

Name: _____

Chem 203
December 14, 2013

Final Exam Part II
Problem 1 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.

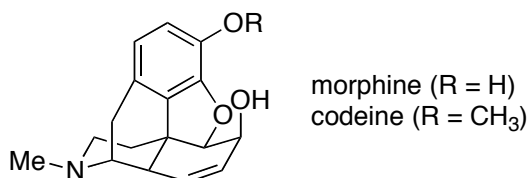
Books, notes, lecture videos, calculators, rulers, and laptop computers are permitted as is wireless (or wired) internet access and appropriate software (e.g, Pymol, Macromodel/Maestro, Excel, NMRPrediction, Chemdraw, ElComp, MolE, etc.). Catalogs of molecular structures (e.g., the Aldrich catalog, the 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 $C_{18}H_{25}NO$: 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. 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 2-5.

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-r) 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:

p:

q:

r:

c. Redraw the structure of the molecule below and write the letter (a-r) 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 (1-18) 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:

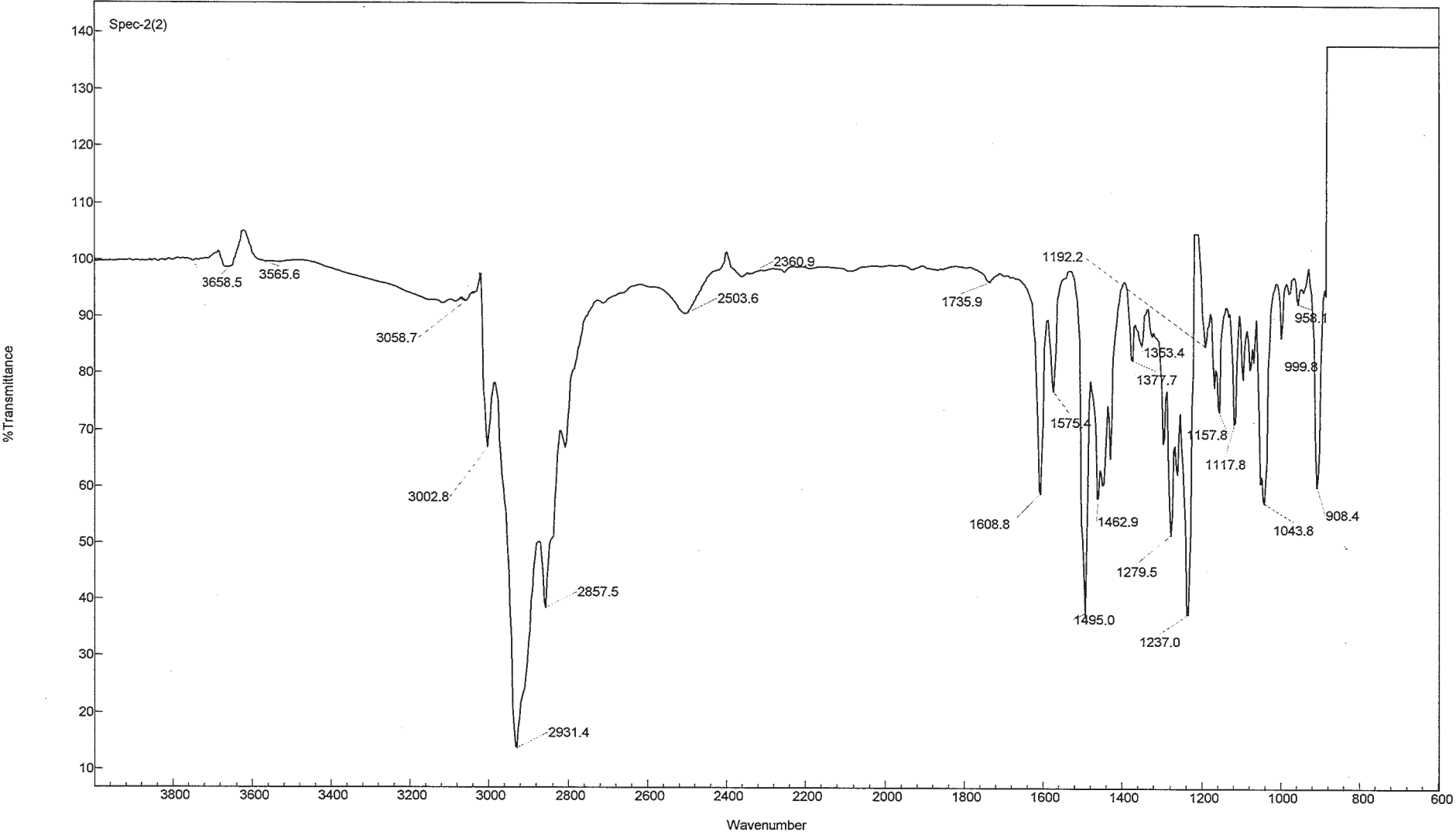
16:

17:

18:

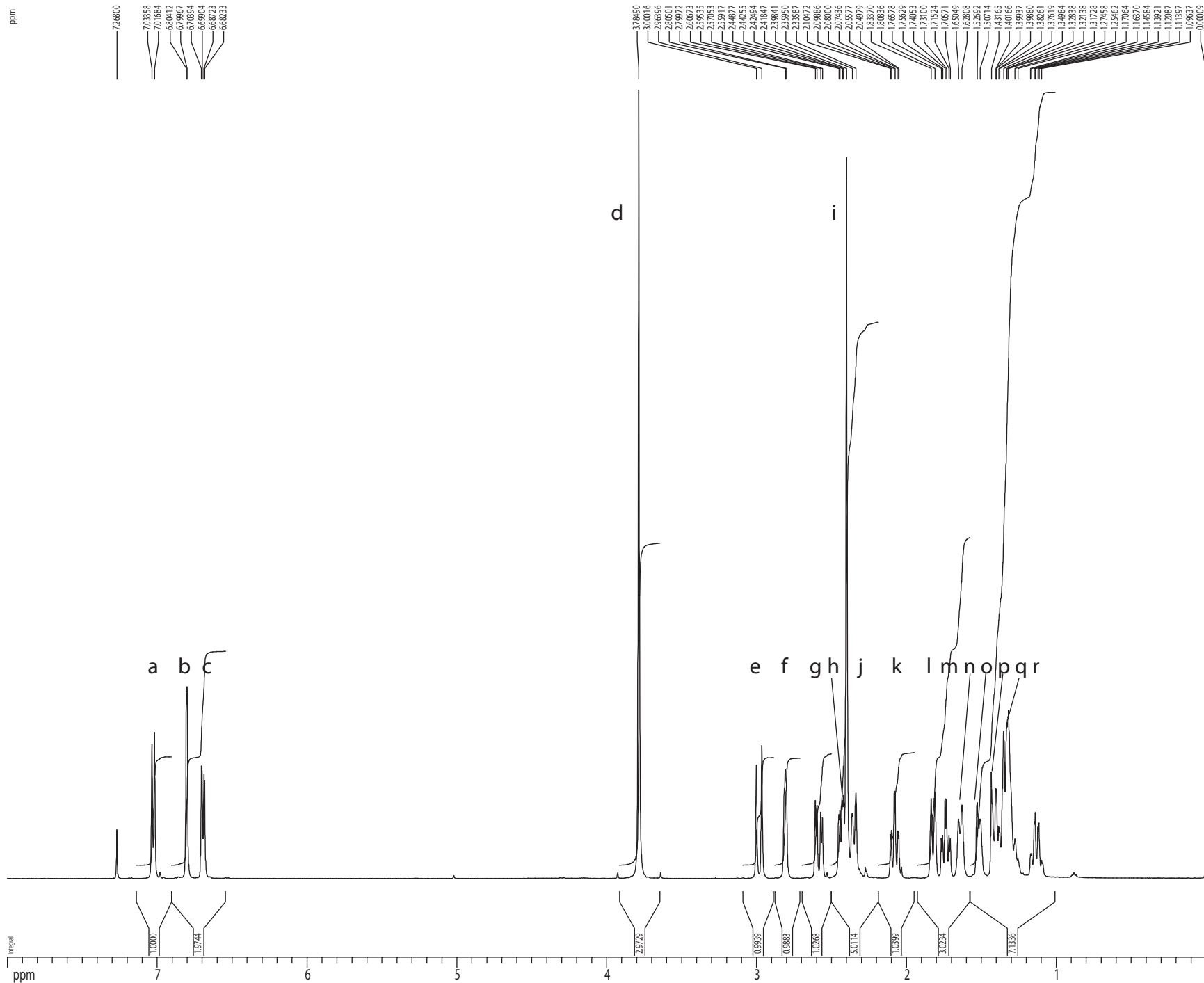
e. Redraw the structure of the molecule below and write the number (1-18) of each ^{13}C resonance next to the carbon or carbons to which it corresponds. If the assignment of particular resonance is uncertain, please indicate this.

