Electronic Supplementary Material (ESI) for MedChemComm.

Supplementary Information

Design, synthesis and cytotoxicity of bengamide analogues and their epimers

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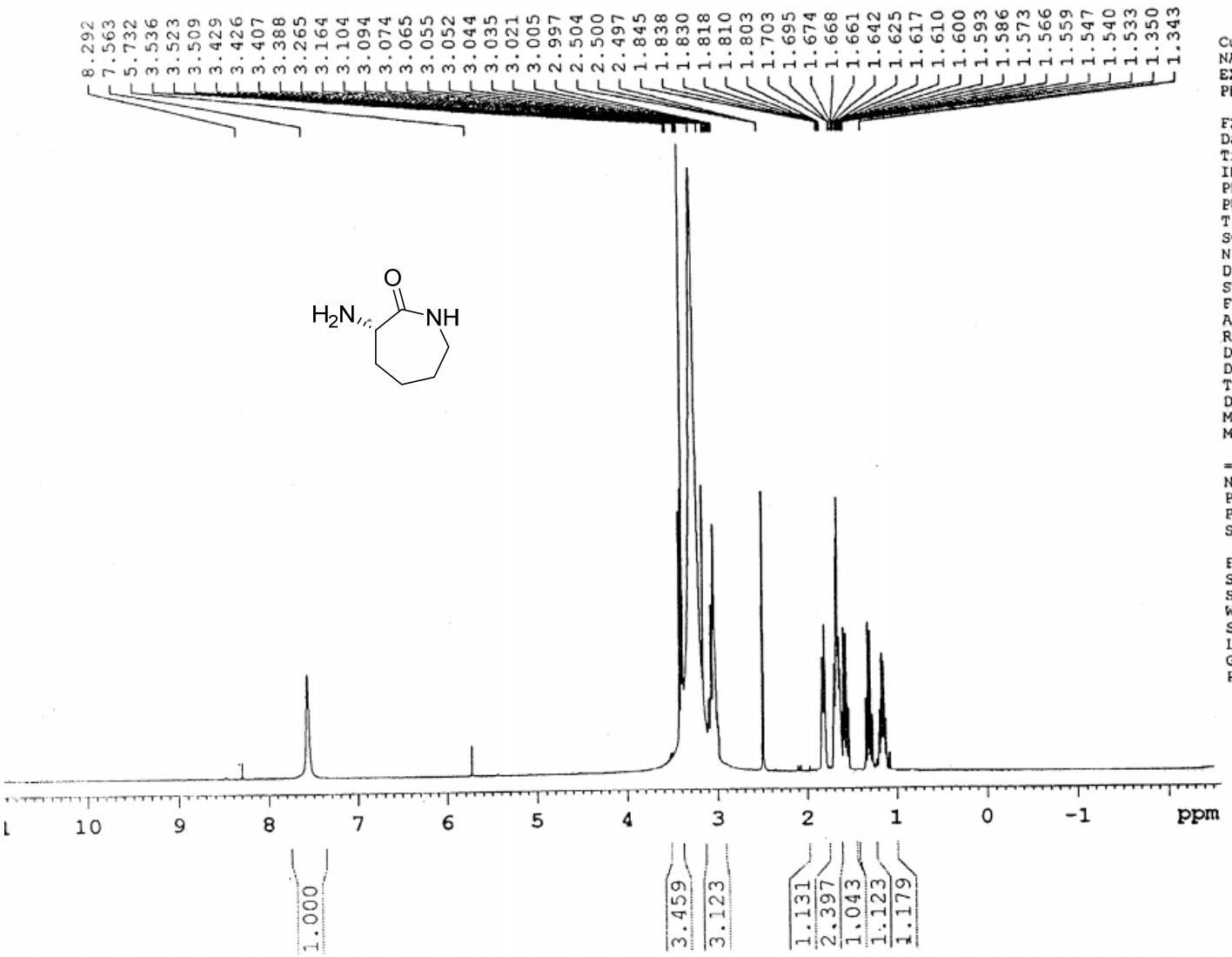
^{1}H NMR spectrum of **3a** (500 MHz, DMSO-d_6)

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Current Data Parameters
NAME          2LOI_06Sel4
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140908
Time               16.25
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     0
SWH          10000.000 Hz
FIDRES           0.152588 Hz
AQ             3.2769001 sec
RG                    57
DW             50.000 usec
DE              6.00 usec
TE              300.0 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1              8.50 usec
PL1             -3.00 dB
SFO1       500.1337510 MHz

F2 - Processing parameters
SI                 32768
SF         500.1300052 MHz
WDW                   EM
SSB                    0
LB              0.30 Hz
GB                     0
PC                  1.00
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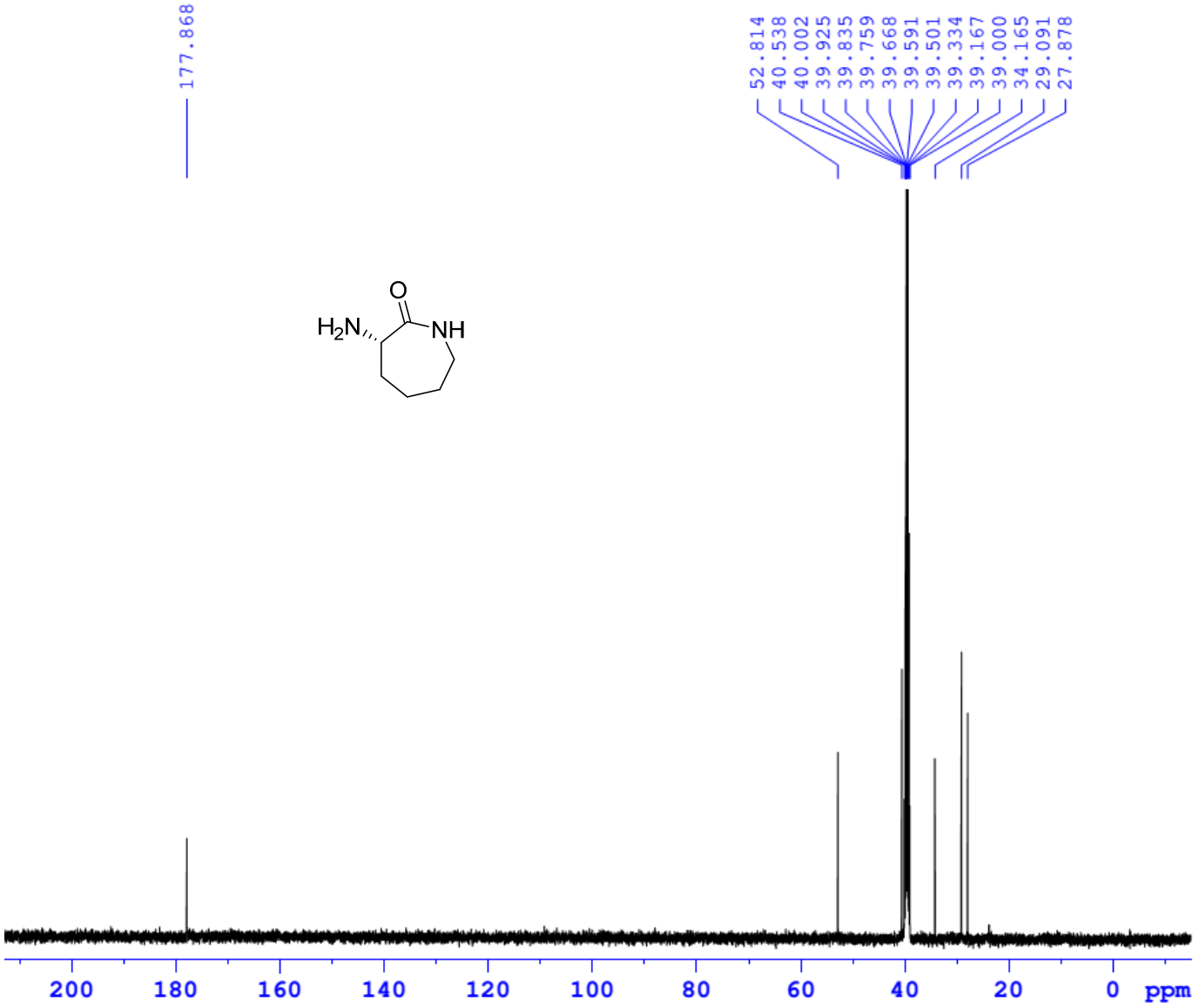
^{13}C NMR spectrum of **3a** (125 MHz, DMSO-d_6)

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Current Data Parameters
NAME          2DAO14Oct14
EXPNO                   2
PROCNO                  1

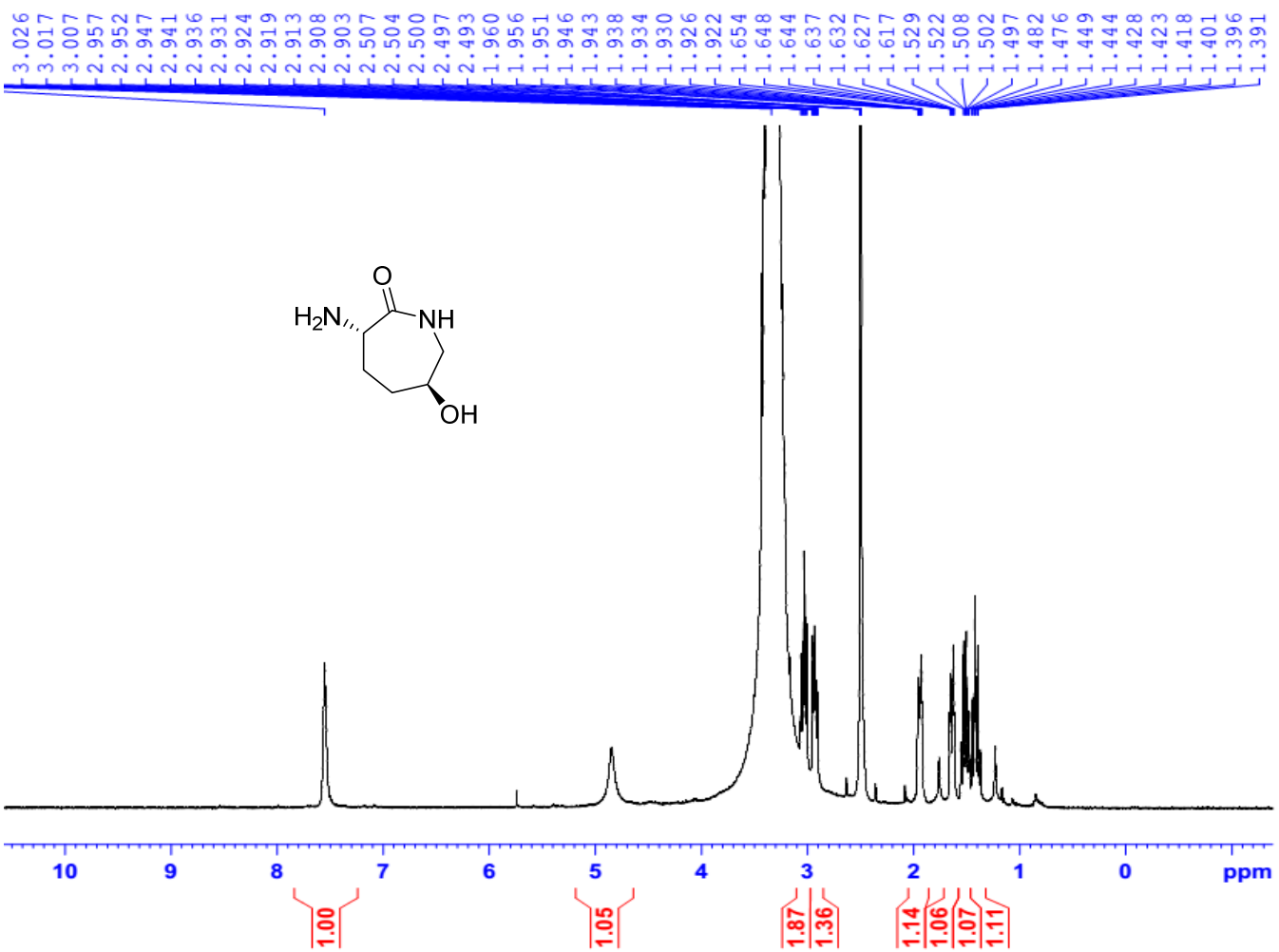
F2 - Acquisition Paramet
Date_            20141014
Time                16.12
INSTRUM             spect
PROBHD   5 mm Multinucl
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   128
DS                     2
SWH            31446.541
FIDRES         0.479836
AQ             1.0420883
RG                 32768
DW                15.900
DE                 6.00
TE                300.0
D1             2.00000000
d11            0.03000000
DELTA          1.89999998
MCREST         0.00000000
MCWRK          0.01500000

======== CHANNEL f1 ====
NUC1                13C
P1                 7.50
PL1                0.00
SFO1         125.7715724

======== CHANNEL f2 ====
CPDPRG2          waltz16
NUC2                1H
PCPD2              80.00
PL2                -3.00
PL12               16.47
PL13               22.00
SFO2         500.1320005

F2 - Processing paramete
SI                 32768
SF           125.7578450
WDW                   EM
SSB                    0
LB                  1.00
GB                     0
```

^{1}H NMR spectrum of *rac*-**4a** (500 MHz, DMSO-d_6)

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Current Data Parameters
NAME      2NGAN_BGCYCLOA
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150918
Time              11.41
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG               111.09
DW               50.000 usec
DE                6.50 usec
TE                301.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                 1H
P1                10.00 usec
PLW1        22.00000000 W

F2 - Processing parameters
SI                65536
SF           500.2000043 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```
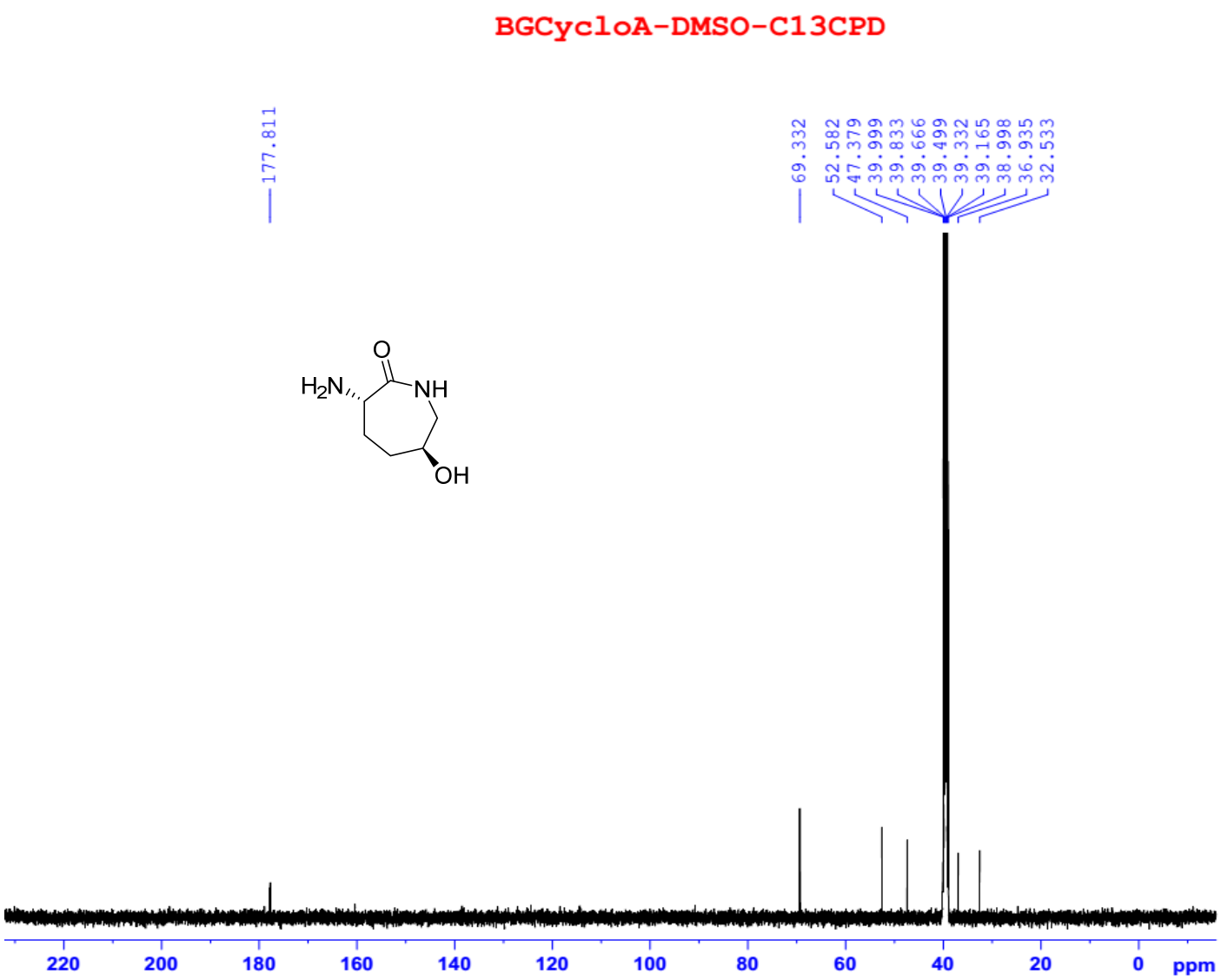

^{13}C NMR spectrum of *rac*-**4a** (125 MHz, DMSO-d_6)

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Current Data Parameters
NAME      2NGAN_BGCycloA
EXPNO                  2
PROCNO                 1

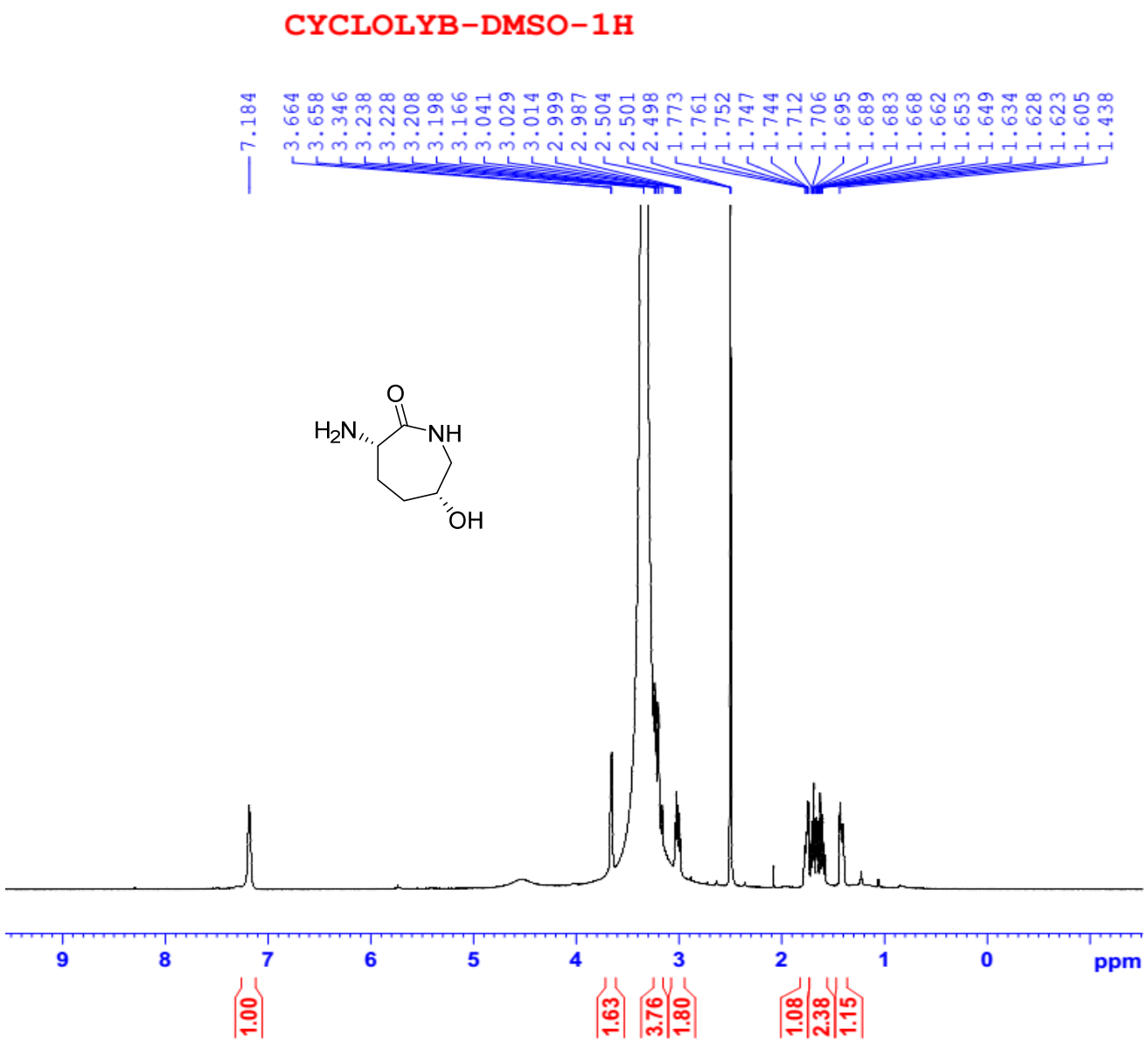
F2 - Acquisition Parameters
Date_          20151030
Time              10.23
INSTRUM           spect
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                 1065
DS                    2
SWH           31446.541 Hz
FIDRES         0.479836 Hz
AQ            1.0420383 sec
RG                32768
DW               15.900 usec
DE                6.00 usec
TE               296.8 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST   0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                  7.20 usec
PL1       0 dB
SFO1         125.7715724 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2               80.00 usec
PL2                 -3.00 dB
PL12                14.89 dB
PL13                22.00 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                  32768
SF           125.7578414 MHz
WDW                  EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

^{1}H NMR spectrum of *rac*-**4b** (500 MHz, DMSO-d_6)

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Current Data Parameters
NAME      2NGAN_CYCLOLYB
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160122
Time              16.32
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                89.63
DW               50.000 usec
DE                6.50 usec
TE                299.7 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                1H
P1                10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                65536
SF           500.2000038 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```
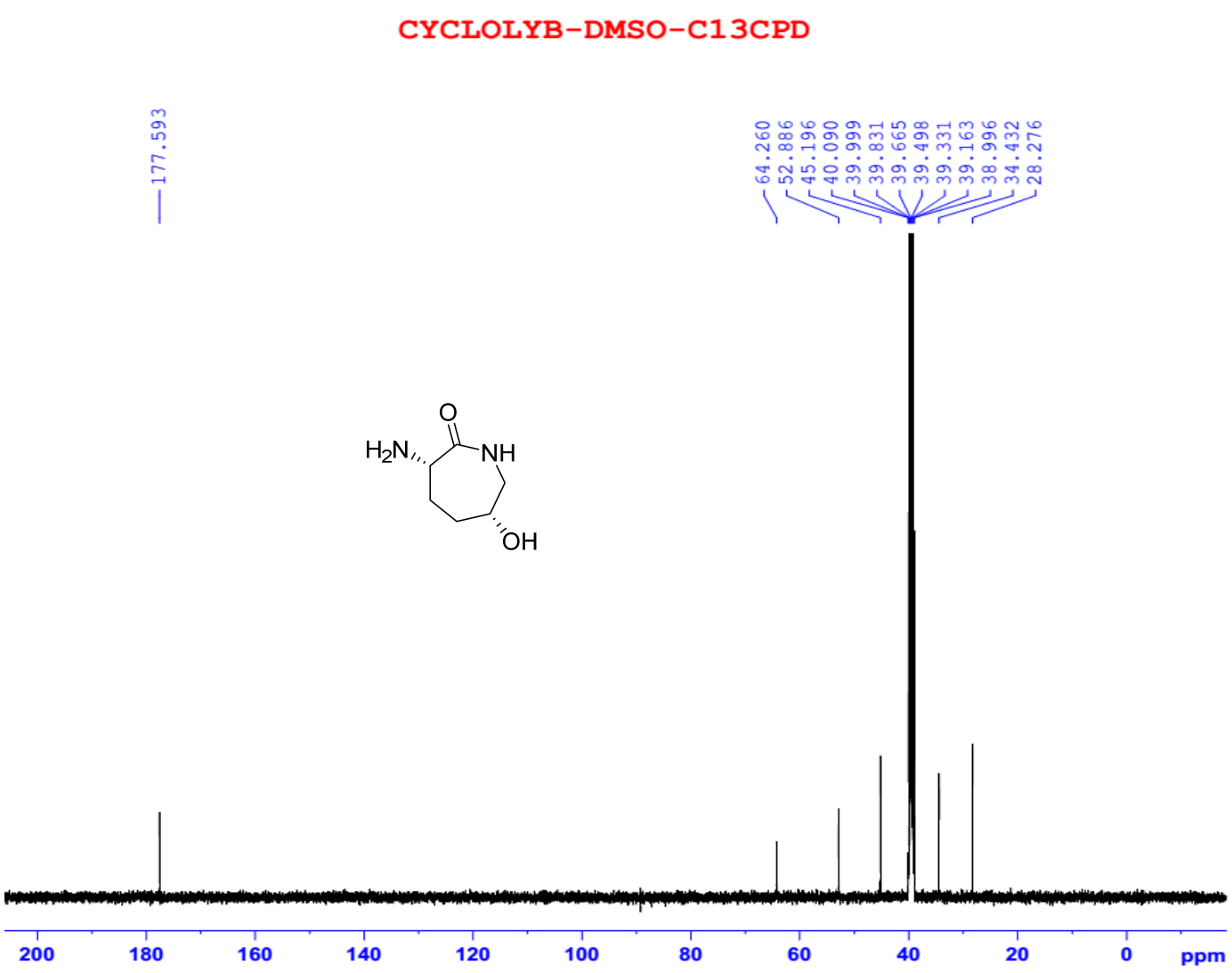

^{13}C NMR spectrum of *rac*-**4b** (125 MHz, DMSO-d_6)

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Current Data Parameters
NAME      2NGAN_CYCLOLYB
EXPNO                  2
PROCNO                 1

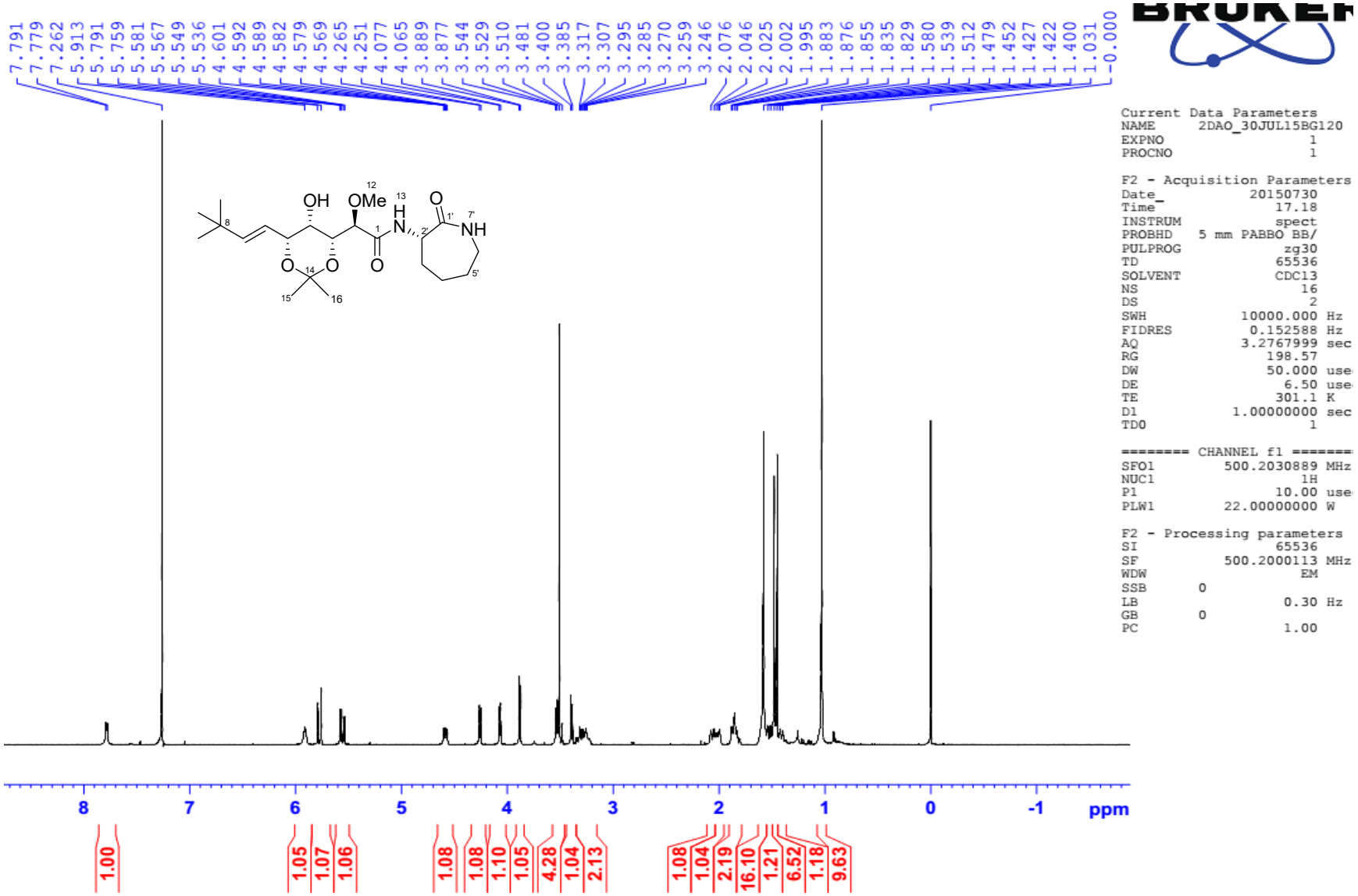
F2 - Acquisition Parameters
Date_           20160125
Time               19.27
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG               198.57
DW               16.800 usec
DE                6.50 usec
TE               298.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7879670 MHz
NUC1               13C
P1               10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                32768
SF          125.7754445 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

^{1}H NMR spectrum of **6a** (500 MHz, $CDCl_3$)

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Current Data Parameters
NAME      2DAO_30JUL15BG120
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150730
Time                 17.18
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              10000.000 Hz
FIDRES               0.152588 Hz
AQ                3.2767999 sec
RG                   198.57
DW                   50.000 use
DE                    6.50 use
TE                   301.1 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 =======
SFO1           500.2030889 MHz
NUC1                    1H
P1                   10.00 use
PLW1           22.00000000 W

F2 - Processing parameters
SI                   65536
SF              500.2000113 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```
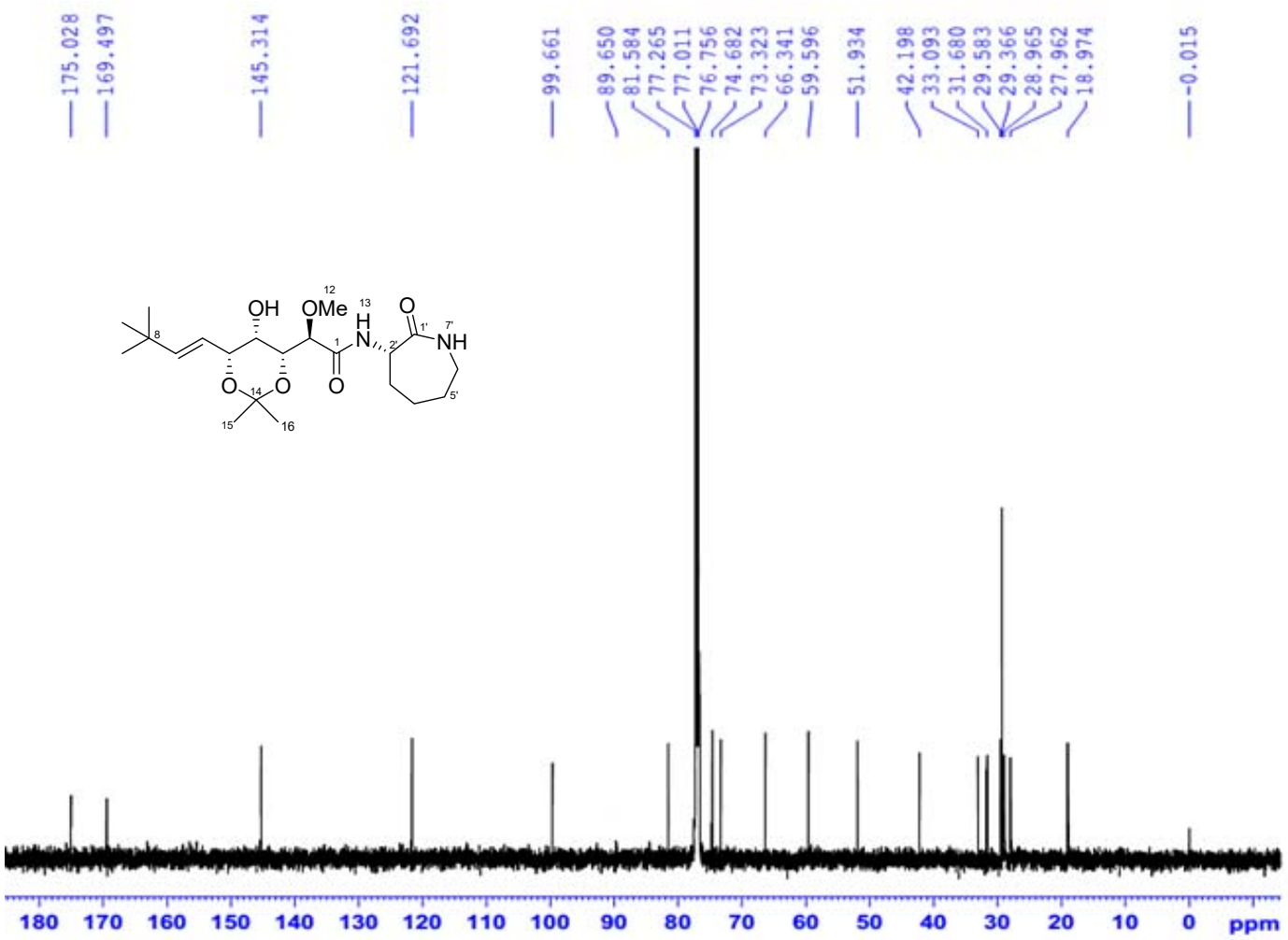
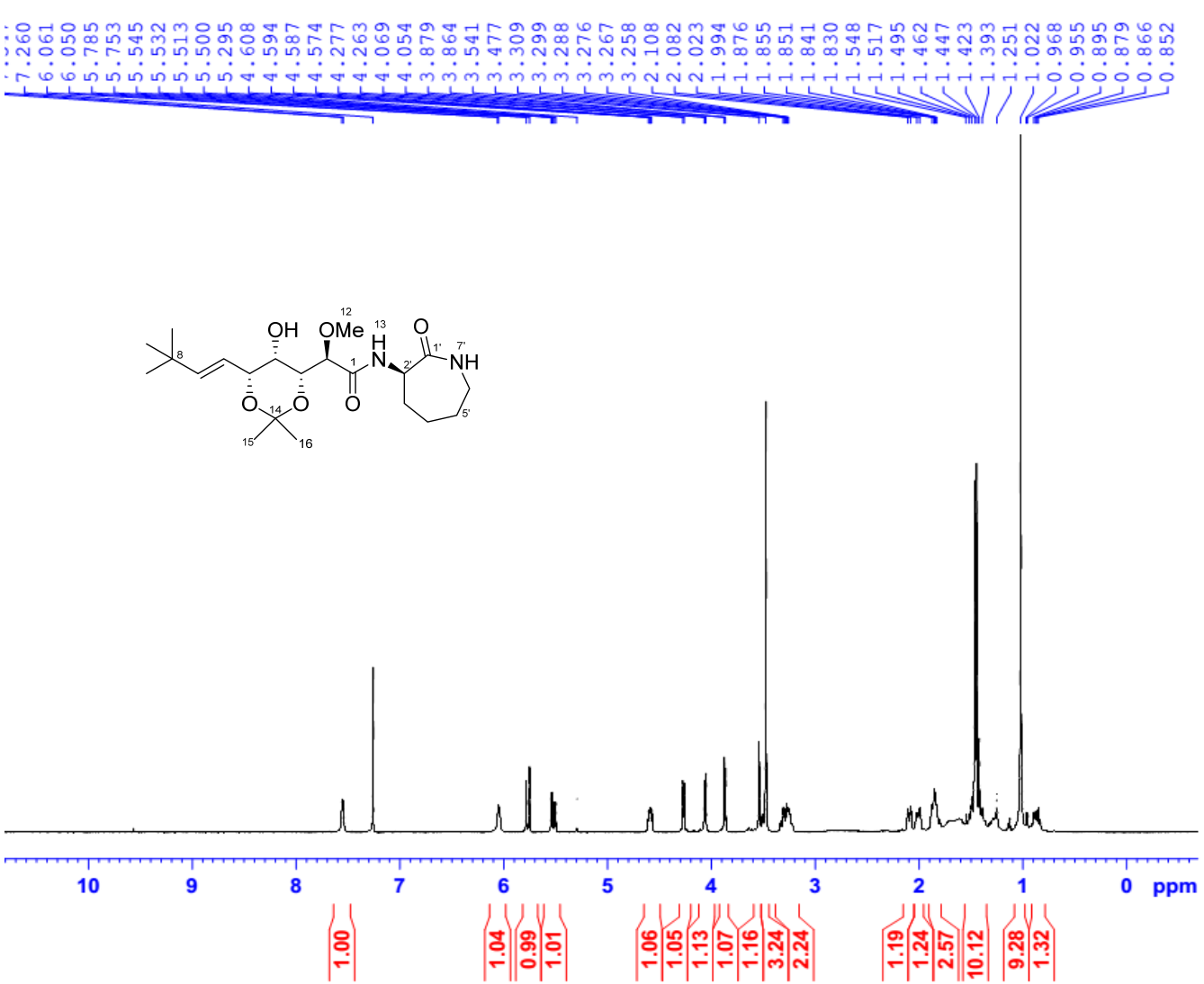

^{13}C NMR spectrum of **6a** (500 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      2DAO_30JUL15BG120
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150731
Time                 18.13
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    4096
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                  198.57
DW                  16.800 usec
DE                    6.50 usec
TE                   301.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          125.7879670 MHz
NUC1                    13C
P1                    10.00 usec
PLW1          88.00000000 W

======== CHANNEL f2 ========
SFO2          500.2020008 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                 80.00 usec
PLW2          22.00000000 W
PLW12          0.34375000 W
PLW13          0.22000000 W

F2 - Processing parameters
SI                    32768
SF          125.7753900 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

^{1}H NMR spectrum of **6b** (500 MHz, $CDCl_3$)

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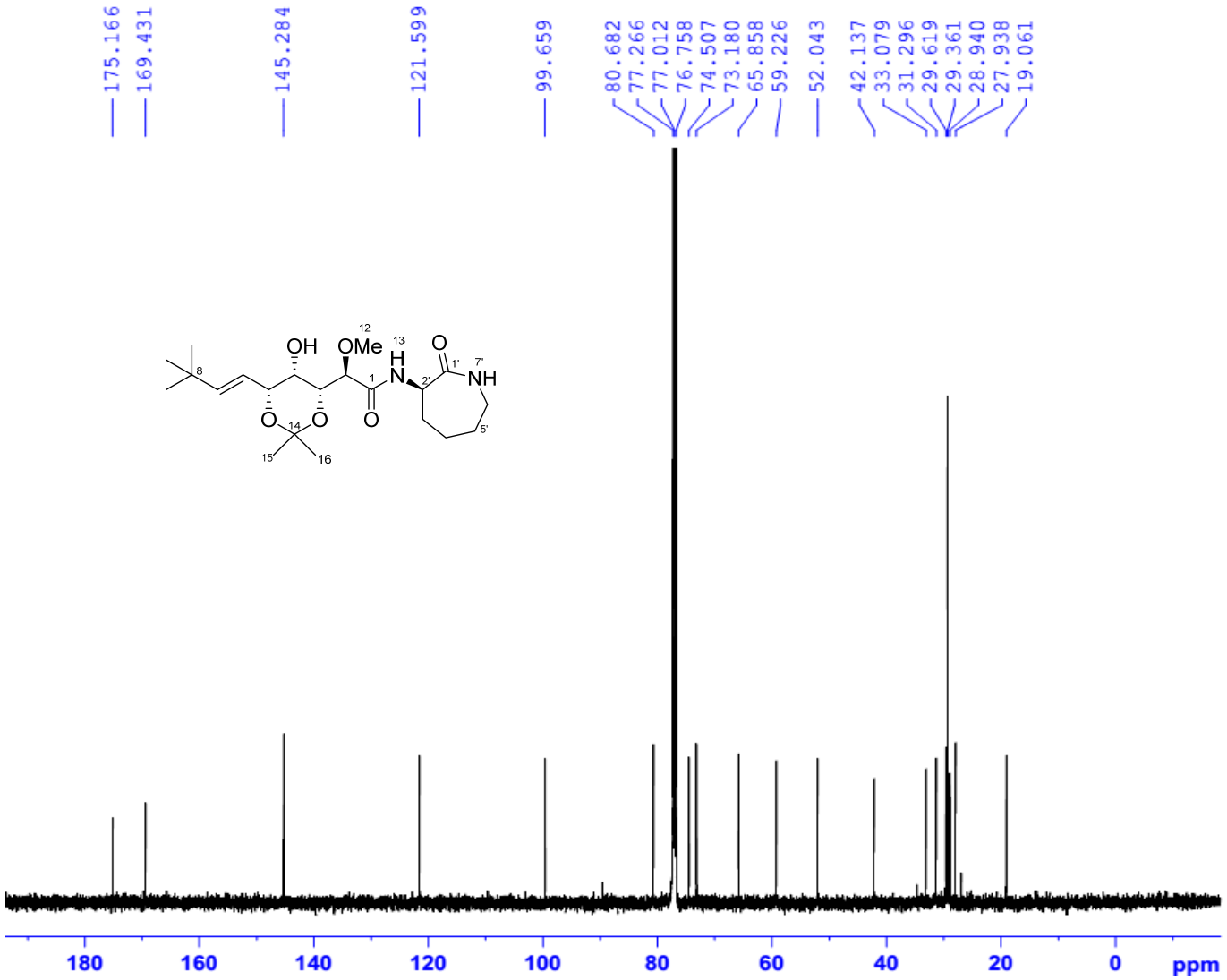
Current Data Parameters
NAME                  2HIEU_HD2
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20151007
Time                      17.36
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                  10000.000 Hz
FIDRES                0.152588 Hz
AQ                    3.2767999 sec
RG                       142.98
DW                        50.000 usec
DE                         6.50 usec
TE                        300.8 K
D1                   1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                500.2030889 MHz
NUC1                        1H
P1                        10.00 usec
PLW1                22.00000000 W

F2 - Processing parameters
SI                           65536
SF                  500.2000123 MHz
WDW                            EM
SSB                 0
LB                        0.30 Hz
GB                  0
PC                        1.00
```

