

Name: _____

Chem 203
December 20, 2014

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.

The following spectral data are provided for a compound with a molecular formula $C_{10}H_{17}NO_2$: IR (thin film from $CHCl_3$ on salt plates), 500 MHz 1H NMR, 125.8 MHz ^{13}C NMR, DEPT-90, DEPT-135, COSY, HMQC, HMBC, TOCSY (100 ms mixing time), NOESY, and a 1D NOE experiment. All NMR spectra were measured in $CDCl_3$ 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.

MAKE SURE TO COMPLETELY ANSWER THE QUESTIONS **a-f** 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. Build an energy-minimized molecular model of the molecule using PyMOL and the "clean" function. 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 Problem_II.1.pse . E-mail the .pse files to me (jsnowick@uci.edu).

Alternatively, you may build an energy-minimized model of the correct diastereomer using Maestro/MacroModel with the MMFF force field. E-mail me (jsnowick@uci.edu) the -out.maegz file associated with that model.

c. Tabulate the shifts of the ^1H resonances (a-j) 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:

d. Redraw the structure of the molecule below and write the letter (a-j) 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.

e. Tabulate the shifts of the ^{13}C resonances (1-10) 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:

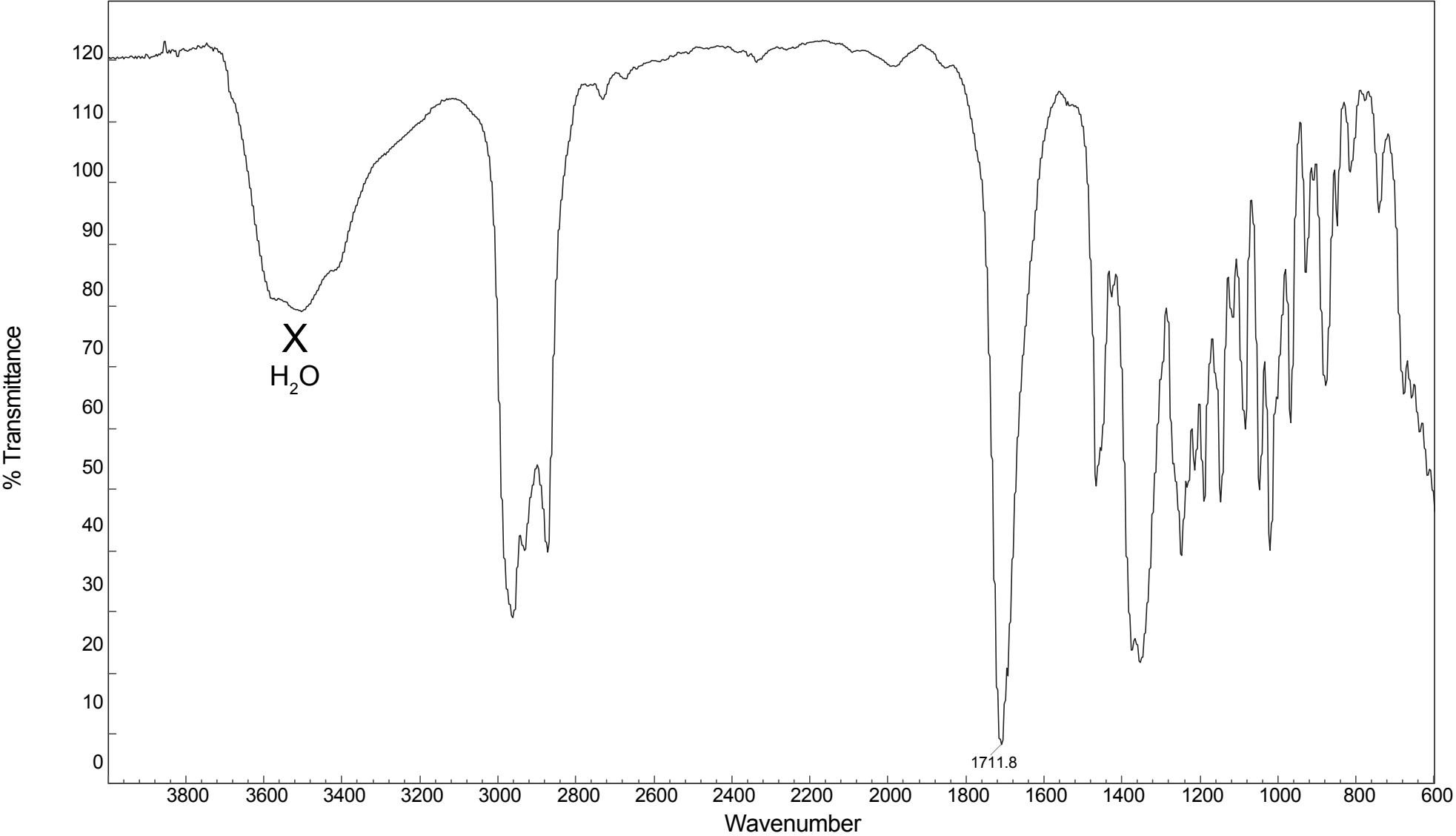
8:

9:

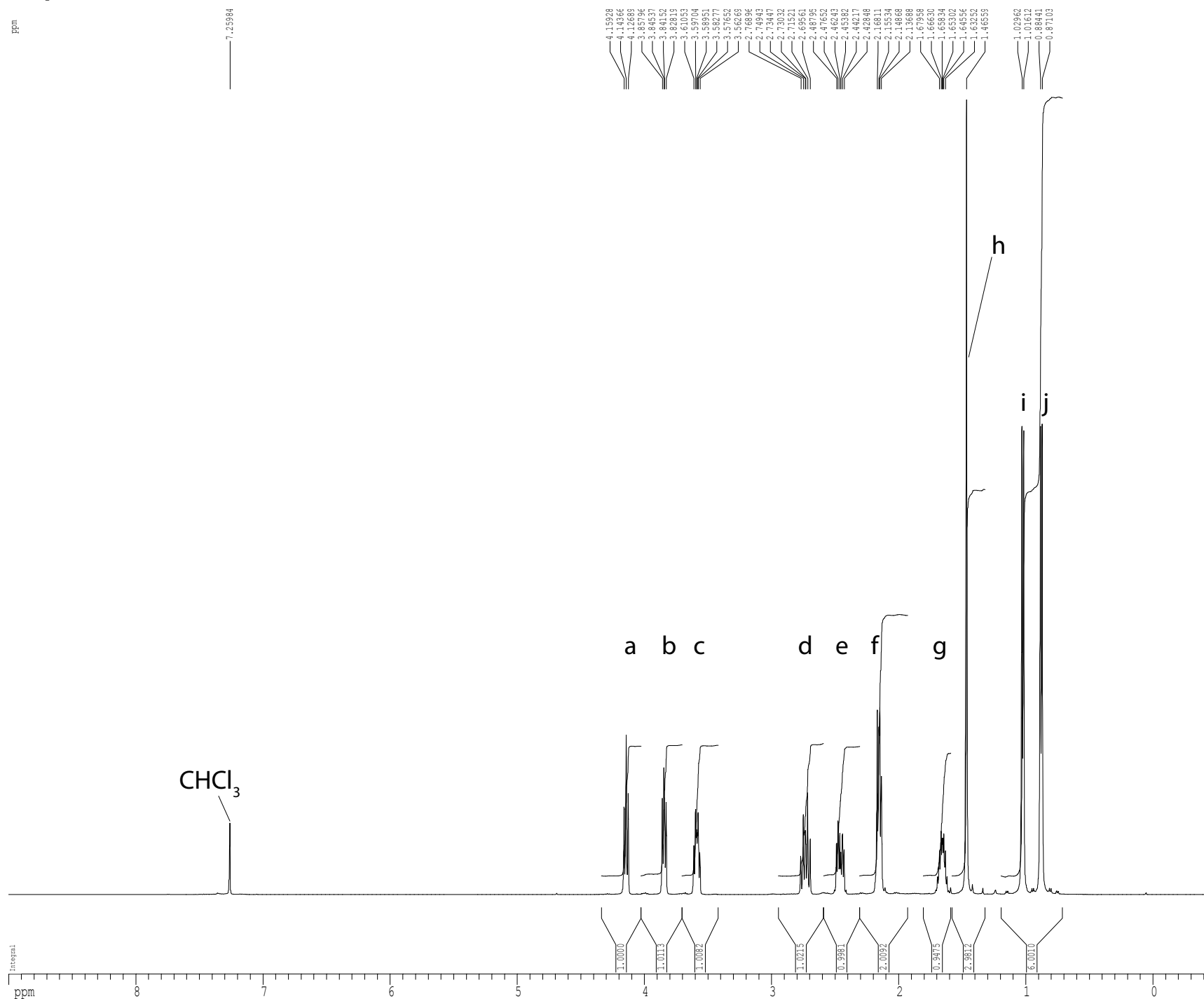
10:

f. 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.

