Name: _____

Chem 203
December 10, 2011

Final Exam Part I
(40 points)

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 DISHNONESTY, WILL RESULT IN A FAILING GRADE (F) IN THE CLASS, AND MAY RESULT IN EXPULSION FROM THE Ph.D. PROGRAM.

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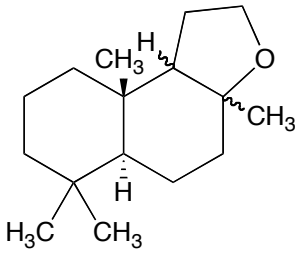
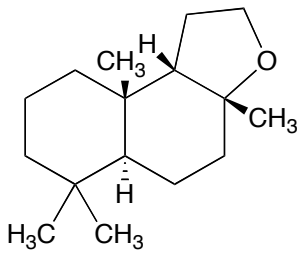
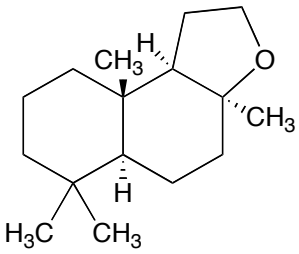
1. The following spectral data are provided for a tricyclic compound: 500.22 MHz ^{1}H NMR, 125.79 MHz ^{13}C NMR, DEPT, COSY, TOCSY, HMQC, HMBC, NOESY, and HSQC-TOCSY spectra with 5-, 10-, 20-, and 100-ms mixing times. All NMR spectra were measured in C_6D_6 solution.



Using these data, determine the stereochemistry and assign all of the ^{1}H 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.



1



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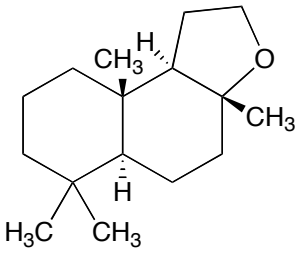

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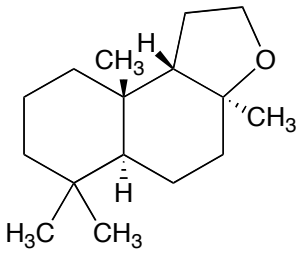

4

MAKE SURE TO COMPLETELY ANSWER THE QUESTIONS **a-g** ON PAGES 2-6.

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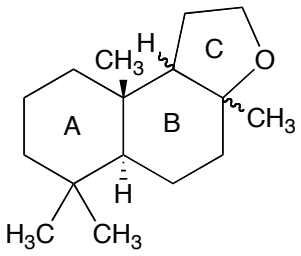
a. Build energy-minimized molecular models of diastereomers **1**, **2**, **3**, and **4** using PyMOL and the "clean" function. Rotate each molecule into an appropriate orientation. Use the side menu (S) to show each molecule as sticks (Show-sticks). Use the pulldown menu to display each molecule in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

Feel free to use the *trans*-decalin template .pse file or .pdb file on the course web page "Simple Conformational Analysis of Cyclic and Bicyclic Compounds" which is linked to the "Assignments" and "Class Materials" web pages. You are also welcome to just make your own *trans*-decalin.

NOTE: For diastereomer **4** you will have to build the B ring in a boat conformation, because the B–C ring junction does not allow the B ring to adopt a chair conformation. After minimization, the B ring should be in a twist-boat conformation. The A–B ring junction will look like that of the other diasteromers, but the B–C ring junction will be enforcing a twist-boat conformation of the B ring.

If you would like to review the conformations of cyclohexane, please see my Chem H52A course web page "Cyclohexanes" at: https://eee.uci.edu/10f/40600/cyclohexane.html . The page contains links to .pdb files of boat and twist-boat cyclohexane, which can be opened in PyMOL. If you would like to see an example of a related exercise in which ring fusion induces a twist boat conformation in a cyclohexane ring, please see my course web page "Perhydroanthracenes" and the associated .pdb files at: https://eee.uci.edu/10f/40600/perhydroanthracenes.html .



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

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b. Examine the ^{1}H NMR spectra and familiarize yourself with the resonances, which have been lettered *a–l* for you. Examine the ^{13}C NMR spectra and number the sixteen unique resonances associated with the molecule 1–16.

Examine the DEPT spectra and identify the quaternary (C), methine (CH), methylene (CH_2), and methyl (CH_3) peaks. NOTE: Although the DEPT 90 contains small resonances associated with the methyl and methylene groups, it is easy to identify the methine groups.

Examine the HMQC spectra and correlate the numbers of ^{13}C resonances with the letters of the ^{1}H resonances.

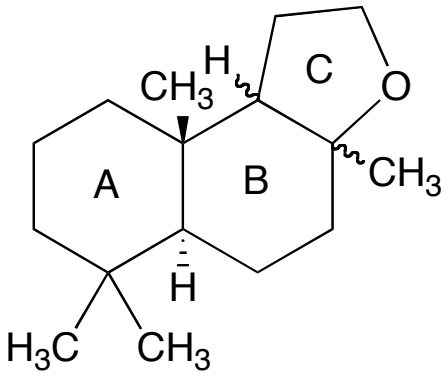
Finally, examine the HSQC-TOCSY spectrum with 100-ms mixing time and identify which methine and methylene resonances are associated with the three main spin systems in the molecule, which we will call the A-ring spin system, the B-ring spin system, and the C-ring spin system:

Numbers associated with the ^{13}C resonances associated with the A-ring spin system: ___, ___, ___.

Numbers associated with the ^{13}C resonances associated with the B-ring spin system: ___, ___, ___.

Numbers associated with the ^{13}C resonances associated with the C-ring spin system: ___, ___, ___.

c. Examine the HSQC-TOCSY spectra with 5, 10, 20, and 100-ms mixing times. Assign the *six* methine and methylene ^{13}C resonances from the B- and C-ring spin systems, to the corresponding atoms in the structure, below. That is, write the number next to the atom in the structure below.



NOTE: Work the problem the way we did in class and is described in the assigned reading in "Two-Dimensional NMR Spectroscopy: Applications for Chemists and Biochemists." Start with the track that grows in under ^{1}H resonances *a* and *b* and assign one spin system. Then work with the track that grows in under ^{1}H resonance *c* and assign another spin system.

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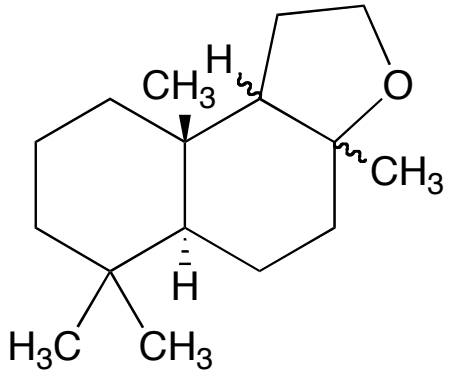
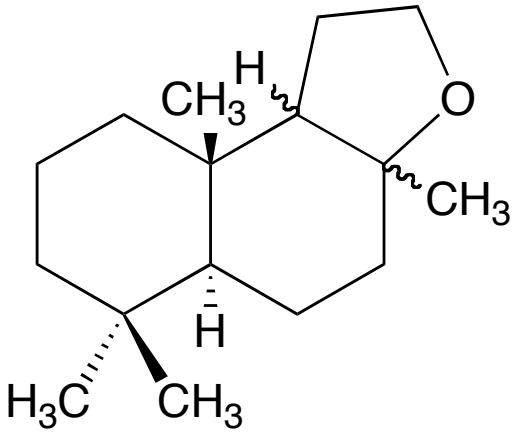
d. Use the HMBC spectrum and particularly the expansion that gives the higher-level contours of the isolated methyl groups to assign the remaining ^{13}C resonances to the corresponding atoms in the structure, below. That is, write the number next to the atom in the structure below.



e. Use the NOESY spectrum to stereospecifically assign the diastereotopic geminal dimethyl ^{13}C resonances to the corresponding atoms in the structure, below. That is, write the number next to the atom in the structure below. HINT: Consider the proximity of the methyl groups to each other; use the models that you have built in Part **a** for insights.

Transcribe your other numbers from Parts **c** and **d**, so that every carbon is numbered. Write the letters of the corresponding ^{1}H resonances next to the numbers.



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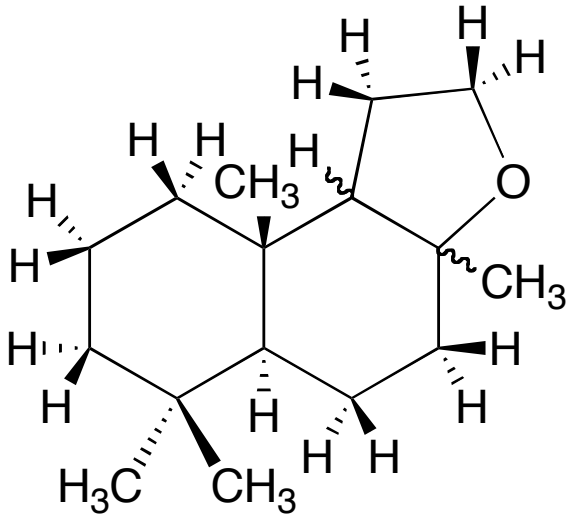
f. Determine the stereochemistry of the molecule. Which diastereomer is it? _____

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.

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



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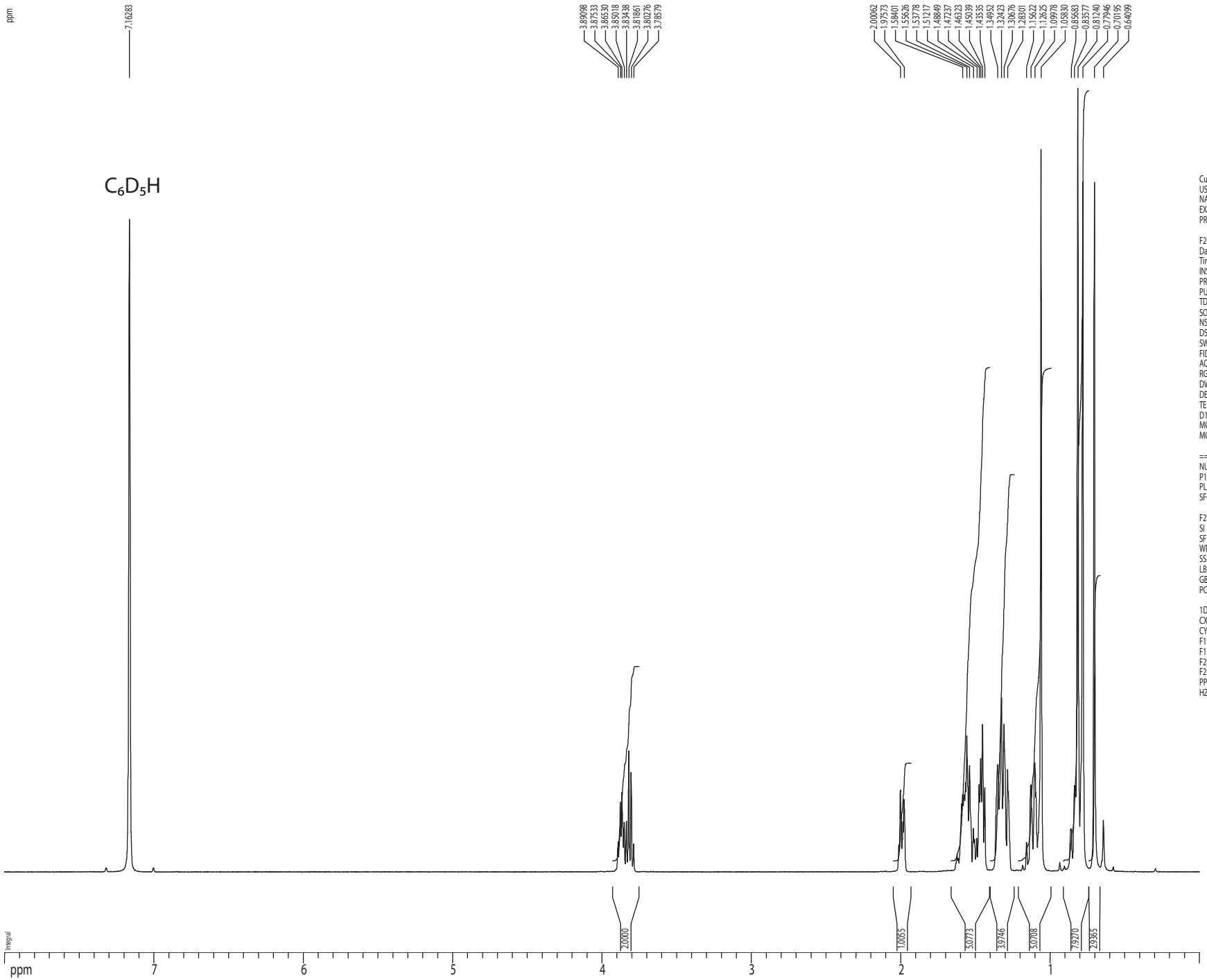
1H spectrum at 500 MHz in C_6D_6



