

Name: _____

Chem 203
December 20, 2014

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.

The following spectral data are provided for a compound with a molecular formula $C_{17}H_{22}O_3$: IR (KBr pellet), 500 MHz 1H NMR, 125.8 MHz ^{13}C NMR, DEPT-90, DEPT-135, COSY, HMQC, HMBC, TOCSY (150 ms mixing time), HSQC-TOCSY with increasing mixing times (5, 10, 25, and 50 ms), and NOESY. All NMR spectra were measured in CD_3SOCD_3 solution.

NOTE: Chemical exchange of exchangeable protons with each other and with H_2O (3.3 ppm) in the CD_3SOCD_3 gives crosspeaks in the TOCSY spectrum and shows up as EXSY (negative) peaks in the NOESY spectrum.

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 2-5.

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.3.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-r) 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:

o:

p:

q:

r:

d. Redraw the structure of the molecule below and write the letter (a-r) 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 (1-17) 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:

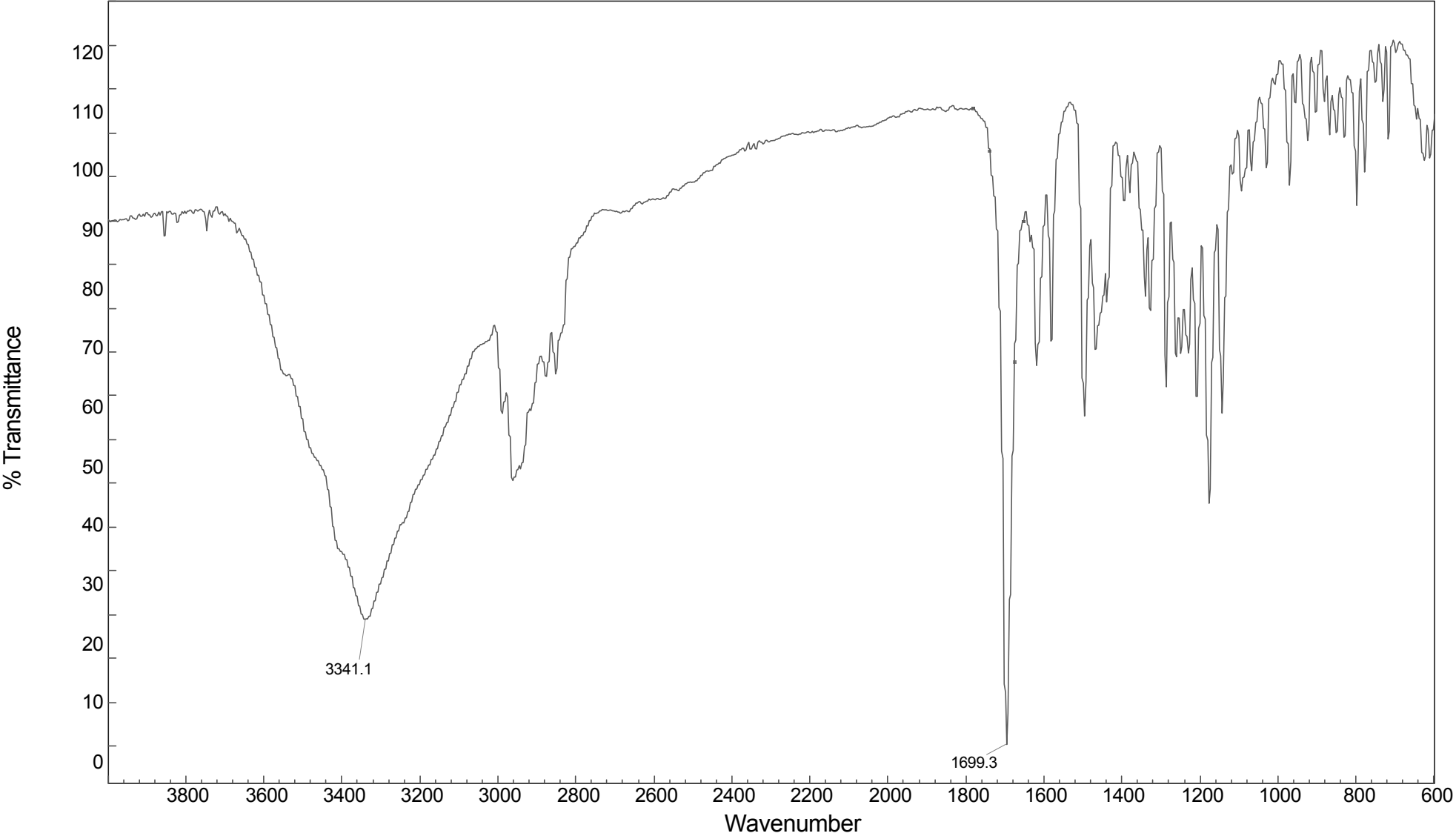
15:

16:

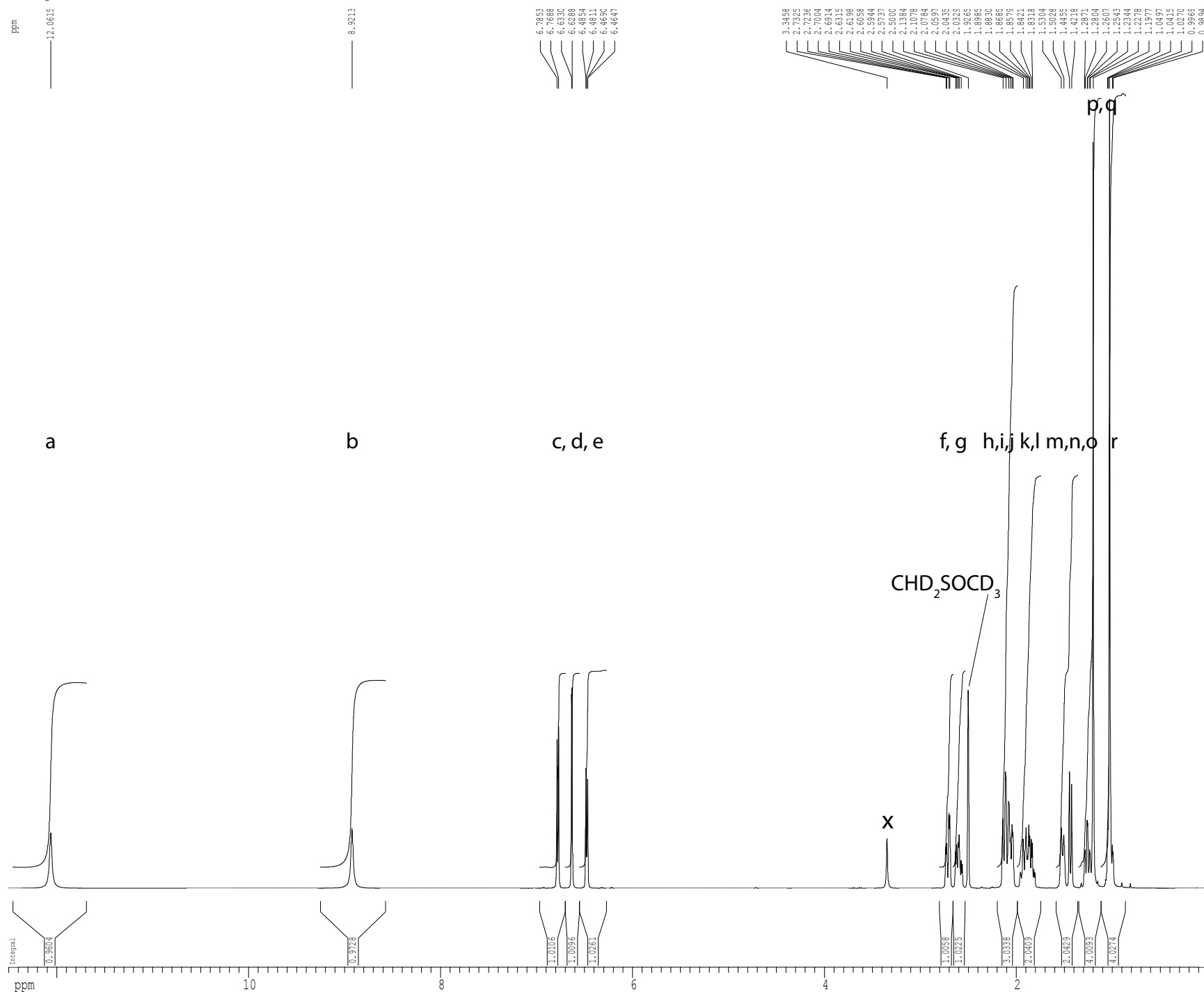
17:

f. 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.

Varian Resolutions Pro



¹H spectrum



Current Data Parameters
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 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
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 Time_ 22.21
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 PULPROG zg30
 TD 128202
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.062502 Hz
 AQ 7.9998546 sec
 RG 4.5
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 DL 0.10000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

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 P1 7.50 usec
 PL1 1.60 dB
 SF01 500.2235015 MHz

F2 - Processing parameters
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 GB 0
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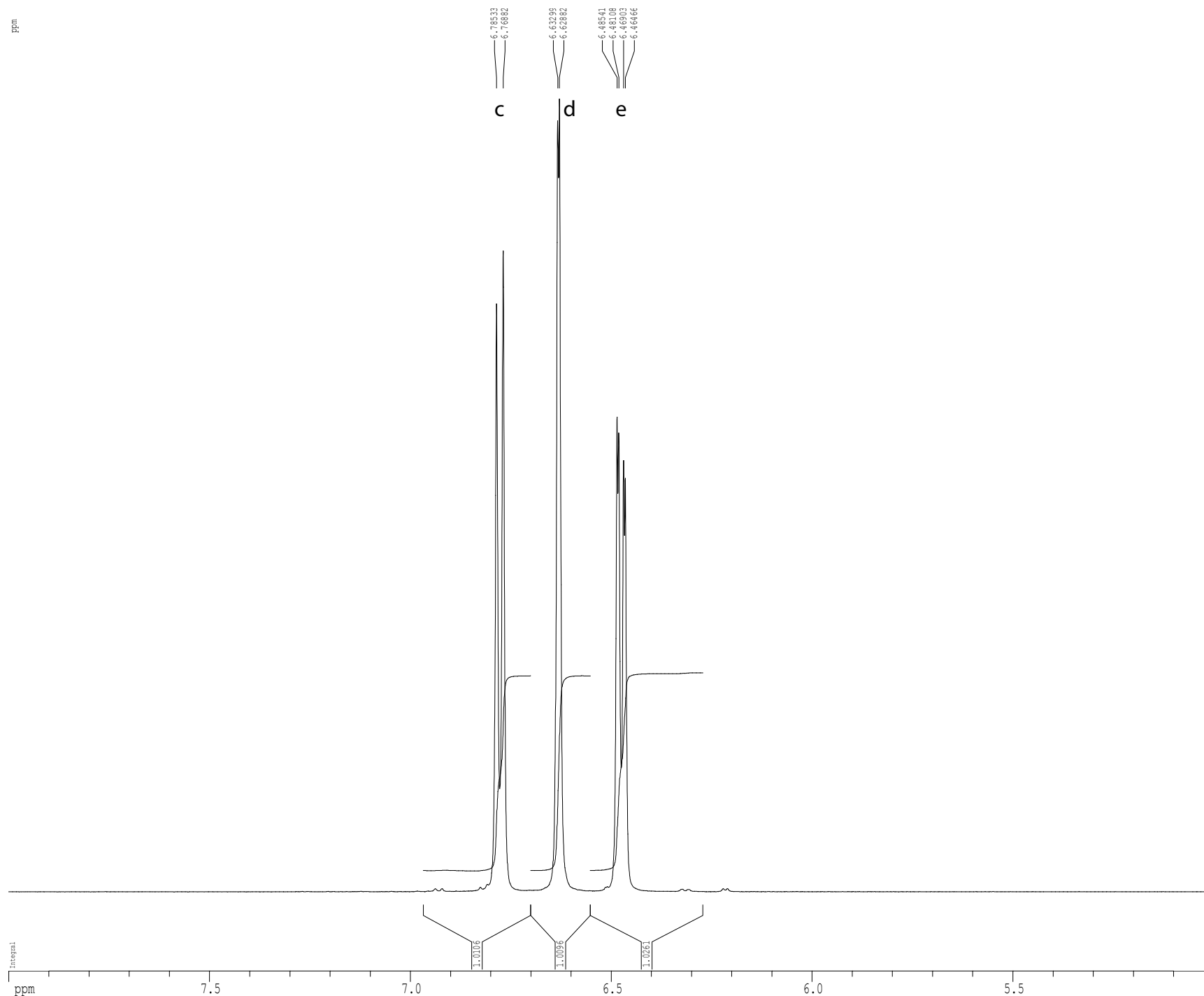
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 CY 15.00 cm
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 F1 6252.75 Hz
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 F2 0.00 Hz
 PPMCM 0.54825 ppm/cm
 HZCM 274.24344 Hz/cm

