Date Run: 11-10-2012 (Time Run: 09:52:18)

COMPOUND 2

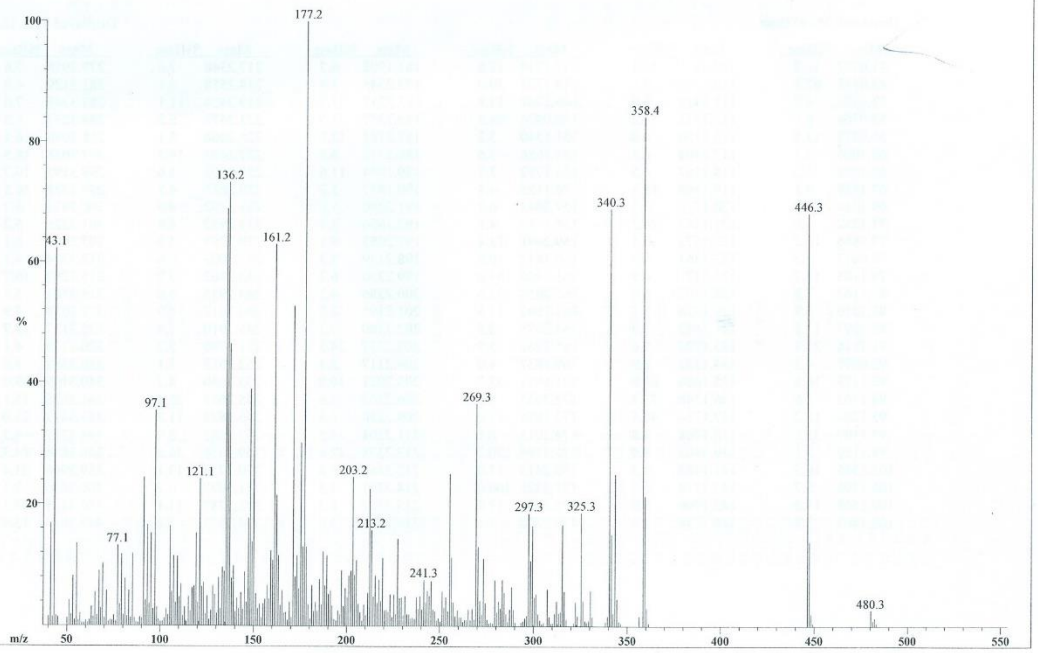
Instrument: JEOL MSRoute
Inlet: My Inlet

