

Degradation characteristics of a novel PAF receptor antagonist

SY0916 in aqueous solution

Supplementary data

Fig. A The MS³ spectra of D2

Fig.A.1 MS³ spectrum of m/z 193 ion from m/z 211 of D2

Fig.A.2 MS³ spectrum of m/z 165 ion from m/z 211 of D2

Fig.A.3 MS³ spectrum of m/z 137 ion from m/z 211 of D2

Fig. B The NMR spectra of D1

Fig.B.1 ¹H spectrum of synthesized D1

Fig.B.2 ¹³C spectrum of synthesized D1

Fig.B.3 HSQC spectrum of synthesized D1

Fig.B.4 partial-enlarged HSQC spectrum of synthesized D1

Fig.B.5 HMBC spectrum of synthesized D1

Fig.B.6 partial-enlarged HMBC spectrum of synthesized D1

Fig. C The NMR spectra of D2

Fig.C.1 ¹H spectrum of D2 by LC-SPE-NMR

Fig.C.2 ¹³C spectrum of D2 by LC-SPE-NMR

Fig.C.3 HSQC spectrum of D2 by LC-SPE-NMR

Fig.C.4 partial-enlarged HSQC spectrum of D2 by LC-SPE-NMR

Fig.C.5 HMBC spectrum of D2 by LC-SPE-NMR