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		[Hz]	[PPM]	
1	11916.8	6033.402	12.0615	1.05
2	24764.0	4462.635	8.9213	1.14
3	33502.9	3394.156	6.7853	2.83
4	33570.5	3385.900	6.7688	3.09
5	34126.2	3317.953	6.6330	3.71
6	34143.2	3315.868	6.6288	3.81
7	34730.0	3244.133	6.4854	2.28
8	34747.7	3241.964	6.4811	2.21
9	34797.0	3235.939	6.4690	2.08
10	34814.9	3233.750	6.4647	1.99
11	47575.1	1673.612	3.3458	0.94
12	50084.0	1366.856	2.7325	0.79
13	50120.3	1362.419	2.7236	0.85
14	50215.2	1350.812	2.7004	1.43
15	50252.1	1346.310	2.6914	1.39
16	50497.2	1316.334	2.6315	0.70
17	50545.2	1310.467	2.6198	0.82
18	50602.4	1303.476	2.6058	0.87
19	50648.9	1297.789	2.5944	1.02
20	50733.8	1287.412	2.5737	0.53
21	51035.3	1250.549	2.5000	3.76
22	52514.6	1069.683	2.1384	1.32
23	52639.7	1054.379	2.1078	2.21
24	52760.1	1039.663	2.0784	1.65
25	52836.6	1030.312	2.0597	0.96
26	52903.0	1022.189	2.0435	1.21
27	52946.2	1016.906	2.0329	1.07
28	53381.7	963.659	1.9265	0.94
29	53496.1	949.678	1.8985	1.16
30	53559.7	941.897	1.8830	0.61
31	53619.0	934.643	1.8685	1.21
32	53662.3	929.350	1.8579	1.00
33	53726.9	921.450	1.8421	0.93
34	53769.1	916.296	1.8318	0.86
35	55002.1	765.547	1.5304	1.15
36	55114.9	751.746	1.5028	1.01
37	55349.5	723.060	1.4455	2.22
38	55446.3	711.236	1.4218	1.97
39	55997.3	643.857	1.2871	0.69
40	56024.8	640.503	1.2804	0.73
41	56105.5	630.634	1.2607	1.30
42	56131.8	627.420	1.2543	1.24
43	56213.2	617.463	1.2344	0.73
44	56240.3	614.153	1.2278	0.67
45	56363.3	599.119	1.1977	14.19
46	56968.7	525.093	1.0497	0.83
47	57002.3	520.980	1.0415	1.15
48	57061.9	513.704	1.0270	15.00
49	57184.9	498.664	0.9969	0.83
50	57215.5	494.915	0.9894	0.69

¹H spectrum

ppm



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PROCNO        1

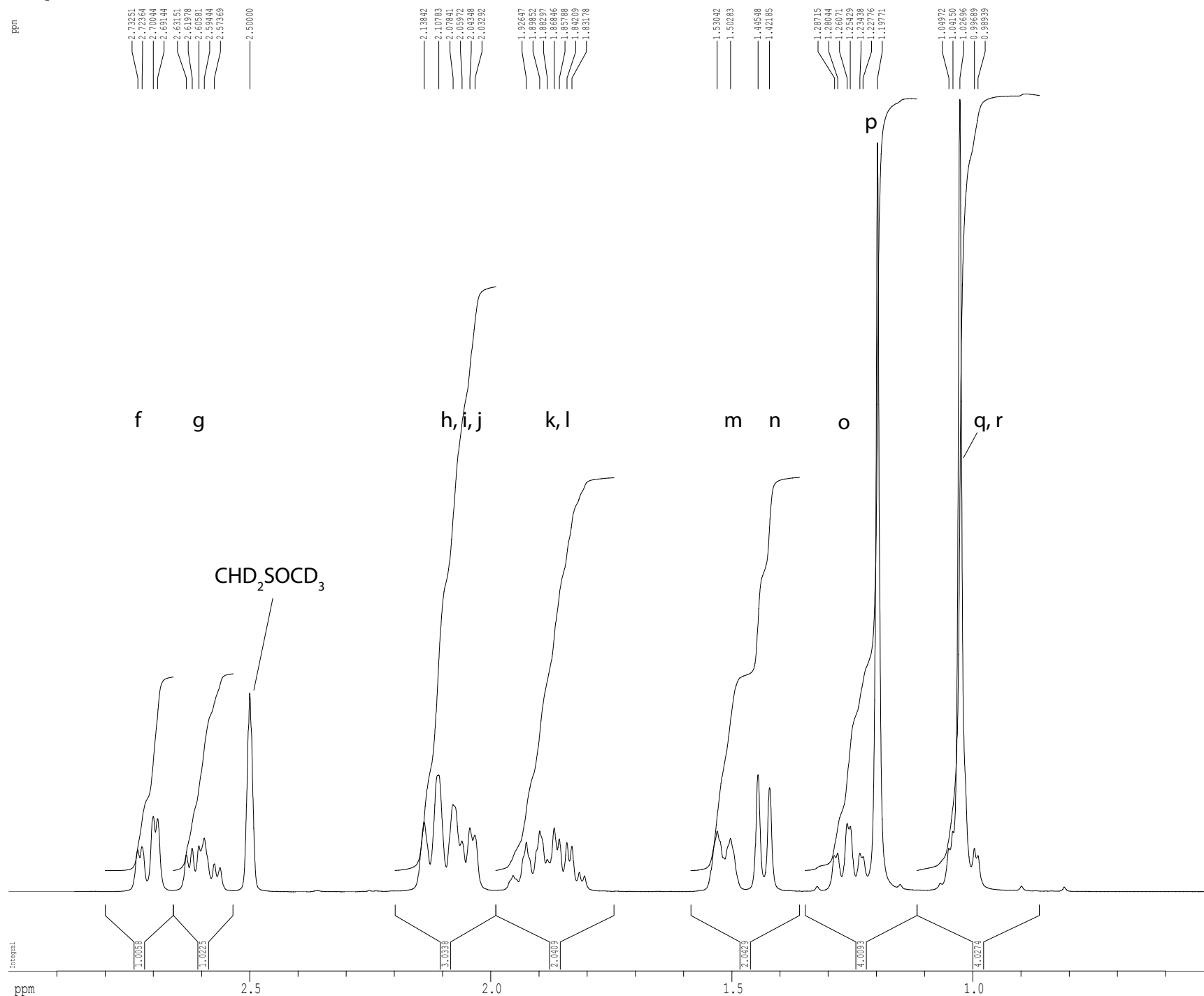
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FIDRES        0.062502 Hz
AQ            7.9998546 sec
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===== CHANNEL f1 =====
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PL1           1.60 dB
SF01          500.2235015 MHz

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           8.000 ppm
F1            4001.76 Hz
F2P           5.000 ppm
F2            2501.10 Hz
PPMCM         0.13158 ppm/cm
HZCM          65.81843 Hz/cm
    
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¹H spectrum



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Current Data Parameters
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NAME          partII B
EXPNO         21
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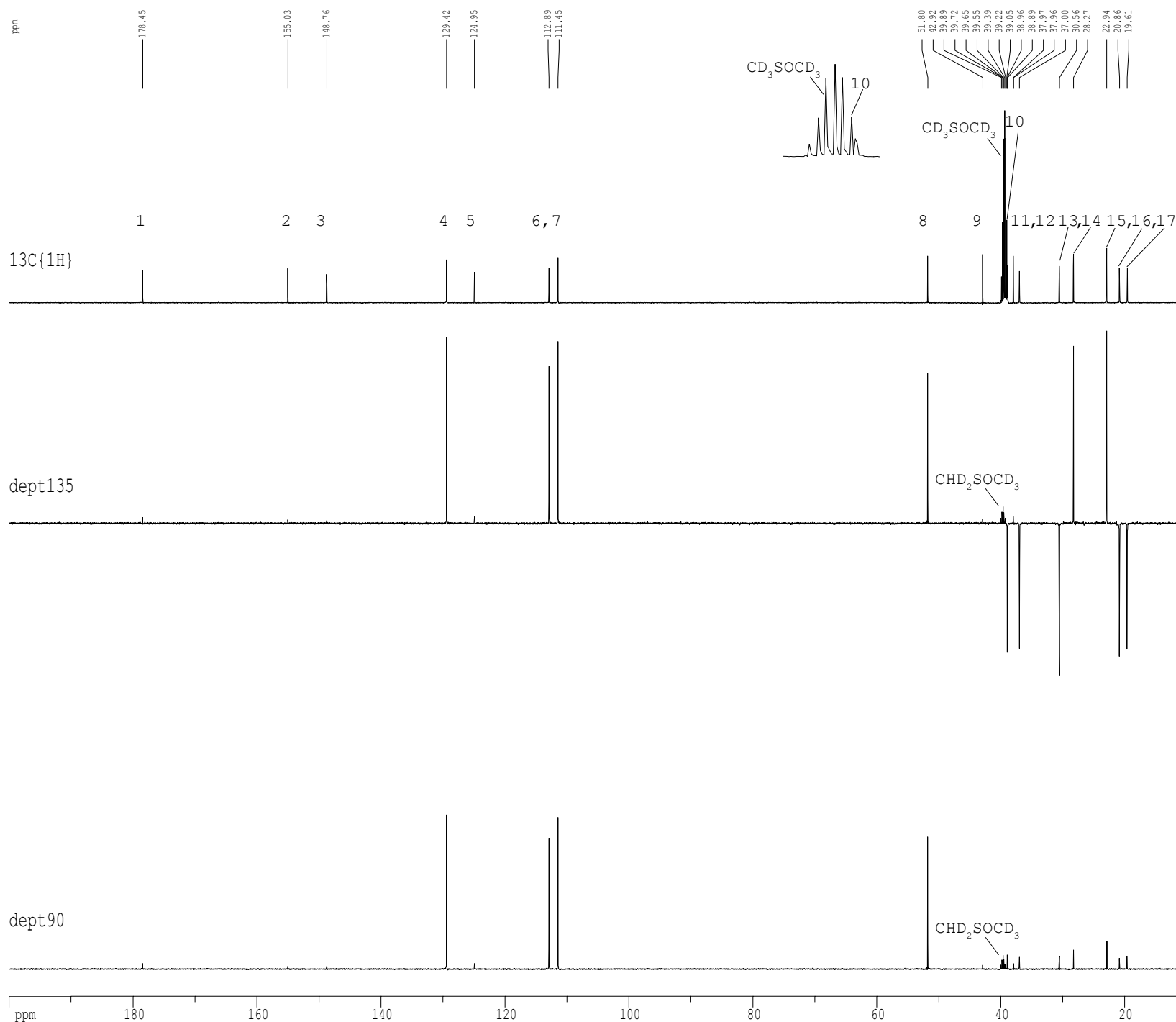
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PULPROG       zg30
TD            128202
SOLVENT       DMSO
NS            64
DS            2
SWH           8012.820 Hz
FIDRES        0.062502 Hz
AQ            7.9998546 sec
RG            4.5
DW            62.400 usec
DE            6.00 usec
TE            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            500.2200175 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           0.500 ppm
F2            250.11 Hz
PPMCM         0.10965 ppm/cm
HZCM          54.84869 Hz/cm
  
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Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters
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 SOLVENT DMSO
 NS 1024
 DS 16
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813940 sec
 RG 4597.6
 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
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 MCWRRK 0.01500000 sec
 P2 33.10 usec

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 P11 500.00 usec
 P12 2000.00 usec
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 PL1 -1.00 dB
 SFO1 125.7942548 MHz
 SF1 2.70 dB
 SF2 2.70 dB
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 SPNAM2 Crp60comp,4
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 SPOFF2 0.00 Hz

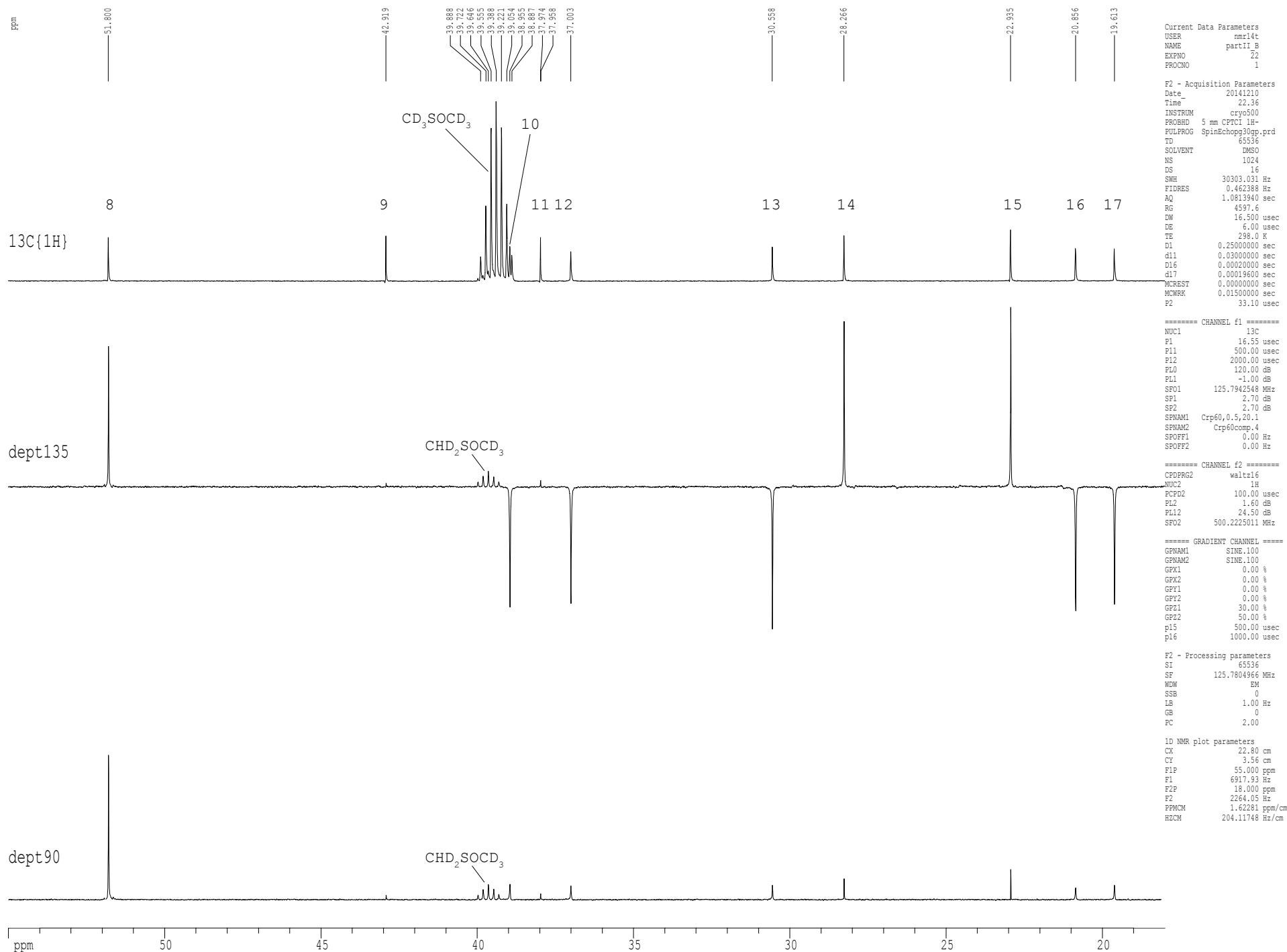
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 PL12 24.50 dB
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===== GRADIENT CHANNEL =====
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 GPT2 0.00 %
 GP21 30.00 %
 GP22 50.00 %
 p15 500.00 usec
 p16 1000.00 usec

