Name: _____

Chem 203
December 15, 2012

Final Exam Part I
(40 points)

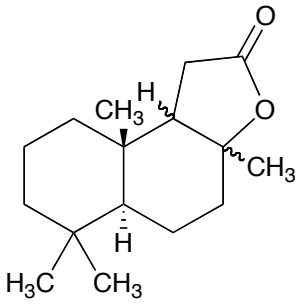
THIS FINAL EXAM CONSISTS OF PART I
AND TWO OUT OF THE THREE PROBLEMS FROM PART II

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

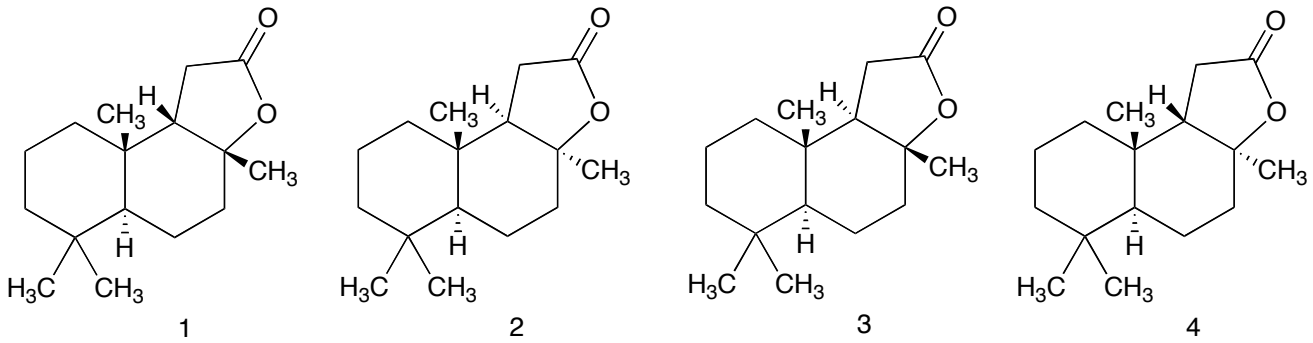
If you wish to unstaple the pages, please initial each page.

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.

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.



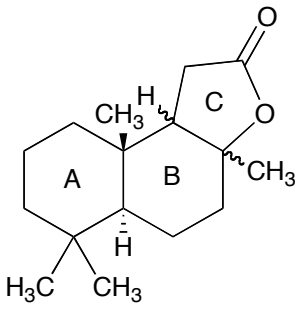
MAKE SURE TO COMPLETELY ANSWER THE QUESTIONS **a-g** ON PAGES 2-6.

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).

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.

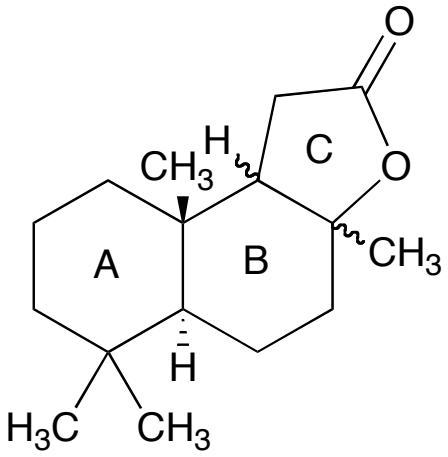
Finally, examine the HSQC-TOCSY spectrum with 100-ms mixing time and identify which methine and methylene resonances are associated with the three main spin systems in the molecule, which we will call the A-ring spin system, the B-ring spin system, and the C-ring spin system:

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: ___, ___, ___.

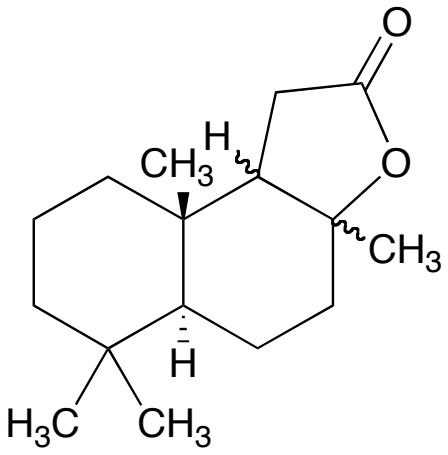
Numbers associated with the ^{13}C resonances associated with the C-ring spin system: ___, ___.

c. Examine the HSQC-TOCSY spectra with 5, 10, 20, and 100-ms mixing times. Assign the *five* 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.



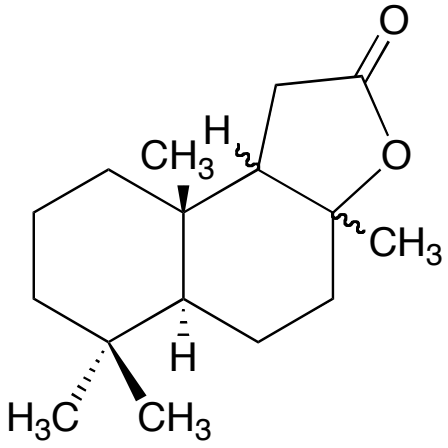
NOTE: Work the problem the way we did in class and is described in the assigned reading in "Two-Dimensional NMR Spectroscopy: Applications for Chemists and Biochemists." Start with the track that grows in under ^{1}H resonances *a* and *b* and assign one spin system. Then work with the track that grows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

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.

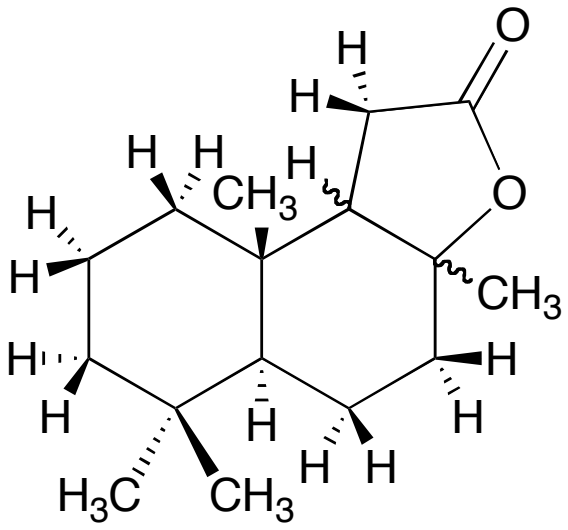
Transcribe your other numbers from Parts **c** and **d**, so that every carbon is numbered. Write the letters of the corresponding ^{1}H resonances next to the numbers.



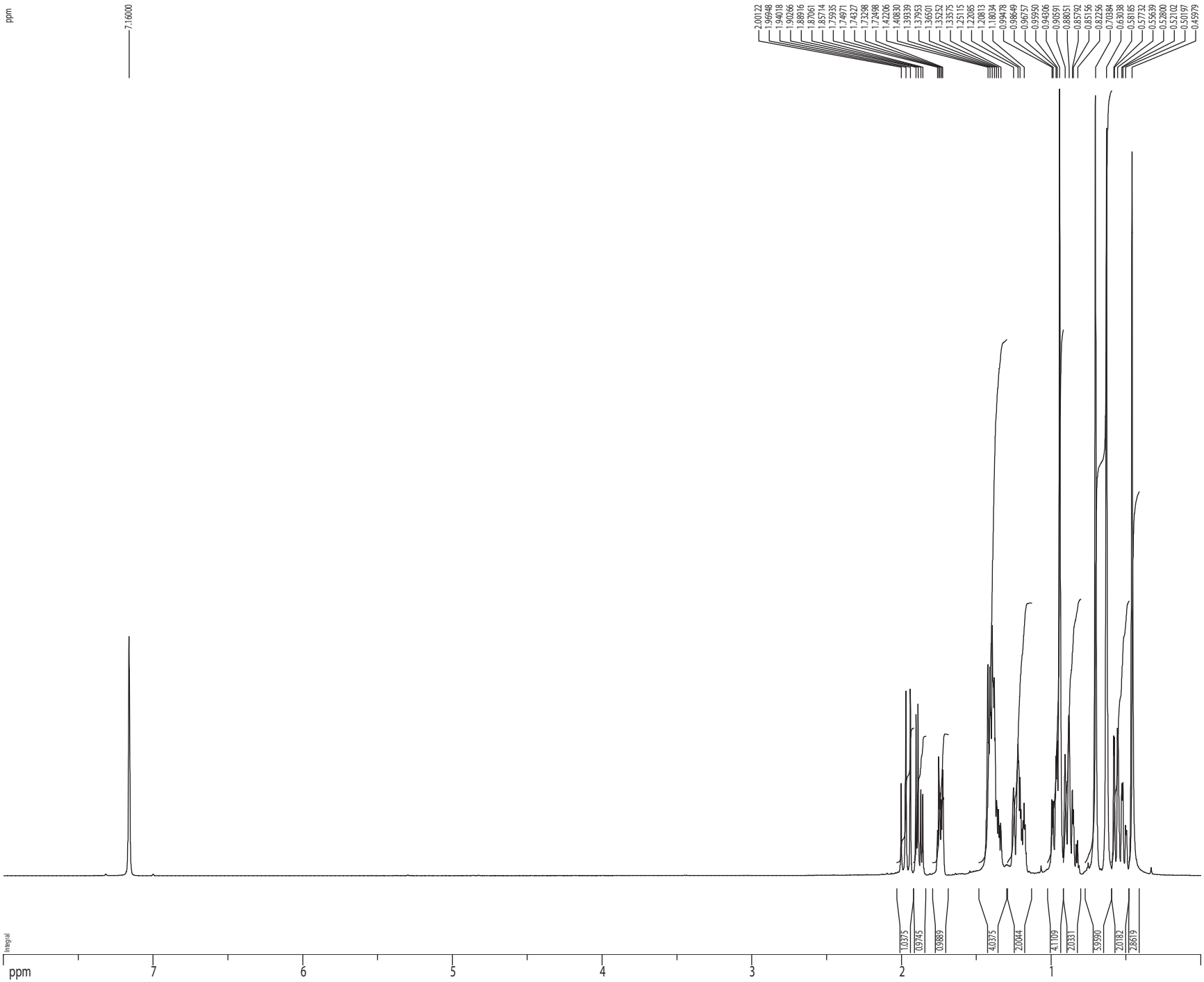
f. Determine the stereochemistry of the molecule. Which diastereomer is it? _____

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.