Varian Resolutions Pro



Name
Spec-2 (2) —

¹H spectrum



Current Data Parameters
 USER nmrl3t
 NAME Banana_Rama_2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131204
 Time 19:40
 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 3.2
 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 500.2200276 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 0.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 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

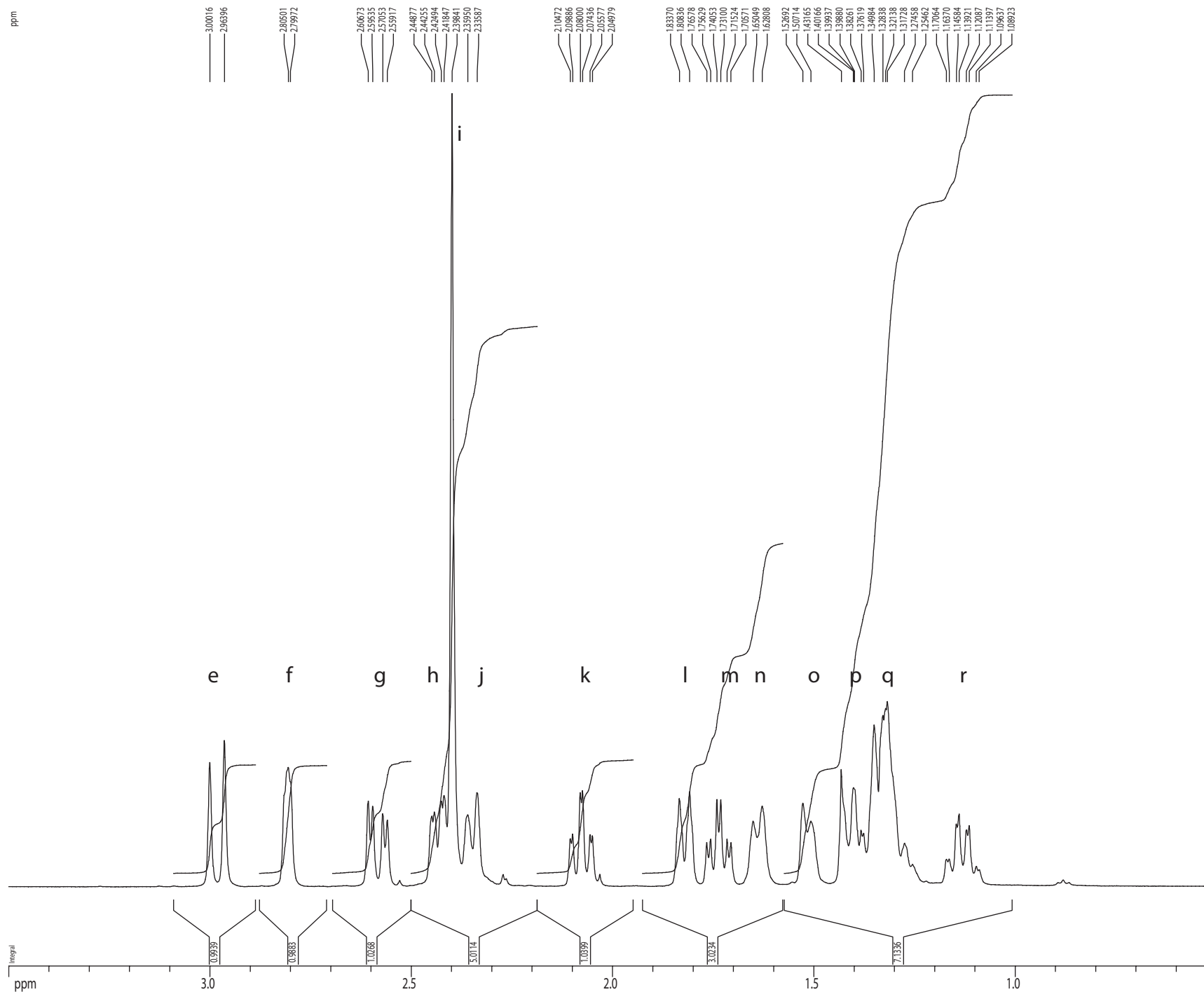
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#	ADDRESS	FREQUENCY [Hz]	INTENSITY [PPM]
1	31445.8	3635.598	0.93
2	32404.9	3518.337	2.55
3	32473.4	3509.964	2.78
4	33343.6	3403.558	3.52
5	33361.8	3401.333	3.65
6	33753.5	3353.446	2.14
7	33773.6	3350.991	2.05
8	33821.9	3345.083	1.98
9	33841.9	3342.634	1.87
10	45696.0	1893.284	15.00
11	48906.6	1500.741	2.15
12	49054.7	1482.634	2.53
13	49705.0	1403.119	2.06
14	49726.6	1400.477	1.81
15	50516.2	1303.937	1.48
16	50562.8	1298.244	1.39
17	50664.3	1285.828	1.26
18	50710.8	1280.145	1.16
19	51162.4	1224.926	1.22
20	51187.9	1221.811	1.29
21	51259.9	1213.005	1.48
22	51286.4	1209.769	1.58
23	51368.5	1199.731	13.73
24	51527.7	1180.268	1.24
25	51624.4	1168.450	1.62
26	52570.0	1052.824	0.83
27	52594.1	1049.889	0.92
28	52671.2	1040.459	1.63
29	52694.3	1037.634	1.66
30	52770.3	1028.338	0.90
31	52794.8	1025.344	0.88
32	53678.9	917.255	1.53
33	53782.5	904.579	1.64
34	53956.7	883.280	0.77
35	53995.6	878.533	0.82
36	54060.1	870.645	1.51
37	54099.1	865.878	1.51
38	54163.5	857.996	0.83
39	54202.5	853.231	0.76
40	54428.4	825.606	1.14
41	54520.1	814.396	1.40
42	54934.0	763.795	1.44
43	55014.9	753.903	1.13
44	55323.8	716.139	2.03
45	55446.5	701.136	1.71
46	55455.8	699.993	1.69
47	55458.1	699.710	1.69
48	55524.4	691.611	0.98
49	55550.7	688.397	0.93
50	55658.4	675.218	2.80
51	55746.2	664.483	2.97
52	55774.9	660.983	3.08

53	55791.7	658.931	1.3173	3.20
54	55966.4	637.571	1.2746	0.75
55	56048.0	627.585	1.2546	0.38
56	56391.6	585.580	1.1706	0.48
57	56420.0	582.108	1.1637	0.48
58	56493.1	573.171	1.1458	1.08
59	56520.2	569.854	1.1392	1.26
60	56595.2	560.683	1.1209	0.99
61	56623.4	557.231	1.1140	1.06
62	56695.5	548.426	1.0964	0.35
63	61180.6	0.043	0.0001	1.56

¹H spectrum

ppm



Current Data Parameters
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 NAME Banana_Rama_2
 EXPNO 1
 PROCNO 1

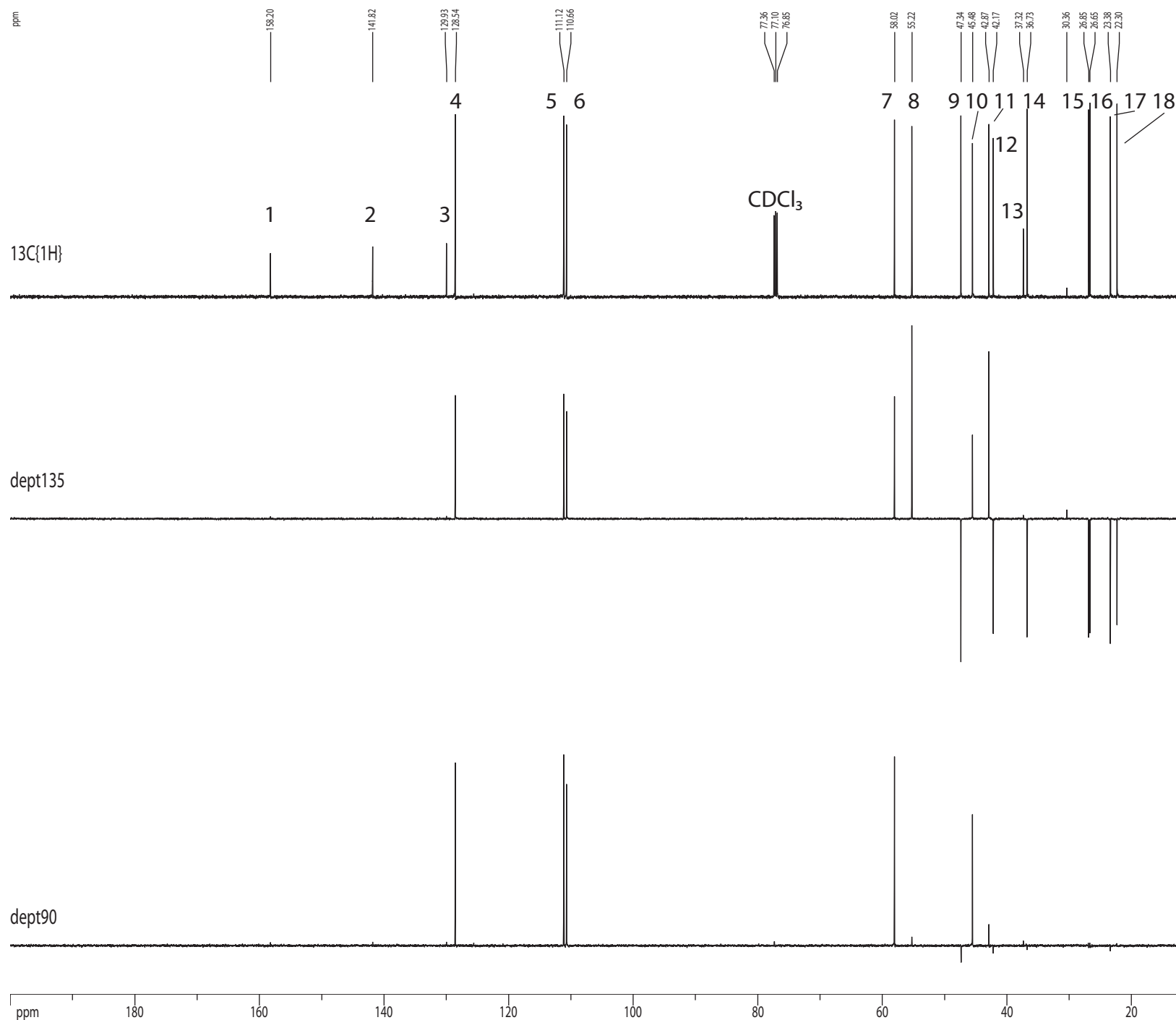
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 Date_ 20131204
 Time 19:40
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG zg30
 TD 81728
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 3.2
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCOREST 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 500.2200276 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 0.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 FIP 3.500 ppm
 F1 1750.77 Hz
 F2P 0.500 ppm
 F2 250.11 Hz
 PPMCM 0.13158 ppm/cm
 HZCM 65.81843 Hz/cm

