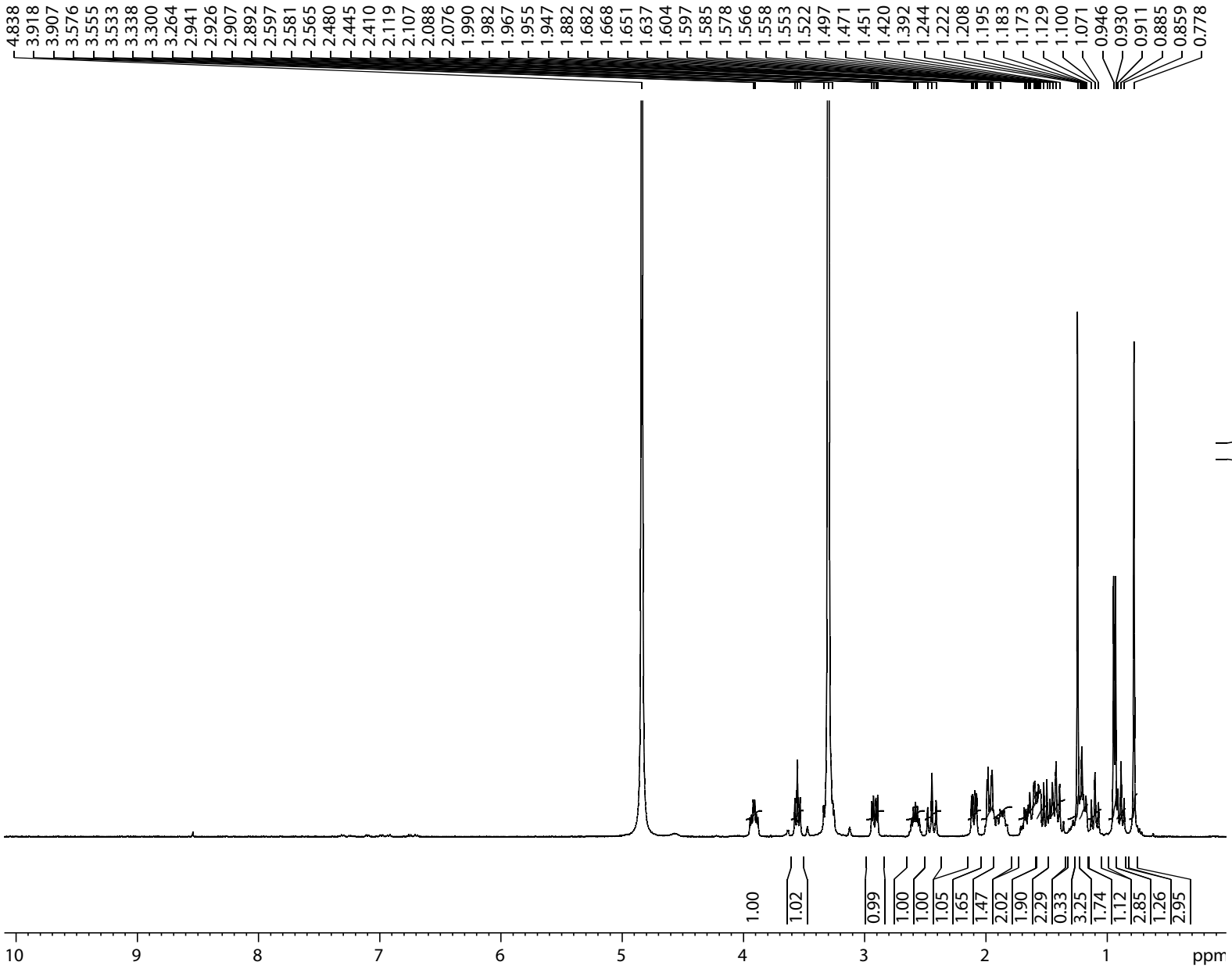
Compound 1
1H-NMR

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME nov07-13
EXPNO 1
PROCNO 1

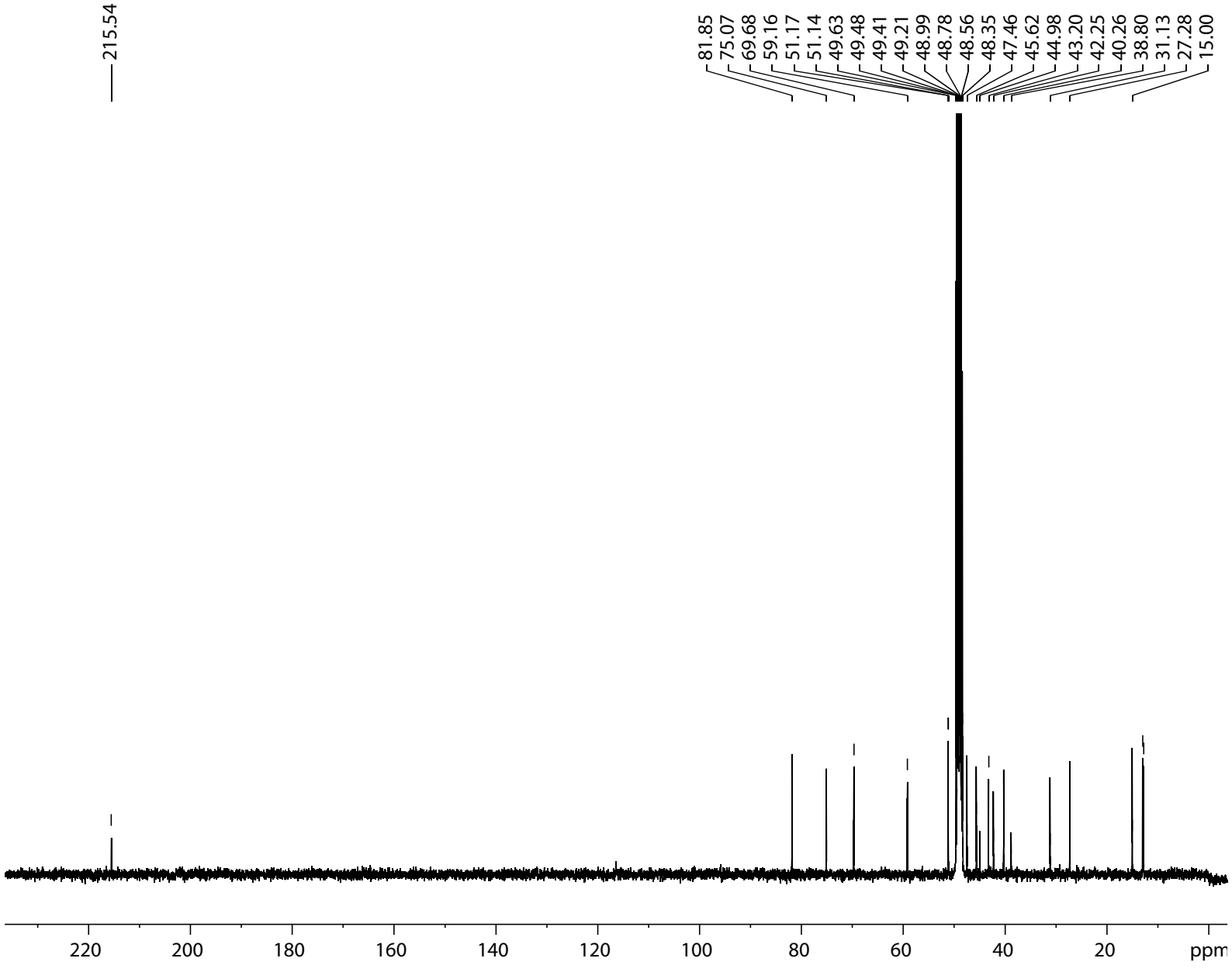
F2 - Acquisition Parameters
Date_ 20131107
Time 15.42
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT MeOD
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 322.5
DW 62.400 usec
DE 6.50 usec
TE 299.1 K
D1 1.50000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 400.0332002 MHz

F2 - Processing parameters
SI 16384
SF 400.0300087 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Compound 2
BB

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME nov07-13
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131109
Time 0.14
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg
TD 32768
SOLVENT MeOD
NS 20480
DS 2
SWH 24154.590 Hz
FIDRES 0.737140 Hz
AQ 0.6782976 sec
RG 32768
DW 20.700 usec
DE 6.50 usec
TE 297.7 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 20

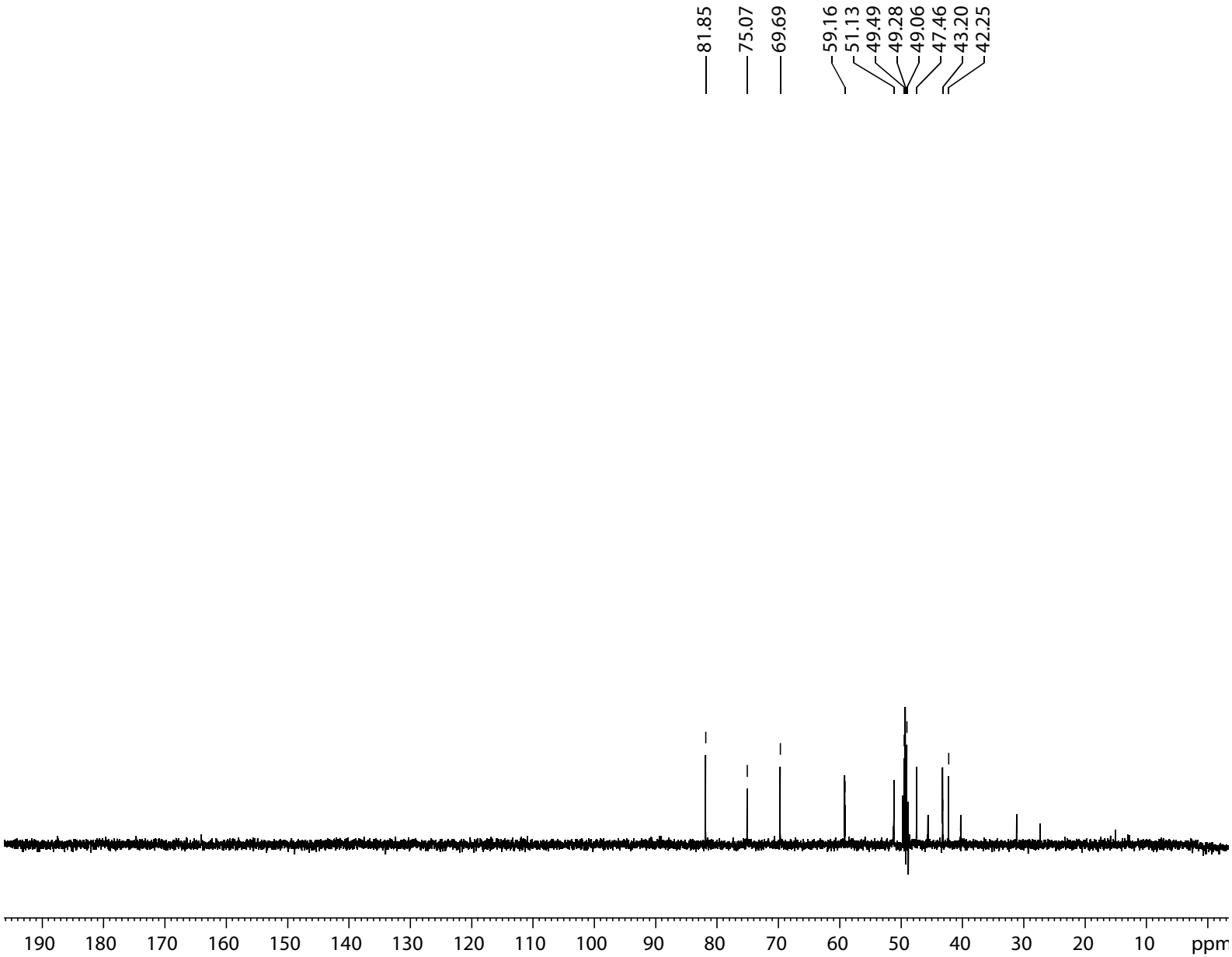
======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
PL1 -6.00 dB
SFO1 100.5991916 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
PL13 22.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874816 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Compound 2
DEPT90

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME nov07-13
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131109
Time 22.26
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG dept90
TD 32768
SOLVENT MeOD
NS 7168
DS 2
SWH 20080.320 Hz
FIDRES 0.612803 Hz
AQ 0.8159232 sec
RG 16384
DW 24.900 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 7

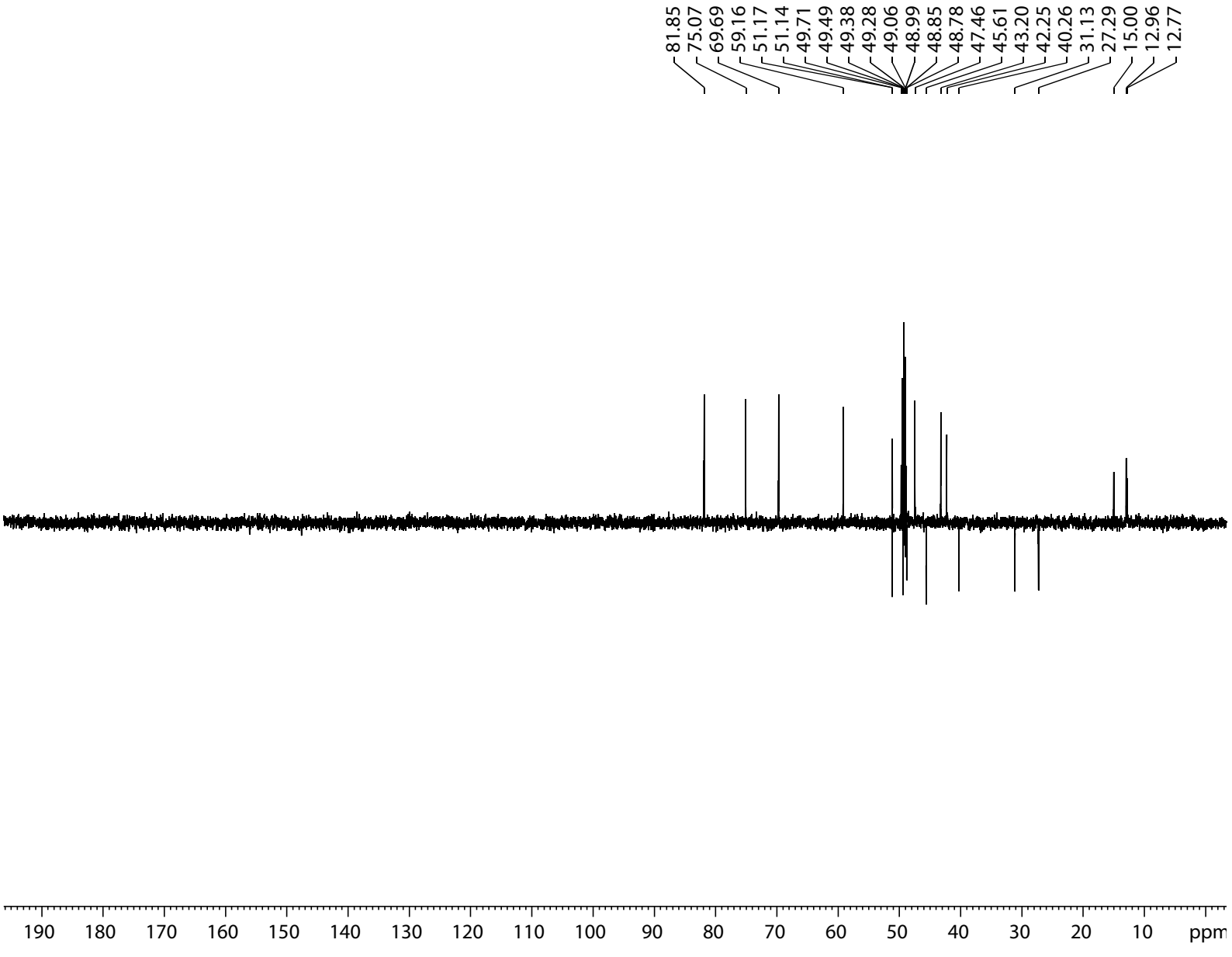
======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
P2 24.60 usec
PL1 -6.00 dB
SFO1 100.5971798 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 10.50 usec
P4 21.00 usec
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874816 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20

Compound 2
DEPT135

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME nov07-13
EXPNO 7
PROCNO 1

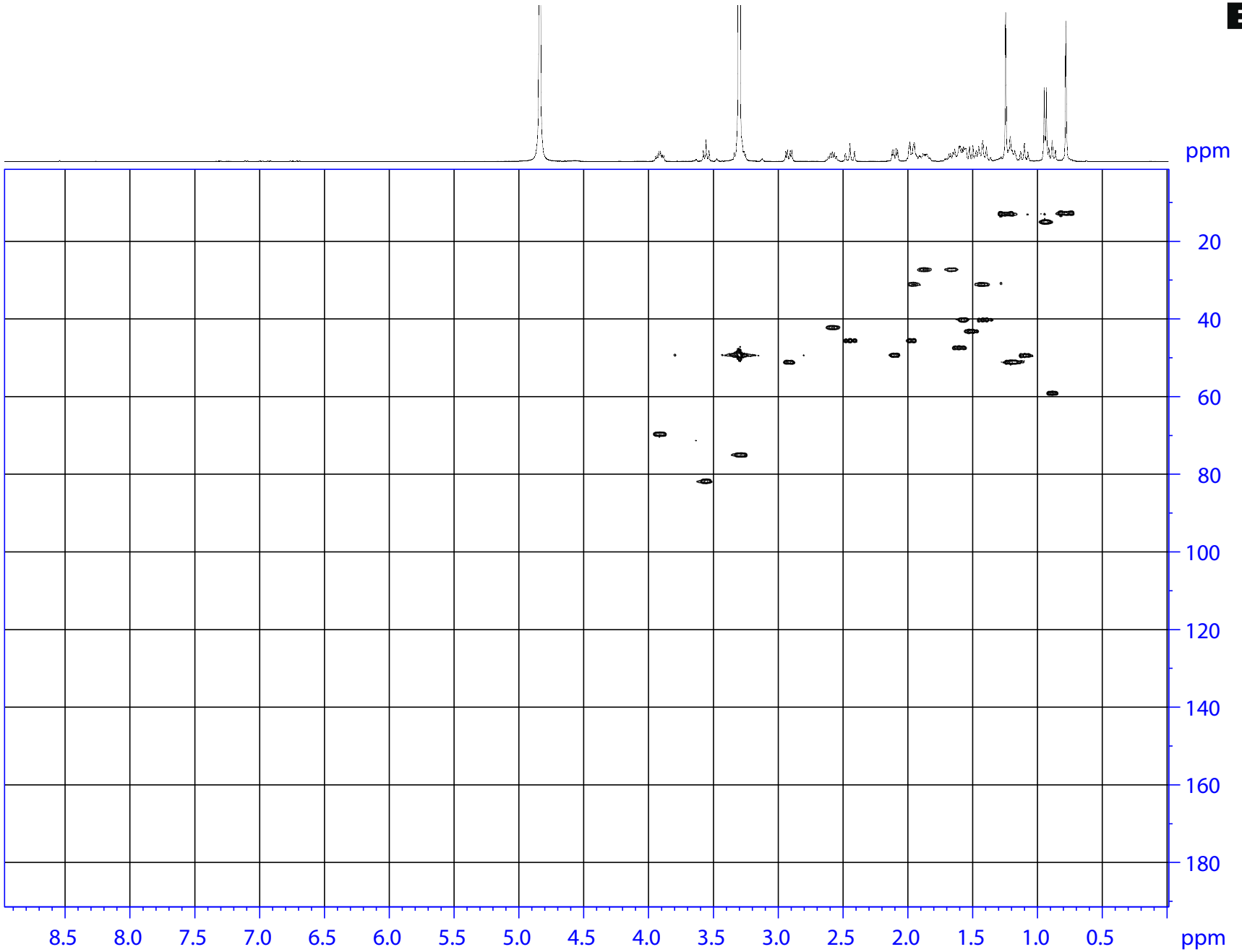
F2 - Acquisition Parameters
Date_ 20131109
Time 13.02
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG dept135
TD 32768
SOLVENT MeOD
NS 14336
DS 2
SWH 20080.320 Hz
FIDRES 0.612803 Hz
AQ 0.8159232 sec
RG 16384
DW 24.900 usec
DE 6.50 usec
TE 299.9 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 14

======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
P2 24.60 usec
PL1 -6.00 dB
SFO1 100.5971798 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 10.50 usec
P4 21.00 usec
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874816 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20

Compound 2
HSQC



Current Data Parameters
NAME nov07-13
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131108
Time 3.05
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG hsqcetgpsi
TD 1024
SOLVENT MeOD
NS 64
DS 2
SWH 3591.954 Hz
FIDRES 3.507768 Hz
AQ 0.1425408 sec
RG 14596.5
DW 139.200 usec
DE 6.50 usec
TE 297.6 K
CNST2 145.0000000
D0 0.00000300 sec
D1 2.00000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00010000 sec
D24 0.00110000 sec
IN0 0.00002615 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
P28 2000.00 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp
NUC2 13C
P3 11.40 usec
P4 22.80 usec
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 17.00 dB
SFO2 100.5971798 MHz

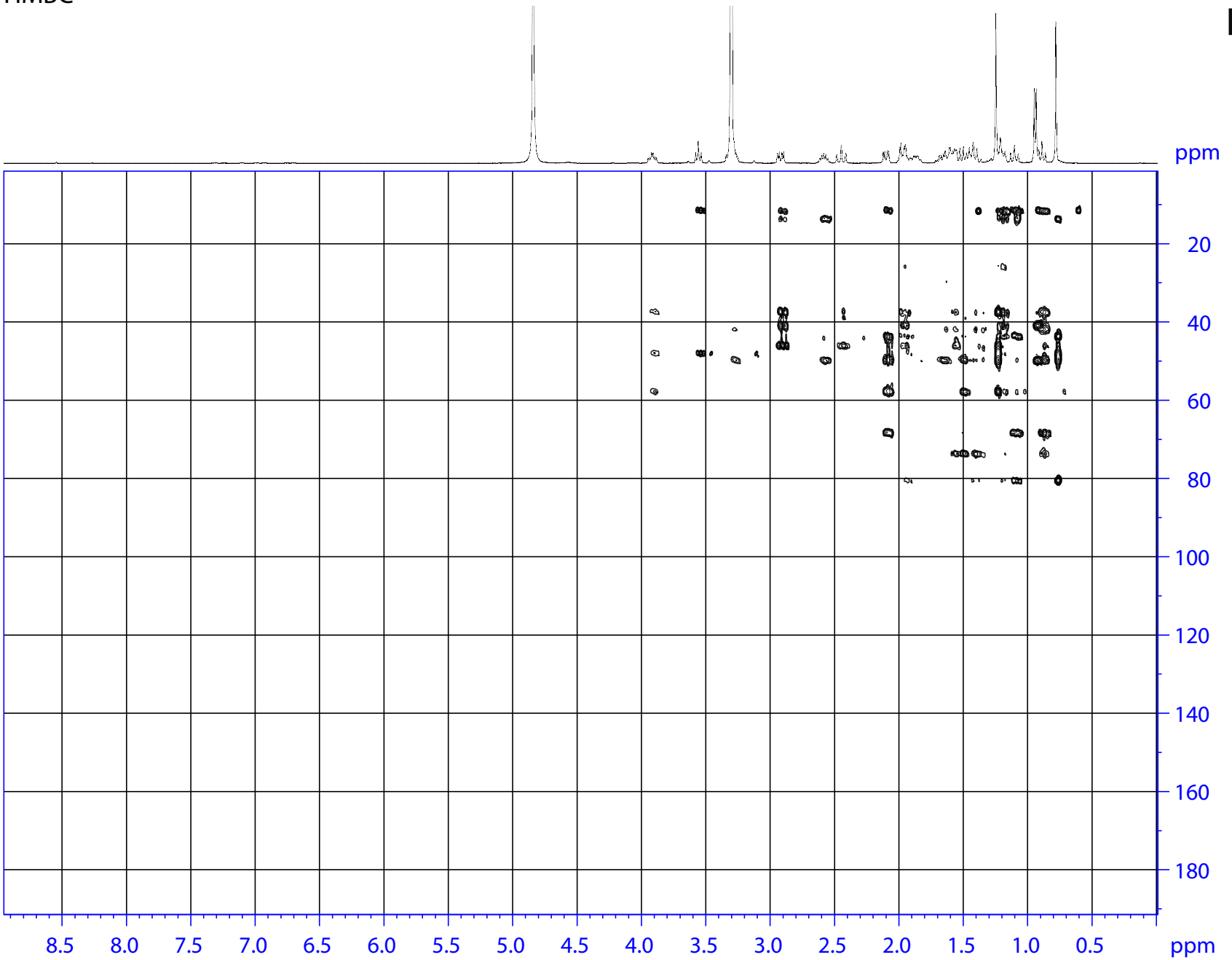
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.5972 MHz
FIDRES 149.323944 Hz
SW 190.000 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.5874816 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

Compound 2
HMBC



Current Data Parameters
NAME nov07-13
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131108
Time 12.56
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG hmbcgplpndqf
TD 2048
SOLVENT MeOD
NS 64
DS 2
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 14596.5
DW 139.200 usec
DE 6.50 usec
TE 299.1 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 0.00002160 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 11.40 usec
PL2 -6.00 dB
SFO2 100.5991916 MHz

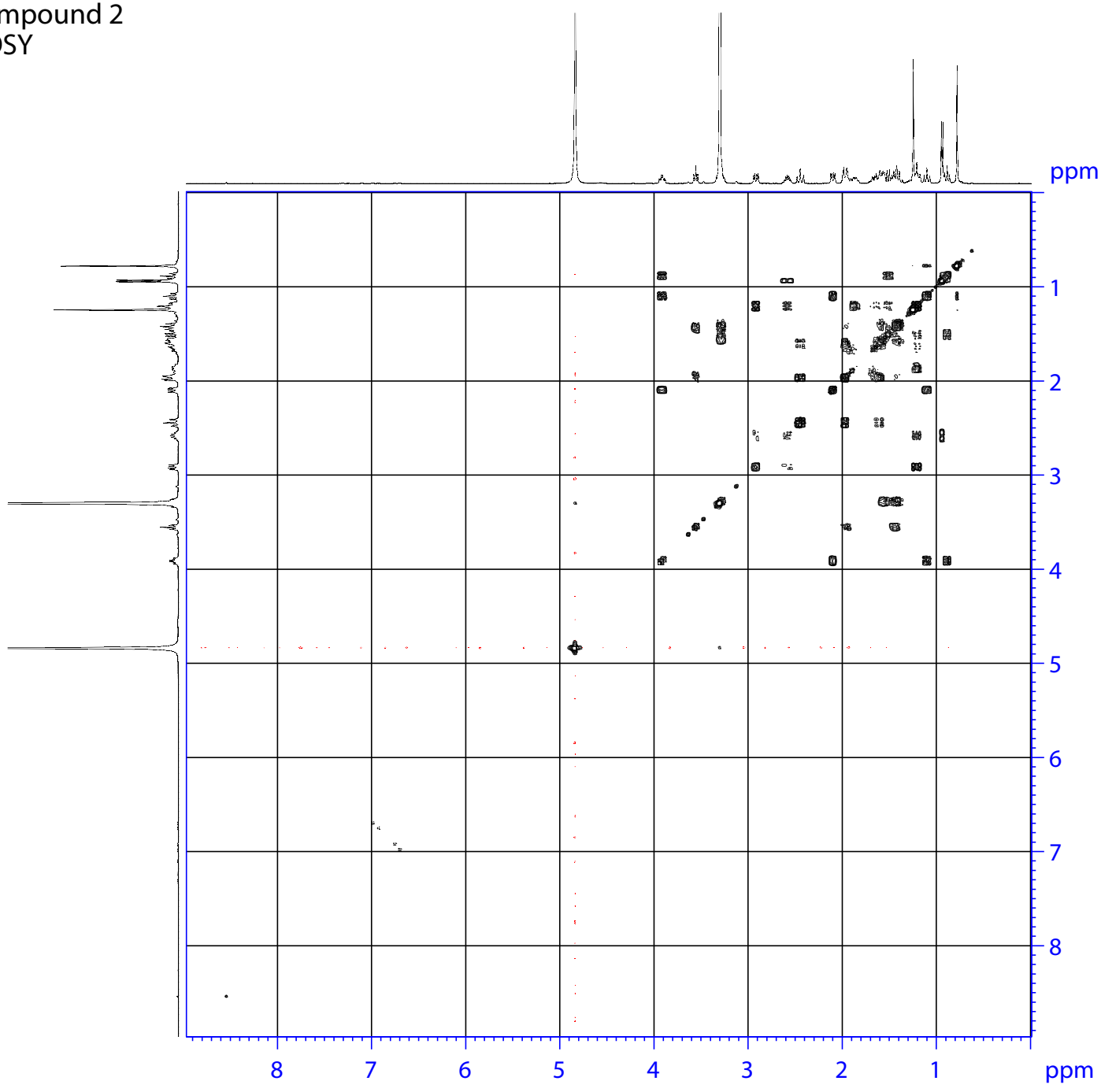
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPNAM[3] SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.5992 MHz
FIDRES 180.764175 Hz
SW 230.000 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.0300147 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.5876227 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Compound 2
COSY



AVANCE NEO 400 MHz
LAb # 115

Current Data Parameters
NAME nov07-13
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131107
Time 15.49
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG cosygpqf
TD 2048
SOLVENT MeOD
NS 32
DS 8
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 362
DW 139.200 usec
DE 6.50 usec
TE 299.1 K
D0 0.00000300 sec
D1 1.50000000 sec
D13 0.00000400 sec
D16 0.00010000 sec
IN0 0.00027840 sec

======== CHANNEL f1 ========
NUC1 1H
P0 10.80 usec
P1 10.80 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPZ1 10.00 %
P16 1000.00 usec

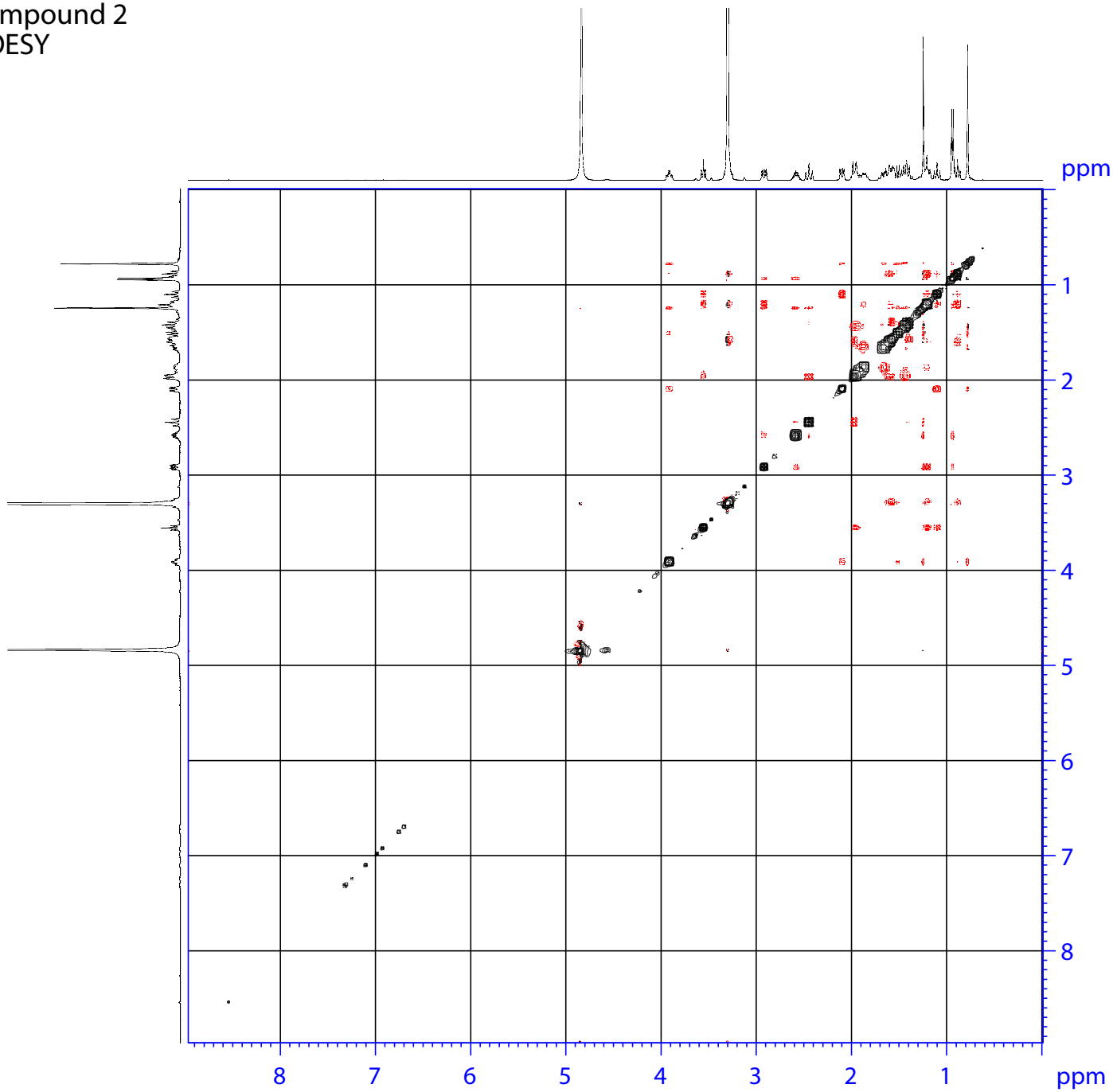
F1 - Acquisition parameters
TD 256
SFO1 400.0318 MHz
FIDRES 28.062141 Hz
SW 8.979 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.0300087 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Compound 2
NOESY

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME nov07-13
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131107
Time 20.00
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG noesygpph
TD 2048
SOLVENT MeOD
NS 32
DS 8
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 456.1
DW 139.200 usec
DE 6.50 usec
TE 299.1 K
D0 0.00012545 sec
D1 2.00000000 sec
D8 0.80000001 sec
D16 0.00010000 sec
IN0 0.00027840 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 400.0318 MHz
FIDRES 28.062141 Hz
SW 8.979 ppm
FnMODE States-TPPI