Fig.C.6 partial-enlarged HMBC spectrum of D2 by LC-SPE-NMR

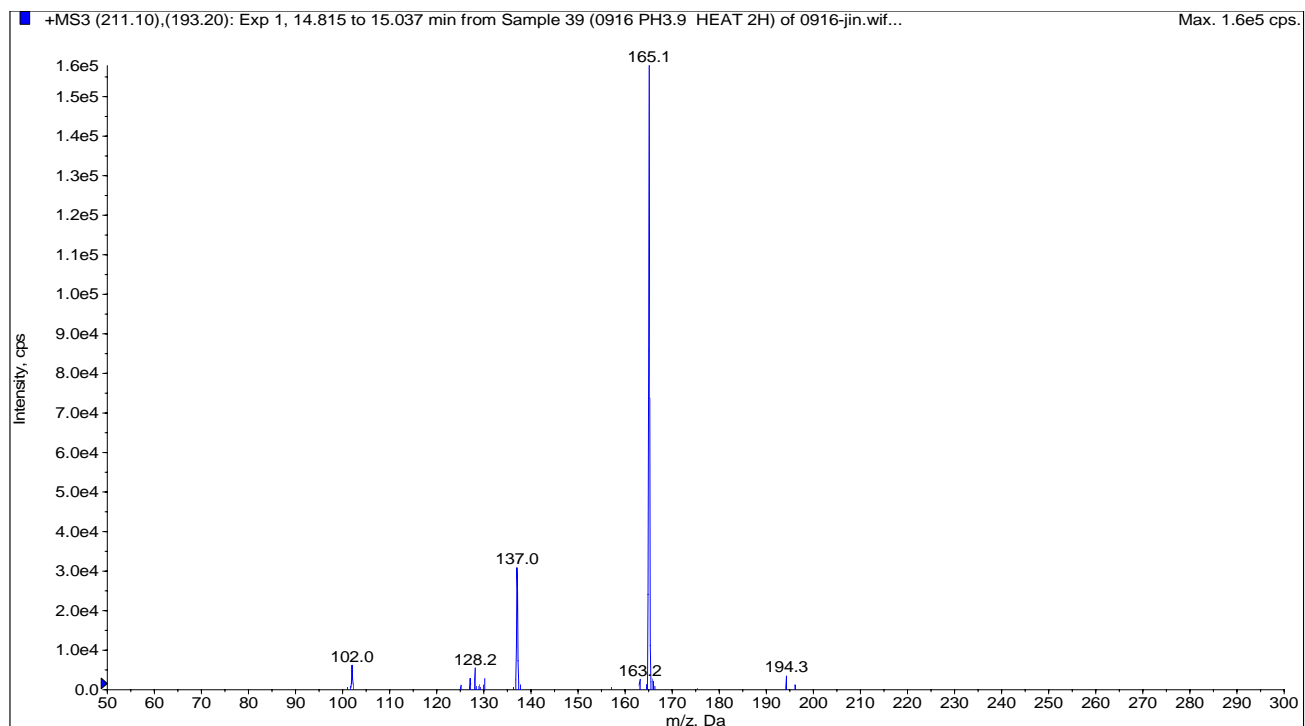


Fig.A.1 MS³ spectrum of m/z 193 ion from m/z 211 of D2

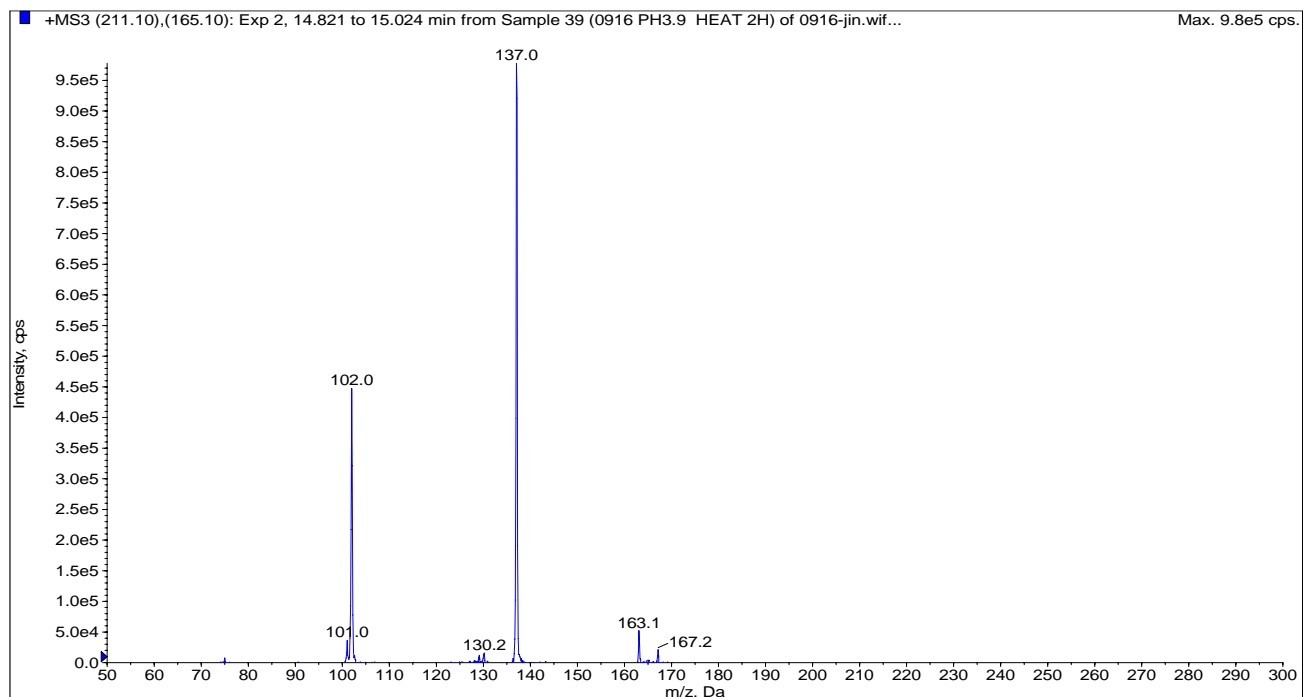


Fig.A.2 MS³ spectrum of m/z 165 ion from m/z 211 of D2

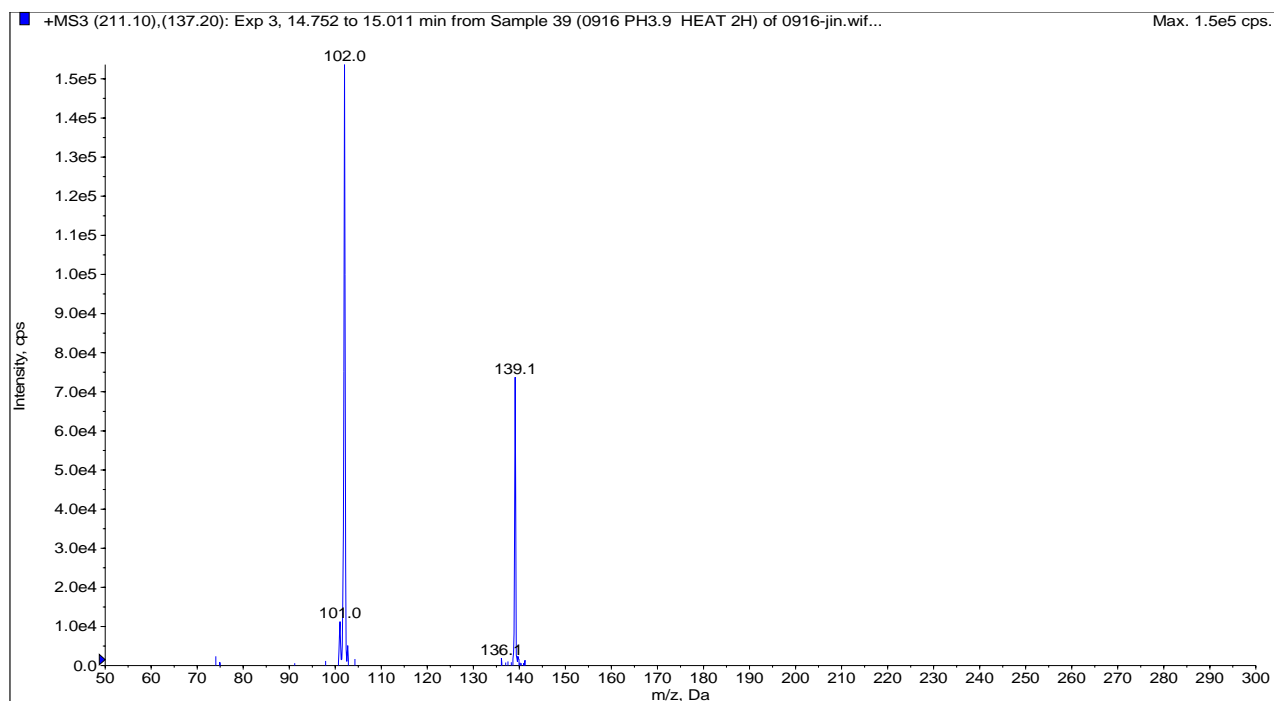


Fig.A.3 MS³ spectrum of m/z 137 ion from m/z 211 of D2

Bruker AVIII HD 600 20171102
PROTON CD3OD D:\ DATA2017 24



Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
TD 65536
SOLVENT CD3OD
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 12.7
DW 41.600 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.2537068 MHz
NUC1 1H
P1 11.50 usec
PLW1 12.93200016 W

F2 - Processing parameters
SI 65536
SF 600.2500172 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

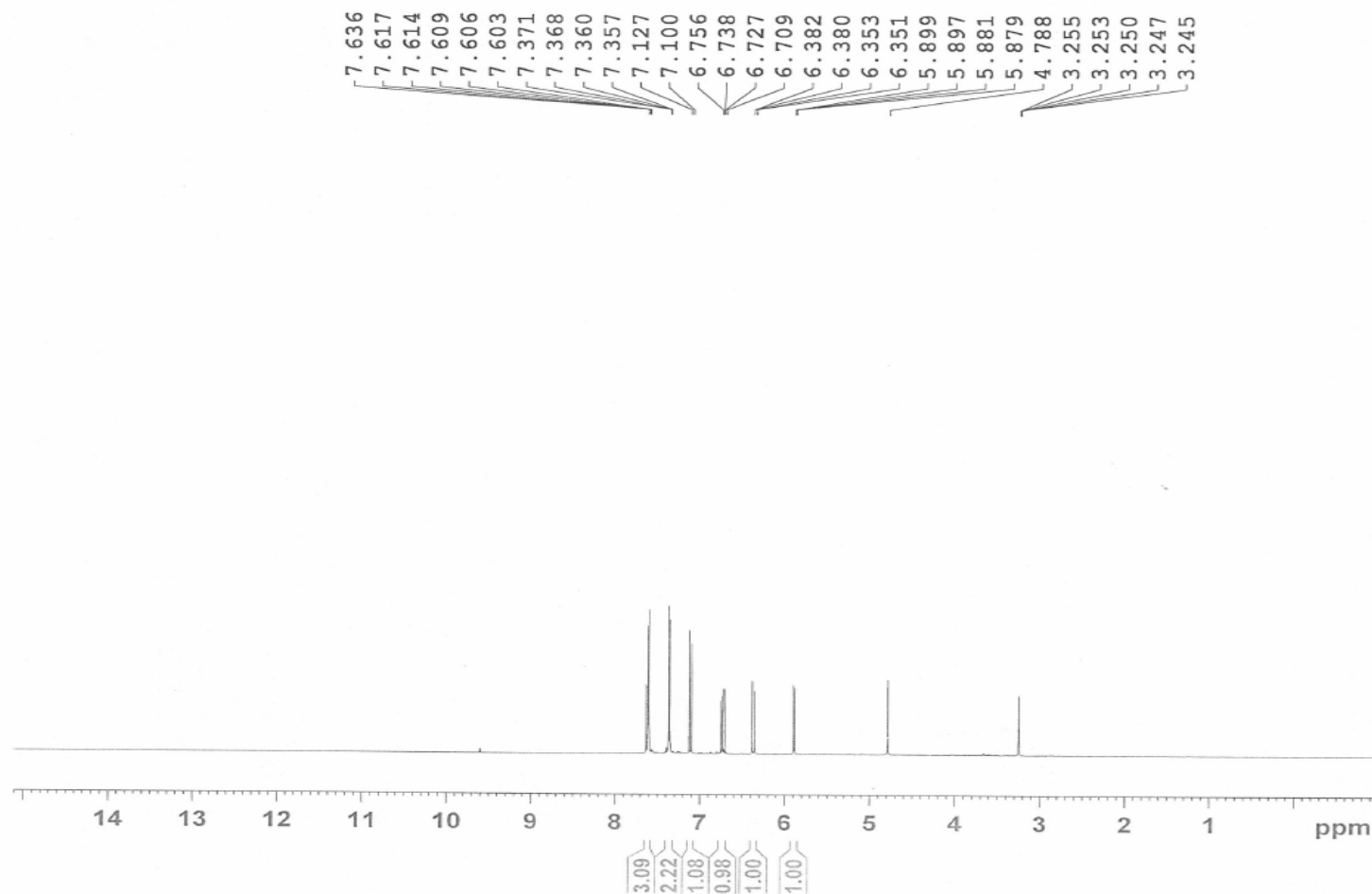
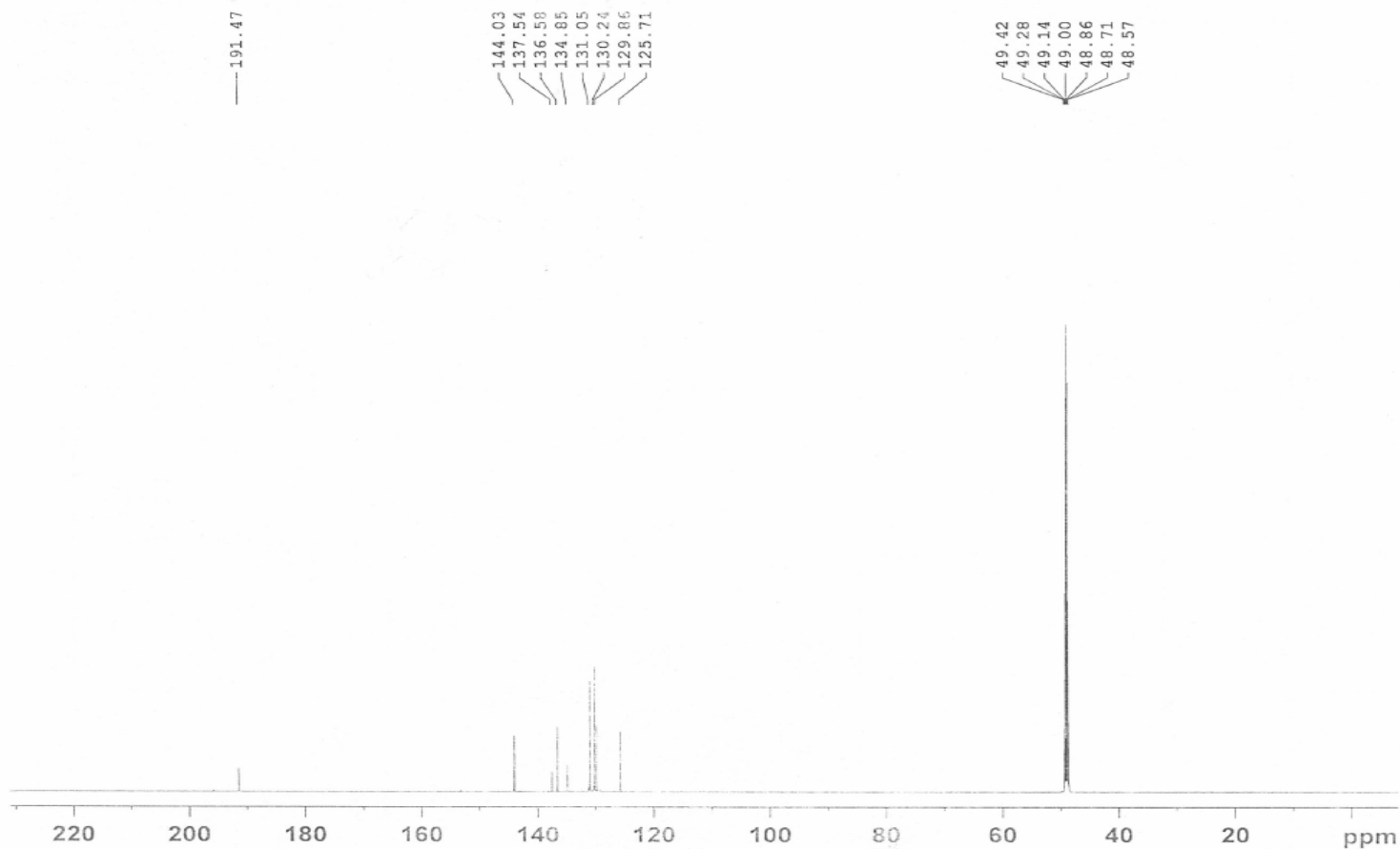