1H spectrum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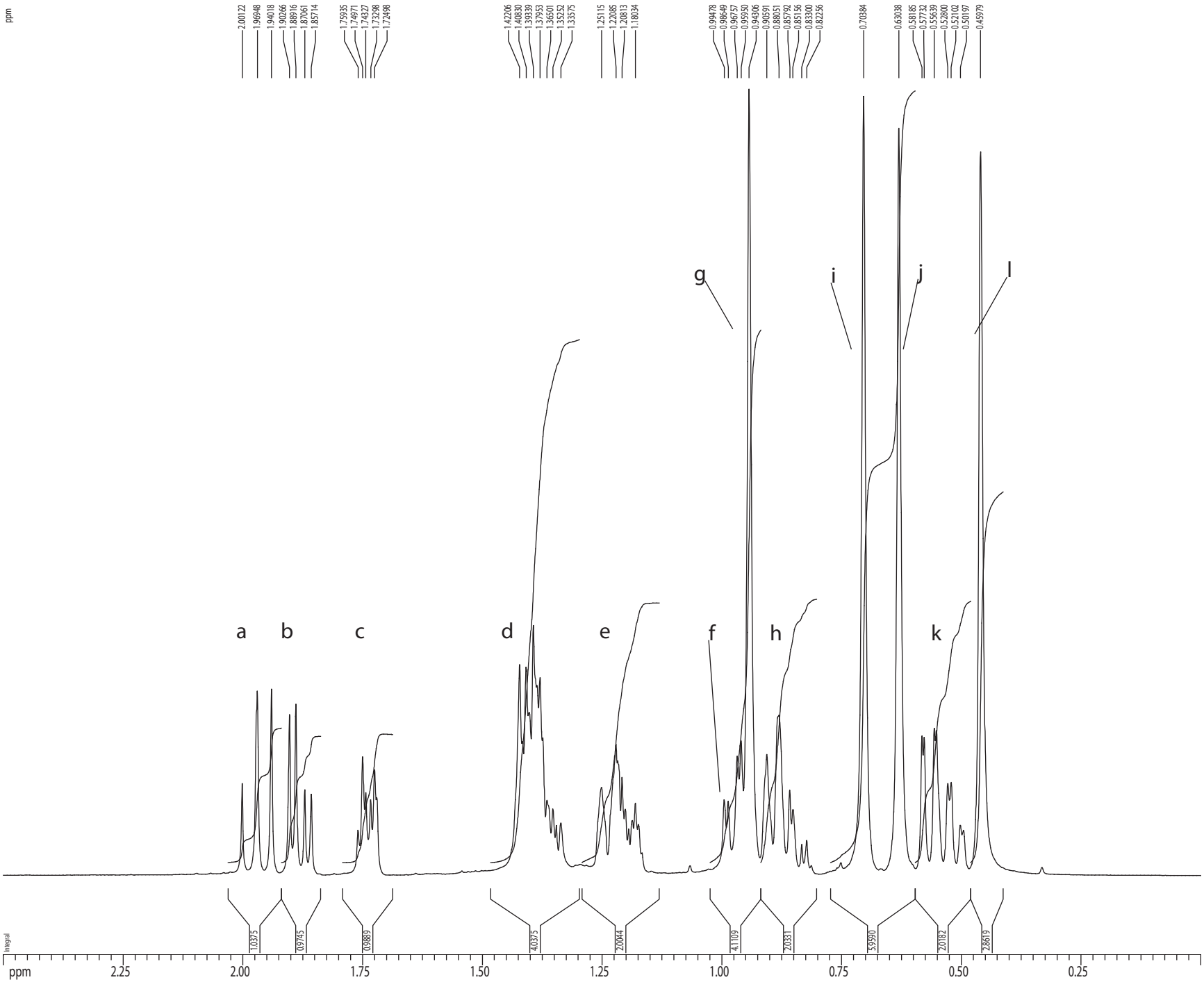
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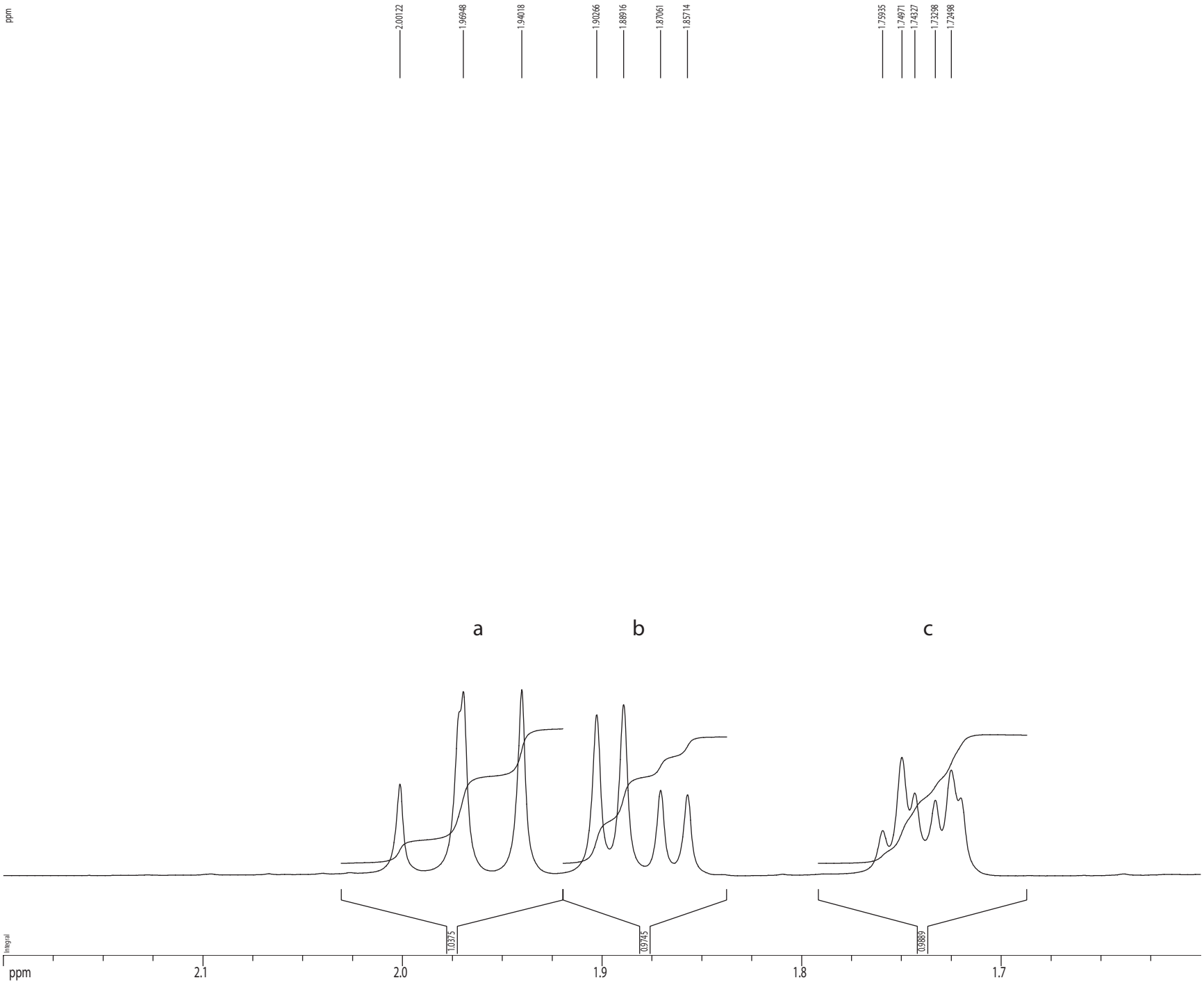
1H spectrum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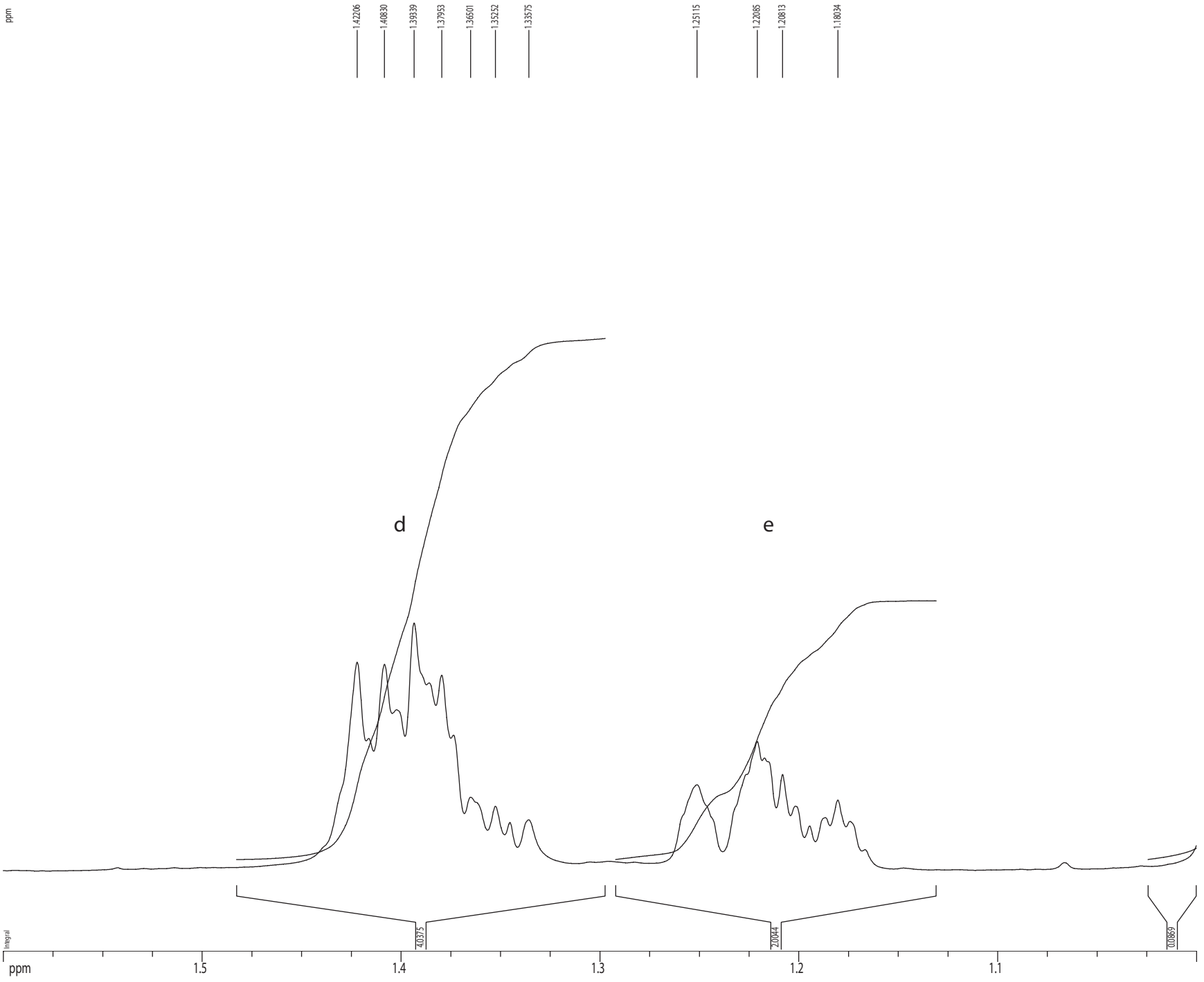
