

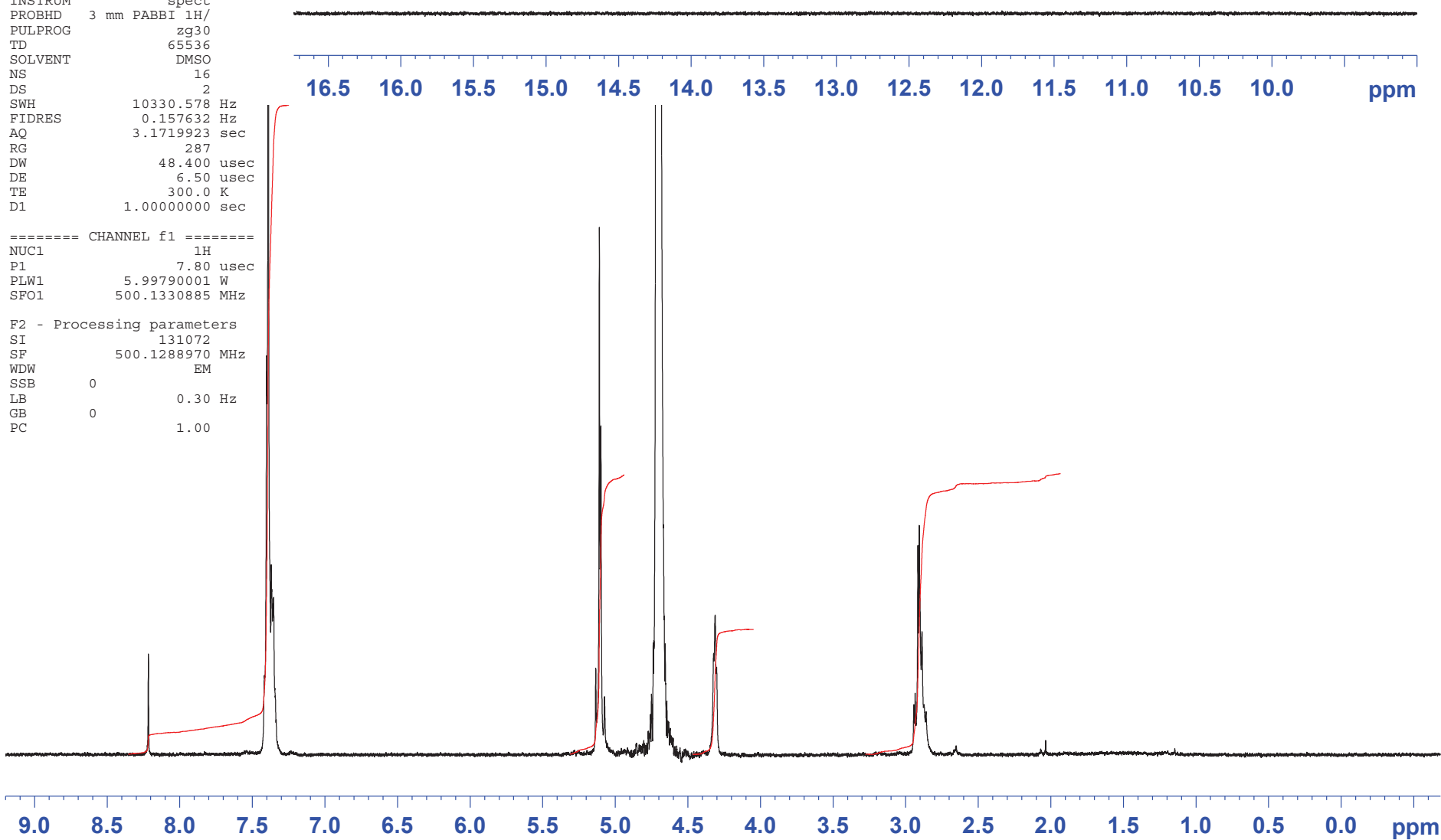
compound 3a

Current Data Parameters
NAME 305936
EXPNO 200
PROCNO 1

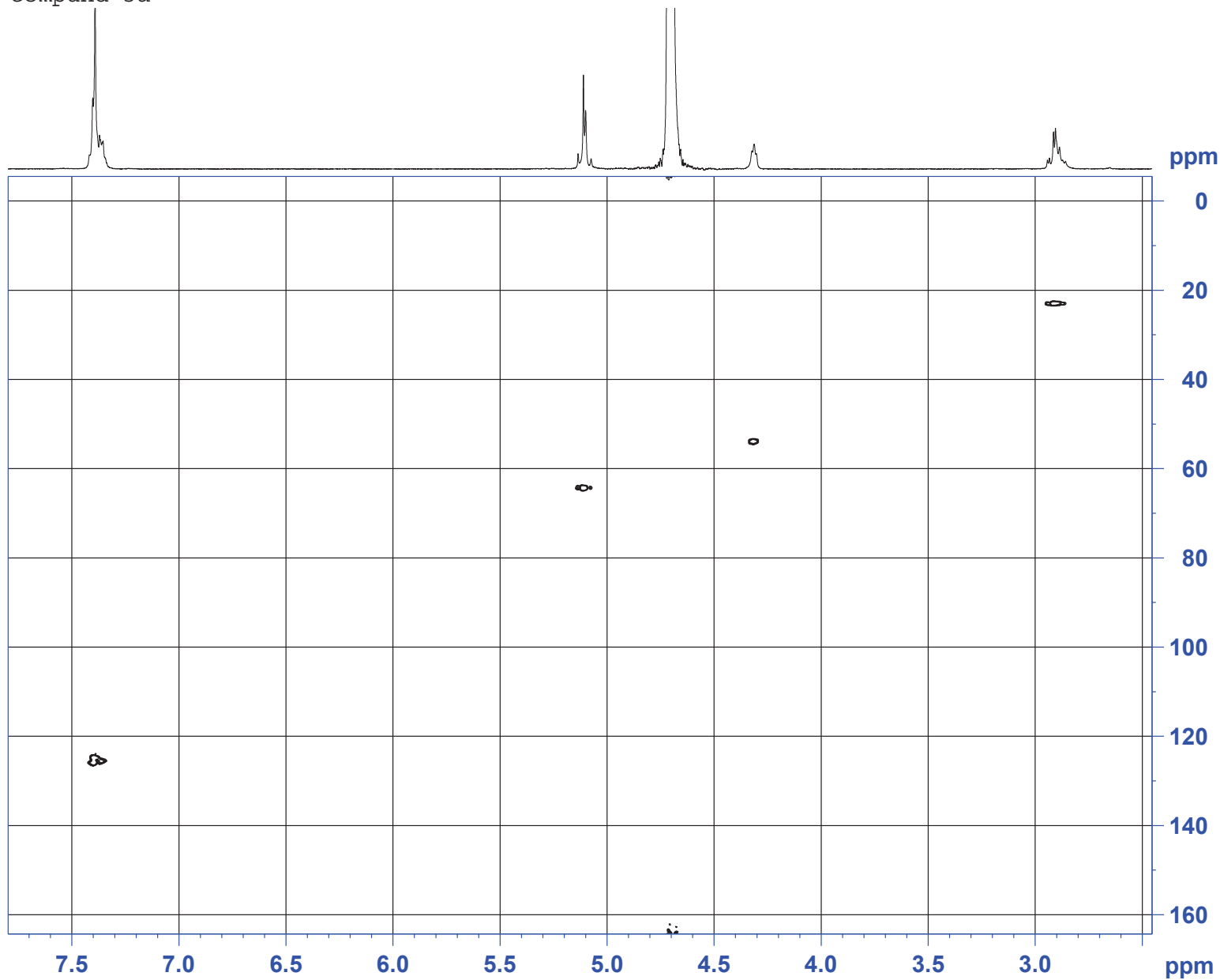
F2 - Acquisition Parameters
Date_ 20130824
Time 13.53
INSTRUM spect
PROBHD 3 mm PABBI 1H/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 287
DW 48.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 7.80 usec
PLW1 5.99790001 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 131072
SF 500.1288970 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



compound 3a



```
Current Data Parameters
NAME          305936
EXPNO         201
PROCNO        1

F2 - Acquisition Parameters
Date_         20130824
Time_         13.55
INSTRUM       spect
PROBHD        3 mm PABBI 1H/
PULPROG       hsqcqtgpsi
TD            1024
SOLVENT       DMSO
NS            4
DS            16
SWH           2673.797 Hz
FIDRES        2.611130 Hz
AQ            0.1915380 sec
RG            2050
DW            187.000 usec
DE            6.50 usec
TE            300.1 K
CNST2         145.0000000
D0            0.0000300 sec
D1            1.33697903 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D24           0.00110000 sec
IN0           0.00002340 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1          1H
P1            7.80 usec
P2            15.60 usec
P28           1000.00 usec
PLW1          5.99790001 W
SFO1          500.1314653 MHz

===== CHANNEL f2 =====
CPDPRG2       garp
NUC2          13C
P3            11.00 usec
P4            22.00 usec
PCPD2         70.00 usec
PLW2          130.00000000 W
PLW12         3.21020007 W
SFO2          125.7678496 MHz

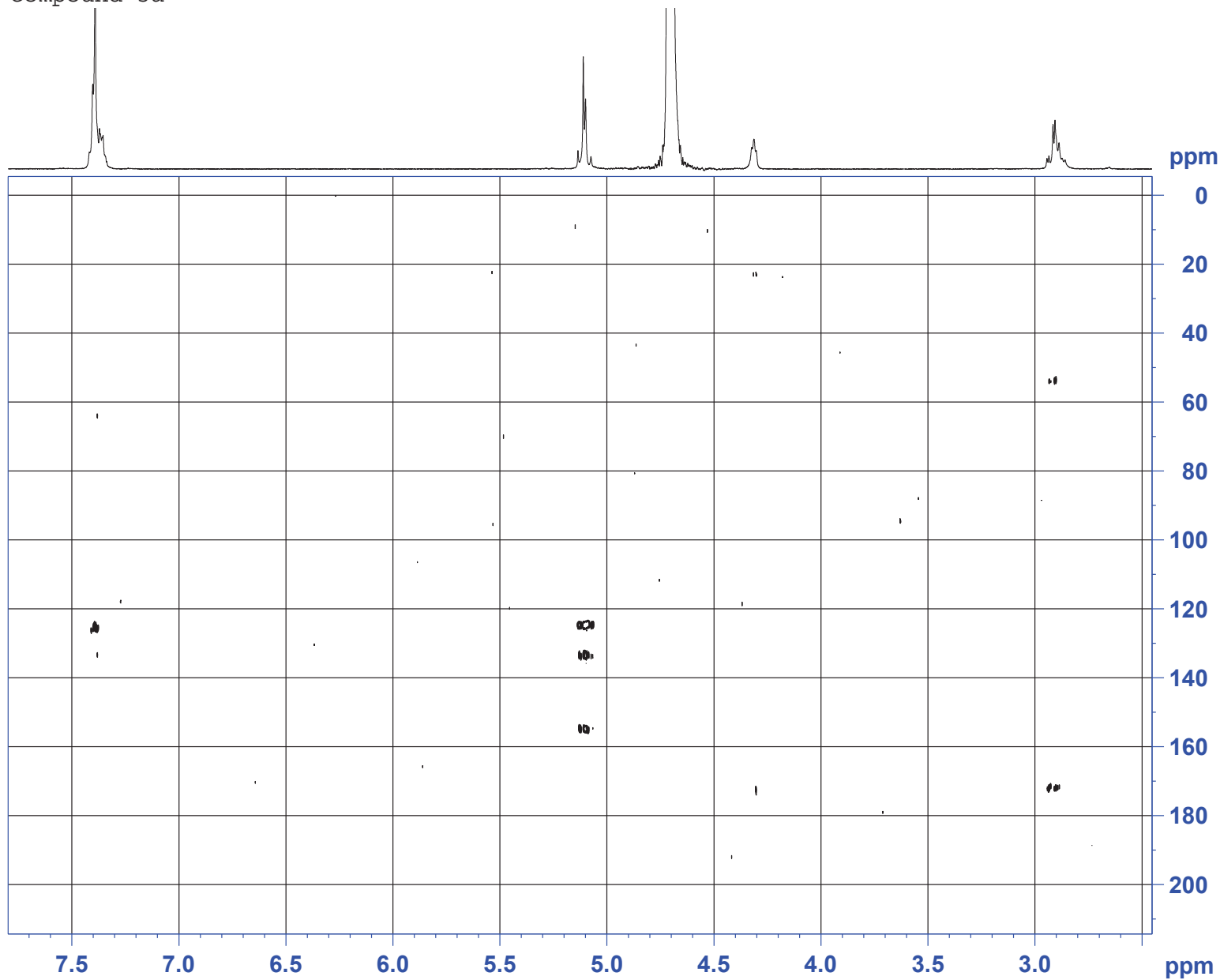
===== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1          80.00 %
GPZ2          20.10 %
P16           1000.00 usec

F1 - Acquisition parameters
TD            256
SFO1          125.7678 MHz
FIDRES        83.517296 Hz
SW            169.999 ppm
FnMODE        Echo-Antiecho

F2 - Processing parameters
SI            2048
SF            500.1289021 MHz
WDW           QSINE
SSB           2
LB            0 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI            1024
MC2           echo-antiecho
SF            125.7578713 MHz
WDW           SINE
SSB           2
LB            0 Hz
GB            0
```

compound 3a



```
Current Data Parameters
NAME          305936
EXPNO         202
PROCNO        1

F2 - Acquisition Parameters
Date_         20130824
Time          14.22
INSTRUM       spect
PROBHD        3 mm PABBI 1H/
PULPROG       hmbcetgpl3nd
TD            2048
SOLVENT       DMSO
DS            16
SWH           2673.797 Hz
FIDRES        1.305565 Hz
AQ            0.3830260 sec
RG            1820
DW            187.000 usec
DE            6.50 usec
TE            299.9 K
CNST6         120.0000000
CNST7         170.0000000
CNST13        8.0000000
CNST30        0.5981131
D0            0.00000300 sec
D1            1.64856303 sec
D6            0.06250000 sec
D16           0.00020000 sec
IN0           0.00001805 sec

===== CHANNEL f1 =====
NUC1           1H
P1             7.80 usec
P2            15.60 usec
PLW1          5.99790001 W
SFO1          500.1314653 MHz

===== CHANNEL f2 =====
NUC2           13C
P3            11.00 usec
P24           2000.00 usec
PLW2          130.00000000 W
SFO2          125.7709936 MHz
SPNAM7        Crp60comp.4
SPOAL7        0 Hz
SPOFFS7       0 Hz
SPW7          24.03400040 W

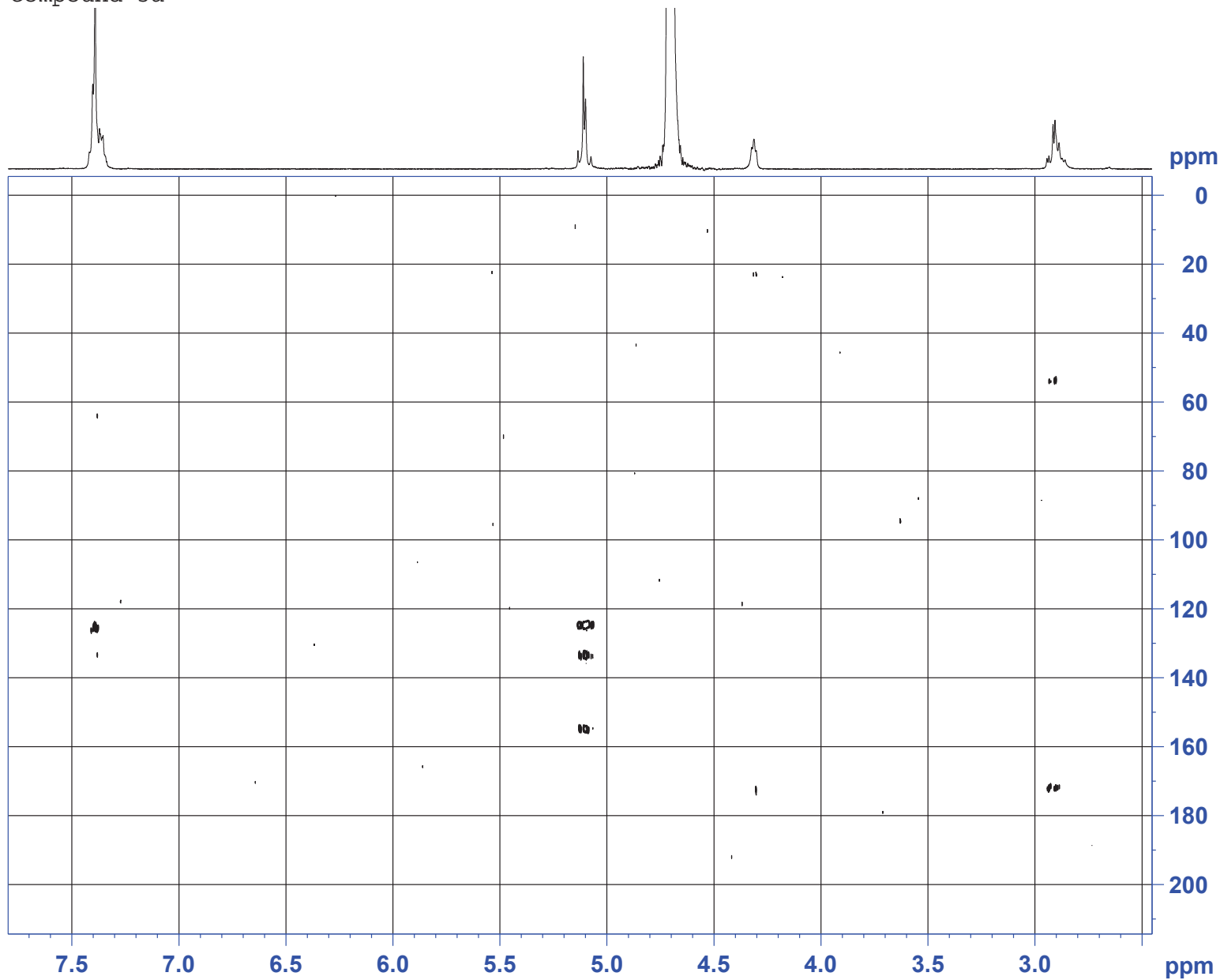
===== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM3        SMSQ10.100
GPNAM4        SMSQ10.100
GPNAM5        SMSQ10.100
GPNAM6        SMSQ10.100
GPZ1          80.00 %
GPZ3          14.00 %
GPZ4          -8.00 %
GPZ5          -4.00 %
GPZ6          -2.00 %
P16           1000.00 usec

F1 - Acquisition parameters
TD            256
SFO1          125.771 MHz
FIDRES        108.083908 Hz
SW            219.999 ppm
FbMODE        Echo-Antiecho

F2 - Processing parameters
SI            4096
SF            500.1289021 MHz
WDW           SINE
SSB           0
LB            0 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI            1024
MC2           echo-antiecho
SF            125.7578713 MHz
WDW           GM
SSB           0
LB            0 Hz
GB            0cc
```

compound 3a



```
Current Data Parameters
NAME          305936
EXPNO         202
PROCNO        1

F2 - Acquisition Parameters
Date_         20130824
Time          14.22
INSTRUM       spect
PROBHD        3 mm PABBI 1H/
PULPROG       hmbcetgpl3nd
TD            2048
SOLVENT       DMSO
DS            16
SWH           2673.797 Hz
FIDRES        1.305565 Hz
AQ            0.3830260 sec
RG            1820
DW            187.000 usec
DE            6.50 usec
TE            299.9 K
CNST6         120.0000000
CNST7         170.0000000
CNST13        8.0000000
CNST30        0.5981131
D0            0.00000300 sec
D1            1.64856303 sec
D6            0.06250000 sec
D16           0.00020000 sec
IN0           0.00001805 sec

===== CHANNEL f1 =====
NUC1           1H
P1             7.80 usec
P2            15.60 usec
PLW1          5.99790001 W
SFO1          500.1314653 MHz

===== CHANNEL f2 =====
NUC2           13C
P3            11.00 usec
P24           2000.00 usec
PLW2          130.00000000 W
SFO2          125.7709936 MHz
SPNAM7        Crp60comp.4
SPOAL7        0 Hz
SPOFFS7       0 Hz
SPW7          24.03400040 W

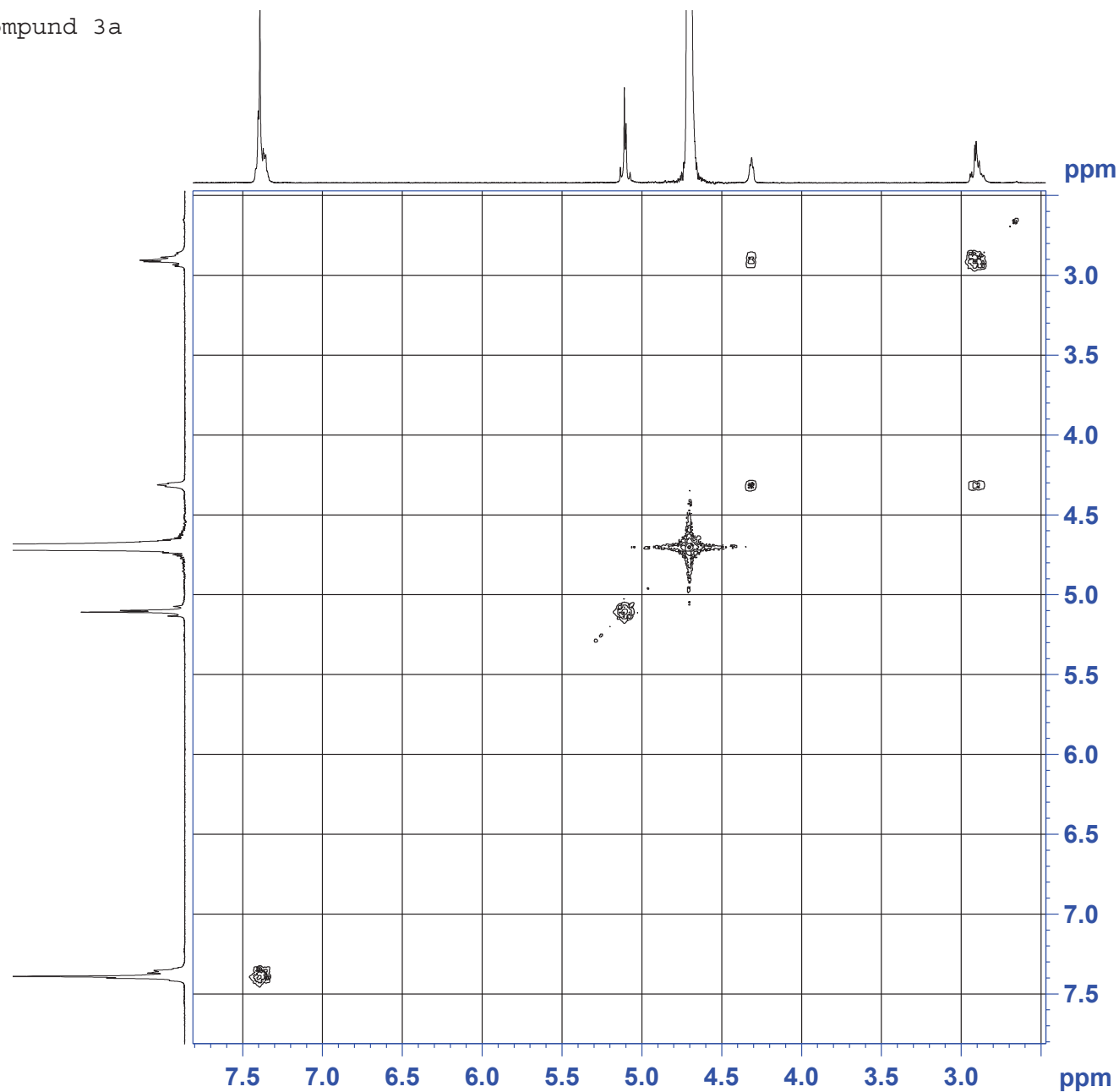
===== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM3        SMSQ10.100
GPNAM4        SMSQ10.100
GPNAM5        SMSQ10.100
GPNAM6        SMSQ10.100
GPZ1          80.00 %
GPZ3          14.00 %
GPZ4          -8.00 %
GPZ5          -4.00 %
GPZ6          -2.00 %
P16           1000.00 usec

F1 - Acquisition parameters
TD            256
SFO1          125.771 MHz
FIDRES        108.083908 Hz
SW            219.999 ppm
FbMODE        Echo-Antiecho

F2 - Processing parameters
SI            4096
SF            500.1289021 MHz
WDW           SINE
SSB           0
LB            0 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI            1024
MC2           echo-antiecho
SF            125.7578713 MHz
WDW           GM
SSB           0
LB            0 Hz
GB            0cc
```

compound 3a



Current Data Parameters
NAME 305936
EXPNO 203
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130824
Time 16.47
INSTRUM spect
PROBHD 3 mm PABBI 1H/
PULPROG cosygpgf
TD 2048
SOLVENT DMSO
NS 4
DS 8
SWH 2673.797 Hz
FIDRES 1.30565 Hz
AQ 0.3830260 sec
RG 575
DW 187.000 usec
DE 6.50 usec
TE 300.0 K
D0 0.0000300 sec
D1 1.74481905 sec
D13 0.0000400 sec
D16 0.00020000 sec
IN0 0.00037400 sec

