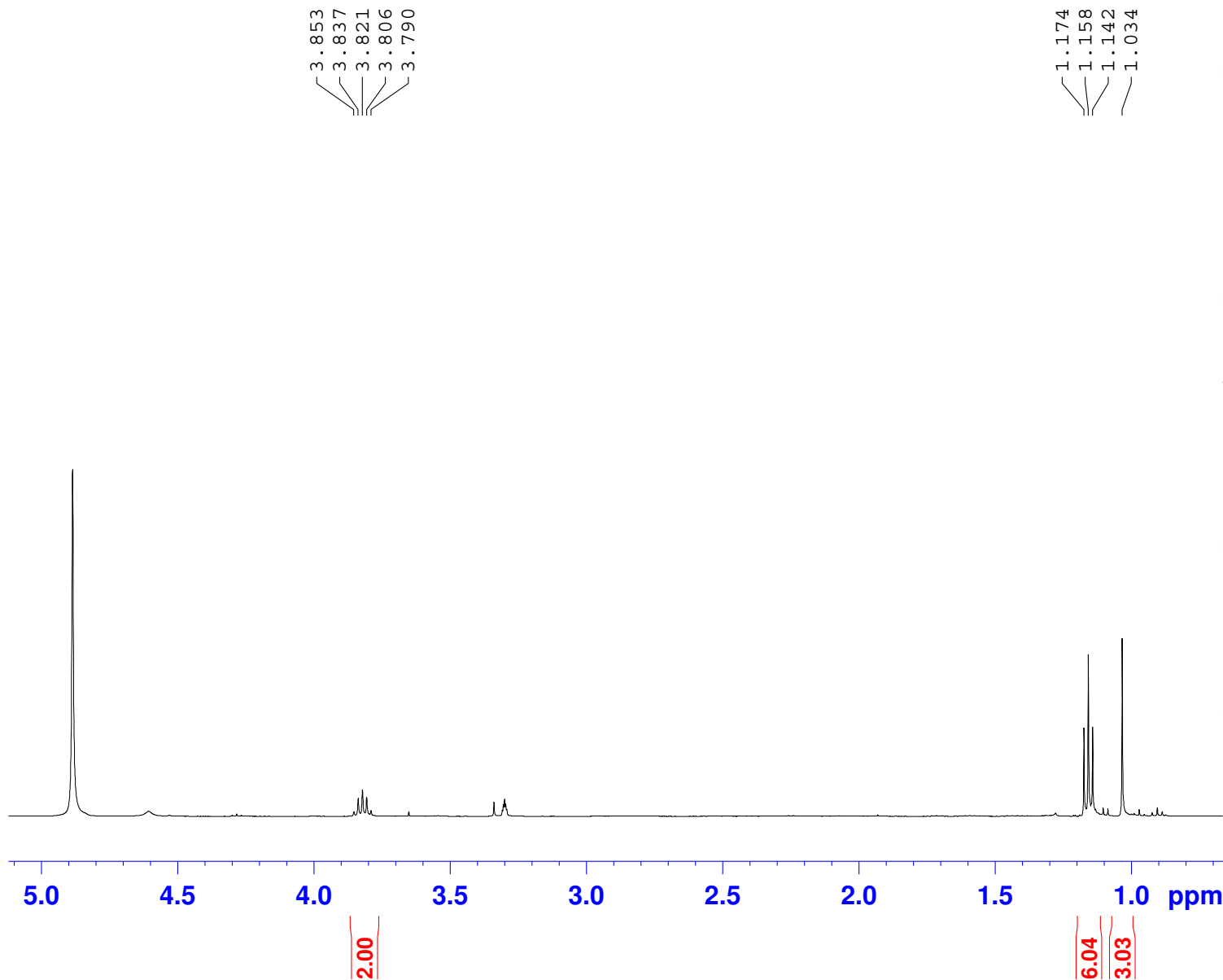
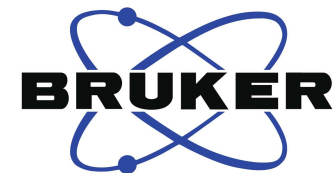


