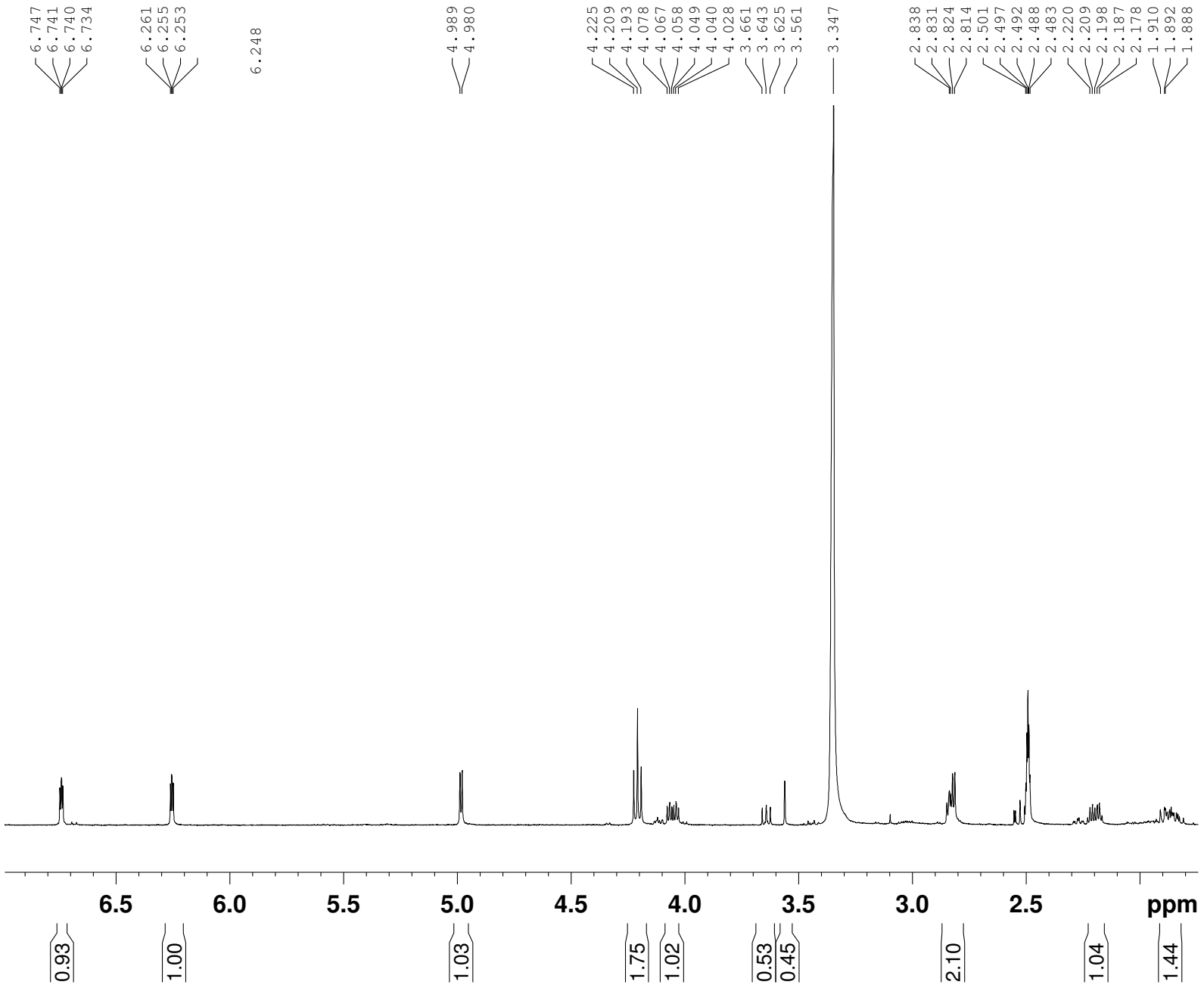
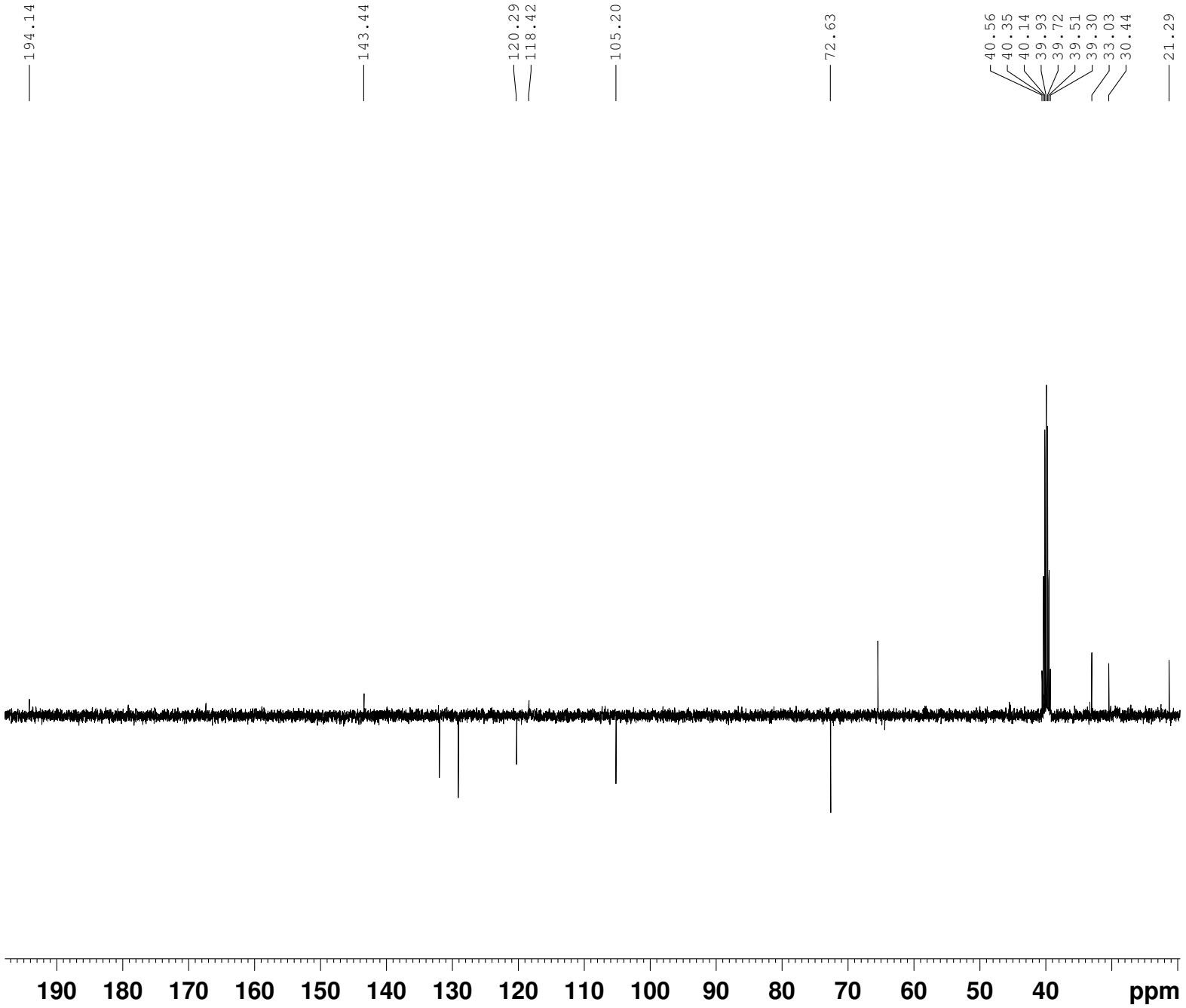
Figure S1. ^{1}H (400MHz) NMR spectrum of **1** in DMSO-d_6.