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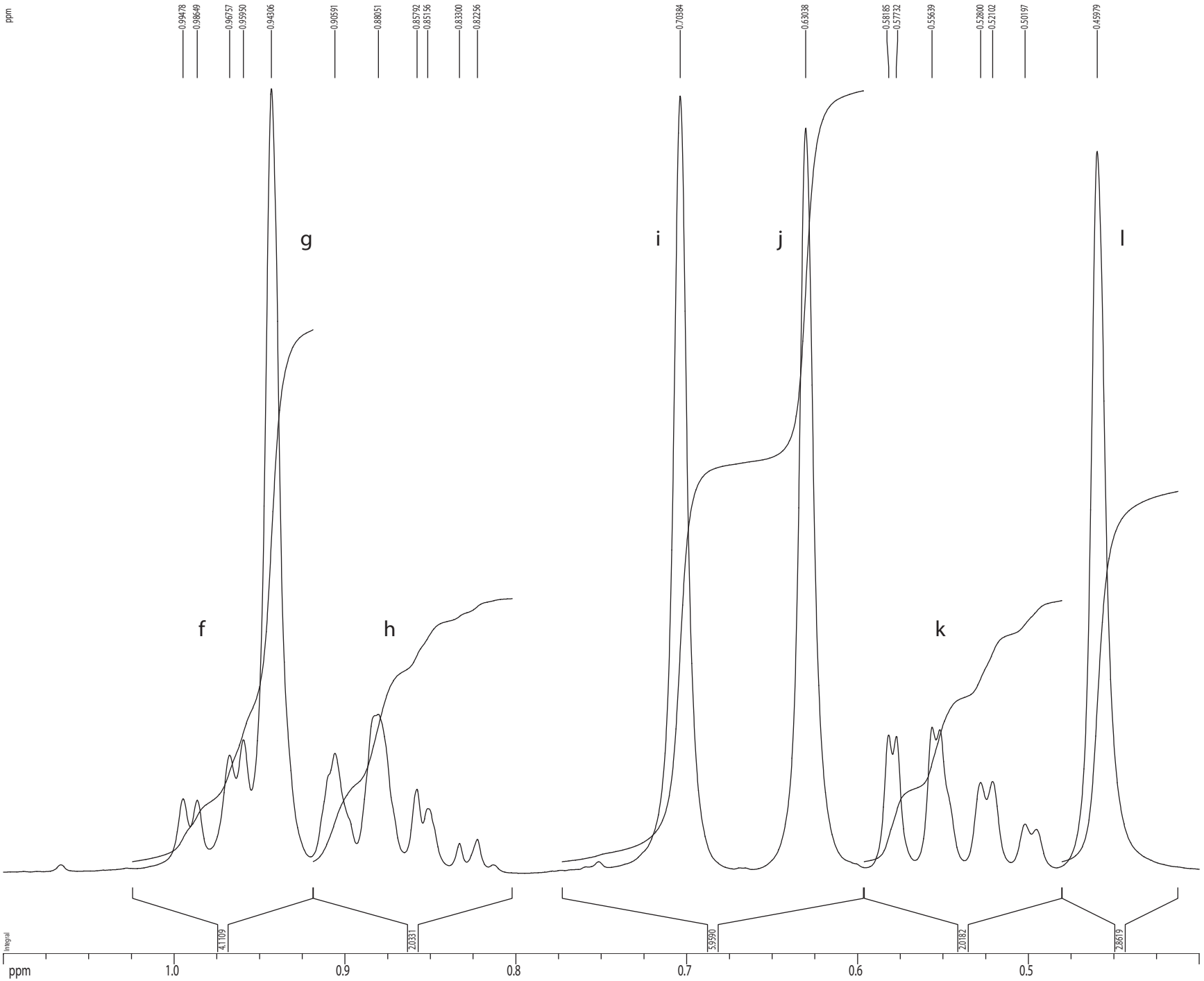
1H spectrum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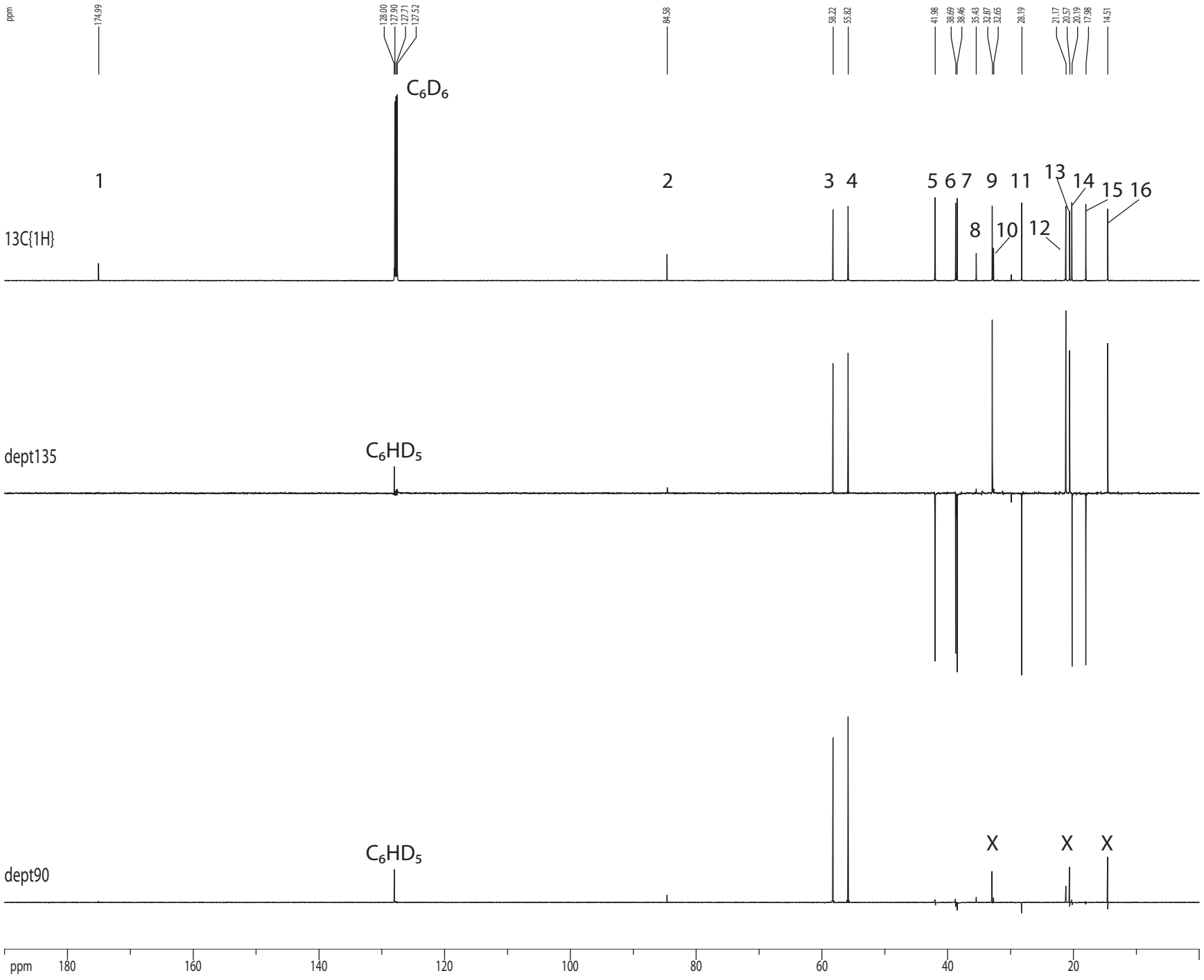
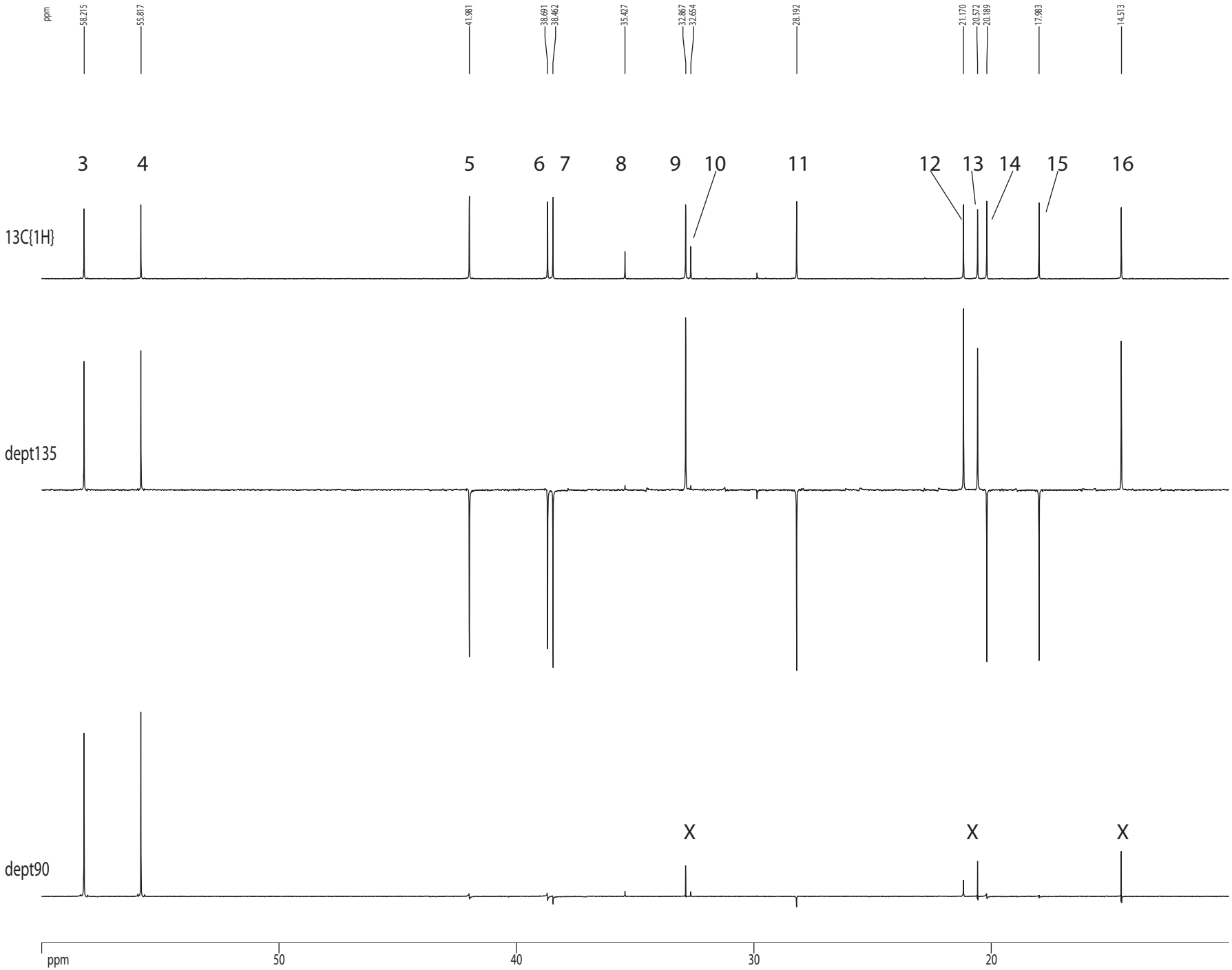


