

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

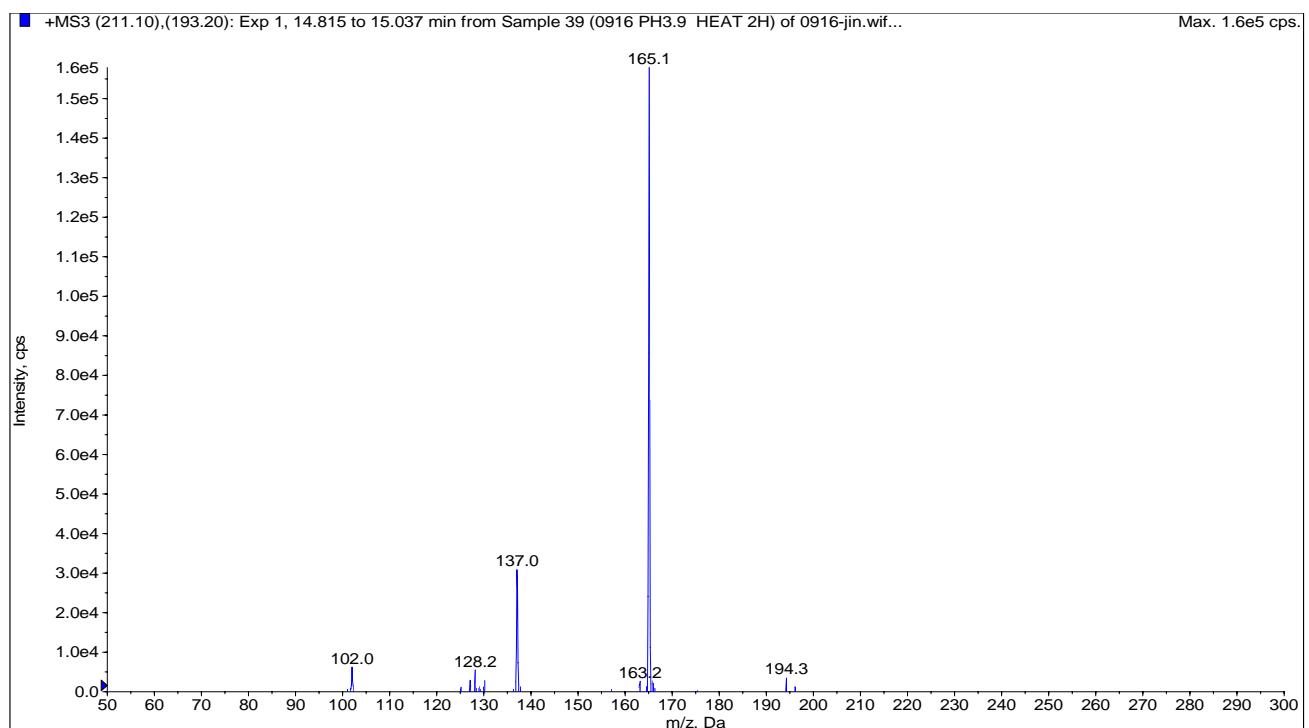


Fig.A.1 MS³ spectrum of m/z 193 ion from m/z 211 of D2

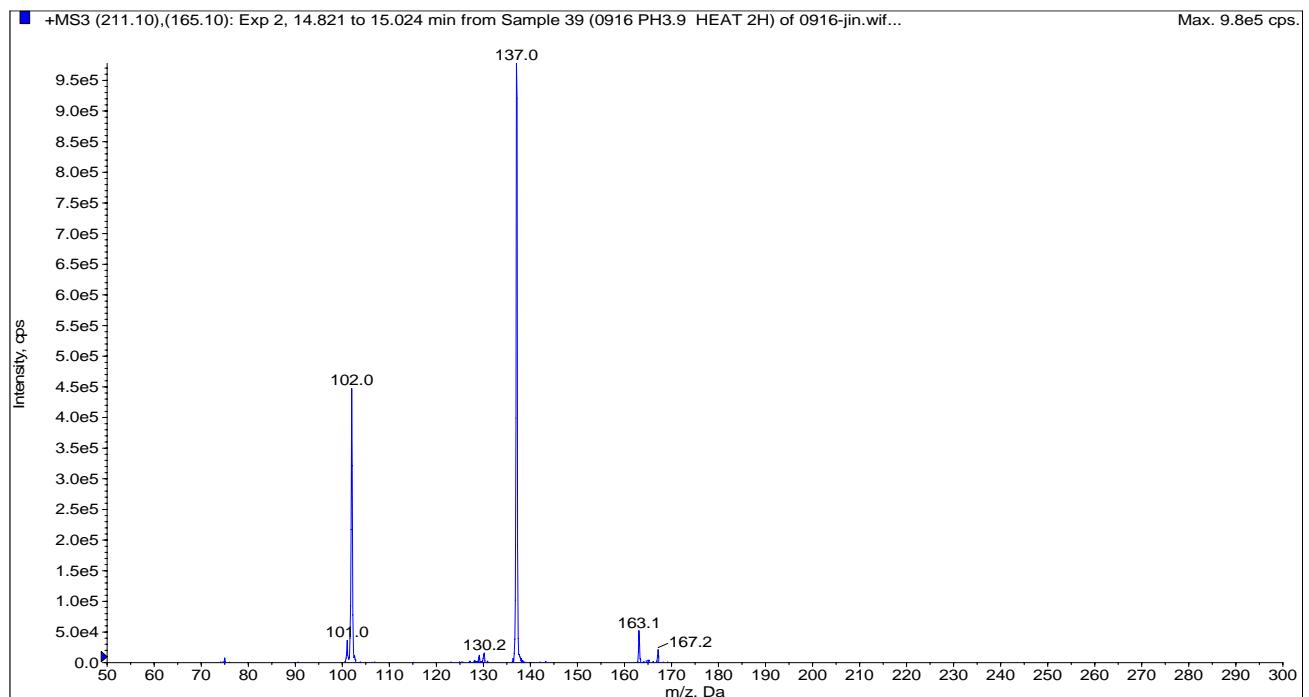


Fig.A.2 MS³ spectrum of m/z 165 ion from m/z 211 of D2

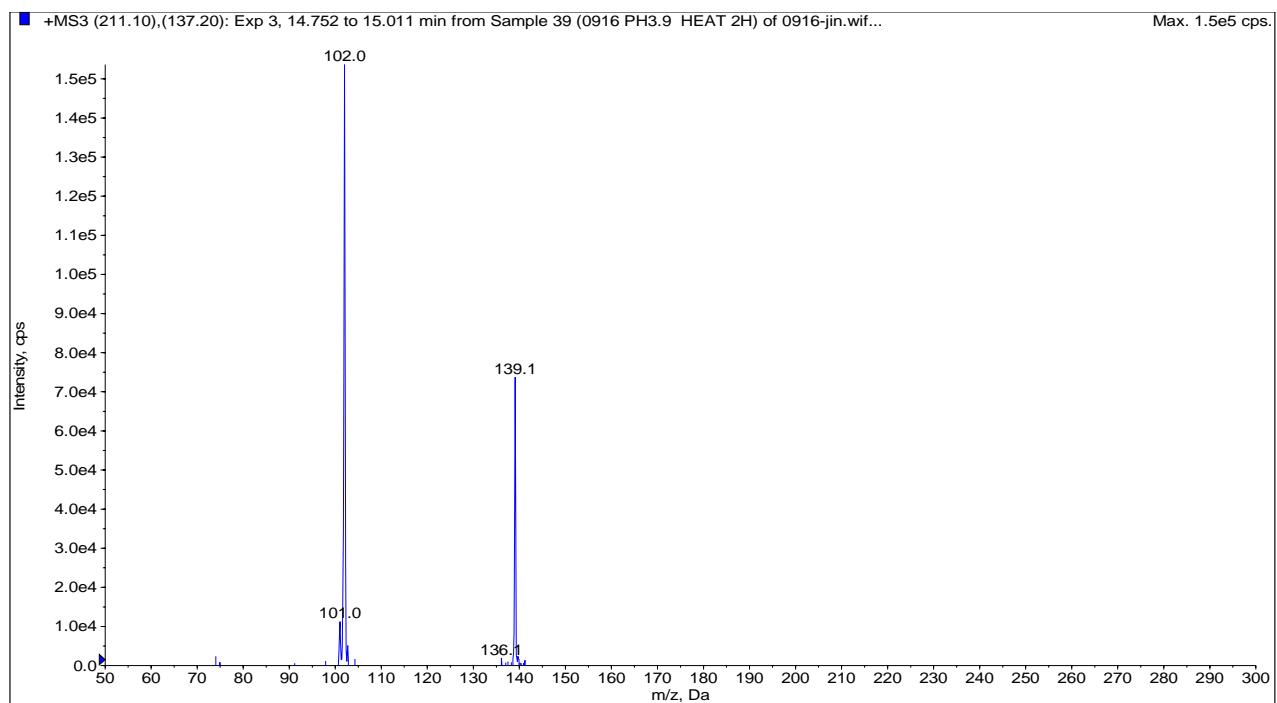
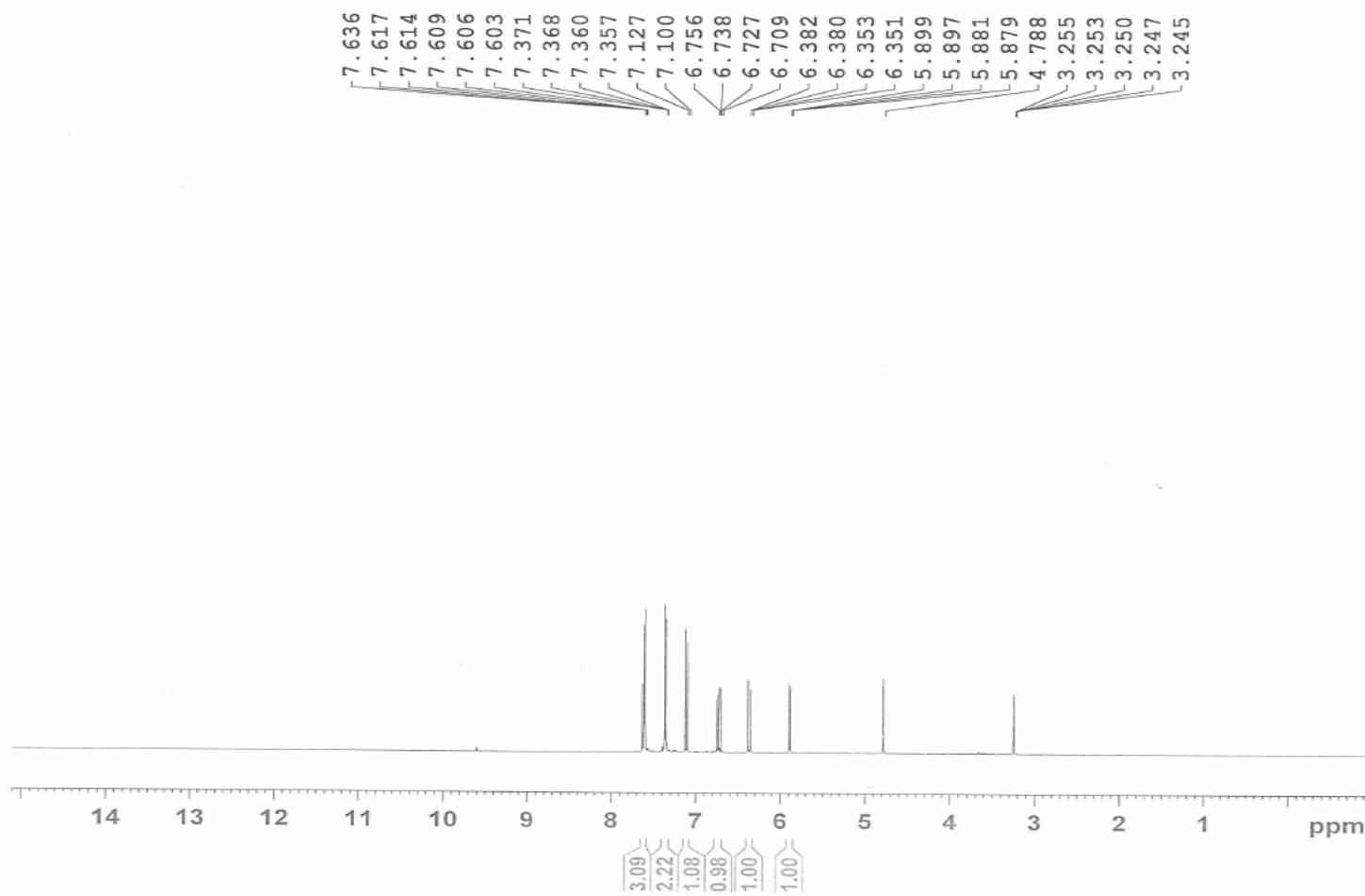


Fig.A.3 MS³ spectrum of m/z 137 ion from m/z 211 of D2

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



