

Name: _____

Chem 203
December 10, 2011

Final Exam Part II
Problem 3 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 $C_{10}H_{16}O$: IR (Thin Film on NaCl), 500 MHz 1H NMR, 125.7 MHz ^{13}C NMR, DEPT-90, DEPT-135, COSY, HMQC, HMBC, TOCSY, and NOESY. 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 $CDCl_3$. The 1H resonance at 7.27 ppm corresponds to $CHCl_3$.

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-j) 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:

c. Redraw the structure of the molecule below and write the letter (a-j) 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 (1-10) 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:

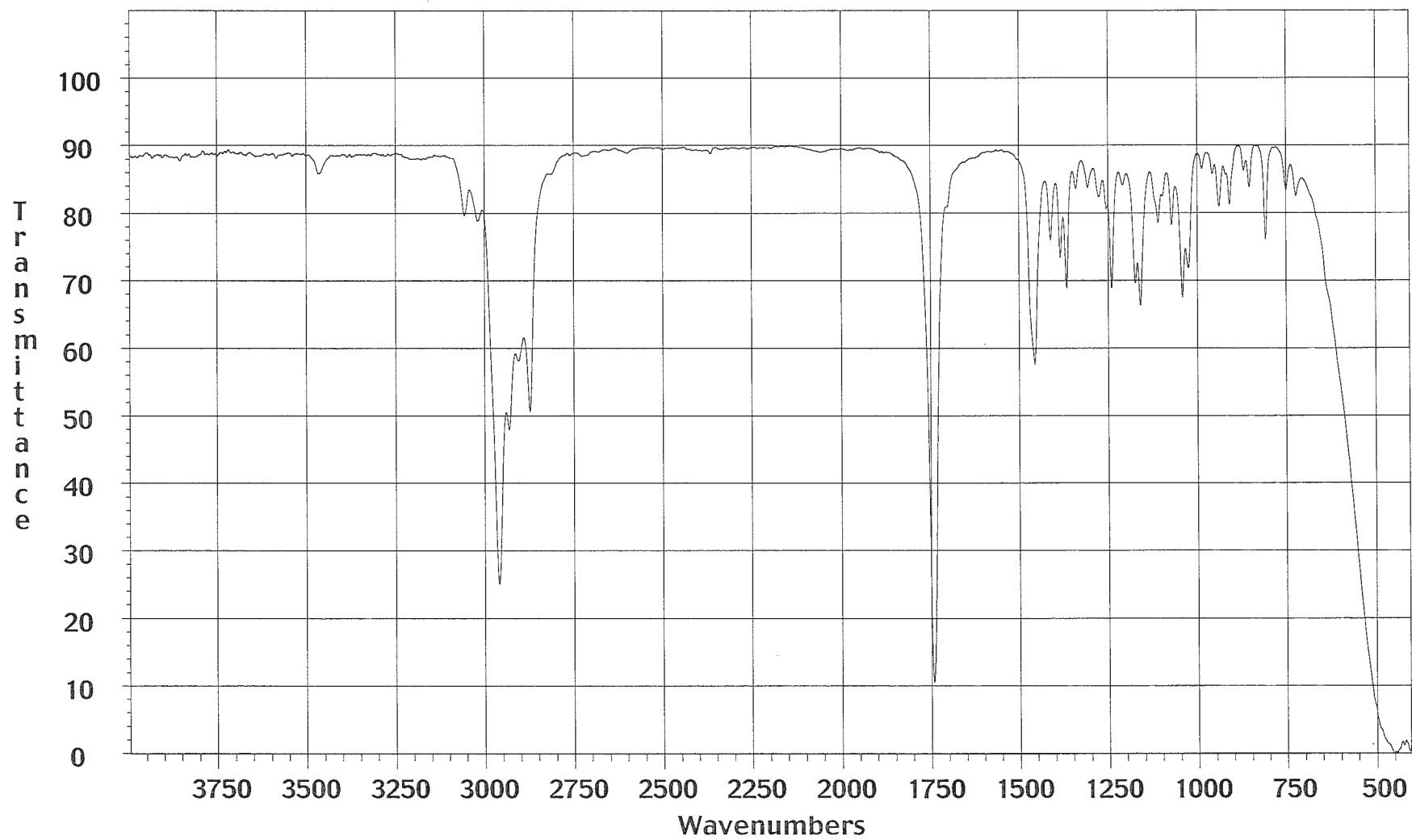
e. Redraw the structure of the molecule below and write the number (1-10) of each ^{13}C resonance next to the carbon or carbons to which it corresponds. If the assignment of particular resonance is uncertain, please indicate this.

f. Build an energy-minimized molecular model of the molecule using PyMOL and the "clean" function. Save the .pse file as problem3.pse.

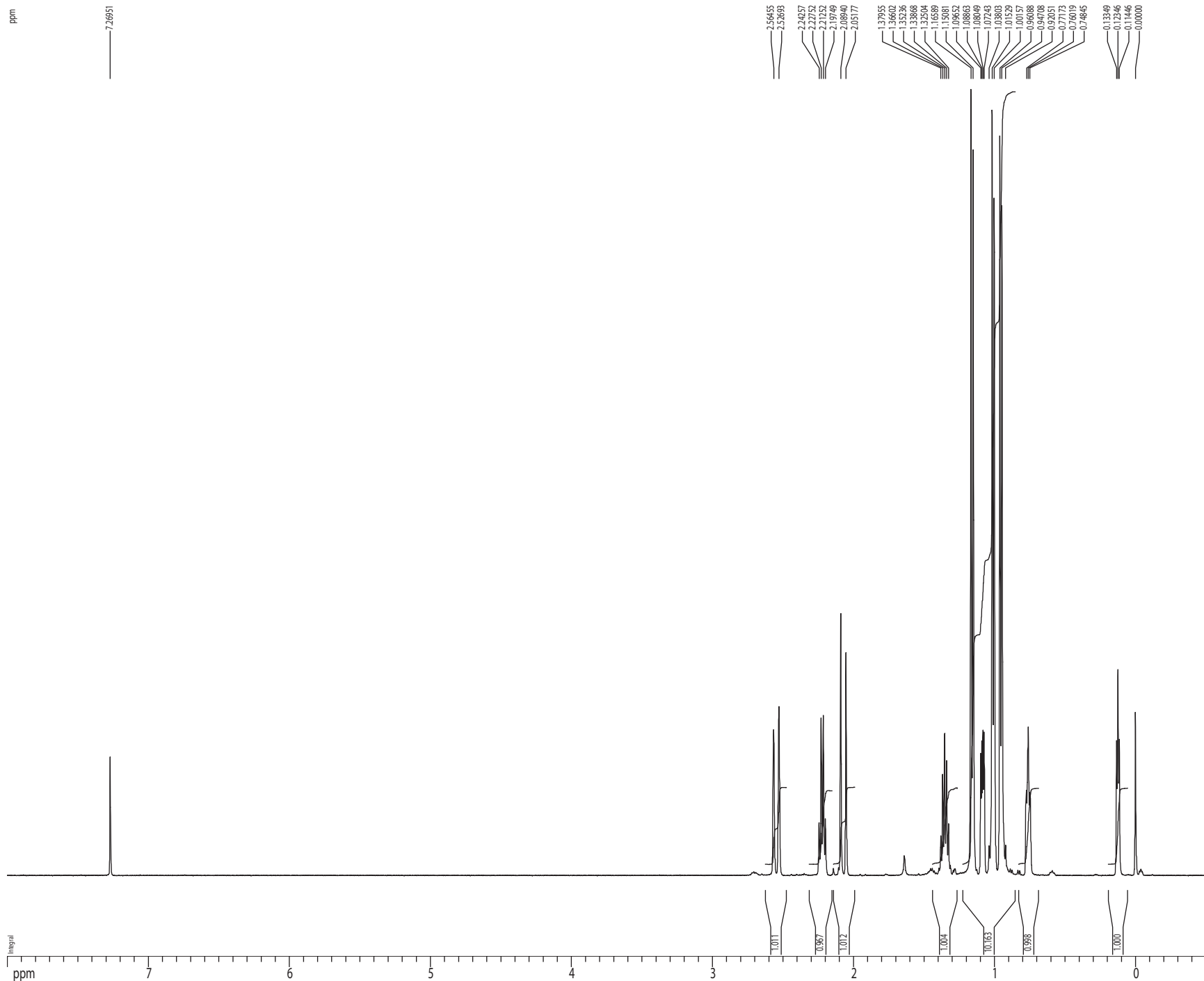
E-mail the .pse file to me (jsnowick@uci.edu).

