

Name: _____

Chem 203
December 14, 2013

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.

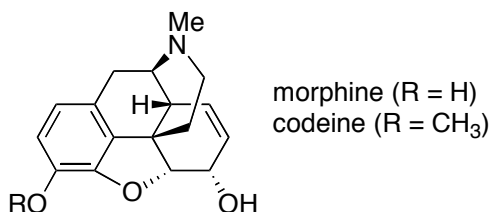
Books, notes, lecture videos, calculators, rulers, and laptop computers are permitted as is wireless (or wired) internet access and appropriate software (e.g, Pymol, Macromodel/Maestro, Excel, NMRPrediction, Chemdraw, ElComp, MolE, etc.). Catalogs of molecular structures (e.g., the Aldrich catalog, the 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.

The following spectral data are provided for a compound with a molecular formula $C_{16}H_{25}NO_2$: IR (solution in $CHCl_3$), 500 MHz 1H NMR, 125.8 MHz ^{13}C NMR, DEPT-90, DEPT-135, COSY, HMQC, HMBC, TOCSY (150 ms mixing time) and NOESY. Also included are select regions of the HSQC-TOCSY spectra with increasing mixing times. All NMR spectra were measured in $CDCl_3$ solution.

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.

HINT: The compound is related in structure to codeine, the methyl ether of morphine.



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

a. Write the structure of the molecule.

If there are any aspects of your structure that don't seem to make sense, please feel free to comment on them below:

b. Tabulate the shifts of the ^1H resonances (a-o) 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:

n:

o:

c. Redraw the structure of the molecule below and write the letter (a-o) 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 (1-15) 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:

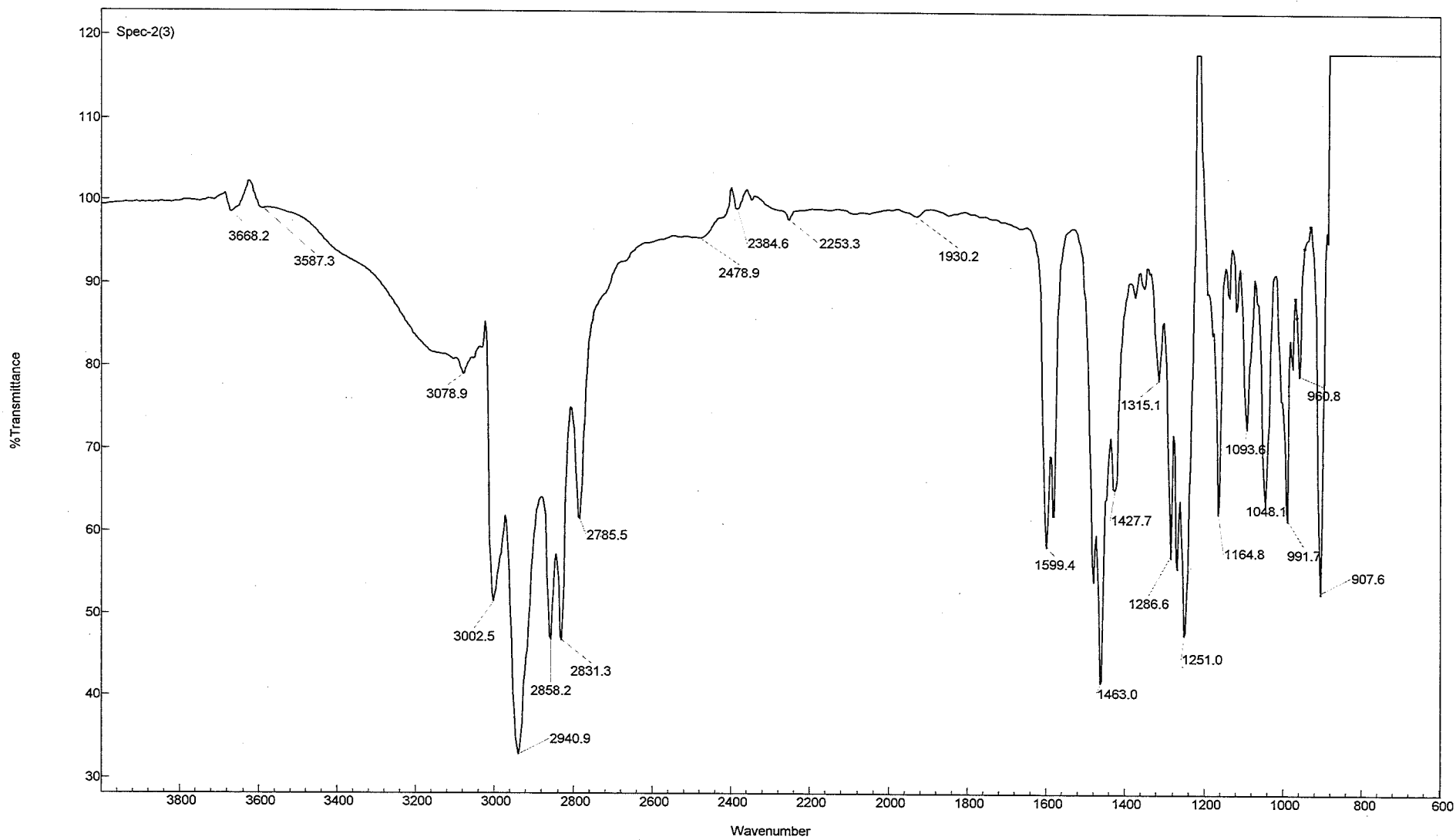
13:

14:

15:

e. Redraw the structure of the molecule below and write the number (1-15) 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.

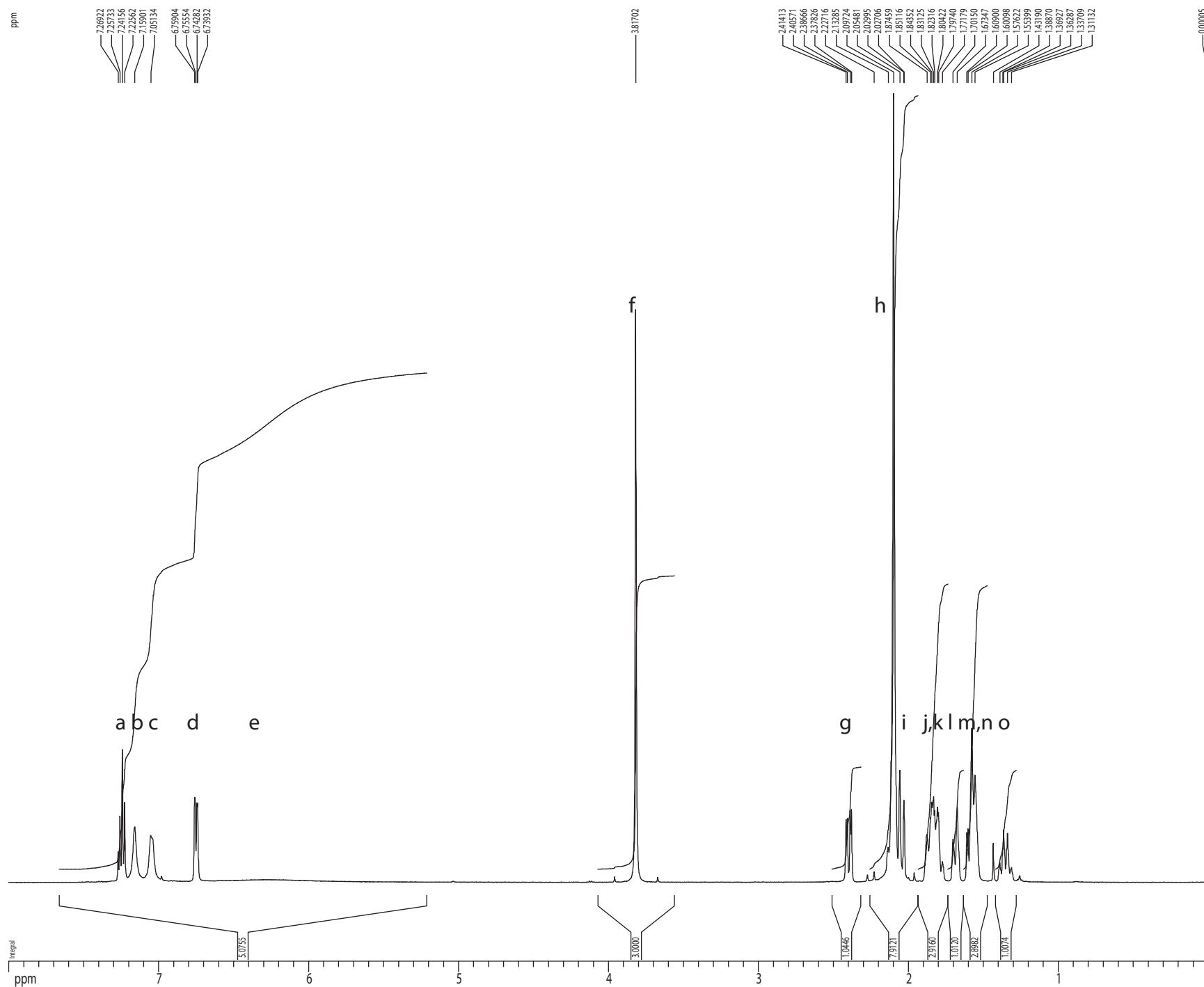
Varian Resolutions Pro



Name

Spec-2 (3)

