

Supporting Information

An Antibiotic Indole Sesquiterpene Alkaloid from *Greenwayodendron suaveolens* with a New Natural Product Framework

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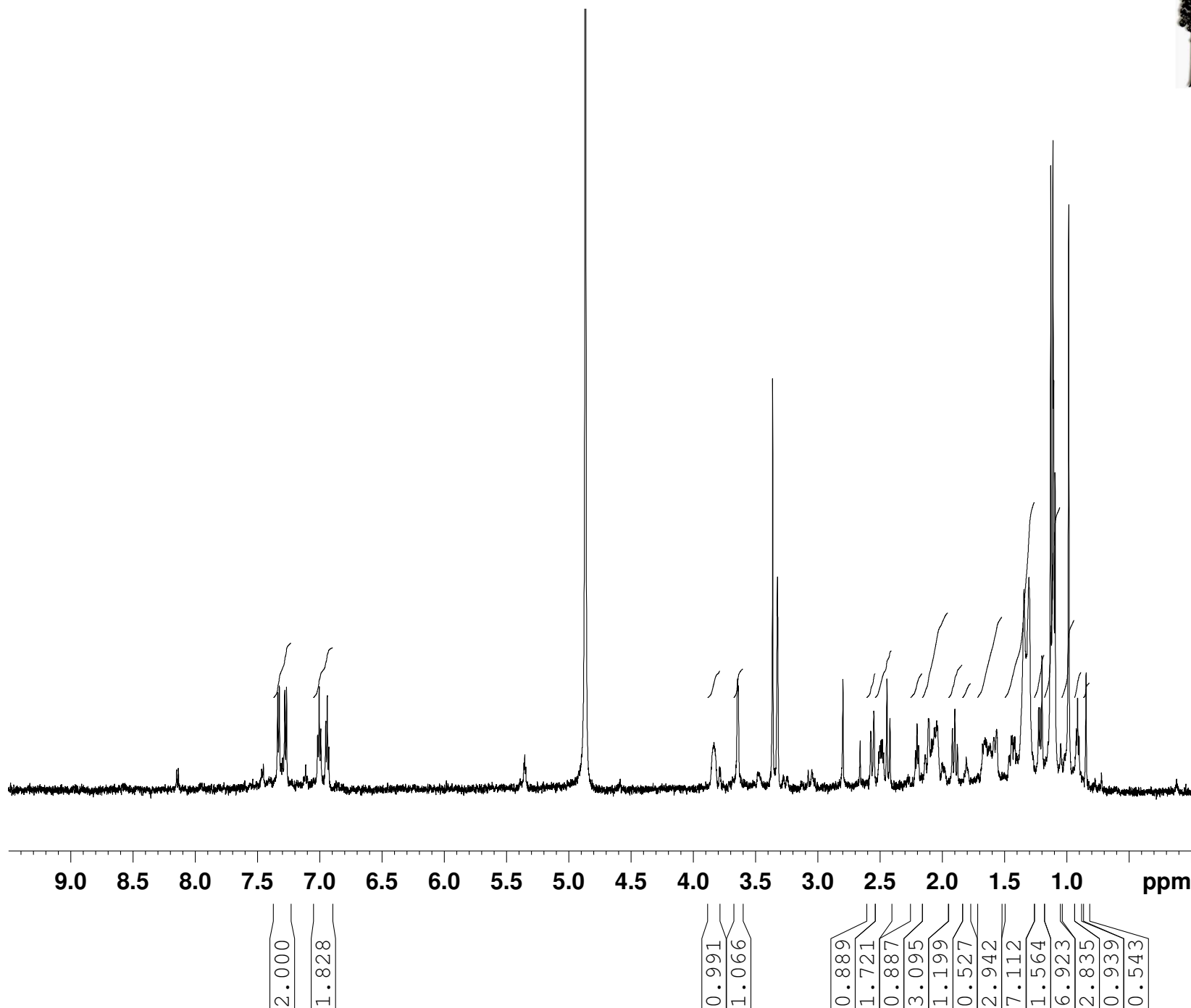
¹ H NMR spectrum for 1	S2
COSY spectrum for 1	S3
HSQC spectrum for 1	S4
HMBC spectrum for 1	S5
ROESY spectrum for 1	S6
¹ H NMR spectrum for 2	S7
COSY spectrum for 2	S8
HSCQ spectrum for 2	S9
HMBC spectrum for 2	S10
ROESY spectrum for 2	S11
¹ H NMR spectrum for 3	S12
COSY spectrum for 3	S13
HSQC spectrum for 3	S14
HMBC spectrum for 3	S15
ROESY spectrum for 3	S16
¹ H NMR spectrum for 4	S17
COSY spectrum for 4	S18
HSQC spectrum for 4	S19
HMBC spectrum for 4	S20
ROESY spectrum for 4	S21

¹H NMR Spectrum for **1** in MeOD

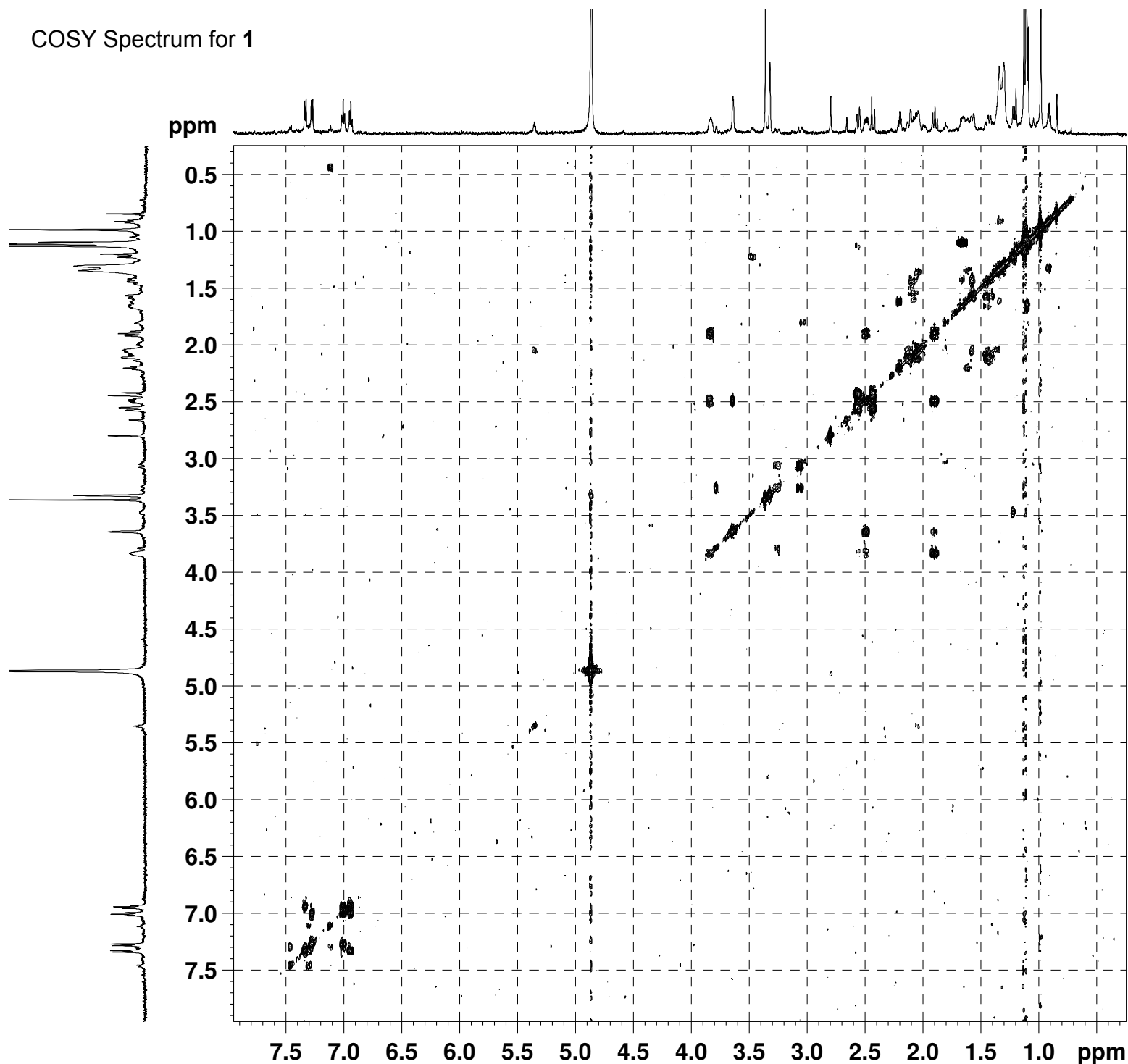


NAME SF_17357
EXPNO 1
PROCNO 1
Date_ 20081113
Time 16.33
INSTRUM spect
PROBHD 1 mm CapLC 1H-
PULPROG zg
TD 65536
SOLVENT MeOD
NS 64
DS 2
SWH 9615.385 Hz
FIDRES 0.146719 Hz
AQ 3.4079220 sec
RG 2048
DW 52.000 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 5.00 usec
PL1 13.00 dB
SFO1 600.1324005 MHz
SI 32768
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 2.00