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 500 Mhz in CDCl₃



Current Data Parameters
 USER nmr11t
 NAME sample 18
 EXPNO 99
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111205
 Time 21.17
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG zg30
 TD 81728
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 4
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.2235015 MHz

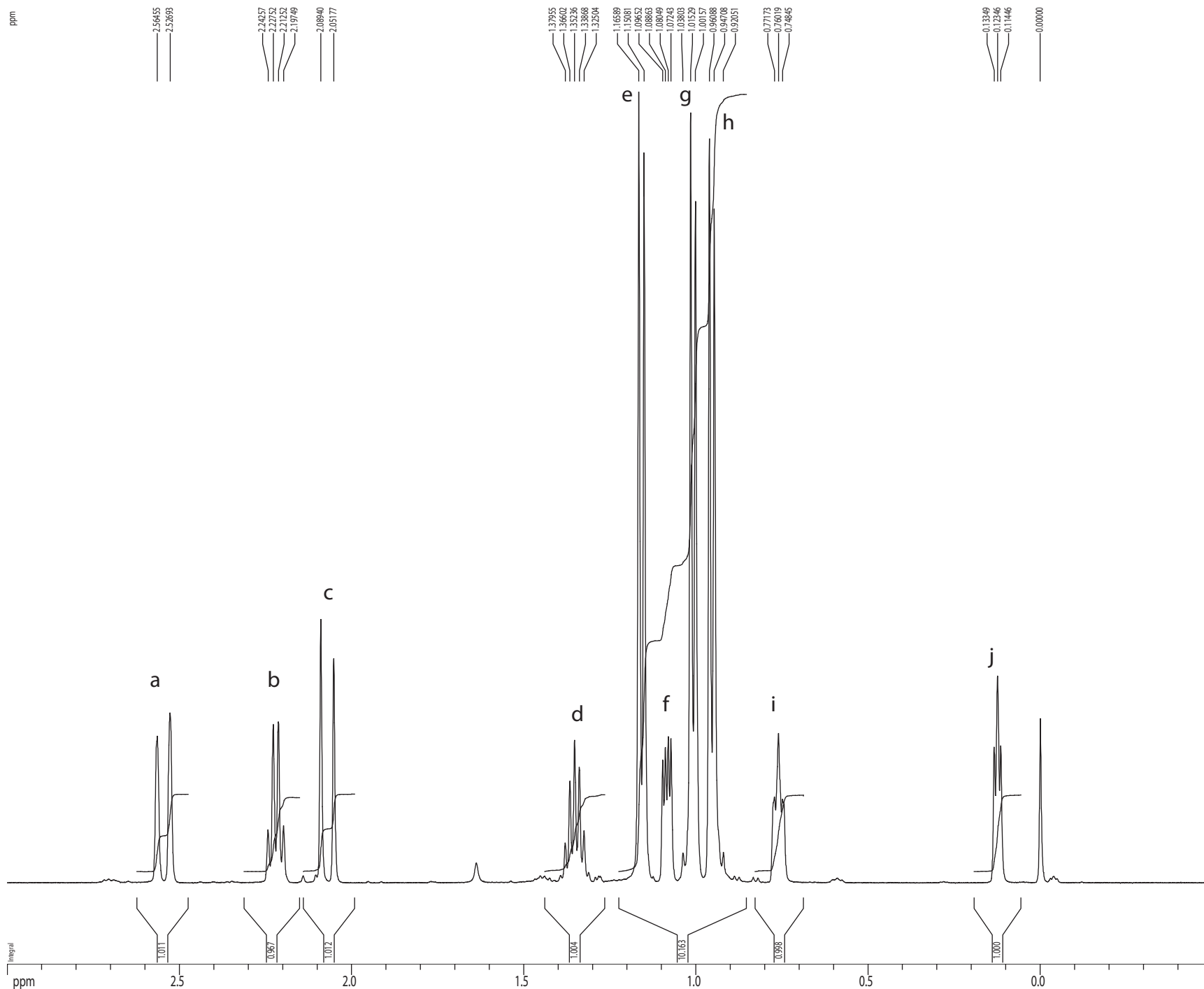
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 SF 500.2200266 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
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 CY 15.00 cm
 F1P 8.000 ppm
 F1 4001.76 Hz
 F2P -0.500 ppm
 F2 -250.11 Hz
 PPMCM 0.37281 ppm/cm
 HZCM 186.48555 Hz/cm

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#	ADDRESS	FREQUENCY		INTENSITY
		[Hz]	[PPM]	
1	50696.8	1282.838	2.5645	2.82
2	50850.7	1264.019	2.5269	3.26
3	52014.1	1121.778	2.2426	1.05
4	52075.7	1114.248	2.2275	3.04
5	52137.0	1106.748	2.2125	3.09
6	52198.5	1099.230	2.1975	1.12
7	52640.8	1045.160	2.0894	5.02
8	52794.7	1026.336	2.0518	4.28
9	55544.9	690.077	1.3795	0.80
10	55600.3	683.312	1.3660	1.97
11	55656.2	676.477	1.3524	2.74
12	55712.1	669.636	1.3387	2.23
13	55767.9	662.812	1.3250	1.02
14	56419.1	583.202	1.1659	15.00
15	56480.8	575.656	1.1508	13.86
16	56702.9	548.502	1.0965	2.36
17	56735.2	544.552	1.0886	2.60
18	56768.5	540.481	1.0805	2.81
19	56801.4	536.452	1.0724	2.77
20	56942.2	519.243	1.0380	0.61
21	57035.2	507.870	1.0153	14.61
22	57091.3	501.007	1.0016	12.94
23	57257.8	480.651	0.9609	14.12
24	57314.3	473.746	0.9471	12.80
25	57423.0	460.455	0.9205	0.62
26	58031.7	386.035	0.7717	1.66
27	58078.9	380.260	0.7602	2.87
28	58126.9	374.388	0.7484	1.62
29	60642.9	66.773	0.1335	2.61
30	60683.9	61.759	0.1235	3.95
31	60720.7	57.253	0.1145	2.64
32	61189.0	-0.000	-0.0000	3.15

¹H spectrum at 500 MHz in CDCl₃



Current Data Parameters
 USER nmr11t
 NAME sample 18
 EXPNO 99
 PROCNO 1

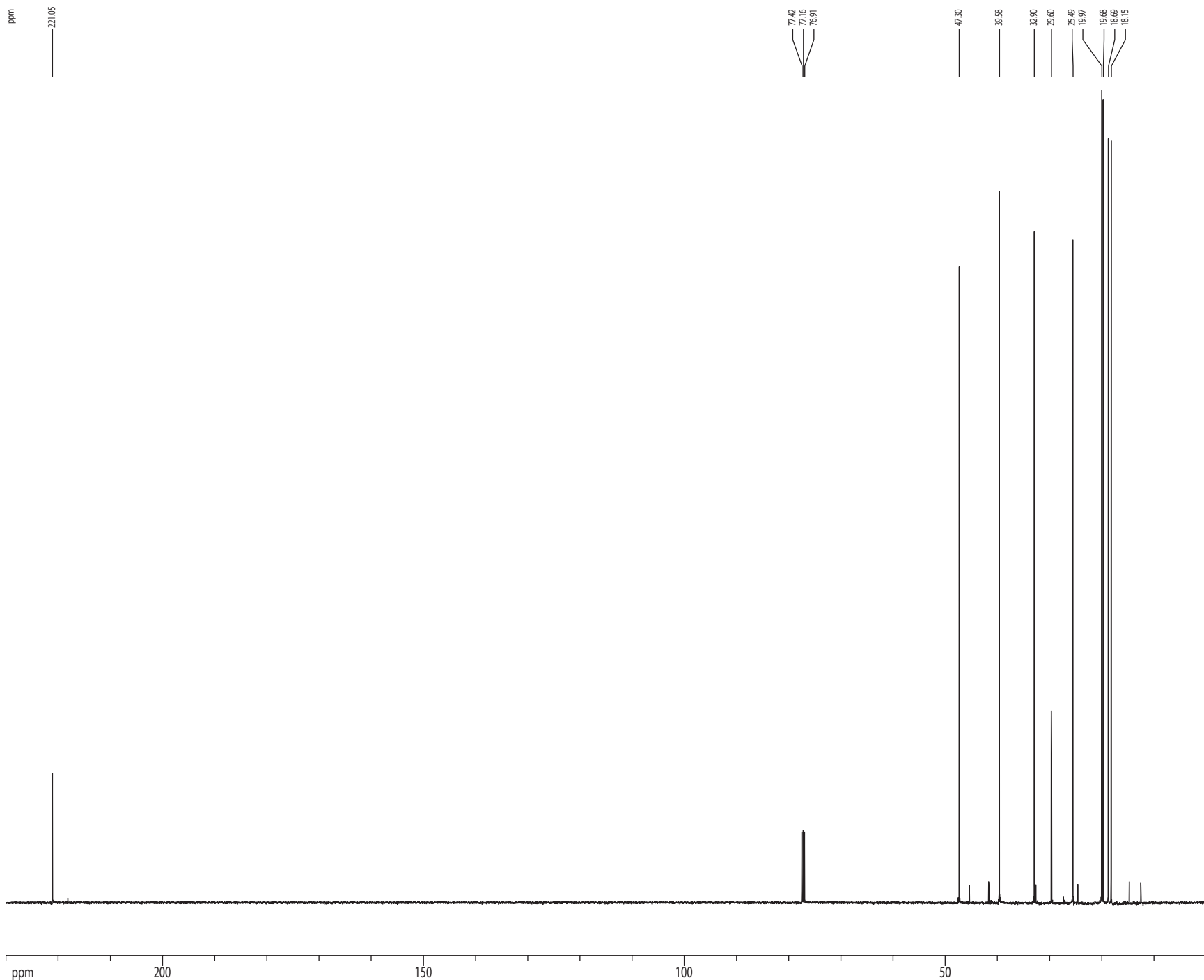
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 Date_ 20111205
 Time 21.17
 INSTRUM cryo500
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 PULPROG zg30
 TD 81728
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 4
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.2235015 MHz

