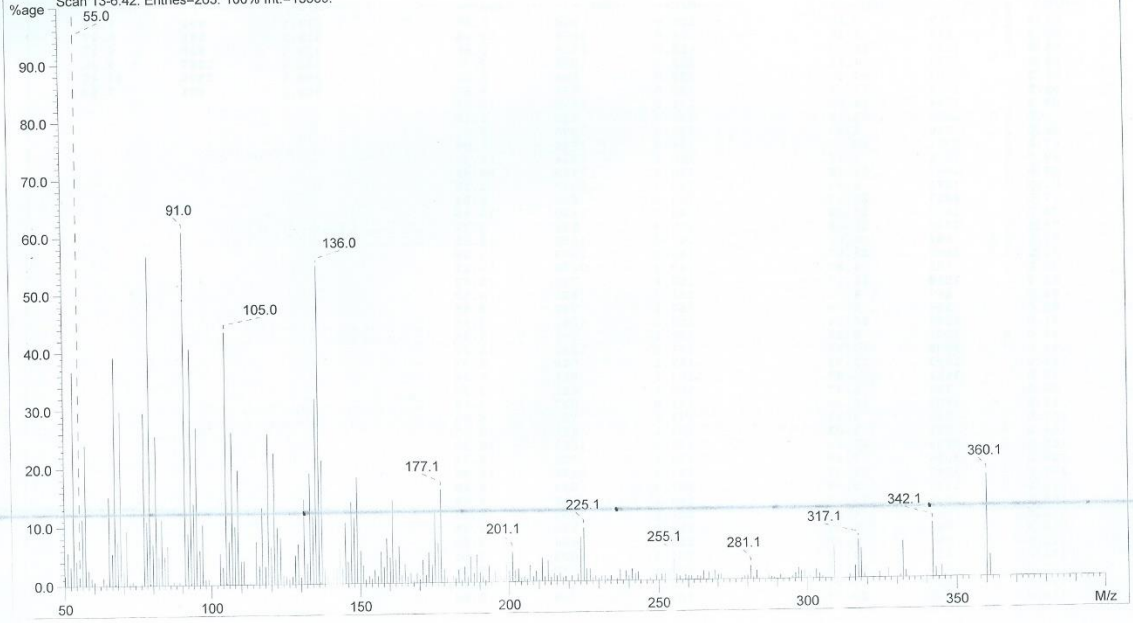
50/52

COMPOUND 8
EI-MS

Instrument : MAT312

SCAN GRAPH. Flagging=M/z.
Scan 13-6:42. Entries=263. 100% Int.=13589.

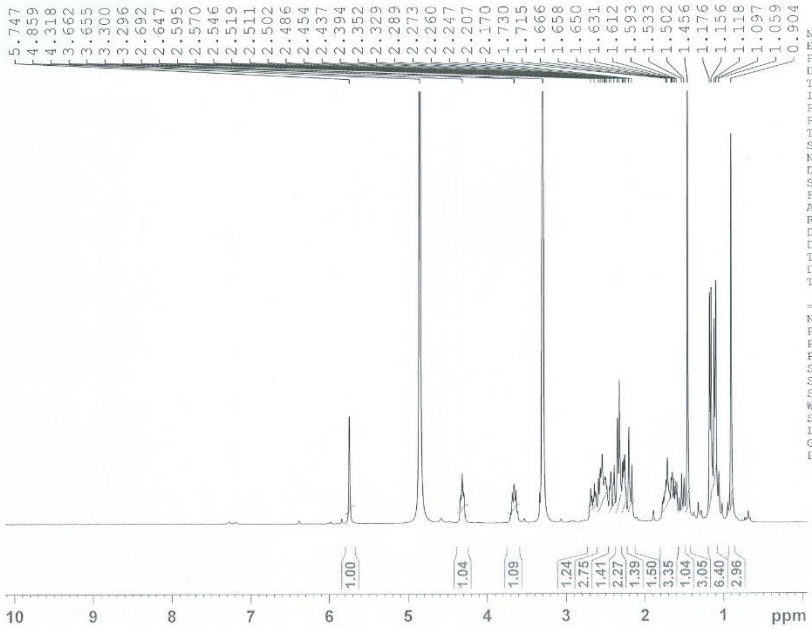


COMPOUND 6
HREI-MS

Mass	Relative Intensity	Theoretical Mass	Delta [mmu]	RDB	Composition
354.9792	1.6	354.9873	-8.1	19.5	$C_{20}H_3O_7$
360.2295	8.0	360.2295	0.0	7.0	$C_{22}H_{32}O_4$
361.2343	1.9	361.2373	-3.1	6.5	$C_{22}H_{33}O_4$
366.9792	1.0	366.9873	-8.1	20.5	$C_{21}H_3O_7$