COSY Spectrum for 1

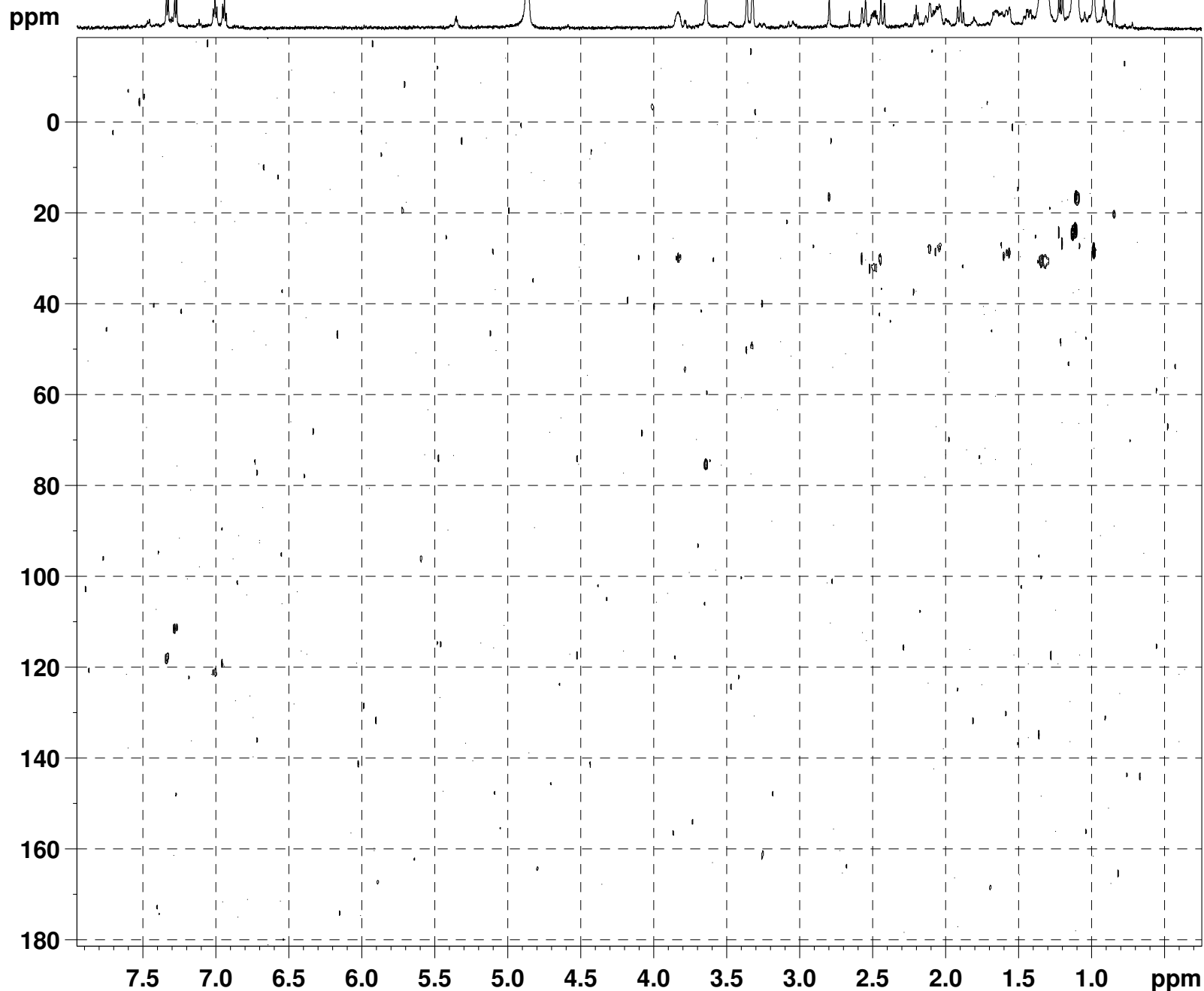


NAME SF_17357
 EXPNO 2
 PROCNO 1
 Date_ 20081113
 Time 16.36
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG cosygpcqf
 TD 2048
 SOLVENT MeOD
 NS 16
 DS 16
 SWH 4629.629 Hz
 FIDRES 2.260561 Hz
 AQ 0.2212340 sec
 RG 2048
 DW 108.000 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 1.32550597 sec
 d13 0.00000400 sec
 D16 0.00025000 sec
 IN0 0.00021600 sec

===== CHANNEL f1 =====
 NUC1 1H
 P0 10.10 usec
 P1 10.10 usec
 PL1 13.00 dB
 SFO1 600.1324573 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPZ1 6.00 %
 GPZ2 6.00 %
 P16 1000.00 usec
 ND0 1
 TD 256
 SFO1 600.1325 MHz
 FIDRES 18.084490 Hz
 SW 7.714 ppm
 FMODE QF
 SI 1024
 SF 600.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 2.00
 SI 1024
 MC2 QF
 SF 600.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

HSQC Spectrum for 1



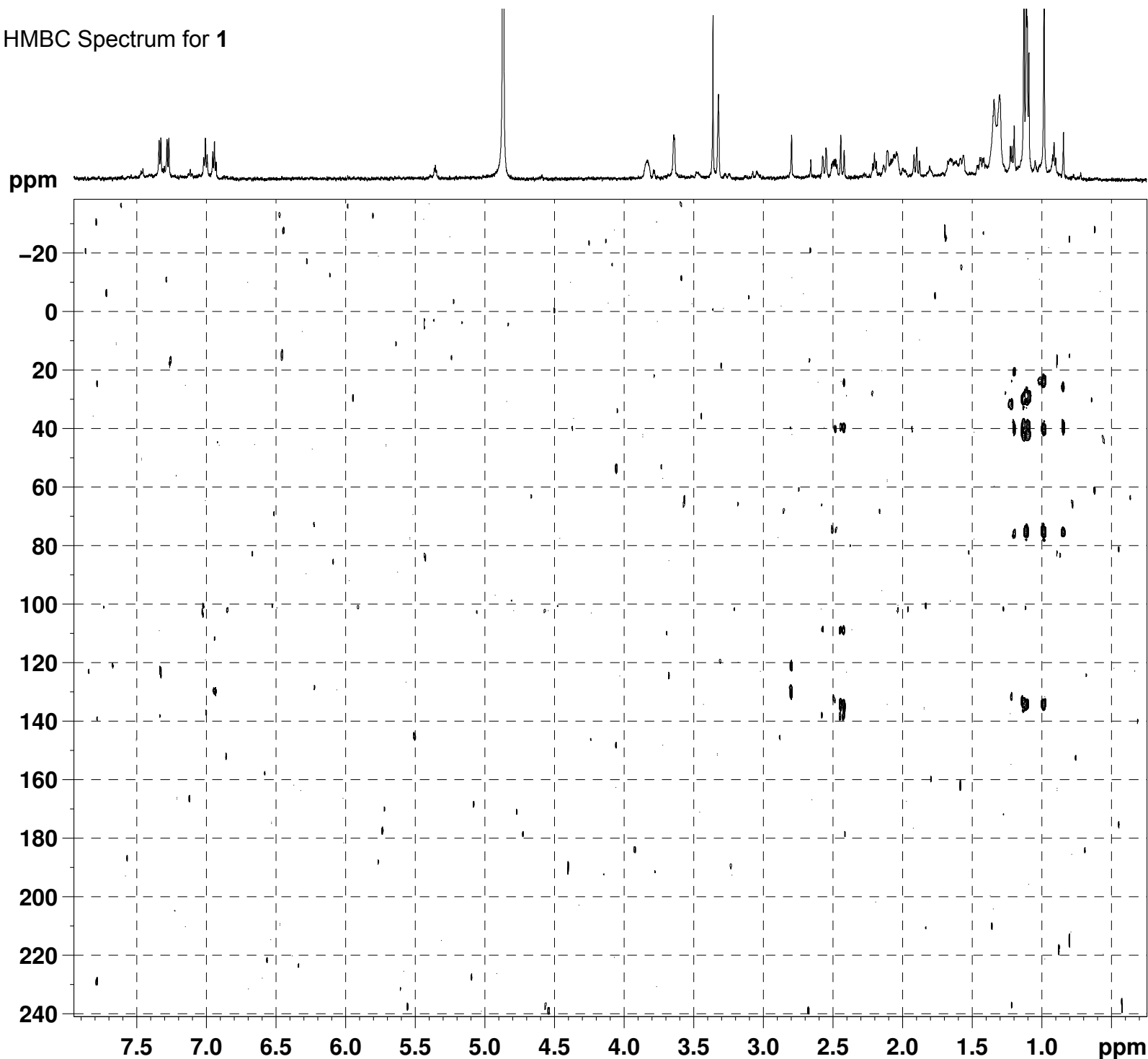
NAME SF_17357
 EXPNO 3
 PROCNO 1
 Date 20081113
 Time 18.27
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG hsqcetgpsisp.2
 TD 2048
 SOLVENT MeOD
 NS 128
 DS 32
 SWH 4629.629 Hz
 FIDRES 2.260561 Hz
 AQ 0.2212340 sec
 RG 2048
 DW 108.000 usec
 DE 115.71 usec
 TE 298.0 K
 CNST2 145.0000000
 CNST17 -0.5000000
 d0 0.00000300 sec
 D1 1.01646495 sec
 d4 0.00172414 sec
 d11 0.03000000 sec
 D16 0.00025000 sec
 D24 0.00086000 sec
 DELTA 0.00127220 sec
 DELTA1 0.00125800 sec
 DELTA2 0.00147014 sec
 DELTA3 0.00135600 sec
 IN0 0.00001655 sec
 ST1CNT 0

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.10 usec
 p2 20.20 usec
 P28 2000.00 usec
 PL1 13.00 dB
 SFO1 600.1324573 MHz

===== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 13C
 P3 10.00 usec
 P14 500.00 usec
 P24 2000.00 usec
 PCPD2 60.00 usec
 PL0 120.00 dB
 PL2 18.00 dB
 PL12 34.00 dB
 SFO2 150.9148810 MHz
 SP3 27.00 dB
 SP7 27.00 dB
 SPNAM3 Crp60,0.5,20.1
 SPNAM7 Crp60comp.4
 SPOAL3 0.500
 SPOAL7 0.500
 SPOFFS3 0.00 Hz
 SPOFFS7 0.00 Hz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPZ1 20.00 %
 GPZ2 5.03 %
 P16 1000.00 usec
 ND0 2
 TD 100
 SFO1 150.9149 MHz
 FIDRES 302.114807 Hz
 SW 200.189 ppm
 FnMODE Echo-Antiecho
 SI 1024
 SF 600.1300000 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024

HMBC Spectrum for 1



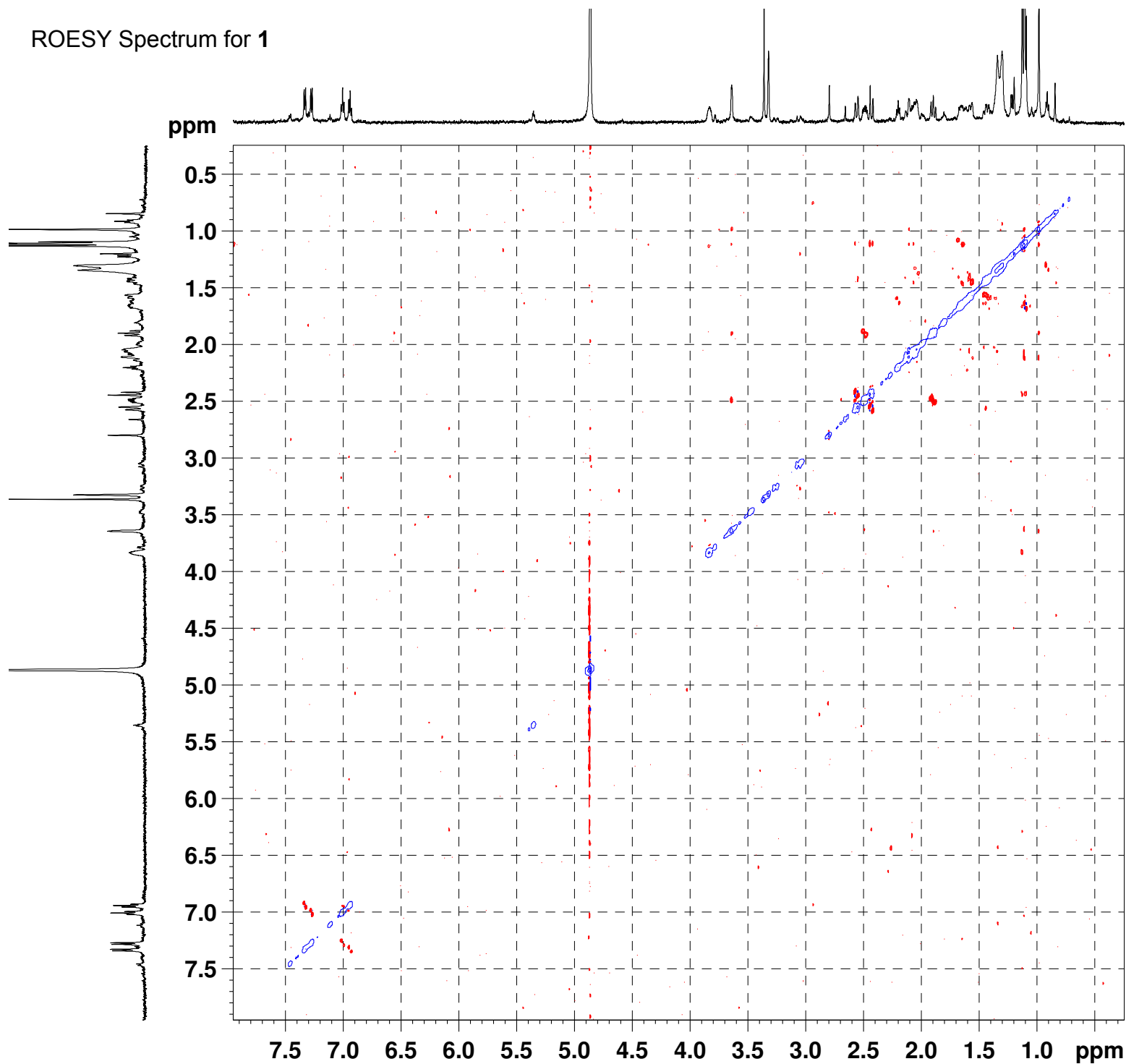
NAME SF_17357
 EXPNO 5
 PROCNO 1
 Date_ 20081114
 Time 10.54
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG inv4gpglrm
 TD 2048
 SOLVENT MeOD
 NS 1024
 DS 32
 SWH 4629.629 Hz
 FIDRES 2.260561 Hz
 AQ 0.2212340 sec
 RG 2048
 DW 108.000 usec
 DE 6.00 usec
 TE 298.0 K
 CNST2 145.000000
 d0 0.00000300 sec
 D1 1.14224303 sec
 d2 0.00344828 sec
 D6 0.06600000 sec
 d13 0.00000300 sec
 D16 0.00025000 sec
 INO 0.00001185 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.10 usec
 P2 20.20 usec
 PL1 13.00 dB
 SFO1 600.1324573 MHz