Z-restored spin-echo 13C spectrum with 1H decoupling



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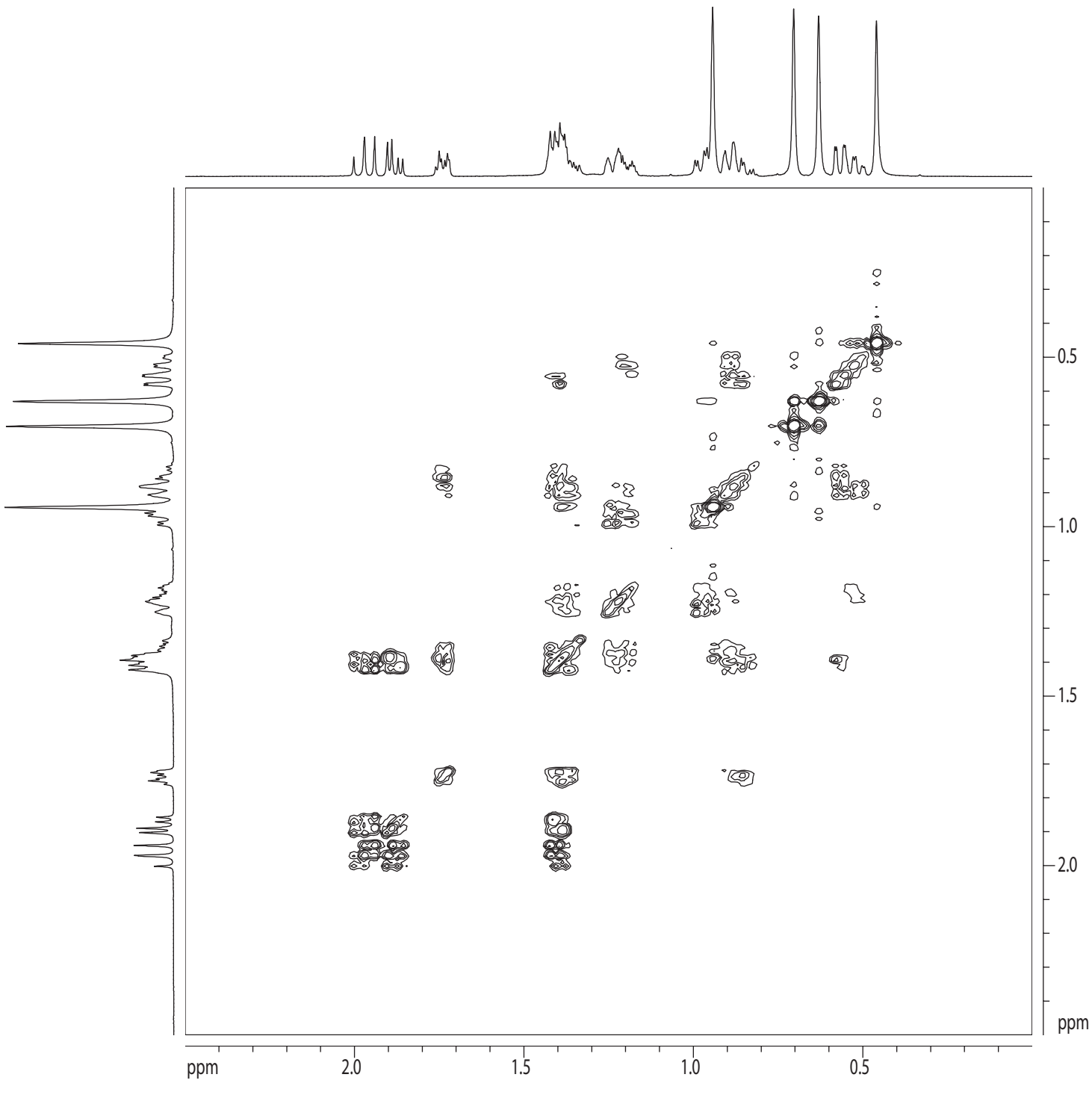

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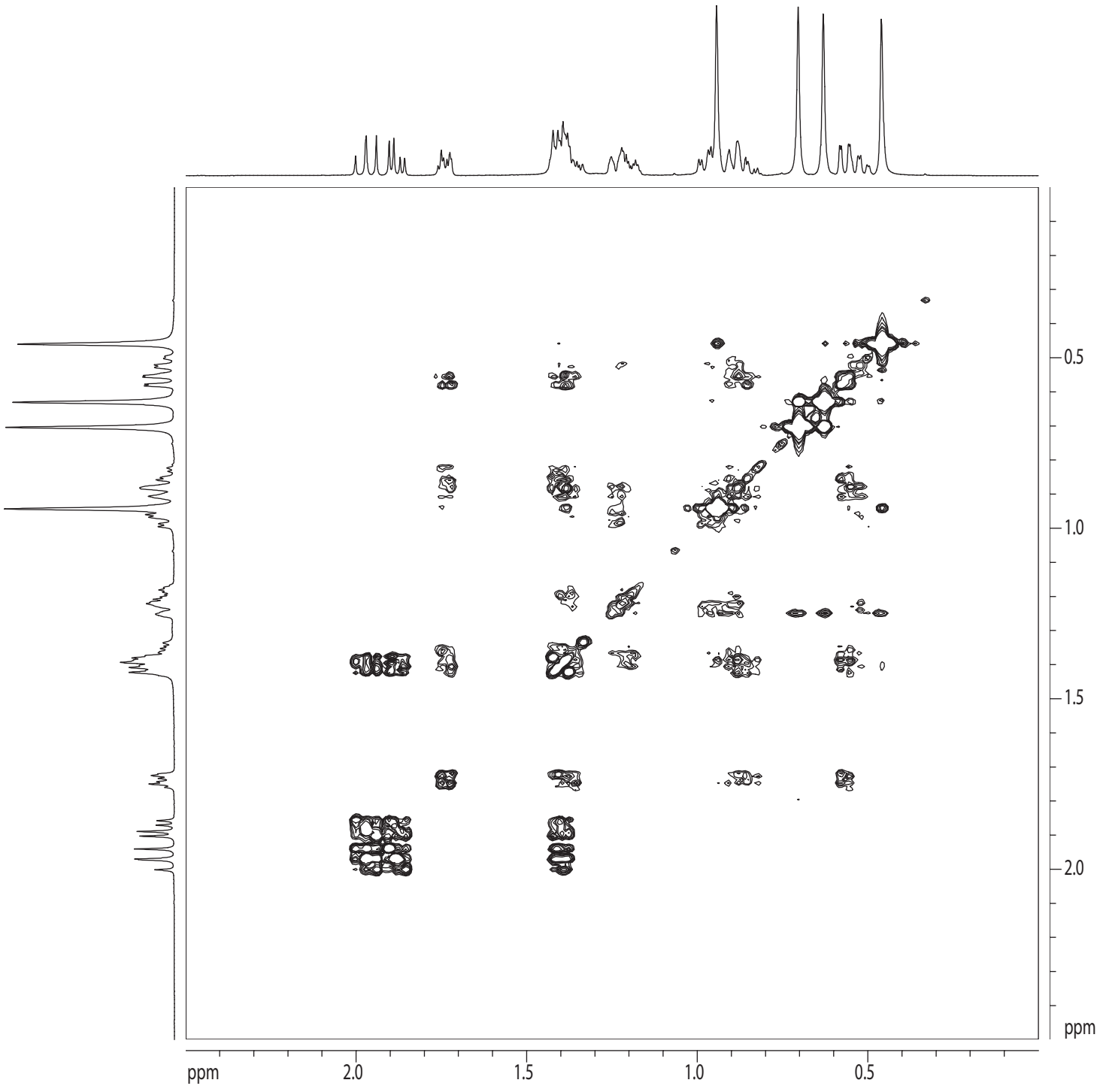

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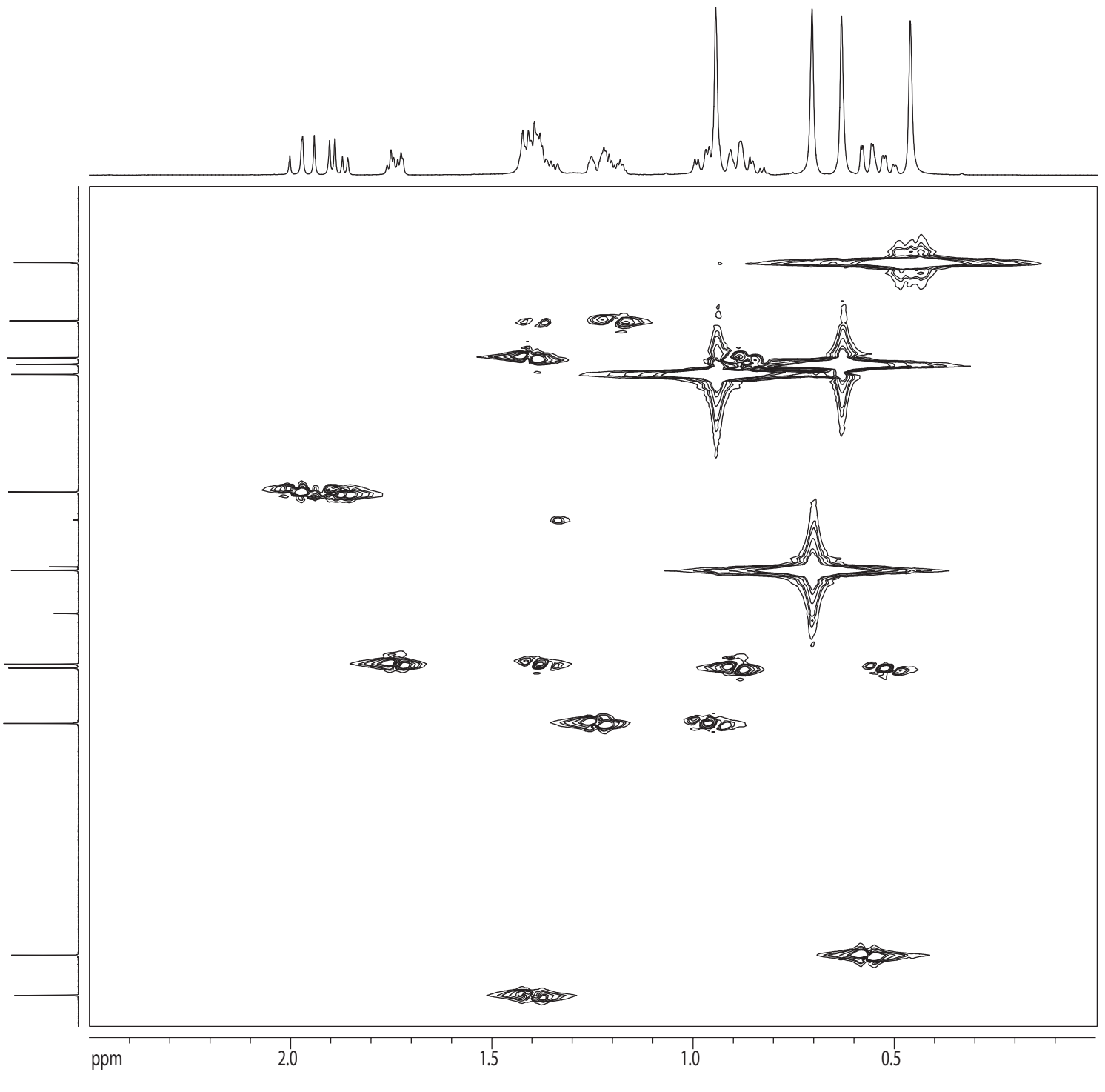

