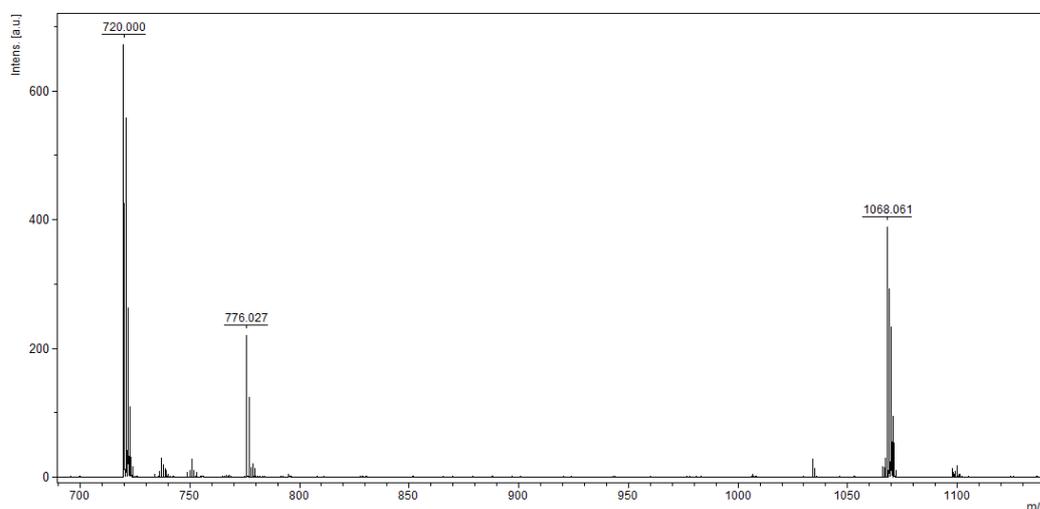


Synthesis of [60]fulleropyrrolidine–dithienylethene conjugates and DFT calculations of their photochromic properties

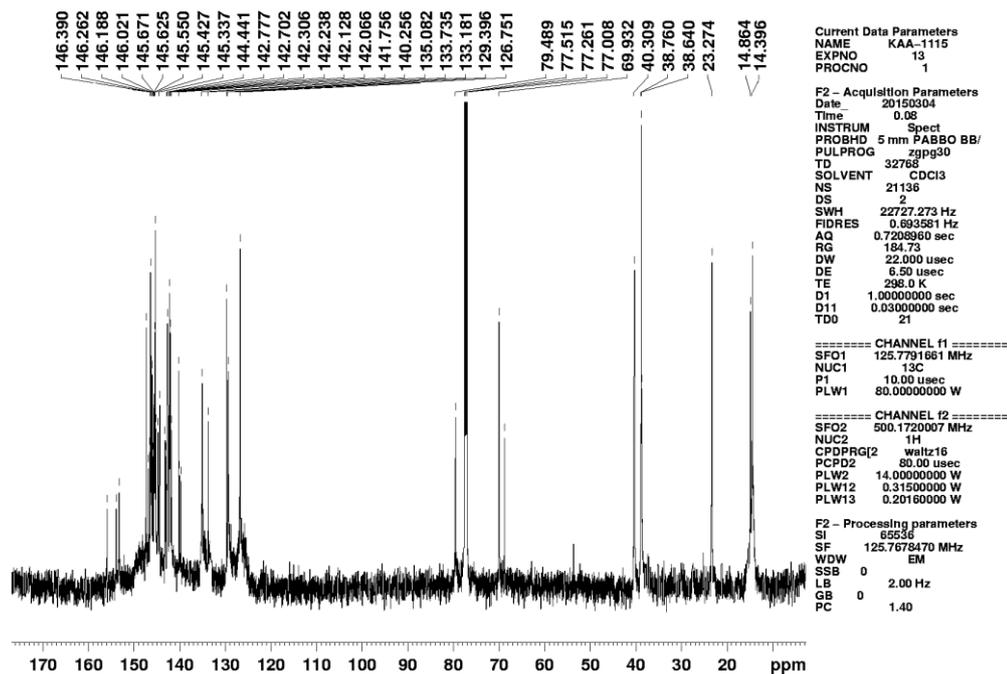
Airat R. Tuktarov, Artur A. Khuzin, Leonard M. Khalilov, Artur R. Tulyabaev, Arslan R. Akhmetov and Usein M. Dzhemilev