Fig.B.1 ^1H spectrum of synthesized D1



Bruker AVIII HD 600 20171102
C13 CD3OD D:\\ DATA2017 24



Current Data Parameters
NAME 20171102 M192
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171106
Time 10.24
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 65536
SOLVENT CD3OD
NS 400
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 31.37 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 50

===== CHANNEL f1 =====
SFO1 150.9495843 MHz
NUC1 13C
P1 12.54 usec
PLW1 19.39800072 W

===== CHANNEL f2 =====
SFO2 600.2524010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 12.93200016 W
PLW12 0.34902999 W
PLW13 0.17556000 W

F2 - Processing parameters
SI 32768
SF 150.9327649 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

Fig.B.2 ^{13}C spectrum of synthesized D1

Bruker AVIII HD 600 20171102
 {HSQC (phase sensitive)} CD3OD D:\ DATA2017 24

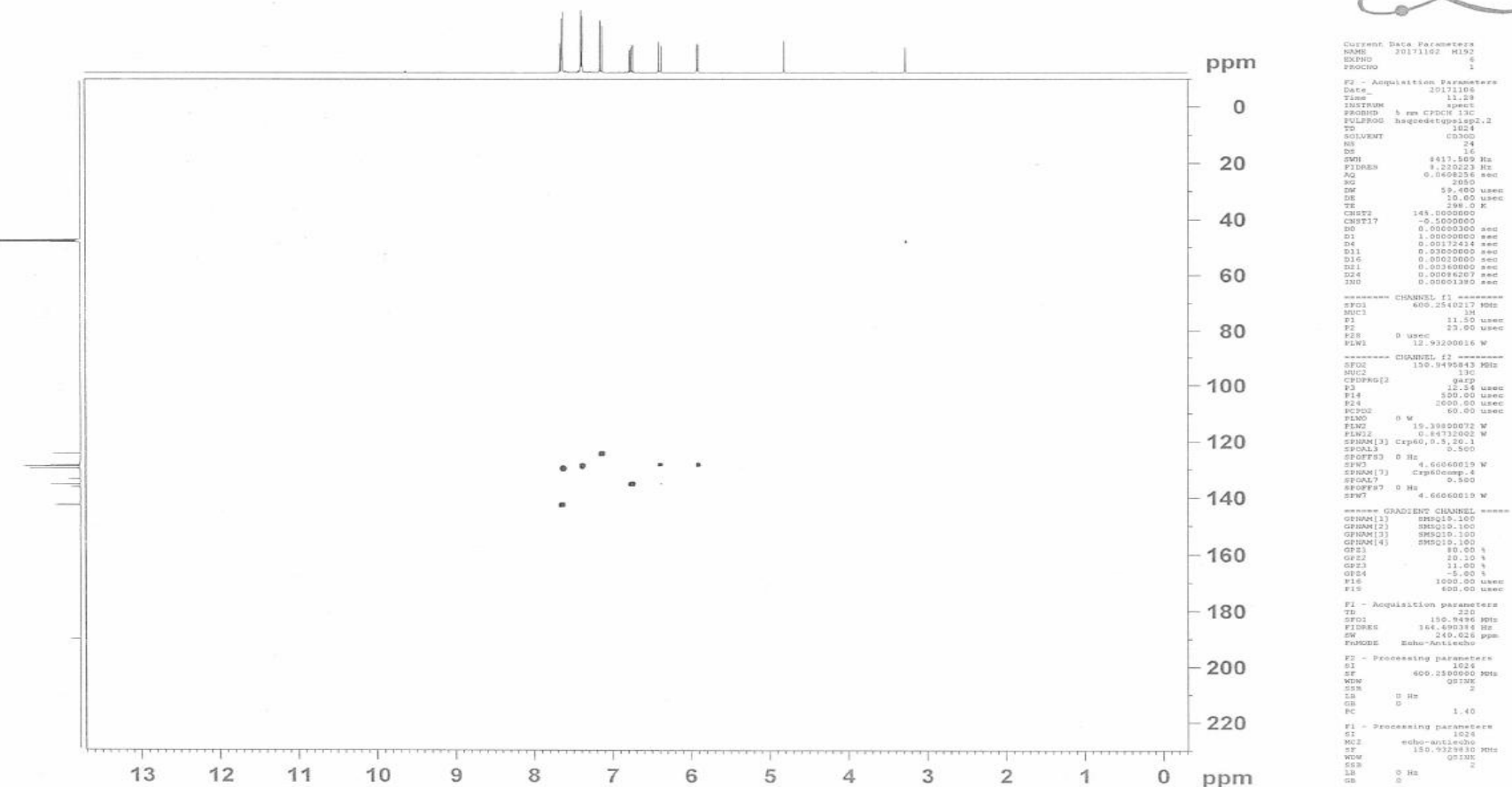


Fig.B.3 HSQC spectrum of synthesized D1

Bruker AVIII HD 600 20171102
 {HSQC_(phase sensitive)} CD3OD D:\ DATA2017 24

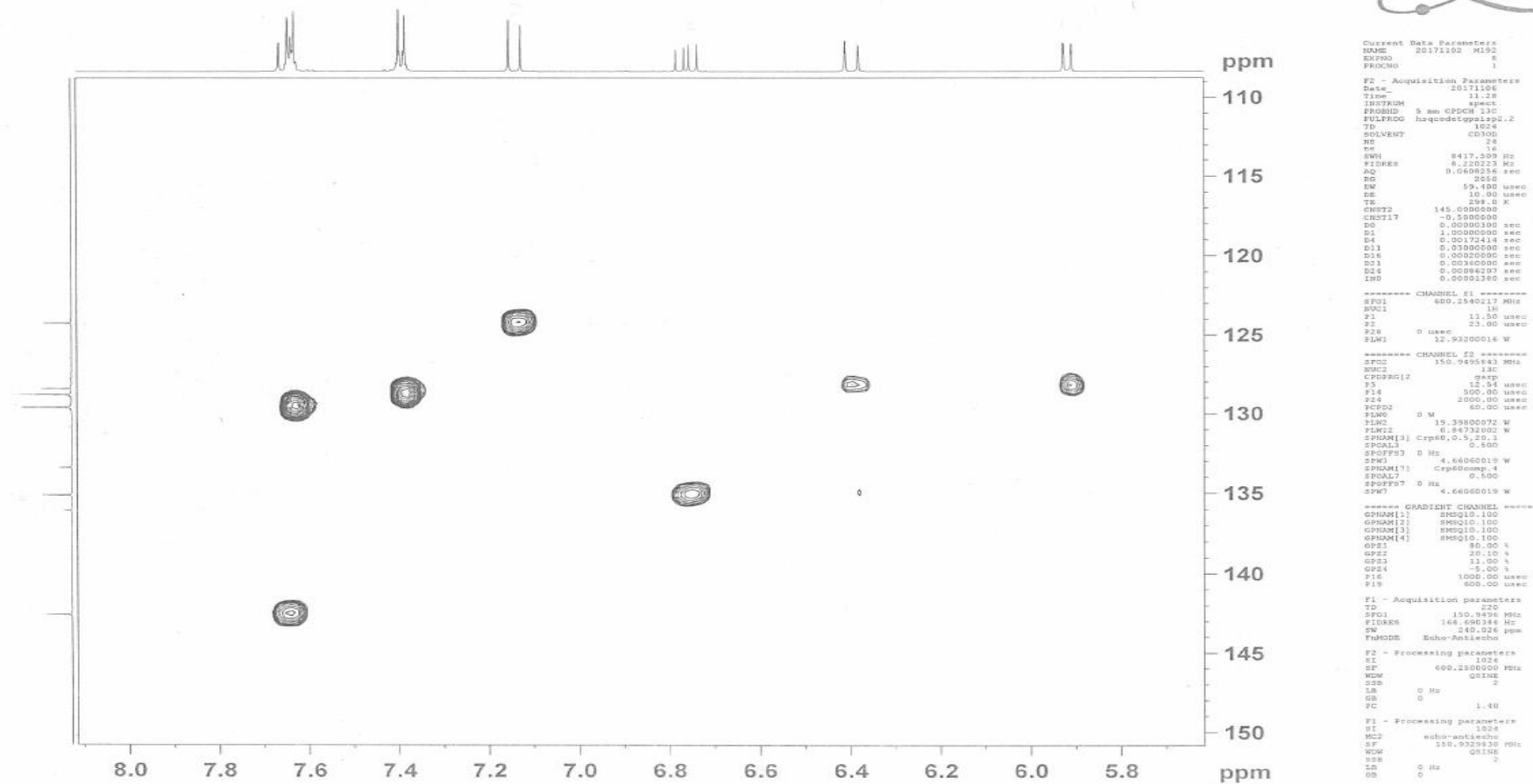


Fig.B.4 partial-enlarged HSQC spectrum of synthesized D1

Bruker AVIII HD 600 20171102
HMBC CD3OD D:\ DATA2017 24

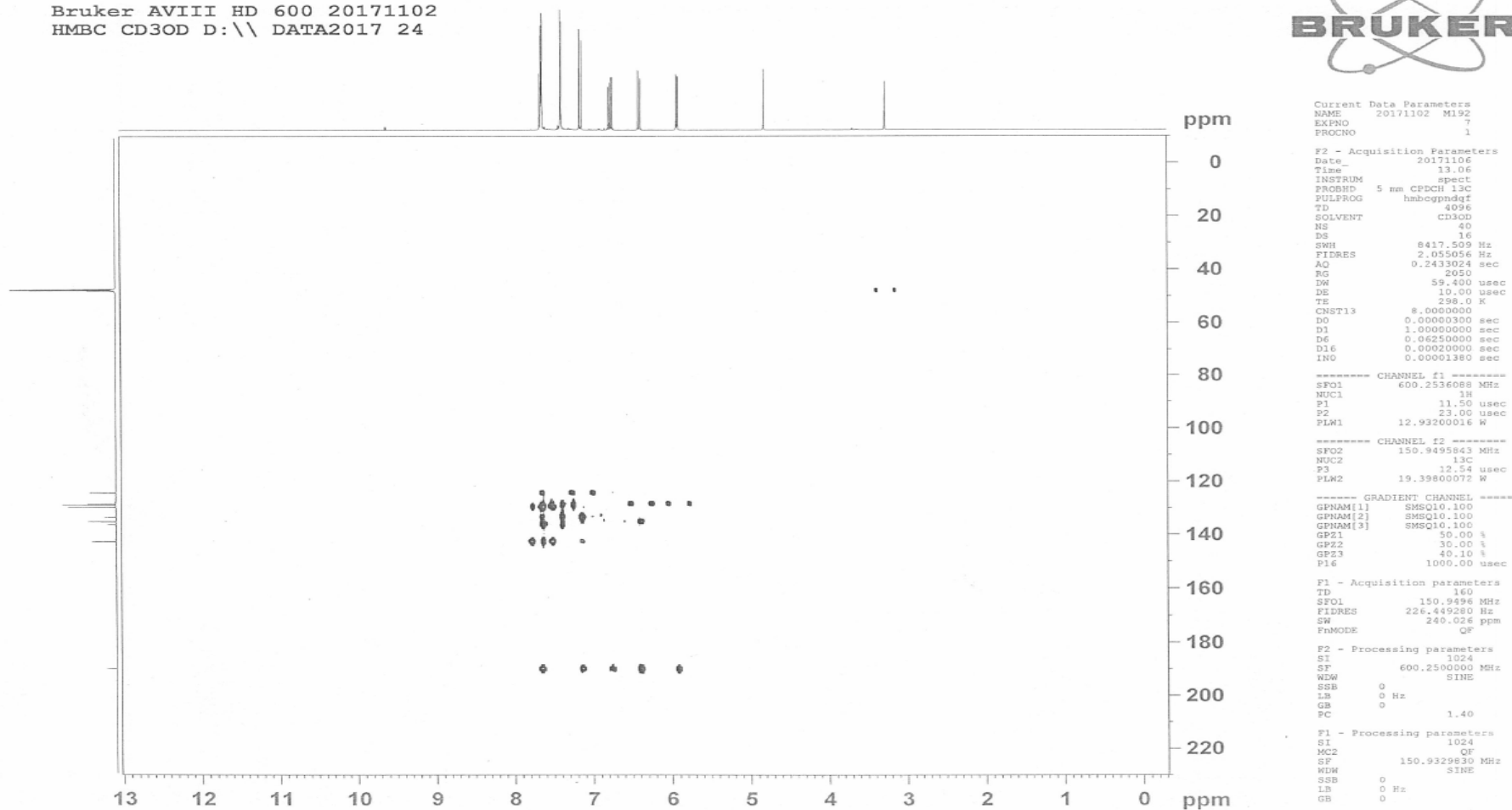


Fig.B.5 HMBC spectrum of synthesized D1

Bruker AVIII HD 600 20171102
HMBC CD3OD D:\DATA2017 24

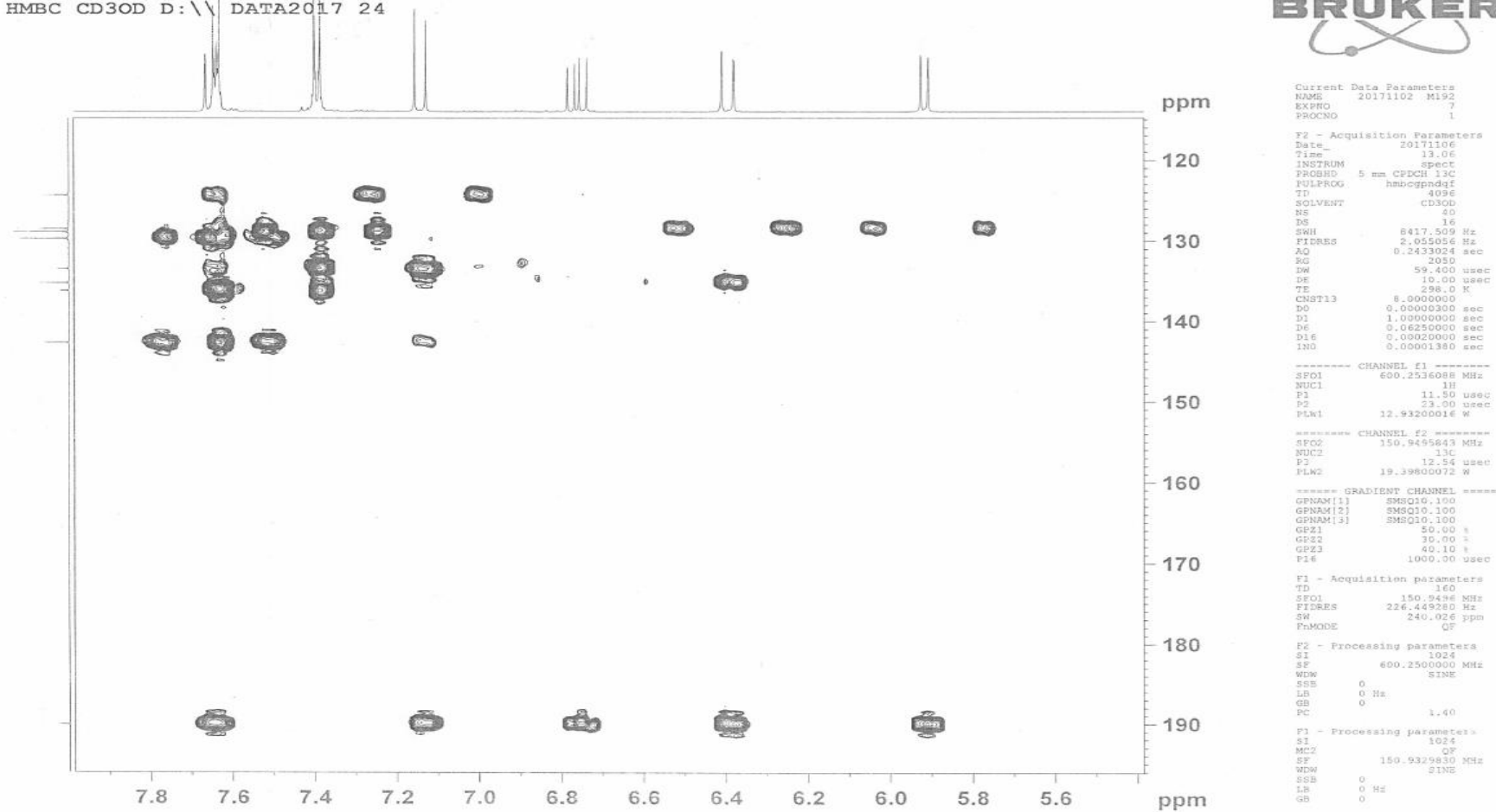