COMPOUND 8
H-NMR

AVANCE AV - III
300 MHz, LAB # 116



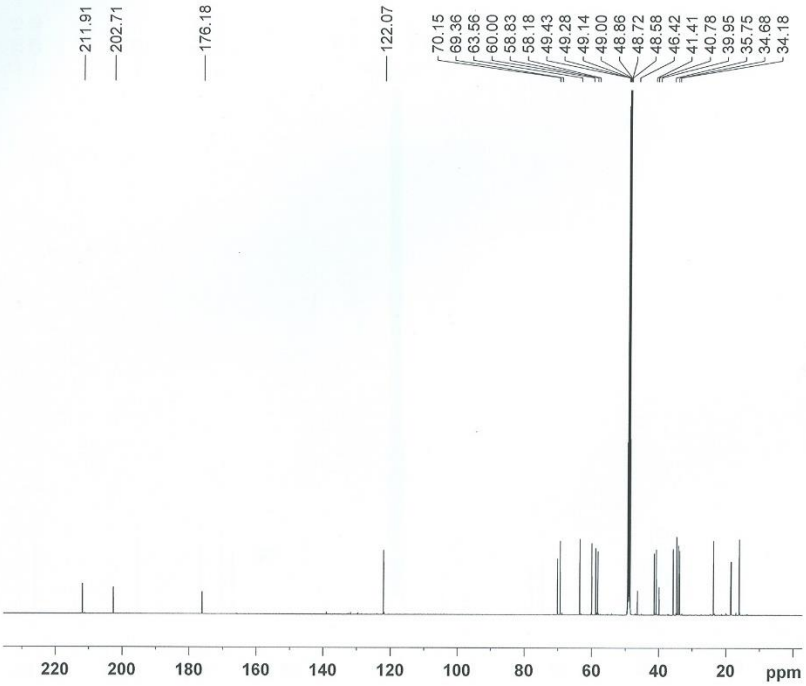

```
NAME                Nov08
EXPNO                   2
PROCNO                  1
Date_            20121108
Time                10.57
INSTRUM             Spect
PROBHD    5 mm BBO BB-1H
PULPROG              zg30
TD                  32768
SOLVENT              MeOD
NS                     32
DS                      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          300.1300073 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.00
```

H.E.J. Research Institute of Chemistry.

COMPOUND 8
BB

AVANCE AV-600
CRYO PROBE
LAB NO: 108

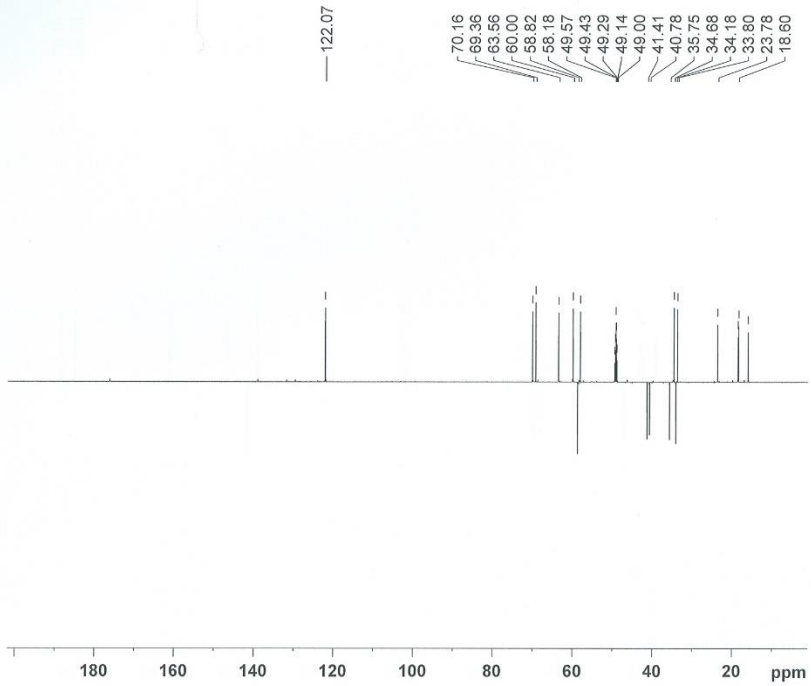



```
NAME            nov-13-12
EXPNO                   6
PROCNO                  1
Date_            20121113
Time                21.11
INSTRUM             spect
PROBHD    5 mm CPTCI 1H-
PULPROG              zgpg
TD                  65536
SOLVENT              MeOD
NS                   8192
DS                      2
SWH            35971.223 Hz
FIDRES          0.548877 Hz
AQ             0.9110143 sec
RG                  32768
DW               13.900 usec
DE                 6.50 usec
TE                298.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                     8

======== CHANNEL f1 ========
NUC1                   13C
P1                 15.40 usec
PL1                 1.00 dB
PL1W        83.60149384 W
SFO1       150.9453107 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2              65.00 usec
PL2                 3.30 dB
PL12               22.06 dB
PL13               27.00 dB
PL2W        9.16420078 W
PL12W       0.12192553 W
PL13W       0.03909260 W
SFO2        600.2336014 MHz
SI                 32768
SF         150.9277408 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.10
```

