

Name: _____

Chem 203
December 10, 2011

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 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.

2. The following spectral data are provided for a compound with a molecular formula $C_{15}H_{22}O_2$: IR (Thin Film on NaCl), 500 MHz 1H NMR, 125.7 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 $CDCl_3$. The 1H resonance at 7.25 ppm corresponds to $CHCl_3$.

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

a. Write the structure of the molecule.

b. Tabulate the shifts of the ^1H resonances (a-i) 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:

c. Redraw the structure of the molecule below and write the letter (a-i) 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 (1-12) 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:

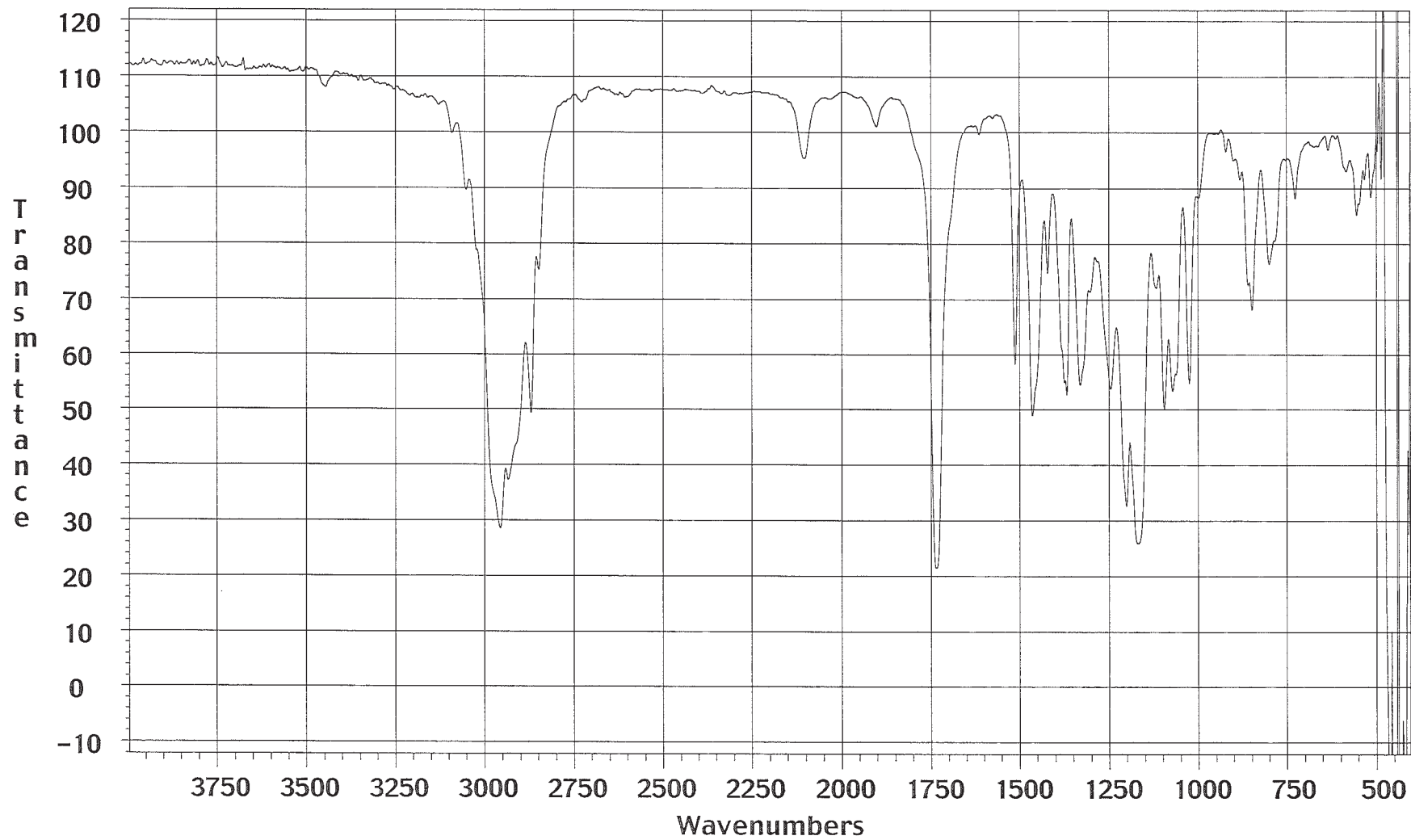
11:

12:

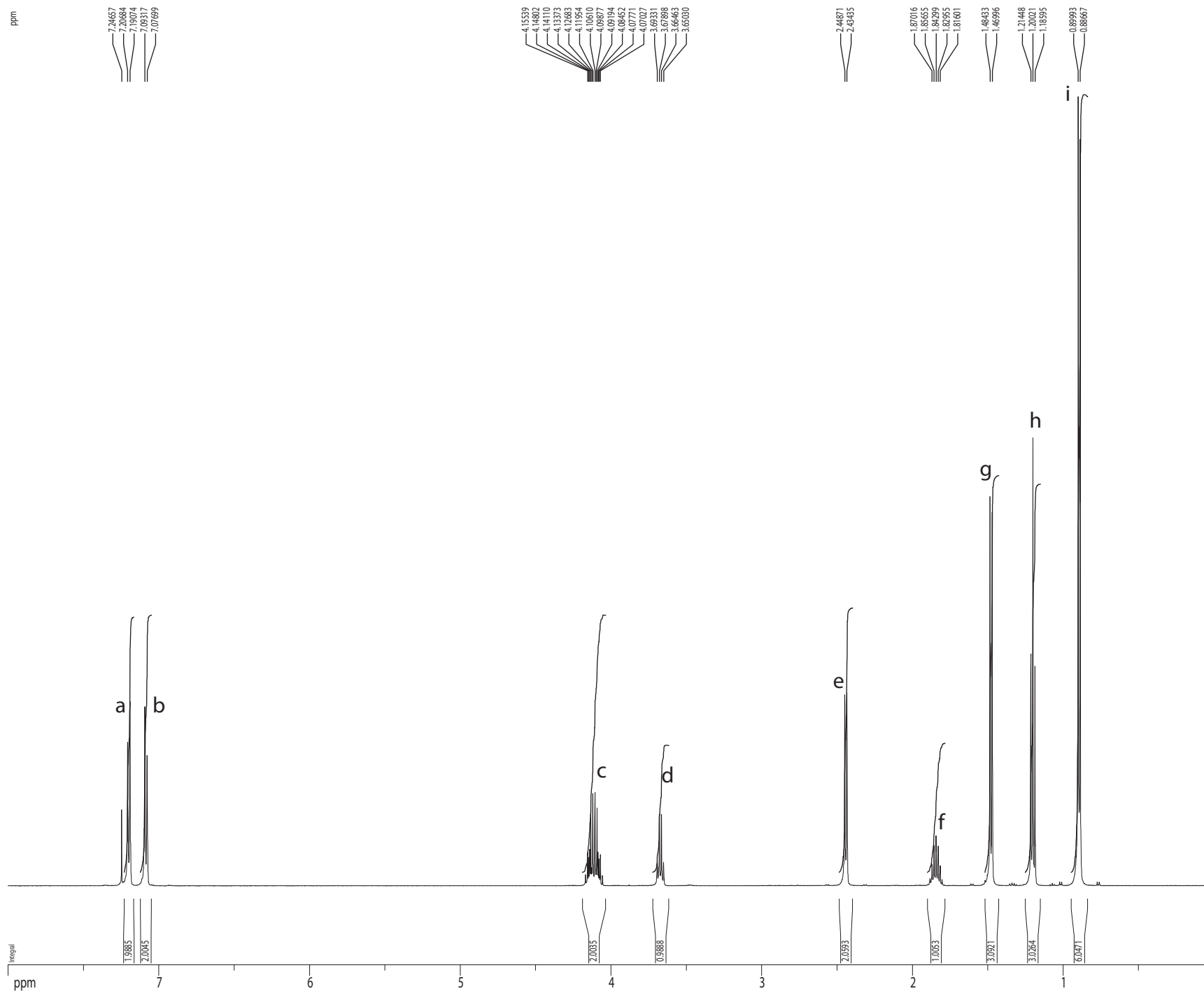
e. Redraw the structure of the molecule below and write the number (1-10) of each ^{13}C resonance next to the carbon or carbons to which it corresponds. If the assignment of particular resonance is uncertain, please indicate this.