===== CHANNEL f2 =====
 NUC2 13C
 P3 10.00 usec
 PL2 18.00 dB
 SFO2 150.9178393 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 12.50 %
 GPZ2 7.50 %
 GPZ3 10.02 %
 P16 1000.00 usec
 ND0 2
 TD 100
 SFO1 150.9178 MHz
 FIDRES 421.940918 Hz
 SW 279.583 ppm
 FnmODE QF
 SI 1024
 SF 600.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 QF
 SF 150.9025700 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

ROESY Spectrum for 1



NAME SF_17357
 EXPNO 4
 PROCNO 1
 Date_ 20081113
 Time_ 22.56
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG roesyph
 TD 2048
 SOLVENT MeOD
 NS 32
 DS 16
 SWH 4629.629 Hz
 FIDRES 2.260561 Hz
 AQ 0.2212340 sec
 RG 2048
 DW 108.000 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00009757 sec
 D1 1.46805000 sec
 d12 0.00002000 sec
 IN0 0.00021600 sec
 ST1CNT 0

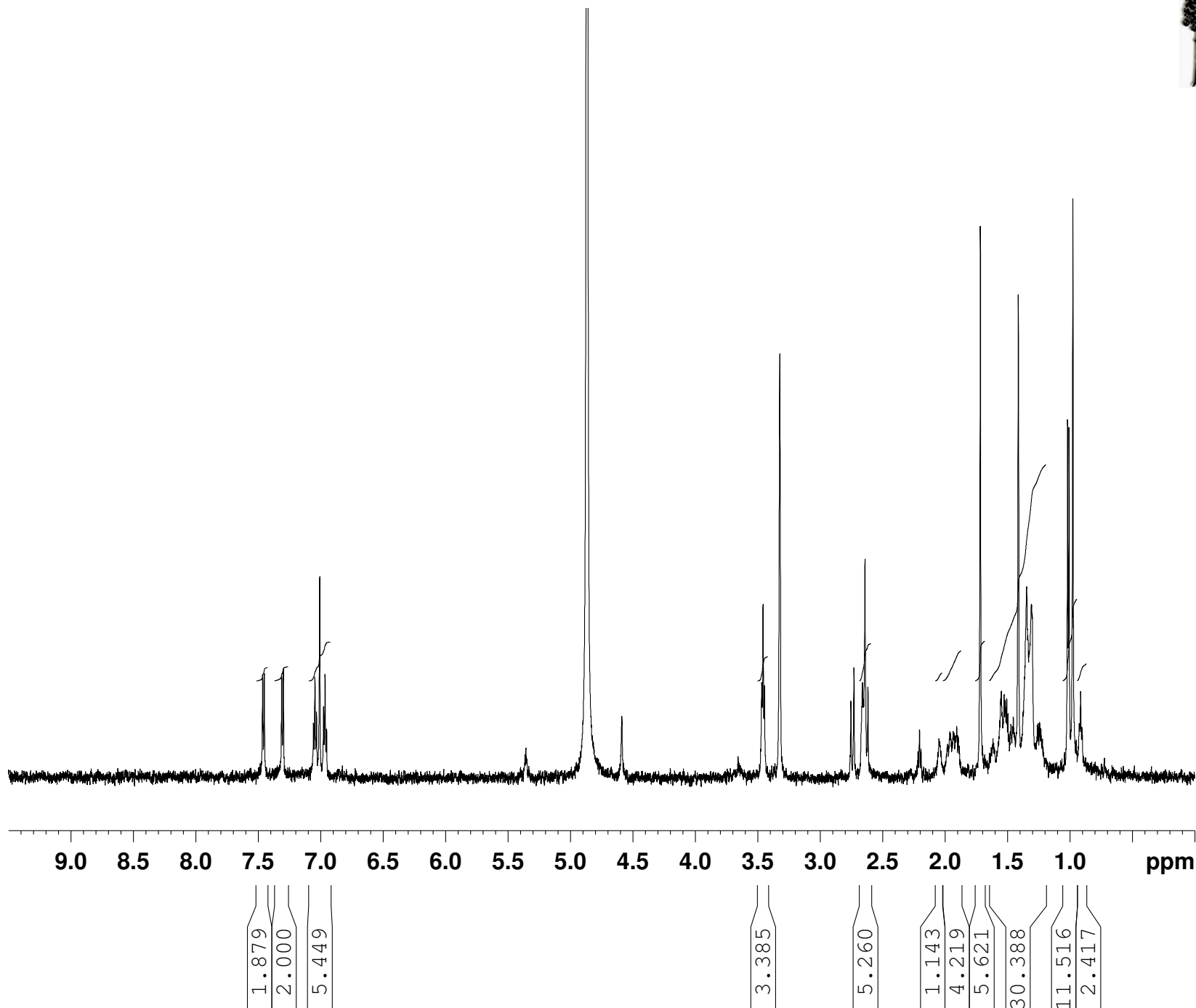
===== CHANNEL f1 =====
 NUC1 1H
 P1 10.10 usec
 P15 250000.00 usec
 PL1 13.00 dB
 PL11 35.50 dB
 SFO1 600.1324573 MHz
 ND0 1
 TD 256
 SFO1 600.1325 MHz
 FIDRES 18.084490 Hz
 SW 7.714 ppm
 FnmODE States-TPPI
 SI 1024
 SF 600.1300000 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.00
 SI 1024
 MC2 States-TPPI
 SF 600.1300000 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

¹H NMR Spectrum for **2** in MeOD

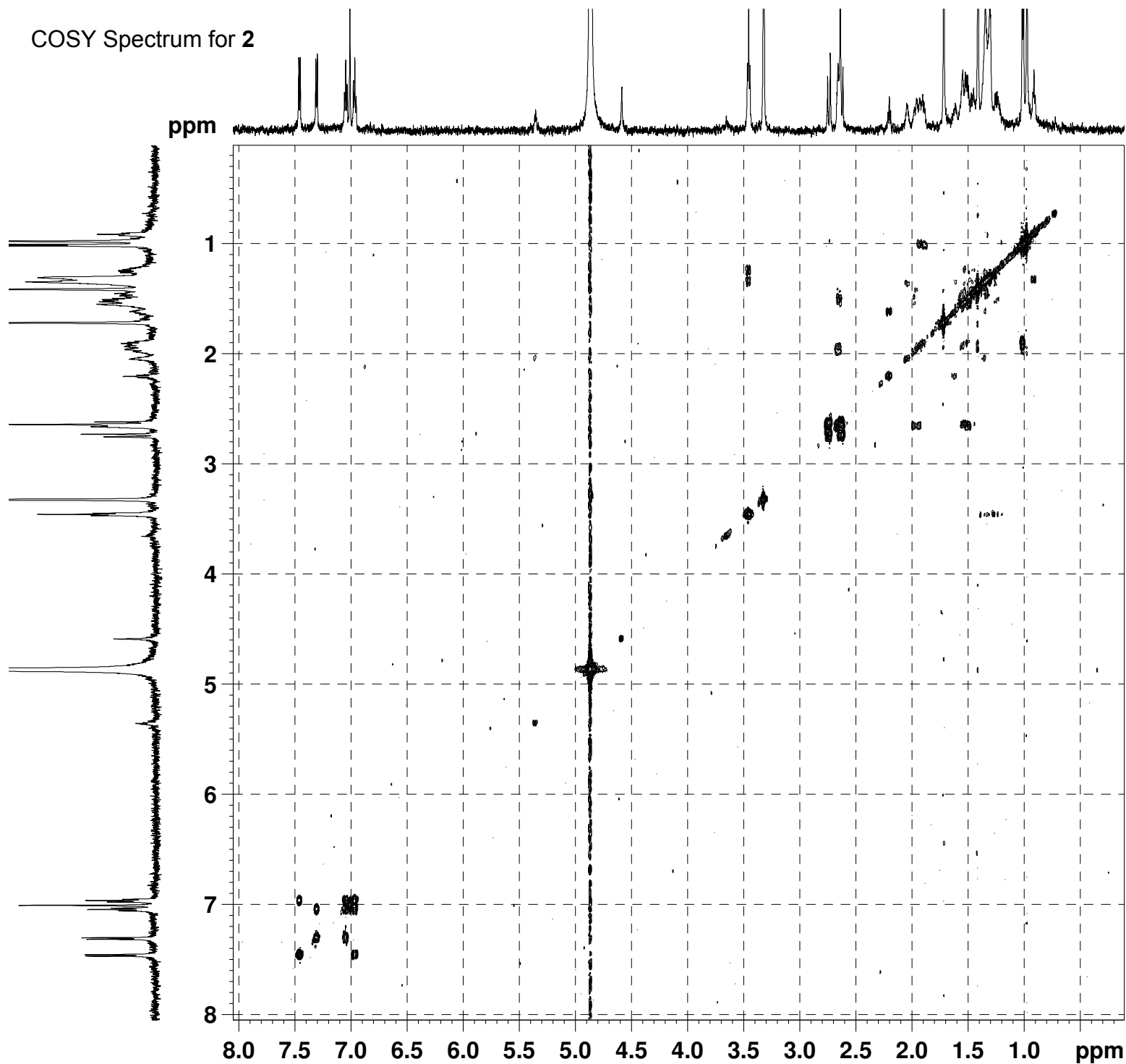


NAME SF_17355
EXPNO 1
PROCNO 1
Date_ 20081117
Time 15.53
INSTRUM spect
PROBHD 1 mm CapLC 1H-
PULPROG zg
TD 65536
SOLVENT MeOD
NS 64
DS 2
SWH 9615.385 Hz
FIDRES 0.146719 Hz
AQ 3.4079220 sec
RG 2048
DW 52.000 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 5.00 usec
PL1 13.00 dB
SFO1 600.1324005 MHz
SI 32768
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 2.00



