

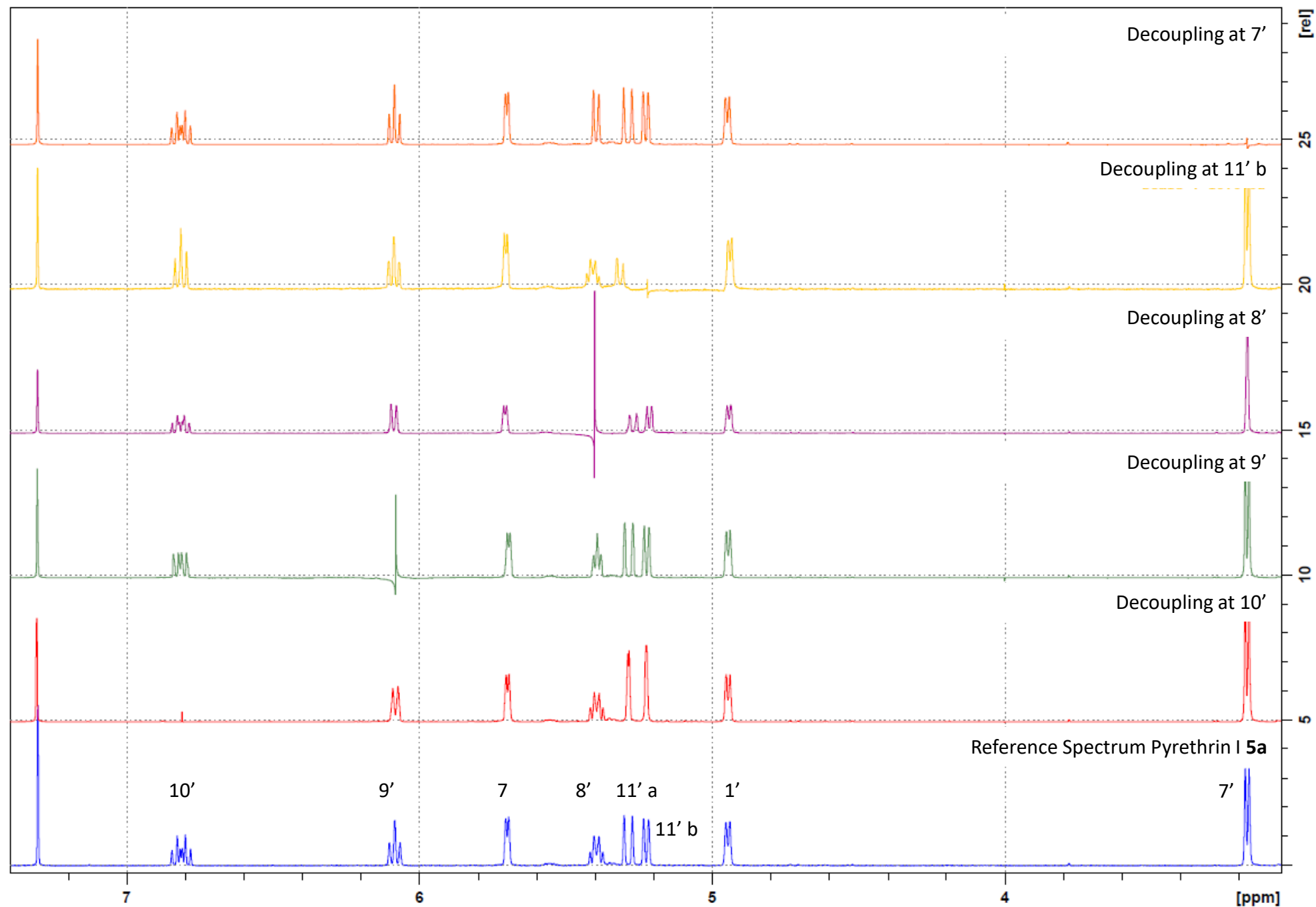
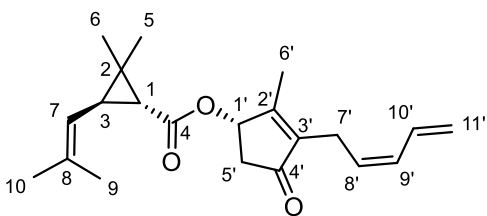
Supporting Information

Synthetic Modification of the Natural Pyrethrins

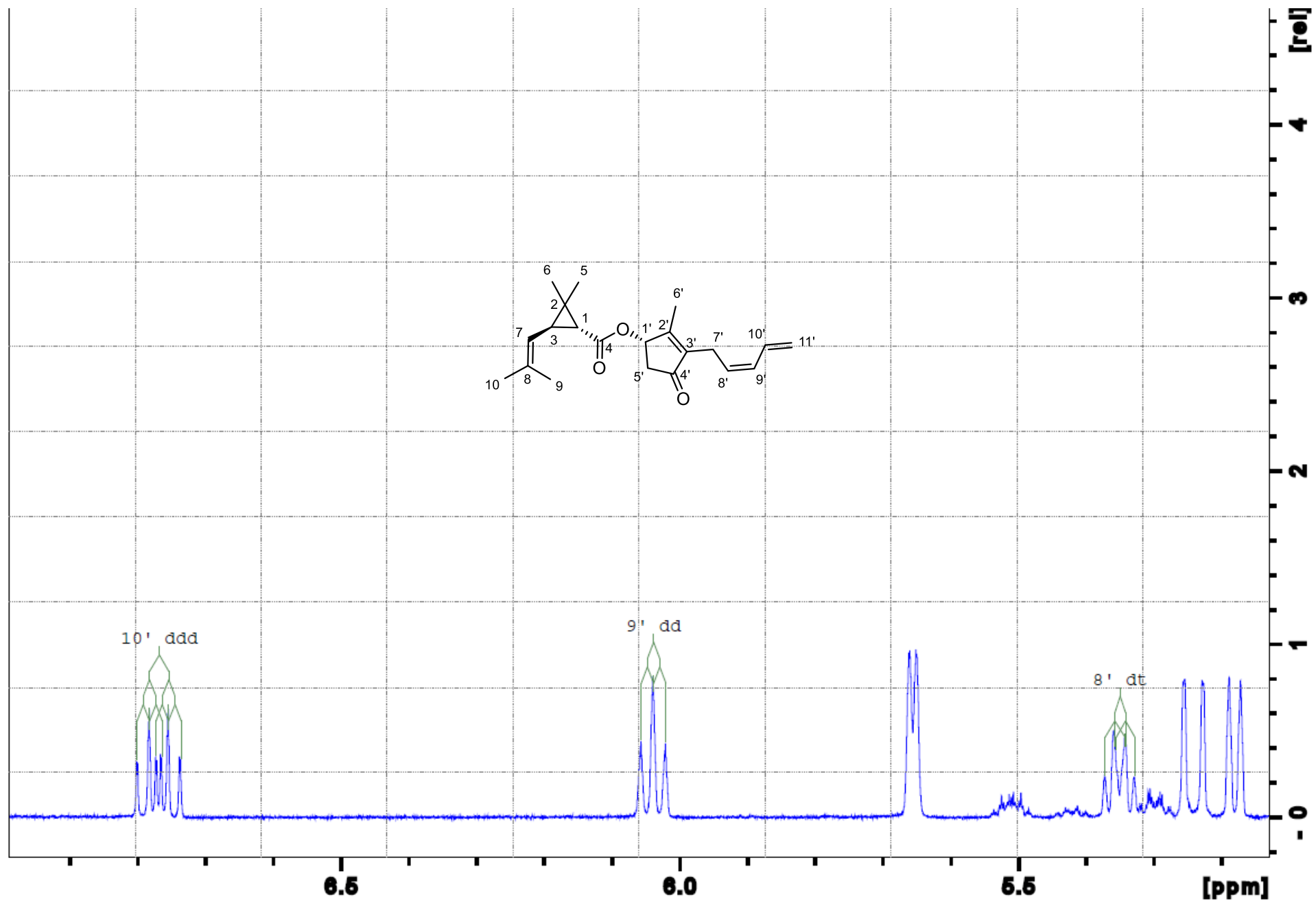
Todd E. Markham

General Supporting Information

Representative Homonuclear Decoupling Experiments



Representative Multiplet Analysis



Reduction Chemistry Characterisation Data

4'R-51a NMR Characterisation

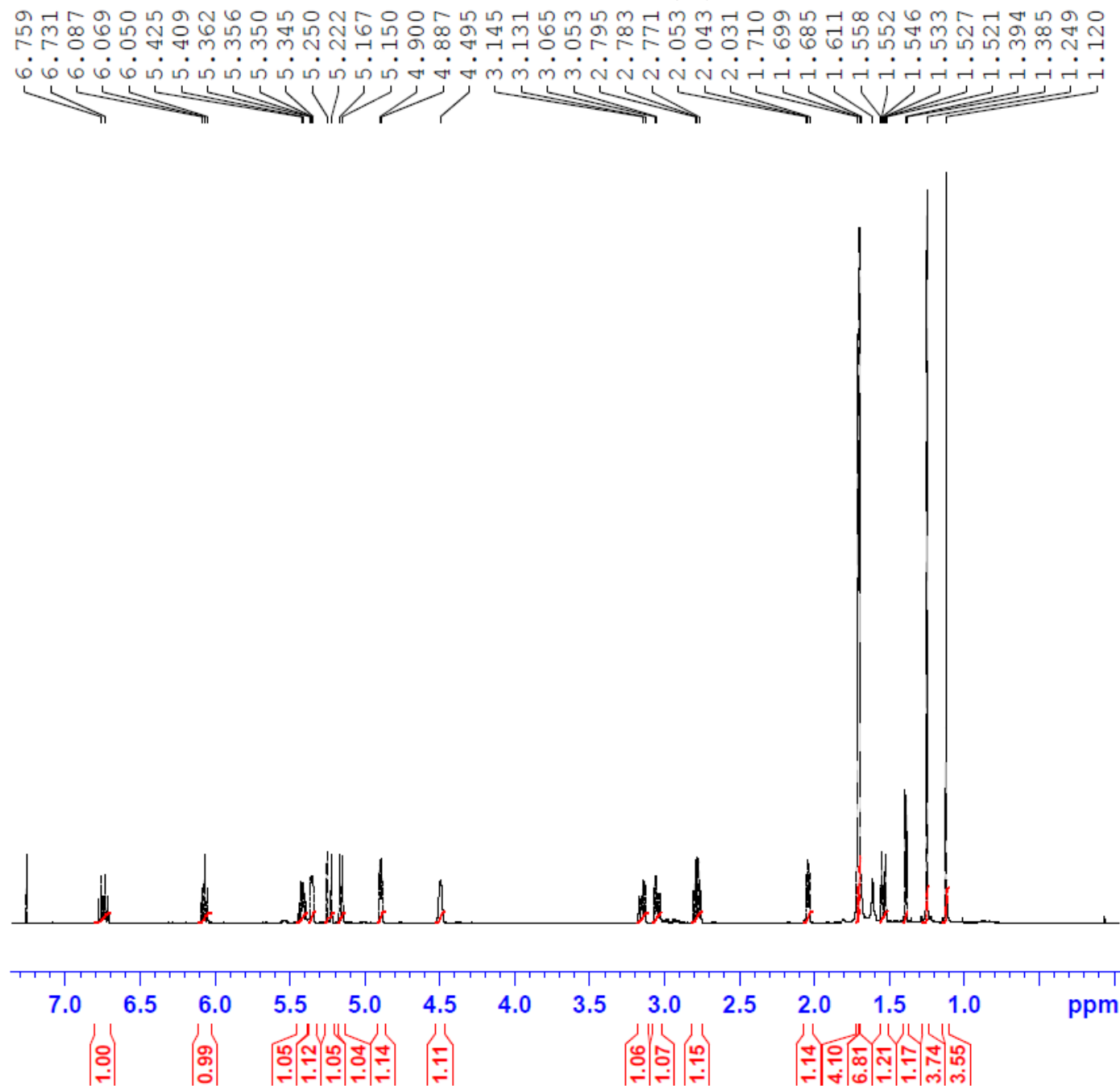


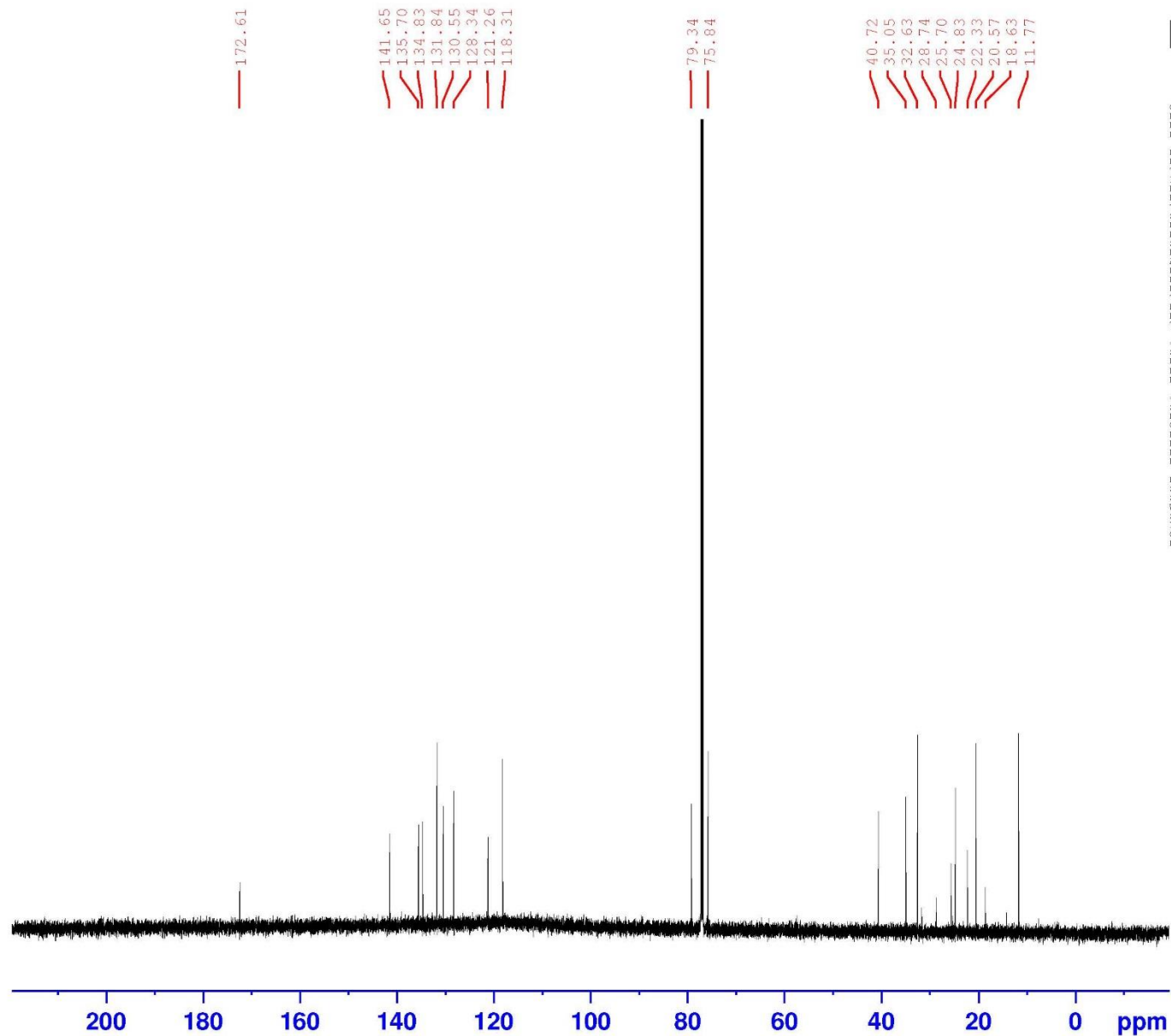
Current Data Parameters
NAME 20180914 Pyrethrin I Alcohol
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180914
Time_ 18.43
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 80.6
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 8.40 usec
PLW1 12.55000019 W

F2 - Processing parameters
SI 65536
SF 600.1300266 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00





Current Data Parameters
NAME 20190118 Pyrethrin I Alcohol Major diastereomer
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190119
Time 23.30
INSTRUM spect
PROBHD 5 mm PABBI 1H/7
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087559 sec
RG 1620
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 16.00 usec
PLW1 110.7600014 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPOWPG2 waltz16
PCPD2 70.00 usec
PLW2 13.55000019 W
PLW12 0.18071000 W
PLW13 0.08855400 W

F2 - Processing parameters
SI 32768
SF 150.9027905 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20190118 Pyrethrin I Alcohol Major diastereomer
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190119
Time 20.13
INSTRUM spect
PROBHD 5 mm F4HH1 1H/
PULPROG carygpmphpp
TD 2048
SOLVENT CDCl3
NS 10
DS 4
SS 4504.504 Hz
FIDRES 2.199463 Hz
AQ 0.2273280 sec
RG 2050
DM 111.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00010030 sec
D1 1.9111636 sec
D11 0.03000000 sec
D12 0.00020000 sec
D16 0.00020000 sec
IN0 0.00022000 sec

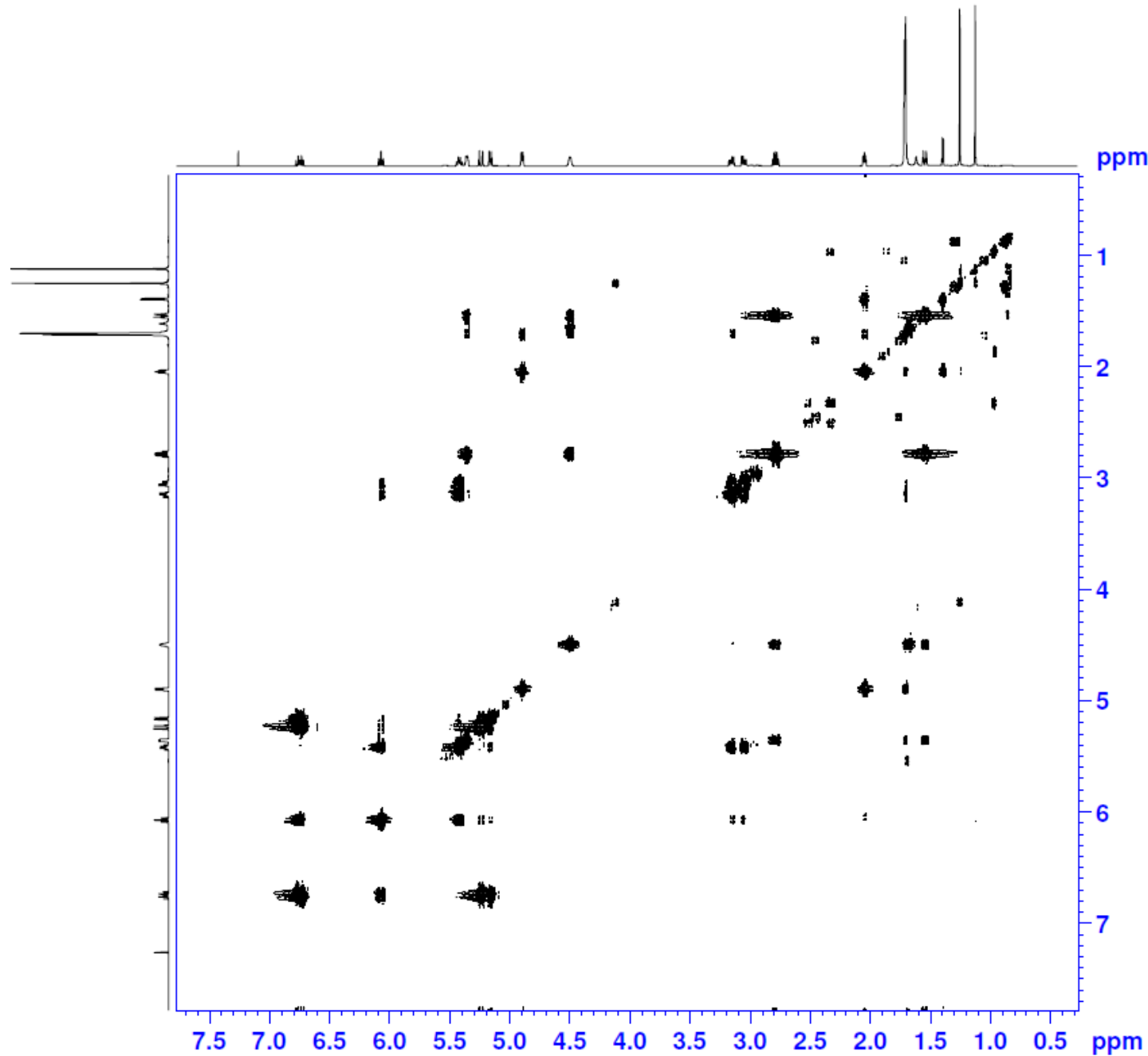
----- CHANNEL f1 -----
SFO1 600.1324422 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P17 2500.00 usec
PCW1 12.55000019 W
P1W10 1.30999994 W

----- GRADIENT CHANNEL -----
GPRAM[1] SMSQ10.100
GPRAM[2] SMSQ10.100
GPE1 10.00 Hz
GPE2 20.00 Hz
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1324 MHz
FIDRES 17.595720 Hz
SN 7.506 ppm
PnMODE States-TFF1

F2 - Processing parameters
SI 1024
SF 600.1300296 MHz
WDW QSIK
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TFF1
SF 600.1300214 MHz
WDW QSIK
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190118 Pyrethrin 1 Alcohol Major diastereomer
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190119
Time 23.35
INSTRUM spect
PROBHD 5 mm F4HH1 1H/
PULPROG zgpg30
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 4629.629 Hz
FIDRES 4.521122 Hz
AQ 0.1105920 sec
RG 2050
EW 108.000 usec
DE 6.50 usec
TE 298.3 K
CHST2 145.0000000
CB 0.000000000 usec
D1 1.45494401 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
EGGPTNS

CHANNEL F1
SFO1 600.1324577 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P28 1000.00 usec
P1M1 12.55000019 W

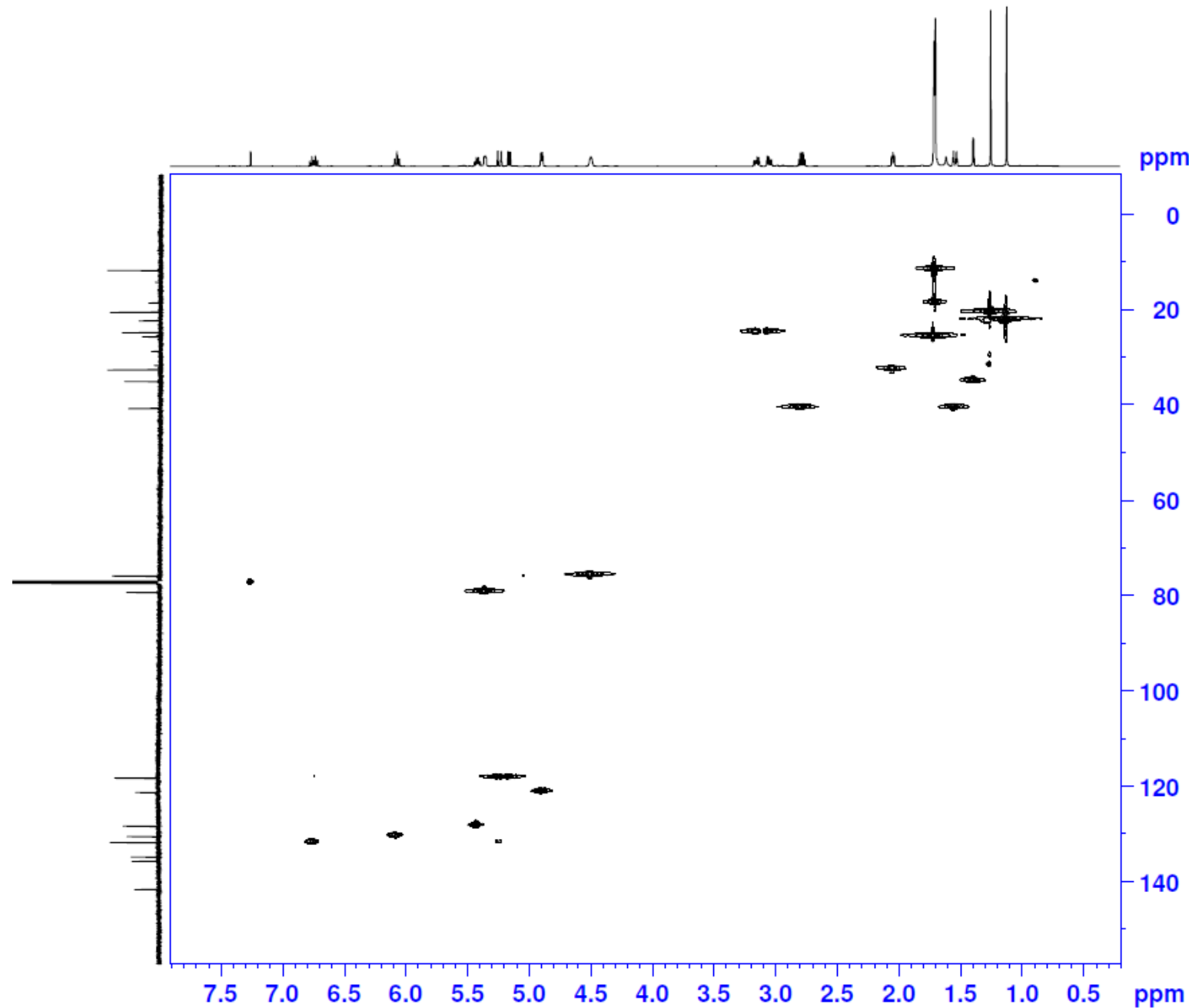
CHANNEL F2
SFO2 150.9140636 MHz
NUC2 13C
CHRGPG[2] zgpg
P3 16.00 usec
P4 32.00 usec
PCTD2 60.00 usec
P1M2 110.76000214 W
P1M12 7.87610006 W

GRADIENT CHANNEL
GPMAM[1] SMSQ10.100
GPMAM[2] SMSQ10.100
GPE1 80.00 A
GPE2 20.10 A
P1G 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656210 Hz
SM 165.657 ppm
FAMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300245 MHz
WDW QNINE
SSB 2
LA 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028261 MHz
WDW QNINE
SSB 2
LA 0 Hz
GB 0





Current Data Parameters
NAME 20190122 Pyrethrin I Alcohol MAJOR
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190122
Time 9.11
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG noesygpph
TD 4096
SOLVENT CDC13
NS 2
DS 16
SWH 5411.255 Hz
FIDRES 1.321107 Hz
AQ 0.3784704 sec
RG 203
DW 92.400 usec
DE 6.50 usec
TE 298.2 K
D0 0.00008170 sec
D1 3.00000000 sec
D8 0.60000002 sec
D16 0.00020000 sec
IN0 0.00018480 sec

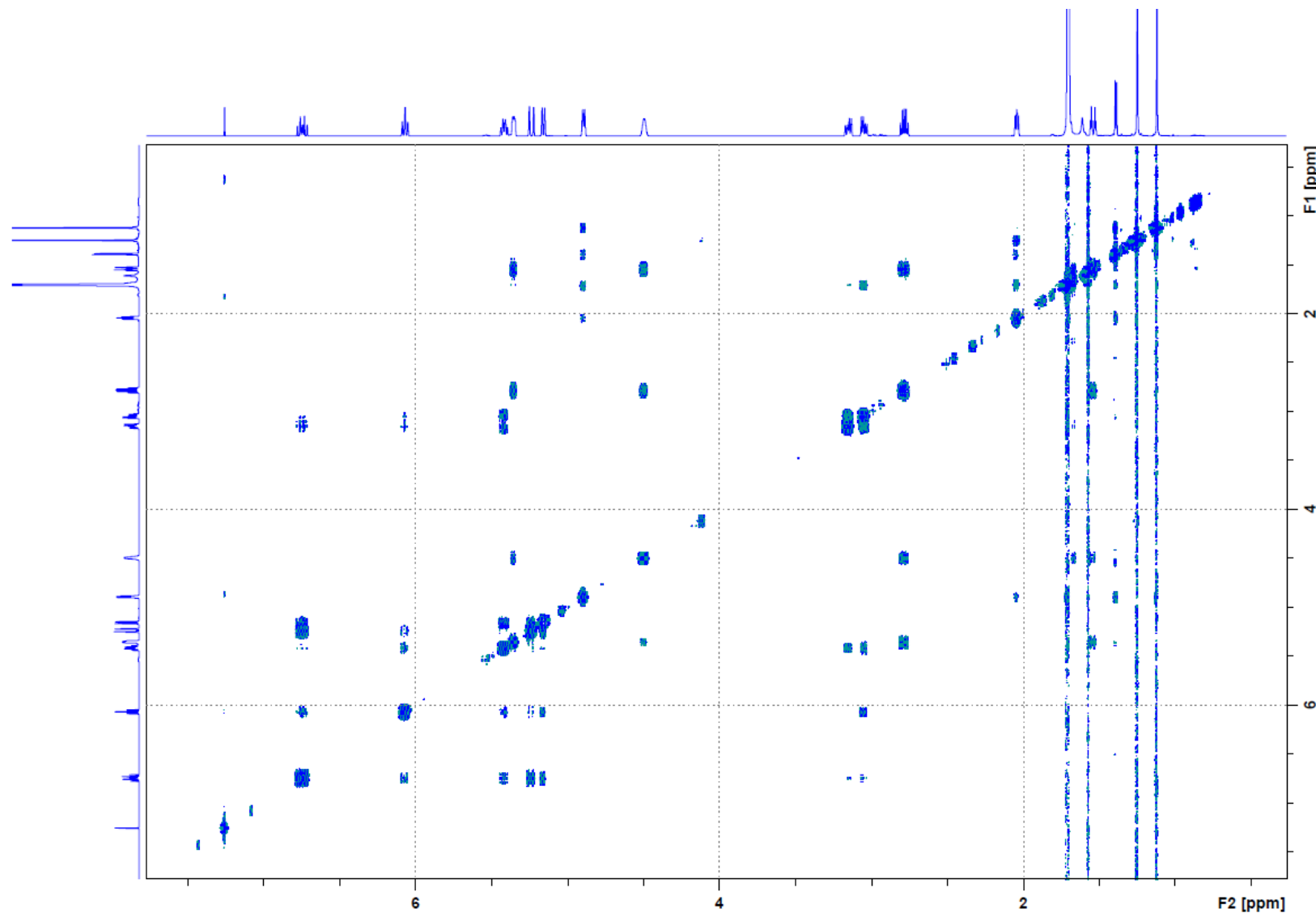
===== CHANNEL f1 =====
SFO1 600.1323960 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P1M1 12.55000019 W

===== GRADIENT CHANNEL =====
CPN1M1 SMSQ10.100
GP1 40.00 %
P16 1000.00 usec

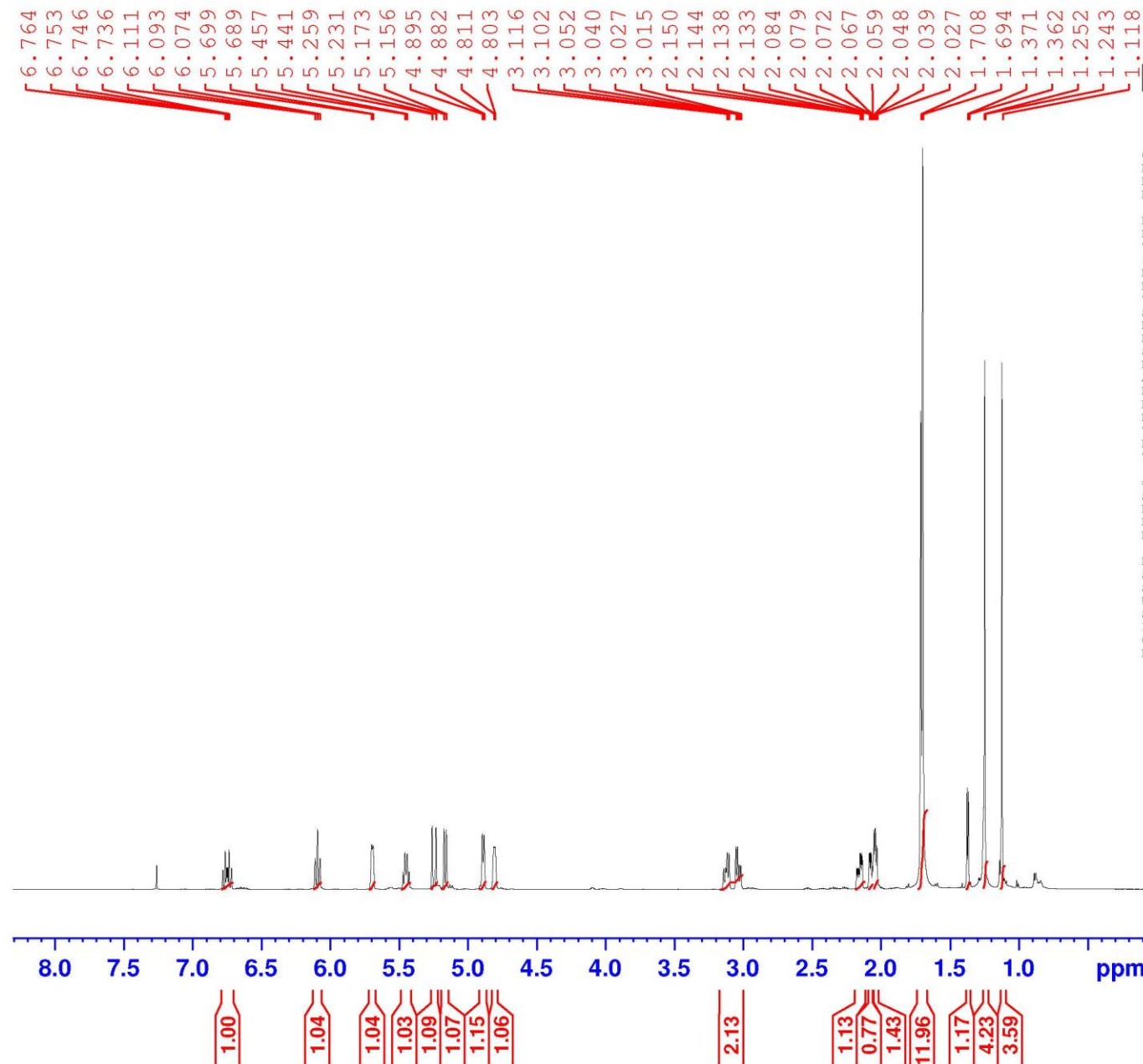
F1 - Acquisition parameters
TD 472
SFO1 600.1324 MHz
FIDRES 11.464524 Hz
SW 9.017 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 4096
SF 600.1300256 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300234 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0



4'S-51a NMR Characterisation

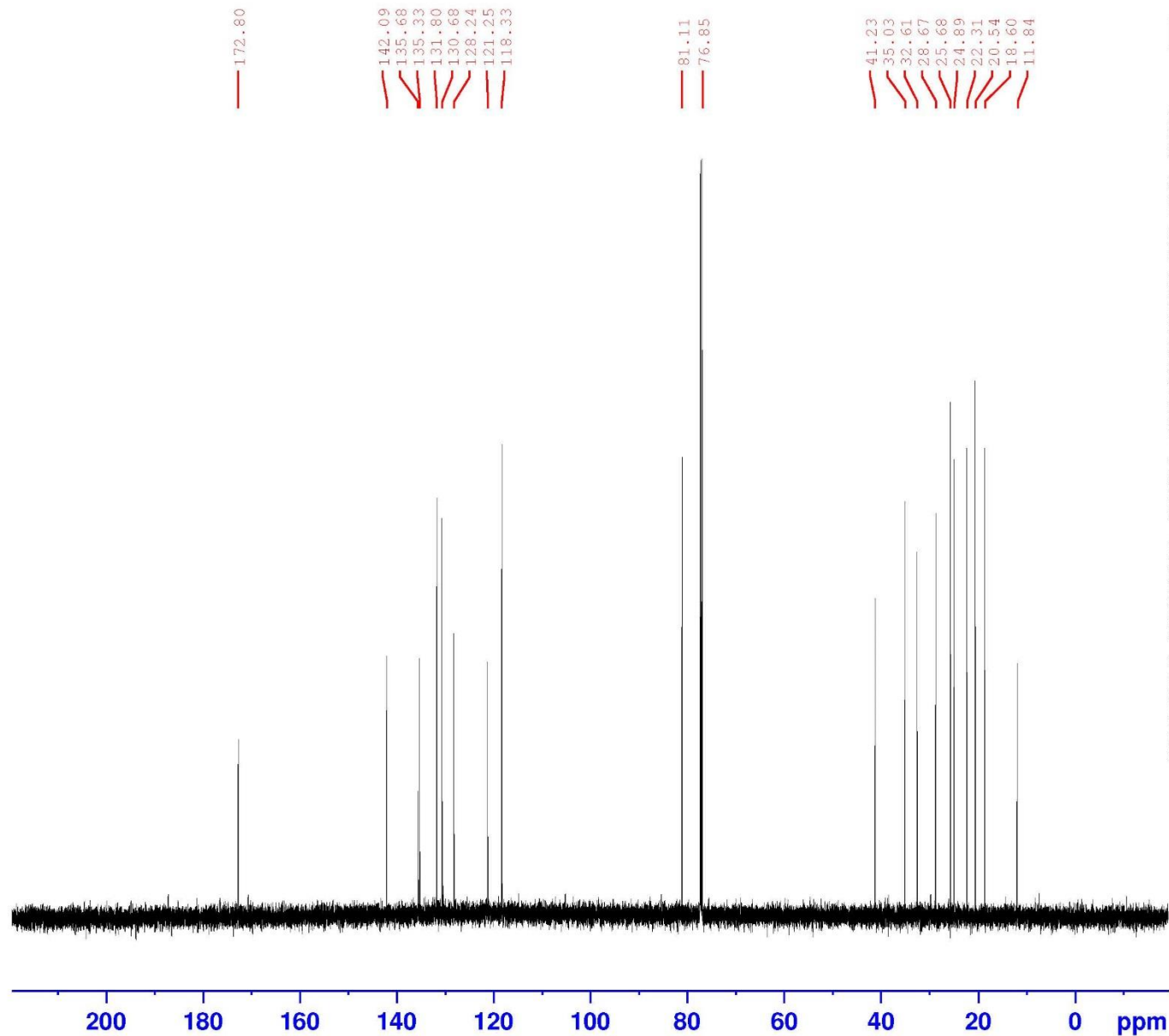


Current Data Parameters
 NAME 20190123 Pyrethrin I OH MINOR
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190123
 Time 18.09
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 32
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 8.40 usec
 PLW1 12.55000019 W

F2 - Processing parameters
 SI 65536
 SF 600.1300240 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20190122 Pyrethrin I OH MINOR
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190122
Time 16.43
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 215
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 1440
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 16.00 usec
PLW1 110.76000214 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
PCPDFRG[2] waltz16
PCPD2 70.00 usec
PLW2 12.55000019 W
PLW12 0.18072000 W
PLW13 0.08855400 W

F2 - Processing parameters
SI 32768
SF 150.9027917 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20190118 Pyrethrin I Alcohol Minor diastereomer
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190120
Time 7.29
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG cosygpc1p7pp
TD 2048
SOLVENT CDCl3
NS 20
DS 4
SWH 4716.301 Hz
FIDRES 2.303213 Hz
AQ 0.2170380 sec
RG 2050
DW 106.000 usec
DE 6.50 usec
TE 298.2 K
DO 0.00009530 sec
D1 1.32135704 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021200 sec

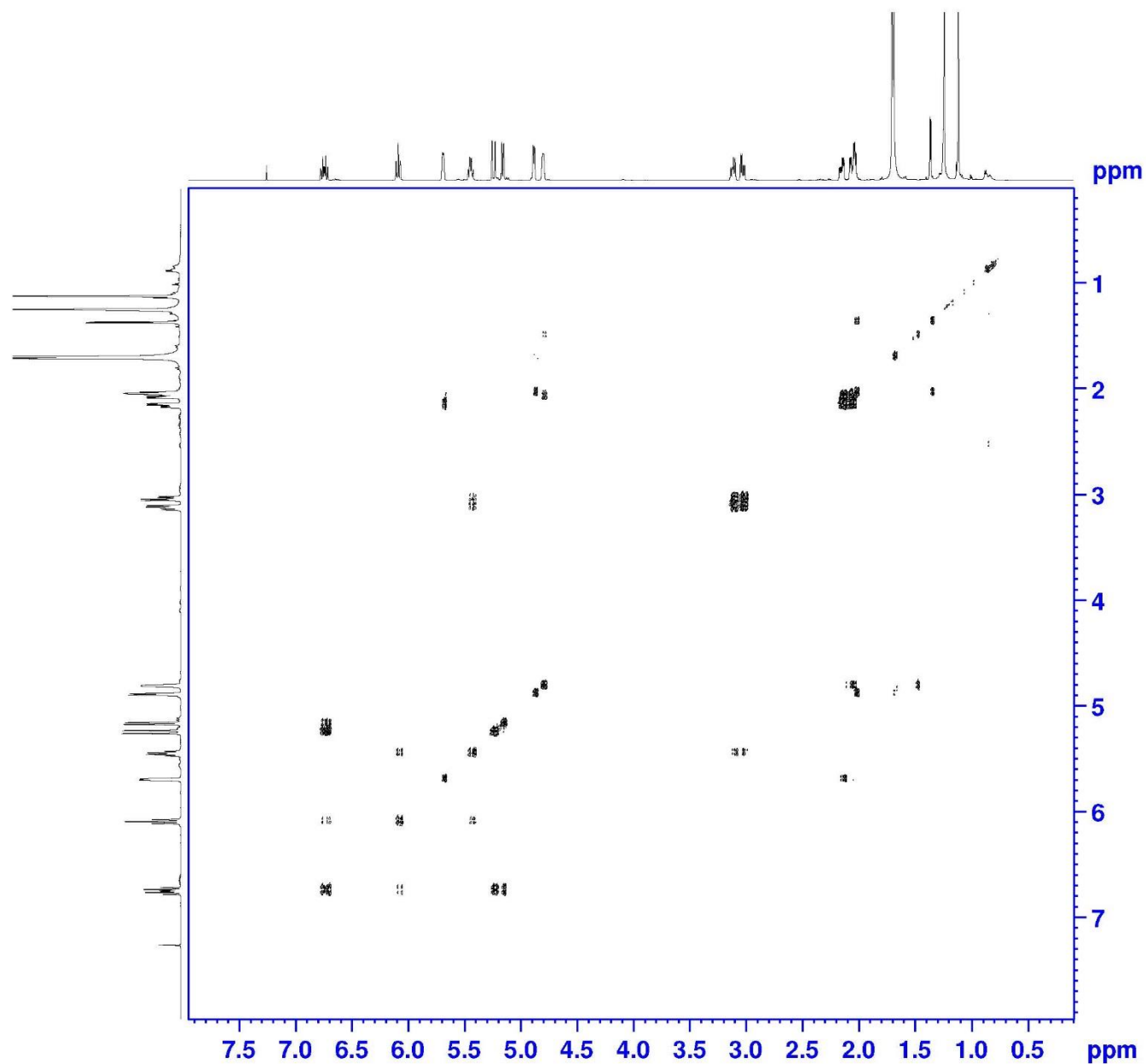
===== CHANNEL f1 =====
SFO1 600.1324547 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P17 2500.00 usec
PLW1 12.55000019 W
PLW0 1.30999994 W

===== GRADIENT CHANNEL =====
GPNM(1) SMSQ10.100
GPNM(2) SMSQ10.100
GP11 10.00 %
GP12 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 356
SFO1 600.1325 MHz
FIDRES 18.425707 Hz
SM 7.860 ppm
P0MODE States-TPP1

F2 - Processing parameters
SI 1024
SF 600.1300392 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPP1
SF 600.1300336 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190116 Pyrethrin I Alcohol Minor diastereomer
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190120
Time 14:57
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG hsqcetpp
TD 1024
SOLVENT CDCl3
NS 70
DS 16
SWH 4629.629 Hz
FIDRES 4.921122 Hz
AQ 0.1105920 sec
RG 2050
RW 108.000 usec
DE 6.50 usec
TE 298.3 K
CHST2 145.0000000
DO 0.0000200 sec
D1 1.45494401 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
TMO 0.00002000 sec
ZGPGTMS

===== CHANNEL f1 =====
SFO1 600.1324815 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P28 1000.00 usec
PLW1 12.85000019 W

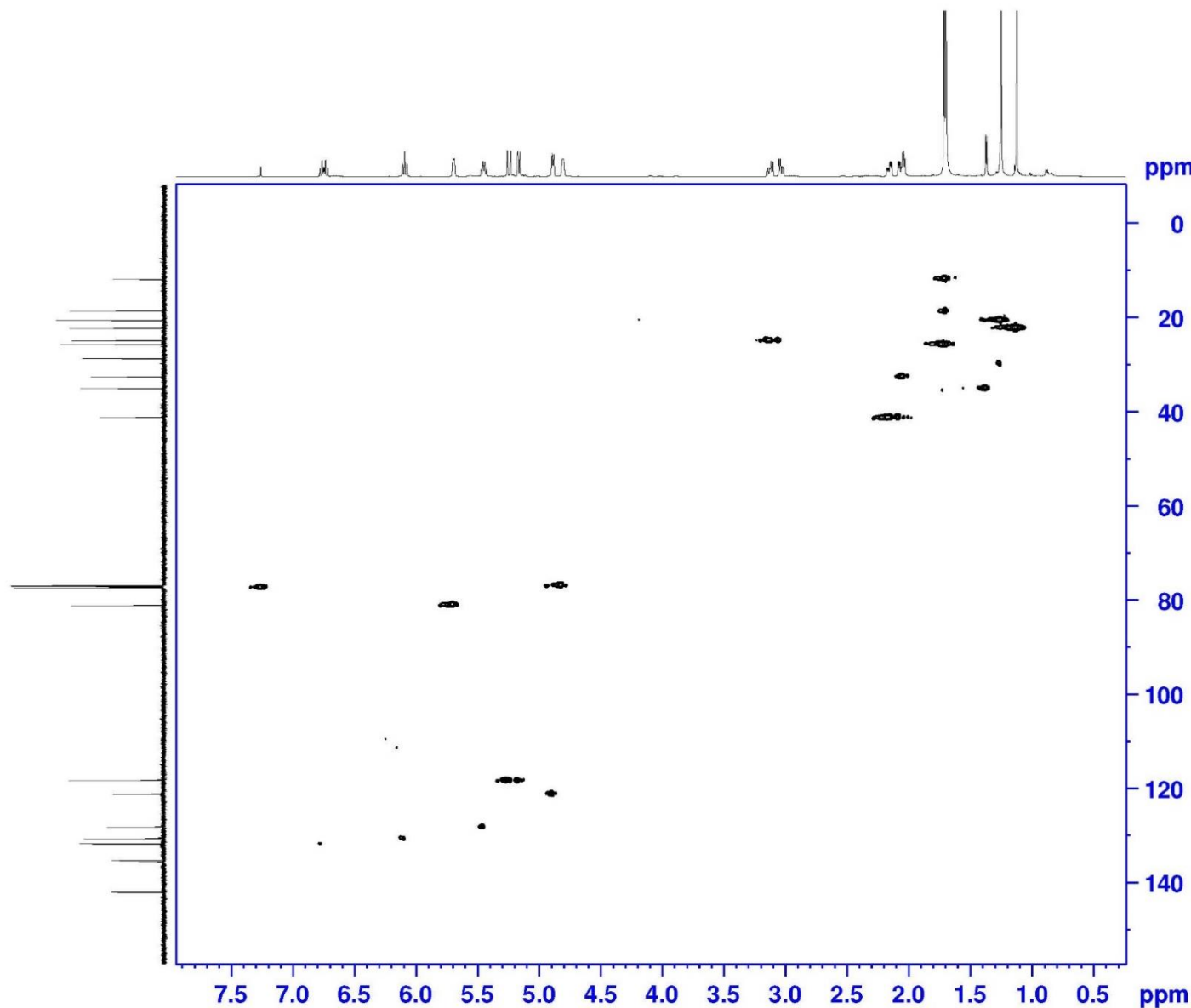
===== CHANNEL f2 =====
SFO2 150.9140616 MHz
NUC2 13C
P3 16.00 usec
P4 32.00 usec
PCPD2 60.00 usec
PLW2 110.76000314 W
PLW12 7.87610006 W

===== GRADIENT CHANNEL =====
GPRAM[1] SMSQ10.100
GPRAM[2] SMSQ10.100
SP21 80.00 %
SP22 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
PRMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300257 MHz
WDW Q5INE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9026140 MHz
WDW Q5INE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190122 Pyrethrin I OH MINOR
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190122
Time 16.54
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG noesygpph
TD 4096
SOLVENT CDCl3
NS 2
DS 16
SWH 5411.255 Hz
FIDRES 1.321107 Hz
AQ 0.3784704 sec
RG 50.8
DW 92.400 usec
DE 6.50 usec
TE 298.2 K
D0 0.00008170 sec
D1 3.00000000 sec
D8 0.60000002 sec
D16 0.00020000 sec
INO 0.00018480 sec

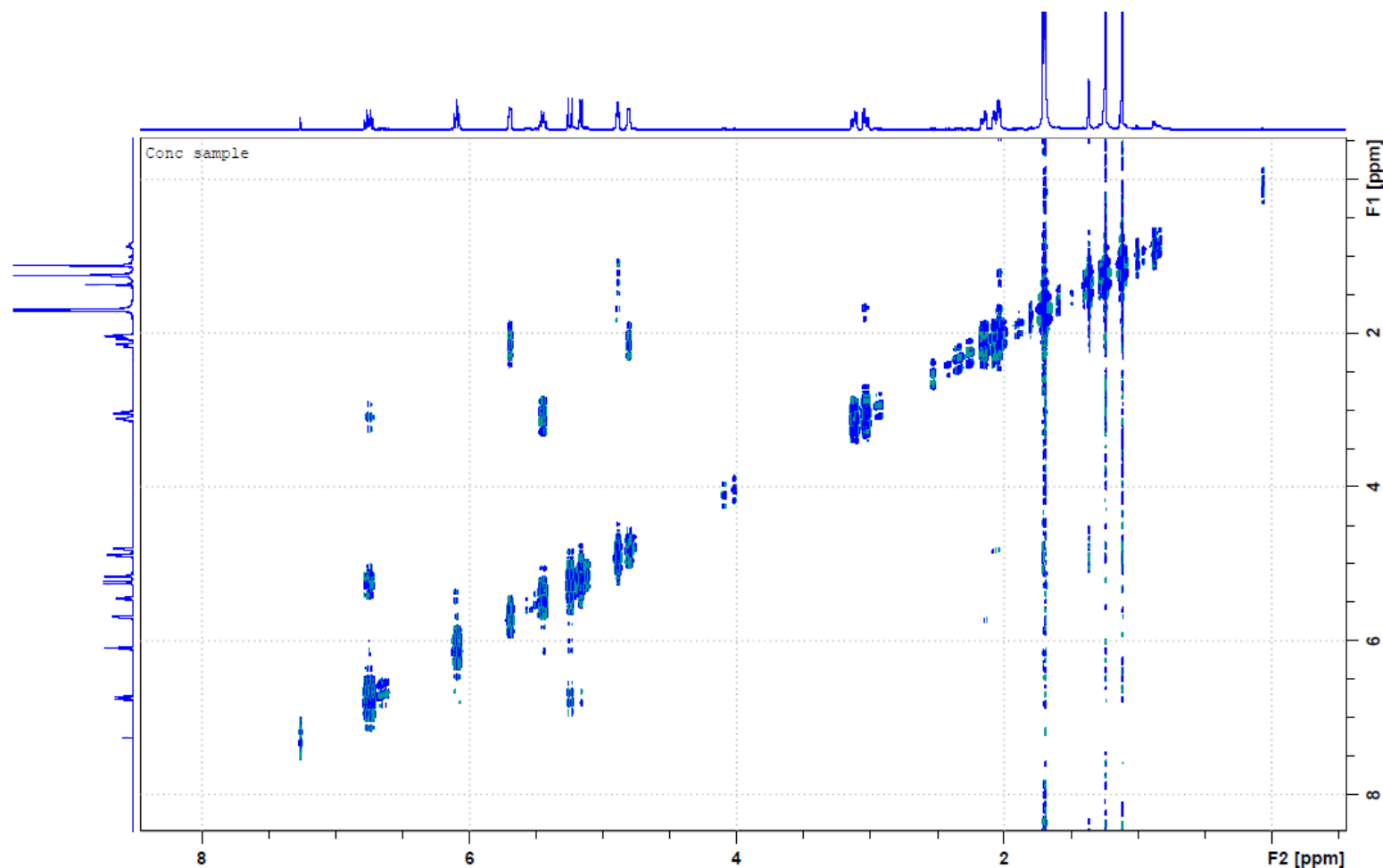
----- CHANNEL f1 -----
SFO1 600.1323960 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
PLW1 12.55000019 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

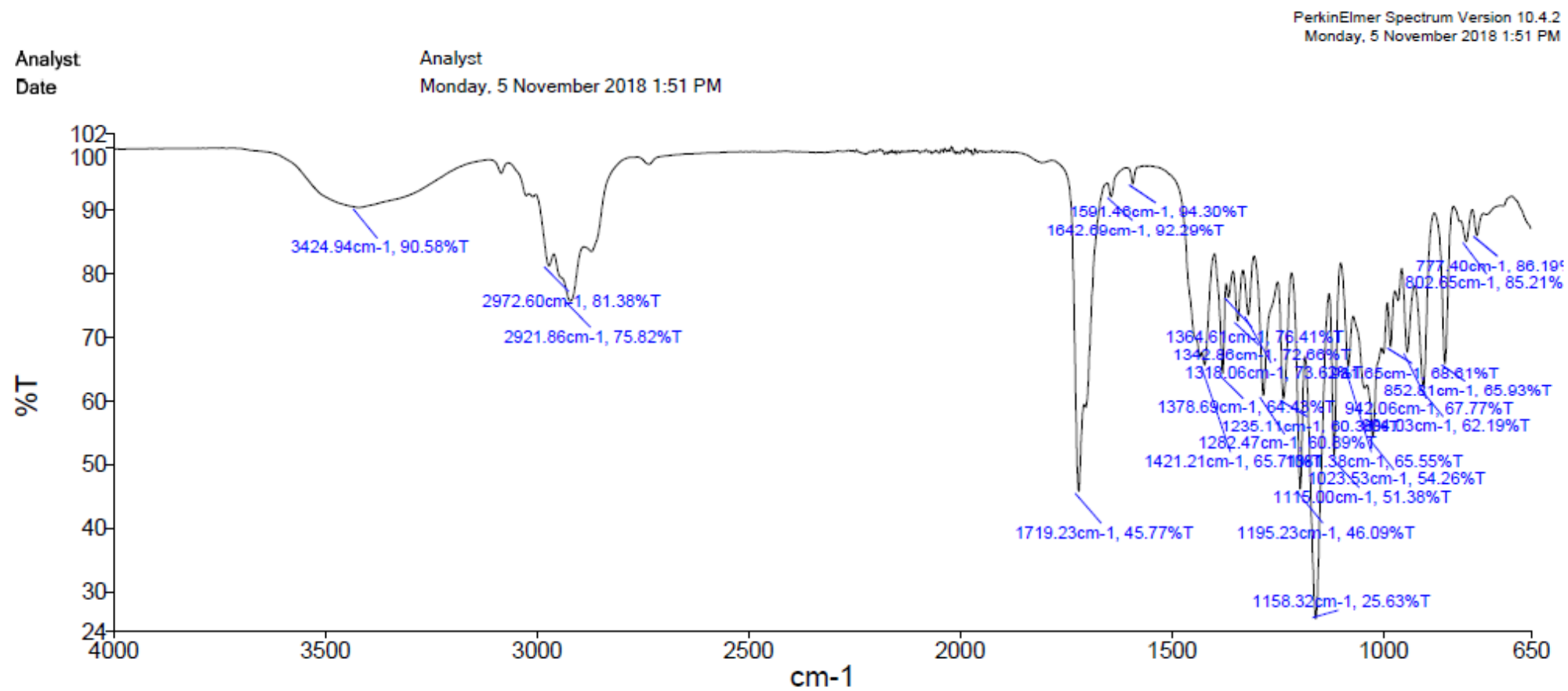
F1 - Acquisition parameters
TD 127
SFO1 600.1324 MHz
FIDRES 42.608311 Hz
SW 9.017 ppm
FMODE States-TPPI

F2 - Processing parameters
SI 4096
SF 600.1300253 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