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



Current Data Parameters
 USER nmrl3t
 NAME Banana_Rama_2
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131204
 Time 19:42
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG SpinEchopg30pp.prd
 TD 65536
 SOLVENT CDCl3
 NS 154
 DS 16
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813940 sec
 RG 11585.2
 DW 16.500 usec
 DE 6.00 usec
 TE 298.2 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 Cp60.0.5.20.1
 SPNAM2 Cp60comp.4
 SPOFF1 0.00 Hz
 SPOFF2 0.00 Hz

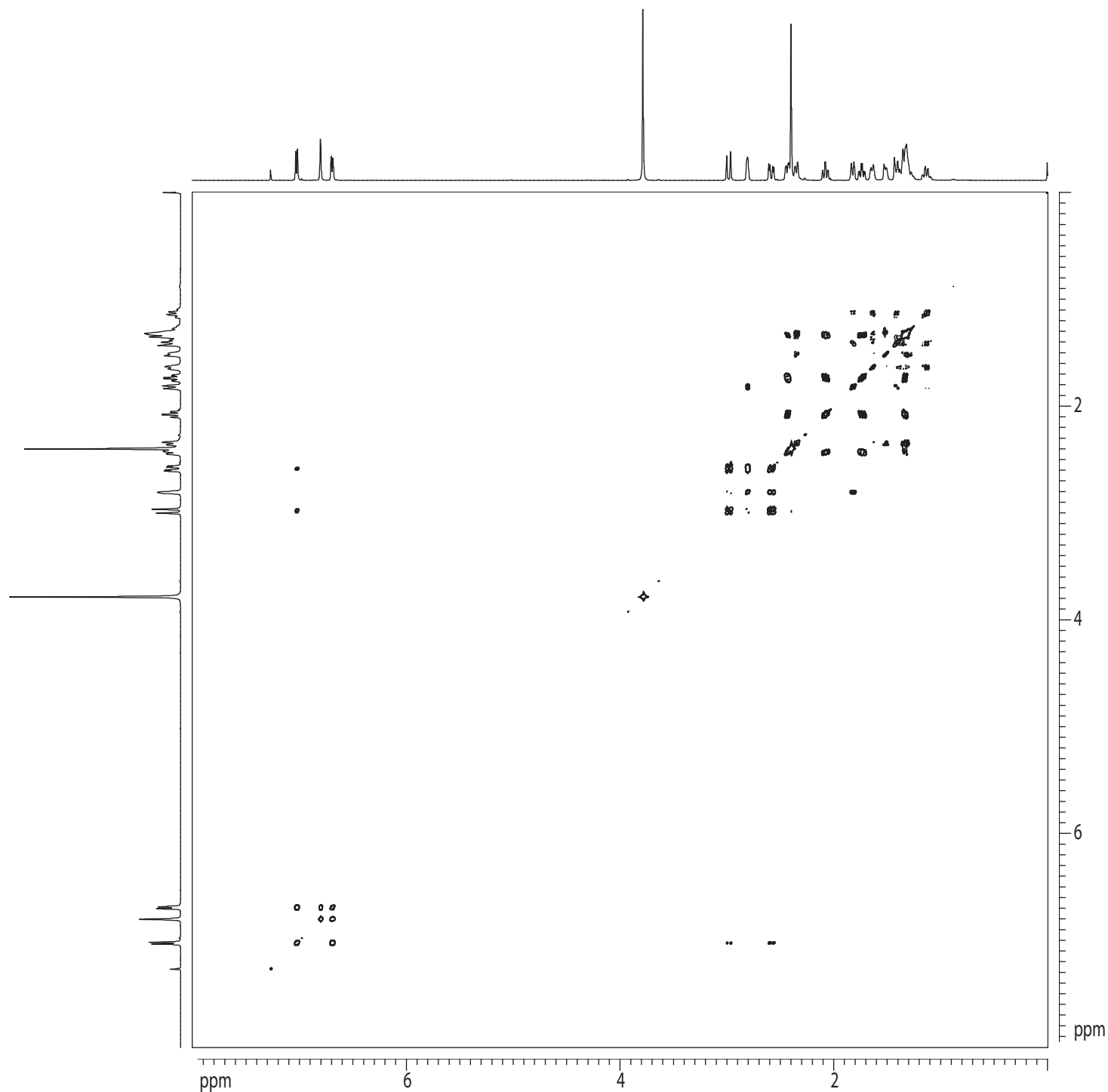
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 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 1.60 dB
 PL12 24.60 dB
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPK1 0.00 %
 GPK2 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 3.55 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 Banana_Rama_2
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131204
 Time 19:56
 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 3.2
 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

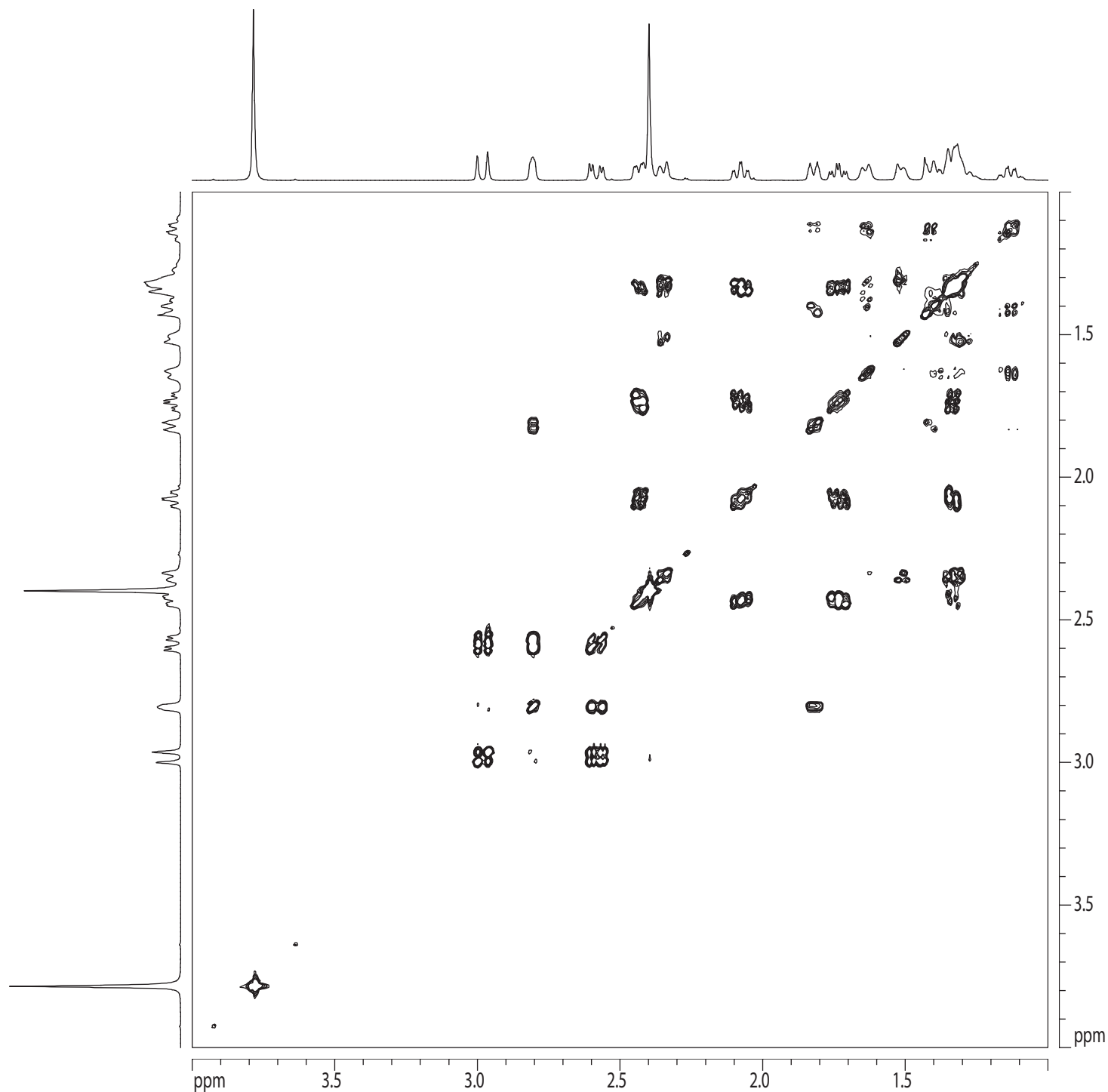
F1 - Acquisition parameters
 ND0 1
 TD 512
 SFO1 500.222 MHz
 FIDRES 7.825020 Hz
 SW 8.009 ppm
 FnmODE undefined

F2 - Processing parameters
 SI 1024
 SF 500.2200276 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 500.2200276 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 Banana_Rama_2
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131204
 Time 19:56
 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 3.2
 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

