Date Run: 10-16-2012 (Time Run: 12:00:03)

COMPOUND 4

Instrument: JEOL MSRoute
Inlet: Direct Probe

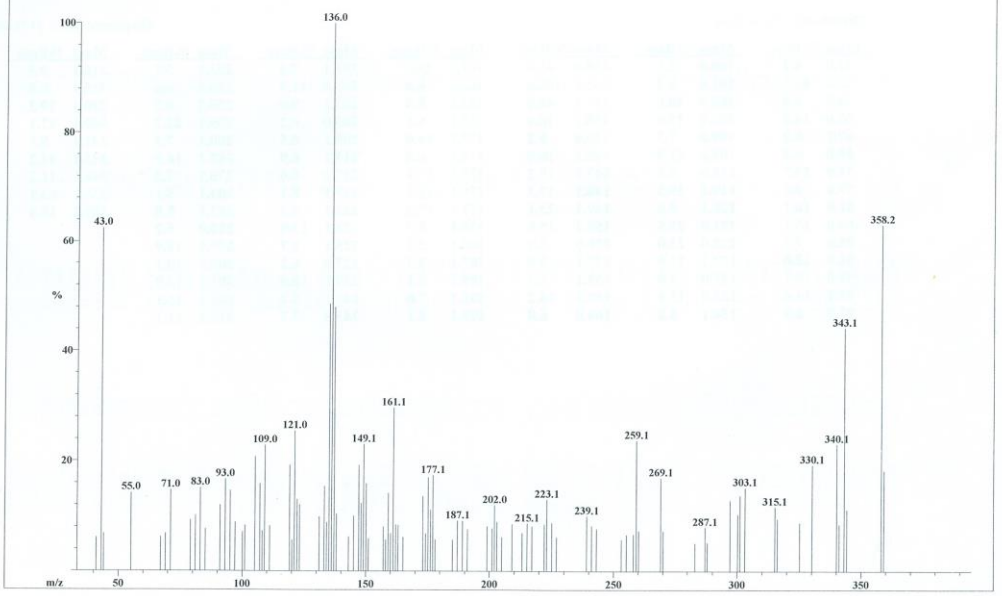
Ionization mode: EI+

Run By: HEJ

Scan: 24
Base: m/z 136; 14.8%FS TIC: 2178480

R.T.: 2.07

#Ions: 99

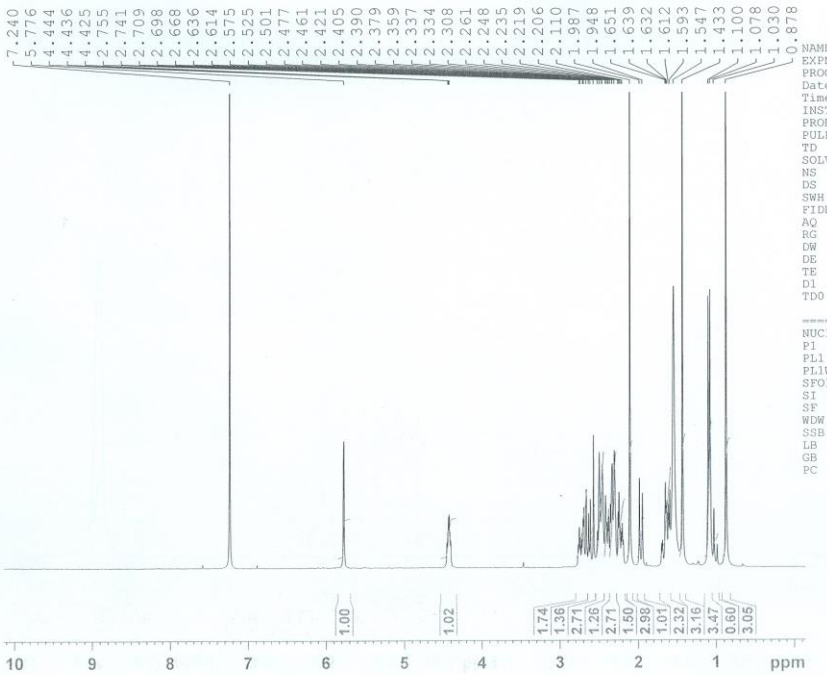


COMPOUND 4

Mass	Relative Intensity	Theoretical Mass	Delta [mmu]	RDB	Composition
242.9856	11.2				
251.1437	1.8	251.1430	0.7	9.5	$C_{18}H_{19}O_1$
		251.1489	-5.2	0.5	$C_{11}H_{23}O_6$
253.1583	1.7	253.1587	-0.4	8.5	$C_{18}H_{21}O_1$
254.1644	1.2	254.1665	-2.1	8.0	$C_{18}H_{22}O_1$
254.9856	3.4				
255.1684	2.7	255.1743	-5.9	7.5	$C_{18}H_{23}O_1$
258.1612	1.2	258.1614	-0.3	7.0	$C_{17}H_{22}O_2$
259.1678	3.1	259.1693	-1.4	6.5	$C_{17}H_{23}O_2$
265.1563	1.5	265.1587	-2.4	9.5	$C_{19}H_{21}O_1$
266.9853	1.6				
267.1434	1.0	267.1438	-0.4	0.5	$C_{11}H_{23}O_7$
		267.1380	5.5	9.5	$C_{18}H_{19}O_2$
268.9824	2.4	268.9869	-4.5	17.5	$C_{17}H_1O_4$
269.1546	4.6	269.1536	1.0	8.5	$C_{18}H_{21}O_2$
270.1585	2.2	270.1614	-2.9	8.0	$C_{18}H_{22}O_2$
279.1743	1.6	279.1743	-0.0	9.5	$C_{20}H_{23}O_1$
		279.1802	-5.9	0.5	$C_{13}H_{27}O_6$
280.9824	6.9	280.9869	-4.5	18.5	$C_{18}H_1O_4$
281.1584	1.3	281.1595	-1.1	0.5	$C_{12}H_{25}O_7$
		281.1536	4.8	9.5	$C_{19}H_{21}O_2$
282.1612	1.7	282.1614	-0.2	9.0	$C_{19}H_{22}O_2$