¹H spectrum



Current Data Parameters
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 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131205
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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 2.8
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

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 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.2235015 MHz

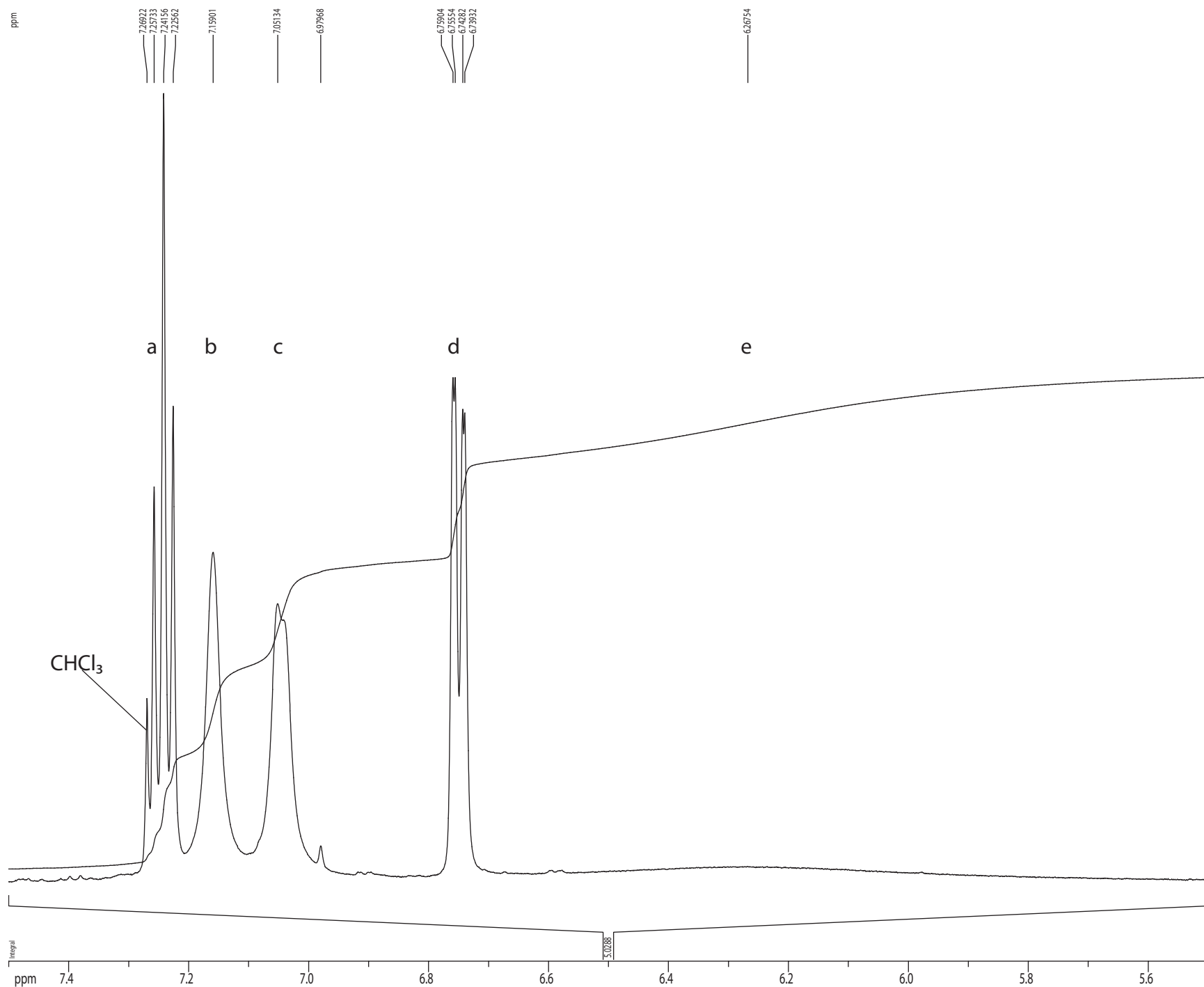
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 SF 500.2200260 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 FIP 8.000 ppm
 F1 4001.76 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 0.35088 ppm/cm
 HZCM 175.51581 Hz/cm

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#	ADDRESS	FREQUENCY	INTENSITY
	[Hz]	[PPM]	
1	31453.8	3636.209	7.2692 0.59
2	31502.5	3630.260	7.2573 1.27
3	31567.0	3622.374	7.2416 2.53
4	31632.2	3614.400	7.2256 1.53
5	31904.7	3581.078	7.1590 1.06
6	32345.2	3527.220	7.0513 0.89
7	33541.1	3381.007	6.7590 1.62
8	33555.4	3379.254	6.7555 1.62
9	33607.5	3372.892	6.7428 1.52
10	33621.8	3371.144	6.7393 1.50
11	45577.6	1909.347	3.8170 10.89
12	51317.2	1207.597	2.4141 1.20
13	51351.6	1203.385	2.4057 1.22
14	51429.6	1193.856	2.3867 1.37
15	51464.0	1189.651	2.3783 1.39
16	52082.2	1114.068	2.2272 0.20
17	52468.0	1066.896	2.1329 0.67
18	52613.7	1049.082	2.0972 15.00
19	52787.3	1027.856	2.0548 2.14
20	52889.0	1015.422	2.0300 1.53
21	52900.8	1013.977	2.0271 1.56
22	53524.6	937.704	1.8746 0.92
23	53620.5	925.985	1.8512 1.23
24	53651.7	922.166	1.8435 1.53
25	53701.9	916.028	1.8312 1.63
26	53735.0	911.979	1.8232 1.36
27	53812.5	902.506	1.8042 1.44
28	53840.4	899.097	1.7974 1.33
29	53945.2	886.286	1.7718 0.40
30	54232.7	851.125	1.7015 0.83
31	54347.4	837.104	1.6735 1.43
32	54611.2	804.854	1.6090 0.95
33	54644.0	800.841	1.6010 1.02
34	54745.3	788.456	1.5762 2.93
35	54836.2	777.338	1.5540 2.04
36	55335.7	716.265	1.4319 0.75
37	55512.5	694.654	1.3887 0.37
38	55592.0	684.936	1.3693 0.65
39	55618.2	681.734	1.3629 1.00
40	55723.6	668.841	1.3371 0.93
41	55829.1	655.946	1.3113 0.29
42	61193.8	0.025	0.0001 0.87

¹H spectrum



Current Data Parameters
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 NAME Coconut_fun
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131205
 Time 19.11
 INSTRUM cryo500
 PROBHID 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 2.8
 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 500.2200260 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 FIP 7.500 ppm
 F1 3751.65 Hz
 F2P 5.500 ppm
 F2 2751.21 Hz
 PPMCM 0.08772 ppm/cm
 HZCM 43.87895 Hz/cm

¹H spectrum

ppm

241413
240571
238666
237826
222716
213285
209724
205481
202995
202706
187459
185116
184552
183125
182316
180422
179740
177179
170150
167347
160900
160098
157622
155399
143190
138870
136927
136287
133709
131132

h

g

i

j k

l

m n

o

ppm

2.8

2.6

2.4

2.2

2.0

1.8

1.6

1.4

1.2

Current Data Parameters
USER nmr13t
NAME Coconut_fun
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131205
Time 19:11
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 2.8
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 500.2200260 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
FIP 3.000 ppm
F1 1500.66 Hz
F2 1.000 ppm
FZ 500.22 Hz
PPMCM 0.08772 ppm/cm
HZCM 43.87895 Hz/cm

