

Name: _____

Chem 203
December 14, 2013

Final Exam Part I
(40 points + 5 points extra credit)

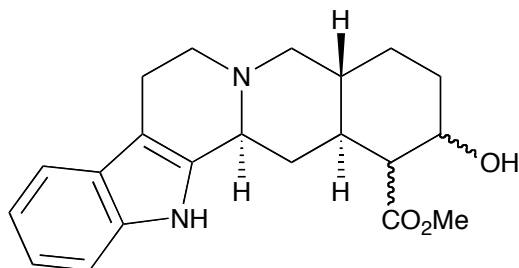
**THIS FINAL EXAM CONSISTS OF PART I
AND TWO OUT OF THE THREE PROBLEMS FROM PART II**

**IF THREE PROBLEMS FROM PART II ARE SUBMITTED,
ONLY THE FIRST TWO (Part II, PROBLEMS 1-2) WILL BE GRADED**

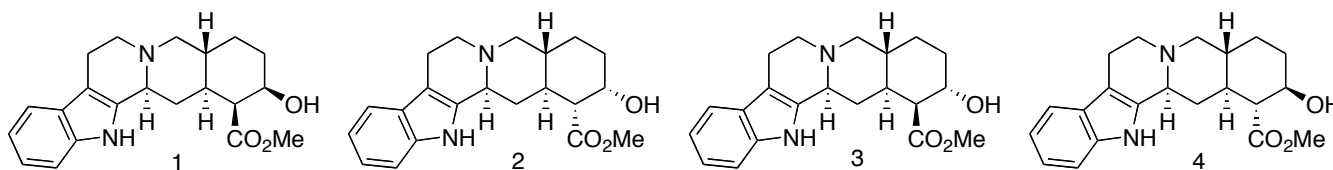
If you wish to unstaple the pages, please initial each page.

Books, notes, lecture videos, calculators, rulers, and laptop computers are permitted as is wireless (or wired) internet access and appropriate software (e.g, PyMOL, Maestro/MacroModel, Excel, ChemDoodle, Chemdraw, ElComp, MolE, etc.). Communication with other students by e-mail, text, or in person is not permitted. 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. INAPPROPRIATE COMMUNICATION OR 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.

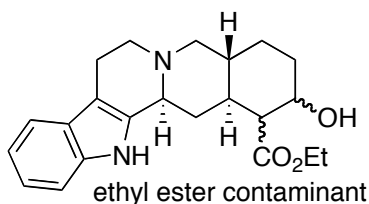
The following spectral data are provided for a pentacyclic compound: 500 MHz ^1H NMR, 125.8 MHz ^{13}C NMR, DEPT, COSY, TOCSY (20 ms mixing time), HMQC, HMBC, NOESY, and HSQC-TOCSY spectra with 5-, 10-, 25-, and 50-ms mixing times. All NMR spectra were measured in CDCl_3 solution.



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

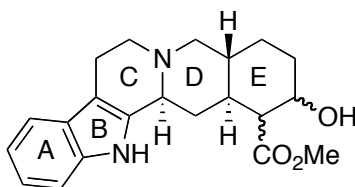


NOTE: The compound, which is a methyl ester, is contaminated with about 20 mol % of the ethyl ester. The spectrum of the ethyl ester is virtually identical, except that there are resonances for the CO_2Et group, and resonance a is slightly shifted.



a. Build energy-minimized molecular models of diastereomers **1**, **2**, **3**, and **4** using PyMOL and the "clean" function. Rotate each molecule into an appropriate orientation. Use the side menu (S) to show each molecule as sticks (Show-sticks). Use the pulldown menu to display each molecule in maximum quality with (Display-Quality-Maximum Quality). Save the .pse files as diastereomer1.pse, diastereomer2.pse, diastereomer3.pse, and diastereomer4.pse.

NOTE: The C, D, and E rings adopt stable *trans*-decalin type conformations.

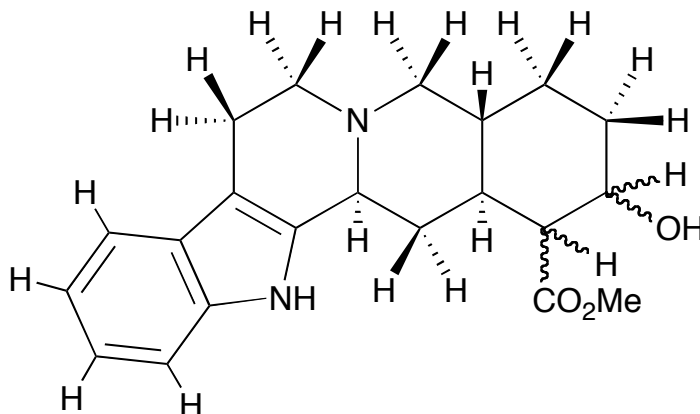


E-mail the .pse files to me (jsnowick@uci.edu).

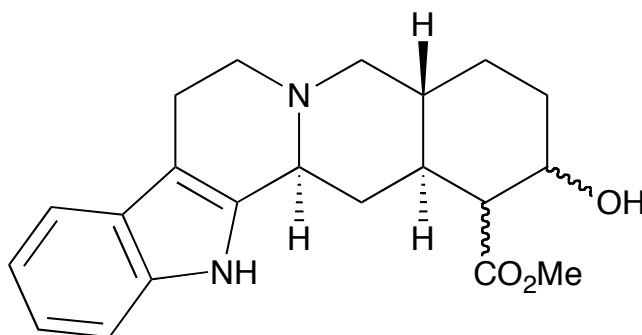
b. Determine the stereochemistry of the molecule. Which diastereomer is it? _____

Explain how you determined the stereochemistry of the molecule. Make a conformationally realistic drawing of the molecule to help aid in your explanation. If there are any aspects of the stereochemistry you are uncertain about, please include this in your explanation.

c. Insofar as possible, assign the ^1H resonances to the corresponding atoms in the structure, below. That is, write the letter (a–r) next to the atom in the structure below. You may not be able to assign them all. Explain briefly about those that you are uncertain.

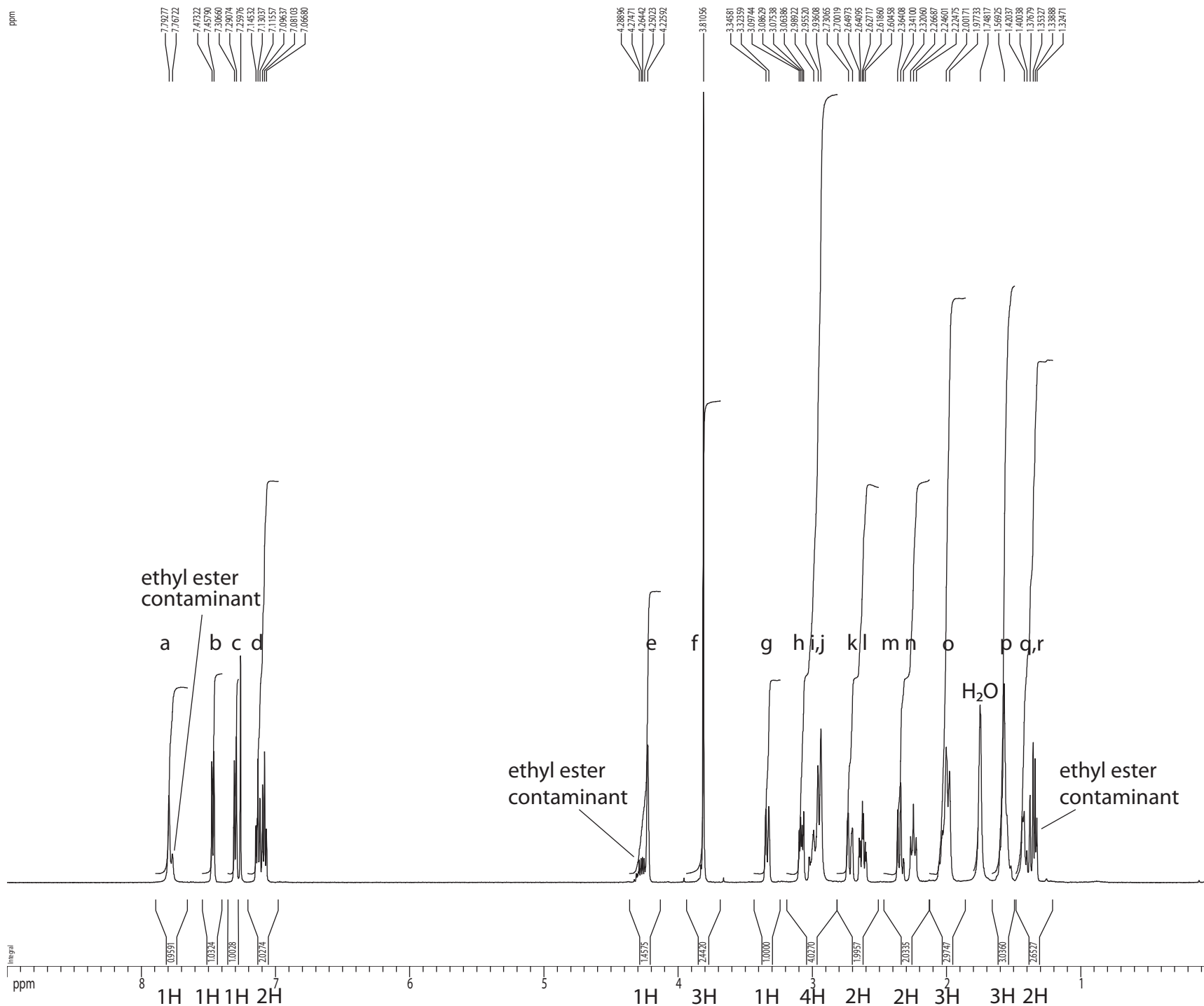


d. Insofar as possible, assign the ^{13}C resonances to the corresponding atoms in the structure, below. That is, write the number (1–21) next to the atom in the structure below. You may not be able to assign them all. Explain briefly about those that you are uncertain.



EXTRA CREDIT (5 points). Build an energy-minimized model of the correct diastereomer using Maestro/MacroModel with the MMFF force field. E-mail me (jsnowick@uci.edu) the -out.maegz file associated with that model.

¹H spectrum



Current Data Parameters
 USER nmr13t
 NAME Apple_pie_2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131206
 Time 1924
 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 5
 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 =====
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 P1 7.50 usec
 PL1 1.60 dB
 SF01 500.2235015 MHz

F2 - Processing parameters
 SI 65536
 SF 500.2200309 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 FIP 9.000 ppm
 F1 4501.98 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 0.39474 ppm/cm
 HZCM 197.45528 Hz/cm

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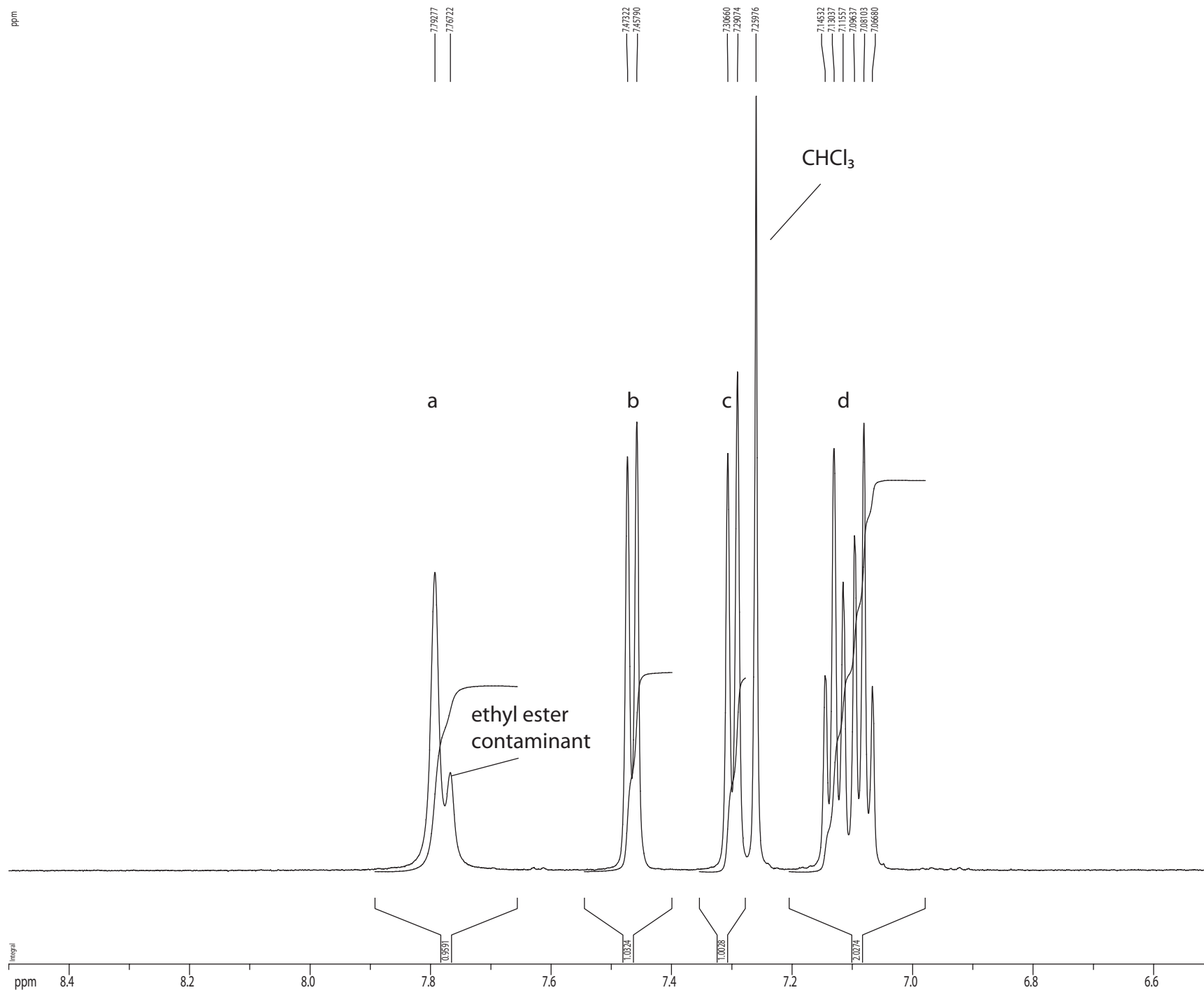
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2	29376.4	3885.318	7.7672	0.62
3	30579.2	3738.252	7.4732	2.37
4	30641.9	3730.592	7.4579	2.56
5	31260.9	3654.909	7.3066	2.39
6	31325.8	3646.974	7.2907	2.84
7	31452.5	3631.476	7.2598	4.38
8	31920.7	3574.233	7.1453	1.16
9	31981.9	3566.756	7.1304	2.41
10	32042.4	3559.351	7.1156	1.68
11	32121.0	3549.744	7.0964	1.93
12	32183.8	3542.072	7.0810	2.55
13	32242.0	3534.956	7.0668	1.10
14	43606.8	2145.421	4.2890	0.51
15	43665.1	2138.294	4.2747	0.54
16	43707.2	2133.150	4.2644	0.56
17	43765.2	2126.050	4.2502	0.54
18	43864.7	2113.888	4.2259	2.68
19	45564.0	1906.120	3.8106	15.00
20	47465.5	1673.641	3.3458	1.47
21	47556.4	1662.524	3.3236	1.52
22	48481.6	1549.401	3.0974	1.06
23	48527.2	1543.826	3.0863	1.32
24	48571.9	1538.364	3.0754	1.16
25	48619.0	1532.602	3.0639	1.42
26	48924.3	1495.268	2.9892	1.07
27	49063.5	1478.251	2.9552	2.29
28	49141.8	1468.683	2.9361	2.98
29	49982.2	1365.926	2.7306	1.39
30	50106.8	1350.689	2.7002	1.11
31	50313.3	1325.448	2.6497	0.92
32	50349.2	1321.056	2.6409	0.87
33	50405.6	1314.160	2.6272	1.62
34	50440.7	1309.874	2.6186	1.39
35	50498.0	1302.861	2.6046	0.85
36	51482.0	1182.559	2.3641	1.46
37	51576.4	1171.016	2.3410	1.96
38	51659.8	1160.810	2.3206	0.53
39	51879.7	1133.933	2.2669	0.95
40	51965.0	1123.496	2.2460	1.56
41	52052.0	1112.865	2.2248	0.93
42	52964.5	1001.293	2.0017	2.64
43	53064.2	989.100	1.9773	2.19
44	54001.8	874.468	1.7482	3.43
45	54733.8	784.968	1.5692	3.83
46	55342.9	710.496	1.4204	1.43
47	55424.7	700.497	1.4004	0.69
48	55521.2	688.697	1.3768	1.73
49	55617.4	676.931	1.3533	2.73