Ionization mode: EI+

Scan: 7
Base: m/z 177; 54.4%FS TIC: 13337782

R.T.: .53

#Ions: 310

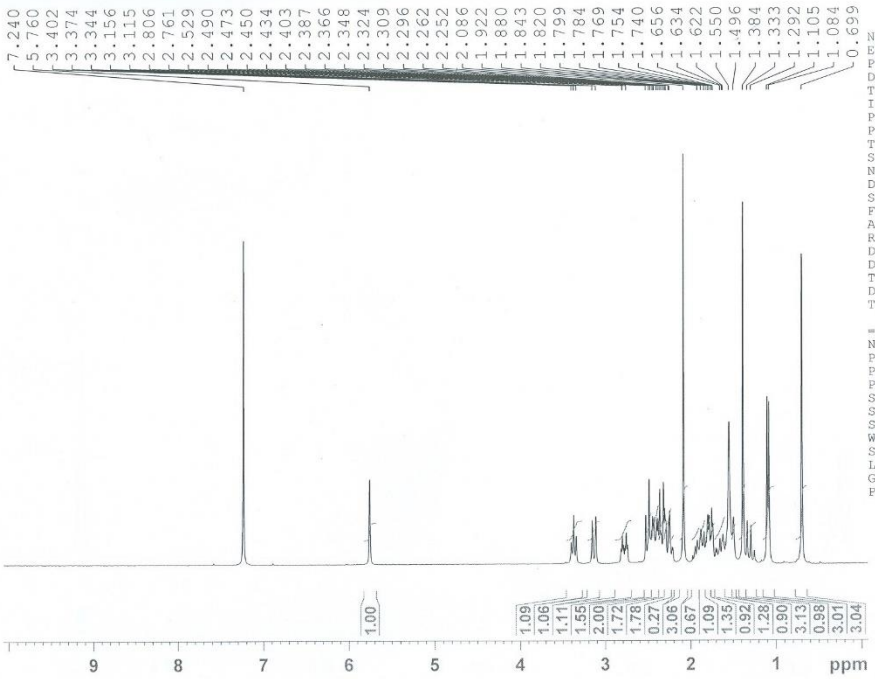


COMPOUND-2
HREI-MS

Mass	Relative Intensity	Theoretical Mass	Delta [mmu]	RDB	Composition
255.1710	2.8	255.1743	-3.3	7.5	$C_{18} H_{23} O_1$
255.2250	3.3				
256.1263	1.6	256.1247	1.6	13.0	$C_{20} H_{16}$
256.1642	1.5	256.1669	-2.8	3.0	$C_{14} H_{24} O_4$
256.2220	10.2	256.2186	3.4	6.0	$C_{19} H_{28}$
257.2119	3.4	257.2111	0.8	1.5	$C_{15} H_{29} O_3$
260.1710	1.2				
262.1231	2.2	262.1200	3.1	7.0	$C_{15} H_{18} O_4$
264.0250	1.1	264.0206	4.4	18.0	$C_{19} H_4 O_2$
264.1125	5.4	264.1145	-2.0	11.0	$C_{18} H_{16} O_2$
265.1064	2.0	265.1012	5.3	15.5	$C_{21} H_{13}$
267.1076	1.3				
268.9824	4.7	268.9869	-4.5	17.5	$C_{17} H_1 O_4$
270.0010	2.8				
271.0074	1.2	271.0026	4.8	16.5	$C_{17} H_3 O_4$
273.0327	1.6	273.0335	-0.8	19.5	$C_{21} H_5 O_1$
279.1469	2.5				
280.9824	2.9	280.9869	-4.5	18.5	$C_{18} H_1 O_4$
281.1646	1.5				
282.1629	1.5	282.1614	1.5	9.0	$C_{19} H_{22} O_2$
283.1731	1.7	283.1693	3.9	8.5	$C_{19} H_{23} O_2$
284.2822	6.1				
285.2877	2.4				
292.9824	7.0	292.9869	-4.5	19.5	$C_{19} H_1 O_4$
297.1860	3.7	297.1849	1.1	8.5	$C_{20} H_{25} O_2$
297.2738	2.0	297.2788	-5.0	1.5	$C_{19} H_{37} O_2$
298.1955	2.5	298.1927	2.8	8.0	$C_{20} H_{26} O_2$
299.1965	1.6	299.2006	-4.1	7.5	$C_{20} H_{27} O_2$
304.9824	1.3	304.9869	-4.5	20.5	$C_{20} H_1 O_4$
307.1650	2.2	307.1693	-4.3	10.5	$C_{21} H_{23} O_2$
311.2221	1.5	311.2217	0.4	3.5	$C_{18} H_{31} O_4$
312.2060	1.2	312.2084	-2.4	8.0	$C_{21} H_{28} O_2$
313.2715	3.7	313.2737	-2.2	1.5	$C_{19} H_{37} O_3$
315.1980	1.0	315.1955	2.5	7.5	$C_{20} H_{27} O_3$
322.1974	1.1	322.1927	4.7	10.0	$C_{22} H_{26} O_2$
325.1805	3.9	325.1798	0.7	9.5	$C_{21} H_{25} O_3$
330.9792	2.0				
339.2643	2.0	339.2682	-3.9	7.5	$C_{24} H_{35} O_1$
340.2055	11.6	340.2033	2.2	9.0	$C_{22} H_{28} O_3$
341.2092	3.0	341.2111	-1.9	8.5	$C_{22} H_{29} O_3$
342.9792	2.3				
343.1983	2.0				
356.1931	1.1	356.1982	-5.1	9.0	$C_{22} H_{28} O_4$
358.2126	4.8	358.2139	-1.3	8.0	$C_{22} H_{30} O_4$
367.2746	3.1				
368.3366	3.1				
369.3414	1.1	369.3363	5.1	1.5	$C_{23} H_{45} O_3$
380.9760	1.1				
392.9760	2.5				
393.2989	1.3	393.2999	-1.0	4.5	$C_{24} H_{41} O_4$
423.3491	1.2	423.3469	2.2	3.5	$C_{26} H_{47} O_4$
430.9729	1.0				
551.5206	2.7	551.5186	2.0	6.5	$C_{39} H_{67} O_1$
576.5173	1.4				
577.5380	2.0	577.5343	3.7	7.5	$C_{41} H_{69} O_1$

