Date Run: 10-05-2012 (Time Run: 10:01:56)

COMPOUND 3

Instrument: JEOL MSRoute

Inlet: Direct Probe

Ionization mode: EI+

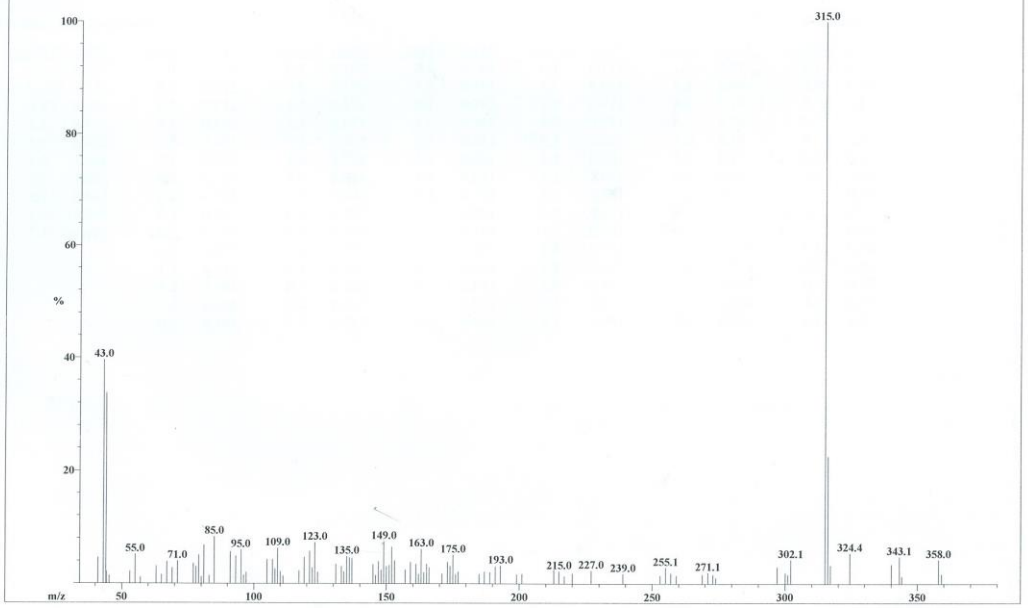
Run By: HEJ

Scan: 21

R.T.: 1.78

Base: m/z 315; 53.6%FS TIC: 2824128

#Ions: 100



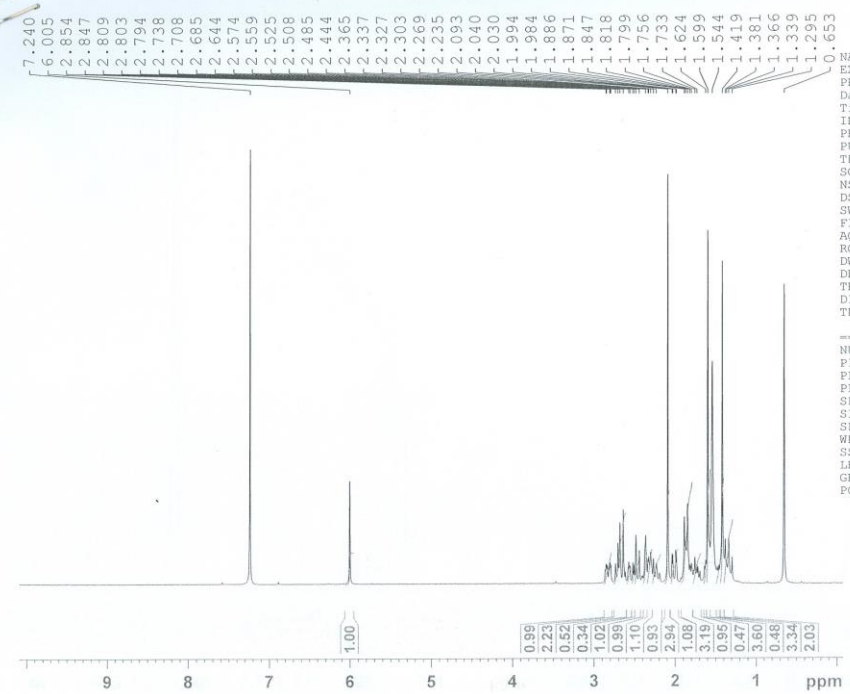
COMPOUND 3
HREI-MS

Mass	Relative Intensity	Theoretical Mass	Delta [mmu]	RDB	Composition
152.0781	1.7	152.0832	-5.1	4.0	$C_9 H_{12} O_2$
154.9920	3.3				
157.1015	1.7	157.1012	0.4	6.5	$C_{12} H_{13}$
159.0800	3.3	159.0804	-0.5	6.5	$C_{11} H_{11} O_1$
161.0945	2.1	161.0961	-1.6	5.5	$C_{11} H_{13} O_1$
161.9919	4.0	161.9948	-2.8	8.0	$C_8 H_2 O_4$
163.1141	1.2	163.1117	2.3	4.5	$C_{11} H_{15} O_1$
165.0721	1.2	165.0699	2.3	9.5	$C_{13} H_9$
165.0947	1.0	165.0910	3.6	4.5	$C_{10} H_{13} O_2$
168.9888	18.4	168.9920	-3.2	10.5	$C_{10} H_1 O_3$
173.0945	2.8	173.0961	-1.6	6.5	$C_{12} H_{13} O_1$
174.1065	6.1	174.1039	2.6	6.0	$C_{12} H_{14} O_1$
175.1076	4.2	175.1117	-4.1	5.5	$C_{12} H_{15} O_1$
176.1195	1.0	176.1196	-0.1	5.0	$C_{12} H_{16} O_1$
180.9888	21.7	180.9920	-3.2	11.5	$C_{11} H_1 O_3$
181.9897	1.1				
185.9926	1.6	185.9948	-2.2	10.0	$C_{10} H_2 O_4$
187.1140	1.9	187.1117	2.2	6.5	$C_{13} H_{15} O_1$
192.9888	5.7	192.9920	-3.2	12.5	$C_{12} H_1 O_3$
193.1212	2.2	193.1223	-1.1	4.5	$C_{12} H_{17} O_2$
199.1171	1.4	199.1117	5.3	7.5	$C_{14} H_{15} O_1$
204.9888	3.4	204.9920	-3.2	13.5	$C_{13} H_1 O_3$
211.1108	1.1	211.1117	-1.0	8.5	$C_{15} H_{15} O_1$
211.9924	1.3	211.9893	3.1	16.0	$C_{15} O_2$
