

Supporting Information File 2

for

A macrolactonization approach to the total synthesis of the antimicrobial cyclic depsipeptide LI-F04a and diastereoisomeric analogues

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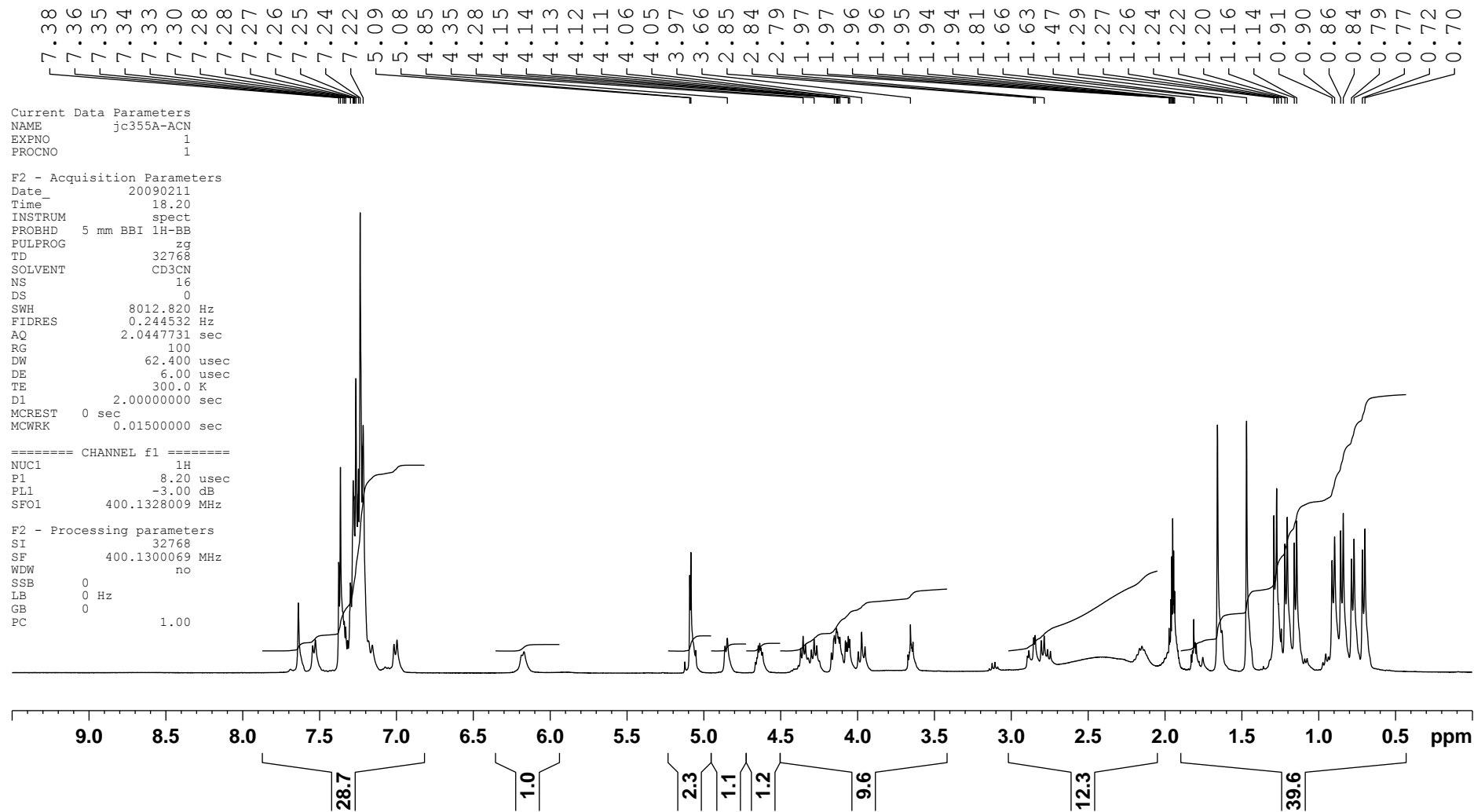
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^1H , ^{13}C and 2D NMR data for all new compounds

Cbz-L-Thr-D-Val-L-Val-D-*allo*-Thr(Ψ Pro)-D-Asn(Trt)-D-Ala-OH (6)



Cbz-L-Thr-D-Val-L-Val-D-*allo*-Thr(Ψ Pro)-D-Asn(Trt)-D-Ala-OH (6) COSY

Current Data Parameters
NAME jc355A-ACN
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090212
Time 3.34
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG cosygmfph
TD 4000
SOLVENT MeOH
NS 4
DS 16
SWH 3591.954 Hz
FIDRES 0.897988 Hz
AQ 0.5568500 sec
RG 1024
DW 139.200 usec
DE 6.00 usec
TE 300.0 K
d0 0.00012840 sec
d1 2.5000000 sec
d13 0.00000400 sec
d16 0.00015000 sec
d20 0.00165400 sec
INO 0.00027769 sec
MCREST 0 sec
MCRWK 1.25000000 sec
ST1CNT 0

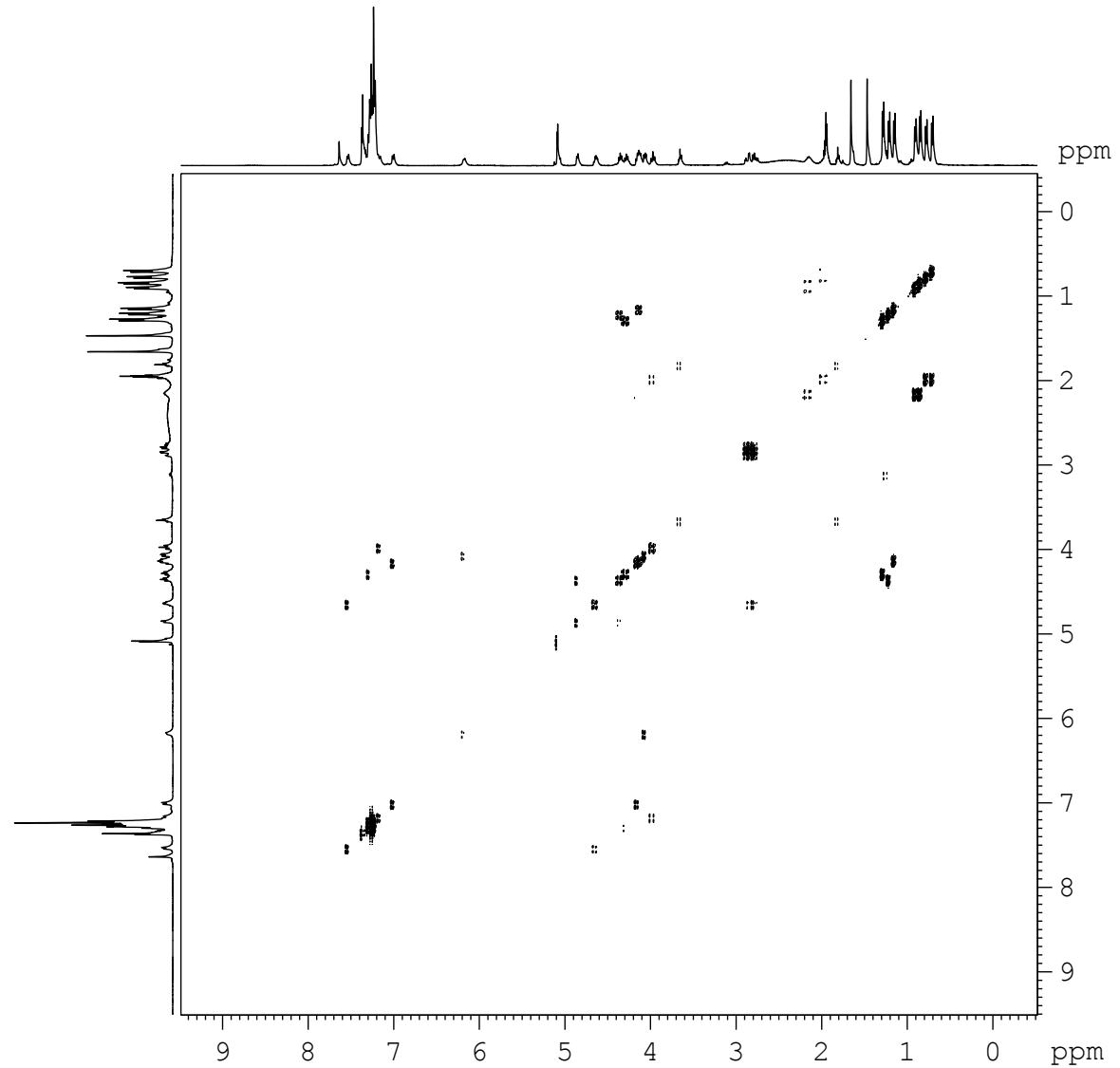
==== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
p2 16.40 usec
PL1 -3.00 dB
SFO1 400.1318006 MHz

==== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPX1 0 %
GPX2 0 %
GPY1 0 %
GPY2 0 %
GPZ1 10.00 %
GPZ2 20.00 %
P16 1500.00 usec

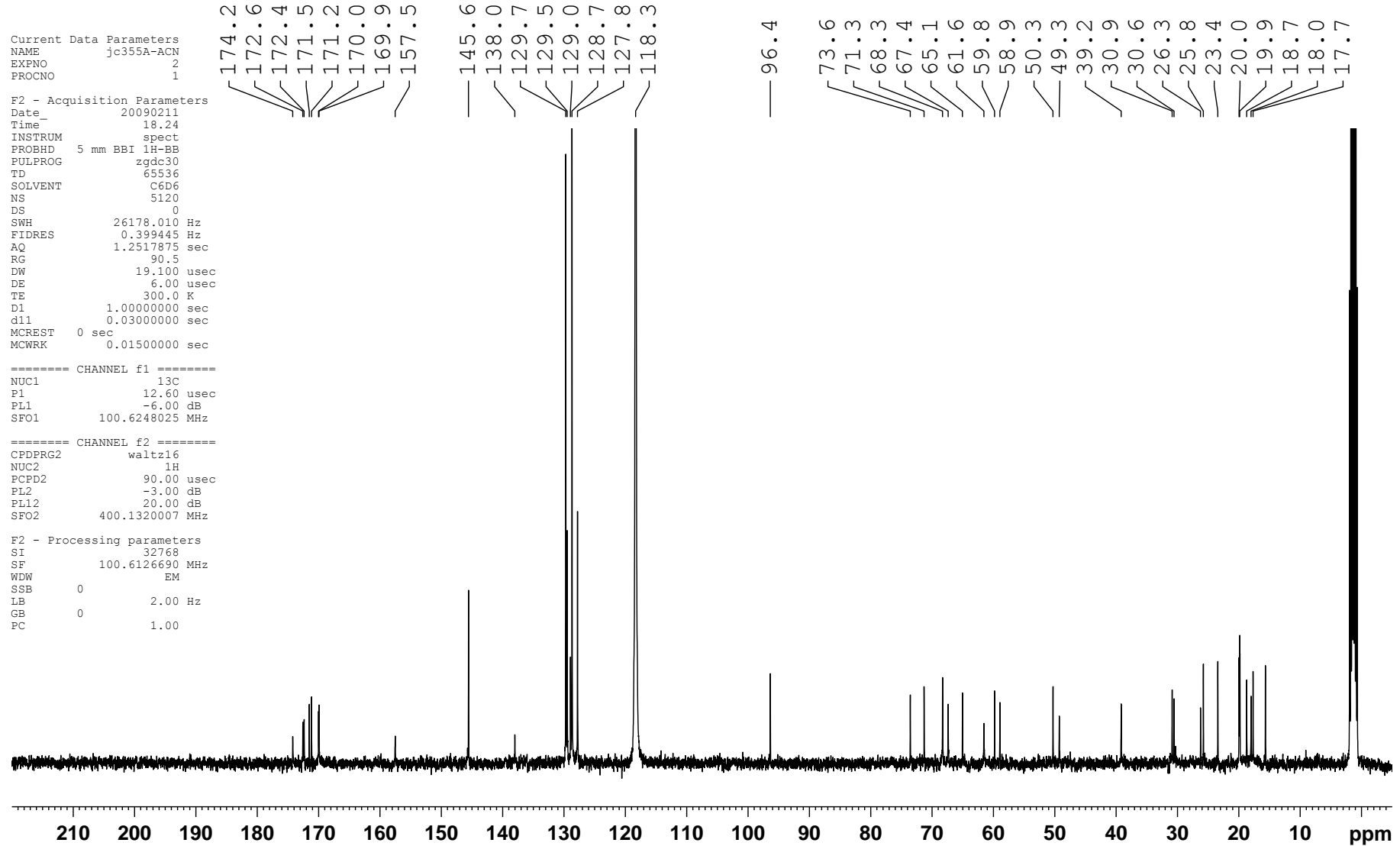
F1 - Acquisition parameters
TD 256
SFO1 400.1318 MHz
FIDRES 14.067072 Hz
SW 9.000 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 2048
SF 400.1300000 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 States-TPPI
SF 400.1300000 MHz
WDW
SSB 2
LB 0 Hz
GB 0



Cbz-L-Thr-D-Val-L-Val-D-*allo*-Thr(Ψ Pro)-D-Asn(Trt)-D-Ala-OH (6)



Cbz-L-Thr-D-Val-L-Val-D-*allo*-Thr(Ψ Pro)-D-Asn(Trt)-D-Ala-OH (6) HSQC

Current Data Parameters
 NAME jc355A-ACN
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090211
 Time_ 21.39
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG invletgpsi
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.876942 Hz
 AQ 0.5702132 sec
 RG 1024
 DW 139.200 usec
 DE 6.00 usec
 TE 300.0 K
 CNST2 140.0000000
 d0 0.00000300 sec
 D1 2.00000000 sec
 d4 0.00178571 sec
 d11 0.03000000 sec
 d13 0.00000400 sec
 D16 0.00015000 sec
 D24 0.00178500 sec
 DELTA 0.00172240 sec
 DELTA1 0.00165800 sec
 INO 0.00002259 sec
 MCREST 0 sec
 MCWRR 0.33333400 sec
 STICNT 0

==== CHANNEL f1 =====
 NUC1 1H
 P1 8.20 usec
 p2 16.40 usec
 P28 0.50 usec
 PL1 -3.00 dB
 SFO1 400.1318006 MHz

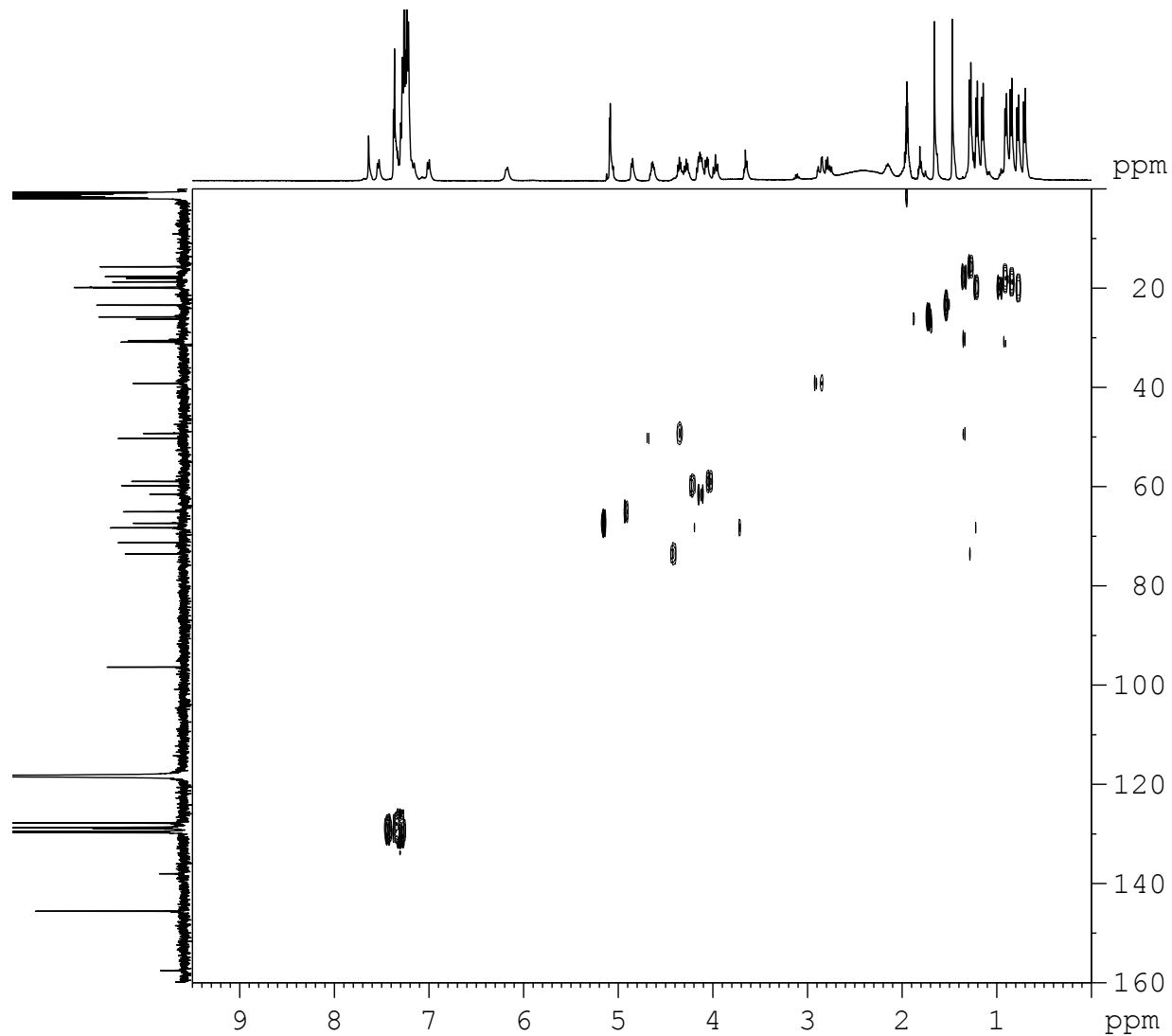
==== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 13C
 P3 12.00 usec
 p4 24.00 usec
 PCPD2 70.00 usec
 PL2 -6.00 dB
 PL12 10.70 dB
 SFO2 100.6227903 MHz

==== GRADIENT CHANNEL =====
 GPNAM1 sine.100
 GPNAM2 sine.100
 GPX1 0 %
 GPX2 0 %
 GPY1 0 %
 GPY2 0 %
 GPZ1 80.00 %
 GPZ2 20.10 %
 F16 1500.00 usec

F1 - Acquisition parameters
 TD 256
 SFO1 100.6228 MHz
 FIDRES 86.469284 Hz
 SW 219.991 ppm
 FhMODE Echo-Antiecho

F2 - Processing parameters
 SI 1024
 SF 400.1299808 MHz
 WDW QSINE
 SSB 0
 LB 0 Hz
 CB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 echo-antiecho
 SF 100.6126591 MHz
 WDW
 SSB 0
 LB 0 Hz
 GB 0



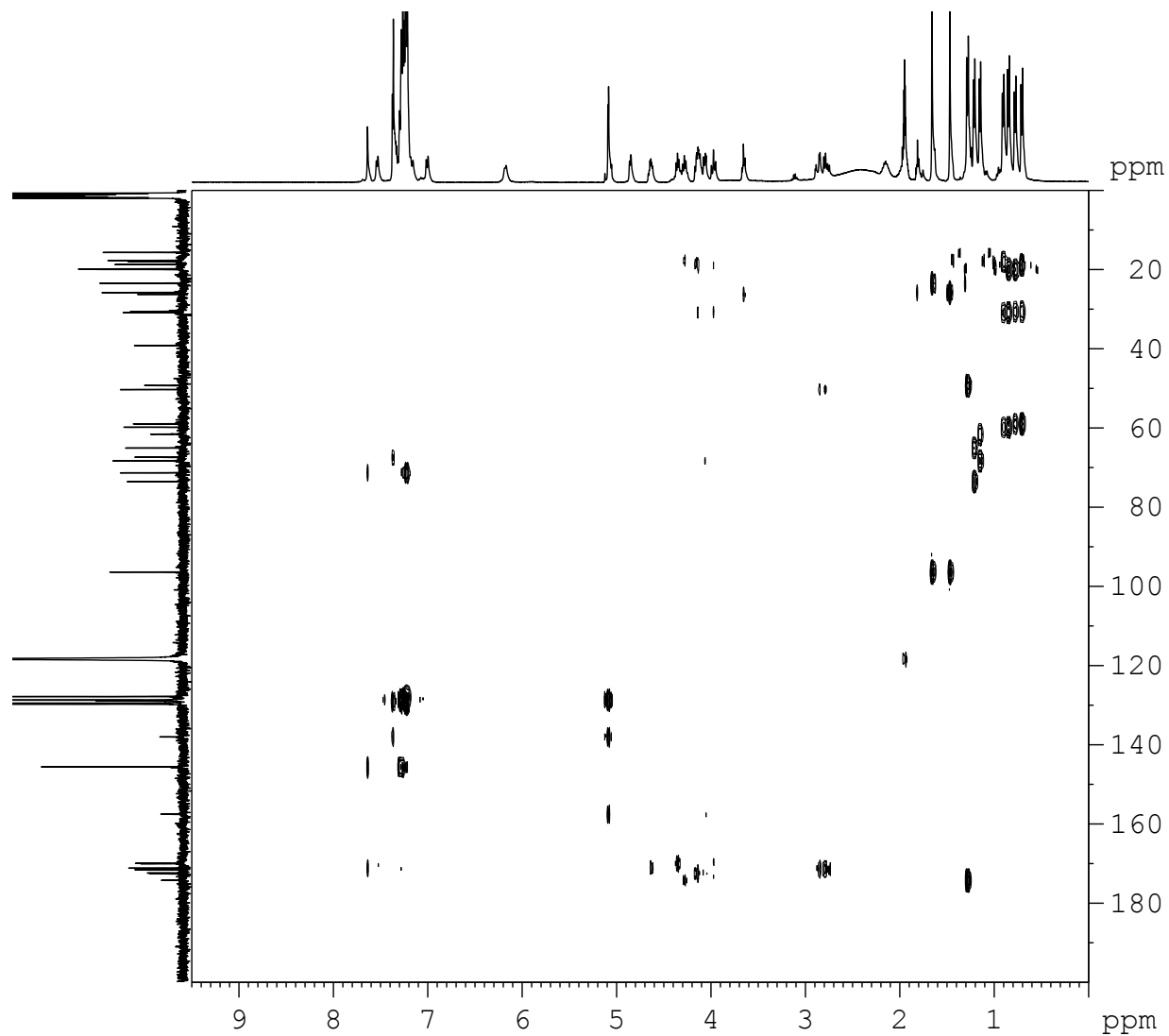
Cbz-L-Thr-D-Val-L-Val-D-*allo*-Thr(Ψ Pro)-D-Asn(Trt)-D-Ala-OH (6) HMBC

Current Data Parameters
NAME jc355A-ACN
EXPNO 1
PROCNO 1

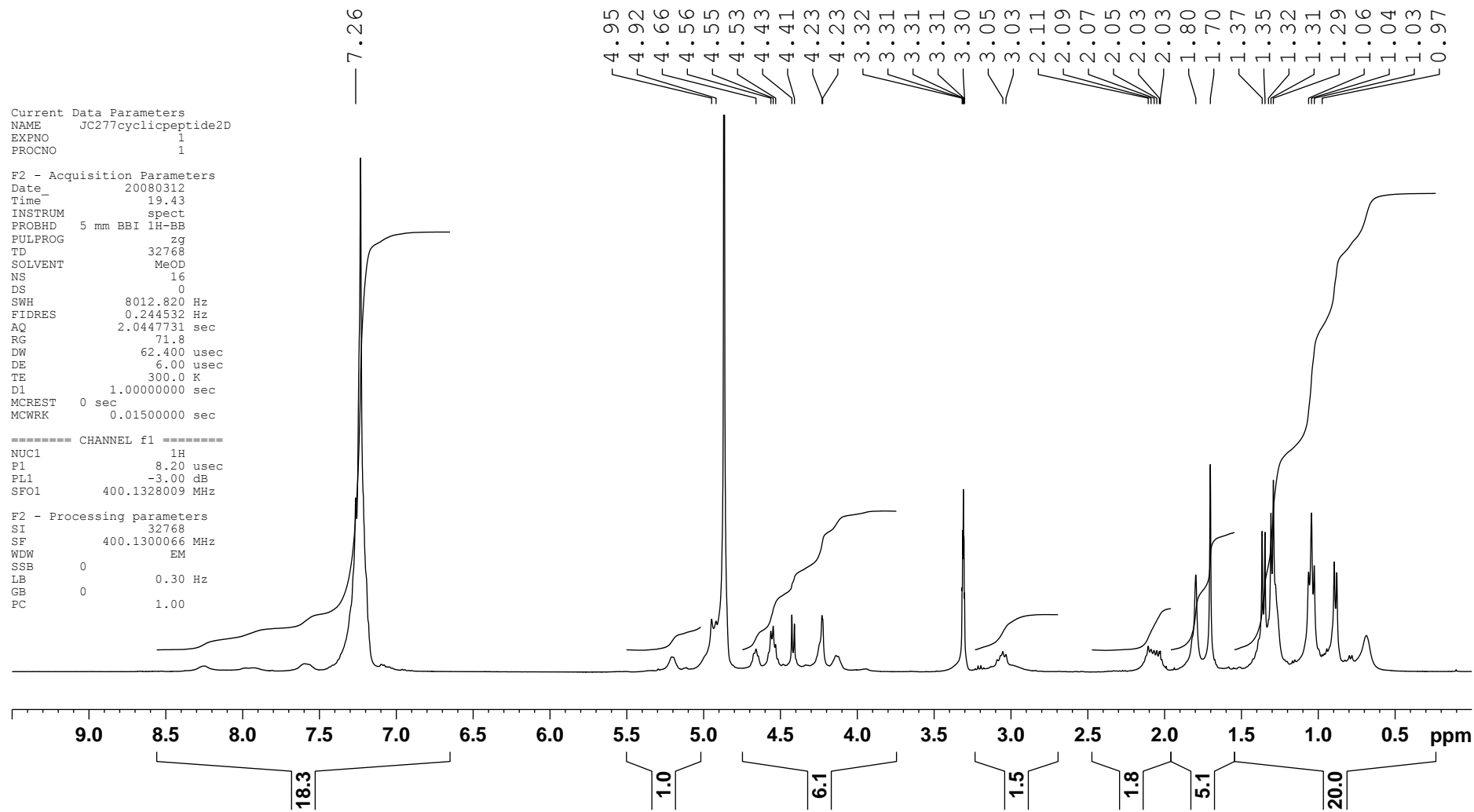
F2 - Acquisition Parameters
Date_ 20090211
Time 18.20
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg
TD 32768
SOLVENT CD3CN
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 100
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
MCREST 0 sec
MCWRK 0.0150000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 -3.00 dB
SFO1 400.1328009 MHz

F2 - Processing parameters
SI 32768
SF 400.1300069 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



Cyclic depsipeptide (11)