2-{4-[2-(5-Chloro-2-methylthiophen-3-yl)cyclopenten-1-yl]-5-methylthiophen-2-yl}-1-methyl-3,4-fulleropyrrolidine 2a

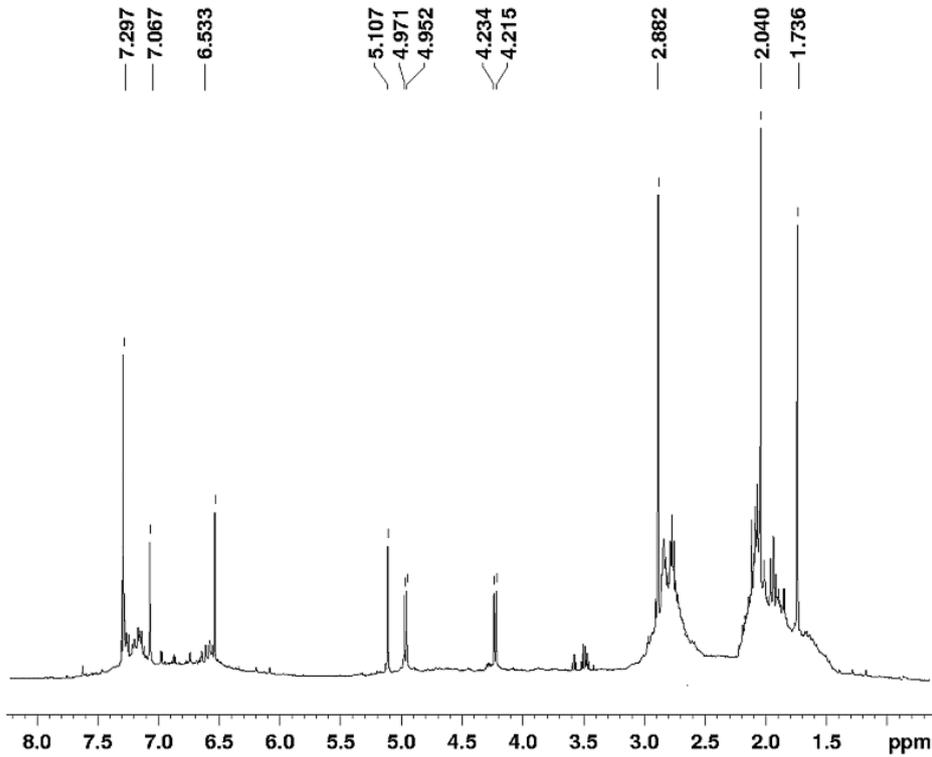
MS MALDI TOF/TOF



¹³C



¹H



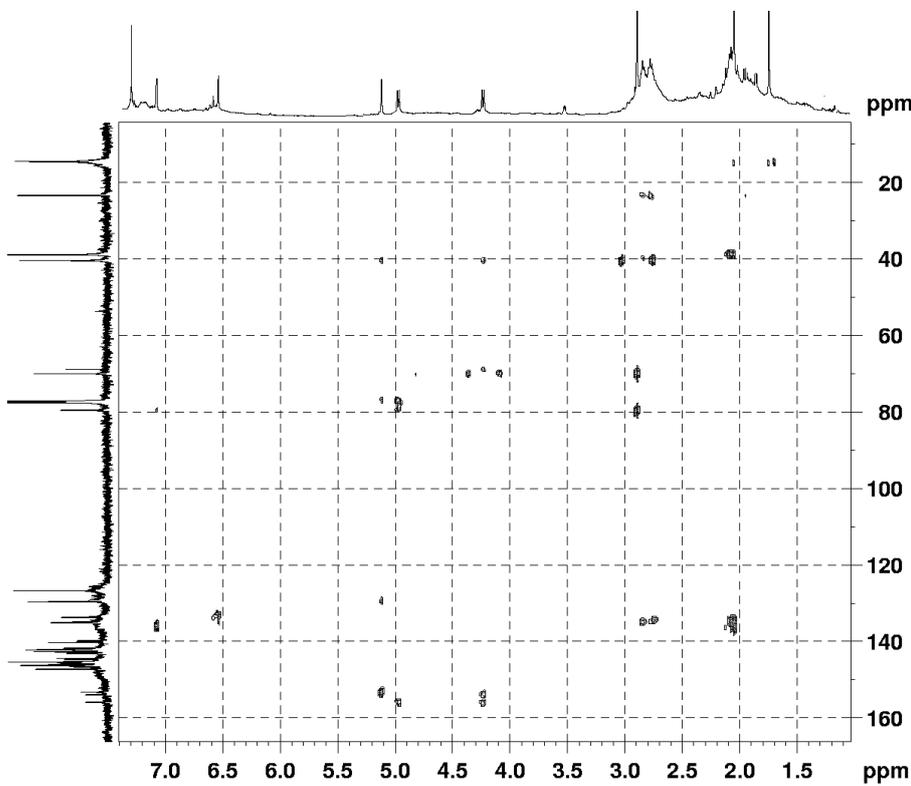
Current Data Parameters
NAME KAA-1115
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150521
Time 11.06
INSTRUM Spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192000 sec
RG 106.44
DW 50.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1740014 MHz
NUC1 1H
P1 12.00 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 500.1700000 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

HMBC



Current Data Parameters
NAME KAA-1115
EXPNO 107
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150303