^{13}C NMR spectrum of **6b** (500 MHz, $CDCl_3$)

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Current Data Parameters
NAME                  2HIEU_HD2
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20151009
Time                       7.58
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                         65536
SOLVENT                   CDCl3
NS                          1024
DS                             4
SWH                    29761.904 Hz
FIDRES                 0.454131 Hz
AQ                     1.1010048 sec
RG                        198.57
DW                        16.800 usec
DE                         6.50 usec
TE                        302.3 K
D1                     2.00000000 sec
D11                    0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                 125.7879670 MHz
NUC1                        13C
P1                        10.00 usec
PLW1                 88.00000000 W

======== CHANNEL f2 ========
SFO2                 500.2020008 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     80.00 usec
PLW2                 22.00000000 W
PLW12                 0.34375000 W
PLW13                 0.22000000 W

F2 - Processing parameters
SI                         32768
SF                   125.7753900 MHz
WDW                           EM
SSB                0
LB                         1.00 Hz
GB                 0
PC                         1.40
```
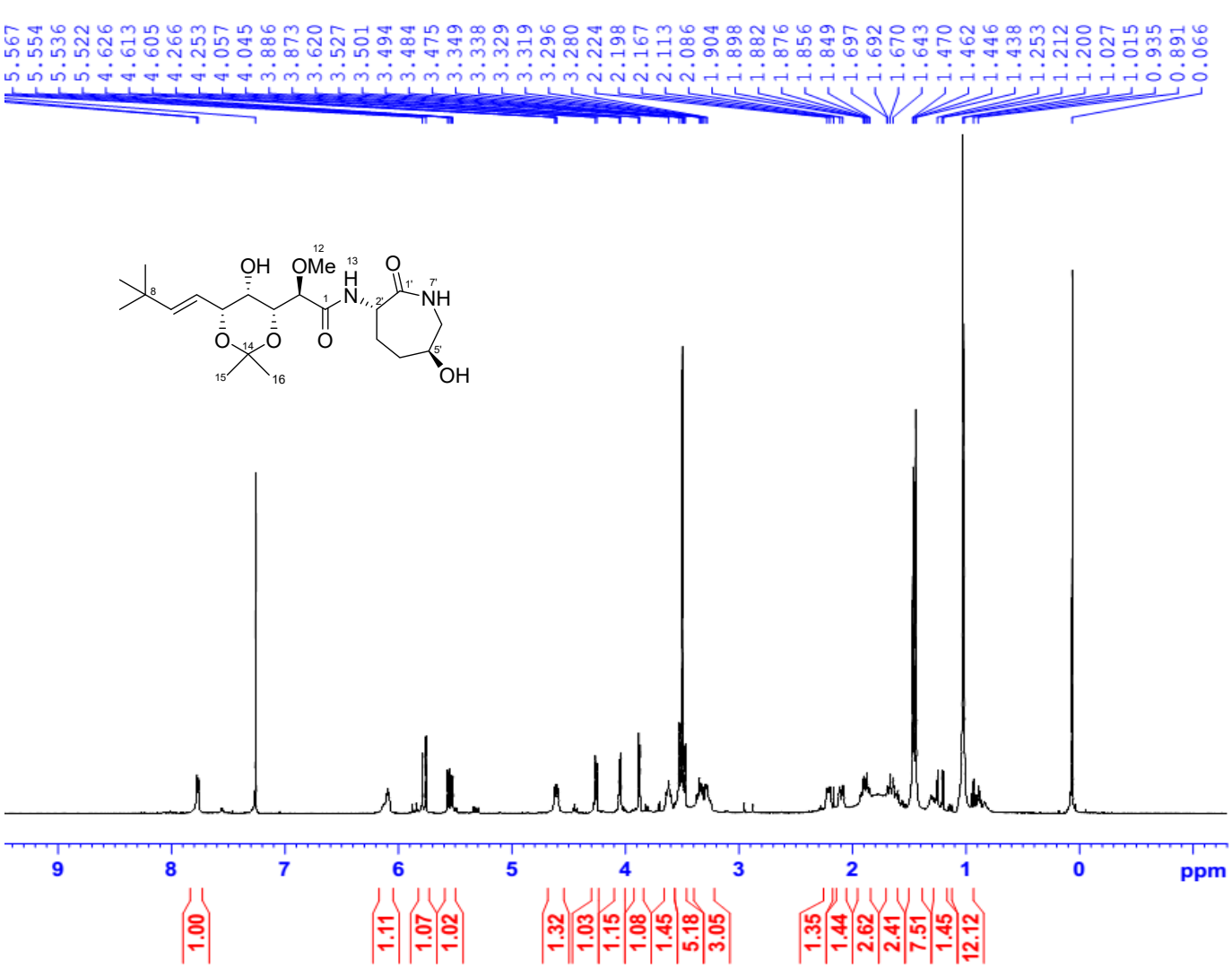

^{1}H NMR spectrum of **7a** (500 MHz, $CDCl_3$)

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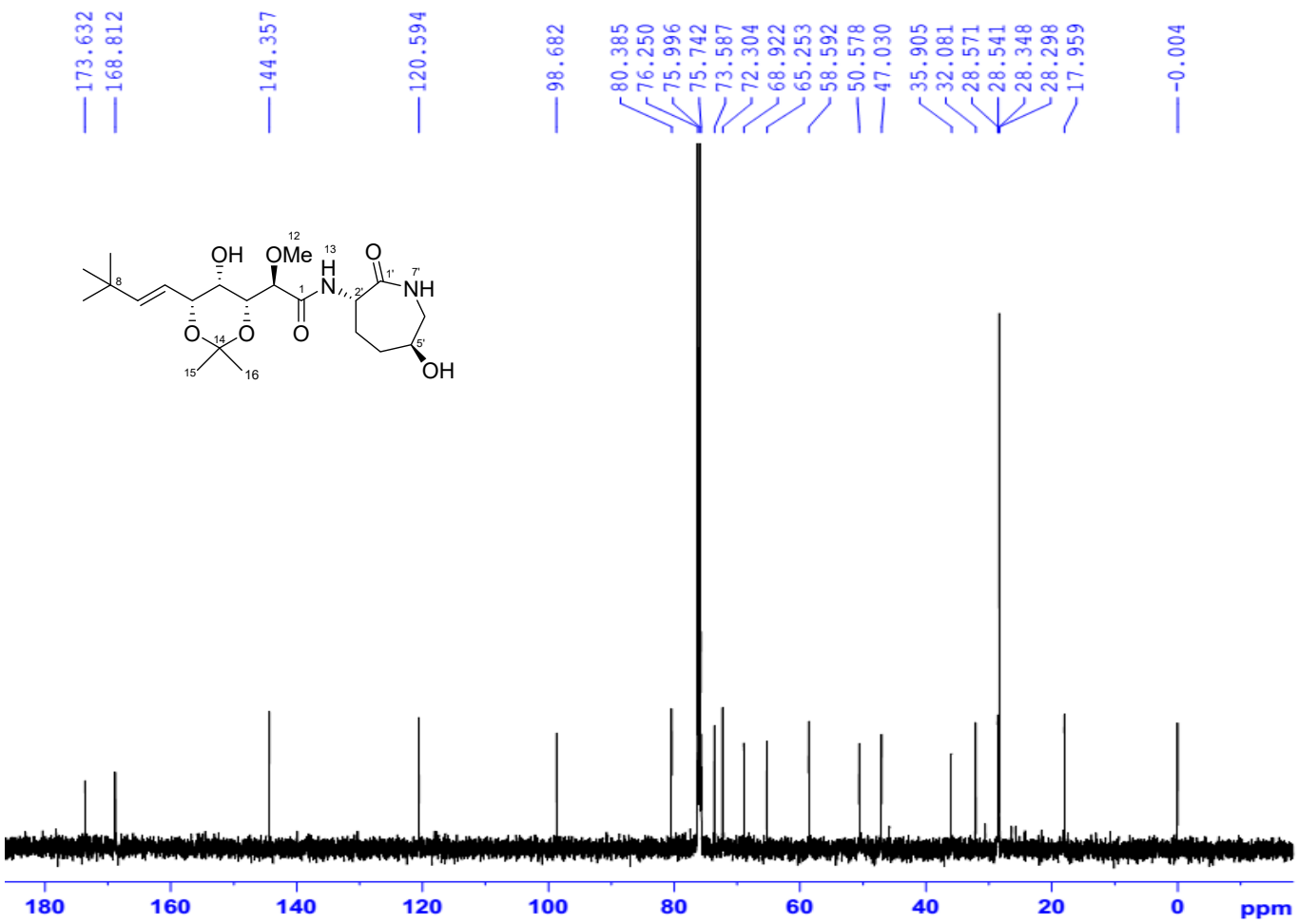
Current Data Parameters
NAME      2DAO_4JA16BG102A
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameter
Date_             20160108
Time                  4.37
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 se
RG                 157.35
DW                 50.000 us
DE                  6.50 us
TE                 301.7 K
D1           1.00000000 se
TD0                      1

======== CHANNEL f1 ======
SFO1         500.2030889 MH
NUC1                  1H
P1                10.00 us
PLW1         22.00000000 W

F2 - Processing parameters
SI                   65536
SF           500.2000122 MH
WDW                    EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C NMR spectrum of **7a** (500 MHz, $CDCl_3$)

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Current Data Parameters
NAME      2DAO_4JA16BG102A
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20160108
Time                  5.59
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1536
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                  198.57
DW                  16.800 usec
DE                   6.50 usec
TE                  302.3 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          125.7879670 MHz
NUC1                   13C
P1                   10.00 usec
PLW1          88.00000000 W

======== CHANNEL f2 ========
SFO2          500.2020008 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                80.00 usec
PLW2          22.00000000 W
PLW12          0.34375000 W
PLW13          0.22000000 W

F2 - Processing parameters
SI                    32768
SF           125.7755173 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```
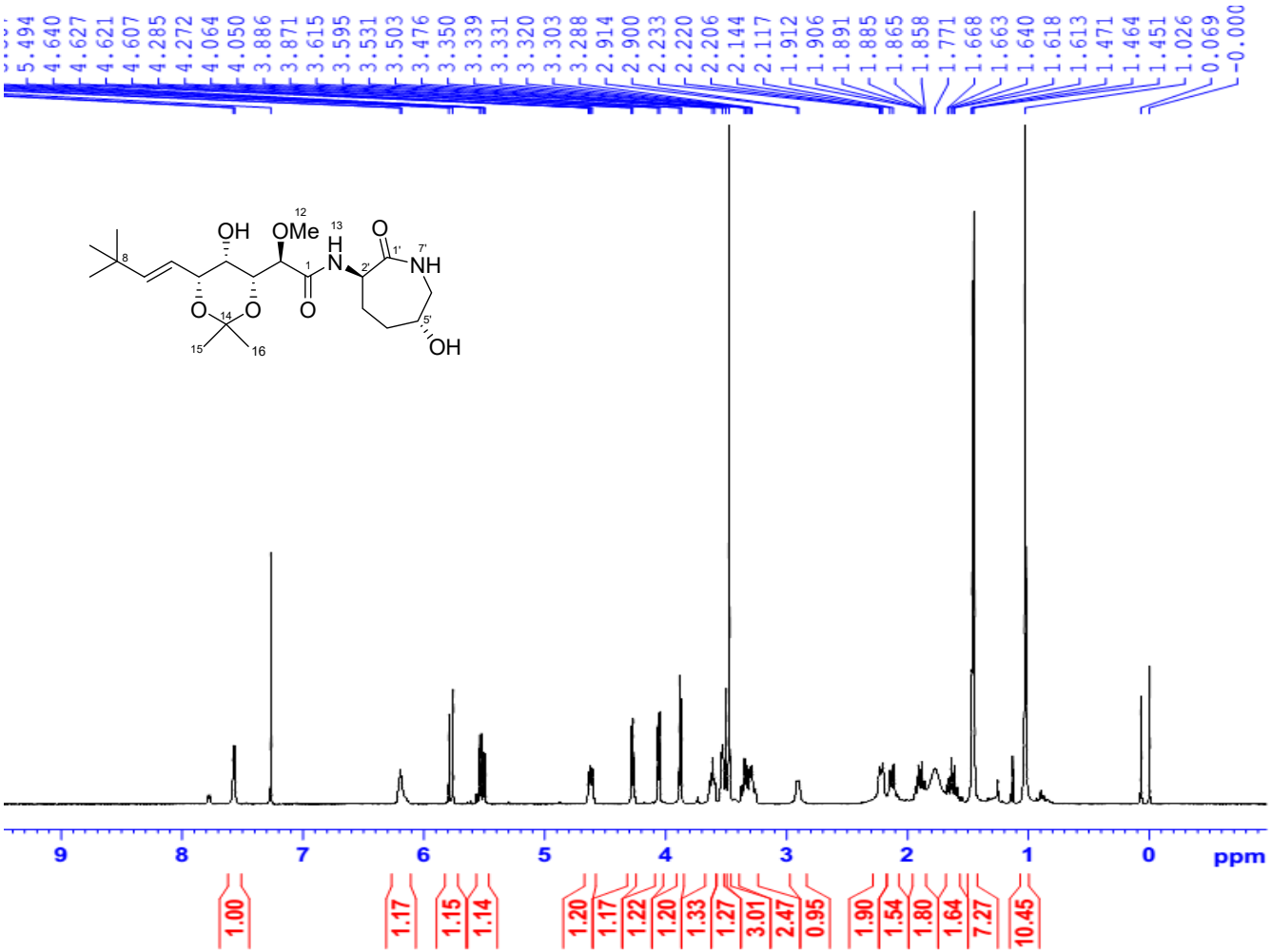

^{1}H NMR spectrum of **7b** (500 MHz, $CDCl_3$)

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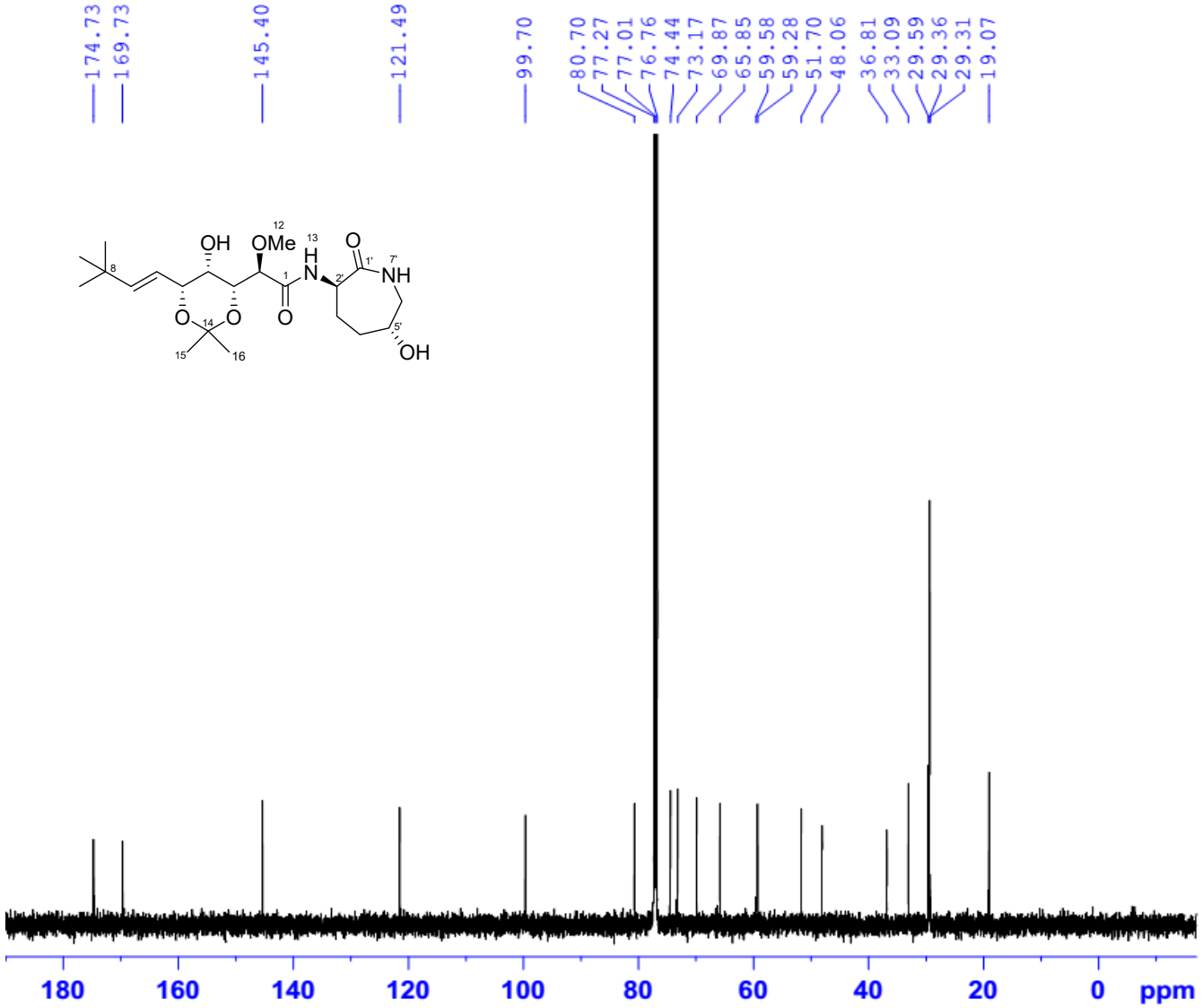
Current Data Parameters
NAME      2HIEU_BG102AB2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160427
Time              16.53
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ            3.2767999 sec
RG                127.68
DW                50.000 usec
DE                 6.50 usec
TE                301.1 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                   1H
P1                10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                    65536
SF           500.2000094 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C NMR spectrum of **7b** (500 MHz, $CDCl_3$)

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Current Data Parameters
NAME      2HIEU_BG102AB2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160502