Varian Resolutions Pro



¹H spectrum



Current Data Parameters
 USER nmrl4t
 NAME Act II A
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
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 Time_ 22.32
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 PROBHD 5 mm CPTCI 1H-
 PULPROG zg30
 TD 128202
 SOLVENT CDCl₃
 NS 64
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.062502 Hz
 AQ 7.9998546 sec
 RG 3.2
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCREST 0.00000000 sec
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 PL1 1.60 dB
 SF01 500.2235015 MHz

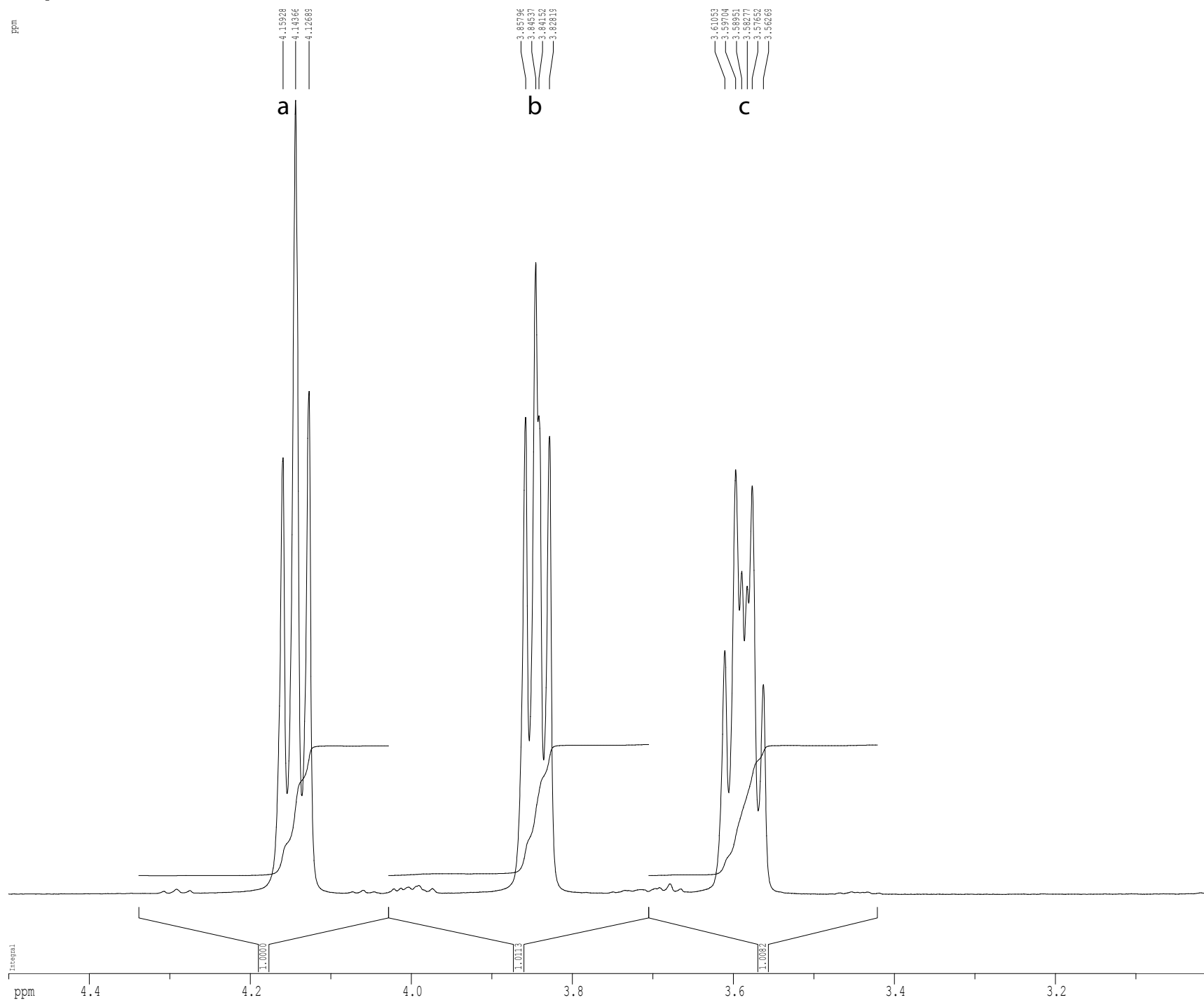
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1D NMR plot parameters
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 CY 15.00 cm
 F1P 9.000 ppm
 F1 4501.98 Hz
 F2P -0.500 ppm
 F2 -250.11 Hz
 PPMCM 0.41667 ppm/cm
 HZCM 208.42502 Hz/cm

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#	ADDRESS	FREQUENCY		INTENSITY
		[Hz]	[PPM]	
1	31431.7	3631.516	7.2598	1.35
2	44116.8	2080.552	4.1593	1.66
3	44180.7	2072.742	4.1437	3.02
4	44249.3	2064.353	4.1269	1.91
5	45349.6	1929.829	3.8580	1.81
6	45401.1	1923.530	3.8454	2.40
7	45416.8	1921.605	3.8415	1.82
8	45471.4	1914.936	3.8282	1.74
9	46361.9	1806.061	3.6105	0.92
10	46417.1	1799.312	3.5970	1.61
11	46447.9	1795.543	3.5895	1.23
12	46475.5	1792.173	3.5828	1.17
13	46501.0	1789.046	3.5765	1.55
14	46557.6	1782.129	3.5627	0.80
15	49805.0	1385.088	2.7690	0.73
16	49884.9	1375.317	2.7494	1.51
17	49946.1	1367.837	2.7345	1.22
18	49963.0	1365.761	2.7303	0.98
19	50024.8	1358.204	2.7152	1.92
20	50105.0	1348.397	2.6956	1.04
21	50954.6	1244.523	2.4880	0.97
22	51001.4	1238.807	2.4765	1.39
23	51059.0	1231.757	2.4624	1.15
24	51094.3	1227.448	2.4538	0.80
25	51141.9	1221.620	2.4422	1.15
26	51197.9	1214.776	2.4285	0.84
27	52263.2	1084.531	2.1681	3.48
28	52315.4	1078.143	2.1553	3.17
29	52342.7	1074.812	2.1487	3.54
30	52391.0	1068.907	2.1369	2.24
31	54261.9	840.159	1.6796	0.83
32	54316.2	833.517	1.6663	1.20
33	54348.8	829.532	1.6583	1.06
34	54370.5	826.874	1.6530	1.07
35	54401.1	823.141	1.6456	1.15
36	54454.4	816.619	1.6325	0.82
37	55137.4	733.117	1.4656	15.00
38	56921.0	515.037	1.0296	8.84
39	56976.3	508.281	1.0161	8.76
40	57515.1	442.401	0.8844	8.84
41	57569.9	435.705	0.8710	8.88

¹H spectrum



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Current Data Parameters
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NAME          Act II A
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PROCNO        1

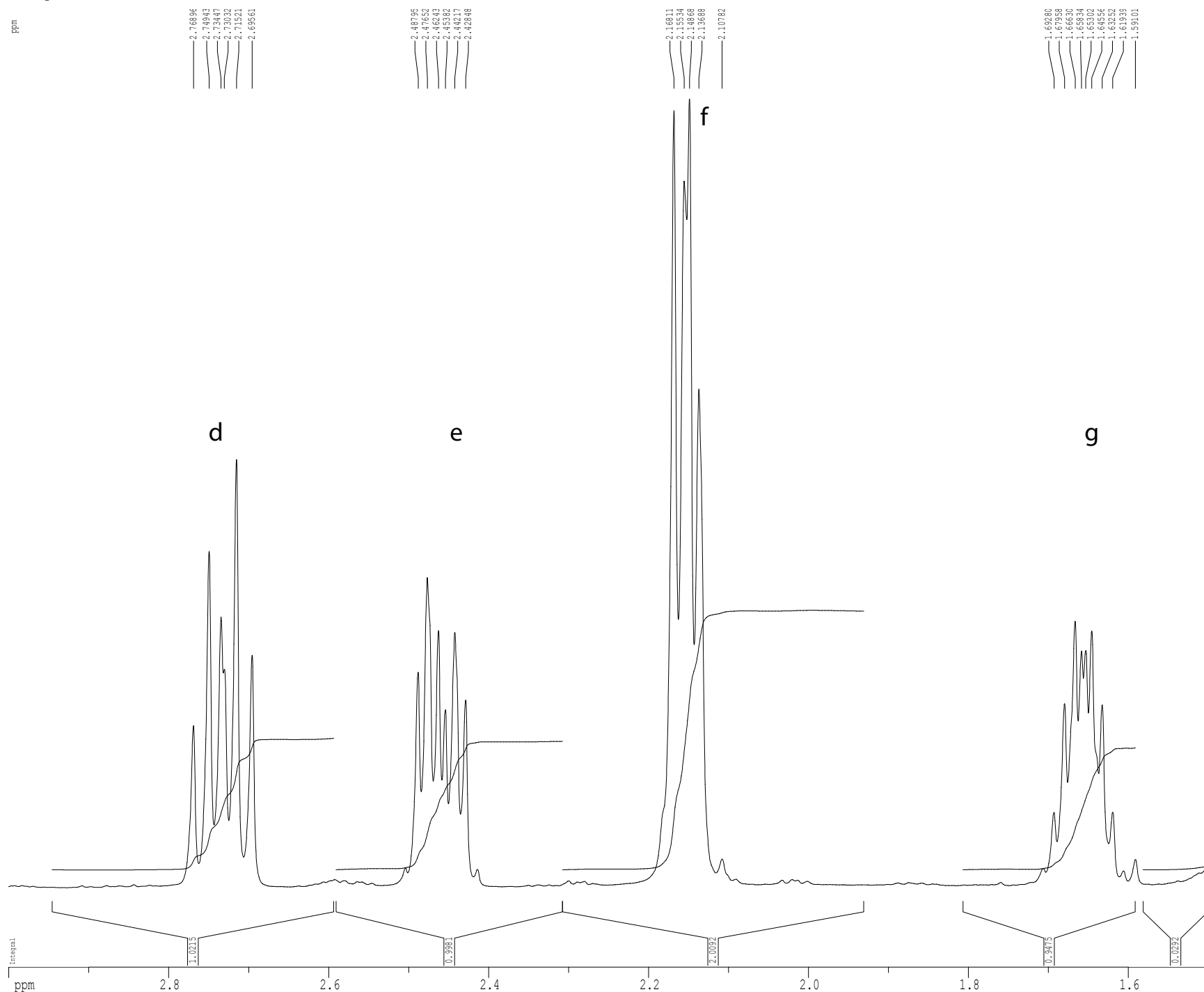
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SOLVENT       CDCl3
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FIDRES        0.062502 Hz
AQ            7.9998546 sec
RG            3.2
DW            62.400 usec
DE            6.00 usec
TE            298.0 K
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MCREST        0.00000000 sec
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===== CHANNEL f1 =====
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PL1            1.60 dB
SF01          500.2235015 MHz

