

Name: _____

Chem 203
December 14, 2013

Final Exam Part II
Problem 3 of 3 (30 points)

Select and submit TWO OUT OF THE THREE PROBLEMS FROM PART II for grading.
Do not submit three problems.

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

Books, notes, lecture videos, calculators, rulers, and laptop computers are permitted as is wireless (or wired) internet access and appropriate software (e.g, Pymol, Macromodel/Maestro, Excel, NMRPrediction, Chemdraw, ElComp, MolE, etc.). Catalogs of molecular structures (e.g., the Aldrich catalog, the Merck Index, etc.) or databases of molecular structures (such as wireless access to SciFinder Scholar, the Sigma-Aldrich website, etc.) are NOT PERMITTED. USE OF SUCH ITEMS CONSTITUTES ACADEMIC DISHONESTY, WILL RESULT IN A FAILING GRADE (F) IN THE CLASS, AND MAY RESULT IN EXPULSION FROM THE Ph.D. PROGRAM.

If you wish to use a laptop computer, please be willing to share briefly with others when needed.

The following spectral data are provided for a compound with a molecular formula $C_{16}H_{24}O$: IR (solution in $CHCl_3$), 500 MHz 1H NMR, 125.8 MHz ^{13}C NMR, DEPT-90, DEPT-135, COSY, TOCSY (20 ms mixing time), HMQC, HMBC, 1D NOE (irradiation at 3.36 ppm), and NOESY. All NMR spectra were measured in C_6D_6 solution.

Using these data, determine the structure of the compound and assign all of the 1H and ^{13}C resonances to their respective atoms in the structure. Make sure to determine the stereochemistry of the compound and to clearly assign 1H resonances to the appropriate diastereotopic protons.

HINT: In the 1H NMR spectrum, the alcohol OH resonance is directly underneath one of the other resonances. Also, the alcohol OH group exchanges slowly on the NMR time scale, which results in coupling to the adjacent CH group.

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

a. Write the structure of the molecule.

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

b. Tabulate the shifts of the ^1H resonances (a-n) in order of descending chemical shift. Provide an appropriate name for each multiplet (e.g., s, d, t, q, quintet, sextet, septet, octet, dd, ddd, dt, td, dddd, tt, qd, dq, etc.) and list its coupling constants in appropriate order; also list its integral [e.g., a: 3.30 (t, $J = 7.3$ Hz, 3 H)]. If a resonance is not described by a well-defined multiplet, name it as m and give its range [e.g., c: 4.43-4.37 (m, 2 H)].

a:

b:

c:

d:

e:

f:

g:

h:

i:

j:

k:

l:

m:

n:

c. Redraw the structure of the molecule below and write the letter (a-n) of each ^1H resonance next to the proton or protons to which it corresponds. If the assignment of a particular resonance is uncertain, please indicate this.

d. Tabulate the shifts of the ^{13}C resonances (1-14) in order of descending chemical shift. Make sure to report the chemical shift of each carbon resonances to the nearest tenth of ppm, unless two have the same value, in which case you may report it to the nearest hundredth.

1:

2:

3:

4:

5:

6:

7:

8:

9:

10:

11:

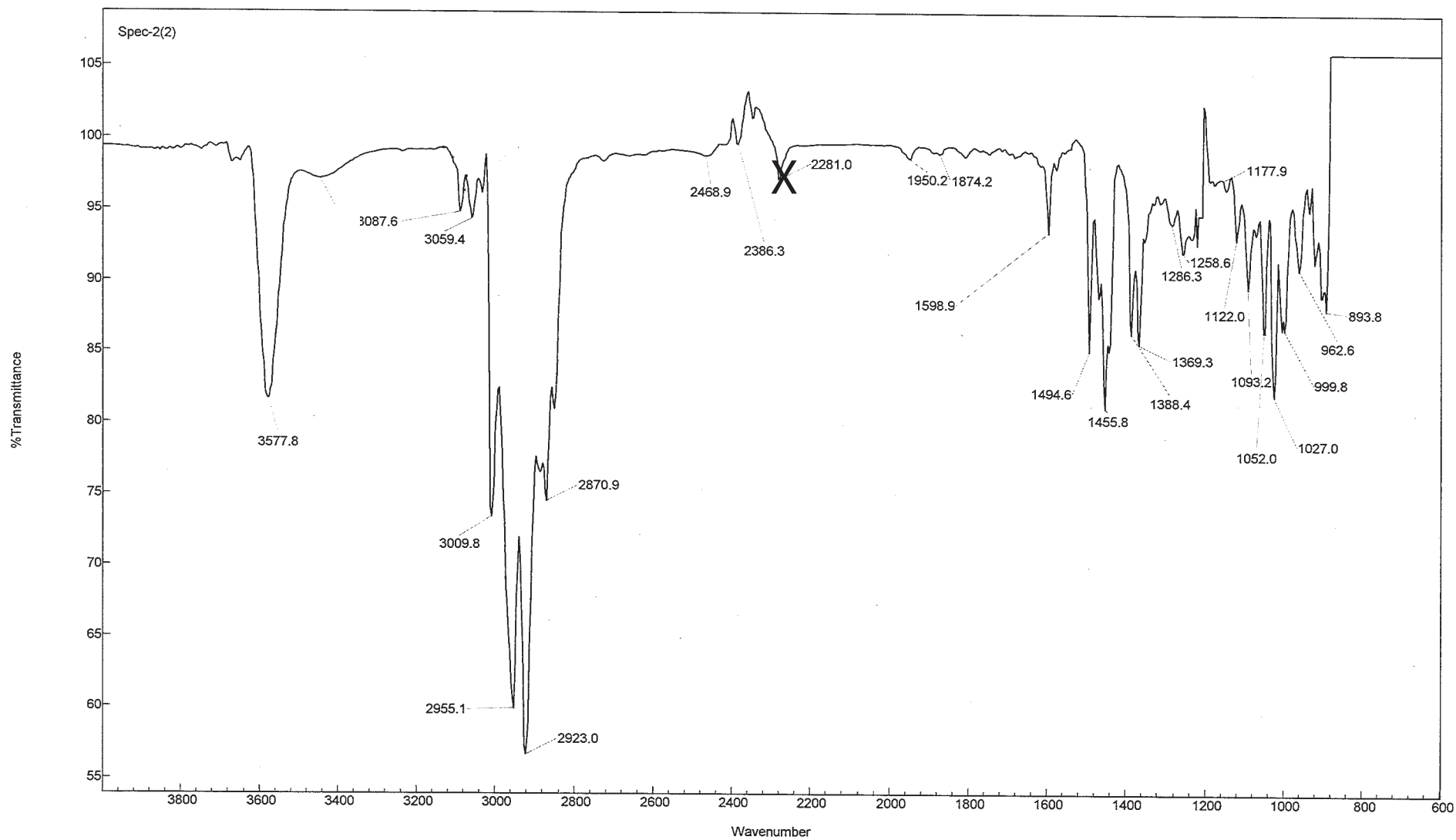
12:

13:

14:

e. Redraw the structure of the molecule below and write the number (1-14) of each ^{13}C resonance next to the carbon or carbons to which it corresponds. If the assignment of particular resonance is uncertain, please indicate this.

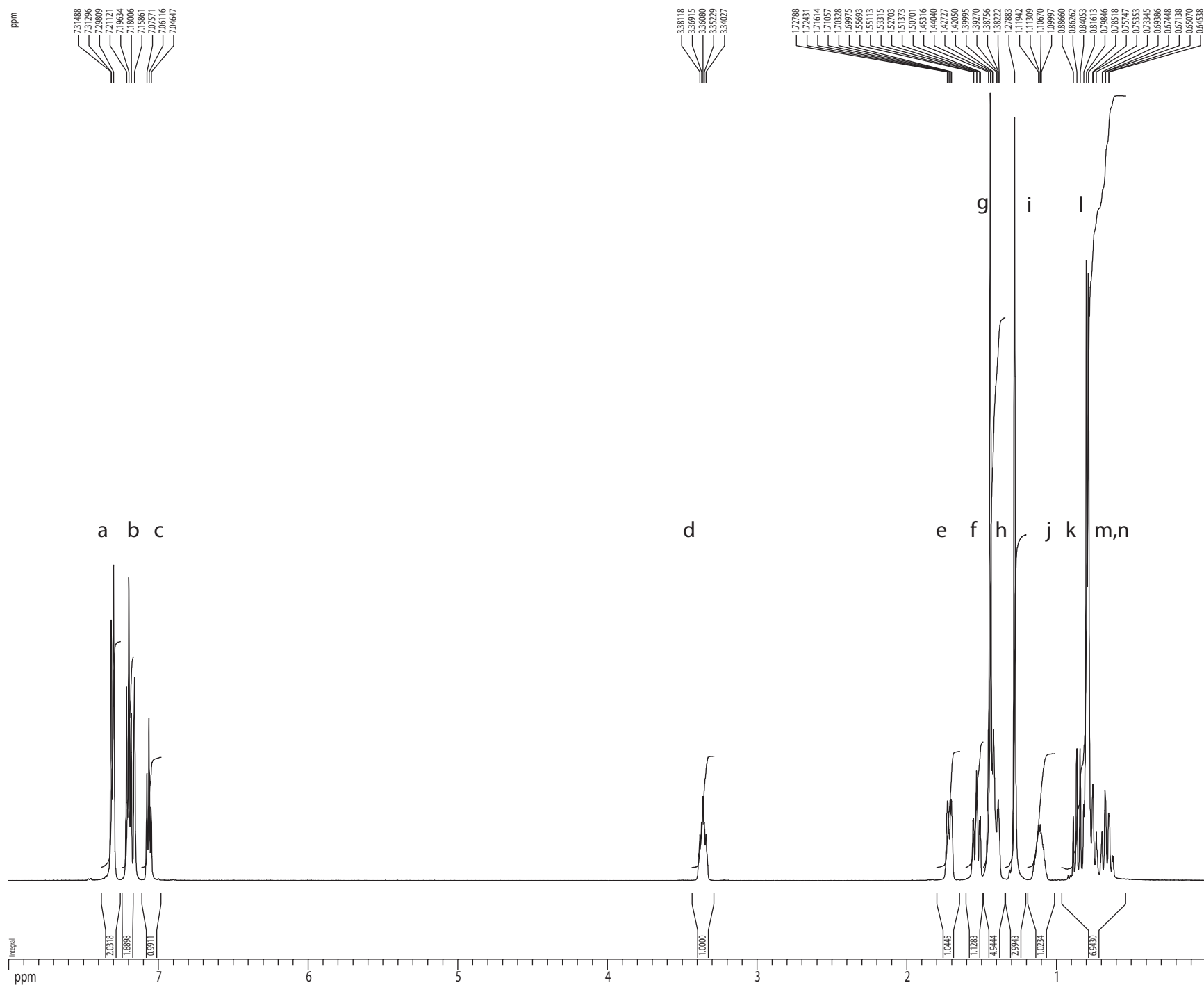
Varian Resolutions Pro



Name

Spec-2 (2)