F2 - Processing parameters
 SI 65536
 SF 500.2200266 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
 F1P 3.000 ppm
 F1 1500.66 Hz
 F2P -0.500 ppm
 F2 -250.11 Hz
 PPMCM 0.15351 ppm/cm
 HZCM 76.78816 Hz/cm

Z-restored spin-echo ¹³C spectrum with ¹H decoupling at 125 MHz in CDCl₃



Current Data Parameters
 USER nmr11t
 NAME sample 17
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111204
 Time 20.09
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG SpinEchogg30gp.prd
 TD 65536
 SOLVENT CDCl3
 NS 108
 DS 16
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813940 sec
 RG 7298.2
 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
 PLO 120.00 dB
 PL1 -1.00 dB
 SFO1 125.7942548 MHz
 SP1 3.20 dB
 SP2 3.20 dB
 SPNAM1 Crg60.0.5.20.1
 SPNAM2 Crg60comp.4
 SPOFF1 0.00 Hz
 SPOFF2 0.00 Hz

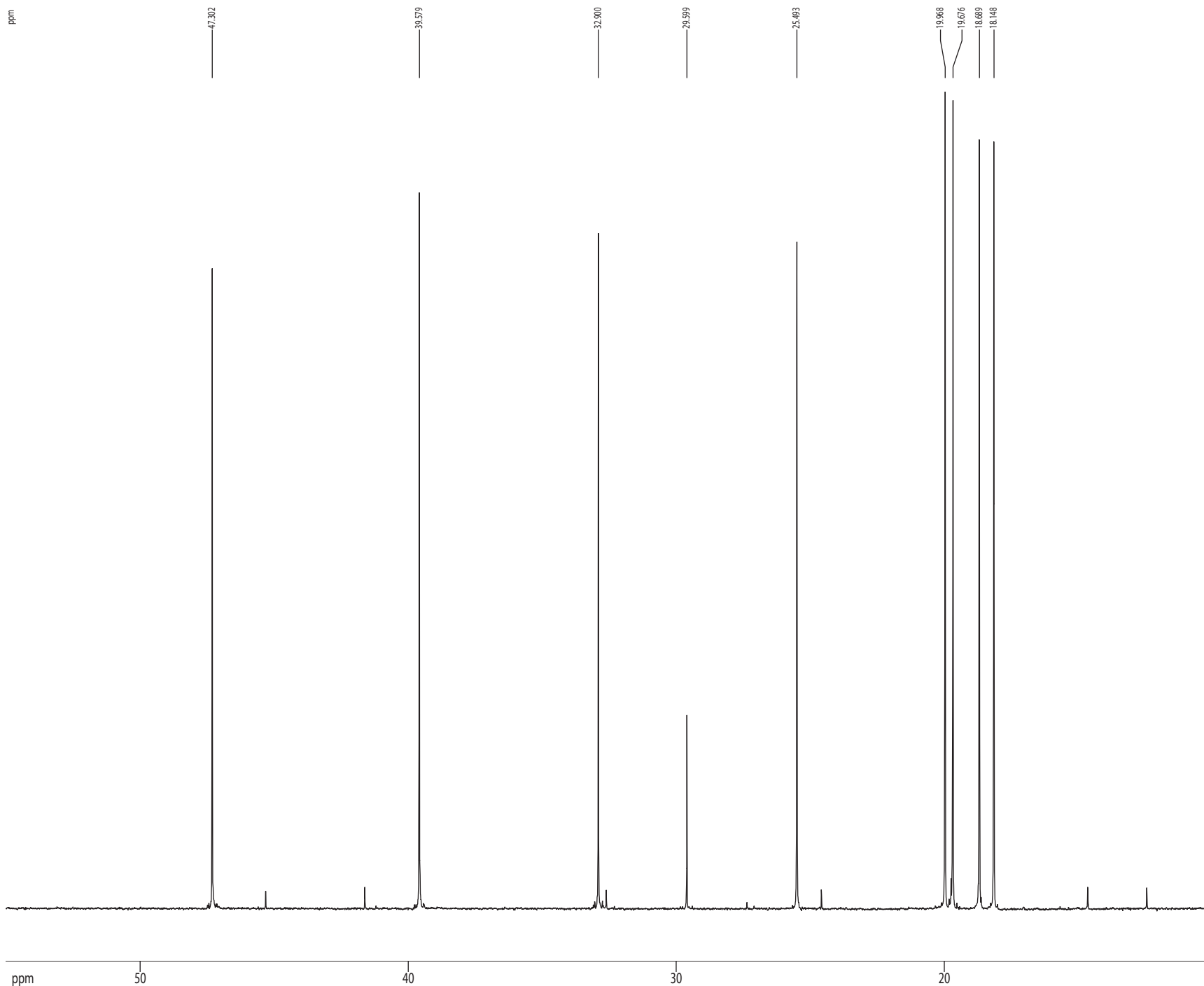
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 100.00 usec
 PL2 1.60 dB
 PL12 24.60 dB
 SFO2 500.2225011 MHz

==== 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 125.7804190 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
 F1P 230.000 ppm
 F1 28929.50 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.08772 ppm/cm
 HZCM 1268.83765 Hz/cm