F2 - Processing parameters
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SSB           0
LB            0.30 Hz
GB            0
PC            4.00

1D NMR plot parameters
CX            22.80 cm
CY            15.00 cm
F1P           4.500 ppm
F1            2250.99 Hz
F2P           3.000 ppm
F2            1500.66 Hz
PPMCM         0.06579 ppm/cm
HZCM          32.90921 Hz/cm
    
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¹H spectrum



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Current Data Parameters
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EXPNO         1
PROCNO        1

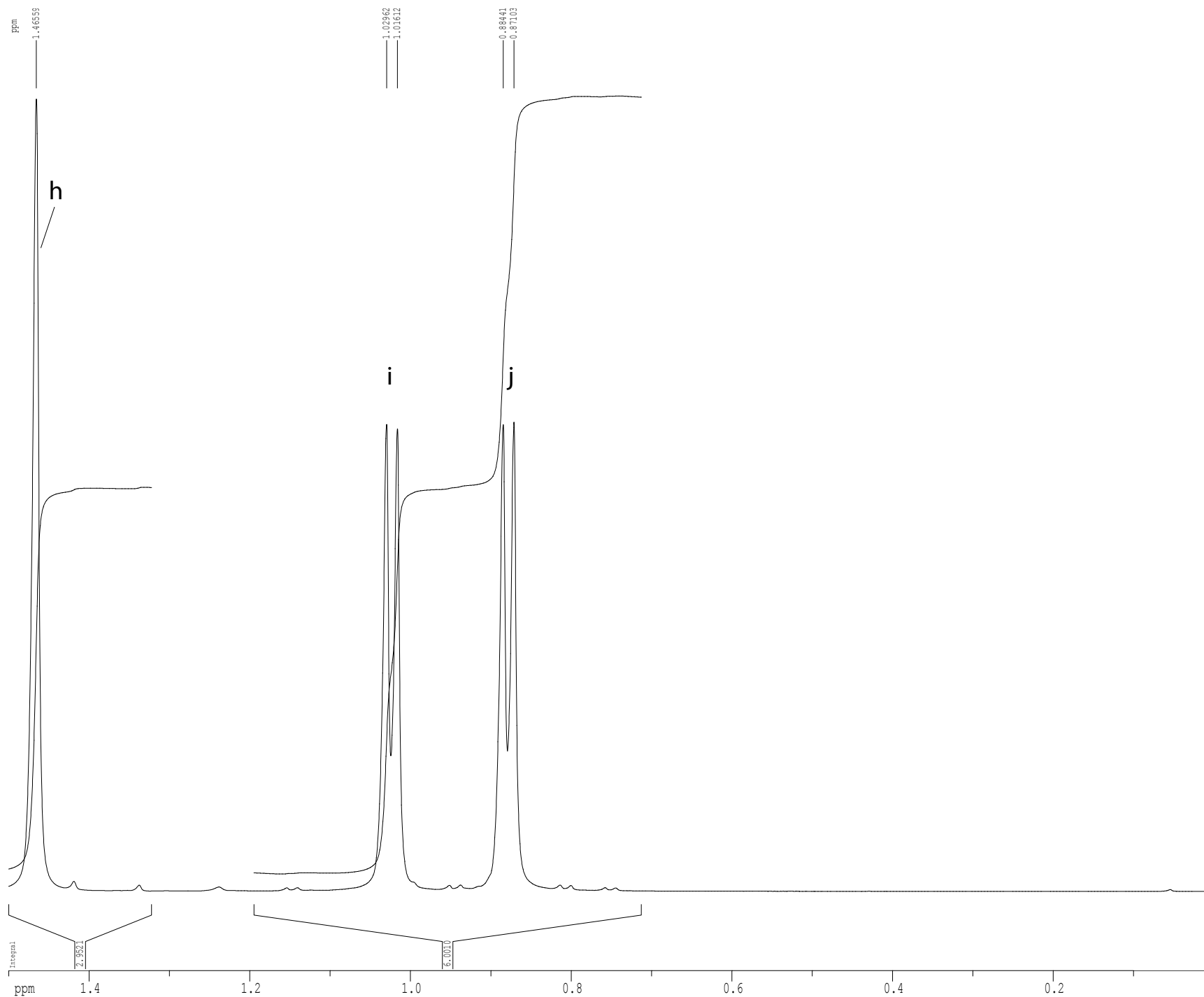
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PULPROG       zg30
TD            128202
SOLVENT       CDCl3
NS            64
DS            2
SWH           8012.820 Hz
FIDRES        0.062502 Hz
AQ            7.9998546 sec
RG            3.2
DW            62.400 usec
DE            6.00 usec
TE            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
SF01          500.2235015 MHz

F2 - Processing parameters
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SF           500.2200334 MHz
WDW           EM
SSB            0
LB            0.30 Hz
GB            0
PC            4.00

1D NMR plot parameters
CX            22.80 cm
CY            15.00 cm
F1P           3.000 ppm
F1            1500.66 Hz
F2P           1.500 ppm
F2            750.33 Hz
PPMCM         0.06579 ppm/cm
HZCM          32.90921 Hz/cm
    