Time              10.18
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               198.57
DW               16.800 usec
DE                6.50 usec
TE               303.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7879670 MHz
NUC1                13C
P1                10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                32768
SF          125.7753900 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```
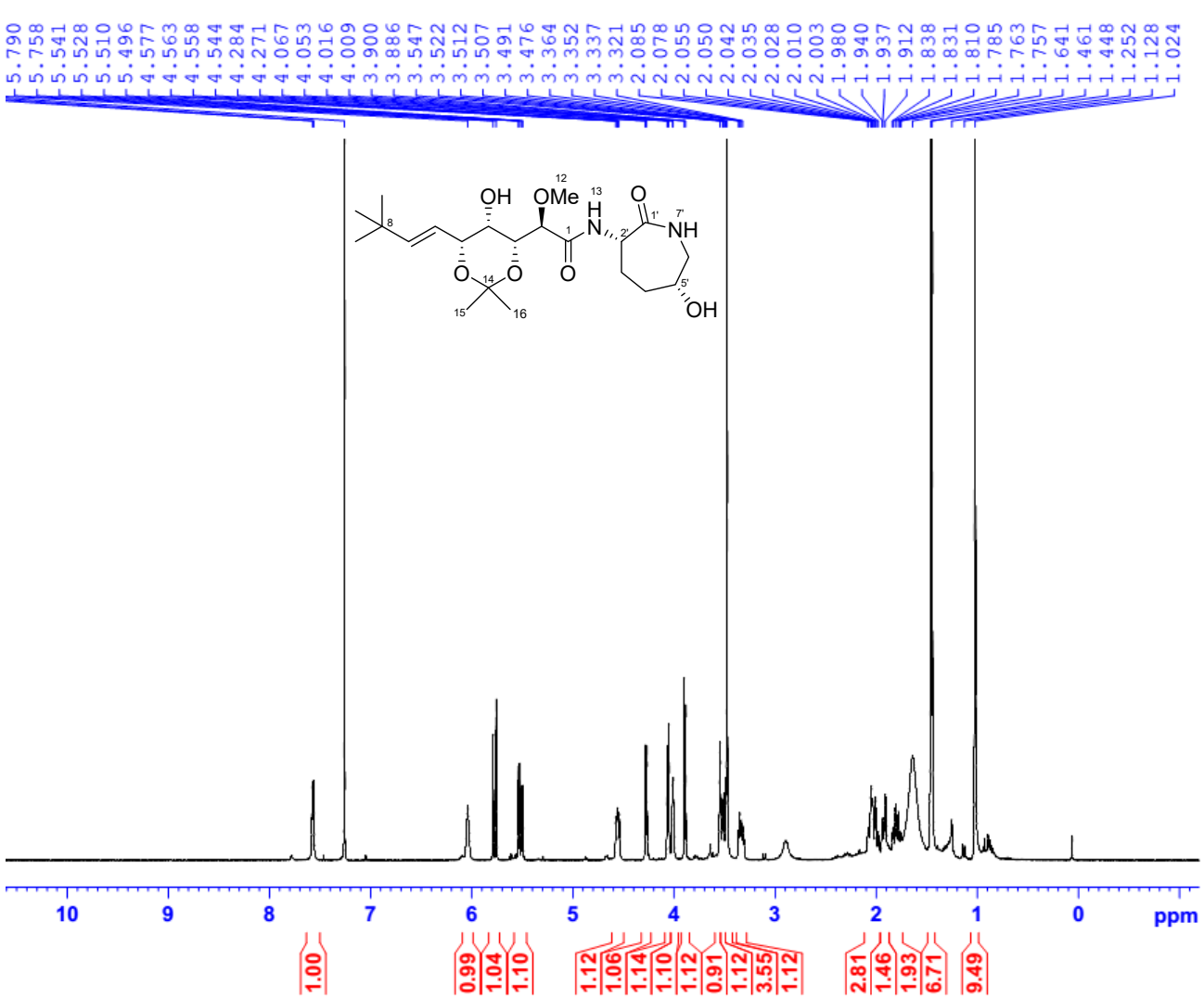

^{1}H NMR spectrum of **7c** (500 MHz, $CDCl_3$)

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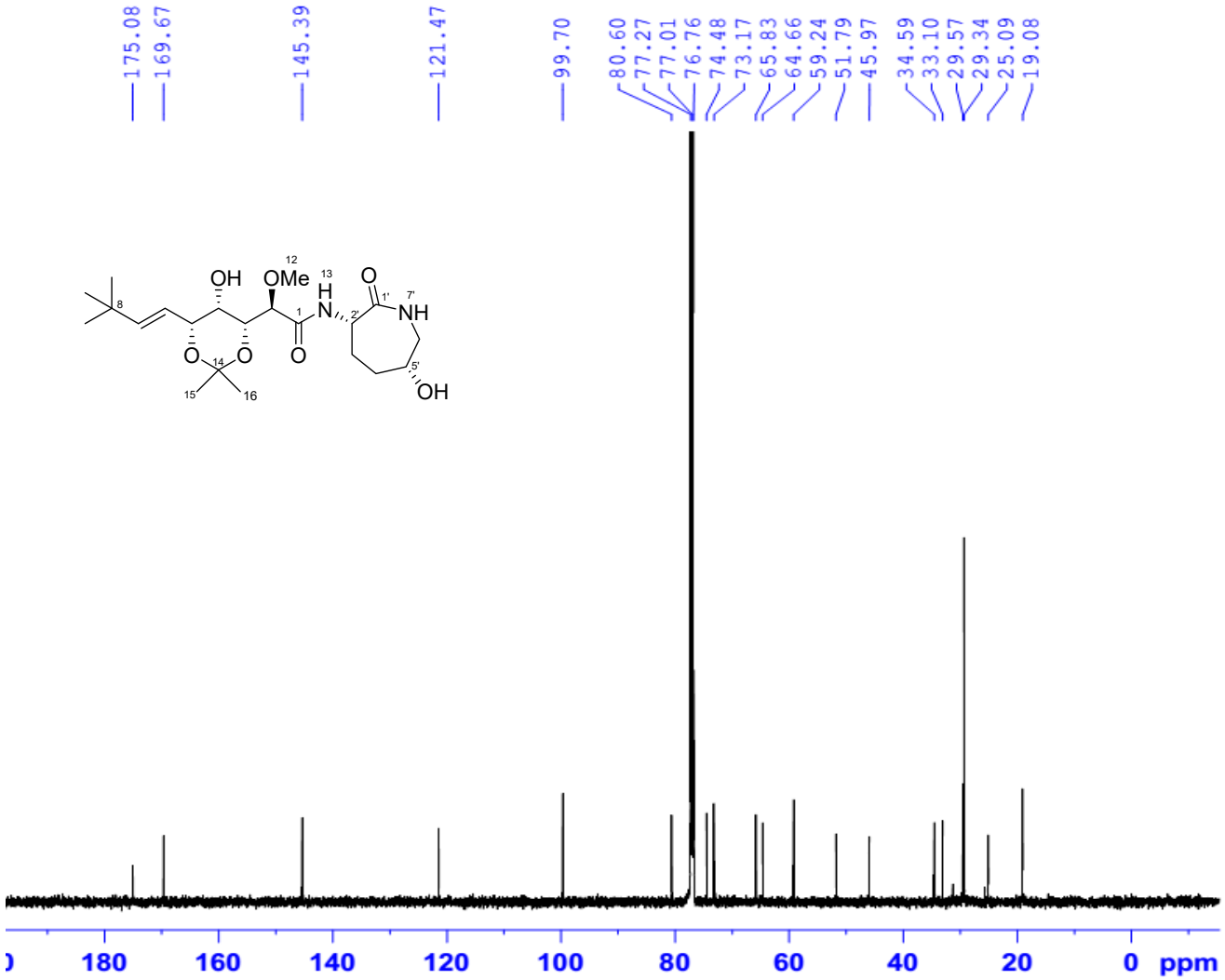
Current Data Parameters
NAME      2HIEU_BG102.2A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160324
Time              17.50
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG               175.34
DW               50.000 usec
DE                6.50 usec
TE               300.5 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                 1H
P1                10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                65536
SF           500.2000124 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C NMR spectrum of **7c** (500 MHz, $CDCl_3$)

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Current Data Parameters
NAME       2HIEUBG102.2A
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20160406
Time              22.26
INSTRUM           spect
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 4096
DS                    2
SWH           31446.541 Hz
FIDRES         0.479836 Hz
AQ             1.0420383 sec
RG                32768
DW               15.900 usec
DE                6.00 usec
TE                296.3 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST    0 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                  7.40 usec
PL1       0 dB
SFO1        125.7715724 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2               80.00 usec
PL2                 -3.00 dB
PL12                14.89 dB
PL13                22.00 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                   32768
SF           125.7577906 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```
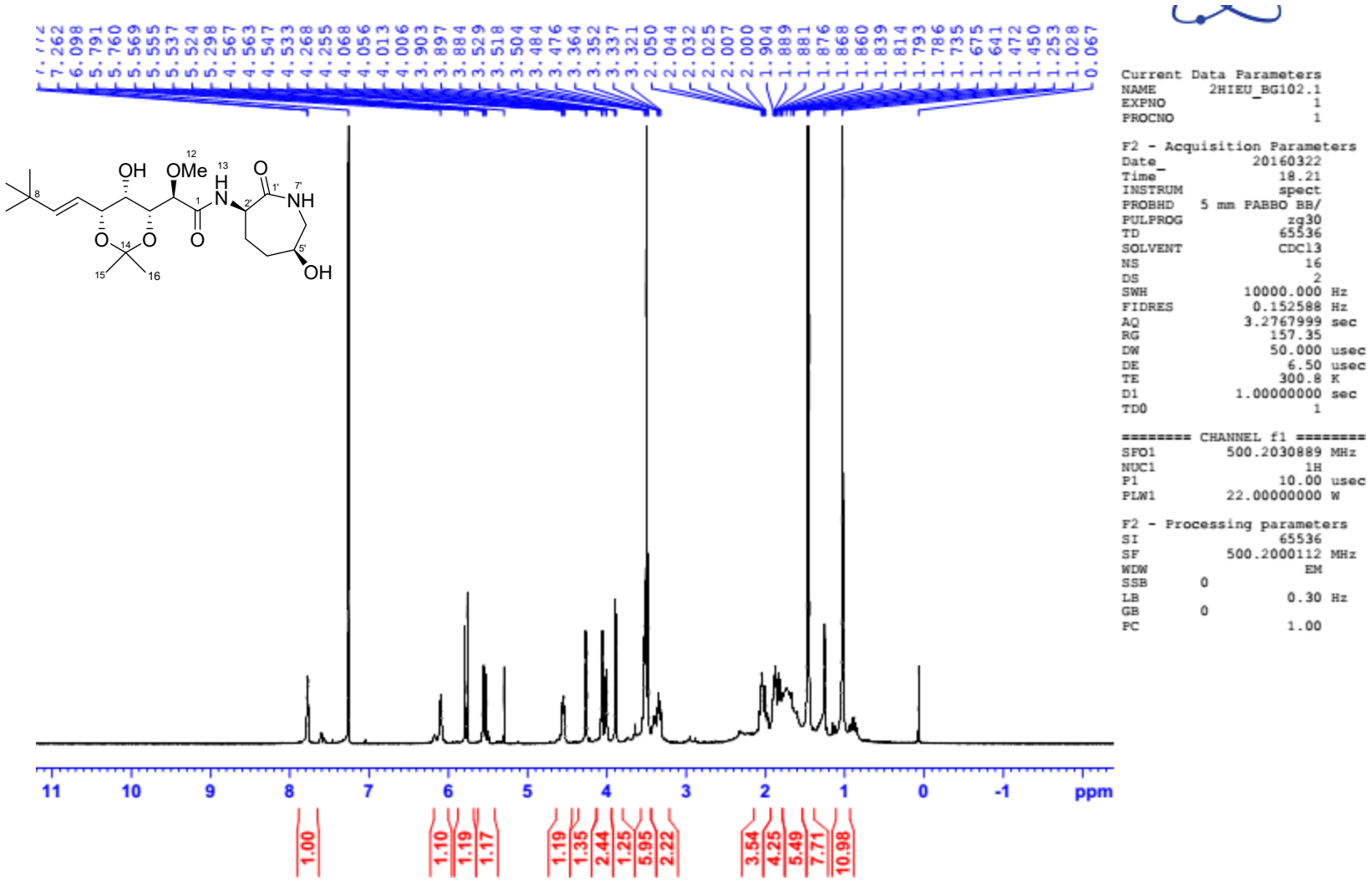
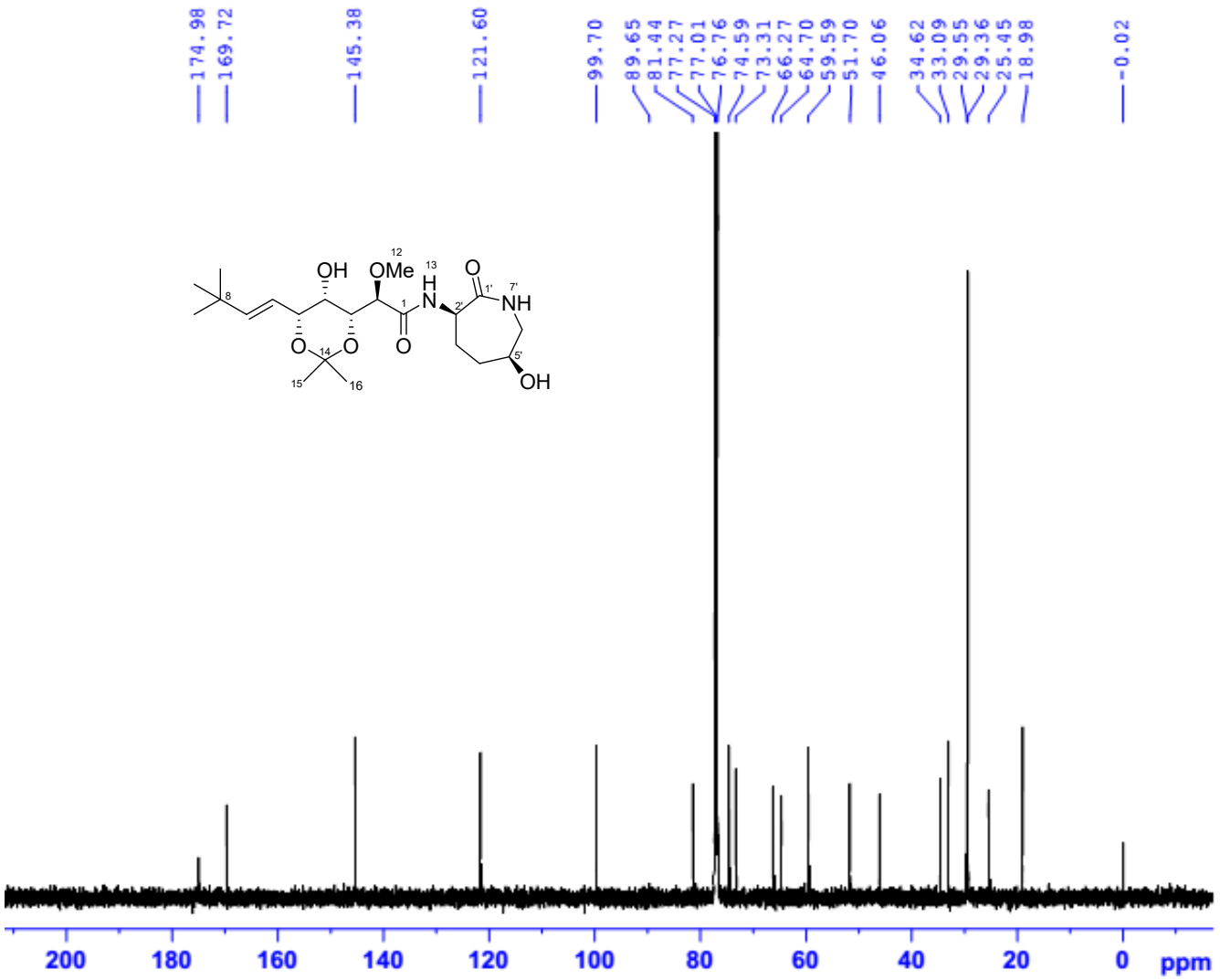

^{1}H NMR spectrum of **7d** (500 MHz, $CDCl_3$)



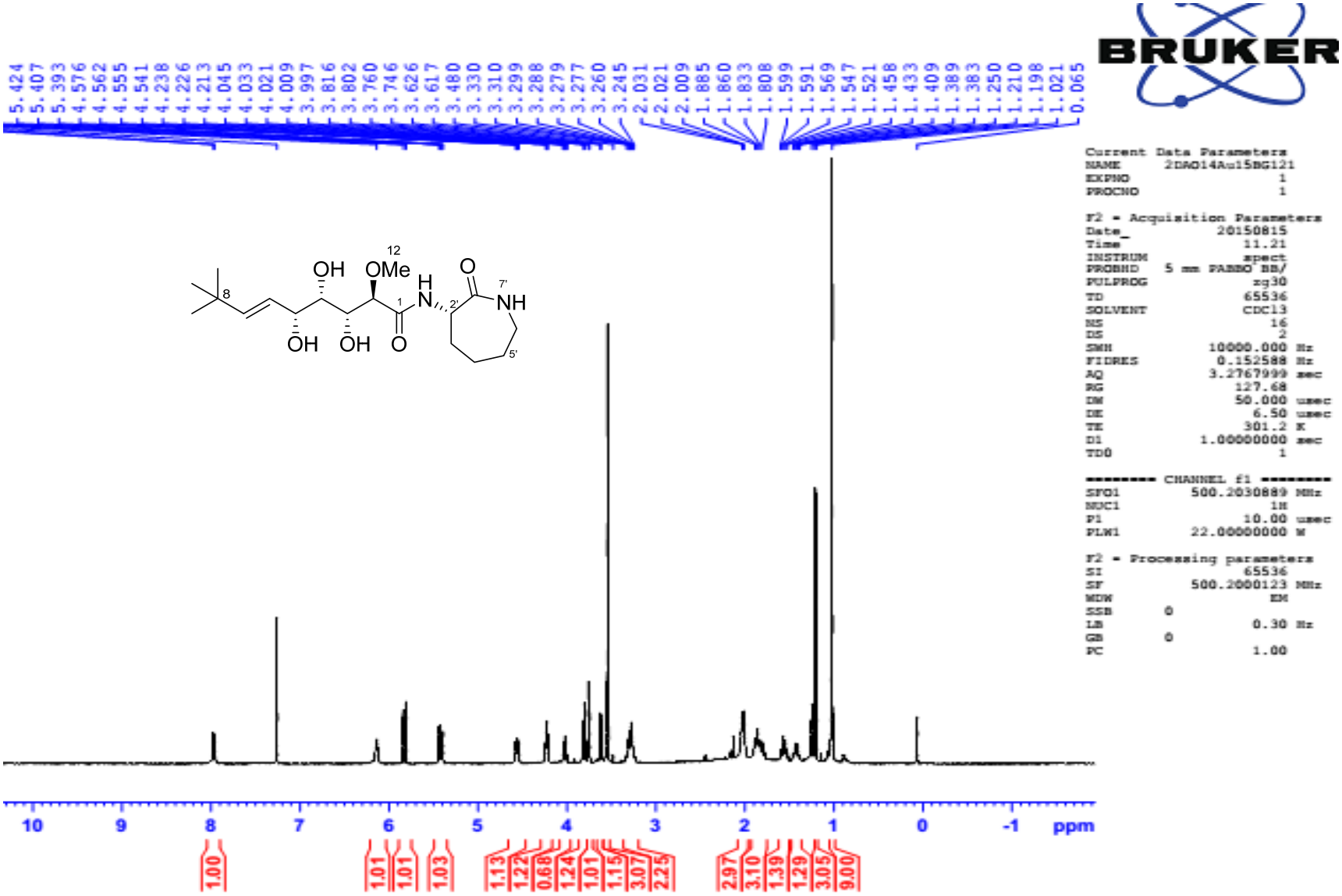

```
Current Data Parameters
NAME       2HIEU_BG102.1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160322
Time              18.21
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                157.35
DW                50.000 usec
DE                 6.50 usec
TE                300.8 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                  1H
P1                 10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000112 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C NMR spectrum of **7d** (500 MHz, $CDCl_3$)

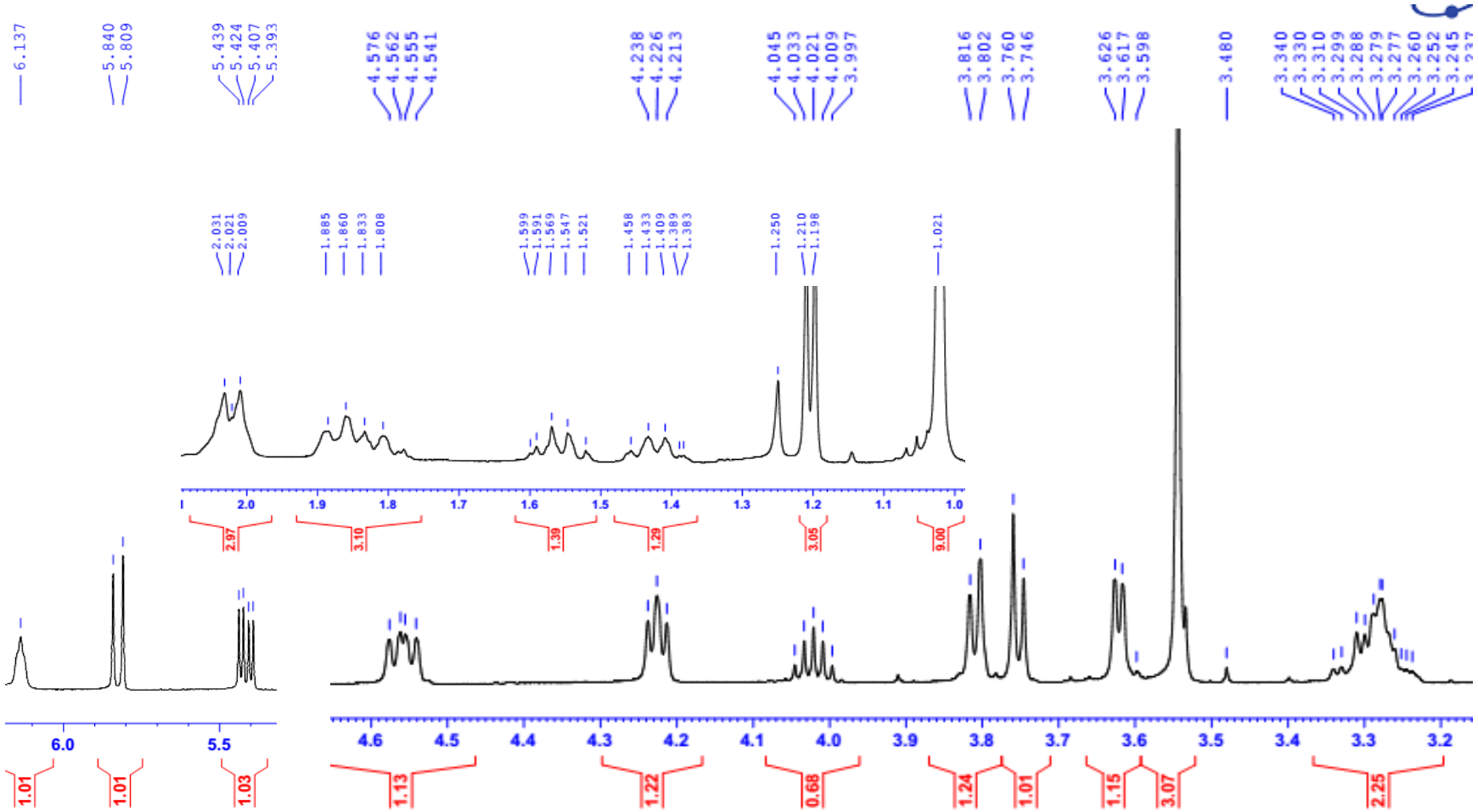



```
Current Data Parameters
NAME      2HIEU_BG102.1
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20160409
Time              16.37
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              65536
SOLVENT         CDCl3
NS               2117
DS                  4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG               198.57
DW               16.800 usec
DE                6.50 usec
TE               301.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         125.7879670 MHz
NUC1                13C
P1                10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                32768
SF           125.7753900 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

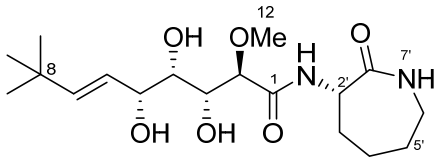
^{1}H NMR spectrum of **8a** (500 MHz, $CDCl_3$)

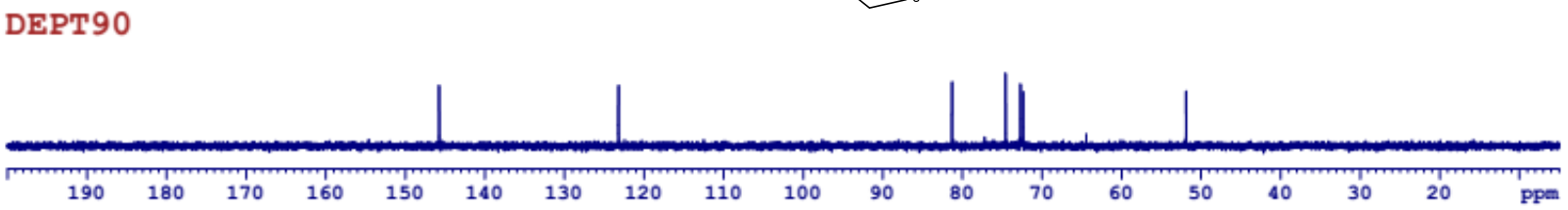


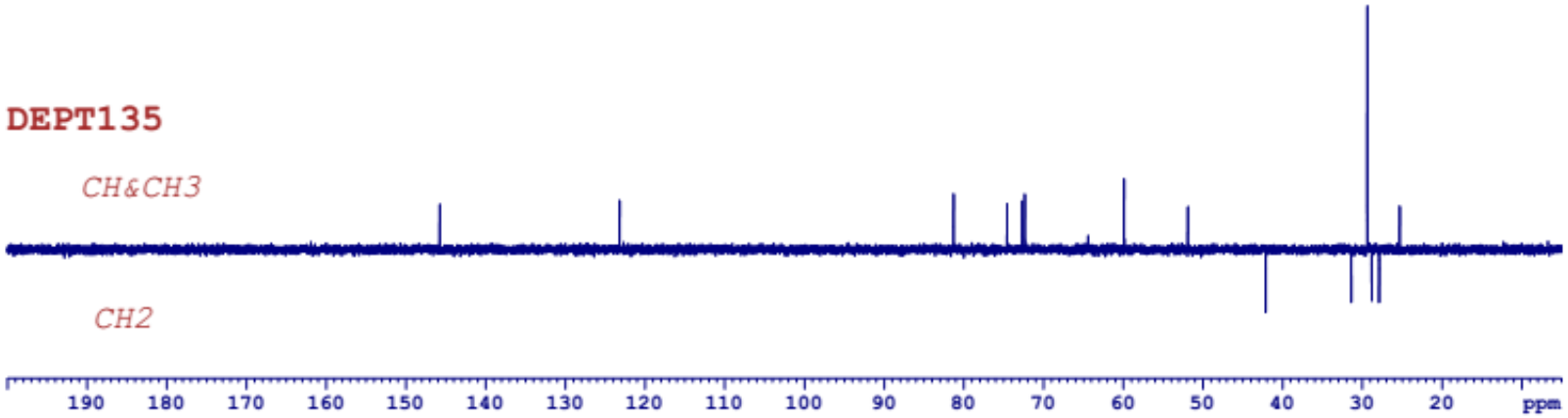
Expanded parts of ^{1}H NMR spectrum of **8a** (500 MHz, $CDCl_3$)

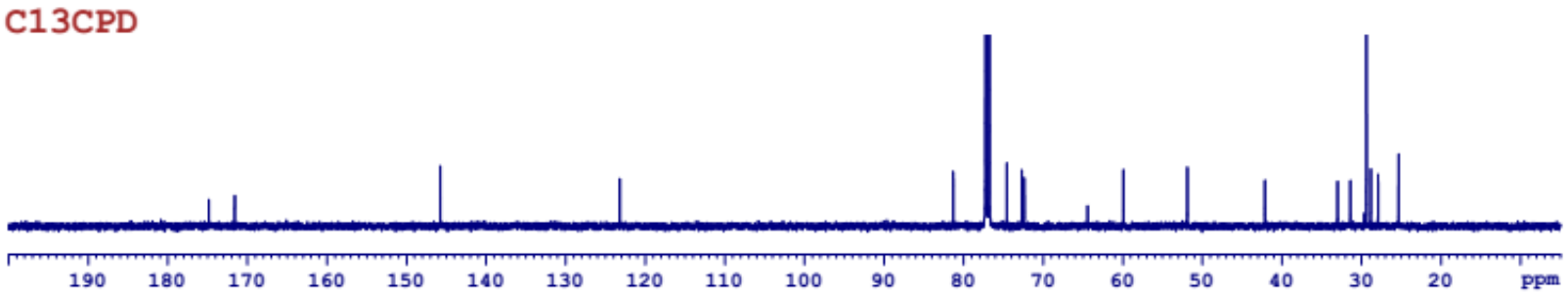


^{13}C NMR and DEPT spectra of **8a** (125 MHz, $CDCl_3$)

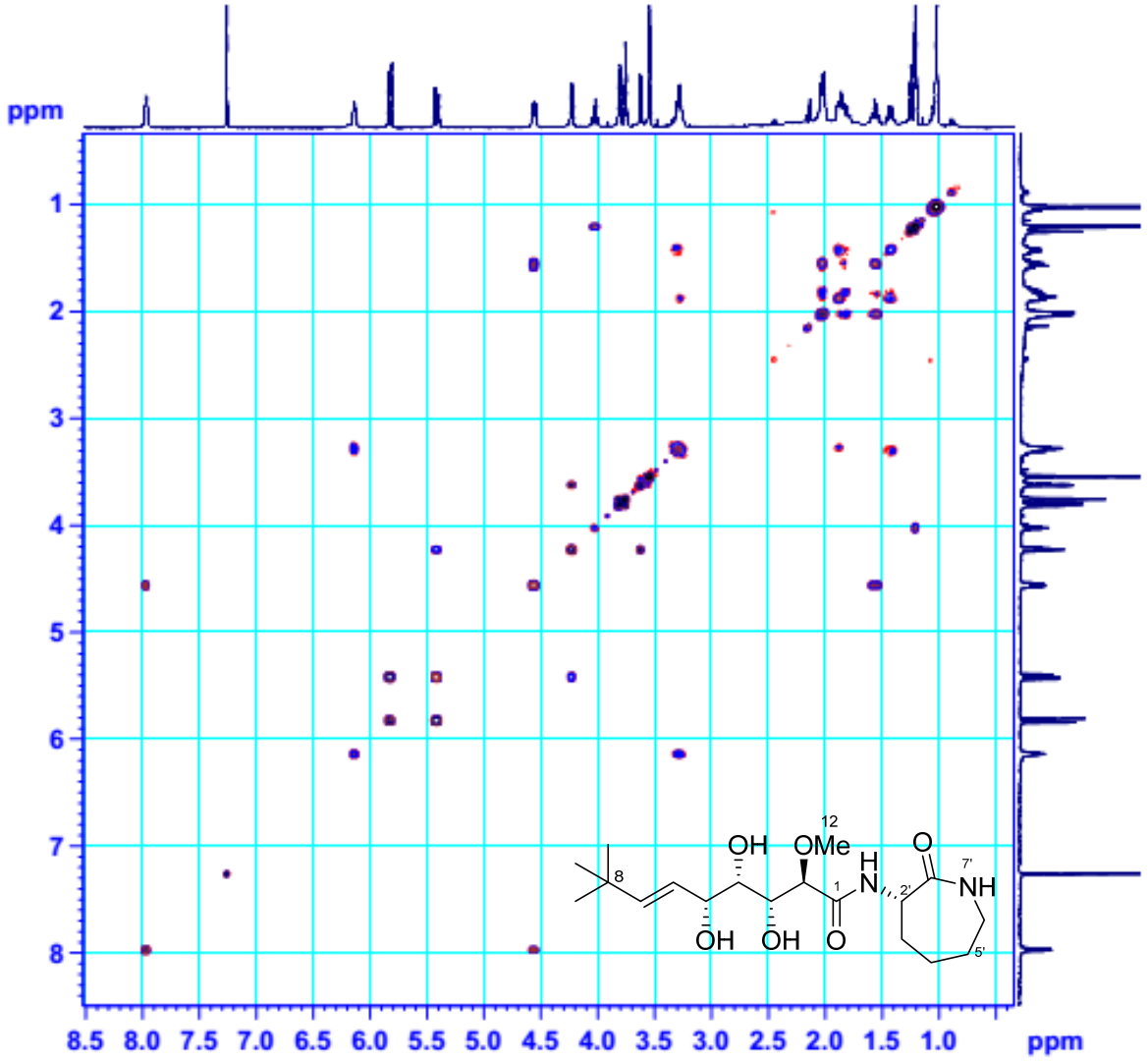








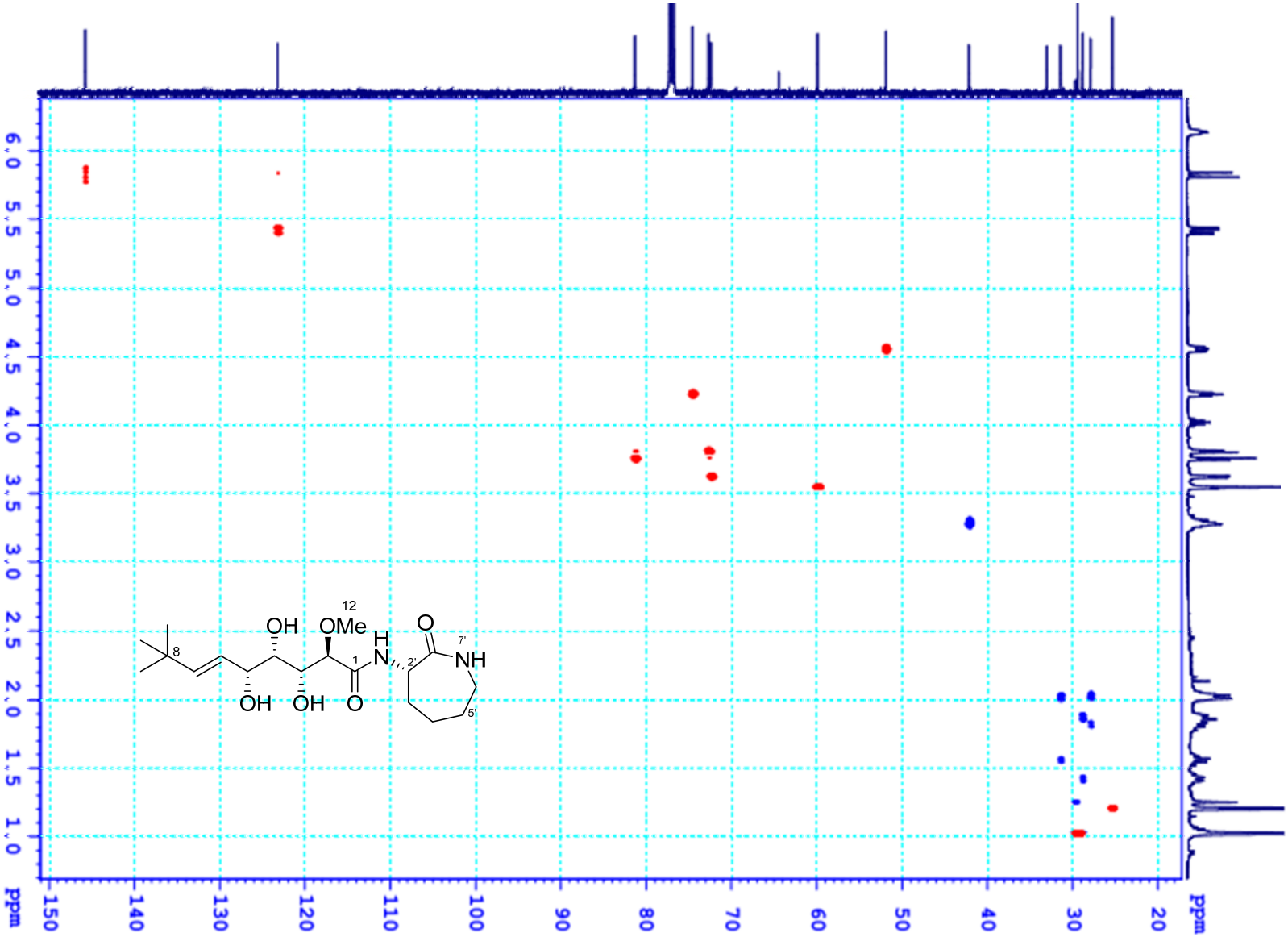
COSY spectrum of **8a** (500 MHz, $CDCl_3$)



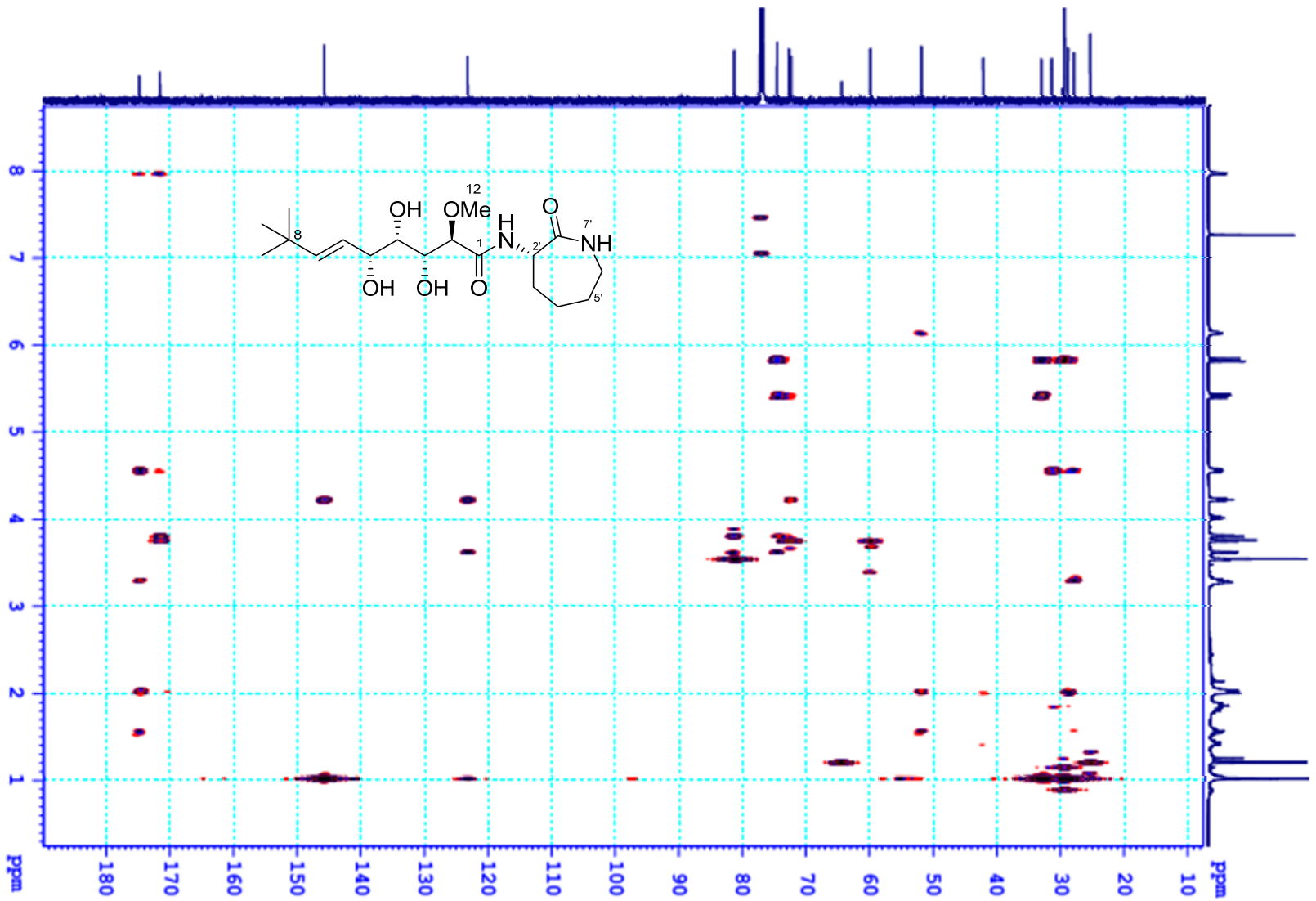
BRUKER