¹H spectrum



Current Data Parameters
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 NAME Donut_Yummy
 EXPNO 2
 PROCNO 1

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 Date_ 20131210
 Time 19:36
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 PROBHD 5 mm CPTCI 1H-
 PULPROG zg30
 TD 81728
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 3.2
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

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

F2 - Processing parameters
 SI 65536
 SF 500.2200000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 0.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 FIP 8.000 ppm
 F1 4001.76 Hz
 F2 0.000 Hz
 F2 0.000 Hz
 PPMCM 0.35088 ppm/cm
 HZCM 175.51579 Hz/cm

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	[Hz]	[PPM]	

1	31479.8	3659.049	7.3149	4.84
2	31487.6	3658.090	7.3130	4.97
3	31548.5	3650.649	7.2981	6.02
4	31903.9	3607.193	7.2112	3.69
5	31964.7	3599.755	7.1963	5.78
6	32031.3	3591.610	7.1801	3.19
7	32119.1	3580.879	7.1586	3.88
8	32458.3	3539.410	7.0757	2.05
9	32517.8	3532.135	7.0612	3.10
10	32577.9	3524.787	7.0465	1.40
11	47573.5	1691.335	3.3812	0.88
12	47622.7	1685.318	3.3692	1.12
13	47656.9	1681.137	3.3608	1.61
14	47691.7	1676.883	3.3523	1.11
15	47740.9	1670.867	3.3403	0.88
16	54337.5	864.321	1.7279	1.52
17	54352.2	862.534	1.7243	1.49
18	54385.6	858.448	1.7161	0.91
19	54408.4	855.660	1.7106	0.97
20	54438.2	852.017	1.7033	1.55
21	54452.6	850.250	1.6998	1.52
22	55037.0	778.806	1.5569	1.15
23	55060.7	775.907	1.5511	1.19
24	55134.2	766.914	1.5332	2.09
25	55159.3	763.849	1.5270	1.53
26	55213.7	757.196	1.5137	1.15
27	55241.2	753.838	1.5070	1.24
28	55461.5	726.901	1.4532	2.93
29	55513.7	720.516	1.4404	15.00
30	55567.4	713.947	1.4273	2.24
31	55595.1	710.562	1.4205	2.88
32	55679.2	700.281	1.3999	1.00
33	55708.9	696.654	1.3927	1.35
34	55729.9	694.087	1.3876	1.55
35	55751.7	691.413	1.3822	1.20
36	56174.7	639.698	1.2788	14.53
37	56700.8	575.378	1.1502	0.38
38	56730.7	571.716	1.1429	0.45
39	56758.3	568.342	1.1362	0.54
40	56785.0	565.081	1.1297	0.74
41	56799.3	563.335	1.1262	0.81
42	56826.9	559.959	1.1194	1.01
43	56852.8	556.789	1.1131	1.02
44	56878.9	553.595	1.1067	1.07
45	56906.5	550.229	1.1000	0.91
46	56948.1	545.139	1.0898	0.69
47	56973.9	541.979	1.0835	0.59
48	57001.8	538.575	1.0767	0.38
49	57779.4	443.496	0.8866	1.22

50	57877.6	431.498	0.8626	2.52
51	57967.9	420.451	0.8405	2.51
52	58067.7	408.247	0.8161	1.46
53	58140.0	399.406	0.7985	11.82
54	58194.4	392.763	0.7852	11.57
55	58307.7	378.902	0.7575	1.70
56	58323.9	376.929	0.7535	1.84
57	58406.0	366.886	0.7334	0.93
58	58568.0	347.081	0.6939	0.93
59	58647.3	337.388	0.6745	1.73
60	58659.9	335.839	0.6714	1.59
61	58744.6	325.495	0.6507	1.29
62	58766.3	322.834	0.6454	1.24
63	58847.9	312.853	0.6254	0.47
64	58874.7	309.579	0.6189	0.46

¹H spectrum

ppm

731488
731296
72809
721121
719634
718006
715861
707571
706116
704647

a b c

C₆D₅H

Current Data Parameters
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NAME Donut_Yummy
EXPNO 2
PROCNO 1

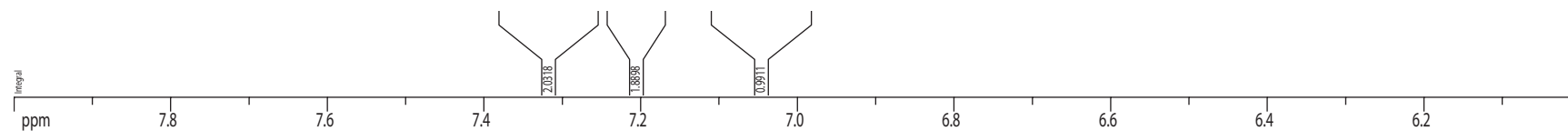
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Time 19:36
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PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 3.2
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

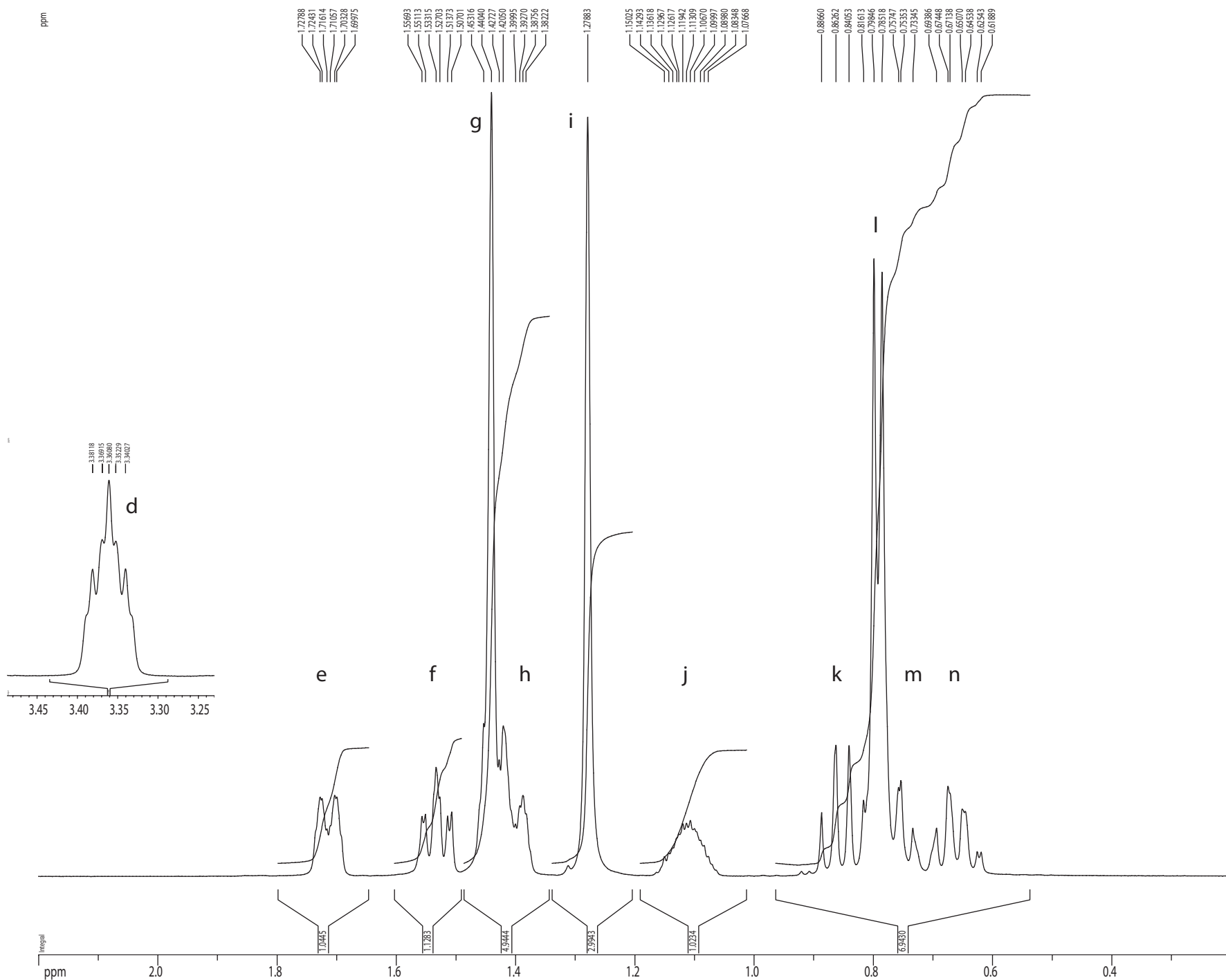
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SSB 0
LB 0.30 Hz
GB 0
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1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
FIP 8.000 ppm
F1 4001.76 Hz
F2P 6.000 ppm
F2 3001.332 Hz
PPMCM 0.08772 ppm/cm
HZCM 43.87895 Hz/cm

ppm



¹H spectrum



Current Data Parameters
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 NAME Donut_Yummy
 EXPNO 2
 PROCNO 1