283.1695	1.9	283.1693	0.2	8.5	$C_{19}H_{23}O_2$
292.9824	12.3	292.9869	-4.5	19.5	$C_{19}H_1O_4$
293.9846	1.0	293.9795	5.1	15.0	$C_{15}H_2O_7$
295.1712	1.3	295.1693	2.0	9.5	$C_{20}H_{23}O_2$
		295.1751	-3.9	0.5	$C_{13}H_{27}O_7$
296.1801	1.3	296.1830	-2.8	0.0	$C_{13}H_{28}O_7$
		296.1771	3.0	9.0	$C_{20}H_{24}O_2$
297.1872	5.9	297.1849	2.3	8.5	$C_{20}H_{25}O_2$
298.1939	2.4	298.1927	1.2	8.0	$C_{20}H_{26}O_2$
300.1783	1.9				
301.1814	2.0	301.1798	1.5	7.5	$C_{19}H_{25}O_3$
304.9824	2.1	304.9869	-4.5	20.5	$C_{20}H_1O_4$
307.1691	1.2	307.1693	-0.2	10.5	$C_{21}H_{23}O_2$
315.1918	1.4	315.1955	-3.7	7.5	$C_{20}H_{27}O_3$
316.1784	1.1	316.1822	-3.8	12.0	$C_{23}H_{24}O_1$
316.9827	1.3	316.9869	-4.2	21.5	$C_{21}H_1O_4$
325.1817	2.0	325.1798	1.9	9.5	$C_{21}H_{25}O_3$
		325.1857	-3.9	0.5	$C_{14}H_{29}O_8$
330.2135	1.6	330.2189	-5.5	7.0	$C_{21}H_{30}O_3$
330.9792	3.6				
338.1862	1.8	338.1876	-1.4	10.0	$C_{22}H_{26}O_3$
340.2040	13.0	340.2033	0.7	9.0	$C_{22}H_{28}O_3$
		340.2092	-5.2	0.0	$C_{15}H_{32}O_8$
341.2046	3.5				
342.9792	4.0				
343.1908	2.0	343.1904	0.4	8.5	$C_{21}H_{27}O_4$
354.9792	1.5				
358.2128	4.0	358.2139	-1.0	8.0	$C_{22}H_{30}O_4$
359.2164	1.1	359.2217	-5.3	7.5	$C_{22}H_{31}O_4$
381.0255	2.9				
393.1095	2.7	393.1121	-2.7	18.5	$C_{26}H_{17}O_4$