```
Current Data Parameters
NAME      2DAO14Au15RG121
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150817
Time                18.01
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     4
DS                     8
SWH              4761.905 Hz
FIDRES           2.325149 Hz
AQ               0.2150400 sec
RG                  64.21
DW                105.000 usec
DE                  6.50 usec
TE                300.1 K
D0               0.00000300 sec
D1               1.93815005 sec
D11              0.03000000 sec
D12              0.00002000 sec
D13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00021000 sec

======== CHANNEL f1 ========
SFO1          500.2019934 MHz
NUC1                  1H
P0                 10.00 usec
P1                 10.00 usec
P17              2500.00 usec
PLW1          22.00000000 W
PLW10          3.25440001 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   128
SFO1          500.202 MHz
FIDRES        37.202381 Hz
SW                9.520 ppm
FnMODE               QF

F2 - Processing parameters
SI                  1024
SF          500.2000098 MHz
WDW                 QSINE
SSB          0
LB           0 Hz
GB           0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF          500.2000097 MHz
WDW                 QSINE
SSB          0
LB           0 Hz
GB           0
```

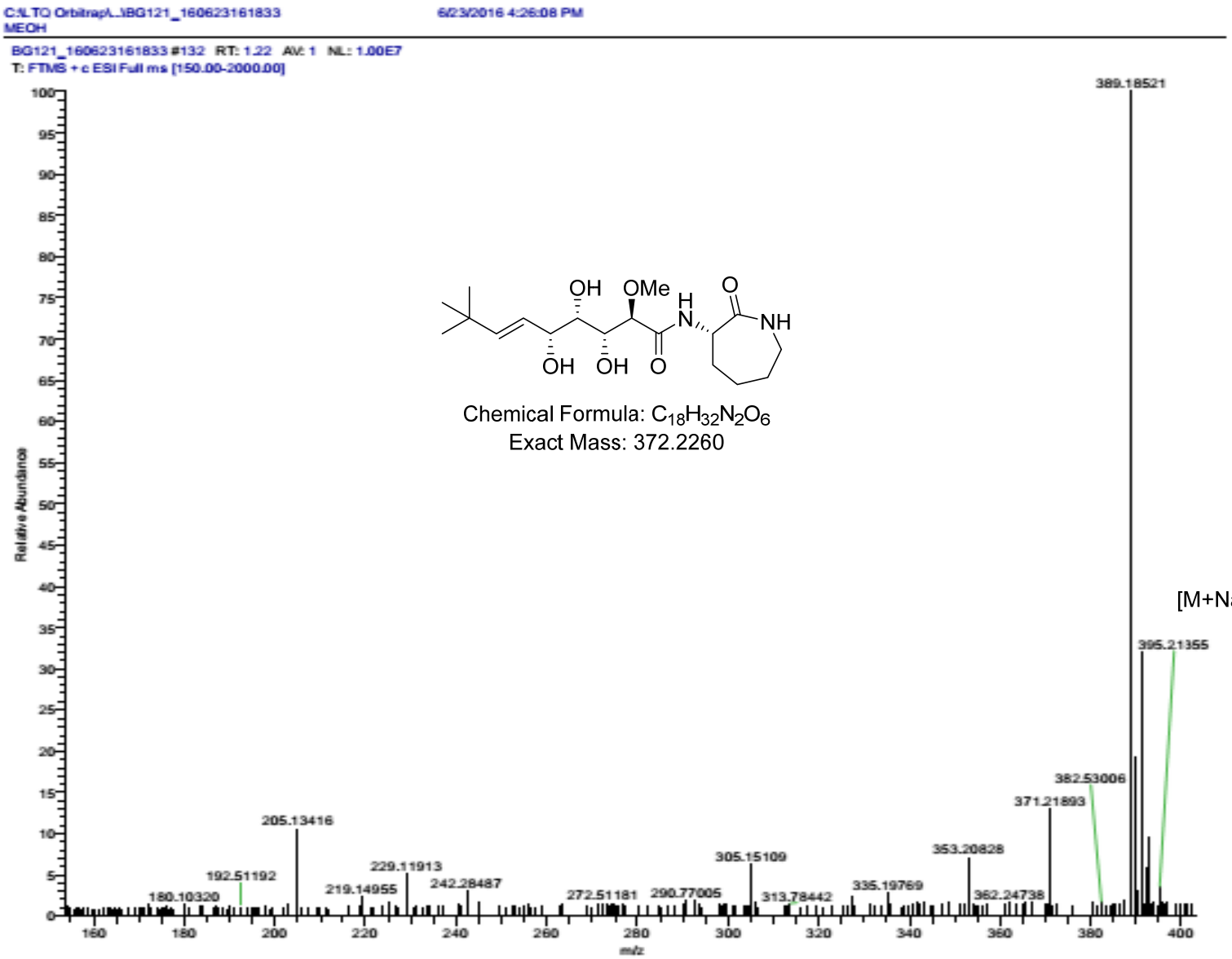
HSQC spectrum of **8a** (^{1}H: 500 MHz, ^{13}C: 125 MHz, $CDCl_3$)



HMBC spectrum of **8a** (^{1}H: 500 MHz, ^{13}C: 125 MHz, $CDCl_3$)

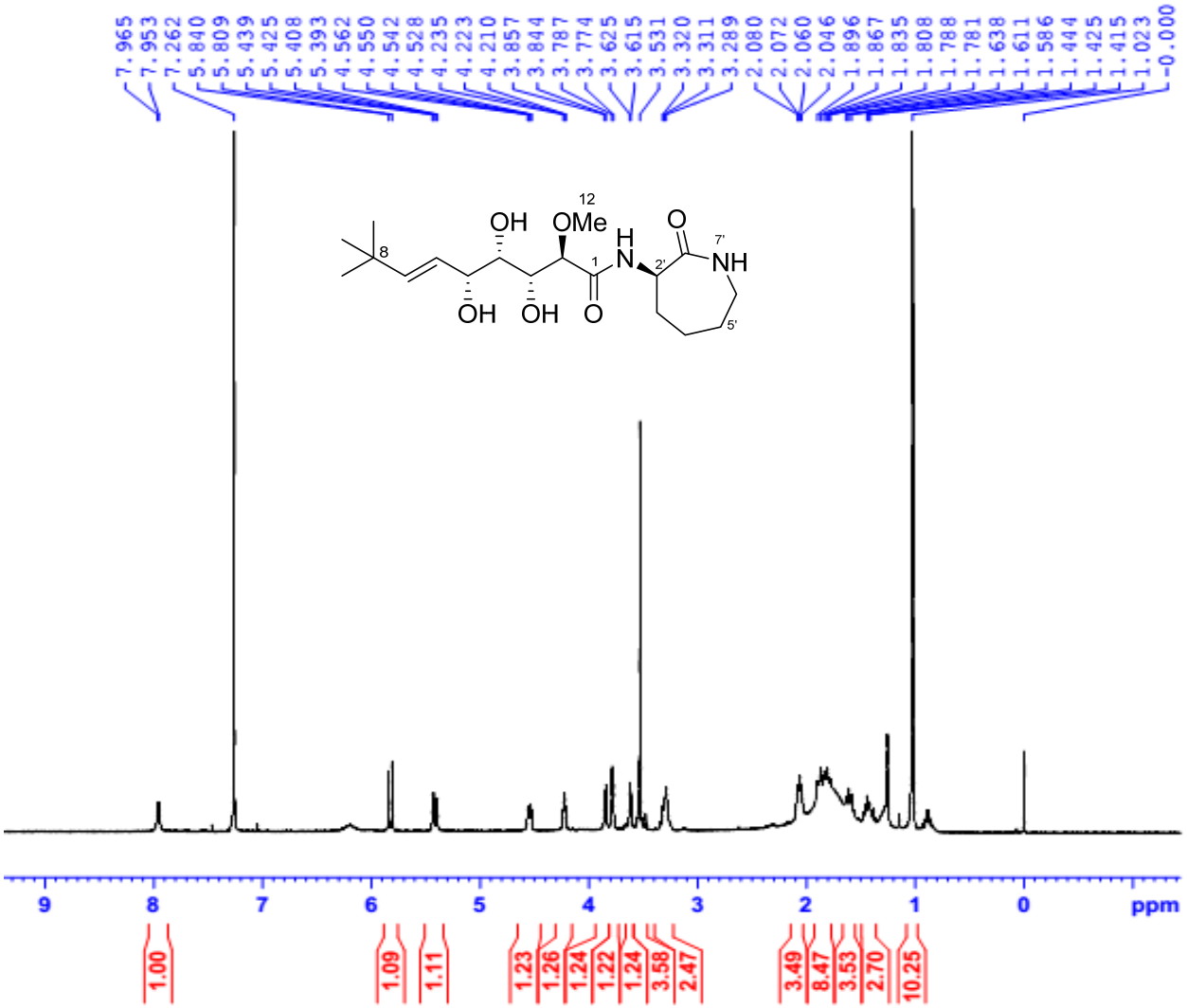


HRESI Mass spectrum of **8a**



Chemical Formula: $C_{18}H_{32}N_2O_6$
Exact Mass: 372.2260

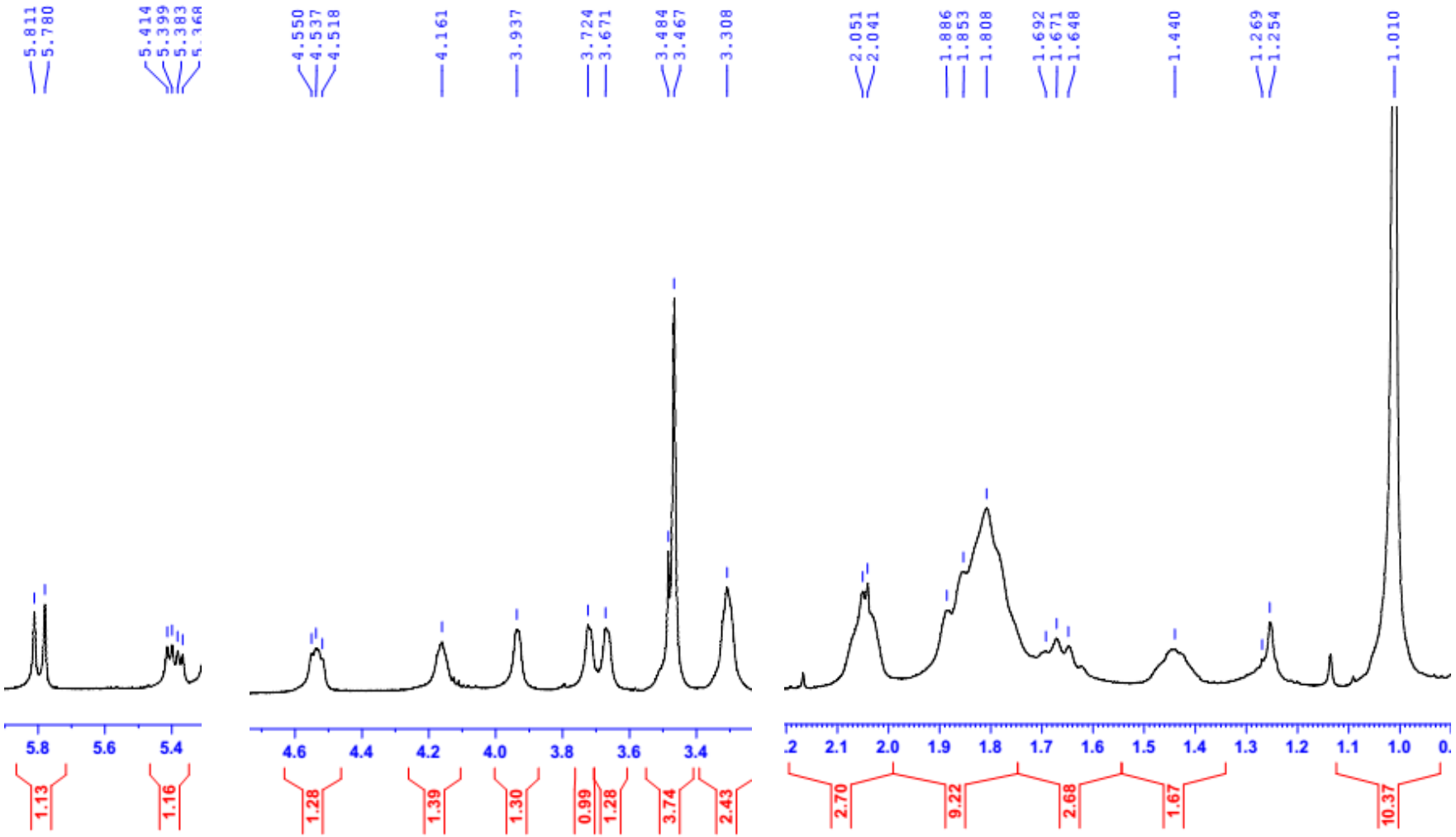
^{1}H NMR spectrum of **8b** (500 MHz, $CDCl_3$)



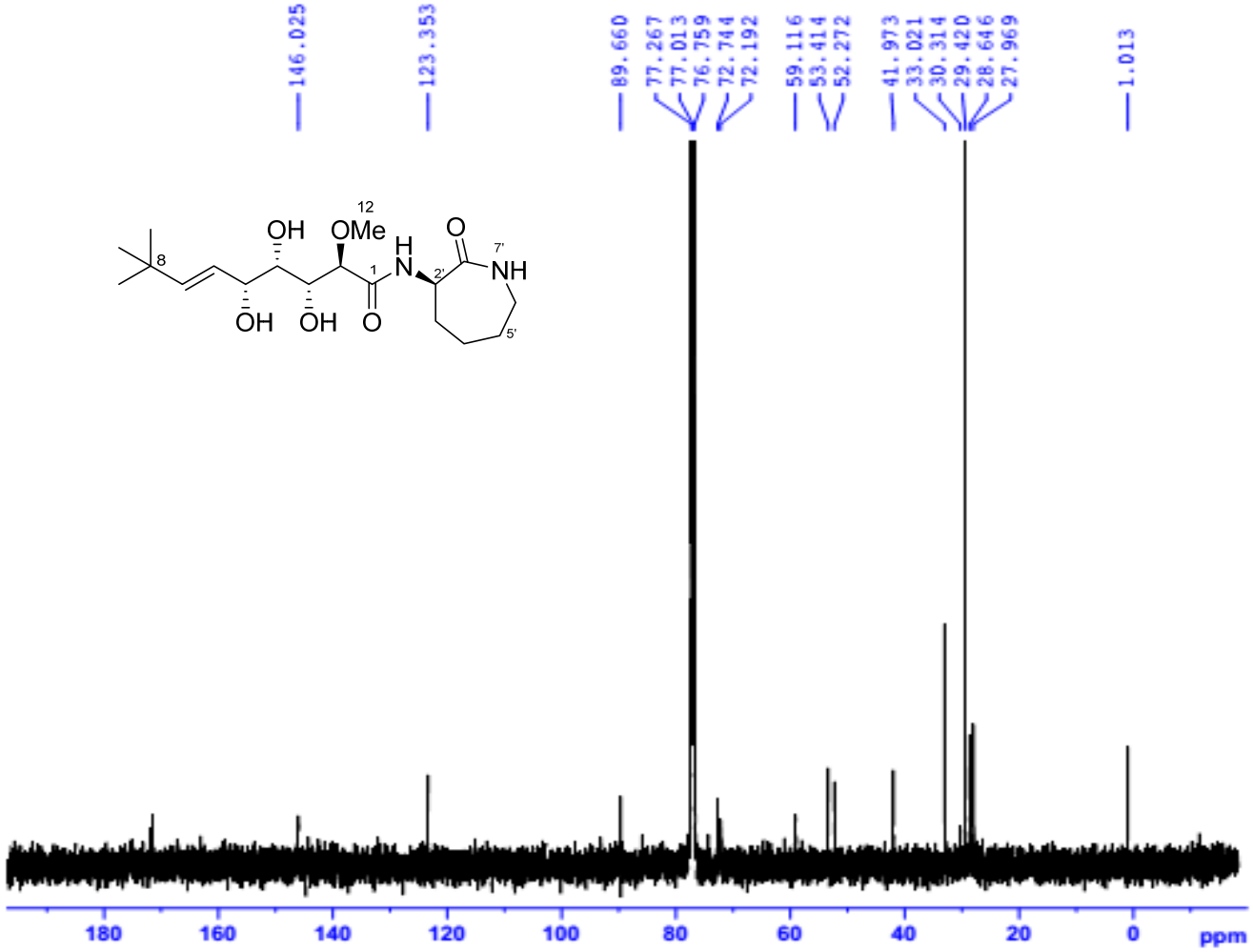
BRUKER

```
Current Data Parameters
NAME      2DAO12Oc15BG129
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151013
Time              10.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                198.57
DW                50.000 usec
DE                 6.50 usec
TE                300.0 K
D1             1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                  1H
P1                 10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                65536
SF            500.2000114 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Expanded parts of ^{1}H NMR spectrum of **8b** (500 MHz, $CDCl_3$)

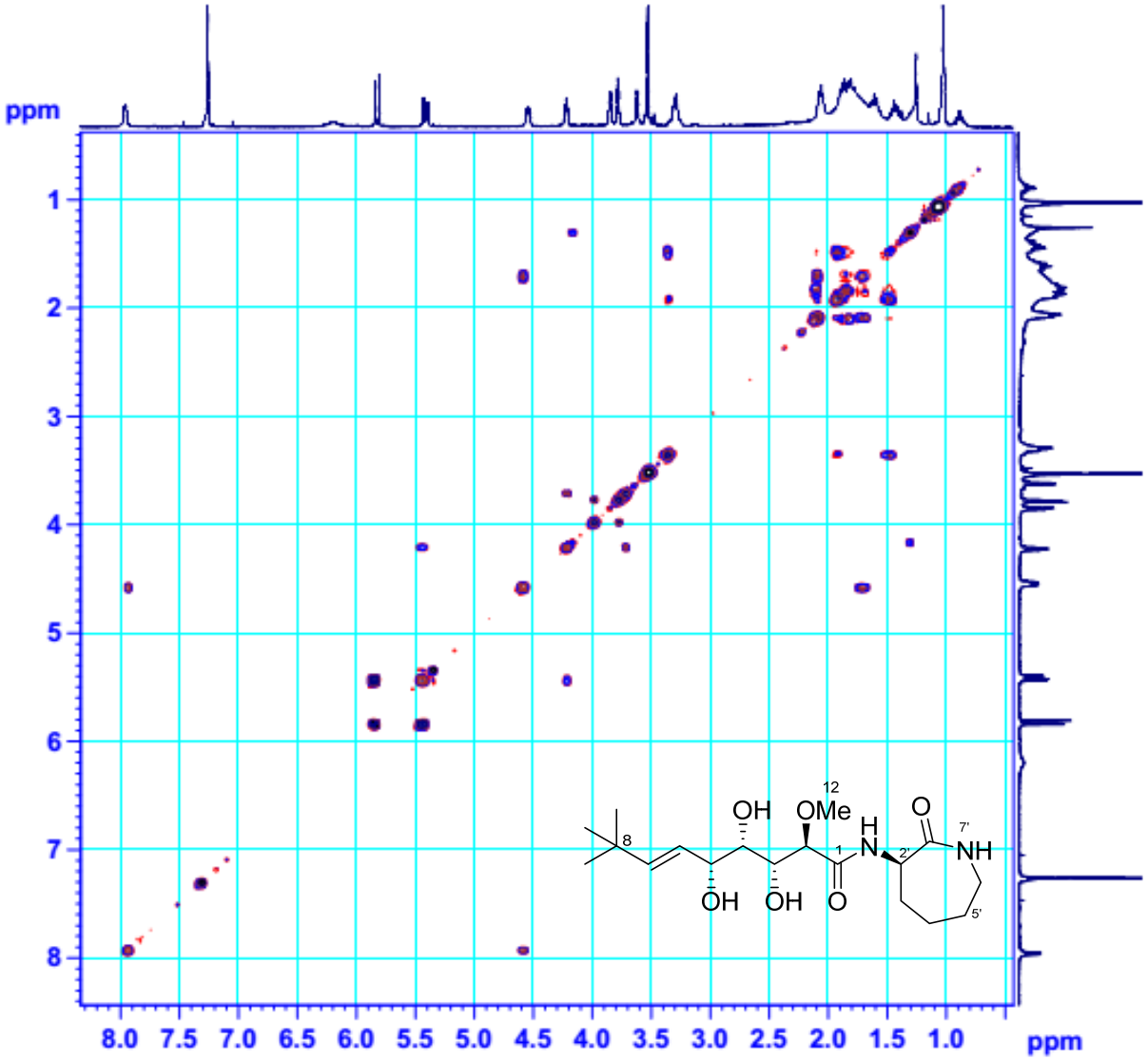


^{13}C NMR spectrum of **8b** (125 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      2DAO12Oc15BG129
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151014
Time                 0.24
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 4096
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG                198.57
DW                16.800 usec
DE                 6.50 usec
TE                301.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7879670 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                32768
SF           125.7753900 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