1.0446

7.9121

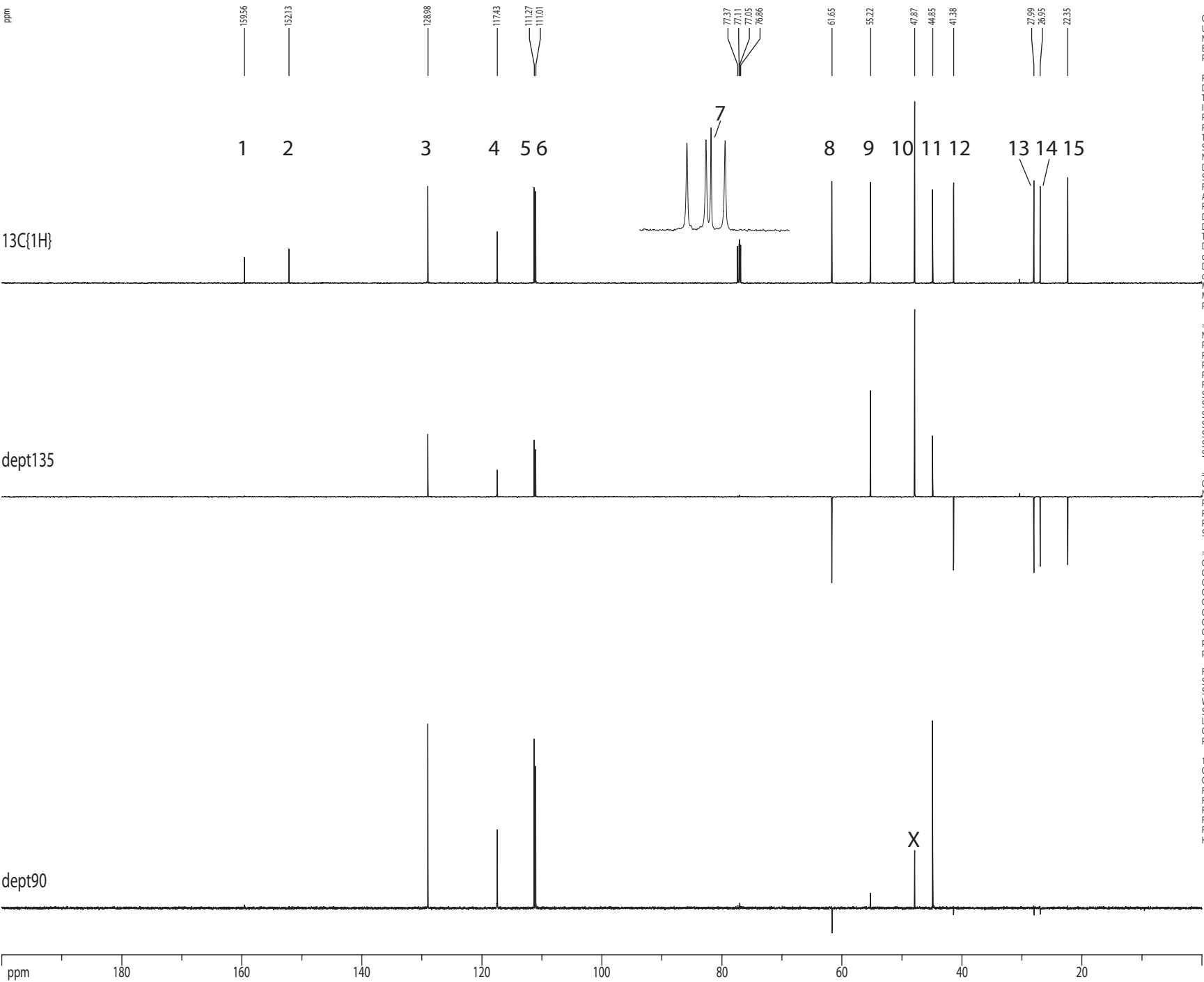
2.9760

1.0720

2.8982

1.0074

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters
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NAME Coconut_fun
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131205
Time 19.14
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG Spinechop30gp.prd
TD 65536
SOLVENT CDCl3
NS 172
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813940 sec
RG 14596.5
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
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SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz

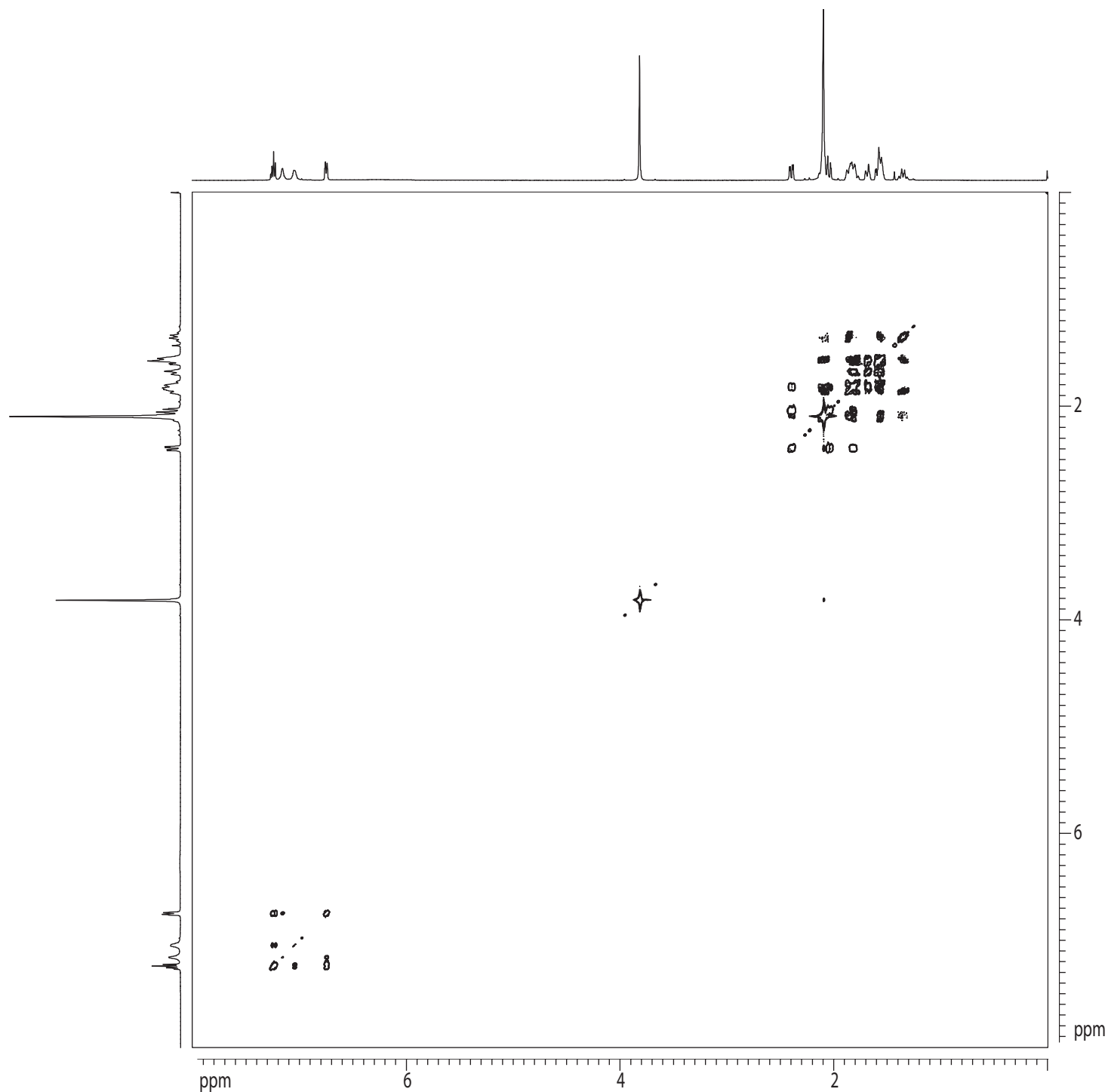
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NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====
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GPNAM2 SINE100
GPX1 0.00 %
GPX2 0.00 %
GPV1 0.00 %
GPV2 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 200.000 ppm
F1 25156.08 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 8.77193 ppm/cm
HZCM 1103.33704 Hz/cm

gcosy60



Current Data Parameters
 USER nmr13t
 NAME Coconut_fun
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131205
 Time 19:28
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG cosygp60.prd
 TD 2048
 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 4006.410 Hz
 FIDRES 1.956255 Hz
 AQ 0.2556404 sec
 RG 2.8
 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 =====
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 GPNAM2 sine.100
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 GPX2 0.00 %
 GPY1 0.00 %
 GPY2 0.00 %
 GPZ1 17.00 %
 GPZ2 17.00 %
 P16 1000.00 usec