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GPY3 0.00 %
GPZ1 30.00 %
GPZ2 18.00 %
GPZ3 24.00 %
P16 1000.00 usec

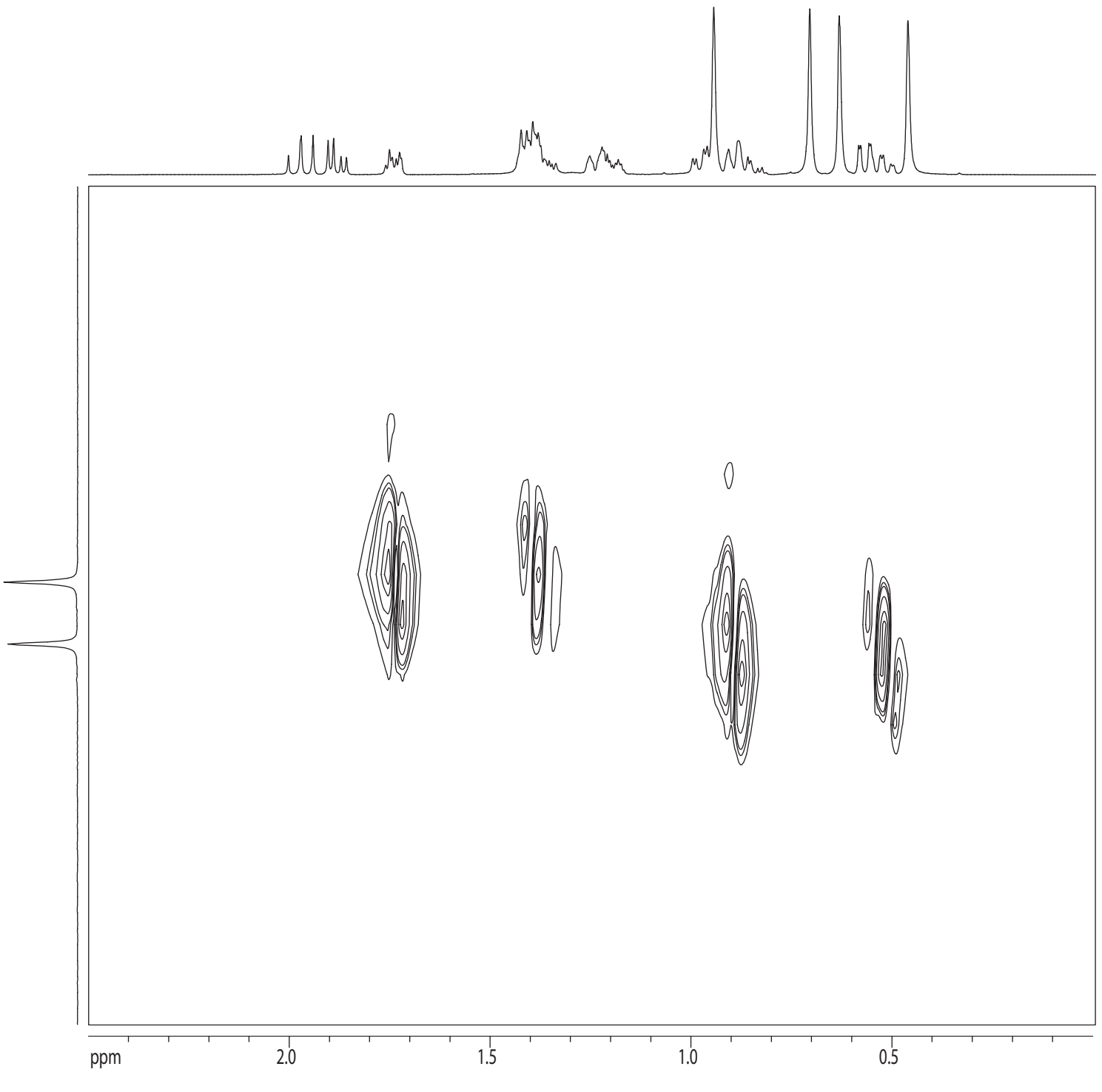
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7924 MHz
FIDRES 46.502975 Hz
SW 189.276 ppm
FnMODE undefined

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 2.499 ppm
F2LO 1250.27 Hz
F2PHI -0.004 ppm
F2HI -2.17 Hz
F1PLO 60.062 ppm
F1LO 7554.60 Hz
F1PHI 9.965 ppm
F1HI 1253.45 Hz
F2PPMCM 0.13910 ppm/cm
F2HZCM 69.58008 Hz/cm
F1PPMCM 3.33976 ppm/cm
F1HZCM 420.07687 Hz/cm

ghmqc



Current Data Parameters
USER nmr12t
NAME Fin_1_500
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121208
Time 1.10
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG inv4gp.wu
TD 2048
SOLVENT C6D6
NS 4
DS 16
SWH 1250.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 2048
DW 400.000 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 0.00002100 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2206253 MHz

======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7923681 MHz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 30.00 %
GPZ2 18.00 %
GPZ3 24.00 %
P16 1000.00 usec

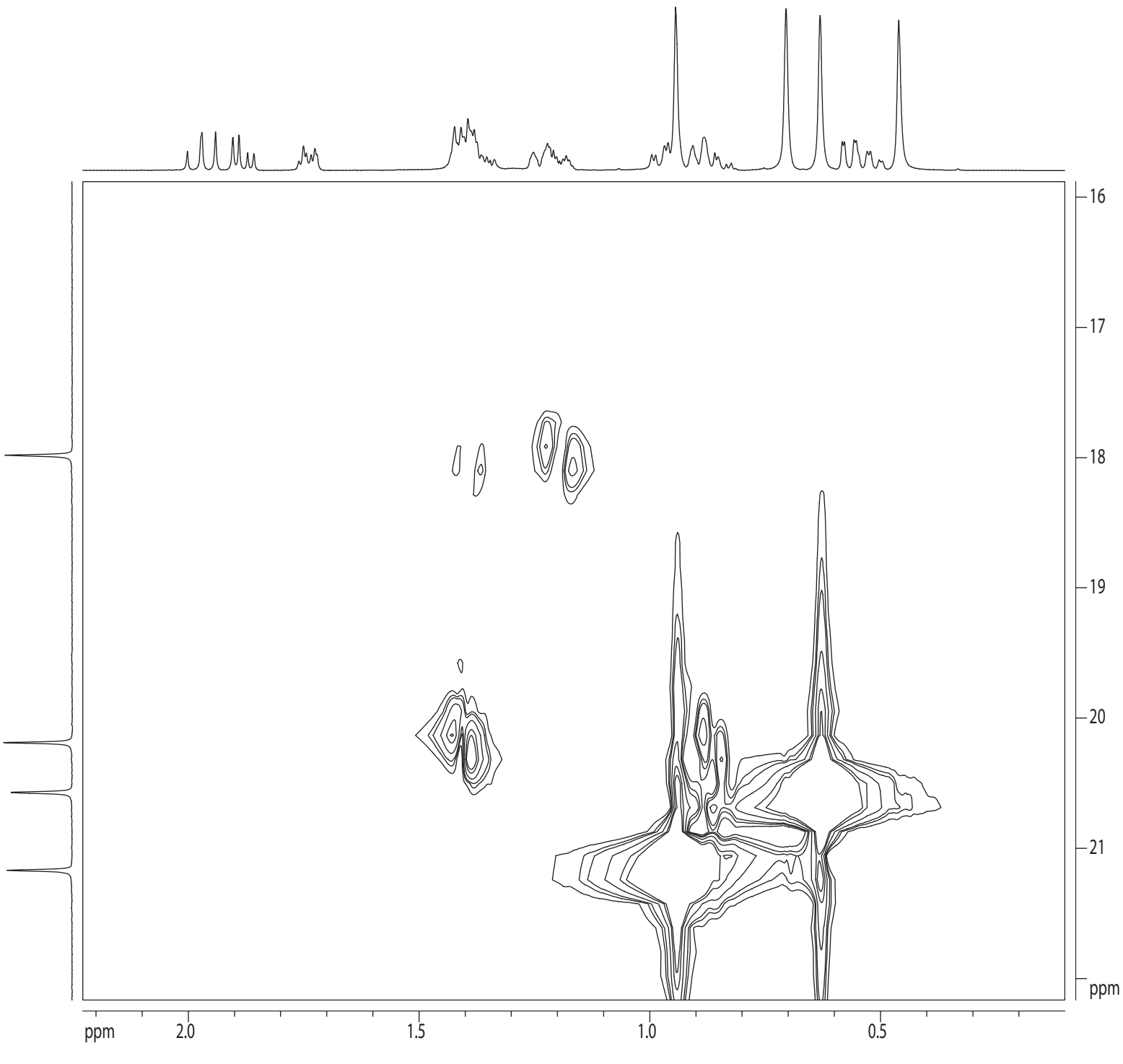
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7924 MHz
FIDRES 46.502975 Hz
SW 189.276 ppm
FnMODE undefined

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 2.499 ppm
F2LO 1250.27 Hz
F2PHI -0.007 ppm
F2HI -3.39 Hz
F1PLO 40.097 ppm
F1LO 5043.44 Hz
F1PHI 37.000 ppm
F1HI 4653.88 Hz
F2PPMCM 0.13923 ppm/cm
F2HZCM 69.64790 Hz/cm
F1PPMCM 0.20648 ppm/cm
F1HZCM 25.97078 Hz/cm

ghmqc



Current Data Parameters
USER nmr12t
NAME Fin_1_500
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121208
Time 1.10
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG inv4gp.wu
TD 2048
SOLVENT C6D6
NS 4
DS 16
SWH 1250.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 2048
DW 400.000 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 0.00002100 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2206253 MHz

======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7923681 MHz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 30.00 %
GPZ2 18.00 %
GPZ3 24.00 %
P16 1000.00 usec

