Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

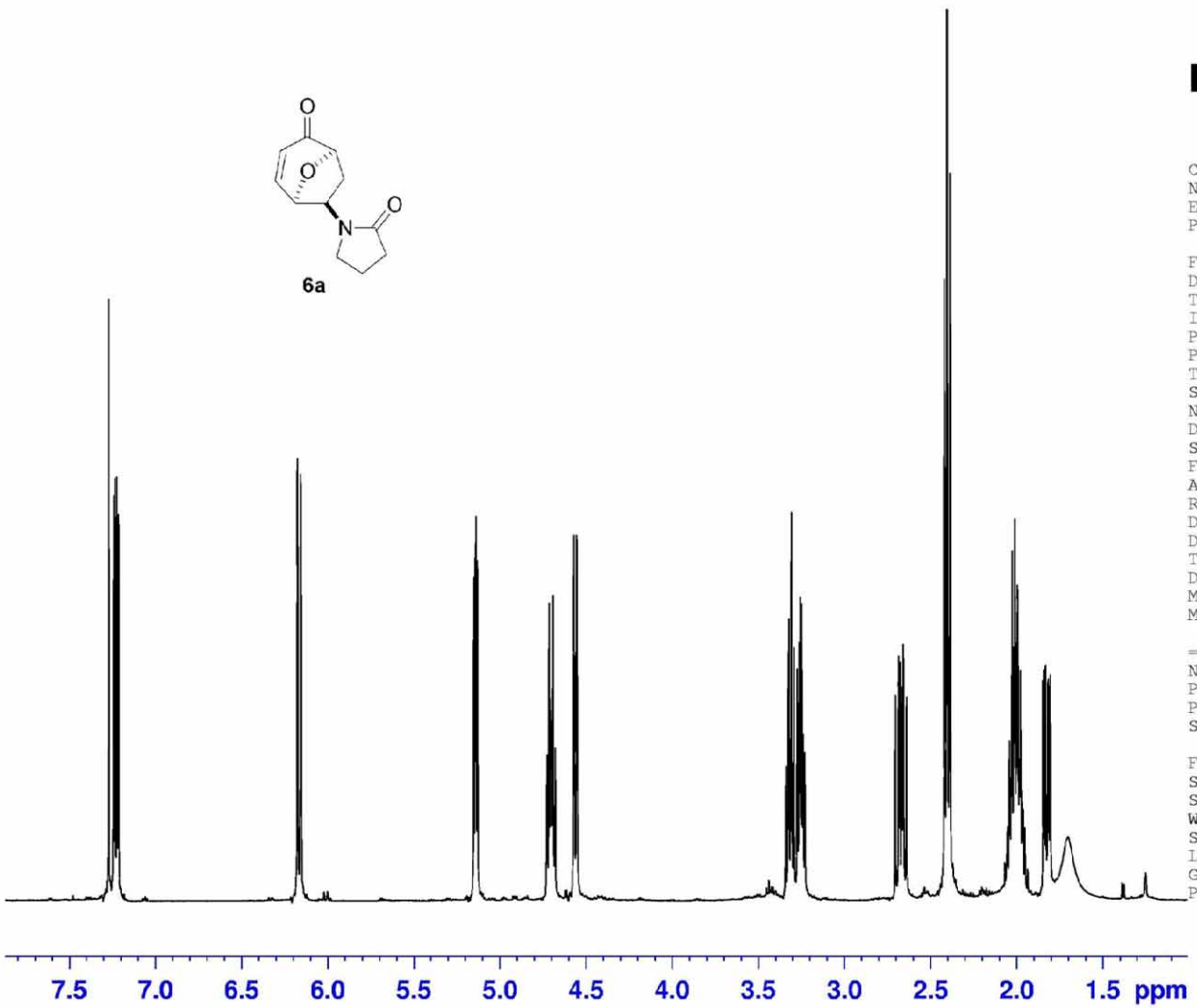
Diastereoselective 1,3-Dipolar Cycloaddition of Pyrylium Ylides with Chiral Enamides

Kirill Tchabanenko,[*a] Colleen Sloan,[a] Yves-Mael Bunetel[a] and Philip Mullen[a]

School of Chemistry and Chemical Engineering, Queen's University Belfast, David Keir Building, Stranmillis Road, Belfast BT9 5AG, United Kingdom.

k.tchabanenko@qub.ac.uk

Supporting Information.