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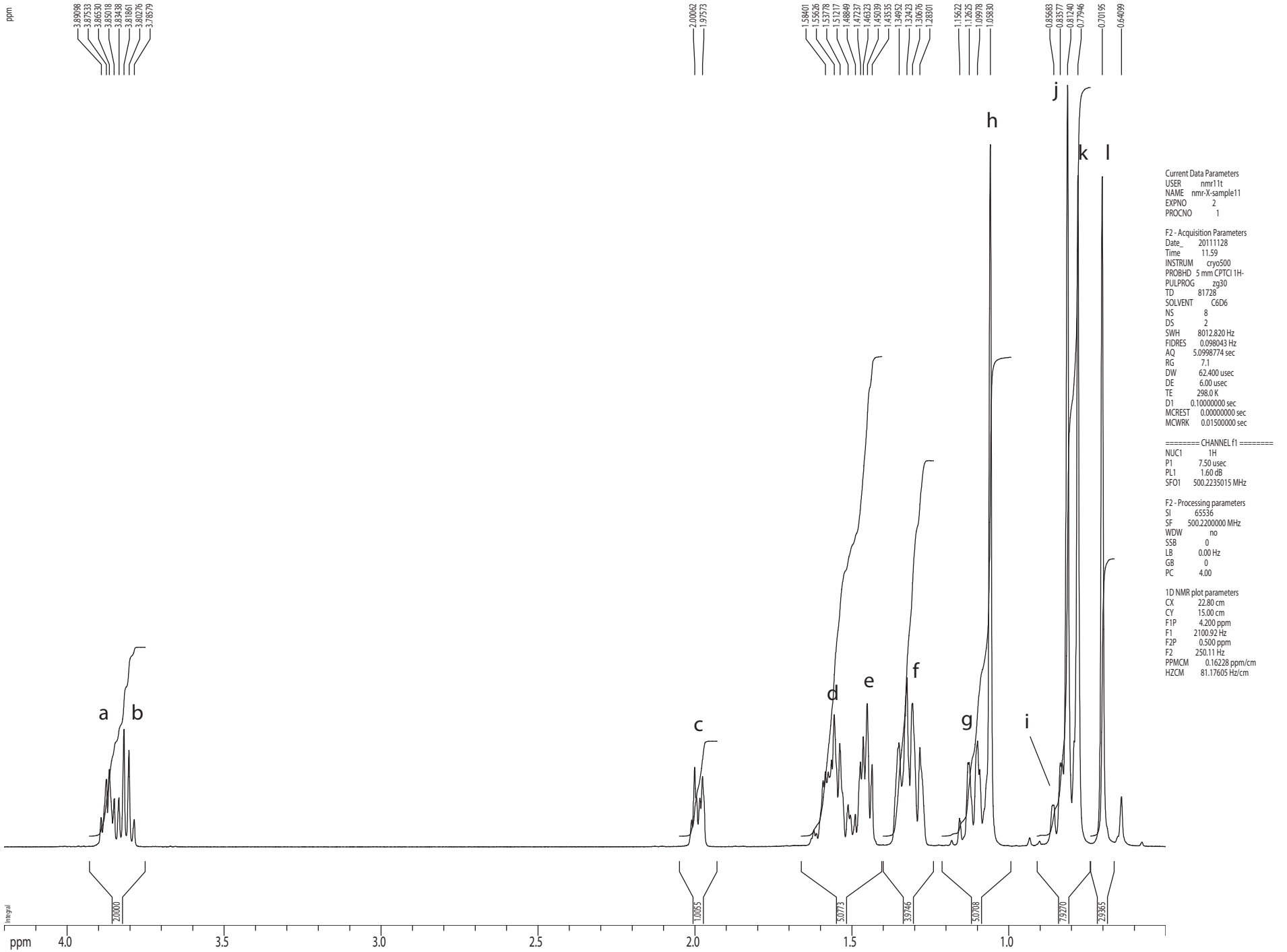
2	45551.8	1938.519	3.8753	1.37
3	45592.8	1933.502	3.8653	1.56
4	45654.7	1925.939	3.8502	0.99
5	45719.3	1918.036	3.8344	1.01
6	45783.9	1910.146	3.8186	2.35
7	45848.7	1902.217	3.8028	1.94
8	45918.1	1893.729	3.7858	0.58
9	53221.7	1000.748	2.0006	1.60
10	53323.6	988.298	1.9757	1.43
11	54926.2	792.353	1.5840	1.52
12	55039.7	778.472	1.5563	2.64
13	55115.3	769.226	1.5378	2.07
14	55220.1	756.417	1.5122	0.87
15	55317.0	744.573	1.4885	0.68
16	55382.9	736.512	1.4724	1.71
17	55420.3	731.938	1.4632	2.20
18	55472.8	725.515	1.4504	2.86
19	55534.3	717.993	1.4354	1.65
20	55885.5	675.057	1.3495	2.09
21	55989.0	662.406	1.3242	3.36
22	56060.4	653.669	1.3068	2.86
23	56157.6	641.786	1.2830	1.99
24	56676.4	578.362	1.1562	0.61
25	56799.0	563.371	1.1262	1.70
26	56907.3	550.131	1.0998	2.12
27	57077.0	529.382	1.0583	13.83
28	57901.2	428.605	0.8568	0.86
29	57987.4	418.071	0.8358	1.69
30	58083.0	406.376	0.8124	15.00
31	58217.8	389.900	0.7795	13.22
32	58534.9	351.131	0.7020	13.21
33	58784.3	320.638	0.6410	1.03

1H spectrum at 500 MHz in C_6D_6



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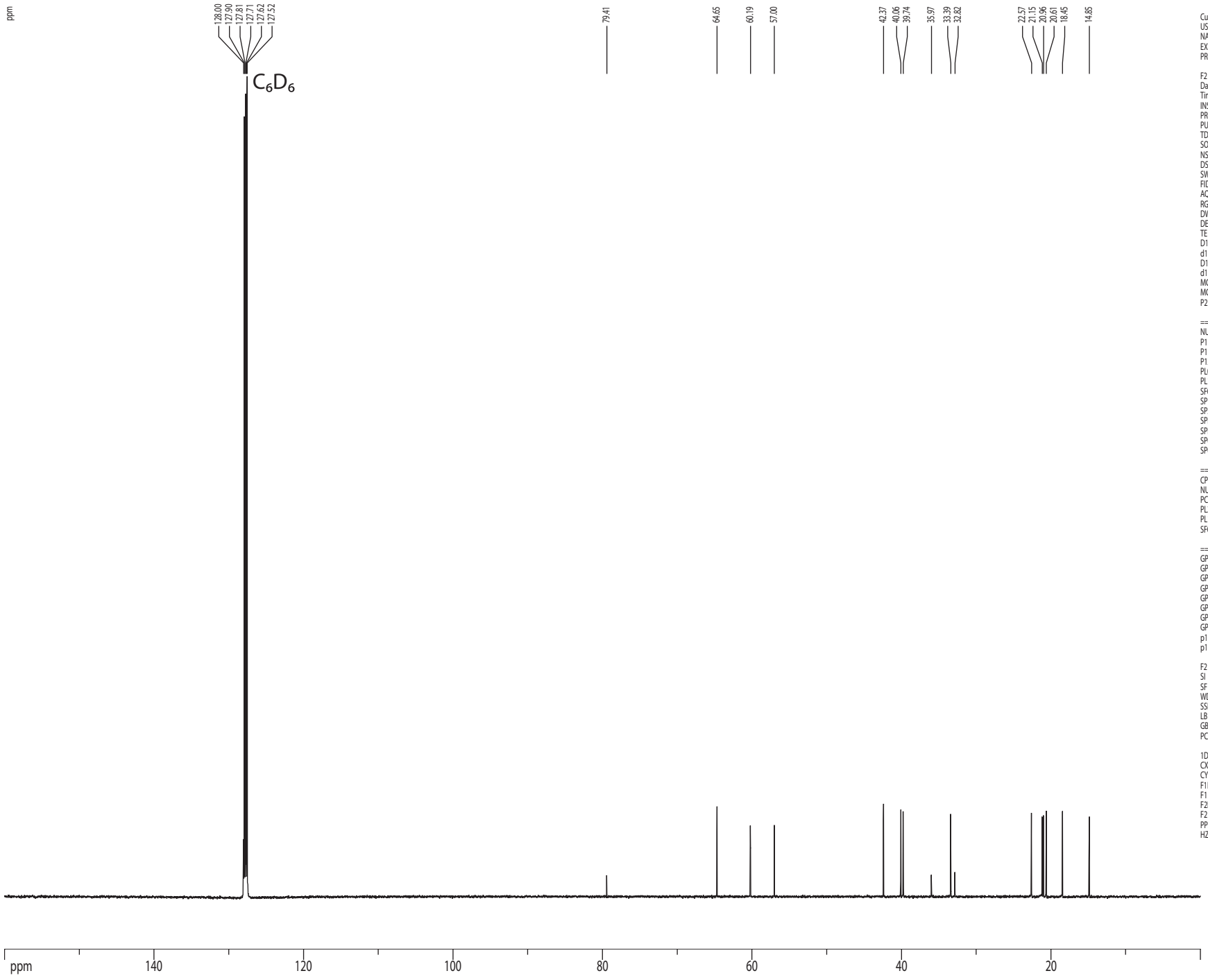
Time 11.59
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT C6D6
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 7.1
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 4.200 ppm
F1 2100.92 Hz
F2P 0.500 ppm
F2 250.11 Hz
PPMCM 0.16228 ppm/cm
HZCM 81.17605 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling at 125 MHz in C_6D_6



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PROCNO 1

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PULPROG SpinEchopg30gp.prd
TD 65536
SOLVENT C6D6
NS 330
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813940 sec
RG 32768
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00019600 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7942548 MHz
SP1 3.20 dB
SP2 3.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz

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

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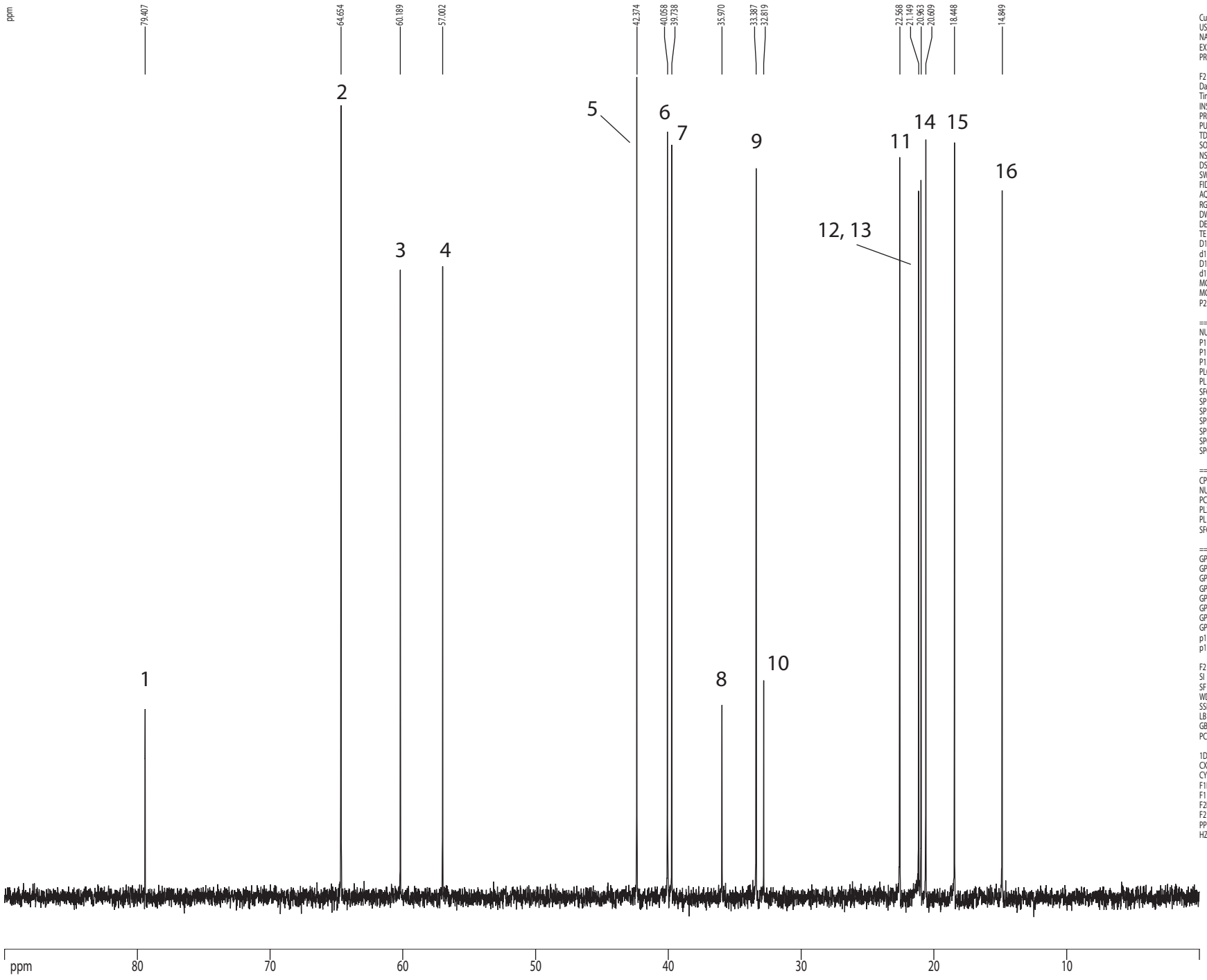
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.7804190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 160.000 ppm
F1 20124.87 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 7.01754 ppm/cm
HZCM 882.66962 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling at 125 MHz in C_6D_6



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NS 330
DS 16
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FIDRES 0.462388 Hz
AQ 1.0813940 sec
RG 32768
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00019600 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7942548 MHz
SP1 3.20 dB
SP2 3.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz

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

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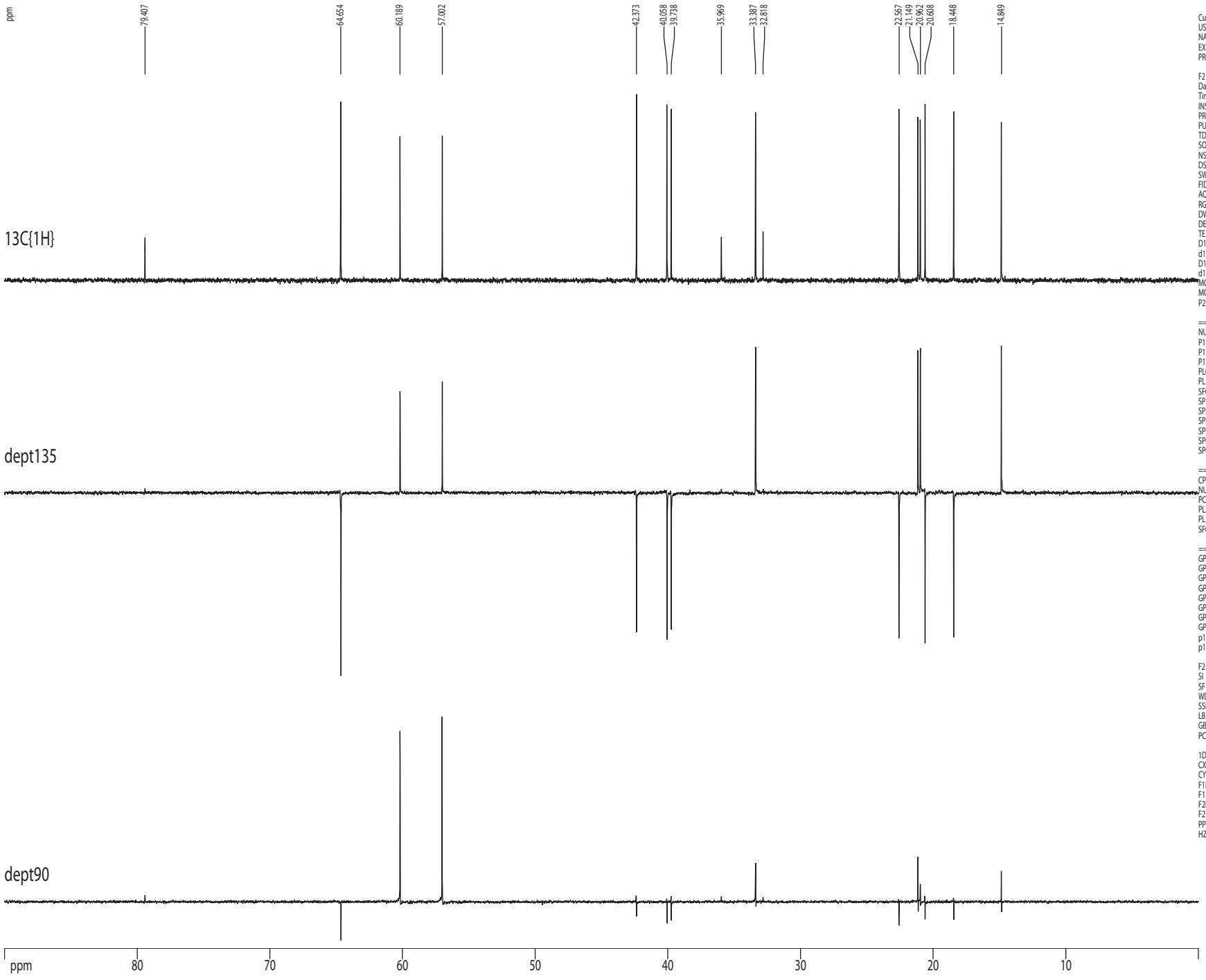
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.7804190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 90.000 ppm
F1 11320.24 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 3.94737 ppm/cm
HZCM 496.50168 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling at 125 MHz in C_6D_6



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NS 330
DS 16
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FIDRES 0.462388 Hz
AQ 1.0813940 sec
RG 32768
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00019600 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7942548 MHz
SP1 3.20 dB
SP2 3.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz

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

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

F2 - Processing parameters
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WDW EM
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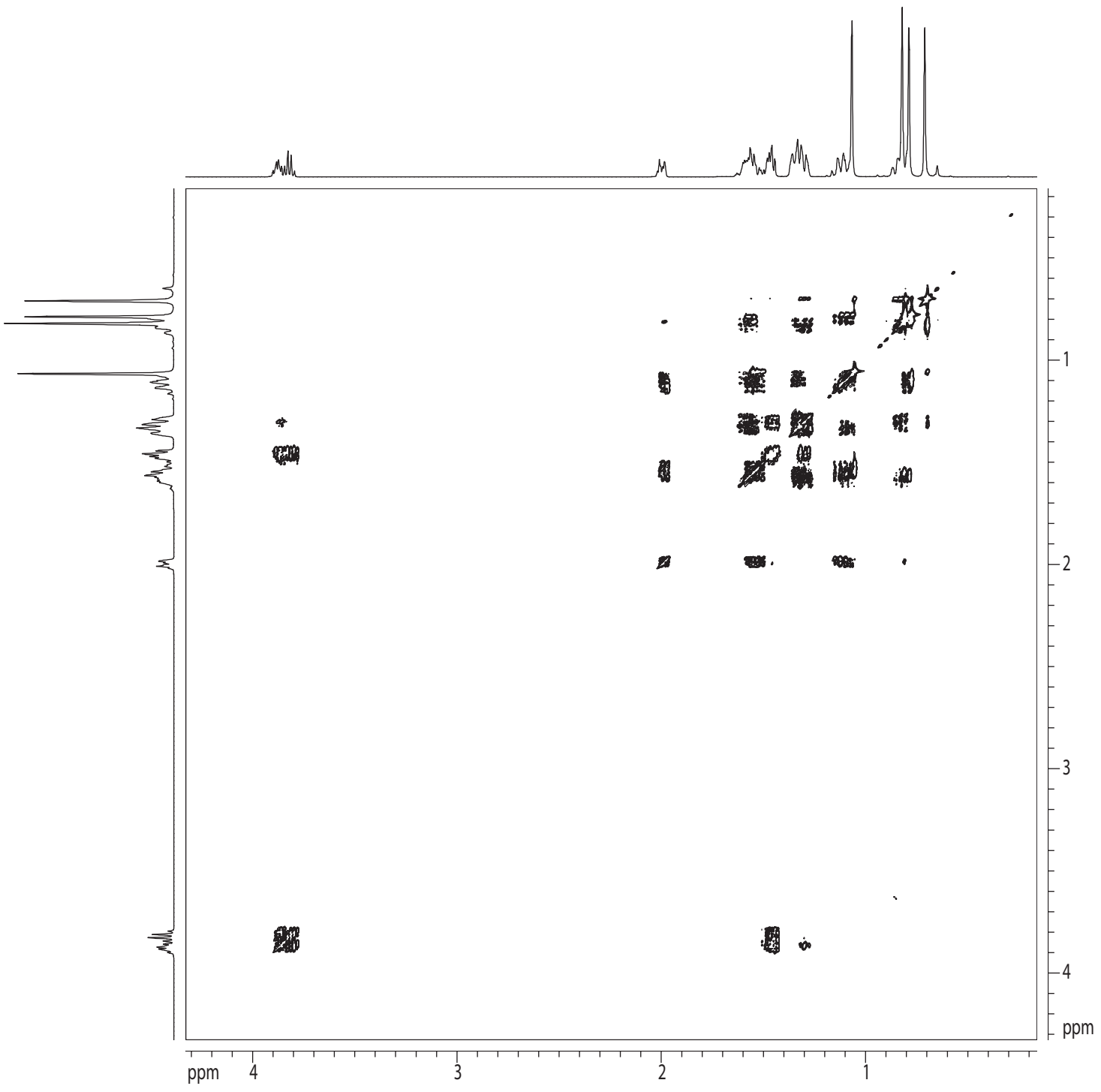
LB 1.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 3.56 cm
F1P 90.000 ppm
F1 11320.24 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 3.94737 ppm/cm
HZCM 496.50168 Hz/cm

gcosy60



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TD 2048
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NS 4
DS 16
SWH 2083.333 Hz
FIDRES 1.017253 Hz
AQ 0.4915700 sec
RG 35.9
DW 240.000 usec
DE 6.00 usec
TE 298.0 K
d0 0.00000300 sec
D1 1.00000000 sec
d13 0.00000300 sec
D16 0.00020000 sec
IN0 0.00048000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2211225 MHz