COMPOUND 4
H-NMR

AVANCE AV - III
300 MHz, LAB # 116



NAME	oct15
EXPNO	2
PROCNO	1
Date_	20121015
Time	9.15
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

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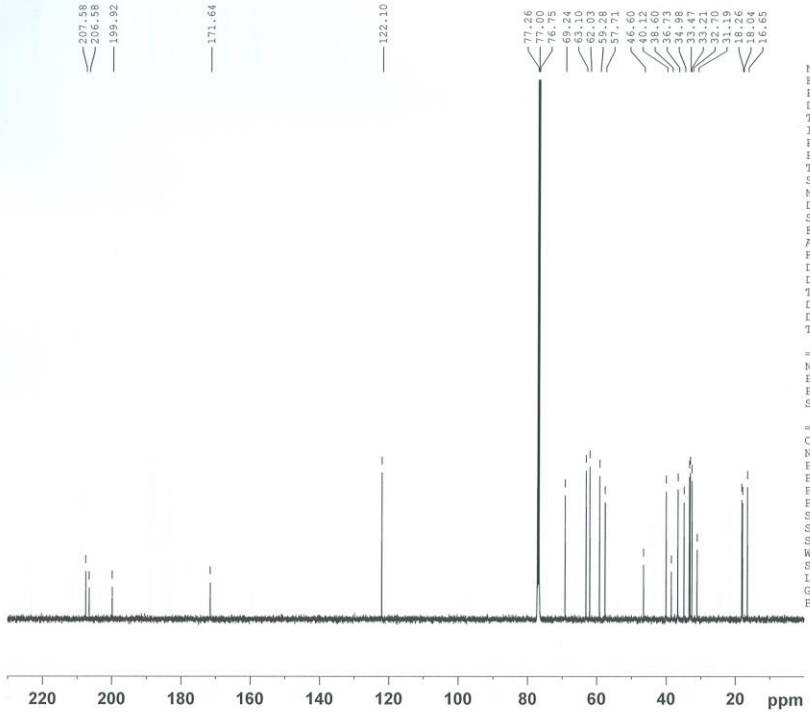
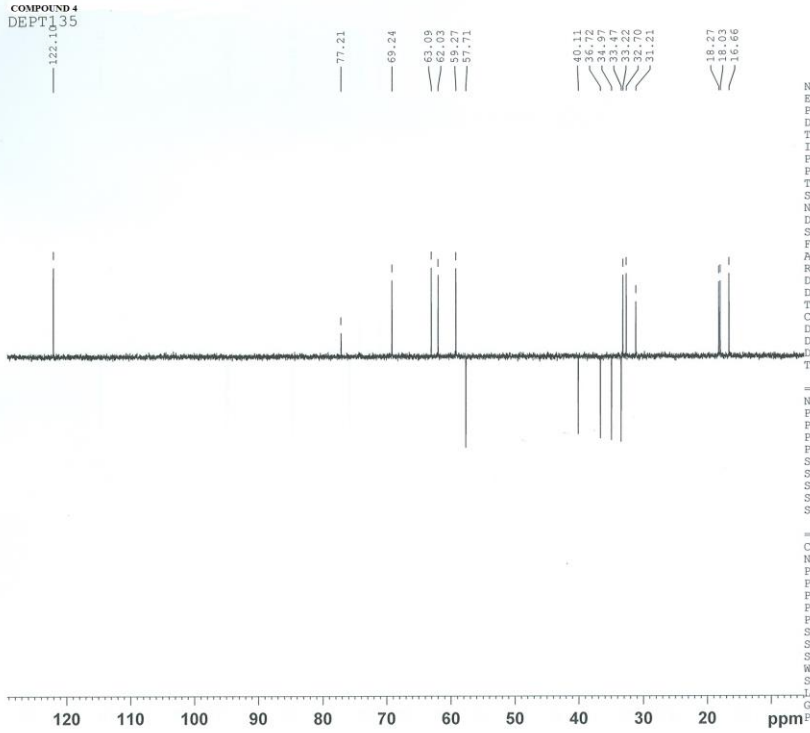
COMPOUND 4
BB