==== CHANNEL f1 =====
NUC1 1H
P0 7.80 usec
P1 7.80 usec
PLW1 5.99790001 W
SFO1 500.1314653 MHz

==== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 500.1315 MHz
FIDRES 10.444519 Hz
SW 5.346 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 500.1288954 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1288954 MHz
WDW TRAP
SSB 0
LB 0 Hz
GB 0c

Current Data Parameters
NAME 50039067
EXPNO 500
PROCNO 1

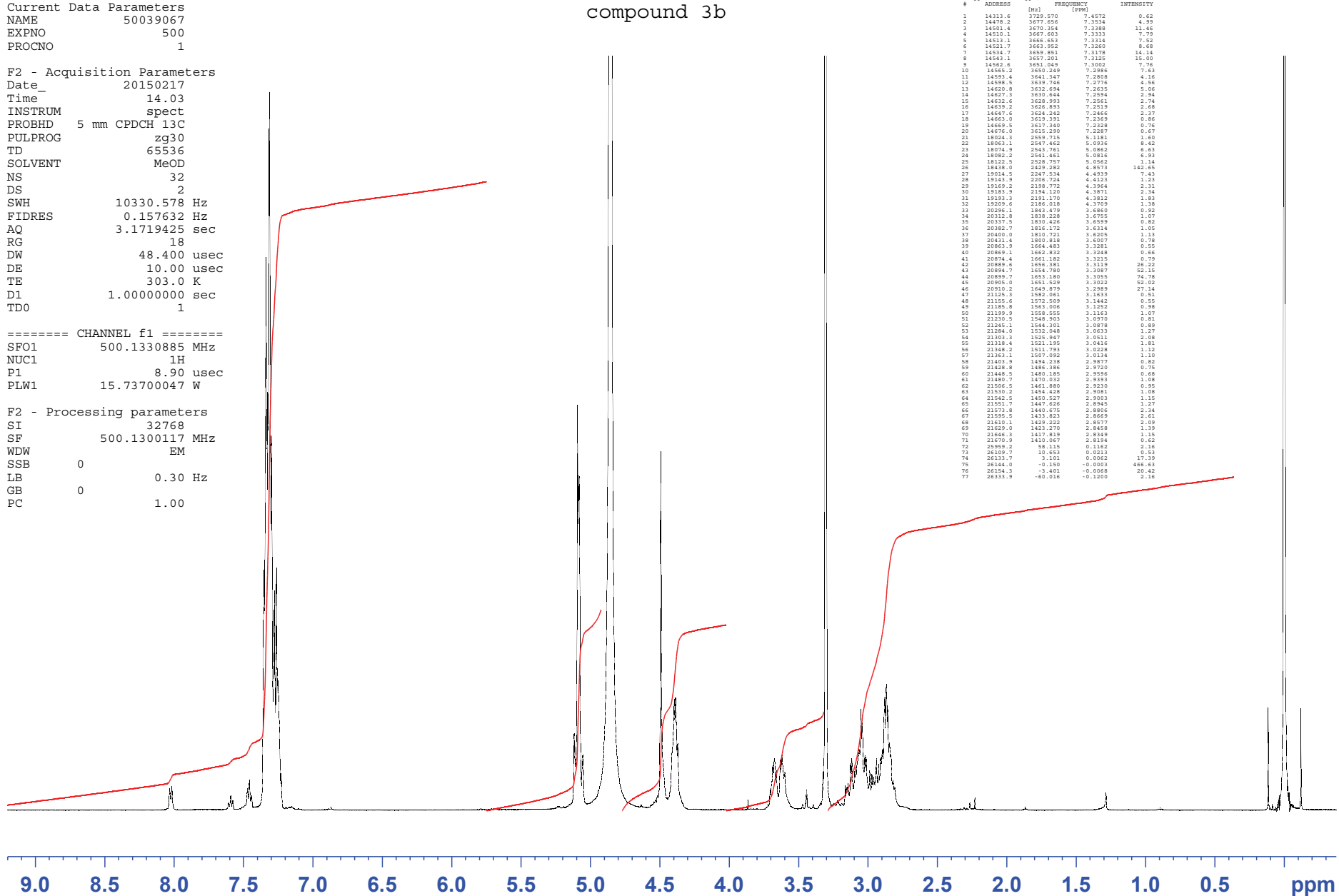
F2 - Acquisition Parameters
Date_ 20150217
Time 14.03
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 32
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 18
DW 48.400 usec
DE 10.00 usec
TE 303.0 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 8.90 usec
PLW1 15.73700047 W

F2 - Processing parameters
SI 32768
SF 500.1300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

compound 3b

U-C:/Bruker/TopSpin3.2\data\smTrack\smr_USER-hwup0081_NAME=50039067_EXPNO=500_PROCNO=1
F1=16.48ppm F2=4.17ppm M1=0.50cm M2=1.0000.00cm PC=1.000



Current Data Parameters
NAME 50039067
EXPNO 501
PROCNO 1

compound 3b

F2 - Acquisition Parameters
Date_ 20150217
Time 17.05
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg
TD 65536
SOLVENT MeOD
NS 2048
DS 4
SWH 30864.197 Hz
FIDRES 0.470950 Hz
AQ 1.0616832 sec
RG 724
DW 16.200 usec
DE 18.000 usec
TE 303.0 K
D1 4.00000000 sec
D11 0.03000000 sec
TDO 1

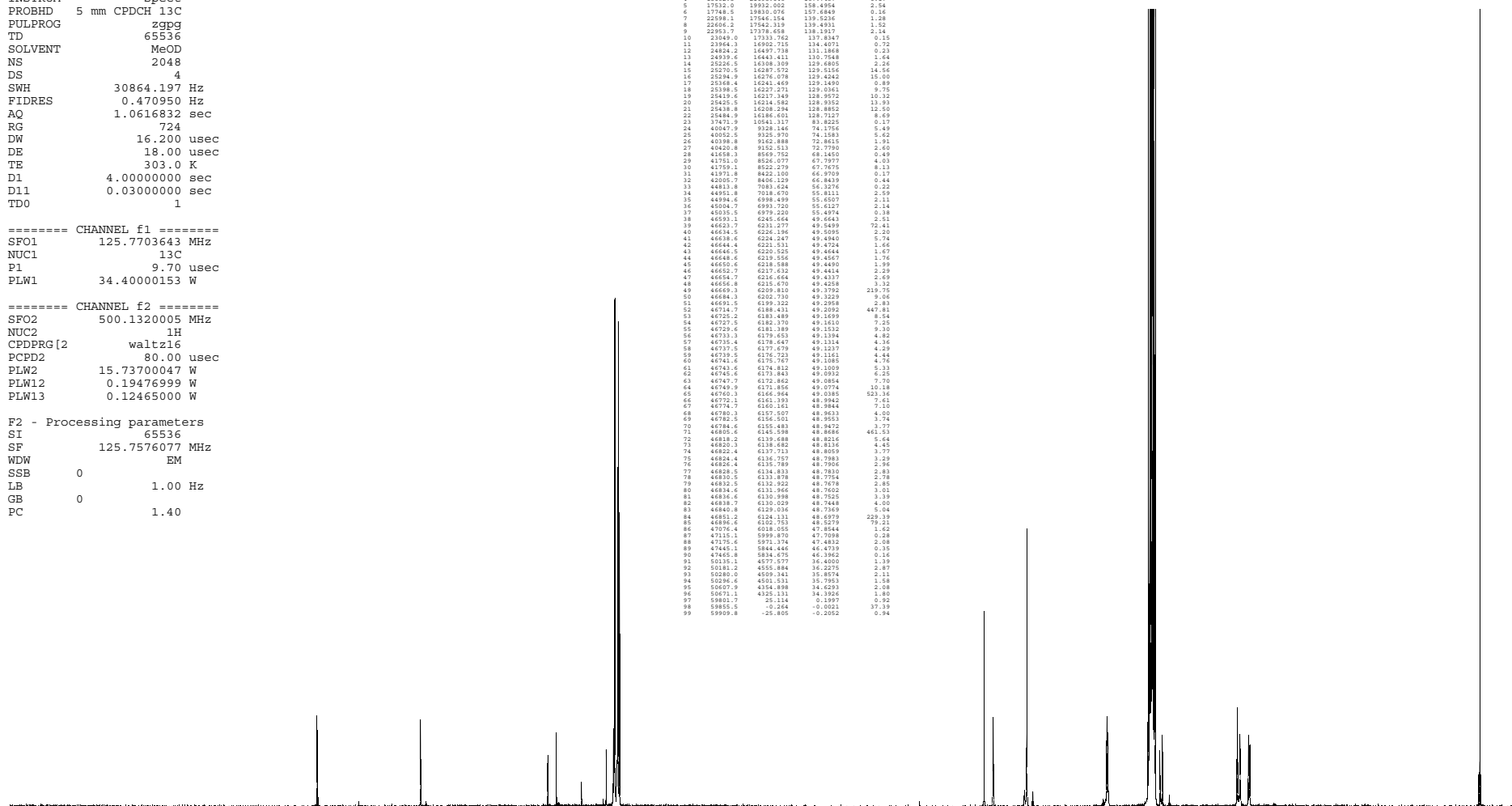
==== CHANNEL f1 =====
SFO1 125.7703643 MHz
NUC1 13C
P1 9.70 usec
PLW1 34.40000153 W

==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 15.73700047 W
PLW12 0.19476999 W
PLW13 0.12465000 W

F2 - Processing parameters
SI 65536
SF 125.7576077 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DD=C:/Bruker/TopSpin3.2\data\dataTrack\msr_USER\hwg0081_MMR-50039067_EXPNO=501_PROCNO=1
F1=224.131800 F2=21.276900 MC=0.00000 WALTZ160000.00000 PC=1.40000

[Hz]	ADDRESS	PPM	INTENSITY
1	13385.4	21884.814	174.6241
2	13386.1	21879.812	171.9840
3	13438.0	21860.068	173.8270
4	15052.5	21395.046	167.7437
5	17512.0	19932.002	158.4984
6	17748.5	19811.076	157.6849
7	22598.1	17546.154	139.5236
8	22598.2	17546.319	139.4931
9	22953.7	17378.658	138.1917
10	23049.0	17333.762	137.4947
11	23964.3	16902.715	134.4071
12	24042.2	16897.738	131.4868
13	24939.6	16443.411	130.7548
14	25206.5	16308.309	129.8895
15	25270.5	16287.572	129.5156
16	25294.9	16276.078	129.4042
17	25368.4	16241.469	129.1490
18	25398.5	16227.271	129.0361
19	25419.6	16217.349	128.9572
20	25425.5	16214.582	128.9325
21	25438.8	16208.294	128.8852
22	25484.9	16186.401	128.7127
23	37471.9	10541.117	83.8225
24	40087.9	9328.146	74.3765
25	40052.5	9325.970	74.1883
26	40398.8	9152.888	72.8615
27	40420.8	9152.511	72.7790
28	41458.3	8569.752	68.1450
29	41751.0	8524.077	67.7977
30	41759.1	8522.279	67.7875
31	41971.8	8422.100	66.8709
32	42005.7	8406.129	66.8439
33	44813.8	7083.624	56.3276
34	44851.8	7083.670	55.8111
35	44904.6	6998.499	55.6507
36	45004.7	6939.720	55.2127
37	45035.5	6929.220	55.4974
38	45093.1	6845.664	49.6843
39	46623.7	6231.277	49.5499
40	46634.5	6226.196	49.5095
41	46638.6	6224.247	49.4940
42	46644.4	6221.531	49.4724
43	46646.5	6220.525	49.4644
44	46648.6	6219.556	49.4567
45	46650.6	6218.588	49.4490
46	46652.7	6217.632	49.4414
47	46654.7	6216.664	49.4337
48	46656.8	6215.670	49.4258
49	46669.3	6209.810	49.3792
50	46684.3	6202.730	49.3229
51	46691.5	6199.322	49.2958
52	46714.7	6188.431	49.2092
53	46725.2	6183.489	49.1699
54	46727.5	6182.370	49.1610
55	46729.6	6181.389	49.1532
56	46733.3	6179.653	49.1394
57	46735.4	6178.647	49.1334
58	46737.5	6177.679	49.1277
59	46739.5	6176.723	49.1161
60	46741.6	6175.767	49.1085
61	46743.6	6174.812	49.1009
62	46745.6	6173.843	49.0932
63	46747.7	6172.862	49.0854
64	46749.9	6171.856	49.0774
65	46750.3	6166.964	49.0385
66	46772.1	6161.393	48.9942
67	46774.7	6160.161	48.9844
68	46780.3	6157.507	48.9633
69	46782.5	6156.501	48.9553
70	46784.6	6155.483	48.9472
71	46805.6	6145.598	48.8686
72	46818.2	6139.688	48.8216
73	46820.3	6138.682	48.8136
74	46822.4	6137.713	48.8059
75	46824.4	6136.757	48.7983
76	46826.4	6135.789	48.7908
77	46828.5	6134.833	48.7830
78	46830.5	6133.878	48.7754
79	46832.5	6132.922	48.7678
80	46834.6	6131.966	48.7602
81	46836.6	6130.998	48.7525
82	46838.7	6130.029	48.7448
83	46840.8	6129.036	48.7369
84	46851.2	6124.121	48.6979
85	46896.6	6102.753	48.5279
86	47076.4	6038.055	47.8644
87	47115.1	5999.870	47.7098
88	47375.6	5971.374	47.4832
89	47445.1	5844.446	46.4739
90	47465.8	5834.675	46.3962
91	50135.1	4577.577	36.4000
92	50181.2	4555.884	36.2275
93	50280.0	4509.341	35.8574
94	50296.6	4501.531	35.7953
95	50607.9	4354.898	34.6293
96	50671.1	4325.131	34.3924
97	59801.7	25.114	0.1997
98	59855.5	-0.264	-0.0021
99	59909.8	-25.805	-0.2052



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

DU=C:\Bruker\TopSpin3.2\data\SamTrack\mr, USER=hwp008, NAME=50039067, EXPRNO=502, PROCNO=1
F1=219.769ppm, F2=16.892ppm, MI=0.50cm, MAXZ=10000.00cm, PC=1.400

#	ADDRESS	FREQUENCY	INTENSITY	
1	21637.2	16903.193	134.4109	0.56
2	24648.6	16443.901	130.7587	1.17
3	24846.2	16308.762	129.6841	1.79
4	24991.8	16286.050	129.5194	15.00
5	25037.0	16276.568	129.4281	12.69
6	25091.4	16246.815	129.1997	0.61
7	25124.5	16227.749	129.0399	7.11
8	25146.4	16217.827	128.9610	9.06
9	25152.6	16210.014	128.9186	13.12
10	25156.1	16208.795	128.8951	13.19
11	40221.4	8161.099	74.1458	6.12
12	40316.6	8128.574	74.1790	-6.21
13	40321.4	8128.189	74.1458	-6.13
14	40680.7	8163.240	72.8643	-2.15
15	40703.4	8152.880	72.7824	-2.96
16	42082.7	8526.517	67.8012	-4.11
17	42091.1	8525.759	67.7112	-8.99
18	45401.8	7019.224	55.8155	2.15
19	45446.4	6998.952	55.8543	1.72
20	45456.9	6994.185	55.8164	1.75
21	47106.1	6246.167	49.4663	8.45
22	47151.4	6224.687	49.4975	17.73
23	47196.6	6203.233	49.1209	26.55
24	47231.7	6188.205	49.2074	0.58
25	47245.9	6181.754	49.1561	17.06
26	47276.4	6167.393	49.0462	-0.66
27	47291.3	6160.236	48.9850	8.76
28	47321.8	6146.165	48.8747	-0.91
29	47371.2	6124.848	48.7036	-0.68
30	47405.4	6118.520	47.8381	1.25
31	47705.3	5975.776	47.4864	1.58
32	50777.2	4578.080	36.4040	-1.46
33	50820.3	4556.263	36.2105	-1.00
34	50927.6	4509.794	35.8610	-2.19
35	50944.8	4501.997	35.7990	-1.64
36	51267.7	4355.318	34.6328	-2.25
37	51331.1	4325.659	34.1968	-1.87
38	59126.8	781.747	6.2163	-0.77
39	60280.0	241.211	2.0771	-0.80
40	60801.7	25.667	0.2041	1.70
41	60820.0	0.289	0.0021	66.76
42	60911.9	-25.302	-0.2012	1.55
43	61815.4	-240.771	-2.0746	-0.77
44	62976.4	-781.206	-6.2120	-0.84
45	63724.4	-1102.609	-11.3033	0.93

CH,CH3-Signals positive, CH2-Signals negative

DU=C:\Bruker\TopSpin3.2\data\SamTrack\mr, USER=hwp008, NAME=50039067, EXPRNO=503, PROCNO=1
F1=219.769ppm, F2=16.892ppm, MI=0.50cm, MAXZ=10000.00cm, PC=1.400

