Name: _____

Chem 203
December 15, 2012

Final Exam Part II
Problem 1 of 3 (30 points)

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

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

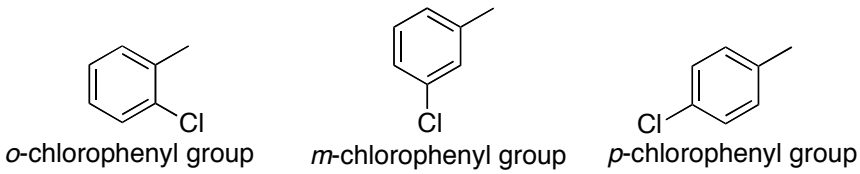
Books, notes, lecture videos, calculators, rulers, and laptop computers are permitted as is wireless (or wired) internet access and appropriate software (e.g, Pymol, Macromodel/Maestro, Excel, NMRPrediction, Chemdraw, ElComp, MolE, etc.). Catalogs of molecular structures (e.g., the Aldrich catalog, the Merck Index, etc.) or databases of molecular structures (such as wireless access to SciFinder Scholar, the Sigma-Aldrich website, etc.) are NOT PERMITTED. USE OF SUCH ITEMS CONSTITUTES ACADEMIC DISHNONESTY, 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 $C_{17}H_{19}ClO$: IR (solution in $CHCl_3$), 600 MHz ^1H NMR, 150.9 MHz ^{13}C NMR, DEPT-90, DEPT-135, COSY, HMQC, HMBC, TOCSY and NOESY. 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.

All NMR spectra were measured in deuterotoluene, $C_6D_5CD_3$. ^1H resonances associated with ^1H isotopic impurities in the solvent are marked.

HINT: The molecule contains a chlorophenyl group.



o-chlorophenyl group *m*-chlorophenyl group *p*-chlorophenyl 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 ^{1}H resonances (a-l) 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:

c. Redraw the structure of the molecule below and write the letter (a-l) of each ^{1}H 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 (1-17) in order of descending chemical shift. Make sure to report the chemical shift of each carbon resonances to the nearest tenth of ppm, unless two have the same value, in which case you may report it to the nearest hundredth.

1:

2:

3:

4:

5:

6:

7:

8:

9:

10:

11:

12:

13:

14:

15:

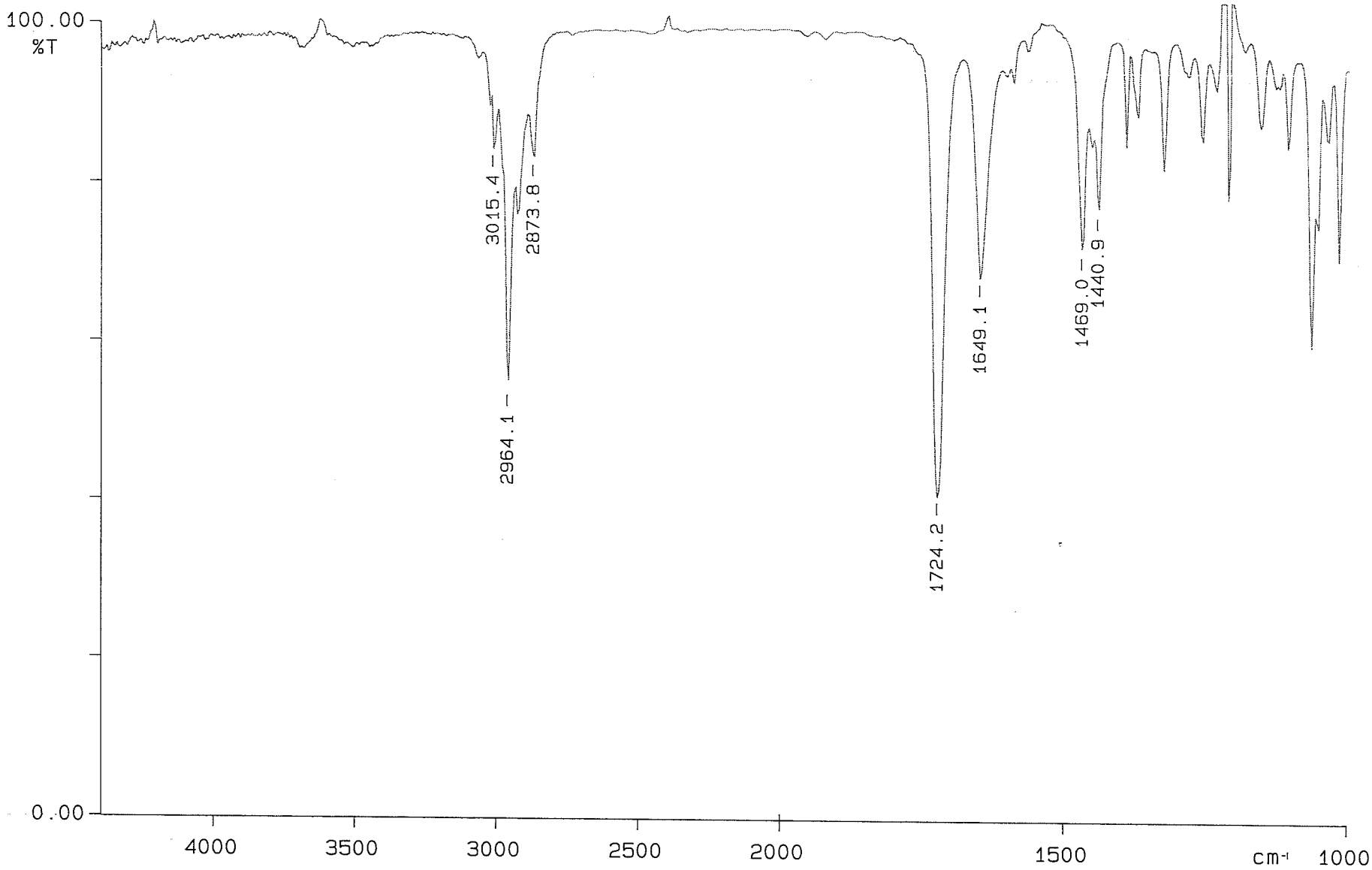
16:

17:

e. Redraw the structure of the molecule below and write the number (1-17) 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.

