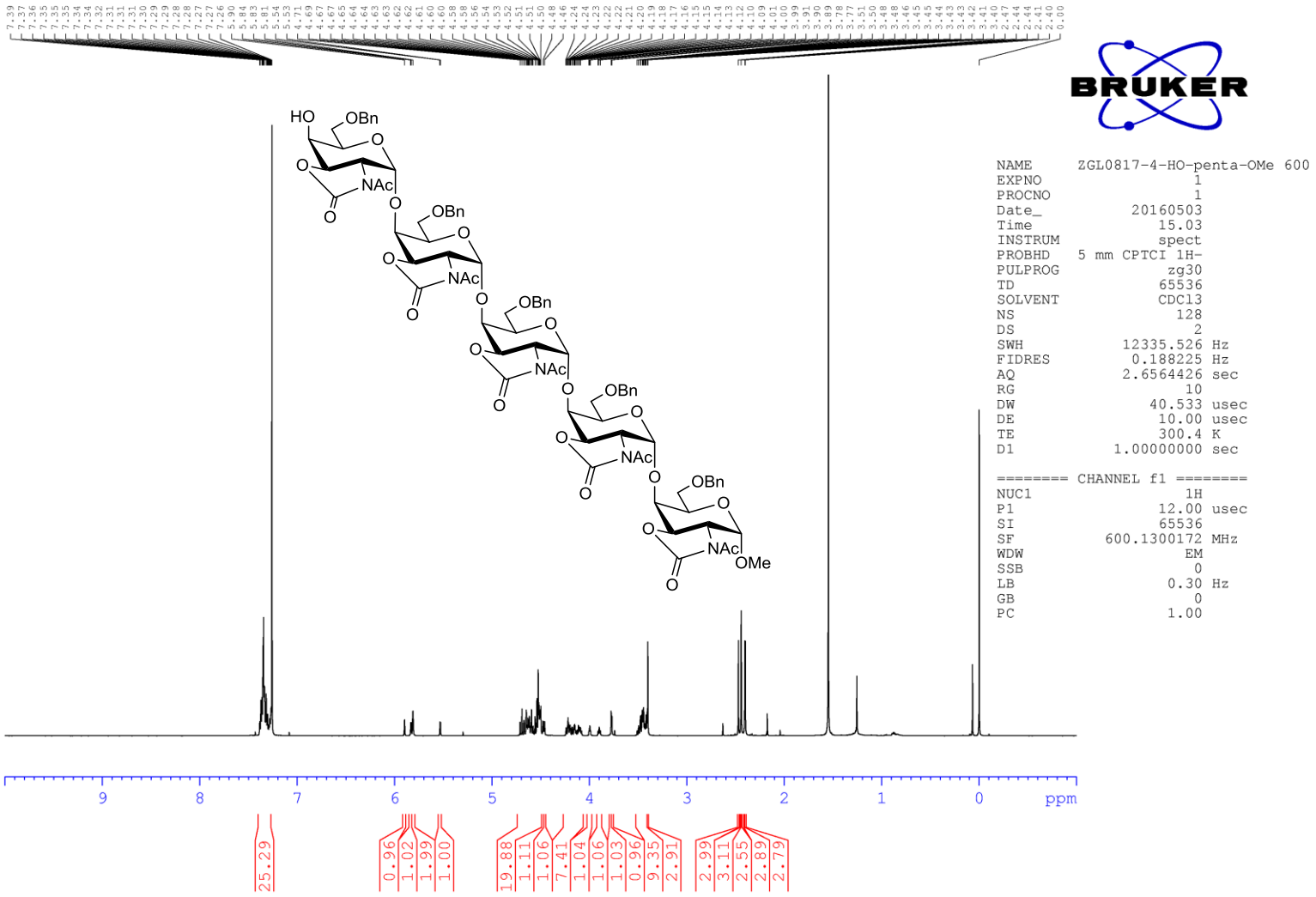
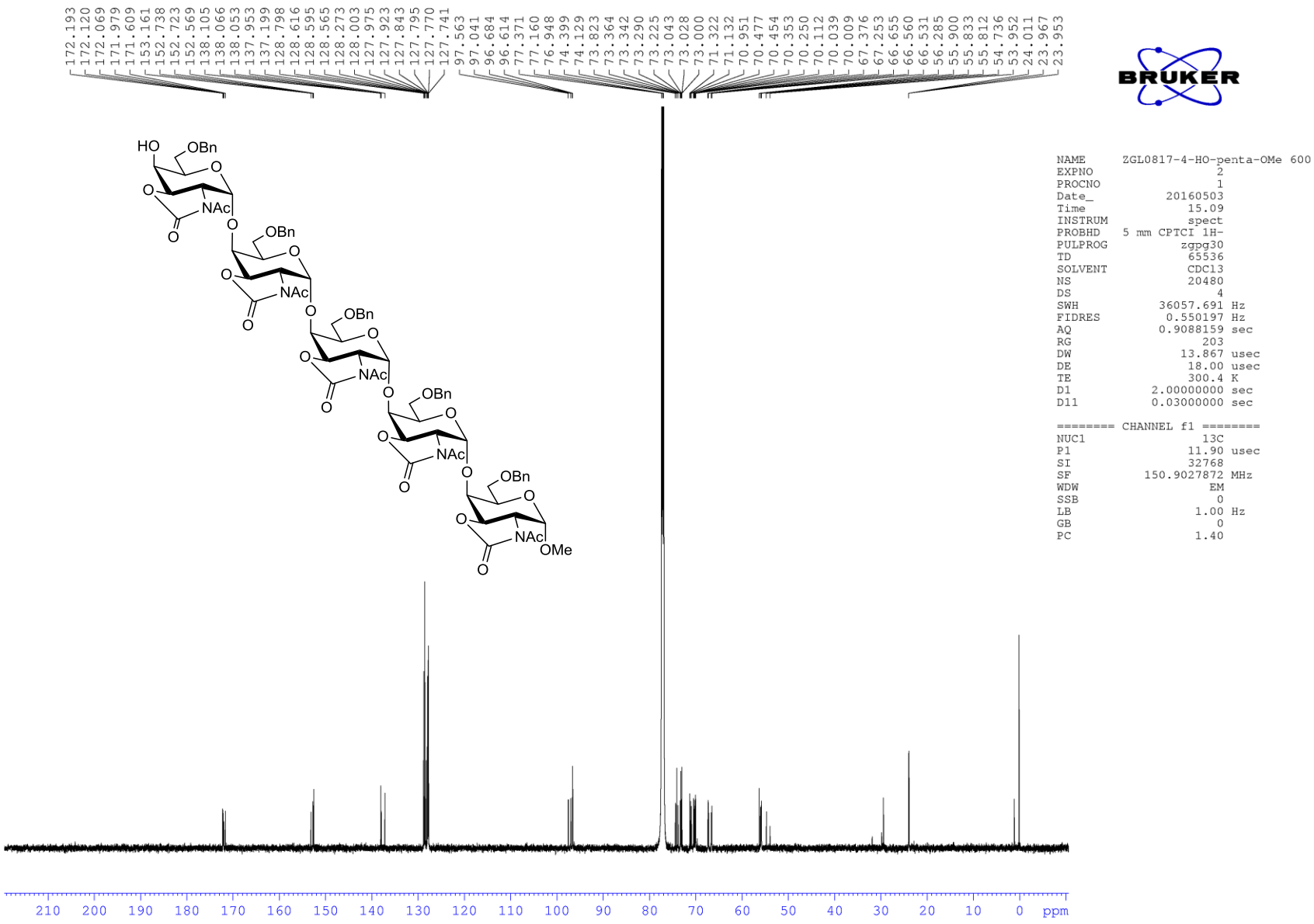
Time                        17.09
INSTRUM                     spect
PROBHD    5 mm CPTCI 1H-
PULPROG              hmbcgpndqf
TD                           2048
SOLVENT                      D2O
NS                            16
DS                            16
SWH                     4006.410 Hz
FIDRES                  1.956255 Hz
AQ                      0.2556404 sec
RG                            203
DW                       124.800 usec
DE                        10.00 usec
TE                         300.4 K
CNST13                  8.0000000
D0                      0.00000300 sec
D1                      1.50000000 sec
D6                      0.06250000 sec
D16                     0.00020000 sec
IN0                     0.00001840 sec

======== CHANNEL f1 ========
NUC1                          1H
P1                        13.10 usec
P2                        26.20 usec
ND0                           2
TD                          512
SFO1                  150.9177 MHz
FIDRES                53.074162 Hz
SW                      180.058 ppm
FnMODE                       QF
SI                          2048
SF                  600.1299507 MHz
WDW                       SINE
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.40
SI                          1024
MC2                          QF
SF                  150.9026765 MHz
WDW                       SINE
SSB                          0
LB                        0.00 Hz
GB                           0
```

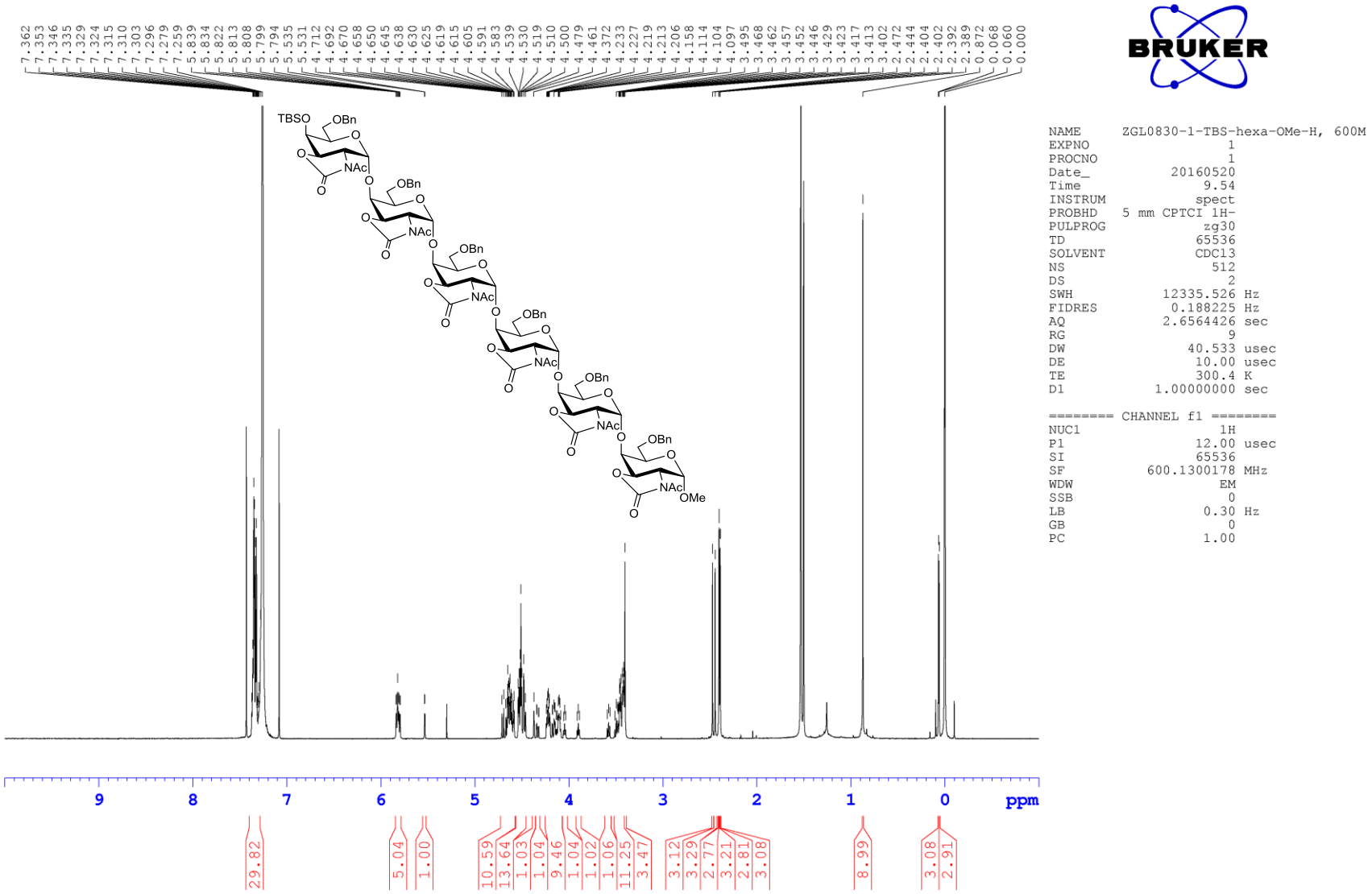
HMBC NMR spectrum of compound **6**



^{1}H NMR spectrum of compound **7**



^{13}C NMR spectrum of compound **7**

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PROCNO               1
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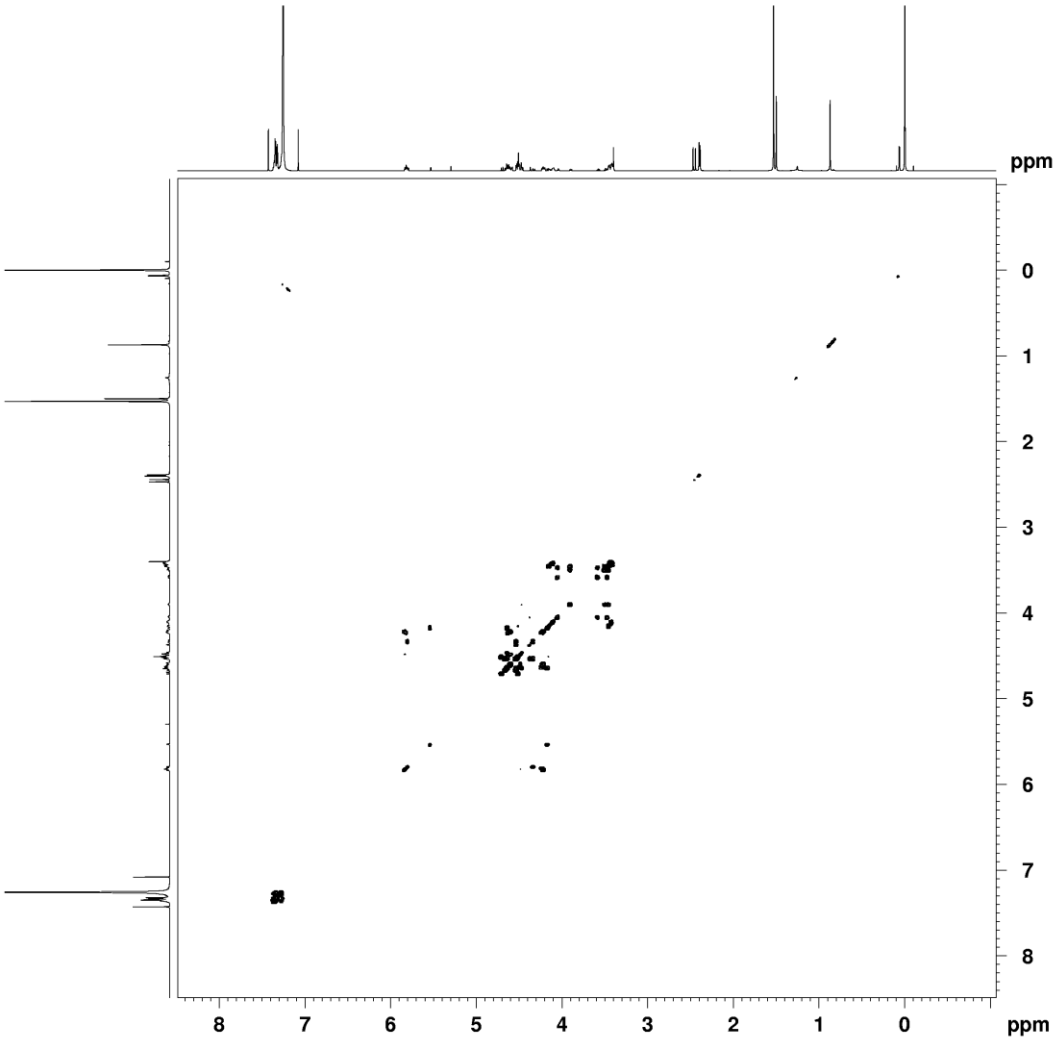
Time              9.54
INSTRUM          spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zg30
TD              65536
SOLVENT         CDCl3
NS                512
DS                  2
SWH         12335.526 Hz
FIDRES        0.188225 Hz
AQ            2.6564426 sec
RG                  9
DW             40.533 usec
DE             10.00 usec
TE              300.4 K
D1          1.00000000 sec

======== CHANNEL f1 ========
NUC1                1H
P1             12.00 usec
SI                65536
SF        600.1300178 MHz
WDW                EM
SSB                 0
LB              0.30 Hz
GB                  0
PC              1.00
```