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

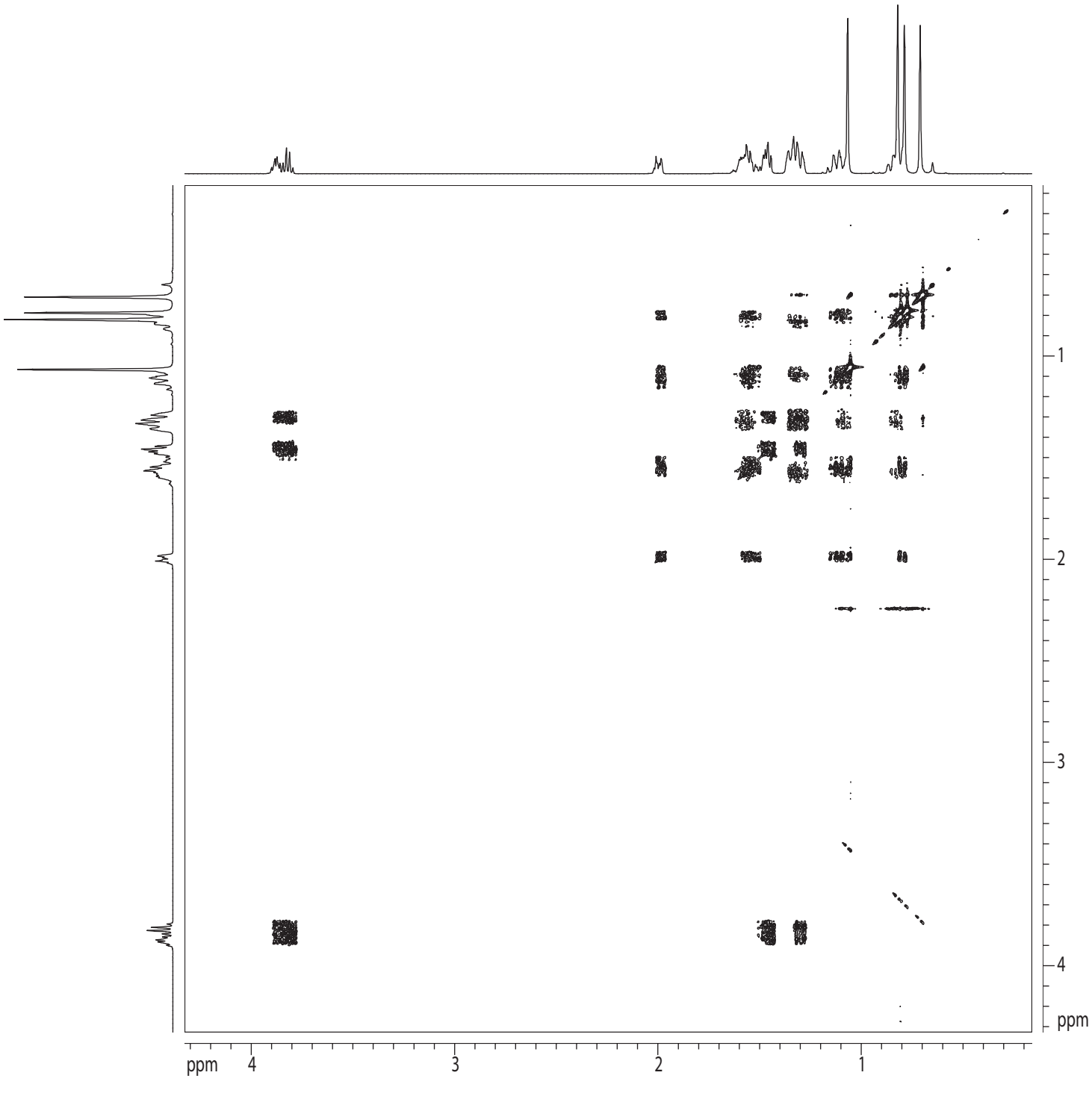
F1 - Acquisition parameters
ND0 1
TD 512
SFO1 500.2211 MHz
FIDRES 4.069010 Hz
SW 4.165 ppm
FnMODE undefined

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

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 4.326 ppm
F2LO 2164.12 Hz
F2PHI 0.162 ppm
F2HI 80.79 Hz
F1PLO 4.326 ppm
F1LO 2164.12 Hz
F1PHI 0.162 ppm
F1HI 80.79 Hz
F2PPMCM 0.27766 ppm/cm
F2HZCM 138.88889 Hz/cm
F1PPMCM 0.27766 ppm/cm
F1HZCM 138.88889 Hz/cm

gtocsy



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PROCNO 1

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Time 22.32
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG mlevgp_mo
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 2083.333 Hz
FIDRES 1.017253 Hz
AQ 0.4915700 sec
RG 35.9
DW 240.000 usec
DE 6.00 usec
TE 298.0 K
d0 0.00000300 sec
D1 2.00000000 sec
D9 0.06000000 sec
d12 0.00002000 sec
D16 0.00020000 sec
FACTOR1 4
IN0 0.00048000 sec
l1 24
SCALEF 6

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p5 23.34 usec
P6 35.00 usec
p7 70.00 usec
P17 2500.00 usec
PL1 1.60 dB
PL10 15.20 dB
SFO1 500.2211225 MHz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1000.00 usec

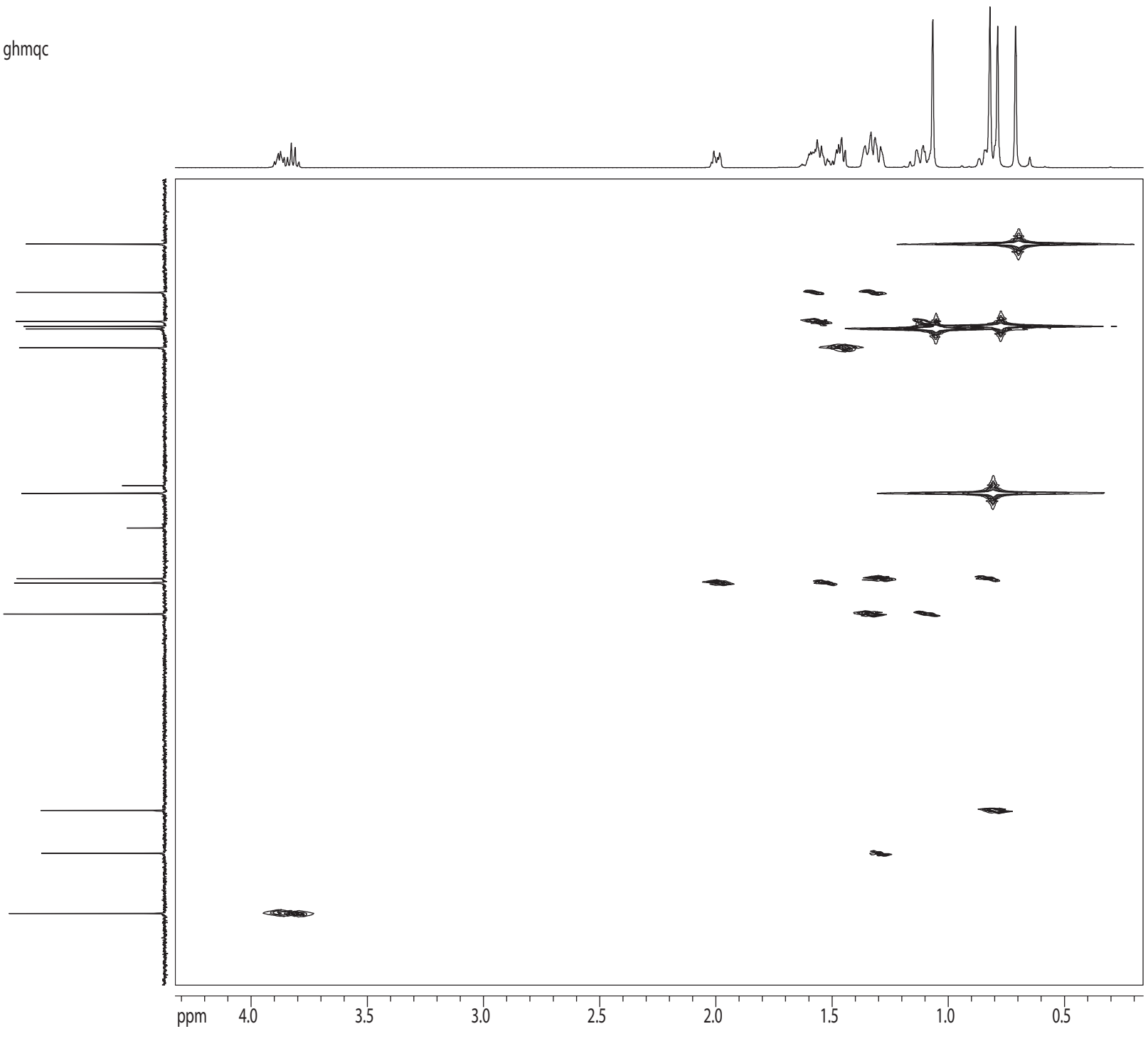
F1 - Acquisition parameters
ND0 1
TD 512
SFO1 500.2211 MHz
FIDRES 4.069010 Hz
SW 4.165 ppm
FnMODE undefined

F2 - Processing parameters
SI 1024
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 4.326 ppm
F2LO 2164.12 Hz
F2PHI 0.162 ppm
F2HI 80.79 Hz
F1PLO 4.326 ppm
F1LO 2164.12 Hz
F1PHI 0.162 ppm
F1HI 80.79 Hz
F2PPMCM 0.27766 ppm/cm
F2HZCM 138.88889 Hz/cm
F1PPMCM 0.27766 ppm/cm
F1HZCM 138.88889 Hz/cm

ghmqc



Current Data Parameters
USER nmr11t
NAME nmr-X-sample11
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111201
Time 0.04
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG inv4gp.wu
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 2083.333 Hz
FIDRES 1.017253 Hz
AQ 0.4915700 sec
RG 7298.2
DW 240.000 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 0.00004960 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2211225 MHz