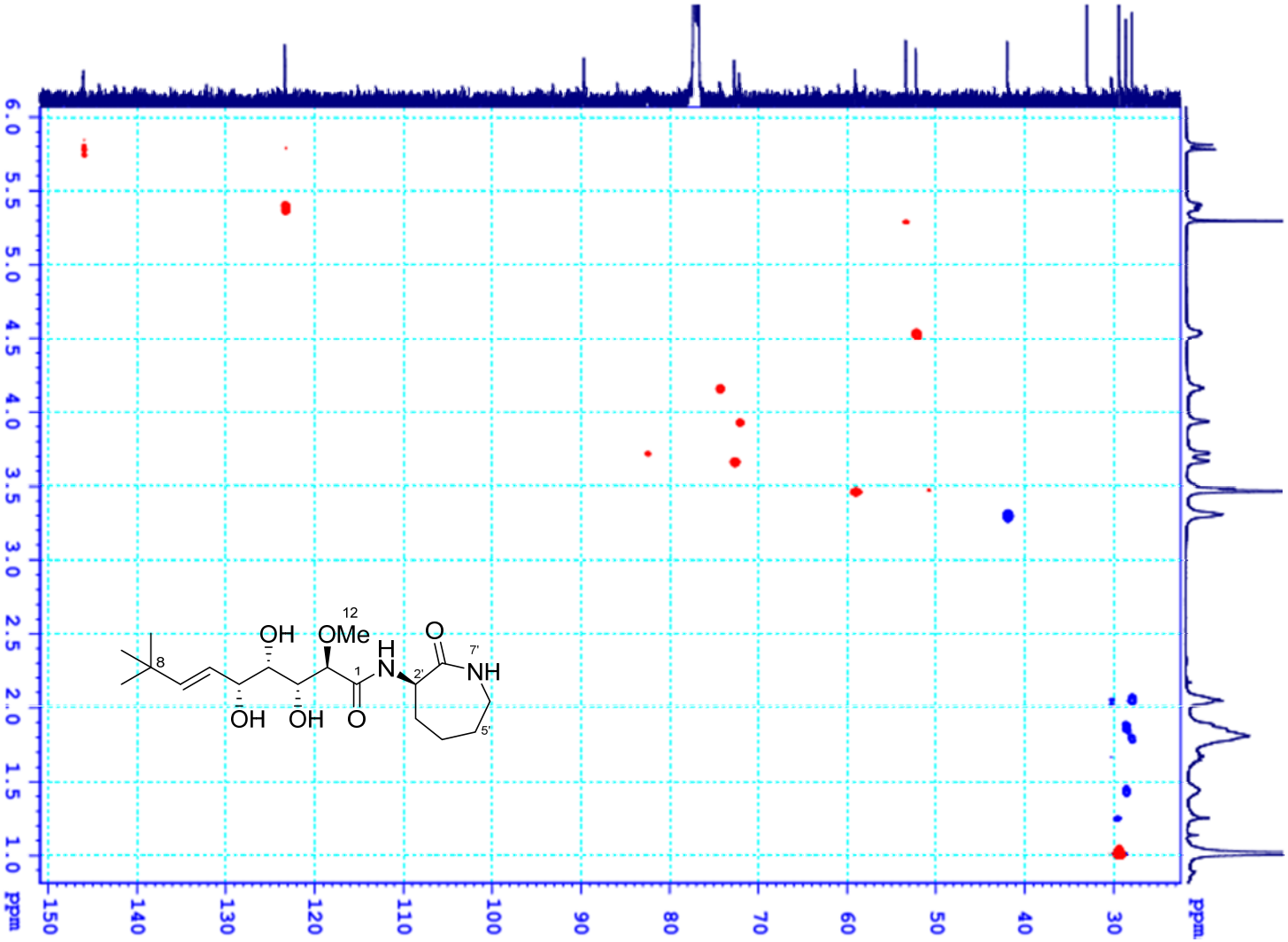
COSY spectrum of **8b** (500 MHz, $CDCl_3$)



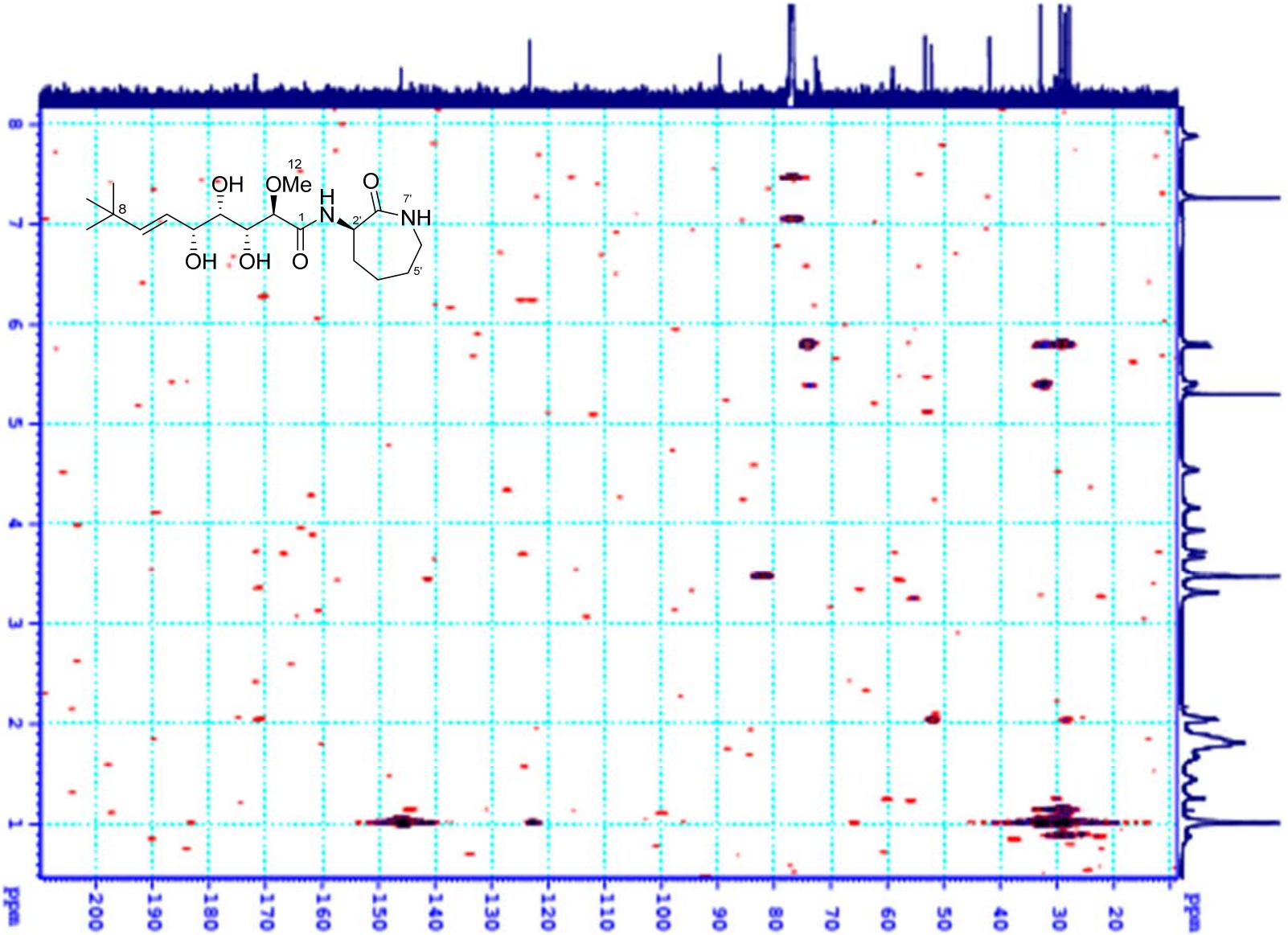
BRUKER

```
Current Data Parameters
NAME      20AO12Oc15BG129
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151014
Time                1.41
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     8
DS                     8
SWH             4672.897 Hz
FIDRES          2.281688 Hz
AQ              0.2191360 sec
RG                 64.21
DW                107.000 usec
DE                  6.50 usec
TE                300.3 K
D0              0.00000300 sec
D1              1.93405402 sec
D11             0.03000000 sec
D12             0.00002000 sec
D13             0.00000400 sec
D16             0.00020000 sec
IN0             0.00021400 sec

======== CHANNEL f1 ========
SFO1          500.2019858 MHz
NUC1                  1H
P0                 10.00 usec
P1                 10.00 usec
P17              2500.00 usec
PLW1          22.00000000 W
PLW10          3.25440001 W

====== GRADIENT CHANNEL =====
GPNAM[1]       SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   128
SFO1          500.202 MHz
FIDRES        36.507008 Hz
SW                9.342 ppm
FnMODE               QF

F2 - Processing parameters
SI                  1024
SF          500.1999853 MHz
WDW                 QSINE
SSB                    0
LB                  0 Hz
GB                     0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF          500.1999873 MHz
WDW                 QSINE
SSB                    0
LB                  0 Hz
GB                     0
```

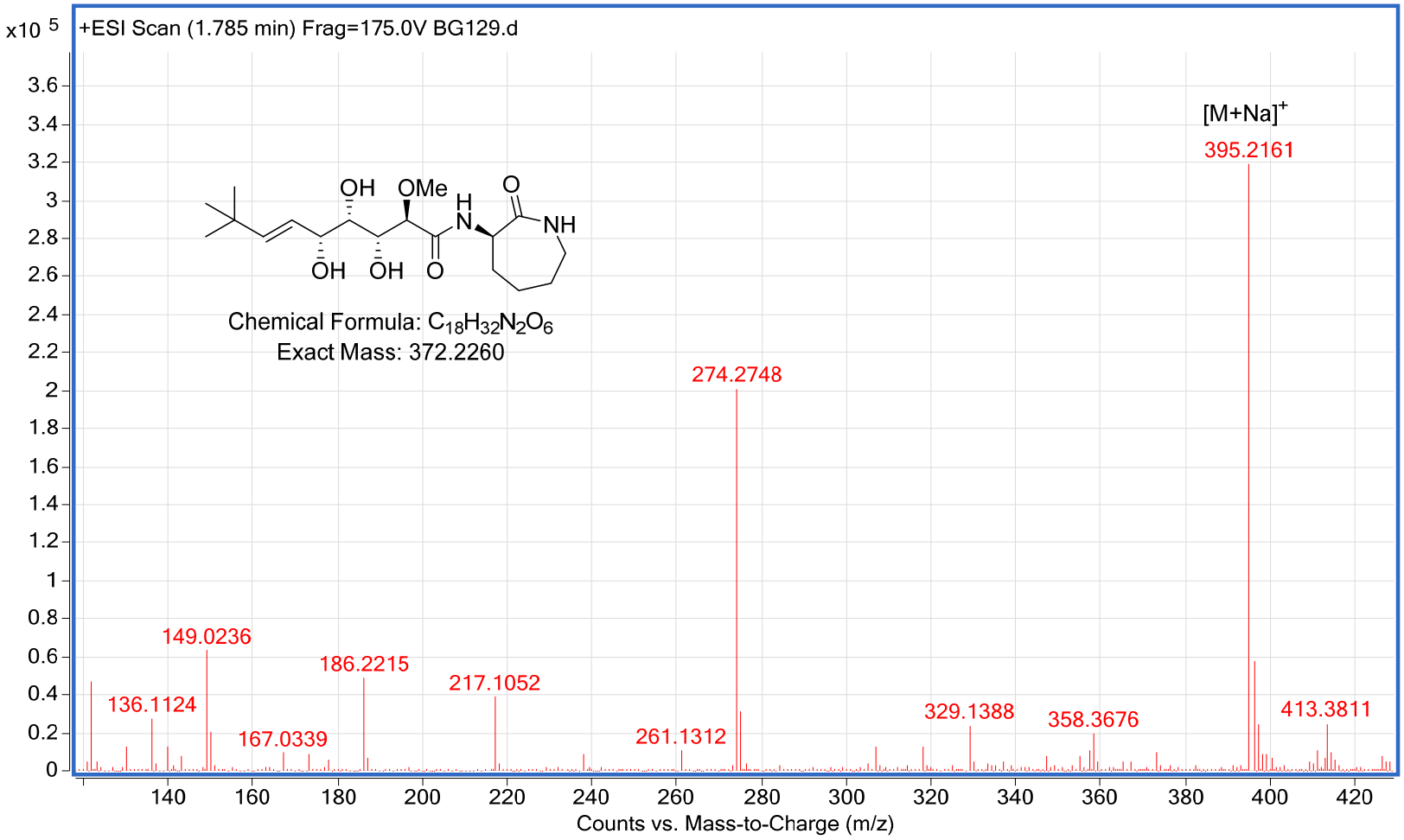
HSQC spectrum of **8b** (^{1}H: 500 MHz, ^{13}C: 125 MHz, $CDCl_3$)



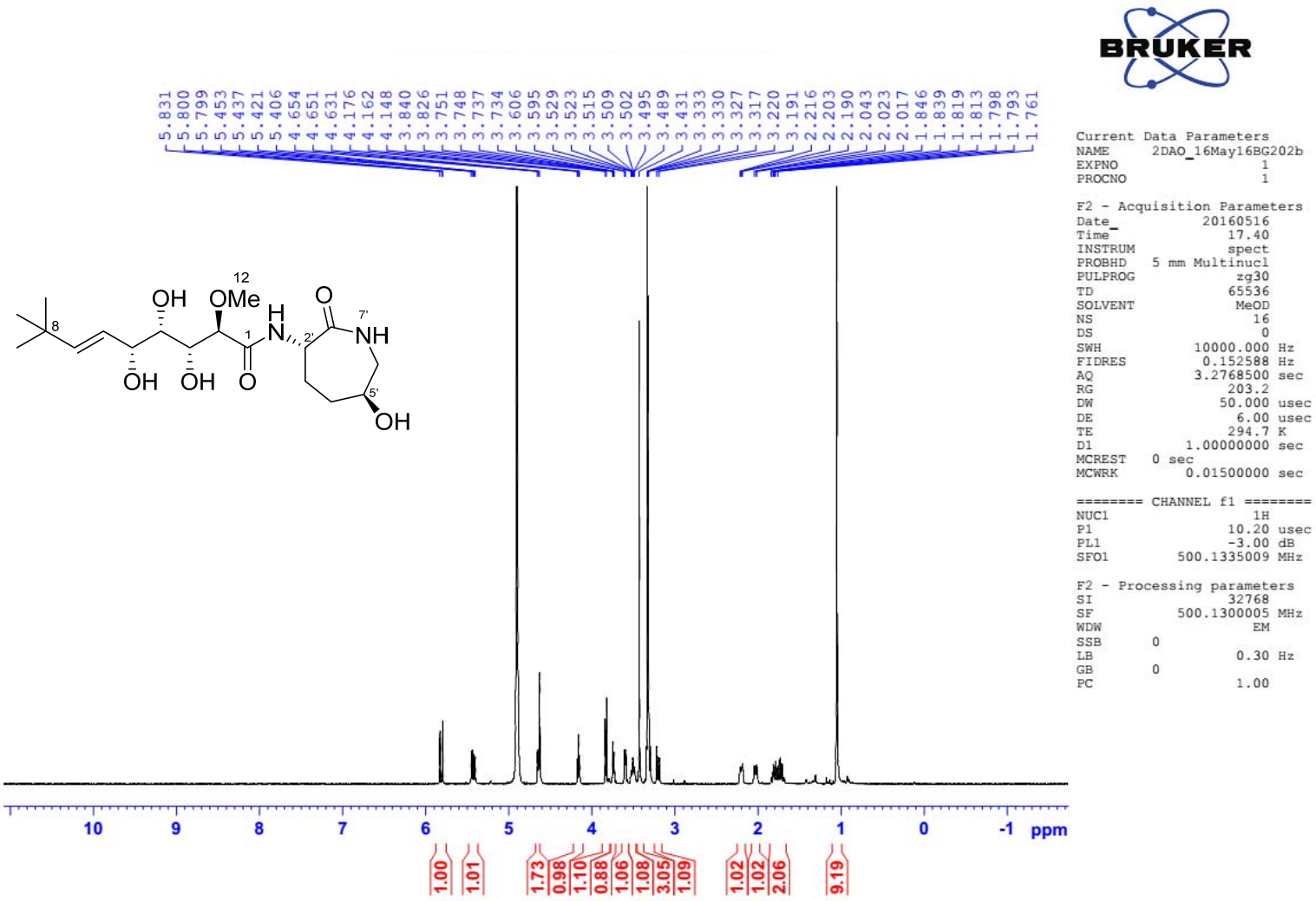
HMBC spectrum of **8b** (^{1}H: 500 MHz, ^{13}C: 125 MHz, $CDCl_3$)



HRESI Mass spectrum of **8b**

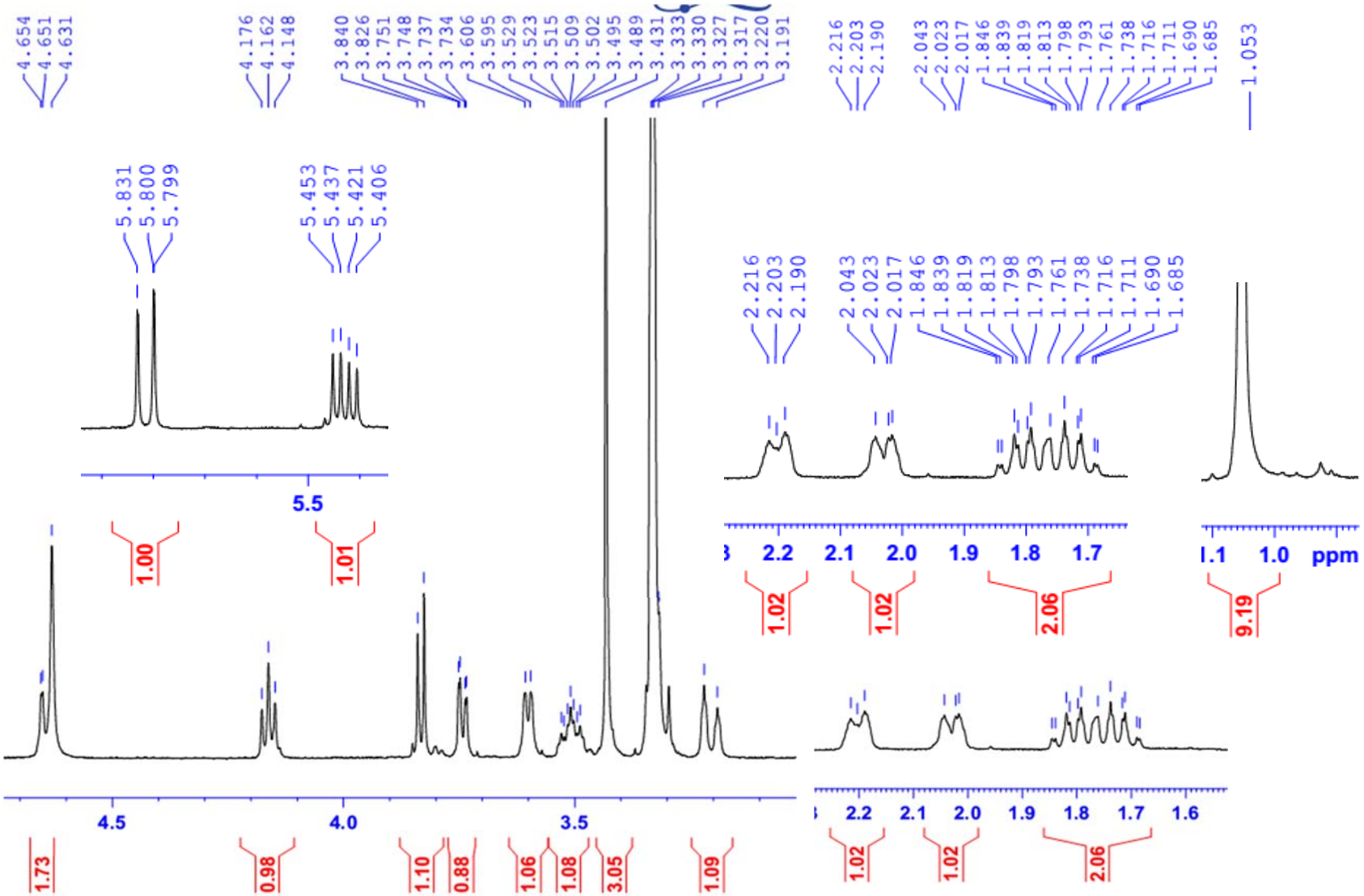


^{1}H NMR spectrum of **9a** (500 MHz, CD_3OD)

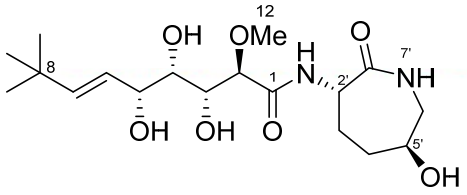


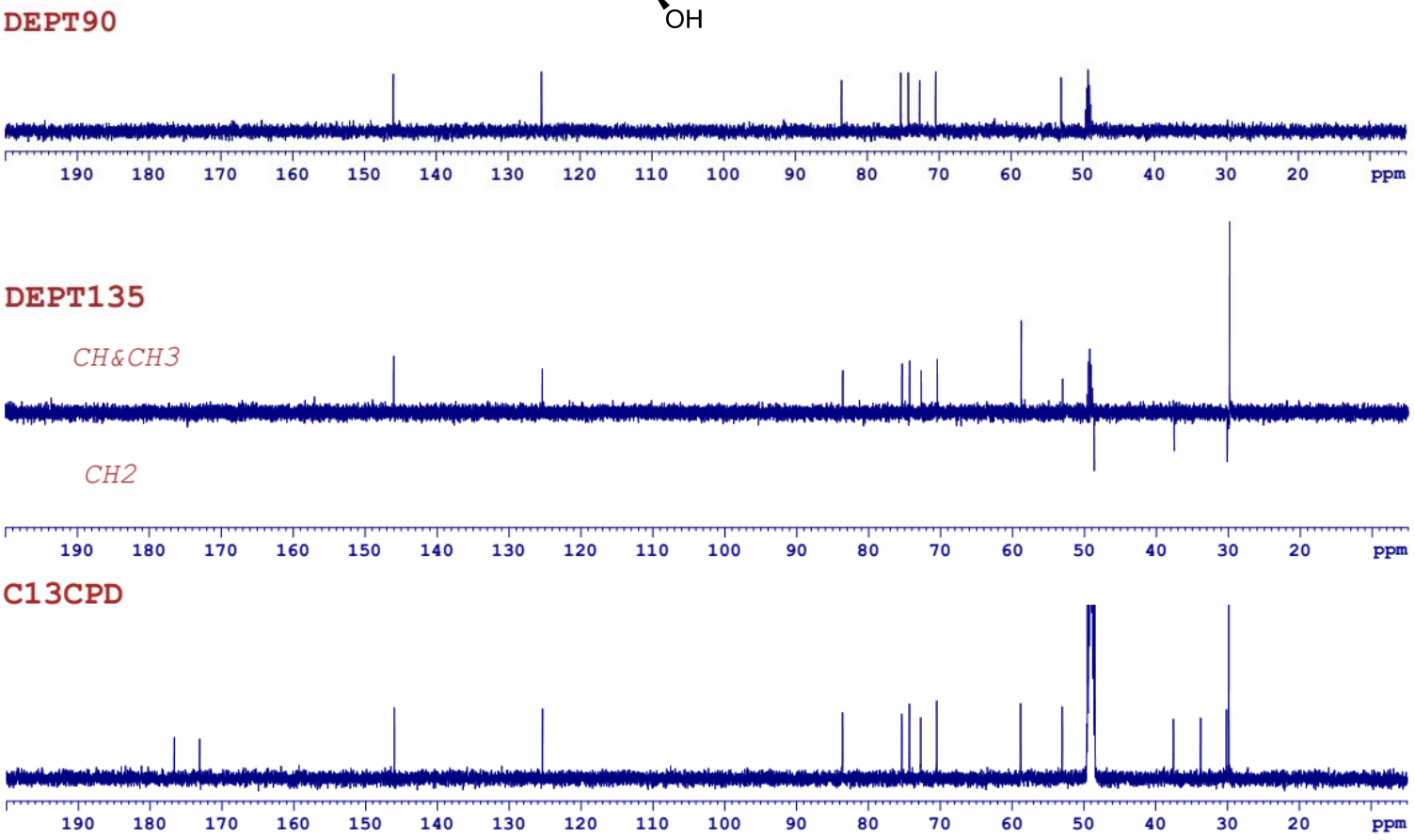

```
Current Data Parameters
NAME      2DAO_16May16BG202b
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20160516
Time                 17.40
INSTRUM              spect
PROBHD   5 mm Multinucl
PULPROG              zg30
TD                  65536
SOLVENT              MeOD
NS                     16
DS                      0
SWH             10000.000 Hz
FIDRES              0.152588 Hz
AQ                3.2768500 sec
RG                    203.2
DW                   50.000 usec
DE                    6.00 usec
TE                   294.7 K
D1              1.00000000 sec
MCREST    0 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.20 usec
PL1                 -3.00 dB
SFO1           500.1335009 MHz

F2 - Processing parameters
SI                     32768
SF             500.1300005 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

Expanded parts of ^{1}H NMR spectrum of **9a** (500 MHz, CD_3OD)

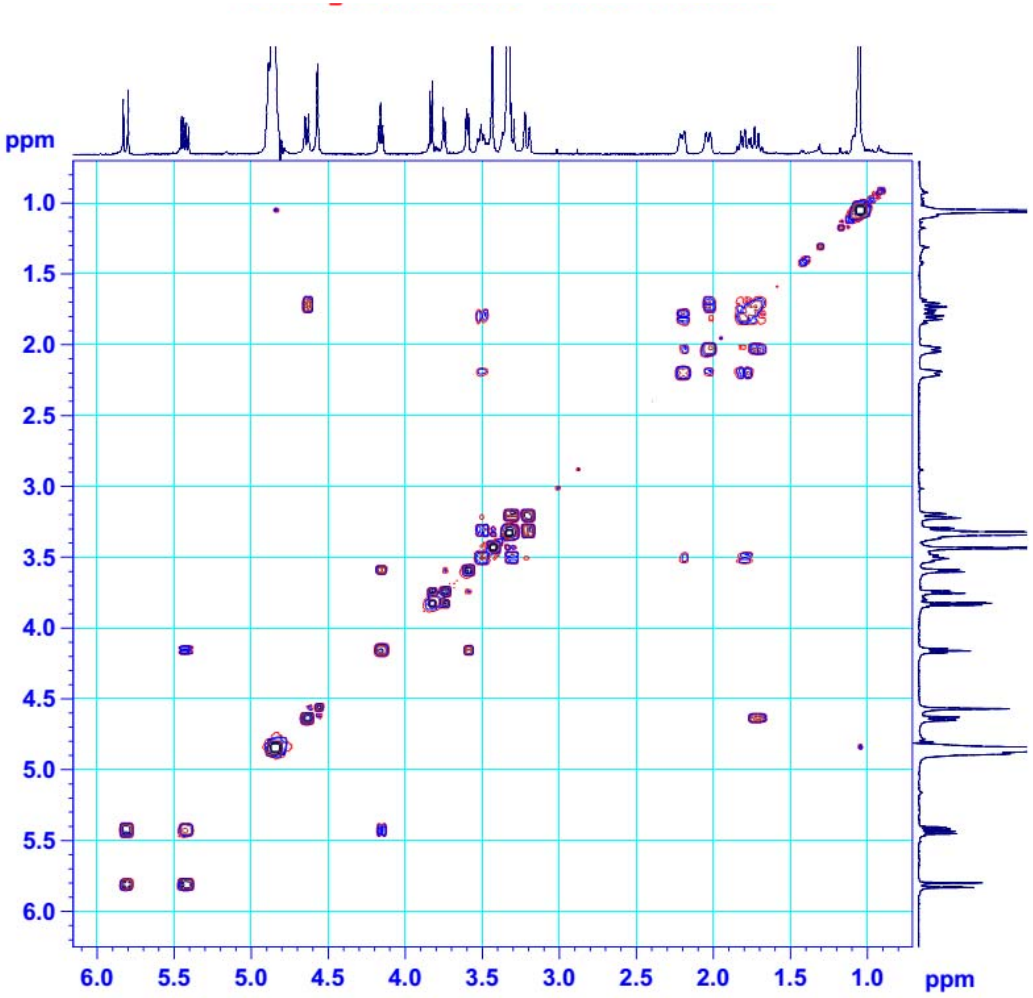


^{13}C NMR and DEPT spectra of **9a** (125 MHz, CD_3OD)





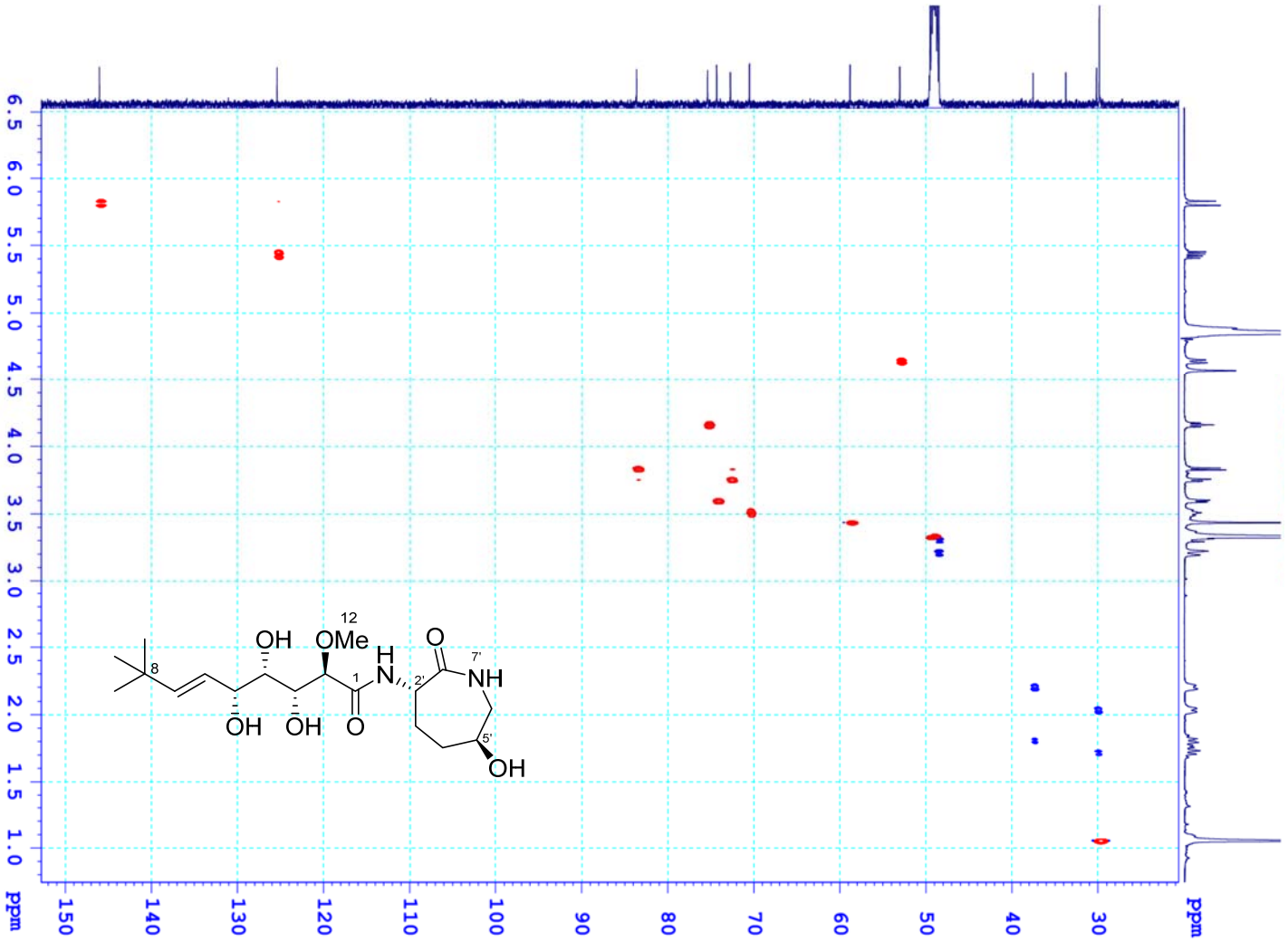
COSY spectrum of **9a** (500 MHz, CD_3OD)



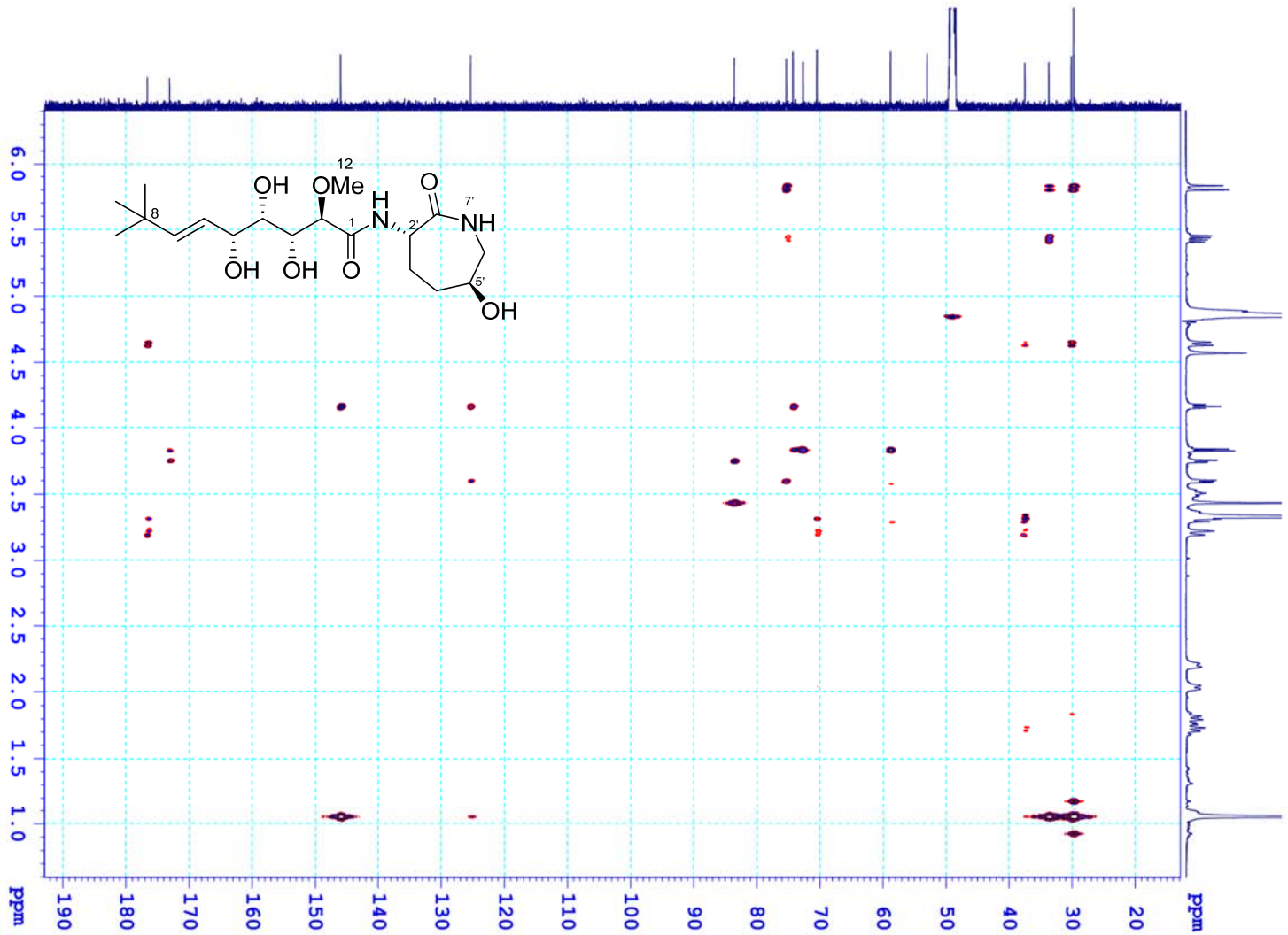
BRUKER

