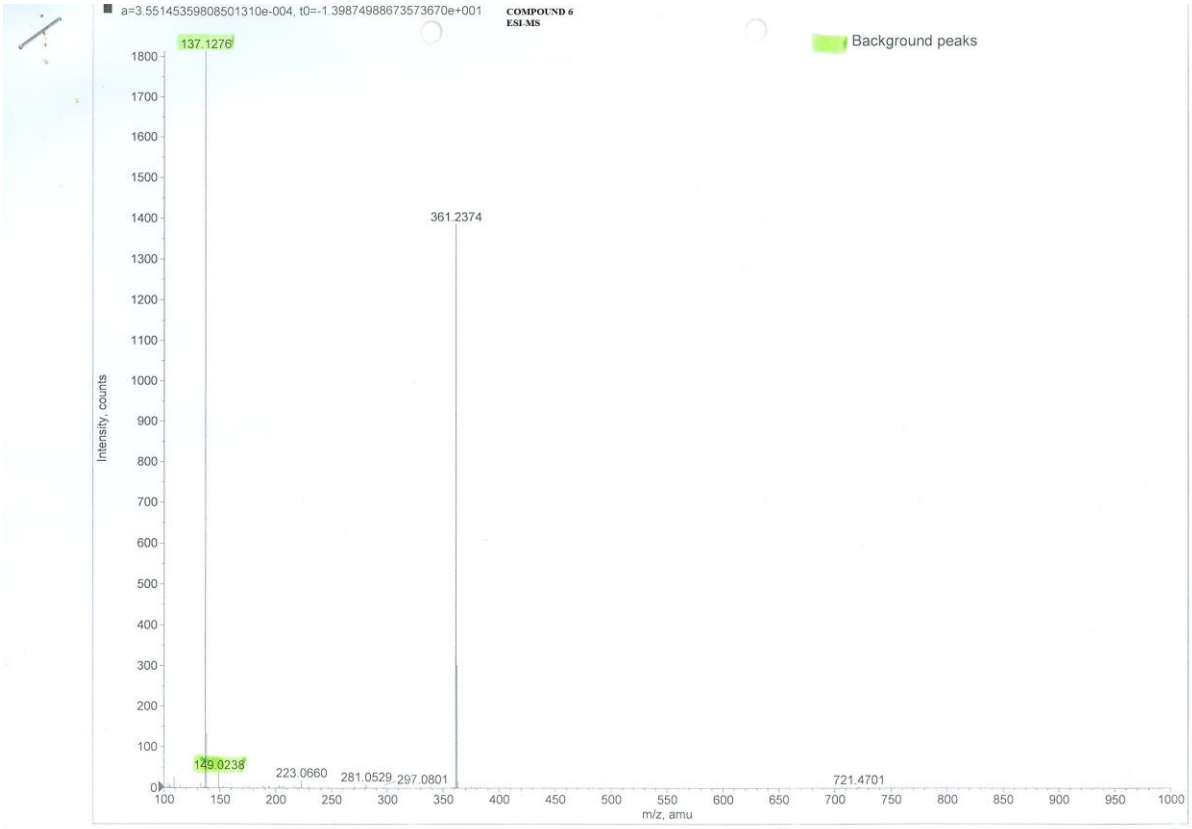


COMPOUND 6
HRESI-MS

B

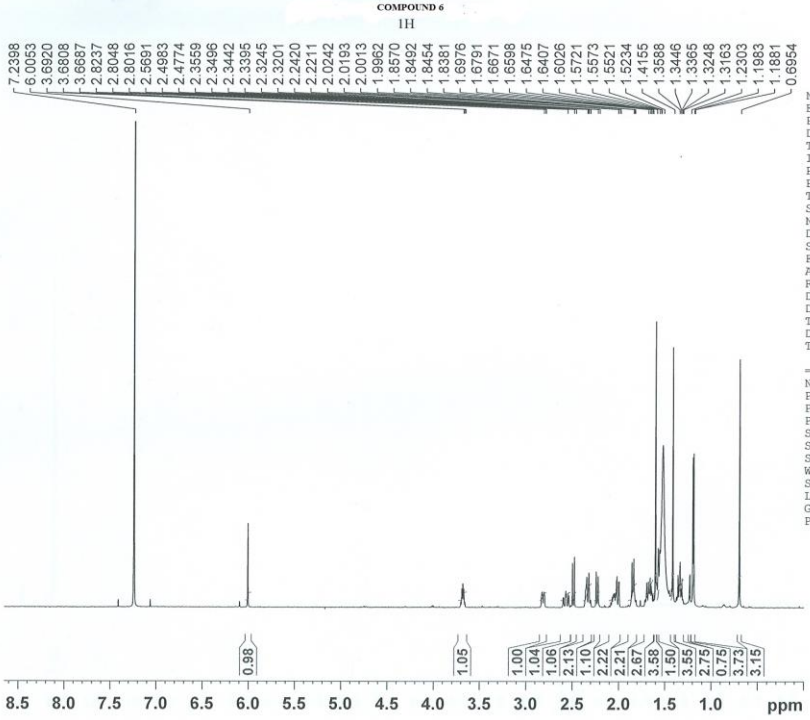
Target m/z: +361.2382 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 100
Min DBE: -0.5000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: MEDCB-4a 25-2-13.wiff

	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	0.3151	0.8723	6.5

COMPOUND 6

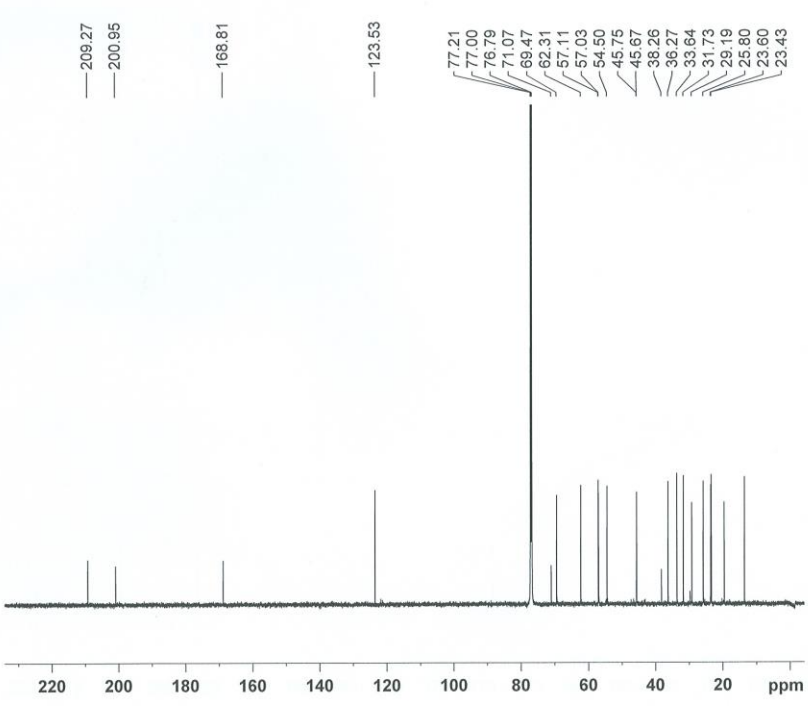
1H



AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	dec-16-12
EXPNO	1
PROCNO	1
Date_	20121216
Time	10.32
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3632404 sec
RG	9
DW	41.600 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	7.20 usec
PL1	3.30 dB
PL1W	9.16420078 W
SFO1	600.2354021 MHz
SI	16384
SF	600.2300251 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	0.50

