

Name: _____

Chem 203
December 10, 2011

Final Exam Part II
Problem 2 of 3 (30 points)

Select and submit TWO OUT OF THE THREE PROBLEMS FROM PART II for grading.
Do not submit three problems.

If you wish to unstaple the pages, please initial each page.

Books, notes, lecture videos, calculators, rulers, and laptop computers are permitted as is wireless (or wired) internet access and appropriate software (e.g., Pymol, Macromodel/Maestro, Excel, NMRPrediction, Chemdraw, ElComp, MolE, etc.). Catalogs of molecular structures (e.g., the Aldrich catalog, the Merck Index, etc.) or databases of molecular structures (such as wireless access to SciFinder Scholar, the Sigma-Aldrich website, etc.) are NOT PERMITTED. USE OF SUCH ITEMS CONSTITUTES ACADEMIC DISHONESTY, WILL RESULT IN A FAILING GRADE (F) IN THE CLASS, AND MAY RESULT IN EXPULSION FROM THE Ph.D. PROGRAM.

If you wish to use a laptop computer, please be willing to share briefly with others when needed.

2. The following spectral data are provided for a compound with a molecular formula $C_{16}H_{22}O$: IR (Thin film on NaCl), 400 MHz 1H NMR, 125.7 MHz ^{13}C NMR, DEPT-90, DEPT-135, COSY, HMQC, HMBC, TOCSY, and NOESY. The COSY, HMQC, HMBC, TOCSY, and NOESY were recorded at 500 MHz, however the 400 MHz 1H NMR spectra are shown along the axes. Using these data, determine the structure of the compound and assign all of the 1H and ^{13}C resonances to their respective atoms in the structure. Make sure to determine the stereochemistry of the compound and to clearly assign 1H resonances to the appropriate diastereotopic protons.

All NMR spectra were measured in C_6D_6 . The 1H resonance at 7.1 ppm corresponds to $C_6D_5H + 2H$.

MAKE SURE TO COMPLETELY ANSWER THE QUESTIONS **a-f** ON PAGES 2-4.

a. Write the structure of the molecule.

b. Tabulate the shifts of the ^1H resonances (a-m) in order of descending chemical shift. Provide an appropriate name for each multiplet (e.g., s, d, t, q, quintet, sextet, septet, octet, dd, ddd, dt, td, dddd, tt, qd, dq, etc.) and list its coupling constants in appropriate order; also list its integral [e.g., a: 3.30 (t, $J = 7.3$ Hz, 3 H)]. If a resonance is not described by a well-defined multiplet, name it as m and give its range [e.g., c: 4.43-4.37 (m, 2 H)].

a:

b:

c:

d:

e:

f:

g:

h:

i:

j:

k:

l:

m:

c. Redraw the structure of the molecule below and write the letter (a-m) of each ^1H resonance next to the proton or protons to which it corresponds. If the assignment of a particular resonance is uncertain, please indicate this.

d. Tabulate the shifts of the ^{13}C resonances (1-14) in order of descending chemical shift. Make sure to report the chemical shift of each carbon resonances to the nearest tenth of ppm, unless two have the same value, in which case you may report it to the nearest hundredth.

1:

2:

3:

4:

5:

6:

7:

8:

9:

10:

11:

12:

13:

14:

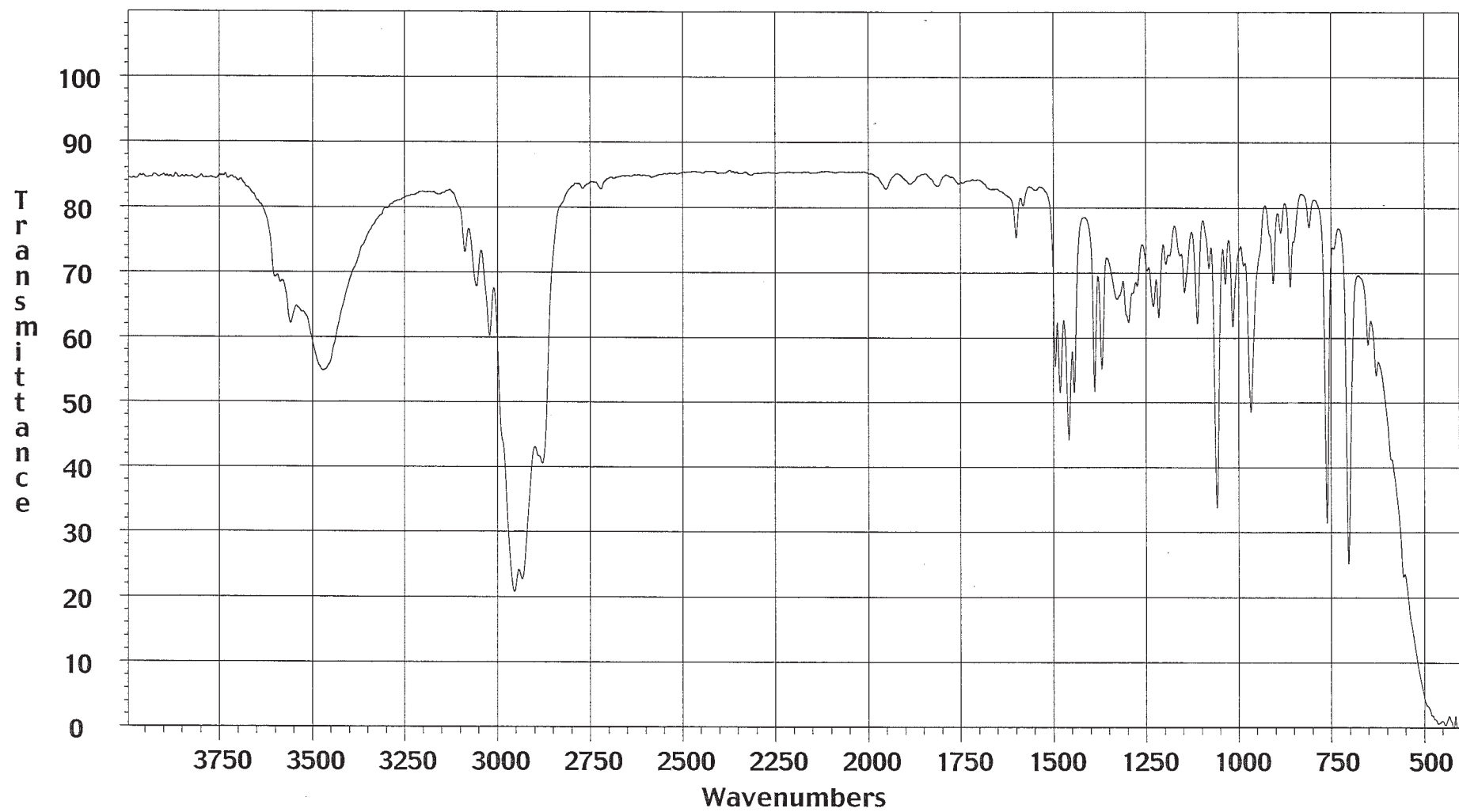
e. Redraw the structure of the molecule below and write the number (1-14) of each ^{13}C resonance next to the carbon or carbons to which it corresponds. If the assignment of particular resonance is uncertain, please indicate this.

f. Build an energy-minimized molecular model of the the molecule using PyMOL and the "clean" function. Save the .pse file as problem2.pse.

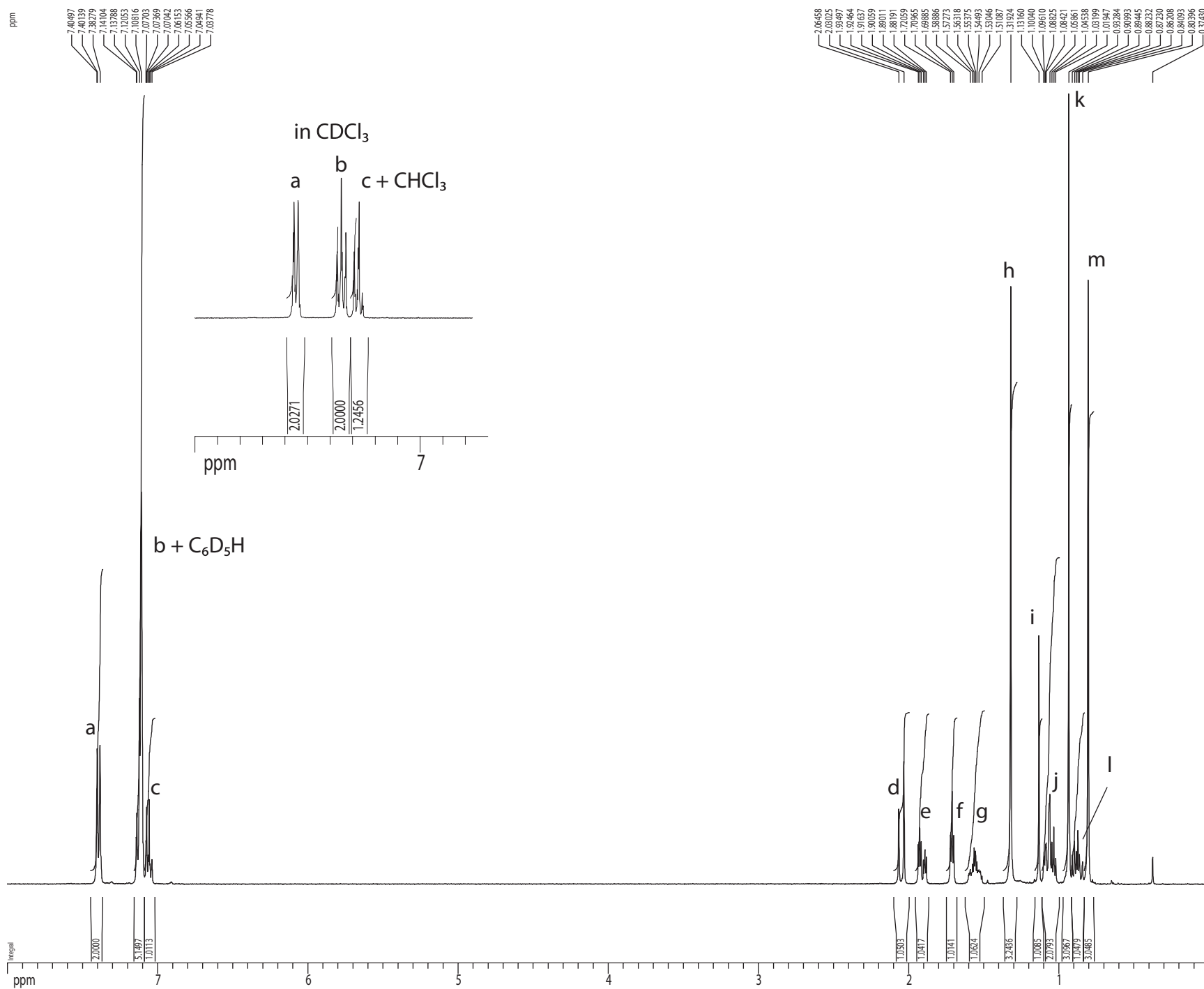
E-mail the .pse file to me (jsnowick@uci.edu).

If you have encountered any problems of which I should be aware in grading this problem, please let me know, below.

Thin Film on NaCl plates



¹H spectrum at 400 MHz in C₆D₆



Current Data Parameters
USER nmr11t
NAME sample 16
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111202
Time 13.31
INSTRUM drx400
PROBHD 5 mm QNP H₂/P
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 8
DS 2
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1118579 sec
RG 128
DW 78.000 usec
DE 4.50 usec
TE 298.1 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 ¹H
P1 12.00 usec
PL1 -0.60 dB
SFO1 400.1328009 MHz

F2 - Processing parameters
SI 65536
SF 400.1300175 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
FIP 8.000 ppm
F1 3201.04 Hz
F2 0.000 ppm
F3 0.00 Hz
PPMCM 0.35088 ppm/cm
HZCM 140.39650 Hz/cm

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		[Hz]	[PPM]	
1	30932.2	2962.950	7.4050	1.80
2	30946.8	2961.518	7.4014	2.57
3	31022.9	2954.077	7.3828	2.64
4	32011.9	2857.343	7.1410	0.89
5	32024.8	2856.079	7.1379	1.35
6	32095.8	2849.137	7.1205	3.52
7	32146.4	2844.189	7.1082	7.44
8	32273.7	2831.732	7.0770	0.82
9	32287.4	2830.397	7.0737	1.47
10	32300.8	2829.087	7.0704	0.94
11	32337.1	2825.531	7.0615	0.55
12	32361.2	2823.180	7.0557	1.60
13	32386.7	2820.679	7.0494	0.38
14	32434.3	2816.028	7.0378	0.47
15	52778.5	826.101	2.0646	1.43
16	52919.0	812.363	2.0302	2.32
17	53308.8	774.238	1.9350	0.76
18	53351.0	770.108	1.9246	1.05
19	53384.8	766.796	1.9164	0.81
20	53449.4	760.483	1.9006	0.46
21	53492.2	756.291	1.8901	0.65
22	53525.8	753.007	1.8819	0.51
23	54185.7	688.458	1.7206	0.93
24	54230.5	684.081	1.7096	1.76
25	54274.6	679.761	1.6989	0.92
26	54724.6	635.751	1.5889	0.28
27	54790.6	629.297	1.5727	0.38
28	54829.6	625.475	1.5632	0.69
29	54868.2	621.700	1.5537	0.63
30	54904.3	618.172	1.5449	0.42
31	54963.5	612.383	1.5305	0.27
32	55043.6	604.545	1.5109	0.15
33	55195.1	589.731	1.4738	0.07
34	55827.5	527.869	1.3192	11.35
35	56473.1	464.720	1.1614	0.09
36	56595.1	452.787	1.1316	4.71
37	56722.8	440.305	1.1004	0.45
38	56740.4	438.580	1.0961	0.53
39	56772.5	435.440	1.0882	0.76
40	56789.0	433.825	1.0842	0.78
41	56893.7	423.583	1.0586	1.70
42	56947.9	418.286	1.0454	0.80
43	57002.6	412.930	1.0320	1.08
44	57053.8	407.921	1.0195	0.49
45	57408.2	373.259	0.9328	15.00
46	57502.0	364.089	0.9099	0.55
47	57565.3	357.896	0.8944	0.81
48	57614.9	353.044	0.8823	0.62
49	57655.9	349.032	0.8723	1.02
50	57697.7	344.943	0.8621	0.57