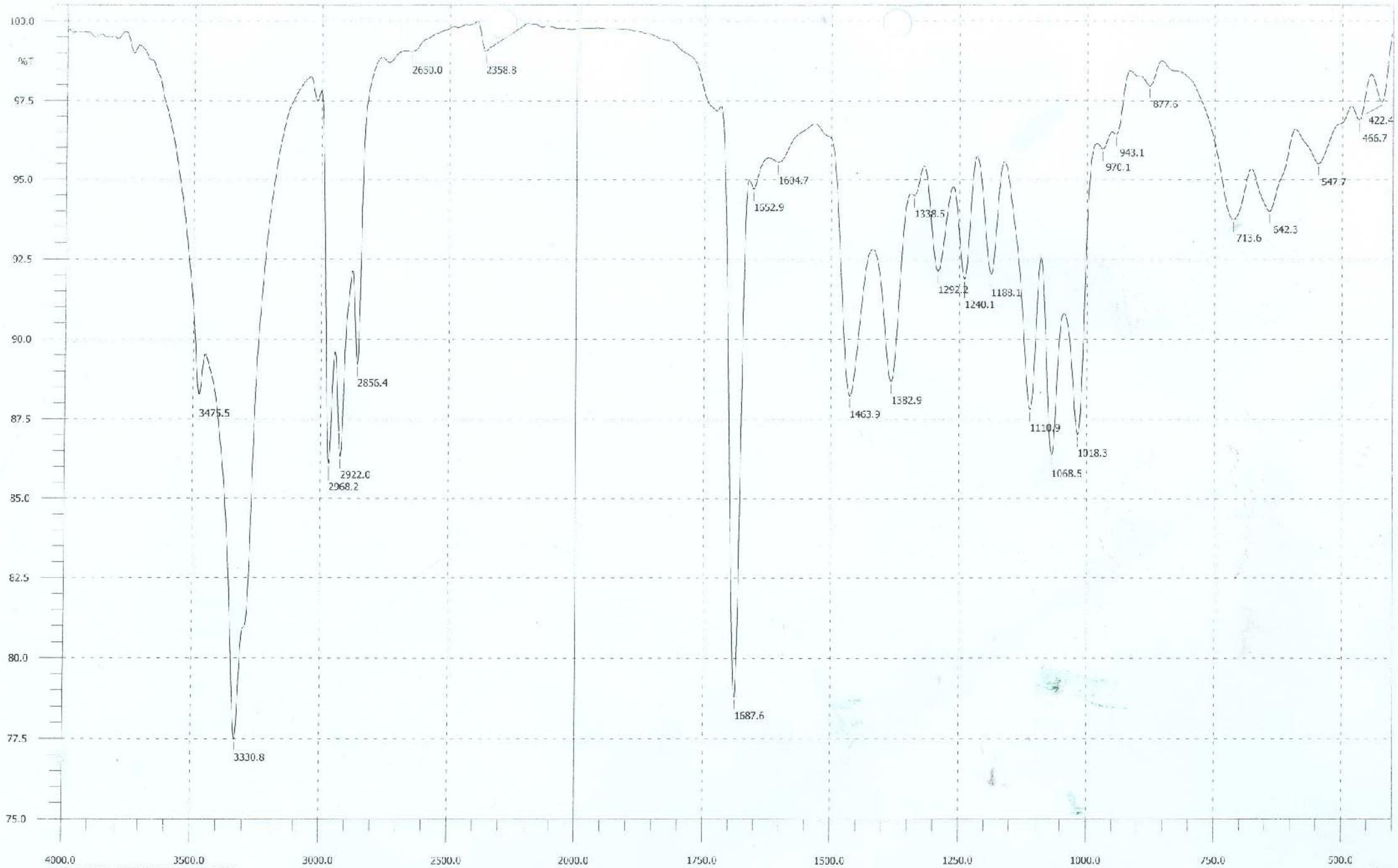
F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

JEOL HX 110 MASS SPECTROMETER (FAB-HR)

STUDENT NAME	Zahid Hussain	SAMPLE CODE	DATE	
SUPERVISOR NAME	Prof. Dr. M. Iqbal	ZDB 10	FAB (+VE / -VE)	

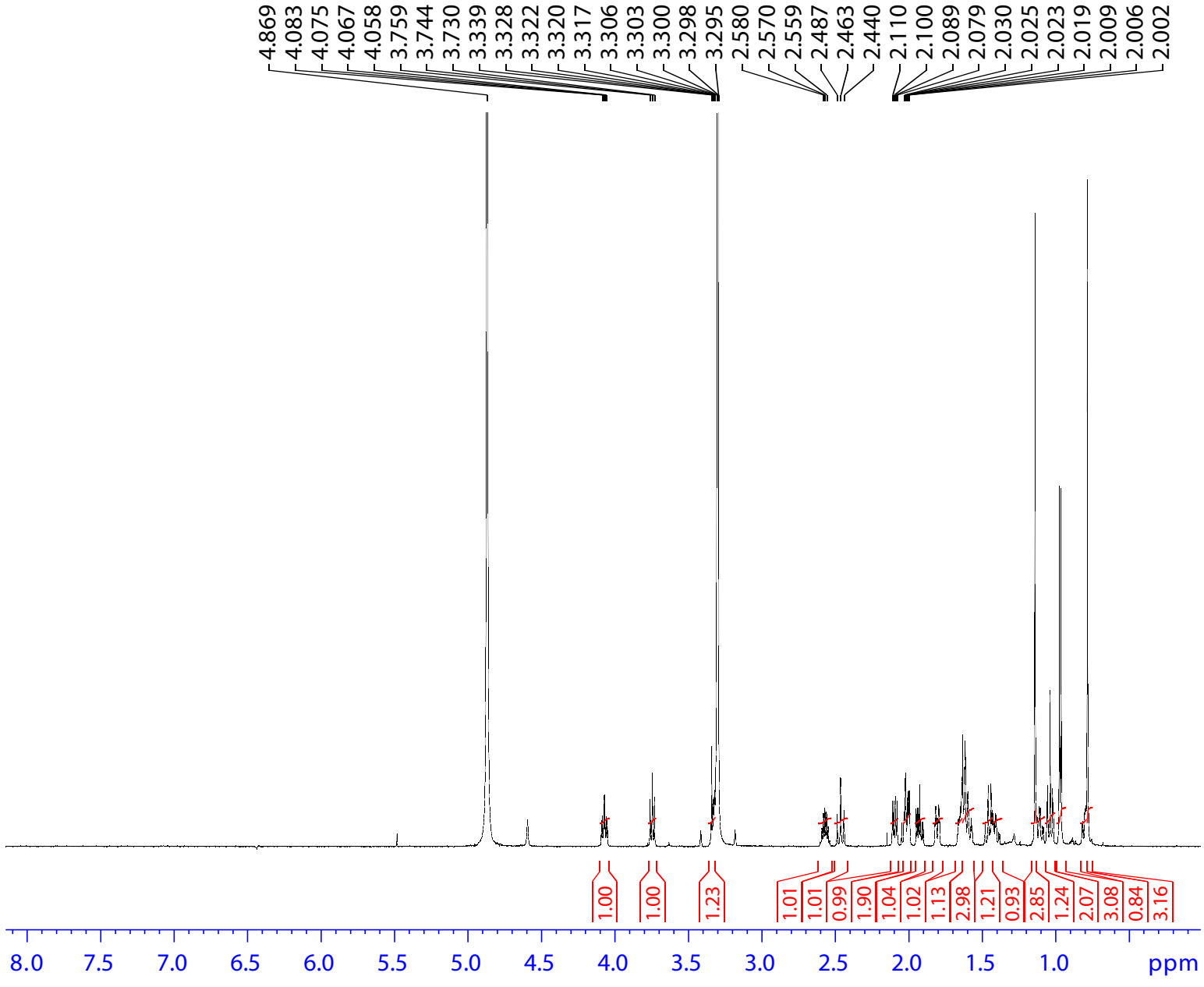
Mass	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
337.2356	337.2379	-6.8	-2.3	4.5	$C_{20}H_{33}O_4$



ZDB-10.IRS: K-631/Zahid Hussain/MIC

Date:	12/17/2014	Time:	09:21:51	NScans:	5		
Type:	HYPER IR	User:	ZUBAIR AHMED			Detector:	standard
Abscissa:	1/cm	Ordinate:	%T	Apodization:	Happ		
Min:	401.17	Max:	3998.16	Range:	1/cm		
Ndp:	1866	Data Interval:	1.92868	Resolution:	4.0		
Gain:	auto	Aperture:	auto	Mirror Speed:	2.8(low)		

Compound 3
1H



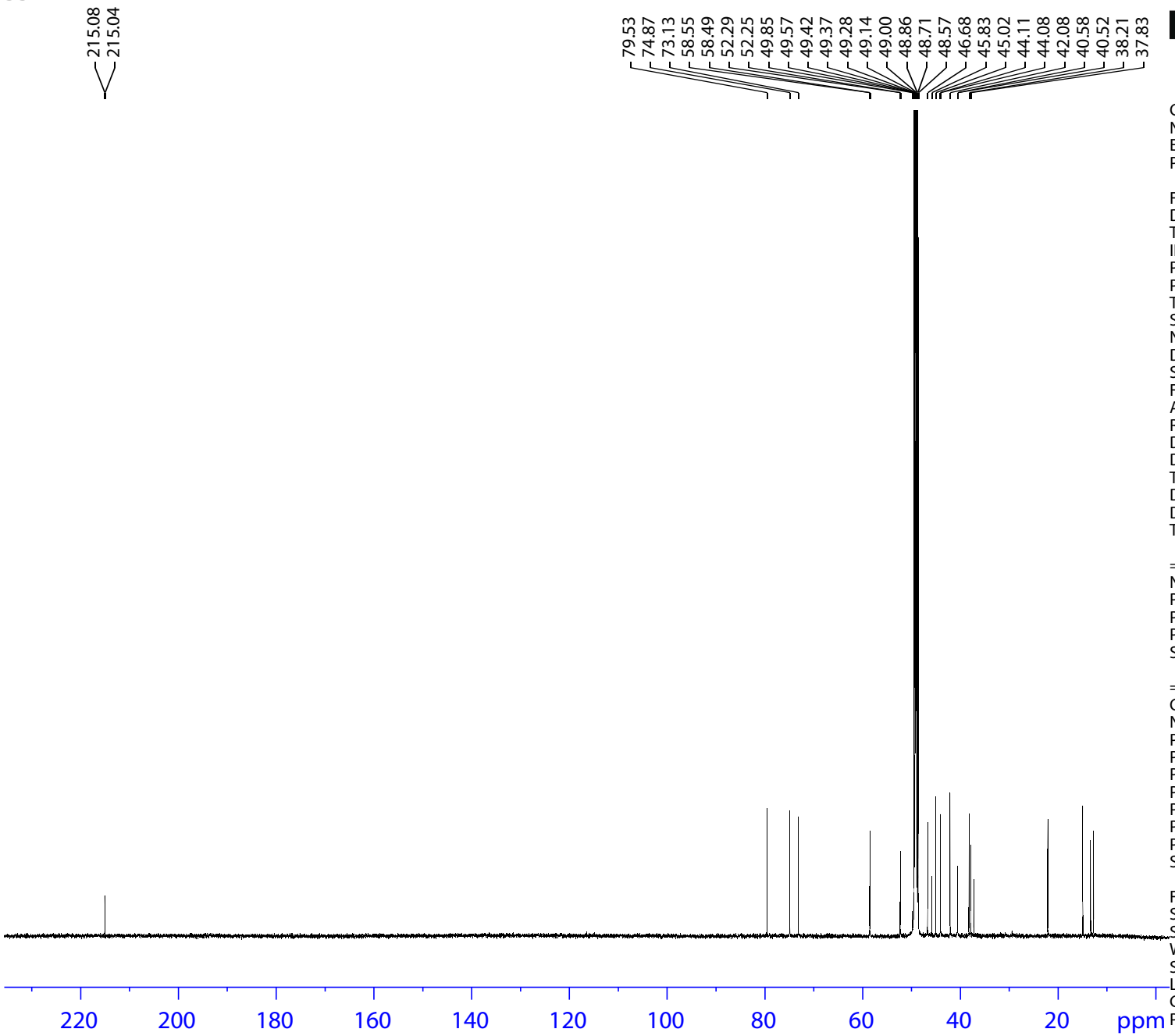
Current Data Parameters
NAME jan26-14
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140126
Time 17.52
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32768
SOLVENT MeOD
NS 8
DS 0
SWH 9615.385 Hz
FIDRES 0.293438 Hz
AQ 1.7039360 sec
RG 8
DW 52.000 usec
DE 6.50 usec
TE 297.9 K
D1 1.50000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 8.00 usec
PL1 3.31 dB
PL1W 6.79873323 W
SFO1 600.0345002 MHz

F2 - Processing parameters
SI 32768
SF 600.0300172 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40

Compound 3
BB



Current Data Parameters
NAME jan26-14
EXPNO 6
PROCNO 1

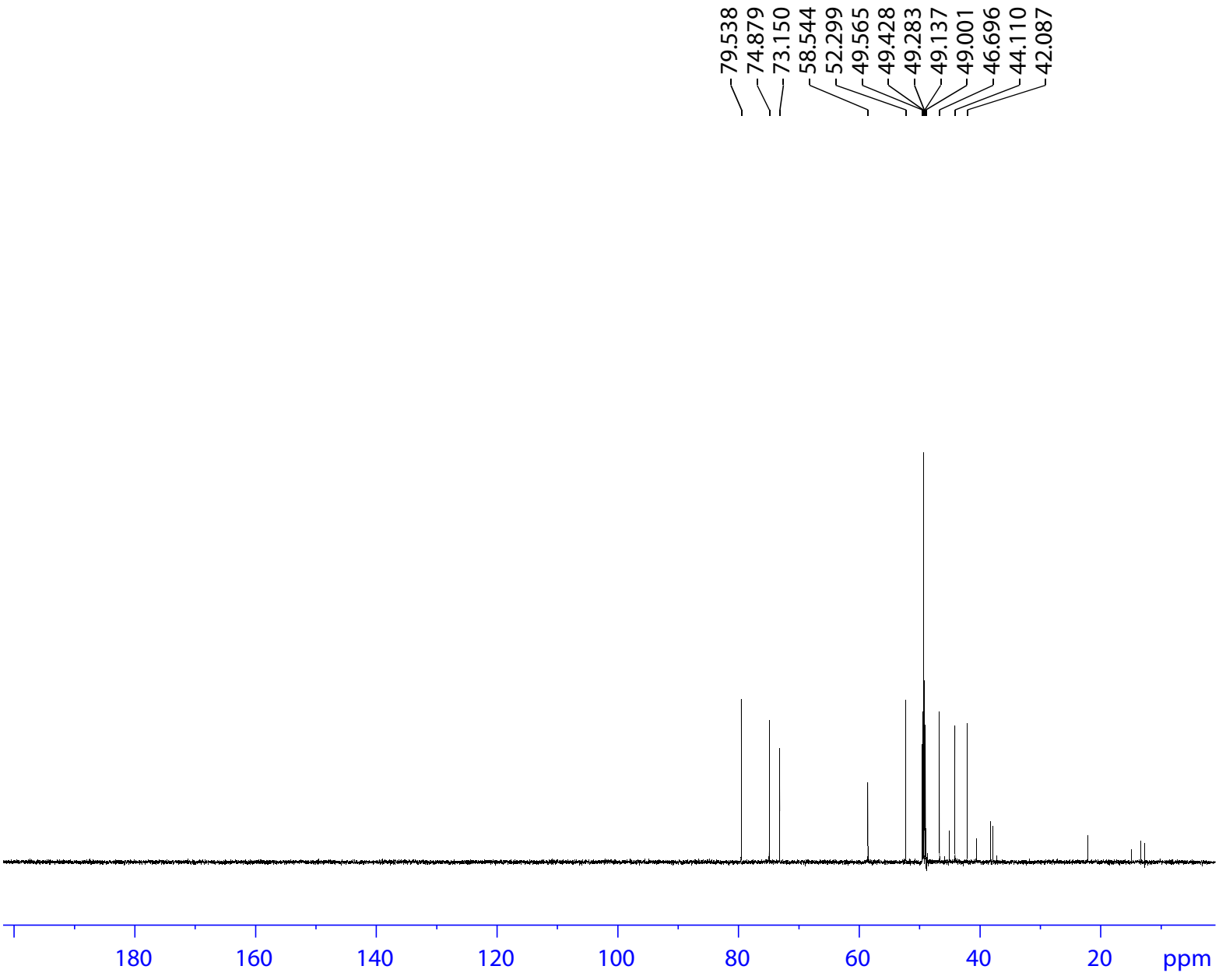
F2 - Acquisition Parameters
Date_ 20140127
Time 11.18
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg
TD 32768
SOLVENT MeOD
NS 4806
DS 4
SWH 35971.223 Hz
FIDRES 1.097755 Hz
AQ 0.4554752 sec
RG 32768
DW 13.900 usec
DE 6.50 usec
TE 288.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 12

======== CHANNEL f1 ========
NUC1 13C
P1 12.70 usec
PL1 -1.81 dB
PL1W 81.92915344 W
SFO1 150.8950149 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.31 dB
PL12 23.31 dB
PL13 22.50 dB
PL2W 6.79873323 W
PL12W 0.06798734 W
PL13W 0.08192718 W
SFO2 600.0336002 MHz

F2 - Processing parameters
SI 16384
SF 150.8774509 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Compound 3
deptsp 90



Current Data Parameters
NAME jan26-14
EXPNO 8
PROCNO 1

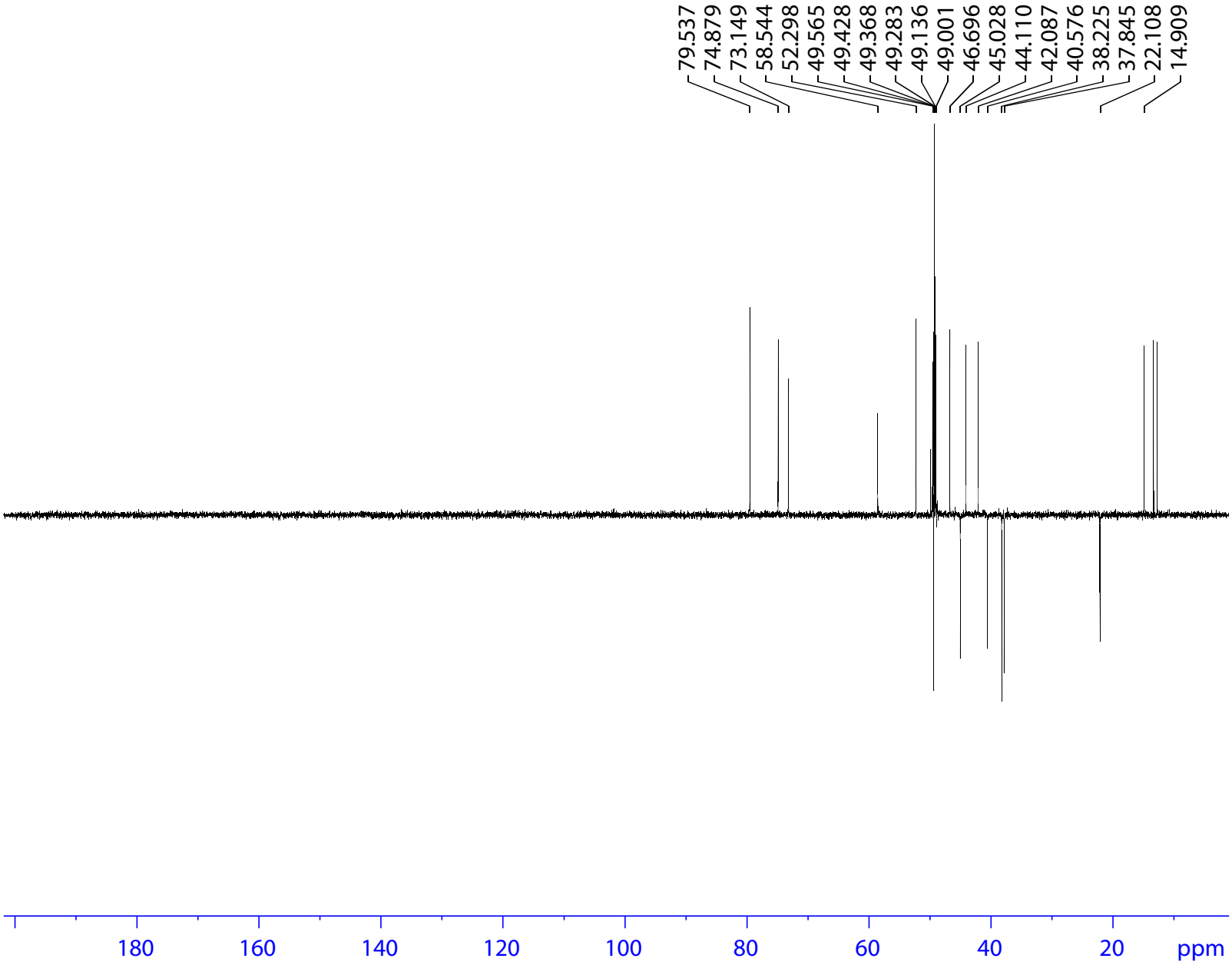
F2 - Acquisition Parameters
Date_ 20140127
Time 15.33
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG deptsp90
TD 32768
SOLVENT MeOD
NS 2507
DS 2
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5406720 sec
RG 32768
DW 16.500 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 3

======== CHANNEL f1 ========
NUC1 13C
P1 12.70 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.81 dB
PL0W 0 W
PL1W 81.92915344 W
SFO1 150.8927518 MHz
SP2 4.19 dB
SPNAM[2] Crp60comp.4
SPOAL2 0.500
SPOFFS2 0 Hz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 8.00 usec
P4 16.00 usec
PCPD2 80.00 usec
PL2 3.31 dB
PL12 23.31 dB
PL2W 6.79873323 W
PL12W 0.06798734 W
SFO2 600.0330002 MHz

F2 - Processing parameters
SI 16384
SF 150.8774509 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 3
deptsp135



Current Data Parameters
NAME jan26-14
EXPNO 7
PROCNO 1

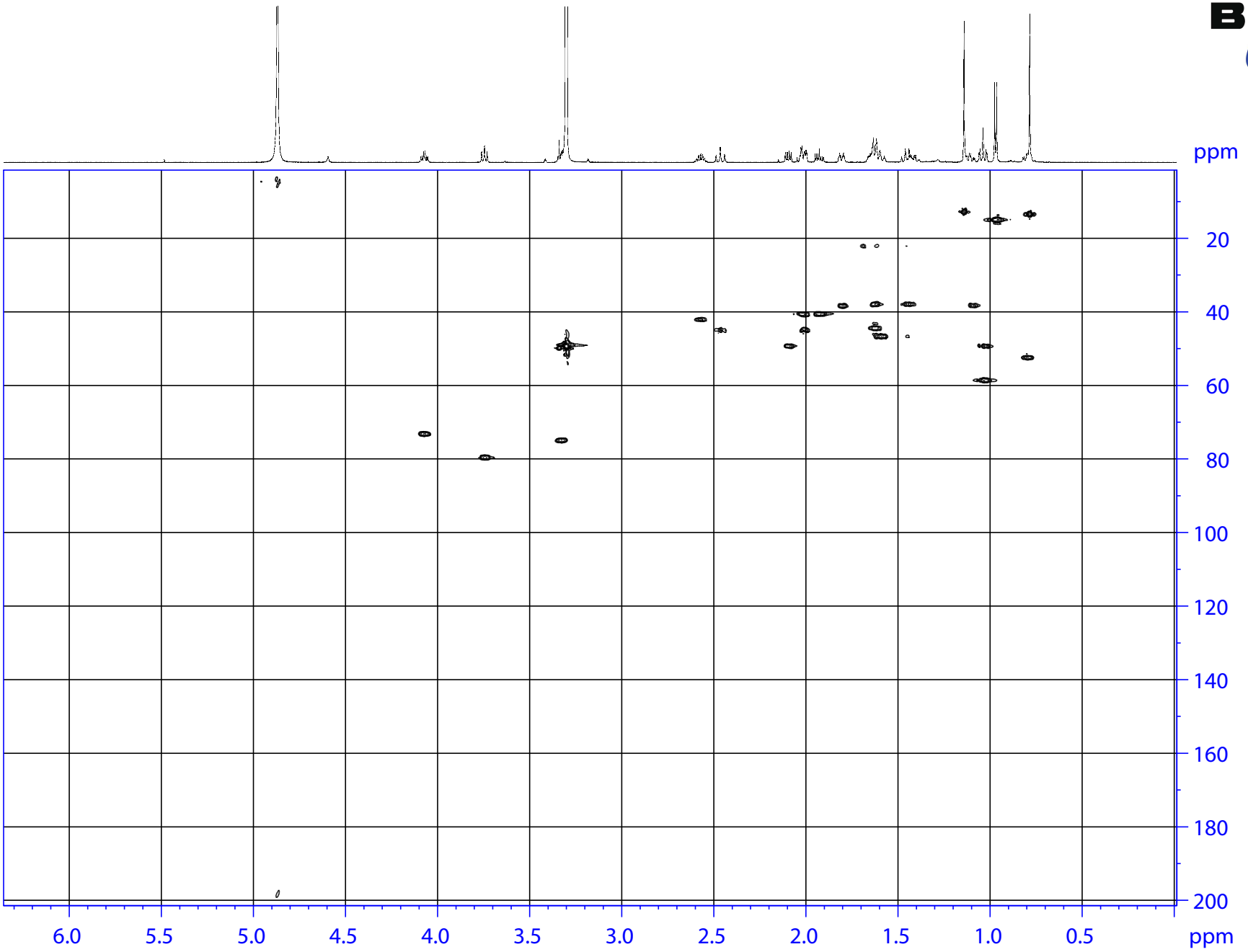
F2 - Acquisition Parameters
Date_ 20140127
Time 14.33
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG deptsp135
TD 32768
SOLVENT MeOD
NS 2348
DS 2
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5406720 sec
RG 32768
DW 16.500 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 6

======== CHANNEL f1 ========
NUC1 13C
P1 12.70 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.81 dB
PL0W 0 W
PL1W 81.92915344 W
SFO1 150.8927518 MHz
SP2 4.19 dB
SPNAM[2] Crp60comp.4
SPOAL2 0.500
SPOFFS2 0 Hz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 8.00 usec
P4 16.00 usec
PCPD2 80.00 usec
PL2 3.31 dB
PL12 23.31 dB
PL2W 6.79873323 W
PL12W 0.06798734 W
SFO2 600.0330002 MHz

F2 - Processing parameters
SI 16384
SF 150.8774509 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 3
hsqc



Current Data Parameters
NAME jan26-14
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140126
Time 22.31
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpsi
TD 1024
SOLVENT MeOD
NS 32
DS 8
SWH 3822.630 Hz
FIDRES 3.733037 Hz
AQ 0.1339392 sec
RG 36780.8
DW 130.800 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 0.00020000 sec
D24 0.00110000 sec
IN0 0.00001655 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 8.00 usec
P2 16.00 usec
P28 1000.00 usec
PL1 3.31 dB
PL1W 6.79873323 W
SFO1 600.0319201 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp
NUC2 13C
P3 11.50 usec
P4 23.00 usec
PCPD2 55.00 usec
PL2 -1.81 dB
PL12 11.70 dB
PL2W 81.92915344 W
PL12W 3.65122390 W
SFO2 150.8927518 MHz

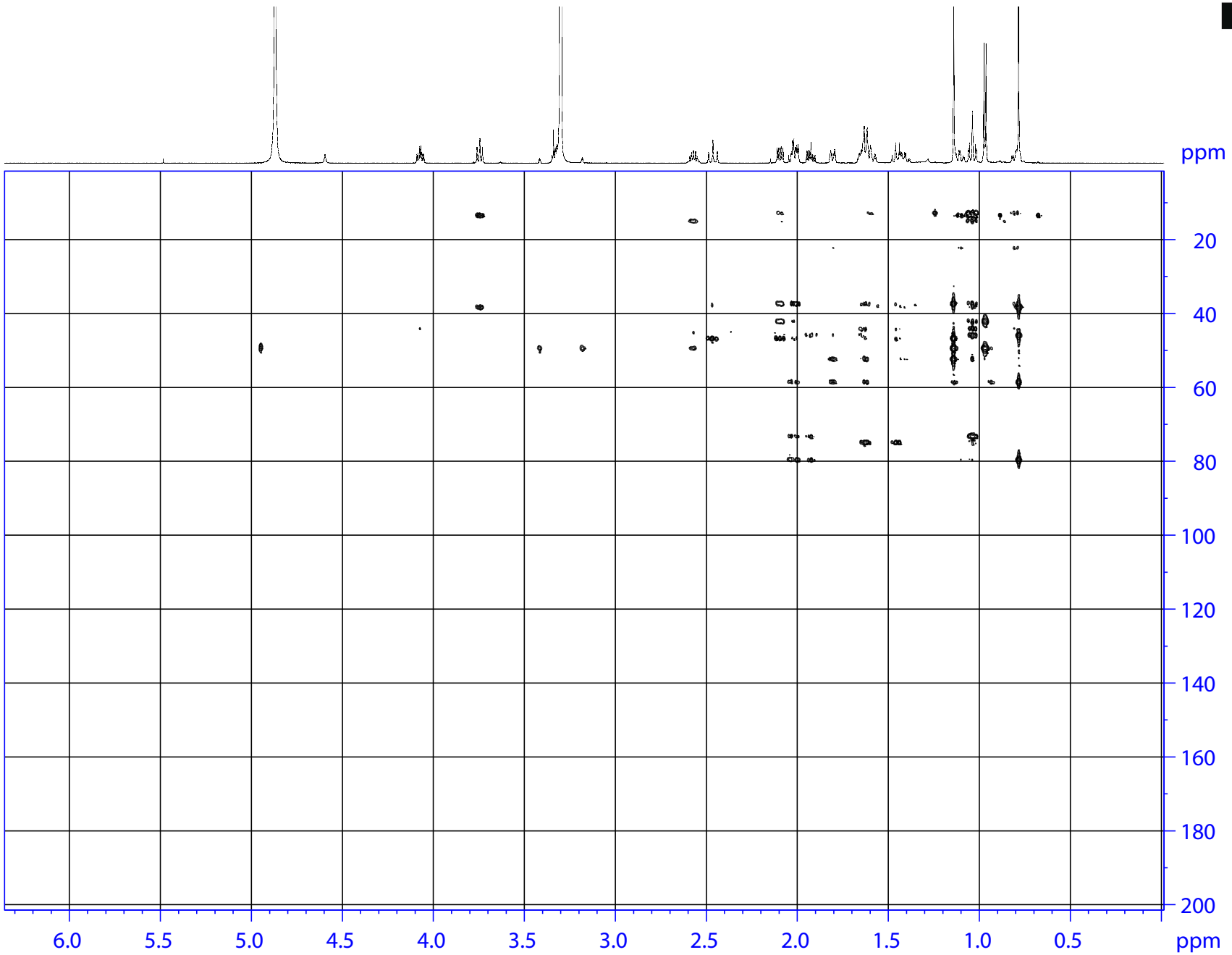
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8928 MHz
FIDRES 235.769928 Hz
SW 200.000 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.0300172 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.8774509 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Compound 3
HMBC



Current Data Parameters
NAME jan26-14
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140127
Time 2.19
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG hmbcgplpndqf
TD 2048
SOLVENT MeOD
NS 64
DS 16
SWH 3822.630 Hz
FIDRES 1.866518 Hz
AQ 0.2678784 sec
RG 41285.1
DW 130.800 usec
DE 6.50 usec
TE 288.5 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 8.00 usec
P2 16.00 usec
PL1 3.31 dB
PL1W 6.79873323 W
SFO1 600.0319201 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 11.50 usec
PL2 -1.81 dB
PL2W 81.92915344 W
SFO2 150.8950149 MHz

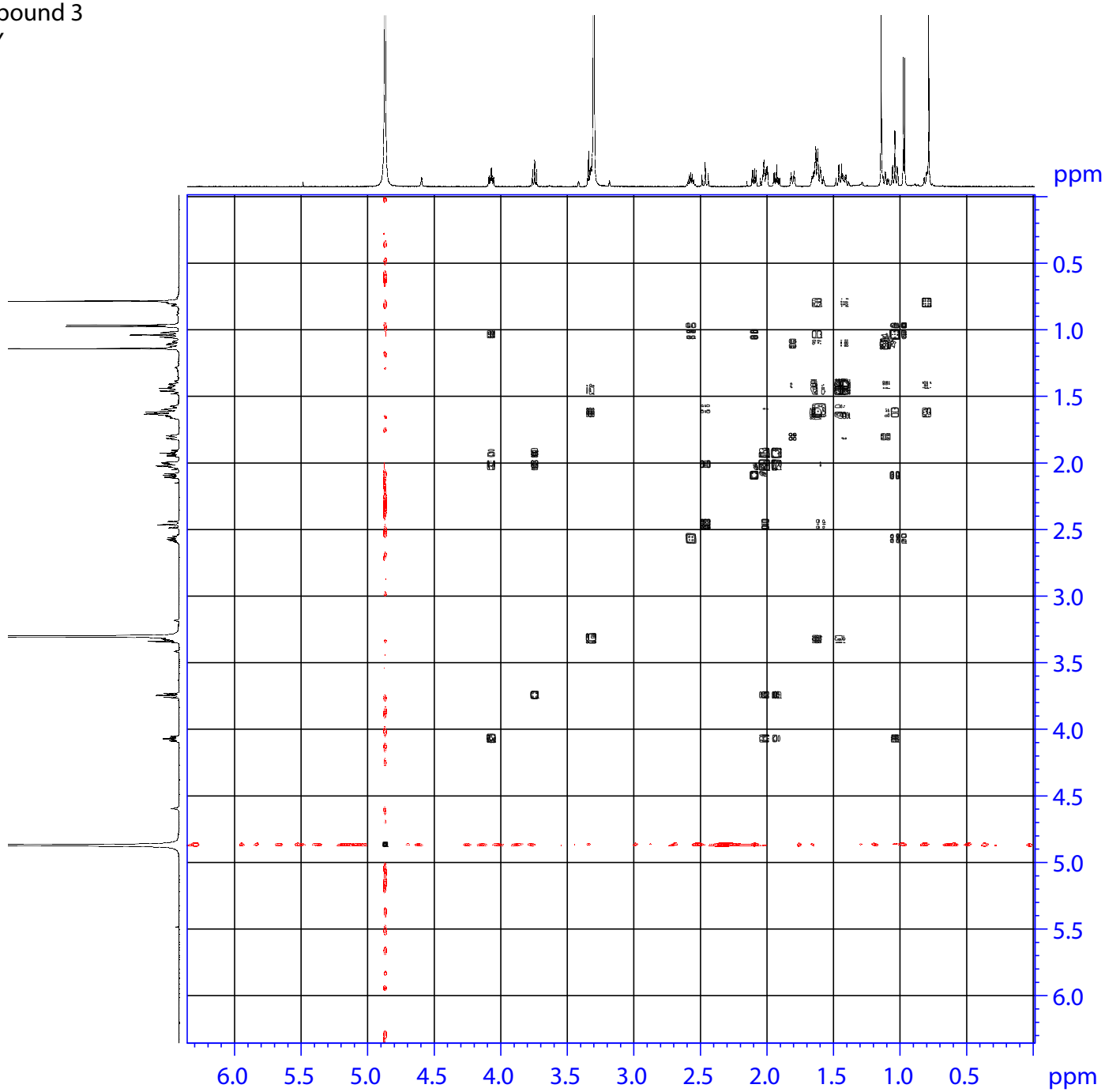
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPNAM[3] SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 2000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.895 MHz
FIDRES 271.139465 Hz
SW 230.000 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.0300172 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8774509 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