COMPOUND 2
1H-NMR

AVANCE AV - III
300 MHz, LAB # 116

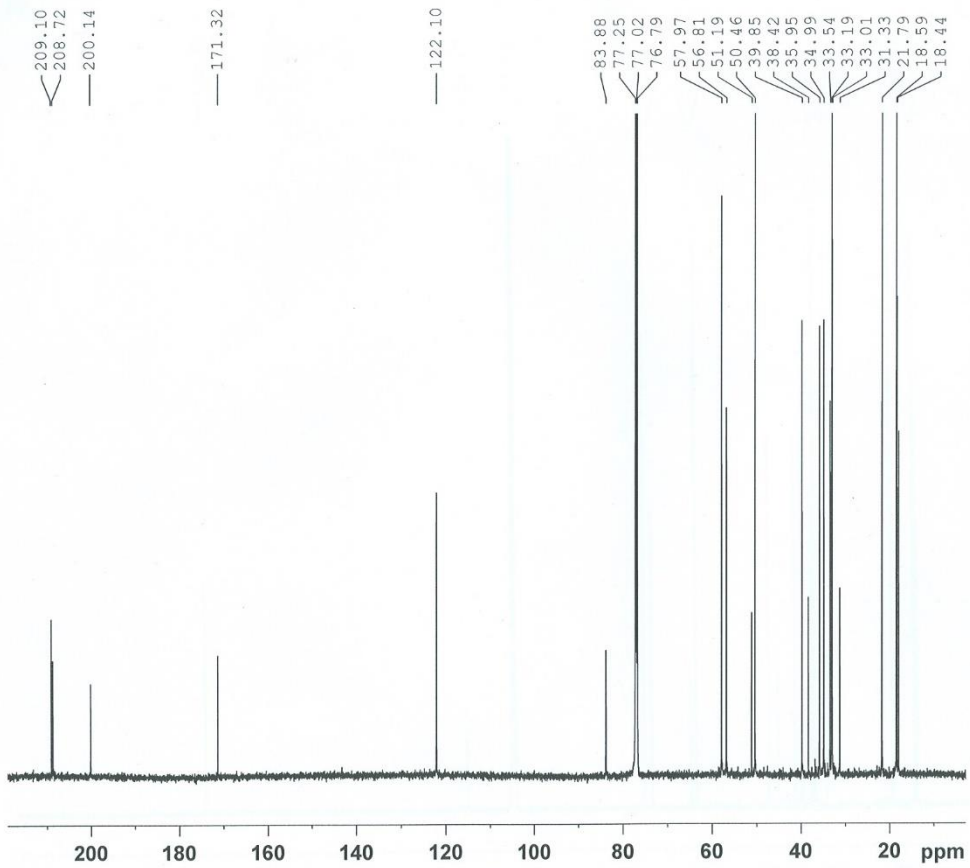


NAME	Nov07	
EXPNO	3	
PROCNO	1	
Date_	20121107	
Time	10.41	
INSTRUM	Spect	
PROBHD	5 mm BBO BB-1H	
PULPROG	zg30	
TD	32768	
SOLVENT	CDCl3	
NS	32	
DS	0	
SWH	6188.119	Hz
FIDRES	0.188846	Hz
AQ	2.6477044	sec
RG	203	
DW	80.800	usec
DE	6.50	usec
TE	300.0	K
D1	1.50000000	sec
TD0	1	
======== CHANNEL f1 ========		
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	

H.E.J. Research Institute of Chemistry.