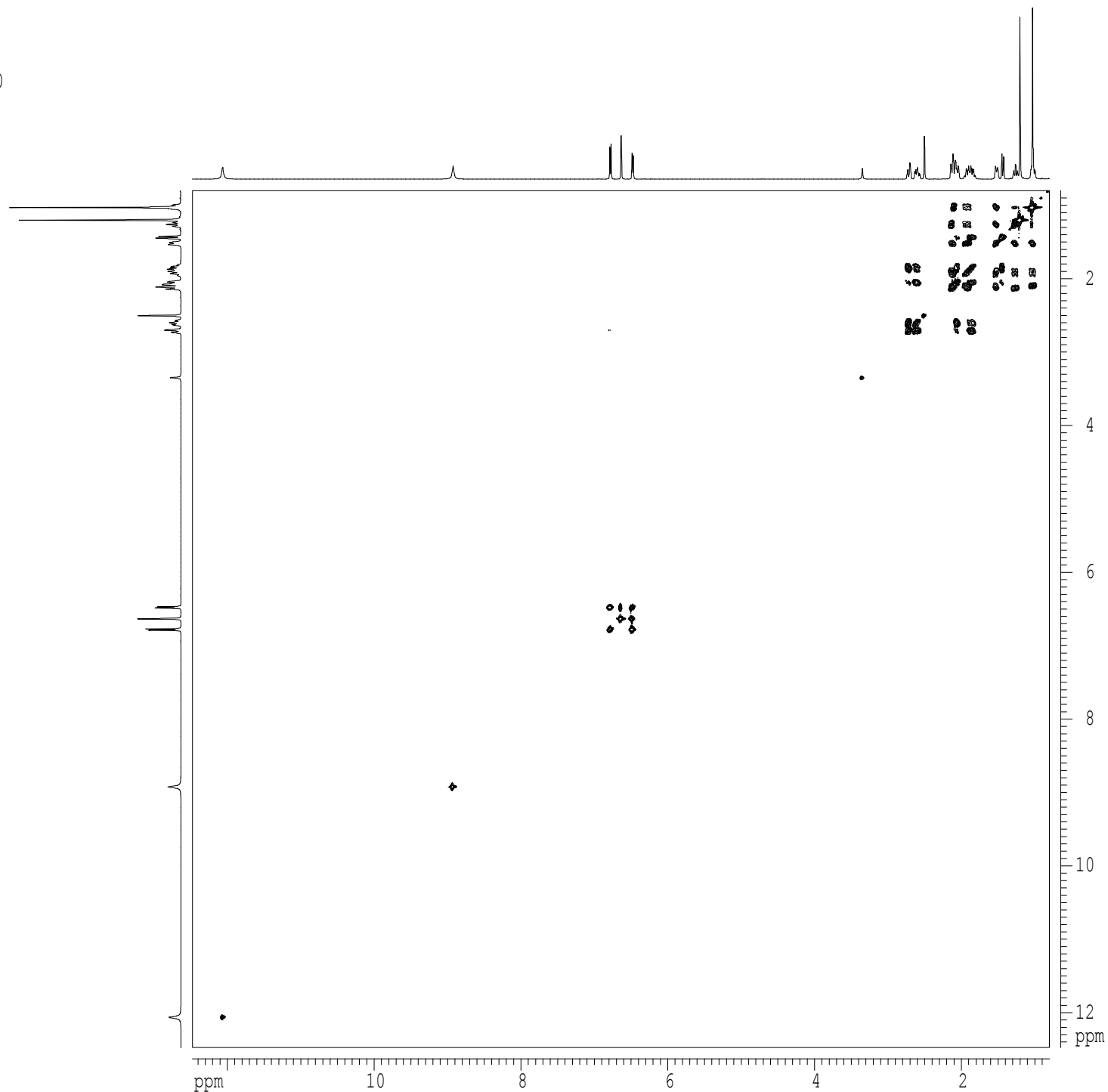
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1D NMR plot parameters
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 CY 3.56 cm
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 F1 25156.10 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 8.77193 ppm/cm
 HSCM 1103.33777 Hz/cm

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



gcosy60



Current Data Parameters
USER nmrl4t
NAME partII_B
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
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Time 22.58
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PROBHD 5 mm CPTCI 1H-
PULPROG cosygp60.prd
TD 2048
SOLVENT DMSO
NS 8
DS 16
SWH 6265.664 Hz
FIDRES 3.059406 Hz
AQ 0.1634804 sec
RG 5
DW 79.800 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
IN0 0.00015960 sec

===== CHANNEL f1 =====
NUC1 1H
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PL1 1.60 dB
SFO1 500.2231250 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

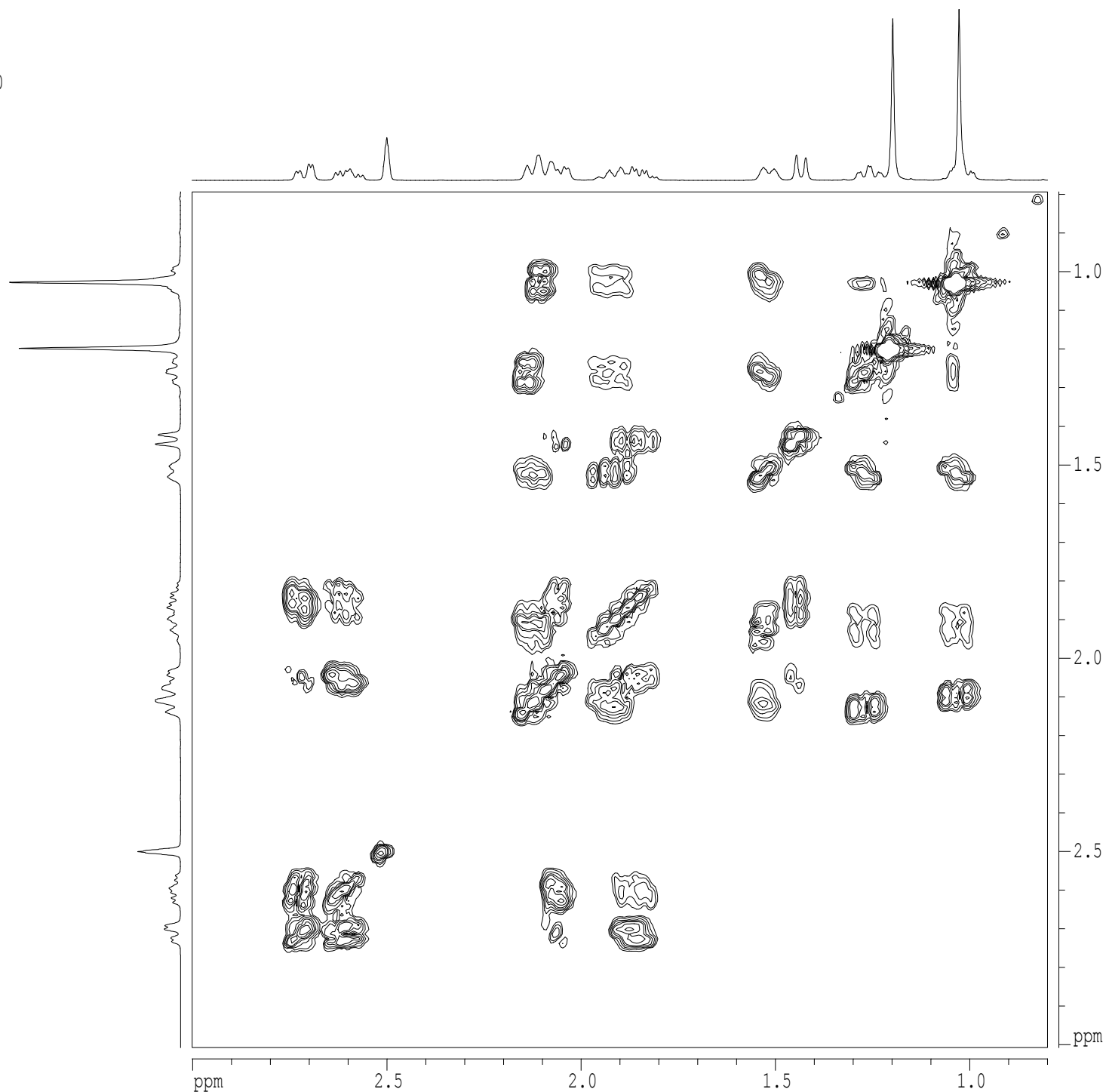
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SW 12.526 ppm
FnMODE undefined

F2 - Processing parameters
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SF 500.2200175 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.2200175 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 12.475 ppm
F2LO 6240.31 Hz
F2PHI 0.800 ppm
F2HI 400.18 Hz
F1PLO 12.475 ppm
F1LO 6240.31 Hz
F1PHI 0.800 ppm
F1HI 400.18 Hz
F2PPMCM 0.77834 ppm/cm
F2HZCM 389.34225 Hz/cm
F1PPMCM 0.77834 ppm/cm
F1HZCM 389.34225 Hz/cm

gcosy60



Current Data Parameters
 USER nmrl4t
 NAME partII B
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
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 Time 22.58
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 TD 2048
 SOLVENT DMSO
 NS 8
 DS 16
 SWH 6265.664 Hz
 FIDRES 3.059406 Hz
 AQ 0.1634804 sec
 RG 5
 DW 79.800 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
 IN0 0.00015960 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.2231250 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

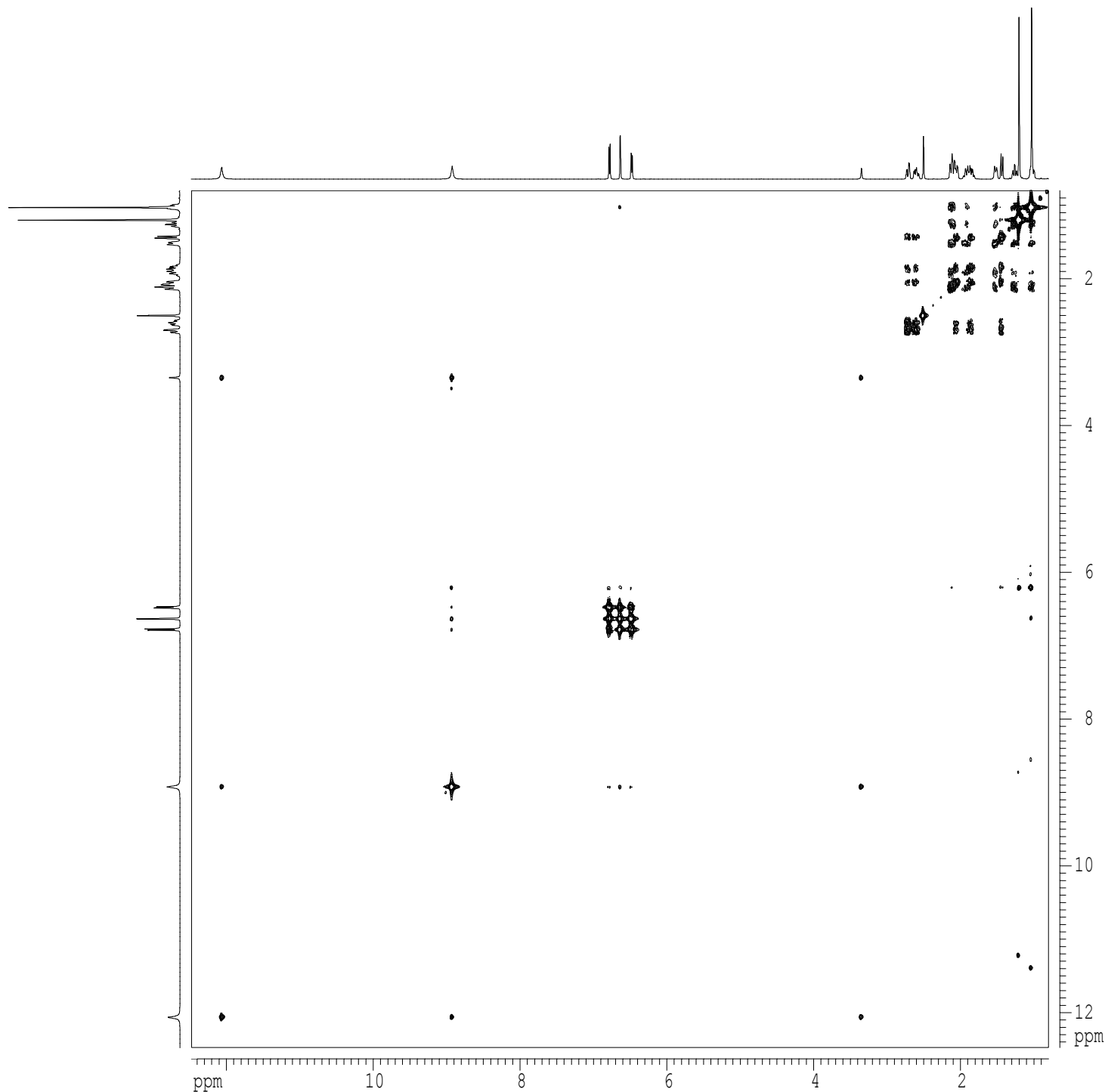
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 SW 12.526 ppm
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 SF 500.2200175 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
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 MC2 QF
 SF 500.2200175 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
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 CX1 15.00 cm
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 F2LO 1501.29 Hz
 F2PHI 0.799 ppm
 F2HI 399.90 Hz
 F1PLO 3.007 ppm
 F1LO 1504.35 Hz
 F1PHI 0.793 ppm
 F1HI 396.84 Hz
 F2PPMCM 0.14679 ppm/cm
 F2HZCM 73.42575 Hz/cm
 F1PPMCM 0.14760 ppm/cm
 F1HZCM 73.83368 Hz/cm