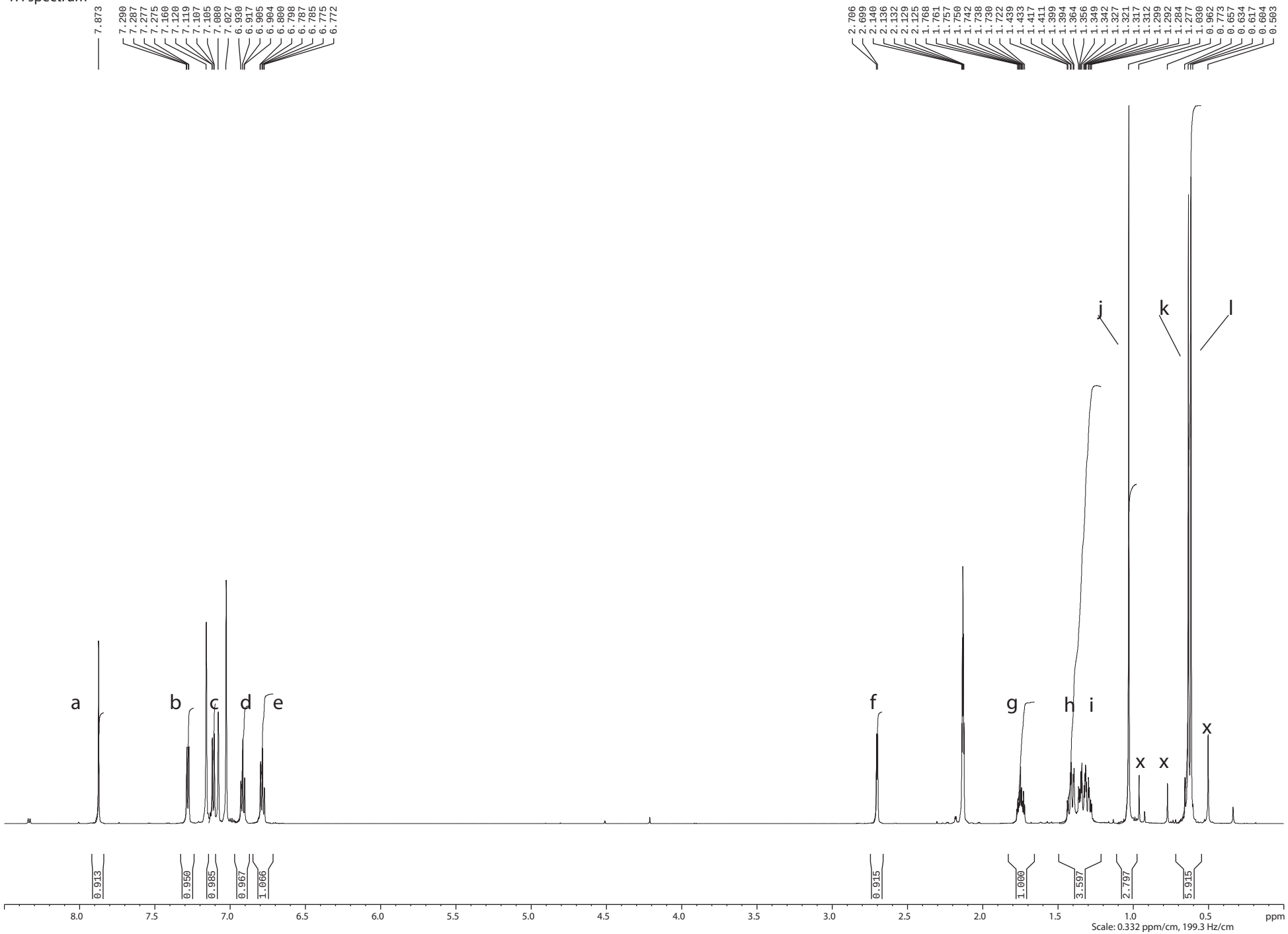
II 2 solution

PERKIN ELMER



12/12/12 14: 41
X: 4 scans, 4.0cm-1

1H spectrum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7.160
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7.080
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6.917
6.905
6.904
6.800
6.798
6.787
6.785
6.775
6.772
2.706
2.699
2.140
2.136
2.132
2.129
2.125
1.768
1.761
1.757
1.750
1.742
1.738
1.730
1.722
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1.417
1.411
1.399
1.394
1.364
1.356
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1.327
1.321
1.317
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1.299
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0.657
0.634
0.617
0.604
0.503
a
b
c
d
e
f
g
h
i
j
k
l
x
x
x
0.913
0.950
0.985
0.967
1.066
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1.000
3.597
2.797
5.915
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
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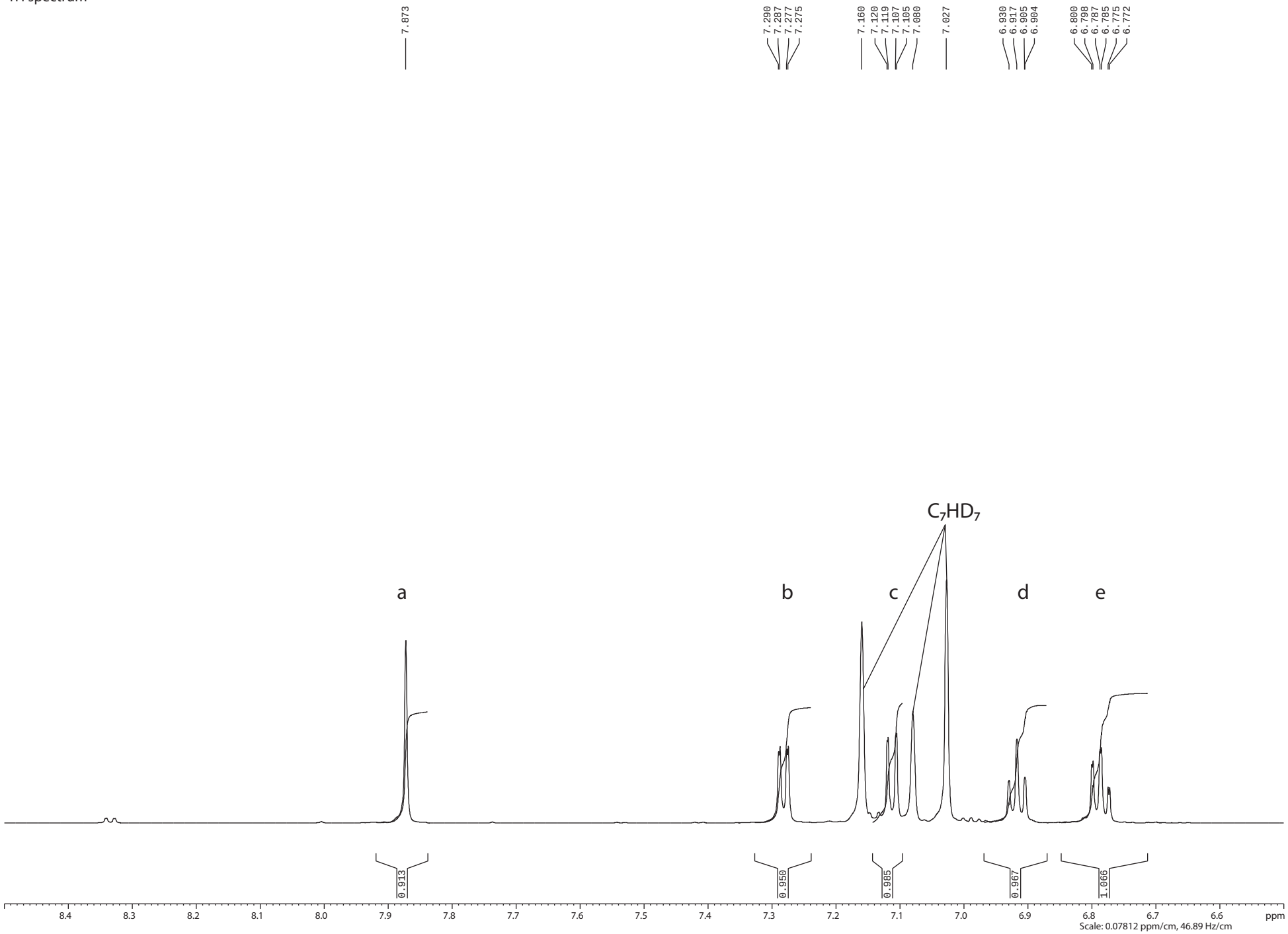
3	31591.4	4373.542	7.2877	1.61
4	31634.5	4367.214	7.2771	1.56
5	31644.0	4365.815	7.2748	1.62
6	32114.0	4296.862	7.1599	4.22
7	32160.1	4290.100	7.1486	0.23
8	32223.9	4280.743	7.1330	0.24
9	32276.3	4273.047	7.1202	1.74
10	32282.7	4272.104	7.1186	1.80
11	32331.0	4265.031	7.1068	1.85
12	32337.4	4264.087	7.1053	1.89
13	32440.6	4248.942	7.0800	2.35
14	32656.3	4217.297	7.0273	5.10
15	33052.1	4159.225	6.9305	0.87
16	33055.5	4158.725	6.9297	0.90
17	33106.6	4151.229	6.9172	1.76
18	33154.7	4144.174	6.9055	0.96
19	33158.4	4143.631	6.9046	0.97
20	33584.7	4081.075	6.8003	1.23
21	33593.6	4079.782	6.7982	1.31
22	33637.9	4073.280	6.7873	1.54
23	33646.3	4072.050	6.7853	1.58
24	33689.0	4065.774	6.7748	0.76
25	33699.6	4064.229	6.7722	0.75
26	50330.5	1624.157	2.7063	1.89
27	50359.4	1619.910	2.6993	1.88
28	52647.7	1284.179	2.1398	2.10
29	52662.4	1282.024	2.1362	3.90
30	52677.3	1279.835	2.1326	5.39
31	52692.1	1277.663	2.1290	3.96
32	52706.9	1275.485	2.1253	2.11
33	54142.3	1064.890	1.7744	0.31
34	54168.6	1061.026	1.7680	0.53
35	54196.6	1056.924	1.7612	0.44
36	54214.5	1054.295	1.7568	0.70
37	54243.3	1050.065	1.7497	1.19
38	54272.9	1045.729	1.7425	0.75
39	54292.2	1042.902	1.7378	0.47
40	54323.4	1038.316	1.7302	0.68
41	54354.1	1033.815	1.7227	0.40
42	55513.0	863.775	1.4393	0.48

43	55539.6	859.884	1.4328	0.56
44	55601.6	850.787	1.4177	1.07
45	55626.5	847.124	1.4116	1.28
46	55679.6	839.338	1.3986	1.04
47	55698.9	836.502	1.3939	1.15
48	55746.8	829.477	1.3822	0.24
49	55781.9	824.332	1.3736	0.25
50	55820.2	818.703	1.3642	0.78
51	55851.6	814.099	1.3565	0.72
52	55882.0	809.646	1.3491	1.09
53	55912.1	805.224	1.3417	1.27
54	55971.9	796.453	1.3271	0.80
55	55996.8	792.793	1.3210	1.06
56	56011.7	790.610	1.3174	1.22
57	56033.2	787.450	1.3121	0.87
58	56087.8	779.446	1.2988	0.96
59	56113.1	775.730	1.2926	0.76
60	56148.6	770.524	1.2839	0.50
61	56175.7	766.544	1.2773	0.42
62	57185.9	618.329	1.0303	15.00
63	57466.2	577.205	0.9618	1.01
64	57614.0	555.521	0.9257	0.25
65	58236.3	464.218	0.7735	0.84
66	58712.1	394.408	0.6572	0.96
67	58806.1	380.624	0.6342	13.14
68	58875.6	370.418	0.6172	13.54
69	58929.2	362.555	0.6041	0.40
70	59341.2	302.104	0.5034	1.85
71	60016.8	202.984	0.3382	0.35