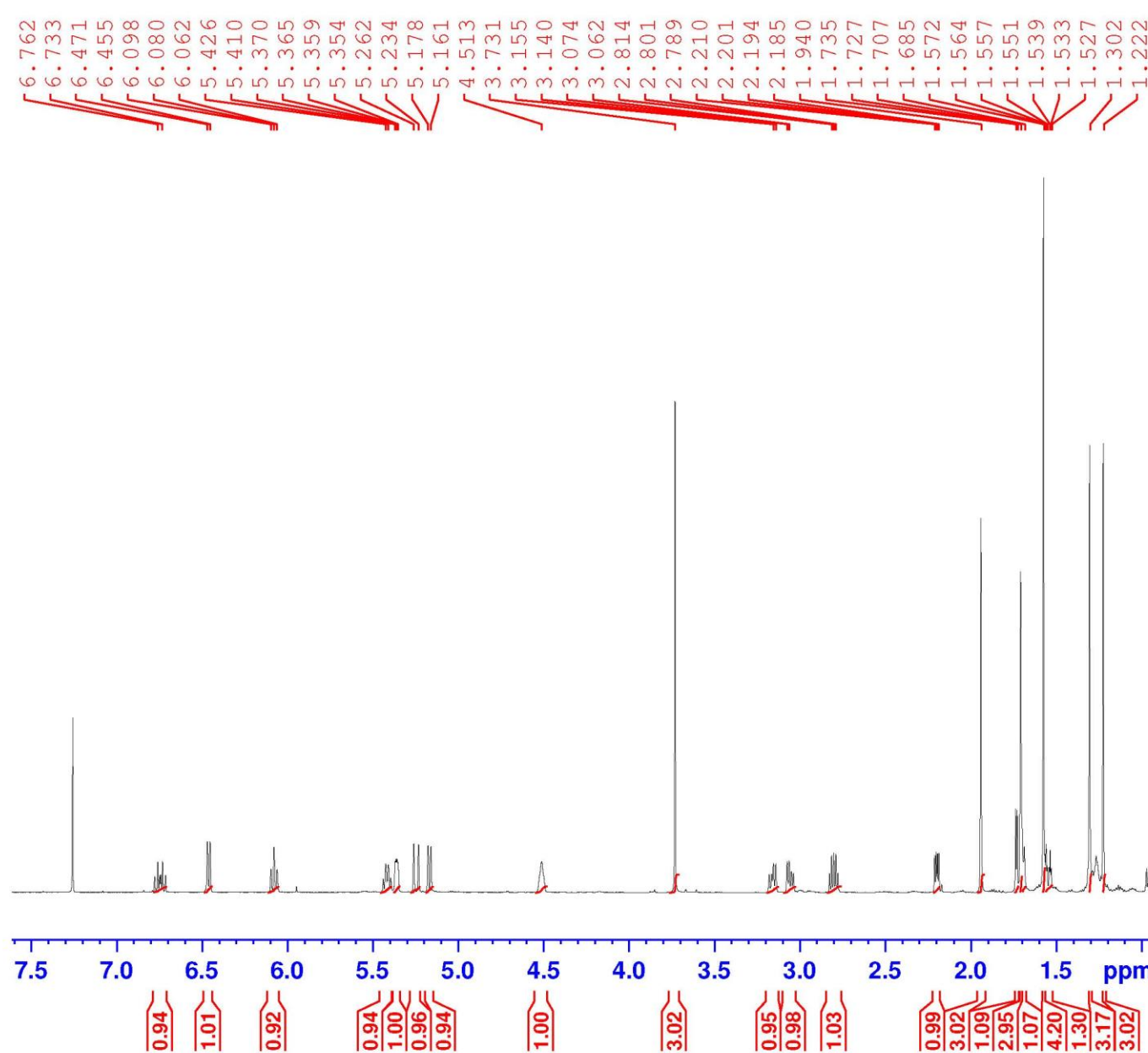
F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300135 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0



51a IR Spectrum



4'R-51b NMR Characterisation

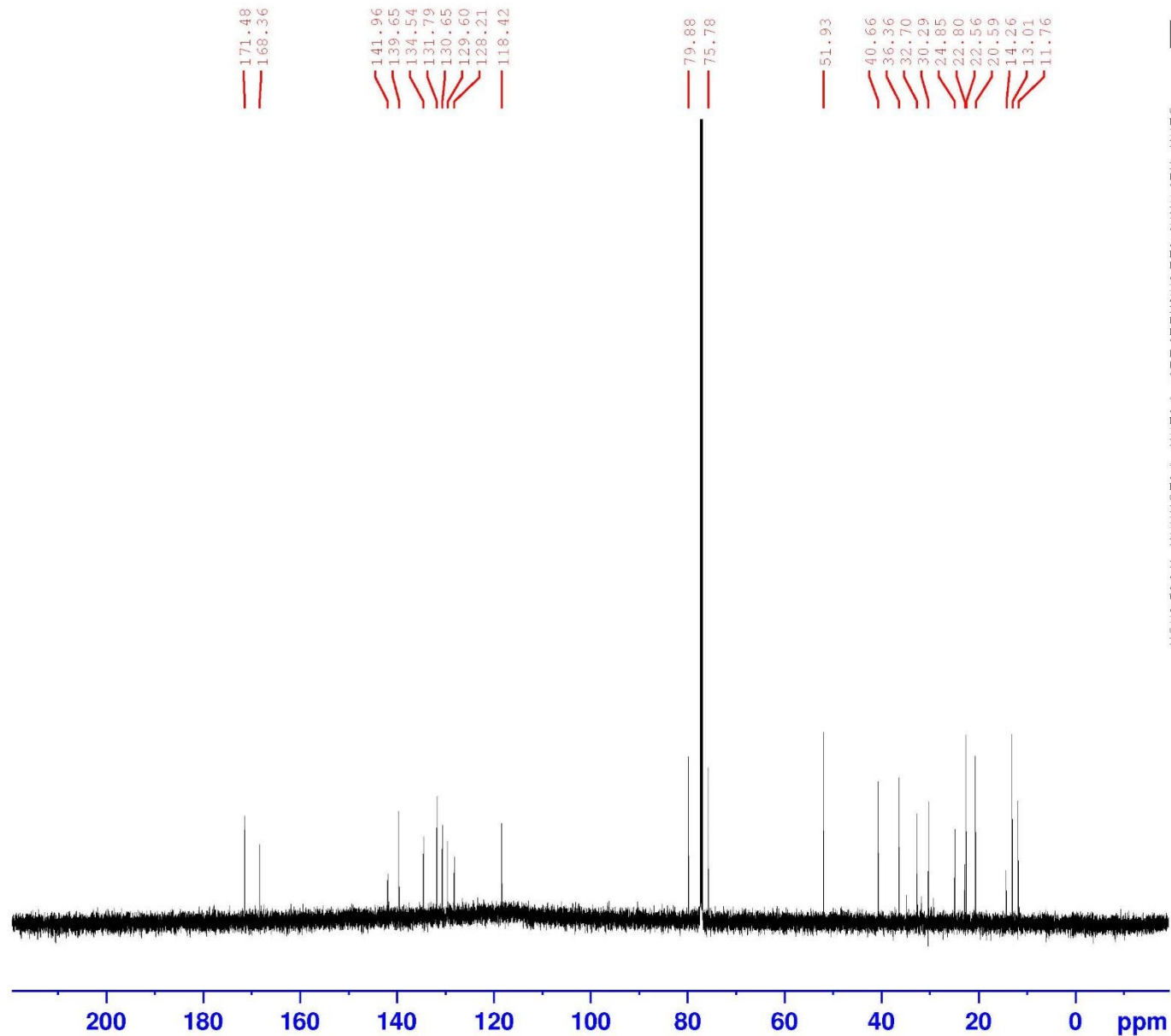


Current Data Parameters
 NAME 20190117 Pyrethrin II Allylic alcohol
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190117
 Time_ 17.14
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 228
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 600.1337060 MHz
 NUC1 1H
 P1 8.40 usec
 PLW1 12.55000019 W

F2 - Processing parameters
 SI 65536
 SF 600.1300258 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20190117 Pyrethrin II Allylic alcohol
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190117
Time 19.45
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 1440
DW 13.867 usec
DE 6.50 usec
TK 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 150.9178968 MHz
NUC1 13C
P1 16.00 usec
PLM1 110.76000214 W

----- CHANNEL f2 -----
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 12.55000019 W
PLM2 0.18072000 W
PLM3 0.08855400 W

F2 - Processing parameters
SI 32768
SF 150.9027891 MHz
WDW no
SSE 0
LB 0 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20190117 Pyrethrin II Allylic alcohol
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190117
Time 17.16
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG cosygmphpp
TD 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 4464.286 Hz
FIDRES 2.179827 Hz
AQ 0.2293760 sec
RG 2050
DW 112.000 usec
DE 6.50 usec
TK 298.2 K
D0 0.00010130 sec
D1 1.90906894 sec
D11 0.03000000 sec
D12 0.00020000 sec
D16 0.00020000 sec
LNO 0.00022400 sec

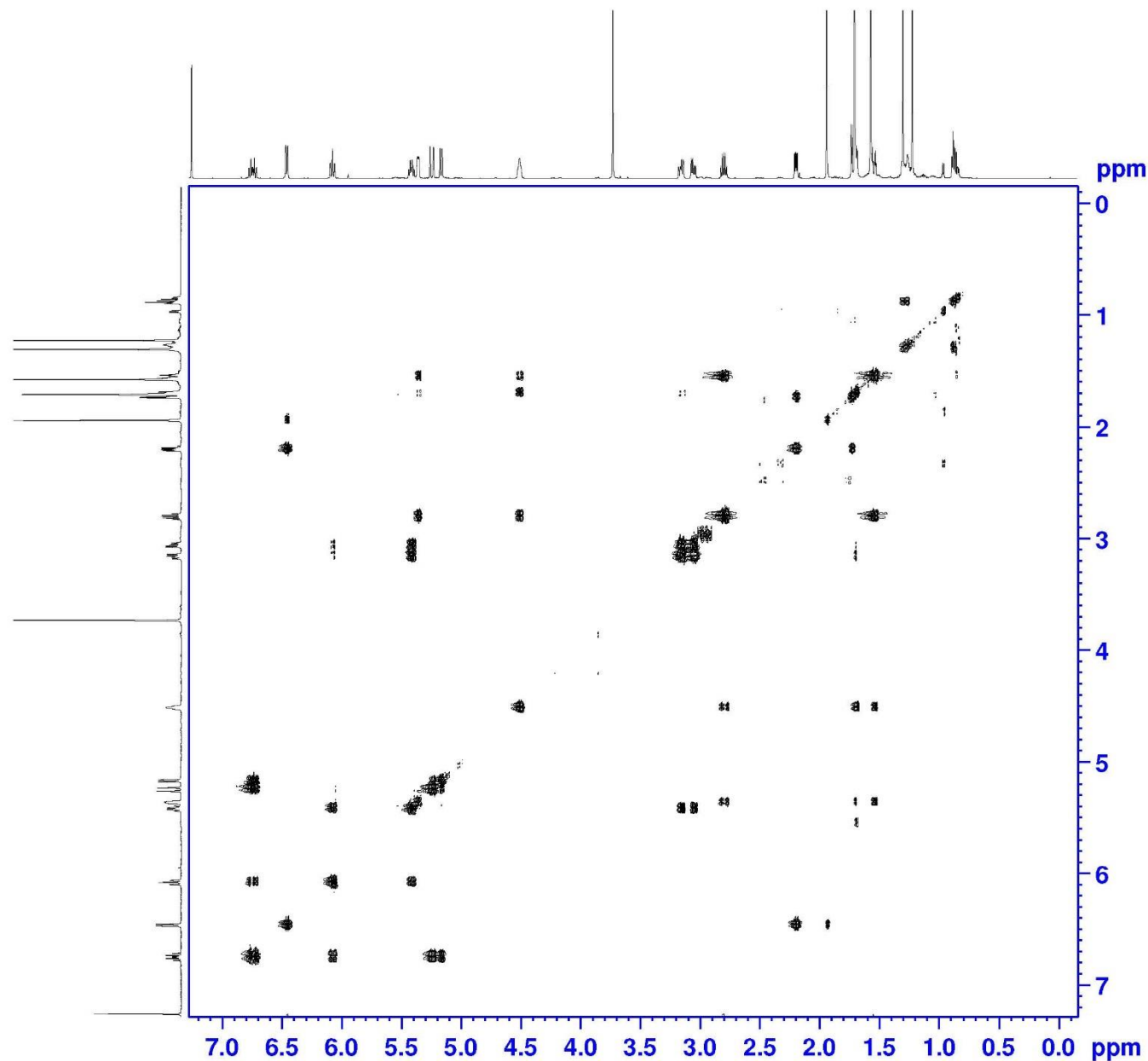
===== CHANNEL f1 =====
SFO1 600.1321673 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P17 2500.00 usec
PLM1 12.55000019 W
PLM10 1.30999994 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GP21 10.00 %
GP22 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1322 MHz
FIDRES 17.438616 Hz
SW 7.439 ppm
EnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.1300296 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
WDW States-TPPI
SF 600.1300274 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190117 Pyrethrin II Allylic alcohol
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190117
Time 19.51
INSTRUM spect
PROBHD 5 mm PABBE 1H/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 45
DS 16
SWH 4201.681 Hz
FIDRES 4.103204 Hz
AQ 0.1218560 sec
RG 2050
DW 119.0000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.44368005 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
INO 0.00002000 sec
EGOPTNS

===== CHANNEL f1 =====
SFO1 600.1322686 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P28 1000.00 usec
PLM1 12.55000019 W

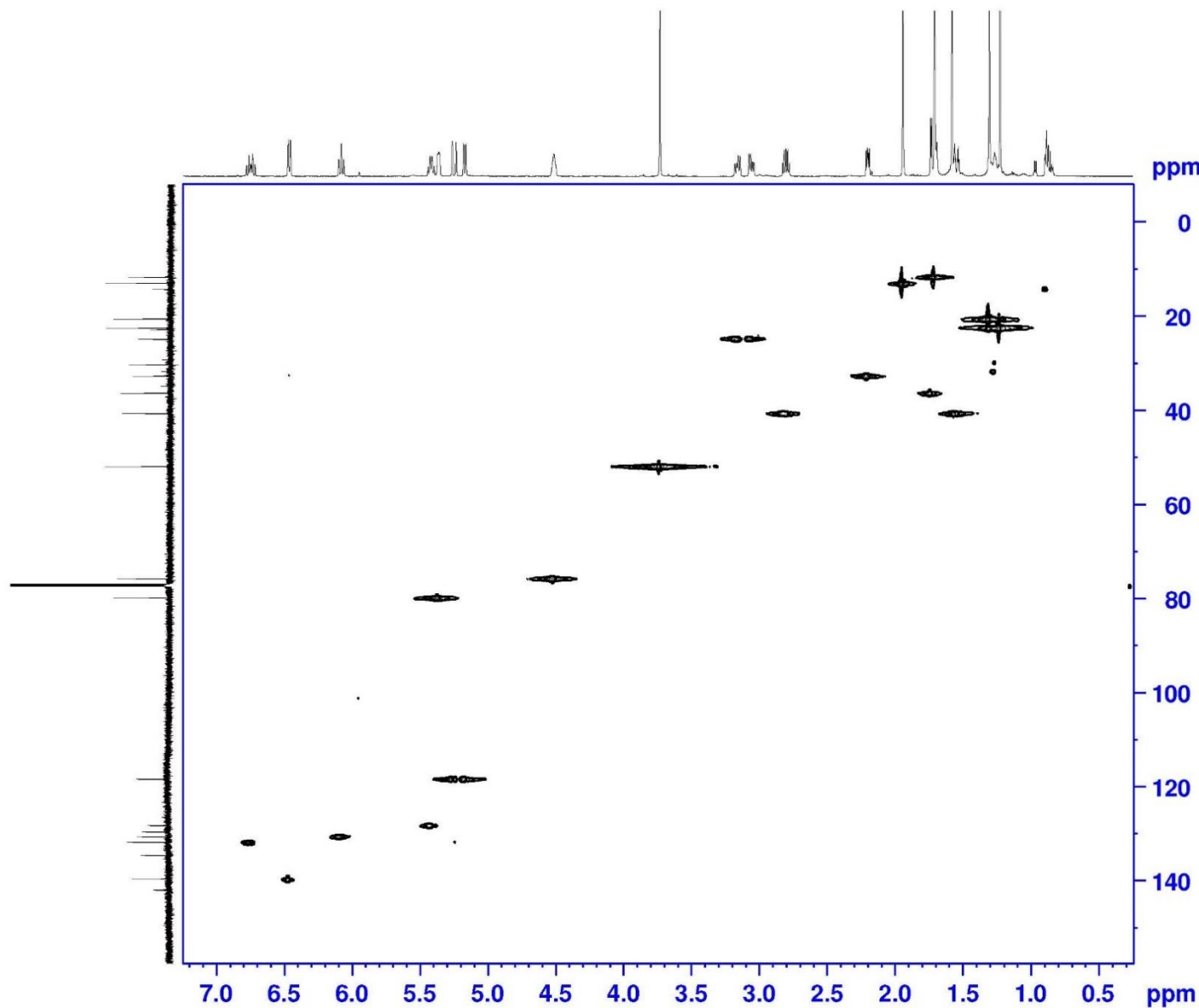
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 16.00 usec
P4 32.00 usec
PCPD2 60.00 usec
PLM2 110.76000214 W
PLM12 7.87610006 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
PL6 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.856250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300209 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9027813 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190121 Pyrethrin II OH MAJOR
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20190121
Time 8.41
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG noesygpph
TD 4096
SOLVENT CDCl3
NS 2
DS 16
SWH 5411.255 Hz
FIDRES 1.321107 Hz
AQ 0.3784704 sec
RG 203
DW 92.400 usec
DE 6.50 usec
TE 298.2 K
D0 0.00008170 sec
D1 3.00000000 sec
D8 0.60000002 sec
D16 0.00020000 sec
IN0 0.00018480 sec

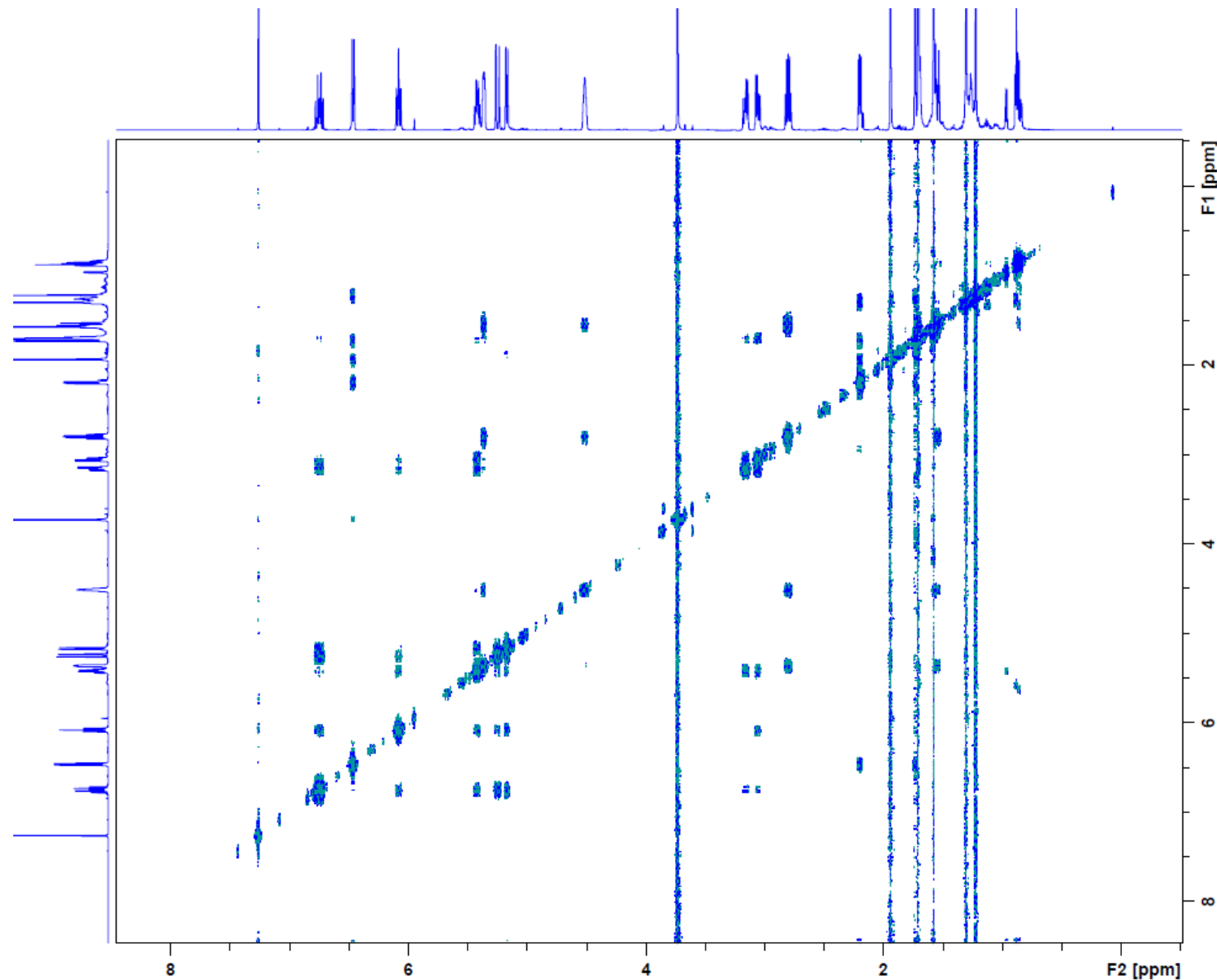
----- CHANNEL f1 -----
SFO1 600.1323960 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
PLW1 12.55000019 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 397
SFO1 600.1324 MHz
FIDRES 13.630366 Hz
SW 9.017 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 4096
SF 600.1300252 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300210 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0



4'S-51b NMR Characterisation

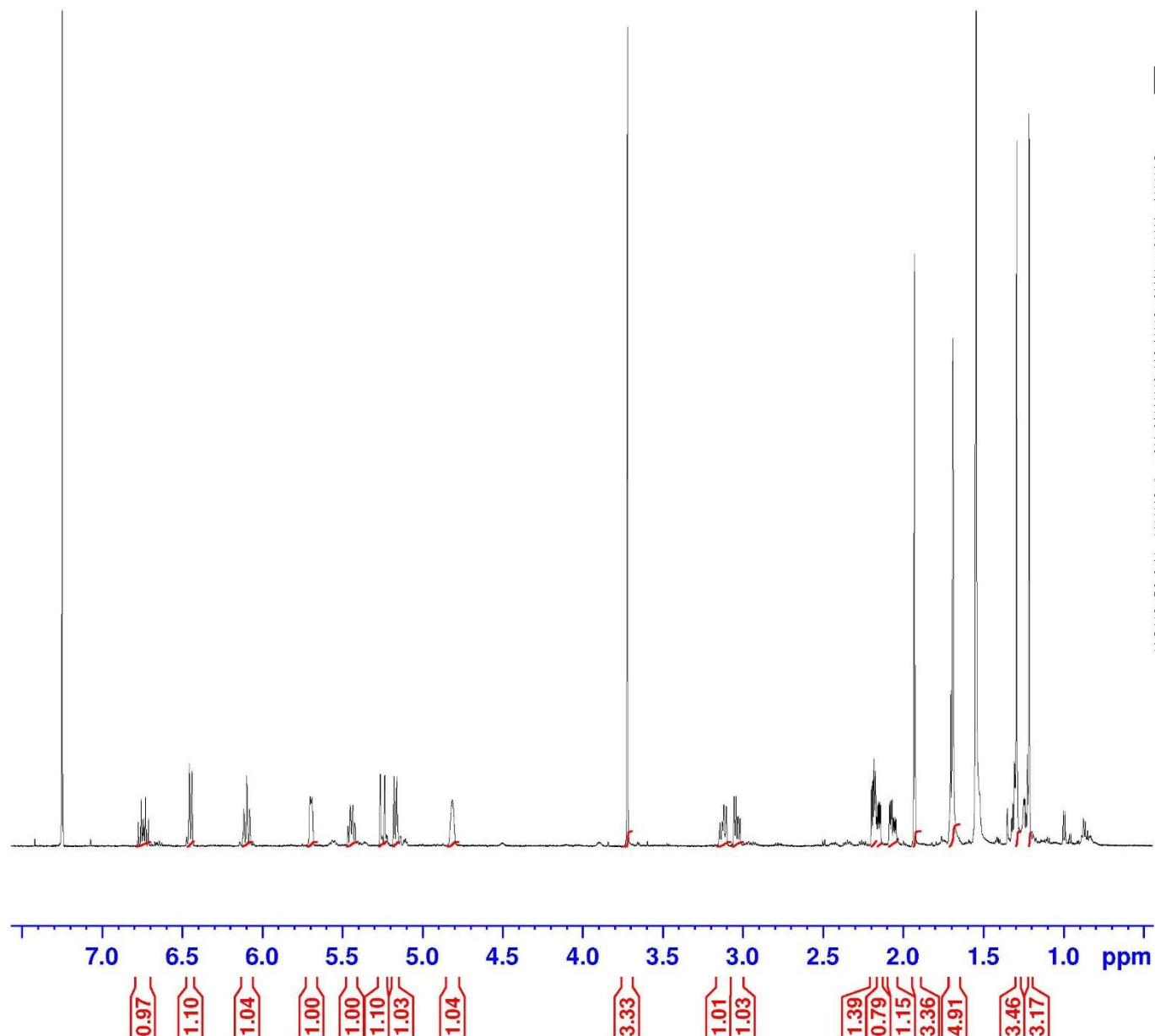


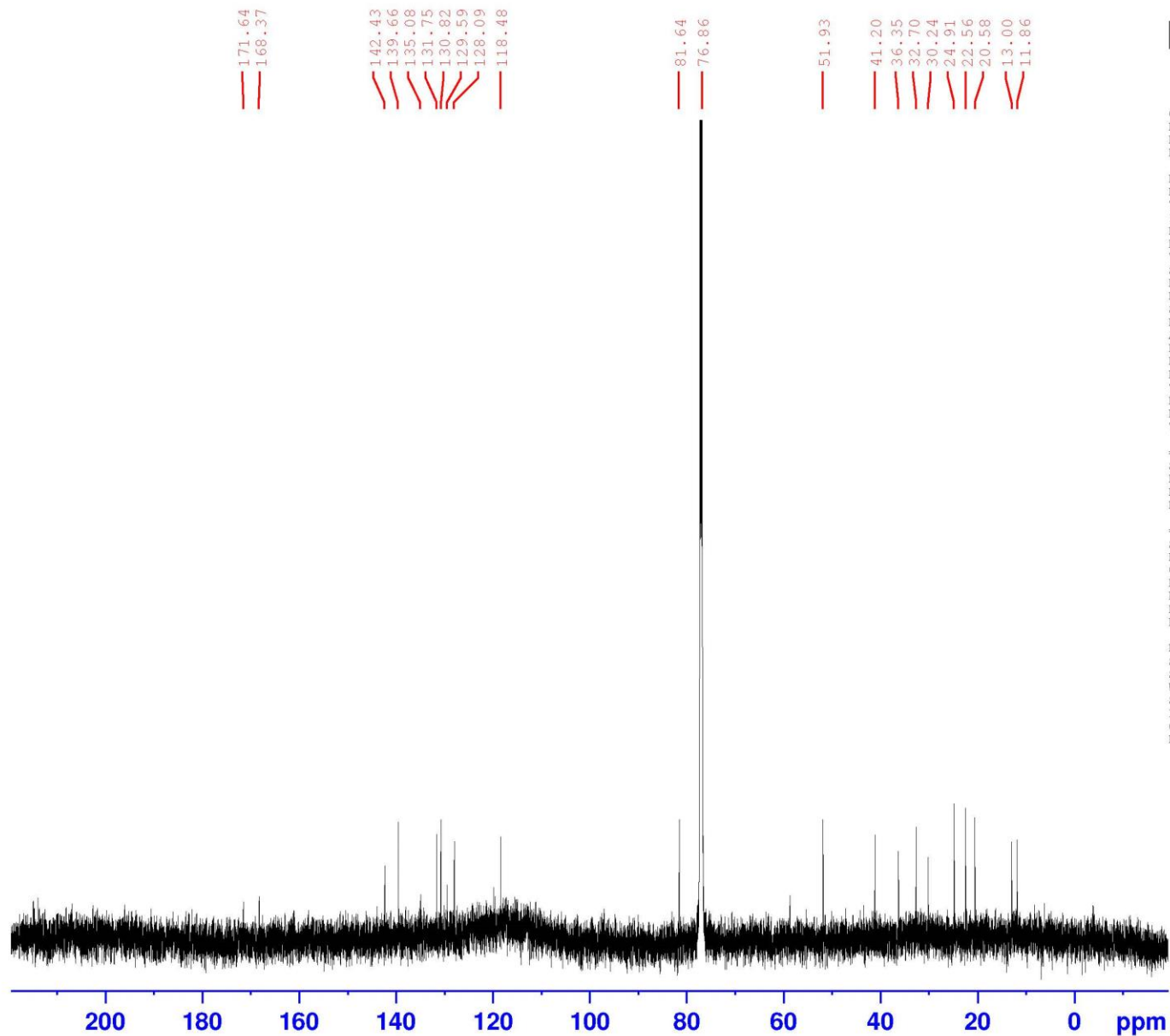
Current Data Parameters
 NAME 20190123 Pyrethrin II OH MINOR
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190123
 Time 18.28
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 362
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 8.40 usec
 PLW1 12.55000019 W

F2 - Processing parameters
 SI 65536
 SF 600.1300305 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00





Current Data Parameters
NAME 20190121 Pyrethrin II Minor OH
EXFNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190121
Time 22.33
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 6144
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 1440
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 16.00 usec
PLW1 110.76000214 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 12.55000019 W
PLW12 0.18072000 W
PLW13 0.08855400 W

F2 - Processing parameters
SI 32768
SF 150.9027895 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20190125 Pyrethrin II OH MINOR
EXFNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190125
Time 10.54
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 6
DS 4
SWH 4201.681 Hz
FIDRES 2.051602 Hz
AQ 0.2437120 sec
RG 2050
DW 119.000 usec
DE 6.50 usec
TE 298.2 K
DO 0.00010830 sec
D1 1.89473295 sec
D11 0.03000000 sec
D12 0.00020000 sec
D16 0.00020000 sec
INO 0.00023800 sec

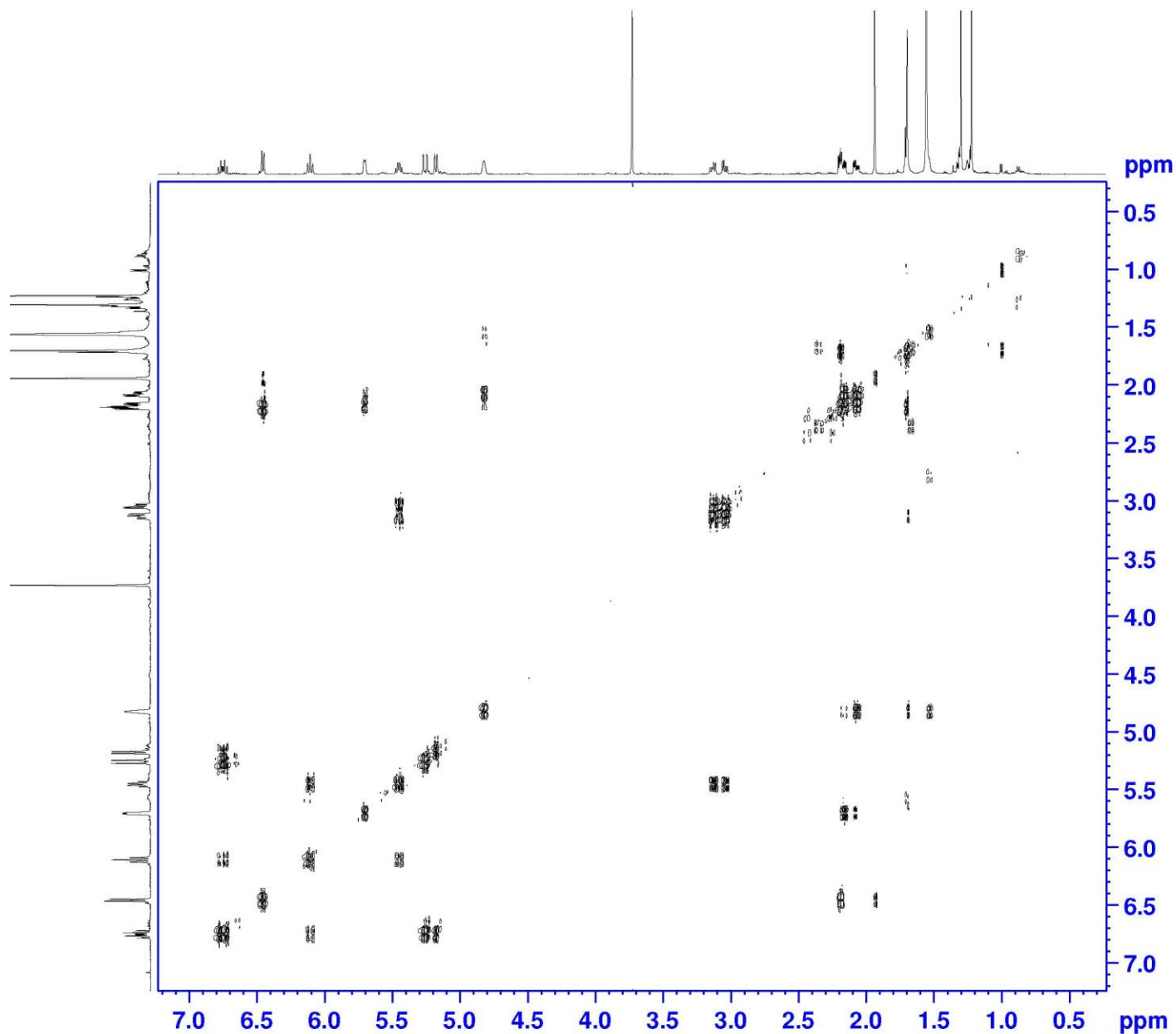
===== CHANNEL f1 =====
SF01 600.1322665 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P17 2500.00 usec
PLW1 12.55000019 W
PLW10 1.309999994 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 124
SF01 600.1323 MHz
FIDRES 33.884521 Hz
SW 7.001 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.1300272 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300209 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190118 Pyrethrin II Alcohol Minor diastereomer
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190119
Time 8.26
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 1024
SOLVENT CDCl3
NS 76
DS 16
SWH 4347.926 Hz
FIDRES 4.245924 Hz
AQ 0.1177508 sec
RG 2050
DW 115.908 usec
DE 6.50 usec
TE 298.3 K
SMT2 145.000000
D1 0.0000000 sec
D11 1.44777596 sec
D4 0.00172414 sec
D11 0.03600000 sec
D16 0.00620000 sec
ID0 0.00692000 sec
ZGPGTMS

----- CHANNEL F1 -----
SFO1 600.1322932 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P21 1000.00 usec
PL11 12.5300019 W

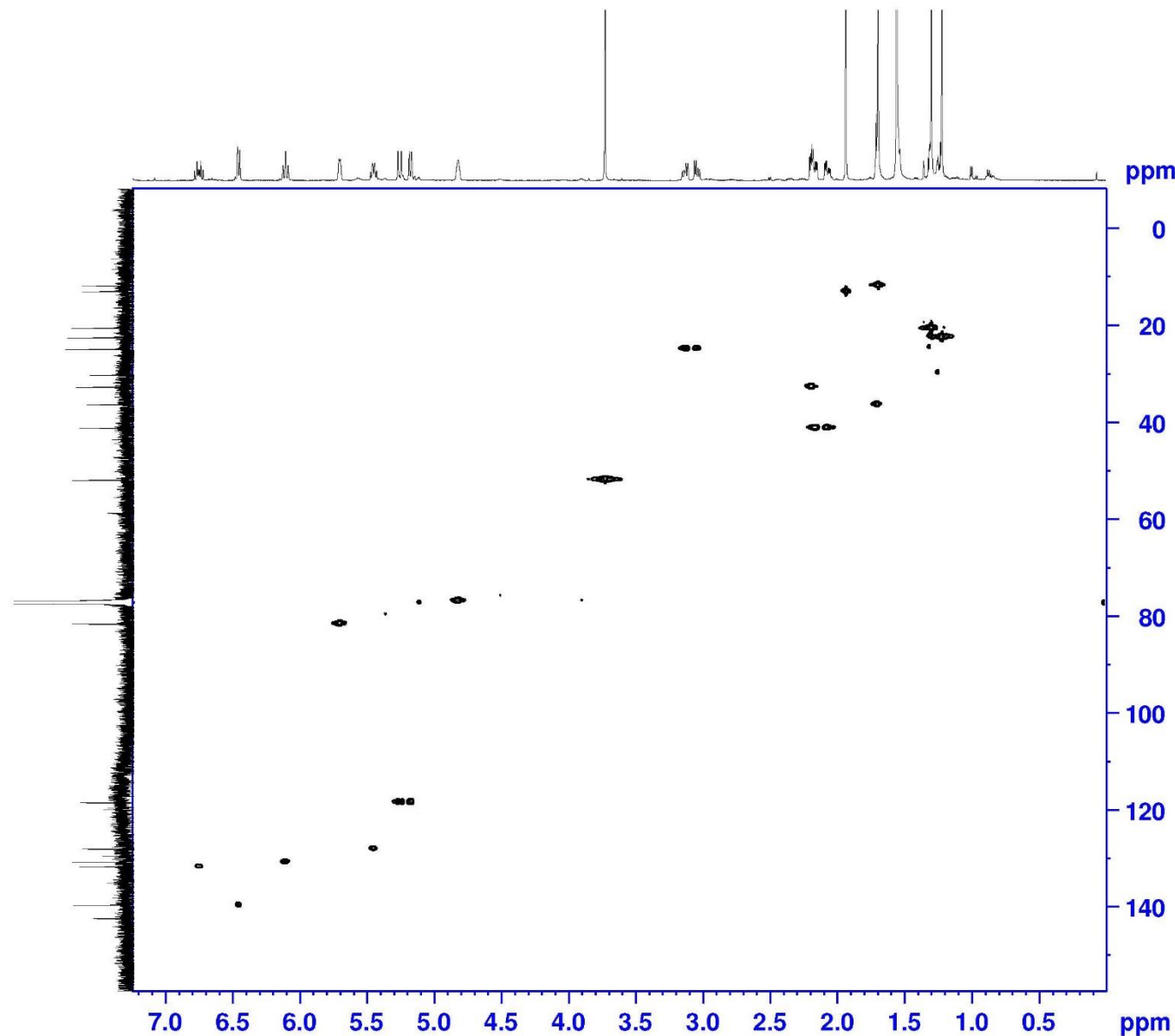
----- CHANNEL F2 -----
SFO2 150.9140636 MHz
NUC2 13C
CDEPG(2) gprp
P3 16.00 usec
P4 32.00 usec
PCPD2 60.00 usec
PLM12 110.7600014 W
PLM12 7.87610006 W

===== GRADIENT CHANNEL =====
GPRAM(1) ZMSQ10.100
GPRAM(2) ZMSQ10.100
GF21 80.00 %
GF22 20.10 %
F16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.456256 Hz
SN 145.457 ppm
PnMODE Echo-Antlecho

F2 - Processing parameters
SI 1024
SF 600.1300289 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antlecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190121 Pyrethrin II OH MINOR
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190121
Time 13.10
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG noesygpph
TD 4096
SOLVENT CDCl3
NS 2
DS 16
SWH 5411.255 Hz
FIDRES 1.321107 Hz
AQ 0.3784704 sec
RG 575
DW 92.400 usec
DE 6.50 usec
TE 298.2 K
D0 0.00008170 sec
D1 3.00000000 sec
D8 0.60000002 sec
D16 0.00020000 sec
INO 0.00018480 sec

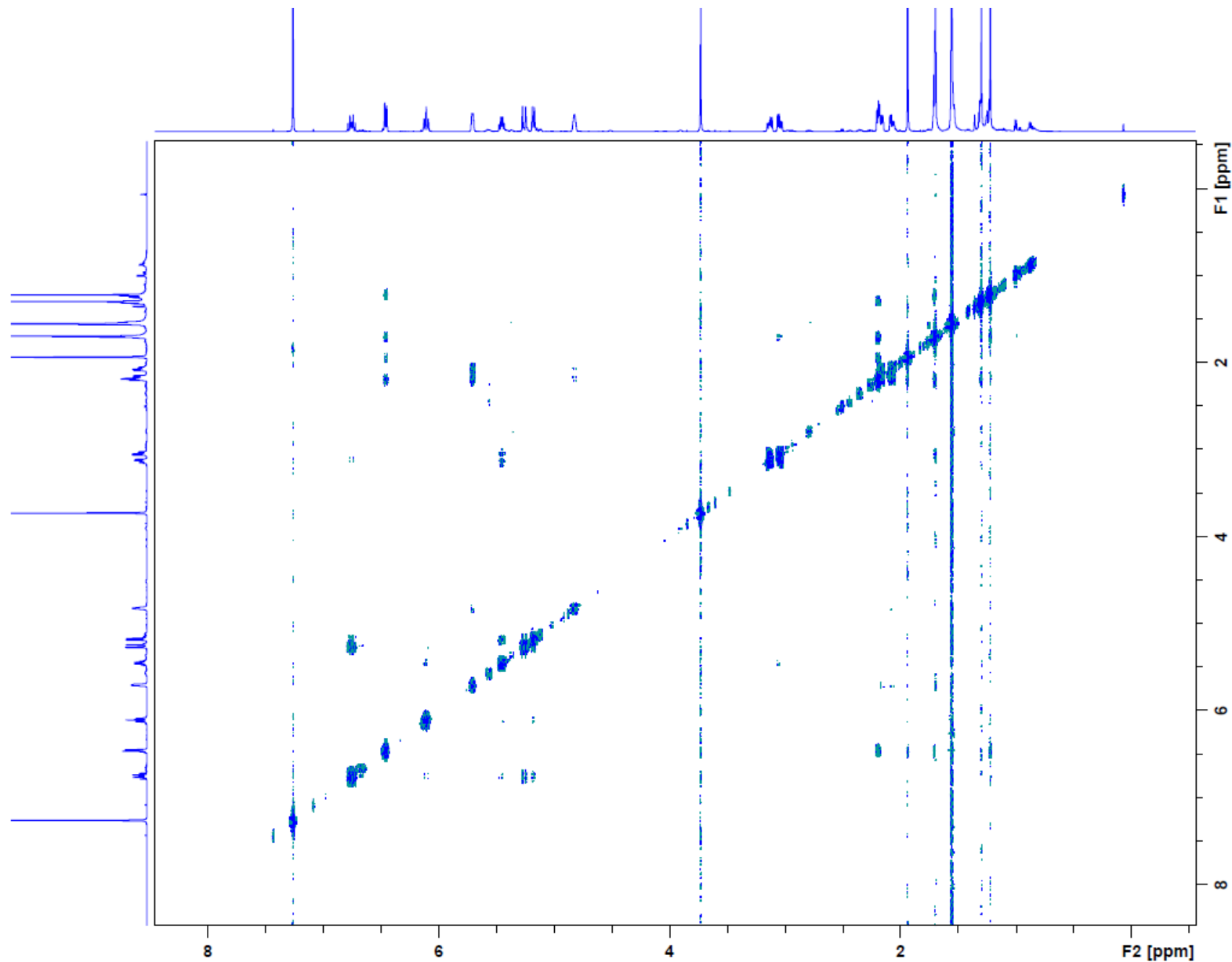
----- CHANNEL f1 -----
SFO1 600.1323960 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
PLW1 12.55000019 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

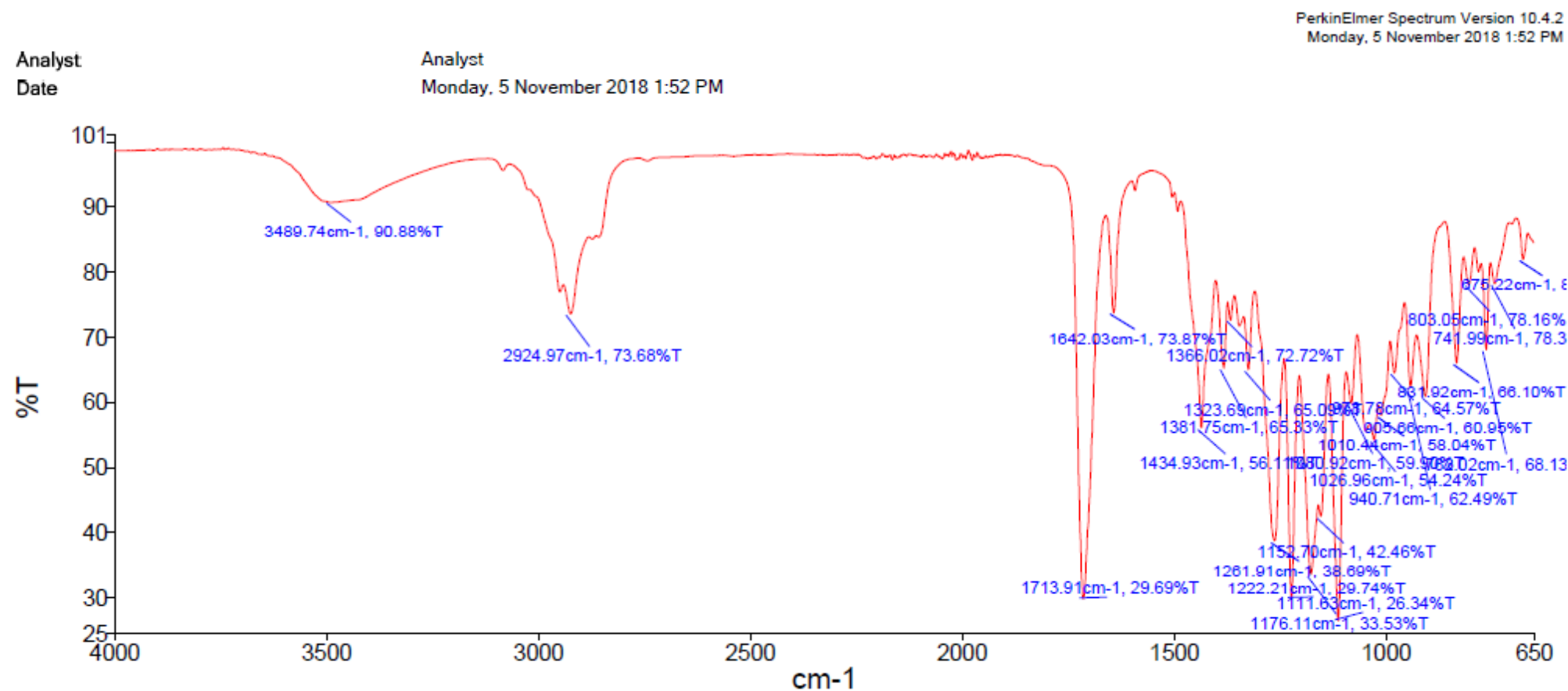
F1 - Acquisition parameters
TD 384
SFO1 600.1324 MHz
FIDRES 14.091811 Hz
SW 9.017 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 4096
SF 600.1300256 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

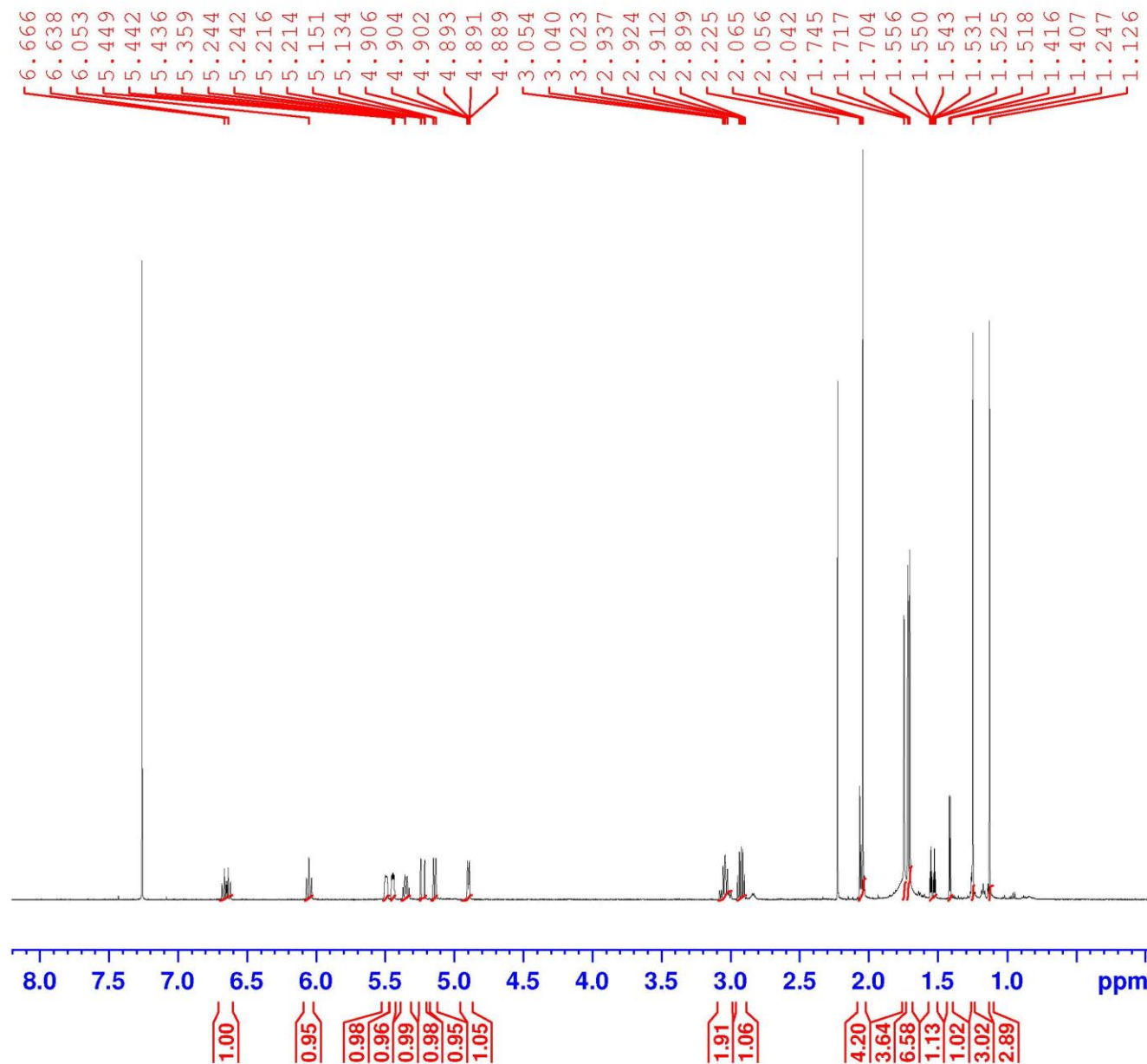
F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300184 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0



51b IR Spectrum



4'R-52a NMR Characterisation

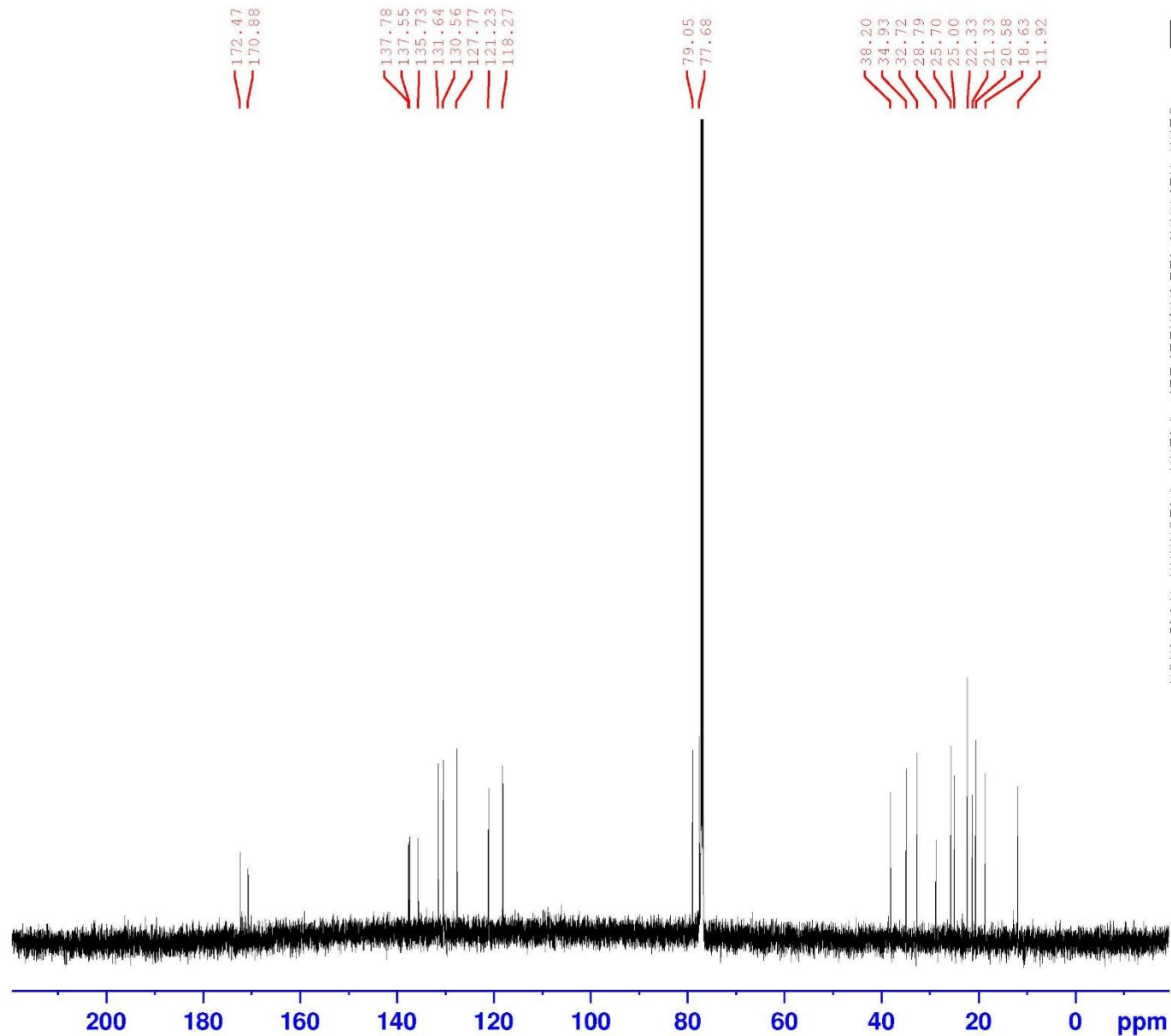


Current Data Parameters
 NAME 20190218 Pyrethrin I Acetate MAJOR
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190218
 Time_ 18.32
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 322
 DW 41.600 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 600.1337061 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300256 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20190218 Pyrethrin I Acetate MAJOR
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190218
Time 21.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CEDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9027902 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20190218 Pyrethrin I Acetate MAJOR
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190218
Time 18.54
INSTRUM spect
PROBHD 5 mm PARBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 4587.156 Hz
FIDRES 2.239822 Hz
AQ 0.2232320 sec
RG 161
DW 109.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.90456295 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00021800 sec

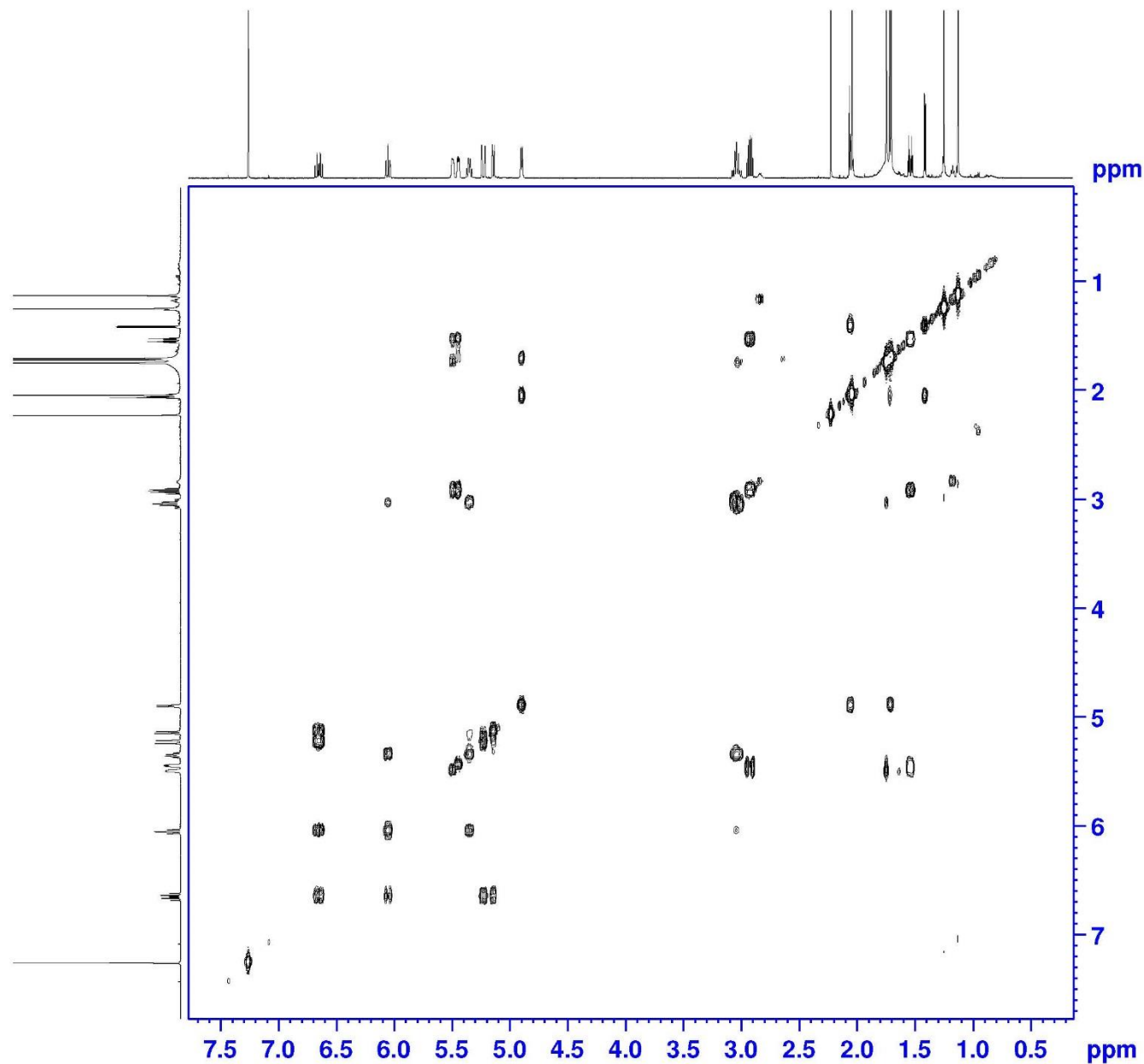
===== CHANNEL f1 =====
SFO1 600.1323992 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