50	55676.3	669.732	1.3389	2.42
51	55734.3	662.646	1.3247	1.30
52	61155.1	-0.133	-0.0003	8.40

¹H spectrum

ppm



Current Data Parameters
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 NAME Apple_pie_2
 EXPNO 1
 PROCNO 1

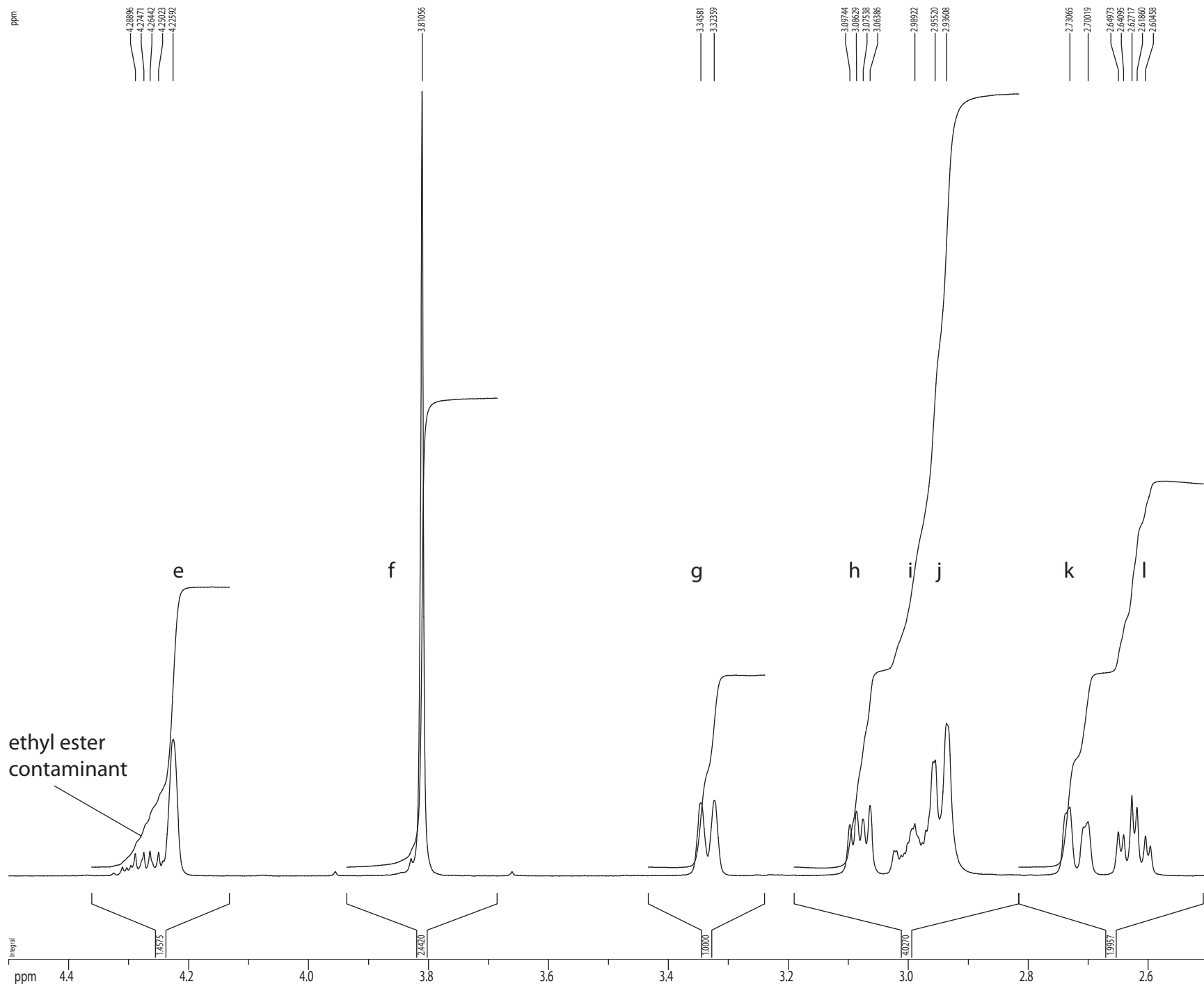
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 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 5
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
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 PL1 1.60 dB
 SFO1 500.2235015 MHz

F2 - Processing parameters
 SI 65536
 SF 500.2200309 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 8.500 ppm
 F1 4251.87 Hz
 F2P 6.500 ppm
 F2 3251.43 Hz
 PPMCM 0.08772 ppm/cm
 HZCM 43.87895 Hz/cm

¹H spectrum



Current Data Parameters
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 EXPNO 1
 PROCNO 1

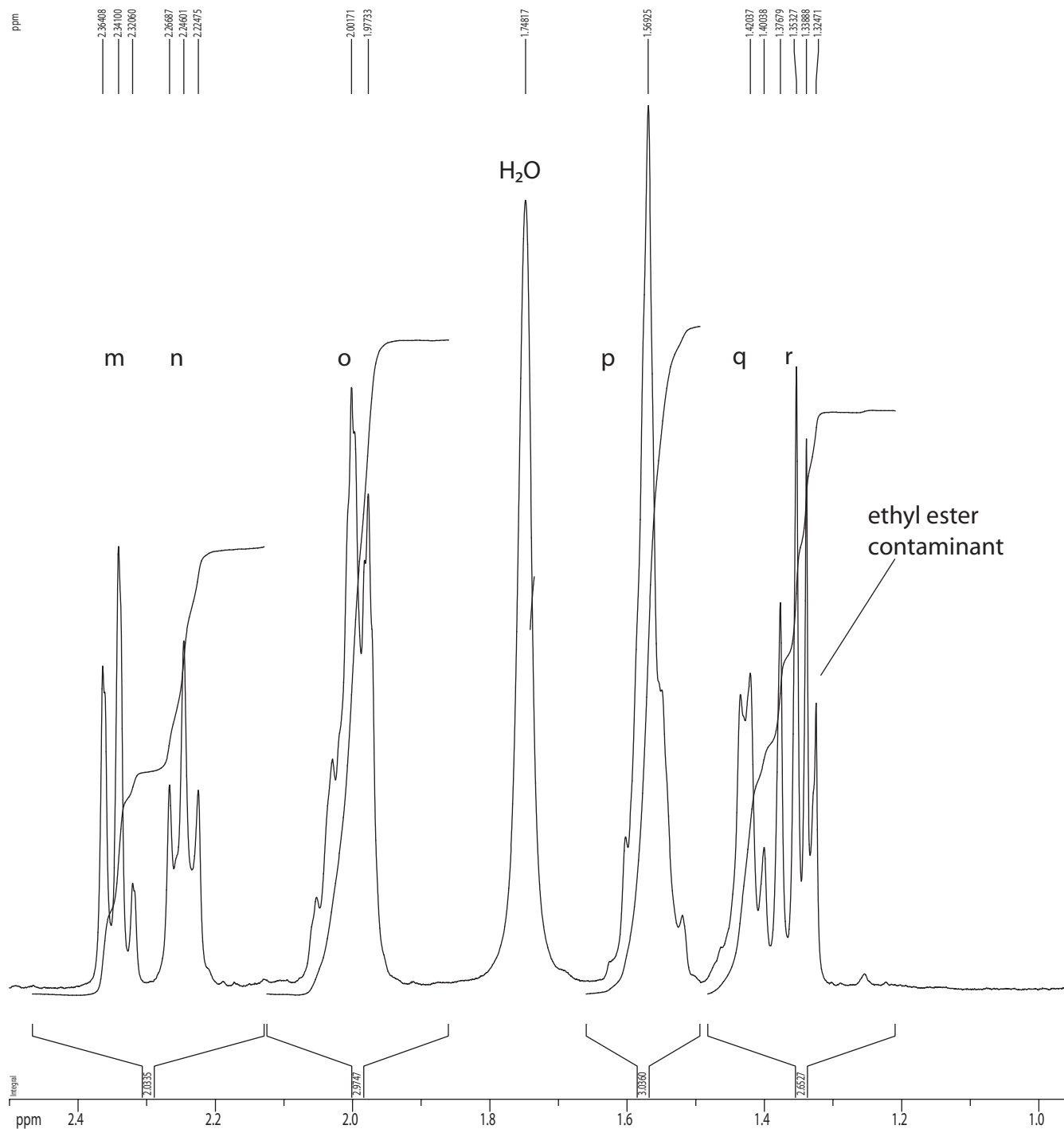
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 Date_ 20131206
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 TD 81728
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 5
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
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 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.2235015 MHz

F2 - Processing parameters
 SI 65536
 SF 500.2200309 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 4.500 ppm
 F1 2250.99 Hz
 F2P 2.500 ppm
 F2 1250.55 Hz
 PPMCM 0.08772 ppm/cm
 HZCM 43.87895 Hz/cm

1H spectrum



Current Data Parameters
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 EXPNO 1
 PROCNO 1

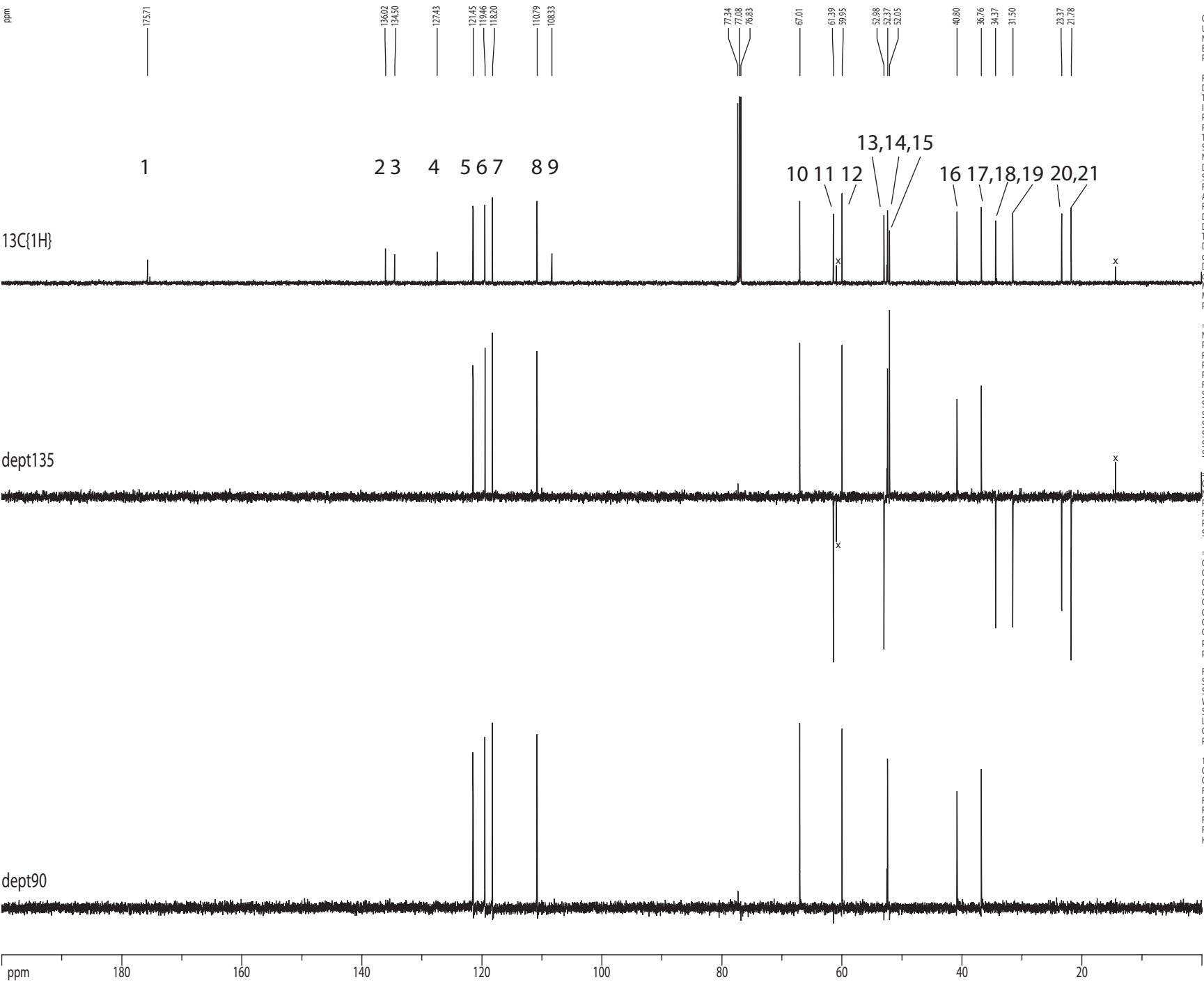
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 TD 81728
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 5
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 DT 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

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

F2 - Processing parameters
 SI 65536
 SF 500.2200309 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 2.500 ppm
 F1 1250.55 Hz
 F2P 0.500 ppm
 F2 250.11 Hz
 PPMCM 0.08772 ppm/cm
 HZCM 43.87895 Hz/cm

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



Current Data Parameters
USER nmrl3t
NAME Apple_ple_2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131206
Time 19.30
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PULPROG SpinEchopg30gp.prd
TD 65536
SOLVENT CDCl3
NS 376
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

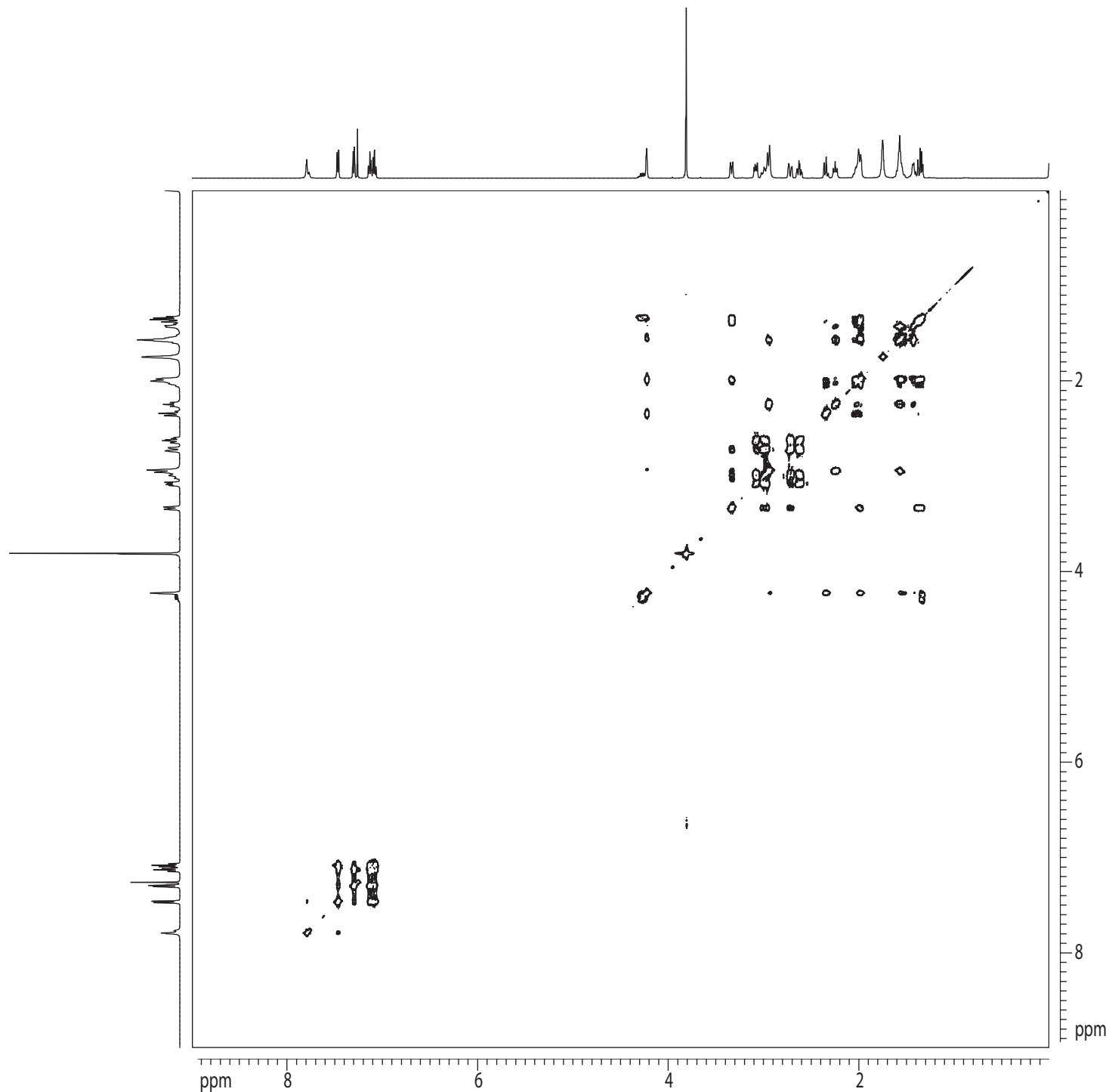
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PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
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
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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
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NAME Apple_pie_2
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
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Time 19:49
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PULPROG cosygp60.prd
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 4496.403 Hz
FIDRES 2.195509 Hz
AQ 0.2277876 sec
RG 5
DW 111.200 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 0.00022240 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.222510 MHz