Time 18.33
INSTRUM Spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 64
DS 16
SWH 4504.504 Hz
FIDRES 1.099733 Hz
AQ 0.454650 sec
RG 184.73
DW 111.000 usec
DE 6.50 usec
TE 298.0 K
CNST13 8.0000000
D0 0.0000300 sec
D1 1.5000000 sec
D6 0.0625000 sec
D16 0.0002000 sec
IN0 0.00001530 sec

===== CHANNEL f1 =====
SFO1 500.1722508 MHz
NUC1 1H
P1 12.00 usec
P2 24.00 usec
PLW1 15.00000000 W

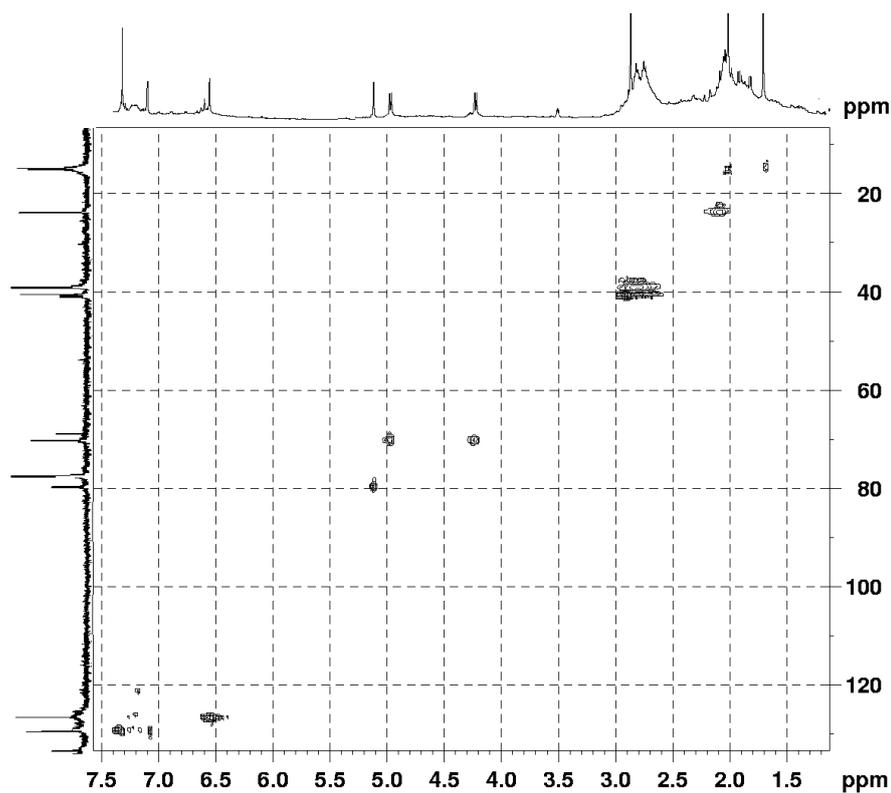
===== CHANNEL f2 =====
SFO2 125.7829387 MHz
NUC2 13C
P3 10.00 usec
PLW2 81.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 125.7829 MHz
FIDRES 246.676102 Hz
SW 250.006 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 500.1700000 MHz
WDW SINE
SSB 0 Hz
LB 0 Hz
GB 0
PC 1.40

