Date Run: 03-08-2012 (Time Run: 11:12:03)

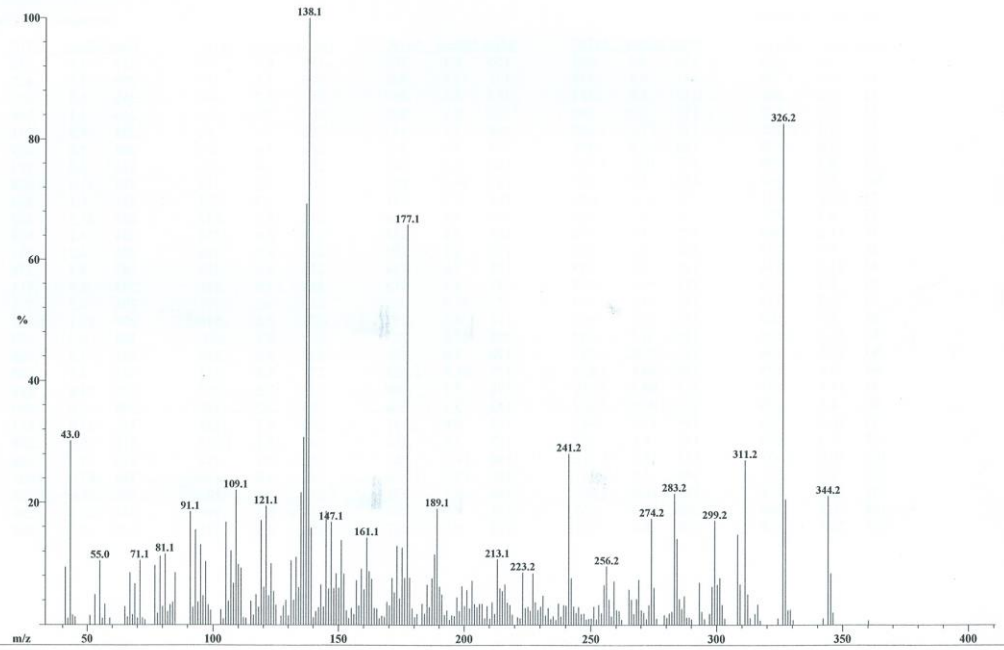
COMPOUND 1
Instrument: JEOL MSRoute
Inlet: Direct Probe

Ionization mode: EI+

Scan: 11
Base: m/z 138; 86.7%FS TIC: 15261897 (Max Inten : 909503)