Cyclic depsipeptide (11) COSY

Current Data Parameters
NAME JC277cyclicpeptide2D
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20080312
Time 19.43
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG cosygpcqf
TD 2048
SOLVENT MeOH
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 3.912510 Hz
AQ 0.1278452 sec
RG 90.5
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
d0 0.0000300 sec
d1 2.00000000 sec
d13 0.00000400 sec
d16 0.00015000 sec
INO 0.00012480 sec
MCREST 0 sec
MCWRK 2.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
P0 8.20 usec
P1 8.20 usec
PL1 -3.00 dB
SFO1 400.1320007 MHz

===== GRADIENT CHANNEL =====

GPNAME1 sine.100
GPNAME2 sine.100
GPX1 0 %
GPX2 0 %
GPY1 0 %
GPY2 0 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1500.00 usec

F1 - Acquisition parameters

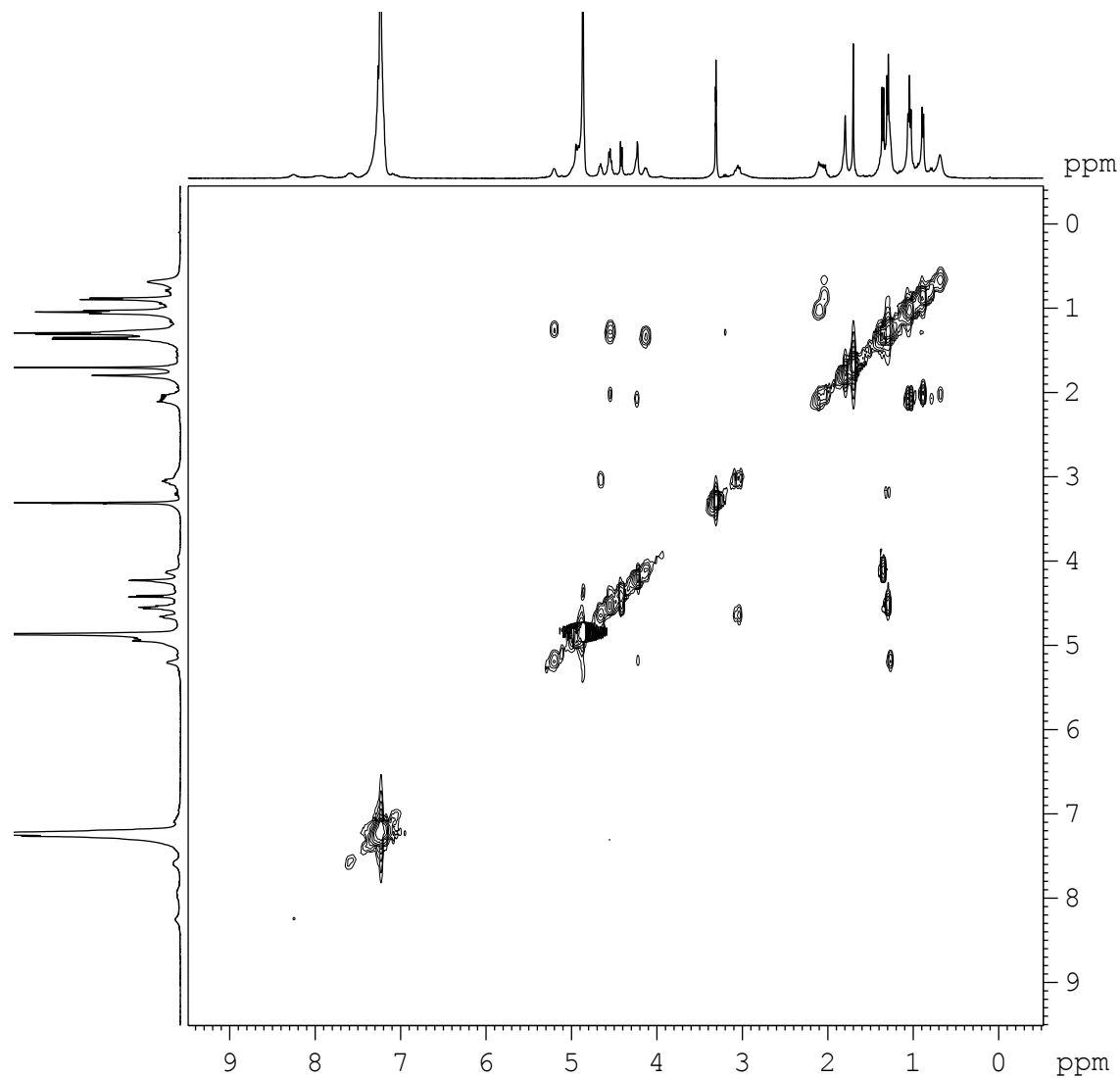
TD 256
SFO1 400.132 MHz
FIDRES 31.300079 Hz
SW 20.025 ppm
FnMODE QF

F2 - Processing parameters

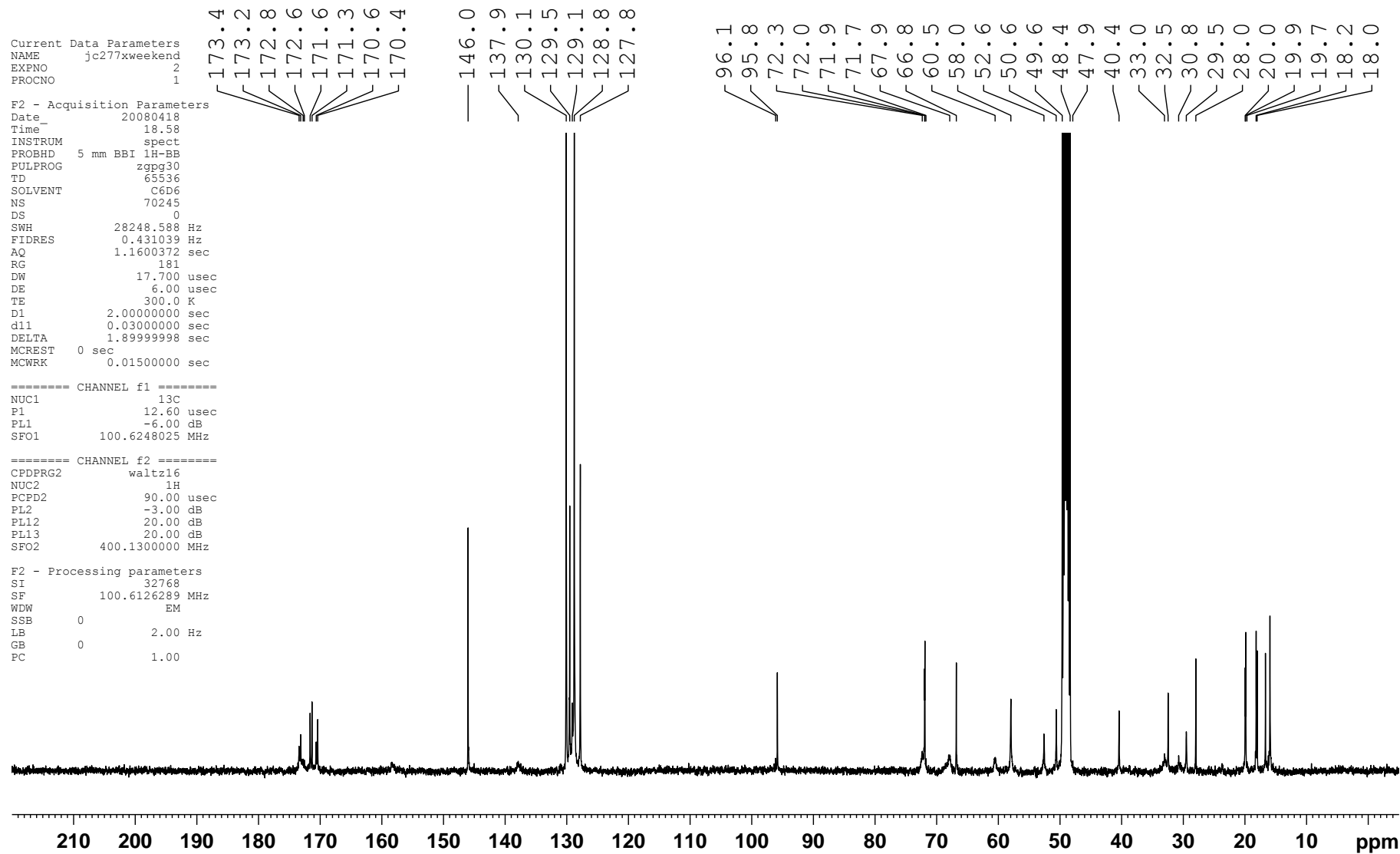
SI 4096
SF 400.1300066 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters

SI 256
MC2 QF
SF 400.1300000 MHz
WDW States
SSB 0
LB 0 Hz
GB 0



Cyclic depsipeptide (11)



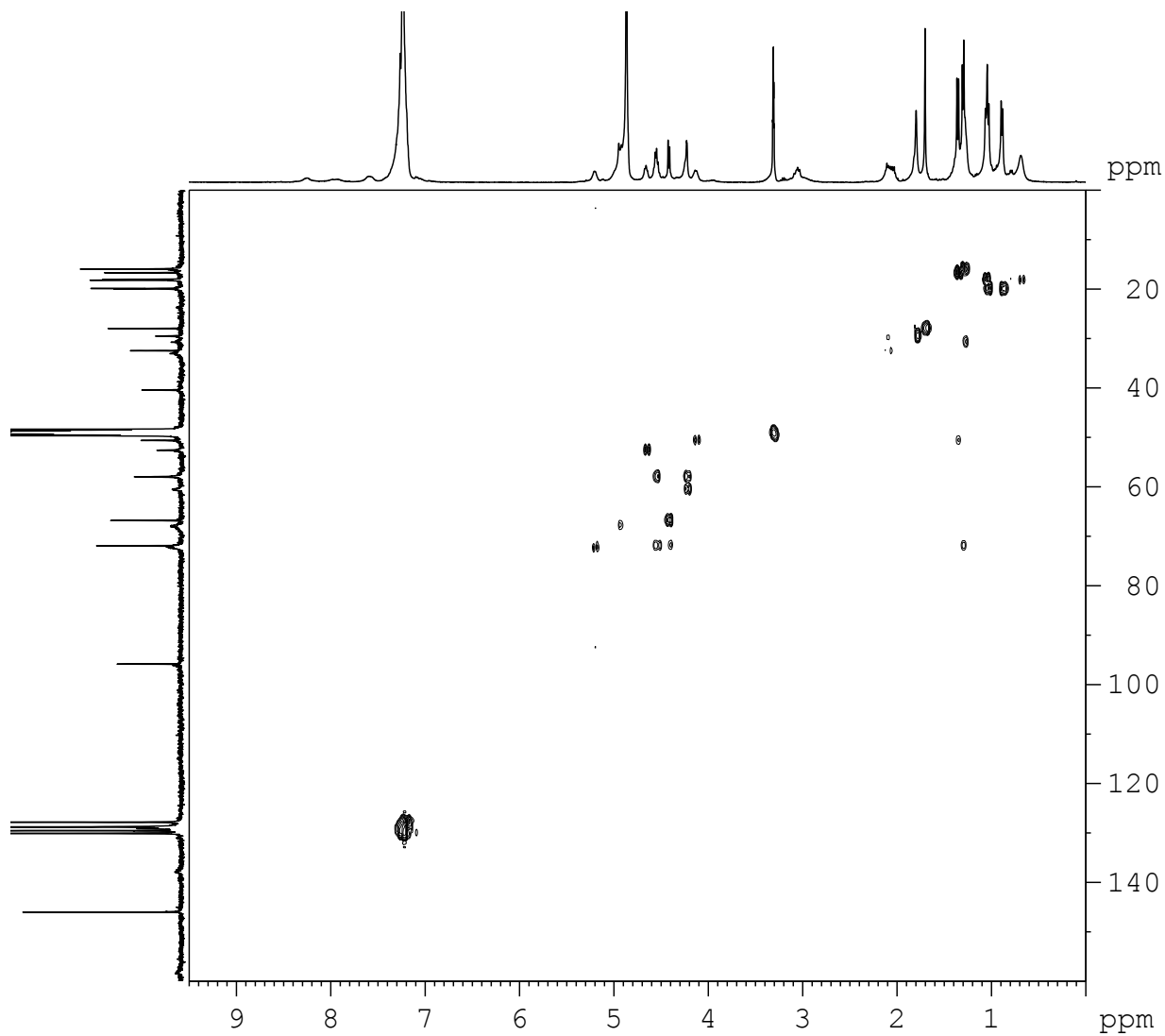
Cyclic depsipeptide (11) HSQC

Current Data Parameters
NAME JC277cyclicpeptide2D
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080312
Time_ 19.43
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg
TD 32768
SOLVENT MeOD
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 71.8
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 -3.00 dB
SFO1 400.1328009 MHz

F2 - Processing parameters
SI 32768
SF 400.1300066 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Cyclic depsipeptide (11) HMBC

```
Current Data Parameters
NAME          JC277hsqc
EXPNO         4
PROCNO        1

F2 - Acquisition Parameters
Date_         20080511
Time          19.07
INSTRUM       spect
PROBHD        5 mm BBI 1H-BB
PULPROG       inv4gp1plrndqf
TD            2048
SOLVENT       MeOH
NS            64
DS            16
SWH           8012.820 Hz
FIDRES        3.912510 Hz
AQ            0.1278452 sec
RG            8192
DW            62.400 usec
DE            6.00 usec
TE            300.0 K
CNST2         140.0000000
d0            0.00000300 sec
D1            0.80000001 sec
d2            0.00357143 sec
D6            0.07200000 sec
d13           0.00000400 sec
D16           0.00015000 sec
IN0           0.00001988 sec
MCREST        0 sec
MCWRK         0.80000001 sec

===== CHANNEL f1 =====
NUC1           1H
P1             8.20 usec
P2            16.40 usec
PL1            -3.00 dB
SFO1          400.1320007 MHz

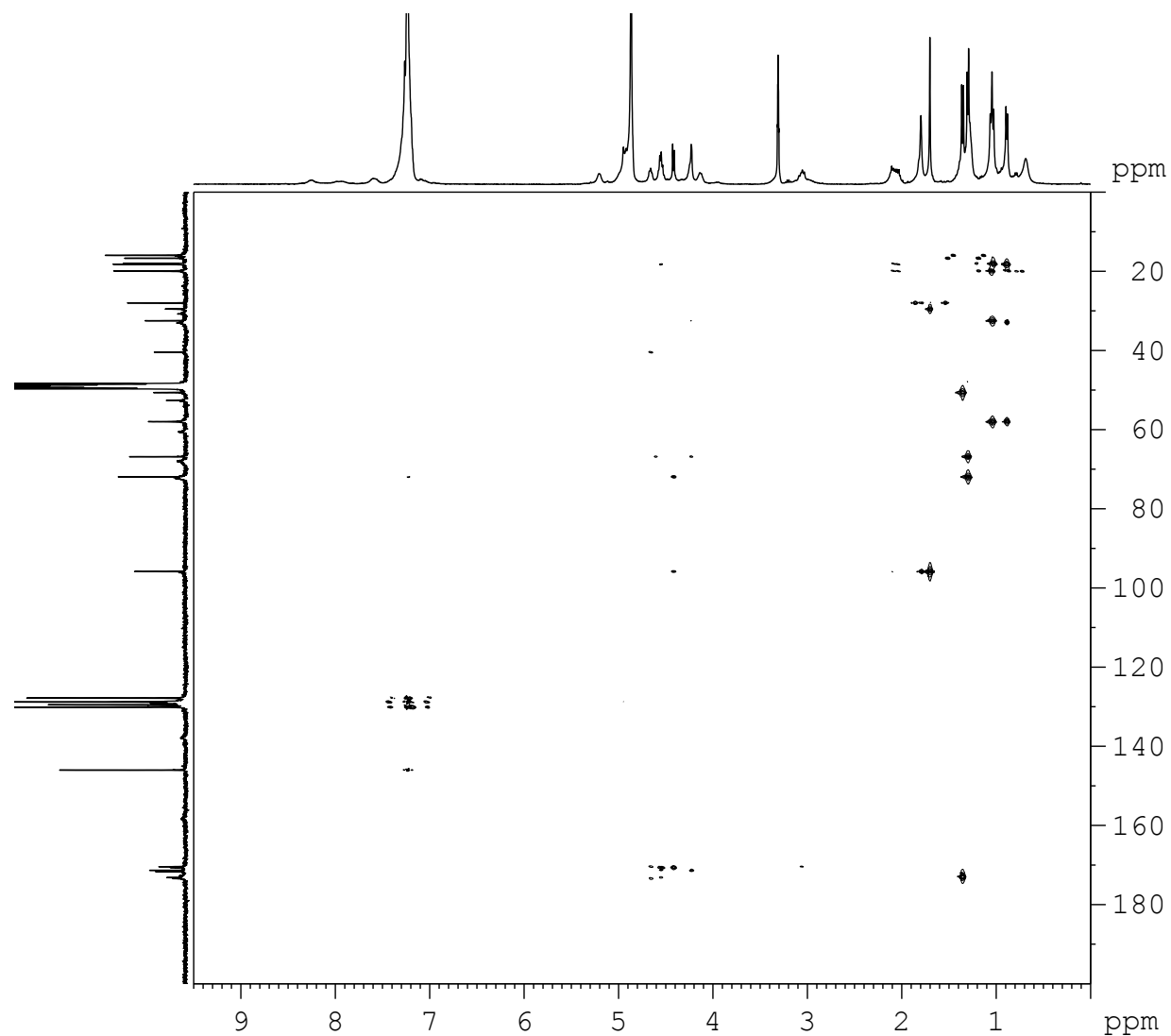
===== CHANNEL f2 =====
NUC2           13C
P3            12.00 usec
PL2            -6.00 dB
SFO2          100.6227903 MHz

===== GRADIENT CHANNEL =====
GPNAM1         sine.100
GPNAM2         sine.100
GPNAM3         sine.100
GPX1           0 %
GPX2           0 %
GPX3           0 %
GPY1           0 %
GPY2           0 %
GPY3           0 %
GPZ1           50.00 %
GPZ2           30.00 %
GPZ3           40.10 %
P16            1500.00 usec

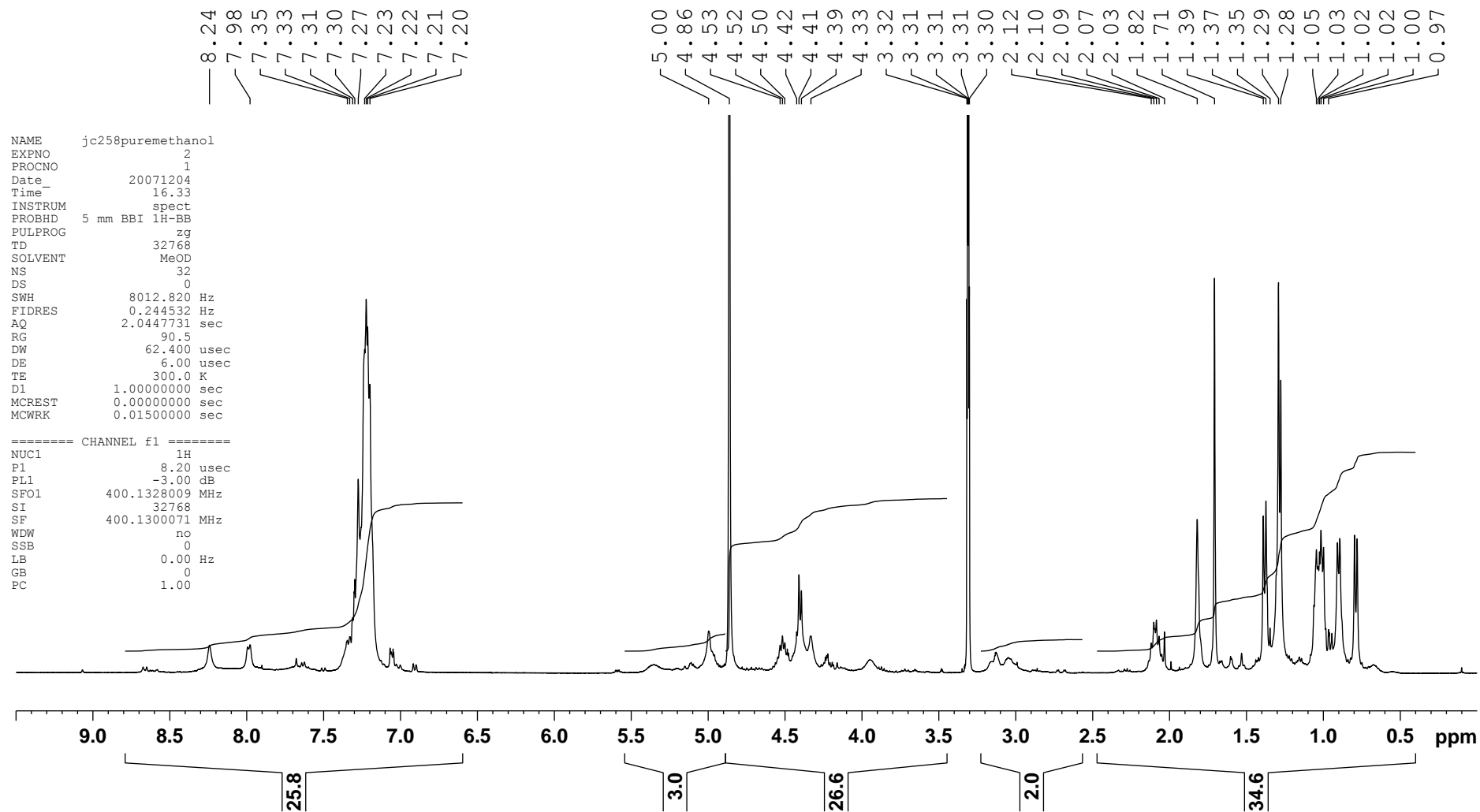
F1 - Acquisition parameters
TD             512
SFO1          100.6228 MHz
FIDRES         49.135220 Hz
SW             250.015 ppm
FhMODE         QF

F2 - Processing parameters
SI             4096
SF            400.1300097 MHz
WDW            SINE
SSB            2
LB             0 Hz
GB             0
PC             1.40

F1 - Processing parameters
SI             2048
SF            100.6126243 MHz
WDW            States
SSB            2
LB             0 Hz
GB             0
```



Cyclic depsipeptide (10)



Cyclic depsipeptide (10) COSY

```

Current Data Parameters
NAME      jc258pure
EXPNO    2
PROCNO    1

F2 - Acquisition Parameters
Date_    20071206
Time     19.20
INSTRUM  spect
PROBHD   5 mm BBI 1H-BB
PULPROG  cosygmfph
TD       2048
SOLVENT  MeOH
NS       15
DS       0
SWH      4006.410 Hz
FIDRES   1.956255 Hz
AQ       0.2556404 sec
RG       4597.6
DW       124.800 usec
DE       6.00 usec
TE       300.0 K
d0       0.00011390 sec
d1       2.50000000 sec
d13      0.00000400 sec
d16      0.00015000 sec
d20      0.00165400 sec
INO      0.00024960 sec
MCREST   0 sec
MCWRK    1.25000000 sec
ST1CNT   0

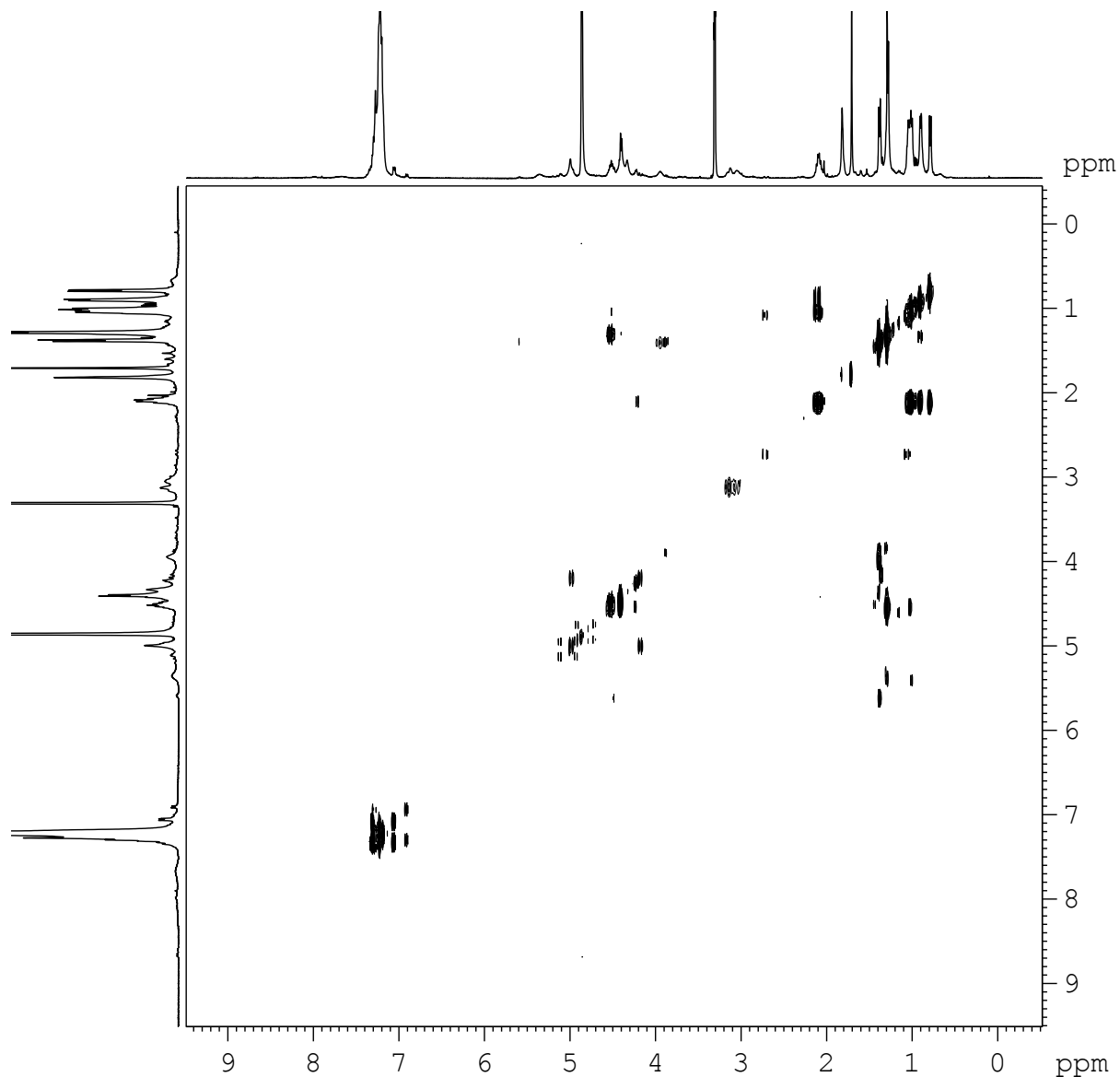
===== CHANNEL f1 =====
NUC1     1H
P1       8.56 usec
p2       17.12 usec
PL1      -3.00 dB
SFO1     400.1320007 MHz

===== GRADIENT CHANNEL =====
GPNAM1   sine.100
GPNAM2   sine.100
GPX1     0 %
GPX2     0 %
GPY1     0 %
GPY2     0 %
GPZ1     10.00 %
GPZ2     20.00 %
P16      1500.00 usec

F1 - Acquisition parameters
TD       256
SFO1     400.132 MHz
FIDRES   15.650040 Hz
SW       10.013 ppm
FnMODE   States-TPPI

F2 - Processing parameters
SI       2048
SF       400.1300035 MHz
WDW      SINE
SSB      0
LB       0 Hz
GB       0
PC       1.00

F1 - Processing parameters
SI       256
MC2      States-TPPI
SF       400.1299891 MHz
WDW      SINE
SSB      0
LB       0 Hz
GB       0
    
```