HSQC



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Current Data Parameters
NAME      KAA-1115
EXPNO    106
PROCNO   1

F2 - Acquisition Parameters
Date_    20150303
Time     17.13
INSTRUM  Spec1
PROBHD   5 mm PABBO BB/
PULPROG  hsgcqdpph
TD       1024
SOLVENT  CDCl3
NS       32
DS       16
SWH      4504.504 Hz
FIDRES   4.398930 Hz
AQ       0.1136640 sec
RG       184.73
DW       111.000 usec
DE       6.50 usec
TE       298.0 K
CNST2    145.000000
D0       0.00000300 sec
D1       1.00000000 sec
D4       0.00172414 sec
D11      0.03000000 sec
D13      0.00004000 sec
D16      0.00020000 sec
D21      0.00344827 sec
IN0      0.00002480 sec

===== CHANNEL f1 =====
SFO1    500.1722508 MHz
NUC1     1H
P1      12.00 usec
P2      24.00 usec
PLW1    15.00000000 W

===== CHANNEL f2 =====
SFO2    125.7779080 MHz
NUC2     13C
CPDPRG2  garp
P3      10.00 usec
P4      20.00 usec
PCPD2    70.00 usec
PLW2    81.00000000 W
PLW12   1.65310001 W

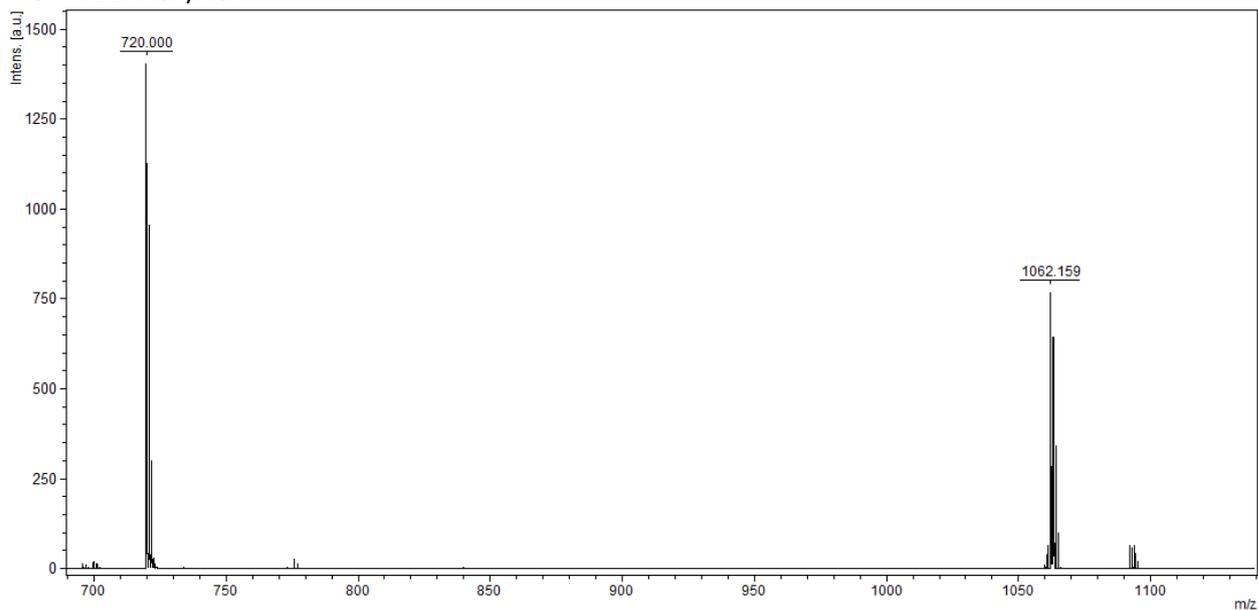
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1    30.00 %
GPZ2    80.00 %
GPZ3    20.10 %
P16     1000.00 usec