213.1273	2.2	213.1274	-0.1	7.5	$C_{15} H_{17} O_1$
216.9896	1.4	216.9920	-2.4	14.5	$C_{14} H_1 O_3$
218.9856	6.8				
227.1451	1.2	227.1430	2.0	7.5	$C_{16} H_{19} O_1$
230.9856	10.8				
235.9866	1.2	235.9893	-2.7	18.0	$C_{17} O_2$
237.1296	1.2	237.1274	2.2	9.5	$C_{17} H_{17} O_1$
238.1432	1.1				
239.1415	1.6	239.1430	-1.6	8.5	$C_{17} H_{19} O_1$
242.9856	14.3				
243.9825	1.0	243.9791	3.4	16.0	$C_{15} O_4$
253.1642	1.9	253.1587	5.5	8.5	$C_{18} H_{21} O_1$
254.9856	3.5				
255.1405	1.9	255.1380	2.5	8.5	$C_{17} H_{19} O_2$
255.1686	1.7	255.1743	-5.7	7.5	$C_{18} H_{23} O_1$
266.9924	1.3				
268.9824	1.9	268.9869	-4.5	17.5	$C_{17} H_1 O_4$
269.1488	1.0	269.1536	-4.8	8.5	$C_{18} H_{21} O_2$
279.1740	1.4	279.1743	-0.4	9.5	$C_{20} H_{23} O_1$
280.9824	6.7	280.9869	-4.5	18.5	$C_{18} H_1 O_4$
292.9824	14.8	292.9869	-4.5	19.5	$C_{19} H_1 O_4$
296.1757	1.3	296.1771	-1.4	9.0	$C_{20} H_{24} O_2$
297.1898	1.6	297.1849	4.9	8.5	$C_{20} H_{25} O_2$
304.9824	2.2	304.9869	-4.5	20.5	$C_{20} H_1 O_4$
315.1971	16.2	315.1955	1.6	7.5	$C_{20} H_{27} O_3$
316.2055	3.8	316.2033	2.2	7.0	$C_{20} H_{28} O_3$
316.9834	1.3	316.9869	-3.5	21.5	$C_{21} H_1 O_4$
325.1941	1.4	325.1951	-1.0	13.5	$C_{25} H_{25}$
330.9792	4.1				
340.1995	8.3	340.2033	-3.8	9.0	$C_{22} H_{28} O_3$
341.2047	1.7				
342.9792	5.4				
343.1874	1.1	343.1904	-3.0	8.5	$C_{21} H_{27} O_4$
354.9792	1.5				
358.2115	1.3	358.2139	-2.4	8.0	$C_{22} H_{30} O_4$
380.9760	2.1				
392.9760	3.8				
404.9760	1.5				
442.9728	1.9				
492.9697	1.1				

