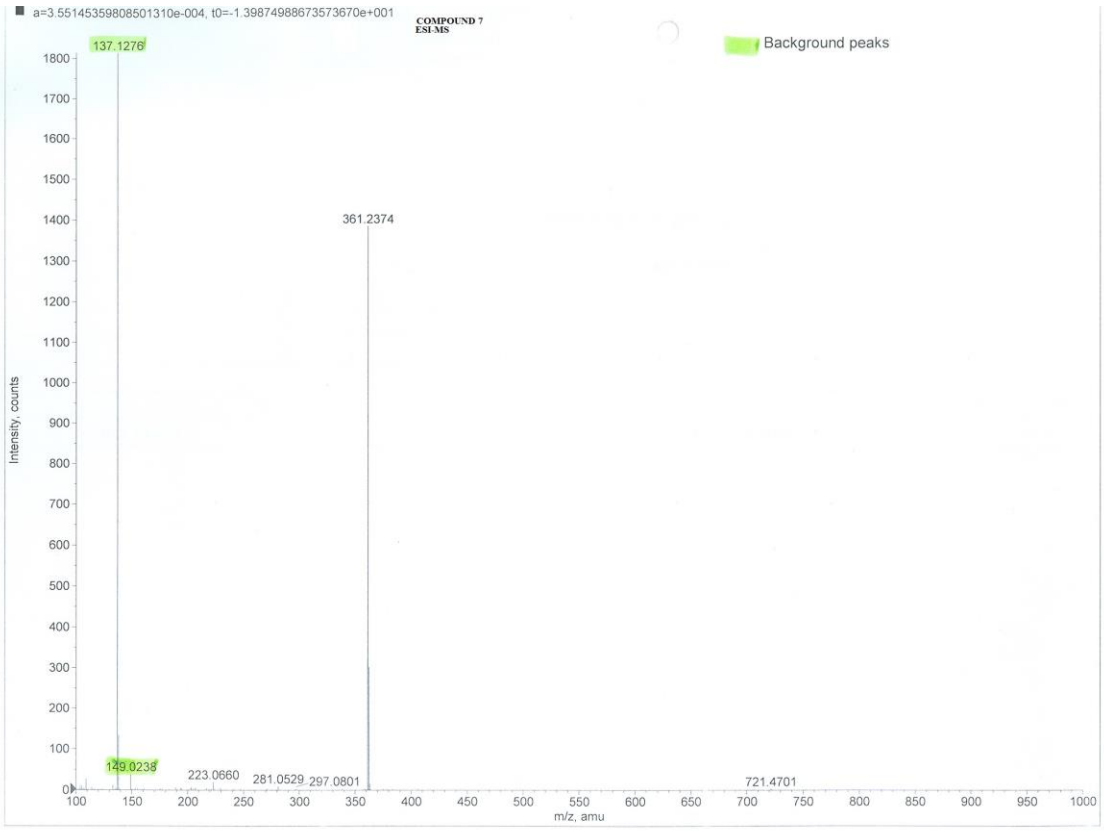


COMPOUND 7
HRESI-MS

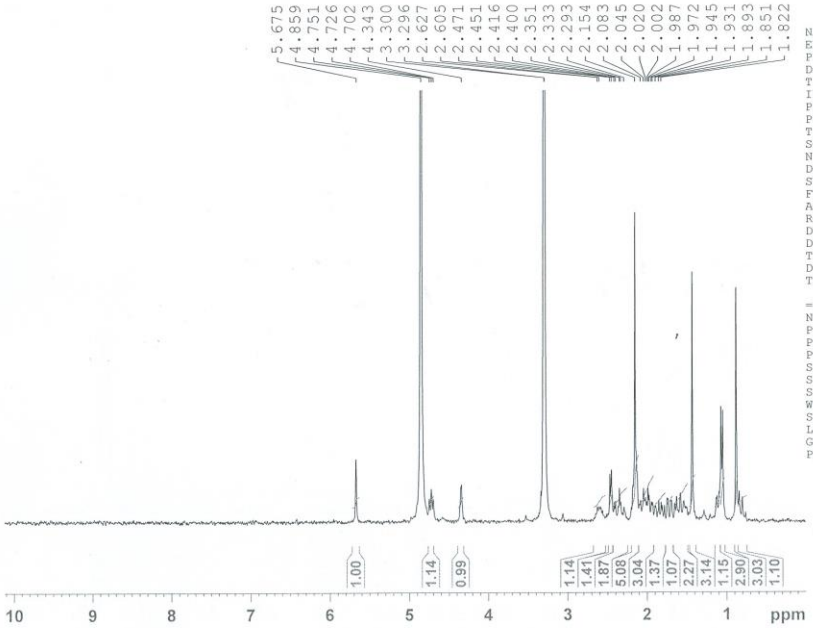
Target m/z: +361.2374 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 100
Min DBE: -0.5000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: MEDCB-4 25-2-13.wiff