NAME	oct17-12
EXPNO	10
PROCNO	1
Date_	20121018
Time	9.20
INSTRUM	spect
PROBHD	5 mm BBI 1H/D-
PULPROG	zgpg
TD	65536
SOLVENT	CDCl3
NS	18432
DS	4
SWH	29498.525 Hz
FIDRES	0.450112 Hz
AQ	1.1109022 sec
RG	32768
DW	16.950 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	18
======== CHANNEL f1 ========	
NUC1	13C
P1	13.70 usec
PL1	-3.00 dB
SFO1	125.7723529 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	6.00 dB
PL12	25.25 dB
PL13	25.25 dB
SFO2	500.1325007 MHz
SI	32768
SF	125.7577898 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

COMPOUND 4

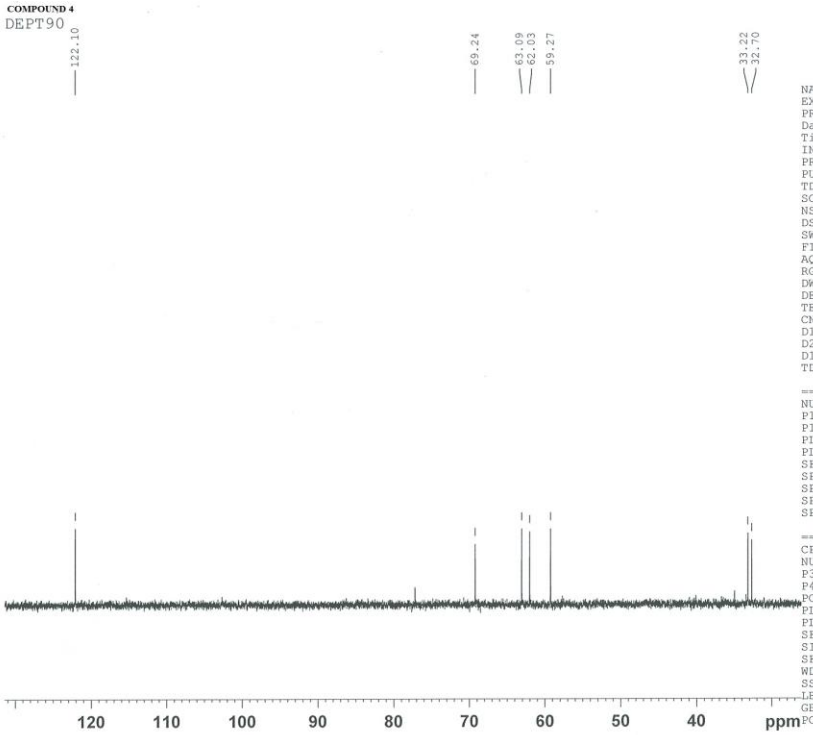
DEPT135




```
NAME            oct17-12
EXPNO                11
PROCNO                1
Date_          20121019
Time               1.19
INSTRUM           spect
PROBHD    5 mm BBI 1H/D-
PULPROG        deptsp135
TD                32768
SOLVENT            CDCl3
NS                11951
DS                    2
SWH            23809.523 Hz
FIDRES          0.726609 Hz
AQ             0.6881990 sec
RG                32768
DW                21.000 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                   12

======== CHANNEL f1 ========
NUC1                 13C
P1                 13.70 usec
P12             2000.00 usec
PL0              120.00 dB
PL1               -3.00 dB
SFO1         125.7697360 MHz
SP2                2.42 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                6.00 dB
PL12              25.25 dB
SFO2         500.1335009 MHz
SI                32768
SF           125.7577898 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

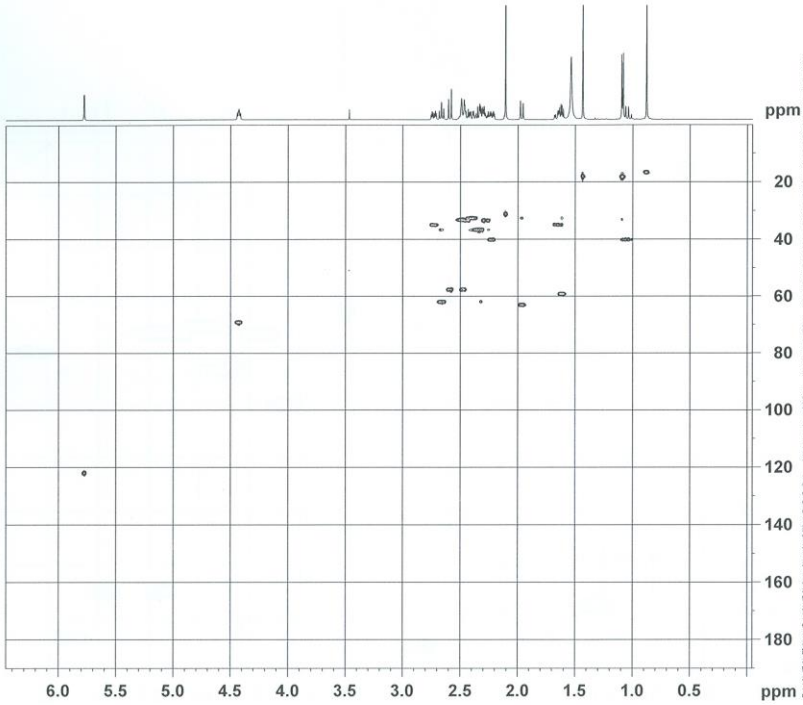
COMPOUND 4

DEPT90