Z-restored spin-echo ¹³C spectrum with ¹H decoupling at 125 MHz in CDCl₃



```

Current Data Parameters
USER      nmr11t
NAME      sample 17
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20111204
Time      20.09
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchogg30gppr
TD         65536
SOLVENT   CDCl3
NS         108
DS         16
SWH        30303.031 Hz
FIDRES     0.462388 Hz
AQ         1.0813940 sec
RG         7298.2
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
PLO        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

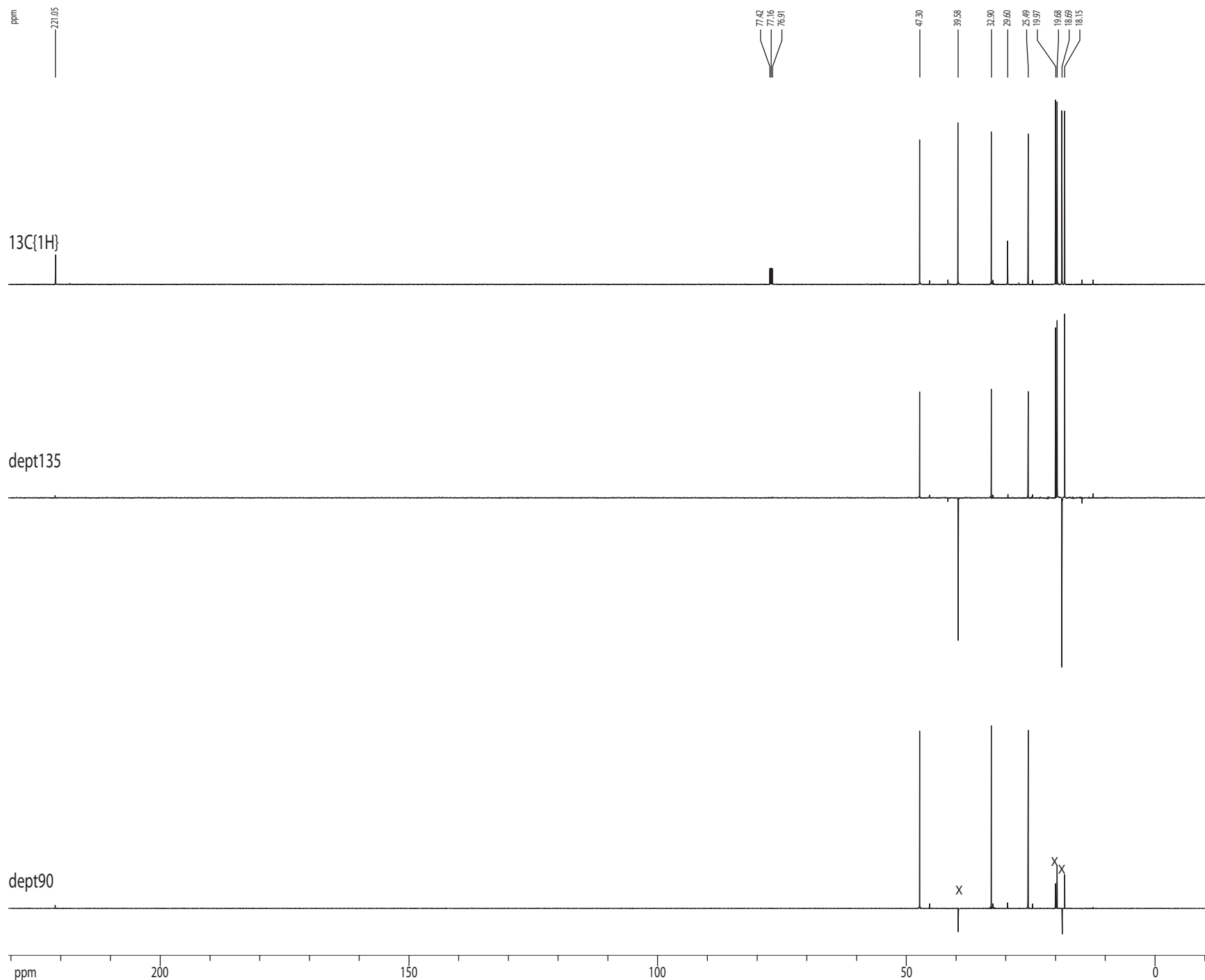
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      100.00 usec
PL2        1.50 dB
PL12       24.60 dB
SFO2      500.2225011 MHz

===== 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         125.7804190 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
F1P        55.000 ppm
F1         6917.92 Hz
F2P        10.000 ppm
F2         1257.80 Hz
PPMCM      1.97368 ppm/cm
HZCM       248.25084 Hz/cm
    
```

Z-restored spin-echo ¹³C spectrum with ¹H decoupling at 125 MHz in CDCl₃



```

Current Data Parameters
USER      nmr11t
NAME      sample 17
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20111204
Time      20.09
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchogg30gpprd
TD         65536
SOLVENT   CDCl3
NS         108
DS         16
SWH        30303.031 Hz
FIDRES     0.462388 Hz
AQ         1.0813940 sec
RG         7298.2
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

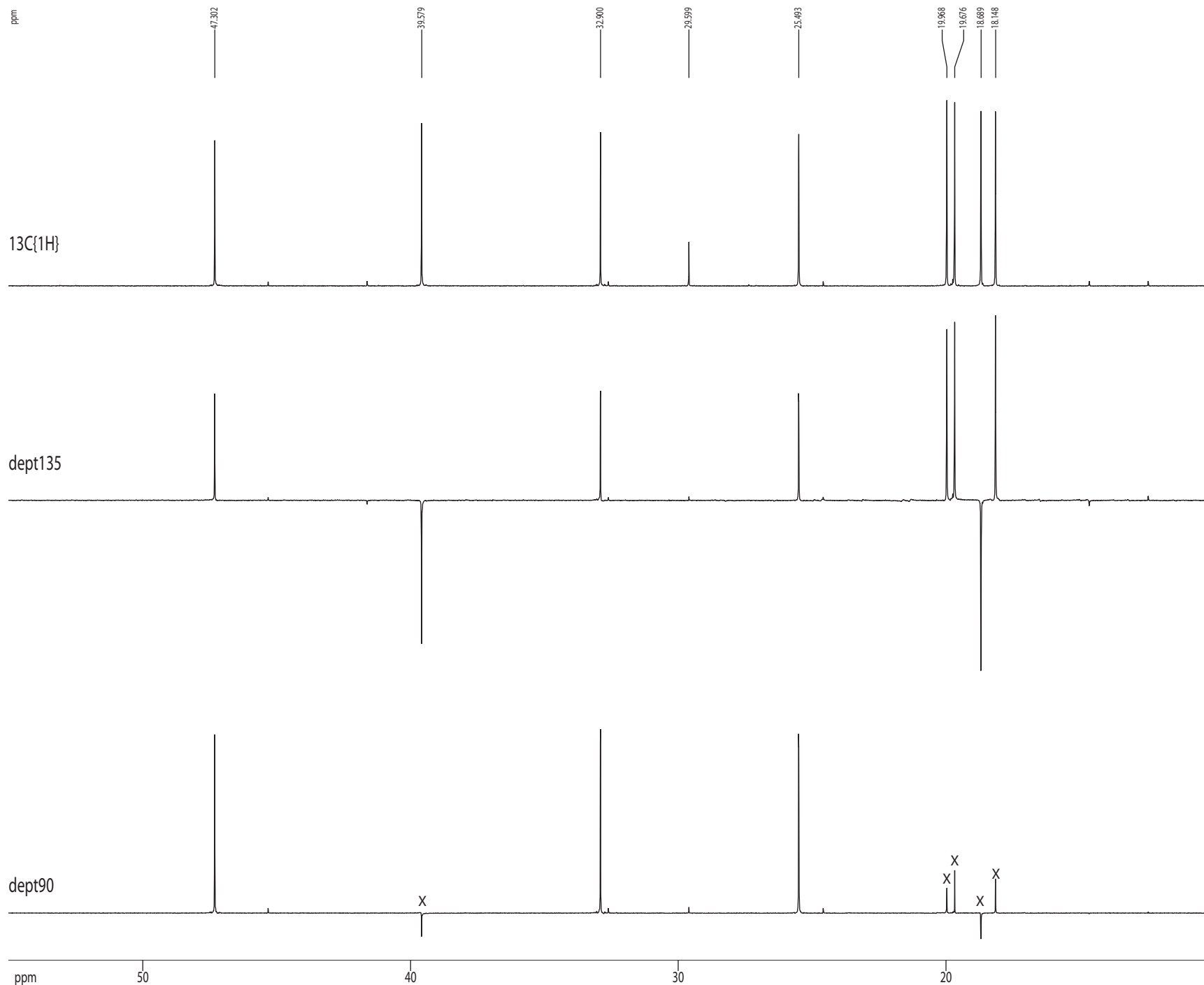
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      100.00 usec
PL2        1.60 dB
PL12       24.60 dB
SFO2      500.2225011 MHz

===== 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         125.7804190 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        230.460 ppm
F1         28987.37 Hz
F2P        -10.460 ppm
F2         -1315.66 Hz
PPMCM      10.56667 ppm/cm
HZCM       1329.08032 Hz/cm
    
```

Z-restored spin-echo ¹³C spectrum with ¹H decoupling at 125 MHz in CDCl₃



Current Data Parameters
 USER nmr11t
 NAME sample 17
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111204
 Time 20.09
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG SpinEchogg30gpprd
 TD 65536
 SOLVENT CDCl3
 NS 108
 DS 16
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813940 sec
 RG 7298.2
 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
 PLO 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