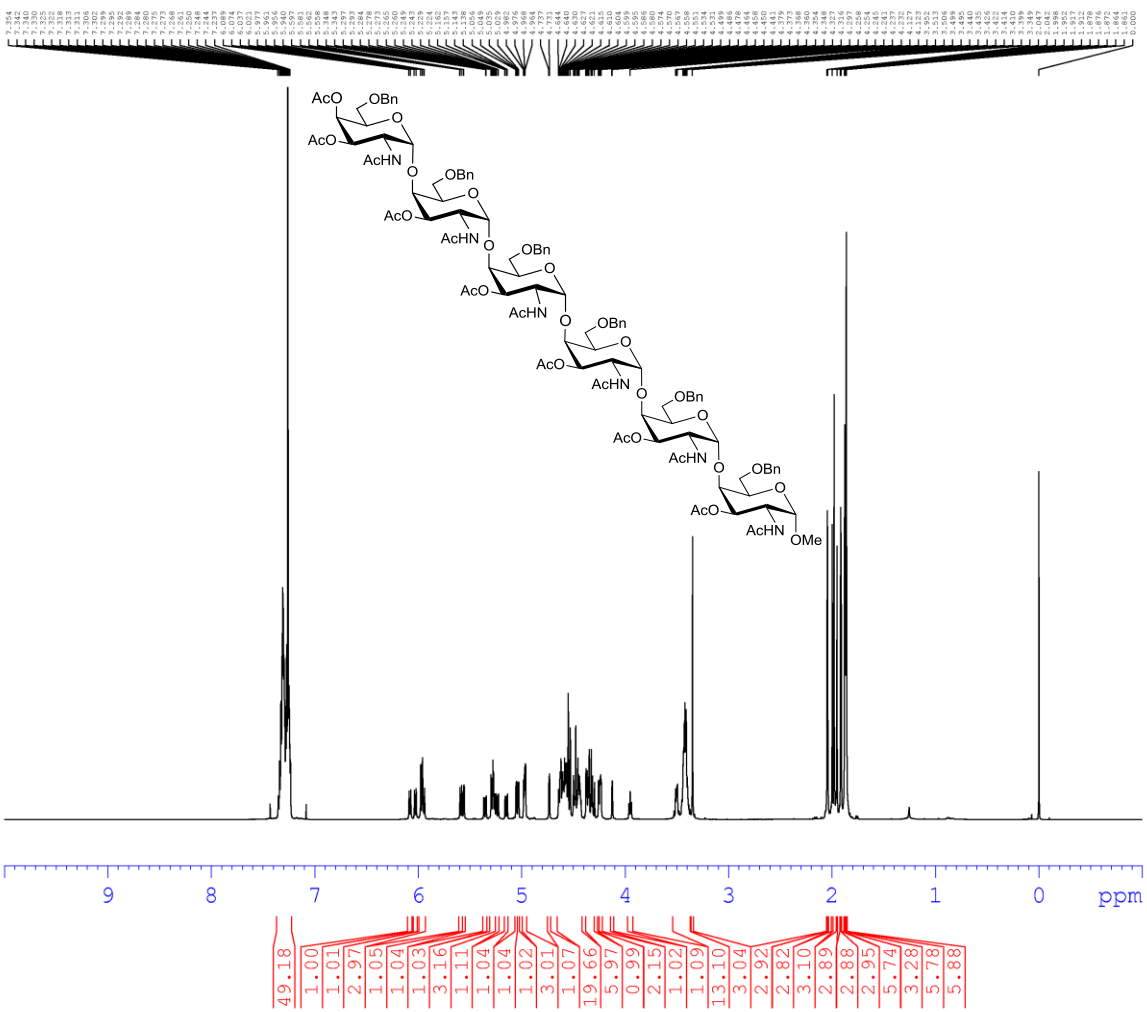
^{1}H NMR spectrum of compound **8**




```
NAME          ZGL0830-1-TBS-hexa-OMe-H, 600M
EXPNO                    3
PROCNO                   1
Date_             20160522
Time                 16.19
INSTRUM              spect
PROBHD     5 mm CPTCI 1H-
PULPROG          cosygpmfqf
TD                    2048
SOLVENT               CDCl3
NS                      16
DS                       8
SWH               5733.945 Hz
FIDRES            2.799778 Hz
AQ               0.1786356 sec
RG                     203
DW                  87.200 usec
DE                  10.00 usec
TE                  300.4 K
D0               0.00000300 sec
D1               2.00000000 sec
D13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00017440 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.00 usec
ND0                      1
TD                    1024
SFO1              600.1322 MHz
FIDRES            5.599528 Hz
SW                   9.554 ppm
FnMODE                  QF
SI                    2048
SF             600.1300167 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.40
SI                    1024
MC2                     QF
SF             600.1300158 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
```

COSY NMR spectrum of compound **8**

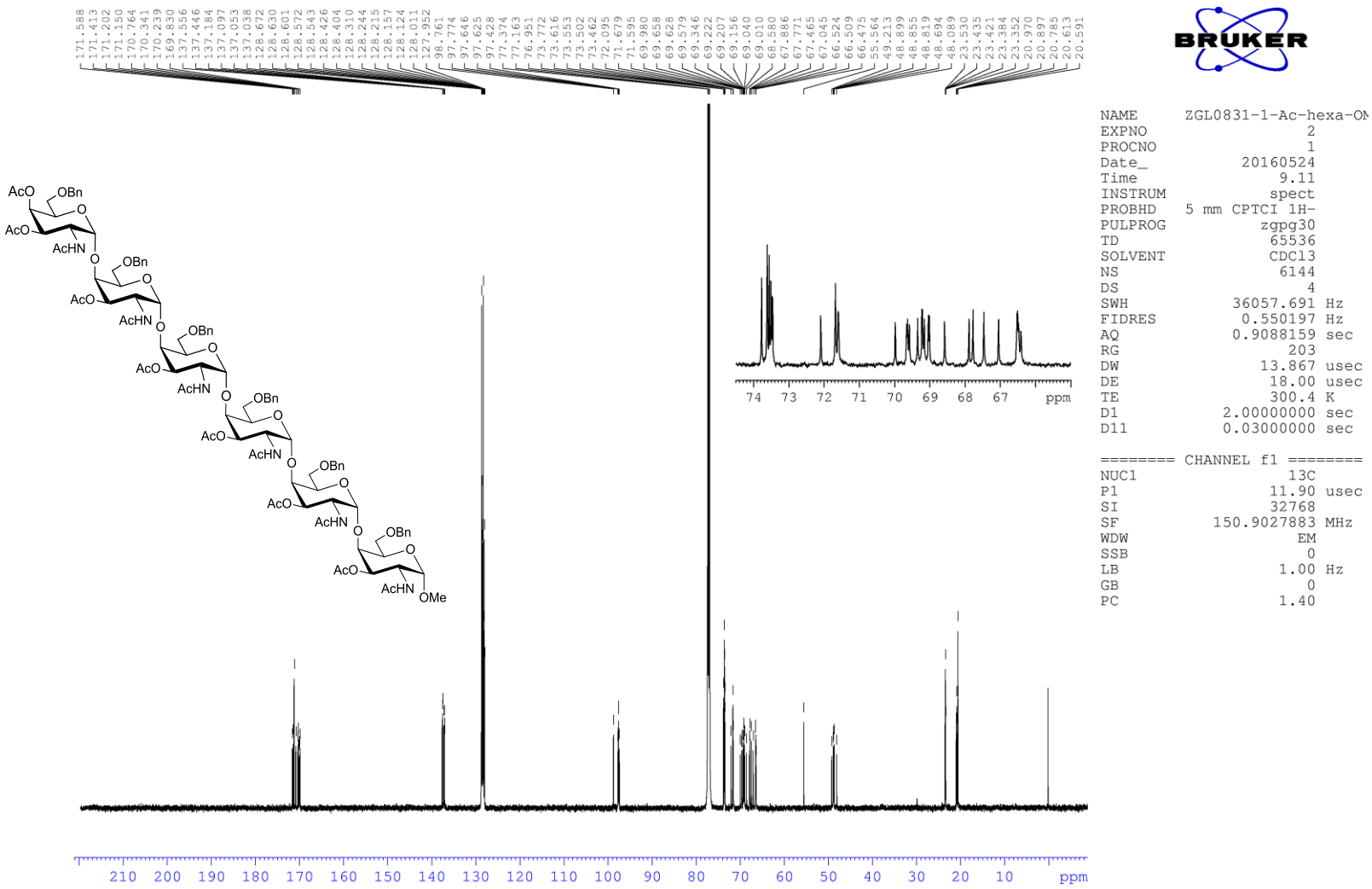


BRUKER

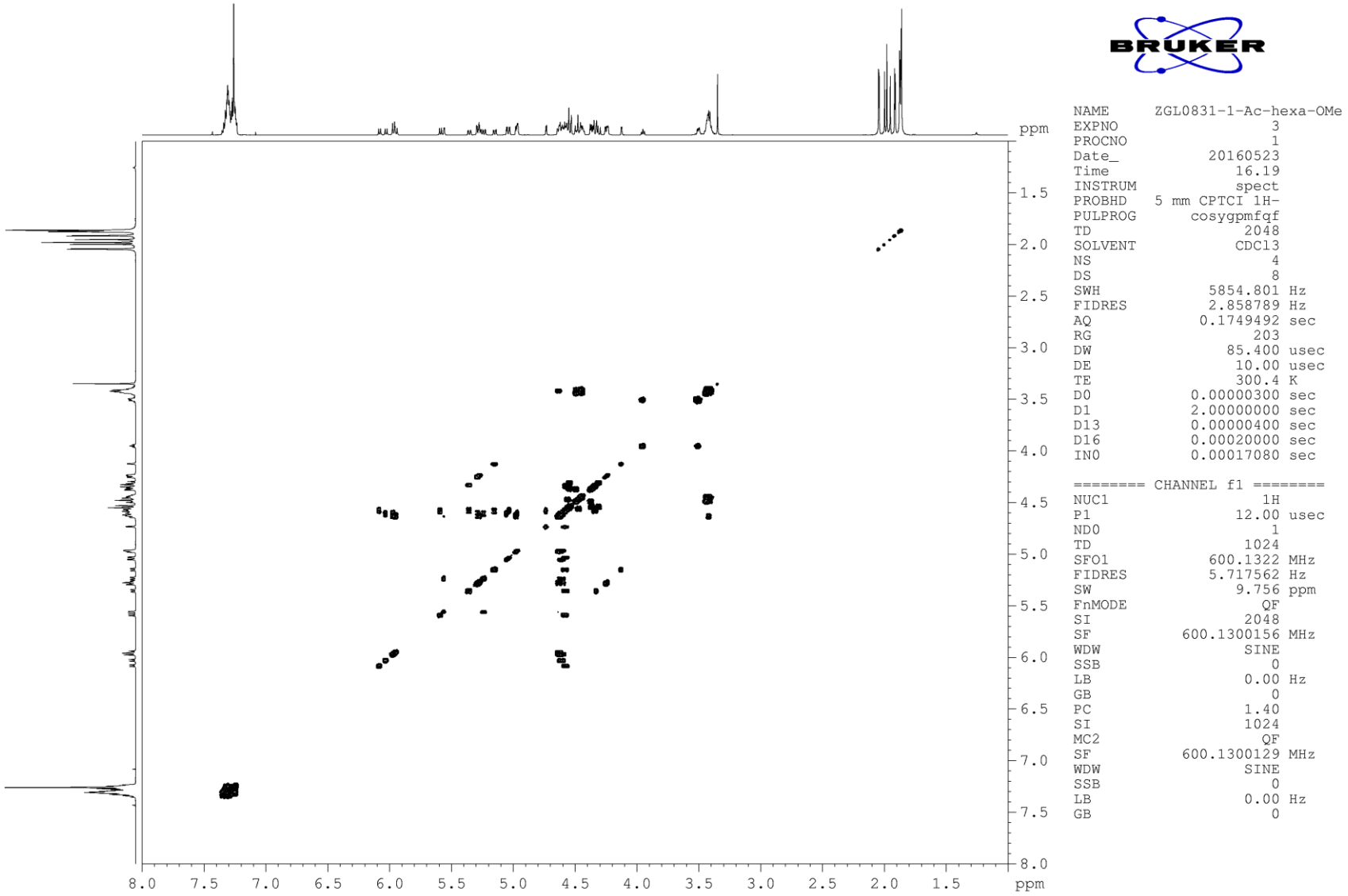
```
NAME        ZGL0831-1-Ac-hexa-OMe
EXPNO                           1
PROCNO                          1
Date_                    20160523
Time                        16.03
INSTRUM                     spect
PROBHD    5 mm CPTCI 1H-
PULPROG                      zg30
TD                          65536
SOLVENT                     CDCl3
NS                            128
DS                              2
SWH                    12335.526 Hz
FIDRES                  0.188225 Hz
AQ                     2.6564426 sec
RG                              8
DW                         40.533 usec
DE                         10.00 usec
TE                         300.4 K
D1                    1.00000000 sec

======== CHANNEL f1 ========
NUC1                           1H
P1                         12.00 usec
SI                          65536
SF                  600.1300166 MHz
WDW                            EM
SSB                             0
LB                           0.30 Hz
GB                              0
PC                           1.00
```

^{1}H NMR spectrum of compound **9**



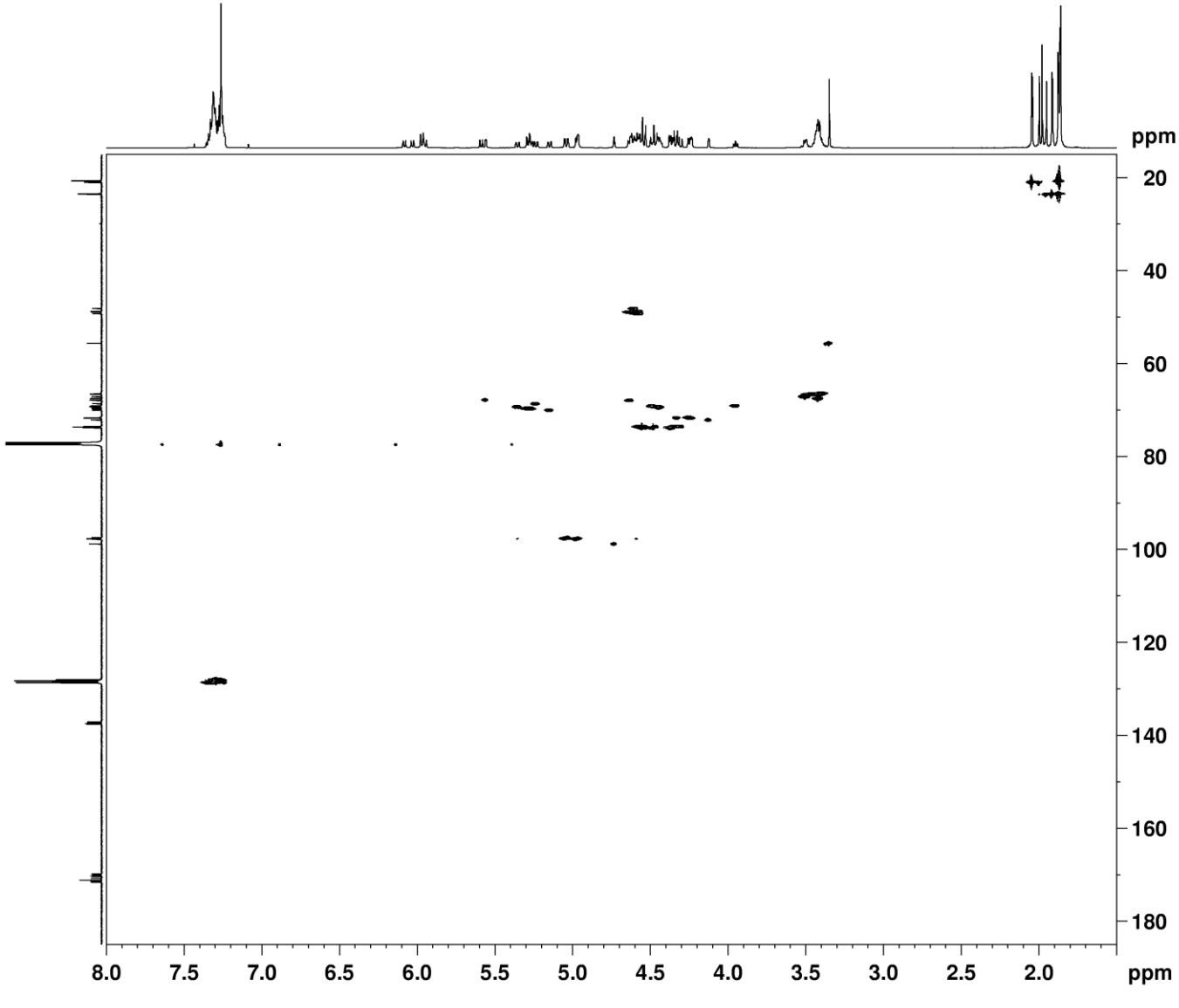
^{13}C NMR spectrum of compound **9**



BRUKER

NAME	ZGL0831-1-Ac-hexa-OMe
EXPNO	3
PROCNO	1
Date_	20160523
Time	16.19
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygpmfqf
TD	2048
SOLVENT	CDCl3
NS	4
DS	8
SWH	5854.801 Hz
FIDRES	2.858789 Hz
AQ	0.1749492 sec
RG	203
DW	85.400 usec
DE	10.00 usec
TE	300.4 K
D0	0.00000300 sec
D1	2.00000000 sec
D13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00017080 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	12.00 usec
ND0	1
TD	1024
SFO1	600.1322 MHz
FIDRES	5.717562 Hz
SW	9.756 ppm
FnMODE	QF
SI	2048
SF	600.1300156 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	600.1300129 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