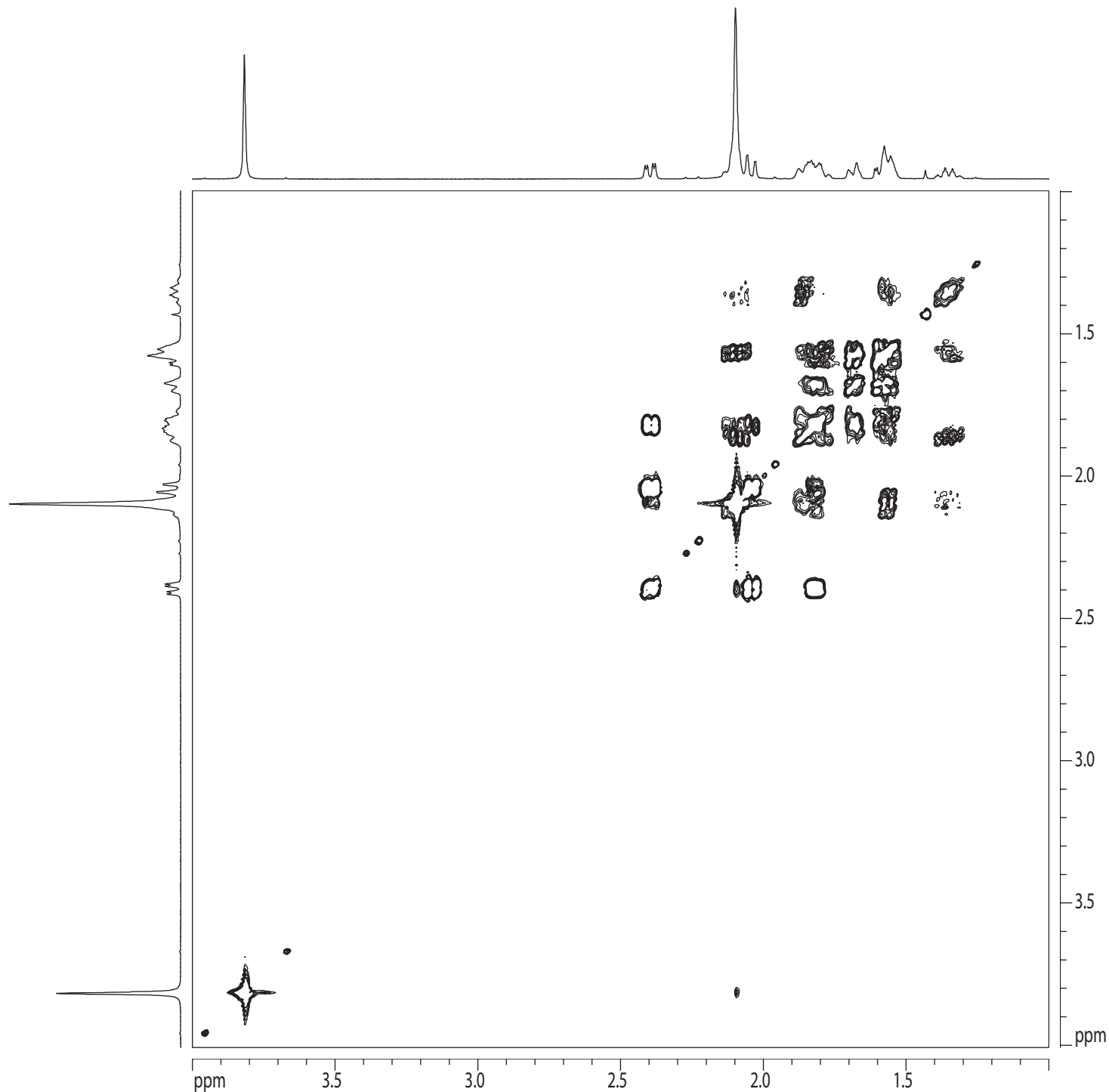
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 FIDRES 7.825020 Hz
 SW 8.009 ppm
 FnMODE undefined

F2 - Processing parameters
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 SF 500.2200260 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 500.2200260 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 nmr13t
 NAME Coconut_fun
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131205
 Time 19:28
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG cosygp60.prd
 TD 2048
 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 4006.410 Hz
 FIDRES 1.956255 Hz
 AQ 0.2556404 sec
 RG 2.8
 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
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 GPX2 0.00 %
 GPY1 0.00 %
 GPY2 0.00 %
 GPZ1 17.00 %
 GPZ2 17.00 %
 P16 1000.00 usec

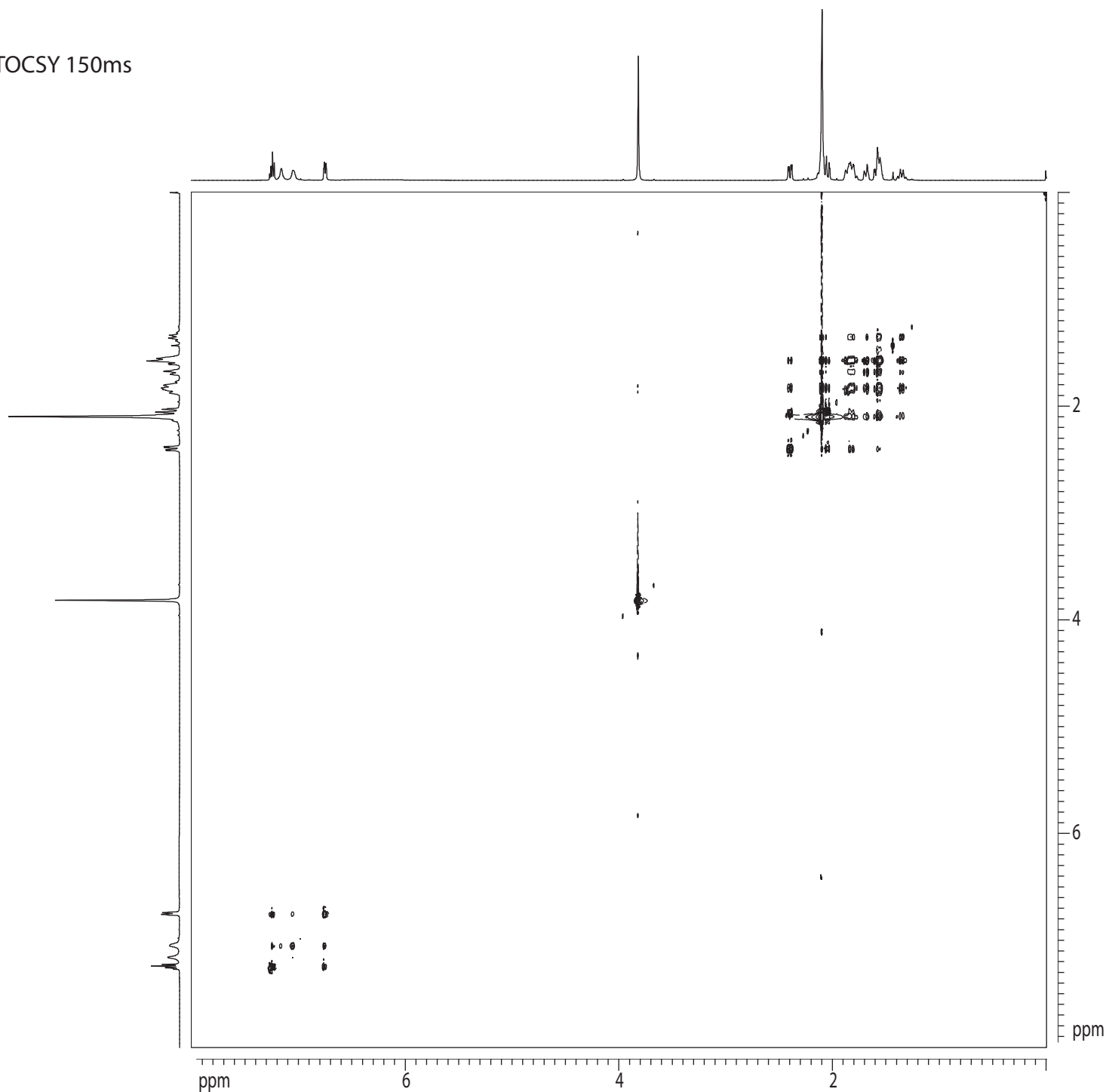
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F2 - Processing parameters
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 SF 500.2200260 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
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 MC2 QF
 SF 500.2200260 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 4.000 ppm
 F2LO 2000.88 Hz
 F2PHI 1.000 ppm
 F2HI 500.22 Hz
 F1PLO 4.008 ppm
 F1LO 2004.79 Hz
 F1PHI 0.997 ppm
 F1HI 498.47 Hz
 F2PPMCM 0.20000 ppm/cm
 F2HZCM 100.04401 Hz/cm
 F1PPMCM 0.20075 ppm/cm
 F1HZCM 100.42110 Hz/cm

TOCSY 150ms



Current Data Parameters
 USER nmr13t
 NAME Coconut_fun
 EXPNO 22
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131213
 Time 11.52
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG tocsytp.wu
 TD 2048
 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 4006.410 Hz
 FIDRES 1.956255 Hz
 AQ 0.2557652 sec
 RG 80.6
 DW 124.800 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 2.00000000 sec
 d8 0.14985408 sec
 d12 0.00002000 sec
 INO 0.00012480 sec
 L1 64