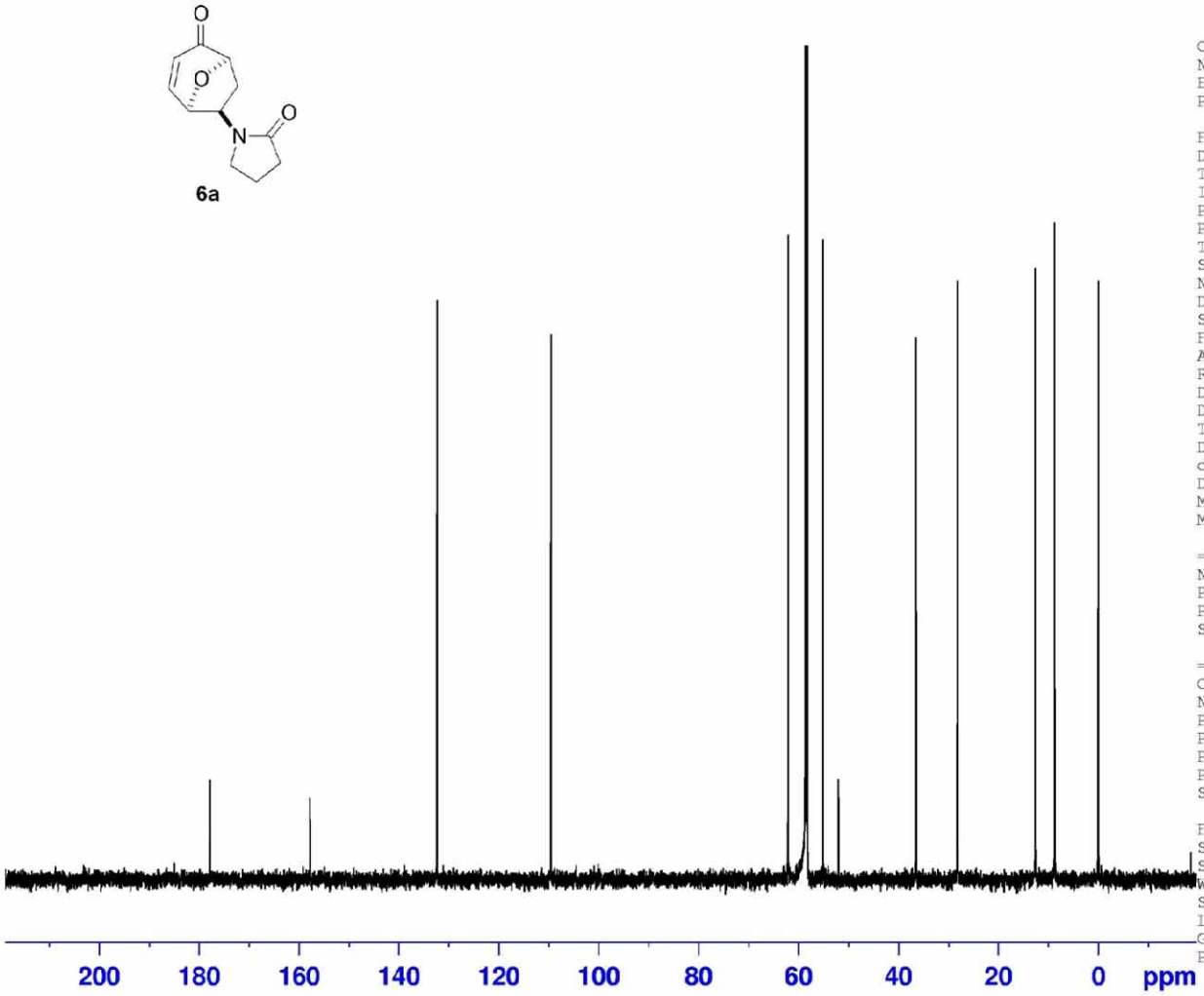
BRUKER

```
Current Data Parameters
NAME       Cycloadduct6a
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110621
Time                1.42
INSTRUM            spect
PROBHD   5 mm BBO 1H-BB
PULPROG               zg
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894966 sec
RG                   256
DW                62.400 usec
DE                 6.00 usec
TE                292.6 K
D1             2.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1                -3.00 dB
SFO1         500.1320005 MHz

F2 - Processing parameters
SI                 16384
SF          500.1300080 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



BRUKER

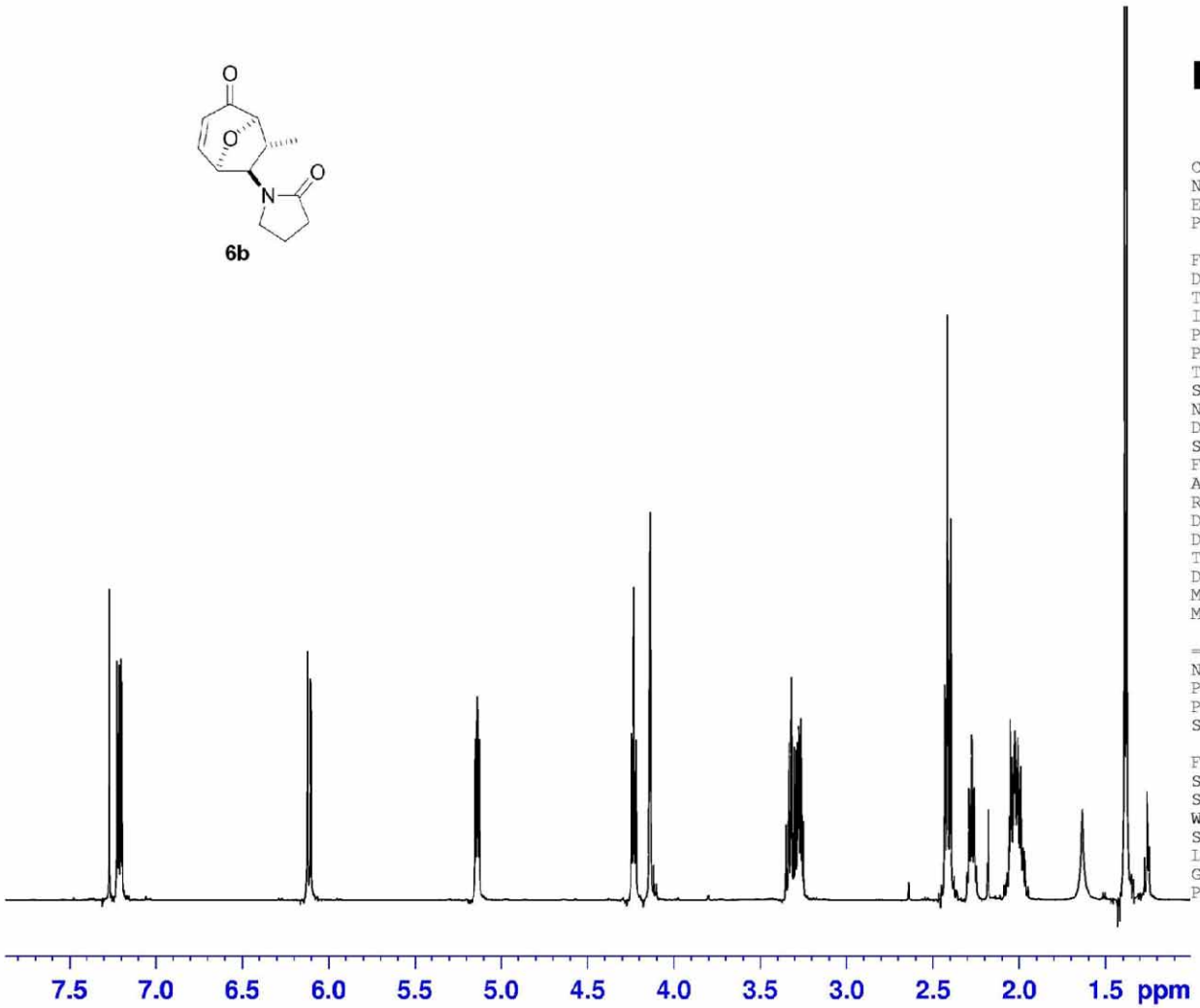
```
Current Data Parameters
NAME       Cycloadduct6a
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110621
Time                3.59
INSTRUM            spect
PROBHD   5 mm BBO 1H-BB
PULPROG             zgpg
TD                135168
SOLVENT             CDCl3
NS                   2048
DS                      4
SWH           35211.270 Hz
FIDRES         0.260500 Hz
AQ             1.9194356 sec
RG                 16384
DW                14.200 usec
DE                 6.00 usec
TE                292.8 K
D1            2.00000000 sec
d11           0.03000000 sec
DELIA         1.89999998 sec
MCRESI        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 6.00 usec
PL1               -3.00 dB
SFO1         125.7725760 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             100.00 usec
PL2               120.00 dB
PL12               18.00 dB
PL13               20.00 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                 65536
SF          125.7601250 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



