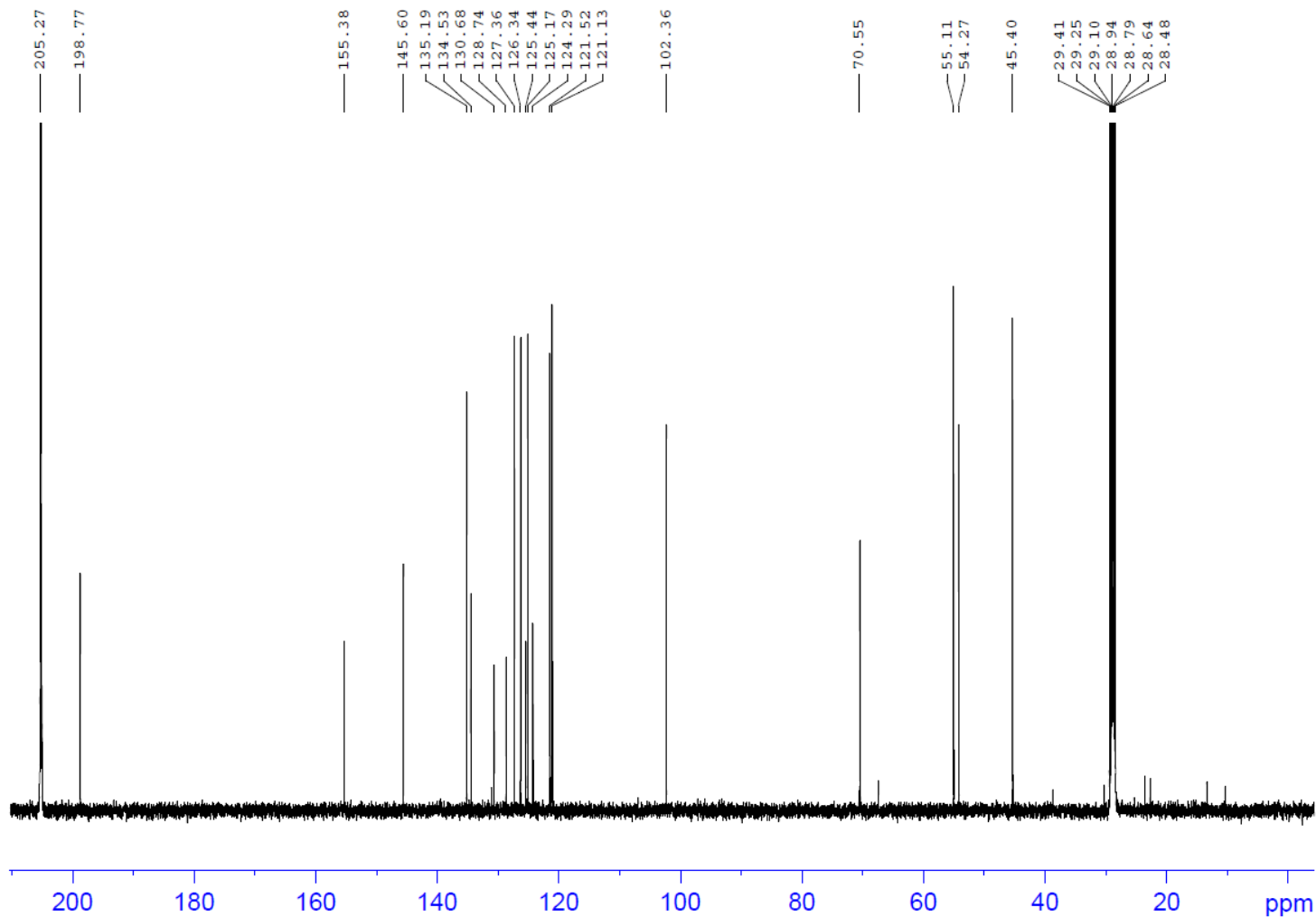


Supporting Information

¹³C of Compound 1

W007-4



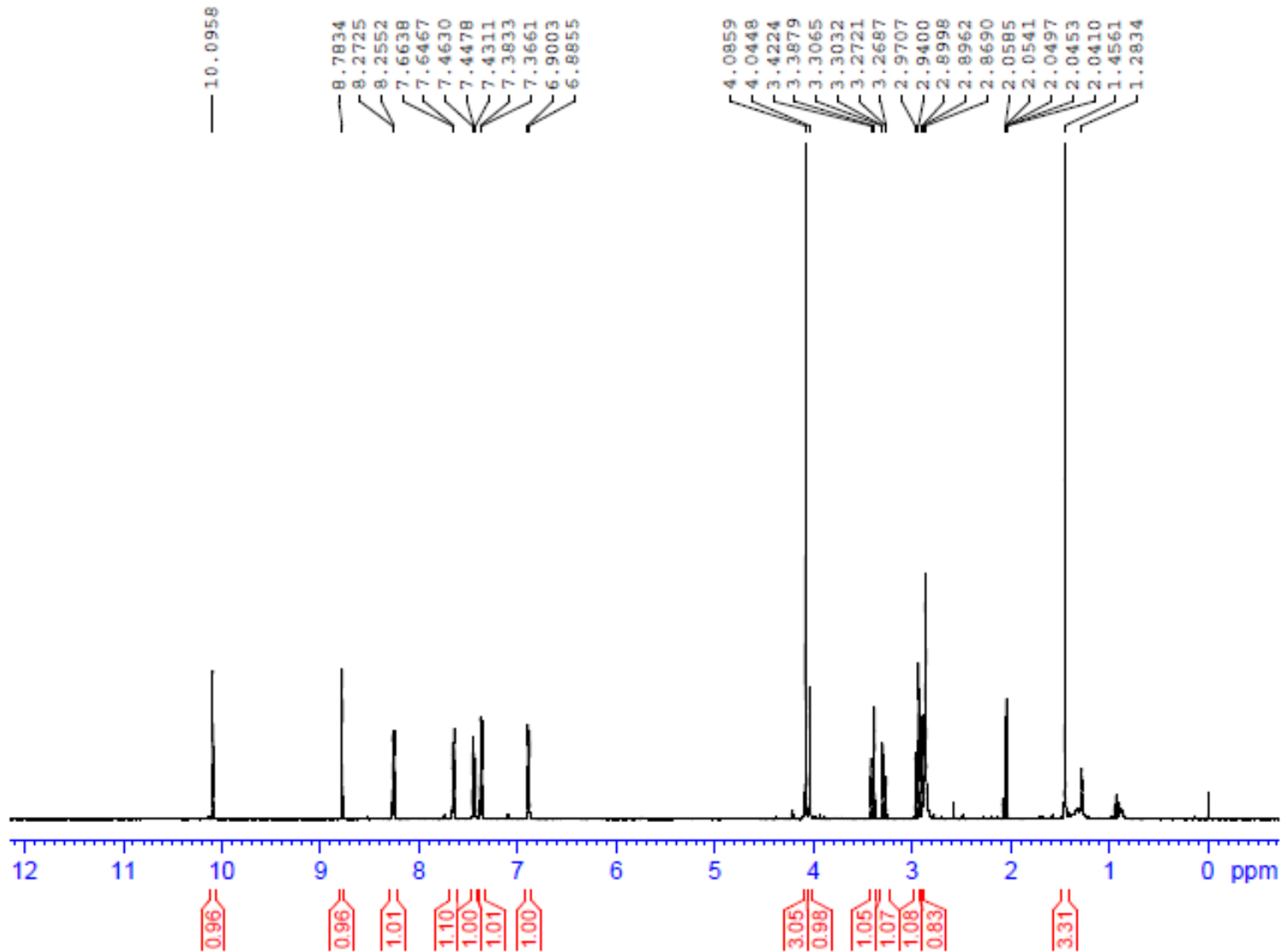
```
NAME          101118
EXPNO         2
PROCNO        1
Date_         20101118
Time_         11.17
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       Acetone
NS            1024
DS            4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG            203