Fig.B.6 partial-enlarged HMBC spectrum of synthesized D1

Bruker AVIIIHD 600 20160713
PROTON CD3OD D:\\ DATA2016 6



Current Data Parameters
NAME 20160713 0916210
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160714
Time_ 7.25
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT CD3OD
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 12.7
DW 41.600 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 600.2537068 MHz
NUC1 1H
P1 11.50 usec
PLW1 12.93200016 W

F2 - Processing parameters
SI 65536
SF 600.2500168 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

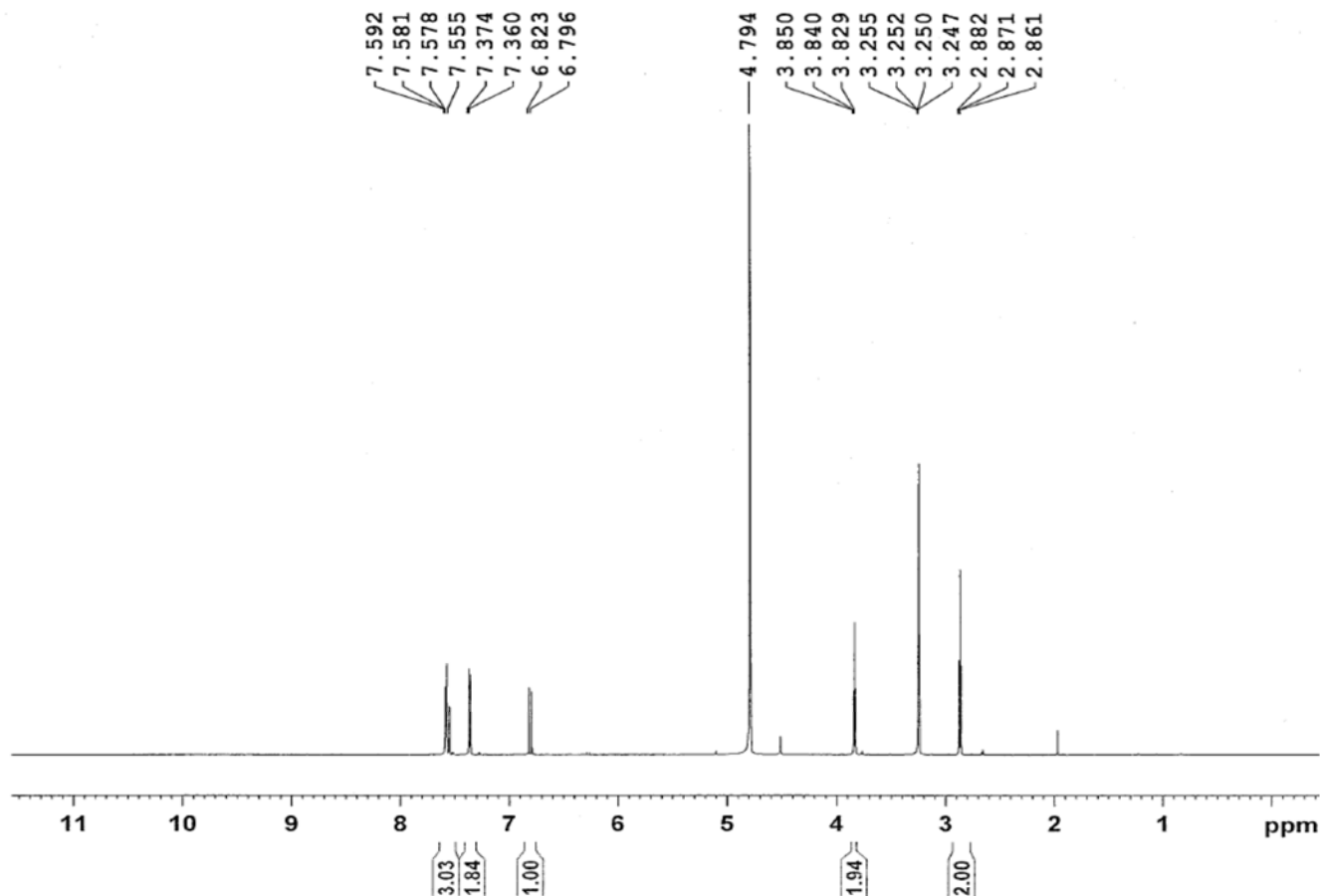
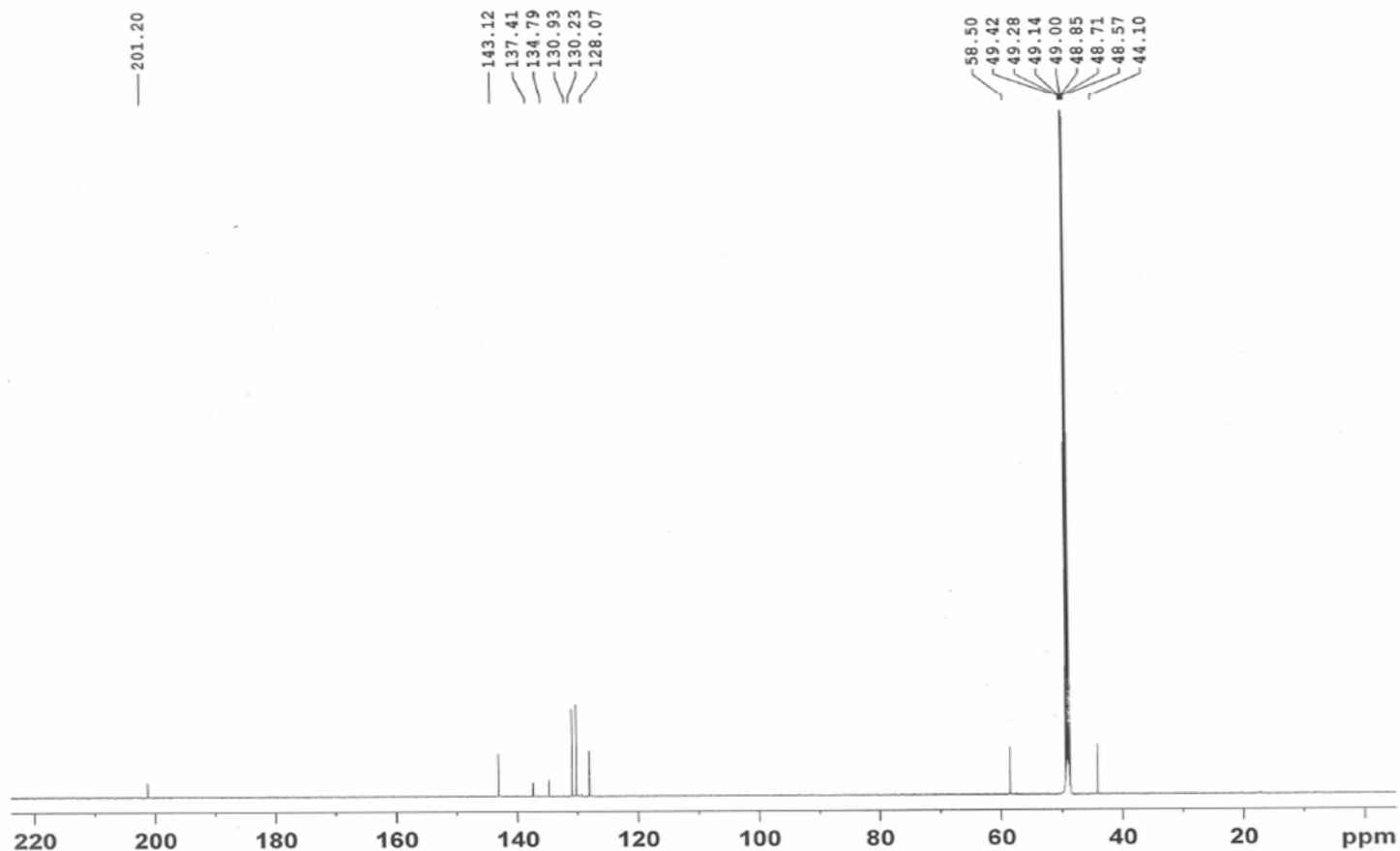