```

¹H spectrum



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Current Data Parameters
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NAME          Act II A
EXPNO         1
PROCNO        1

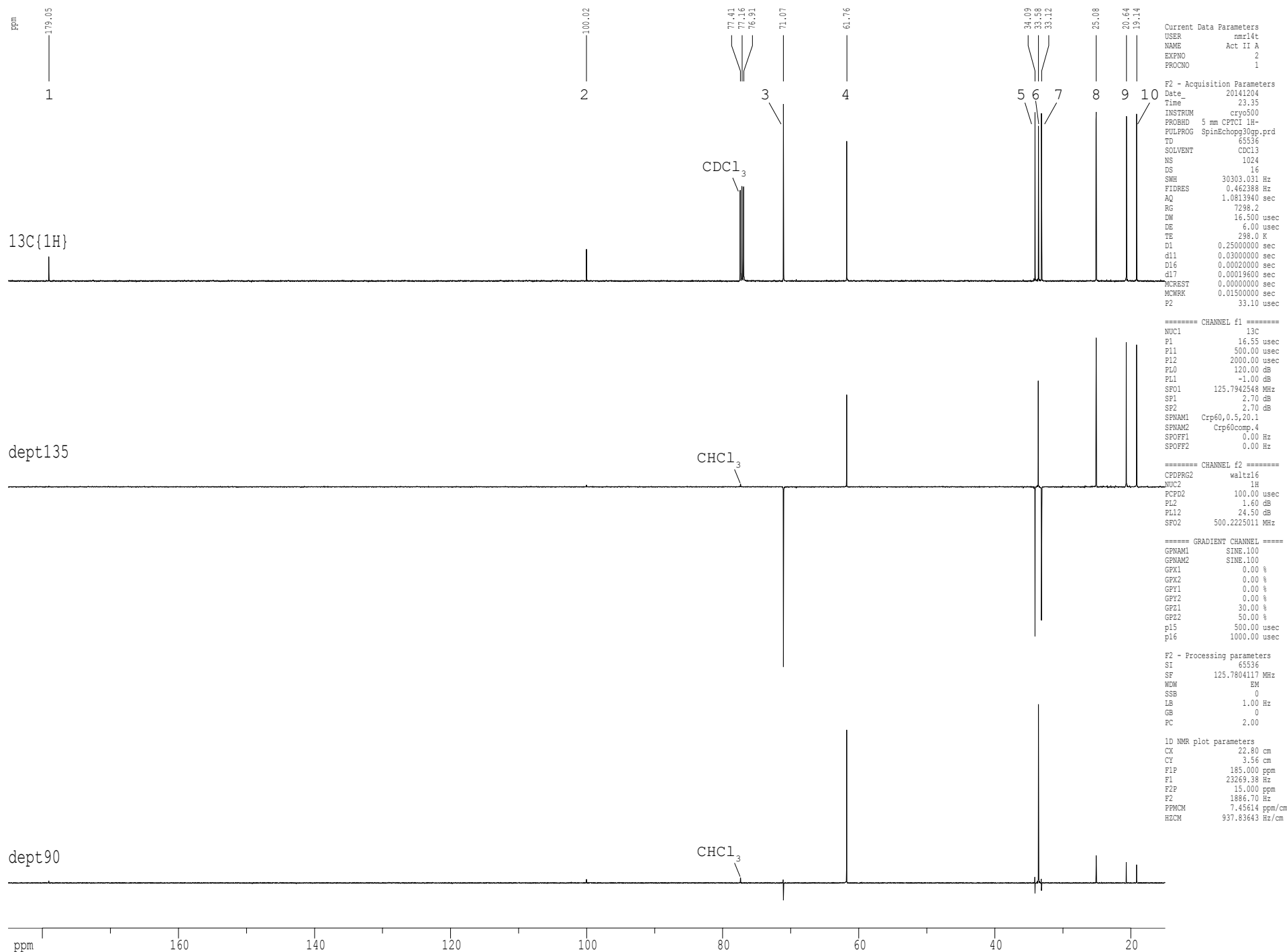
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PULPROG       zg30
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SOLVENT       CDCl3
NS            64
DS            2
SWH           8012.820 Hz
FIDRES        0.062502 Hz
AQ            7.9998546 sec
RG            3.2
DW            62.400 usec
DE            6.00 usec
TE            298.0 K
D1            0.10000000 sec
MCREST        0.00000000 sec
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===== CHANNEL f1 =====
NUC1           1H
P1             7.50 usec
PL1            1.60 dB
SF01          500.2235015 MHz

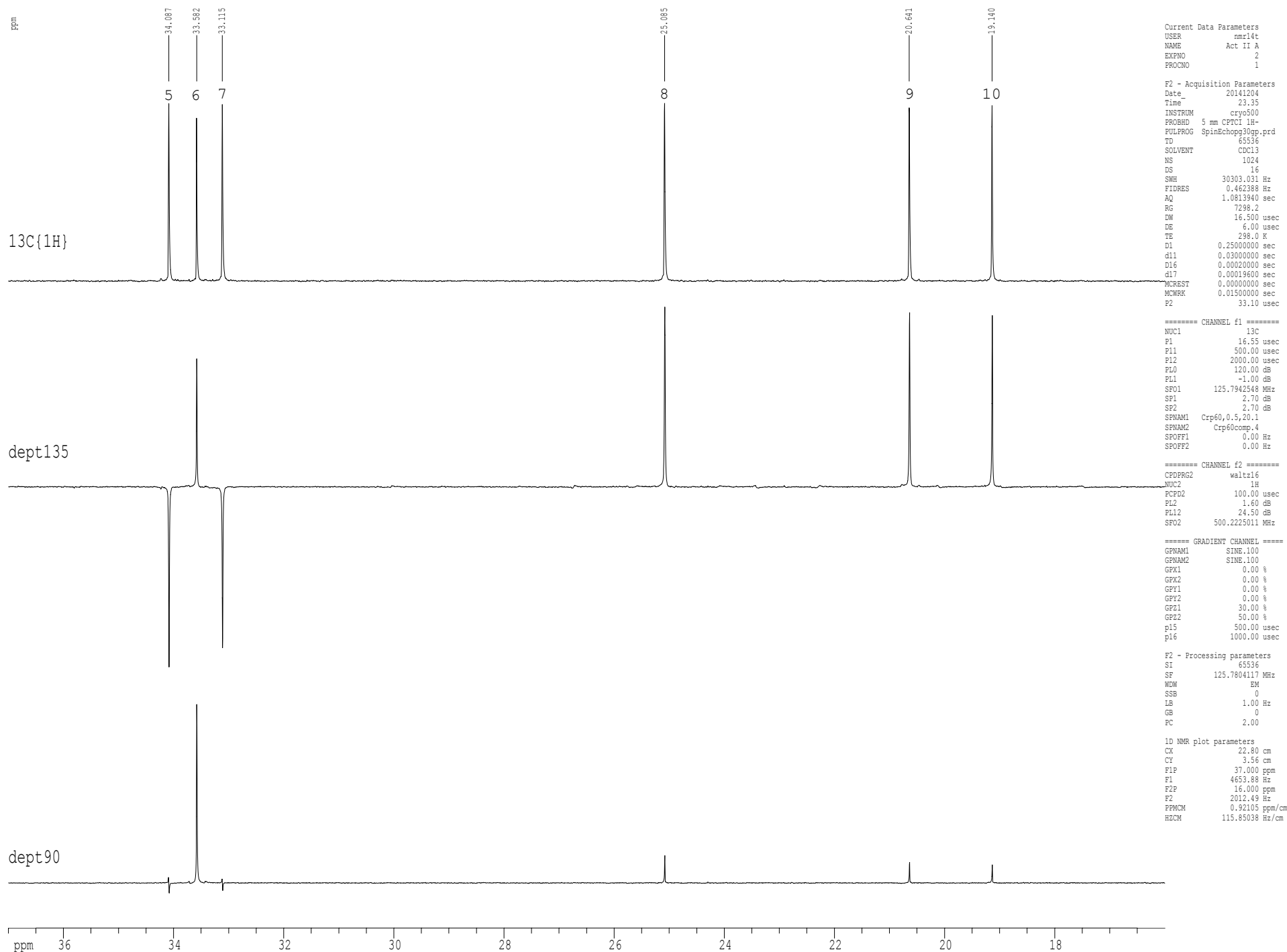
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GB            0
PC            4.00

1D NMR plot parameters
CX            22.80 cm
CY            15.00 cm
F1P           1.500 ppm
F1            750.33 Hz
F2P          -0.000 ppm
F2           -0.00 Hz
PPMCM         0.06579 ppm/cm
HZCM          32.90921 Hz/cm
    
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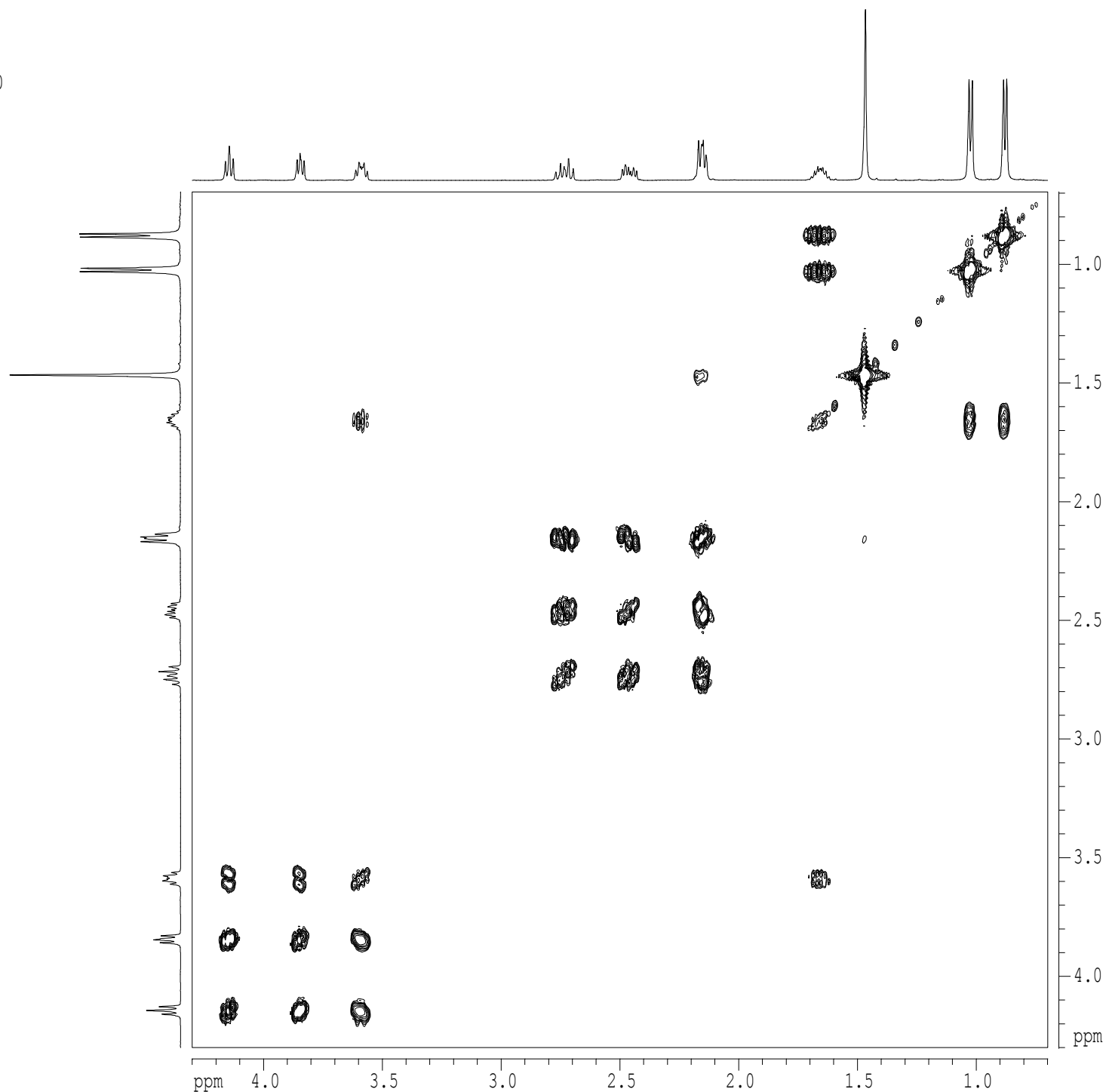
Z-restored spin-echo 13C spectrum with 1H decoupling



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



gcosy60



Current Data Parameters
USER nmrl4t
NAME Act II A
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141205
Time 0.30
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG cosygp60.prd
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 5000.000 Hz
FIDRES 2.441406 Hz
AQ 0.2048500 sec
RG 5
DW 100.000 usec
DE 6.00 usec
TE 298.0 K
d0 0.00000300 sec
D1 1.00000000 sec
d13 0.00000300 sec
D16 0.00020000 sec
IN0 0.00020000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2225000 MHz

===== GRADIENT CHANNEL =====
GPNAM1 sine.100
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

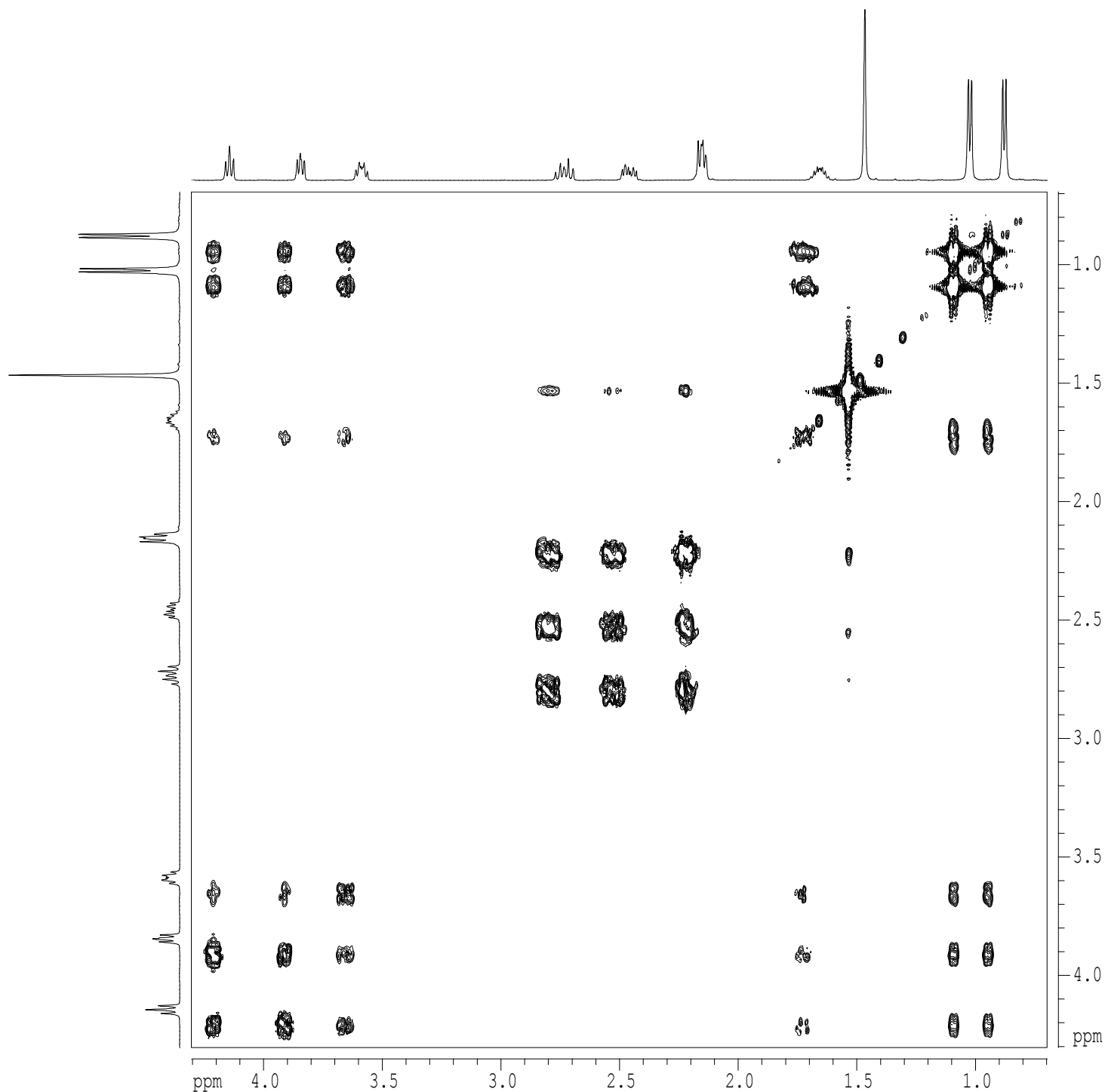
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TD 256