Compound 3
COSY



Current Data Parameters
NAME jan26-14
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140126
Time 17.58
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG cosydfqf
TD 2048
SOLVENT MeOD
NS 16
DS 4
SWH 3822.630 Hz
FIDRES 1.866518 Hz
AQ 0.2678784 sec
RG 28.5
DW 130.800 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 0.00026160 sec

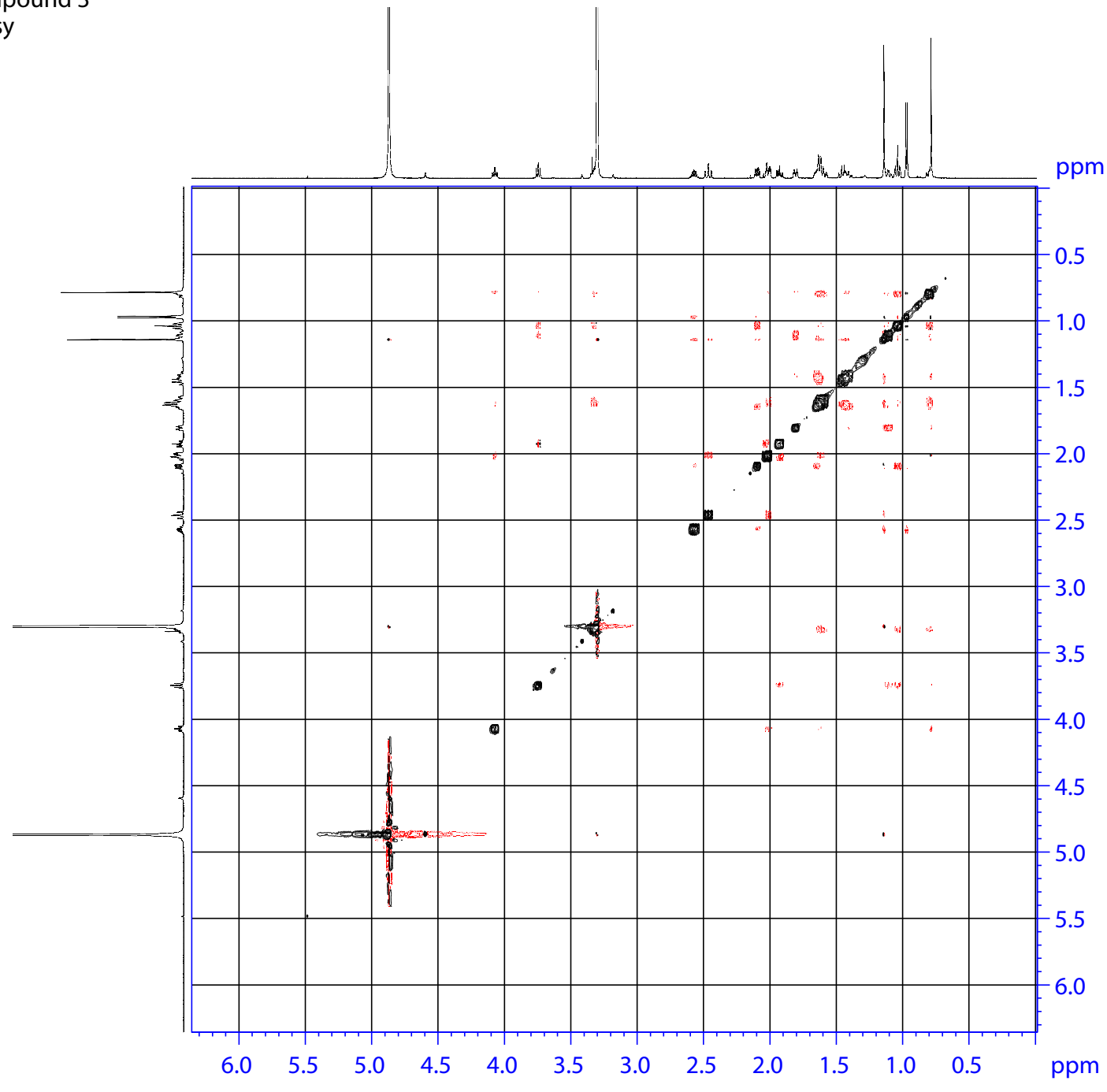
======== CHANNEL f1 ========
NUC1 1H
P1 8.00 usec
PL1 3.31 dB
PL1W 6.79873323 W
SFO1 600.0319201 MHz

F1 - Acquisition parameters
TD 128
SFO1 600.0319 MHz
FIDRES 59.728592 Hz
SW 6.371 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.0300172 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.0300172 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Compound 3
noesy



Current Data Parameters
NAME jan26-14
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140126
Time 19.00
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG noesygpph
TD 2048
SOLVENT MeOD
NS 16
DS 4
SWH 3822.630 Hz
FIDRES 1.866518 Hz
AQ 0.2678784 sec
RG 25.4
DW 130.800 usec
DE 6.50 usec
TE 298.1 K
D0 0.00012061 sec
D1 2.00000000 sec
D8 0.80000001 sec
D16 0.00020000 sec
IN0 0.00026160 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.00 usec
P2 16.00 usec
PL1 3.31 dB
PL1W 6.79873323 W
SFO1 600.0319201 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.0319 MHz
FIDRES 29.864296 Hz
SW 6.371 ppm
FnMODE States-TPPI

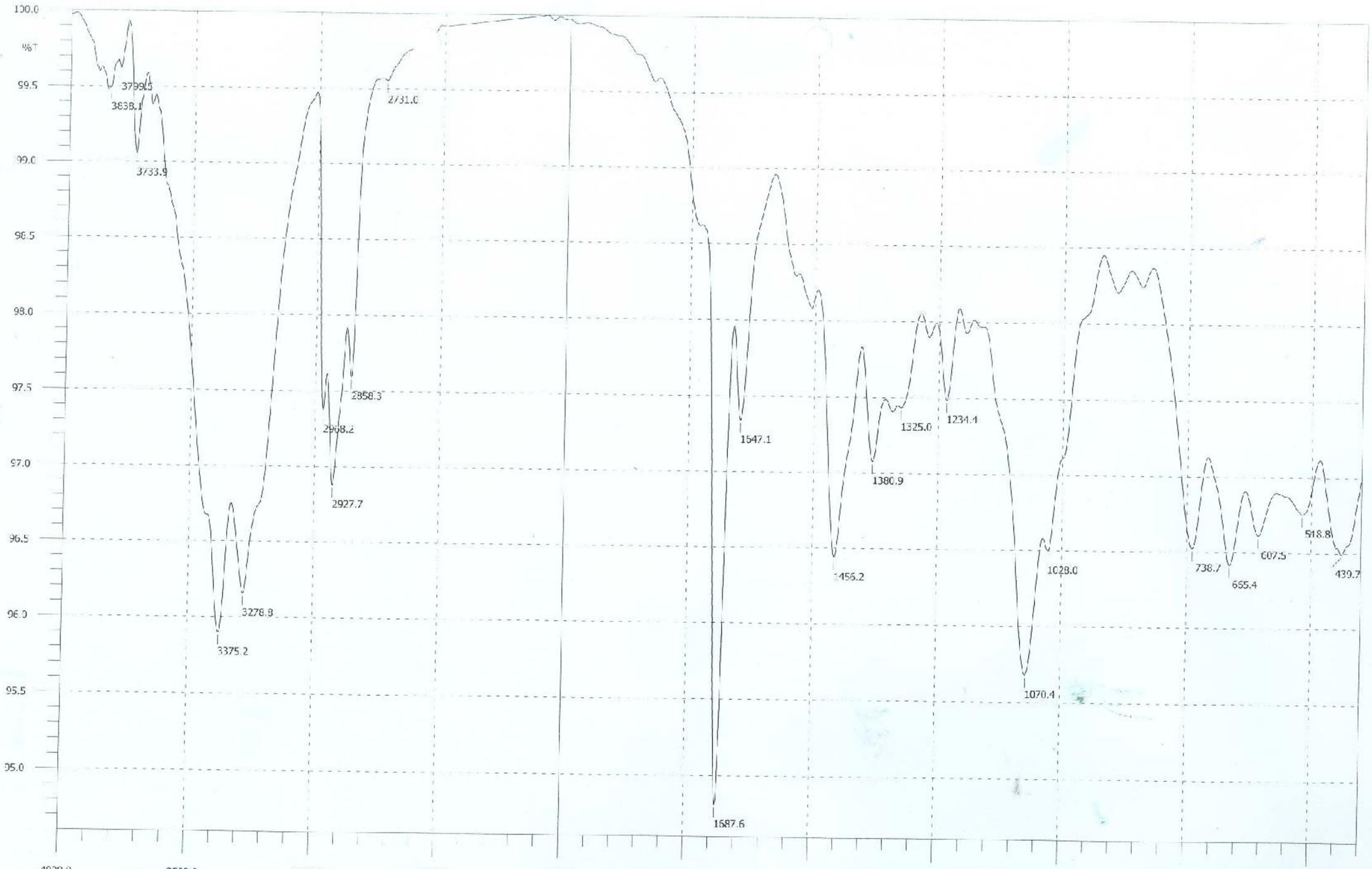
F2 - Processing parameters
SI 1024
SF 600.0300172 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 512
MC2 States-TPPI
SF 600.0300172 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

JEOL HX 110 MASS SPECTROMETER (EI-HR)

STUDENT NAME	Zahid Hussain	SAMPLE CODE	DATED
SUPERVISOR NAME	Prof. Dr. M. Iqbal Ch.	ZDB - 12B	

Mass	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
337.2372	337.2379	-2.0	-0.7	4.5	$C_{20}H_{33}O_4$

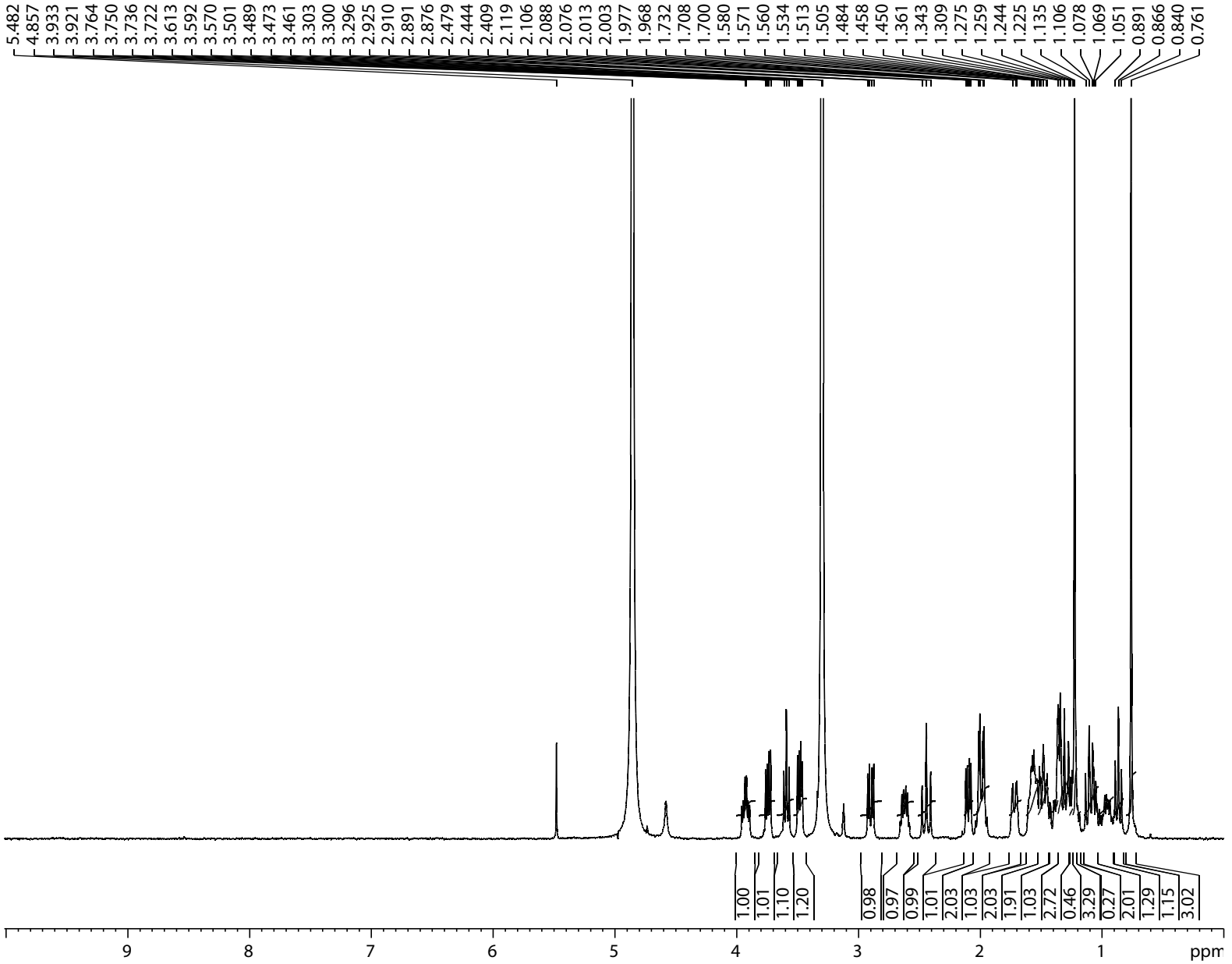


ZDB-12B.IRS: ZDB-12B/Zahid Hussain/MIC

Date:	12/17/2014	Time:	09:24:21	NScans:	5		
Type:	HYPER IR	User:	ZUBAIR AHMED			Detector:	standard
Abscissa:	1/cm	Ordinate:	%T	Apodization:	Happ		
Min:	401.17	Max:	3998.16	Range:	1/cm		
Ndp:	1866	Data Interval:	1.92868	Resolution:	4.0		
Gain:	auto	Aperture:	auto	Mirror Speed:	2.8(low)		

Compound 4
1H

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME jan05-14
EXPNO 1
PROCNO 1

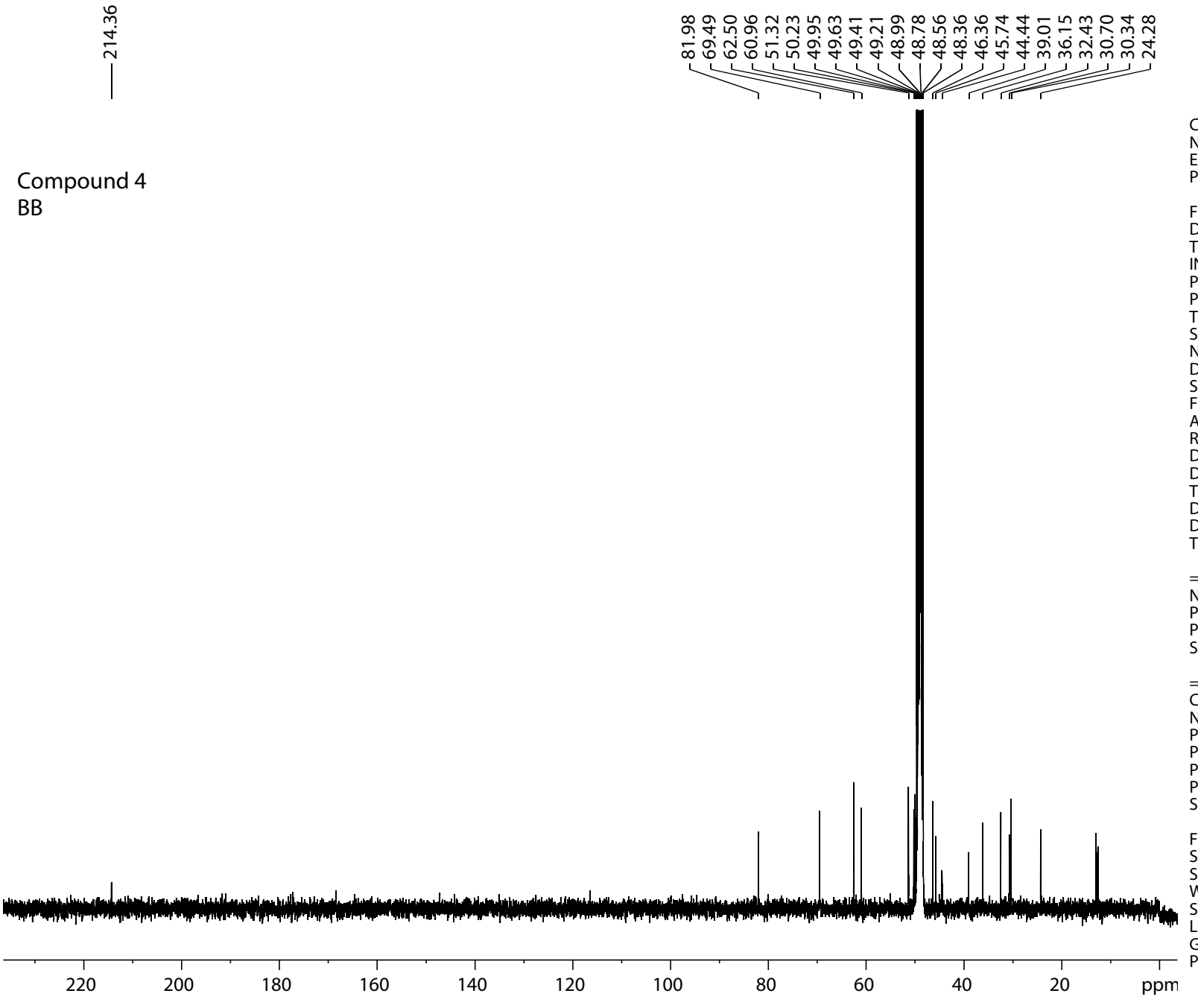
F2 - Acquisition Parameters
Date_ 20140105
Time 15.02
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT MeOD
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 322.5
DW 62.400 usec
DE 6.50 usec
TE 297.2 K
D1 1.50000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 400.0332002 MHz

F2 - Processing parameters
SI 16384
SF 400.0300087 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

AVANCE NEO 400 MHz
LAb # 115

Compound 4
BB



Current Data Parameters
NAME jan05-14
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140106
Time 19.20
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg
TD 32768
SOLVENT MeOD
NS 20480
DS 2
SWH 24154.590 Hz
FIDRES 0.737140 Hz
AQ 0.6782976 sec
RG 32768
DW 20.700 usec
DE 6.50 usec
TE 296.5 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 20

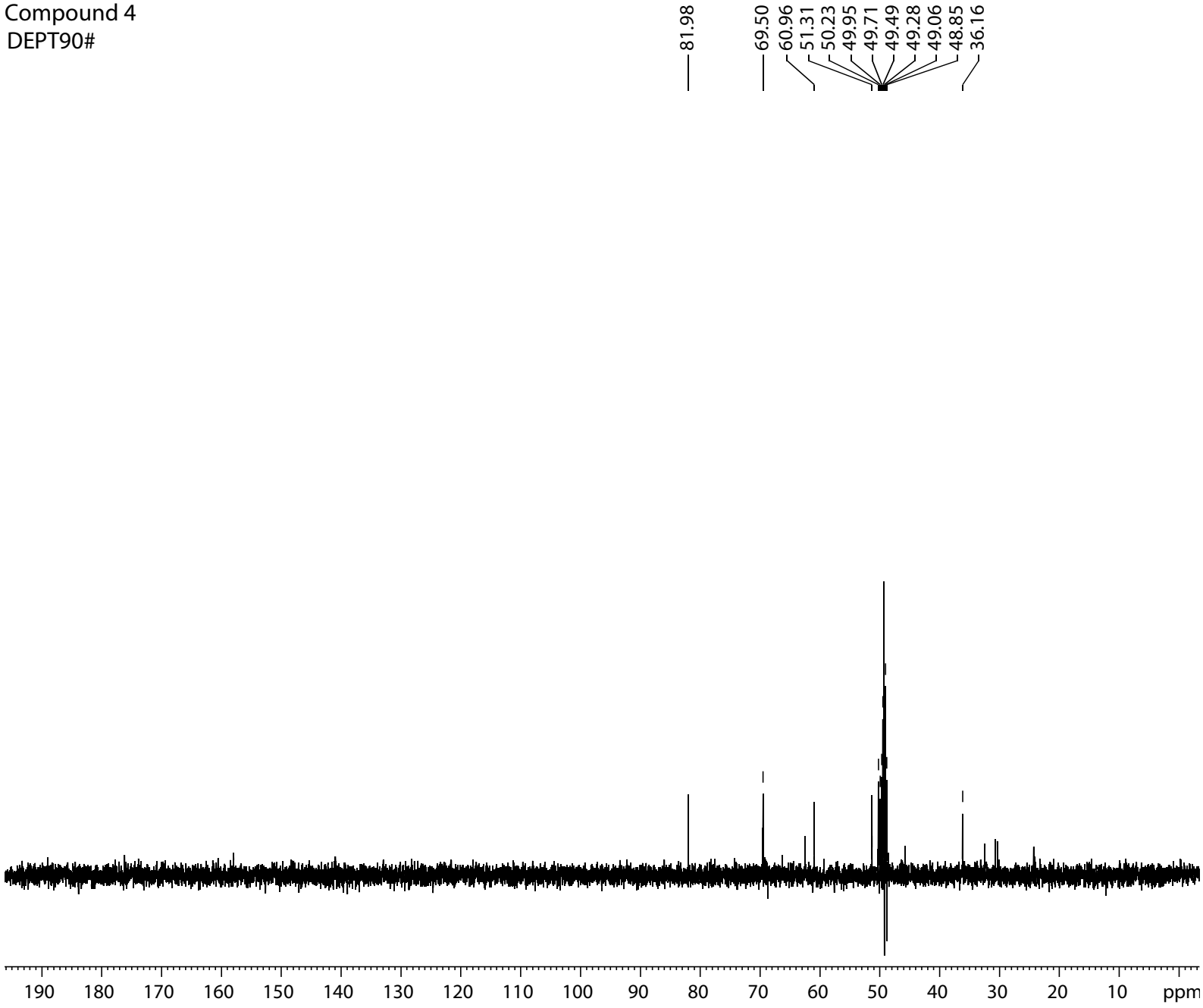
======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
PL1 -6.00 dB
SFO1 100.5991916 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
PL13 22.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874816 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Compound 4
DEPT90#

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME jan05-14
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140107
Time 14.50
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG dept90
TD 32768
SOLVENT MeOD
NS 6144
DS 2
SWH 20080.320 Hz
FIDRES 0.612803 Hz
AQ 0.8159232 sec
RG 16384
DW 24.900 usec
DE 6.50 usec
TE 296.8 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 6

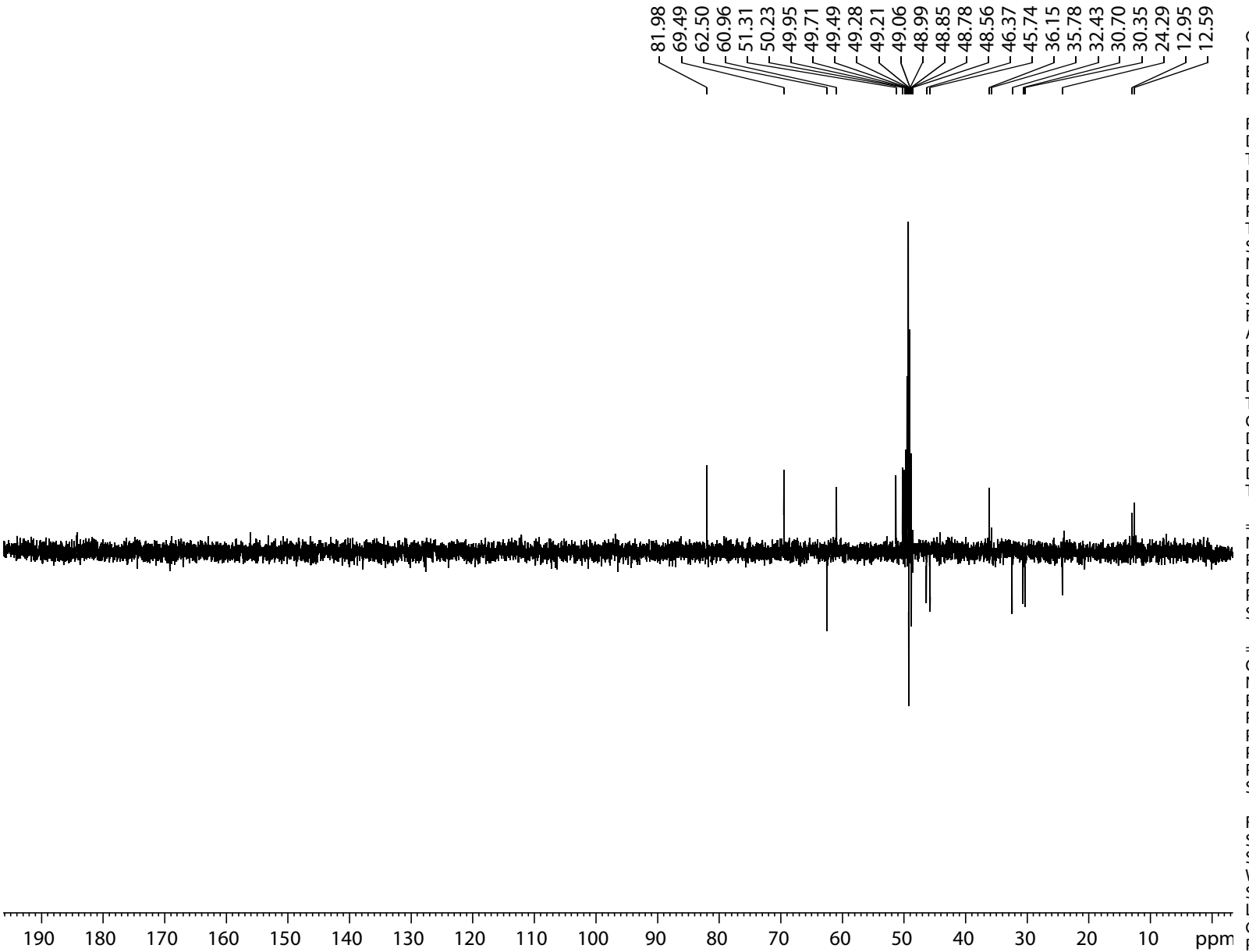
======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
P2 24.60 usec
PL1 -6.00 dB
SFO1 100.5971798 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 10.50 usec
P4 21.00 usec
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874816 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20

Compound 4
DEP135#//

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME jan05-14
EXPNO 7
PROCNO 1

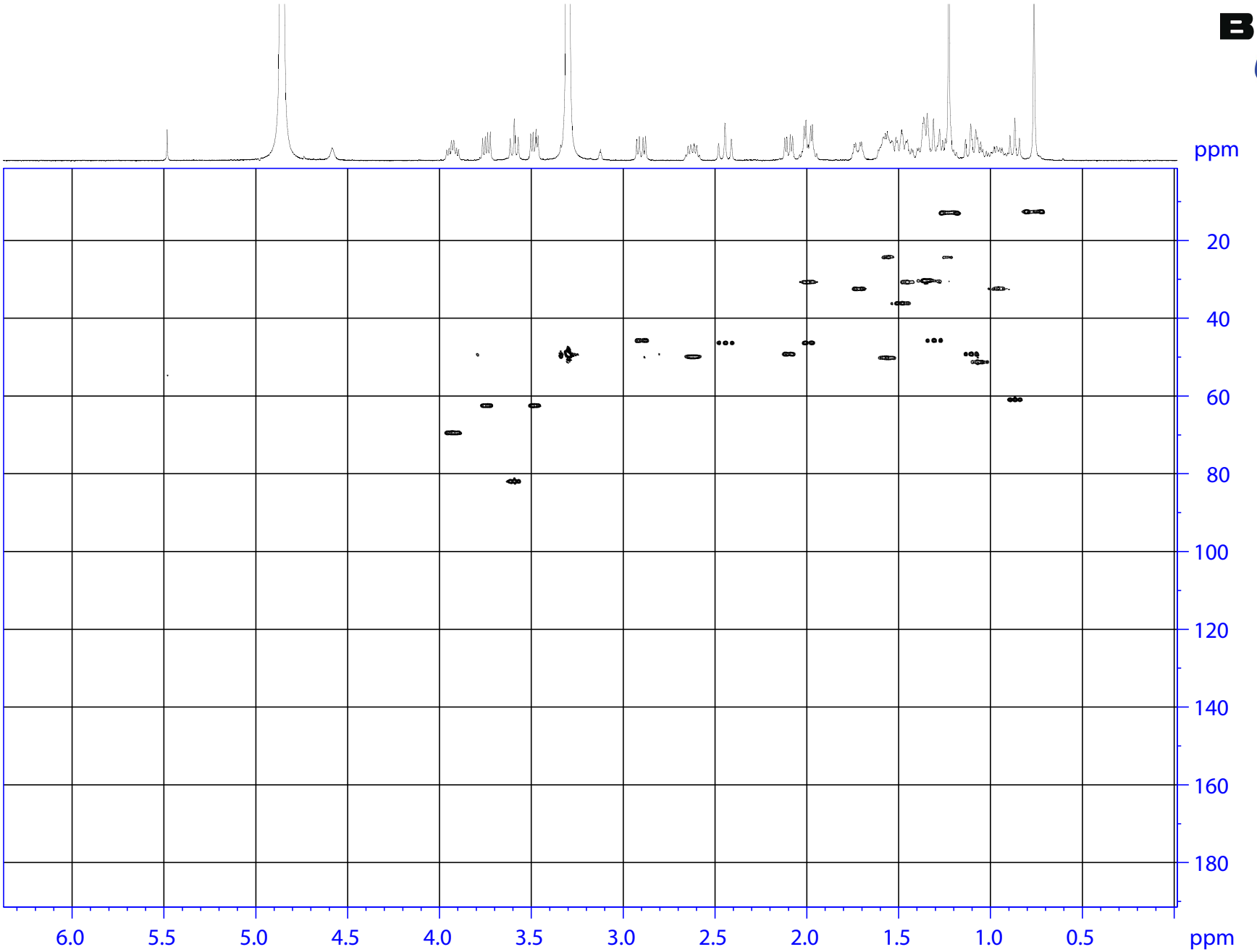
F2 - Acquisition Parameters
Date_ 20140107
Time 8.08
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG dept135
TD 32768
SOLVENT MeOD
NS 10240
DS 2
SWH 20080.320 Hz
FIDRES 0.612803 Hz
AQ 0.8159232 sec
RG 16384
DW 24.900 usec
DE 6.50 usec
TE 296.4 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 10

======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
P2 24.60 usec
PL1 -6.00 dB
SFO1 100.5971798 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 10.50 usec
P4 21.00 usec
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874816 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20

Compound 4
HSQC//



Current Data Parameters
NAME jan05-14
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140105
Time 23.39
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG hsqcetgpsi
TD 1024
SOLVENT MeOD
NS 64
DS 2
SWH 2556.237 Hz
FIDRES 2.496325 Hz
AQ 0.2002944 sec
RG 14596.5
DW 195.600 usec
DE 6.50 usec
TE 297.0 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 0.00002615 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
P28 2000.00 usec
PL1 3.00 dB
SFO1 400.0312801 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp
NUC2 13C
P3 11.40 usec
P4 22.80 usec
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 17.00 dB
SFO2 100.5971798 MHz

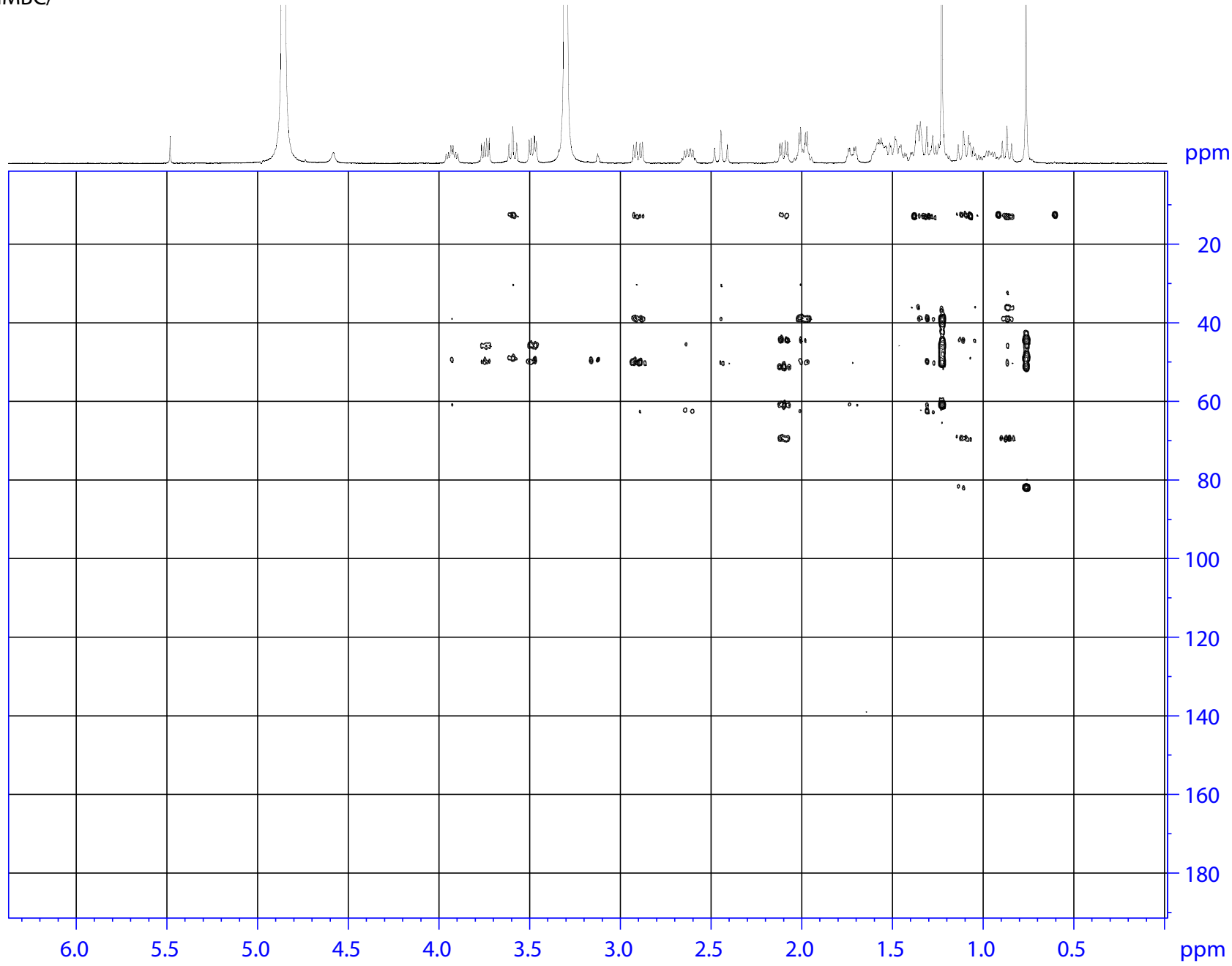
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.5972 MHz
FIDRES 149.323944 Hz
SW 190.000 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.5874816 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