1H spectrum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6.905
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6.800
6.798
6.787
6.785
6.775
6.772
C7HD7
a
b
c
d
e
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8.4
8.3
8.2
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8.0
7.9
7.8
7.7
7.6
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7.4
7.3
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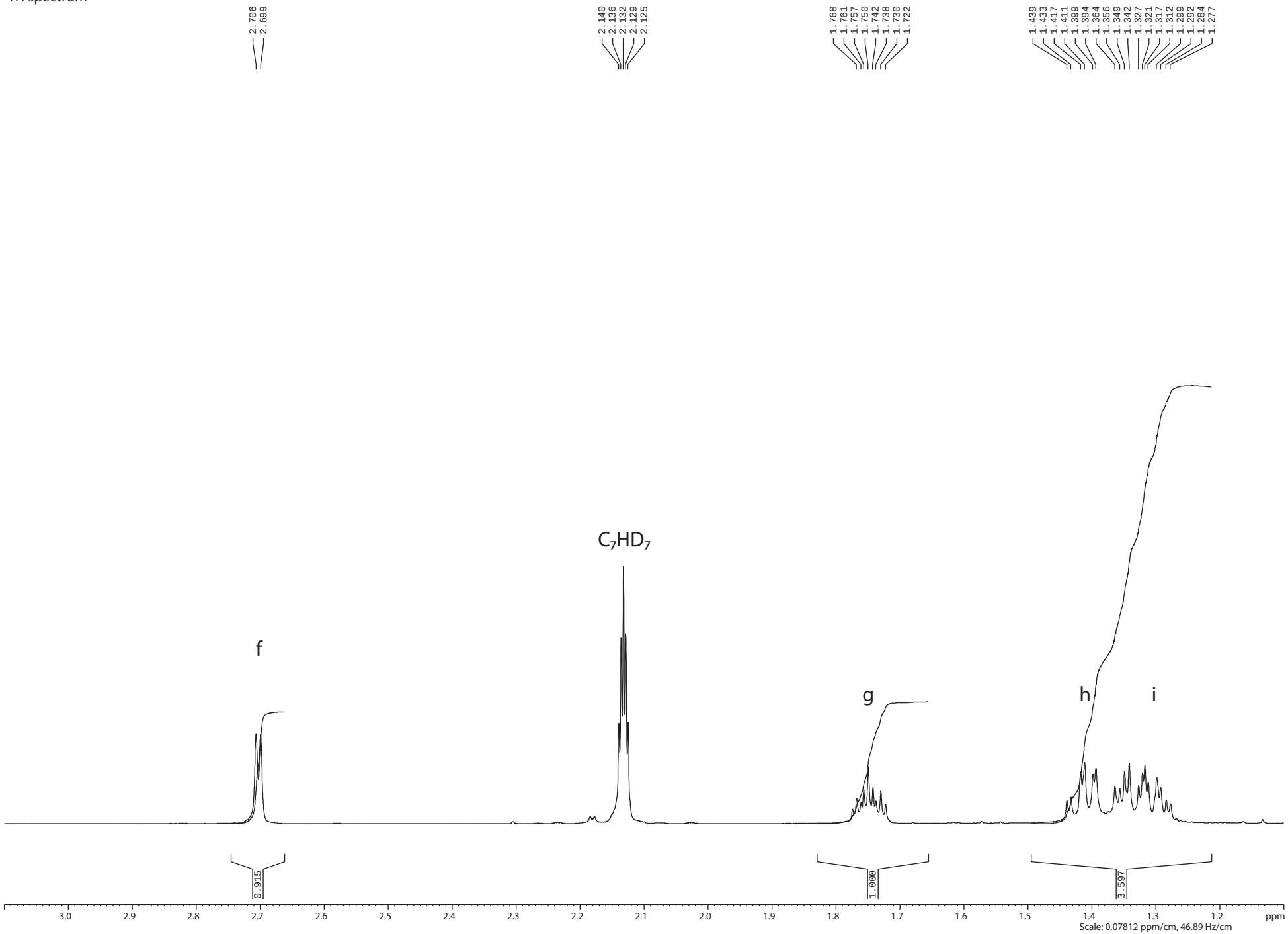
1H spectrum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1.292
1.284
1.277
C7HD7
f
g
h
i
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1.000
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2.9
2.8
2.7
2.6
2.5
2.4
2.3
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1.8
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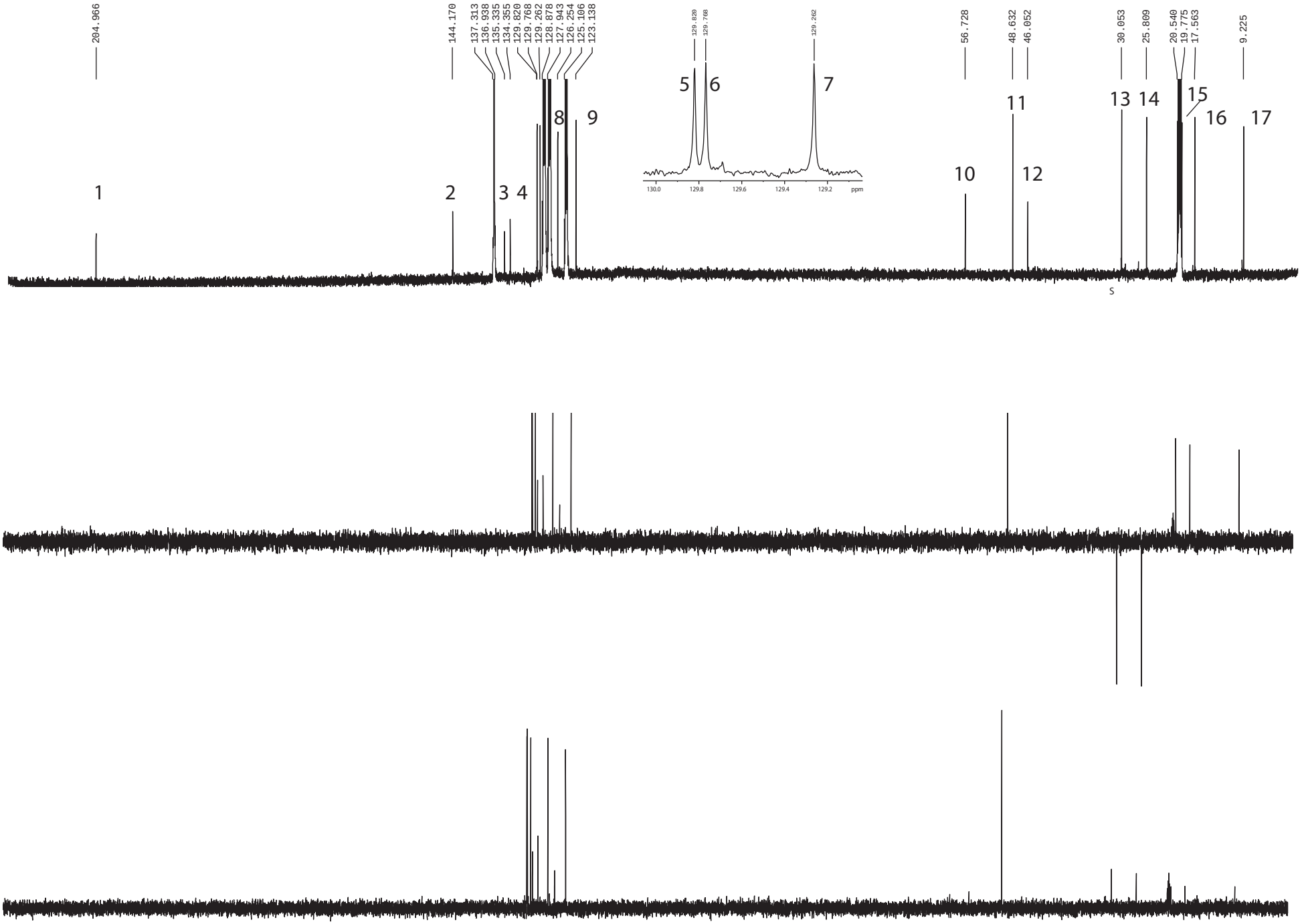
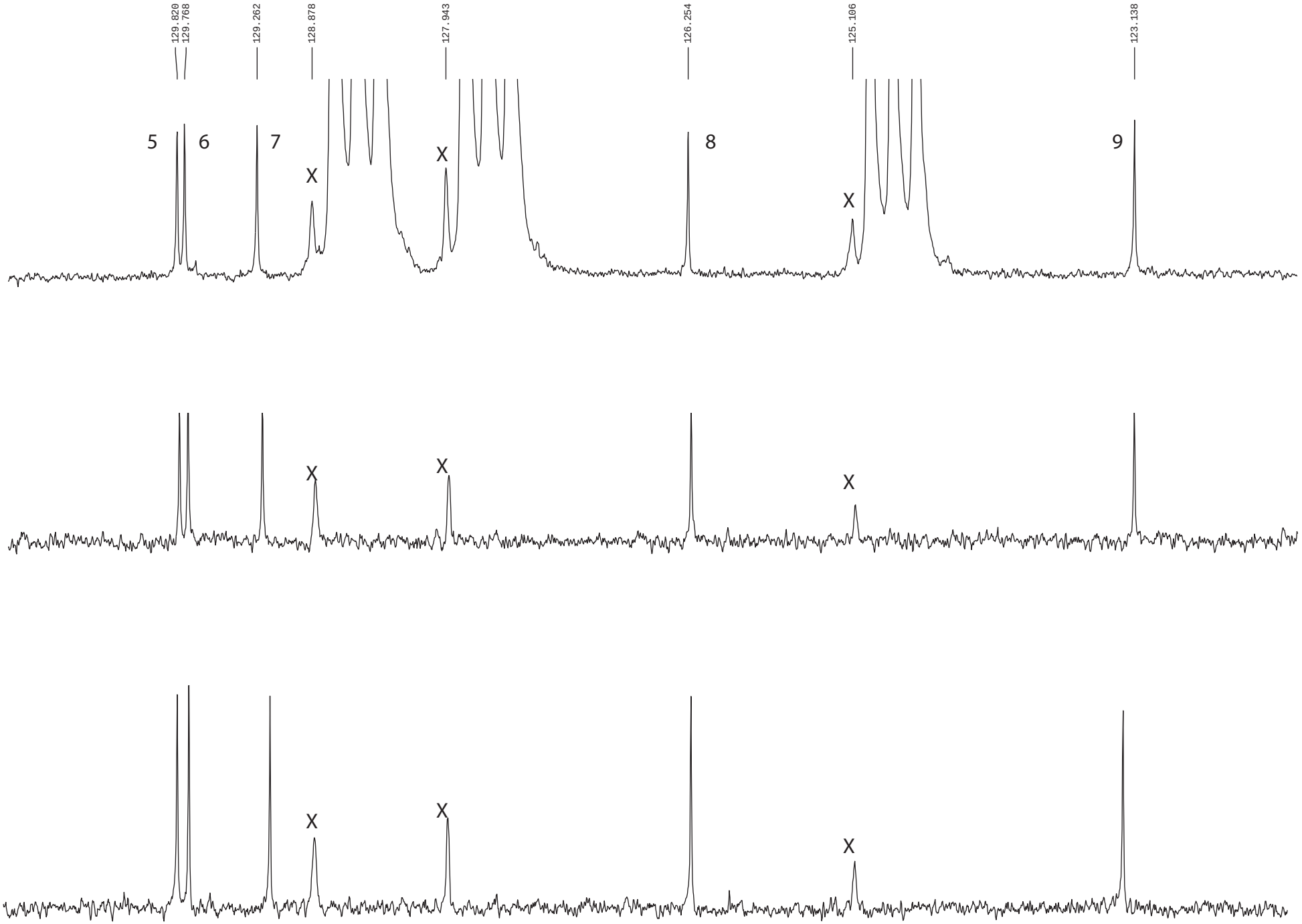
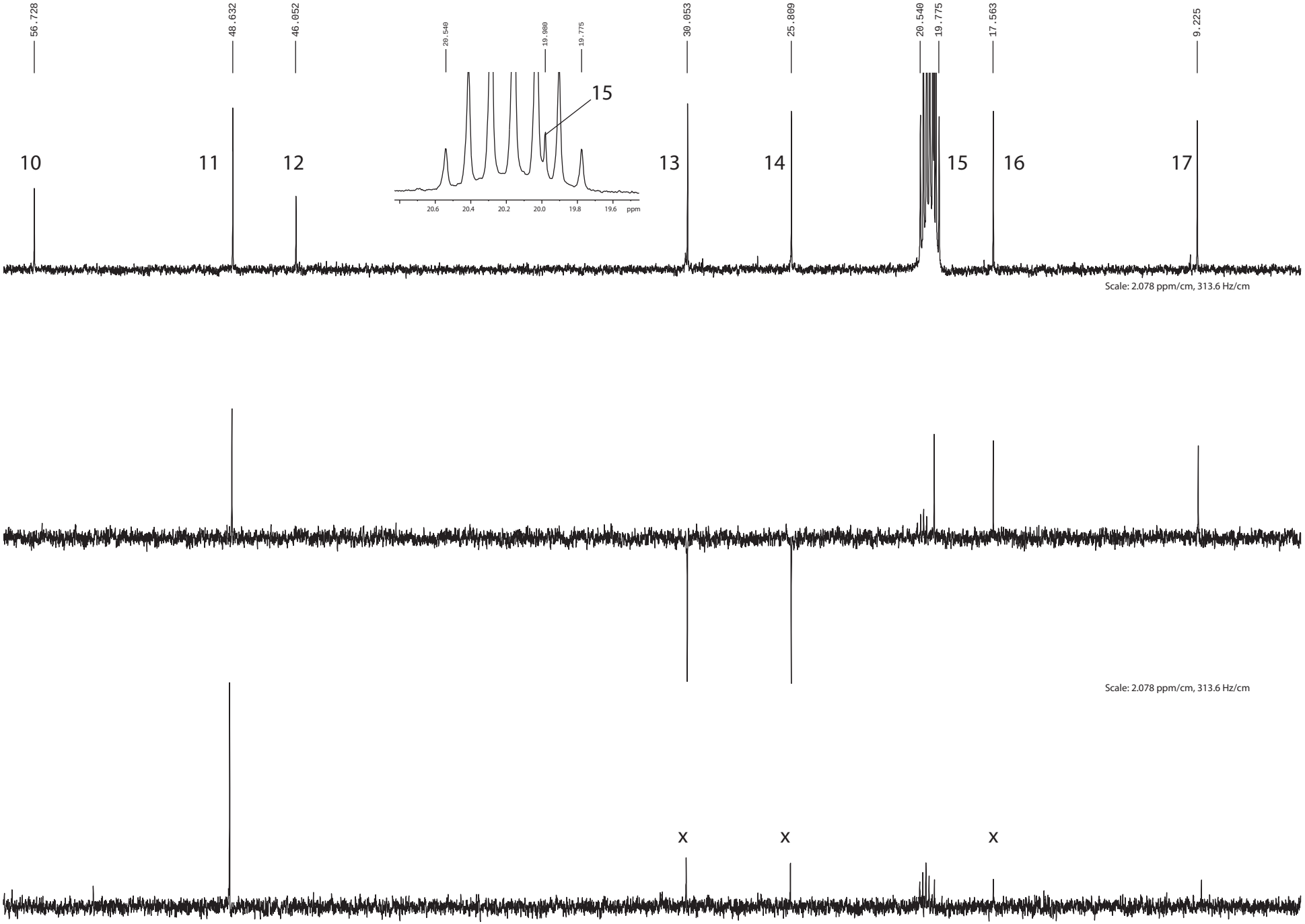
13C spectrum with 1H decoupling