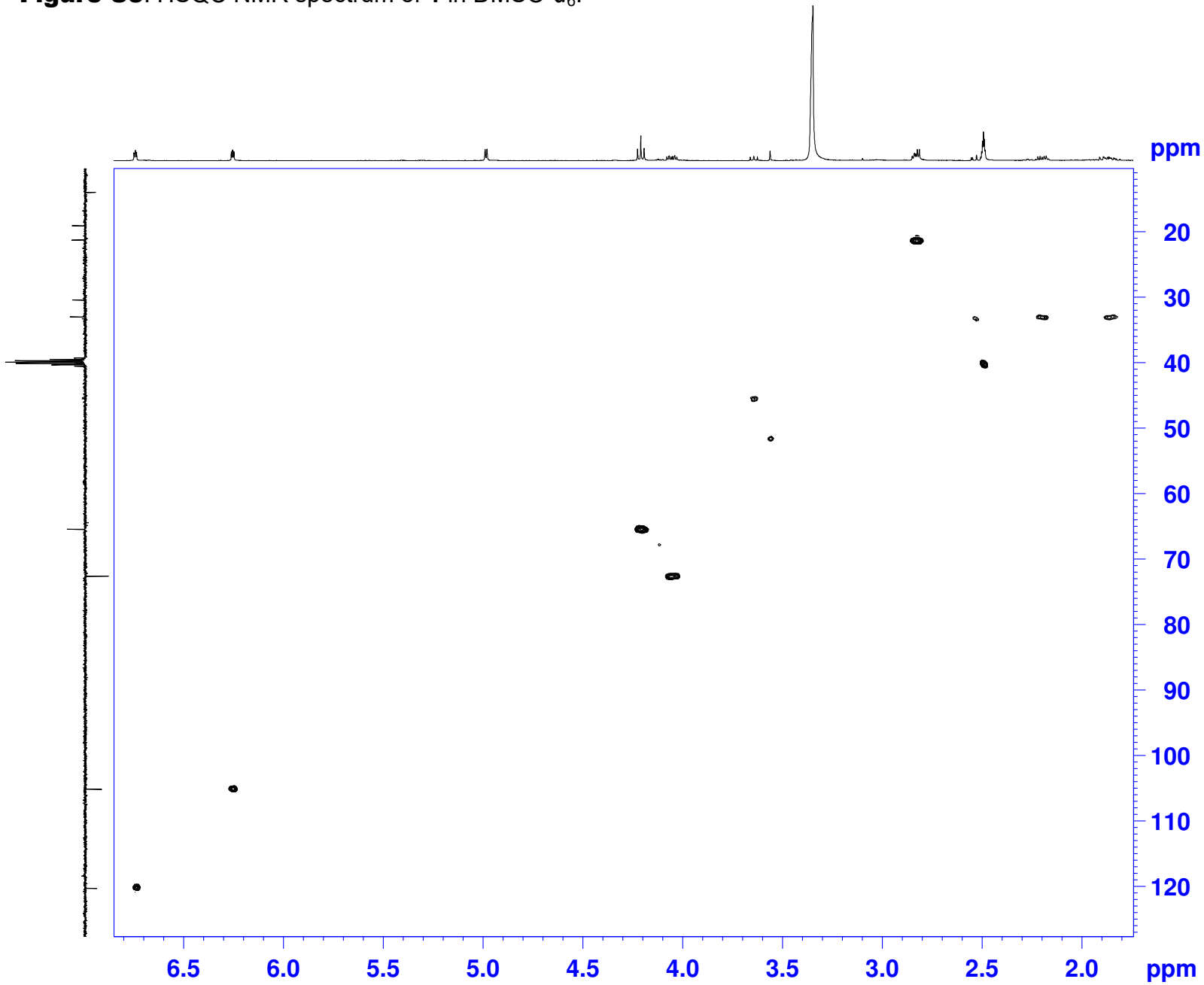

```
Current Data Parameters
NAME                 TW43-4-6
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20151106
Time                   23.55
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                      50.8
DW                    60.800 usec
DE                     6.50 usec
TE                    293.9 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      13.09 usec
PL1                     -1.00 dB
PL1W             12.14314651 W
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                      32768
SF                400.1300000 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

Figure S2. ^{13}C (100 MHz) NMR spectrum of **1** in DMSO-d_6.