Compound 4
HMBC/



Current Data Parameters
NAME jan05-14
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140106
Time 7.31
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG hmbcgplpndqf
TD 2048
SOLVENT MeOD
NS 64
DS 2
SWH 2556.237 Hz
FIDRES 1.248163 Hz
AQ 0.4005888 sec
RG 14596.5
DW 195.600 usec
DE 6.50 usec
TE 296.8 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 0.00002160 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
PL1 3.00 dB
SFO1 400.0312801 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 11.40 usec
PL2 -6.00 dB
SFO2 100.5991916 MHz

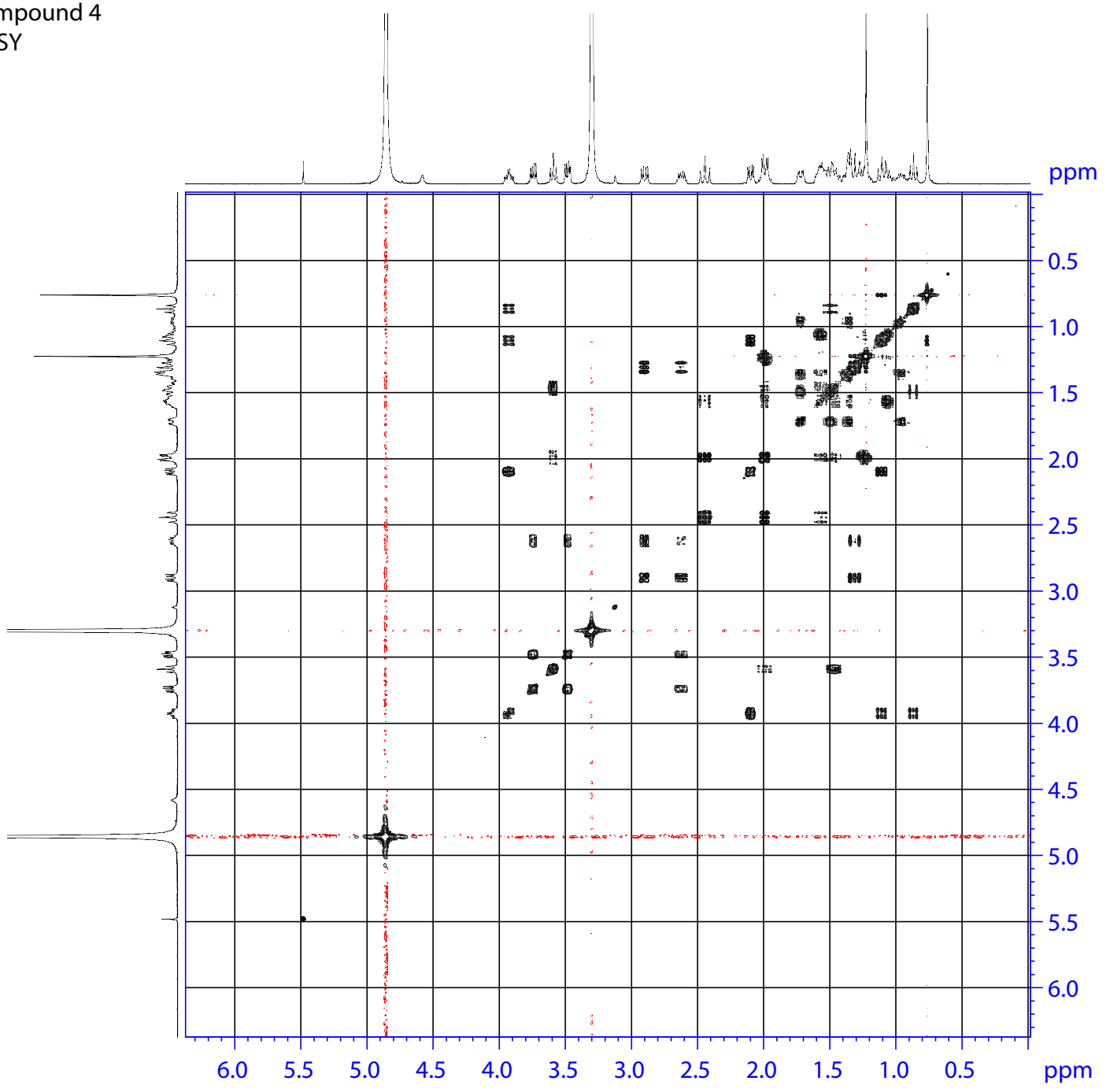
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPNAM[3] SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.5992 MHz
FIDRES 180.764175 Hz
SW 230.000 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.5874816 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Compound 4
COSY



AVANCE NEO 400 MHz
LAb # 115

Current Data Parameters
NAME jan05-14
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140105
Time 15.11
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG cosygpqf
TD 2048
SOLVENT MeOD
NS 16
DS 8
SWH 2556.237 Hz
FIDRES 1.248163 Hz
AQ 0.4005888 sec
RG 1024
DW 195.600 usec
DE 6.50 usec
TE 297.3 K
D0 0.00000300 sec
D1 1.50000000 sec
D13 0.00000400 sec
D16 0.00010000 sec
IN0 0.00039120 sec

======== CHANNEL f1 ========
NUC1 1H
P0 10.80 usec
P1 10.80 usec
PL1 3.00 dB
SFO1 400.0312801 MHz

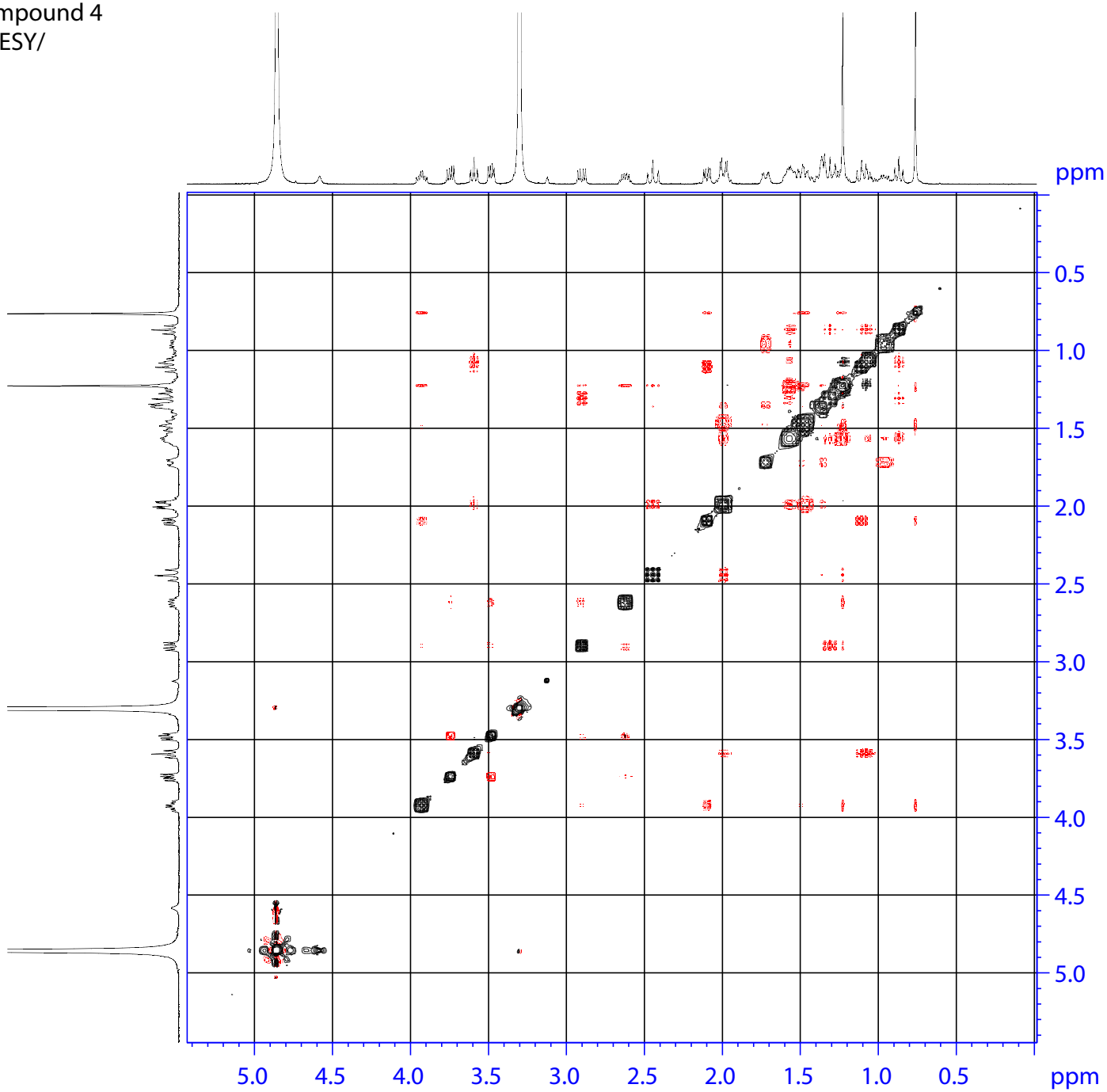
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 400.0313 MHz
FIDRES 19.970602 Hz
SW 6.390 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.0300087 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Compound 4
NOESY/



AVANCE NEO 400 MHz
LAb # 115

Current Data Parameters
NAME jan05-14
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140105
Time 17.26
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG noesygpph
TD 2048
SOLVENT MeOD
NS 32
DS 8
SWH 2556.237 Hz
FIDRES 1.248163 Hz
AQ 0.4005888 sec
RG 256
DW 195.600 usec
DE 6.50 usec
TE 296.9 K
D0 0.00018185 sec
D1 1.50000000 sec
D8 0.80000001 sec
D16 0.00010000 sec
IN0 0.00039120 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
PL1 3.00 dB
SFO1 400.0312801 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 400.0313 MHz
FIDRES 19.970602 Hz
SW 6.390 ppm
FnMODE States-TPPI

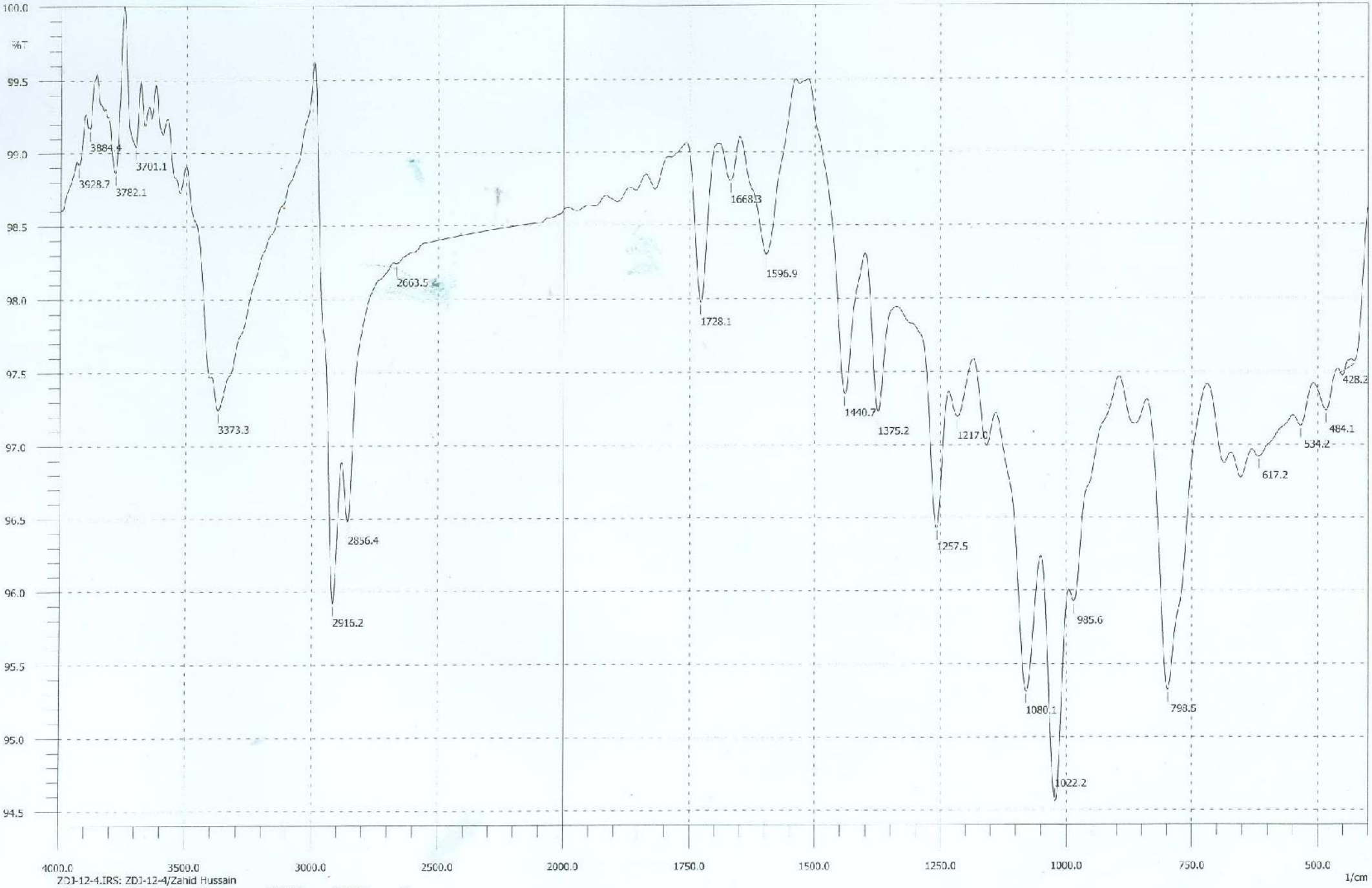
F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

JEOL HX 110 MASS SPECTROMETER (FAB-HR)

STUDENT NAME	Zahid	SAMPLE CODE	DATE	
SUPERVISOR NAME	Prof. Dr. M. Iqbal	ZDB - 14	FAB (+VE / -VE)	

Mass	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
337.2366	337.2379	-3.8	-1.3	4.5	$C_{20}H_{33}O_4$

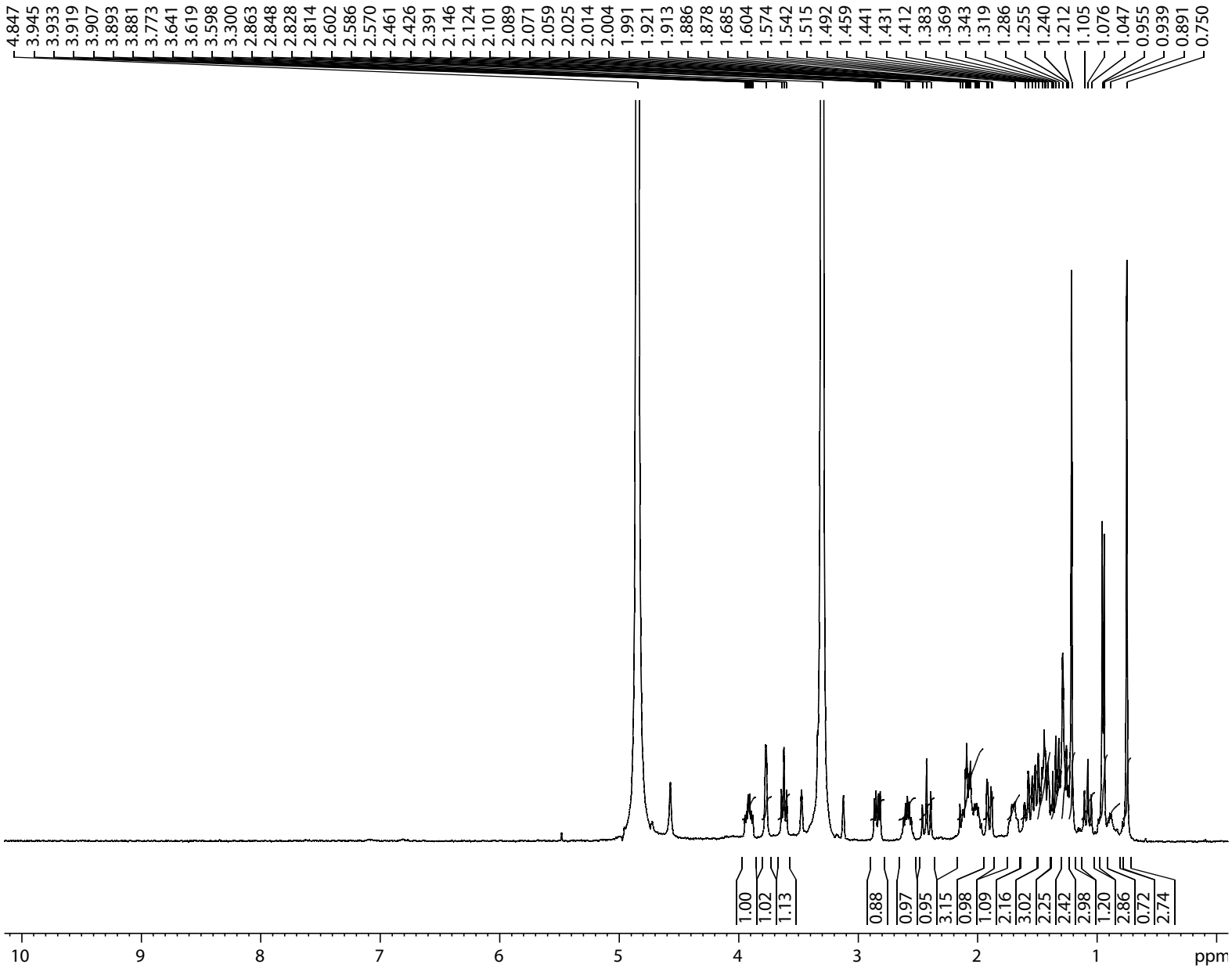


ZD1-12-4.IRS: ZD1-12-4/Zahid Hussain

Date:	04/02/2015	Time:	15:51:48	NScans:	5	
Type:	HYPER IR	User:	ZUBAIR AHMED		Detector:	standard
Abscissa:	1/cm	Ordinate:	%T	Apodization:	Happ	
Min:	401.17	Max:	3998.16	Range:	1/cm	
Ndp:	1866	Data Interval:	1.92868	Resolution:	4.0	
Gain:	auto	Aperture:	auto	Mirror Speed:	2.8(low)	

Compound 5
1H

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME dec26-13
EXPNO 1
PROCNO 1

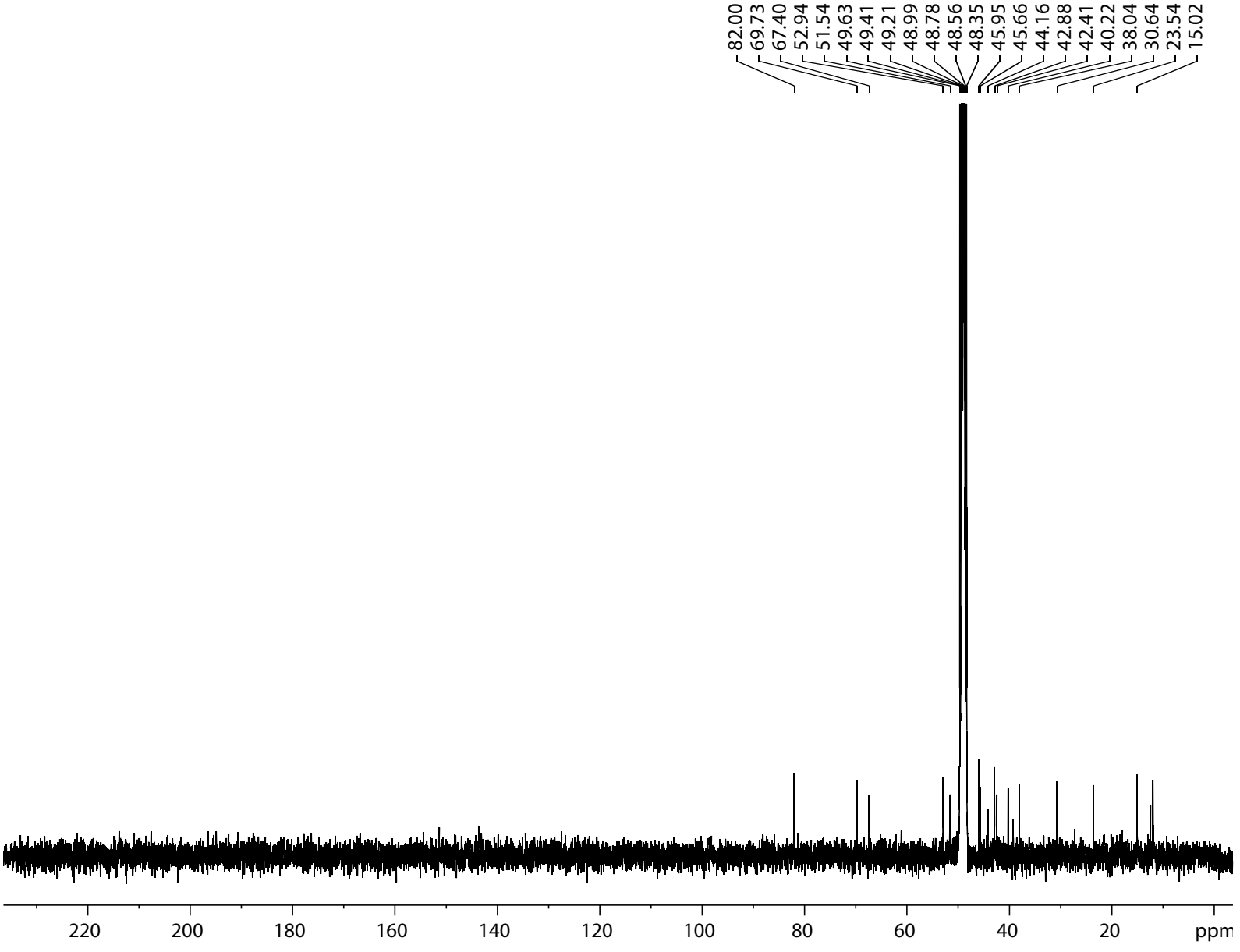
F2 - Acquisition Parameters
Date_ 20131226
Time 15.25
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT MeOD
NS 64
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 362
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.50000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 400.0332002 MHz

F2 - Processing parameters
SI 16384
SF 400.0300087 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Compound 5
BB

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME dec26-13
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131227
Time 23.57
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg
TD 32768
SOLVENT MeOD
NS 20480
DS 2
SWH 24154.590 Hz
FIDRES 0.737140 Hz
AQ 0.6782976 sec
RG 32768
DW 20.700 usec
DE 6.50 usec
TE 297.7 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 20

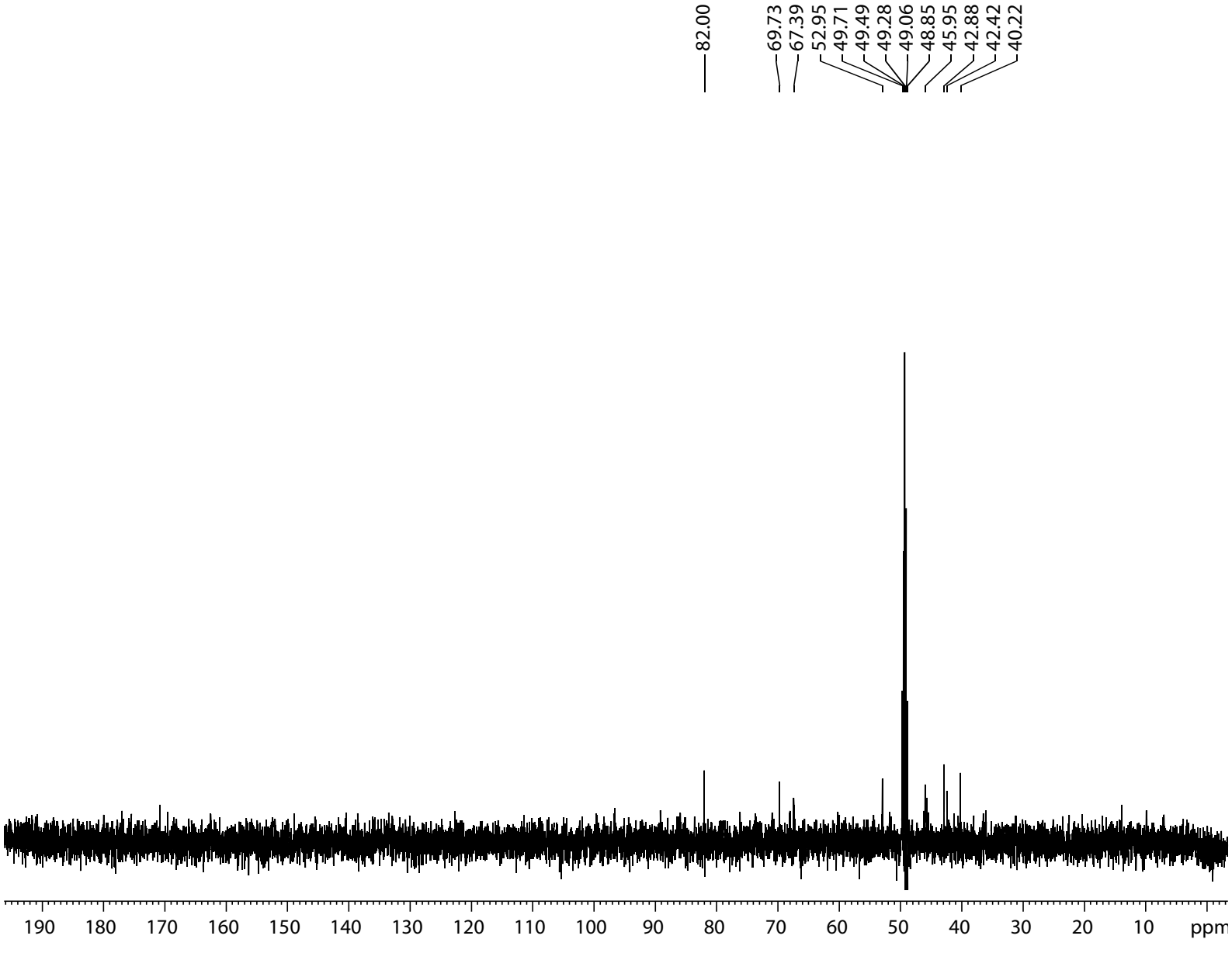
======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
PL1 -6.00 dB
SFO1 100.5991916 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
PL13 22.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874816 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Compound 5
DEPT90#

AVANCE NEO 400 MH
LAb # 115



Current Data Parameters
NAME dec26-13
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131228
Time 20.48
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG dept90
TD 32768
SOLVENT MeOD
NS 7168
DS 2
SWH 20080.320 Hz
FIDRES 0.612803 Hz
AQ 0.8159232 sec
RG 16384
DW 24.900 usec
DE 6.50 usec
TE 297.3 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 7

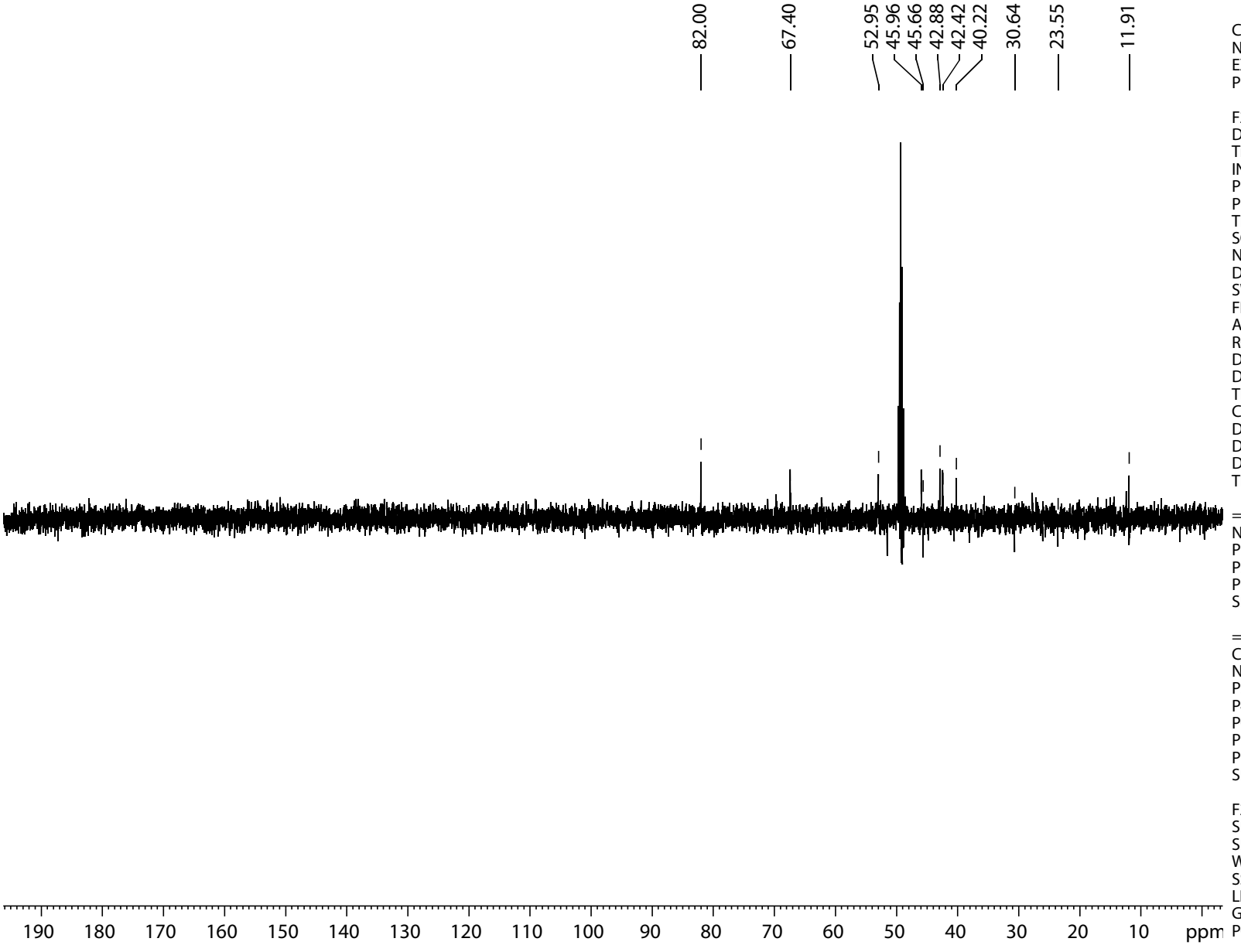
======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
P2 24.60 usec
PL1 -6.00 dB
SFO1 100.5971798 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 10.50 usec
P4 21.00 usec
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874816 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20

Compound 5
DEP135#//

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME dec26-13
EXPNO 7
PROCNO 1

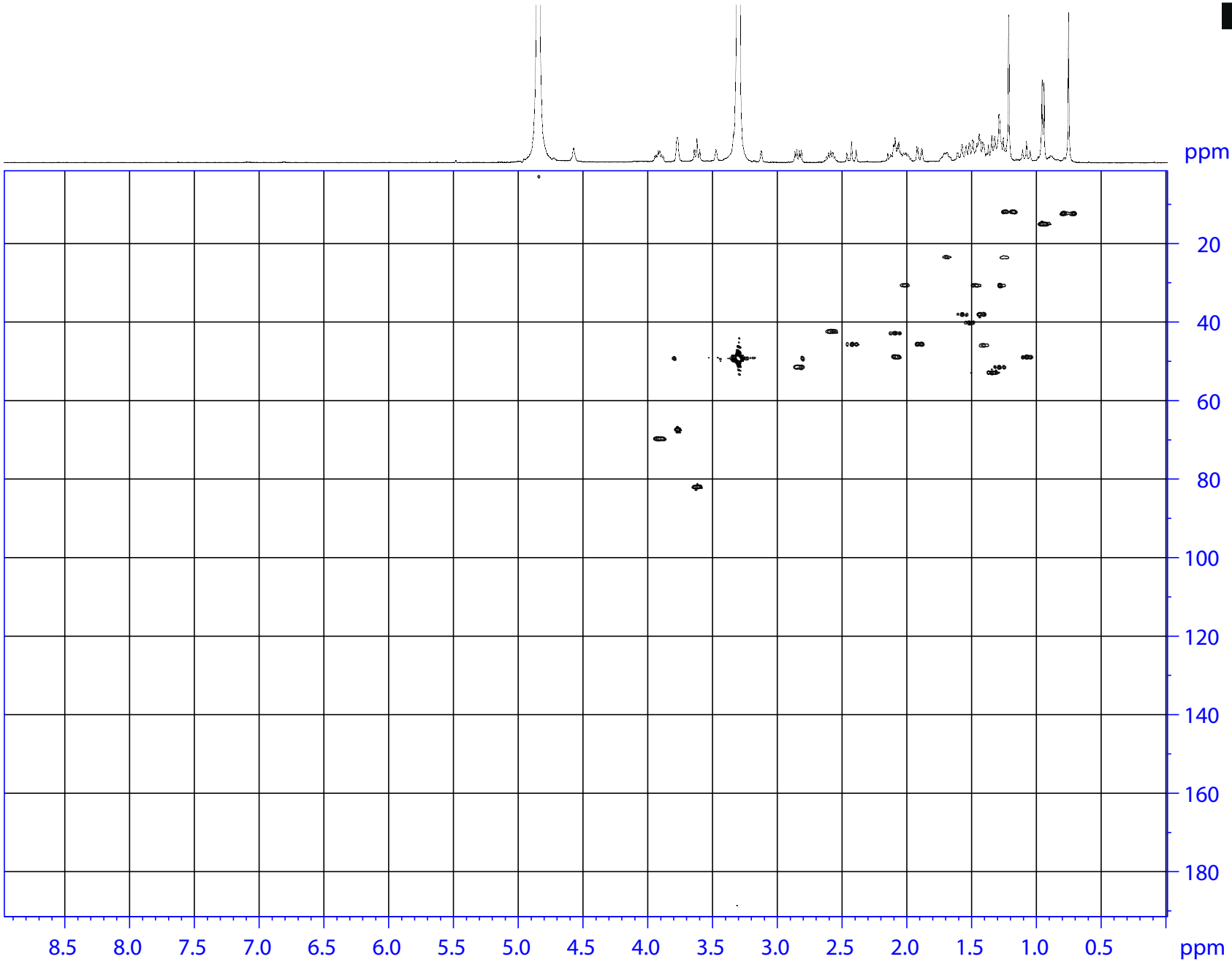
F2 - Acquisition Parameters
Date_ 20131228
Time 12.44
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG dept135
TD 32768
SOLVENT MeOD
NS 12288
DS 2
SWH 20080.320 Hz
FIDRES 0.612803 Hz
AQ 0.8159232 sec
RG 16384
DW 24.900 usec
DE 6.50 usec
TE 296.4 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 12