gtocsy



```
Current Data Parameters
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NAME      partII_B
EXPNO     6
PROCNO    1

F2 - Acquisition Parameters
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Time      0.21
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PULPROG   mlevpg mo
TD        2048
SOLVENT   DMSO
NS         8
DS        16
SWH        6265.664 Hz
FIDRES     3.059406 Hz
AQ         0.1634804 sec
RG         5
DW         79.800 usec
DE         6.00 usec
TE         298.0 K
d0         0.00000300 sec
d1         2.00000000 sec
d9         0.15000001 sec
d12        0.00002000 sec
d16        0.00020000 sec
FACTOR1    11
IN0        0.00015960 sec
l1         66
SCALEF     6

===== CHANNEL f1 =====
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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       500.2231250 MHz

===== GRADIENT CHANNEL =====
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GPNAM2     sine.100
GPX1       0.00 %
GPX2       0.00 %
GPT1       0.00 %
GPT2       0.00 %
GPE1       10.00 %
GPE2       10.00 %
P16        1000.00 usec

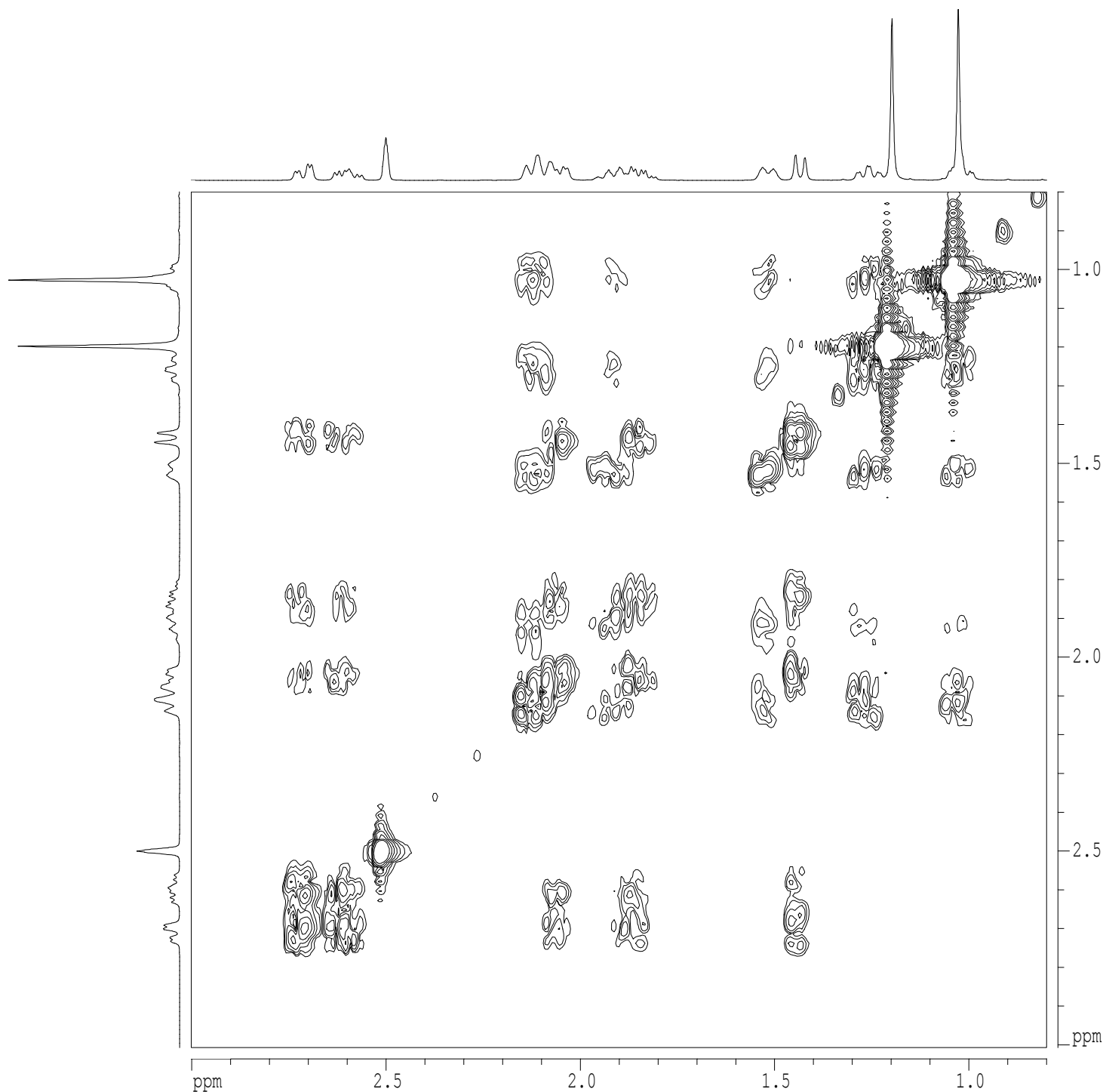
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FnMODE     undefined

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SF         500.2200175 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
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MC2        QF
SF         500.2200175 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0

2D NMR plot parameters
CX2        15.00 cm
CX1        15.00 cm
F2PLO      12.475 ppm
F2LO       6240.31 Hz
F2EHI      0.800 ppm
F2EHL      400.18 Hz
F1PLO      12.475 ppm
F1LO       6240.31 Hz
F1EHI      0.800 ppm
F1EHL      400.18 Hz
F2PPMCM    0.77834 ppm/cm
F2HZCM     389.34225 Hz/cm
F1PPMCM    0.77834 ppm/cm
F1HZCM     389.34225 Hz/cm
```

gtocsy



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Current Data Parameters
USER      nmrl4t
NAME      partII_B
EXPNO     6
PROCNO    1

F2 - Acquisition Parameters
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Time      0.21
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PULPROG   mlevpg mo
TD        2048
SOLVENT   DMSO
NS        8
DS        16
SWH       6265.664 Hz
FIDRES    3.059406 Hz
AQ        0.1634804 sec
RG        5
DW        79.800 usec
DE        6.00 usec
TE        298.0 K
d0        0.00000300 sec
D1        2.00000000 sec
D9        0.15000001 sec
d12       0.00002000 sec
D16       0.00020000 sec
FACTOR1   11
IN0       0.00015960 sec
l1        66
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      500.2231250 MHz

===== GRADIENT CHANNEL =====
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GPNAM2    sine.100
GPX1      0.00 %
GPX2      0.00 %
GPT1      0.00 %
GPT2      0.00 %
GPT1      10.00 %
GPT2      10.00 %
P16       1000.00 usec

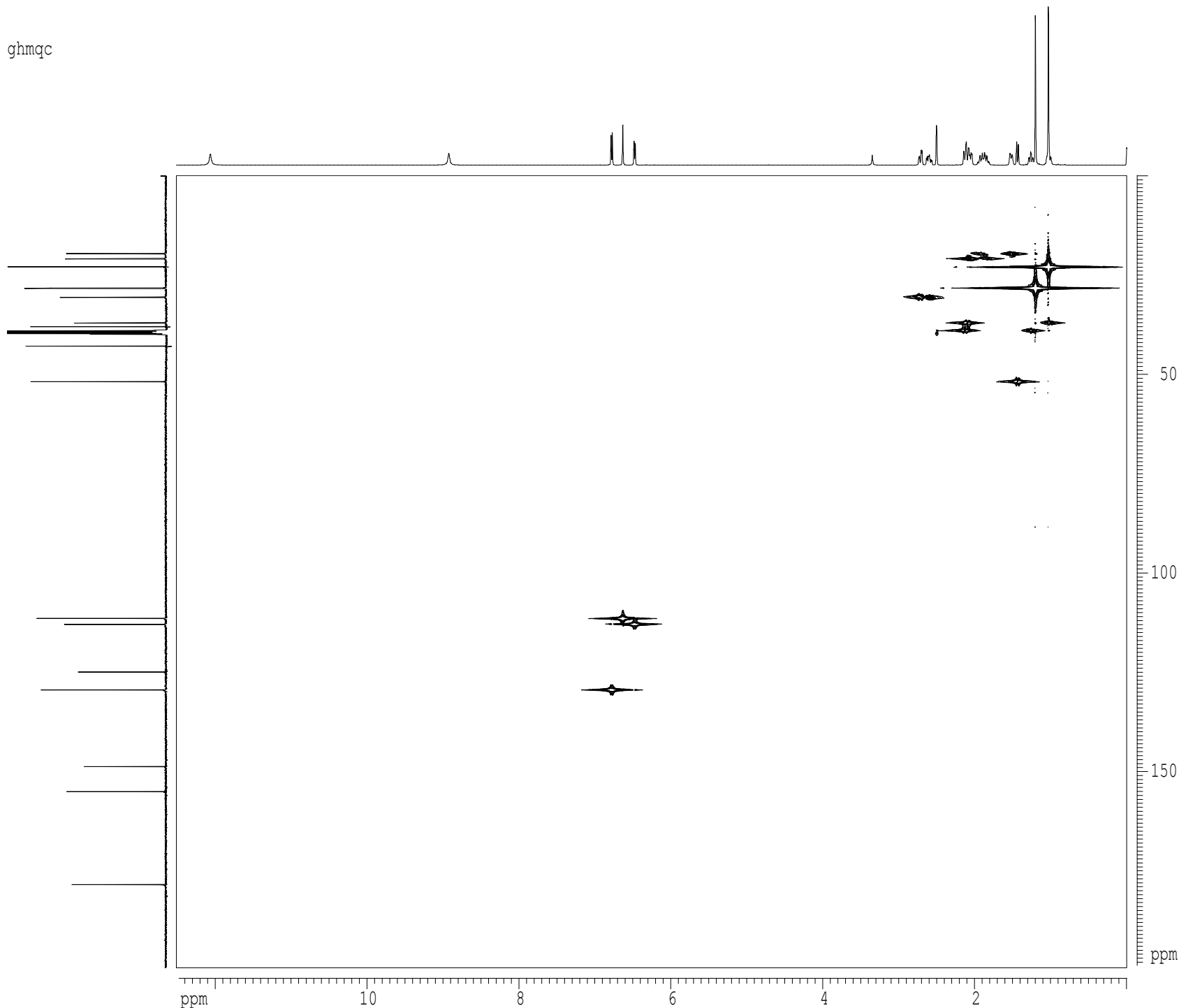
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SW        12.526 ppm
FnMODE    undefined

F2 - Processing parameters
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SF        500.2200175 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
MC2       QF
SF        500.2200175 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0

2D NMR plot parameters
CX2       15.00 cm
CX1       15.00 cm
F2PLO     3.001 ppm
F2LO      1501.29 Hz
F2PHI     0.800 ppm
F2HT      400.18 Hz
F1PLO     3.007 ppm
F1LO      1504.35 Hz
F1PHI     0.800 ppm
F1HT      400.18 Hz
F2PPMCM   0.14675 ppm/cm
F2HZCM    73.40756 Hz/cm
F1PPMCM   0.14716 ppm/cm
F1HZCM    73.61153 Hz/cm
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ghmqc



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Current Data Parameters
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NAME      partII B
EXPNO     25
PROCNO    1

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PULPROG   inv4gp.wu
TD         2048
SOLVENT   DMSO
NS         8
DS         16
SWH        6265.664 Hz
FIDRES     3.059406 Hz
AQ         0.1634804 sec
RG         4000
DW         79.800 usec
DE         6.50 usec
TE         298.0 K
CNS2       145.0000000
d0         0.00000300 sec
d1         1.00000000 sec
d2         0.00344828 sec
d12        0.0002000 sec
d13        0.00000300 sec
d16        0.00020000 sec
d20        0.00242528 sec
IN0        0.00001988 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
P2         15.00 usec
PL1        1.60 dB
SFO1       500.2231250 MHz

===== CHANNEL f2 =====
CPDPRG2    garp
NUC2       13C
P3         15.50 usec
PCPD2      65.00 usec
PL2        -1.00 dB
PL12       11.30 dB
SFO2       125.7929190 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

