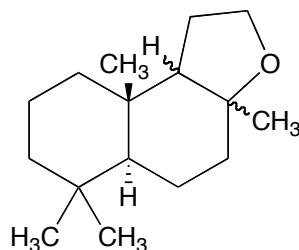
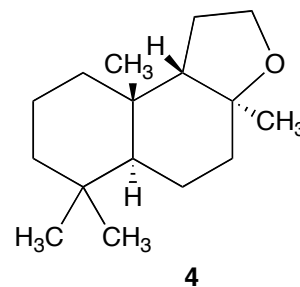
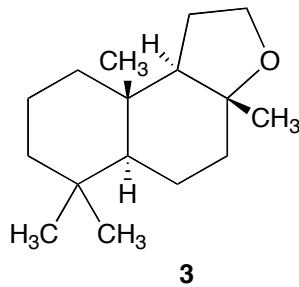
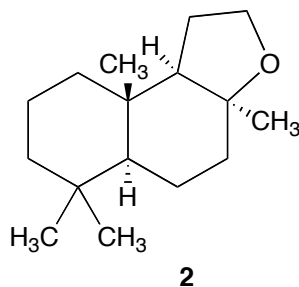
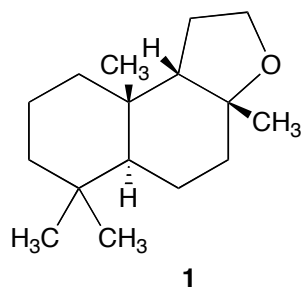


1. The following spectral data are provided for a tricyclic compound: 500.22 MHz ^1H NMR, 125.79 MHz ^{13}C NMR, DEPT, COSY, TOCSY, HMQC, HMBC, NOESY, and HSQC-TOCSY spectra with 5-, 10-, 20-, and 100-ms mixing times. All NMR spectra were measured in C_6D_6 solution.

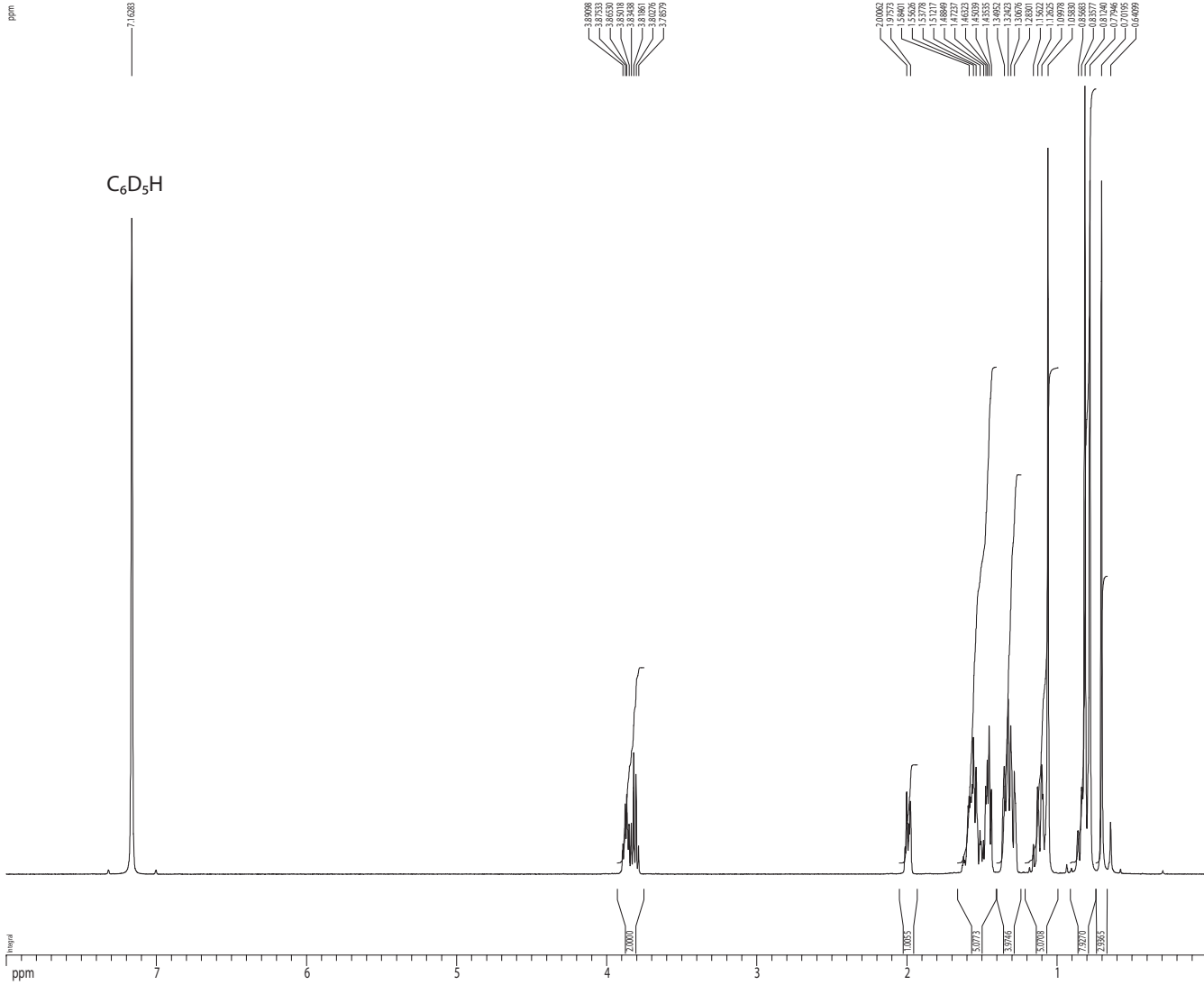


Using these data, determine the stereochemistry and assign all of the ^1H and ^{13}C resonances to their respective atoms in the structure. Specifically, assign the stereochemistry of the two stereocenters shown with squiggly lines, and hence which of the four possible diastereomers (**1**, **2**, **3**, or **4**) is consistent with these data.



MAKE SURE TO COMPLETELY ANSWER THE QUESTIONS **a-g** ON PAGES 2-6.

1H spectrum at 500 MHz in C₆D₆



3.8098
3.8753
3.8650
3.8418
3.8241
3.8181
3.8076
3.7879

2.1452
1.9351
1.5601
1.5506
1.5179
1.4869
1.4727
1.4529
1.4335
1.3952
1.3821
1.3676
1.3502
1.3201
1.0978
1.0800
0.8563
0.8340
-0.1796
-0.1405
-0.4079

Current Data Parameters
 USER nmr11t
 NAME nmr-X-sample11
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111128
 Time 11.59
 INSTRUM cryo200
 PROBRID 5mm EPTCI 1H-
 PULPROG zg30
 TD 81728
 SOLVENT C6D6
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 71
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 INCRST 0.00000000 sec
 MCWRC 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.223015 MHz

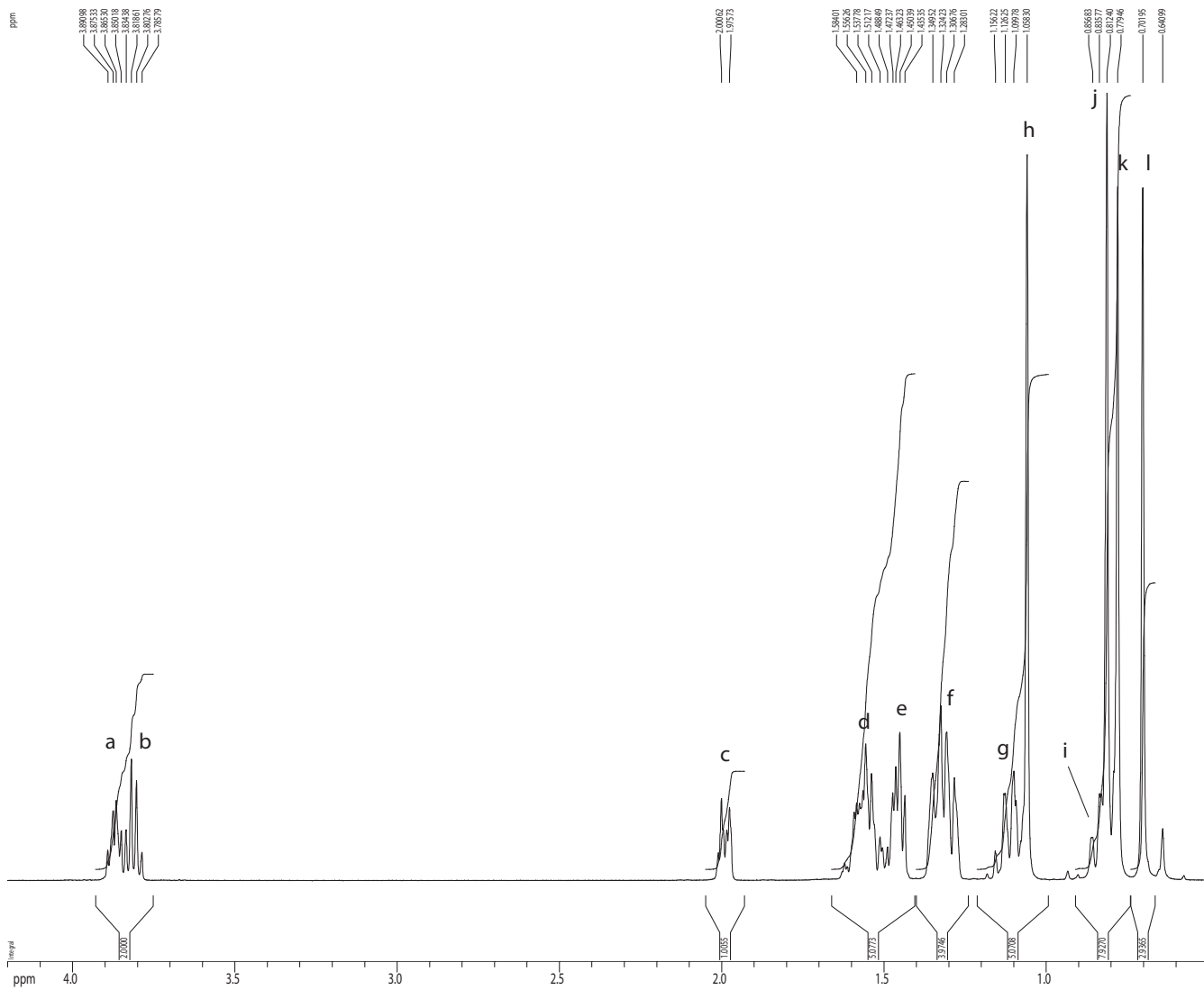
F2 - Processing parameters
 SI 6556
 SF 500.220000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F*P 8.000 ppm
 F1 4001.76 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PRGCM 0.33088 ppm/cm
 HZCM 175.51579 Hz/cm

DU=/v, USER=nmr11t, NAME=nmr-X-sample11, EXPNO=2, PROCNO=1
F1=4.200ppm, F2=0.500ppm, MI=0.50cm, MAXI=10000.00cm, PC=4.000

#	ADDRESS	FREQUENCY		INTENSITY
		[Hz]	[PPM]	
1	45487.8	1946.347	3.8910	0.62
2	45551.8	1938.519	3.8753	1.37
3	45592.8	1933.502	3.8653	1.56
4	45654.7	1925.939	3.8502	0.99
5	45719.3	1918.036	3.8344	1.01
6	45783.9	1910.146	3.8186	2.35
7	45848.7	1902.217	3.8028	1.94
8	45918.1	1893.729	3.7858	0.58
9	53221.7	1000.748	2.0006	1.60
10	53323.6	988.298	1.9757	1.43
11	54926.2	792.353	1.5840	1.52
12	55039.7	778.472	1.5563	2.64
13	55115.3	769.226	1.5378	2.07
14	55220.1	756.417	1.5122	0.87
15	55317.0	744.573	1.4885	0.68
16	55382.9	736.512	1.4724	1.71
17	55420.3	731.938	1.4632	2.20
18	55472.8	725.515	1.4504	2.86
19	55534.3	717.993	1.4354	1.65
20	55885.5	675.057	1.3495	2.09
21	55989.0	662.406	1.3242	3.36
22	56060.4	653.669	1.3068	2.86
23	56157.6	641.786	1.2830	1.99
24	56676.4	578.362	1.1562	0.61
25	56799.0	563.371	1.1262	1.70
26	56907.3	550.131	1.0998	2.12
27	57077.0	529.382	1.0583	13.83
28	57901.2	428.605	0.8568	0.86
29	57987.4	418.071	0.8358	1.69
30	58083.0	406.376	0.8124	15.00
31	58217.8	389.900	0.7795	13.22
32	58534.9	351.131	0.7020	13.21
33	58784.3	320.638	0.6410	1.03