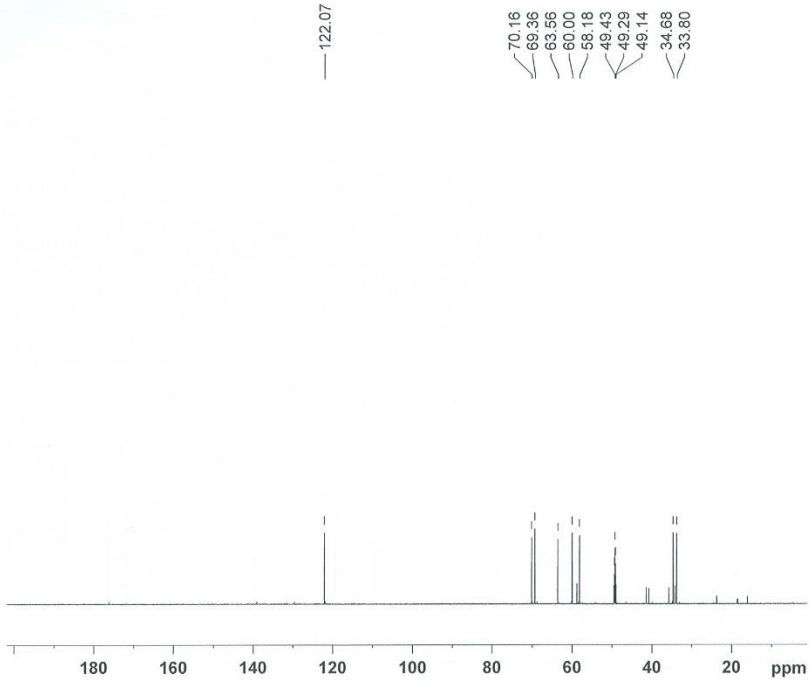
COMPOUND 8
DEPT-135



AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	nov-13-12
EXPNO	7
PROCNO	1
Date_	20121114
Time	2.52
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	deptsp135
TD	65536
SOLVENT	MeOD
NS	6144
DS	2
SWH	30303.031 Hz
FIDRES	0.462388 Hz
AQ	1.0814105 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	16.00 usec
P12	2000.00 usec
PL0	120.00 dB
PL1	2.00 dB
PL0W	0.00000000 W
PL1W	66.40702820 W
SFO1	150.9430468 MHz
SP2	1.99 dB
SPNAM2	Crp60comp.4
SPOAL2	0.500
SPOFFS2	0.00 Hz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
P3	7.50 usec
P4	15.00 usec
PCPD2	65.00 usec
PL2	3.30 dB
PL12	22.06 dB
PL2W	9.16420078 W
PL12W	0.12192553 W
SFO2	600.2324009 MHz
SI	32768
SF	150.9277408 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