51	57784.2	336.483	0.8409	0.42
52	57935.4	321.690	0.8040	11.47
53	58053.3	310.159	0.7751	0.08
54	58578.1	258.830	0.6469	0.06
55	59693.1	149.769	0.3743	0.50

^1H spectrum at 400 MHz in C_6D_6

ppm

in CDCl_3

7.40497
7.40139
7.38279

7.14104
7.13788
7.12053
7.10816
7.07703
7.07369
7.07042
7.06153
7.05566
7.04941
7.03778

a

b

c + CHCl_3

b + $\text{C}_6\text{D}_5\text{H}$

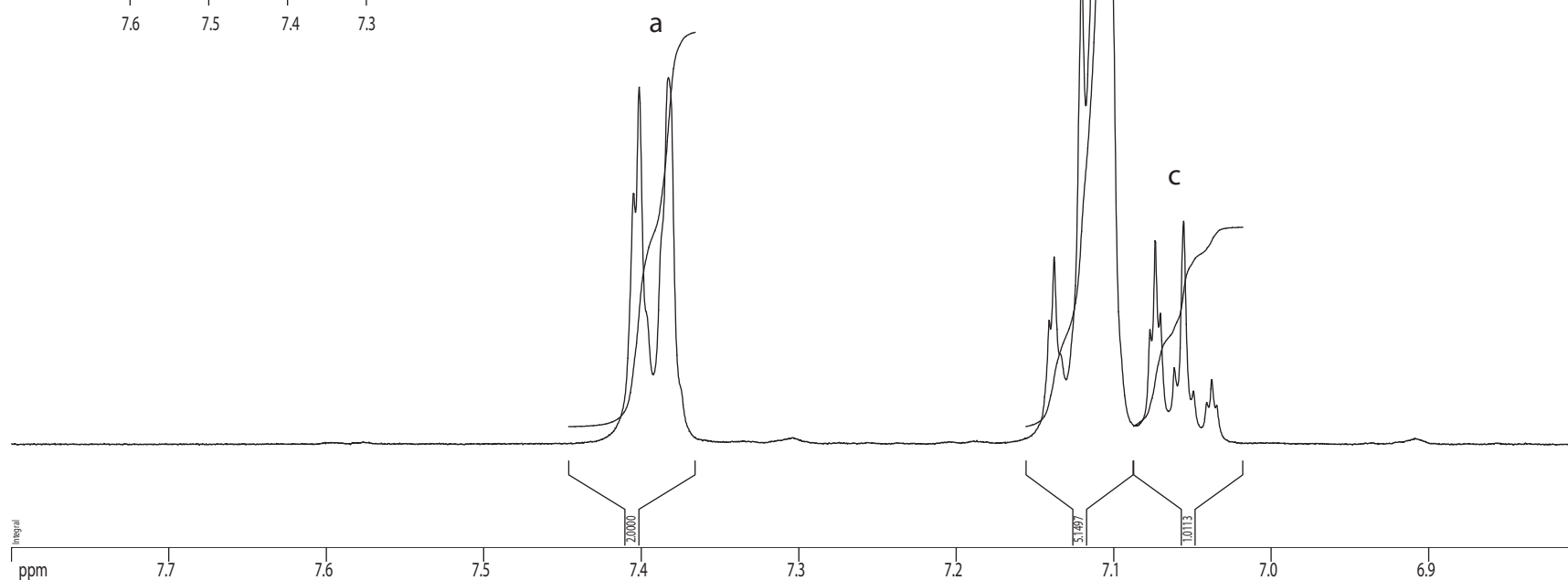
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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 8
DS 2
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1118579 sec
RG 128
DW 78.000 usec
DE 4.50 usec
TE 298.1 K
D1 0.10000000 sec
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MCWRK 0.01500000 sec

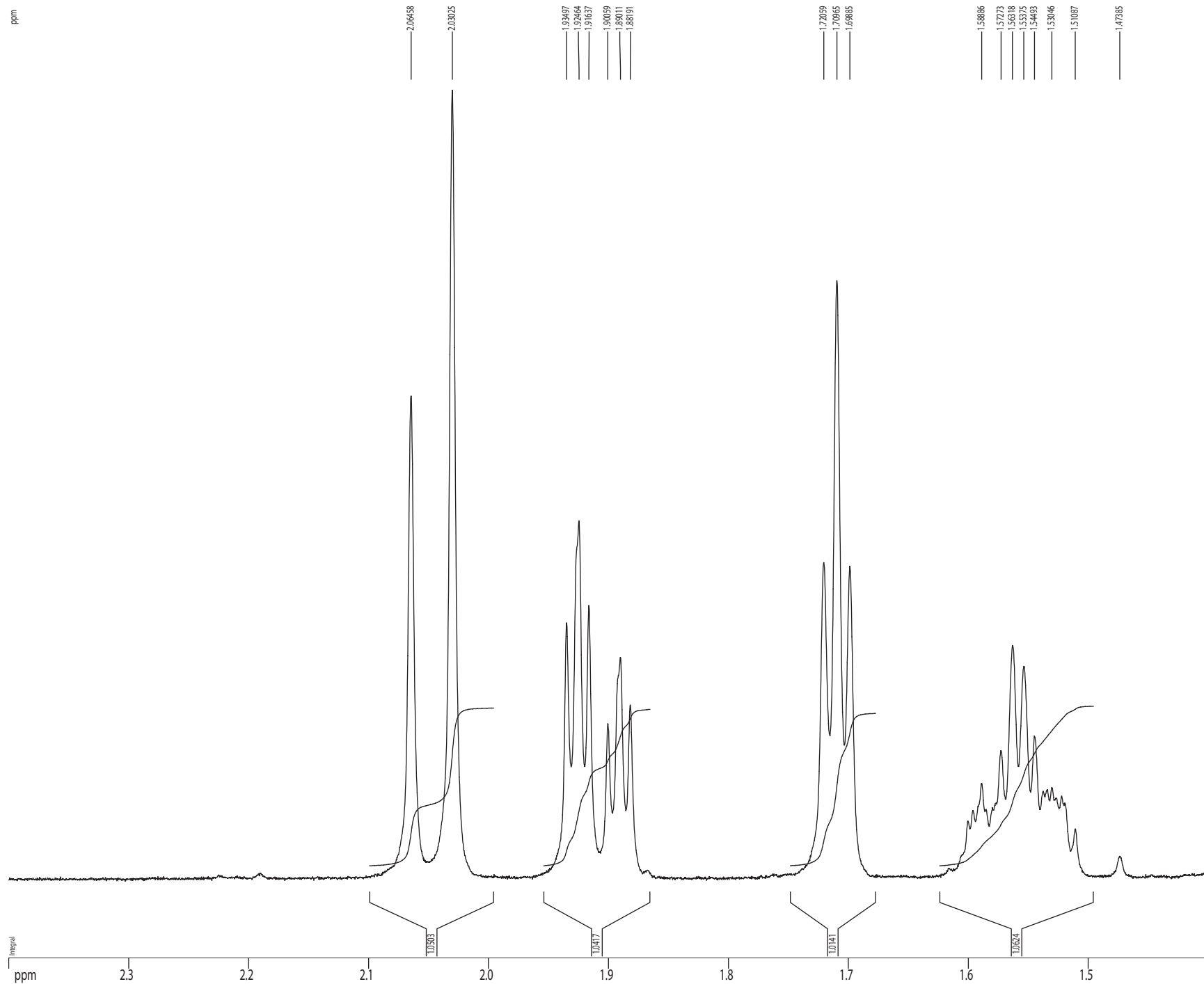
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NUC1 ^1H
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SFO1 400.1328009 MHz

F2 - Processing parameters
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SF 400.1300175 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 7.800 ppm
F1 3121.01 Hz
F2P 6.800 ppm
F2 2720.88 Hz
PPMCM 0.04386 ppm/cm
HZCM 17.54956 Hz/cm



¹H spectrum at 400 MHz in C₆D₆



Current Data Parameters
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 NAME sample 16
 EXPNO 1
 PROCNO 1

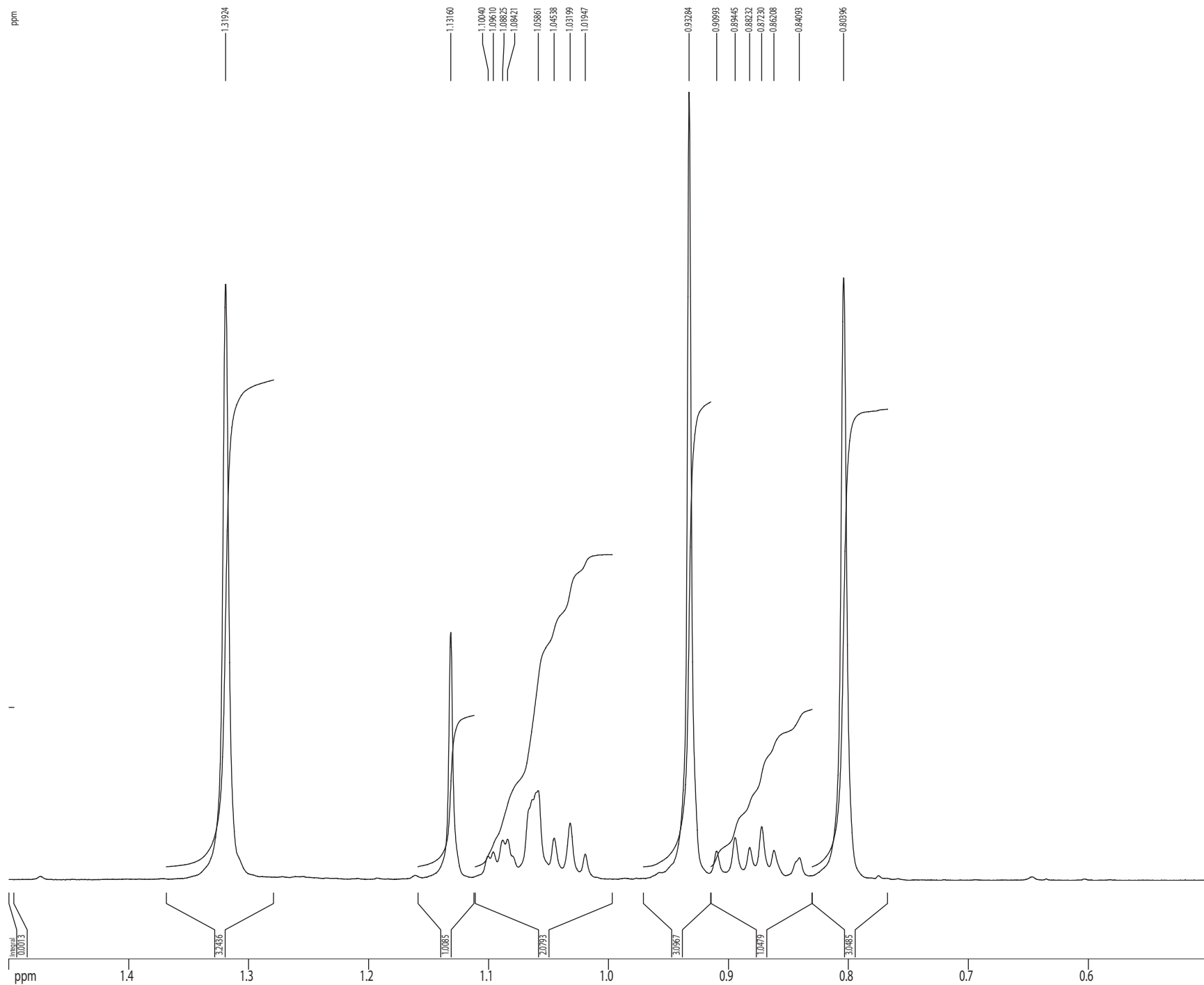
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 6410.256 Hz
 FIDRES 0.097813 Hz
 AQ 5.1118579 sec
 RG 128
 DW 78.000 usec
 DE 4.50 usec
 TE 298.1 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 12.00 usec
 PL1 -0.60 dB
 SFO1 400.1328009 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300175 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 2.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 2.400 ppm
 F1 960.31 Hz
 F2P 1.400 ppm
 F2 560.18 Hz
 PPMCM 0.04386 ppm/cm
 HZCM 17.54956 Hz/cm

¹H spectrum at 400 MHz in C₆D₆



Current Data Parameters
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 PROCNO 1

