

**Phaeochromycins F–H, three new polyketide metabolites from *Streptomyces* sp. DSS-18**

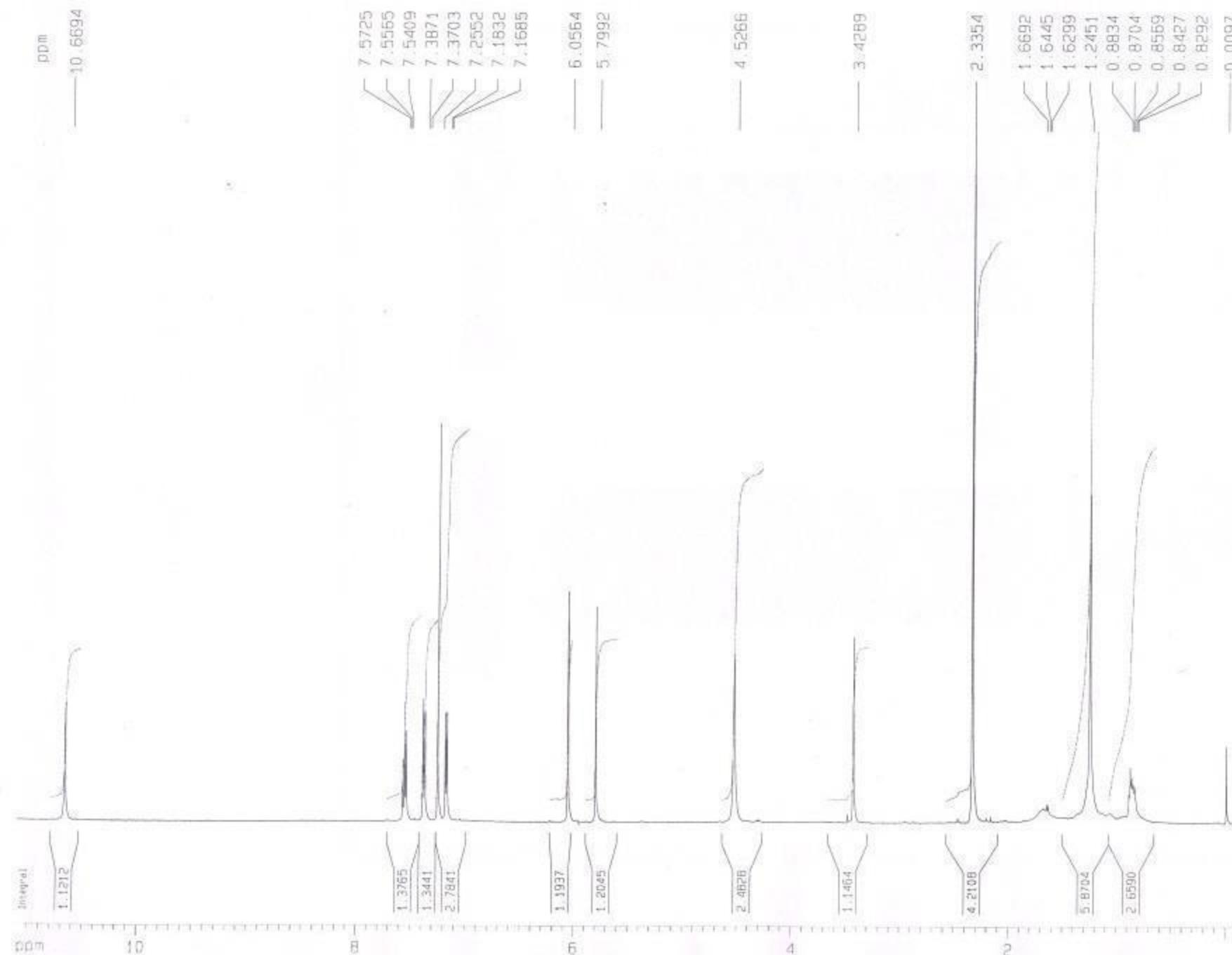
Jian Li, Chun-Hua Lu, Bao-Bing Zhao, Zhong-Hui Zheng<sup>\*</sup> and Yue-Mao Shen

Index

- Page SI 2–18 NMR spectra of compounds **1–3**.  
Page SI 19 HPLC data of compound **1** and crude extract.

1-1H

2



## Current Data Parameters

NAME mds20  
EXPNO 21  
PROCNO 1

## F2 - Acquisition Parameters

Date\_ 20051125  
Time 17.17  
INSTRUM DRX500  
PROBHD 5 mm BB1 1H-BB  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 1  
DS 0  
SWH 5127.451 Hz  
F1ORES 0.186995 Hz  
AQ 2.6739187 sec  
RG 80.6  
DW B1.600 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 sec

## \*\*\*\*\* CHANNEL f1 \*\*\*\*\*

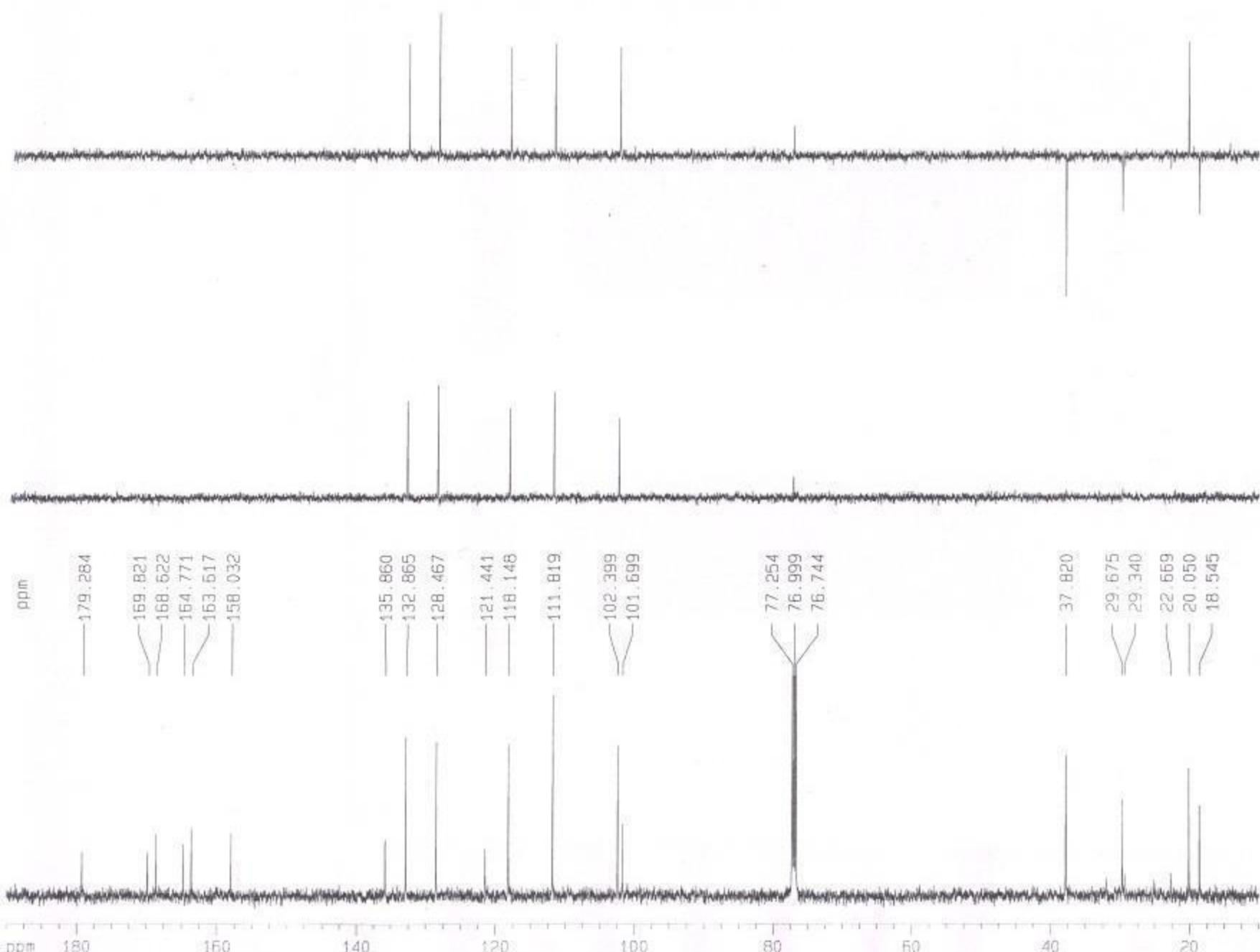
NUC1 1H  
P1 10.00 usec  
PL1 -4.00 dB  
SF01 500.1329931 MHz

## F2 - Processing parameters

SI 16384  
SF 500.1300150 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

## 1D NMR plot parameters

CX 22.00 cm  
CY 14.00 cm  
F1P 11.095 ppm  
F1 5548.92 Hz  
F2P -0.152 ppm  
F2 -75.93 Hz  
PPMCN 0.51122 ppm/cm  
HZCM 255.67503 Hz/cm



Current Data Parameters  
 NAME: nds2D  
 EXPNO: 22  
 PAGEID: 1

F2 - Acquisition Parameters  
 Date: 20051126  
 Time: 12.48  
 INSTRUM: DRX500  
 PROBHD: 5 mm DUL 13C-1  
 PULPROG: zgdc  
 TD: 32768  
 SOLVENT: CDCl3  
 NS: 203  
 DS: 0  
 SWH: 29498.525 Hz  
 FIDRES: 0.900224 Hz  
 AQ: 0.5554676 sec  
 RG: 8192  
 DM: 16.950 usec  
 DE: 6.00 usec  
 TE: 300.0 K  
 D1: 3.0000000 sec  
 d11: 0.03000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1: 13C  
 P1: 5.90 usec  
 PL1: 0.00 dB  
 SF01: 125.7716224 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPB2: waitz16  
 NUC2: 1H  
 PCPD2: 84.00 usec  
 PL2: -4.00 dB  
 PL12: 18.00 dB  
 SF02: 500.1338510 MHz