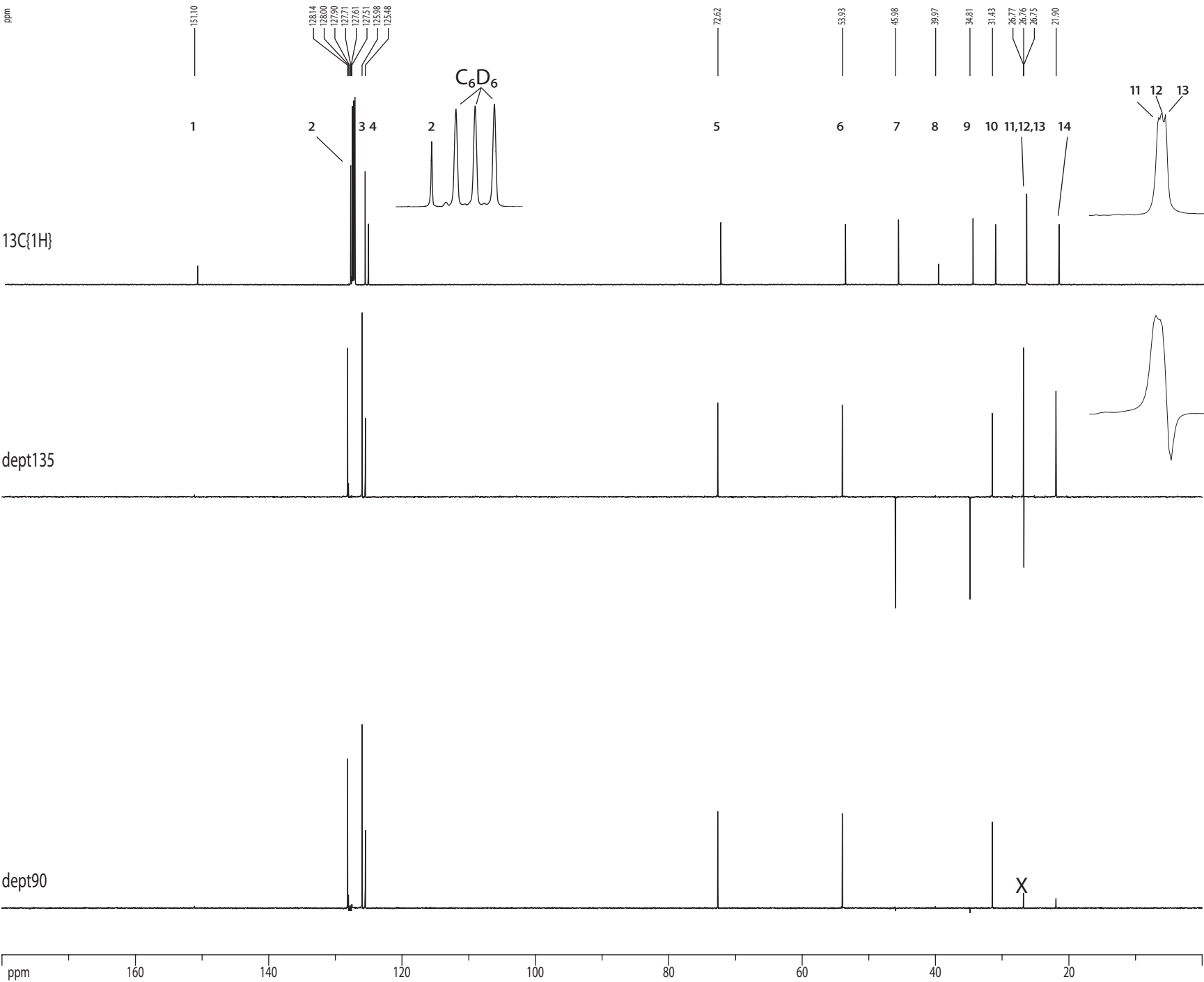
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 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 3.2
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

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

F2 - Processing parameters
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 SF 500.2200000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 0.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 2.200 ppm
 F1 1100.48 Hz
 F2P 0.200 ppm
 F2 100.04 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 Donut_Yummy
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
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Time 19:42
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PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchopg30gp.prd
TD 65536
SOLVENT CDCl3
NS 146
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813940 sec
RG 3649.1
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 125.7942348 MHz
SP1 3.20 dB
SP2 3.20 dB
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SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz

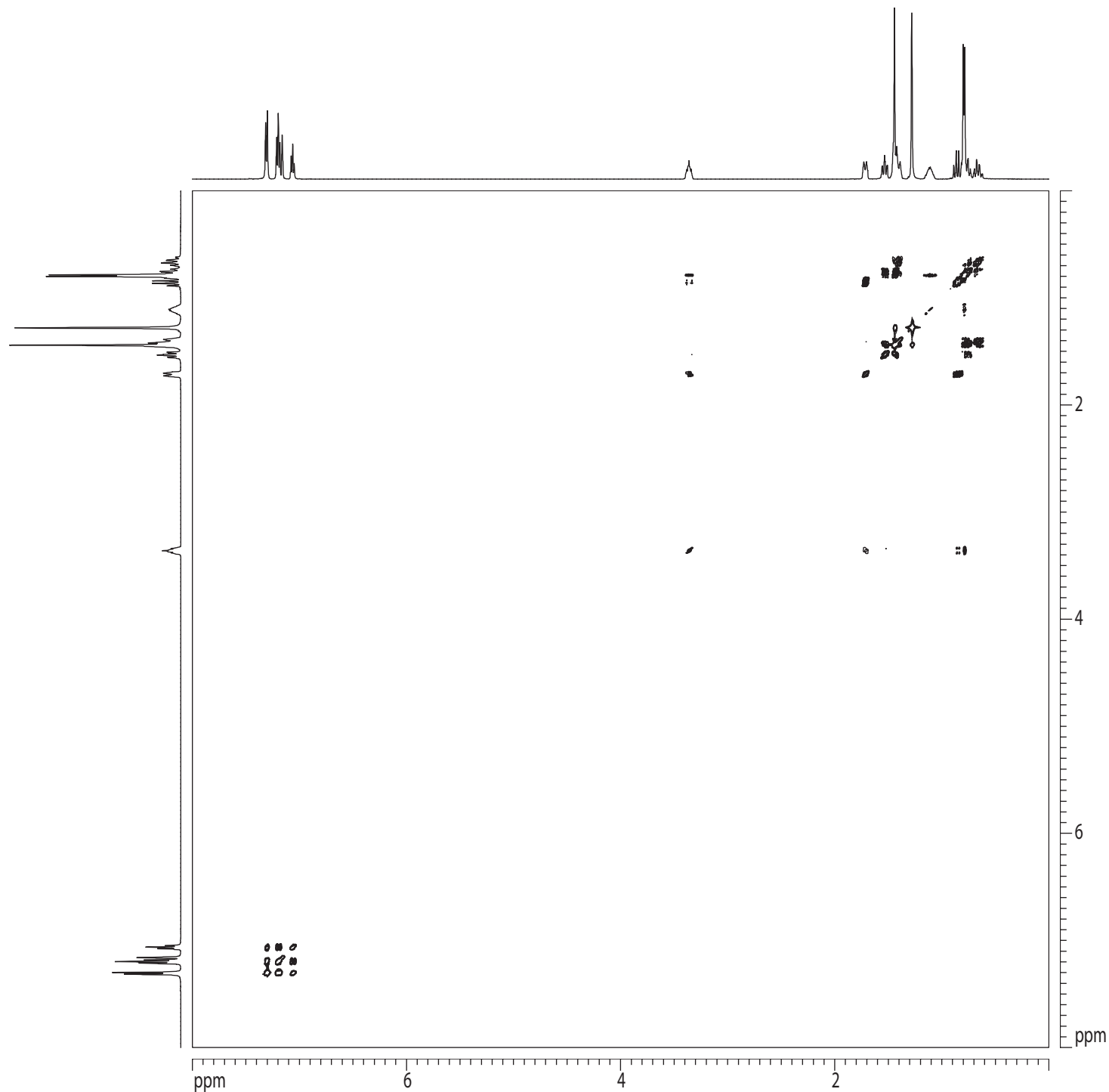
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NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz

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GPNAM1 SINE.100
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 3.56 cm
F1P 180.000 ppm
F1 22640.47 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 7.89474 ppm/cm
HZCM 993.00336 Hz/cm

gcosy60



Current Data Parameters
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 NAME Donut_Yummy
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
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 Time 19:51
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 PROBHD 5 mm CPTCI 1H-
 PULPROG cosygp60.prd
 TD 2048
 SOLVENT C6D6
 NS 8
 DS 16
 SWH 4006.410 Hz
 FIDRES 1.956255 Hz
 AQ 0.2556404 sec
 RG 3.2
 DW 124.800 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 1.00000000 sec
 d13 0.00000300 sec
 D16 0.00020000 sec
 INO 0.00024960 sec

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 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.2220009 MHz

===== GRADIENT CHANNEL =====
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 GPNAM2 sine.100
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 GPX2 0.00 %
 GPY1 0.00 %
 GPY2 0.00 %
 GPZ1 17.00 %
 GPZ2 17.00 %
 P16 1000.00 usec

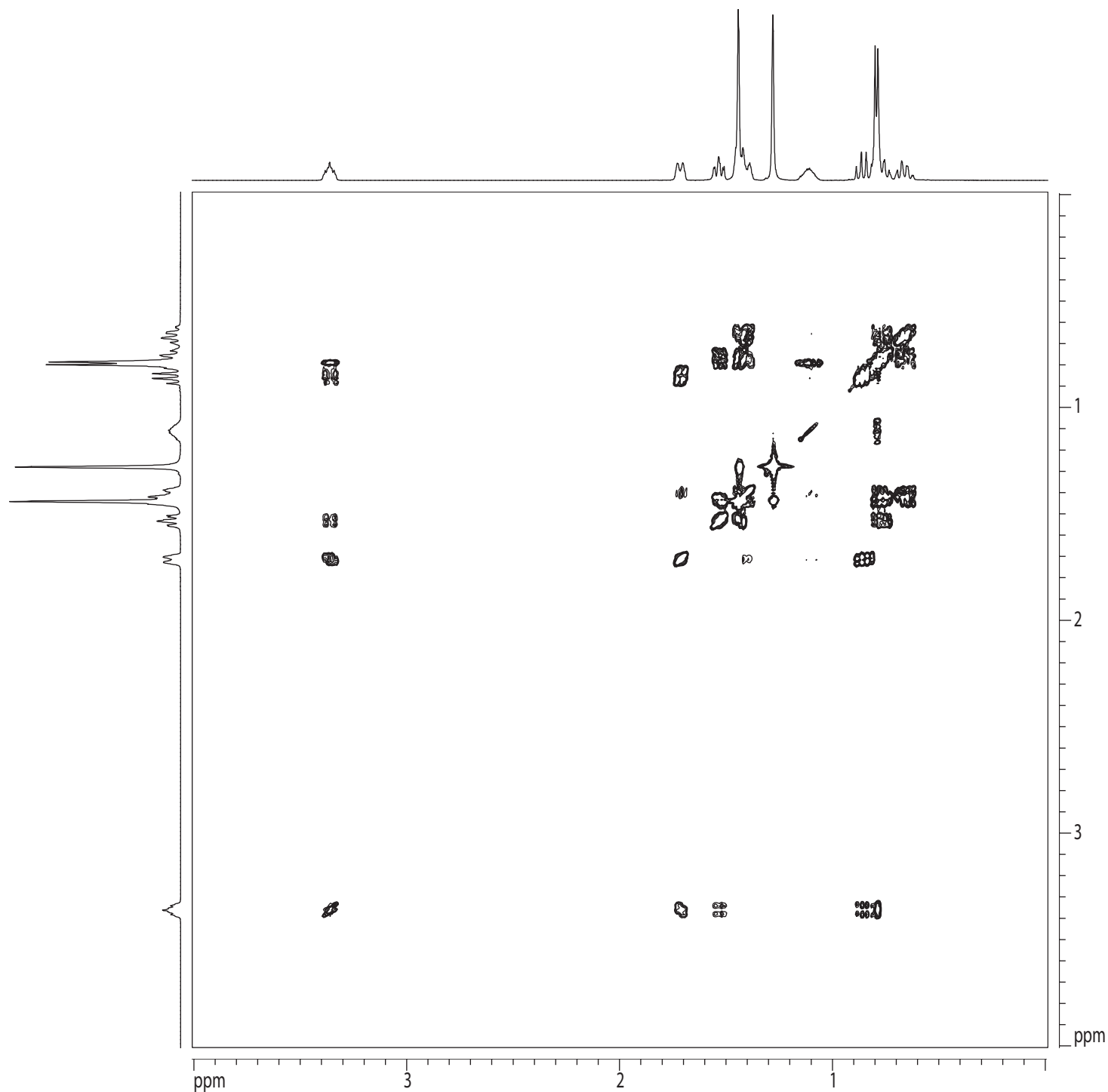
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 TD 512
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 FIDRES 7.825020 Hz
 SW 8.009 ppm
 FnmODE undefined