Fig.C.1 ^1H spectrum of D2 by LC-SPE-NMR



Bruker AVIIIHD 600 20160713
C13 CD3OD D:\ DATA2016 6



Current Data Parameters
NAME 20160713 0916210
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160714
Time 7.27
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 65536
SOLVENT CD3OD
NS 3200
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 31.37 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 400

===== CHANNEL f1 =====
SFO1 150.9495843 MHz
NUC1 13C
P1 12.54 usec
PLW1 19.39800072 W

===== CHANNEL f2 =====
SFO2 600.2524010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 12.93200016 W
PLW12 0.34902999 W
PLW13 0.17556000 W

F2 - Processing parameters
SI 32768
SF 150.9327626 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

Fig.C.2 ^{13}C spectrum of D2 by LC-SPE-NMR

Bruker AVIIIHD 600 20160713
HSQC CD3OD D:\ DATA2016 6

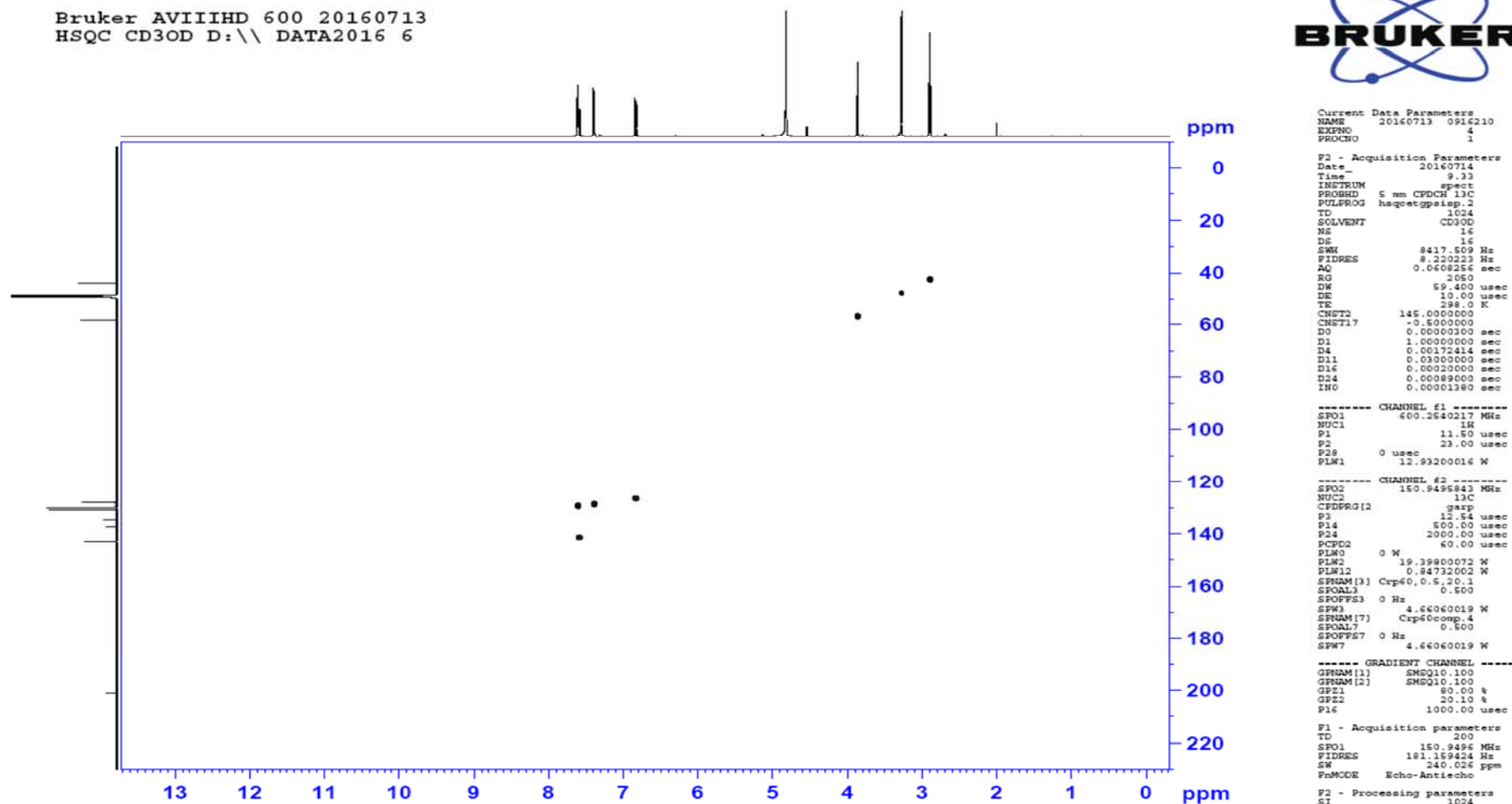
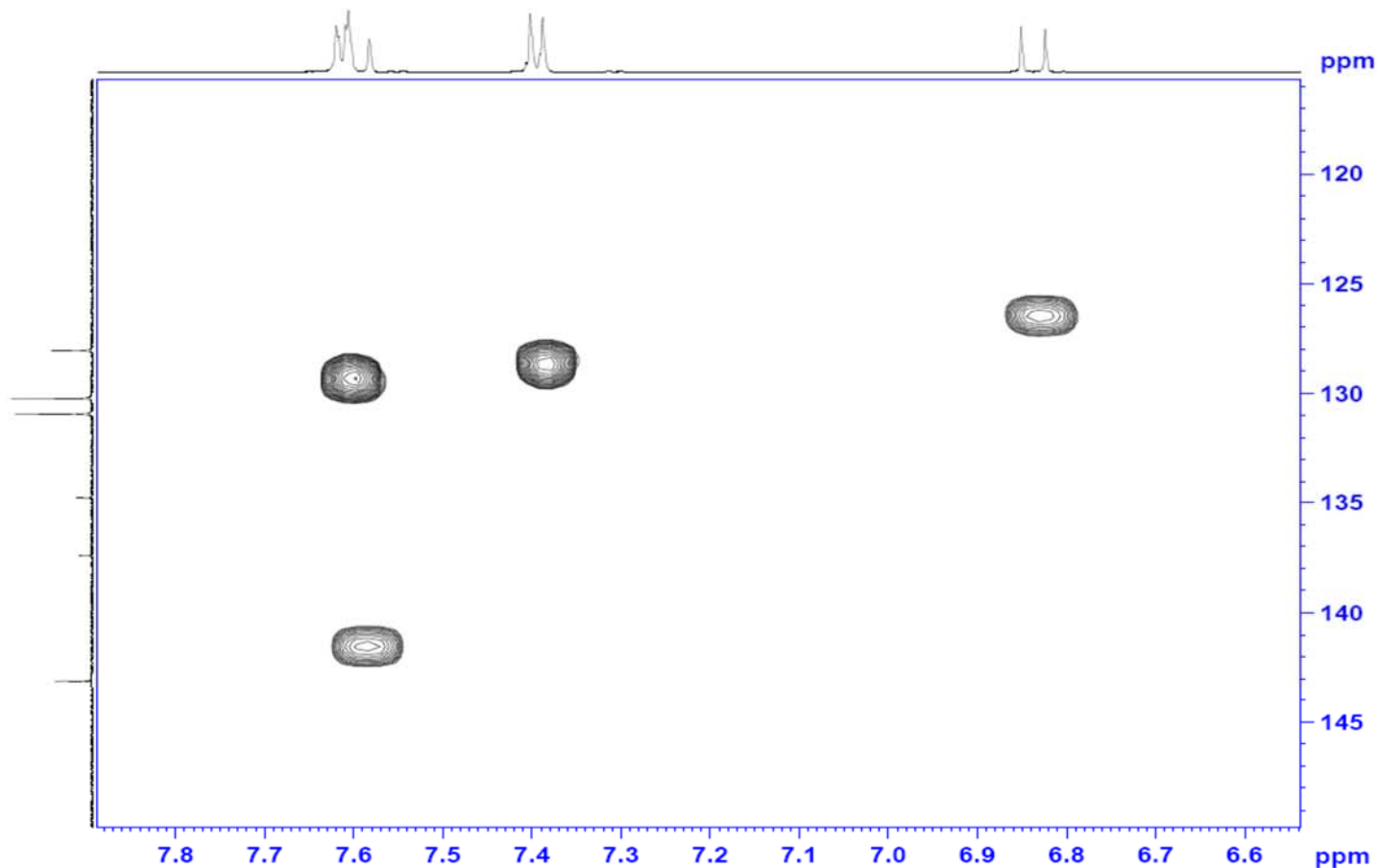


Fig.C.3 HSQC spectrum of D2 by LC-SPE-NMR

Bruker AVIIIHD 600 20160713
HSQC CD3OD D:\ DATA2016 6



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Current Data Parameters
NAME      20160713_0916210
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20160714
Time      9.33