f. Explain briefly the appearance of resonance **c** in the ^1H NMR spectrum

Thin Film on NaCl



1H spectrum at 500 MHz in CDCl₃



Current Data Parameters
 USER nmr11t
 NAME RKS-X-sample1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111005
 Time 20.40
 INSTRUM gn500
 PROBHD 5 mm broadband
 PULPROG zg30
 TD 81728
 SOLVENT CDCl3T
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 40.3
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
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 P1 12.20 usec
 PL1 -5.00 dB
 SFO1 499.5134966 MHz

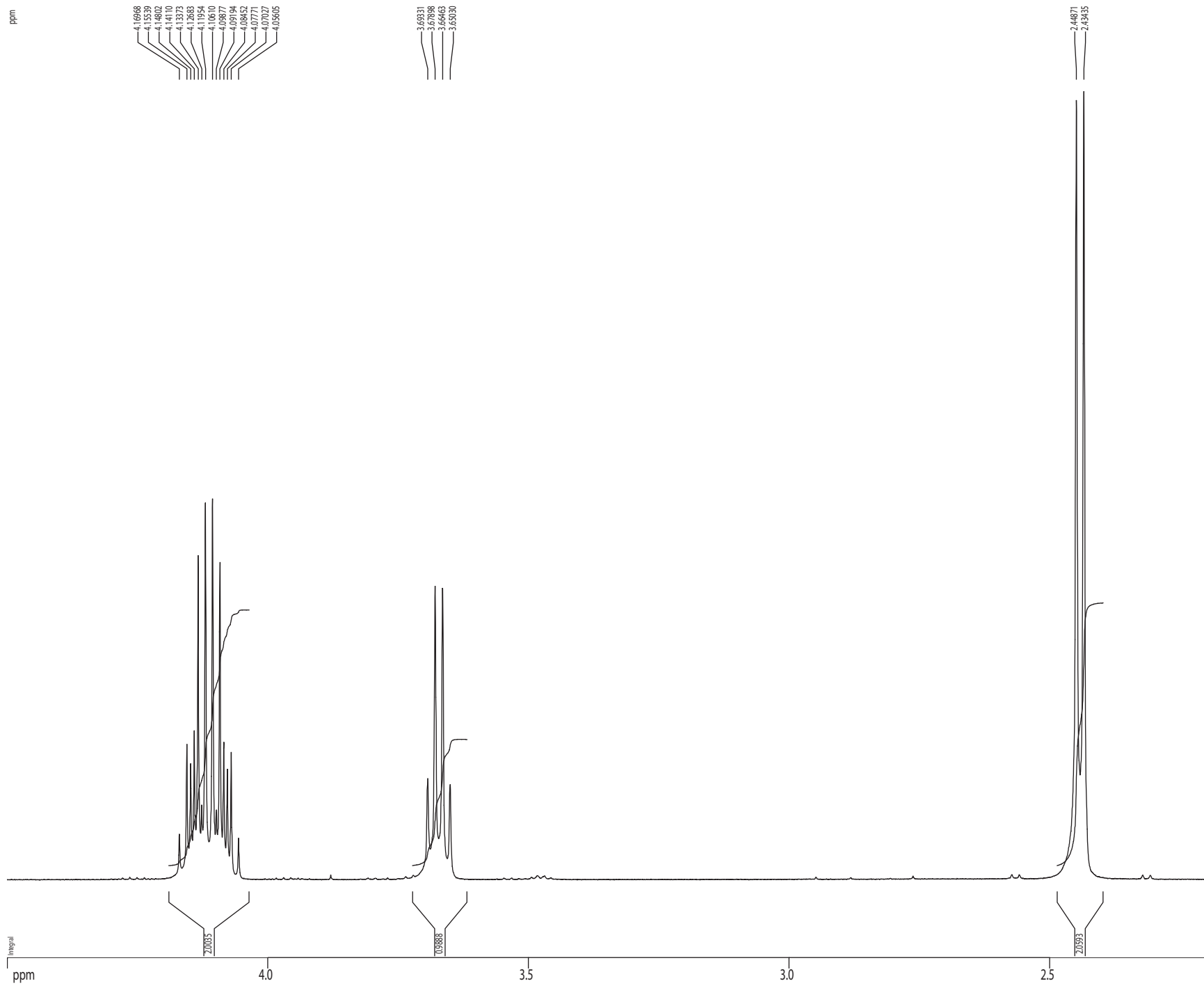
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 SF 499.5100341 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 8.000 ppm
 F1 3996.08 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 0.35088 ppm/cm
 HZCM 175.26669 Hz/cm

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#	ADDRESS	FREQUENCY		INTENSITY
		[Hz]	[PPM]	
1	31481.6	3619.736	7.2466	1.46
2	31643.9	3599.891	7.2068	2.71
3	31709.7	3591.846	7.1907	3.49
4	32108.3	3543.112	7.0932	3.38
5	32174.4	3535.030	7.0770	2.46
6	44110.4	2075.660	4.1554	0.63
7	44140.5	2071.976	4.1480	0.54
8	44168.8	2068.522	4.1411	0.69
9	44198.9	2064.839	4.1337	1.50
10	44227.1	2061.395	4.1268	0.34
11	44256.9	2057.751	4.1195	1.74
12	44311.8	2051.037	4.1061	1.76
13	44341.7	2047.376	4.0988	0.32
14	44369.6	2043.963	4.0919	1.48
15	44399.9	2040.258	4.0845	0.63
16	44427.8	2036.857	4.0777	0.51
17	44458.2	2033.140	4.0703	0.59
18	45998.2	1844.846	3.6933	0.46
19	46056.8	1837.685	3.6790	1.36
20	46115.4	1830.521	3.6646	1.35
21	46173.9	1823.364	3.6503	0.44
22	51082.9	1223.154	2.4487	3.61
23	51141.6	1215.980	2.4343	3.65
24	53446.6	934.165	1.8702	0.40
25	53502.2	927.365	1.8566	0.76
26	53557.6	920.591	1.8430	0.94
27	53612.5	913.877	1.8295	0.75
28	53667.8	907.115	1.8160	0.38
29	55022.8	741.440	1.4843	7.36
30	55081.5	734.263	1.4700	7.13
31	56125.3	606.647	1.2145	4.40
32	56183.6	599.519	1.2002	8.56
33	56241.9	592.395	1.1860	4.15
34	57410.4	449.523	0.8999	15.00
35	57464.6	442.901	0.8867	14.24