```
Current Data Parameters
NAME                 TW43-4-6
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20151107
Time                    0.21
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                 jmod
TD                     65536
SOLVENT                 DMSO
NS                      3072
DS                         4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                       203
DW                    20.800 usec
DE                     6.50 usec
TE                    294.9 K
CNST2             145.0000000
CNST11              1.0000000
D1                  2.00000000 sec
D20                 0.00689655 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                    12.37 usec
P2                    24.74 usec
PL1                    1.00 dB
PL1W             28.13319778 W
SFO1            100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2              waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                   -1.00 dB
PL12                  14.72 dB
PL2W             12.14314651 W
PL12W             0.32533529 W
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF              100.6127690 MHz
WDW                         EM
SSB           0
LB                     1.00 Hz
GB            0
PC                     1.40
```

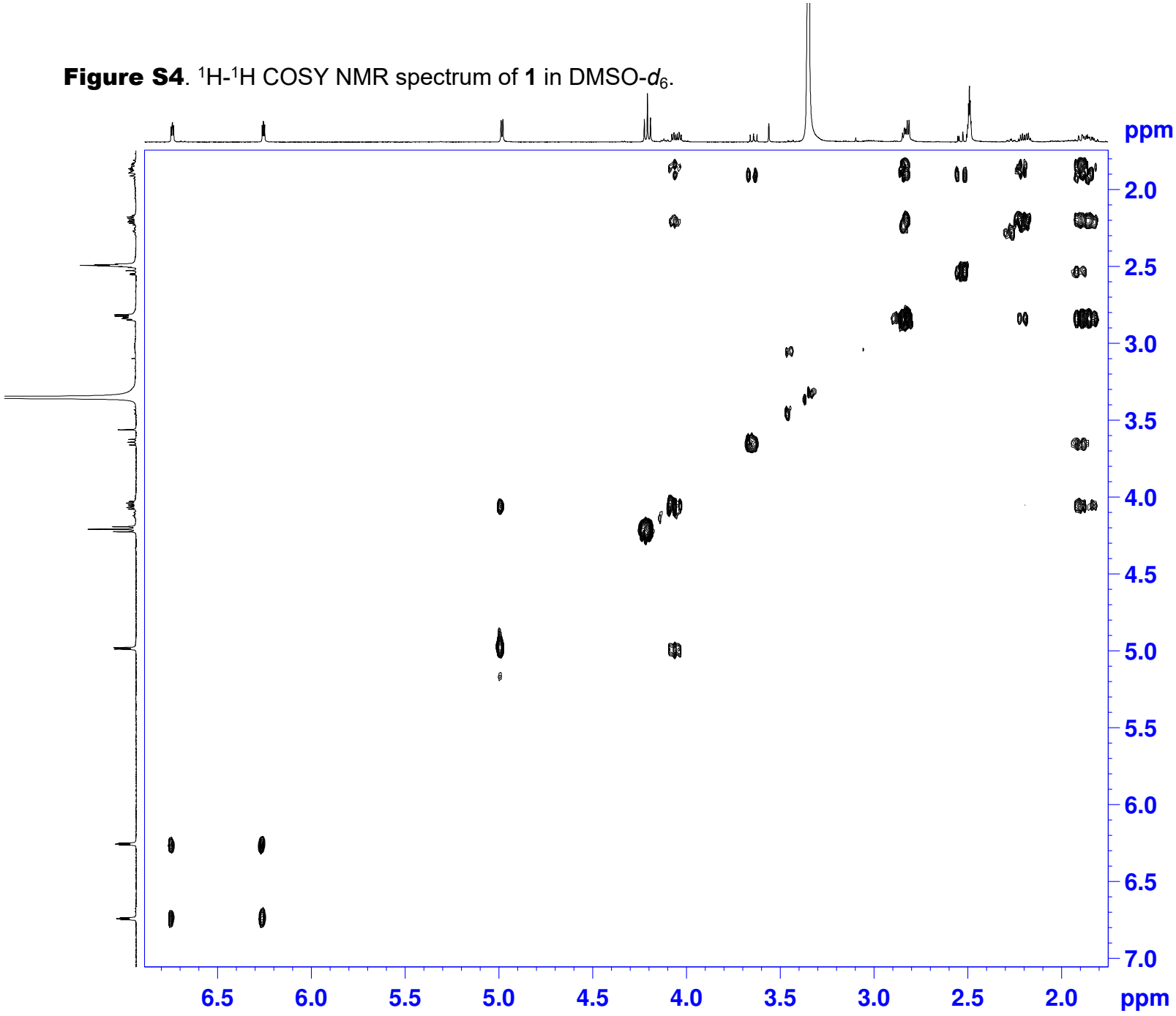
Figure S3. HSQC NMR spectrum of **1** in DMSO-d_6.



BRUKER

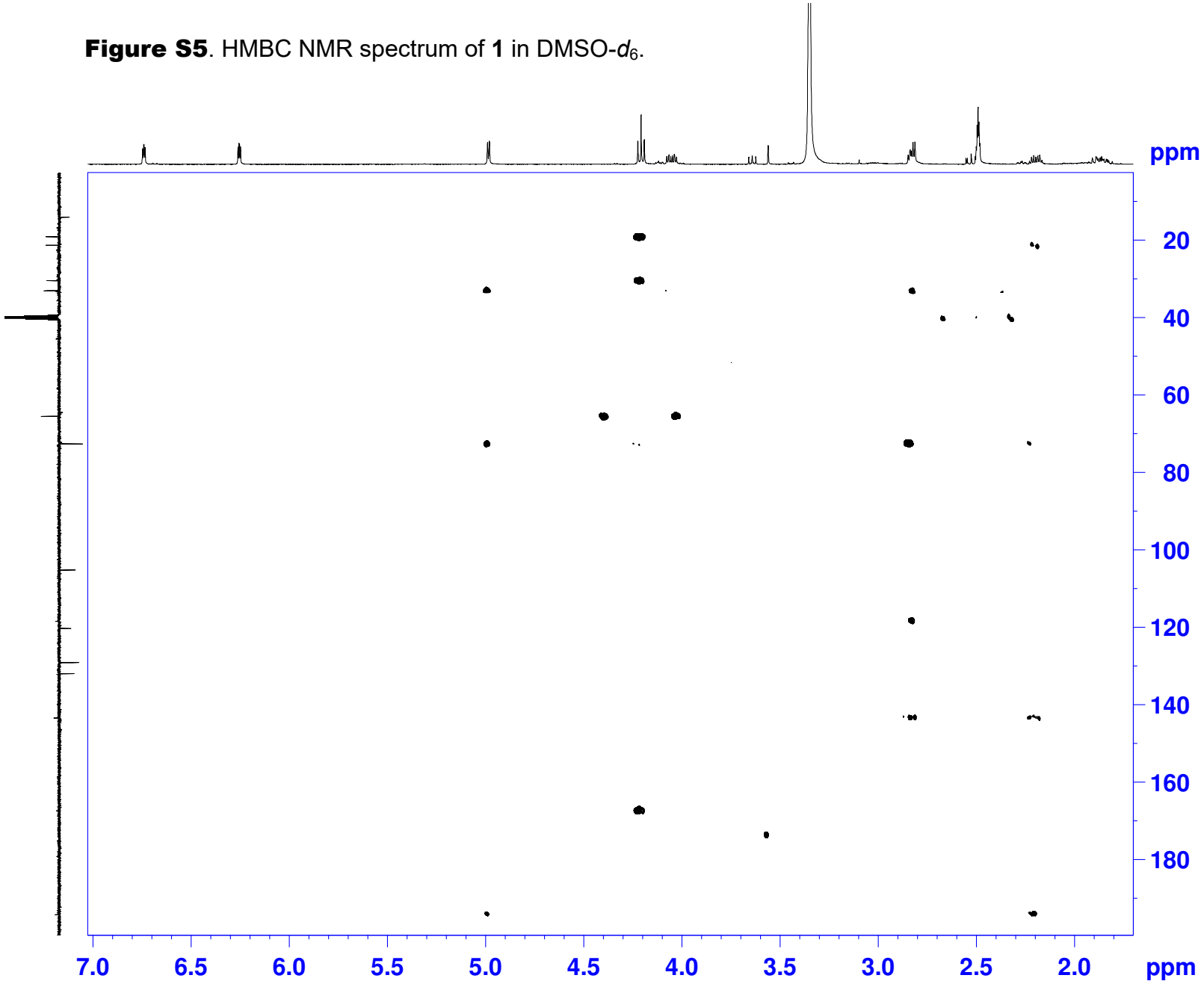
```
Current Data Parameters
NAME                  TW43-4-6
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_              20151107
Time                    2.55
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG         hsqcedetgp
TD                      1024
SOLVENT                 DMSO
NS                         8
DS                        16
SWH                4000.000 Hz
FIDRES             3.906250 Hz
AQ                 0.1280000 sec
RG                       203
DW                   125.000 usec
DE                     6.50 usec
TE                    294.6 K
CNST2             145.0000000
D0                 0.00000300 sec
D1                 1.50000000 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
D21                0.00345000 sec
IN0                0.00003105 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                       1H
P1                      13.09 usec
P2                      26.18 usec
P28                      1.00 usec
PL1                     -1.00 dB
PL1W              12.14314651 W
SFO1              400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2                 garp
NUC2                      13C
P3                      12.37 usec
P4                      24.74 usec
PCPD2                   75.00 usec
PL2                      1.00 dB
PL12                    16.65 dB
PL2W              28.13319778 W
PL12W              0.76598305 W
SFO2              100.6208180 MHz