COMPOUND 2

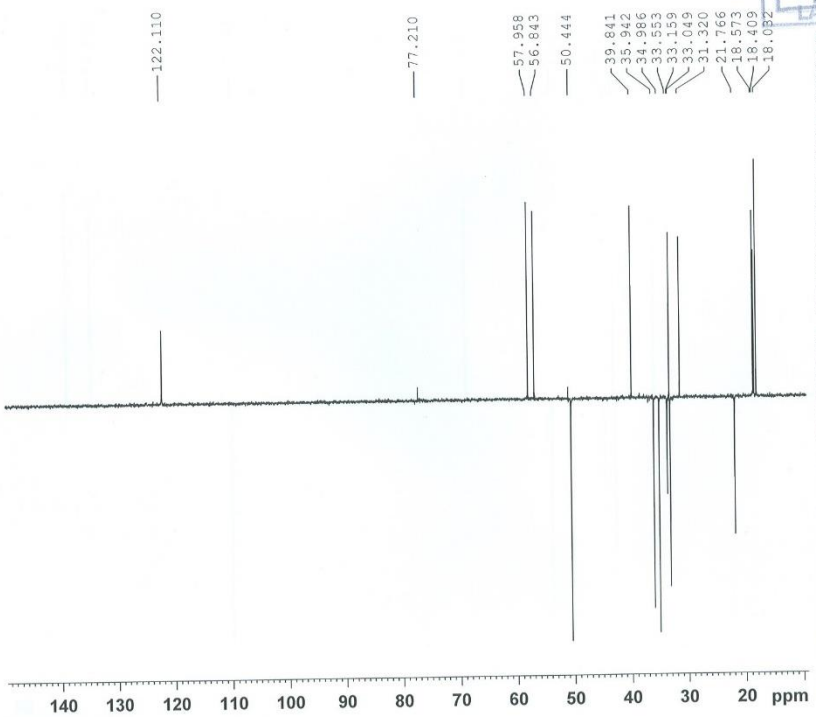
BB




```
NAME            oct09-15
EXPNO                   8
PROCNO                  1
Date_            20151009
Time               15.48
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG             zgpg
TD                  32768
SOLVENT             CDCl3
NS                  12288
DS                      4
SWH            35971.223 Hz
FIDRES          1.097755 Hz
AQ             0.4555391 sec
RG                  32768
DW                 13.900 usec
DE                   6.50 usec
TE                  298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    12

======== CHANNEL f1 ========
NUC1                  13C
P1                  12.70 usec
PL1                 -1.81 dB
PL1W          81.92915344 W
SFO1         150.8950149 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  3.31 dB
PL12                23.31 dB
PL13                22.50 dB
PL2W          6.79873323 W
PL12W         0.06798734 W
PL13W         0.08192718 W
SFO2         600.0336002 MHz
SI                 16384
SF           150.8776659 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.00
```