F1 - Acquisition parameters
TD      128
SFO1    125.7779 MHz
FIDRES   157.510086 Hz
SW      160.293 ppm
FnMODE   TPPI

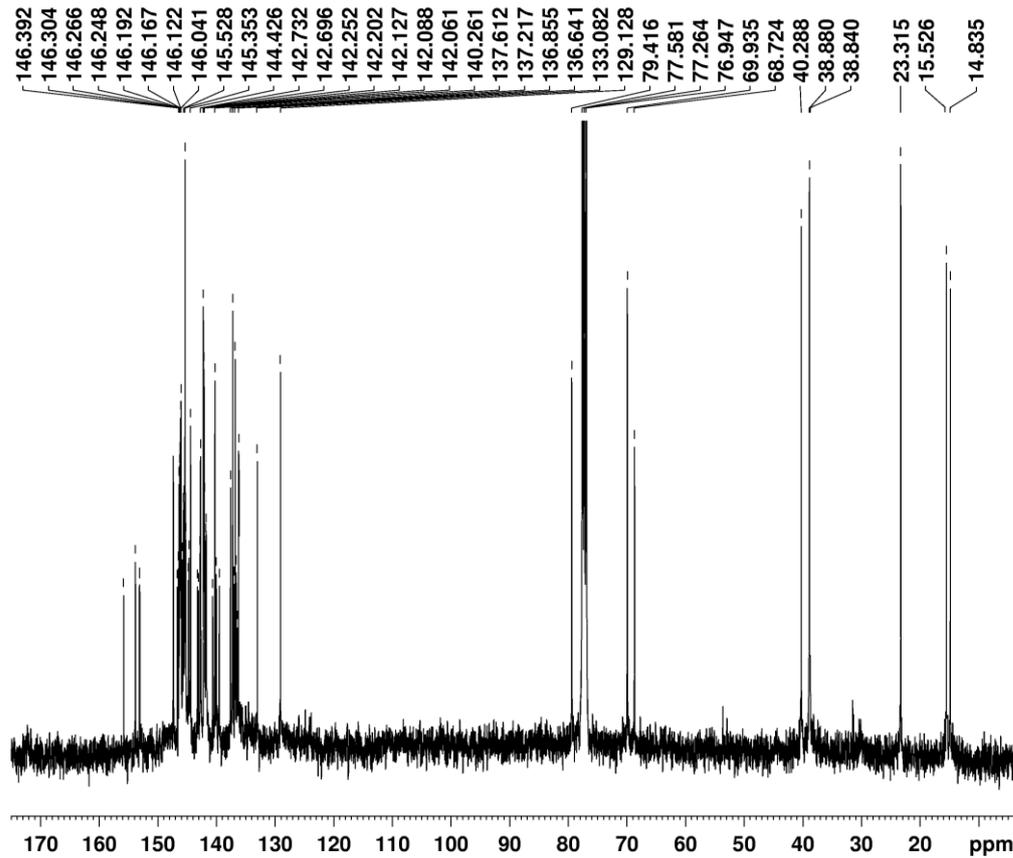
F2 - Processing parameters
    
```

2-{4-[2-(5-Formyl-2-methylthiopen-3-yl)cyclopent-1-yl]-5-methylthiophen-2-yl}-1-methyl-3,4-fulleropyrrolidine 2b

MS MALDI TOF/TOF



¹³C



Current Data Parameters
NAME KAA-942
EXPNO 5
PROCNO 1

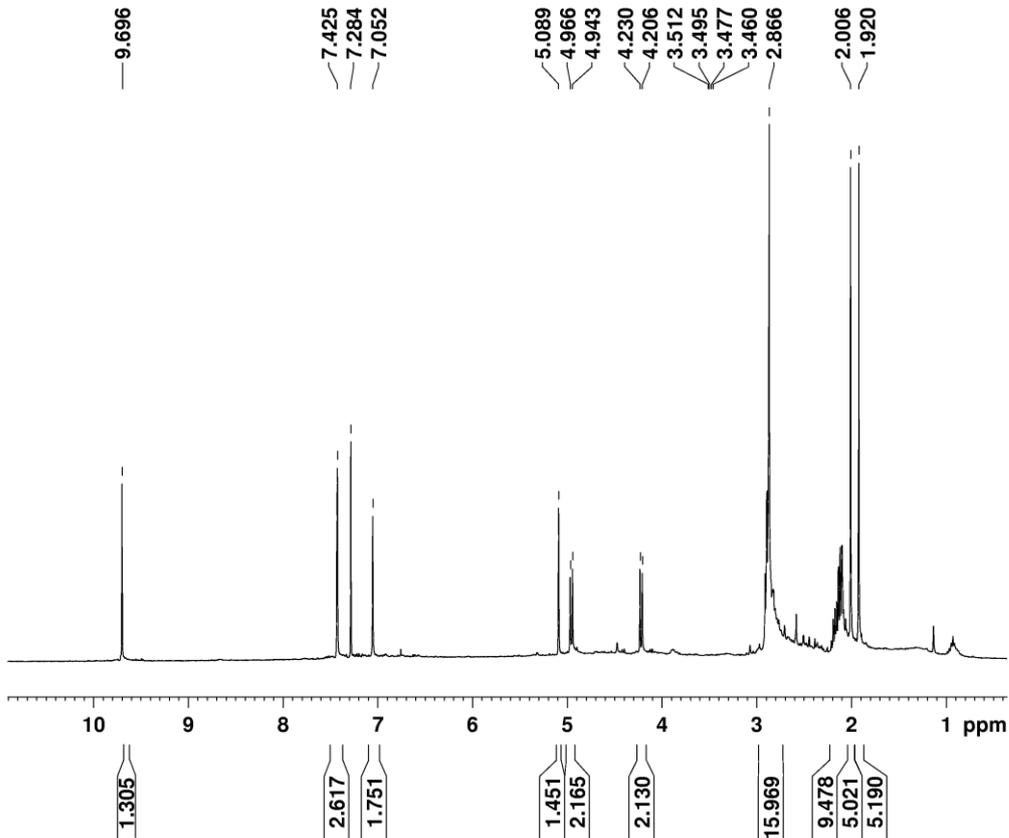
F2 - Acquisition Parameters
Date_ 20131106
Time 0.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 19623
DS 2
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 0.9043968 sec
RG 2050
DW 27.600 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 10

===== CHANNEL f1 =====
SFO1 100.6218241 MHz
NUC1 13C
P1 10.00 usec
PLW1 34.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 8.89999962 W