Current Data Parameters
NAME 20171102 M192
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20171106
Time 10.22
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 1.0000000 sec
TDO 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

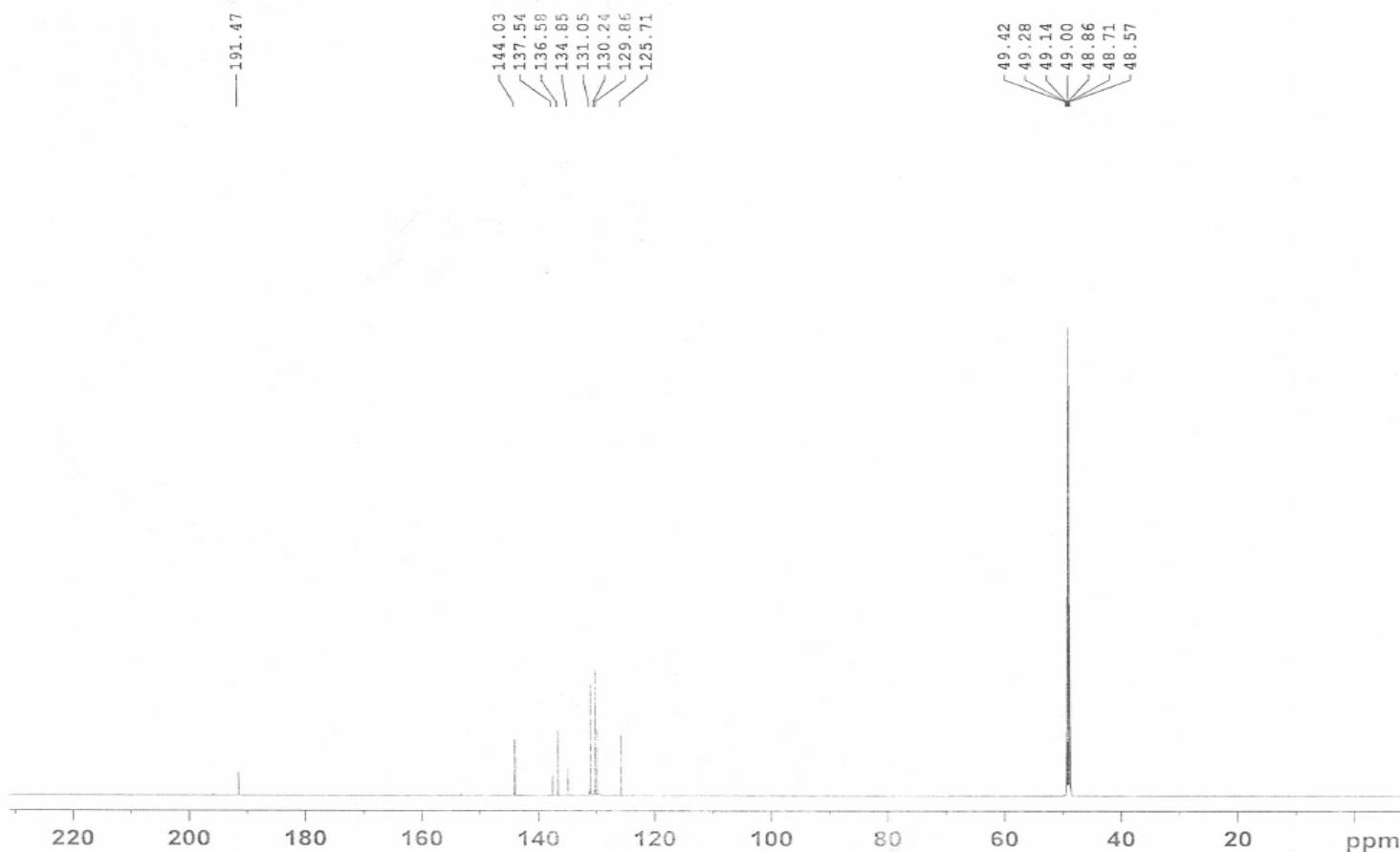


Fig.B.2 ¹³C spectrum of synthesized D1

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 1.0000000 sec
D11 0.0300000 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