Cyclic depsipeptide (10) HMBC

```

Current Data Parameters
NAME          JC493pseudolb
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20100728
Time_         18.19
INSTRUM       spect
PROBHD        5 mm BBI 1H-BB
PULPROG       inv4gpipirndqf
TD            4096
SOLVENT       CD3CN
NS            64
DS            8
SWH           4006.410 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG            2048
DW            124.800 usec
DE            6.00 usec
TE            0 K
CNST2         145.0000000
d0            0.00000300 sec
D1            1.500000000 sec
d2            0.00344828 sec
D6            0.06230000 sec
d13           0.00000400 sec
D16           0.00015000 sec
IN0           0.00002484 sec
MCREST        0 sec
MCWRK         1.50000000 sec

===== CHANNEL f1 =====
NUC1          1H
F1            6.07 usec
p2            12.14 usec
PL1           -3.00 dB
SFO1          400.2101790 MHz

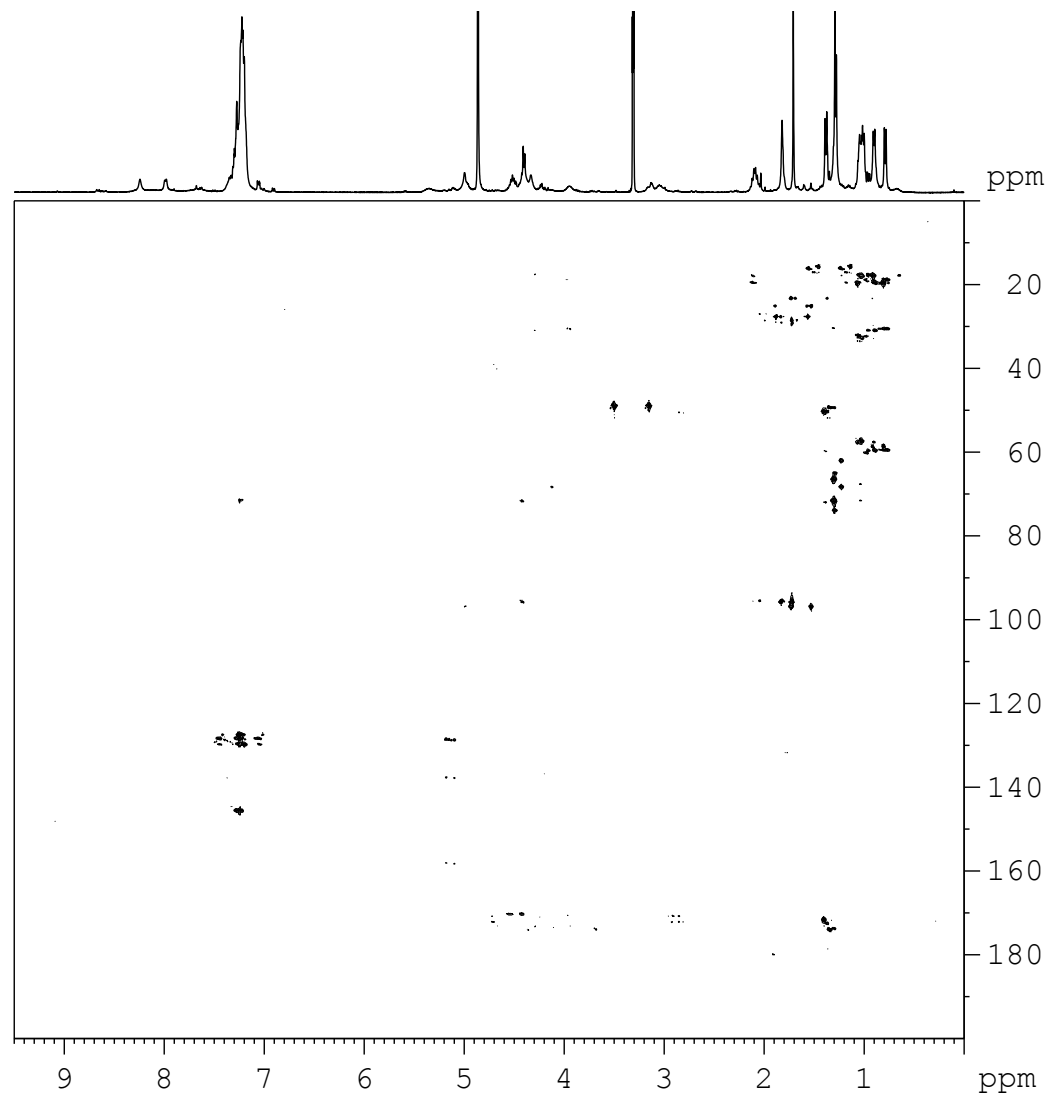
===== CHANNEL f2 =====
NUC2          13C
F2            12.00 usec
PL2           -6.00 dB
SFO2          100.6424892 MHz

===== GRADIENT CHANNEL =====
GPNAM1        sine.100
GPNAM2        sine.100
GPNAM3        sine.100
GPX1          0 %
GPX2          0 %
GPX3          0 %
GPY1          0 %
GPY2          0 %
GPY3          0 %
GPZ1          50.00 %
GPZ2          30.00 %
GPZ3          40.10 %
P16           1500.00 usec

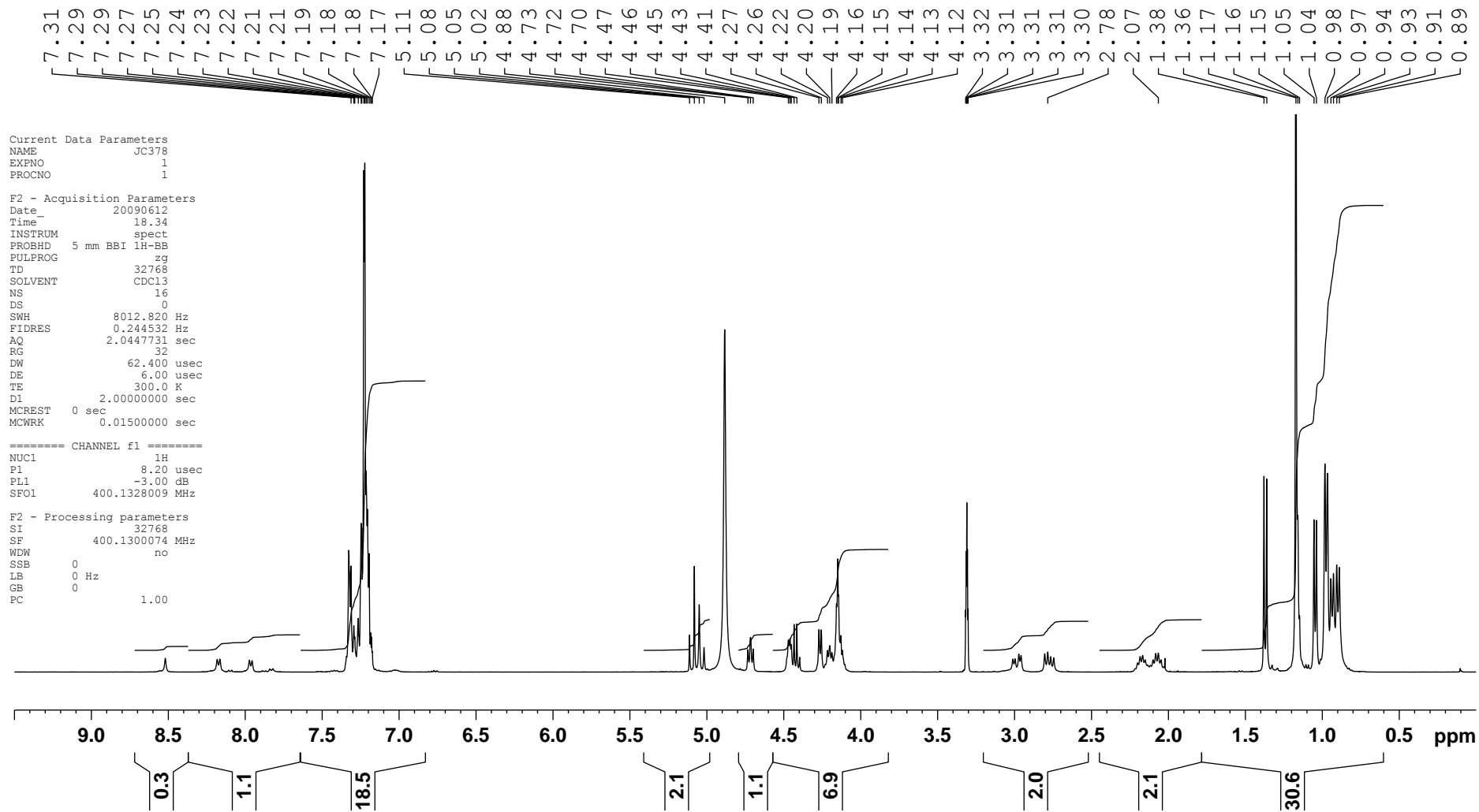
F1 - Acquisition parameters
TD            512
SFO1          100.6425 MHz
FIDRES        39.318066 Hz
SW            200.023 ppm
FAMODE        QF

F2 - Processing parameters
SI            2048
SF            400.2081726 MHz
WDW           SINE
SSB           2
LB            0 Hz
GB            0
PC            1.00

F1 - Processing parameters
SI            1024
MC2           QF
SF            100.6323106 MHz
WDW           States
SSB           2
LB            0 Hz
GB            0
    
```



Cbz-L-Thr-D-Val-L-Val-D-allo-Thr(*tert*-butyl)-D-Asn(Trt)-L-Ala-OH (9)



Cbz-L-Thr-D-Val-L-Val-D-*allo*-Thr(*tert*-butyl)-D-Asn(Trt)-L-Ala-OH (9) COSY

```

Current Data Parameters
NAME          JC378
EXPNO         3
PROCNO        1

F2 - Acquisition Parameters
Date_         20090612
Time          21.54
INSTRUM       spect
PROBHD        5 mm BBI 1H-BB
PULPROG       cosygmzph
TD            4096
SOLVENT       MeOH
NS            16
DS            8
SWH           4006.410 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG            1448.15
DW            124.800 usec
DE            6.00 usec
TE            300.0 K
d0            0.00011452 sec
d1            3.00000000 sec
d13           0.00000400 sec
d16           0.00015000 sec
d20           0.00165400 sec
IN0           0.00024991 sec
MCREST        0 sec
MCWRK         1.5000000 sec
ST1CNT        0

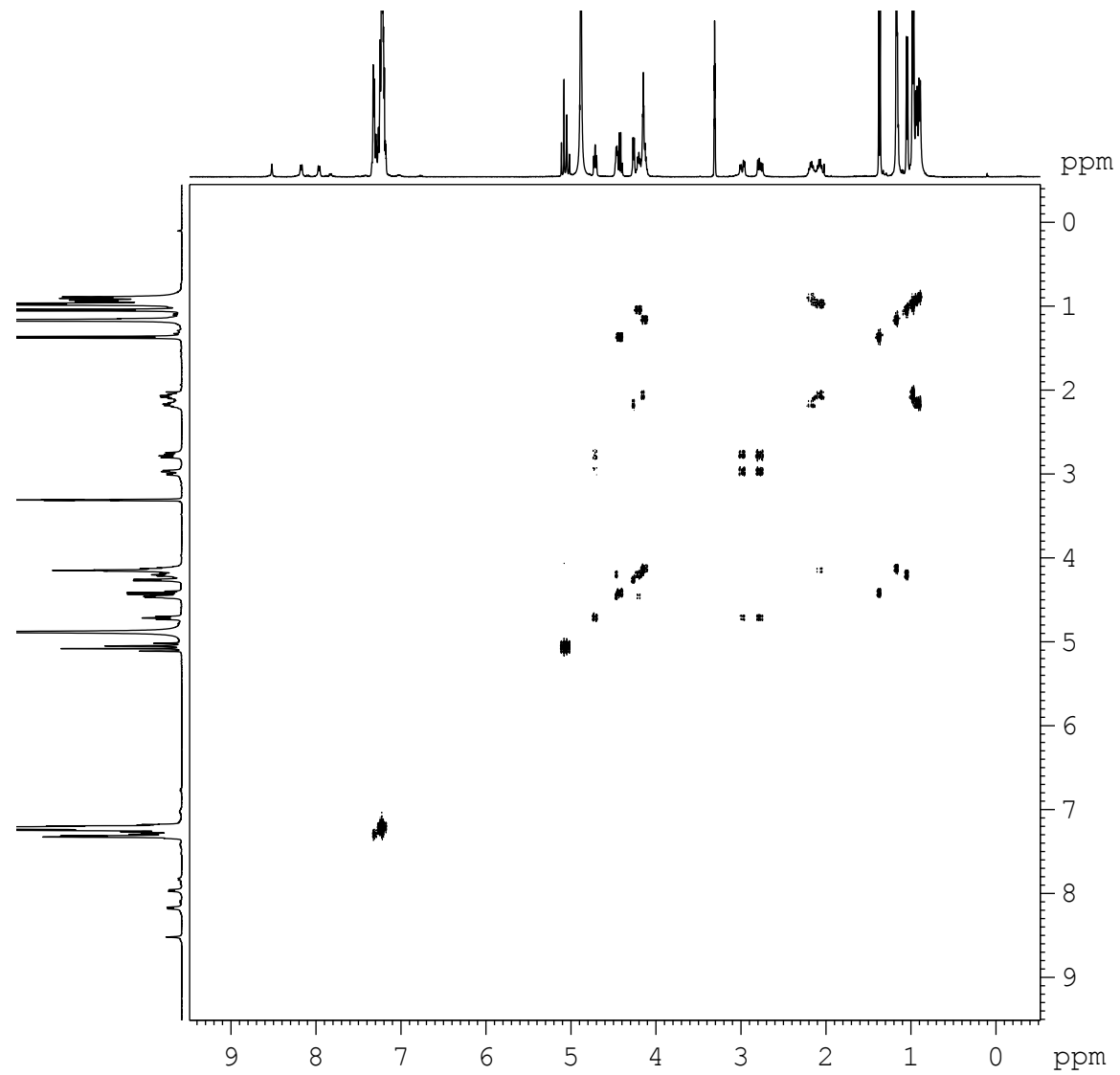
===== CHANNEL f1 =====
NUC1           1H
P1             8.20 usec
p2            16.40 usec
PL1           -3.00 dB
SFO1          400.1318006 MHz

===== GRADIENT CHANNEL =====
GPNAM1        sine.100
GPNAM2        sine.100
GPX1          0 %
GPX2          0 %
GPY1          0 %
GPY2          0 %
GPZ1          10.00 %
GPZ2          20.00 %
P16           1500.00 usec

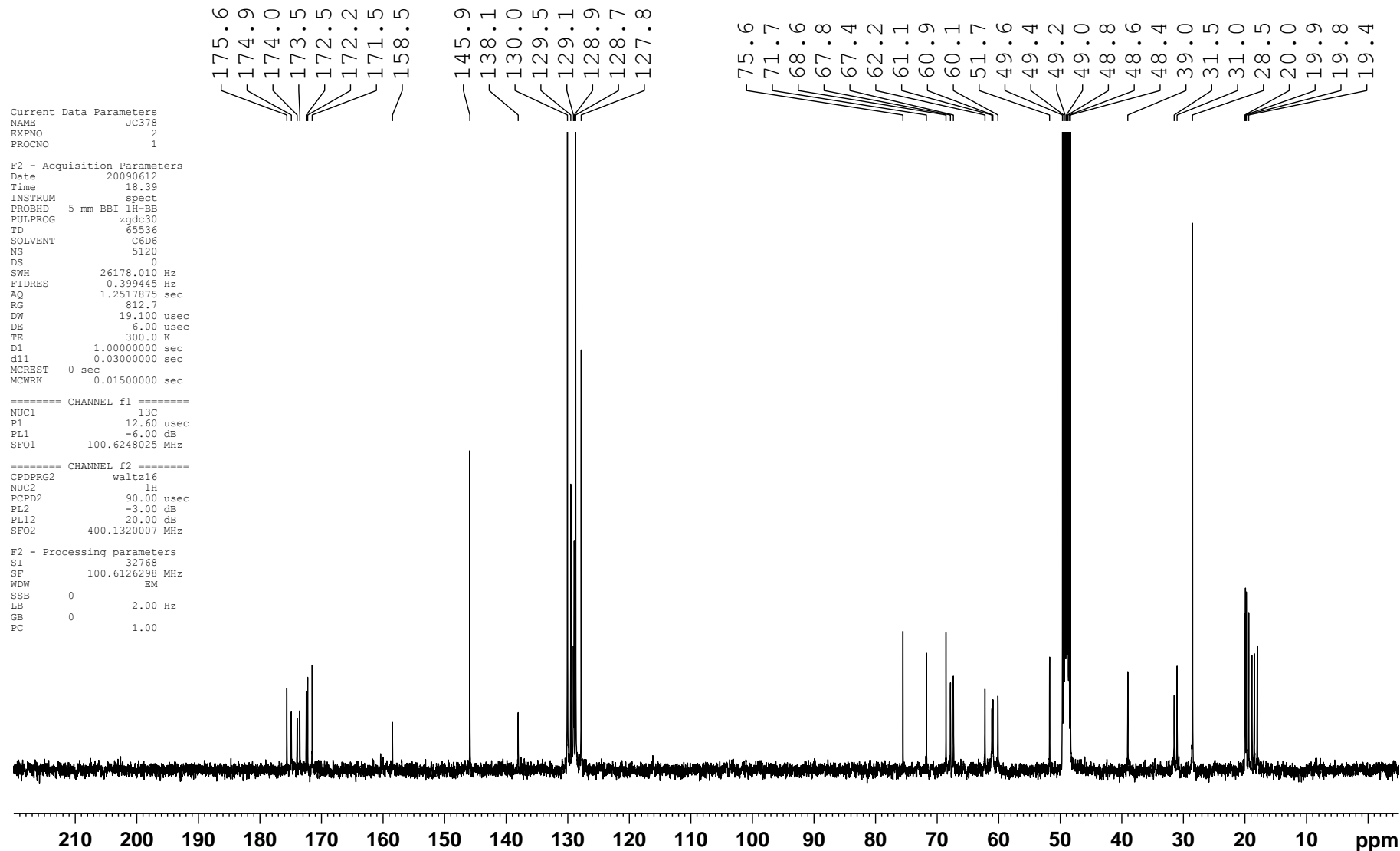
F1 - Acquisition parameters
TD            256
SFO1          400.1318 MHz
FIDRES        15.630470 Hz
SW            10.000 ppm
FnMODE        States-TPPI

F2 - Processing parameters
SI            4096
SF            400.1300076 MHz
WDW           SINE
SSB           2
LB            0 Hz
GB            0
PC            1.00

F1 - Processing parameters
SI            1024
MC2           States-TPPI
SF            400.1300076 MHz
WDW           SINE
SSB           2
LB            0 Hz
GB            0
    
```



Cbz-L-Thr-D-Val-L-Val-D-*allo*-Thr(*tert*-butyl)-D-Asn(Trt)-L-Ala-OH (9)



Cbz-L-Thr-D-Val-L-Val-D-*allo*-Thr(*tert*-butyl)-D-Asn(Trt)-L-Ala-OH (9) HSQC

```

Current Data Parameters
NAME          JC378
EXPNO         5
PROCNO        1

F2 - Acquisition Parameters
Date_         20090613
Time_         6.52
INSTRUM       spect
PROBHD        5 mm BBI 1H-BB
PULPROG       invetgpsi
TD            4096
SOLVENT       CDCl3
NS            16
DS            8
SWH           4006.410 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG            2048
DW            124.800 usec
DE            6.00 usec
TE            300.0 K
CNST2         140.0000000
d0            0.00000300 sec
d1            3.00000000 sec
d4            0.00178571 sec
d11           0.03000000 sec
d13           0.00000400 sec
D16           0.00015000 sec
D24           0.00178500 sec
DELTA         0.00172240 sec
DELTA1        0.00168800 sec
INO           0.00002259 sec
MCREST        0 sec
MCWRK         0.50000101 sec
ST1CNT        0

===== CHANNEL f1 =====
NUC1          1H
P1            8.20 usec
P2            16.40 usec
P28           0.50 usec
PL1           -3.00 dB
SFO1          400.1318006 MHz

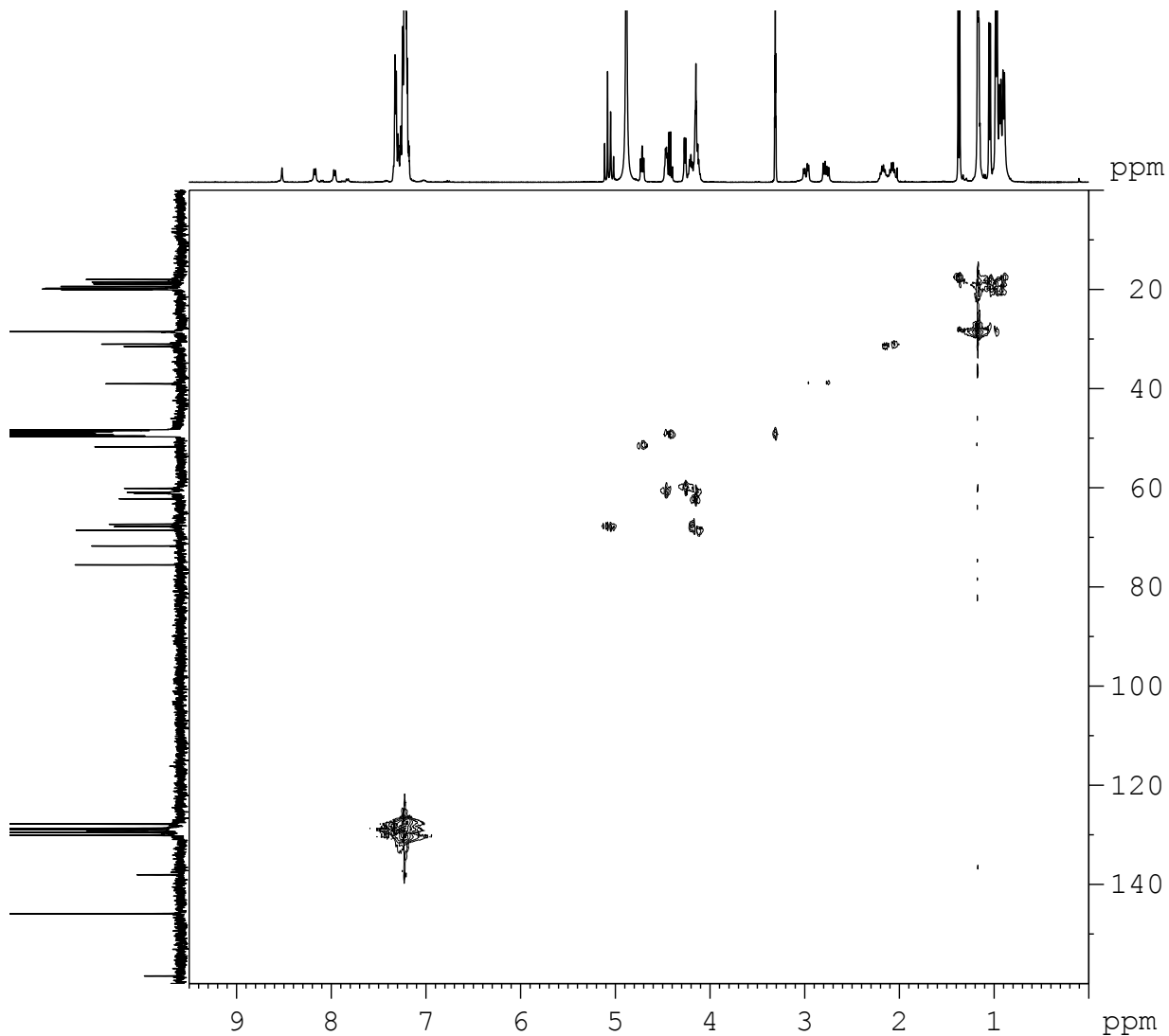
===== CHANNEL f2 =====
CPDPRG2       garp
NUC2          13C
P3            12.00 usec
P4            24.00 usec
PCPD2         70.00 usec
PL2           -6.00 dB
PL12          10.70 dB
SFO2          100.6227903 MHz

===== GRADIENT CHANNEL =====
GPNAM1        sine.100
GPNAM2        sine.100
GFX1          0 %
GFX2          0 %
GPV1          0 %
GPV2          0 %
GFZ1          80.00 %
GFZ2          20.10 %
P16           1500.00 usec

F1 - Acquisition parameters
TD            256
SFO1          100.6228 MHz
FIDRES        86.469284 Hz
SW            219.991 ppm
FMODE         Echo-Antiecho

F2 - Processing parameters
SI            2048
SF            400.1300049 MHz
WDW           SINE
SSB           2
LB            0 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI            512
MC2           echo-antiecho
SF            100.6126295 MHz
WDW           SINE
SSB           1
LB            0 Hz
GB            0
    
```