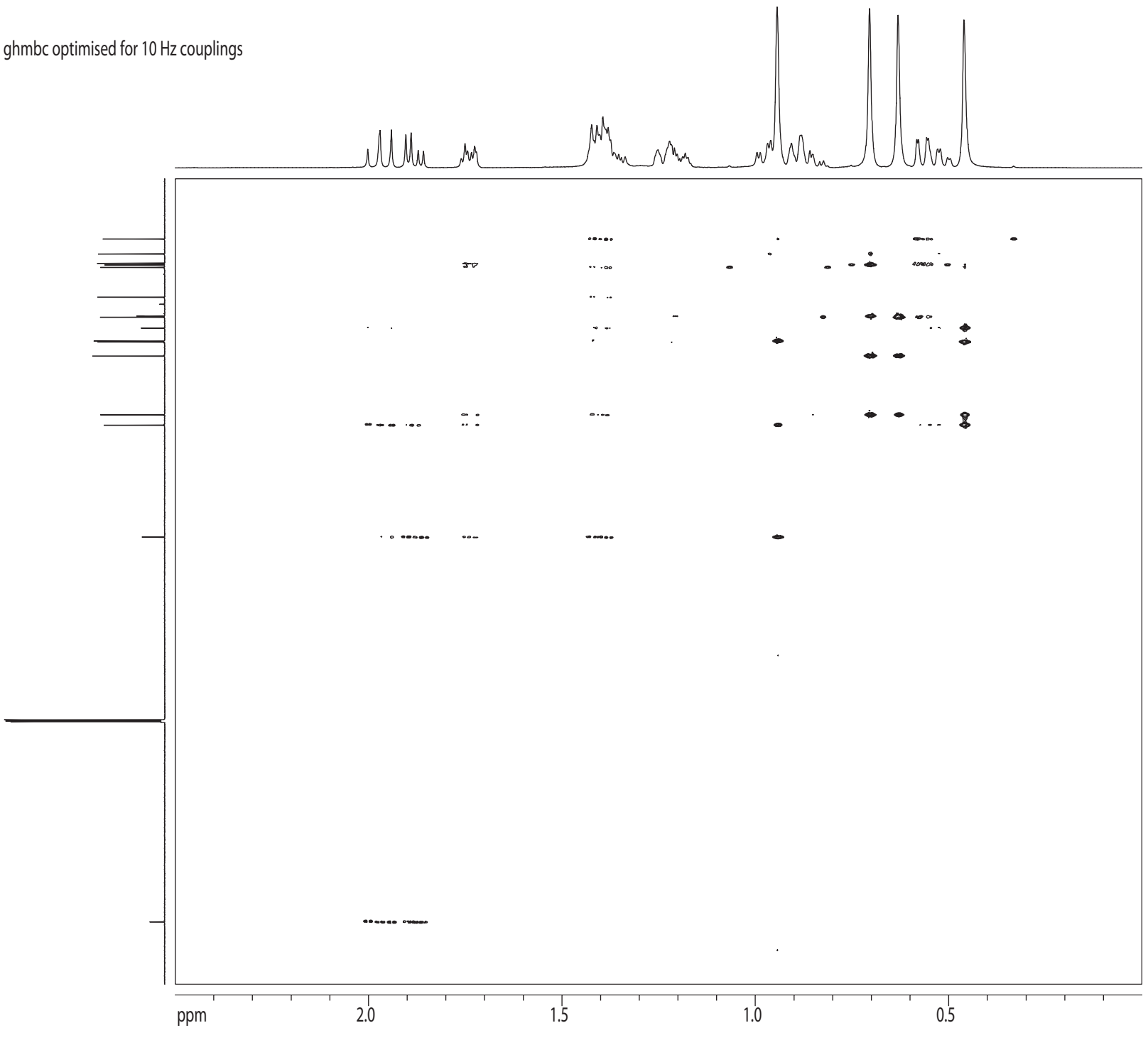
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7924 MHz
FIDRES 46.502975 Hz
SW 189.276 ppm
FnMODE undefined

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 2.229 ppm
F2LO 1114.77 Hz
F2PHI 0.101 ppm
F2HI 50.32 Hz
F1PLO 22.166 ppm
F1LO 2788.04 Hz
F1PHI 15.881 ppm
F1HI 1997.49 Hz
F2PPMCM 0.11822 ppm/cm
F2HZCM 59.13629 Hz/cm
F1PPMCM 0.41901 ppm/cm
F1HZCM 52.70337 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters
USER nmr12t
NAME Fin_1_500
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121208
Time 2.14
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT C6D6
NS 2
DS 16
SWH 1250.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384500 sec
RG 1824.6
DW 400.000 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 0.00002100 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2206253 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7923681 MHz

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

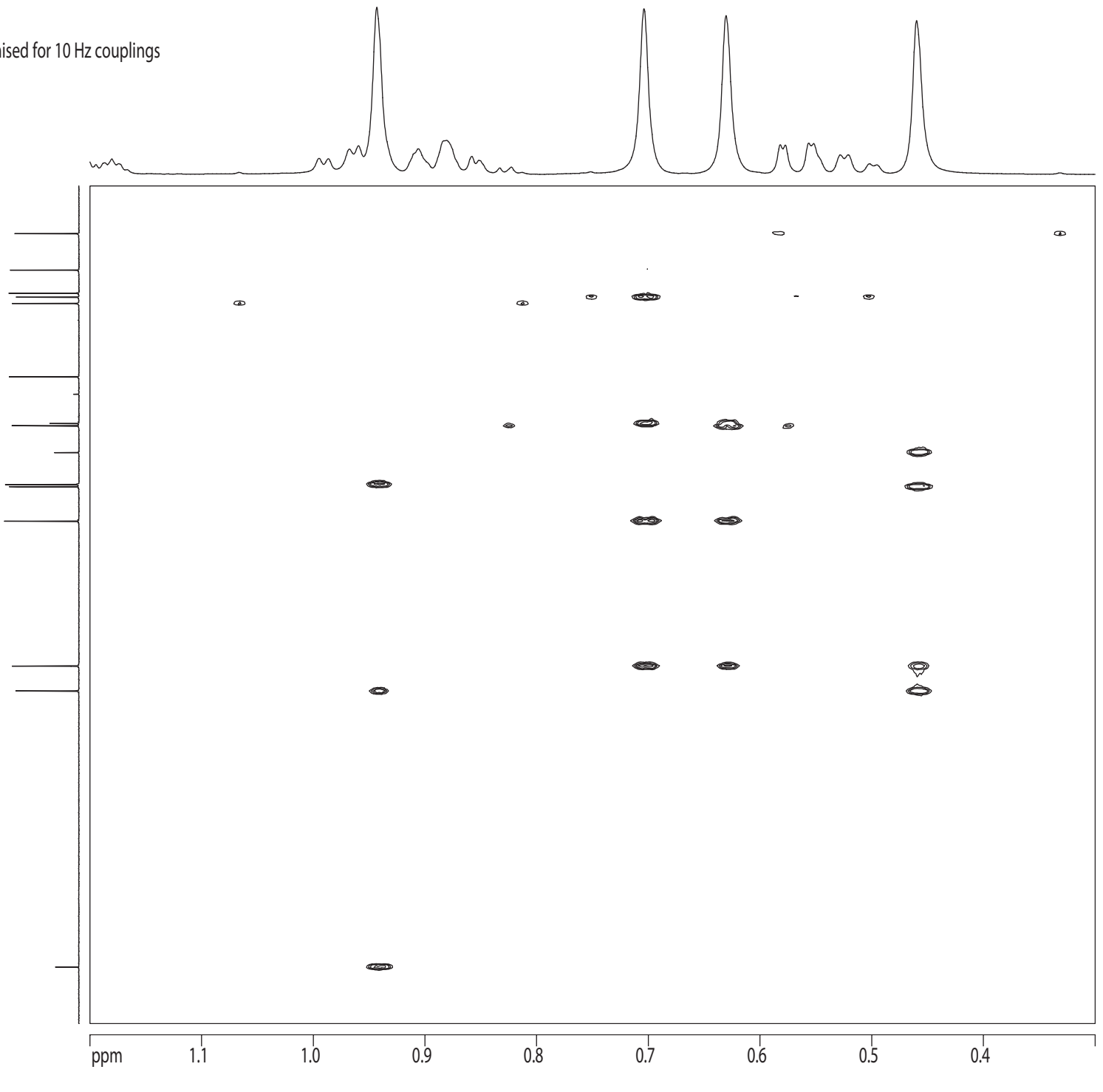
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7924 MHz
FIDRES 46.502975 Hz
SW 189.276 ppm
FnMODE undefined

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 2.499 ppm
F2LO 1250.27 Hz
F2PHI 0.001 ppm
F2HI 0.27 Hz
F1PLO 189.647 ppm
F1LO 23853.89 Hz
F1PHI 0.353 ppm
F1HI 44.37 Hz
F2PPMCM 0.13883 ppm/cm
F2HZCM 69.44444 Hz/cm
F1PPMCM 12.61962 ppm/cm
F1HZCM 1587.30151 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters
USER nmr12t
NAME Fin_1_500
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121208
Time 2.14
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT C6D6
NS 2
DS 16
SWH 1250.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384500 sec
RG 1824.6
DW 400.000 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 0.00002100 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2206253 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7923681 MHz

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

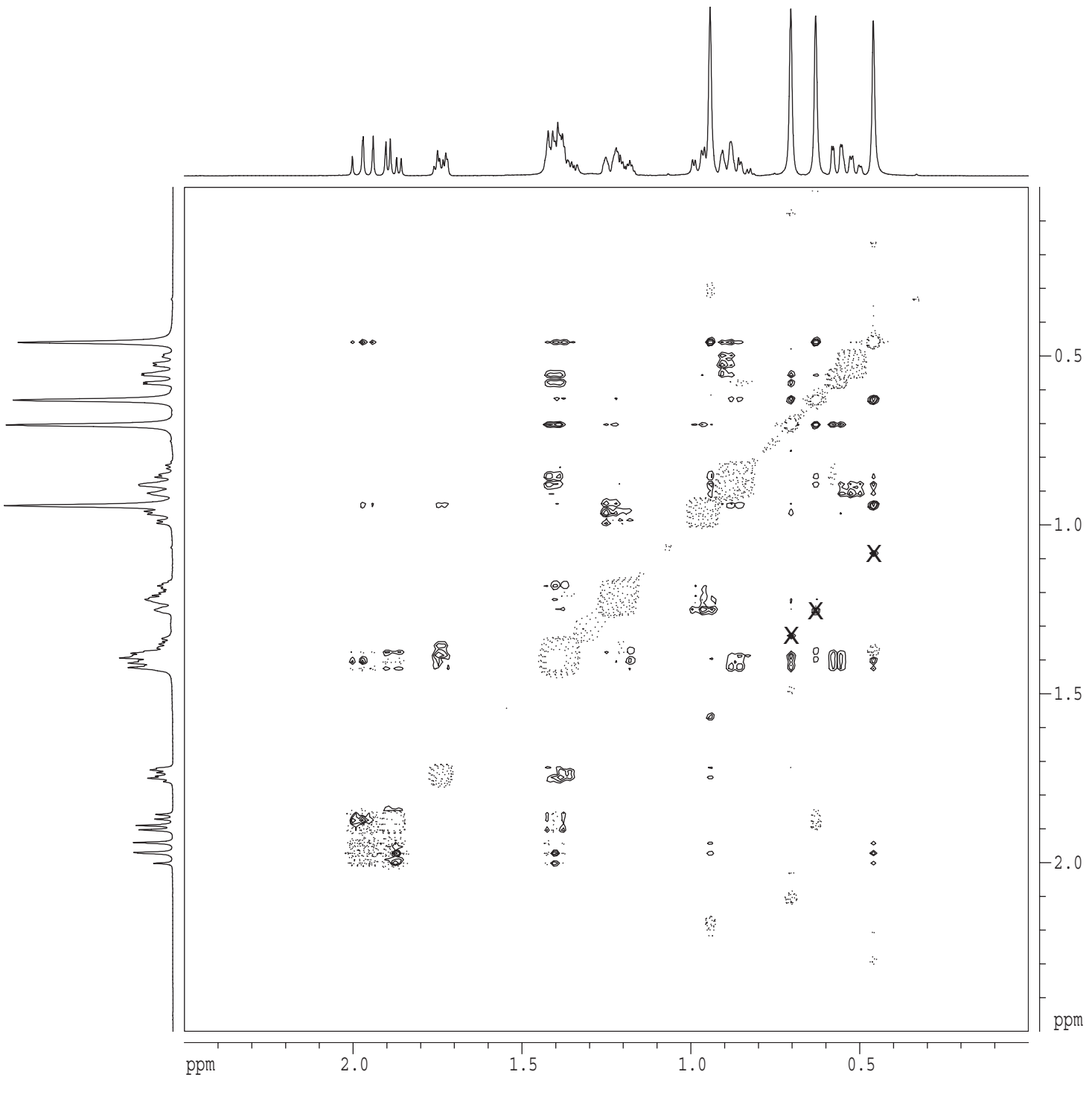
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7924 MHz
FIDRES 46.502975 Hz
SW 189.276 ppm
FnMODE undefined