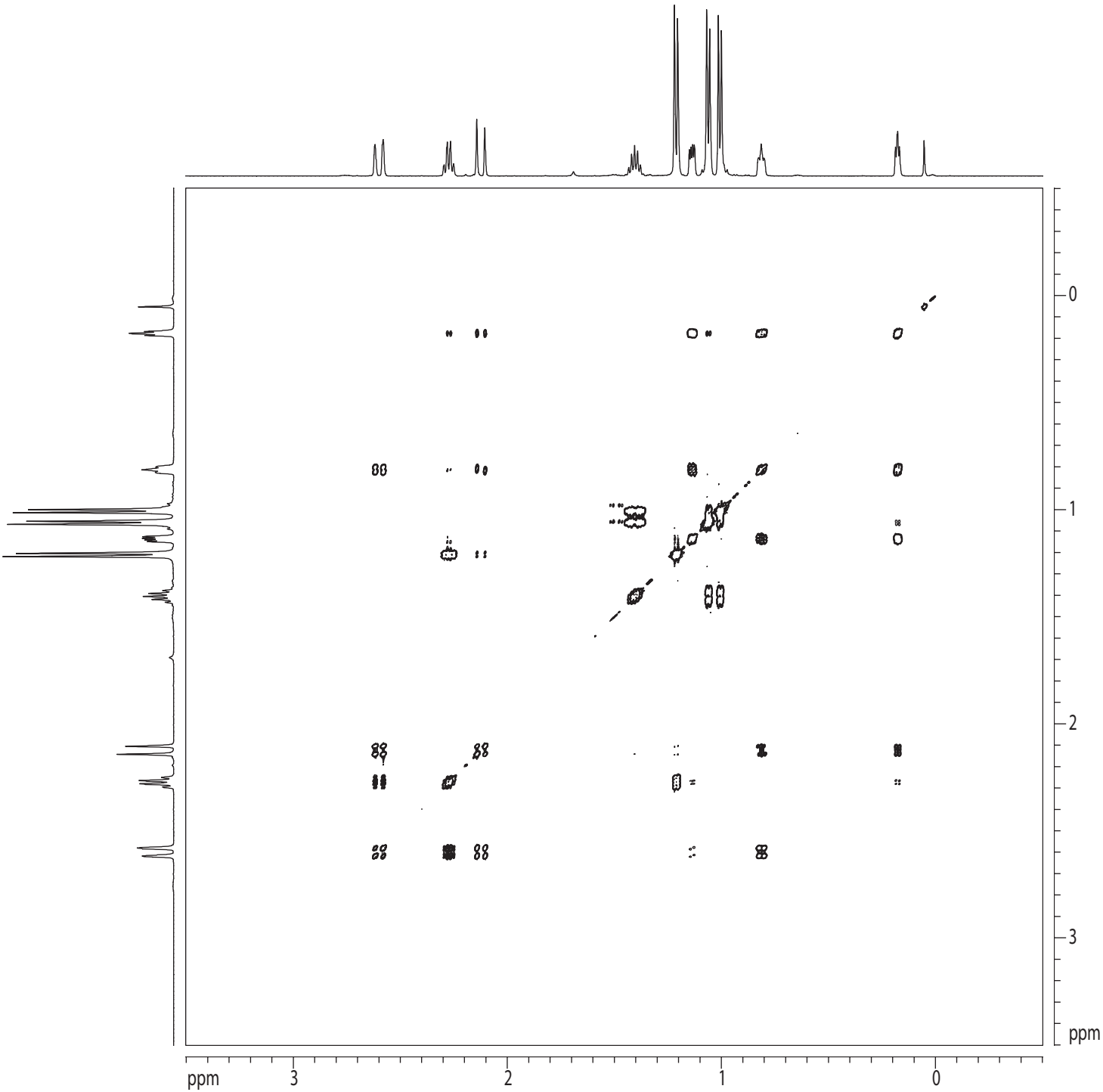
===== CHANNEL f2 =====
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 NUC2 ¹H
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 PL2 1.60 dB
 PL12 24.60 dB
 SFO2 500.2225011 MHz

===== 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 125.7804190 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 55.000 ppm
 F1 6917.92 Hz
 F2P 10.000 ppm
 F2 1257.80 Hz
 PPMCM 1.97368 ppm/cm
 HZCM 248.25084 Hz/cm

gcosy60



Current Data Parameters
USER nmr11t
NAME sample 18
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111205
Time 22.48
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG cosp60.prd
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 2003.205 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 35.9
DW 249.600 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 0.00049920 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2207503 MHz

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

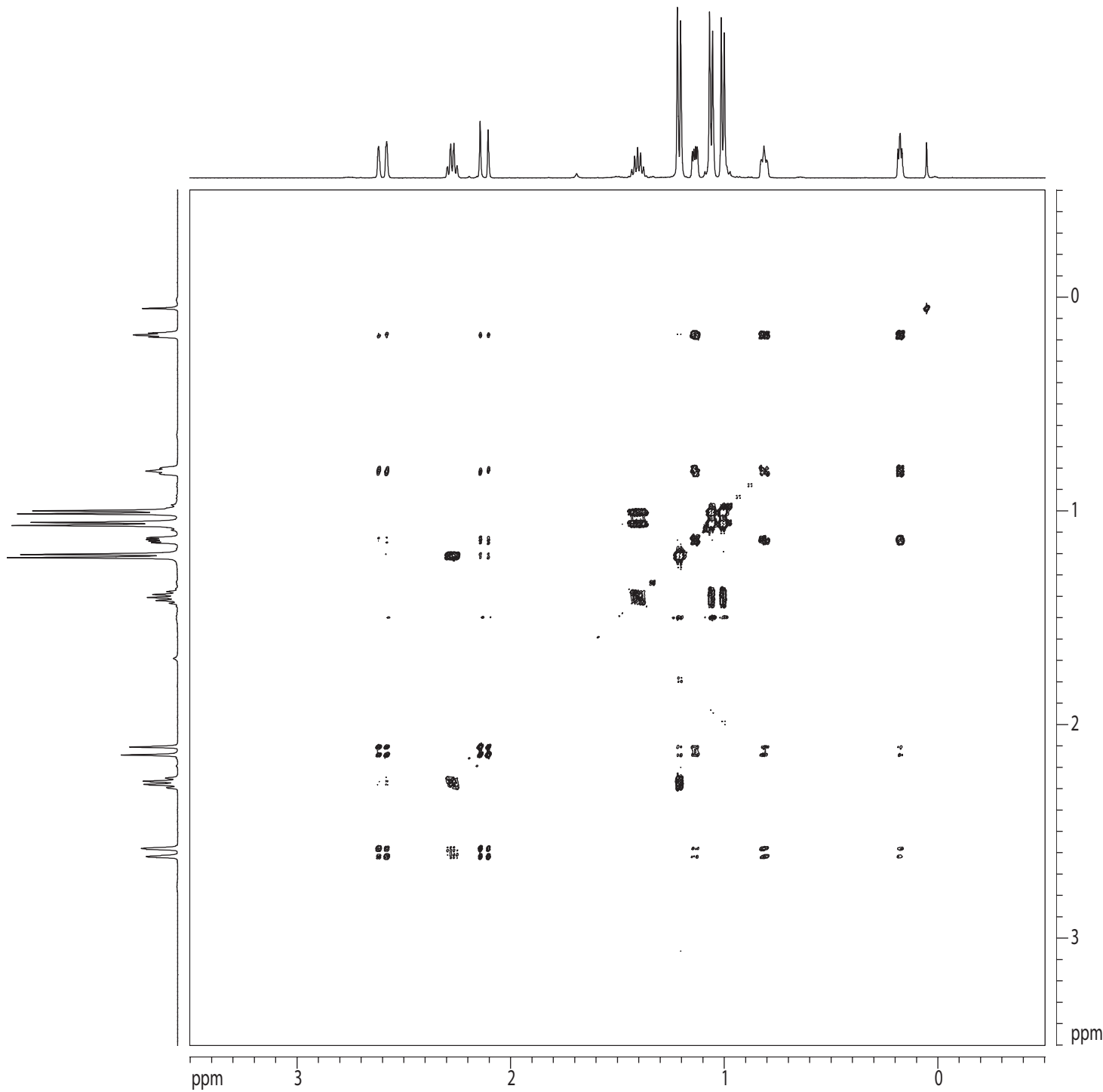
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ND0 1
TD 512
SFO1 500.2208 MHz
FIDRES 3.912510 Hz
SW 4.005 ppm
FnMODE undefined

F2 - Processing parameters
SI 1024
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 2.00

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 3.502 ppm
F2LO 1751.93 Hz
F2PHI -0.502 ppm
F2HI -251.27 Hz
F1PLO 3.502 ppm
F1LO 1751.93 Hz
F1PHI -0.502 ppm
F1HI -251.27 Hz
F2PPMCM 0.26698 ppm/cm
F2HZCM 133.54701 Hz/cm
F1PPMCM 0.26698 ppm/cm
F1HZCM 133.54701 Hz/cm

gtocsy



Current Data Parameters
USER nmr11t
NAME sample 18
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111205
Time 23.45
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG mlevvgp_mo
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 2003.205 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 4
DW 249.600 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 0.00049920 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 500.2207503 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