COSY Spectrum for 2

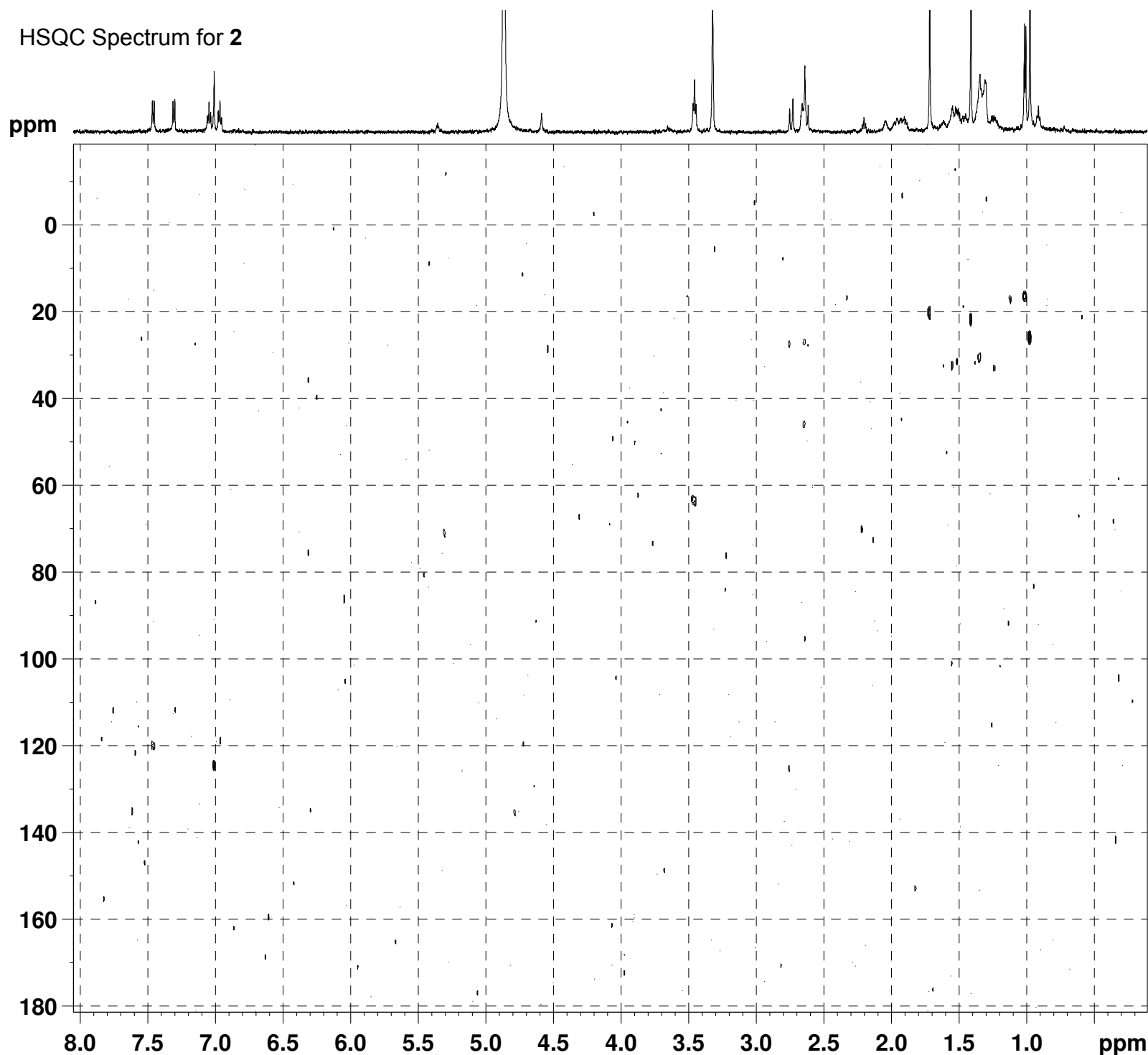


NAME SF_17355
 EXPNO 2
 PROCNO 1
 Date_ 20081117
 Time 16.01
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG cosygpcqf
 TD 2048
 SOLVENT MeOD
 NS 16
 DS 16
 SWH 4770.992 Hz
 FIDRES 2.329586 Hz
 AQ 0.2146804 sec
 RG 2048
 DW 104.800 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 1.33165002 sec
 d13 0.00000400 sec
 D16 0.00025000 sec
 INO 0.00020960 sec

===== CHANNEL f1 =====
 NUC1 1H
 P0 10.30 usec
 P1 10.30 usec
 PL1 13.00 dB
 SFO1 600.1324457 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPZ1 6.00 %
 GPZ2 6.00 %
 P16 1000.00 usec
 ND0 1
 TD 200
 SFO1 600.1324 MHz
 FIDRES 23.854961 Hz
 SW 7.950 ppm
 FnMODE QF
 SI 1024
 SF 600.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 2.00
 SI 1024
 MC2 QF
 SF 600.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

HSQC Spectrum for 2



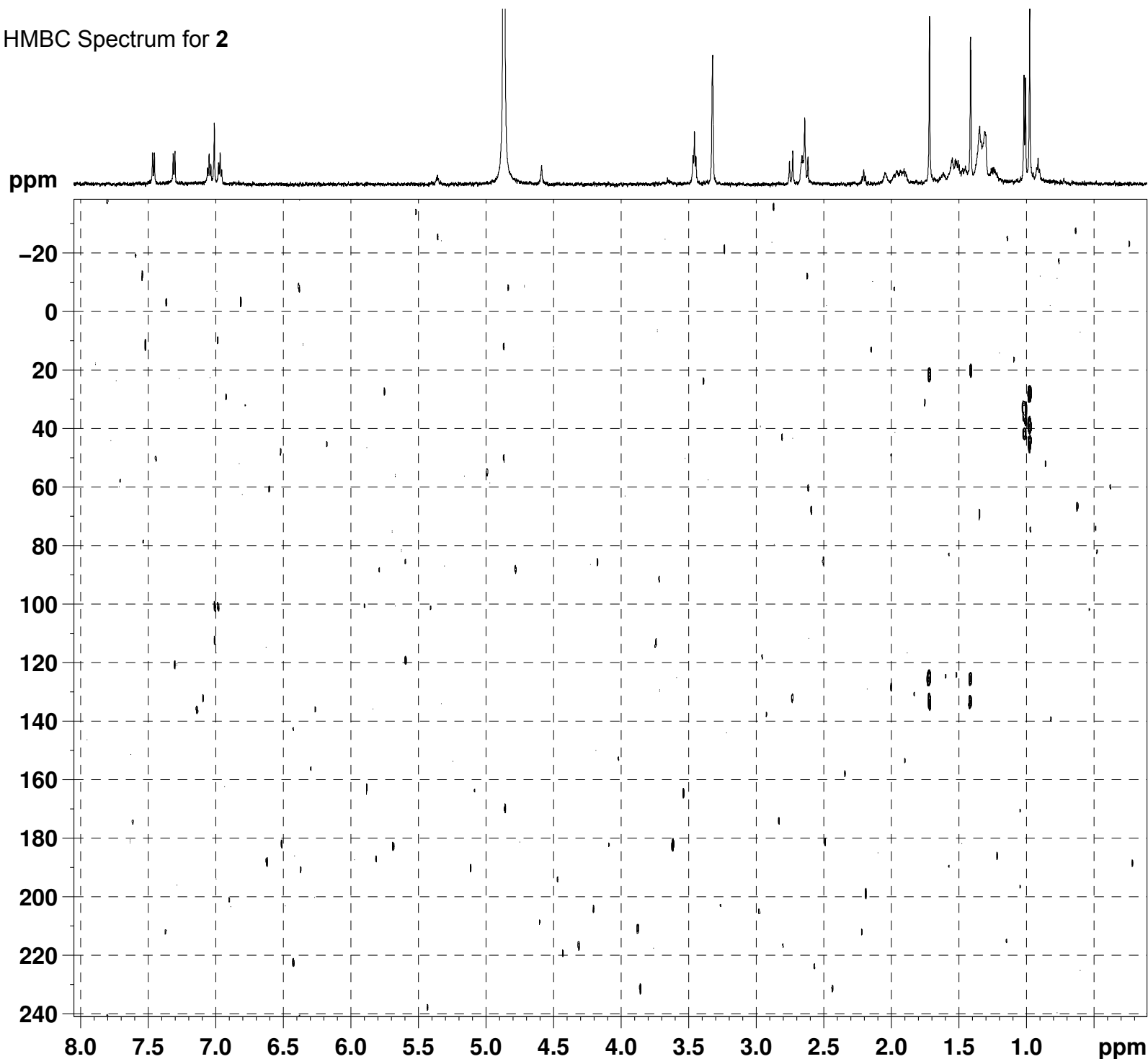
NAME SF_17355
EXPNO 3
PROCNO 1
Date_ 20081117
Time 17.28
INSTRUM spect
PROBHD 1 mm CapLC 1H-
PULPROG hsqcetgpsisp.2
TD 2048
SOLVENT MeOD
NS 128
DS 32
SWH 4770.992 Hz
FIDRES 2.329586 Hz
AQ 0.2146804 sec
RG 2048
DW 104.800 usec
DE 115.71 usec
TE 298.0 K
CNST2 145.0000000
CNST17 -0.5000000
d0 0.00000300 sec
D1 1.02260900 sec
d4 0.00172414 sec
d11 0.03000000 sec
D16 0.00025000 sec
D24 0.00086000 sec
DELTA 0.00127260 sec
DELTA1 0.00125800 sec
DELTA2 0.00147014 sec
DELTA3 0.00135600 sec
IN0 0.00001655 sec
ST1CNT 0

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
p2 20.60 usec
P28 2000.00 usec
PL1 13.00 dB
SFO1 600.1324457 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 10.00 usec
P14 500.00 usec
P24 2000.00 usec
PCPD2 60.00 usec
PL0 120.00 dB
PL2 18.00 dB
PL12 34.00 dB
SFO2 150.9148810 MHz
SP3 27.00 dB
SP7 27.00 dB
SPNAM3 Crp60,0.5,20.1
SPNAM7 Crp60comp.4
SPOAL3 0.500
SPOAL7 0.500
SPOFFS3 0.00 Hz
SPOFFS7 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 20.00 %
GPZ2 5.03 %
P16 1000.00 usec
ND0 2
TD 100
SFO1 150.9149 MHz
FIDRES 302.114807 Hz
SW 200.189 ppm
FnMODE Echo-Antiecho
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024

HMBC Spectrum for 2



NAME SF_17355
 EXPNO 5
 PROCNO 1
 Date_ 20081118
 Time 2.35
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG inv4gpglrmnd
 TD 2048
 SOLVENT MeOD
 NS 512
 DS 32
 SWH 4770.992 Hz
 FIDRES 2.329586 Hz
 AQ 0.2146804 sec
 RG 2048
 DW 104.800 usec
 DE 6.00 usec
 TE 298.0 K
 CNST2 145.0000000
 d0 0.00000300 sec
 D1 1.14838696 sec
 d2 0.00344828 sec
 D6 0.06600000 sec
 d13 0.00000300 sec
 D16 0.00025000 sec
 INO 0.00001185 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.30 usec
 P2 20.60 usec
 PL1 13.00 dB
 SFO1 600.1324457 MHz

===== CHANNEL f2 =====
 NUC2 13C
 P3 10.00 usec
 PL2 18.00 dB
 SFO2 150.9178393 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 12.50 %
 GPZ2 7.50 %
 GPZ3 10.02 %
 P16 1000.00 usec
 ND0 2
 TD 67
 SFO1 150.9178 MHz
 FIDRES 629.762573 Hz
 SW 279.583 ppm
 FnmODE QF
 SI 1024
 SF 600.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 QF
 SF 150.9025700 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