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 1.200 ppm
F2LO 600.26 Hz
F2PHI 0.300 ppm
F2HI 150.07 Hz
F1PLO 90.009 ppm
F1LO 11321.34 Hz
F1PHI 9.965 ppm
F1HI 1253.44 Hz
F2PPMCM 0.05000 ppm/cm
F2HZCM 25.01100 Hz/cm
F1PPMCM 5.33623 ppm/cm
F1HZCM 671.19299 Hz/cm

NOESY



Current Data Parameters

USER	nmr12t
NAME	Fin_1_500
EXPNO	9
PROCNO	2

F2 - Acquisition Parameters

Date_	20121208
Time	3.06
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	noesygptp
TD	2048
SOLVENT	C6D6
NS	4
DS	16
SWH	1250.000 Hz
FIDRES	0.610352 Hz
AQ	0.8192500 sec
RG	9
DW	400.000 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	0.00040000 sec

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

NUC1	1H
P1	7.50 usec
P2	15.00 usec
PL1	1.60 dB
SFO1	500.2206253 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	500.2206 MHz
FIDRES	2.441406 Hz
SW	2.499 ppm
FnMODE	undefined

F2 - Processing parameters

SI	256
SF	500.2200000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40

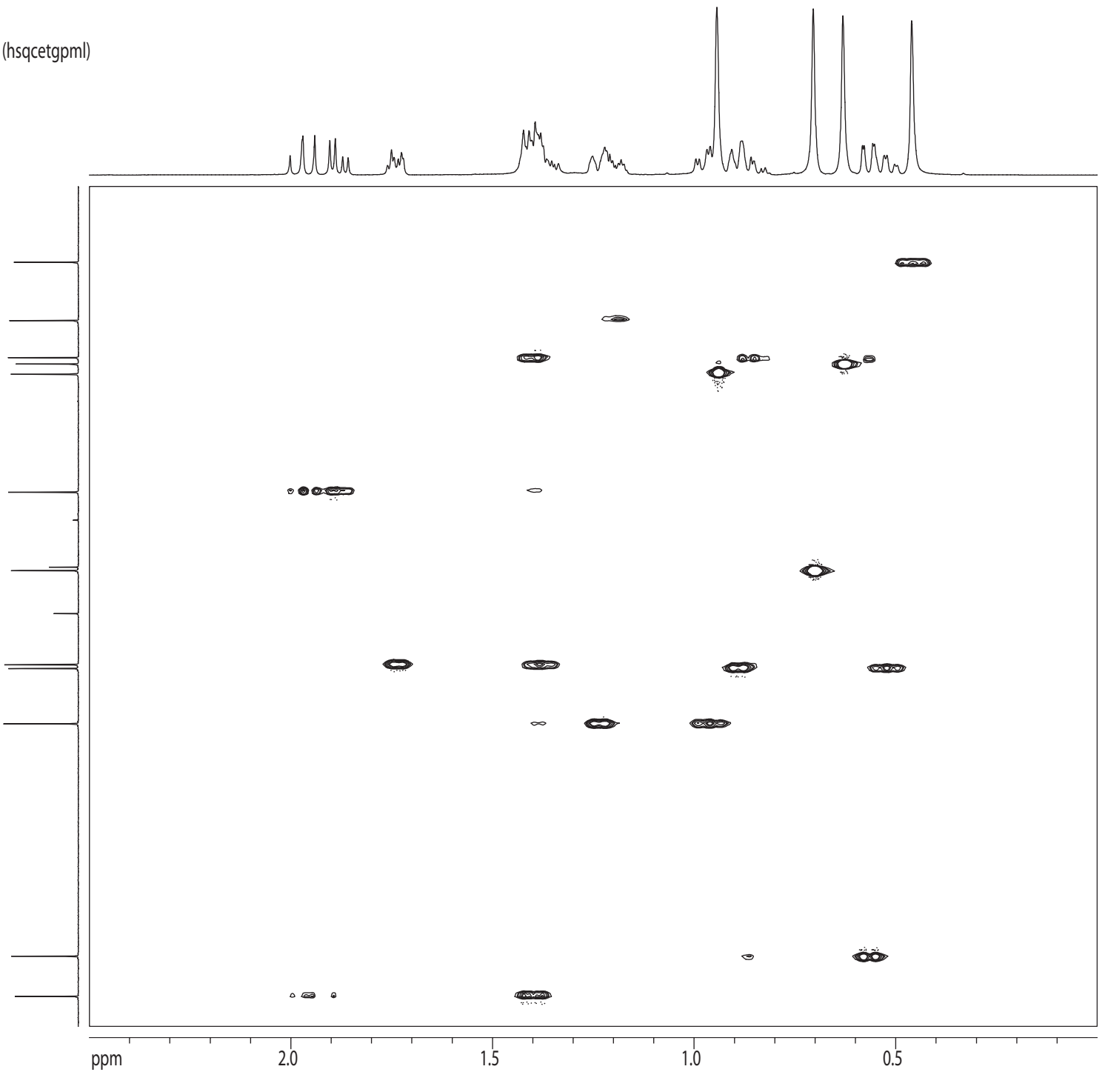
F1 - Processing parameters

SI	256
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	2.499 ppm
F2LO	1250.27 Hz
F2PHI	0.001 ppm
F2HI	0.27 Hz
F1PLO	2.499 ppm
F1LO	1250.27 Hz
F1PHI	0.001 ppm
F1HI	0.27 Hz
F2PPMCM	0.16659 ppm/cm
F2HZCM	83.33334 Hz/cm
F1PPMCM	0.16659 ppm/cm
F1HZCM	83.33334 Hz/cm

5ms
HSQC-TOCSY (hsqcetgpml)



Current Data Parameters
USER nmr12t
NAME Fin_1_500
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121208
Time 5.15
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpml
TD 2048
SOLVENT C6D6
NS 2
DS 32
SWH 1250.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 1824.6
DW 400.000 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 0.00002100 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 500.2206253 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 125.7923681 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

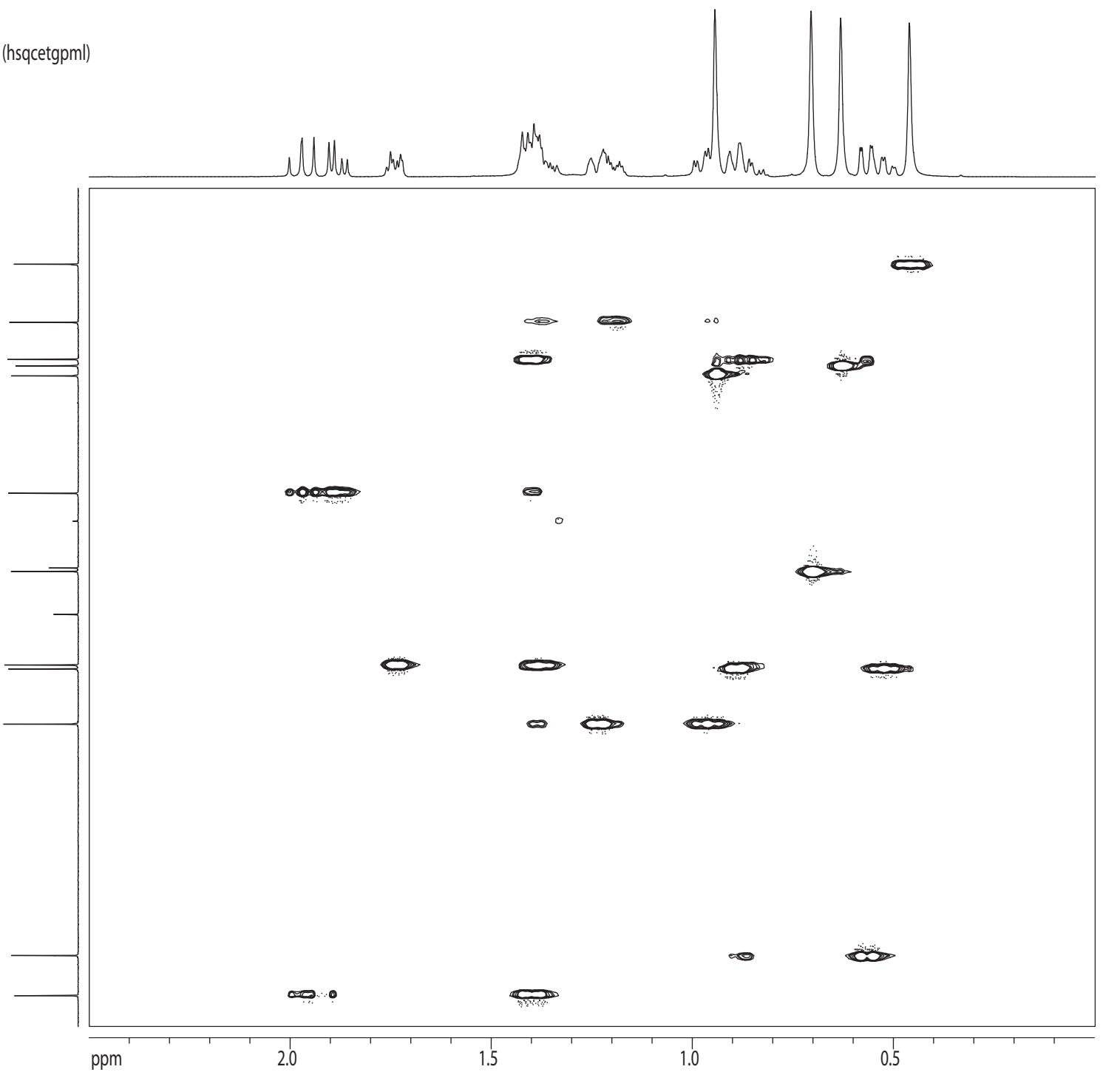
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7924 MHz
FIDRES 46.502975 Hz
SW 189.276 ppm
FnMODE Echo-Antiecho