```
NAME            oct17-12
EXPNO                12
PROCNO                1
Date_          20121019
Time               8.44
INSTRUM           spect
PROBHD    5 mm BBI 1H/D-
PULPROG        deptsp90
TD                32768
SOLVENT            CDCl3
NS                 2068
DS                    2
SWH            23809.523 Hz
FIDRES          0.726609 Hz
AQ             0.6881990 sec
RG                32768
DW                21.000 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                    8

======== CHANNEL f1 ========
NUC1                 13C
P1                 13.70 usec
P12             2000.00 usec
PL0              120.00 dB
PL1               -3.00 dB
SFO1         125.7697360 MHz
SP2                2.42 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                6.00 dB
PL12              25.25 dB
SFO2         500.1335009 MHz
SI                32768
SF           125.7577898 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

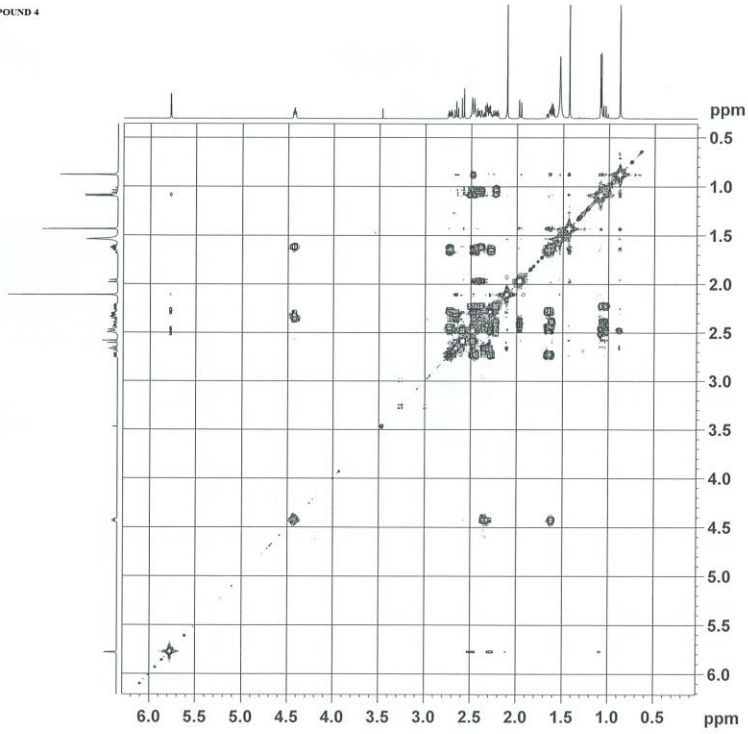
COMPOUND 4
HSQC




```
NAME            oct17-12
EXPNO                  8
PROCNO                 1
Date_           20121017
Time               18.46
INSTRUM            spect
PROBHD   5 mm BBI 1H/D-
PULPROG      hsqcetgpsi
TD                  1024
SOLVENT             CDCl3
NS                     32
DS                      8
SWH            3255.208 Hz
FIDRES         3.178914 Hz
AQ            0.1574900 sec
RG              23170.5
DW              153.600 usec
DE                 6.50 usec
TE               298.0 K
CNST2          145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00010000 sec
D24            0.00110000 sec
IN0            0.00002090 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.60 usec
P2                  15.20 usec
P28                  0.00 usec
PL1                  6.00 dB
SFO1        500.1316254 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                  13.70 usec
P4                  27.40 usec
PCPD2               65.00 usec
PL2                 -2.85 dB
PL12                10.67 dB
SFO2        125.76973360 MHz

======= GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPZ1                80.00 %
GPZ2                20.10 %
P16               1000.00 usec
ND0                     2
TD                    256
SFO1            125.7697 MHz
FIDRES          93.344727 Hz
SW              190.000 ppm
FnMODE     Echo-Antiecho
SI                   1024
SF          500.1300233 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
PC                   4.00
SI                   1024
MC2        echo-antiecho
SF         125.7577898 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
```