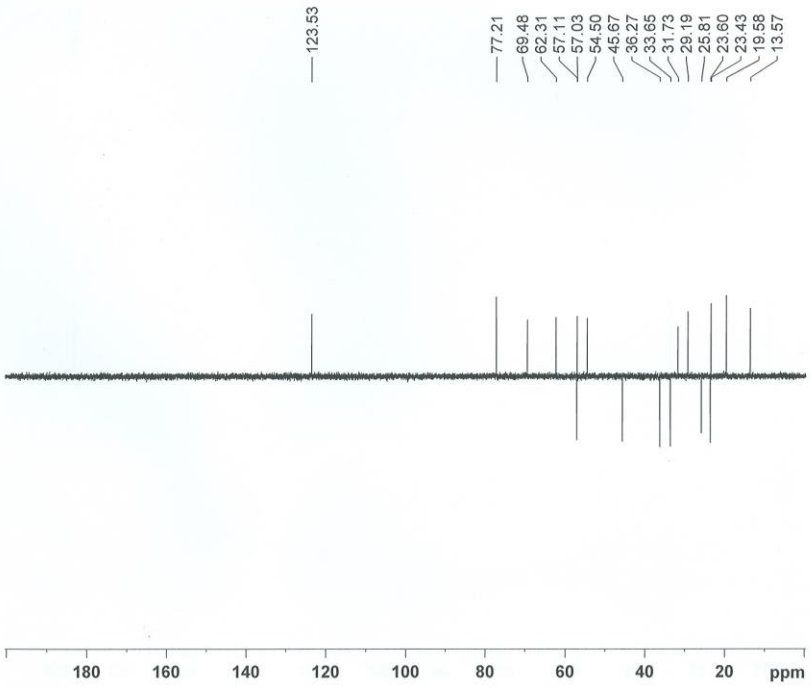
COMPOUND 6
BB



AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	dec-16-12
EXPNO	6
PROCNO	1
Date_	20121216
Time	21.47
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	zgpg
TD	65536
SOLVENT	CDCl3
NS	12288
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	294.5 K
D1	1.50000000 sec
D11	0.03000000 sec
TD0	12
======== 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	150.9279594 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.10

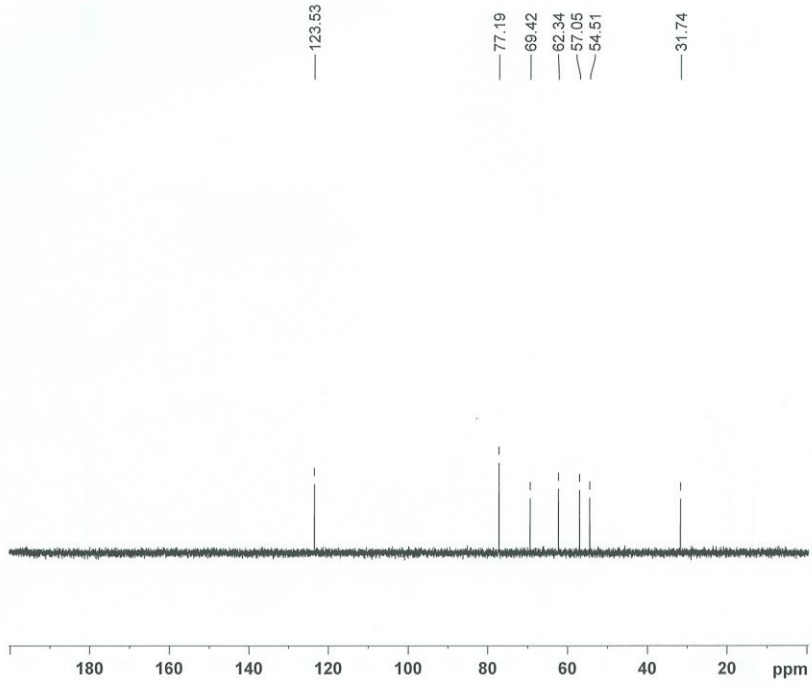
COMPOUND 6
DEPT-135



AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	dec-16-12
EXPNO	7
PROCNO	1
Date_	20121217
Time	6.18
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	deptsp135
TD	65536
SOLVENT	CDCl3
NS	2486
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	294.3 K
CNST2	145.0000000
D1	1.50000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	6
======== CHANNEL f1 ========	
NUC1	13C
P1	15.40 usec
P12	2000.00 usec
PL0	120.00 dB
PL1	1.00 dB
PL0W	0.00000000 W
PL1W	83.60149384 W
SFO1	150.9430468 MHz
SP2	5.40 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	150.9279594 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