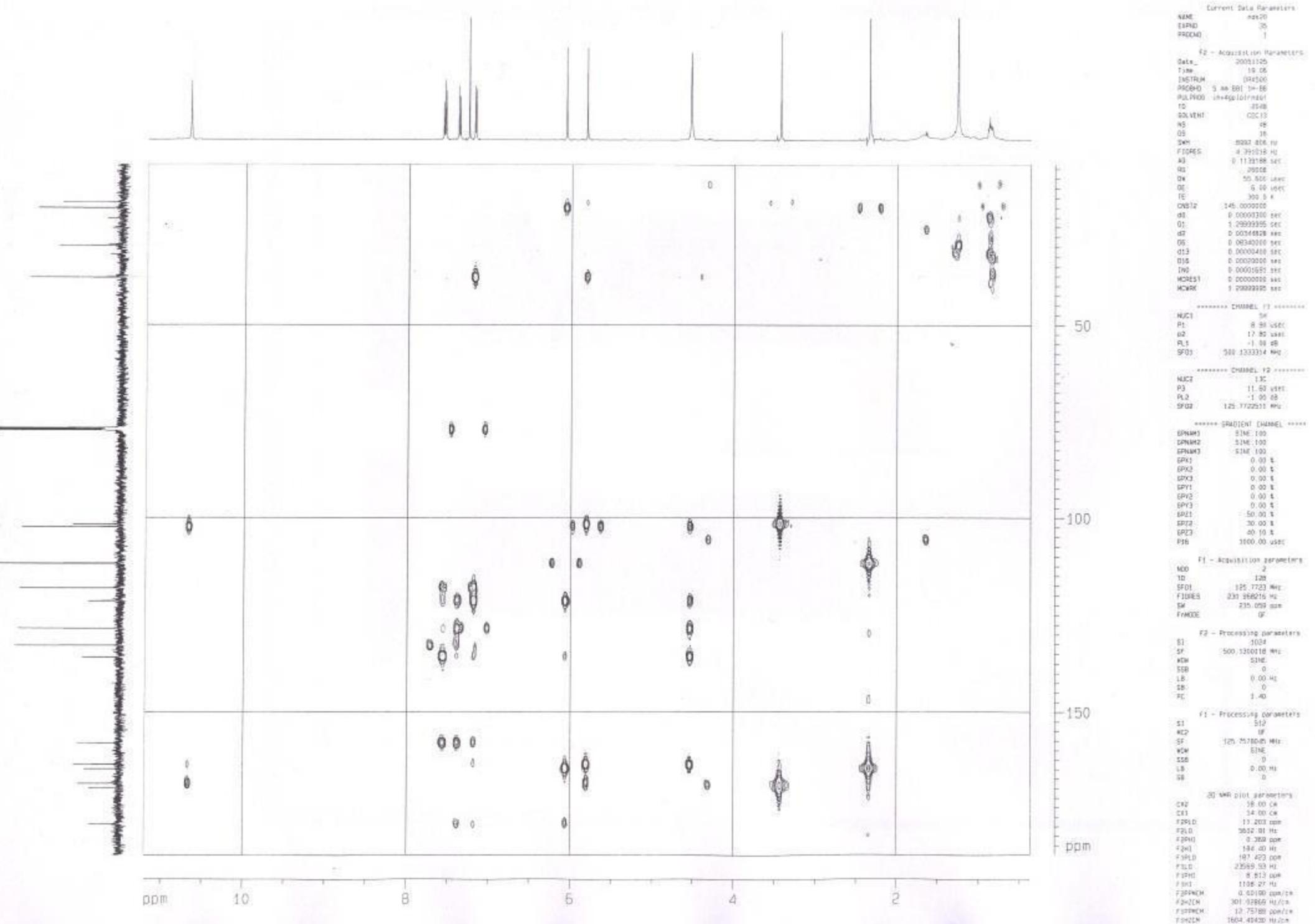
F2 - Processing parameters  
 S1: 16384  
 SF: 125.7577900 MHz  
 WM: EM  
 SS9: 0  
 LB: 2.00 Hz  
 SB: 0  
 PC: 1.50

1D NMR plot parameters  
 CX: 22.00 cm  
 CY: 12.00 cm  
 F1P: 190.000 ppm  
 F1: 23893.98 Hz  
 F2P: 10.000 ppm  
 F2: 1257.58 Hz  
 PPMCH: 8.18182 ppm/cm  
 HzCH: 1028.92737 Hz/cm