AVANCE AV-500
LAB NO: 109-B

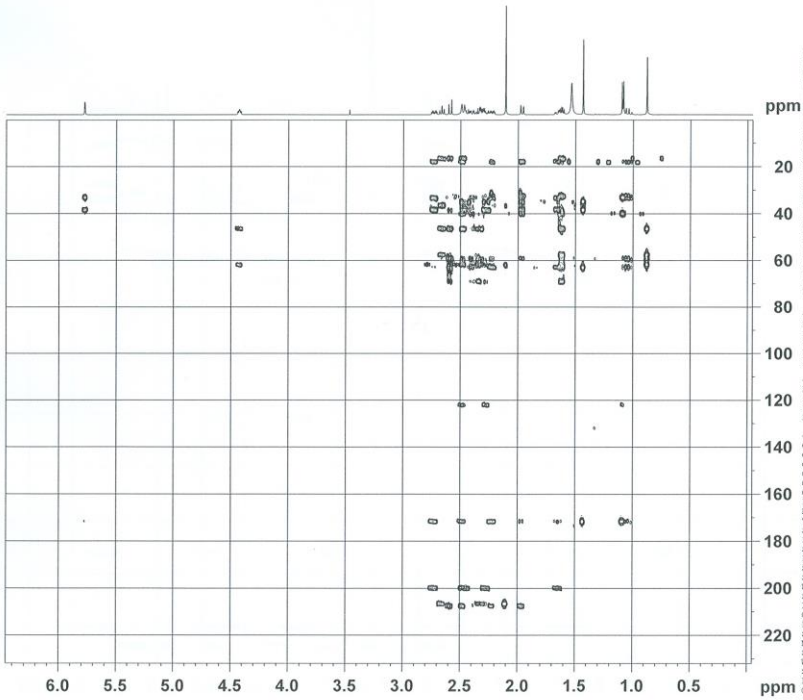
COMPOUND 4
COSY




```
NAME            oct17-12
EXPNO                  6
PROCNO                 1
Date_           20121017
Time               14.41
INSTRUM            spect
PROBHD   5 mm BBI 1H/D-
PULPROG          cosygpqf
TD                   2048
SOLVENT             CDCl3
NS                      8
DS                      8
SWH            3255.208 Hz
FIDRES         1.589457 Hz
AQ            0.3147764 sec
RG                    362
DW              153.600 usec
DE                 6.50 usec
TE               298.0 K
D0             0.00000300 sec
D1             1.50000000 sec
D13            0.00000400 sec
D16            0.00010000 sec
IN0            0.00030720 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                   7.60 usec
P1                   7.60 usec
PL1                  6.00 dB
SFO1        500.1316254 MHz

======= GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPZ1                10.00 %
P16               1000.00 usec
ND0                     1
TD                    256
SFO1            500.1316 MHz
FIDRES         12.715656 Hz
SW                  6.509 ppm
FnMODE                 QF
SI                   1024
SF          500.1300233 MHz
WDW                 SINE
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   4.00
SI                   1024
MC2                    QF
SF          500.1300233 MHz
WDW                 SINE
SSB                     0
LB                   0.00 Hz
GB                      0
```