Cbz-L-Thr-D-Val-L-Val-D-*allo*-Thr(*tert*-butyl)-D-Asn(Trt)-L-Ala-OH (9) HMBC

```

Current Data Parameters
NAME          JC378
EXPNO         6
PROCNO        1

F2 - Acquisition Parameters
Date_         20090613
Time_         10.56
INSTRUM       spect
PROBHD        5 mm BBI 1H-5B
PULPROG       invgpp1prndqf
TD            4096
SOLVENT       MeOH
NS            32
DS            8
SWH           4006.410 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG            2048
DW            124.800 usec
DE            6.00 usec
TE            300.0 K
CNST2         140.0000000
d0            0.00000300 sec
D1            3.00000000 sec
d2            0.00357143 sec
D6            0.07200000 sec
d13           0.00004000 sec
D16           0.00015000 sec
IN0           0.00002259 sec
MCREST        0 sec
MCWRK         3.00000000 sec

===== CHANNEL f1 =====
NUC1           1H
P1             8.20 usec
P2            16.40 usec
PL1           -3.00 dB
SFO1          400.1318006 MHz

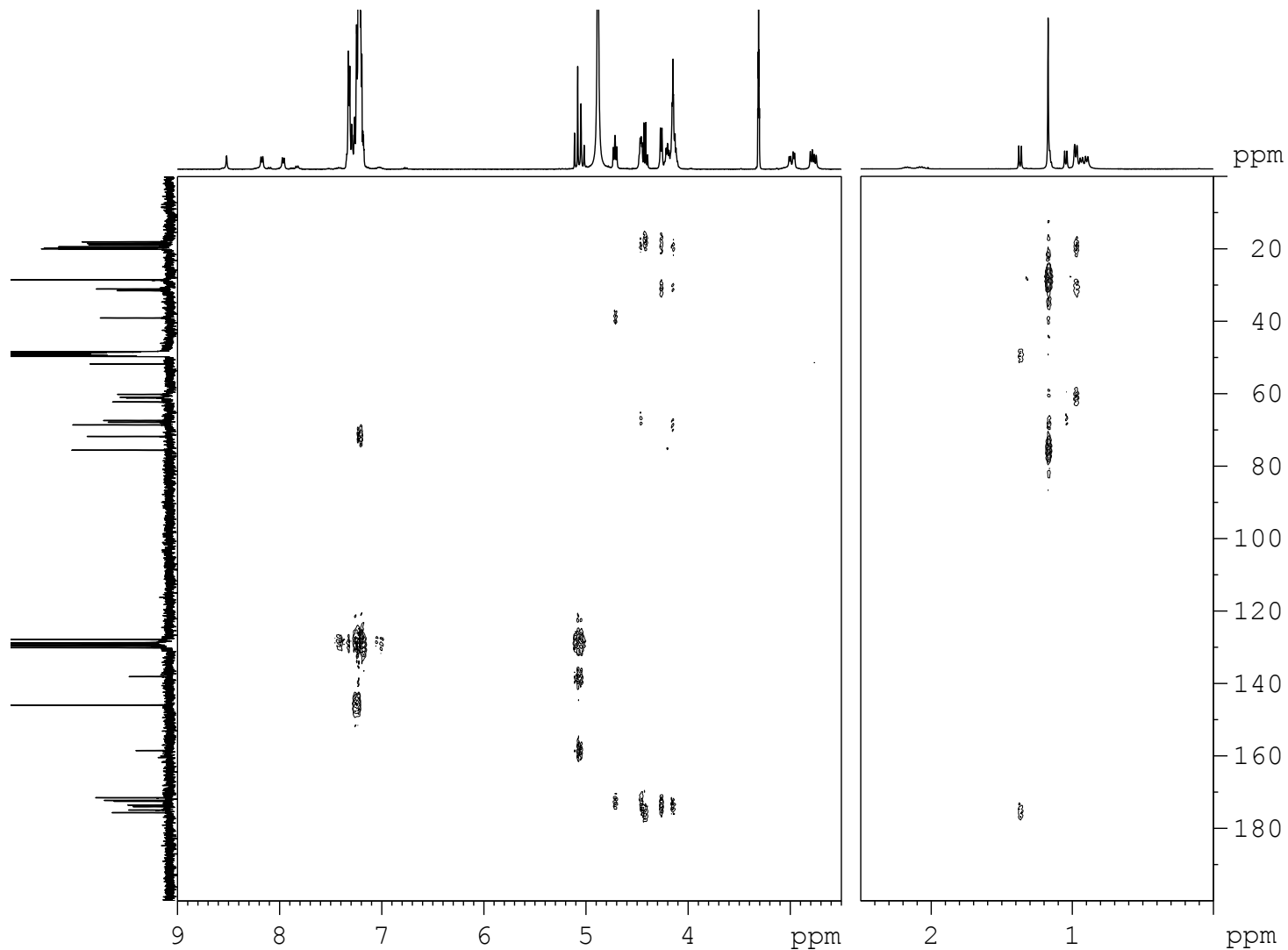
===== CHANNEL f2 =====
NUC2           13C
P3            12.00 usec
PL2           -6.00 dB
SFO2          100.6227903 MHz

===== GRADIENT CHANNEL =====
GPNAM1        sine.100
GPNAM2        sine.100
GPNAM3        sine.100
GPX1          0 %
GPX2          0 %
GPX3          0 %
GPY1          0 %
GPY2          0 %
GPY3          0 %
GPZ1          50.00 %
GPZ2          30.00 %
GPZ3          40.10 %
P16           1500.00 usec

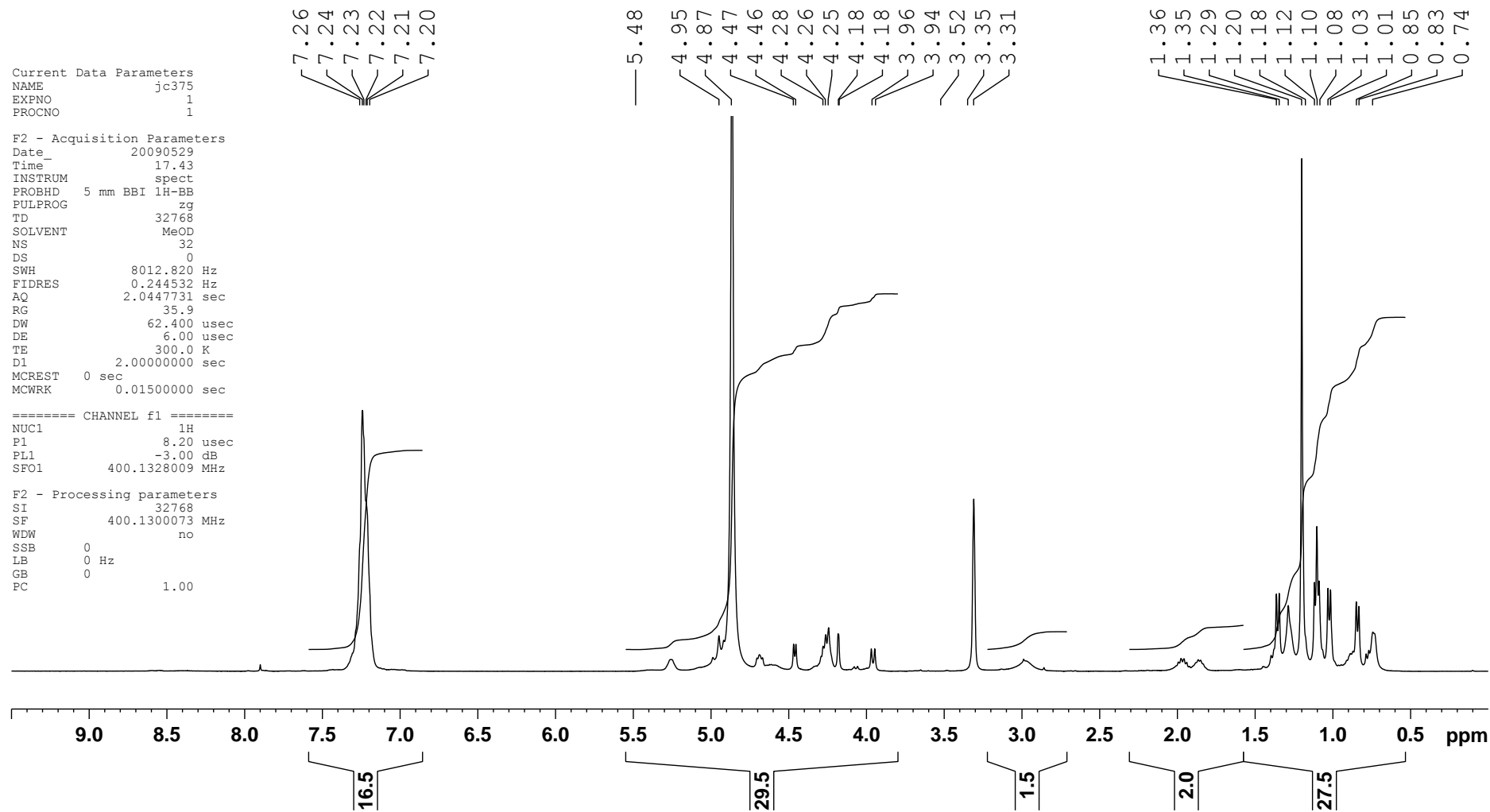
F1 - Acquisition parameters
TD            129
SFO1          100.6228 MHz
FIDRES        171.597961 Hz
SW            219.991 ppm
FhMODE        QF

F2 - Processing parameters
SI            1024
SF            400.1300076 MHz
WDW           SINE
SSB           2
LB            0 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI            512
MC2           QF
SF            100.6126298 MHz
WDW           States
SSB           2
LB            0 Hz
GB            0
    
```



Cyclic depsipeptide (8)



Cyclic depsipeptide (8) COSY

Current Data Parameters
NAME jc375
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090531
Time 16.54
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG cosygpmfph
TD 4096
SOLVENT MeOD
NS 16
DS 8
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 812.75
DW 124.800 usec
DE 6.00 usec
TE 300.0 K
d0 0.00011174 sec
d1 2.5000000 sec
d13 0.00000400 sec
d16 0.00015000 sec
d20 0.00165400 sec
IN0 0.00024991 sec
MCREST 0 sec
MCWRK 1.25000000 sec
ST1CNT 0

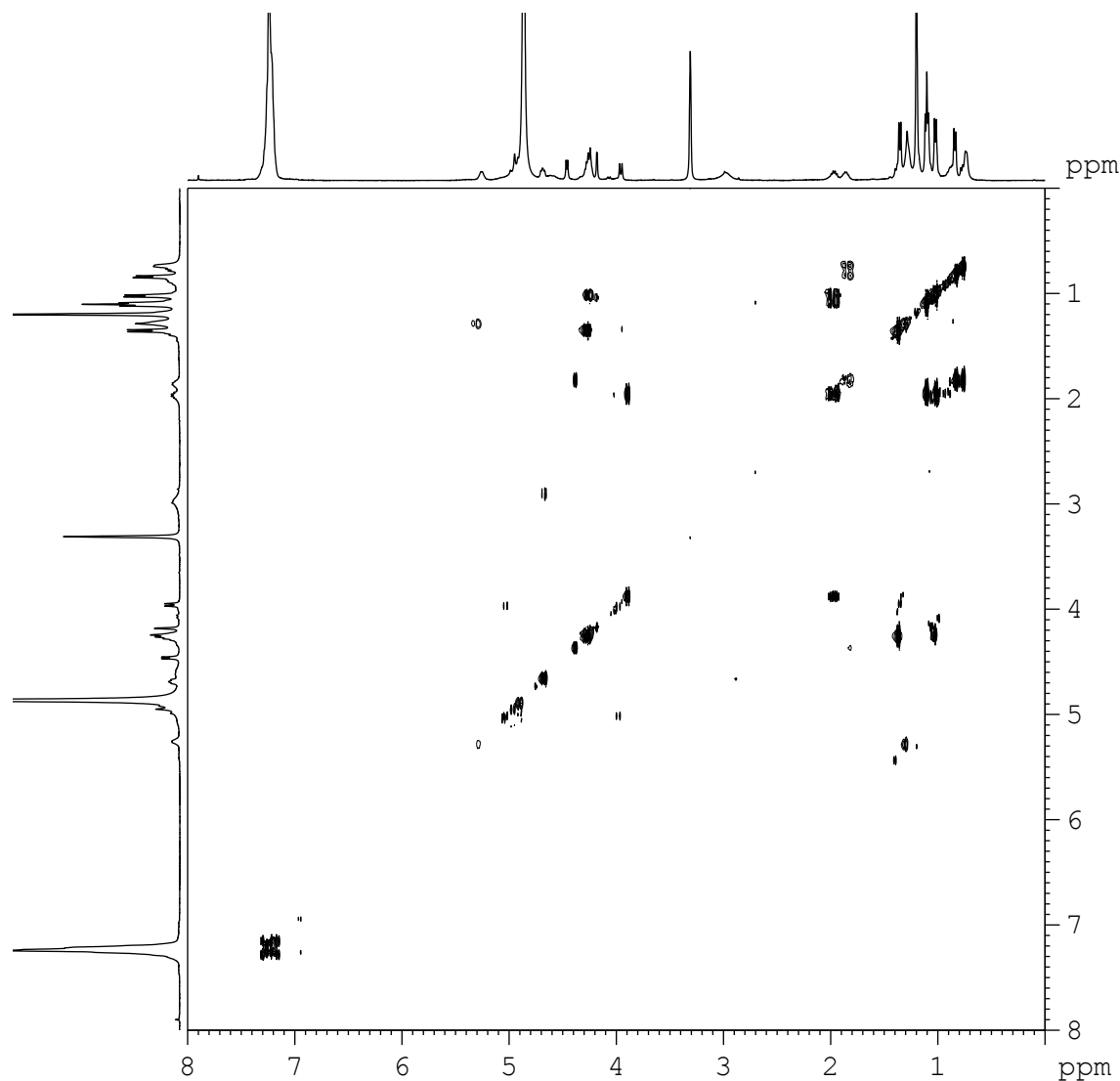
==== CHANNEL f1 =====
NUC1 1H
P1 10.38 usec
p2 20.76 usec
PL1 -3.00 dB
SFO1 400.1320007 MHz

==== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPX1 0 %
GPX2 0 %
GPY1 0 %
GPY2 0 %
GPZ1 10.00 %
GPZ2 20.00 %
P16 1500.00 usec

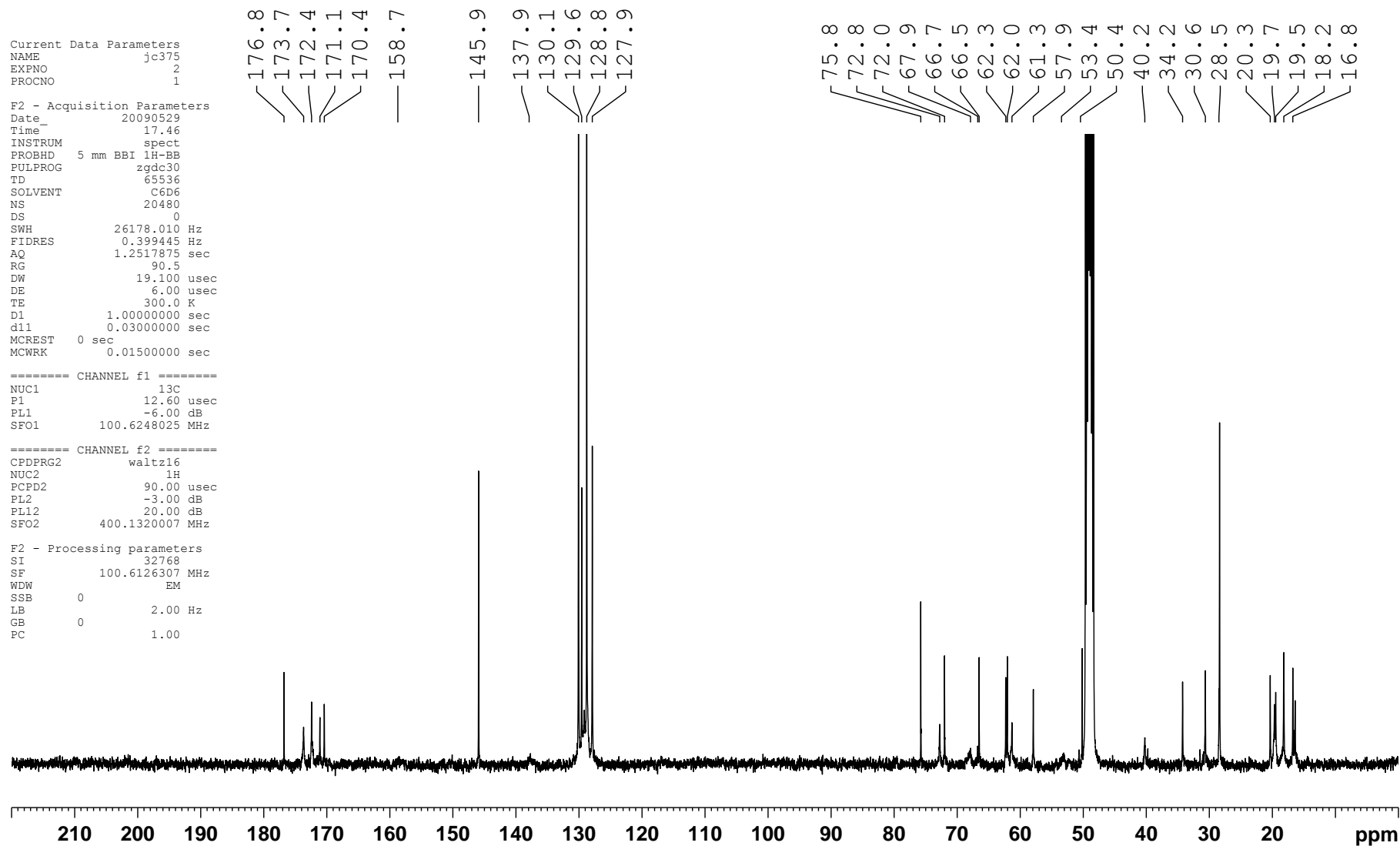
F1 - Acquisition parameters
TD 256
SFO1 400.132 MHz
FIDRES 15.630470 Hz
SW 10.000 ppm
FnMODE States-TFPI

F2 - Processing parameters
SI 4096
SF 400.1300051 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TFPI
SF 400.1300089 MHz
WDW
SSB 2
LB 0 Hz
GB 0



Cyclic depsipeptide (8)



Cyclic depsipeptide (8) HSQC

```

Current Data Parameters
NAME          jc375
EXPNO         7
PROCNO        1

F2 - Acquisition Parameters
Date_         20090601
Time          0.45
INSTRUM       spect
PROBHD        5 mm BBI 1H-BB
PULPROG       invietgpsai
TD            4096
SOLVENT       CDCl3
NS            32
DS            8
SWH           4006.410 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG            2298.8
DW            124.800 usec
DE            6.00 usec
TE            300.0 K
CNST2         140.0000000
d0            0.00000300 sec
d1            2.50000000 sec
d4            0.00178571 sec
d11           0.03000000 sec
d13           0.00000400 sec
d16           0.00015000 sec
D24           0.00178500 sec
DELTA         0.00172676 sec
DELTA1        0.00165800 sec
IN0           0.00002259 sec
MCWREST       0 sec
MCWRK         0.41666749 sec
ST1CNT        0

===== CHANNEL f1 =====
NUC1           1H
P1            10.38 usec
P2            20.76 usec
P28           0.50 usec
PL1           -3.00 dB
SFO1          400.1320007 MHz

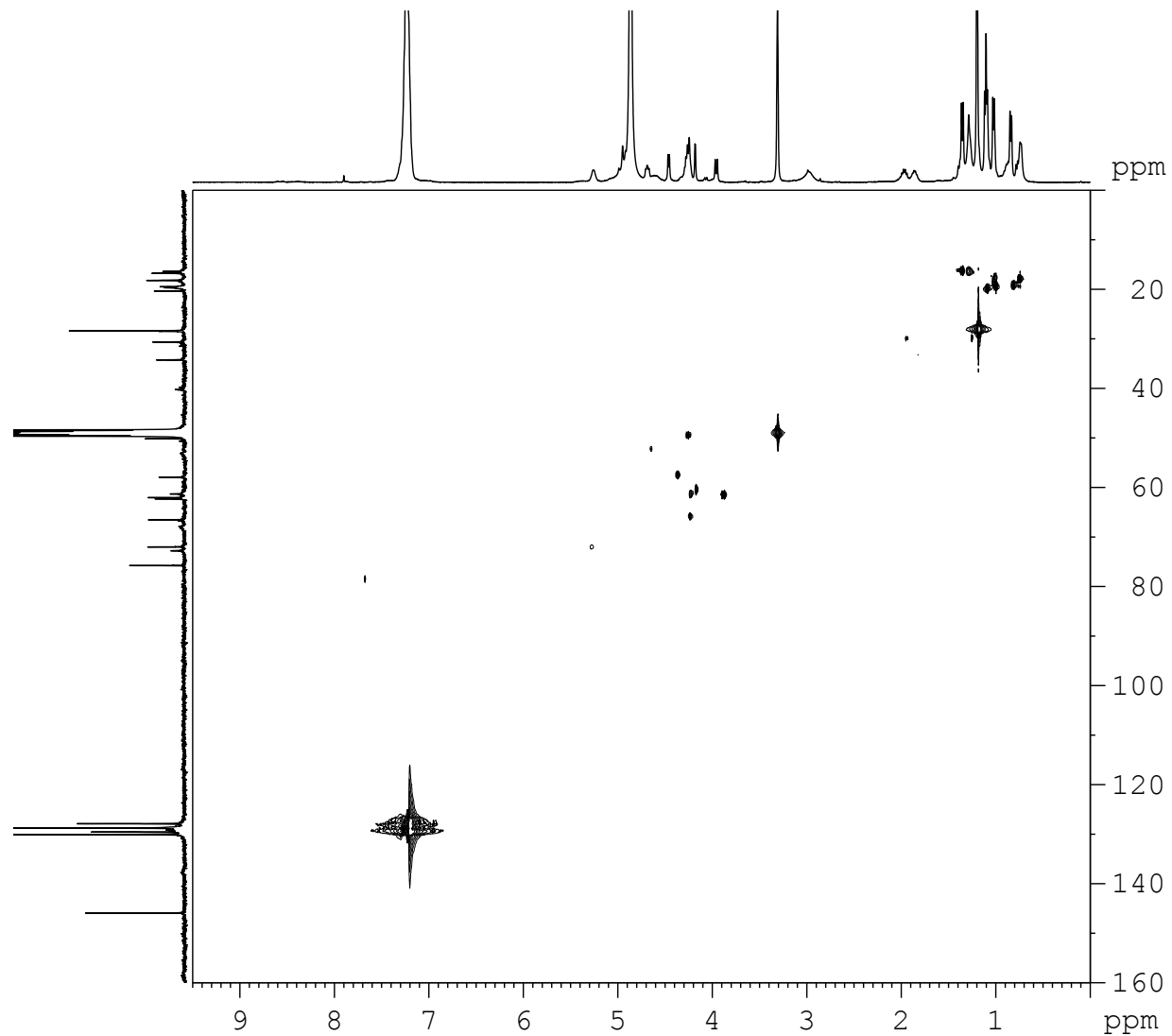
===== CHANNEL f2 =====
CPDPRG2       garp
NUC2           13C
P3            12.00 usec
p4            24.00 usec
PCPD2         70.00 usec
PL2           -6.00 dB
PL12          10.70 dB
SFO2          100.6227903 MHz

===== GRADIENT CHANNEL =====
GPNAM1        sine.100
GPNAM2        sine.100
GPX1          0 %
GPX2          0 %
GPY1          0 %
GPY2          0 %
GPE1          80.00 %
GPE2          20.10 %
P16           1500.00 usec

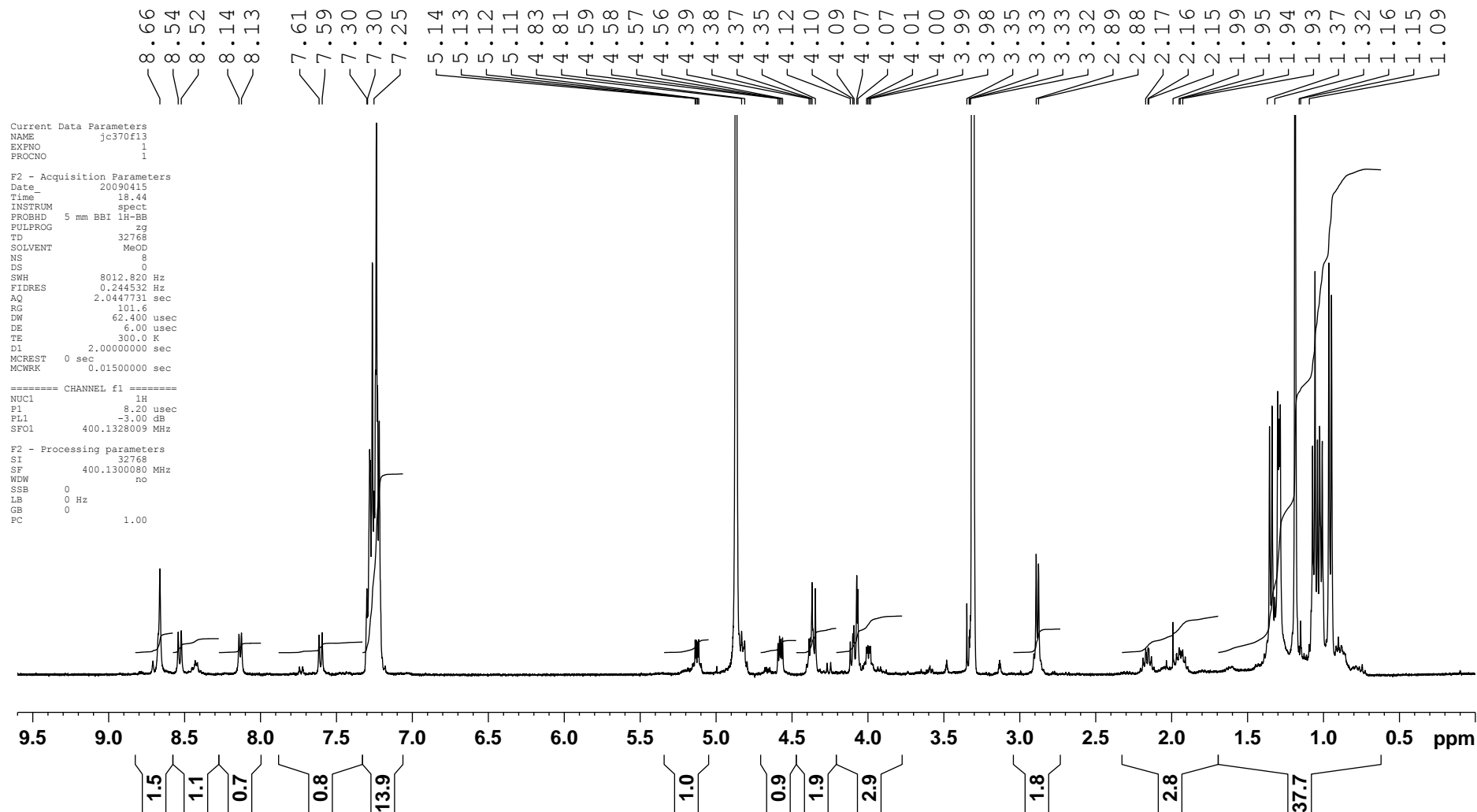
F1 - Acquisition parameters
TD            256
SFO1          100.6228 MHz
FIDRES        86.469284 Hz
SW            219.991 ppm
FnMODE        Echo-Antiecho

F2 - Processing parameters
SI            2048
SF            400.1300067 MHz
WDW           SINE
SSB           2
LB            0 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI            1024
MC2           echo-antiecho
SF            100.6126976 MHz
WDW           2
SSB           2
LB            0 Hz
GB            0
    
```



Cyclic depsipeptide (17)



Cyclic depsipeptide (17) COSY

Current Data Parameters
NAME JC377hsqc
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090626
Time 18.37
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG cosygmfch
TD 4096
SOLVENT MeOH
NS 48
DS 8
SWH 2394.636 Hz
FIDRES 0.584628 Hz
AQ 0.8552948 sec
RG 645.075
DW 208.800 usec
DE 6.00 usec
TE 300.0 K
d0 0.00019712 sec
d1 1.29999995 sec
d13 0.00000400 sec
d16 0.00015000 sec
d20 0.00165400 sec
INO 0.00041652 sec
MCREST 0 sec
MCWRK 0.64999998 sec
STICNT 0