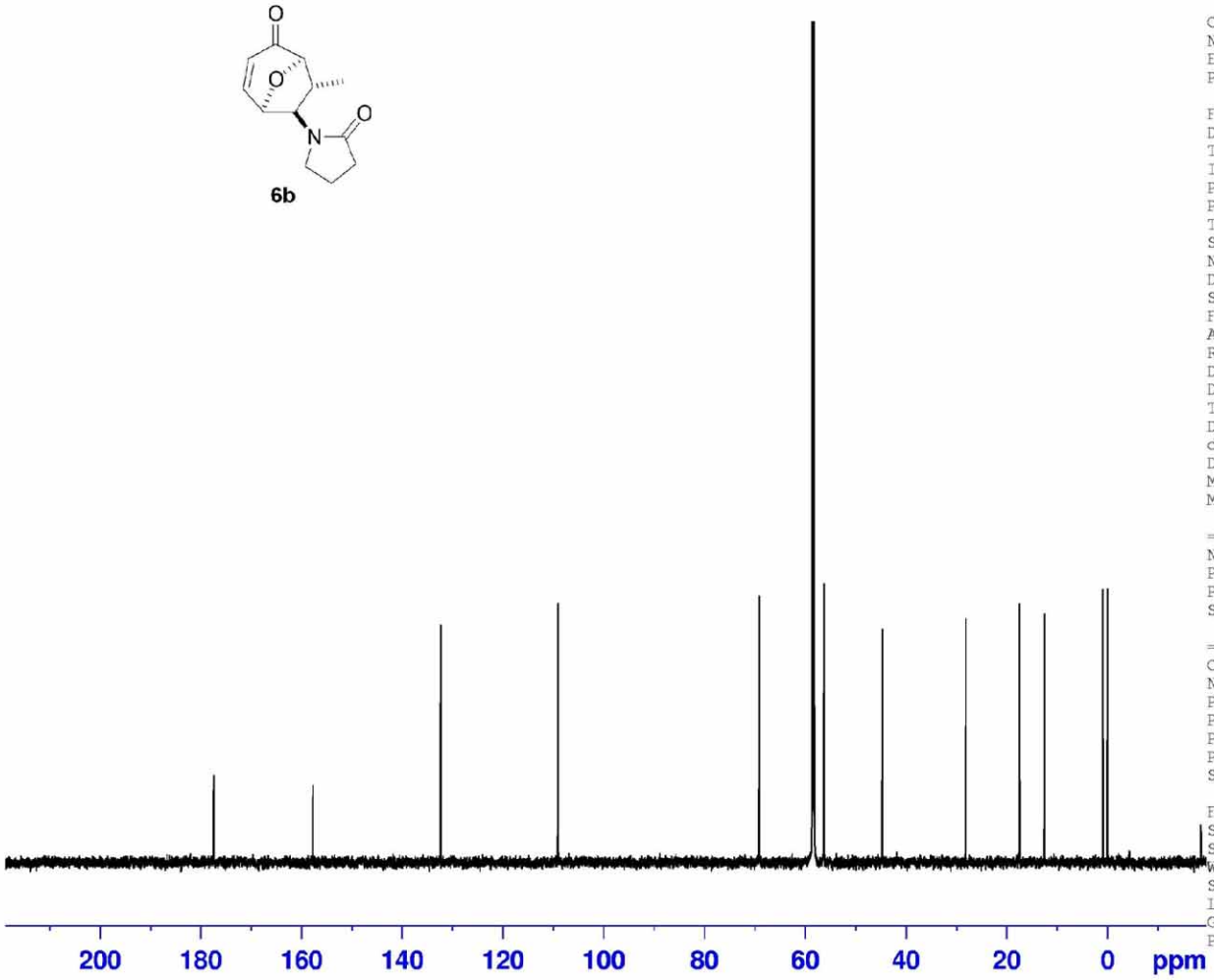
BRUKER

```
Current Data Parameters
NAME       Cycloadduct6b
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110111
Time               15.59
INSTRUM            spect
PROBHD   5 mm DUI 1H-13
PULPROG               zg
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894966 sec
RG                   181
DW                62.400 usec
DE                 6.00 usec
TE                510.3 K
D1             2.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1               -3.00 dB
SFO1         500.1320005 MHz

F2 - Processing parameters
SI                 16384
SF           500.1300093 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



BRUKER

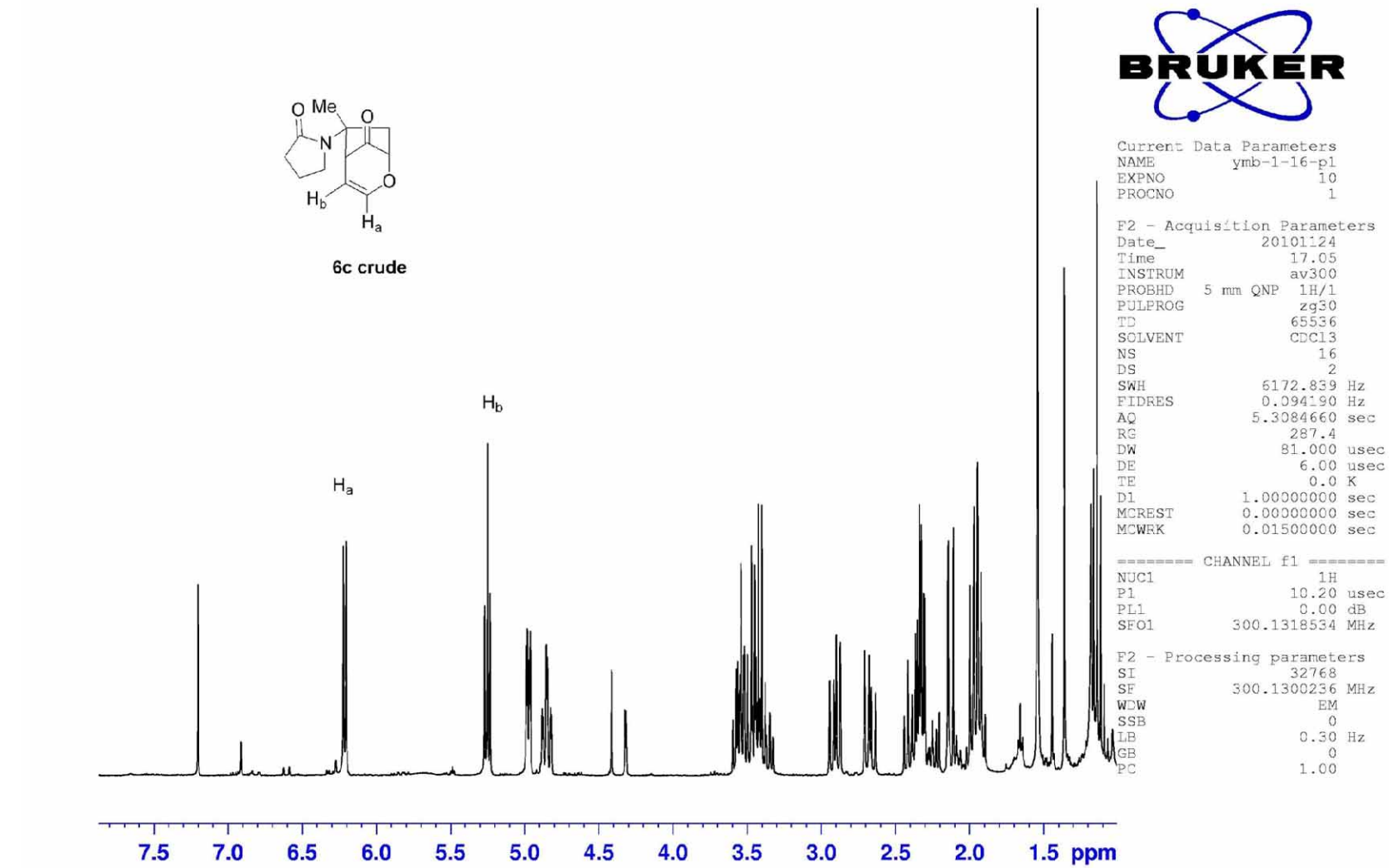
```
Current Data Parameters
NAME       Cycloadduct6b
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110111
Time               20.32
INSTRUM            spect
PROBHD   5 mm DUI 1H-13
PULPROG            zgpg
TD               135168
SOLVENT            CDCl3
NS                 4096
DS                    4
SWH           35211.270 Hz
FIDRES         0.260500 Hz
AQ             1.9194356 sec
RG                645.1
DW               14.200 usec
DE                6.00 usec
TE                510.3 K
D1            2.00000000 sec
d11           0.03000000 sec
DELIA         1.89999998 sec
MCRESI        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 5.50 usec
PL1                0.00 dB
SFO1        125.7725760 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2           100.00 usec
PL2             120.00 dB
PL12             18.00 dB
PL13             20.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                 65536
SF          125.7601292 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