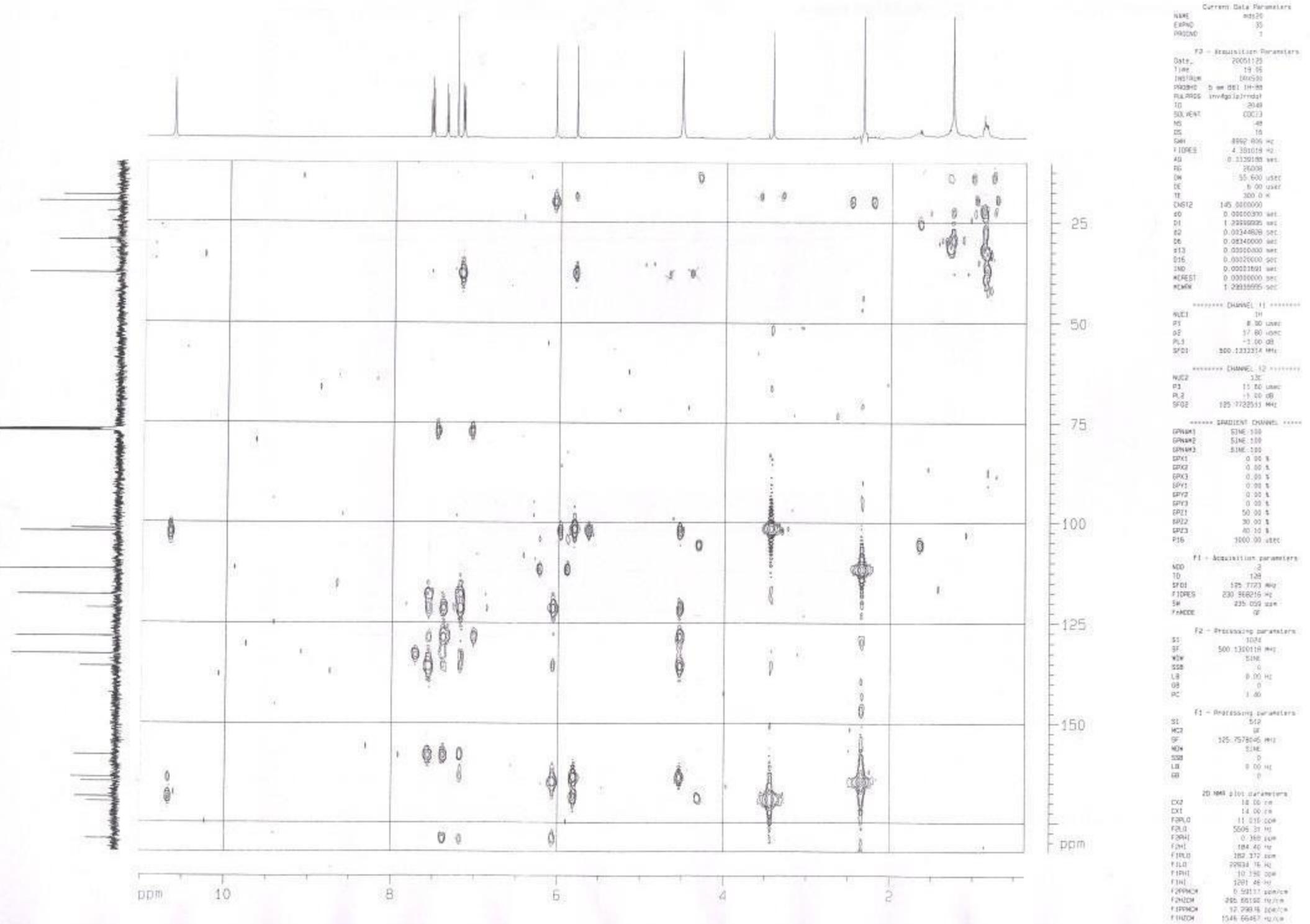
# 1-HMBC

5



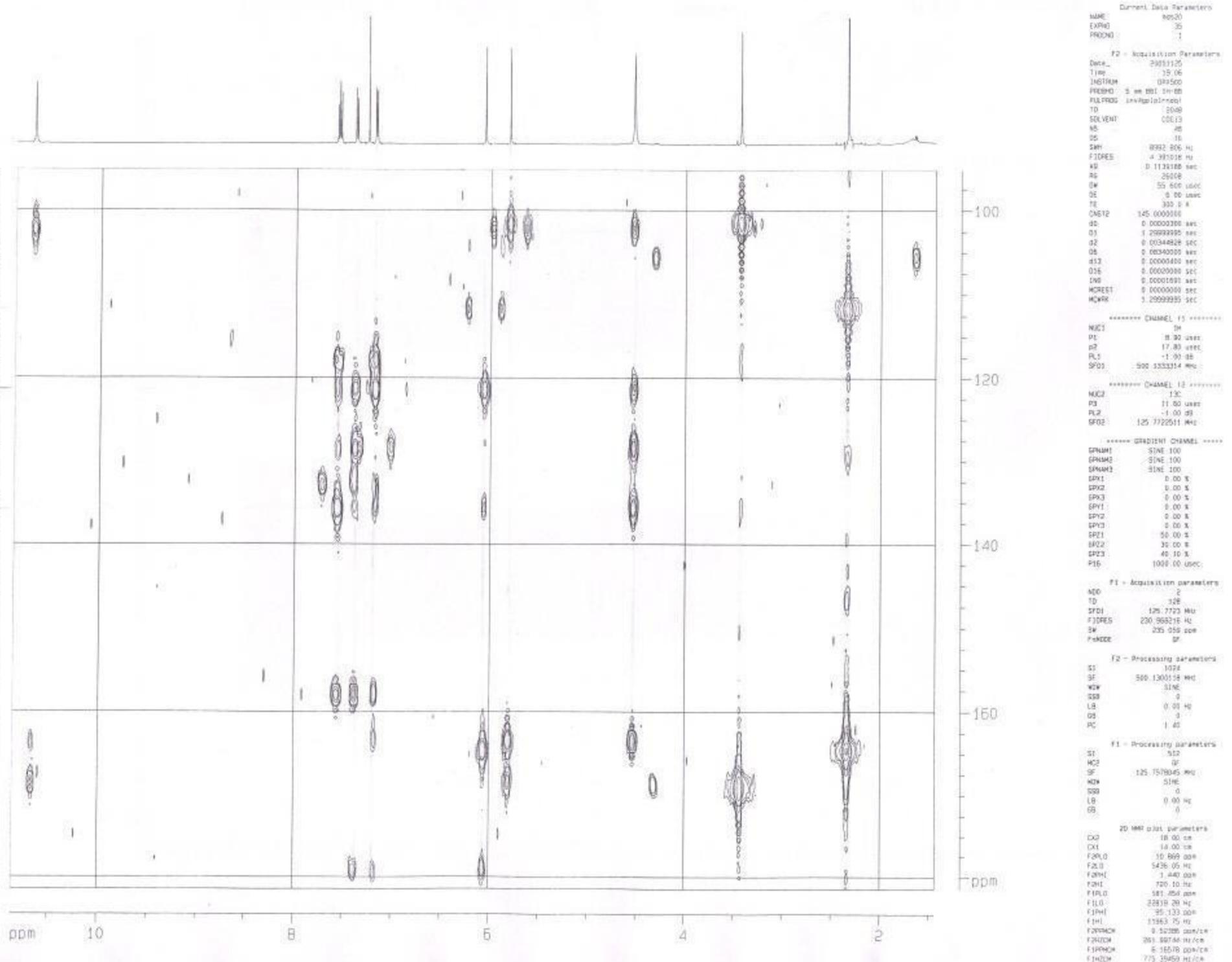
# 1-HMBC

6



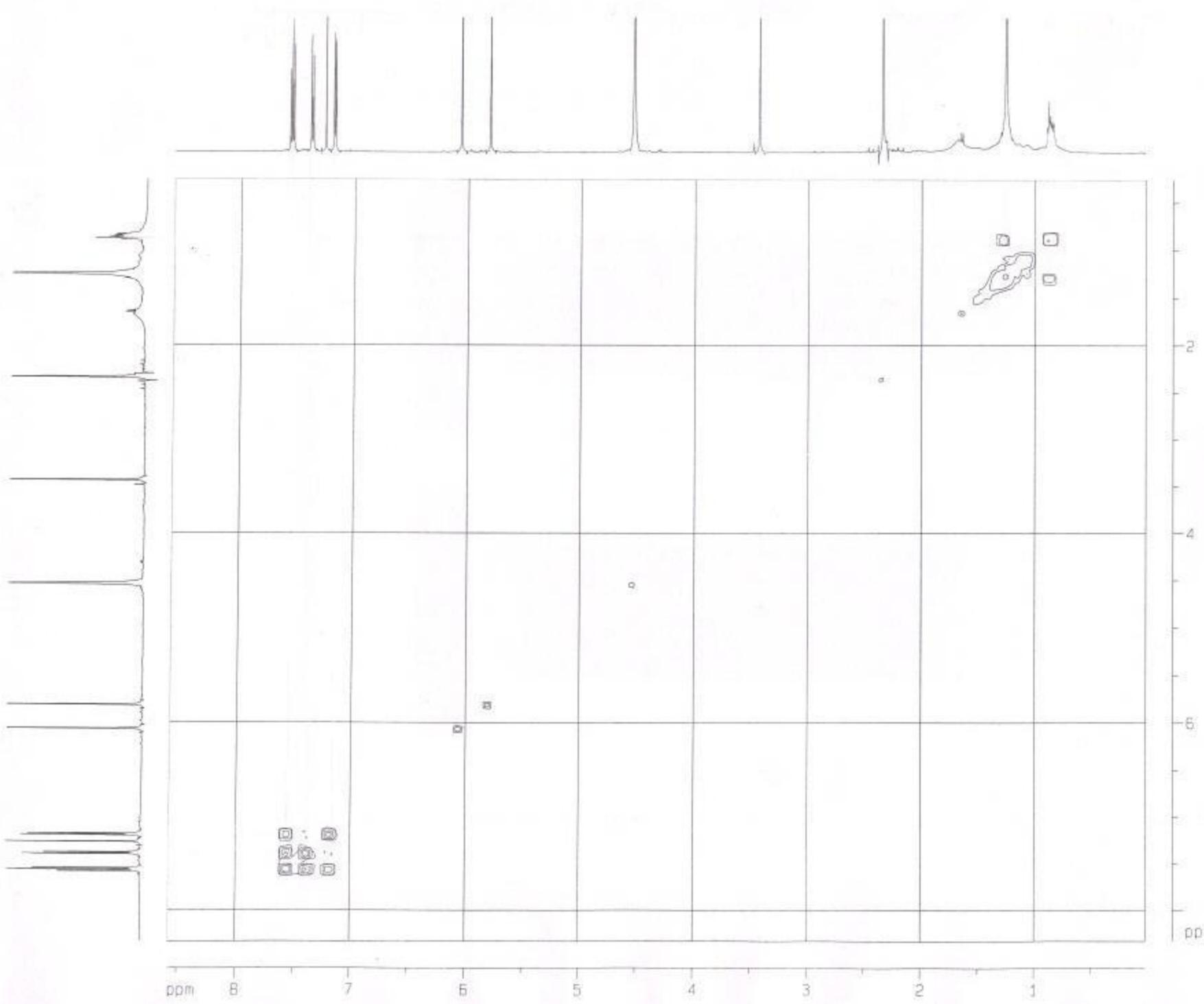
# 1-HMBC

7



# 1- H-H- COSY

8



Current Data Parameters:  
 NAME: mds20  
 EXPNO: 33  
 PROCNO: 1

F2 - Acquisition Parameters:  
 Date: 20051125  
 Time: 18:43  
 INSTRUM: DRX500  
 PROBHD: 5 mm BB1:1H-BB  
 PULPROG: cosygated1d  
 TD: 1024  
 SOLVENT: DDC13  
 NS: 2  
 DS: 16  
 SWH: 8012.820 Hz  
 FIDRES: 7.825020 Hz  
 AB: 0.0539475 sec  
 RS: 26008  
 DM: 62.400 usec  
 DE: 6.00 usec  
 TE: 300.0 K  
 DD: 0.00000300 sec  
 Q1: 2.0000000 sec  
 A1: 0.0000400 sec  
 Q1S: 0.0002000 sec  
 Q1E: 0.0002000 sec  
 JNO: 0.00012486 sec  
 PRREST: 0.0000000 sec  
 NOSEK: 2.0000000 sec

\*\*\*\*\* CHANNEL F1 \*\*\*\*\*  
 NUC1: 1H  
 P1: 8.90 usec  
 PL1: -1.00 dB  
 SF01: 500.1318310 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: 10.00 %  
 GPZ2: 10.00 %  
 GPZ3: 30.00 %  
 P16: 1000.00 usec

F1 - Acquisition parameters:  
 NOD: 1  
 TD: 1024  
 SF01: 500.1318310 MHz  
 FIDRES: 7.825020 Hz  
 SW: 15.001 sec  
 F MODE: GF