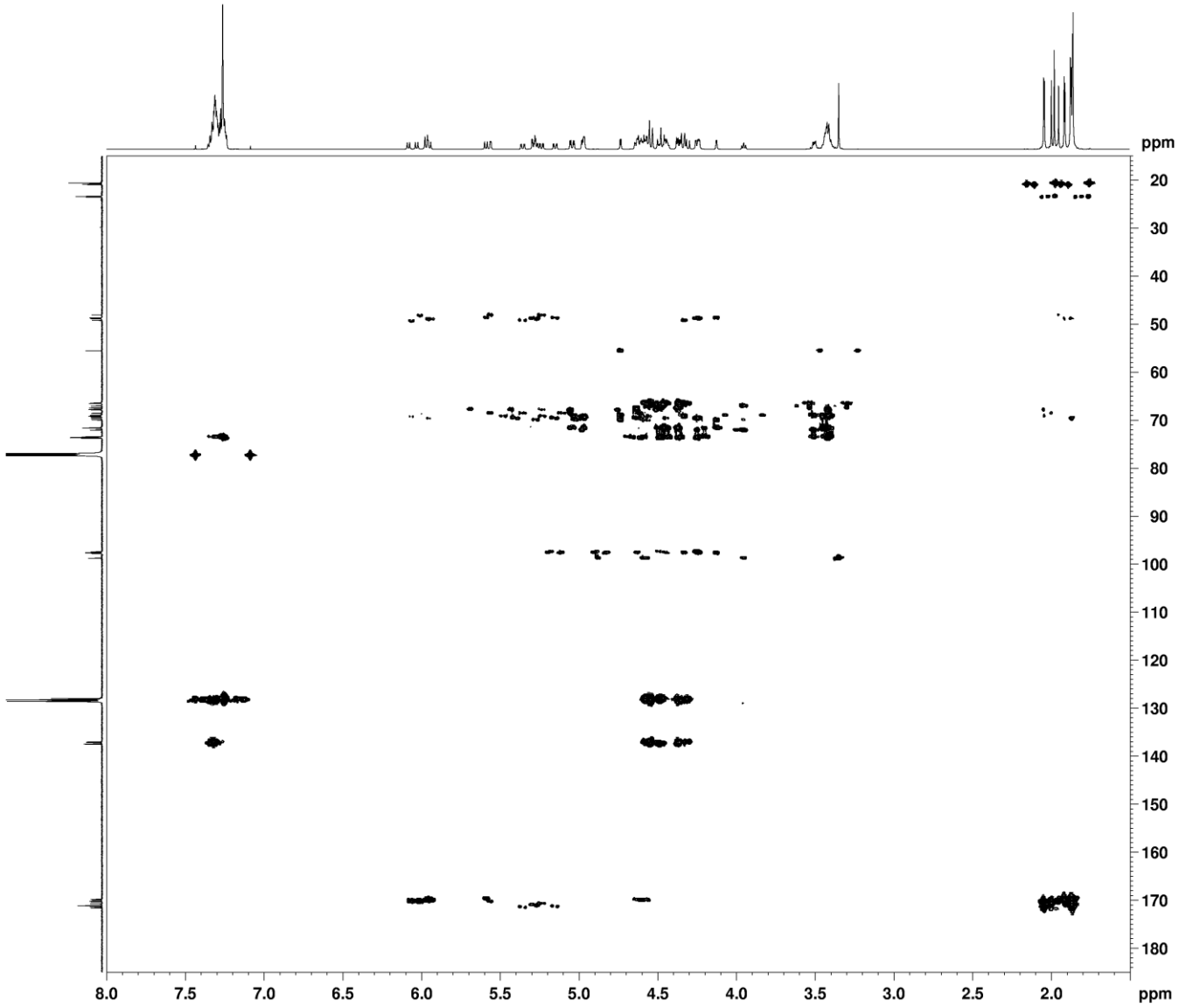
COSY NMR spectrum of compound **9**



BRUKER

NAME	ZGL0831-1-Ac-hexa-OMe
EXPNO	4
PROCNO	1
Date_	20160523
Time	18.56
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	hsqcetgp
TD	2048
SOLVENT	CDCl3
NS	16
DS	16
SWH	5854.801 Hz
FIDRES	2.858789 Hz
AQ	0.1749492 sec
RG	203
DW	85.400 usec
DE	10.00 usec
TE	300.4 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
IN0	0.00002000 sec
ZGOPTNS	
======== CHANNEL f1 ========	
NUC1	1H
P1	12.00 usec
P2	24.00 usec
P28	0.00 usec
ND0	2
TD	512
SFO1	150.9141 MHz
FIDRES	48.822838 Hz
SW	165.639 ppm
FnMODE	Echo-Antiecho
SI	2048
SF	600.1300142 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	150.9027862 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

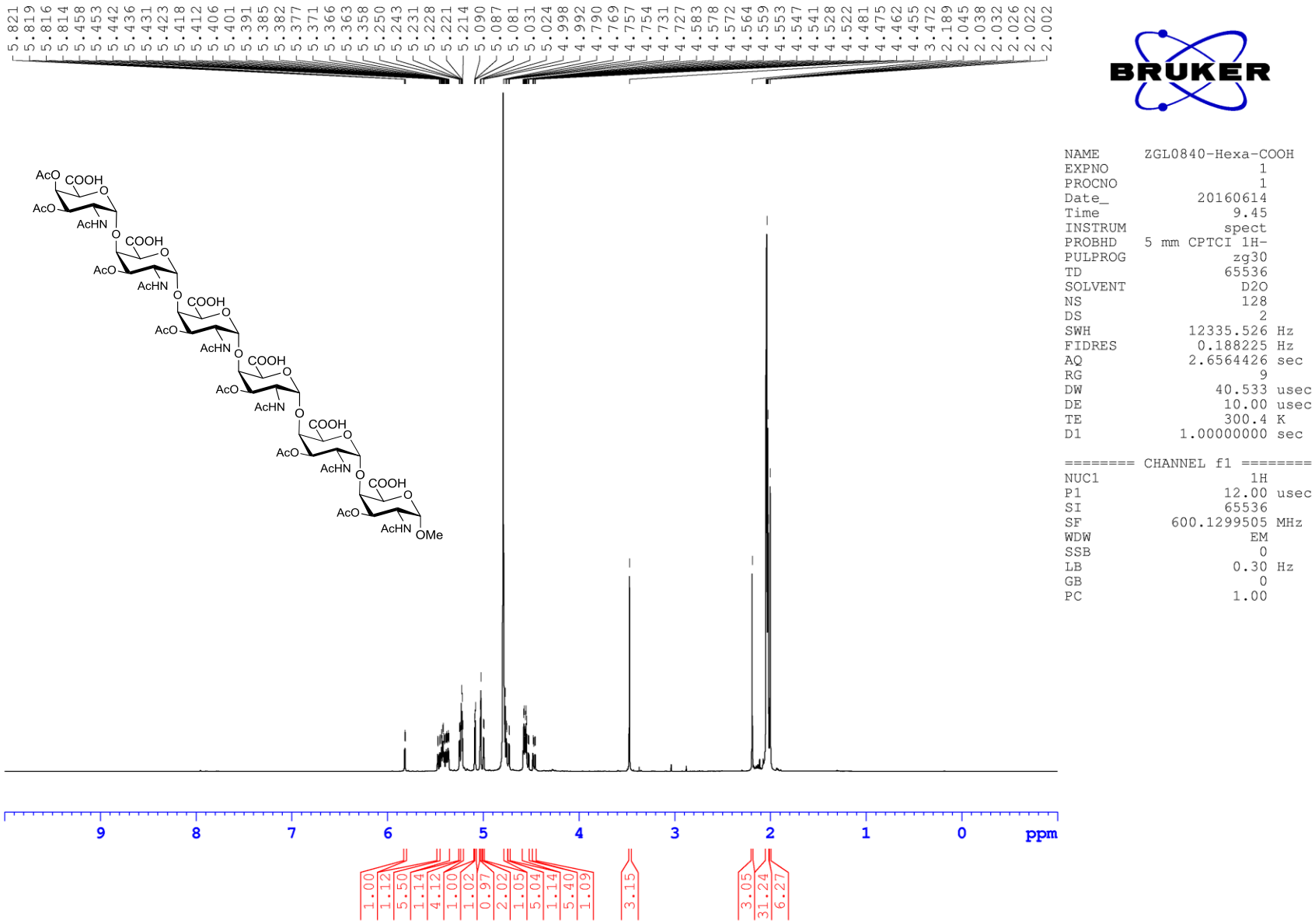
HSQC NMR spectrum of compound **9**



BRUKER

NAME	ZGL0831-1-Ac-hexa-(
EXPNO	5
PROCNO	1
Date_	20160523
Time	22.48
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	hmbcgpndqf
TD	2048
SOLVENT	CDCl3
NS	24
DS	16
SWH	5854.801 Hz
FIDRES	2.858789 Hz
AQ	0.1749492 sec
RG	203
DW	85.400 use(
DE	10.00 use(
TE	300.4 K
CNST13	8.0000000
D0	0.00000300 sec
D1	1.50000000 sec
D6	0.06250000 sec
D16	0.00020000 sec
IN0	0.00001490 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	12.00 use(
P2	24.00 use(
ND0	2
TD	512
SFO1	150.9179 MHz
FIDRES	65.465065 Hz
SW	222.095 ppm
FnMODE	QF
SI	2048
SF	600.1300142 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	150.9028056 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

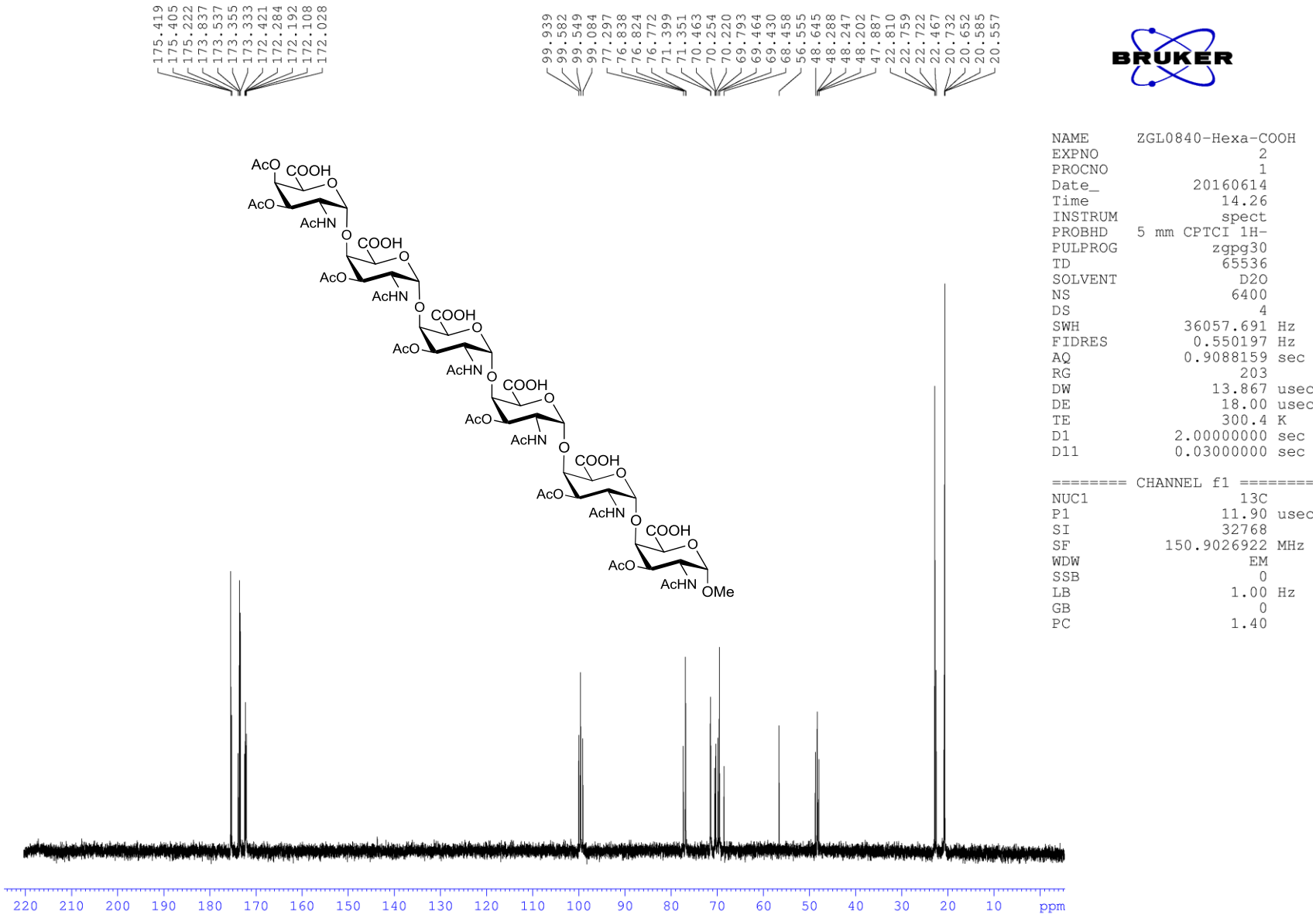
HMBC NMR spectrum of compound **9**



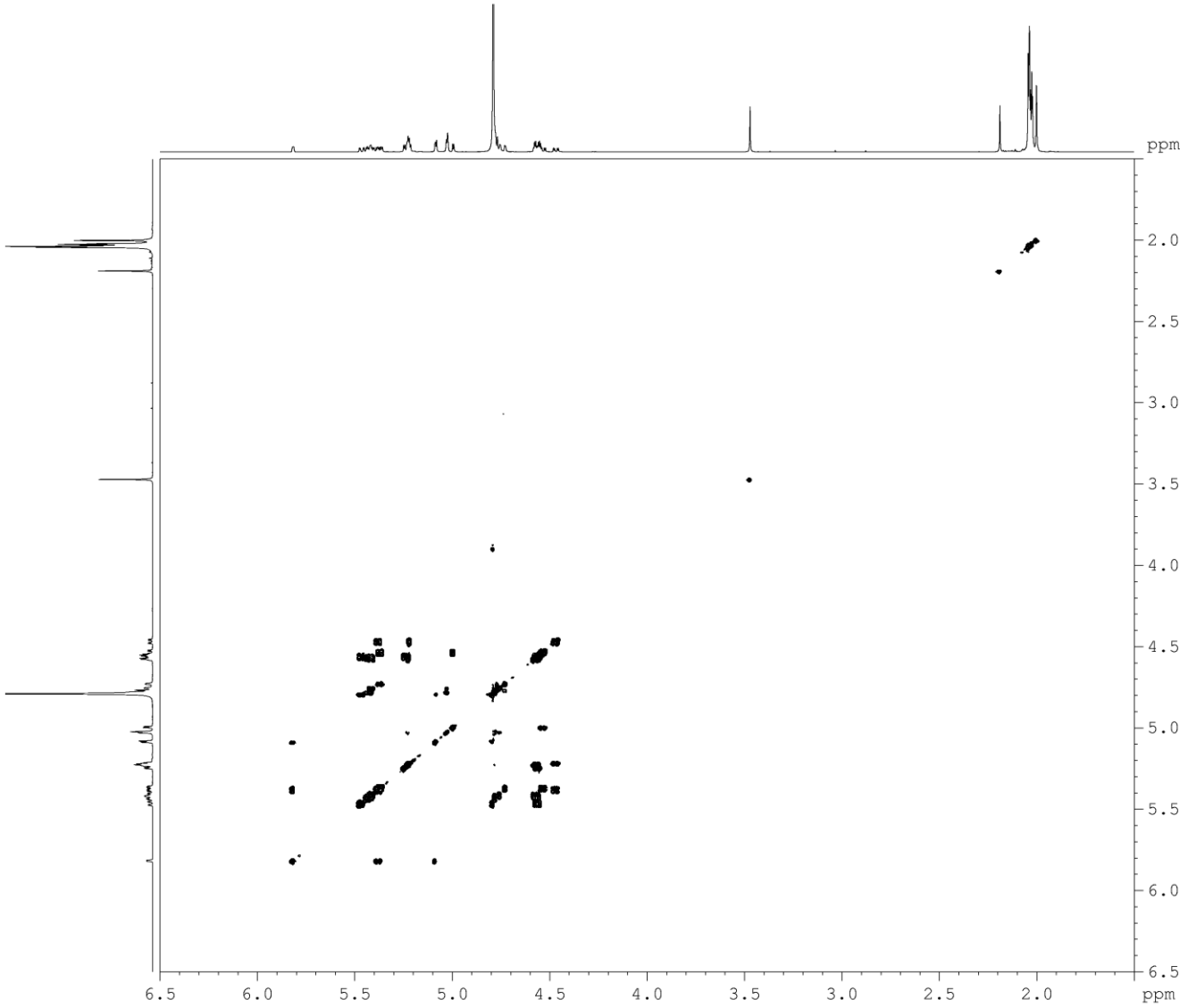

```
NAME      ZGL0840-Hexa-COOH
EXPNO                    1
PROCNO                   1
Date_             20160614
Time                 9.45
INSTRUM             spect
PROBHD   5 mm CPTCI 1H-
PULPROG              zg30
TD                  65536
SOLVENT               D2O
NS                    128
DS                      2
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                      9
DW                 40.533 usec
DE                 10.00 usec
TE                 300.4 K
D1             1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.00 usec
SI                  65536
SF          600.1299505 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```

^{1}H NMR spectrum of compound **10**



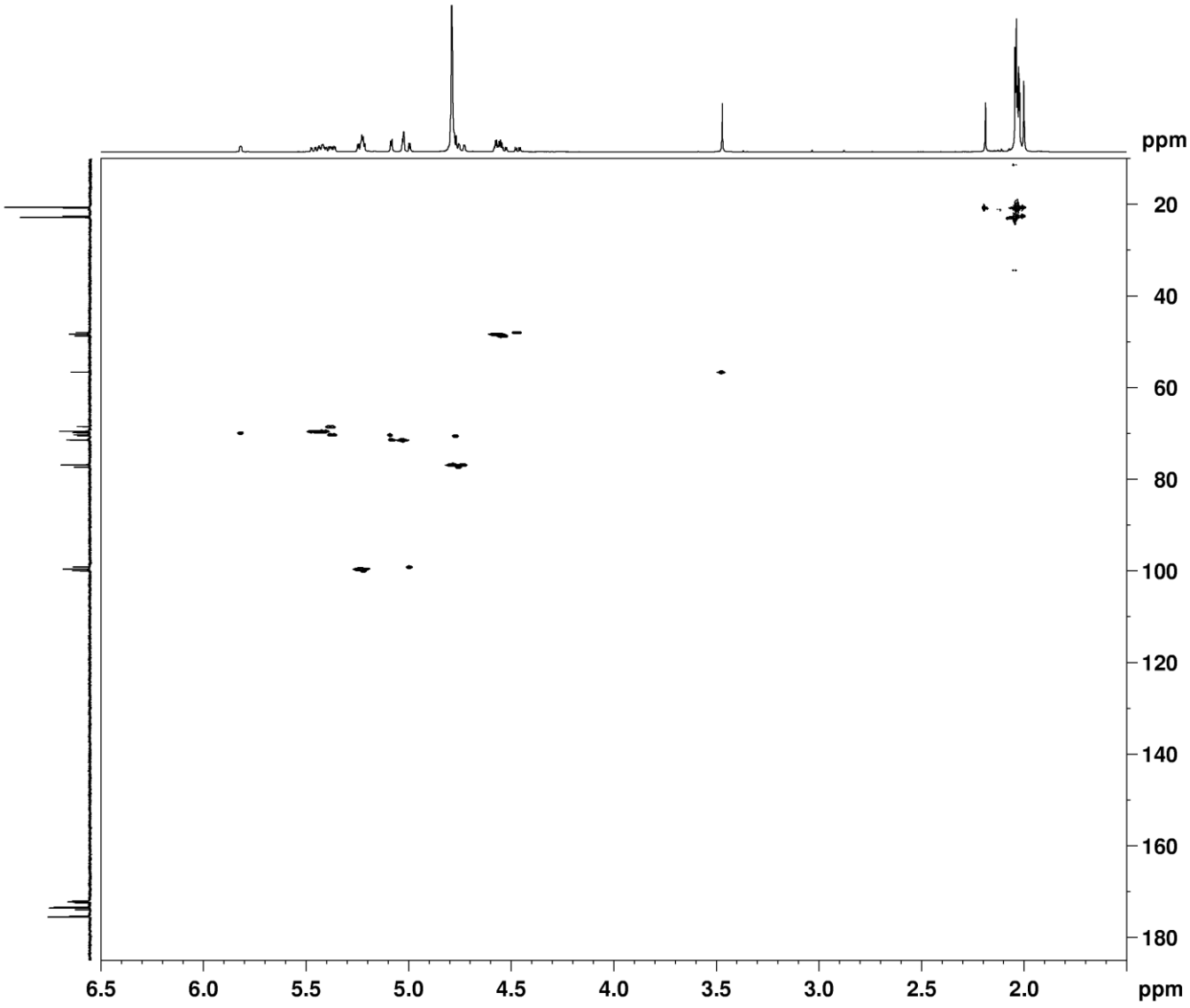
^{13}C NMR spectrum of compound **10**