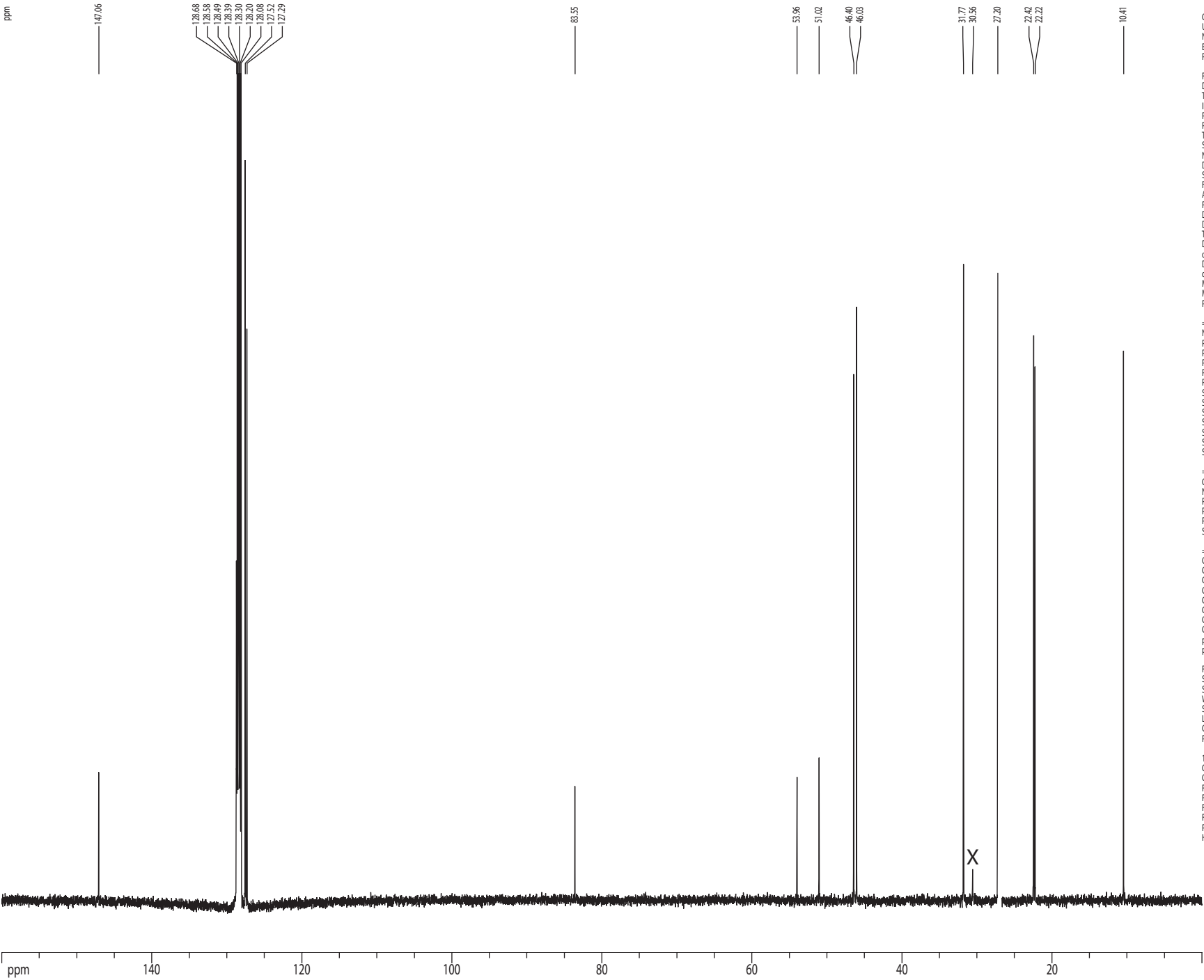
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 PROBHD 5 mm QNP H/F/P
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 6410.256 Hz
 FIDRES 0.097813 Hz
 AQ 5.1118579 sec
 RG 128
 DW 78.000 usec
 DE 4.50 usec
 TE 298.1 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 12.00 usec
 PL1 -0.60 dB
 SFO1 400.1328009 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300175 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 2.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 1.500 ppm
 F1 600.19 Hz
 F2P 0.500 ppm
 F2 200.06 Hz
 PPMCM 0.04386 ppm/cm
 HZCM 17.54956 Hz/cm

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



Current Data Parameters
USER nmr11t
NAME Sample 16
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111203
Time 21.07
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchogg30gp.prd
TD 65536
SOLVENT CDCl3
NS 365
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813940 sec
RG 3251
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00019600 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 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 Cyp60.0.5.20.1
SPNAM2 Cyp60.comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz

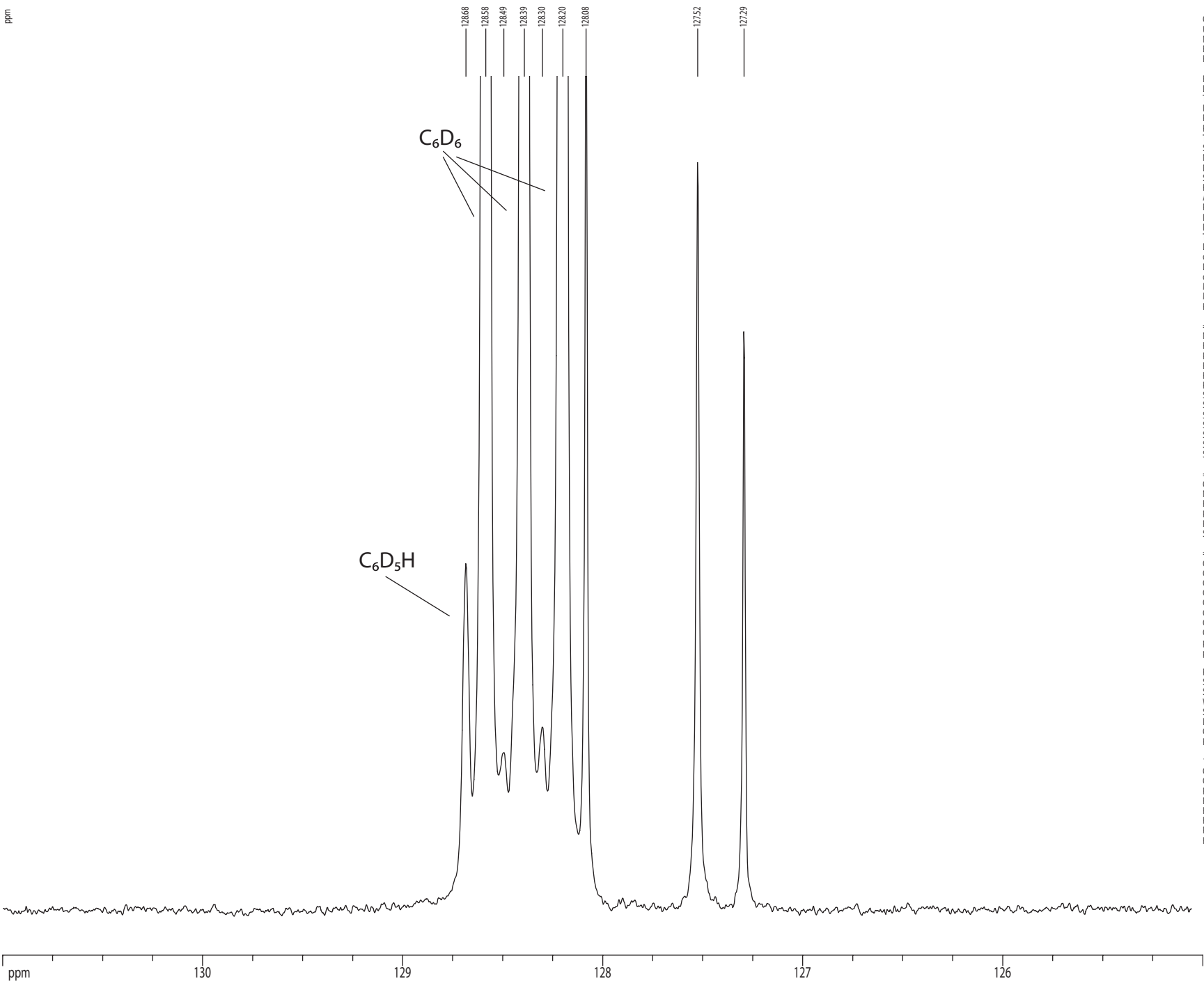
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.7803328 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 911.1 cm
F1P 160.000 ppm
F1 20124.85 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 7.01754 ppm/cm
HZCM 882.66907 Hz/cm

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



Current Data Parameters

USER nmr11t
NAME Sample 16
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20111203
Time 21.07
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchopg30gp.prd
TD 65536
SOLVENT CDCl3
NS 365
DS 16
SWH 30903.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813940 sec
RG 3251
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00019600 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 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 Crp60.0.5.20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz

===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz

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

GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec

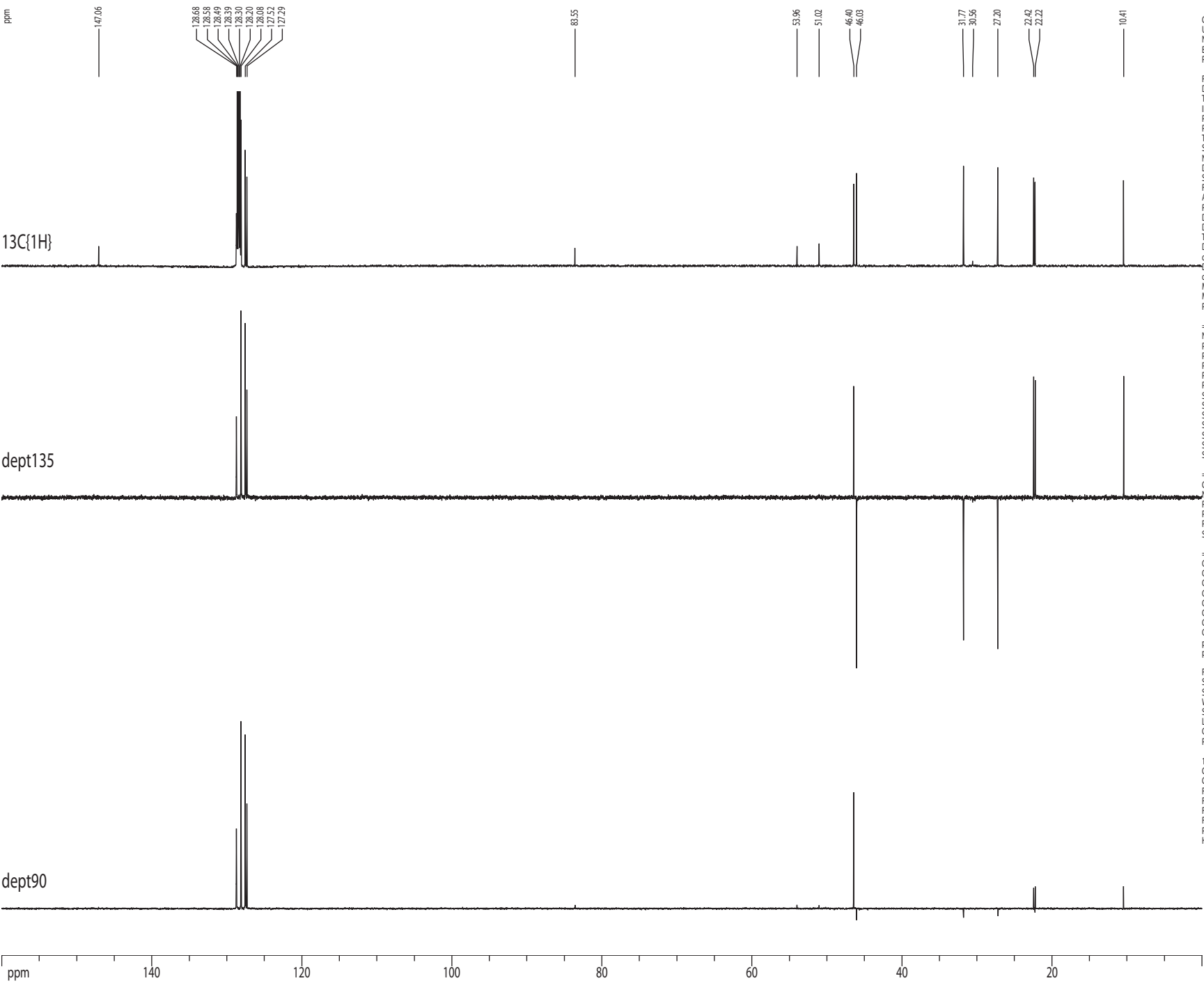
F2 - Processing parameters

SI 65536
SF 125.7803328 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

1D NMR plot parameters

CX 22.80 cm
CY 91.11 cm
F1P 131.000 ppm
F1 16472.22 Hz
F2P 125.000 ppm
F2 15722.54 Hz
PPMCM 0.26316 ppm/cm
HZCM 33.10009 Hz/cm

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



Current Data Parameters
USER nmr11t
NAME Sample 16
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111203
Time 21.07
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchogg30gp.prd
TD 65536
SOLVENT CDCl3
NS 365
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813940 sec
RG 3251
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d16 0.00020000 sec
d17 0.00019600 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 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 Cnp60.0.5.20.1
SPNAM2 Cnp60.comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz

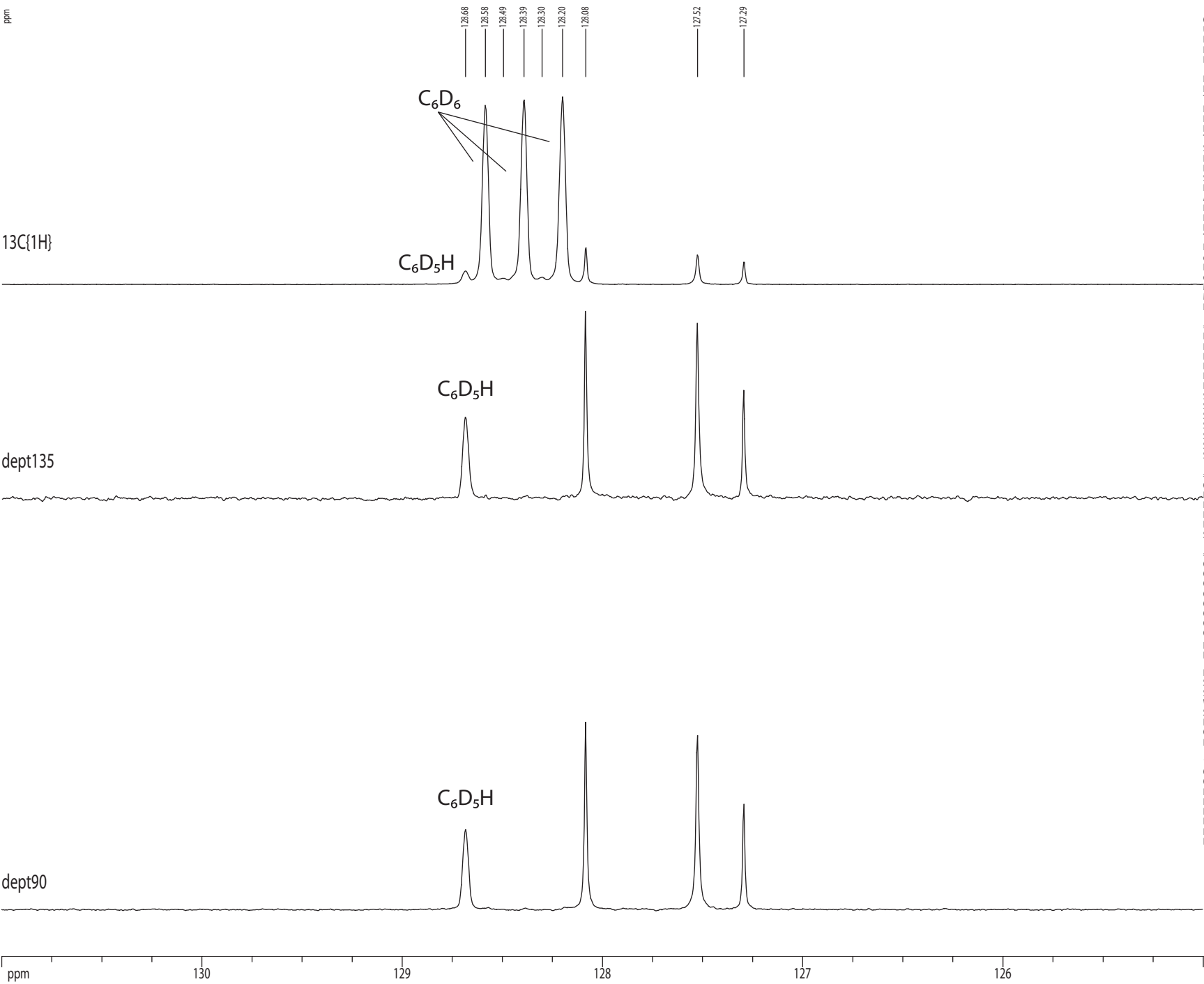
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CPDPRG2 waltz16
NUC2 ¹H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.7803328 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