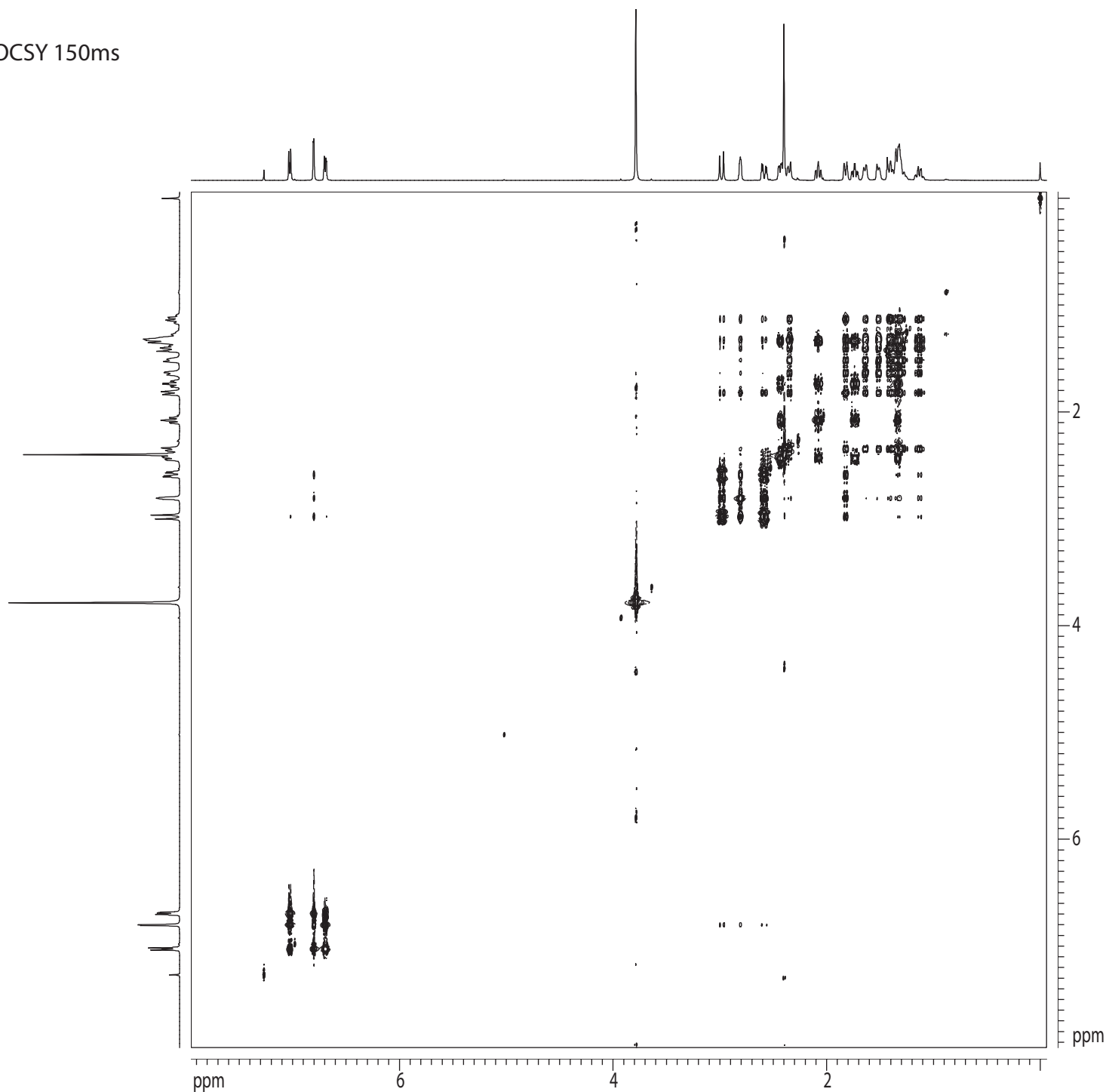
F1 - Acquisition parameters
 ND0 1
 TD 512
 SFO1 500.222 MHz
 FIDRES 7.825020 Hz
 SW 8.009 ppm
 FnmODE undefined

F2 - Processing parameters
 SI 1024
 SF 500.2200276 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 500.2200276 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 4.000 ppm
 F1LO 2000.88 Hz
 F1PHI 1.000 ppm
 F1HI 500.22 Hz
 F2PPMCM 0.20000 ppm/cm
 F2HZCM 100.04401 Hz/cm
 F1PPMCM 0.20000 ppm/cm
 F1HZCM 100.04401 Hz/cm

TOCSY 150ms



Current Data Parameters
 USER nmr13t
 NAME Banana_Rama_2
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131213
 Time 10:35
 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 0.2556404 sec
 RG 3.6
 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

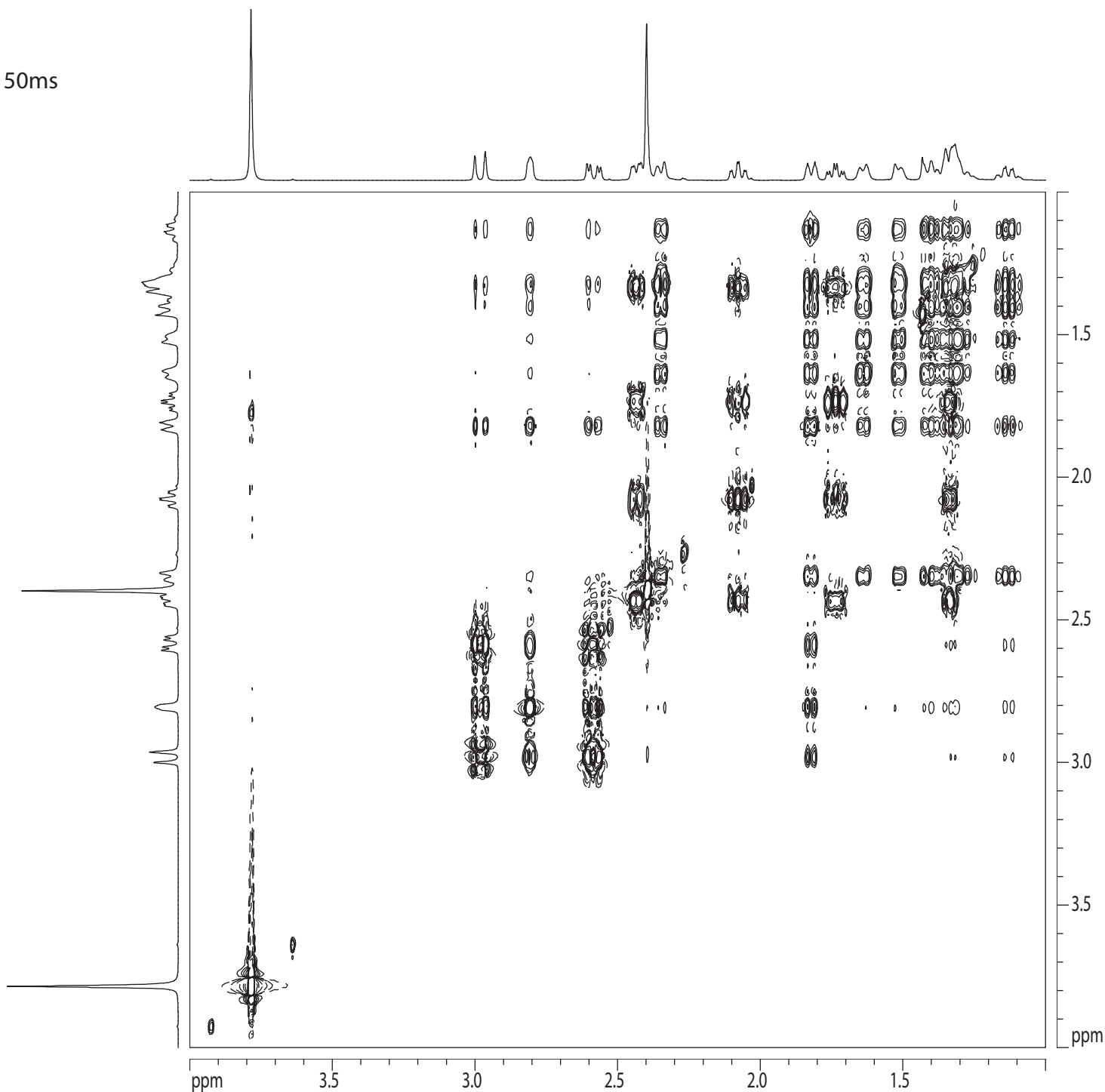
F1 - Acquisition parameters
 ND0 2
 TD 218
 SFO1 500.222 MHz
 FIDRES 18.378029 Hz
 SW 8.009 ppm
 FnMODE undefined

F2 - Processing parameters
 SI 1024
 SF 500.2200276 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0
 PC 4.00

F1 - Processing parameters
 SI 1024
 MC2 TPPI
 SF 500.2200276 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 7.949 ppm
 F2LO 3976.48 Hz
 F2PHI -0.060 ppm
 F2HI -29.93 Hz
 F1PLO 7.949 ppm
 F1LO 3976.48 Hz
 F1PHI -0.060 ppm
 F1HI -29.93 Hz
 F2PPMCM 0.53395 ppm/cm
 F2HZCM 267.09399 Hz/cm
 F1PPMCM 0.53395 ppm/cm
 F1HZCM 267.09399 Hz/cm

TOCSY 150ms



Current Data Parameters
 USER nmr13t
 NAME Banana_Rama_2
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131213
 Time 10.35
 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 0.2556404 sec
 RG 3.6
 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