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

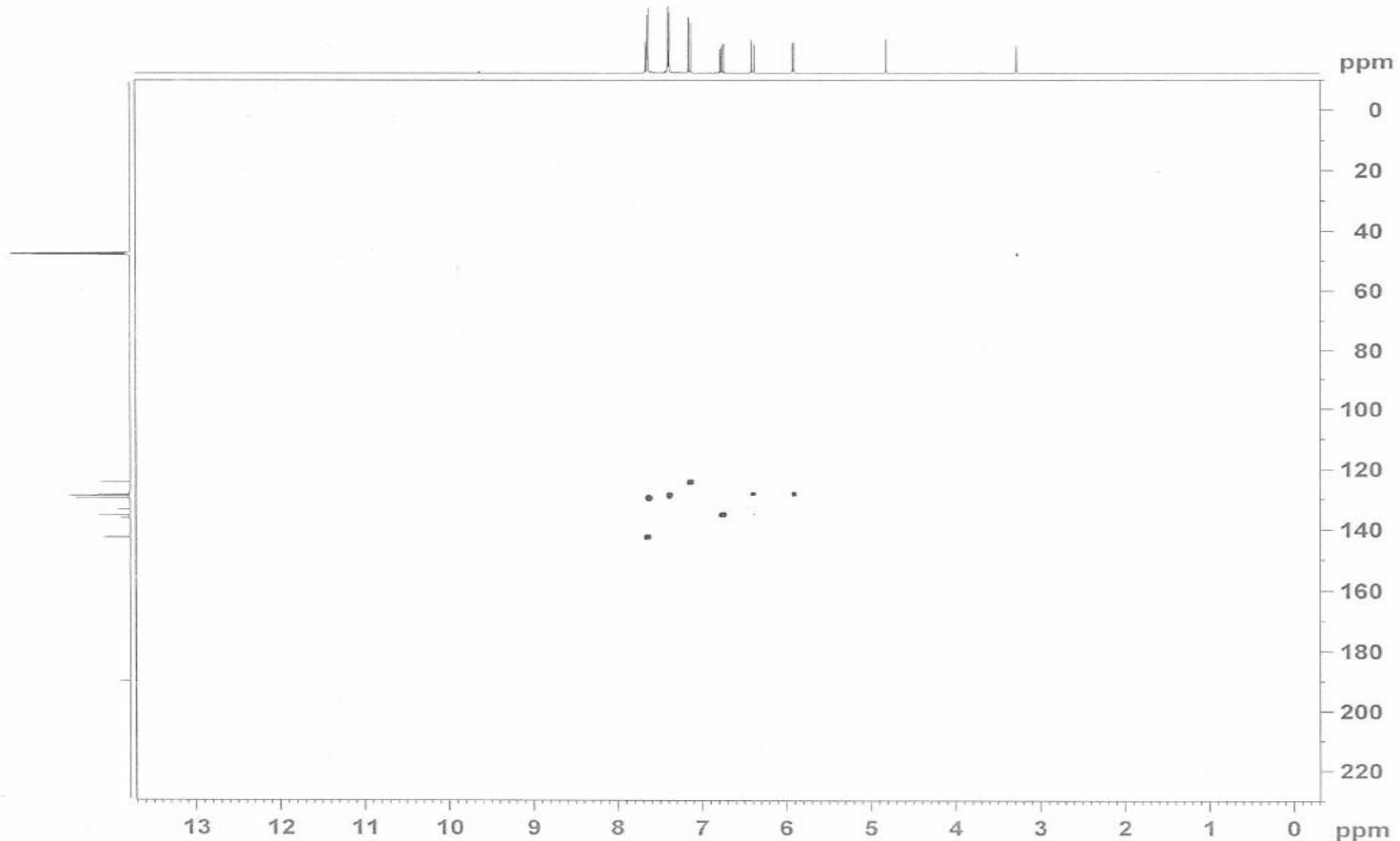
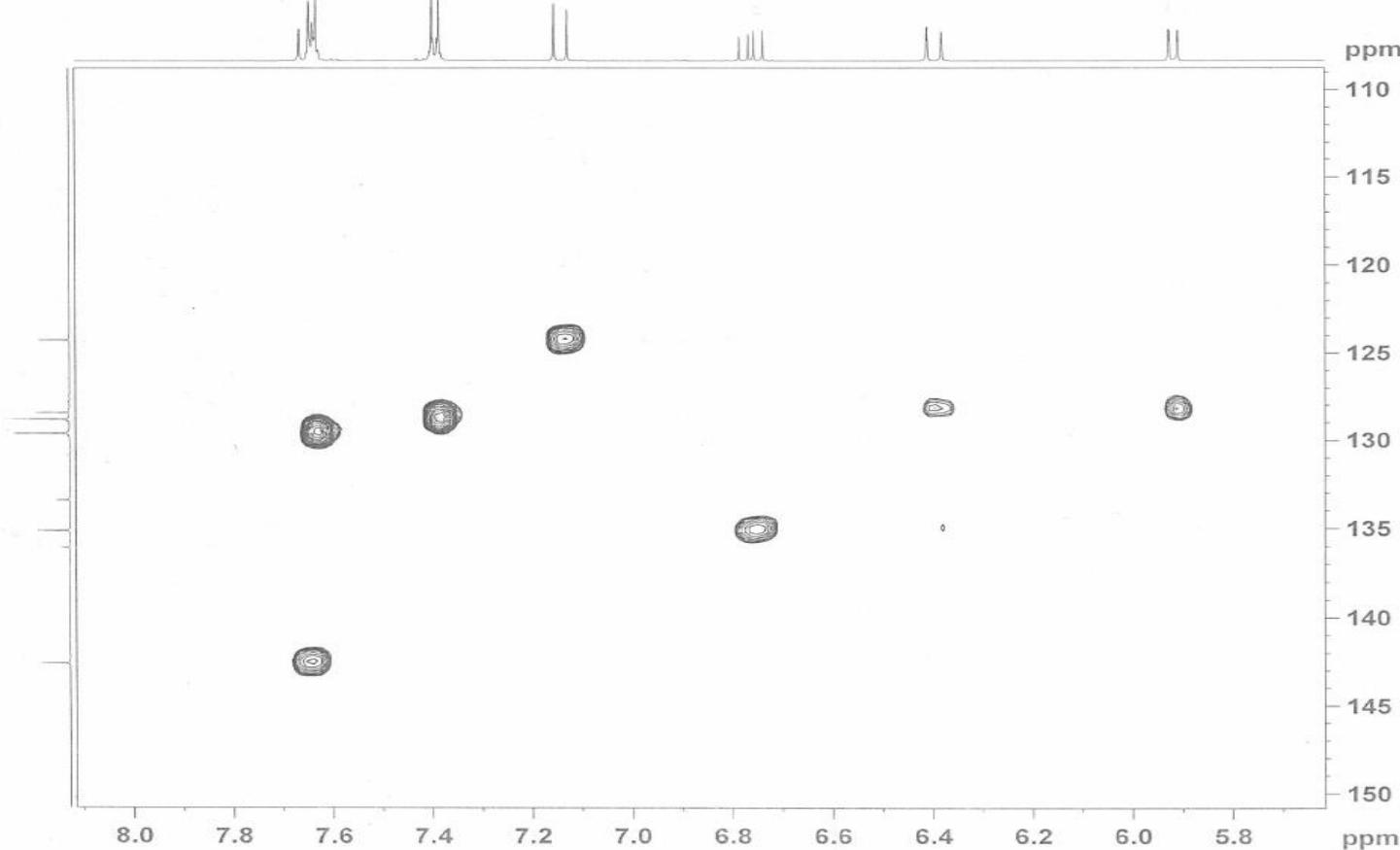