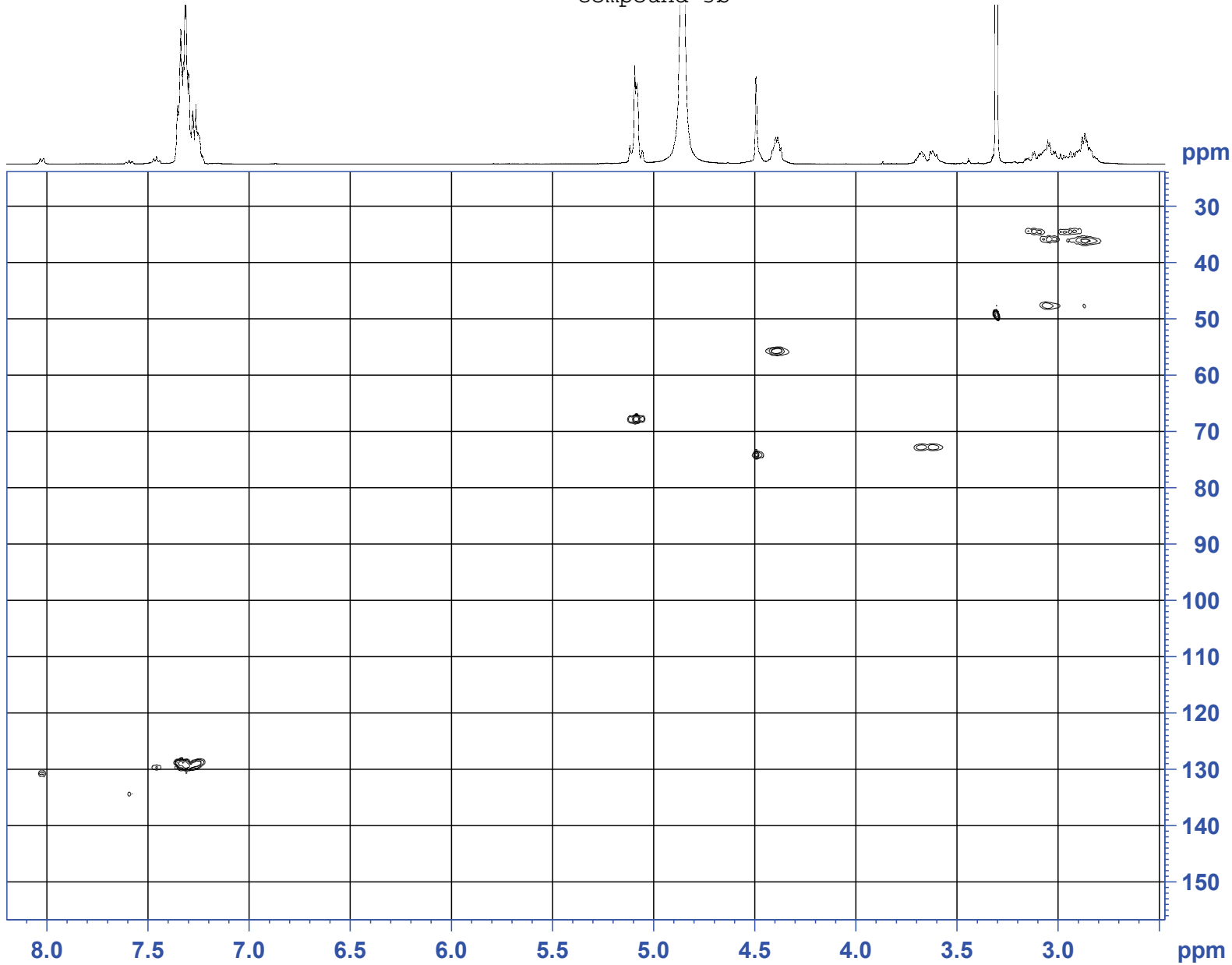
#	ADDRESS	FREQUENCY	INTENSITY	
1	21638.3	16902.680	134.4069	0.59
2	24649.6	16443.436	130.7550	1.36
3	24847.2	16308.287	129.6824	1.77
4	24992.8	16287.585	129.5167	15.00
5	25038.1	16276.090	129.4243	12.66
6	25088.4	16244.148	129.1703	0.55
7	25120.6	16227.284	129.0362	7.09
8	25147.4	16217.349	128.9572	9.06
9	25150.6	16214.545	128.9347	13.22
10	25157.4	16208.307	128.8853	13.69
11	40221.4	8161.099	74.1458	6.15
12	40316.6	8128.574	74.1790	-6.13
13	40321.4	8128.189	74.1458	-6.13
14	40680.7	8163.240	72.8643	-2.17
15	40703.4	8152.878	72.8111	-2.99
16	42082.7	8526.517	67.8111	1.69
17	42091.1	8525.776	67.7111	1.69
18	45401.8	7019.224	55.8111	8.29
19	45447.5	6998.970	55.8111	1.69
20	45456.9	6998.970	55.8111	1.69
21	47106.1	6246.174	49.6447	8.29
22	47151.4	6224.224	49.4939	17.73
23	47196.6	6202.780	49.3333	26.00
24	47231.7	6187.891	49.2049	0.91
25	47245.9	6181.288	49.1524	16.71
26	47276.4	6166.449	49.0344	1.02
27	47291.3	6159.784	48.9814	8.60
28	47321.8	6146.107	48.8839	0.79
29	47371.2	6124.722	47.8839	1.27
30	47405.4	6117.123	47.4828	1.61
31	60858.6	-0.176	-0.0014	2.89

CH-Signals

compound 3b

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

compound 3b



```
Current Data Parameters
NAME      50039067
EXPNO    504
PROCNO   1

F2 - Acquisition Parameters
Date_    20150217
Time     20.04
INSTRUM  spect
PROBHD   5 mm CPDCH 13C
PULPROG  hsqcetgpsi2.2
TD       2048
SOLVENT  MeOD
NS       16
DS       16
SWH      4504.504 Hz
FIDRES   2.199465 Hz
AQ       0.2273280 sec
RG       2050
DW       111.000 usec
DE       10.00 usec
TE       303.0 K
CNST2    145.0000000
CNST17   -0.5000000
D0       0.00000300 sec
D1       1.40046704 sec
D4       0.00172414 sec
D11      0.03000000 sec
D16      0.00020000 sec
D24      0.00110000 sec
IN0      0.00002090 sec

===== CHANNEL f1 =====
SF01    500.1319832 MHz
NUC1    1H
P1      8.90 usec
P2      17.80 usec
PLW1    0 usec
P28     15.73700047 W

===== CHANNEL f2 =====
SF02    125.7678496 MHz
NUC2    13C
CPDPRG2 garp
P3      9.70 usec
P14     500.00 usec
P24     2000.00 usec
PCPD2   70.00 usec
PLW0    0 W
PLW2    34.40000153 W
PLW12   0.66055000 W
SPNAM[3] Crp60,0.5,20,1
SPOAL3  0.500
SPOFFS3 0 Hz
SPW3    4.94530010 W
SPNAM[7] Crp60comp.4
SPOAL7  0.500
SPOFFS7 0 Hz
SPW7    4.94530010 W

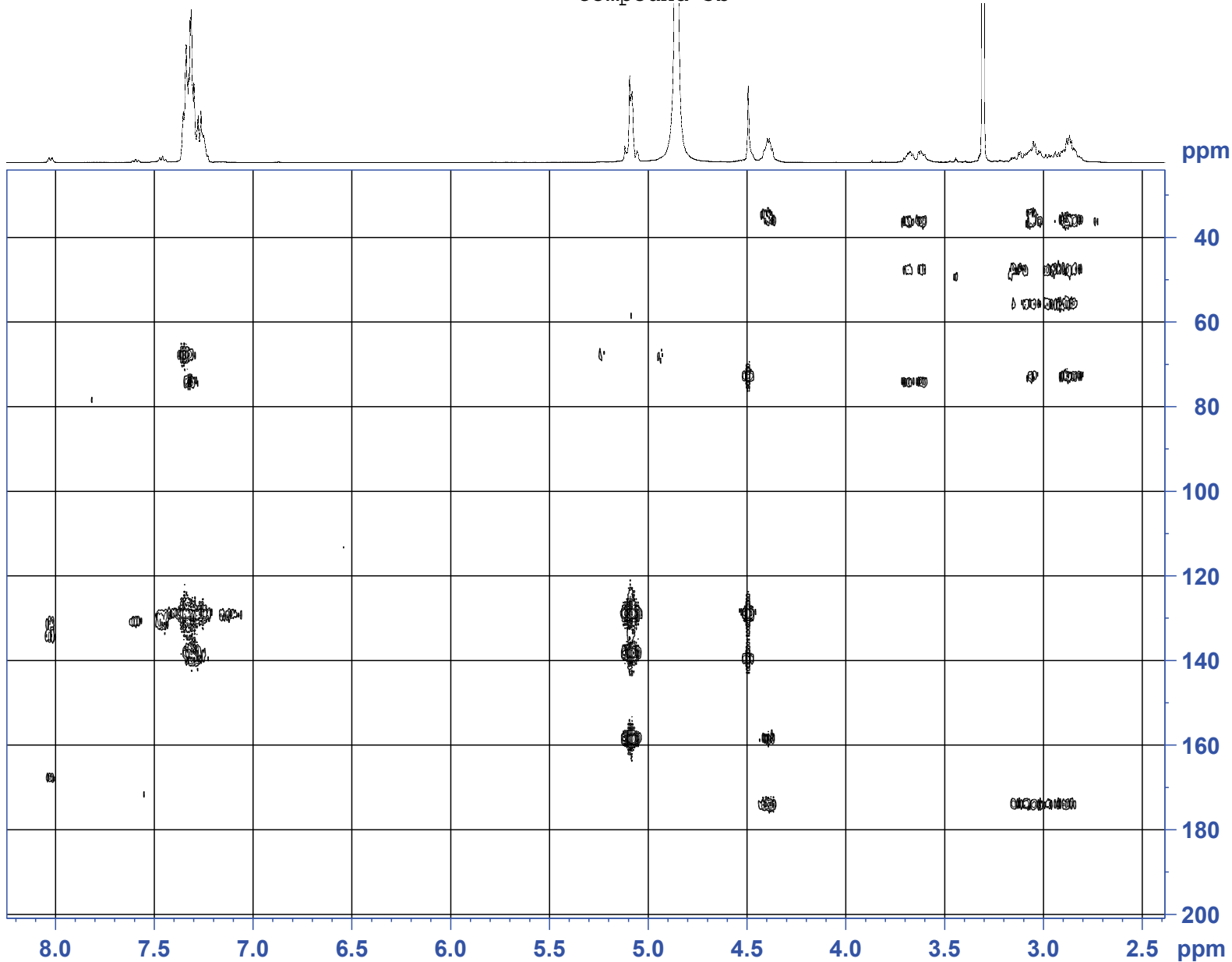
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1    80.00 %
GPZ2    20.10 %
GPZ3    11.00 %
GPZ4    -5.00 %
P16     1000.00 usec
P19     600.00 usec

F1 - Acquisition parameters
TD      256
SF01    125.7678 MHz
FIDRES  93.450958 Hz
SW      130.219 ppm
PhMODE  Echo-Antiecho

F2 - Processing parameters
SI      2048
SF      500.1300117 MHz
WDW     QSINE
SSB     2
LB      0 Hz
GB      0
PC      1.40

F1 - Processing parameters
SI      1024
NC2     echo-antiecho
SF      125.7576077 MHz
WDW     QSINE
SSB     2
LB      0 Hz
GB      0cc
```

compound 3b



```

Current Data Parameters
NAME      50039067
EXPNO    505
PROCNO   1

F2 - Acquisition Parameters
Date_    20150217
Time     22.01
INSTRUM  spect
PROBHD   5 mm CPDCH 13C
PULPROG  hmbcetgp12nd
TD       2048
SOLVENT  MeOD
NS       32
DS       16
SWH      4504.504 Hz
FIDRES   2.199465 Hz
AQ       0.2273280 sec
RG       2050
DW       111.000 usec
DE       10.00 usec
TE       303.0 K

===== CHANNEL f1 =====
SFO1     500.1319832 MHz
NUC1     1H
P1       8.90 usec
P2       17.80 usec
PLW1     15.73700047 W

===== CHANNEL f2 =====
SFO2     125.7703443 MHz
NUC2     13C
P3       9.70 usec
P24      2000.00 usec
PLW2     34.40000153 W
SFOAL7   Crp60comp.4
SFOAL7   0.500
SPOFFS7  0 Hz
SPW7     4.94530010 W

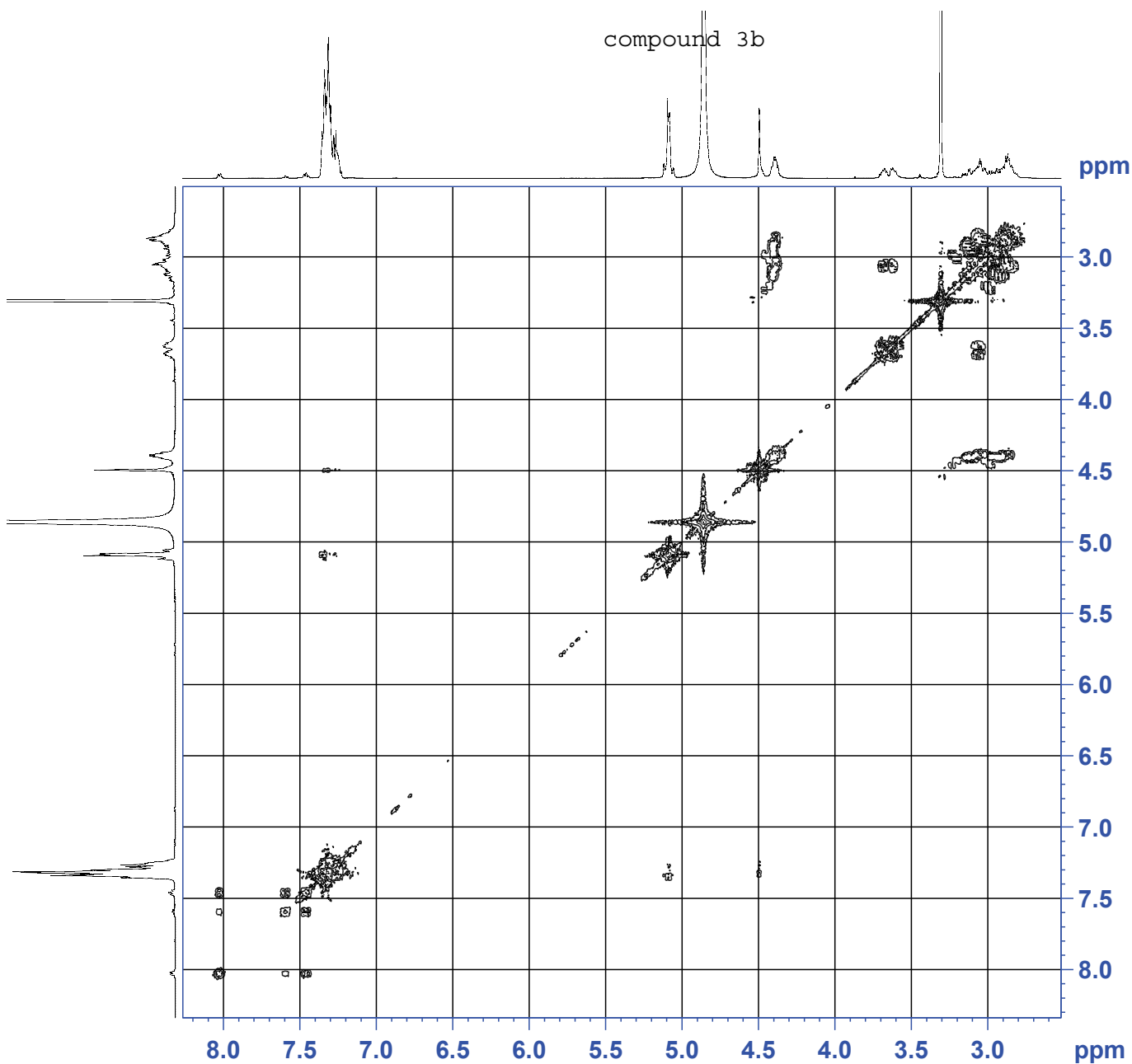
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPNAM[5] SMSQ10.100
GPZ1     80.00 %
GPZ3     15.00 %
GPZ4     -10.00 %
GPZ5     -15.00 %
P16      1000.00 usec

F1 - Acquisition parameters
TD       256
SFO1     125.7703 MHz
FIDRES   109.113129 Hz
SW       222.095 ppm
PnMODE   Echo-Antiecho

F2 - Processing parameters
SI       2048
SF       500.1300117 MHz
WDW      SINE
SSB      0 Hz
LB       0 Hz
GB       0
PC       1.40

F1 - Processing parameters
SI       1024
MC2      echo-antiecho
SF       125.7576077 MHz
WDW      SINE
SSB      0 Hz
LB       0 Hz
GB       0
    
```

compound 3b



```
Current Data Parameters
NAME      50039067
EXPNO    506
PROCNO   1

F2 - Acquisition Parameters
Date_    20150218
Time     1.56
INSTRUM spect
PROBHD   5 mm CPDCH 13C
PULPROG cosygpppgf
TD       2048
SOLVENT  MeOD
NS       8
DS       16
SWH      4504.504 Hz
FIDRES   2.199465 Hz
AQ       0.2273280 sec
RG       25.4
DW       111.000 usec
DE       10.00 usec
TE       303.0 K
D0       0.00000300 sec
D1       1.38735902 sec
D11      0.03000000 sec
D12      0.00002000 sec
D13      0.00000400 sec
D16      0.00020000 sec
INO      0.00022200 sec

===== CHANNEL f1 =====
SFO1    500.1319832 MHz
        NUC1      1H
P0       8.90 usec
P1       8.90 usec
P17      2500.00 usec
PLW1    15.73700047 W
PLW10   1.84399998 W

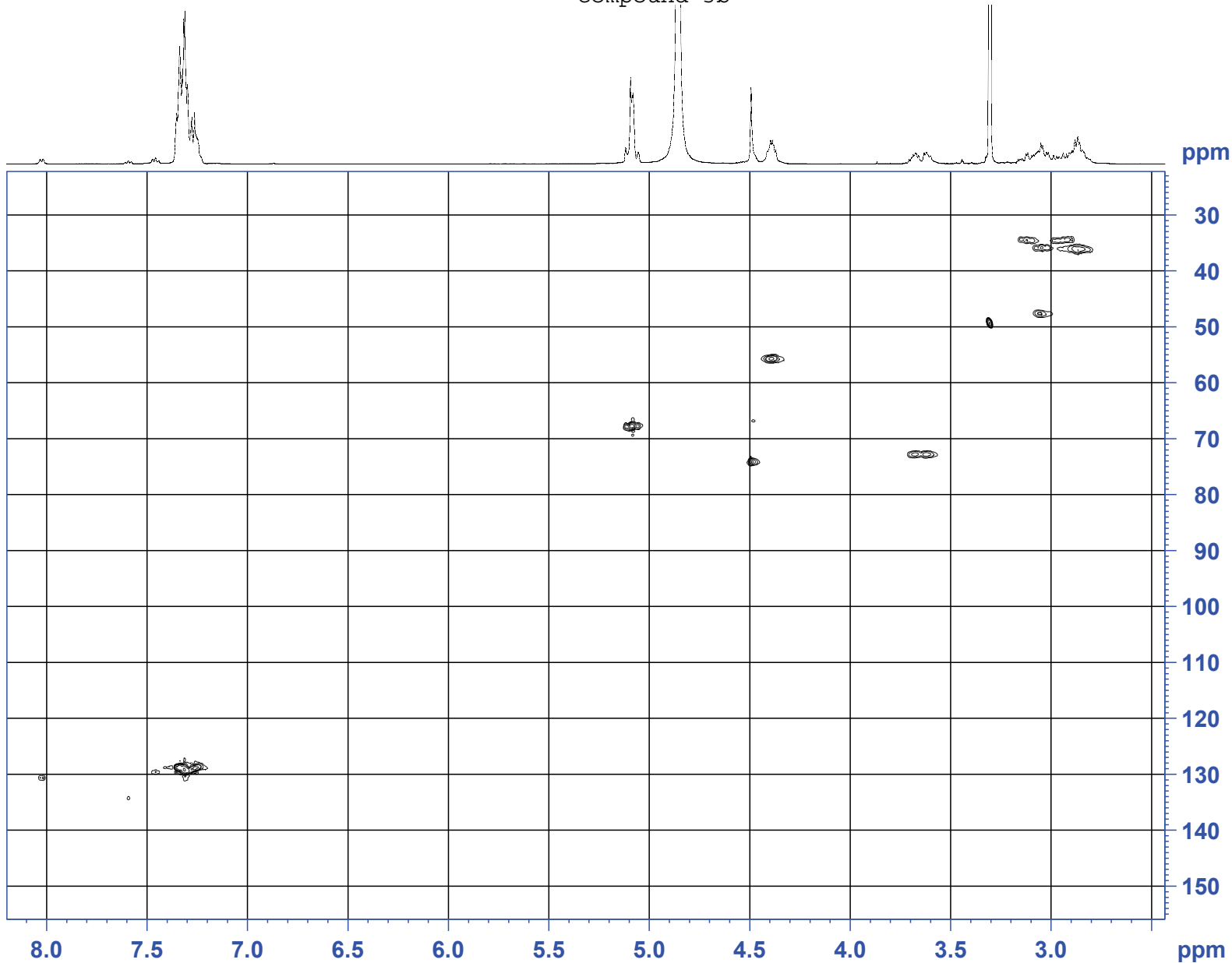
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1     10.00 %
P16      1000.00 usec

F1 - Acquisition parameters
TD       512
SFO1    500.132 MHz
FIDRES   8.797860 Hz
SW       9.007 ppm
        FnMODE    QF

F2 - Processing parameters
SI       2048
SF       500.1300117 MHz
WDW      SINE
        SSB       0
        LB       0 Hz
        GB       0
        PC       1.40

F1 - Processing parameters
SI       2048
MC2     QF
SF       500.1300117 MHz
WDW      SINE
        SSB       0
        LB       0 Hz
        GB       0
```

compound 3b



```
Current Data Parameters
NAME      50039067
EXPNO    507
PROCNO   1

F2 - Acquisition Parameters
Date_    20150218
Time     3.54
INSTRUM  spect
PROBHD   5 mm CPDCH 13C
PULPROG  hsqcdecfg
TD       2048
SOLVENT  MeOD
NS       16
DS       16
SWH      4504.504 Hz
FIDRES   2.199465 Hz
AQ       0.2273280 sec
RG       2050
DW       111.000 usec
DE       10.00 usec
TE       303.0 K
CNST2    145.0000000
D0       0.00000300 sec
D1       1.40046704 sec
D4       0.00172414 sec
D11      0.03000000 sec
D13      0.00000400 sec
D16      0.00020000 sec
D21      0.00345000 sec
IN0      0.00002090 sec
ZGPGTNS

===== CHANNEL f1 =====
SF01    500.1319832 MHz
NUC1    1H
P1      8.90 usec
P2      17.80 usec
PLM1    15.73700047 W

===== CHANNEL f2 =====
SF02    125.7678491 MHz
NUC2    13C
CPDPRG2  garp
P3      9.70 usec
P4      19.40 usec
PCPD2   70.00 usec
PLM2    34.40000153 W
PLM12   0.66055000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1    80.00 %
GPZ2    20.10 %
P16     1000.00 usec

F1 - Acquisition parameters
TD      256
SF01    125.7678 MHz
FIDRES   93.450958 Hz
SW       130.219 ppm
PnMODE   Echo-Antiecho

F2 - Processing parameters
SI       2048
SF       500.1300117 MHz
WDW      QSINE
SSB      2
LB       0 Hz
GB       0
PC       1.40

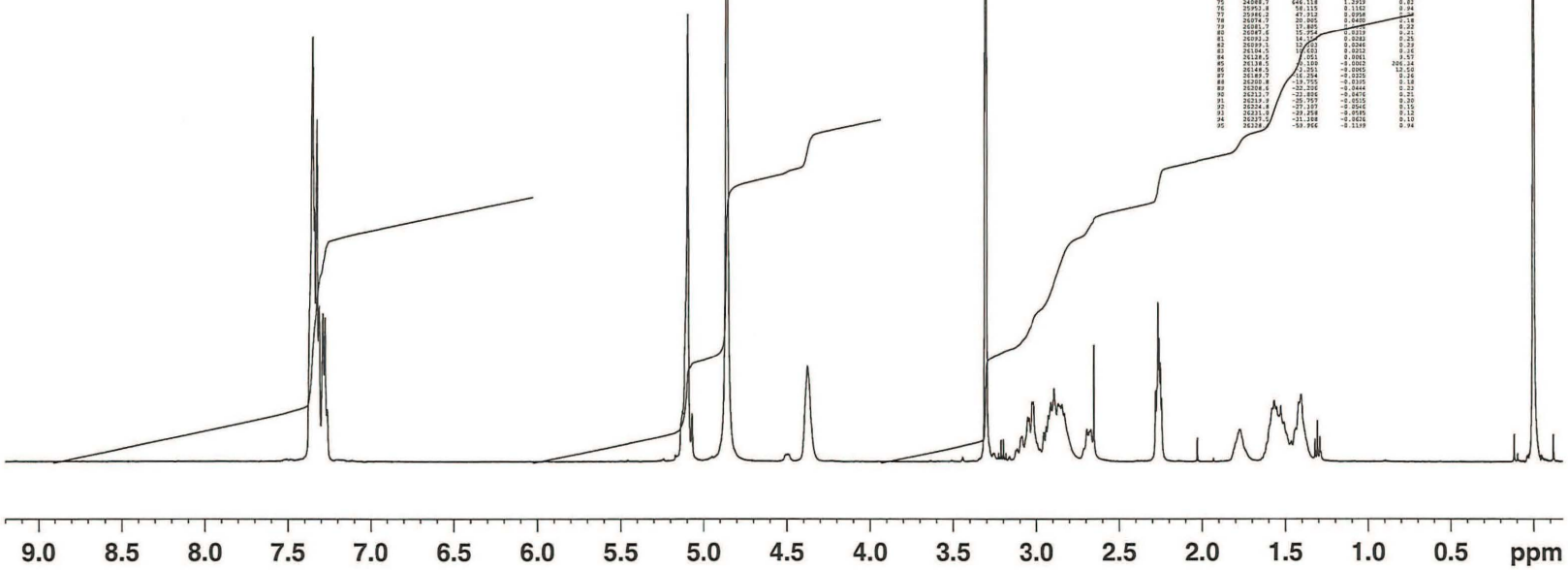
F1 - Processing parameters
SI       1024
WC2      echo-antiecho
SF       125.7576072 MHz
WDW      QSINE
SSB      2
LB       0 Hz
GB       0
```

compound 3c

NAME 62155052
EXPNO 500
PROCNO 1
Date_ 20140116
Time 8.06
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 32
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 8
DW 48.400 usec
DE 6.50 usec
TE 303.0 K
DL 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.90 usec
PL1 3.00 dB
PL1W 15.73656750 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
EC 1.00