======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7865620 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

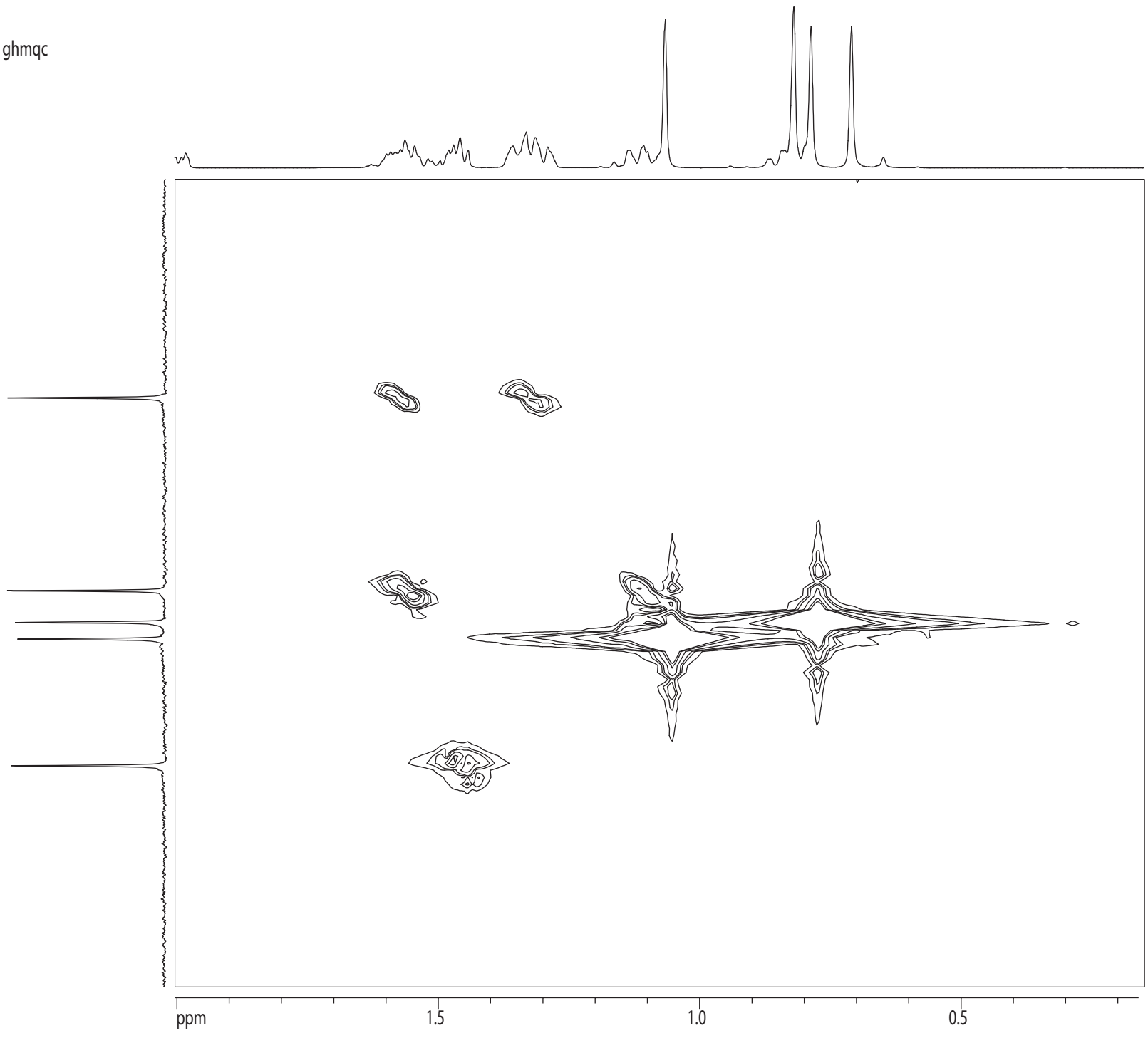
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7866 MHz
FIDRES 19.688761 Hz
SW 80.141 ppm
FnMODE undefined

F2 - Processing parameters
SI 1024
SF 500.2200000 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 125.7804190 MHz
WDW QSINE
SSB 3
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 18.00 cm
CX1 15.00 cm
F2PLO 4.326 ppm
F2LO 2164.12 Hz
F2PHI 0.162 ppm
F2HI 80.79 Hz
F1PLO 70.000 ppm
F1LO 8804.63 Hz
F1PHI 10.000 ppm
F1HI 1257.80 Hz
F2PPMCM 0.23138 ppm/cm
F2HZCM 115.74074 Hz/cm
F1PPMCM 4.00000 ppm/cm
F1HZCM 503.12167 Hz/cm

ghmqc



Current Data Parameters
USER nmr11t
NAME nmr-X-sample11
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111201
Time 0.04
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG inv4gp.wu
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 2083.333 Hz
FIDRES 1.017253 Hz
AQ 0.4915700 sec
RG 7298.2
DW 240.000 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 0.00004960 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2211225 MHz

======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7865620 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

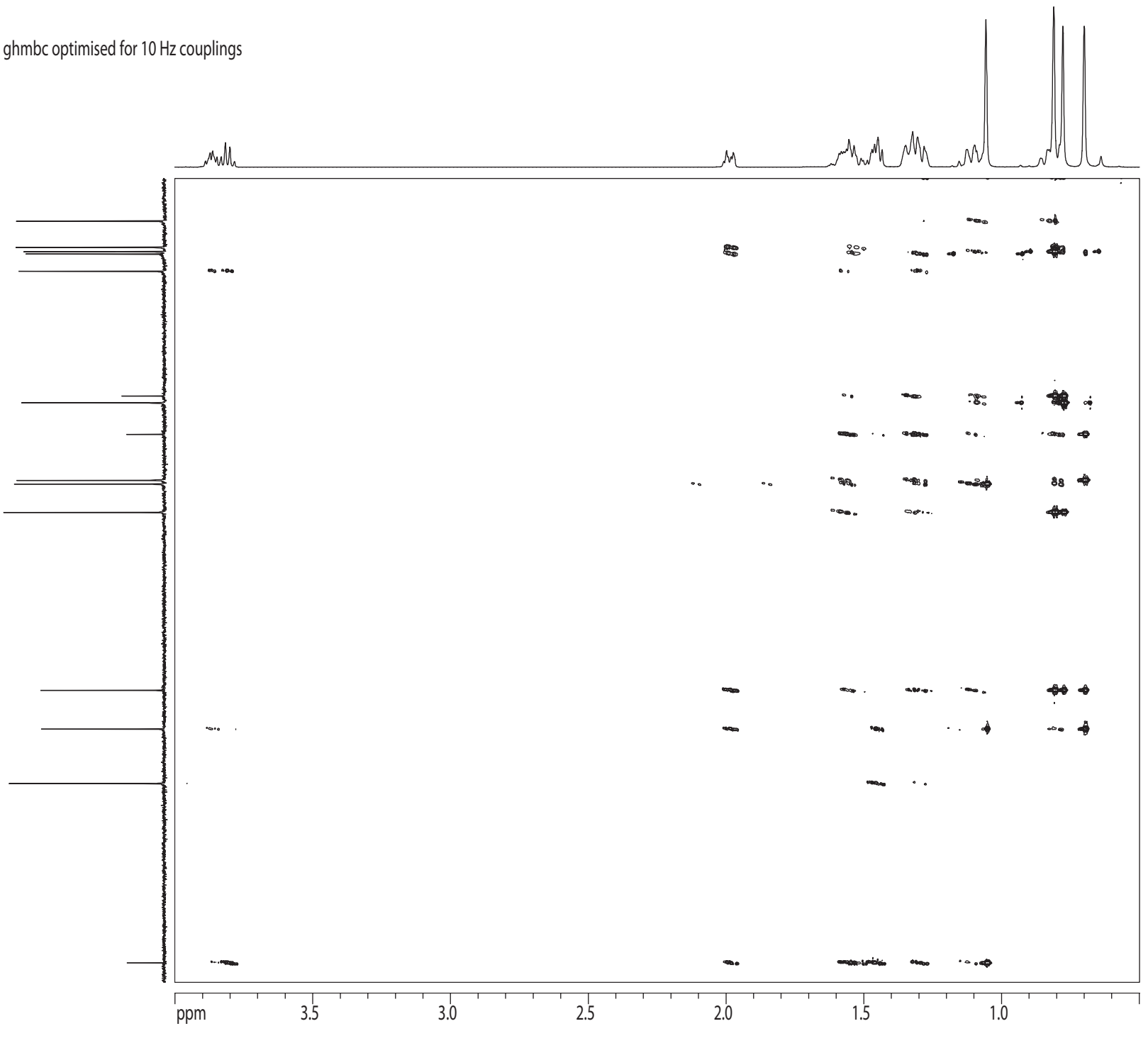
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7866 MHz
FIDRES 19.688761 Hz
SW 80.141 ppm
FnMODE undefined

F2 - Processing parameters
SI 1024
SF 500.2200000 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 125.7804190 MHz
WDW QSINE
SSB 3
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 18.00 cm
CX1 15.00 cm
F2PLO 2.004 ppm
F2LO 1002.42 Hz
F2PHI 0.149 ppm
F2HI 74.69 Hz
F1PLO 25.046 ppm
F1LO 3150.33 Hz
F1PHI 16.000 ppm
F1HI 2012.49 Hz
F2PPMCM 0.10304 ppm/cm
F2HZCM 51.54080 Hz/cm
F1PPMCM 0.60308 ppm/cm
F1HZCM 75.85626 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters
USER nmr11t
NAME nmr-X-sample11
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111201
Time 0.57
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT CDCl3
NS 4
DS 16
SWH 2083.333 Hz
FIDRES 0.508626 Hz
AQ 0.9830900 sec
RG 8192
DW 240.000 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 0.00004960 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2211225 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7865620 MHz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.00 %
P16 1000.00 usec