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

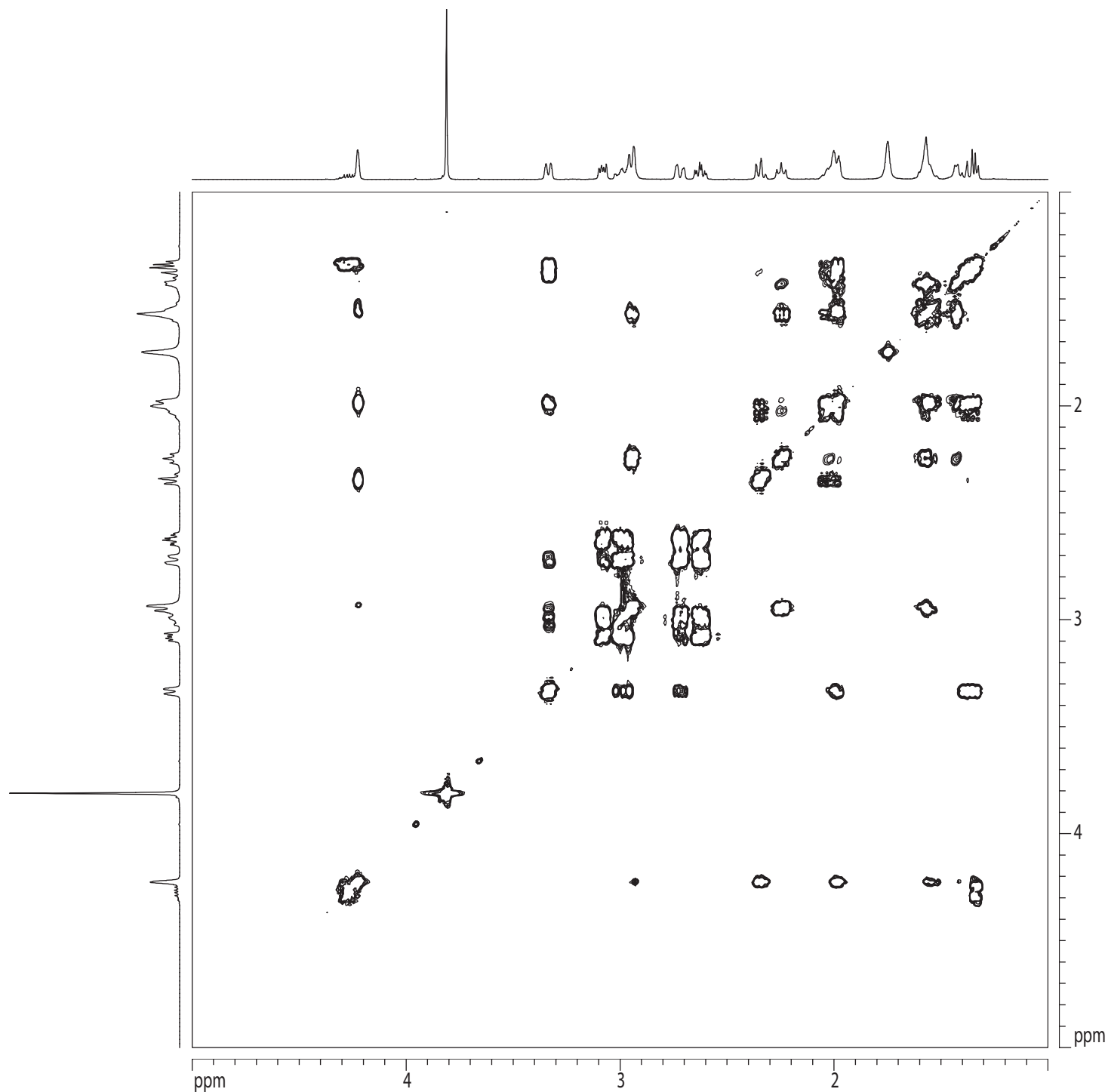
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SF 500.2200309 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.2200309 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 8.994 ppm
F2LO 4499.19 Hz
F2PHI 0.006 ppm
F2HI 2.79 Hz
F1PLO 8.994 ppm
F1LO 4499.19 Hz
F1PHI 0.006 ppm
F1HI 2.79 Hz
F2PPMCM 0.59926 ppm/cm
F2HZCM 299.76022 Hz/cm
F1PPMCM 0.59926 ppm/cm
F1HZCM 299.76022 Hz/cm

gcosy60



Current Data Parameters
 USER nmr13t
 NAME Apple_pie_2
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131206
 Time 19:49
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 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 4496.403 Hz
 FIDRES 2.195509 Hz
 AQ 0.2277876 sec
 RG 5
 DW 111.200 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 0.00022240 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.222510 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

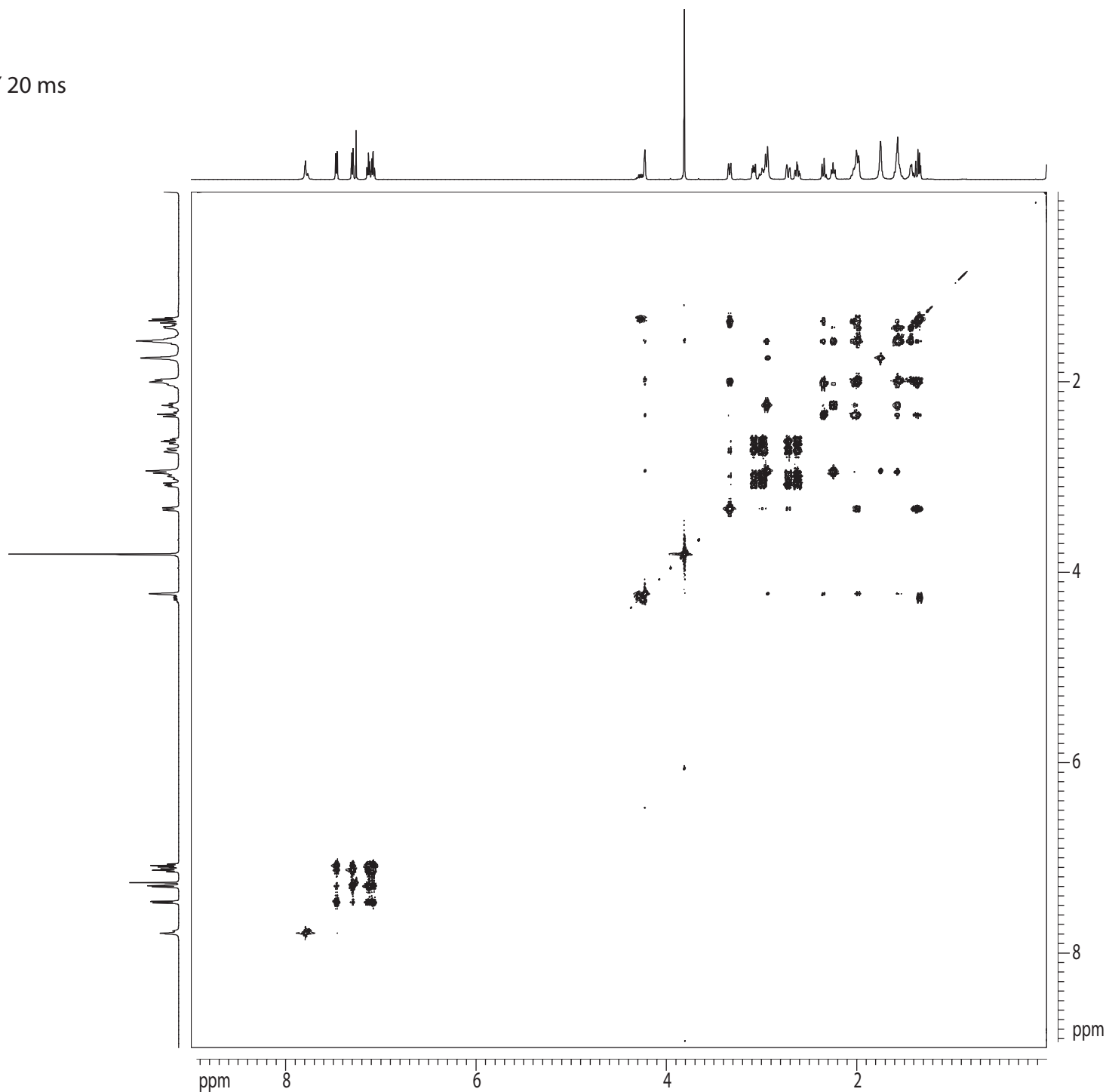
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 FIDRES 8.782037 Hz
 SW 8.989 ppm
 FhMODE undefined

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 SF 500.2200309 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 500.2200309 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.000 ppm
 F2LO 2501.10 Hz
 F2PHI 1.000 ppm
 F2HI 500.22 Hz
 F1PLO 5.000 ppm
 F1LO 2501.10 Hz
 F1PHI 1.000 ppm
 F1HI 500.22 Hz
 F2PPMCM 0.26667 ppm/cm
 F2HZCM 133.39201 Hz/cm
 F1PPMCM 0.26667 ppm/cm
 F1HZCM 133.39201 Hz/cm

TOCSY 20 ms



Current Data Parameters
 USER nmr13t
 NAME Apple_pie_2
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
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 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 4496.403 Hz
 FIDRES 2.195509 Hz
 AQ 0.2277876 sec
 RG 5
 DW 111.200 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 2.00000000 sec
 d8 0.02084341 sec
 d12 0.00002000 sec
 INO 0.00011120 sec
 L1 7

===== 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 500.2222510 MHz

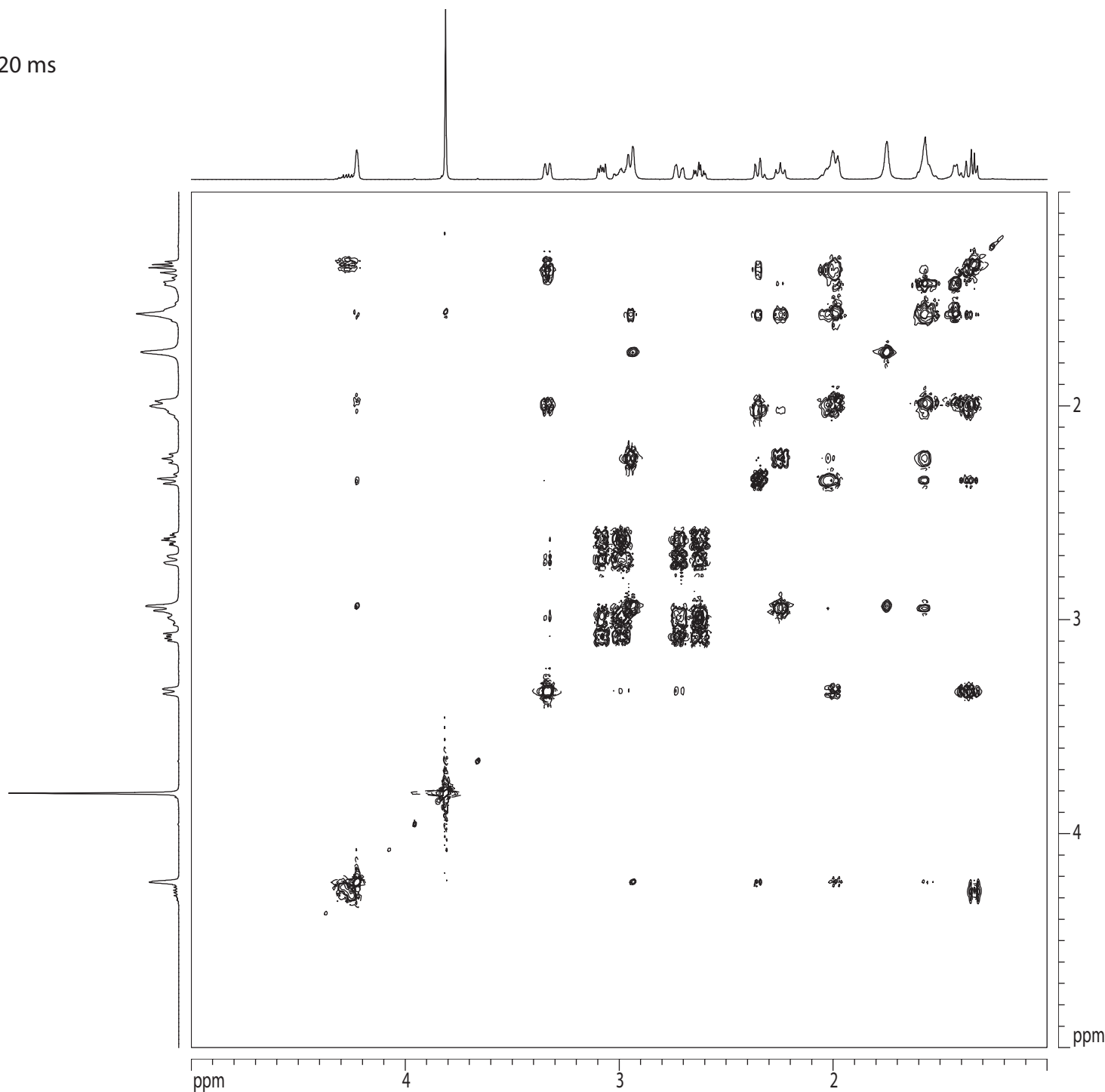
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 FIDRES 8.782037 Hz
 SW 8.989 ppm
 FnMODE undefined

F2 - Processing parameters
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 SF 500.2200309 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0
 PC 4.00

F1 - Processing parameters
 SI 1024
 MC2 TPPI
 SF 500.2200309 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
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 F2LO 4499.19 Hz
 F2PHI 0.006 ppm
 F2HI 2.79 Hz
 F1PLO 8.994 ppm
 F1LO 4499.19 Hz
 F1PHI 0.006 ppm
 F1HI 2.79 Hz
 F2PPMCM 0.59926 ppm/cm
 F2HZCM 299.76022 Hz/cm
 F1PPMCM 0.59926 ppm/cm
 F1HZCM 299.76022 Hz/cm

TOCSY 20 ms



Current Data Parameters
 USER nmr13t
 NAME Apple_pie_2
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131206
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 PROBHD 5 mm CPTCI 1H-
 PULPROG tocsytp.wu
 TD 2048
 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 4496.403 Hz
 FIDRES 2.195509 Hz
 AQ 0.2277876 sec
 RG 5
 DW 111.200 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 2.00000000 sec
 d8 0.02084341 sec
 d12 0.00002000 sec
 INO 0.00011120 sec
 L1 7