R.T.: .4

#Ions: 247

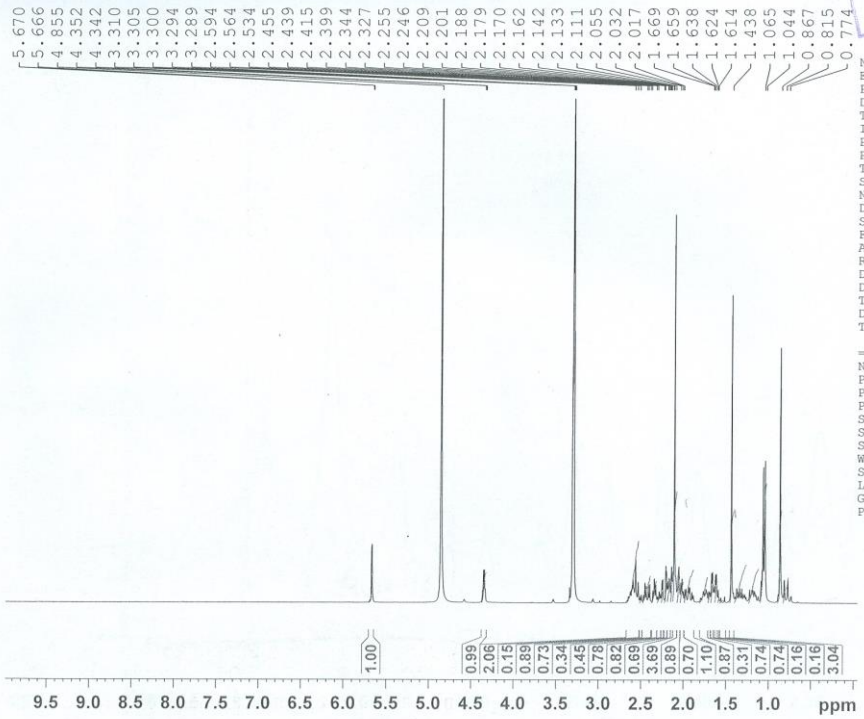


COMPOUND 1
HREI-MS

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
229.1558	1.1433	229.1592	-15.1	-3.5	6.5	$C_{16}H_{21}O_1$
230.1647	1.1235	230.1671	-10.2	-2.4	6.0	$C_{16}H_{22}O_1$
230.9856	10.1973					
235.1461	2.3050	235.1487	-10.9	-2.6	9.5	$C_{18}H_{19}$
235.9903	1.5915	235.9898	2.1	0.5	18.0	$C_{17}O_2$
237.1281	6.4994	237.1279	0.6	0.1	9.5	$C_{17}H_{17}O_1$
238.1317	1.6528	238.1358	-17.0	-4.1	9.0	$C_{17}H_{18}O_1$
238.1719	1.5974	238.1722	-1.2	-0.3	8.0	$C_{18}H_{22}$
239.1445	8.5158	239.1436	3.7	0.9	8.5	$C_{17}H_{19}O_1$
240.1504	3.5755	240.1514	-4.3	-1.0	8.0	$C_{17}H_{20}O_1$
241.1595	34.3282	241.1592	1.0	0.2	7.5	$C_{17}H_{21}O_1$
242.1613	8.0068	242.1671	-23.8	-5.8	7.0	$C_{17}H_{22}O_1$
242.9856	10.7517					
243.1680	2.6426					
244.1800	1.3706	244.1827	-11.1	-2.7	6.0	$C_{17}H_{24}O_1$
249.1641	1.2879	249.1643	-0.9	-0.2	9.5	$C_{19}H_{21}$
251.1567	2.5020					
251.1719	2.5436					
253.1576	9.4321	253.1592	-6.6	-1.7	8.5	$C_{18}H_{21}O_1$
254.1609	2.9978					
254.9856	3.1008					
255.1765	4.7361	255.1749	6.1	1.6	7.5	$C_{18}H_{23}O_1$
256.1792	5.3710	256.1827	-13.6	-3.5	7.0	$C_{18}H_{24}O_1$
257.1801	1.5230					
259.1601	1.4768					
265.1876	3.7302					
266.1636	1.9155	266.1671	-13.0	-3.4	9.0	$C_{19}H_{22}O_1$
266.1934	1.7699	266.1882	19.6	5.2	4.0	$C_{16}H_{26}O_3$
266.9826	2.2321					
267.1765	5.1427	267.1749	6.0	1.6	8.5	$C_{19}H_{23}O_1$
268.1781	3.8653	268.1827	-17.3	-4.6	8.0	$C_{19}H_{24}O_1$
268.9824	3.2185					
269.1880	6.3470	269.1905	-9.5	-2.5	7.5	$C_{19}H_{25}O_1$
270.1949	1.4897	270.1984	-12.8	-3.5	7.0	$C_{19}H_{26}O_1$
274.1938	3.5868	274.1933	2.0	0.6	6.0	$C_{18}H_{26}O_2$
275.1837	1.5065	275.1800	13.5	3.7	10.5	$C_{21}H_{23}$
279.1820	1.5170					
280.9824	7.4444					
281.1917	3.9565	281.1905	4.1	1.2	8.5	$C_{20}H_{25}O_1$
282.1968	2.3667	282.1984	-5.7	-1.6	8.0	$C_{20}H_{26}O_1$
283.2082	10.3496	283.2062	7.0	2.0	7.5	$C_{20}H_{27}O_1$
284.2158	6.7966	284.2140	6.2	1.8	7.0	$C_{20}H_{28}O_1$
285.2192	1.5294	285.2218	-9.2	-2.6	6.5	$C_{20}H_{29}O_1$
287.2091	1.0827					
291.1752	1.2563	291.1749	1.1	0.3	10.5	$C_{21}H_{23}O_1$
292.9824	11.0504					
293.1918	7.8888	293.1905	4.3	1.3	9.5	$C_{21}H_{25}O_1$
294.1981	1.8412	294.1984	-0.7	-0.2	9.0	$C_{21}H_{26}O_1$
295.1985	1.0957					
297.1860	1.0710	297.1855	2.0	0.6	8.5	$C_{20}H_{25}O_2$
298.1901	2.3438	298.1933	-10.6	-3.2	8.0	$C_{20}H_{26}O_2$
298.2272	2.3886	298.2297	-8.1	-2.4	7.0	$C_{21}H_{30}O_1$
299.2031	3.4644	299.2011	6.7	2.0	7.5	$C_{20}H_{27}O_2$
300.2091	1.5522	300.2089	0.4	0.1	7.0	$C_{20}H_{28}O_2$
301.2118	1.4331	301.2168	-16.5	-5.0	6.5	$C_{20}H_{29}O_2$
304.9824	2.3586					
307.1707	1.0914	307.1698	2.9	0.9	10.5	$C_{21}H_{23}O_2$
308.2144	4.8190	308.2140	1.1	0.3	9.0	$C_{22}H_{28}O_1$
309.1909	7.9338	309.1855	17.6	5.4	9.5	$C_{21}H_{25}O_2$
310.1917	2.6948	310.1933	-5.2	-1.6	9.0	$C_{21}H_{26}O_2$
311.1993	45.8148	311.2011	-5.7	-1.8	8.5	$C_{21}H_{27}O_2$
312.2023	11.1425					
313.2109	1.4069	313.2168	-18.8	-5.9	7.5	$C_{21}H_{29}O_2$
316.9794	1.3110					
324.2056	7.1655	324.2089	-10.3	-3.3	9.0	$C_{22}H_{28}O_2$
325.2178	1.7057	325.2168	3.3	1.1	8.5	$C_{22}H_{29}O_2$
326.2232	44.0701	326.2246	-4.2	-1.4	8.0	$C_{22}H_{30}O_2$
327.2266	11.4459	327.2324	-17.8	-5.8	7.5	$C_{22}H_{31}O_2$
328.2291	2.4050					
330.9792	3.5883					
342.2260	1.1861					
342.9792	4.4157					
344.2348	4.3784	344.2351	-1.0	-0.4	7.0	$C_{22}H_{32}O_3$
345.2387	1.3757	345.2430	-12.3	-4.2	6.5	$C_{22}H_{33}O_3$
354.9792	1.6937					