Figure S1. <sup>1</sup>H NMR spectrum of compound 1 in CD<sub>3</sub>OD



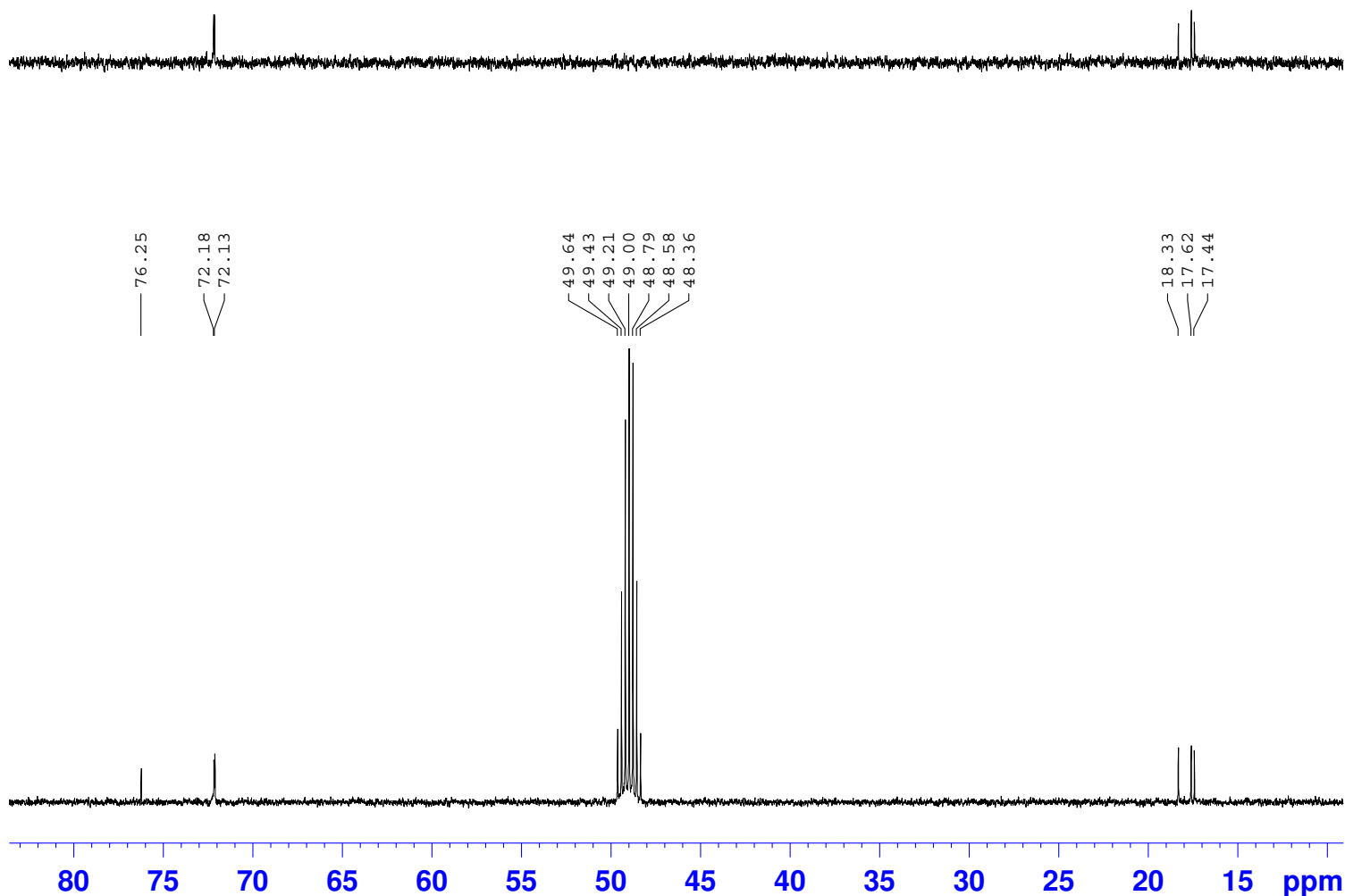
Current Data Parameters  
NAME 1K00610-20  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160607  
Time\_ 17.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT MeOD  
NS 64  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 203  
DW 60.800 usec  
DE 6.50 usec  
TE 295.7 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 400.1300070 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S2. <sup>13</sup>C NMR spectrum of compound 1 in CD<sub>3</sub>OD



Current Data Parameters

NAME 1K00610-20  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20160607  
 Time\_ 18.38  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT MeOD  
 NS 926  
 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 296.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====

NUC1 13C  
 P1 12.37 usec  
 PL1 1.00 dB  
 PL1W 28.13319778 W  
 SFO1 100.6228298 MHz