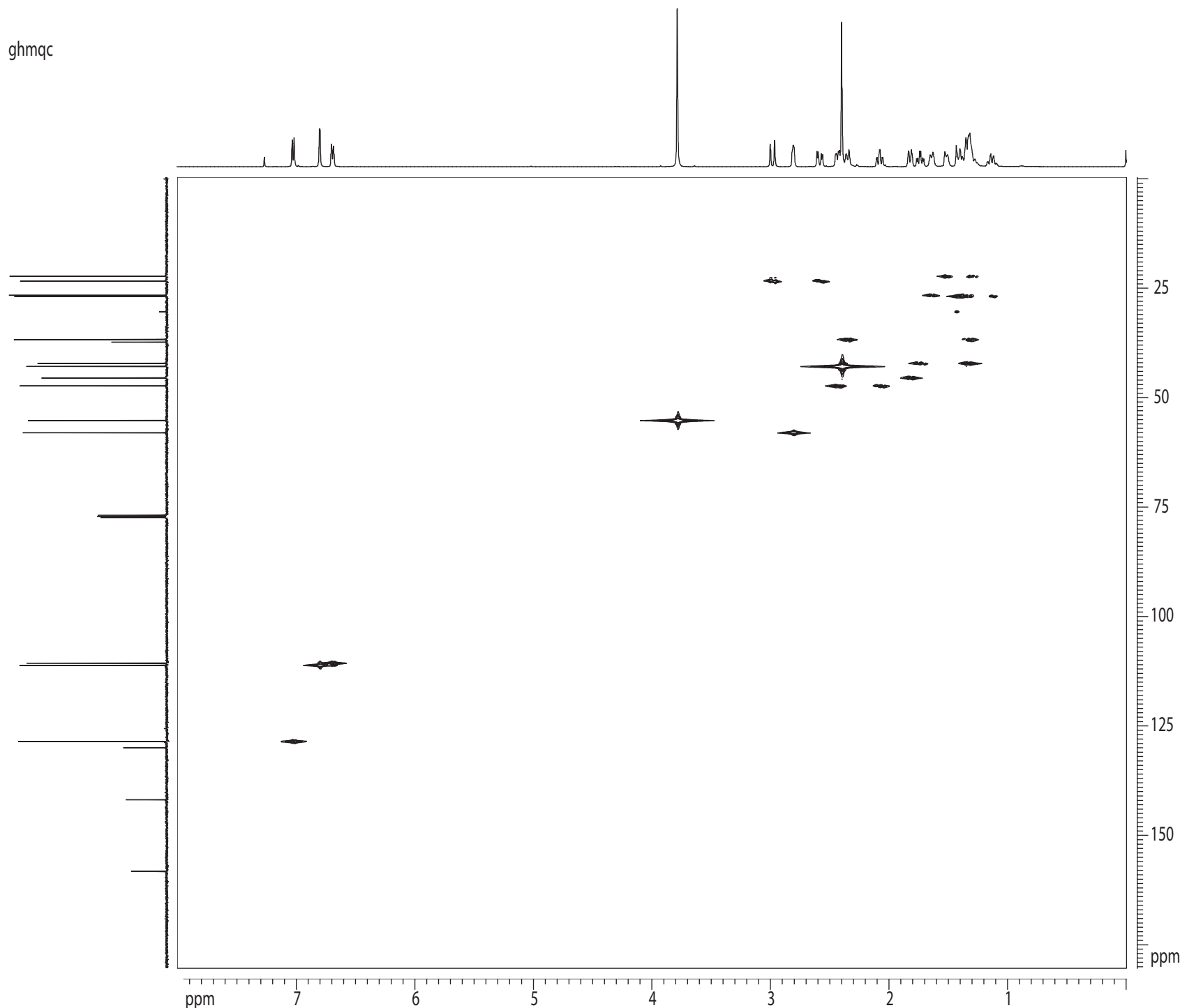
F1 - Acquisition parameters
 ND0 2
 TD 218
 SFO1 500.222 MHz
 FIDRES 18.378029 Hz
 SW 8.009 ppm
 FnMODE undefined

F2 - Processing parameters
 SI 1024
 SF 500.2200276 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0
 PC 4.00

F1 - Processing parameters
 SI 1024
 MC2 TPPI
 SF 500.2200276 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0

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

ghmqc



Current Data Parameters

USER nmr13t
NAME Banana_Rama_2
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131205
Time 3.56
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 2896.3
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 0.00003000 sec
D16 0.00020000 sec
d20 0.00242528 sec
INO 0.00002200 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 125.7917392 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 125.7917 MHz
FIDRES 44.389206 Hz
SW 180.674 ppm
FnmODE undefined

F2 - Processing parameters

SI 1024
SF 500.2200276 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

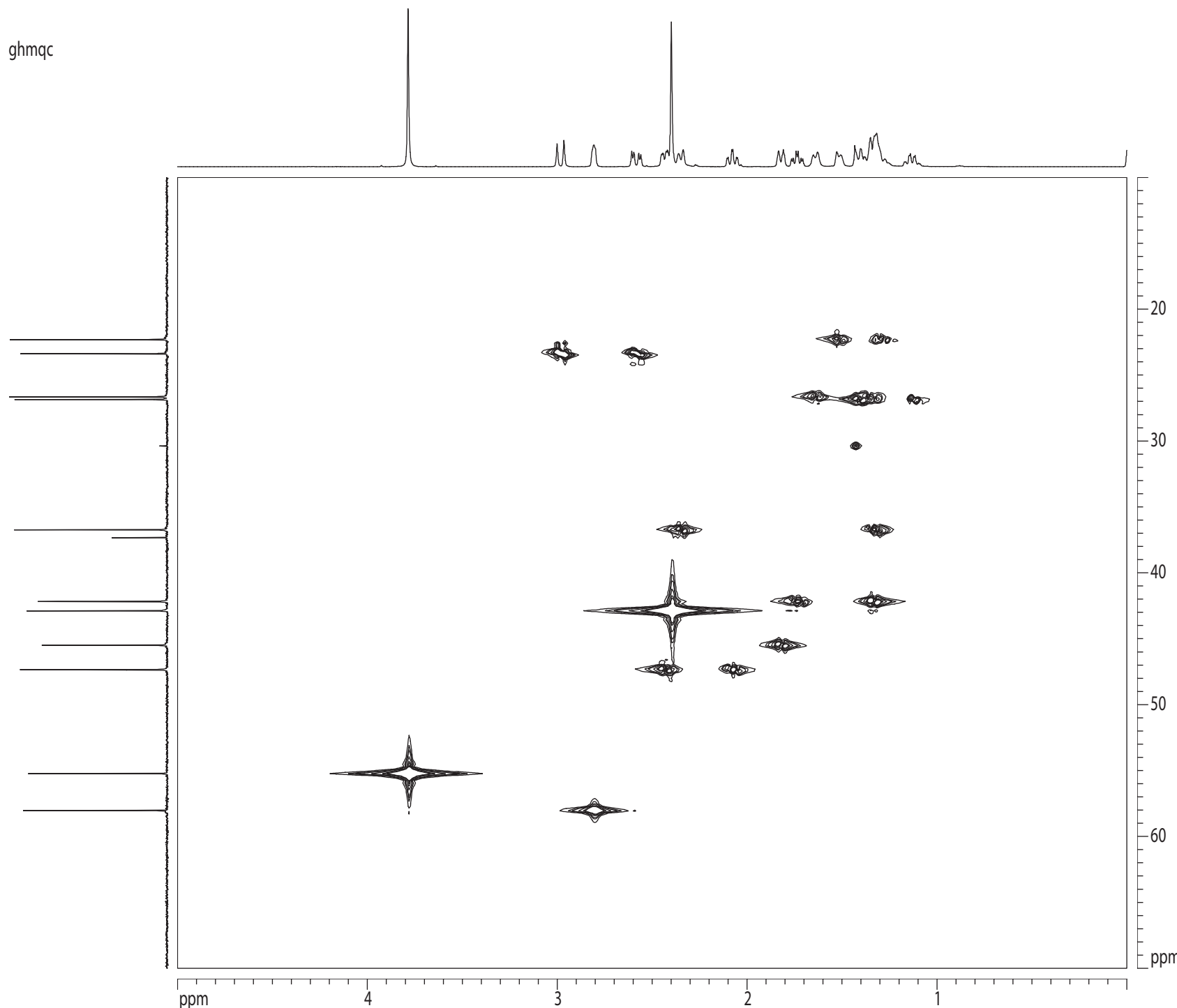
F1 - Processing parameters

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 180.345 ppm
F1LO 22683.87 Hz
F1PHI -0.345 ppm
F1HI -43.40 Hz
F2PPMCM 0.44496 ppm/cm
F2HZCM 222.57837 Hz/cm
F1PPMCM 12.04600 ppm/cm
F1HZCM 1515.15149 Hz/cm

ghmqc



Current Data Parameters

USER nmrl3t
NAME Banana_Rama_2
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131205
Time 3.56
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 2896.3
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 0.00002200 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 125.7917392 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 125.7917 MHz
FIDRES 44.399206 Hz
SIW 180.674 ppm
FnMODE undefined