Fig.B.3 HSQC spectrum of synthesized D1

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



```
Current Data Parameters
NAME: 20171102_M152
EXPNO: 6
PROCNO: 1

FID - Acquisition Parameters
Date: 2017-11-02
Time: 11:28
INSTRUM: spect
PROBHD: 5 mm CPDMH DCC
PULPROG: hsquicetpsisp2.2
TD: 65536
SOLVENT: CD3OD
NS: 24
SWH: 8417.509 Hz
VRAM: 16384
AQ: 0.0609256 sec
RG: 2510
DW: 59.00 usec
DE: 10.00 usec
TE: 299.0 K
D1: 0.5000000 sec
C1: 145.0000000 sec
C2: 0.0000000 sec
D2: 0.0002414 sec
D3: 0.0000000 sec
D4: 0.0002000 sec
D5: 0.0034000 sec
D6: 0.0000000 sec
IMD: 0.0001380 sec

CHANNEL F1 =====
RF01: 400.2540217 MHz
RF02: 11.50 usec
F1: 11.50 usec
F2: 23.00 usec
D1: 0 usec
PLW1: 12.93200014 W

CHANNEL F2 =====
RF02: 150.9495843 MHz
RF03: 12.00 usec
CPDPRG[2]: garp
P1: 12.00 usec
T1A: 500.00 usec
T2A: 2000.00 usec
PCP02: 40.00 usec
PLW0: 0 W
PLW2: 15.39800072 W
T1B: 500.00 usec
SPNM[1]: Cpmg0.0,20,1
SPNM[2]: 0.500
SPDPFS3: 0 Hz
SPNM[3]: 4.66060019 W
SPNM[4]: Cpmg0.0,20,1
SPNM[5]: 0.500
SPDPFS7: 0 Hz
SPNM[6]: 4.66060019 W

GRADIENT: G100Z1
GPHAM[1]: SH9210.100
GPHAM[2]: SH9210.100
GPHAM[3]: SH9210.100
GPHAM[4]: SH9210.100
GPI1: 80.00 %
GPI2: 10.00 %
GPI3: 11.00 %
GPI4: 5.00 %
PL1: 1000.00 usec
PL9: 600.00 usec

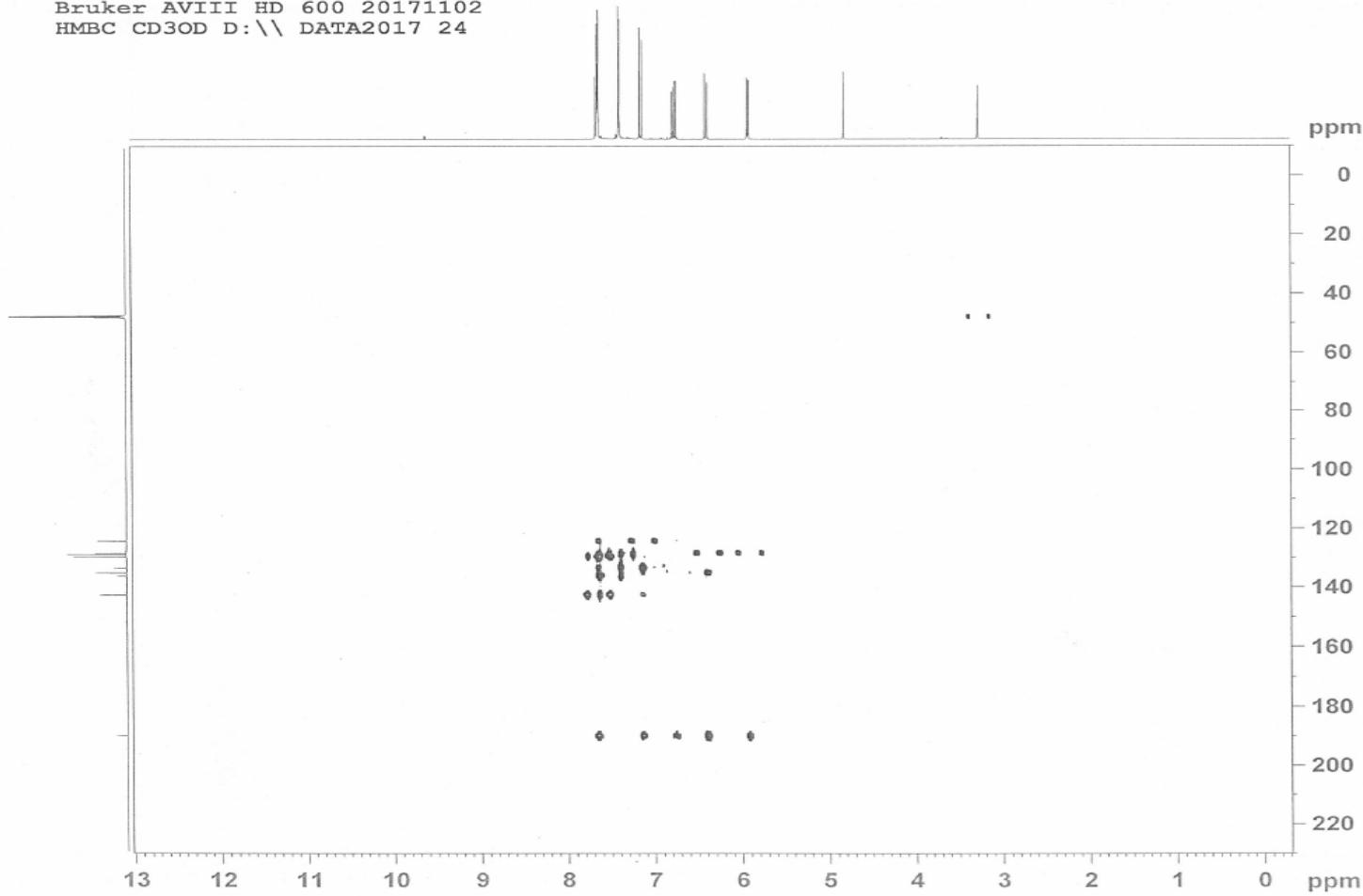
FID - Acquisition parameters
TD: 65536
FID01: 130.0000000 Hz
FIDRES: 144.680344 Hz
SW: 240.026 ppm
WMDME: Echo-Antiecho

F2 - Processing parameters
IL: 1024
SF: 600.12500000 MHz
WM: 2048
SSB: 0 Hz
LB: 0 Hz
GS: 1.40

F2 - Processing parameters
SF1: 152.8444444 Hz
SF2: echo-antiecho
SF: 150.9329930 MHz
WM: 2048
SSB: 0 Hz
LB: 0 Hz
GS: 0.00
```

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

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



Current Data Parameters
NAME: 20171102_M192
EXPNO: 7
PROCNO: 1

F2 - Acquisition Parameters
Date: 20171106
Time: 13.06
INSTRUM: spect
PROBHD: 5 mm CPDCH 13C
PULPROG: hmbcgp3d
TD: 4096
SOLVENT: CD3OD
NS: 40
DS: 16
SWH: 8417.500 Hz
FIDRES: 2.055056 Hz
AQ: 0.2433024 sec
RG: 2050
DW: 59.400 usec
DE: 13.000 usec
TE: 298.0 K
CNST13: 8.0000000
D0: 0.00000300 sec
D1: 1.00000000 sec
D2: 0.00000000 sec
D16: 0.000020000 sec
INO: 0.00001380 sec

CHANNEL f1 -----
SF01: 600.2536088 MHz
NUC1: 1H
P1: 11.50 usec
P2: 23.00 usec
PLW1: 12.93200016 W

CHANNEL f2 -----
SF02: 150.9495843 MHz
NUC2: 13C
P3: 12.54 usec
PLW2: 19.39800072 W