¹H spectrum at 500 Mhz in CDCl₃



Current Data Parameters
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 NAME RKS-X-sample1
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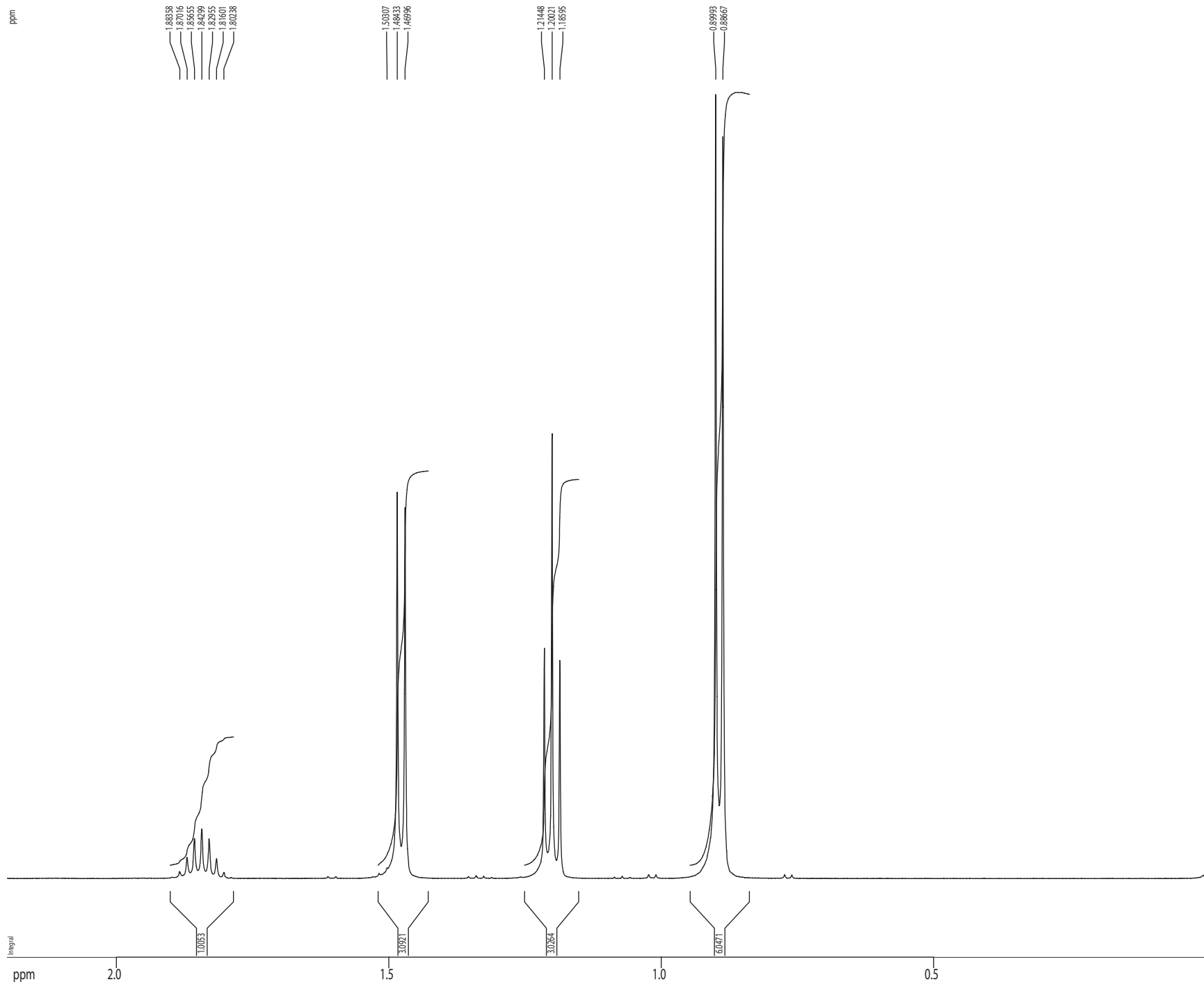
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 SOLVENT CDCl3T
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 DS 2
 SWH 8012820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 40.3
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 ¹H
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 PL1 -5.00 dB
 SFO1 499.5134966 MHz

F2 - Processing parameters
 SI 65536
 SF 499.5100341 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1 2247.80 Hz
 F2 2.200 ppm
 F2 1098.92 Hz
 PPMCM 0.10088 ppm/cm
 HZCM 50.38917 Hz/cm

¹H spectrum at 500 MHz in CDCl₃



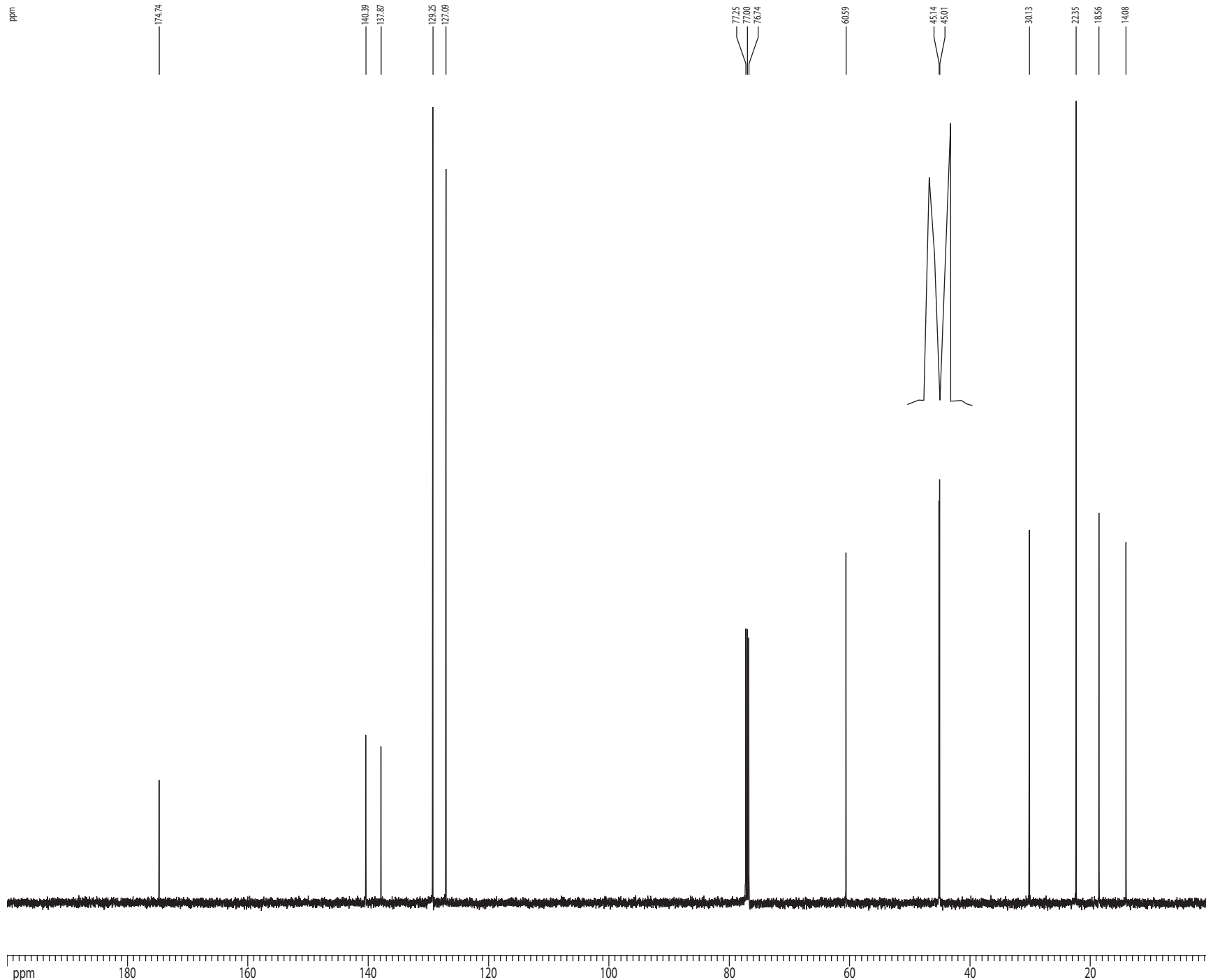
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 PULPROG zg30
 TD 81728
 SOLVENT CDCl3T
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.098043 Hz
 AQ 5.0998774 sec
 RG 40.3
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.20 usec
 PL1 -5.00 dB
 SFO1 499.5134966 MHz