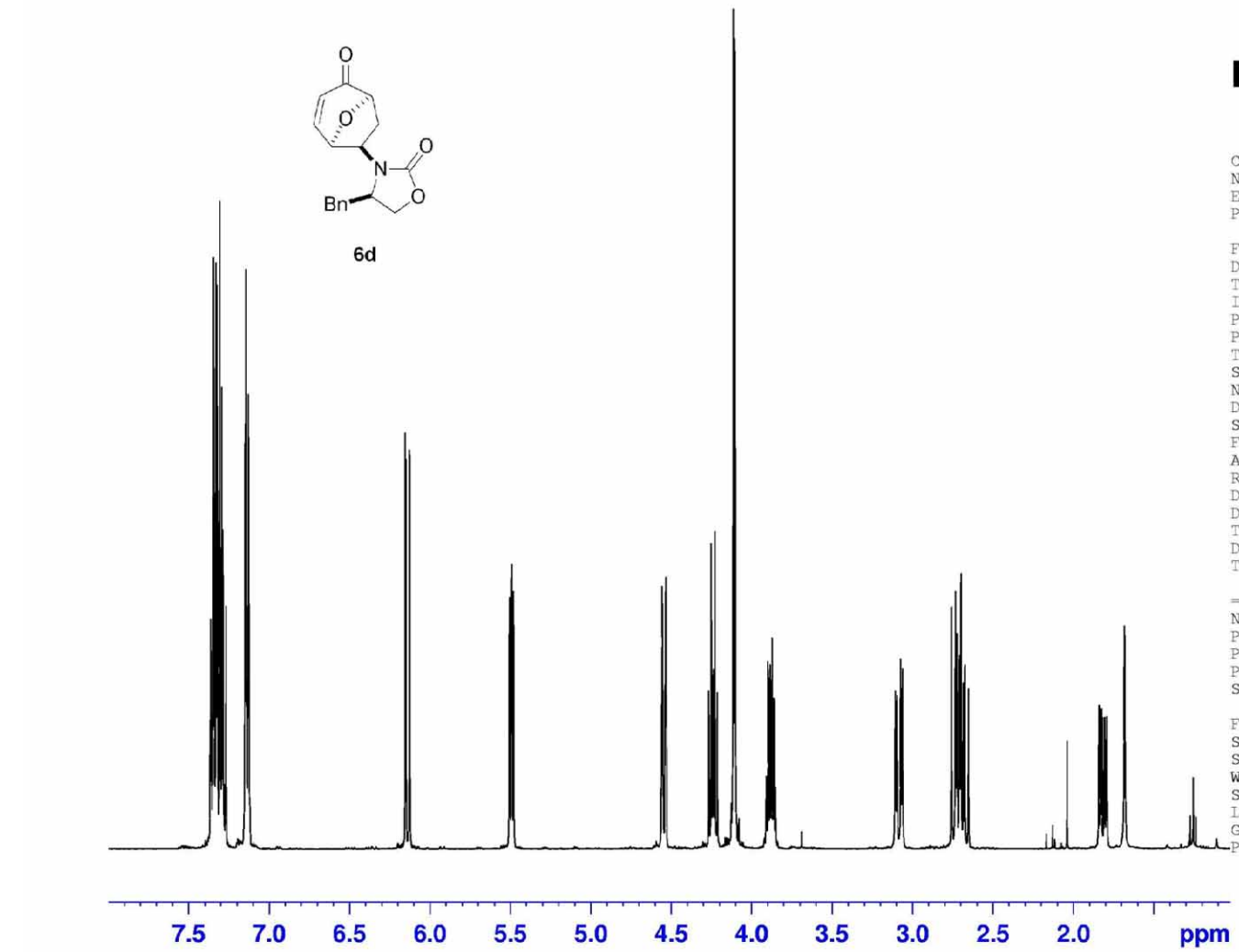
BRUKER

```
Current Data Parameters
NAME          ymb-1-16-p1
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20101124
Time               17.05
INSTRUM            av300
PROBHD   5 mm QNP  1H/1
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6172.839 Hz
FIDRES         0.094190 Hz
AQ             5.3084660 sec
RG                287.4
DW               81.000 usec
DE                6.00 usec
TE                 0.0 K
D1             1.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.20 usec
PL1                0.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                32768
SF           300.1300236 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

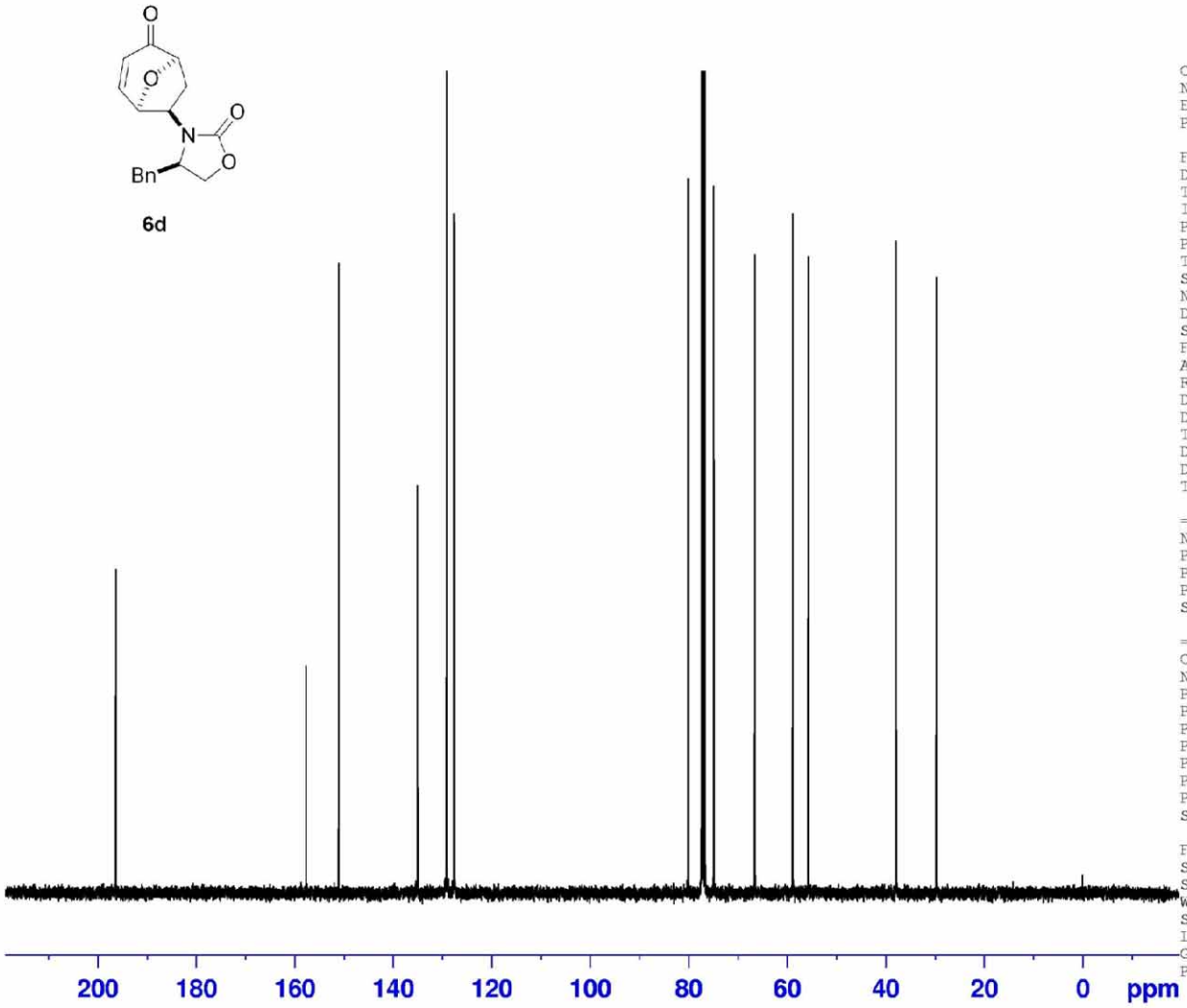



```
Current Data Parameters
NAME       Cycloadduct6d
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100727
Time               15.51
INSTRUM         AVIII_400
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                  90.5
DW                60.800 usec
DE                17.19 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 8.50 usec
PL1                -5.66 dB
PL1W        27.00118637 W
SFO1        400.1124708 MHz

F2 - Processing parameters
SI                 32768
SF          400.1100079 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



BRUKER

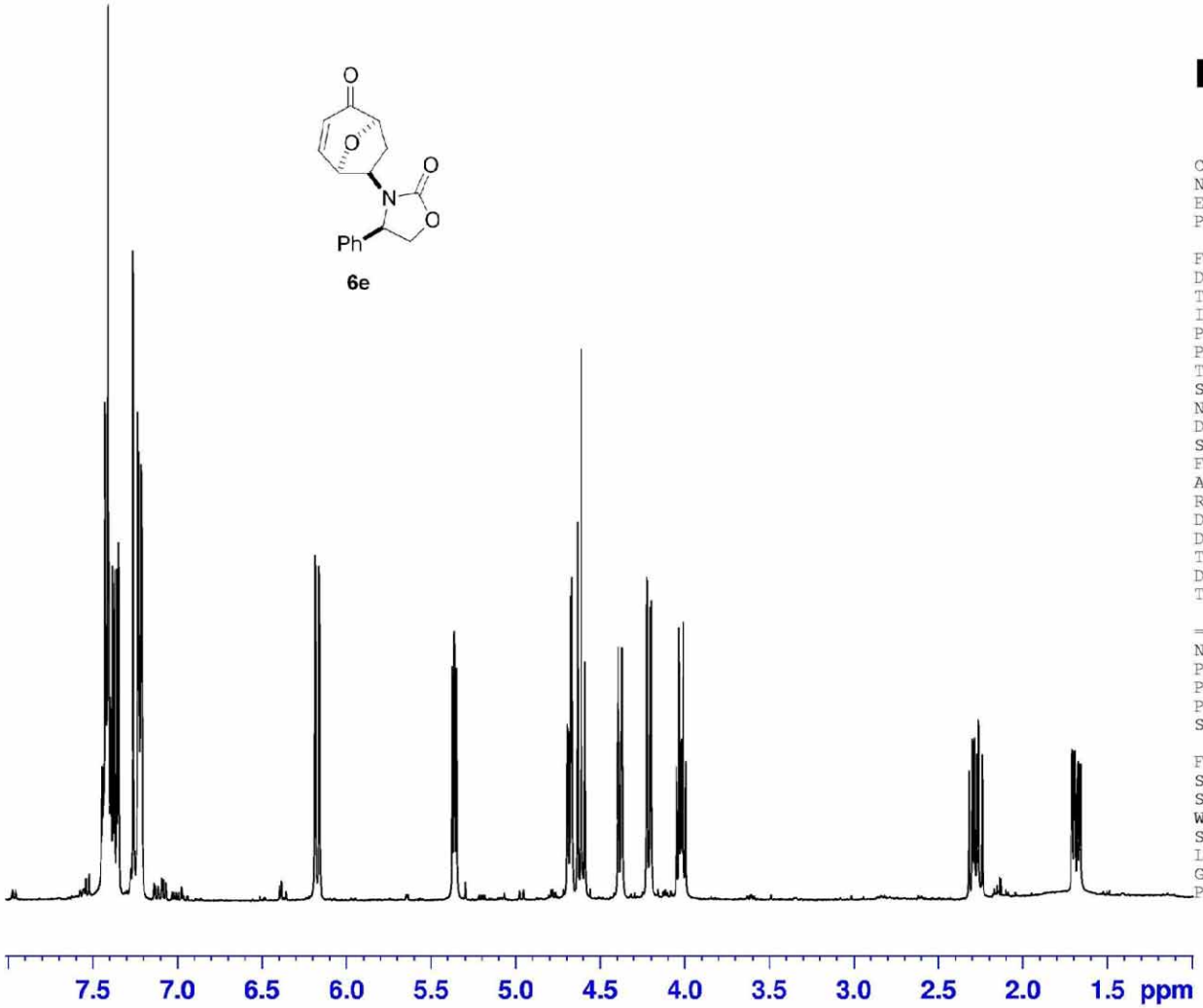
```
Current Data Parameters
NAME       Cycloadduct6d
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100727
Time               16.45
INSTRUM         AVIII_400
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 96150
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           24038.461 Hz
FIDRES         0.250010 Hz
AQ             1.9999700 sec
RG                    64
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   7.85 usec
PL1                 -3.30 dB
PL1W         69.27709961 W
SFO1        100.6178003 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz64
NUC2                  1H
PCPD2              60.00 usec
PL2                -5.66 dB
PL12               11.31 dB
PL13               14.31 dB
PL2W         27.00118637 W
PL12W         0.54247886 W
PL13W         0.27188349 W
SFO2        400.1116004 MHz

F2 - Processing parameters
SI                  131072
SF          100.6077400 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

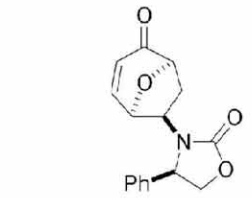



