

Supporting Information File 2

for

Design, automated synthesis and immunological evaluation of NOD2-ligand–antigen conjugates

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Email: Jeroen D. C. Codée - jcodee@chem.leidenuniv.nl; Dmitri V. Filippov - filippov@chem.leidenuniv.nl

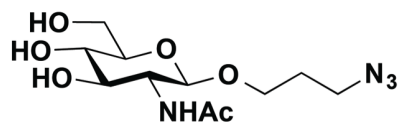
*Corresponding author

NMR spectra

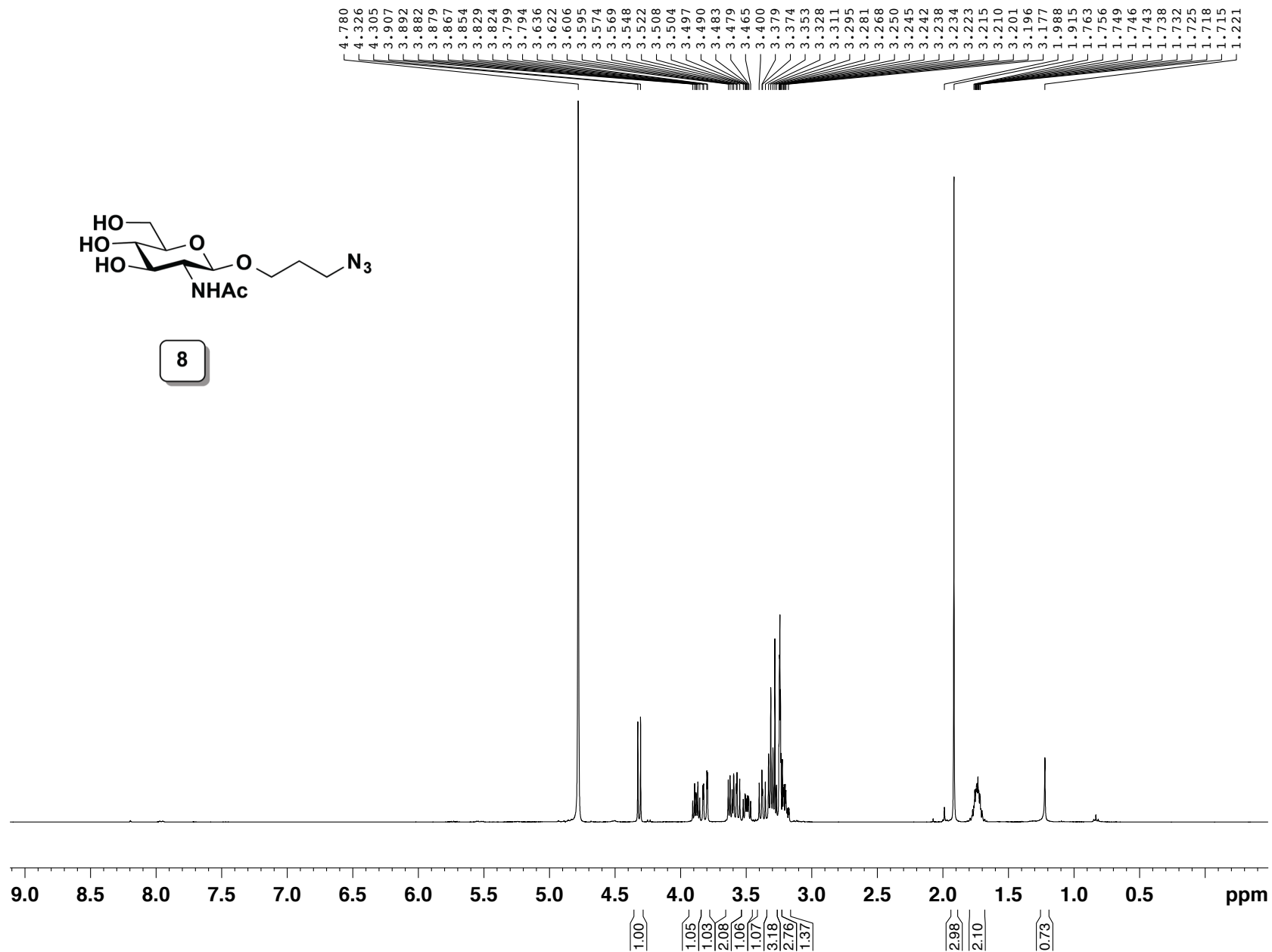
Contents:

Compound 8	¹ H NMR 400 MHz CD ₃ CD	p S2-S3
Compound 8	¹³ C NMR 100 MHz CD ₃ CD	p S4
Compound 9	¹ H NMR 400 MHz DMSO-d ₆	p S5
Compound 9	¹³ C NMR 100 MHz DMSO-d ₆	p S6
Compound 10	¹ H NMR 400 MHz CD ₃ CD	p S7
Compound 10	¹³ C NMR 100 MHz CD ₃ CD	p S8
Compound 12	¹ H NMR 400 MHz DMSO-d ₆	p S9
Compound 12	¹³ C NMR 100 MHz DMSO-d ₆	p S10
Compound 13	¹ H NMR 400 MHz DMSO-d ₆	p S11
Compound 13	¹³ C NMR 100 MHz DMSO-d ₆	p S12
Compound 14	¹ H NMR 400 MHz CD ₃ CD	p S13-S14
Compound 14	¹³ C NMR 100 MHz CD ₃ CD	p S15
Compound 15	¹ H NMR 400 MHz DMSO-d ₆	p S16
Compound 15	¹³ C NMR 100 MHz DMSO-d ₆	p S17
Compound 16	¹ H NMR 600 MHz DMSO-d ₆	p S18
Compound 16	¹³ C NMR 150 MHz DMSO-d ₆	p S19
Compound 17	¹ H NMR 600 MHz DMSO-d ₆	p S20
Compound 17	¹³ C NMR 150 MHz DMSO-d ₆	p S21
Compound 17	¹ H NMR 400 MHz D ₂ O	p S22-S23
Compound 18 (crude)	¹ H NMR 400 MHz CD ₃ CD	p S24
Compound 18 (crude)	¹³ C NMR 100 MHz CD ₃ CD	p S25
Compound 19	¹ H NMR 400 MHz CD ₃ CD	p S26
Compound 19	¹³ C NMR 100 MHz CD ₃ CD	p S27
Compound 20	¹ H NMR 400 MHz D ₂ O	p S28
Compound 20	¹³ C NMR 100 MHz CD ₃ CD	p S29

S2

1h NMR av400liq
mw034

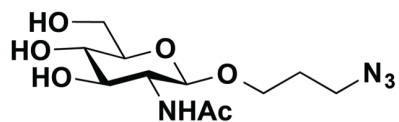
8



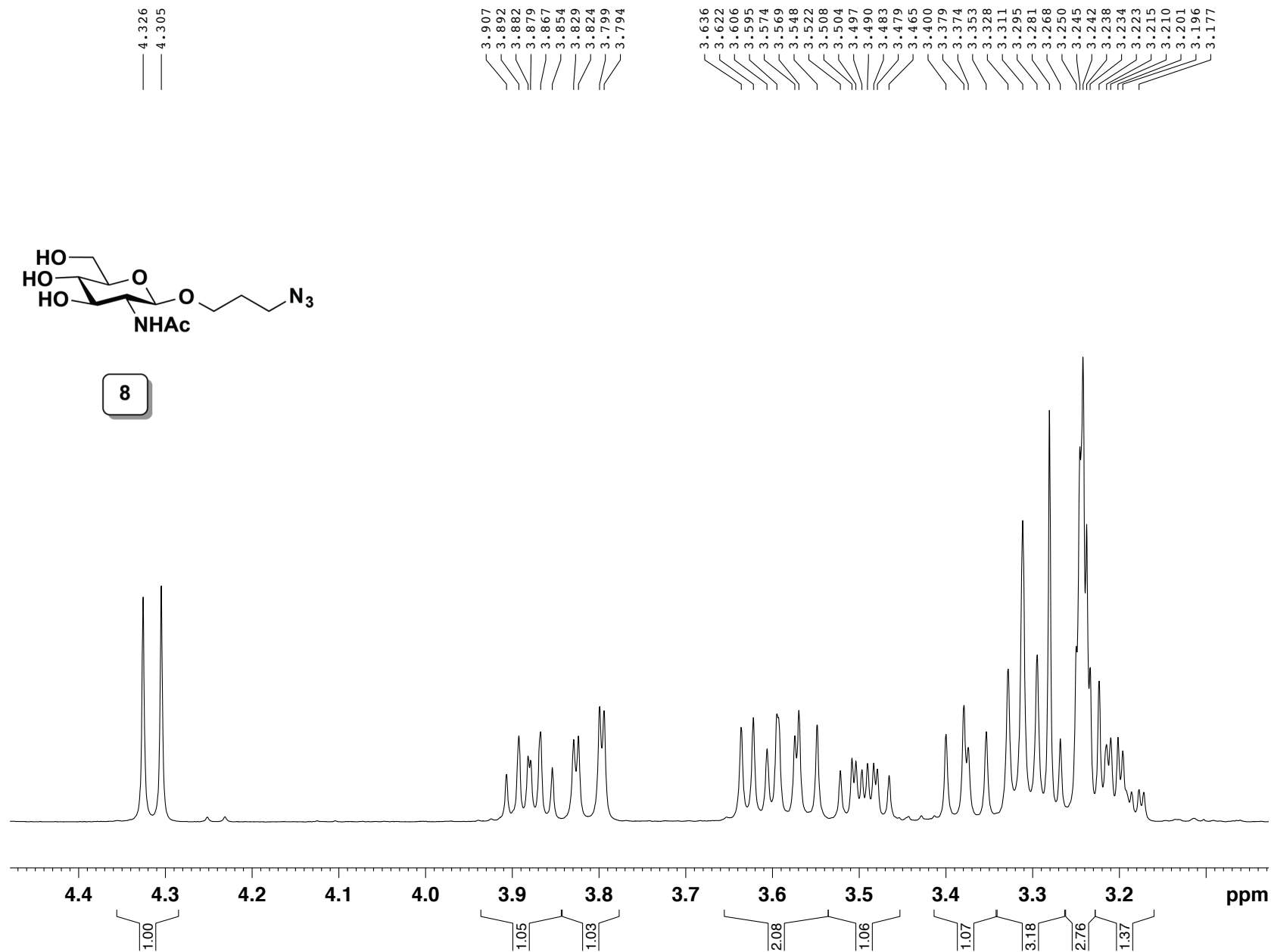
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PULPROG zg30
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SOLVENT MeOD
NS 16
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FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.10 usec
PL1 0.00 dB
PL1W 8.41481972 W
SFO1 400.2324716 MHz
SI 65536
SF 400.2300373 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S3

1h NMR av400liq
mw034

8

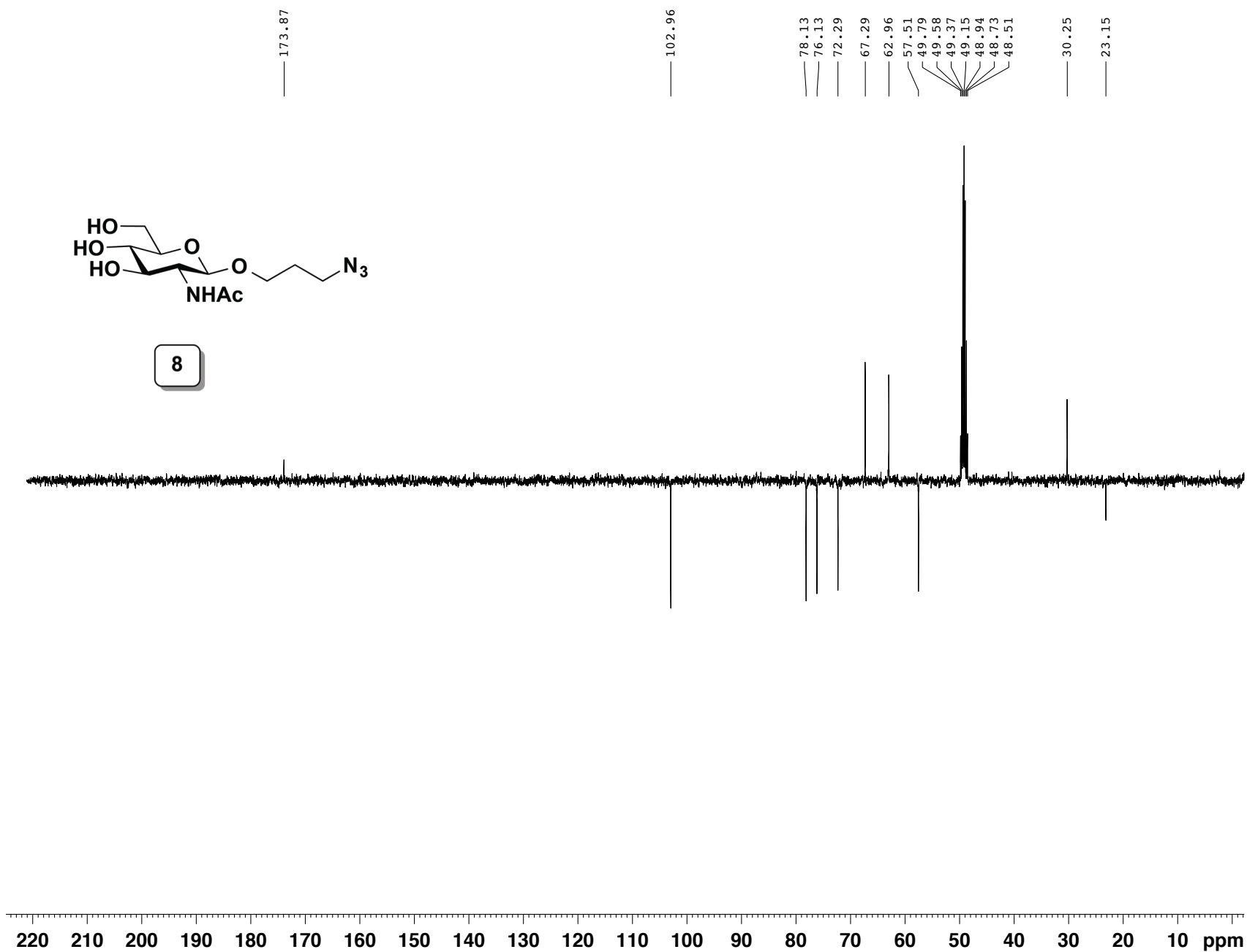


NAME 0807marian
EXPNO 57
PROCNO 1
Date_ 20080716
Time 9.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 0
SWH 8223.685 Hz
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AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.10 usec
PL1 0.00 dB
PL1W 8.41481972 W
SFO1 400.2324716 MHz
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SF 400.2300373 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S4