===== 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 500.2222510 MHz

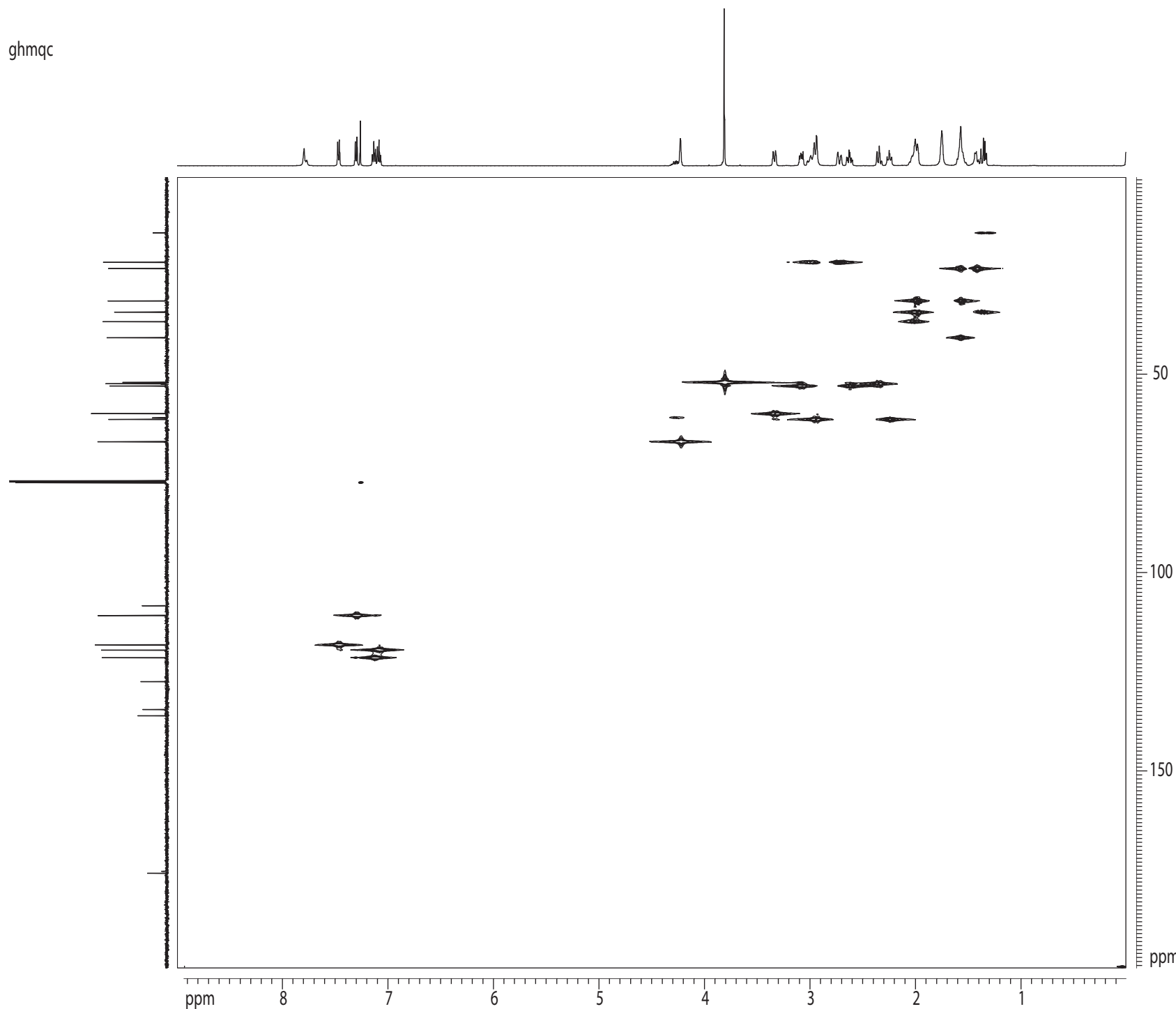
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 TD 512
 SFO1 500.2223 MHz
 FIDRES 8.782037 Hz
 SW 8.989 ppm
 FnMODE undefined

F2 - Processing parameters
 SI 1024
 SF 500.2200309 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0
 PC 4.00

F1 - Processing parameters
 SI 1024
 MC2 TPPI
 SF 500.2200309 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.000 ppm
 F2LO 2501.10 Hz
 F2PHI 1.000 ppm
 F2HI 500.22 Hz
 F1PLO 5.000 ppm
 F1LO 2501.10 Hz
 F1PHI 1.000 ppm
 F1HI 500.22 Hz
 F2PPMCM 0.26667 ppm/cm
 F2HZCM 133.39201 Hz/cm
 F1PPMCM 0.26667 ppm/cm
 F1HZCM 133.39201 Hz/cm

ghmqc



Current Data Parameters

USER nmrl3t
NAME Apple_ple_2
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131207
Time 3.38
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG inv4gpcw
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 4496.403 Hz
FIDRES 2.195509 Hz
AQ 0.2277876 sec
RG 11585.2
DW 111.200 usec
DE 6.50 usec
TE 298.0 K
CHST2 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 0.00001995 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2222510 MHz

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

CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7929970 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 125.793 MHz
FIDRES 48.950500 Hz
SIW 199.237 ppm
FnMODE undefined

F2 - Processing parameters

SI 1024
SF 500.2200309 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

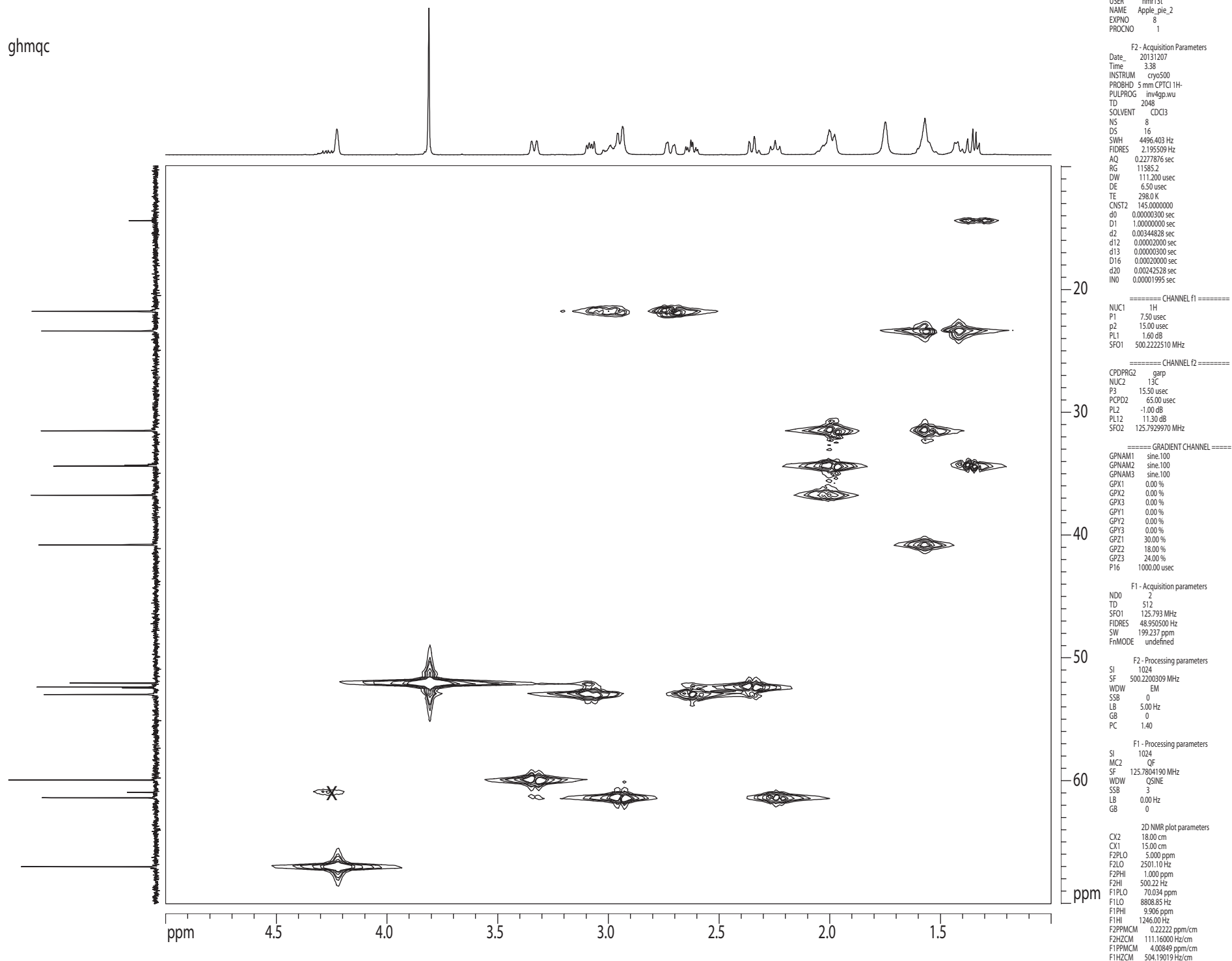
F1 - Processing parameters

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

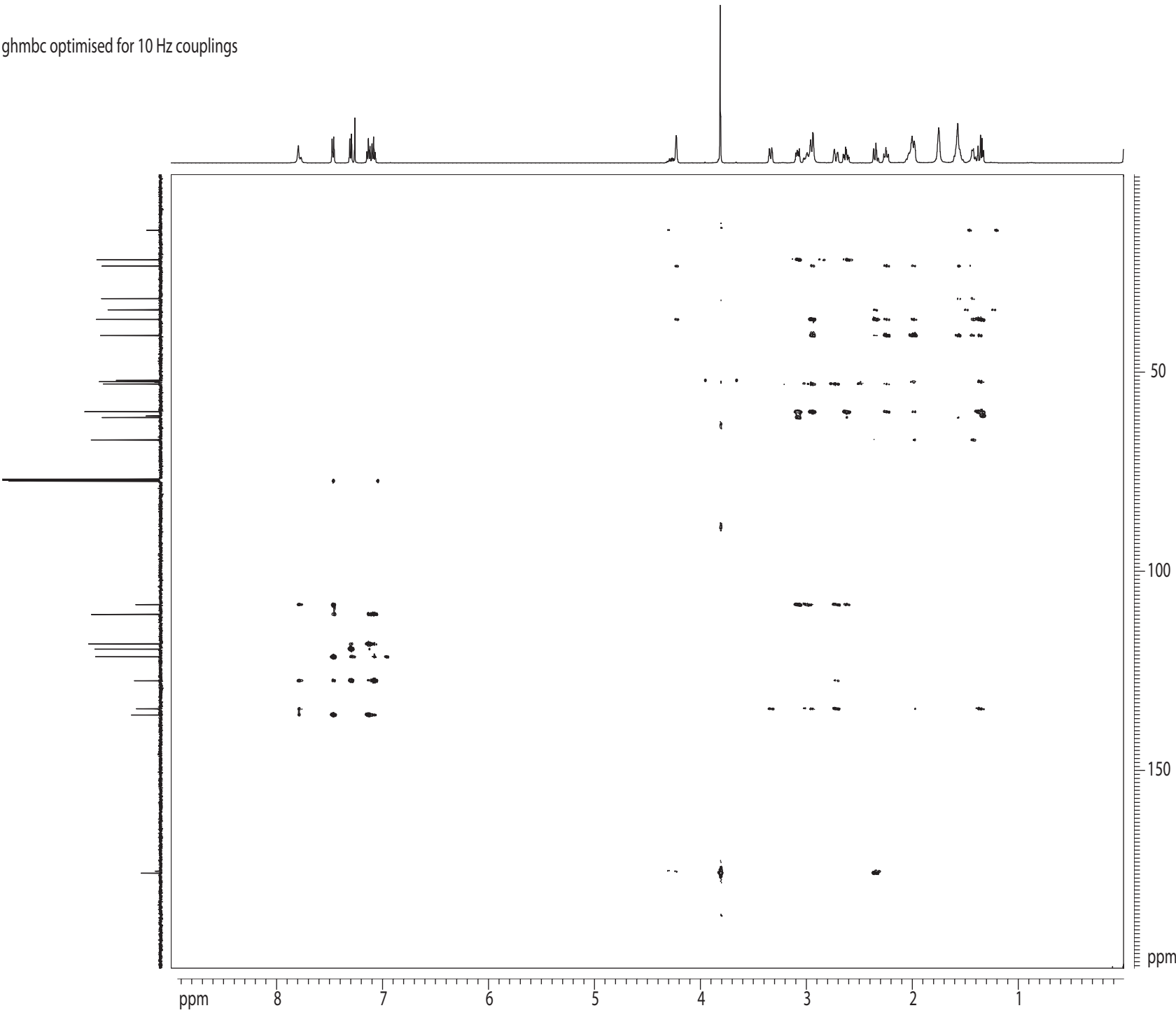
2D NMR plot parameters

CX2 18.00 cm
CX1 15.00 cm
F2PLO 8.994 ppm
F2LO 4499.19 Hz
F2PHI 0.006 ppm
F2HI 2.79 Hz
F1PLO 199.629 ppm
F1LO 25109.37 Hz
F1PHI 0.371 ppm
F1HI 46.71 Hz
F2PPMCM 0.49938 ppm/cm
F2HZCM 249.80017 Hz/cm
F1PPMCM 13.28382 ppm/cm
F1HZCM 1670.84387 Hz/cm

ghmqc



ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr13t
NAME Apple_pie_2
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131207
Time 5:04
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT CDCl3
NS 8
DS 16
SWH 4496.403 Hz
FIDRES 1.097755 Hz
AQ 0.455252 sec
RG 14596.5
DW 111.200 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 0.0001995 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2222510 MHz

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

NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7929970 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 125.793 MHz
FIDRES 48.950500 Hz
SW 199.237 ppm
FnMODE undefined

F2 - Processing parameters

SI 2048
SF 500.2200309 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

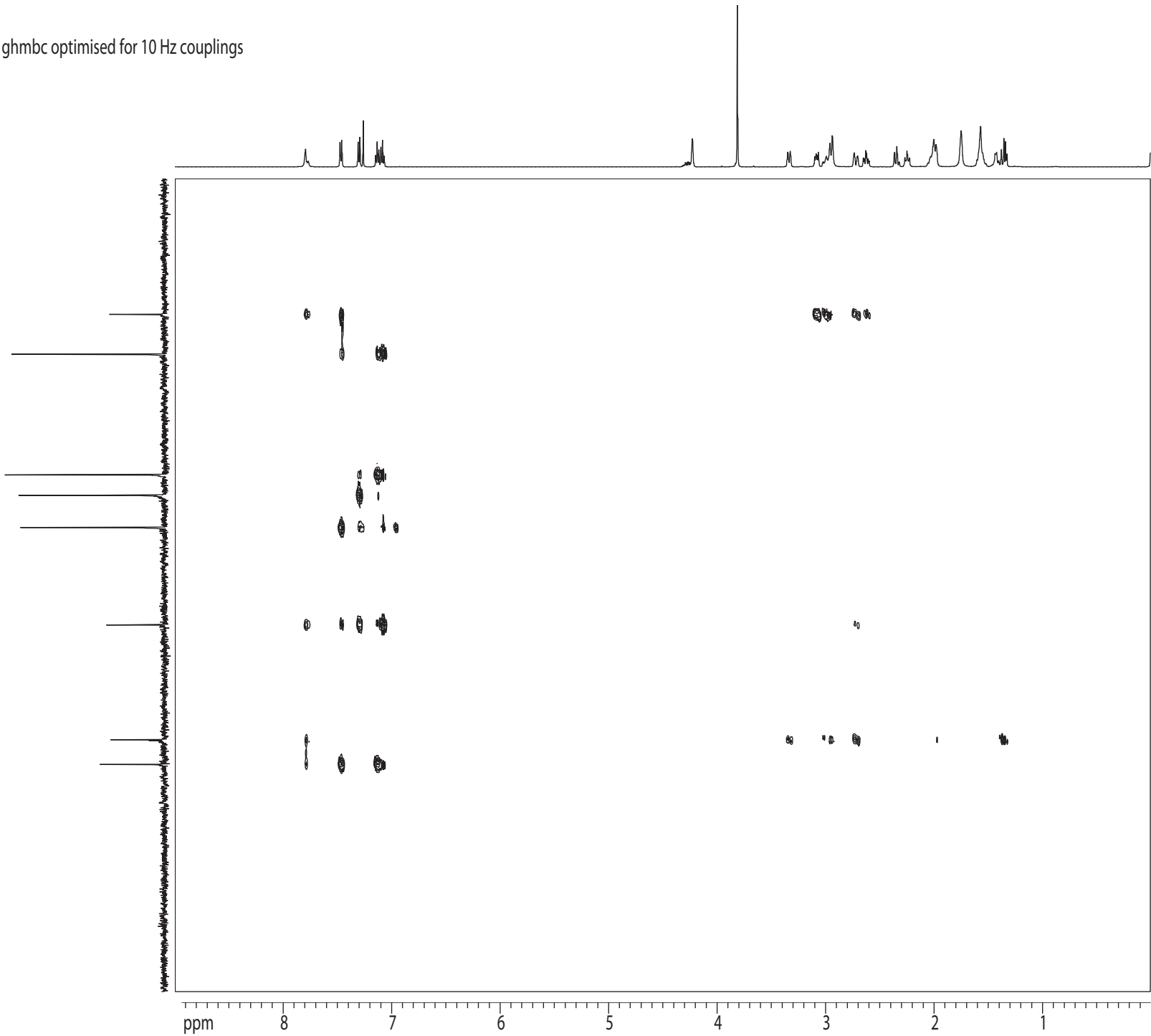
F1 - Processing parameters

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 8.994 ppm
F2LO 4499.19 Hz
F2PHI 0.006 ppm
F2HI 2.79 Hz
F1PLO 199.629 ppm
F1LO 25109.37 Hz
F1PHI 0.371 ppm
F1HI 46.71 Hz
F2PPMCM 0.49938 ppm/cm
F2HZCM 249.80017 Hz/cm
F1PPMCM 13.28382 ppm/cm
F1HZCM 1670.84387 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr13t
NAME Apple_pie_2
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131207
Time 5:04
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT CDCl3
NS 8
DS 16
SWH 4496.403 Hz
FIDRES 1.097755 Hz
AQ 0.455252 sec
RG 145965
DW 111.200 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
INO 0.0001995 sec