```
NAME      ZGL0840-Hexa-COOH
EXPNO                    3
PROCNO                   1
Date_             20160614
Time                 9.55
INSTRUM             spect
PROBHD   5 mm CPTCI 1H-
PULPROG       cosygpmfqf
TD                    2048
SOLVENT                D2O
NS                       8
DS                       8
SWH               3765.060 Hz
FIDRES            1.838408 Hz
AQ                0.2720244 sec
RG                     203
DW                 132.800 usec
DE                  10.00 usec
TE                  300.4 K
D0              0.00000300 sec
D1              2.00000000 sec
D13             0.00000400 sec
D16             0.00020000 sec
IN0             0.00026560 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.50 usec
ND0                      1
TD                     512
SFO1             600.1323 MHz
FIDRES             7.353629 Hz
SW                    6.274 ppm
FnMODE                  QF
SI                    2048
SF            600.1299502 MHz
WDW                  SINE
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                    1024
MC2                     QF
SF            600.1299483 MHz
WDW                  SINE
SSB                     0
LB                   0.00 Hz
GB                      0
```

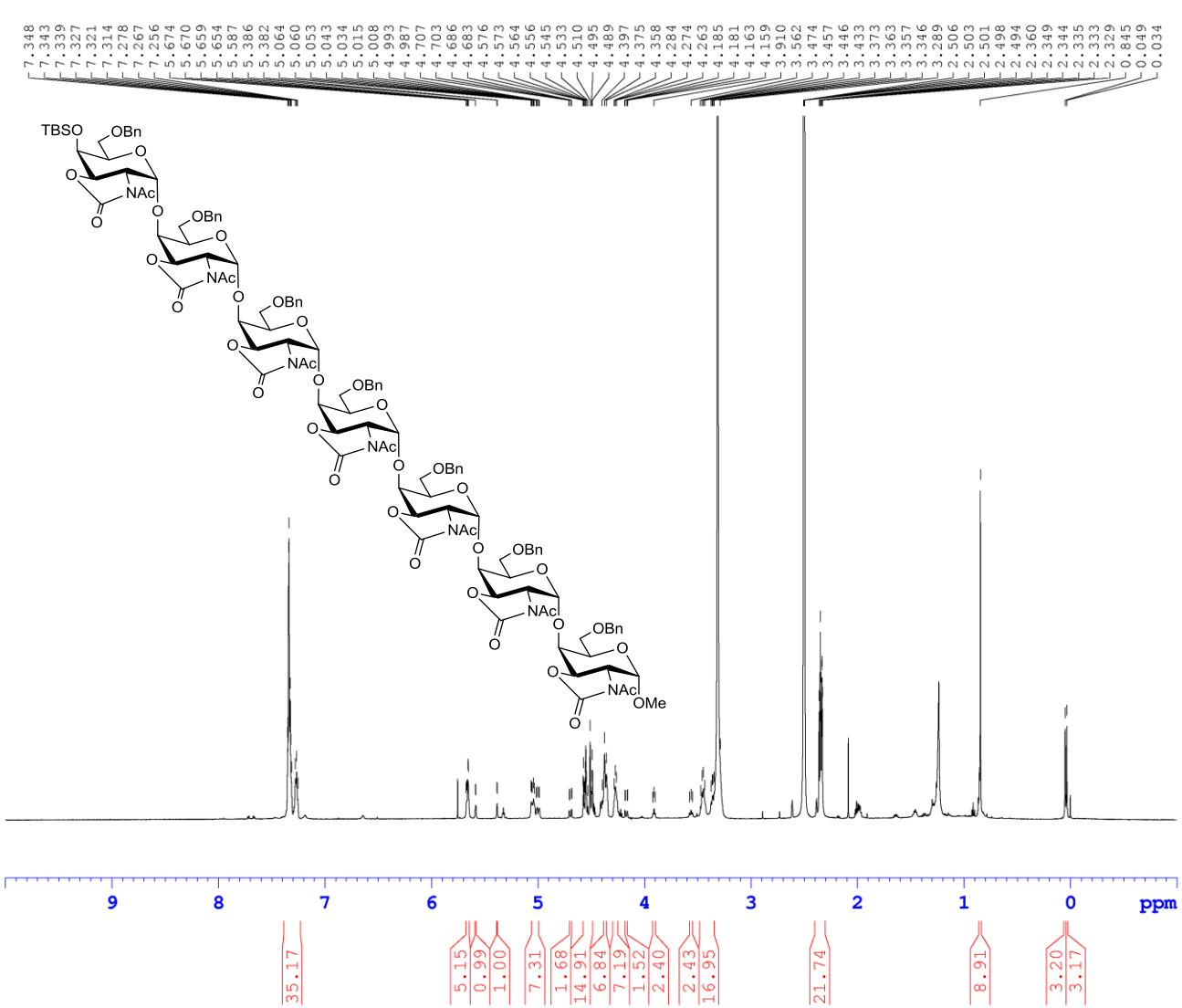
COSY NMR spectrum of compound **10**




```
NAME        ZGL0840-Hexa-COOH
EXPNO                       4
PROCNO                      1
Date_                20160615
Time                     2.21
INSTRUM                 spect
PROBHD    5 mm CPTCI 1H-
PULPROG              hsqcetgp
TD                       2048
SOLVENT                   D2O
NS                         16
DS                         16
SWH                  3765.060 Hz
FIDRES               1.838408 Hz
AQ                   0.2720244 sec
RG                         203
DW                     132.800 usec
DE                      10.00 usec
TE                      300.4 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
IN0                  0.00002000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                        1H
P1                      12.50 usec
P2                      25.00 usec
P28                      0.00 usec
ND0                         2
TD                        512
SFO1                 150.9141 MHz
FIDRES                48.822838 Hz
SW                     165.639 ppm
FnMODE          Echo-Antiecho
SI                       2048
SF                 600.1299492 MHz
WDW                      QSINE
SSB                         2
LB                       0.00 Hz
GB                          0
PC                       1.40
SI                       1024
MC2              echo-antiecho
SF                 150.9026841 MHz
WDW                      QSINE
SSB                         2
LB                       0.00 Hz
GB                          0
```

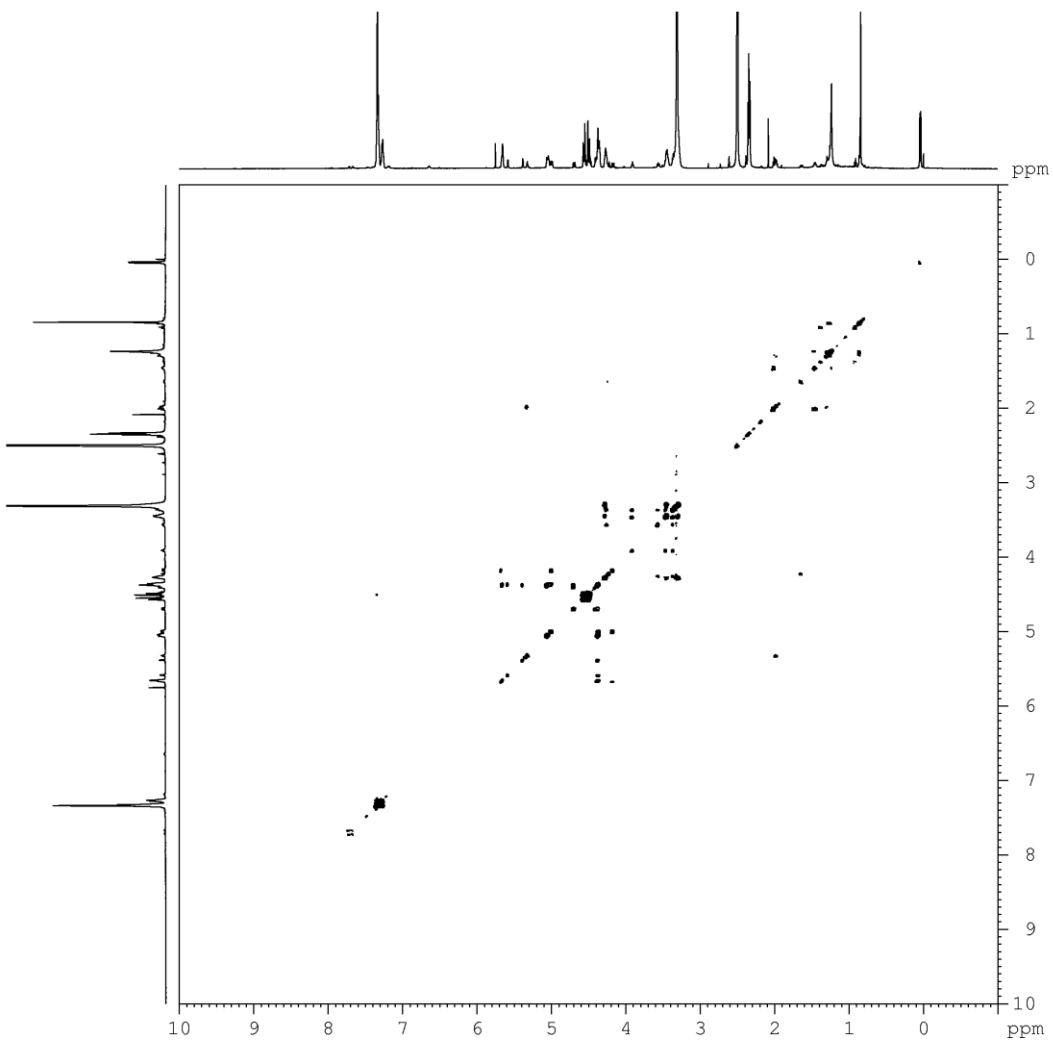
HSQC NMR spectrum of compound **10**




```
NAME            ZGL0899d
EXPNO                  1
PROCNO                 1
Date_           20170510
Time               16.11
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                   128
DS                     2
SWH          12335.526 Hz
FIDRES        0.188225 Hz
AQ           2.6564426 sec
RG                  11.3
DW                40.533 usec
DE                10.00 usec
TE                300.4 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                12.00 usec
SI                65536
SF          600.1300073 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

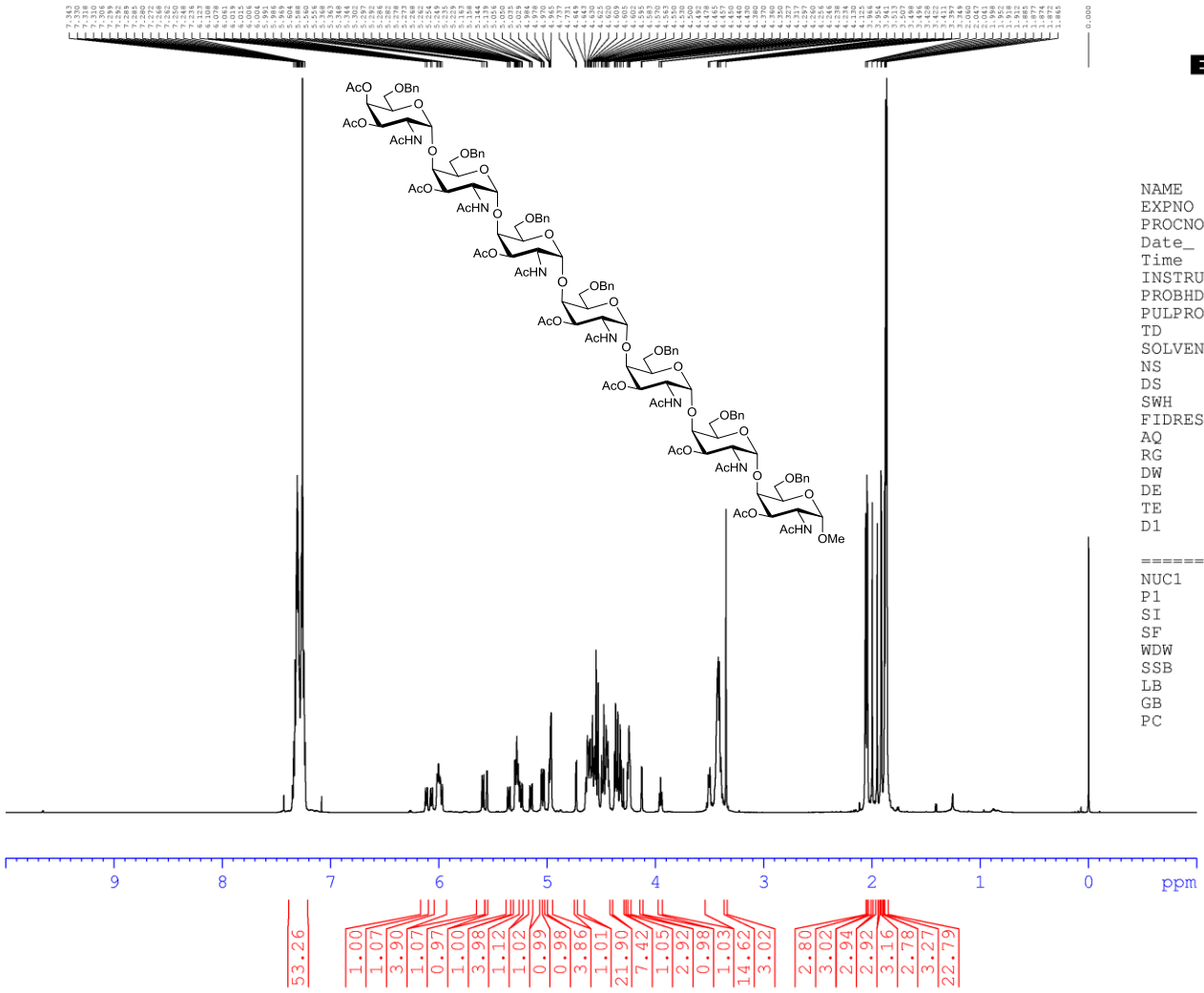
^{1}H NMR spectrum of compound **11**




```
NAME                ZGL0899d
EXPNO                      2
PROCNO                     1
Date_               20170512
Time                   11.00
INSTRUM                spect
PROBHD    5 mm CPTCI 1H-
PULPROG         cosygpmfqf
TD                      2048
SOLVENT                 DMSO
NS                         8
DS                         8
SWH                5102.041 Hz
FIDRES             2.491231 Hz
AQ                 0.2007540 sec
RG                       203
DW                    98.000 usec
DE                    10.00 usec
TE                    300.4 K
D0                 0.00000300 sec
D1                 2.00000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00019600 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                    12.60 usec
ND0                        1
TD                       512
SFO1               600.1323 MHz
FIDRES             9.964913 Hz
SW                    8.502 ppm
FnMODE                    QF
SI                       2048
SF              600.1300066 MHz
WDW                     SINE
SSB                        0
LB                    0.00 Hz
GB                         0
PC                     1.40
SI                     1024
MC2                       QF
SF              600.1300037 MHz
WDW                     SINE
SSB                        0
LB                    0.00 Hz
```