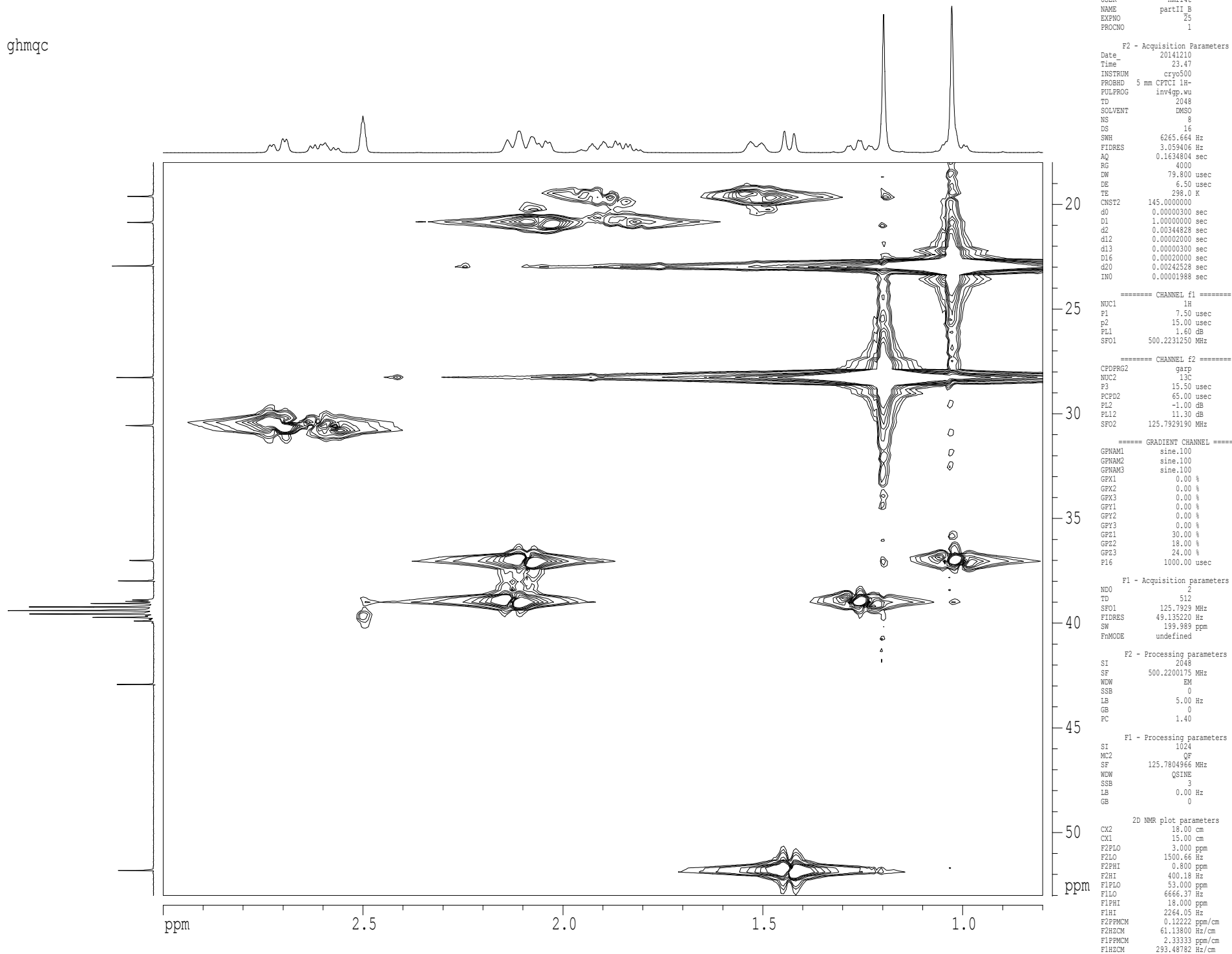
F1 - Acquisition parameters
ND0        2
TD          512
SFO1       125.7929 MHz
FIDRES     49.135220 Hz
SW         199.989 ppm
FhMODE     undefined

F2 - Processing parameters
SI          2048
SF          500.2200175 MHz
WDW         EM
SSB         0
LB          5.00 Hz
GB          0
PC          1.40

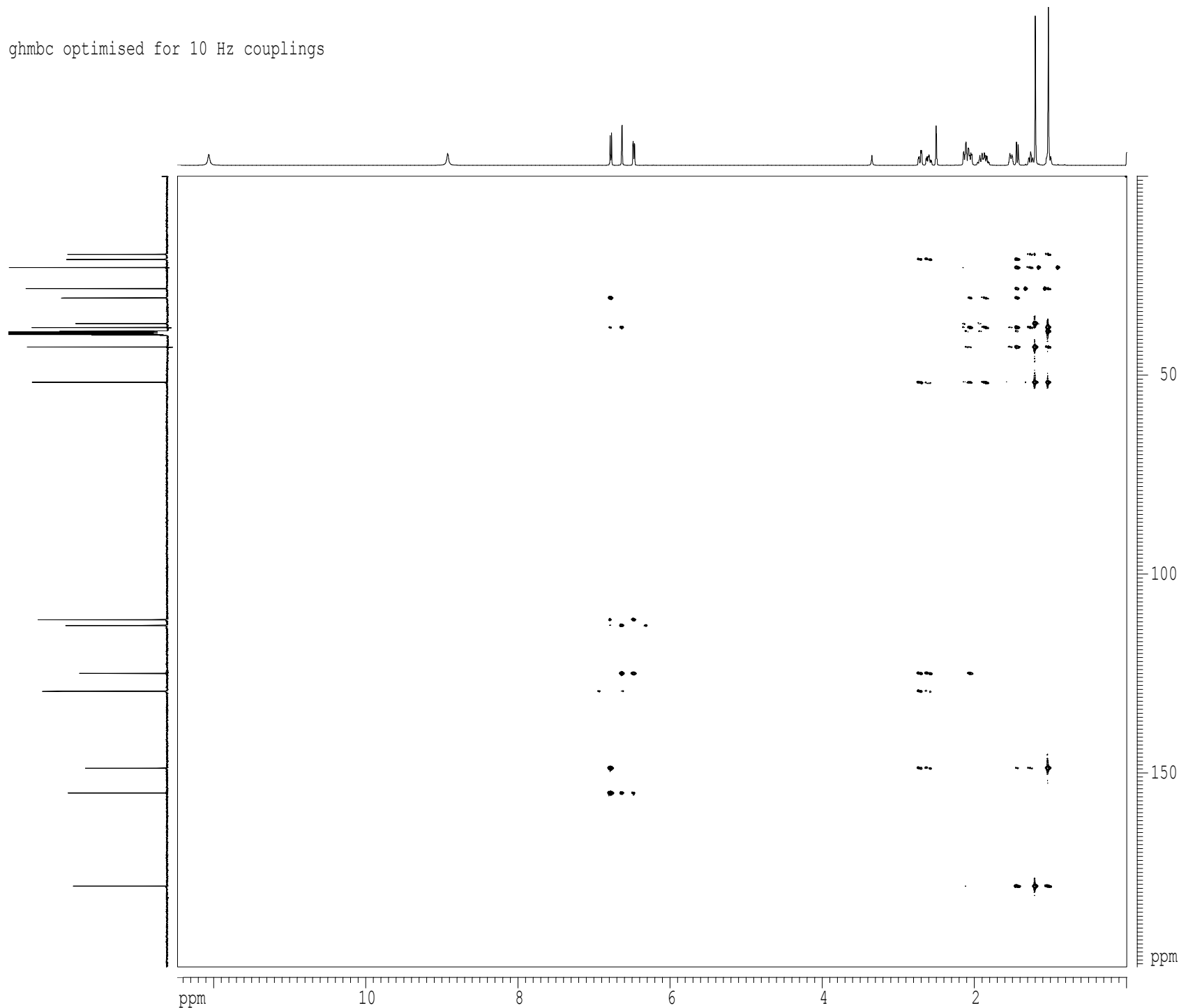
F1 - Processing parameters
SI          1024
MC2         QF
SF          125.7804966 MHz
WDW         QSINE
SSB         3
LB          0.00 Hz
GB          0

2D NMR plot parameters
CX2         18.00 cm
CX1         15.00 cm
F2PL0       12.510 ppm
F2LO        6257.83 Hz
F2PHI       -0.003 ppm
F2HI        -1.71 Hz
F1PL0       199.384 ppm
F1LO        25078.63 Hz
F1PHI       -0.039 ppm
F1HI        -4.92 Hz
F2PPMCM     0.69520 ppm/cm
F2HZCM      347.75256 Hz/cm
F1PPMCM     13.29488 ppm/cm
F1HZCM      1672.23633 Hz/cm
```

ghmqc



ghmbc optimised for 10 Hz couplings



```
Current Data Parameters
USER      nmr14t
NAME      partII_B
EXPNO     26
PROCNO    1

F2 - Acquisition Parameters
Date_     20141211
Time      1.09
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   ghmbc.wu
TD         4096
SOLVENT   DMSO
NS         8
DS         16
SWH        6265.664 Hz
FIDRES     1.529703 Hz
AQ         0.3269108 sec
RG         4000
DW         79.800 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        0.00001988 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
P2         15.00 usec
PL1        1.60 dB
SFO1       500.2231250 MHz

===== CHANNEL F2 =====
NUC2       13C
P3         15.50 usec
PL2        -1.00 dB
SFO2       125.7929190 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

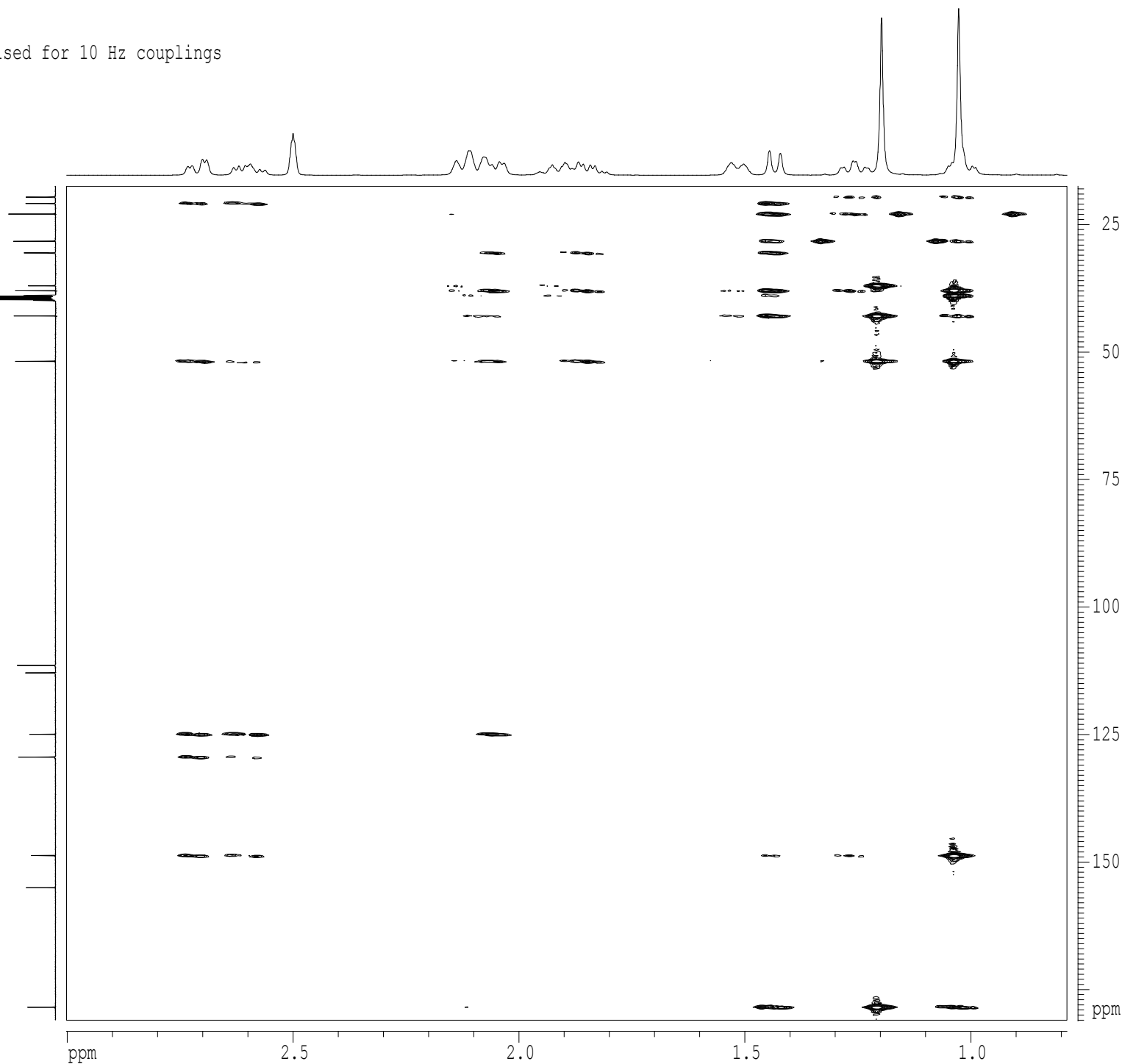
F1 - Acquisition parameters
ND0        2
TD          512
SFO1       125.7929 MHz
FIDRES     49.135220 Hz
SW         199.989 ppm
FnMODE     undefined

F2 - Processing parameters
SI         2048
SF         500.2200175 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        QF
SF         125.7804966 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0

2D NMR plot parameters
CX2        18.00 cm
CX1        15.00 cm
F2PLO      12.475 ppm
F2LO       6240.31 Hz
F2PHI      -0.002 ppm
F2HI       -0.88 Hz
F1PLO      198.767 ppm
F1LO       25001.01 Hz
F1PHI      -0.070 ppm
F1HI       -8.82 Hz
F2PPMCM    0.69316 ppm/cm
F2HZCM     346.73273 Hz/cm
F1PPMCM    13.25581 ppm/cm
F1HZCM     1667.32190 Hz/cm
```

ghmbc optimised for 10 Hz couplings



```
Current Data Parameters
USER      nmrl4t
NAME      partII B
EXPNO     26
PROCNO    1

F2 - Acquisition Parameters
Date_     20141211
Time      1.09
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   ghmbc.wu
TD         4096
SOLVENT   DMSO
NS         8
DS         16
SWH        6265.664 Hz
FIDRES     1.529703 Hz
AQ         0.3269108 sec
RG         4000
DW         79.800 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        0.00001988 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
p2         15.00 usec
PL1        1.60 dB
SFO1       500.2231250 MHz

===== CHANNEL f2 =====
NUC2       13C
P3         15.50 usec
PL2        -1.00 dB
SFO2       125.7929190 MHz

===== GRADIENT CHANNEL =====
GPNAM1     sine.100
GPNAM2     sine.100
GPNAM3     sine.100
GPX1       0.00 %
GPX2       0.00 %
GPX3       0.00 %
GPV1       0.00 %
GPV2       0.00 %
GPV3       0.00 %
GPZ1       50.00 %
GPZ2       30.00 %
GPZ3       40.00 %
P16        1000.00 usec