F2	F1	Phase	Amplitude	Phase
1	14454.8	1921	1.1814	6.34
2	14454.4	2879.554	1.2188	6.49
3	14377.3	2879.552	1.2188	6.49
4	14377.3	2879.552	1.2188	6.49
5	14377.3	2879.552	1.2188	6.49
6	14377.3	2879.552	1.2188	6.49
7	14377.3	2879.552	1.2188	6.49
8	14377.3	2879.552	1.2188	6.49
9	14377.3	2879.552	1.2188	6.49
10	17925.1	2588.222	1.1709	6.22
11	18025.3	2588.222	1.1709	6.22
12	18025.3	2588.222	1.1709	6.22
13	18025.3	2588.222	1.1709	6.22
14	18025.3	2588.222	1.1709	6.22
15	18025.3	2588.222	1.1709	6.22
16	18025.3	2588.222	1.1709	6.22
17	18025.3	2588.222	1.1709	6.22
18	18025.3	2588.222	1.1709	6.22
19	20977.0	1571.038	1.4425	5.14
20	20977.0	1571.038	1.4425	5.14
21	20977.0	1571.038	1.4425	5.14
22	20977.0	1571.038	1.4425	5.14
23	20977.0	1571.038	1.4425	5.14
24	20977.0	1571.038	1.4425	5.14
25	20977.0	1571.038	1.4425	5.14
26	20977.0	1571.038	1.4425	5.14
27	20977.0	1571.038	1.4425	5.14
28	20977.0	1571.038	1.4425	5.14
29	20977.0	1571.038	1.4425	5.14
30	20977.0	1571.038	1.4425	5.14
31	20977.0	1571.038	1.4425	5.14
32	20977.0	1571.038	1.4425	5.14
33	20977.0	1571.038	1.4425	5.14
34	20977.0	1571.038	1.4425	5.14
35	20977.0	1571.038	1.4425	5.14
36	20977.0	1571.038	1.4425	5.14
37	20977.0	1571.038	1.4425	5.14
38	20977.0	1571.038	1.4425	5.14
39	20977.0	1571.038	1.4425	5.14
40	20977.0	1571.038	1.4425	5.14
41	20977.0	1571.038	1.4425	5.14
42	21477.4	1489.287	1.2755	6.43
43	21477.4	1489.287	1.2755	6.43
44	21477.4	1489.287	1.2755	6.43
45	21477.4	1489.287	1.2755	6.43
46	21477.4	1489.287	1.2755	6.43
47	21477.4	1489.287	1.2755	6.43
48	21477.4	1489.287	1.2755	6.43
49	21477.4	1489.287	1.2755	6.43
50	21477.4	1489.287	1.2755	6.43
51	21477.4	1489.287	1.2755	6.43
52	21477.4	1489.287	1.2755	6.43
53	21477.4	1489.287	1.2755	6.43
54	21477.4	1489.287	1.2755	6.43
55	21477.4	1489.287	1.2755	6.43
56	21477.4	1489.287	1.2755	6.43
57	21477.4	1489.287	1.2755	6.43
58	21477.4	1489.287	1.2755	6.43
59	21477.4	1489.287	1.2755	6.43
60	21477.4	1489.287	1.2755	6.43
61	21477.4	1489.287	1.2755	6.43
62	21477.4	1489.287	1.2755	6.43
63	21477.4	1489.287	1.2755	6.43
64	21477.4	1489.287	1.2755	6.43
65	21477.4	1489.287	1.2755	6.43
66	21477.4	1489.287	1.2755	6.43
67	21477.4	1489.287	1.2755	6.43
68	21477.4	1489.287	1.2755	6.43
69	21477.4	1489.287	1.2755	6.43
70	21477.4	1489.287	1.2755	6.43
71	21477.4	1489.287	1.2755	6.43
72	21477.4	1489.287	1.2755	6.43
73	21477.4	1489.287	1.2755	6.43
74	21477.4	1489.287	1.2755	6.43
75	21477.4	1489.287	1.2755	6.43
76	21477.4	1489.287	1.2755	6.43
77	21477.4	1489.287	1.2755	6.43
78	21477.4	1489.287	1.2755	6.43
79	21477.4	1489.287	1.2755	6.43
80	21477.4	1489.287	1.2755	6.43
81	21477.4	1489.287	1.2755	6.43
82	21477.4	1489.287	1.2755	6.43
83	21477.4	1489.287	1.2755	6.43
84	21477.4	1489.287	1.2755	6.43
85	21477.4	1489.287	1.2755	6.43
86	21477.4	1489.287	1.2755	6.43
87	21477.4	1489.287	1.2755	6.43
88	21477.4	1489.287	1.2755	6.43
89	21477.4	1489.287	1.2755	6.43
90	21477.4	1489.287	1.2755	6.43
91	21477.4	1489.287	1.2755	6.43
92	21477.4	1489.287	1.2755	6.43
93	21477.4	1489.287	1.2755	6.43
94	21477.4	1489.287	1.2755	6.43
95	21477.4	1489.287	1.2755	6.43
96	21477.4	1489.287	1.2755	6.43



2

```

NAME          62155052
EXPNO         501
PROCNO        1
Date_         20140116
Time          11.07
INSTRUM       spect
PROBHD        5 mm CPDCH 13C
PULPROG       zgpg
TD            65536
SOLVENT       MeOD
NS            1024
DS            4
SWH           30864.197 Hz
FIDRES        0.470950 Hz
AQ            1.0617332 sec
RG            645
DW            16.200 usec
DE            20.00 usec
TE            303.0 K
DL            4.0000000 sec
D11           0.03000000 sec
TDD           1

===== CHANNEL f1 =====
NUC1           13C
P1             9.70 usec
PL1            4.00 dB
PL1W          34.40000153 W
SFO1          125.7703643 MHz

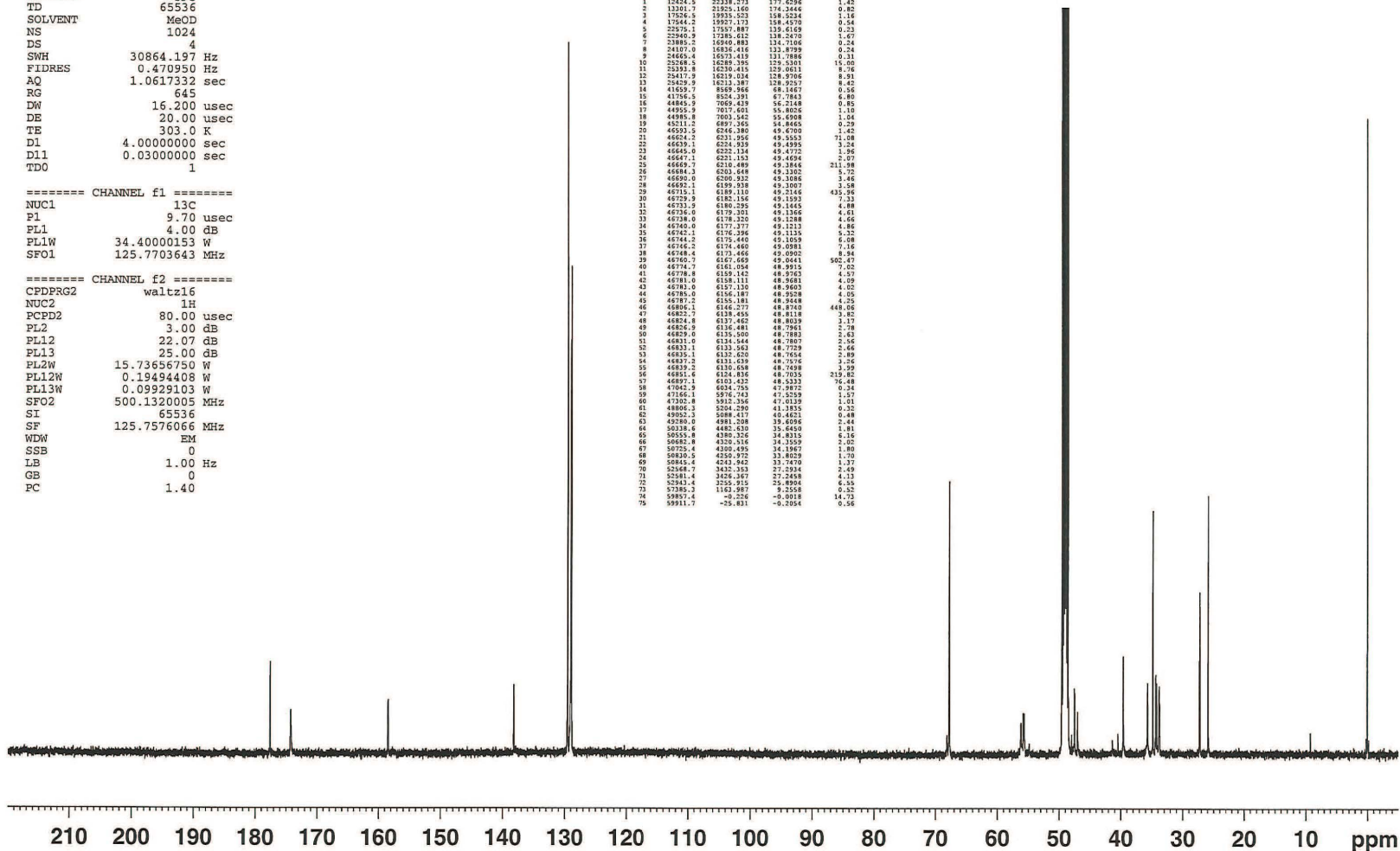
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 usec
PL2            3.00 dB
PL12          22.07 dB
PL13          25.00 dB
PL2W          15.73656750 W
PL12W         0.19494408 W
PL13W         0.0929103 W
SFO2          500.1320005 MHz
SI            65536
SF            125.7576066 MHz
WDW            EM
SSB            0
LB            1.00 Hz
GB            0
PC            1.40

```

compound 3c

EM/CPD/Topspin, UCDM=Eastrock, NAME=62155052, EXPNO=501, PROCNO=1
F1=234.160ppm, F2=21.266ppm, MI=0.00cm, MAXT=10000.00cm, PC=1.400

#	ABSCISSA	FREQUENCY	INTENSITY
1	12424.5	22338.773	177.4526
2	13201.7	21925.160	174.2446
3	17524.5	19325.523	198.2524
4	17544.2	19327.173	198.4570
5	22575.1	17527.887	198.6169
6	22940.9	17385.612	198.2470
7	23885.2	16940.183	197.2106
8	24107.0	16836.416	197.8739
9	24650.4	16373.419	197.7886
10	25268.5	16280.395	199.5301
11	25393.8	16290.415	199.0611
12	25417.9	16219.034	198.9706
13	25429.9	16212.387	198.9611
14	41659.7	8549.966	68.1467
15	41756.5	8524.293	67.7863
16	44845.9	7069.439	56.2148
17	44955.9	7077.603	56.8026
18	44985.8	7003.542	55.4908
19	45111.2	6897.365	54.8465
20	45203.5	6746.380	49.6700
21	46624.2	6231.956	49.5523
22	46639.1	6234.939	49.4995
23	46645.0	6222.134	49.4772
24	46647.1	6231.153	49.4634
25	46659.7	6210.489	49.2846
26	46684.3	6203.648	49.2302
27	46690.0	6200.322	49.2086
28	46692.1	6199.938	49.2007
29	46715.1	6189.110	49.2146
30	46729.9	6182.156	49.1993
31	46731.9	6180.729	49.1465
32	46736.0	6179.301	49.1366
33	46738.0	6178.320	49.1288
34	46740.0	6177.377	49.1213
35	46742.1	6176.396	49.1135
36	46744.2	6175.460	49.1059
37	46746.2	6174.460	49.0981
38	46748.4	6173.460	49.0902
39	46750.7	6172.460	49.0841
40	46774.7	6161.094	48.9915
41	46778.8	6159.113	48.9808
42	46781.0	6158.113	48.9808
43	46783.0	6157.130	48.9603
44	46785.0	6156.187	48.9608
45	46787.2	6155.181	48.9448
46	46809.0	6144.272	48.9708
47	46822.7	6138.455	48.8118
48	46824.8	6137.452	48.8039
49	46826.9	6136.481	48.7961
50	46829.0	6135.500	48.7883
51	46831.0	6134.544	48.7807
52	46833.1	6133.563	48.7729
53	46835.1	6132.620	48.7654
54	46837.2	6131.639	48.7576
55	46839.2	6130.658	48.7498
56	46841.4	6129.678	48.7420
57	46847.1	6103.432	48.5332
58	47042.9	6024.793	47.9872
59	47164.1	5976.743	47.5259
60	47302.8	5928.396	47.0199
61	48806.3	5204.290	41.1835
62	48952.3	5088.417	40.4633
63	49280.0	4981.208	39.6096
64	50138.4	4822.530	38.6450
65	50555.8	4780.326	34.8315
66	50602.8	4720.316	33.2509
67	50725.4	4700.495	34.1967
68	50810.5	4620.972	33.8079
69	50845.4	4243.942	33.7470
70	52668.7	3425.353	27.2834
71	52881.4	3426.367	27.2458
72	52843.4	2526.915	25.8906
73	57385.3	1163.987	9.2558
74	59897.4	-9.226	-0.0018
75	59911.7	-25.831	-0.2054



L

compound 3c

CH,CH3-signals positive, CH2-signals negative

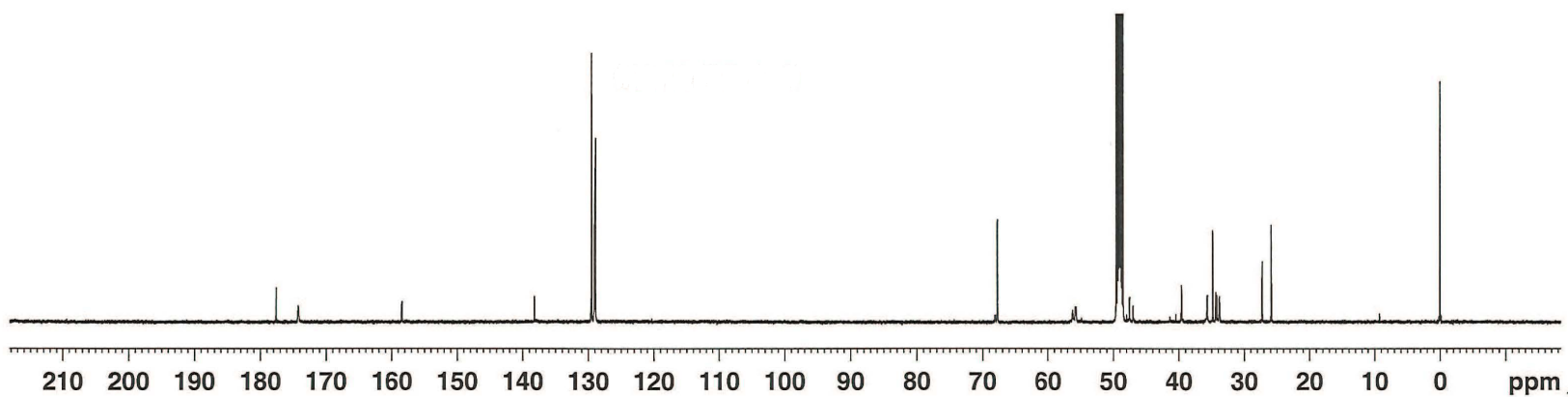
DE=cpt/topspin, USER=SamTrack, NAME=62155052, EXPNO=502, PROCNO=1
F1=215.778ppm, F2=16.883ppm, MI=0.50cm, MAXI=10000.00cm, PC=1.400

#	ADDRESS	FREQUENCY [PPM]	INTENSITY	
1	24992.0	16288.842	129.5257	15.00
2	25123.7	16229.019	129.0500	6.15
3	25146.6	16218.644	128.9678	9.06
4	25159.2	16212.897	128.9218	10.92
5	25178.8	16204.056	128.8815	1.52
6	42089.8	8524.228	67.7830	-5.91
7	45399.7	7066.486	56.1944	0.60
8	45442.2	7051.769	55.8767	0.74
9	47105.7	6246.355	49.6698	1.99
10	47152.9	6234.913	49.4993	4.58
11	47200.1	6203.459	49.3287	6.84
12	47247.4	6161.980	49.1579	4.37
13	47294.8	6160.463	48.9868	2.31
14	47698.9	5976.997	47.5276	1.07
15	47839.4	5913.148	47.0202	0.68
16	49892.2	4980.819	39.6073	-1.78
17	50989.7	4482.504	35.6440	-1.43
18	51214.3	4380.490	34.8328	-4.53
19	51345.7	4330.809	34.3582	-1.33
20	51389.4	4300.973	34.2005	-1.12
21	51499.4	4251.035	33.8034	-1.49
22	53301.7	3432.341	27.2949	-1.38
23	53315.1	3426.442	27.2464	-2.16
24	53889.1	3256.619	26.8960	-4.20
25	60860.2	0.013	0.0001	20.63
26	60916.4	-25.529	-0.2030	0.70

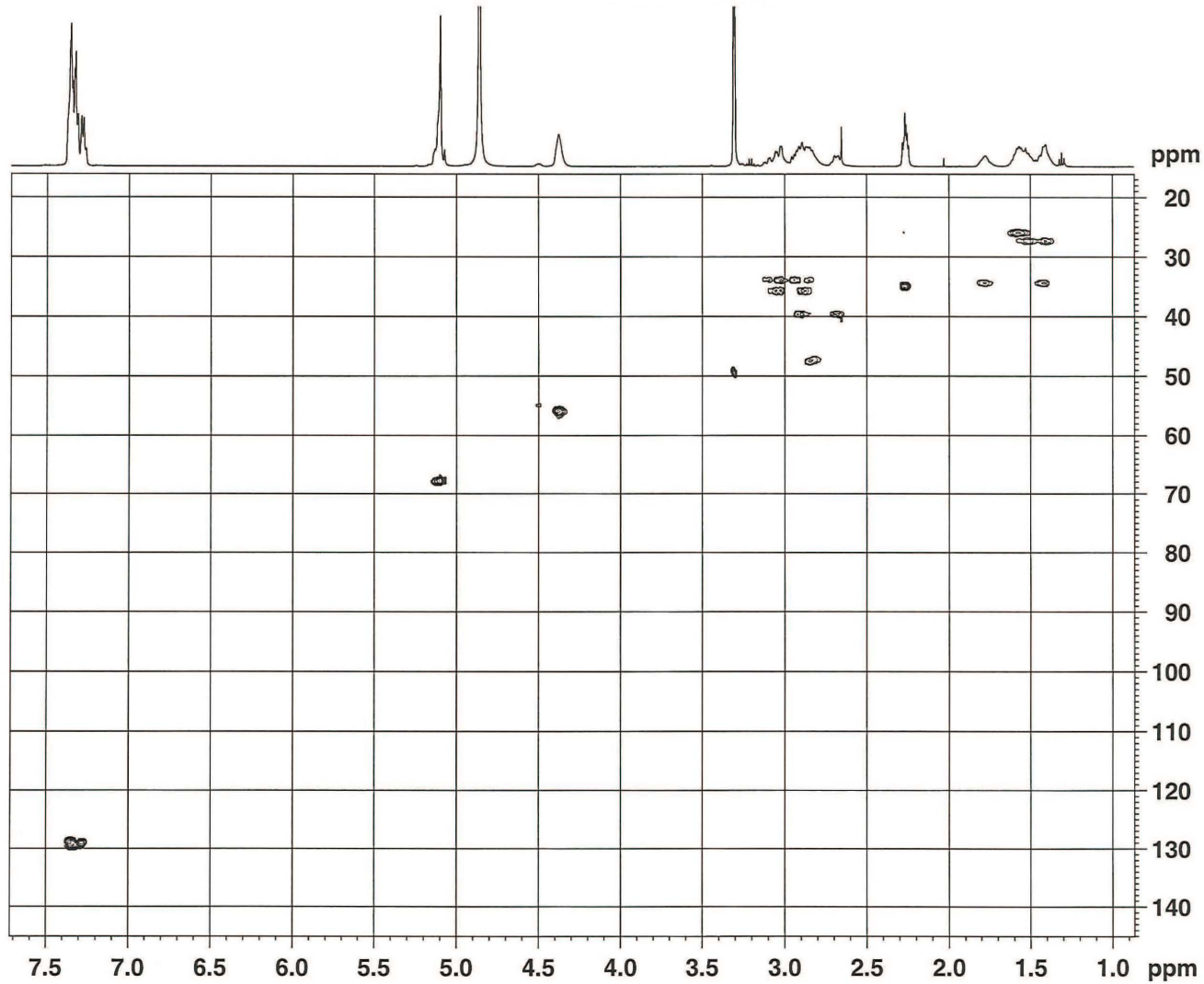
DE=cpt/topspin, USER=SamTrack, NAME=62155052, EXPNO=503, PROCNO=1
F1=215.778ppm, F2=16.883ppm, MI=0.50cm, MAXI=10000.00cm, PC=1.400