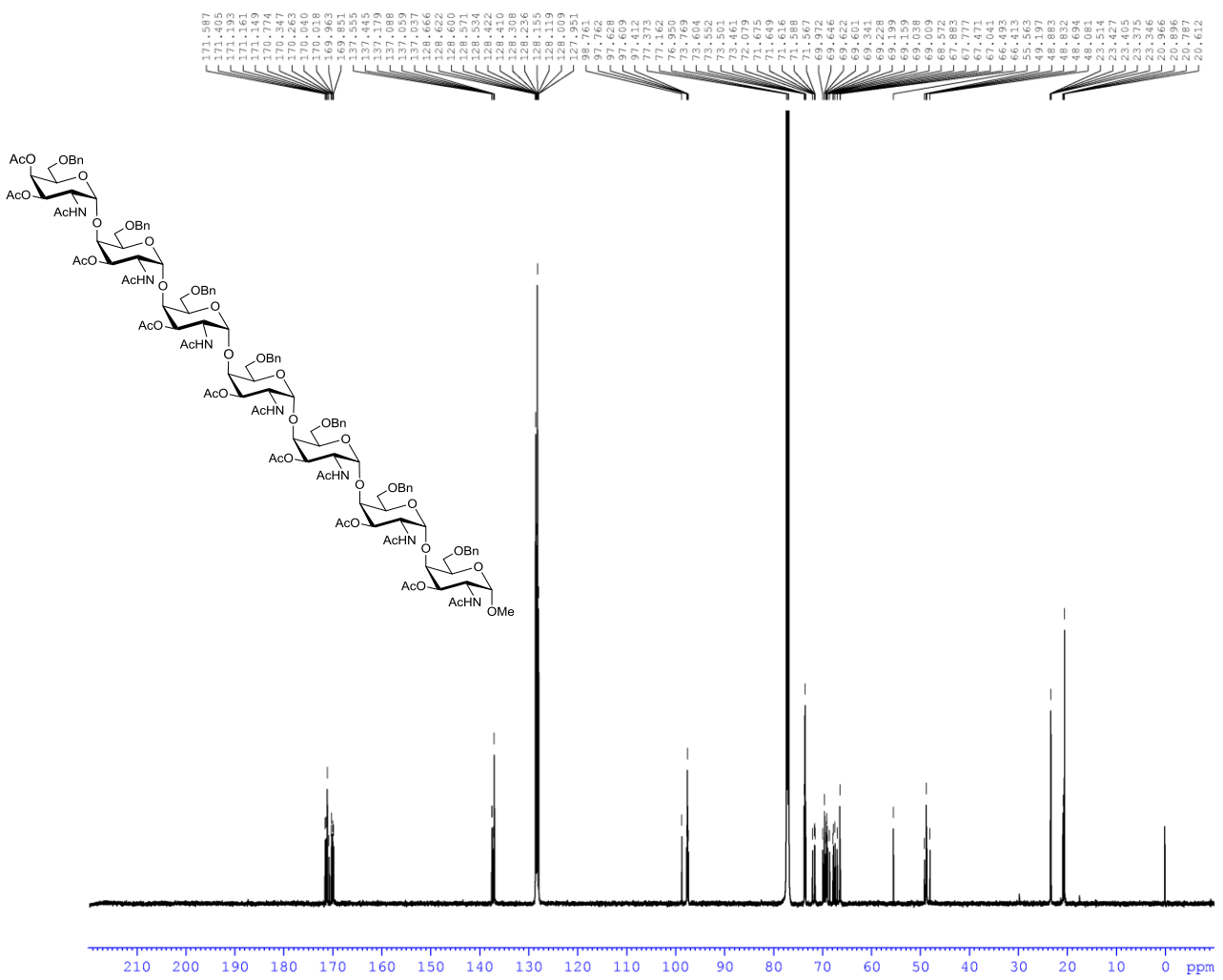
COSY NMR spectrum of compound **11**




```
NAME      ZGL0853a-Ac-hepta-OMe
EXPNO                 1
PROCNO                1
Date_          20160626
Time               6.58
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   64
DS                    2
SWH           12335.526 Hz
FIDRES         0.188225 Hz
AQ            2.6564426 sec
RG                    9
DW               40.533 usec
DE                10.00 usec
TE                300.4 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                12.00 usec
SI                65536
SF          600.1300161 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

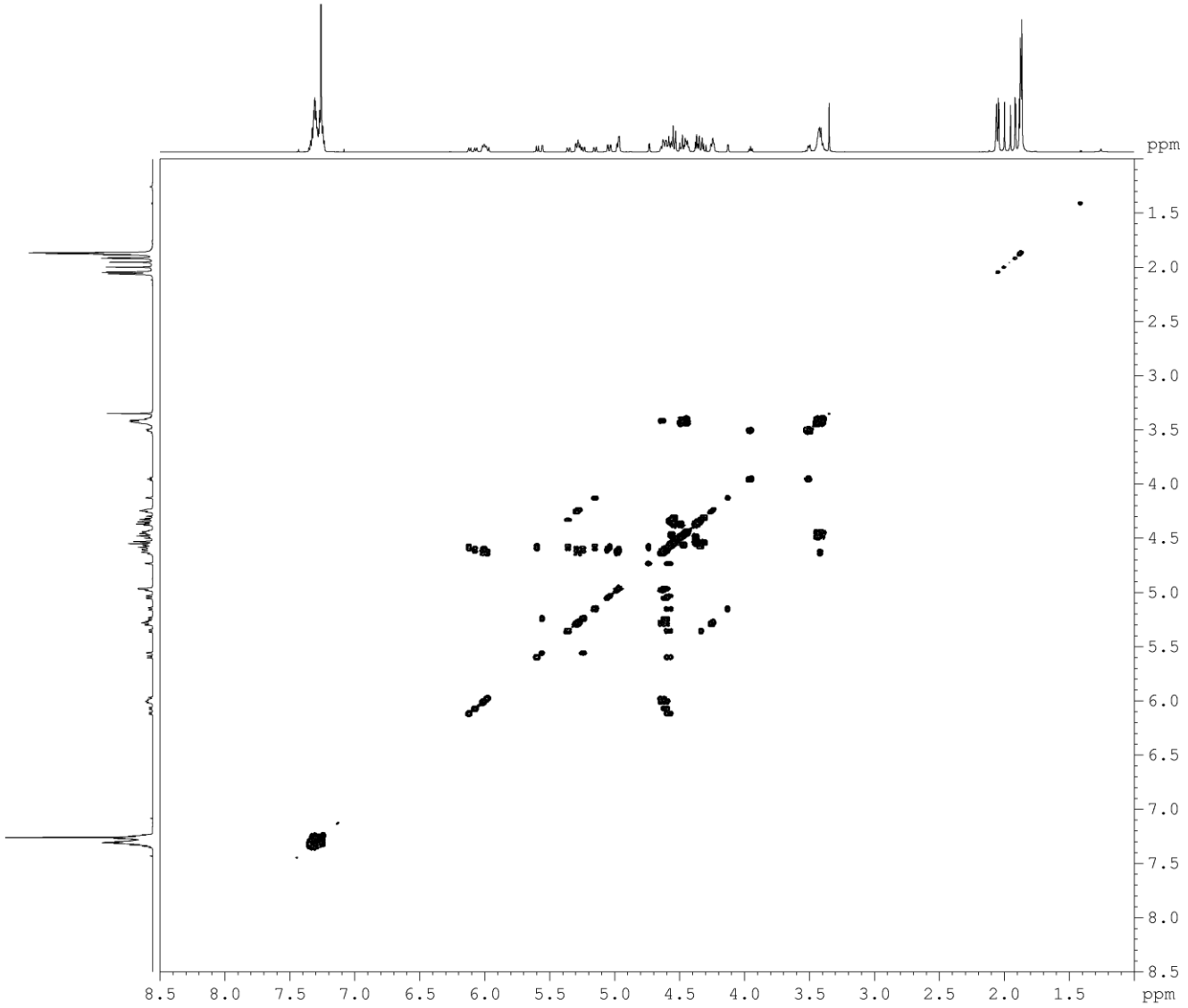
^{1}H NMR spectrum of compound **12**



BRUKER

NAME	ZGL0853a-Ac-hepta-OM
EXPNO	2
PROCNO	1
Date_	20160627
Time	10.58
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	9440
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	203
DW	13.867 usec
DE	18.00 usec
TE	300.4 K
D1	2.00000000 sec
D11	0.03000000 sec
======== CHANNEL f1 ========	
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9027885 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

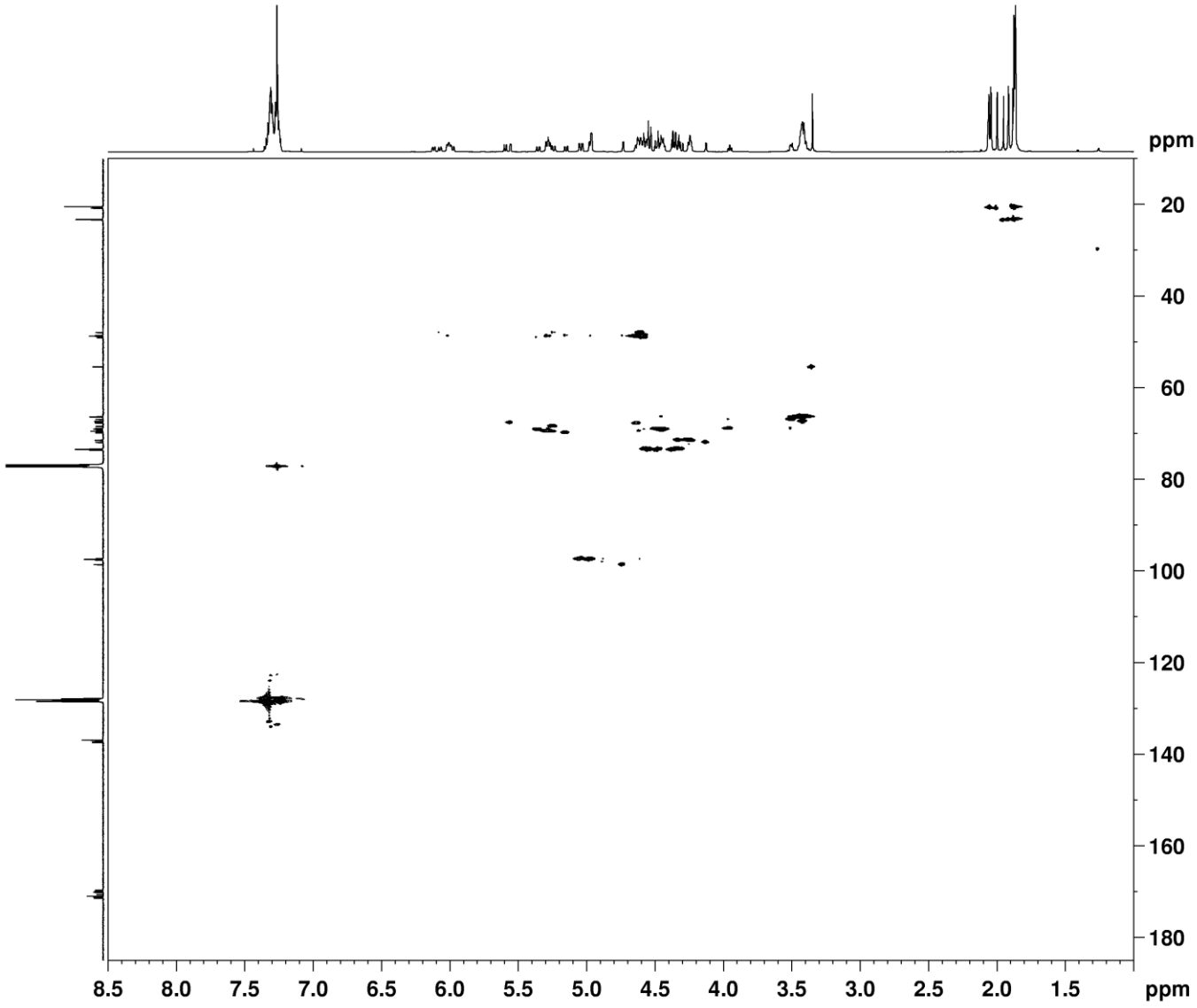
^{13}C NMR spectrum of compound **12**




```
NAME          ZGL0853a-Ac-hepta-OMe
EXPNO                             3
PROCNO                            1
Date_                      20160626
Time                          12.47
INSTRUM                       spect
PROBHD       5 mm CPTCI 1H-
PULPROG             cosygpmfqf
TD                             2048
SOLVENT                     CDCl3
NS                                4
DS                                8
SWH                    6775.068 Hz
FIDRES                 3.308139 Hz
AQ                     0.1511924 sec
RG                              203
DW                        73.800 usec
DE                        10.00 usec
TE                        300.4 K
D0                     0.00000300 sec
D1                     2.00000000 sec
D13                    0.00000400 sec
D16                    0.00020000 sec
IN0                    0.00014760 sec

======== CHANNEL f1 ========
NUC1                          1H
P1                        12.00 usec
ND0                               1
TD                             1024
SFO1                   600.1329 MHz
FIDRES                 6.616297 Hz
SW                       11.289 ppm
FnMODE                         QF
SI                             2048
SF                  600.1300146 MHz
WDW                         SINE
SSB                               0
LB                        0.00 Hz
GB                                0
PC                             1.40
SI                             1024
MC2                            QF
SF                  600.1300143 MHz
WDW                         SINE
SSB                               0
LB                        0.00 Hz
GB                                0
```

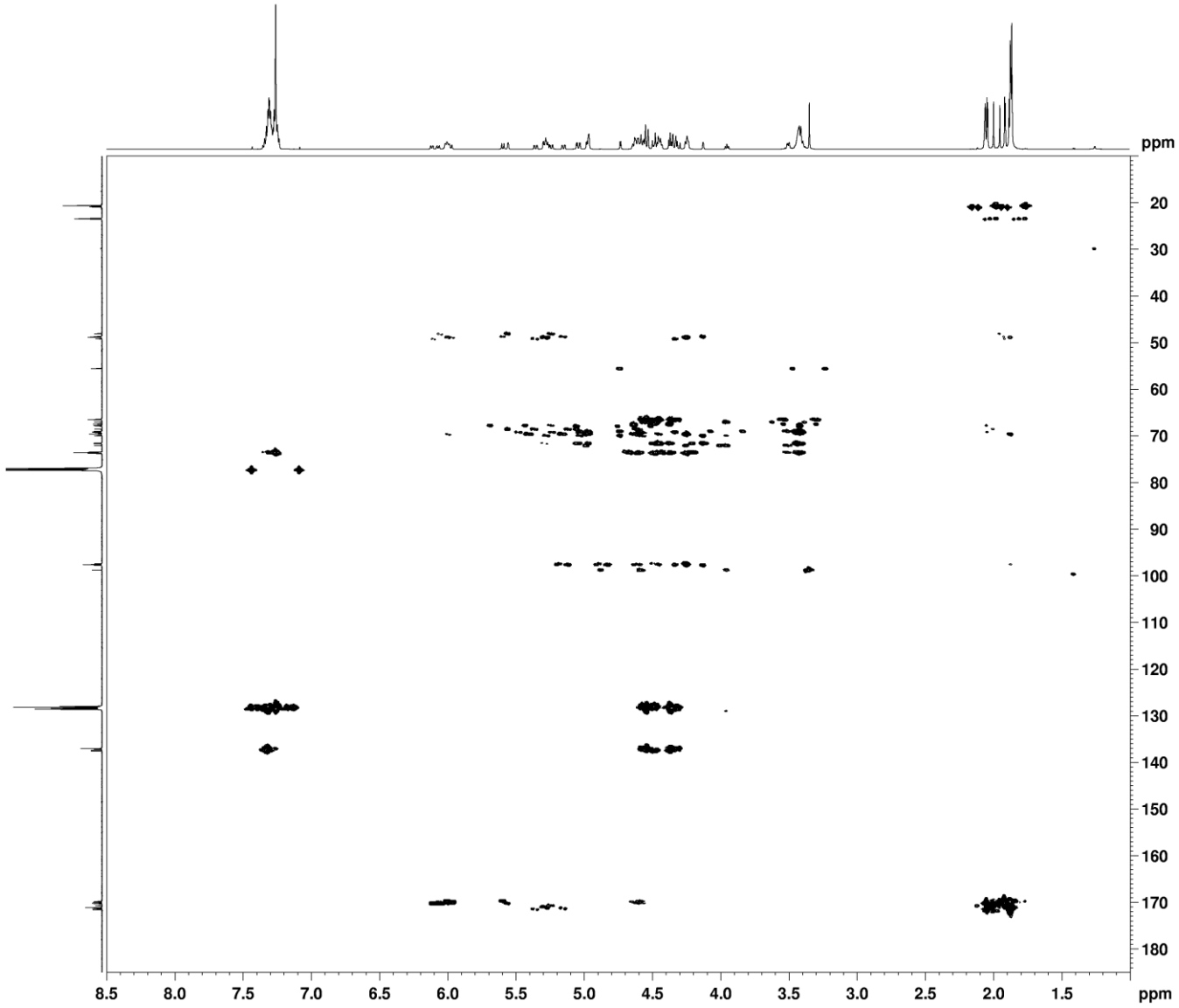
COSY NMR spectrum of compound **12**