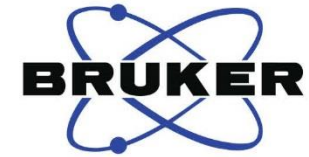
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GP21 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1324 MHz
FIDRES 35.837154 Hz
SW 7.644 ppm
F1MODE QF

F2 - Processing parameters
SI 1024
SF 600.1300252 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300274 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190218 Pyrethrin I Acetate MAJOR
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters

Date_ 20190218
Time 21.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
DS 16
SWH 4672.897 Hz
FIDRES 4.563376 Hz
AQ 0.1095680 sec
RG 2050
DW 107.000 usec
DE 6.50 usec
TE 298.3 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45596802 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS

===== CHANNEL f1 =====
SFO1 600.1324365 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

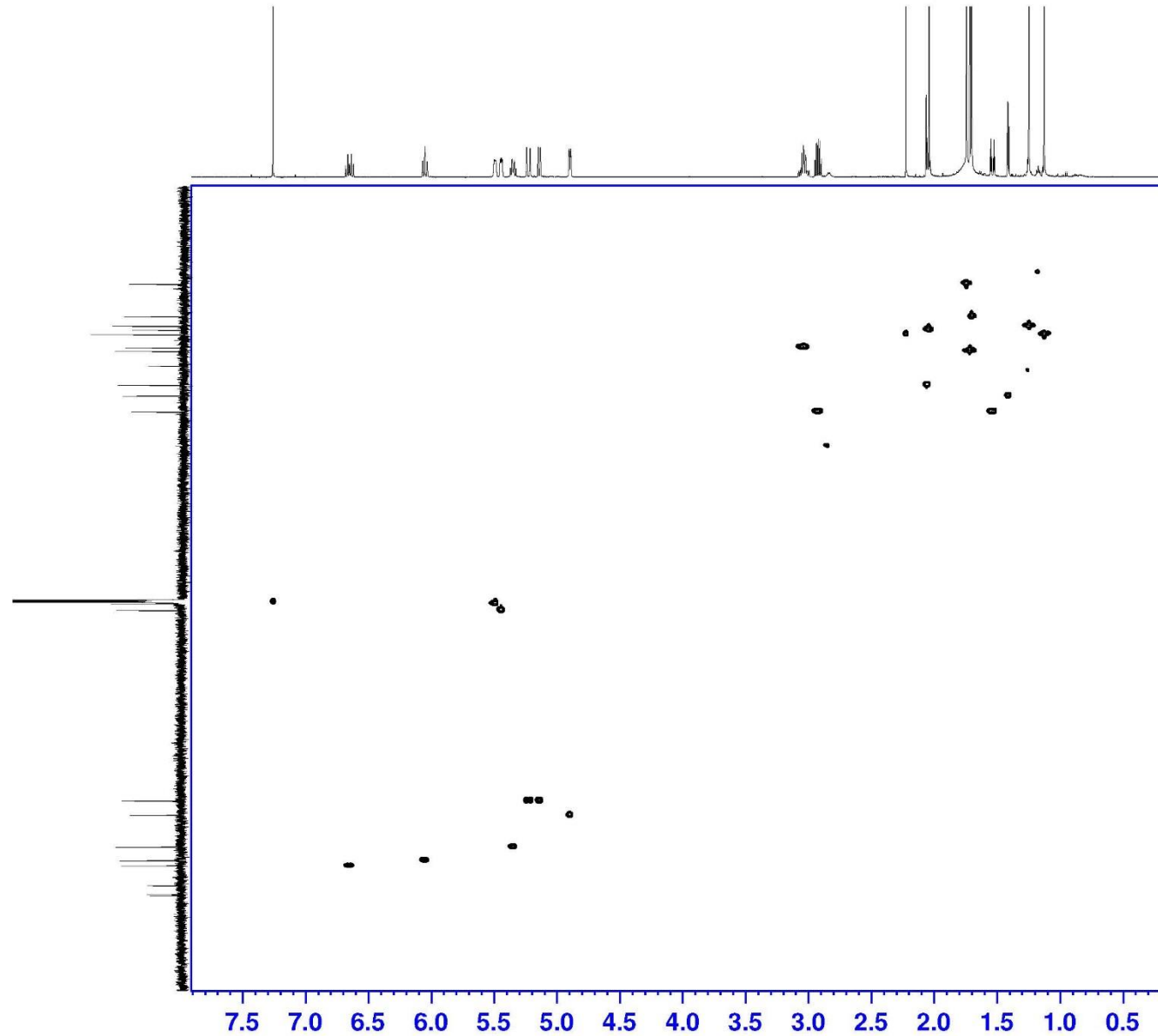
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CDDPRG[2] garrp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 80.00000000 W
PLW12 3.20000005 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

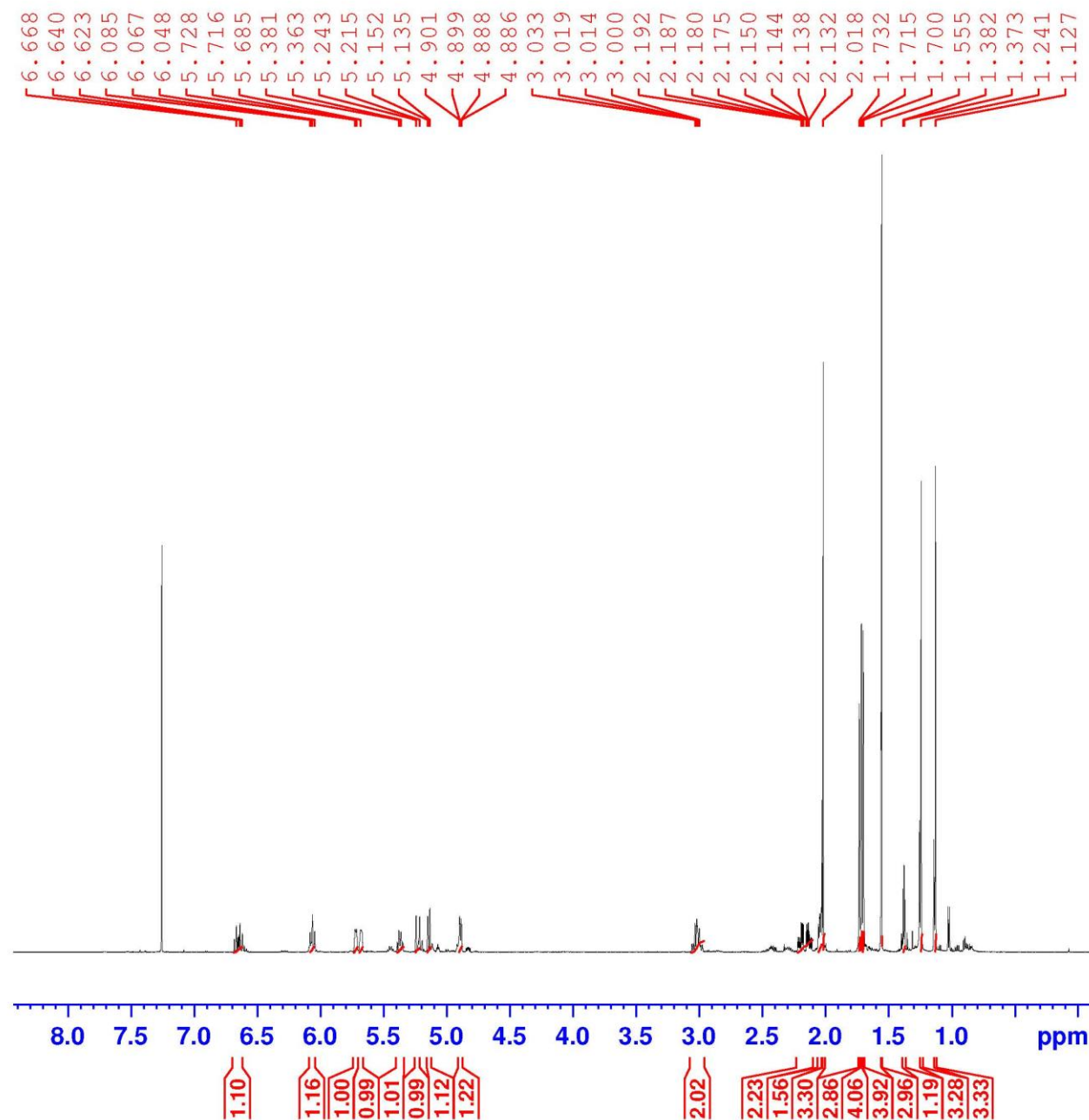
F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300252 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028159 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



4'S-52a NMR Characterisation

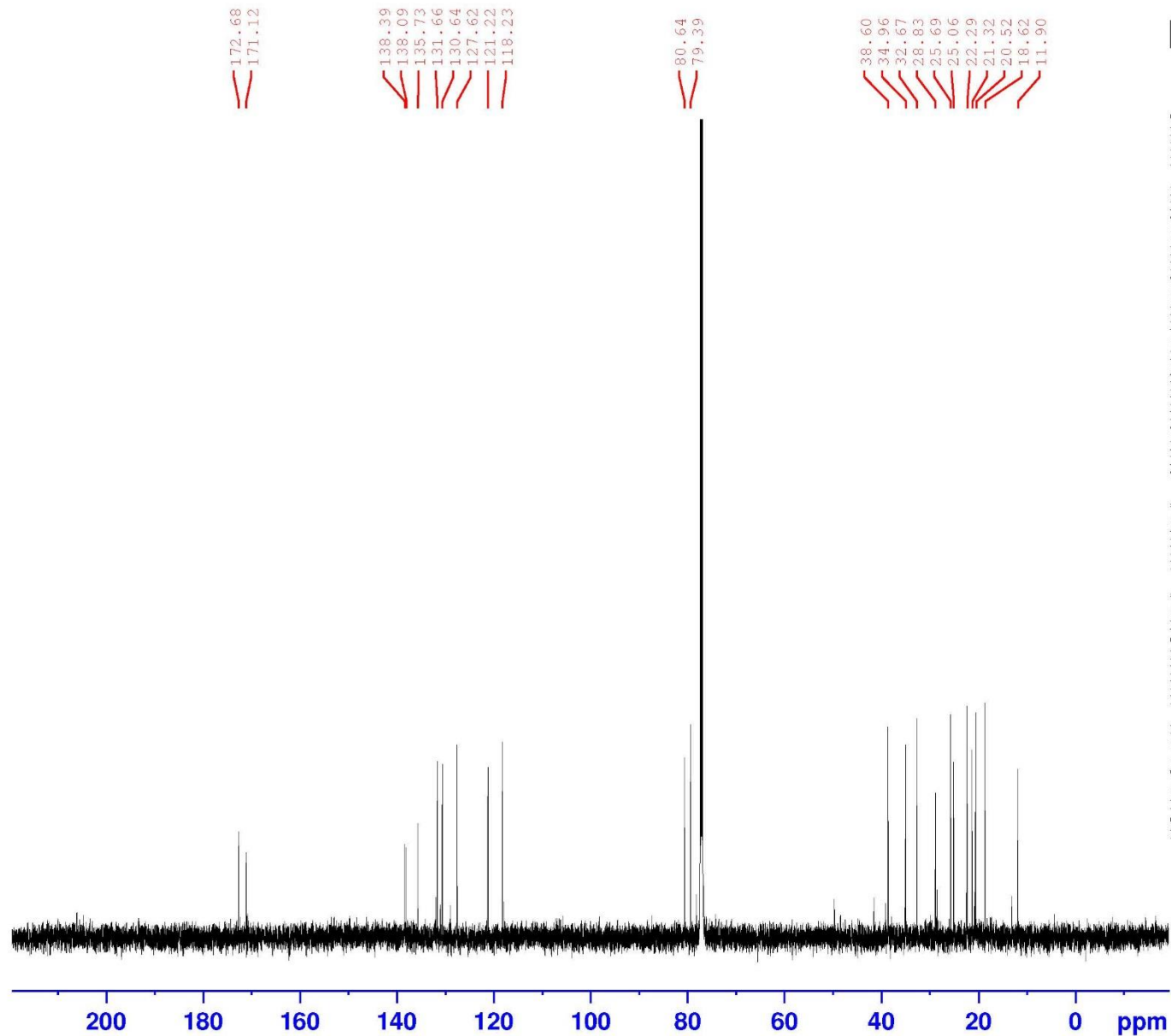


Current Data Parameters
 NAME 20190225 PI Acetate Minor
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190225
 Time 18.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 256
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 600.1337061 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300258 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20190225 PI Acetate Minor
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190225
Time 21.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SF01 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.0000000 W

===== CHANNEL f2 =====
SF02 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.0000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9027908 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20190225 PI Acetate Minor
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190225
Time 18.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 4587.156 Hz
FIDRES 2.239822 Hz
AQ 0.2232320 sec
RG 144
DW 109.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.90456295 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00021800 sec

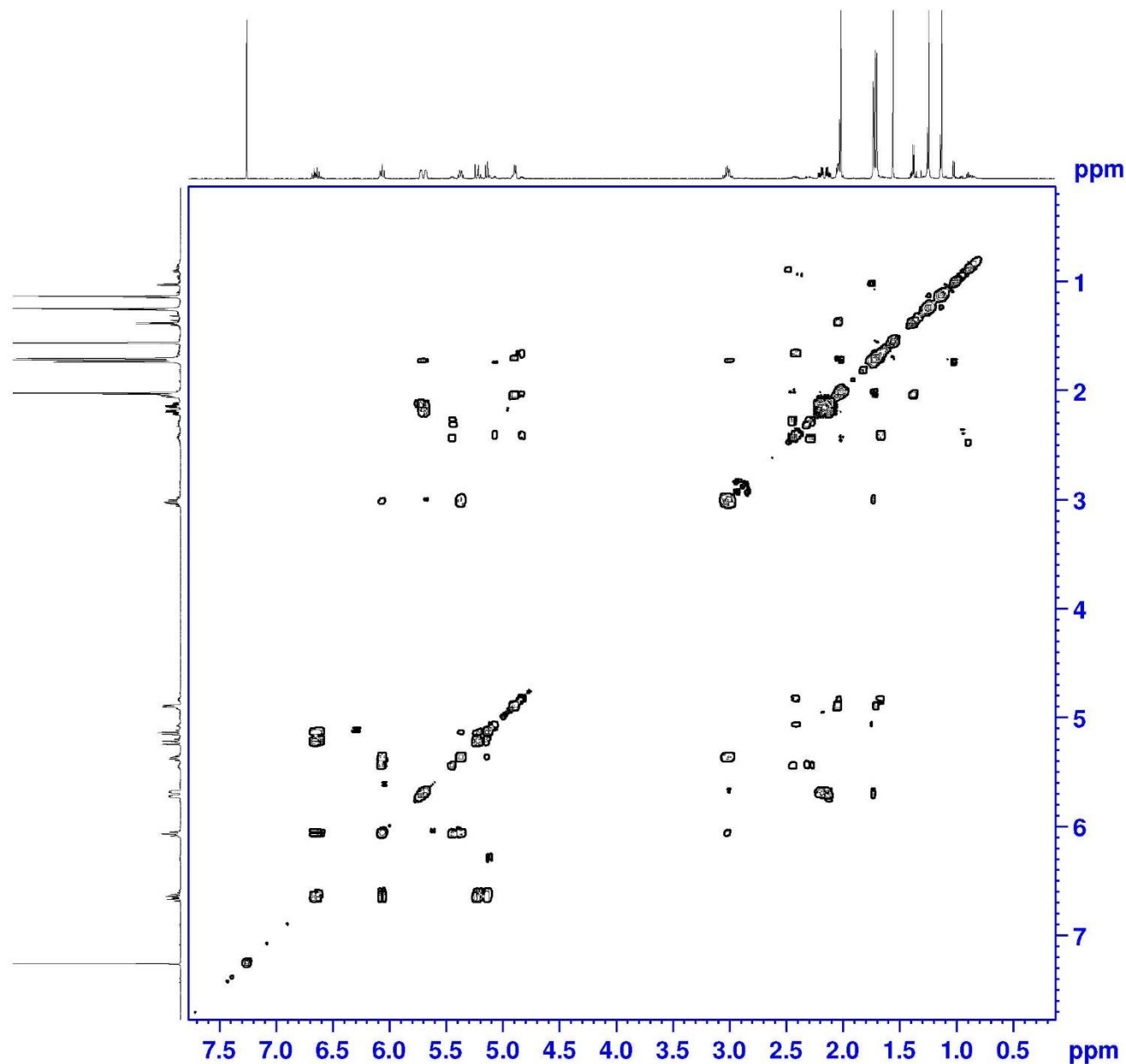
===== CHANNEL f1 =====
SFO1 600.1323978 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1324 MHz
FIDRES 35.837154 Hz
SW 7.644 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300256 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

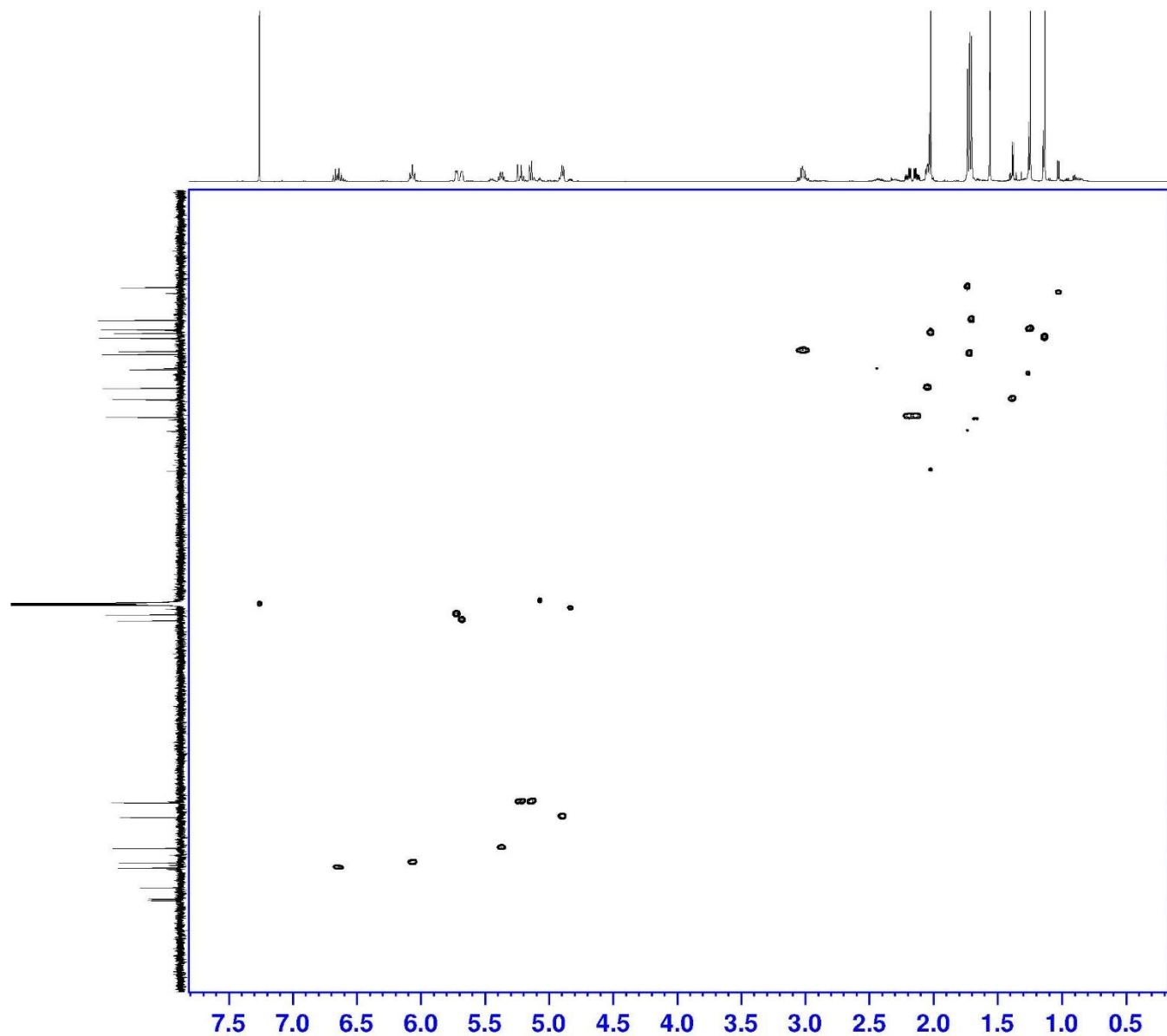
F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300261 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0



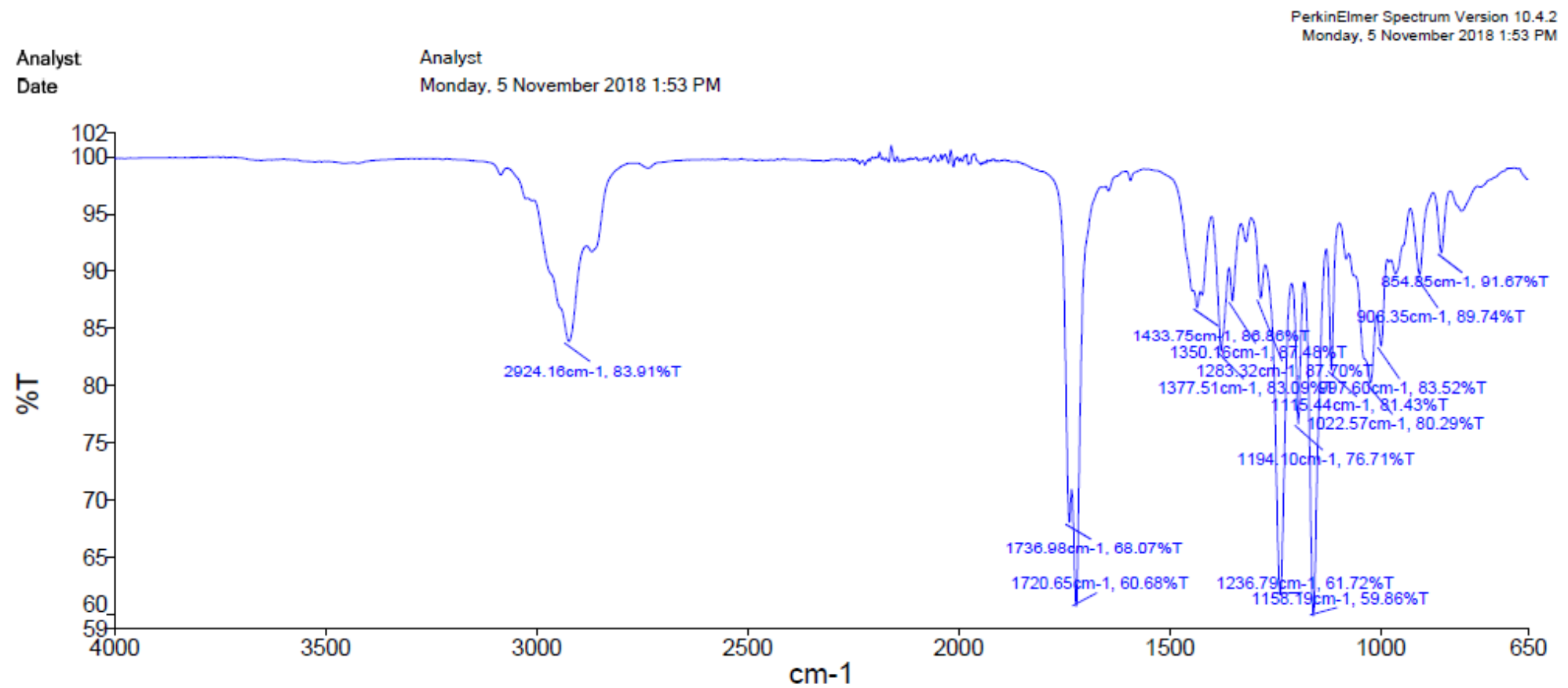


Current Data Parameters
NAME 20190225 PI Acetate Minor
EXPNO 24
PROCNO 1

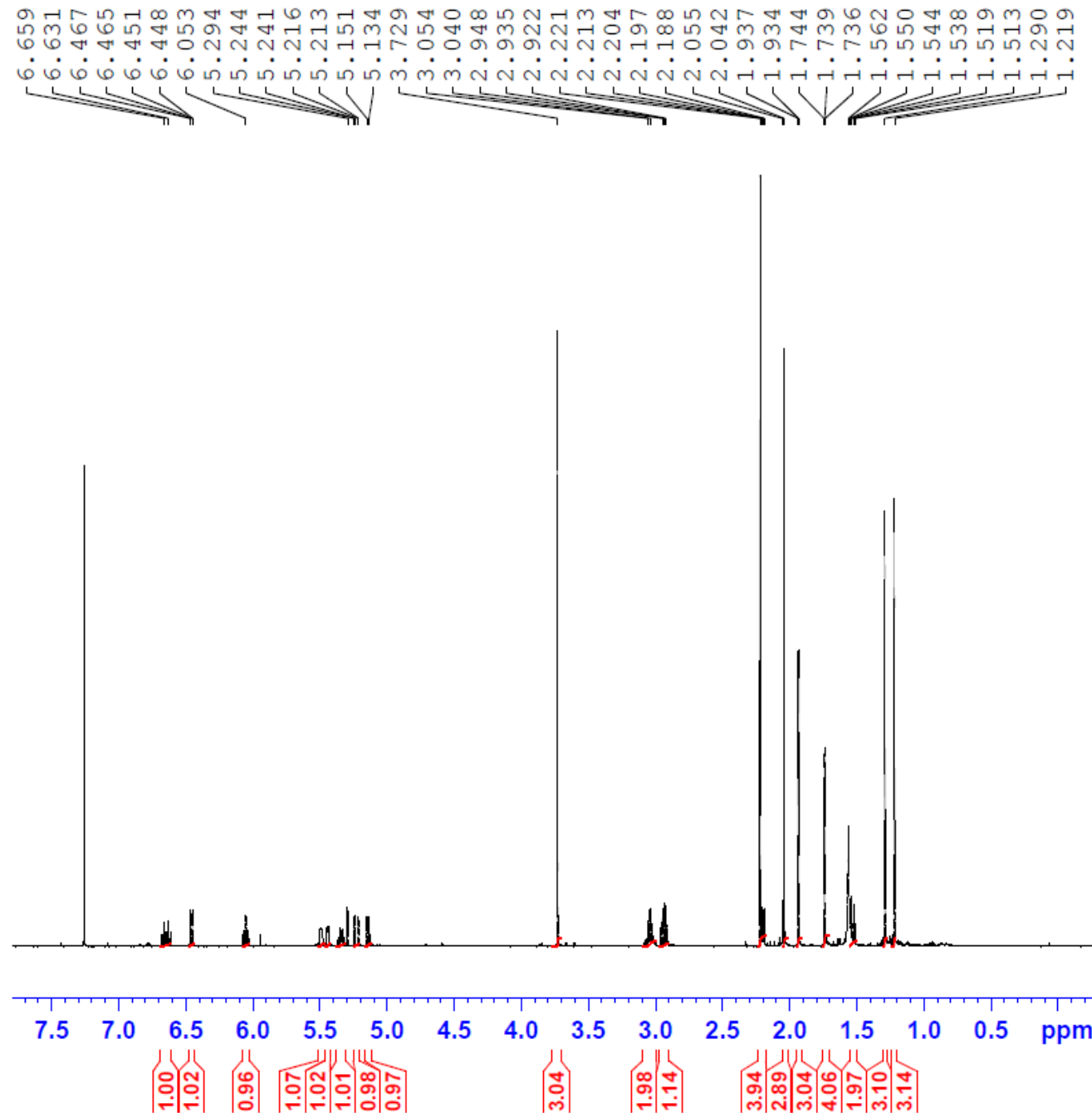
F2 - Acquisition Parameters
Date_ 20190225
Time 21.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcstgpp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 4587.156 Hz
FIDRES 4.479644 Hz
AQ 0.1116160 sec
RG 2050
DW 109.000 usec
DE 6.50 usec
TE 298.3 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45392001 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS
===== CHANNEL f1 =====
SFO1 600.1324175 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CDDPRG[2] garrp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 80.00000000 W
PLW12 3.20000005 W
===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
PL6 1000.00 usec
F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FMODE Echo-Antiecho
F2 - Processing parameters
SI 1024
SF 600.1300234 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40
F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9026227 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



52a IR Spectrum



4'R-52b NMR Characterisation

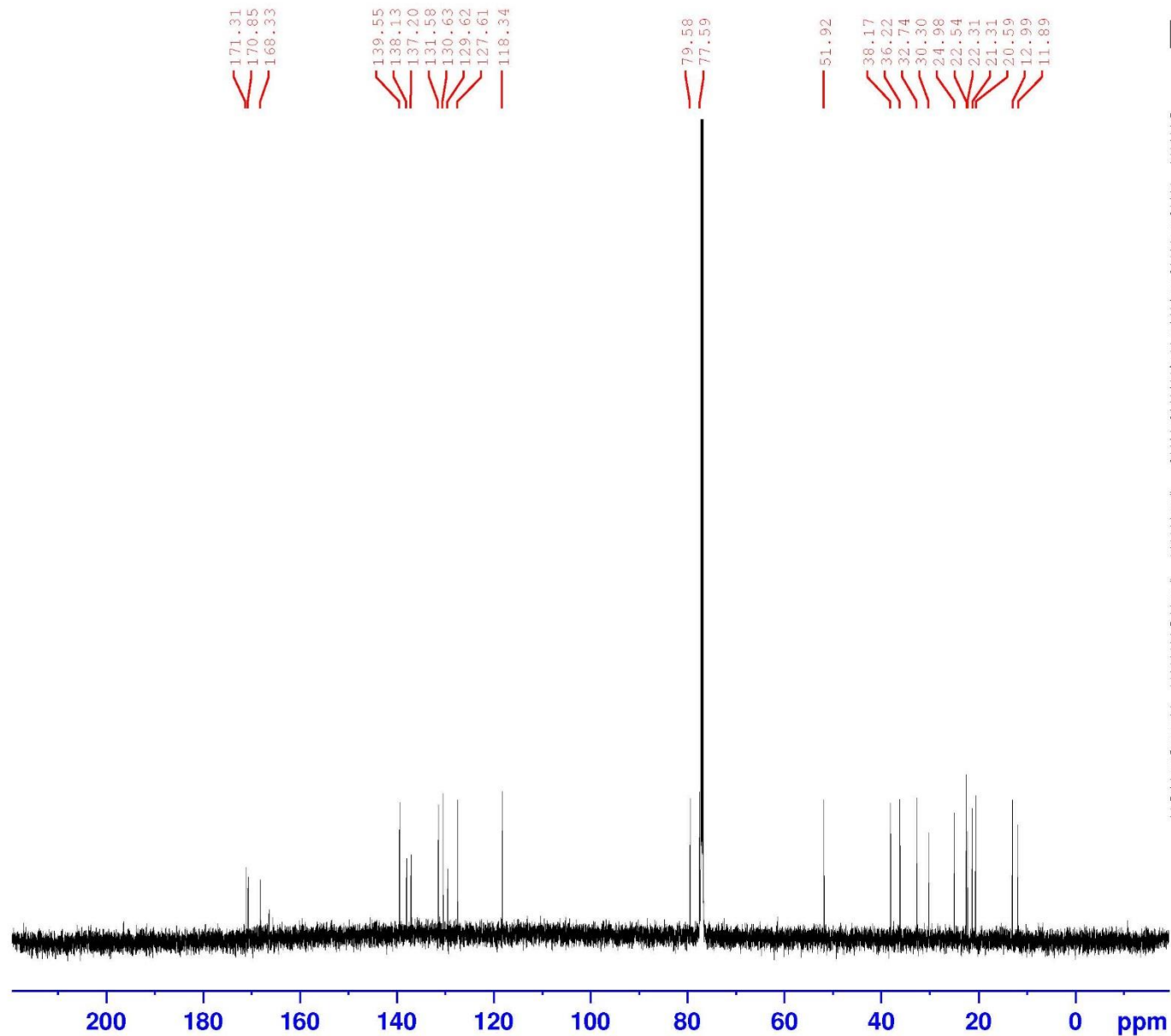


Current Data Parameters
 NAME 20190220 F11 Acetate MAJOR
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190220
 Time_ 17.35
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 322
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 600.1337061 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300283 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20190220 PII Acetate MAJOR
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190220
Time 20.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9027925 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20190220 PII Acetate MAJOR
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190220
Time 17.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 4237.288 Hz
FIDRES 2.068988 Hz
AQ 0.2416640 sec
RG 161
DW 118.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.88613105 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00023600 sec

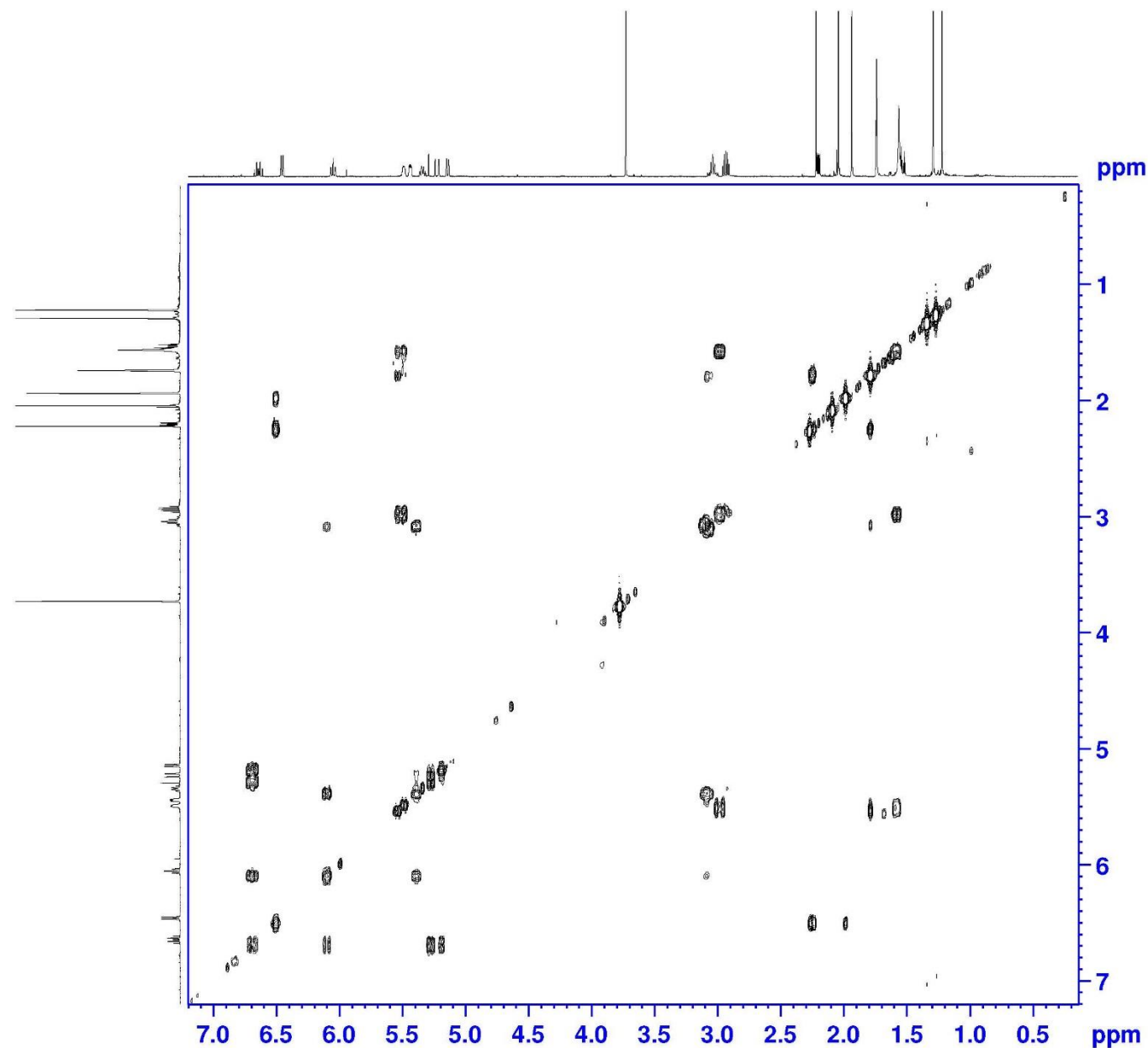
===== CHANNEL f1 =====
SFO1 600.1322008 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

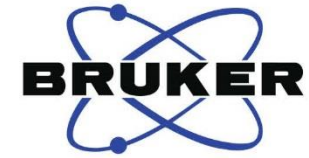
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1322 MHz
FIDRES 33.103813 Hz
SW 7.061 ppm
F1MODE QF

F2 - Processing parameters
SI 1024
SF 600.1299971 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1299966 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190220 F11 Acetate MAJOR
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190220
Time 20.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
DS 16
SWH 4201.681 Hz
FIDRES 4.103204 Hz
AQ 0.1218560 sec
RG 2050
DW 119.000 usec
DE 6.50 usec
TE 298.3 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.44368005 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS

===== CHANNEL f1 =====
SFO1 600.1322258 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

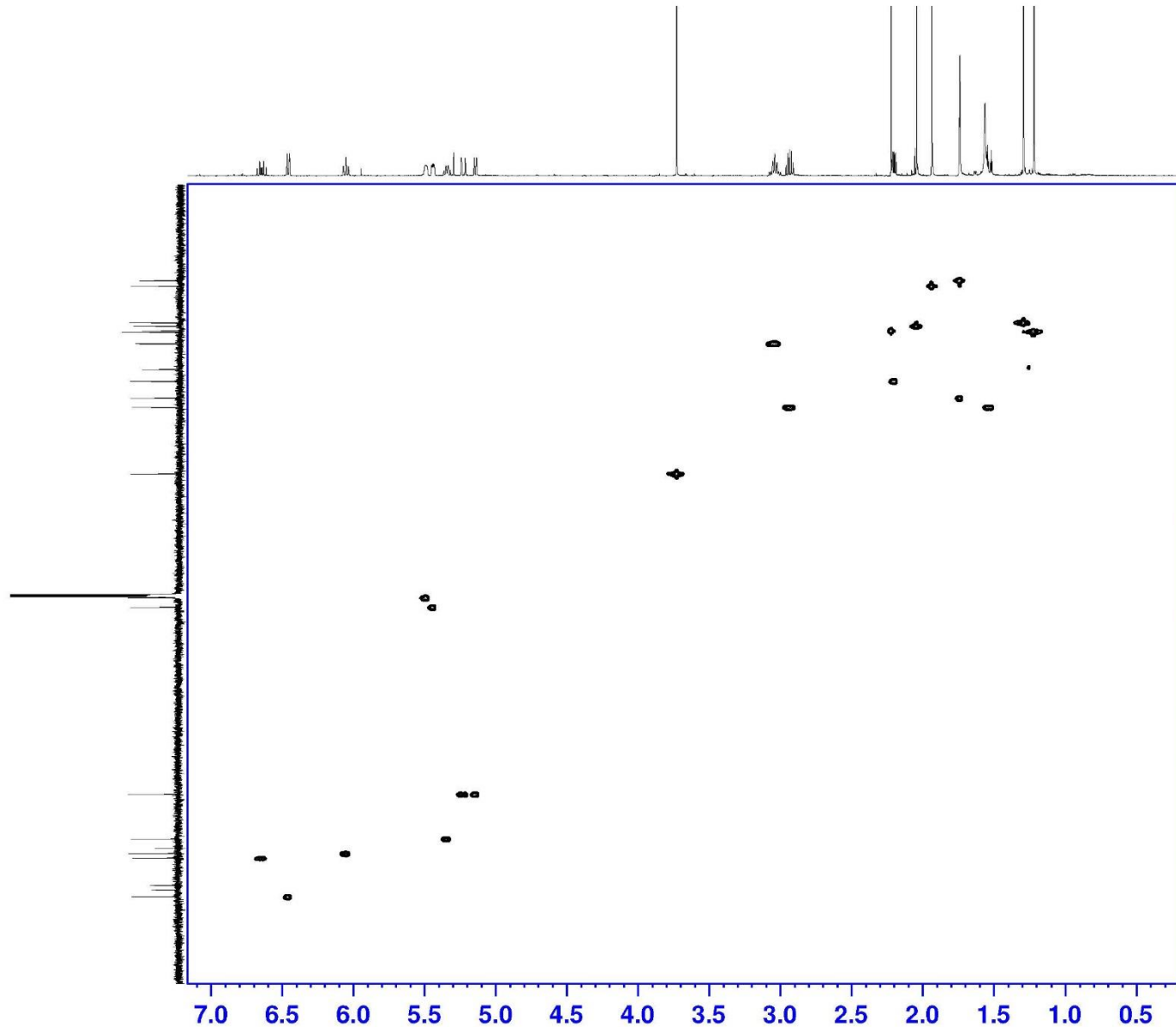
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CDDPRG[2] garrp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 80.00000000 W
PLW12 3.20000005 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

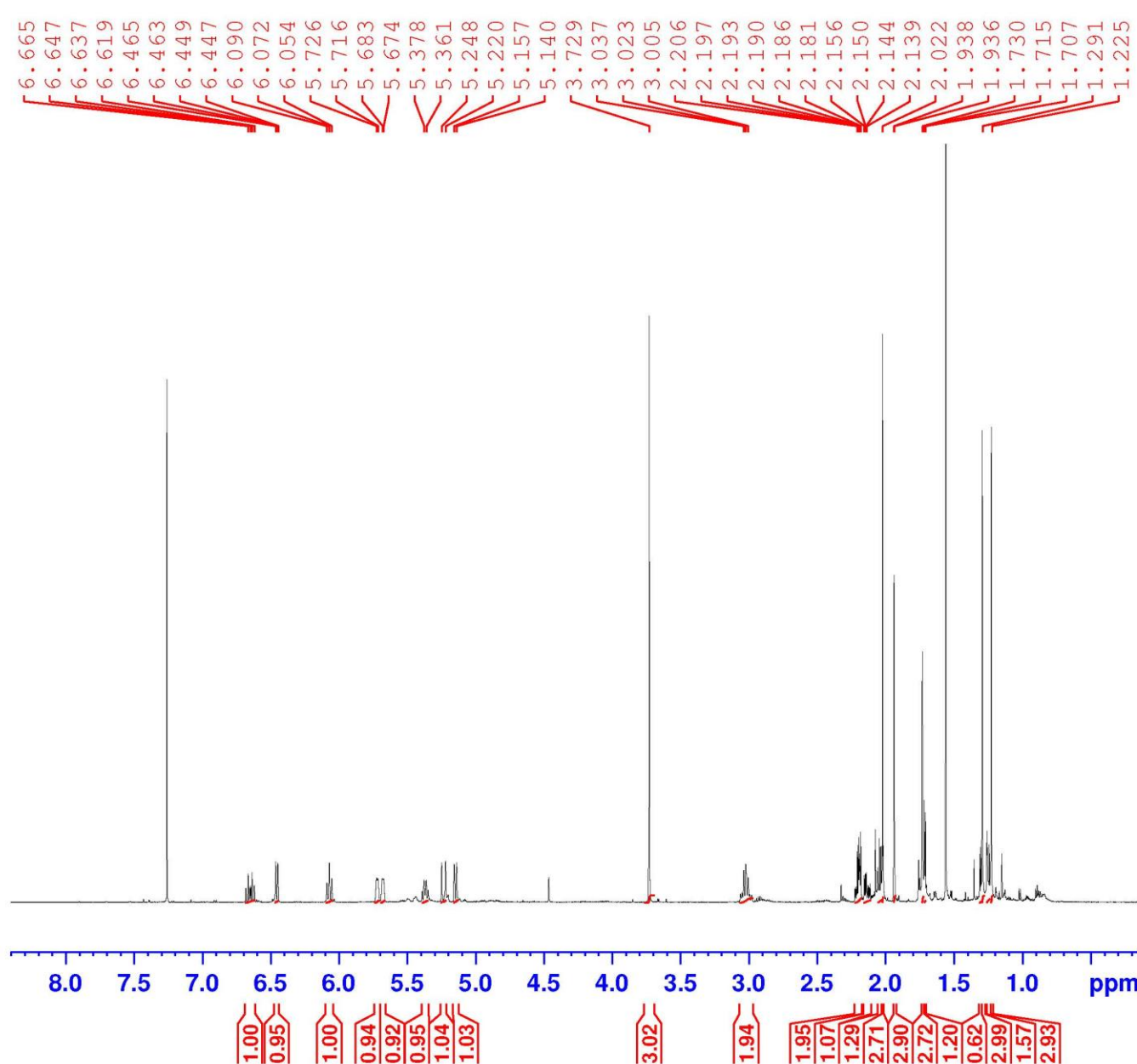
F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300260 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9027807 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



4'S-52b NMR Characterisation

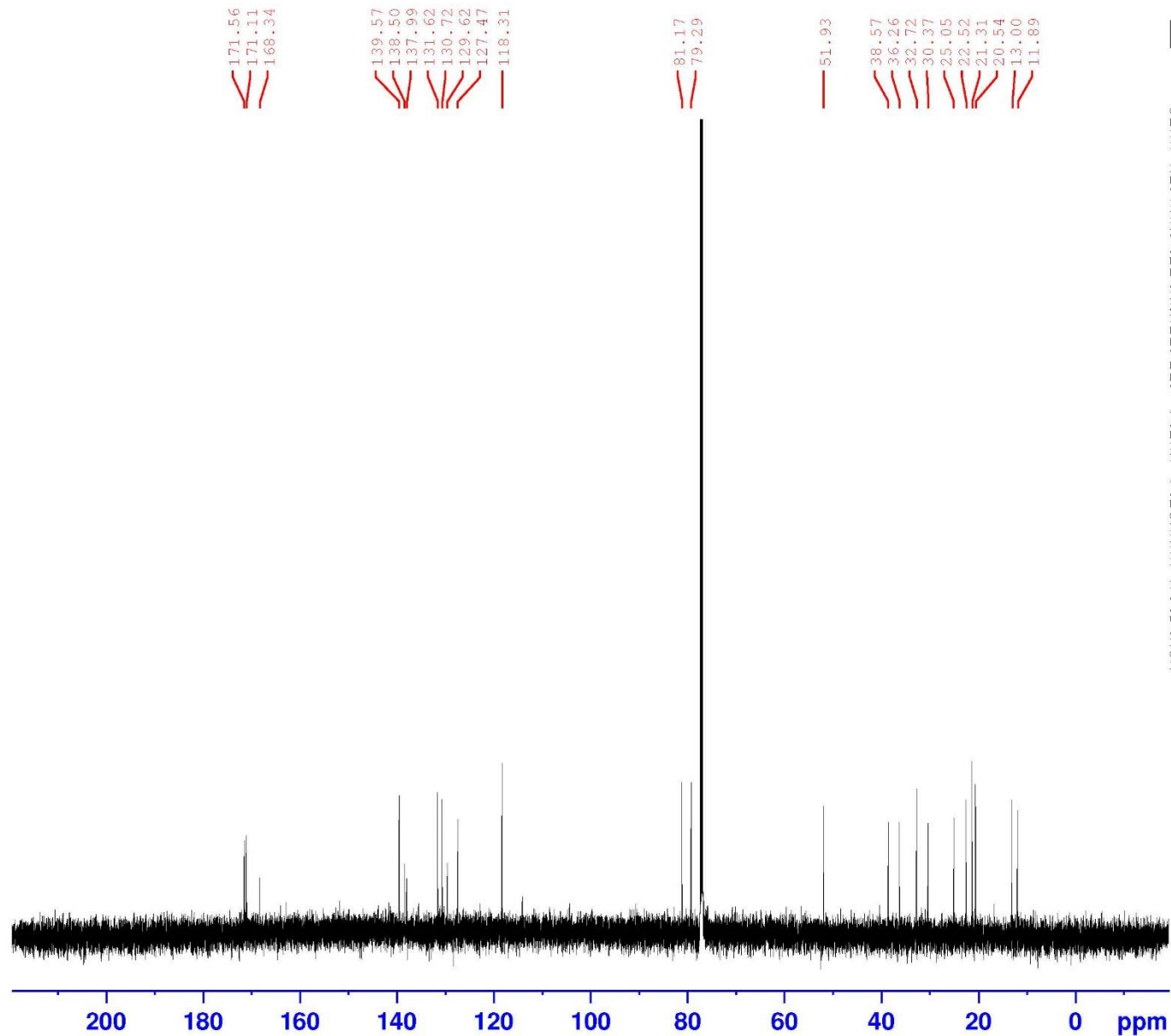


Current Data Parameters
NAME 20190226 Pyrethrin II Acetate Minor
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190226
Time 17.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 287
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337061 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300261 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 20190226 Pyrethrin II Acetate Minor
 EXPNO 22
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190226
 Time 21.20
 INSTRUM spect
 PROBRD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 3096
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9027906 MHz
 WDW no
 SSB 0
 LE 0 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20190226 Pyrethrin II Acetate Minor
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190226
Time 17:59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 4629.629 Hz
FIDRES 2.260561 Hz
AQ 0.2211840 sec
RG 144
FW 108.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.90661097 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00021600 sec

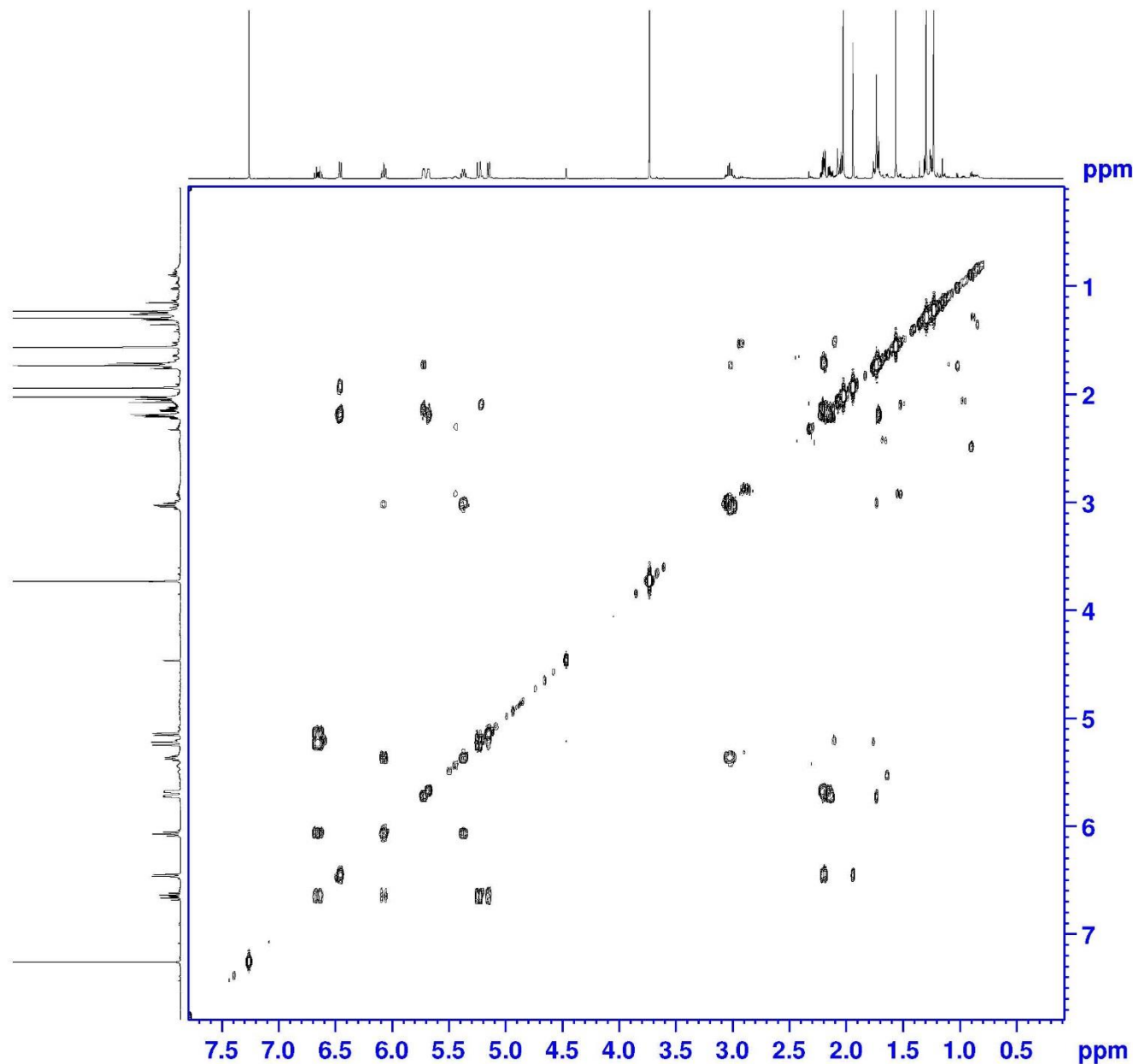
===== CHANNEL f1 =====
SFO1 600.1323879 MHz
NUC1 1H
FO 13.50 usec
PI 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GP21 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1324 MHz
FIDRES 36.168980 Hz
SW 7.714 ppm
PnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300249 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300256 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190226 Pyrethrin II Acetate Minor
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters

Date_ 20190226
Time 21.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 4629.629 Hz
FIDRES 4.521122 Hz
AQ 0.1105920 sec
RG 2050
RW 108.000 usec
DE 6.50 usec
TE 298.3 K
CNS12 145.0000000
D0 0.0000300 sec
D1 1.45494401 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGFTNS

===== CHANNEL f1 =====
SFO1 600.1323855 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

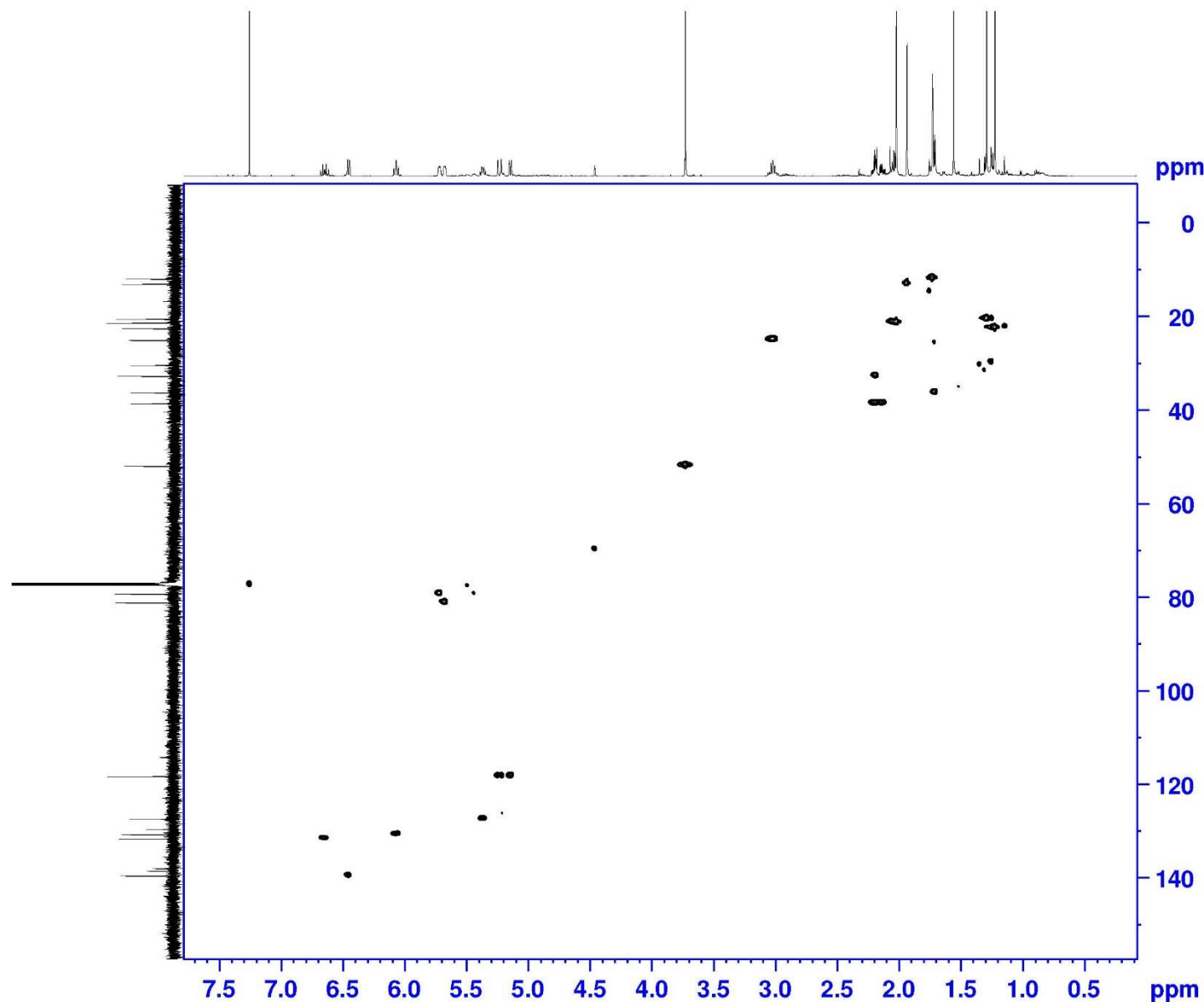
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 80.00000000 W
PLW12 3.20000005 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GEF1 80.00 %
GEF2 20.10 %
PL6 1000.00 usec