```
Current Data Parameters
NAME      2DAO_16MAY16BG202b
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_               20160517
Time                   13.52
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG        cosygpppqf
TD                     2048
SOLVENT                MeOD
NS                        4
DS                        8
SWH                5000.000 Hz
FIDRES             2.441406 Hz
AQ                 0.2048000 sec
RG                    198.57
DW                  100.000 usec
DE                    6.50 usec
TE                   302.5 K
D0                 0.00000300 sec
D1                 2.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00020000 sec

======== CHANNEL f1 ========
SFO1              500.2022509 MHz
NUC1                       1H
P0                    10.00 usec
P1                    10.00 usec
P17                 2500.00 usec
PLW1             22.00000000 W
PLW10             3.25440001 W

====== GRADIENT CHANNEL =====
GPNAM[1]       SMSQ10.100
GPZ1                  10.00 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                       128
SFO1                500.2023 MHz
FIDRES             39.062500 Hz
SW                     9.996 ppm
FnMODE                    QF

F2 - Processing parameters
SI                       1024
SF                500.2000014 MHz
WDW                     QSINE
SSB          0
LB           0 Hz
GB           0
PC                       1.00

F1 - Processing parameters
SI                       1024
MC2                       QF
SF                500.2000000 MHz
WDW                     QSINE
SSB          0
LB           0 Hz
GB           0
```

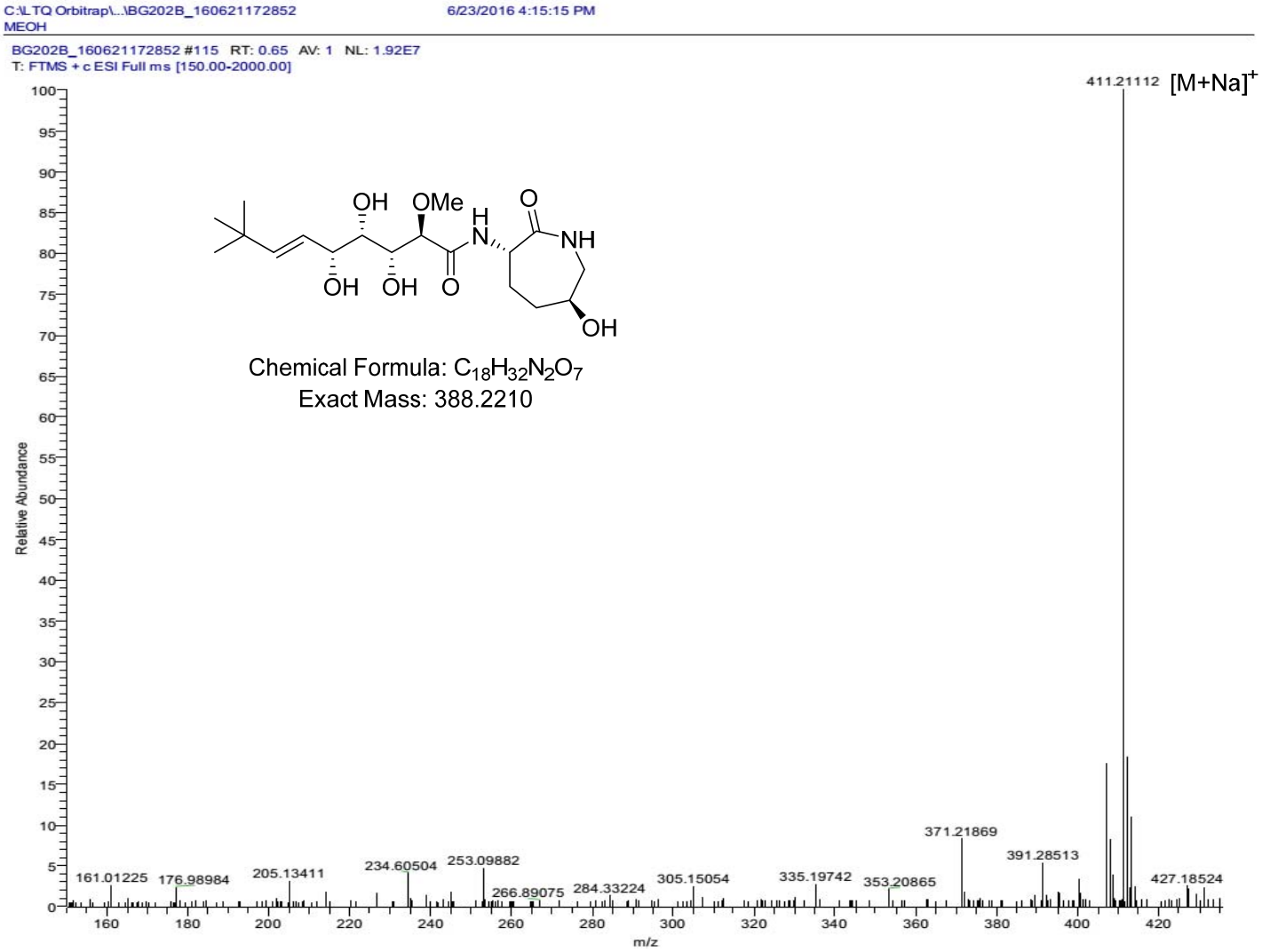
HSQC spectrum of **9a** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)



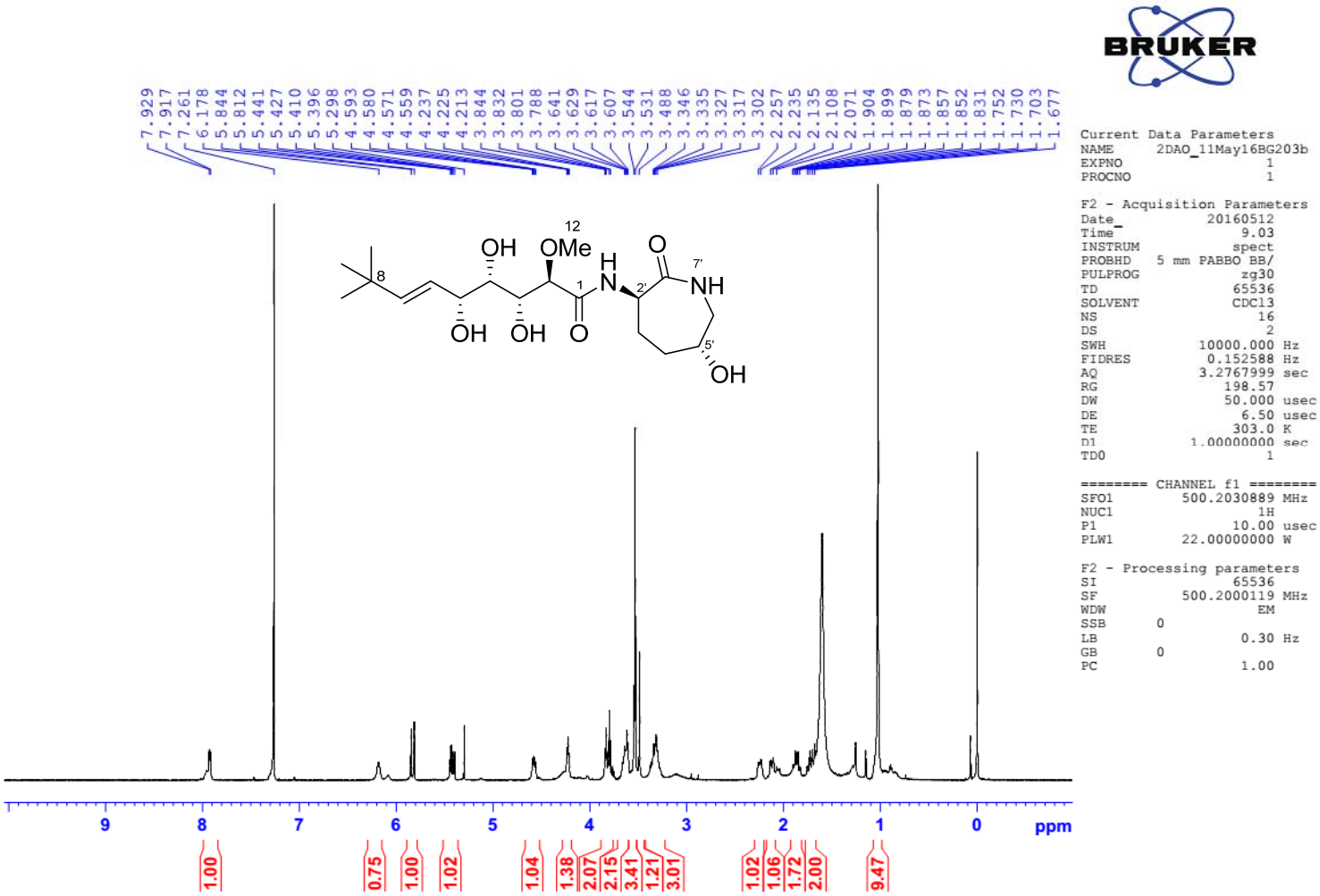
HMBC spectrum of **9a** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)



HRESI Mass spectrum of **9a**

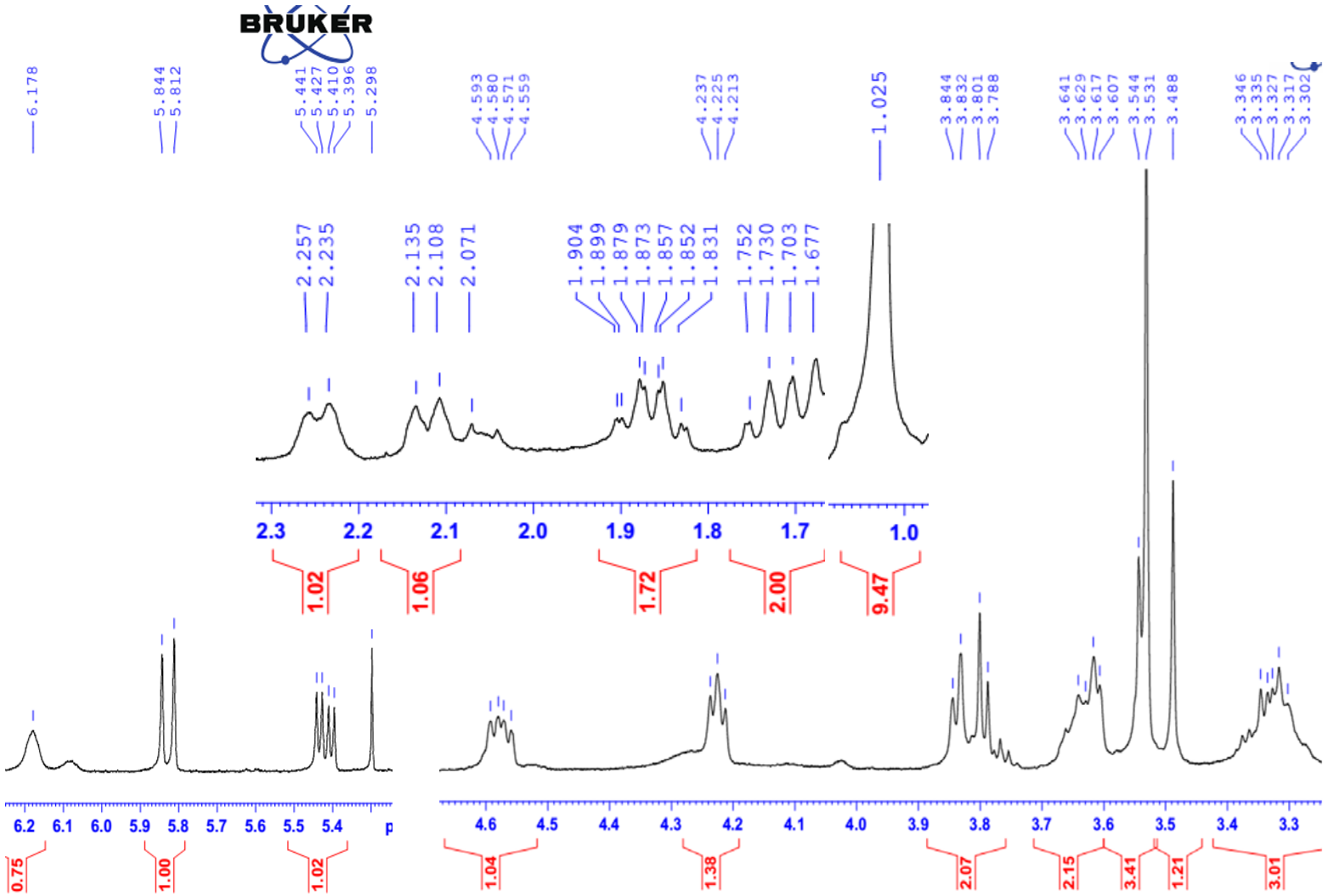


^{1}H NMR spectrum of **9b** (500 MHz, CD_3OD)

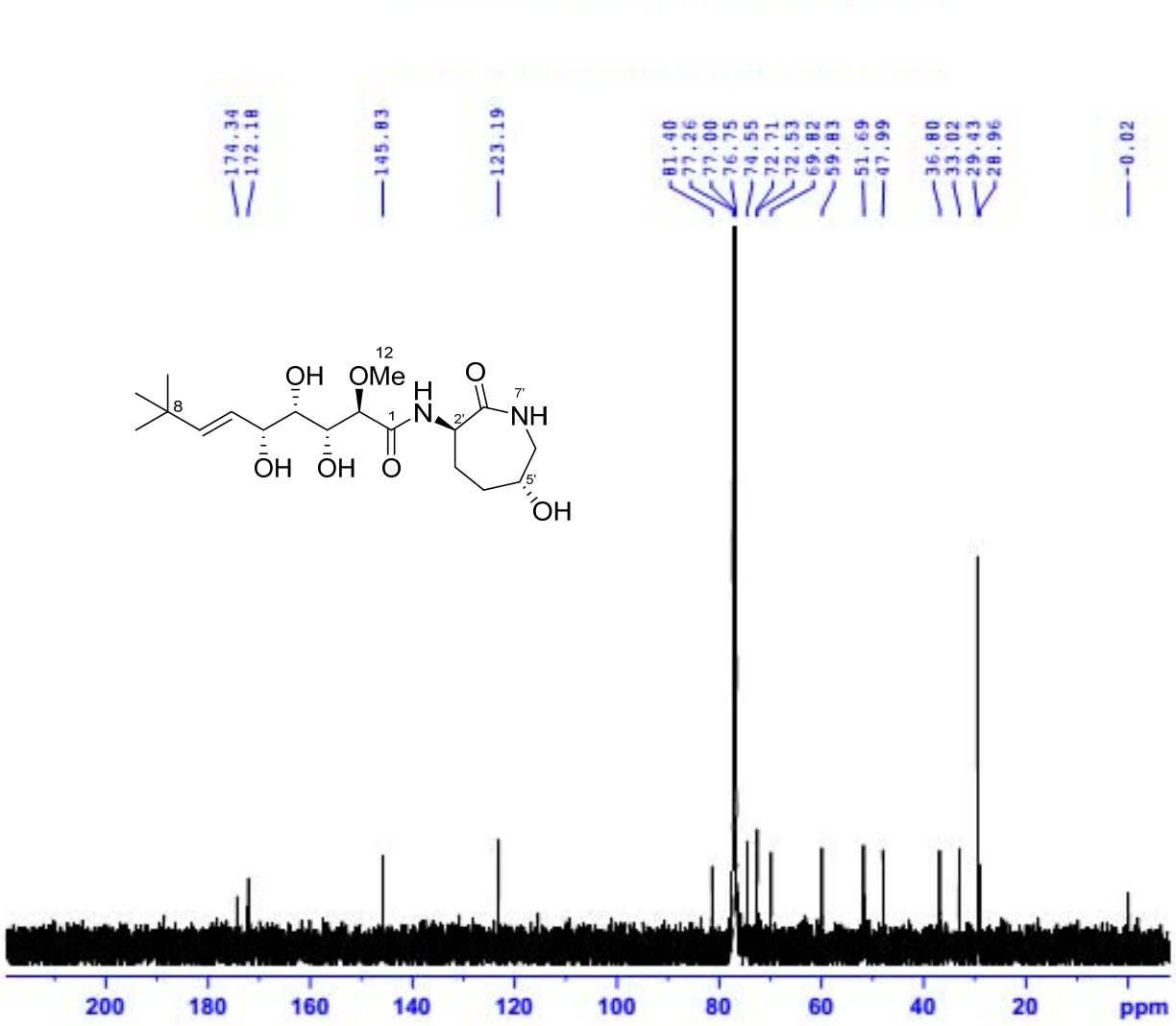



```
Current Data Parameters
NAME      2DAO_11May16BG203b
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20160512
Time                   9.03
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              10000.000 Hz
FIDRES               0.152588 Hz
AQ                3.2767999 sec
RG                   198.57
DW                   50.000 usec
DE                    6.50 usec
TE                   303.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                    1H
P1                   10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                   65536
SF            500.2000119 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

Expanded parts of ^{1}H NMR spectrum of **9b** (500 MHz, CD_3OD)