#	ADDRESS	FREQUENCY [PPM]	INTENSITY	
1	24992.0	16288.842	129.5257	15.00
2	25123.8	16228.994	129.0498	6.21
3	25146.5	16218.682	128.9678	9.01
4	25159.2	16212.897	128.9218	11.05
5	25178.8	16204.056	128.8815	1.62
6	45408.3	7017.174	55.7992	0.69
7	47105.5	6246.405	49.6702	2.20
8	47152.8	6234.926	49.4994	4.42
9	47200.1	6203.484	49.3289	6.73
10	47247.3	6182.018	49.1592	4.42
11	47294.7	6160.500	48.9871	2.18
12	47699.4	5976.718	47.5257	0.94
13	47840.9	5912.481	47.0149	0.61
14	60860.2	-0.013	-0.0001	0.99

CH-signals



compound 3c



```
NAME 62155052
EXPNO 1
PROCNO 504
Date_ 20140116
Time 8.43
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG hsqcetgpsisp2.2
TD 7948
SOLVENT MeOD
NS 2
DS 16
SWH 4347.826 Hz
FIDRES 2.122952 Hz
AQ 0.2355700 sec
RG 2050
DW 115.000 usec
DE 6.50 usec
TE 303.0 K
CNS22 145.0000000
CNS17 -0.5000000
DO 0.00000300 sec
DL 1.39227498 sec
D4 0.00175414 sec
D11 0.03000000 sec
D16 0.00200000 sec
D24 0.00110000 sec
IN0 0.00002090 sec

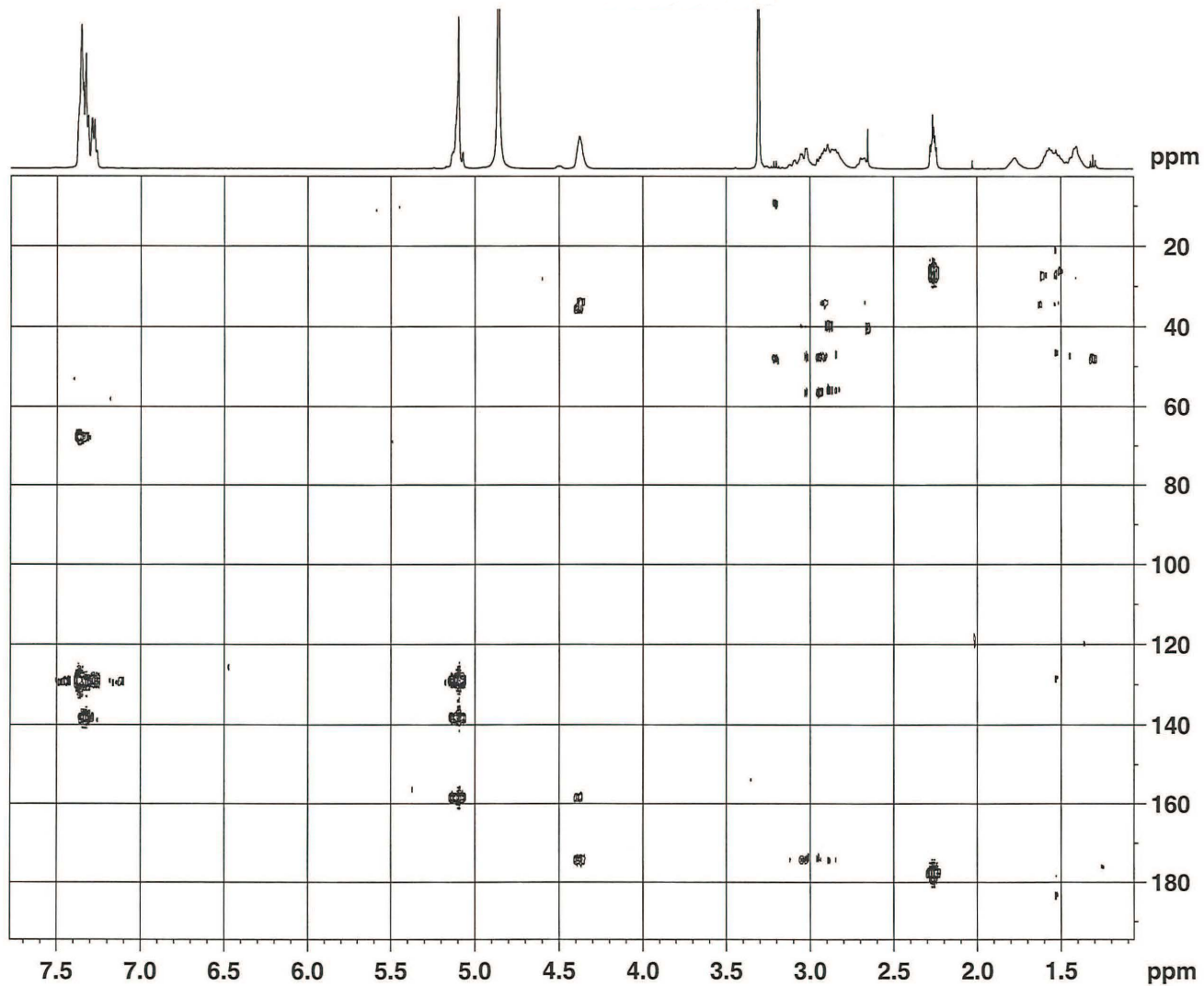
***** CHANNEL f1 *****
NUC1 1H
P1 8.90 usec
P2 17.80 usec
P28 1000.00 usec
PL1 3.00 dB
PL1W 15.7365750 W
SFO1 500.1318645 MHz

***** CHANNEL f2 *****
CPDPRG2 garp
NUC2 13C
P3 9.70 usec
P14 500.00 usec
P24 2000.00 usec
PCPD2 65.00 usec
PL0 120.00 dB
PL2 4.00 dB
PL12 20.52 dB
PL0W 0.00000000 W
PL2W 34.40000153 W
PL12W 0.7658159 W
SFO2 125.7678496 MHz
SP3 12.42 dB
SP7 12.42 dB
SFO3 Crp60,0.5,20.1
SFO4 Crp60comp,4
SFOAL3 0.500
SFOAL7 0.500
SPOFFS3 0.00 Hz
SPOFFS7 0.00 Hz

***** GRADIENT CHANNEL *****
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPNAM4 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec
ND0 2
TD 256
SFO1 125.7678 MHz
FIDRES 93.342123 Hz
SW 190.000 ppm
FmMODE Echo-Antiecho
SI 2048
SF 500.1300132 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 125.7576066 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
```

K

compound 3c



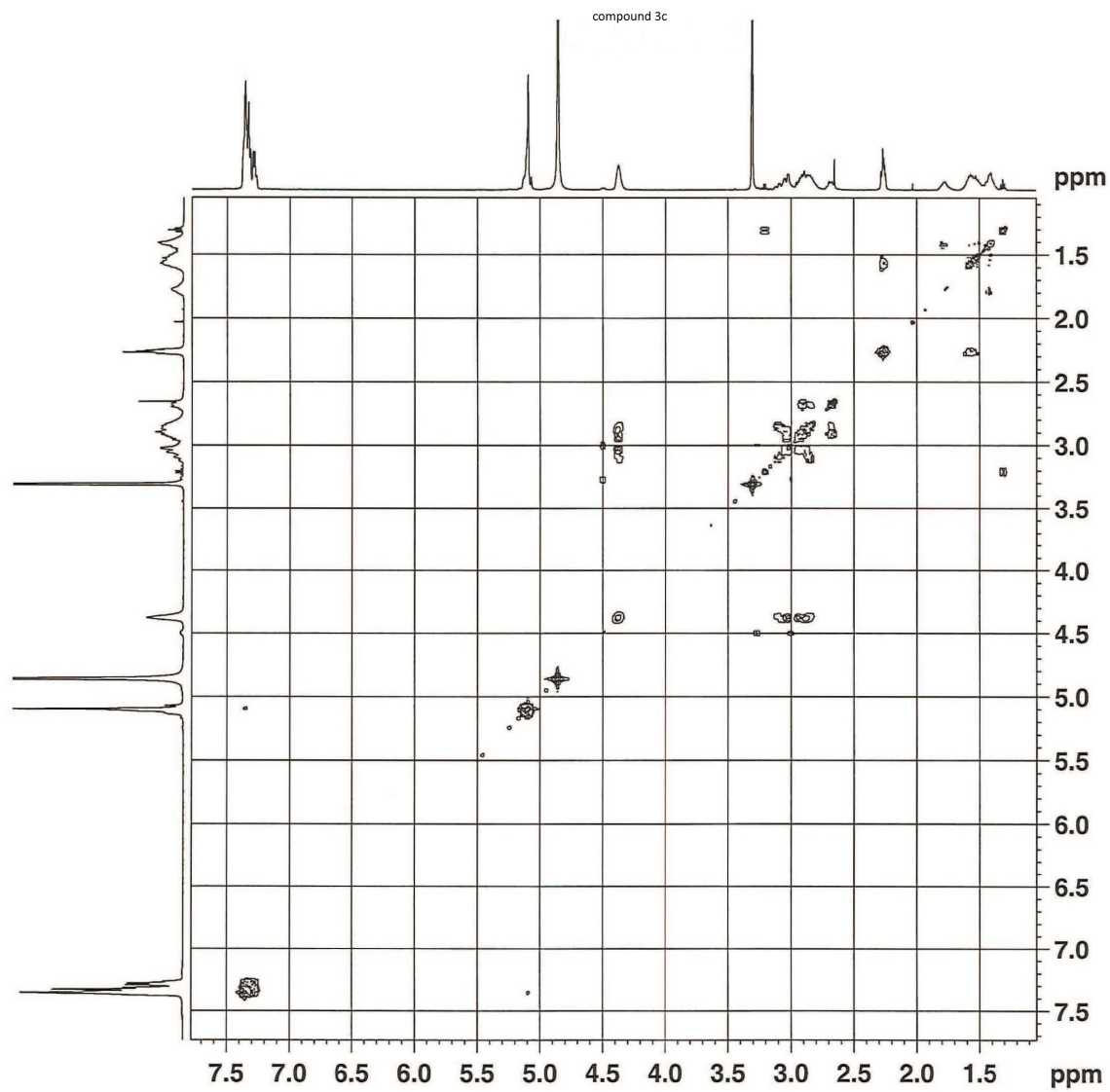
```
NAME 62155052
EXPNO 505
PROCNO 1
Date_ 20140116
Time 11.08
INSTRUM spect
PROBHD 5 mm CPDCH 13C
FULPROG hmbcetsp12nd
TD 2048
SOLVENT MeOD
NS 16
DS 16
SWH 4347.826 Hz
FIDRES 2.122962 Hz
AQ 0.2355700 sec
RG 2050
DW 115.000 usec
DE 6.50 usec
TE 303.0 K
CNS*6 125.0000000
CNS*7 160.0000000
CNS*13 10.0000000
CNS*30 0.5981150
D0 0.00000300 sec
D1 1.42176604 sec
D5 0.05000000 sec
D16 0.00020000 sec
IN0 0.00001790 sec

===== CHANNEL f1 =====
NUC1 1H
P1 8.90 usec
P2 17.80 usec
PL1 3.00 dB
PL1W 15.73656750 W
SFO1 500.1318645 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 9.70 usec
P24 2000.00 usec
PL2 4.00 dB
PL2W 34.40000153 W
SFO2 125.7703443 MHz
SP7 12.42 dB
SPNAM7 Crp60comp.4
SFOAL7 0.500
SPOFFS7 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM3 SINE.100
GPNAM4 SINE.100
GPNAM5 SINE.100
GPZ1 80.00 %
GPZ3 15.00 %
GPZ4 -10.00 %
GPZ5 -5.00 %
P16 NDO 1000.00 usec 2
TD 256
SFO1 125.7703 MHz
FIDRES 109.113174 Hz
SW 222.095 ppm
FnMODE Echo-Antiecho
SI 2048
SF 500.1300132 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 125.7576066 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
```

6



```

NAME          62155052
EXPNO         506
PROCNO        1
Date_         20140116
Time          9.13
INSTRUM       spect
PROBHD        5 mm CPDCH 13C
PULPROG       cosygpppqf
TD            2048
SOLVENT       MeOD
NS            1
DS            16
SWH           4347.826 Hz
FIDRES        2.122962 Hz
AQ            0.2355700 sec
RG            18
DW            115.000 usec
DE            6.50 usec
TE            303.0 K
DO            0.0000300 sec
D1            1.37916696 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00023000 sec

```

```

===== CHANNEL f1 =====
NUC1          1H
P0            8.90 usec
P1            8.90 usec
P17           2500.00 usec
  PL1         3.00 dB
  PL10        13.84 dB
  PL1W        15.73656750 W
  PL10W       1.29691052 W
SFO1          500.1318645 MHz

```

```

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPZ1          10.00 %
P16           1000.00 usec
  NDO         1
  TD          512
SFO1          500.1319 MHz
FIDRES        8.491848 Hz
SW            8.693 ppm
  F1MODE      QF
  SI          2048
SF            500.1300132 MHz
  WDW         SINE
  SSB         0
  LB          0.00 Hz
  GB          0
  PC          1.40
  SI          2048
  MC2         QF
SF            500.1300132 MHz
  WDW         SINE
  SSB         0
  LB          0.00 Hz
  GB          0

```

u-

```

NAME      62155052
EXPNO    500
PROCNO   1
Date_    20140116
Time     8.06
INSTRUM  spect
PROBHD   5 mm CPDCH 13C
PULPROG  zg30
TD       65536
SOLVENT  MeOD
NS       32
DS       2
SWH      10330.578 Hz
FIDRES   0.157632 Hz
AQ       3.1719923 sec
RG       8
DW       48.400 usec
DE       6.50 usec
TE       303.0 K
DL       1.00000000 sec
TD0      1

```

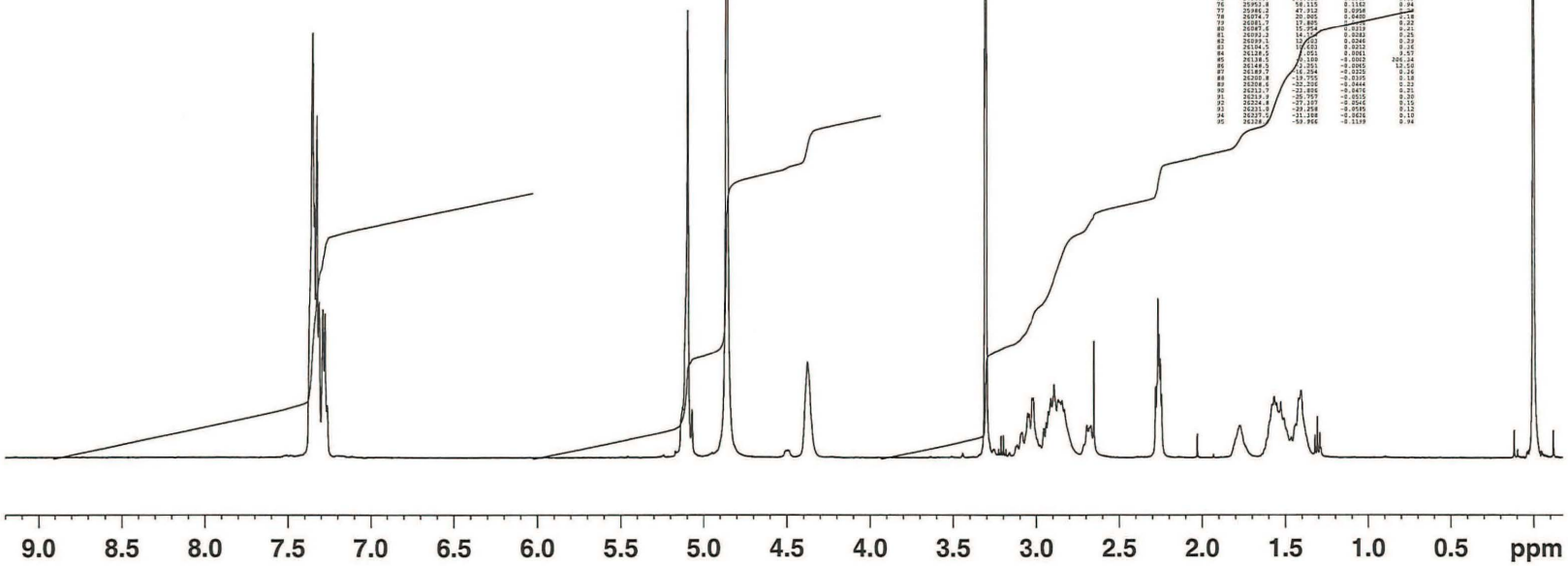
```

===== CHANNEL f1 =====
NUC1      1H
P1        8.90 usec
PL1       3.00 dB
PL1W     15.73656750 W
SFO1     500.1330885 MHz
SI        32768
SF       500.1300132 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
EC        1.00

```

compound 3d

1	14454.8	212.254	1.2114	6.34
2	14454.4	2079.954	7.2398	8.49
3	14453.3	2081.052	7.2398	1.45
4	14452.9	2079.954	7.2398	1.45
5	14452.0	2079.954	7.2398	5.17
6	14451.1	2079.954	7.2398	2.04
7	14450.5	2079.954	7.2398	4.05
8	14450.4	2079.954	7.2398	4.05
9	14450.3	2079.954	7.2398	1.77
10	17925.1	2088.222	5.1709	0.22
11	18025.3	2088.222	5.1709	0.22
12	18025.3	2088.222	5.1709	15.05
13	18025.8	2088.222	5.1709	0.22
14	18029.9	2074.202	4.9973	1.18
15	18032.5	2420.232	4.8526	89.55
16	18032.5	2420.232	4.8526	0.22
17	18032.5	2420.232	4.8526	0.22
18	18126.2	2188.513	4.7309	0.22
19	20077.0	1571.038	3.4427	0.14
20	20242.2	1702.249	3.4222	0.10
21	20884.7	1834.214	3.2564	0.17
22	20885.1	1832.212	3.2564	0.16
23	20884.9	1834.181	3.2564	12.68
24	20889.8	1874.880	3.2082	26.64
25	20895.0	1852.289	3.2051	37.78
26	20895.1	1851.279	3.2089	39.80
27	20925.0	1848.237	3.2089	14.89
28	20964.5	1831.074	3.2613	14.29
29	20976.1	1827.423	3.2565	0.24
30	21037.5	1834.279	3.2279	8.29
31	21042.6	1827.424	3.2222	0.74
32	21052.8	1839.744	3.1887	0.74
33	21087.0	1832.464	3.1841	0.28
34	21129.4	1821.011	3.1532	0.19
35	21139.3	1840.411	3.1090	0.15
36	21139.4	1838.420	3.1054	0.44
37	21239.7	1844.401	3.0880	0.47
38	21239.7	1838.447	3.0835	0.19
39	21239.7	1838.447	3.0835	1.49
40	21242.1	1833.242	3.0821	2.02
41	21252.6	1838.422	3.0402	0.02
42	21477.4	1489.287	2.9759	0.43
43	21481.0	1479.488	2.9644	0.19
44	21481.0	1479.488	2.9644	0.19
45	21481.9	1453.328	2.9261	1.56
46	21525.8	1455.378	2.9261	2.05
47	21559.7	1446.276	2.9118	2.46
48	21559.4	1432.322	2.9055	1.77
49	21575.9	1432.322	2.9055	1.77
50	21575.9	1432.322	2.9055	1.94
51	21594.0	1434.788	2.8984	1.64
52	21644.3	1387.488	2.8791	1.10
53	21688.4	1332.788	2.8788	1.04
54	21702.3	1334.444	2.8703	1.06
55	21731.2	1326.299	2.8519	1.99
56	21732.0	1318.664	2.8501	0.41
57	21745.0	1323.794	2.8503	5.18
58	21755.0	1327.844	2.8379	4.17
59	21755.0	1327.844	2.8379	1.17
60	21774.9	1323.792	2.8425	2.15
61	21792.8	1314.314	2.8266	0.50
62	21794.4	1305.201	2.8233	0.10
63	21794.4	1305.201	2.8233	0.10
64	21813.8	1290.261	2.8081	0.79
65	21813.8	1290.261	2.8081	0.79
66	21813.8	1290.261	2.8081	3.06
67	21813.8	1290.261	2.8081	0.81
68	21813.8	1290.261	2.8081	1.87
69	21813.8	1290.261	2.8081	1.87
70	21813.8	1290.261	2.8081	1.87
71	21813.8	1290.261	2.8081	1.87
72	21813.8	1290.261	2.8081	1.87
73	21813.8	1290.261	2.8081	1.87
74	21813.8	1290.261	2.8081	1.87
75	21813.8	1290.261	2.8081	1.87
76	21813.8	1290.261	2.8081	1.87
77	21813.8	1290.261	2.8081	1.87
78	21813.8	1290.261	2.8081	1.87
79	21813.8	1290.261	2.8081	1.87
80	21813.8	1290.261	2.8081	1.87
81	21813.8	1290.261	2.8081	1.87
82	21813.8	1290.261	2.8081	1.87
83	21813.8	1290.261	2.8081	1.87
84	21813.8	1290.261	2.8081	1.87
85	21813.8	1290.261	2.8081	1.87
86	21813.8	1290.261	2.8081	1.87
87	21813.8	1290.261	2.8081	1.87
88	21813.8	1290.261	2.8081	1.87
89	21813.8	1290.261	2.8081	1.87
90	21813.8	1290.261	2.8081	1.87
91	21813.8	1290.261	2.8081	1.87
92	21813.8	1290.261	2.8081	1.87
93	21813.8	1290.261	2.8081	1.87
94	21813.8	1290.261	2.8081	1.87
95	21813.8	1290.261	2.8081	1.87
96	21813.8	1290.261	2.8081	1.87