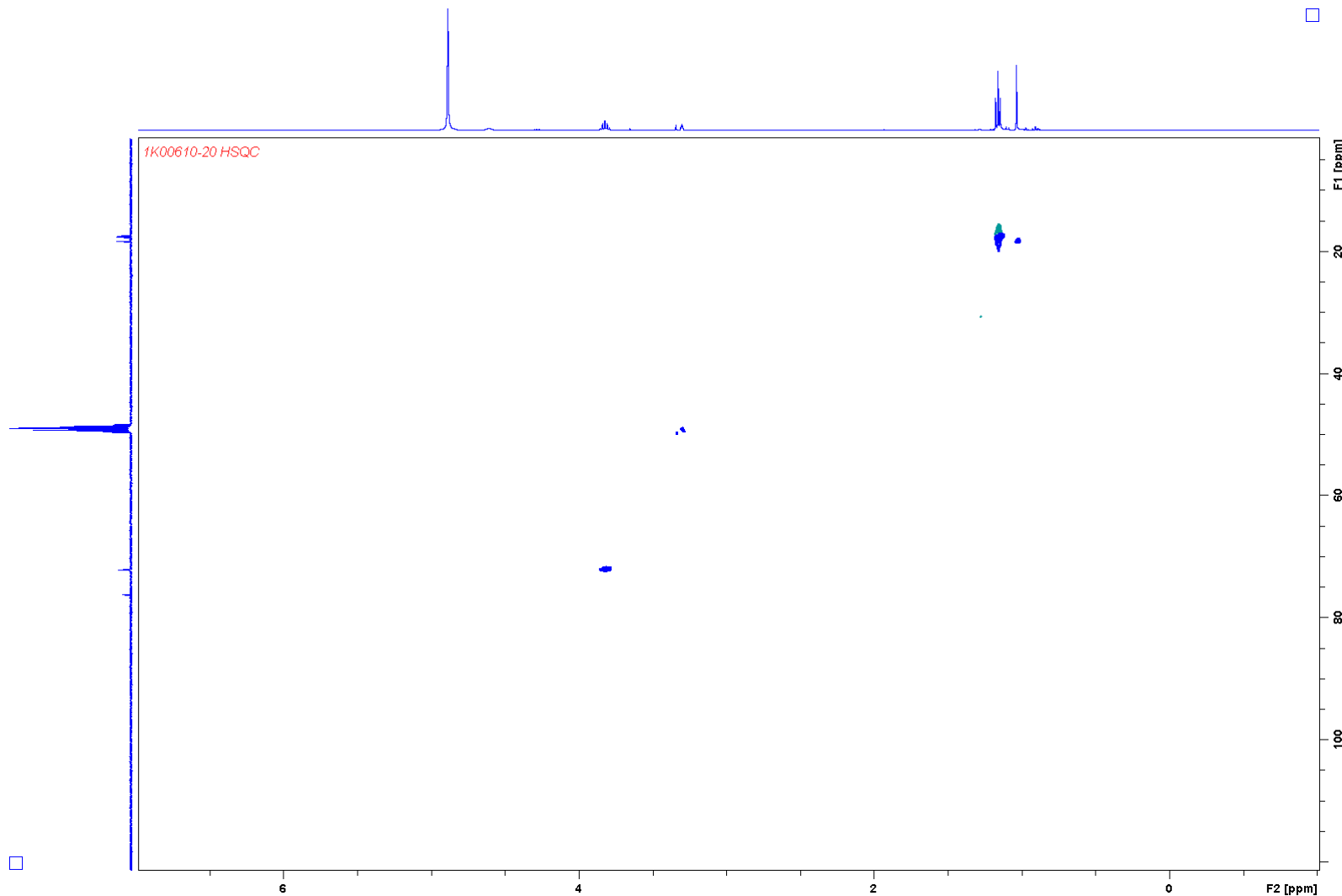
==== CHANNEL f2 =====

CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 14.72 dB  
 PL13 14.50 dB  
 PL2W 12.14314651 W  
 PL12W 0.32533529 W  
 PL13W 0.34224036 W  
 SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768  
 SF 100.6126271 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

Figure S3. HSQC spectrum of compound 1 in CD<sub>3</sub>OD



Current Data Parameters  
 NAME 1K00610-20  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160610  
 Time 19.33  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hsqcedetgp  
 TD 1024  
 SOLVENT MeOD  
 NS 8  
 DS 32  
 SWH 3201.024 Hz  
 FIDRES 3.126000 Hz  
 AQ 0.1599488 sec  
 RG 203  
 DW 156.200 usec  
 DE 6.50 usec  
 TE 295.6 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  
 INO 0.00004140 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 400.1312004 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 100.6188058 MHz

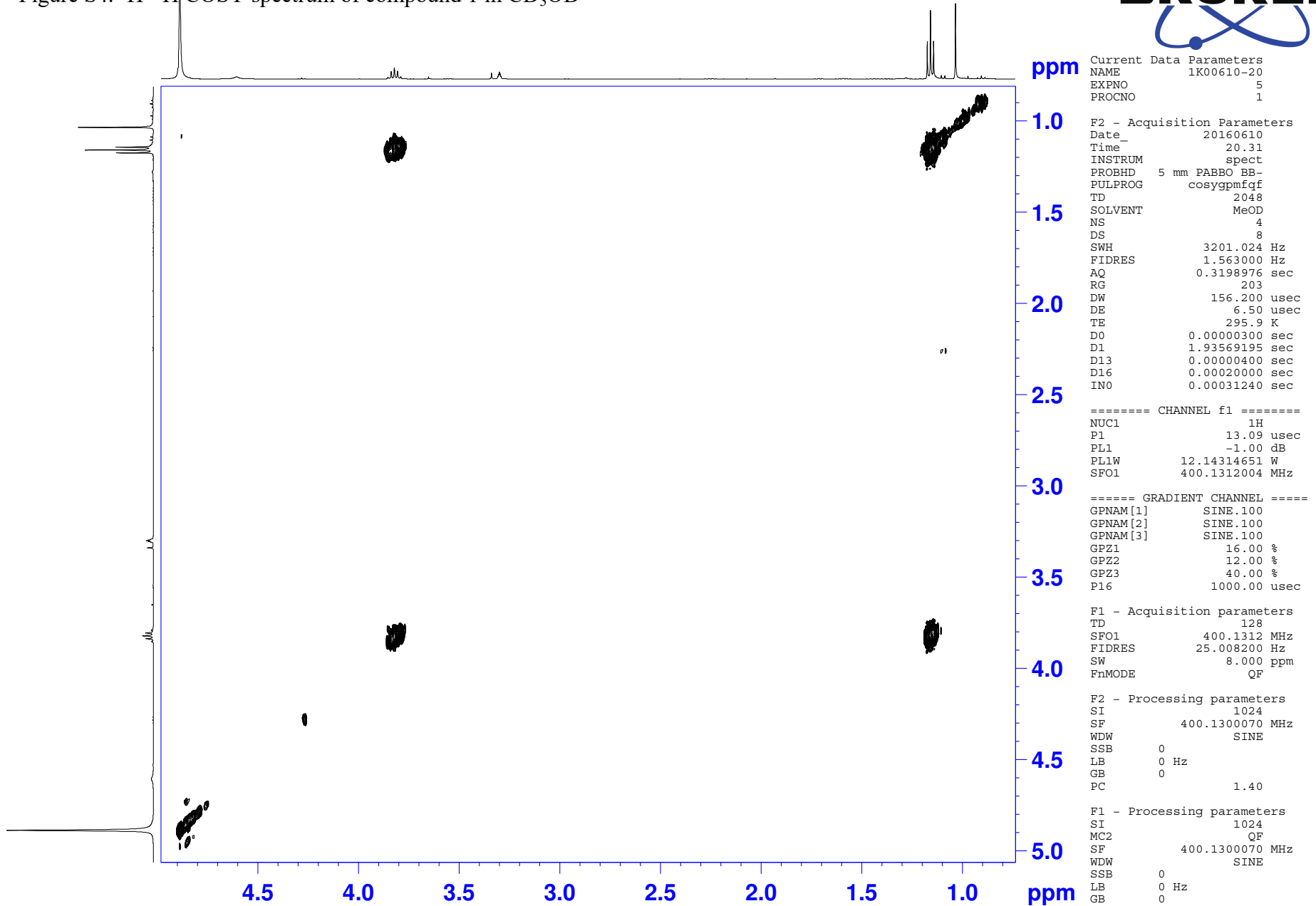
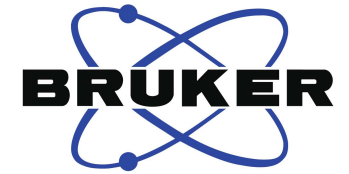
===== GRADIENT CHANNEL =====  
 GPNAM[1] SINE.100  
 GPNAM[2] SINE.100  
 GPZ1 80.00 %  
 GPZ2 20.10 %  
 P16 1000.00 usec