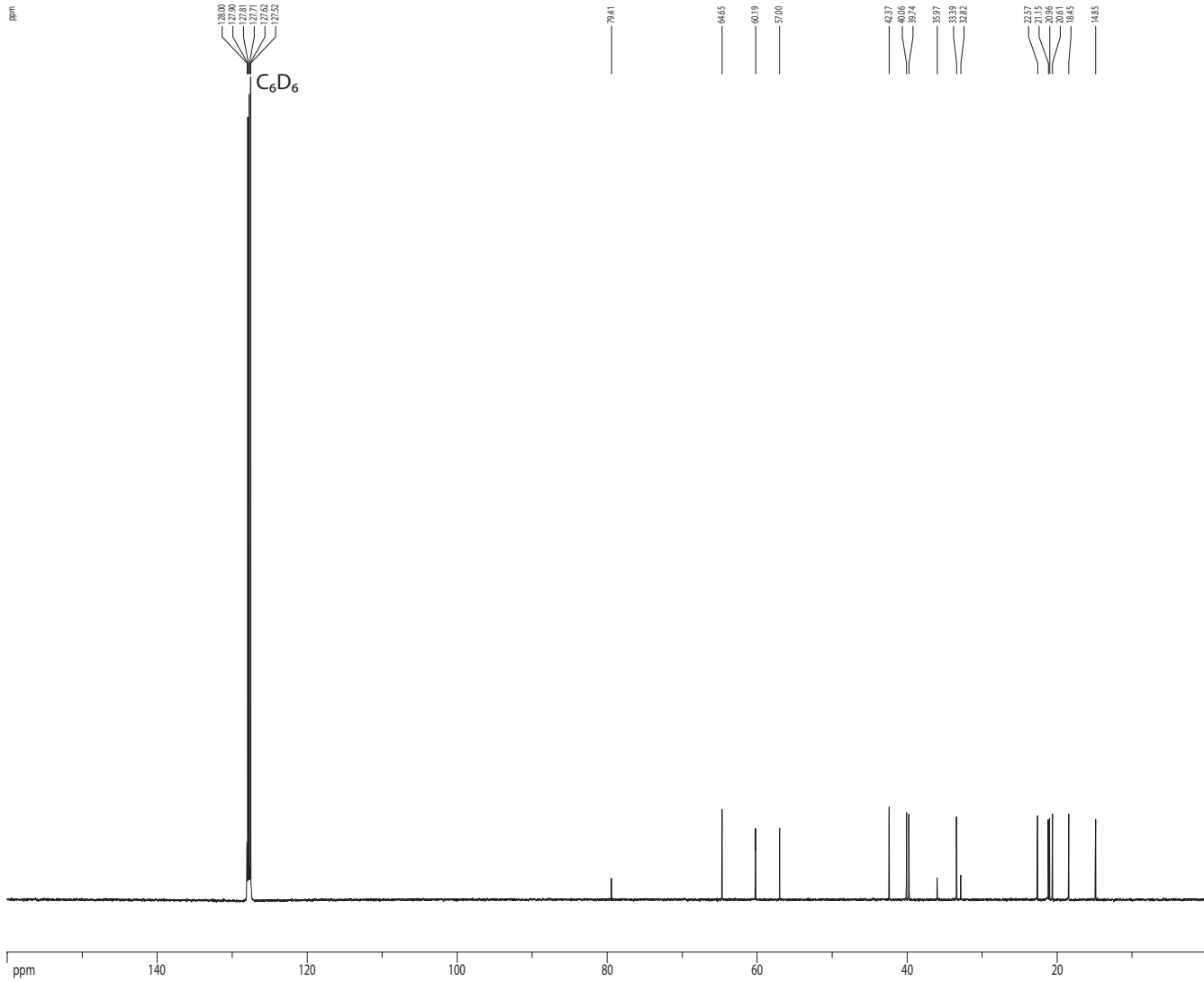
1H spectrum at 500 MHz in C₆D₆



Current Data Parameters
 USER nmr11t
 NAME nmr-X-sample11
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20111128
 Time 11:59
 INSTRUM cryo500
 PROBHD 5mm CPXI 1H-
 PULPROG zg30
 TD 81728
 SOLVENT C6D6
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 7.1
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.1000000 sec
 MCREST 0.0000000 sec
 MCNPRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.235015 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.220000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 4.00
 1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 FIP 4.210 ppm
 F1 2100.52 Hz
 F2P 0.500 ppm
 F2 250.11 Hz
 PPMCM 0.16228 ppm/cm
 HZCM 81.17655 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling at 125 MHz in C₆D₆



```

Current Data Parameters
USER          nmr11t
NAME         nmr-x-sample11
EXPNO        3
PROCNO       1

F2 - Acquisition Parameters
Date_        20111128
Time         12.02
INSTRUM      cryo500
PROBHD       5 mm CFC 1H-
PULPROG      SpinEcho30gpgp
TD           65536
SOLVENT      C6D6
NS           330
DS           16
SWH          30393.031 Hz
FIDRES       0.462388 Hz
AQ           1.0815940 sec
RG           327.08
DW           16.500 usec
DE           6.00 usec
TE           296.0 K
D1           0.25000000 sec
d11          0.03000000 sec
D16          0.00300000 sec
d17          0.00019000 sec
MCREST      0.00000000 sec
MCWRRK      0.01500000 sec
F2           31.00 usec

===== CHANNEL f1 =====
NUC1         13C
P1           15.50 usec
P11          500.00 usec
P12          2000.00 usec
PL0          120.00 dB
PL1          -1.00 dB
SFO1         125.7942548 MHz
SP1          3.20 dB
SP2          3.20 dB
SFO1M1       Ccp60.5.20.1
SFO1M2       Ccp60comp.4
SFOFF1       0.00 Hz
SFOFF2       0.00 Hz

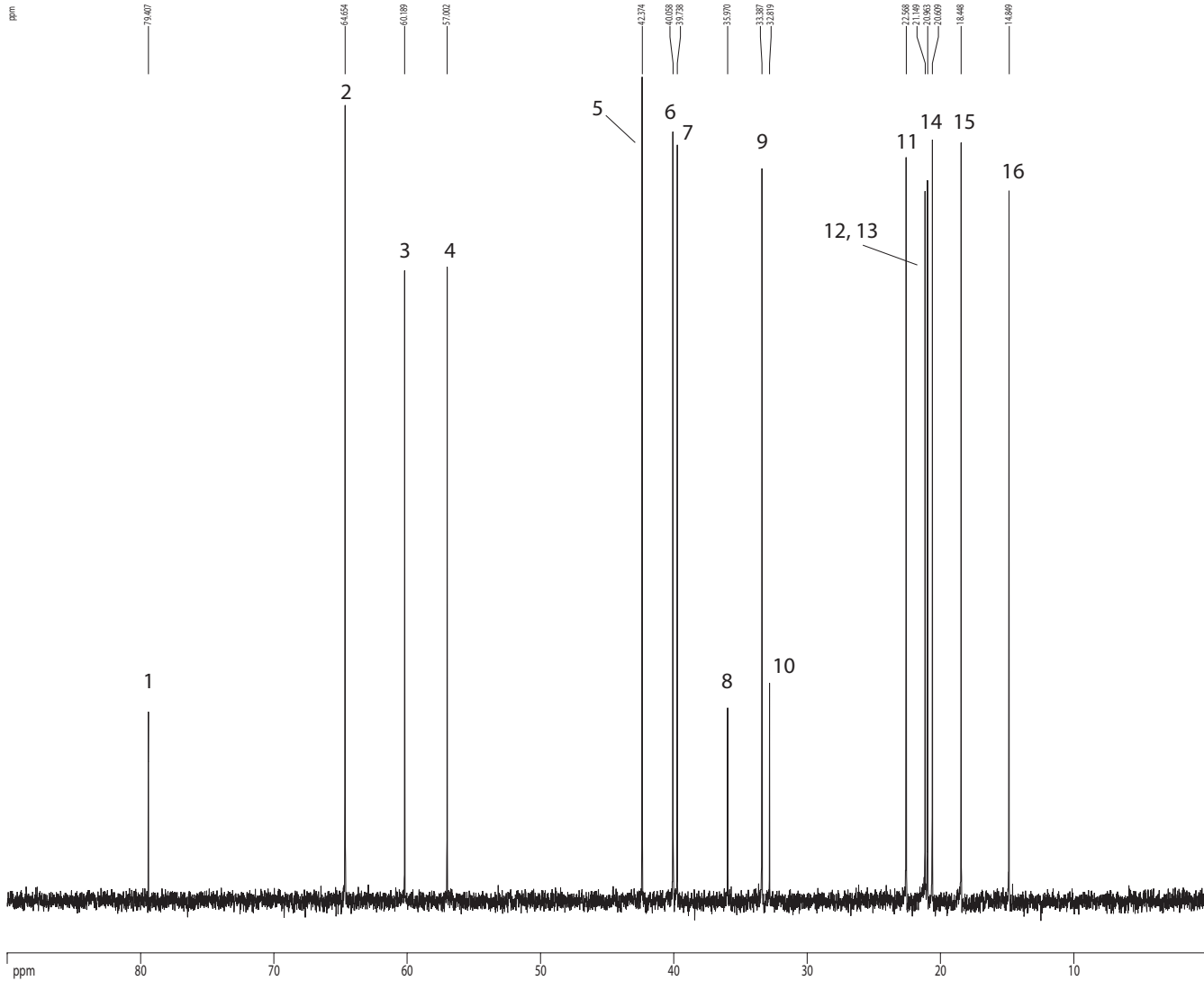
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2         1H
PCPD2        100.00 usec
PL2          1.60 dB
PL12         24.50 dB
SFO2         500.2225011 MHz

===== GRADIENT CHANNEL =====
GPNAM1       SINE.100
GPNAM2       SINE.100
GPR1         0.00 %
GPR2         0.00 %
GPR3         0.00 %
GPR4         0.00 %
GPR5         0.00 %
GPR6         0.00 %
GPR7         0.00 %
GPR8         0.00 %
GPR9         0.00 %
GPR10        0.00 %
GPR11        0.00 %
GPR12        0.00 %
GPR13        0.00 %
GPR14        0.00 %
GPR15        0.00 %
GPR16        0.00 %
GPR17        0.00 %
GPR18        0.00 %
GPR19        0.00 %
GPR20        0.00 %
GPR21        30.00 %
GPR22        50.00 %
p15          500.00 usec
d16          1000.00 usec

F2 - Processing parameters
SI           65536
SF           125.7804190 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           2.00

1D NMR plot parameters
CX           22.80 cm
CY           15.65 cm
FIP         160.000 ppm
F1           201.24371 Hz
F2P         0.000 ppm
F2           0.00 Hz
FPMCM       7.01754 ppm/cm
HECM        882.66963 Hz/cm
    
```