COMPOUND 2

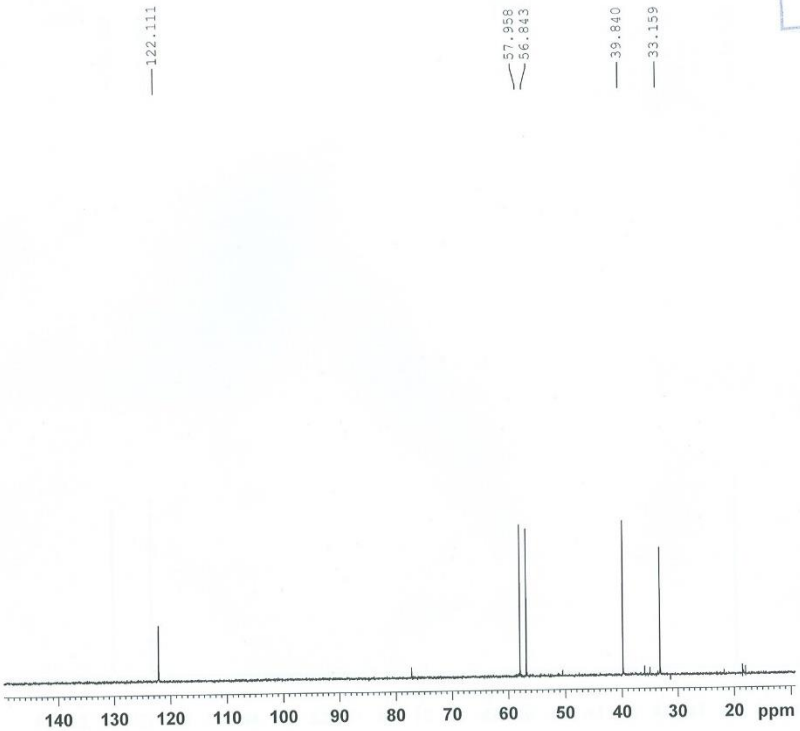
dept135



NAME	oct09-15
EXPNO	9
PROCNO	1
Date_	20151010
Time	0.17
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	deptsp135
TD	32768
SOLVENT	CDCl3
NS	6144
DS	2
SWH	30303.031 Hz
FIDRES	0.924775 Hz
AQ	0.5407385 sec
RG	32768
DW	16.500 usec
DE	6.50 usec
TE	298.0 K
CNST2	145.0000000
D1	1.50000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	6
======== CHANNEL f1 ========	
NUC1	13C
P1	12.70 usec
P12	2000.00 usec
PL0	120.00 dB
PL1	-1.81 dB
PL0W	0.00000000 W
PL1W	81.92915344 W
SFO1	150.8927518 MHz
SP2	4.19 dB
SPNAM2	Crp60comp.4
SPOAL2	0.500
SPOFFS2	0.00 Hz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
P3	8.00 usec
P4	16.00 usec
PCPD2	80.00 usec
PL2	3.31 dB
PL12	23.31 dB
PL2W	6.79873323 W
PL12W	0.06798734 W
SFO2	600.0330002 MHz
SI	16384
SF	150.8776659 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

COMPOUND 2

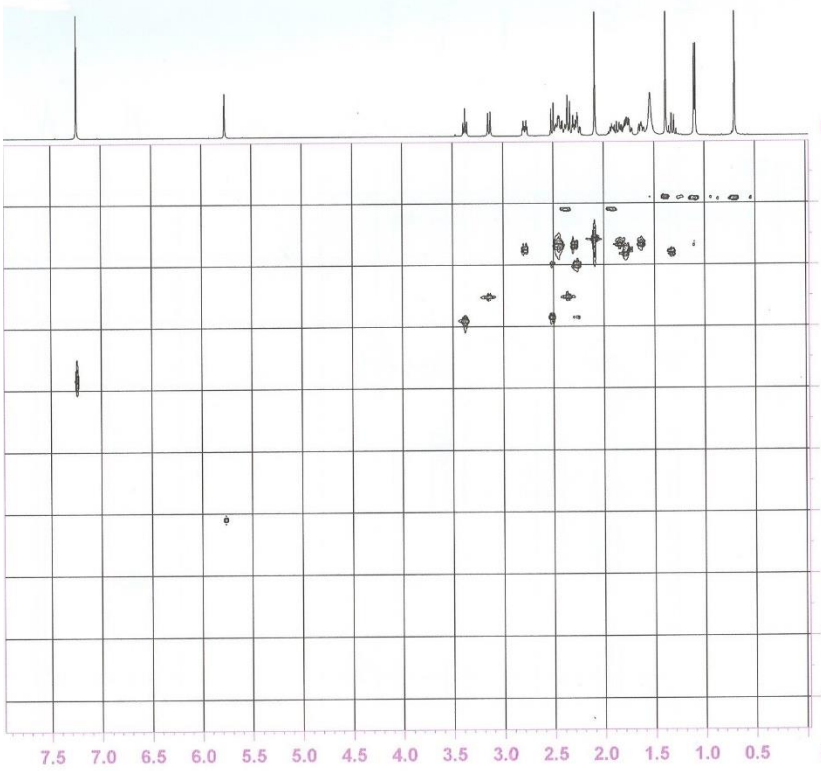
dept 90



AVANCE AV-600-LC
CRYOPROBE
LAB NO: 108

NAME	oct09-15
EXPNO	10
PROCNO	1
Date_	20151010
Time	3.51
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	deptsp90
TD	32768
SOLVENT	CDCl3
NS	3072
DS	2
SWH	30303.031 Hz
FIDRES	0.924775 Hz
AQ	0.5407385 sec
RG	32768
DW	16.500 usec
DE	6.50 usec
TE	298.0 K
CNST2	145.0000000
D1	1.50000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	3
======== CHANNEL f1 ========	
NUC1	13C
P1	12.70 usec
P12	2000.00 usec
PL0	120.00 dB
PL1	-1.81 dB
PLOW	0.00000000 W
PL1W	81.92915344 W
SFO1	150.8927518 MHz
SP2	4.19 dB
SPNAM2	Crp60comp.4
SPOAL2	0.500
SPOFFS2	0.00 Hz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
P3	8.00 usec
P4	16.00 usec
PCPD2	80.00 usec
PL2	3.31 dB
PL12	23.31 dB
PL2W	6.79873323 W
PL12W	0.06798734 W
SFO2	600.0330002 MHz
SI	16384
SF	150.8776659 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