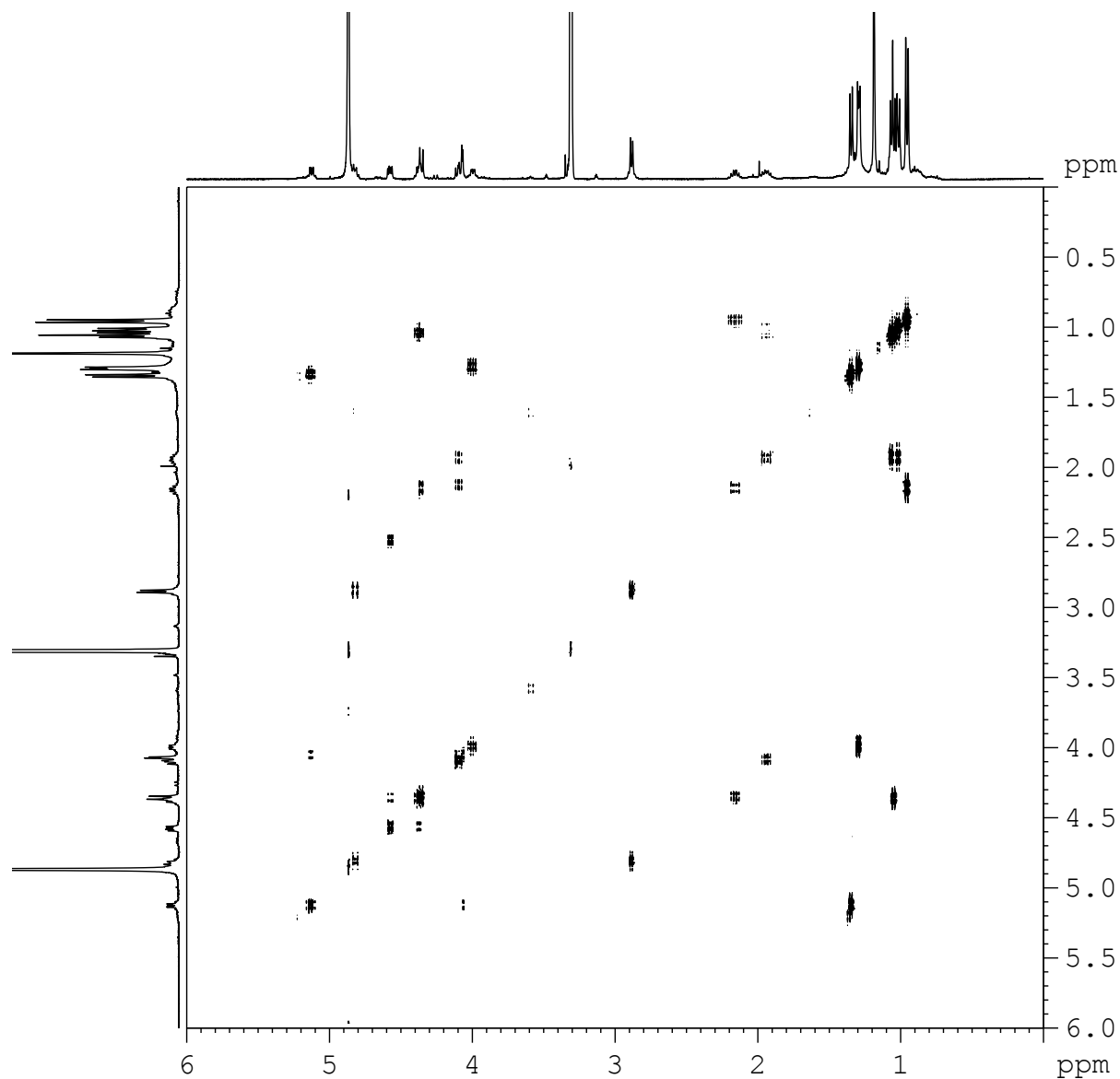
==== CHANNEL f1 =====
NUC1 1H
P1 8.75 usec
p2 17.50 usec
PL1 -3.00 dB
SFO1 400.1312004 MHz

==== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPX1 0 %
GPX2 0 %
GPY1 0 %
GPY2 0 %
GPZ1 10.00 %
GPZ2 20.00 %
P16 1500.00 usec

F1 - Acquisition parameters
TD 256
SFO1 400.1312 MHz
FIDRES 9.378188 Hz
SW 6.000 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 2048
SF 400.1300078 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 256
MC2 States-TPPI
SF 400.1300078 MHz
WDW
SSB 0
LB 0 Hz
GB 0



Cyclic depsipeptide (17) HSQC

```

Current Data Parameters
NAME          JC377hsqc
EXPNO         3
PROCNO        1

F2 - Acquisition Parameters
Date_         20090627
Time          2.07
INSTRUM       spect
PROBHD        5 mm BBI 1H-5B
PULPROG       invietqpsi
TD            4096
SOLVENT       CDCl3
NS            64
DS            8
SWH           4006.410 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG            1625.5
DW           124.800 usec
DE            6.00 usec
TE            300.0 K
CNST2         140.000000
d0            0.00000300 sec
D1            1.29999995 sec
d4            0.00178571 sec
d11           0.03000000 sec
d13           0.00000400 sec
D16           0.00015000 sec
D24           0.00178500 sec
DELTA         0.00172350 sec
DELTA1        0.00165800 sec
INO           0.00003549 sec
MCREST        0 sec
MCWRK         0.21666709 sec
ST1CNT        0

===== CHANNEL f1 =====
NUC1           1H
P1             8.75 usec
P2            17.50 usec
P28           0.50 usec
PL1           -3.00 dB
SFO1          400.1318006 MHz

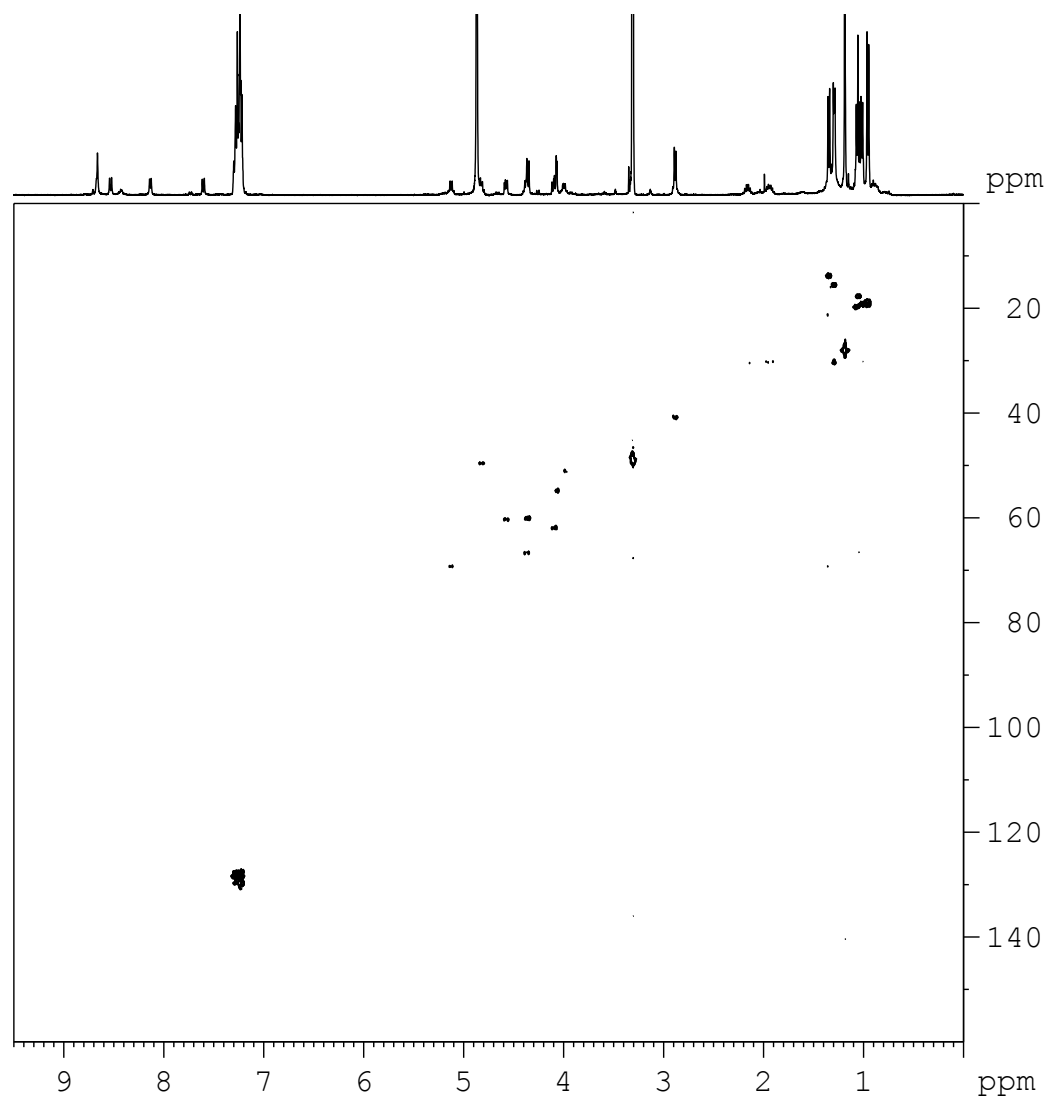
===== CHANNEL f2 =====
CPDPRG2       garp
NUC2           13C
P3            12.00 usec
P4            24.00 usec
PCPD2         70.00 usec
PL2           -6.00 dB
PL12          10.70 dB
SFO2          100.6197719 MHz

===== GRADIENT CHANNEL =====
GPNAM1        sine.100
GPNAM2        sine.100
GPX1          0 %
GPX2          0 %
GPY1          0 %
GPY2          0 %
GPZ1          80.00 %
GPZ2          20.10 %
P16           1500.00 usec

F1 - Acquisition parameters
TD            512
SFO1          100.6198 MHz
FIDRES        27.518492 Hz
SW            140.027 ppm
FnMODE        Echo-Antiecho

F2 - Processing parameters
SI            1024
SF            400.1300073 MHz
WDW           SINE
SSB           1
LB            0 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI            512
MC2           echo-antiecho
SF            100.6126510 MHz
WDW           SSB
SSB           1
LB            0 Hz
GB            0
    
```



Cyclic depsipeptide (17) HMBC

Current Data Parameters
 Date 20090627
 NAME JC377hsqc
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date 20090627
 Time 18.53
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG inv4gpgplrndf
 TD 4096
 SOLVENT MeOH
 NS 64
 DS 16
 SWH 4006.410 Hz
 FIDRES 0.978127 Hz
 AQ 0.5112308 sec
 RG 2048
 DW 124.800 usec
 DE 6.00 usec
 TE 300.0 K
 CNST2 140.0000000
 d0 0.00000300 sec
 D1 1.29999995 sec
 d2 0.00357143 sec
 D6 0.07200000 sec
 d13 0.00000400 sec
 D16 0.00015000 sec
 IN0 0.00002485 sec
 MCREST 0 sec
 MCWRK 1.29999995 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 8.75 usec
 p2 17.50 usec
 PL1 -3.00 dB
 SFO1 400.1318000 MHz

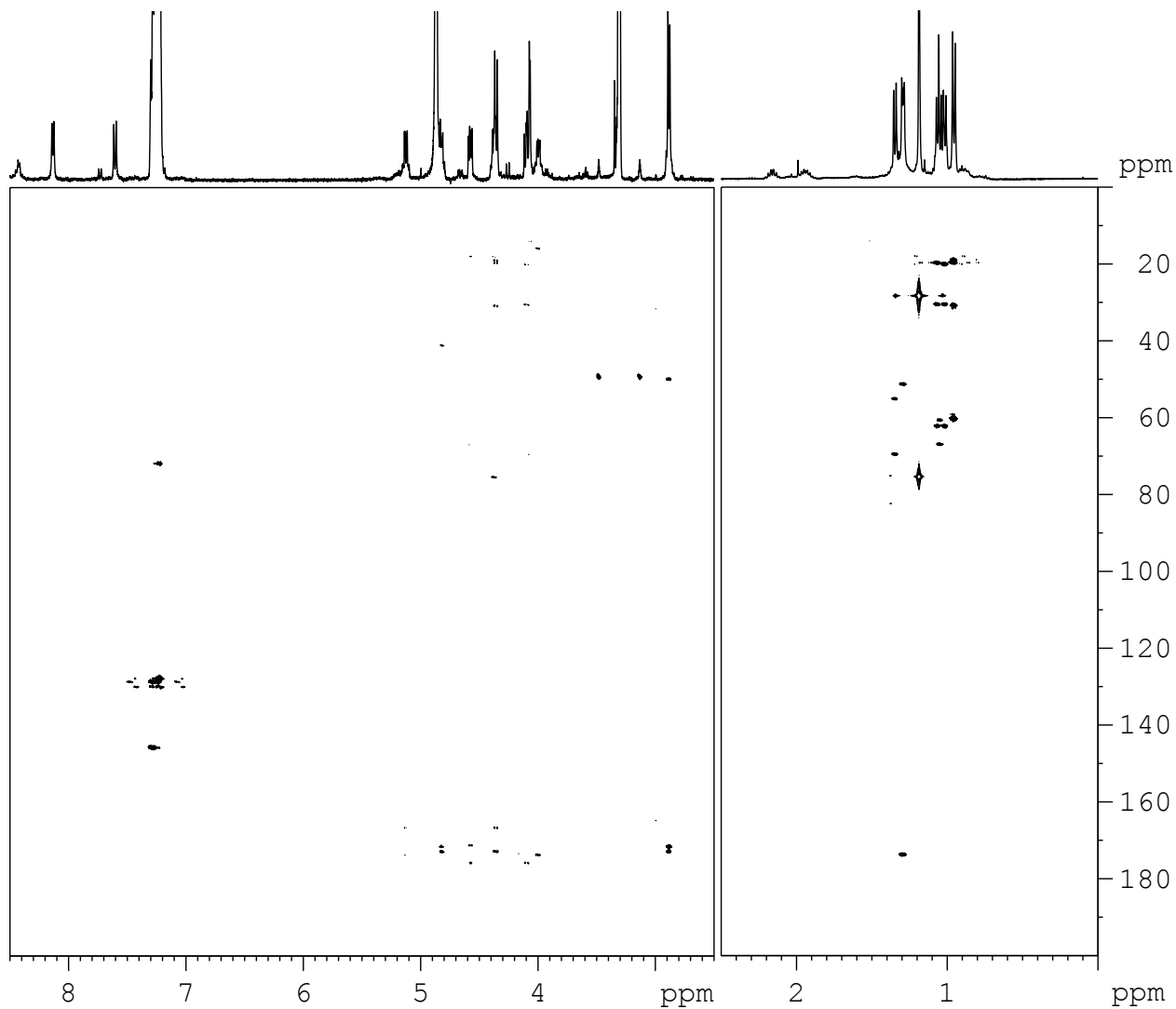
==== CHANNEL f2 =====
 NUC2 13C
 P3 12.00 usec
 PL2 -6.00 dB
 SFO2 100.6227903 MHz

==== GRADIENT CHANNEL =====
 GPNAM1 sine.100
 GPNAM2 sine.100
 GPNAM3 sine.100
 GPX1 0 %
 GPX2 0 %
 GPX3 0 %
 GPY1 0 %
 GPY2 0 %
 GPY3 0 %
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1500.00 usec

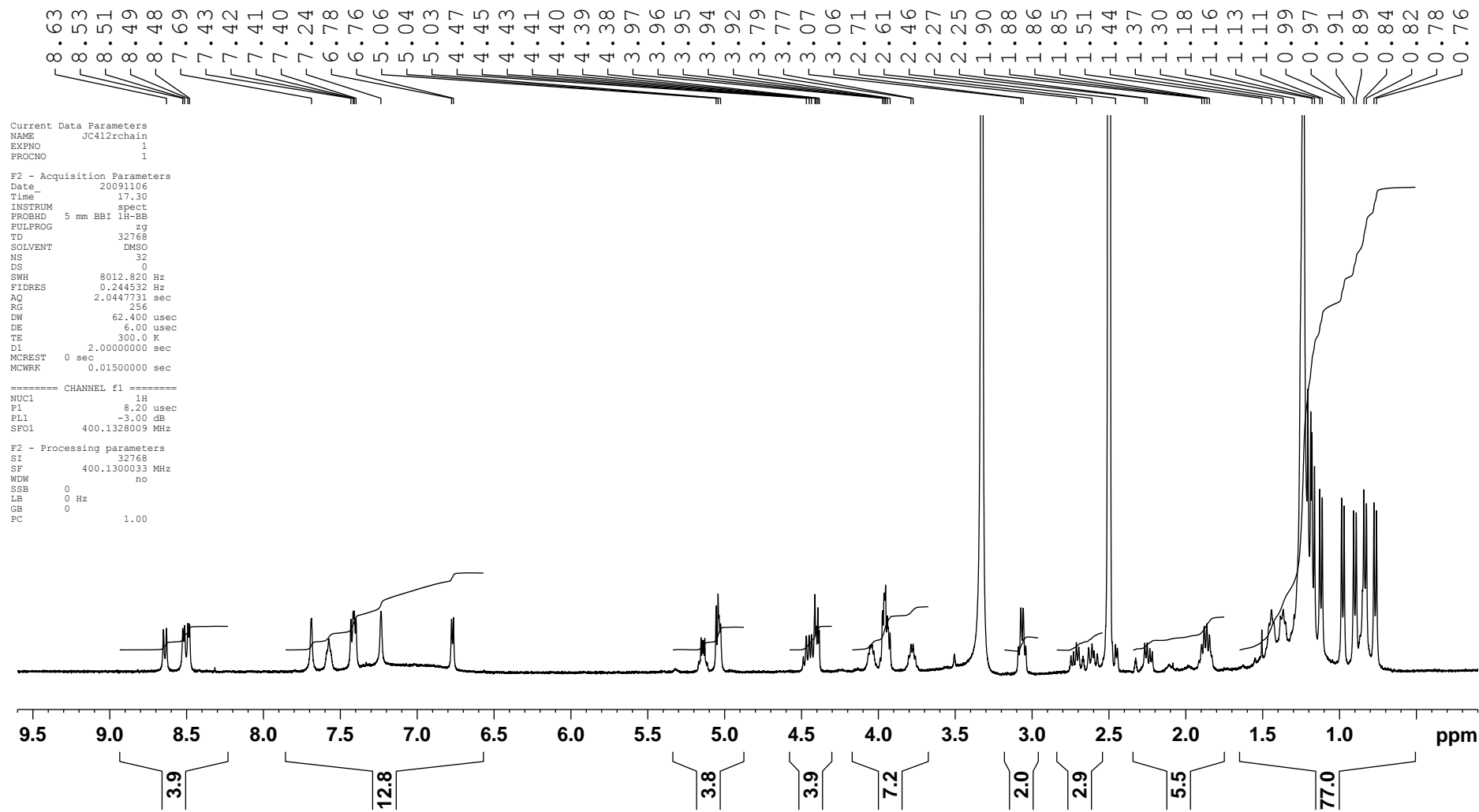
F1 - Acquisition parameters
 TD 512
 SFO1 100.6228 MHz
 FIDRES 39.298290 Hz
 SW 199.962 ppm
 FMODE QF

F2 - Processing parameters
 SI 4096
 SF 400.1300078 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 100.6126295 MHz
 WDW States
 SSB 2
 LB 0 Hz
 GB 0



Cyclic depsipeptide (22)



Cyclic depsipeptide (22) COSY

Current Data Parameters
NAME JC398DMS01b
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090918
Time 18.36
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG cosygpgf
TD 4096
SOLVENT CDCl3
NS 128
DS 16
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 1024
DW 124.800 usec
DE 6.00 usec
TE 300.0 K
d0 0.00000300 sec
D1 2.00000000 sec
d13 0.00000400 sec
D16 0.00015000 sec
IN0 0.00024988 sec
MCREST 0 sec
MCWRK 2.00000000 sec

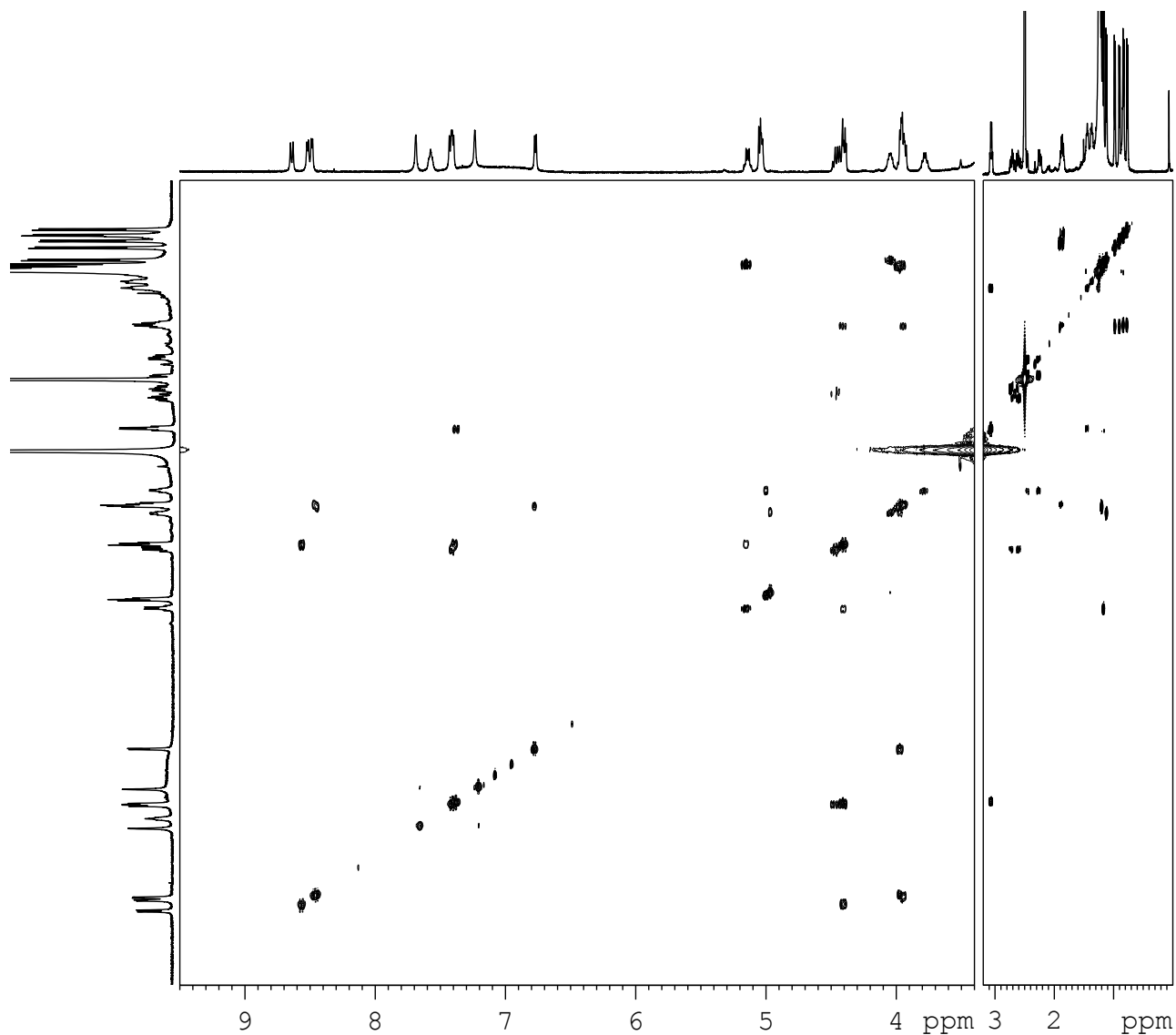
===== CHANNEL f1 =====
NUC1 1H
P0 5.30 usec
P1 5.30 usec
PL1 -3.00 dB
SFO1 400.2099789 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0 %
GPX2 0 %
GPY1 0 %
GPY2 0 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1500.00 usec

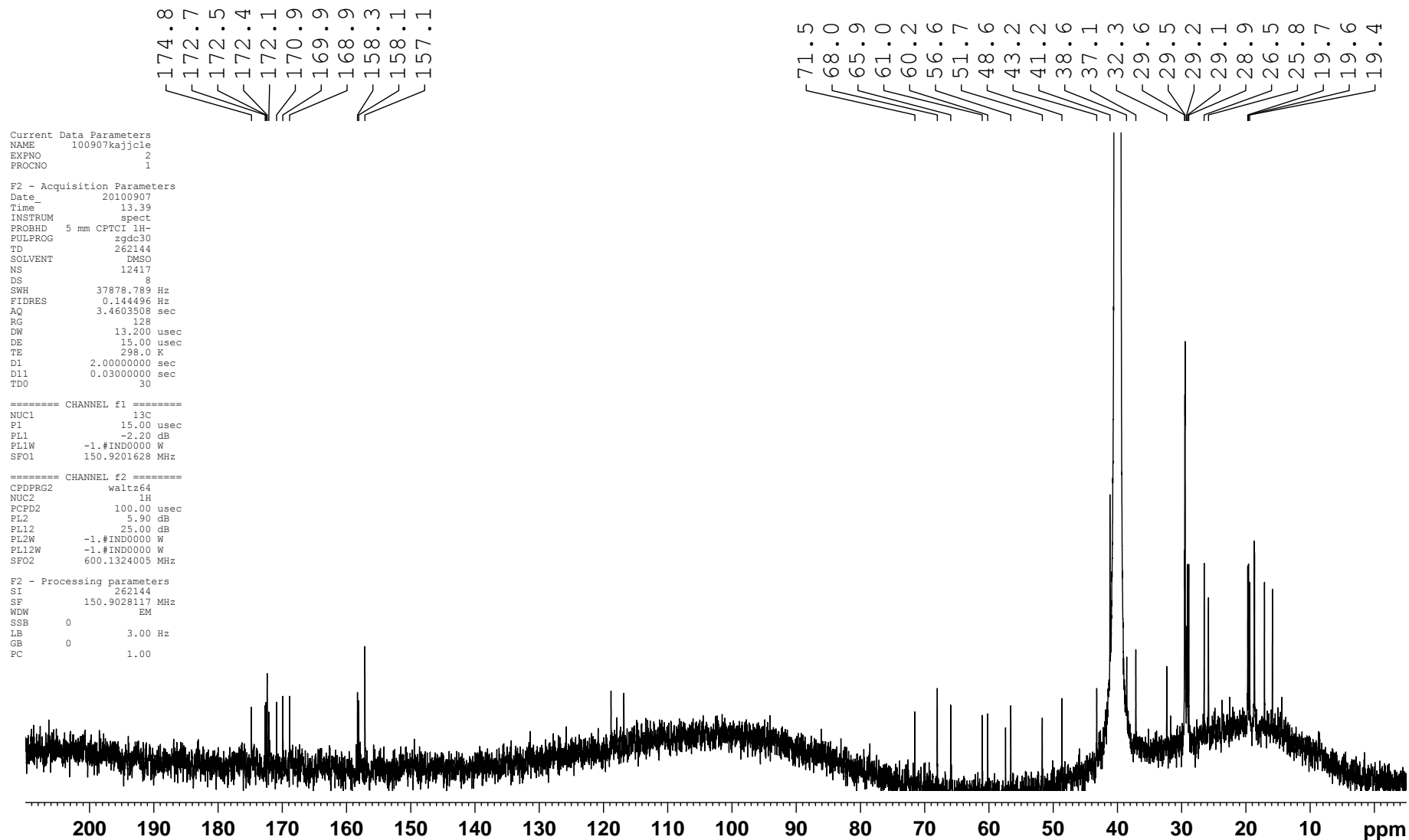
F1 - Acquisition parameters
TD 128
SFO1 400.21 MHz
FIDRES 31.265633 Hz
SW 10.000 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 400.2081745 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.2081743 MHz
WDW States
SSB 0
LB 0 Hz
GB 0