F2 - Processing parameters
 SI 65536
 SF 499.5100341 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1 1098.92 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 0.09649 ppm/cm
 HZCM 48.19834 Hz/cm

¹³C spectrum with ¹H decoupling at 125 MHz in CDCl₃



```

Current Data Parameters
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NAME      RKS-X-sample1
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
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Time      20.44
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PROBHD    5 mm broadband
PULPROG   zgdc30
TD         65536
SOLVENT   CDCl3
NS         182
DS         4
SWH        30303.031 Hz
FIDRES     0.462388 Hz
AQ         1.0813940 sec
RG         4597.6
DW         16.500 usec
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TE         298.0 K
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d11        0.03000000 sec
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MCWRK     0.01500000 sec

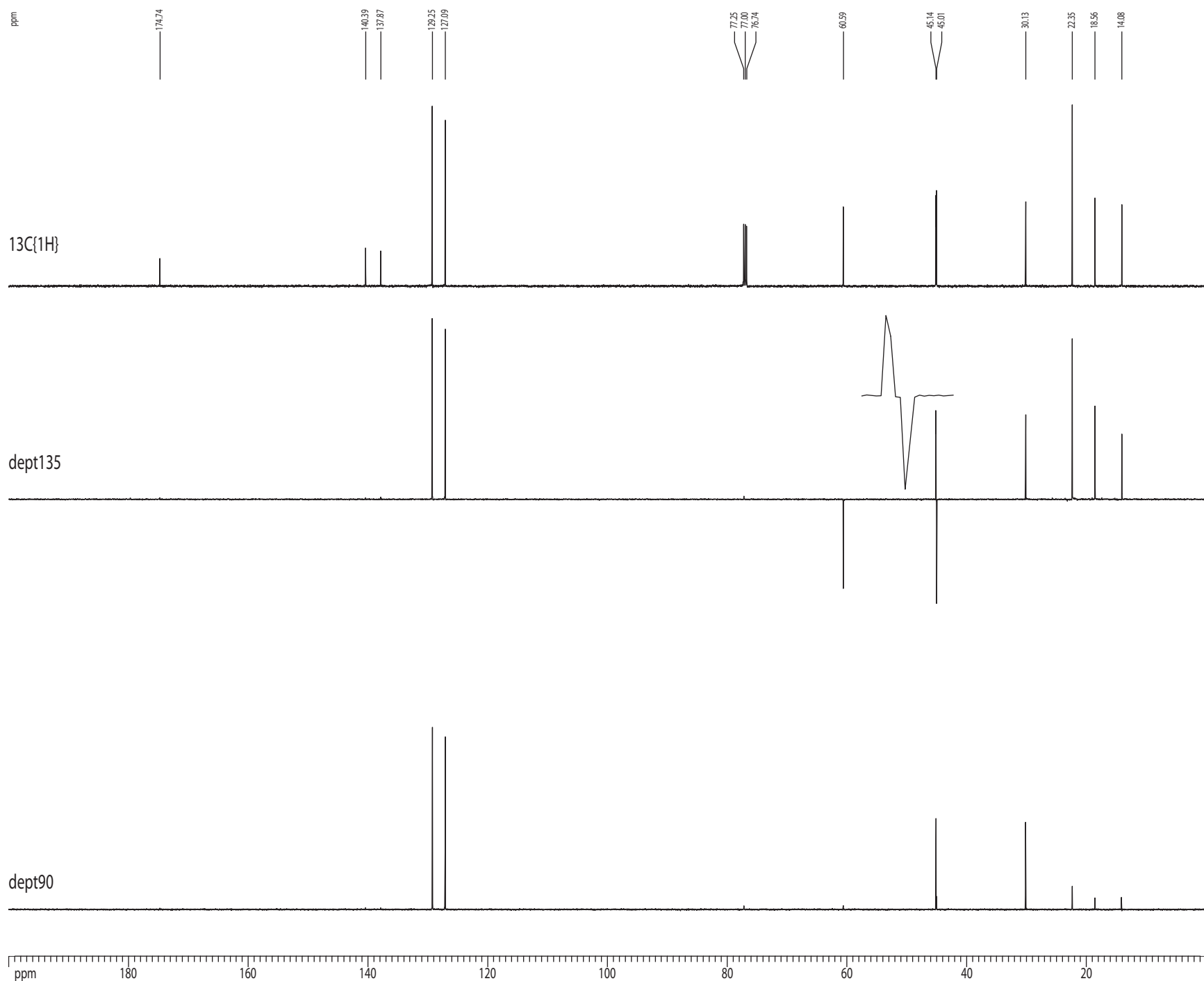
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NUC1      13C
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PL1       0.00 dB
SFO1      125.6157052 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -3.00 dB
PL12      13.20 dB
SFO2      499.5124975 MHz

F2 - Processing parameters
SI         65536
SF         125.6019001 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
FIP        200.000 ppm
F1         25120.38 Hz
F2         0.000 ppm
F2         0.00 Hz
PPMCM      8.77193 ppm/cm
HZCM       1101.77112 Hz/cm
    
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¹³C spectrum with ¹H decoupling at 125 MHz in CDCl₃



Current Data Parameters
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 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111005
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 PROBHD 5 mm broadband
 PULPROG zgdc30
 TD 65536
 SOLVENT CDCl3
 NS 182
 DS 4
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813940 sec
 RG 4597.6
 DW 16.500 usec
 DE 4.50 usec
 TE 298.0 K
 D1 0.25000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
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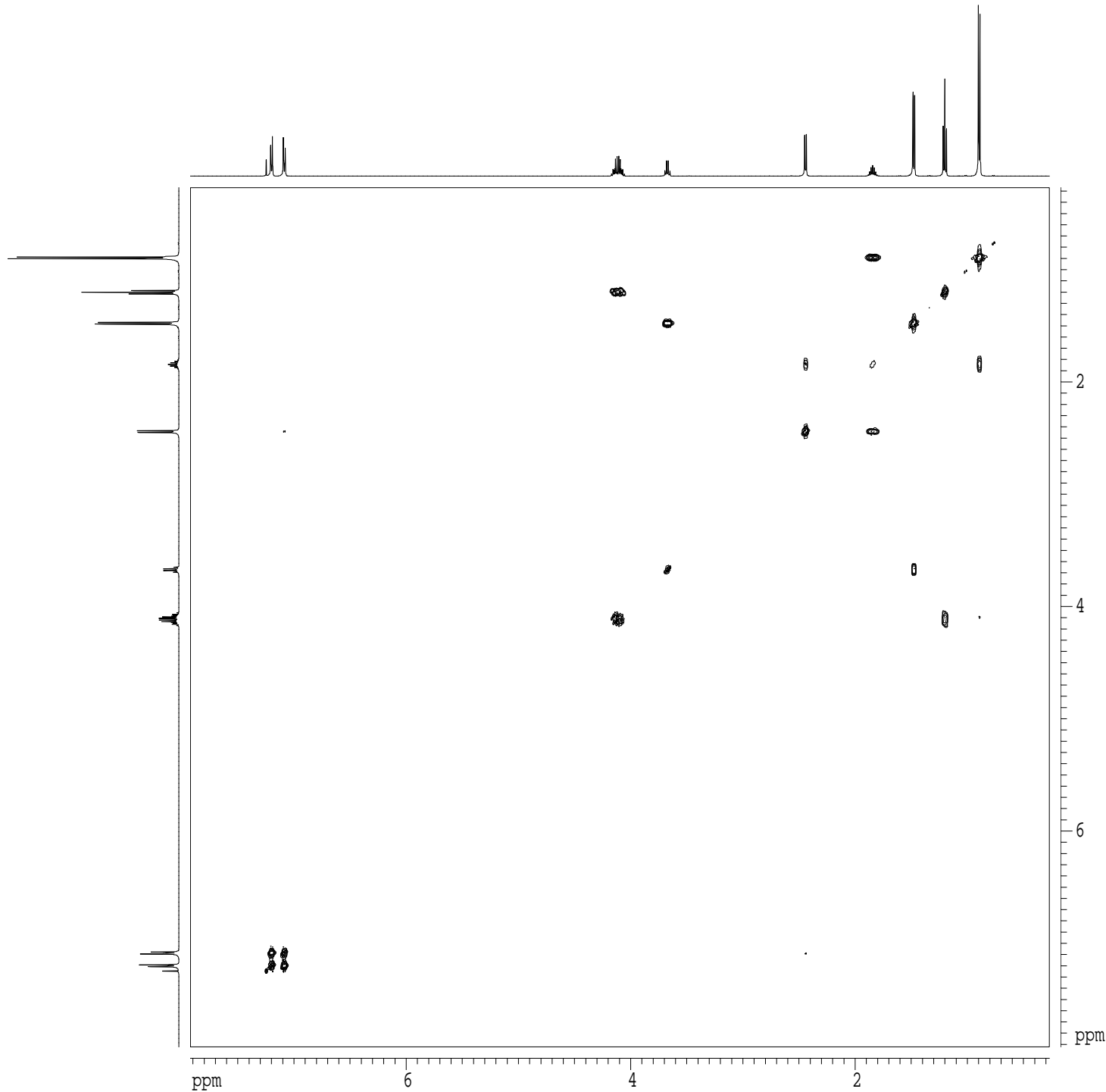