F2 - Processing parameters

SI 1024
SF 500.2200276 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

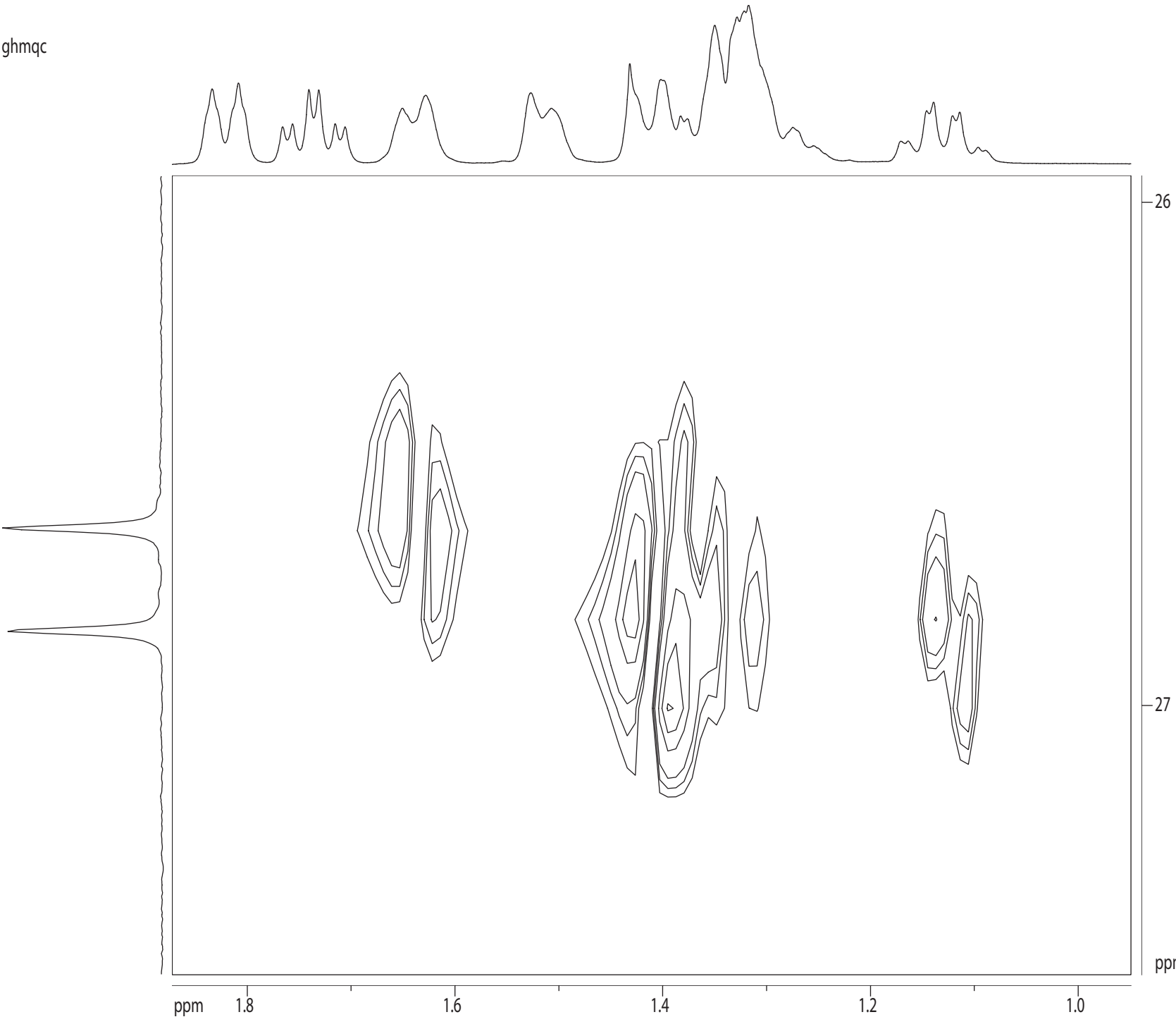
F1 - Processing parameters

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 5.000 ppm
F2LO 2501.10 Hz
F2PHI 0.000 ppm
F2HI 0.00 Hz
F1PLO 70.000 ppm
F1LO 8804.63 Hz
F1PHI 10.000 ppm
F1HI 1257.80 Hz
F2PPMCM 0.2778 ppm/cm
F2HZCM 138.95001 Hz/cm
F1PPMCM 4.00000 ppm/cm
F1HZCM 503.12167 Hz/cm

ghmqc



Current Data Parameters

USER nmrl3t
NAME Banana_Rama_2
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131205
Time 3.56
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG inv4gpcw
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 2896.3
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 0.00002200 sec

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

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

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

CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7917392 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 125.7917 MHz
FIDRES 44.389206 Hz
SIW 180.674 ppm
FnMODE undefined

F2 - Processing parameters

SI 1024
SF 500.2200276 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

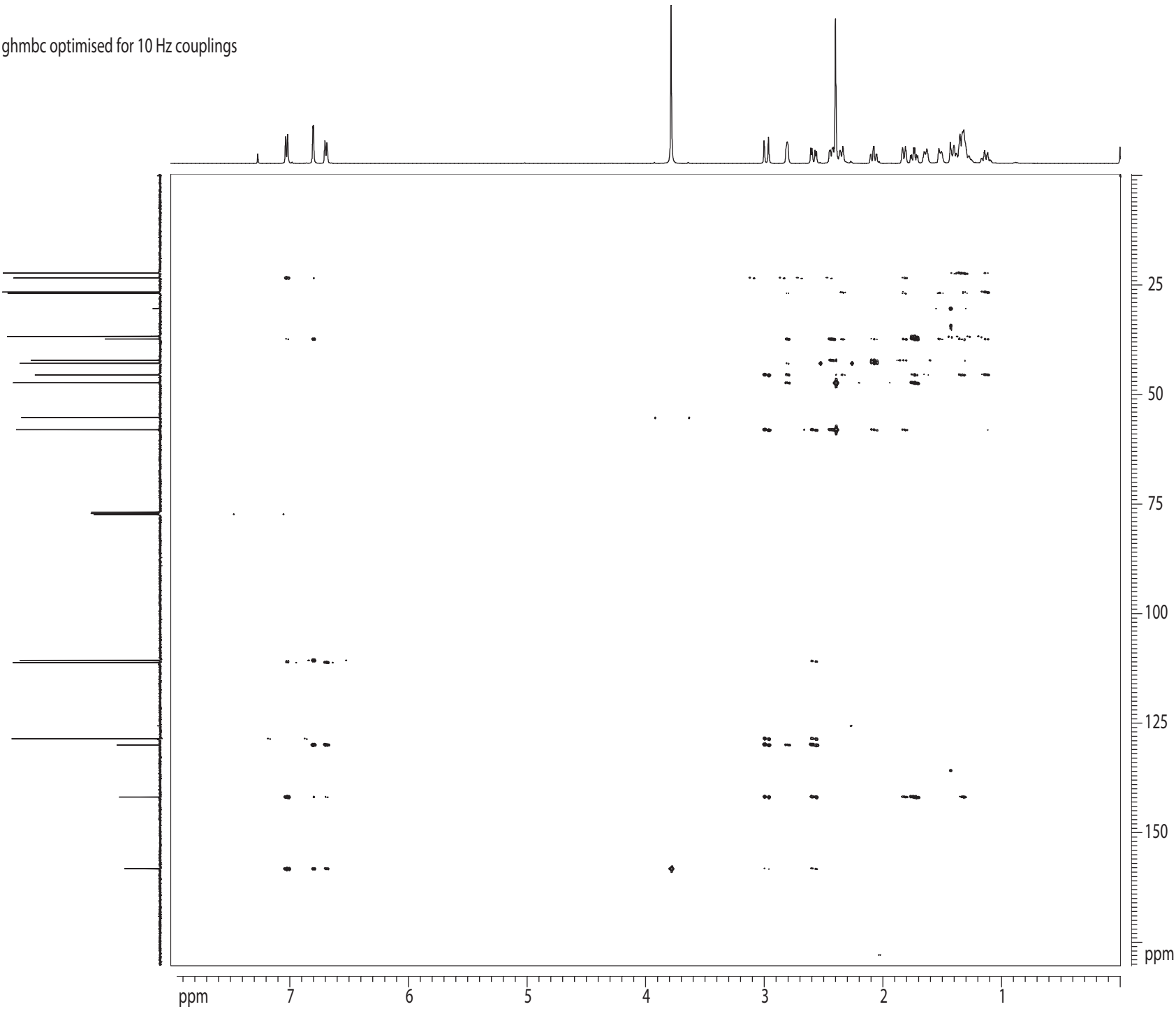
CX2 18.00 cm
CX1 15.00 cm
F2PLO 1.872 ppm
F2LO 936.46 Hz
F2PHI 0.949 ppm
F2HI 474.79 Hz
F1PLO 27.535 ppm
F1LO 3463.34 Hz
F1PHI 25.947 ppm
F1HI 3263.59 Hz
F2PPMCM 0.05127 ppm/cm
F2HZCM 25.64868 Hz/cm
F1PPMCM 0.10587 ppm/cm
F1HZCM 13.31676 Hz/cm

26

27

ppm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr13t
NAME Banana_Rama_2
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131205
Time 5:24
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 7298.2
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 0.00002200 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 125.7917392 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 125.7917 MHz
FIDRES 44.389206 Hz
SW 180.674 ppm
FnMODE undefined