Z-restored spin-echo 13C spectrum with 1H decoupling at 125 MHz in C₆D₆



```

Current Data Parameters
USER          nmr11t
NAME         nmr-x-sample11
EXPNO        3
PROCNO       1

F2 - Acquisition Parameters
Date_        2011128
Time         12.02
INSTRUM      cryo500
PROBHD       5 mm CFC 1H-
PULPROG      SpinEcho30gp.prd
TD           65536
SOLVENT      C6D6
NS           330
DS           16
SWH          30393.031 Hz
FIDRES       0.462388 Hz
AQ           1.0815940 sec
RG           32768
DW           16.500 usec
DE           6.00 usec
TE           298.2 K
D1           0.25000000 sec
d11          0.03000000 sec
D16          0.00030000 sec
d17          0.00019000 sec
MCREST      0.00000000 sec
MCWRRK      0.01500000 sec
F2           31.00 usec

===== CHANNEL f1 =====
NUC1         13C
P1           15.50 usec
P11          500.00 usec
P12          2000.00 usec
PL0          120.00 dB
PL1          -1.00 dB
SFO1         125.7942548 MHz
SP1          3.20 dB
SP2          3.20 dB
SPNAM1       Cp60.0.5.20.1
SPNAM2       Cp60comp.4
SFOFF1       0.00 Hz
SFOFF2       0.00 Hz

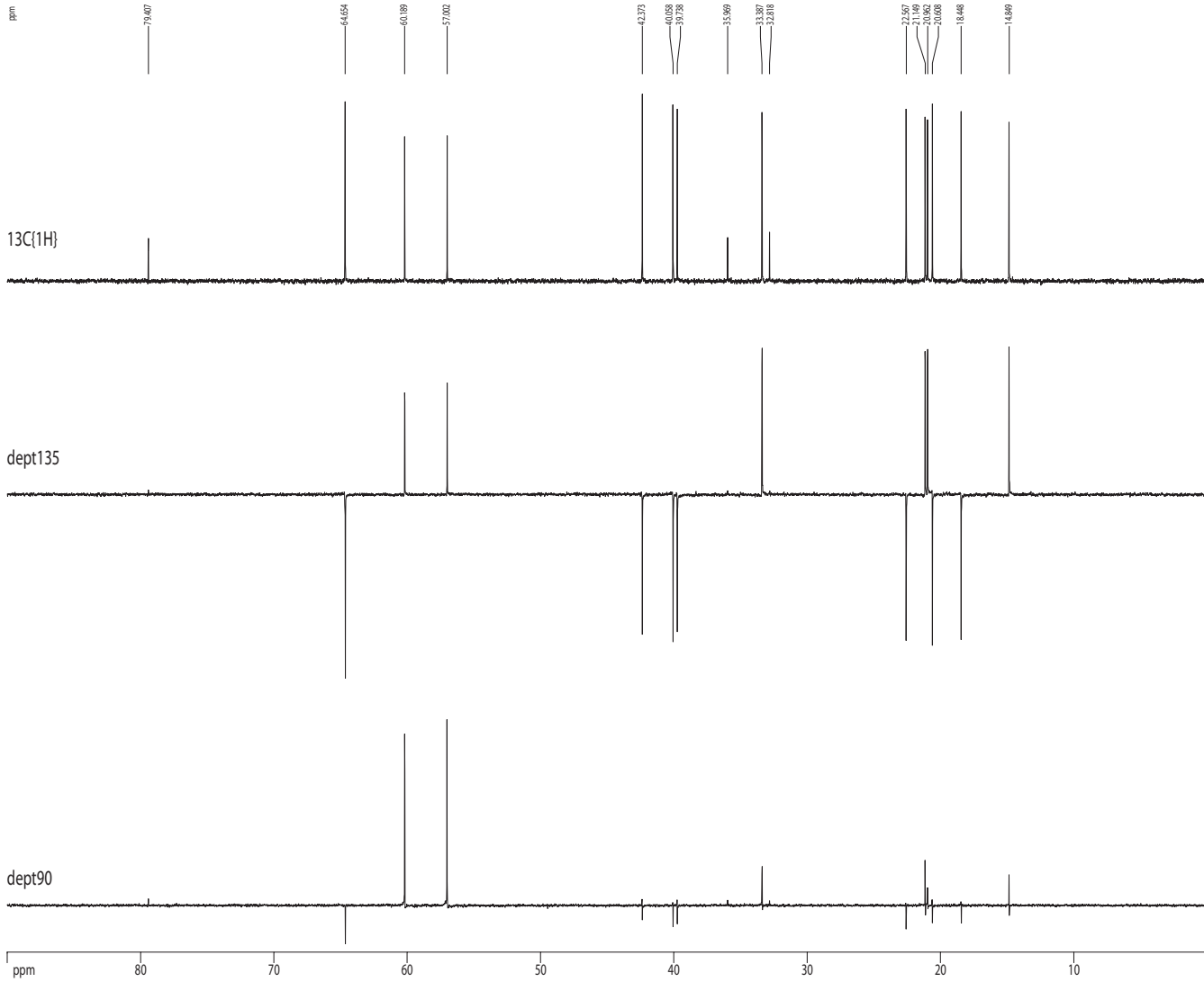
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2         1H
PCPD2        100.00 usec
PL2          1.60 dB
PL12         24.50 dB
SFO2         500.2225011 MHz

===== GRADIENT CHANNEL =====
GPNAM1       SINE.100
GPNAM2       SINE.100
GPI1         0.00 %
GPI2         0.00 %
GPI3         0.00 %
GPI4         0.00 %
GPI5         0.00 %
GPI6         0.00 %
GPI7         0.00 %
GPI8         0.00 %
GPI9         0.00 %
GPI10        0.00 %
GPI11        0.00 %
GPI12        0.00 %
GPI13        0.00 %
GPI14        0.00 %
GPI15        0.00 %
GPI16        0.00 %
GPI17        0.00 %
GPI18        0.00 %
GPI19        0.00 %
GPI20        0.00 %
GPI21        30.00 %
GPI22        50.00 %
GPI23        50.00 %
GPI24        50.00 %
GPI25        50.00 %
GPI26        50.00 %
GPI27        50.00 %
GPI28        50.00 %
GPI29        50.00 %
GPI30        50.00 %
GPI31        50.00 %
GPI32        50.00 %
GPI33        50.00 %
GPI34        50.00 %
GPI35        50.00 %
GPI36        50.00 %
GPI37        50.00 %
GPI38        50.00 %
GPI39        50.00 %
GPI40        50.00 %
GPI41        50.00 %
GPI42        50.00 %
GPI43        50.00 %
GPI44        50.00 %
GPI45        50.00 %
GPI46        50.00 %
GPI47        50.00 %
GPI48        50.00 %
GPI49        50.00 %
GPI50        50.00 %

F2 - Processing parameters
SI           65536
SF           125.7804190 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           2.00

TD NMR plot parameters
CX           22.80 cm
CY           15.65 cm
FIP          90.00 ppm
F1           11320.24 Hz
F2P          0.000 ppm
F2           0.00 Hz
FPMCM        3.94732 ppm/cm
HECM         496.50168 Hz/cm
    
```

Z-restored spin-echo 13C spectrum with 1H decoupling at 125 MHz in C₆D₆



```

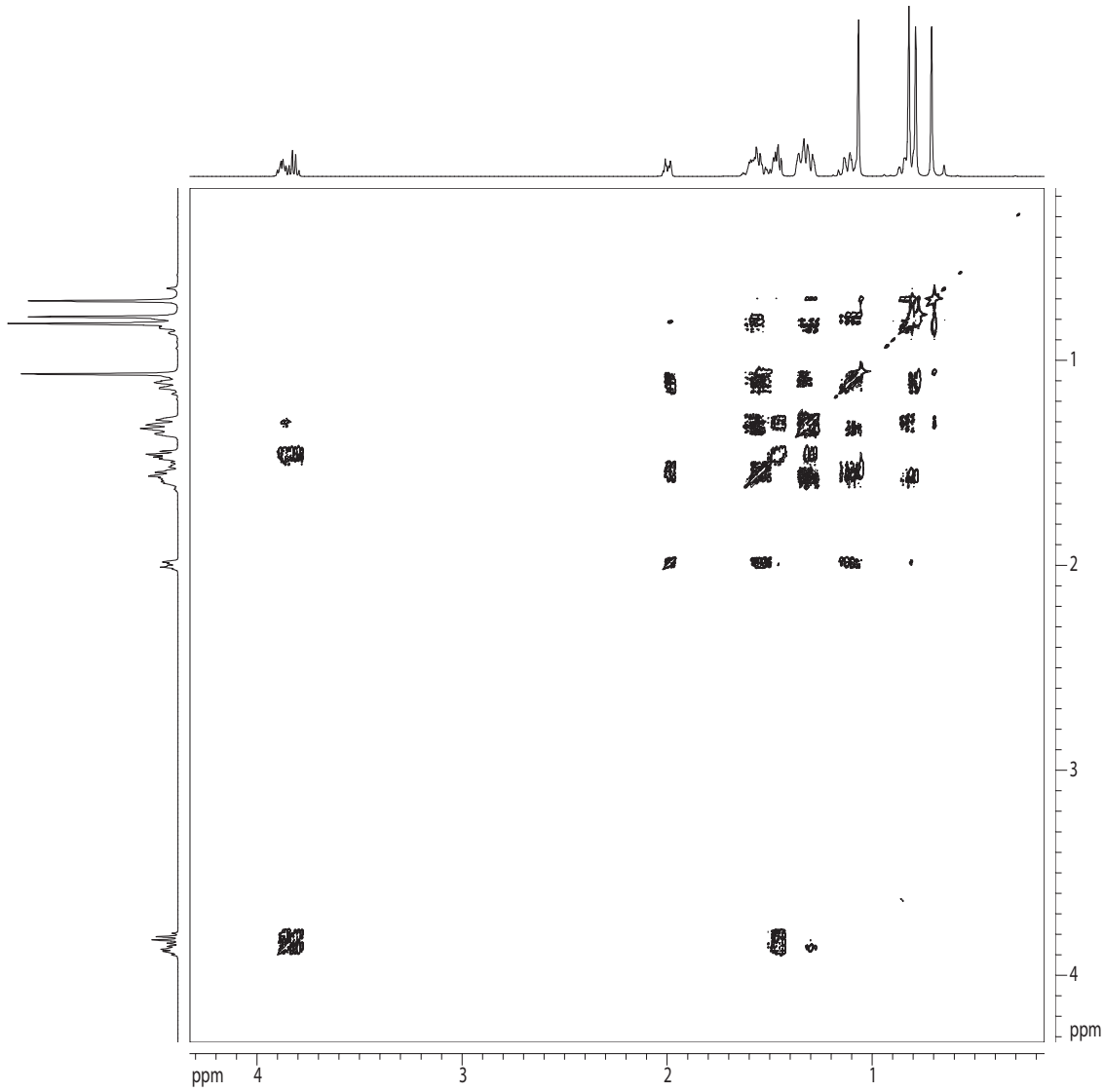
Current Data Parameters
USER          nmr11t
NAME         nmr-x-sample11
EXPNO        5
PROCNO       1

F2 - Acquisition Parameters
Date_        20111128
Time         12.02
INSTRUM      cryo500
PROBHD       5 mm CFC1 1H-
PULPROG      SpinEcho30ppg.prd
TD           65536
SOLVENT      CDCl3
NS           330
DS           16
SWH          30393.031 Hz
FIDRES       0.462388 Hz
AQ           1.0815940 sec
RG           32768
DW           16.500 usec
DE           6.00 usec
TE           298.2 K
D1           0.25000000 sec
d11          0.03000000 sec
D16          0.00300000 sec
d17          0.00019000 sec
dCREST       0.00000000 sec
NUC1PROG     13C
===== CHANNEL f1 =====
NUC1         13C
P1           15.50 usec
P11          500.00 usec
P12          2000.00 usec
PL0          120.00 dB
PL1          -1.00 dB
SFO1         125.760548 MHz
SP1          3.20 dB
SP2          3.20 dB
SFO2         125.760548 MHz
SFO1         125.760548 MHz
SFO2         500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1       SINE.100
GPNAM2       SINE.100
GP11         0.00 %
GP12         0.00 %
GP21         0.00 %
GP22         0.00 %
GP31         30.00 %
GP32         50.00 %
p15          500.00 usec
p16          1000.00 usec

F2 - Processing parameters
SI           65536
SF           125.7604190 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           2.00

TD NMR plot parameters
CX           22.80 cm
CY           3.56 cm
FIP          90.000 ppm
F1           11320.24 Hz
F2P          0.000 ppm
F2           0.00 Hz
FPMCM        3.94737 ppm/cm
FECM         496.50168 Hz/cm
    
```

gcosy60



```
Current Data Parameters
USER nmr11t
NAME nmr-X-sample11
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111130
Time 21.35
INSTRUM cryo500
PROBHD 5 mm CPYCI 1H-
PULPROG cosygp60.prd
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 2083.333 Hz
FIDRES 1.017253 Hz
AQ 0.4915700 sec
RG 35.9
DW 240.000 usec
DE 6.00 usec
TE 298.0 K
d0 0.0000300 sec
D1 1.0000000 sec
d13 0.00000300 sec
D16 0.0002000 sec
IN0 0.0004800 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 1.80 dB
SFO1 500.2211225 MHz

===== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 17.00 %
GPZ2 17.00 %
P16 1000.00 usec

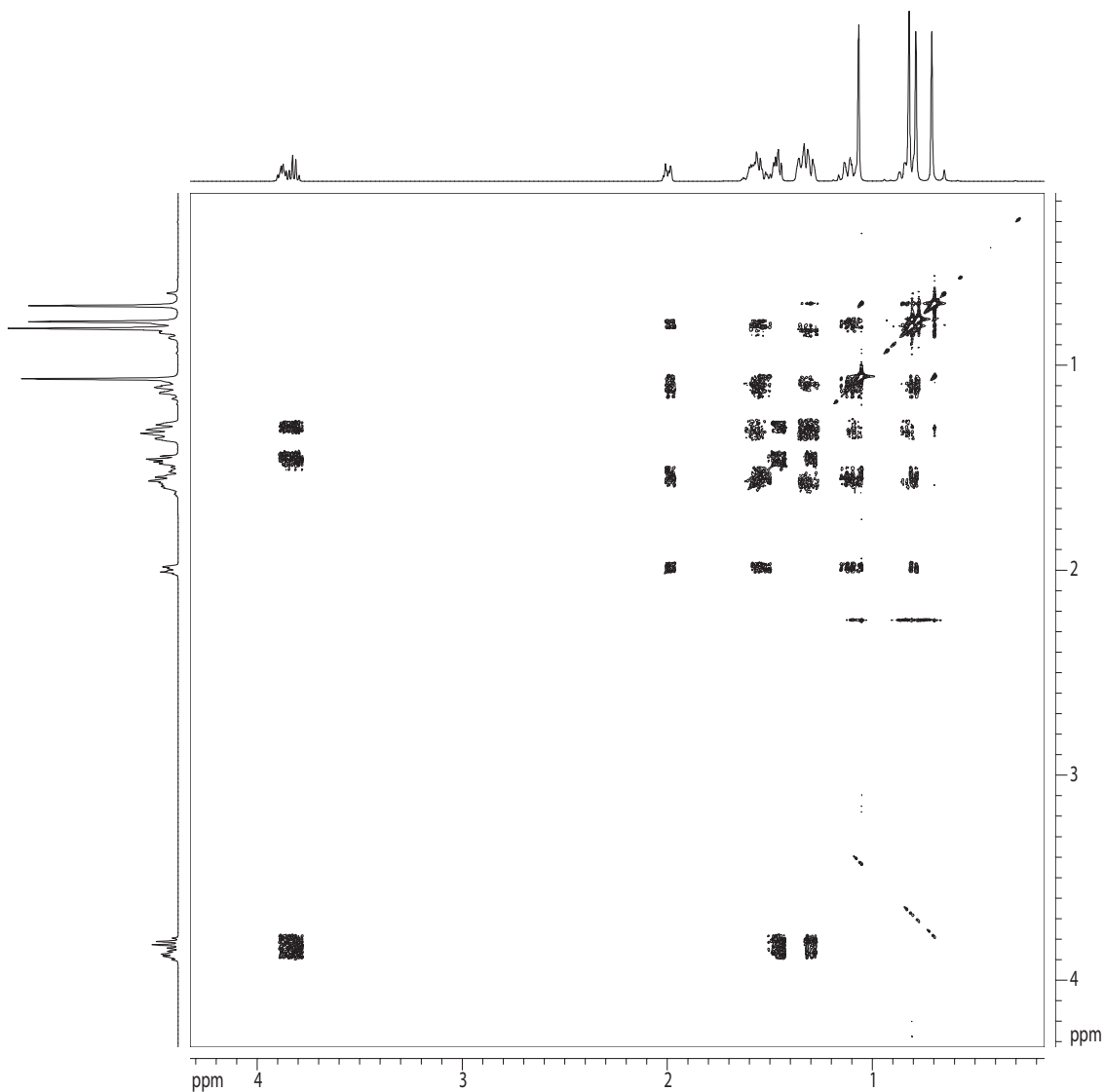
F1 - Acquisition parameters
ND0 1
TD 512
SFO1 500.2211 MHz
FIDRES 4.059010 Hz
SW 4.165 ppm
FnMODE undefined

F2 - Processing parameters
SI 1024
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 4.326 ppm
F2LO 2164.12 Hz
F2PHI 0.162 ppm
F2HI 80.79 Hz
F1PLO 4.326 ppm
F1LO 2164.12 Hz
F1PHI 0.162 ppm
F1HI 80.79 Hz
F2PPMCM 0.27766 ppm/cm
F2HZCM 138.88889 Hz/cm
F1PPMCM 0.27766 ppm/cm
F1HZCM 138.88889 Hz/cm
```