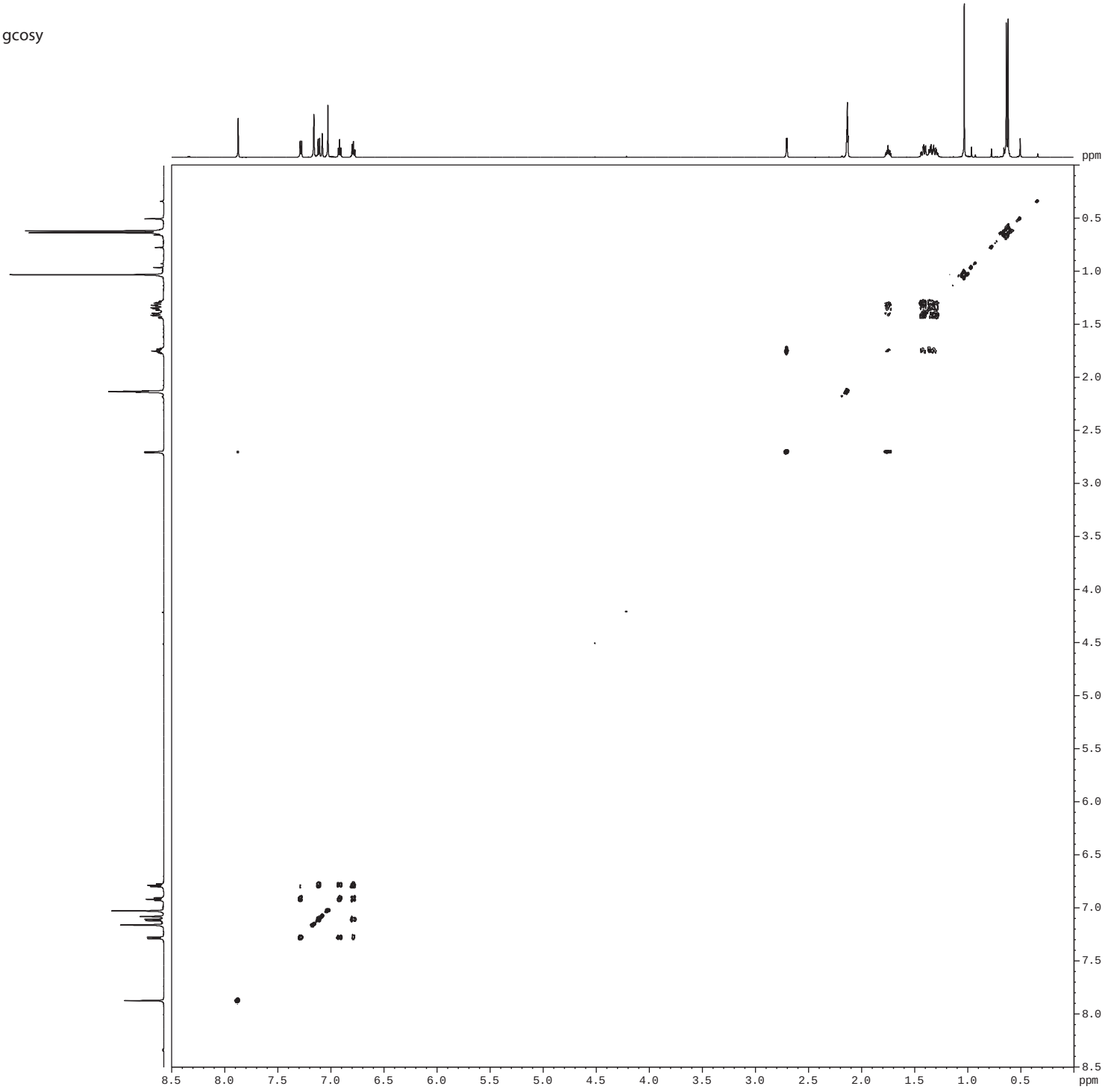
13C spectrum with 1H decoupling



13C spectrum with 1H decoupling



gcosy

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RG                 203
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DE               6.00 usec
TE              264.2 K
D0          0.00000300 sec
D1          1.48689198 sec
D13         0.00000400 sec
D16         0.00020000 sec
IN0         0.00019600 sec

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NUC1                1H
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P1               8.00 usec
PLW1        23.01441956 W
SFO1       600.1325505 MHz

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GPZ1            10.00 %
P16           1000.00 usec

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SFO1          600.1326 MHz
FIDRES        9.964924 Hz
SW               8.502 ppm
FnMODE              QF

F2 - Processing parameters
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SF          600.1300000 MHz
WDW               SINE
SSB       0
LB        0 Hz
GB        0
PC                1.00

F1 - Processing parameters
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WDW             States
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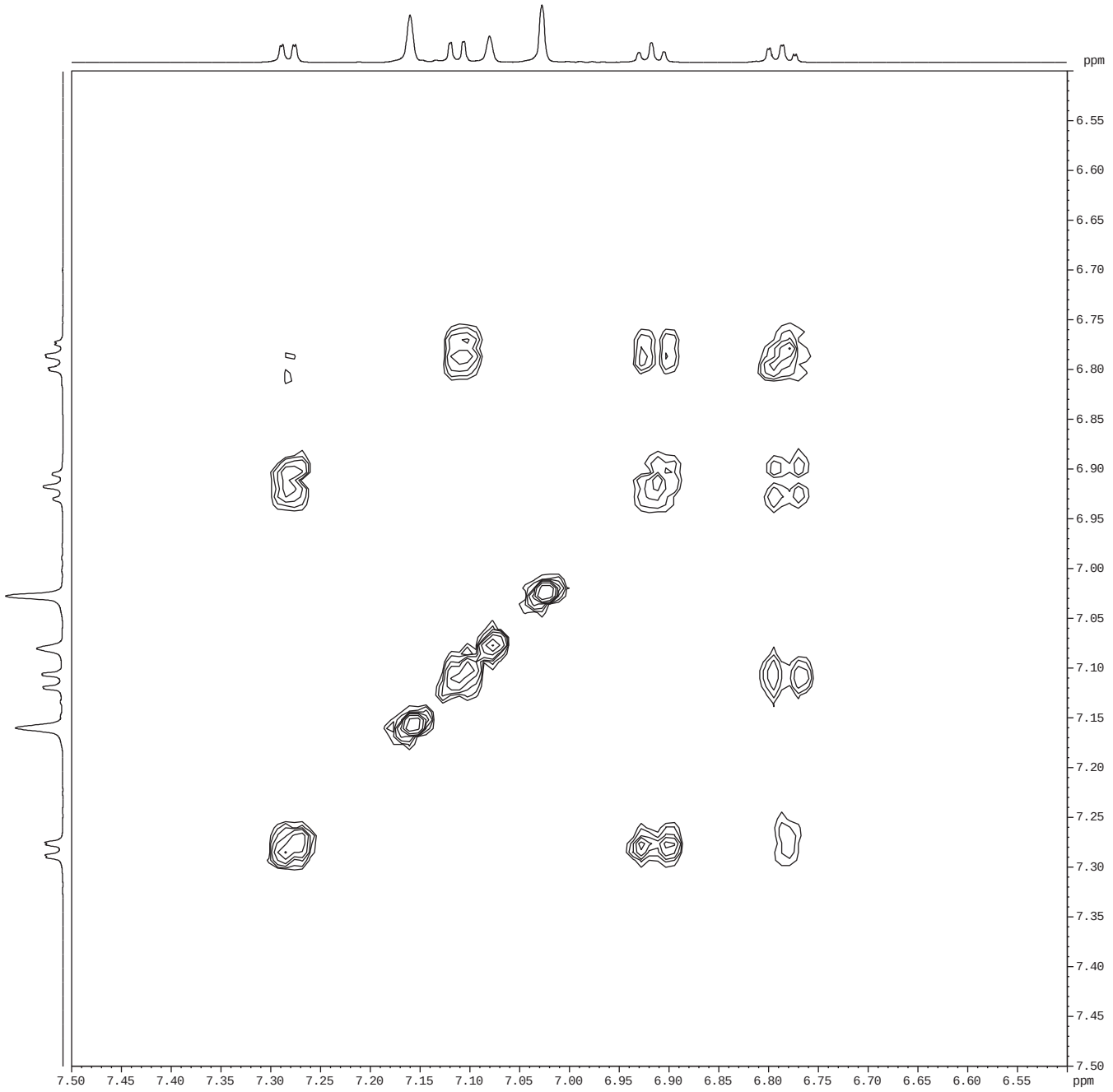
gcosy

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======== CHANNEL f1 ========
NUC1                1H
P0               8.00 usec
P1               8.00 usec
PLW1        23.01441956 W
SFO1       600.1325505 MHz

====== GRADIENT CHANNEL =====
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SW              8.502 ppm
FnMODE             QF

F2 - Processing parameters
SI                1024
SF          600.1300000 MHz
WDW               SINE
SSB       0
LB        0 Hz
GB        0
PC                1.00

F1 - Processing parameters
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MC2                QF
SF          600.1300000 MHz
WDW             States
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LB        0 Hz
GB        0
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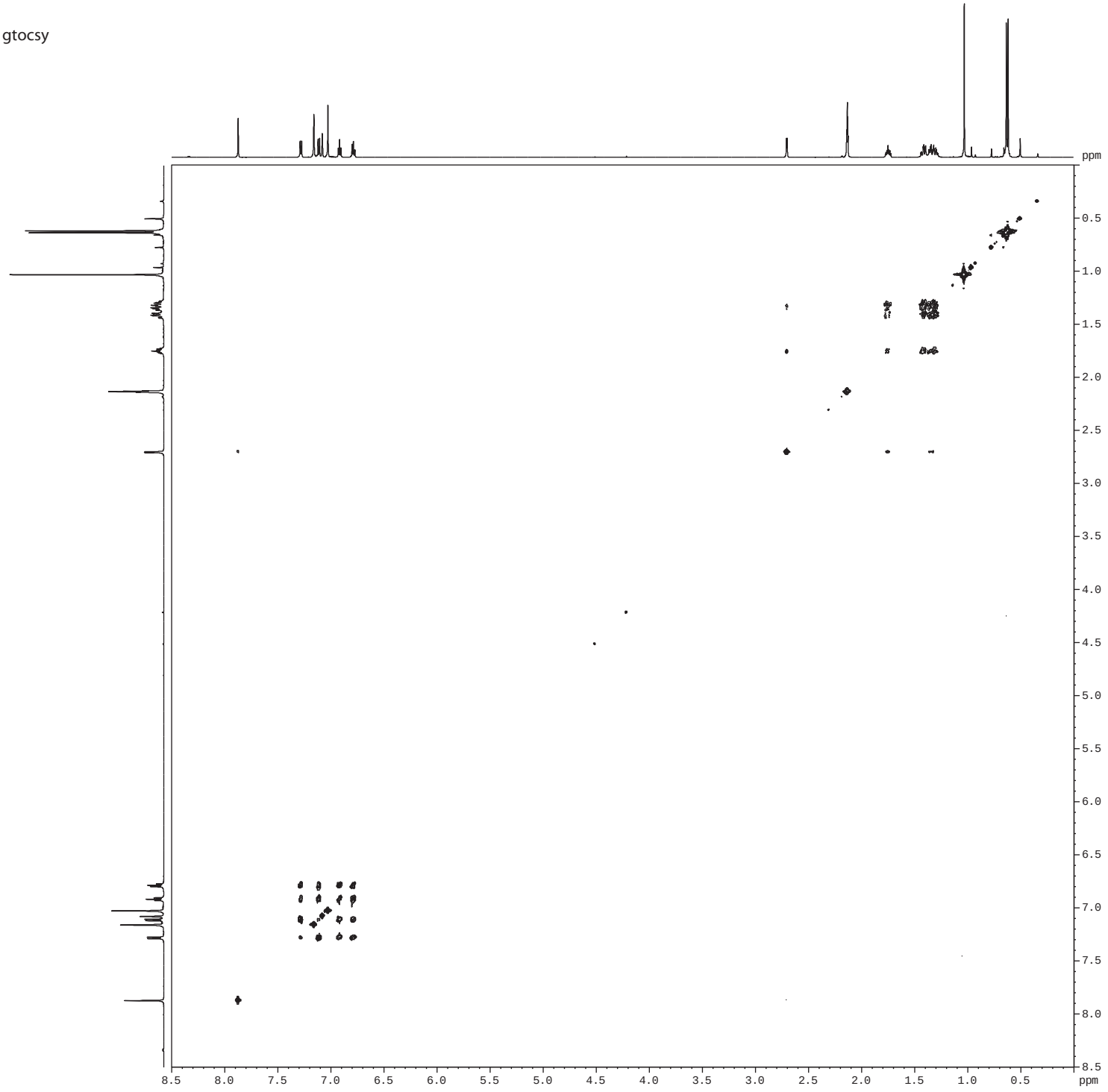
gtocsy

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DS                   16
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FIDRES        2.491231 Hz
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RG                  203
DW               98.000 usec
DE                6.00 usec
TE               265.0 K
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D1           2.00000000 sec
D9           0.06000000 sec
D12          0.00002000 sec
D16          0.00020000 sec
IN0          0.00019600 sec
L1                   30

======== CHANNEL f1 ========
NUC1                 1H
P1                8.00 usec
P5               23.34 usec
P6               35.00 usec
P7               70.00 usec
P17            2500.00 usec
PLW1        23.01441956 W
PLW10        1.20226395 W
SFO1        600.1325505 MHz

====== GRADIENT CHANNEL =====
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GPNAM2          SINE.100
GPZ1              10.00 %
GPZ2             -10.00 %
P16             1000.00 usec

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FIDRES         9.964924 Hz
SW                8.502 ppm
FnMODE               QF