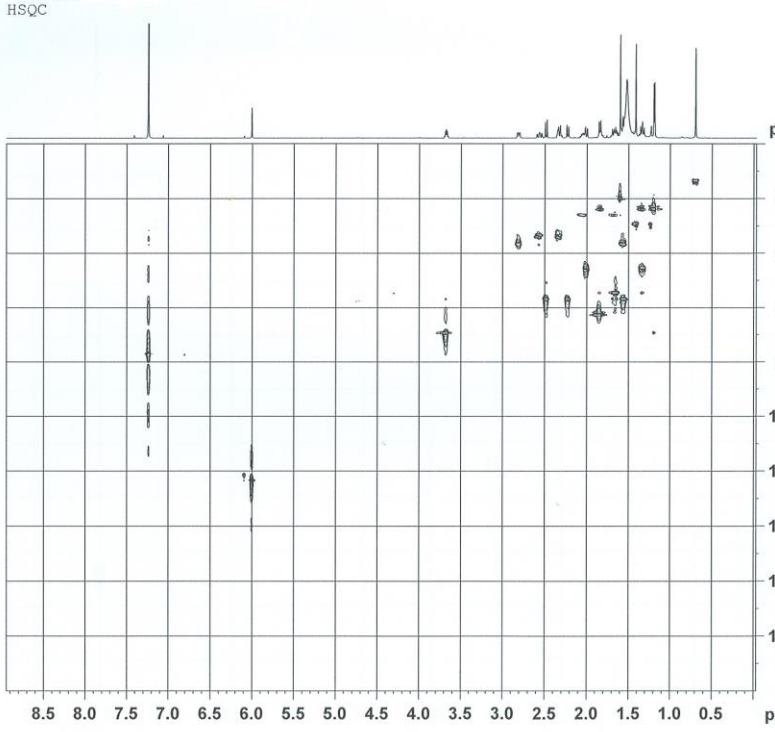
COMPOUND 6
DEPT-90



AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	dec-16-12
EXPNO	8
PROCNO	1
Date_	20121217
Time	8.00
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	deptsp90
TD	65536
SOLVENT	CDCl3
NS	864
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	15.40 usec
P12	2000.00 usec
PL0	120.00 dB
PL1	1.00 dB
PL0W	0.00000000 W
PL1W	83.60149384 W
SFO1	150.9430468 MHz
SP2	5.40 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	150.9279594 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