COMPOUND 8
DEPT-90

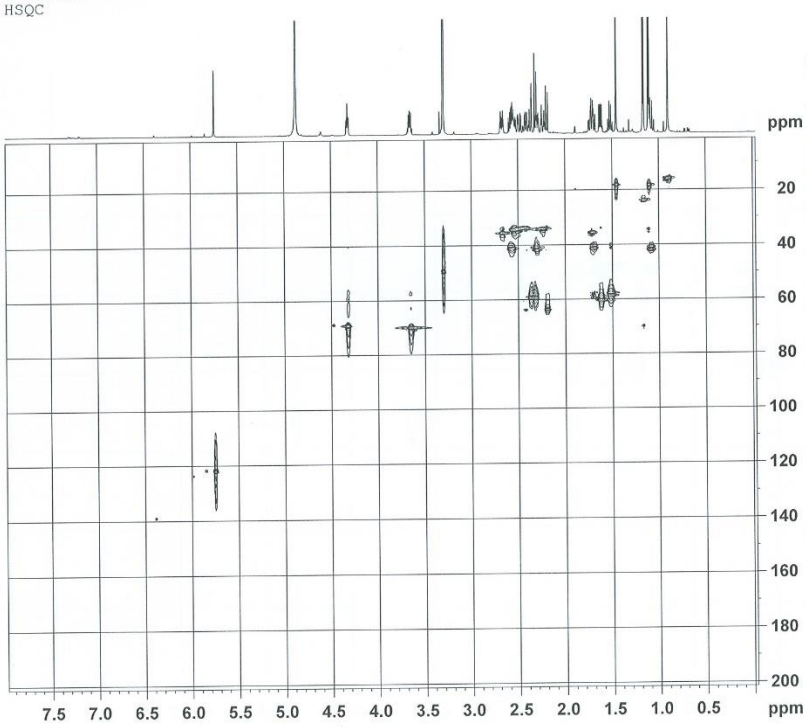


AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	nov-13-12
EXPNO	8
PROCNO	1
Date_	20121114
Time	7.22
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	deptsp90
TD	65536
SOLVENT	MeOD
NS	1166
DS	2
SWH	30303.031 Hz
FIDRES	0.462388 Hz
AQ	1.0814105 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	4
======== CHANNEL f1 ========	
NUC1	13C
P1	16.00 usec
P12	2000.00 usec
PL0	120.00 dB
PL1	2.00 dB
PL0W	0.00000000 W
PL1W	66.40702820 W
SFO1	150.9430468 MHz
SP2	1.99 dB
SPNAM2	Crp60comp.4
SPOAL2	0.500
SPOFFS2	0.00 Hz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
P3	7.50 usec
P4	15.00 usec
PCPD2	65.00 usec
PL2	3.30 dB
PL12	22.06 dB
PL2W	9.16420078 W
PL12W	0.12192553 W
SFO2	600.2324009 MHz
SI	32768
SF	150.9277408 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