mw034 13CNMR

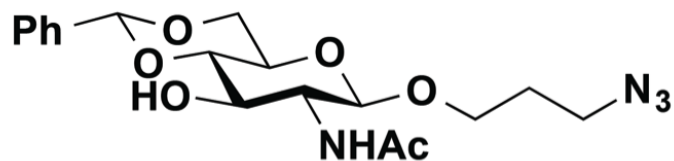


S5
1h NMR av400liq mw173

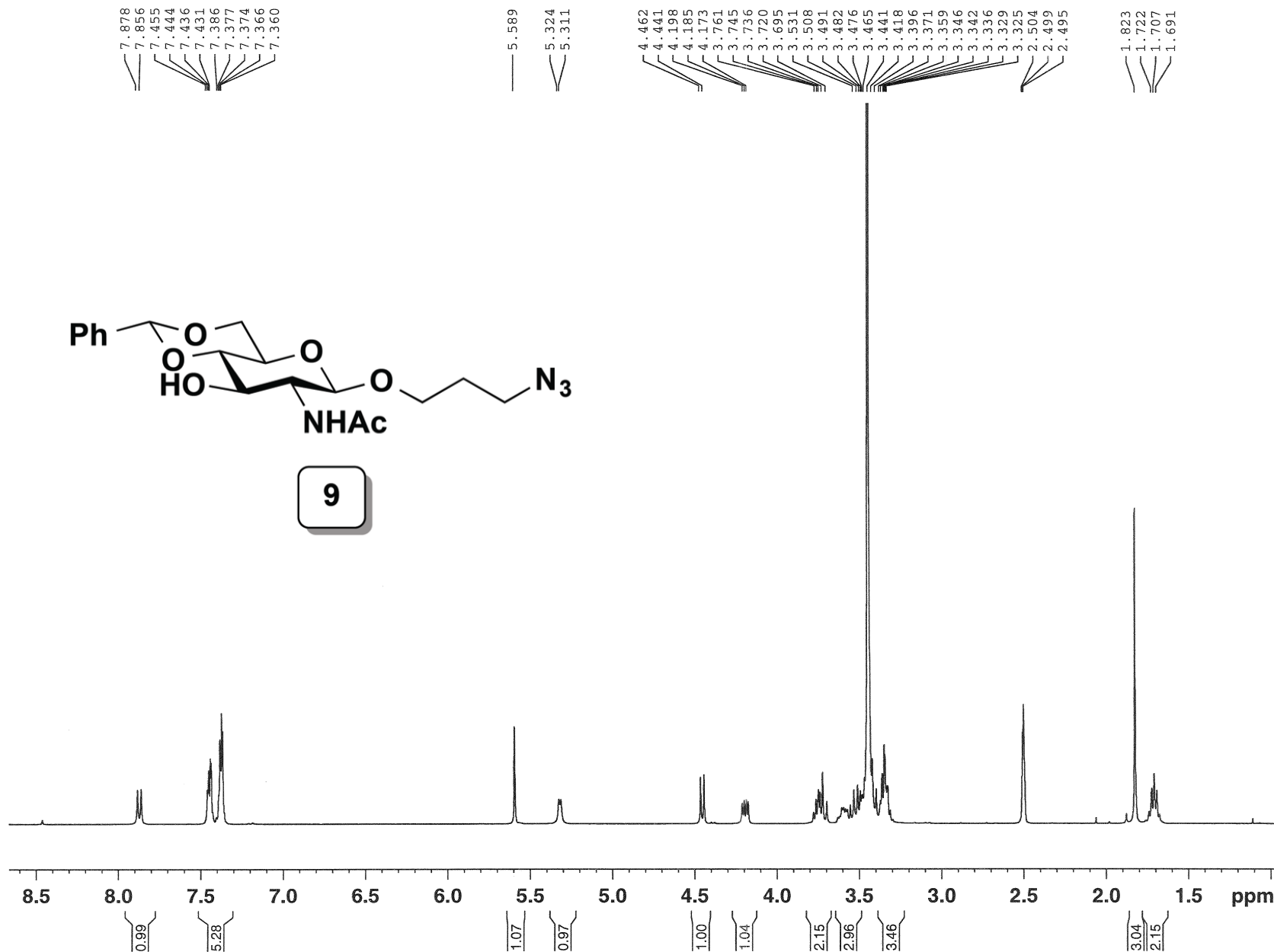
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PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         8
DS         0
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         114
DW         60.800 usec
DE         6.50 usec
TE         295.9 K
D1         1.00000000 sec
TD0        1

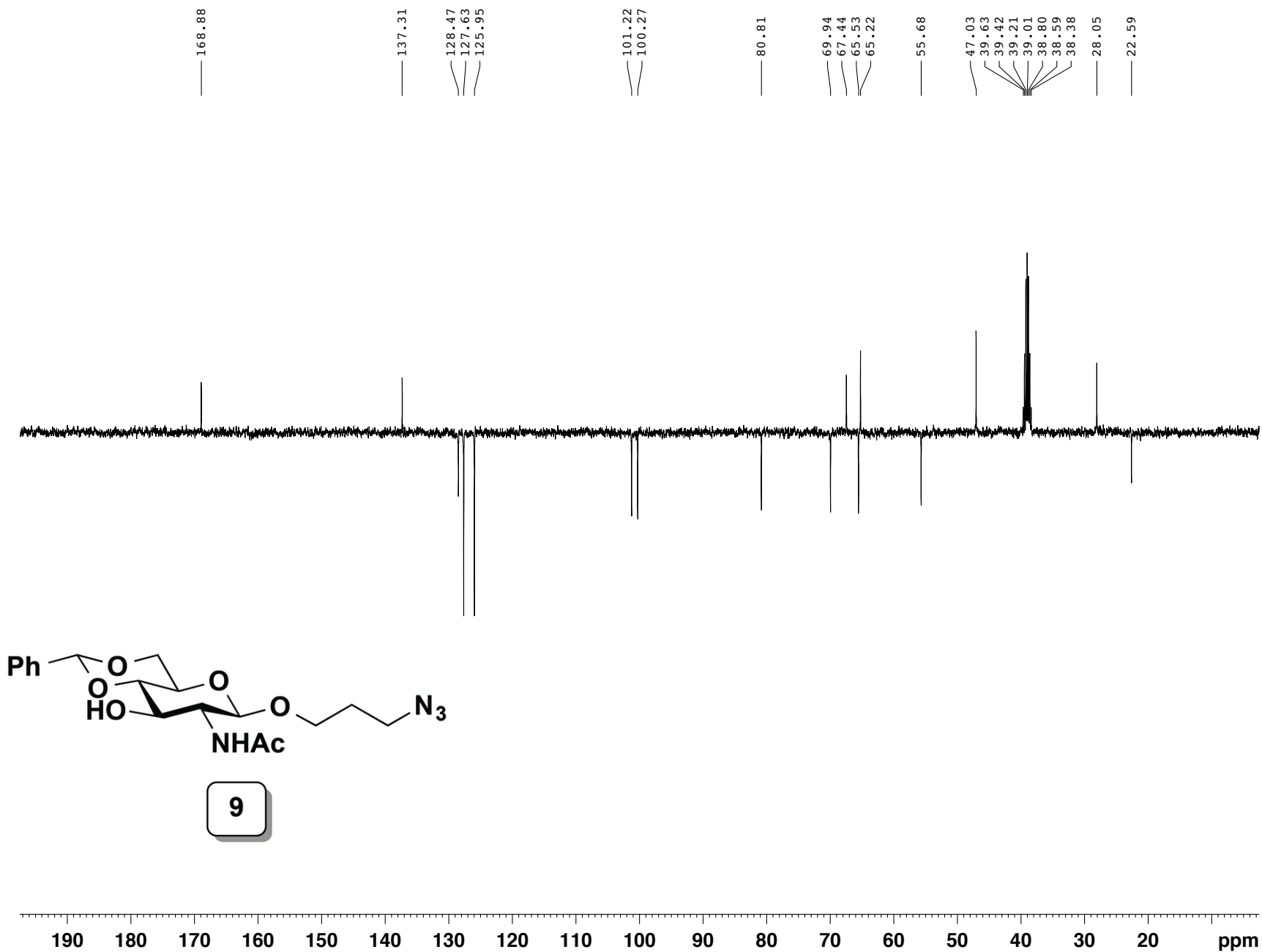
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SF01       400.2324716 MHz
SI         65536
SF         400.2300059 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
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9



S6

¹³C APT av400liq mw173

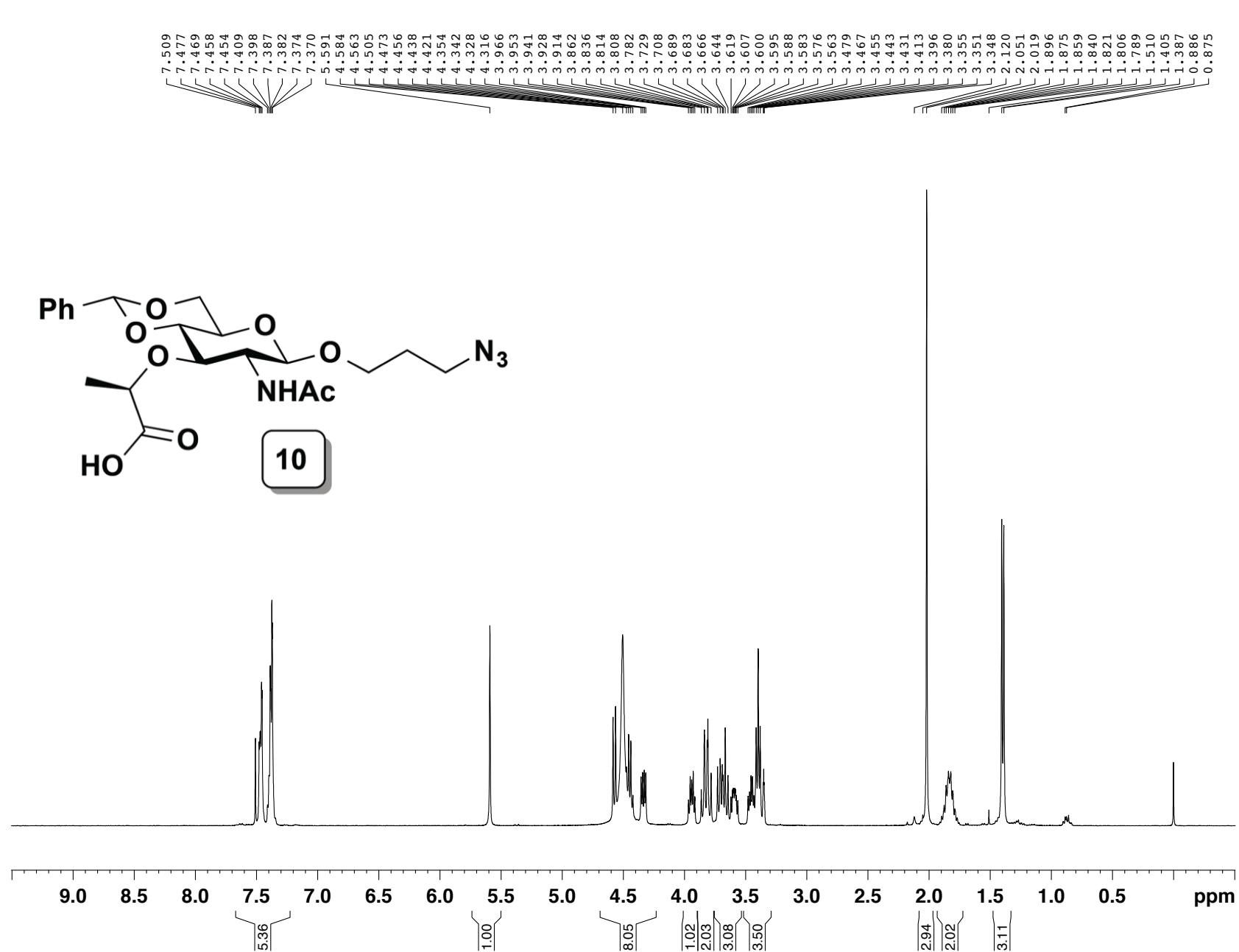
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EXPNO 13
PROCNO 1
Date_ 20090612
Time 9.49
INSTRUM spect
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PULPROG jmod
TD 65536
SOLVENT DMSO
NS 88
DS 1
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 295.9 K
CNST2 155.0000000
CNST11 1.0000000
D1 1.50000000 sec
D20 0.00645161 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 9.10 usec
P2 18.20 usec
PL1 -1.00 dB
PL1W 44.27188873 W
SFO1 100.6479773 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL2W 8.41481972 W
PL12W 0.26609996 W
SFO2 400.2316009 MHz
SI 32768
SF 100.6380019 MHz
WDW EM
SSB 0
LB 2.50 Hz
GB 0
PC 1.40

S7

1h NMR av400liq BvB 7



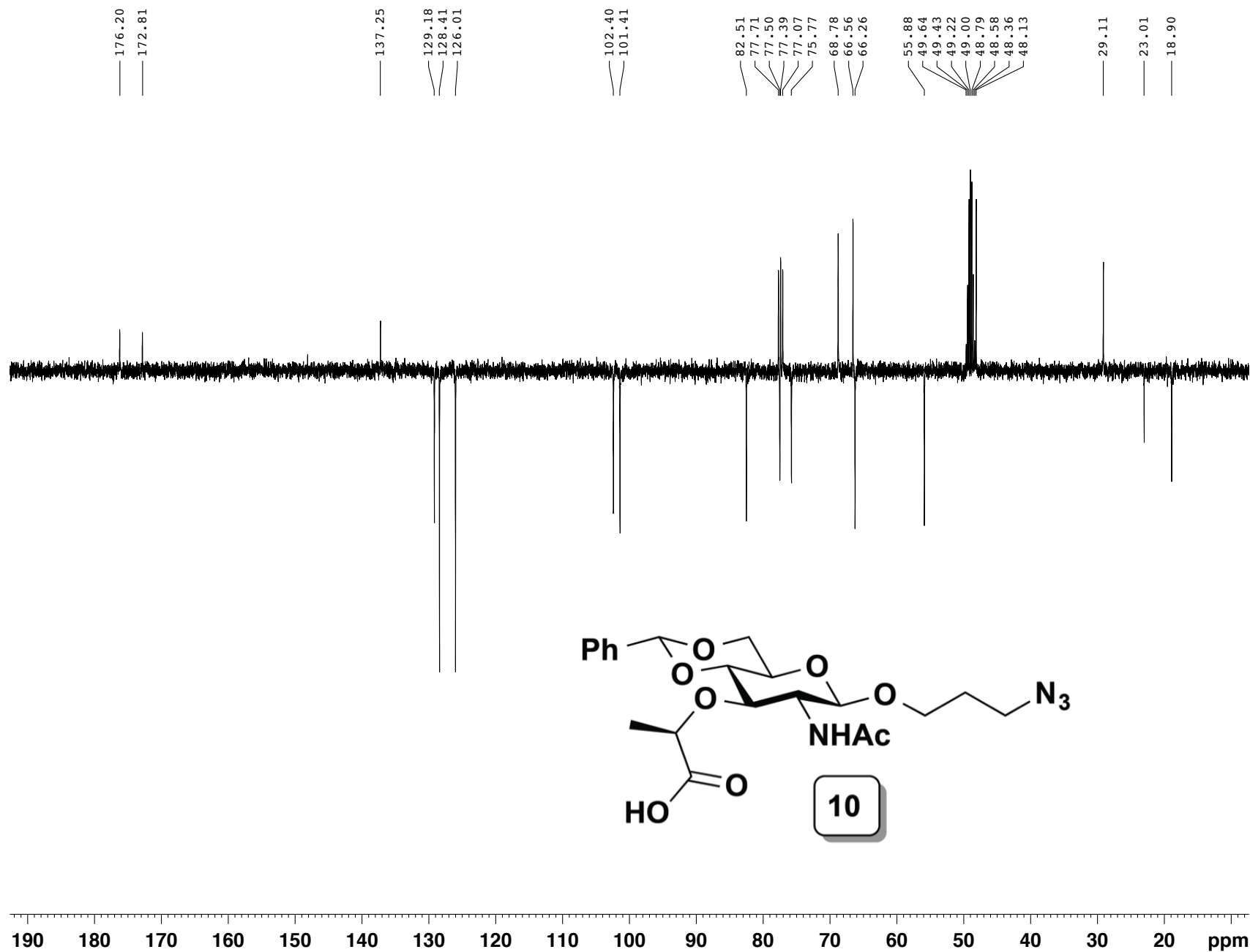
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PROCNO 1
Date_ 20100603
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PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.50 usec
TE 300.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 -3.00 dB
PL1W 16.78977203 W
SFO1 400.2324716 MHz
SI 65536
SF 400.2299939 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S8