GRADIENT CHANNEL -----

GPNAME[1]: SMSQ10.100

GPNAME[2]: SMSQ10.100

GPNAME[3]: SMSQ10.100

GPZ1: 50.00 %

GPZ2: 30.00 %

GPZ3: 40.10 %

P16: 1000.00 usec

F1 - Acquisition parameters

TD: 4096

SF01: 150.9496 MHz

FIDRES: 226.44926 Hz

SW: 240.026 ppm

PRMode: QF

F2 - Processing parameters

S1: 1024

SF: 600.2500000 MHz

WDW: SINE

SSB: 0

LB: 0 Hz

GB: 0

PC: 1.40

F1 - Processing parameters

S1: 1024

MC2: QF

SF: 150.9329630 MHz

WDW: SINE

SSB: 0

LB: 0 Hz

GB: 0

Fig.B.5 HMBC spectrum of synthesized D1

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

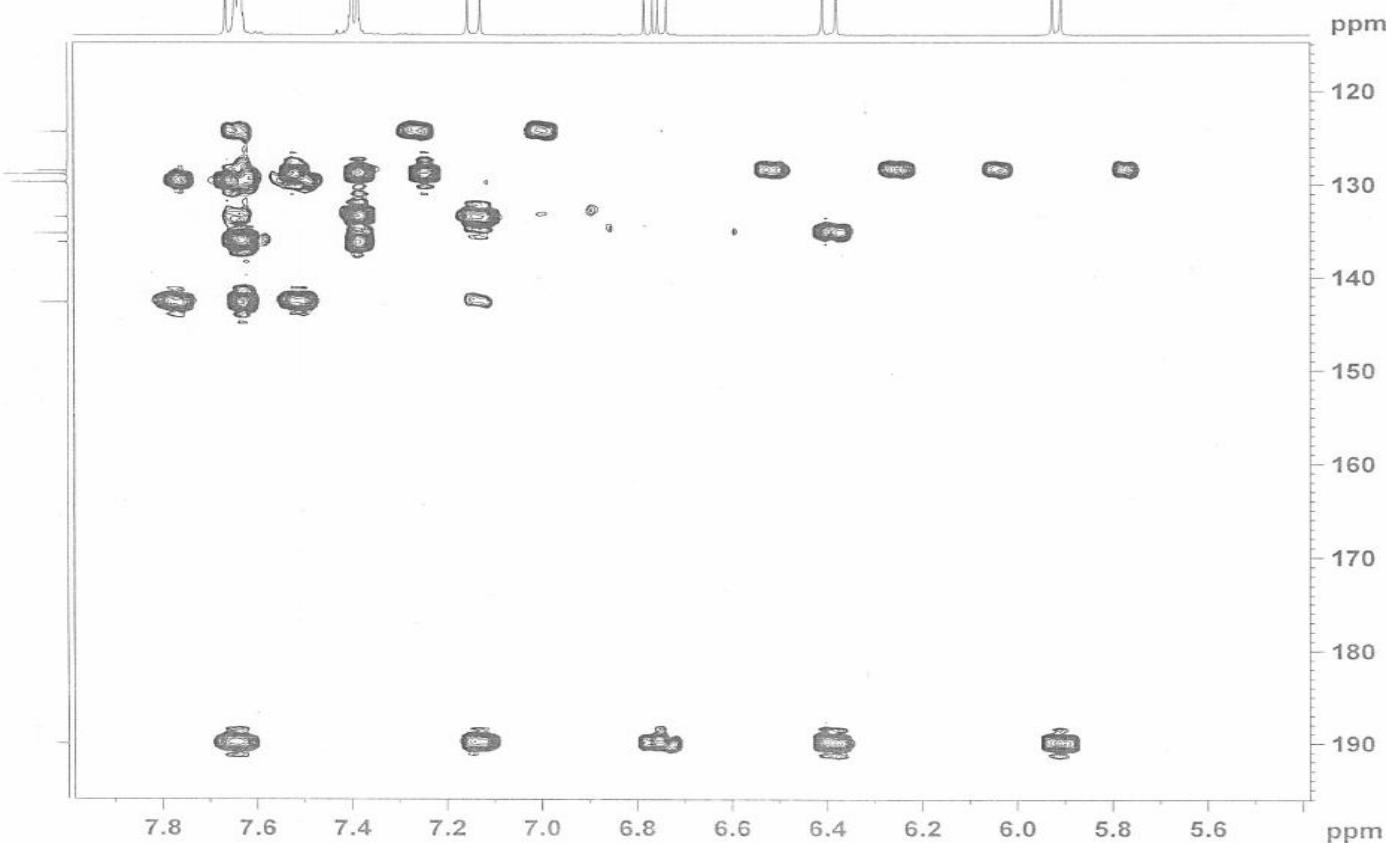


Fig.B.6 partial-enlarged HMBC spectrum of synthesized D1

Current Data Parameters
NAME: 20171102_M192
EXPNO: 7
PROCNO: 1

F2 - Acquisition Parameters
Date: 20171106
Time: 13.06
INSTRUM: spect
PROBHD: 5 mm CPDCH 13C
PULPROG: hmbcgrf
TD: 4096
SOLVENT: CD3OD
NS: 40
DS: 16
SWH: 8417.506 Hz
FIDRES: 2.055056 Hz
AQ: 0.2433024 sec
RG: 2050
DW: 59.400 usec
DPF: 1.00 usec
TE: 298.0 M
CNST13: 8.0000000
D0: 0.00000300 sec
D1: 1.0000000 sec
D6: 0.06250000 sec
D16: 0.00020000 sec
INO: 0.00001380 sec

CHANNEL F1
SF01: 600.2536088 MHz
NUC1: 1H
P1: 11.50 usec
P2: 23.00 usec
PLW1: 12.93200016 W

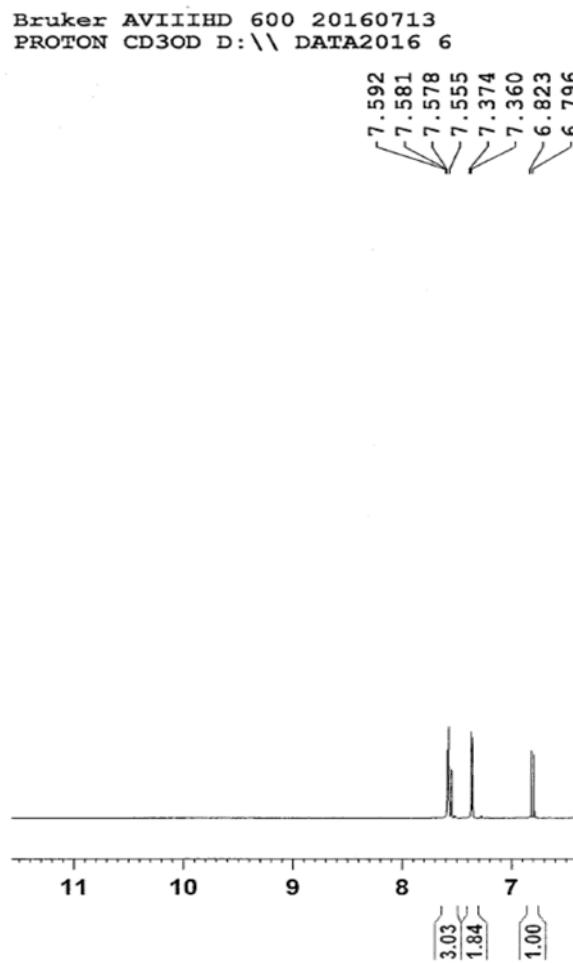
CHANNEL F2
SF02: 150.9495843 MHz
NUC2: 13C
P1: 12.54 usec
PLW2: 19.39800072 W

GRADIENT CHANNEL
GPNAME[1]: SMCQ10_100
GPNAME[2]: SMCQ10_100
GPNAME[3]: SMCQ10_100
GPZ1: 50.00 °
GPZ2: 30.00 °
GPZ3: 40.10 °
P16: 1000.00 usec

F1 - Acquisition parameters
TD: 160
SF01: 150.9495 MHz
FIDRES: 226.449280 Hz
SW: 240.024 ppm
PwMode: QF

F2 - Processing parameters
SI: 1024
SF: 600.2500000 MHz
WDW: SINE
SSB: 0
LB: 0 Hz
GB: 0
PC: 1.40