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 NUC1 ¹³C
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 PL1 0.00 dB
 SFO1 125.6157052 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PL2 -3.00 dB
 PL12 13.20 dB
 SFO2 499.5124975 MHz

F2 - Processing parameters
 SI 65536
 SF 125.6019001 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 200.000 ppm
 F1 25120.38 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 8.77193 ppm/cm
 HZCM 1101.77112 Hz/cm

gcosy60



Current Data Parameters
USER nmrlit
NAME RKS-X-sample1
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111006
Time 21.57
INSTRUM gn500
PROBHD 5 mm broadband
PULPROG cosygp60.prd
TD 2048
SOLVENT CDCl3
NS 16
DS 16
SWH 3822.630 Hz
FIDRES 1.866518 Hz
AQ 0.2679284 sec
RG 645.1
DW 130.800 usec
DE 6.00 usec
TE 298.0 K
d0 0.00000300 sec
D1 1.00000000 sec
d13 0.00000300 sec
D16 0.00025000 sec
IN0 0.00026160 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -5.00 dB
SF01 499.5120801 MHz

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

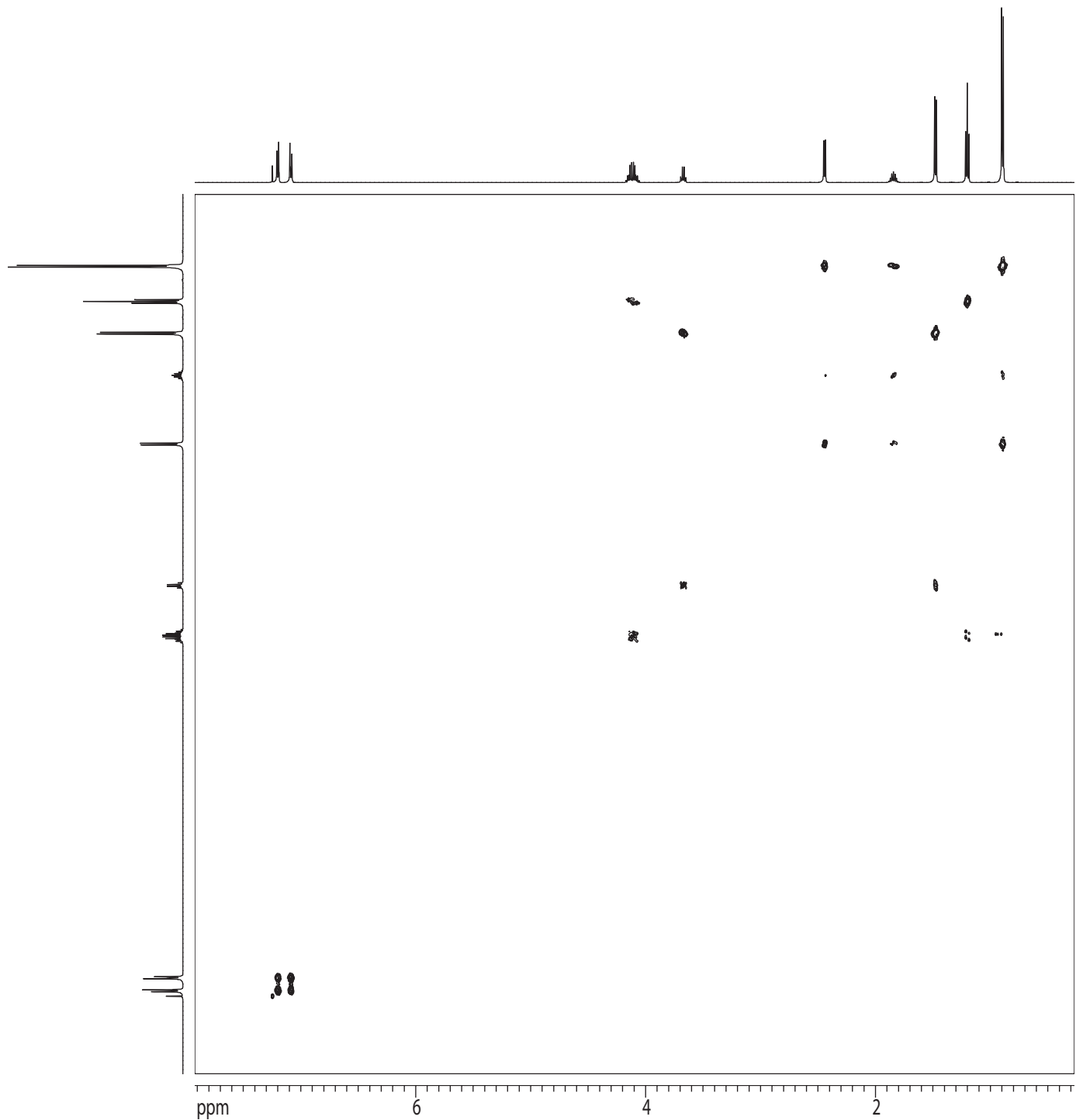
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TD 256
SF01 499.5121 MHz
FIDRES 14.932148 Hz
SW 7.653 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 499.5100341 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 499.5100341 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 7.922 ppm
F2LO 3957.27 Hz
F2PHI 0.270 ppm
F2HI 134.64 Hz
F1PLO 7.922 ppm
F1LO 3957.27 Hz
F1PHI 0.270 ppm
F1HI 134.64 Hz
F2PPMCM 0.51018 ppm/cm
F2HZCM 254.84200 Hz/cm
F1PPMCM 0.51018 ppm/cm
F1HZCM 254.84200 Hz/cm

gtocsy



Current Data Parameters
USER nmr11t
NAME RKS-X-sample1
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111006
Time 23.28
INSTRUM gn500
PROBHD 5 mm broadband
PULPROG mlevgp_mo
TD 2048
SOLVENT CDCl3
NS 16
DS 16
SWH 3822.630 Hz
FIDRES 1.866518 Hz
AQ 0.2679284 sec
RG 80.6
DW 130.800 usec
DE 6.00 usec
TE 298.0 K
d0 0.00000300 sec
D1 2.00000000 sec
D9 0.10000000 sec
d12 0.00002000 sec
D16 0.00050000 sec
FACTOR1 7
IN0 0.00026160 sec
I1 42
SCALEF 6

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
p5 23.34 usec
P6 35.00 usec
p7 70.00 usec
P17 2500.00 usec
PL1 -5.00 dB
PL10 5.90 dB
SFO1 499.5120801 MHz

===== GRADIENT CHANNEL =====