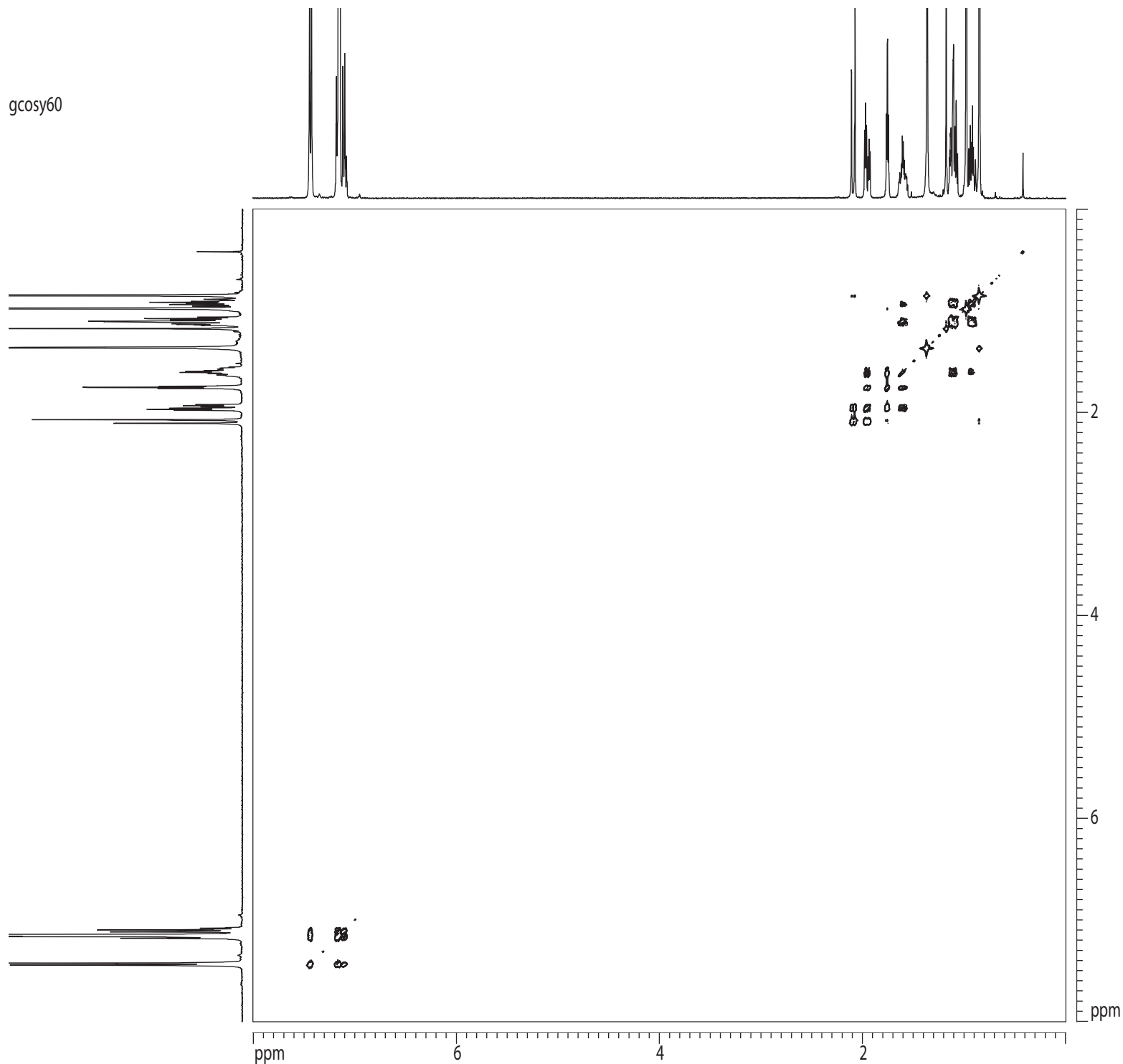
1D NMR plot parameters
CX 22.80 cm
CY 3.56 cm
F1P 160.000 ppm
F1 20124.85 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 7.01754 ppm/cm
HZCM 882.66907 Hz/cm

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



Current Data Parameters	
USER	nmr11t
NAME	Sample 16
EXPNO	2
PROCNO	1
F2 - Acquisition Parameters	
Date_	20111203
Time	21.07
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	SpinEchogg30gp.prd
TD	65536
SOLVENT	CDCl3
NS	365
DS	16
SWH	30303.031 Hz
FIDRES	0.462388 Hz
AQ	1.0813940 sec
RG	3251
DW	16.500 usec
DE	6.00 usec
TE	298.0 K
D1	0.25000000 sec
d11	0.03000000 sec
D16	0.00020000 sec
d17	0.00019600 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
P2	31.00 usec
===== CHANNEL f1 =====	
NUC1	^{13}C
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	Cyp60.0.5.20.1
SPNAM2	Cyp60comp.4
SPOFF1	0.00 Hz
SPOFF2	0.00 Hz
===== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	1.60 dB
PL12	24.60 dB
SFO2	500.2225011 MHz
===== GRADIENT CHANNEL =====	
GPAM1	SINE.100
GPAM2	SINE.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	30.00 %
GPZ2	50.00 %
p15	500.00 usec
p16	1000.00 usec
F2 - Processing parameters	
SI	65536
SF	125.7803328 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	2.00
1D NMR plot parameters	
CX	22.80 cm
CY	3.56 cm
F1P	131.000 ppm
F1	16477.22 Hz
F2P	125.000 ppm
F2	15722.54 Hz
PPMCM	0.26316 ppm/cm
HZCM	33.10009 Hz/cm

gcosy60



Current Data Parameters
 USER nmr11t
 NAME Sample 16
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
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 Time 21.36
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG cosygp60.prd
 TD 2048
 SOLVENT C6D6
 NS 4
 DS 16
 SWH 4006.410 Hz
 FIDRES 1.956255 Hz
 AQ 0.2556404 sec
 RG 35.9
 DW 124.800 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 1.00000000 sec
 d13 0.00000300 sec
 D16 0.00020000 sec
 INO 0.00024960 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.2220009 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

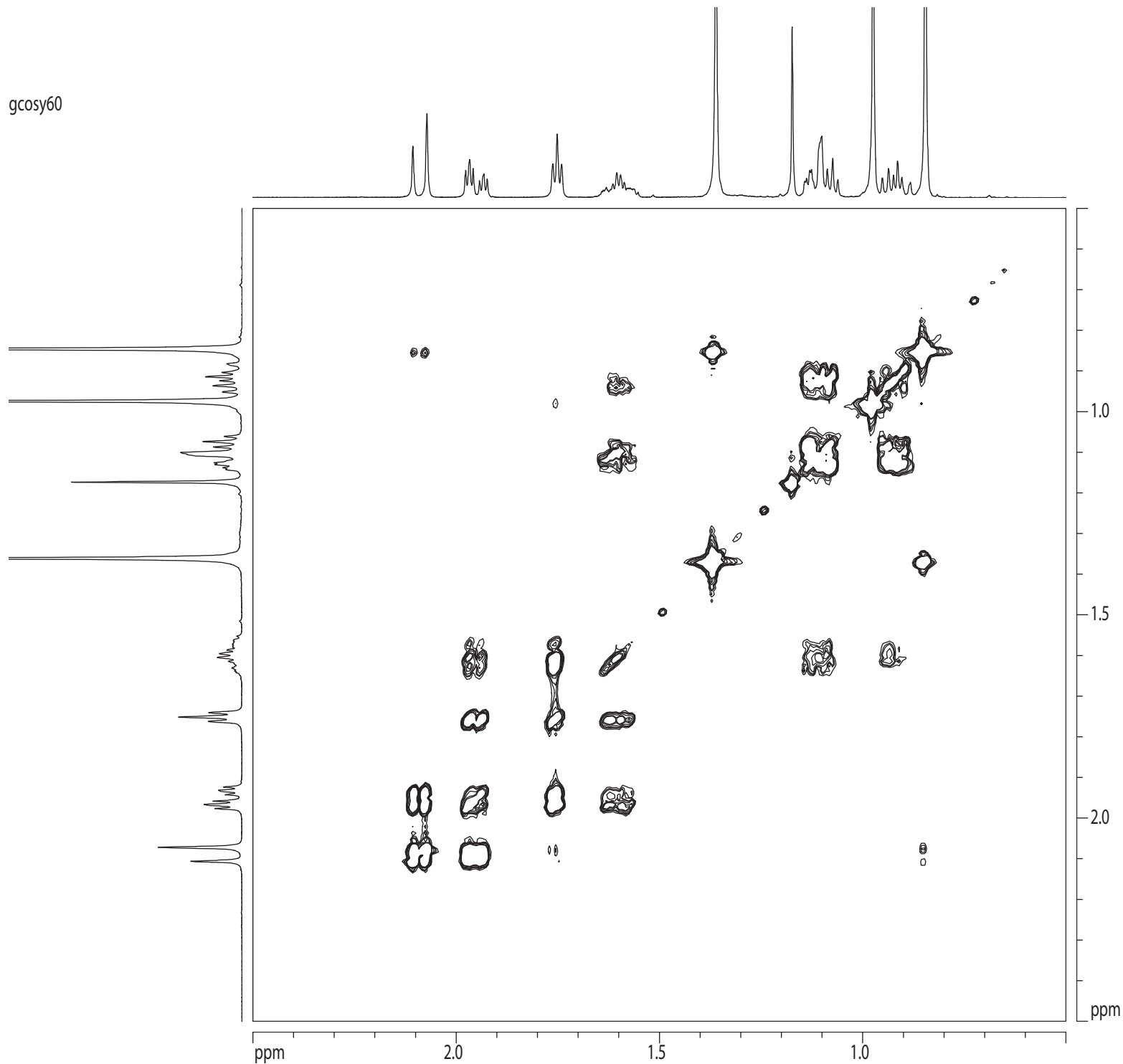
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 ND0 1
 TD 512
 SFO1 500.222 MHz
 FIDRES 7.825020 Hz
 SW 8.009 ppm
 FnmODE undefined

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 8.005 ppm
 F2LO 4004.08 Hz
 F2PHI -0.005 ppm
 F2HI -2.33 Hz
 F1PLO 8.005 ppm
 F1LO 4004.08 Hz
 F1PHI -0.005 ppm
 F1HI -2.33 Hz
 F2PPMCM 0.53395 ppm/cm
 F2HZCM 267.09402 Hz/cm
 F1PPMCM 0.53395 ppm/cm
 F1HZCM 267.09402 Hz/cm

gcosy60



Current Data Parameters

USER	nmr11t
NAME	Sample 16
EXPNO	5
PROCNO	1

F2 - Acquisition Parameters

Date_	20111203
Time	21.36
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	C6D6
NS	4
DS	16
SWH	4006.410 Hz
FIDRES	1.956255 Hz
AQ	0.2556404 sec
RG	35.9
DW	124.800 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00024960 sec

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

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2220009 MHz

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

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GRZ1	17.00 %
GRZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	512
SFO1	500.222 MHz
FIDRES	7.825020 Hz
SW	8.009 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

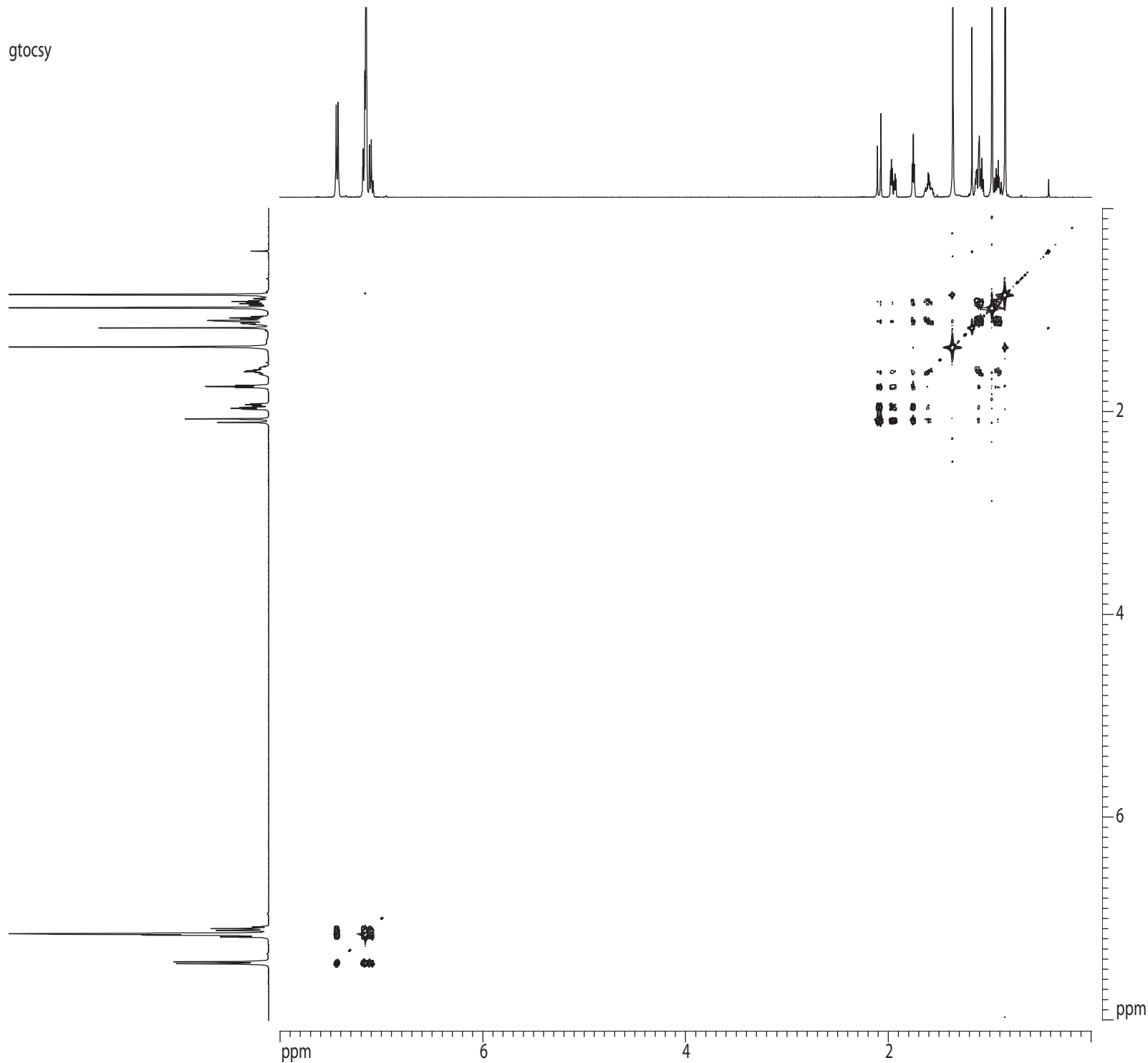
F1 - Processing parameters

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	2.500 ppm
F2LO	1250.55 Hz
F2PHI	0.500 ppm
F2HI	250.11 Hz
F1PLO	2.500 ppm
F1LO	1250.55 Hz
F1PHI	0.500 ppm
F1HI	250.11 Hz
F2PPMCM	0.13333 ppm/cm
F2HZCM	66.69600 Hz/cm
F1PPMCM	0.13333 ppm/cm
F1HZCM	66.69600 Hz/cm

gtocsy



Current Data Parameters
USER nmr11t
NAME Sample 16
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111203
Time 22.22
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG mlevup_mo
TD 2048
SOLVENT C6D6
NS 1
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 4
DW 124.800 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
D16 0.00020000 sec
FACTOR1 4
INO 0.00024960 sec
I1 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 500.222009 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