===== 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

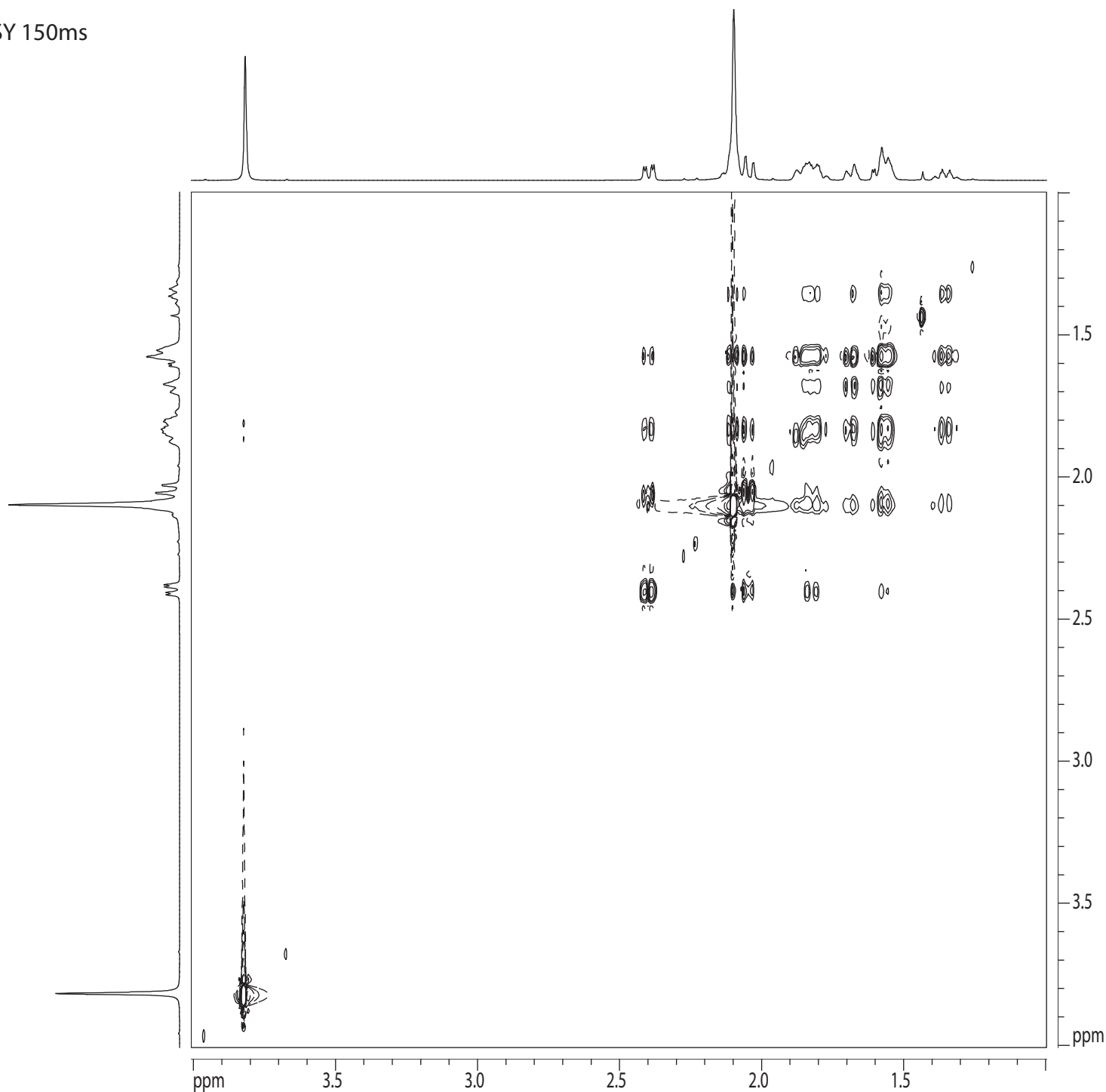
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 SFO1 500.222 MHz
 FIDRES 22.257835 Hz
 SW 8.009 ppm
 FnMODE undefined

F2 - Processing parameters
 SI 1024
 SF 500.2200260 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0
 PC 4.00

F1 - Processing parameters
 SI 1024
 MC2 TPPI
 SF 500.2200260 MHz
 WDW QSINE
 SSB 3
 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

TOCSY 150ms



Current Data Parameters
 USER nmr13t
 NAME Coconut_fun
 EXPNO 22
 PROCNO 1

F2 - Acquisition Parameters
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 Time 11.52
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 PROBHD 5 mm CPTCI 1H-
 PULPROG tocsytp.wu
 TD 2048
 SOLVENT CDCl₃
 NS 8
 DS 16
 SWH 4006.410 Hz
 FIDRES 1.956255 Hz
 AQ 0.2557652 sec
 RG 80.6
 DW 124.800 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 2.00000000 sec
 d8 0.14985408 sec
 d12 0.00002000 sec
 INO 0.00012480 sec
 L1 64

===== 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

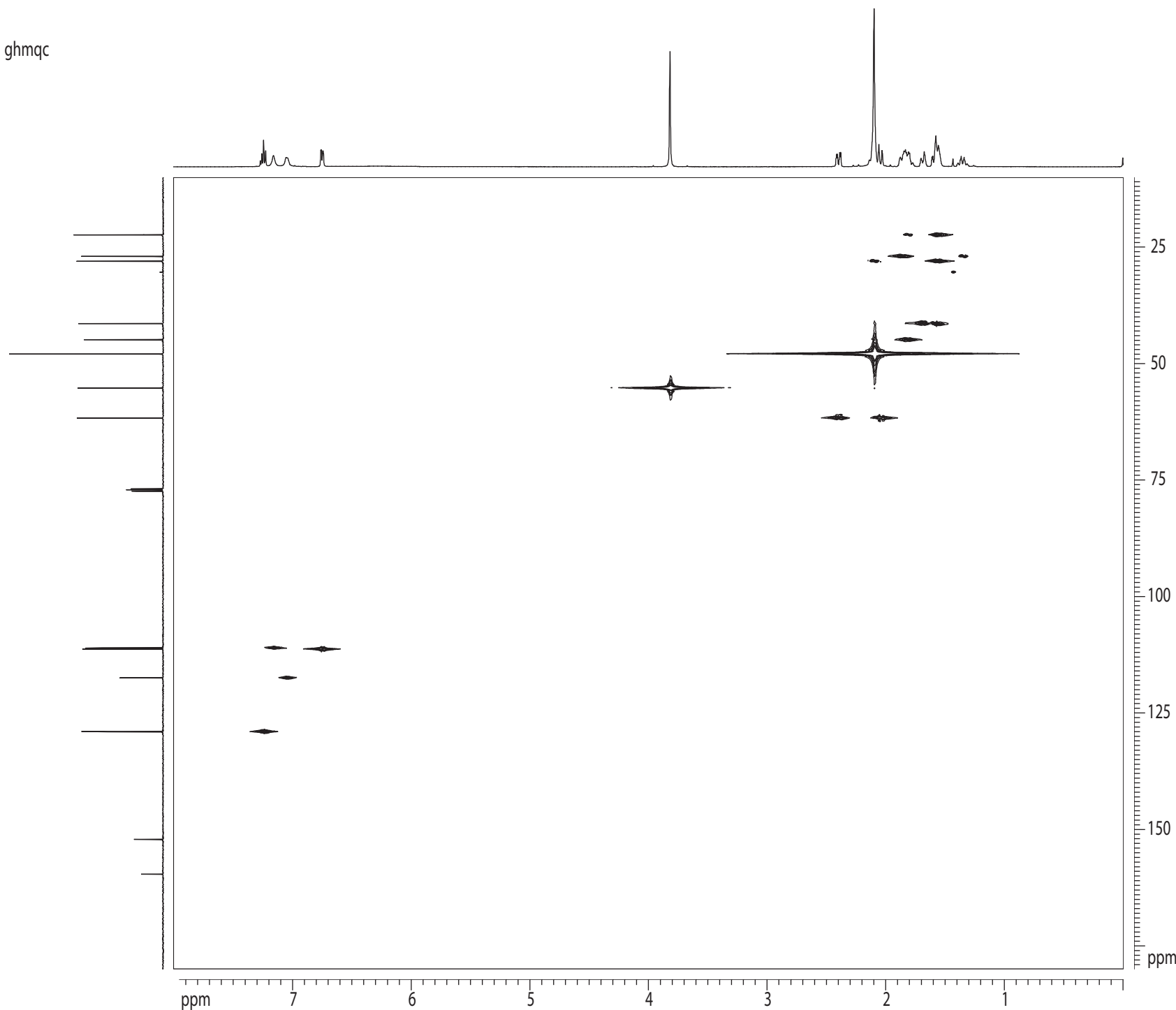
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 TD 177
 SFO1 500.222 MHz
 FIDRES 22.635086 Hz
 SW 8.009 ppm
 FnMODE undefined

F2 - Processing parameters
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 SF 500.2200260 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0
 PC 4.00

F1 - Processing parameters
 SI 1024
 MC2 TPPI
 SF 500.2200260 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 4.008 ppm
 F2LO 2004.79 Hz
 F2PHI 0.997 ppm
 F2HI 498.47 Hz
 F1PLO 4.008 ppm
 F1LO 2004.79 Hz
 F1PHI 0.997 ppm
 F1HI 498.47 Hz
 F2PPMCM 0.20075 ppm/cm
 F2HZCM 100.42110 Hz/cm
 F1PPMCM 0.20075 ppm/cm
 F1HZCM 100.42110 Hz/cm

ghmqc



Current Data Parameters

USER nmr13t
NAME Coconut_fun
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131206
Time 3.23
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PROBHD 5 mm CPTCI 1H-
PULPROG inv4gp.wu
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 1824.6
DW 124.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000300 sec
D16 0.00020000 sec
d20 0.00242528 sec
IN0 0.00002340 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 125.7923681 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 125.7924 MHz
FIDRES 41.733440 Hz
SIW 169.863 ppm
FnMODE undefined