PLW12 0.24067000 W
PLW13 0.19495000 W

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

¹H



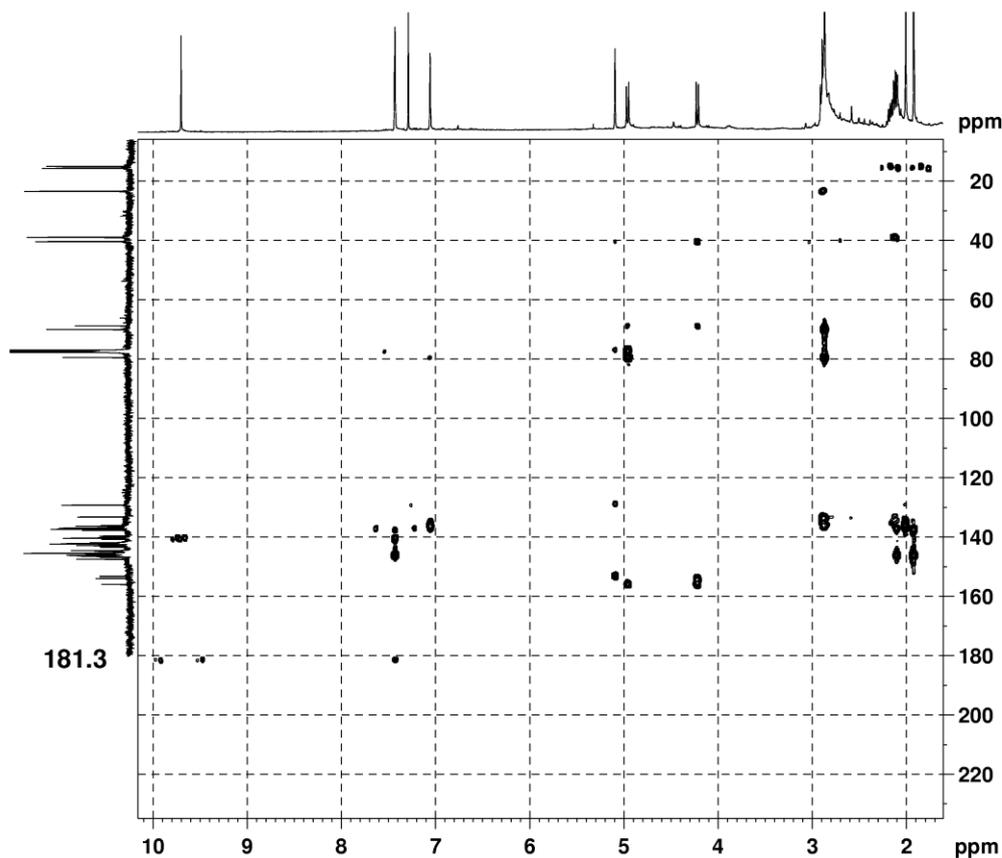
Current Data Parameters
NAME KAA-942
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131105
Time 18.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 228
DW 62.400 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1332010 MHz
NUC1 1H
P1 14.80 usec
PLW1 8.89999962 W

F2 - Processing parameters
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

HMBC



Current Data Parameters
 NAME KAA-942
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131105
 Time 19.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG hmbcgp1ndqf
 TD 1024
 SOLVENT CDCl3
 NS 64
 DS 16
 SWH 4401.409 Hz
 FIDRES 4.298251 Hz
 AQ 0.1163264 sec
 RG 2050