F2 - Processing parameters
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SF          600.1300000 MHz
WDW                SINE
SSB      0
LB       0 Hz
GB       0
PC                 1.00

F1 - Processing parameters
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MC2                  QF
SF          600.1300000 MHz
WDW              States
SSB      0
LB       0 Hz
GB       0
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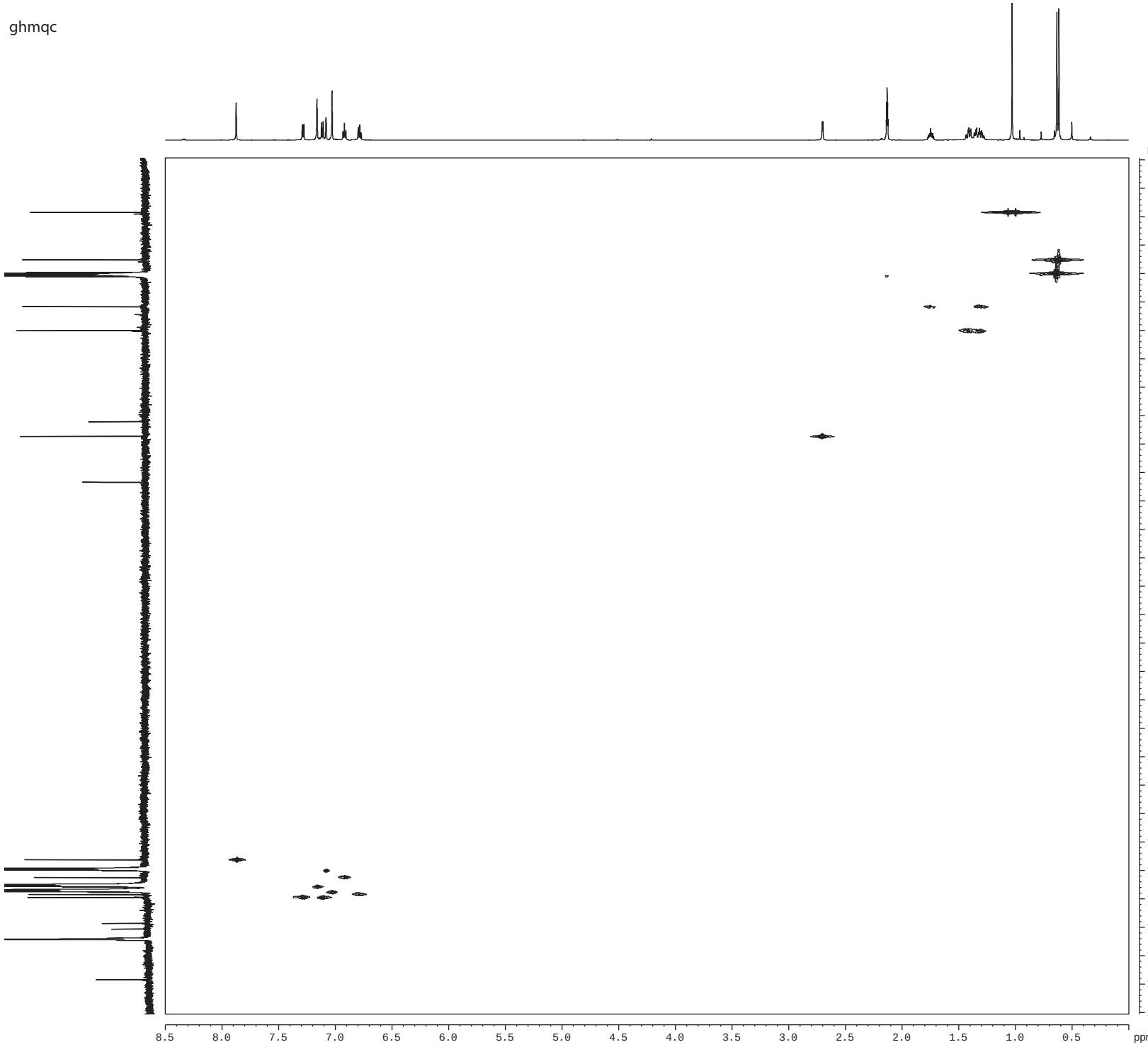
ghmqc

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======== CHANNEL f1 ========
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P1                8.00 usec
P2               16.00 usec
PLW1        23.01441956 W
SFO1       600.1325505 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                13C
P3               15.00 usec
PCPD2            70.00 usec
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PLW12        4.89778900 W
SFO2       150.9141262 MHz

====== GRADIENT CHANNEL =====
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GPNAM2       SMSQ10.100
GPNAM3       SMSQ10.100
GPZ1             50.00 %
GPZ2             30.00 %
GPZ3             40.10 %
P16            1000.00 usec

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FIDRES        44.389210 Hz
SW              150.597 ppm
FnMODE               QF

F2 - Processing parameters
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SF          600.1300000 MHz
WDW                EM
SSB      0
LB               5.00 Hz
GB       0
PC               1.00

F1 - Processing parameters
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WDW         States-TPPI
SSB                  3
LB       0 Hz
GB       0
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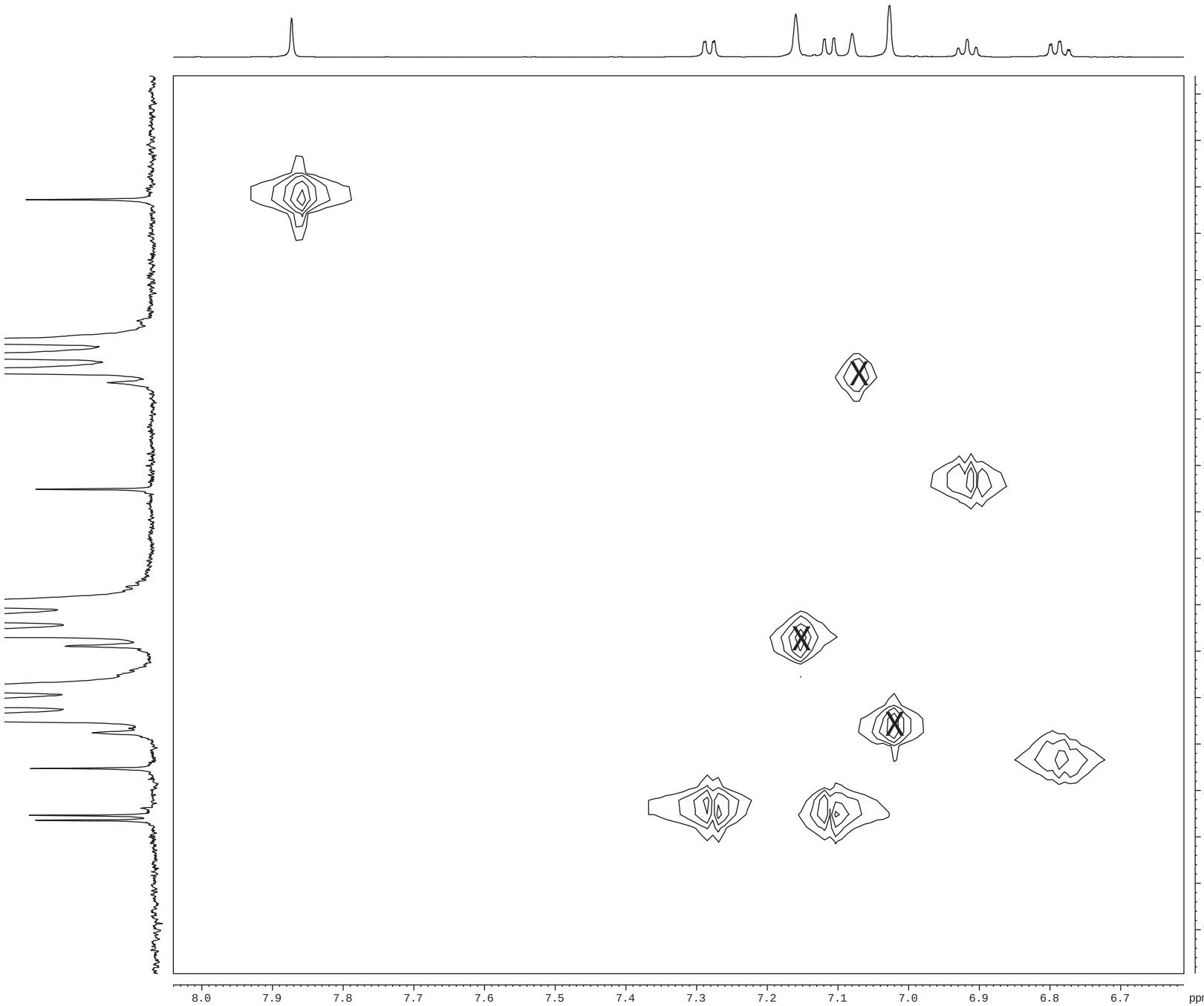
ghmqc

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DS                   16
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======== CHANNEL f1 ========
NUC1                 1H
P1                8.00 usec
P2               16.00 usec
PLW1        23.01441956 W
SFO1       600.1325505 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                13C
P3               15.00 usec
PCPD2            70.00 usec
PLW2       107.15190125 W
PLW12        4.89778900 W
SFO2       150.9141262 MHz

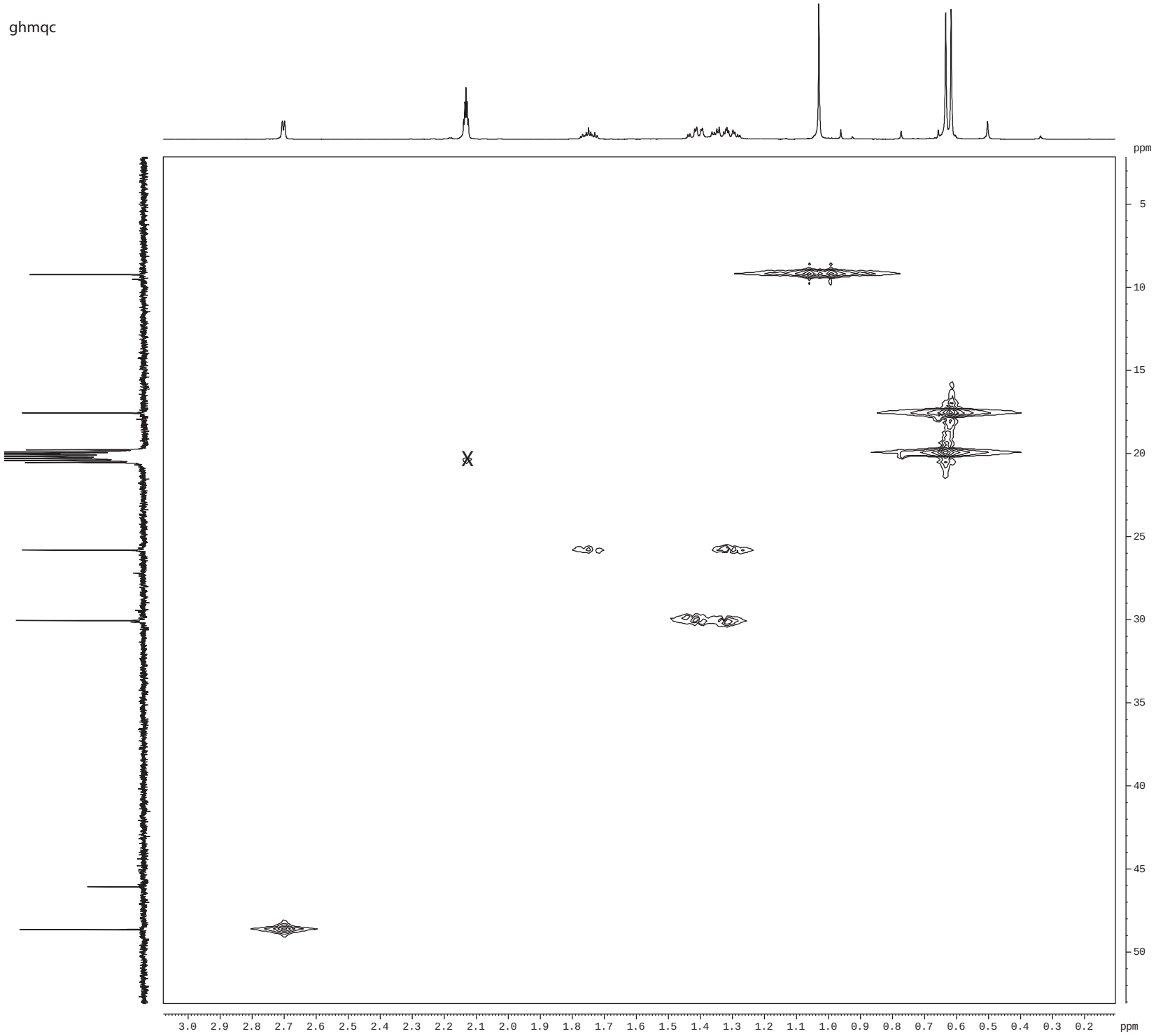
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPNAM2       SMSQ10.100
GPNAM3       SMSQ10.100
GPZ1              50.00 %
GPZ2              30.00 %
GPZ3              40.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                  512
SFO1          150.9141 MHz
FIDRES        44.389210 Hz
SW              150.597 ppm
FnMODE               QF