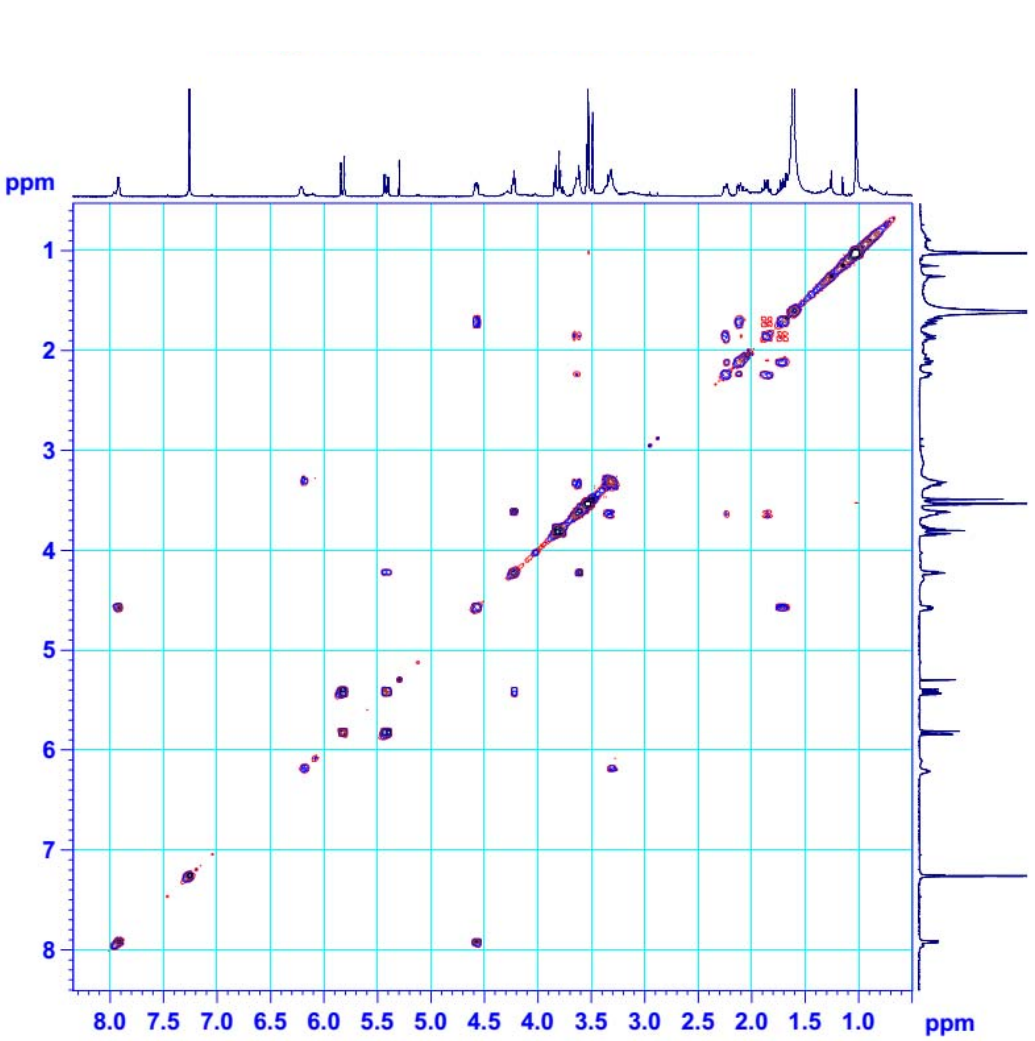


^{13}C NMR spectrum of **9b** (125 MHz, CD_3OD)




```
Current Data Parameters
NAME      2DAO_11May16BG203b
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20160516
Time                 20.42
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   4096
DS                      4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                  198.57
DW                 16.800 usec
DE                  6.50 usec
TE                 303.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          125.7892253 MHz
NUC1                  13C
P1                  10.00 usec
PLW1          88.00000000 W

======== CHANNEL f2 ========
SFO2          500.2020008 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2               80.00 usec
PLW2          22.00000000 W
PLW12          0.34375000 W
PLW13          0.22000000 W

F2 - Processing parameters
SI                   32768
SF          125.7753900 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

COSY spectrum of **9b** (500 MHz, CD_3OD)



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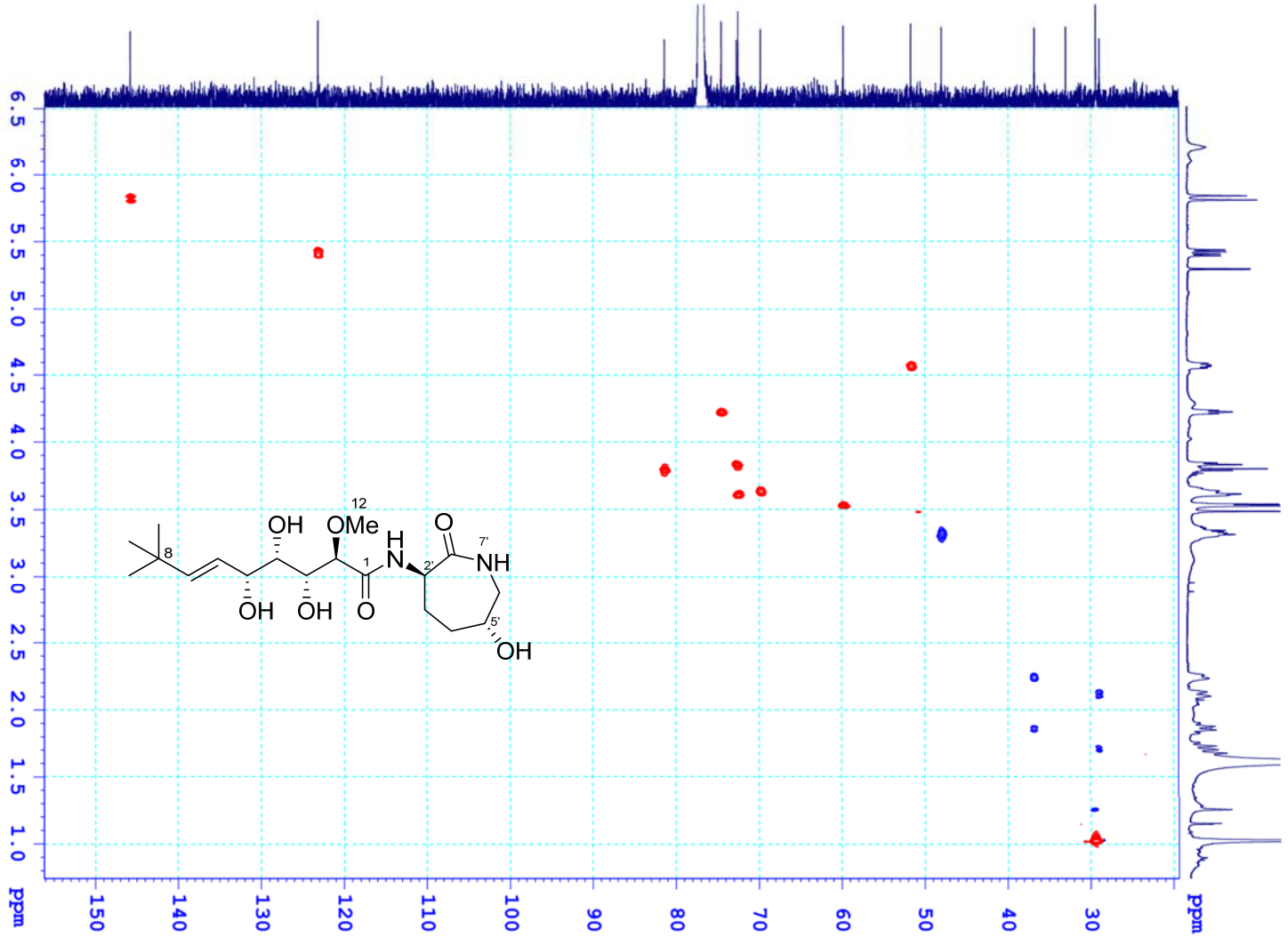
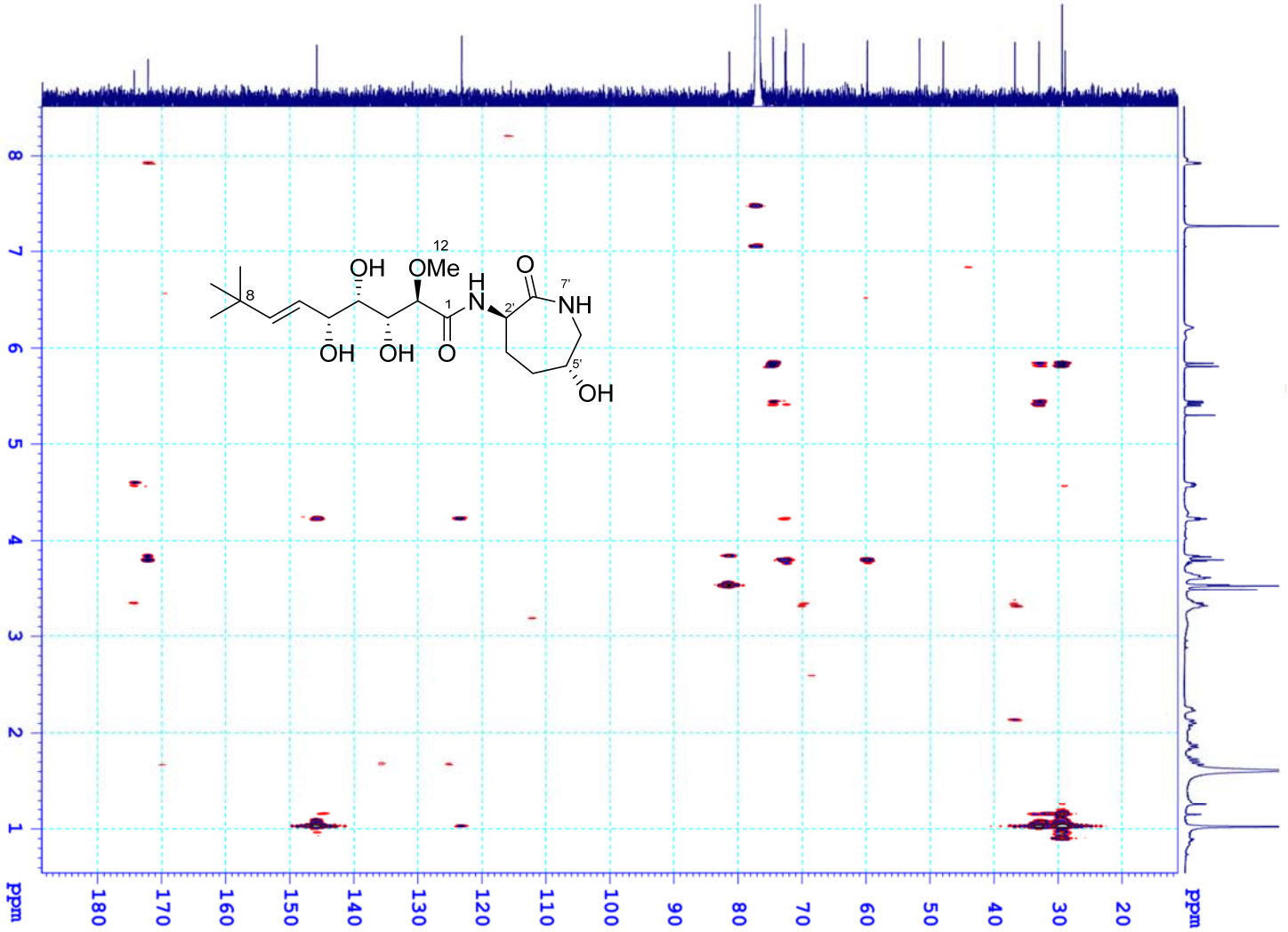
```
Current Data Parameters
NAME      2DAO_11May16BG203b
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_              20160516
Time                  21.50
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG        cosygpppqf
TD                     2048
SOLVENT             CDCl3
NS                        8
DS                        8
SWH                5000.000 Hz
FIDRES             2.441406 Hz
AQ                 0.2048000 sec
RG                    198.57
DW                 100.000 usec
DE                   6.50 usec
TE                   303.1 K
D0                 0.00000300 sec
D1                 2.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00020000 sec

======== CHANNEL f1 ========
SFO1              500.2022509 MHz
NUC1                      1H
P0                    10.00 usec
P1                    10.00 usec
P17                 2500.00 usec
PLW1             22.00000000 W
PLW10             3.25440001 W

====== GRADIENT CHANNEL =====
GPNAM[1]       SMSQ10.100
GPZ1                  10.00 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                       160
SFO1               500.2023 MHz
FIDRES            31.250000 Hz
SW                    9.996 ppm
FnMODE                   QF

F2 - Processing parameters
SI                       1024
SF              500.2000133 MHz
WDW                    QSINE
SSB          0
LB           0 Hz
GB           0
PC                     1.00

F1 - Processing parameters
SI                       1024
MC2                      QF
SF              500.2000128 MHz
WDW                    QSINE
SSB          0
LB           0 Hz
GB           0
```

HSQC spectrum of **9b** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)



HMBC spectrum of **9b** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)



HRESI Mass spectrum of **9b**

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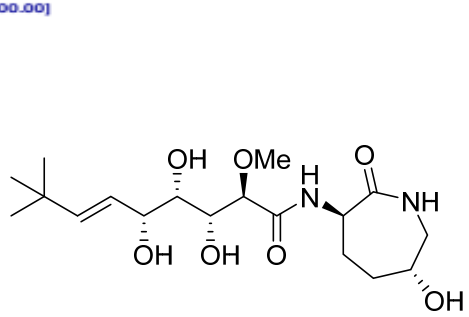
19 Le Thanh Tong, Hoan Kiem, Ha Noi
Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

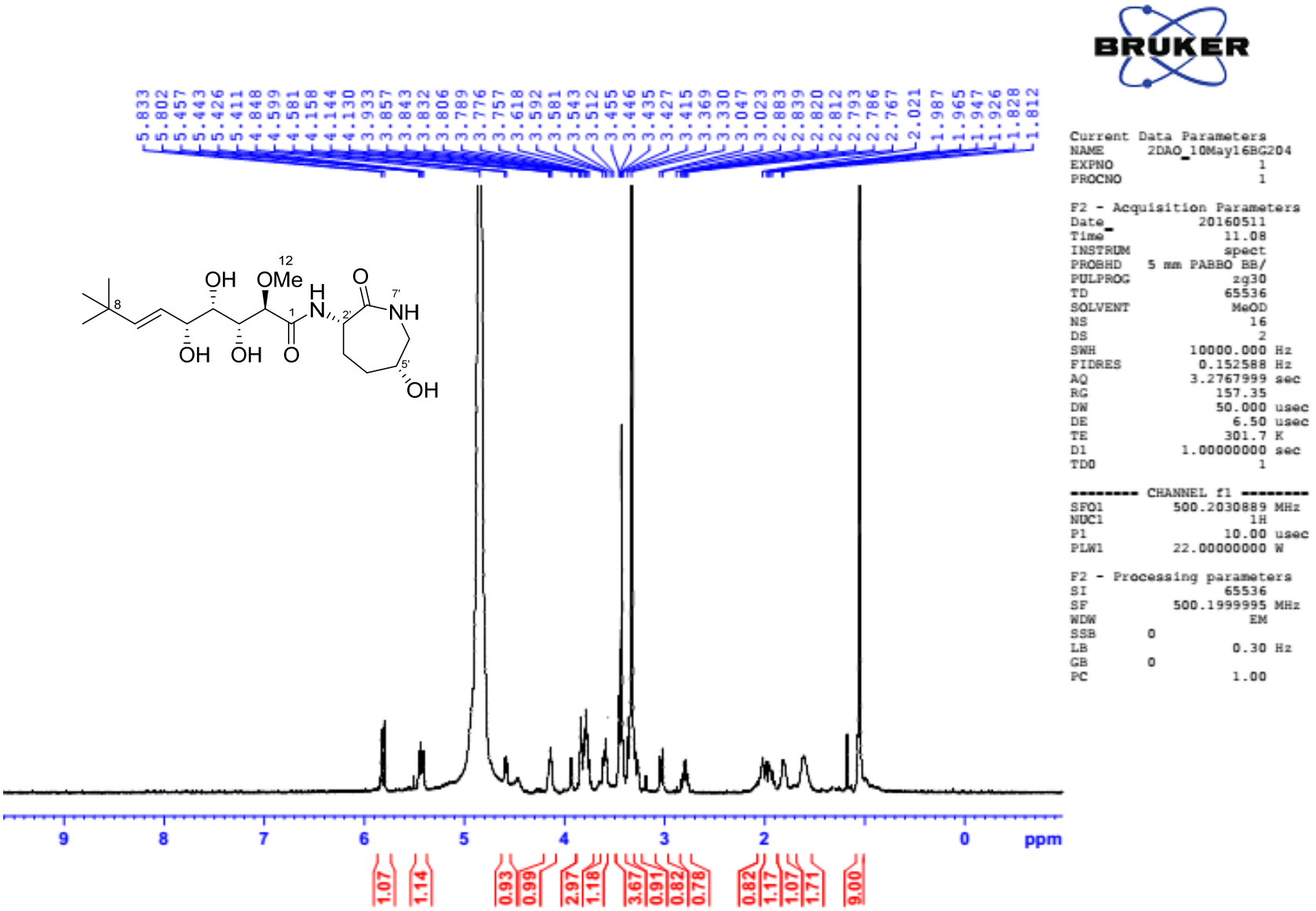
C:\LTQ Orbitrap\...\BG203_160621172852 6/23/2016 3:38:15 PM
MEOH

BG203_160621172852 #233 RT: 1.01 AV: 1 NL: 1.18E7
T: FTMS + c ESI Full ms [150.00-2000.00]



Chemical Formula: $C_{18}H_{32}N_2O_7$
Exact Mass: 388.2210

^{1}H NMR spectrum of **9c** (500 MHz, CD_3OD)



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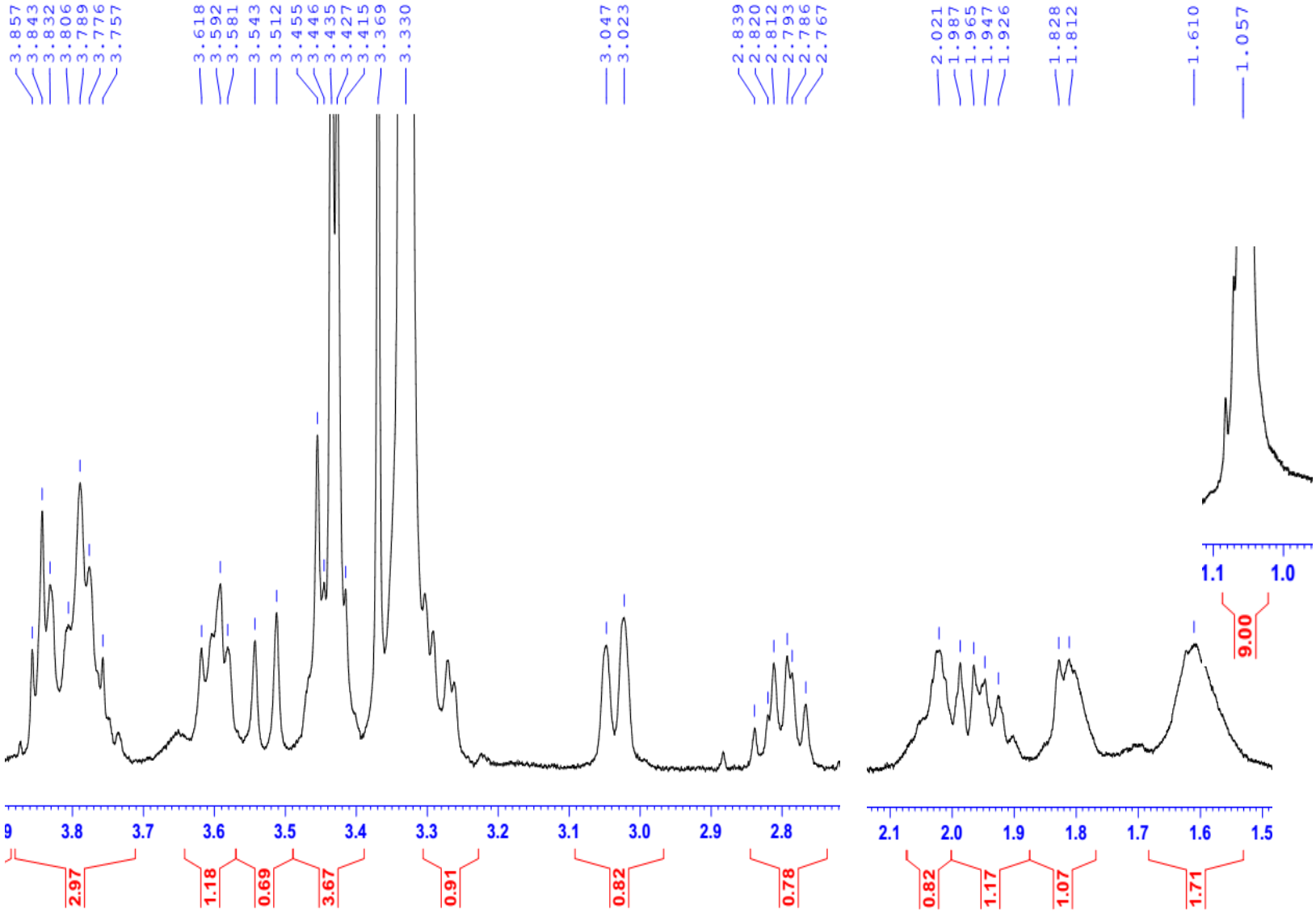
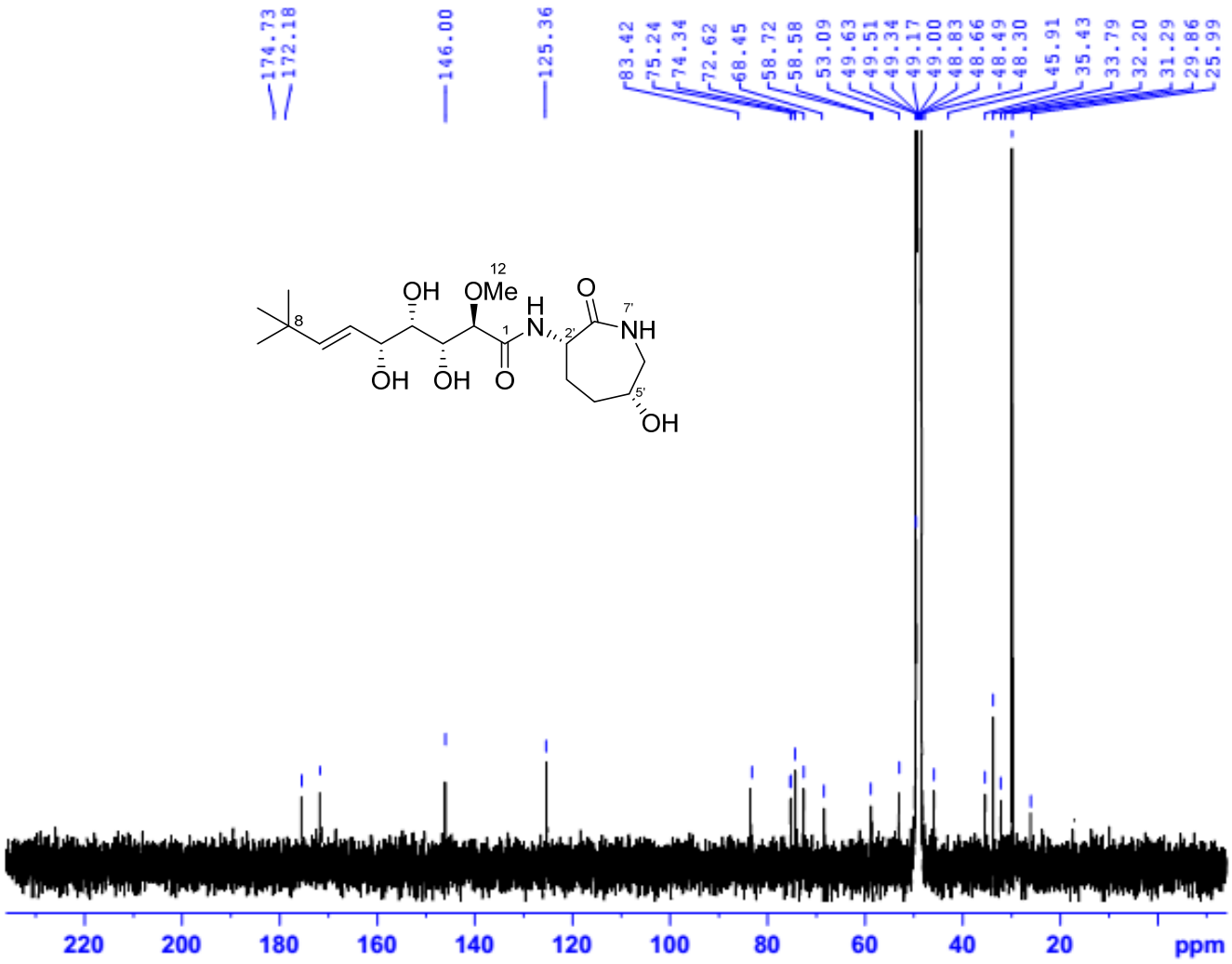
```
Current Data Parameters
NAME      2DAO_10May16BG204
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20160511
Time                 11.08
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              MeOD
NS                     16
DS                      2
SWH            10000.000 Hz
FIDRES          0.152588 Hz
AQ             3.2767999 sec
RG                 157.35
DW                 50.000 usec
DE                  6.50 usec
TE                 301.7 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                   1H
P1                  10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                  65536
SF            500.1999995 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

Expanded parts of ^{1}H NMR spectrum of **9c** (500 MHz, CD_3OD)

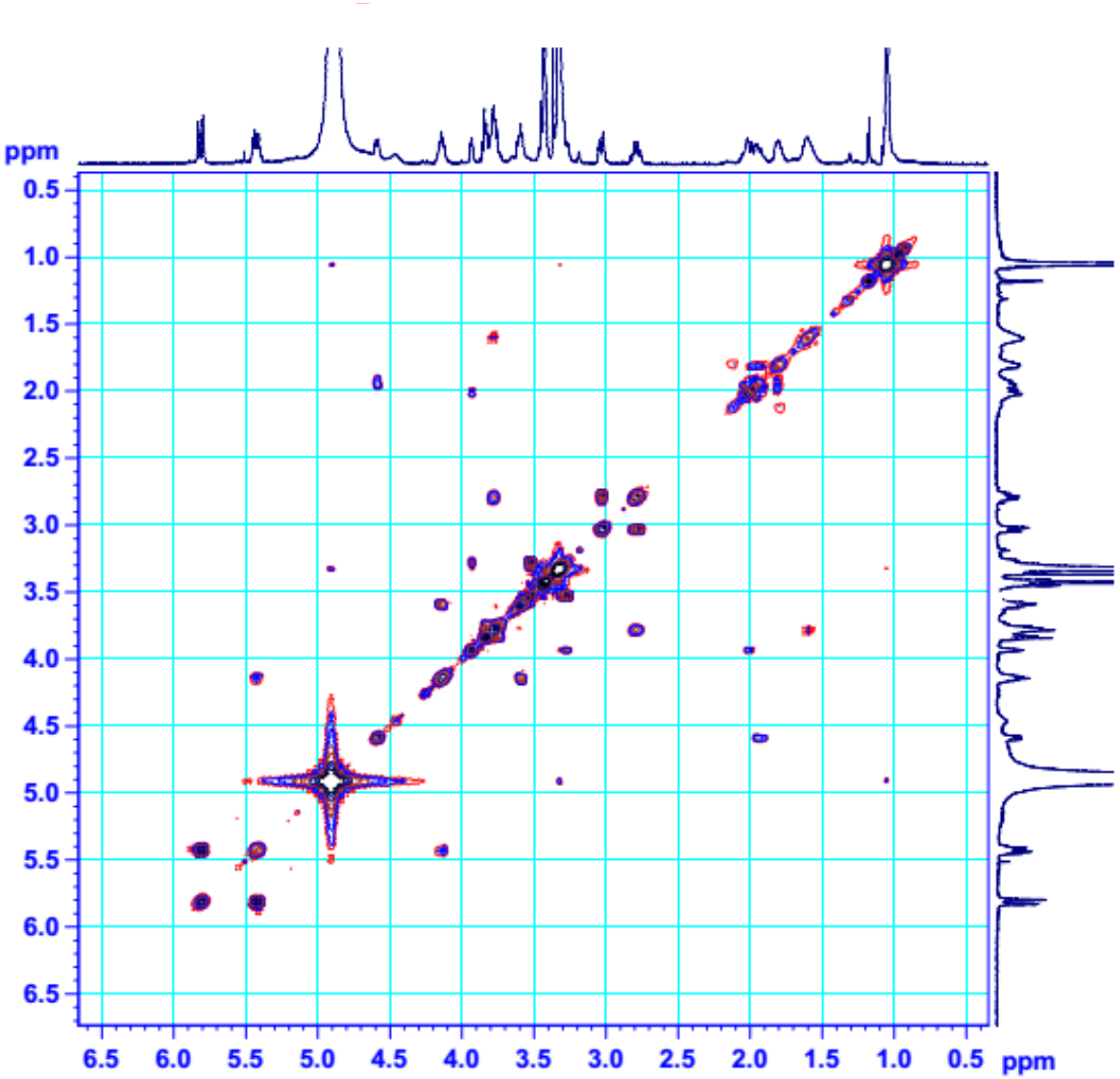


^{13}C NMR spectrum of **9c** (125 MHz, CD_3OD)




```
Current Data Parameters
NAME      2DAO_10May16BG204
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20160512
Time                   0.51
INSTRUM               spect
PROBHD   5 mm Multinucl
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                    10240
DS                        2
SWH               31446.541 Hz
FIDRES             0.479836 Hz
AQ                 1.0420383 sec
RG                    32768
DW                   15.900 usec
DE                    6.00 usec
TE                   294.4 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST    0 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                    7.40 usec
PL1       0 dB
SFO1          125.7715724 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                  -3.00 dB
PL12                 14.89 dB
PL13                 22.00 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF            125.7576123 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.00
```

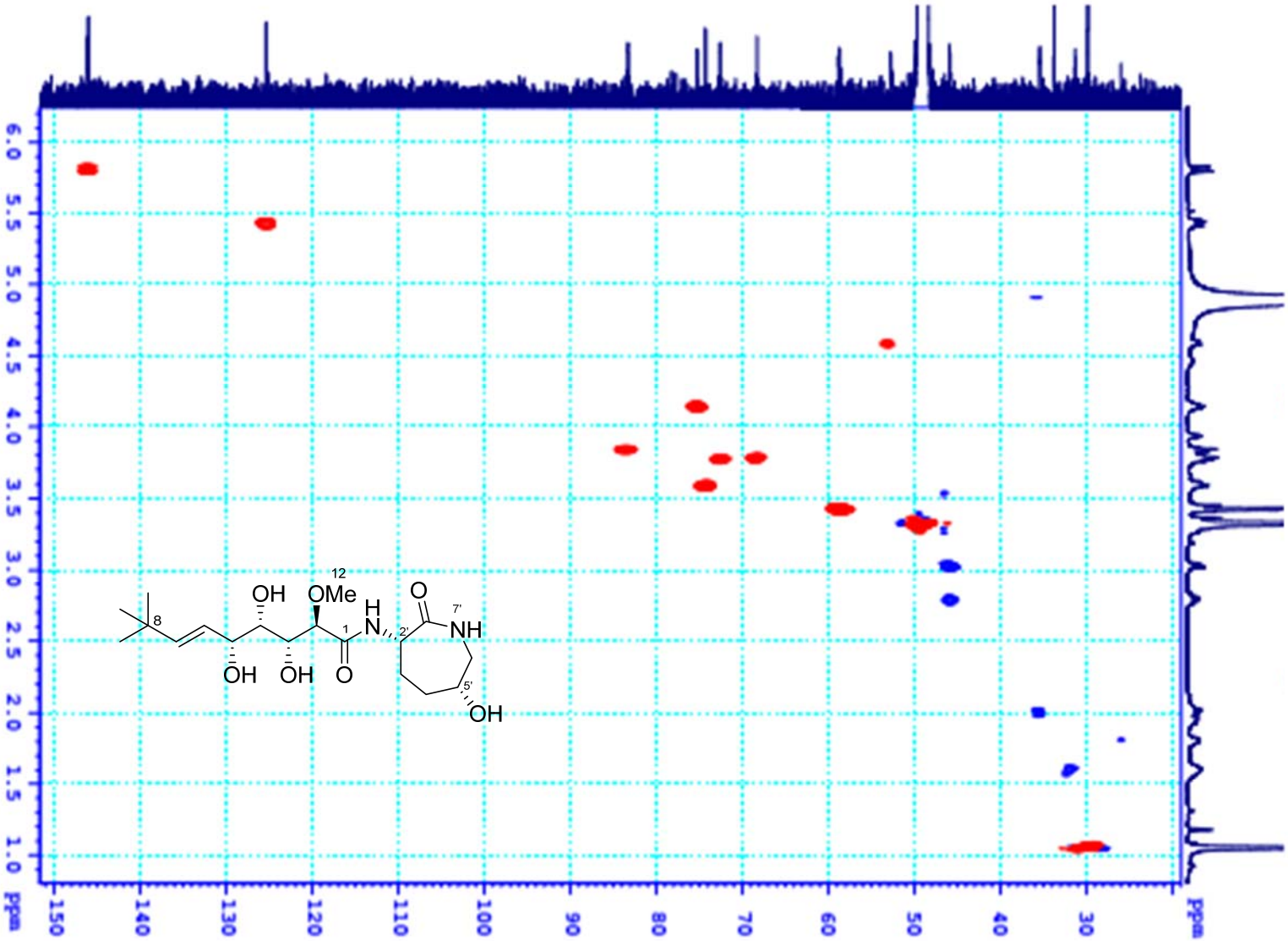
COSY spectrum of **9c** (500 MHz, CD_3OD)



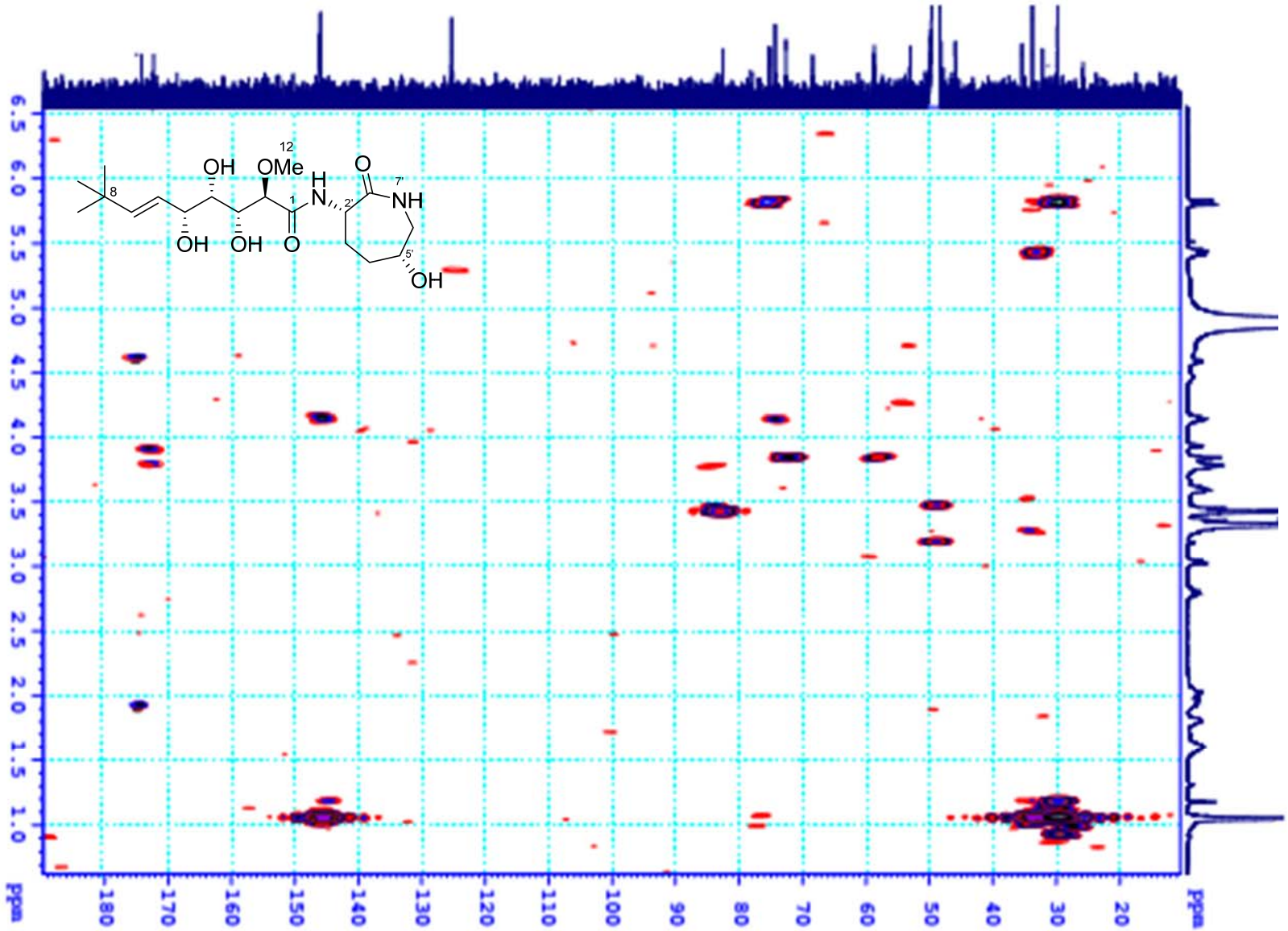
BRUKER

```
Current Data Parameters
NAME      2DAO_10May16BG204
EXPNO                     5
PROCNO                    1

F2 - Acquisition Parameters
Date_              20160512
Time                   3.18
INSTRUM               spect
PROBHD   5 mm Multinucl
PULPROG          cosygpqf
TD                     2048
SOLVENT                MeOD
NS                       16
DS                       16
SWH                5000.000 Hz
FIDRES             2.441406 Hz
AQ                 0.2049000 sec
RG                     574.7
DW                   100.000 usec
DE                      6.00 usec
TE                     294.2 K
d0                0.00000300 sec
D1                1.48689198 sec
d13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00020000 sec
MCREST    0 sec
MCWRK             1.48689198 sec

======== CHANNEL f1 ========
NUC1                      1H
P0                     10.20 usec
P1                     10.20 usec
PL1                    -3.00 dB
SFO1           500.1322506 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]          SINE.100
GPNAM[2]          SINE.100
GPX1        0 %
GPX2        0 %
GPY1        0 %
GPY2        0 %
GPZ1                   10.00 %
GPZ2                   10.00 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                       128
SFO1           500.1323 MHz
FIDRES          39.062500 Hz
SW                   9.997 ppm
FnMODE                  QF

F2 - Processing parameters
SI                      1024
SF             500.1300009 MHz
WDW                     SINE
SSB         0
LB          0 Hz
GB          0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                     QF
SF             500.1300020 MHz
WDW                     SINE
SSB         0
LB          0 Hz
GB          0
```