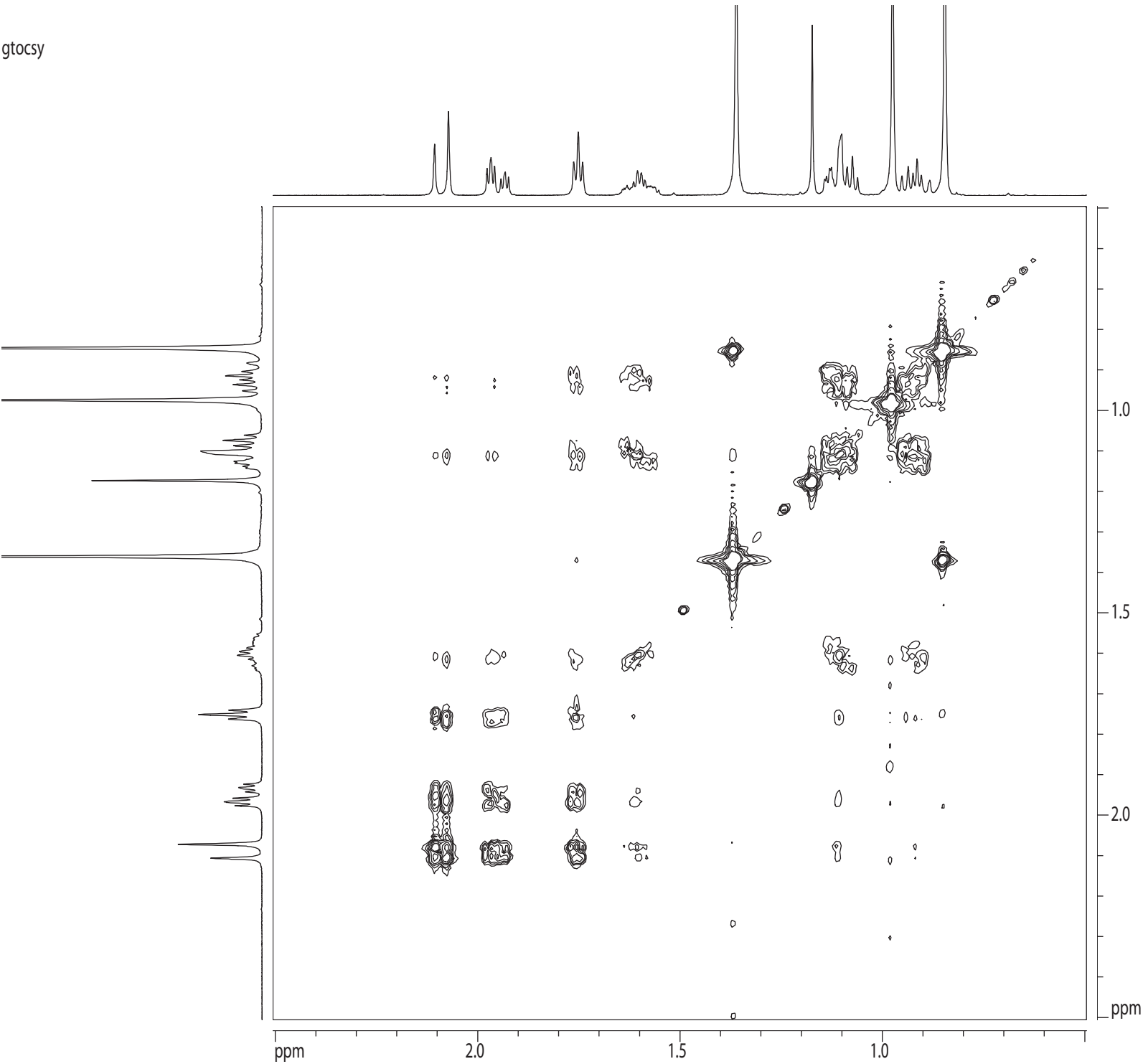
F1 - Acquisition parameters
ND0 1
TD 512
SFO1 500.222 MHz
FIDRES 7.825020 Hz
SW 8.009 ppm
FnMODE undefined

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 8.005 ppm
F2LO 4004.08 Hz
F2PHI -0.005 ppm
F2HI -2.33 Hz
F1PLO 8.005 ppm
F1LO 4004.08 Hz
F1PHI -0.005 ppm
F1HI -2.33 Hz
F2PPMCM 0.53395 ppm/cm
F2HZCM 267.09402 Hz/cm
F1PPMCM 0.53395 ppm/cm
F1HZCM 267.09402 Hz/cm

gtocsy



Current Data Parameters
USER nmr11t
NAME Sample 16
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111203
Time 22.22
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG mlevup_mo
TD 2048
SOLVENT C6D6
NS 1
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 4
DW 124.800 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
D16 0.00002000 sec
FACTOR1 4
INO 0.00024960 sec
I1 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 500.2220009 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

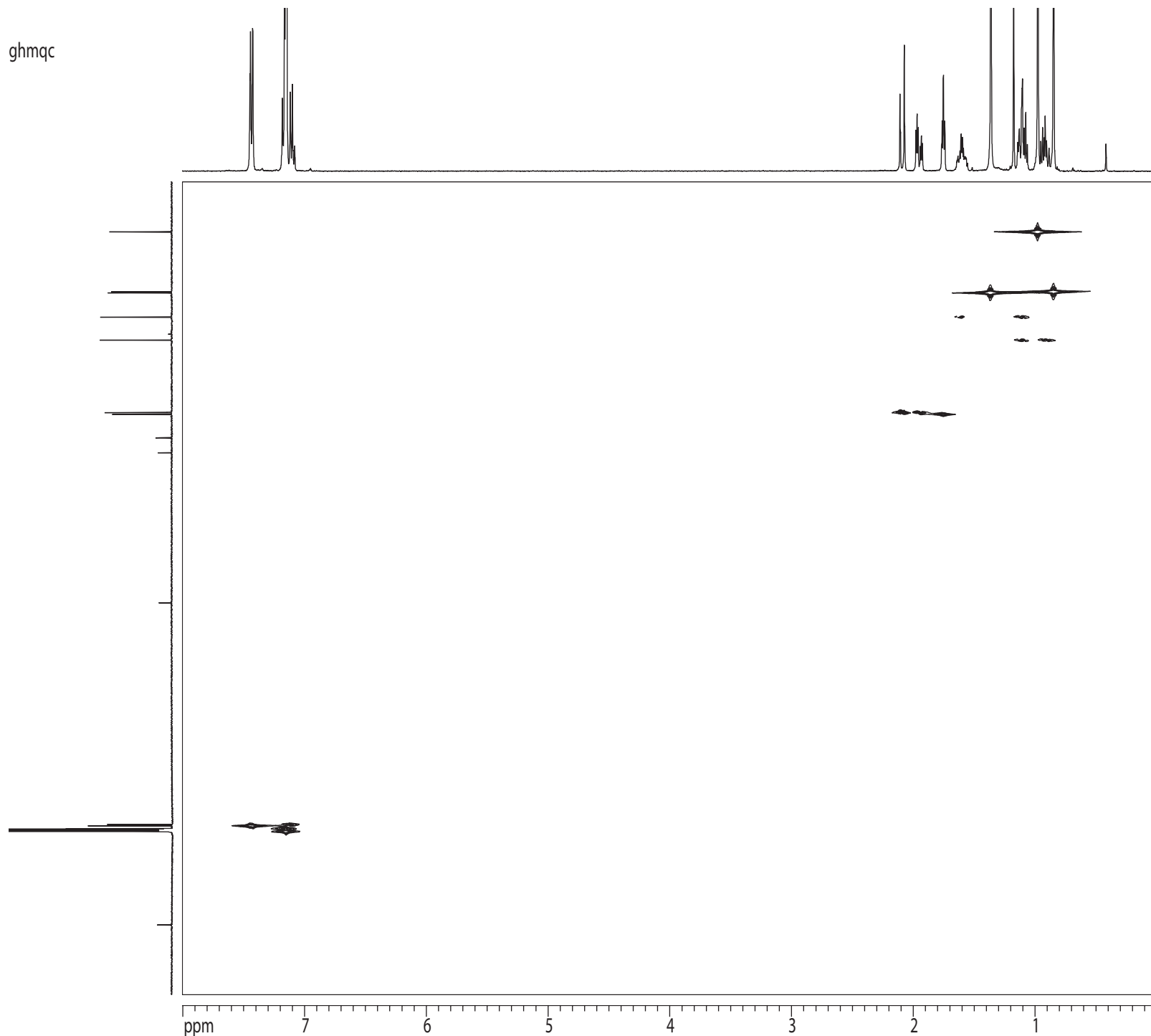
F1 - Acquisition parameters
ND0 1
TD 512
SFO1 500.222 MHz
FIDRES 7.825020 Hz
SW 8.009 ppm
FnMODE undefined

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 OF
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 2.506 ppm
F2LO 1253.59 Hz
F2PHI 0.496 ppm
F2HI 248.07 Hz
F1PLO 2.506 ppm
F1LO 1253.59 Hz
F1PHI 0.496 ppm
F1HI 248.07 Hz
F2PPMCM 0.13401 ppm/cm
F2HZCM 67.03434 Hz/cm
F1PPMCM 0.13401 ppm/cm
F1HZCM 67.03434 Hz/cm

ghmqc



Current Data Parameters

USER nmr11t
NAME Sample 16
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters

Date_ 20111203
Time 22.43
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG inv4gpcw
TD 2048
SOLVENT C6D6
NS 4
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 7298.2
DW 124.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.000000
d0 0.00000300 sec
D1 1.00000000 sec
d2 0.00344028 sec
d12 0.00002000 sec
d13 0.00000300 sec
D16 0.00020000 sec
d20 0.00242528 sec
IN0 0.00002480 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 MHz

===== CHANNEL f2 =====

CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7904814 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 30.00 %
GPZ2 18.00 %
GPZ3 24.00 %
P16 1000.00 usec

F1 - Acquisition parameters

ND0 2
TD 512
SFO1 125.7905 MHz
FIDRES 39.377522 Hz
SW 160.277 ppm
FnMODE undefined

F2 - Processing parameters

SI 1024
SF 500.2200000 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

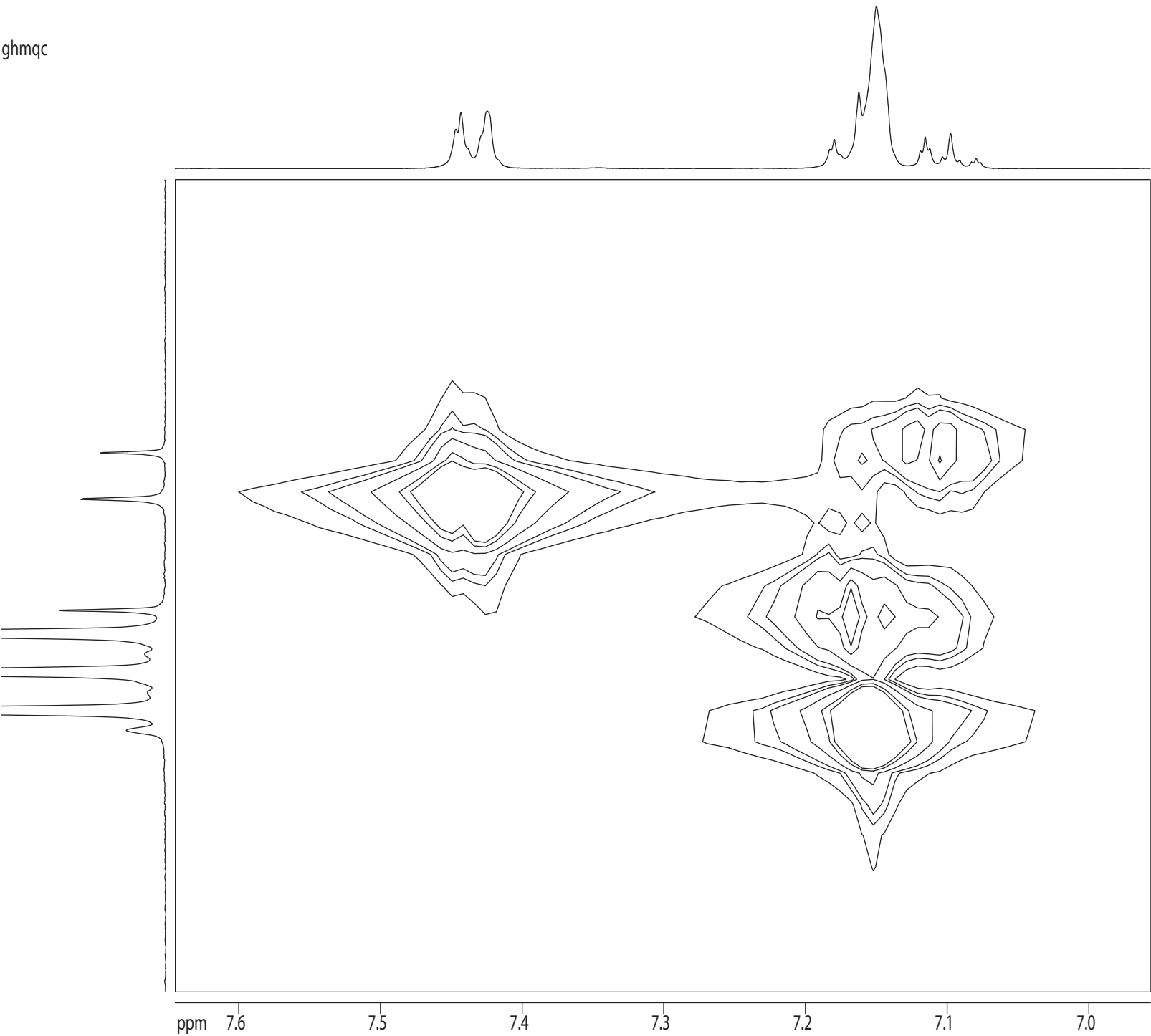
F1 - Processing parameters

SI 1024
MC2 QF
SF 125.7804190 MHz
WDW QSINE
SSB 3
LB 0.00 Hz
GB 0

2D NMR plot parameters

CX2 18.00 cm
CX1 15.00 cm
F2PLO 8.005 ppm
F2LO 4004.08 Hz
F2PHI -0.005 ppm
F2HI -2.33 Hz
F1PLO 160.145 ppm
F1LO 20143.07 Hz
F1PHI -0.145 ppm
F1HI -18.22 Hz
F2PPMCM 0.44496 ppm/cm
F2HZCM 222.57835 Hz/cm
F1PPMCM 10.68597 ppm/cm
F1HZCM 1344.08606 Hz/cm