BvB 7

biosynAPTfast MeOD /opt/DATA nmrafd 4



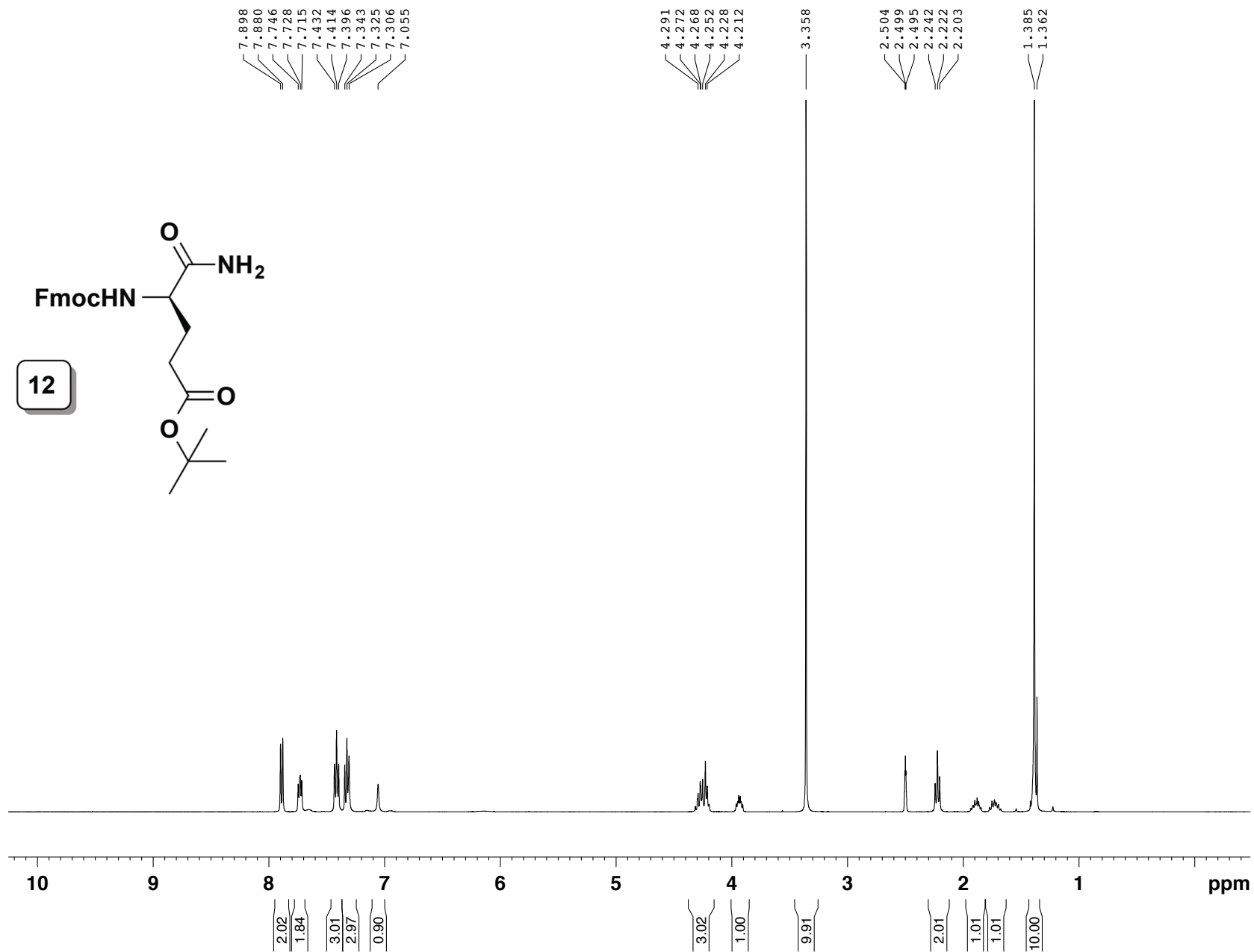
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PULPROG jmod
TD 65536
SOLVENT MeOD
NS 256
DS 1
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 301.2 K
CNST2 155.0000000
CNST11 1.0000000
D1 1.50000000 sec
D20 0.00645161 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.10 usec
P2 18.20 usec
PL1 -1.00 dB
PL1W 44.27188873 W
SFO1 100.6479773 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.89 dB
PL2W 16.78977203 W
PL12W 0.54455876 W
SFO2 400.2316009 MHz
SI 32768
SF 100.6378953 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S9

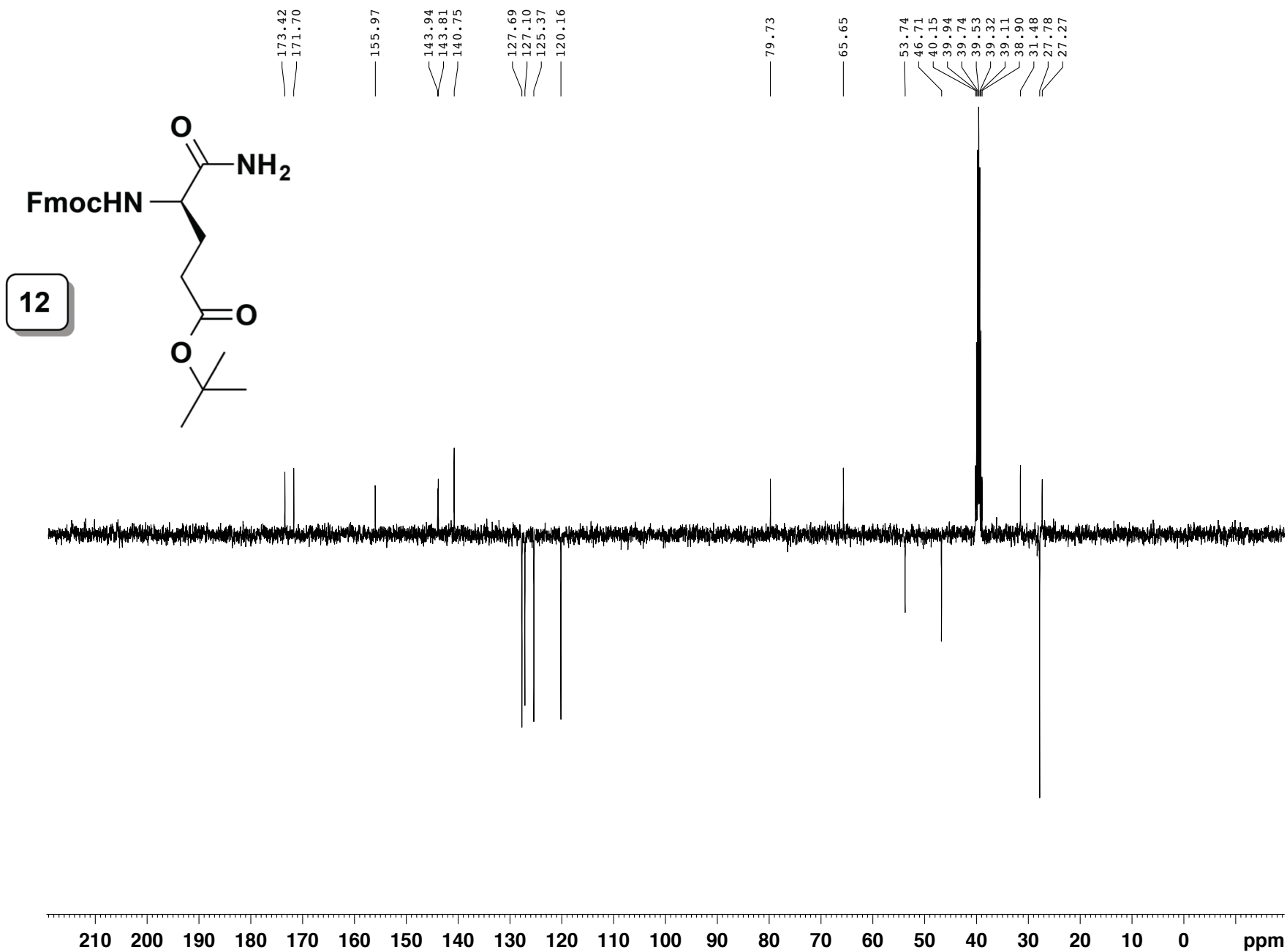
1h NMR av400liq mw308



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EXPNO 6
PROCNO 1
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Time 13.12
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 14
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.40 usec
PL1 0.00 dB
PL1W 8.41481972 W
SFO1 400.2324716 MHz
SI 65536
SF 400.2300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S10

¹³C APT av400liq mw308

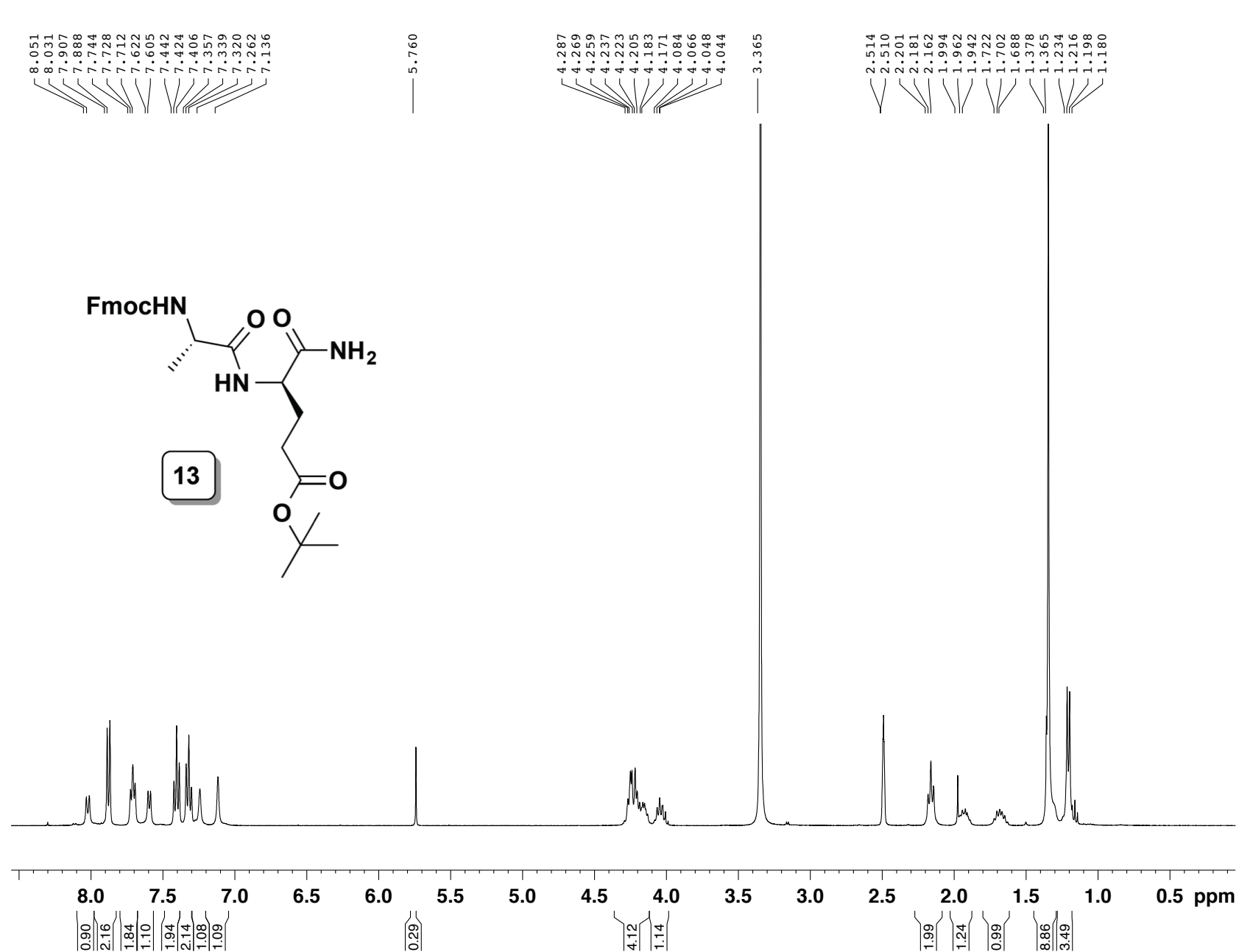
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EXPNO 7
PROCNO 1
Date_ 20100906
Time 13.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT DMSO
NS 114
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 296.5 K
CNST2 155.0000000
CNST11 1.0000000
D1 1.50000000 sec
D20 0.00645161 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.10 usec
P2 18.20 usec
PL1 -1.00 dB
PL1W 44.27188873 W
SFO1 100.6479773 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 14.89 dB
PL2W 8.41481972 W
PL12W 0.27292591 W
SFO2 400.2316009 MHz
SI 32768
SF 100.6379571 MHz
WDW EM
SSB 0
LB 2.50 Hz
GB 0
PC 1.40