```
NAME      ZGL0853a-Ac-hepta-OMe
EXPNO                         4
PROCNO                        1
Date_                  20160626
Time                       7.04
INSTRUM                  spect
PROBHD    5 mm CPTCI 1H-
PULPROG       hsqcetgpsi
TD                         2048
SOLVENT                  CDCl3
NS                           24
DS                           16
SWH                   6775.068 Hz
FIDRES                3.308139 Hz
AQ                    0.1511924 sec
RG                           203
DW                       73.800 usec
DE                       10.00 usec
TE                       300.4 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                   0.00002000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                         1H
P1                       12.00 usec
P2                       24.00 usec
P28                       0.00 usec
ND0                          2
TD                         512
SFO1                  150.9141 MHz
FIDRES                48.822838 Hz
SW                     165.639 ppm
FnMODE     Echo-Antiecho
SI                        2048
SF                  600.1300134 MHz
WDW                      QSINE
SSB                          2
LB                        0.00 Hz
GB                           0
PC                        1.40
SI                        1024
MC2               echo-antiecho
SF                  150.9028094 MHz
WDW                      QSINE
SSB                          2
LB                        0.00 Hz
GB                           0
```

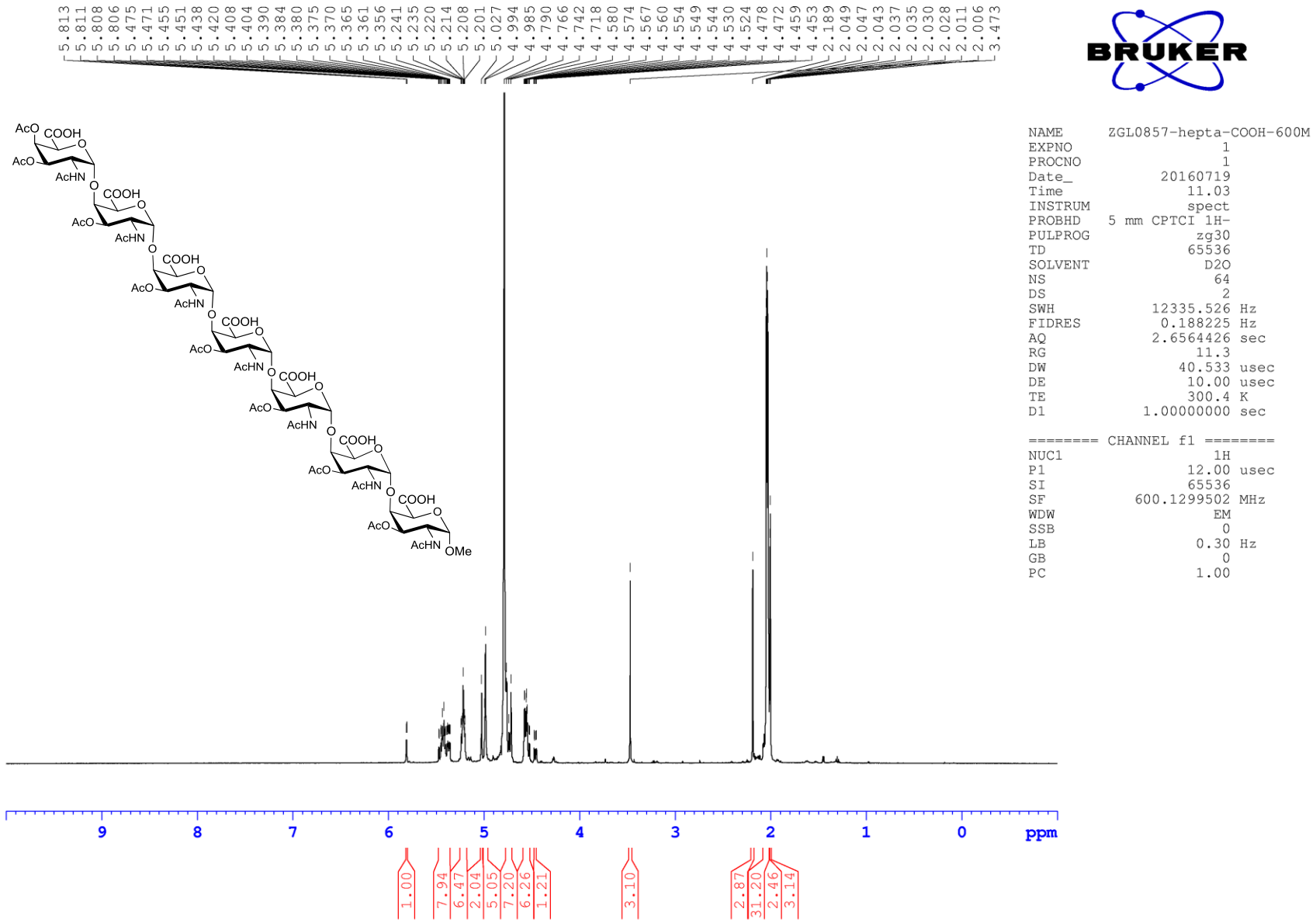
HSQC NMR spectrum of compound **12**



BRUKER

NAME	ZGL0853a-Ac-hepta-OM
EXPNO	5
PROCNO	1
Date_	20160626
Time	15.20
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	hmbcgpndqf
TD	2048
SOLVENT	CDCl3
NS	24
DS	16
SWH	6775.068 Hz
FIDRES	3.308139 Hz
AQ	0.1511924 sec
RG	203
DW	73.800 usec
DE	10.00 usec
TE	300.4 K
CNST13	8.0000000
D0	0.00000300 sec
D1	1.50000000 sec
D6	0.06250000 sec
D16	0.00020000 sec
IN0	0.00001490 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	12.00 usec
P2	24.00 usec
ND0	2
TD	1024
SFO1	150.9179 MHz
FIDRES	32.732533 Hz
SW	222.095 ppm
FnMODE	QF
SI	2048
SF	600.1300143 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	150.9027958 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

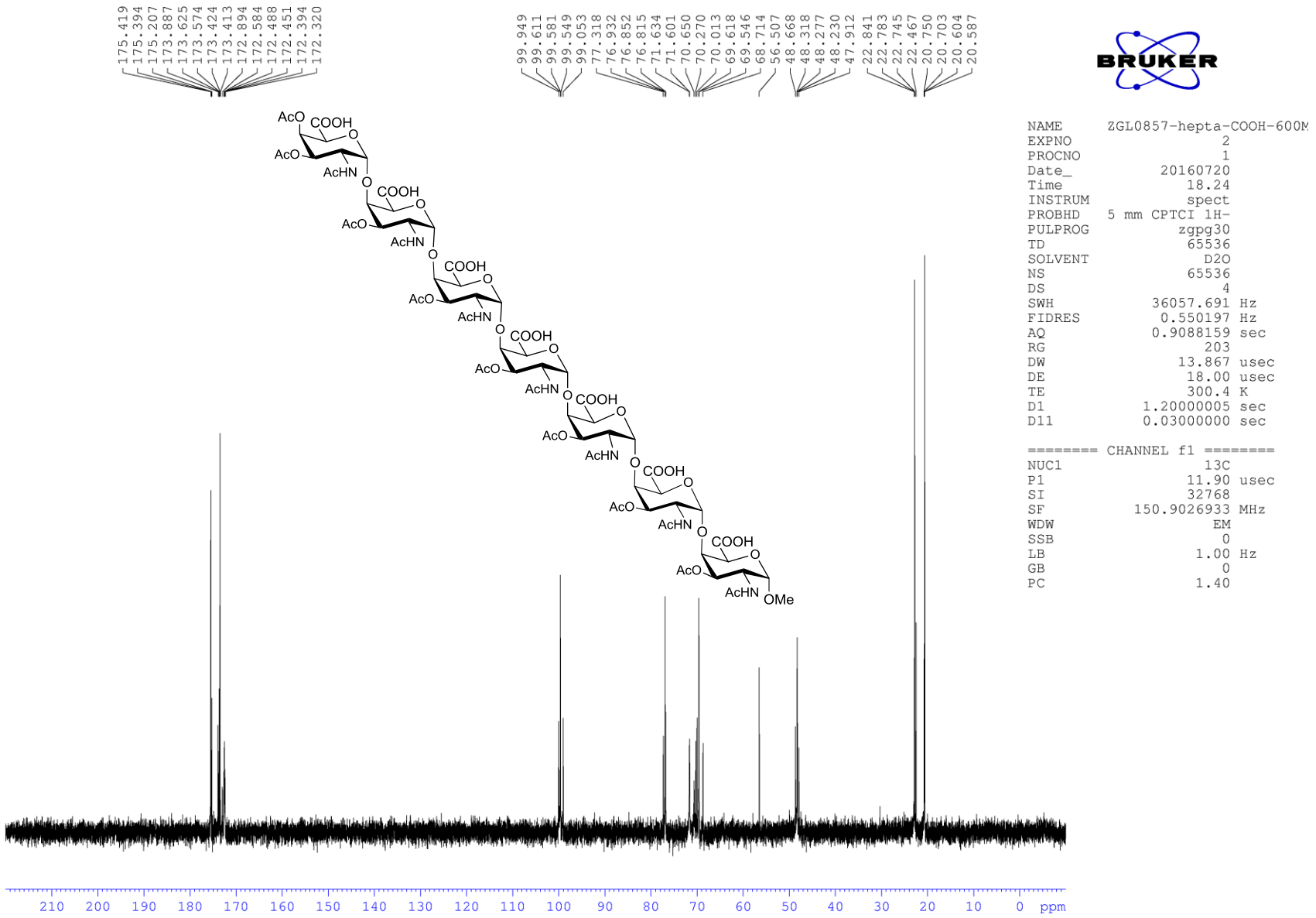
HMBC NMR spectrum of compound **12**



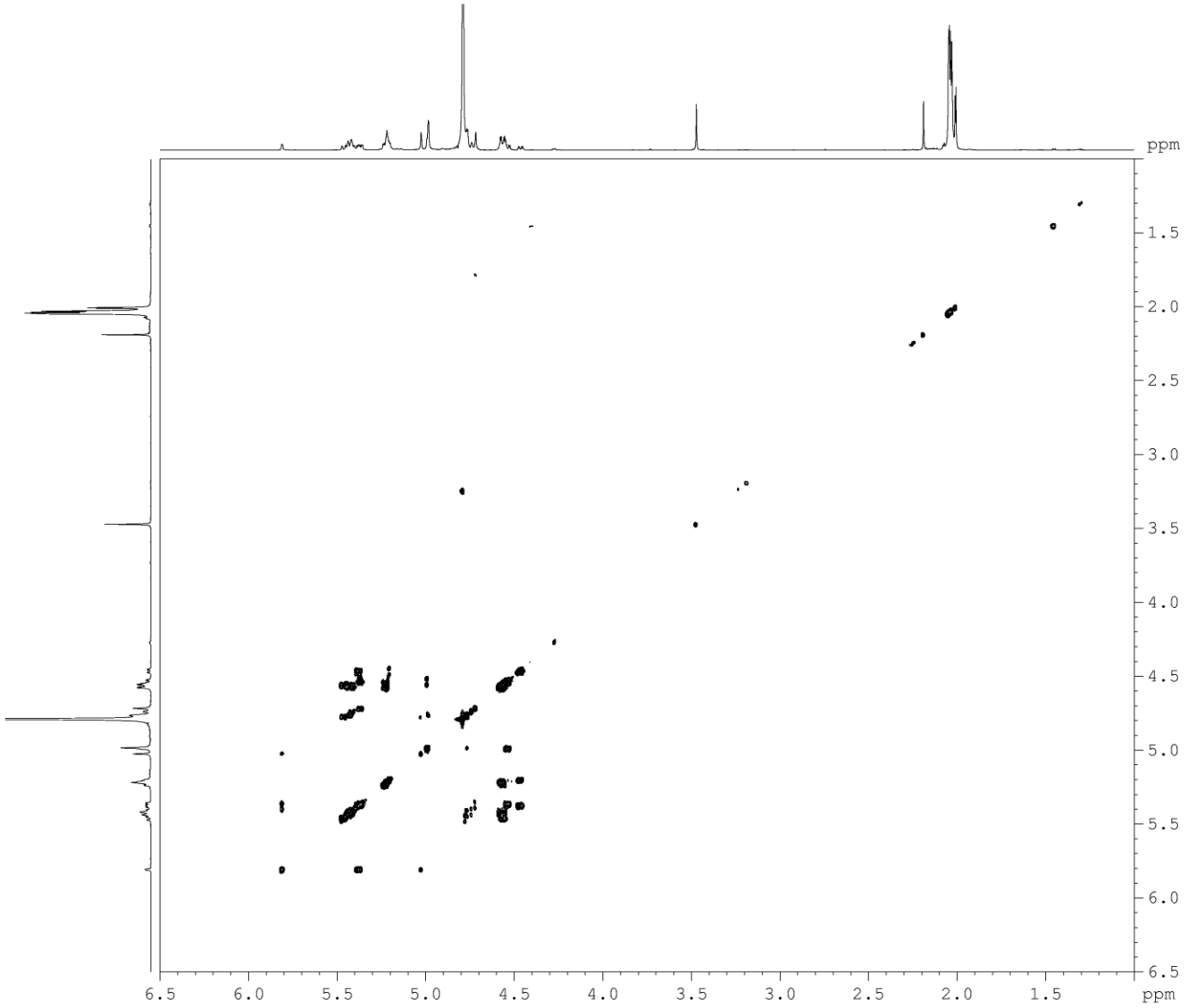

```
NAME      ZGL0857-hepta-COOH-600M
EXPNO                1
PROCNO               1
Date_         20160719
Time             11.03
INSTRUM          spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               65536
SOLVENT            D2O
NS                 64
DS                  2
SWH          12335.526 Hz
FIDRES        0.188225 Hz
AQ            2.6564426 sec
RG               11.3
DW               40.533 usec
DE               10.00 usec
TE               300.4 K
D1          1.00000000 sec

======== CHANNEL f1 ========
NUC1                1H
P1              12.00 usec
SI              65536
SF         600.1299502 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```

^{1}H NMR spectrum of compound **13**



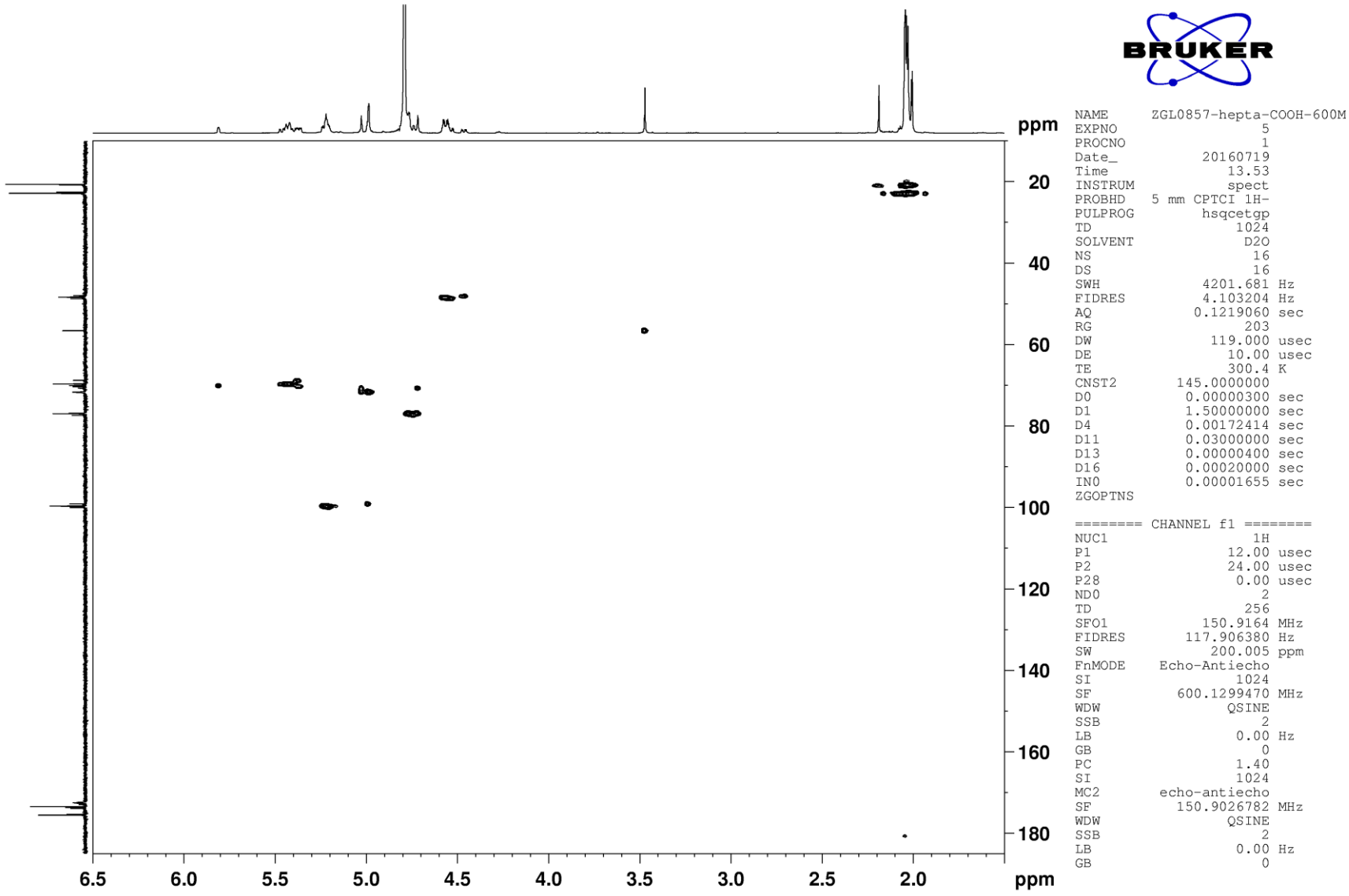
^{13}C NMR spectrum of compound **13**




```
NAME      ZGL0857-hepta-COOH-600M
EXPNO                  4
PROCNO                 1
Date_           20160719
Time               11.16
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG      cosygpmfqf
TD                  2048
SOLVENT              D2O
NS                    16
DS                    16
SWH            4201.681 Hz
FIDRES         2.051602 Hz
AQ             0.2437620 sec
RG                   203
DW               119.000 usec
DE                10.00 usec
TE                300.4 K
D0           0.00000300 sec
D1           2.00000000 sec
D13          0.00000400 sec
D16          0.00020000 sec
IN0          0.00023805 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                12.00 usec
ND0                    1
TD                   256
SFO1           600.1319 MHz
FIDRES        16.409874 Hz
SW                7.000 ppm
FnMODE                QF
SI                  1024
SF          600.1299492 MHz
WDW                 SINE
SSB                    0
LB                 0.00 Hz
GB                     0
PC                  1.40
SI                  1024
MC2                   QF
SF          600.1299478 MHz
WDW                 SINE
SSB                    0
LB                 0.00 Hz
GB                     0
```