F2 - Processing parameters
SI                 1024
SF          600.1300000 MHz
WDW                EM
SSB      0
LB                5.00 Hz
GB       0
PC                1.00

F1 - Processing parameters
SI                 1024
MC2                QF
SF          150.9028136 MHz
WDW         States-TPPI
SSB                   3
LB       0 Hz
GB       0
```

ghmqc




```
Current Data Parameters
NAME          Fin_2_600
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20121207
Time               3.14
INSTRUM           av600
PROBHD   5 mm TBI 1H/13
PULPROG        hmqcgpqf
TD                2048
SOLVENT         Toluene
NS                   8
DS                  16
SWH           5102.041 Hz
FIDRES        2.491231 Hz
AQ           0.2007540 sec
RG                2050
DW             98.000 usec
DE              6.00 usec
TE             266.6 K
CNST2       145.0000000
D0          0.00000300 sec
D1          1.10000002 sec
D2          0.00344828 sec
D12         0.00002000 sec
D13         0.00000400 sec
D16         0.00020000 sec
IN0         0.00002200 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                8.00 usec
P2               16.00 usec
PLW1        23.01441956 W
SFO1       600.1325505 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                13C
P3               15.00 usec
PCPD2            70.00 usec
PLW2       107.15190125 W
PLW12        4.89778900 W
SFO2       150.9141262 MHz

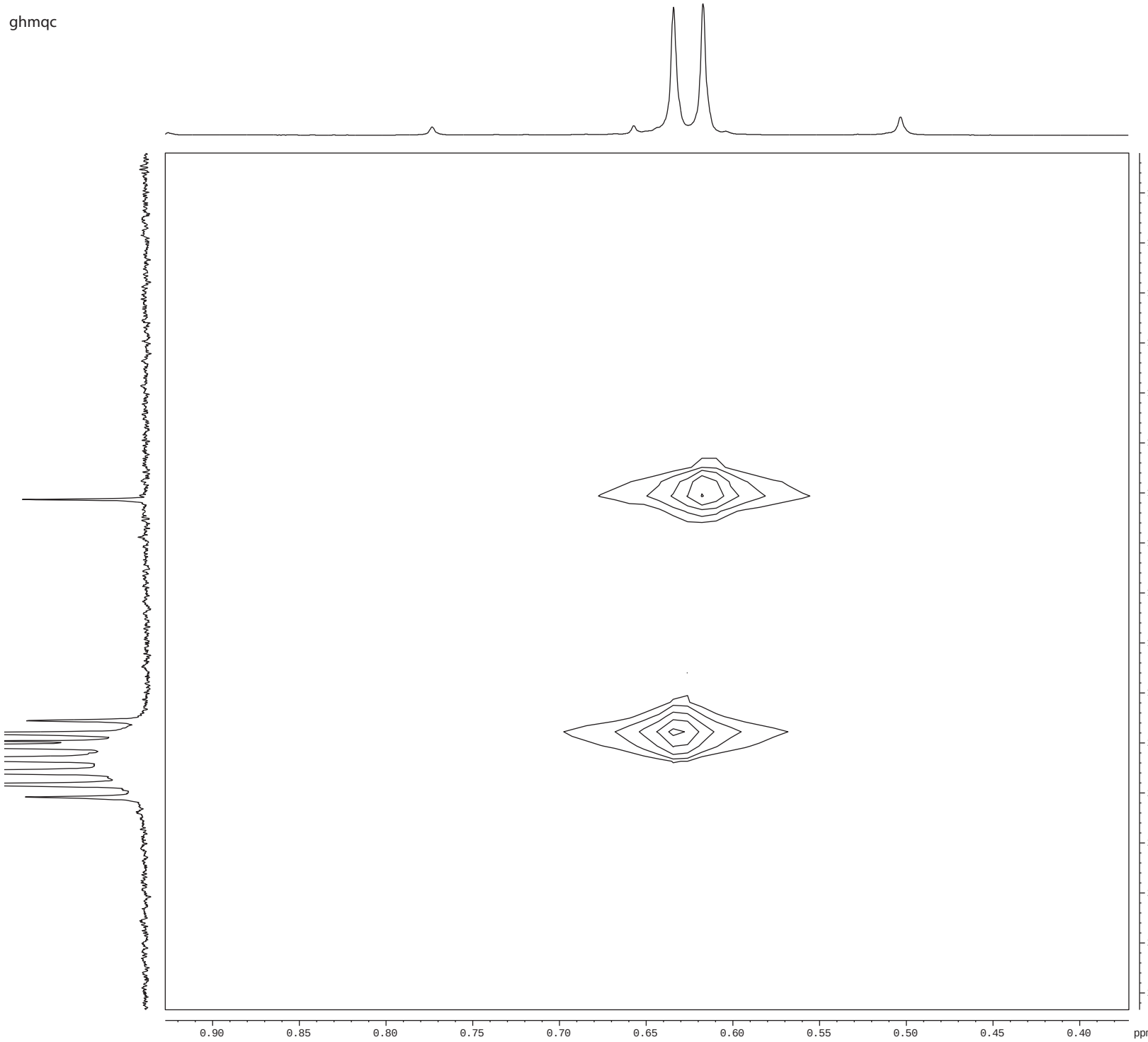
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPNAM2       SMSQ10.100
GPNAM3       SMSQ10.100
GPZ1             50.00 %
GPZ2             30.00 %
GPZ3             40.10 %
P16            1000.00 usec

F1 - Acquisition parameters
TD                 512
SFO1          150.9141 MHz
FIDRES       44.389210 Hz
SW             150.597 ppm
FnMODE              QF

F2 - Processing parameters
SI                1024
SF          600.1300000 MHz
WDW                EM
SSB      0
LB               5.00 Hz
GB       0
PC               1.00

F1 - Processing parameters
SI                1024
MC2                QF
SF          150.9028136 MHz
WDW         States-TPPI
SSB                  3
LB       0 Hz
GB       0
```

ghmqc




```
Current Data Parameters
NAME          Fin_2_600
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20121207
Time               3.14
INSTRUM           av600
PROBHD   5 mm TBI 1H/13
PULPROG        hmqcgpqf
TD                2048
SOLVENT         Toluene
NS                   8
DS                  16
SWH           5102.041 Hz
FIDRES        2.491231 Hz
AQ           0.2007540 sec
RG                2050
DW             98.000 usec
DE              6.00 usec
TE             266.6 K
CNST2       145.0000000
D0           0.00000300 sec
D1           1.10000002 sec
D2           0.00344828 sec
D12          0.00002000 sec
D13          0.00000400 sec
D16          0.00020000 sec
IN0          0.00002200 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                8.00 usec
P2               16.00 usec
PLW1        23.01441956 W
SFO1       600.1325505 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                13C
P3               15.00 usec
PCPD2            70.00 usec
PLW2       107.15190125 W
PLW12        4.89778900 W
SFO2       150.9141262 MHz

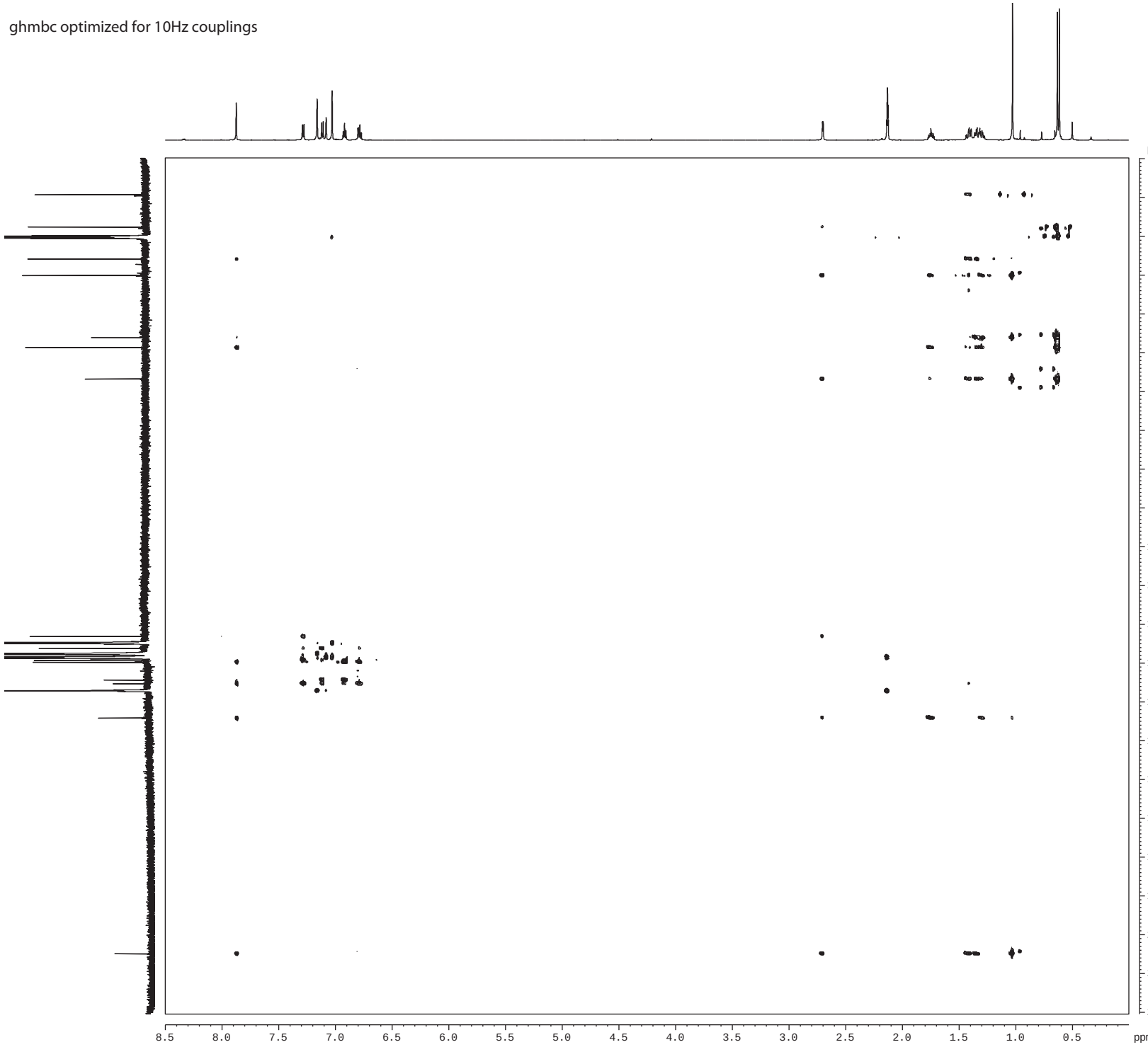
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPNAM2       SMSQ10.100
GPNAM3       SMSQ10.100
GPZ1             50.00 %
GPZ2             30.00 %
GPZ3             40.10 %
P16            1000.00 usec