DW            16.800 usec
DE            6.50 usec
TE            299.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
```

```
----- CHANNEL f1 -----
NUC1          13C
P1            10.04 usec
PL1           -1.00 dB
PL1W          106.25253296 W
SFO1          125.7703643 MHz
```

```
----- CHANNEL f2 -----
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.35 dB
PL12          16.90 dB
PL13          17.00 dB
PL2W          19.76737595 W
PL12W         0.43747079 W
PL13W         0.42751271 W
SFO2          500.1320005 MHz
SI            32768
SF            125.7577890 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

¹H of Compound 1

W007-4

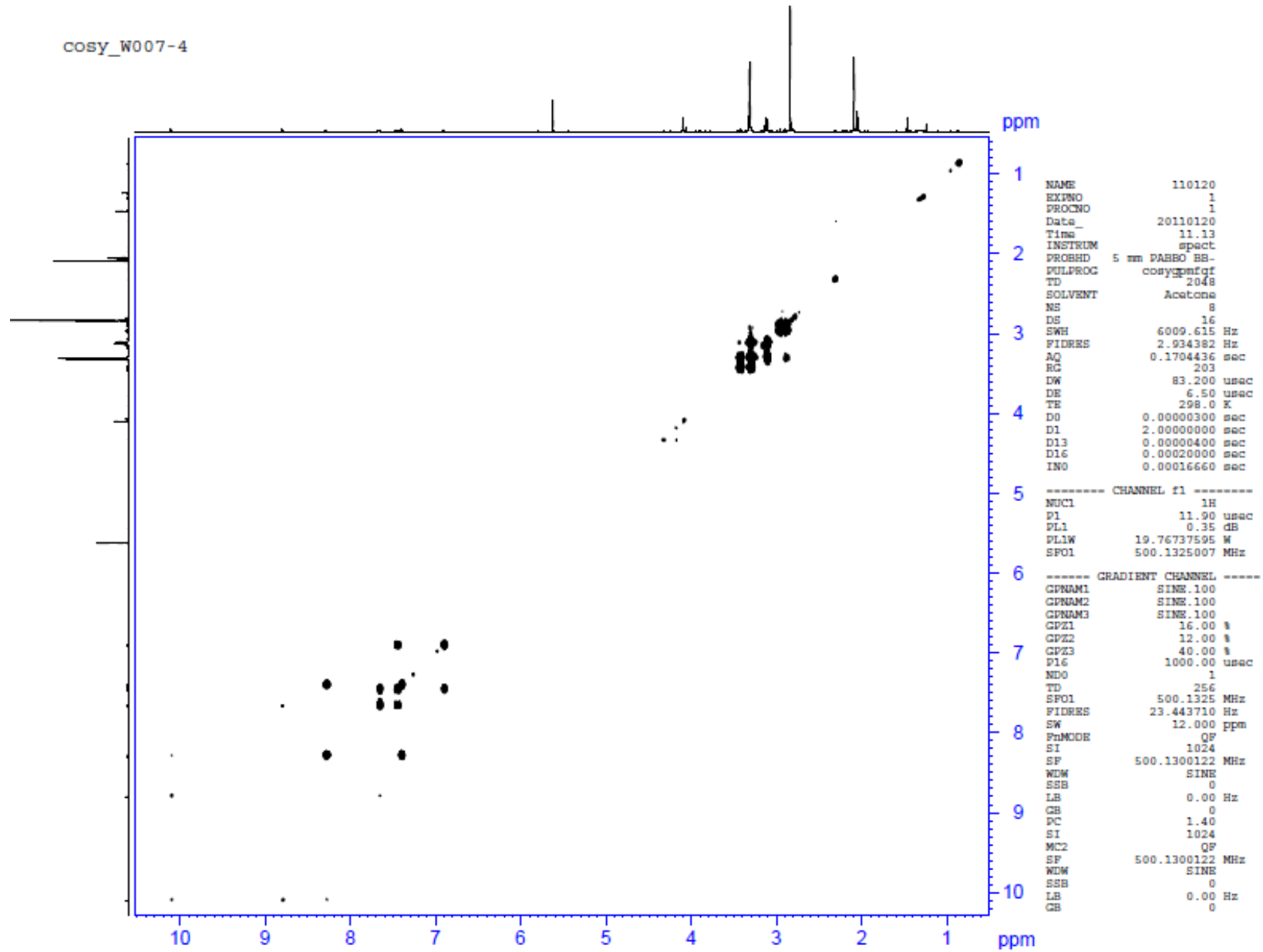