S11

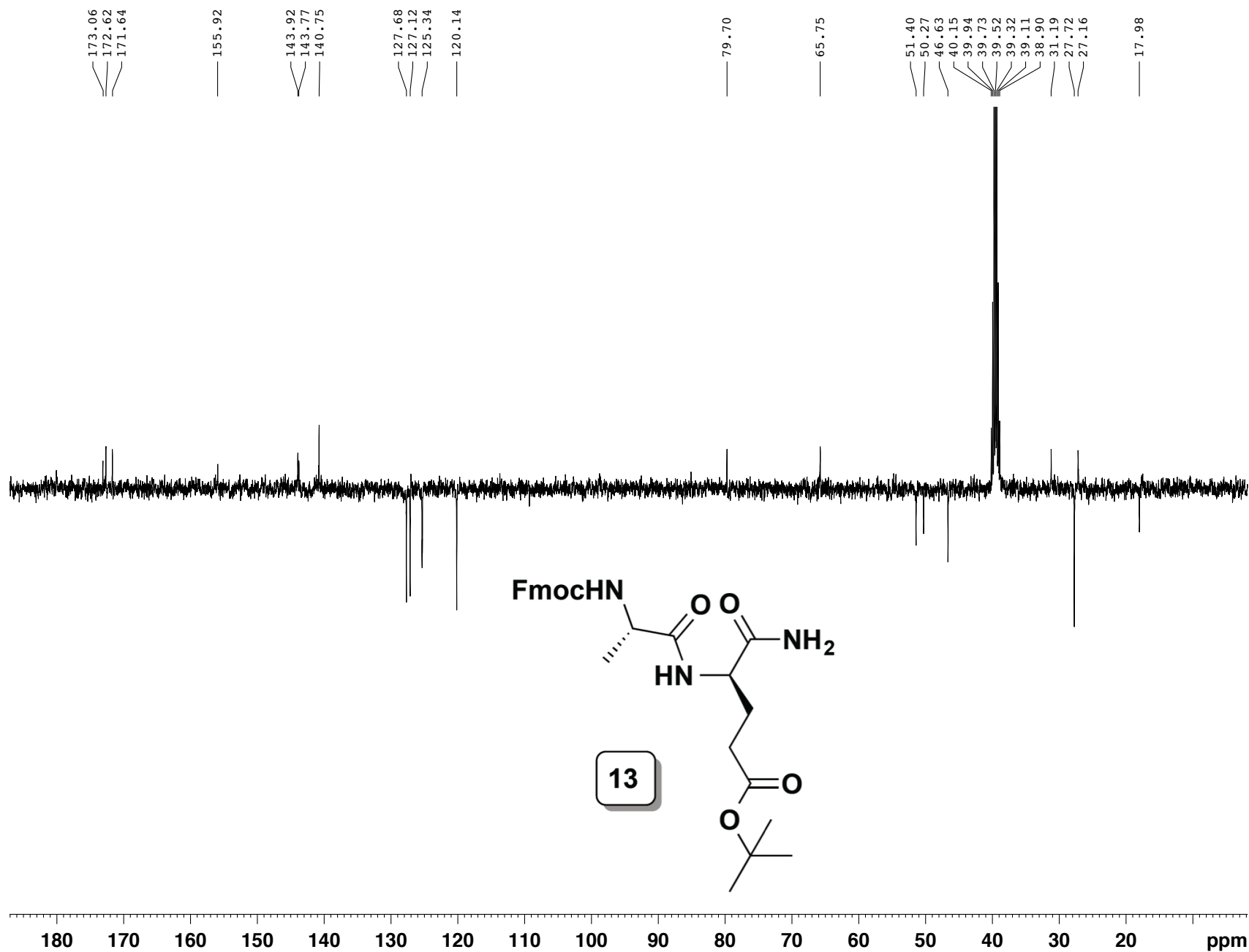
1h NMR av400liq mw313



NAME 1009Marian
EXPNO 27
PROCNO 1
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Time 13.26
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.40 usec
PL1 0.00 dB
PL1W 8.41481972 W
SFO1 400.2324716 MHz
SI 65536
SF 400.2300086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S12

¹³C APT av400liq mw313

NAME 1009Marian
EXPNO 28
PROCNO 1
Date_ 20100913
Time 13.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT DMSO
NS 81
DS 0
SWH 24038.461 H
FIDRES 0.366798 H
AQ 1.3631988 s
RG 2050
DW 20.800 us
DE 6.00 us
TE 297.9 K
CNST2 155.0000000
CNST11 1.0000000
D1 1.50000000 s
D20 0.00645161 s
TD0 1

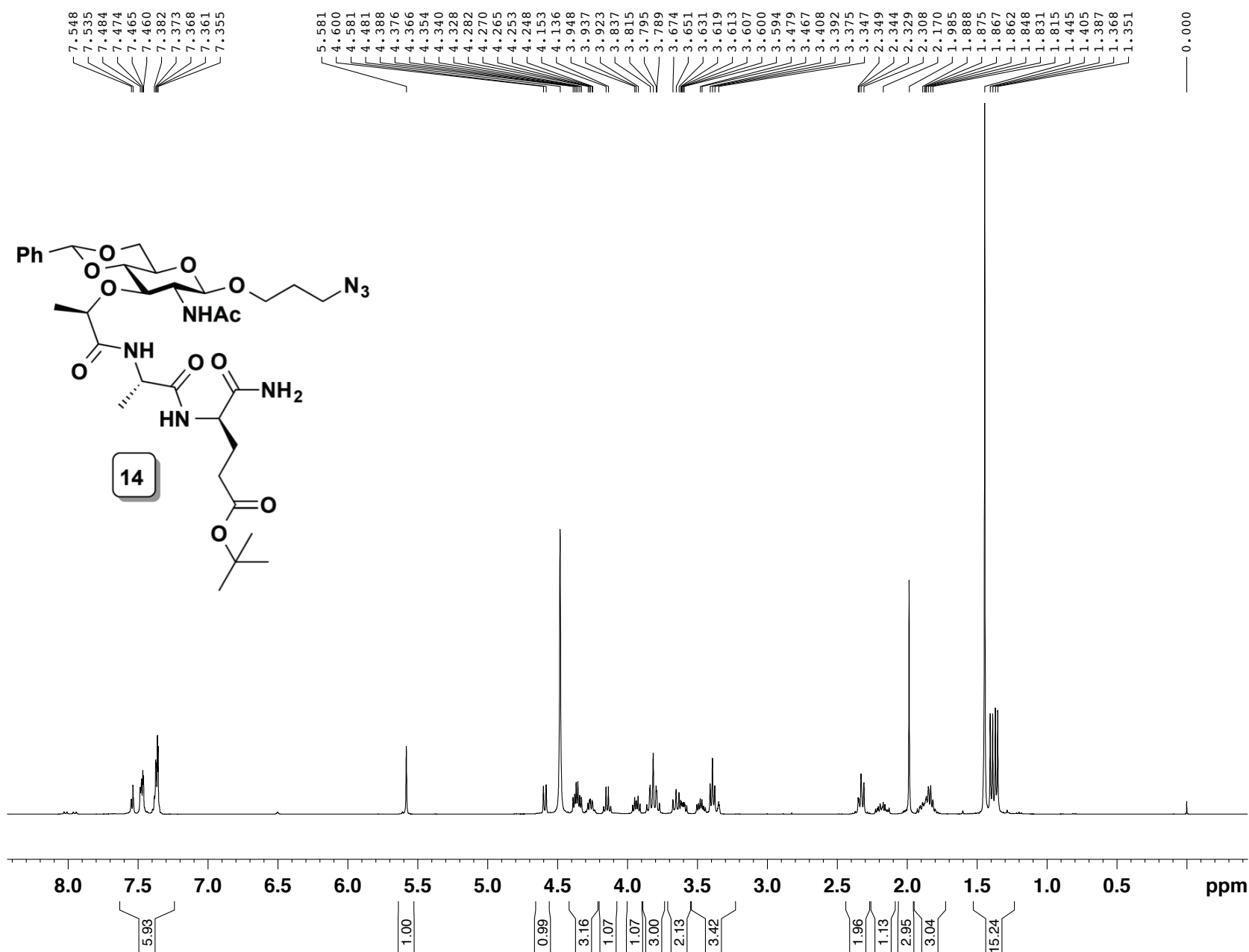
===== CHANNEL f1 =====
NUC1 13C
P1 9.10 us
P2 18.20 us
PL1 -1.00 dB
PL1W 44.27188873 W
SFO1 100.6479773 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 us
PL2 0.00 dB
PL12 14.89 dB
PL2W 8.41481972 W
PL12W 0.27292591 W
SFO2 400.2316009 MHz
SI 32768
SF 100.6379578 MHz
WDW EM
SSB 0
LB 2.50 Hz
GB 0
PC 1.40

S13

mw295

biosyn1Hfast MeOD /opt/DATA nmrafd 1



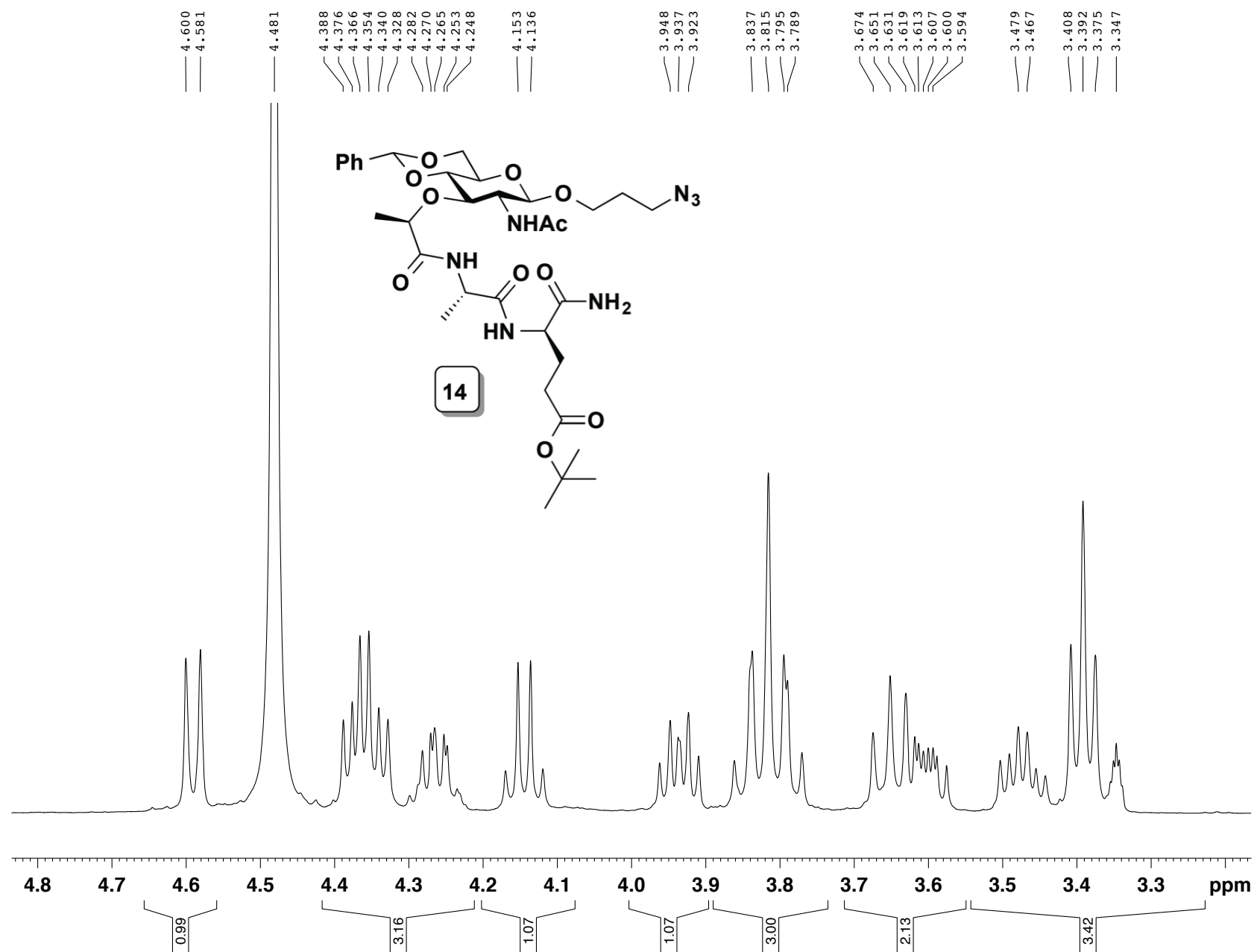
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PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 1
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 80.6
DW 60.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.10 usec
PL1 0.00 dB
PL1W 8.41481972 W
SFO1 400.2324716 MHz
SI 65536
SF 400.2299953 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S14

mw295

biosyn1Hfast MeOD /opt/DATA nmrafd 1



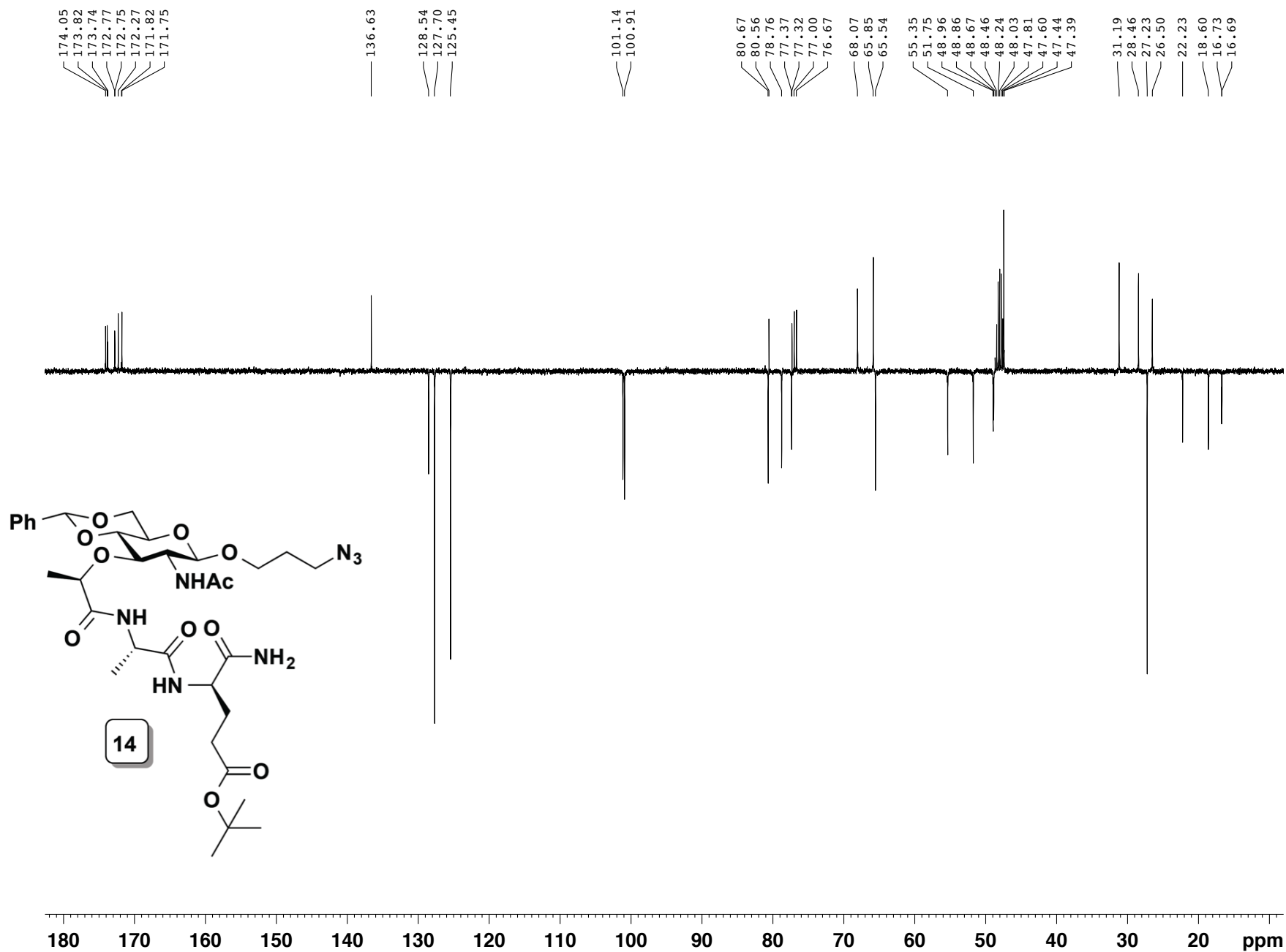
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PROCNO 1
Date_ 20100825
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PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 1
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 80.6
DW 60.800 use
DE 6.50 use
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.10 use
PL1 0.00 dB
PL1W 8.41481972 W
SFO1 400.2324716 MHz
SI 65536
SF 400.2299953 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S15

mw295

biosynAPTfast MeOD /opt/DATA nmrafd 1



NAME 1008Marian
EXPNO 85
PROCNO 1
Date_ 20100825
Time 17.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT MeOD
NS 512
DS 1
SWH 24038.461 H
FIDRES 0.366798 H
AQ 1.3631988 s
RG 2050
DW 20.800 us
DE 6.00 us
TE 300.2 K
CNST2 155.0000000
CNST11 1.0000000
D1 1.50000000 s
D20 0.00645161 s
TD0 1