COMPOUND 1

1H

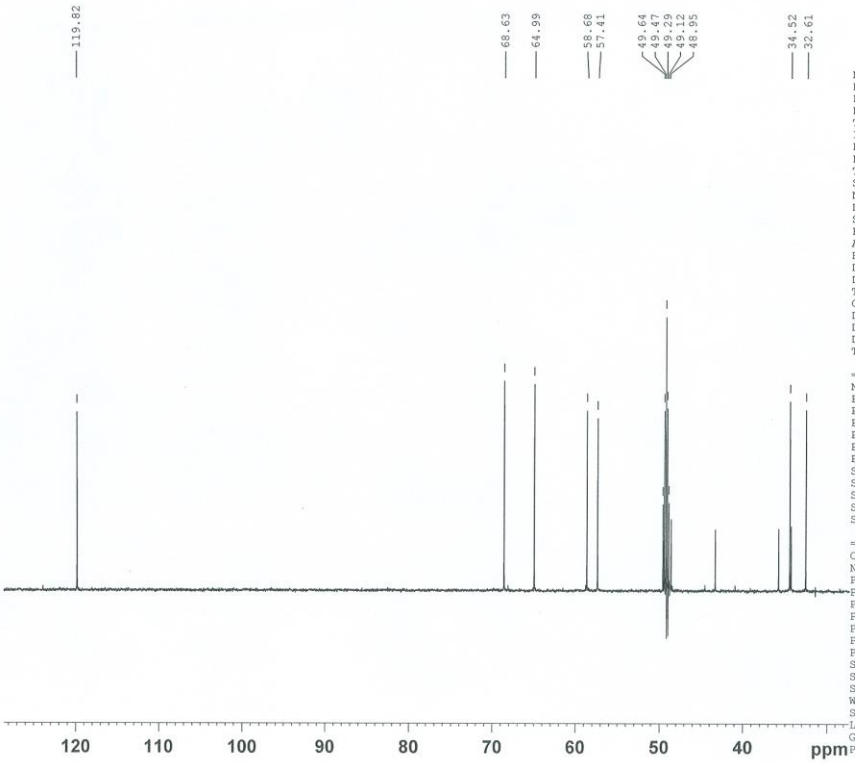


NAME	fab14
EXPNO	1
PROCNO	1
Date_	20120214
Time	9.28
INSTRUM	Spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	MeOD
NS	128
DS	0
SWH	6188.119 Hz
FIDRES	0.188846 Hz
AQ	2.6477044 sec
RG	203
DW	80.800 usec
DE	6.50 usec
TE	300.0 K
D1	1.50000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.00 usec
PL1	0.00 dB
PL1W	13.16228485 W
SFO1	300.1321009 MHz
SI	16384
SF	300.1300074 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