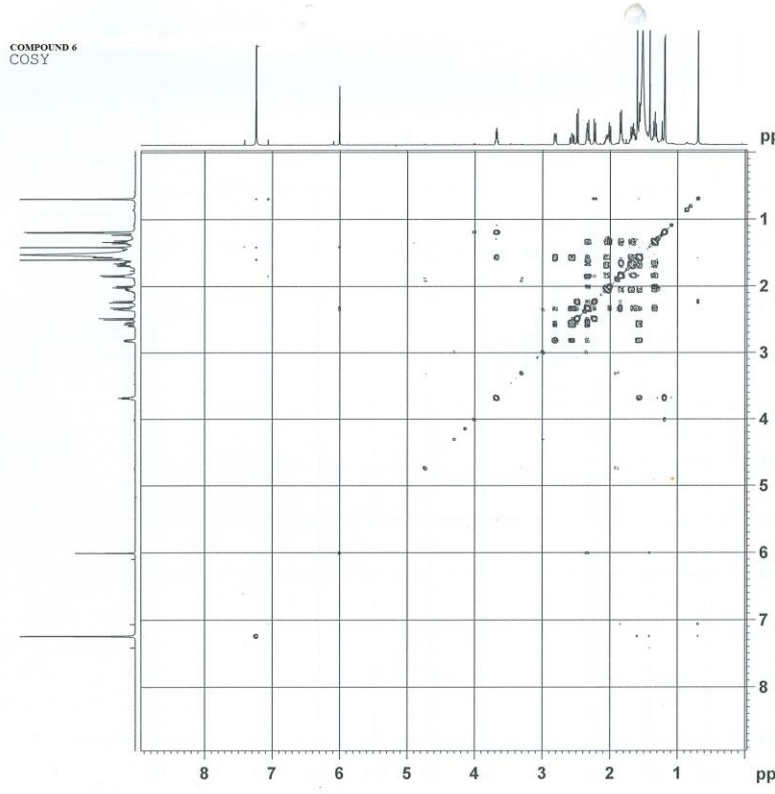
COMPOUND 6
HSQC



AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	dec-16-12
EXPNO	4
PROCNO	1
Date_	20121216
Time	13.00
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	hsqcetgpsi
TD	1024
SOLVENT	CDCl3
NS	32
DS	8
SWH	5387.931 Hz
FIDRES	5.261652 Hz
AQ	0.0951700 sec
RG	46341
DW	92.800 usec
DE	6.50 usec
TE	298.0 K
CNST2	145.00000000
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	600.2327010 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

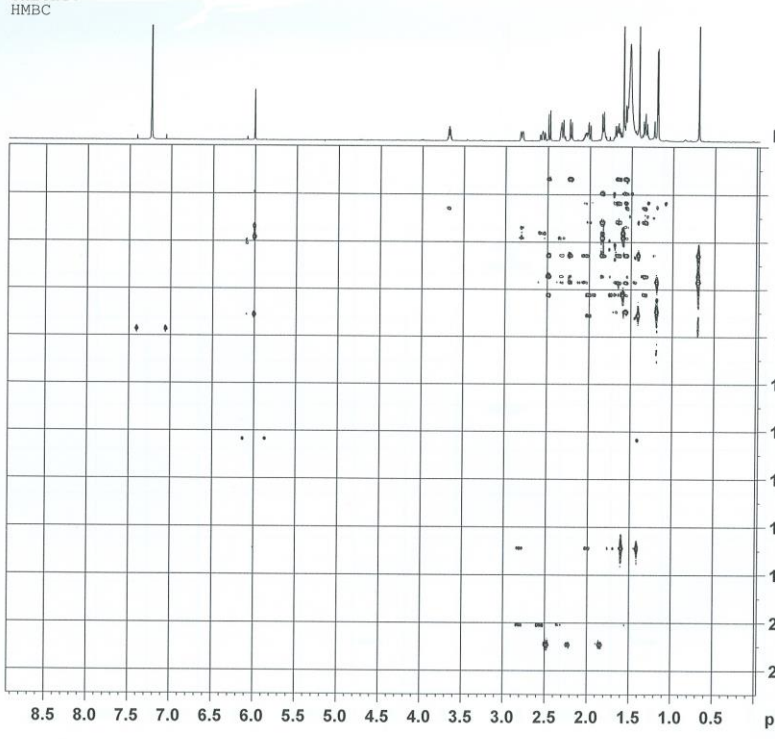
COMPOUND 6
COSY



AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	dec-16-12
EXPNO	2
PROCNO	1
Date_	20121216
Time	10.38
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	cosydfqf
TD	2048
SOLVENT	CDCl3
NS	8
DS	4
SWH	5387.931 Hz
FIDRES	2.630826 Hz
AQ	0.1901972 sec
RG	35.9
DW	92.800 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	0.00018560 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	7.20 usec
PL1	3.30 dB
PL1W	9.16420078 W
SFO1	600.2327010 MHz
ND0	1
TD	256
SFO1	600.2327 MHz
FIDRES	21.046606 Hz
SW	8.976 ppm
FnMODE	QF
SI	1024
SF	600.2300251 MHz
WDW	QSINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	600.2300251 MHz
WDW	QSINE
SSB	0
LB	0.00 Hz
GB	0