gtocsy



```
Current Data Parameters
USER      nmr11t
NAME      nmr-X-sample11
EXPNO     9
PROCNO    1

F2 - Acquisition Parameters
Date_     20111130
Time      22.32
INSTRUM   cryo500
PROBHD    5mm CPTCI 1H-
PULPROG   mzgpg_me
TD         2048
SOLVENT   CDCl3
NS         4
DS         16
SWH        2083.333 Hz
FIDRES     1.017253 Hz
AQ         0.4915700 sec
RG         35.9
DW         240.000 usec
DE         6.00 usec
TE         298.0 K
d0         0.00000300 sec
D1         2.00000000 sec
D9         0.06000000 sec
d12        0.00002000 sec
D15        0.00000000 sec
FACTOR1    4
INO         0.00048000 sec
II         24
SCALEF     6

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
p5         23.34 usec
P6         35.00 usec
p7         70.00 usec
P17        2500.00 usec
PL1        1.60 dB
PL10       15.20 dB
SFO1       500.2211225 MHz

===== GRADIENT CHANNEL =====
GPNAM1     sine.100
GPNAM2     sine.100
GPX1       0.00 %
GPX2       0.00 %
GPY1       0.00 %
GPY2       0.00 %
GPZ1       10.00 %
GPZ2       10.00 %
P16        1000.00 usec

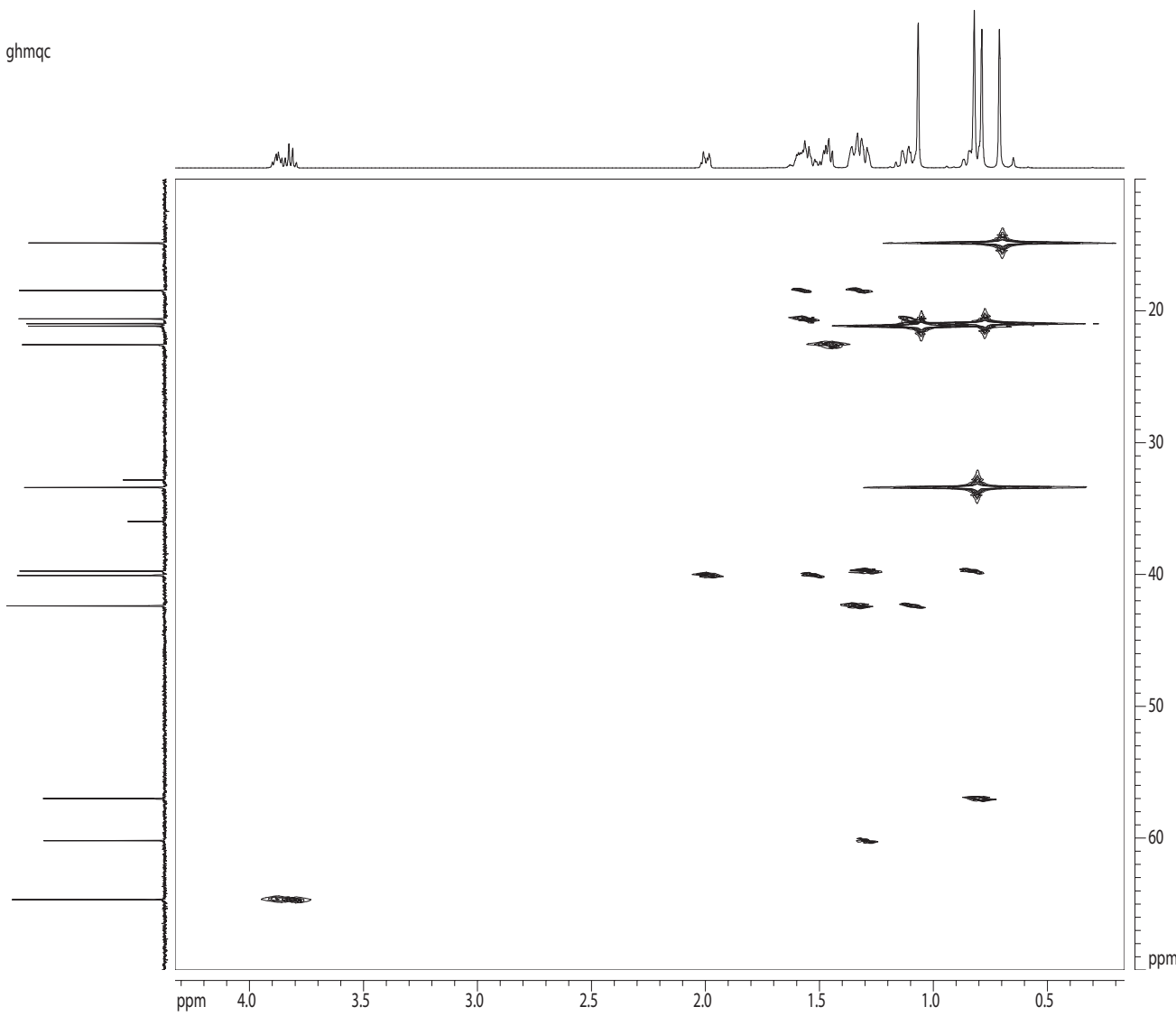
F1 - Acquisition parameters
ND0        1
TD         512
SFO1       500.2211 MHz
FIDRES     4.069010 Hz
SW         4.165 ppm
FmMODE     undefined

F2 - Processing parameters
SI         1024
SF         500.2200000 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        QF
SF         500.2200000 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0

2D NMR plot parameters
CX2        15.00 cm
CX1        15.00 cm
F2PLO      4.326 ppm
F2LO       2164.12 Hz
F2PHI      0.162 ppm
F2HI       80.79 Hz
F1PLO      4.326 ppm
F1LO       2164.12 Hz
F1PHI      0.162 ppm
F1HI       80.79 Hz
F2PPMCM    0.27766 ppm/cm
F2HZCM     138.88889 Hz/cm
F1PPMCM    0.27766 ppm/cm
F1HZCM     138.88889 Hz/cm
```

ghmqc



Current Data Parameters
USER: nmr11
NAME: nmr11-sample11
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20111201
Time: 0:04
INSTRUM: cryo500
PROBHD: 5 mm CPFI 1H-
PULPROG: jw4gpgwuu
TD: 2048
SOLVENT: CDCl3
NS: 4
DS: 16
SWH: 2083.333 Hz
FIDRES: 1.017253 Hz
AQ: 0.4915700 sec
RG: 729.2
DW: 240.000 usec
DE: 6.50 usec
TE: 298.0 K
CNST2: 145.000000
d0: 0.00000000 usec
D1: 1.0000000 sec
d2: 0.00344828 sec
d12: 0.00000000 sec
d13: 0.00000000 sec
D16: 0.00000000 sec
d20: 0.00242528 sec
W0: 0.0004966 usec

===== CHANNEL f1 =====
NUC1: 1H
P1: 7.50 usec
p2: 15.00 usec
PL1: 1.00 dB
SFO1: 500.2211225 MHz

===== CHANNEL f2 =====
CPDPRG2: gpgp
NUC2: 13C
P3: 15.50 usec
PCPD2: 65.00 usec
PL2: -1.00 dB
PL12: 11.30 dB
SFO2: 125.7665620 MHz

===== GRADIENT CHANNEL =====
GPNAM1: sine100
GPNAM2: sine100
GPNAM3: sine100
GPX1: 0.00 %
GPX2: 0.00 %
GPX3: 0.00 %
GPY1: 0.00 %
GPY2: 0.00 %
GPY3: 0.00 %
GPZ1: 30.00 %
GPZ2: 18.00 %
GPZ3: 24.00 %
P16: 1000.00 usec

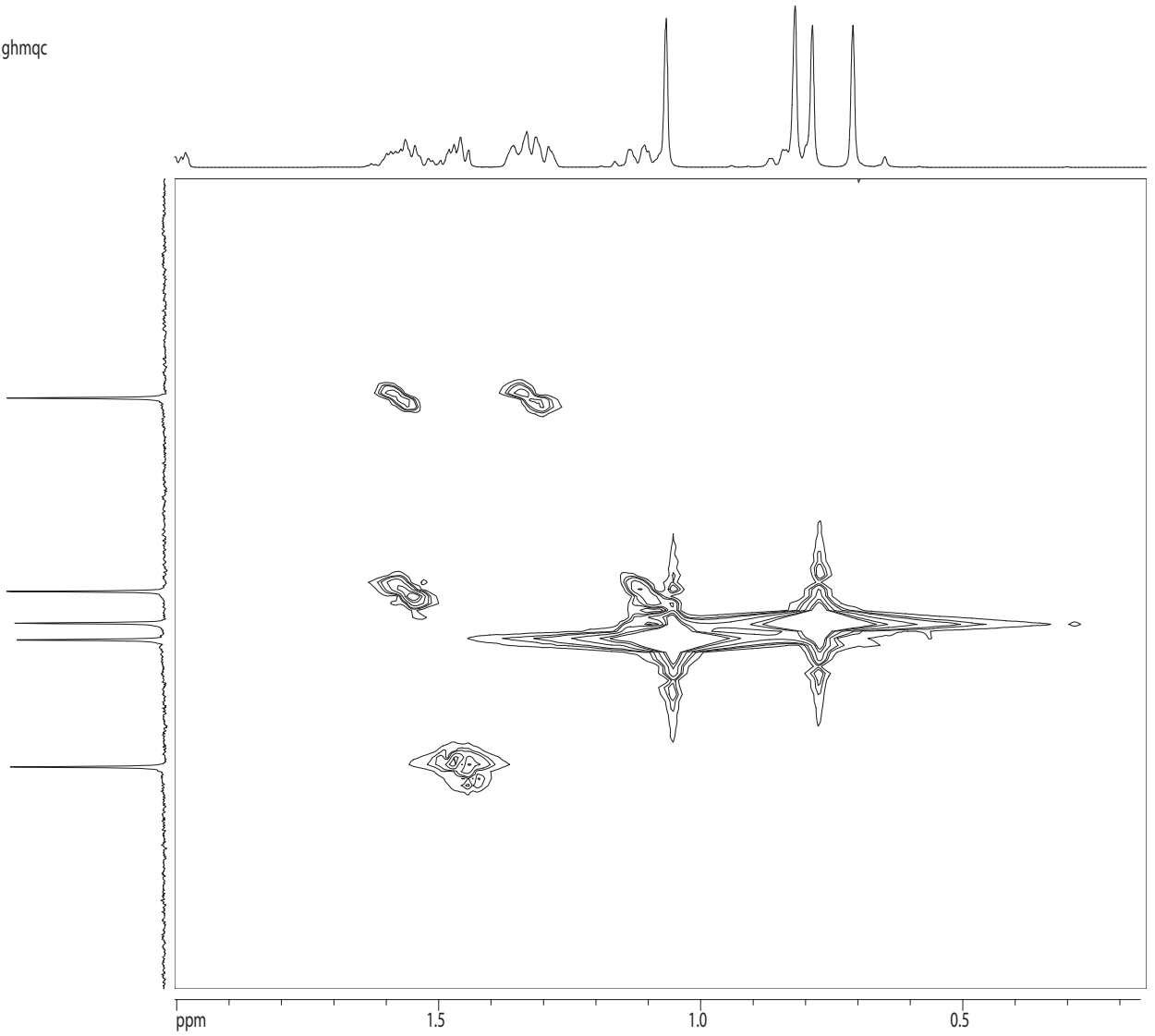
F1 - Acquisition parameters
ND0: 2
TD: 512
SFO1: 125.7866 MHz
FIDRES: 19.888761 Hz
SW: 80.141 ppm
FMODE: undefined