AVANCE A
LAB NO. 116

COMPOUND 1
BB

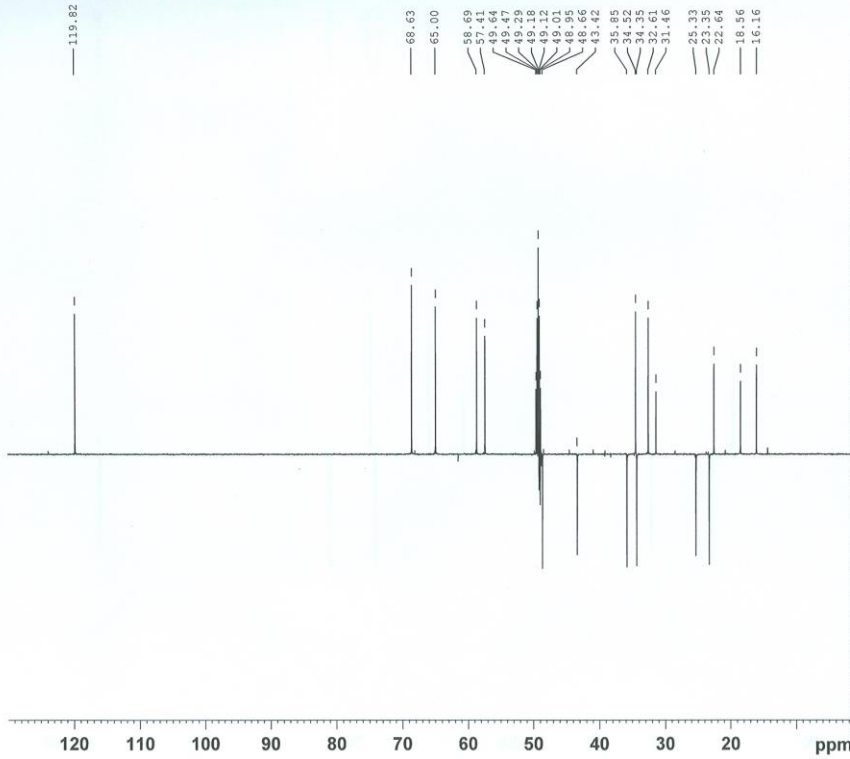
AVANCE AV-500
CRYOPROBE
LAB NO: 108




```
NAME            mar09-12
EXPNO                   9
PROCNO                  1
Date_            20120310
Time                 8.40
INSTRUM             spect
PROBHD    5 mm CPDUL 13C
PULPROG          deptsp90
TD                  32768
SOLVENT              MeOD
NS                   1153
DS                      2
SWH            25252.525 Hz
FIDRES          0.770646 Hz
AQ             0.6488762 sec
RG                  32768
DW                 19.800 usec
DE                  6.50 usec
TE                 293.5 K
CNST2        145.0000000
D1            1.50000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                     4

======== CHANNEL f1 ========
NUC1                  13C
P1                   7.80 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                  3.00 dB
PL0W          0.00000000 W
PL1W         33.36152267 W
SFO1         125.8206598 MHz
SP2                  1.99 dB
SPNAM2       Crp60comp.4
SPOAL2             0.500
SPOFFS2             0.00 Hz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
P3                  13.50 usec
P4                  27.00 usec
PCPD2               80.00 usec
PL2                  2.00 dB
PL12                18.50 dB
PL2W         11.25274181 W
PL12W         0.25191751 W
SFO2         500.3330020 MHz
SI                  32768
SF           125.8079004 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00
```