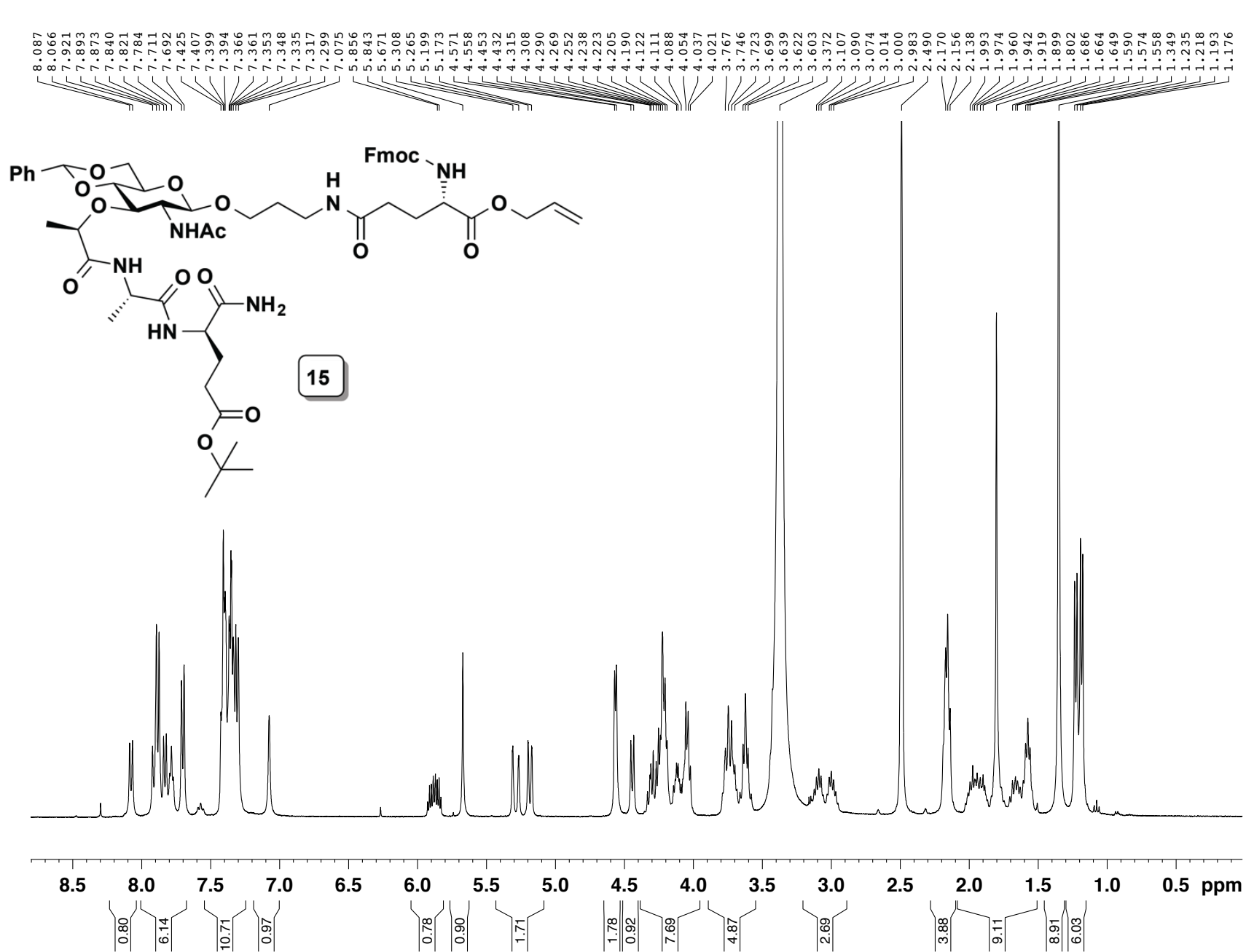
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NUC1 13C
P1 9.10 us
P2 18.20 us
PL1 -1.00 dB
PL1W 44.27188873 W
SFO1 100.6479773 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 us
PL2 0.00 dB
PL12 15.00 dB
PL2W 8.41481972 W
PL12W 0.26609996 W
SFO2 400.2316009 MHz
SI 32768
SF 100.6379580 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S16

mw396

biosyn1Hfast DMSO /opt/DATA nmrafd 8



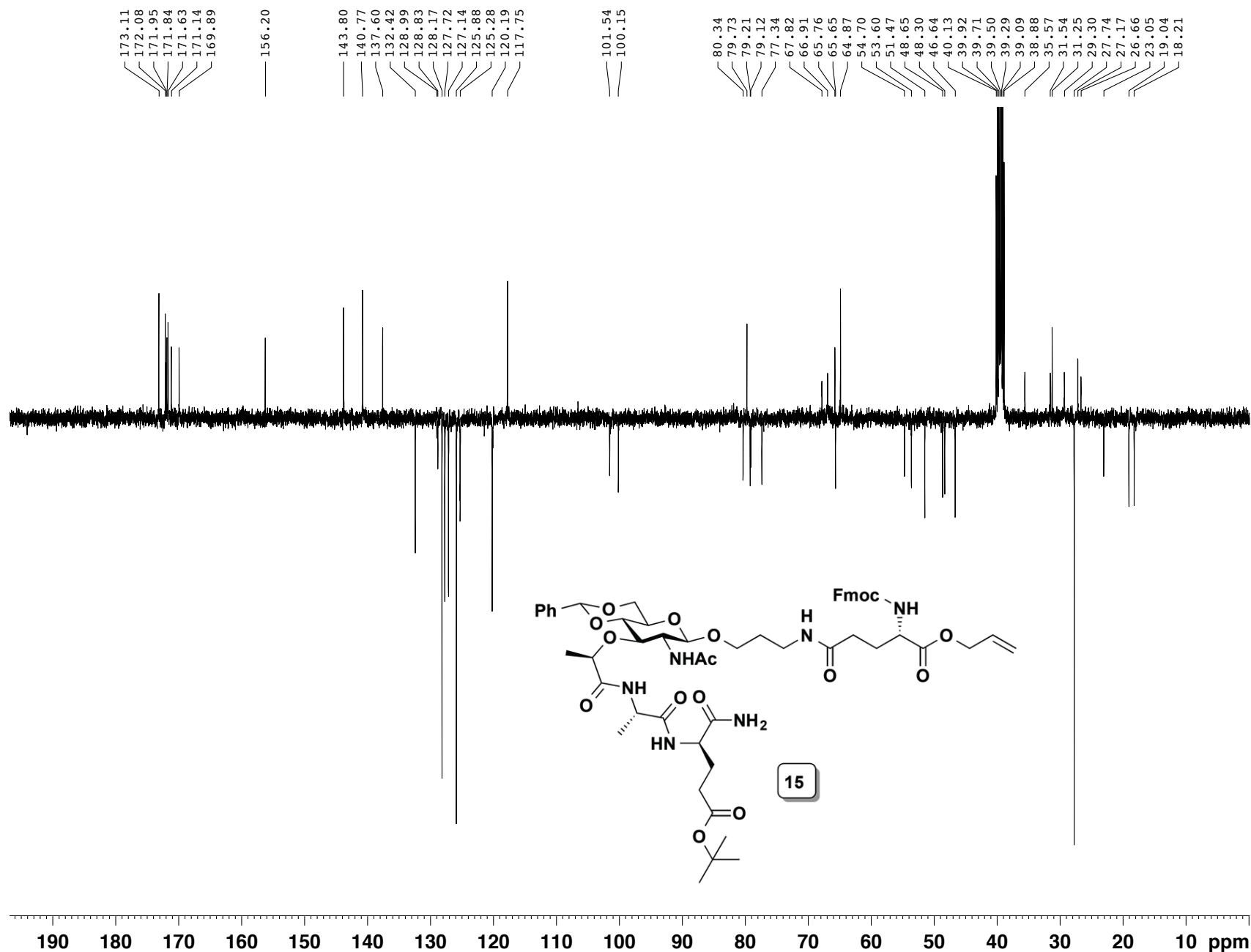
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EXPNO 69
PROCNO 1
Date_ 20110331
Time 2.16
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 1
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.40 usec
PL1 0.00 dB
PL1W 8.41481972 W
SFO1 400.2324716 MHz
SI 65536
SF 400.2300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S17

mw342

biosynAPTfast DMSO /opt/DATA nmrafd 8



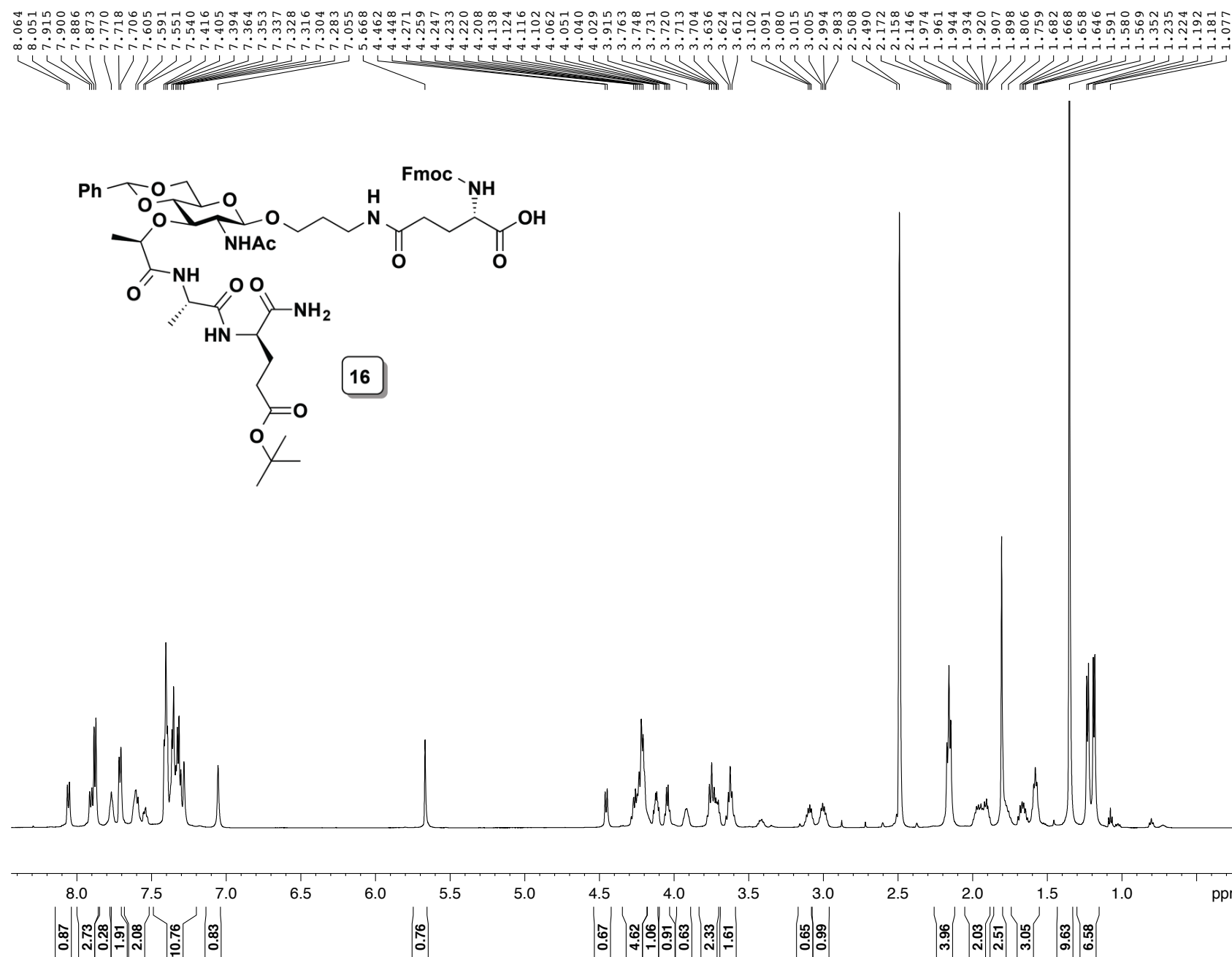
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EXPNO 33
PROCNO 1
Date_ 20101117
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PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT DMSO
NS 3072
DS 1
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 295.0 K
CNST2 155.0000000
CNST11 1.0000000
D1 1.50000000 sec
D20 0.00645161 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.10 usec
P2 18.20 usec
PL1 -1.00 dB
PL1W 44.27188873 W
SFO1 100.6479773 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL2W 8.41481972 W
PL12W 0.26609996 W
SFO2 400.2316009 MHz
SI 32768
SF 100.6379561 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S18