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GPNAM2 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 2000.00 usec

F1 - Acquisition parameters
ND0 1
TD 256
SFO1 499.5121 MHz
FIDRES 14.932148 Hz
SW 7.653 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 499.5100341 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 499.5100341 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 7.922 ppm
F2LO 3957.27 Hz
F2PHI 0.270 ppm
F2HI 134.64 Hz
F1PLO 7.922 ppm
F1LO 3957.27 Hz
F1PHI 0.270 ppm
F1HI 134.64 Hz
F2PPMCM 0.51018 ppm/cm
F2HZCM 254.84200 Hz/cm
F1PPMCM 0.51018 ppm/cm
F1HZCM 254.84200 Hz/cm

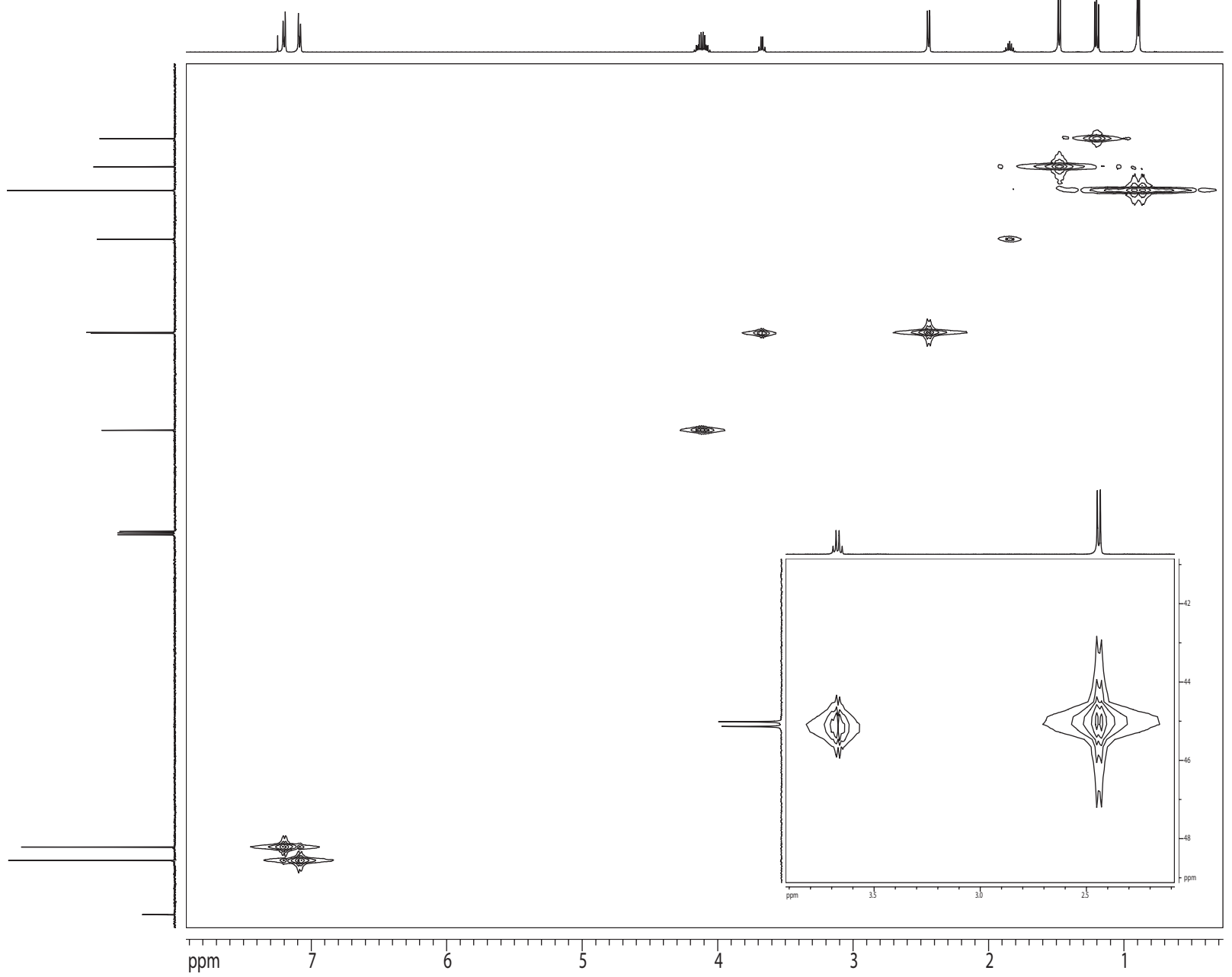
2

4

6

ppm

ghmqc



Current Data Parameters
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NAME RKS-X-sample1
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
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Time 4.16
INSTRUM gn500
PROBHD 5 mm broadband
PULPROG inv4gp.wu
TD 2048
SOLVENT CDCl3
NS 16
DS 16
SWH 3822.630 Hz
FIDRES 1.866518 Hz
AQ 0.2679284 sec
RG 9195.2
DW 130.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.000000
d0 0.00000300 sec
D1 1.00000000 sec
D2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000300 sec
D16 0.00025000 sec
d20 0.00242528 sec
IN0 0.00002020 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
p2 24.00 usec
PL1 -5.00 dB
SFO1 499.5120801 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 7.70 usec
PCPD2 70.00 usec
PL2 0.00 dB
PL12 20.40 dB
SFO2 125.6145482 MHz

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

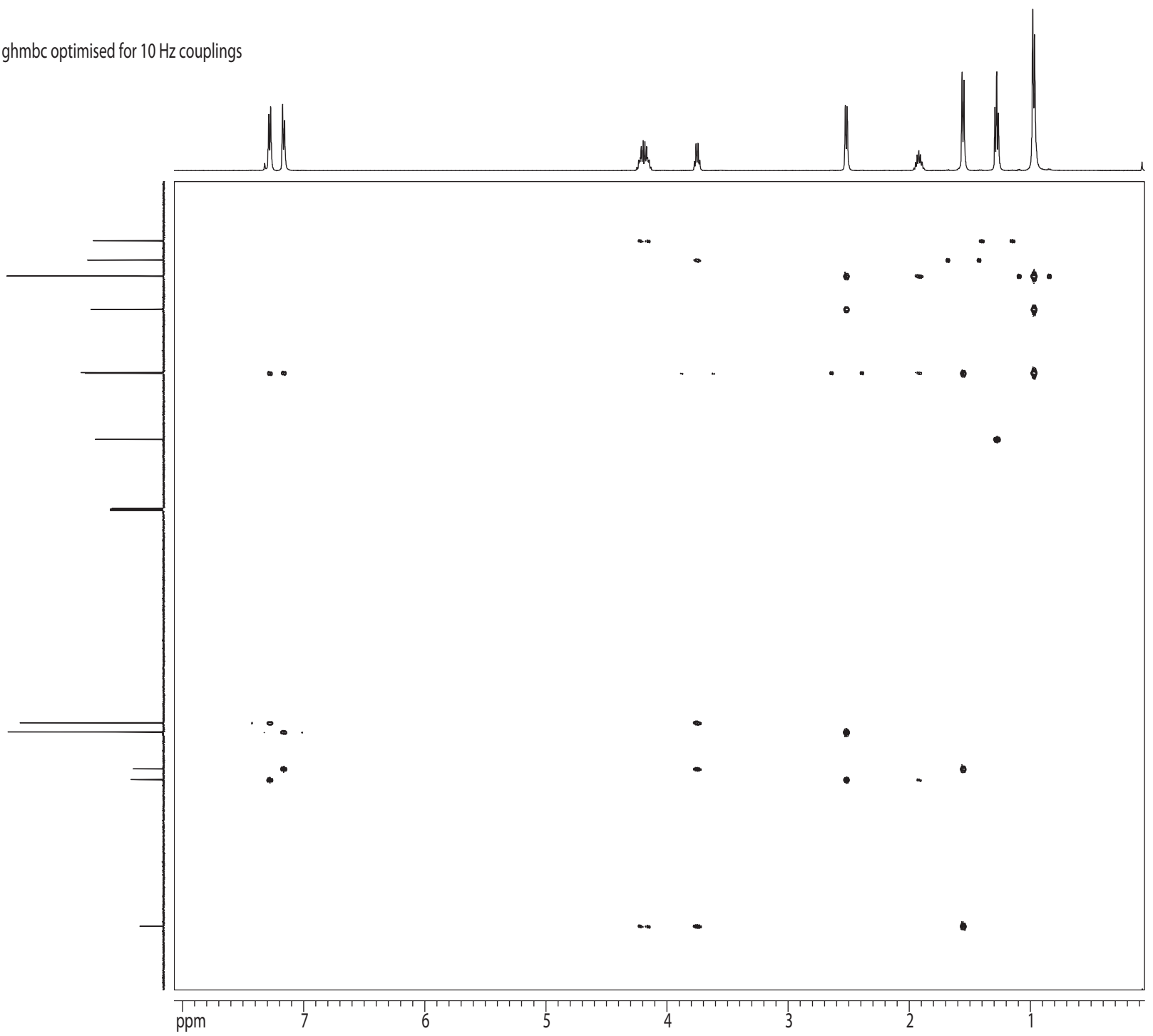
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FIDRES 96.689354 Hz
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FMODE QF

F2 - Processing parameters
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SF 499.5100341 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 125.6019001 MHz
WDW QSINE
SSB 3
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 18.00 cm
CX1 15.00 cm
F2PLO 7.922 ppm
F2LO 3957.27 Hz
F2PHI 0.270 ppm
F2HI 134.64 Hz
F1PLO 140.000 ppm
F1LO 17584.26 Hz
F1PHI 2.165 ppm
F1HI 271.93 Hz
F2PPMCM 0.42515 ppm/cm
F2HZCM 212.36835 Hz/cm
F1PPMCM 9.18900 ppm/cm
F1HZCM 1154.15552 Hz/cm

ghmbc optimised for 10 Hz couplings