COMPOUND 2
HSQC

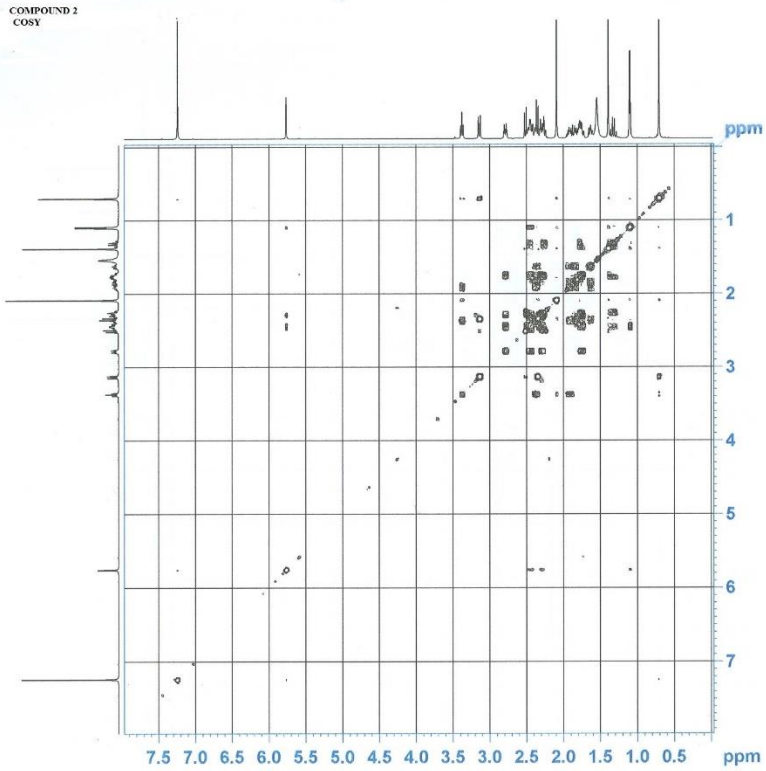


BRUKER

BRUKER AVANCE 500 CHANNEL 18

```
NAME                nov08-12
EXPNO                      5
PROCNO                     1
Date_            20121108
Time                    20.31
INSTRUM                 spect
PROBHD     5 mm PABBI 1H/
PULPROG          hsqcetgpsi
TD                      1024
SOLVENT                 CDCl3
NS                        32
DS                         8
SWH                 4006.410 Hz
FIDRES              3.912510 Hz
AQ                0.1279700 sec
RG                   20642.5
DW                   124.800 usec
DE                     6.50 usec
TE                    297.5 K
CNST2            145.0000000
D0                0.00000300 sec
D1                2.00000000 sec
D4                0.00172414 sec
D11               0.03000000 sec
D13               0.00000400 sec
D16               0.00020000 sec
D24               0.00110000 sec
IN0               0.00002090 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                      1H
P1                      7.05 usec
P2                     14.10 usec
P28                  1000.00 usec
PL1                     5.00 dB
SFO1             500.2320009 MHz

======== CHANNEL f2 ========
CPDPRG2                garp
NUC2                      13C
P3                     15.25 usec
P4                     30.50 usec
PCPD2                  70.00 usec
PL2                    -3.00 dB
PL12                    9.00 dB
SFO2             125.7948834 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPZ1                    80.00 %
GPZ2                    20.10 %
P16                  1000.00 usec
ND0                        2
TD                       256
SFO1             125.7949 MHz
FIDRES           93.363388 Hz
SW                   190.000 ppm
FnMODE        Echo-Antiecho
SI                      1024
SF               500.2300183 MHz
WDW                     QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
PC                      1.00
SI                      1024
MC2            echo-antiecho
SF               125.7829370 MHz
WDW                     QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
```