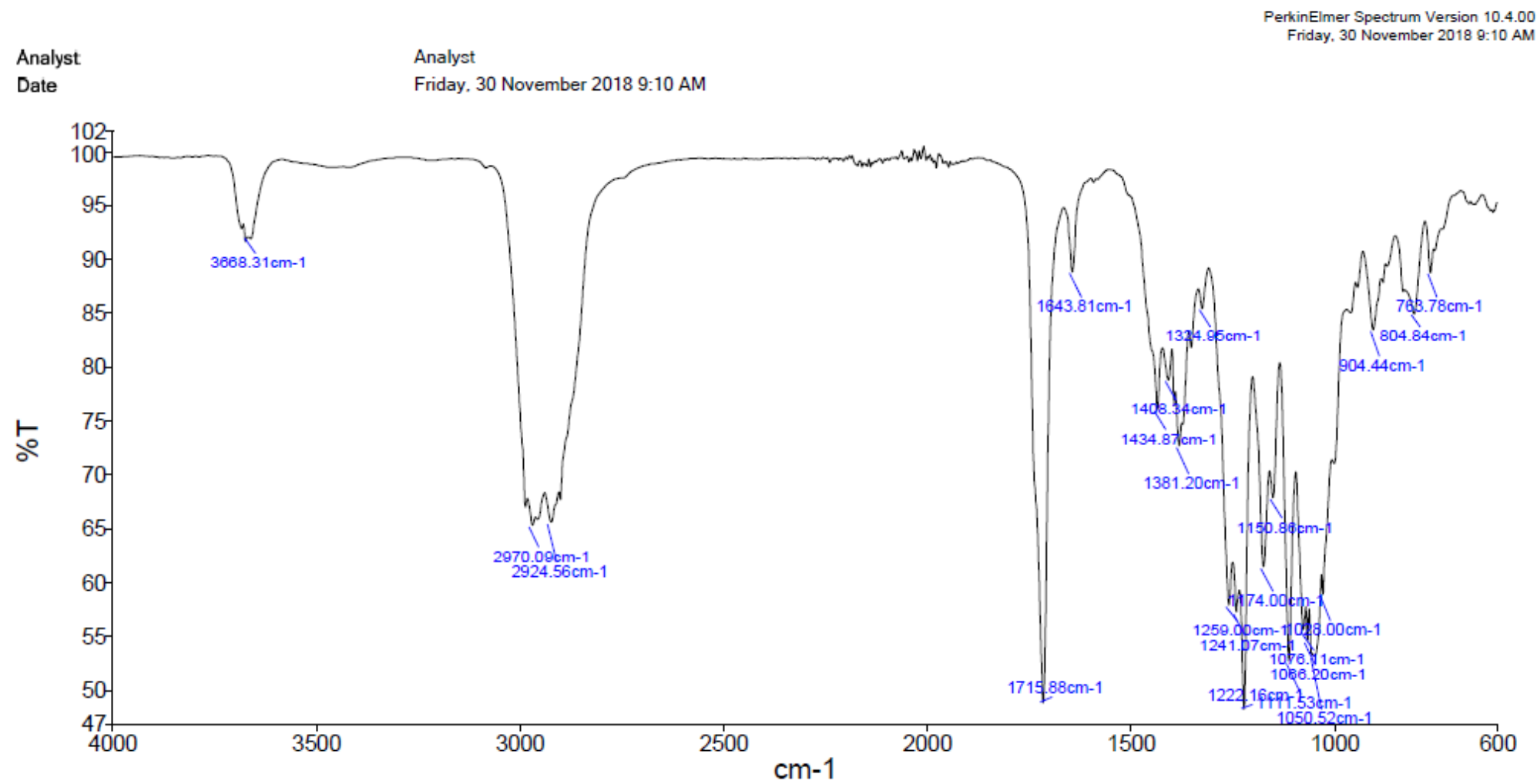
F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300250 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

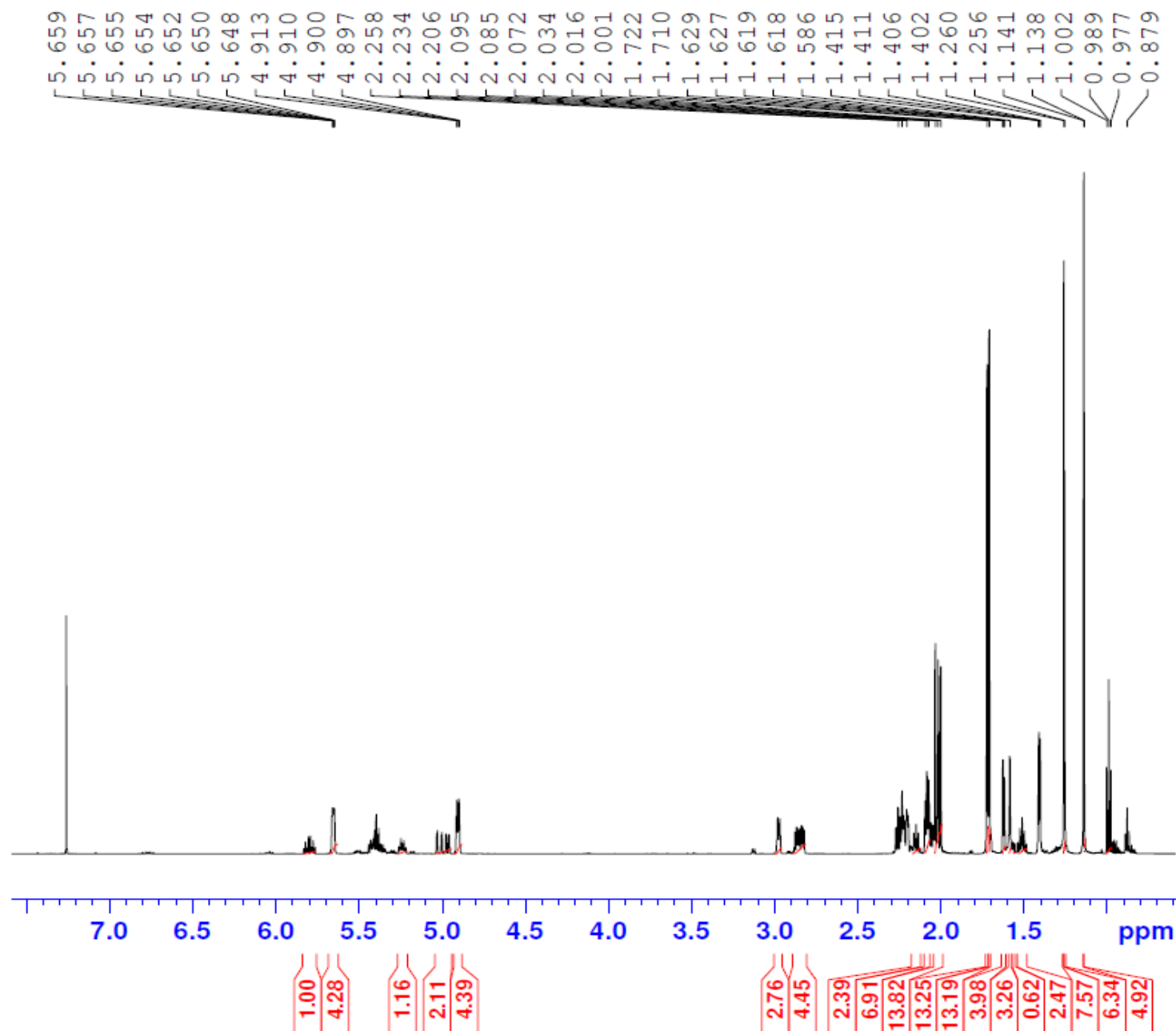
F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028175 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



52b IR Spectrum



Representative ^1H NMR showing dihydropyrethrin 55



Current Data Parameters
NAME 20180614 Hydrogenation Pyrethrin I
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180614
Time 10.25
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 114
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 8.40 usec
PLW1 12.55000019 W

F2 - Processing parameters
SI 65536
SF 600.1300249 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

53a NMR Characterisation

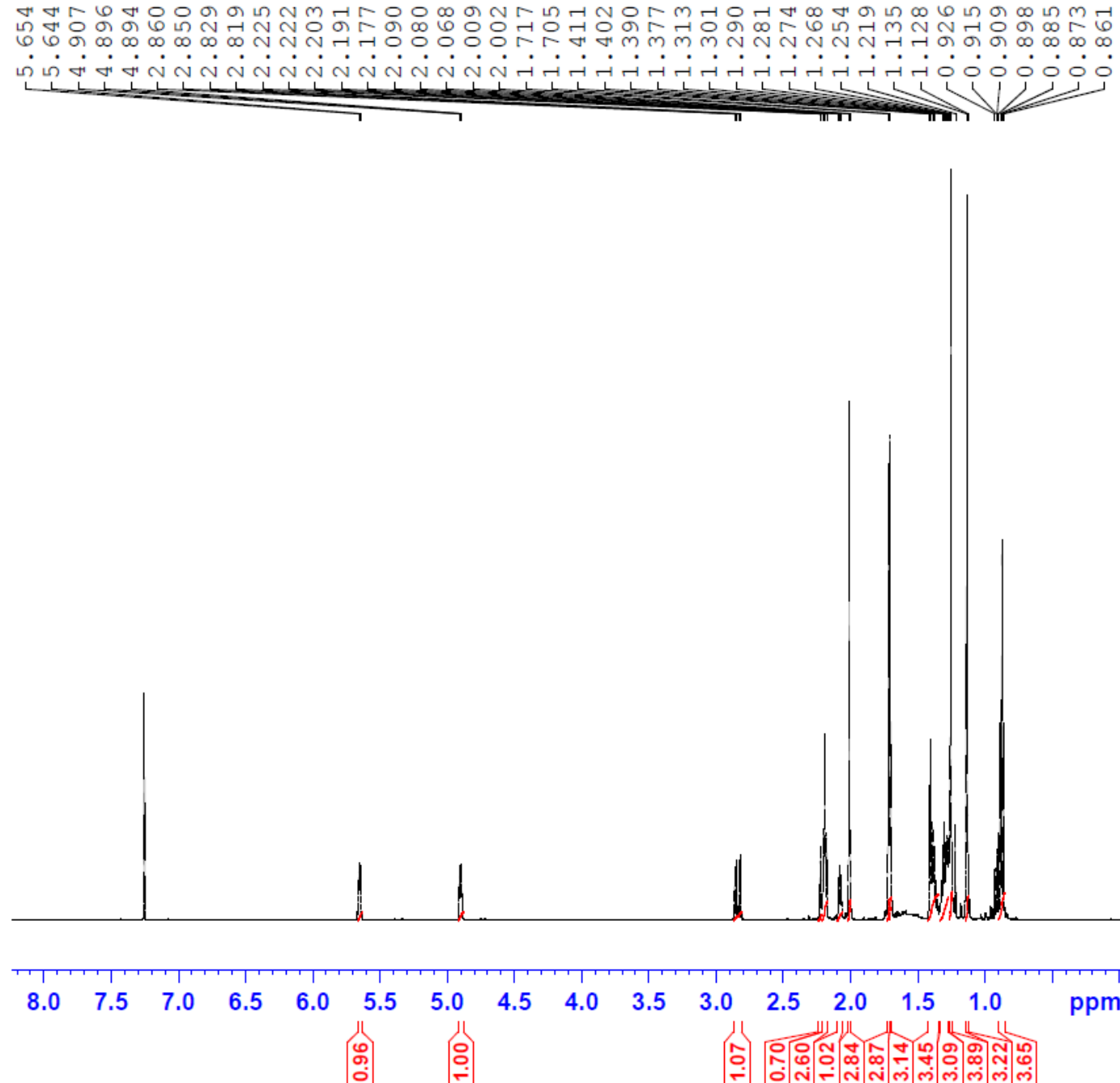


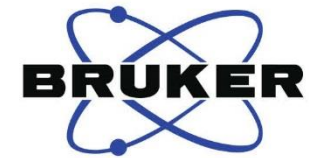
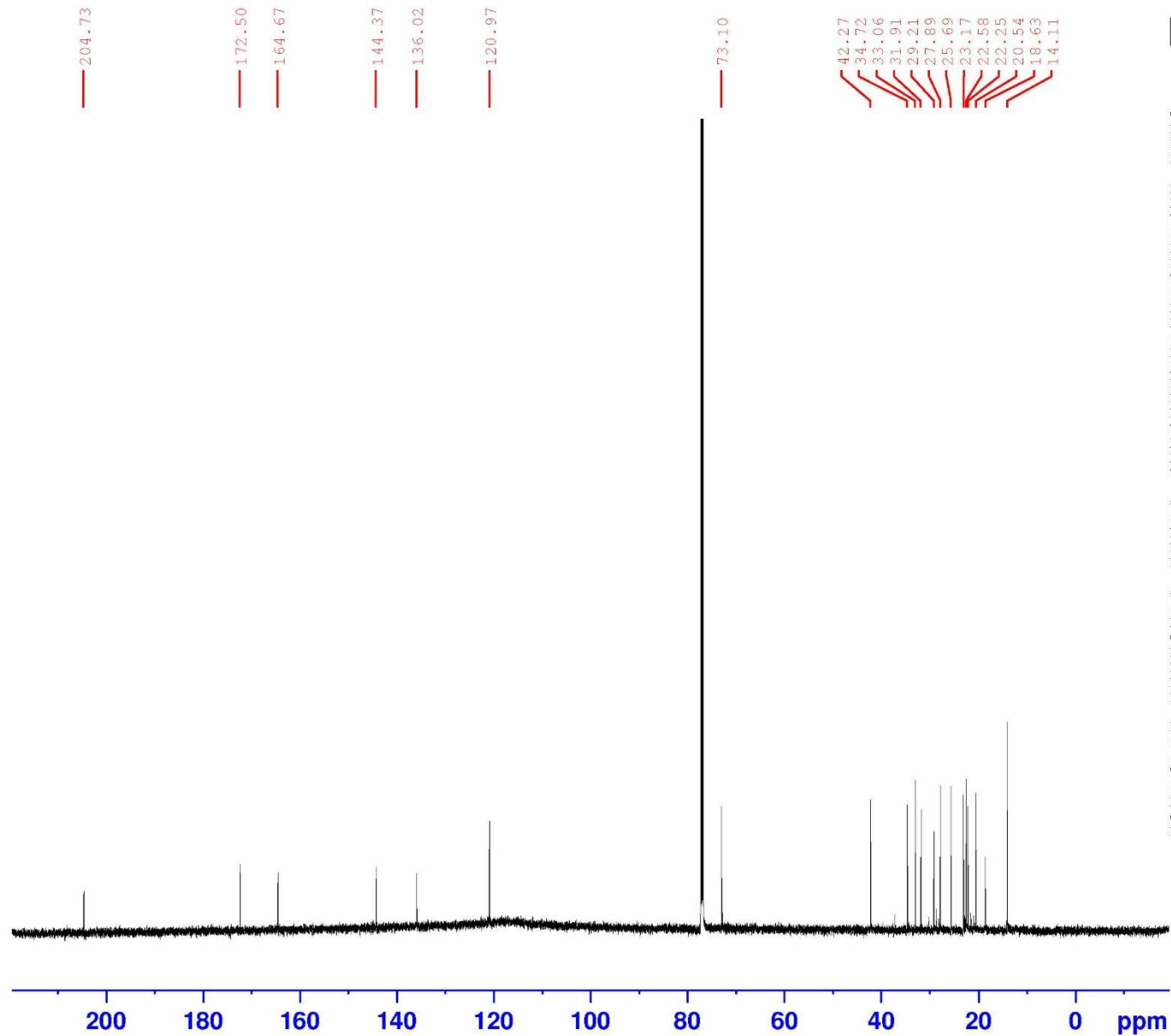
Current Data Parameters
 NAME 20180904 Hydrogenation PI
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180904
 Time_ 18.28
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 161
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 600.1337060 MHz
 NUC1 1H
 P1 8.40 usec
 PLW1 12.85000019 W

F2 - Processing parameters
 SI 65536
 SF 600.1300297 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
NAME 20180904 Hydrogenation PI
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180904
Time 20.13
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 1820
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 150.9178988 MHz
NUC1 13C
P1 16.00 usec
PLW1 110.76000214 W

===== CHANNEL f2 =====
SF02 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 12.55000019 W
PLW12 0.18072000 W
PLW13 0.08855400 W

F2 - Processing parameters
SI 32768
SF 150.9027920 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20180904 Hydrogenation PI
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180904
Time 20.20
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 3816.794 Hz
FIDRES 1.863669 Hz
AQ 0.2682880 sec
RG 2050
DW 131.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00012030 sec
D1 1.87015700 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00026200 sec

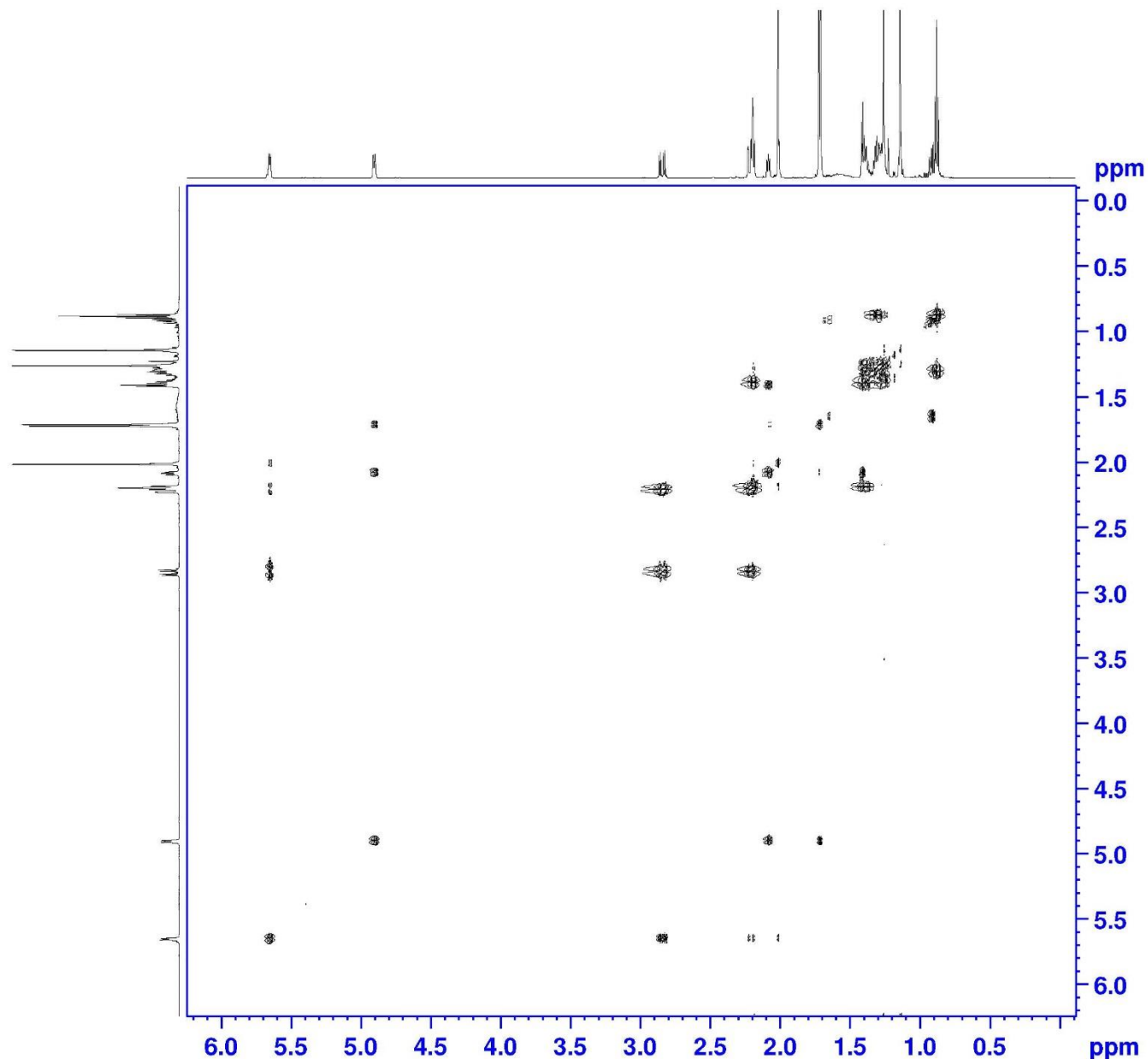
===== CHANNEL f1 =====
SF01 600.1318677 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P17 2500.00 usec
PLW1 12.55000019 W
PLW10 1.30999994 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.1319 MHz
FIDRES 14.909351 Hz
SW 6.360 ppm
EnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.1300271 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

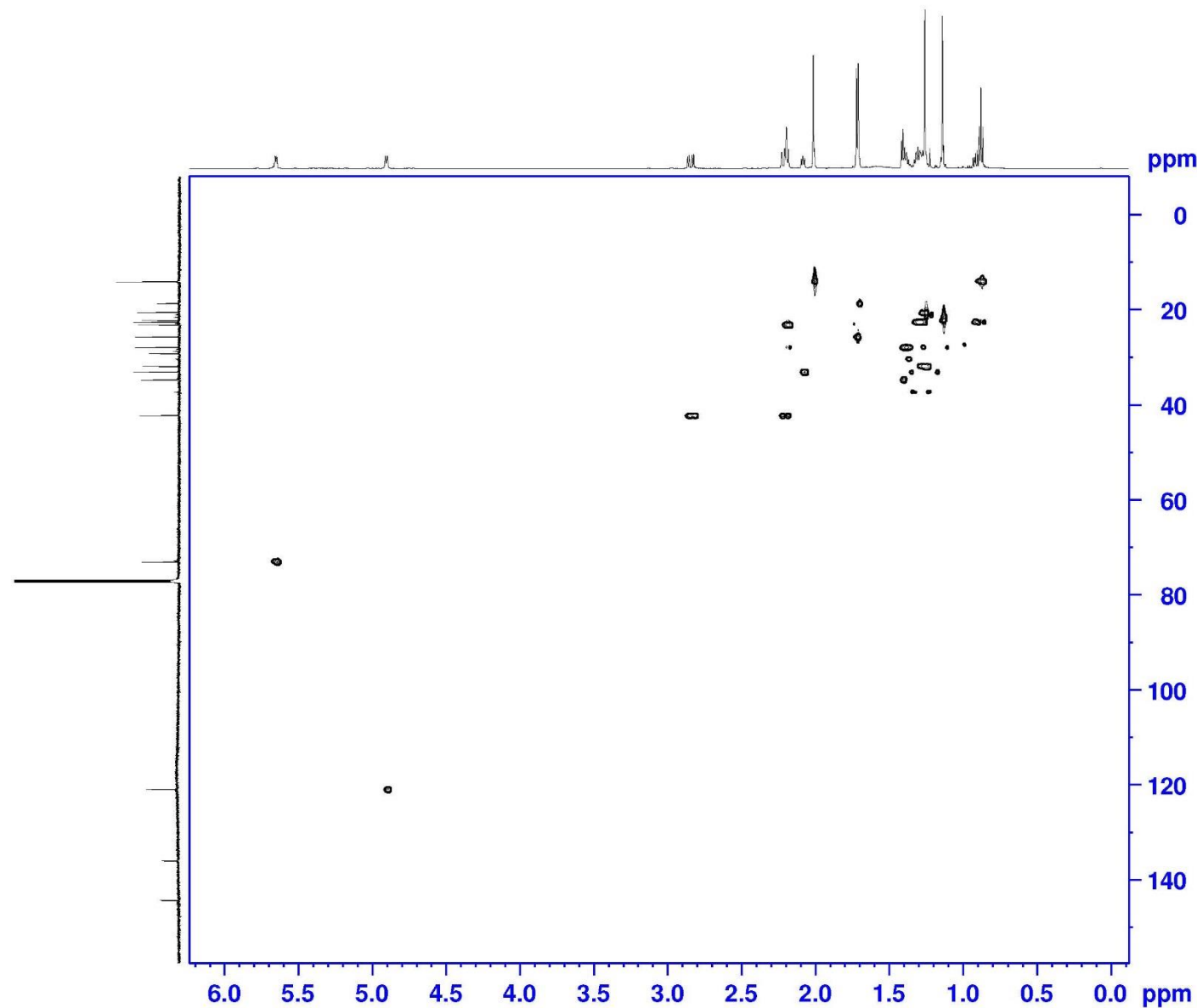
F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300277 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20180904 Hydrogenation PI
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180904
Time 21.10
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG hsqcztgp
TD 1024
SOLVENT CDCl3
DS 16
SWH 3816.794 Hz
FIDRES 3.727338 Hz
AQ 0.1341440 sec
RG 2050
DW 131.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.43139195 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS
===== CHANNEL f1 =====
SFO1 600.1318677 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P28 1000.00 usec
PLW1 12.55000019 W
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CDDPRG[2] garrp
P3 16.00 usec
P4 32.00 usec
PCPD2 60.00 usec
PLW2 110.76000214 W
PLW12 7.87610006 W
===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec
F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FMODE Echo-Antiecho
F2 - Processing parameters
SI 1024
SF 600.1300315 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40
F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9027851 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

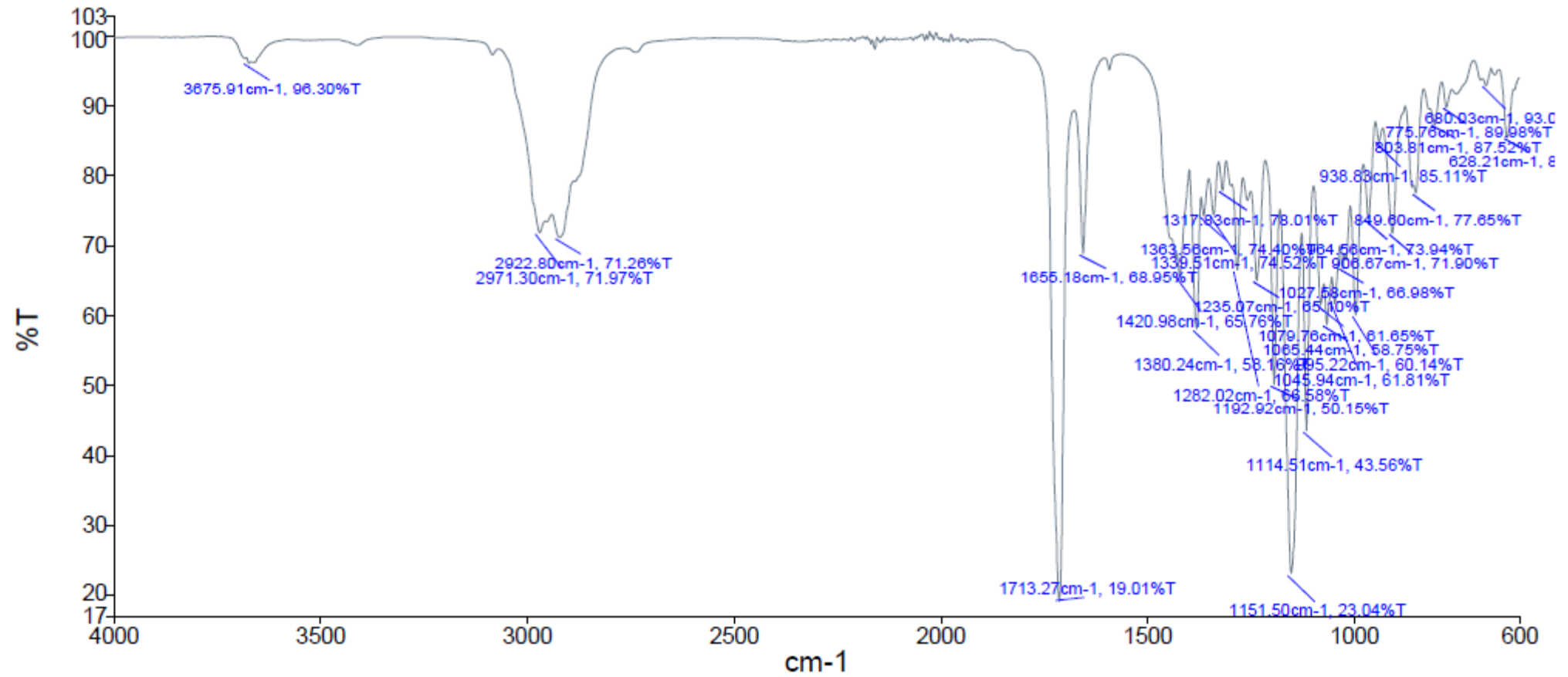


53a IR Spectrum

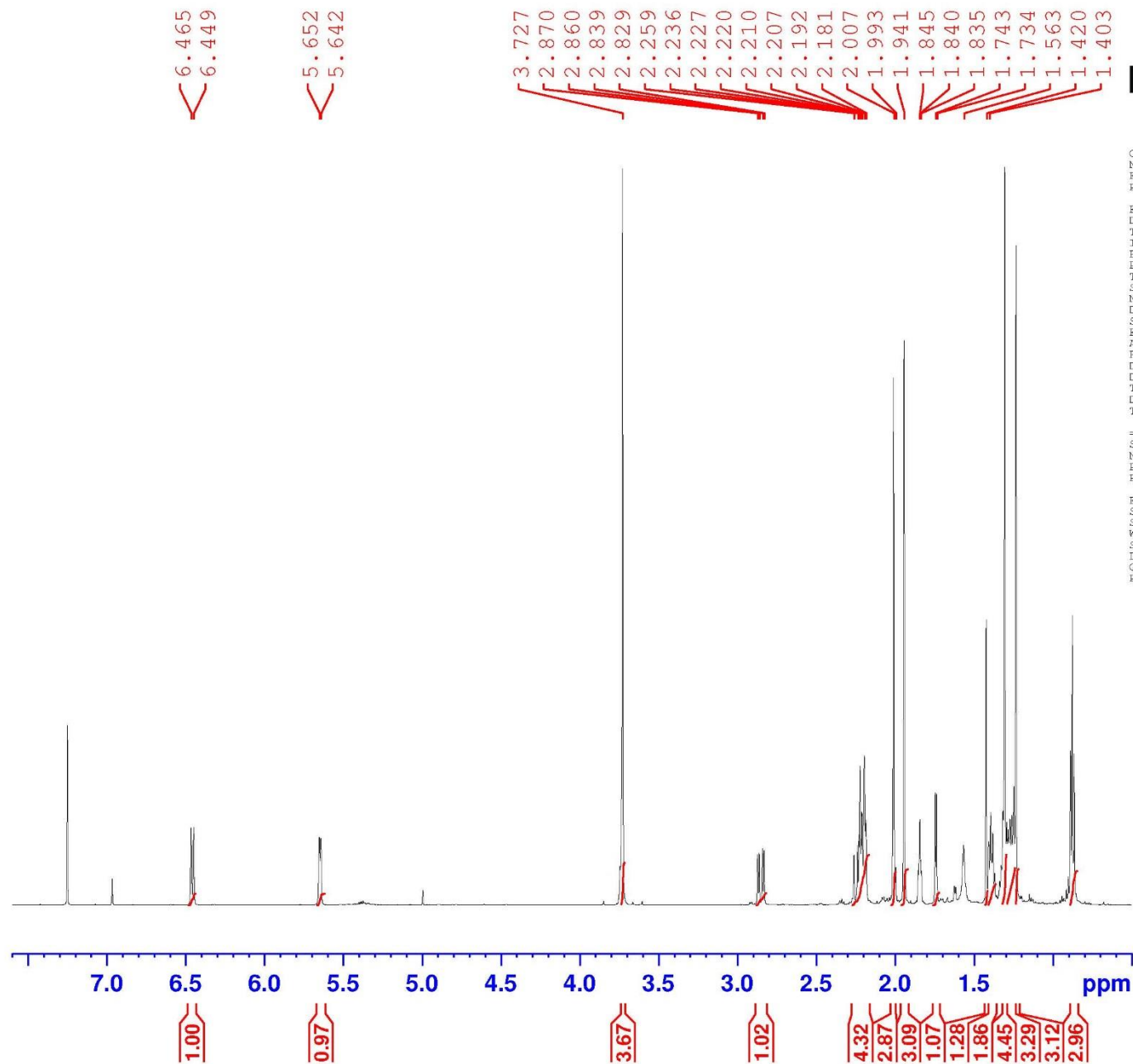
PerkinElmer Spectrum Version 10.4.2
Wednesday, 17 October 2018 3:00 PM

Analyst
Date

Analyst
Wednesday, 17 October 2018 3:00 PM



53b NMR Characterisation

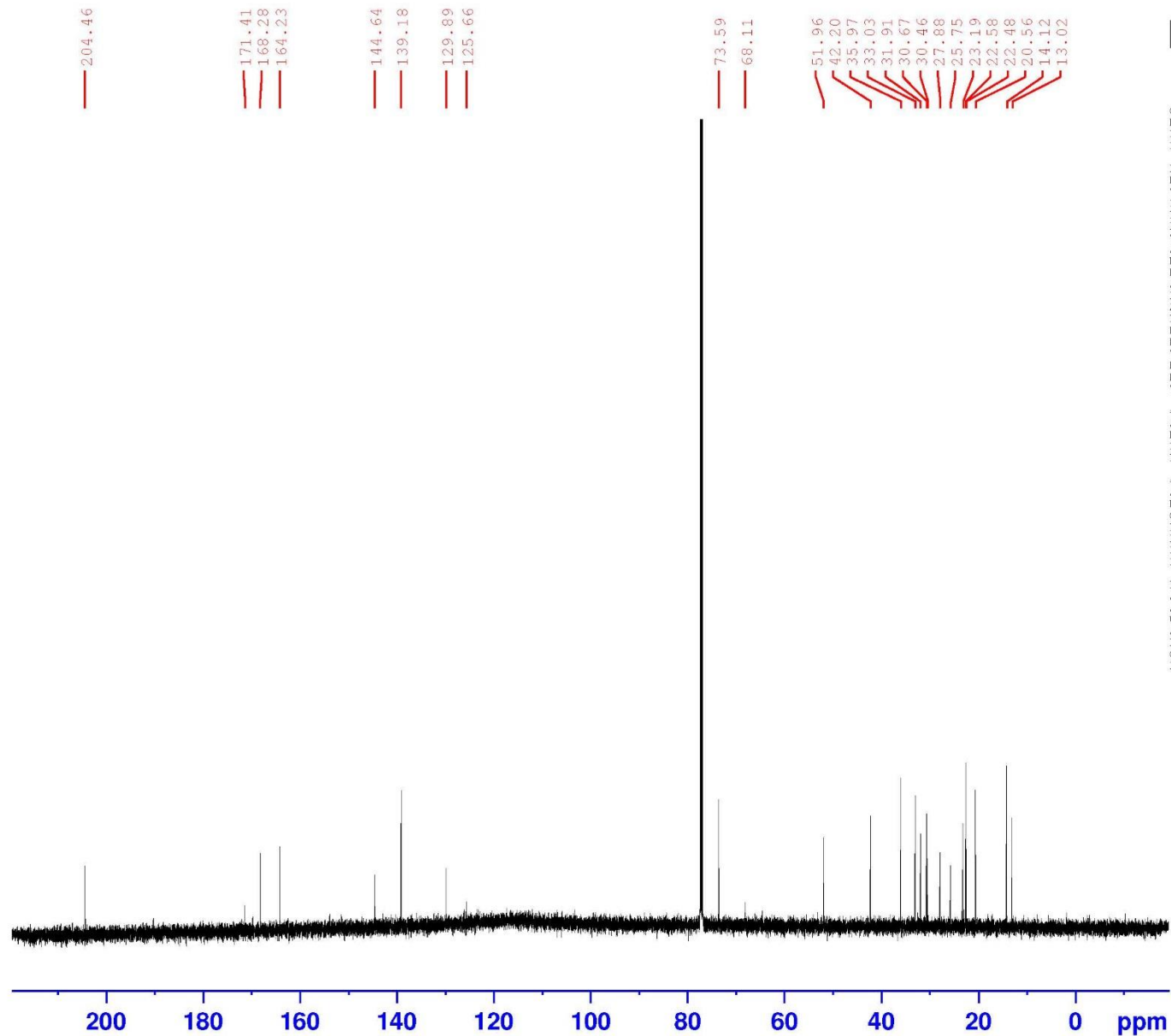


Current Data Parameters
 NAME 20180914 Hydrogenation Pyrethrin II
 EXPNO 31
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180914
 Time 21.24
 INSTRUM spect
 PROBRD 5 mm PABBI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 161
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUCL1 1H
 P1 8.40 usec
 PLW1 12.55000019 W

F2 - Processing parameters
 SI 65536
 SF 600.1300304 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20180914 Hydrogenation Pyrethrin II
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180914
Time 21.08
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 1440
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 16.00 usec
PLW1 110.76000214 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 12.55000019 W
PLW12 0.18072000 W
PLW13 0.08855400 W

F2 - Processing parameters
SI 32768
SF 150.9027904 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20180914 Hydrogenation Pyrethrin II
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180914
Time 21.35
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG cosygmphpp
TD 2048
SOLVENT CDCl3
NS 10
DS 4
SWH 4132.231 Hz
FIDRES 2.017691 Hz
AQ 0.2478080 sec
RG 2050
RW 121.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00011030 sec
D1 1.89063704 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
TNO 0.00024200 sec

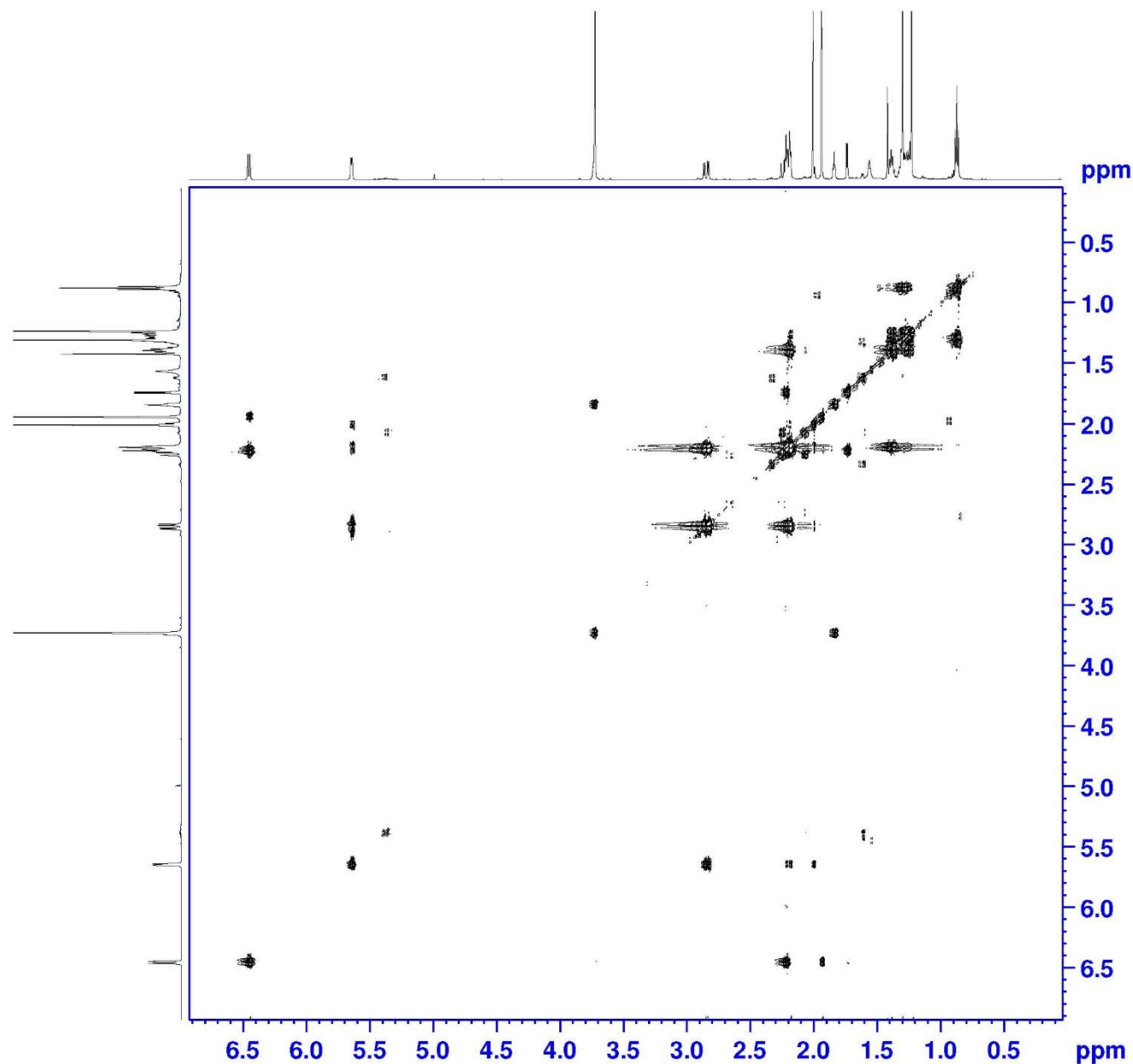
===== CHANNEL f1 =====
SFO1 600.1321235 MHz
NUC1 1H
P1 6.40 usec
P2 16.80 usec
P17 2500.00 usec
PLW1 12.55000019 W
PLW10 1.309999994 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1321 MHz
FIDRES 16.141529 Hz
SW 6.886 ppm
F0MODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.1300327 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300295 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20180914 Hydrogenation Pyrethrin II
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180914
Time 23.37

INSTRUM spect
PROBHD 5 mm FABB1 1H/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 4464.286 Hz
FIDRES 4.359654 Hz
AQ 0.1146880 sec
RG 2050
RW 112.000 usec
DE 6.50 usec
TE 298.0 K
CNS12 145.0000000
D0 0.00000300 sec
D1 1.45084798 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGFTNS

===== CHANNEL f1 =====
SFO1 600.1319837 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P28 1000.00 usec
PLW1 12.55000019 W

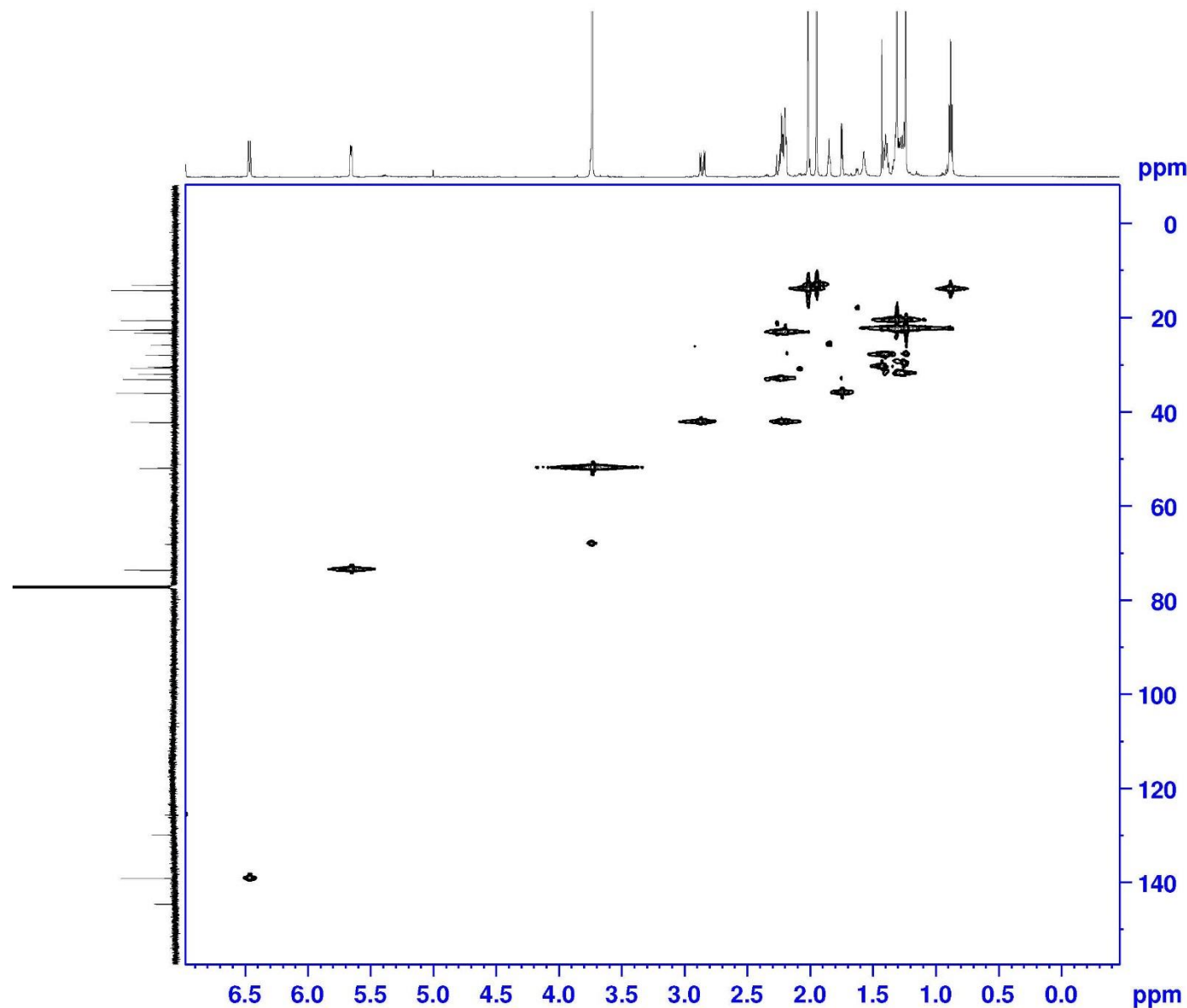
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 16.00 usec
P4 32.00 usec
PCPD2 60.00 usec
PLW2 110.76000214 W
PLW12 7.87610006 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GEF1 80.00 %
GEF2 20.10 %
PL6 1000.00 usec

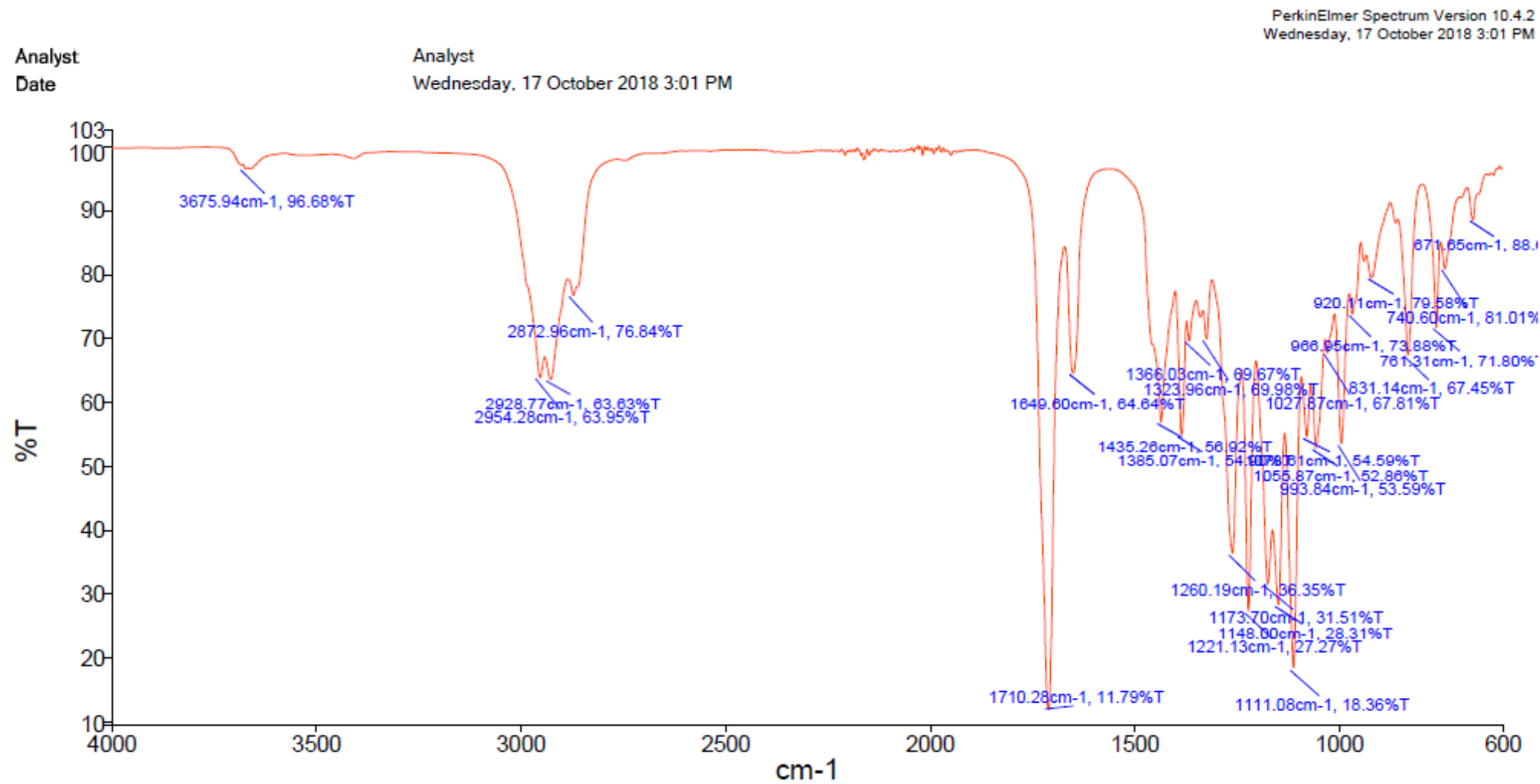
F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FhMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300268 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

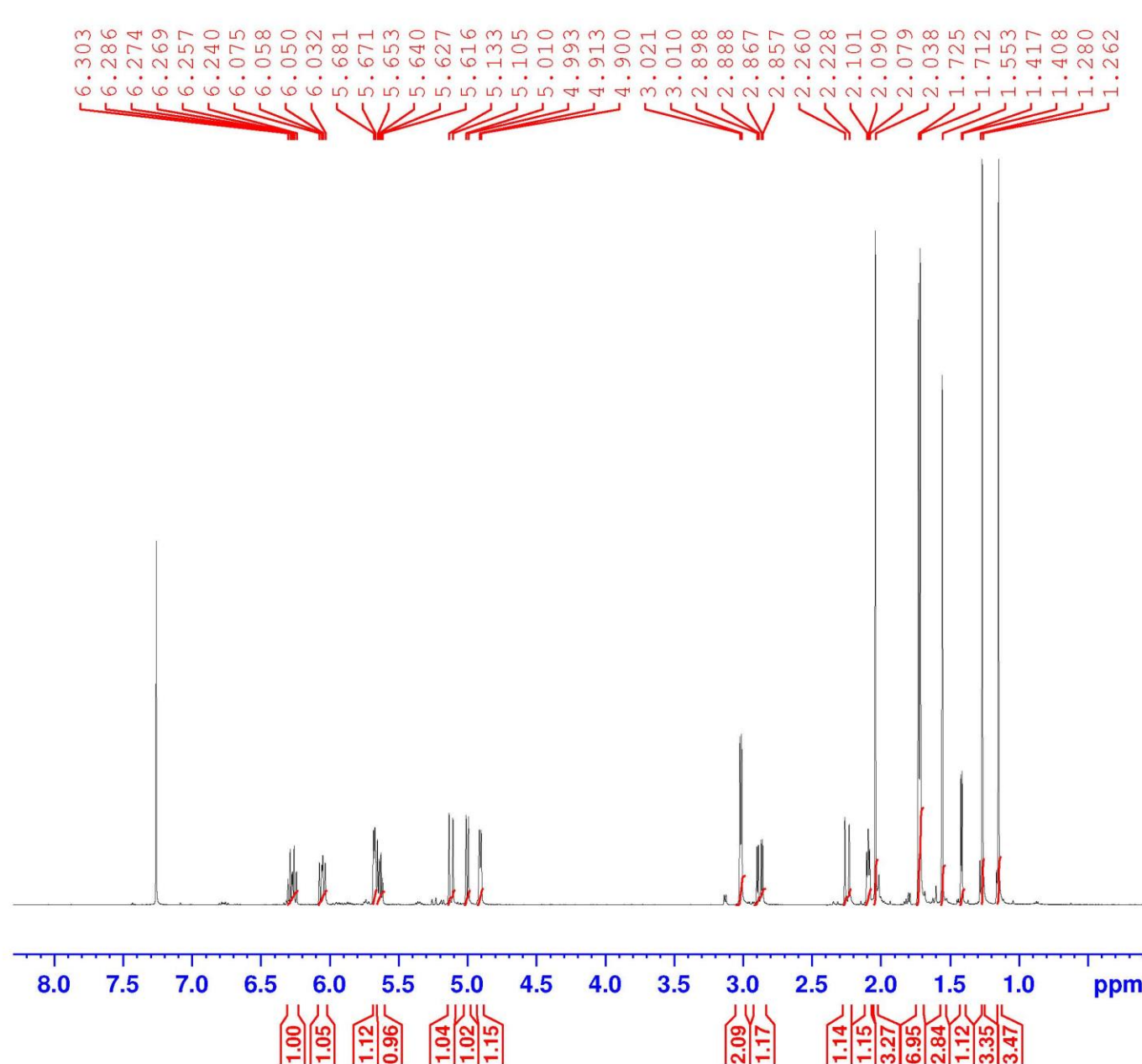
F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



53b IR Spectrum



34a NMR Characterisation

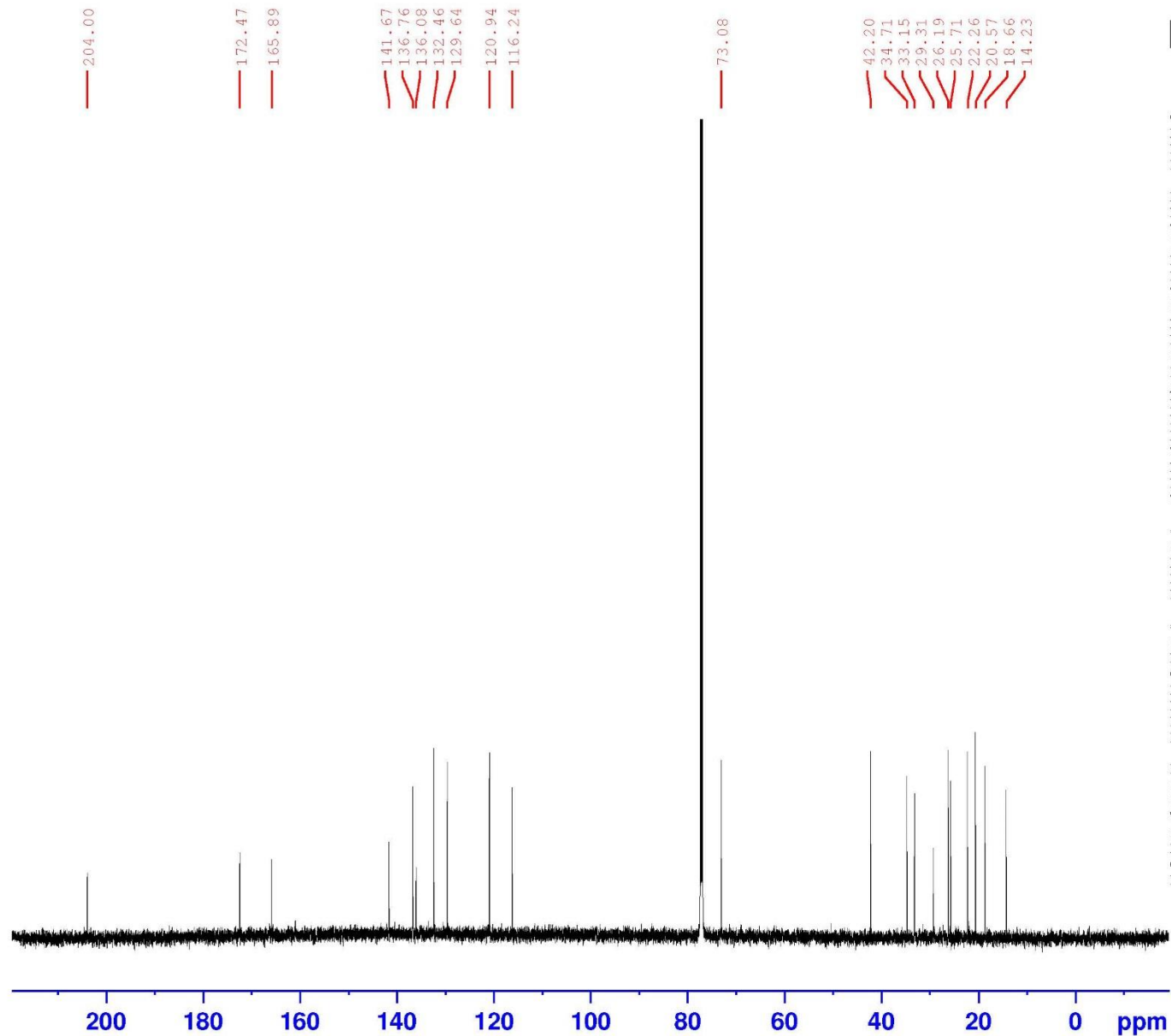


Current Data Parameters
 NAME 20190404 Trans PI CLEAN
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190405
 Time 3.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 287
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300263 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20190404 Trans PI CLEAN
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190405
Time 5.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9027893 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20190404 Trans PI CLEAN
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190405
Time 3.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 4545.455 Hz
FIDRES 2.219460 Hz
AQ 0.2252800 sec
RG 144
DW 110.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.90251505 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00022000 sec