COMPOUND 3

^{1}H

AVANCE AV - III
300 MHz, LAB # 116

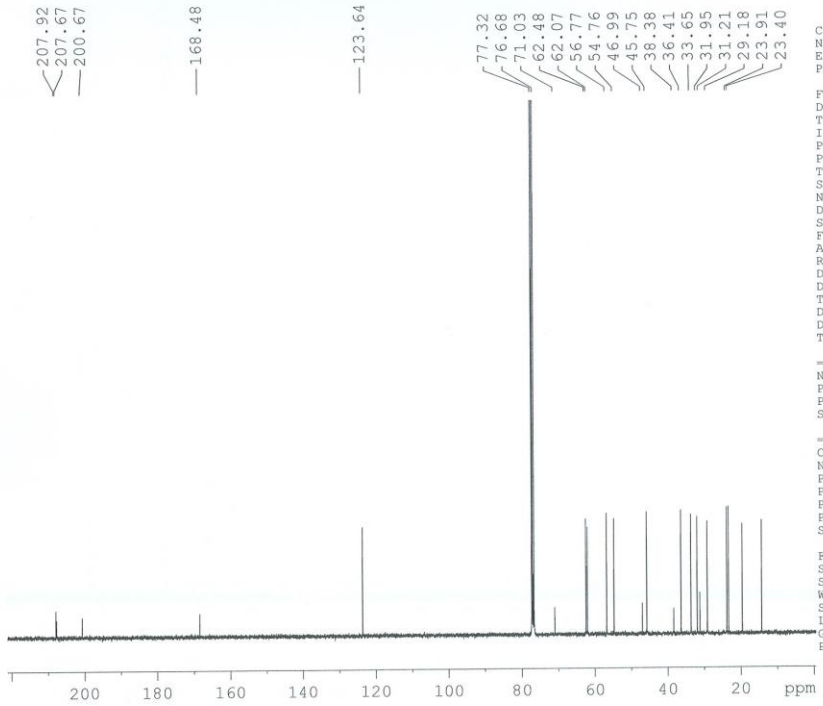



```
NAME                oct04
EXPNO                   1
PROCNO                  1
Date_            20121004
Time                11.36
INSTRUM             Spect
PROBHD    5 mm BBO BB-1H
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH             6188.119 Hz
FIDRES          0.188846 Hz
AQ            2.6477044 sec
RG                    203
DW                 80.800 usec
DE                   6.50 usec
TE                  300.0 K
D1             1.50000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  12.50 usec
PL1                  0.00 dB
PL1W        13.16228485 W
SFO1        300.1321009 MHz
SI                  16384
SF          300.1300118 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.00
```

COMPOUND 3

BB

AVANCE - III AV 400 MHz (A)
LAB # 109

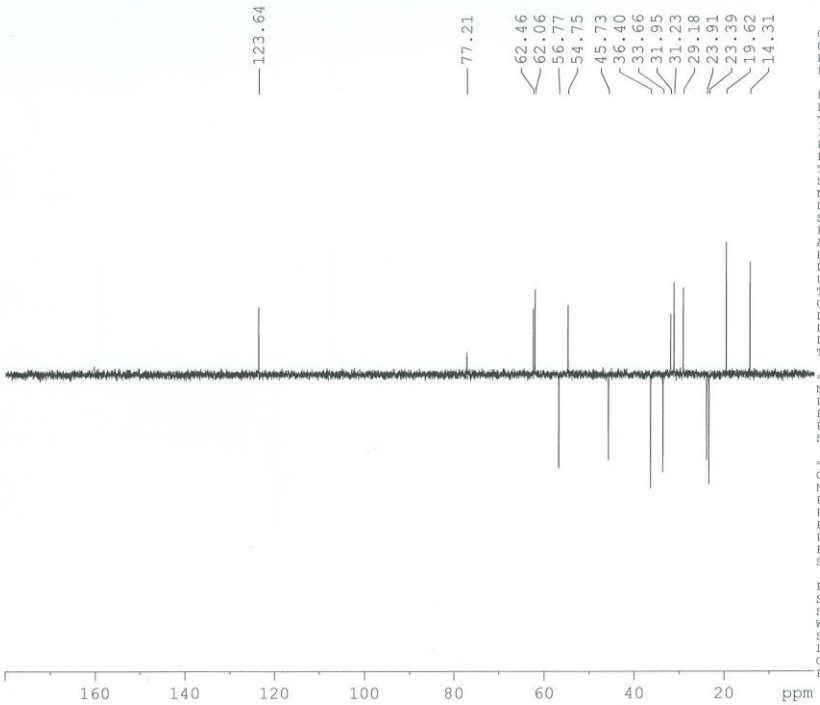



```
Current Data Parameters
NAME             oct-06-12
EXPNO                    6
PROCNO                   1

F2 - Acquisition Parameters
Date_            20121007
Time                17.06
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg
TD                  32768
SOLVENT             CDCl3
NS                  20480
DS                      4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ             0.6816244 sec
RG                 196.51
DW                 20.800 usec
DE                   6.50 usec
TE                  302.6 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0                    20

======== CHANNEL f1 ========
NUC1                  13C
P1                  10.20 usec
PLW1        70.00000000 W
SFO1       100.6494874 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2               90.00 usec
PLW2        17.00000000 W
PLW12        0.19746999 W
PLW13        0.15995000 W
SFO2       400.2316009 MHz

F2 - Processing parameters
SI                  32768
SF         100.6379133 MHz
WDW                    EM
SSB      0
LB                   1.00 Hz
GB       0
PC                   1.40
```