AVANCE AV-500
LAB NO: 109-B

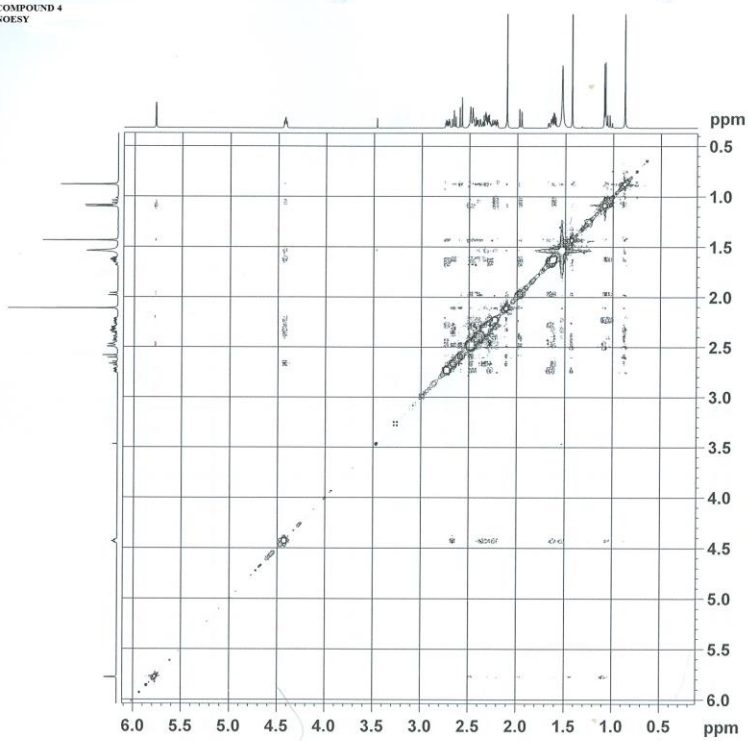
COMPOUND 4
HMBC




```
NAME            oct17-12
EXPNO                  9
PROCNO                 1
Date_           20121017
Time               22.37
INSTRUM            spect
PROBHD   5 mm BBI 1H/D-
PULPROG     hmbcgplpndqf
TD                  4096
SOLVENT             CDCl3
NS                     64
DS                      8
SWH             3255.208 Hz
FIDRES          0.794729 Hz
AQ              0.6293492 sec
RG                23170.5
DW                153.600 usec
DE                   6.50 usec
TE                  298.0 K
CNST2         145.0000000
CNST13         10.0000000
D0              0.00000300 sec
D1              2.00000000 sec
D2              0.00344828 sec
D6              0.05000000 sec
D16             0.00010000 sec
IN0             0.00001715 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.60 usec
P2                  15.20 usec
PL1                  6.00 dB
SFO1          500.1316254 MHz

======== CHANNEL f2 ========
NUC2                  13C
P3                  13.70 usec
PL2                 -2.85 dB
SFO2          125.7723769 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                    205
SFO1            125.7724 MHz
FIDRES        142.337524 Hz
SW                232.000 ppm
FnMODE                 QF
SI                   1024
SF            500.1300233 MHz
WDW                 QSINE
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   4.00
SI                   1024
MC2                    QF
SF            125.7577898 MHz
WDW                 QSINE
SSB                     0
LB                   0.00 Hz
GB                      0
```

AVANCE AV-500
LAB NO: 109-B

COMPOUND 4
NOESY




```
NAME            oct17-12
EXPNO                  7
PROCNO                 1
Date_           20121017
Time               15.45
INSTRUM            spect
PROBHD   5 mm BBI 1H/D-
PULPROG         noesygpph
TD                   2048
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             3255.208 Hz
FIDRES          1.589457 Hz
AQ              0.3147764 sec
RG                 1625.5
DW                153.600 usec
DE                   6.50 usec
TE                  298.0 K
D0              0.00014392 sec
D1              1.50000000 sec
D8              0.80000001 sec
D16             0.00010000 sec
IN0             0.00030720 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.60 usec
P2                  15.20 usec
PL1                  6.00 dB
SFO1          500.1316254 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            500.1300233 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
PC                   4.00
SI                   1024
MC2           States-TPPI
SF            500.1300233 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
```

AVANCE AV-500
LAB NO: 109-B