	Elements	Min Number	Max Number
1	C	0	30
2	H	0	50
3	O	0	4

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C22 H33 O4	361.2378	-0.4848	-1.3422	6.5

COMPOUND 7
H-NMR

AVANCE AV - III
300 MHz, LAB # 116



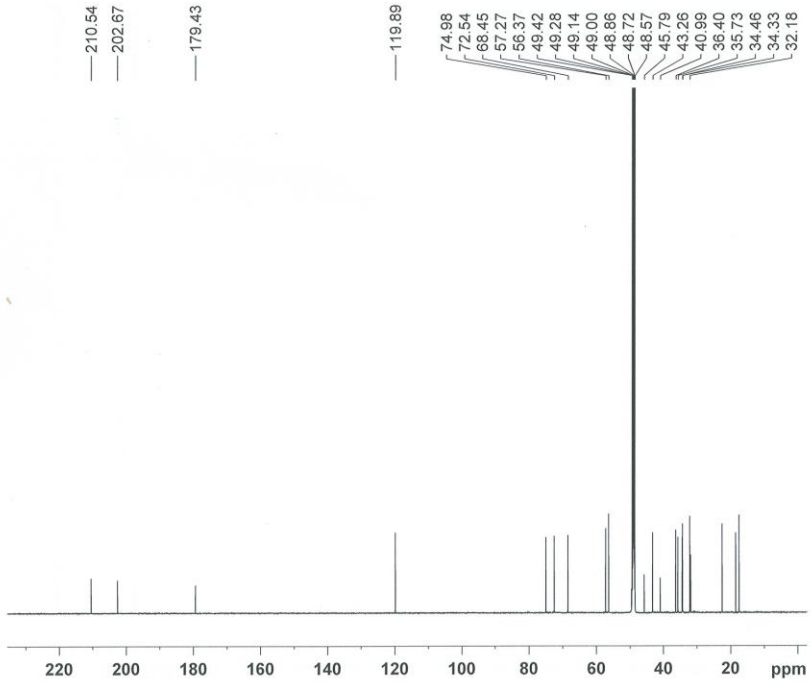

```
NAME              Nov08
EXPNO               1
PROCNO              1
Date_           20121108
Time               10.49
INSTRUM            Spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT             MeOD
NS                    32
DS                     0
SWH            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          300.1300072 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.00
```

H.E.J. Research Institute of Chemistry.