```
Current Data Parameters
NAME      400MHZ Product 6E
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20110907
Time                9.54
INSTRUM         AVIII_400
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   181
DW                60.800 usec
DE                17.19 usec
TE                300.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  8.50 usec
PL1                -5.66 dB
PL1W        27.00118637 W
SFO1        400.1124708 MHz

F2 - Processing parameters
SI                 32768
SF          400.1100090 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



6e

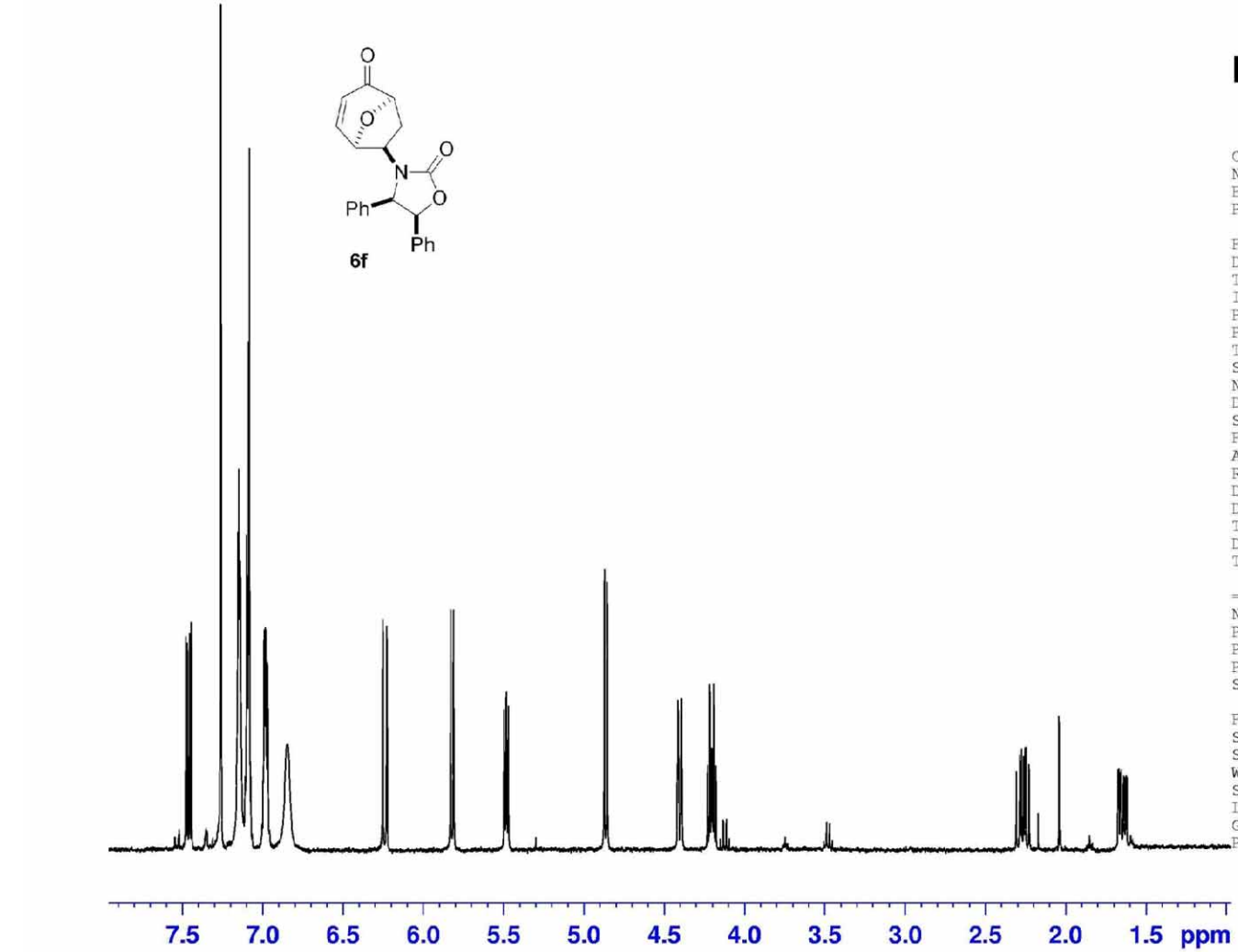

```
Current Data Parameters
NAME      400MHZ Product 6E
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_           20110907
Time               10.48
INSTRUM         AVIII_400
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                96150
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.250010 Hz
AQ             1.9999700 sec
RG                  144
DW                20.800 usec
DE                 6.50 usec
TE                300.1 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                 7.85 usec
PL1               -3.30 dB
PL1W        69.27709961 W
SFO1       100.6178003 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz64
NUC2                1H
PCPD2              60.00 usec
PL2                -5.66 dB
PL12               11.31 dB
PL13               14.31 dB
PL2W        27.00118637 W
PL12W        0.54247886 W
PL13W        0.27188349 W
SFO2       400.1116004 MHz

F2 - Processing parameters
SI                131072
SF         100.6077400 MHz
WDW                 EM
SSB                  0
LB                2.00 Hz
GB                   0
PC                1.40
```

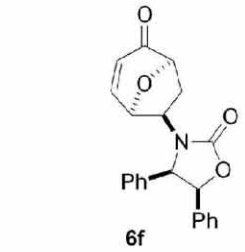



```
Current Data Parameters
NAME      400MHZ Product 6F
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20110907
Time                8.55
INSTRUM        AVIII_400
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                    362
DW                60.800 usec
DE                17.19 usec
TE                299.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 8.50 usec
PL1                -5.66 dB
PL1W        27.00118637 W
SFO1        400.1124708 MHz

F2 - Processing parameters
SI                 32768
SF          400.1100103 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



6f

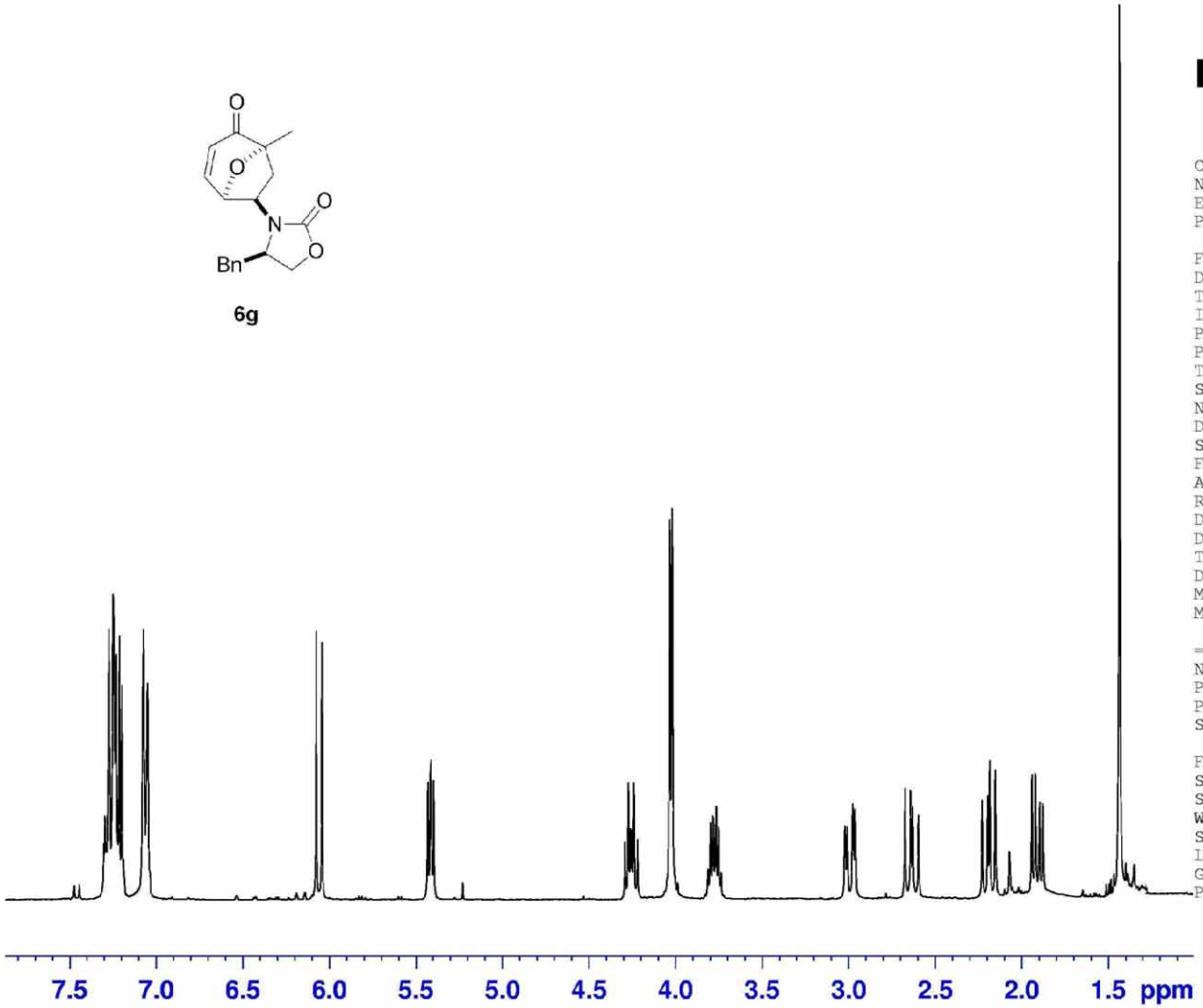