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FIDRES 19.531250 Hz
SW 9.996 ppm
FnMODE undefined

F2 - Processing parameters
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SF 500.2200334 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.2200334 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 4.300 ppm
F2LO 2150.95 Hz
F2PHI 0.699 ppm
F2HI 349.89 Hz
F1PLO 4.300 ppm
F1LO 2150.95 Hz
F1PHI 0.695 ppm
F1HI 347.45 Hz
F2PPMCM 0.24004 ppm/cm
F2HZCM 120.07034 Hz/cm
F1PPMCM 0.24036 ppm/cm
F1HZCM 120.23310 Hz/cm

gtocsy



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Current Data Parameters
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NAME      Act II A
EXPNO     6
PROCNO    1

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INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   mlevpg mo
TD        2048
SOLVENT   CDCl3
NS         8
DS         16
SWH        5000.000 Hz
FIDRES     2.441406 Hz
AQ         0.2048500 sec
RG         5
DW         100.000 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        0.00020000 sec
FACTOR1    7
IN0        0.00020000 sec
l1         42
SCALEF     6

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
p5         23.34 usec
P6         35.00 usec
p7         70.00 usec
P17        2500.00 usec
PL1        1.60 dB
PL10       15.20 dB
SFO1       500.2225000 MHz

===== GRADIENT CHANNEL =====
GPNAM1     sine.100
GPNAM2     sine.100
GPX1       0.00 %
GPX2       0.00 %
GPY1       0.00 %
GPY2       0.00 %
GPE1       10.00 %
GPE2       10.00 %
P16        1000.00 usec

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FnMODE     undefined

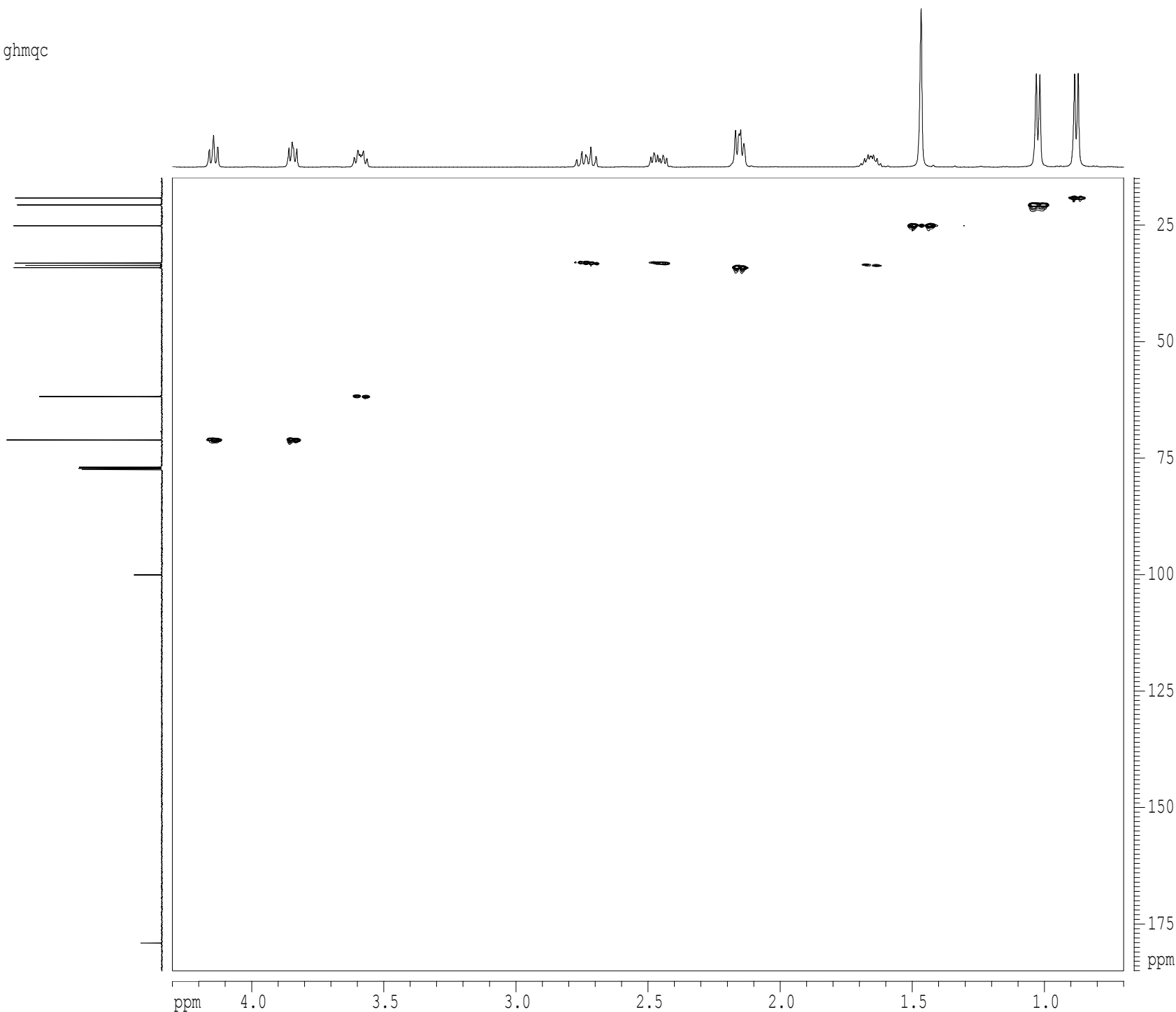
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LB         0.00 Hz
GB         0

2D NMR plot parameters
CX2        15.00 cm
CX1        15.00 cm
F2PLO      4.305 ppm
F2L0       2153.32 Hz
F2PHI      0.698 ppm
F2H1       349.12 Hz
F1PLO      4.305 ppm
F1L0       2153.32 Hz
F1PHI      0.693 ppm
F1H1       346.68 Hz
F2PPMCM    0.24045 ppm/cm
F2HZCM     120.27995 Hz/cm
F1PPMCM    0.24078 ppm/cm
F1HZCM     120.44271 Hz/cm

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ghmqc