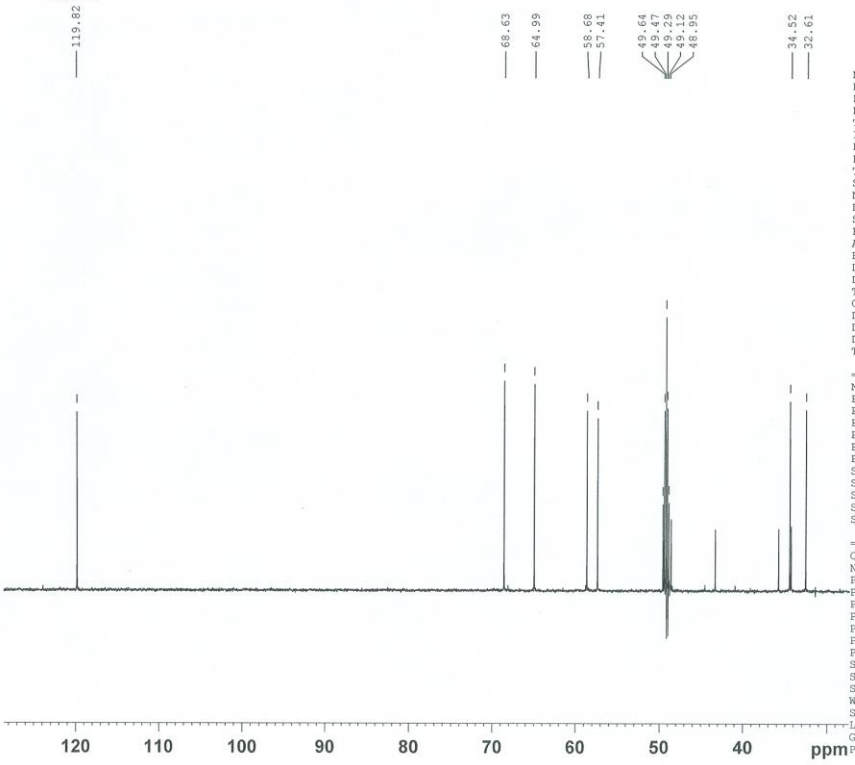
COMPOUND 1
DEPT-135

AVANCE AV-500
CRYOPROBE
LAB NO: 108




```
NAME            mar09-12
EXPNO                   8
PROCNO                  1
Date_            20120310
Time                 6.12
INSTRUM             spect
PROBHD    5 mm CPDUL 13C
PULPROG         deptsp135
TD                  32768
SOLVENT              MeOD
NS                   4506
DS                      2
SWH            25252.525 Hz
FIDRES          0.770646 Hz
AQ             0.6488762 sec
RG                  32768
DW                 19.800 usec
DE                  6.50 usec
TE                 294.2 K
CNST2        145.0000000
D1            1.50000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                     7

======== CHANNEL f1 ========
NUC1                  13C
P1                   7.80 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                  3.00 dB
PL0W          0.00000000 W
PL1W         33.36152267 W
SFO1         125.8206598 MHz
SP2                  1.99 dB
SPNAM2       Crp60comp.4
SPOAL2             0.500
SPOFFS2             0.00 Hz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
P3                  13.50 usec
P4                  27.00 usec
PCPD2               80.00 usec
PL2                  2.00 dB
PL12                18.50 dB
PL2W         11.25274181 W
PL12W         0.25191751 W
SFO2         500.3330020 MHz
SI                  32768
SF           125.8079004 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00
```