```
Current Data Parameters
NAME                  CS-CA1
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_              20110909
Time                  14.58
INSTRUM               spect
PROBHD   5 mm BBO 1H-BB
PULPROG                zgpg
TD                   135168
SOLVENT               CDCl3
NS                     1406
DS                        4
SWH               35211.270 Hz
FIDRES            0.260500 Hz
AQ                1.9194356 sec
RG                    16384
DW                   14.200 usec
DE                    6.00 usec
TE                   300.0 K
D1               1.00000000 sec
d11              0.03000000 sec
DELIA            0.89999998 sec
MCRESI           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                    6.00 usec
PL1                  -3.00 dB
SFO1          125.7725760 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               100.00 usec
PL2                 120.00 dB
PL12                 18.00 dB
PL13                 20.00 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                     65536
SF            125.7600000 MHz
WDW                       EM
SSB                        0
LB                    2.00 Hz
GB                         0
PC                    1.00
```

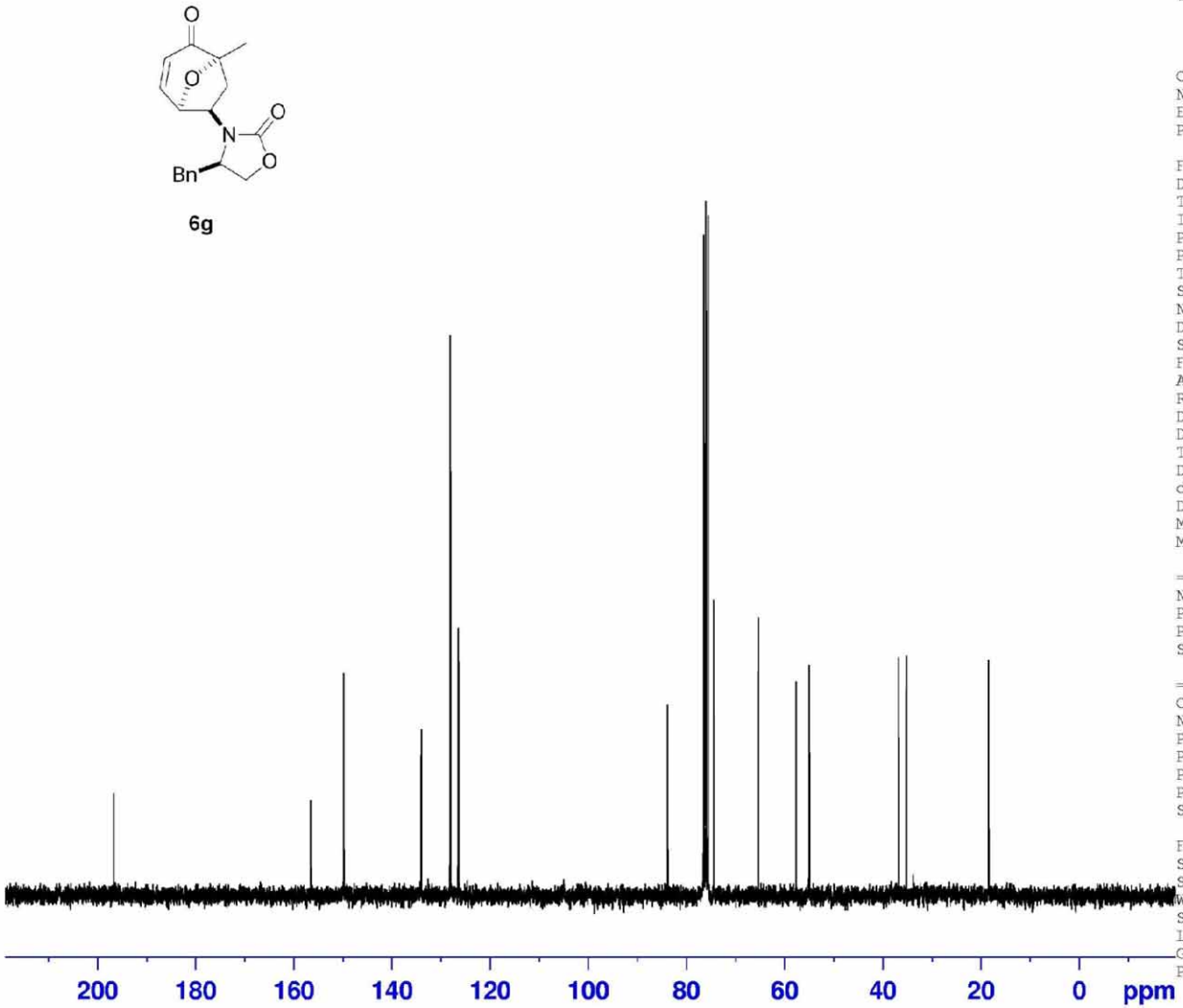



```
Current Data Parameters
NAME       PHM-005-06-01
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110620
Time               14.16
INSTRUM            av300
PROBHD   5 mm QNP  1H/1
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6172.839 Hz
FIDRES         0.094190 Hz
AQ             5.3084660 sec
RG                  181
DW               81.000 usec
DE                6.00 usec
TE                 0.0 K
D1          1.00000000 sec
MCREST      0.00000000 sec
MCWRK       0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.20 usec
PL1                0.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                32768
SF          300.1300245 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