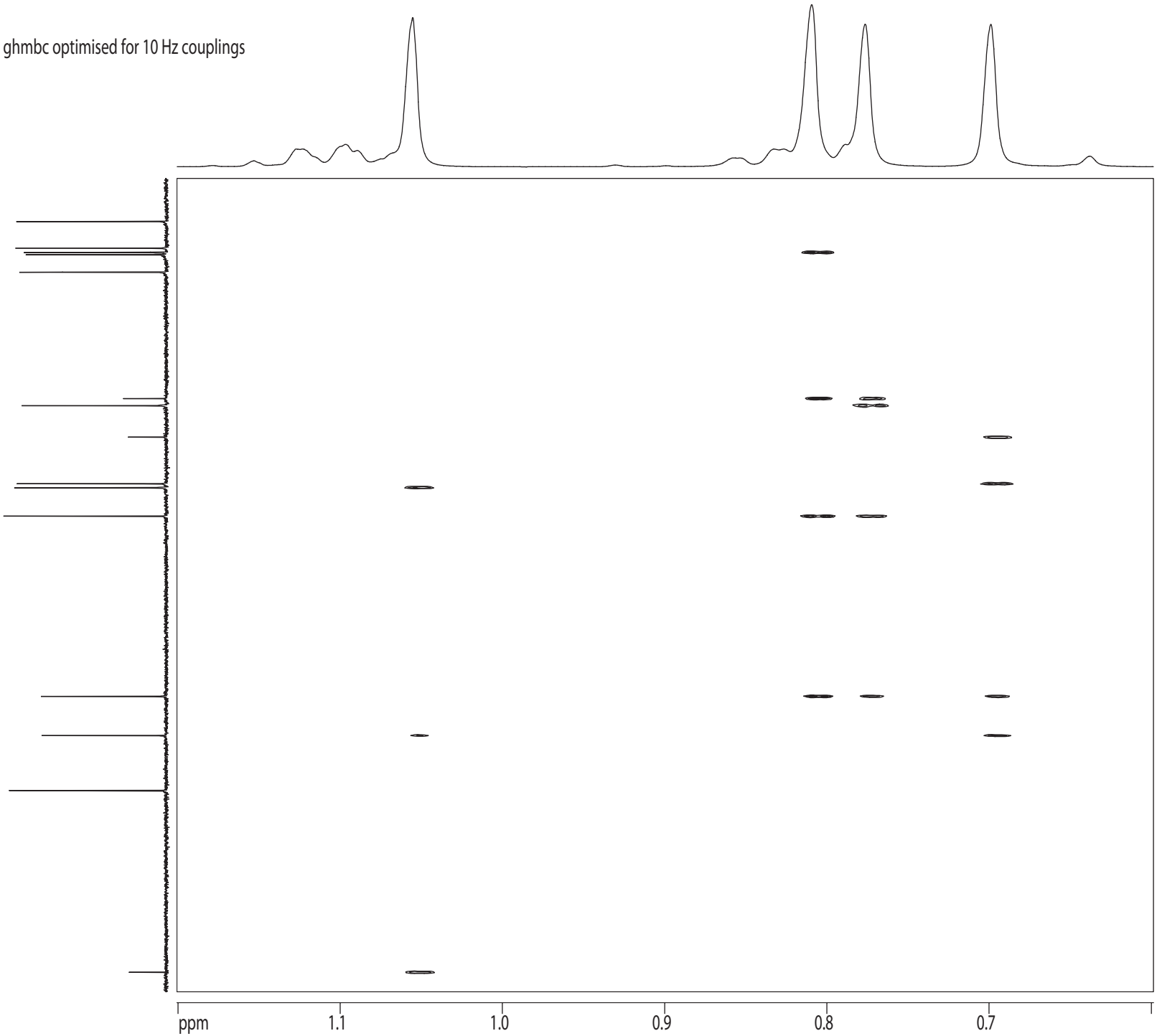
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7866 MHz
FIDRES 19.688761 Hz
SW 80.141 ppm
FnMODE undefined

F2 - Processing parameters
SI 2048
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 125.7804190 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 18.00 cm
CX1 15.00 cm
F2PLO 4.001 ppm
F2LO 2001.36 Hz
F2PHI 0.499 ppm
F2HI 249.65 Hz
F1PLO 81.007 ppm
F1LO 10189.06 Hz
F1PHI 14.950 ppm
F1HI 1880.41 Hz
F2PPMCM 0.19455 ppm/cm
F2HZCM 97.31716 Hz/cm
F1PPMCM 4.40379 ppm/cm
F1HZCM 553.91046 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters
USER nmr11t
NAME nmr-X-sample11
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111201
Time 0.57
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT CDCl3
NS 4
DS 16
SWH 2083.333 Hz
FIDRES 0.508626 Hz
AQ 0.9830900 sec
RG 8192
DW 240.000 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 0.00004960 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2211225 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7865620 MHz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.00 %
P16 1000.00 usec

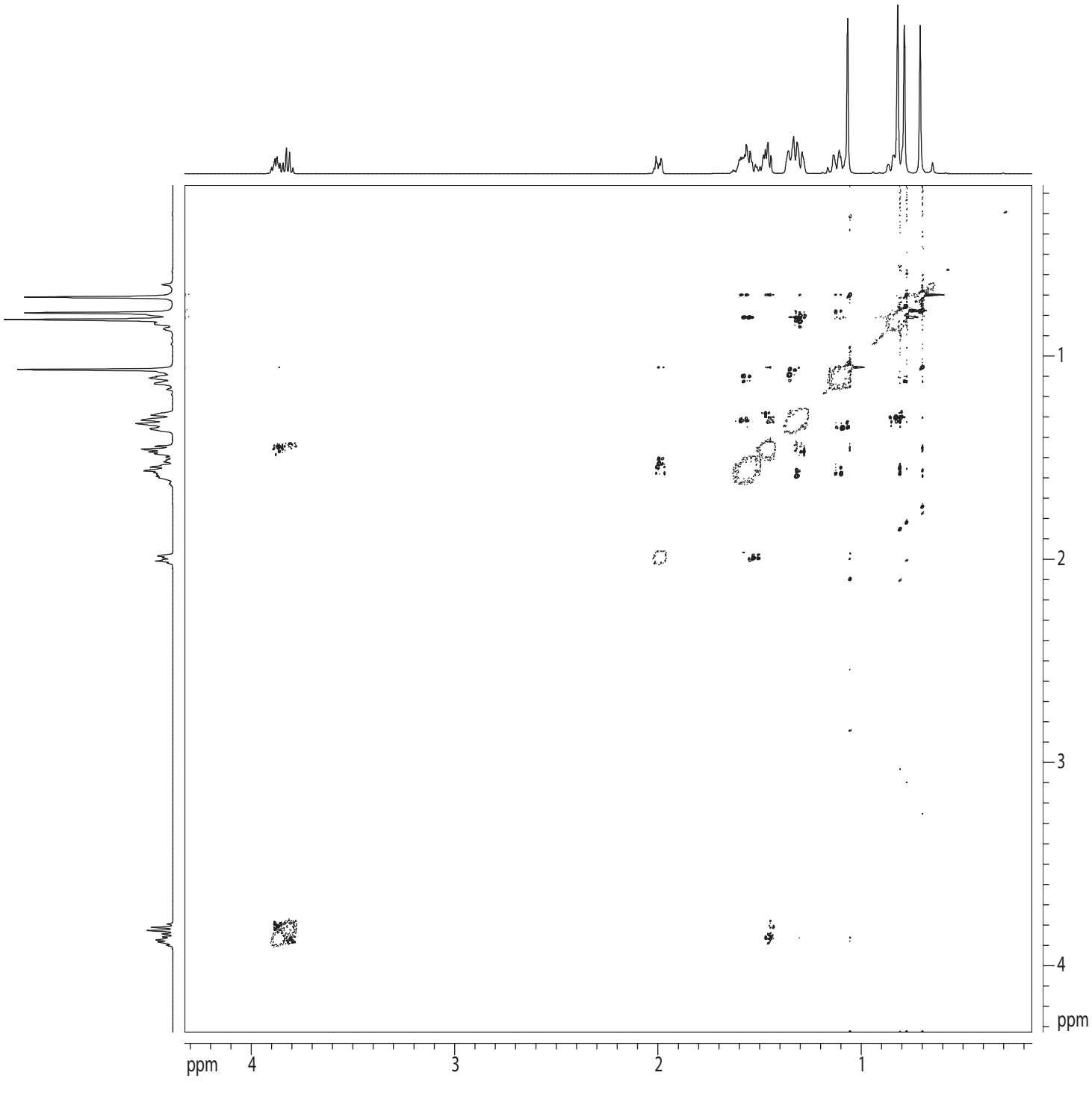
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7866 MHz
FIDRES 19.688761 Hz
SW 80.141 ppm
FnMODE undefined

F2 - Processing parameters
SI 2048
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 125.7804190 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 18.00 cm
CX1 15.00 cm
F2PLO 1.201 ppm
F2LO 600.61 Hz
F2PHI 0.599 ppm
F2HI 299.50 Hz
F1PLO 81.000 ppm
F1LO 10188.21 Hz
F1PHI 14.950 ppm
F1HI 1880.41 Hz
F2PPMCM 0.03344 ppm/cm
F2HZCM 16.72815 Hz/cm
F1PPMCM 4.40334 ppm/cm
F1HZCM 553.85388 Hz/cm

gnoesy



Current Data Parameters
USER nmr11t
NAME nmr-X-sample11
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111201
Time 2.17
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG noesygptp
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 2083.333 Hz
FIDRES 1.017253 Hz
AQ 0.4915700 sec
RG 25.4
DW 240.000 usec
DE 6.00 usec
TE 298.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D8 0.80000001 sec
D16 0.00020000 sec
d20 0.39880002 sec
IN0 0.00024000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
P2 15.00 usec
PL1 1.60 dB
SFO1 500.2211225 MHz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec

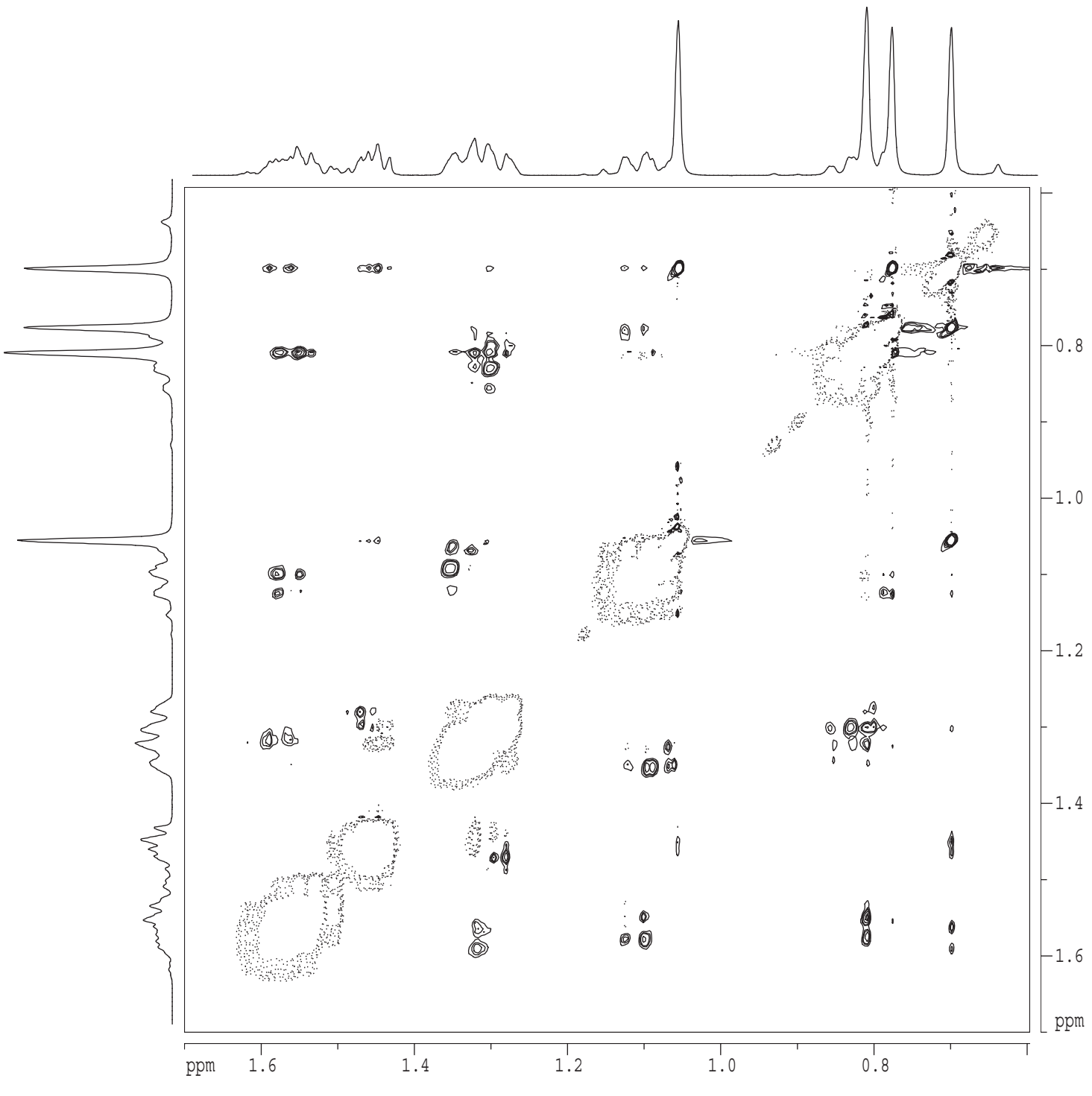
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 500.2211 MHz
FIDRES 4.069010 Hz
SW 4.165 ppm
FnMODE undefined