F1 - Acquisition parameters  
 TD 256  
 SFO1 100.6188 MHz  
 FIDRES 47.165066 Hz  
 SW 120.000 ppm  
 FhMODE Echo-Antiecho

F2 - Processing parameters  
 SI 1024  
 SF 400.1300070 MHz  
 WDW QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0  
 PC 1.40

F1 - Processing parameters  
 SI 1024  
 MC2 echo-antiecho  
 SF 100.6126271 MHz  
 WDW QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0

Figure S4.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 1 in  $\text{CD}_3\text{OD}$



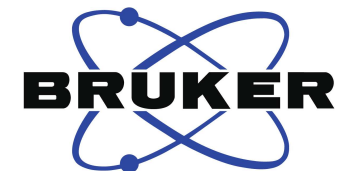
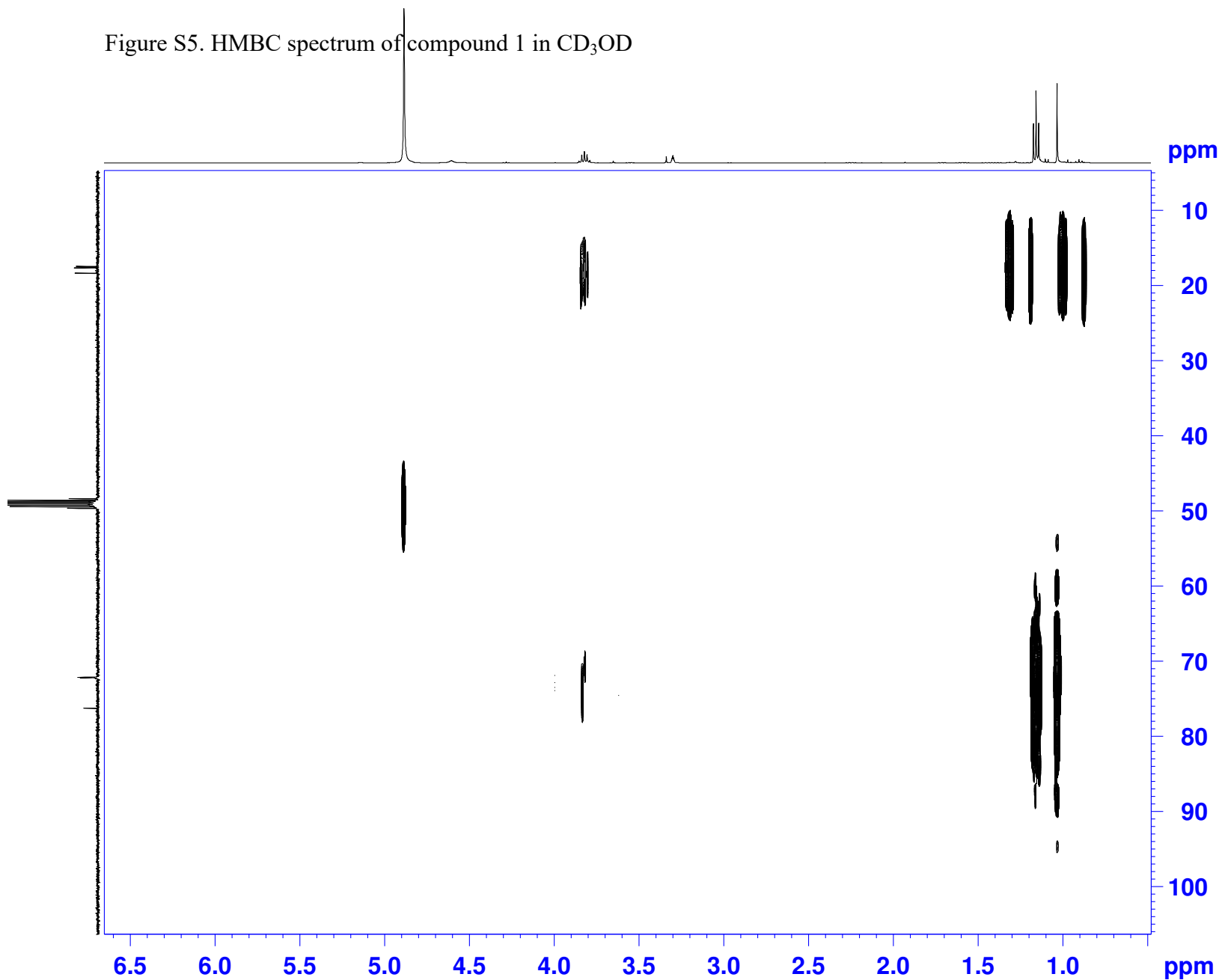