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

F1 - Acquisition parameters
TD                         256
SFO1                100.6208 MHz
FIDRES             62.888012 Hz
SW                   160.000 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                        1024
SF                400.1300000 MHz
WDW                      QSINE
SSB                          2
LB             0 Hz
GB             0
PC                       1.40

F1 - Processing parameters
SI                        1024
MC2            echo-antiecho
SF                100.6127690 MHz
WDW                      QSINE
SSB                          2
LB             0 Hz
GB             0
```

Figure S4. ^{1}H-^{1}H COSY NMR spectrum of **1** in DMSO-d_6.




```
Current Data Parameters
NAME                  TW43-4-6
EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_              20151107
Time                    3.52
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG         cosygpmfqf
TD                      2048
SOLVENT                 DMSO
NS                         6
DS                         8
SWH                4000.000 Hz
FIDRES             1.953125 Hz
AQ                 0.2560000 sec
RG                       203
DW                   125.000 usec
DE                     6.50 usec
TE                    294.0 K
D0                 0.00000300 sec
D1                 1.93569195 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00024990 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      13.09 usec
PL1                     -1.00 dB
PL1W              12.14314651 W
SFO1              400.1320007 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]             SINE.100
GPNAM[2]             SINE.100
GPNAM[3]             SINE.100
GPZ1                    16.00 %
GPZ2                    12.00 %
GPZ3                    40.00 %
P16                   1000.00 usec

F1 - Acquisition parameters
TD                         128
SFO1                   400.132 MHz
FIDRES              31.260313 Hz
SW                     10.000 ppm
FnMODE                      QF

F2 - Processing parameters
SI                        1024
SF                400.1299958 MHz
WDW                       SINE
SSB          0
LB           0 Hz
GB           0
PC                        1.40

F1 - Processing parameters
SI                        1024
MC2                         QF
SF                400.1299958 MHz
WDW                       SINE
SSB          0
LB           0 Hz
GB           0
```

Figure S5. HMBC NMR spectrum of **1** in DMSO-d_6.




```
Current Data Parameters
NAME            TW43-4-6
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151107
Time                4.22
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG      hmbcgpndqf
TD                 4096
SOLVENT            DMSO
NS                   56
DS                   16
SWH           4000.000 Hz
FIDRES        0.976563 Hz
AQ            0.5120000 sec
RG                 203
DW              125.000 usec
DE                6.50 usec
TE               293.9 K
CNST13         8.0000000
D0            0.00000300 sec
D1            1.37220395 sec
D6            0.06250000 sec
D16           0.00020000 sec
IN0           0.00002485 sec

======== CHANNEL f1 ========
NUC1                1H
P1                13.09 usec
P2                26.18 usec
PL1               -1.00 dB
PL1W        12.14314651 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
NUC2               13C
P3                12.37 usec
PL2                1.00 dB
PL2W        28.13319778 W
SFO2        100.6228303 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]        SINE.100
GPNAM[2]        SINE.100
GPNAM[3]        SINE.100
GPZ1               50.00 %
GPZ2               30.00 %
GPZ3               40.10 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                  128
SFO1           100.6228 MHz
FIDRES       157.223175 Hz
SW             200.000 ppm
FnMODE              QF

F2 - Processing parameters
SI                 1024
SF          400.1299958 MHz
WDW                SINE
SSB       0
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2                 QF
SF          100.6127690 MHz
WDW                SINE
SSB       0
LB        0 Hz
GB        0
```