```
NAME 101118
EXPNO 1
PROCNO 1
Date_ 20101118
Time_ 11.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 114
DW 48.400 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 11.90 usec
PL1 0.35 dB
PL1W 19.76737595 W
SPO1 500.1330885 MHz
SI 32768
SP 500.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```

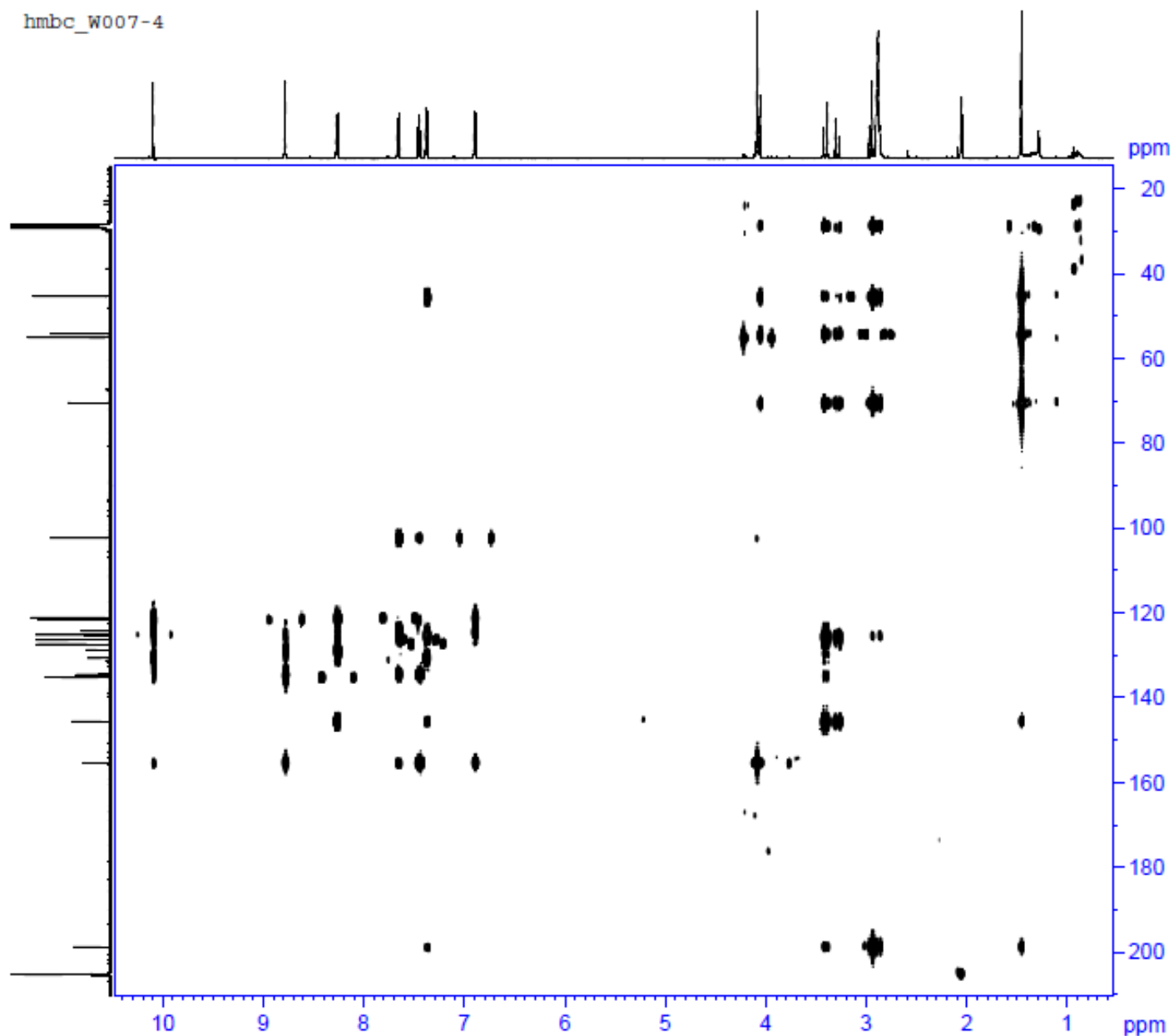
COSY of Compound 1

cosy_W007-4



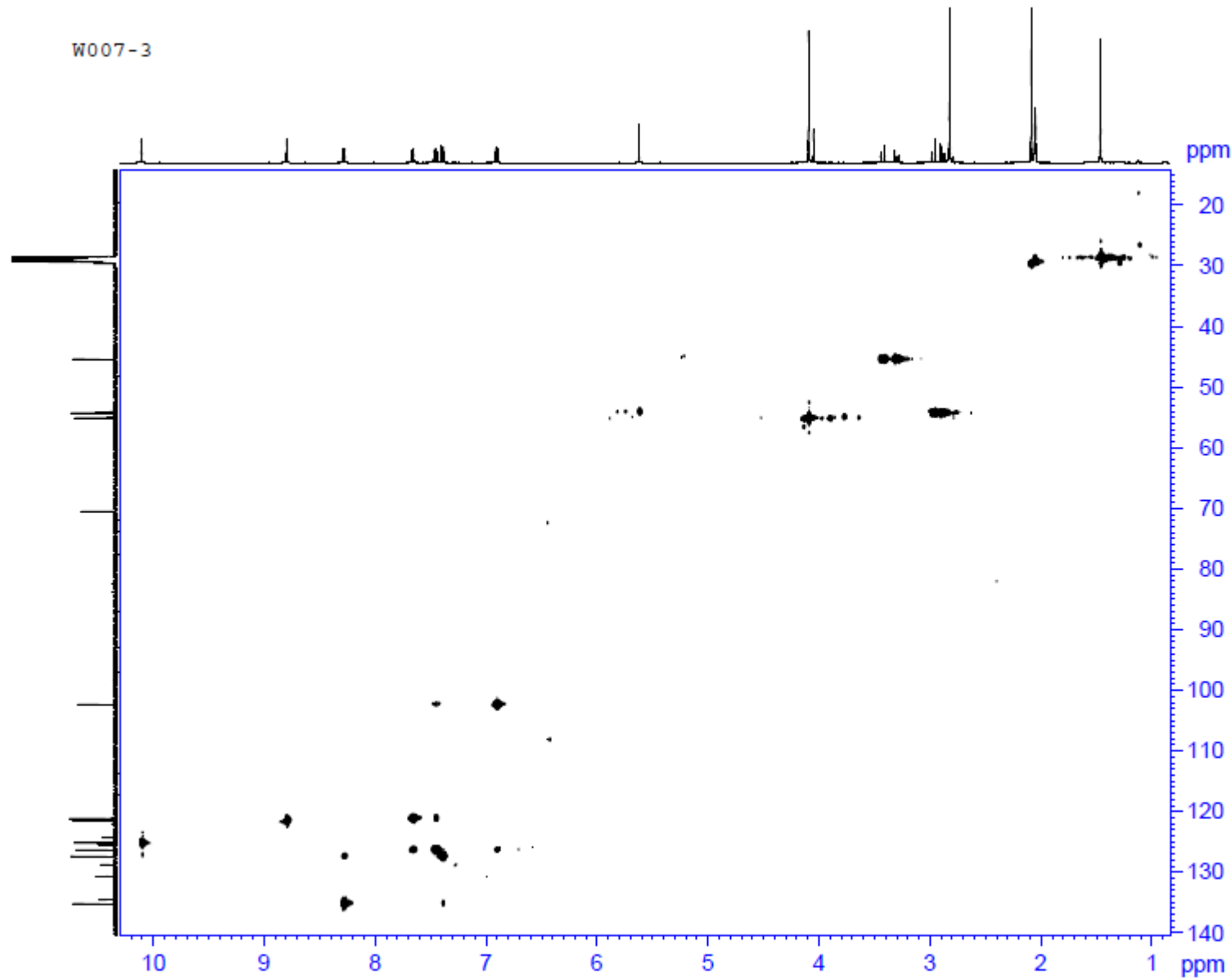
HMBC of Compound 1

hmbc_w007-4



HSQC of Compound 1

W007-3



```

NAME          101110
EXPNO         2
PROCNO        1
Date_         20101110
Time          8.51
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       hsqcetpp1qc2