F2 - Processing parameters
SI 1024
SF 500.2200000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 TPPI
SF 500.2200000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 4.326 ppm
F2LO 2164.12 Hz
F2PHI 0.162 ppm
F2HI 80.79 Hz
F1PLO 4.326 ppm
F1LO 2164.12 Hz
F1PHI 0.162 ppm
F1HI 80.79 Hz
F2PPMCM 0.27766 ppm/cm
F2HZCM 138.88889 Hz/cm
F1PPMCM 0.27766 ppm/cm
F1HZCM 138.88889 Hz/cm

gnoesy



Current Data Parameters

USER	nmr11t
NAME	nmr-X-sample11
EXPNO	12
PROCNO	1

F2 - Acquisition Parameters

Date_	20111201
Time	2.17
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	noesygptp
TD	2048
SOLVENT	CDCl3
NS	4
DS	16
SWH	2083.333 Hz
FIDRES	1.017253 Hz
AQ	0.4915700 sec
RG	25.4
DW	240.000 usec
DE	6.00 usec
TE	298.0 K
D0	0.00000300 sec
D1	2.00000000 sec
D8	0.80000001 sec
D16	0.00020000 sec
d20	0.39880002 sec
IN0	0.00024000 sec

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

NUC1	1H
P1	7.50 usec
P2	15.00 usec
PL1	1.60 dB
SFO1	500.2211225 MHz

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

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	40.00 %
GPZ2	-40.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	2
TD	512
SFO1	500.2211 MHz
FIDRES	4.069010 Hz
SW	4.165 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40

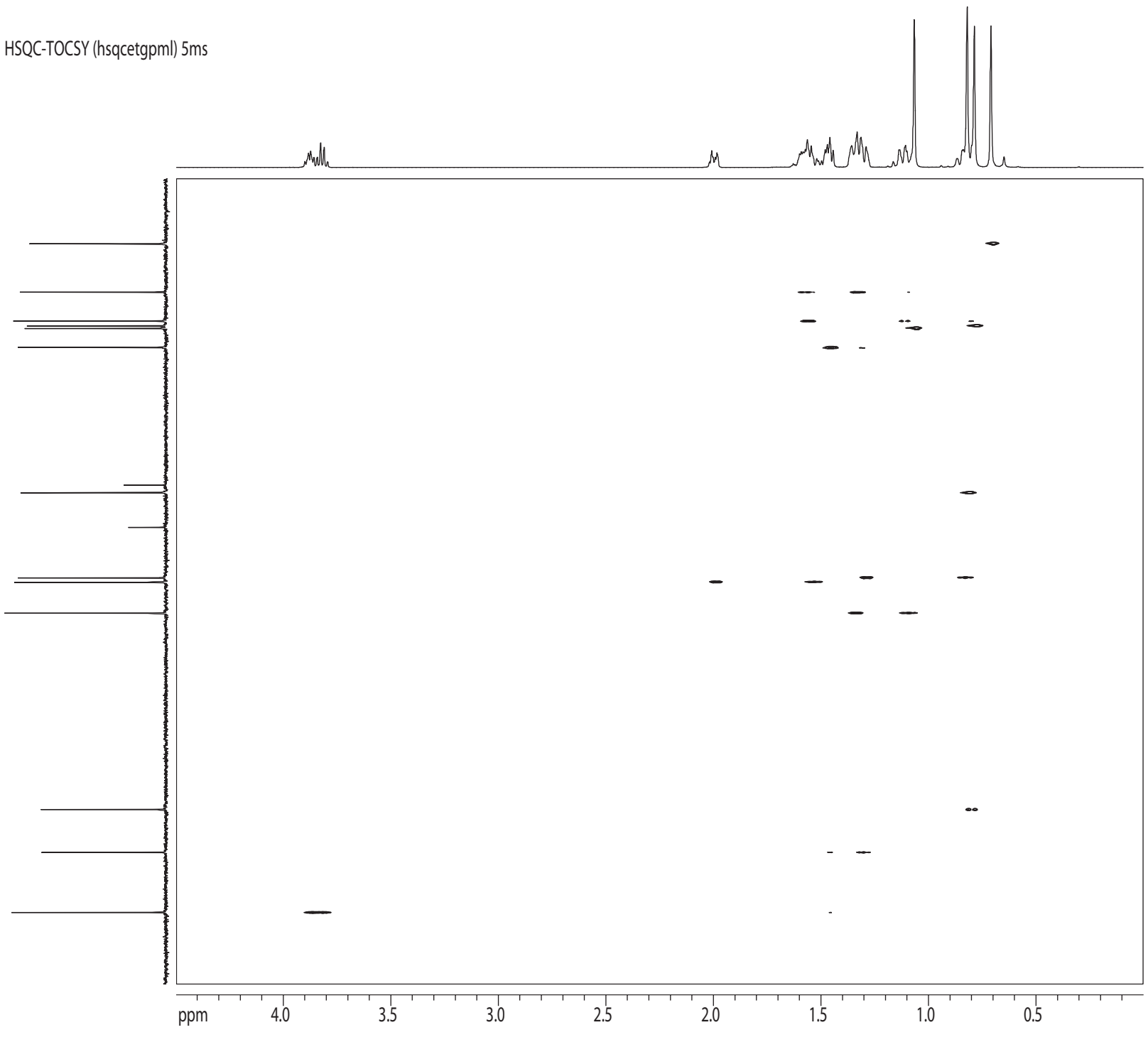
F1 - Processing parameters

SI	1024
MC2	TPPI
SF	500.2200000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	1.700 ppm
F2LO	850.37 Hz
F2PHI	0.597 ppm
F2HI	298.48 Hz
F1PLO	1.700 ppm
F1LO	850.37 Hz
F1PHI	0.593 ppm
F1HI	296.45 Hz
F2PPMCM	0.07355 ppm/cm
F2HZCM	36.79276 Hz/cm
F1PPMCM	0.07382 ppm/cm
F1HZCM	36.92840 Hz/cm

HSQC-TOCSY (hsqcetgpml) 5ms



Current Data Parameters
USER nmr11t
NAME nmr-X-sample11
EXPNO 18
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111206
Time 21.27
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpml
TD 2048
SOLVENT C6D6
NS 4
DS 32
SWH 2248.201 Hz
FIDRES 1.097755 Hz
AQ 0.4555252 sec
RG 5160.6
DW 222.400 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 0.00020000 sec
DELTA 0.00122100 sec
DELTA1 0.00120800 sec
FACTOR1 0
IN0 0.00004680 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 500.2211251 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 125.7863936 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

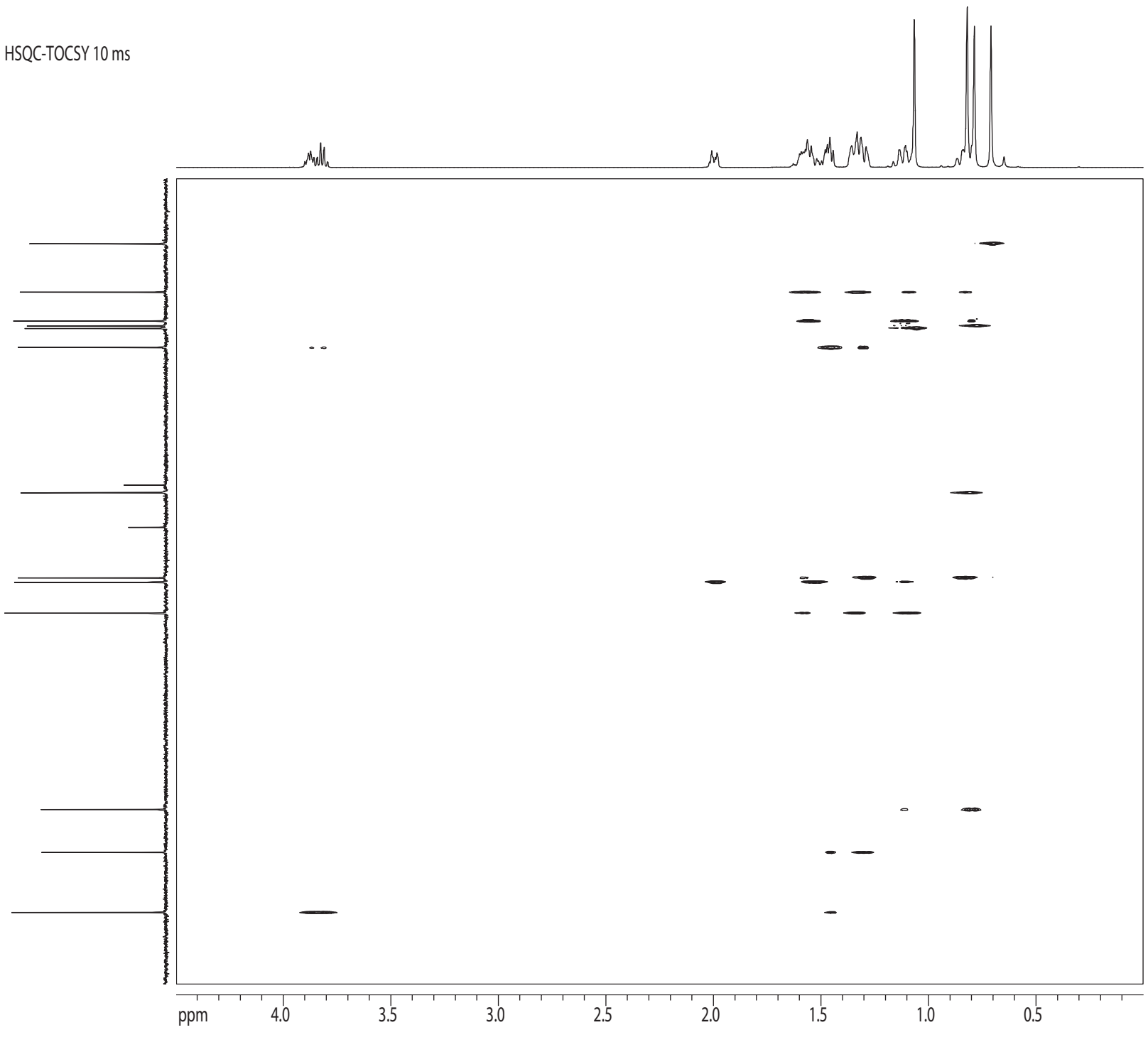
F1 - Acquisition parameters
ND0 2
TD 1024
SFO1 125.7864 MHz
FIDRES 10.433360 Hz
SW 84.936 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.2200000 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.00