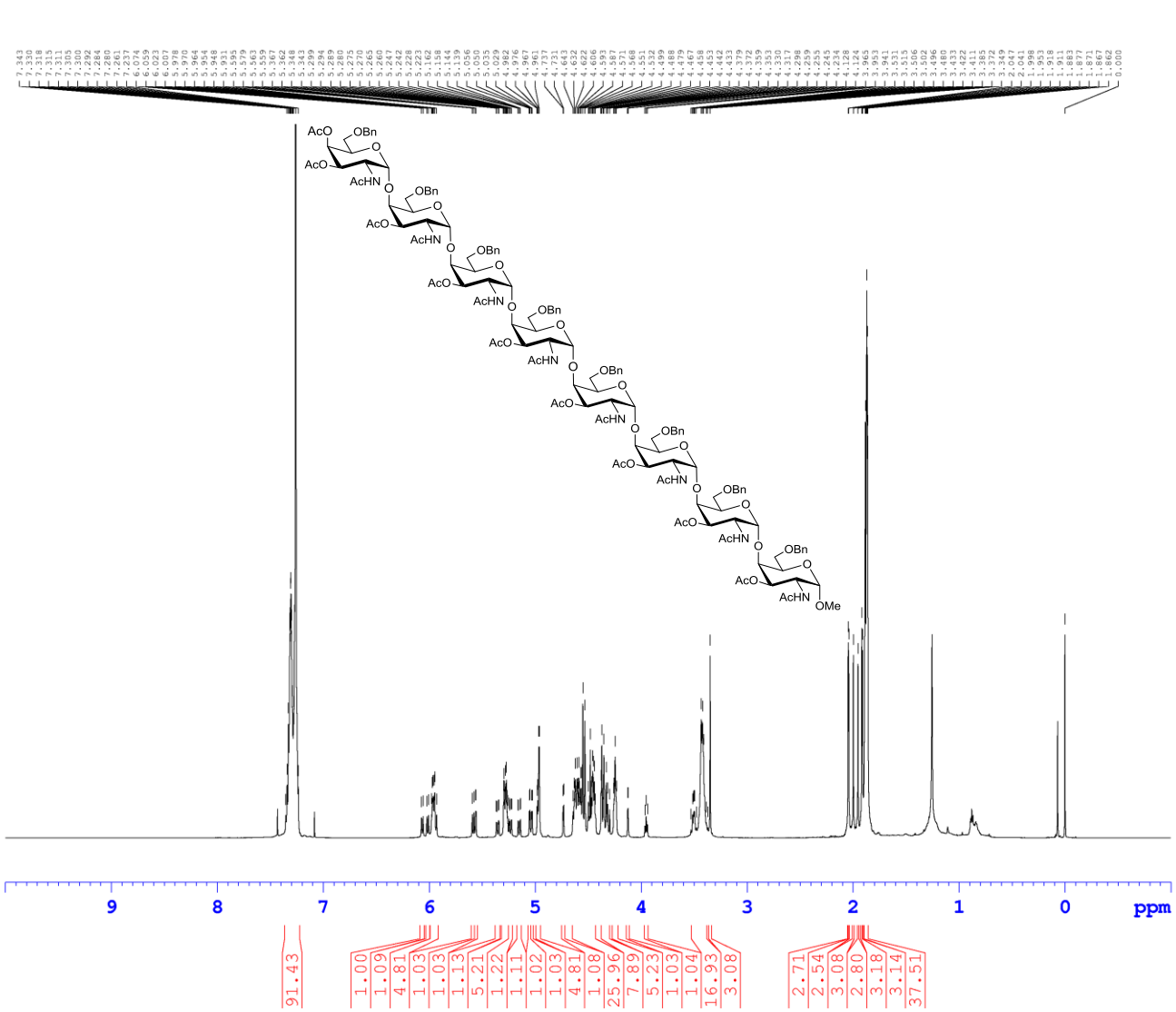
COSY NMR spectrum of compound **13**




```
NAME      ZGL0857-hepta-COOH-600M
EXPNO                           5
PROCNO                          1
Date_                    20160719
Time                        13.53
INSTRUM                     spect
PROBHD   5 mm CPTCI 1H-
PULPROG                 hsqcetgp
TD                          1024
SOLVENT                      D2O
NS                            16
DS                            16
SWH                     4201.681 Hz
FIDRES                  4.103204 Hz
AQ                      0.1219060 sec
RG                            203
DW                      119.000 usec
DE                       10.00 usec
TE                        300.4 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
IN0                   0.00001655 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                          1H
P1                       12.00 usec
P2                       24.00 usec
P28                       0.00 usec
ND0                           2
TD                          256
SFO1                  150.9164 MHz
FIDRES                117.906380 Hz
SW                       200.005 ppm
FnMODE            Echo-Antiecho
SI                          1024
SF                    600.1299470 MHz
WDW                        QSINE
SSB                           2
LB                        0.00 Hz
GB                            0
PC                        1.40
SI                          1024
MC2               echo-antiecho
SF                    150.9026782 MHz
WDW                        QSINE
SSB                           2
LB                        0.00 Hz
GB                            0
```

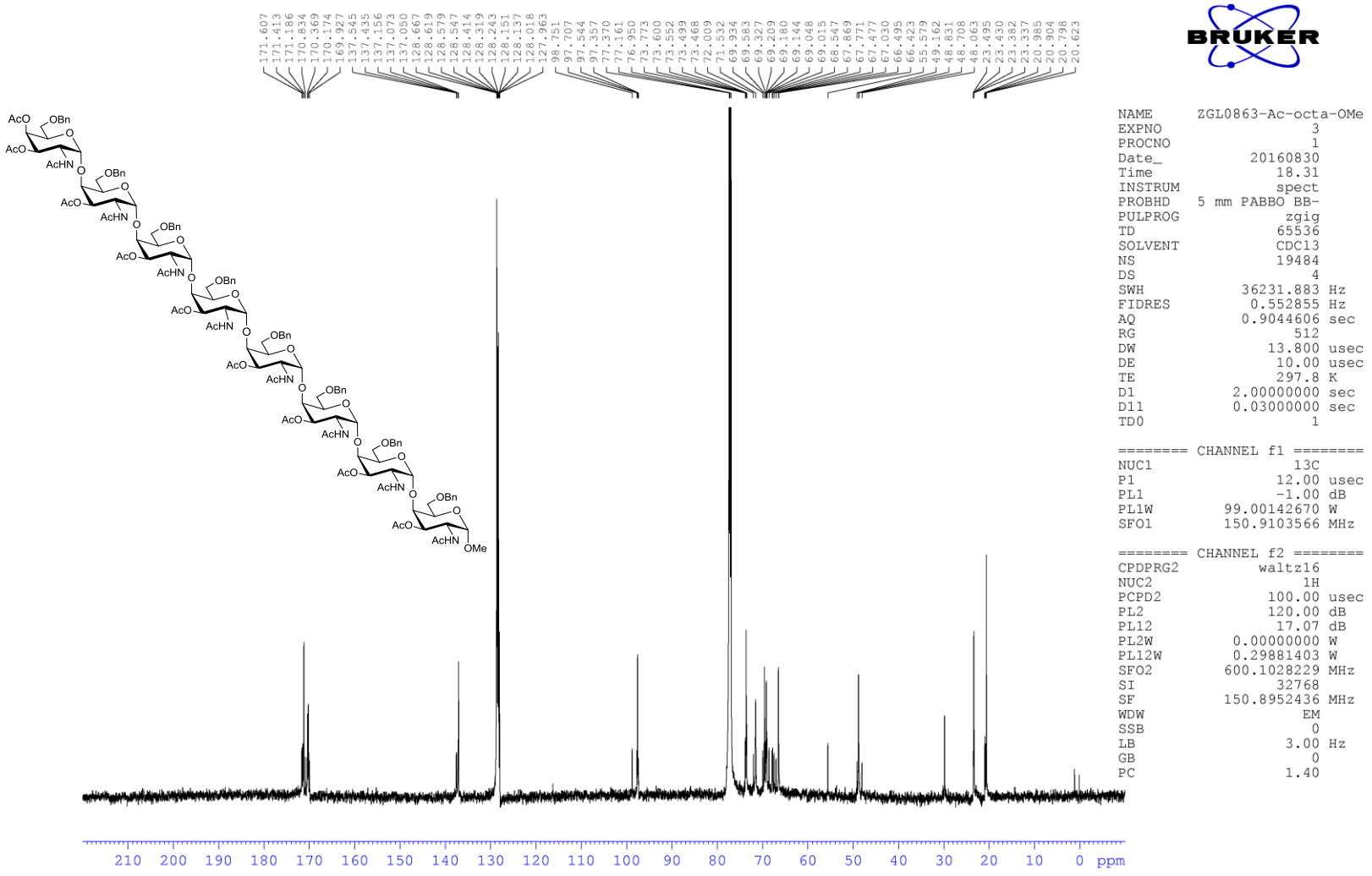
HSQC NMR spectrum of compound **13**




```
NAME      ZGL0863-Ac-octa-OMe-1
EXPNO                         1
PROCNO                        1
Date_                  20160902
Time                      15.08
INSTRUM                   spect
PROBHD    5 mm CPTCI 1H-
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          64
DS                           2
SWH                  12335.526 Hz
FIDRES                0.188225 Hz
AQ                   2.6564426 sec
RG                           9
DW                      40.533 usec
DE                      10.00 usec
TE                        300.4 K
D1                  1.00000000 sec

======== CHANNEL f1 ========
NUC1                         1H
P1                      12.00 usec
SI                       65536
SF                600.1300167 MHz
WDW                         EM
SSB                          0
LB                      0.30 Hz
GB                           0
PC                      1.00
```

^{1}H NMR spectrum of compound **14**

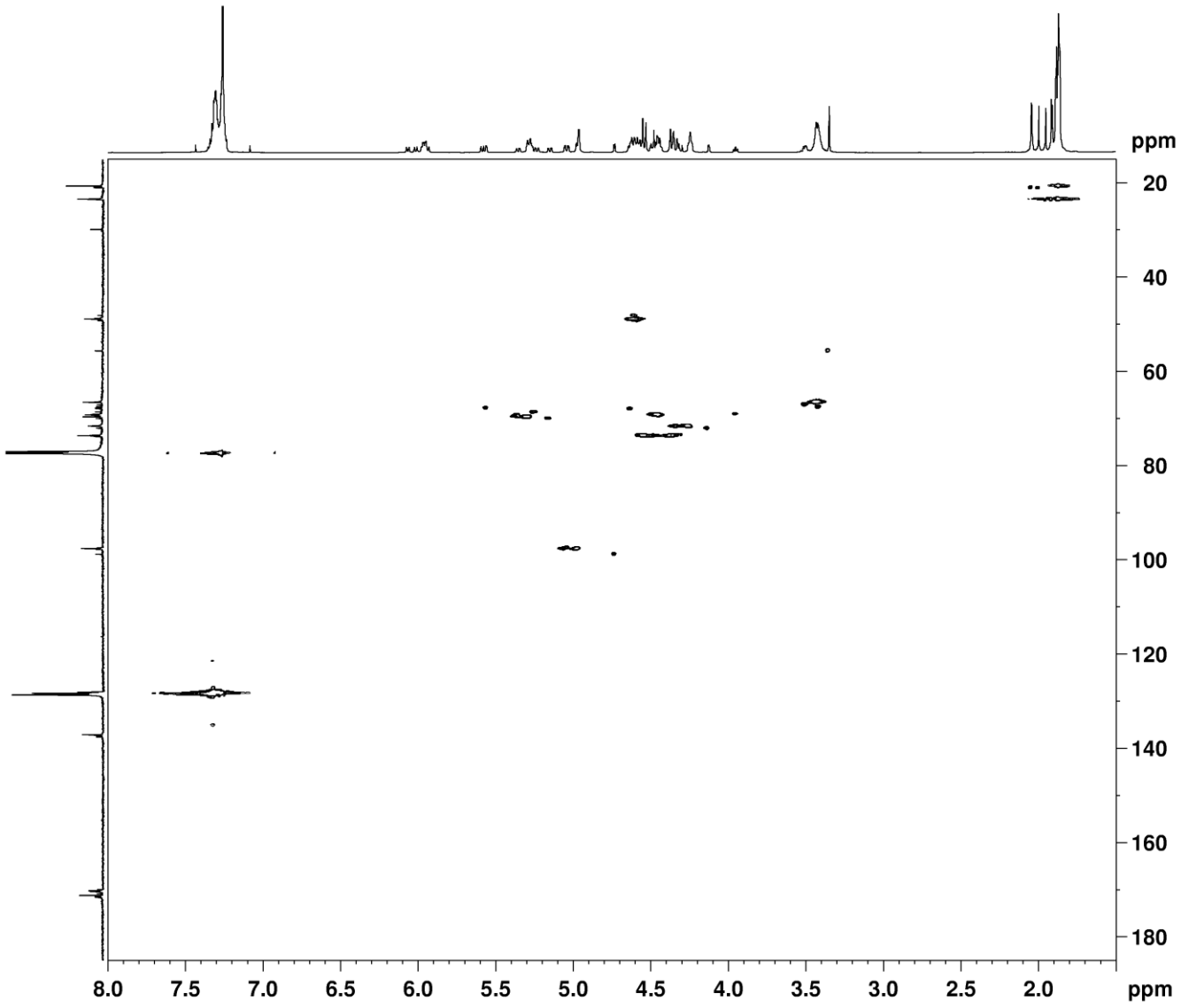



```
NAME      ZGL0863-Ac-octa-OMe
EXPNO                       3
PROCNO                      1
Date_                20160830
Time                    18.31
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG                  zgig
TD                      65536
SOLVENT                 CDCl3
NS                      19484
DS                          4
SWH                36231.883 Hz
FIDRES             0.552855 Hz
AQ                 0.9044606 sec
RG                        512
DW                     13.800 usec
DE                     10.00 usec
TE                     297.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                     12.00 usec
PL1                    -1.00 dB
PL1W              99.00142670 W
SFO1             150.9103566 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  100.00 usec
PL2                    120.00 dB
PL12                    17.07 dB
PL2W               0.00000000 W
PL12W              0.29881403 W
SFO2             600.1028229 MHz
SI                       32768
SF               150.8952436 MHz
WDW                        EM
SSB                         0
LB                      3.00 Hz
GB                          0
PC                      1.40
```

^{13}C NMR spectrum of compound **14**



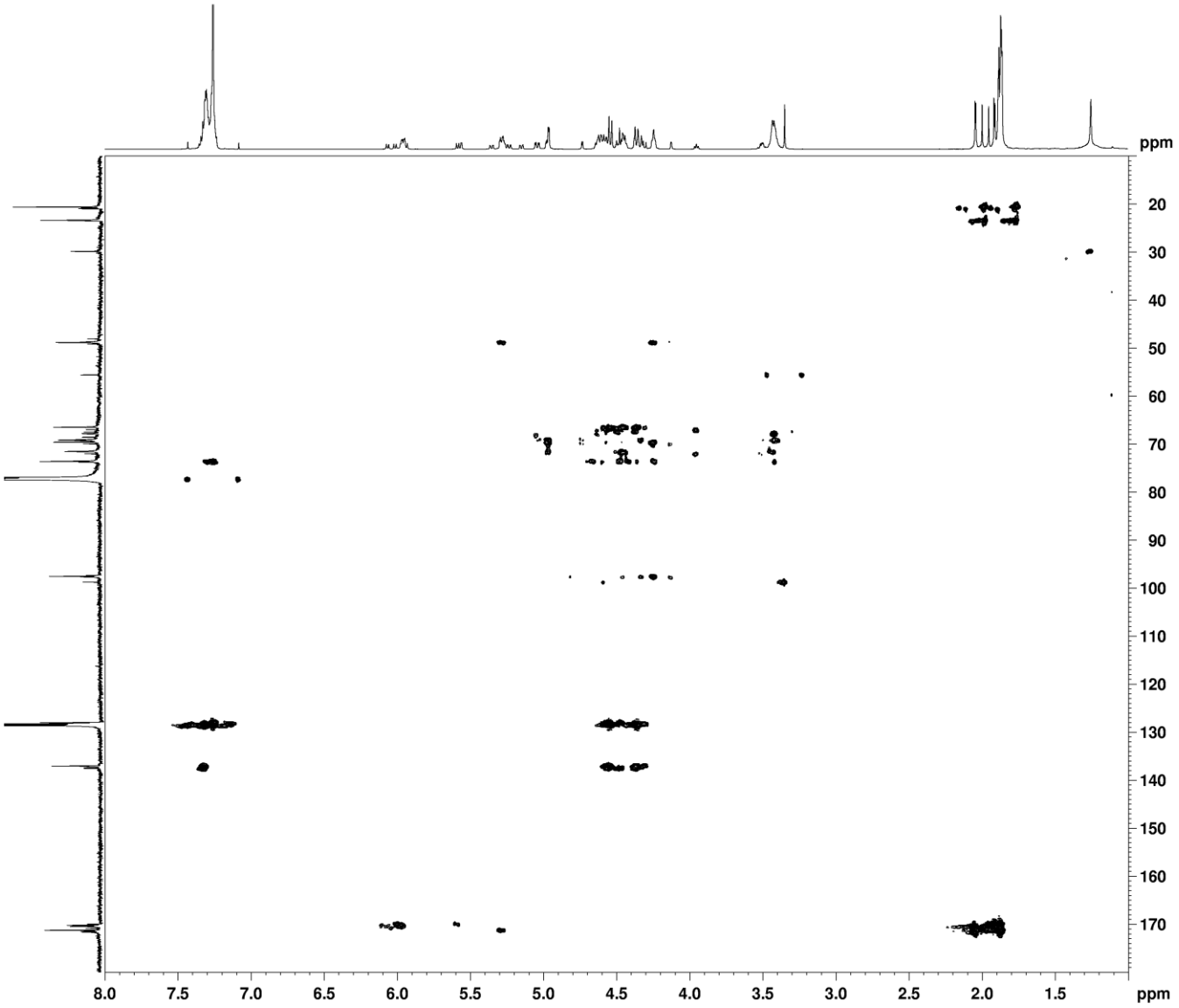

```
NAME          ZGL0863-Ac-octa-OMe
EXPNO                           4
PROCNO                          1
Date_                    20160831
Time                        18.26
INSTRUM                     spect
PROBHD       5 mm PABBO BB-
PULPROG            hsqcetgpsi
TD                           2048
SOLVENT                   CDCl3
NS                             32
DS                             16
SWH                    6009.615 Hz
FIDRES                 2.934382 Hz
AQ                     0.1705268 sec
RG                           512
DW                        83.200 usec
DE                        10.00 usec
TE                        297.9 K
CNST2                145.0000000
D0                    0.00000300 sec
D1                    2.00000000 sec
D4                    0.00172414 sec
D11                   0.03000000 sec
D13                   0.00000400 sec
D16                   0.00020000 sec
D24                   0.00172400 sec
IN0                   0.00002000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                          1H
P1                        11.33 usec
P2                        22.66 usec
P28                        0.00 usec
PL1                       -1.85 dB
PL1W                23.30241585 W
SFO1                600.1024004 MHz

======== CHANNEL f2 ========
CPDPRG2                    garp
NUC2                        13C
P3                        12.00 usec
P4                        24.00 usec
PCPD2                     75.00 usec
PL2                       -1.00 dB
PL12                      14.92 dB
PL2W                99.00142670 W
PL12W                2.53303647 W
SFO2                150.9065195 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SMSQ10.100
GPNAM2               SMSQ10.100
GPZ1                      80.00 %
GPZ2                      20.10 %
P16                     1000.00 usec
ND0                           2
TD                          400
SFO1                 150.9065 MHz
FIDRES                62.490108 Hz
SW                      165.639 ppm
FnMODE           Echo-Antiecho
SI                         4096
SF                 600.1000073 MHz
WDW                       QSINE
SSB                           2
LB                        0.00 Hz
GB                            0
PC                         1.40
SI                         1024
MC2              echo-antiecho
SF                 150.8952432 MHz
WDW                       QSINE
SSB                           2
LB                        0.00 Hz
GB                            0
```