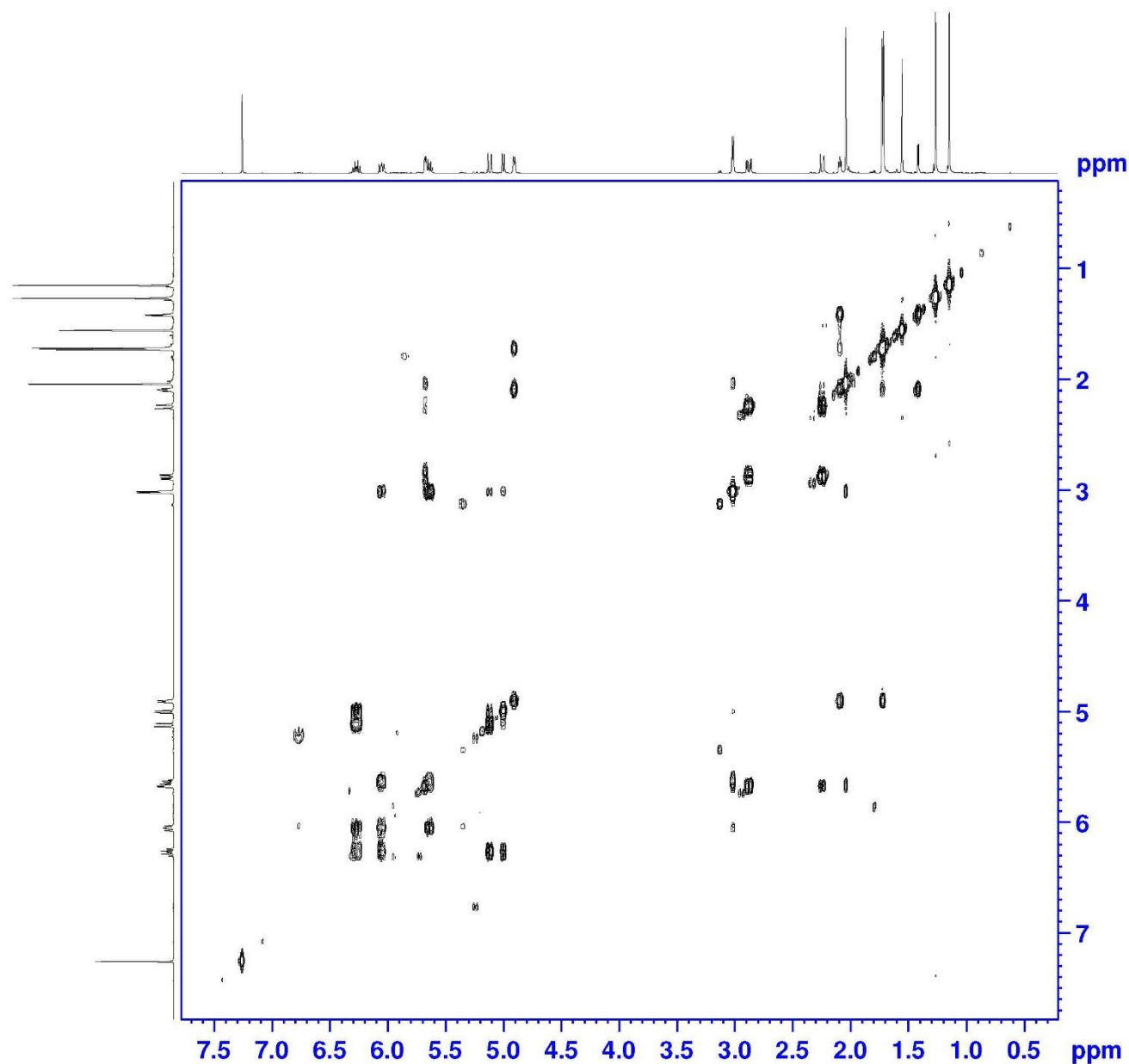
===== CHANNEL f1 =====
SFO1 600.1324241 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1324 MHz
FIDRES 35.511364 Hz
SW 7.574 ppm
F1MODE QF

F2 - Processing parameters
SI 1024
SF 600.1300250 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

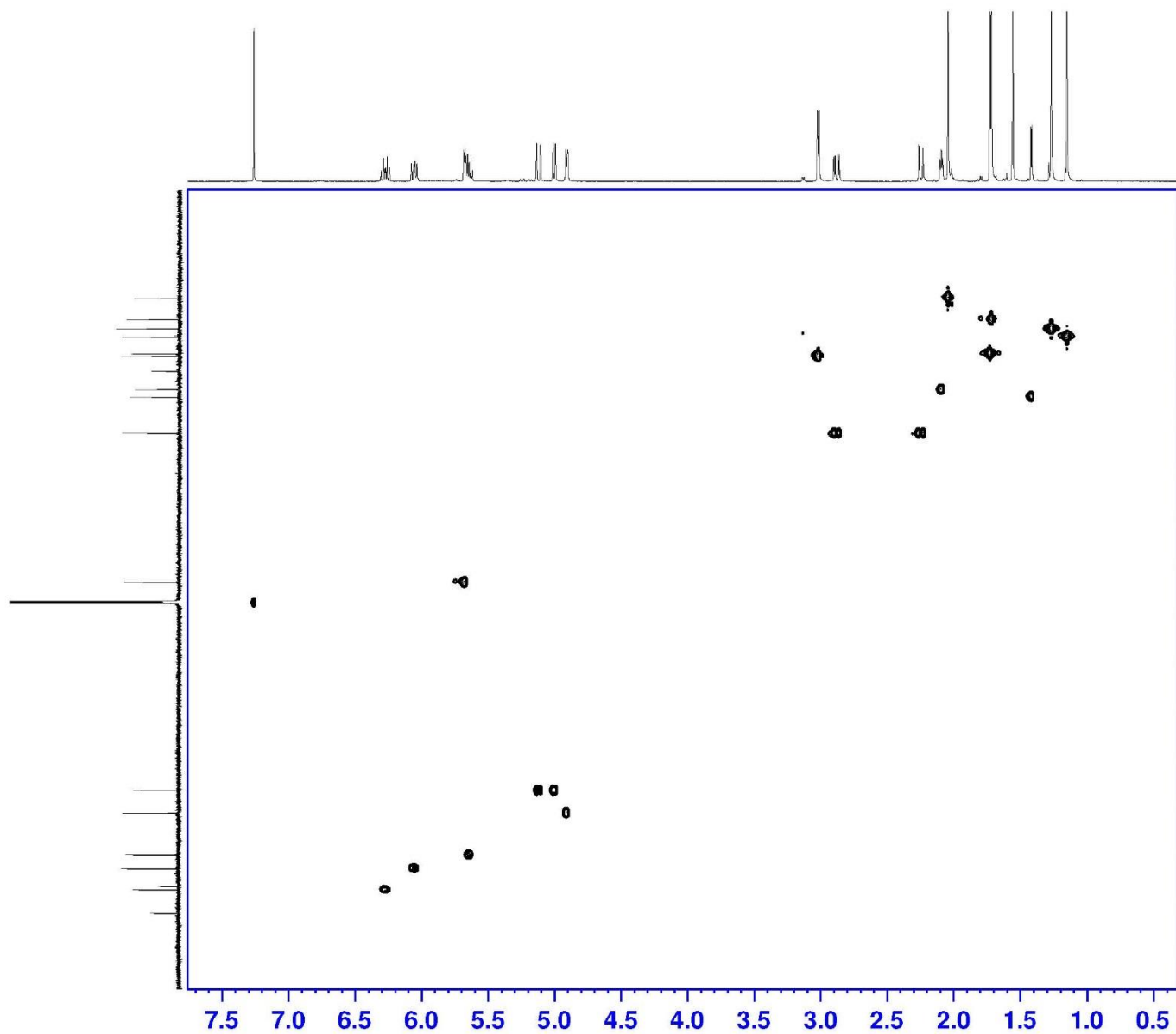
F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300264 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190404 Trans PI CLEAN
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190405
Time 6.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcztgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 4464.286 Hz
FIDRES 4.359654 Hz
AQ 0.1146880 sec
RG 2050
DW 112.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45084798 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS
===== CHANNEL f1 =====
SFO1 600.1324484 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CDDPRG[2] garrp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 80.00000000 W
PLW12 3.20000005 W
===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
PL6 1000.00 usec
F1 - Acquisition parameters
TD 137
SFO1 150.9141 MHz
FIDRES 182.481750 Hz
SW 165.657 ppm
FMODE Echo-Antiecho
F2 - Processing parameters
SI 1024
SF 600.1300246 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40
F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028116 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

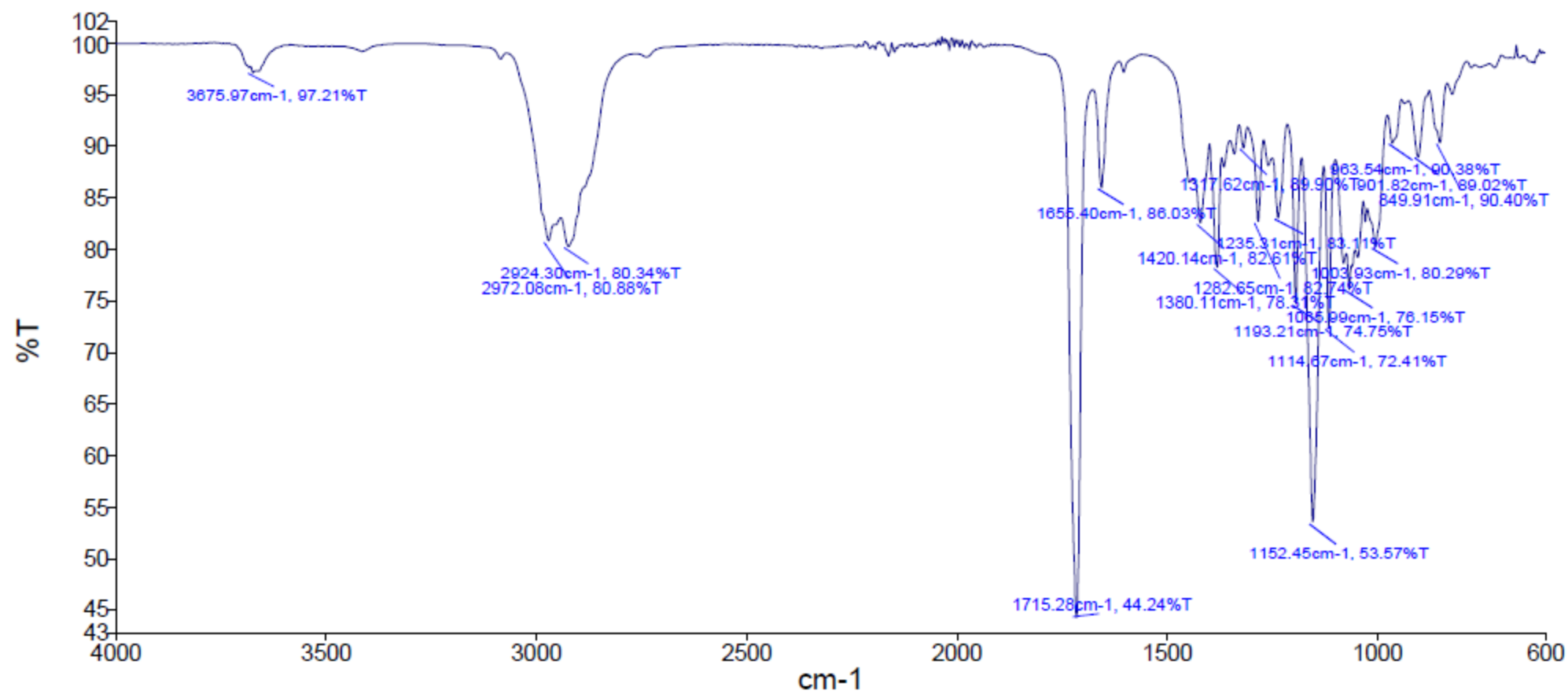


34a IR Spectrum

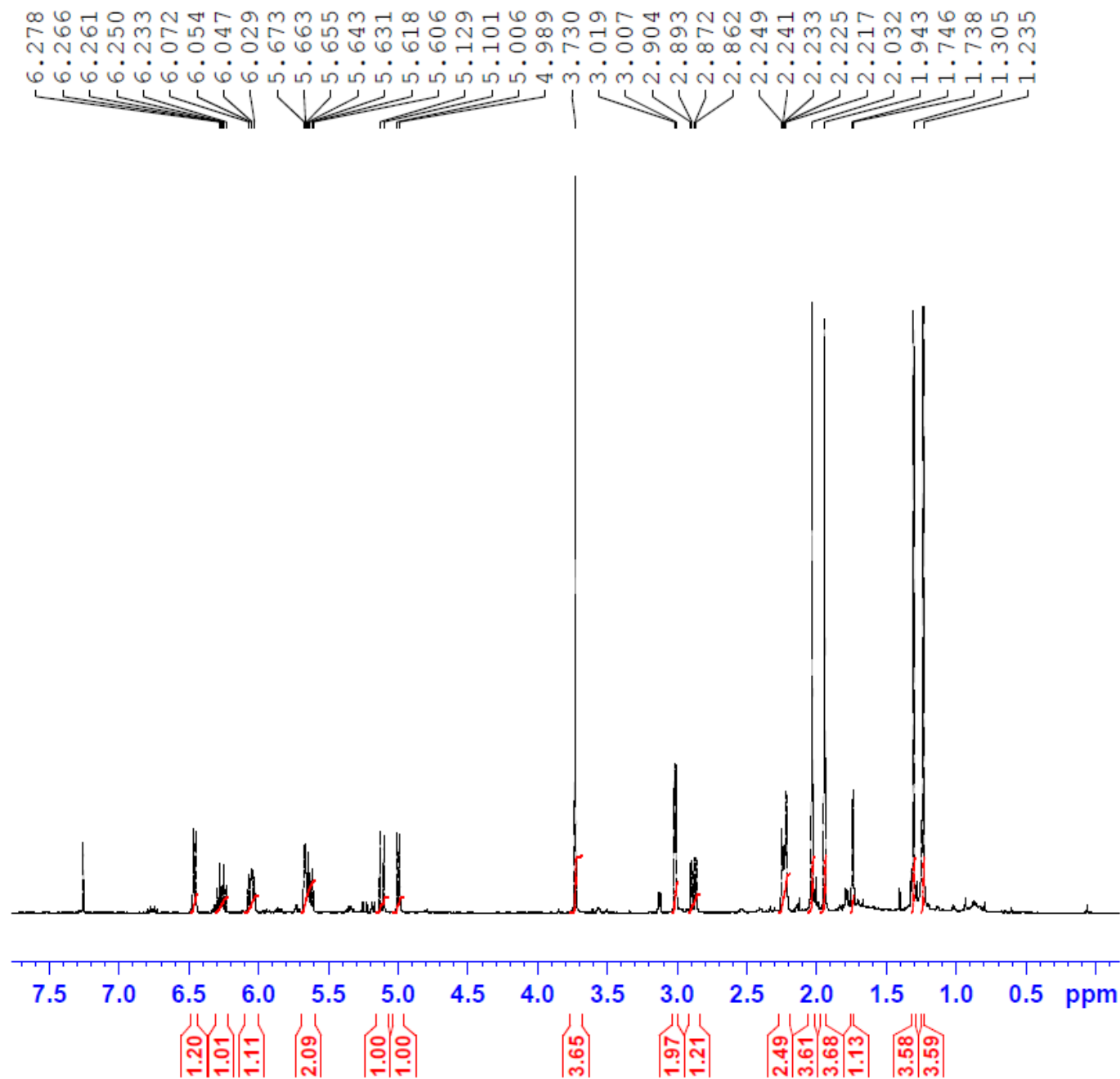
PerkinElmer Spectrum Version 10.4.2
Wednesday, 17 October 2018 3:01 PM

Analyst
Date

Analyst
Wednesday, 17 October 2018 3:01 PM



34b NMR Characterisation

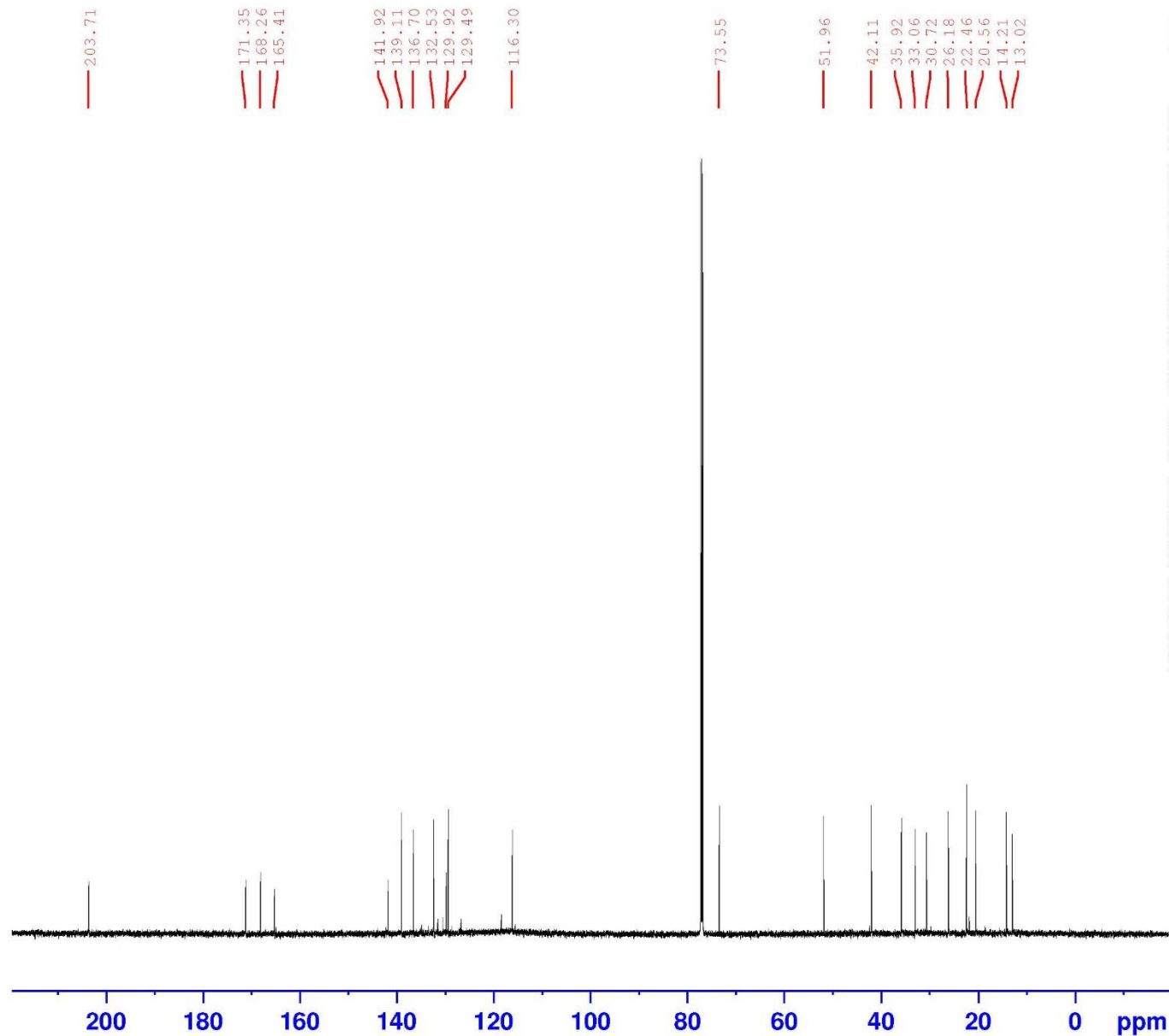


Current Data Parameters
 NAME 20181008 Transfer Hydrogenation PII
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181008
 Time_ 17.10
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 90.5
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 8.40 usec
 PLW1 12.55000019 W

F2 - Processing parameters
 SI 65536
 SF 600.1300270 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20181008 Transfer Hydrogenation PII
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181008
Time 18.16
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 1620
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 16.00 usec
PLW1 110.76000214 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 12.55000019 W
PLW12 0.18072000 W
PLW13 0.08855400 W

F2 - Processing parameters
SI 32768
SF 150.9027908 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20181008 Transfer Hydrogenation PII
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181008
Time 18.23
INSTRUM spect
PROBHD 5 mm FBB1 1H/
PULPROG cosygmphpp
TD 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 4716.981 Hz
FIDRES 2.303213 Hz
AQ 0.2170880 sec
RG 2050
RW 106.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00009530 sec
D1 1.92135704 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021200 sec

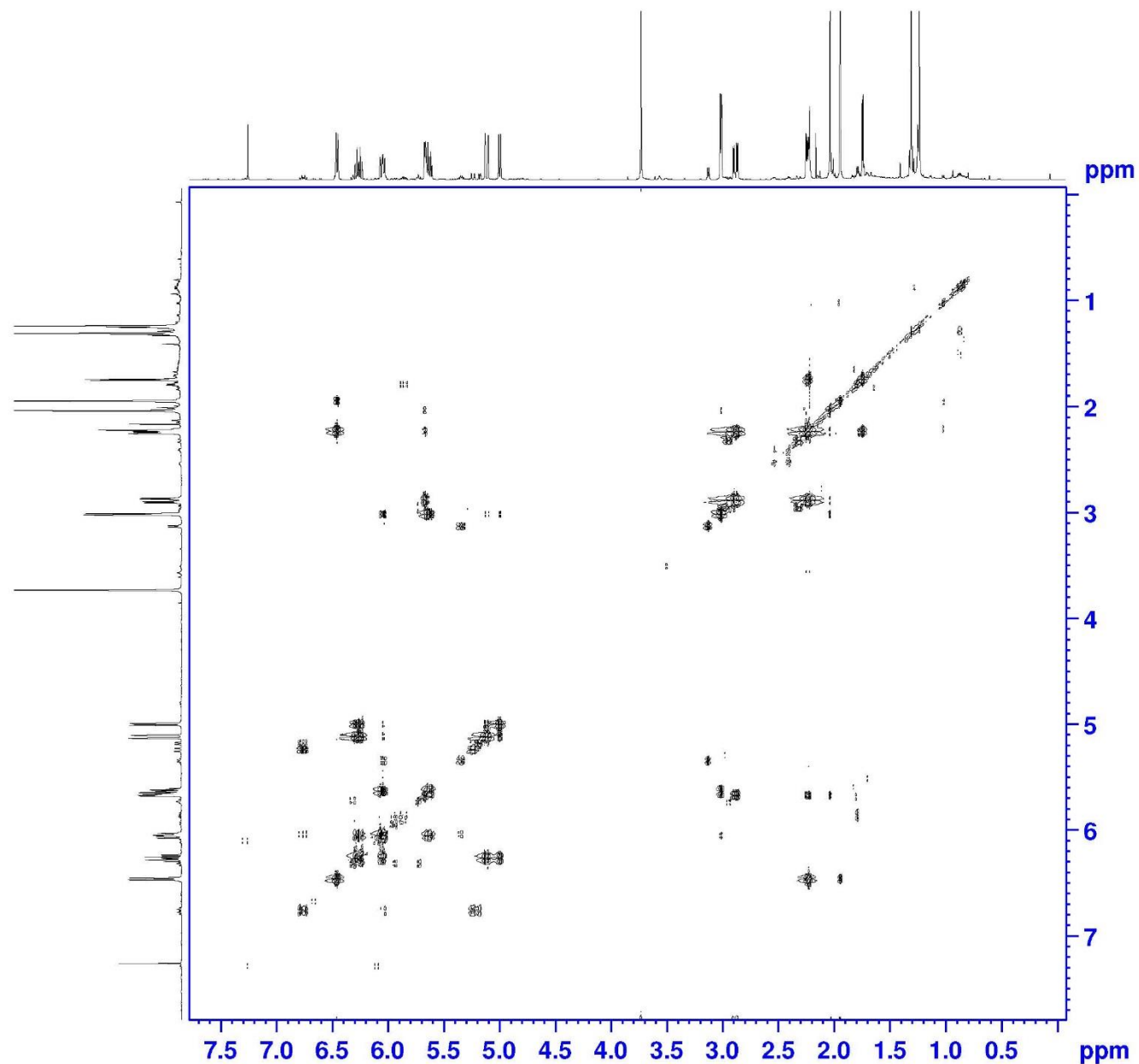
===== CHANNEL f1 =====
SFO1 600.1323382 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P17 2500.00 usec
PLW1 12.55000019 W
PLW10 1.30999994 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1323 MHz
FIDRES 18.425707 Hz
SW 7.860 ppm
FbMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.1300250 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300203 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20181008 Transfer Hydrogenation PII
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181008
Time 19.12

INSTRUM spect
PROBHD 5 mm FABB1 1H/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 35
DS 16
SWH 4716.981 Hz
FIDRES 4.606427 Hz
AQ 0.1085440 sec
RG 2050
RW 106.000 usec
DE 6.50 usec
TE 298.1 K
CNS12 145.0000000
D0 0.00000300 sec
D1 1.45699203 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGFTNS

===== CHANNEL f1 =====
SFO1 600.1323382 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P28 1000.00 usec
PLW1 12.55000019 W

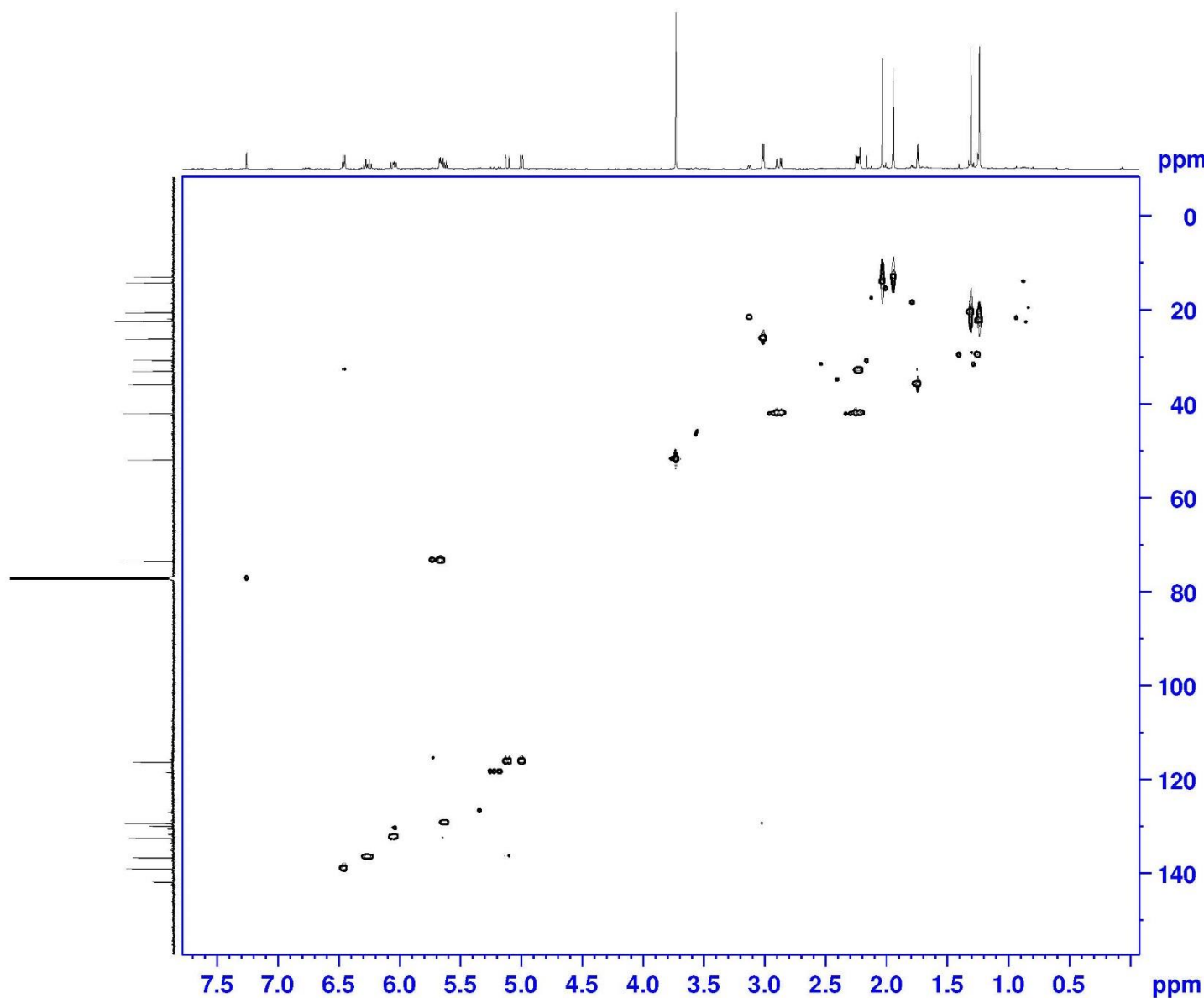
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 16.00 usec
P4 32.00 usec
PCPD2 60.00 usec
PLW2 110.76000214 W
PLW12 7.87610006 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GEF1 80.00 %
GEF2 20.10 %
PL6 1000.00 usec

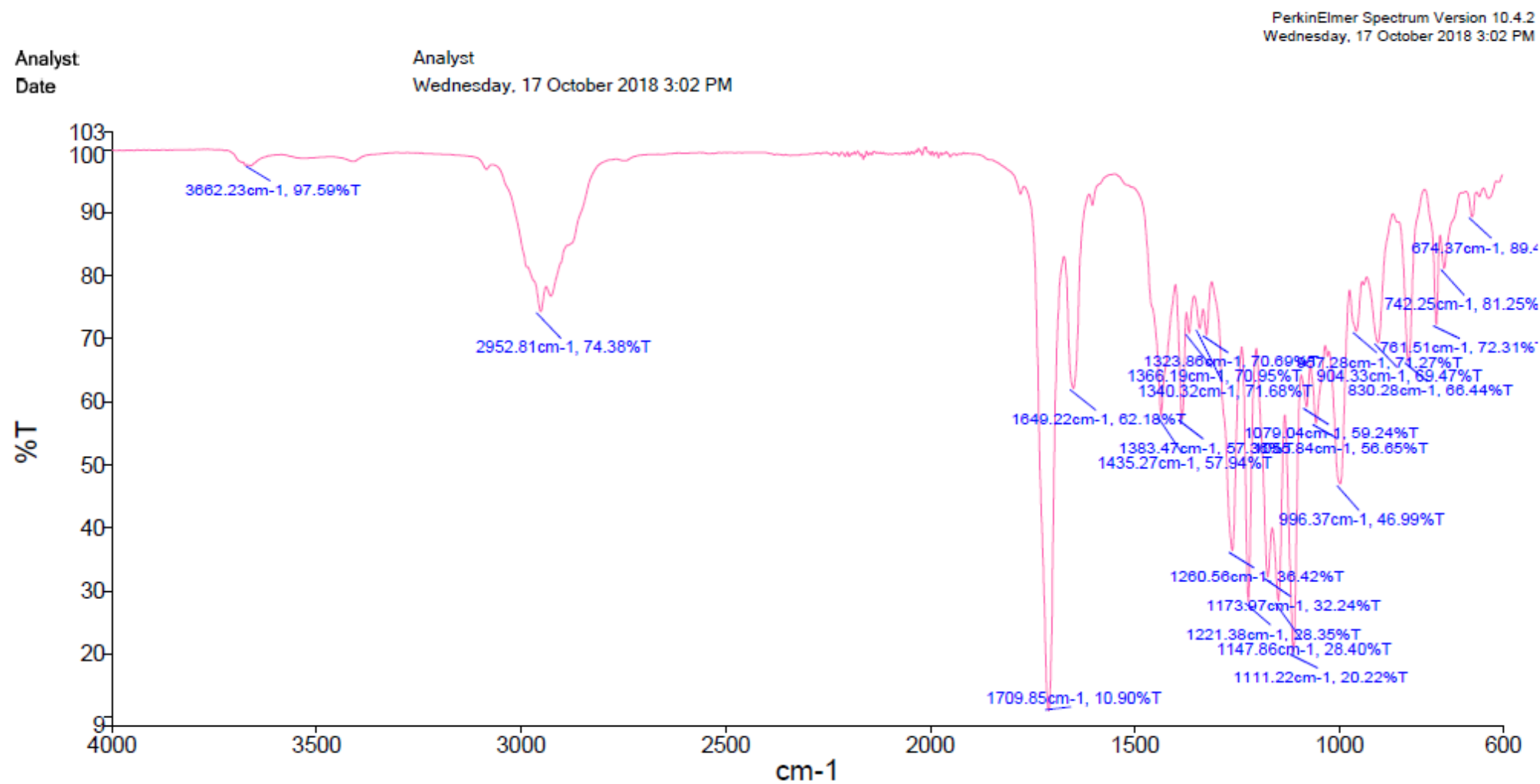
F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300239 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

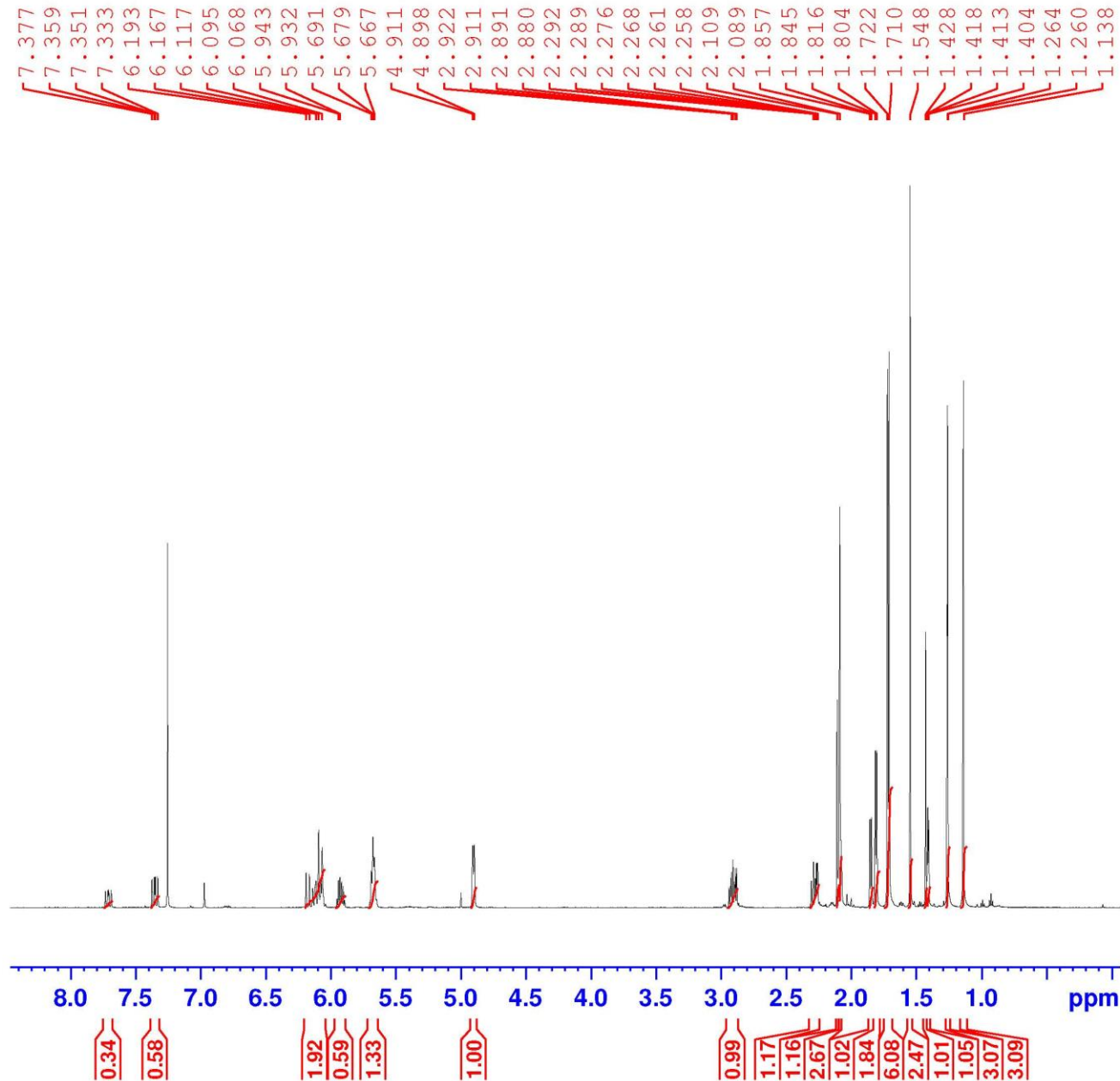
F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028240 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



34b IR Spectrum



25a NMR Characterisation

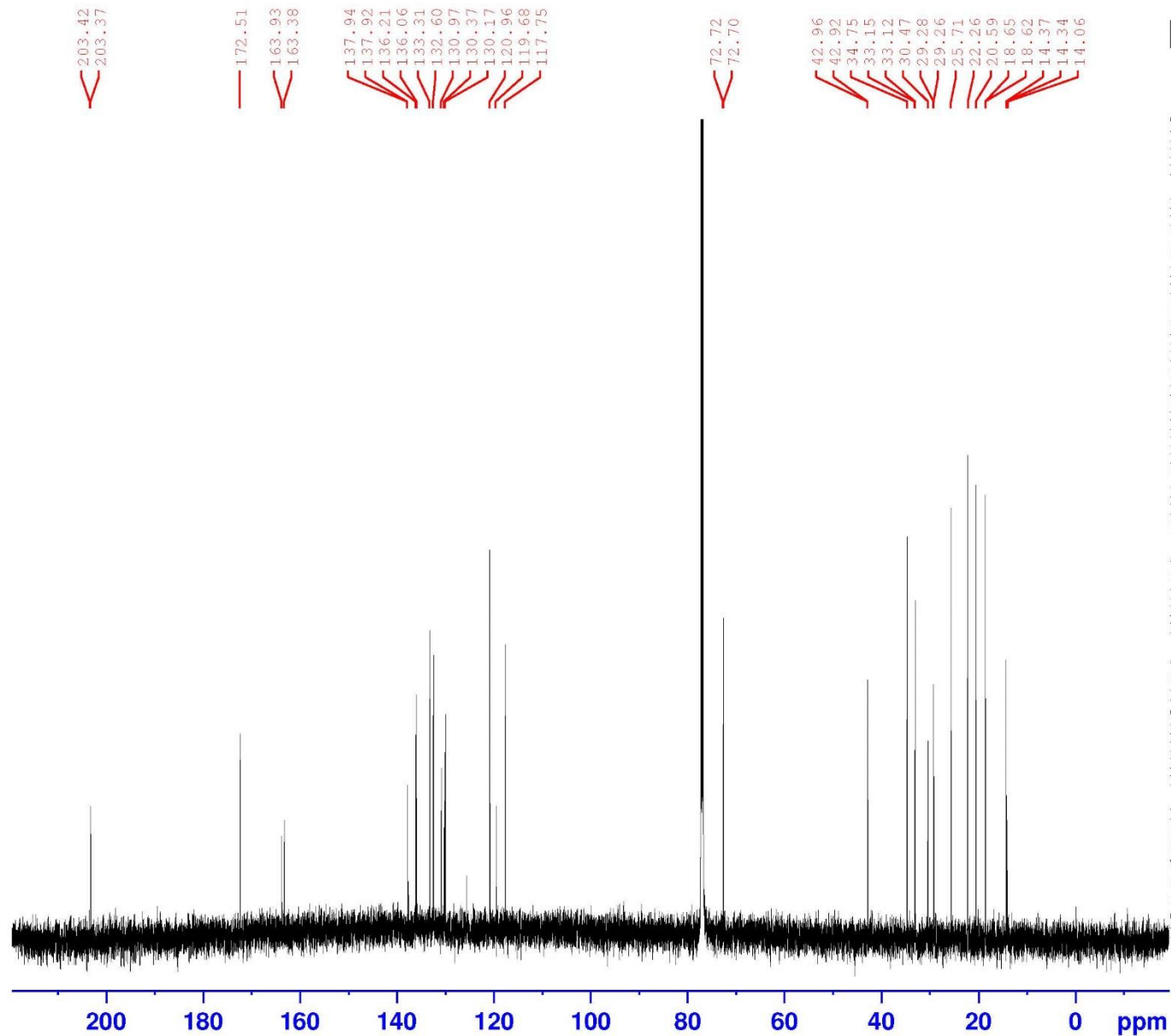


Current Data Parameters
 NAME 20190404 Iso PI CLEAN
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190404
 Time 19.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 287
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300277 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



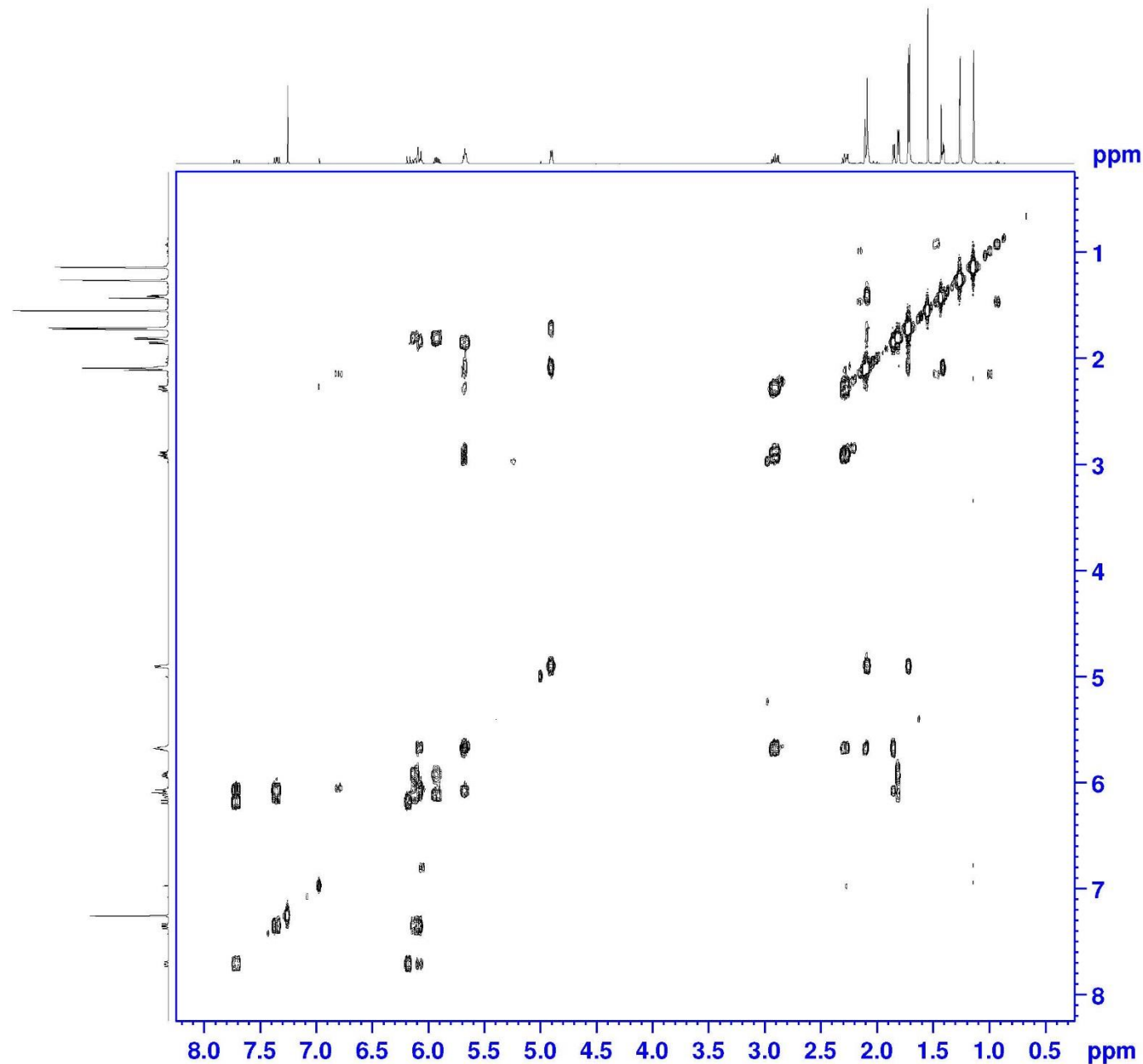
Current Data Parameters
NAME 20190404 Iso PI CLEAN
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190404
Time 21.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9027898 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20190404 Iso PI CLEAN
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190404
Time 19.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 4807.692 Hz
FIDRES 2.347506 Hz
AQ 0.2129920 sec
RG 144
DW 104.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.91480303 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00020800 sec

===== CHANNEL f1 =====
SFO1 600.1325742 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1326 MHz
FIDRES 37.560097 Hz
SW 8.011 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300254 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300271 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0



Current Data Parameters
NAME 20190404 Iso PI CLEAN
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190404
Time 21.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcstgpp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 4761.905 Hz
FIDRES 4.650298 Hz
AQ 0.1075200 sec
RG 2050
DW 105.000 usec
DE 6.50 usec
TE 298.3 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45801604 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS

===== CHANNEL f1 =====
SFO1 600.1325854 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

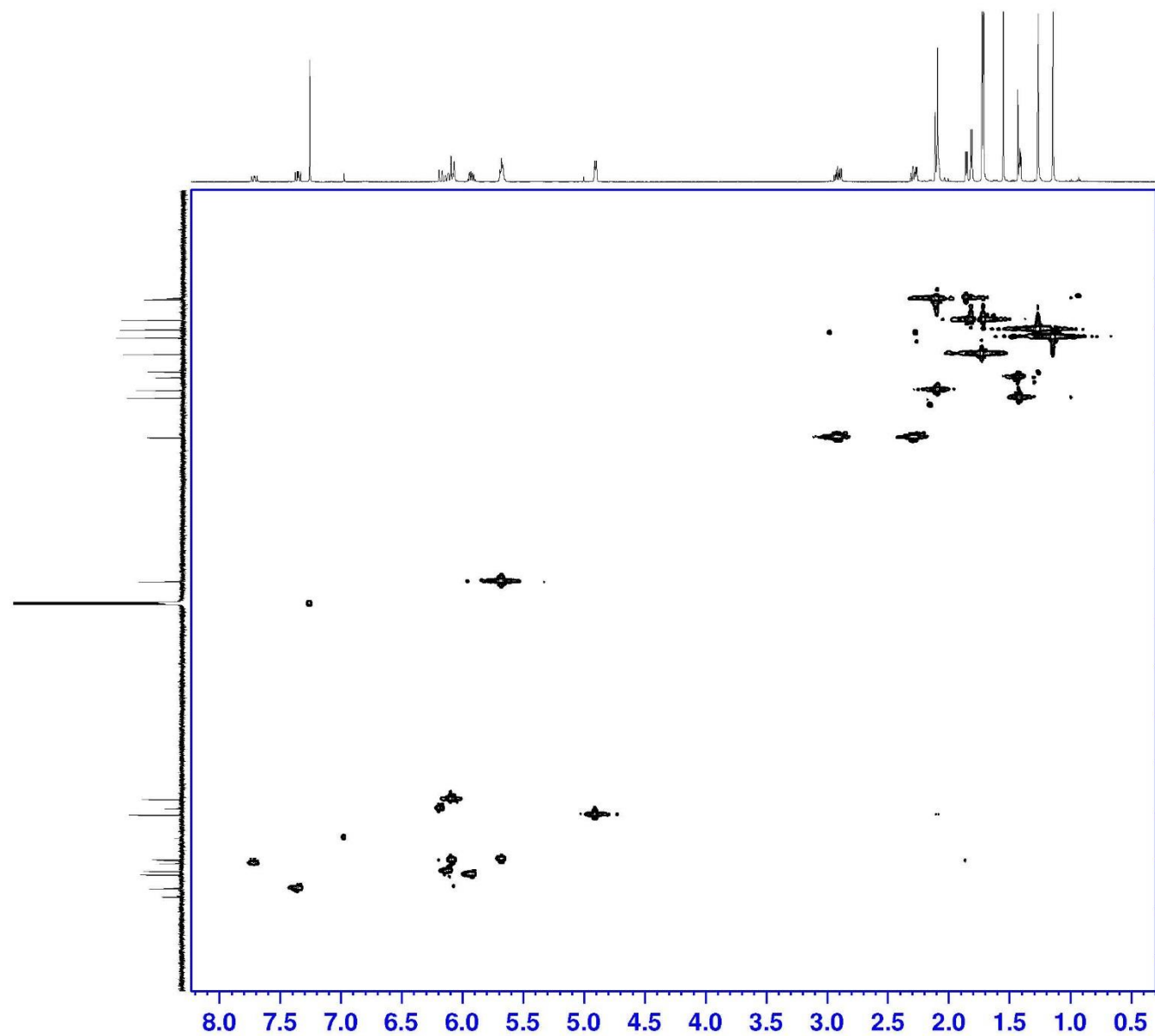
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CDDPRG[2] garrp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 80.00000000 W
PLW12 3.20000005 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

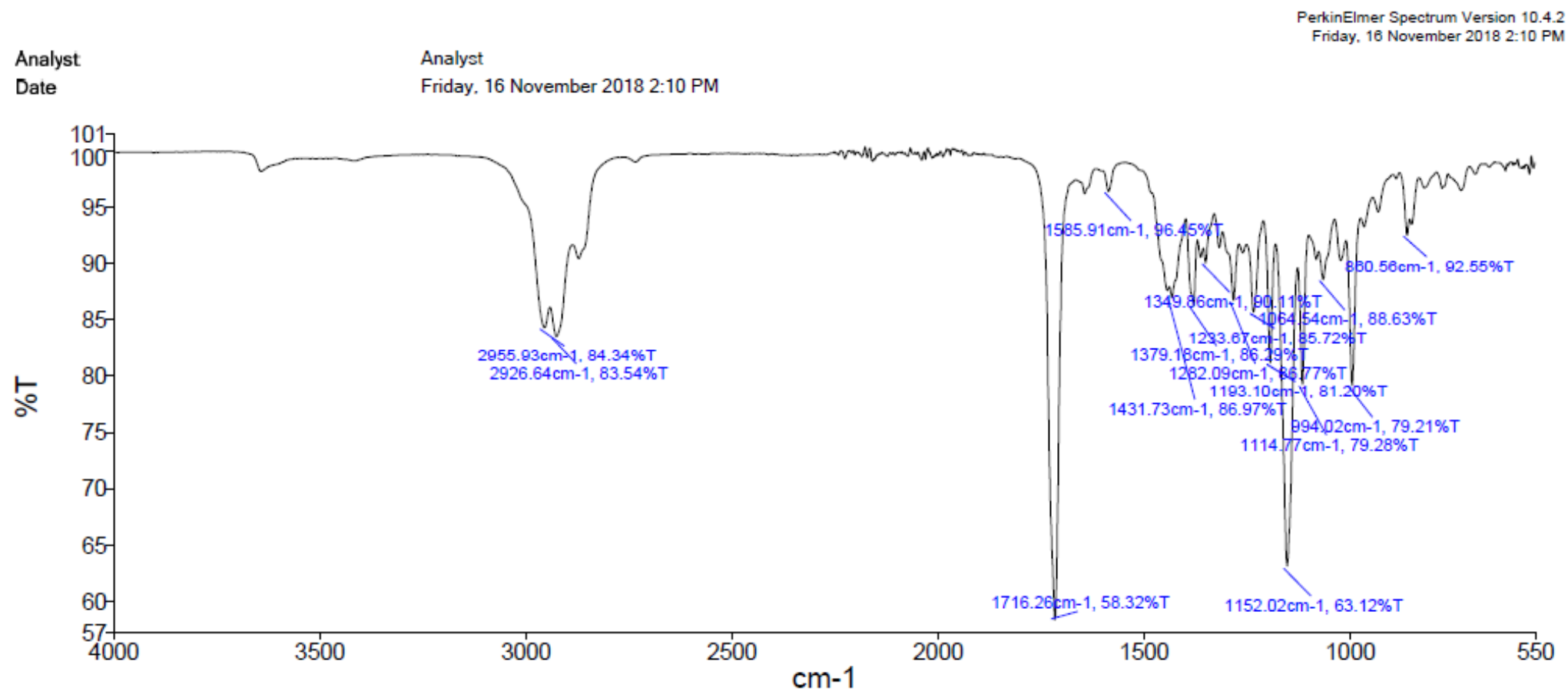
F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300256 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

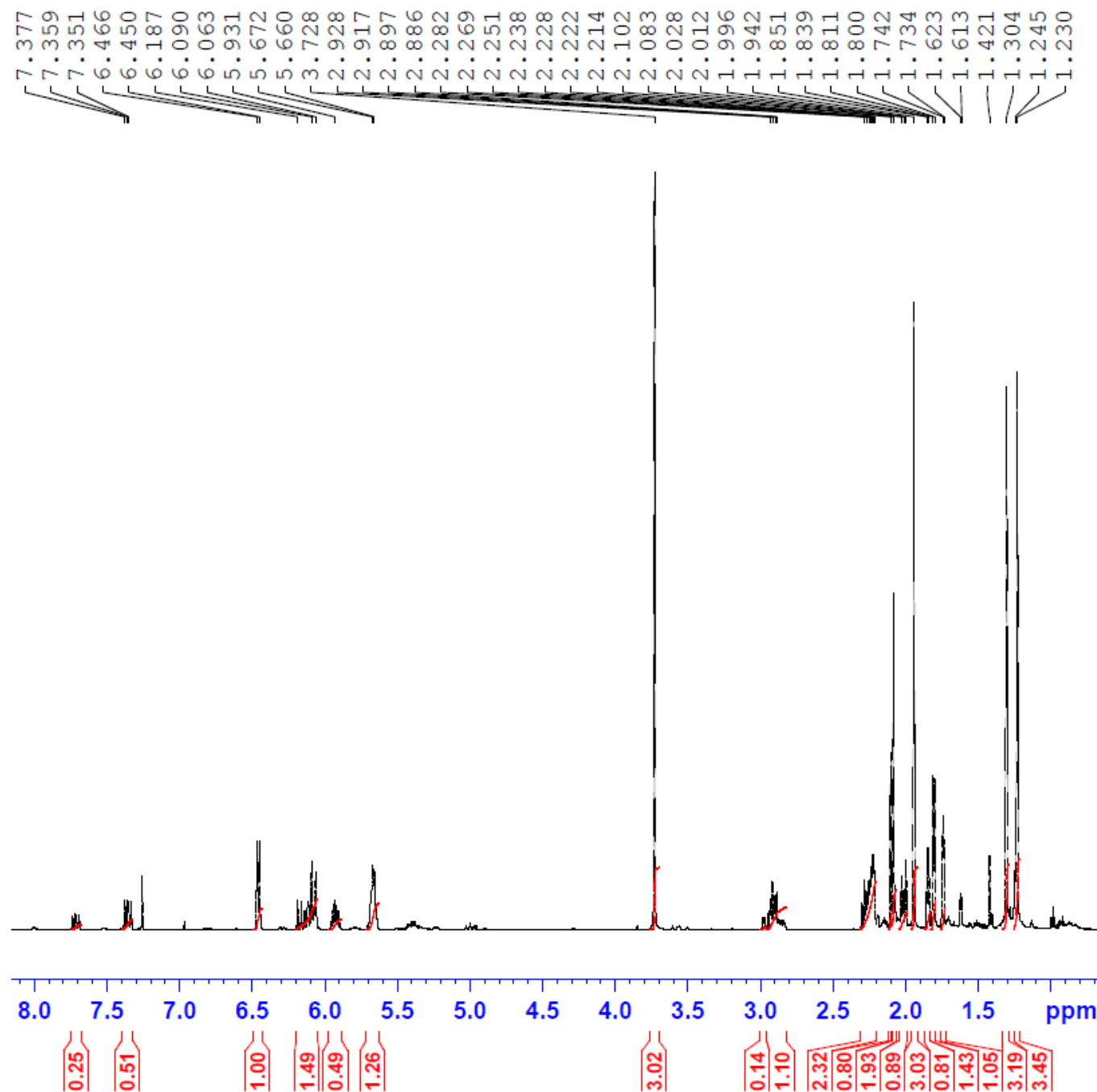
F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028165 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