```

Current Data Parameters
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NAME      RKS-X-sample1
EXPNO     11
PROCNO    1

F2 - Acquisition Parameters
Date_     20111204
Time      10.10
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   ghmbc.wu
TD         4096
SOLVENT   CDCl3
NS         4
DS         16
SWH        4006.410 Hz
FIDRES     0.978127 Hz
AQ         0.5112308 sec
RG         2048
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
INO        0.00002097 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
p2         15.00 usec
PL1        1.60 dB
SFO1       500.2220322 MHz

===== CHANNEL f2 =====
NUC2       13C
P3         15.50 usec
PL2        -1.00 dB
SFO2       125.7923623 MHz

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GPNAM2     sine.100
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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 %
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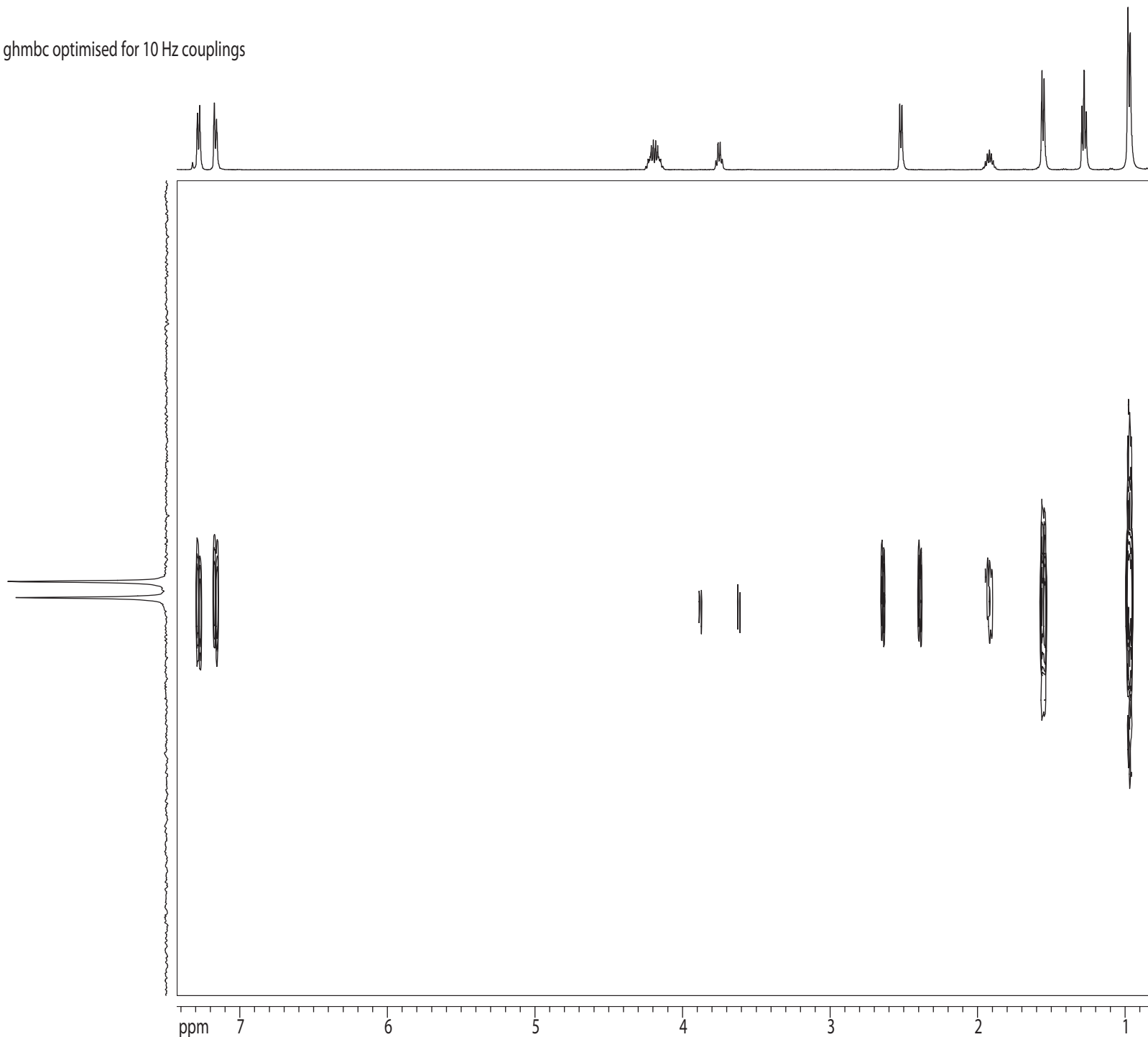
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FhMODE     undefined