F2 - Processing parameters
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 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 8.000 ppm
 F2LO 4001.76 Hz
 F2PHI 0.000 ppm
 F2HI 0.00 Hz
 F1PLO 8.000 ppm
 F1LO 4001.76 Hz
 F1PHI 0.000 ppm
 F1HI 0.00 Hz
 F2PPMCM 0.53333 ppm/cm
 F2HZCM 266.78400 Hz/cm
 F1PPMCM 0.53333 ppm/cm
 F1HZCM 266.78400 Hz/cm

gcosy60



Current Data Parameters
 USER nmr13t
 NAME Donut_Yummy
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
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 Time 19:51
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 PROBHD 5 mm CPTCI 1H-
 PULPROG cosygp60.prd
 TD 2048
 SOLVENT C6D6
 NS 8
 DS 16
 SWH 4006.410 Hz
 FIDRES 1.956255 Hz
 AQ 0.2556404 sec
 RG 3.2
 DW 124.800 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 1.00000000 sec
 d13 0.00000300 sec
 D16 0.00020000 sec
 INO 0.00024960 sec

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

===== GRADIENT CHANNEL =====
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 GPNAM2 sine.100
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 GPX2 0.00 %
 GPY1 0.00 %
 GPY2 0.00 %
 GPZ1 17.00 %
 GPZ2 17.00 %
 P16 1000.00 usec

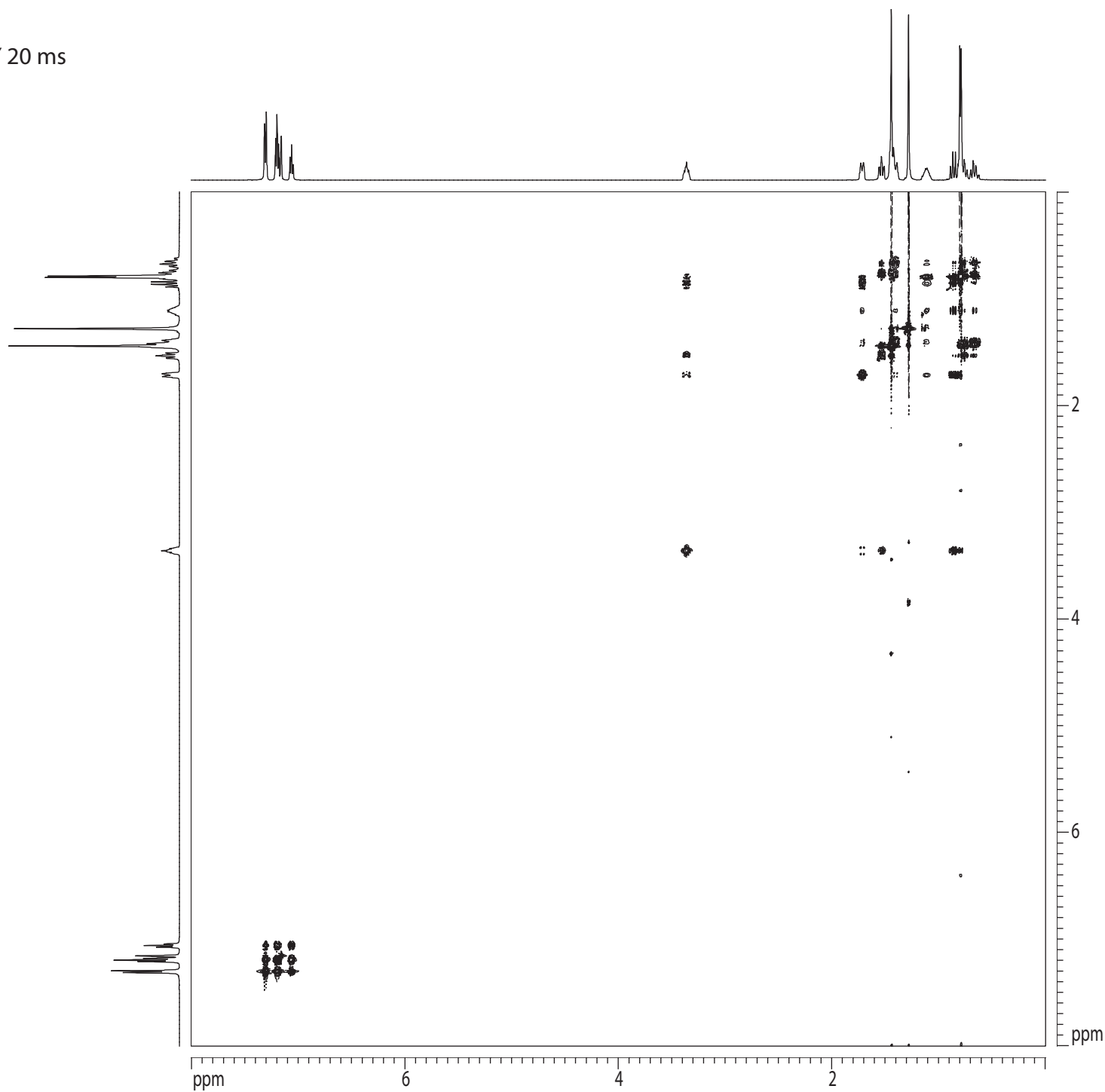
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 FnmODE undefined

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 4.008 ppm
 F2LO 2004.79 Hz
 F2PHI -0.012 ppm
 F2HI -6.24 Hz
 F1PLO 4.008 ppm
 F1LO 2004.79 Hz
 F1PHI -0.012 ppm
 F1HI -6.24 Hz
 F2PPMCM 0.26802 ppm/cm
 F2HZCM 134.06868 Hz/cm
 F1PPMCM 0.26802 ppm/cm
 F1HZCM 134.06868 Hz/cm

TOCSY 20 ms



Current Data Parameters
 USER nmr13t
 NAME Donut_Yummy
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131210
 Time 21.23
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 PULPROG tocsytp.wu
 TD 2048
 SOLVENT C6D6
 NS 8
 DS 16
 SWH 4006.410 Hz
 FIDRES 1.956255 Hz
 AQ 0.2556404 sec
 RG 3.2
 DW 124.800 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 2.00000000 sec
 d8 0.02084341 sec
 d12 0.00002000 sec
 INO 0.00012480 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 500.2220009 MHz

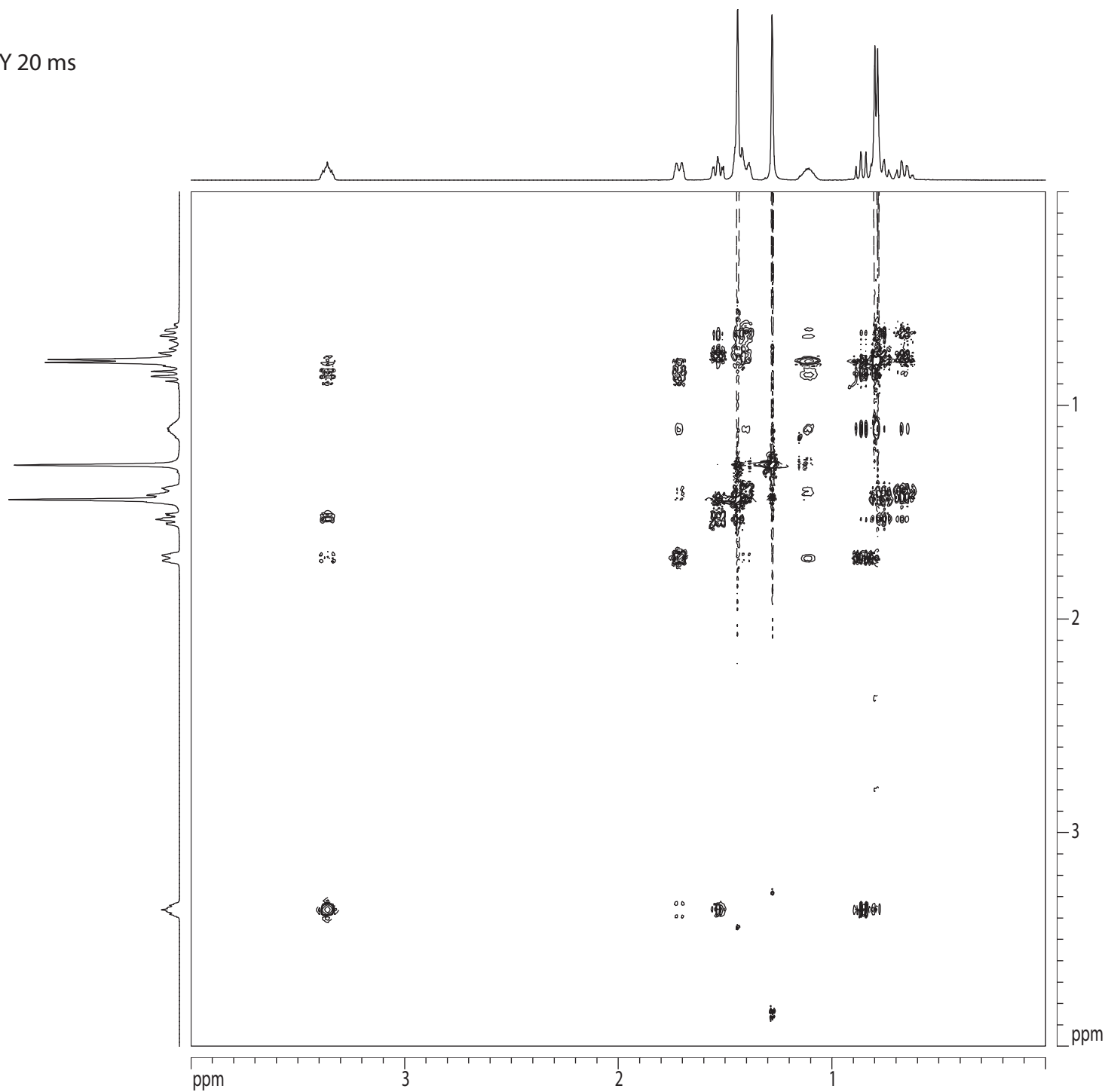
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F2 - Processing parameters
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 SF 500.2200000 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 TPPI
 SF 500.2200000 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 8.005 ppm
 F2LO 4004.08 Hz
 F2PHI -0.005 ppm
 F2HI -2.33 Hz
 F1PLO 8.005 ppm
 F1LO 4004.08 Hz
 F1PHI -0.005 ppm
 F1HI -2.33 Hz
 F2PPMCM 0.53395 ppm/cm
 F2HZCM 267.09402 Hz/cm
 F1PPMCM 0.53395 ppm/cm
 F1HZCM 267.09402 Hz/cm