presat GP dmx600 MW-401 in dms0(d6) 300K



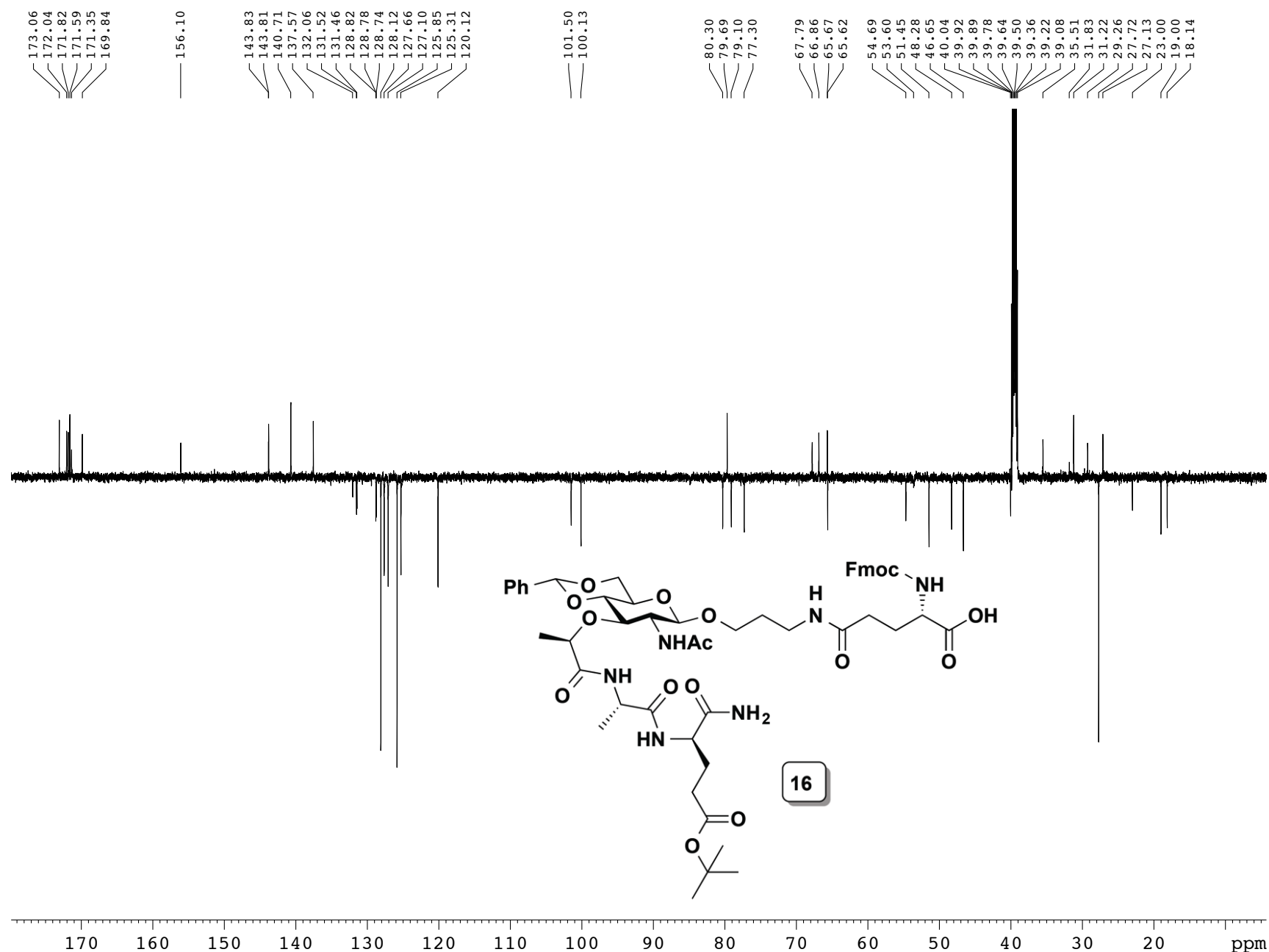
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EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
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PROBHD 5 mm CPTCI 1H-
PULPROG noesygpgpr1d
TD 65536
SOLVENT DMSO
NS 16
DS 4
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 32
DW 41.600 use
DE 10.00 use
TE 305.5 K
D1 4.00000000 sec
D8 0.01000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1 1H
P0 8.76 use
P1 8.76 use
PLW1 5.00029993 W
PLW9 0.00000316 W
SFO1 600.1320258 MHz

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 50.00 %
GPZ2 -10.00 %
P16 1000.00 use

F2 - Processing parameters
SI 65536
SF 600.1300144 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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Current Data Parameters
NAME      biosyn042011Maria
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20110411
Time      9.08
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PROBHD    5 mm CPTCI 1H-
PULPROG   jmod
TD         131072
SOLVENT   DMSO
NS         777
DS         0
SWH        34722.223 Hz
FIDRES     0.264910 Hz
AQ         1.8874367 sec
RG         2050
DW         14.400000 usec
DE         7.400000 usec
TE         305.5 K
CNST2     155.0000000 W
CNST11    1.0000000 W
D1         1.50000000 sec
D20        0.00645161 sec

===== CHANNEL f1 =====
NUC1       13C
P1         12.500000 usec
P2         25.000000 usec
PLW1       105.8000003 W
SF01       150.9185940 MHz

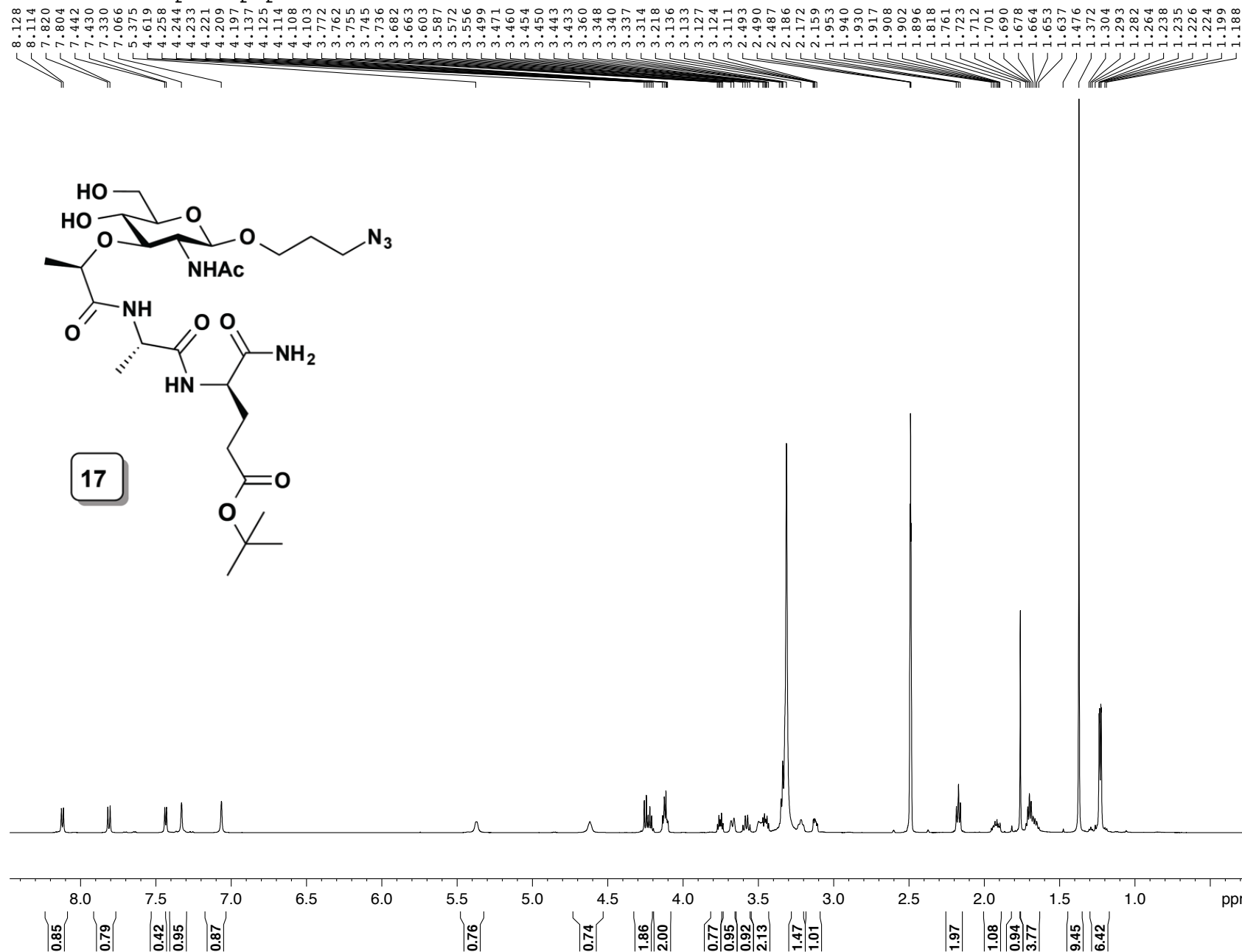
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     70.000000 usec
PLW2      5.00000000 W
PLW12     0.06530600 W
SF02      600.1324000 MHz

F2 - Processing parameters
SI         131072
SF         150.9028792 MHz
WDW        EM
SSB        0
LB         0
GB         0
PC         1.40

```

S20

mw197 in dms0(d6)
PROTON DMSO /opt/topspin nmrafd 3



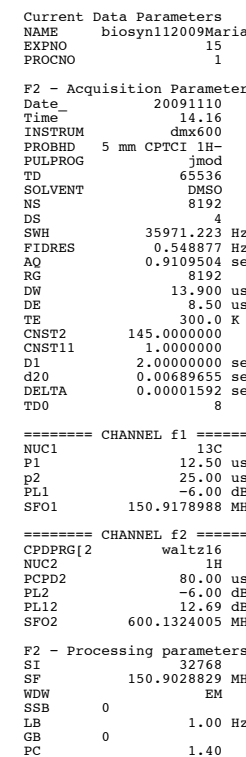
Current Data Parameters
NAME biosyn112009Maria
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091110
Time 9.39
INSTRUM dm600
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 12376.237 Hz
FIDRES 0.188846 Hz
AQ 2.6476543 sec
RG 128
DW 40.400 usec
DE 8.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.30 usec
PL1 -6.00 dB
SFO1 600.1337060 MHz

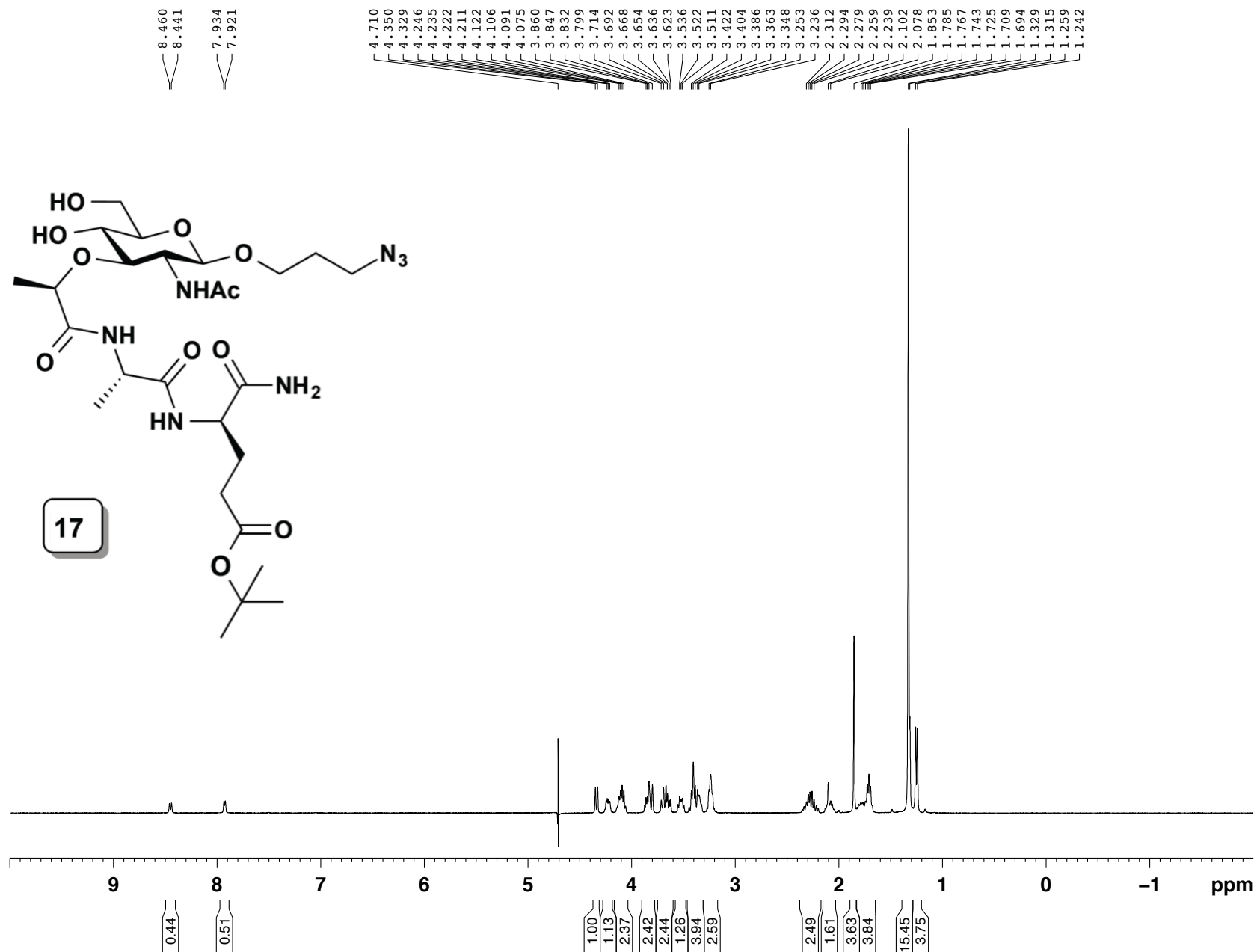
F2 - Processing parameters
SI 32768
SF 600.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```
mw197 in dms0(d6)
C13APT DMSO /opt/topspin nmrafd 3
```