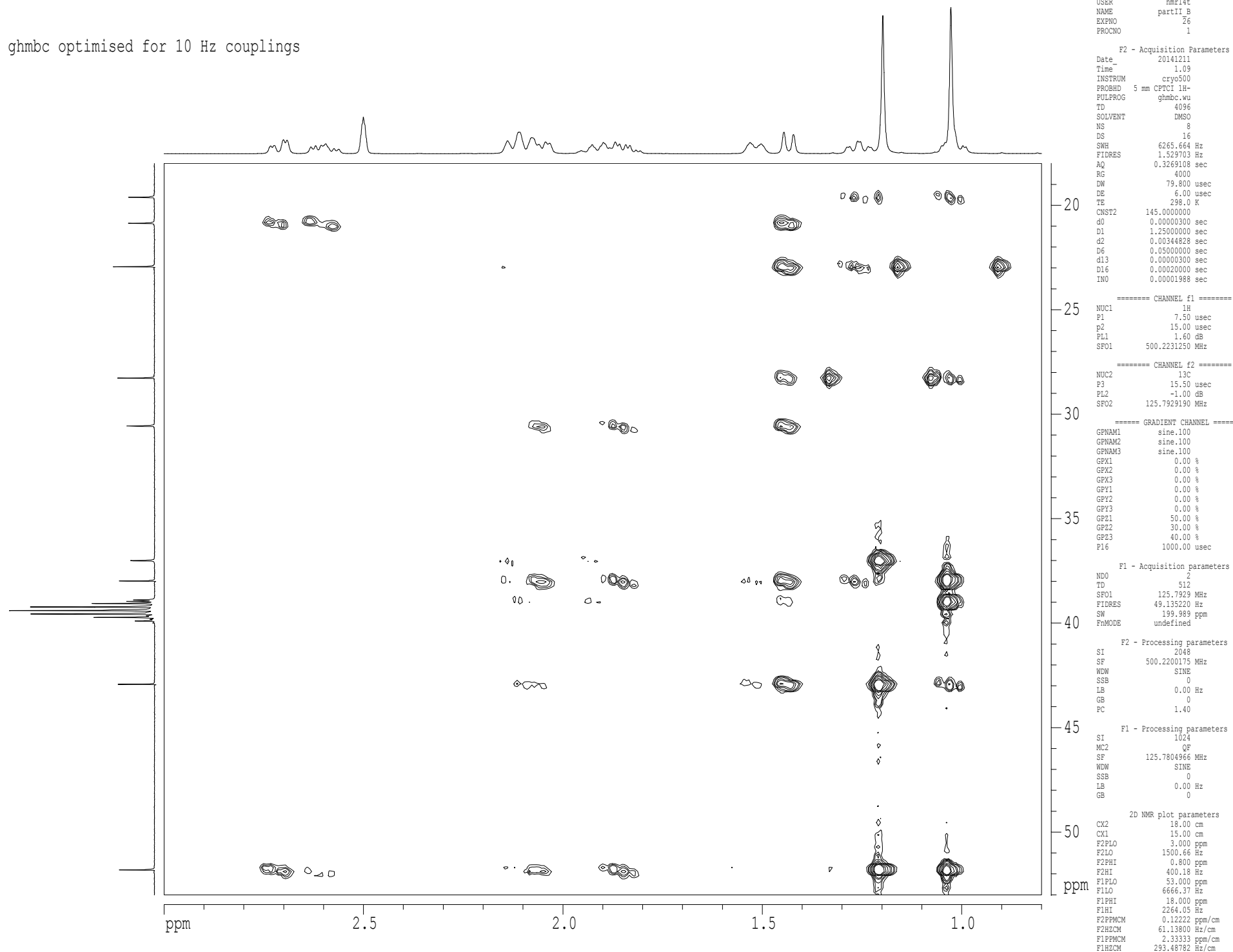
F1 - Acquisition parameters
ND0        2
TD         512
SFO1       125.7929 MHz
FIDRES     49.135220 Hz
SW         199.989 ppm
FhMODE     undefined

F2 - Processing parameters
SI         2048
SF         500.2200175 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

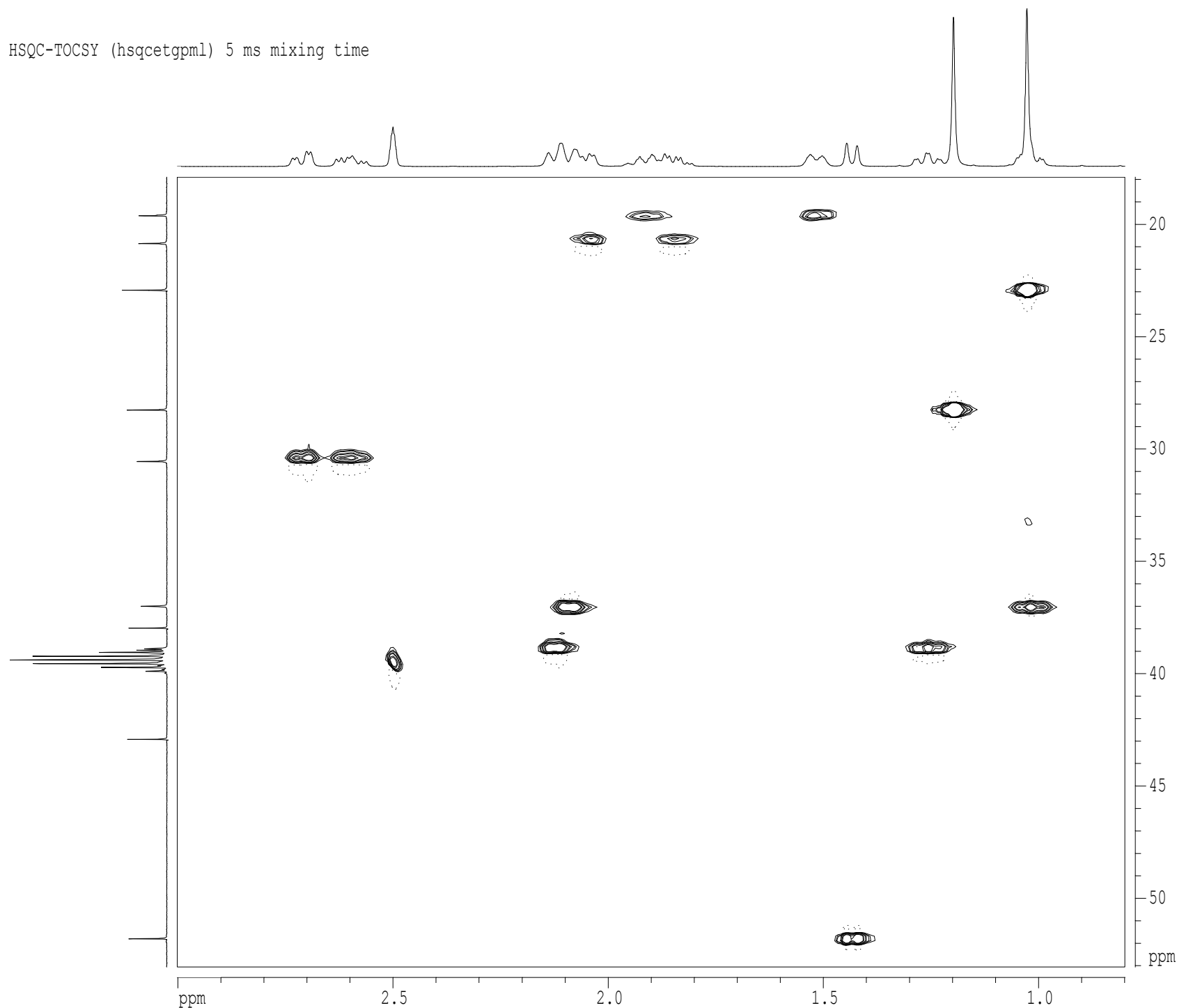
F1 - Processing parameters
SI         1024
MC2        QF
SF         125.7804966 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0

2D NMR plot parameters
CX2        18.00 cm
CX1        15.00 cm
F2PLO      3.001 ppm
F2LO       1501.29 Hz
F2PHI      0.787 ppm
F2HI       393.78 Hz
F1PLO      181.000 ppm
F1LO       22766.27 Hz
F1PHI      17.509 ppm
F1HI       2202.27 Hz
F2PPMCM    0.12300 ppm/cm
F2HZCM     61.52806 Hz/cm
F1PPMCM    10.89941 ppm/cm
F1HZCM     1370.93335 Hz/cm
```

ghmbc optimised for 10 Hz couplings



HSQC-TOCSY (hsgcetgpml) 5 ms mixing time



```

Current Data Parameters
USER      rnr14t
NAME      part11 B
EXFNO     28
PROCNO    1

F2 - Acquisition Parameters
Date_     20141211
Time      4.52
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   hsgcetgpml
TD         2048
SOLVENT   DMSO
NS         2
DS         32
SWH        6265.664 Hz
FIDRES     3.059406 Hz
AQ         0.1634804 sec
RG         500
DW         79.800 usec
DE         6.50 usec
TE         298.0 K
CNST2     145.0000000
d0         0.00000300 sec
d1         2.00000000 sec
d4         0.00172414 sec
d9         0.00500000 sec
d11        0.03000000 sec
d12        0.00002000 sec
d13        0.00000400 sec
d16        0.00020000 sec
DELTA      0.0012100 sec
DELTA1     0.00120800 sec
FACTOR1    0
IN0        0.00001988 sec
I1         11
MCREST     0.0000000 sec
MCWRK      0.40000001 sec
SCALEF     6
STICNT     256

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
p2         15.00 usec
p5         23.34 usec
p6         35.00 usec
p7         70.00 usec
P17        2500.00 usec
P28        1000.00 usec
PL1        1.60 dB
PL10       15.20 dB
SFO1       500.2231250 MHz

===== CHANNEL f2 =====
CPDPRG2    98rp
NUC2       13C
P3         15.50 usec
p4         31.00 usec
PCPD2      65.00 usec
PL2        -1.00 dB
PL12       11.30 dB
SFO2       125.7929190 MHz

===== GRADIENT CHANNEL =====
GPRM1      SINE.100
GPRM2      SINE.100
GPX1       0.00 %
GPX2       0.00 %
GPY1       0.00 %
GPY2       0.00 %
GZF1       80.00 %
GPF2       20.10 %
P16        1000.00 usec

F1 - Acquisition parameters
ND0        2
TD         512
SFO1       125.7929 MHz
FIDRES     49.135220 Hz
SW         199.989 ppm
FhMODE     Echo-Antiecho

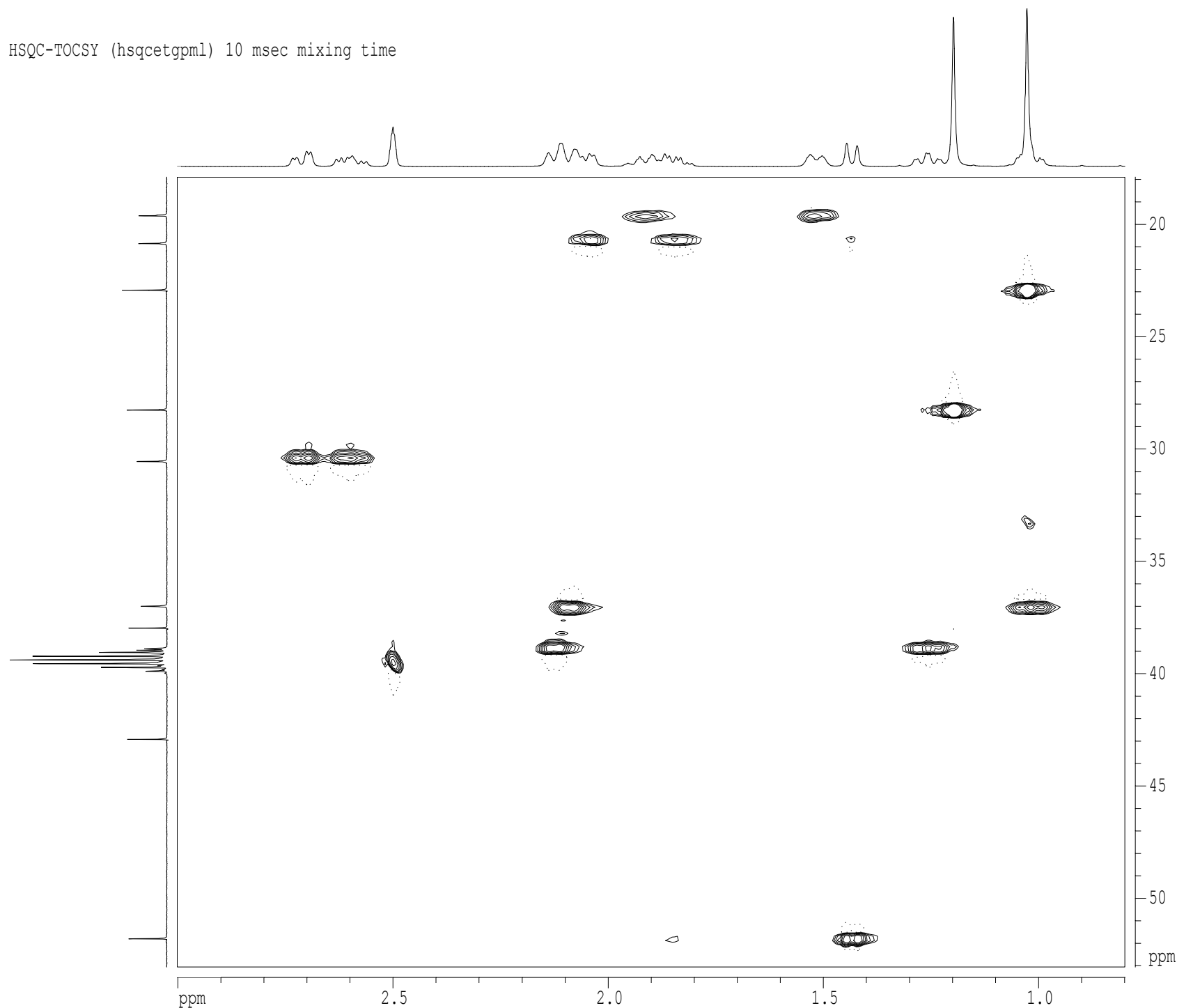
F2 - Processing parameters
SI         2048
SF         500.2200175 MHz
WDW        EM
SSB        0
LB         5.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        echo-antiecho
SF         125.7804966 MHz
WDW        Q8SINE
SSB        3
LB         0.00 Hz
GB         0