COMPOUND 1
DEPT-90

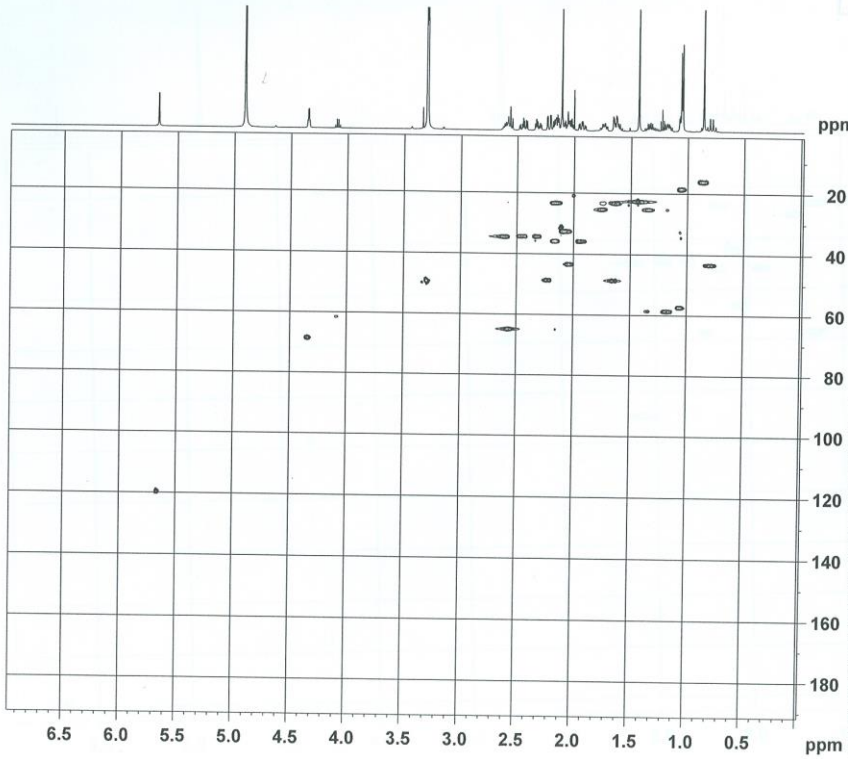


AVANCE AV-500
CRYOPROBE
1996

NAME	mar09-12	
EXPNO	9	
PROCNO	1	
Date_	20120310	
Time	8.40	
INSTRUM	spect	
PROBHD	5 mm CPDUL 13C	
PULPROG	deptsp90	
TD	32768	
SOLVENT	MeOD	
NS	1153	
DS	2	
SWH	25252.525	Hz
FIDRES	0.770646	Hz
AQ	0.6488762	sec
RG	32768	
DW	19.800	usec
DE	6.50	usec
TE	293.5	K
CNST2	145.0000000	
D1	1.50000000	sec
D2	0.00344828	sec
D12	0.00002000	sec
TD0	4	
======== CHANNEL f1 ========		
NUC1	13C	
P1	7.80	usec
P12	2000.00	usec
PL0	120.00	dB
PL1	3.00	dB
PL0W	0.00000000	W
PL1W	33.36152267	W
SFO1	125.8206598	MHz
SP2	1.99	dB
SPNAM2	Crp60comp.4	
SPOAL2	0.500	
SPOFFS2	0.00	Hz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
P3	13.50	usec
P4	27.00	usec
PCPD2	80.00	usec
PL2	2.00	dB
PL12	18.50	dB
PL2W	11.25274181	W
PL12W	0.25191751	W
SFO2	500.3330020	MHz
SI	32768	
SF	125.8079004	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	2.00	

COMPOUND 1
HSQC

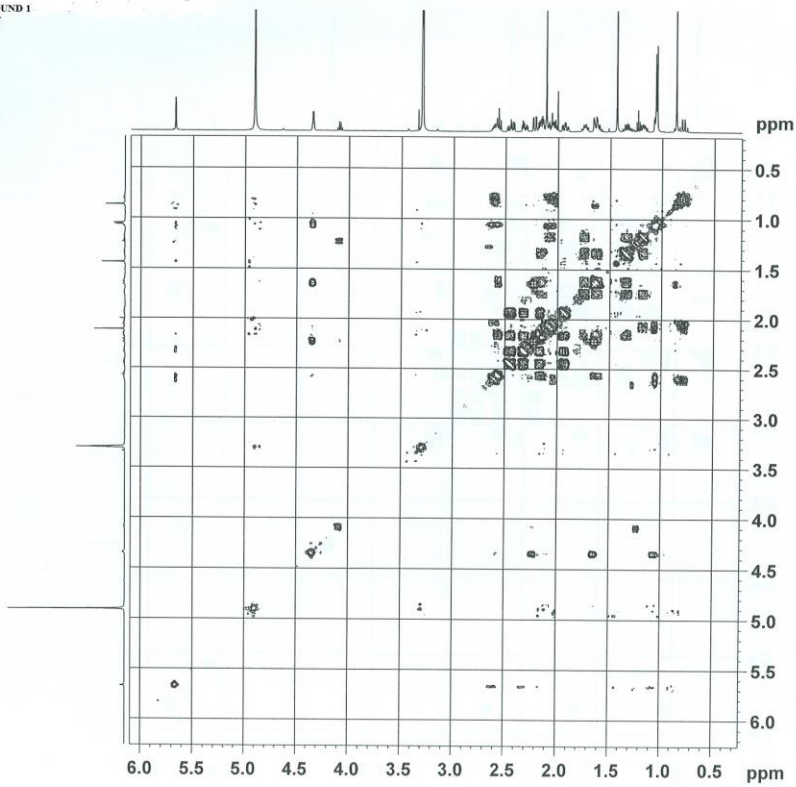
AVANCE AV-500
CRYOPROBE
LAB NO: 108




```
NAME            mar09-12
EXPNO                  5
PROCNO                 1
Date_           20120309
Time               13.46
INSTRUM            spect
PROBHD   5 mm CPDUL 13C
PULPROG        hsqcetgpsi
TD                  1024
SOLVENT             MeOD
NS                    32
DS                     8
SWH            3501.401 Hz
FIDRES         3.419337 Hz
AQ             0.1464200 sec
RG                 26008
DW               142.800 usec
DE                 6.50 usec
TE                294.0 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           0.00015000 sec
D24           0.00110000 sec
IN0           0.00002090 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                  13.50 usec
P2                  27.00 usec
P28                  0.50 usec
PL1                  2.00 dB
PL1W          11.25274181 W
SFO1         500.3317512 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                  13C
P3                   7.80 usec
P4                  15.60 usec
PCPD2               65.00 usec
PL2                  3.00 dB
PL12                21.50 dB
PL2W          33.36152267 W
PL12W          0.47124404 W
SFO2         125.8200308 MHz

====== GRADIENT CHANNEL =====
GPNAM1            SINE.100
GPNAM2            SINE.100
GPZ1                 80.00 %
GPZ2                 20.10 %
P16                2000.00 usec
ND0                     2
TD                    256
SFO1               125.82 MHz
FIDRES          93.382057 Hz
SW                190.000 ppm
FnMODE        Echo-Antiecho
SI                     1024
SF           500.3300143 MHz
WDW                   QSINE
SSB                       2
LB                     0.00 Hz
GB                        0
PC                     4.00
SI                     1024
MC2           echo-antiecho
SF           125.8079004 MHz
WDW                   QSINE
SSB                       2
LB                     0.00 Hz
GB                        0
```