F1 - Acquisition parameters
TD                 512
SFO1          150.9141 MHz
FIDRES       44.389210 Hz
SW             150.597 ppm
FnMODE              QF

F2 - Processing parameters
SI                1024
SF          600.1300000 MHz
WDW                EM
SSB      0
LB              5.00 Hz
GB       0
PC              1.00

F1 - Processing parameters
SI                1024
MC2                QF
SF          150.9028136 MHz
WDW         States-TPPI
SSB                  3
LB       0 Hz
GB       0
```

ghmbc optimized for 10Hz couplings




```
Current Data Parameters
NAME          Fin_2_600
EXPNO                 9
PROCNO                1

F2 - Acquisition Parameters
Date_          20121207
Time               4.45
INSTRUM           av600
PROBHD   5 mm TBI 1H/13
PULPROG    hmbcgplpndqf
TD                 4096
SOLVENT         Toluene
NS                    8
DS                   16
SWH           5102.041 Hz
FIDRES        1.245615 Hz
AQ            0.4014580 sec
RG                 2050
DW              98.000 usec
DE               6.00 usec
TE               268.5 K
CNST2       145.0000000
CNST13       10.0000000
D0          0.00000300 sec
D1          1.10000002 sec
D2          0.00344828 sec
D6          0.05000000 sec
D16         0.00020000 sec
IN0         0.00001500 sec

======== CHANNEL f1 ========
NUC1                1H
P1                8.00 usec
P2               16.00 usec
PLW1        23.01441956 W
SFO1       600.1325505 MHz

======== CHANNEL f2 ========
NUC2               13C
P3               15.00 usec
PLW2       107.15190125 W
SFO2        150.9194141 MHz

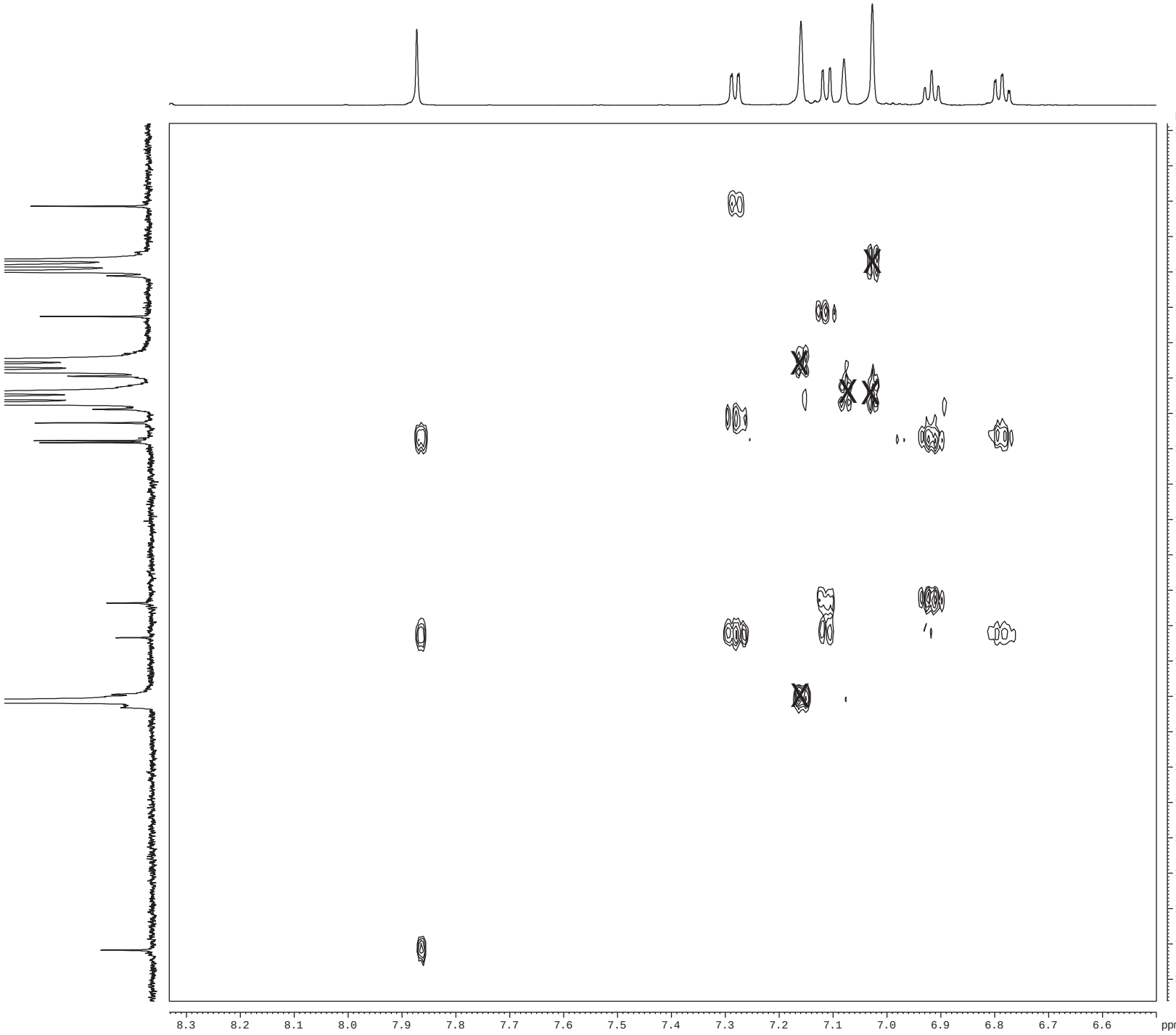
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPNAM2       SMSQ10.100
GPNAM3       SMSQ10.100
GPZ1              50.00 %
GPZ2              30.00 %
GPZ3              40.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                 512
SFO1          150.9194 MHz
FIDRES        65.104156 Hz
SW             220.868 ppm
FnMODE               QF

F2 - Processing parameters
SI                2048
SF          600.1300000 MHz
WDW               SINE
SSB      0
LB       0 Hz
GB       0
PC                1.00

F1 - Processing parameters
SI                1024
MC2                 QF
SF          150.9028136 MHz
WDW              States
SSB      0
LB       0 Hz
GB       0
```

ghmbc optimized for 1**0** Hz couplings




```
Current Data Parameters
NAME          Fin_2_600
EXPNO                 9
PROCNO                1

F2 - Acquisition Parameters
Date_          20121207
Time               4.45
INSTRUM           av600
PROBHD   5 mm TBI 1H/13
PULPROG    hmbcgplpndqf
TD                 4096
SOLVENT         Toluene
NS                    8
DS                   16
SWH            5102.041 Hz
FIDRES         1.245615 Hz
AQ            0.4014580 sec
RG                 2050
DW               98.000 usec
DE                6.00 usec
TE                268.5 K
CNST2        145.0000000
CNST13        10.0000000
D0           0.00000300 sec
D1           1.10000002 sec
D2           0.00344828 sec
D6           0.05000000 sec
D16          0.00020000 sec
IN0          0.00001500 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                 8.00 usec
P2                16.00 usec
PLW1         23.01441956 W
SFO1        600.1325505 MHz

======== CHANNEL f2 ========
NUC2                13C
P3                15.00 usec
PLW2        107.15190125 W
SFO2         150.9194141 MHz

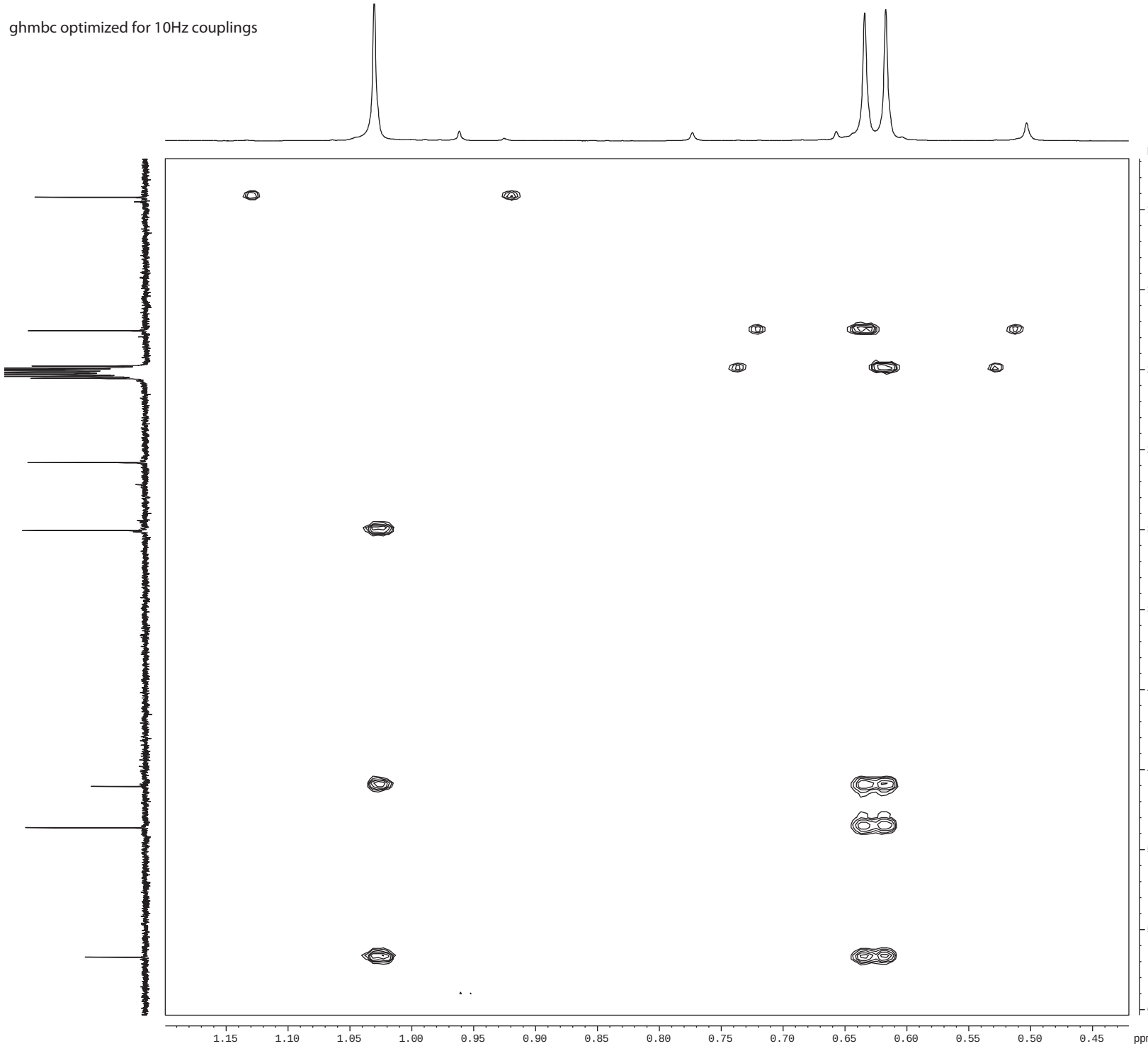
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPNAM3        SMSQ10.100
GPZ1               50.00 %
GPZ2               30.00 %
GPZ3               40.10 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                  512
SFO1           150.9194 MHz
FIDRES         65.104156 Hz
SW               220.868 ppm
FnMODE                QF

F2 - Processing parameters
SI                 2048
SF          600.1300000 MHz
WDW                SINE
SSB       0
LB        0 Hz
GB        0
PC                 1.00

F1 - Processing parameters
SI                 1024
MC2                  QF
SF          150.9028136 MHz
WDW              States
SSB       0
LB        0 Hz
GB        0
```

ghmbc optimized for 10Hz couplings