Figure S5. HMBC spectrum of compound 1 in CD<sub>3</sub>OD



Current Data Parameters  
NAME 1K00610-20  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160610  
Time 20.54  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hmbcgpndqf  
TD 4096  
SOLVENT MeOD  
NS 64  
DS 16  
SWH 3201.024 Hz  
FIDRES 0.781500 Hz  
AQ 0.6397952 sec  
RG 203  
DW 156.200 usec  
DE 6.50 usec  
TE 295.7 K  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.37220395 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00004140 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 13.09 usec  
P2 26.18 usec  
PL1 -1.00 dB  
PL1W 12.14314651 W  
SFO1 400.1312004 MHz

==== CHANNEL f2 =====  
NUC2 13C  
P3 12.37 usec  
PL2 1.00 dB  
PL2W 28.13319778 W  
SFO2 100.6188058 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 11  
SFO1 100.6188 MHz  
FIDRES 1097.659668 Hz  
SW 120.000 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 400.1300070 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 100.6126271 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

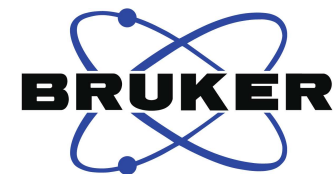
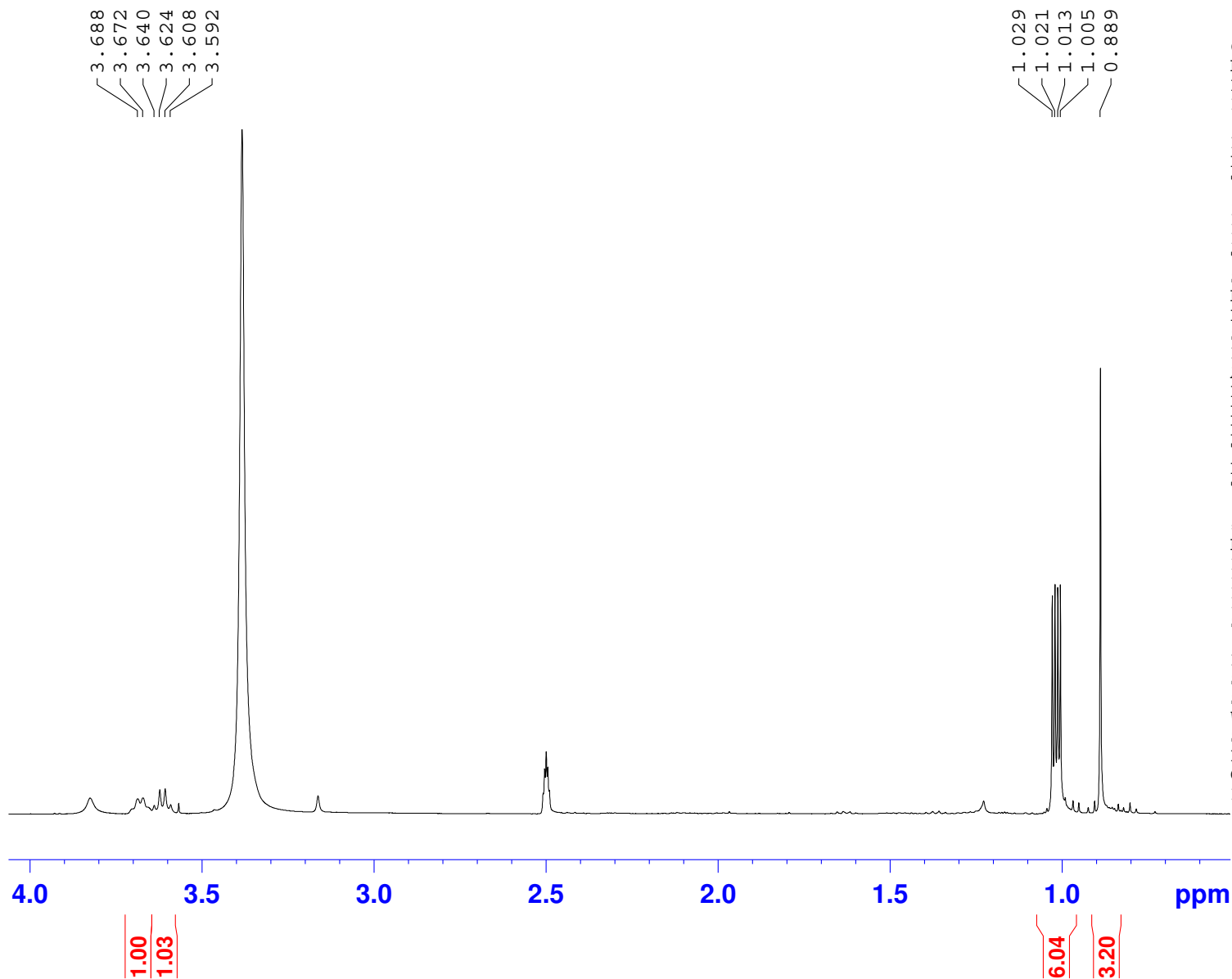