HSQC NMR spectrum of compound **14**



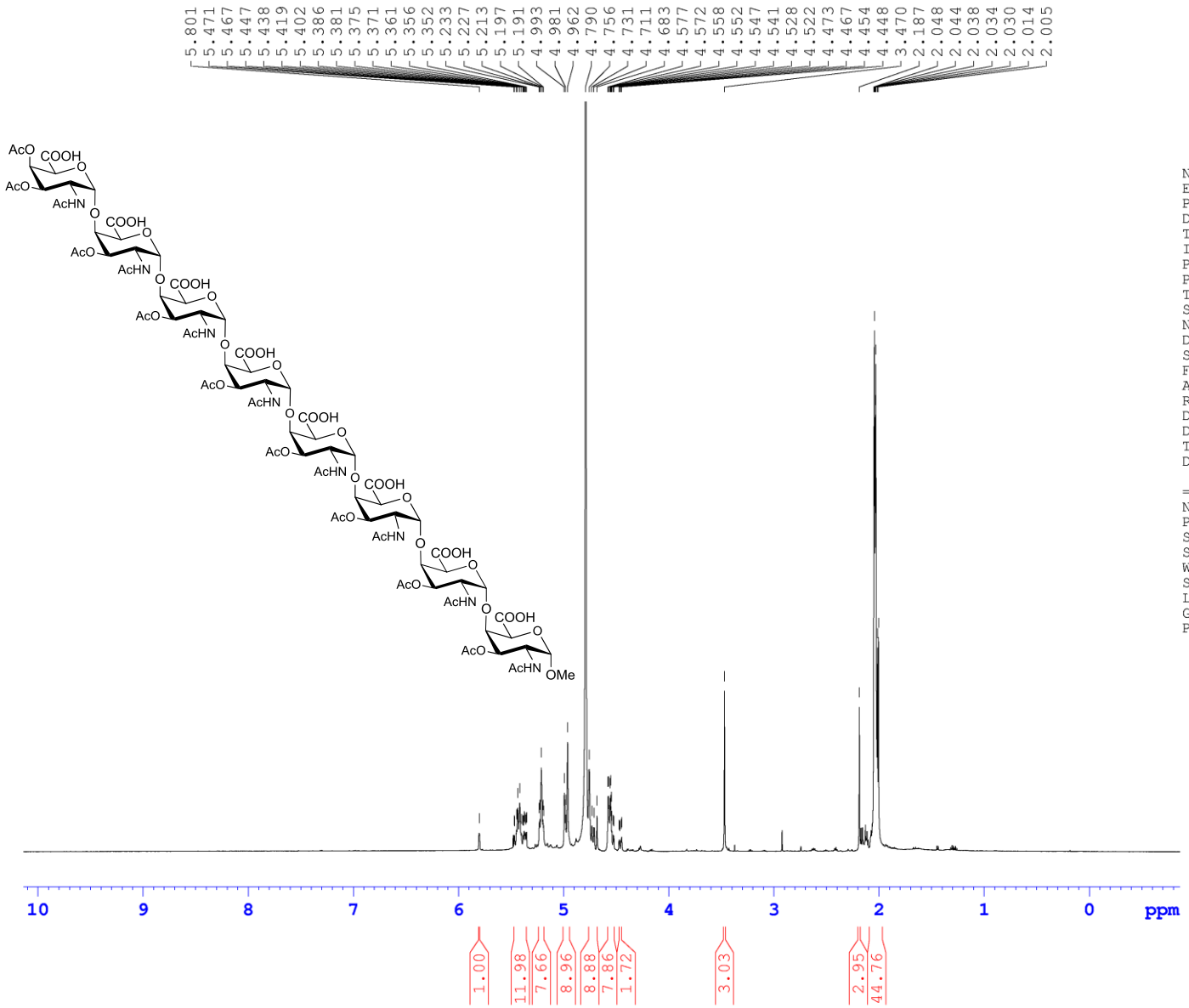

```
NAME          ZGL0863-Ac-octa-OMe
EXPNO                           5
PROCNO                          1
Date_                    20160901
Time                         2.16
INSTRUM                     spect
PROBHD       5 mm PABBO BB-
PULPROG        hmbcgplpndqf
TD                           2048
SOLVENT                    CDCl3
NS                             64
DS                             16
SWH                    6009.615 Hz
FIDRES                 2.934382 Hz
AQ                     0.1705268 sec
RG                           512
DW                        83.200 usec
DE                        10.00 usec
TE                        298.0 K
CNST2                145.0000000
CNST13                 8.0000000
D0                     0.00000300 sec
D1                     2.00000000 sec
D2                     0.00344828 sec
D6                     0.06250000 sec
D16                    0.00020000 sec
IN0                    0.00001745 sec

======== CHANNEL f1 ========
NUC1                           1H
P1                        11.33 usec
P2                        22.66 usec
PL1                       -1.85 dB
PL1W                 23.30241585 W
SFO1                600.1024004 MHz

======== CHANNEL f2 ========
NUC2                          13C
P3                        12.00 usec
PL2                       -1.00 dB
PL2W                 99.00142670 W
SFO2                150.9080911 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SMSQ10.100
GPNAM2               SMSQ10.100
GPNAM3               SMSQ10.100
GPZ1                      50.00 %
GPZ2                      30.00 %
GPZ3                      40.10 %
P16                     1000.00 usec
ND0                            2
TD                           512
SFO1                 150.9081 MHz
FIDRES                56.001049 Hz
SW                       190.000 ppm
FnMODE                        QF
SI                          1024
SF                  600.1000079 MHz
WDW                        SINE
SSB                           0
LB                         0.00 Hz
GB                            0
PC                         1.40
SI                          1024
MC2                           QF
SF                  150.8952309 MHz
WDW                        SINE
SSB                           0
LB                         0.00 Hz
GB                            0
```

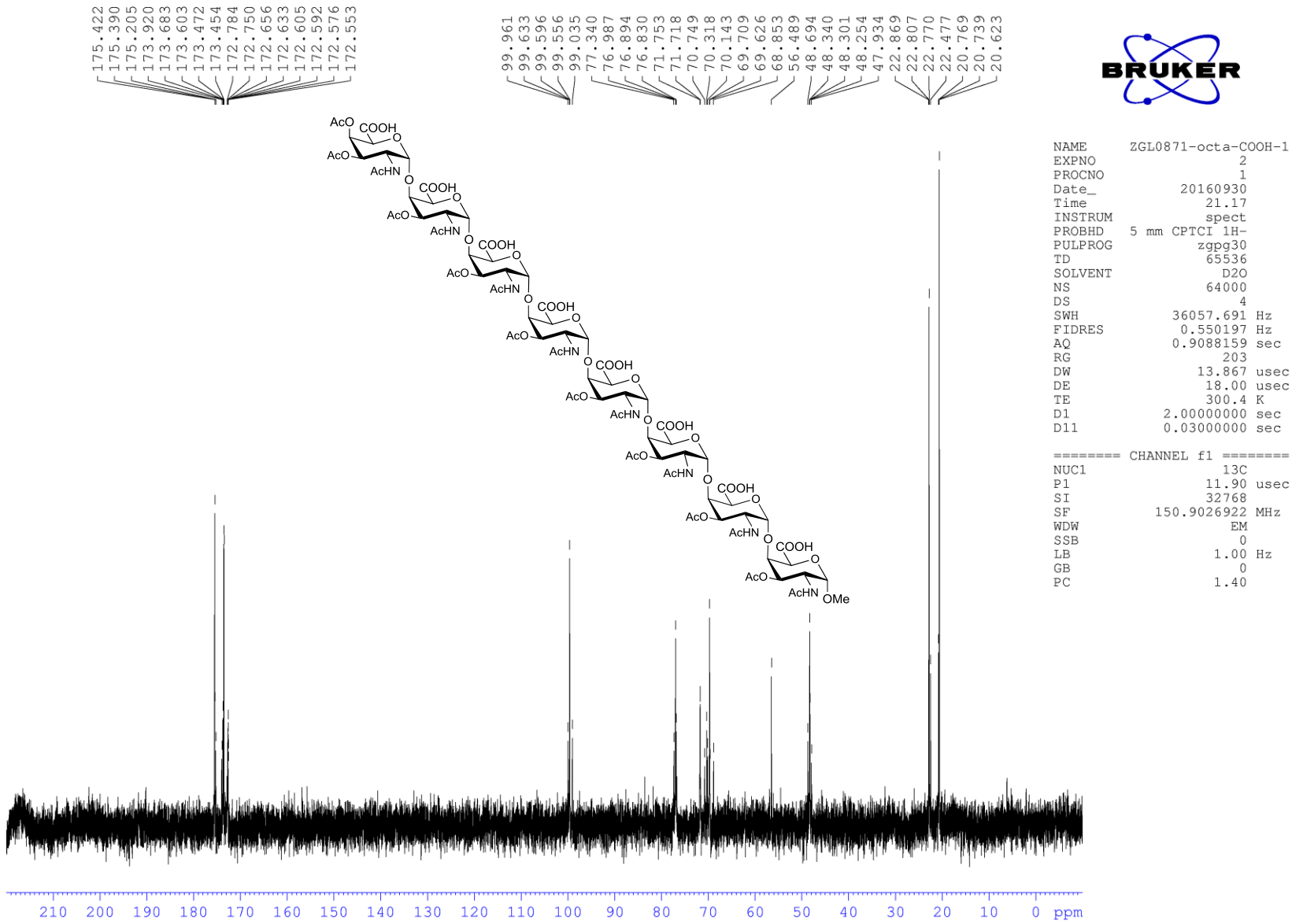
HMBC NMR spectrum of compound **14**



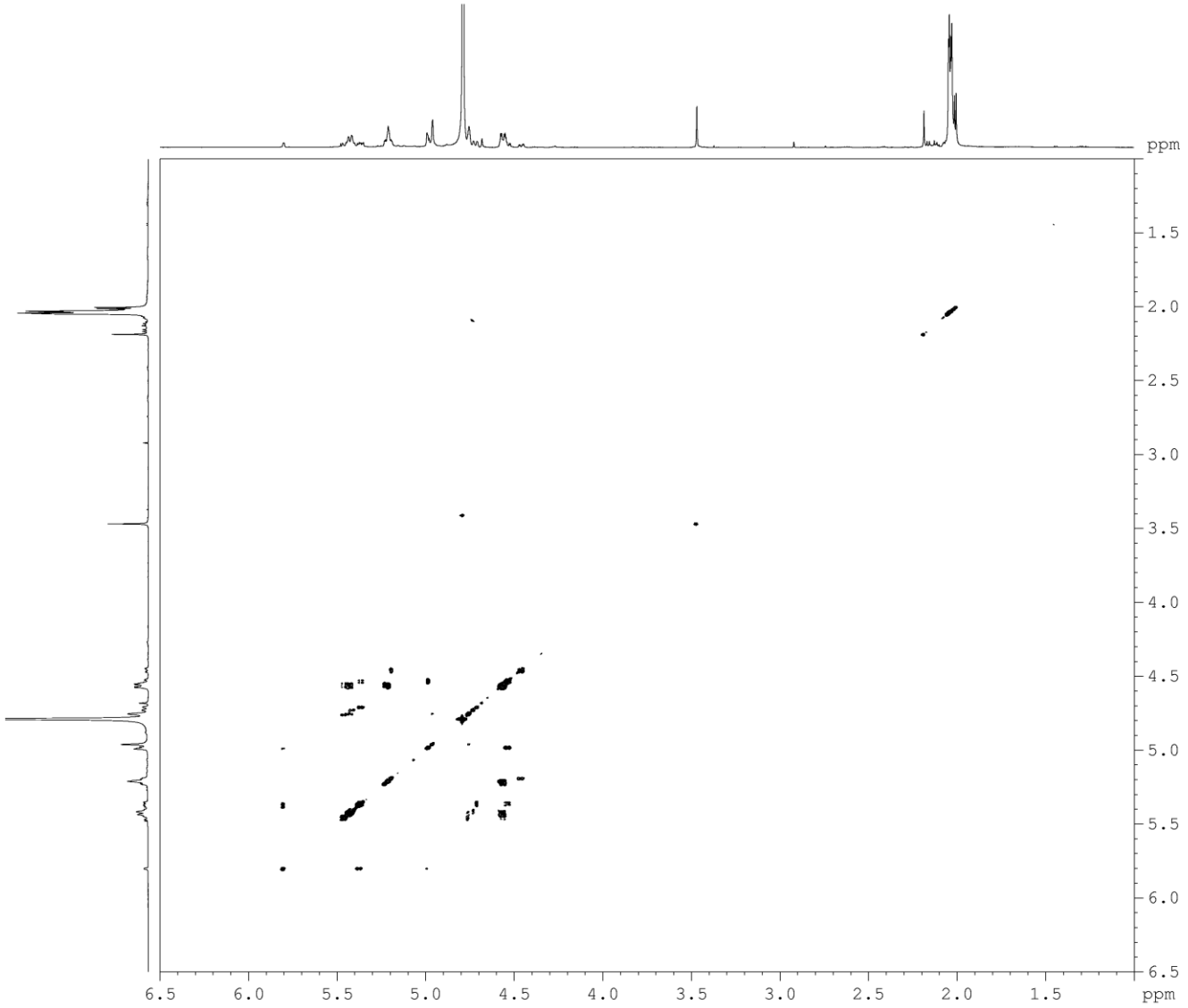
BRUKER

NAME	ZGL0871-octa-COOH
EXPNO	1
PROCNO	1
Date_	20160930
Time	18.51
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	zg30
TD	65536
SOLVENT	D2O
NS	258
DS	2
SWH	12335.526 Hz
FIDRES	0.188225 Hz
AQ	2.6564426 sec
RG	10
DW	40.533 usec
DE	10.00 usec
TE	300.4 K
D1	1.00000000 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	12.00 usec
SI	65536
SF	600.1299500 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{1}H NMR spectrum of compound **15**



^{13}C NMR spectrum of compound **15**




```
NAME      ZGL0871-octa-COOH
EXPNO                    3
PROCNO                   1
Date_             20161003
Time                 23.54
INSTRUM              spect
PROBHD   5 mm CPTCI 1H-
PULPROG       cosygpmfqf
TD                    2048
SOLVENT                D2O
NS                      16
DS                       8
SWH             4058.442 Hz
FIDRES          1.981661 Hz
AQ              0.2523636 sec
RG                     203
DW               123.200 usec
DE                10.00 usec
TE                 300.4 K
D0            0.00000300 sec
D1            2.00000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00024640 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                 12.00 usec
ND0                      1
TD                     512
SFO1             600.132 MHz
FIDRES          7.926687 Hz
SW                 6.763 ppm
FnMODE                  QF
SI                    1024
SF           600.1299486 MHz
WDW                  SINE
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                    1024
MC2                     QF
SF           600.1299487 MHz
WDW                  SINE
SSB                     0
LB                   0.00 Hz
GB                      0
```

COSY NMR spectrum of compound **15**