F2 - Processing parameters
SI: 1024
SF: 500.220000 MHz
WDW: EM
SSB: 0
LB: 5.00 Hz
GB: 0
PC: 1.40

F1 - Processing parameters
SI: 1024
MC2: QF
SF: 125.780490 MHz
WDW: GSNR
SSB: 3
LB: 0.00 Hz
GB: 0

2D NMR plot parameters
CX2: 18.00 cm
CX1: 15.00 cm
F2PLO: 4.326 ppm
F2LO: 2164.12 Hz
F2PH: 0.162 ppm
F2HI: 80.79 Hz
F1PLO: 70.000 ppm
F1LO: 8804.63 Hz
F1PH: 10.000 ppm
F1HI: 1257.80 Hz
F2PPMCM: 0.23138 ppm/cm
F2HZCM: 115.74076 Hz/cm
F1PPMCM: 4.00000 ppm/cm
F1HZCM: 303.12167 Hz/cm

ghmqc



Current Data Parameters
USER: nmr11
NAME: nmr11-sample11
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20111201
Time: 0:04
INSTRUM: cryo500
PROBHD: 5 mm CPFI 1H-
PULPROG: jw4gpgw
TD: 2048
SOLVENT: CDCl3
NS: 4
DS: 16
SWH: 2083.333 Hz
FIDRES: 1.017253 Hz
AQ: 0.4915700 sec
RG: 7298.2
DW: 240.000 usec
DE: 6.50 usec
TE: 298.0 K
CNST2: 145.000000
d0: 0.00000000 usec
D1: 1.00000000 usec
d2: 0.00344828 sec
d12: 0.00000000 sec
d13: 0.00000000 sec
D16: 0.00000000 sec
d20: 0.00242528 sec
W0: 0.0004966 usec

==== CHANNEL f1 =====
NUC1: 1H
P1: 7.50 usec
p2: 15.00 usec
PL1: -1.00 dB
SF01: 500.2211225 MHz

==== CHANNEL f2 =====
CPDPRG2: gpgp
NUC2: 13C
P3: 15.50 usec
PCPD2: 65.00 usec
PL2: -1.00 dB
PL12: 1.30 dB
SF02: 125.7665620 MHz

==== GRADIENT CHANNEL =====
GPNAM1: sine100
GPNAM2: sine100
GPNAM3: sine100
GPX1: 0.00 %
GPX2: 0.00 %
GPX3: 0.00 %
GPY1: 0.00 %
GPY2: 0.00 %
GPY3: 0.00 %
GPZ1: 30.00 %
GPZ2: 18.00 %
GPZ3: 24.00 %
PI6: 1000.00 usec

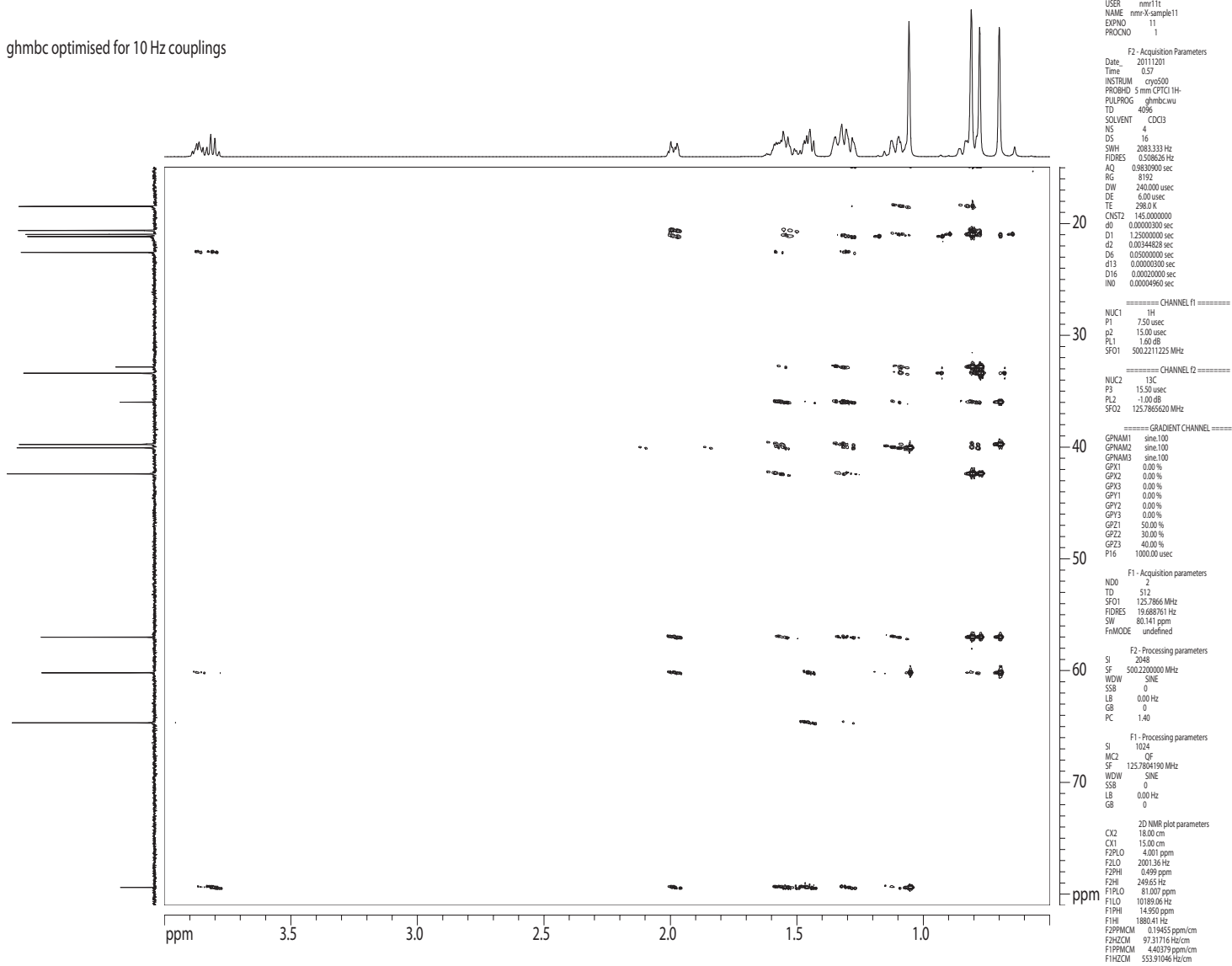
F1 - Acquisition parameters
ND0: 2
TD: 512
SF01: 125.7866 MHz
FIDRES: 19.888761 Hz
SW: 881.141 ppm
FMODE: undefined

F2 - Processing parameters
SI: 1024
SF: 500.220000 MHz
WDW: EM
SSB: 0
LB: 5.00 Hz
GB: 0
PC: 1.40

F1 - Processing parameters
SI: 1024
MC2: CF
SF: 125.7804190 MHz
WDW: GSNR
SSB: 3
LB: 0.00 Hz
GB: 0

2D NMR plot parameters
CX2: 18.00 cm
CX1: 15.00 cm
F2PLO: 2.004 ppm
F2LO: 1002.42 Hz
F2PH: 0.149 ppm
F2HI: 74.69 Hz
F1PLO: 25.96 ppm
F1LO: 3150.33 Hz
F1PH: 16.000 ppm
F1HI: 2012.49 Hz
F2PPMCM: 0.10304 ppm/cm
F2HZCM: 51.56800 Hz/cm
F1PPMCM: 0.60308 ppm/cm
F1HZCM: 75.85626 Hz/cm

ghmbc optimised for 10 Hz couplings



```
Current Data Parameters
USER nm111
NAME nm11-sample11
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111201
Time 0.57
INSTRUM crys500
PROBHD 5 mm CP131H-
PULPROG ghmbc.wu
TD 4096
SOLVENT CDCl3
NS 4
DS 16
SWH 2083.333 Hz
FIDRES 0.508626 Hz
AQ 0.983090 sec
RG 8192
DW 240.000 usec
DE 6.00 usec
TE 298.0 K
CNS2 145.000000
d0 0.00000300 sec
D1 1.2500000 sec
d2 0.00344828 sec
D6 0.00500000 sec
d13 0.00000300 sec
D16 0.00020000 sec
IN0 0.00004960 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2217225 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7865620 MHz

===== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.00 %
P16 1000.00 usec

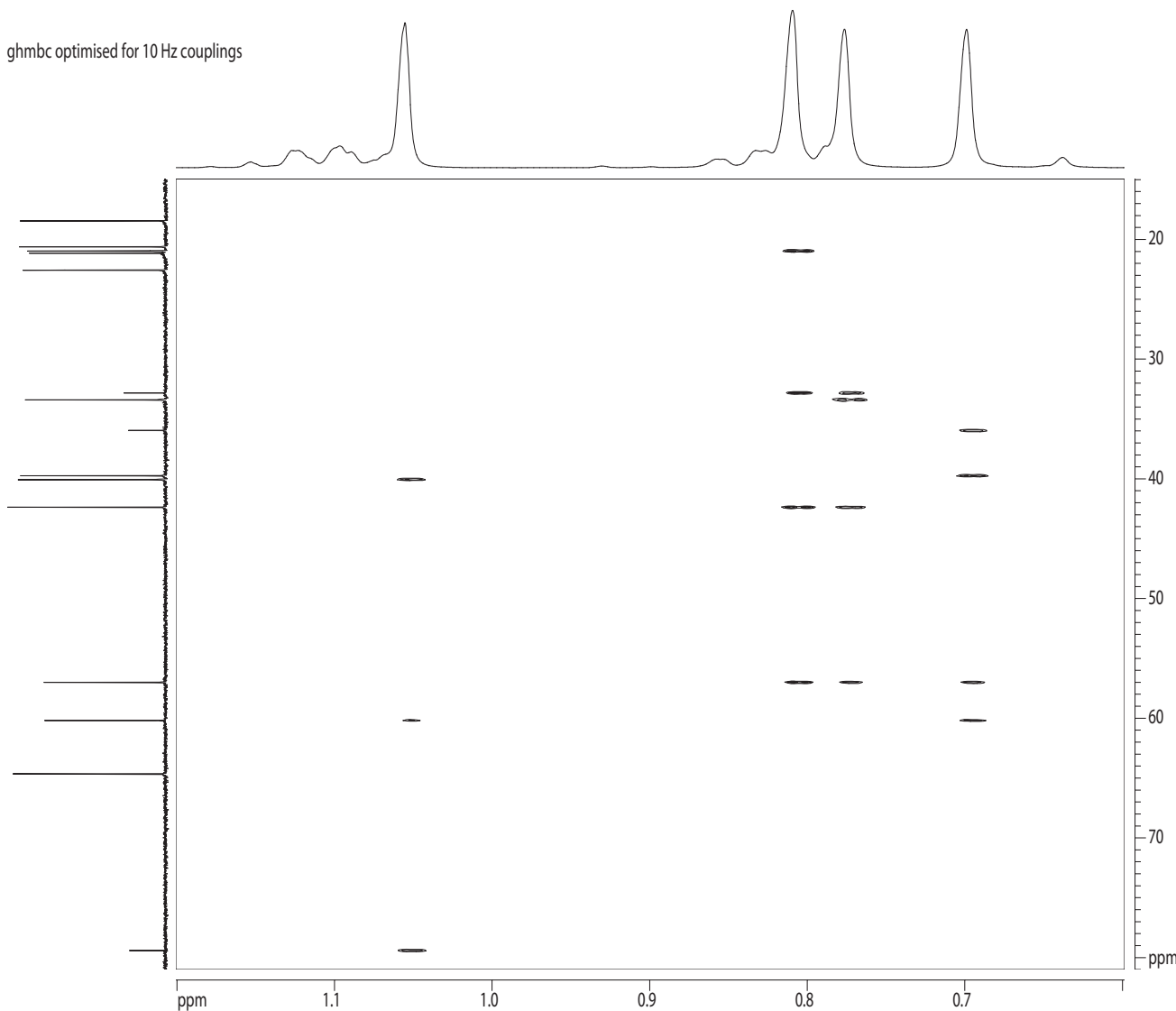
F1 - Acquisition parameters
IND0 2
TD 512
SFO1 125.7866 MHz
FIDRES 19.688761 Hz
SW 80.141 ppm
F0MODE undefined

F2 - Processing parameters
SI 2048
SF 500.220000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 OF
SF 125.7804190 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 18.00 cm
CX1 15.00 cm
F2PLO -4.001 ppm
F2LO 2001.36 Hz
F2HI 6.499 ppm
F2H1 249.65 Hz
F1PLO 81.007 ppm
F1LO 10189.89 Hz
F1PHI 14.950 ppm
F1H 1880.41 Hz
F2PPMCM 0.19455 ppm/cm
F2HZCM 97.31716 Hz/cm
F1PPMCM 4.40379 ppm/cm
F1HZCM 553.91046 Hz/cm
```

ghmbc optimised for 10 Hz couplings



Current Data Parameters
USER nm111
NAME nm-X-sample11
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111201
Time 0.57
INSTRUM crys500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT CDCl3
NS 4
DS 16
SWH 2083.333 Hz
FIDRES 0.508626 Hz
AQ 0.983090 sec
RG 8192
DW 240.000 usec
DE 6.00 usec
TE 298.0 K
CNS2 145.000000
d0 0.00000300 sec
D1 1.2500000 sec
d2 0.00344828 sec
D6 0.00500000 sec
d13 0.00000300 sec
D16 0.00020000 sec
IN0 0.00004960 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2217225 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7865620 MHz

===== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.00 %
P16 1000.00 usec

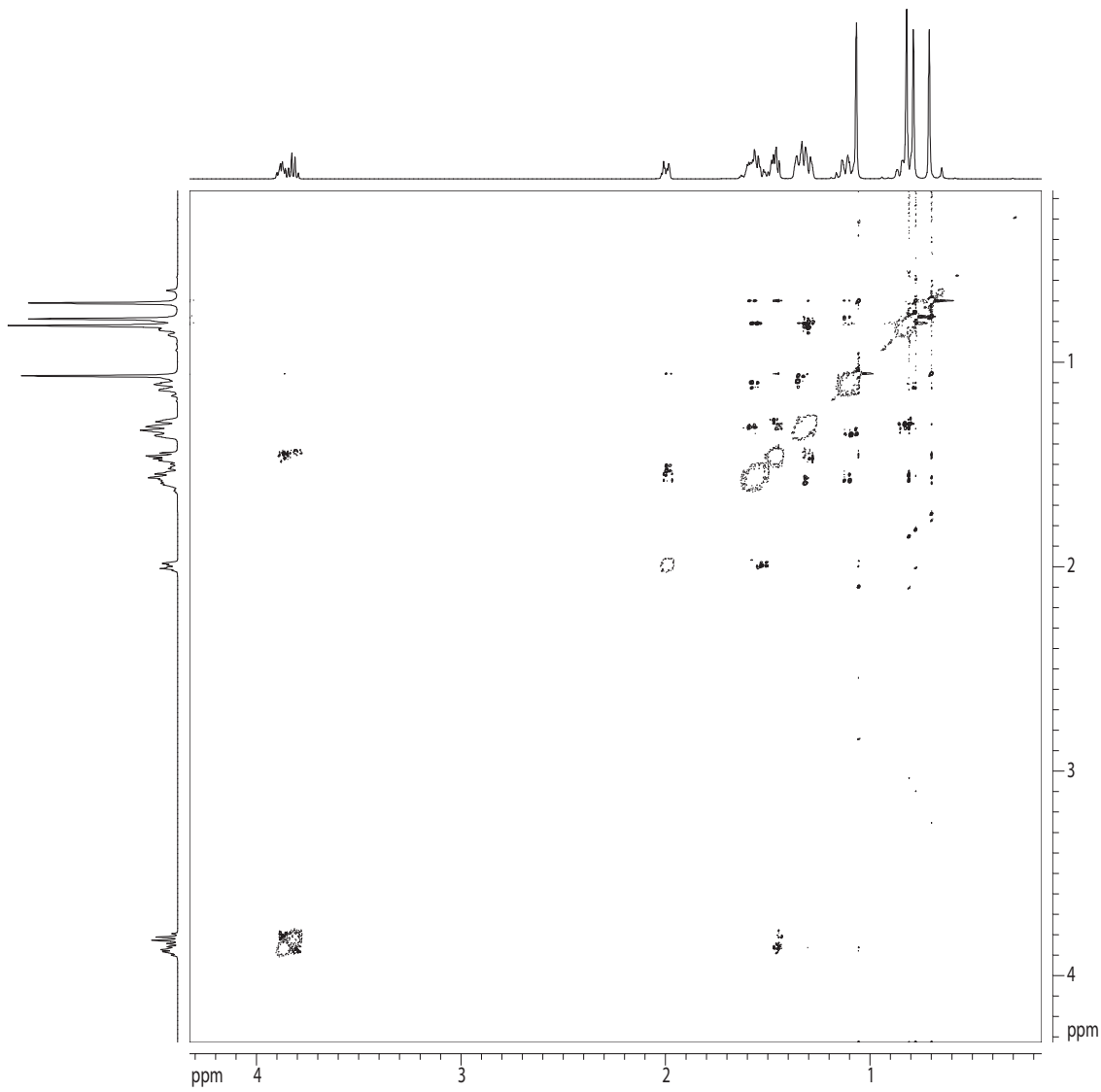
F1 - Acquisition parameters
IND0 2
TD 512
SFO1 125.7866 MHz
FIDRES 19.688761 Hz
SW 80.141 ppm
F0MODE undefined

F2 - Processing parameters
SI 2048
SF 500.220000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 OF
SF 125.7804190 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 18.00 cm
CX1 15.00 cm
F2PLO 1.201 ppm
F2LO 600.61 Hz
F2PHI 0.599 ppm
F2HI 299.50 Hz
F1PLO 81.000 ppm
F1LO 10188.21 Hz
F1PHI 14.950 ppm
F1HI 1880.41 Hz
F2PPMCM 0.03344 ppm/cm
F2HZCM 16.2815 Hz/cm
F1PPMCM 4.40334 ppm/cm
F1HZCM 553.85388 Hz/cm

gnoesy



```
Current Data Parameters
USER nmr11t
NAME nmr-x-sample11
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111201
Time 2.17
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG noesygptp
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 2083.333 Hz
FIDRES 1.017253 Hz
AQ 0.4915700 sec
RG 25.4
DW 240.000 usec
DE 6.00 usec
TE 298.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D8 0.80000001 sec
D16 0.00020000 sec
d20 0.39880002 sec
IN0 0.00024000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
P2 15.00 usec
PL1 1.60 dB
SFO1 500.2211235 MHz

===== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec

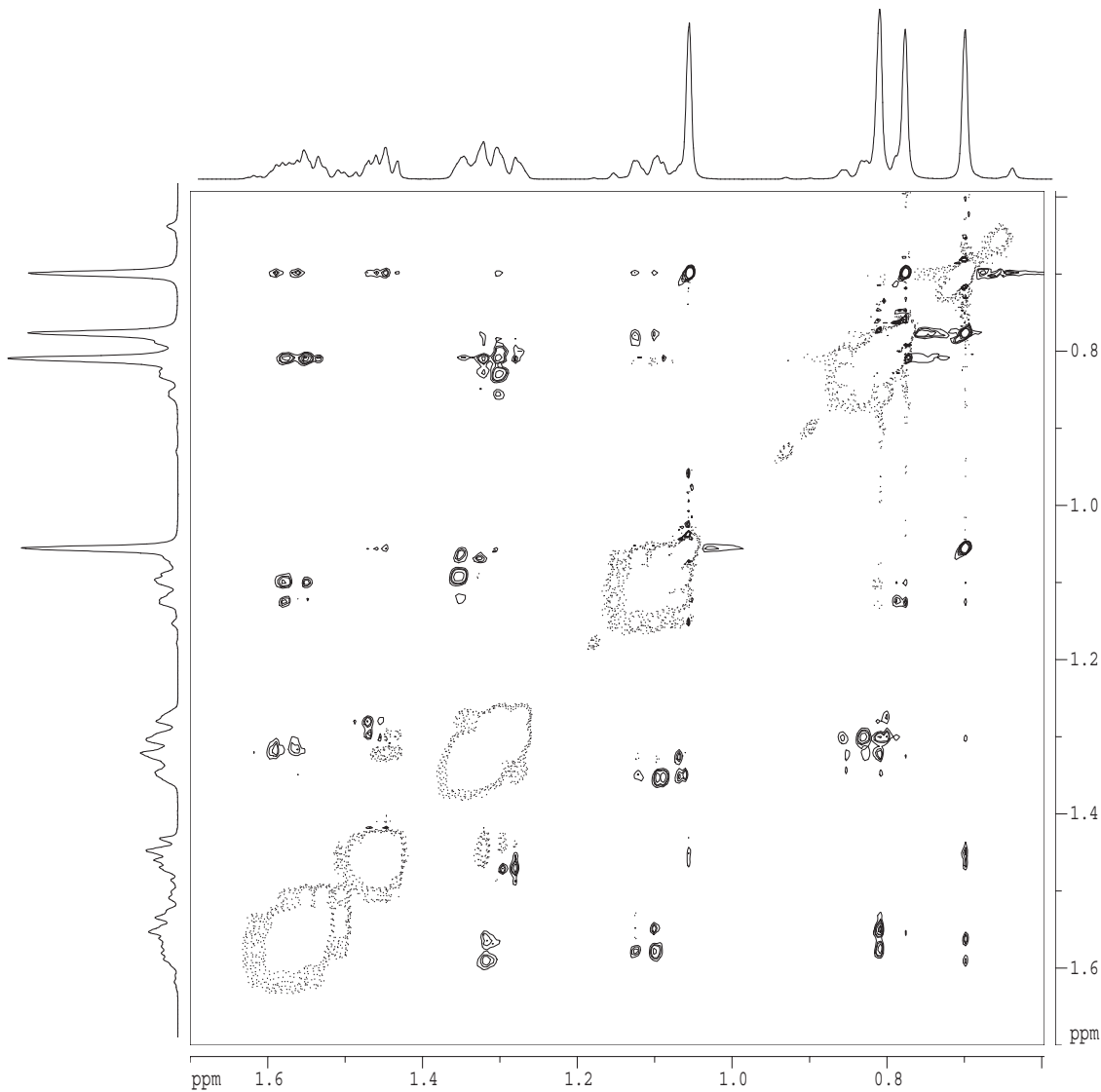
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 500.22111 MHz
FIDRES 4.069010 Hz
SW 4.165 ppm
FnMODE undefined

F2 - Processing parameters
SI 1024
SF 500.2200000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 TPPI
SF 500.2200000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 4.326 ppm
F2LO 2164.12 Hz
F2PHI 0.162 ppm
F2HI 80.79 Hz
F1PLO 4.326 ppm
F1LO 2164.12 Hz
F1PHI 0.162 ppm
F1HI 80.79 Hz
F2PPMCM 0.27766 ppm/cm
F2HZCM 138.88889 Hz/cm
F1PPMCM 0.27766 ppm/cm
F1HZCM 138.88889 Hz/cm
```

gnoesy



```
Current Data Parameters
USER          nmrlit
NAME          nmr-X-sample11
EXPNO        12
PROCNO        1

F2 - Acquisition Parameters
Date_         2011201
Time          2.17
INSTRUM      cryo500
PROBHD       5 mm CPTCI 1H-
PULPROG      noesygptp
TD            2048
SOLVENT      CDCl3
NS            4
DS            16
SWH           2083.333 Hz
FIDRES       1.017253 Hz
AQ            0.4915700 sec
RG            25.4
DW            240.000 usec
DE            6.00 usec
TE            298.0 K
D0            0.0000300 sec
D1            2.0000000 sec
D8            0.8000001 sec
D16           0.0002000 sec
d20           0.3988002 sec
d30           0.0002400 sec
INO

===== CHANNEL f1 =====
NUC1          1H
P1            7.50 usec
P2            15.00 usec
PL1           1.60 dB
SFO1          500.2211225 MHz

===== GRADIENT CHANNEL =====
GPNAM1       sine.100
GPNAM2       sine.100
GFX1         0.00 %
GYZ1         0.00 %
GPY1         0.00 %
GPZ1         0.00 %
GPE1         40.00 %
GPE2         -40.00 %
P16          1000.00 usec

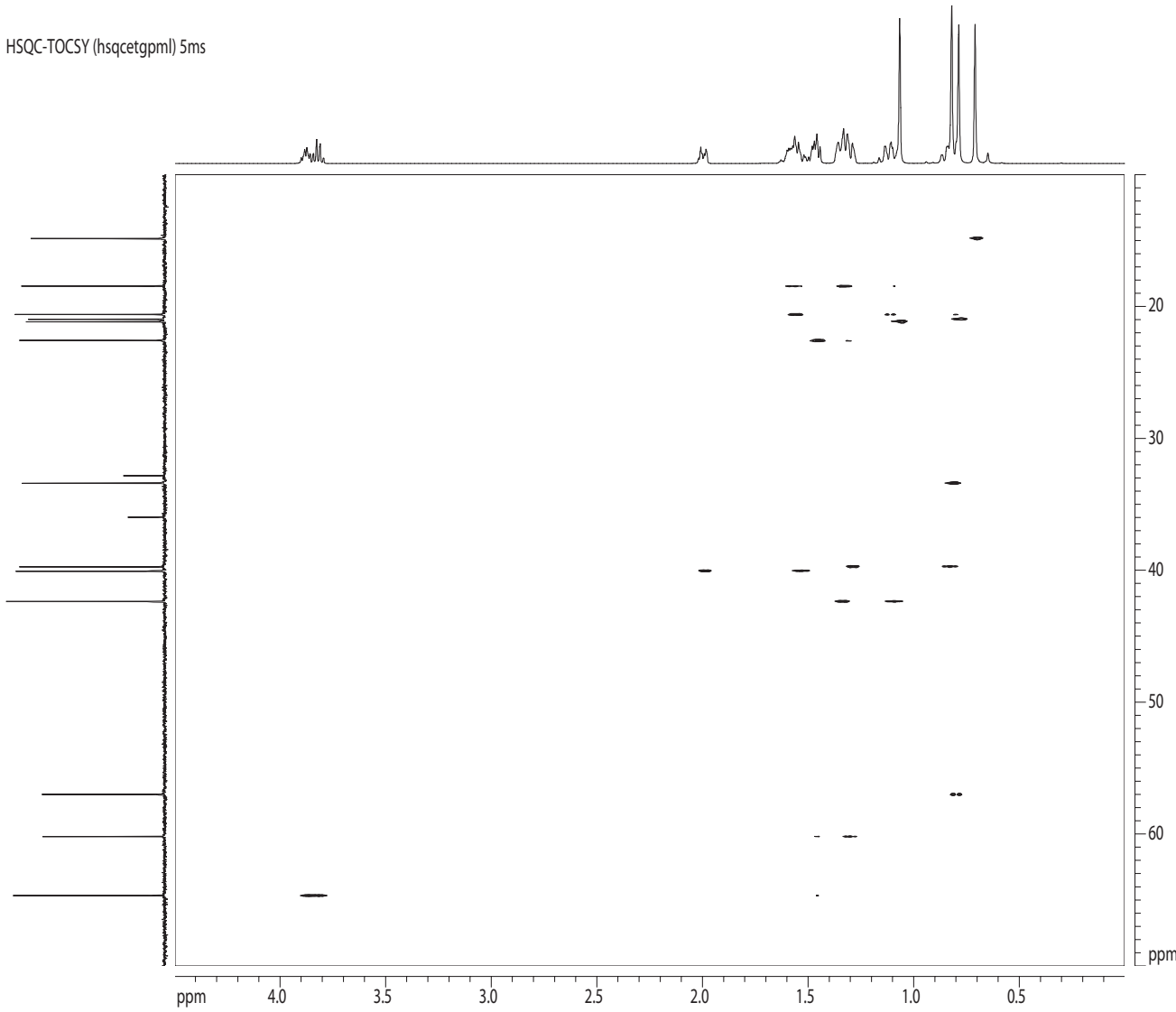
F1 - Acquisition parameters
ND0           2
TD            512
SFO1          500.2211 MHz
FIDRES       4.069010 Hz
SW            4.165 ppm
F0MODE        undefined

F2 - Processing parameters
SI            1024
SF            500.2200000 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI            1024
WCZ           TPP1
SF            500.2200000 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0

2D NMR plot parameters
CX2           15.00 cm
CX1           15.00 cm
F2FLO         1.700 ppm
F2LO          850.37 Hz
F2FHI         0.597 ppm
F2FHI         298.48 Hz
F1FLO         1.700 ppm
F1LO          850.37 Hz
F1FHI         0.593 ppm
F1FHI         296.45 Hz
F2PPMCM      0.07355 ppm/cm
F2HZCM       36.79276 Hz/cm
F1PPMCM      0.07382 ppm/cm
F1HZCM       36.92840 Hz/cm
```