F2 - Processing parameters

SI 1024
SF 500.2200260 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

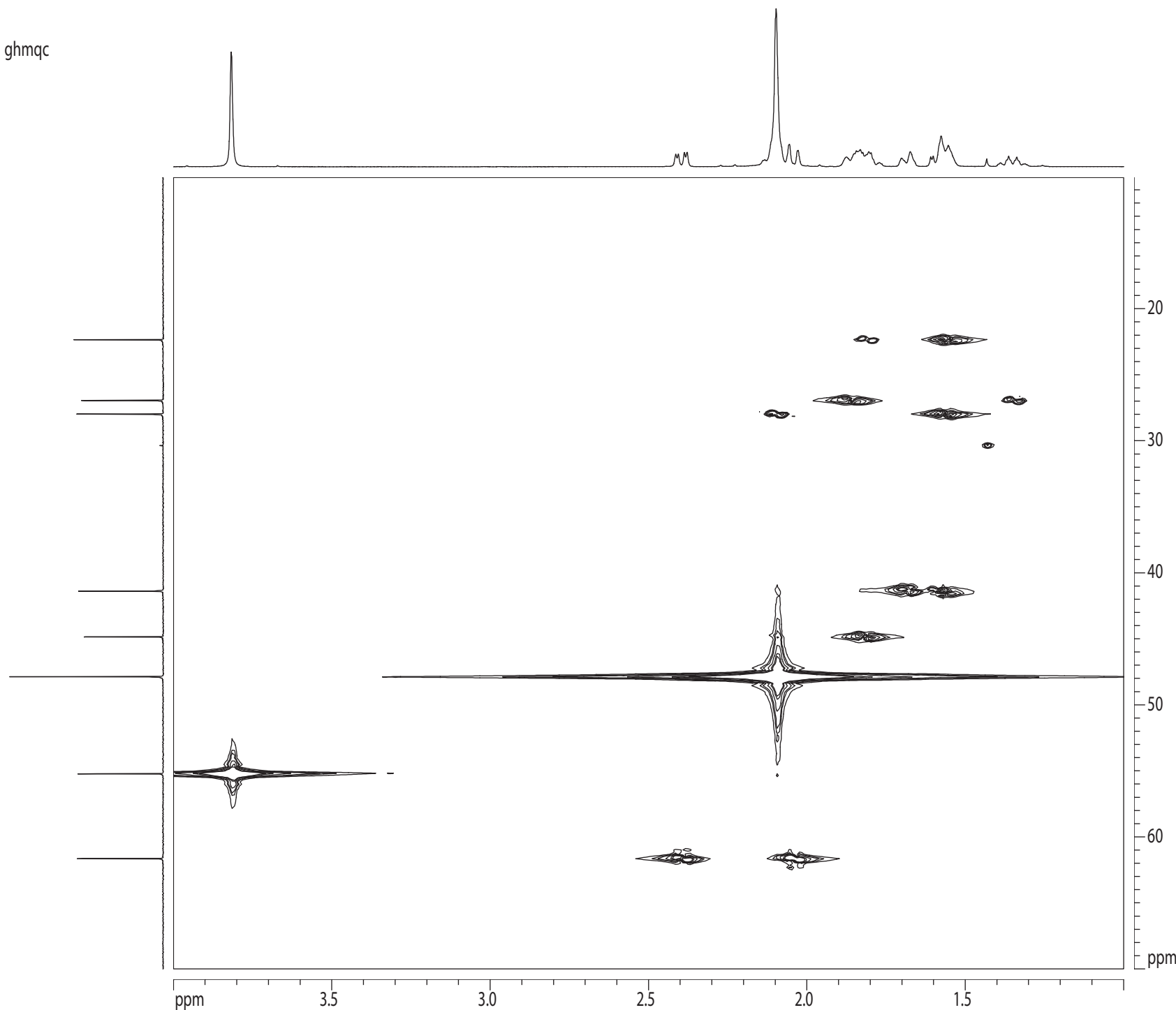
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MC2 QF
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WDW QSINE
SSB 3
LB 0.00 Hz
GB 0

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 179.940 ppm
F1LO 22632.89 Hz
F1PHI 10.060 ppm
F1HI 1265.37 Hz
F2PPMCM 0.44496 ppm/cm
F2HZCM 222.57837 Hz/cm
F1PPMCM 11.32530 ppm/cm
F1HZCM 1424.50146 Hz/cm

ghmqc



Current Data Parameters

USER nmr13t
NAME Coconut_fun
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131206
Time 3.23
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG inv4gp.wu
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 1824.6
DW 124.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
d1 1.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000300 sec
d16 0.00020000 sec
d20 0.00242528 sec
IN0 0.00002340 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 125.7923681 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 30.00 %
GPZ2 18.00 %
GPZ3 24.00 %
P16 1000.00 usec

F1 - Acquisition parameters

ND0 2
TD 512
SFO1 125.7924 MHz
FIDRES 41.733440 Hz
SW 169.863 ppm
FnMODE undefined