BRUKER

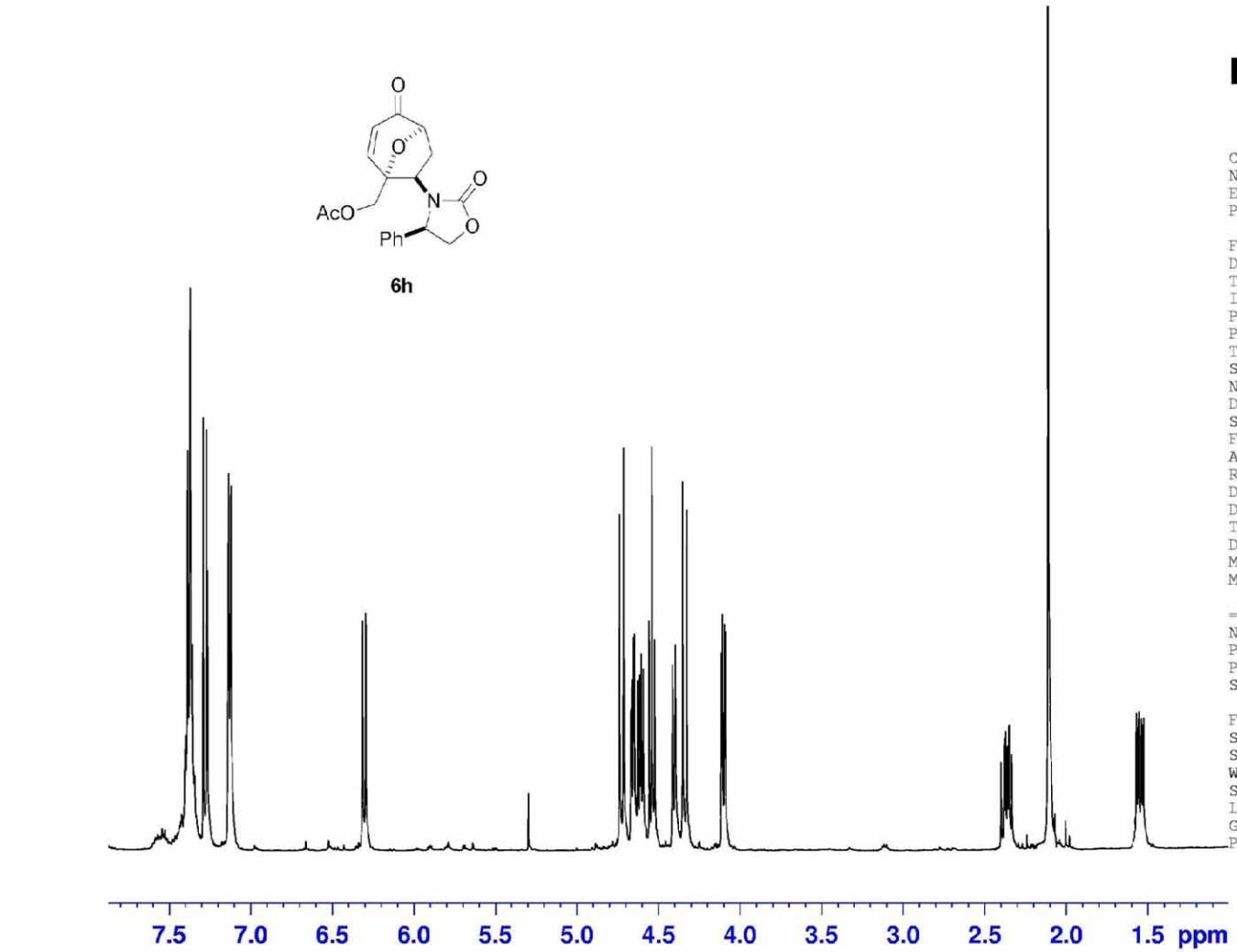
```
Current Data Parameters
NAME       PHM-005-06-01
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110620
Time               14.49
INSTRUM            av300
PROBHD   5 mm QNP  1H/1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    2
SWH           22675.736 Hz
FIDRES         0.346004 Hz
AQ             1.4451188 sec
RG                5792.6
DW                22.050 usec
DE                 6.00 usec
TE                  0.0 K
D1            1.00000000 sec
d11           0.03000000 sec
DELIA         0.89999998 sec
MCRESI        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 9.00 usec
PL1                0.00 dB
SFO1         75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12              19.00 dB
PL13              19.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4678257 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



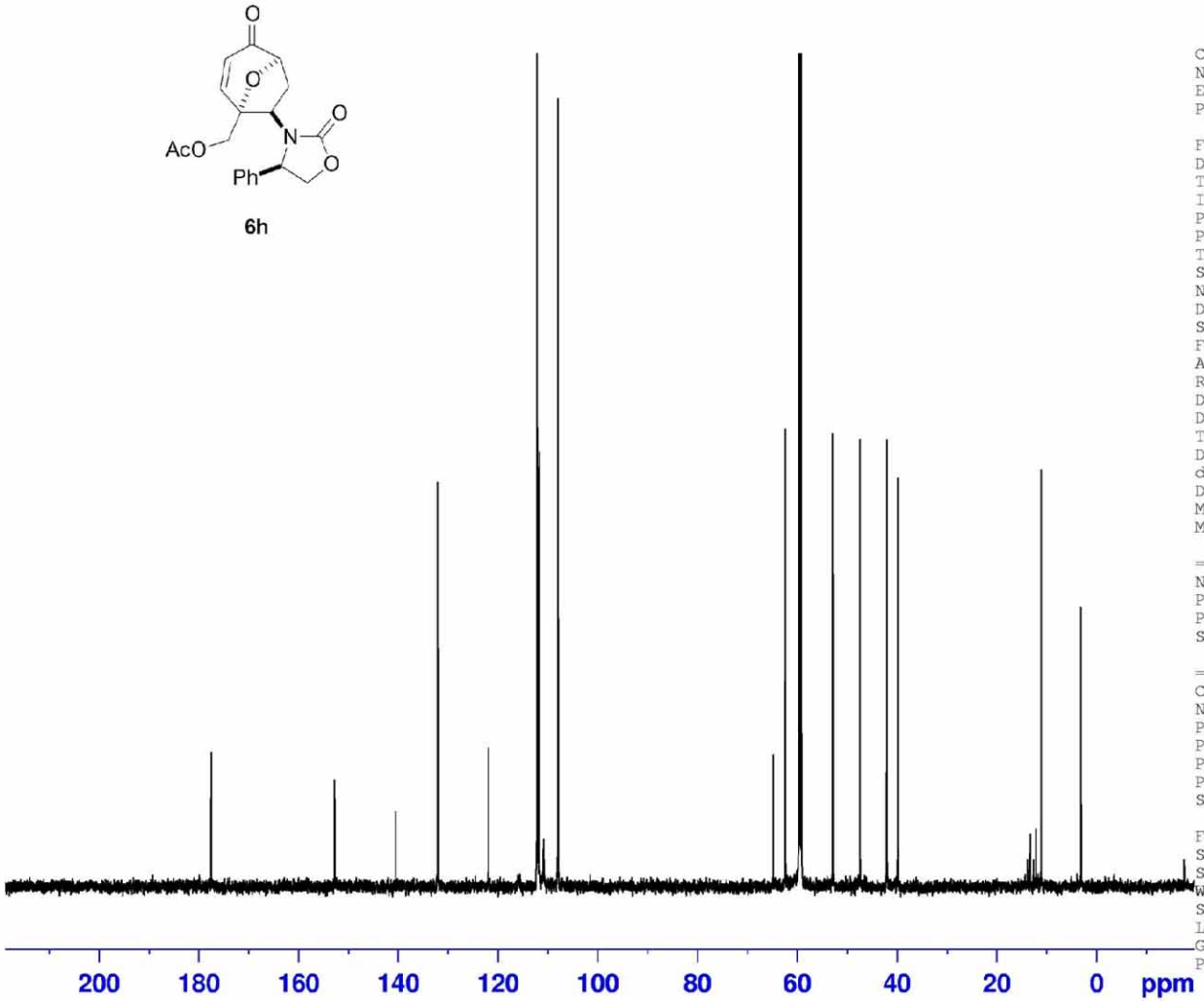
BRUKER

```
Current Data Parameters
NAME       Cycloadduct6h
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20101101
Time               16.50
INSTRUM            spect
PROBHD   5 mm BBO 1H-BB
PULPROG               zg
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894966 sec
RG                 143.7
DW                62.400 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1               -3.00 dB
SFO1         500.1320005 MHz

F2 - Processing parameters
SI                 16384
SF           500.1300110 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