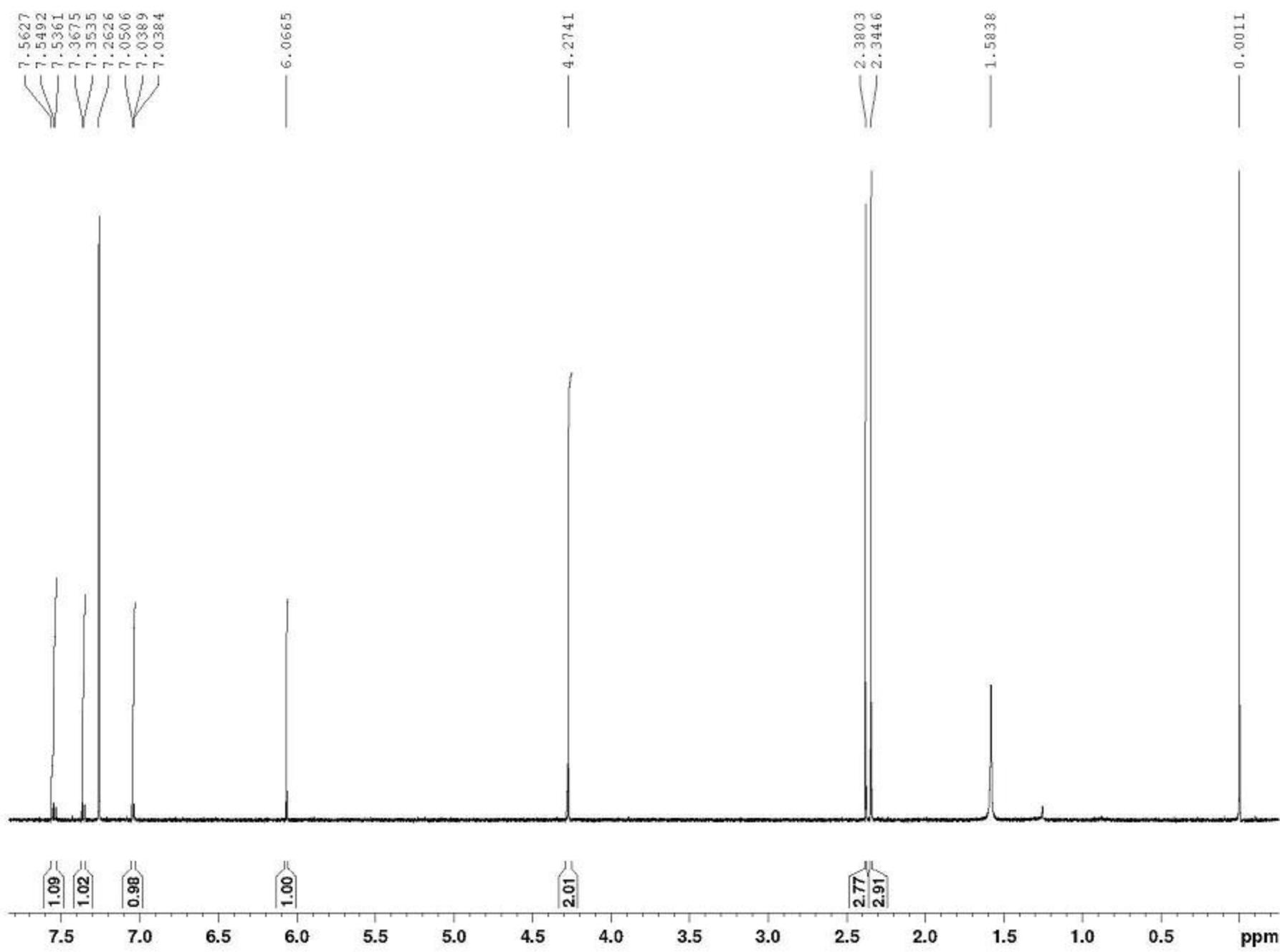
F2 - Processing parameters:  
 S1: 1024  
 SF: 500.1300119 MHz  
 NW: SINE  
 SS1: b  
 LB: 0.00 Hz  
 GS: b  
 PC: 1.00

F1 - Processing parameters:  
 S1: 1024  
 MC2: GF  
 SF: 500.1311765 MHz  
 NW: SINE  
 SS1: b  
 LB: 0.00 Hz  
 GS: b

2D NMR plot parameters:  
 C1R: 18.00 cm  
 C1I: 14.00 cm  
 F2PL0: 8.581 ppm  
 F2LD: 4291.83 Hz  
 F2RD: 0.023 ppm  
 F2HI: 11.54 Hz  
 F1PL0: 11.335 ppm  
 F1LD: 4181.78 Hz  
 F1RI: 0.257 ppm  
 F1HI: 128.51 Hz  
 F2PROMH: 0.475465 ppm/cbr  
 F2NDMH: 237.79357 Hz/cbr  
 F2PDMH: 0.57703 ppm/cbr  
 F2NDCH: 288.59103 Hz/cbr

2-1H

9



Current Data Parameters  
NAME DS-25-1  
EXPNO 1  
PROCNO 1

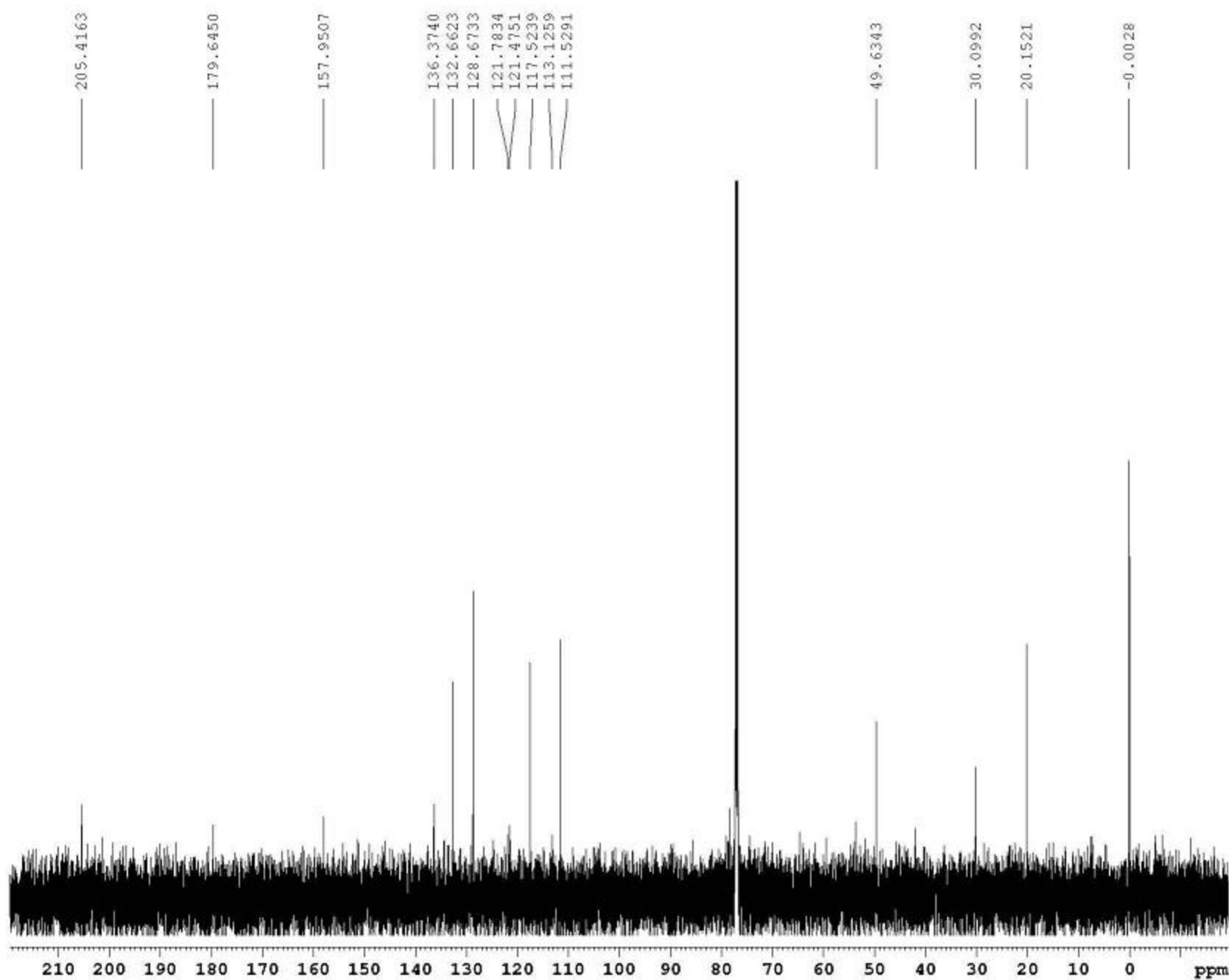
F2 - Acquisition Parameters  
Data\_ 20070828  
Time 9.23  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 40  
DS 2  
SWH 4854.369 Hz  
FIDRES 0.074072 Hz  
AQ 6.7502580 sec  
RG 1150  
DW 103.000 usec  
DE 6.00 usec  
TE 296.2 K  
D1 3.0000000 sec  
TD0 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 9.70 usec  
PL1 2.00 dB  
SFO1 600.1322845 MHz

F2 - Processing parameters  
SI 32768  
SF 600.1300087 MHz  
NDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

2-13C

10



Current Data Parameters  
 NAME DS-25-1  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20070830  
 Time 3.09  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg3d30  
 TD 65536  
 SOLVENT CDCl3  
 NS 4096  
 DS 4  
 SWH 36057.691 Hz  
 FIDRES 0.550197 Hz  
 AQ 0.9086159 sec  
 RG 2550  
 DM 13.867 usec  
 DE 6.00 usec  
 TE 299.9 K  
 D1 3.00000000 sec  
 d11 0.03000000 sec  
 ID0 1