COMPOUND 1
COSY

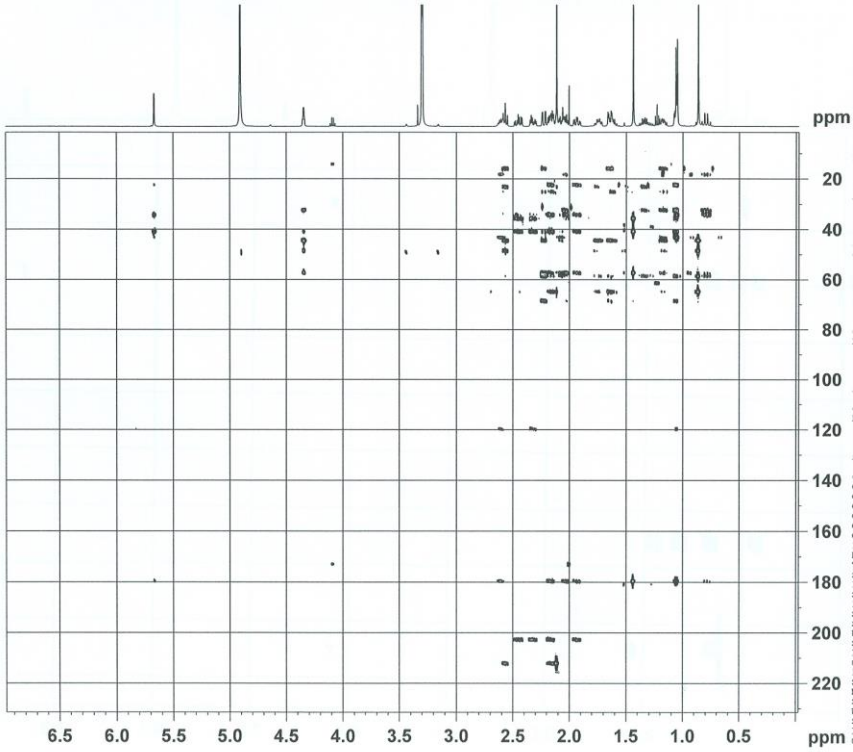
AVANCE AV-500
CRYOPROBE
LAB NO: 108




```
NAME            mar09-12
EXPNO                  3
PROCNO                 1
Date_           20120309
Time               11.13
INSTRUM            spect
PROBHD   5 mm CPDUL 13C
PULPROG          cosydfqf
TD                  2048
SOLVENT             MeOD
NS                     8
DS                     2
SWH            3501.401 Hz
FIDRES         1.709668 Hz
AQ             0.2926472 sec
RG                  71.8
DW               142.800 usec
DE                 6.50 usec
TE                293.1 K
D0            0.00000300 sec
D1            1.50000000 sec
D13           0.00000400 sec
D20           0.00000400 sec
IN0           0.00028560 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  13.50 usec
PL1                  2.00 dB
PL1W          11.25274181 W
SFO1         500.3317512 MHz
ND0                     1
TD                    256
SFO1            500.3318 MHz
FIDRES         13.677347 Hz
SW                  6.998 ppm
FnMODE                 QF
SI                     1024
SF           500.3300143 MHz
WDW                   SINE
SSB                       0
LB                     0.00 Hz
GB                        0
PC                     4.00
SI                     1024
MC2                    QF
SF           500.3300143 MHz
WDW                   SINE
SSB                       0
LB                     0.00 Hz
GB                        0
```