ROESY Spectrum for 2

ppm

1

2

3

4

5

6

7

8

8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm



NAME	SF_17355
EXPNO	4
PROCNO	1
Date_	20081117
Time	21.56
INSTRUM	spect
PROBHD	1 mm CapLC 1H-
P1,PROG	mesyph
TD	2048
SOLVENT	MeOD
NS	32
DS	16
SWH	4770.992 Hz
FIDRES	2.7329586 Hz
AQ	0.2146804 sec
RG	2048
DW	104.800 usec
DE	6.00 usec
TE	298.0 K
d0	0.00009424 sec
D1	1.47419405 sec
d12	0.00002000 sec
IN0	0.00020960 sec
ST1CNT	0

```

===== CHANNEL f1 =====
NUC1          1H
P1            10.30 usec
P15           250000.00 usec
PL1           13.00 dB
PL11          35.50 dB
SFO1          600.1324457 MHz
ND0           1
TD            256
SFO1          600.1324 MHz
FIDRES        18.636688 Hz
SW            7.950 ppm
FnMODE        States-TPPI
SI            1024
SF            600.1300000 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.00
SI            1024
MC2           States-TPPI
SF            600.1300000 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0

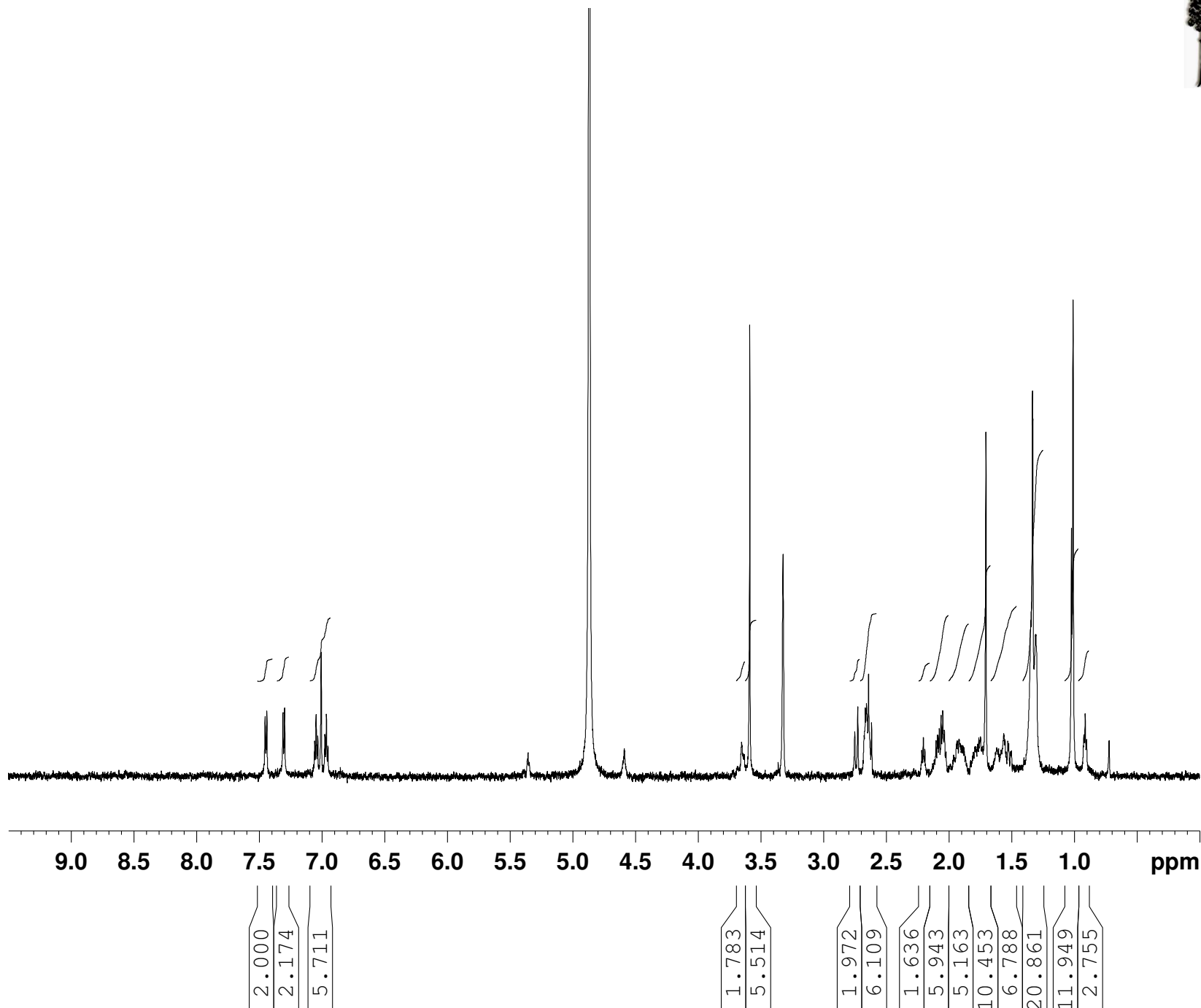
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¹H NMR Spectrum for **3** in MeOD

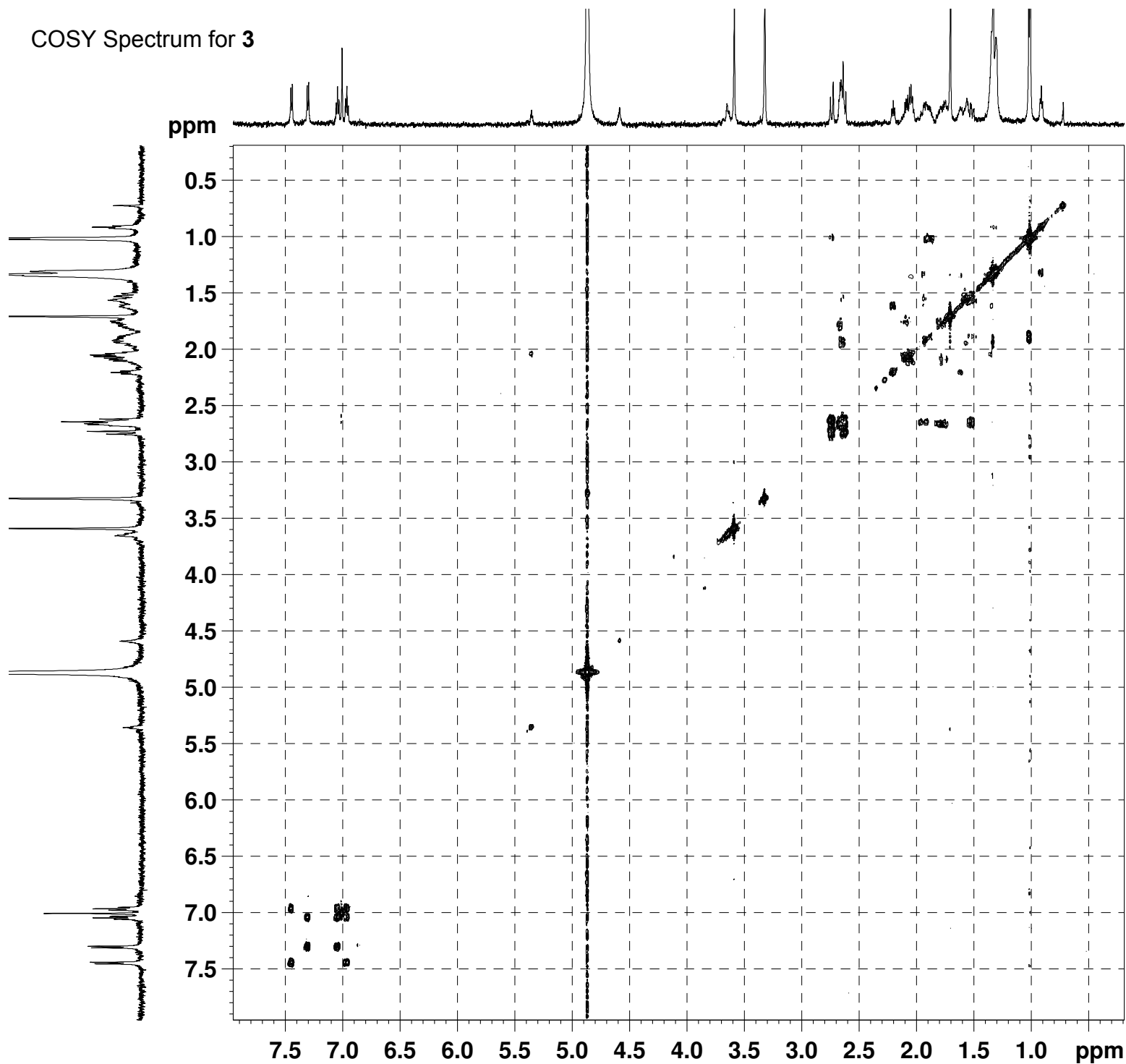


NAME SF_17359
EXPNO 1
PROCNO 1
Date_ 20081118
Time 16.26
INSTRUM spect
PROBHD 1 mm CapLC 1H-
PULPROG zg
TD 65536
SOLVENT MeOD
NS 64
DS 2
SWH 9615.385 Hz
FIDRES 0.146719 Hz
AQ 3.4079220 sec
RG 2048
DW 52.000 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 5.00 usec
PL1 13.00 dB
SFO1 600.1324005 MHz
SI 32768
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 2.00



COSY Spectrum for 3

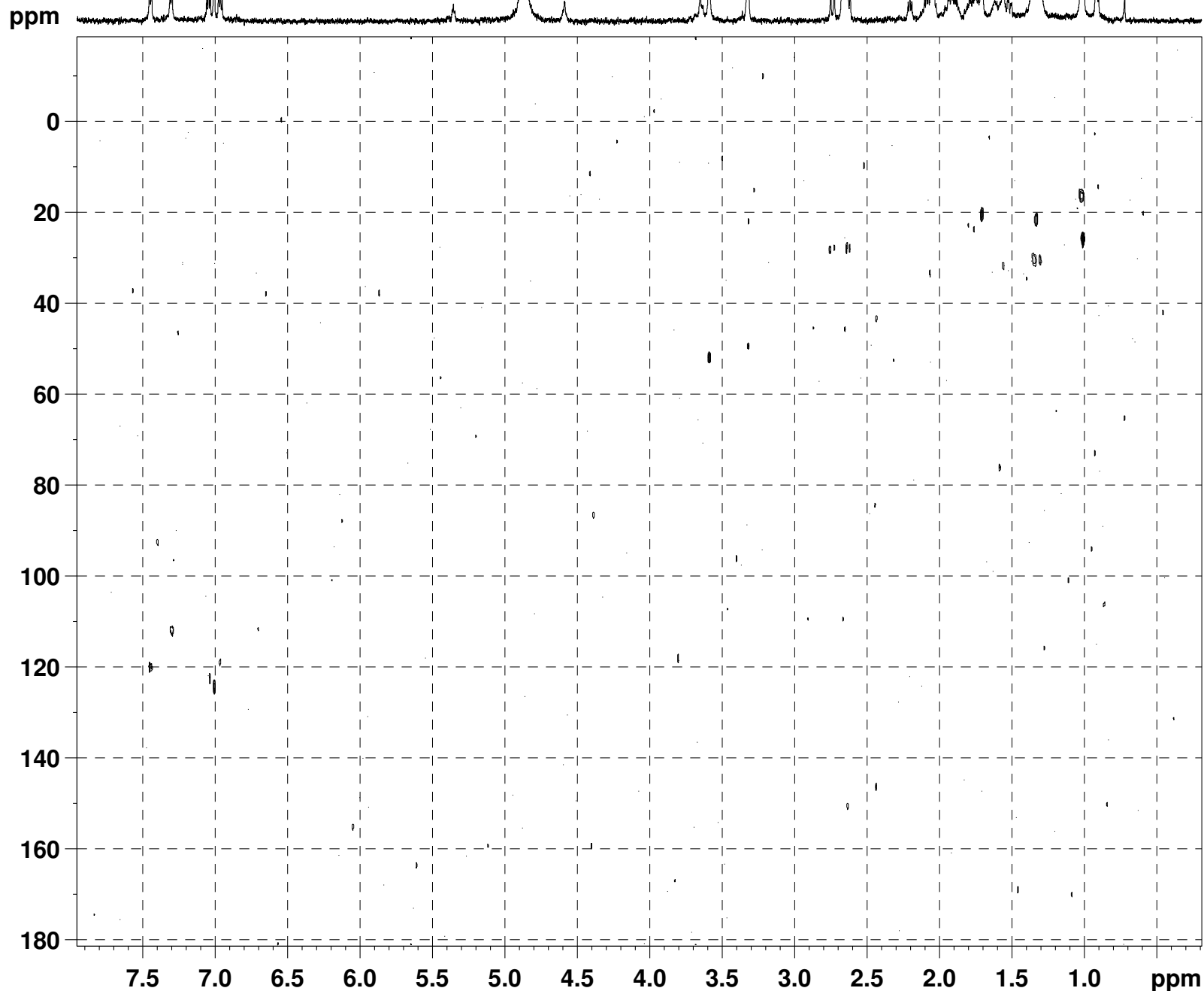


NAME SF_17359
 EXPNO 2
 PROCNO 1
 Date_ 20081118
 Time 16.37
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG cosygpcqf
 TD 2048
 SOLVENT MeOD
 NS 16
 DS 16
 SWH 4664.179 Hz
 FIDRES 2.277431 Hz
 AQ 0.2195956 sec
 RG 2048
 DW 107.200 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 1.32755399 sec
 d13 0.00000400 sec
 D16 0.00025000 sec
 INO 0.00021440 sec

===== CHANNEL f1 =====
 NUC1 1H
 P0 10.50 usec
 P1 10.50 usec
 PL1 13.00 dB
 SFO1 600.1324414 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPZ1 6.00 %
 GPZ2 6.00 %
 P16 1000.00 usec
 ND0 1
 TD 256
 SFO1 600.1324 MHz
 FIDRES 18.219450 Hz
 SW 7.772 ppm
 FnMODE QF
 SI 1024
 SF 600.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 2.00
 SI 1024
 MC2 QF
 SF 600.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

HSQC Spectrum for 3



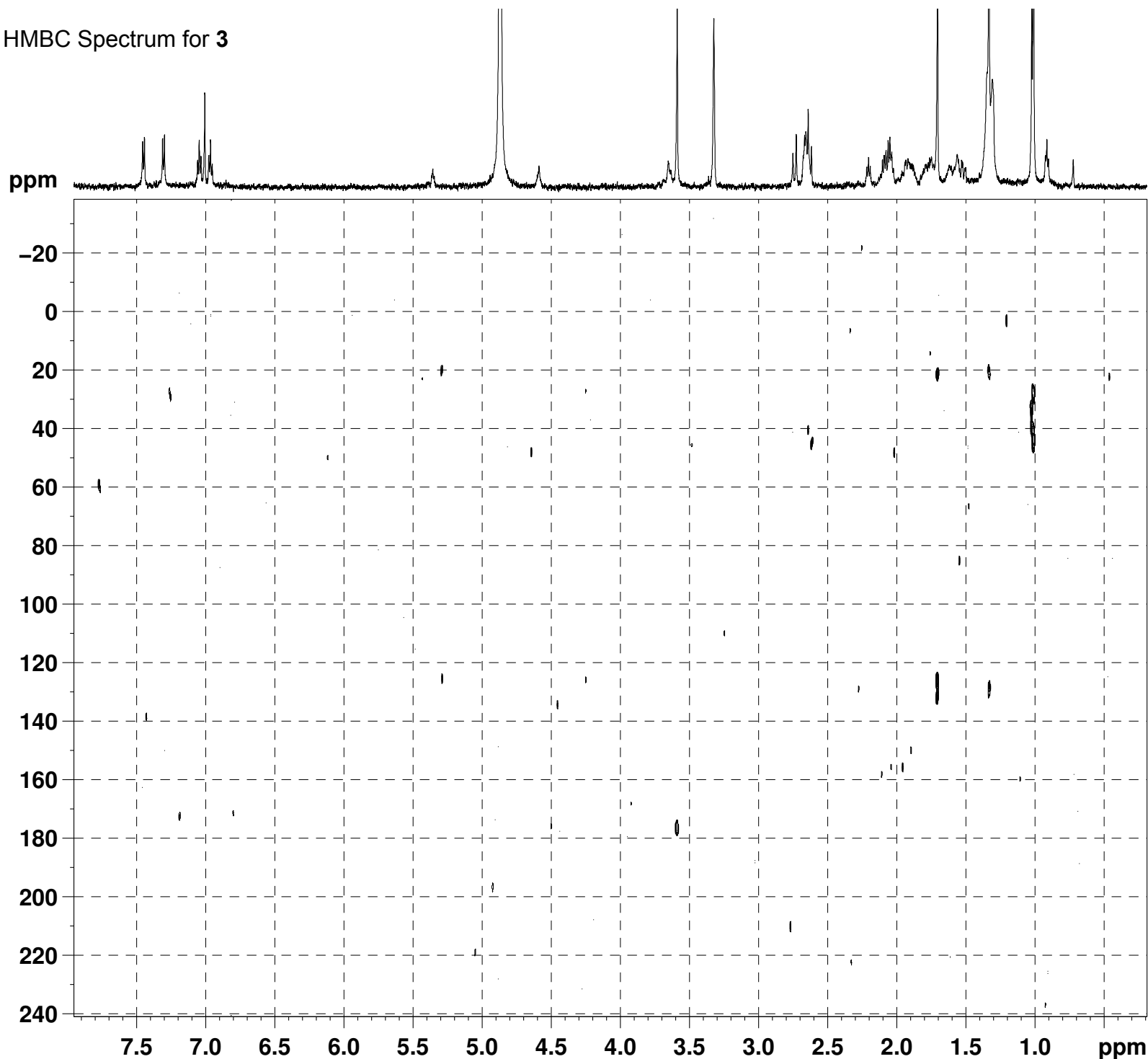
NAME SF_17359
 EXPNO 3
 PROCNO 1
 Date 20081118
 Time 18.28