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

110 NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2222510 MHz

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

120 NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7929970 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

130 ND0 2
TD 512
SFO1 125.793 MHz
FIDRES 48.950500 Hz
SW 199.237 ppm
FnMODE undefined

F2 - Processing parameters

SI 2048
SF 500.2200309 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

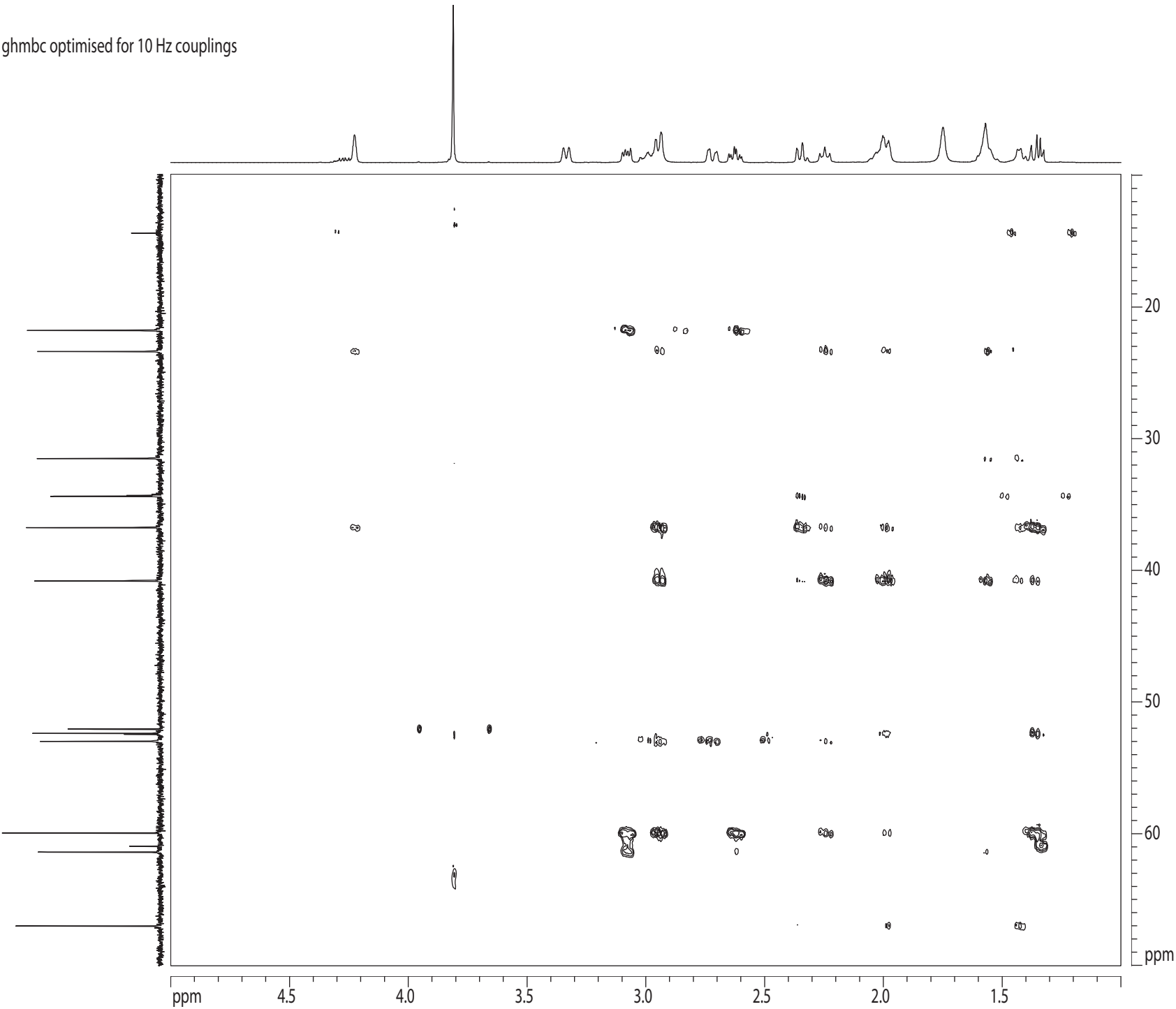
F1 - Processing parameters

140 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 8.994 ppm
F2LO 4499.19 Hz
F2PHI 0.006 ppm
F2HI 2.79 Hz
F1PLO 150.000 ppm
F1LO 18867.06 Hz
F1PHI 100.000 ppm
F1HI 12578.04 Hz
F2PPMCM 0.49938 ppm/cm
F2HZCM 249.80017 Hz/cm
F1PPMCM 3.33333 ppm/cm
F1HZCM 419.26807 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr13t
NAME Apple_pie_2
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131207
Time 5:04
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT CDCl3
NS 8
DS 16
SWH 4496.403 Hz
FIDRES 1.097755 Hz
AQ 0.455252 sec
RG 145965
DW 111.200 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
INO 0.0001995 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2222510 MHz

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

NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7929970 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 125.793 MHz
FIDRES 48.950500 Hz
SW 199.237 ppm
FnMODE undefined

F2 - Processing parameters

SI 2048
SF 500.2200309 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

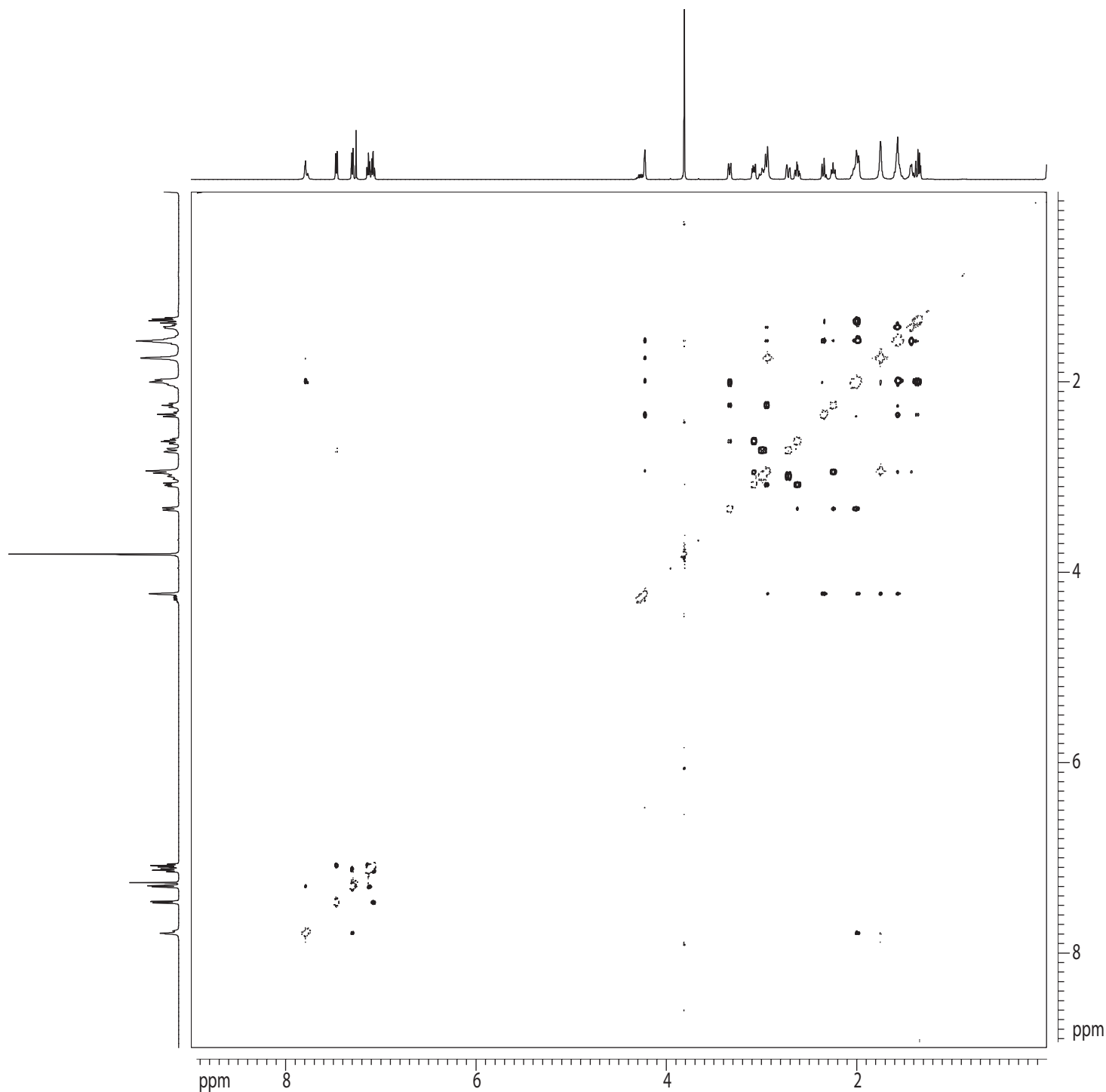
F1 - Processing parameters

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 5.000 ppm
F2LO 2501.10 Hz
F2PHI 1.000 ppm
F2HI 500.22 Hz
F1PLO 70.034 ppm
F1LO 8808.85 Hz
F1PHI 9.906 ppm
F1HI 1246.00 Hz
F2PPMCM 0.2222 ppm/cm
F2HZCM 111.16000 Hz/cm
F1PPMCM 4.00849 ppm/cm
F1HZCM 504.19019 Hz/cm

noesy



Current Data Parameters
 USER nmr13t
 NAME Apple_pie_2
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131206
 Time 23.55
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG noesyrvtp
 TD 2048
 SOLVENT CDCl₃
 NS 8
 DS 16
 SWH 4496.403 Hz
 FIDRES 2.195509 Hz
 AQ 0.2277876 sec
 RG 18
 DW 111.200 usec
 DE 6.00 usec
 TE 298.0 K
 D0 0.0000300 sec
 D1 2.00000000 sec
 D8 1.00000000 sec
 INO 0.00011120 sec

===== CHANNEL f1 =====
 NUC1 ^1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.2222510 MHz

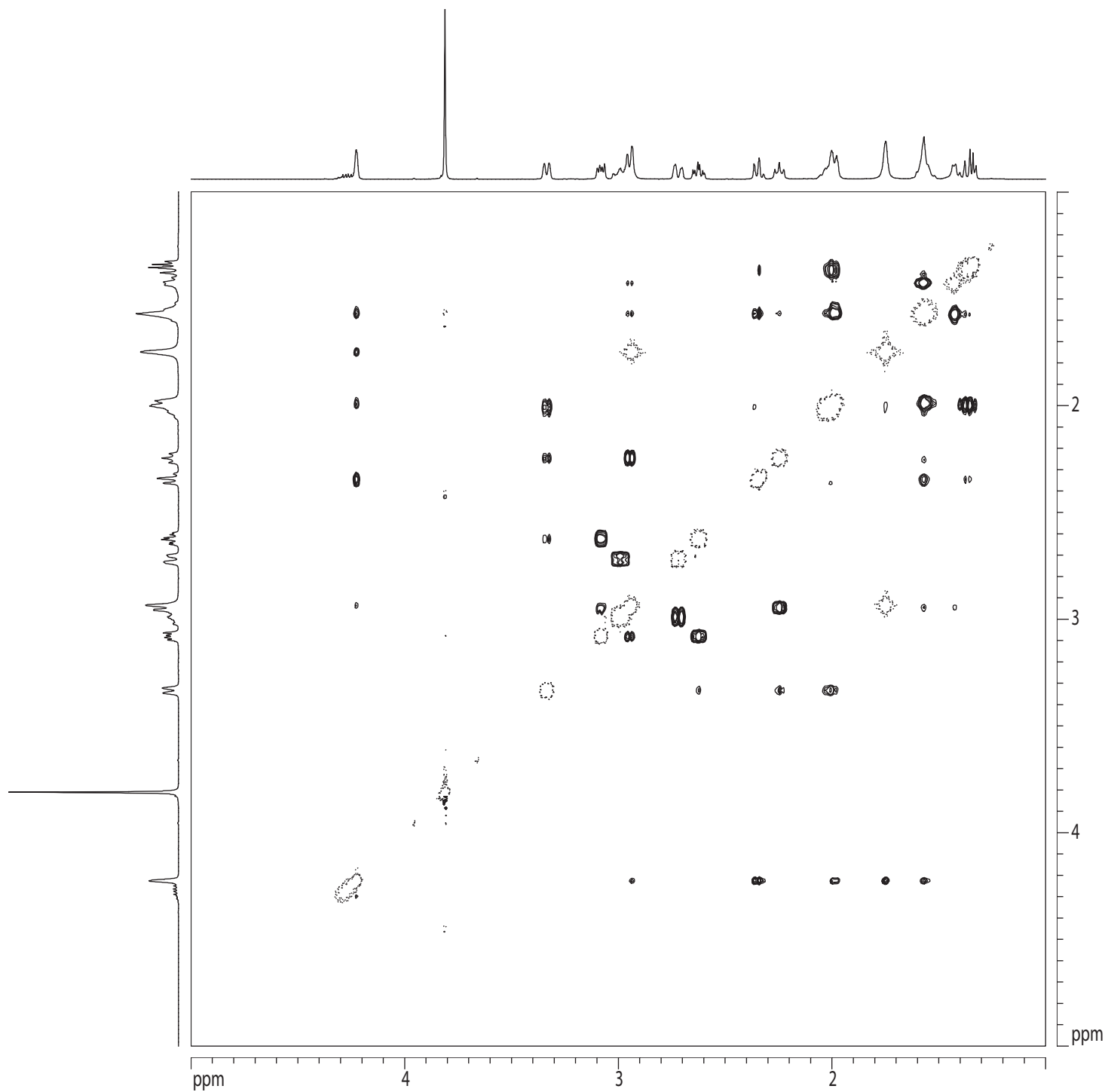
F1 - Acquisition parameters
 ND0 2
 TD 512
 SFO1 500.2223 MHz
 FIDRES 8.782037 Hz
 SW 8.989 ppm
 FnMODE undefined

F2 - Processing parameters
 SI 1024
 SF 500.2200309 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 2.00