Figure S6. <sup>1</sup>H NMR spectrum of compound 1 in DMSO-d<sub>6</sub>



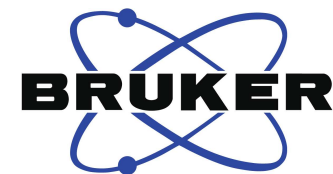
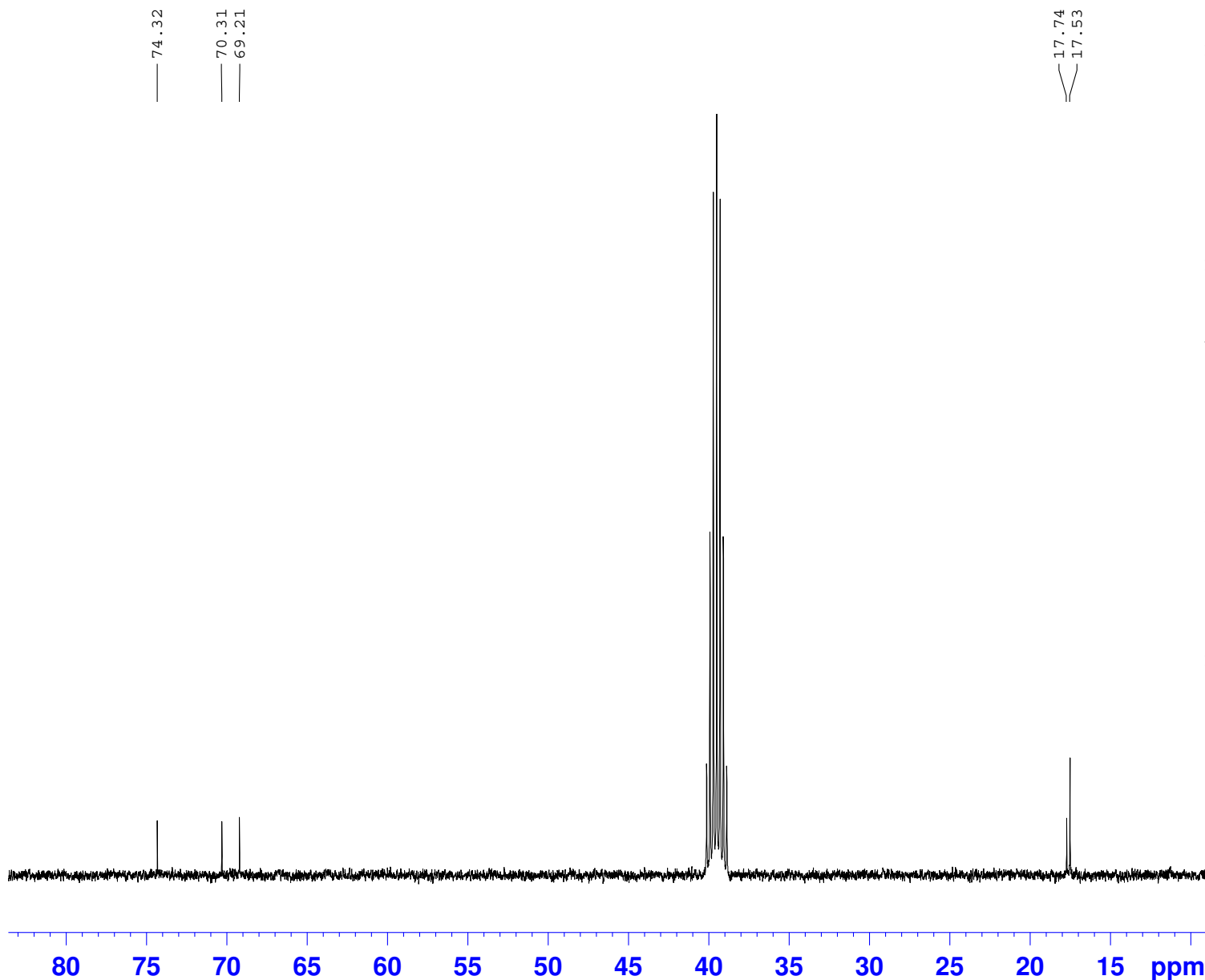
Current Data Parameters  
NAME 1K00610-20 DMSO  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160815  
Time\_ 18.10  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 128  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 203  
DW 60.800 usec  
DE 6.50 usec  
TE 295.8 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 400.1299972 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S7.  $^{13}\text{C}$  NMR spectrum of compound 1 in  $\text{DMSO-}d_6$