2

NAME 62155052
EXPNO 501
PROCNO 1
Date_ 20140116
Time 11.07
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg
TD 65536
SOLVENT MeOD
NS 1024
DS 4
SWH 30864.197 Hz
FIDRES 0.470950 Hz
AQ 1.0617332 sec
RG 645
DW 16.200 usec
DE 20.00 usec
TE 303.0 K
DL 4.0000000 sec
D11 0.03000000 sec
TDD 1

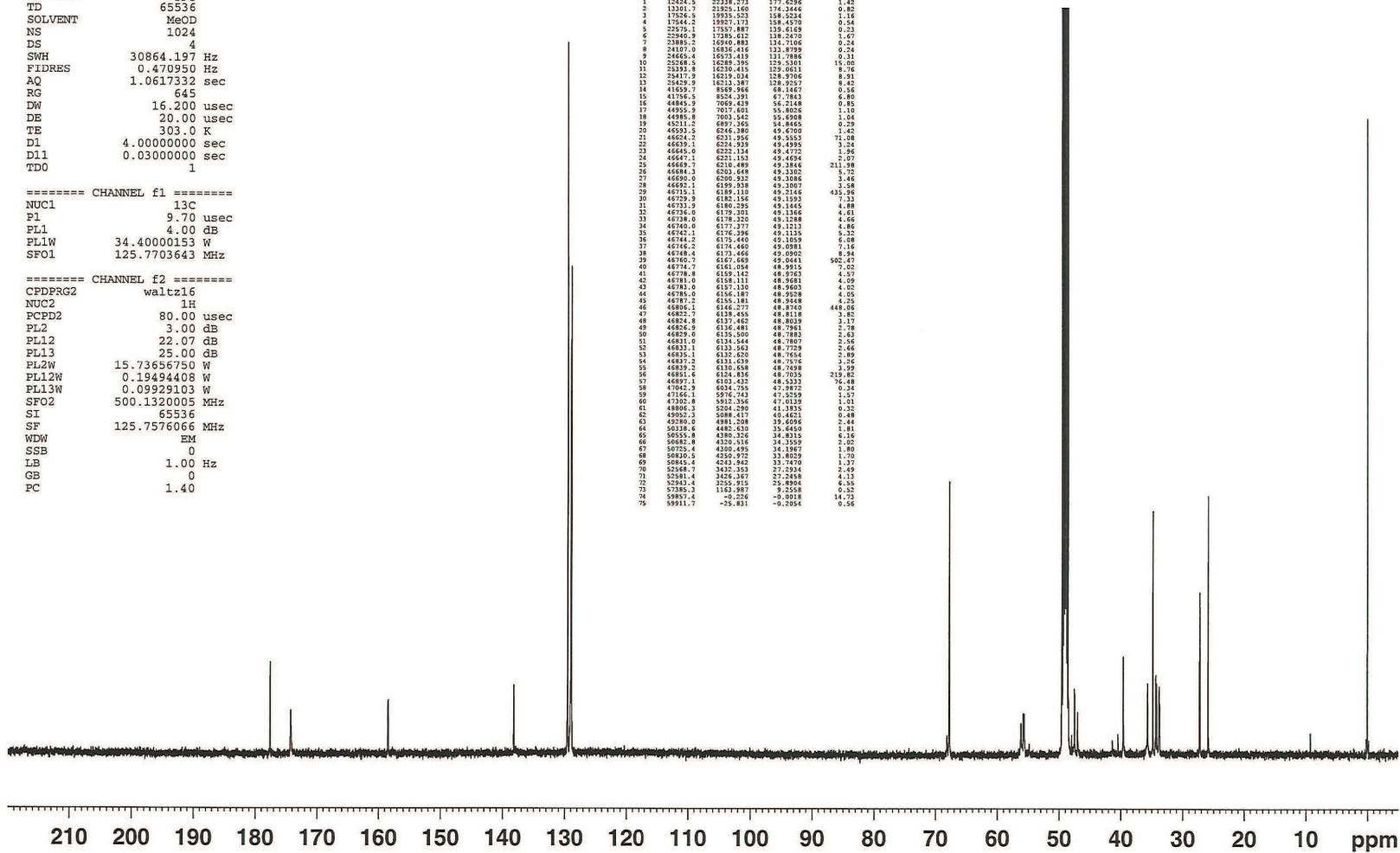
===== CHANNEL f1 =====
NUC1 13C
P1 9.70 usec
PL1 4.00 dB
PL1W 34.40000153 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.07 dB
PL13 25.00 dB
PL2W 15.73656750 W
PL12W 0.19494408 W
PL13W 0.0929103 W
SFO2 500.1320005 MHz
SI 65536
SF 125.7576066 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

compound 3d

EM/CPD/Topspin, UCDM=FastTrack, NAME=62155052, EXPNO=501, PROCNO=1
F1=234.160ppm, F2=21.266ppm, MI=0.00cm, MAXF=10000.00cm, PC=1.400

#	NAME	F1 (ppm)	F2 (ppm)	INTENSITY
1		12424.5	22338.773	177.4526
2		13201.7	21925.160	174.2446
3		17524.5	19235.523	198.2524
4		17544.2	19271.173	158.4570
5		22575.1	17527.887	139.6169
6		22940.9	17385.612	138.2470
7		23885.2	16940.883	134.2106
8		24107.0	16836.416	133.8739
9		24650.4	16273.419	131.7886
10		25268.5	16280.395	129.5301
11		25393.8	16230.415	129.0611
12		25417.9	16219.034	128.9706
13		25429.9	16212.387	128.9623
14		41659.7	8549.966	68.1467
15		41756.5	8524.293	67.7863
16		44845.9	7069.439	56.2148
17		44955.2	7077.603	56.8026
18		44985.8	7003.542	55.4908
19		45111.2	6897.365	54.8465
20		45233.5	6246.380	49.6700
21		44624.2	6231.356	49.5523
22		44639.1	6234.939	49.4995
23		44645.0	6222.134	49.4772
24		44647.1	6231.153	49.4634
25		44649.7	6210.489	49.2846
26		44684.3	6203.648	49.2302
27		44690.0	6200.322	49.2086
28		44692.1	6199.938	49.2007
29		44715.1	6189.110	49.2146
30		44729.9	6182.156	49.1993
31		44731.9	6180.729	49.1465
32		44736.0	6179.301	49.1366
33		44738.0	6178.320	49.1288
34		44740.0	6177.377	49.1213
35		44742.1	6176.396	49.1135
36		44744.2	6175.460	49.1059
37		44746.2	6174.460	49.0981
38		44748.4	6173.460	49.0902
39		44750.7	6172.460	49.0841
40		44774.7	6161.094	48.9915
41		44778.8	6159.113	48.9808
42		44781.0	6158.113	48.9808
43		44783.0	6157.130	48.9603
44		44785.0	6156.187	48.9608
45		44787.2	6155.181	48.9448
46		44809.0	6144.272	48.9708
47		44822.7	6138.455	48.8118
48		44824.8	6137.462	48.8039
49		44826.9	6136.481	48.7961
50		44829.0	6135.500	48.7883
51		44831.0	6134.544	48.7807
52		44833.1	6133.563	48.7729
53		44835.1	6132.620	48.7654
54		44837.2	6131.639	48.7576
55		44839.2	6130.658	48.7498
56		44841.3	6129.678	48.7420
57		44843.3	6128.735	48.7342
58		47042.9	6204.793	67.9872
59		47164.1	5976.743	47.5259
60		47302.8	5924.396	47.5139
61		48806.3	5204.290	41.1835
62		48952.3	5088.417	40.4633
63		49280.0	4981.208	39.6096
64		50138.4	4821.530	38.6450
65		50555.8	4780.326	34.8315
66		50602.8	4720.316	33.2509
67		50725.4	4700.495	34.1967
68		50810.5	4520.972	33.8079
69		50845.4	4243.942	33.7470
70		52668.7	3425.353	27.2834
71		52881.4	3426.367	27.2458
72		52843.4	2526.915	25.8906
73		57385.3	1163.987	9.2558
74		59897.4	-9.226	-0.0018
75		59911.7	-25.831	-0.2054



L

DI=cpt/topspin, USER=SamTrack, NAME=62155052, EXPNO=502, PROCNO=1
 F1=215.778ppm, F2=16.883ppm, MI=0.50cm, MAXI=10000.00cm, PC=1.400

CH,CH3-signals positive, CH2-signals negative

#	ADDRESS	FREQUENCY [PPM]	INTENSITY
1	24992.0	16288.842	129.5257
2	25123.7	16229.019	129.0500
3	25146.6	16218.644	128.9678
4	25159.2	16212.897	128.9218
5	25178.8	16204.056	128.8815
6	42089.8	8524.238	67.7830
7	45399.7	7066.486	56.1934
8	45442.2	7051.769	55.8767
9	47105.7	6246.355	49.6698
10	47152.9	6234.913	49.4993
11	47200.1	6203.459	49.3287
12	47247.4	6161.980	49.1579
13	47294.8	6160.463	48.9868
14	47698.9	5976.997	47.5276
15	47839.4	5913.148	47.0202
16	49892.2	4980.819	39.6073
17	50989.7	4462.504	35.6440
18	51214.3	4380.490	34.8328
19	51345.7	4330.809	34.3582
20	51389.4	4300.973	34.2005
21	51499.4	4251.035	33.8034
22	53301.7	3432.341	27.2949
23	53315.1	3426.442	27.2464
24	53889.1	3256.619	26.8960
25	60860.2	0.013	0.0001
26	60916.4	-25.529	-0.2030



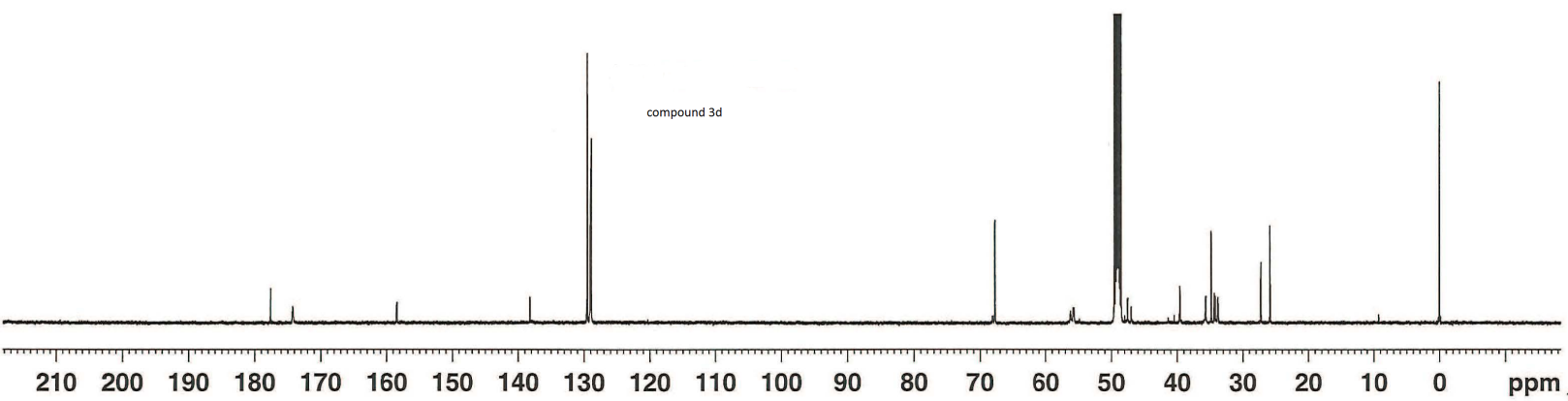
DI=cpt/topspin, USER=SamTrack, NAME=62155052, EXPNO=503, PROCNO=1
 F1=215.778ppm, F2=16.883ppm, MI=0.50cm, MAXI=10000.00cm, PC=1.400

CH-signals

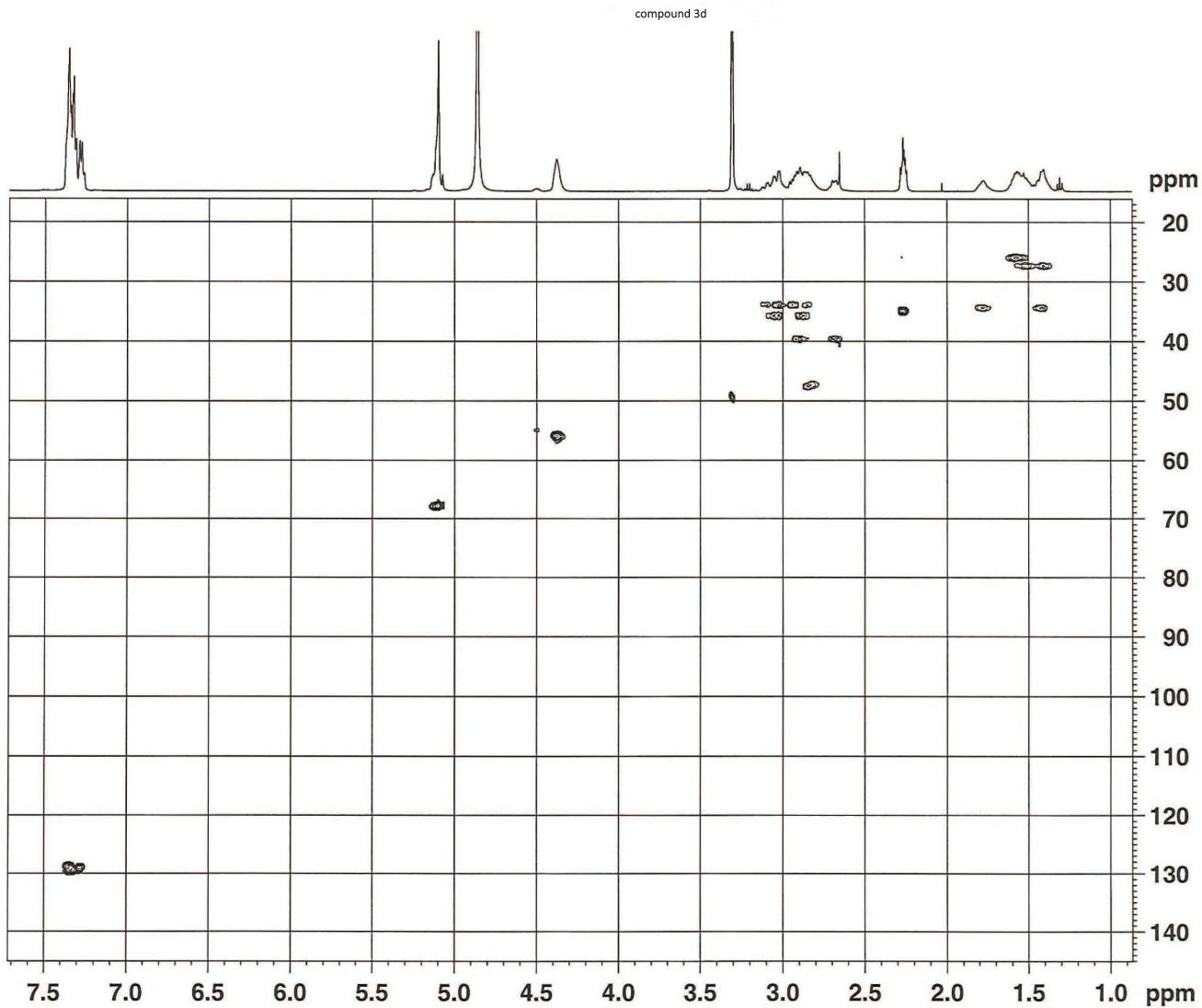
#	ADDRESS	FREQUENCY [PPM]	INTENSITY
1	24992.0	16288.842	129.5257
2	25123.8	16228.994	129.0498
3	25146.5	16218.682	128.9678
4	25159.2	16212.897	128.9218
5	25178.8	16204.056	128.8815
6	45408.3	7017.174	55.7992
7	47105.5	6246.405	49.6702
8	47152.8	6234.926	49.4994
9	47200.1	6203.484	49.3289
10	47247.3	6182.018	49.1592
11	47294.7	6160.500	48.9871
12	47699.4	5976.718	47.5257
13	47840.9	5912.481	47.0149
14	60860.2	-0.013	-0.0001



compound 3d



W



```

NAME          62155052
EXPNO         1
PROCNO        1
Date_         20140116
Time          8.43
INSTRUM       spect
PROBHD        5 mm CPDCH 13C
PULPROG       hsqcetgpsisp2.2
TD            7948
SOLVENT       MeOD
NS            2
DS            16
SWH           4347.826 Hz
FIDRES        2.122952 Hz
AQ            0.2355700 sec
RG            2050
DW            115.000 usec
DE            6.50 usec
TE            303.0 K
CNS22         145.0000000
CNS17         -0.5000000
DO            0.00000300 sec
DL            1.39227498 sec
D4            0.00175414 sec
D11           0.03000000 sec
D16           0.00200000 sec
D24           0.00110000 sec
IN0           0.00002090 sec

***** CHANNEL f1 *****
NUC1           1H
P1             8.90 usec
P2            17.80 usec
P28           1000.00 usec
PL1            3.00 dB
PL1W          15.7365750 W
SFO1          500.1318645 MHz

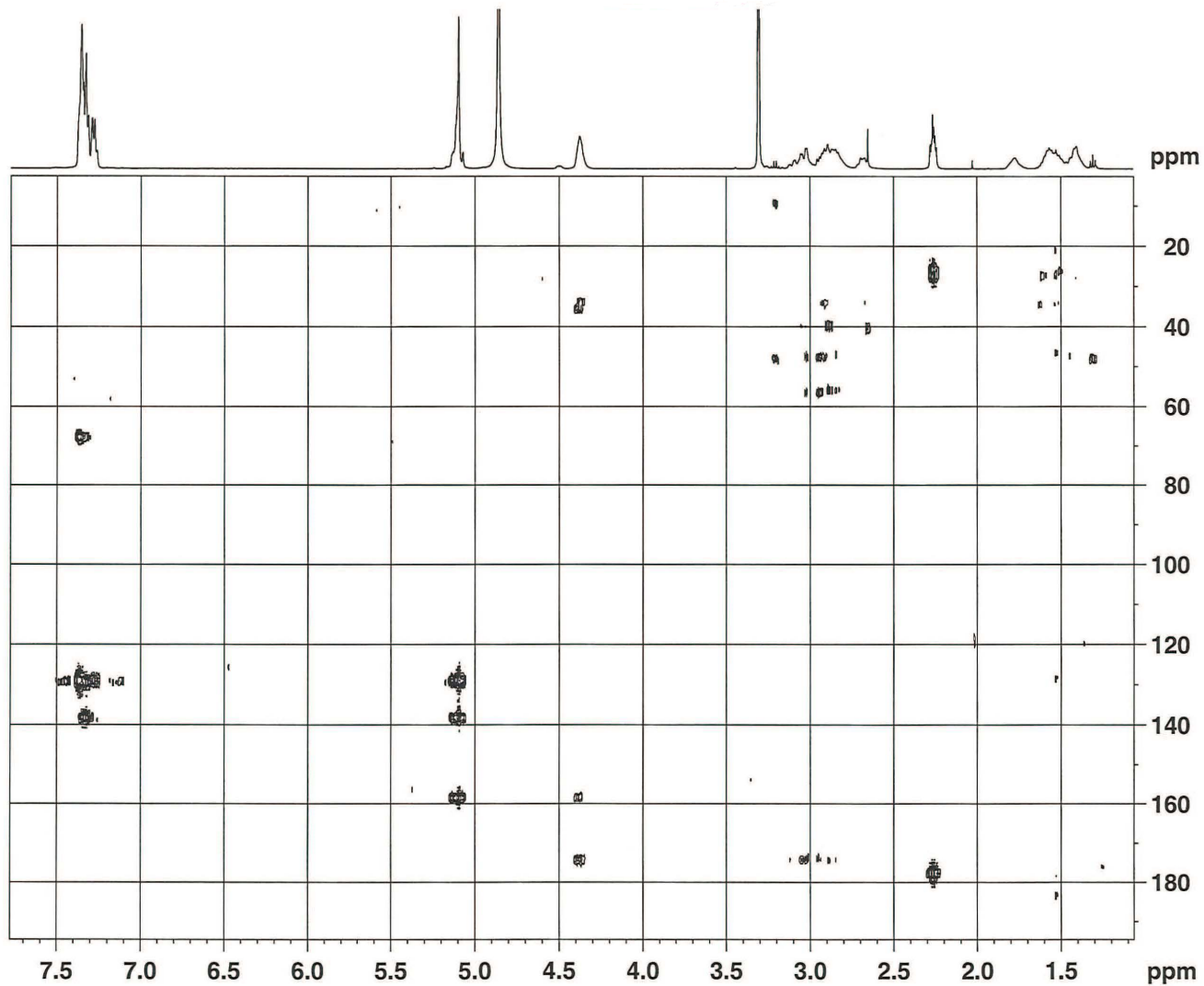
***** CHANNEL f2 *****
CPDPRG2       garp
NUC2          13C
P3             9.70 usec
P14           500.00 usec
P24           2000.00 usec
PCPD2         65.00 usec
PL0            120.00 dB
PL2            4.00 dB
PL12           20.52 dB
PL0W           0.00000000 W
PL2W           34.40000153 W
PL12W          0.7658159 W
SFO2          125.7678496 MHz
SP3            12.42 dB
SP7            12.42 dB
SPNAM3        Crp60,0.5,20.1
SPNAM7        Crp60comp.4
SFOAL3         0.500
SFOAL7         0.500
SPOFFS3        0.00 Hz
SPOFFS7        0.00 Hz

***** GRADIENT CHANNEL *****
GPNAM1        SINE.100
GPNAM2        SINE.100
GPNAM3        SINE.100
GPNAM4        SINE.100
GPZ1           80.00 %
GPZ2           20.10 %
GPZ3           11.00 %
GPZ4           -5.00 %
P16           1000.00 usec
P19           600.00 usec
ND0            2
TD            256
SFO1          125.7678 MHz
FIDRES         93.342123 Hz
SW            190.000 ppm
FIRNODE       Echo-Antiecho
SI            2048
SF            500.1300132 MHz
WDW           QSINE
SSB            2
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           echo-antiecho
SF            125.7576066 MHz
WDW           QSINE
SSB            2
LB            0.00 Hz
GB            0