ghmqc



Current Data Parameters

USER nmr11t
NAME Sample 16
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters

Date_ 20111203
Time 22.43
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG inv4gq.wu
TD 2048
SOLVENT C6D6
NS 4
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 7298.2
DW 124.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.00000000 sec
d2 0.00344028 sec
d12 0.00002000 sec
d13 0.00000300 sec
D16 0.00020000 sec
d20 0.00242528 sec
IN0 0.00002480 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 MHz

===== CHANNEL f2 =====

CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7904814 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 30.00 %
GPZ2 18.00 %
GPZ3 24.00 %
P16 1000.00 usec

F1 - Acquisition parameters

ND0 2
TD 512
SFO1 125.7905 MHz
FIDRES 39.377522 Hz
SW 160.277 ppm
FnMODE undefined

F2 - Processing parameters

SI 1024
SF 500.2200000 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

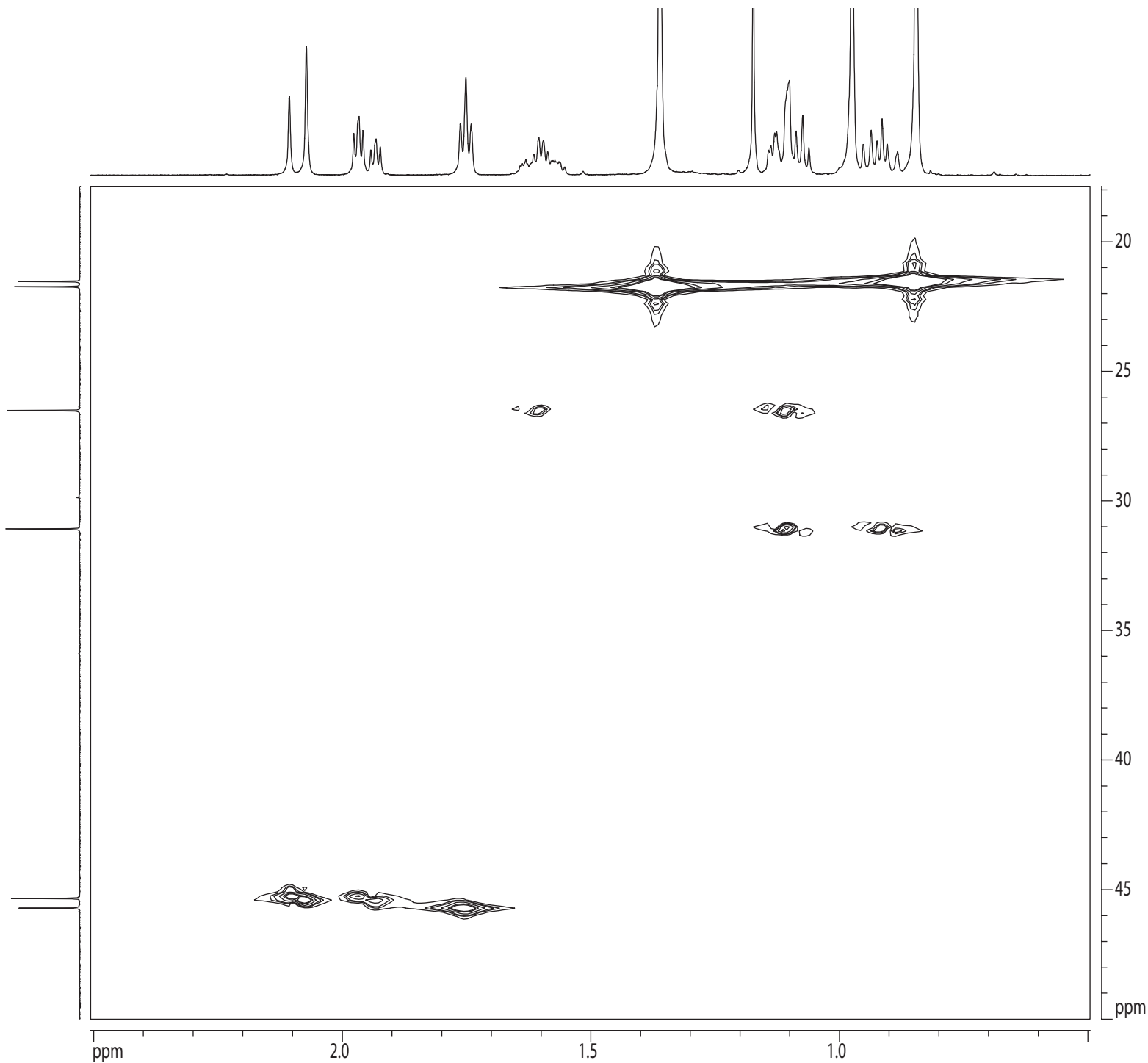
F1 - Processing parameters

SI 1024
MC2 QF
SF 125.7804190 MHz
WDW QSINE
SSB 3
LB 0.00 Hz
GB 0

2D NMR plot parameters

CX2 18.00 cm
CX1 15.00 cm
F2PLO 7.645 ppm
F2LO 3824.11 Hz
F2PHI 6.957 ppm
F2HI 3479.81 Hz
F1PLO 129.308 ppm
F1LO 16264.58 Hz
F1PHI 125.238 ppm
F1HI 15752.47 Hz
F2PPMCM 0.03824 ppm/cm
F2HZCM 19.12782 Hz/cm
F1PPMCM 0.27132 ppm/cm
F1HZCM 34.12720 Hz/cm

ghmqc



Current Data Parameters

USER nmr11t
NAME Sample 16
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters

Date_ 20111203
Time 22:43
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG invgpgw
TD 2048
SOLVENT C6D6
NS 4
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 7298.2
DW 124.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.000000
d0 0.00000300 sec
D1 1.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000300 sec
D16 0.00020000 sec
d20 0.00242528 sec
IN0 0.00002480 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 MHz

===== CHANNEL f2 =====

CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7904814 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 30.00 %
GPZ2 18.00 %
GPZ3 24.00 %
P16 1000.00 usec

F1 - Acquisition parameters

ND0 2
TD 512
SFO1 125.7905 MHz
FIDRES 39.377522 Hz
SW 160.277 ppm
FnMODE undefined

F2 - Processing parameters

SI 1024
SF 500.2200000 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

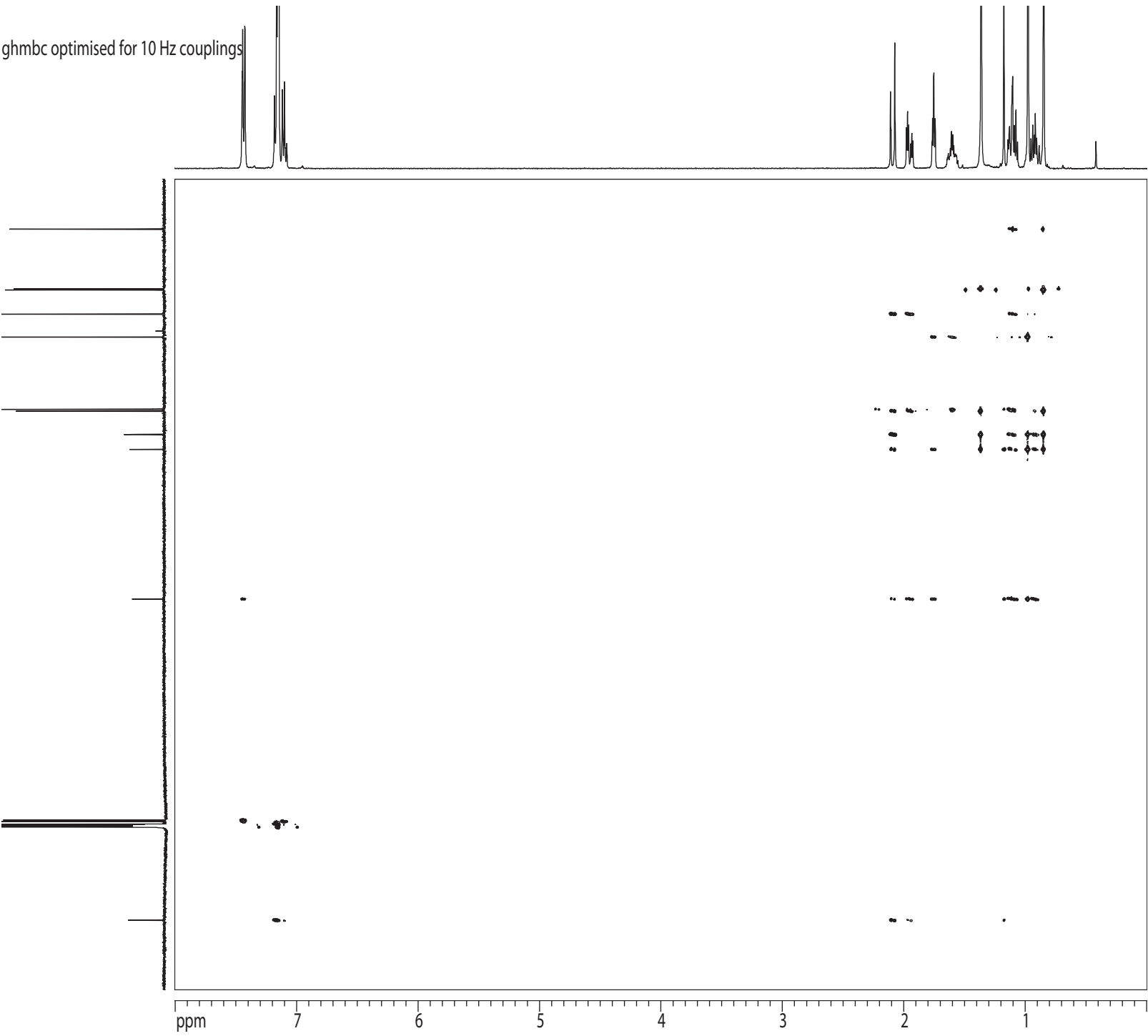
F1 - Processing parameters

SI 1024
MC2 QF
SF 125.7804190 MHz
WDW QSINE
SSB 3
LB 0.00 Hz
GB 0

2D NMR plot parameters

CX2 18.00 cm
CX1 15.00 cm
F2PLO 2.506 ppm
F2LO 1253.59 Hz
F2PHI 0.496 ppm
F2HI 248.07 Hz
F1PLO 50.000 ppm
F1LO 6289.02 Hz
F1PHI 17.856 ppm
F1HI 2245.98 Hz
F2PPMCM 0.11167 ppm/cm
F2HZCM 55.86195 Hz/cm
F1PPMCM 2.14291 ppm/cm
F1HZCM 269.53577 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr11t
NAME Sample 16
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters

Date_ 201111203
Time 23.27
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.cwv
TD 4096
SOLVENT C6D6
NS 4
DS 16
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 5160.6
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.25000000 sec
d2 0.00344828 sec
D6 0.05000000 sec
d13 0.00000300 sec
D16 0.00020000 sec
IN0 0.00002480 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 MHz

===== CHANNEL f2 =====

NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7904814 MHz

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

GPNAME1 sine.100
GPNAME2 sine.100
GPNAME3 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

ND0 2
TD 512
SFO1 125.7905 MHz
FIDRES 39.377522 Hz
SW 160.277 ppm
FhMODE undefined