======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
P2 24.60 usec
PL1 -6.00 dB
SFO1 100.5971798 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 10.50 usec
P4 21.00 usec
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874816 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20

Compound 5
HSQC//



Current Data Parameters
NAME dec26-13
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131227
Time 2.47
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG hsqcetgpsi
TD 1024
SOLVENT MeOD
NS 64
DS 2
SWH 3591.954 Hz
FIDRES 3.507768 Hz
AQ 0.1425408 sec
RG 14596.5
DW 139.200 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D0 0.00000300 sec
D1 2.00000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00010000 sec
D24 0.00110000 sec
IN0 0.00002615 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
P28 2000.00 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp
NUC2 13C
P3 11.40 usec
P4 22.80 usec
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 17.00 dB
SFO2 100.5971798 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

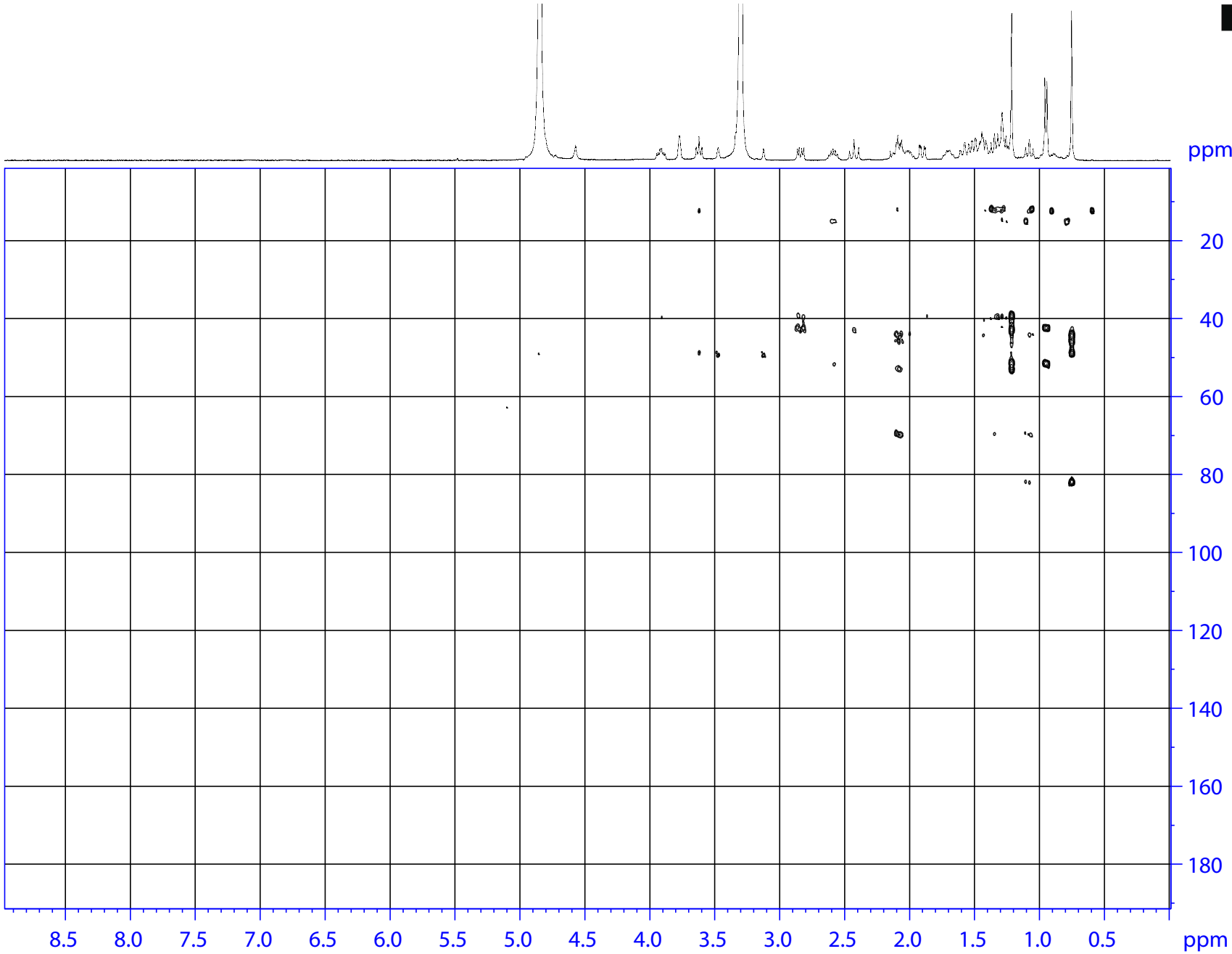
F1 - Acquisition parameters
TD 256
SFO1 100.5972 MHz
FIDRES 149.323944 Hz
SW 190.000 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.5874816 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

Compound 5

HMBC/



Current Data Parameters
NAME dec26-13
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131227
Time 12.39
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG hmbcgplpndqf
TD 2048
SOLVENT MeOD
NS 64
DS 2
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 14596.5
DW 139.200 usec
DE 6.50 usec
TE 296.8 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 0.00002160 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 11.40 usec
PL2 -6.00 dB
SFO2 100.5991916 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPNAM[3] SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

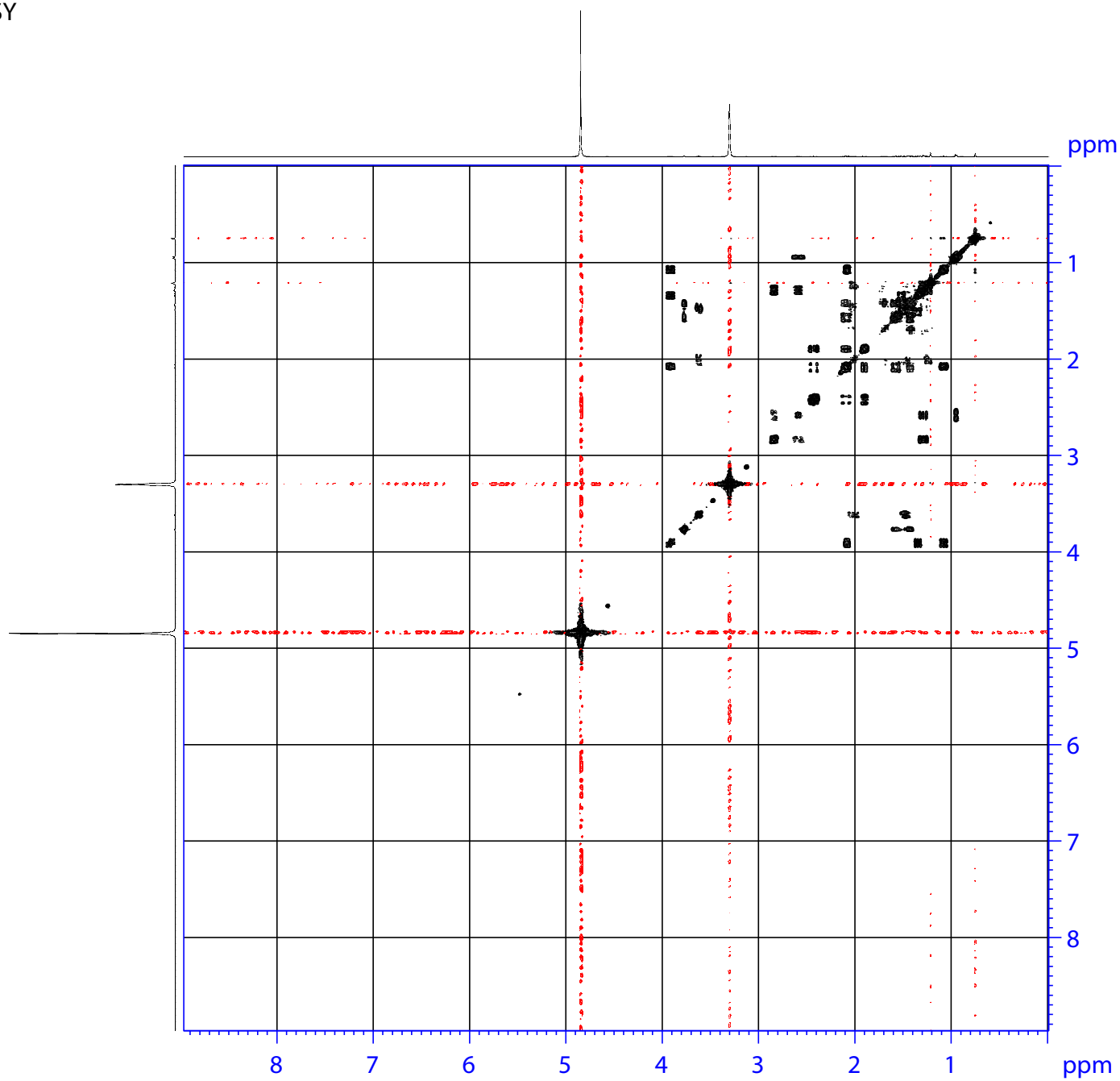
F1 - Acquisition parameters
TD 256
SFO1 100.5992 MHz
FIDRES 180.764175 Hz
SW 230.000 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.5874816 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Compound 5
COSY

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME dec26-13
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131226
Time 15.31
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG cosygpqf
TD 2048
SOLVENT MeOD
NS 32
DS 8
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 2048
DW 139.200 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.50000000 sec
D13 0.00000400 sec
D16 0.00010000 sec
IN0 0.00027840 sec

======== CHANNEL f1 ========
NUC1 1H
P0 10.80 usec
P1 10.80 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

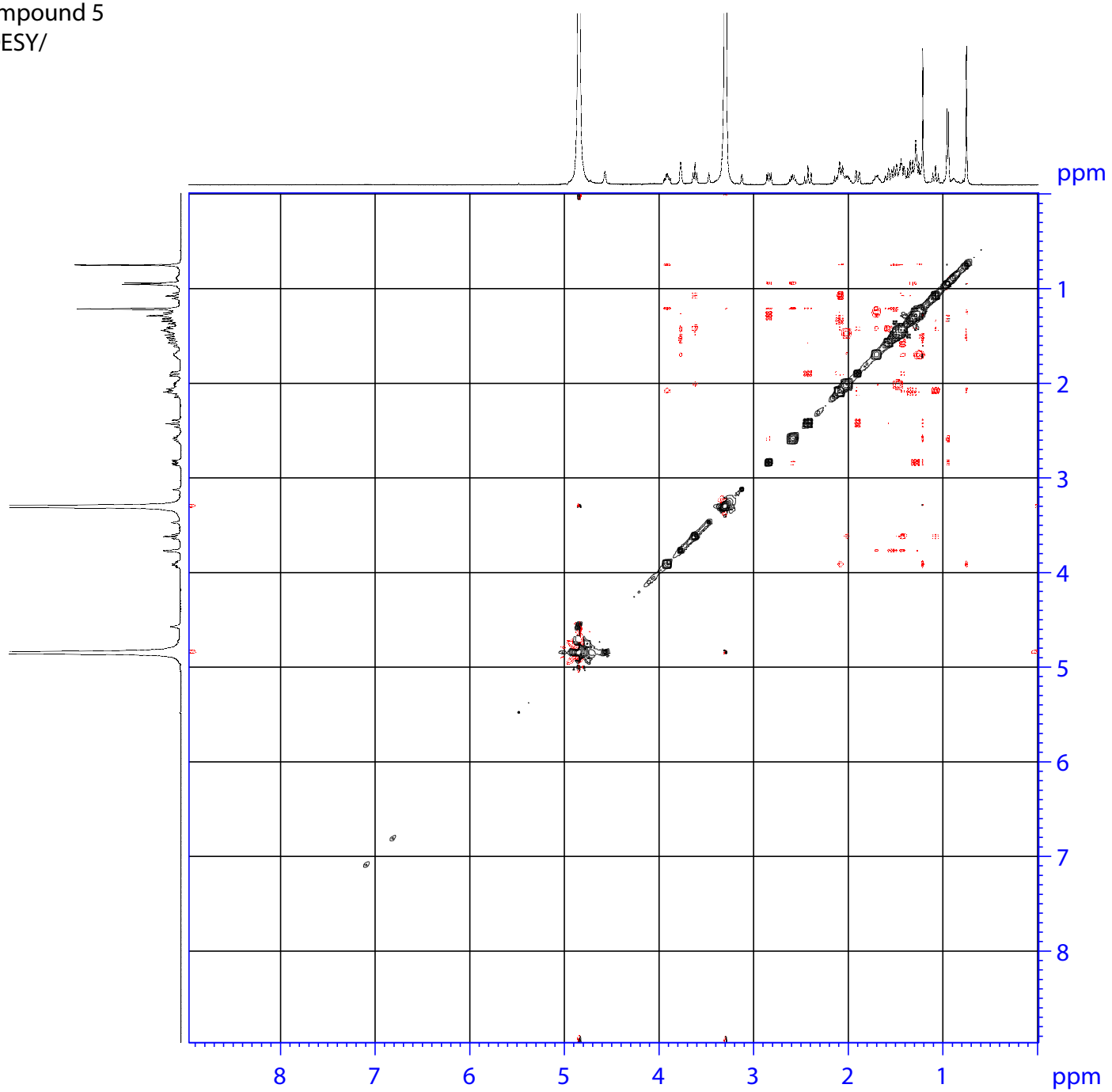
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 400.0318 MHz
FIDRES 28.062141 Hz
SW 8.979 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.0300087 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Compound 5
NOESY/



AVANCE NEO 400 MHz
LAb # 115

Current Data Parameters
NAME dec26-13
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131226
Time 19.42
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG noesygpph
TD 2048
SOLVENT MeOD
NS 32
DS 8
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 1149.4
DW 139.200 usec
DE 6.50 usec
TE 299.1 K
D0 0.00012545 sec
D1 2.00000000 sec
D8 0.80000001 sec
D16 0.00010000 sec
IN0 0.00027840 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 400.0318 MHz
FIDRES 28.062141 Hz
SW 8.979 ppm
FnMODE States-TPPI

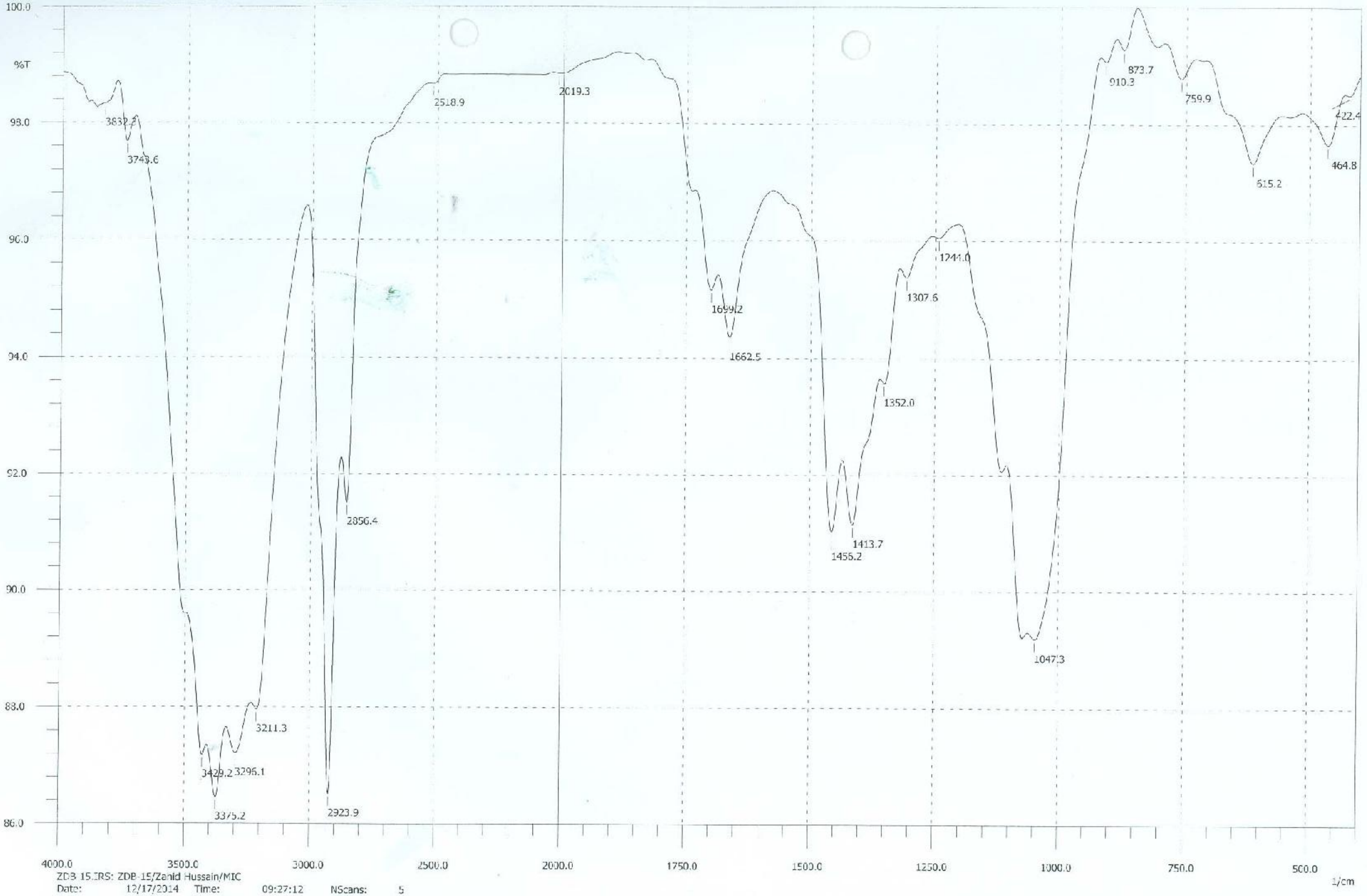
F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

JEOL HX 110 MASS SPECTROMETER (FAB-HR)

STUDENT NAME	Zahid	SAMPLE CODE	DATE	
SUPERVISOR NAME	Prof. Dr. M. Iqbal	ZDB-15	FAB (+VE / -VE)	

Mass	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
337.2365	337.2379	-4.1	-1.4	4.5	$C_{21} H_{33} O_4$

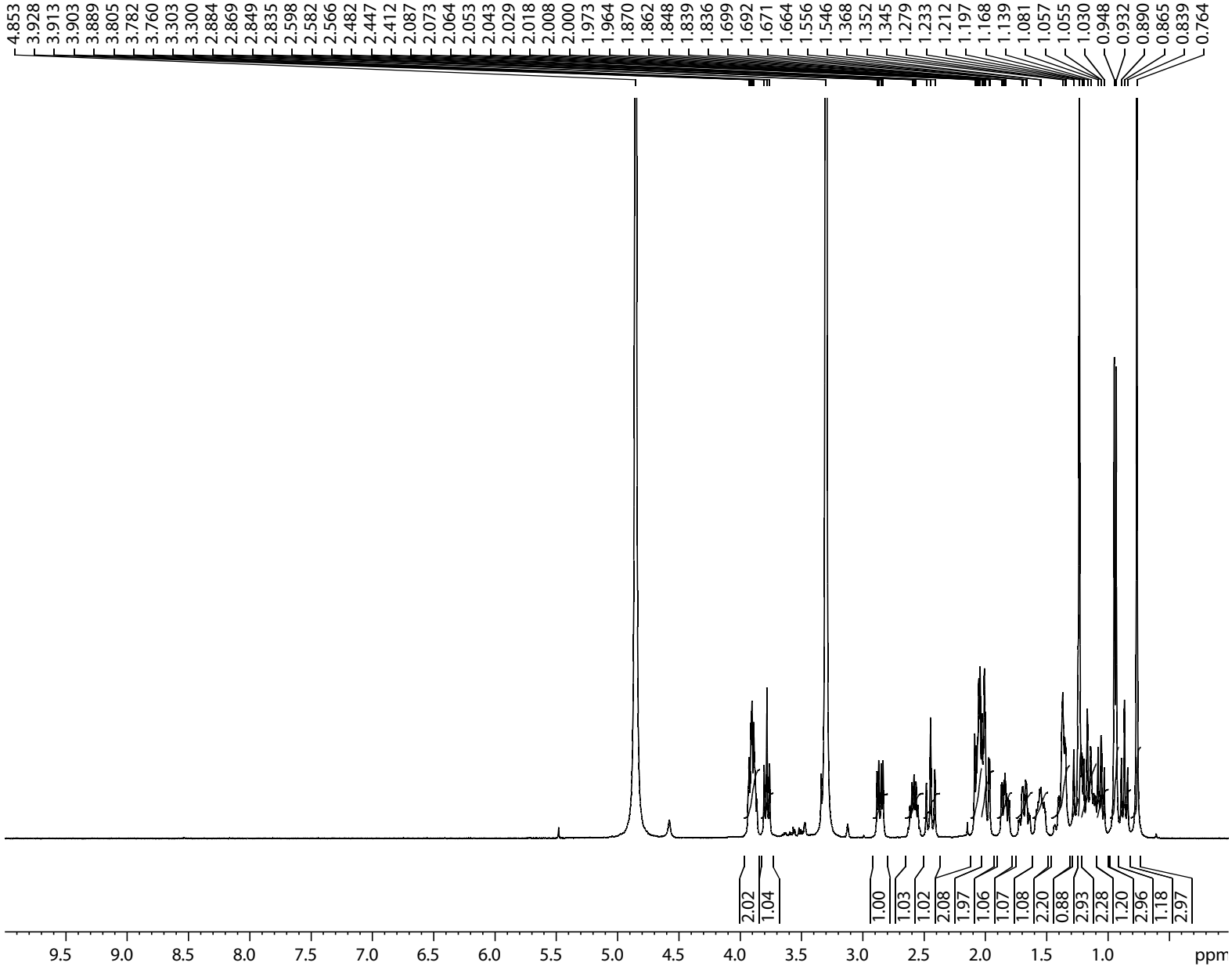


ZDB-15.CRS: ZDB-15/Zahid Hussain/MIC

Date:	12/17/2014	Time:	09:27:12	NScans:	5		
Type:	HYPER IR	User:	ZUBAIR AHMED			Detector:	standard
Abscissa:	1/cm	Ordinate:	%T	Apodization:	Happ		
Min:	401.17	Max:	3998.16	Range:	1/cm		
Ndp:	1866	Data Interval:	1.92868	Resolution:	4.0		
Gain:	auto	Aperture:	auto	Mirror Speed:	2.8(low)		

Compound 6
1H

AVANCE NEO 400 MHz
LAb # 115



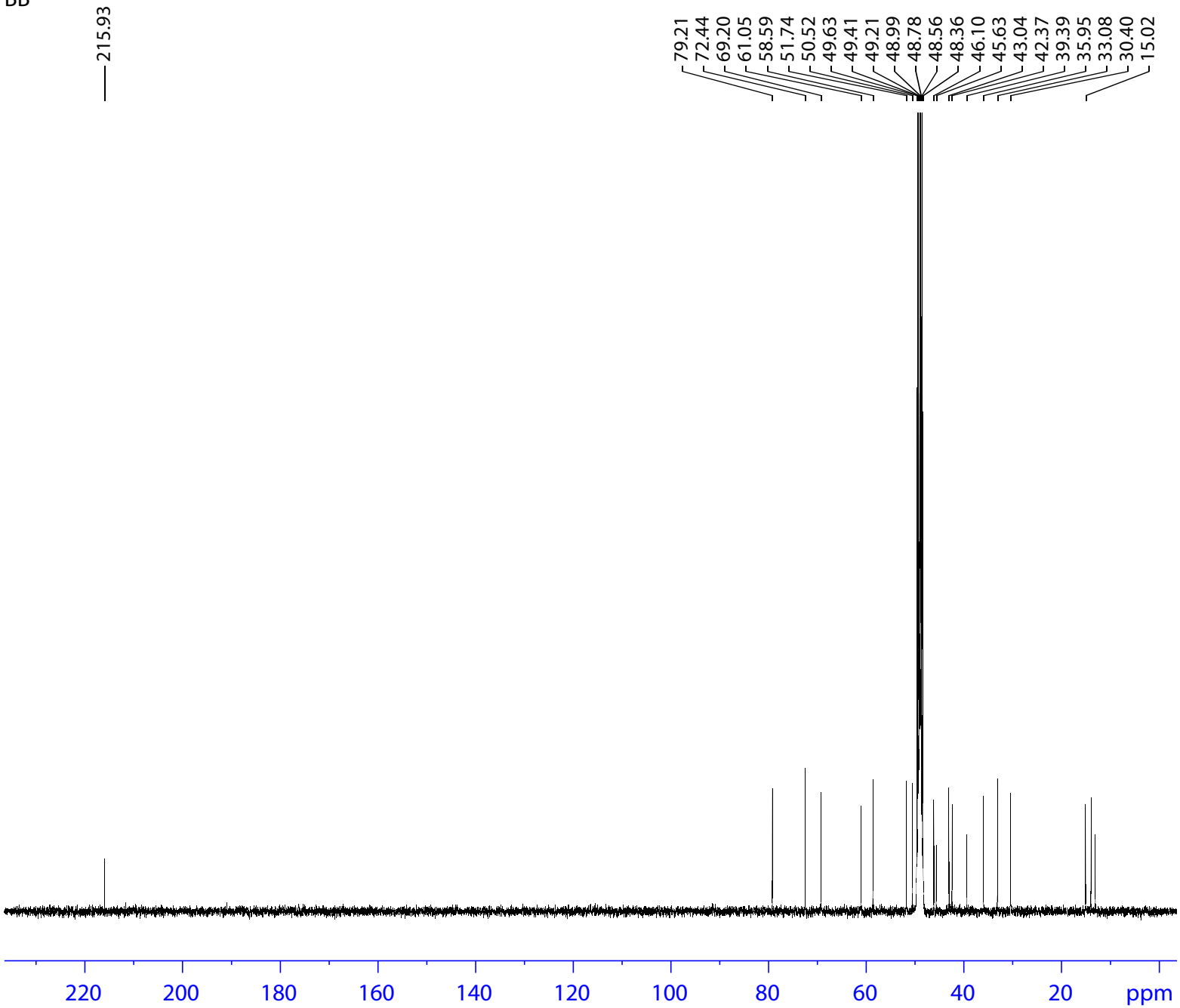
Current Data Parameters
NAME jan10-14
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140110
Time 18.54
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT MeOD
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 256
DW 62.400 usec
DE 6.50 usec
TE 297.5 K
D1 1.50000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 400.0332002 MHz

F2 - Processing parameters
SI 16384
SF 400.0300087 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Compound 6
BB



Current Data Parameters
NAME jan10-14
EXPNO 6
PROCNO 1

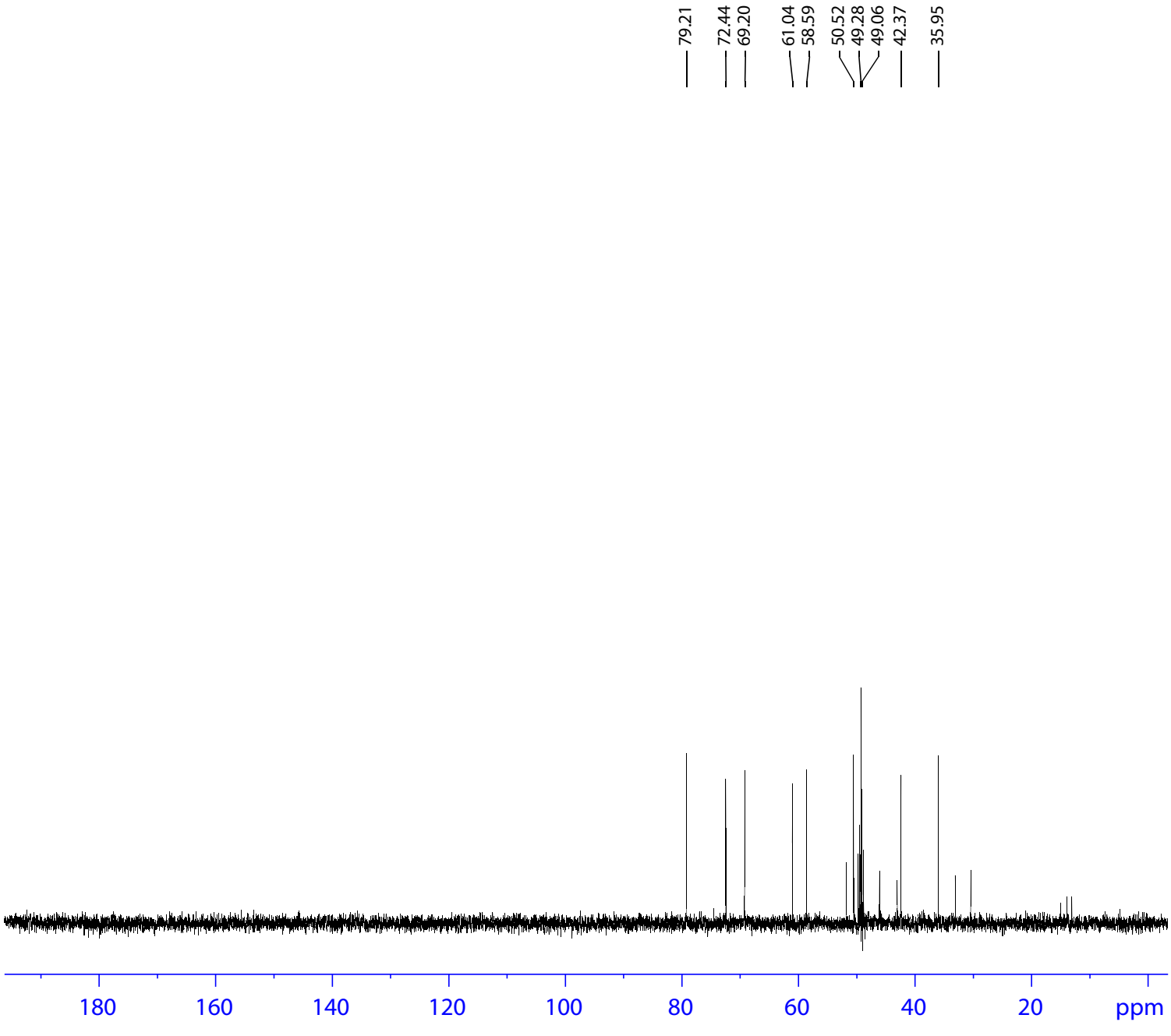
F2 - Acquisition Parameters
Date_ 20140112
Time 1.14
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg
TD 32768
SOLVENT MeOD
NS 20480
DS 2
SWH 24154.590 Hz
FIDRES 0.737140 Hz
AQ 0.6782976 sec
RG 32768
DW 20.700 usec
DE 6.50 usec
TE 296.9 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 20

======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
PL1 -6.00 dB
SFO1 100.5991916 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
PL13 22.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874816 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Compound 6
DEPT90#



Current Data Parameters
NAME jan10-14
EXPNO 8
PROCNO 1

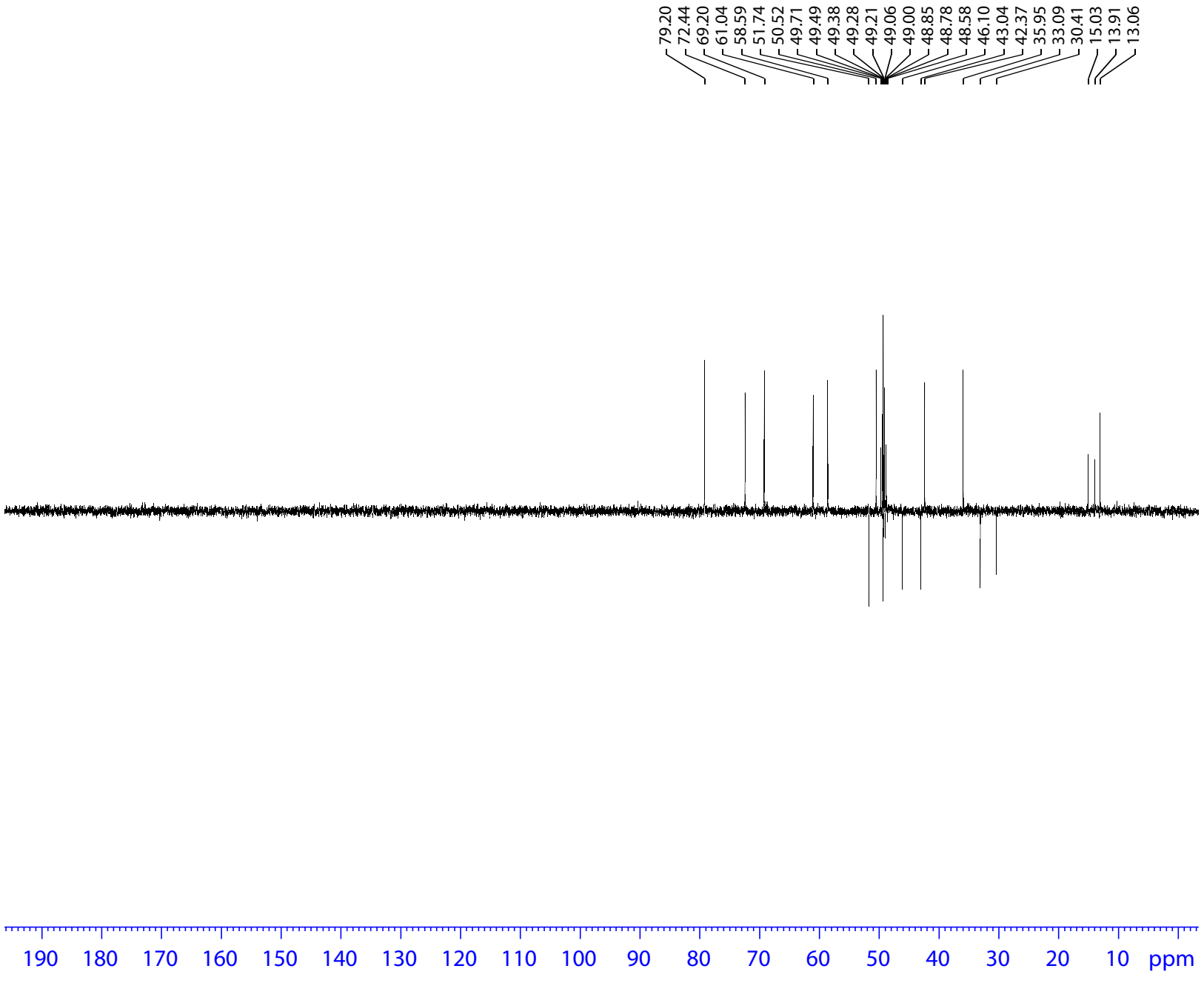
F2 - Acquisition Parameters
Date_ 20140115
Time 4.08
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG dept90
TD 32768
SOLVENT MeOD
NS 7168
DS 2
SWH 20080.320 Hz
FIDRES 0.612803 Hz
AQ 0.8159232 sec
RG 16384
DW 24.900 usec
DE 6.50 usec
TE 297.0 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 7