```
Current Data Parameters
USER      nmrl4t
NAME      Act II A
EXPNO     7
PROCNO    1

F2 - Acquisition Parameters
Date_     20141205
Time      2.12
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   inv4gp.wu
TD         2048
SOLVENT   CDCl3
NS         8
DS         16
SWH        5000.000 Hz
FIDRES     2.441406 Hz
AQ         0.2048500 sec
RG         5792.6
DW         100.000 usec
DE         6.50 usec
TE         298.0 K
CNST2     145.0000000
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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        0.00001806 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
P2         15.00 usec
PL1        1.60 dB
SFO1       500.2225000 MHz

===== CHANNEL f2 =====
CPDPRG2    9atp
NUC2       13C
P3         15.50 usec
PCPD2      65.00 usec
PL2        -1.00 dB
PL12       11.30 dB
SFO2       125.7941690 MHz

===== GRADIENT CHANNEL =====
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GPNAM2     sine.100
GPNAM3     sine.100
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GPX2       0.00 %
GPX3       0.00 %
GPY1       0.00 %
GPY2       0.00 %
GPY3       0.00 %
GPZ1       30.00 %
GPZ2       18.00 %
GPZ3       24.00 %
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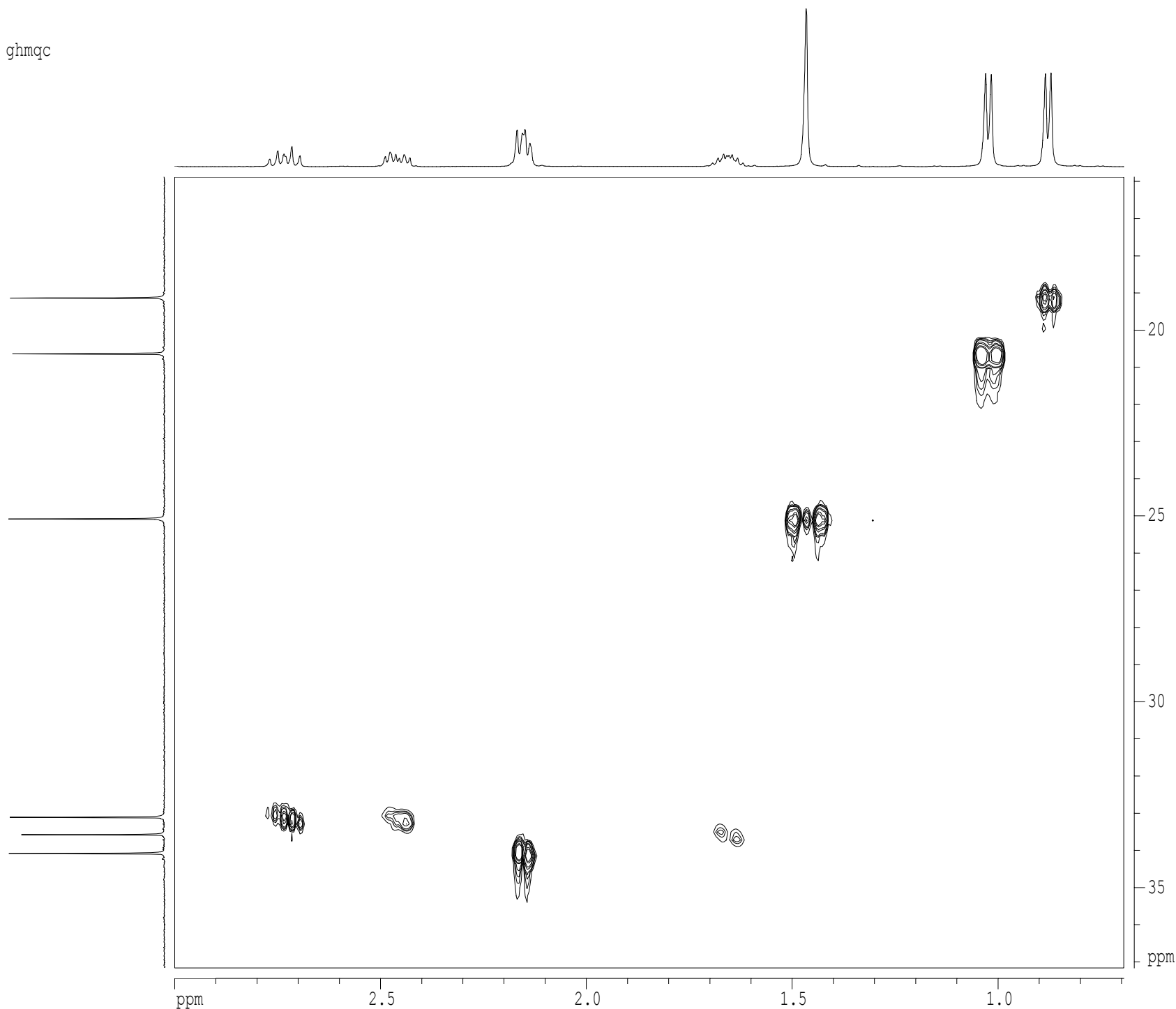
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SSB        0
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
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MC2        QF
SF         125.7804117 MHz
WDW        QSINE
SSB        3
LB         0.00 Hz
GB         0

2D NMR plot parameters
CX2        18.00 cm
CX1        15.00 cm
F2PLO      4.300 ppm
F2LO       2150.95 Hz
F2PHI      0.700 ppm
F2HI       350.15 Hz
F1PLO      185.028 ppm
F1LO       23272.85 Hz
F1PHI      14.810 ppm
F1HI       1862.81 Hz
F2PPMCM    0.20000 ppm/cm
F2HZCM     100.04401 Hz/cm
F1PPMCM    11.34784 ppm/cm
F1HZCM     1427.33569 Hz/cm
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ghmqc



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NAME      Act II A
EXPNO     7
PROCNO    1

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PULPROG   inv4gp.wu
TD         2048
SOLVENT   CDCl3
NS         8
DS         16
SWH        5000.000 Hz
FIDRES     2.441406 Hz
AQ         0.2048500 sec
RG         5792.6
DW         100.000 usec
DE         6.50 usec
TE         298.0 K
CMST2     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        0.00001806 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
p2         15.00 usec
PL1        1.60 dB
SFO1       500.2225000 MHz

===== CHANNEL f2 =====
CPDPRG2    9atp
NUC2       13C
P3         15.50 usec
PCPD2      65.00 usec
PL2        -1.00 dB
PL12       11.30 dB
SFO2       125.7941690 MHz

===== GRADIENT CHANNEL =====
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GPNAM2     sine.100
GPNAM3     sine.100
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GPX2        0.00 %
GPX3        0.00 %
GPY1        0.00 %
GPY2        0.00 %
GPY3        0.00 %
GPZ1        30.00 %
GPZ2        19.00 %
GPZ3        24.00 %
P16         1000.00 usec

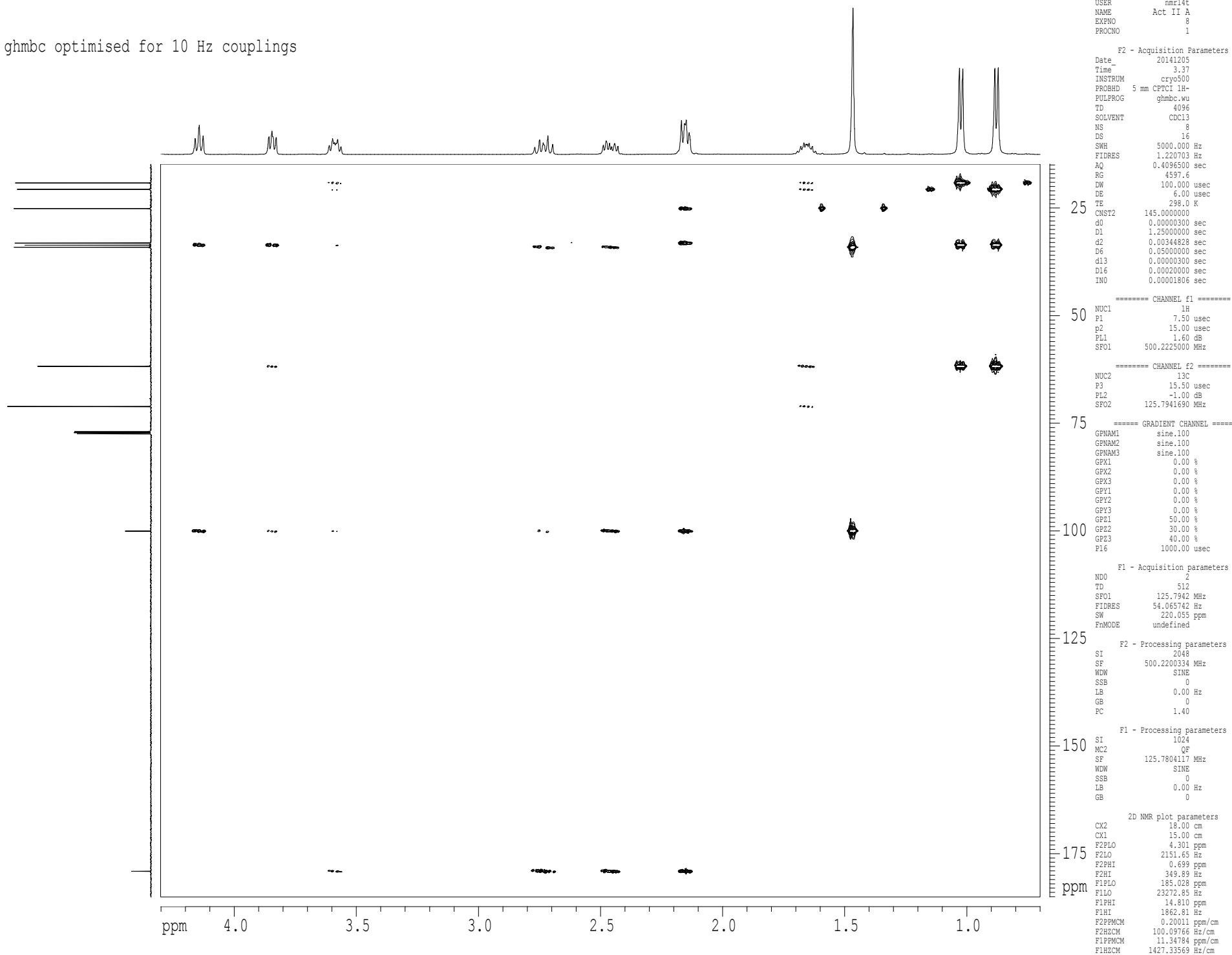
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TD         512
SFO1       125.7942 MHz
FIDRES     54.065742 Hz
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PC         1.40