F2 - Processing parameters

SI 2048
SF 500.2200276 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

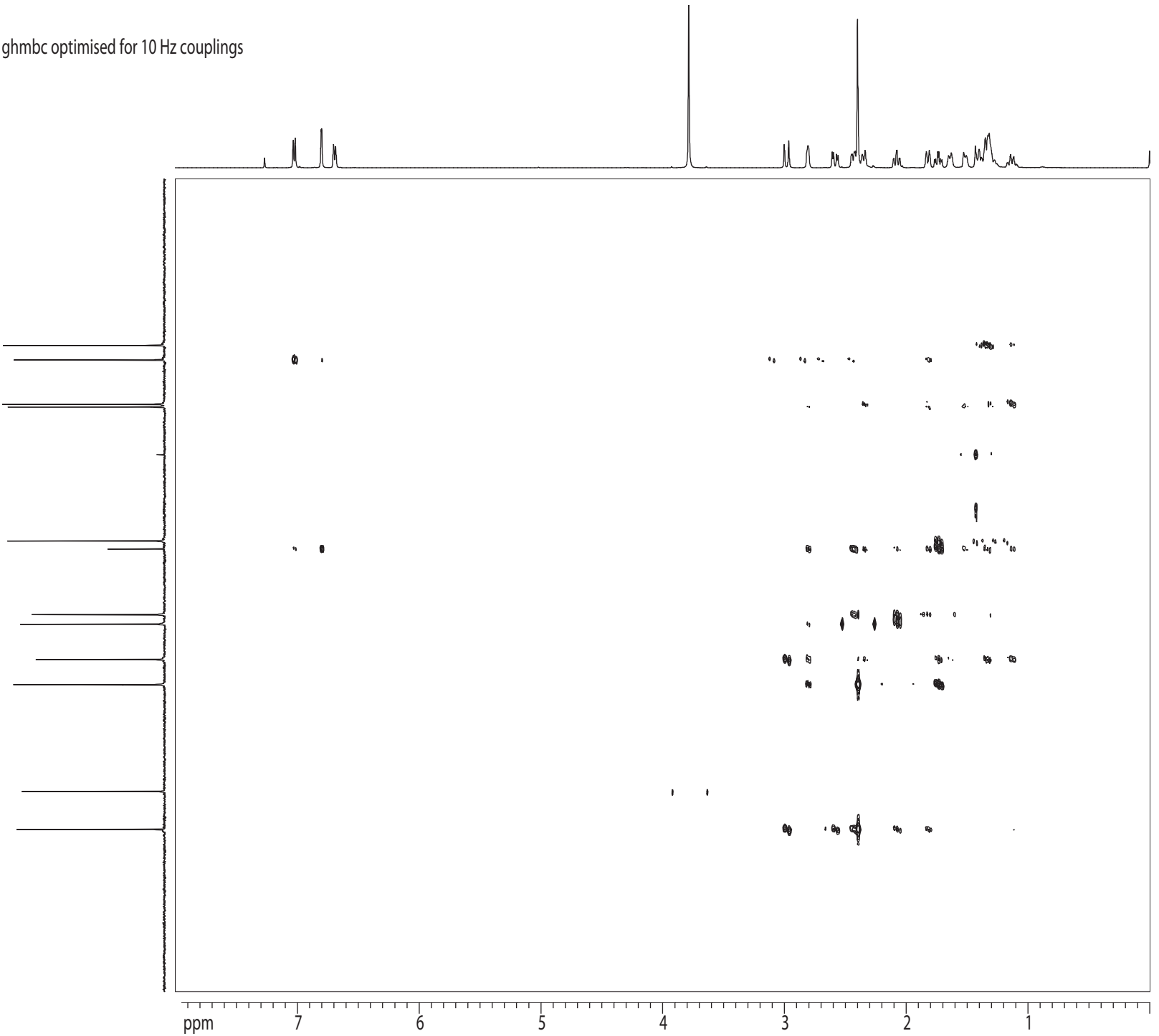
F1 - Processing parameters

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 180.345 ppm
F1LO 22683.87 Hz
F1PHI -0.345 ppm
F1HI 43.40 Hz
F2PPMCM 0.44496 ppm/cm
F2HZCM 222.57837 Hz/cm
F1PPMCM 12.04600 ppm/cm
F1HZCM 1515.15149 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr13t
NAME Banana_Rama_2
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131205
Time 5:24
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 7298.2
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.000000
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 0.00002200 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 125.7917392 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 125.7917 MHz
FIDRES 44.389206 Hz
SW 180.674 ppm
FnMODE undefined

F2 - Processing parameters

SI 2048
SF 500.2200276 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

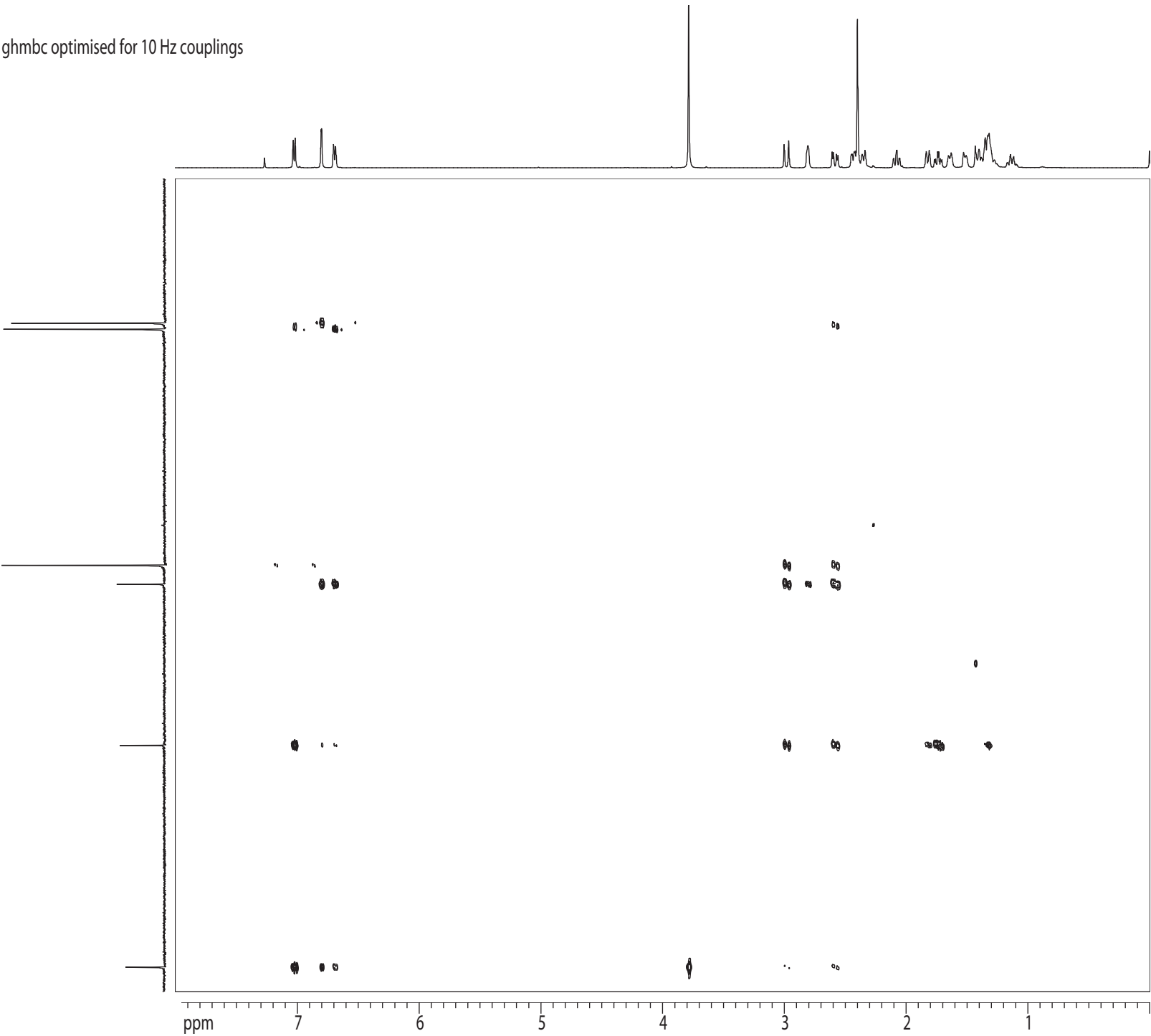
F1 - Processing parameters

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 8.005 ppm
F2LO 4004.08 Hz
F2PHI -0.005 ppm
F2HI -2.33 Hz
F1PLO 70.000 ppm
F1LO 8804.63 Hz
F1PHI 10.000 ppm
F1HI 1257.80 Hz
F2PPMCM 0.44496 ppm/cm
F2HZCM 222.57837 Hz/cm
F1PPMCM 4.00000 ppm/cm
F1HZCM 503.12167 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr13t
NAME Banana_Rama_2
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131205
Time 5:24
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 7298.2
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 0.00002200 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 125.7917392 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 125.7917 MHz
FIDRES 44.389206 Hz
SW 180.674 ppm
FnMODE undefined

F2 - Processing parameters

SI 2048
SF 500.2200276 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

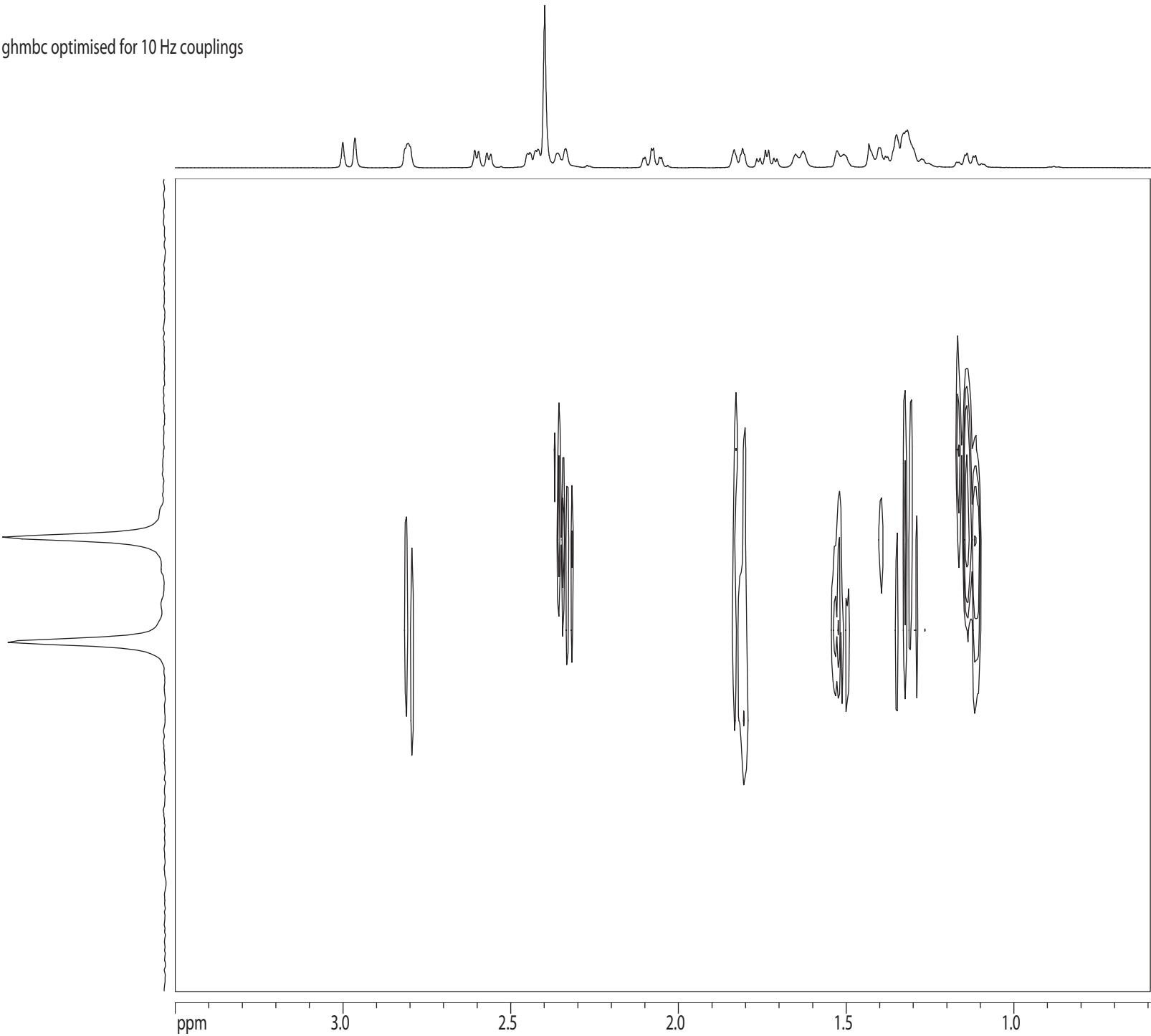
F1 - Processing parameters

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 8.005 ppm
F2LO 4004.08 Hz
F2PHI -0.005 ppm
F2HI -2.33 Hz
F1PLO 160.000 ppm
F1LO 20124.87 Hz
F1PHI 100.000 ppm
F1HI 12578.04 Hz
F2PPMCM 0.44496 ppm/cm
F2HZCM 222.57837 Hz/cm
F1PPMCM 4.00000 ppm/cm
F1HZCM 503.12167 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr13t
NAME Banana_Rama_2
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131205
Time 5:24
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 7298.2
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.000000
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 0.0002200 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 125.7917392 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 125.7917 MHz
FIDRES 44.389206 Hz
SW 180.674 ppm
FnMODE undefined