======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
P2 24.60 usec
PL1 -6.00 dB
SFO1 100.5971798 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 10.50 usec
P4 21.00 usec
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874816 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20

Compound 6
DEP135



Current Data Parameters
NAME jan10-14
EXPNO 7
PROCNO 1

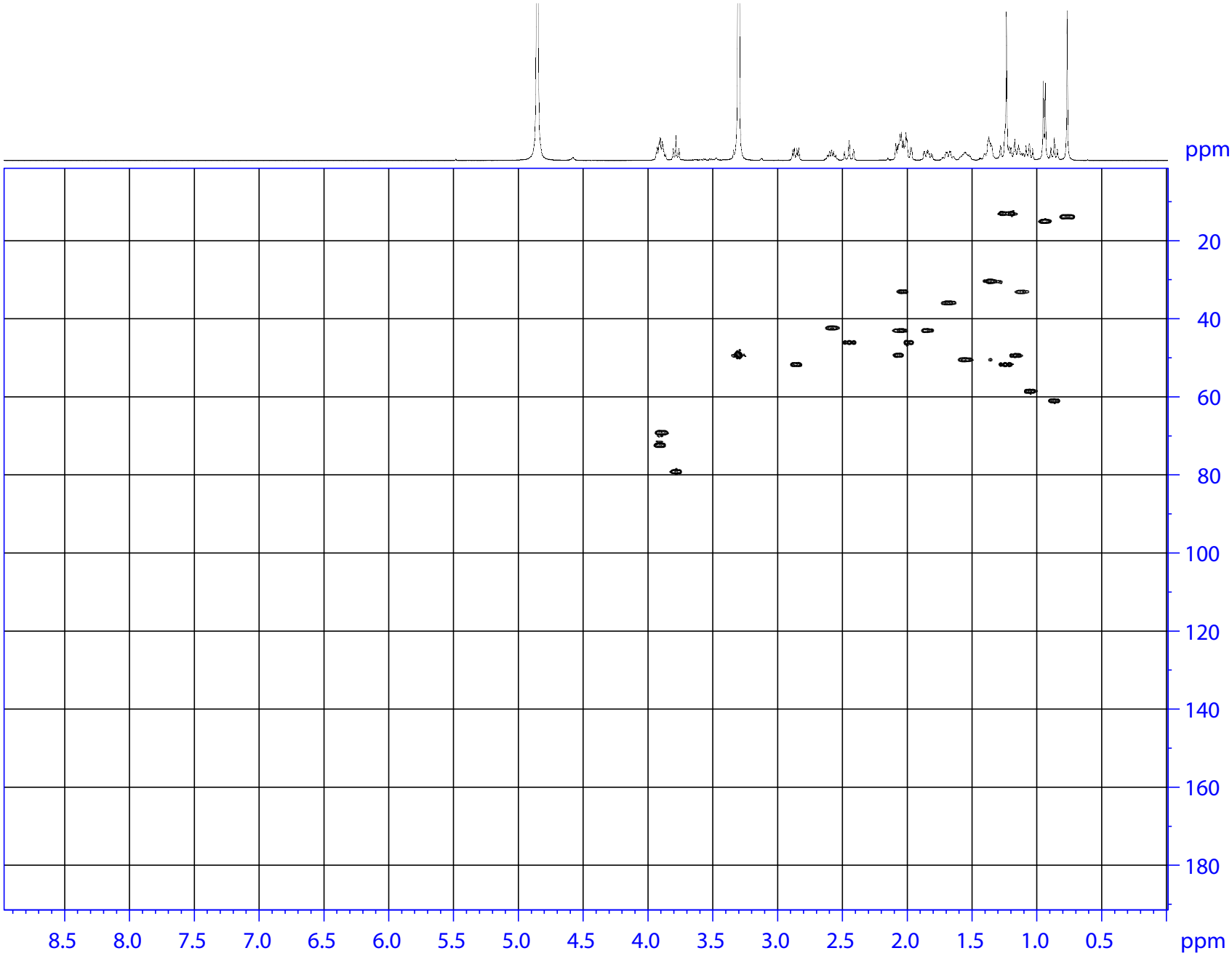
F2 - Acquisition Parameters
Date_ 20140114
Time 17.24
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG dept135
TD 32768
SOLVENT MeOD
NS 16384
DS 2
SWH 20080.320 Hz
FIDRES 0.612803 Hz
AQ 0.8159232 sec
RG 16384
DW 24.900 usec
DE 6.50 usec
TE 297.2 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 16

======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
P2 24.60 usec
PL1 -6.00 dB
SFO1 100.5971798 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 10.50 usec
P4 21.00 usec
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874816 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20

Compound 6
HSQC//



Current Data Parameters
NAME jan10-14
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140111
Time 6.21
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG hsqcetgpsi
TD 1024
SOLVENT MeOD
NS 64
DS 2
SWH 3591.954 Hz
FIDRES 3.507768 Hz
AQ 0.1425408 sec
RG 14596.5
DW 139.200 usec
DE 6.50 usec
TE 296.7 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 0.00002615 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
P28 2000.00 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp
NUC2 13C
P3 11.40 usec
P4 22.80 usec
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 17.00 dB
SFO2 100.5971798 MHz

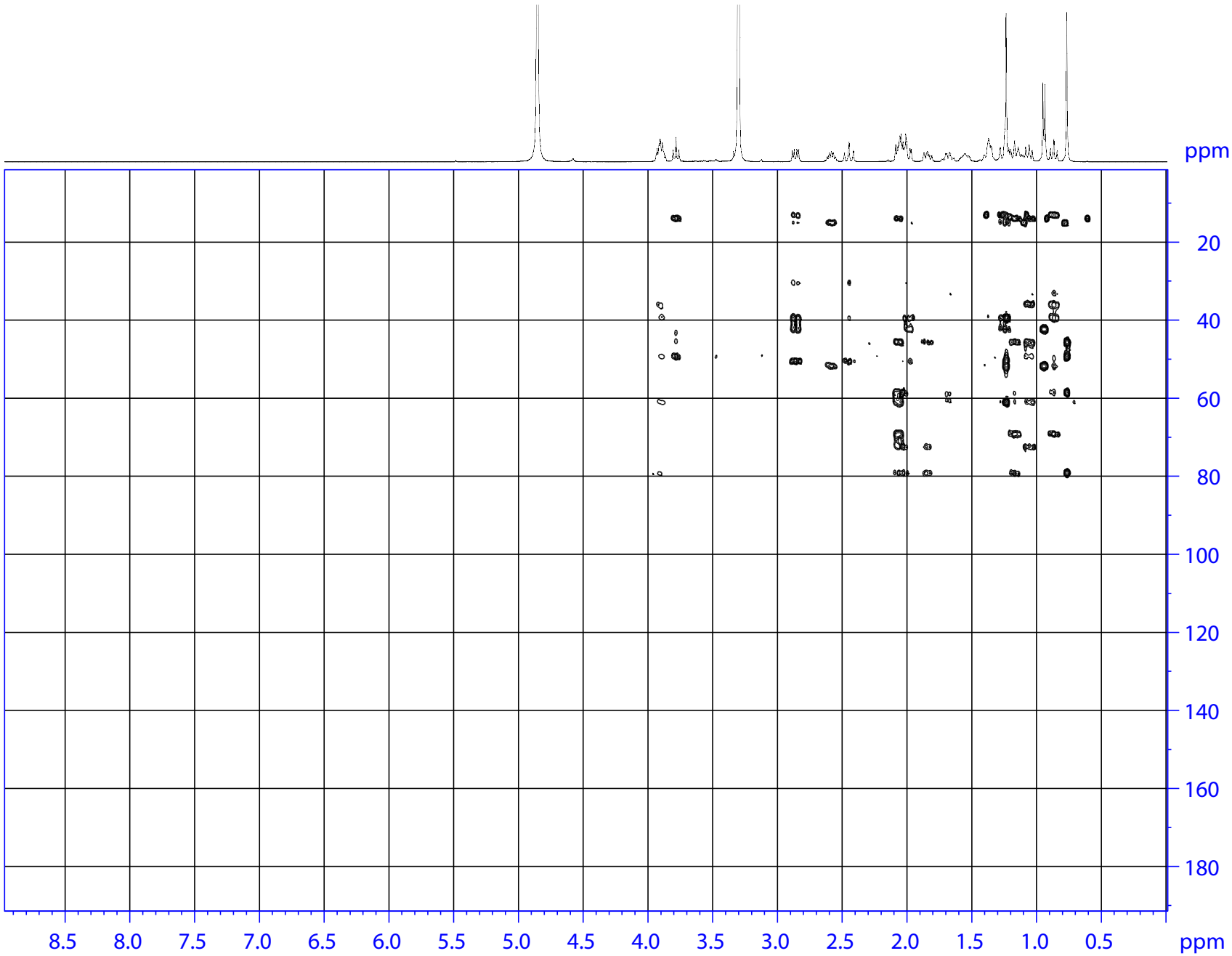
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.5972 MHz
FIDRES 149.323944 Hz
SW 190.000 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.5874816 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

Compound 6
HMBC



Current Data Parameters
NAME jan10-14
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140111
Time 13.56
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG hmbcgplpndqf
TD 2048
SOLVENT MeOD
NS 64
DS 2
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 14596.5
DW 139.200 usec
DE 6.50 usec
TE 296.7 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 0.00002160 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 11.40 usec
PL2 -6.00 dB
SFO2 100.5991916 MHz

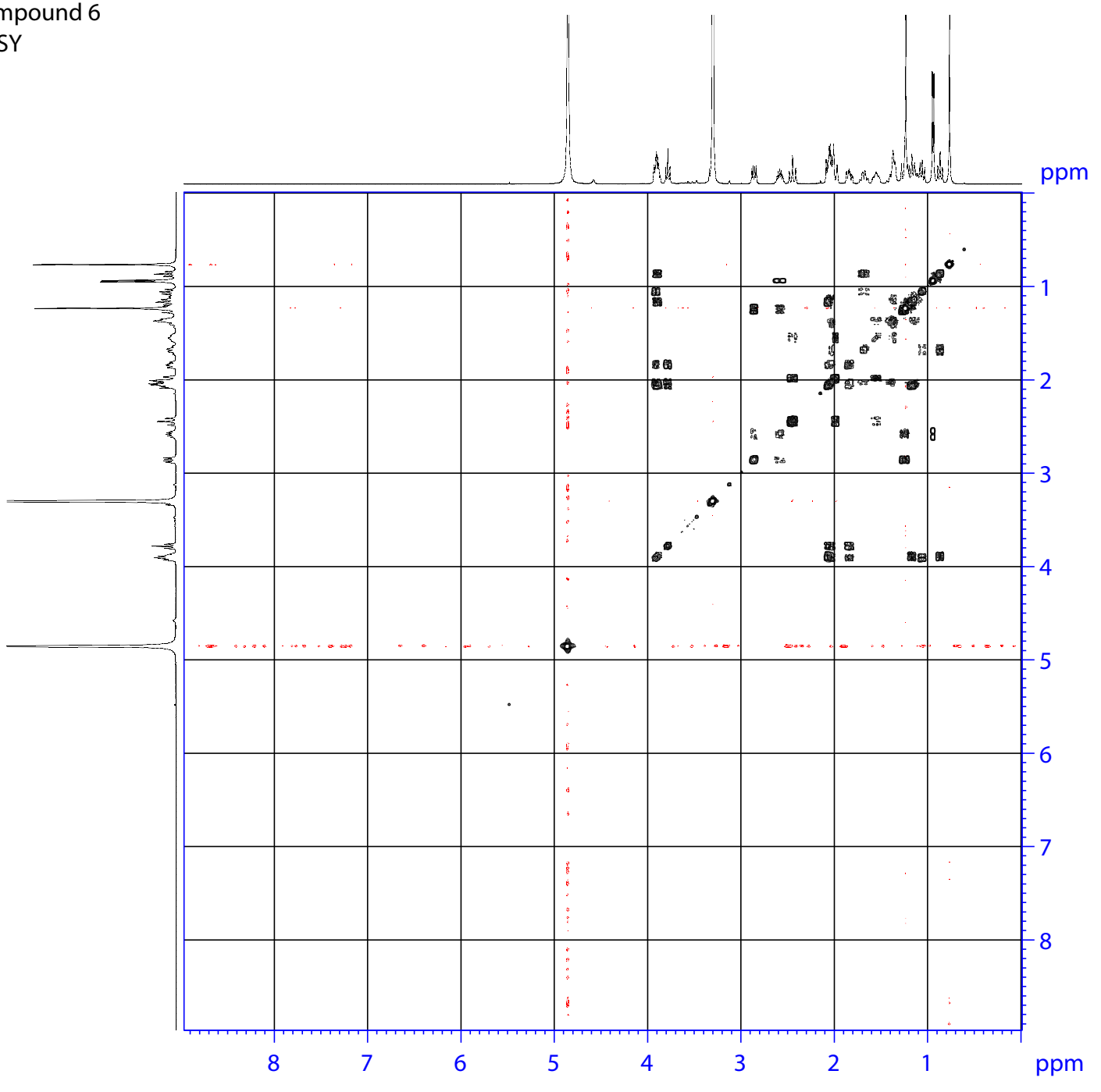
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPNAM[3] SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.5992 MHz
FIDRES 180.764175 Hz
SW 230.000 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.5874816 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Compound 6
COSY



AVANCE NEO 400 MHz
LAb # 115

Current Data Parameters
NAME jan10-14
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140110
Time 19.06
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG cosygpqf
TD 2048
SOLVENT MeOD
NS 32
DS 8
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 574.7
DW 139.200 usec
DE 6.50 usec
TE 297.5 K
D0 0.00000300 sec
D1 1.50000000 sec
D13 0.00000400 sec
D16 0.00010000 sec
IN0 0.00027840 sec

======== CHANNEL f1 ========
NUC1 1H
P0 10.80 usec
P1 10.80 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPZ1 10.00 %
P16 1000.00 usec

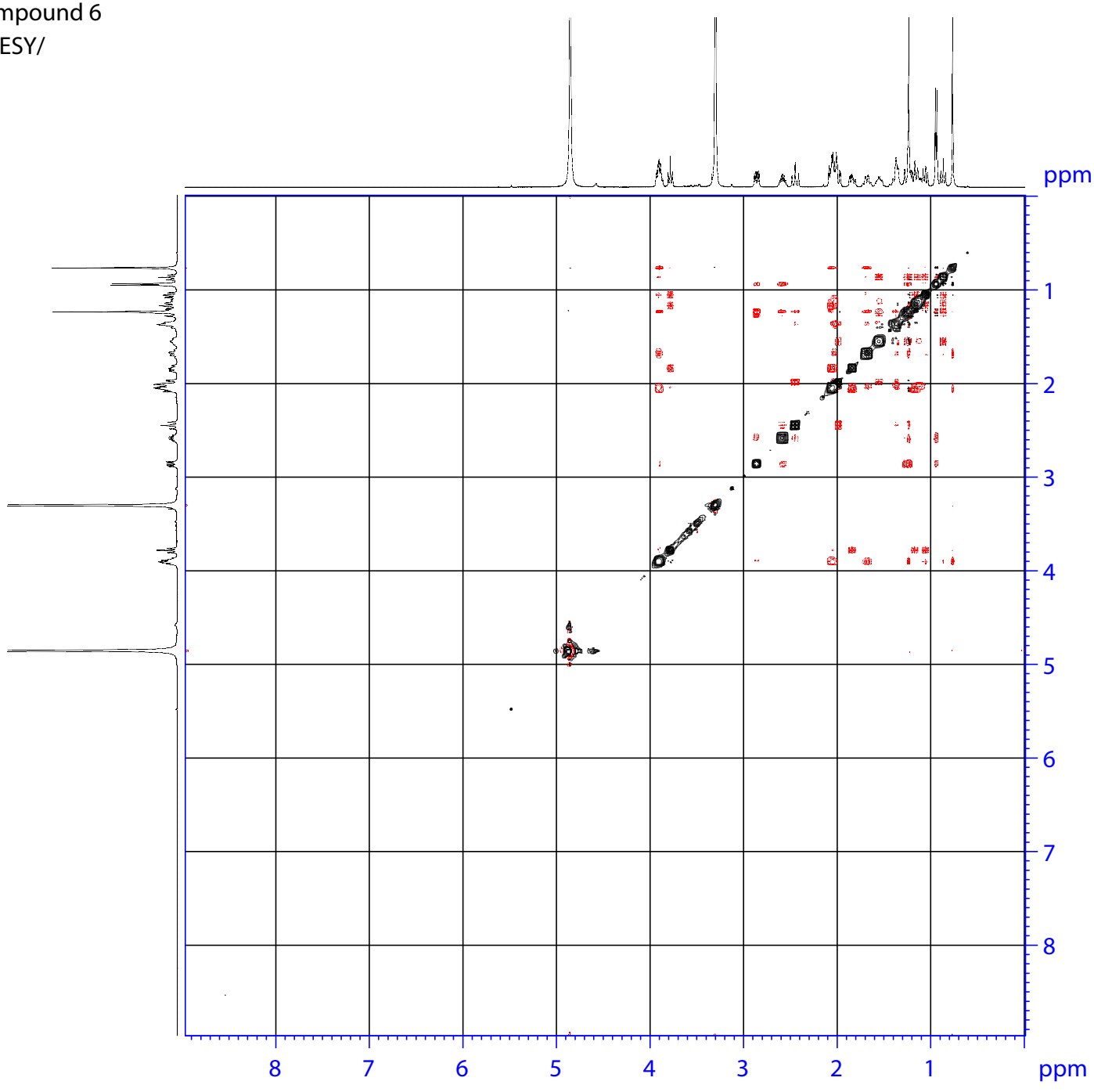
F1 - Acquisition parameters
TD 256
SFO1 400.0318 MHz
FIDRES 28.062141 Hz
SW 8.979 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.0300087 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Compound 6
NOESY/

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME jan10-14
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140110
Time 23.16
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG noesygpph
TD 2048
SOLVENT MeOD
NS 32
DS 8
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 362
DW 139.200 usec
DE 6.50 usec
TE 297.2 K
D0 0.00012545 sec
D1 2.00000000 sec
D8 0.80000001 sec
D16 0.00010000 sec
IN0 0.00027840 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 400.0318 MHz
FIDRES 28.062141 Hz
SW 8.979 ppm
FnMODE States-TPPI

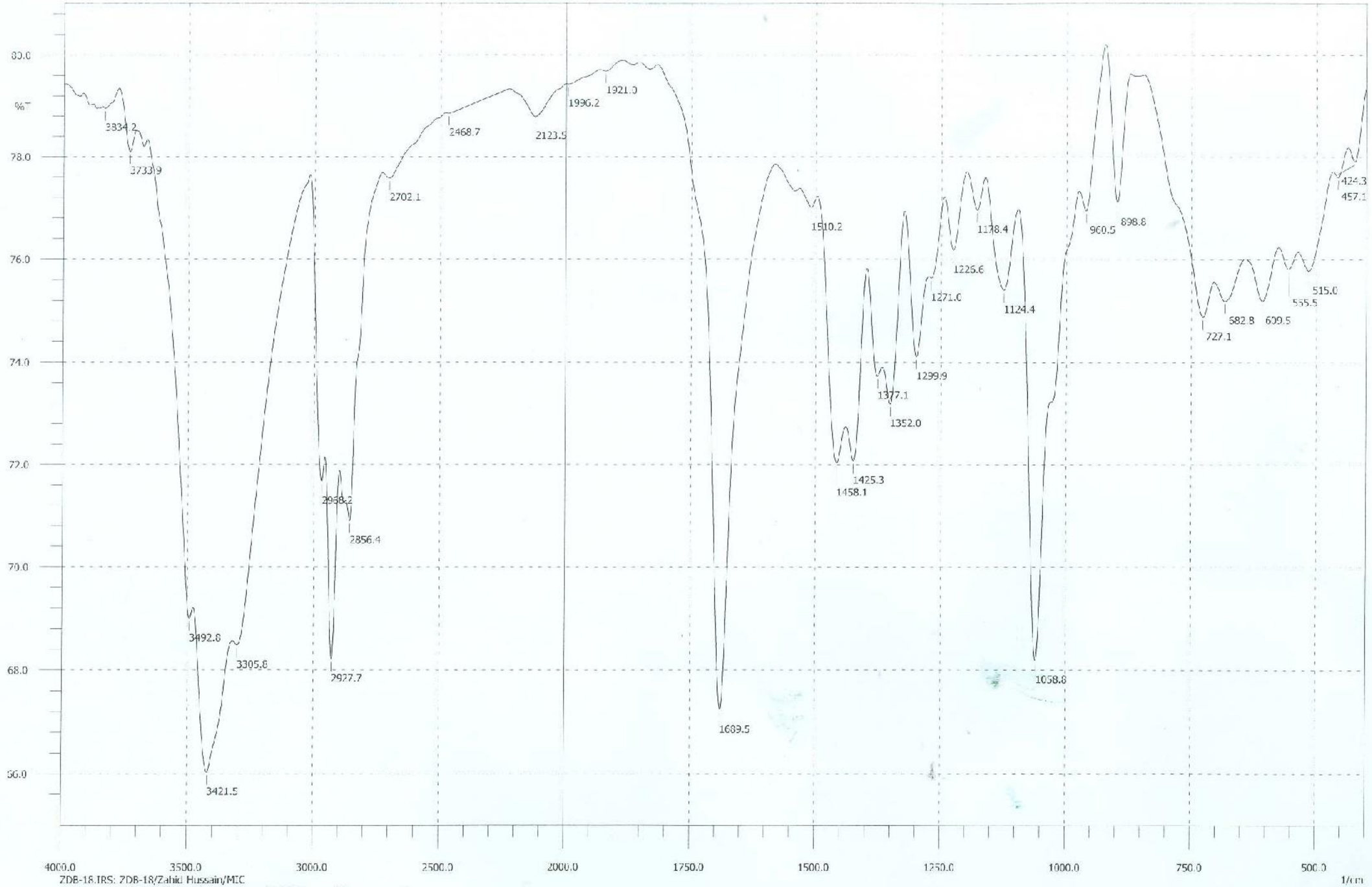
F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

JEOL HX 110 MASS SPECTROMETER (FAB-HR)

STUDENT NAME	Zahid	SAMPLE CODE	DATE	
SUPERVISOR NAME	Prof. Dr. M. Iqbal	ZDB-18	FAB (+VE / -VE)	

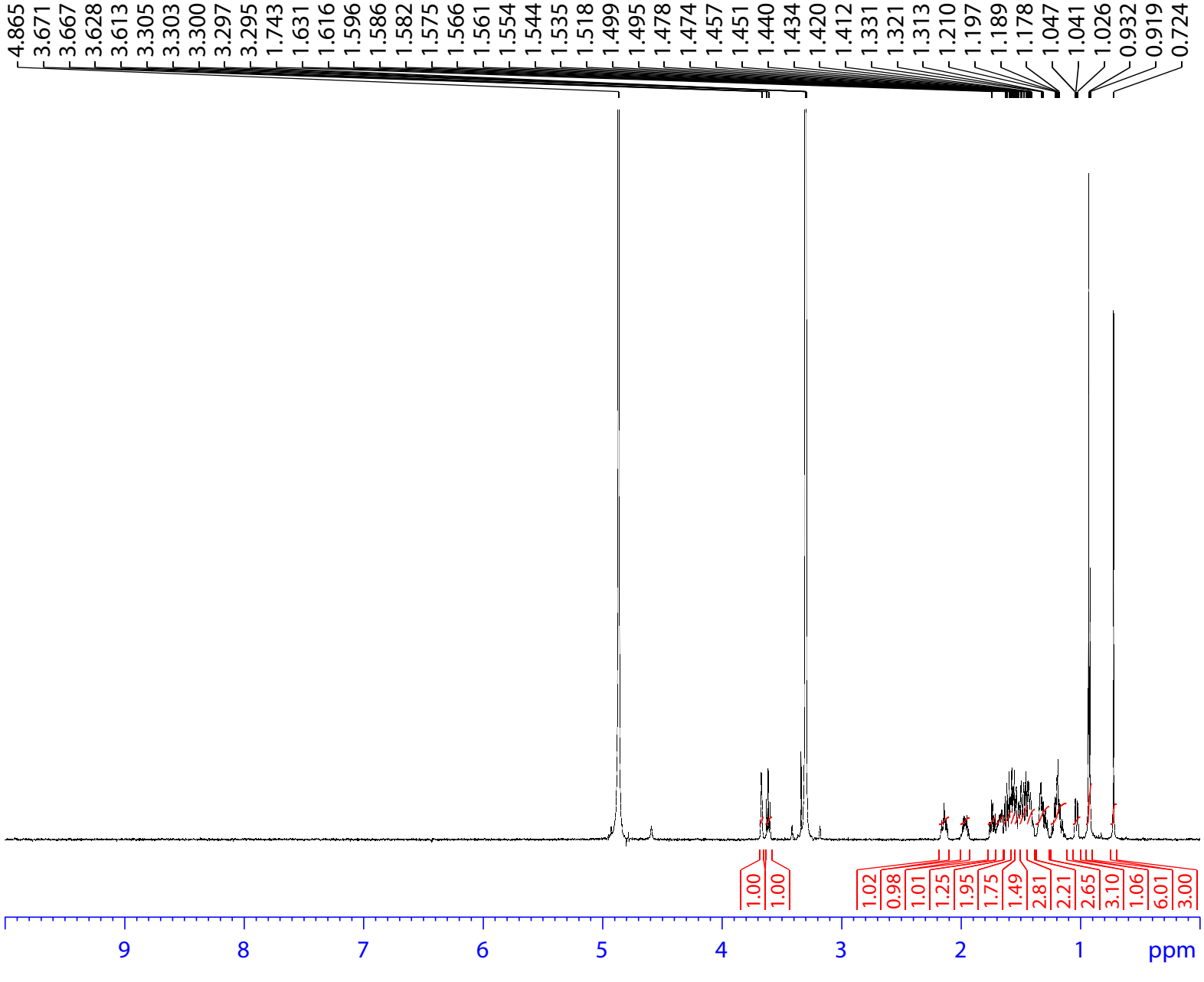
Mass	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
337.2372	337.2379	-2.0	-0.7	4.5	$C_{20}H_{33}O_4$



ZDB-18.IRS: ZDB-18/Zahid Hussain/MIC

Date:	12/17/2014	Time:	09:28:25	NScans:	5		
Type:	HYPER IR	User:	ZUBAIR AHMED			Detector:	standard
Abscissa:	1/cm	Ordinate:	%T	Apodization:	Happ		
Min:	401.17	Max:	3998.16	Range:	1/cm		
Ndp:	1866	Data Interval:	1.92868	Resolution:	4.0		
Gain:	auto	Aperture:	auto	Mirror Speed:	2.8(low)		

Compound 7
1H



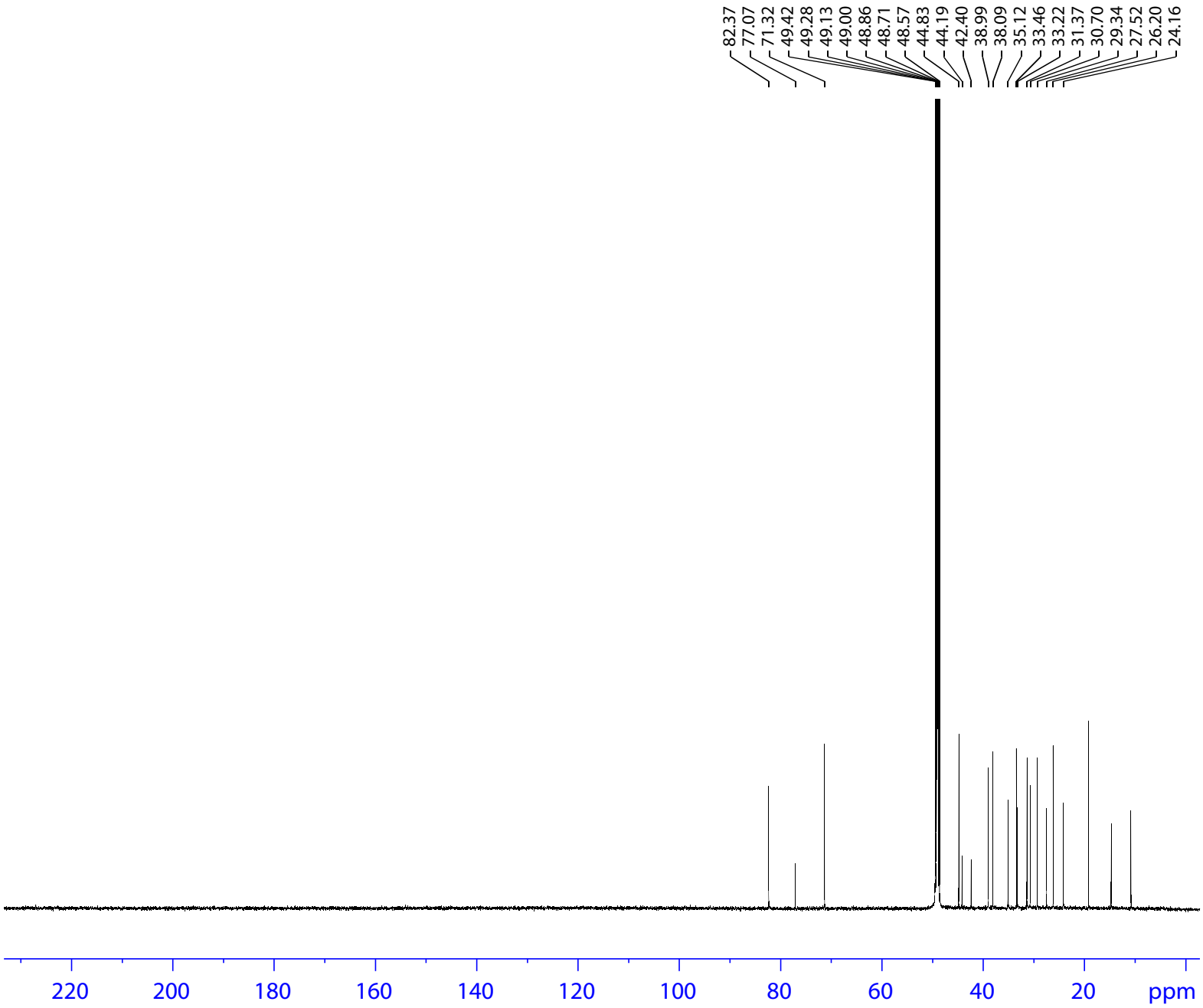
Current Data Parameters
NAME apr25-14
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140425
Time 19.18
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32768
SOLVENT MeOD
NS 1
DS 0
SWH 9615.385 Hz
FIDRES 0.293438 Hz
AQ 1.7039360 sec
RG 8
DW 52.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 8.00 usec
PL1 3.31 dB
PL1W 6.79873323 W
SFO1 600.0345002 MHz

F2 - Processing parameters
SI 32768
SF 600.0300172 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40

Compound 7
BB



Current Data Parameters
NAME apr25-14
EXPNO 6
PROCNO 1

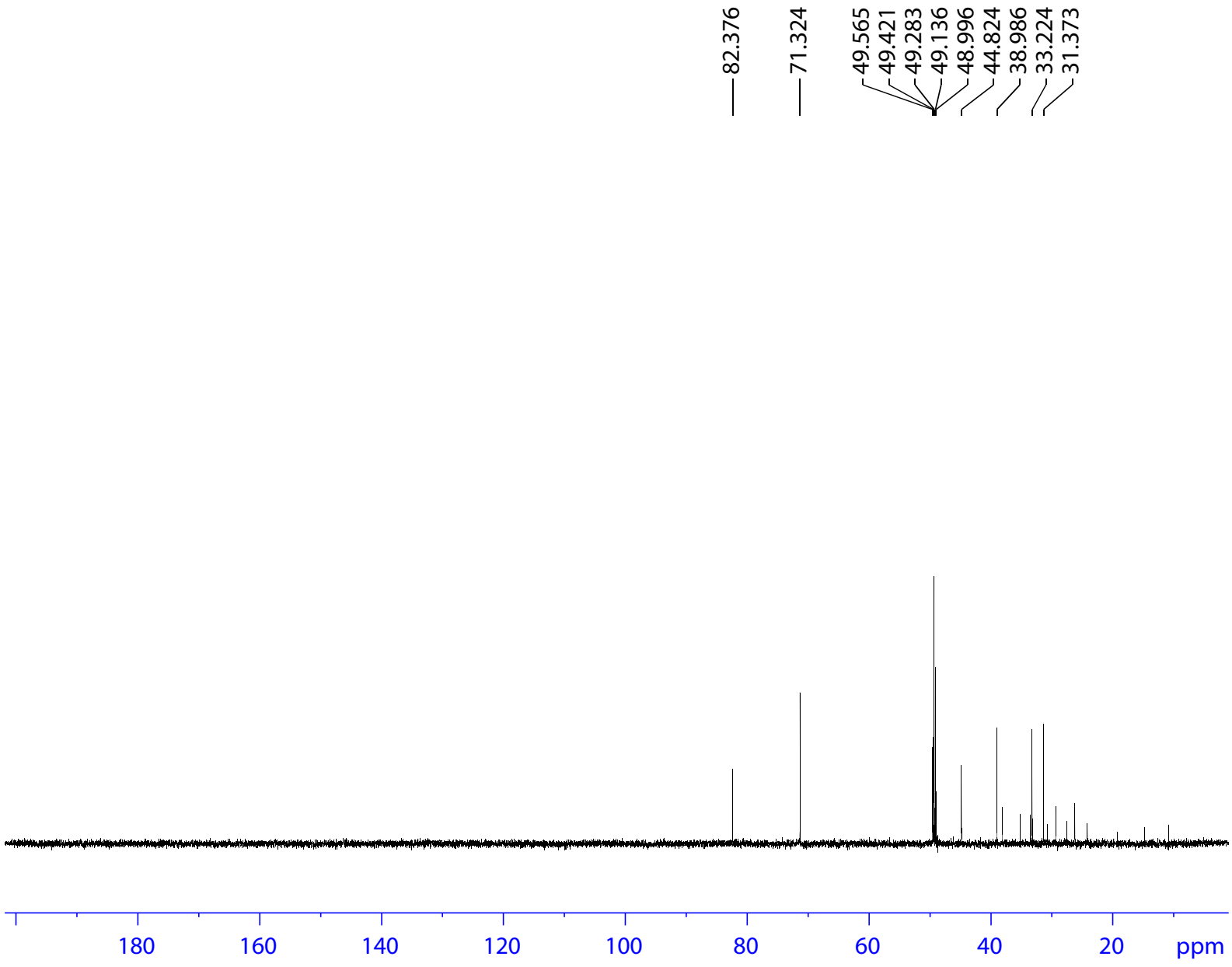
F2 - Acquisition Parameters
Date_ 20140426
Time 14.17
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg
TD 32768
SOLVENT MeOD
NS 3791
DS 4
SWH 35971.223 Hz
FIDRES 1.097755 Hz
AQ 0.4554752 sec
RG 32768
DW 13.900 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 12