F2 - Processing parameters

SI 2048
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

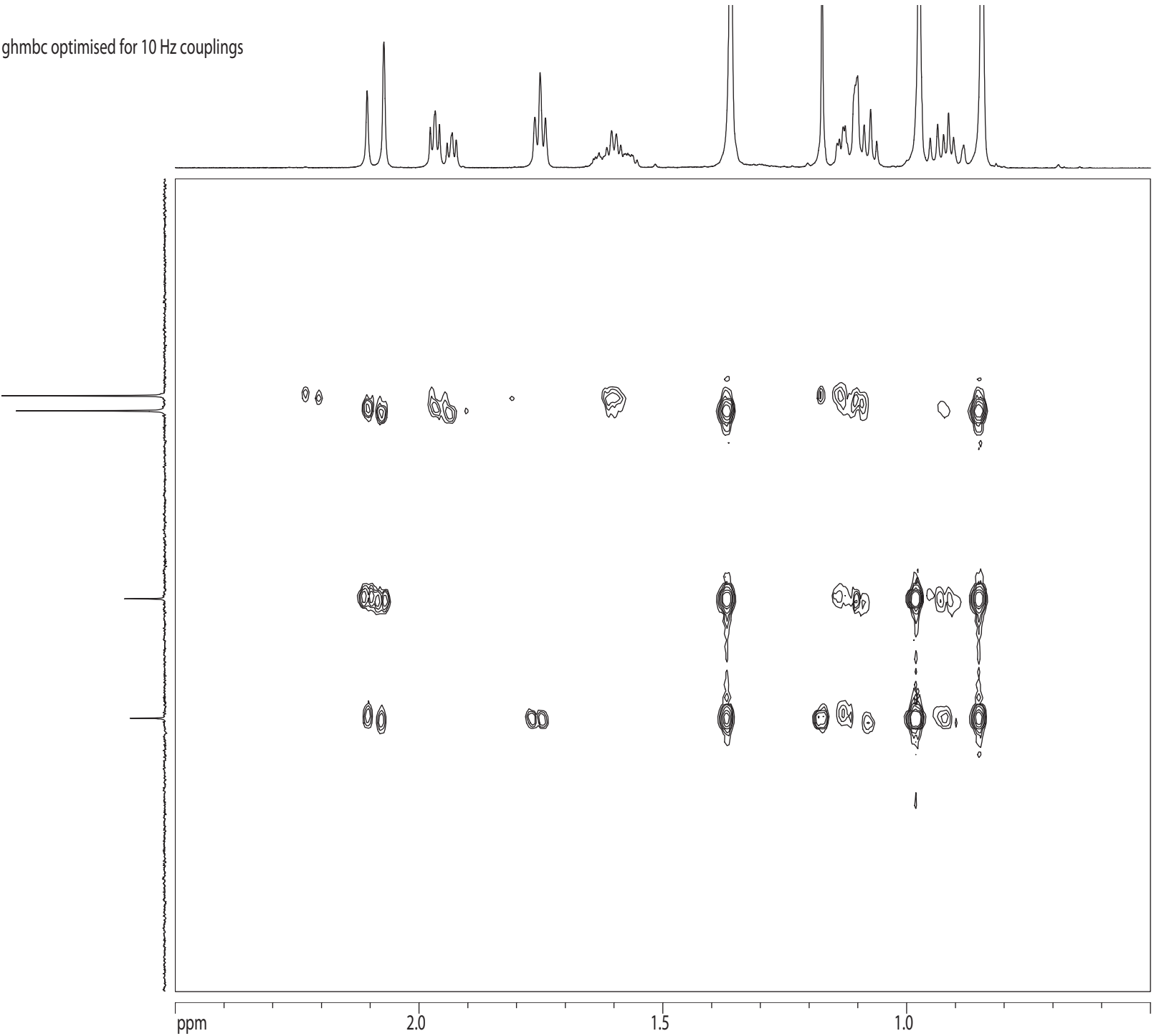
F1 - Processing parameters

SI 1024
MC2 QF
SF 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 8.005 ppm
F2LO 4004.08 Hz
F2PHI -0.005 ppm
F2HI -2.33 Hz
F1PLO 160.145 ppm
F1LO 20143.07 Hz
F1PHI -0.145 ppm
F1HI -18.22 Hz
F2PPMCM 0.44496 ppm/cm
F2HZCM 222.57835 Hz/cm
F1PPMCM 10.68597 ppm/cm
F1HZCM 1344.08606 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr11t
NAME Sample 16
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters

Date_ 201111203
Time 23.27
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT C6D6
NS 4
DS 16
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 5160.6
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.25000000 sec
d2 0.00344828 sec
D6 0.05000000 sec
d13 0.00000300 sec
D16 0.00020000 sec
INO 0.0002480 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.222009 MHz

===== CHANNEL f2 =====

NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7904814 MHz

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

GP1AM1 sine.100
GP1AM2 sine.100
GP1AM3 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

ND0 2
TD 512
SFO1 125.7905 MHz
FIDRES 39.377522 Hz
SW 160.277 ppm
FnMODE undefined

F2 - Processing parameters

SI 2048
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

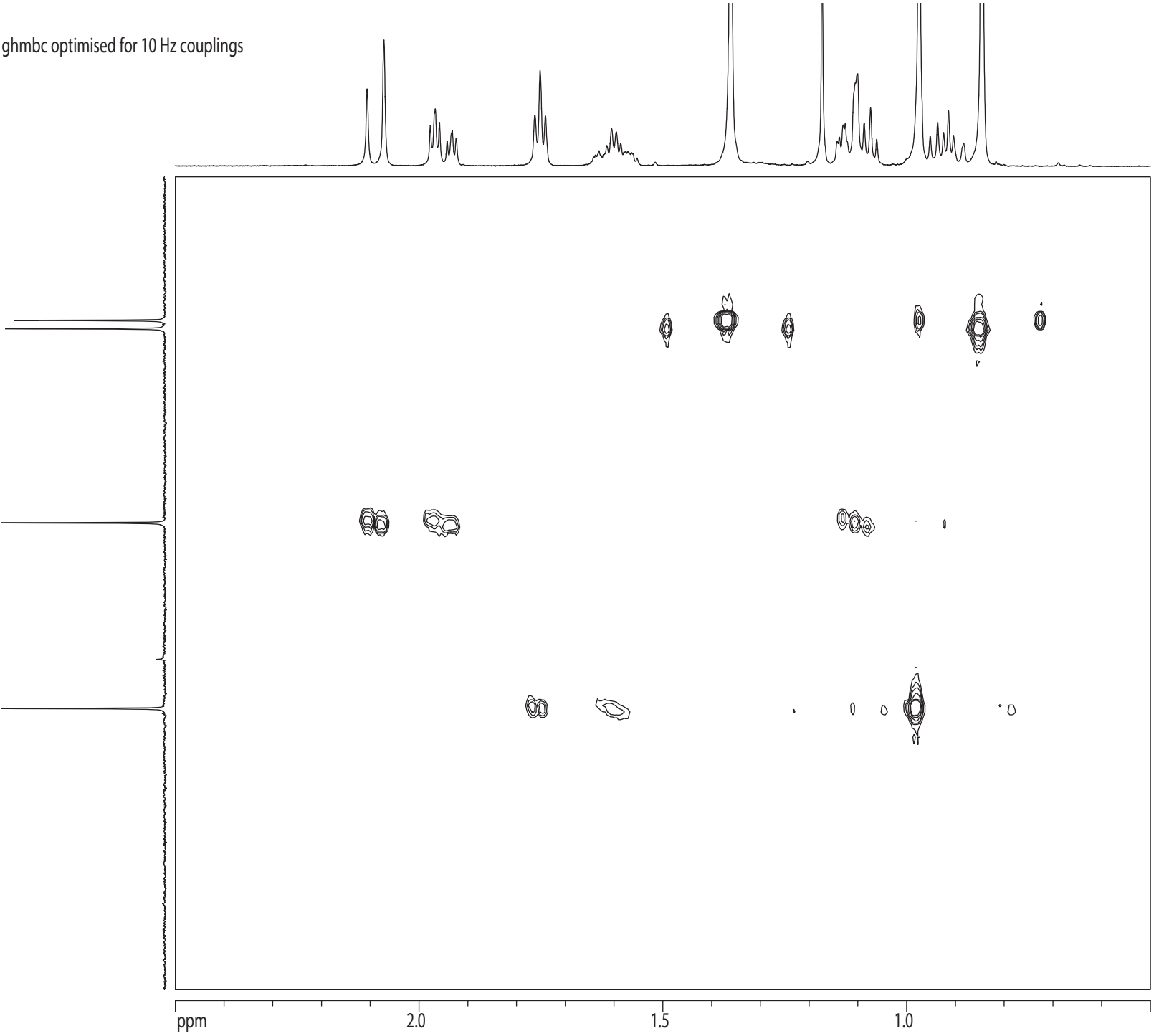
F1 - Processing parameters

SI 1024
MC2 QF
SF 125.7804190 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters

CY2 18.00 cm
CX1 15.00 cm
F2PLO 2.500 ppm
F2LO 1250.55 Hz
F2PHI 0.500 ppm
F2HI 250.11 Hz
F1PLO 60.000 ppm
F1LO 7546.83 Hz
F1PHI 40.000 ppm
F1HI 5031.22 Hz
F2PPMCM 0.11111 ppm/cm
F2HZCM 55.58000 Hz/cm
F1PPMCM 1.33333 ppm/cm
F1HZCM 167.70723 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr11t
NAME Sample 16
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters

Date_ 201111203
Time 23.27
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wvu
TD 4096
SOLVENT C6D6
NS 4
DS 16
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 5160.6
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.25000000 sec
d2 0.00344828 sec
D6 0.05000000 sec
d13 0.00000300 sec
D16 0.00020000 sec
INO 0.00002480 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 MHz

===== CHANNEL f2 =====

NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7904814 MHz

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

GPNAME1 sine.100
GPNAME2 sine.100
GPNAME3 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

ND0 2
TD 512
SFO1 125.7905 MHz
FIDRES 39.377522 Hz
SW 160.277 ppm
F1MODE undefined

F2 - Processing parameters

SI 2048
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

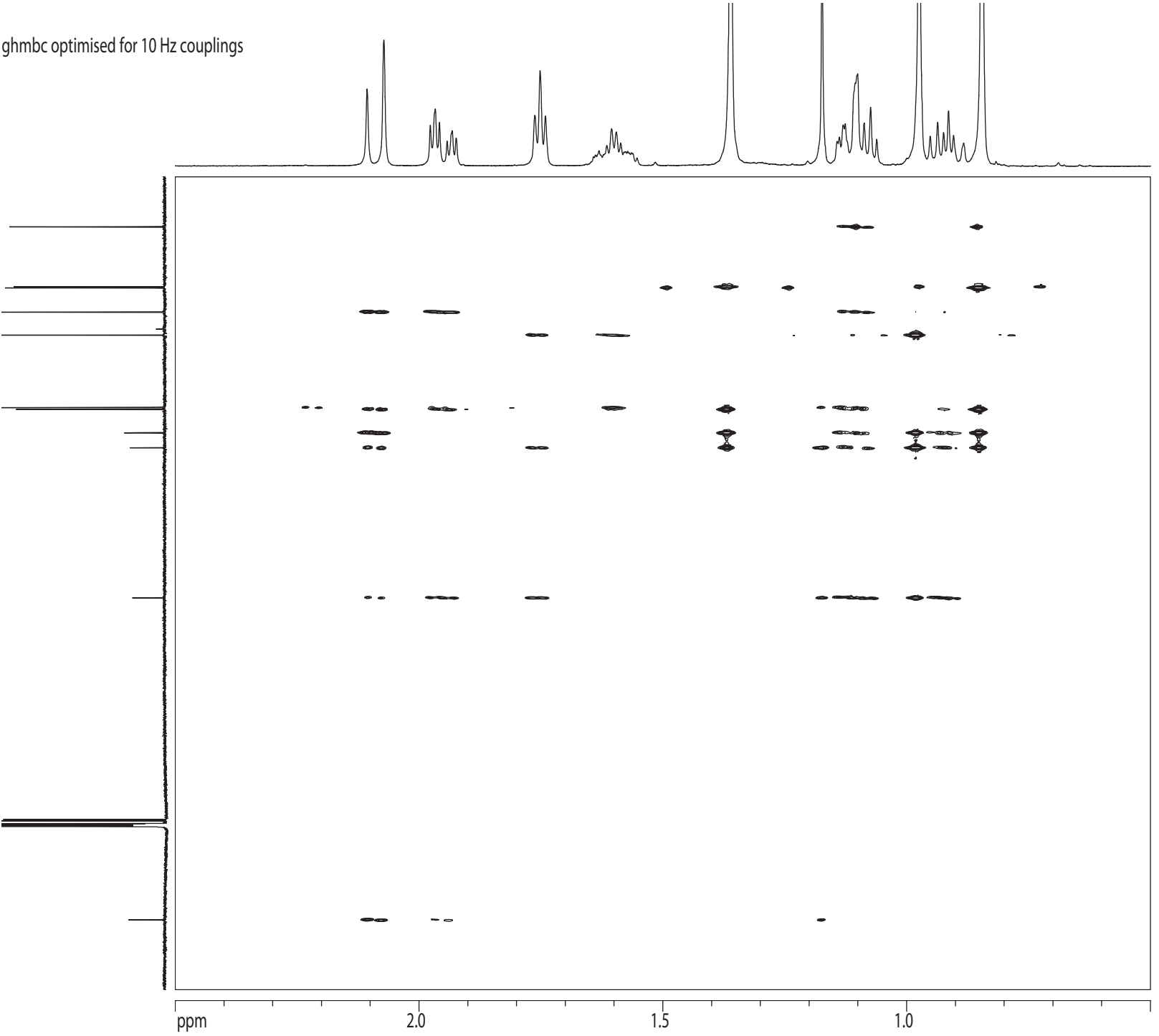
F1 - Processing parameters

SI 1024
MC2 QF
SF 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 2.500 ppm
F2LO 1250.55 Hz
F2PHI 0.500 ppm
F2HI 250.11 Hz
F1PLO 38.000 ppm
F1LO 4779.66 Hz
F1PHI 18.000 ppm
F1HI 2264.05 Hz
F2PPMCM 0.11111 ppm/cm
F2HZCM 55.58000 Hz/cm
F1PPMCM 1.33333 ppm/cm
F1HZCM 167.70723 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr11t
NAME Sample 16
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters

Date_ 201111203
Time 23.27
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT C6D6
NS 4
DS 16
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 5160.6
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.25000000 sec
d2 0.00344828 sec
D6 0.05000000 sec
d13 0.00000300 sec
D16 0.00020000 sec
IN0 0.00002480 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 MHz

===== CHANNEL f2 =====

NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7904814 MHz

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

GPNAME1 sine.100
GPNAME2 sine.100
GPNAME3 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

ND0 2
TD 512
SFO1 125.7905 MHz
FIDRES 39.377522 Hz
SW 160.277 ppm
F1MODE undefined