TOCSY 20 ms



Current Data Parameters
 USER nmr13t
 NAME Donut_Yummy
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131210
 Time 21.23
 INSTRUM cryo500
 PROBHD 5 mm CPTCI 1H-
 PULPROG tocsytp.wu
 TD 2048
 SOLVENT C6D6
 NS 8
 DS 16
 SWH 4006.410 Hz
 FIDRES 1.956255 Hz
 AQ 0.2556404 sec
 RG 3.2
 DW 124.800 usec
 DE 6.00 usec
 TE 298.0 K
 d0 0.00000300 sec
 D1 2.00000000 sec
 d8 0.02084341 sec
 d12 0.00002000 sec
 INO 0.00012480 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 500.2220009 MHz

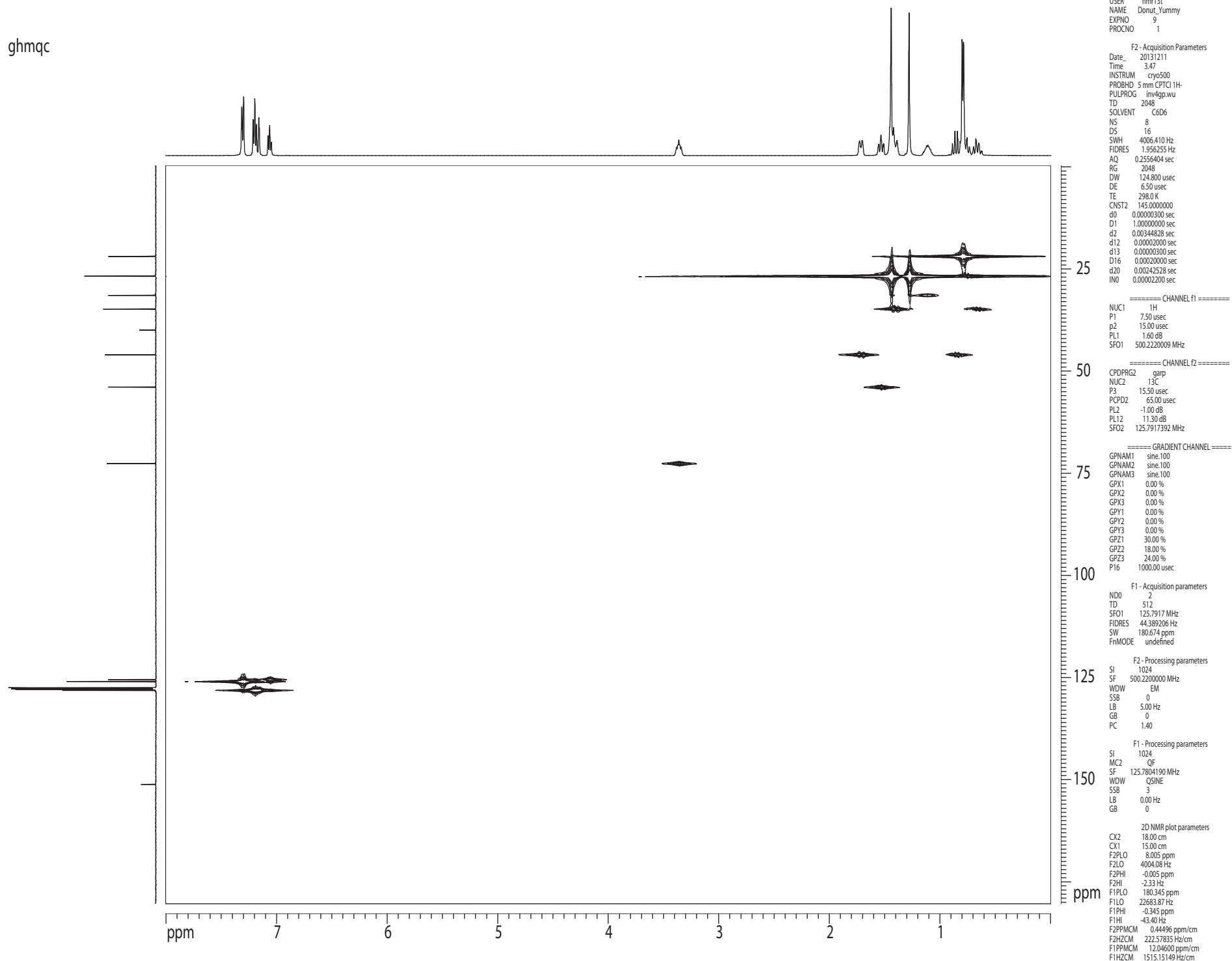
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F2 - Processing parameters
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 SSB 3
 LB 0.00 Hz
 GB 0
 PC 1.40

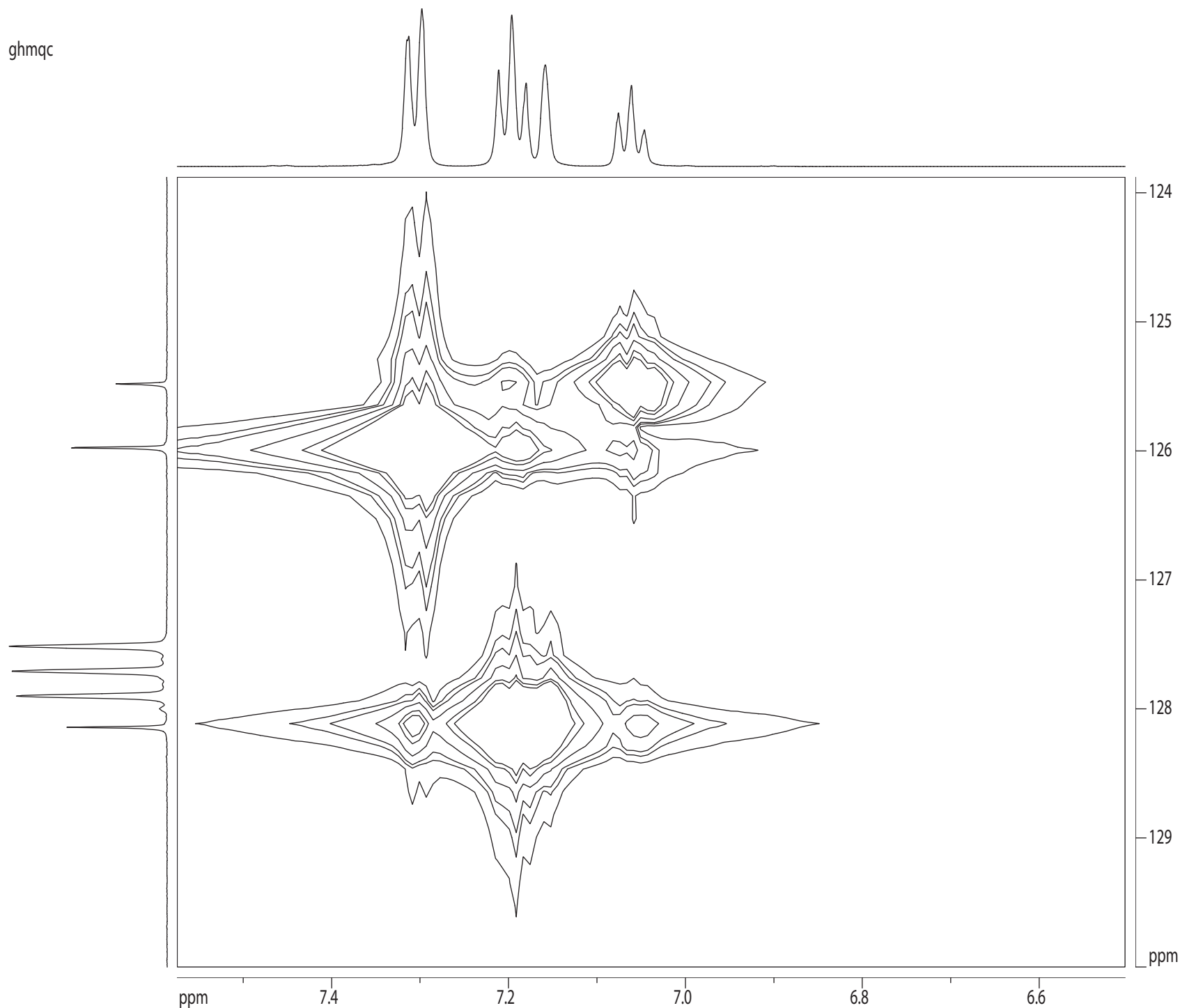
F1 - Processing parameters
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 SF 500.2200000 MHz
 WDW QSINE
 SSB 3
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 4.000 ppm
 F2LO 2000.88 Hz
 F2PHI 0.000 ppm
 F2HI 0.00 Hz
 F1PLO 4.000 ppm
 F1LO 2000.88 Hz
 F1PHI 0.000 ppm
 F1HI 0.00 Hz
 F2PPMCM 0.26667 ppm/cm
 F2HZCM 133.39200 Hz/cm
 F1PPMCM 0.26667 ppm/cm
 F1HZCM 133.39200 Hz/cm

ghmqc



ghmqc



Current Data Parameters

USER nmrl3t
NAME Donut_Yummy
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131211
Time 3.47
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PULPROG inv4gp.wu
TD 2048
SOLVENT C6D6
NS 8
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 2048
DW 124.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
d1 1.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000300 sec
d16 0.00020000 sec
d20 0.00242528 sec
IN0 0.00002200 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 MHz

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

CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7917392 MHz

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

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

F1 - Acquisition parameters

ND0 2
TD 512
SFO1 125.7917 MHz
FIDRES 44.389206 Hz
SIW 180.674 ppm
FnMODE undefined