F1 - Processing parameters
 SI 1024
 MC2 TPPI
 SF 500.2200309 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 8.994 ppm
 F2LO 4499.19 Hz
 F2PHI 0.006 ppm
 F2HI 2.79 Hz
 F1PLO 8.994 ppm
 F1LO 4499.19 Hz
 F1PHI 0.006 ppm
 F1HI 2.79 Hz
 F2PPMCM 0.59926 ppm/cm
 F2HZCM 299.76022 Hz/cm
 F1PPMCM 0.59926 ppm/cm
 F1HZCM 299.76022 Hz/cm

noesy



Current Data Parameters
 USER nmr13t
 NAME Apple_pie_2
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131206
 Time 23.55
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG noesyrvtp
 TD 2048
 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 4496.403 Hz
 FIDRES 2.195509 Hz
 AQ 0.2277876 sec
 RG 18
 DW 111.200 usec
 DE 6.00 usec
 TE 298.0 K
 D0 0.00000300 sec
 D1 2.00000000 sec
 D8 1.00000000 sec
 INO 0.00011120 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.222510 MHz

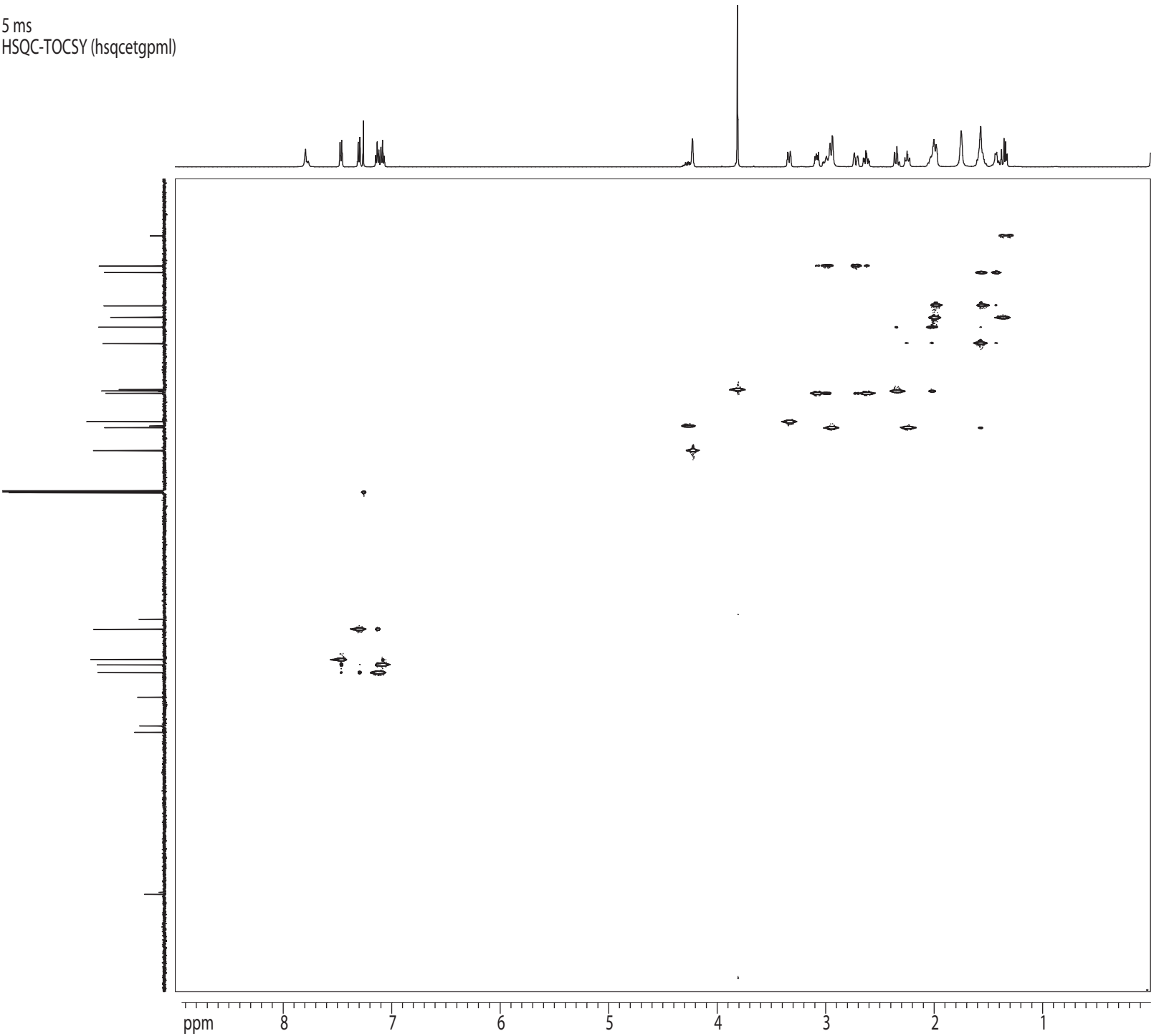
F1 - Acquisition parameters
 ND0 2
 TD 512
 SFO1 500.2223 MHz
 FIDRES 8.782037 Hz
 SW 8.989 ppm
 FnMODE undefined

F2 - Processing parameters
 SI 1024
 SF 500.2200309 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 2.00

F1 - Processing parameters
 SI 1024
 MC2 TPPI
 SF 500.2200309 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.000 ppm
 F2LO 2501.10 Hz
 F2PHI 1.000 ppm
 F2HI 500.22 Hz
 F1PLO 5.000 ppm
 F1LO 2501.28 Hz
 F1PHI 0.998 ppm
 F1HI 498.97 Hz
 F2PPMCM 0.26667 ppm/cm
 F2HZCM 133.39201 Hz/cm
 F1PPMCM 0.26686 ppm/cm
 F1HZCM 133.48697 Hz/cm

5 ms
HSQC-TOCSY (hsqcetgpm1)



Current Data Parameters
USER nmr13t
NAME Apple_pse_2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131207
Time 7:07
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpm1
TD 2048
SOLVENT CDCl3
NS 2
DS 32
SWH 4496.403 Hz
FIDRES 2.195599 Hz
AQ 0.2277876 sec
RG 11585.2
DW 111.200 usec
DE 6.50 usec
TE 298.0 K
CNS2 145.0000000
d0 0.00000300 sec
d1 2.000000000 sec
d4 0.00172414 sec
d9 0.005000000 sec
d11 0.030000000 sec
d12 0.000020000 sec
d13 0.000004000 sec
d16 0.000020000 sec
DELTA 0.00122100 sec
DELTA1 0.00120800 sec
FACTOR1 0
INO 0.00011995 sec
I1 0
MCREST 0.00000000 sec
MCWRK 0.40000001 sec
SCALEF 6
ST1CNT 256

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p2 15.00 usec
p5 23.34 usec
P6 35.00 usec
p7 70.00 usec
P17 2500.00 usec
P28 1000.00 usec
PL1 1.60 dB
PL10 15.30 dB
SFO1 500.2222510 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 15.50 usec
p4 31.00 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7929970 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE100
GPNAM2 SINE100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

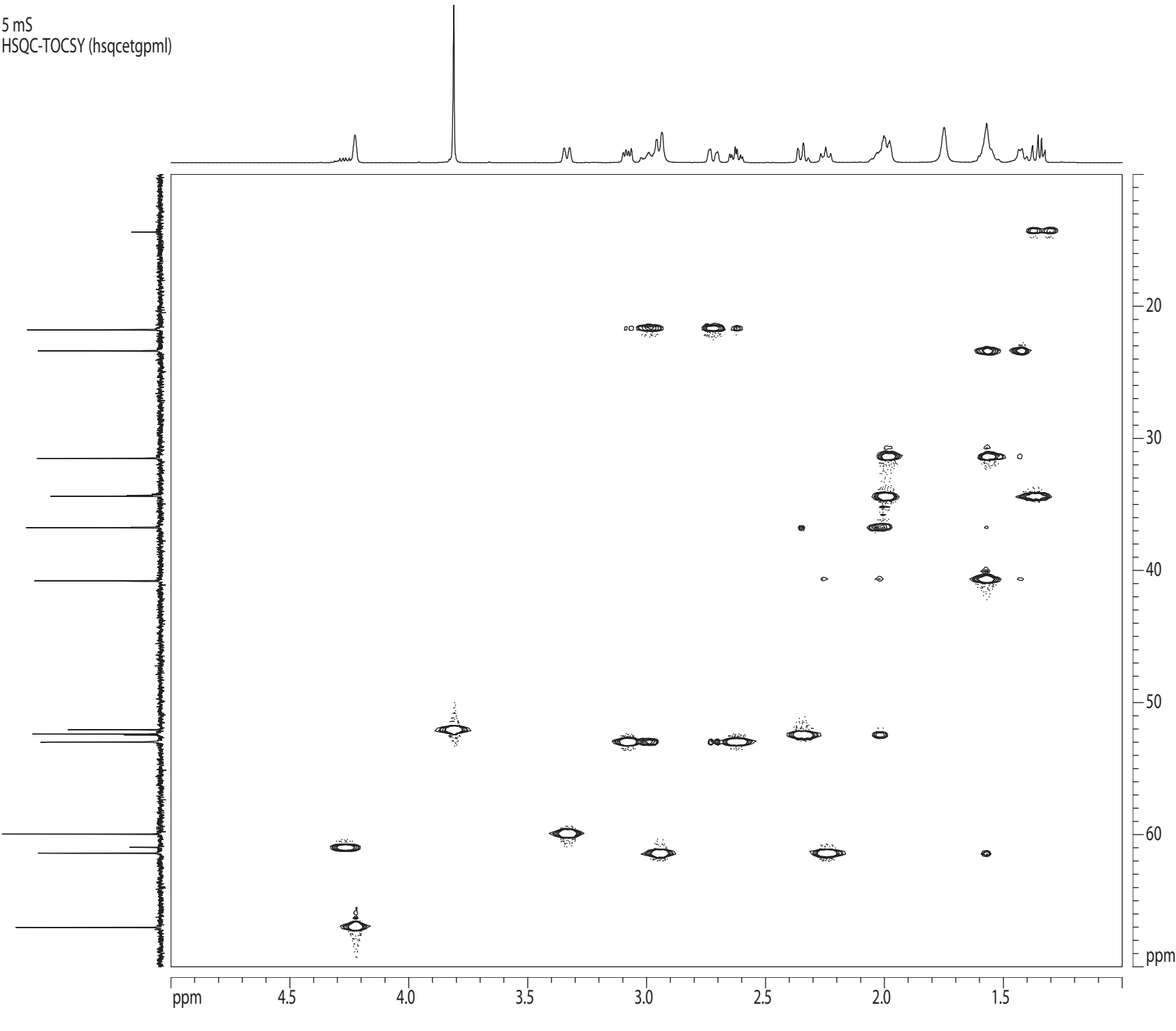
F1 - Acquisition parameters
NDO 2
TD 512
SFO1 125.793 MHz
FIDRES 48.950500 Hz
SW 199.237 ppm
FhMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.2209309 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 125.7804190 MHz
WDW QSI
SSB 3
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 18.00 cm
CX1 15.00 cm
F2PLO 8.994 ppm
F2PLO 4499.19 Hz
F2PHI 0.006 ppm
F2HI 2.79 Hz
F1PLO 199.629 ppm
F1LO 25109.37 Hz
F1PHI 0.371 ppm
F1HI 46.71 Hz
F2PPMCM 0.49938 ppm/cm
F2HZCM 249.80017 Hz/cm
F1PPMCM 13.28382 ppm/cm
F1HZCM 1670.84387 Hz/cm

5 mS
HSQC-TOCSY (hsqcetgpm1)



Current Data Parameters
USER nmrl3t
NAME Apple_pie_2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131207
Time 7.07
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpm1
TD 2048
SOLVENT CDCl3
NS 2
DS 32
SWH 4496.403 Hz
FIDRES 2.195599 Hz
AQ 0.2277876 sec
RG 11585.2
DW 111.200 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
d1 2.00000000 sec
d4 0.00172414 sec
d9 0.00500000 sec
d11 0.03000000 sec
d12 0.00002000 sec
d13 0.00000400 sec
d16 0.00002000 sec
DELTA 0.00122100 sec
DELTA1 0.00120800 sec
FACTOR1 0
INO 0.00001995 sec
I1 0
MCREST 0.00000000 sec
MCWRK 0.40000001 sec
SCALEF 6
STCNT 256

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p2 15.00 usec
p5 23.34 usec
P6 35.00 usec
p7 70.00 usec
P17 2500.00 usec
P28 1000.00 usec
PL1 1.60 dB
PL10 15.30 dB
SFO1 500.2222510 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 15.50 usec
p4 31.00 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7929970 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE100
GPNAM2 SINE100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

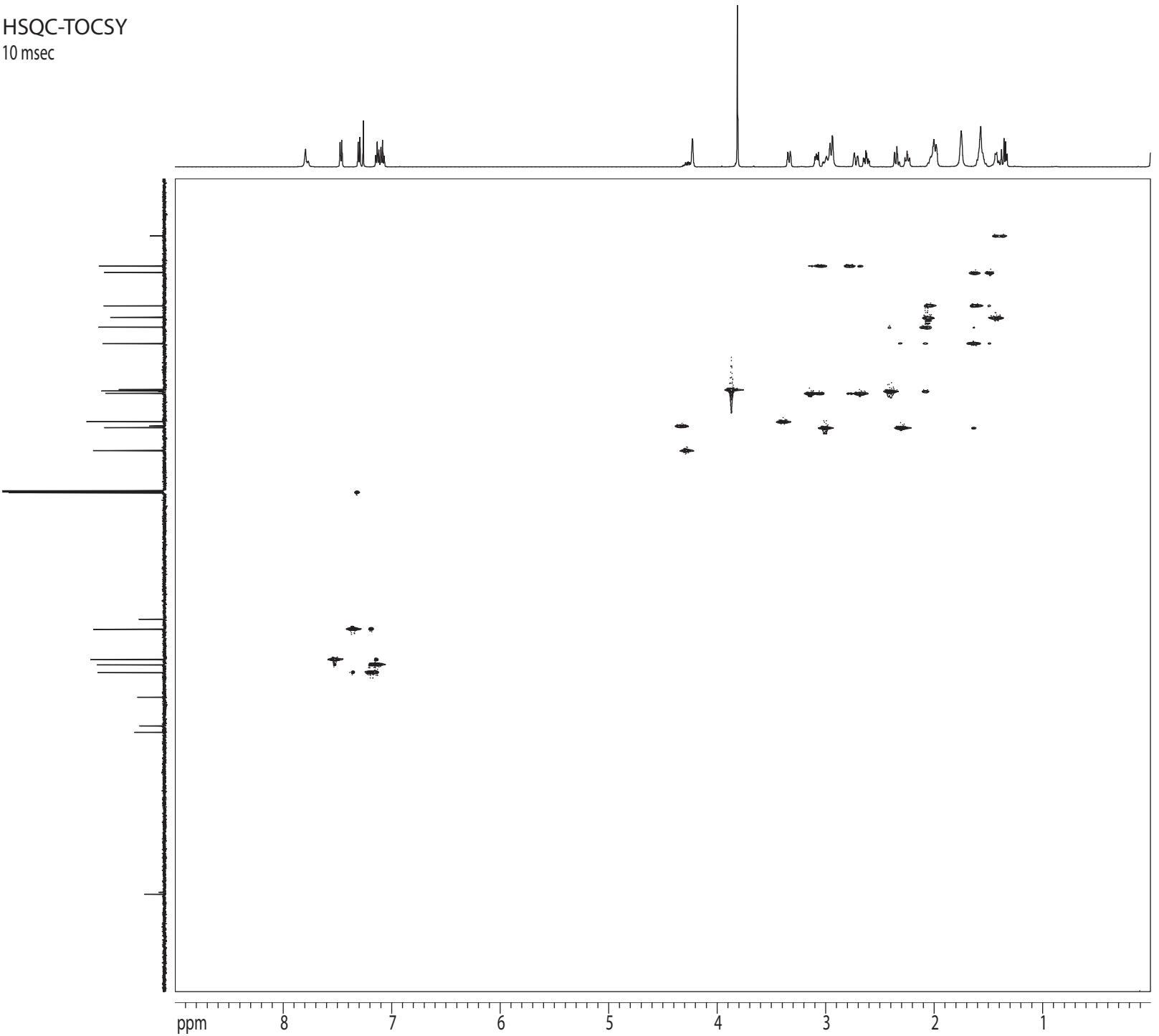
F1 - Acquisition parameters
NDO 2
TD 512
SFO1 125.793 MHz
FIDRES 48.950500 Hz
SW 199.237 ppm
FhMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.220309 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
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 1.000 ppm
F2HI 500.22 Hz
F1PLO 70.000 ppm
F1LO 8804.63 Hz
F1PHI 10.000 ppm
F1HI 1257.80 Hz
F2PPMCM 0.22222 ppm/cm
F2HZCM 111.16000 Hz/cm
F1PPMCM 4.00000 ppm/cm
F1HZCM 503.12167 Hz/cm