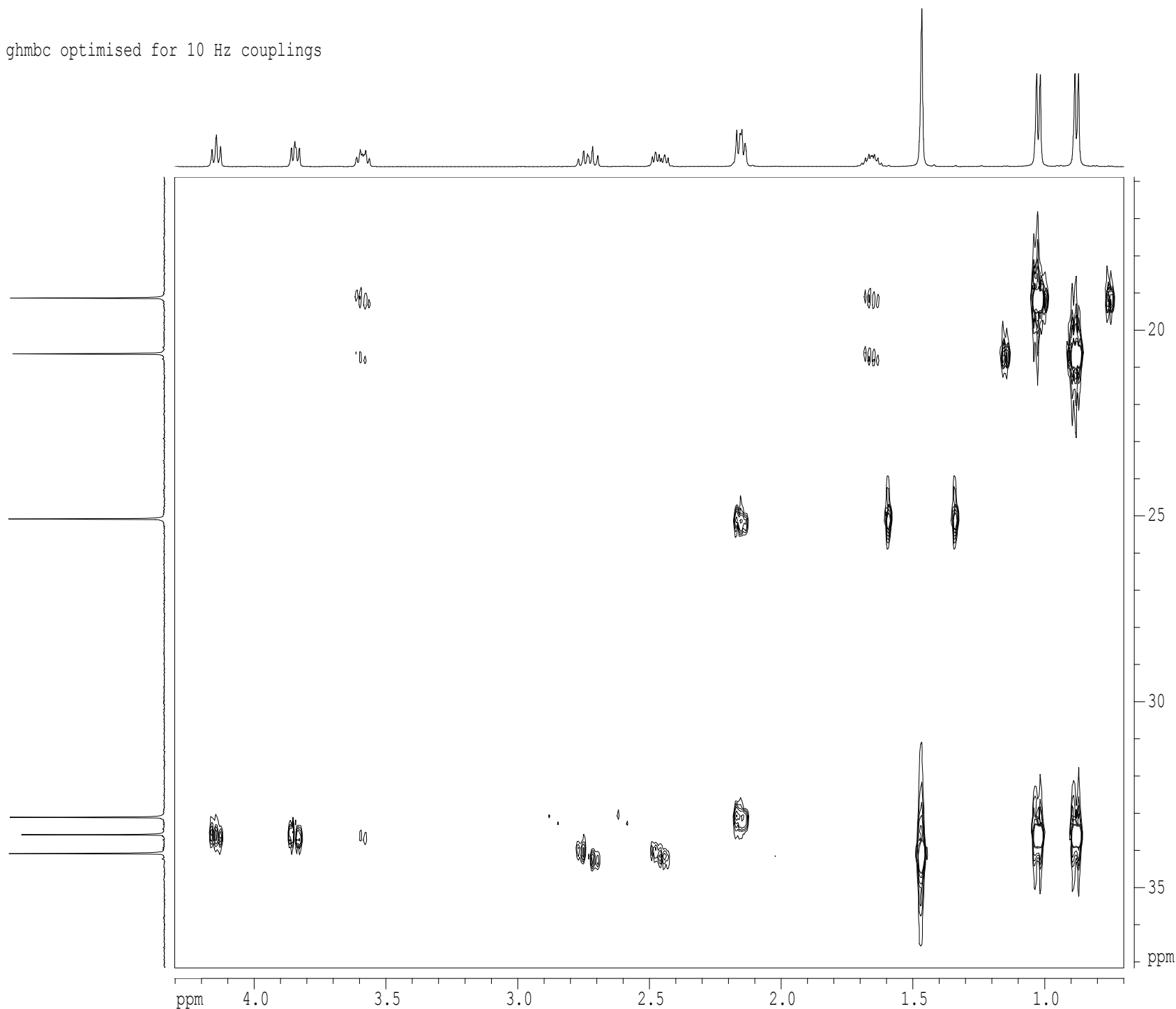
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GB         0

2D NMR plot parameters
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CX1        15.00 cm
F2PL0      3.000 ppm
F2LO       1500.66 Hz
F2PHI      0.695 ppm
F2H1       347.45 Hz
F1PL0      37.162 ppm
F1LO       4674.23 Hz
F1PHI      15.885 ppm
F1H1       1997.98 Hz
F2PPMCM    0.12808 ppm/cm
F2HZCM     64.06725 Hz/cm
F1PPMCM    1.41848 ppm/cm
F1HZCM     178.41696 Hz/cm
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ghmbc optimised for 10 Hz couplings



ghmbc optimised for 10 Hz couplings



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Current Data Parameters
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NAME      partII_A
EXPNO     8
PROCNO    1

F2 - Acquisition Parameters
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Time      3.37
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PULPROG   ghmbc.wu
TD         4096
SOLVENT   CDCl3
NS         8
DS         16
SWH        5000.000 Hz
FIDRES     1.220703 Hz
AQ         0.4096500 sec
RG         4597.6
DW         100.000 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        0.00001806 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
P2         15.00 usec
PL1        1.60 dB
SFO1       500.2225000 MHz

===== CHANNEL f2 =====
NUC2       13C
P3         15.50 usec
PL2        -1.00 dB
SFO2       125.7941690 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

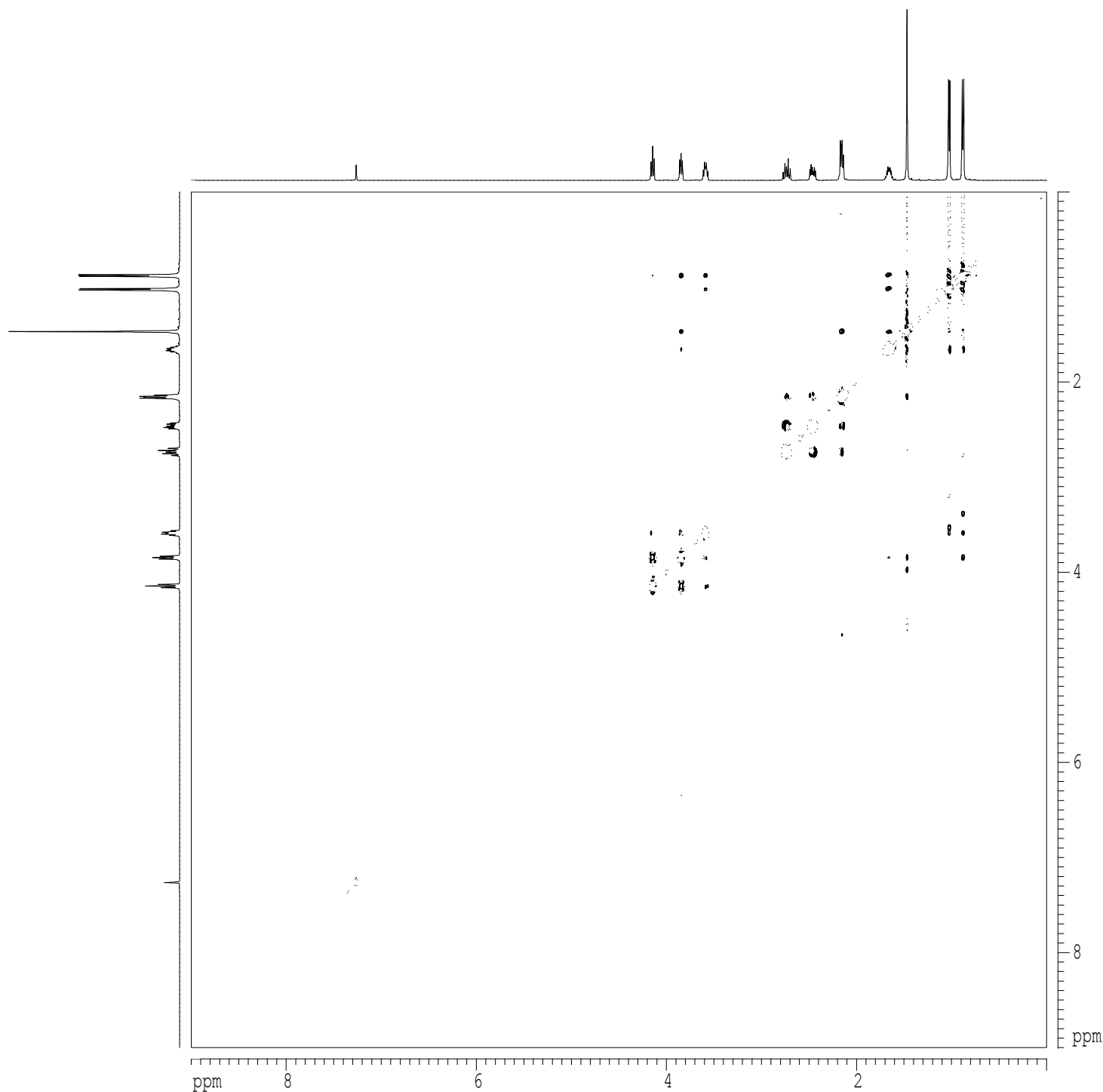
F1 - Acquisition parameters
ND0        2
TD         512
SFO1       125.7942 MHz
FIDRES     54.065742 Hz
SW         220.055 ppm
FnMODE     undefined

F2 - Processing parameters
SI         2048
SF         500.2200334 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        QF
SF         125.7804117 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0