Cyclic depsipeptide (22)



Cyclic depsipeptide (22) HSQC

Current Data Parameters
NAME JC398403DMSOHMBC
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090929
Time_ 19.08
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG invietcpai
TD 2948
SOLVENT DMSO
NS 256
DS 8
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 4096
DW 124.800 usec
DE 6.00 usec
TE 300.0 K
CNS2 145.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d4 0.00172414 sec
d11 0.03000000 sec
d13 0.00000400 sec
D16 0.00015000 sec
D24 0.00172000 sec
DELTA 0.00171660 sec
DELTA1 0.00165800 sec
IN0 0.00004140 sec
MCREST 0 sec
MCWRK 0.33333400 sec
STICW 0

===== CHANNEL f1 =====
NUC1 1H
P1 5.30 usec
p2 10.60 usec
P28 2000.00 usec
PL1 -3.00 dB
SFO1 400.2099789 MHz

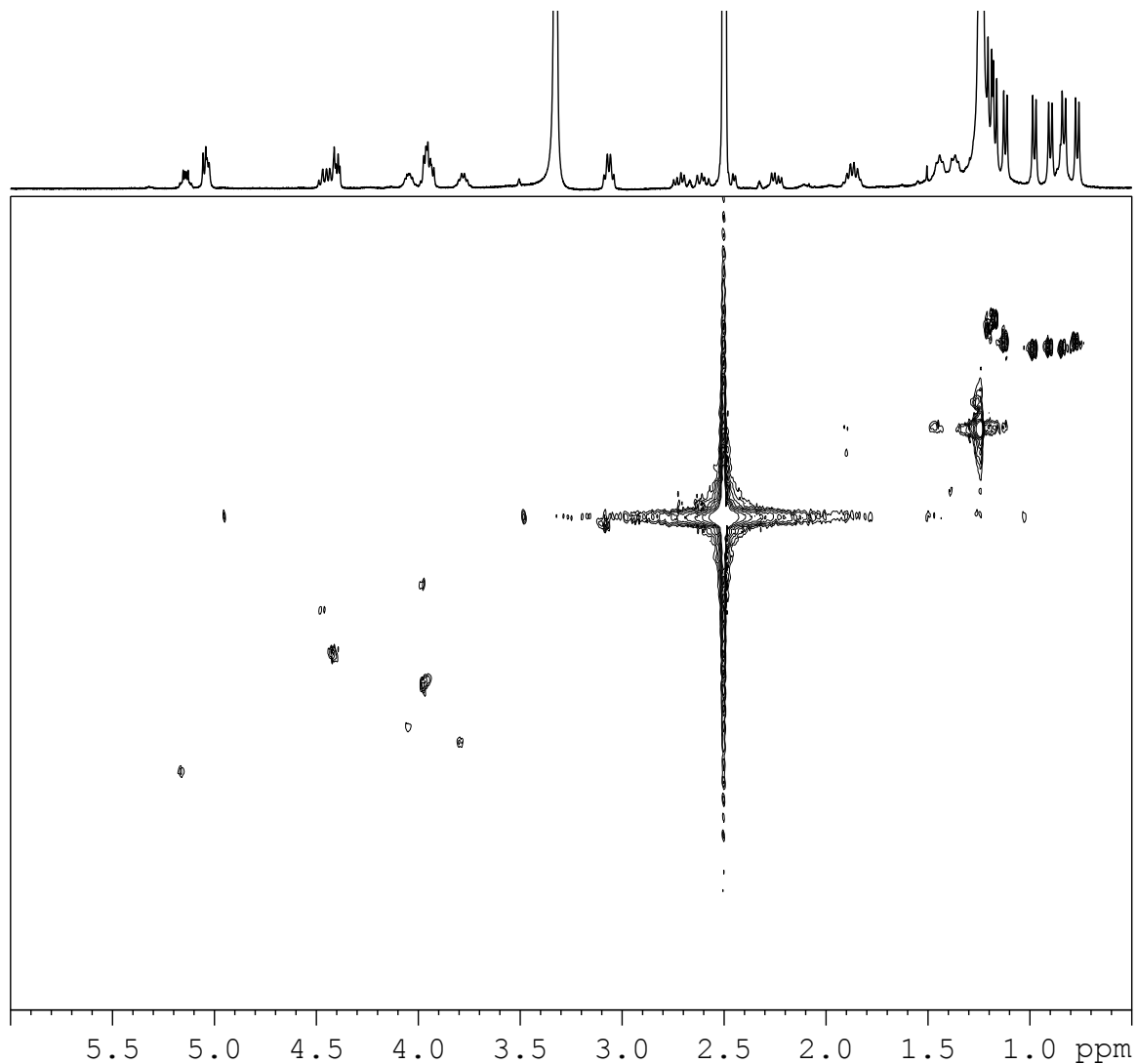
===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 12.00 usec
p4 24.00 usec
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 10.48 dB
SFO2 100.6374576 MHz

===== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPX1 0 %
GPX2 0 %
GPY1 0 %
GPY2 0 %
GPZ1 80.00 %
GPZ2 20.10 %
P16 1500.00 usec

F1 - Acquisition parameters
TD 110
SFO1 100.6375 MHz
FIDRES 109.793587 Hz
SW 120.008 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 2048
SF 400.2081751 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 512
MC2 echo-antiecho
SF 100.6325017 MHz
WDW SSB
LB 0 Hz
GB 0



Cyclic depsipeptide (22) HMBC

```

Current Data Parameters
NAME JC398403DMSOHMBC
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090929
Time 18.08
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG invietgpsi
TD 2048
SOLVENT DMSO
NS 256
DS 8
SWH 4006.410 Hz
FIDRES 1.986255 Hz
AQ 0.2556404 sec
RG 4096
DW 124.800 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
d0 0.00000300 sec
d1 2.00000000 sec
d4 0.00172414 sec
d11 0.03000000 sec
d13 0.00000400 sec
d16 0.00015000 sec
D24 0.00172000 sec
DELTA 0.00171660 sec
DELTA1 0.00165800 sec
IN0 0.00004140 sec
MCREST 0 sec
MCWRK 0.33333400 sec
STICNT 0

===== CHANNEL f1 =====
NUC1 1H
P1 5.30 usec
p2 10.60 usec
P28 2000.00 usec
PL1 -3.00 dB
SFO1 400.2099789 MHz

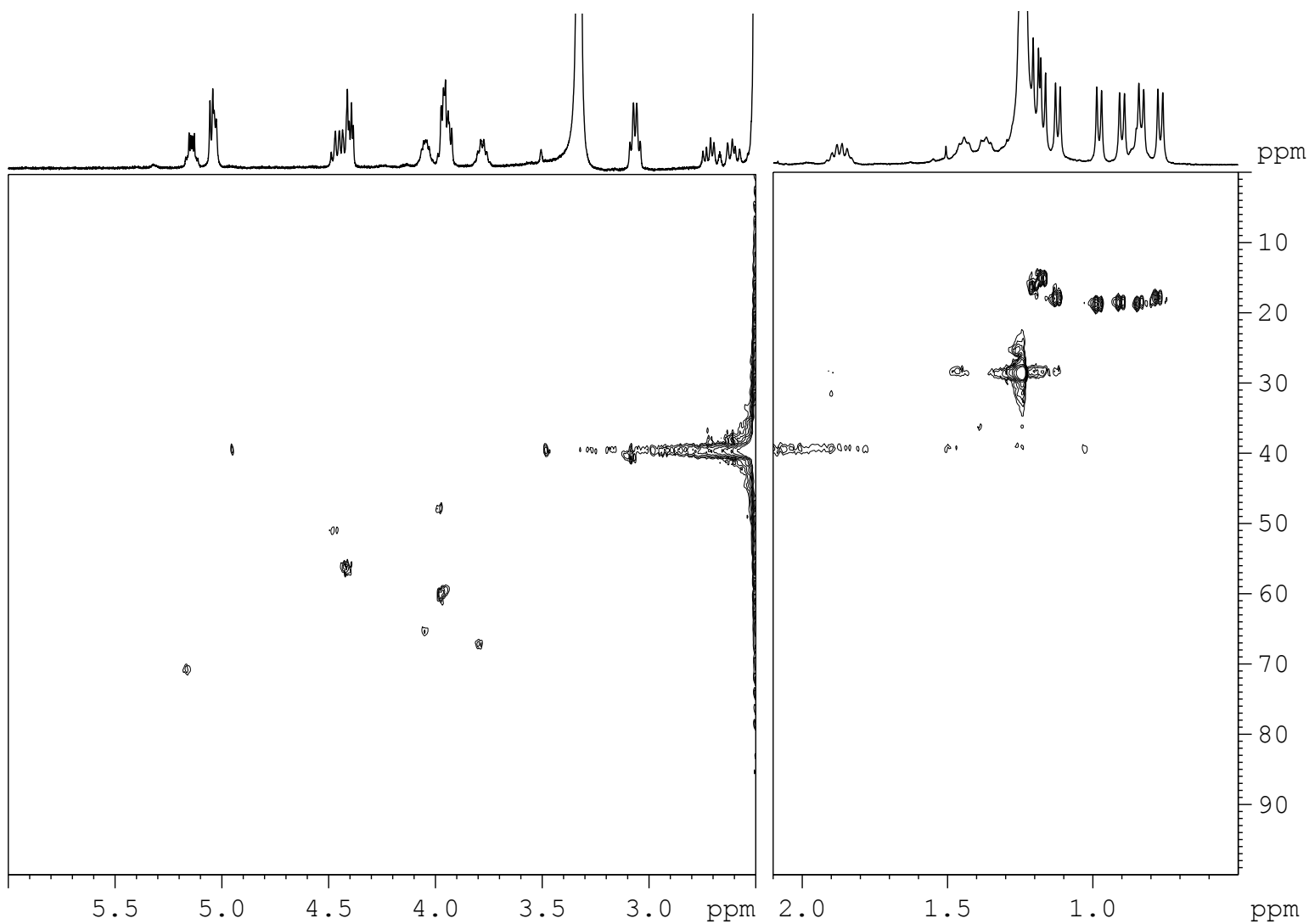
===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 12.00 usec
p4 24.00 usec
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 10.48 dB
SFO2 100.6374576 MHz

===== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPX1 0 %
GPX2 0 %
GPF1 0 %
GPY2 0 %
GPZ1 80.00 %
GPZ2 20.10 %
F16 1500.00 usec

F1 - Acquisition parameters
TD 110
SFO1 100.6375 MHz
FIDRES 109.793587 Hz
SW 120.008 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 2048
SF 400.2081751 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 512
MC2 echo-antiecho
SF 100.6325017 MHz
WDW
SSB 2
LB 0 Hz
GB 0
    
```



Cyclic depsipeptide (22) HMBC

```

Current Data Parameters
NAME      JC398403DMSORHMC
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20091002
Time      16.53
INSTRUM   spect
PROBHD    5 mm BBI 1H-BB
PULPROG   inv4gpplrndgf
TD        4096
SOLVENT   DMSO
NS        512
DS        8
SWH       4006.410 Hz
FDRRES    0.978127 Hz
AQ        0.5112308 sec
RG        11585.3
DW        124.800 usec
DE        6.00 usec
TE        300.0 K
CNST2    145.0000000
d0        0.00000300 sec
D1        2.00000000 sec
d2        0.00044828 sec
D6        0.06250000 sec
d13       0.00000400 sec
D16       0.00015000 sec
IN0       0.00002259 sec
MCREST    0 sec
MCWRK     2.00000000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        5.30 usec
p2        10.60 usec
PL1       -3.00 dB
SFO1      400.2099789 MHz

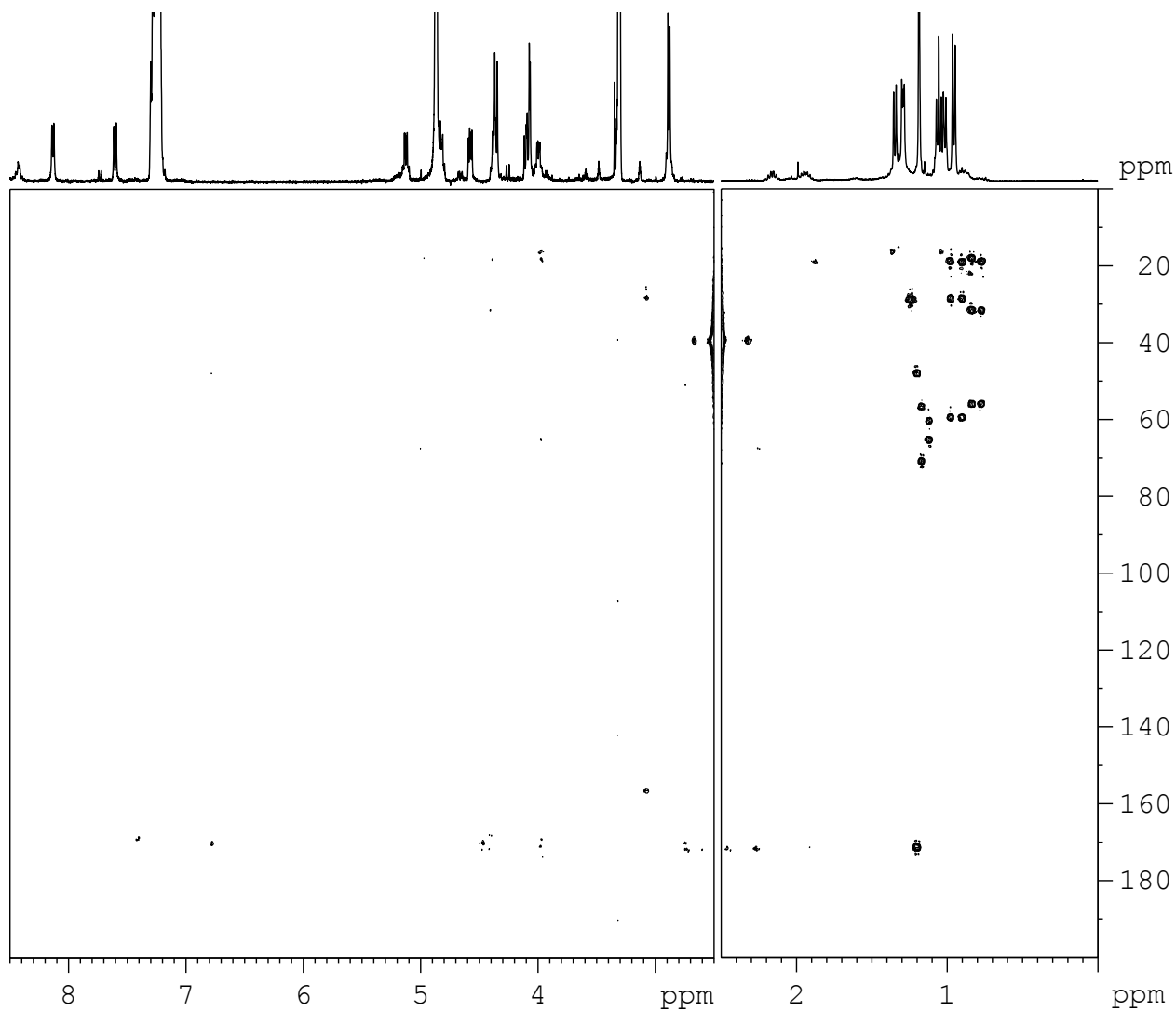
===== CHANNEL f2 =====
NUC2      13C
P3        12.00 usec
PL2       -6.00 dB
SFO2      100.6424892 MHz

===== GRADIENT CHANNEL =====
GPNAM1    sine.100
GPNAM2    sine.100
GPNAM3    sine.100
GPX1      0 %
GPX2      0 %
GPX3      0 %
GPY1      0 %
GPY2      0 %
GPY3      0 %
GPZ1      50.00 %
GPZ2      30.00 %
GPZ3      40.10 %
P16       1500.00 usec

F1 - Acquisition parameters
TD        240
SFO1      100.6425 MHz
FDRRES    92.233902 Hz
SW        219.948 ppm
F1MODE    QF

F2 - Processing parameters
SI        2048
SF        400.2081767 MHz
WDW       SINE
SSB       2
LB        0 Hz
GB        0
PC        1.00

F1 - Processing parameters
SI        1024
MC2       QF
SF        100.6324924 MHz
WDW       States
SSB       2
LB        0 Hz
GB        0
    
```



Cyclic depsipeptide (22) HMBC

```
Current Data Parameters
NAME JC398403DMSOHRMBC
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date 20091002
Time 16.53
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG inv4gpplrndqf
TD 4096
SOLVENT DMSO
NS 512
DS 8
SWH 4006.410 Hz
FIDRES 0.378127 Hz
AQ 0.5112308 sec
RG 11585.3
DW 124.800 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
d0 0.00000300 sec
d1 2.00000000 sec
d2 0.00344828 sec
d6 0.06250000 sec
d13 0.00000400 sec
d16 0.00015000 sec
IN0 0.00002259 sec
MCREST 0 sec
MCWRK 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 5.30 usec
p2 10.60 usec
PL1 -3.00 dB
SFO1 400.2099789 MHz

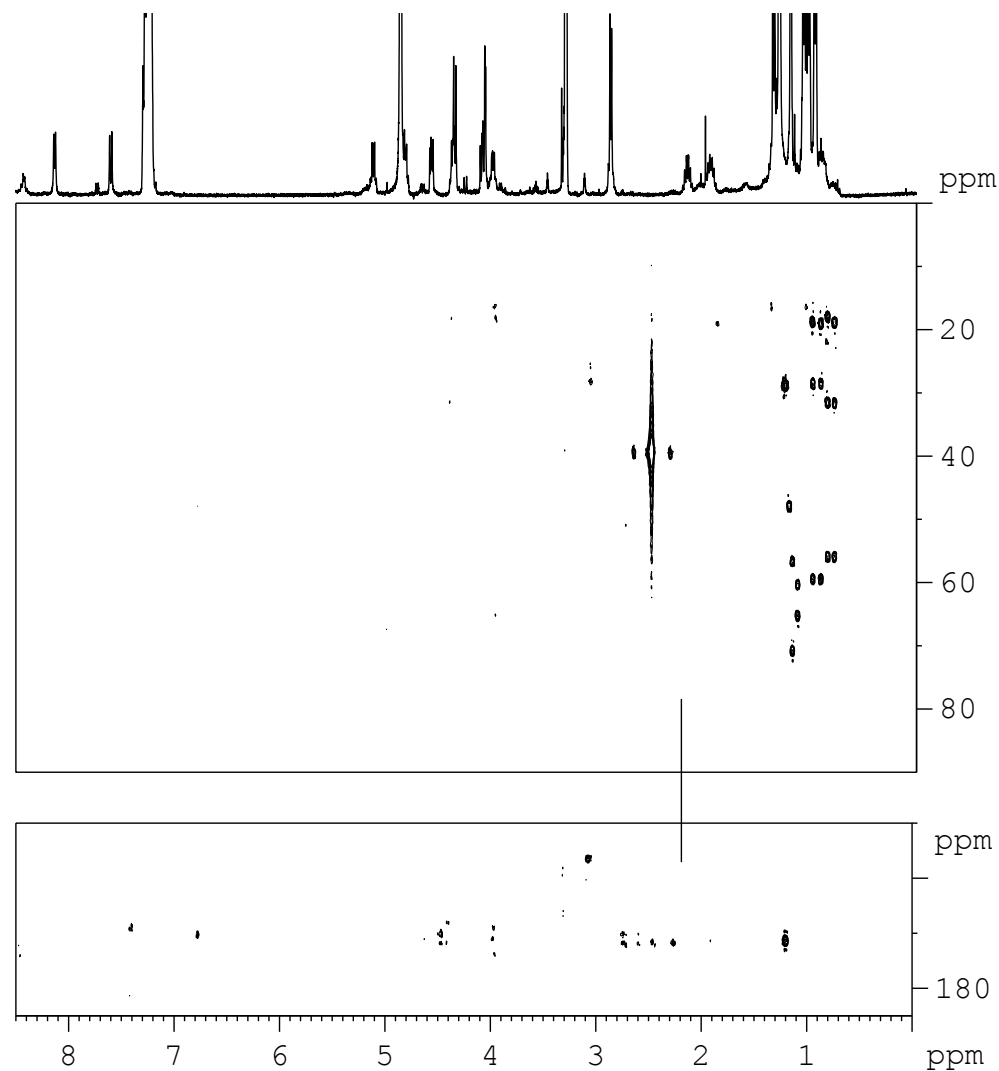
===== CHANNEL f2 =====
NUC2 13C
P3 12.00 usec
PL2 -6.00 dB
SFO2 100.6424892 MHz

===== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPX1 0 %
GPX2 0 %
GPX3 0 %
GPY1 0 %
GPY2 0 %
GPY3 0 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1500.00 usec

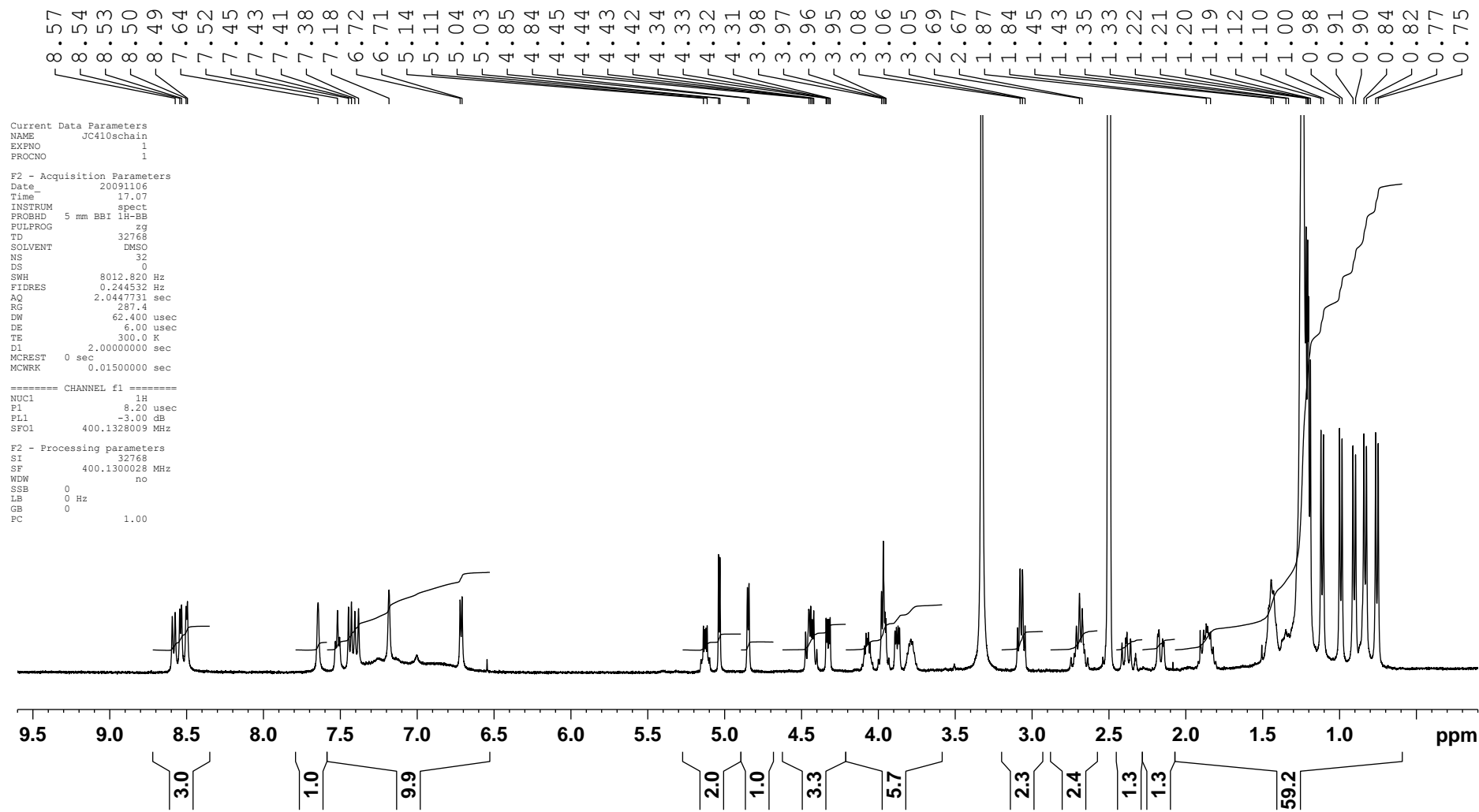
F1 - Acquisition parameters
TD 240
SFO1 100.6425 MHz
FIDRES 92.233902 Hz
SW 219.948 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 400.2081767 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6324924 MHz
WDW States
SSB 2
LB 0 Hz
GB 0
```



Cyclic depsipeptide (23)



Cyclic depsipeptide (23) COSY

Current Data Parameters
NAME EpimerS
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20090619
Time 21.13
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG cosygpmfph
TD 4096
SOLVENT MeOH
NS 64
DS 8
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 1625.5
DW 124.800 usec
DE 6.00 usec
TE 323.1 K
d0 0.00011452 sec
D1 2.00000000 sec
d13 0.00000400 sec
D16 0.00015000 sec
d20 0.00165400 sec
IN0 0.00024991 sec
MCREST 0 sec
MCWRK 1.00000000 sec
ST1CNT 0

===== CHANNEL f1 =====

NUC1 1H
P1 8.20 usec
p2 16.40 usec
PL1 -3.00 dB
SFO1 400.1318006 MHz

===== GRADIENT CHANNEL =====

GPNAM1 sine.100
GPNAM2 sine.100
GPX1 0 %
GPX2 0 %
GPY1 0 %
GPY2 0 %
GPZ1 10.00 %
GPZ2 20.00 %
P16 1500.00 usec