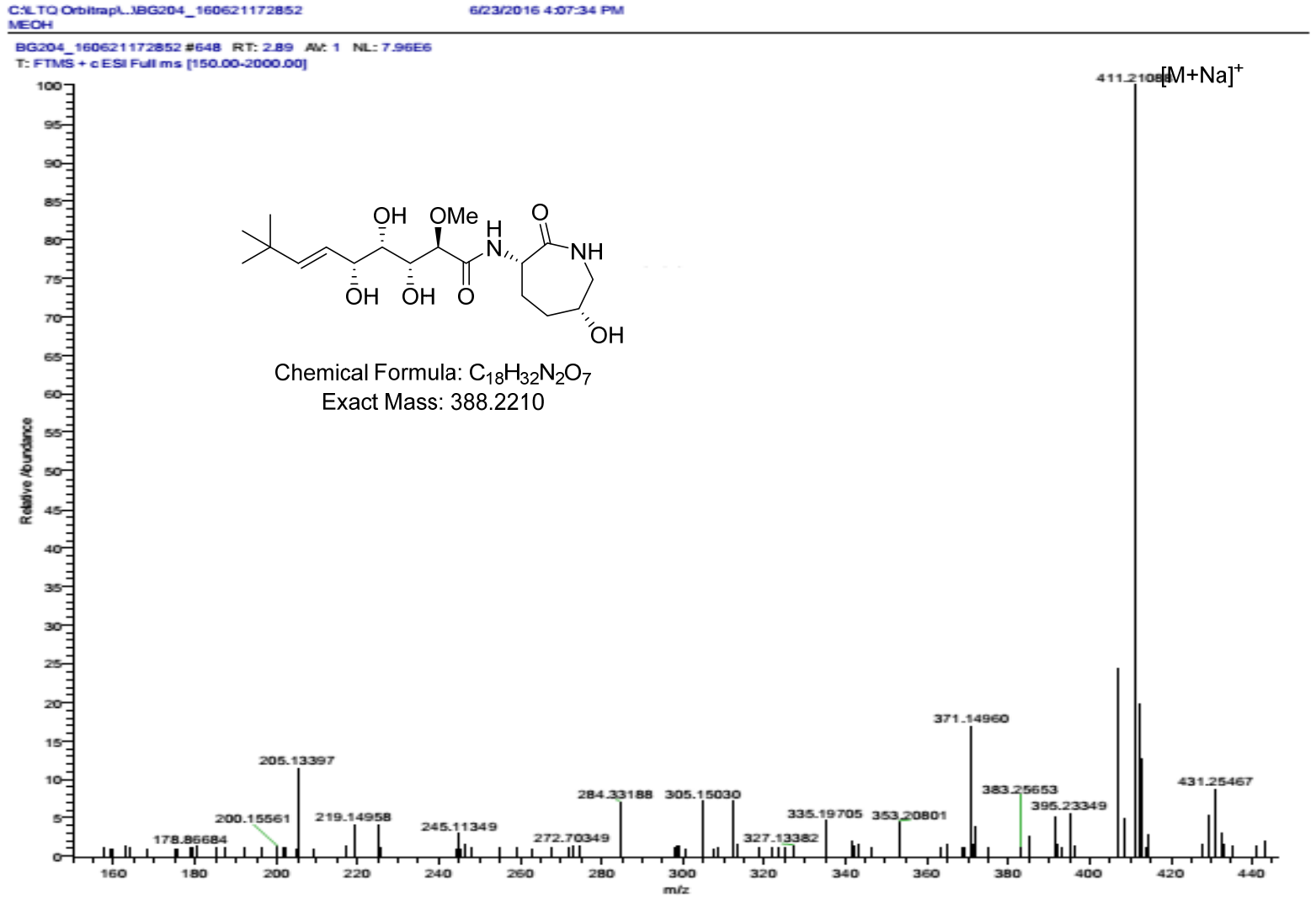
HSQC spectrum of **9c** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)



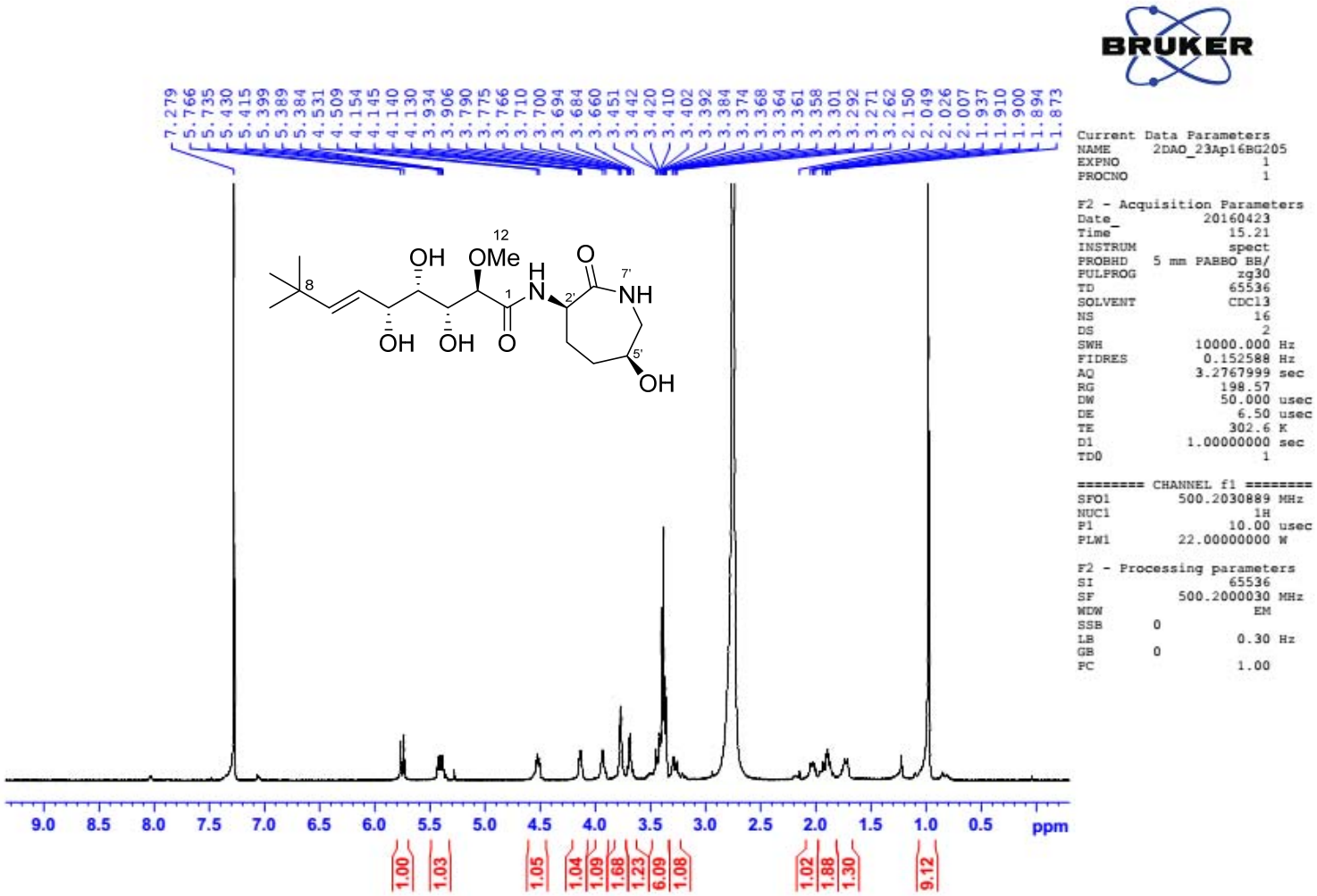
HMBC spectrum of **9c** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)



HRESI Mass spectrum of **9c**

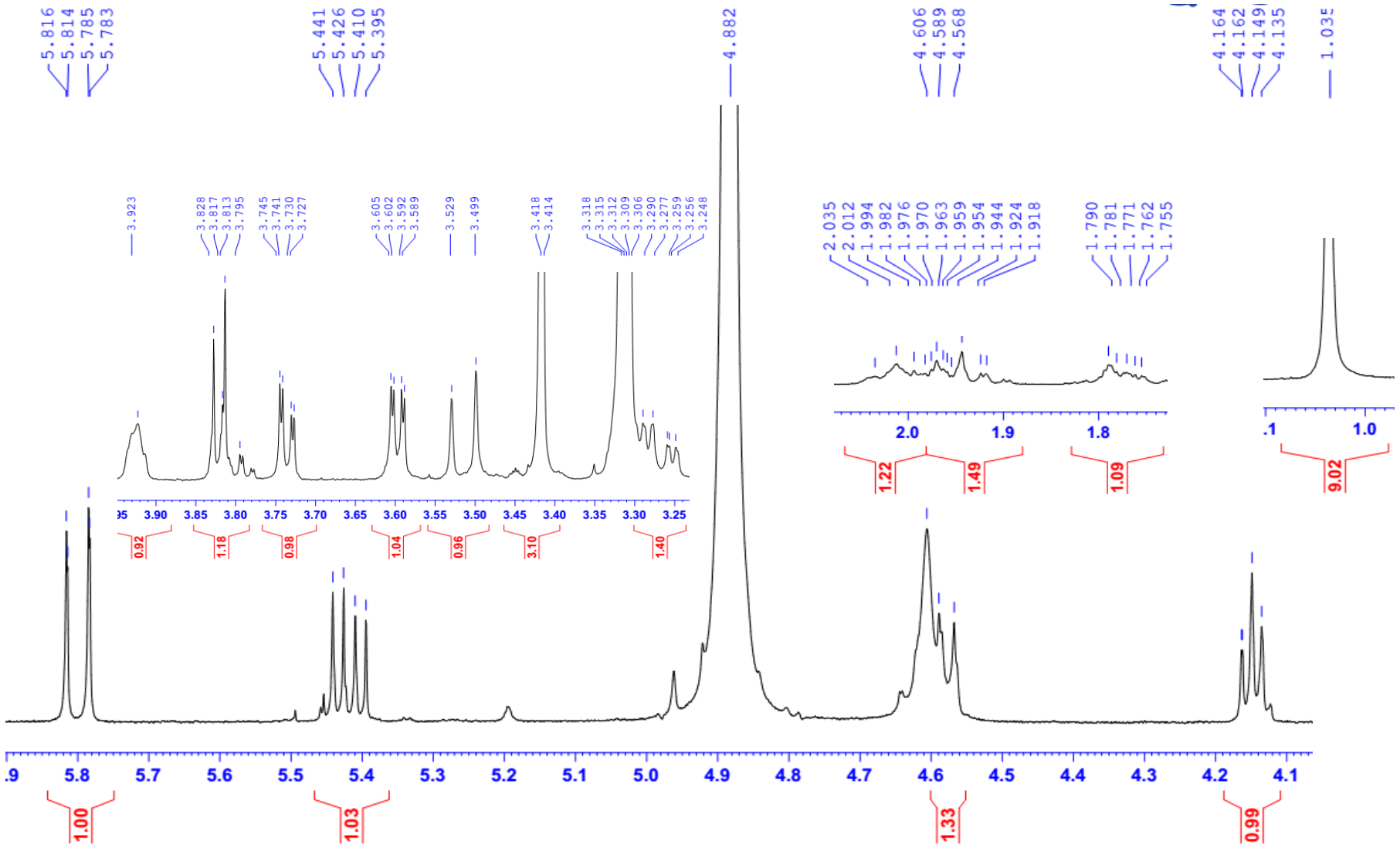


^{1}H NMR spectrum of **9d** (500 MHz, CD_3OD)

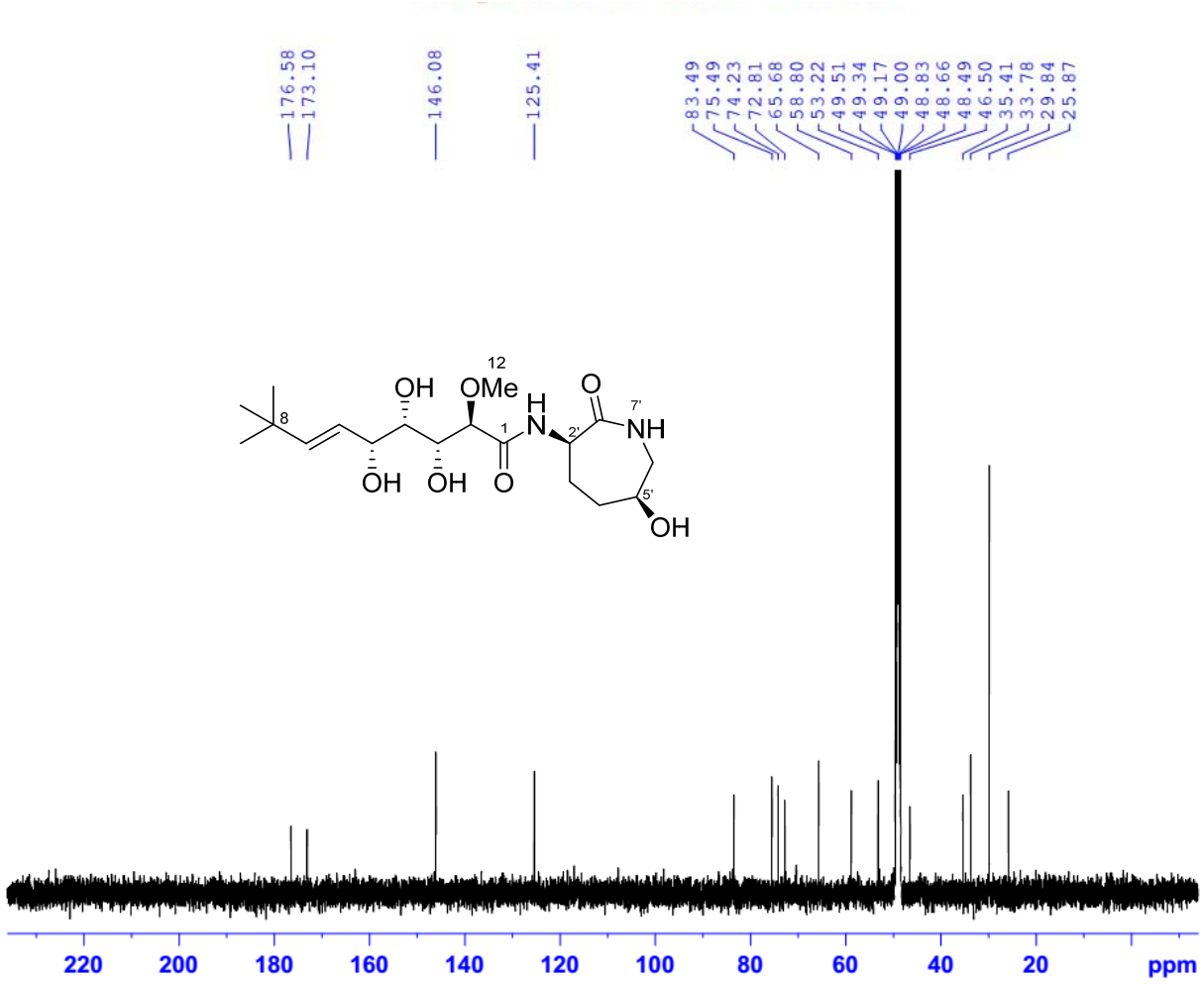



```
Current Data Parameters
NAME      2DAO_23Ap16BG205
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20160423
Time                 15.21
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              10000.000 Hz
FIDRES           0.152588 Hz
AQ               3.2767999 sec
RG                  198.57
DW                  50.000 usec
DE                    6.50 usec
TE                   302.6 K
D1               1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                    1H
P1                   10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                   65536
SF            500.2000030 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

Expanded parts of ^{1}H NMR spectrum of **9d** (500 MHz, CD_3OD)

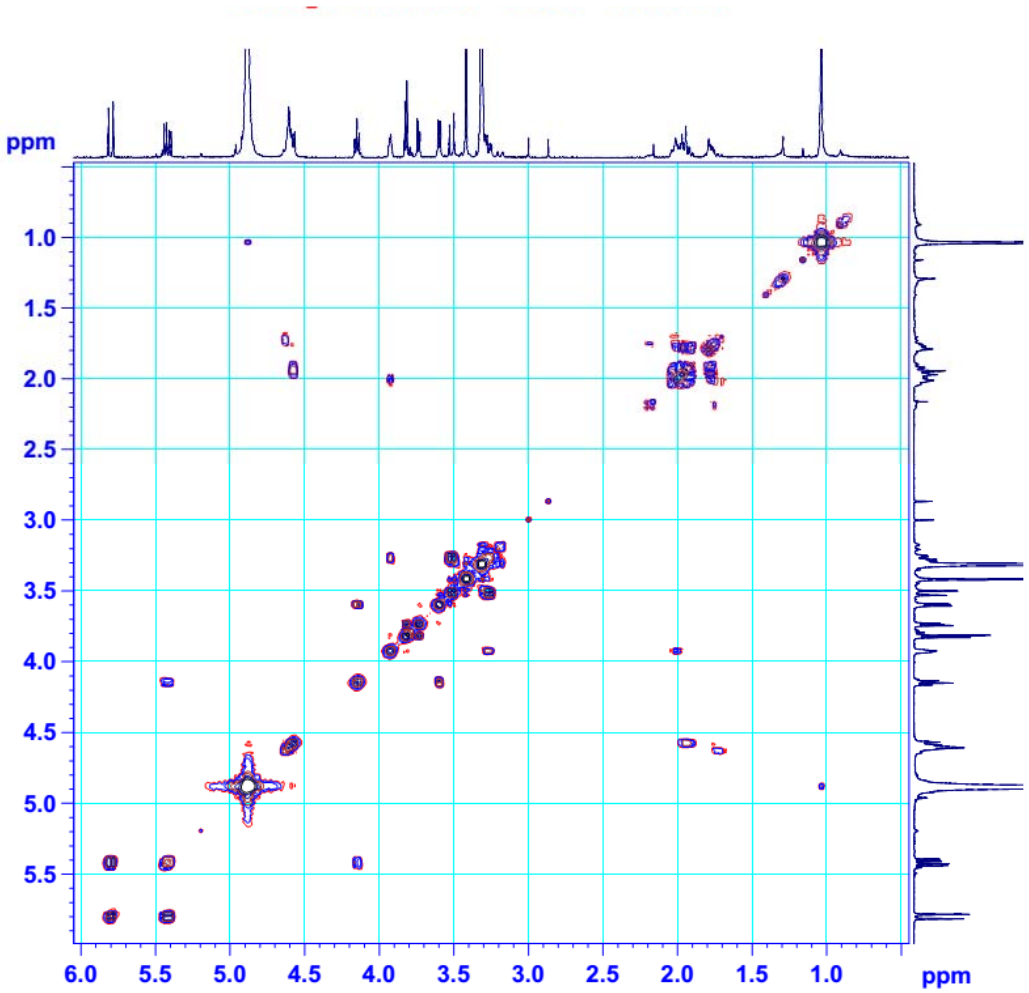


^{13}C NMR spectrum of **9d** (125 MHz, CD_3OD)




```
Current Data Parameters
NAME      2DAO_25Ap16BG205
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20160426
Time              21.45
INSTRUM           spect
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT            MeOD
NS                 4096
DS                    2
SWH           31446.541 Hz
FIDRES         0.479836 Hz
AQ            1.0420383 sec
RG                32768
DW               15.900 usec
DE                6.00 usec
TE                295.9 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST   0 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                  7.40 usec
PL1       0 dB
SFO1        125.7715724 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               14.89 dB
PL13               22.00 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                  32768
SF           125.7576120 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

COSY spectrum of **9d** (500 MHz, CD_3OD)



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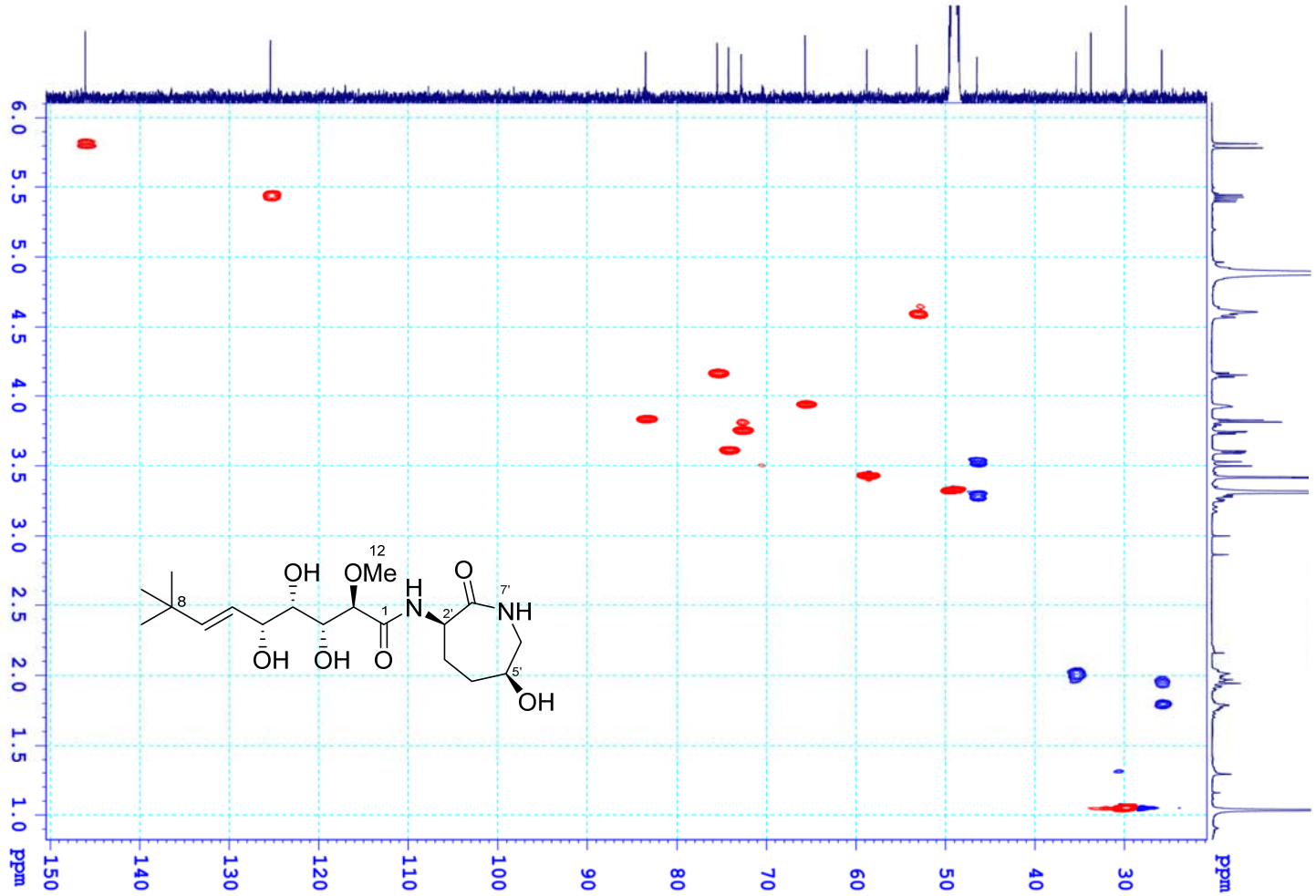
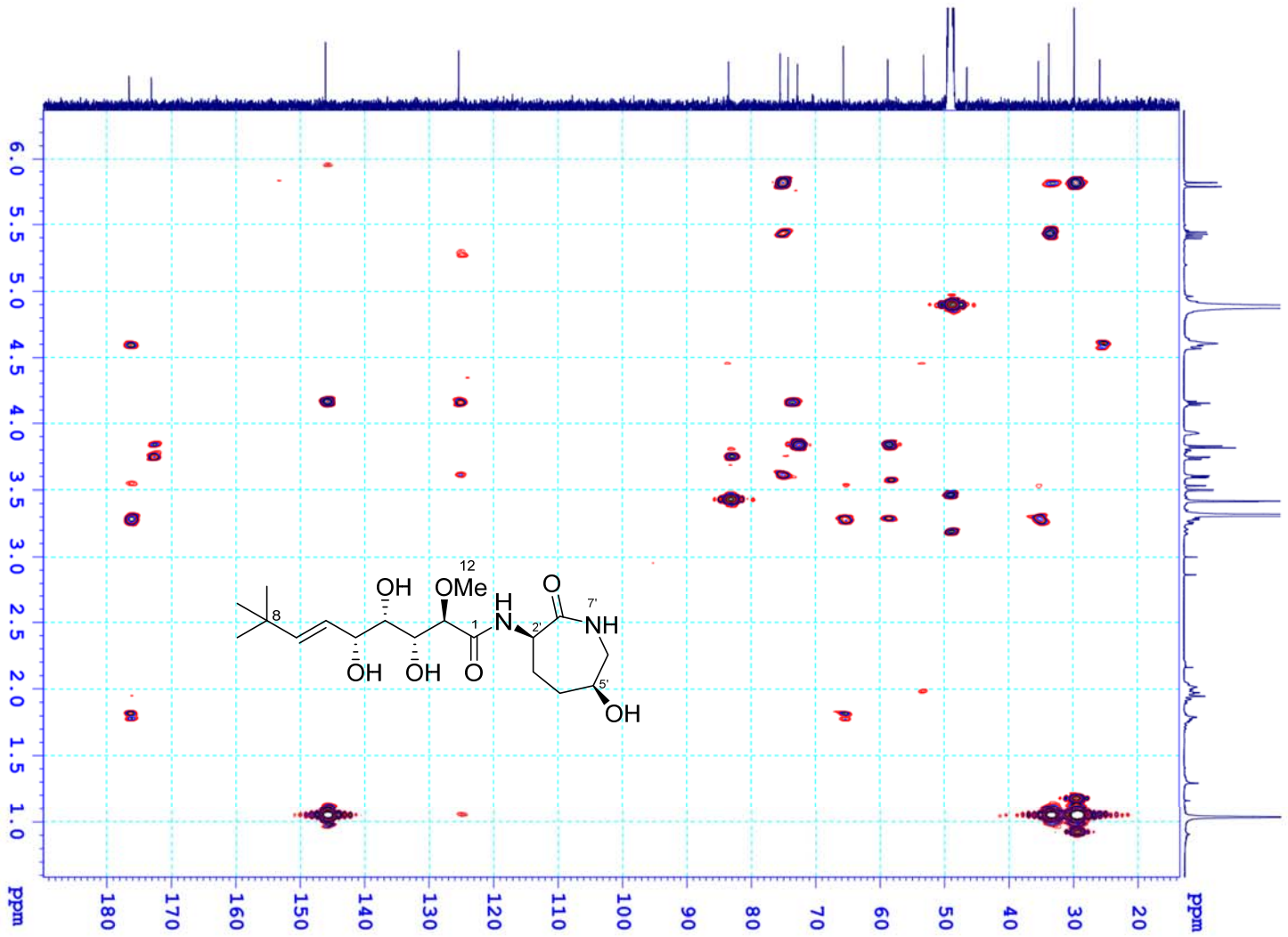
```
Current Data Parameters
NAME      2DAO_25Ap16BG205
EXPNO                    5
PROCNO                   1

F2 - Acquisition Parameters
Date_              20160426
Time                 22.59
INSTRUM              spect
PROBHD    5 mm Multinucl
PULPROG          cosygpqf
TD                   2048
SOLVENT              MeOD
NS                      8
DS                      8
SWH               5000.000 Hz
FIDRES            2.441406 Hz
AQ                0.2049000 sec
RG                      256
DW                100.000 usec
DE                  6.00 usec
TE                  295.6 K
d0                0.00000300 sec
D1                1.48689198 sec
d13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00020000 sec
MCREST    0 sec
MCWRK             1.48689198 sec

======== CHANNEL f1 ========
NUC1                     1H
P0                    10.20 usec
P1                    10.20 usec
PL1                   -3.00 dB
SFO1           500.1322506 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]          SINE.100
GPNAM[2]          SINE.100
GPX1        0 %
GPX2        0 %
GPY1        0 %
GPY2        0 %
GPZ1                  10.00 %
GPZ2                  10.00 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                       128
SFO1              500.1323 MHz
FIDRES           39.062500 Hz
SW                    9.997 ppm
FnMODE                   QF

F2 - Processing parameters
SI                      1024
SF             500.1300092 MHz
WDW                     SINE
SSB         0
LB          0 Hz
GB          0
PC                    1.40

F1 - Processing parameters
SI                      1024
MC2                     QF
SF             500.1300091 MHz
WDW                     SINE
SSB         0
LB          0 Hz
GB          0
```

HSQC spectrum of **9d** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)



HMBC spectrum of **9d** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)



HRESI Mass spectrum of **9d**