F2 - Processing parameters

SI 1024
SF 500.2200260 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

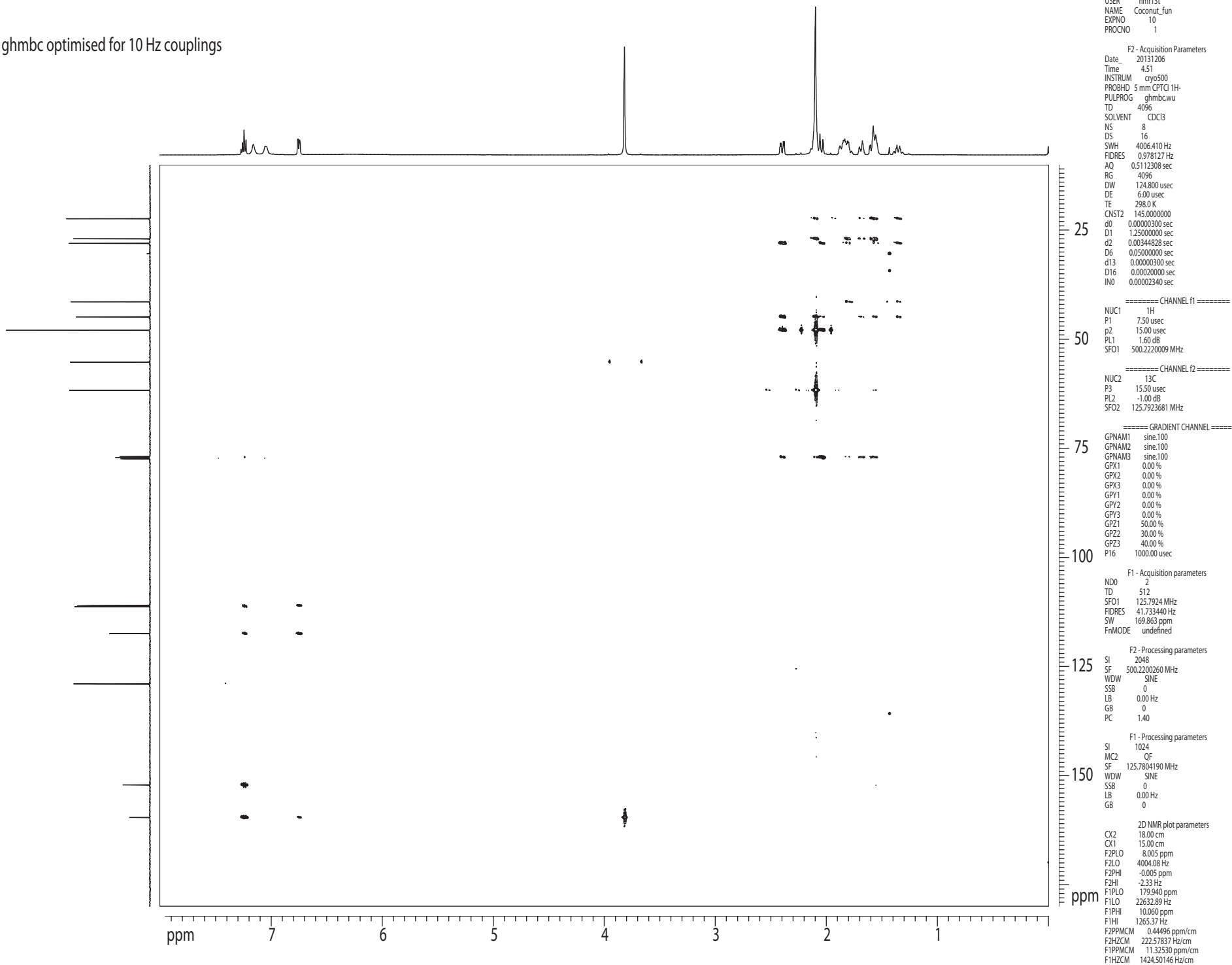
F1 - Processing parameters

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

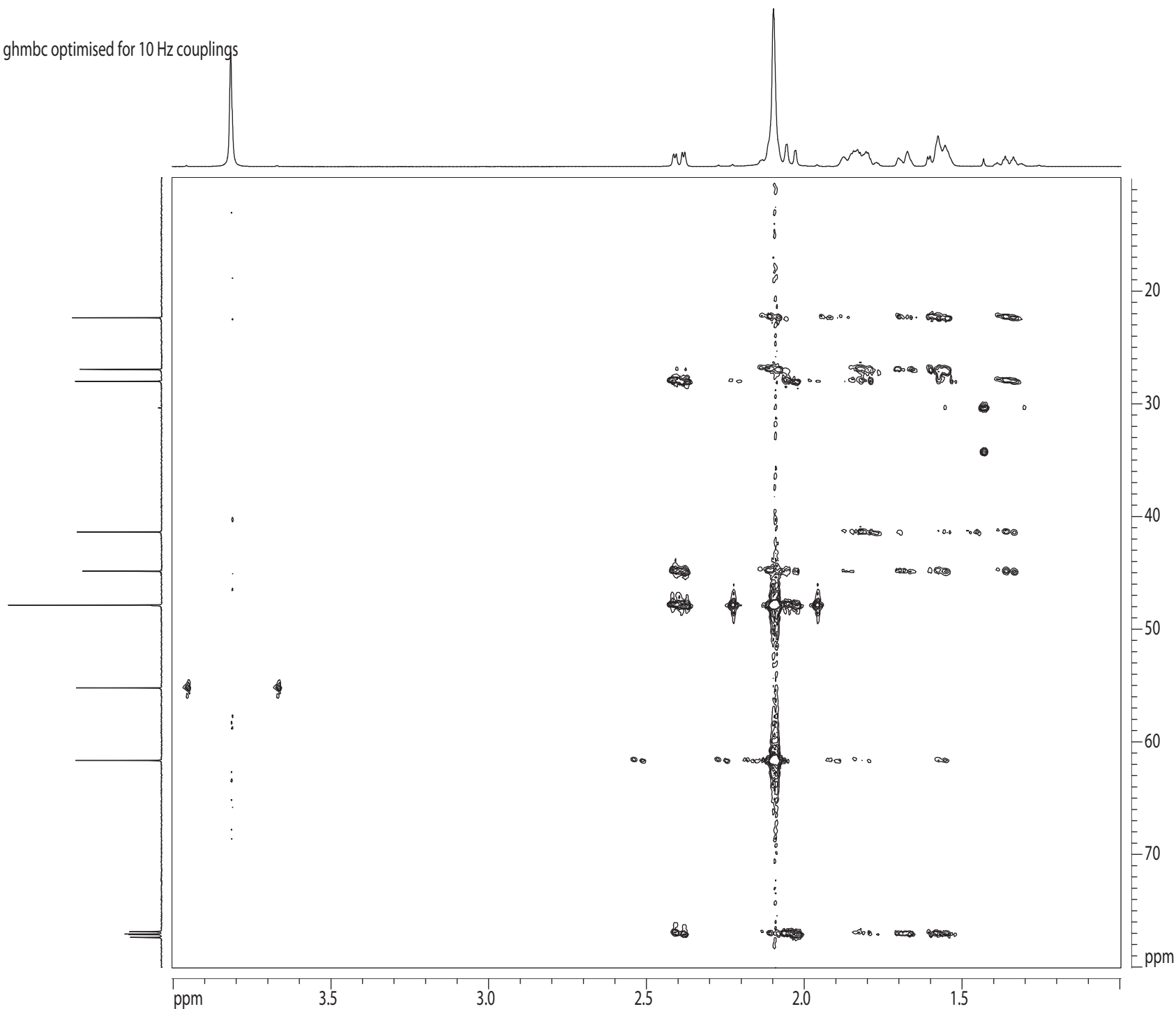
2D NMR plot parameters

CX2 18.00 cm
CX1 15.00 cm
F2PLO 4.000 ppm
F2LO 2000.88 Hz
F2PHI 1.000 ppm
F2HI 500.22 Hz
F1PLO 70.000 ppm
F1LO 8804.63 Hz
F1PHI 10.060 ppm
F1HI 1265.37 Hz
F2PPMCM 0.16667 ppm/cm
F2HZCM 83.37000 Hz/cm
F1PPMCM 3.99599 ppm/cm
F1HZCM 502.61737 Hz/cm

ghmbc optimised for 10 Hz couplings



ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER	nmr13t
NAME	Coconut_fun
EXPNO	10
PROCNO	1

F2 - Acquisition Parameters

Date_	20131206
Time	4.51
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	ghmbc.wu
TD	4096
SOLVENT	CDCl3
NS	8
DS	16
SWH	4006.410 Hz
FIDRES	0.978127 Hz
AQ	0.5112308 sec
RG	4096
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	0.00002340 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	125.7923681 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	125.7924 MHz
FIDRES	41.733440 Hz
SW	169.863 ppm
FnMODE	undefined

F2 - Processing parameters

SI	2048
SF	500.2200260 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

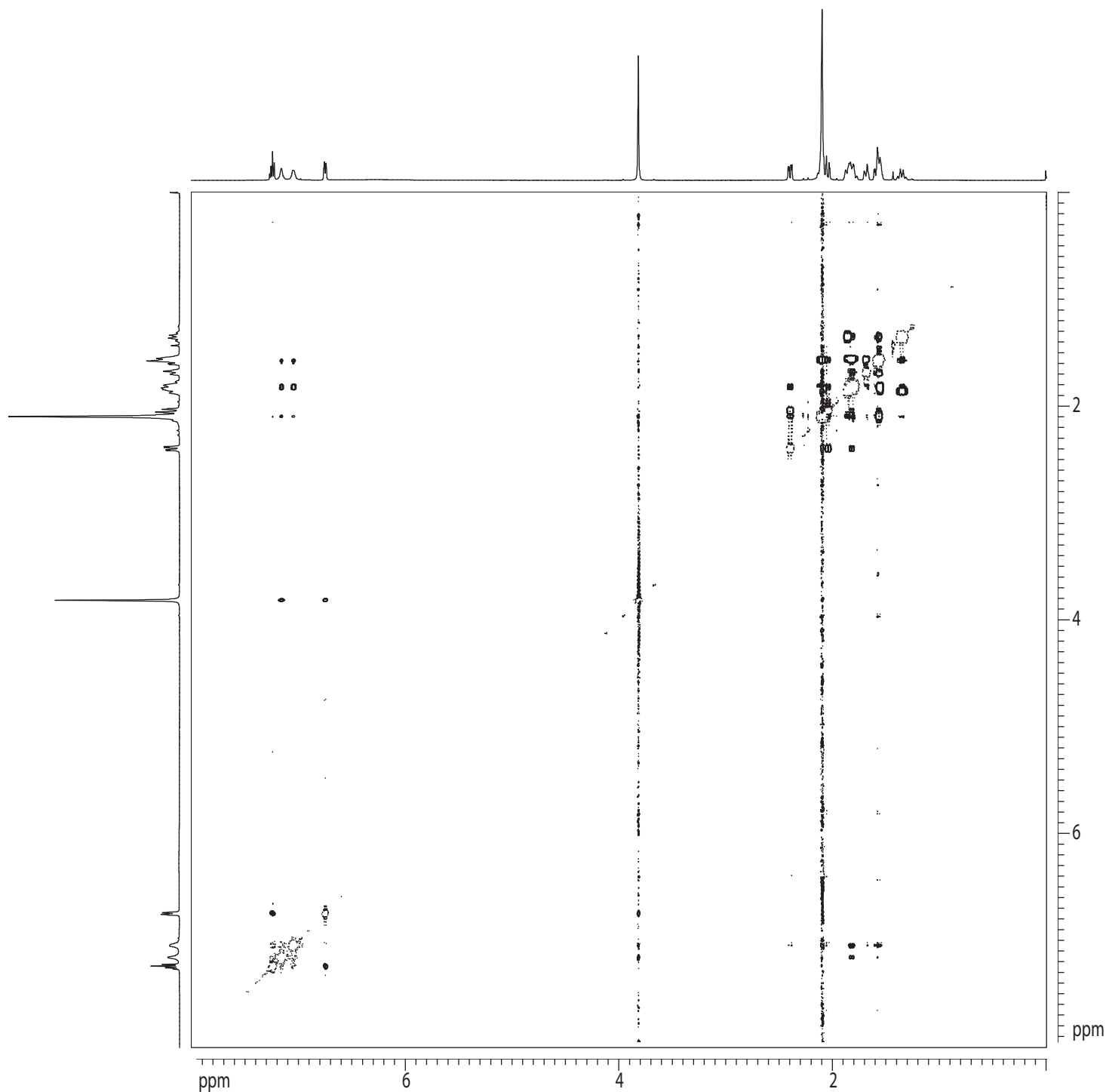
F1 - Processing parameters

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
CY1	15.00 cm
F2PLO	4.004 ppm
F2LO	2002.83 Hz
F2PHI	0.997 ppm
F2HI	498.47 Hz
F1PLO	80.069 ppm
F1LO	10071.12 Hz
F1PHI	9.894 ppm
F1HI	1244.50 Hz
F2PPMCM	0.16708 ppm/cm
F2HZCM	83.57557 Hz/cm
F1PPMCM	4.67832 ppm/cm
F1HZCM	588.44153 Hz/cm

noesy



Current Data Parameters
 USER nmr13t
 NAME Coconut_fun
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131205
 Time 23.38
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG noesyrvtp
 TD 2048
 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 4006.410 Hz
 FIDRES 1.956255 Hz
 AQ 0.2556404 sec
 RG 2.8
 DW 124.800 usec
 DE 6.00 usec
 TE 298.0 K
 D0 0.0000300 sec
 D1 2.00000000 sec
 D8 1.0000000 sec
 INO 0.00012480 sec