COMPOUND 3

DEPT 135

AVANCE - III AV 400 MHz (A)
LAB # 109

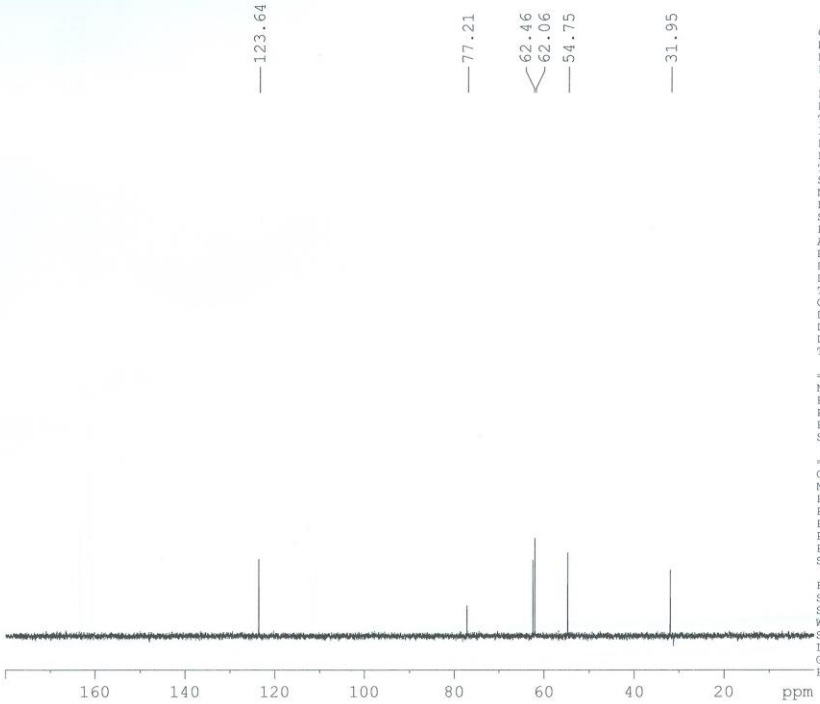



```
Current Data Parameters
NAME              oct-06-12
EXPNO                     7
PROCNO                    1

F2 - Acquisition Parameters
Date_             20121008
Time                  5.56
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            dept135
TD                    32768
SOLVENT               CDCl3
NS                     4345
DS                        8
SWH              18115.941 Hz
FIDRES            0.552855 Hz
AQ               0.9044468 sec
RG                   196.51
DW                  27.600 usec
DE                    6.50 usec
TE                   302.1 K
CNST2           145.0000000
D1               1.50000000 sec
D2               0.00344828 sec
D12              0.00002000 sec
TD0                      10

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.20 usec
P2                     20.40 usec
PLW1            70.00000000 W
SFO1            100.6469714 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
P3                      9.70 usec
P4                     19.40 usec
PCPD2                  90.00 usec
PLW2            17.00000000 W
PLW12            0.19746999 W
SFO2            400.2312800 MHz

F2 - Processing parameters
SI                      16384
SF               100.6379133 MHz
WDW                        EM
SSB        0
LB                      1.00 Hz
GB         0
PC                      1.40
```