TD            2048
SOLVENT       Acetone
NS            8
DS            8
SFO          600.615 Hz
FIDRES        2.934382 Hz
AQ            0.1704436 sec
RG            203
SW            81.200 usec
DS            6.50 usec
TE            298.2 K
CQ1T2         145.0000000
D0            0.0000000 sec
D1            2.0000000 sec
D4            0.00172414 sec
D11           0.0000000 sec
D16           0.0000000 sec
D24           0.00086207 sec
IN0           0.00002650 sec
ZDROPPING

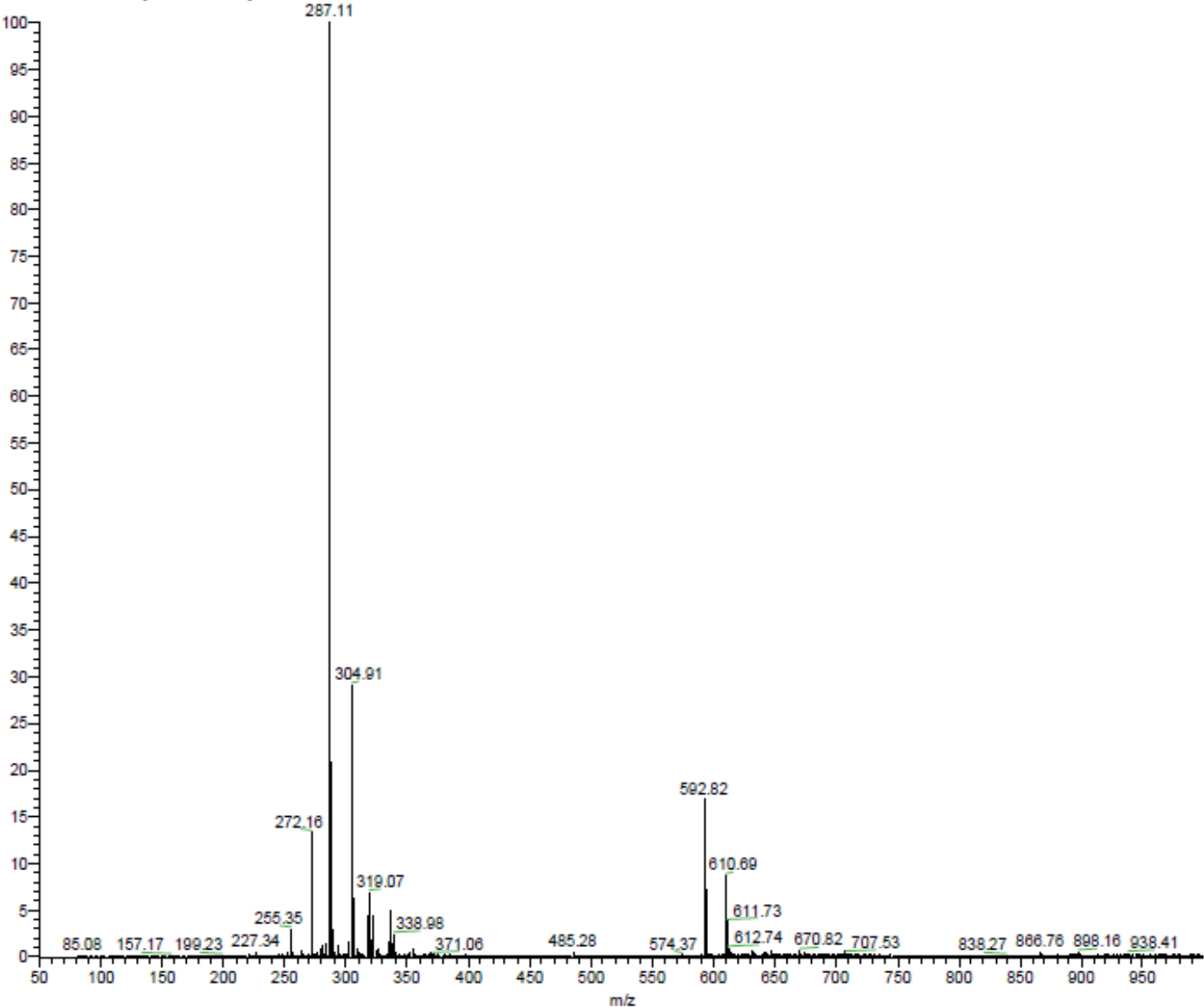
----- CHANNEL f1 -----
NUC1          1H
P1            11.90 usec
P2            23.80 usec
P20           0.00 usec
P21           0.35 dB