COMPOUND 7
BB

AVANCE AV-600
CRYO PROBE
LAB NO: 108

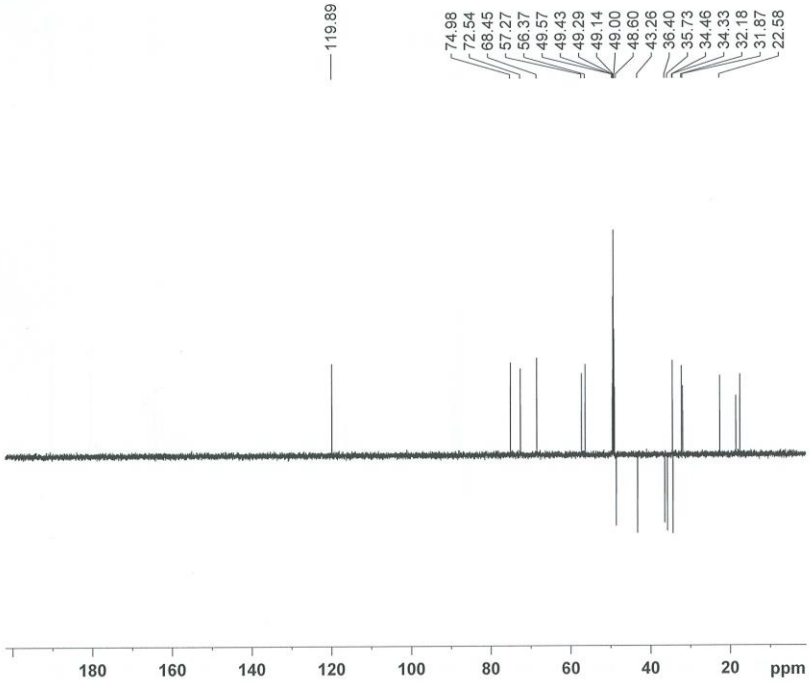



```
NAME            nov-15-12
EXPNO                  11
PROCNO                  1
Date_           20121116
Time                 3.14
INSTRUM             spect
PROBHD   5 mm CPTCI 1H-
PULPROG             zgpg
TD                  65536
SOLVENT              MeOD
NS                   8192
DS                      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          150.9277406 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.10
```

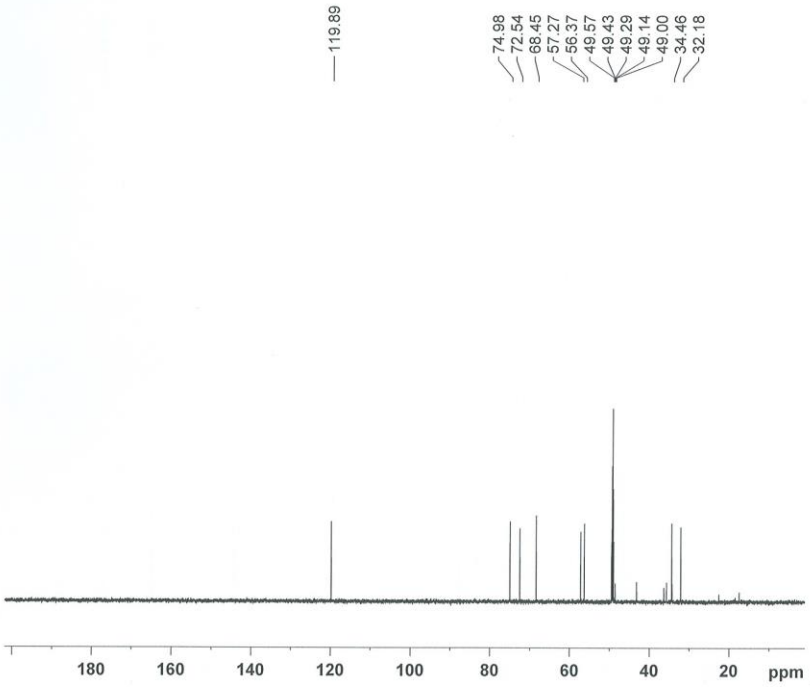
COMPOUND 6
DEPT-135



AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	nov-15-12
EXPNO	12
PROCNO	1
Date_	20121116
Time	8.34
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	deptsp135
TD	65536
SOLVENT	MeOD
NS	560
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	150.9277406 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