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

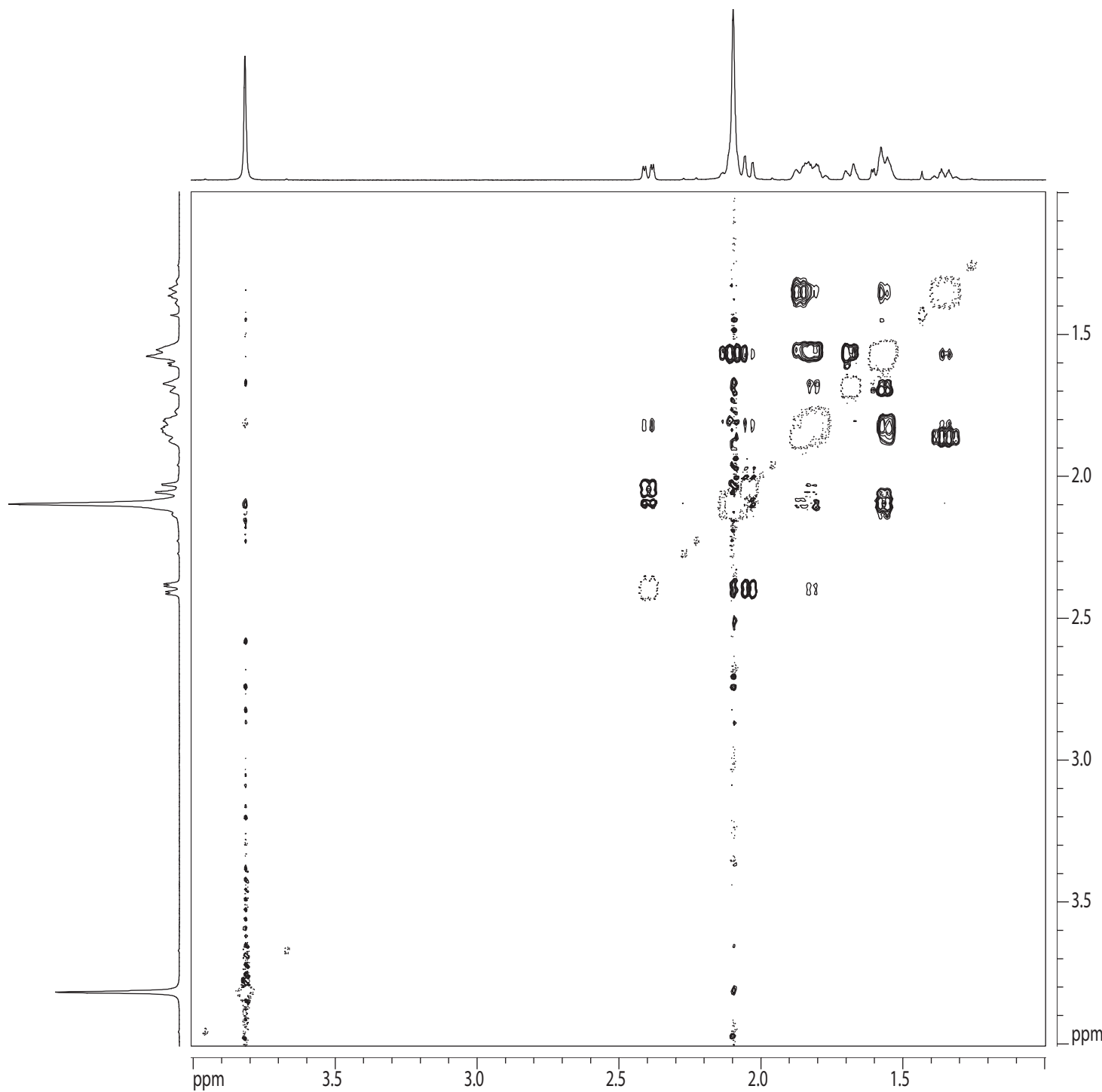
F1 - Acquisition parameters
 ND0 2
 TD 512
 SFO1 500.222 MHz
 FIDRES 7.825020 Hz
 SW 8.009 ppm
 FnMODE undefined

F2 - Processing parameters
 SI 1024
 SF 500.2200260 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 TPPI
 SF 500.2200260 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

noesy



Current Data Parameters
 USER nmr13t
 NAME Coconut_fun
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131205
 Time 23.38
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG noesyrvtp
 TD 2048
 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 4006.410 Hz
 FIDRES 1.956255 Hz
 AQ 0.2556404 sec
 RG 2.8
 DW 124.800 usec
 DE 6.00 usec
 TE 298.0 K
 D0 0.00000300 sec
 D1 2.00000000 sec
 D8 1.00000000 sec
 INO 0.00012480 sec

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

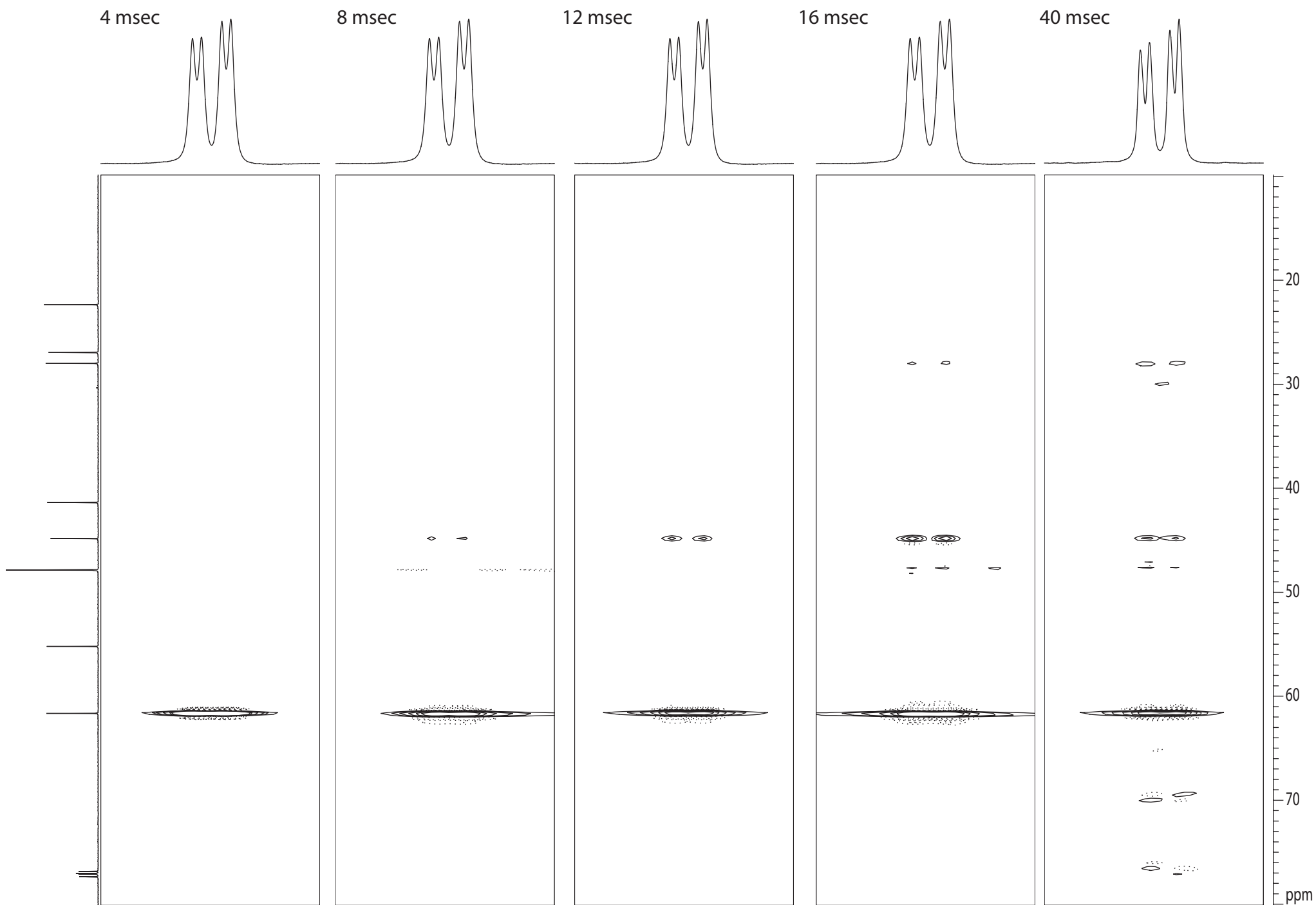
F1 - Acquisition parameters
 ND0 2
 TD 512
 SFO1 500.222 MHz
 FIDRES 7.825020 Hz
 SW 8.009 ppm
 FnMODE undefined

F2 - Processing parameters
 SI 1024
 SF 500.2200260 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 TPPI
 SF 500.2200260 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 4.008 ppm
 F2LO 2004.79 Hz
 F2PHI 0.997 ppm
 F2HI 498.47 Hz
 F1PLO 4.008 ppm
 F1LO 2004.79 Hz
 F1PHI 0.997 ppm
 F1HI 498.47 Hz
 F2PPMCM 0.20075 ppm/cm
 F2HZCM 100.42110 Hz/cm
 F1PPMCM 0.20075 ppm/cm
 F1HZCM 100.42110 Hz/cm

HSQC-TOCSY of peak 'g' (2.4 ppm) at 4 msec, 8 msec, 12 msec, 16 msec, 40 msec.



HSQC-TOCSY of peak 'o' (1.36 ppm) at 4 msec, 8 msec, 12 msec, 16 msec, 32 msec.

4 msec

8 msec

12 msec

16 msec

32 msec