P2LW          19.76737595 W
SFO1          500.1329008 MHz

----- CHANNEL f2 -----
CQ1PRG2       gsrp
NUC2          13C
P3            11.90 usec
P4            23.80 usec
P14           500.00 usec
PCPD2         70.00 usec
P20           120.00 dB
P21           1.00 dB
P2L2          16.39 dB
P2LW          0.00000000 W
P2LW          67.04081726 W
P2LW          1.93792559 W
SFO2          125.7665920 MHz
SFO2          7.65 dB
SFO2          Crp60, 0.5, 20.1
SFOCAL3       0.500
SFOFFS3       0.00 Hz

----- GRADIENT CHANNEL -----
GRNAM1        SINE.100
GRNAM2        SINE.100
GRNAM3        SINE.100
GRNAM4        SINE.100
GRP1          80.00 %
GRP2          20.10 %
GRP3          11.00 %
GRP4          -5.00 %
P16           1000.00 usec
P19           500.00 usec
NUC           2
TD            256
SFO1          125.7666 MHz
FIDRES        73.691260 Hz
SW            150.000 ppm
PRMODE       Echo-AntiEcho
SI            1024
SF            500.1300091 MHz
WDM          QGINH
SGB          2
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           echo-antiEcho
SF            125.767890 MHz
WDM          QGINH
SGB          2
LB            0.00 Hz
GB            0
    
```

Mass Spectra of Compound 1

QS-ZHY-3-N_101117094618 #11-36 RT: 0.16-0.48 AV: 26 NL: 3.38E4
T: ITMS - e ESI Full ms [50.00-2000.00]



NOESY of Compound 1

noesy_W007-4