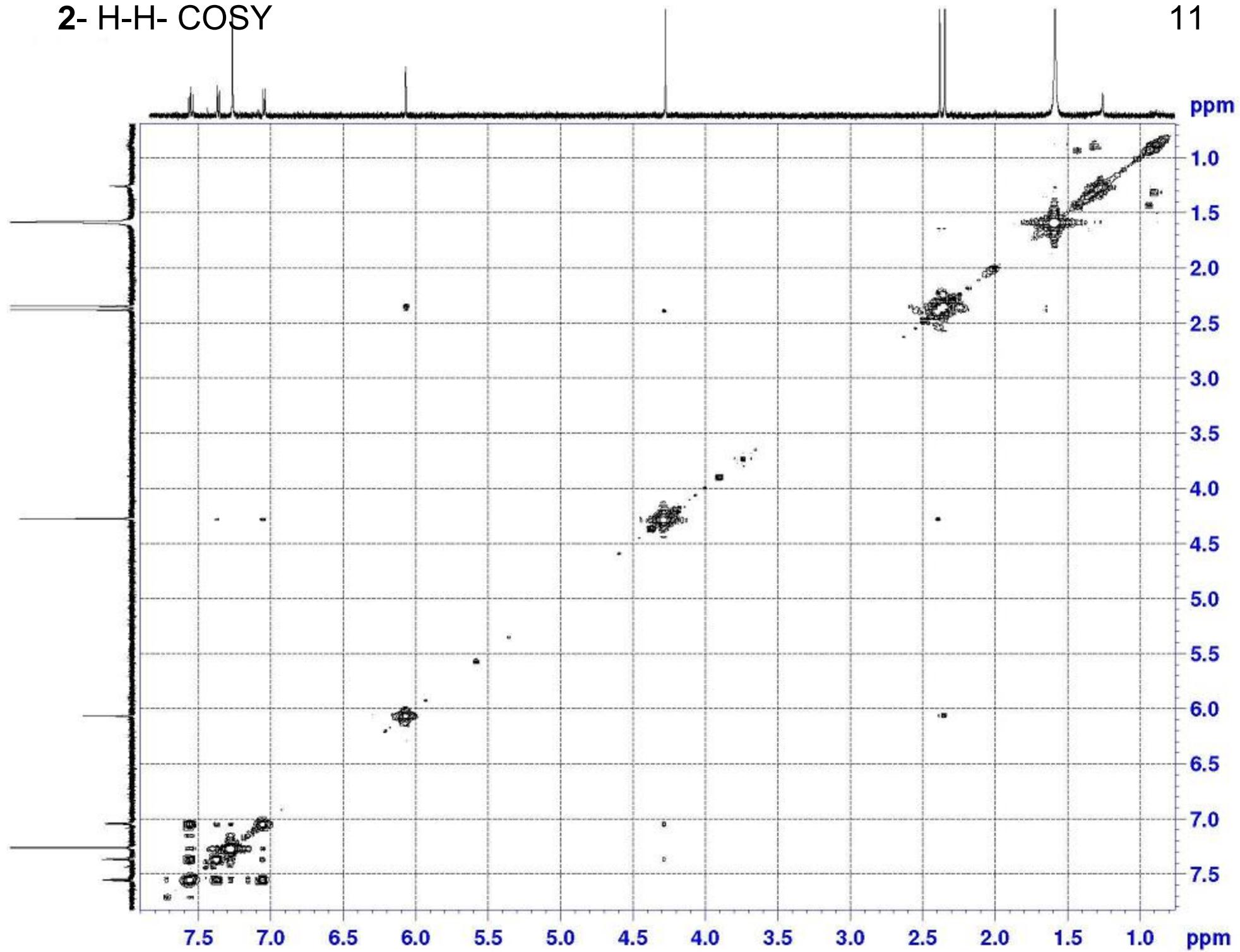
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.80 usec  
 PL1 2.00 dB  
 SF01 150.9176908 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 70.00 usec  
 PLJ2 12.50 dB  
 PL2 -1.00 dB  
 SF02 600.1324005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 150.9028057 MHz  
 NDW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 0.40

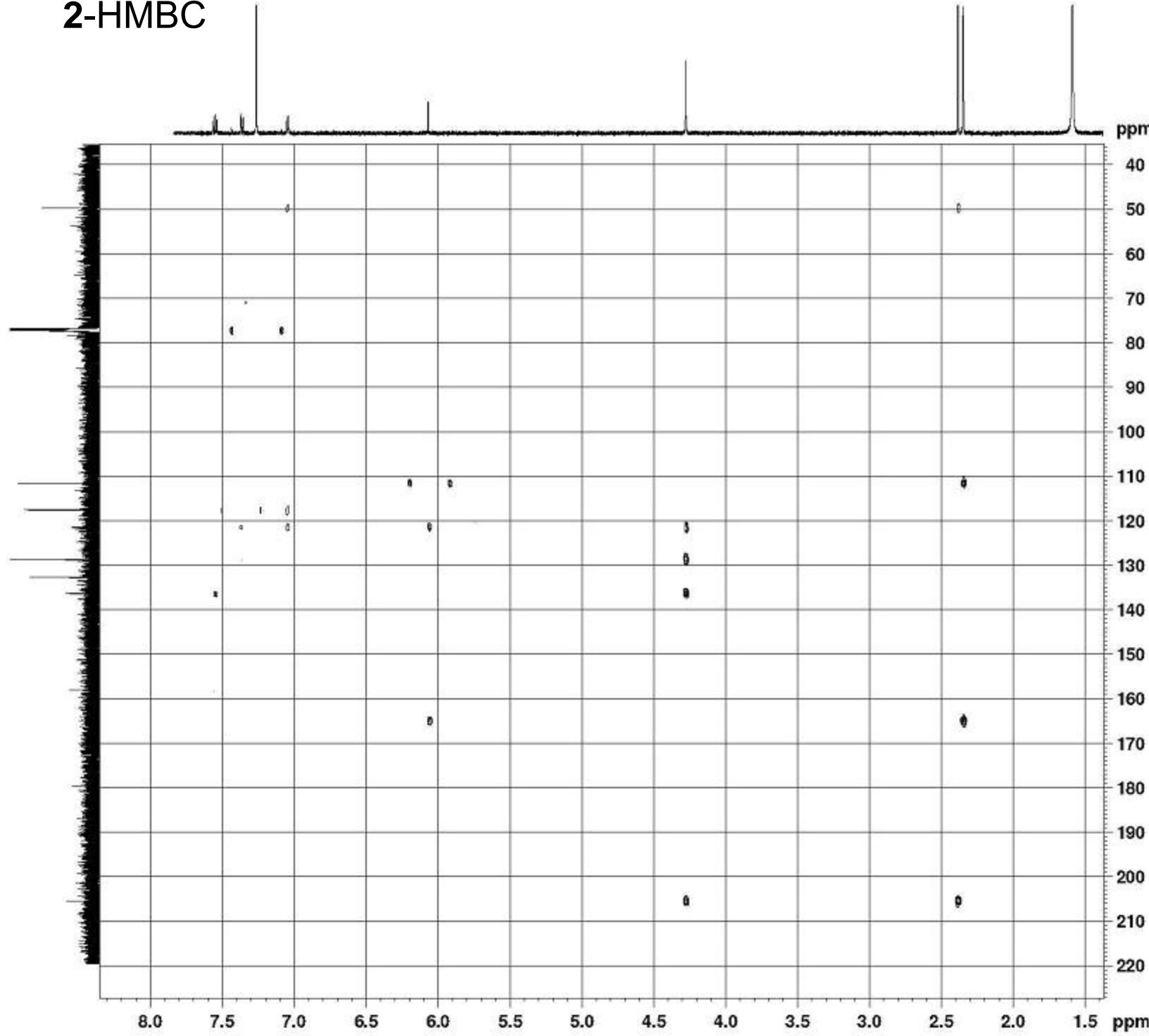
2-H-H-COSY

11



2-HMBC

12



Current Data Parameters  
NAME DS-2S-1  
EXPNO 7  
PROCNO 1

P2 - Acquisition Parameters  
Date 20070830  
Time 7.09  
INSTRUM spect  
PROBHD 5 mm PARBO BB-  
PULFRQ hmbcognqf  
TD 2048  
SOLVENT CDCl3  
NS 16  
DS 16  
SWH 4054.369 Hz  
FIDRES 2.370297 Hz  
AQ 0.2109940 sec  
RG 2050  
DW 103.000 usec  
DE 6.00 usec  
TE 296.4 K  
CNST13 8.000000  
d0 0.00000300 sec  
D1 1.5000000 sec  
D16 0.0002000 sec  
d6 0.0625000 sec  
IN0 0.00001490 sec

----- CHANNEL f1 -----  
NUC1 1H  
P1 14.90 usec  
p2 29.00 usec  
PL1 -1.00 dB  
SFO1 600.1322758 MHz