 DW 113.600 usec
 DE 6.50 usec
 TE 299.5 K
 CNST2 145.0000000
 CNST13 10.0000000
 D0 0.00000300 sec
 D1 0.85781398 sec
 D2 0.00344828 sec
 D6 0.05000000 sec
 D16 0.00020000 sec
 IN0 0.00001990 sec

===== CHANNEL f1 =====
 SFO1 400.1322007 MHz
 NUC1 1H
 P1 14.80 usec
 P2 29.60 usec
 PLW1 8.89999962 W

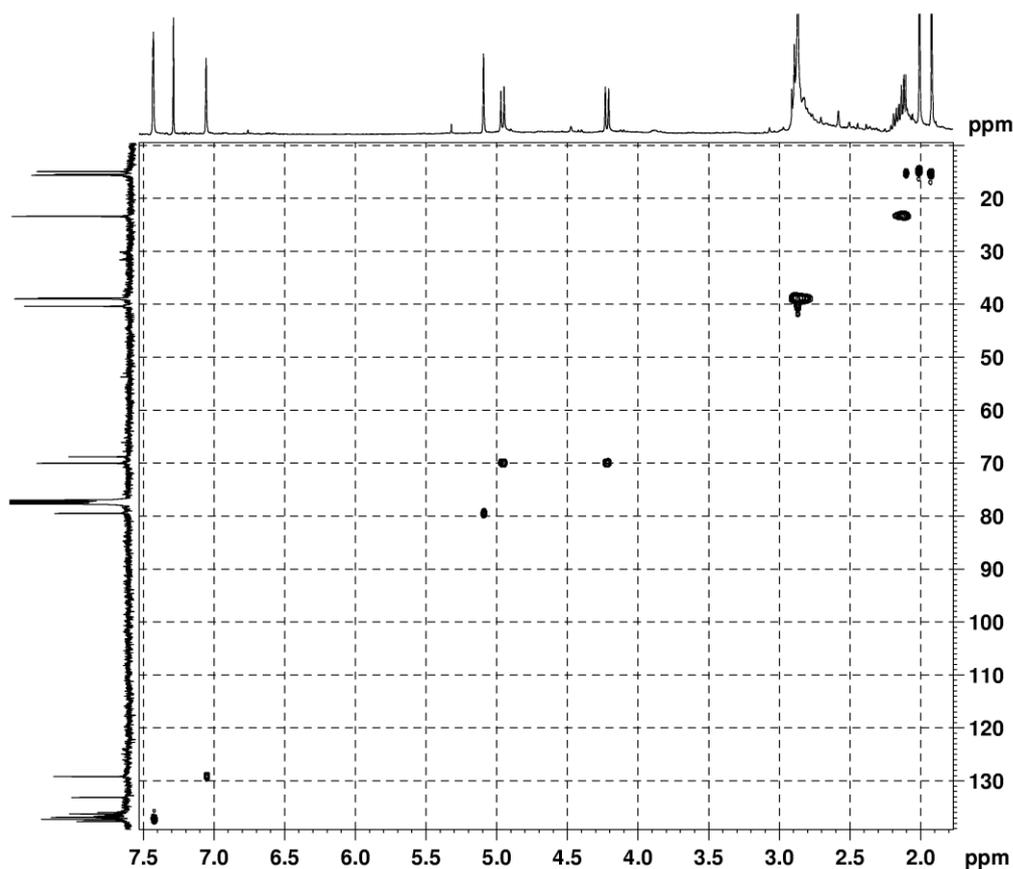
===== CHANNEL f2 =====
 SFO2 100.6248425 MHz
 NUC2 13C
 P3 10.00 usec
 PLW2 34.00000000 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SFO1 100.6248 MHz
 FIDRES 198.293976 Hz
 SW 249.696 ppm
 FnmODE QF

F2 - Processing parameters
 SI 2048
 SF 400.1300000 MHz
 WDW QSINE
 SSB 3

HSQC



Current Data Parameters
 NAME KAA-942
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131105
 Time 18.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG hsqcetgp