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG hsqcetgpsisp.2
 TD 2048
 SOLVENT MeOD
 NS 128
 DS 32
 SWH 4664.179 Hz
 FIDRES 2.277431 Hz
 AQ 0.2195956 sec
 RG 2048
 DW 107.200 usec
 DE 115.71 usec
 TE 298.0 K
 CNST2 145.0000000
 CNST17 -0.5000000
 d0 0.00000300 sec
 D1 1.01851296 sec
 d4 0.00172414 sec
 d11 0.03000000 sec
 D16 0.00025000 sec
 D24 0.00086000 sec
 DELTA 0.00127300 sec
 DELTA1 0.00125800 sec
 DELTA2 0.00147014 sec
 DELTA3 0.00135600 sec
 IN0 0.00001655 sec
 ST1CNT 0

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 p2 21.00 usec
 P28 2000.00 usec
 PL1 13.00 dB
 SFO1 600.1324414 MHz

===== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 13C
 P3 10.00 usec
 P14 500.00 usec
 P24 2000.00 usec
 PCPD2 60.00 usec
 PL0 120.00 dB
 PL2 18.00 dB
 PL12 34.00 dB
 SFO2 150.9148810 MHz
 SP3 27.00 dB
 SP7 27.00 dB
 SPNAM3 Crp60,0.5,20.1
 SPNAM7 Crp60comp.4
 SPOAL3 0.500
 SPOAL7 0.500
 SPOFFS3 0.00 Hz
 SPOFFS7 0.00 Hz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPZ1 20.00 %
 GPZ2 5.03 %
 P16 1000.00 usec
 ND0 2
 TD 100
 SFO1 150.9149 MHz
 FIDRES 302.114807 Hz
 SW 200.189 ppm
 FnMODE Echo-Antiecho
 SI 1024
 SF 600.1300000 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024

HMBC Spectrum for 3



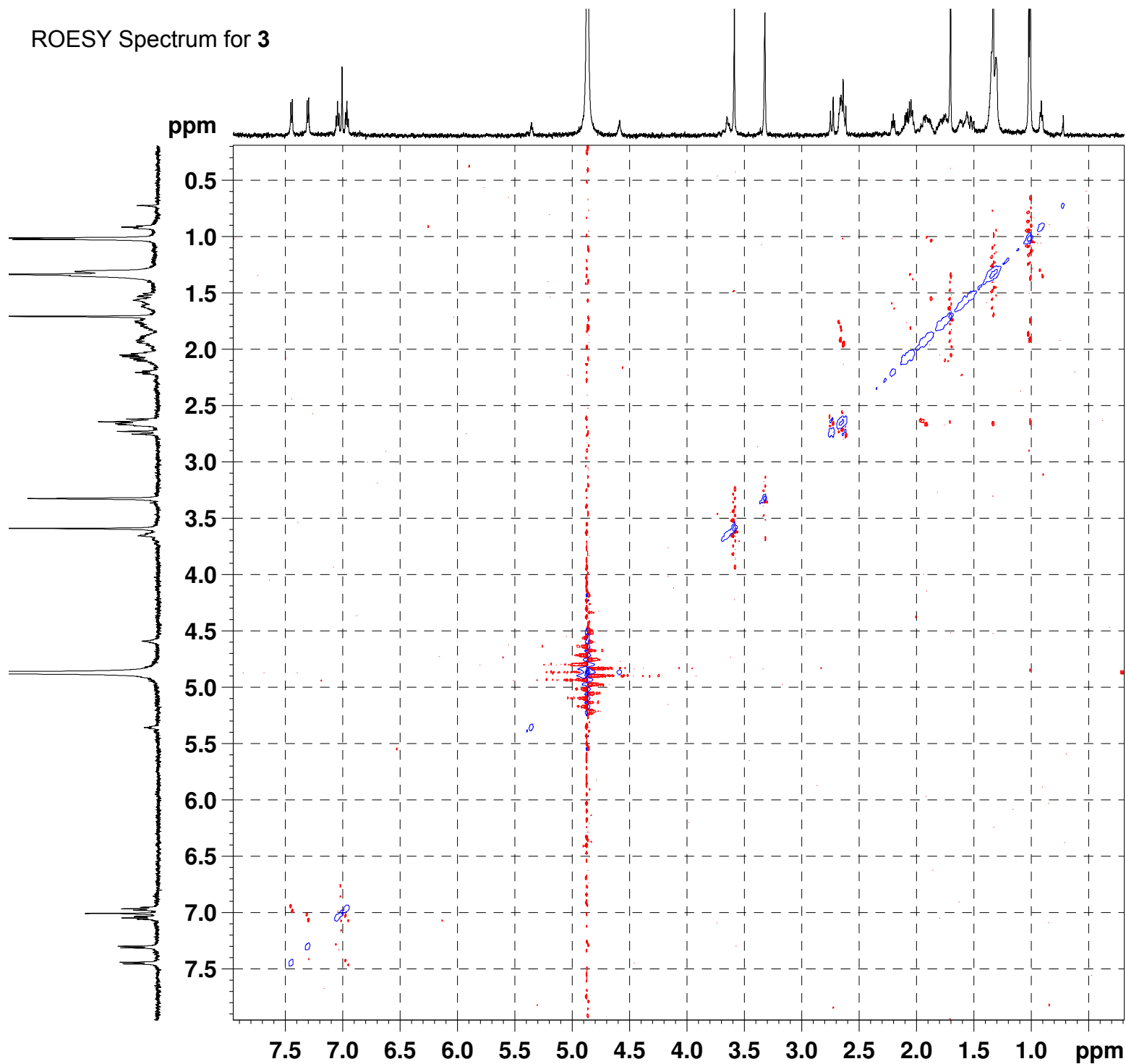
NAME SF_17359
EXPNO 5
PROCNO 1
Date_ 20081119
Time 3.36
INSTRUM spect
PROBHD 1 mm CapLC 1H-
PULPROG inv4gpglrmnd
TD 2048
SOLVENT MeOD
NS 512
DS 32
SWH 4664.179 Hz
FIDRES 2.277431 Hz
AQ 0.2195956 sec
RG 2048
DW 107.200 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.14429104 sec
d2 0.00344828 sec
D6 0.06600000 sec
d13 0.00000300 sec
D16 0.00025000 sec
IN0 0.00001185 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
P2 21.00 usec
PL1 13.00 dB
SFO1 600.1324414 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 10.00 usec
PL2 18.00 dB
SFO2 150.9178393 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 12.50 %
GPZ2 7.50 %
GPZ3 10.02 %
P16 1000.00 usec
ND0 2
TD 55
SFO1 150.9178 MHz
FIDRES 767.165344 Hz
SW 279.583 ppm
FnMODE QF
SI 1024
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 150.9025700 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

ROESY Spectrum for 3



NAME SF_17359
 EXPNO 4
 PROCNO 1
 Date_ 20081118
 Time_ 22.56
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG roesyph
 TD 2048
 SOLVENT MeOD
 NS 32
 DS 16
 SWH 4664.179 Hz
 FIDRES 2.277431 Hz
 AQ 0.2195956 sec
 RG 2048
 DW 107.200 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00009652 sec
 D1 1.47009802 sec
 d12 0.00002000 sec
 IN0 0.00021440 sec
 ST1CNT 0