2D NMR plot parameters
CX2        18.00 cm
CX1        15.00 cm
F2PLO      3.001 ppm
F2PLO      1501.29 Hz
F2PHI      0.799 ppm
F2HI       399.90 Hz
F1PLO      53.057 ppm
F1LO       6673.58 Hz
F1HI       17.899 ppm
F1HI       2251.41 Hz
F2PVMCM    0.12232 ppm/cm
F2HZCM     61.18813 Hz/cm
F1PVMCM    2.34386 ppm/cm
F1HZCM     294.81131 Hz/cm

```

HSQC-TOCSY (hsgcetgpml) 10 msec mixing time



```

Current Data Parameters
USER      nmrl4t
NAME      part11 B
EXFNO     29
PROCNO    1

F2 - Acquisition Parameters
Date_     20141211
Time      5.31
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   hsgcetgpml
TD         2048
SOLVENT   DMSO
NS         2
DS         32
SWH        6265.664 Hz
FIDRES     3.059406 Hz
AQ         0.1634804 sec
RG         500
DW         79.800 usec
DE         6.50 usec
TE         298.0 K
CNST2     145.0000000
d0         0.0000300 sec
d1         2.0000000 sec
d4         0.00172414 sec
d9         0.0100000 sec
d11        0.0300000 sec
d12        0.0002000 sec
d13        0.0000400 sec
d16        0.0002000 sec
DELTA      0.0012100 sec
DELTA1     0.00120800 sec
FACTOR1    0
IN0        0.0001988 sec
I1         11
MCREST     0.0000000 sec
MCWRK      0.4000001 sec
SCALEF     6
STICNT     256

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
p2         15.00 usec
p5         23.34 usec
p6         35.00 usec
p7         70.00 usec
P17        2500.00 usec
P28        1000.00 usec
PL1        1.60 dB
PL10       15.20 dB
SFO1       500.2231250 MHz

===== CHANNEL f2 =====
CPDPRG2    98rp
NUC2       13C
P3         15.50 usec
p4         31.00 usec
PCPD2      65.00 usec
PL2        -1.00 dB
PL12       11.30 dB
SFO2       125.7929190 MHz

===== GRADIENT CHANNEL =====
GPRM1      SINE.100
GPRM2      SINE.100
GPX1       0.00 %
GPX2       0.00 %
GPY1       0.00 %
GPY2       0.00 %
GZF1       80.00 %
GPF2       20.10 %
P16        1000.00 usec

F1 - Acquisition parameters
ND0        2
TD          512
SFO1       125.7929 MHz
FIDRES     49.135220 Hz
SW         199.989 ppm
FhMODE     Echo-Antiecho

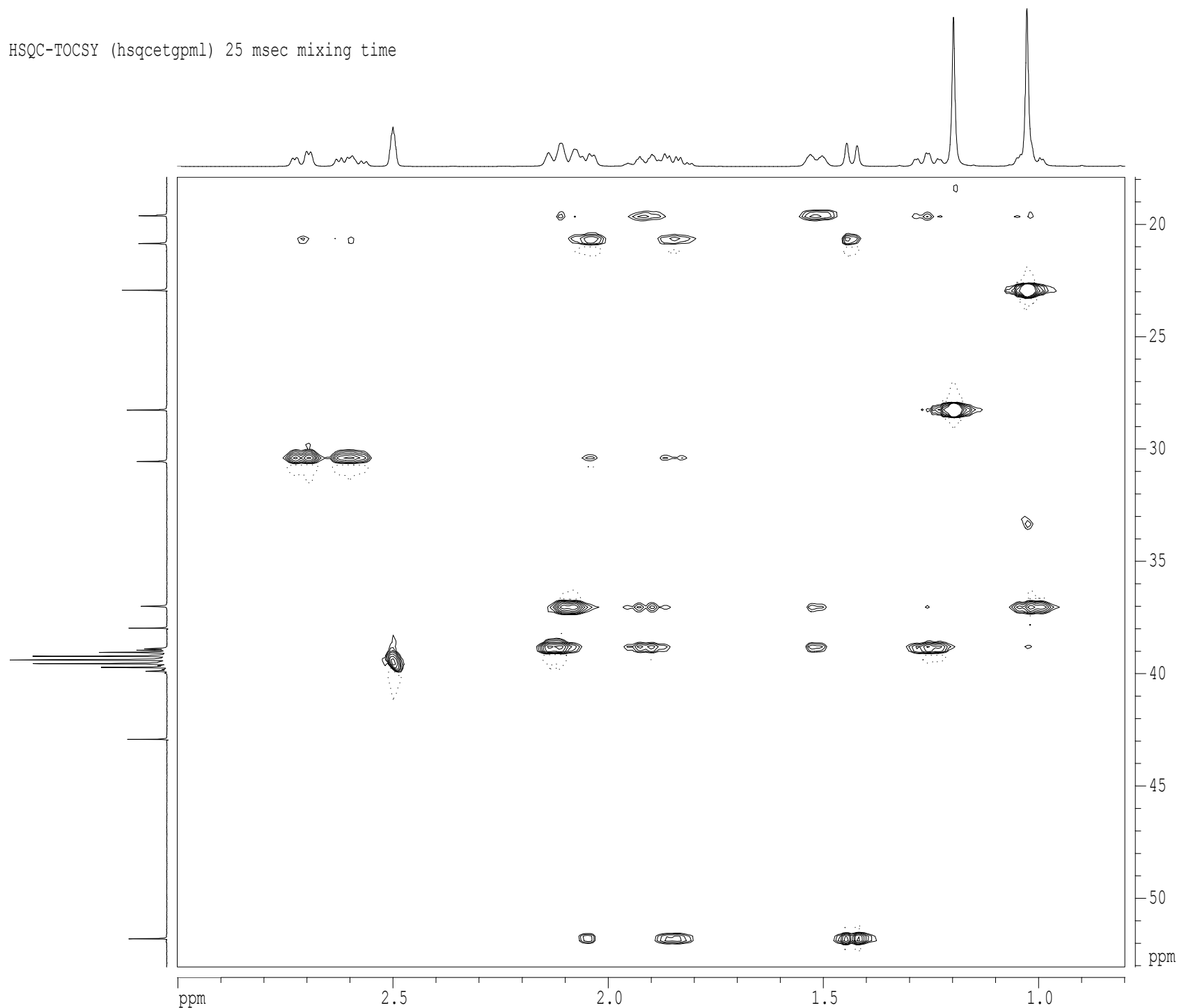
F2 - Processing parameters
SI          2048
SF          500.2200175 MHz
EN          0
SSB         0
LB          5.00 Hz
GB          0
PC          1.40

F1 - Processing parameters
SI          1024
MC2         echo-antiecho
SF          125.7804966 MHz
WDW         Q8SINE
SSB         3
LB          0.00 Hz
GB          0

2D NMR plot parameters
CX2         18.00 cm
CX1         15.00 cm
F2PLO       3.001 ppm
F2PLO       1501.29 Hz
F2PHI       0.799 ppm
F2H1        399.90 Hz
F1PLO       53.057 ppm
F1LO        6673.58 Hz
F1PHI       17.899 ppm
F1H1        2251.41 Hz
F2P2MCM     0.12232 ppm/cm
F2H2CM      61.18813 Hz/cm
F1P2MCM     2.34386 ppm/cm
F1H2CM      294.81131 Hz/cm

```

HSQC-TOCSY (hsgcetgpml) 25 msec mixing time



Current Data Parameters

USER	nmr14t
NAME	part11 B
EXFNO	30
PROCNO	1

F2 - Acquisition Parameters

Date_	20141211
Time	6.10
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	hsgcetgpml
TD	2048
SOLVENT	DMSO
NS	2
DS	32
SWH	6265.664 Hz
FIDRES	3.059406 Hz
AQ	0.1634804 sec
RG	500
DW	79.800 usec
DE	6.50 usec
TE	298.0 K
CNST2	145.0000000
d0	0.00000300 sec
d1	2.00000000 sec
d4	0.00172414 sec
d9	0.02500000 sec
d11	0.03000000 sec
d12	0.00002000 sec
d13	0.00000400 sec
d16	0.00020000 sec
DELTA	0.00121000 sec
DELTA1	0.00120800 sec
FACTOR1	1
INO	0.00001988 sec
l1	
MCREST	0.00000000 sec
MCWRK	0.40000001 sec
SCALEF	6
STICNT	256

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

NUC1	1H
P1	7.50 usec
p2	15.00 usec
p5	23.34 usec
p6	35.00 usec
p7	70.00 usec
P17	2500.00 usec
P28	1000.00 usec
PL1	1.60 dB
PL10	15.20 dB
SFO1	500.2231250 MHz

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

CPDPRG2	gafp
NUC2	13C
F3	15.50 usec
p4	31.00 usec
PCPD2	65.00 usec
PL2	-1.00 dB
PL12	11.30 dB
SFO2	125.7929190 MHz

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

GPRM1	SINE.100
GPRM2	SINE.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	80.00 %
GPZ2	20.10 %
P16	1000.00 usec

f1 - Acquisition parameters

ND0	2
TD	512
SFO1	125.7929 MHz
FIDRES	49.135220 Hz
SW	199.989 ppm
FHMODE	Echo-Antiecho

F2 - Processing parameters

SI	2048
SF	500.2200175 MHz
WDW	EM
SSB	0
LB	5.00 Hz
GB	0
PC	1.40

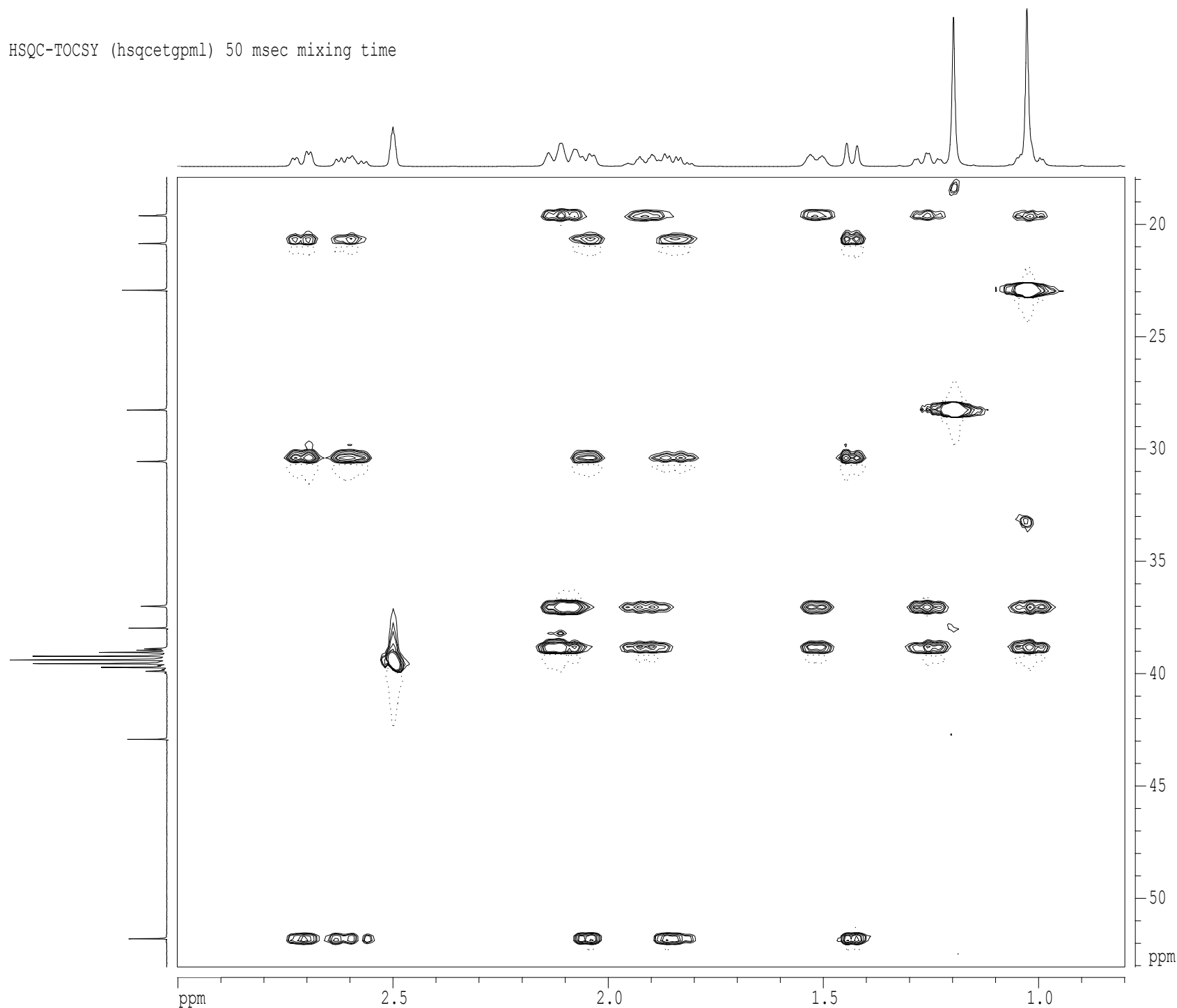
f1 - Processing parameters

SI	1024
MC2	echo-antiecho
SF	125.7804966 MHz
WDW	Q8SINE
SSB	3
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	18.00 cm
CX1	15.00 cm
F2PLO	3.001 ppm
F2PLO	1501.29 Hz
F2PHI	0.799 ppm
F2HI	399.90 Hz
F1PLO	53.057 ppm
F1LO	6673.58 Hz
F1HI	17.899 ppm
F1HI	2251.41 Hz
F2PFCM	0.12232 ppm/cm
F2HFCM	61.18813 Hz/cm
F1PFCM	2.34386 ppm/cm
F1HFCM	294.81131 Hz/cm

HSQC-TOCSY (hsgcetgpm1) 50 msec mixing time