```

k

compound 3d



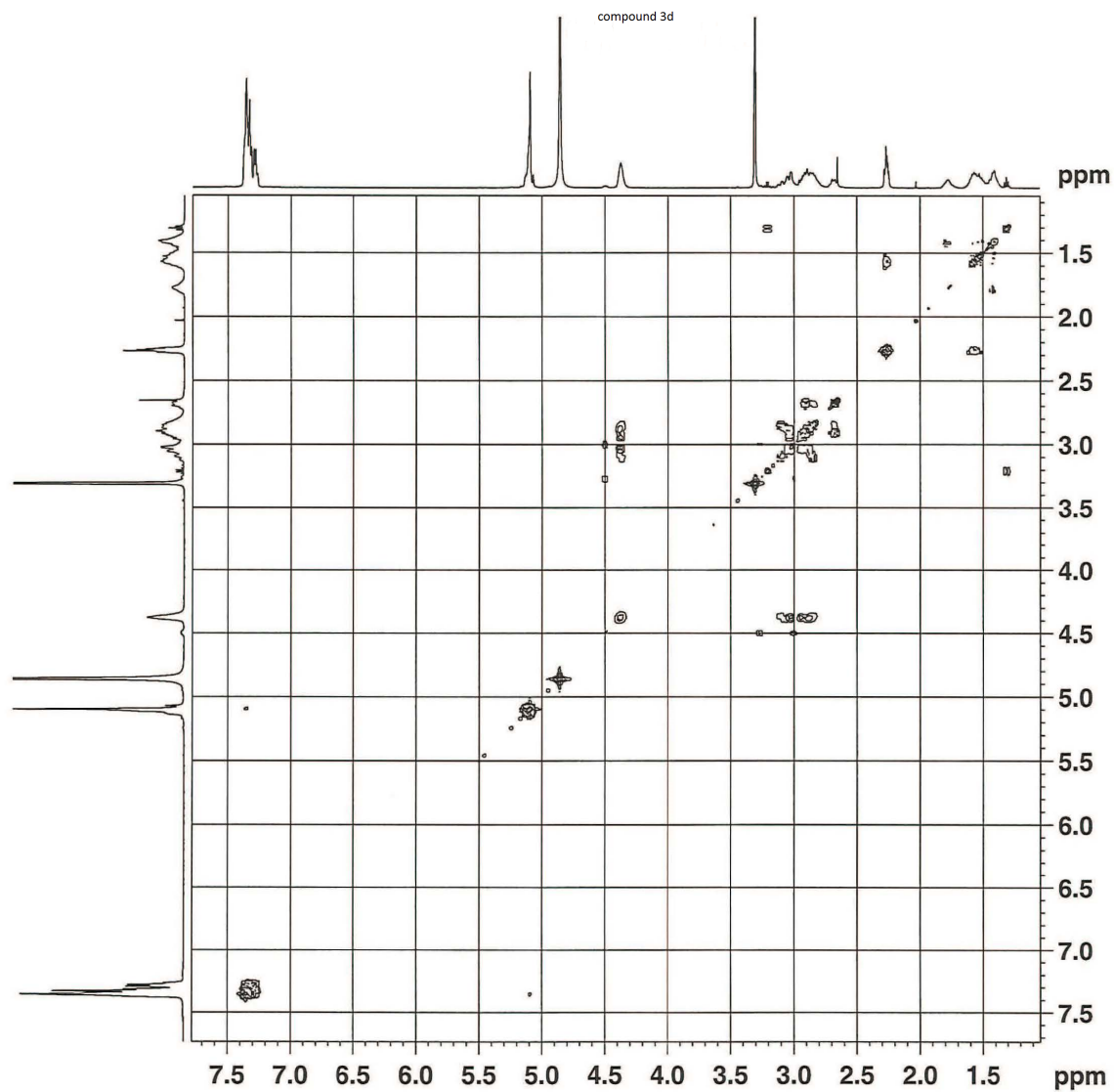
```
NAME 62155052
EXPNO 505
PROCNO 1
Date_ 20140116
Time 11.08
INSTRUM spect
PROBHD 5 mm CPDCH 13C
FULPROG hmbcetsp12nd
TD 2048
SOLVENT MeOD
NS 16
DS 16
SWH 4347.826 Hz
FIDRES 2.122962 Hz
AQ 0.2355700 sec
RG 2050
DW 115.000 usec
DE 6.50 usec
TE 303.0 K
CNS*6 125.0000000
CNS*7 160.0000000
CNS*13 10.0000000
CNS*30 0.5981150
D0 0.00000300 sec
D1 1.42176604 sec
D5 0.05000000 sec
D16 0.00020000 sec
IN0 0.00001790 sec

===== CHANNEL f1 =====
NUC1 1H
P1 8.90 usec
P2 17.80 usec
PL1 3.00 dB
PL1W 15.73656750 W
SFO1 500.1318645 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 9.70 usec
P24 2000.00 usec
PL2 4.00 dB
PL2W 34.40000153 W
SFO2 125.7703443 MHz
SP7 12.42 dB
SPNAM7 Crp60comp.4
SFOAL7 0.500
SPOFFS7 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM3 SINE.100
GPNAM4 SINE.100
GPNAM5 SINE.100
GPZ1 80.00 %
GPZ3 15.00 %
GPZ4 -10.00 %
GPZ5 -5.00 %
P16 NDO 1000.00 usec
TD 2
SFO1 125.7703 MHz
FIDRES 109.113174 Hz
SW 222.095 ppm
FnMODE Echo-Antiecho
SI 2048
SF 500.1300132 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 125.7576066 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
```

6



```

NAME          62155052
EXPNO         506
PROCNO        1
Date_         20140116
Time          9.13
INSTRUM       spect
PROBHD        5 mm CPDCH 13C
PULPROG       cosygpppqf
TD            2048
SOLVENT       MeOD
NS            1
DS            16
SWH           4347.826 Hz
FIDRES        2.122962 Hz
AQ            0.2355700 sec
RG            18
DW            115.000 usec
DE            6.50 usec
TE            303.0 K
DO            0.0000300 sec
D1            1.37916696 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00023000 sec

```

```

===== CHANNEL f1 =====
NUC1          1H
P0            8.90 usec
P1            8.90 usec
P17           2500.00 usec
  PL1          3.00 dB
  PL10         13.84 dB
  PL1W         15.73656750 W
  PL10W        1.29691052 W
SFO1          500.1318645 MHz

```

```

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPZ1          10.00 %
P16           1000.00 usec
  NDO          1
  TD           512
SFO1          500.1319 MHz
FIDRES        8.491848 Hz
SW            8.693 ppm
  F1MODE       QF
  SI           2048
SF            500.1300132 MHz
  WDW          SINE
  SSB          0
  LB           0.00 Hz
  GB           0
  PC           1.40
  SI           2048
  MC2          QF
SF            500.1300132 MHz
  WDW          SINE
  SSB          0
  LB           0.00 Hz
  GB           0

```

u-

Current Data Parameters
 NAME 68952051
 EXPNO 500
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141010
 Time 14.51
 INSTRUM spect
 PROBHD 5 mm CPDCH 13C
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 32
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 10
 DW 48.400 usec
 DE 10.00 usec
 TE 303.0 K
 D1 1.00000000 sec
 TD0 1

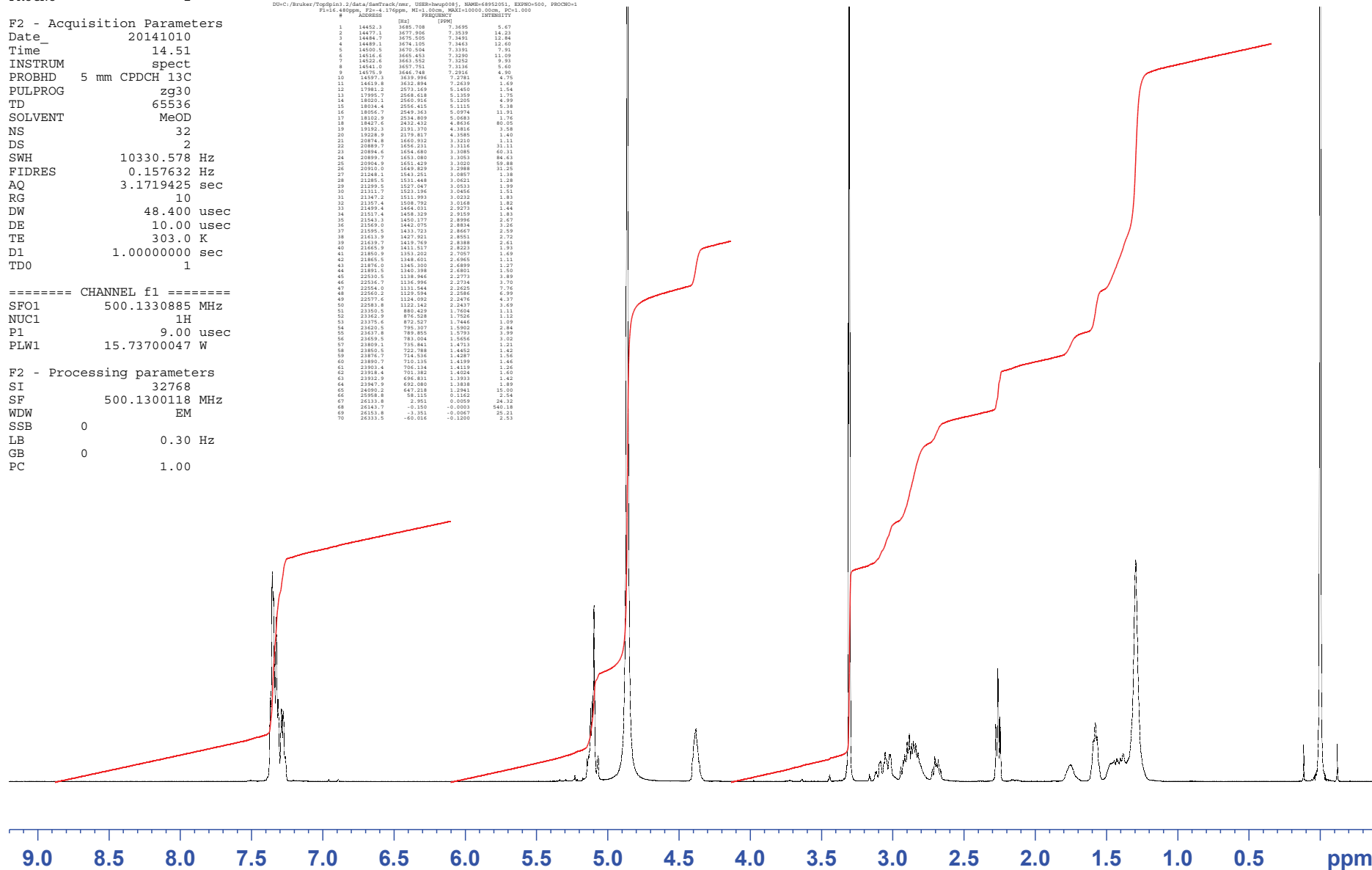
==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 9.00 usec
 PLW1 15.73700047 W

F2 - Processing parameters
 SI 32768
 SF 500.1300118 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

NMR spectra for compound 3e

DOIC:\Bruker\TopSpin1.2\data\5aeTrack\mr_USER\hwg0081_NMR\68952051.EXPNO=500, PROCNO=1
 F1=4.480000, F2=4.174000, M1=1.000000, Q1=0.000000, Q2=0.000000

#	ACQTIME	Hz	PPM	INTEGRITY
1	14443.3	1679.708	7.3650	5.07
2	14477.1	1679.966	7.3539	14.23
3	14489.1	1679.205	7.3459	12.84
4	14489.1	1674.195	7.3463	12.60
5	14505.5	1679.554	7.3390	7.91
6	14516.6	1665.453	7.3290	11.09
7	14523.3	1665.352	7.3222	9.90
8	14541.0	1657.751	7.3136	5.60
9	14575.9	1646.748	7.2916	4.90
10	14597.3	1639.996	7.2781	4.75
11	14638.0	1628.894	7.2639	1.69
12	17981.2	2573.169	5.1450	1.54
13	17995.7	2568.818	5.1329	1.76
14	18020.1	2560.916	5.1205	4.99
15	18034.4	2556.415	5.1113	5.38
16	18056.7	2549.363	5.0974	11.91
17	18062.9	2548.809	5.0953	1.76
18	18427.6	2432.432	4.8636	80.05
19	19322.3	2133.370	4.3816	3.58
20	19228.9	2179.817	4.3585	1.40
21	20874.8	1650.912	3.3210	1.11
22	20889.7	1656.231	3.3116	31.11
23	20884.6	1654.680	3.3085	60.31
24	20899.7	1653.080	3.3053	84.63
25	20904.9	1651.429	3.3020	59.88
26	20910.0	1649.829	3.2988	31.25
27	21248.1	1543.251	3.0857	1.38
28	21285.5	1531.448	3.0621	1.28
29	21279.5	1527.047	3.0513	3.39
30	21311.7	1521.196	3.0408	1.35
31	21347.2	1511.993	3.0230	1.83
32	21371.4	1508.792	3.0168	1.82
33	21499.4	1464.031	2.9273	1.44
34	21517.4	1459.329	2.9159	1.83
35	21541.3	1450.377	2.8996	2.67
36	21548.0	1447.926	2.8944	2.26
37	21598.5	1433.723	2.8667	2.59
38	21613.9	1427.951	2.8501	2.72
39	21618.7	1419.769	2.8388	2.61
40	21665.0	1411.517	2.8223	1.93
41	21850.9	1353.202	2.7057	1.69
42	21865.5	1348.601	2.6965	1.13
43	21876.0	1345.300	2.6899	1.27
44	21881.5	1340.398	2.6801	1.50
45	22510.5	1138.946	2.2773	3.89
46	22516.7	1136.996	2.2734	3.70
47	22554.0	1131.544	2.2625	7.76
48	22562.0	1129.974	2.2586	6.99
49	22577.6	1124.092	2.2476	4.37
50	22581.8	1122.142	2.2437	3.69
51	23350.5	880.429	1.7604	1.11
52	23362.9	876.928	1.7526	1.12
53	23375.6	872.527	1.7446	1.09
54	23625.5	799.207	1.8902	2.84
55	23637.8	789.855	1.8795	3.99
56	23659.5	783.004	1.8656	3.02
57	23809.1	735.841	1.4713	1.21
58	23850.5	722.788	1.4452	1.42
59	23971.7	716.536	1.4287	1.36
60	23990.7	710.335	1.4199	1.46
61	23991.4	709.314	1.4139	1.28
62	23994.4	701.382	1.4024	1.60
63	23992.9	696.911	1.3933	1.42
64	23947.9	692.080	1.3838	1.89
65	24009.2	687.218	1.3741	15.00
66	23958.8	58.115	0.1162	2.54
67	26131.8	2.952	-0.0059	24.32
68	26141.7	-0.150	-0.0053	540.18
69	26131.8	3.353	-0.0067	75.21
70	26333.5	-60.016	-0.1200	2.53



Current Data Parameters
NAME 68952051
EXPNO 501
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141010
Time 15.03
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg
TD 65536
SOLVENT MeOD
NS 128
DS 4
SWH 30864.197 Hz
FIDRES 0.470950 Hz
AQ 1.0616832 sec
RG 456
DW 16.200 usec
DE 18.00 usec
TE 303.0 K
D1 4.0000000 sec
D11 0.0300000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 125.7703643 MHz
NUC1 13C
P1 9.70 usec
PLW1 34.40000153 W

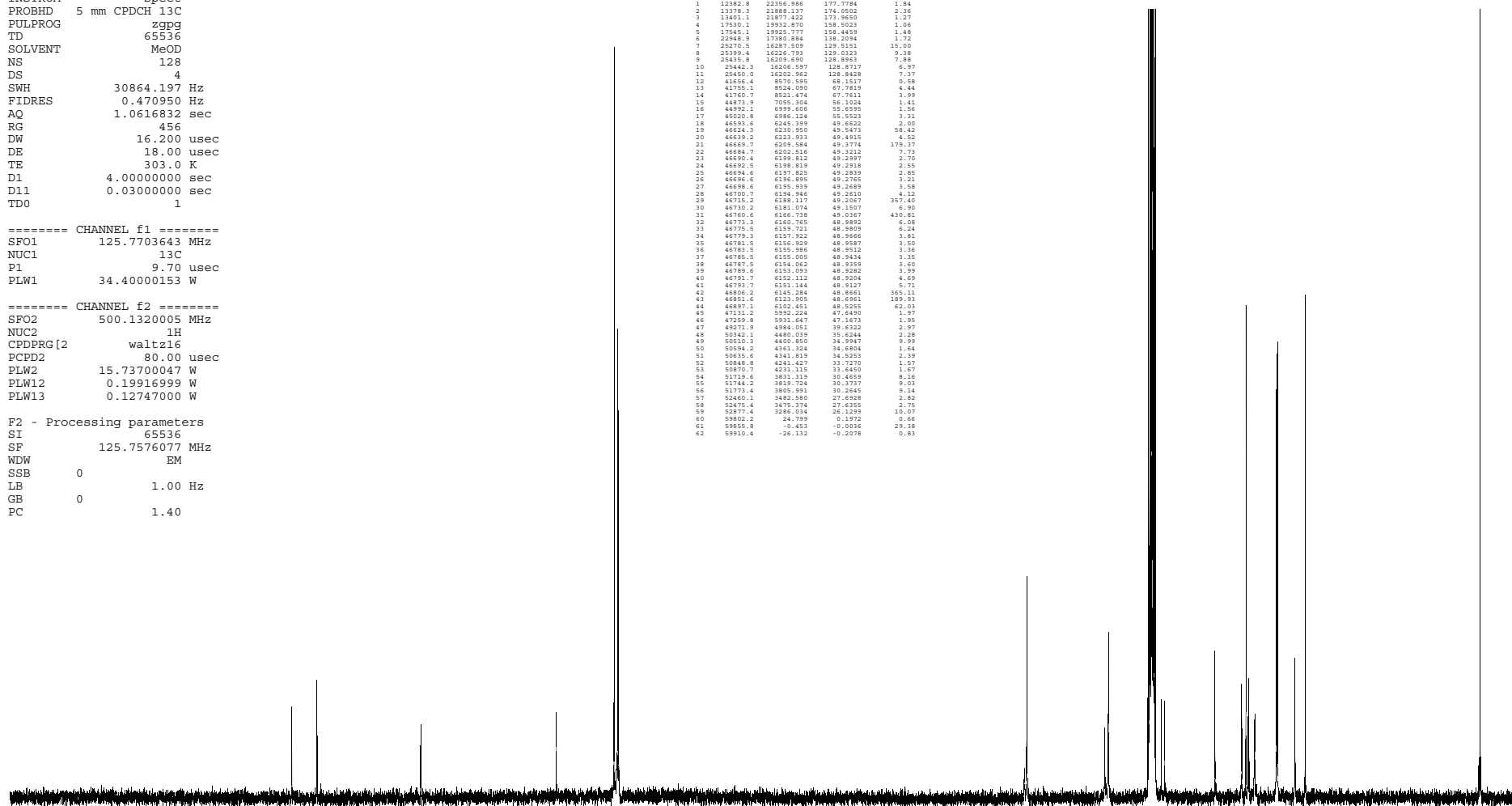
==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.73700047 W
PLW12 0.19916999 W
PLW13 0.12747000 W

F2 - Processing parameters
SI 65536
SF 125.7576077 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

compound 3e

DU=C:\Bruker\TopSpin\2\data\SanTrack\mr_UHSR-huop0081_NAME=68952051_EXPNO=501_PROCNO=1
P1=224.151ppm, F2=-21.275ppm, MI=0.00cm, MAXI=10000.00cm, PC=1.400

[Hz]	ADDSHIFT	PPM	FREQUENCY	INTENSITY
1	12382.8	22386.986	177.7784	1.84
2	13378.3	21886.137	174.0502	2.36
3	13401.1	21877.422	173.9650	1.27
4	17510.1	15932.870	138.5003	1.06
5	17545.1	15925.777	138.4459	1.48
6	22848.9	17386.884	138.2094	1.72
7	25270.5	16287.509	129.5151	15.00
8	25289.4	16226.793	129.0232	3.38
9	25435.8	16209.650	128.8963	7.88
10	25442.3	16206.597	128.8717	6.97
11	25450.0	16202.562	128.8428	7.37
12	41656.4	8570.595	68.1517	0.58
13	41755.1	8524.090	67.7819	4.44
14	41760.7	8521.474	67.7611	3.99
15	44873.9	7053.304	56.1204	1.41
16	44932.1	6999.606	55.6395	1.56
17	45020.8	6986.124	55.5523	3.31
18	46593.6	6245.399	49.6422	2.00
19	46624.3	6230.950	49.5473	88.42
20	46639.2	6223.933	49.4915	4.52
21	46659.7	6209.584	49.3774	179.37
22	46684.7	6202.516	49.3212	7.73
23	46690.4	6199.812	49.2997	2.70
24	46692.5	6198.819	49.2918	2.55
25	46694.6	6197.825	49.2839	2.85
26	46696.6	6196.835	49.2765	3.21
27	46698.6	6195.839	49.2689	3.58
28	46700.7	6194.846	49.2610	6.12
29	46715.2	6188.117	49.2087	357.40
30	46730.2	6181.074	49.1507	6.90
31	46760.6	6166.738	49.0367	430.81
32	46773.3	6160.765	49.0002	6.08
33	46775.5	6159.721	49.9809	6.24
34	46779.3	6157.527	49.9686	3.81
35	46781.5	6156.529	49.9587	3.00
36	46783.5	6155.586	49.9512	3.36
37	46785.5	6154.605	49.9434	3.35
38	46787.5	6154.062	49.9359	3.60
39	46789.6	6153.093	49.9282	3.99
40	46791.7	6152.112	49.9204	4.69
41	46793.7	6151.144	49.9127	5.71
42	46806.2	6145.284	48.8641	165.11
43	46851.6	6123.905	48.6961	189.93
44	46897.1	6102.451	48.5255	62.03
45	47131.2	5992.224	47.6490	1.97
46	47259.8	5931.647	47.1473	1.95
47	49271.9	4984.051	39.6322	2.97
48	50342.1	4460.039	35.6244	2.28
49	50510.3	4400.850	34.9947	9.99
50	50594.2	4361.324	34.6804	1.64
51	50635.6	4341.819	34.5253	2.39
52	50648.8	4341.627	34.5200	1.57
53	50870.7	4231.115	33.6490	1.67
54	51715.6	3821.219	30.6459	8.16
55	51744.2	3819.724	30.3737	9.03
56	51773.4	3805.991	30.2645	9.14
57	52460.1	3482.580	27.6928	2.82
58	52475.4	3476.374	27.6355	2.75
59	52877.4	3266.034	26.1199	10.07
60	59802.2	24.799	0.1972	0.66
61	59835.8	0.483	+0.0036	29.38
62	59910.4	-26.132	-0.2078	0.83