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



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 1.0000000 sec
 TDO 1

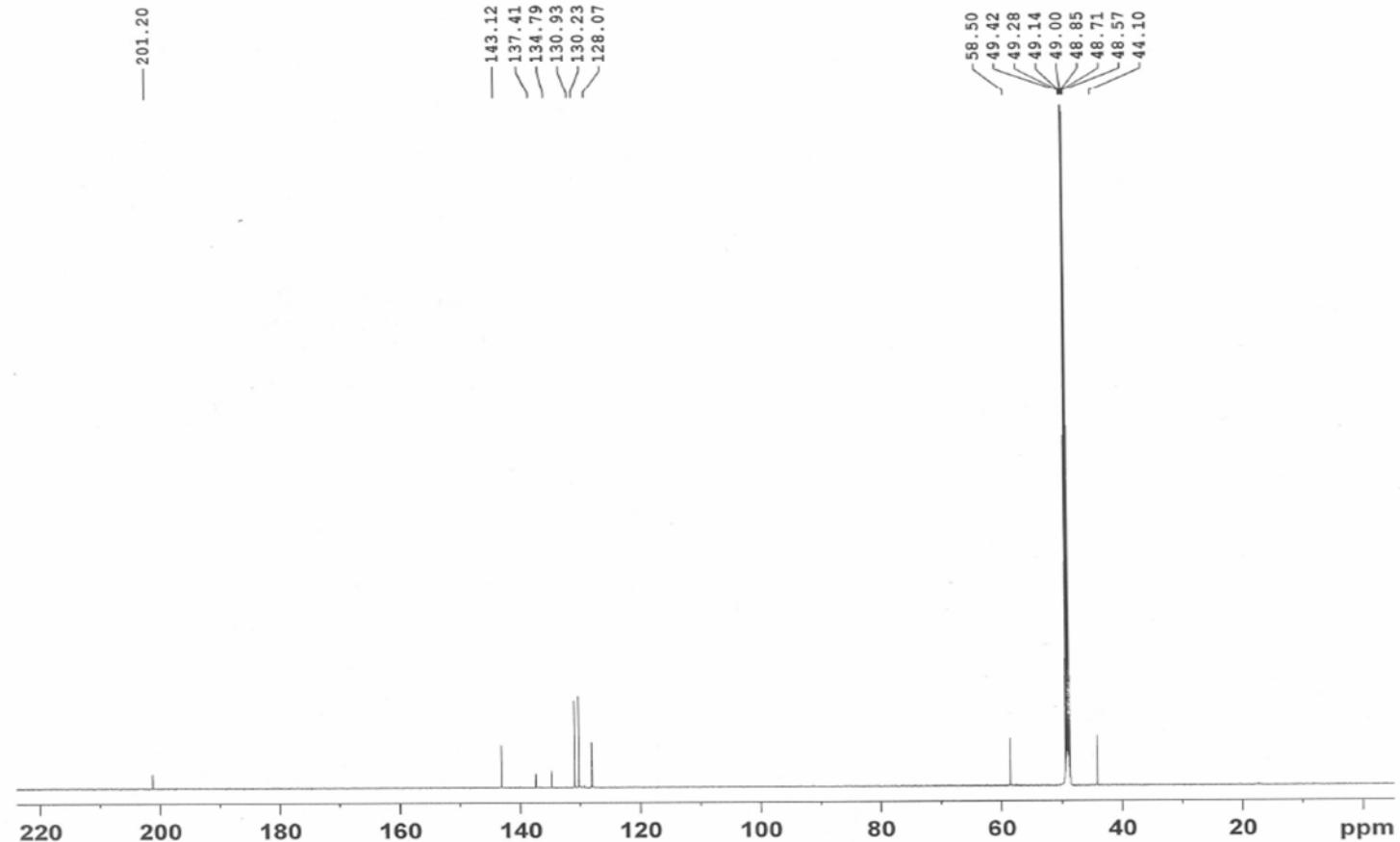
----- CHANNEL f1 -----
 SF01 600.2537068 MHz
 NUC1 1H
 P1 11.50 usec
 PLW1 12.93200016 W

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

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 1.0000000 sec
D11 0.0300000 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 AVIIIHDX 600 20160713
HSQC CD3OD D:\\\\ DATA2016 6



Current Data Parameters
NAME: 20160713_0916210
EXPTNO: 1

P2 - Acquisition Parameters
Date: 20160714
Time: 9.33
INSTRUM: spect
PROBHD: 5 mm CPDCH 13C
PULPROG: hsqcetgpsim2
TD: 65536
TSP: 1024
SOLVENT: CD3OD
NS: 16
DS: 16
SWH: 8417.500 Hz
FIDRES: 0.22053 Hz
AQ: 0.0608266 sec
RG: 2050
DW: 59.400 usec
DE: 6.500 usec
TE: 299.0 K
CNUST2: 145.000000
CNUST1: -0.5000000
DD: 0.0000000 sec
D1: 1.0000000 sec
D4: 0.00172414 sec
D11: 0.03000000 sec
D16: 0.00020000 sec
D24: 0.00089000 sec
IM0: 0.00001380 sec

----- CHANNEL f1 -----
SFO1: 600.2540217 MHz
NUC1: 1H
P1: 11.11 usec
P2: 23.00 usec
P28: 0 usec
PLW1: 12.93200016 W

----- CHANNEL f2 -----
SFO2: 150.9495843 MHz
NUC2: 13C
CPDPKG12: 500.00 usec
D3: 1.54 usec
P14: 500.00 usec
P24: 2000.00 usec
PCPD2: 60.00 usec
D140: 0 W
PLW2: 19.39900072 W
PLW12: 0.84732002 W
SPNAM[3] Crp60,0,5,20.1
SPNAM[7] Crp60,comp.4
SPDOL1: 0.500
SPDOL3: 0 Hz
SPW3: 4.66060019 W
SPW7: 4.66060019 W
SPW9: 4.66060019 W

----- GRADIENT CHANNEL -----
GPNAME[1]: SNSQ10.100
GPNAME[2]: SNSQ10.100
GPIV: 80.00 %
GPZ2: 20.10 %
P16: 1000.00 usec

P1 - Acquisition parameters
TD: 65536
SFO1: 150.9496 MHz
FIDRES: 181.159424 Hz
SW: 240.026 ppm
PmMode: Echo-Antiecho
P2 - Processing parameters
SI: 1024