COMPOUND 3

DEPT 90

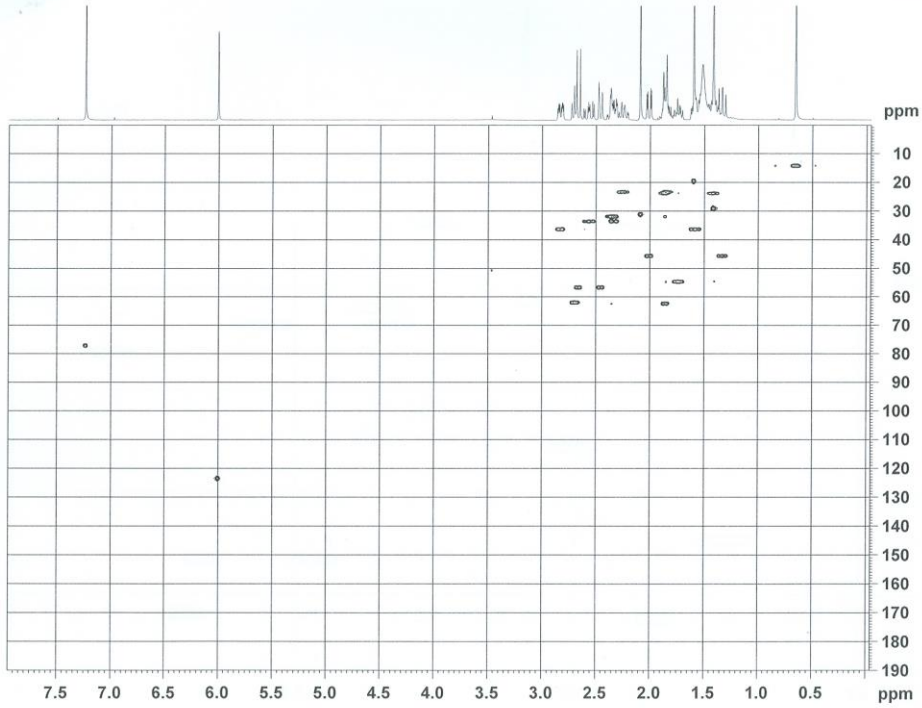
AVANCE - III AV 400 MHz (A)
LAB # 109




```
Current Data Parameters
NAME              oct-06-12
EXPNO                     8
PROCNO                    1

F2 - Acquisition Parameters
Date_             20121008
Time                  8.54
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             dept90
TD                    32768
SOLVENT               CDCl3
NS                     4096
DS                        4
SWH              18115.941 Hz
FIDRES            0.552855 Hz
AQ               0.9044468 sec
RG                   196.51
DW                  27.600 usec
DE                    6.50 usec
TE                   301.8 K
CNST2           145.0000000
D1               1.50000000 sec
D2               0.00344828 sec
D12              0.00002000 sec
TD0                       4

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.20 usec
P2                     20.40 usec
PLW1            70.00000000 W
SFO1            100.6469714 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
P3                      9.70 usec
P4                     19.40 usec
PCPD2                  90.00 usec
PLW2            17.00000000 W
PLW12            0.19746999 W
SFO2            400.2312800 MHz

F2 - Processing parameters
SI                      16384
SF               100.6379133 MHz
WDW                        EM
SSB        0
LB                      1.00 Hz
GB         0
PC                      1.40
```