COMPOUND 7
DEPT-90

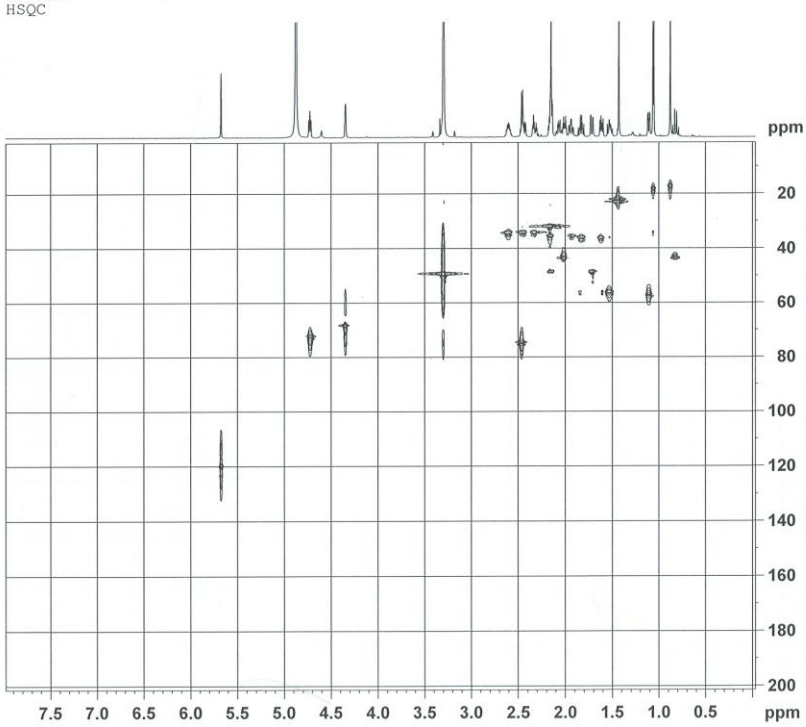


AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	nov-15-12
EXPNO	13
PROCNO	1
Date_	20121116
Time	9.02
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	deptsp90
TD	65536
SOLVENT	MeOD
NS	621
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	150.9277406 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

COMPOUND 7

HSQC

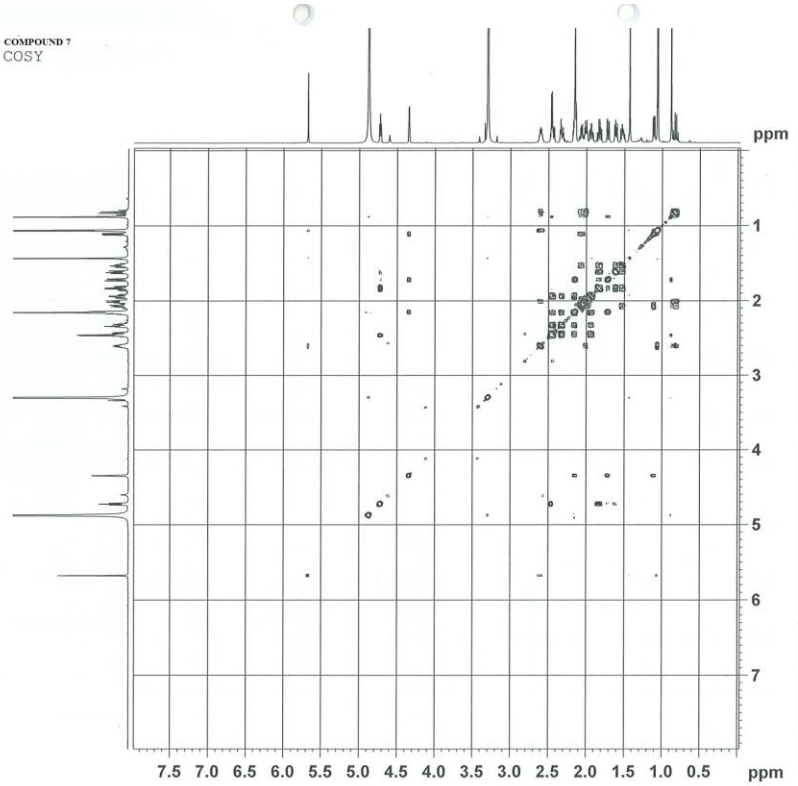


AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	nov-15-12
EXPNO	9
PROCNO	1
Date_	20121115
Time	18.19
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 7