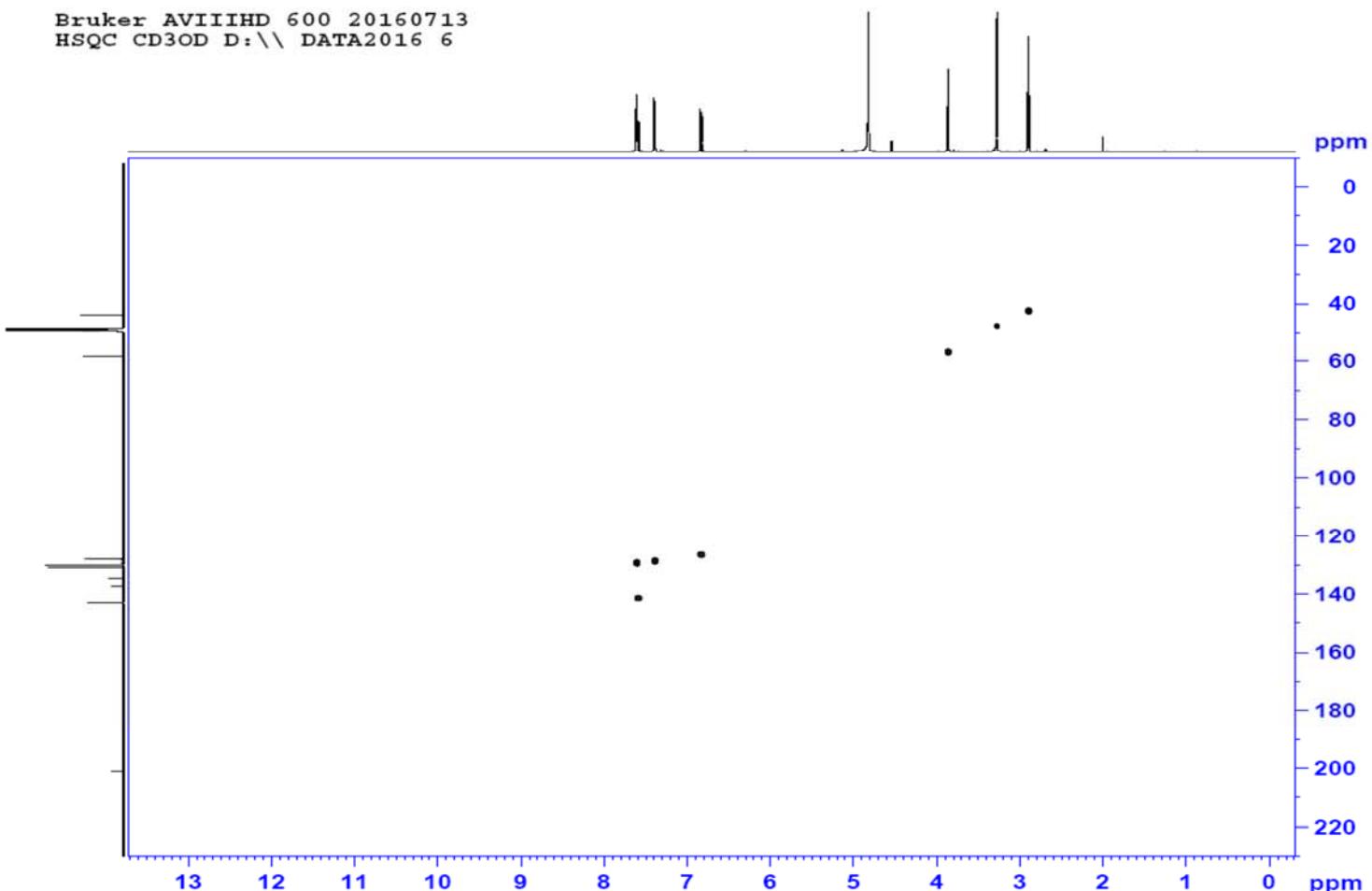
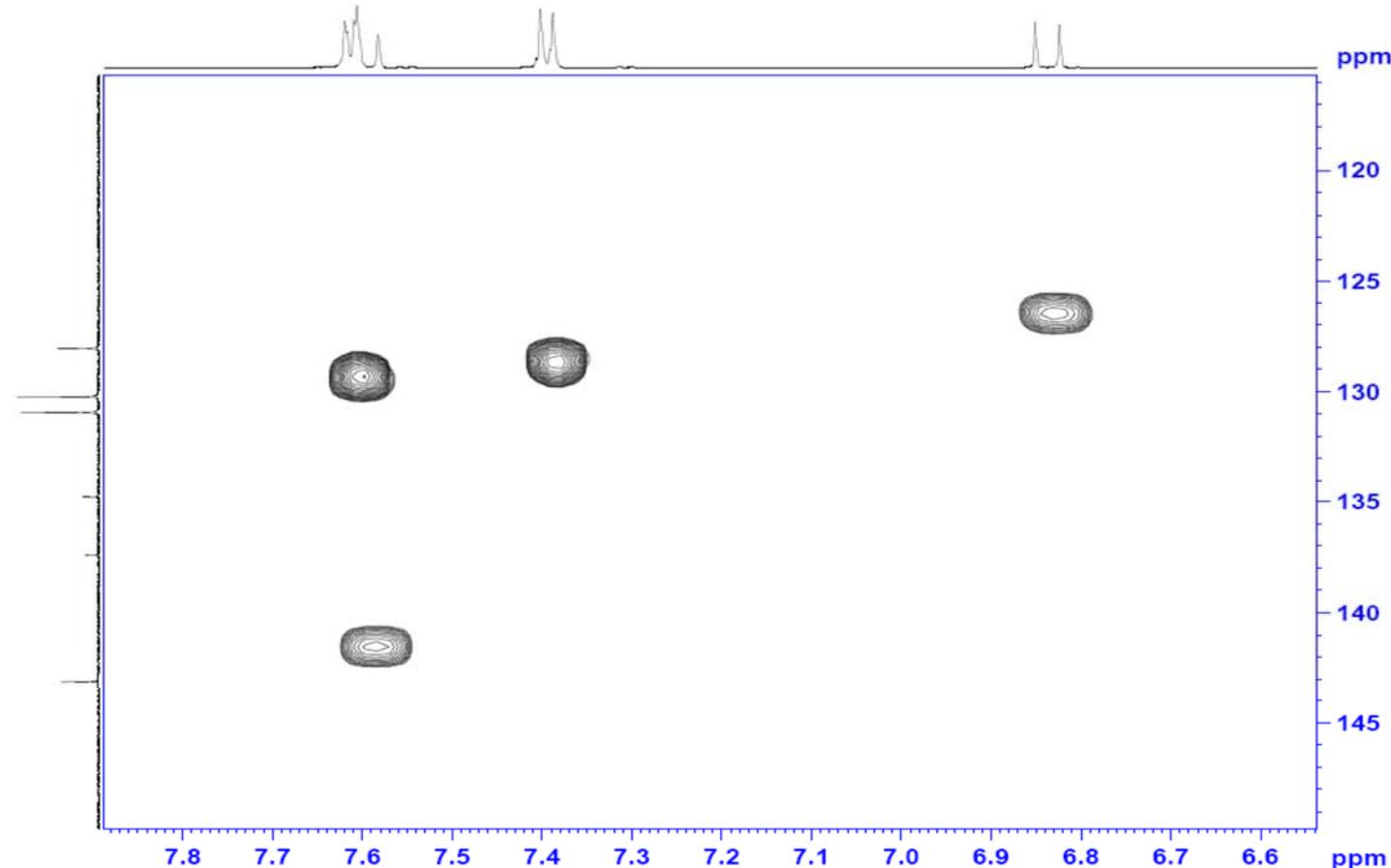


Fig.C.3 HSQC spectrum of D2 by LC-SPE-NMR

Bruker AVIIHHD 600 20160713
HSQC CD3OD D:\\\\ DATA2016 6



Current Data Parameters
NAME 20160713_0916210
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date 20160714
Time 9.19
INSTRUM spect
PROBHDG 5 mm CPDCH 13C
PULPROG hsqctgpsisp.2
TD 1024
SOLVENT CD3OD
NS 14
DS 16
SWH 8417.509 Hz
FIDRES 0.220223 Hz
AQ 0.0608256 sec
RG 2050
DW 50.00 usec
DE 10.00 usec
TE 299.0 K
CNUST2 145.000000
CNUST17 -0.500000
D0 0.000000 sec
D1 1.0000000 sec
D4 0.00172414 sec
D11 0.00300000 sec
D16 0.00020000 sec
D24 0.00089000 sec
INO 0.00001380 sec

----- CHANNEL f1 -----
SPO1 600.2540217 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
P2B 0 usec
PLW1 12.93200016 W

----- CHANNEL f2 -----
SPO2 160.9495843 MHz
NUC2 13C
CPDPRG12 garp
P3 12.54 usec
P14 500.00 usec
P24 2000.00 usec
PCPD2 60.00 usec
PLW2 0 W
PLW2 19.39900072 W
PLW2 0.84732002 W
SPNAM[3] Crp60,0,5,20,1
SPNAM[4] 0.500
SPNAM[5] 0 Hz
SPW3 4.66060019 W
SPNAM[7] Crp60comp,4
SPW4 0.500
SPWPS7 0 Hz
SPW7 4.66060019 W

----- GRADIENT CHANNEL -----
GPNAME[1] SNSQ10.100
GPNAME[2] SNSQ10.100
GPZ1 0 %
GPZ2 20.10 %
P16 1000.00 usec

P1 - Acquisition parameters
TD 200
SPO1 160.9495843 MHz
FIDRES 181.159424 Hz
SW 240.026 ppm
PnMCDE Echo-Antiecho