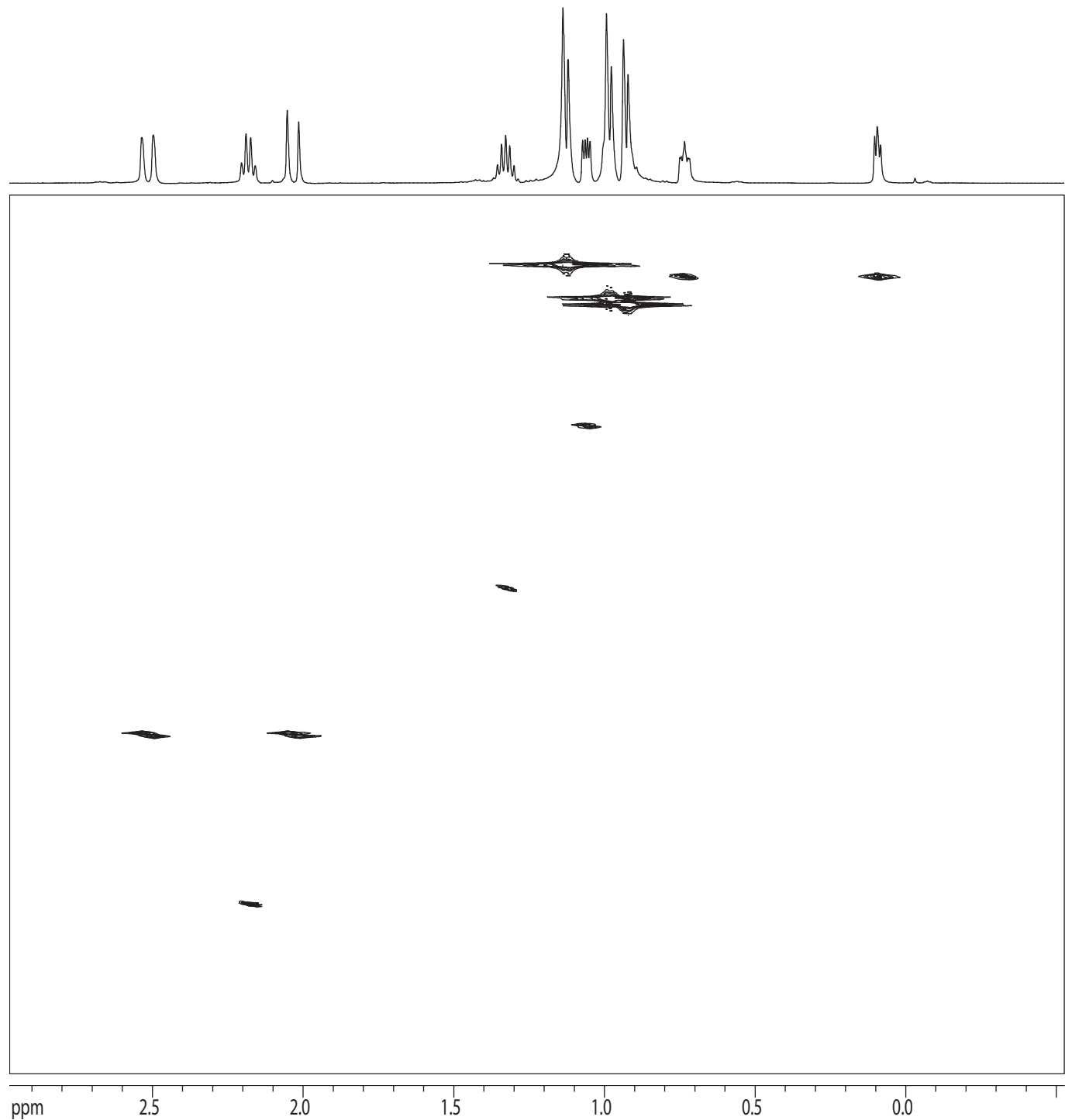
F1 - Acquisition parameters
ND0 1
TD 512
SFO1 500.2208 MHz
FIDRES 3.912510 Hz
SW 4.005 ppm
FnMODE undefined

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 3.502 ppm
F2LO 1751.93 Hz
F2PHI -0.502 ppm
F2HI -251.27 Hz
F1PLO 3.502 ppm
F1LO 1751.93 Hz
F1PHI -0.502 ppm
F1HI -251.27 Hz
F2PPMCM 0.26698 ppm/cm
F2HZCM 133.54701 Hz/cm
F1PPMCM 0.26698 ppm/cm
F1HZCM 133.54701 Hz/cm

ghmqc



Current Data Parameters
USER nmr11t
NAME sample 17
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111204
Time 23.09
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG invgpg.wu
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 1750.700 Hz
FIDRES 0.854834 Hz
AQ 0.5849588 sec
RG 912.3
DW 285.600 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 0.00009919 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2206124 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7848213 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

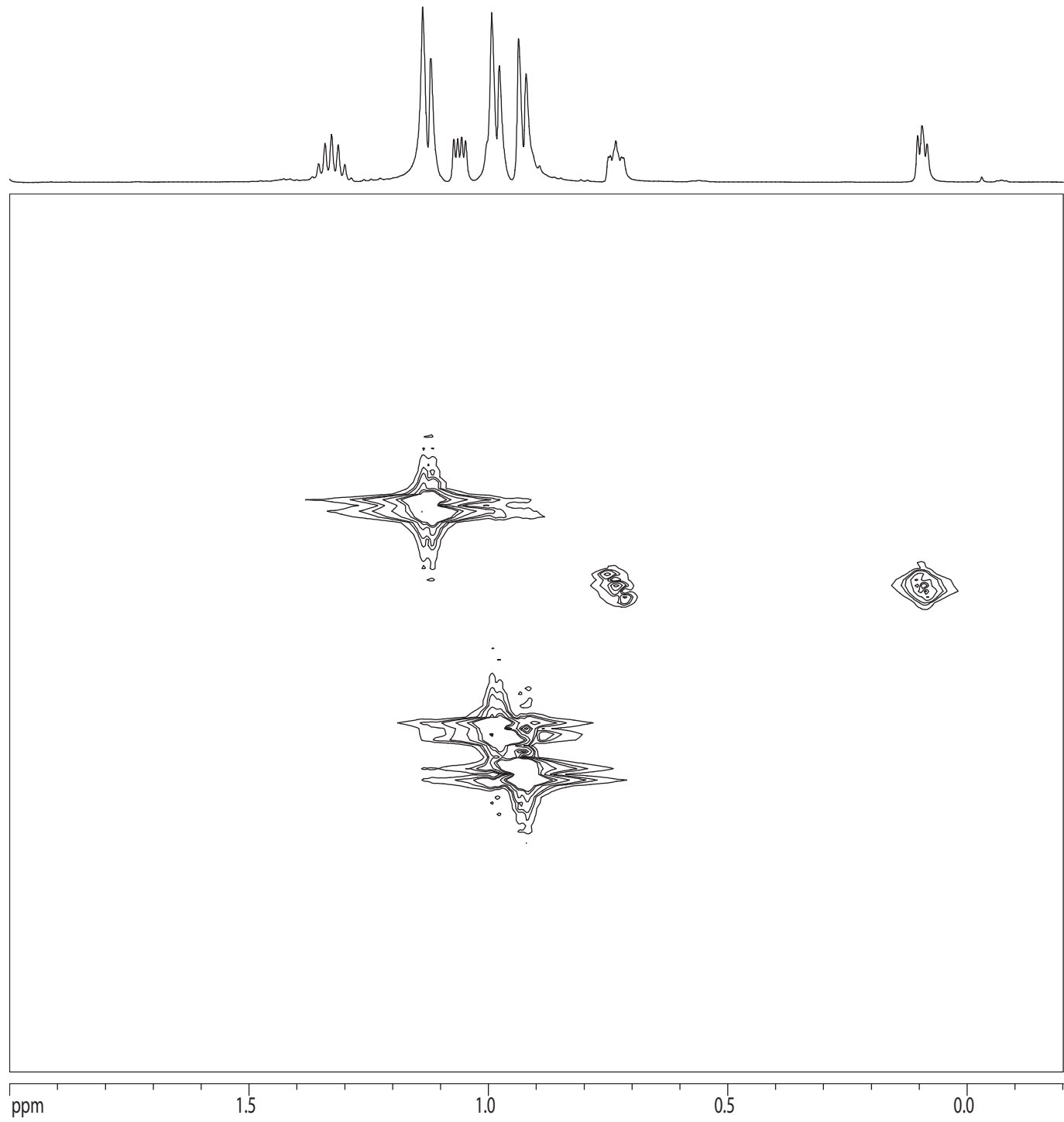
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7848 MHz
FIDRES 9.845621 Hz
SW 40.076 ppm
FMODE undefined