======== CHANNEL f1 ========
NUC1 13C
P1 12.70 usec
PL1 -1.81 dB
PL1W 81.92915344 W
SFO1 150.8950149 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.31 dB
PL12 23.31 dB
PL13 22.50 dB
PL2W 6.79873323 W
PL12W 0.06798734 W
PL13W 0.08192718 W
SFO2 600.0336002 MHz

F2 - Processing parameters
SI 16384
SF 150.8774509 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Compound 7
dept 90



Current Data Parameters
NAME apr25-14
EXPNO 8
PROCNO 1

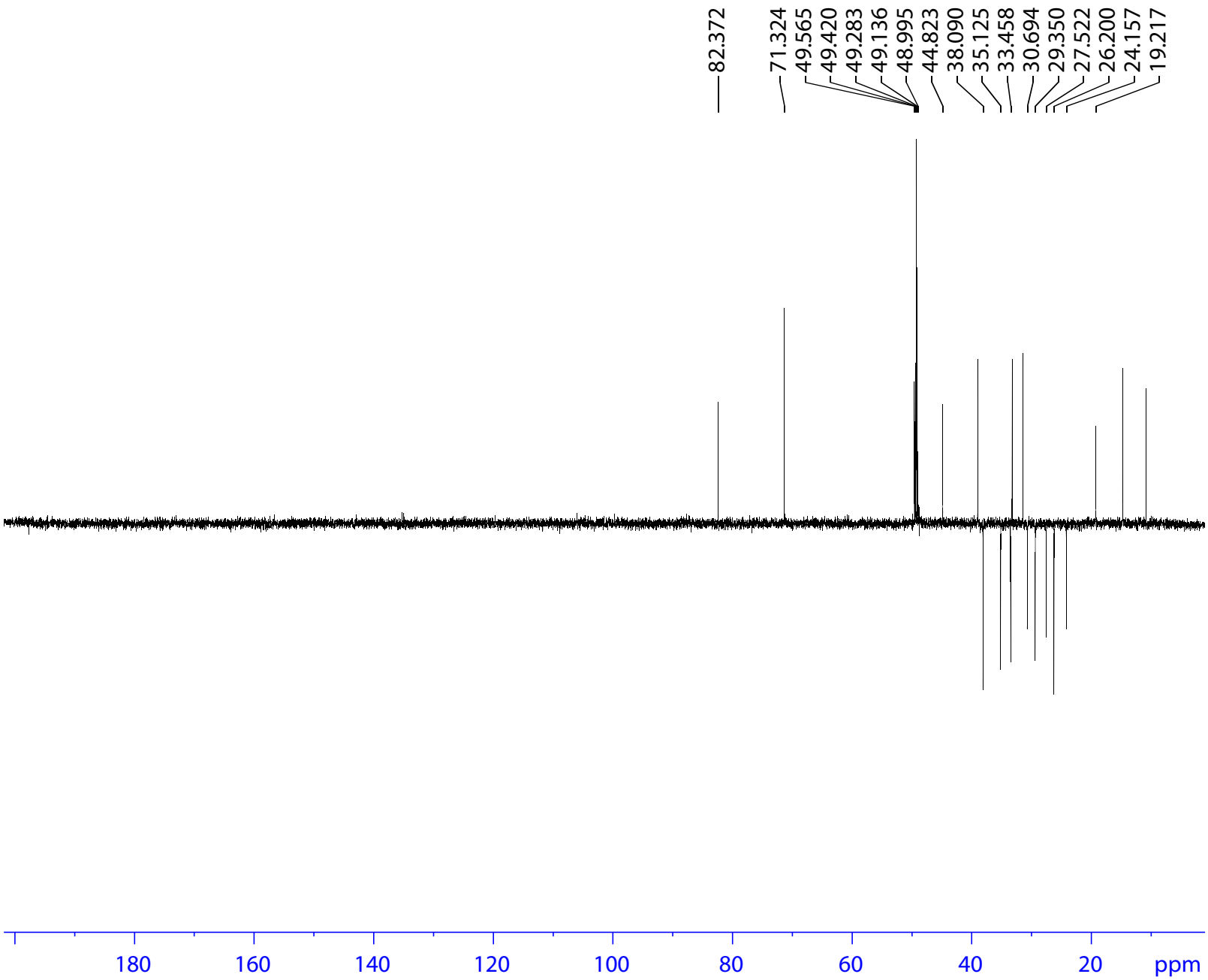
F2 - Acquisition Parameters
Date_ 20140426
Time 16.49
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG deptsp90
TD 32768
SOLVENT MeOD
NS 393
DS 2
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5406720 sec
RG 32768
DW 16.500 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 4

======== CHANNEL f1 ========
NUC1 13C
P1 12.70 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.81 dB
PL0W 0 W
PL1W 81.92915344 W
SFO1 150.8927518 MHz
SP2 4.19 dB
SPNAM[2] Crp60comp.4
SPOAL2 0.500
SPOFFS2 0 Hz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 8.00 usec
P4 16.00 usec
PCPD2 80.00 usec
PL2 3.31 dB
PL12 23.31 dB
PL2W 6.79873323 W
PL12W 0.06798734 W
SFO2 600.0330002 MHz

F2 - Processing parameters
SI 16384
SF 150.8774509 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 7
dept135



Current Data Parameters
NAME apr25-14
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140426
Time 16.35
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG deptsp135
TD 32768
SOLVENT MeOD
NS 651
DS 2
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5406720 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

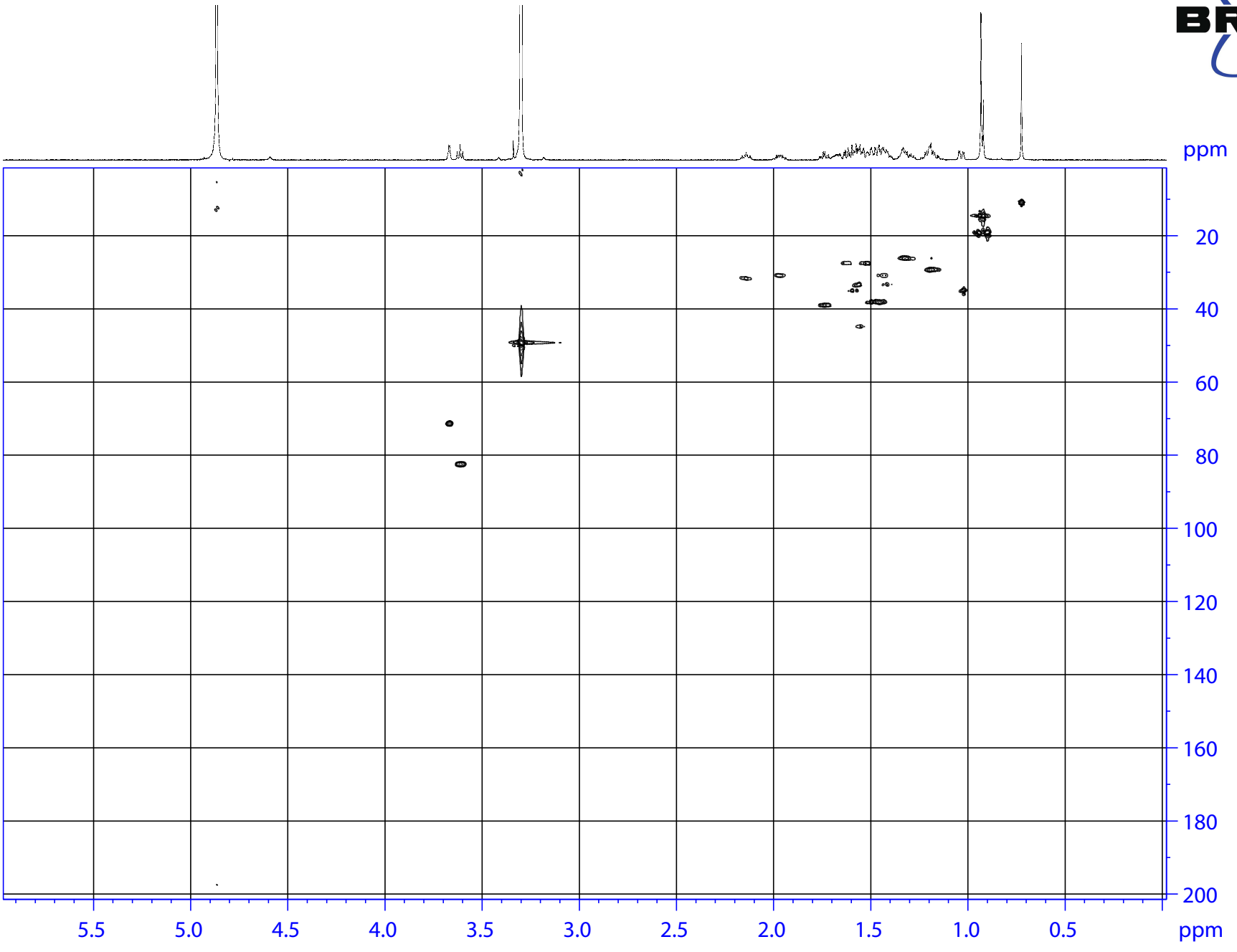
======== CHANNEL f1 ========
NUC1 13C
P1 12.70 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.81 dB
PL0W 0 W
PL1W 81.92915344 W
SFO1 150.8927518 MHz
SP2 4.19 dB
SPNAM[2] Crp60comp.4
SPOAL2 0.500
SPOFFS2 0 Hz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 8.00 usec
P4 16.00 usec
PCPD2 80.00 usec
PL2 3.31 dB
PL12 23.31 dB
PL2W 6.79873323 W
PL12W 0.06798734 W
SFO2 600.0330002 MHz

F2 - Processing parameters
SI 16384
SF 150.8774509 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 7

HSQC



Current Data Parameters
NAME apr25-14
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140426
Time 0.16
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG hsqcetgpsi
TD 1024
SOLVENT MeOD
NS 32
DS 8
SWH 3591.954 Hz
FIDRES 3.507768 Hz
AQ 0.1425408 sec
RG 23170.5
DW 139.200 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 2.00000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
D24 0.00110000 sec
IN0 0.00001655 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 8.00 usec
P2 16.00 usec
P28 1000.00 usec
PL1 3.31 dB
PL1W 6.79873323 W
SFO1 600.0318001 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp
NUC2 13C
P3 11.50 usec
P4 23.00 usec
PCPD2 55.00 usec
PL2 -1.81 dB
PL12 11.70 dB
PL2W 81.92915344 W
PL12W 3.65122390 W
SFO2 150.8927518 MHz

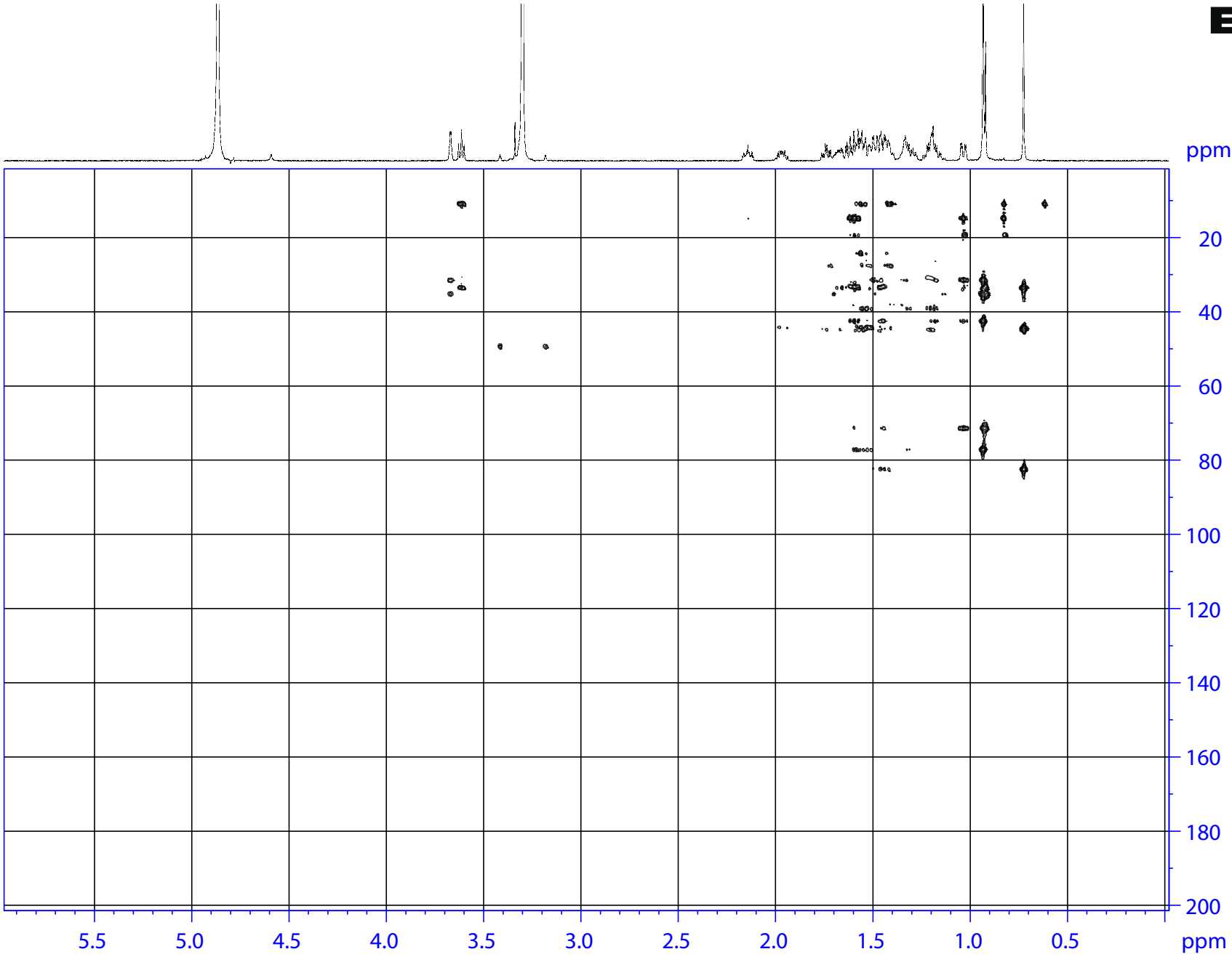
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8928 MHz
FIDRES 235.769928 Hz
SW 200.000 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.0300172 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.8774509 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Compound 7
HMBC



Current Data Parameters
NAME apr25-14
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140426
Time 5.13
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG hmbcgplpndqf
TD 2048
SOLVENT MeOD
NS 64
DS 16
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 41285.1
DW 139.200 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 8.00 usec
P2 16.00 usec
PL1 3.31 dB
PL1W 6.79873323 W
SFO1 600.0318001 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 11.50 usec
PL2 -1.81 dB
PL2W 81.92915344 W
SFO2 150.8950149 MHz

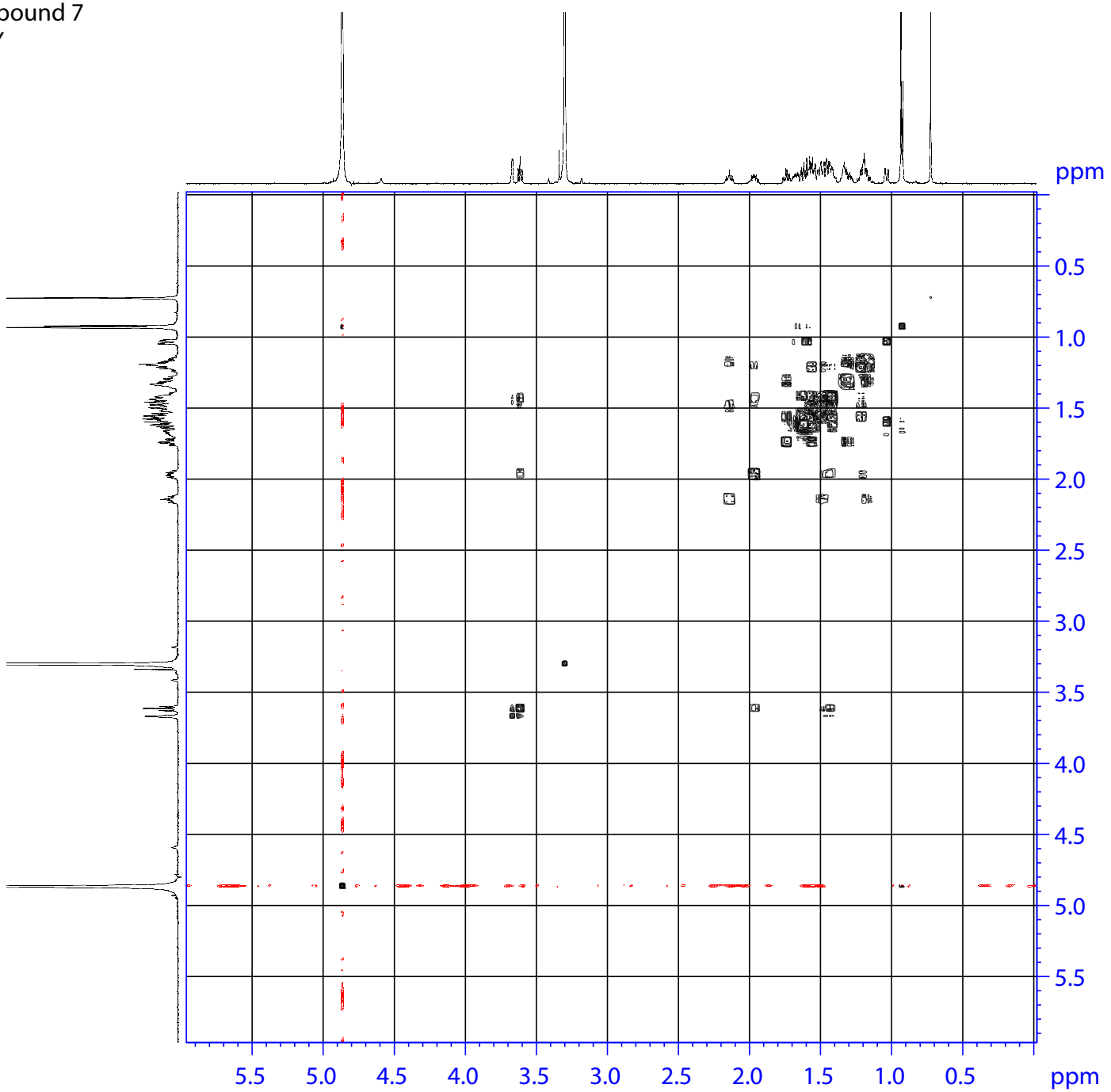
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPNAM[3] SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 2000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.895 MHz
FIDRES 271.139465 Hz
SW 230.000 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.0300172 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8774509 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

Compound 7
COSY



Current Data Parameters
NAME apr25-14
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140425
Time 19.23
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG cosydfqf
TD 2048
SOLVENT MeOD
NS 16
DS 4
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 28.5
DW 139.200 usec
DE 6.50 usec
TE 298.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D20 0.00000200 sec
IN0 0.00027840 sec

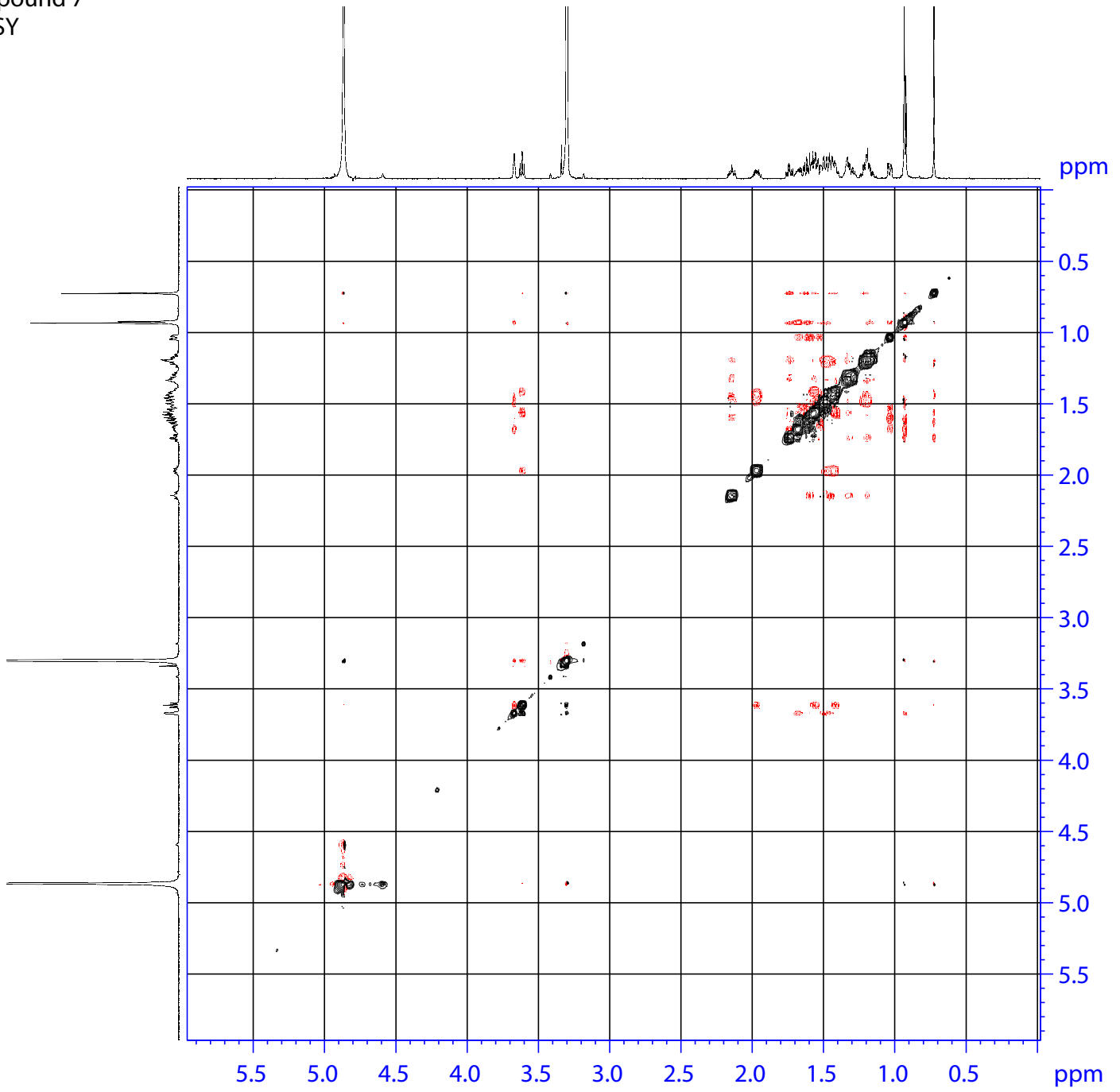
======== CHANNEL f1 ========
NUC1 1H
P1 8.00 usec
PL1 3.31 dB
PL1W 6.79873323 W
SFO1 600.0318001 MHz

F1 - Acquisition parameters
TD 128
SFO1 600.0318 MHz
FIDRES 56.124283 Hz
SW 5.986 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.0300172 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.0300172 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Compound 7
NOESY



Current Data Parameters
NAME apr25-14
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140425
Time 20.43
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG noesygpph
TD 2048
SOLVENT MeOD
NS 16
DS 4
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 25.4
DW 139.200 usec
DE 6.50 usec
TE 298.0 K
D0 0.00012901 sec
D1 2.00000000 sec
D8 0.80000001 sec
D16 0.00020000 sec
IN0 0.00027840 sec

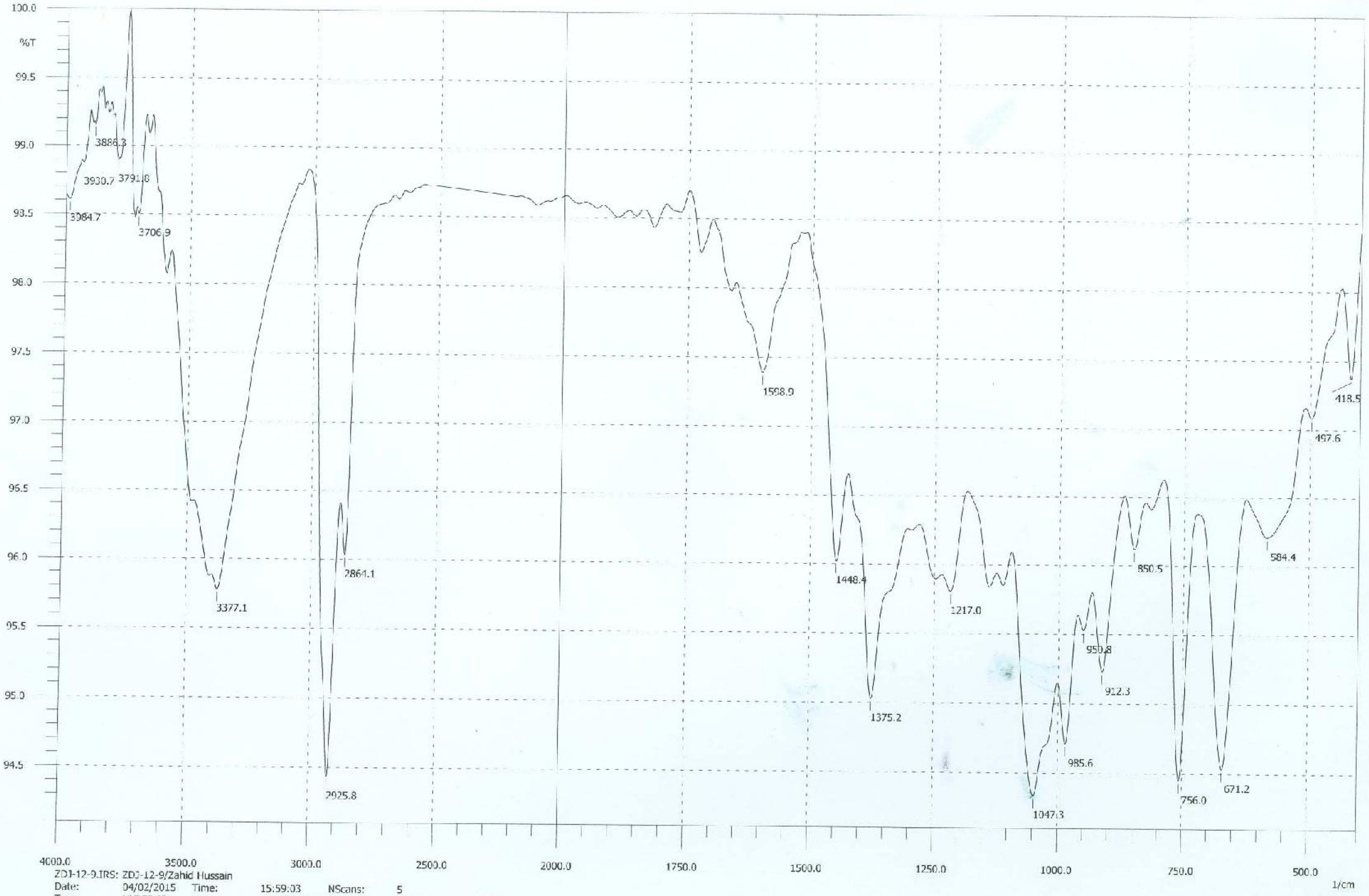
======== CHANNEL f1 ========
NUC1 1H
P1 8.00 usec
P2 16.00 usec
PL1 3.31 dB
PL1W 6.79873323 W
SFO1 600.0318001 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.0318 MHz
FIDRES 28.062141 Hz
SW 5.986 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.0300172 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 512
MC2 States-TPPI
SF 600.0300172 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

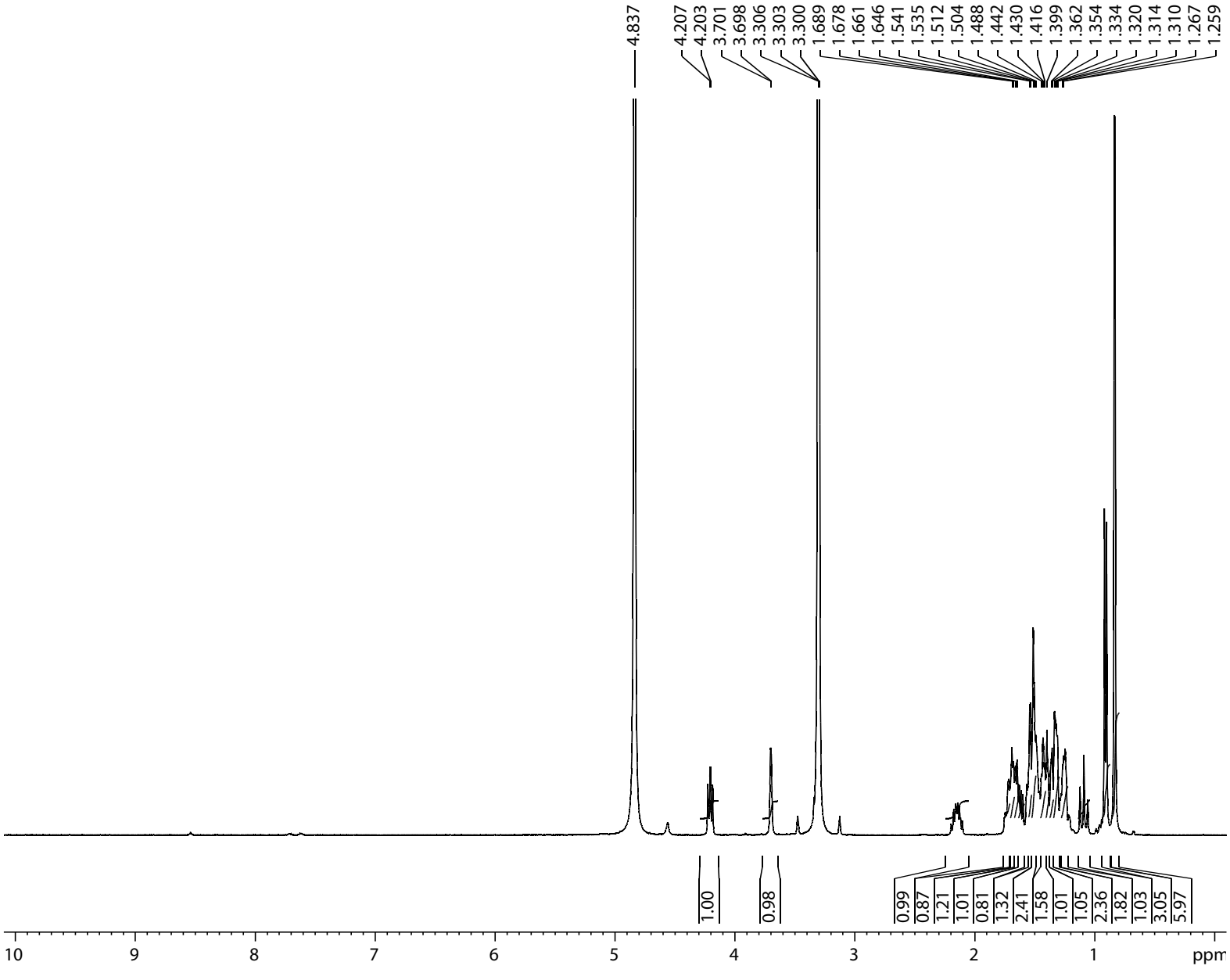


ZD1-12-9.IRS: ZD1-12-9/Zahid Hussain

Date:	04/02/2015	Time:	15:59:03	NScans:	5		
Type:	HYPER IR	User:	ZUBAIR AHMED			Detector:	standard
Abscissa:	1/cm	Ordinate:	%T	Apodization:	Happ		
Min:	401.17	Max:	3998.16	Range:	1/cm		
Ndp:	1866	Data Interval:	1.92868	Resolution:	4.0		
Gain:	auto	Aperture:	auto	Mirror Speed:	2.8(low)		

Compound 8
1H

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME may14-14
EXPNO 1
PROCNO 1