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   hsqcetgpgisip.2
TD        1024
SOLVENT   CD3OD
NS         16
DS         16
SWH        8417.509 Hz
FIDRES     8.220223 Hz
AQ         0.0608256 sec
RG         2050
DW         59.400 usec
DE         10.00 usec
TE         298.0 K
CNET2     145.0000000
CNET17    -0.5000000
D0         0.00000100 sec
D1         1.00000000 sec
D4         0.00172414 sec
D11        0.03000000 sec
D16        0.00020000 sec
D24        0.00089000 sec
INO        0.00001380 sec

----- CHANNEL f1 -----
SFO1      600.2540217 MHz
NUC1       1H
P1         11.50 usec
P2         23.00 usec
P28        0 usec
PLN1      12.93200016 W

----- CHANNEL f2 -----
SFO2      150.9495843 MHz
NUC2       13C
CPDPRG2   gaup
P3         12.54 usec
P14        500.00 usec
P24        2000.00 usec
PCPD2     60.00 usec
PLN0       0 W
PLN2      19.39800072 W
PLN12     0.84732000 W
SPNAM[3]  Crp60.0.5.20.1
SFOAL3     0 Hz
SPOFFS3    0 Hz
SPW3       4.60600019 W
SPNAM[7]   Crp60comp.4
SFOAL7     0 Hz
SPOFFS7    0 Hz
SPW7       4.60600019 W

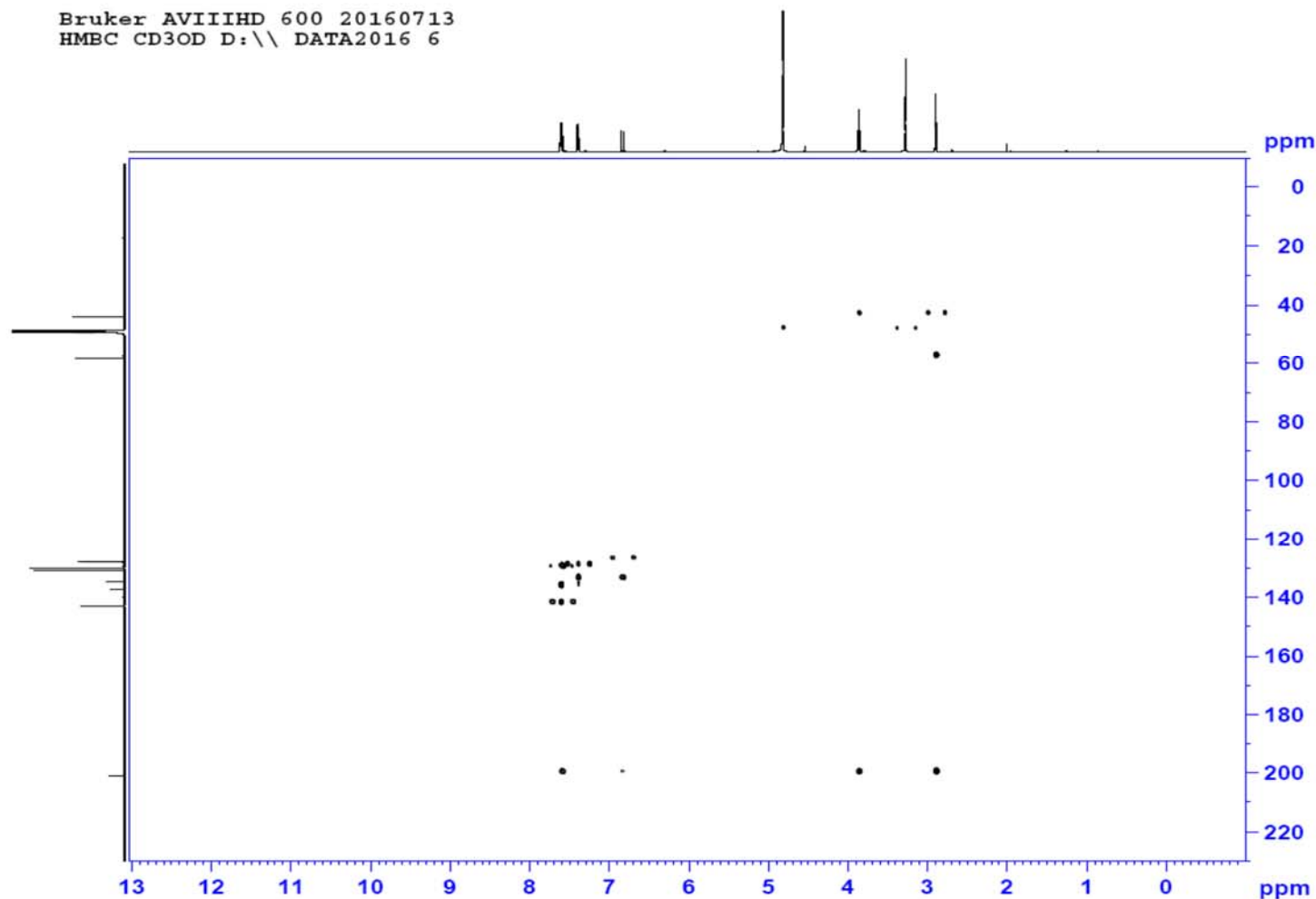
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GRNAM[1]   SMSQ10.100
GRNAM[2]   SMSQ10.100
GFE1       80.00 %
GFE2       20.10 %
P16        1000.00 usec