F1 - Acquisition parameters

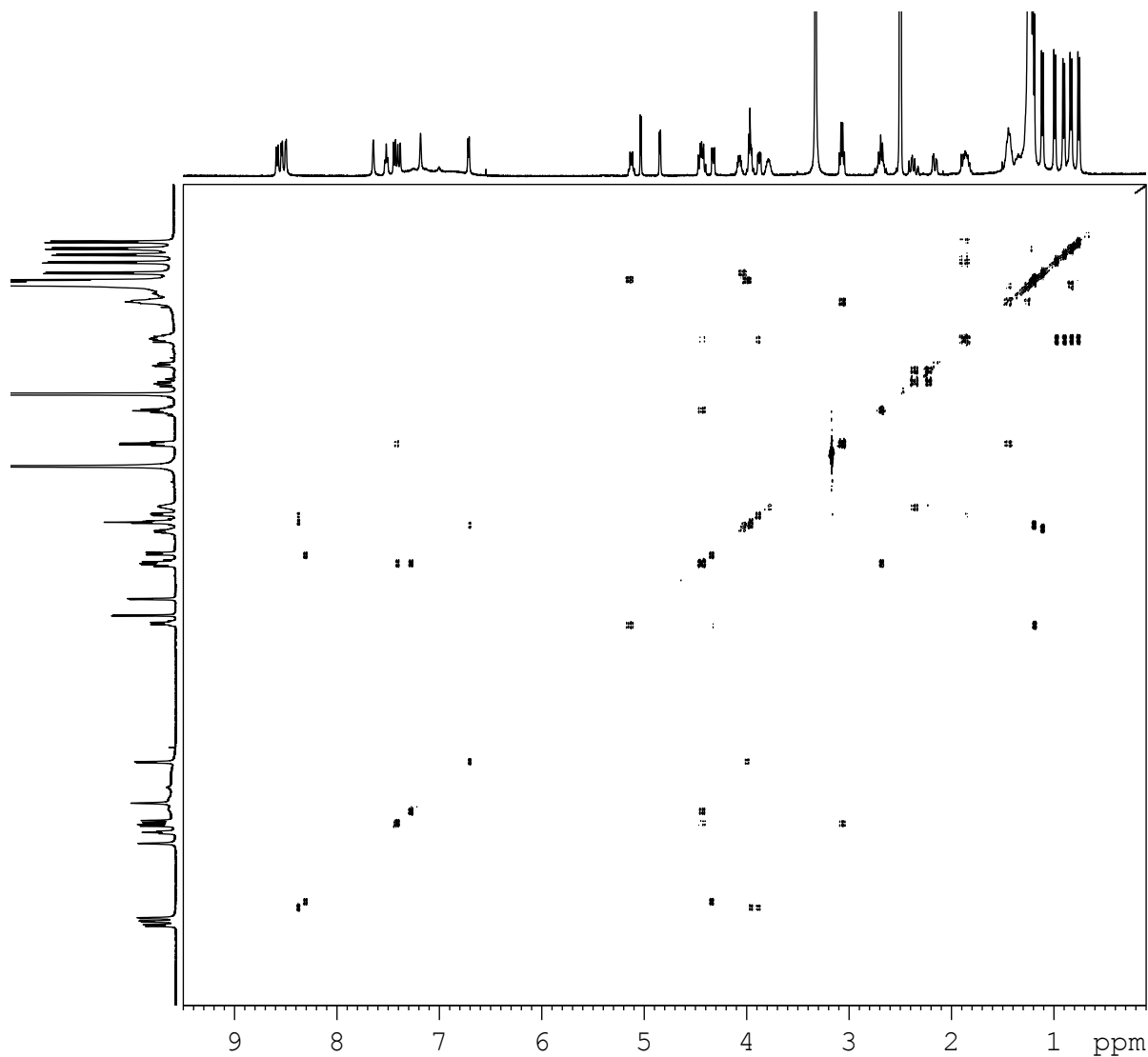
TD 256
SFO1 400.1318 MHz
FIDRES 15.630470 Hz
SW 10.000 ppm
FnMODE States-TPPI

F2 - Processing parameters

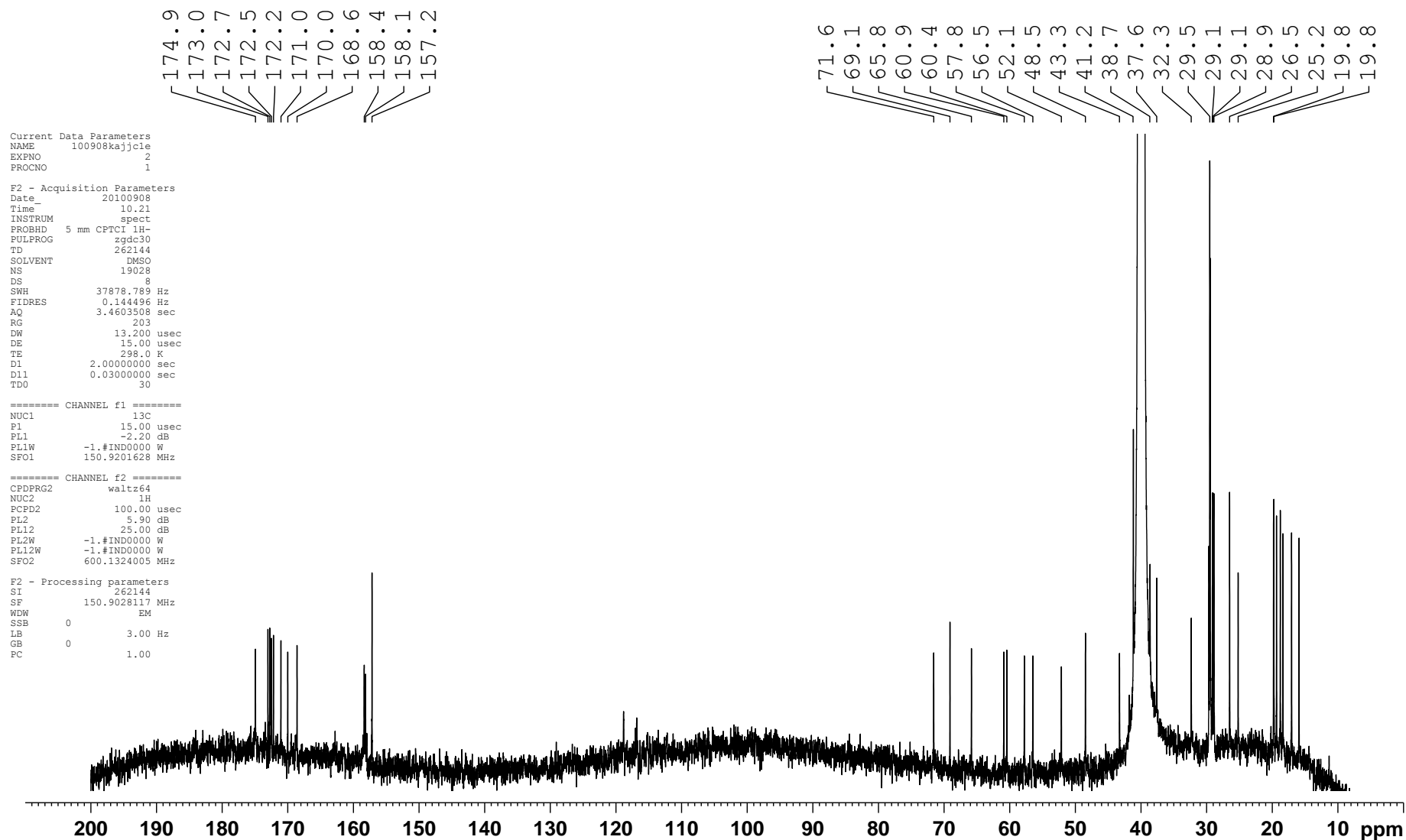
SI 4096
SF 400.1300130 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters

SI 1024
MC2 States-TPPI
SF 400.1300096 MHz
WDW
SSB 2
LB 0 Hz
GB 0



Cyclic depsipeptide (23)



Cyclic depsipeptide (23) HSQC

```

Current Data Parameters
NAME           EpimerS
EXPNO          3
PROCNO        1

F2 - Acquisition Parameters
Date_          20091009
Time           19.20
INSTRUM       spect
PROBHD        5 mm BBI 1H-5B
PULPROG       invietqpsi
TD             4096
SOLVENT       DMSO
NS             1024
DS             8
SWH           4006.410 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG            1024
DW            124.800 usec
DE            6.00 usec
TE            300.0 K
CNST2         140.0000000
d0            0.00000300 sec
D1            2.00000000 sec
d4            0.00178571 sec
d11           0.03000000 sec
d13           0.00000400 sec
D16           0.00015000 sec
D14           0.00178500 sec
DELTA         0.00172240 sec
DELTA1        0.00165800 sec
IN0           0.00004969 sec
MCREST        0 sec
MCWRK         0.33333400 sec
ST1CNT        0

===== CHANNEL f1 =====
NUC1           1H
P1             8.20 usec
P2            16.40 usec
P28           0.50 usec
PL1           -3.00 dB
SFO1          400.1318006 MHz

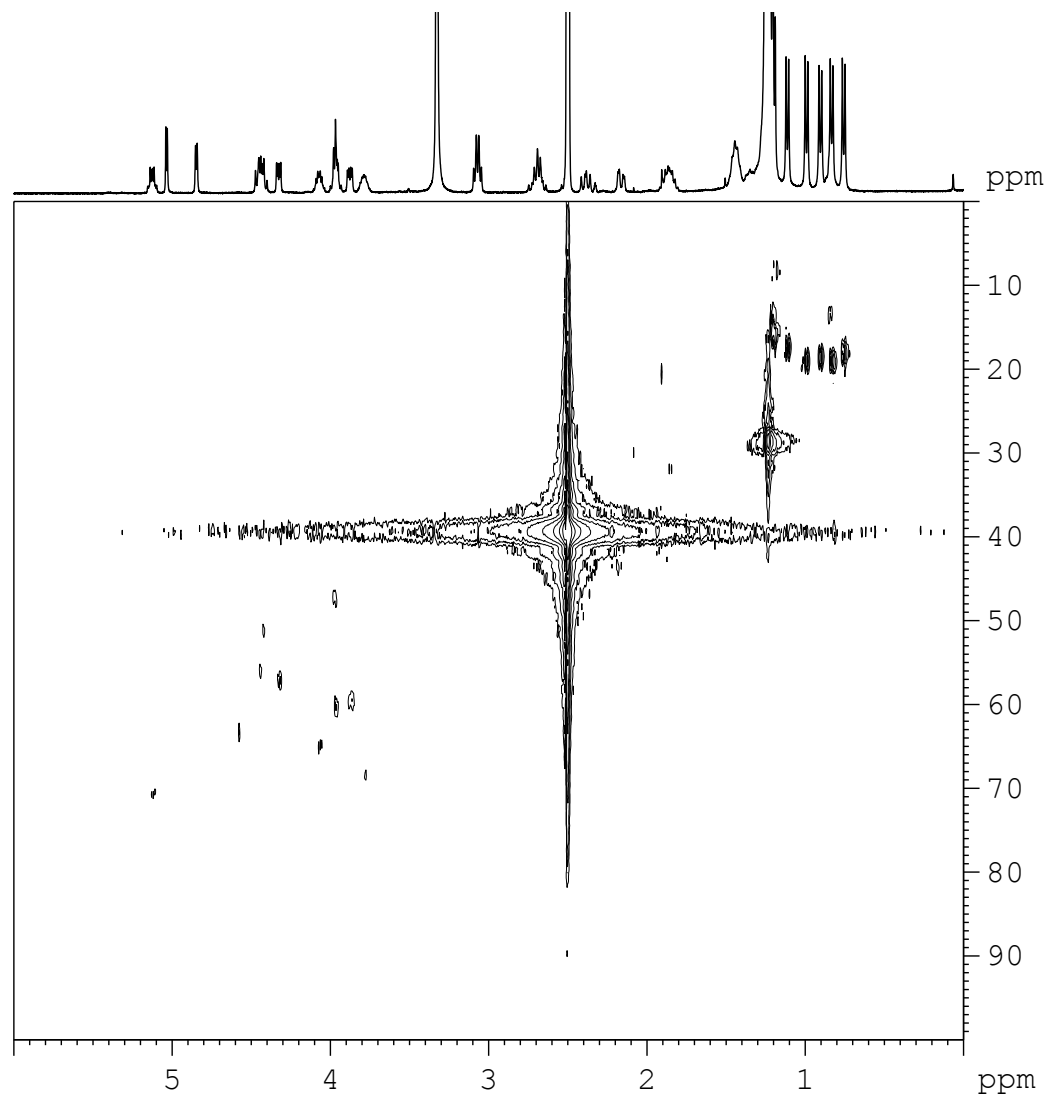
===== CHANNEL f2 =====
CPDPRG2       garp
NUC2           13C
P3            12.00 usec
P4            24.00 usec
PCPD2         70.00 usec
PL2           -6.00 dB
PL12          10.70 dB
SFO2          100.6172566 MHz

===== GRADIENT CHANNEL =====
GPNAM1        sine.100
GPNAM2        sine.100
GPX1          0 %
GPX2          0 %
GPY1          0 %
GPY2          0 %
GPZ1          80.00 %
GPZ2          20.10 %
P16           1500.00 usec

F1 - Acquisition parameters
TD            63
SFO1          100.6173 MHz
FIDRES        159.728455 Hz
SW            100.012 ppm
FnMODE        Echo-Antiecho

F2 - Processing parameters
SI            2048
SF            400.1299998 MHz
WDW           SINE
SSB           2
LB            0 Hz
GB            0
PC            1.00

F1 - Processing parameters
SI            512
MC2           echo-antiecho
SF            100.6128422 MHz
WDW           SINE
SSB           2
LB            0 Hz
GB            0
    
```



Cyclic depsipeptide (23) HMBC

```
Current Data Parameters
NAME JC410schain
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091120
Time 20.23
INSTRUM spect
PROBHD 5 mm BBI 1H-EB
PULPROG inv4gpllrndqf
TD 4096
SOLVENT DMSO
NS 1024
DS 8
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 2048
DW 124.800 usec
DE 6.00 usec
TE 300.0 K
CNST2 140.0000000
d0 0.00000300 sec
D1 1.20000005 sec
d2 0.00357143 sec
D6 0.10000000 sec
d13 0.00000400 sec
D16 0.00015000 sec
INV 0.00002485 sec
MCREST 0 sec
MCWRK 1.20000005 sec

===== CHANNEL f1 =====
NUC1 1H
P1 8.38 usec
p2 16.76 usec
PL1 -3.00 dB
SFO1 400.1320007 MHz

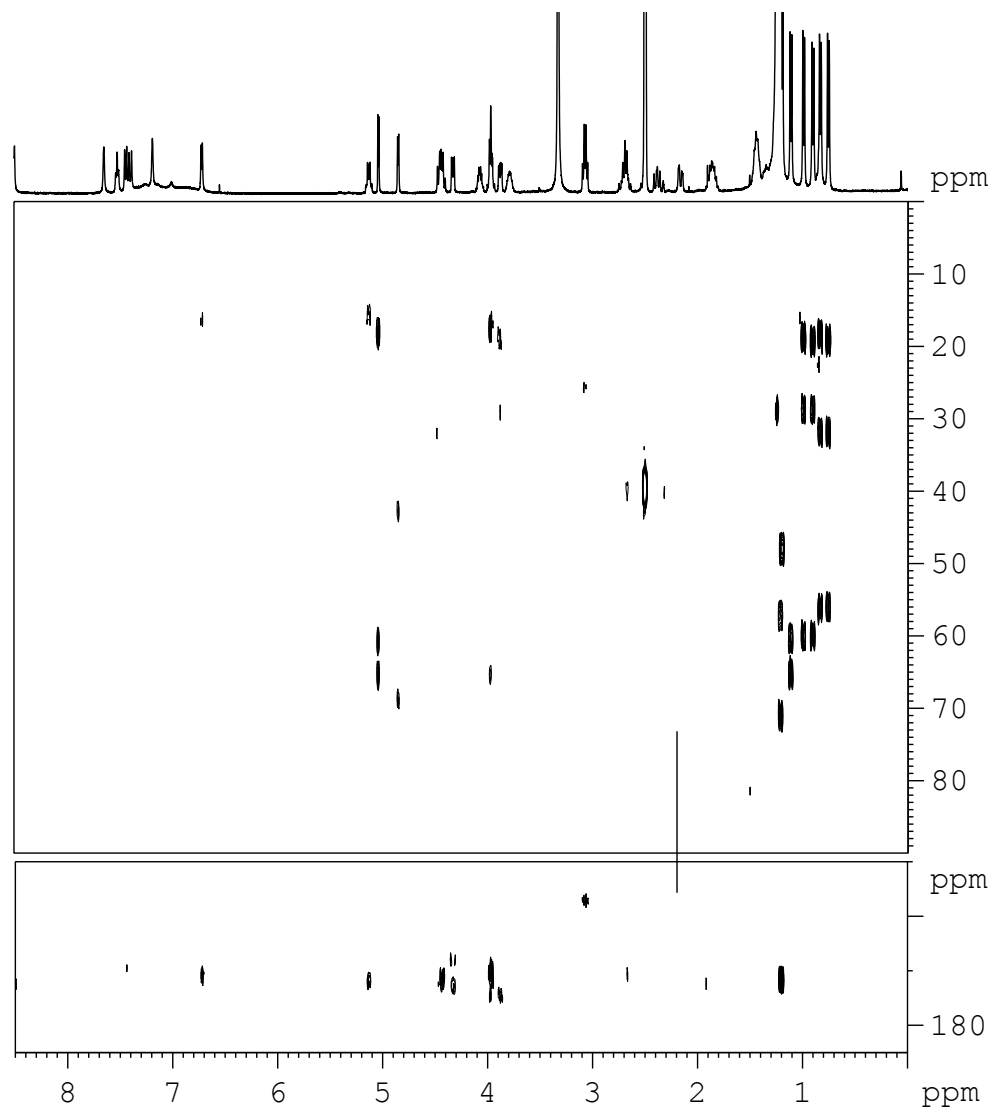
===== CHANNEL f2 =====
NUC2 13C
P3 12.60 usec
PL2 -6.00 dB
SFO2 100.6227903 MHz

===== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPX1 0 %
GPX2 0 %
GPX3 0 %
GPY1 0 %
GPY2 0 %
GPY3 0 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1500.00 usec

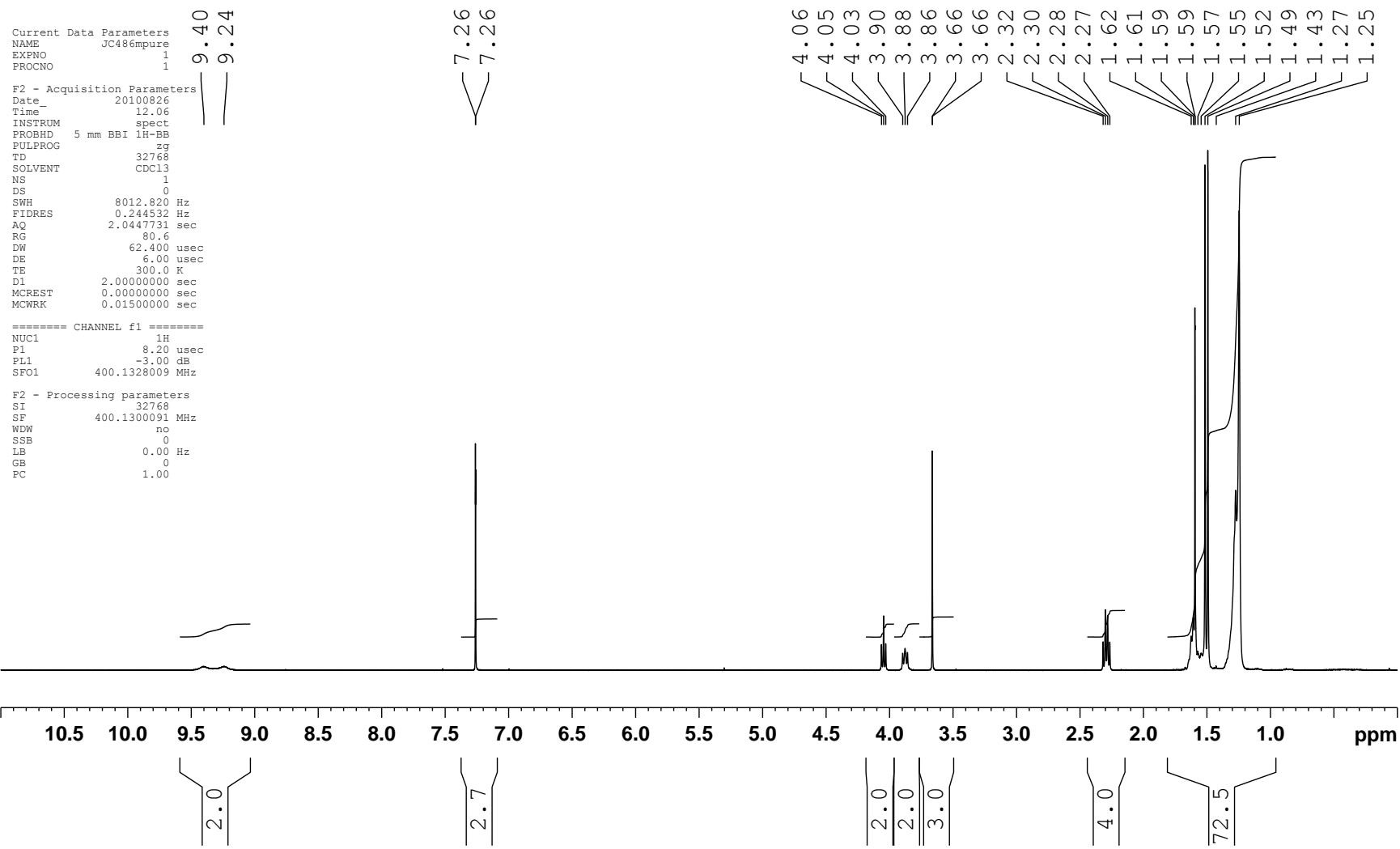
F1 - Acquisition parameters
TD 77
SFO1 100.6228 MHz
FIDRES 261.308105 Hz
SW 199.962 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 2048
MC2 QF
SF 100.6135390 MHz
WDW States-TFPI
SSB 0
LB 0 Hz
GB 0
```



1-Methyl-15-[bis(*tert*-Butoxycarbonyl)guanidino] pentadecanoate (15)