2D NMR plot parameters
CY2        18.00 cm
CX1        15.00 cm
F2PLO      4.301 ppm
F2LO       2151.65 Hz
F2PHI      0.699 ppm
F2HI       349.89 Hz
F1PLO      37.162 ppm
F1LO       4674.23 Hz
F1PHI      15.885 ppm
F1HI       1997.98 Hz
F2PPMCM    0.20011 ppm/cm
F2HZCM     100.09766 Hz/cm
F1PPMCM    1.41848 ppm/cm
F1HZCM     178.41696 Hz/cm
```

gnoesy



Current Data Parameters
USER nmrl4t
NAME Act II A
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141205
Time 5.36
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG noesygptp
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 5000.000 Hz
FIDRES 2.441406 Hz
AQ 0.2048500 sec
RG 5
DW 100.000 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 0.00010000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
P2 15.00 usec
PL1 1.60 dB
SFO1 500.2225000 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

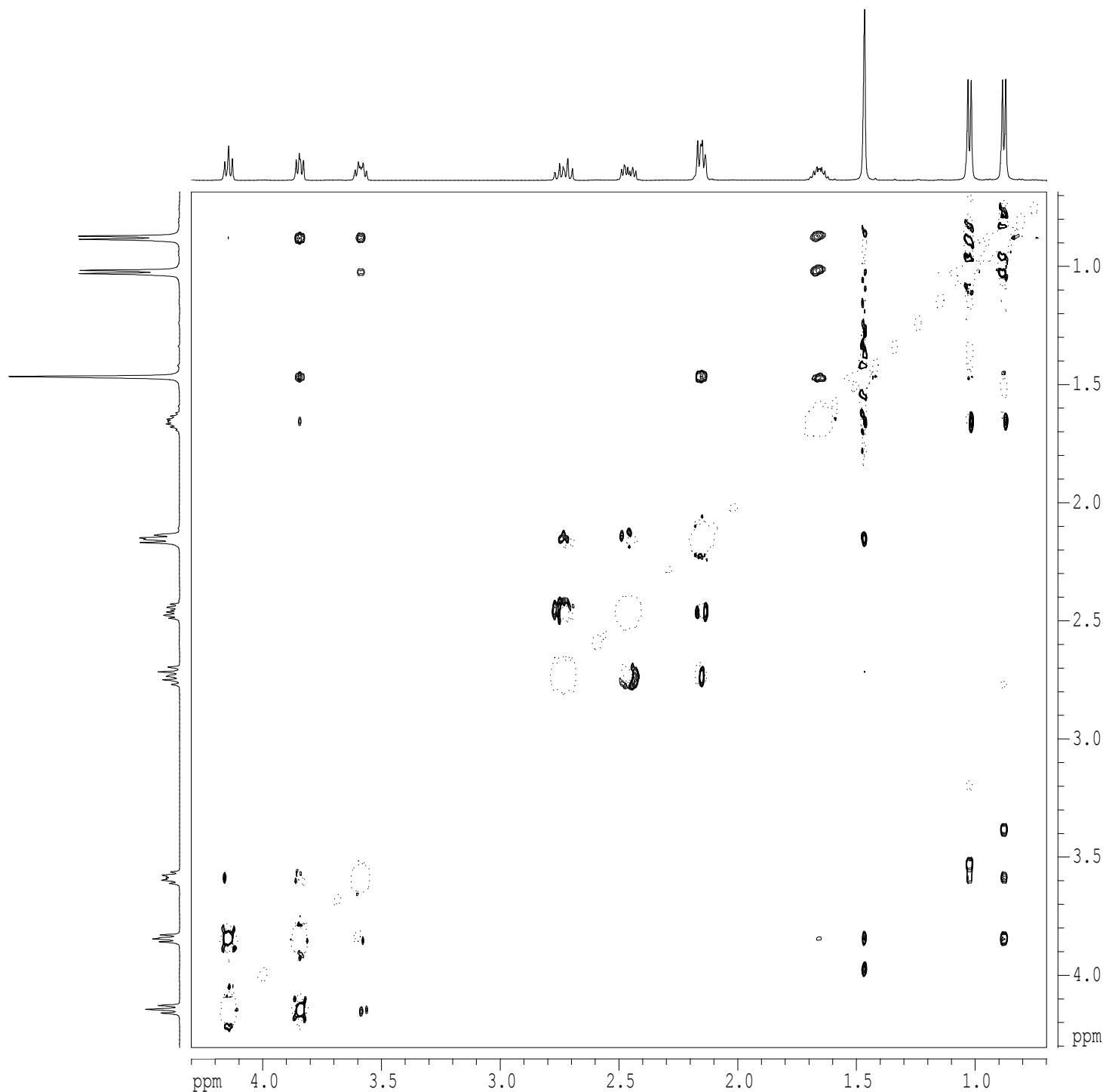
F1 - Acquisition parameters
ND0 2
TD 256
SFO1 500.2225 MHz
FIDRES 19.531250 Hz
SW 9.996 ppm
FnMODE undefined

F2 - Processing parameters
SI 2048
SF 500.2200334 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 TPPI
SF 500.2200334 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 9.000 ppm
F2LO 4501.98 Hz
F2PHI 0.000 ppm
F2HI 0.00 Hz
F1PLO 9.000 ppm
F1LO 4501.98 Hz
F1PHI 0.000 ppm
F1HI 0.00 Hz
F2PPMCM 0.60000 ppm/cm
F2HZCM 300.13202 Hz/cm
F1PPMCM 0.60000 ppm/cm
F1HZCM 300.13202 Hz/cm

gnoesy



```
Current Data Parameters
USER      nmrl4t
NAME      Act II A
EXPNO     9
PROCNO    1

F2 - Acquisition Parameters
Date_     20141205
Time      5.36
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   noesygptp
TD        2048
SOLVENT   CDCl3
NS         8
DS         16
SWH        5000.000 Hz
FIDRES     2.441406 Hz
AQ         0.2048500 sec
RG         5
DW         100.000 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        0.00010000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
P2         15.00 usec
PL1        1.60 dB
SFO1       500.2225000 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

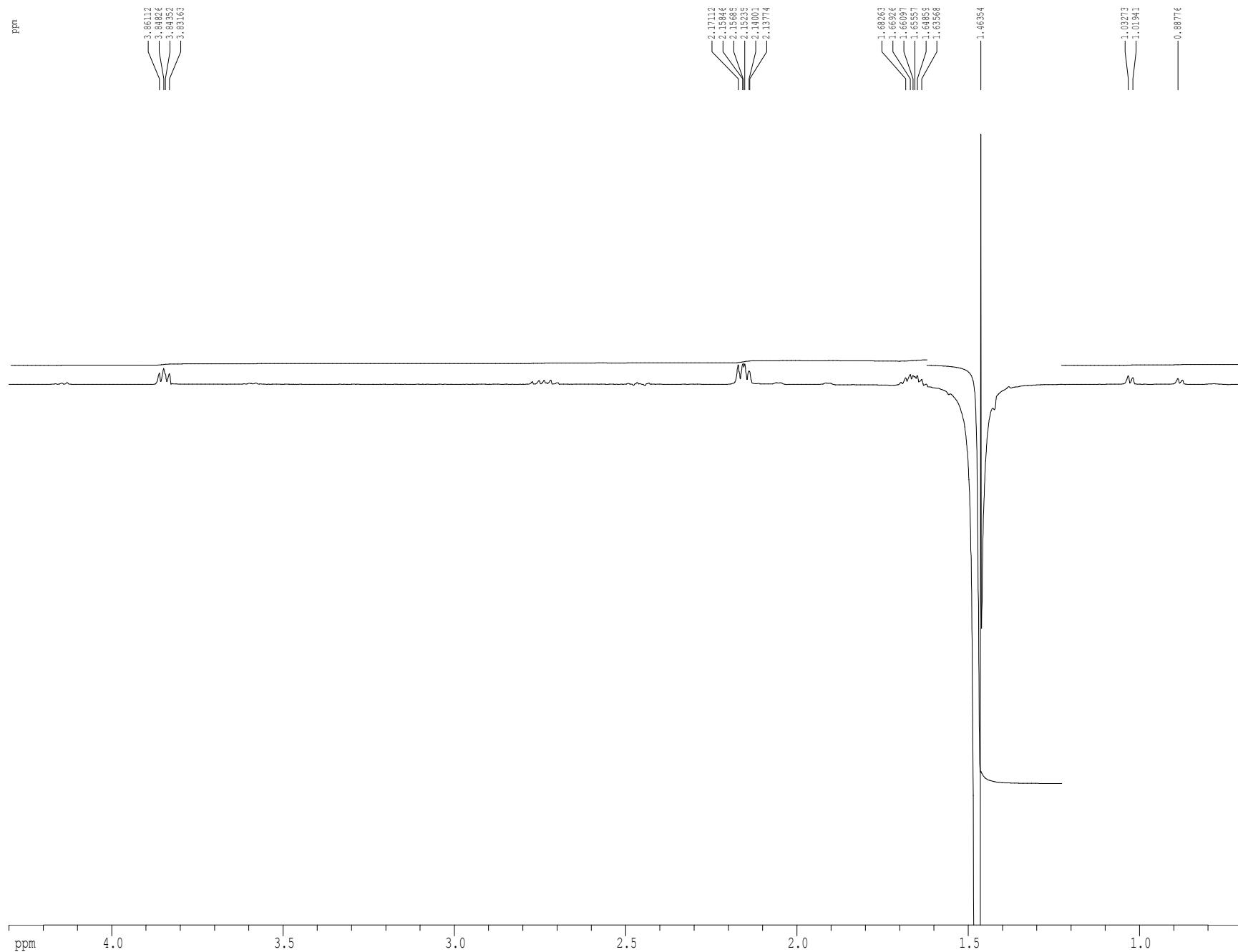
F1 - Acquisition parameters
ND0        2
TD         256
SFO1       500.2225 MHz
FIDRES     19.531250 Hz
SW         9.996 ppm
FnMODE     undefined

F2 - Processing parameters
SI         2048
SF         500.2200334 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        TPPI
SF         500.2200334 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0

2D NMR plot parameters
CX2        15.00 cm
CX1        15.00 cm
F2PLO      4.301 ppm
F2LO       2151.65 Hz
F2PHI      0.699 ppm
F2HI       349.89 Hz
F1PLO      4.306 ppm
F1LO       2154.09 Hz
F1PHI      0.685 ppm
F1HI       342.57 Hz
F2PPMCM    0.24013 ppm/cm
F2HZCM     120.11719 Hz/cm
F1PPMCM    0.24143 ppm/cm
F1HZCM     120.76823 Hz/cm
```

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```

Current Data Parameters
USER      nmrl4t
NAME      partII_A_NOE
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20141215
Time      21.20
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   gnoelcc.wu
TD         65536
SOLVENT   CDCl3
NS         256
DS         8
SWH        10000.000 Hz
FIDRES     0.152588 Hz
AQ         3.2768500 sec
RG         161.3
DW         50.000 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       500.2207673 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         500.2200337 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00

1D NMR plot parameters
CX         22.80 cm
CY         250.00 cm
F1P        4.300 ppm
F1         2150.95 Hz
F2P        0.700 ppm
F2         350.15 Hz
PPMCM      0.15789 ppm/cm
H2CM       78.98212 Hz/cm

```