HSQC-TOCSY (hsqcetgpm) 5ms



```

Current Data Parameters
USER      mm11a
NAME      mmf-X-sample11
EXPNO     18
PROCNO    1

F2 - Acquisition Parameters
Date_     20111206
Time      21:27
INSTRUM   crysco
PROBHD    5 mm CPTCI 1H
PULPROG   hsqcetgpm1
TD         3268
SOLVENT   CDCl3
NS         4
DS         32
SWH        2248.201 Hz
FIDRES     1.195755 Hz
AQ         0.4555252 sec
RG         5166
AQ         22.450 usec
DE         6.50 usec
TE         298.2 K
CHST2     145.000000
d0         0.0000000 sec
D1         2.0000000 sec
d4         0.0012414 sec
D9         0.0500000 sec
d11        0.0300000 sec
d12        0.0000000 sec
d13        0.0000000 sec
D16        0.0002000 sec
DELTA     0.0012100 sec
DELTA1    0.0013000 sec
FACTOR1   0
NUC1      13C
NUC2      1H
P1         7.50 usec
p2         15.00 usec
p5         25.34 usec
P6         35.00 usec
p7         70.00 usec
P17        2500.00 usec
P28        1000.00 usec
PL1        1.60 dB
PL10       15.20 dB
SFO1       900.2211251 MHz

===== CHANNEL f1 =====
NUC1      1H
P1         7.50 usec
p2         15.00 usec
p5         25.34 usec
P6         35.00 usec
p7         70.00 usec
P17        2500.00 usec
P28        1000.00 usec
PL1        1.60 dB
PL10       15.20 dB
SFO1       900.2211251 MHz

===== CHANNEL f2 =====
CPDPRG2   gcp
NUC1      13C
P3         15.50 usec
p4         31.00 usec
PCPD2     65.00 usec
PL1        1.00 dB
PL12       11.20 dB
SFO2       125.7863936 MHz

===== GRADIENT CHANNEL =====
GPNAM1    SINE 100
GPNAM2    SINE 100
GPI1      0.00 %
GPI2      0.00 %
GPI3      0.00 %
GPI4      0.00 %
GPI5      0.00 %
GPI6      80.00 %
GPI7      20.10 %
GPI8      100.00 usec

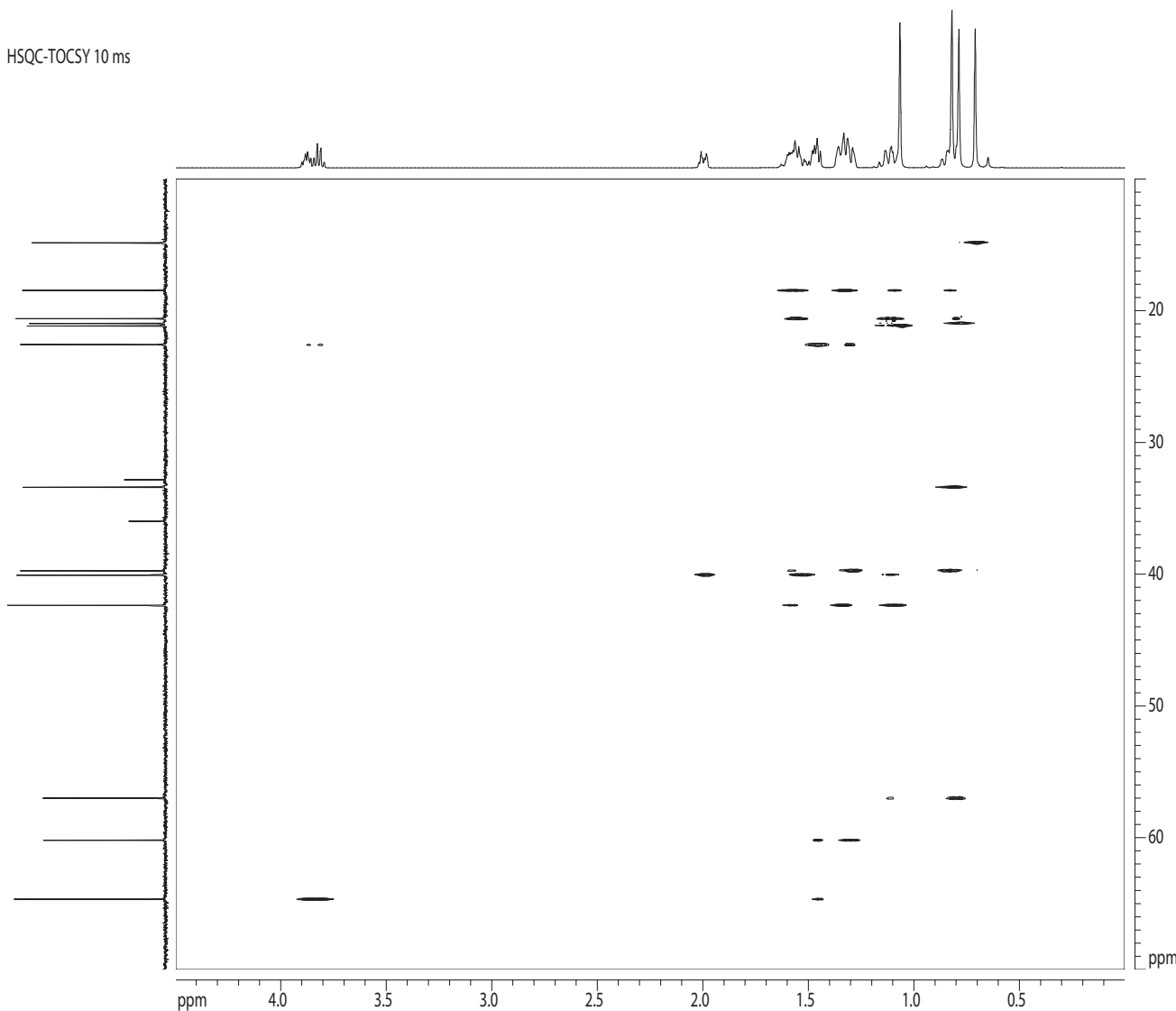
F1 - Acquisition parameters
ND0        2
TD         1024
SFO1       125.7864 MHz
FIDRES     0.1453360 Hz
SW         84.936 ppm
F4MODE     Echo-Antiecho

F2 - Processing parameters
SI         1024
SF         500.2200000 MHz
WDW        EM
SSB        0
LB         5.00 Hz
GB         0
PC         1.00

F1 - Processing parameters
SI         1024
INCR       echo-antiecho
SF         125.7863936 MHz
WDW        OSINE
SSB        3
LB         0.00 Hz
GB         0

2D NMR plot parameters
CQ1        16.00 cm
CX1        15.00 cm
F2P1LO     4.495 ppm
F2P1HI     22491.5 Hz
F2P1F0     0.002 ppm
F2P1F1     0.95 Hz
F2P1F2     70.000 ppm
F2P1F3     8804.63 Hz
F2P1F4     10.000 ppm
F2P1F5     1.25786 Hz
F2P1F6     0.24660 ppm/cm
F2P1F7     124.00000 Hz/cm
F2P1F8     4.00000 ppm/cm
F2P1F9     503.12167 Hz/cm
    
```


HSQC-TOCSY 10 ms



```

Current Data Parameters
USER      mm11a
NAME      mmf-X-sample11
EXPNO    19
PROCNO    1

F2 - Acquisition Parameters
Date_     20111207
Time      0.19
INSTRUM   crys200
PROBHD    5 mm CPTCI 1H
PULPROG   zgpgcgpm1
TD         3268
SOLVENT   CDCl3
NS         4
DS         32
SWH        2246.201 Hz
FIDRES     1.097755 Hz
AQ         0.4555252 sec
RG         4597
AQ         222.400 usec
DE         6.50 usec
TE         298.6 K
CH12      145.000000
d0         0.00000000 sec
D1         2.00000000 sec
d4         0.00172414 sec
D9         0.00100000 sec
d11        0.03000000 sec
d12        0.00002000 sec
d13        0.00000000 sec
D16        0.00020000 sec
DELTA     0.00121100 sec
DELTA1    0.00130000 sec
FACTOR1   0
RG         0.00004680 sec
f1         0
MCREST    0.00000000 sec
MCWBK     0.40000011 sec
SCALEF    6
STOICNT   256

===== CHANNEL f1 =====
NUC1      1H
P1         7.50 usec
p2         15.00 usec
p5         25.34 usec
P6         35.00 usec
p7         70.00 usec
P17        2500.00 usec
P28        1000.00 usec
PL1        1.60 dB
PL10       15.20 dB
SFO1       500.2211251 MHz

===== CHANNEL f2 =====
CPDPRG2   gpgp
NUC2      13C
P3         15.50 usec
p4         31.00 usec
PCPD2     65.00 usec
PL1        1.00 dB
PL12       11.20 dB
SFO2       125.7863936 MHz

===== GRADIENT CHANNEL =====
GPNAM1    SINE 100
GPNAM2    SINE 100
GPR1      0.00 %
GPR2      0.00 %
GPR3      0.00 %
GPR4      0.00 %
GPR5      80.00 %
GPR6      20.10 %
P16        1000.00 usec

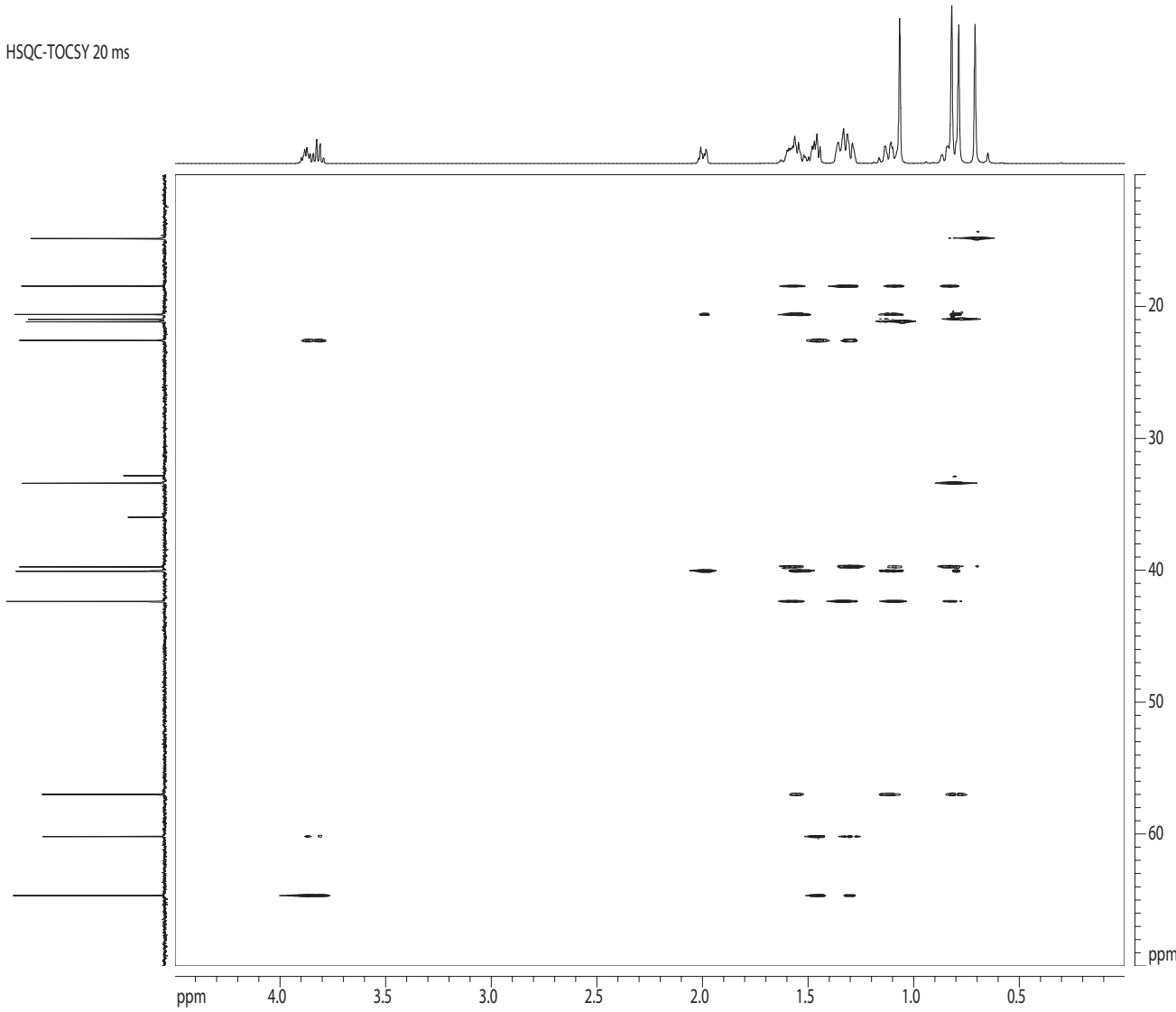
F1 - Acquisition parameters
ND0        2
TD         1024
SFO1       125.7864 MHz
FIDRES     10.453360 Hz
SW         84.936 ppm
FIMODE     Echo-Antiecho

F2 - Processing parameters
SI         1024
SF         500.220000 MHz
WDW        EM
SSB        0
LB         5.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MCA        echo-antiecho
SF         125.7863936 MHz
WDW        OSINE
SSB        3
LB         0.00 Hz
GB         0

2D NMR plot parameters
CQ1        16.00 cm
CX1        15.00 cm
F2P1LO     4.495 ppm
F1LO       224615 Hz
F2P1H      0.002 ppm
F2H         0.95 Hz
F1P1LO     70.000 ppm
F1LO       880463 Hz
F1H         10.460 ppm
F1H1       1257.86 Hz
F2P1MCM    0.24660 ppm/cm
F2P2MCM    1.2400000 Hz/cm
F1P1MCM    4.00000 ppm/cm
F1H2MCM    503.12167 Hz/cm
    
```