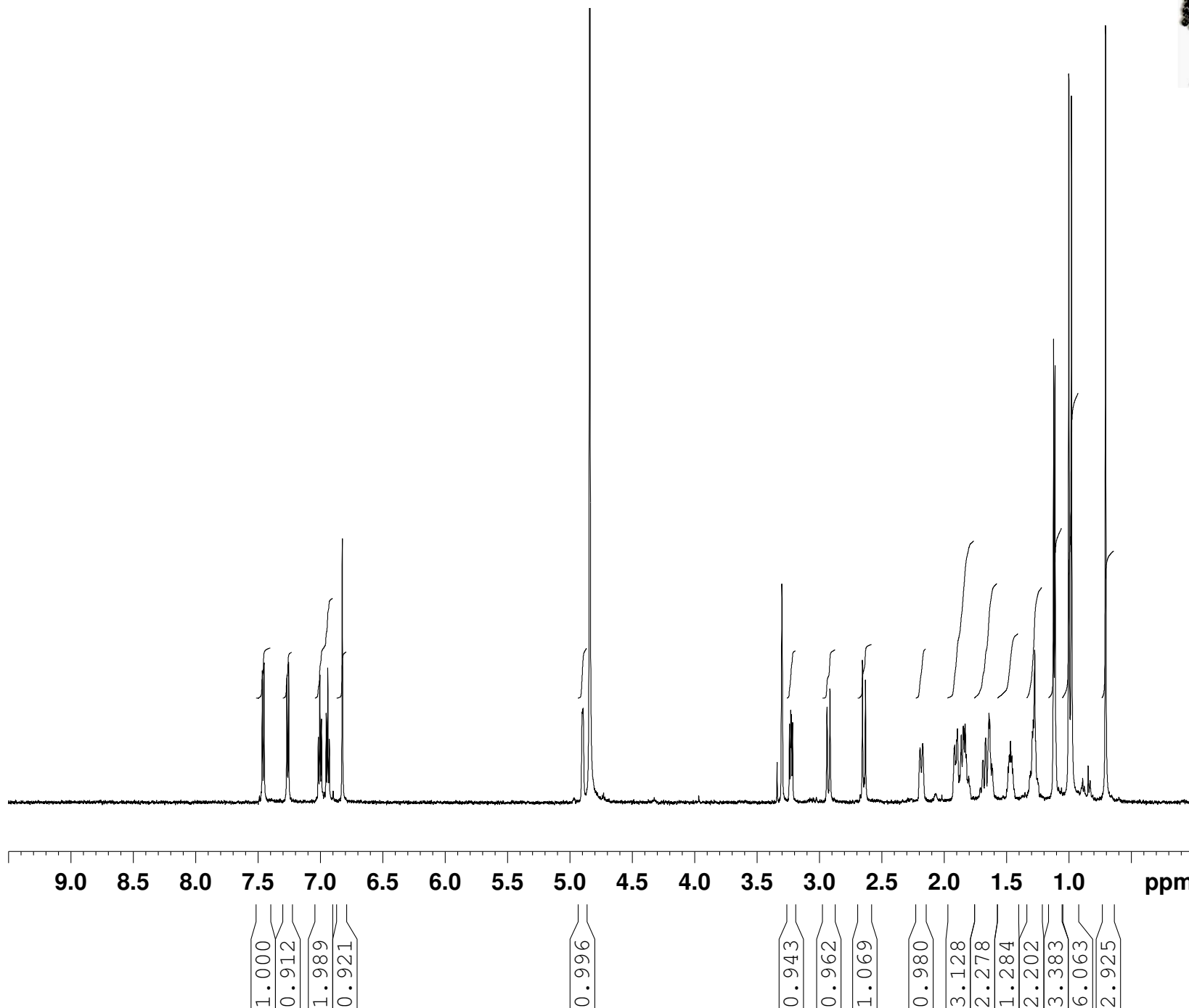
===== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 P15 250000.00 usec
 PL1 13.00 dB
 PL11 35.50 dB
 SFO1 600.1324414 MHz
 ND0 1
 TD 256
 SFO1 600.1324 MHz
 FIDRES 18.219450 Hz
 SW 7.772 ppm
 FnmODE States-TPPI
 SI 1024
 SF 600.1300000 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.00
 SI 1024
 MC2 States-TPPI
 SF 600.1300000 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

¹H NMR Spectrum for **4** in MeOD

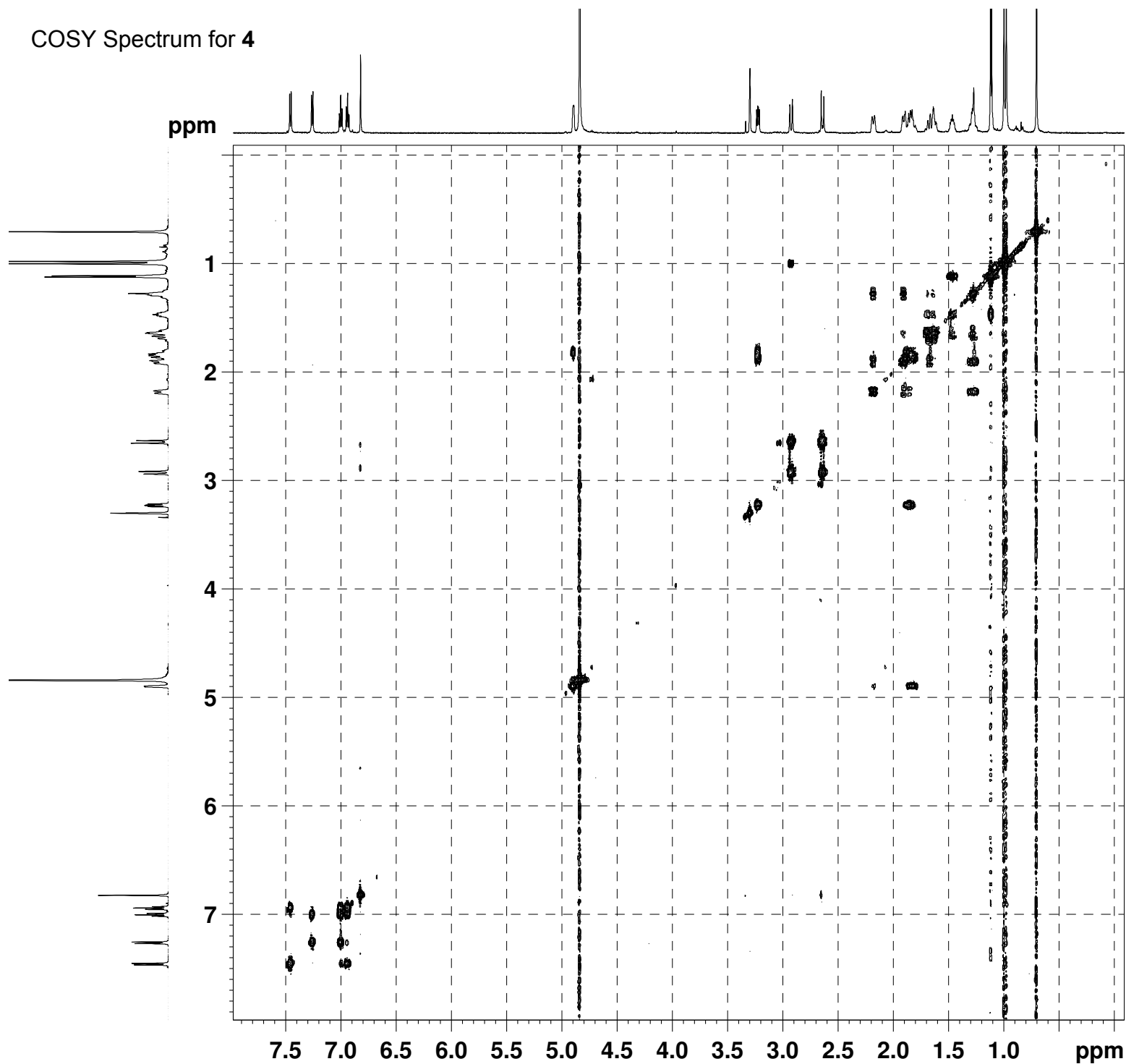


NAME SF_17184
 EXPNO 1
 PROCNO 1
 Date_ 20080827
 Time 15.01
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG zg
 TD 65536
 SOLVENT MeOD
 NS 64
 DS 2
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4079220 sec
 RG 2048
 DW 52.000 usec
 DE 6.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.00 usec
 PL1 13.00 dB
 SFO1 600.1329706 MHz
 SI 32768
 SF 600.1300138 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 2.00



COSY Spectrum for 4

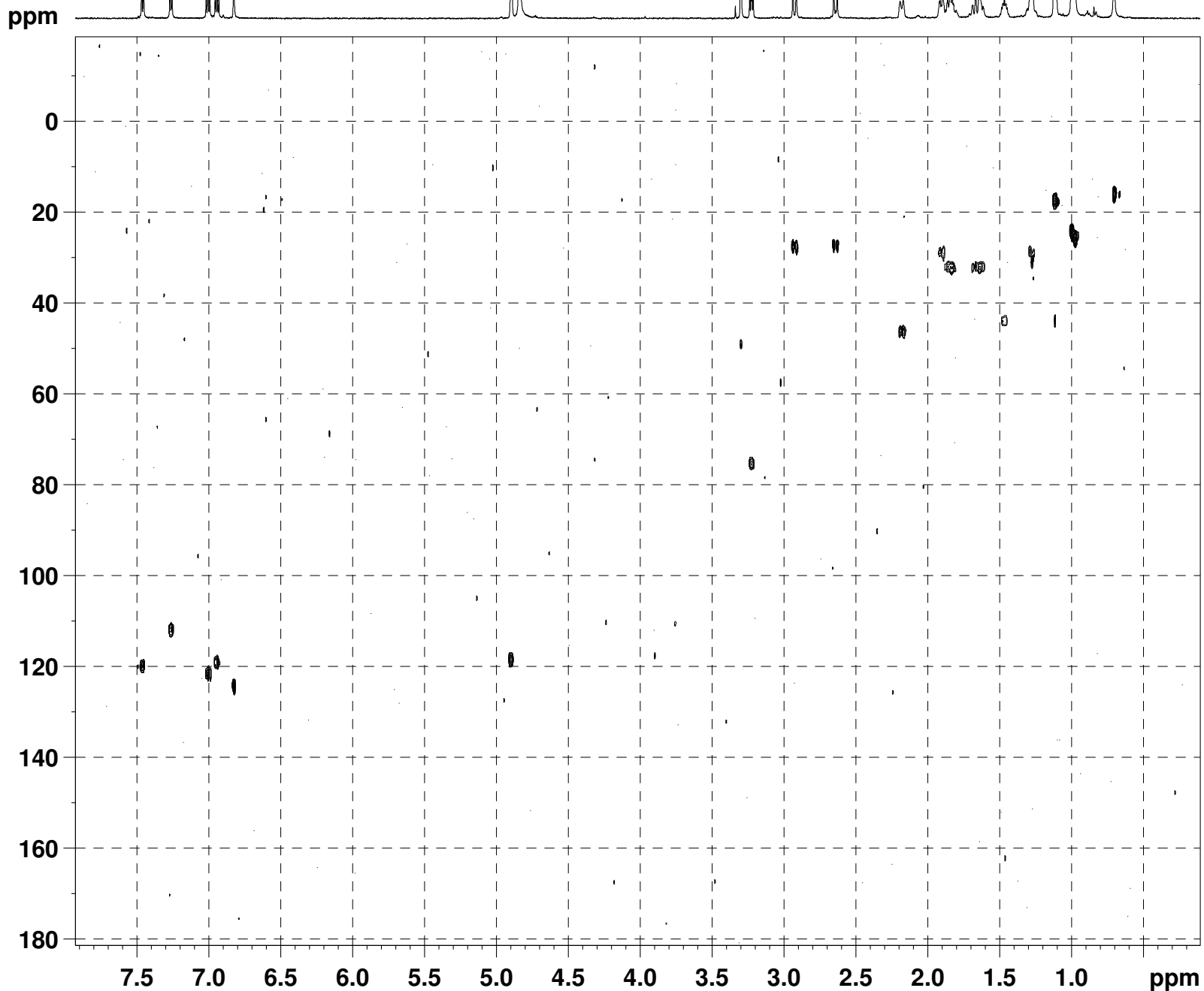


NAME SF_17184
 EXPNO 2
 PROCNO 1
 Date_ 20080827
 Time 15.08
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG cosygpcqf
 TD 2048
 SOLVENT MeOD
 NS 8
 DS 16
 SWH 4844.961 Hz
 FIDRES 2.365704 Hz
 AQ 0.2114036 sec
 RG 2048
 DW 103.200 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 1.33574498 sec
 d13 0.00000400 sec
 D16 0.00025000 sec
 IN0 0.00020640 sec

===== CHANNEL f1 =====
 NUC1 1H
 P0 9.50 usec
 P1 9.50 usec
 PL1 13.00 dB
 SFO1 600.1323774 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPZ1 6.00 %
 GPZ2 6.00 %
 P16 1000.00 usec
 ND0 1
 TD 256
 SFO1 600.1324 MHz
 FIDRES 18.925631 Hz
 SW 8.073 ppm
 FnMODE QF
 SI 1024
 SF 600.1300138 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00
 SI 1024
 MC2 QF
 SF 600.1300138 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

HSQC Spectrum for 4



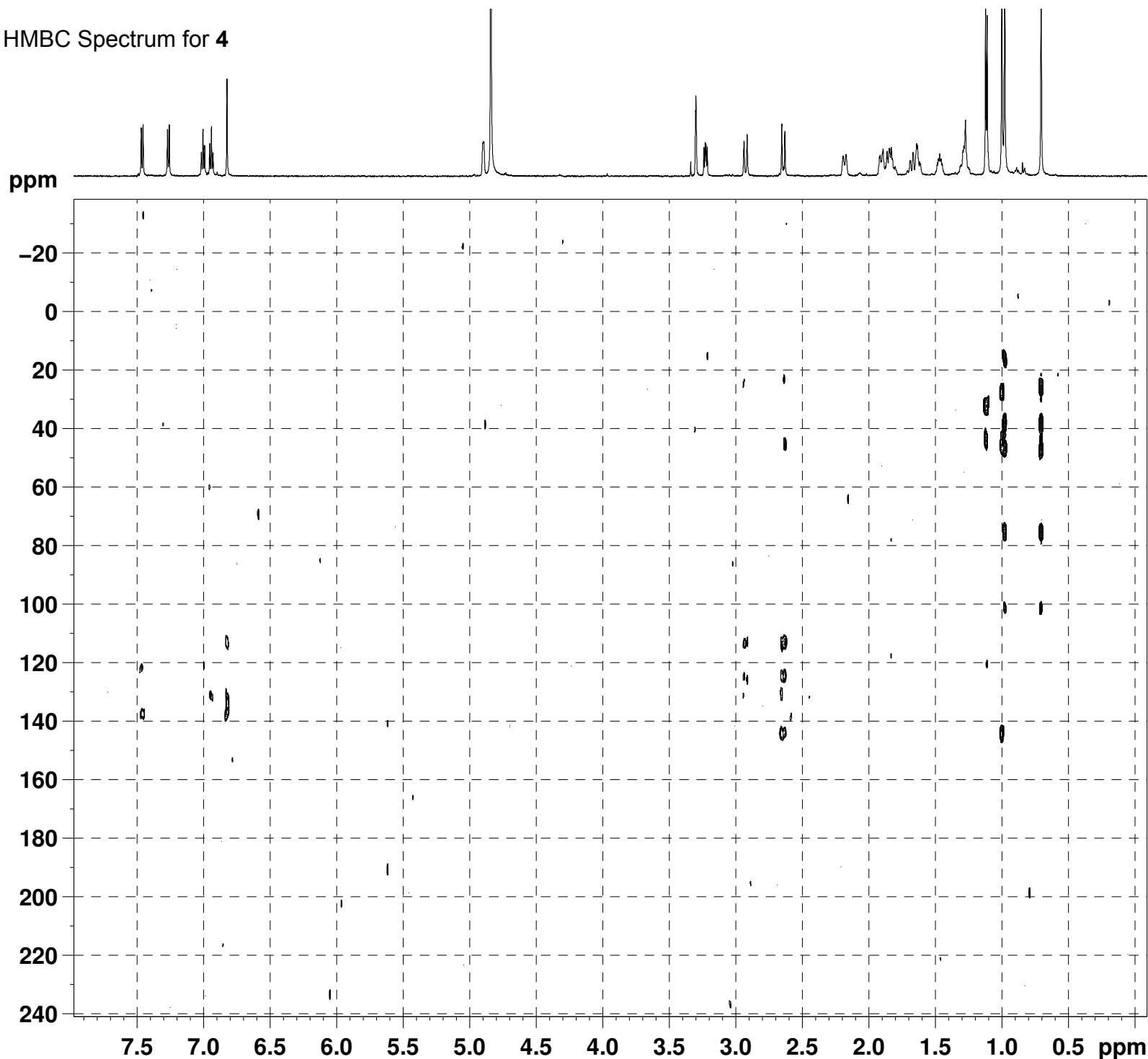
NAME SF_17184
 EXPNO 3
 PROCNO 1
 Date_ 20080827
 Time 16.05
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG hsqcetgpsisp.2
 TD 2048
 SOLVENT MeOD
 NS 128
 DS 32
 SWH 4844.961 Hz
 FIDRES 2.365704 Hz
 AQ 0.2114036 sec
 RG 2048
 DW 103.200 usec
 DE 115.71 usec
 TE 298.0 K
 CNST2 145.0000000
 CNST17 -0.5000000
 d0 0.00000300 sec
 D1 1.02670503 sec
 d4 0.00172414 sec
 d11 0.03000000 sec
 D16 0.00025000 sec
 D24 0.00086000 sec
 DELTA 0.00127100 sec
 DELTA1 0.00125800 sec
 DELTA2 0.00147014 sec
 DELTA3 0.00135600 sec
 IN0 0.00001655 sec
 ST1CNT 0

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.50 usec
 p2 19.00 usec
 P28 2000.00 usec
 PL1 13.00 dB