COMPOUND 8

HSQC

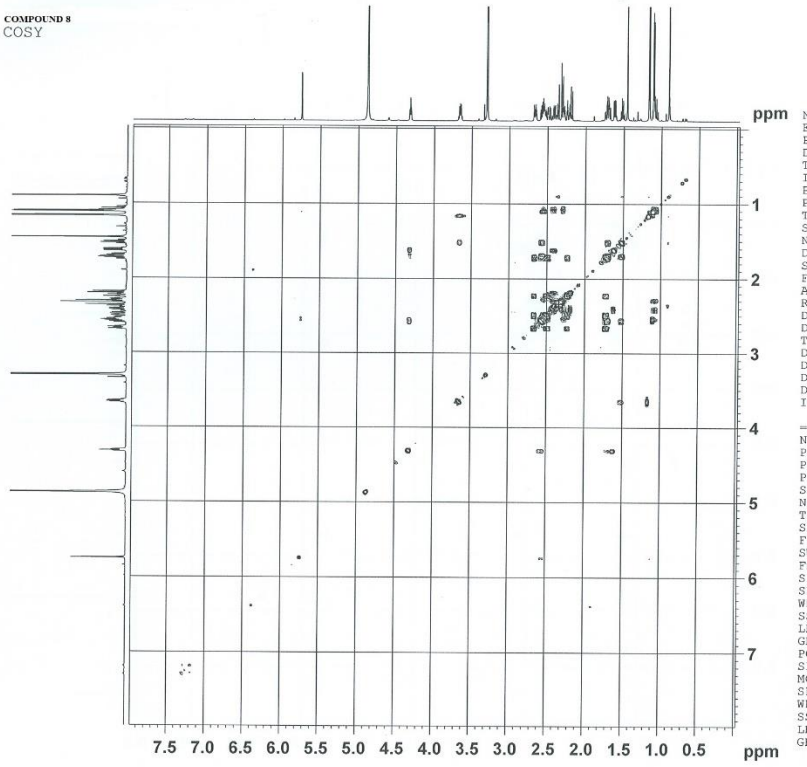


AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	nov-13-12
EXPNO	4
PROCNO	1
Date_	20121113
Time	12.14
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	hsqcetgpsi
TD	1024
SOLVENT	MeOD
NS	32
DS	8
SWH	4807.692 Hz
FIDRES	4.695012 Hz
AQ	0.1066500 sec
RG	26008
DW	104.000 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	0.00015000 sec
D24	0.00110000 sec
IN0	0.00001655 sec
ZGOPTNS	
======== CHANNEL f1 ========	
NUC1	1H
P1	7.20 usec
P2	14.40 usec
P28	0.50 usec
PL1	3.30 dB
PL1W	9.16420078 W
SFO1	600.2324009 MHz
======== CHANNEL f2 ========	
CPDPRG2	garp
NUC2	13C
P3	15.40 usec
P4	30.80 usec
PCPD2	61.00 usec
PL2	1.00 dB
PL12	13.00 dB
PL2W	83.60149384 W
PL12W	5.27489758 W
SFO2	150.9430468 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	80.00 %
GPZ2	20.10 %
P16	2000.00 usec
ND0	2

COMPOUND 8

COSY

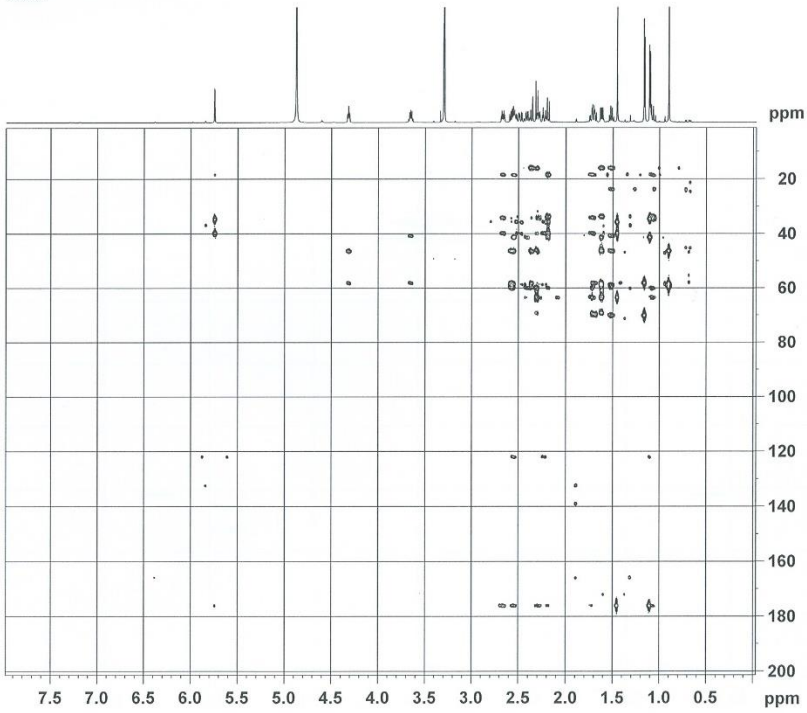


AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	nov-13-12
EXPNO	2
PROCNO	1
Date_	20121113
Time	9.51
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	cosydfqf
TD	2048
SOLVENT	MeOD
NS	8
DS	4
SWH	4807.692 Hz
FIDRES	2.347506 Hz
AQ	0.2131460 sec
RG	32
DW	104.000 usec
DE	6.50 usec
TE	298.0 K
D0	0.00000300 sec
D1	1.50000000 sec
D13	0.00000400 sec
D20	0.00000200 sec
IN0	0.00020800 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	7.20 usec
PL1	3.30 dB
PL1W	9.16420078 W
SFO1	600.2324009 MHz
ND0	1
TD	256
SFO1	600.2324 MHz
FIDRES	18.780046 Hz
SW	8.010 ppm
FnMODE	QF
SI	1024
SF	600.2300156 MHz
WDW	QSINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	600.2300156 MHz
WDW	QSINE
SSB	0
LB	0.00 Hz
GB	0