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 2.974 ppm
F2LO 1487.75 Hz
F2PHI -0.526 ppm
F2HI -262.95 Hz
F1PLO 55.039 ppm
F1LO 6922.79 Hz
F1PHI 1881.83 Hz
F2PPMCM 0.19444 ppm/cm
F2HZCM 97.26112 Hz/cm
F1PPMCM 2.67183 ppm/cm
F1HZCM 336.06387 Hz/cm

ghmqc



Current Data Parameters
USER nmr11t
NAME sample 17
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111204
Time 23.09
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG inv4gp.wu
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 1750.700 Hz
FIDRES 0.854834 Hz
AQ 0.5849588 sec
RG 912.3
DW 285.600 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 0.00009919 sec

==== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2206124 MHz

==== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7848213 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

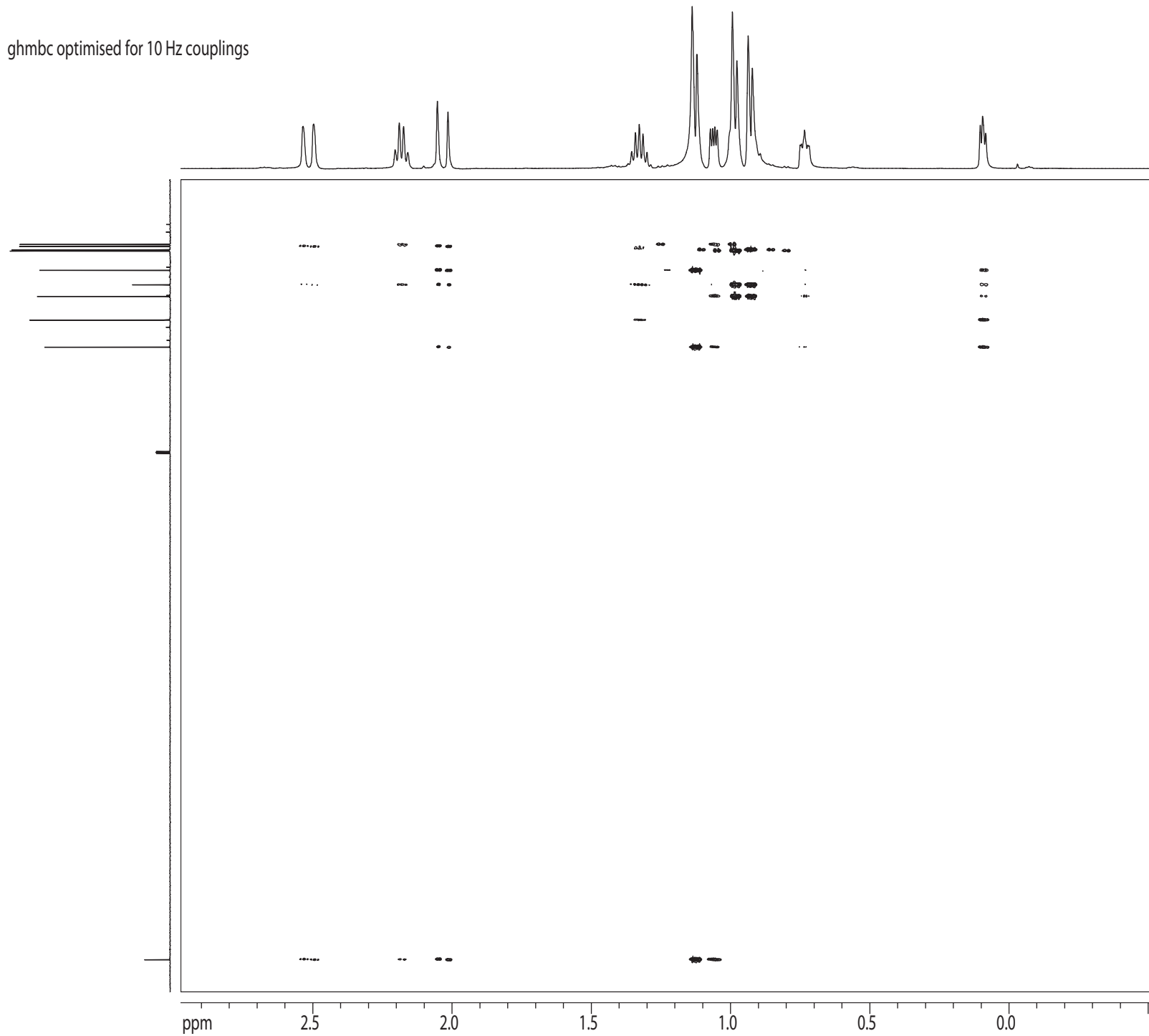
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7848 MHz
FIDRES 9.845621 Hz
SW 40.076 ppm
FnMODE undefined

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 2.000 ppm
F2LO 1000.44 Hz
F2PHI -0.201 ppm
F2HI -100.53 Hz
F1PLO 22.006 ppm
F1LO 2767.94 Hz
F1PHI 16.000 ppm
F1HI 2012.49 Hz
F2PPMCM 0.12228 ppm/cm
F2HZCM 61.16494 Hz/cm
F1PPMCM 0.40041 ppm/cm
F1HZCM 50.36322 Hz/cm

ghmbc optimised for 10 Hz couplings



```

Current Data Parameters
USER      nmr11t
NAME      sample 17
EXPNO     8
PROCNO    1

F2 - Acquisition Parameters
Date_     20111205
Time      0.06
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   ghmbc.wu
TD         4096
SOLVENT   CDCl3
NS         4
DS         16
SWH        1750.700 Hz
FIDRES     0.427417 Hz
AQ         1.1698676 sec
RG         645.1
DW         285.600 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        0.00001725 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
p2         15.00 usec
PL1        1.60 dB
SFO1       500.2206124 MHz

===== CHANNEL f2 =====
NUC2       13C
P3         15.50 usec
PL2        -1.00 dB
SFO2       125.7948837 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

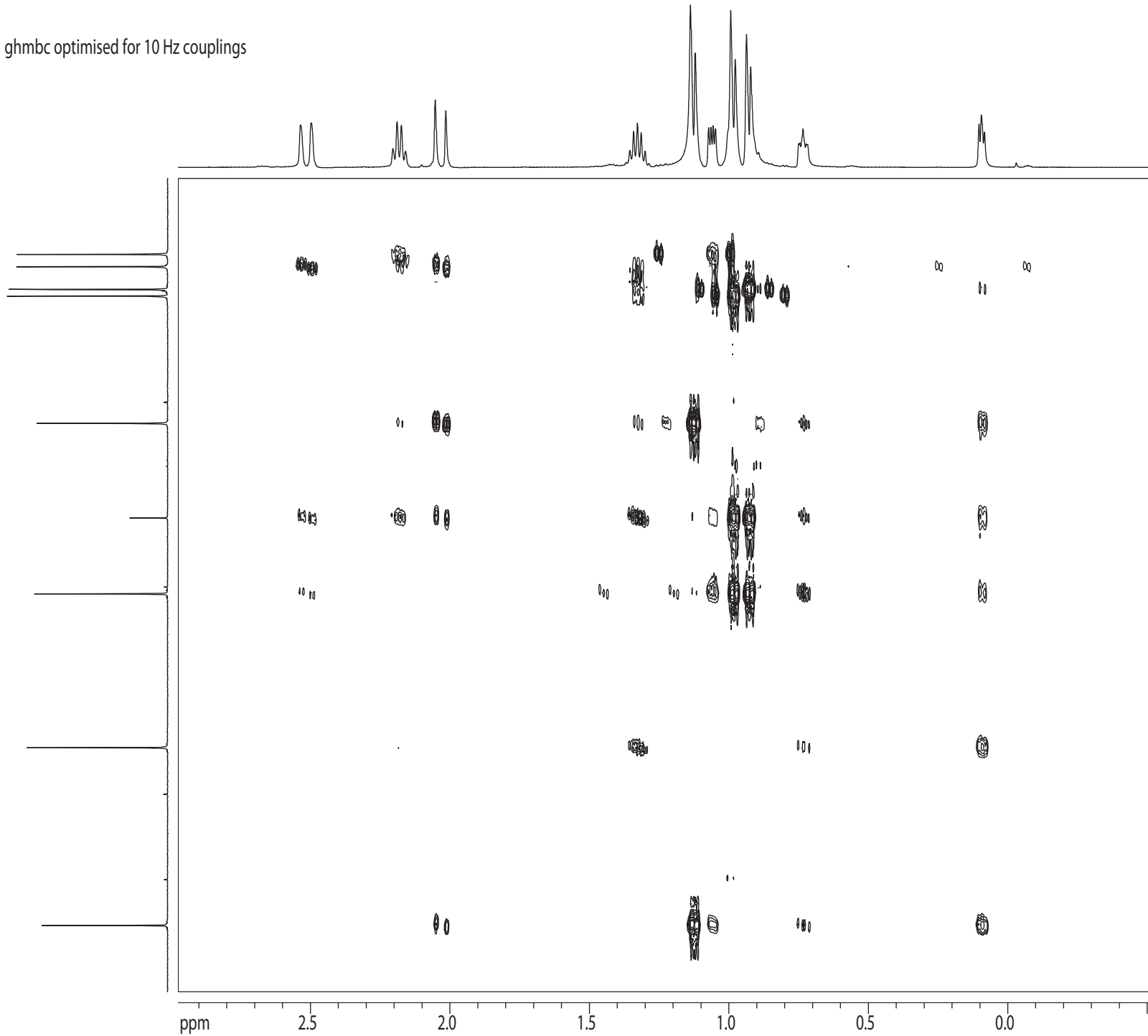
F1 - Acquisition parameters
ND0        2
TD          512
SFO1       125.7949 MHz
FIDRES     56.612320 Hz
SW         230.419 ppm
FhIMODE    undefined

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      2.974 ppm
F2LLO      1487.75 Hz
F2PHI      -0.526 ppm
F2HI       -262.95 Hz
F1PLO      230.223 ppm
F1LLO      28957.49 Hz
F1PHI      -0.223 ppm
F1HI       -28.01 Hz
F2PPMCM    0.19444 ppm/cm
F2HZCM     97.26112 Hz/cm
F1PPMCM    15.36302 ppm/cm
F1HZCM     1932.36719 Hz/cm
    
```