COMPOUND 3
HSQC

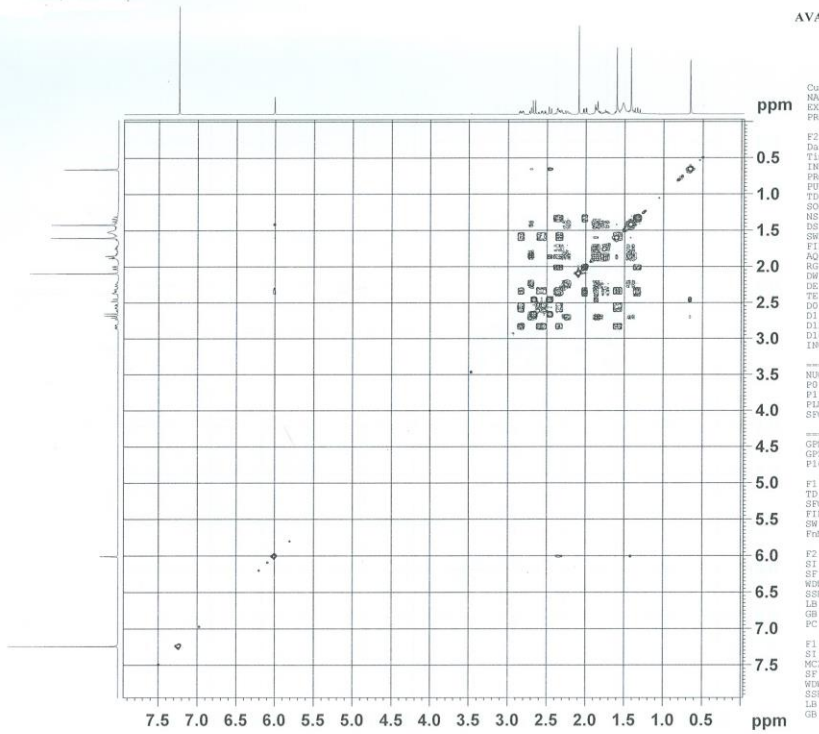
AVANCE - III AV 400 MHz (A)
LAB # 109




```
Current Data Parameters
NAME                 oct-06-12
EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_              20121006
Time                    21.58
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG          hsqcetgpsi
TD                        1024
SOLVENT                   CDCl3
NS                           64
DS                           16
SWH                   3201.024 Hz
FIDRES                3.126000 Hz
AQ                    0.1599988 sec
RG                       196.51
DW                      156.200 usec
DE                        6.50 usec
TE                       301.7 K
CNST2              145.0000000
D0                  0.00000300 sec
D1                  1.50000000 sec
D4                  0.00172414 sec
D11                 0.03000000 sec
D16                 0.00020000 sec
D24                 0.00110000 sec
IN0                 0.00002615 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                         1H
P1                         9.70 usec
P2                        19.40 usec
P28                        1.00 usec
PLW1               17.00000000 W
SFO1              400.2316009 MHz

======== CHANNEL f2 ========
CPDPRG2                   garp
NUC2                         13C
P3                        10.20 usec
P4                        20.40 usec
PCPD2                     80.00 usec
PLW2               70.000000000 W
PLW12               1.13789999 W
SFO2              100.6474746 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SMSQ10.100
GPNAM2             SMSQ10.100
GPZ1                    80.00 %
GPZ2                    20.10 %
P16                   1000.00 usec

F1 - Acquisition parameters
TD                          256
SFO1                  100.6475 MHz
FIDRES               74.697769 Hz
SW                     189.996 ppm
FnMODE          Echo-Antiecho

F2 - Processing parameters
SI                         1024
SF                 400.2300198 MHz
WDW                       QSINE
SSB                           2
LB          0 Hz
GB          0
PC                         1.00

F1 - Processing parameters
SI                         1024
MC2              echo-antiecho
SF                 100.6379133 MHz
WDW
SSB                           2
LB          0 Hz
GB          0
```

COMPOUND 3
COSY

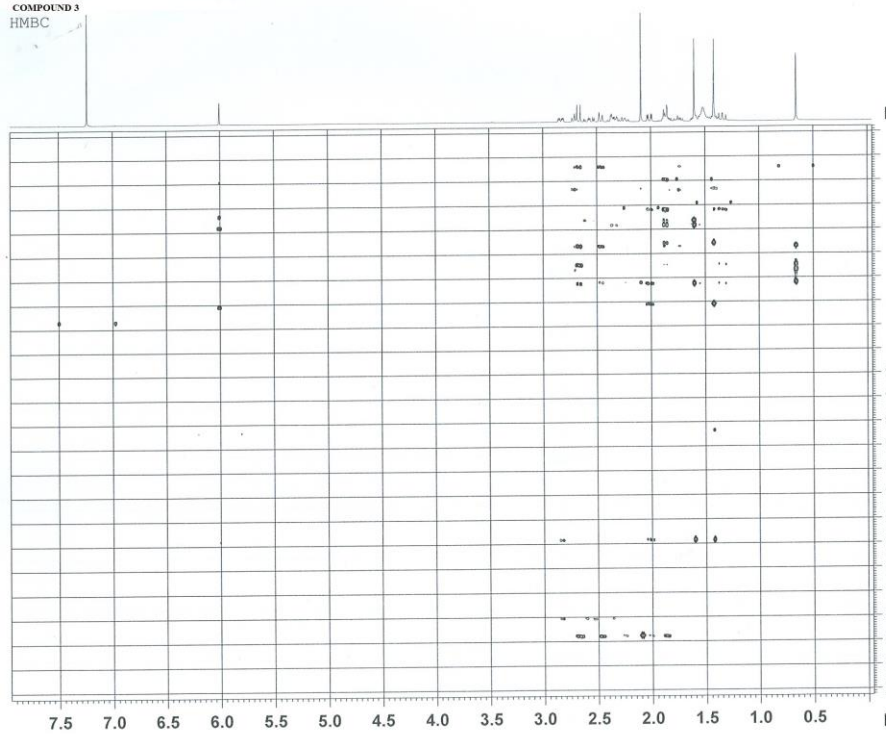
AVANCE - III AV 400 MHz (A)
LAB # 109




```
Current Data Parameters
NAME                 oct-06-12
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20121006
Time                    11.39
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG            cosygpqf
TD                        2048
SOLVENT                   CDCl3
NS                           32
DS                            8
SWH                   3201.024 Hz
FIDRES                1.563000 Hz
AQ                    0.3199476 sec
RG                       196.51
DW                      156.200 usec
DE                        6.50 usec
TE                       301.8 K
D0                  0.00000300 sec
D1                  1.50000000 sec
D13                 0.00000400 sec
D16                 0.00020000 sec
IN0                 0.00031240 sec

======== CHANNEL f1 ========
NUC1                         1H
P0                         9.70 usec
P1                         9.70 usec
PLW1               17.00000000 W
SFO1              400.2316009 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SMSQ10.100
GPZ1                    10.00 %
P16                   1000.00 usec

F1 - Acquisition parameters
TD                          256
SFO1                  400.2316 MHz
FIDRES               12.504000 Hz
SW                       7.998 ppm
FnMODE                      QF

F2 - Processing parameters
SI                         1024
SF                 400.2300198 MHz
WDW                       QSINE
SSB          0
LB          0 Hz
GB          0
PC                         1.00

F1 - Processing parameters
SI                         1024
MC2                          QF
SF                 400.2300198 MHz
WDW                States-TPPI
SSB          0
LB          0 Hz
GB          0
```