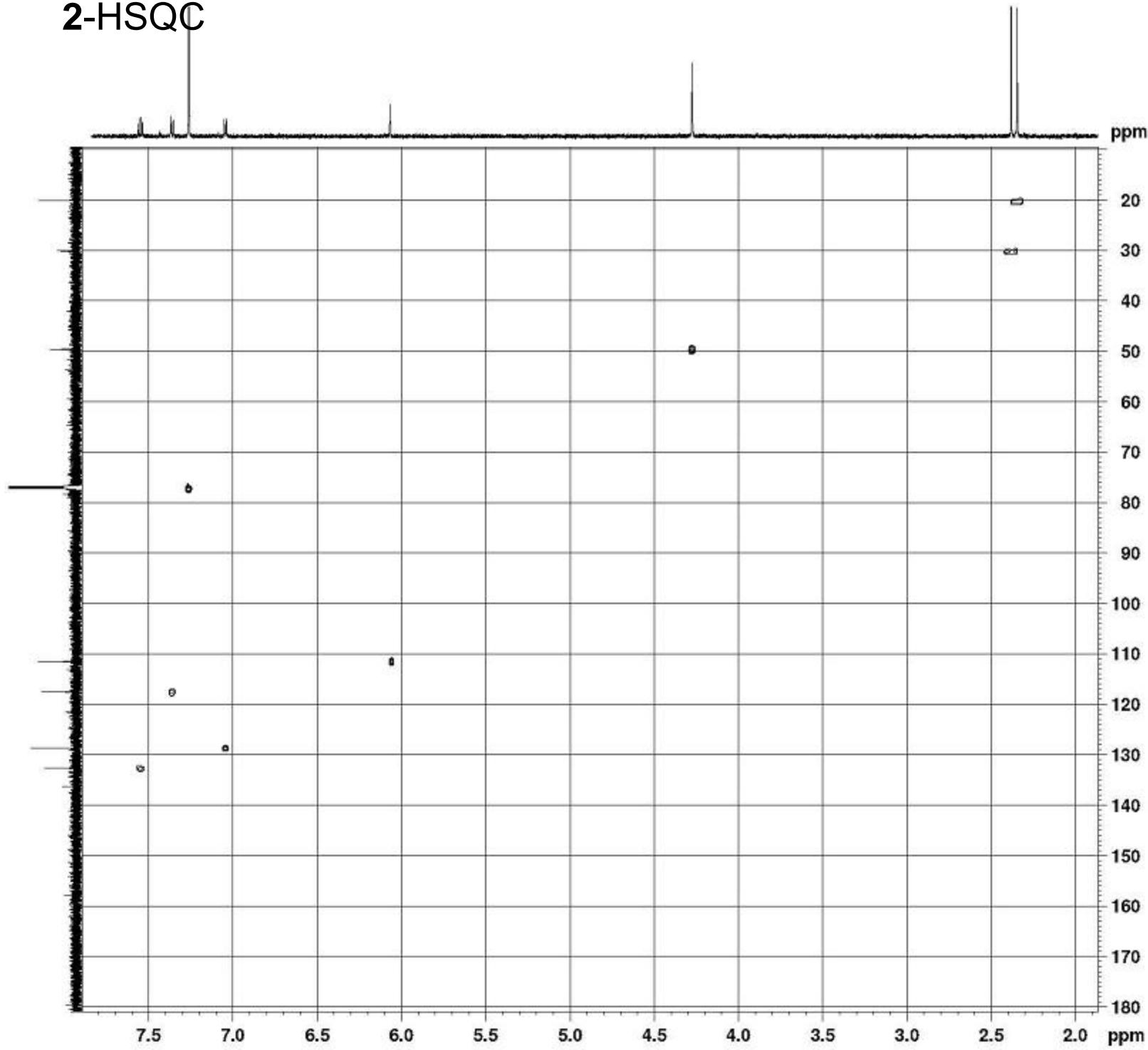
----- CHANNEL f2 -----  
NUC2 13C  
P3 9.80 usec  
PL2 2.00 dB  
SFO2 150.9178748 MHz

----- GRADIENT CHANNEL -----  
GENAM1 SINE,100  
GENAM2 SINE,100  
GENAM3 SINE,100  
GPZ1 50.00 %  
GPZ2 30.00 %  
GPZ3 40.10 %  
P16 1000.00 usec

P1 - Acquisition parameters  
ND0 3  
TD 175  
SFO1 150.9179 MHz  
FIDRES 191.754547 Hz  
SW 222.353 PPM  
PrMODE QF

P2 - Processing parameters  
SI 1024  
SF 600.1300056 MHz  
NDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.40

P1 - Processing parameters  
SI 1024  
MC2 QF  
SF 150.9028035 MHz  
NDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0



```

Current Data Parameters
NAME      D8-25-1
EXPHC     6
PRCNO     1

P2 - Acquisition Parameters
Date      20070830
Time      5.18
INSTRUM  spect
PROBHD  5 mm PABBO BB-
PULPROG hsqcetgp
TD       1024
SOLVENT  CDCl3
NS       16
DS       16
SWH     4054.369 Hz
FIDRES  4.740595 Hz
RQ      0.1055220 sec
RG      2050
DW      103.000 usec
DE      6.00 usec
TE      298.5 K
CPSIG2  145.000000
G0      0.00000300 sec
D1      1.50000000 sec
d11     0.03000000 sec
d13     0.00000400 sec
D16     0.00020000 sec
d4      0.00172414 sec
DELTA   0.00123500 sec
DELTAP1  0.00071614 sec
INO     0.00001640 sec
STIMGT  128
SCOPTNS

CHANNEL f1
NUC1    1H
P1      14.90 usec
P2      29.80 usec
P2B    1000.00 usec
PL1    -1.00 dB
SF01   600.1322758 MHz

CHANNEL f2
CPDPFG2 garp
NUC2    13C
P3      9.80 usec
P4      19.60 usec
PCPD2  70.00 usec
PL12   19.00 dB
PL2    2.00 dB
SF02   150.9171448 MHz

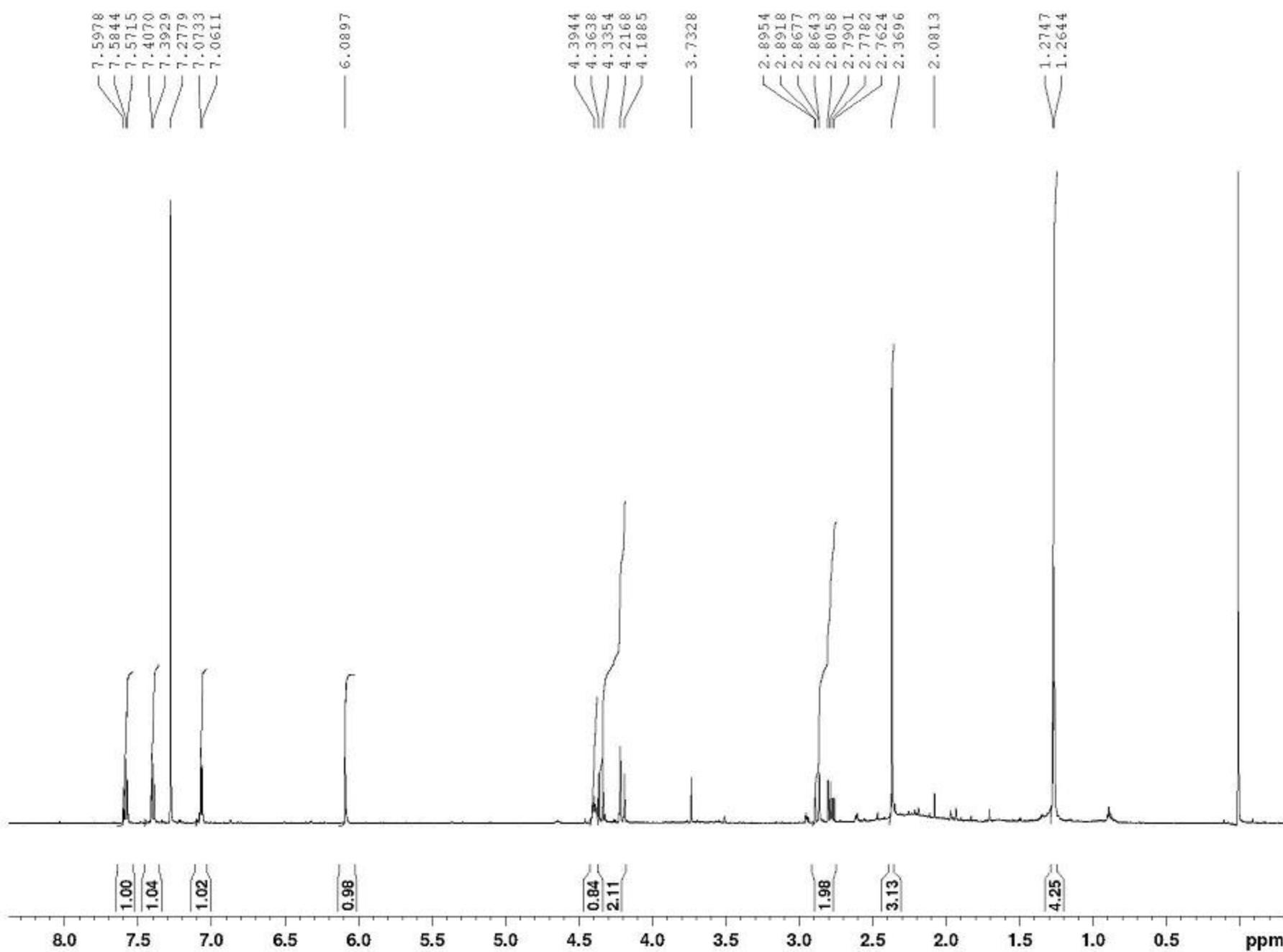
GRADIENT CHANNEL
GPNM1  SINE.100
GPNM2  SINE.100
GP21   80.00 *
GP22   20.10 *
P16    1000.00 usec

P1 - Acquisition parameters
NDO      2
ID       256
SF      150.9171 MHz
FIDRES  135.633682 Hz
SW      230.075 ppm
PnMGE   Echo-Antiecho

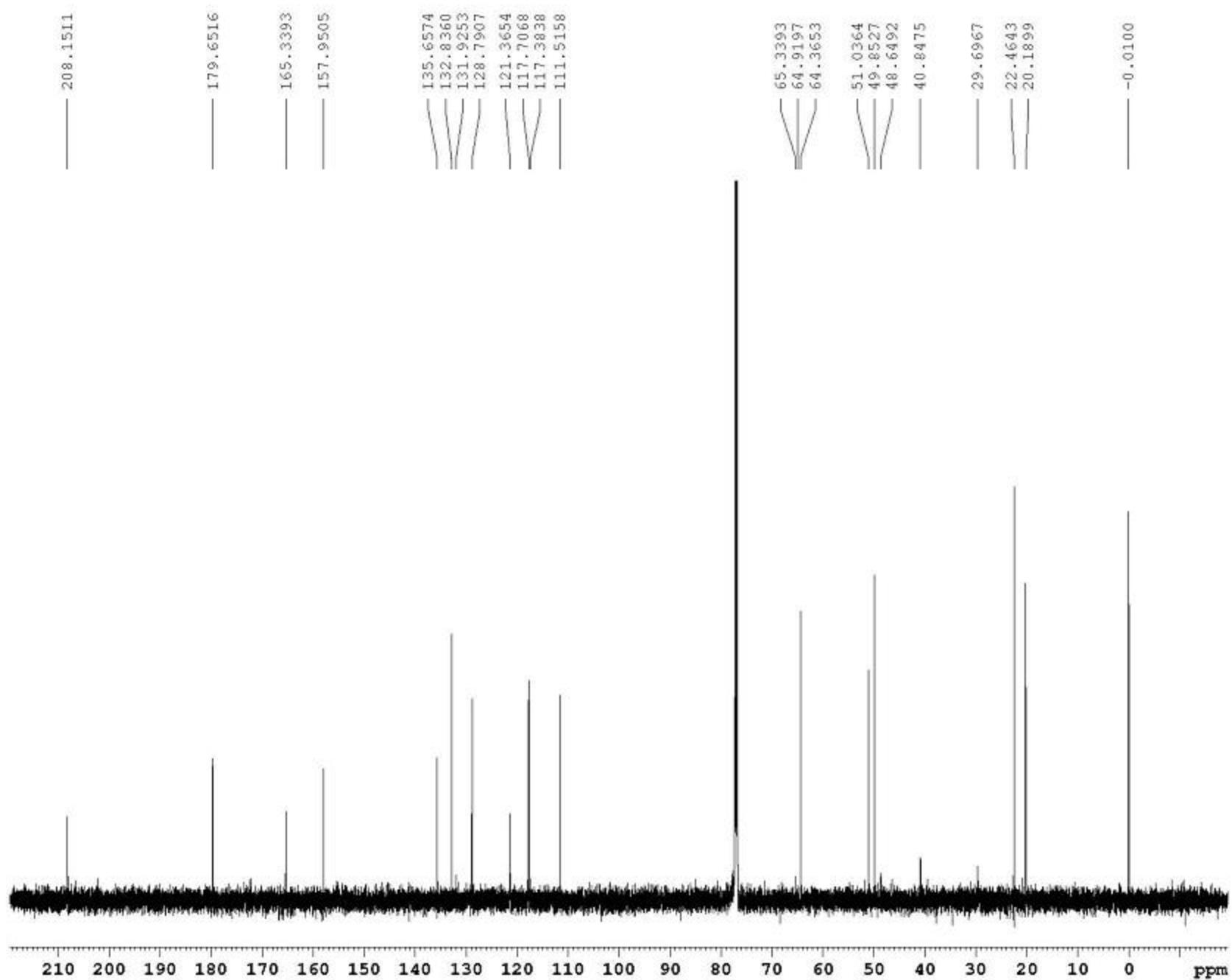
P2 - Processing parameters
SI      1024
SF      600.1300043 MHz
NDW    QSLINE
SSB      2
LB      0.00 Hz
GB      0
PC      1.40

P1 - Processing parameters
SI      1024
MC2   echo-antiecho
SF      150.9027865 MHz
WDW   QSLINE
SSB      2
LB      0.00 Hz
GB      0