BRUKER

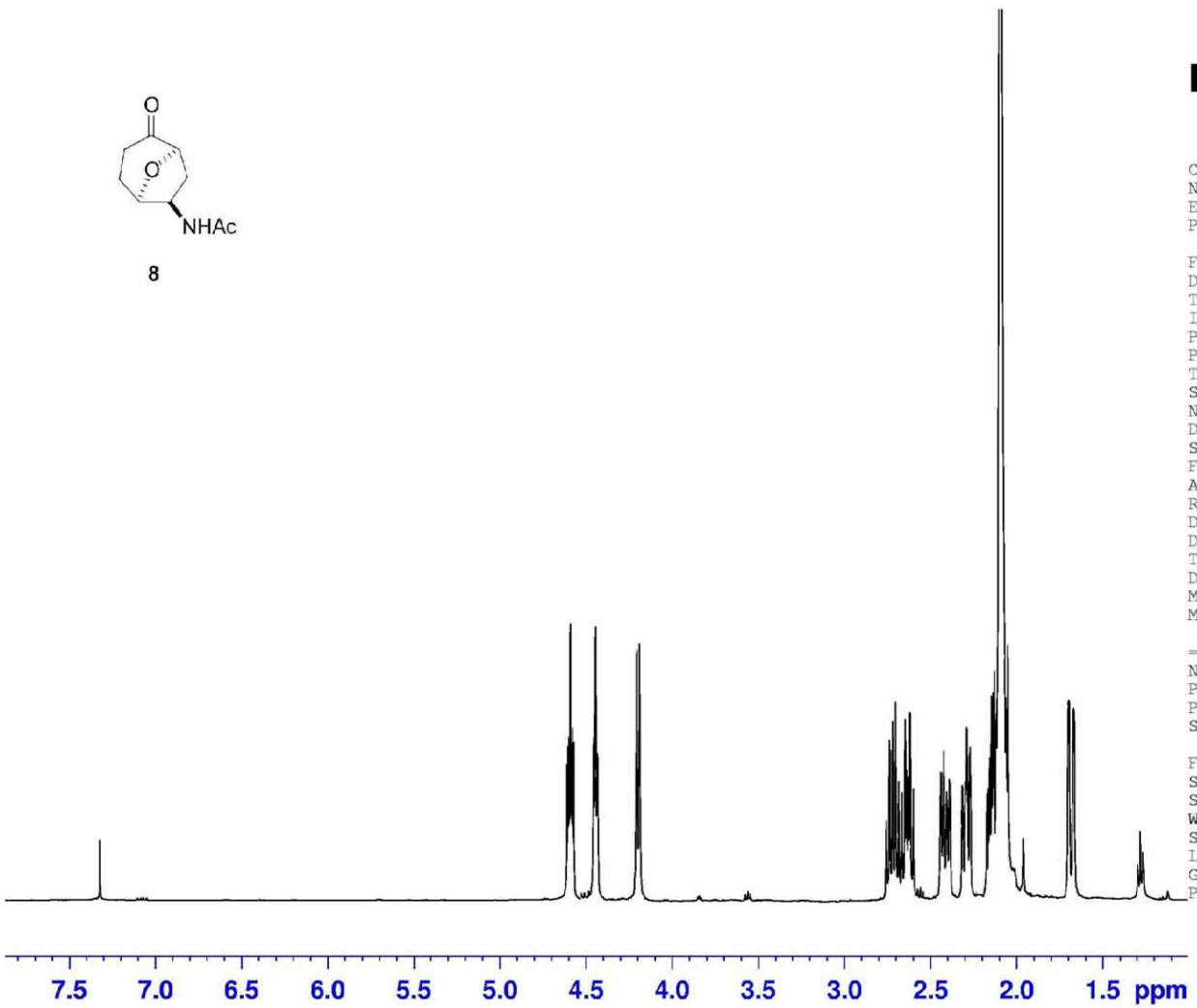
```
Current Data Parameters
NAME       Cycloadduct6h
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20101101
Time               18.40
INSTRUM             spect
PROBHD   5 mm BBO 1H-BB
PULPROG             zgpg
TD                135168
SOLVENT             CDCl3
NS                   2048
DS                      1
SWH           31446.541 Hz
FIDRES         0.232648 Hz
AQ             2.1492212 sec
RG                   8192
DW                15.900 usec
DE                 6.00 usec
TE                300.0 K
D1            1.00000000 sec
d11           0.03000000 sec
DELIA         0.89999998 sec
MCRESI        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                   5.50 usec
PL1                  0.00 dB
SFO1         125.7732048 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                120.00 dB
PL12                18.00 dB
PL13                20.00 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                   65536
SF           125.7600000 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.00
```

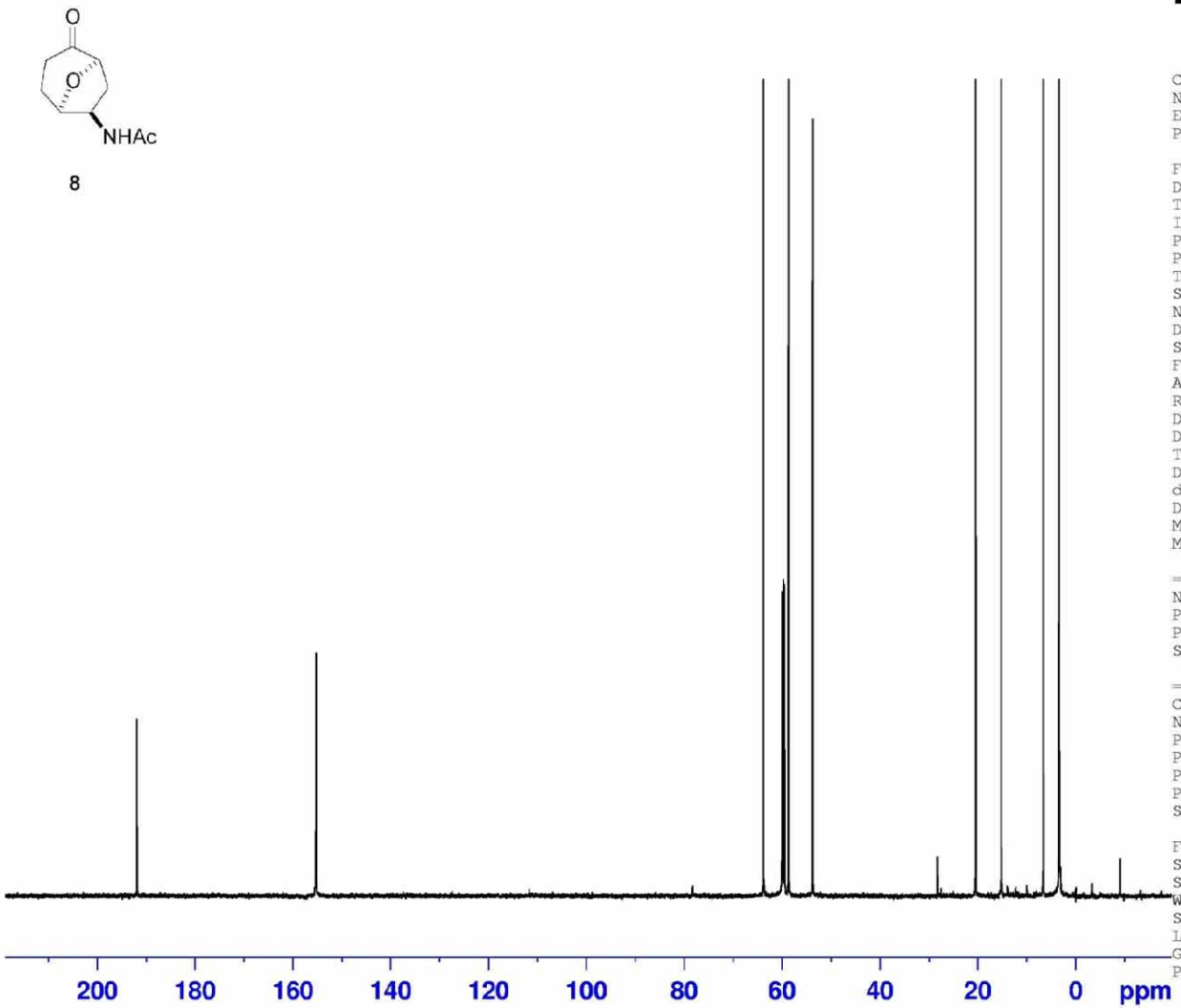



```
Current Data Parameters
NAME                  KI205
EXPNO                    10
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110124
Time                  12.18
INSTRUM               spect
PROBHD    5 mm BBO 1H-BB
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      64
DS                       2
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894966 sec
RG                     14.3
DW                   62.400 usec
DE                    6.00 usec
TE                   300.1 K
D1             2.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.00 usec
PL1                  -3.00 dB
SFO1          500.1320005 MHz

F2 - Processing parameters
SI                   16384
SF            500.1299816 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



BRUKER

```
Current Data Parameters
NAME                  KT205
EXPNO                    11
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110124
Time                  12.20
INSTRUM               spect
PROBHD   5 mm BBO 1H-BB
PULPROG                zgpg
TD                   135168
SOLVENT               CDCl3
NS                     1481
DS                        4
SWH               35211.270 Hz
FIDRES            0.260500 Hz
AQ                1.9194356 sec
RG                   5792.6
DW                   14.200 usec
DE                    6.00 usec
TE                   300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELIA           1.89999998 sec
MCRESI          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                     5.50 usec
PL1                    0.00 dB
SFO1          125.7725760 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                100.00 usec
PL2                  120.00 dB
PL12                  18.00 dB
PL13                  20.00 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                     65536
SF            125.7599646 MHz
WDW                       EM
SSB                        0
LB                    2.00 Hz
GB                         0
PC                      1.00
```