```

Current Data Parameters
USER      nmrl4t
NAME      part11 B
EXPNO     31
PROCNO    1

F2 - Acquisition Parameters
Date_     20141211
Time      6.49
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   hsgcetgpm1
TD        2048
SOLVENT   DMSO
NS         2
DS         32
SWH        6265.664 Hz
FIDRES     3.059406 Hz
AQ         0.1634804 sec
RG         500
DW         79.800 usec
DE         6.50 usec
TE         298.0 K
CNST2     145.0000000
d0         0.00000300 sec
d1         2.00000000 sec
d4         0.00172414 sec
d9         0.05000000 sec
d11        0.03000000 sec
d12        0.00002000 sec
d13        0.00000400 sec
d16        0.00020000 sec
DELTA     0.00122100 sec
DELTA1    0.00120800 sec
FACTOR1    3
IN0        0.00001988 sec
l1         18
MCREST     0.00000000 sec
MCWRK     0.40000001 sec
SCALEF     6
STICNT     256

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
p2         15.00 usec
p5         23.34 usec
p6         35.00 usec
p7         70.00 usec
P17        2500.00 usec
P28        1000.00 usec
PL1        1.60 dB
PL10       15.20 dB
SFO1       500.2231250 MHz

===== CHANNEL f2 =====
PCPDG2     98tp
NUC2       13C
P3         15.50 usec
p4         31.00 usec
PCPD2      65.00 usec
PL2        -1.00 dB
PL12       11.30 dB
SFO2       125.7929190 MHz

===== GRADIENT CHANNEL =====
GPRM1      SINE.100
GPRM2      SINE.100
GPX1       0.00 %
GPX2       0.00 %
GPY1       0.00 %
GPY2       0.00 %
GZ1        80.00 %
GZ2        20.10 %
P16        1000.00 usec

F1 - Acquisition parameters
ND0        2
TD         512
SFO1       125.7929 MHz
FIDRES     49.135220 Hz
SW         199.989 ppm
FAMODE     Echo-Antiecho

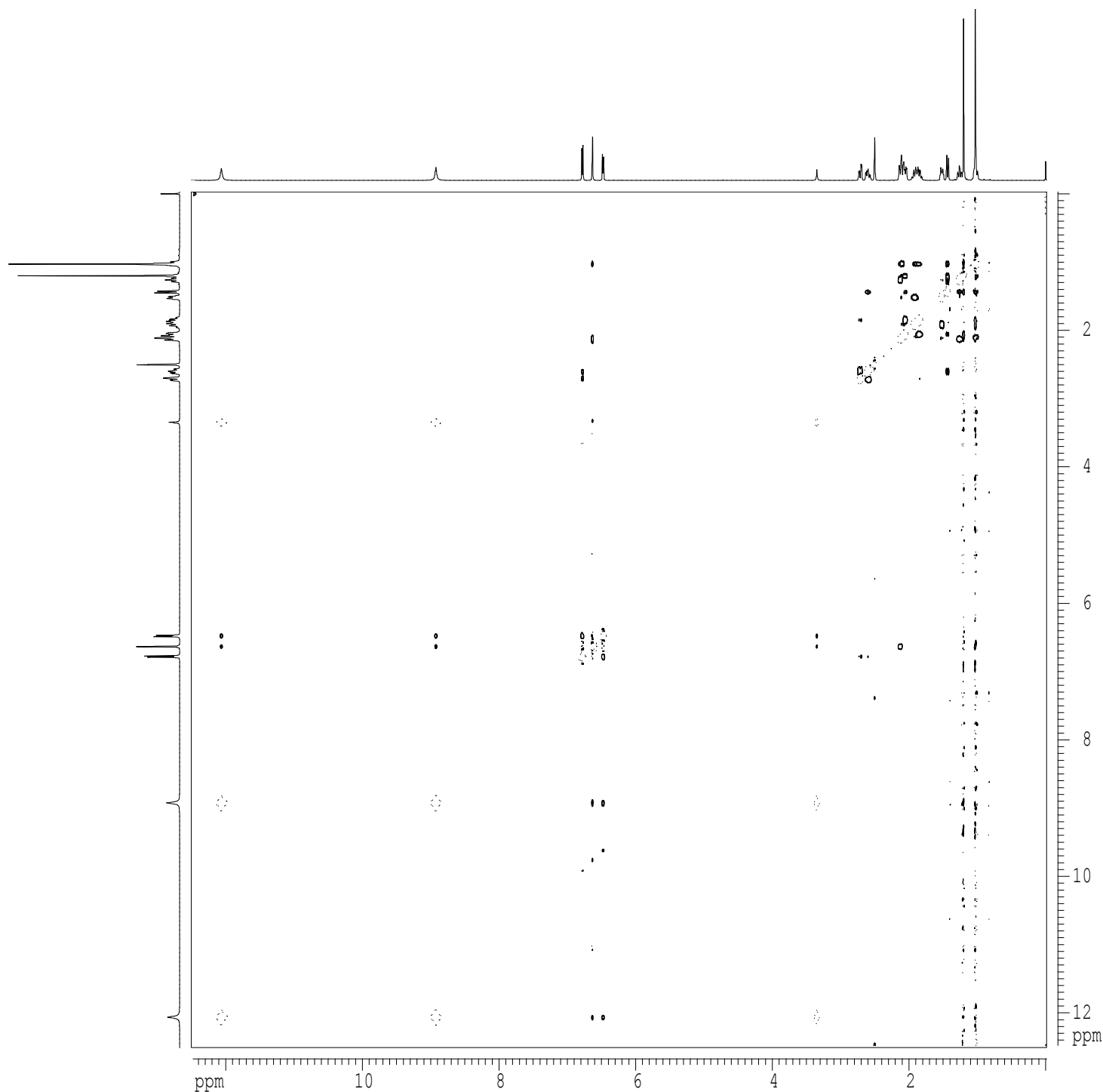
F2 - Processing parameters
SI         2048
SF         500.2200175 MHz
WDW        EM
SSB        0
LB         5.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        echo-antiecho
SF         125.7804965 MHz
WDW        Q8SINE
SSB        3
LB         0.00 Hz
GB         0

2D NMR plot parameters
CX2        18.00 cm
CX1        15.00 cm
F2PLO      3.001 ppm
F2PLO      1501.25 Hz
F2PHI      0.799 ppm
F2HI       399.90 Hz
F1PLO      53.058 ppm
F1LO       6673.66 Hz
F1HI       17.900 ppm
F1HI       2251.45 Hz
F2PVMCM    0.12232 ppm/cm
F2HZCM     61.18813 Hz/cm
F1PVMCM    2.34386 ppm/cm
F1HZCM     294.81131 Hz/cm

```

noesy



```

Current Data Parameters
USER      nmrl4t
NAME      partII B
EXPNO     27
PROCNO    1

F2 - Acquisition Parameters
Date_     20141211
Time      3.03
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   noesyrvtp
TD        2048
SOLVENT   DMSO
NS         8
DS        16
SWH        6265.664 Hz
FIDRES     3.059406 Hz
AQ         0.1634804 sec
RG         5
DW         79.800 usec
DE         6.00 usec
TE         298.0 K
D0         0.00000300 sec
D1         2.00000000 sec
D8         1.00000000 sec
IN0        0.00007980 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
PL1        1.60 dB
SFO1       500.2231250 MHz

F1 - Acquisition parameters
ND0        2
TD         256
SFO1       500.2231 MHz
FIDRES     24.475250 Hz
SW         12.526 ppm
FnMODE     undefined

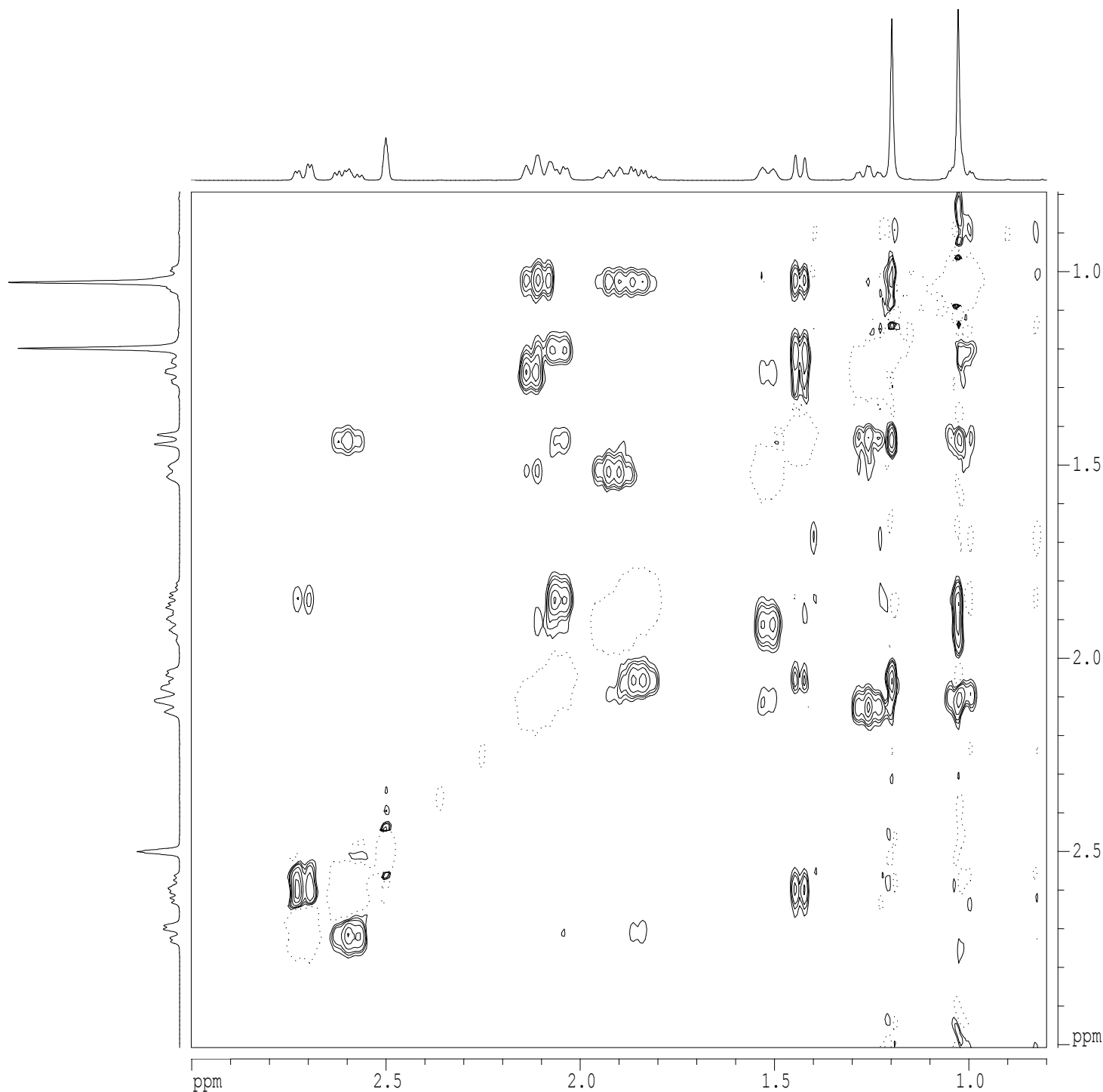
F2 - Processing parameters
SI         2048
SF         500.2200175 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        TPPI
SF         500.2200175 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0

2D NMR plot parameters
CX2        15.00 cm
CX1        15.00 cm
F2PLO      12.504 ppm
F2LO       6254.77 Hz
F2PHI      -0.016 ppm
F2HI       -7.83 Hz
F1PLO      12.510 ppm
F1LO       6257.83 Hz
F1PHI      -0.028 ppm
F1HI       -13.95 Hz
F2PPMCM    0.83465 ppm/cm
F2HZCM     417.50702 Hz/cm
F1PPMCM    0.83587 ppm/cm
F1HZCM     418.11890 Hz/cm

```

noesy



```

Current Data Parameters
USER      nmrl4t
NAME      partII B
EXPNO     27
PROCNO    1

F2 - Acquisition Parameters
Date_     20141211
Time      3.03
INSTRUM   cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   noesyrvtp
TD        2048
SOLVENT   DMSO
NS         8
DS         16
SWH        6265.664 Hz
FIDRES     3.059406 Hz
AQ         0.1634804 sec
RG         5
DW         79.800 usec
DE         6.00 usec
TE         298.0 K
D0         0.00000300 sec
D1         2.00000000 sec
D8         1.00000000 sec
IN0        0.00007980 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
PL1        1.60 dB
SFO1       500.2231250 MHz

F1 - Acquisition parameters
ND0         2
TD         256
SFO1       500.2231 MHz
FIDRES     24.475250 Hz
SW         12.526 ppm
FnMODE     undefined

F2 - Processing parameters
SI         2048
SF         500.2200175 MHz
WDW        QSINE
SSB         2
LB          0.00 Hz
GB          0
PC          1.40

F1 - Processing parameters
SI         1024
MC2        TPPI
SF         500.2200175 MHz
WDW        QSINE
SSB         2
LB          0.00 Hz
GB          0

2D NMR plot parameters
CX2        15.00 cm
CX1        15.00 cm
F2PLO      3.001 ppm
F2LO       1501.29 Hz
F2PHI      0.799 ppm
F2HI       399.90 Hz
F1PLO      3.007 ppm
F1LO       1504.35 Hz
F1PHI      0.793 ppm
F1HI       396.84 Hz
F2PPMCM    0.14679 ppm/cm
F2HZCM     73.42575 Hz/cm
F1PPMCM    0.14760 ppm/cm
F1HZCM     73.83368 Hz/cm

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