```



3-13C



Current Data Parameters  
 NAME D6-27  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20070409  
 Time 11.57  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg3d30  
 TD 65536  
 SOLVENT CDCl3  
 NS 19841  
 DS 4  
 SWH 36057.691 Hz  
 FIDRES 0.550197 Hz  
 AQ 0.9086159 sec  
 RG 2550  
 DM 13.867 usec  
 DE 6.00 usec  
 TE 296.1 K  
 D1 2.0000000 sec  
 d11 0.0300000 sec  
 ID0 1

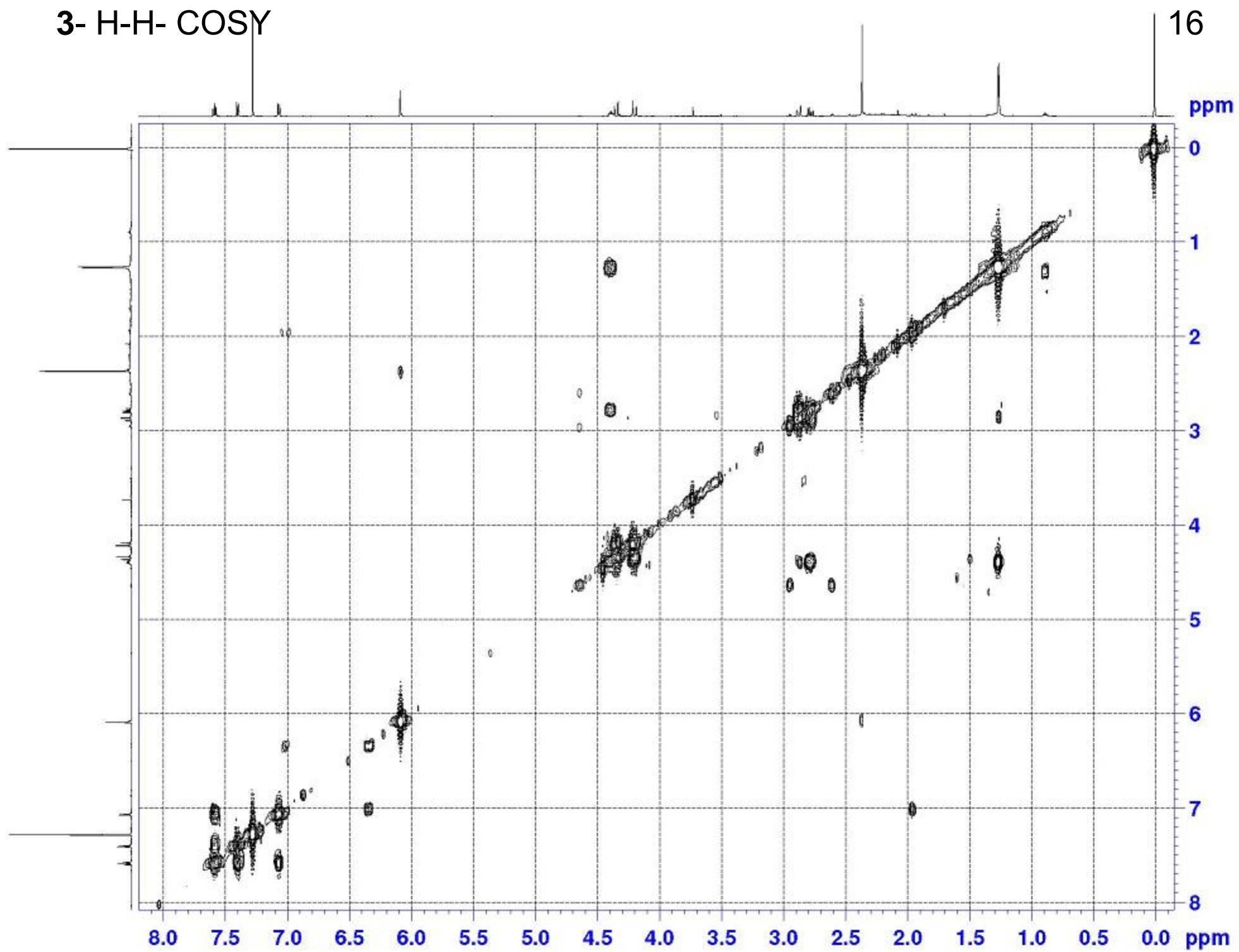
===== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 9.80 usec  
 PL1 2.00 dB  
 SF01 150.9176909 MHz

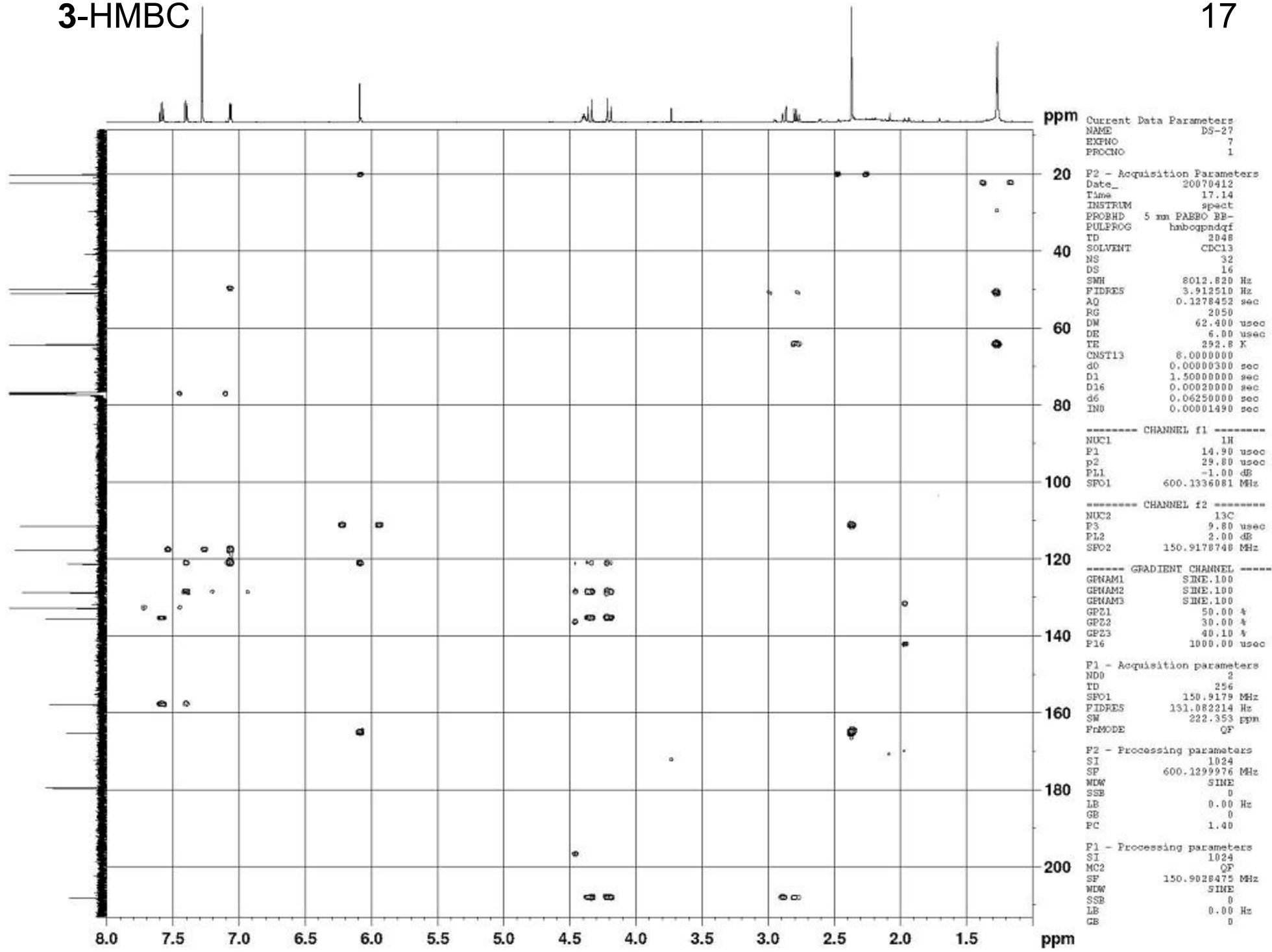
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 70.00 usec  
 PL12 12.50 dB  
 PL2 -1.00 dB  
 SF02 600.1324005 MHz