F2 - Processing parameters

SI 2048
SF 500.2200276 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

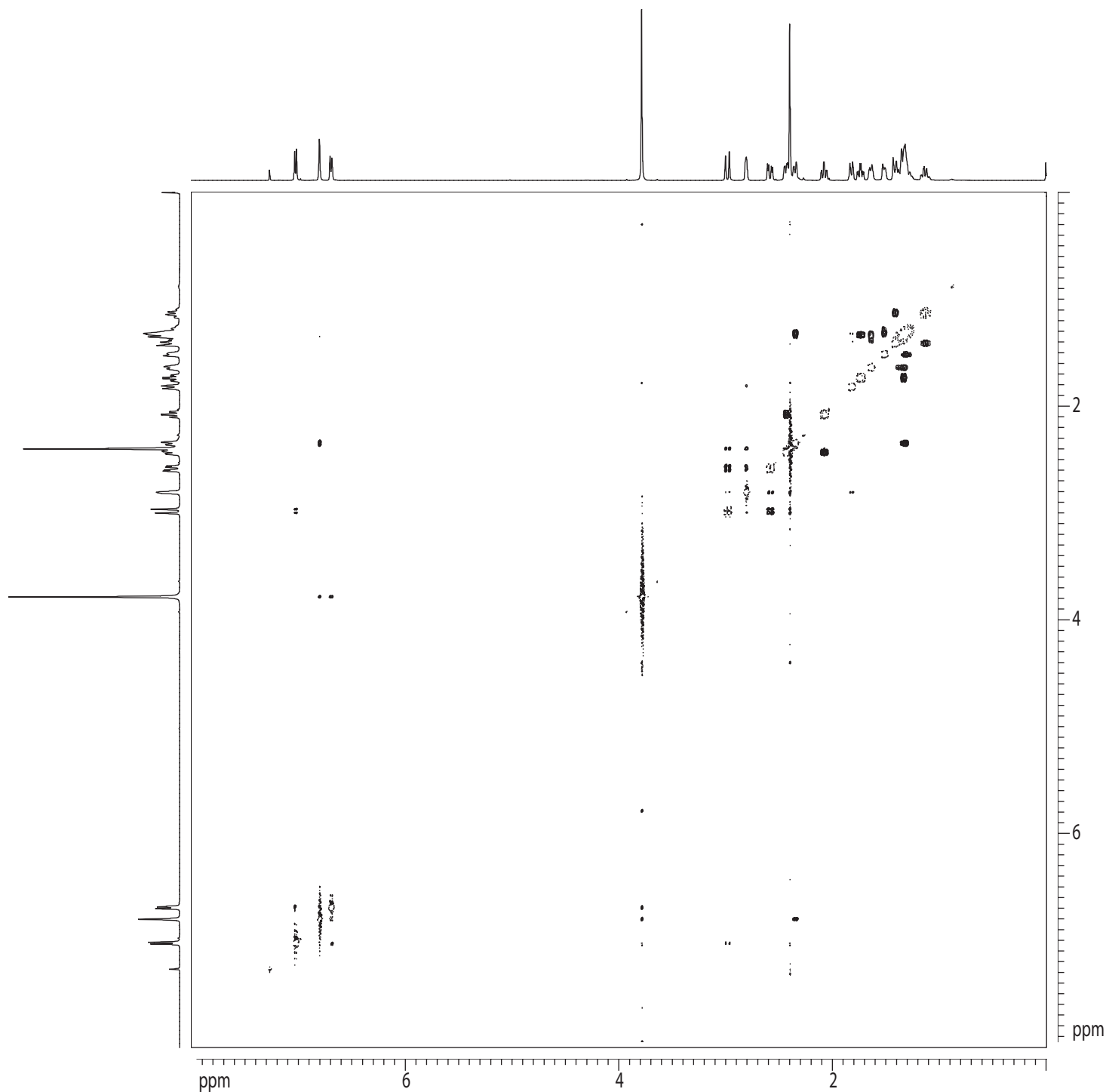
CY2 18.00 cm
CX1 15.00 cm
F2PLO 3.500 ppm
F2LO 1750.77 Hz
F2PHI 0.593 ppm
F2HI 296.77 Hz
F1PLO 27.535 ppm
F1LO 3463.34 Hz
F1PHI 25.947 ppm
F1HI 3263.59 Hz
F2PPMCM 0.16148 ppm/cm
F2HZCM 80.77792 Hz/cm
F1PPMCM 0.10587 ppm/cm
F1HZCM 13.31676 Hz/cm

26

27

ppm

noesy



Current Data Parameters
USER nmr13t
NAME Banana_Rama_2
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131205
Time 0.11
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 3.2
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

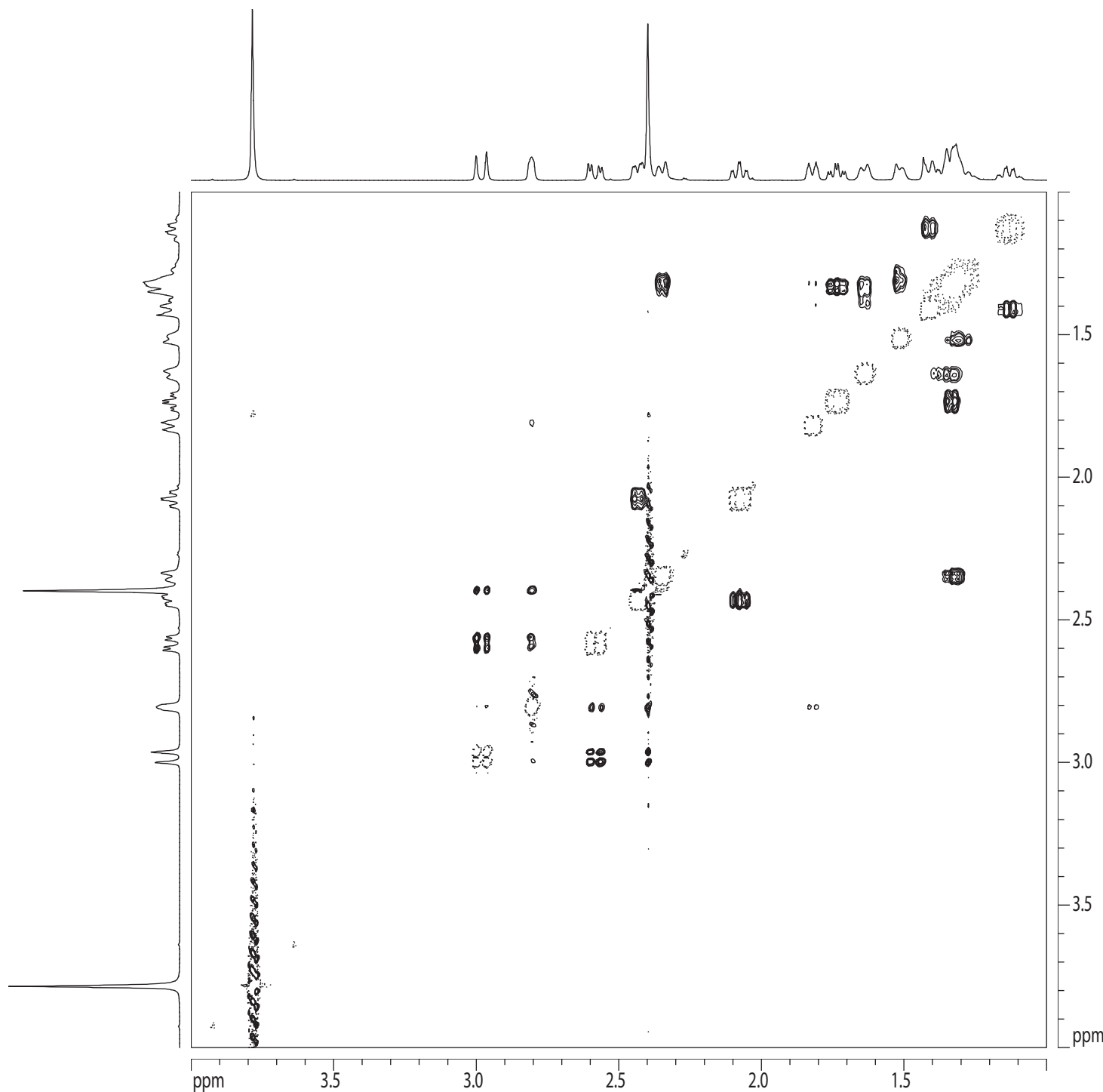
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 500.222 MHz
FIDRES 7.825020 Hz
SW 8.009 ppm
FnMODE undefined

F2 - Processing parameters
SI 1024
SF 500.2200276 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 TPPI
SF 500.2200276 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 Banana_Rama_2
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131205
 Time 0.11
 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 3.2
 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 500.2200276 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 TPPI
 SF 500.2200276 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

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