1-Methyl-15-[bis(*tert*-Butoxycarbonyl)guanidino] pentadecanoate (15)

```

Current Data Parameters
NAME          JC486m
EXPNO         3
PROCNO        1

F2 - Acquisition Parameters
Date_         20100823
Time          15.20
INSTRUM       spect
PROBHD        5 mm BBI 1H-BB
PULPROG       zgdc30
TD            65536
SOLVENT       C6D6
NS            3605
DS            0
SWH           26178.010 Hz
FIDRES        0.399445 Hz
AQ            1.2517875 sec
RG            512
DW            19.100 usec
DE            6.00 usec
TE            300.0 K
D1            1.00000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec
    
```

```

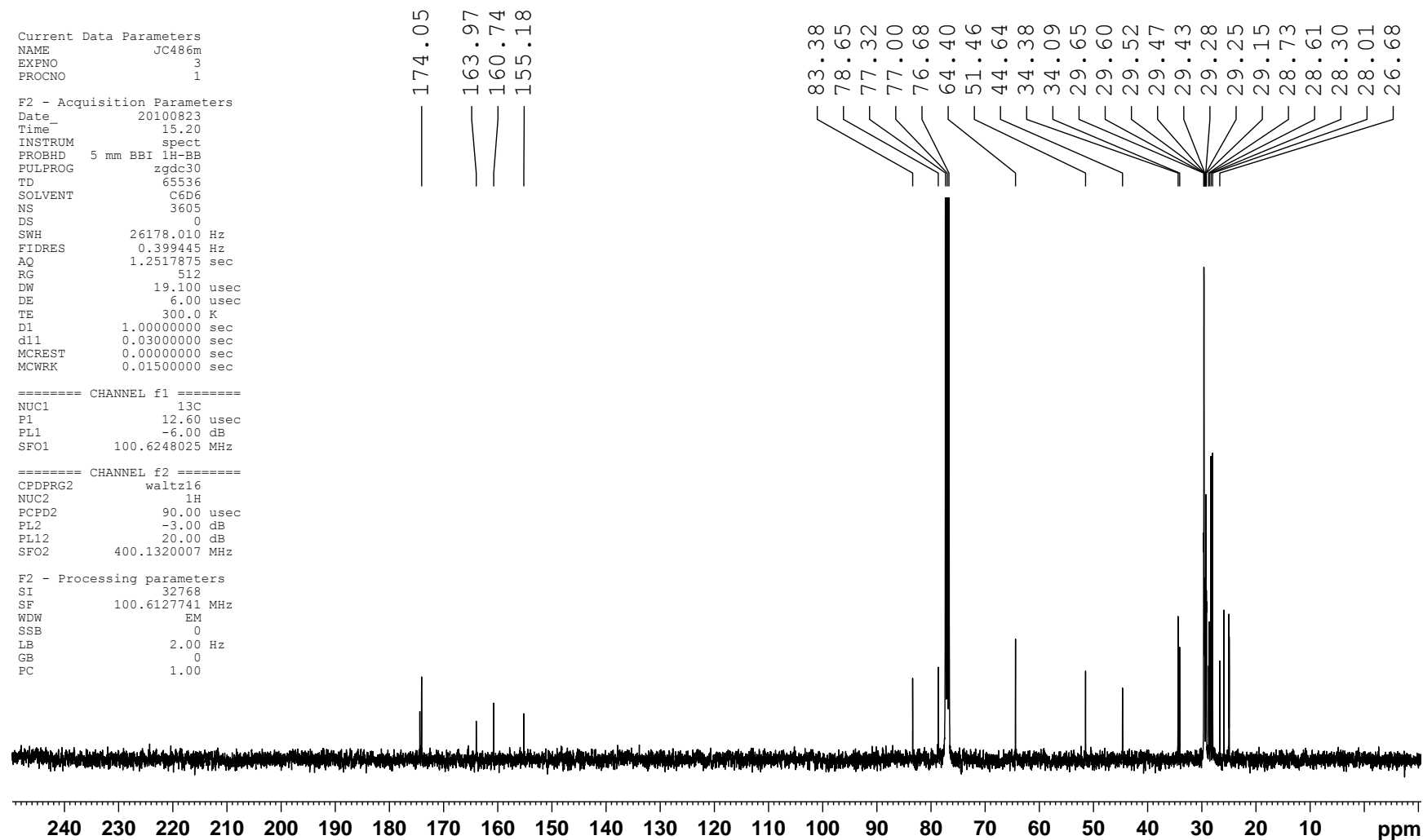
===== CHANNEL f1 =====
NUC1          13C
P1            12.60 usec
PL1           -6.00 dB
SFO1          100.6248025 MHz
    
```

```

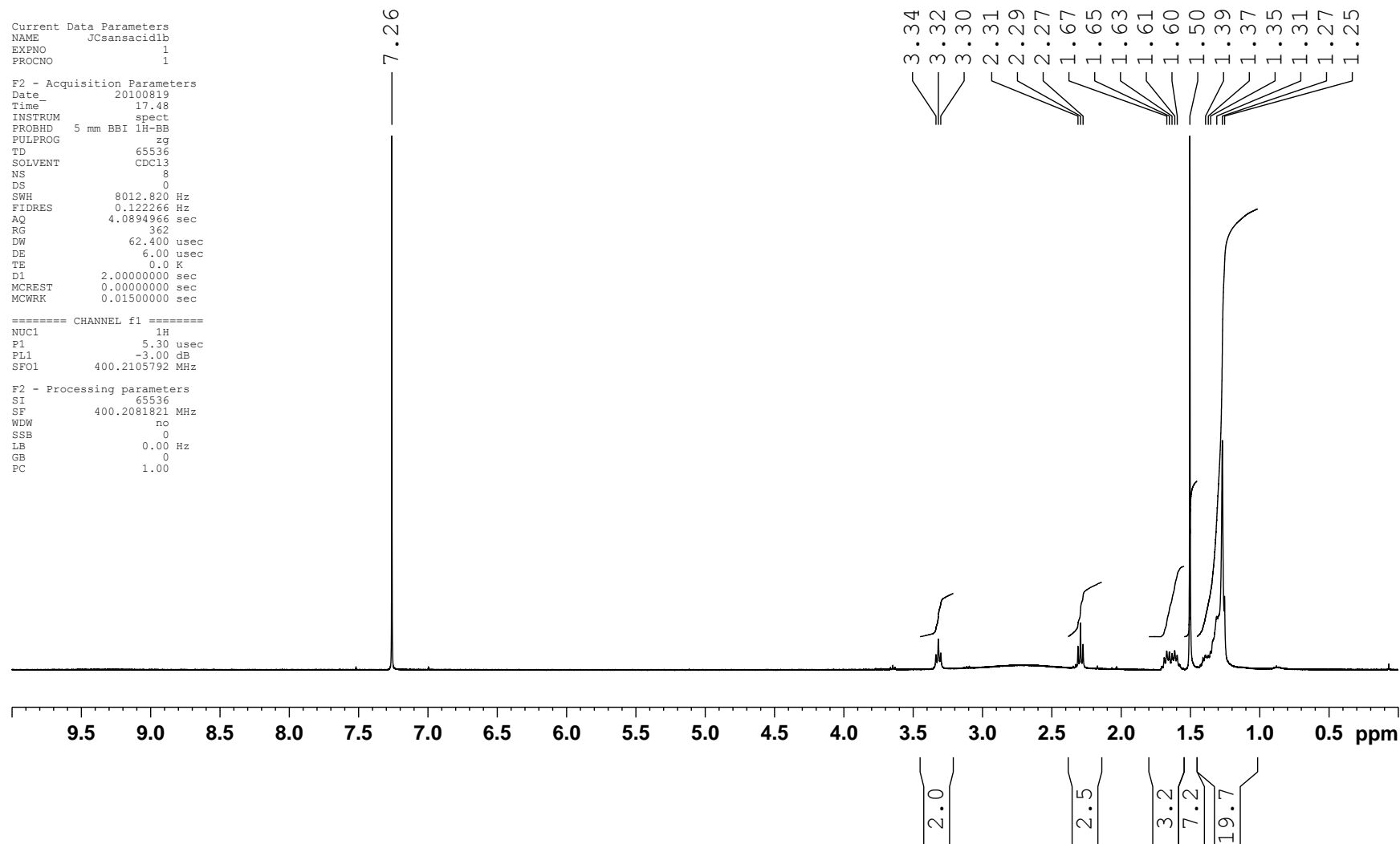
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         90.00 usec
PL2           -3.00 dB
PL12          20.00 dB
SFO2          400.1320007 MHz
    
```

```

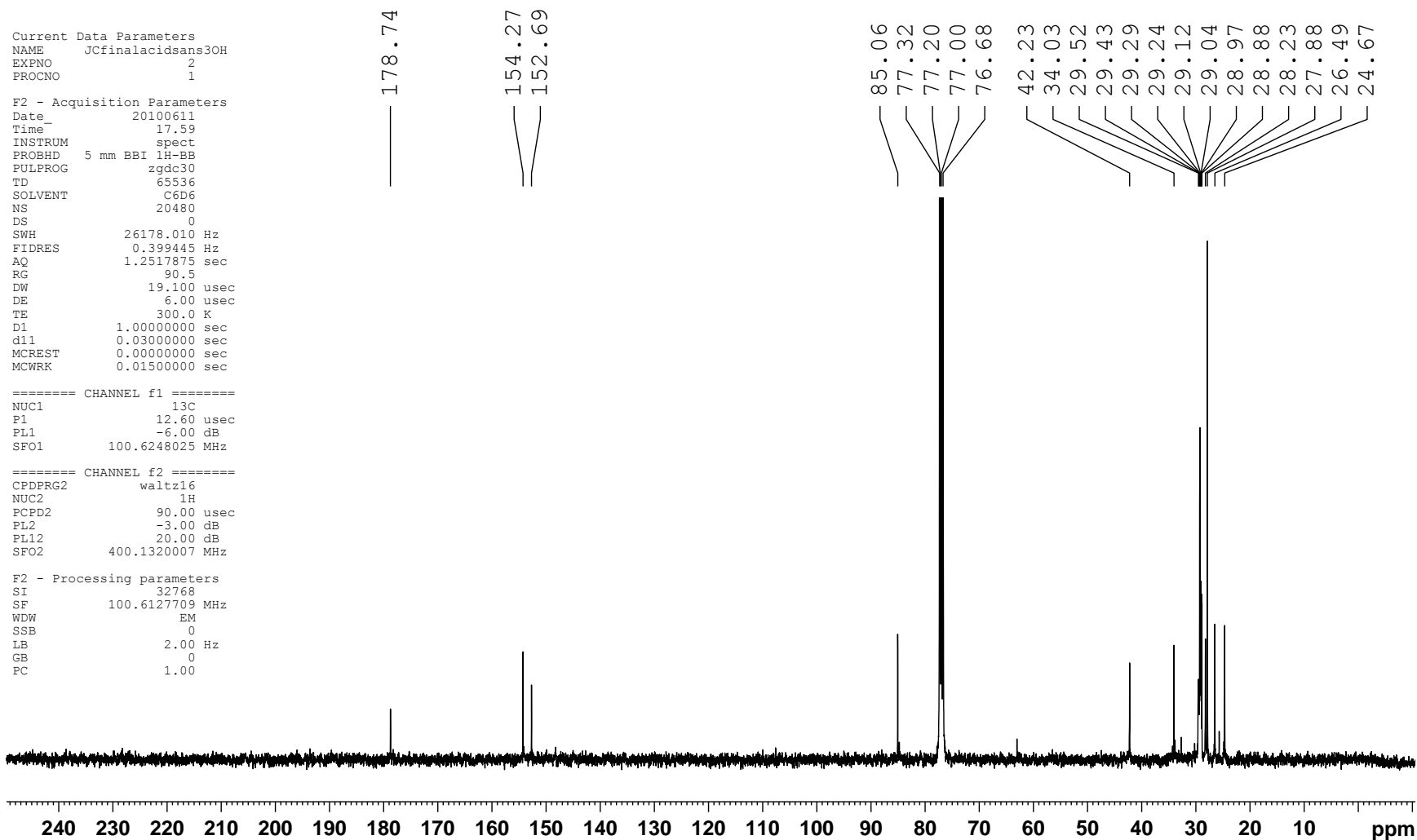
F2 - Processing parameters
SI            32768
SF            100.6127741 MHz
WDW           EM
SSB           0
LB            2.00 Hz
GB            0
PC            1.00
    
```



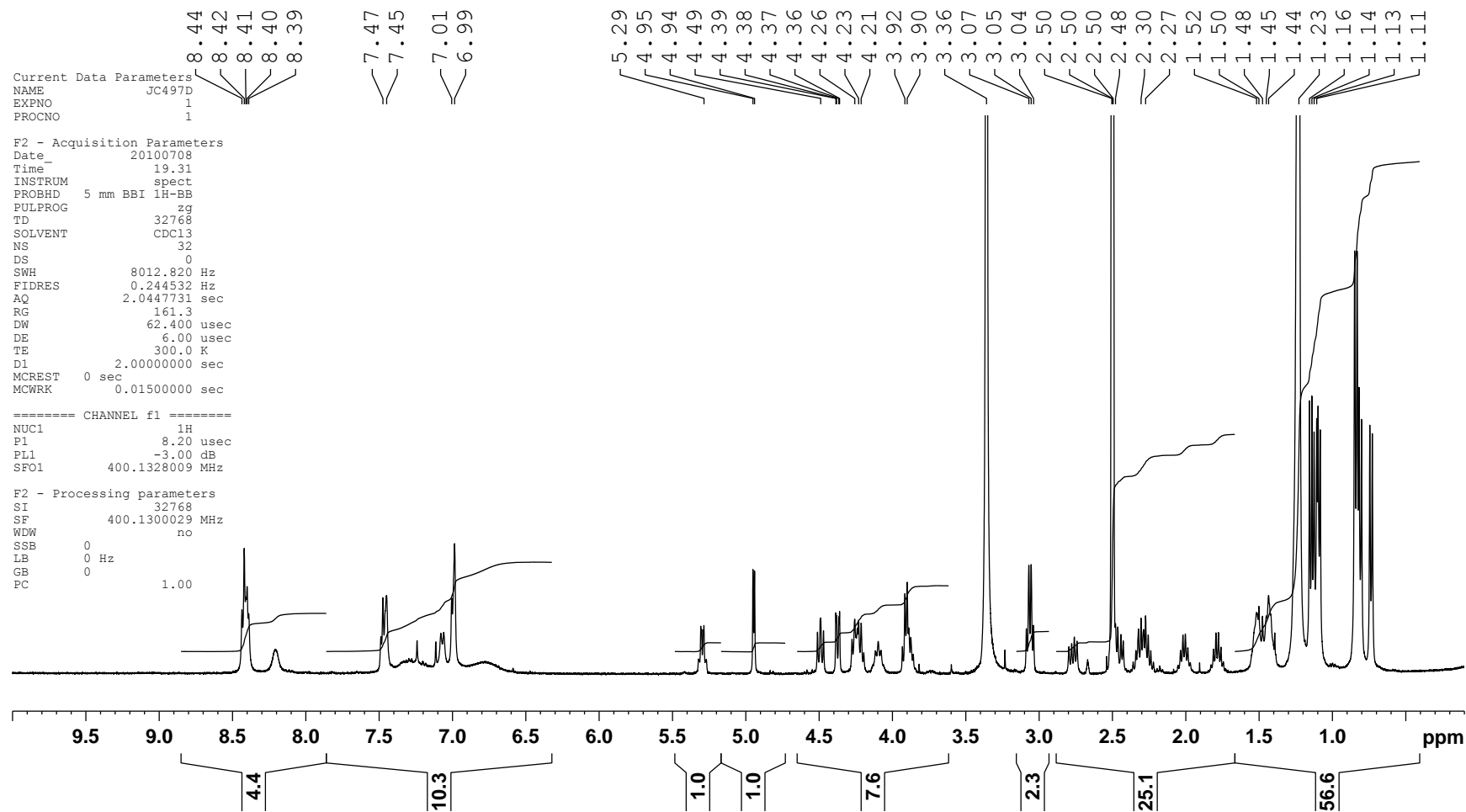
15-(*tert*-Butoxycarbonylguanidino) pentadecanoic acid (12)



15-(tert-Butoxycarbonylguanidino) pentadecanoic acid (12)



Dehydroxy LI-F04a analogue (21)



Dehydroxy LI-F04a analogue (21) COSY

Current Data Parameters
NAME JC497D
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100708
Time_ 19.32
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG cosygpgf
TD 2048
SOLVENT MeOH
NS 32
DS 4
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 114.025
DW 124.800 usec
DE 6.00 usec
TE 300.0 K
d0 0.00000300 sec
D1 1.10000002 sec
d13 0.00000400 sec
D16 0.00015000 sec
IN0 0.00024991 sec
MCREST 0 sec
MCWRK 1.10000002 sec

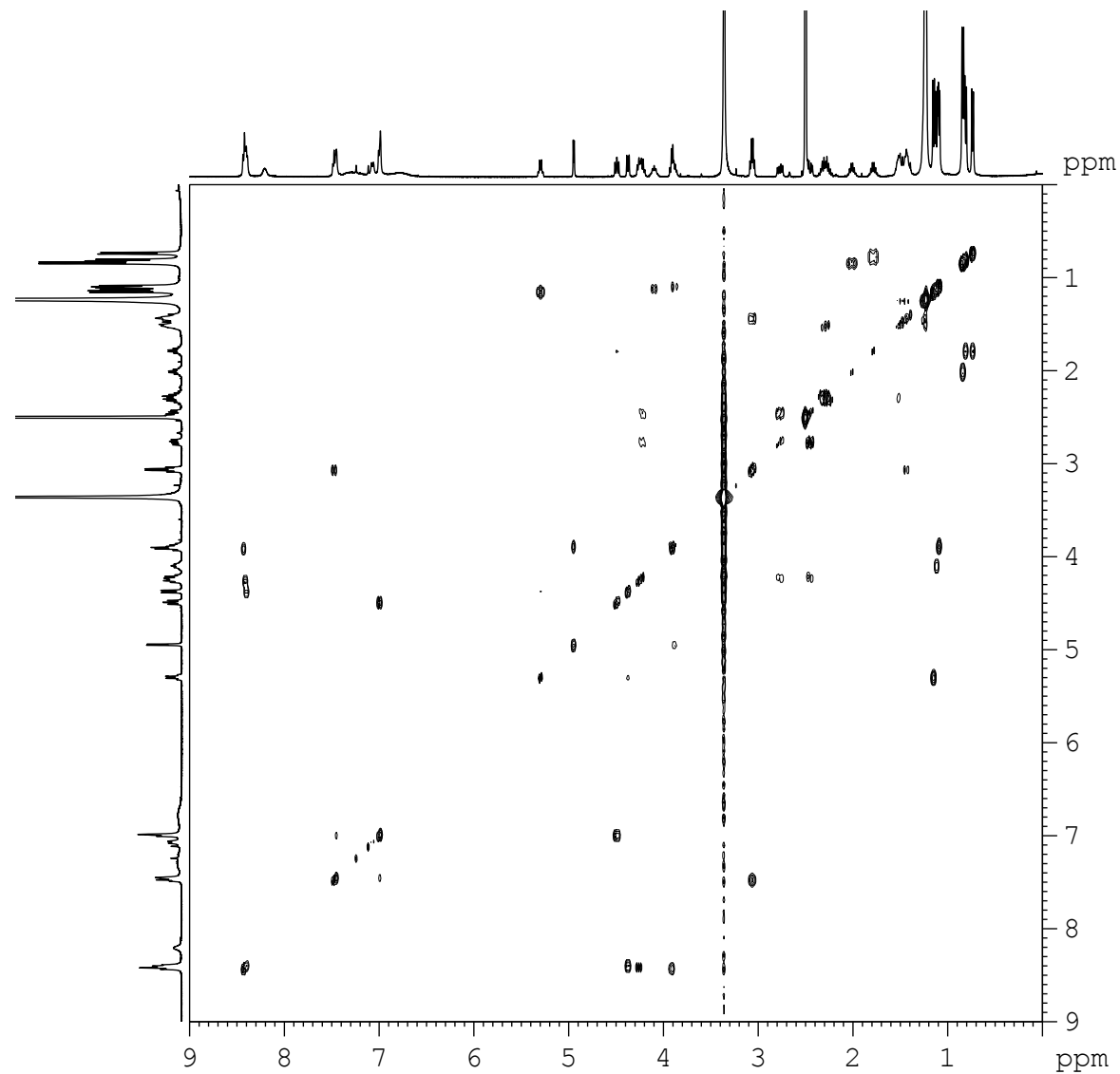
===== CHANNEL f1 =====
NUC1 1H
P0 4.10 usec
P1 8.20 usec
PL1 -3.00 dB
SFO1 400.1320007 MHz

===== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPX1 0 %
GPX2 0 %
GPY1 0 %
GPY2 0 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1500.00 usec

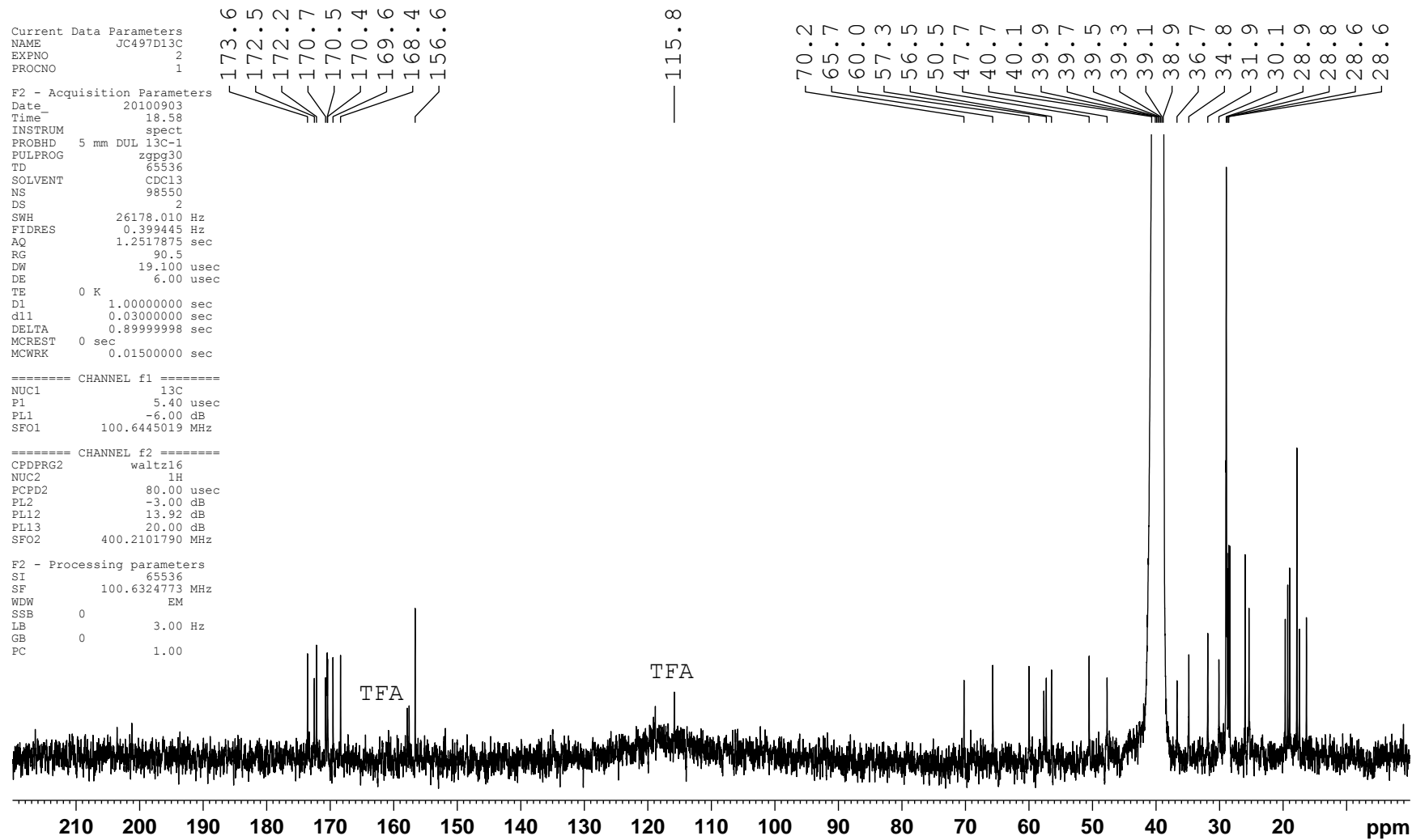
F1 - Acquisition parameters
TD 512
SFO1 400.132 MHz
FIDRES 7.815235 Hz
SW 10.000 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300007 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 256
MC2 QF
SF 400.1299929 MHz
WDW States-TPPI
SSB 0
LB 0 Hz
GB 0



Dehydroxy LI-F04a analogue (21)



Dehydroxy LI-F04a analogue (21) HSQC

```
Current Data Parameters
NAME      JC497D
EXPNO     7
PROCNO    1

F2 - Acquisition Parameters
Date_     20100725
Time      12.54
INSTRUM   spect
PROBHD    5 mm BBI 1H-2B
PULPROG   invietgpsi
TD        2048
SOLVENT   DMSO
NS        64
DS        8
SWH       4006.410 Hz
FIDRES    1.956235 Hz
AQ        0.2556404 sec
RG        512
DM        124.800 usec
DE        6.00 usec
TE        309.9 K
CNST2    140.0000000
d0        0.00000300 sec
d1        1.50000000 sec
d4        0.00178571 sec
d11       0.03000000 sec
d13       0.00000400 sec
d16       0.00015000 sec
D24       0.00178500 sec
DELTA    0.00172240 sec
DELTA1    0.00165900 sec
IN0       0.00004969 sec
MCREST    0 sec
MCWRK     0.25000051 sec
SFICNT    0

===== CHANNEL f1 =====
NUC1      1H
P1        8.20 usec
p2        16.40 usec
P28       0.50 usec
PL1       -3.00 dB
SFO1      400.1320007 MHz

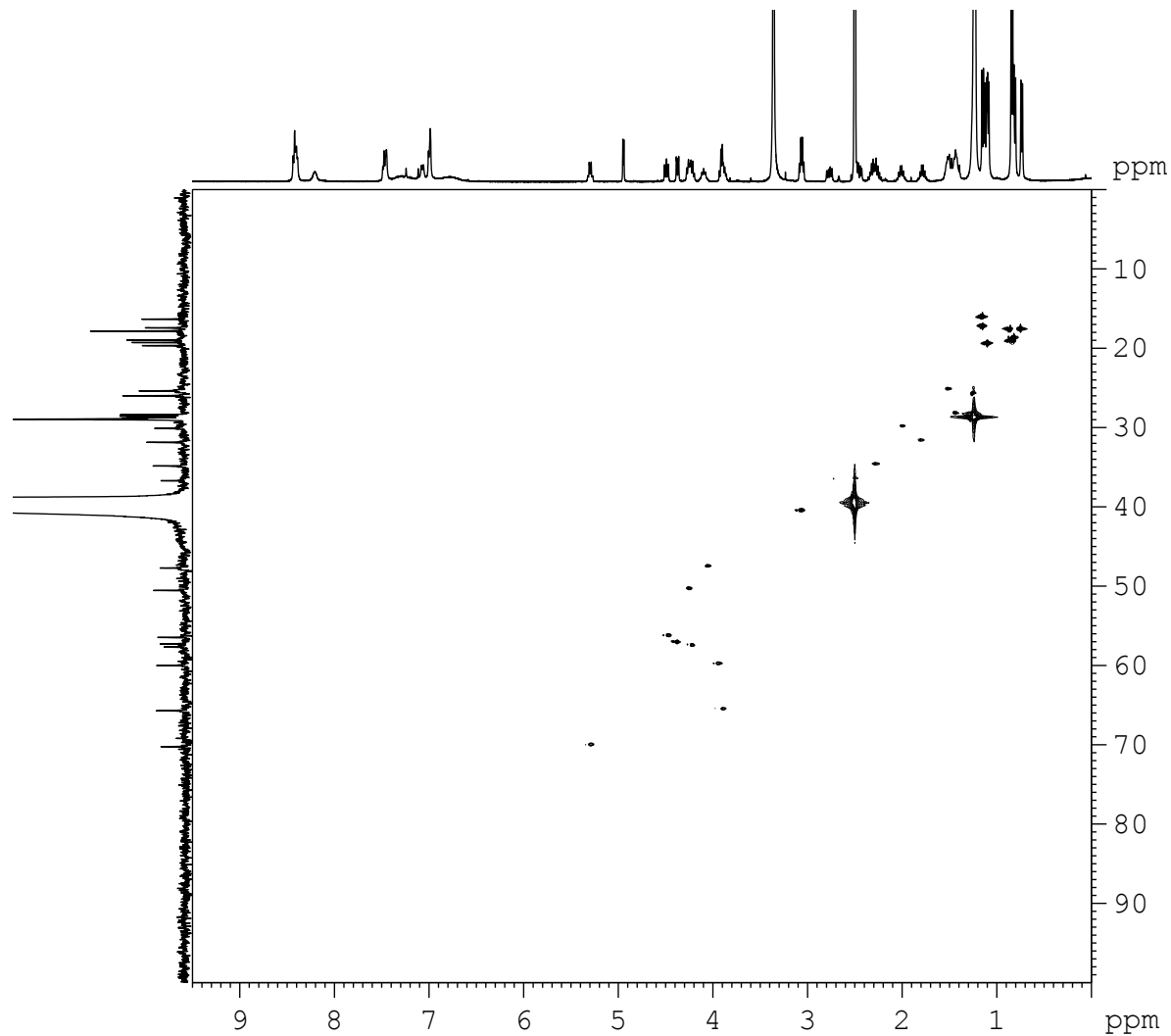
===== CHANNEL f2 =====
CPDPRG2   garp
NUC2      13C
P3        12.00 usec
P4        24.00 usec
PCPD2     70.00 usec
PL2       -6.00 dB
PL12      10.70 dB
SFO2      100.6177596 MHz

===== GRADIENT CHANNEL =====
GPNAM1    sine.100
GPNAM2    sine.100
GFX1      0 %
GFX2      0 %
GFY1      0 %
GFY2      0 %
GPZ1      80.00 %
GPZ2      20.10 %
P16       1500.00 usec

F1 - Acquisition parameters
TD        512
SFO1      100.6178 MHz
FIDRES    19.654089 Hz
SW        100.011 ppm
F1MODE    Echo-Antiecho

F2 - Processing parameters
SI        1024
SF        400.129973 MHz
WDW       SINE
SSB       2
LB        0 Hz
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
MC2       echo-antiecho
SF        100.6128435 MHz
WDW       SINE
SSB       2
LB        0 Hz
GB        0
```



Dehydroxy LI-F04a analogue (21) HMBC

```
Current Data Parameters
NAME      JC497D
EXPNO     7
PROCNO    1

F2 - Acquisition Parameters
Date_     20100725
Time      12.54
INSTRUM   spect
PROBHD    5 mm BBI 1H-BB
PULPROG   invietgpa1
TD        2948
SOLVENT   DMSO
NS        64
DS        8
SWH       4006.410 Hz
FIDRES    1.956255 Hz
AQ        0.2556404 sec
RG        512
DW        124.800 usec
DE        6.00 usec
TE        309.9 K
CNST2     140.0000000
d0        0.00000300 sec
d1        1.50000000 sec
d4        0.00178571 sec
d11       0.03000000 sec
d13       0.00000400 sec
d16       0.00015000 sec
d24       0.00178500 sec
DELTA     0.00172240 sec
DELTA1    0.00165800 sec
IN0       0.00004969 sec
MCREST    0 sec
MCWRK     0.25000051 sec
ST1CNT    0

===== CHANNEL f1 =====
NUC1      1H
P1        8.20 usec
P2        16.40 usec
P28       0.50 usec
PL1       -3.00 dB
SFO1      400.1320007 MHz

===== CHANNEL f2 =====
CPDPRG2   gsrp
NUC2      13C
P3        12.00 usec
p4        24.00 usec
PCPD2     70.00 usec
PL2       -6.00 dB
PL12      10.70 dB
SFO2      100.6177596 MHz

===== GRADIENT CHANNEL =====
GPNAM1    sine.100
GPNAM2    sine.100
GPX1      0 %
GPX2      0 %
GPY1      0 %
GPY2      0 %
GFZ1      80.00 %
GFZ2      20.10 %
P16       1500.00 usec

F1 - Acquisition parameters
TD        512
SFO1      100.6178 MHz
FIDRES    19.654039 Hz
SW        100.011 ppm
FhMODE    Echo-Antiecho

F2 - Processing parameters
SI        1024
SF        400.1299973 MHz
WDW       SINE
SSB       2
LB        0 Hz
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
MC2       echo-antiecho
SF        100.6128435 MHz
WDW       SINE
SSB       2
LB        0 Hz
GB        0
```