ghmbc optimised for 10 Hz couplings



Current Data Parameters
USER nm11t
NAME sample 17
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111205
Time 0.06
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT CDCl3
NS 4
DS 16
SWH 1750.700 Hz
FIDRES 0.427417 Hz
AQ 1.1698676 sec
RG 645.1
DW 285.600 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 0.00001725 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2206124 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7948837 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

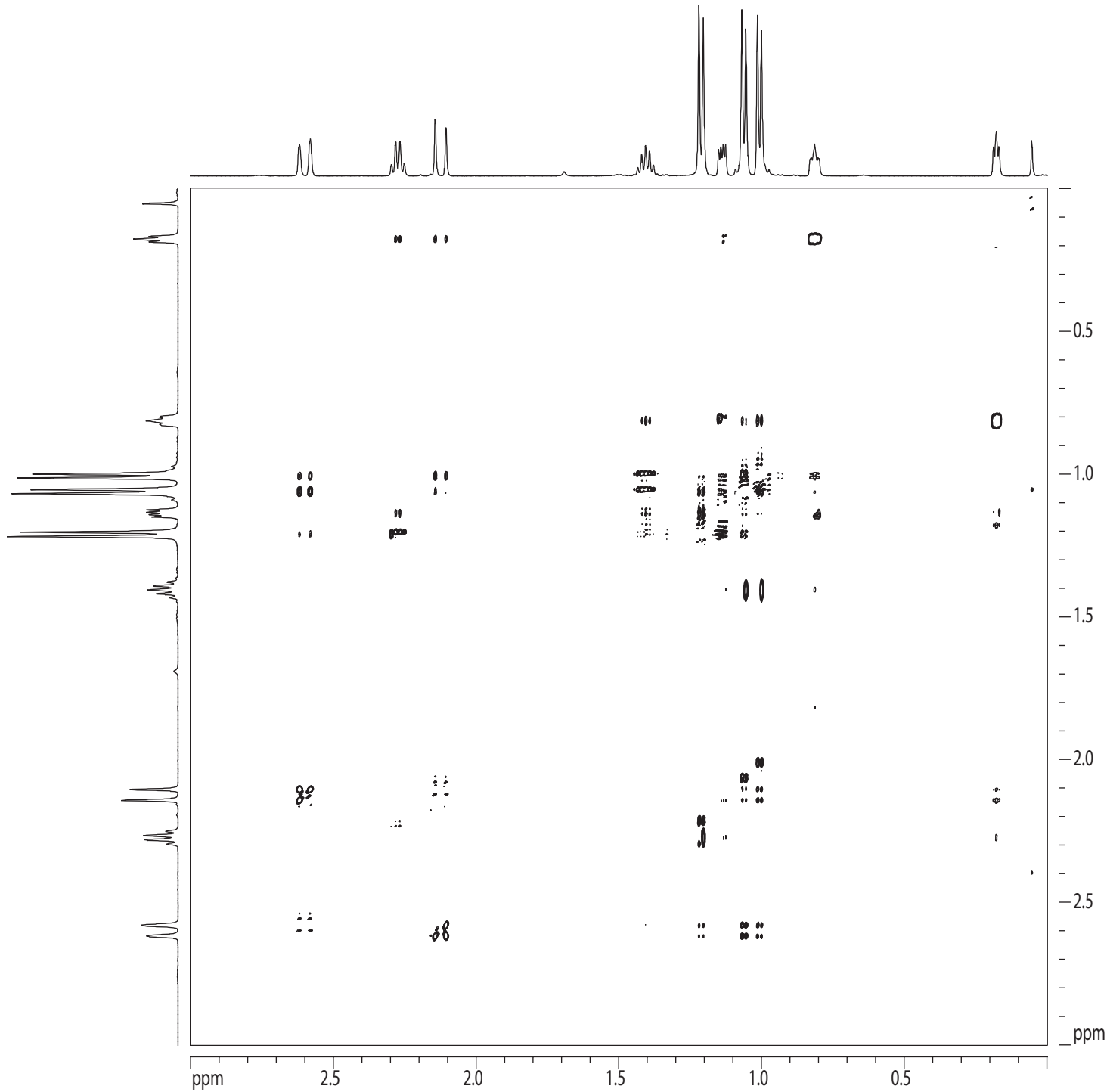
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7949 MHz
FIDRES 56.612320 Hz
SW 230.419 ppm
FhMODE undefined

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 2.974 ppm
F2LO 1487.75 Hz
F2PHI -0.526 ppm
F2HI -262.95 Hz
F1PLO 50.187 ppm
F1LO 6312.57 Hz
F1PHI 14.855 ppm
F1HI 1868.50 Hz
F2PPMCM 0.1944 ppm/cm
F2HZCM 97.26112 Hz/cm
F1PPMCM 2.35546 ppm/cm
F1HZCM 296.27115 Hz/cm

gnoesy



Current Data Parameters
USER nmr11t
NAME sample 18
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111208
Time 20.25
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG noesygptp
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 2003.205 Hz
FIDRES 0.978127 Hz
AQ 0.5114804 sec
RG 57
DW 249.600 usec
DE 6.00 usec
TE 298.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D8 1.50000000 sec
D16 0.00020000 sec
d20 0.74879998 sec
IN0 0.00024960 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
P2 15.00 usec
PL1 1.60 dB
SFO1 500.2207503 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 422
SFO1 500.2208 MHz
FIDRES 4.746932 Hz
SW 4.005 ppm
FnMODE undefined

F2 - Processing parameters
SI 1024
SF 500.2200000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 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
F2PLO 3.002 ppm
F2LO 1501.53 Hz
F2PHI -0.002 ppm
F2HI -0.87 Hz
F1PLO 3.002 ppm
F1LO 1501.53 Hz
F1PHI -0.002 ppm
F1HI -0.87 Hz
F2PPMCM 0.20023 ppm/cm
F2HZCM 100.16026 Hz/cm
F1PPMCM 0.20023 ppm/cm
F1HZCM 100.16026 Hz/cm