S22

noesypr1d mw83 MDP-tBu



```

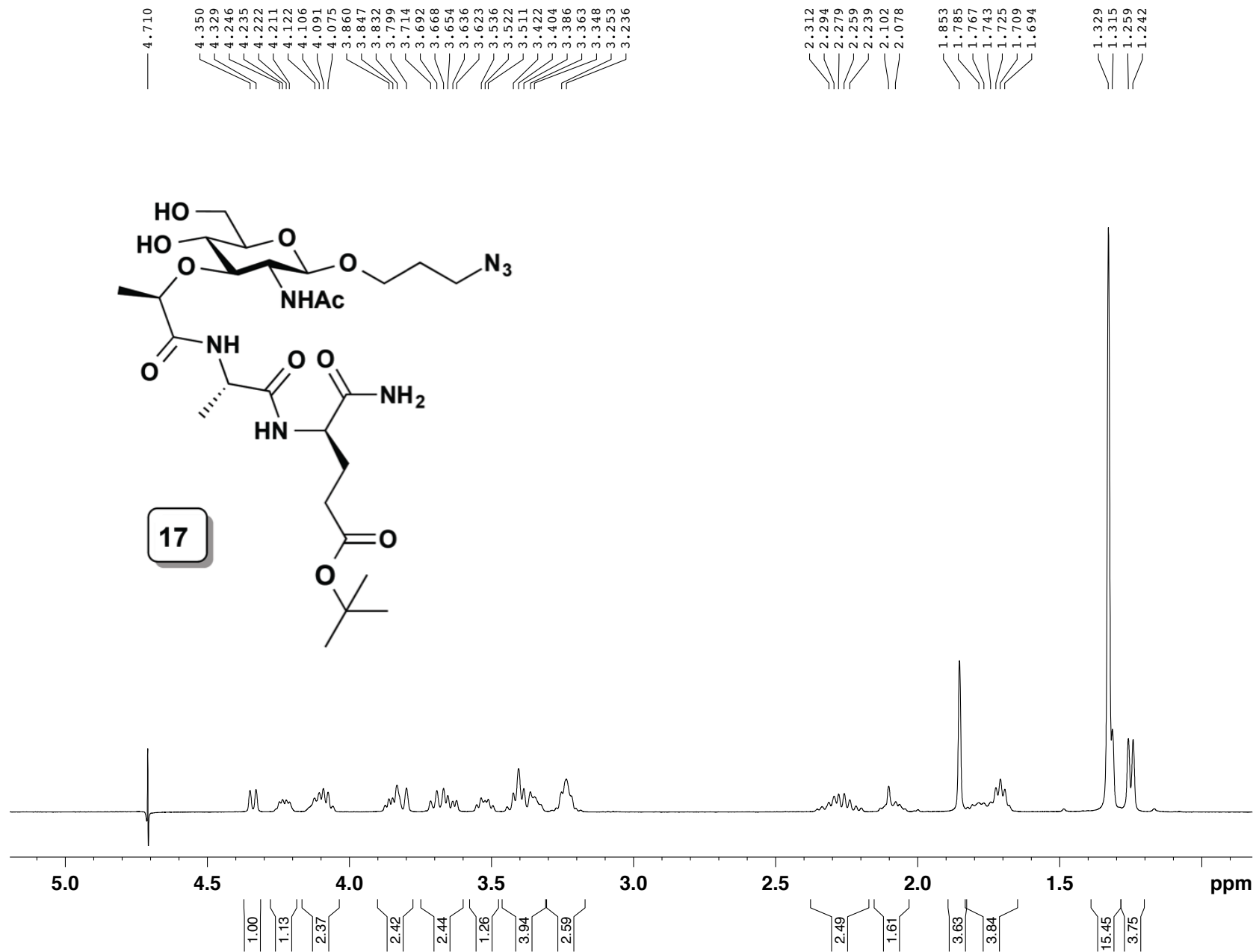
NAME      0810Marian
EXPNO     23
PROCNO    1
Date_     20081028
Time      10.03
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   noesypr1d
TD         32768
SOLVENT   D2O
NS         55
DS         4
SWH        6410.256 Hz
FIDRES     0.195625 Hz
AQ         2.5559540 sec
RG         812
DW         78.000 usec
DE         6.00 usec
TE         293.1 K
D1         1.00000000 sec
D8         0.05000000 sec
D11        0.03000000 sec
D12        0.00002000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.10 usec
PL1        0.00 dB
PL9        51.00 dB
PL1W       8.41481972 W
PL9W       0.00006684 W
SFO1       400.2318811 MHz
SI         65536
SF         400.2299980 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```

S23

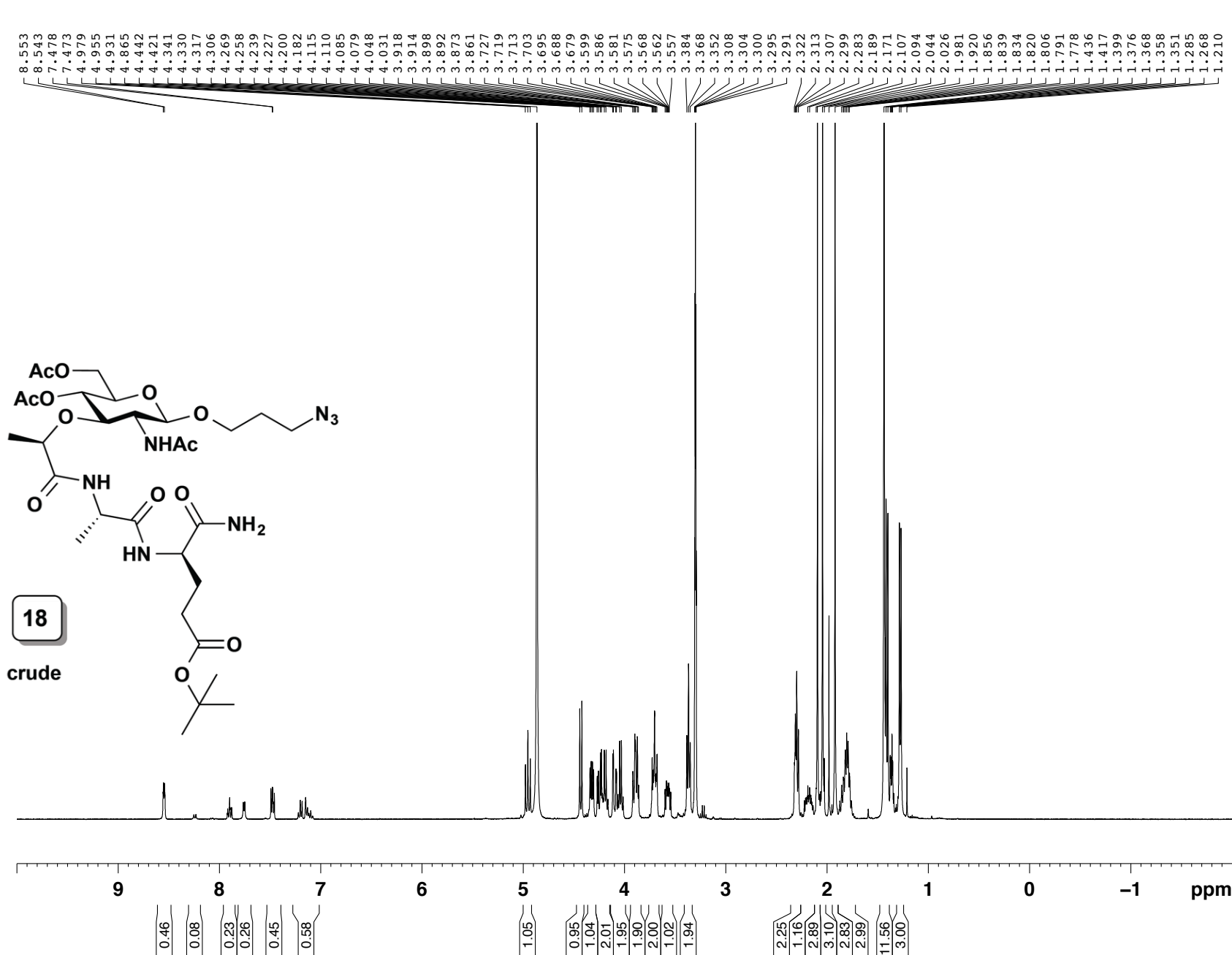
noesypr1d mw83 MDP-tBu



NAME 0810Marian
EXPNO 23
PROCNO 1
Date_ 20081028
Time_ 10.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG noesypr1d
TD 32768
SOLVENT D2O
NS 55
DS 4
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 812
DW 78.000 use
DE 6.00 use
TE 293.1 K
D1 1.00000000 sec
D8 0.05000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.10 use
PL1 0.00 dB
PL9 51.00 dB
PL1W 8.41481972 W
PL9W 0.00006684 W
SFO1 400.2318811 MHz
SI 65536
SF 400.2299980 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```
mw465
biosyn1Hfast MeOD /opt/DATA nmrafd 2
```



```

NAME                1108Marian
EXPNO                121
PROCNO              1
Date_               20110829
Time                18.55
INSTRUM             spect
PROBHD              5 mm PABBO BB-
PULPROG             zg30
TD                  65536
SOLVENT             MeOD
NS                   16
DS                   1
SWH                  8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9846387 sec
RG                   203
DW                   60.800 usec
DE                   6.50 usec
TE                   296.0 K
D1                  1.00000000 sec
TD0                  1

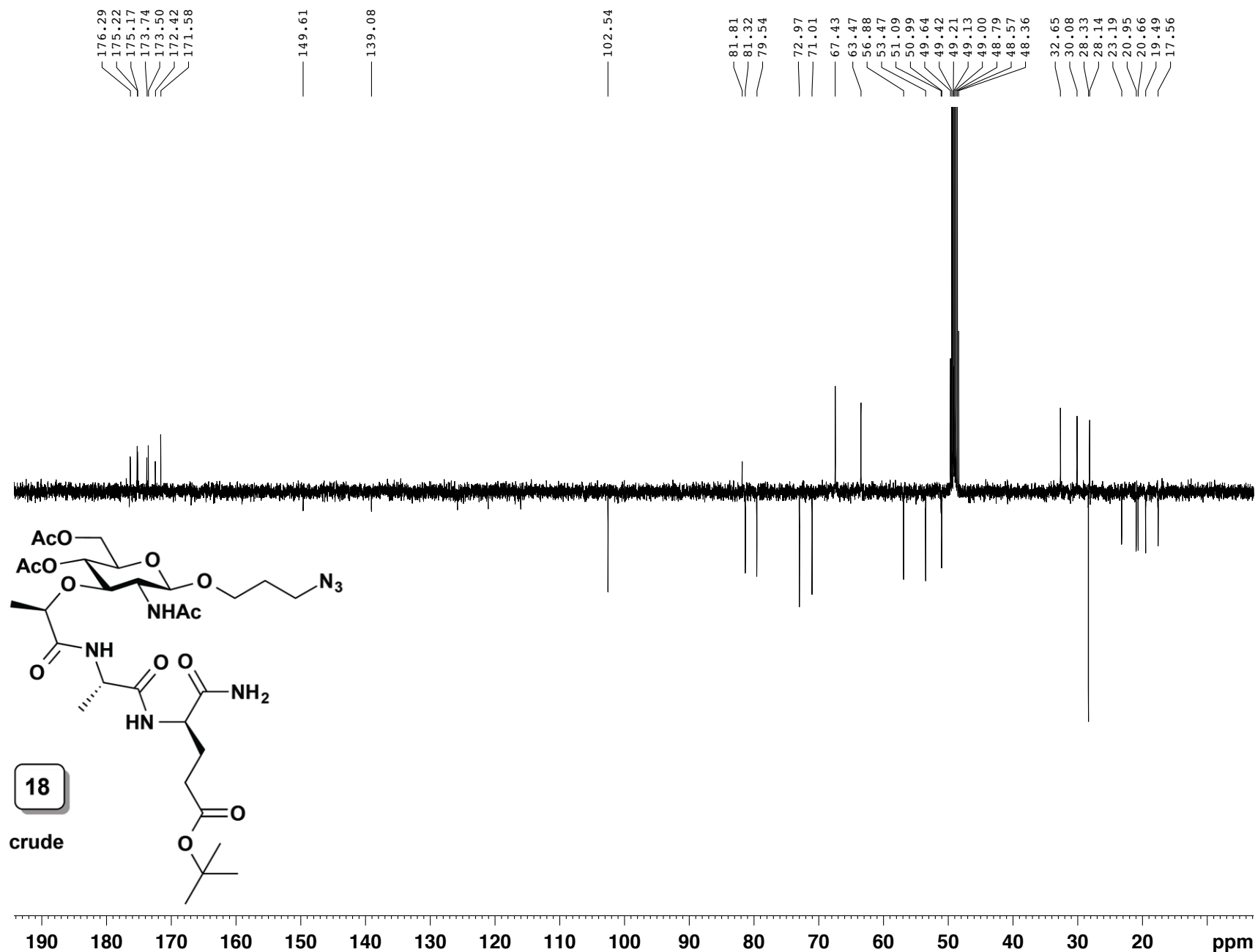
===== CHANNEL f1 =====
NUC1                  1H
P1                    14.40 usec
PL1                   0.00 dB
PL1W                  8.41481972 W
SF01                  400.2324716 MHz
SI                    65536
SF                    400.2300142 MHz
WDW                   EM
SSB                   0
LB                    0.30 Hz
GB                   0
PC                    1.00

```


S25

mw465

biosynAPTfast MeOD /opt/DATA nmrafd 2



```
NAME 1108Marian
EXPNO 122
PROCNO 1
Date_ 20110829
Time 19.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT MeOD
NS 512
DS 1
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 296.8 K
CNST2 155.0000000
CNST11 1.0000000
D1 1.50000000 sec
D20 0.00645161 sec
TD0 1
```