HSQC-TOCSY
10 msec



Current Data Parameters

USER nmr13t
NAME Apple_pse_2
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131207
Time 7:47
INSTRUM cryo500
PROBHD 5 mm CPIC1 1H-
PULPROG hsqcetgpm1
TD 2048
SOLVENT CDCl3
NS 2
DS 32
SWH 4496.403 Hz
FIDRES 2.195599 Hz
AQ 0.2277876 sec
RG 9195.2
DW 111.200 usec
DE 6.50 usec
TE 298.0 K
CNS2 145.0000000
d0 0.00000300 sec
d1 2.00000000 sec
d4 0.00172414 sec
d9 0.01000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
d13 0.00000400 sec
d16 0.00020000 sec
DELTA 0.00122100 sec
DELTA1 0.00120800 sec
FACTOR1 0
INO 0.00011995 sec
I1 0
MCREST 0.00000000 sec
MCWRK 0.40000001 sec
SCALEF 6
ST1CNT 256

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
p5 23.34 usec
P6 35.00 usec
p7 70.00 usec
P17 2500.00 usec
P28 1000.00 usec
PL1 1.60 dB
PL10 15.20 dB
SFO1 500.2222510 MHz

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

CPDPRG2 garp
NUC2 13C
P3 15.50 usec
p4 31.00 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7929970 MHz

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

GPAM1 SINE 100
GPAM2 SINE 100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters

NDO 2
TD 512
SFO1 125.793 MHz
FIDRES 48.950500 Hz
SW 199.237 ppm
FhMODE Echo-Antiecho

F2 - Processing parameters

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

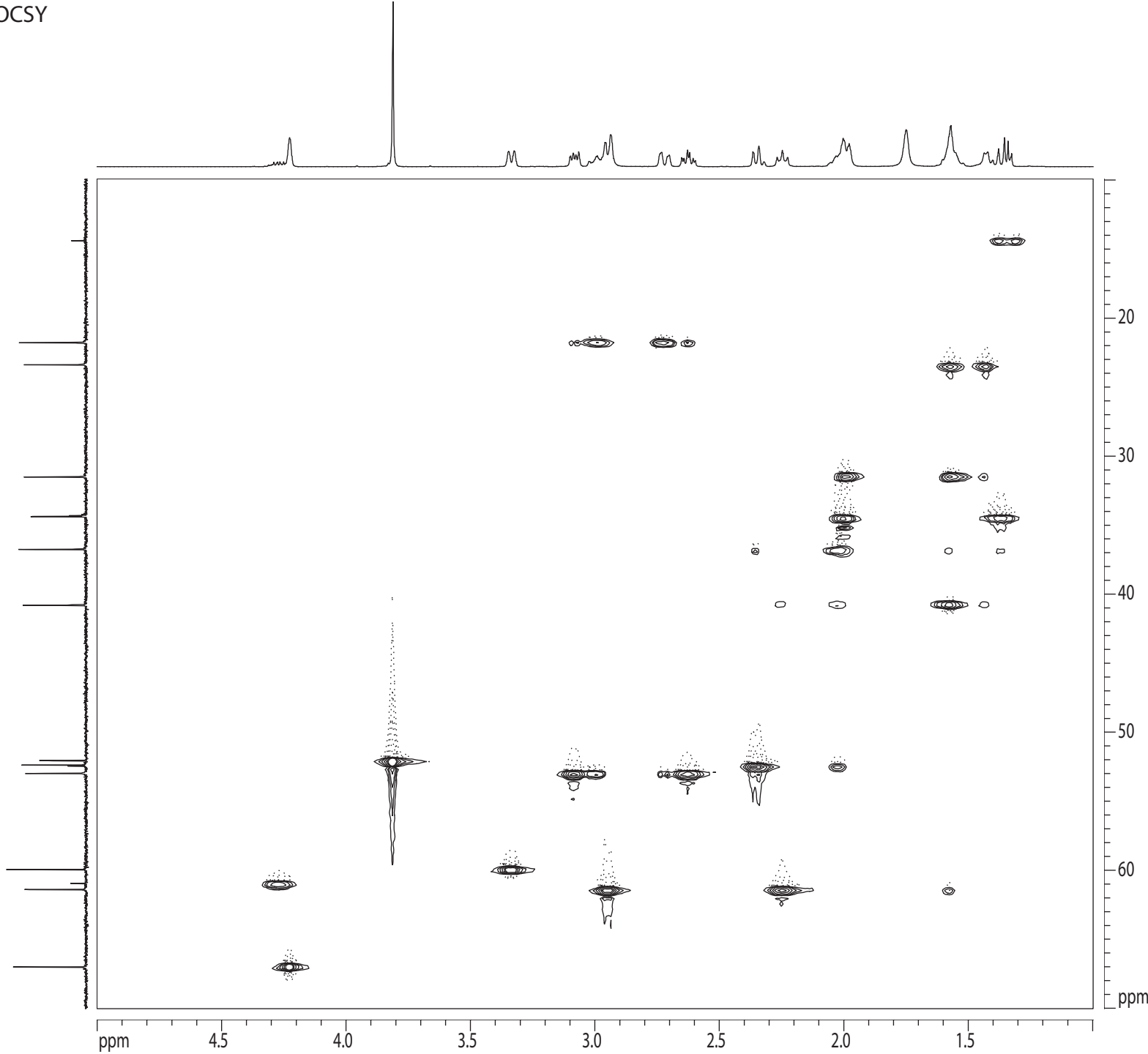
F1 - Processing parameters

SI 1024
MC2 echo-antlecho
SF 125.7804190 MHz
WDW QSINE
SSB 3
LB 0.00 Hz
GB 0

2D NMR plot parameters

CK2 18.00 cm
CK1 15.00 cm
F2PLO 8.994 ppm
F2PLO 4499.19 Hz
F2PHI 0.006 ppm
F2HI 2.79 Hz
F1PLO 199.629 ppm
F1LO 25109.37 Hz
F1PHI 0.371 ppm
F1HI 46.71 Hz
F2PPMCM 0.49938 ppm/cm
F2HZCM 249.80016 Hz/cm
F1PPMCM 13.28382 ppm/cm
F1HZCM 1670.84387 Hz/cm

HSQC-TOCSY
10 msec



Current Data Parameters
USER nmrl3t
NAME Apple_pie_2
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131207
Time 7:47
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpm1
TD 2048
SOLVENT CDCl3
NS 2
DS 32
SWH 4496.403 Hz
FIDRES 2.195509 Hz
AQ 0.2277876 sec
RG 9195.2
DW 111.200 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
d1 2.00000000 sec
d4 0.00172414 sec
d9 0.01000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
d13 0.00000400 sec
d16 0.00020000 sec
DELTA 0.00122100 sec
DELTA1 0.00120800 sec
FACTOR1 0
INO 0.00001995 sec
I1 0
MCREST 0.00000000 sec
MCWRK 0.40000001 sec
SCALEF 6
ST1CNT 256

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p2 15.00 usec
p5 23.34 usec
P6 35.00 usec
p7 70.00 usec
P17 2500.00 usec
P28 1000.00 usec
PL1 1.60 dB
PL10 15.30 dB
SFO1 500.2222510 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 15.50 usec
p4 31.00 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7929970 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE100
GPNAM2 SINE100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

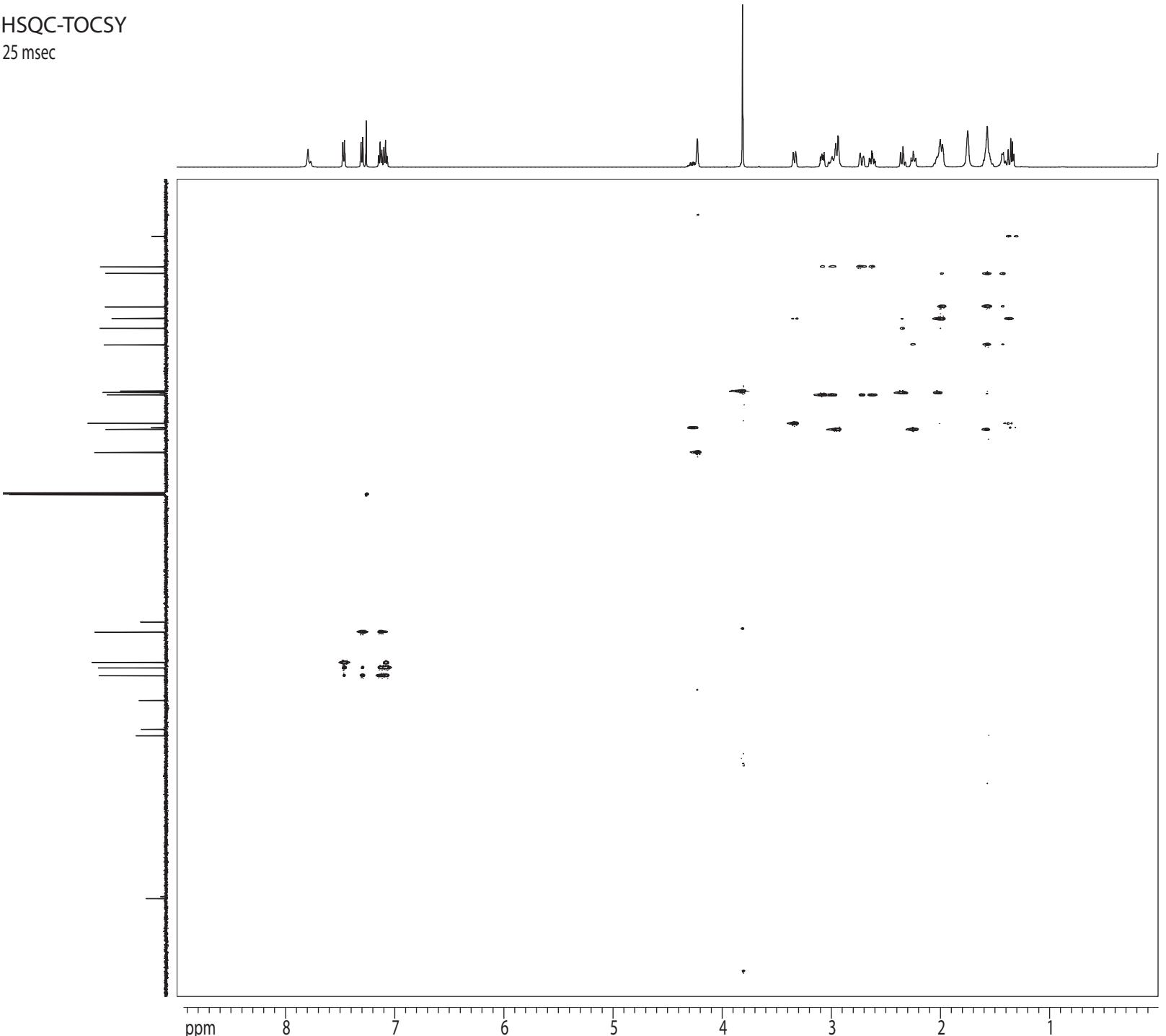
F1 - Acquisition parameters
NDO 2
TD 512
SFO1 125.793 MHz
FIDRES 48.950500 Hz
SW 199.237 ppm
FhMODE Echo-Antiecho

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 echo-antiecho
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
F2LLO 2501.28 Hz
F2PHI 0.998 ppm
F2HI 498.97 Hz
F1PLO 70.034 ppm
F1LLO 8808.85 Hz
F1PHI 9.986 ppm
F1HI 1246.00 Hz
F2PPMCM 0.22238 ppm/cm
F2HZCM 111.23913 Hz/cm
F1PPMCM 4.00849 ppm/cm
F1HZCM 504.19019 Hz/cm

HSQC-TOCSY
25 msec



Current Data Parameters

USER rnm13r
NAME Apple_pie_2
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131207
Time 8.27
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpm1
TD 2048
SOLVENT CDCl3
NS 2
DS 32
SWH 4496.403 Hz
FIDRES 2.195509 Hz
AQ 0.2277876 sec
RG 7298.2
DW 111.200 usec
DE 6.50 usec
TE 298.0 K
CNS2 145.0000000
d0 0.00000300 sec
d1 2.00000000 sec
d4 0.00172414 sec
D9 0.02500000 sec
d11 0.03000000 sec
d12 0.00002000 sec
d13 0.00000400 sec
D16 0.00026000 sec
DELTA 0.00122100 sec
DELTA1 0.00120800 sec
FACTOR1 1
INO 0.00001995 sec
I1 6
MCREST 0.00000000 sec
MCWRK 0.40000001 sec
SCALEF 6
STCNT 256

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
p5 23.34 usec
P6 35.00 usec
p7 70.00 usec
P17 2500.00 usec
P28 1000.00 usec
PL1 1.60 dB
PL10 15.20 dB
SFO1 500.2222510 MHz

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

CPDPRG2 gmp
NUC2 13C
P3 15.50 usec
p4 31.00 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7929970 MHz

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

GP1AM1 SINE100
GP1AM2 SINE100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters

NDO 2
TD 512
SFO1 125.793 MHz
FIDRES 48.950500 Hz
SW 199.237 ppm
F1MODE Echo-Antiecho

F2 - Processing parameters

SI 1024
SF 500.2200300 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

F1 - Processing parameters

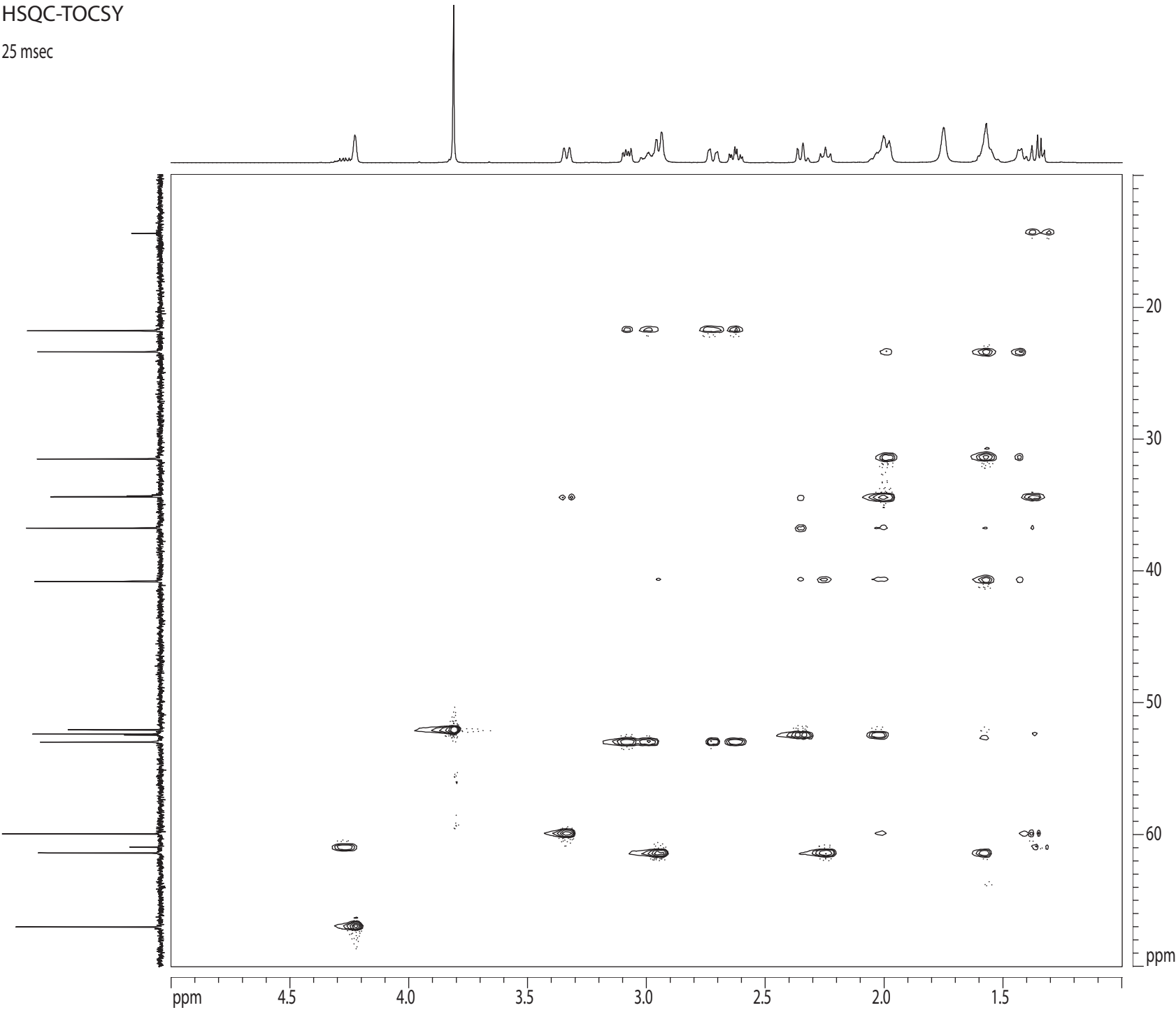
SI 1024
MC2 echo-antiecho
SF 125.7804190 MHz
WDW COSYNE
SSB 3
LB 0.00 Hz
GB 0