 SFO1 600.1323774 MHz

===== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 13C
 P3 10.00 usec
 P14 500.00 usec
 P24 2000.00 usec
 PCPD2 60.00 usec
 PL0 120.00 dB
 PL2 18.00 dB
 PL12 34.00 dB
 SFO2 150.9148810 MHz
 SP3 27.00 dB
 SP7 27.00 dB
 SPNAM3 Crp60,0.5,20.1
 SPNAM7 Crp60comp.4
 SPOAL3 0.500
 SPOAL7 0.500
 SPOFFS3 0.00 Hz
 SPOFFS7 0.00 Hz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPZ1 20.00 %
 GPZ2 5.03 %
 P16 1000.00 usec
 ND0 2
 TD 100
 SFO1 150.9149 MHz
 FIDRES 302.114807 Hz
 SW 200.189 ppm
 FnmODE Echo-Antiecho
 SI 1024
 SF 600.1300138 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024

HMBC Spectrum for 4



NAME SF_17184
 EXPNO 5
 PROCNO 1
 Date_ 20080827
 Time 22.57
 INSTRUM spect
 PROBHD 1 mm CapLC 1H-
 PULPROG inv4gpglrmnd
 TD 2048
 SOLVENT MeOD
 NS 448
 DS 32
 SWH 4844.961 Hz
 FIDRES 2.365704 Hz
 AQ 0.2114036 sec
 RG 2048
 DW 103.200 usec
 DE 6.00 usec
 TE 298.0 K
 CNST2 145.000000
 d0 0.00000300 sec
 D1 1.15248203 sec
 d2 0.00344828 sec
 D6 0.06600000 sec
 d13 0.00000300 sec
 D16 0.00025000 sec
 IN0 0.00001185 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.50 usec
 P2 19.00 usec
 PL1 13.00 dB
 SFO1 600.1323774 MHz

===== CHANNEL f2 =====
 NUC2 13C
 P3 10.00 usec
 PL2 18.00 dB
 SFO2 150.9178393 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPZ1 12.50 %
 GPZ2 7.50 %
 GPZ3 10.02 %
 P16 1000.00 usec
 ND0 2
 TD 100
 SFO1 150.9178 MHz
 FIDRES 421.940918 Hz
 SW 279.583 ppm
 FMODE QF
 SI 1024
 SF 600.1300138 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 QF
 SF 150.9025700 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

ROESY Spectrum for 4

ppm

1

2

3

4

5

6

7

7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm



NAME	SF_17184
EXPNO	4
PROCNO	1
Date_	20080827
Time	20.33
INSTRUM	spect
PROBHD	1 mm CapLC 1H-
PULPROG	zgpg30 presph
TD	2048
SOLVENT	MeOD
NS	16
DS	16
SWH	4844.961 Hz
FIDRES	2.365704 Hz
AQ	0.2114036 sec
RG	2048
DW	103.200 usec
DE	6.00 usec
TE	298.0 K
d0	0.00009315 sec
D1	1.47828901 sec
d12	0.00002000 sec
IN0	0.00020640 sec
ST1CNT	0

```

===== CHANNEL f1 =====
NUC1      1H
P1         9.50 usec
P15        250000.00 usec
PL1        13.00 dB
PL11       35.50 dB
SFO1       600.1323774 MHz
ND0        1
TD         256
SFO1       600.1324 MHz
FIDRES     18.925631 Hz
SW         8.073 ppm
FnMODE     States-TPPI
SI         1024
SF         600.1300138 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.00
SI         1024
MC2        States-TPPI
SF         600.1300138 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0

```