F2 - Processing parameters

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

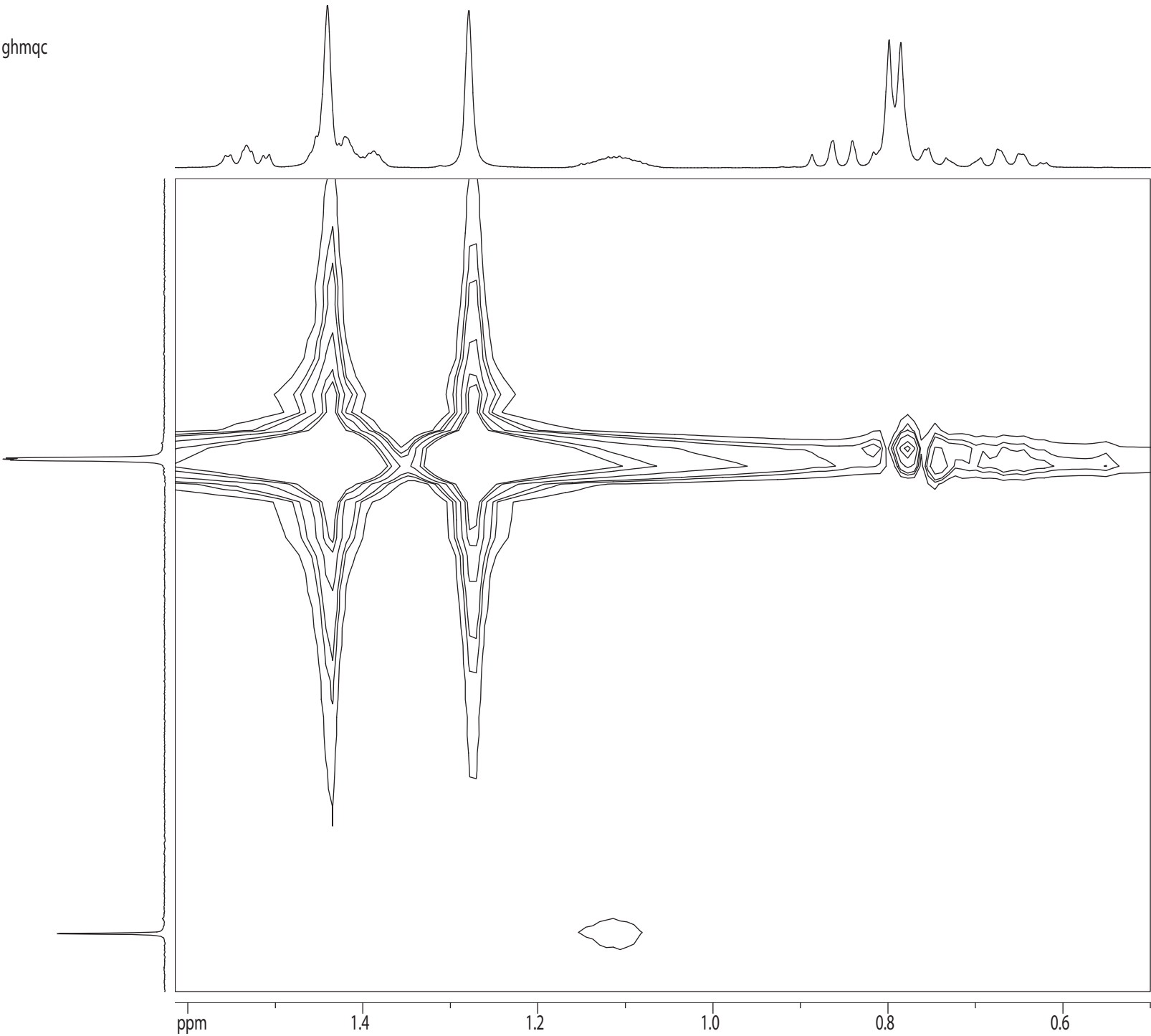
F1 - Processing parameters

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 7.574 ppm
F2LO 3788.90 Hz
F2PHI 6.503 ppm
F2HI 3252.86 Hz
F1PLO 130.000 ppm
F1LO 16351.45 Hz
F1PHI 123.879 ppm
F1HI 15581.60 Hz
F2PPMCM 0.05953 ppm/cm
F2HZCM 29.77854 Hz/cm
F1PPMCM 0.40804 ppm/cm
F1HZCM 51.32381 Hz/cm

ghmqc



Current Data Parameters

USER nmrl3t
NAME Donut_Yummy
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131211
Time 3.47
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG inv4gp.wu
TD 2048
SOLVENT C6D6
NS 8
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 2048
DW 124.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
d1 1.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000300 sec
d16 0.00020000 sec
d20 0.00242528 sec
IN0 0.00002200 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 MHz

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

CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7917392 MHz

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

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

F1 - Acquisition parameters

ND0 2
TD 512
SFO1 125.7917 MHz
FIDRES 44.389206 Hz
SIW 180.674 ppm
FnMODE undefined

F2 - Processing parameters

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

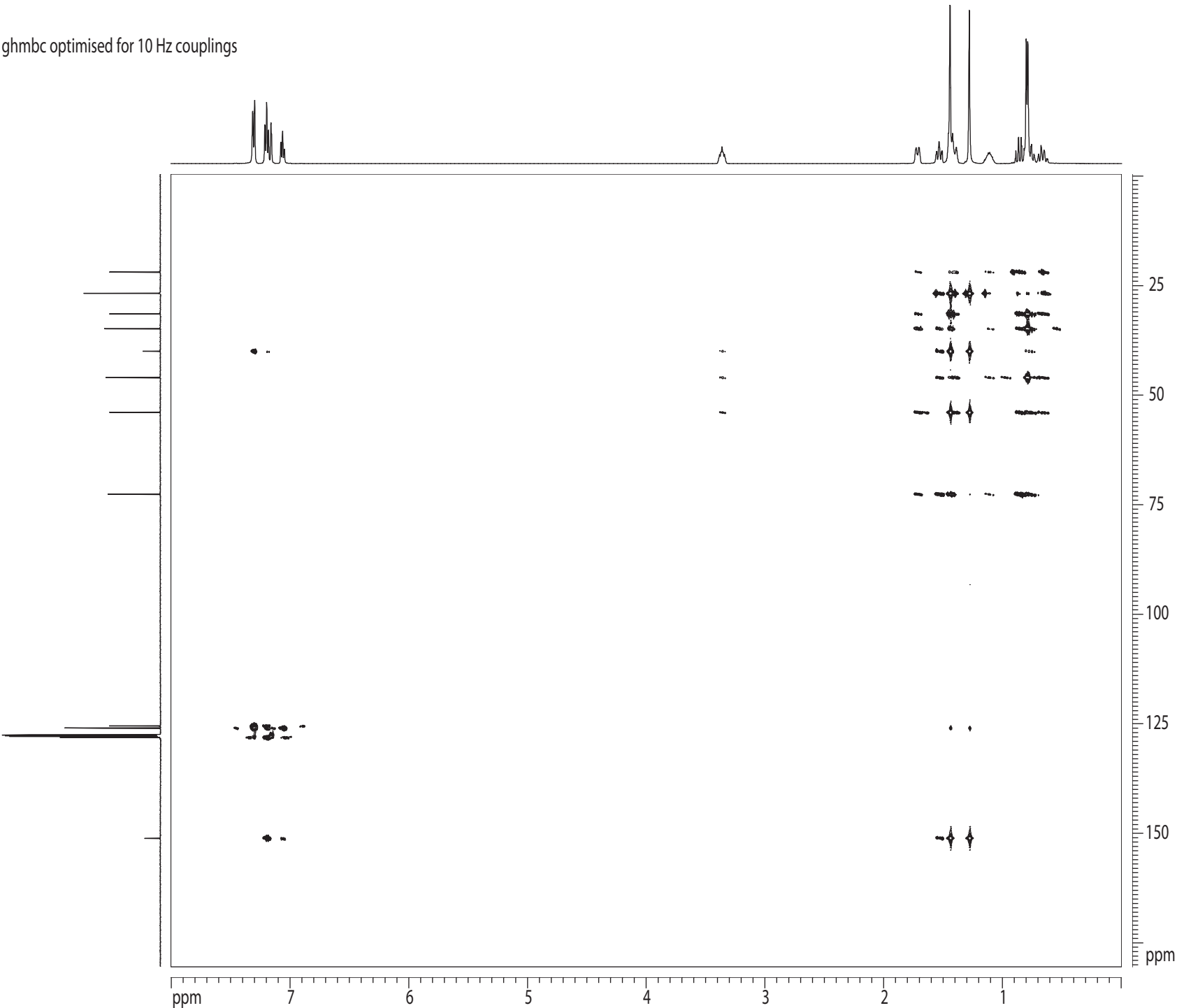
F1 - Processing parameters

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 1.614 ppm
F2LO 807.56 Hz
F2PHI 0.500 ppm
F2HI 250.11 Hz
F1PLO 32.000 ppm
F1LO 4024.97 Hz
F1HI 24.000 ppm
F1HI 3018.73 Hz
F2PPMCM 0.06191 ppm/cm
F2HZCM 30.96959 Hz/cm
F1PPMCM 0.53333 ppm/cm
F1HZCM 67.08289 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr13t
NAME Donut_Yummy
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131211
Time 5:15
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT C6D6
NS 8
DS 16
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 2896.3
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.25000000 sec
d2 0.00344828 sec
D6 0.05000000 sec
d13 0.00000300 sec
D16 0.00020000 sec
IN0 0.00002197 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 MHz

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

NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7917392 MHz

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

GP1AM1 sine.100
GP1AM2 sine.100
GP1AM3 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters

ND0 2
TD 512
SFO1 125.7917 MHz
FIDRES 44.439705 Hz
SW 180.879 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