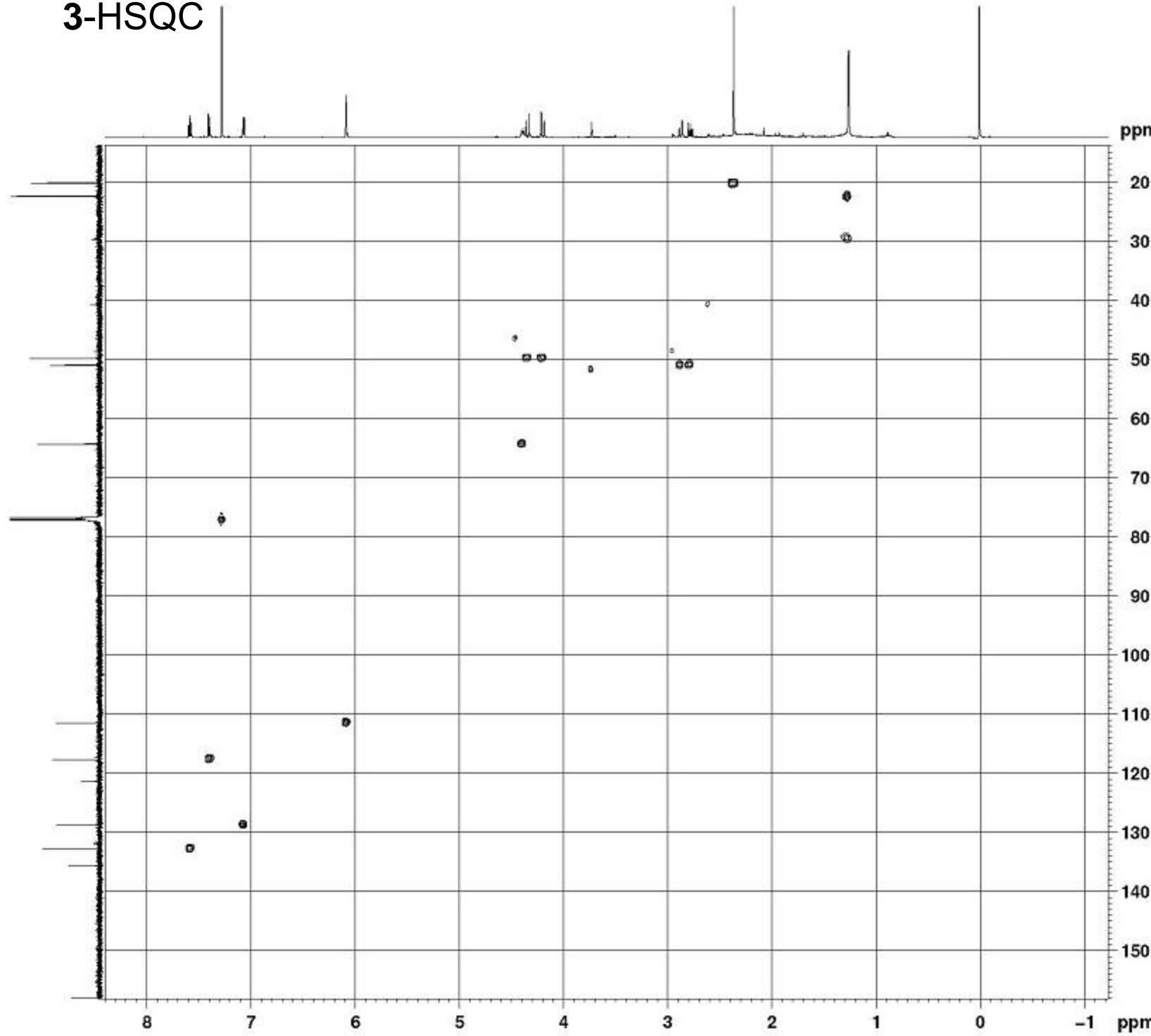
F2 - Processing parameters  
 SI 32768  
 SF 150.9028090 MHz  
 NDW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40

15

### 3- H-H- COSY







Current Data Parameters  
 NAME DS-27  
 EXPNO 6  
 PROCNO 1

P2 - Acquisition Parameters  
 Date\_ 20070412  
 Time 14.32  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hsqcgp  
 TD 1024  
 SOLVENT CDCl3  
 MS 24  
 DS 16  
 SWB 8012.820 Hz  
 FIDRES 7.825020 Hz  
 AQ 0.0639476 sec  
 RG 2500  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 293.2 K  
 CPMG2 1.05.000000  
 D0 0.00000300 sec  
 D1 1.50000000 sec  
 D11 0.03000000 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 d4 0.00172314 sec  
 DELTA 0.00123580 sec  
 DELTA1 0.00071614 sec  
 IND 0.00001655 sec  
 ST1CNT 328  
 ZOOFINS

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 14.90 usec  
 P2 29.80 usec  
 P28 1000.00 usec  
 PL1 -1.00 dB  
 SPO1 600.1336081 MHz

----- CHANNEL f2 -----  
 CPDPRG2 garp  
 NUC2 13C  
 P3 9.80 usec  
 p4 19.60 usec  
 PCPD2 70.00 usec  
 PL12 19.00 dB  
 PL2 2.00 dB  
 SPO2 150.9171948 MHz

----- GRADIENT CHANNEL -----  
 GRADAM1 SINE.100  
 GRADAM2 SINE.100  
 GRT1 80.00 %  
 GRT2 20.10 %  
 P36 1000.00 usec

F1 - Acquisition parameters  
 N1D 2  
 TD 256  
 SPO1 150.9375 MHz  
 FIDRES 118.013596 Hz  
 SW 200.186 ppm  
 F1MODE Echo-Antiecho

F2 - Processing parameters  
 S1 1024  
 SF 600.1299935 MHz  
 N1M QSIME  
 S2B 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.40

F1 - Processing parameters  
 S1 1024  
 MC2 echo-antiecho  
 SF 150.9026276 MHz  
 N1M QSIME  
 S2B 2  
 LB 0.00 Hz  
 GB 0

Compound 1 was examined by reversed-phase HPLC on a 4.6 × 250 mm C-18 (5 µm) column (Merck) with CH<sub>3</sub>CN from 50% to 100% in 15 min (1 mL/min flow rate, 254 nm detection) with a retention time of 11.3 min. Crude extract was examined by the same method. The peak of compound 1 was detected with a retention time of 11.3 min.

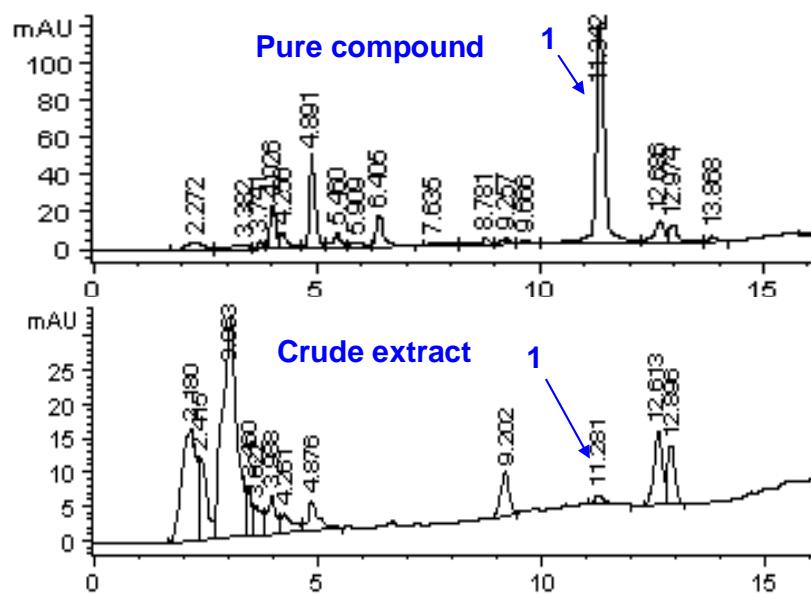


Figure 1: The HPLC result of compound 1 and crude extract.