 TD 1024
 SOLVENT CDCl3
 NS 32
 DS 16
 SWH 4401.409 Hz
 FIDRES 4.298251 Hz
 AQ 0.1163264 sec
 RG 2050
 DW 113.600 usec
 DE 6.50 usec
 TE 298.8 K
 CNST2 140.0000000
 D0 0.00000300 sec
 D1 0.84000123 sec
 D4 0.00178571 sec
 D11 0.03000000 sec
 D16 0.00020000 sec
 IN0 0.00002760 sec
 ZGOPTNS

===== CHANNEL f1 =====
 SFO1 400.1322007 MHz
 NUC1 1H
 P1 14.80 usec
 P2 29.60 usec
 P28 1000.00 usec
 PLW1 8.89999962 W

===== CHANNEL f2 =====
 SFO2 100.6218241 MHz
 NUC2 13C
 CPDPRG[2] garp
 P3 10.00 usec
 P4 20.00 usec
 PCPD2 80.00 usec
 PLW2 34.00000000 W
 PLW12 0.53125000 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPZ1 80.00 %
 GPZ2 20.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SFO1 100.6218 MHz
 FIDRES 141.530792 Hz
 SW 180.040 ppm
 FnmODE Echo-Antiecho

F2 - Processing parameters
 SI 2048