25a IR Spectrum



25b NMR Characterisation

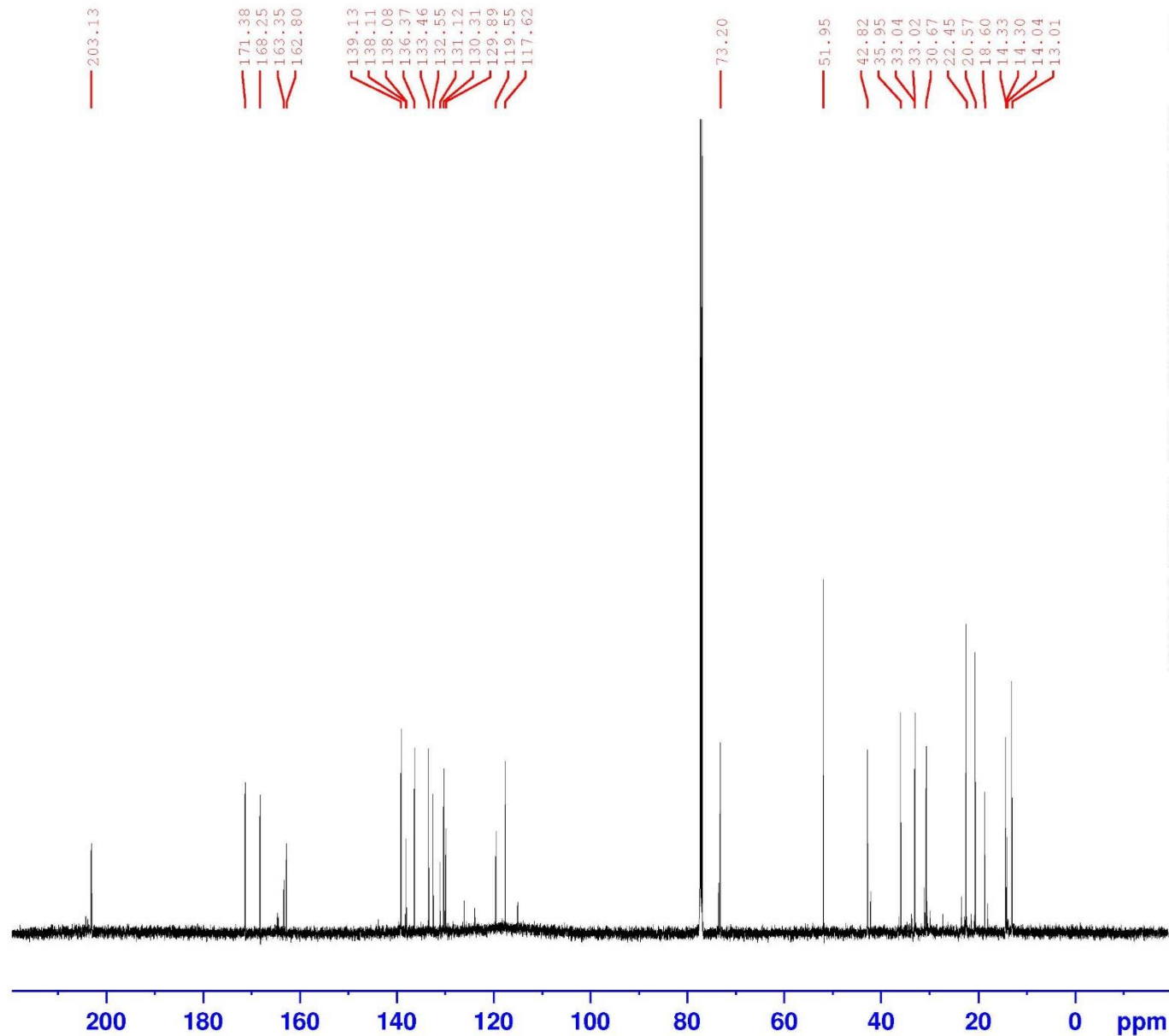


Current Data Parameters
 NAME 20181008 Transfer Hydrogenation PII
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181008
 Time_ 17.03
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 71.8
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 8.40 usec
 PLW1 12.55000019 W

F2 - Processing parameters
 SI 65536
 SF 600.1300267 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20181008 Transfer Hydrogenation PII
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181009
Time 3.59
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 1820
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 16.00 usec
PLW1 110.76000214 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 12.55000019 W
PLW12 0.18072000 W
PLW13 0.08855400 W

F2 - Processing parameters
SI 32768
SF 150.9027924 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20181107 Isopyrethrin II
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181107
Time 9.58
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 5
DS 8
SWH 5000.000 Hz
FIDRES 2.441406 Hz
AQ 0.2048000 sec
RG 64
DW 100.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.92299497 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00020000 sec

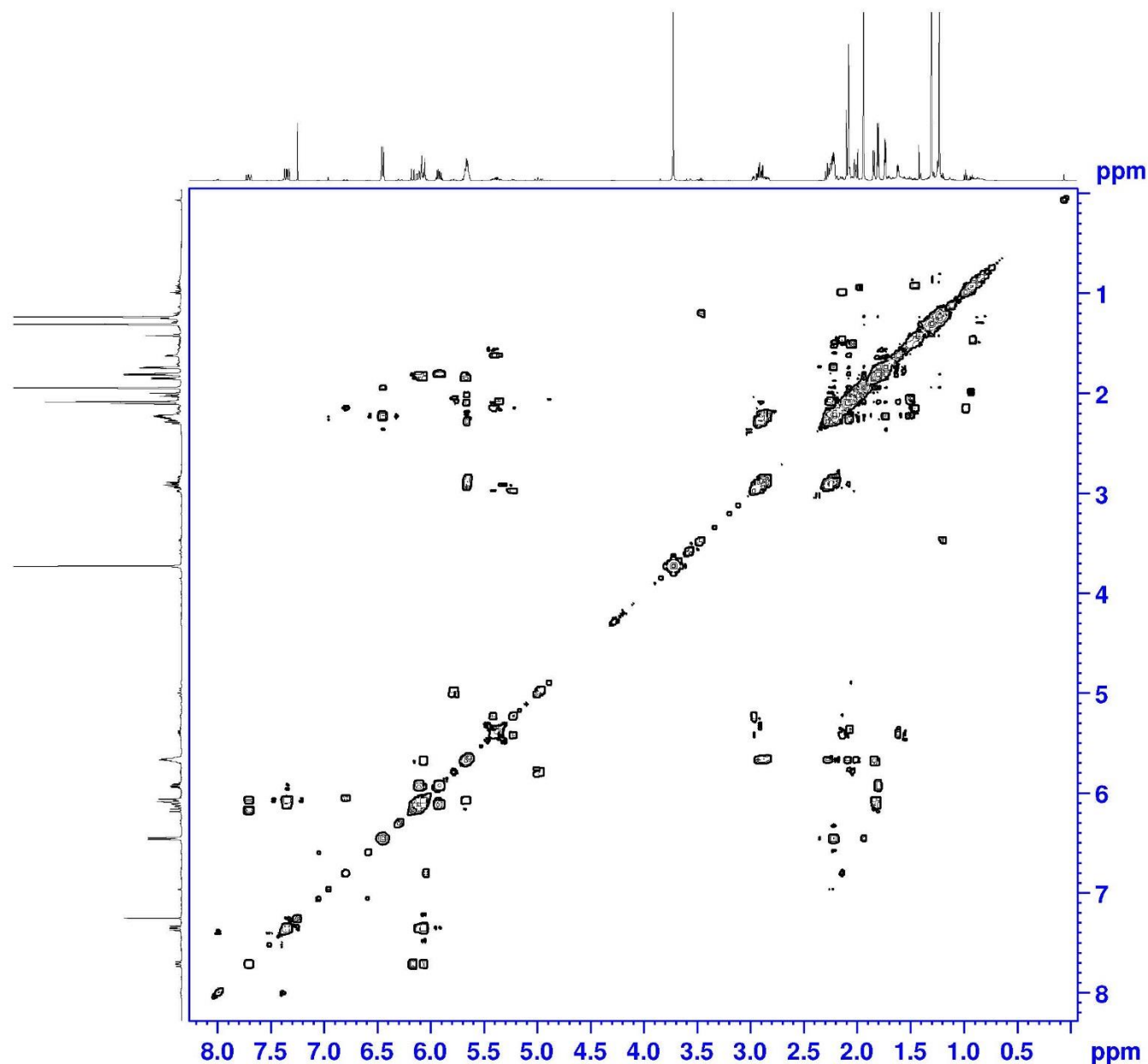
===== CHANNEL f1 =====
SFO1 600.1324960 MHz
NUC1 1H
P0 8.40 usec
P1 8.40 usec
P17 2500.00 usec
PLW1 12.55000019 W
PLW10 1.30999994 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1325 MHz
FIDRES 39.062500 Hz
SW 8.331 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300342 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300265 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20181008 Transfer Hydrogenation PII
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters

Date_ 20181009
Time 4.55
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 35
DS 16
SWH 5050.505 Hz
FIDRES 4.932134 Hz
AQ 0.1013760 sec
RG 2050
RW 99.000 usec
DE 6.50 usec
TE 298.1 K
CNS12 145.0000000
D0 0.00000300 sec
D1 1.46415997 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGFTNS

===== CHANNEL f1 =====
SFO1 600.1324643 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P28 1000.00 usec
PLW1 12.55000019 W

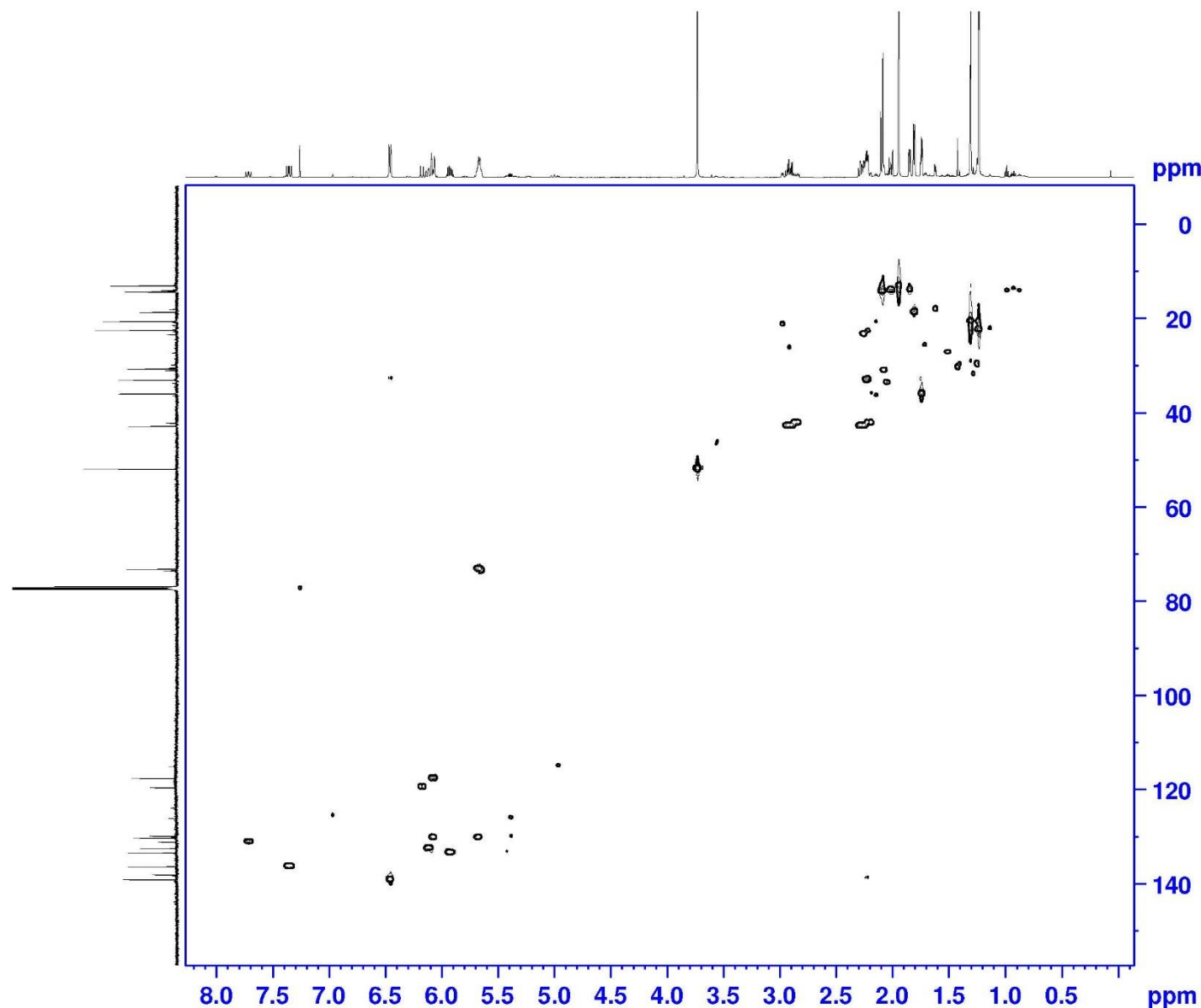
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 16.00 usec
P4 32.00 usec
PCPD2 60.00 usec
PLW2 110.76000214 W
PLW12 7.87610006 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GEF1 80.00 %
GEF2 20.10 %
PL6 1000.00 usec

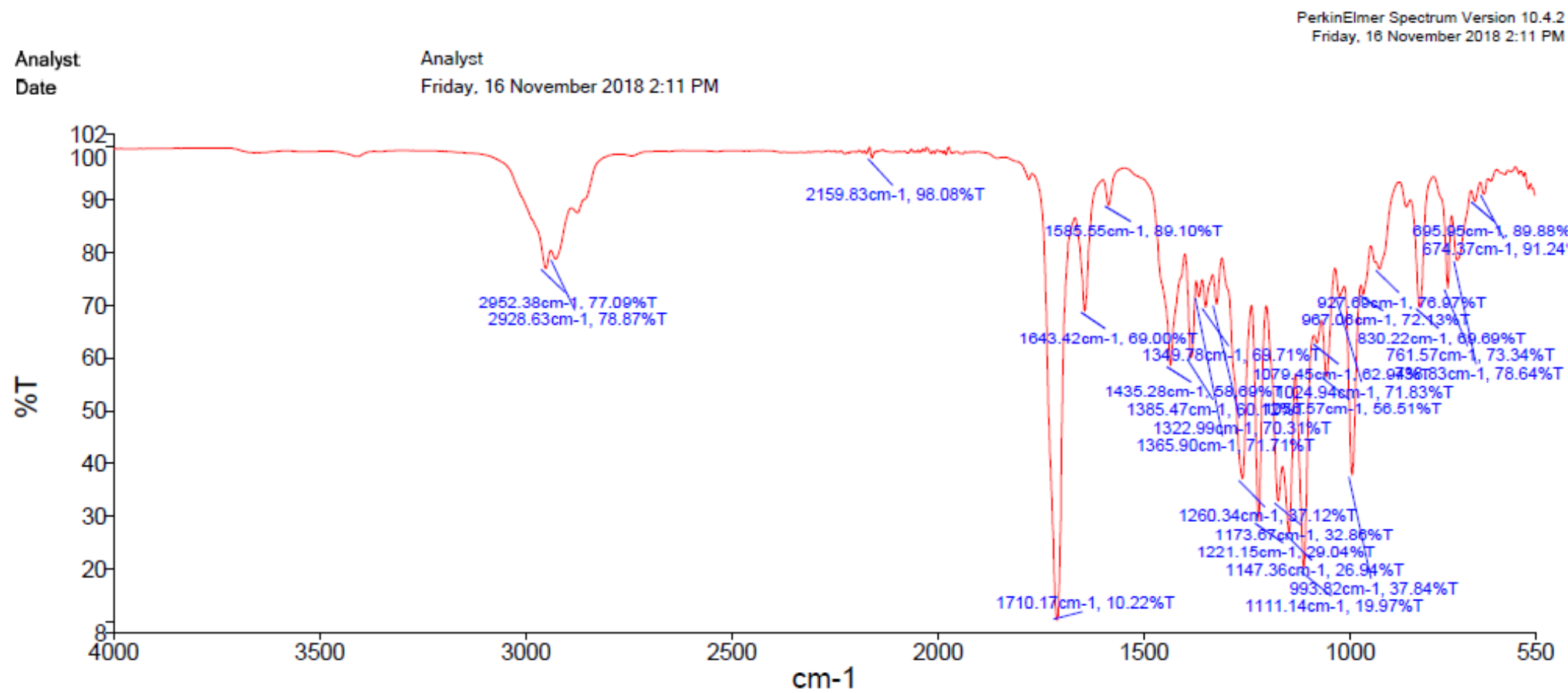
F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FhMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300237 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028198 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



25b IR Spectrum



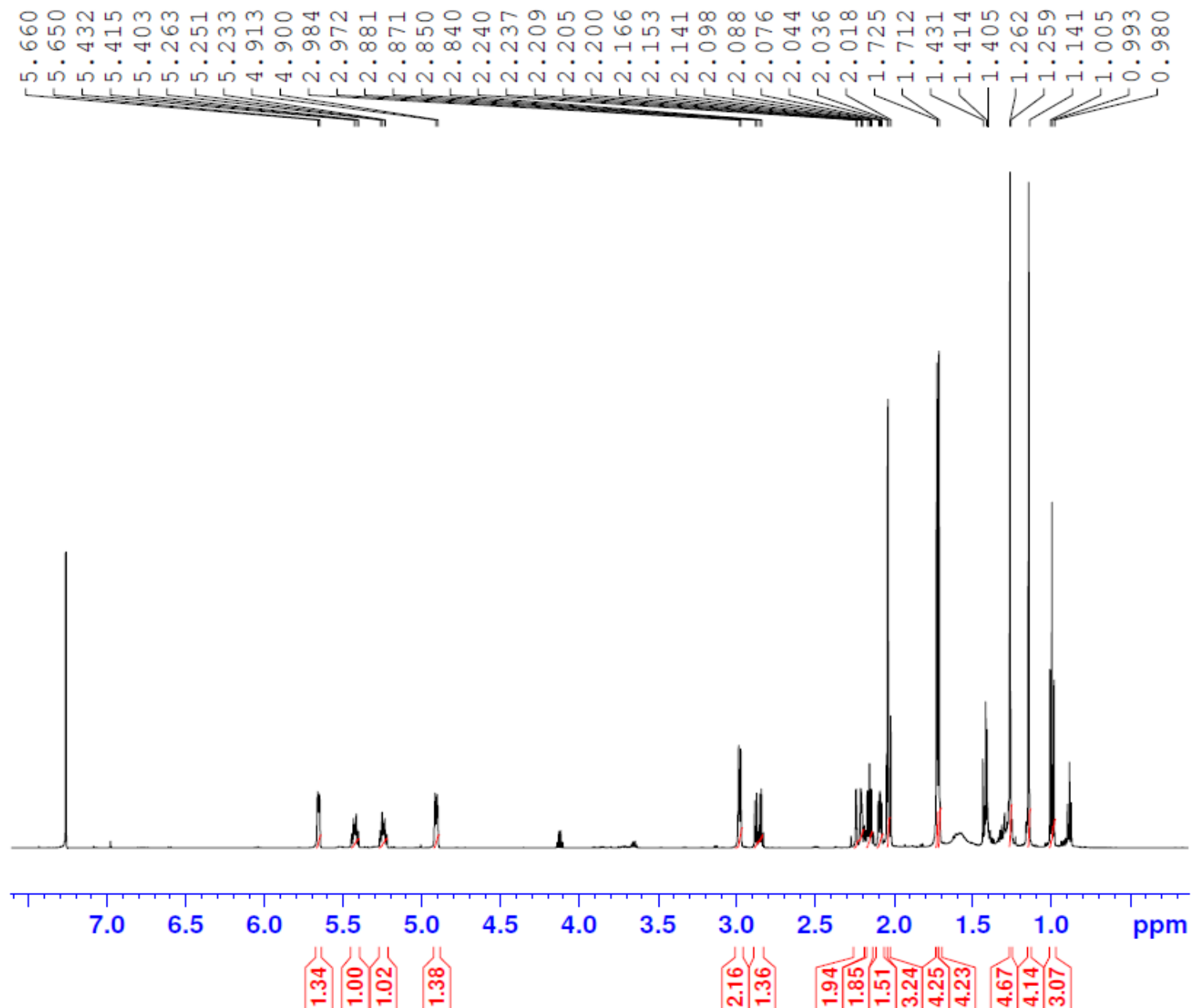
Semi-synthetic **7a** + **53a** mixture NMR Characterisation

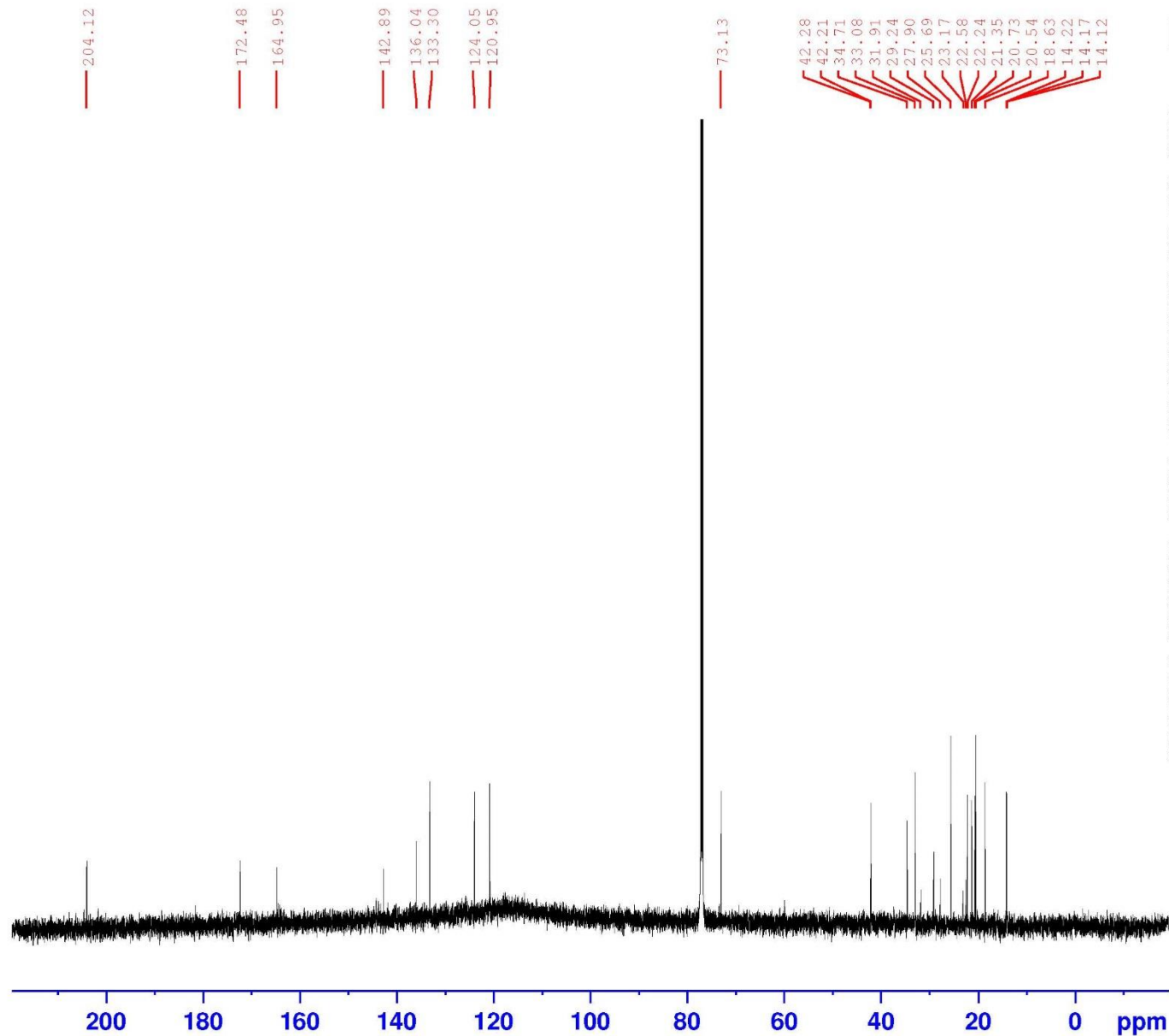
Current Data Parameters
NAME 20180704 Diimide Reduction PI
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180704
Time 18.13
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 181
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 600.1337060 MHz
NUC1 1H
P1 8.40 usec
PLW1 12.55000019 W

F2 - Processing parameters
SI 65536
SF 600.1300237 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00





Current Data Parameters
NAME 20180704 Diimide Reduction PI
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180704
Time 19.12
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 1820
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 16.00 usec
PLW1 110.76000214 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 12.55000019 W
PLW12 0.18072000 W
PLW13 0.08855400 W

F2 - Processing parameters
SI 32768
SF 150.9027915 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20180704 Diimide Reduction PI
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180704
Time 18.15
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG cosygpppgf
TD 2048
SOLVENT CDCl3
NS 1
DS 8
SWH 4672.897 Hz
FIDRES 2.281688 Hz
AQ 0.2191360 sec
RG 64
DW 107.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.90865898 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00021400 sec

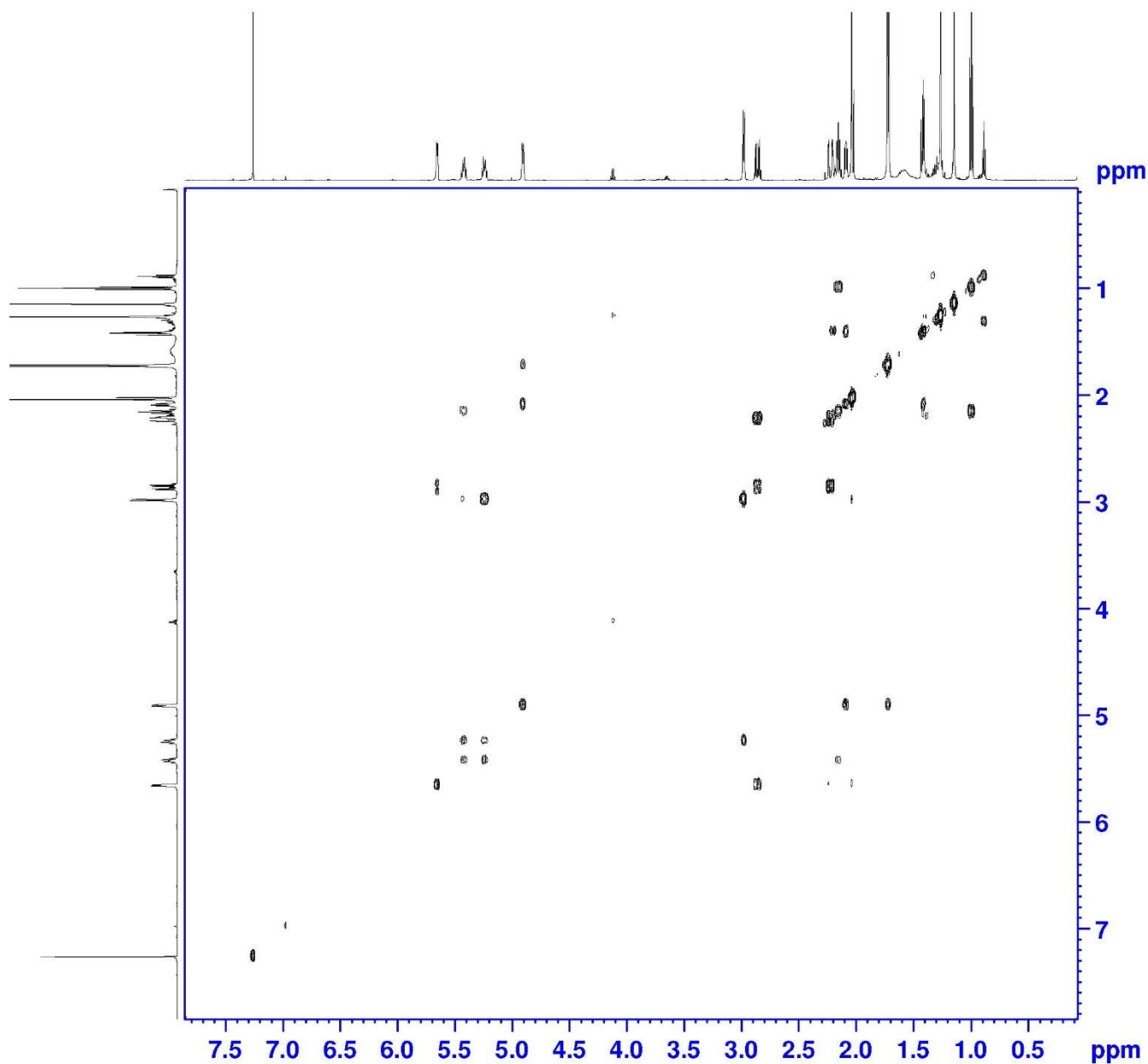
===== CHANNEL f1 =====
SFO1 600.1323996 MHz
NUC1 1H
P0 8.40 usec
P1 8.40 usec
P17 2500.00 usec
PLW1 12.55000019 W
PLW0 1.30999994 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GP21 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1324 MHz
FIDRES 36.507008 Hz
SW 7.786 ppm
EnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300204 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300260 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20180704 Dimide Reduction FI
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180704
Time 19.18

INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG hsqcstgpp
TD 1024
SOLVENT CDCl3
DS 16
SWH 4807.692 Hz
FIDRES 4.695012 Hz
AQ 0.1064960 sec
RG 2050
DW 104.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45904005 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS

===== CHANNEL f1 =====
SFO1 600.1323536 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P28 1000.00 usec
PLW1 12.55000019 W

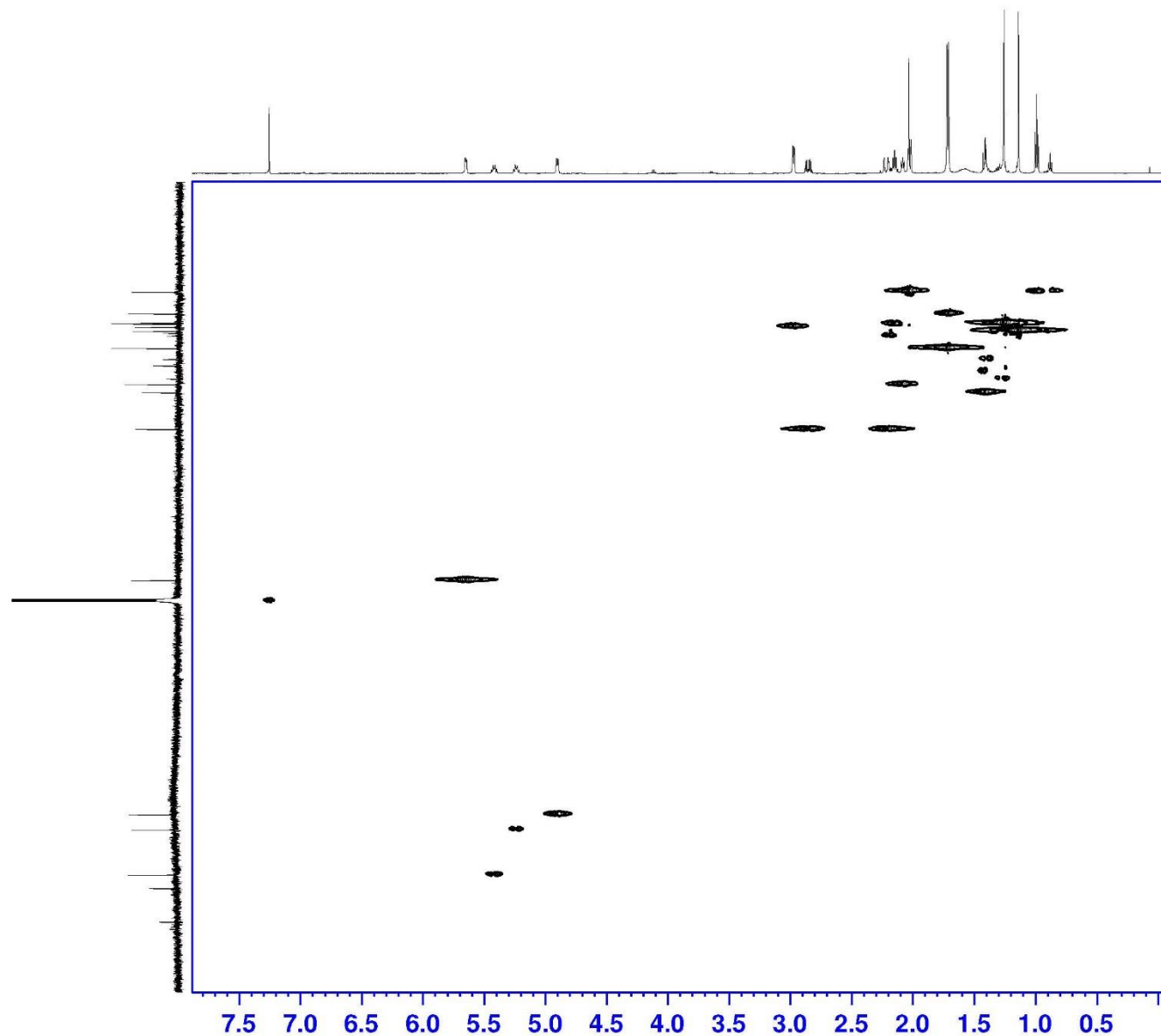
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CDDPRG[2] garrp
P3 16.00 usec
P4 32.00 usec
PCPD2 60.00 usec
PLW2 110.76000214 W
PLW12 7.87610006 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

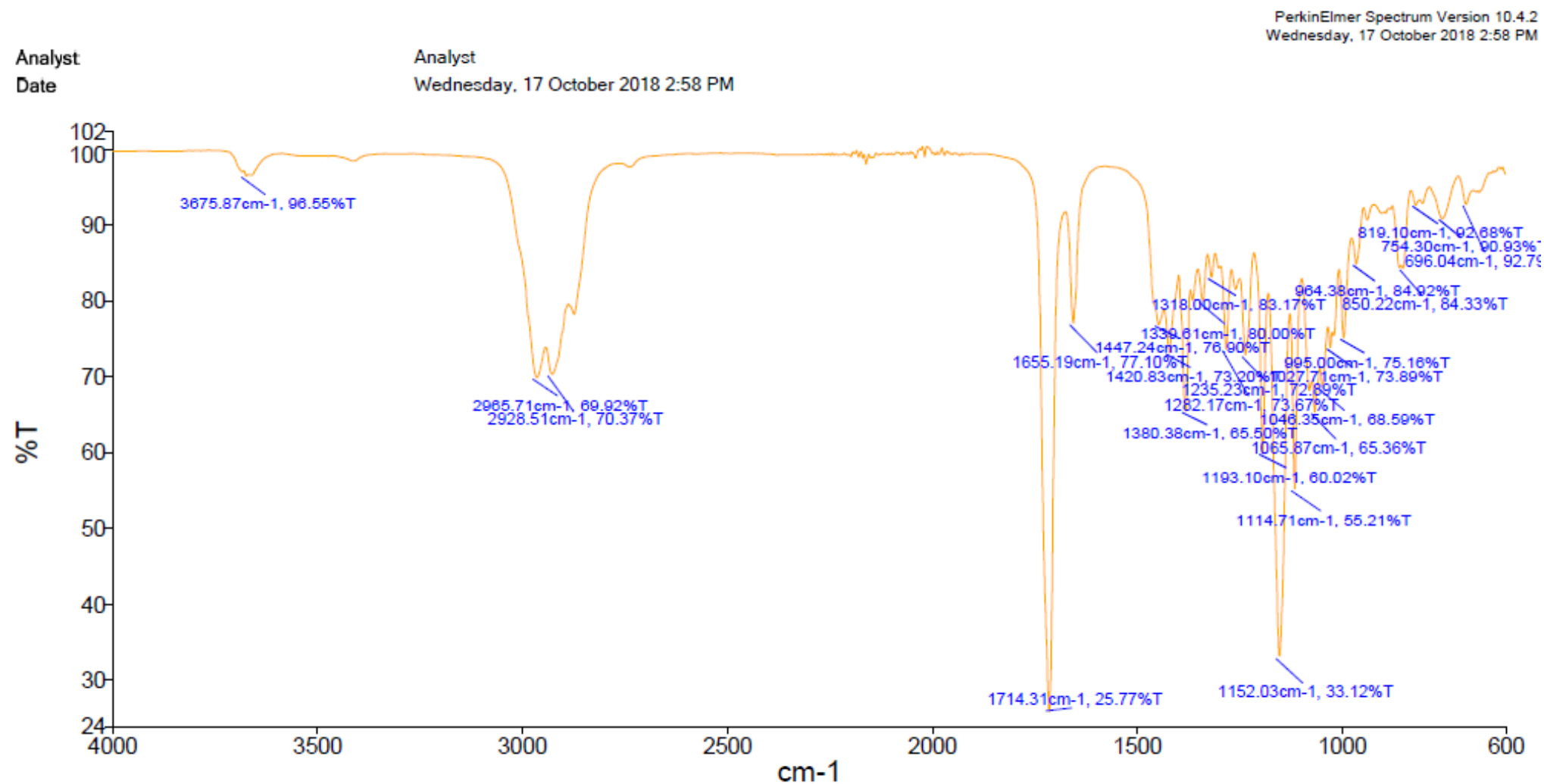
F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300242 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

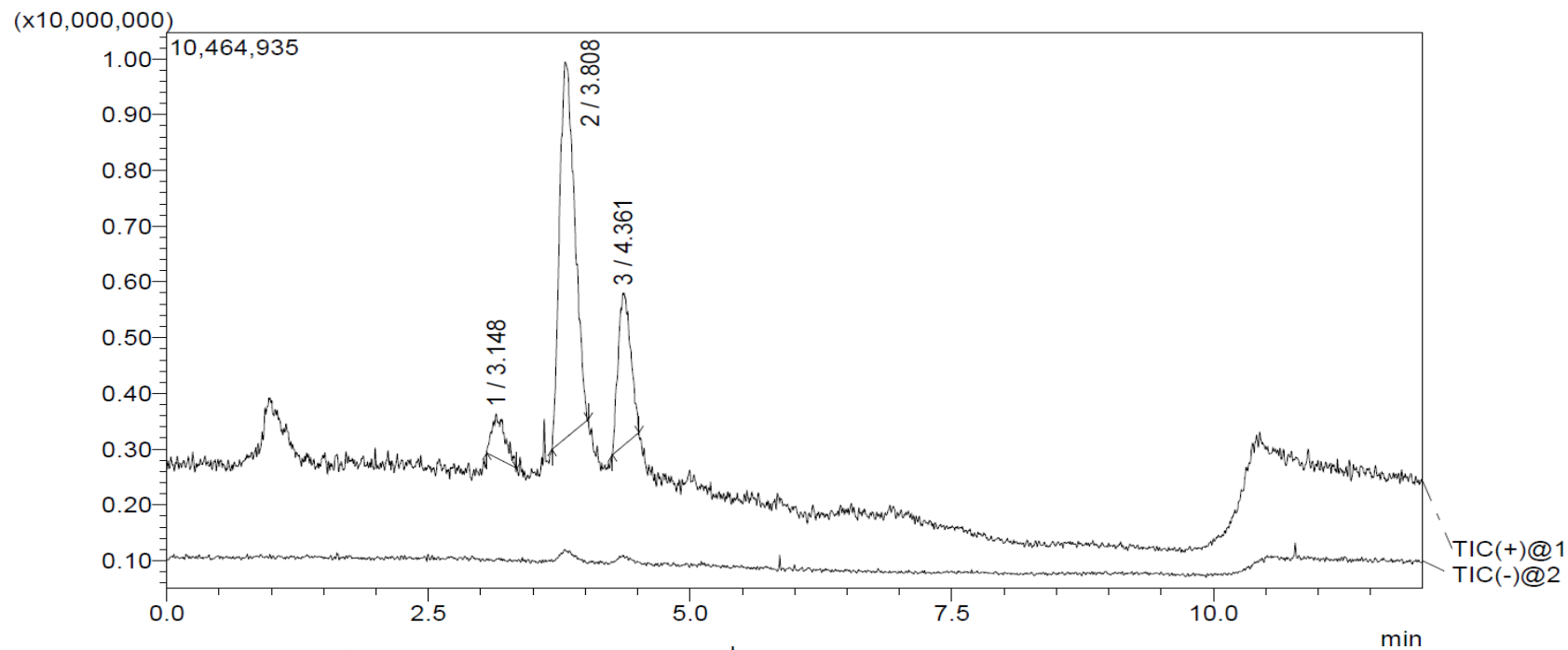
F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9026278 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



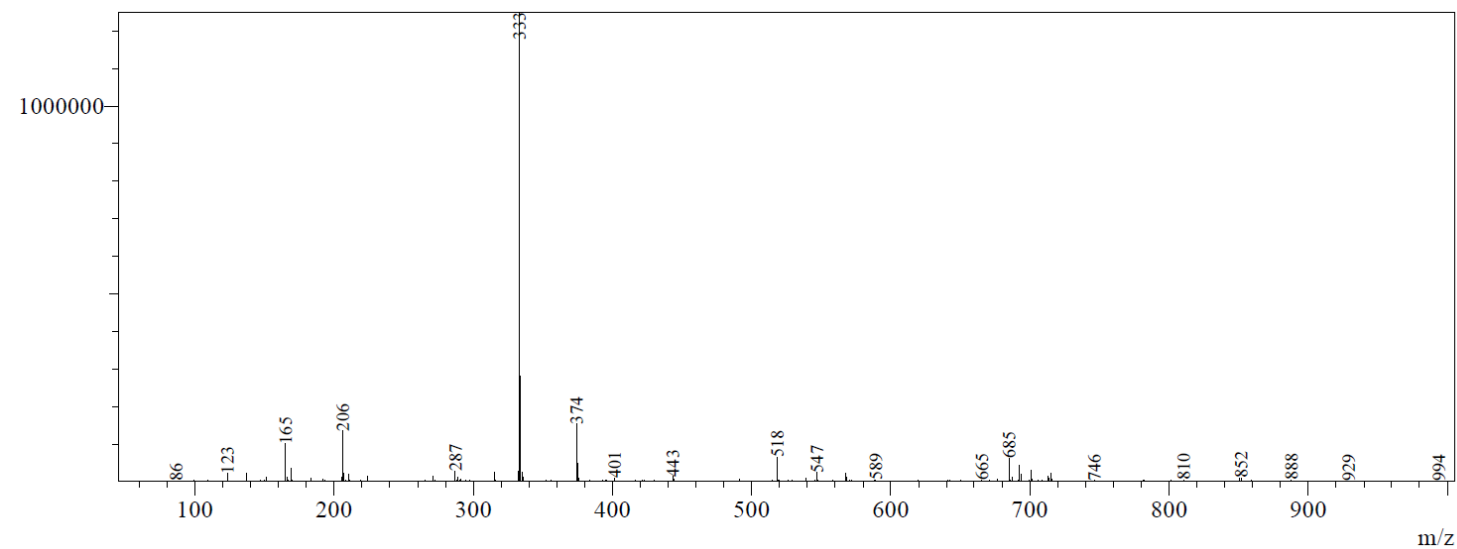
Semi-synthetic 7a + 53a mixture IR Spectrum



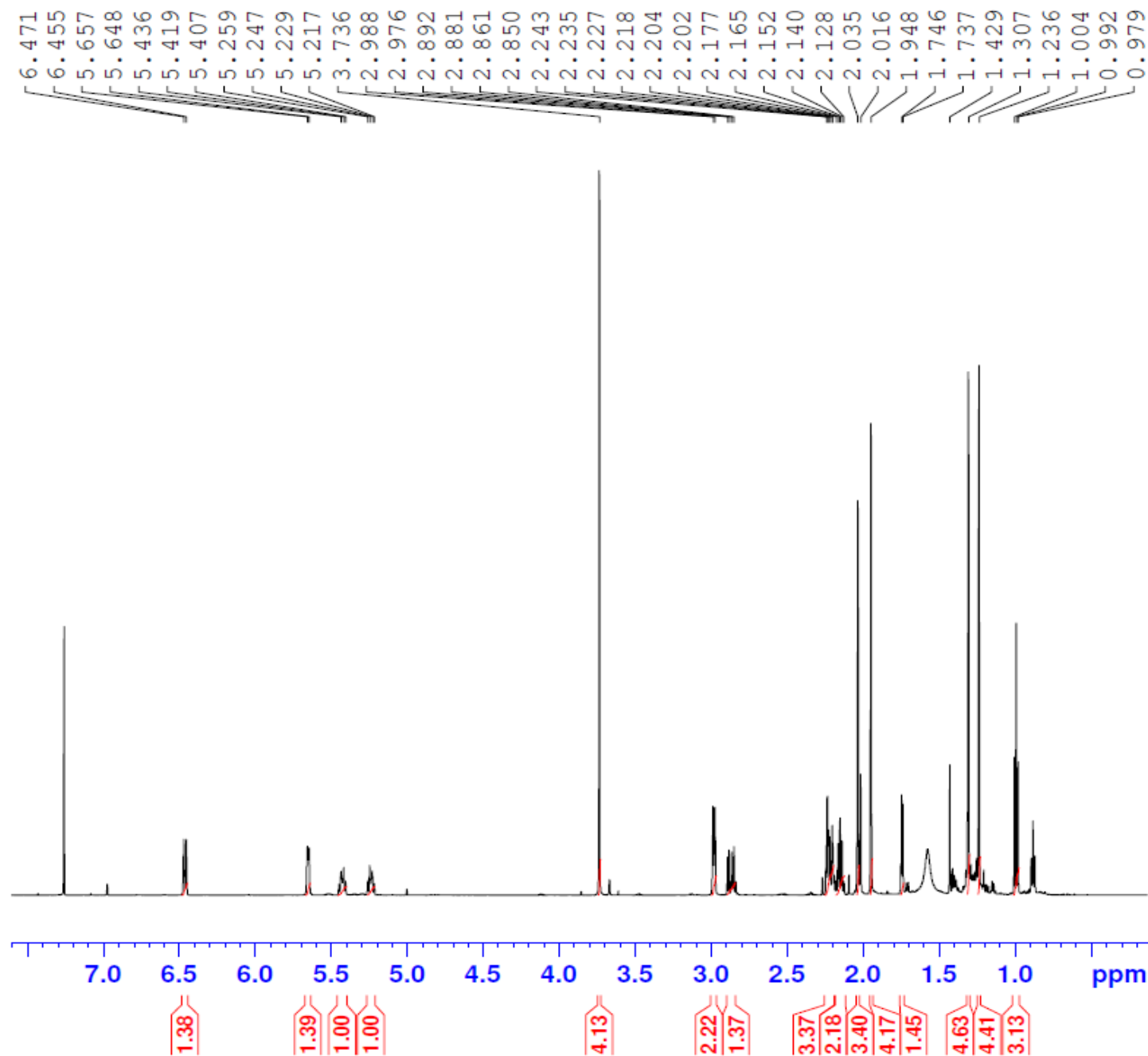
Semi-synthetic 7a + 53a mixture LC-MS



Peak#:3 R.Time:4.361(Scan#:2617)
 MassPeaks:557
 Spectrum Mode:Averaged 4.357-4.363(2615-2619)
 BG Mode:Calc Segment 1 - Event 1



Semi-synthetic **7b** + **53b** mixture NMR Characterisation

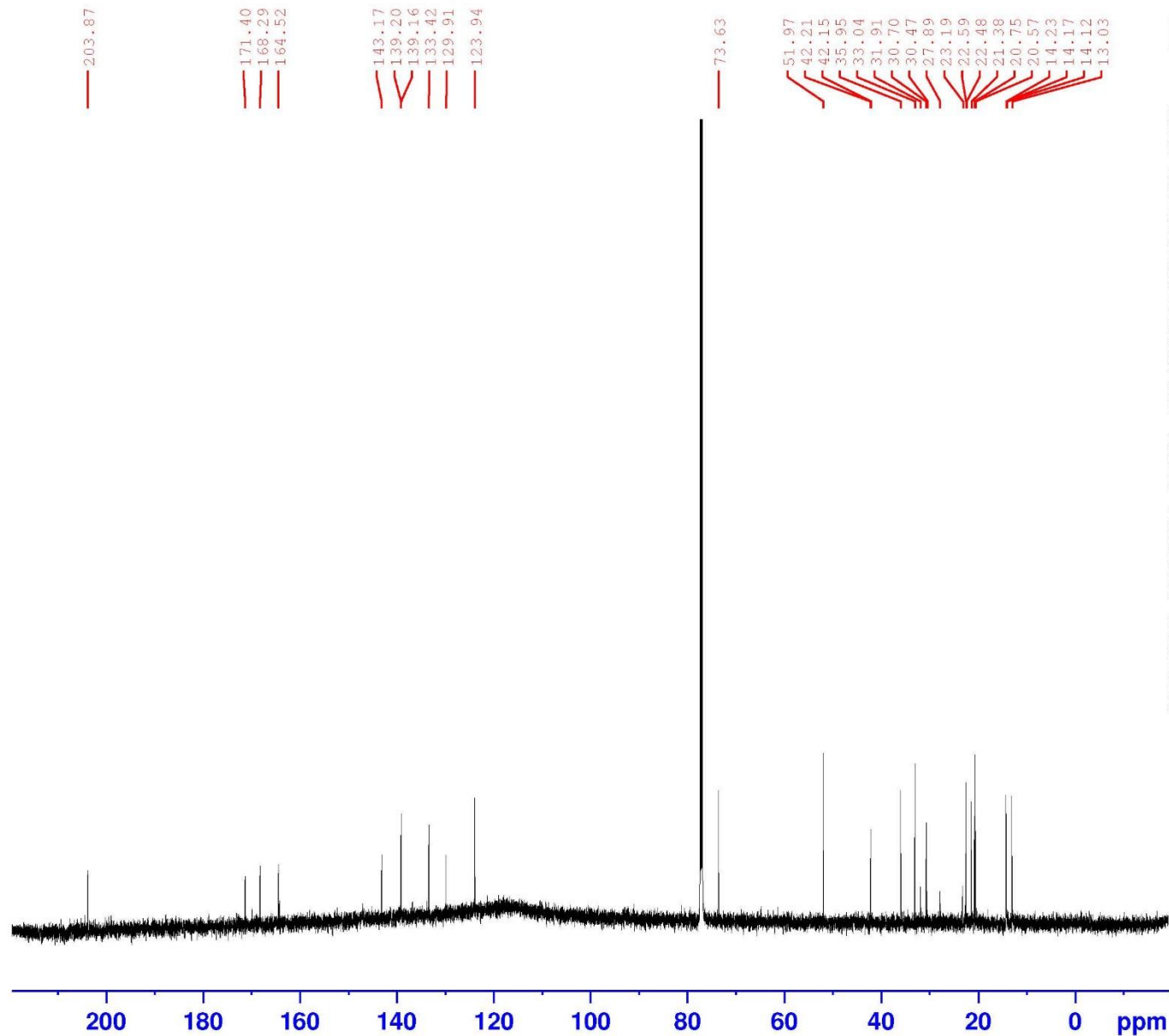


Current Data Parameters
 NAME 20180831 JII (Diimide reduction)
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180831
 Time 18.02
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 203
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 8.40 usec
 PLW1 12.55000019 W

F2 - Processing parameters
 SI 65536
 SF 600.1300252 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20180831 J11 (Diimide reduction)
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180831
Time 19.55
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 1820
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 16.00 usec
PLW1 110.76000214 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 12.55000019 W
PLW12 0.18072000 W
PLW13 0.08855400 W

F2 - Processing parameters
SI 32768
SF 150.9027891 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20180831 JII (Diimide reduction)
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180831
Time 20.19
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG cosygmphpp
TD 2048
SOLVENT CDCl3
NS 15
DS 4
SWH 4854.369 Hz
FIDRES 2.370297 Hz
AQ 0.2109440 sec
RG 2050
DW 103.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00009230 sec
D1 1.32750096 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
TNO 0.00020600 sec

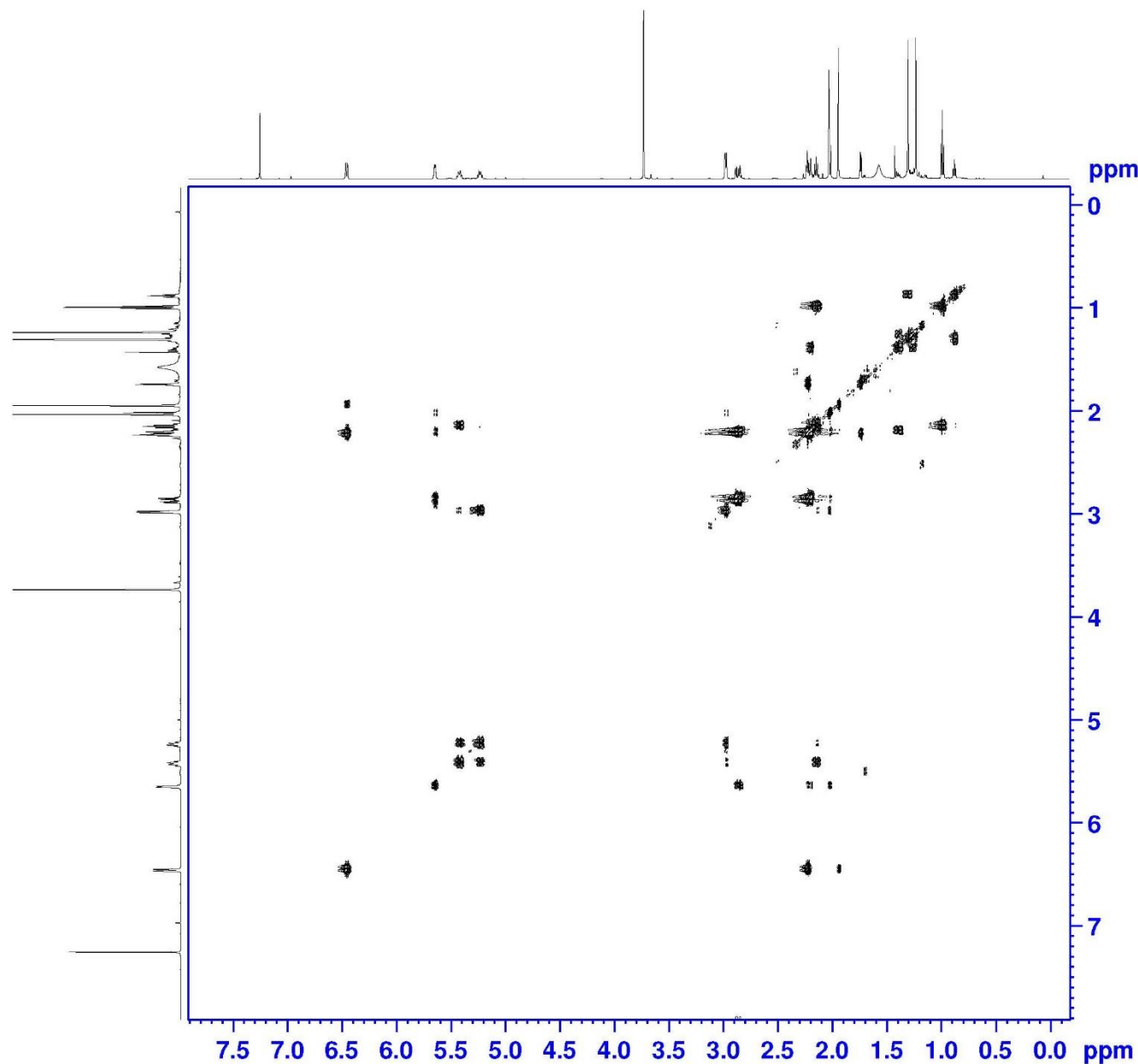
===== CHANNEL f1 =====
SFO1 600.1323522 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P17 2500.00 usec
PLW1 12.55000019 W
PLW10 1.30999994 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GEZ1 10.00 %
GEZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1324 MHz
FIDRES 18.962379 Hz
SW 8.089 ppm
FMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.1300312 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300305 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20180831 J11 (Diimide reduction)
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180831
Time 22:52
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG hsqcstgpp
TD 1024
SOLVENT CDCl3
DS 16
SWH 4854.369 Hz
FIDRES 4.740595 Hz
AQ 0.1054720 sec
RG 2050
DW 103.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46006405 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS

===== CHANNEL f1 =====
SFO1 600.1323522 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P28 1000.00 usec
PLW1 12.55000019 W

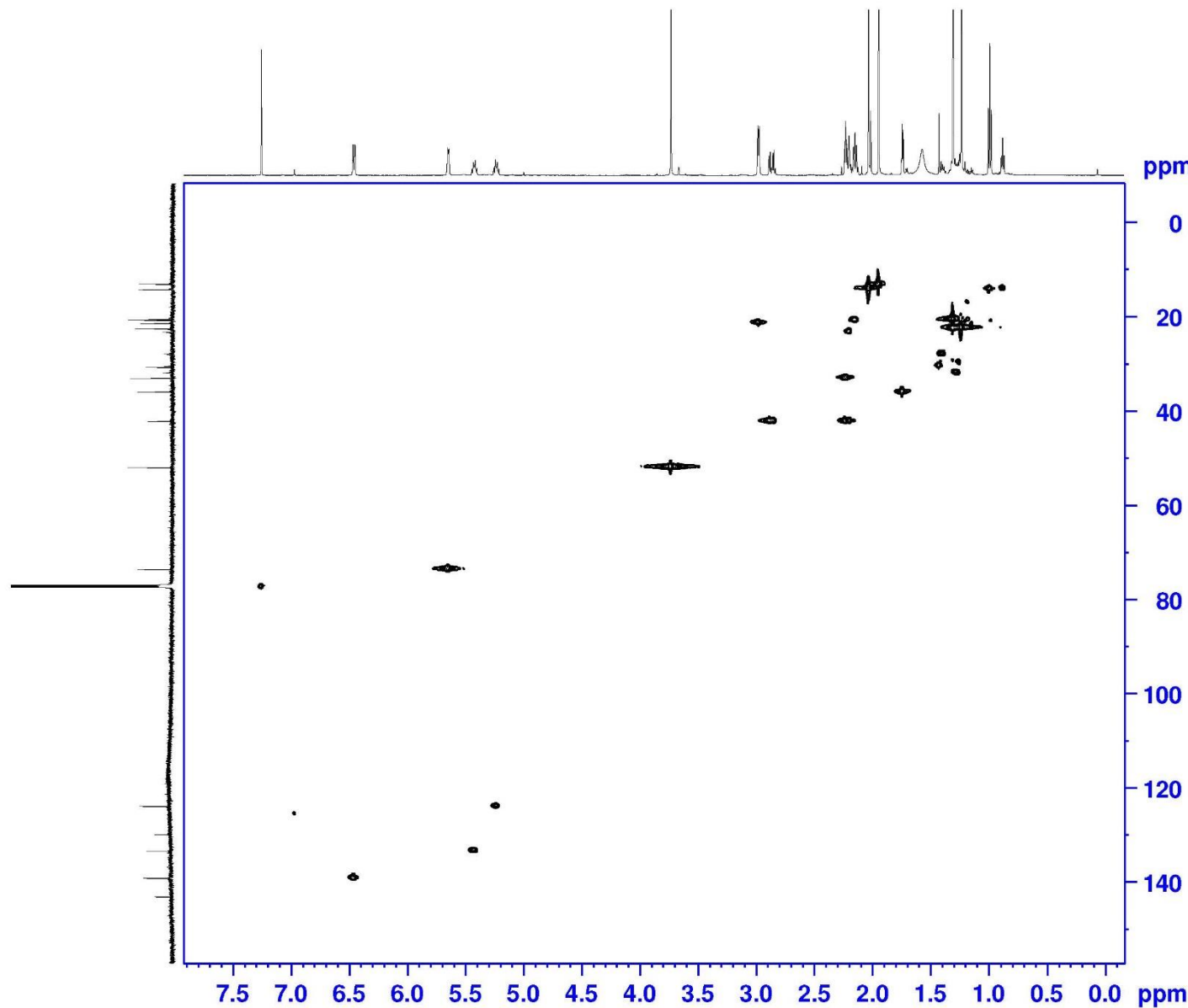
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CDDPRG2 garrp
P3 16.00 usec
P4 32.00 usec
PCPD2 60.00 usec
PLW2 110.76000214 W
PLW12 7.87610006 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

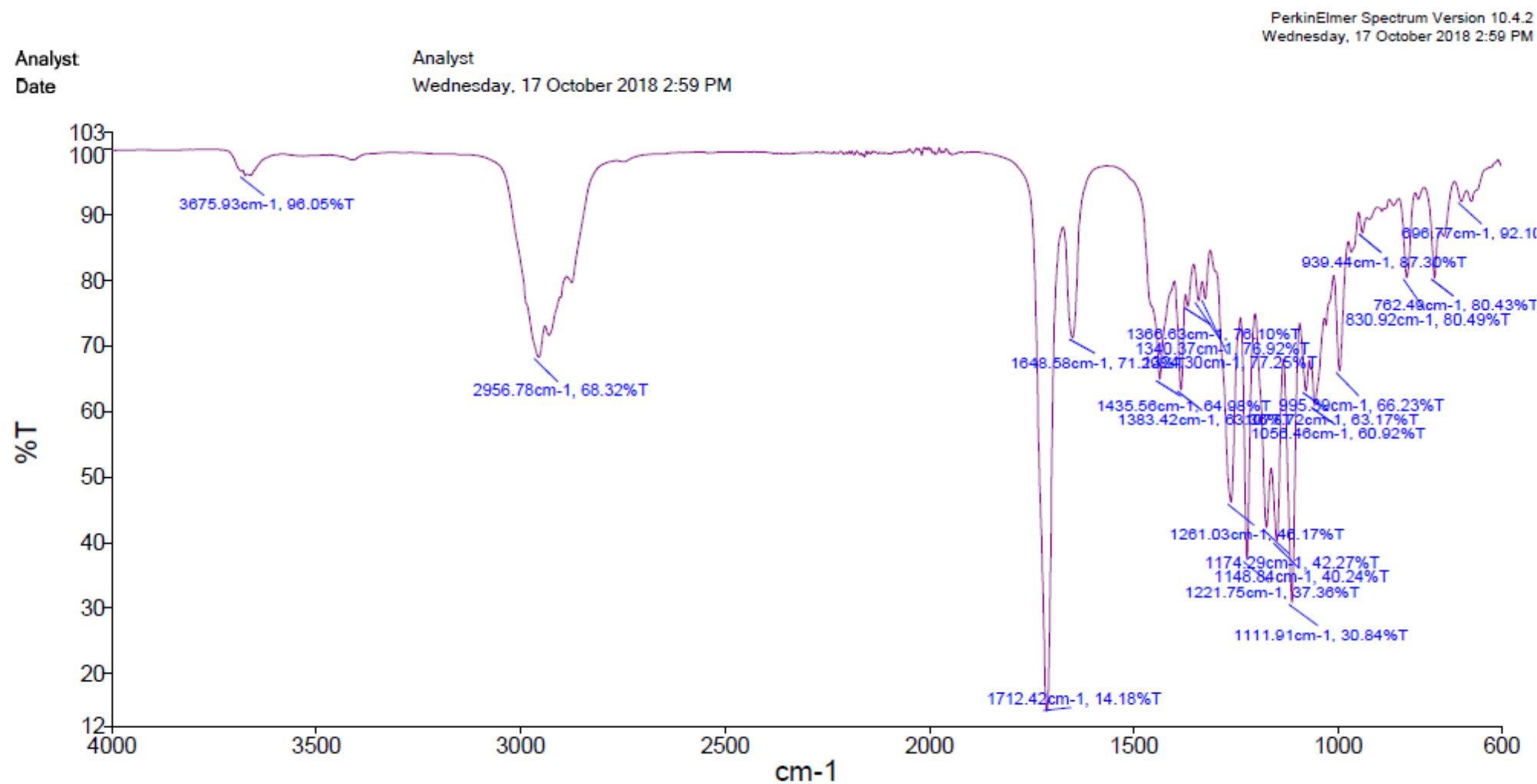
F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300246 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

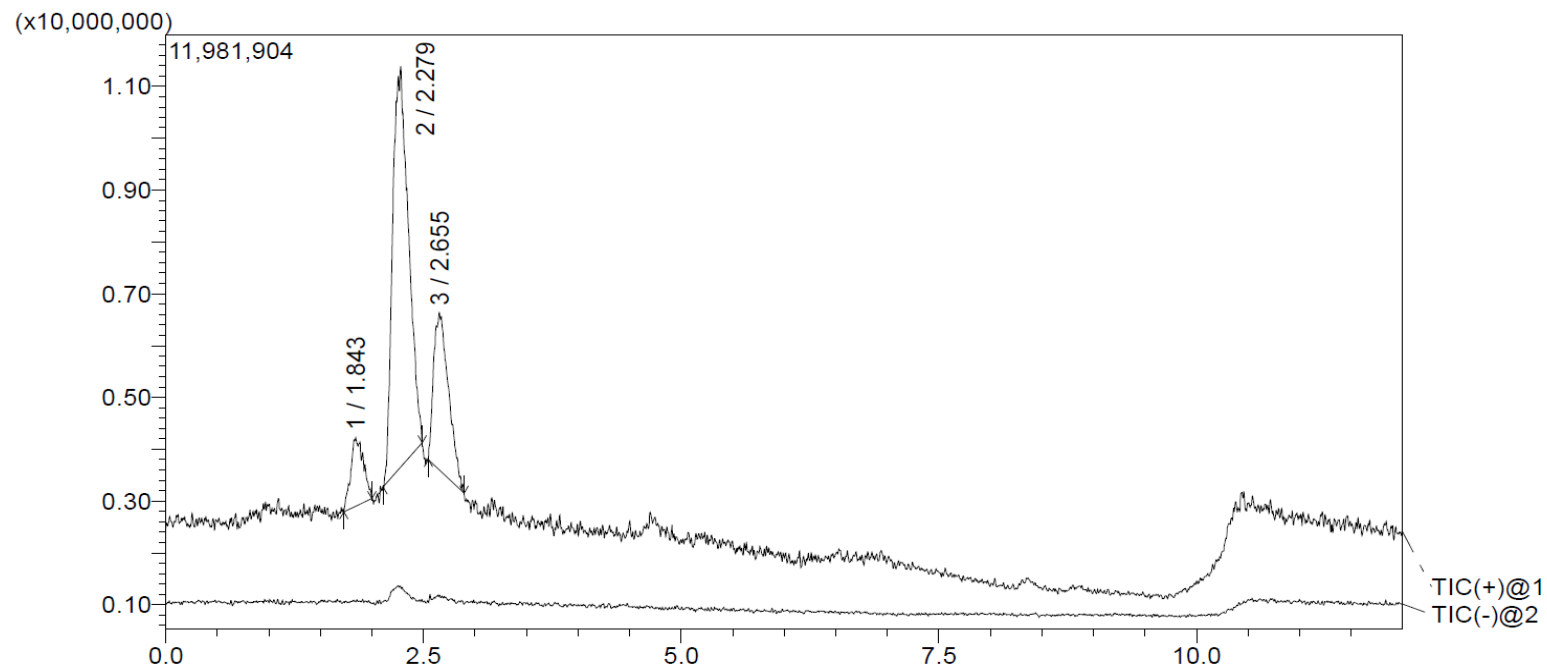
F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028264 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



Semi-synthetic 7b + 53b mixture IR Spectrum

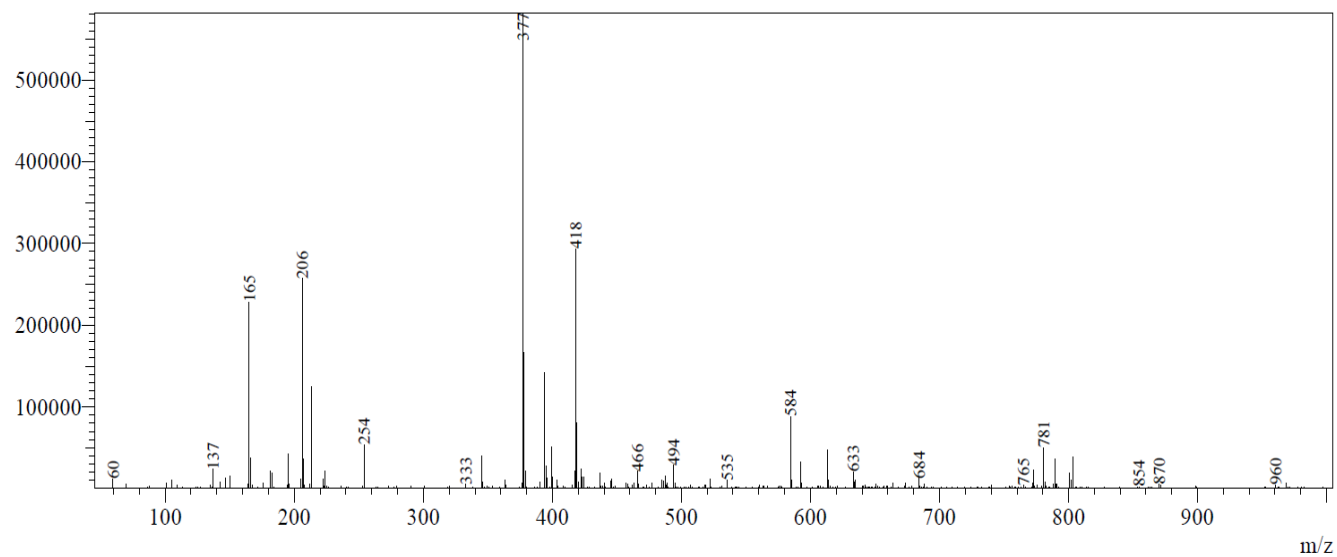


Semi-synthetic **7b** + **53b** mixture LC-MS

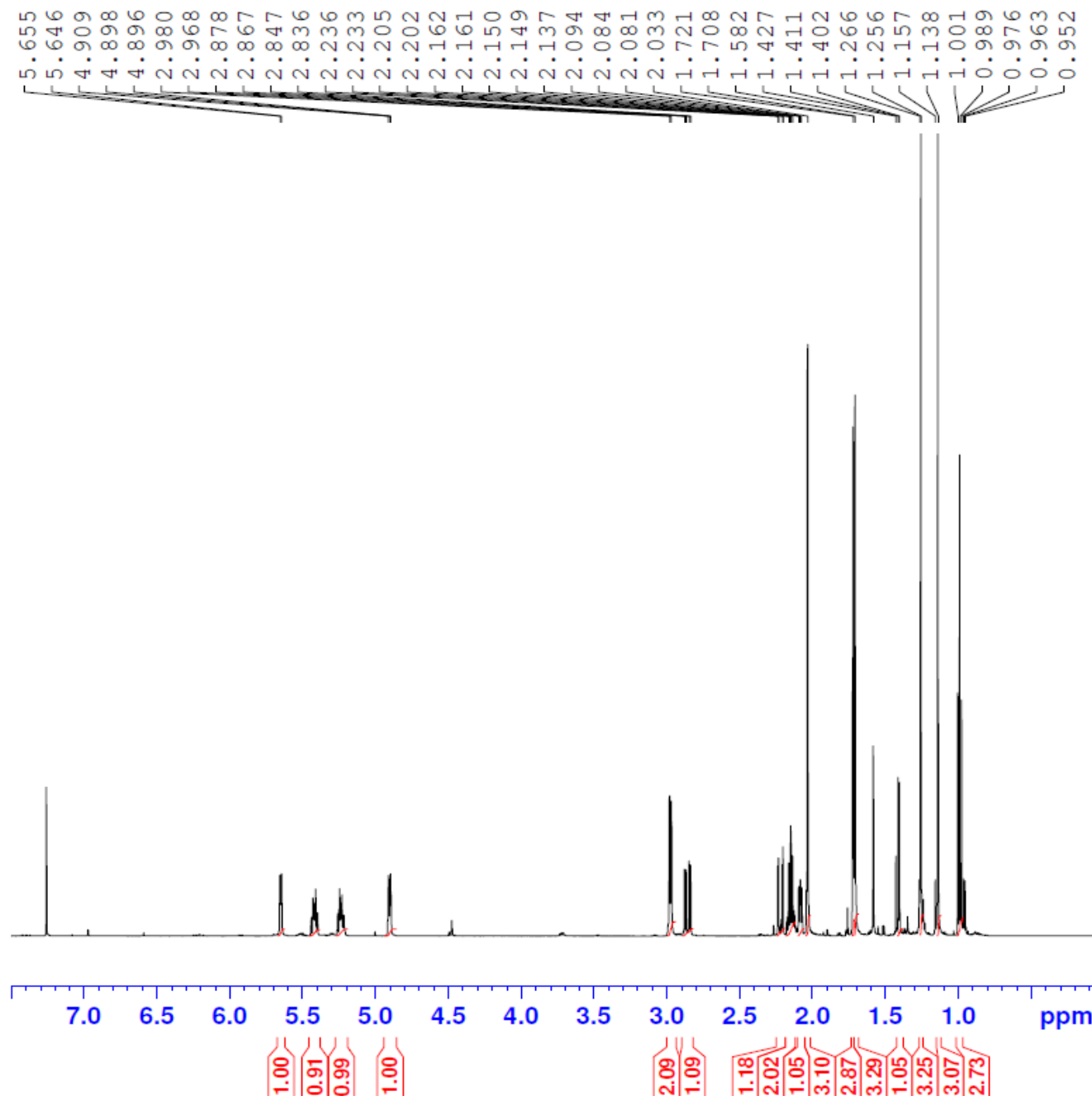


Peak#3 R.Time:2.655(Scan#:1593)
 MassPeaks:607
 Spectrum Mode:Averaged 2.650-2.657(1591-1595)
 BG Mode:Calc Segment 1 - Event 1

7b MS



Natural 7a NMR Characterisation

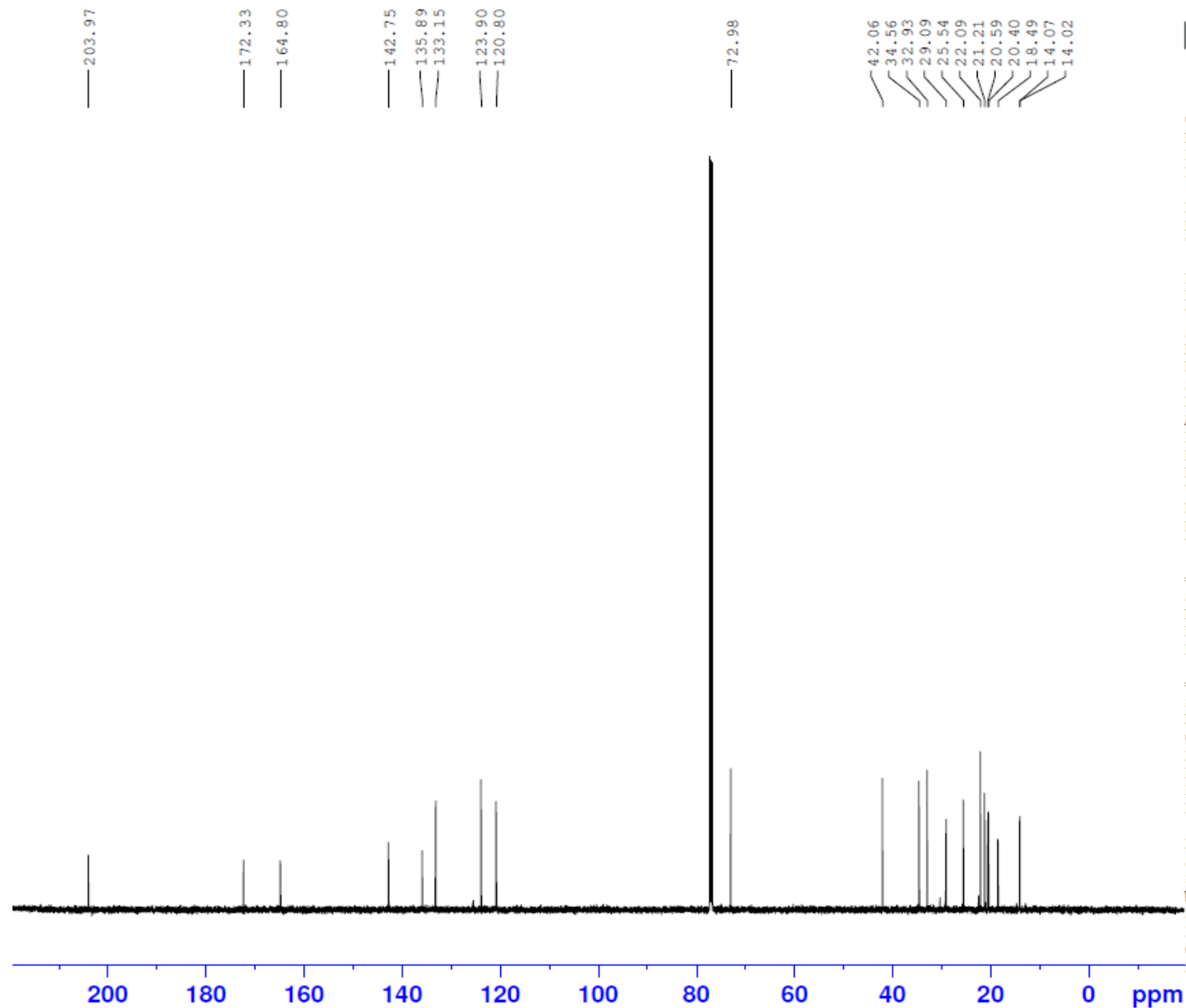


Current Data Parameters
 NAME Natural Jasmolin I
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191022
 Time 17.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 161
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300262 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME Natural Jasmolin I
 EXPNO 11
 PROCNO 1

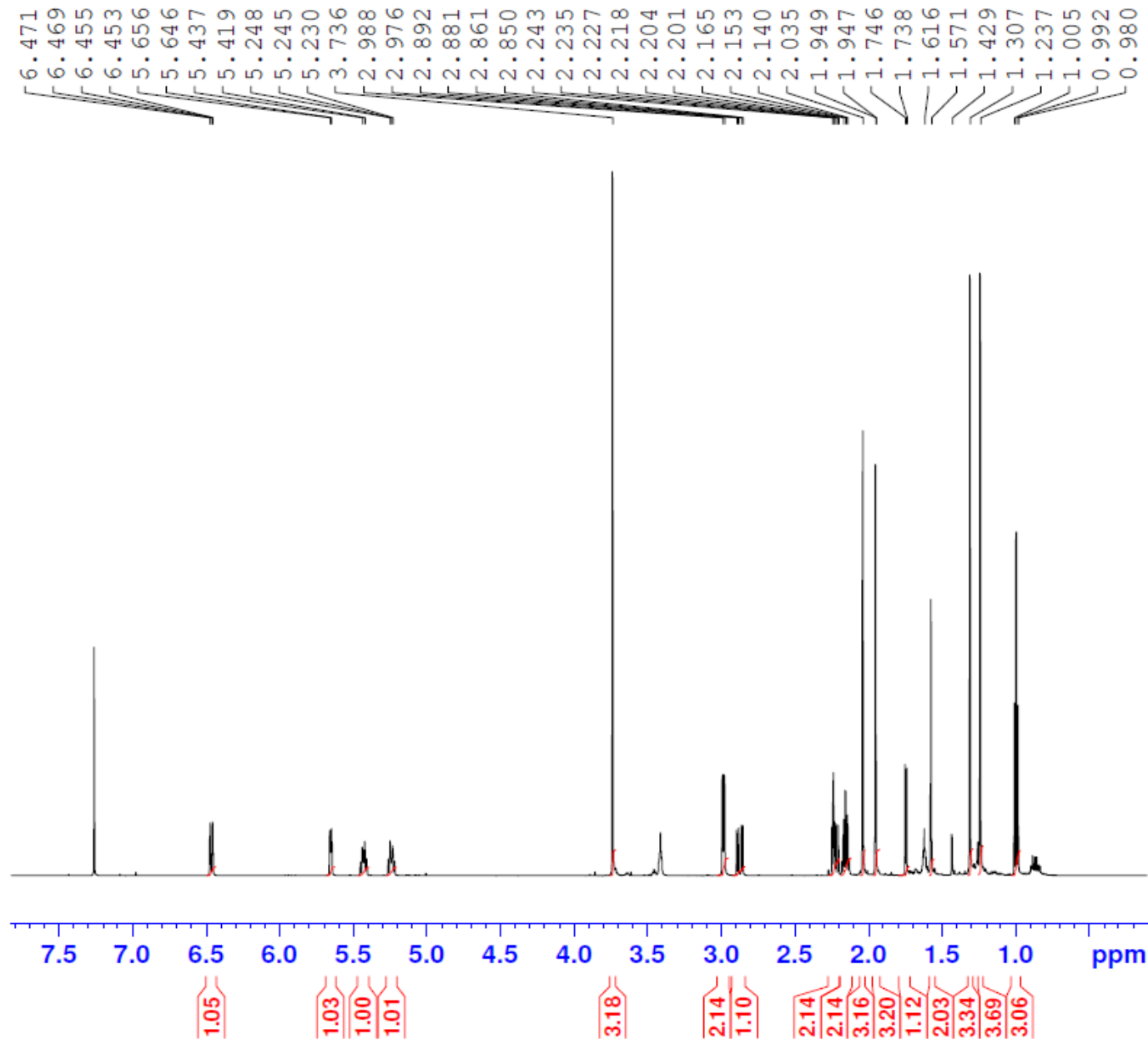
F2 - Acquisition Parameters
 Date_ 20191022
 Time 17.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 603
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028135 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Natural **7b** NMR Characterisation

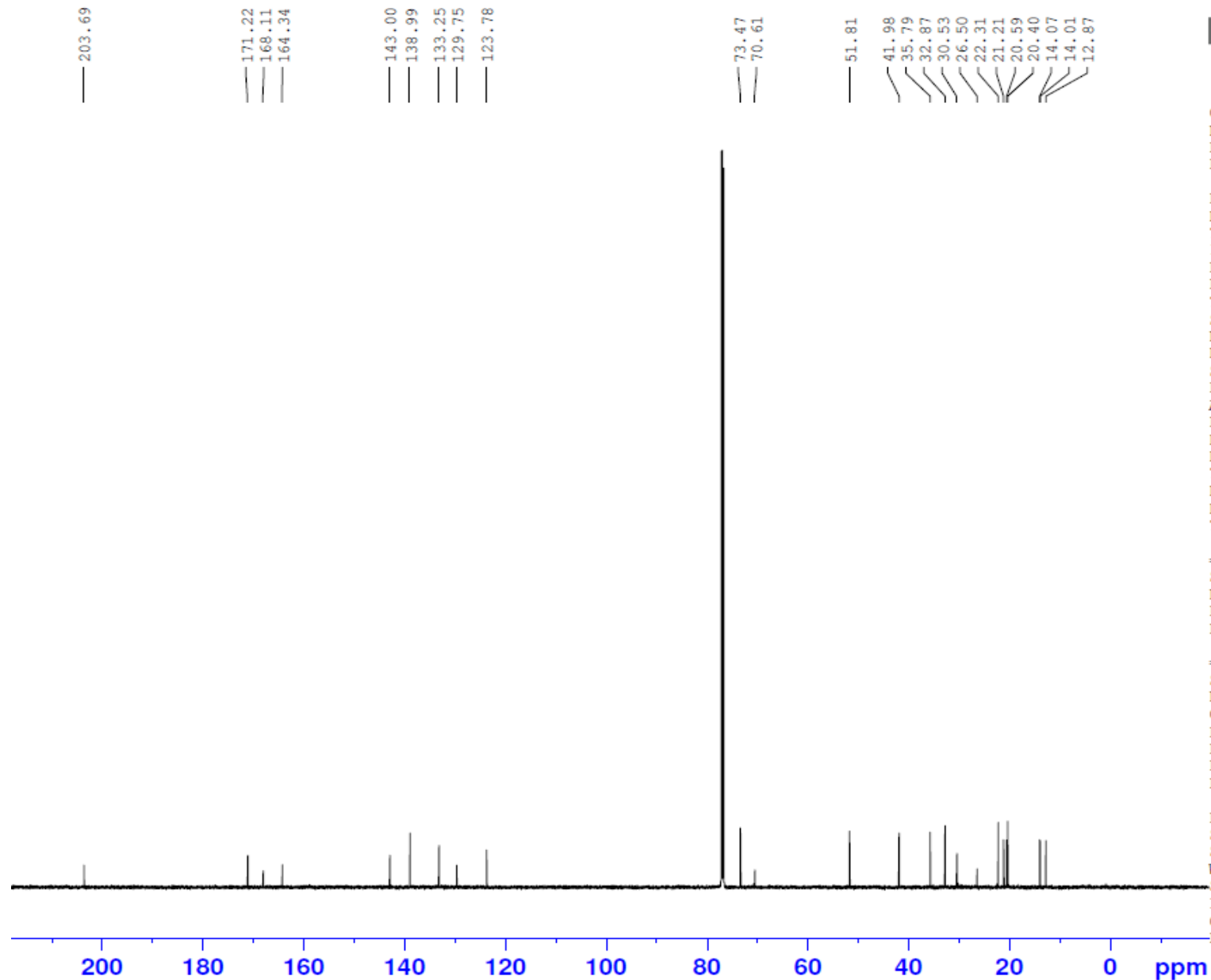


Current Data Parameters
 NAME Natural Jasmolin II
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191022
 Time 17.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 228
 DW 41.600 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300260 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME Natural Jasmolin II
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191022
 Time 19.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

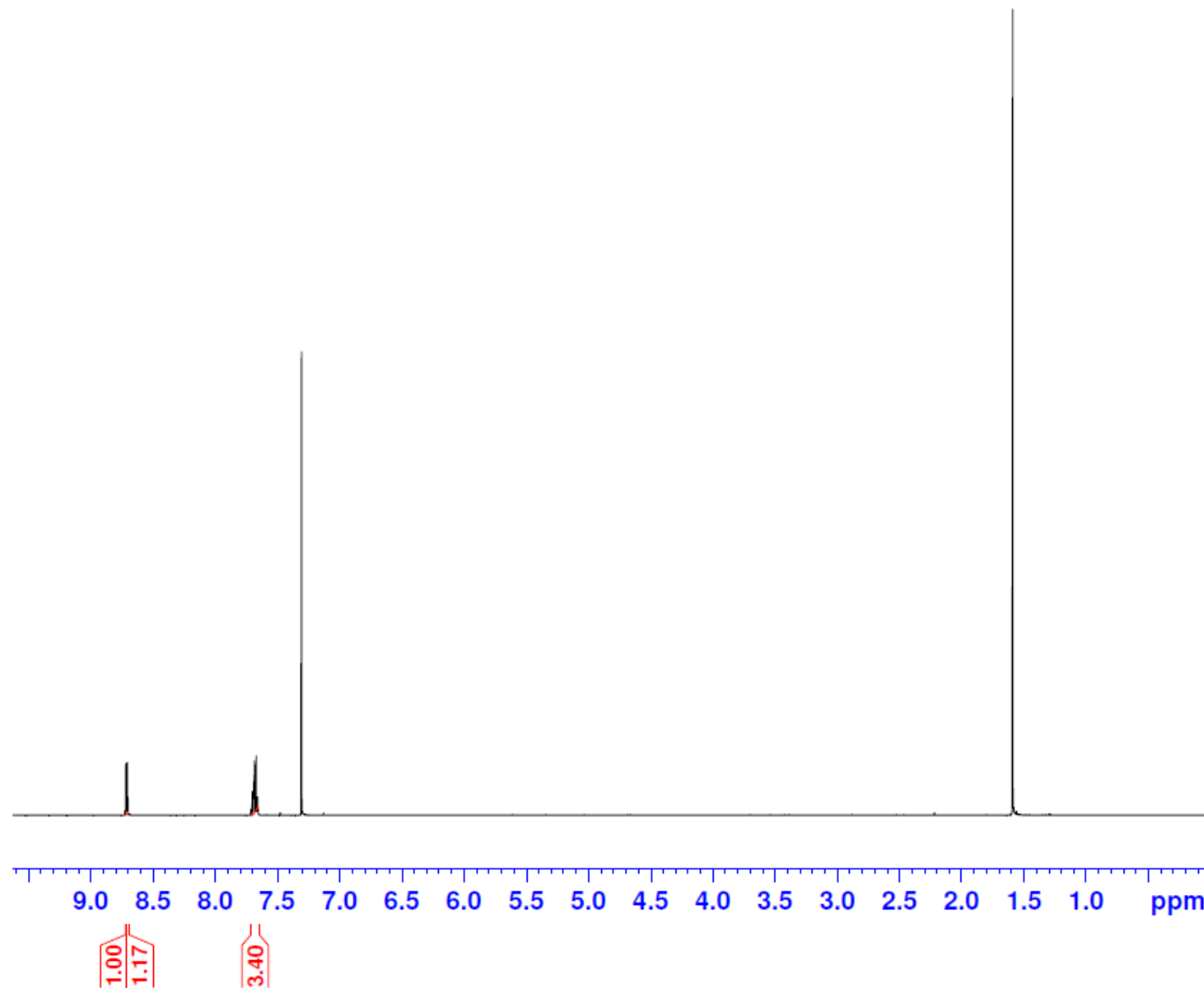
===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028144 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Diels-Alder Chemistry Characterisation Data

71 NMR Characterisation

8.715
8.712
8.704
8.701
7.698
7.689
7.686
7.683
7.680
7.678
7.672
7.670
7.668
7.657
7.654



Current Data Parameters
NAME Bisphenyltetrazine
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191108
Time 16.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 406
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300000 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



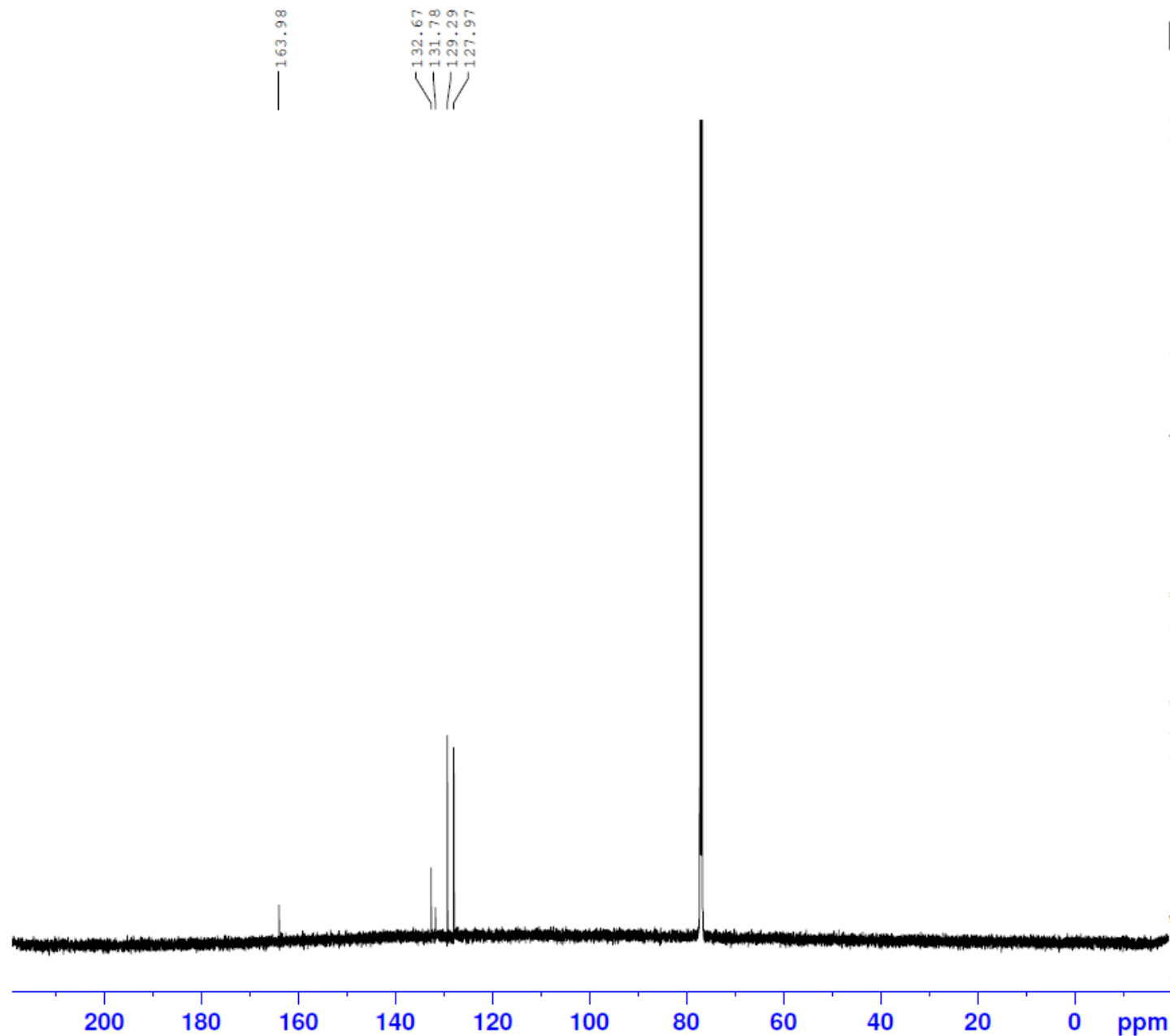
Current Data Parameters
NAME Bisphenyltetrazine
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191109
Time 7.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

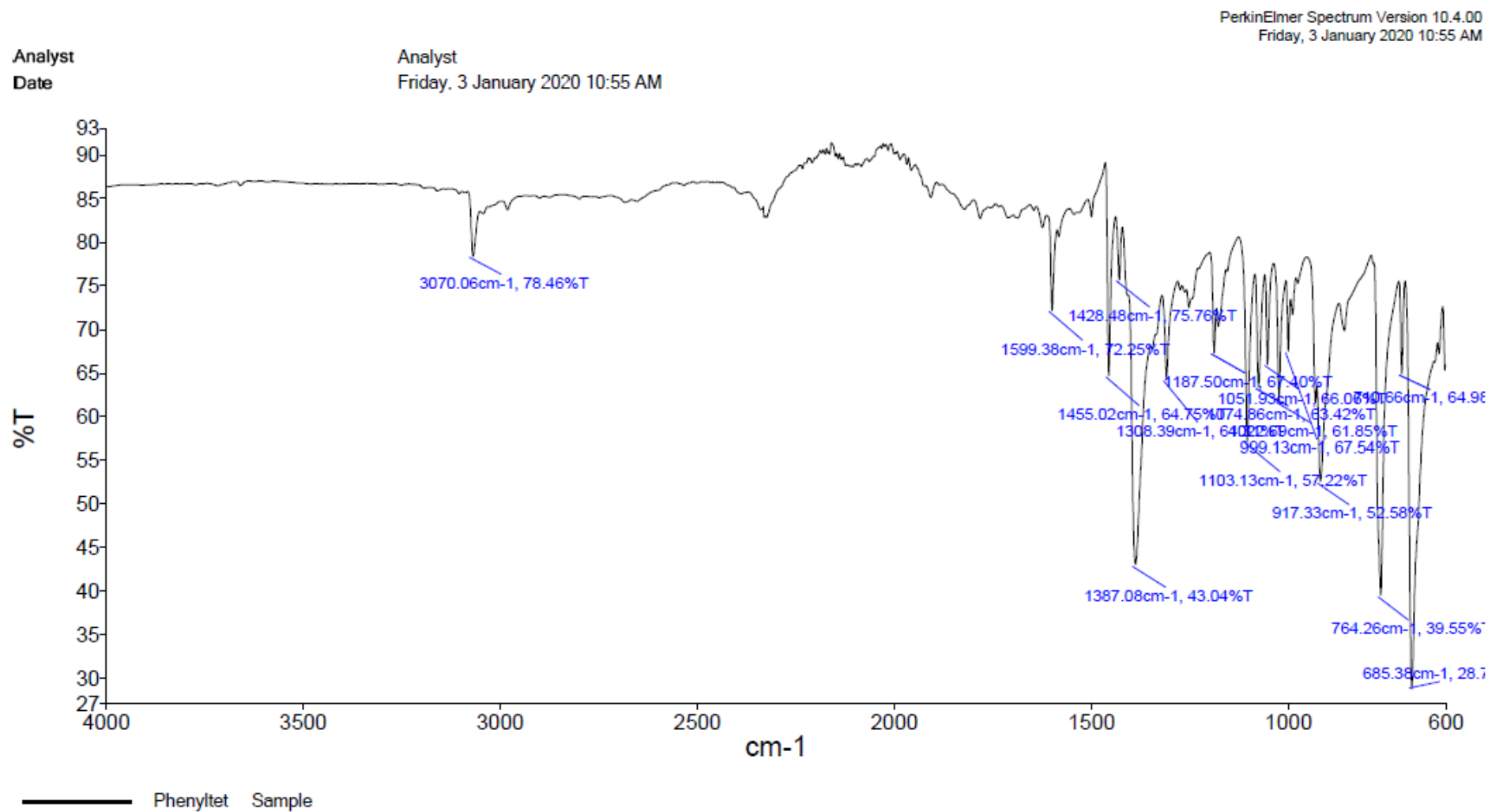
===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

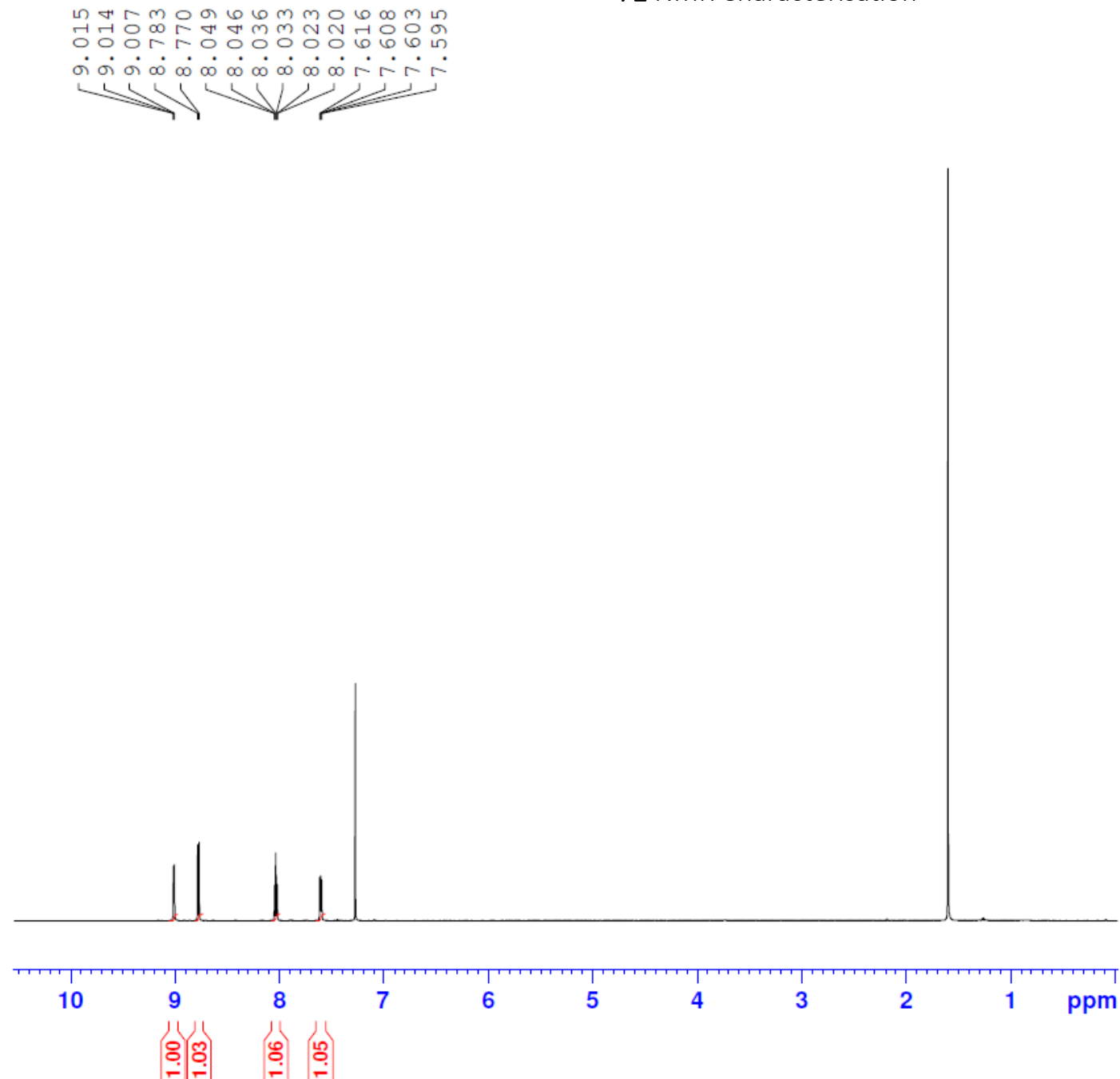
F2 - Processing parameters
SI 32768
SF 150.9028172 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



71 IR Spectrum



72 NMR Characterisation



Current Data Parameters
 NAME 20190929 2pytetrazine
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190929
 Time 11.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 362
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300175 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



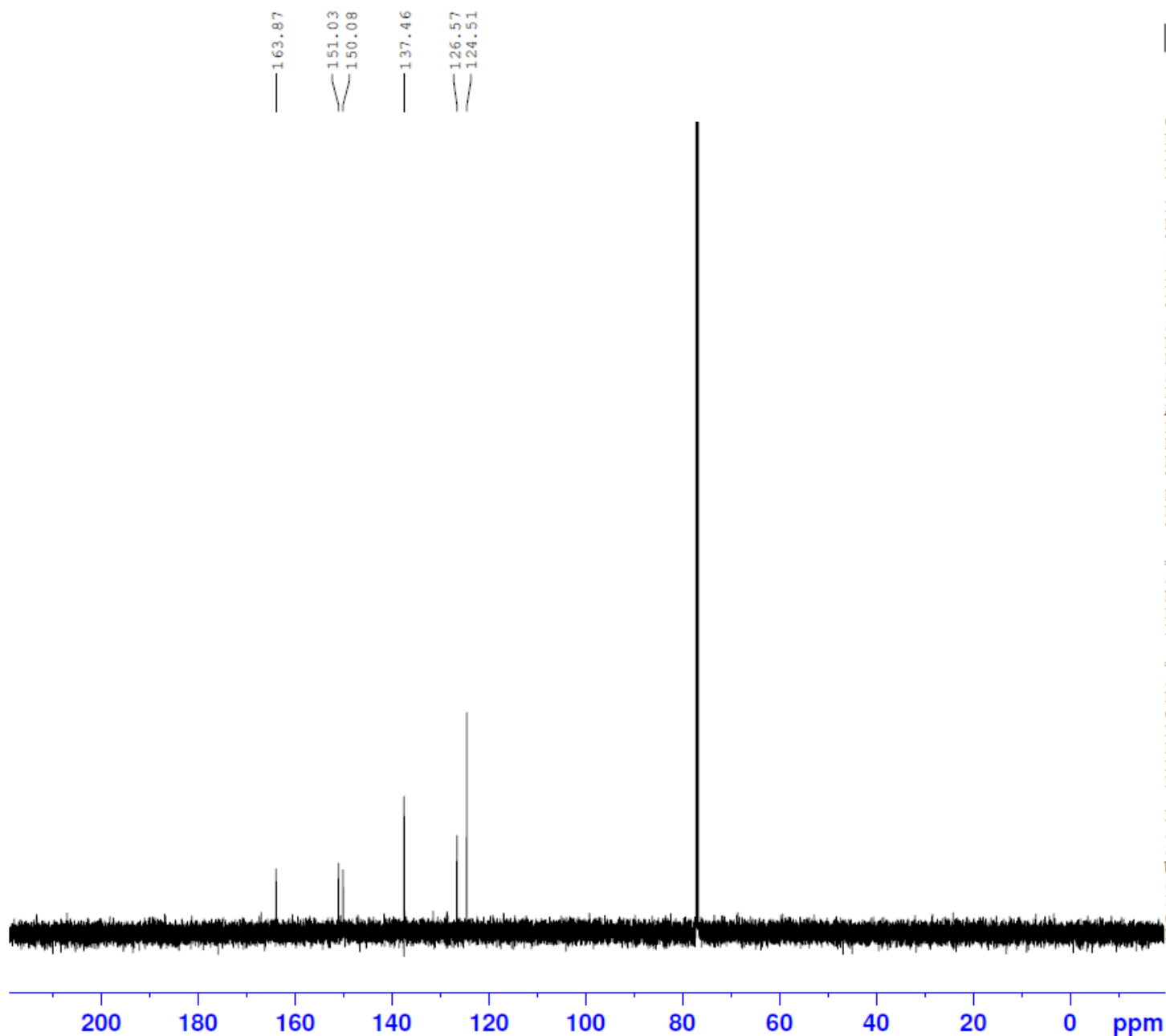
Current Data Parameters
NAME 20190929 2pytetrazine
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190930
Time 9.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 432
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

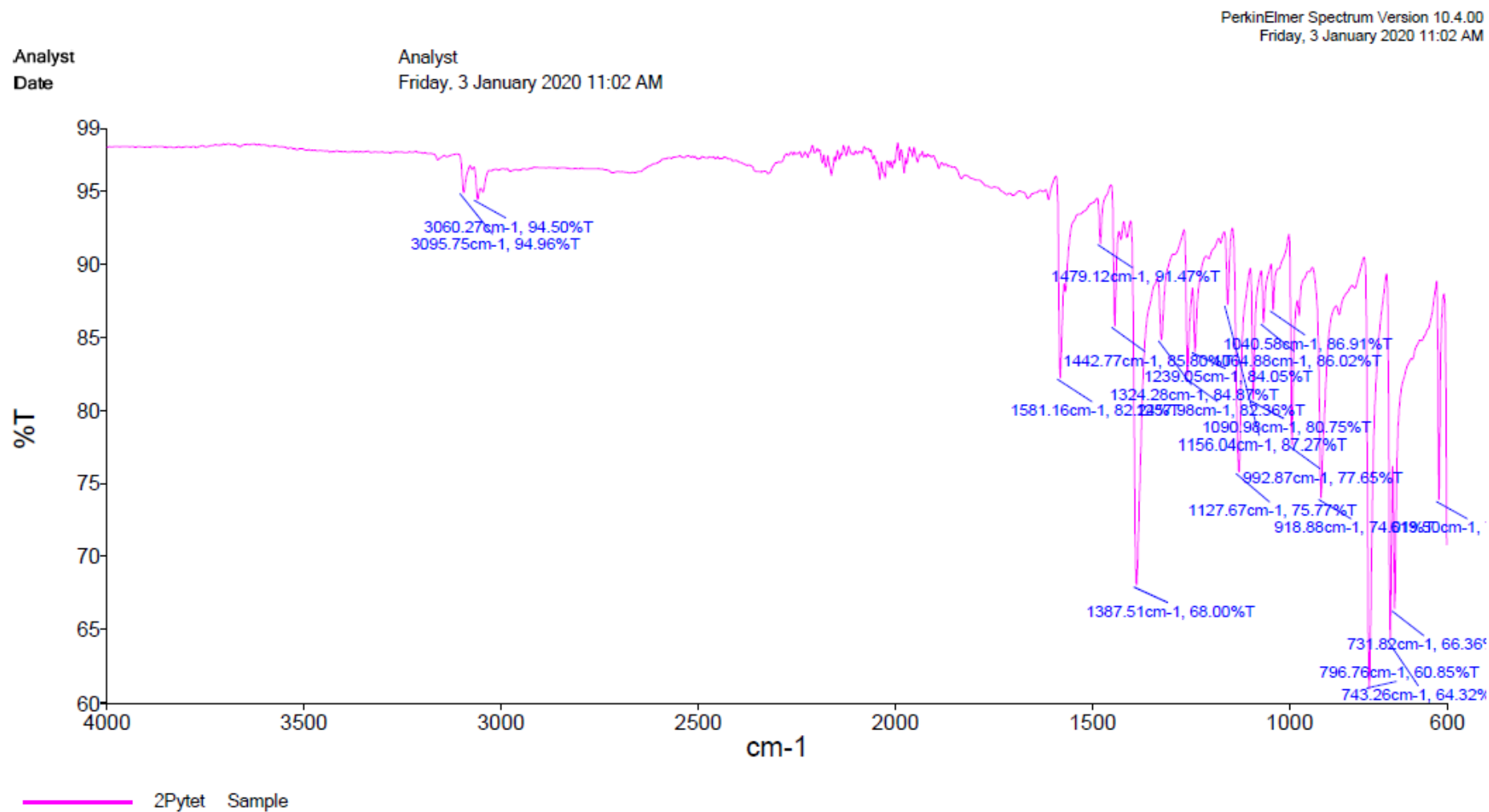
===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028165 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.40



72 IR Spectrum



73 NMR Characterisation

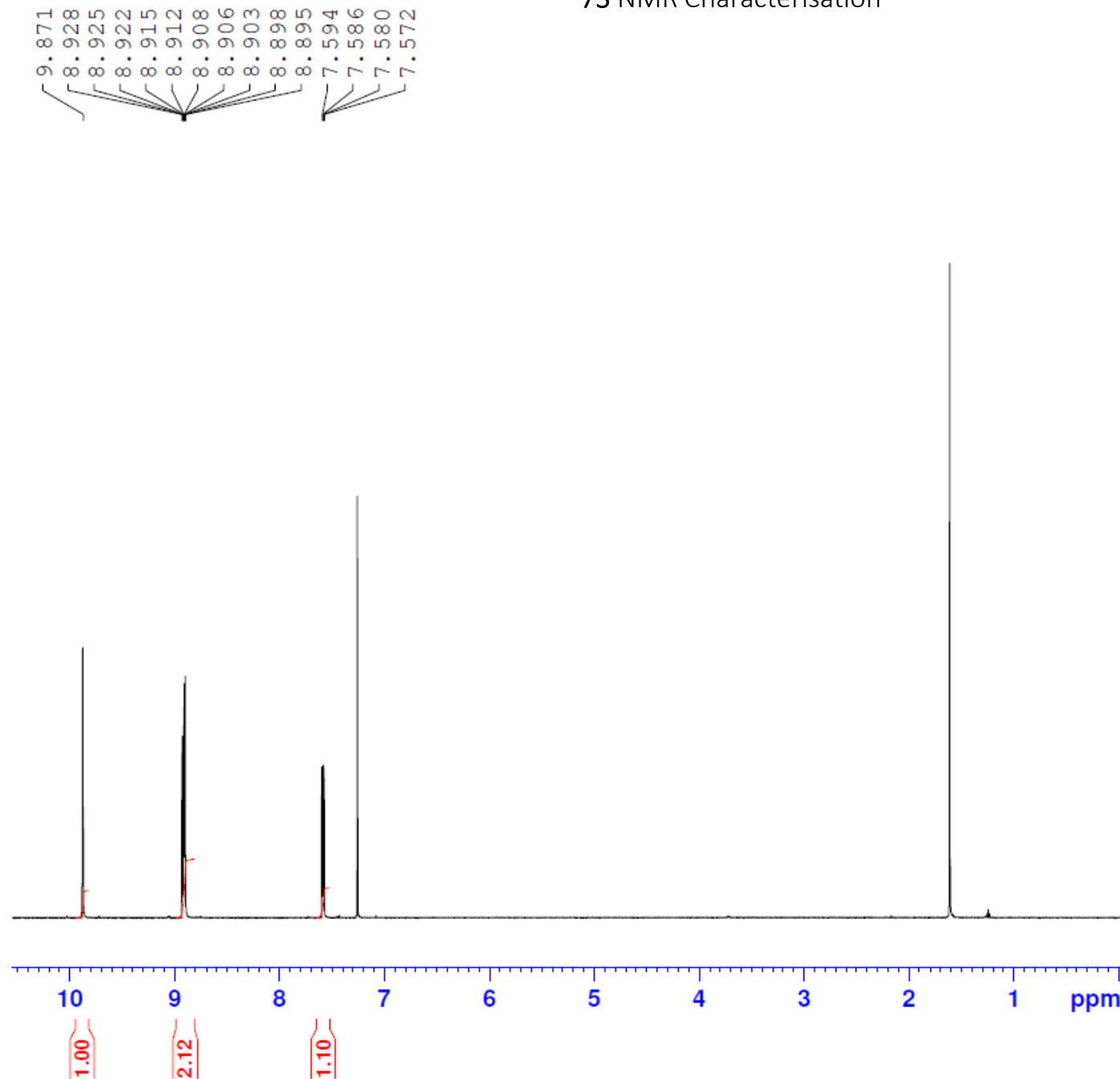


Current Data Parameters
 NAME 3pyridyltetrazine
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191108
 Time 17.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 362
 DW 41.600 usec
 DE 6.50 usec
 TE 298.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300295 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00