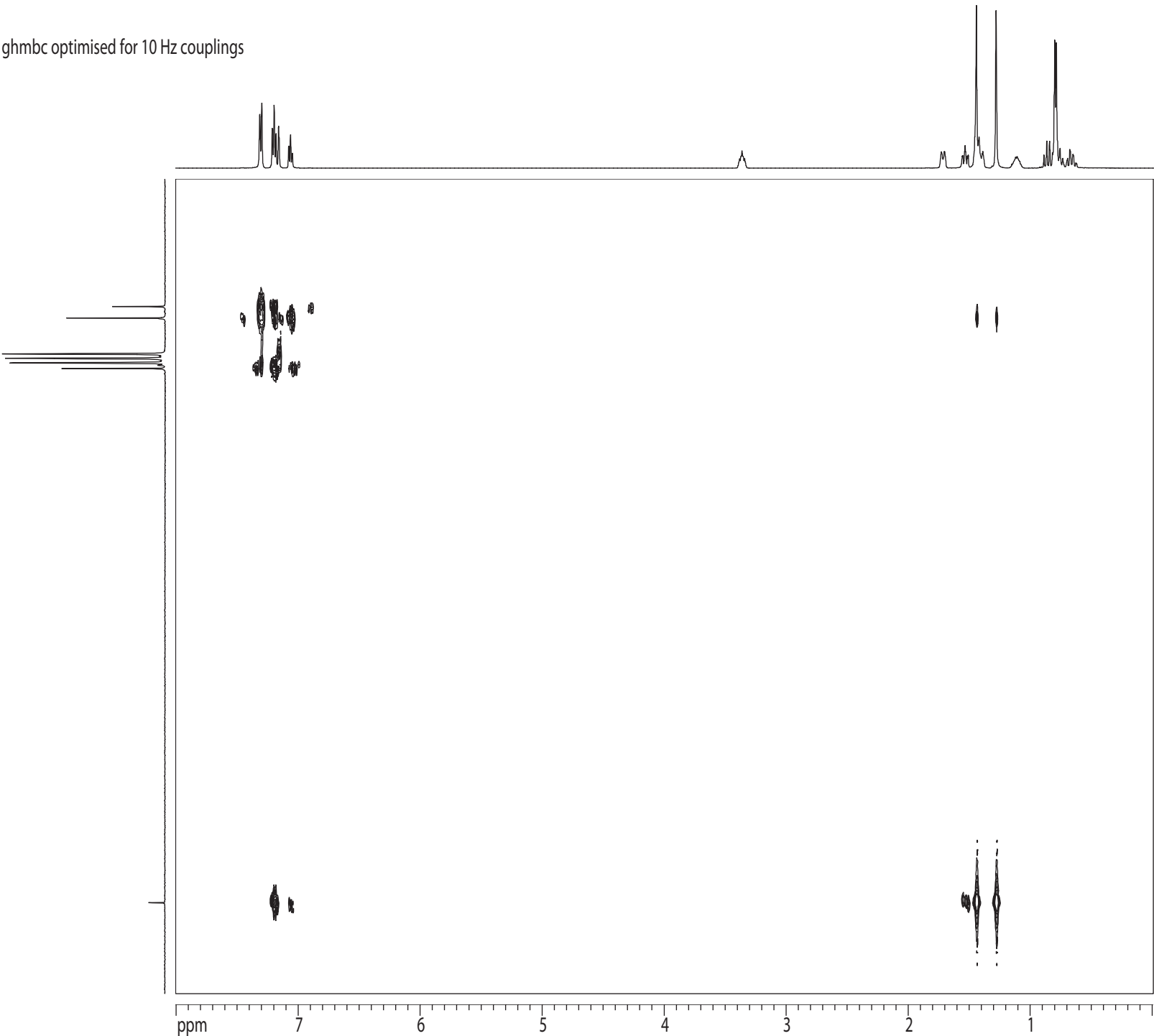
F1 - Processing parameters

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

2D NMR plot parameters

CY2 18.00 cm
CX1 15.00 cm
F2PLO 8.005 ppm
F2LO 4004.08 Hz
F2PHI -0.005 ppm
F2HI -2.33 Hz
F1PLO 180.448 ppm
F1LO 22696.80 Hz
F1PHI -0.448 ppm
F1HI -56.33 Hz
F2PPMCM 0.44496 ppm/cm
F2HZCM 222.57835 Hz/cm
F1PPMCM 12.05971 ppm/cm
F1HZCM 1516.87537 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr13t
NAME Donut_Yummy
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131211
Time 5:15
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT C6D6
NS 8
DS 16
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 2896.3
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.25000000 sec
d2 0.00344828 sec
D6 0.05000000 sec
d13 0.00000300 sec
D16 0.00020000 sec
IN0 0.00002197 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 MHz

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

NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7917392 MHz

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

GP1AM1 sine.100
GP1AM2 sine.100
GP1AM3 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters

ND0 2
TD 512
SFO1 125.7917 MHz
FIDRES 44.439705 Hz
SW 180.879 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

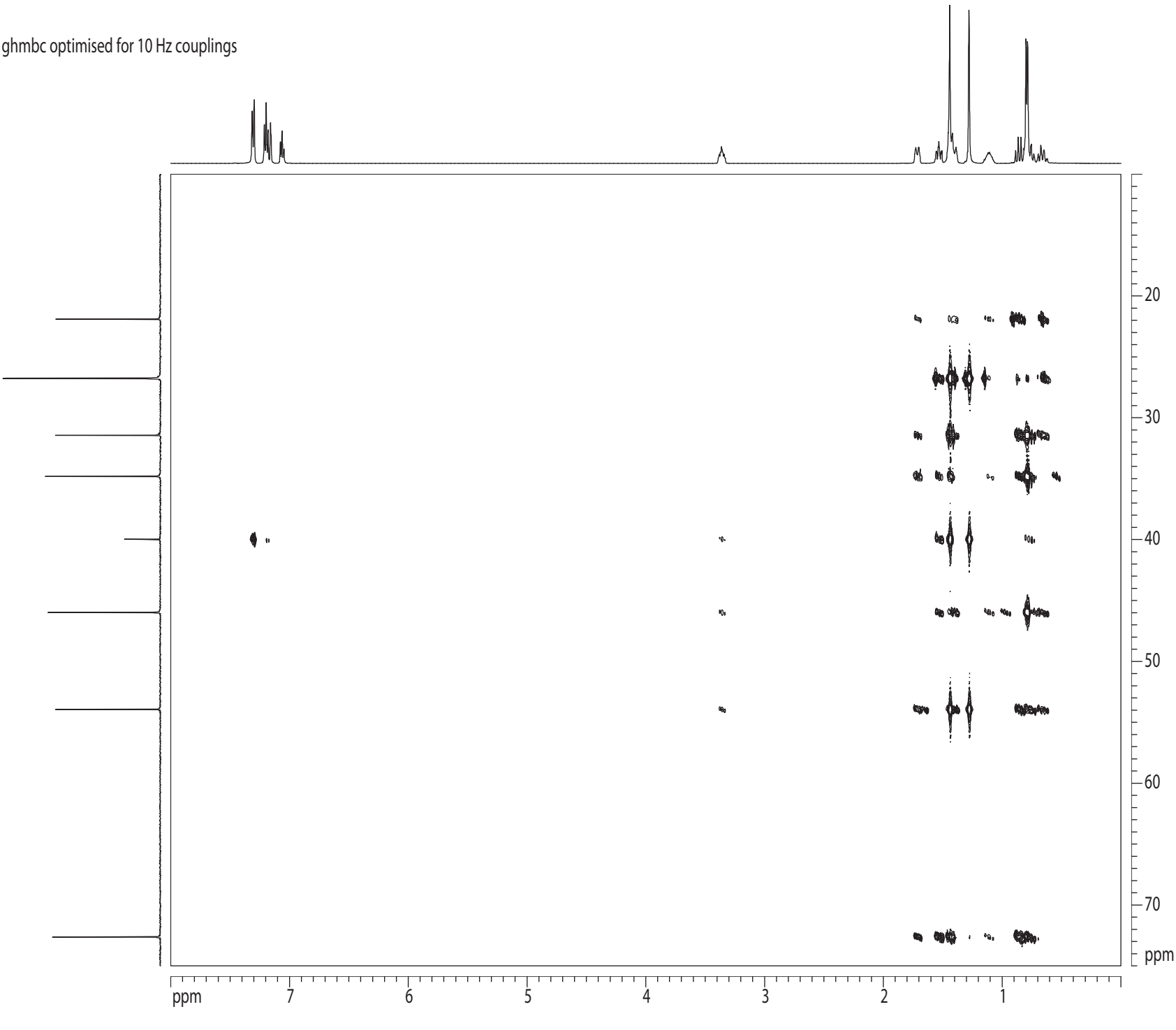
F1 - Processing parameters

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 8.005 ppm
F2LO 4004.08 Hz
F2PHI -0.009 ppm
F2HI -4.28 Hz
F1PLO 155.009 ppm
F1LO 19497.14 Hz
F1PHI 120.000 ppm
F1HI 15093.65 Hz
F2PPMCM 0.44518 ppm/cm
F2HZCM 222.68704 Hz/cm
F1PPMCM 2.33396 ppm/cm
F1HZCM 293.56607 Hz/cm

ghmbc optimised for 10 Hz couplings



Current Data Parameters

USER nmr13t
NAME Donut_Yummy
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131211
Time 5:15
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT C6D6
NS 8
DS 16
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 2896.3
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.25000000 sec
d2 0.00344828 sec
D6 0.05000000 sec
d13 0.00000300 sec
D16 0.00020000 sec
IN0 0.00002197 sec

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

NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220009 MHz

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

NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7917392 MHz

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

GP1AM1 sine.100
GP1AM2 sine.100
GP1AM3 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters

ND0 2
TD 512
SFO1 125.7917 MHz
FIDRES 44.439705 Hz
SW 180.879 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

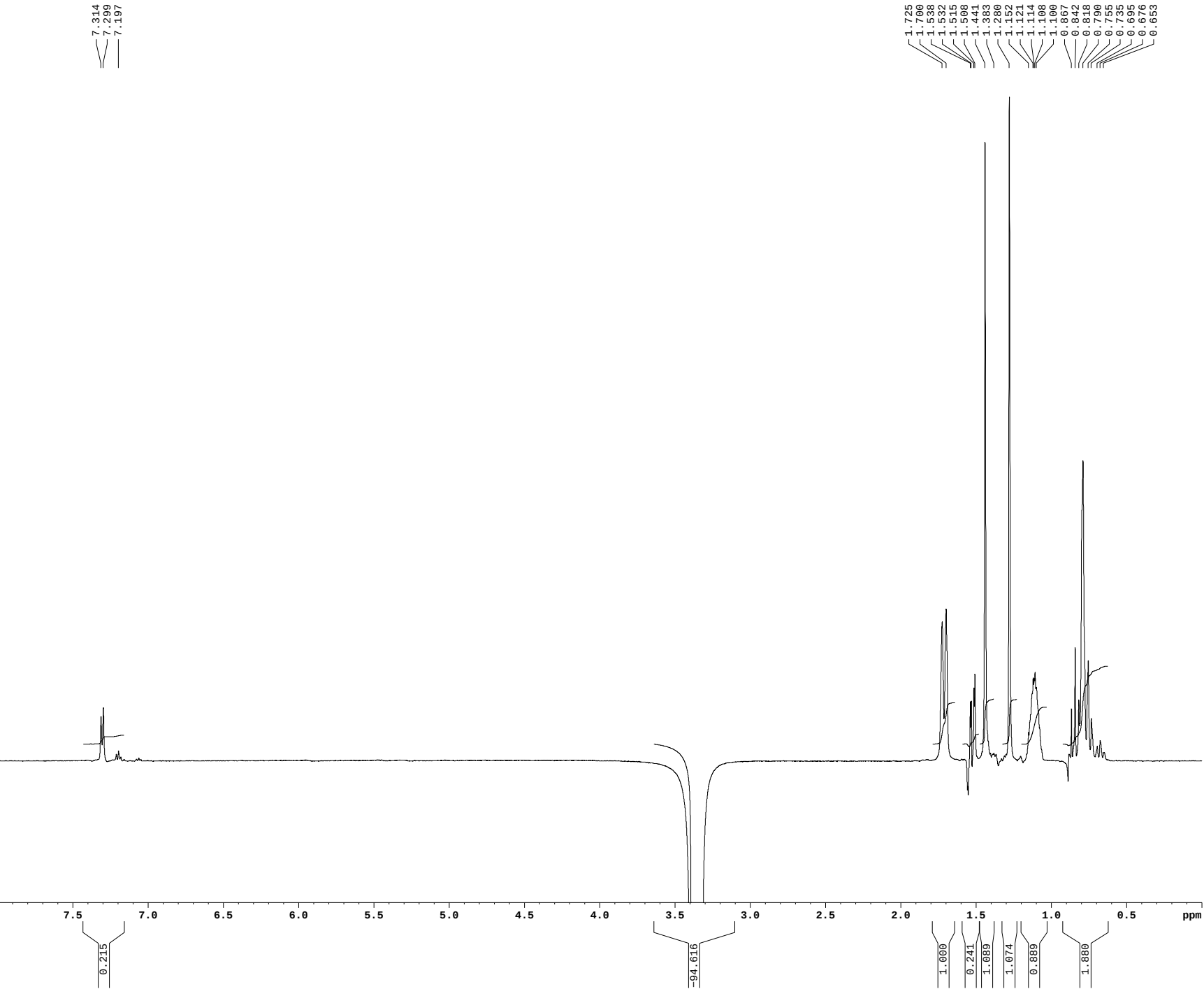
F1 - Processing parameters

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

2D NMR plot parameters

CY2 18.00 cm
CX1 15.00 cm
F2PLO 8.000 ppm
F2LO 4001.76 Hz
F2PHI 0.000 ppm
F2HI 0.00 Hz
F1PLO 75.000 ppm
F1LO 9433.53 Hz
F1PHI 10.000 ppm
F1HI 1257.80 Hz
F2PPMCM 0.44444 ppm/cm
F2HZCM 222.32001 Hz/cm
F1PPMCM 4.33333 ppm/cm
F1HZCM 545.04846 Hz/cm