COMPOUND 3
HMBC

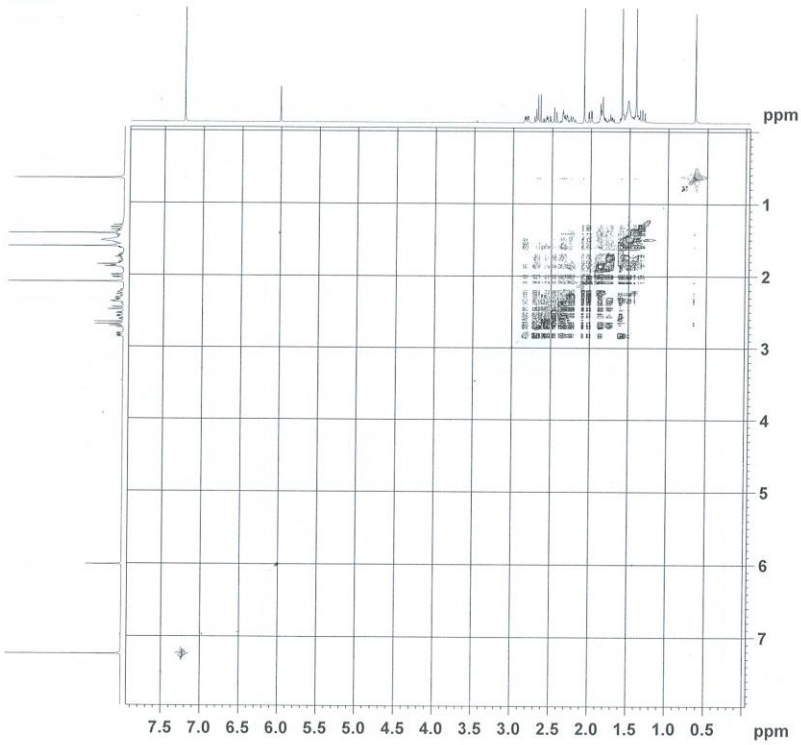
AVANCE - III AV 400 MHz (A)
LAB # 109




```
Current Data Parameters
NAME                oct-06-12
EXPNO                       5
PROCNO                      1

F2 - Acquisition Parameters
Date_              20121007
Time                    5.38
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG     hmbcgplpndqf
TD                      2048
SOLVENT                CDCl3
NS                         64
DS                         16
SWH                  3201.024 Hz
FIDRES               1.563000 Hz
AQ                  0.3199476 sec
RG                     196.51
DW                    156.200 usec
DE                      6.50 usec
TE                     302.2 K
CNST2             145.0000000
CNST13             10.0000000
D0                 0.00000300 sec
D1                 2.00000000 sec
D2                 0.00344828 sec
D6                 0.05000000 sec
D16                0.00020000 sec
IN0                0.00002115 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       9.70 usec
P2                      19.40 usec
PLW1              17.00000000 W
SFO1              400.2316009 MHz

======== CHANNEL f2 ========
NUC2                       13C
P3                      10.20 usec
PLW2              70.00000000 W
SFO2              100.6494874 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SMSQ10.100
GPNAM2             SMSQ10.100
GPNAM3             SMSQ10.100
GPZ1                    50.00 %
GPZ2                    30.00 %
GPZ3                    40.10 %
P16                   1000.00 usec

F1 - Acquisition parameters
TD                         256
SFO1                 100.6495 MHz
FIDRES              92.391670 Hz
SW                     234.996 ppm
FnMODE                     QF

F2 - Processing parameters
SI                        2048
SF                 400.2300198 MHz
WDW                       SINE
SSB          0
LB           0 Hz
GB           0
PC                        1.00

F1 - Processing parameters
SI                        1024
MC2                         QF
SF                 100.6379133 MHz
WDW                       States
SSB          0
LB           0 Hz
GB           0
```