F1 - Acquisition parameters
TD         200
SFO1       150.9496 MHz
FIDRES     181.159424 Hz
SW         240.026 ppm
PnMCOE     Echo-Antiecho

F2 - Processing parameters
SI         1024
```

Fig.C.4 partial-enlarged HSQC spectrum of D2 by LC-SPE-NMR

Bruker AVIIIHD 600 20160713
HMBC CD3OD D:\\ DATA2016 6



```
Current Data Parameters
NAME      20160713_0916210
EXPNO     5
PROCNO    1

F2 - Acquisition Parameters
Date_     20160714
Time      10.33
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   hmbcpgndqf
TD         4096
SOLVENT   CD3OD
NS         40
DS         16
SWH        8417.809 Hz
FIDRES     2.055064 Hz
AQ         0.2433024 sec
RG         2050
DW         59.400 usec
DE         10.00 usec
TE         298.0 K
CNET13    8.0000000
D0         0.00300100 sec
D1         1.00000000 sec
D6         0.06250000 sec
D16        0.00010000 sec
IN0        0.0001380 sec

----- CHANNEL f1 -----
SFO1      400.2536089 MHz
NUC1       1H
P1         11.50 usec
P2         23.00 usec
PLW1      12.93200014 W

----- CHANNEL f2 -----
SFO2      150.9496843 MHz
NUC2       13C
P3         12.54 usec
PLW2      19.39800072 W

----- GRADIENT CHANNEL -----
GPRGM[1]  SMSQ10.100
GPRGM[2]  SMSQ10.100
GPRGM[3]  SMSQ10.100
GFE1      50.00 %
GFE2      30.00 %
GFE3      40.10 %
P16       1000.00 usec

F1 - Acquisition parameters
TD         160
SFO1      150.9496 MHz
FIDRES     226.449280 Hz
SW         240.026 ppm
PnMCOE     QF

F2 - Processing parameters
SI         1024
SF         400.2500000 MHz
WDW        SINE
SSB        0
LB         0 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        QF
SF         150.9329830 MHz
WDW        SINE
SSB        0
LB         0 Hz
GB         0
```

Fig.C.5 HMBC spectrum of D2 by LC-SPE-NMR

Bruker AVIIIHD 600 20160713
HMBC CD3OD D:\\ DATA2016 6

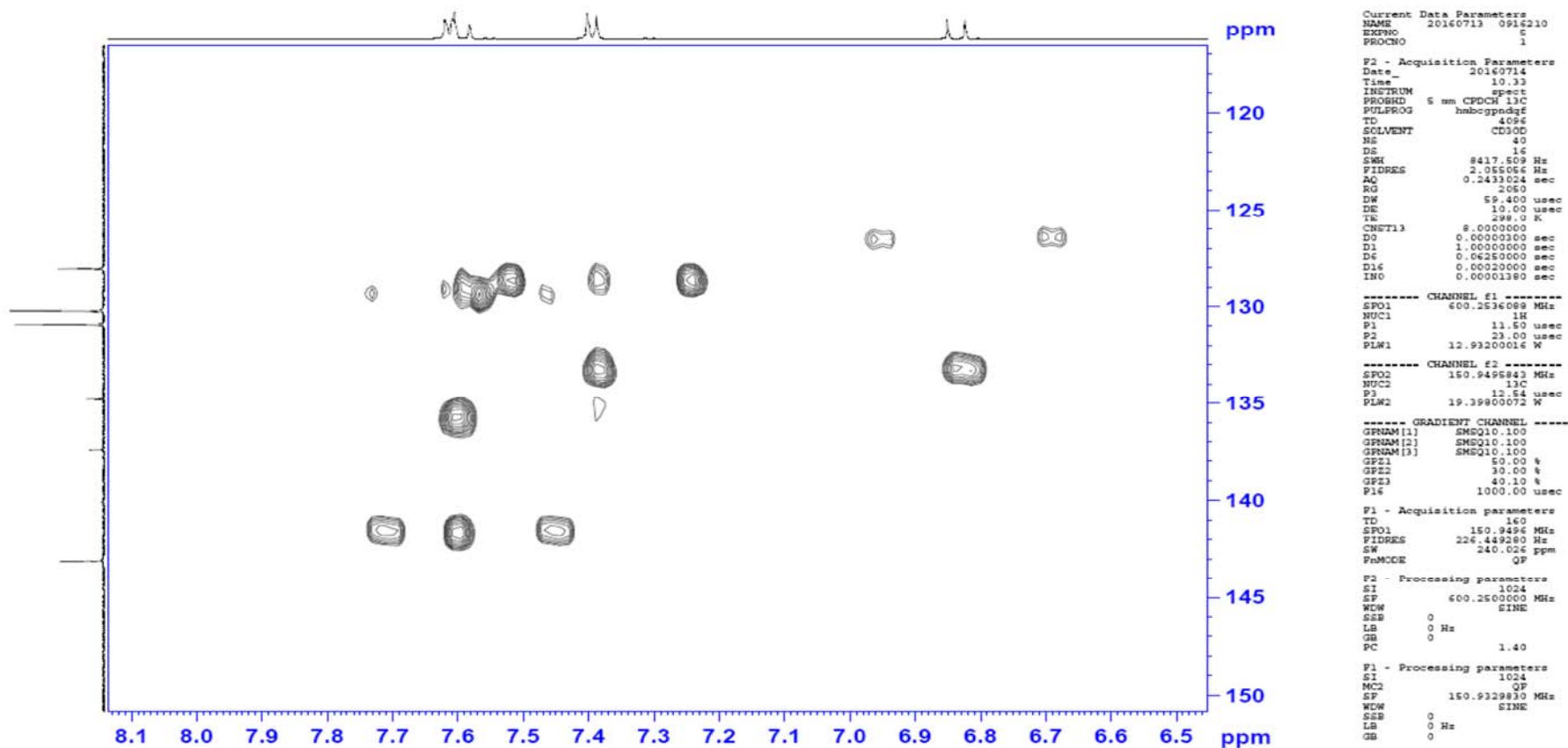


Fig.C.6 partial-enlarged HMBC spectrum of D2 by LC-SPE-NMR