gnoe



Current Data Parameters
USER nmrl3t
NAME Donut_Yummy
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131213
Time 9.17
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 102
DS 8
SWH 5000.000 Hz
FIDRES 0.076294 Hz
AQ 6.5536499 sec
RG 45.3
DW 100.000 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

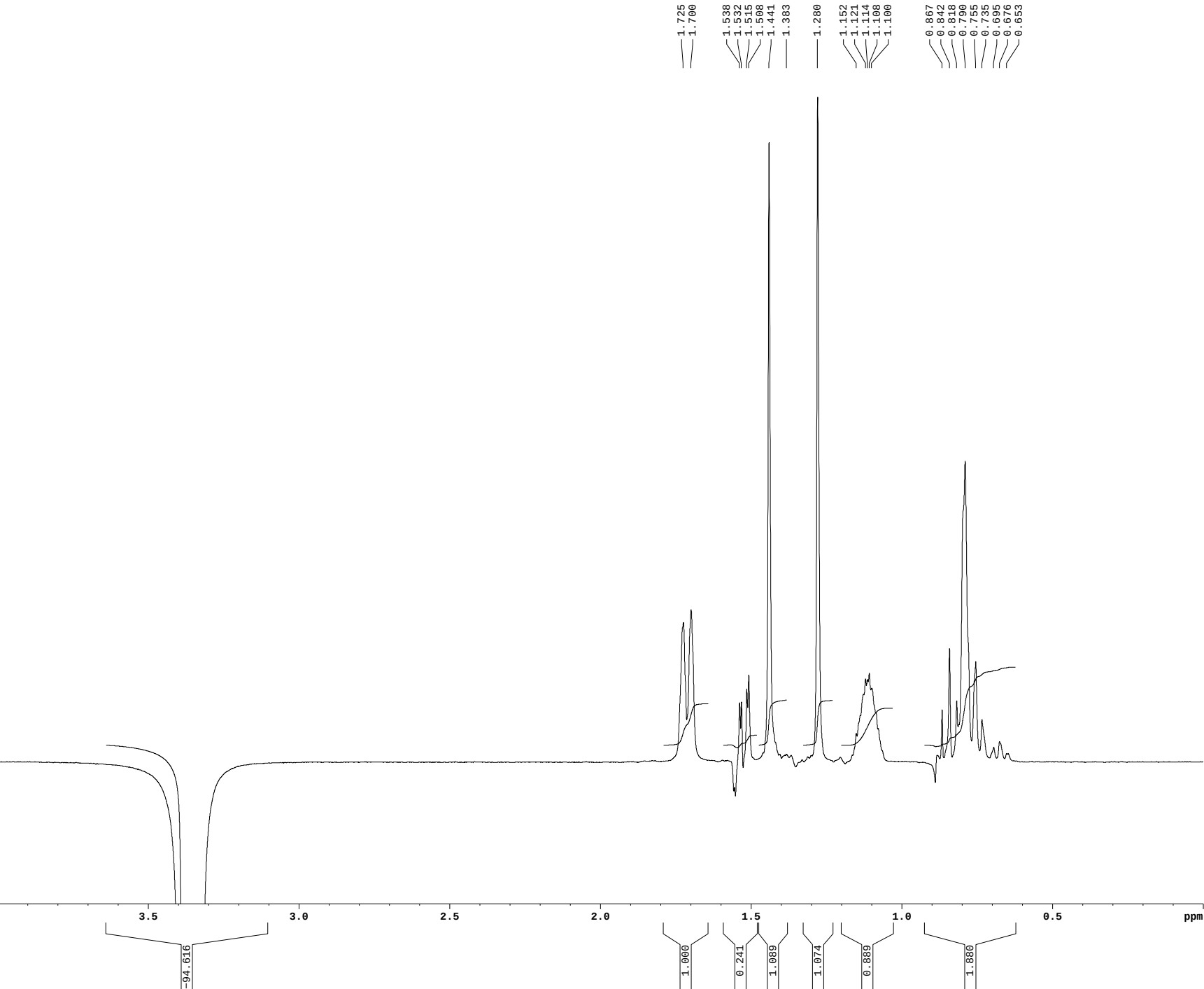
===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SF01 500.2216819 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 14.38 cm
F1P 8.000 ppm
F1 4001.76 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.35088 ppm/cm
HZCM 175.51579 Hz/cm

gnoe



Current Data Parameters
USER nmr13t
NAME Donut_Yummy
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131213
Time 9.17
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 102
DS 8
SWH 5000.000 Hz
FIDRES 0.076294 Hz
AQ 6.5536499 sec
RG 45.3
DW 100.000 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

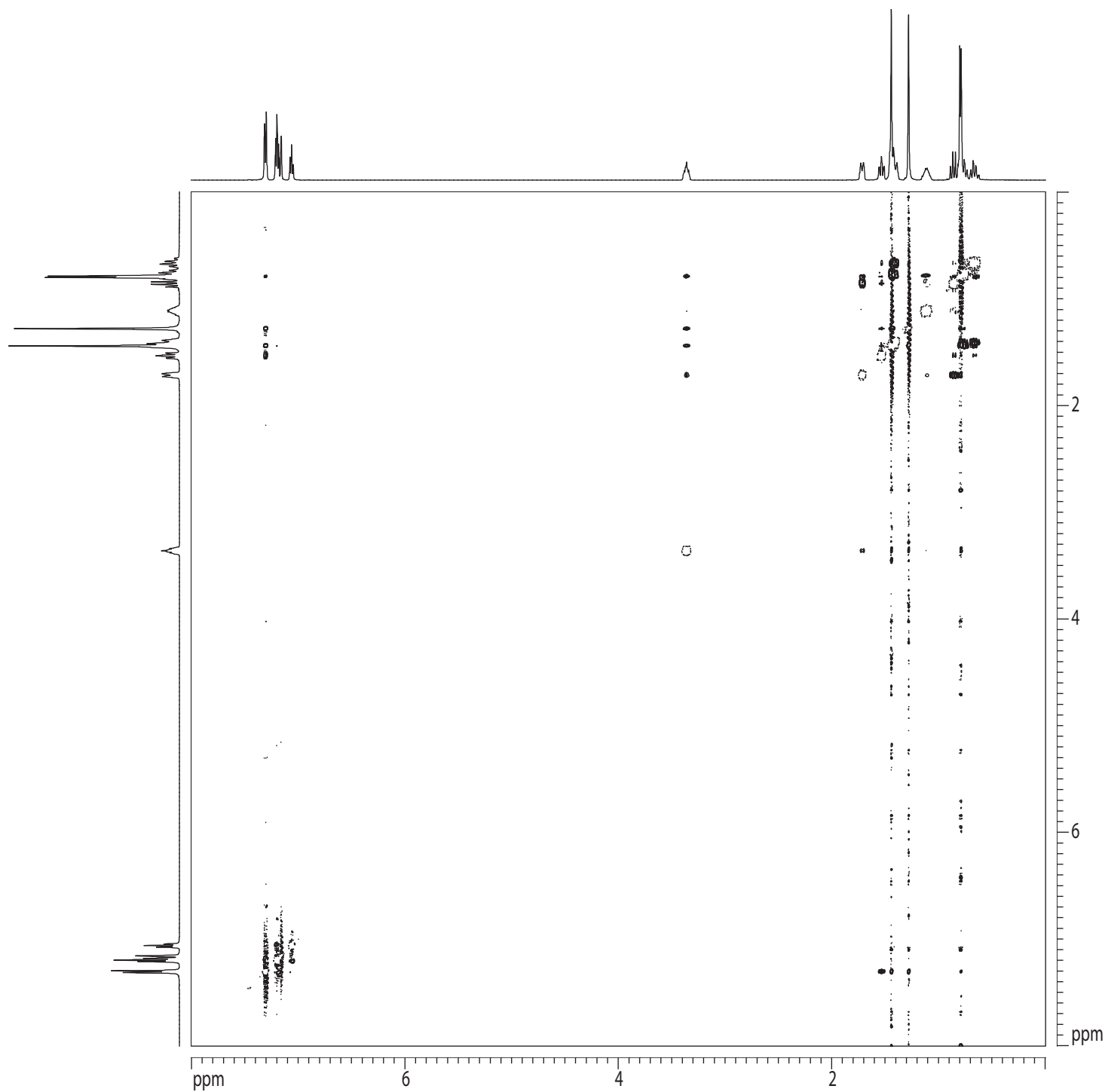
===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SF01 500.2216819 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 14.38 cm
F1P 8.000 ppm
F1 4001.76 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.35088 ppm/cm
HZCM 175.51579 Hz/cm

noesy



Current Data Parameters
USER nmr13t
NAME Donut_Yummy
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131211
Time 0.02
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG noesyrvtp
TD 2048
SOLVENT C6D6
NS 8
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 16
DW 124.800 usec
DE 6.00 usec
TE 298.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D8 1.00000000 sec
INO 0.00012480 sec

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

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

F2 - Processing parameters
SI 1024
SF 500.2200000 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 8.005 ppm
F2LO 4004.08 Hz
F2PHI -0.005 ppm
F2HI -2.33 Hz
F1PLO 8.005 ppm
F1LO 4004.08 Hz
F1PHI -0.005 ppm
F1HI -2.33 Hz
F2PPMCM 0.53395 ppm/cm
F2HZCM 267.09402 Hz/cm
F1PPMCM 0.53395 ppm/cm
F1HZCM 267.09402 Hz/cm

noesy