P2 - 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

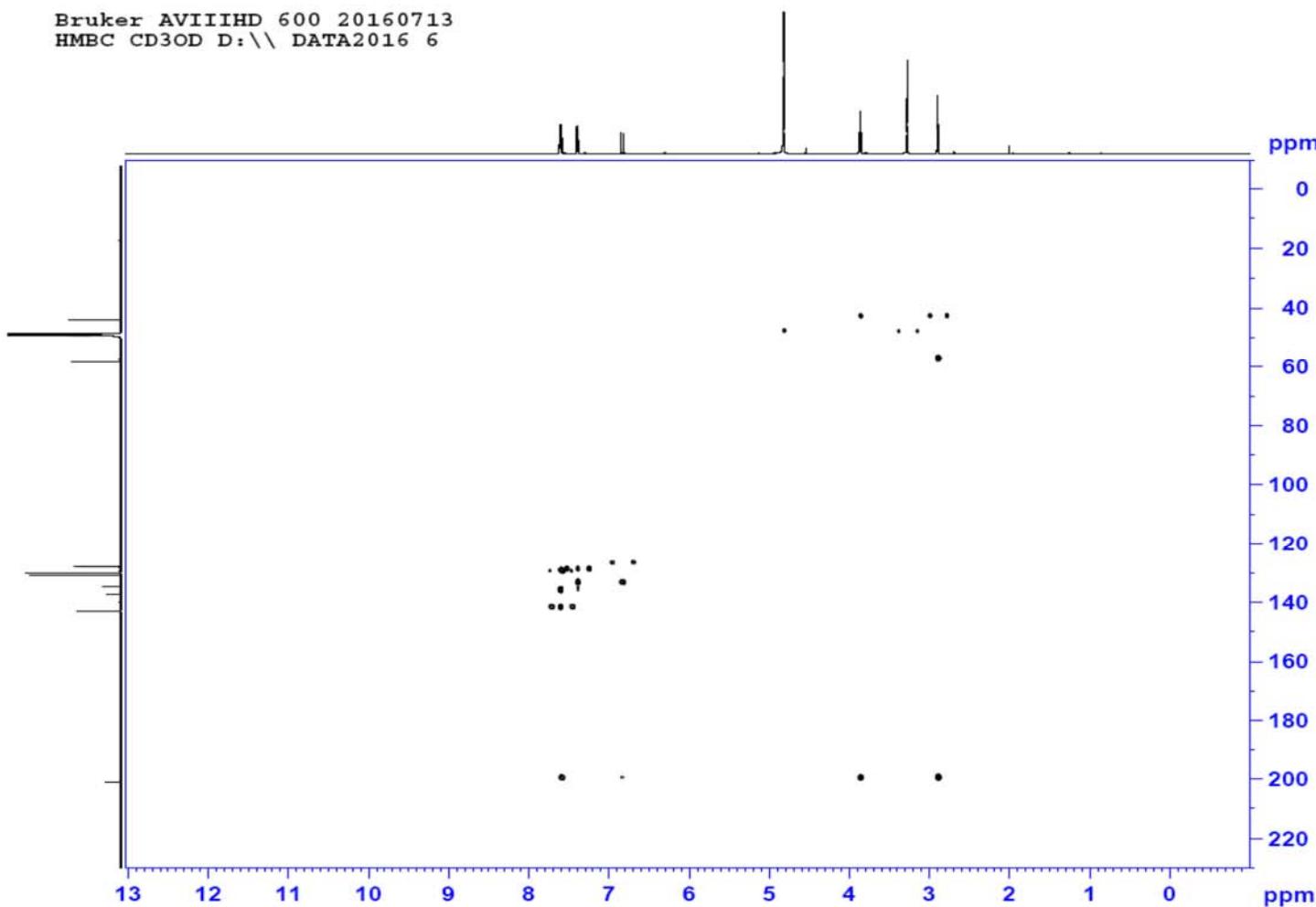
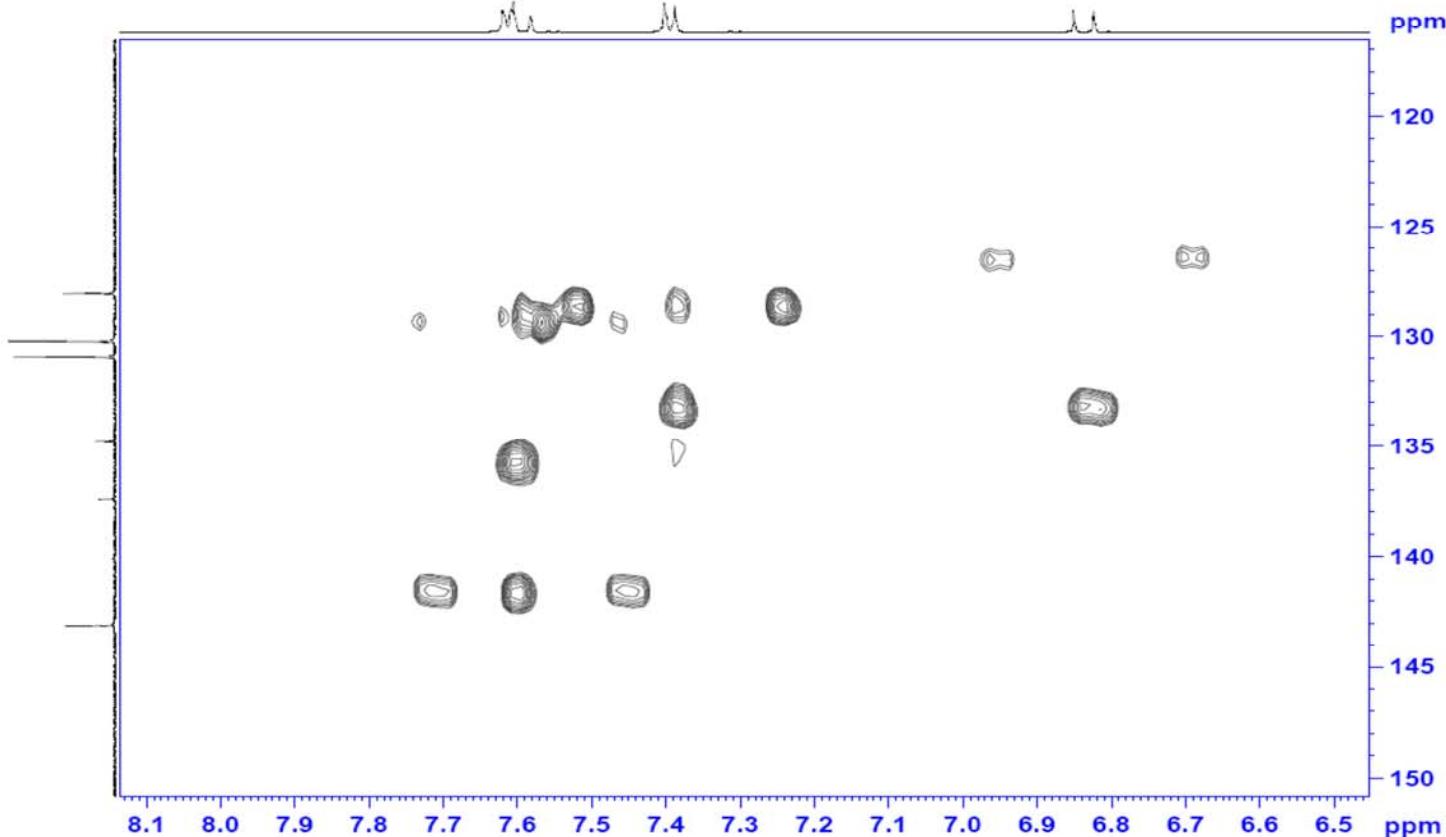


Fig.C.5 HMBC spectrum of D2 by LC-SPE-NMR

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



Current Data Parameters
NAME 20160713_0916210
EXPNO 5
PROCNO 1

P2 - Acquisition Parameters
Date 20160714
Time 10.19
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG hmbcgpndgf
TD 4096
SOLVENT CD3OD
NS 40
DS 16
SWH 8417.509 Hz
FIDRES 2.055056 Hz
AQ 0.241976 sec
RG 2050
DE 59.400 usec
DW 10.00 usec
TE 298.0 K
CPDPLT 0.0900000
D0 0.00000300 sec
D1 1.00000000 sec
D6 0.00250000 sec
D14 0.00020000 sec
INO 0.00001380 sec

----- CHANNEL E1 -----
SPO1 600.2536089 MHz
NUC1 1H
P1 11.00 usec
P2 23.00 usec
PLW1 12.99200016 W

----- CHANNEL E2 -----
SPO2 150.9495842 MHz
NUC2 13C
P3 12.64 usec
PLW2 19.39900072 W

----- GRADIENT CHANNEL -----
GPNUM[1] SMDQ10.100
GPNUM[2] SMDQ10.100
GPNUM[3] SMDQ10.100
GPZ1 0 %
GPZ2 30.00 %
GPZ3 40.10 %
P14 1000.00 usec

P1 - Acquisition parameters
TD 160
SPO1 150.9496 MHz
FIDRES 226.449280 Hz
SW 240.026 ppm
PwMode QF

P2 - Processing parameters
SI 1024
SF 600.2500000 MHz
WMW 0
SSB 0
LB 0 Hz
GB 0
PC 1.40

P1 - Processing parameters
SI 1024
MC2 QF
SF 150.9329830 MHz
WMW 0
SSB 0
LB 0 Hz
GB 0

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