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

DU=C:/Bruker/TopSpin3.2\data/SamTrack/mr, USER=hwup008, NAME=68952051, EXPRNO=502, PROCNO=1
F1=15.768ppm, F2=16.893ppm, MI=0.50cm, MAXI=10000.00cm, PC=1.400

#	ADDRESS	FREQUENCY	INTENSITY	
1	24991.8	16287.974	129.5188	15.00
2	25125.6	16227.210	129.0388	6.78
3	25163.2	16210.130	128.8998	7.96
4	25169.8	16207.137	128.8760	7.14
5	25173.6	16205.415	128.8623	6.03
6	25177.9	16203.453	128.8487	7.63
7	42087.1	8524.467	67.7849	-4.45
8	42093.0	8521.805	67.7637	-4.15
9	45121.0	7955.863	56.1069	1.24
10	45443.7	7922.184	55.6537	1.28
11	47471.8	6245.488	49.1549	2.09
12	47104.6	6245.902	49.4562	6.31
13	47151.8	6234.446	49.4995	12.63
14	47199.2	6202.906	49.1243	19.08
15	47248.0	6181.452	49.1337	13.06
16	47293.7	6159.997	48.9831	6.48
17	47621.4	5991.064	47.6514	1.59
18	47796.1	5991.848	47.1689	1.84
19	49882.3	4984.408	39.6322	-2.89
20	50992.2	4480.404	35.6273	-2.04
21	51165.3	4401.353	34.9957	-1.95
22	51253.9	4361.538	34.6821	-1.37
23	51295.6	4361.384	34.5282	-1.85
24	51517.1	4242.018	33.7317	-1.62
25	51545.4	4231.454	33.6477	-1.66
26	52420.0	3831.998	30.4713	-5.21
27	52445.7	3820.315	30.3784	-5.39
28	52476.1	3806.519	30.2487	-6.10
29	53288.3	3483.031	27.6967	-2.00
30	53294.1	3475.928	27.6399	-1.99
31	53621.1	3286.049	26.1340	-8.47
32	59137.2	781.495	6.2143	-0.65
33	60811.1	261.123	0.0764	-0.84
34	60802.1	25.428	0.2022	1.19
35	60858.0	-0.063	0.0005	45.67
36	60914.4	-26.554	-0.2032	1.24
37	61432.7	-246.960	-2.0751	-0.56
38	62578.6	-781.357	-6.2132	-0.66

H, CH3-Signals positive, CH2-Signals negative

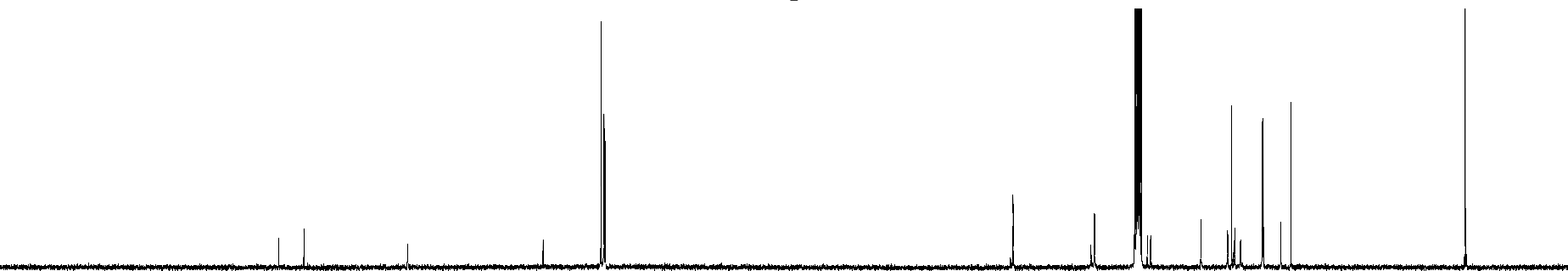


CH-Signals

DU=C:/Bruker/TopSpin3.2\data/SamTrack/mr, USER=hwup008, NAME=68952051, EXPRNO=503, PROCNO=1
F1=15.768ppm, F2=16.893ppm, MI=0.50cm, MAXI=10000.00cm, PC=1.400

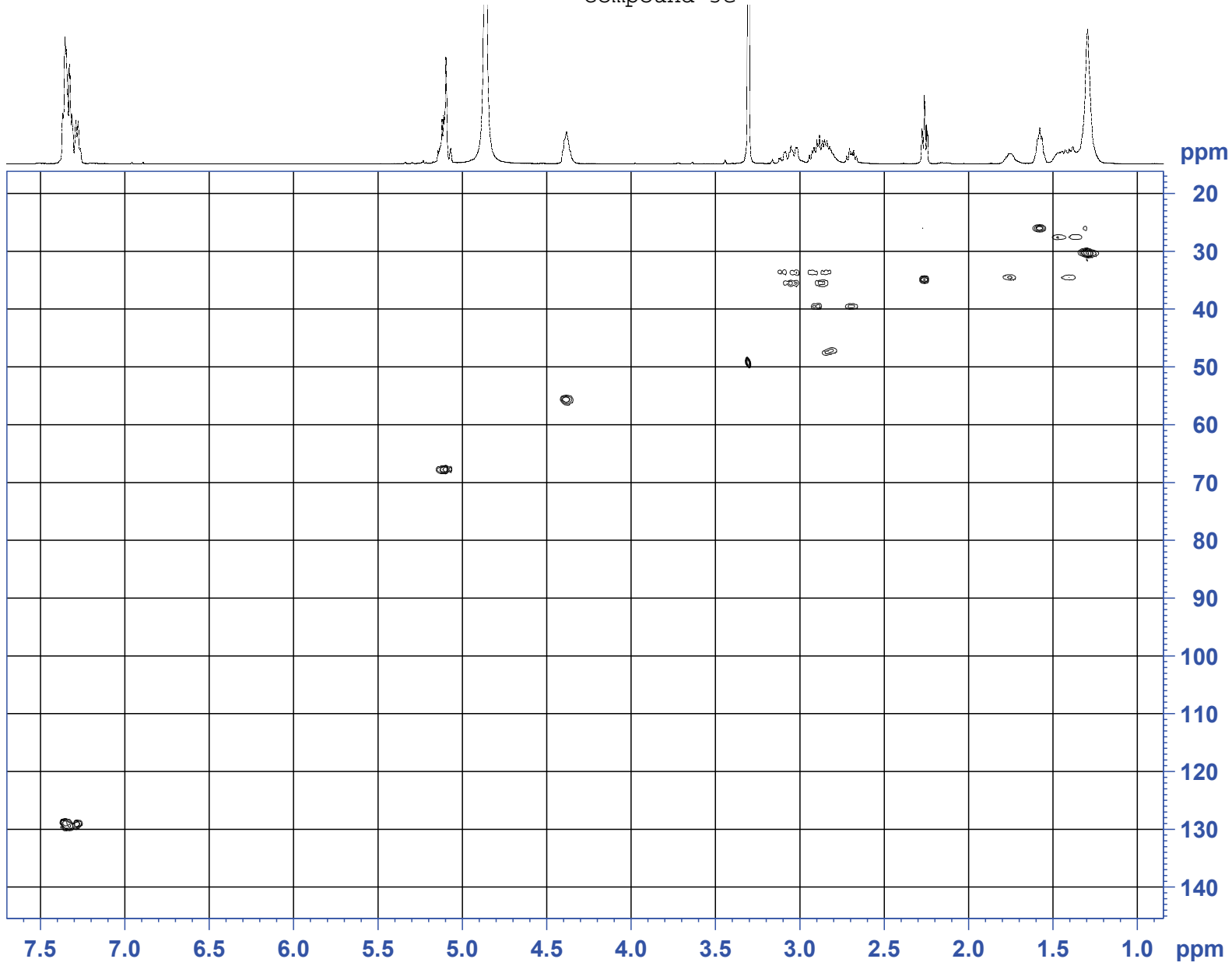
#	ADDRESS	FREQUENCY	INTENSITY	
1	24992.9	16287.497	129.5150	15.00
2	25106.1	16240.602	129.1421	0.54
3	25126.6	16226.768	129.0321	6.71
4	25164.3	16209.640	128.8959	8.37
5	25170.9	16206.660	128.8722	7.21
6	25174.7	16204.937	128.8585	6.02
7	25179.0	16202.962	128.8448	7.88
8	45121.8	7955.517	56.1041	1.24
9	45444.8	7923.643	55.6508	1.37
10	47475.0	6245.948	49.1529	2.19
11	47150.5	6245.970	49.4588	6.47
12	47150.5	6233.970	49.4388	12.37
13	47202.0	6202.441	49.2006	19.22
14	47232.0	6180.941	49.2001	0.62
15	47247.5	6180.986	49.1500	13.15
16	47279.4	6159.532	49.0349	0.51
17	47294.7	6159.532	48.9794	6.37
18	47651.4	5991.126	47.6483	1.61
19	47796.7	5991.171	47.1467	1.61
20	51167.1	4400.976	34.9957	0.60
21	52421.1	3831.507	30.4474	0.79
22	52448.8	3819.824	30.3745	0.76
23	52477.2	3806.041	30.2449	0.82
24	53622.0	3286.189	26.1305	0.87
25	60858.9	-0.377	-0.0030	2.42

Gcompound 3e



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

compound 3e



```
Current Data Parameters
NAME      68952051
EXPNO     504
PROCNO    1

F2 - Acquisition Parameters
Date_     20141010
Time      15.28
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   hsqcetgpsi2p2.2
TD         2048
SOLVENT   MeOD
NS         2
DS         16
SWH        4672.897 Hz
FIDRES     2.281688 Hz
AQ         0.2191360 sec
RG         2050
DW         107.000 usec
DE         10.00 usec
TE         303.0 K
CNST2     145.0000000
CNST17    -0.5000000
D0         0.00000300 sec
D1         1.40865898 sec
D4         0.00172414 sec
D11        0.03000000 sec
D16        0.00020000 sec
D24        0.00110000 sec
IN0        0.00002090 sec

===== CHANNEL f1 =====
SF01      500.1317401 MHz
NUC1      1H
P1         9.00 usec
P2        18.00 usec
PLW1      P2# 0 usec
          15.73700047 W

===== CHANNEL f2 =====
SF02      125.7678496 MHz
NUC2      13C
CPDPRG[2] garp
P3         9.70 usec
P14        500.00 usec
P24        2000.00 usec
PCPD2      70.00 usec
PLW0       0 W
PLW2      34.40000153 W
PLW12     0.66055000 W
SPNAM[3]  Crp60,0.5,20.1
SPOAL3    0.500
SPOFFS3   0 Hz
SPW3      4.94530010 W
SPNAM[7]  Crp60comp.4
SPOAL7    0.500
SPOFFS7   0 Hz
SPW7      4.94530010 W

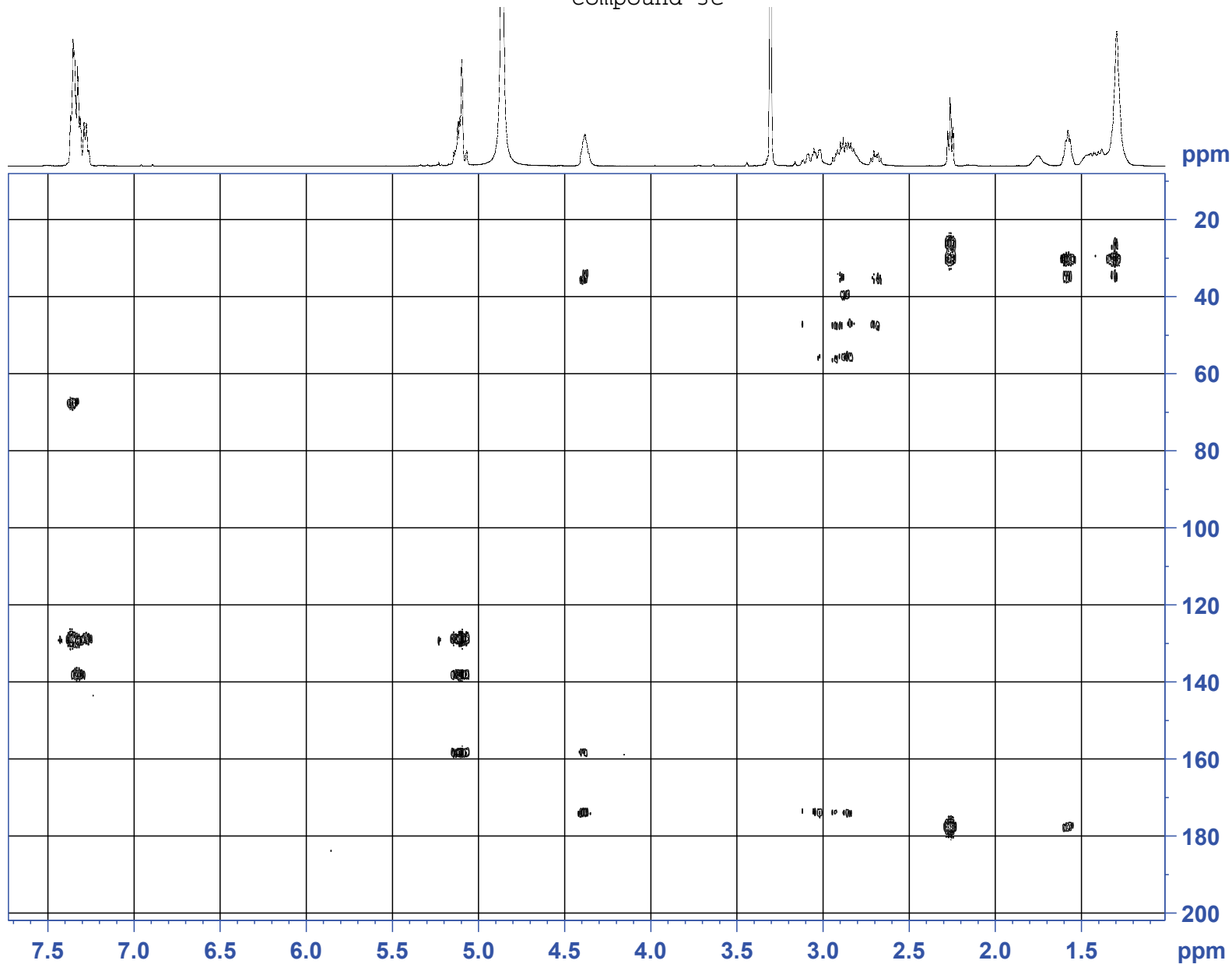
===== GRADIENT CHANNEL =====
GPNAM[1]  SMSQ10.100
GPNAM[2]  SMSQ10.100
GPNAM[3]  SMSQ10.100
GPNAM[4]  SMSQ10.100
GPZ1      80.00 %
GPZ2      20.10 %
GPZ3      11.00 %
GPZ4      -5.00 %
P16       1000.00 usec
P19       600.00 usec

F1 - Acquisition parameters
TD         256
SF01      125.7678 MHz
FIDRES     91.450958 Hz
SW         130.219 ppm
PhMODE     Echo-Antiecho

F2 - Processing parameters
SI         2048
SF         500.1300118 MHz
WDW        QSINE
SSB         2
LB         0 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
NC2        echo-antiecho
SF         125.7576077 MHz
WDW        QSINE
SSB         2
LB         0 Hz
GB         0c ccc
```

compound 3e



```

Current Data Parameters
NAME      68952051
EXPNO    505
PROCNO   1

F2 - Acquisition Parameters
Date_    20141010
Time     15.43
INSTRUM  spect
PROBHD   5 mm CPDCH 13C
PULPROG  hmbcetgp12nd
TD        2048
SOLVENT  MeOD
NS        2
DS        16
SWH       4672.897 Hz
FIDRES    2.281688 Hz
AQ        0.2191360 sec
RG        2050
DW        107.000 usec
DE        10.00 usec
TE        303.0 K

===== CHANNEL f1 =====
SFO1     500.1317401 MHz
NUC1     1H
P1        9.00 usec
P2        18.00 usec
PLW1     15.73700047 W

===== CHANNEL f2 =====
SFO2     125.7703443 MHz
NUC2     13C
P3        9.70 usec
P24       2000.00 usec
PLW2     34.40000153 W
SFOAL7   Crp60comp.4
SPOAL7   0.500
SPOFFS7  0 Hz
SPW7     4.94530010 W

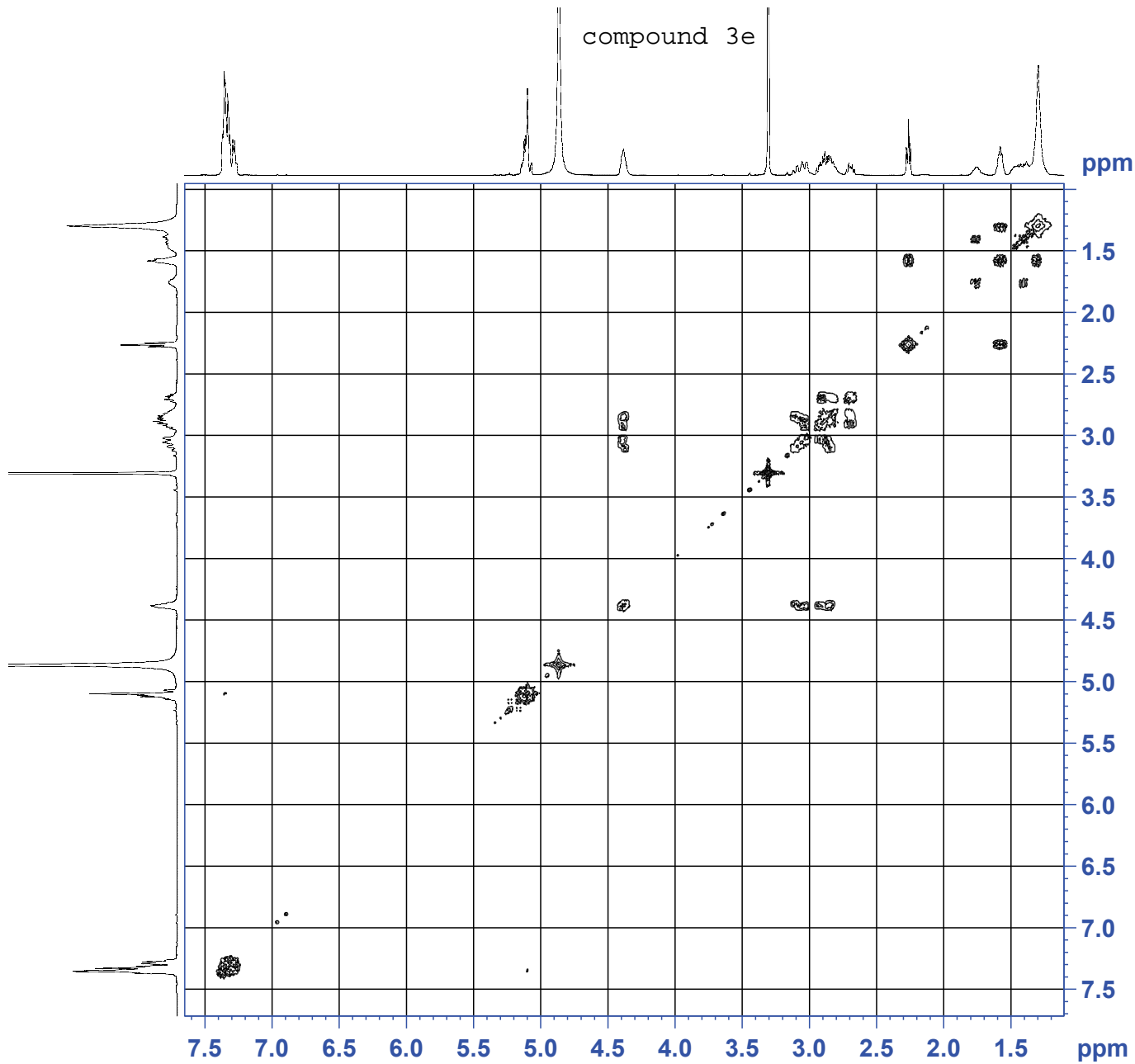
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPNAM[5] SMSQ10.100
GPZ1     80.00 %
GPZ3     15.00 %
GPZ4     -10.00 %
GPZ5     -5.00 %
P16      1000.00 usec

F1 - Acquisition parameters
TD        256
SFO1     125.7703 MHz
FIDRES    109.113129 Hz
SW        222.095 ppm
PnMODE    Echo-Antiecho

F2 - Processing parameters
SI        2048
SF        500.1300118 MHz
WDW       SINE
SSB       0 Hz
LB        0 Hz
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
MC2       echo-antiecho
SF        125.7576077 MHz
WDW       SINE
SSB       0 Hz
LB        0 Hz
GB        0
    
```

compound 3e



```
Current Data Parameters
NAME      68952051
EXPNO    506
PROCNO   1

F2 - Acquisition Parameters
Date_    20141010
Time     15.58
INSTRUM spect
PROBHD   5 mm CPDCH 13C
PULPROG cosygpppgf
TD       2048
SOLVENT MeOD
NS       1
DS       16
SWH      4672.897 Hz
FIDRES   2.281688 Hz
AQ       0.2191360 sec
RG       25.4
DW       107.000 usec
DE       10.00 usec
TE       303.0 K
D0       0.00000300 sec
D1       1.39555001 sec
D11      0.03000000 sec
D12      0.00002000 sec
D13      0.00000400 sec
D16      0.00020000 sec
INO      0.00021400 sec

===== CHANNEL f1 =====
SFO1    500.1317401 MHz
        NUC1      1H
P0       9.00 usec
P1       9.00 usec
P17      2500.00 usec
PLW1     15.73700047 W
PLW10    1.88559997 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1     10.00 %
P16      1000.00 usec

F1 - Acquisition parameters
TD       512
SFO1    500.1317 MHz
FIDRES   9.126752 Hz
SW       9.343 ppm
        FnMODE    QF

F2 - Processing parameters
SI       2048
SF       500.1300118 MHz
WDW      SINE
        SSB       0
        LB       0 Hz
        GB       0
        PC       1.40

F1 - Processing parameters
SI       2048
MC2     QF
SF       500.1300118 MHz
WDW      SINE
        SSB       0
        LB       0 Hz
        GB       0
```