```
Current Data Parameters
NAME          Fin_2_600
EXPNO                 9
PROCNO                1

F2 - Acquisition Parameters
Date_          20121207
Time               4.45
INSTRUM           av600
PROBHD   5 mm TBI 1H/13
PULPROG    hmbcgplpndqf
TD                 4096
SOLVENT         Toluene
NS                    8
DS                   16
SWH            5102.041 Hz
FIDRES         1.245615 Hz
AQ            0.4014580 sec
RG                 2050
DW               98.000 usec
DE                6.00 usec
TE                268.5 K
CNST2        145.0000000
CNST13        10.0000000
D0           0.00000300 sec
D1           1.10000002 sec
D2           0.00344828 sec
D6           0.05000000 sec
D16          0.00020000 sec
IN0          0.00001500 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                 8.00 usec
P2                16.00 usec
PLW1        23.01441956 W
SFO1       600.1325505 MHz

======== CHANNEL f2 ========
NUC2                13C
P3                15.00 usec
PLW2       107.15190125 W
SFO2        150.9194141 MHz

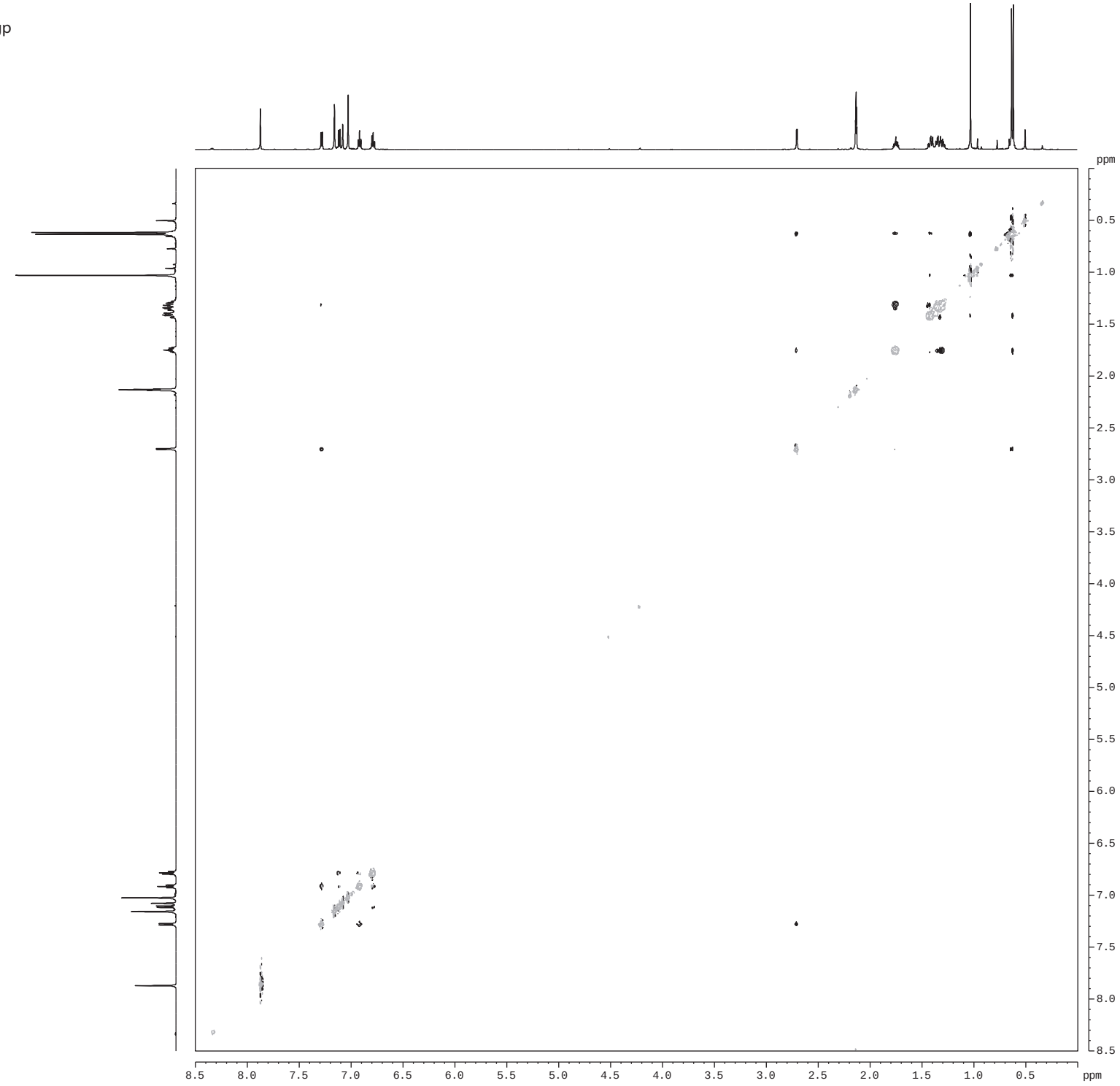
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPNAM2       SMSQ10.100
GPNAM3       SMSQ10.100
GPZ1              50.00 %
GPZ2              30.00 %
GPZ3              40.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                  512
SFO1          150.9194 MHz
FIDRES        65.104156 Hz
SW              220.868 ppm
FnMODE               QF

F2 - Processing parameters
SI                 2048
SF          600.1300000 MHz
WDW                SINE
SSB       0
LB        0 Hz
GB        0
PC                 1.00

F1 - Processing parameters
SI                 1024
MC2                  QF
SF          150.9028136 MHz
WDW              States
SSB       0
LB        0 Hz
GB        0
```

noesygp




```
Current Data Parameters
NAME           Fin_2_600
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20121207
Time                6.34
INSTRUM            av600
PROBHD   5 mm TBI 1H/13
PULPROG        noesygpph
TD                 2048
SOLVENT          Toluene
NS                    8
DS                   16
SWH           5102.041 Hz
FIDRES         2.491231 Hz
AQ            0.2007540 sec
RG                 1030
DW              98.000 usec
DE               6.00 usec
TE              268.9 K
D0           0.00008781 sec
D1           2.00000000 sec
D8           1.00000000 sec
D16          0.00020000 sec
IN0          0.00019600 sec

======== CHANNEL f1 ========
NUC1                1H
P1               8.00 usec
P2              16.00 usec
PLW1        23.01441956 W
SFO1       600.1325505 MHz

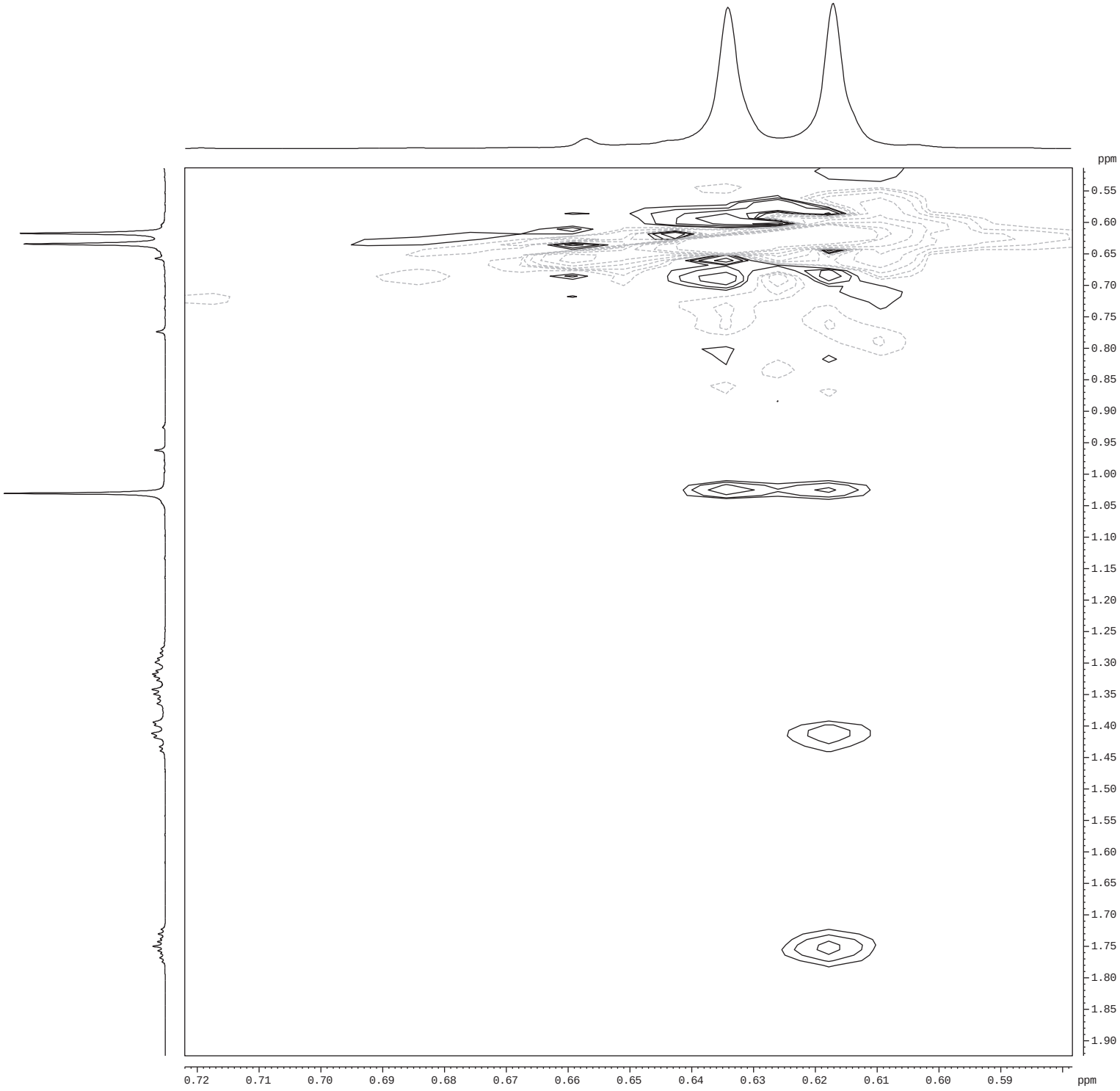
====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPZ1             40.00 %
P16            1000.00 usec

F1 - Acquisition parameters
TD                  512
SFO1          600.1326 MHz
FIDRES        9.964924 Hz
SW               8.502 ppm
FnMODE      States-TPPI

F2 - Processing parameters
SI                 1024
SF          600.1300000 MHz
WDW                QSINE
SSB                   2
LB       0 Hz
GB       0
PC                 1.00

F1 - Processing parameters
SI                 1024
MC2         States-TPPI
SF          600.1300000 MHz
WDW         States-TPPI
SSB                   2
LB       0 Hz
GB       0
```

noesygp




```
Current Data Parameters
NAME           Fin_2_600
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20121207
Time                6.34
INSTRUM            av600
PROBHD   5 mm TBI 1H/13
PULPROG        noesygpph
TD                  2048
SOLVENT          Toluene
NS                     8
DS                    16
SWH           5102.041 Hz
FIDRES         2.491231 Hz
AQ            0.2007540 sec
RG                  1030
DW              98.000 usec
DE               6.00 usec
TE              268.9 K
D0            0.00008781 sec
D1            2.00000000 sec
D8            1.00000000 sec
D16           0.00020000 sec
IN0           0.00019600 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 8.00 usec
P2                16.00 usec
PLW1         23.01441956 W
SFO1        600.1325505 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPZ1               40.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   512
SFO1          600.1326 MHz
FIDRES        9.964924 Hz
SW                8.502 ppm
FnMODE      States-TPPI

F2 - Processing parameters
SI                  1024
SF           600.1300000 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                   1.00

F1 - Processing parameters
SI                  1024
MC2         States-TPPI
SF           600.1300000 MHz
WDW         States-TPPI
SSB                     2
LB        0 Hz
GB        0
```