Current Data Parameters  
 NAME 1K00610-20 DMSO  
 EXPNO 2  
 PROCNO 1

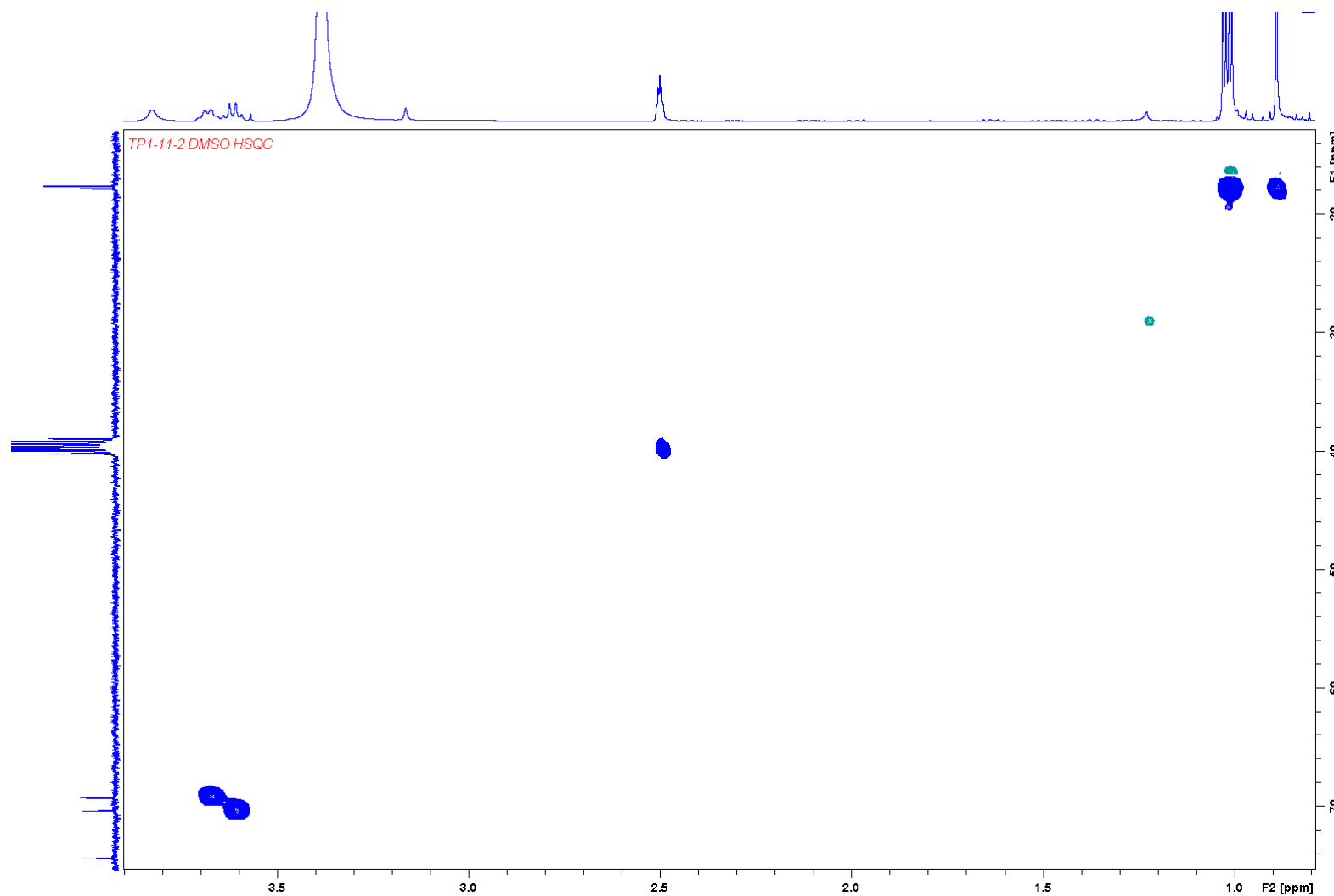
F2 - Acquisition Parameters  
 Date\_ 20160815  
 Time 19.20  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1360  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 203  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 12.37 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  
 PL13 14.50 dB  
 PL2W 12.14314651 W  
 PL12W 0.32533529 W  
 PL13W 0.34224036 W  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6128104 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