COMPOUND 2
COSY

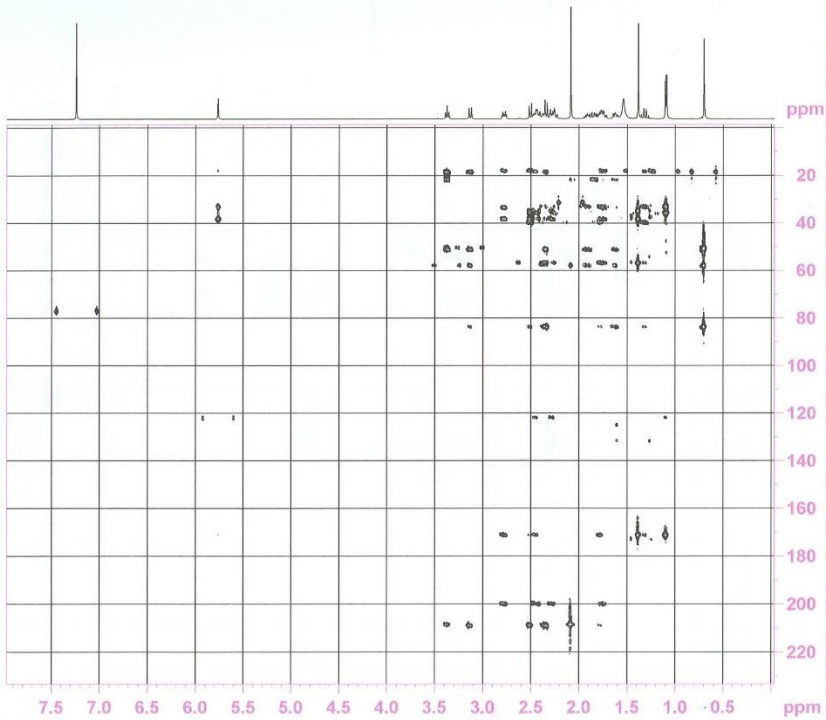


BRUKER

```
NAME                nov08-12
EXPNO                      3
PROCNO                     1
Date_               20121108
Time                   16.32
INSTRUM                spect
PROBHD    5 mm PABBI 1H/
PULPROG             cosygpqf
TD                       2048
SOLVENT                 CDCl3
NS                         8
DS                         8
SWH                 4006.410 Hz
FIDRES              1.956255 Hz
AQ                 0.2557652 sec
RG                     456.1
DW                   124.800 usec
DE                      6.50 usec
TE                     296.5 K
D0                 0.00000300 sec
D1                 1.50000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00024960 sec

======== CHANNEL f1 ========
NUC1                       1H
P0                       7.05 usec
P1                       7.05 usec
PL1                      5.00 dB
SFO1             500.2320009 MHz

====== GRADIENT CHANNEL =====
GPNAM1                SINE.100
GPZ1                     10.00 %
P16                    1000.00 usec
ND0                        1
TD                       256
SFO1                   500.232 MHz
FIDRES              15.650039 Hz
SW                       8.009 ppm
FnMODE                      QF
SI                        1024
SF                 500.2300193 MHz
WDW                      QSINE
SSB                        0
LB                        0.00 Hz
GB                         0
PC                        1.00
SI                        1024
MC2                         QF
SF                 500.2300193 MHz
WDW                      QSINE
SSB                        0
LB                        0.00 Hz
GB                         0
```