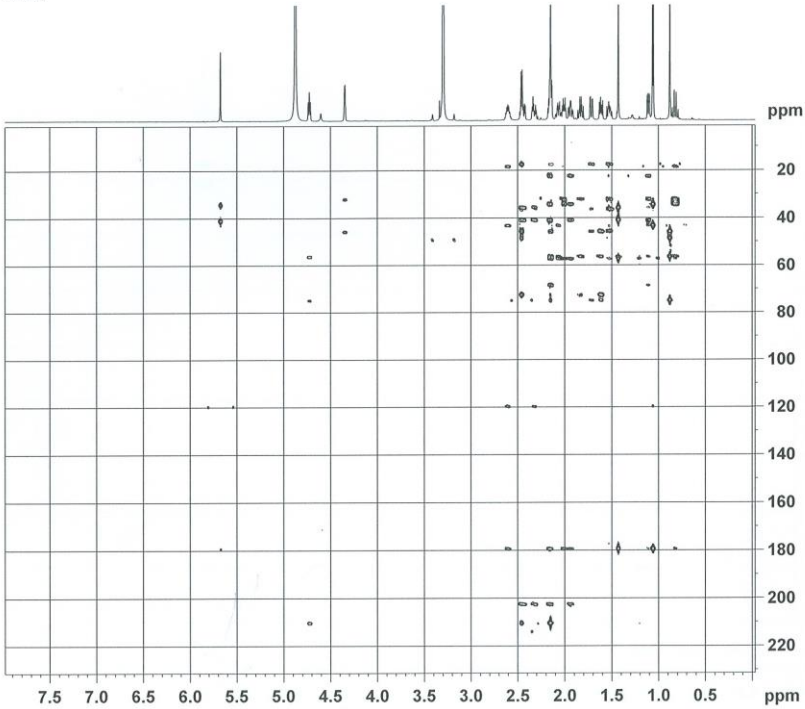
COSY



AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	nov-15-12
EXPNO	7
PROCNO	1
Date_	20121115
Time	15.55
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	298.1 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 7
HMBC



AVANCE AV-600
CRYO PROBE
LAB NO: 108

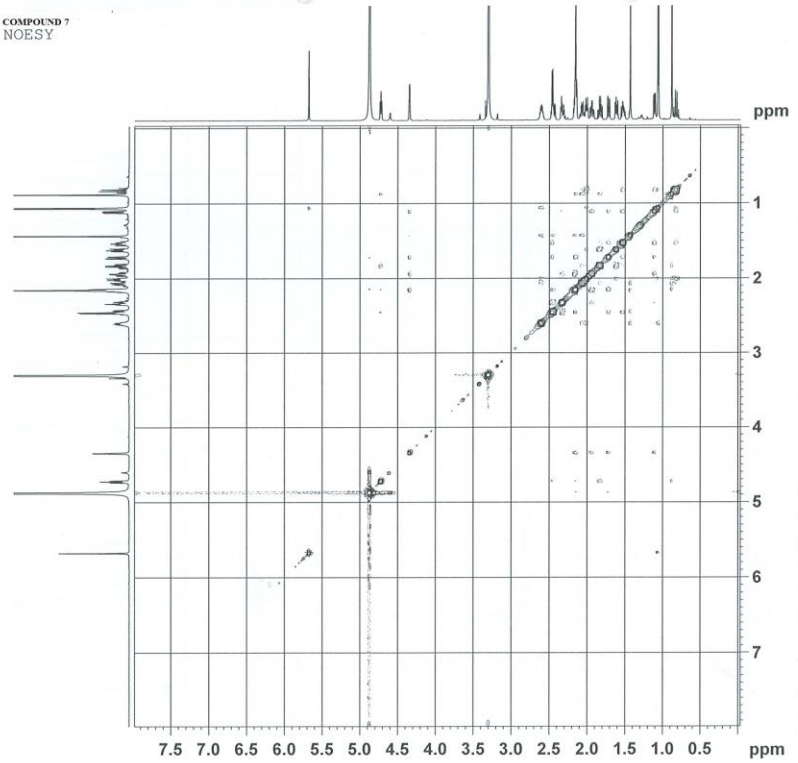
```
NAME          nov-15-12
EXPNO                10
PROCNO                1
Date_          20121115
Time              22.02
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG    hmbcgplpndqf
TD                 4096
SOLVENT            MeOD
NS                   32
DS                    8
SWH            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 7
NOESY



AVANCE AV-600
CRYO PROBE
LAB NO: 108

```
NAME          nov-15-12
EXPNO                 8
PROCNO                1
Date_          20121115
Time              16.55
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                   57
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
```