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 4.496 ppm
F2LO 2249.15 Hz
F2PHI 0.002 ppm
F2HI 0.95 Hz
F1PLO 70.000 ppm
F1LO 8804.63 Hz
F1PHI 10.000 ppm
F1HI 1257.80 Hz
F2PPMCM 0.24969 ppm/cm
F2HZCM 124.90008 Hz/cm
F1PPMCM 4.00000 ppm/cm
F1HZCM 503.12167 Hz/cm

HSQC-TOCSY 10 ms



Current Data Parameters
USER nmr11t
NAME nmr-X-sample11
EXPNO 19
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111207
Time 0.19
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpml
TD 2048
SOLVENT C6D6
NS 4
DS 32
SWH 2248.201 Hz
FIDRES 1.097755 Hz
AQ 0.4555252 sec
RG 4597.6
DW 222.400 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
IN0 0.00004680 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 500.2211251 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 125.7863936 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

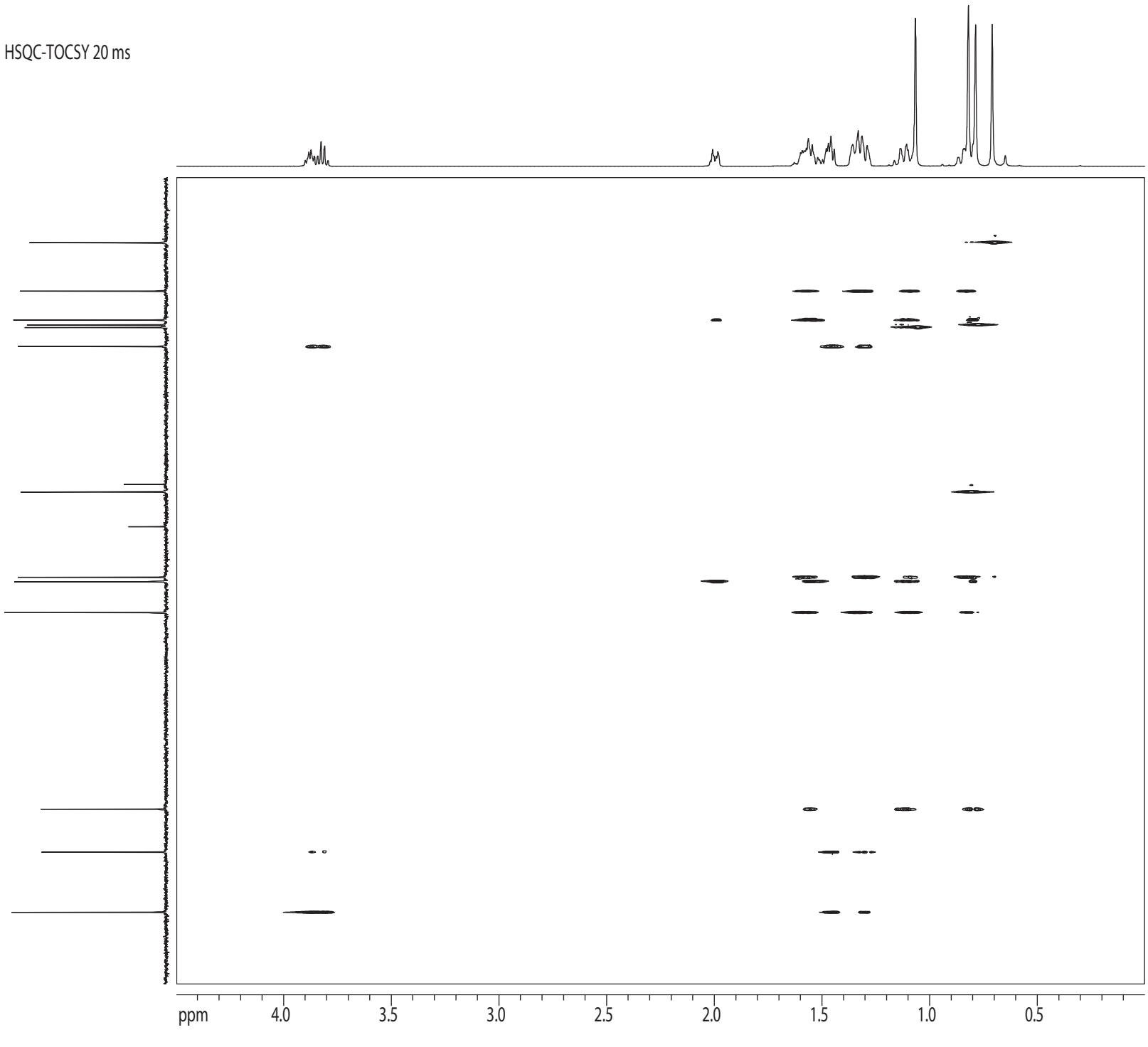
F1 - Acquisition parameters
ND0 2
TD 1024
SFO1 125.7864 MHz
FIDRES 10.433360 Hz
SW 84.936 ppm
FnMODE Echo-Antiecho

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-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 4.496 ppm
F2LO 2249.15 Hz
F2PHI 0.002 ppm
F2HI 0.95 Hz
F1PLO 70.000 ppm
F1LO 8804.63 Hz
F1PHI 10.000 ppm
F1HI 1257.80 Hz
F2PPMCM 0.24969 ppm/cm
F2HZCM 124.90008 Hz/cm
F1PPMCM 4.00000 ppm/cm
F1HZCM 503.12167 Hz/cm

HSQC-TOCSY 20 ms



Current Data Parameters
USER nmr11t
NAME nmr-X-sample11
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111207
Time 3.11
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpml
TD 2048
SOLVENT C6D6
NS 4
DS 32
SWH 2248.201 Hz
FIDRES 1.097755 Hz
AQ 0.4555252 sec
RG 4096
DW 222.400 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 0.02000000 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
IN0 0.00004680 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 15.20 dB
SFO1 500.2211251 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 125.7863936 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

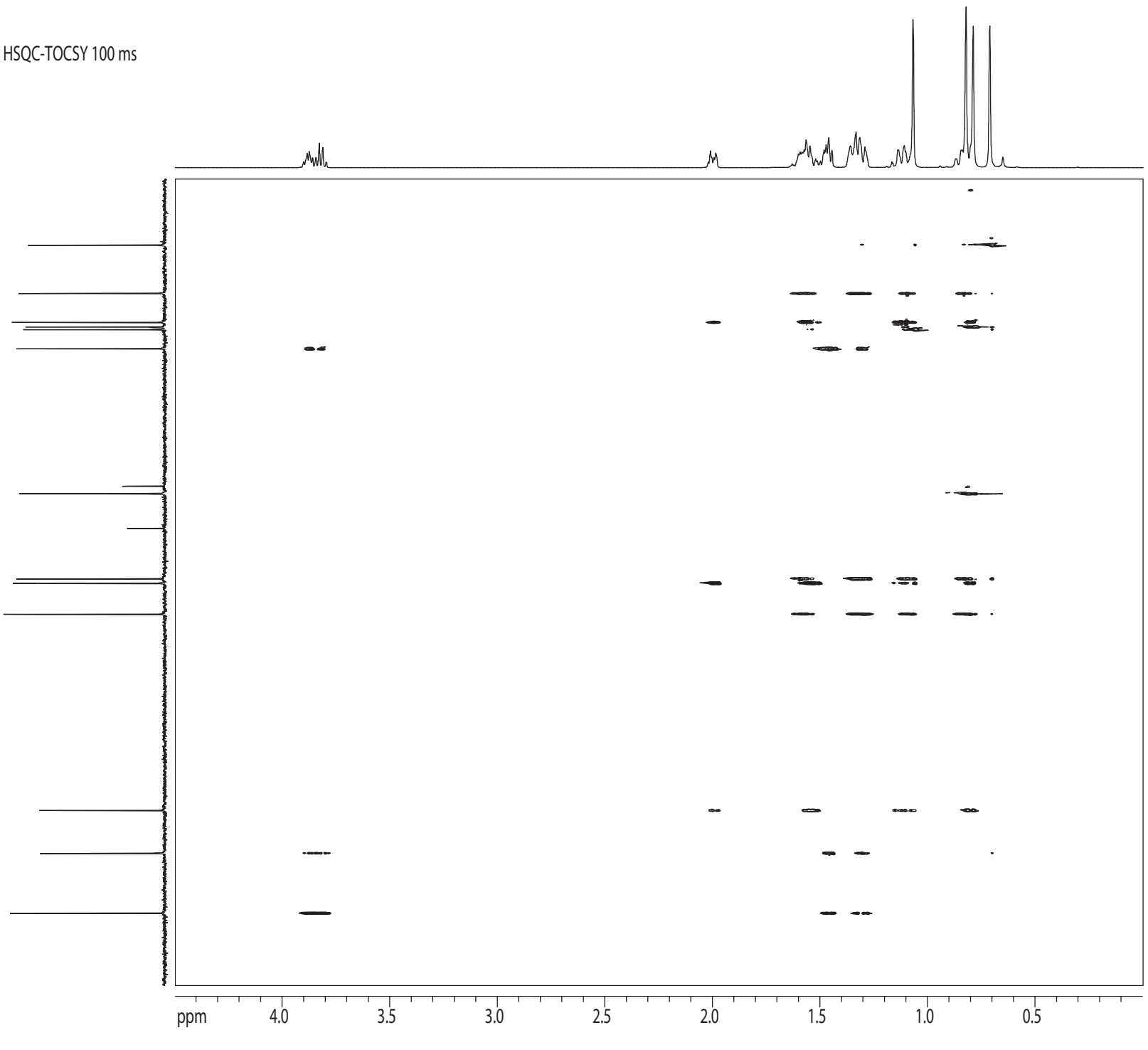
F1 - Acquisition parameters
ND0 2
TD 1024
SFO1 125.7864 MHz
FIDRES 10.433360 Hz
SW 84.936 ppm
FnMODE Echo-Antiecho

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-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 4.496 ppm
F2LO 2249.15 Hz
F2PHI 0.002 ppm
F2HI 0.95 Hz
F1PLO 70.000 ppm
F1LO 8804.63 Hz
F1PHI 10.000 ppm
F1HI 1257.80 Hz
F2PPMCM 0.24969 ppm/cm
F2HZCM 124.90008 Hz/cm
F1PPMCM 4.00000 ppm/cm
F1HZCM 503.12167 Hz/cm

HSQC-TOCSY 100 ms



Current Data Parameters
USER nmr11t
NAME nmr-X-sample11
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111207
Time 6.05
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpml
TD 2048
SOLVENT C6D6
NS 4
DS 32
SWH 2248.201 Hz
FIDRES 1.097755 Hz
AQ 0.4555252 sec
RG 18390.4
DW 222.400 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 0.10000000 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 7
IN0 0.00004680 sec
I1 42
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 500.2211251 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 125.7863936 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
ND0 2
TD 1024
SFO1 125.7864 MHz
FIDRES 10.433360 Hz
SW 84.936 ppm
FnMODE 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-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 4.496 ppm
F2LO 2249.15 Hz
F2PHI -0.002 ppm
F2HI -1.24 Hz
F1PLO 70.062 ppm
F1LO 8812.44 Hz
F1PHI 9.924 ppm
F1HI 1248.25 Hz
F2PPMCM 0.24993 ppm/cm
F2HZCM 125.02204 Hz/cm
F1PPMCM 4.00920 ppm/cm
F1HZCM 504.27905 Hz/cm