MARCE AN 500
LB NO. 118

COMPOUND 2
HMBC

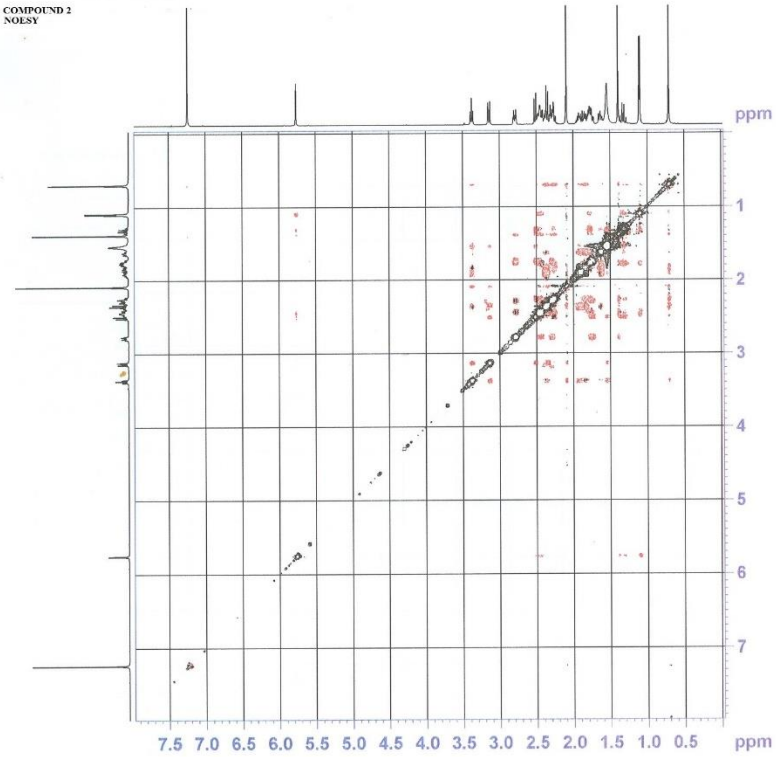


BRUKER

```
NAME                nov08-12
EXPNO                      6
PROCNO                     1
Date_               20121109
Time                   1.26
INSTRUM                spect
PROBHD    5 mm PABBI 1H/
PULPROG           hmbcgplpndqf
TD                       2048
SOLVENT                 CDCl3
NS                        64
DS                         8
SWH                 4006.410 Hz
FIDRES              1.956255 Hz
AQ                 0.2557652 sec
RG                     23170.5
DW                   124.800 usec
DE                      6.50 usec
TE                     297.6 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                0.00001690 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       7.05 usec
P2                      14.10 usec
PL1                      5.00 dB
SFO1             500.2320009 MHz

======== CHANNEL f2 ========
NUC2                      13C
P3                      15.25 usec
PL2                     -3.00 dB
SFO2             125.7974871 MHz

====== GRADIENT CHANNEL =====
GPNAM1                SINE.100
GPNAM2                SINE.100
GPNAM3                SINE.100
GPZ1                     50.00 %
GPZ2                     30.00 %
GPZ3                     40.10 %
P16                    1000.00 usec
ND0                        2
TD                       256
SFO1                 125.7975 MHz
FIDRES              115.478165 Hz
SW                     235.000 ppm
FnMODE                      QF
SI                        1024
SF                 500.2300193 MHz
WDW                      SINE
SSB                        0
LB                        0.00 Hz
GB                         0
PC                        1.00
SI                         512
MC2                         QF
SF                 125.7829370 MHz
WDW                      SINE
SSB                        0
LB                        0.00 Hz
GB                         0
```

MARCE AN 500
LB NO. 118

COMPOUND 2
NOESY



BRUKER

NMRC AV-500
LB NO: 118

```
NAME                nov08-12
EXPNO                      4
PROCNO                     1
Date_            20121108
Time                   17.34
INSTRUM                spect
PROBHD    5 mm PABBI 1H/
PULPROG          noesygpph
TD                      2048
SOLVENT                 CDCl3
NS                         16
DS                          8
SWH                 4006.410 Hz
FIDRES              1.956255 Hz
AQ                  0.2557652 sec
RG                     1149.4
DW                   124.800 usec
DE                      6.50 usec
TE                     297.0 K
D0                  0.00011582 sec
D1                  1.50000000 sec
D8                  0.80000001 sec
D16                 0.00020000 sec
IN0                 0.00024960 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       7.05 usec
P2                      14.10 usec
PL1                      5.00 dB
SFO1             500.2320009 MHz

====== GRADIENT CHANNEL =====
GPNAM1                SINE.100
GPNAM2                SINE.100
GPZ1                     40.00 %
GPZ2                    -40.00 %
P16                   1000.00 usec
ND0                        1
TD                       256
SFO1                 500.232 MHz
FIDRES              15.650039 Hz
SW                       8.009 ppm
FnMODE            States-TPPI
SI                       1024
SF                 500.2300193 MHz
WDW                      QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
PC                      1.00
SI                       1024
MC2               States-TPPI
SF                 500.2300193 MHz
WDW                      QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
```