COMPOUND 8

HMBC

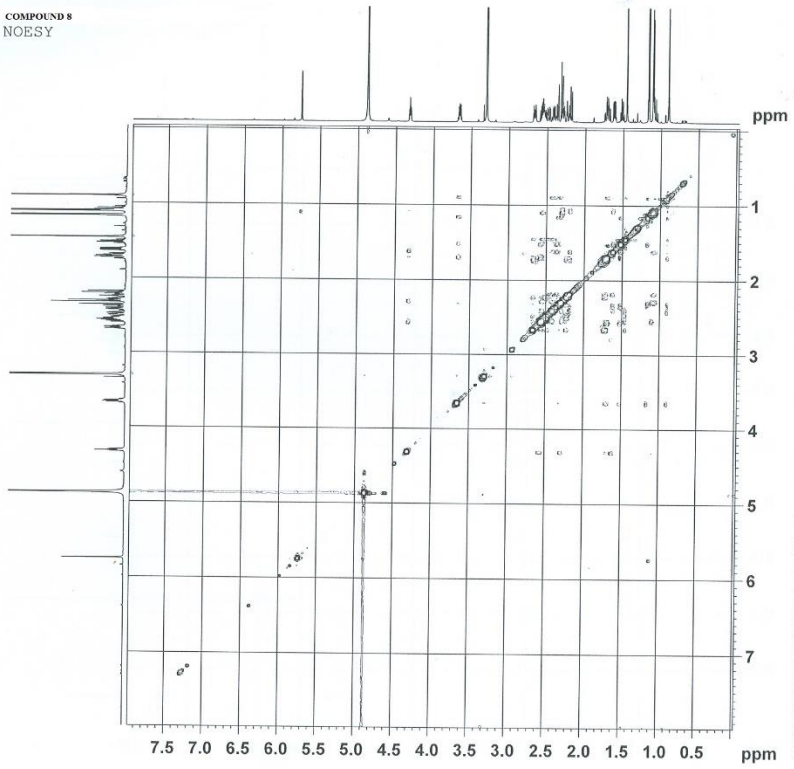


AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	nov-13-12
EXPNO	5
PROCNO	1
Date_	20121113
Time	15.58
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	hmbcgplpndqf
TD	4096
SOLVENT	MeOD
NS	32
DS	8
SWH	4807.692 Hz
FIDRES	1.173753 Hz
AQ	0.4261380 sec
RG	36780.8
DW	104.000 usec
DE	6.50 usec
TE	298.0 K
CNST2	145.0000000
CNST13	13.0000000
D0	0.00000300 sec
D1	1.50000000 sec
D2	0.00344828 sec
D6	0.03846154 sec
D16	0.00015000 sec
IN0	0.00001440 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	7.20 usec
P2	14.40 usec
PL1	3.30 dB
PL1W	9.16420078 W
SFO1	600.2324009 MHz
======== CHANNEL f2 ========	
NUC2	13C
P3	15.40 usec
PL2	1.00 dB
PL2W	83.60149384 W
SFO2	150.9453107 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	150.9453 MHz
FIDRES	135.614929 Hz
SW	230.000 ppm
FnMODE	QF
SI	1024

COMPOUND 8

NOESY



AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	nov-13-12
EXPNO	3
PROCNO	1
Date_	20121113
Time	10.51
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	noesygpph
TD	1024
SOLVENT	MeOD
NS	8
DS	4
SWH	4807.692 Hz
FIDRES	4.695012 Hz
AQ	0.1066500 sec
RG	64
DW	104.000 usec
DE	6.50 usec
TE	298.0 K
D0	0.00009483 sec
D1	1.50000000 sec
D8	0.80000001 sec
D16	0.00015000 sec
IN0	0.00020800 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	7.20 usec
P2	14.40 usec
PL1	3.30 dB
PL1W	9.16420078 W
SFO1	600.2324009 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	40.00 %
GPZ2	-40.00 %
P16	2000.00 usec
ND0	1
TD	256
SFO1	600.2324 MHz
FIDRES	18.780046 Hz
SW	8.010 ppm
FnMODE	States-TPPI
SI	1024
SF	600.2300156 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	States-TPPI
SF	600.2300156 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0