2D NMR plot parameters

CK2 18.00 cm
CK1 15.00 cm
F2PLO 8.994 ppm
F2LO 4999.19 Hz
F2PHI 0.006 ppm
F2HI 2.79 Hz
F1PLO 199.629 ppm
F1LO 25109.37 Hz
F1PHI 0.371 ppm
F1HI 46.71 Hz
F2PPMCM 0.49938 ppm/cm
F2HZCM 249.80017 Hz/cm
F1PPMCM 13.28382 ppm/cm
F1HZCM 1670.84387 Hz/cm

HSQC-TOCSY

25 msec



Current Data Parameters
USER nmrl3t
NAME Apple_pse_2
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131207
Time 8.27
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpm1
TD 2048
SOLVENT CDCl3
NS 2
DS 32
SWH 4496.403 Hz
FIDRES 2.195509 Hz
AQ 0.2277876 sec
RG 7298.2
DW 111.200 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
d1 2.00000000 sec
d4 0.00172414 sec
d9 0.02500000 sec
d11 0.03000000 sec
d12 0.00002000 sec
d13 0.00000400 sec
d16 0.00020000 sec
DELTA 0.00122100 sec
DELTA1 0.00120800 sec
FACTOR1 1
INO 0.00011995 sec
I1 6
MCREST 0.00000000 sec
MCWRK 0.40000001 sec
SCALEF 6
ST1CNT 256

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p2 15.00 usec
p5 23.34 usec
P6 35.00 usec
p7 70.00 usec
P17 2500.00 usec
P28 1000.00 usec
PL1 1.60 dB
PL10 15.30 dB
SFO1 500.2222510 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 15.50 usec
p4 31.00 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7929970 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE 100
GPNAM2 SINE 100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
NDO 2
TD 512
SFO1 125.793 MHz
FIDRES 48.950500 Hz
SW 199.237 ppm
FhMODE Echo-Antiecho

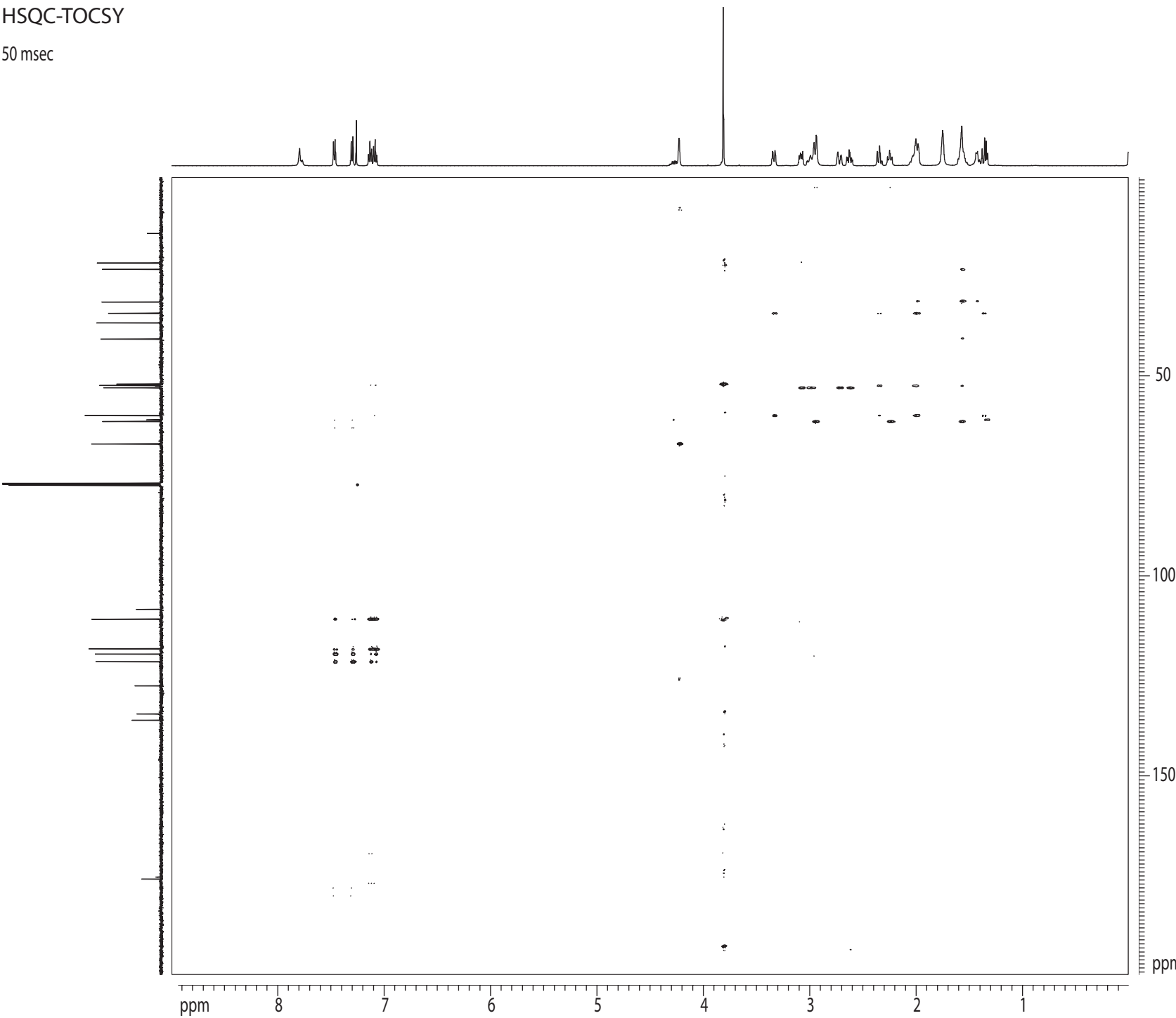
F2 - Processing parameters
SI 1024
SF 500.220309 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antlecho
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 2501.28 Hz
F2PHI 0.998 ppm
F2HI 498.97 Hz
F1PLO 70.034 ppm
F1LO 8808.85 Hz
F1PHI 9.986 ppm
F1HI 1246.00 Hz
F2PPMCM 0.22238 ppm/cm
F2HZCM 111.23913 Hz/cm
F1PPMCM 4.00849 ppm/cm
F1HZCM 504.19019 Hz/cm

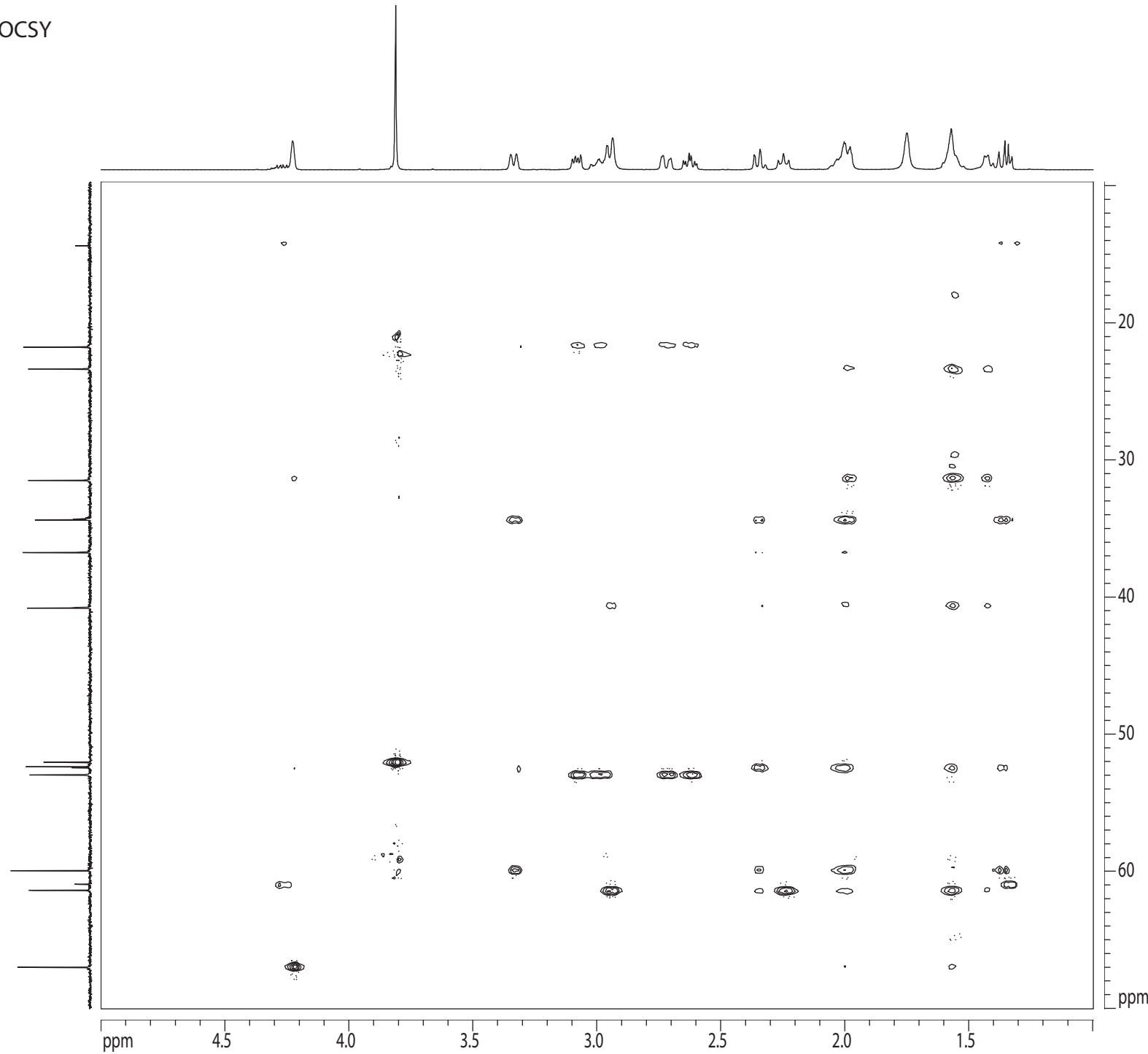
HSQC-TOCSY

50 msec



Current Data Parameters	
USER	nmr13t
NAME	Apple_pse_2
EXPNO	13
PROCNO	1
F2 - Acquisition Parameters	
Date_	20131207
Time	9.07
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	hsqcetgpm1
TD	2048
SOLVENT	CDCl3
NS	2
DS	32
SWH	4496.403 Hz
FIDRES	2.195509 Hz
AQ	0.2277876 sec
RG	20642.5
DW	111.200 usec
DE	6.50 usec
TE	298.0 K
CNST2	145.0000000
do	0.00000300 sec
D1	2.00000000 sec
d4	0.00172414 sec
D9	0.05000000 sec
d11	0.03000000 sec
d12	0.00002000 sec
d13	0.00000400 sec
D16	0.00020000 sec
DELTA	0.00122100 sec
DELTA1	0.00120800 sec
FACTOR1	3
INO	0.0001995 sec
I1	18
MCREST	0.00000000 sec
MCWRK	0.40000001 sec
SCALEF	6
ST1CNT	256
===== CHANNEL f1 =====	
NUC1	1H
P1	7.50 usec
p2	15.00 usec
p5	23.34 usec
P6	35.00 usec
p7	70.00 usec
P17	2500.00 usec
P28	1000.00 usec
PL1	1.60 dB
PL10	15.30 dB
SFO1	500.2222510 MHz
===== CHANNEL f2 =====	
CPDPRG2	garp
NUC2	13C
P3	15.50 usec
p4	31.00 usec
PCPD2	65.00 usec
PL2	-1.00 dB
PL12	11.30 dB
SFO2	125.7929970 MHz
===== GRADIENT CHANNEL =====	
GPNAME1	SINE100
GPNAME2	SINE100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	80.00 %
GPZ2	20.10 %
P16	1000.00 usec
F1 - Acquisition parameters	
NDO	2
TD	512
SFO1	125.793 MHz
FIDRES	48.950500 Hz
SW	199.237 ppm
FnMODE	Echo-Antiecho
F2 - Processing parameters	
SI	1024
SF	500.220309 MHz
WDW	EM
SSB	0
LB	5.00 Hz
GB	0
PC	1.40
F1 - Processing parameters	
SI	1024
MC2	echo-antiecho
SF	125.7804190 MHz
WDW	QSSINE
SSB	3
LB	0.00 Hz
GB	0
2D NMR plot parameters	
CK2	18.00 cm
CK1	15.00 cm
F2PLO	8.994 ppm
F2LLO	4499.19 Hz
F2PHI	0.005 ppm
F2HI	2.79 Hz
F1PLO	199.629 ppm
F1LLO	25109.37 Hz
F1PHI	0.371 ppm
F1HI	46.71 Hz
F2PPMCM	0.49938 ppm/cm
F2HZCM	249.80017 Hz/cm
F1PPMCM	13.28382 ppm/cm
F1HZCM	1670.84387 Hz/cm

HSQC-TOCSY
50 msec



Current Data Parameters
USER nmrl3t
NAME Apple_pie_2
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131207
Time 9.07
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpm1
TD 2048
SOLVENT CDCl3
NS 2
DS 32
SWH 4496.403 Hz
FIDRES 2.195509 Hz
AQ 0.2277876 sec
RG 20642.5
DW 111.200 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
d1 2.00000000 sec
d4 0.00172414 sec
d9 0.02500000 sec
d11 0.03000000 sec
d12 0.00002000 sec
d13 0.00000400 sec
d16 0.00020000 sec
DELTA 0.00122100 sec
DELTA1 0.00120800 sec
FACTOR1 3
INO 0.00011955 sec
I1 18
MCREST 0.00000000 sec
MCWRK 0.40000001 sec
SCALEF 6
ST1CNT 256

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p2 15.00 usec
p5 23.34 usec
P6 35.00 usec
p7 70.00 usec
P17 2500.00 usec
P28 1000.00 usec
PL1 1.60 dB
PL10 15.30 dB
SFO1 500.2222510 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 15.50 usec
p4 31.00 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7929970 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE100
GPNAM2 SINE100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
NDO 2
TD 512
SFO1 125.793 MHz
FIDRES 48.950500 Hz
SW 199.237 ppm
FhMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.220309 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
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 2501.11 Hz
F2PHI 0.997 ppm
F2HI 498.81 Hz
F1PLO 70.034 ppm
F1LO 8808.85 Hz
F1PHI 9.712 ppm
F1HI 1221.52 Hz
F2PPMCM 0.22238 ppm/cm
F2HZCM 111.23913 Hz/cm
F1PPMCM 4.02147 ppm/cm
F1HZCM 505.82184 Hz/cm