Figure S8. HSQC spectrum of compound 1 in DMSO- $d_6$



```

Current Data Parameters
NAME      1K00610-20 DMSO
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20160815
Time      19.30
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   hsqcedetgp
TD         1024
SOLVENT   DMSO
NS         16
DS         32
SWH        4401.409 Hz
FIDRES     4.298251 Hz
AQ         0.1163264 sec
RG         203
DW         113.600 usec
DE         6.50 usec
TE         296.2 K
CNST2     145.000000
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        0.00004140 sec
ZGPTNS

===== 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       400.1318006 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       100.6188058 MHz

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

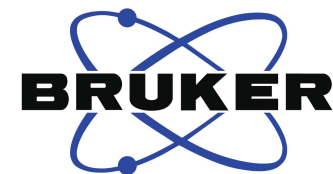
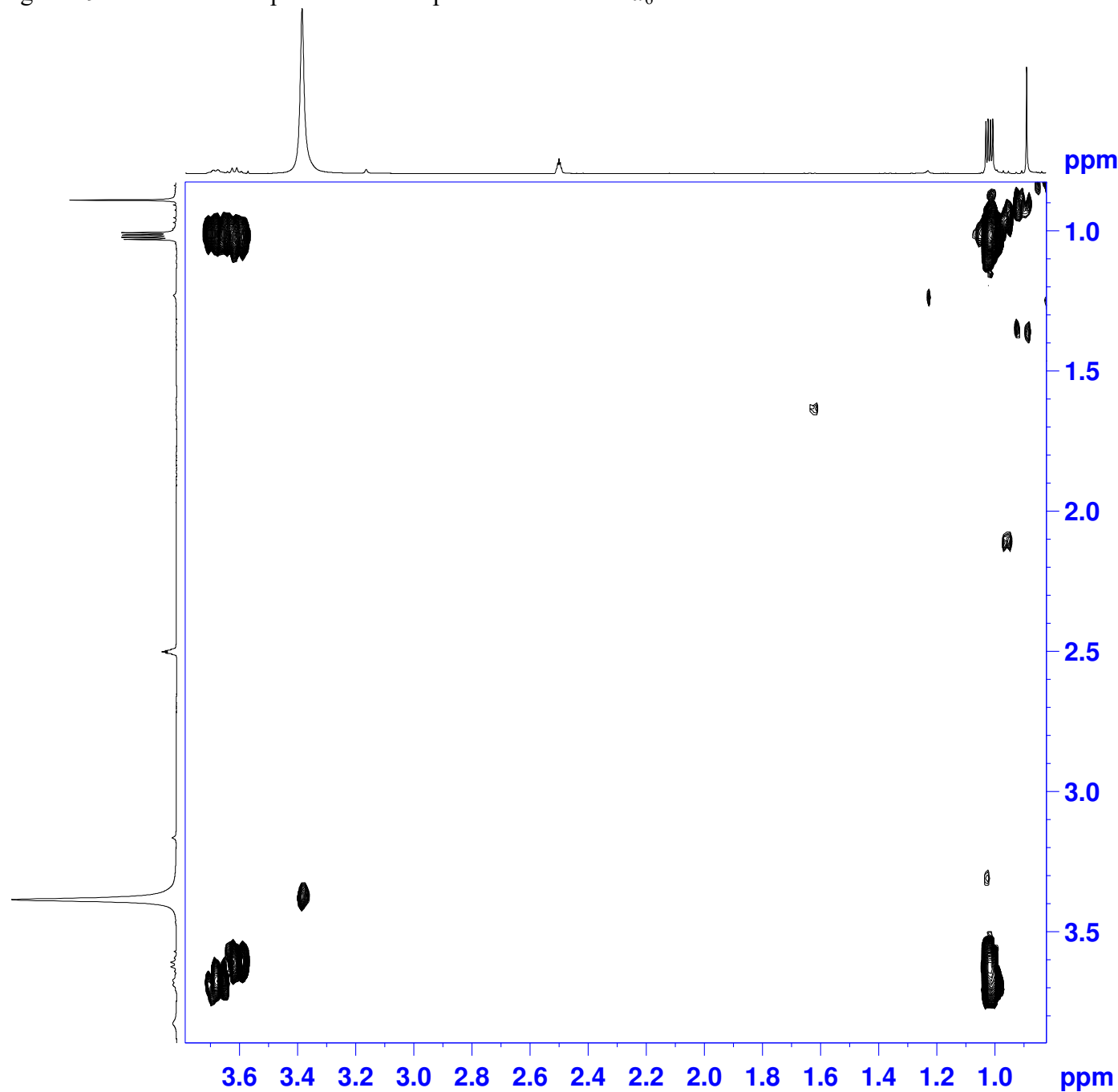
F1 - Acquisition parameters
TD         112
SFO1       100.6188 MHz
FIDRES     107.805862 Hz
SW         120.000 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI         1024
SF         400.1299972 MHz
WDW        QSINE
SSB        2
LB         0 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        echo-antiecho
SF         100.6128104 MHz
WDW        QSINE
SSB        2
LB         0 Hz
GB         0
    
```



Figure S9.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1** in  $\text{DMSO-}d_6$



```

Current Data Parameters
NAME      1K00610-20 DMSO
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20160815
Time      20.19
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   cosygpmfzf
TD        2048
SOLVENT   DMSO
NS        4
DS        8
SWH       4401.409 Hz
FIDRES    2.149125 Hz
AQ        0.2326528 sec
RG        203
DW        113.600 usec
DE        6.50 usec
TE        295.8 K
D0        0.00000300 sec
D1        1.93569195 sec
D13       0.00000400 sec
D16       0.00020000 sec
IN0       0.00022720 sec

===== CHANNEL f1 =====
NUC1      1H
P1        13.09 usec
PL1       -1.00 dB
PL1W      12.14314651 W
SFO1      400.1318006 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      400.1318 MHz
FIDRES    34.386326 Hz
SW        11.000 ppm
FnMODE    QF

F2 - Processing parameters
SI        1024
SF        400.1299972 MHz
WDW       SINE
SSB       0
LB        0 Hz
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
MC2       QF
SF        400.1299972 MHz
WDW       SINE
SSB       0
LB        0 Hz
GB        0
    
```

Figure S10. HMBC spectrum of compound 1 in DMSO-*d*<sub>6</sub>



Current Data Parameters  
 NAME 1K00610-20 DMSO  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160815  
 Time 22.29  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG hmbcgpndqf  
 TD 4096  
 SOLVENT DMSO  
 NS 128  
 DS 16  
 SWH 4401.409 Hz  
 FIDRES 1.074563 Hz  
 AQ 0.4653056 sec  
 RG 203  
 DW 113.600 usec  
 DE 6.50 usec  
 TE 295.5 K  
 CNST13 8.0000000  
 D0 0.00000300 sec  
 D1 1.37220395 sec  
 D6 0.06250000 sec  
 D16 0.00020000 sec  
 IN0 0.00004140 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.09 usec  
 P2 26.18 usec  
 PL1 -1.00 dB  
 PL1W 12.14314651 W  
 SFO1 400.1318006 MHz

==== CHANNEL f2 =====  
 NUC2 13C  
 P3 12.37 usec  
 PL2 1.00 dB  
 PL2W 28.13319778 W  
 SFO2 100.6188058 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 100.6188 MHz  
 FIDRES 94.330132 Hz  
 SW 120.000 ppm  
 FhMODE QF

F2 - Processing parameters  
 SI 1024  
 SF 400.1299972 MHz  
 WDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.40

F1 - Processing parameters  
 SI 1024  
 MC2 QF  
 SF 100.6128104 MHz  
 WDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0