COMPOUND 3
NOESY

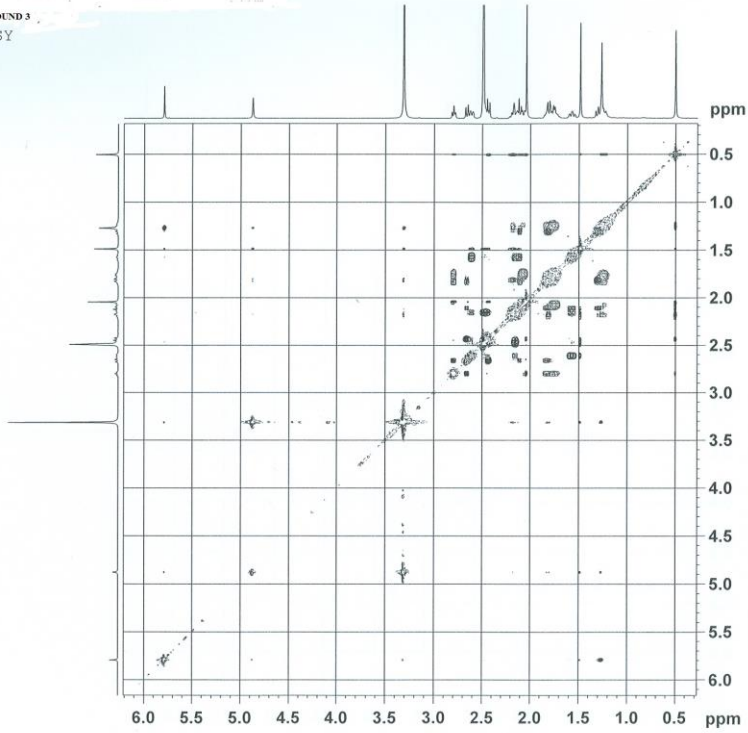
AVANCE - III AV 400 MHz (A)
LAB # 109




```
Current Data Parameters
NAME                oct-06-12
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_              20121006
Time                   15.56
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             noesygpph
TD                      2048
SOLVENT                CDCl3
NS                         32
DS                         32
SWH                  3201.024 Hz
FIDRES               1.563000 Hz
AQ                  0.3199476 sec
RG                     112.56
DW                    156.200 usec
DE                      6.50 usec
TE                     301.9 K
D0                 0.00014385 sec
D1                 1.50000000 sec
D8                 0.80000001 sec
D16                0.00020000 sec
IN0                0.00031240 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       9.70 usec
P2                      19.40 usec
PLW1              17.00000000 W
SFO1              400.2316009 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPZ1                    40.00 %
P16                   1000.00 usec

F1 - Acquisition parameters
TD                         256
SFO1                 400.2316 MHz
FIDRES              12.504000 Hz
SW                      7.998 ppm
FnMODE             States-TPPI

F2 - Processing parameters
SI                        1024
SF                 400.2300198 MHz
WDW                      QSINE
SSB                         2
LB           0 Hz
GB           0
PC                        1.00

F1 - Processing parameters
SI                        1024
MC2                States-TPPI
SF                 400.2300198 MHz
WDW
SSB                         2
LB           0 Hz
GB           0
```

COMPOUND 3

NOESY



AVANCE AV-500
LAB NO: 109B

NAME	feb24-15
EXPNO	12
PROCNO	1
Date_	20150224
Time	15.59
INSTRUM	spect
PROBHD	5 mm BBI 1H/D-
PULPROG	noesygpph
TD	2048
SOLVENT	DMSO
NS	16
DS	2
SWH	3255.208 Hz
FIDRES	1.589457 Hz
AQ	0.3147764 sec
RG	512
DW	153.600 usec
DE	6.50 usec
TE	298.5 K
D0	0.00014341 sec
D1	2.00000000 sec
D8	0.80000001 sec
D16	0.00020000 sec
IN0	0.00030720 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	8.00 usec
P2	16.00 usec
PL1	-1.00 dB
SFO1	500.1316004 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPZ1	40.00 %
P16	1000.00 usec
ND0	1
TD	256
SFO1	500.1316 MHz
FIDRES	12.715656 Hz
SW	6.509 ppm
FnMODE	States-TPPI
SI	1024
SF	500.1300106 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	4.00
SI	1024
MC2	States-TPPI
SF	500.1300106 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0