HSQC-TOCSY 20 ms



```

Current Data Parameters
USER          mm11a
NAME          mmf-X-sample11
EXPNO        20
PROCNO       1

F2 - Acquisition Parameters
Date_         20111207
Time          3.11
INSTRUM      cryo500
PROBHD       5 mm CPTCI 1H
PULPROG      zgpgcgpm1
TD            3268
SOLVENT      CDCl3
NS            4
DS            32
SWH           2246.201 Hz
FIDRES       1.097975 Hz
AQ            0.4555252 sec
RG            4096
DW            222.400 usec
DE            6.50 usec
TE            298.6 K
CH12         145.000000
d0            0.00000000 sec
D1            2.00000000 sec
d4            0.00172414 sec
D9            0.02000000 sec
d11           0.00000000 sec
d12           0.00000000 sec
d13           0.00000000 sec
D16           0.00020000 sec
DELTA        0.00121100 sec
DELTA1       0.00130000 sec
FACTOR1      1
NUC1          13C
NUC2          1H
P1            7.50 usec
p2            15.00 usec
p5            25.34 usec
P6            35.00 usec
p7            70.00 usec
P17           2500.00 usec
P28           1000.00 usec
PL1           1.60 dB
PL10          15.20 dB
SFO1          900.2211251 MHz

===== CHANNEL f2 =====
CPOPRG2      gpgp
NUC2         13C
P3            15.50 usec
p4            31.00 usec
PCPD2        65.00 usec
PL2           1.00 dB
PL12         11.20 dB
SFO2         125.7863936 MHz

===== GRADIENT CHANNEL =====
GPNAM1       SINE 100
GPNAM2       SINE 100
GPI1         0.00 %
GPI2         0.00 %
GPI3         0.00 %
GPI4         0.00 %
GPI5         0.00 %
GPI6         0.00 %
GPI7         80.00 %
GPI8         20.10 %
GPI9         1000.00 usec

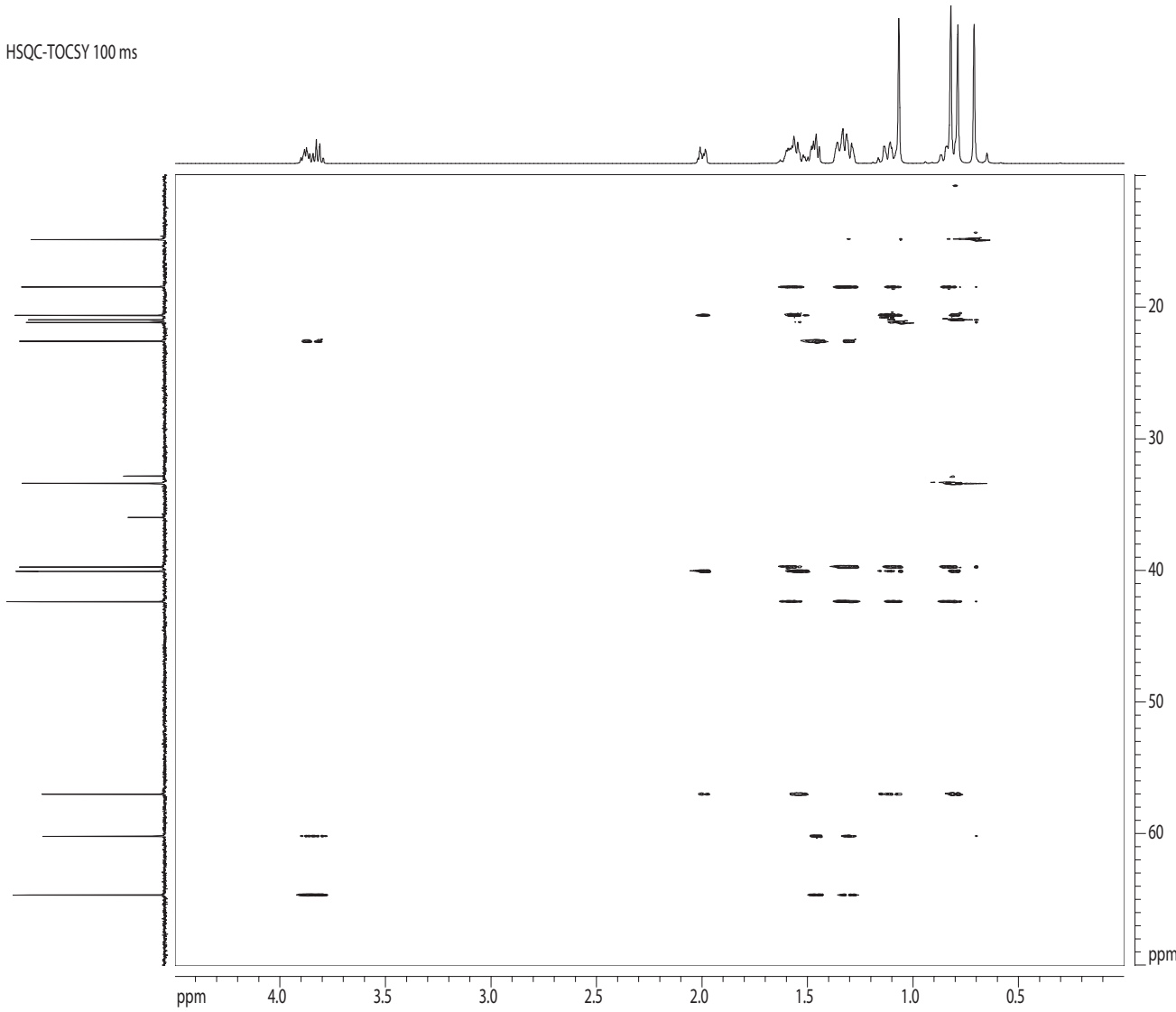
F1 - Acquisition parameters
ND0           2
TD            1024
SFO1         125.7864 MHz
FIDRES       0.1453360 Hz
SW            84.936 ppm
F1MODE       Echo-Antiecho

F2 - Processing parameters
SI            1024
SF            500.220000 MHz
WDW           EM
SSB           0
LB            5.00 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI            1024
INCR         echo-antiecho
SF            125.7863936 MHz
WDW           OSINE
SSB           3
LB            0.00 Hz
GB            0

2D NMR plot parameters
CQ1           16.00 cm
CX1           15.00 cm
F2P10         4.495 ppm
F2LO          224615 Hz
F2P14         0.002 ppm
F2H           0.95 Hz
F2LO          880463 Hz
F2P10         70.000 ppm
F2LO          880463 Hz
F2H           10.000 ppm
F2P14         1.25786 Hz
F2P10         0.24660 ppm/cm
F2P14         124.00000 Hz/cm
F2P10         4.00000 ppm/cm
F2P14         503.12167 Hz/cm
    
```

HSQC-TOCSY 100 ms



```

Current Data Parameters
USER      mmf1a
NAME      mmf-X-sample11
EXPNO    21
PROCNO    1

F2 - Acquisition Parameters
Date_     20111207
Time      6.05
INSTRUM   crys500
PROBHD    5 mm CPTCI 1H
PULPROG   zgpg30
TD         3268
SOLVENT   CDCl3
NS         4
DS         32
SWH        2246.201 Hz
FIDRES    1.097975 Hz
AQ         0.455252 sec
RG         183961
AQ        222.400 usec
DE         6.50 usec
TE         298.2 K
CHST2     145.000000
d0         0.00000000 sec
D1         2.00000000 sec
d4         0.00172414 sec
D9         0.10000000 sec
d11        0.00000000 sec
d12        0.00000000 sec
d13        0.00000000 sec
D16        0.00020000 sec
DELTA     0.00122100 sec
DELTA1    0.00130000 sec
FACTOR1   7
NUC1       1H
NUC2       13C
P1         7.50 usec
p2         15.00 usec
p5         23.34 usec
P6         35.00 usec
p7         70.00 usec
P17        2500.00 usec
P28        1000.00 usec
PL1        1.60 dB
PL10       15.20 dB
SFO1       500.2211251 MHz

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
p2         15.00 usec
p5         23.34 usec
P6         35.00 usec
p7         70.00 usec
P17        2500.00 usec
P28        1000.00 usec
PL1        1.60 dB
PL10       15.20 dB
SFO1       500.2211251 MHz

===== CHANNEL f2 =====
CPOPRG2    gpgp
NUC1       13C
P3         15.50 usec
p4         31.00 usec
PCPD2      65.00 usec
PL1        1.00 dB
PL12       11.20 dB
SFO2       125.7663936 MHz

===== GRADIENT CHANNEL =====
GPNAM1     SINE 100
GPNAM2     SINE 100
GPR1       0.00 %
GPR2       0.00 %
GPR3       0.00 %
GPR4       0.00 %
GPR5       0.00 %
GPR6       0.00 %
GPR7       80.00 %
GPR8       20.10 %
GPR9       100.00 usec
P16        1000.00 usec

F1 - Acquisition parameters
ND0         2
TD          1024
SFO1       125.7664 MHz
FIDRES     0.4453360 Hz
SW          84.936 ppm
F4MODE     Echo-Antiecho

F2 - Processing parameters
SI          1024
SF          500.220000 MHz
WDW         EM
SSB         0
LB          5.00 Hz
GB          0
PC          1.40

F1 - Processing parameters
SI          1024
INSTRUM    echo-antiecho
SF          125.7663936 MHz
WDW         OSINE
SSB         3
LB          0.00 Hz
GB          0

2D NMR plot parameters
CQ         16.00 cm
CX         15.00 cm
F2P1LO     4.495 ppm
F2P1HI     22461.5 Hz
F2P1F0     -0.002 ppm
F2P1F1     -1.24 Hz
F2P1F2     70.062 ppm
F2P1F3     8872.44 Hz
F2P1F4     9.28 ppm
F2P1F5     1248.25 Hz
F2P1F6     0.24993 ppm/cm
F2P1F7     125.02004 Hz/cm
F2P1F8     4.00020 ppm/cm
F2P1F9     5042.7905 Hz/cm
    
```