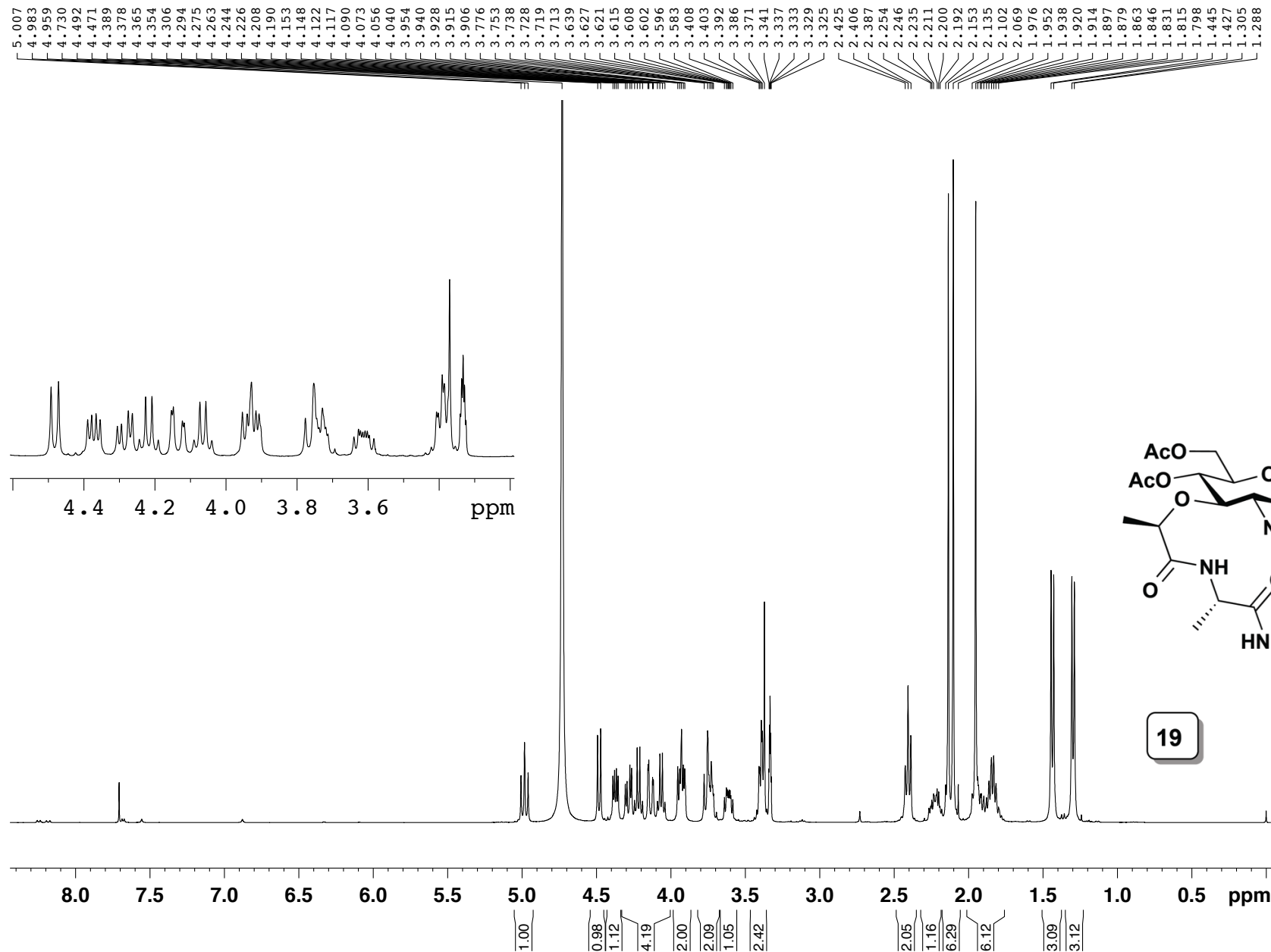
```
===== CHANNEL f1 =====
NUC1 13C
P1 9.10 usec
P2 18.20 usec
PL1 -1.00 dB
PL1W 44.27188873 W
SFO1 100.6479773 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 14.89 dB
PL2W 8.41481972 W
PL12W 0.27292591 W
SFO2 400.2316009 MHz
SI 32768
SF 100.6377734 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

S26

mw332

biosyn1Hfast MeOD /opt/DATA nmrafd 1



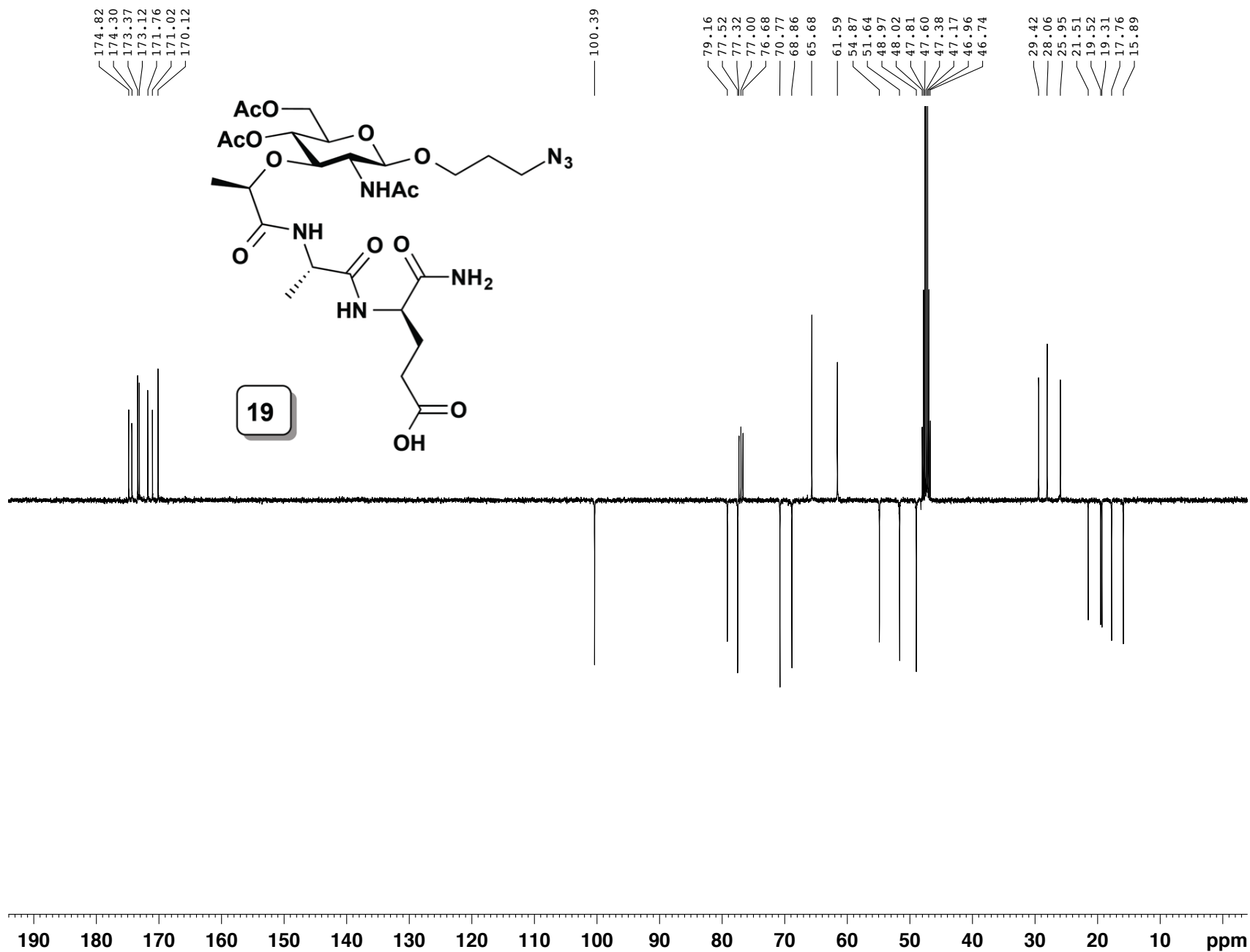
```
NAME      1010Marian
EXPNO     23
PROCNO    1
Date_     20101015
Time_     17.22
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zg30
TD         65536
SOLVENT    MeOD
NS         64
DS         1
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         101
DW         60.800 usec
DE         6.50 usec
TE         295.4 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.10 usec
PL1        0.00 dB
PL1W       8.41481972 W
SFO1       400.2324716 MHz
SI         65536
SF         400.2300008 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

S27

mw332

biosynAPTfast MeOD /opt/DATA nmrafd 1



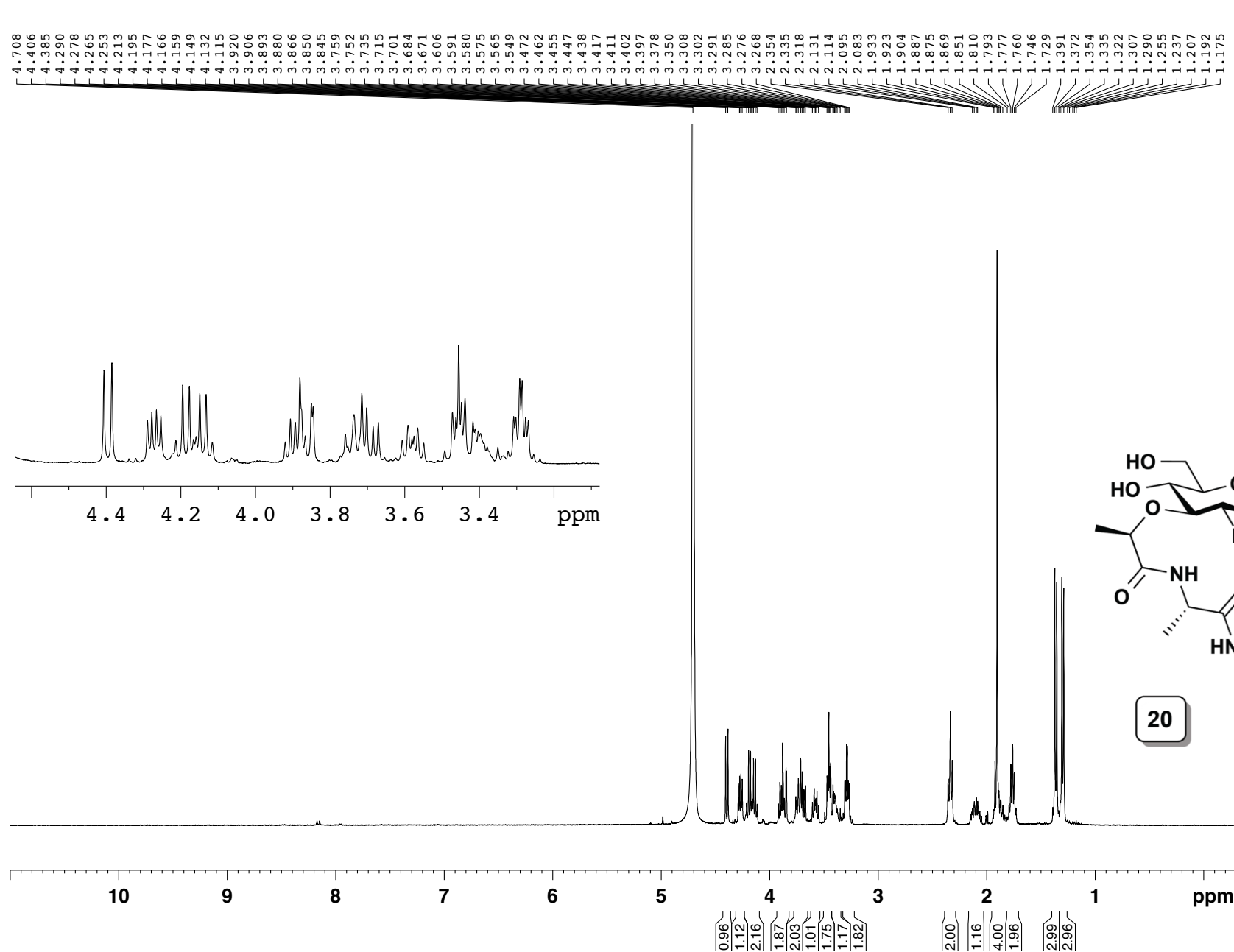
NAME 1010Marian
EXPNO 24
PROCNO 1
Date_ 20101015
Time 19.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT MeOD
NS 3072
DS 1
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 296.7 K
CNST2 155.0000000
CNST11 1.0000000
D1 1.50000000 sec
D20 0.00645161 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.10 usec
P2 18.20 usec
PL1 -1.00 dB
PL1W 44.27188873 W
SFO1 100.6479773 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL2W 8.41481972 W
PL12W 0.26609996 W
SFO2 400.2316009 MHz
SI 32768
SF 100.6379823 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

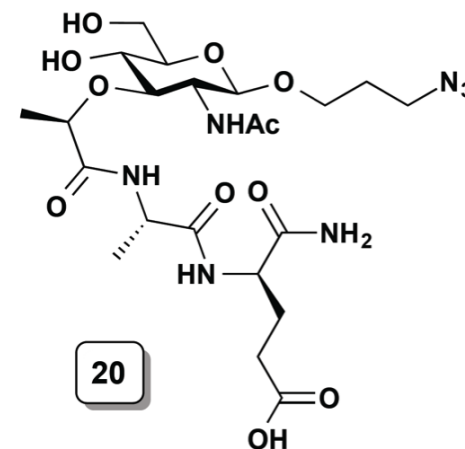
S28

1h NMR av400liq mw278 gezuiverd HB40



NAME 1006Marian
EXPNO 73
PROCNO 1
Date_ 20100622
Time 16.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT D2O
NS 152
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 256
DW 60.800 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1

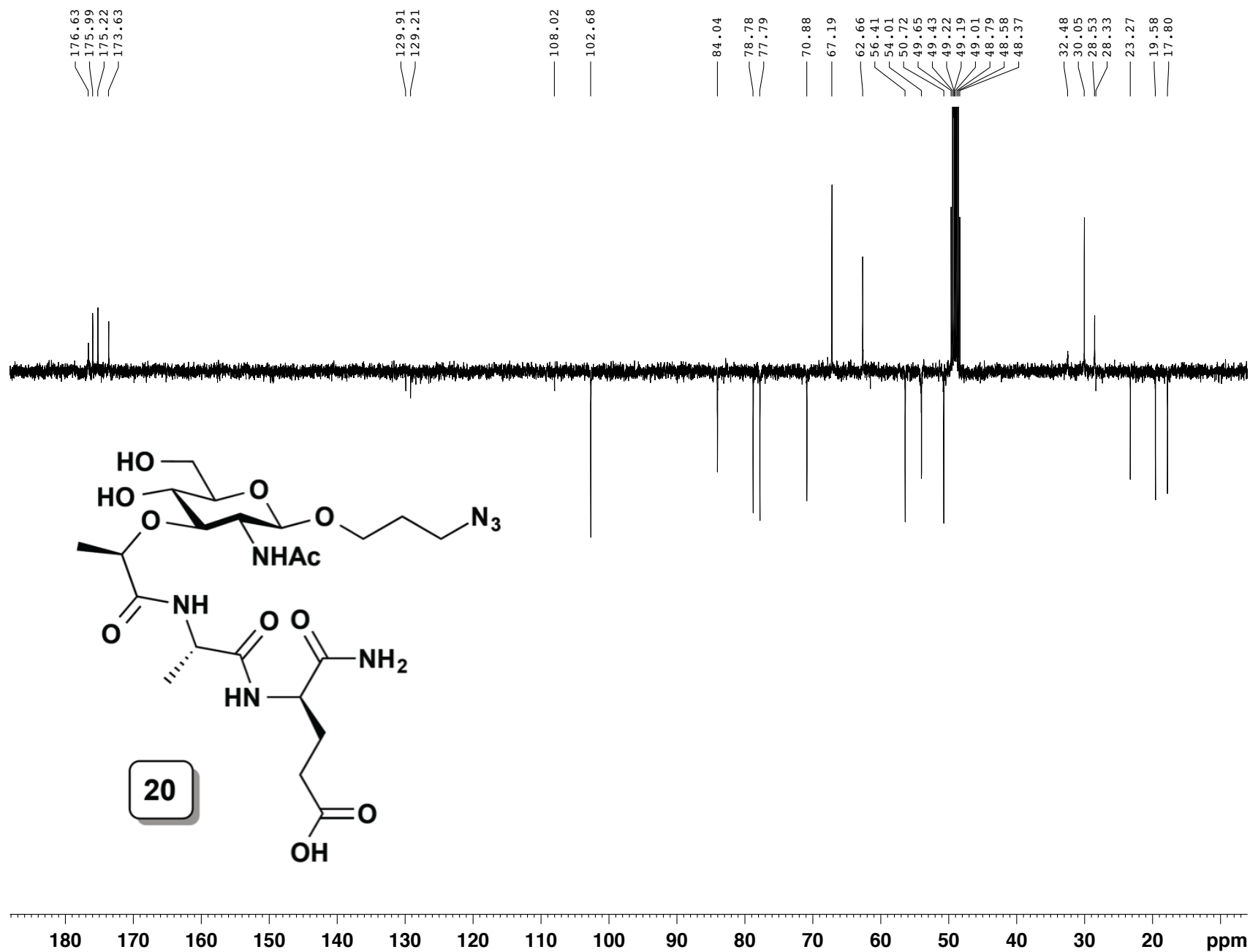
===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 -3.00 dB
PL1W 16.78977203 W
SFO1 400.2324716 MHz
SI 65536
SF 400.2300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S29

mw289

biosynAPTfast MeOD /opt/DATA nmrafd 5



NAME 1008Marian
EXPNO 17
PROCNO 1
Date_ 20100806
Time 23.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT MeOD
NS 512
DS 1
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 297.8 K
CNST2 155.0000000
CNST11 1.0000000
D1 1.50000000 sec
D20 0.00645161 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.10 usec
P2 18.20 usec
PL1 -1.00 dB
PL1W 44.2718873 W
SFO1 100.6479773 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL2W 8.41481972 W
PL12W 0.26609996 W
SFO2 400.2316009 MHz
SI 32768
SF 100.6377751 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40