F2 - Processing parameters

SI 2048
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

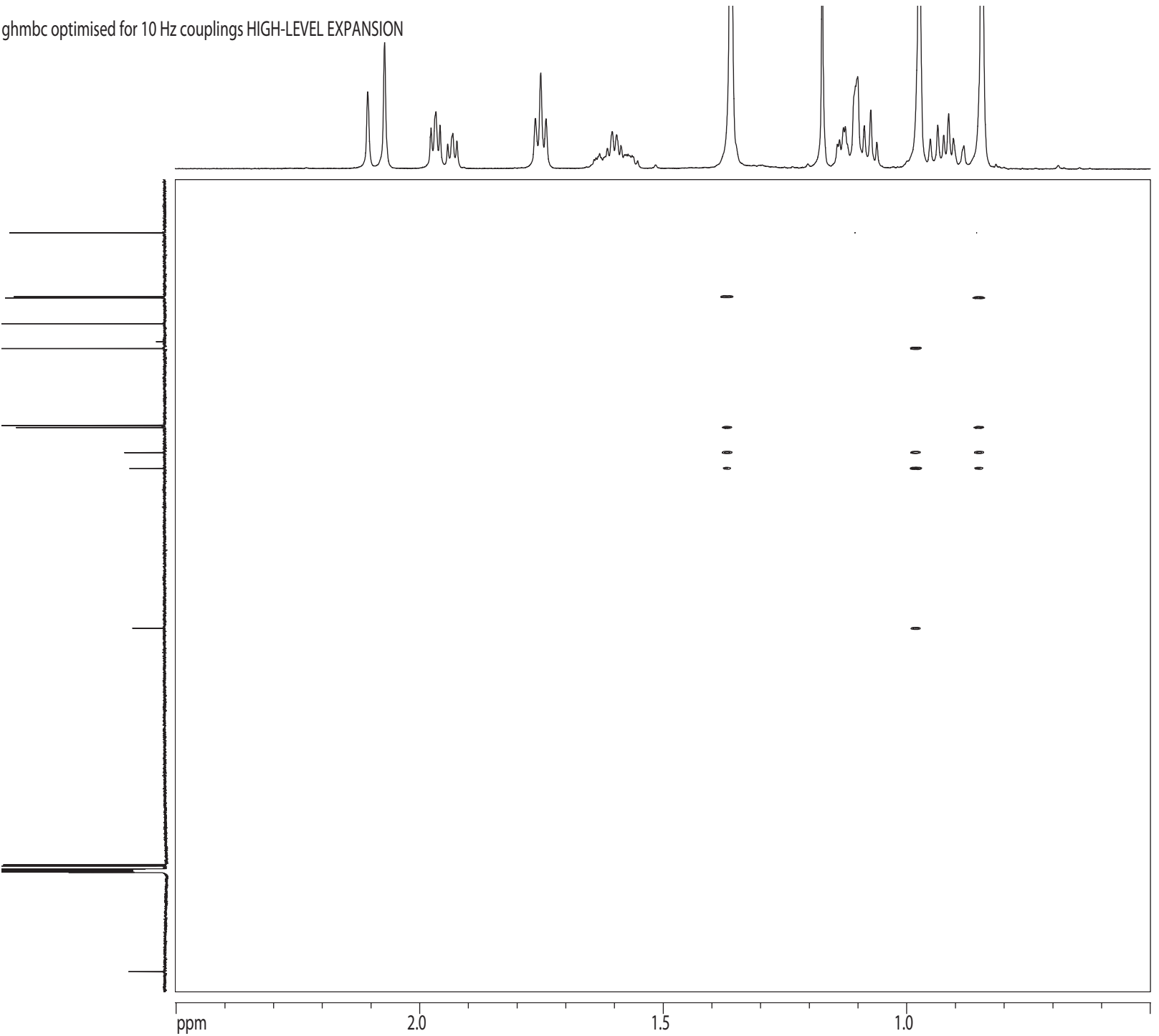
F1 - Processing parameters

SI 1024
MC2 QF
SF 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 2.500 ppm
F2LO 1250.55 Hz
F2PHI 0.500 ppm
F2PHI 250.11 Hz
F1PLO 160.145 ppm
F1LO 20143.07 Hz
F1PHI -0.145 ppm
F1HI -18.22 Hz
F2PPMCM 0.11111 ppm/cm
F2HZCM 55.58000 Hz/cm
F1PPMCM 10.68597 ppm/cm
F1HZCM 1344.08606 Hz/cm

ghmbc optimised for 10 Hz couplings HIGH-LEVEL EXPANSION



Current Data Parameters

USER nmr11t
NAME Sample 16
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters

Date_ 201111203
Time 23.27
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT C6D6
NS 4
DS 16
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 5160.6
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.25000000 sec
d2 0.00344828 sec
D6 0.05000000 sec
d13 0.00000300 sec
D16 0.00020000 sec
IN0 0.00002480 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 MHz

===== CHANNEL f2 =====

NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7904814 MHz

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

GPNAME1 sine.100
GPNAME2 sine.100
GPNAME3 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

ND0 2
TD 512
SFO1 125.7905 MHz
FIDRES 39.377522 Hz
SW 160.277 ppm
F1MODE undefined

F2 - Processing parameters

SI 2048
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

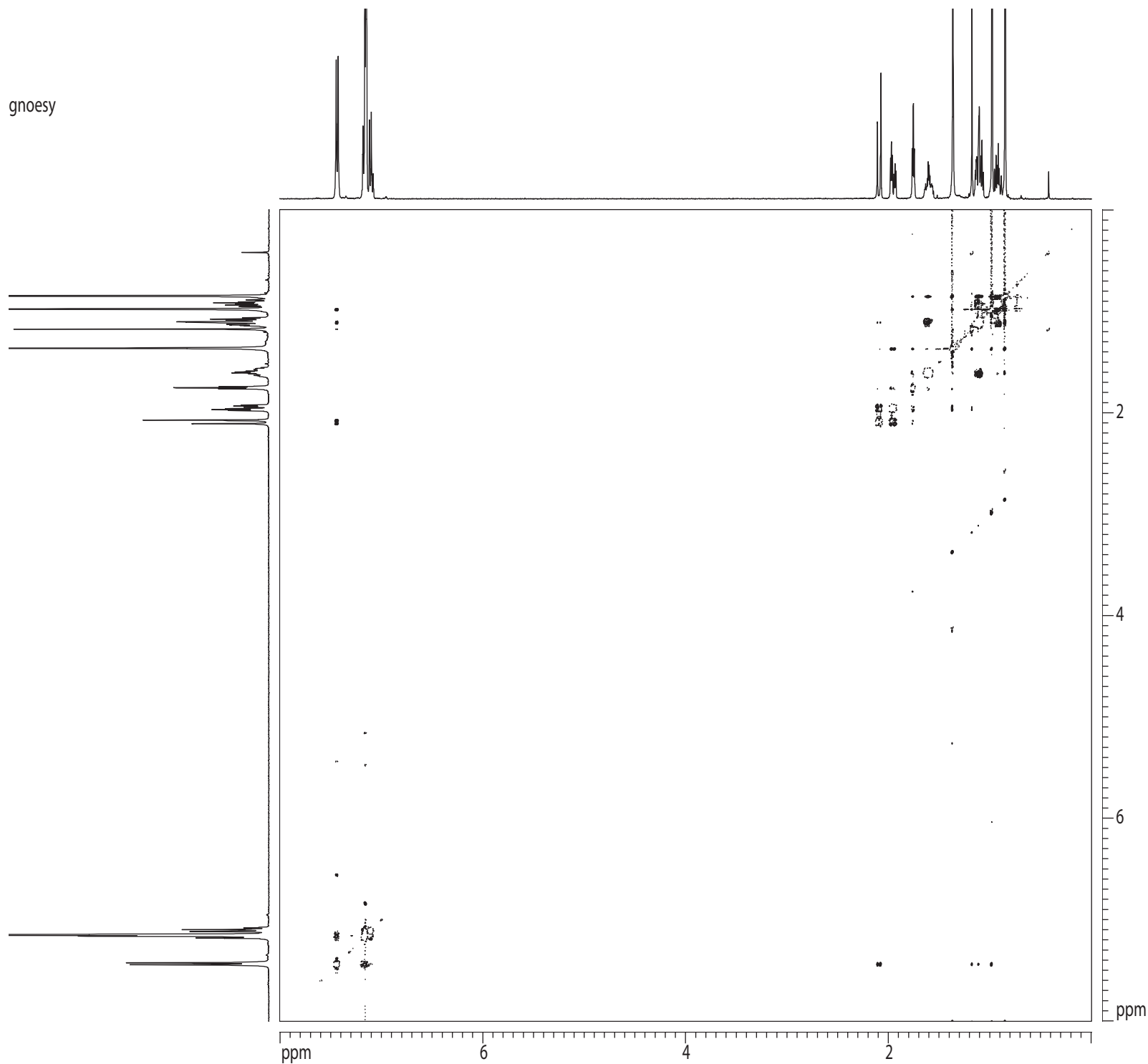
F1 - Processing parameters

SI 1024
MC2 QF
SF 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 2.502 ppm
F2LO 1251.63 Hz
F2PHI 0.500 ppm
F2HI 250.03 Hz
F1PLO 150.127 ppm
F1LO 18882.98 Hz
F1PHI -0.145 ppm
F1HI -18.23 Hz
F2PPMCM 0.11124 ppm/cm
F2HZCM 55.64459 Hz/cm
F1PPMCM 10.01810 ppm/cm
F1HZCM 1260.08069 Hz/cm

gnoesy



Current Data Parameters
USER nmr11t
NAME Sample 16
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111204
Time 0.31
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG noesygptp
TD 2048
SOLVENT C6D6
NS 8
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 128
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d20 0.24879999 sec
IN0 0.00012480 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
P2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 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

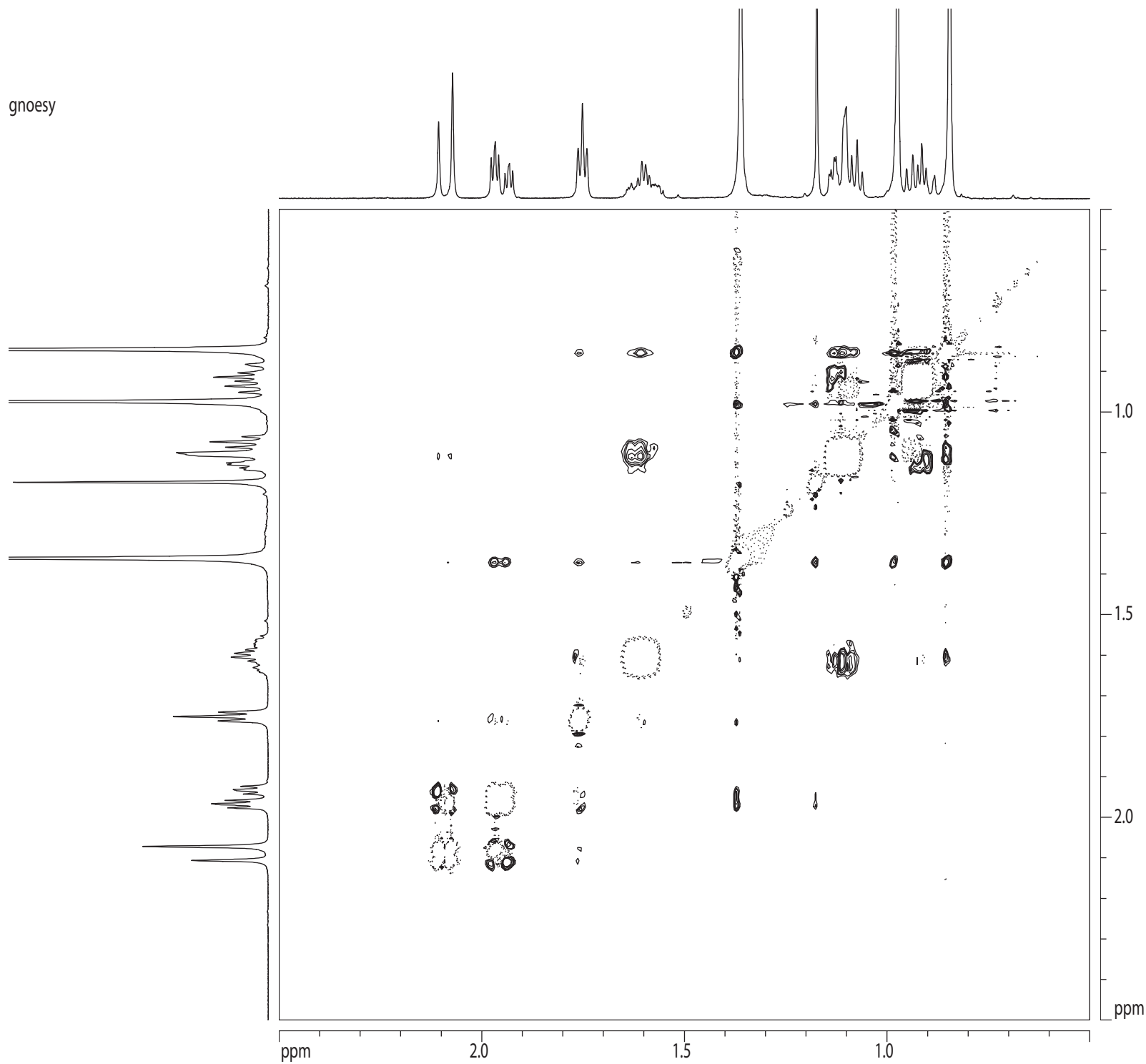
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 500.222 MHz
FIDRES 7.825020 Hz
SW 8.009 ppm
FnMODE undefined

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 8.005 ppm
F2LO 4004.08 Hz
F2PHI -0.005 ppm
F2HI -2.33 Hz
F1PLO 8.005 ppm
F1LO 4004.08 Hz
F1PHI -0.005 ppm
F1HI -2.33 Hz
F2PPMCM 0.53395 ppm/cm
F2HZCM 267.09402 Hz/cm
F1PPMCM 0.53395 ppm/cm
F1HZCM 267.09402 Hz/cm

gnoesy



Current Data Parameters
USER nmr11t
NAME Sample 16
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111204
Time 0.31
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG noesygptp
TD 2048
SOLVENT C6D6
NS 8
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 128
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d20 0.24879999 sec
IN0 0.00012480 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
P2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 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 500.222 MHz
FIDRES 7.825020 Hz
SW 8.009 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 2.500 ppm
F2LO 1250.55 Hz
F2PHI 0.500 ppm
F2HI 250.11 Hz
F1PLO 2.500 ppm
F1LO 1250.55 Hz
F1PHI 0.500 ppm
F1HI 250.11 Hz
F2PPMCM 0.13333 ppm/cm
F2HZCM 66.69600 Hz/cm
F1PPMCM 0.13333 ppm/cm
F1HZCM 66.69600 Hz/cm