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 2.499 ppm
F2LO 1250.27 Hz
F2PHI 0.001 ppm
F2HI 0.27 Hz
F1PLO 60.000 ppm
F1LO 7546.82 Hz
F1PHI 10.000 ppm
F1HI 1257.80 Hz
F2PPMCM 0.13883 ppm/cm
F2HZCM 69.44444 Hz/cm
F1PPMCM 3.33333 ppm/cm
F1HZCM 419.26804 Hz/cm

10ms
HSQC-TOCSY (hsqcetgpml)



Current Data Parameters
USER nmr12t
NAME Fin_1_500
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121208
Time 6.05
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpml
TD 2048
SOLVENT C6D6
NS 2
DS 32
SWH 1250.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 1824.6
DW 400.000 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 0.00002100 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 500.2206253 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 125.7923681 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

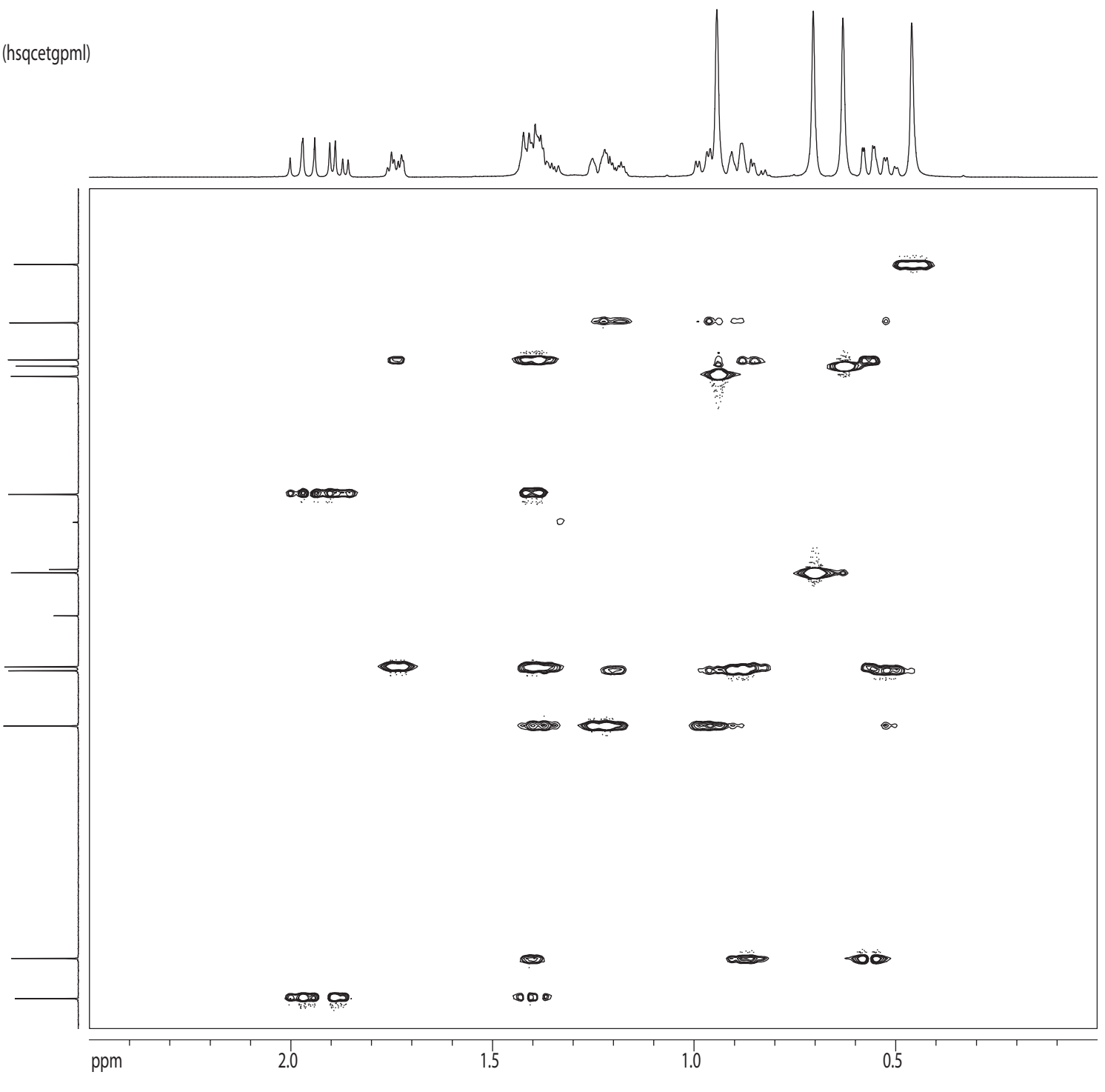
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7924 MHz
FIDRES 46.502975 Hz
SW 189.276 ppm
FnMODE Echo-Antiecho

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 2.499 ppm
F2LO 1250.27 Hz
F2PHI -0.002 ppm
F2HI -0.95 Hz
F1PLO 60.062 ppm
F1LO 7554.60 Hz
F1PHI 9.965 ppm
F1HI 1253.45 Hz
F2PPMCM 0.13896 ppm/cm
F2HZCM 69.51226 Hz/cm
F1PPMCM 3.33976 ppm/cm
F1HZCM 420.07687 Hz/cm

20ms
HSQC-TOCSY (hsqcetgpml)



Current Data Parameters
USER nmr12t
NAME Fin_1_500
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121208
Time 6.55
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpml
TD 2048
SOLVENT C6D6
NS 2
DS 32
SWH 1250.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 1824.6
DW 400.000 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 0.00002100 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 500.2206253 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 125.7923681 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

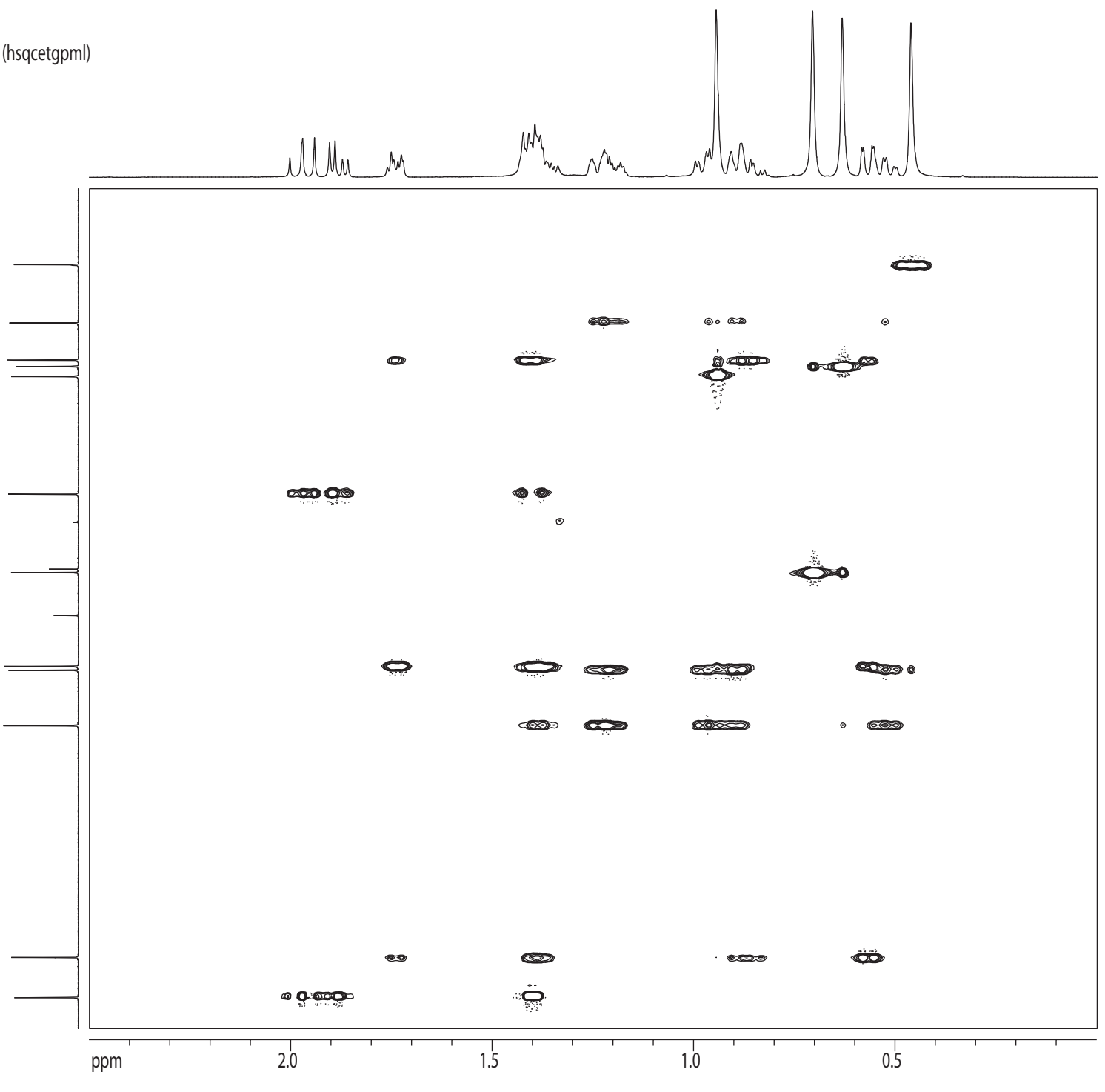
F1 - Acquisition parameters
ND0 2
TD 512
SFO1 125.7924 MHz
FIDRES 46.502975 Hz
SW 189.276 ppm
FnMODE Echo-Antiecho

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 2.499 ppm
F2LO 1250.27 Hz
F2PHI 0.001 ppm
F2HI 0.27 Hz
F1PLO 60.000 ppm
F1LO 7546.82 Hz
F1PHI 10.000 ppm
F1HI 1257.80 Hz
F2PPMCM 0.13883 ppm/cm
F2HZCM 69.44444 Hz/cm
F1PPMCM 3.33333 ppm/cm
F1HZCM 419.26804 Hz/cm

100ms
HSQC-TOCSY (hsqcetgpml)



Current Data Parameters
USER nmr12t
NAME Fin_1_500
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121208
Time 7.46
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpml
TD 2048
SOLVENT C6D6
NS 2
DS 32
SWH 1250.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 1824.6
DW 400.000 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 0.00002100 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 500.2206253 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 125.7923681 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 512
SFO1 125.7924 MHz
FIDRES 46.502975 Hz
SW 189.276 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 2.499 ppm
F2LO 1250.27 Hz
F2PHI -0.002 ppm
F2HI -0.95 Hz
F1PLO 60.062 ppm
F1LO 7554.60 Hz
F1PHI 9.965 ppm
F1HI 1253.45 Hz
F2PPMCM 0.13896 ppm/cm
F2HZCM 69.51226 Hz/cm
F1PPMCM 3.33976 ppm/cm
F1HZCM 420.07687 Hz/cm