F2 - Processing parameters
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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      8.067 ppm
F2LO       4035.37 Hz
F2PHI      0.058 ppm
F2HI       28.96 Hz
F1PLO      189.713 ppm
F1LO       23862.21 Hz
F1PHI      0.193 ppm
F1HI       24.30 Hz
F2PPMCM    0.44496 ppm/cm
F2HZCM     222.57835 Hz/cm
F1PPMCM    12.63466 ppm/cm
F1HZCM     1589.19348 Hz/cm
    
```

ghmbc optimised for 10 Hz couplings



Current Data Parameters
USER nmrl1t
NAME RKS-X-sample1
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111204
Time 10.10
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG ghmbc.wu
TD 4096
SOLVENT CDCl3
NS 4
DS 16
SWH 4006.410 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 2048
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 0.00002097 sec

==== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220322 MHz

==== CHANNEL f2 =====
NUC2 13C
P3 15.50 usec
PL2 -1.00 dB
SFO2 125.7923623 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 290
SFO1 125.7924 MHz
FIDRES 82.199661 Hz
SW 189.502 ppm
FhMODE undefined

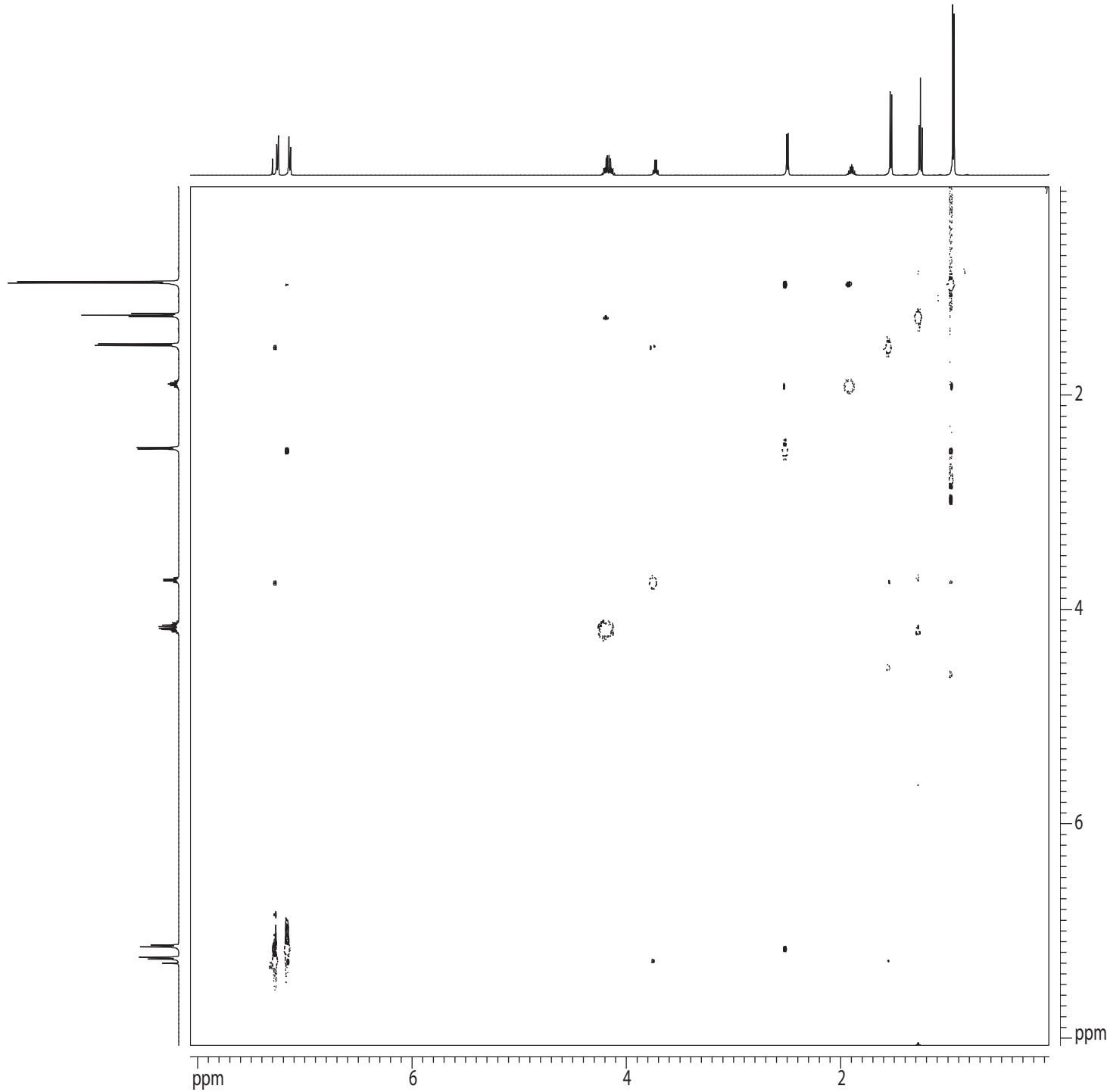
F2 - Processing parameters
SI 2048
SF 500.2200000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

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 7.426 ppm
F2LO 3714.54 Hz
F2PHI 0.801 ppm
F2HI 400.64 Hz
F1PLO 48.128 ppm
F1LO 6053.62 Hz
F1PHI 42.000 ppm
F1HI 5282.78 Hz
F2PPMCM 0.36805 ppm/cm
F2HZCM 184.10535 Hz/cm
F1PPMCM 0.40856 ppm/cm
F1HZCM 51.38922 Hz/cm

43
44
45
46
47
ppm

gnoesy



Current Data Parameters
USER nmr11t
NAME RKS-X-sample1
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111206
Time 14.41
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG noesygptp
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 10.1
DW 124.800 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 0.00012480 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
P2 15.00 usec
PL1 1.60 dB
SFO1 500.2220322 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 206
SFO1 500.222 MHz
FIDRES 19.448593 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 TPII
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 8.067 ppm
F2LO 4035.37 Hz
F2PHI 0.058 ppm
F2HI 28.96 Hz
F1PLO 8.067 ppm
F1LO 4035.37 Hz
F1PHI 0.058 ppm
F1HI 28.96 Hz
F2PPMCM 0.53395 ppm/cm
F2HZCM 267.09402 Hz/cm
F1PPMCM 0.53395 ppm/cm
F1HZCM 267.09402 Hz/cm