COMPOUND 1
HMBC

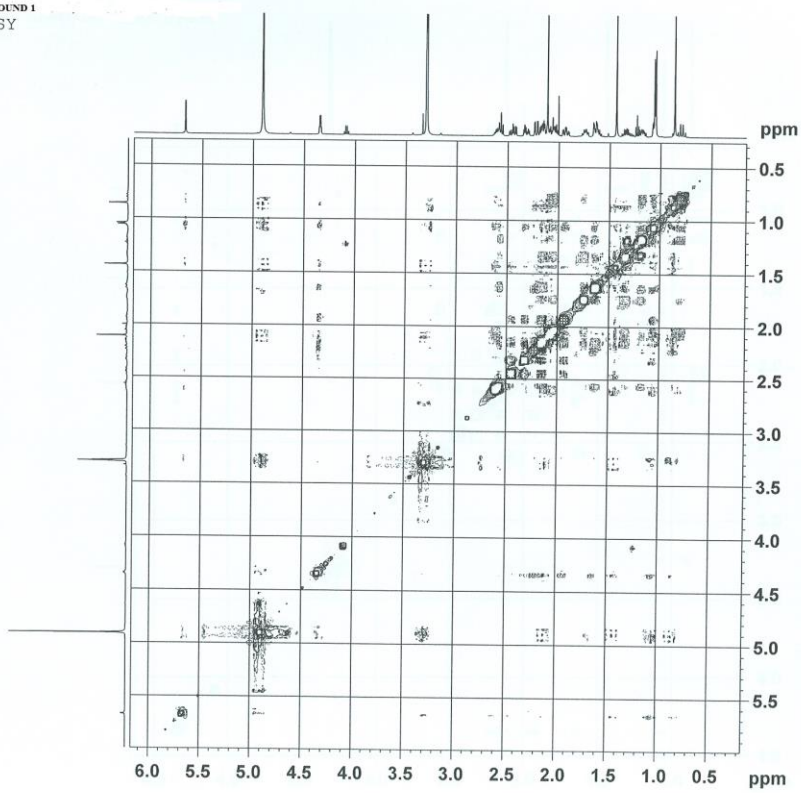
AVANCE AV-500
CRYOPROBE
LAB NO: 108




```
NAME            mar09-12
EXPNO                  6
PROCNO                 1
Date_           20120309
Time               17.35
INSTRUM            spect
PROBHD   5 mm CPDUL 13C
PULPROG     hmbcgplpndqf
TD                  4096
SOLVENT             MeOD
NS                    32
DS                     4
SWH            3501.401 Hz
FIDRES         0.854834 Hz
AQ           0.5851016 sec
RG               41285.1
DW               142.800 usec
DE                  6.50 usec
TE                294.1 K
CNST2        145.0000000
CNST13        13.0000000
D0            0.00000300 sec
D1            2.00000000 sec
D2            0.00344828 sec
D6            0.03846154 sec
D16           0.00015000 sec
IN0           0.00001730 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                13.50 usec
P2                27.00 usec
PL1                2.00 dB
PL1W        11.25274181 W
SFO1        500.3317512 MHz

======== CHANNEL f2 ========
NUC2                 13C
P3                 7.80 usec
PL2                3.00 dB
PL2W        33.36152267 W
SFO2        125.8225469 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPNAM3          SINE.100
GPZ1               50.00 %
GPZ2               30.00 %
GPZ3               40.10 %
P16             2000.00 usec
ND0                    2
TD                   256
SFO1            125.8225 MHz
FIDRES        113.043694 Hz
SW               230.000 ppm
FnMODE                QF
SI                  2048
SF           500.3300143 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  4.00
SI                  1024
MC2                   QF
SF          125.8079004 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0
```

COMPOUND 1
NOESY

AVANCE AV-500




```
NAME            mar09-12
EXPNO                  4
PROCNO                 1
Date_           20120309
Time               12.16
INSTRUM            spect
PROBHD   5 mm CPDUL 13C
PULPROG         noesygpph
TD                  2048
SOLVENT             MeOD
NS                     8
DS                     2
SWH            3501.401 Hz
FIDRES         1.709668 Hz
AQ           0.2926472 sec
RG                  35.9
DW               142.800 usec
DE                  6.50 usec
TE                293.0 K
D0            0.00012561 sec
D1            1.50000000 sec
D8            0.80000001 sec
D16           0.00015000 sec
IN0           0.00028560 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                13.50 usec
P2                27.00 usec
PL1                2.00 dB
PL1W        11.25274181 W
SFO1        500.3317512 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPZ1               40.00 %
GPZ2              -40.00 %
P16             2000.00 usec
ND0                    1
TD                   256
SFO1            500.3318 MHz
FIDRES        13.677347 Hz
SW                6.998 ppm
FnMODE       States-TPPI
SI                  1024
SF           500.3300143 MHz
WDW                QSINE
SSB                    2
LB                  0.00 Hz
GB                     0
PC                  4.00
SI                  1024
MC2          States-TPPI
SF           500.3300143 MHz
WDW                QSINE
SSB                    2
LB                  0.00 Hz
GB                     0
```