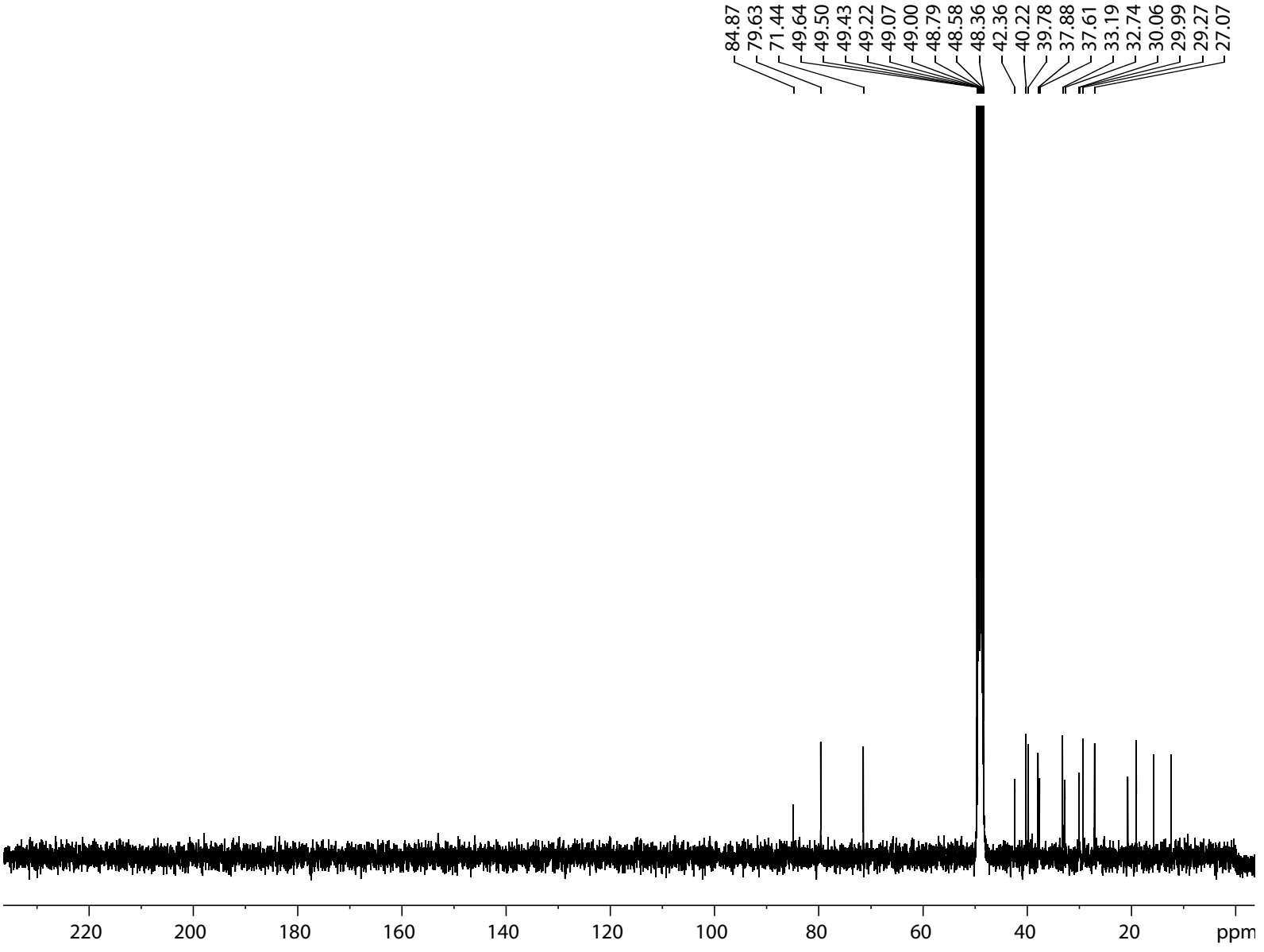
F2 - Acquisition Parameters
Date_ 20140515
Time 15.38
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT MeOD
NS 128
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 362
DW 62.400 usec
DE 6.50 usec
TE 299.4 K
D1 1.50000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 400.0332002 MHz

F2 - Processing parameters
SI 16384
SF 400.0300075 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Compound 8
BB

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME may14-14
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140517
Time 2.04
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg
TD 32768
SOLVENT MeOD
NS 24576
DS 2
SWH 24154.590 Hz
FIDRES 0.737140 Hz
AQ 0.6782976 sec
RG 32768
DW 20.700 usec
DE 6.50 usec
TE 303.1 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 24

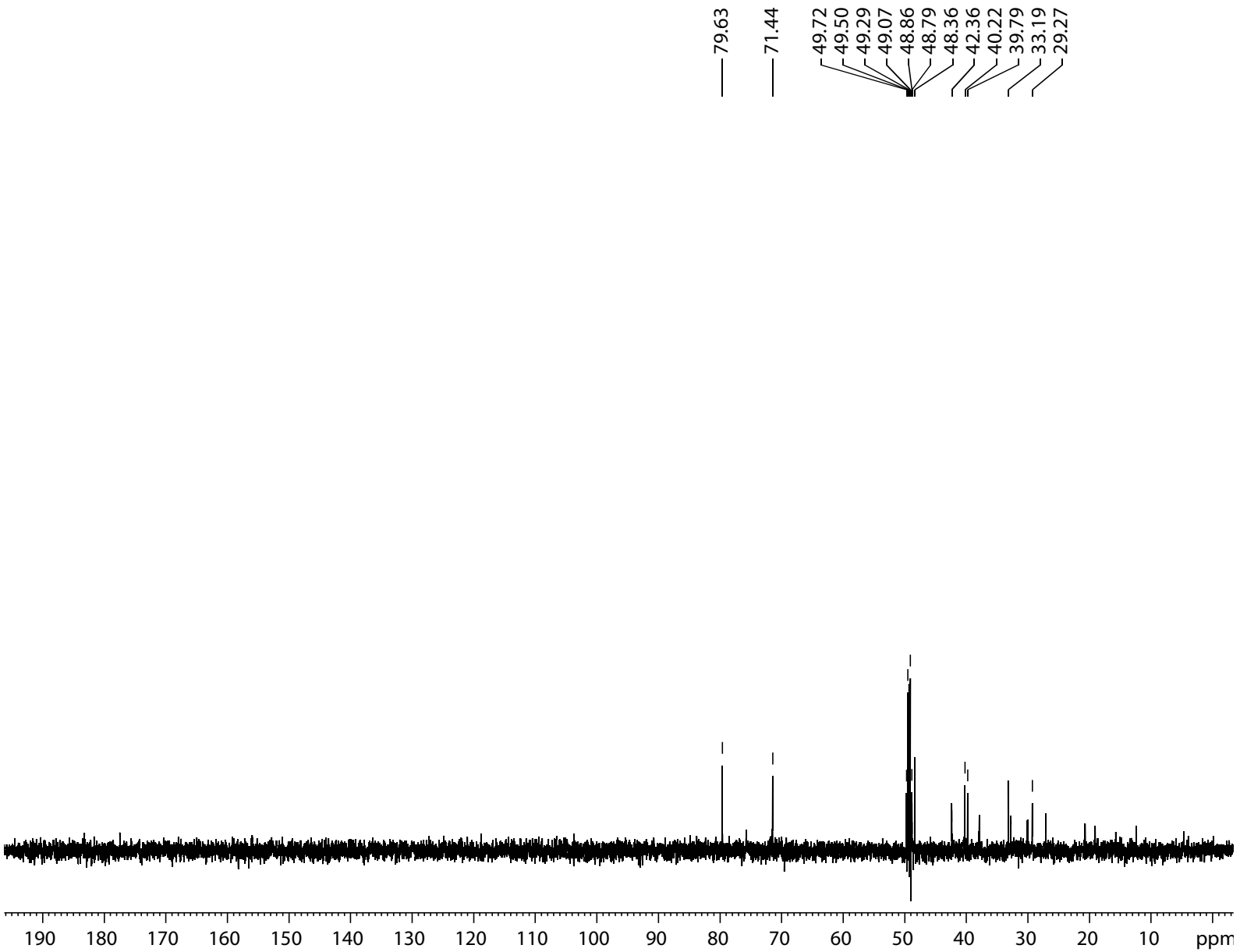
======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
PL1 -6.00 dB
SFO1 100.5991916 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
PL13 22.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874803 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Compound 8
DEPT90#

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME may14-14
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140518
Time 2.49
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG dept90
TD 32768
SOLVENT MeOD
NS 6144
DS 2
SWH 20080.320 Hz
FIDRES 0.612803 Hz
AQ 0.8159232 sec
RG 16384
DW 24.900 usec
DE 6.50 usec
TE 303.8 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 6

======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
P2 24.60 usec
PL1 -6.00 dB
SFO1 100.5971798 MHz

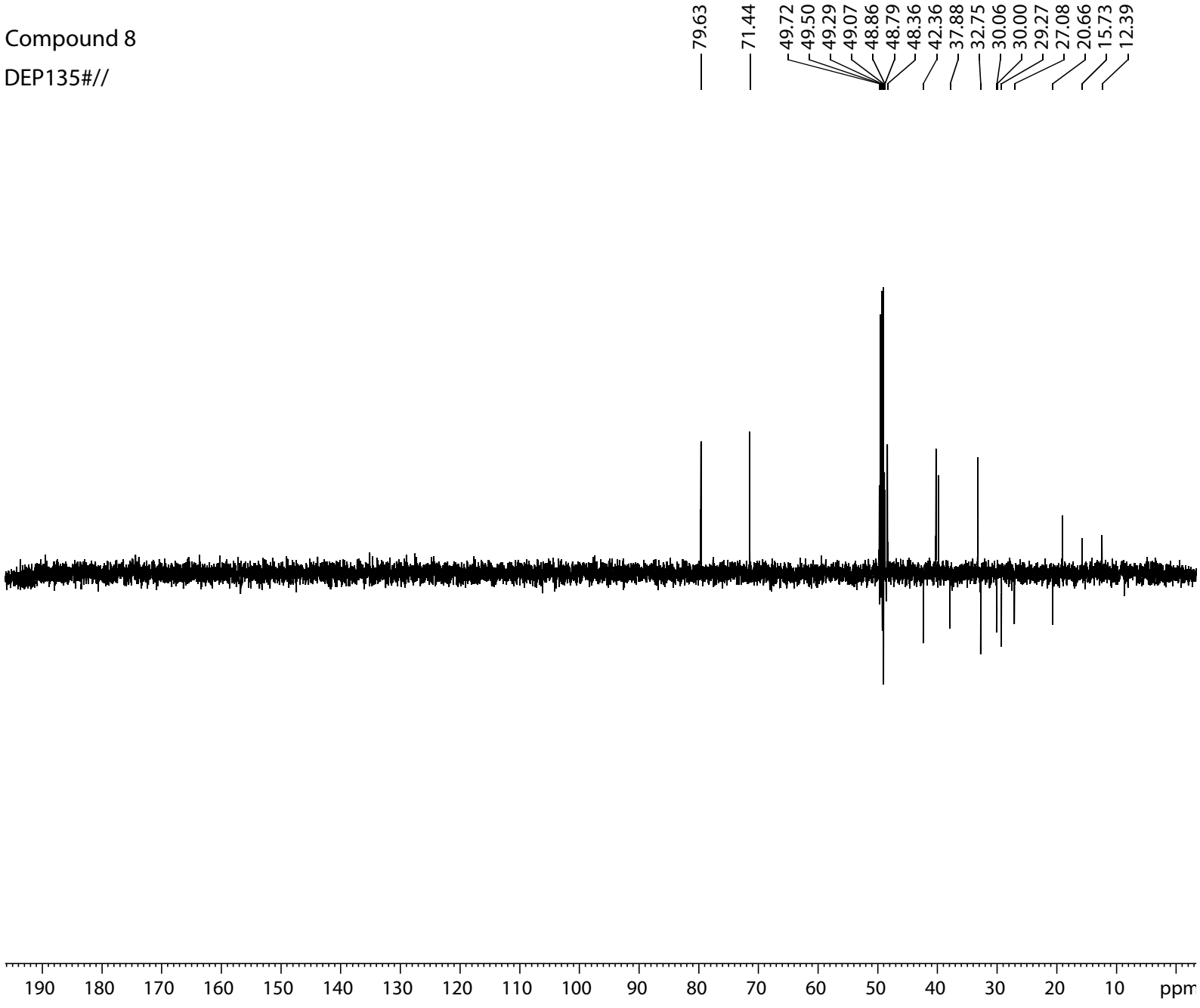
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 10.50 usec
P4 21.00 usec
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874803 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20

Compound 8

DEP135#//

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME may14-14
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140517
Time 17.25
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG dept135
TD 32768
SOLVENT MeOD
NS 14336
DS 2
SWH 20080.320 Hz
FIDRES 0.612803 Hz
AQ 0.8159232 sec
RG 16384
DW 24.900 usec
DE 6.50 usec
TE 303.9 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 14

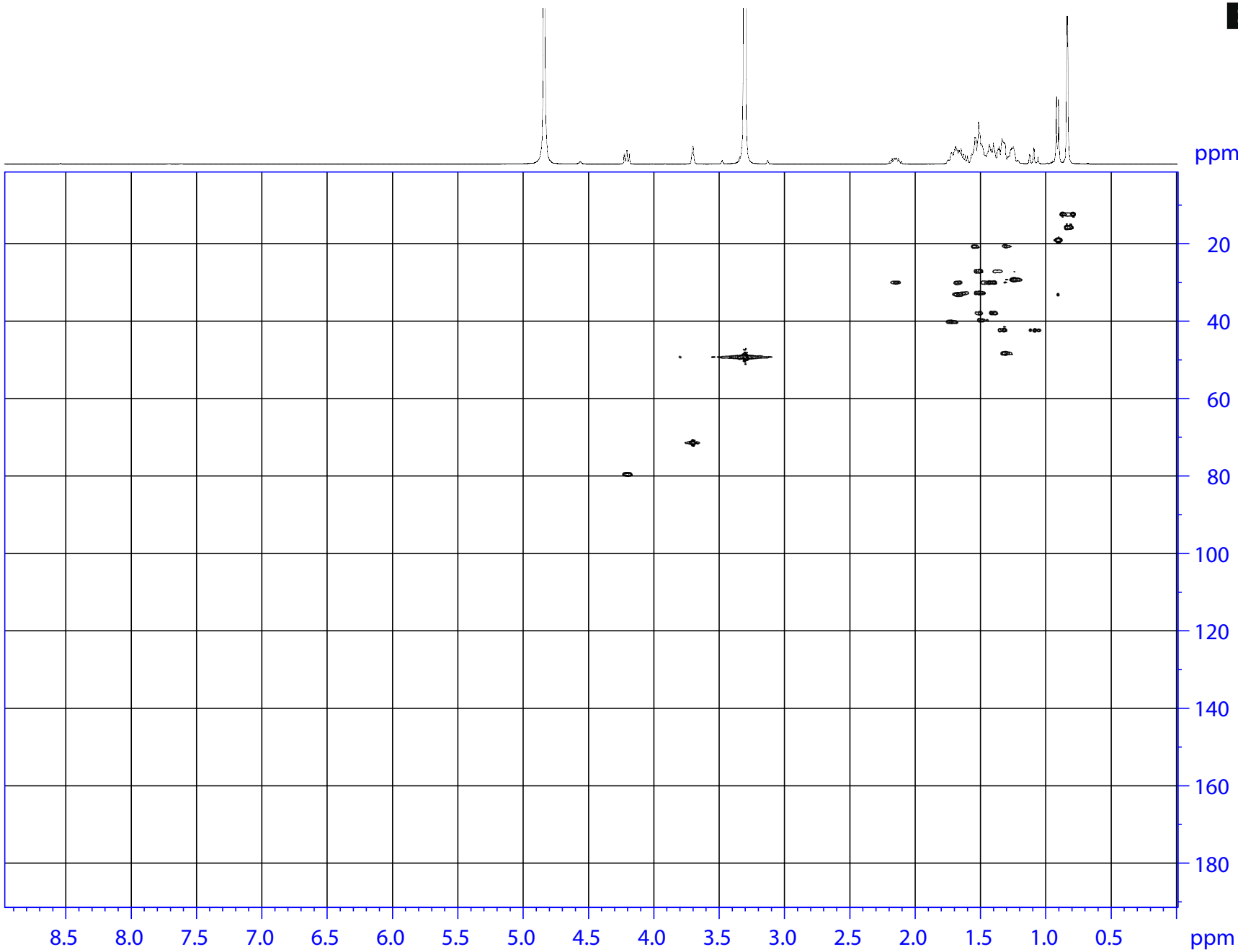
======== CHANNEL f1 ========
NUC1 13C
P1 12.30 usec
P2 24.60 usec
PL1 -6.00 dB
SFO1 100.5971798 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 10.50 usec
P4 21.00 usec
PCPD2 75.00 usec
PL2 3.00 dB
PL12 20.00 dB
SFO2 400.0320001 MHz

F2 - Processing parameters
SI 16384
SF 100.5874803 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20

Compound 8

HSQC//



Current Data Parameters
NAME may14-14
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140516
Time 7.11
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG hsqcetgpsi
TD 1024
SOLVENT MeOD
NS 64
DS 2
SWH 3591.954 Hz
FIDRES 3.507768 Hz
AQ 0.1425408 sec
RG 16384
DW 139.200 usec
DE 6.50 usec
TE 302.8 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 0.00002615 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
P28 2000.00 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp
NUC2 13C
P3 11.40 usec
P4 22.80 usec
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 17.00 dB
SFO2 100.5971798 MHz

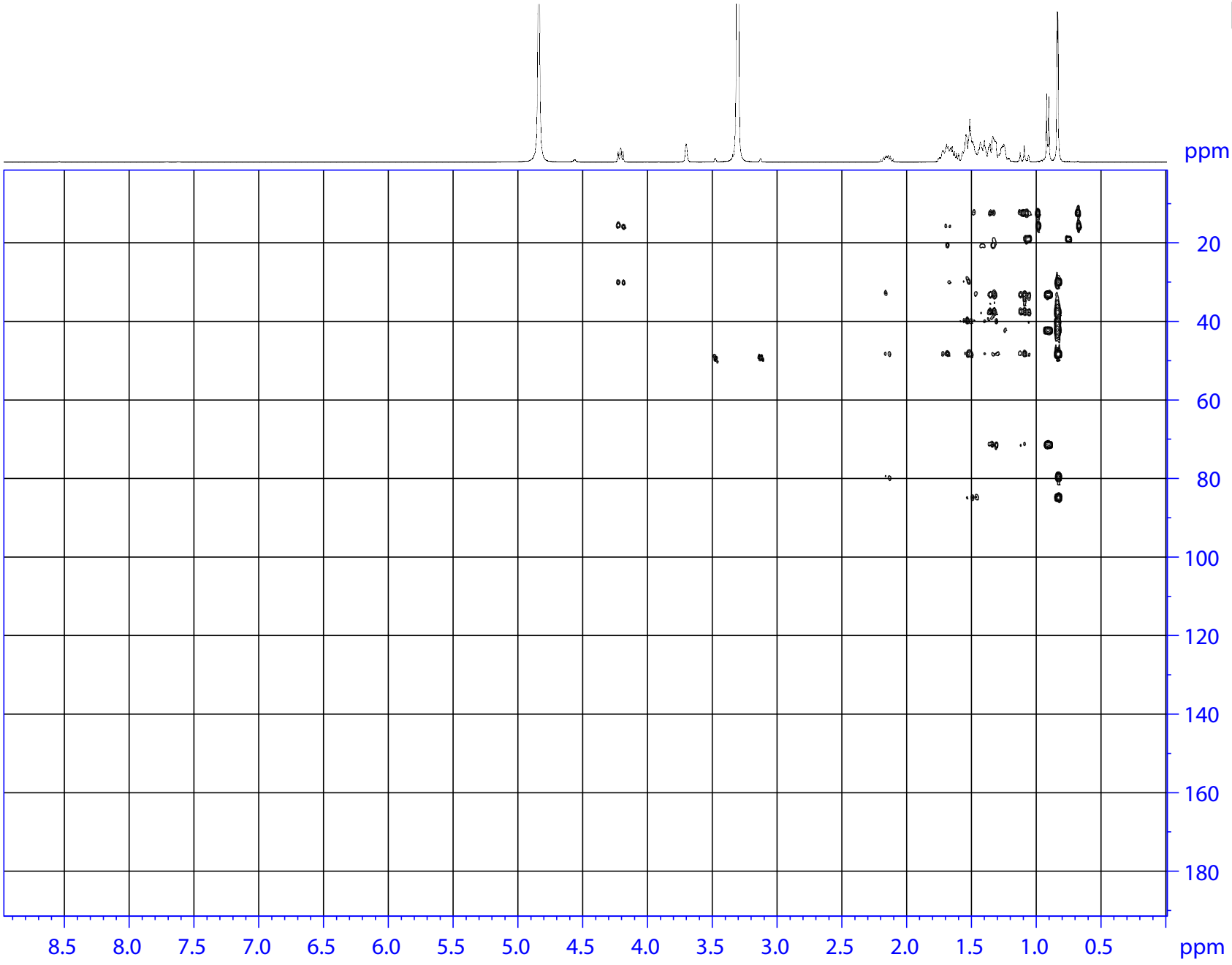
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.5972 MHz
FIDRES 149.323944 Hz
SW 190.000 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.5874803 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

Compound 8
HMBC/



Current Data Parameters
NAME may14-14
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140516
Time 14.46
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG hmbcgplpndqf
TD 2048
SOLVENT MeOD
NS 64
DS 2
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 14596.5
DW 139.200 usec
DE 6.50 usec
TE 300.9 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 0.00002160 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 11.40 usec
PL2 -6.00 dB
SFO2 100.5991916 MHz

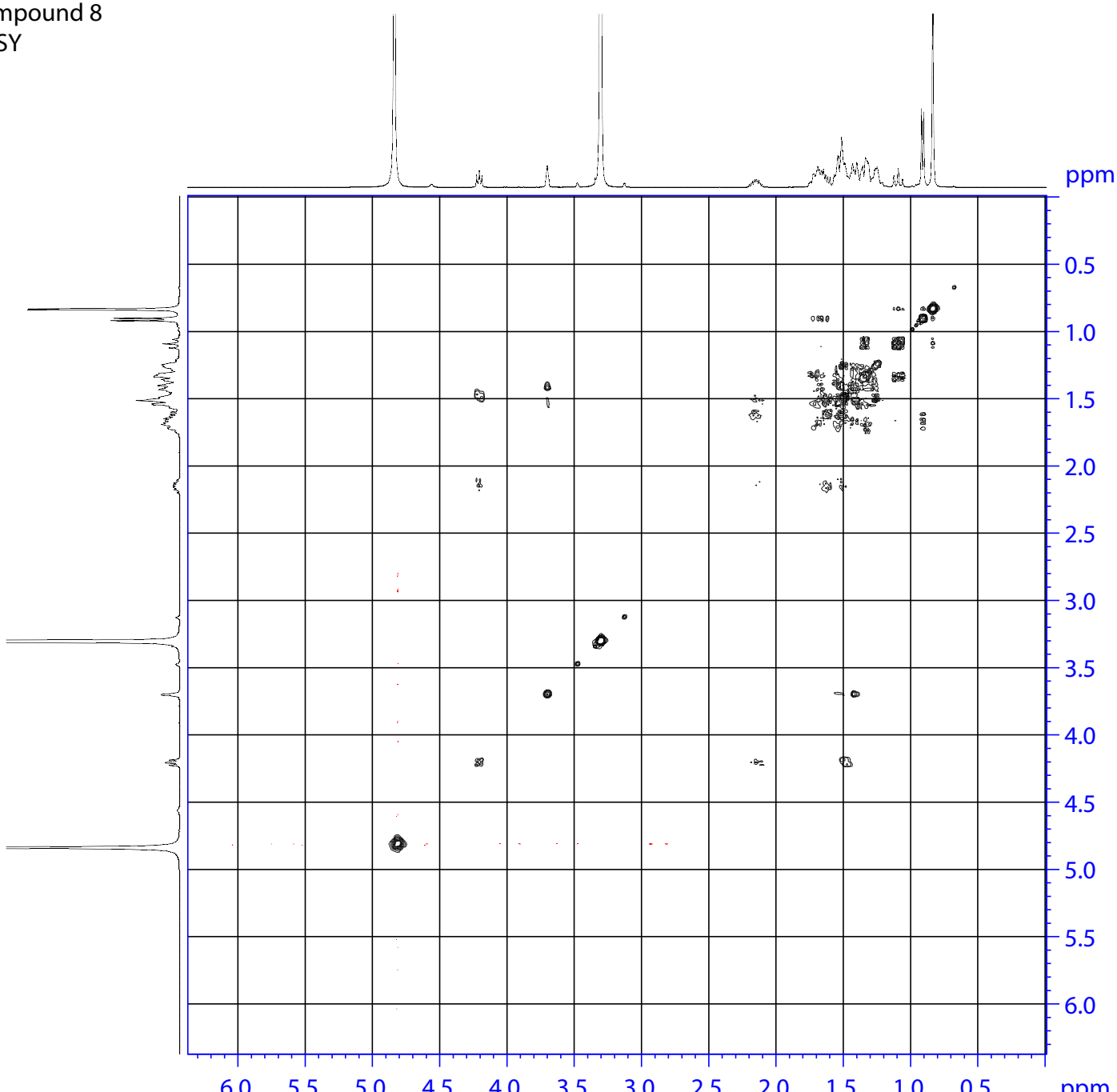
====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPNAM[3] SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.5992 MHz
FIDRES 180.764175 Hz
SW 230.000 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.5874803 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Compound 8
COSY



AVANCE NEO 400 MHz
LAb # 115

Current Data Parameters
NAME may14-14
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140515
Time 19.56
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG cosygpqf
TD 2048
SOLVENT MeOD
NS 32
DS 8
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 456.1
DW 139.200 usec
DE 6.50 usec
TE 298.4 K
D0 0.00000300 sec
D1 1.50000000 sec
D13 0.00000400 sec
D16 0.00010000 sec
IN0 0.00027840 sec

======== CHANNEL f1 ========
NUC1 1H
P0 10.80 usec
P1 10.80 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 400.0318 MHz
FIDRES 28.062141 Hz
SW 8.979 ppm
FnMODE QF

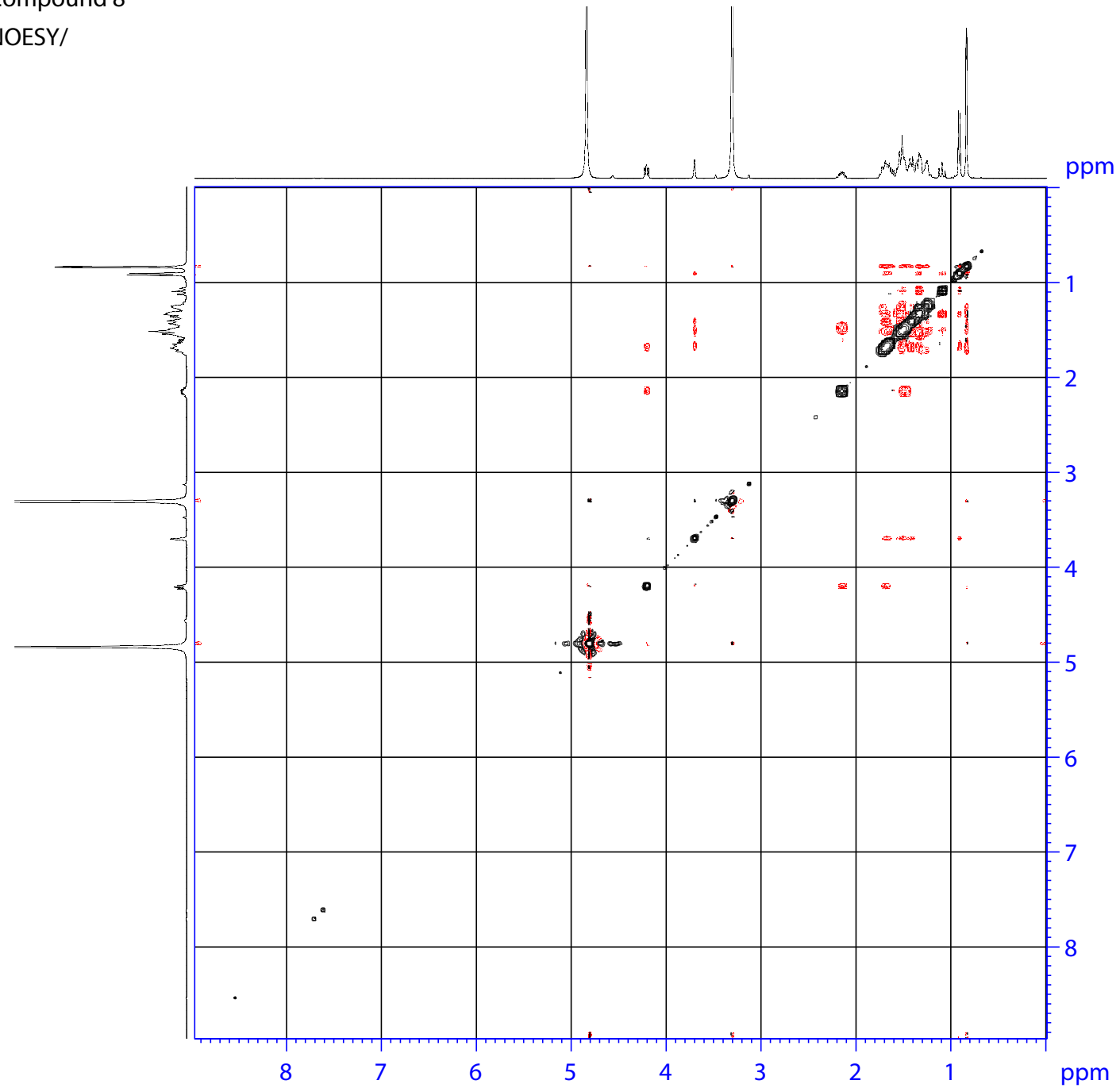
F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.0300087 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Compound 8

NOESY/

AVANCE NEO 400 MHz
LAb # 115



Current Data Parameters
NAME may14-14
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140516
Time 0.06
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG noesygpph
TD 2048
SOLVENT MeOD
NS 32
DS 8
SWH 3591.954 Hz
FIDRES 1.753884 Hz
AQ 0.2850816 sec
RG 645.1
DW 139.200 usec
DE 6.50 usec
TE 302.3 K
D0 0.00012545 sec
D1 2.00000000 sec
D8 0.80000001 sec
D16 0.00010000 sec
IN0 0.00027840 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
P2 21.60 usec
PL1 3.00 dB
SFO1 400.0318001 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 400.0318 MHz
FIDRES 28.062141 Hz
SW 8.979 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 400.0300087 MHz
WDW SINE
SSB 2
LB 0 Hz
GB 0

Elemental composition calculator

Target m/z: +323.2617

Tolerance: +10.0000 ppm

Result type: Elemental

Max num of results: 10

Min DBE: -0.5000 Max DBE: +50.0000

Electron state: OddAndEven

Num of charges: 0

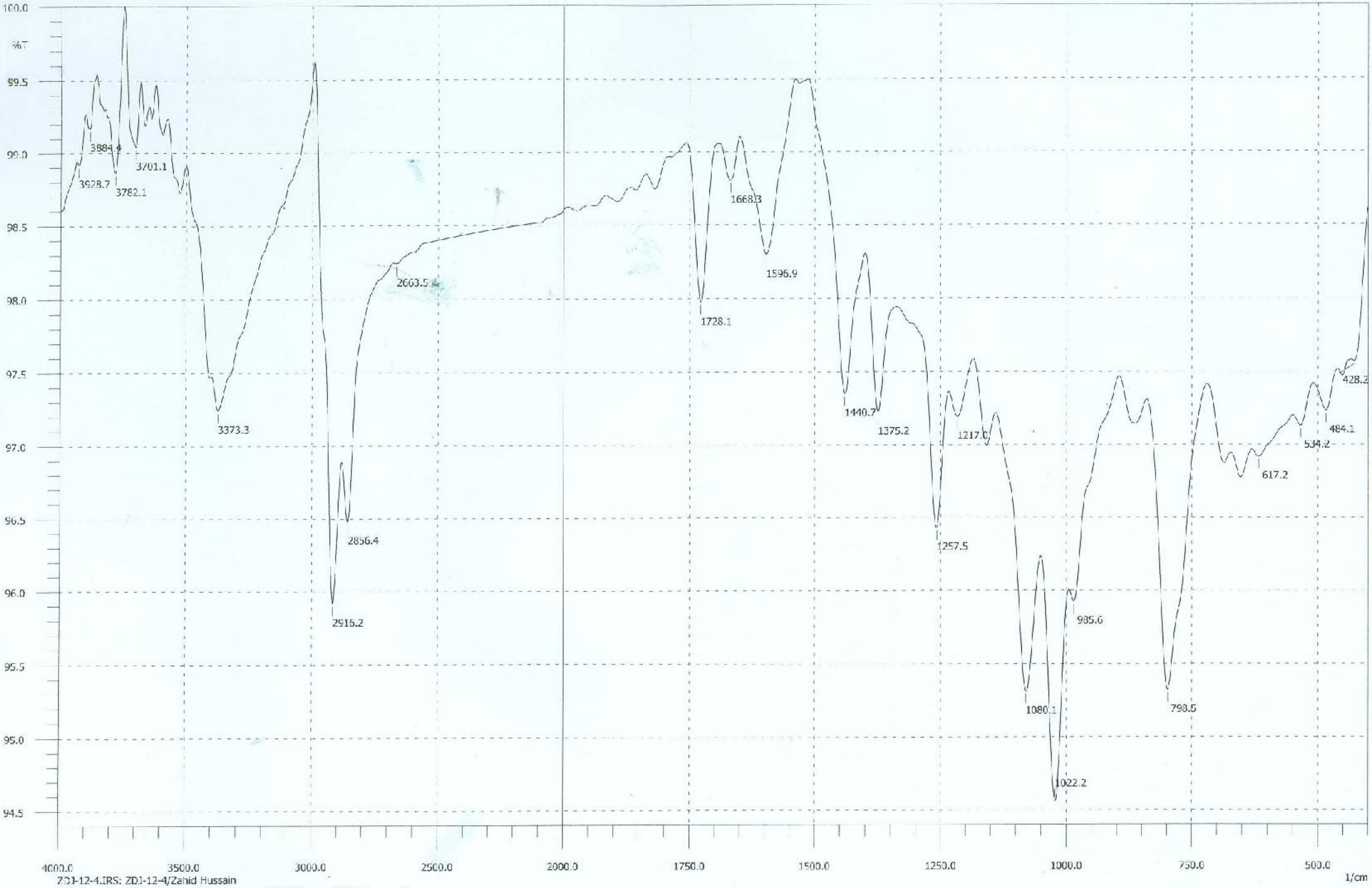
Add water: N/A

Add proton: N/A

File Name: ZDJ-12-4.wiff

	Elements	Min Number	Max Number
1	C	0	23
2	H	0	40
3	O	0	5

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C20 H35 O3	323.2586	3.0796	9.5268	3.5



ZD1-12-4.IRS: ZD1-12-4/Zahid Hussain

Date:	04/02/2015	Time:	15:51:48	NScans:	5	
Type:	HYPER IR	User:	ZUBAIR AHMED		Detector:	standard
Abscissa:	1/cm	Ordinate:	%T	Apodization:	Happ	
Min:	401.17	Max:	3998.16	Range:	1/cm	
Ndp:	1866	Data Interval:	1.92868	Resolution:	4.0	
Gain:	auto	Aperture:	auto	Mirror Speed:	2.8(low)	