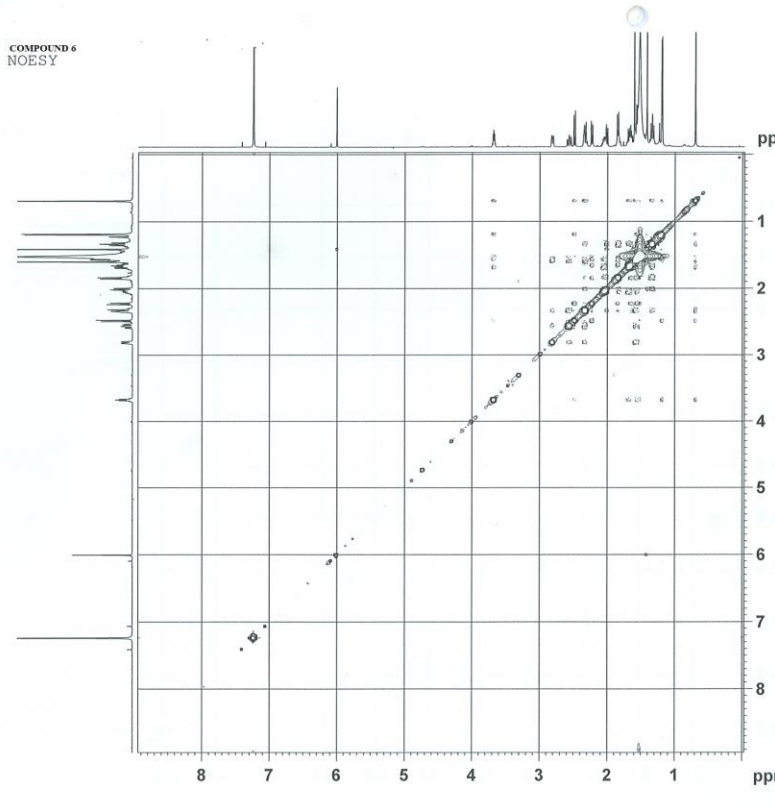
COMPOUND 6
HMBC



AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	dec-16-12
EXPNO	5
PROCNO	1
Date_	20121216
Time	16.42
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	hmbcgplpndqf
TD	4096
SOLVENT	CDCl3
NS	32
DS	8
SWH	5387.931 Hz
FIDRES	1.315413 Hz
AQ	0.3802516 sec
RG	46341
DW	92.800 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	600.2327010 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
NDO	2
TD	256
SFO1	150.9453 MHz
FIDRES	135.614929 Hz
SW	230.000 ppm
FnMODE	QF
SI	1024

COMPOUND 6
NOESY



AVANCE AV-600
CRYO PROBE
LAB NO: 108

NAME	dec-16-12
EXPNO	3
PROCNO	1
Date_	20121216
Time	11.37
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	noesygpph
TD	1024
SOLVENT	CDCl3
NS	8
DS	4
SWH	5387.931 Hz
FIDRES	5.261652 Hz
AQ	0.0951700 sec
RG	71.8
DW	92.800 usec
DE	6.50 usec
TE	298.0 K
D0	0.00008363 sec
D1	1.50000000 sec
D8	0.80000001 sec
D16	0.00015000 sec
IN0	0.00018560 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	7.20 usec
P2	14.40 usec
PL1	3.30 dB
PL1W	9.16420078 W
SFO1	600.2327010 MHz
====== GRADIENT CHANNEL ======	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	40.00 %
GPZ2	-40.00 %
P16	2000.00 usec
NDO	1
TD	256
SFO1	600.2327 MHz
FIDRES	21.046606 Hz
SW	8.976 ppm
FnMODE	States-TPPI
SI	1024
SF	600.2300251 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	States-TPPI
SF	600.2300251 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0