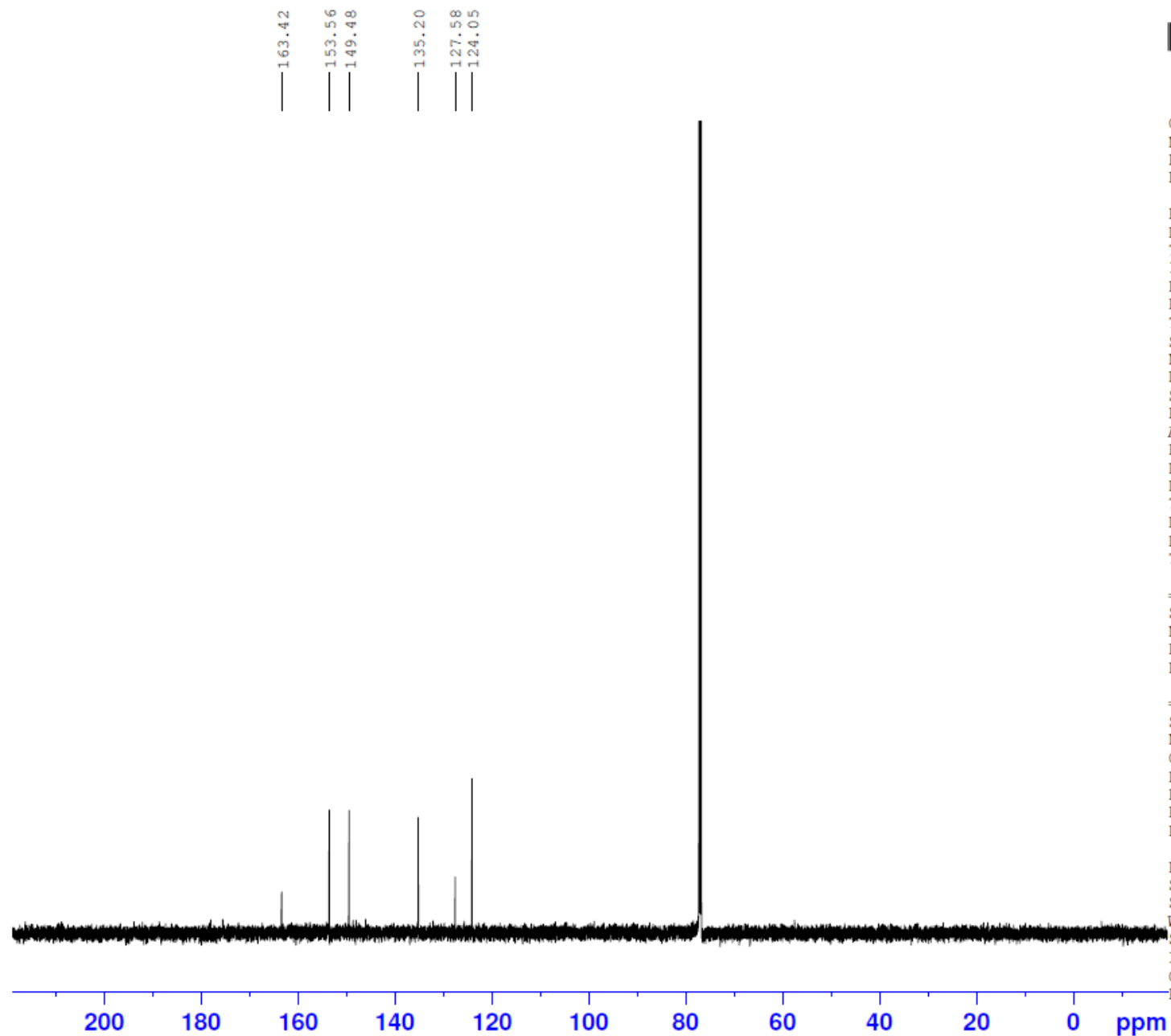
Current Data Parameters
NAME 3pyridyltetrazine
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191108
Time 17.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 189
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

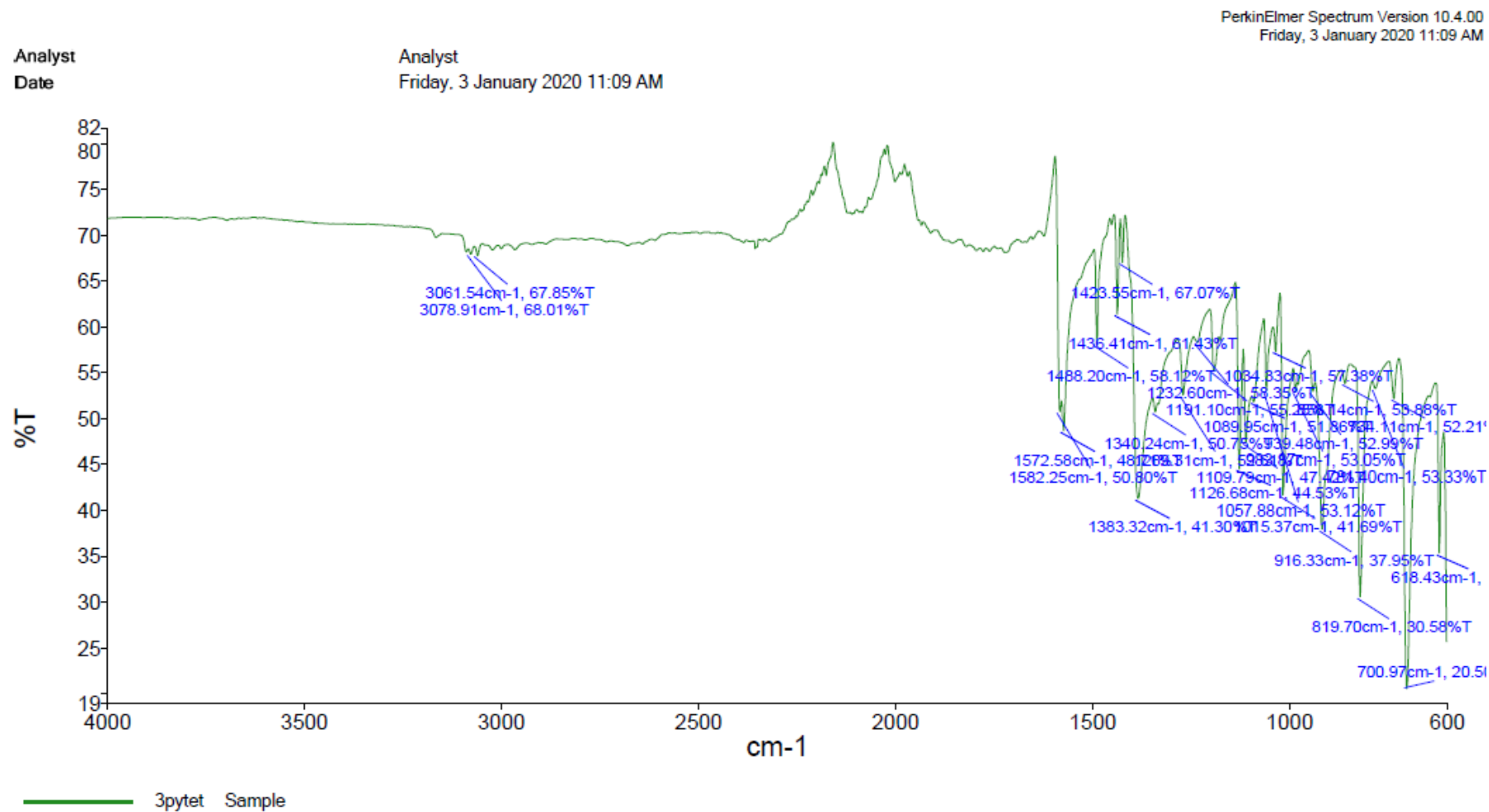
===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028151 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



73 IR Spectrum



74 NMR Characterisation

8.965
8.960
8.958
8.522
8.519
8.514
8.511

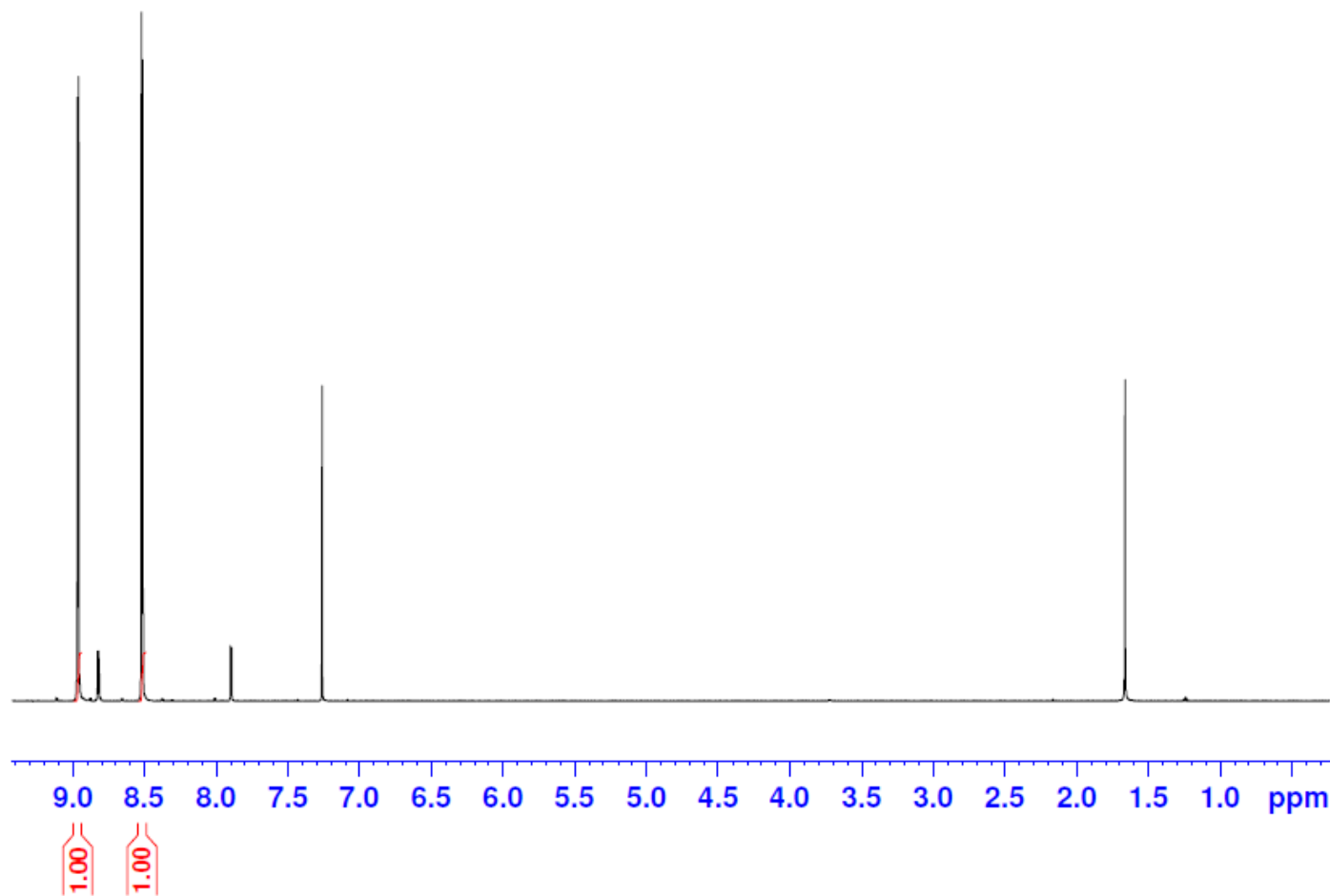


Current Data Parameters
NAME 4pyridyltetrazine
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191108
Time 17.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 322
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300260 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00





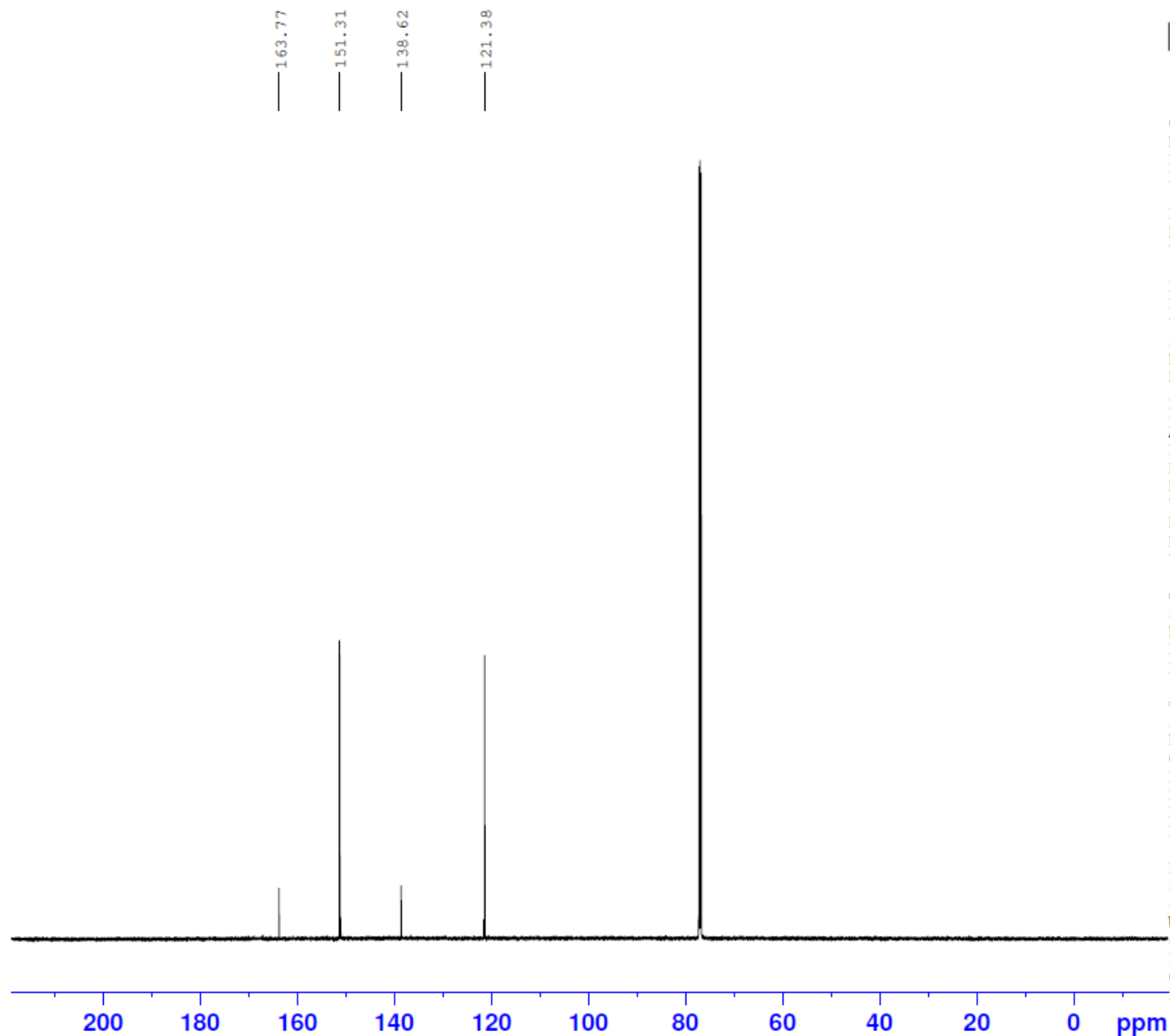
Current Data Parameters
NAME 4pyridyltetrazine
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191108
Time 17.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028163 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

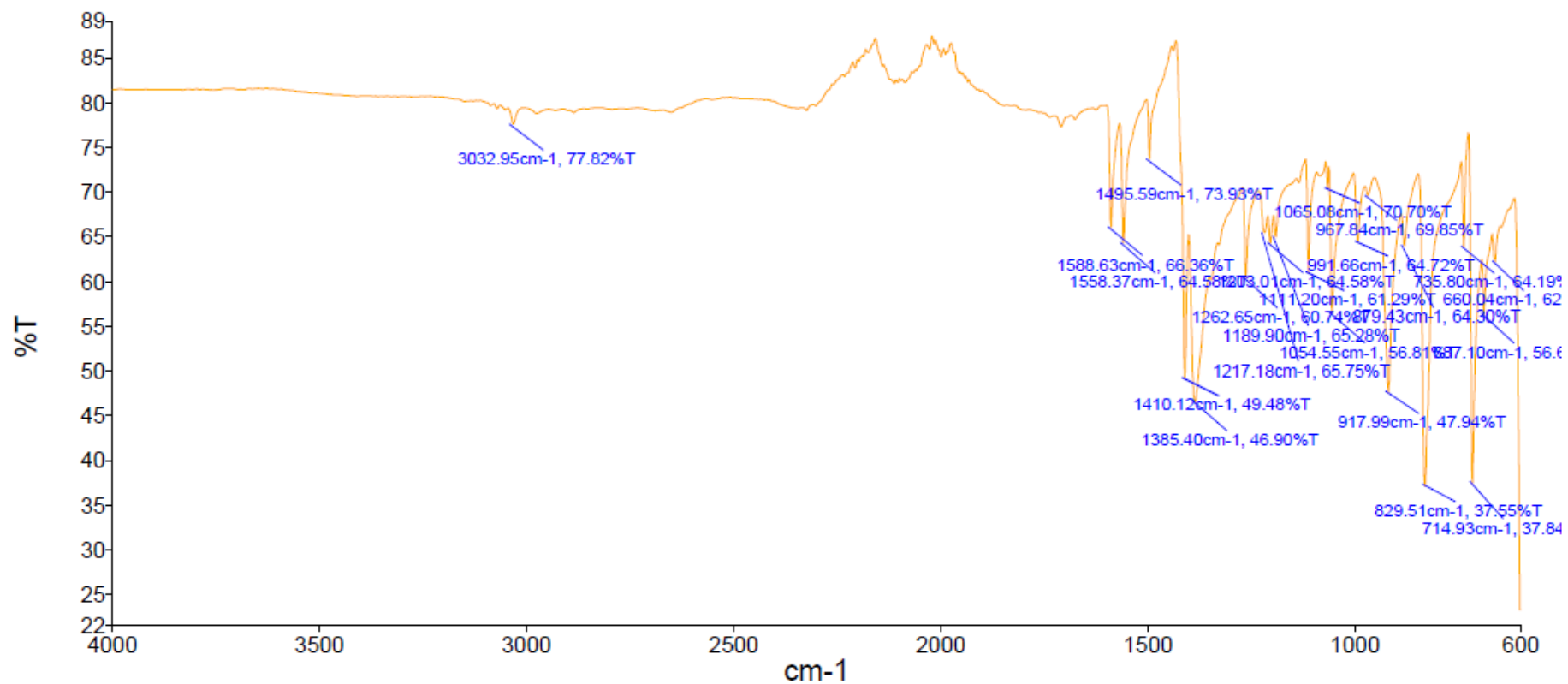


74 IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 3 January 2020 11:15 AM

Analyst
Date

Analyst
Friday, 3 January 2020 11:15 AM



4pytet Sample

76 NMR Characterisation

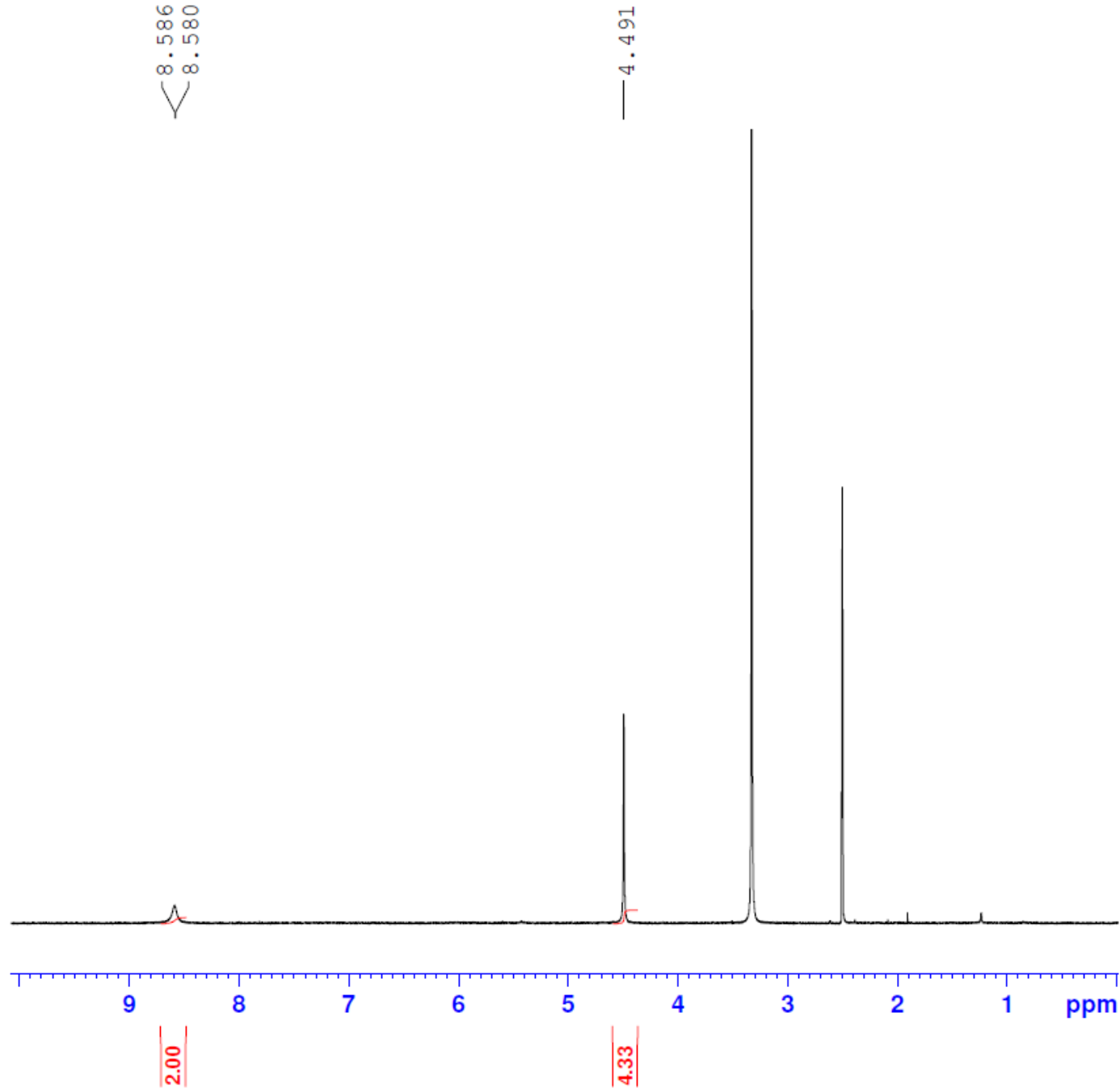


Current Data Parameters
 NAME India Triaminoguanidine HCl
 EXPNO 1210
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190822
 Time 7.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 ID 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 287
 DW 41.600 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 600.1337061 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300041 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00





Current Data Parameters
NAME 20200102 Triaminoguanidine HCl
EXPNO 11
PROCNO 1

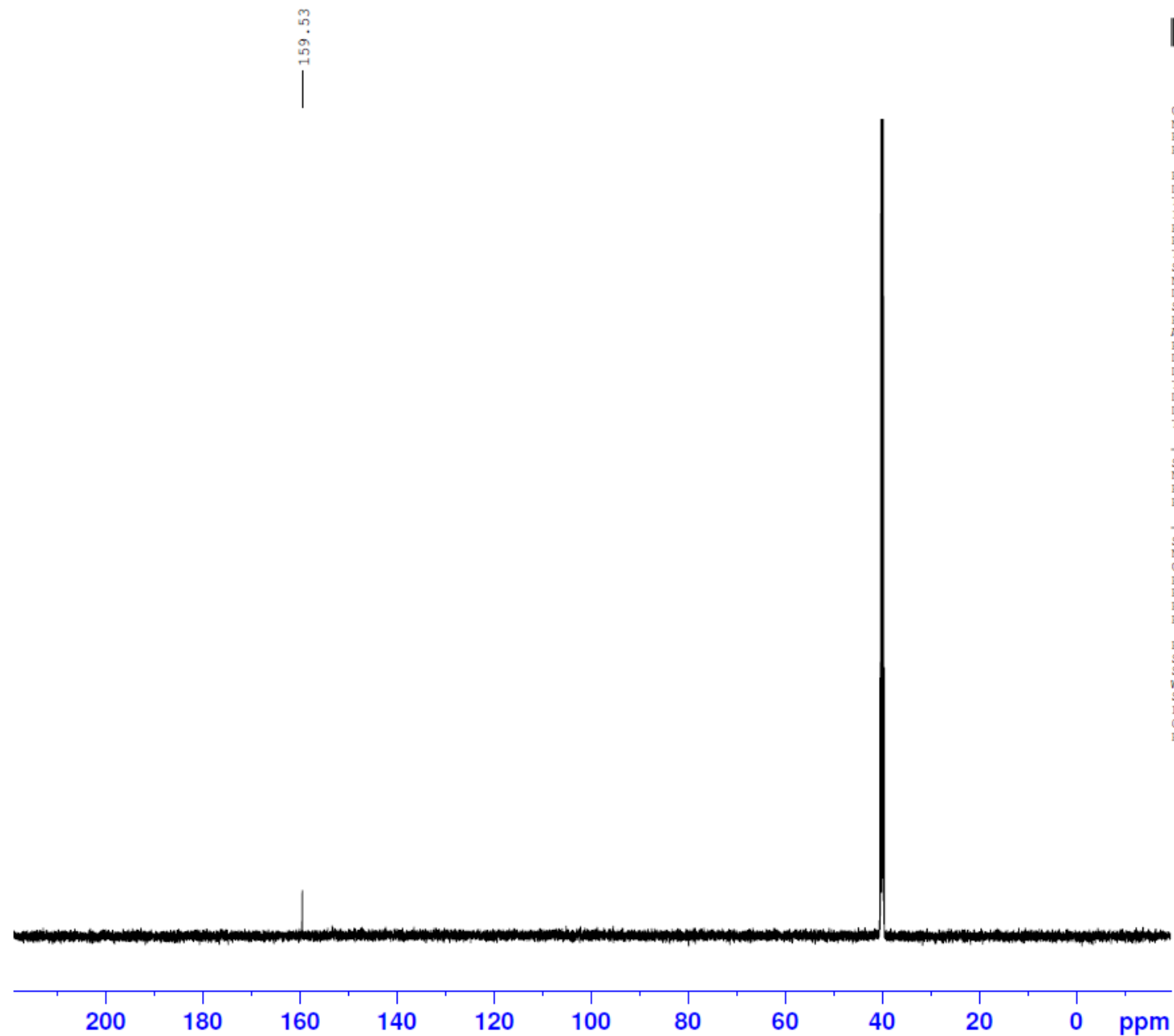
F2 - Acquisition Parameters

Date_ 20200102
Time 11.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 302
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

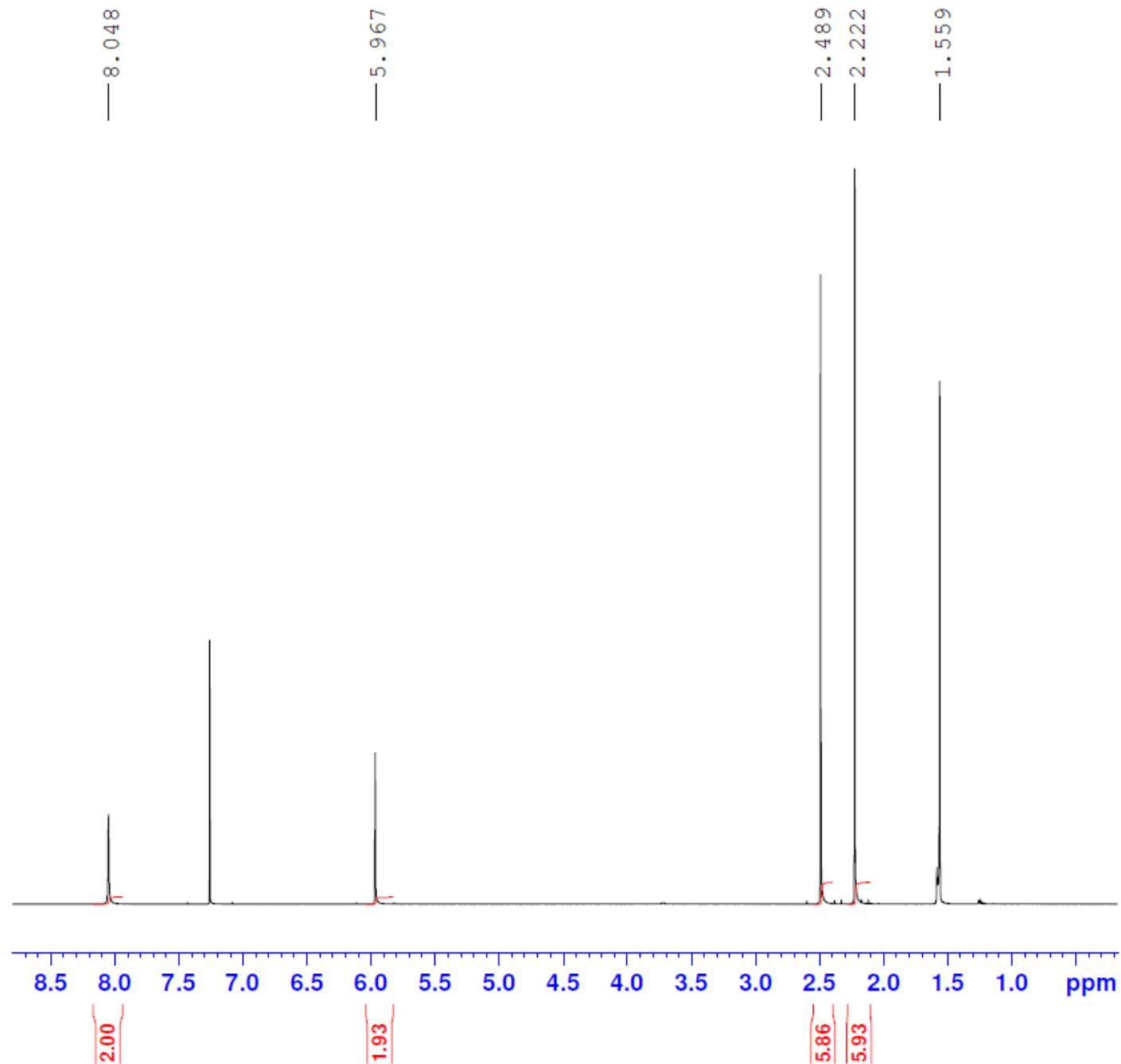
===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



77 NMR Characterisation

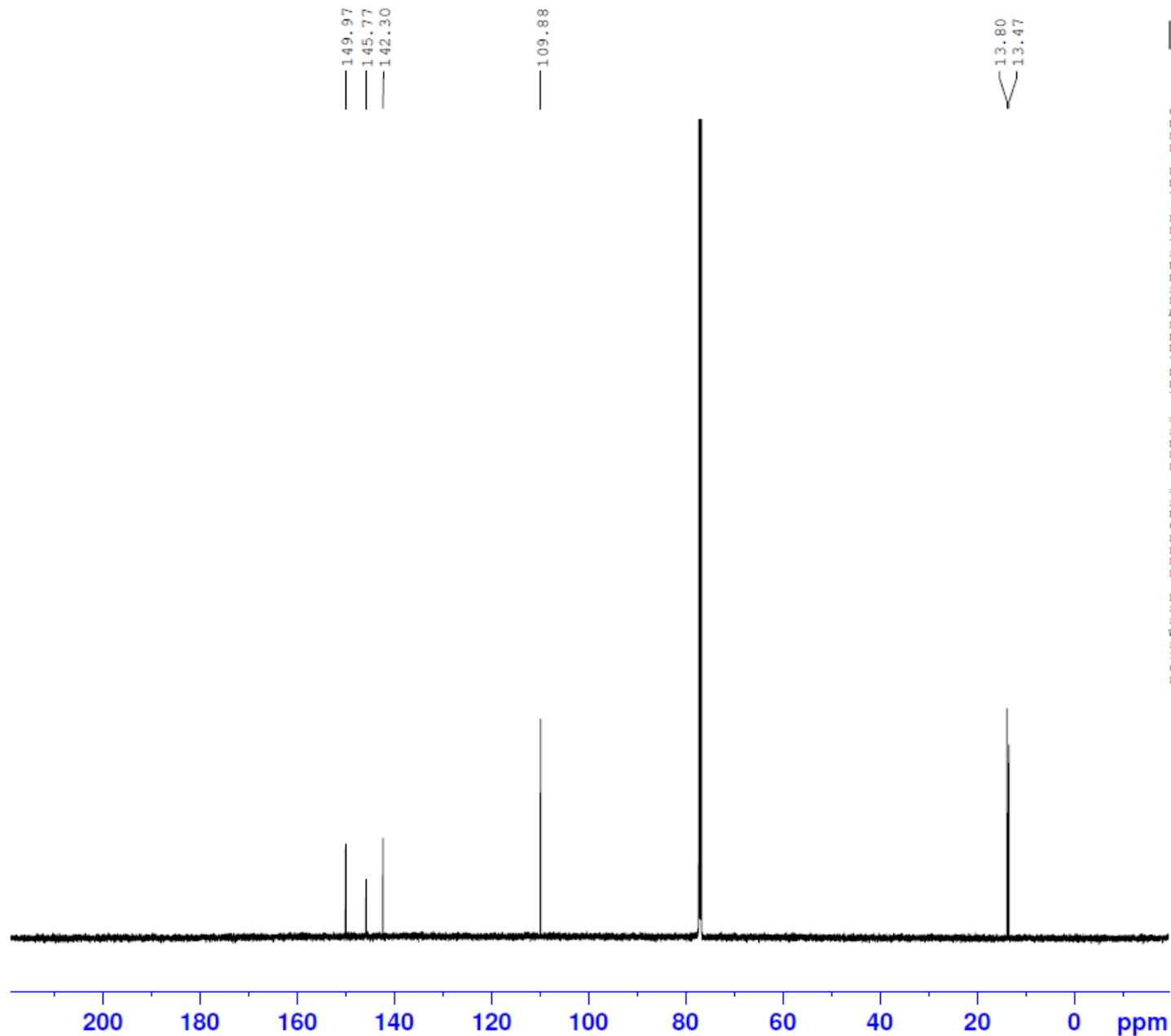


Current Data Parameters
 NAME 20200103 Dihydropyrazolyltetrazine
 EXFNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200103
 Time 10.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 322
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300271 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20200103 Dihydropyrazolyltetrazine
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200103
Time 20.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

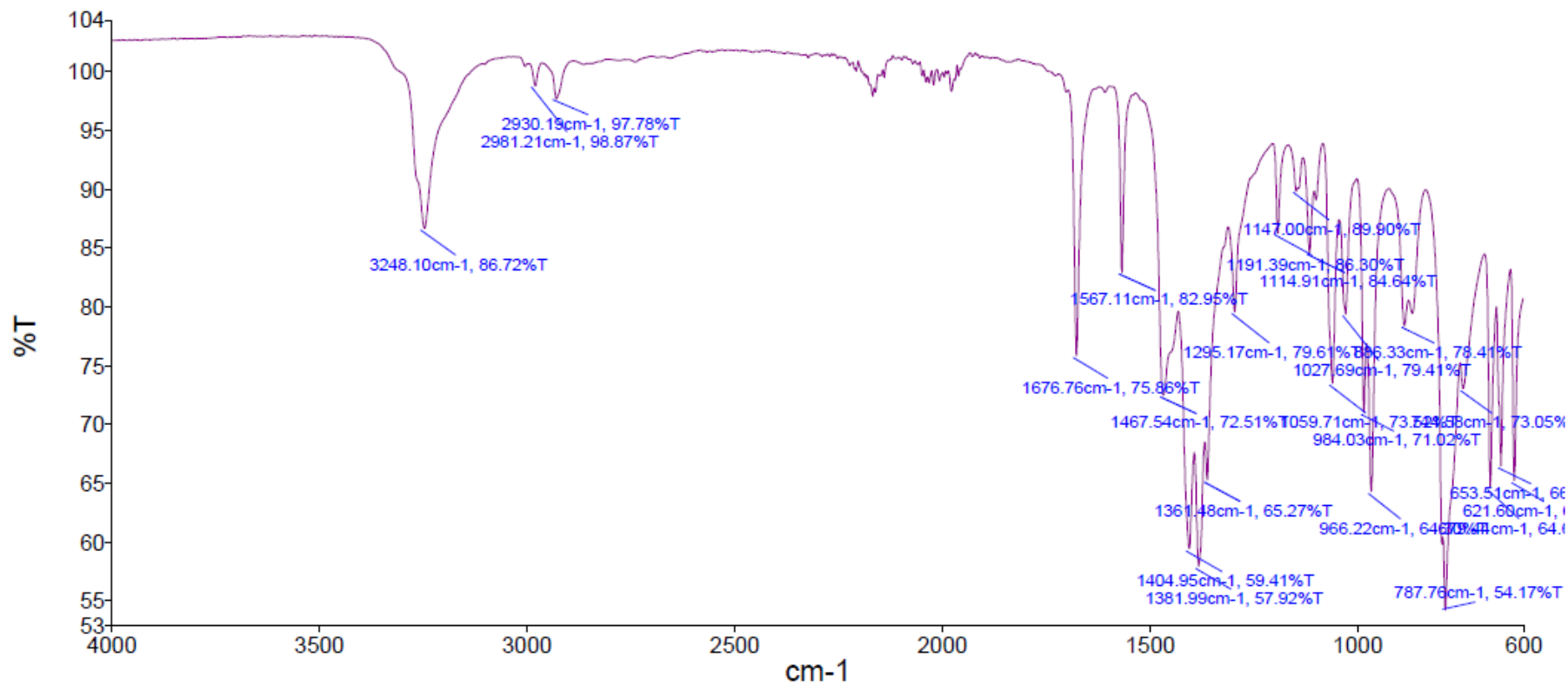
F2 - Processing parameters
SI 32768
SF 150.9028142 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

77 IR Spectrum

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Friday, 3 January 2020 11:26 AM

Analyst
Date

Analyst
Friday, 3 January 2020 11:26 AM



— Dihydropyrtet Sample

78 NMR Characterisation

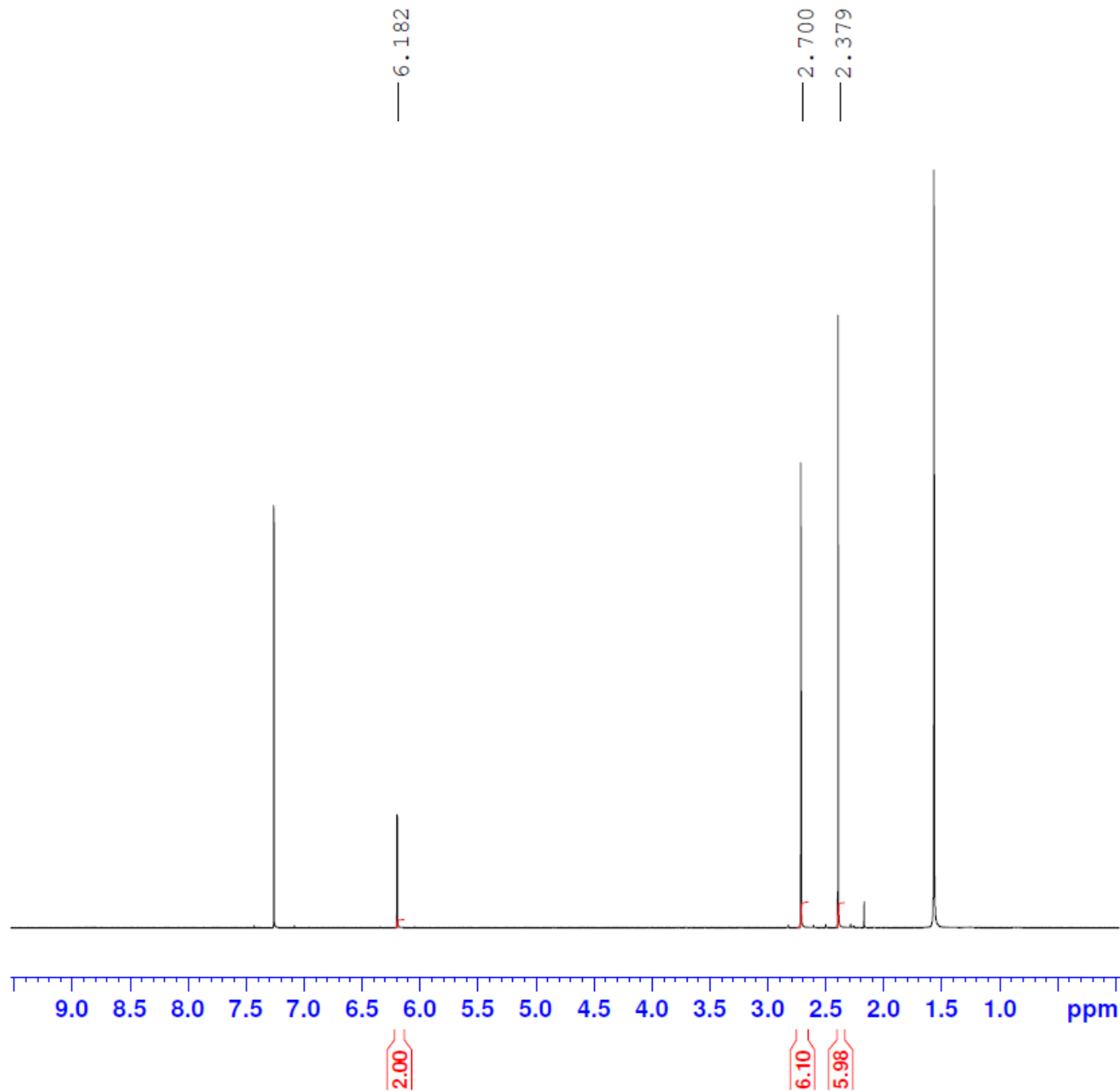


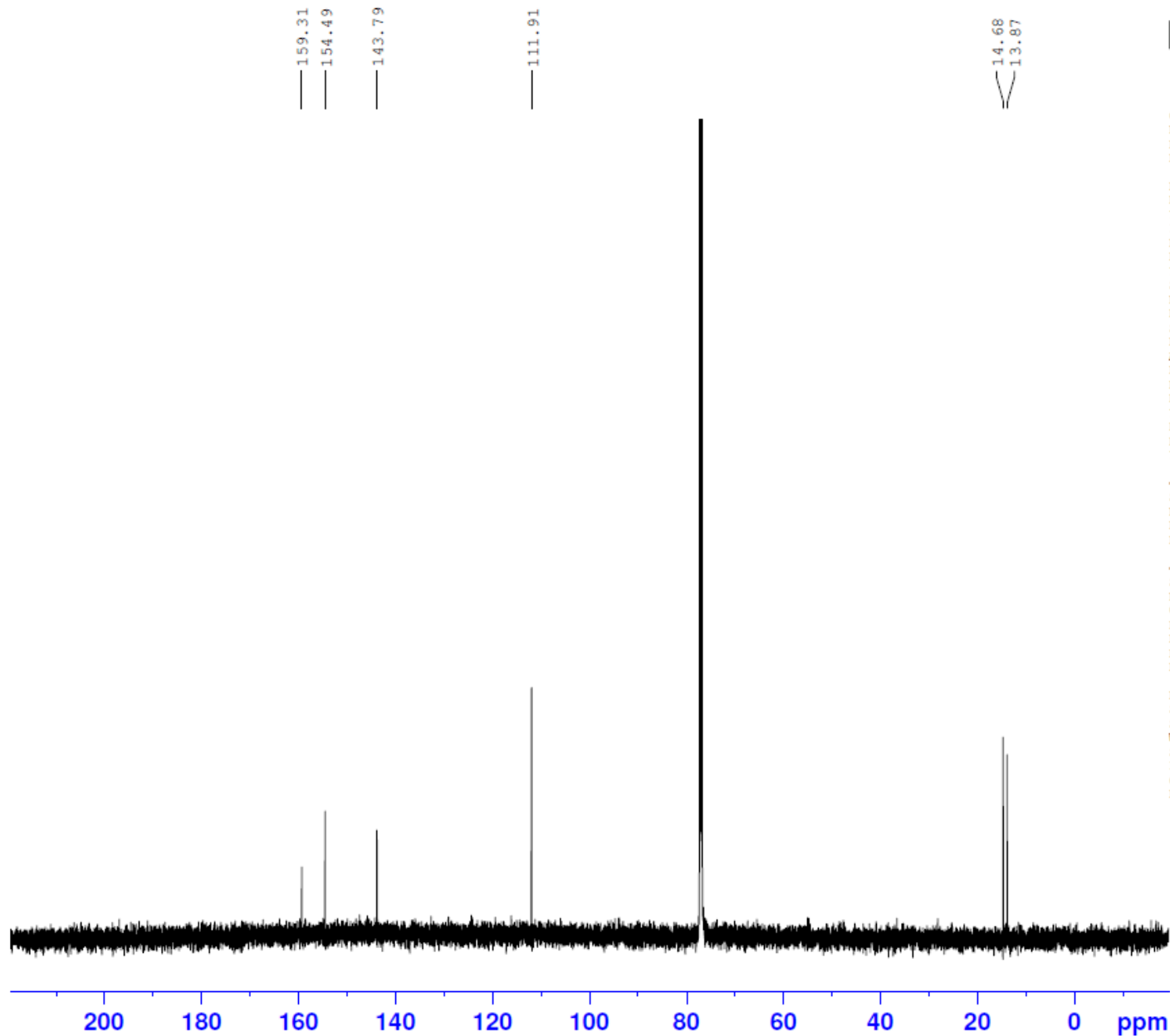
Current Data Parameters
 NAME 20200107 Pyrazolyltetrazine
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200107
 Time_ 17.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 ID 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 362
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300260 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00





Current Data Parameters
 NAME 20200107 Pyrazolyltetrazine
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200107
 Time 19.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 2048
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

----- CHANNEL f2 -----
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

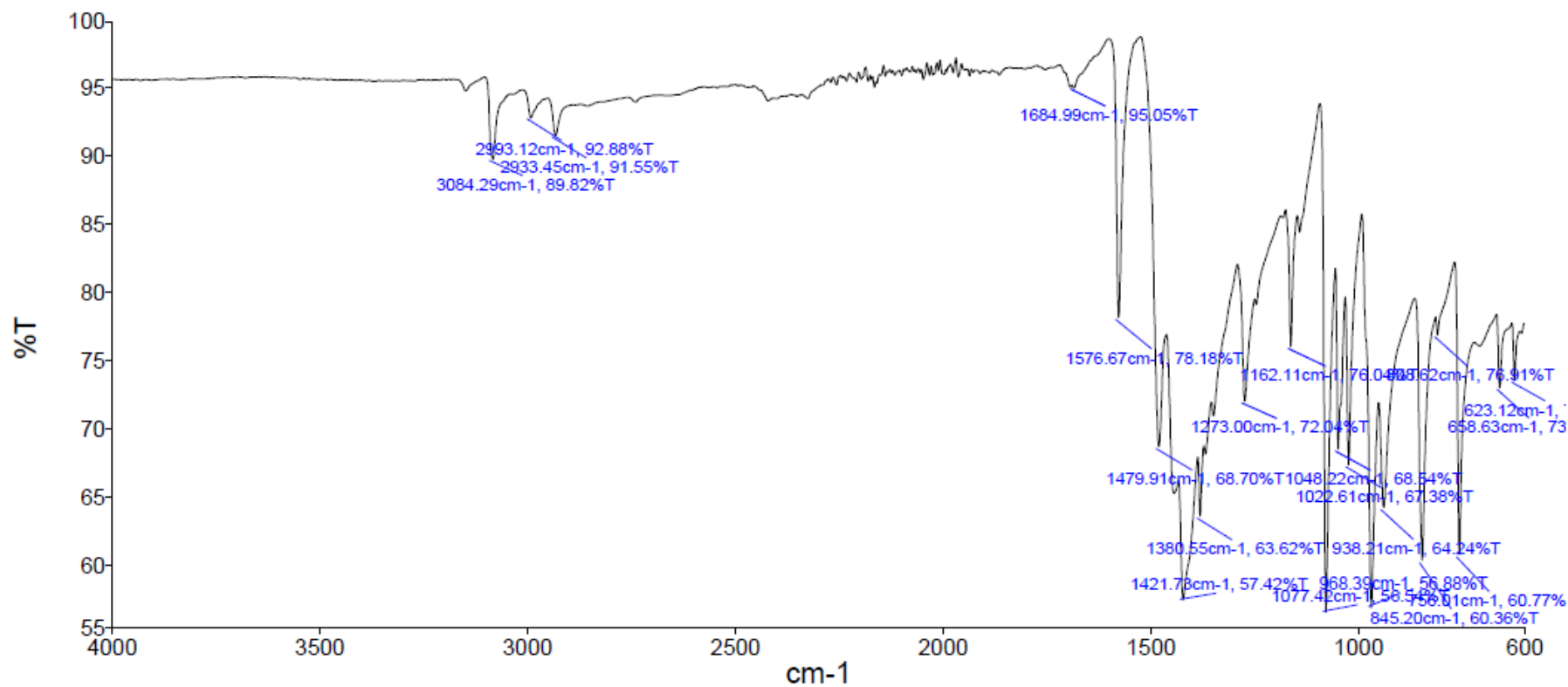
F2 - Processing parameters
 SI 32768
 SF 150.9028144 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

78 IR Spectrum

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Monday, 6 January 2020 10:20 AM

Analyst
Date

Analyst
Monday, 6 January 2020 10:20 AM



Pyrtet Sample

79 NMR Characterisation

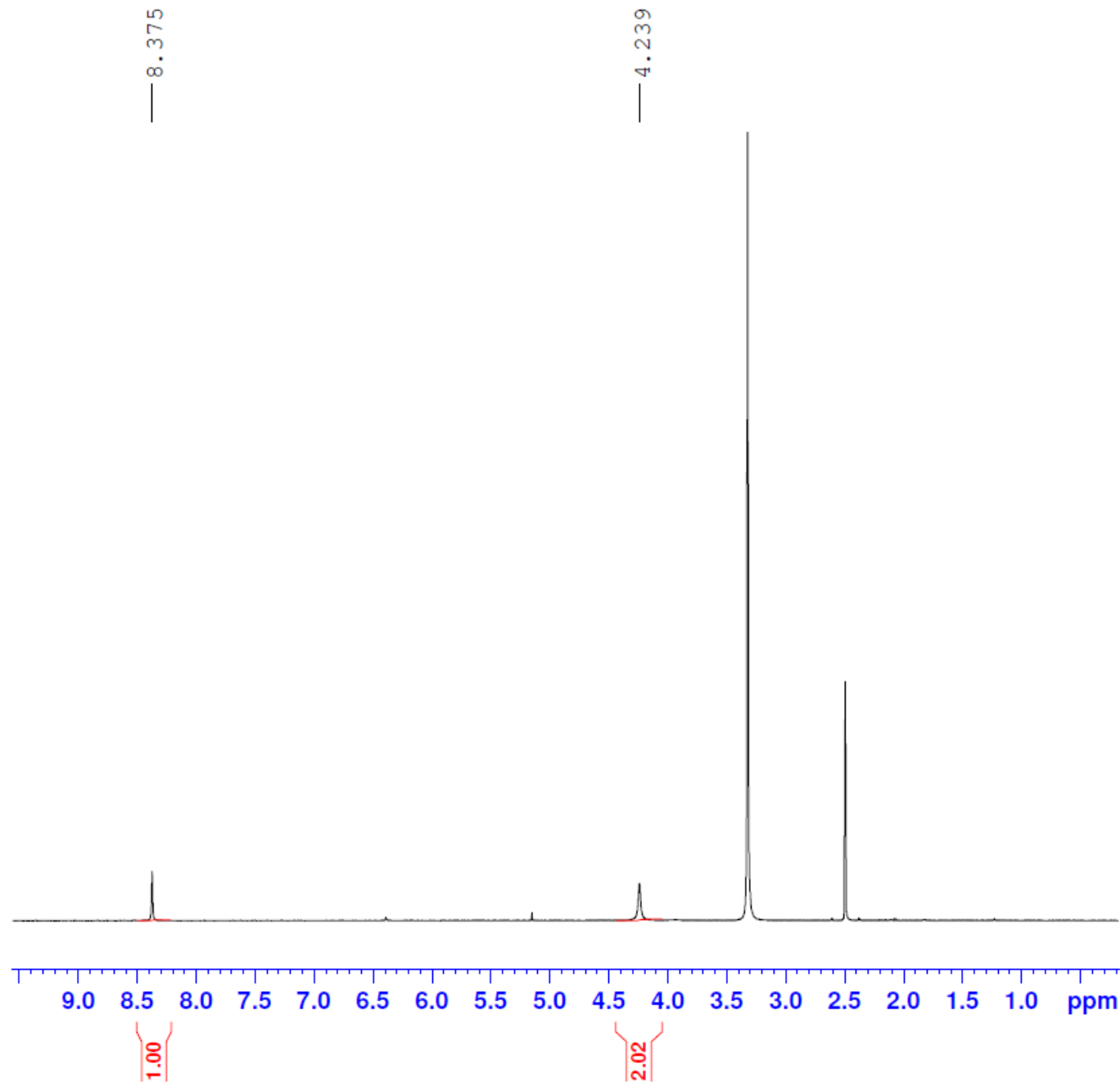


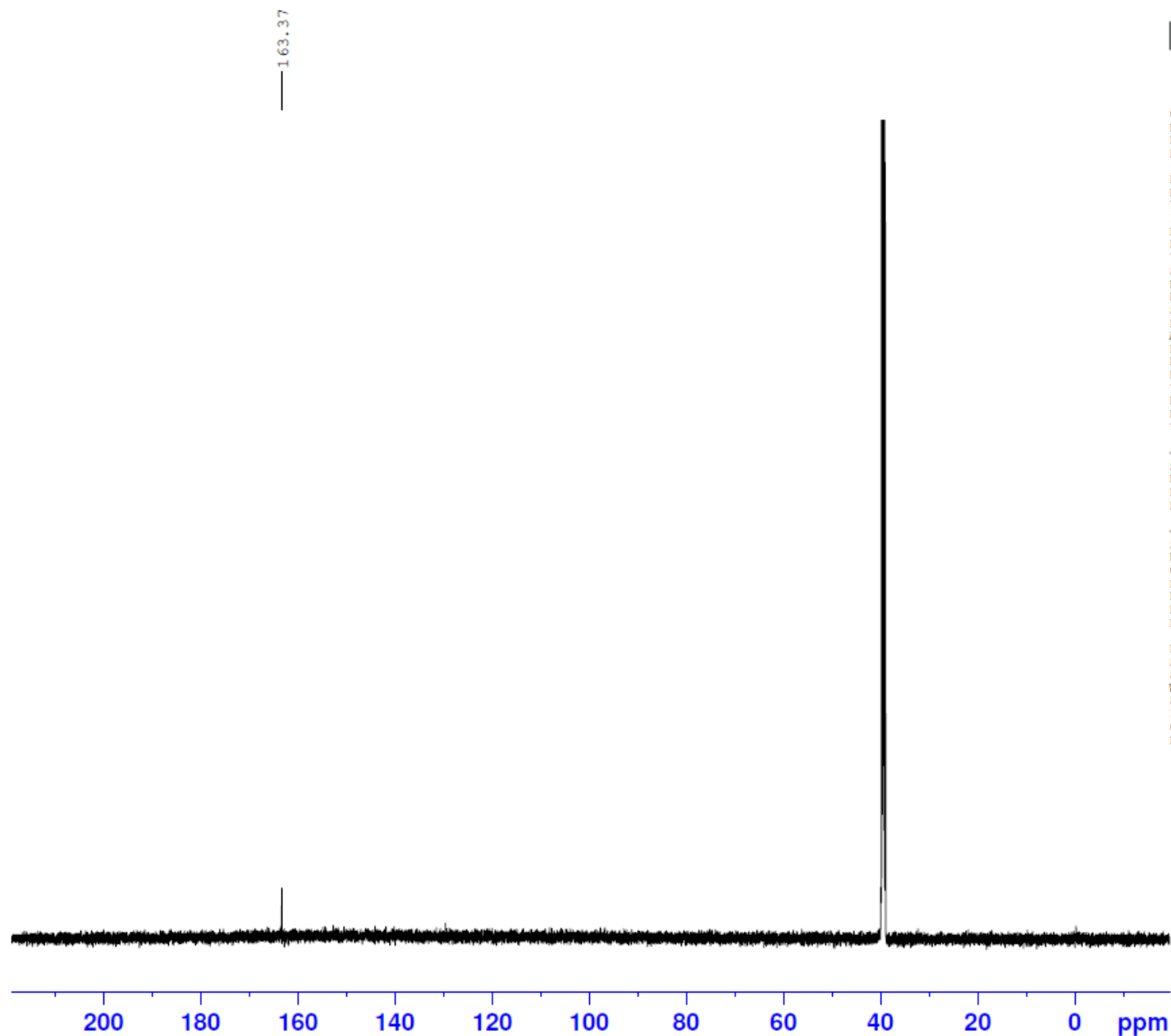
Current Data Parameters
NAME 20200106 Dihydrizinyltetrazine
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200106
Time 17.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 287
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300085 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00





Current Data Parameters
NAME 20200106 Dihydrazinyltetrazine
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200107
Time 9.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

----- CHANNEL f2 -----
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

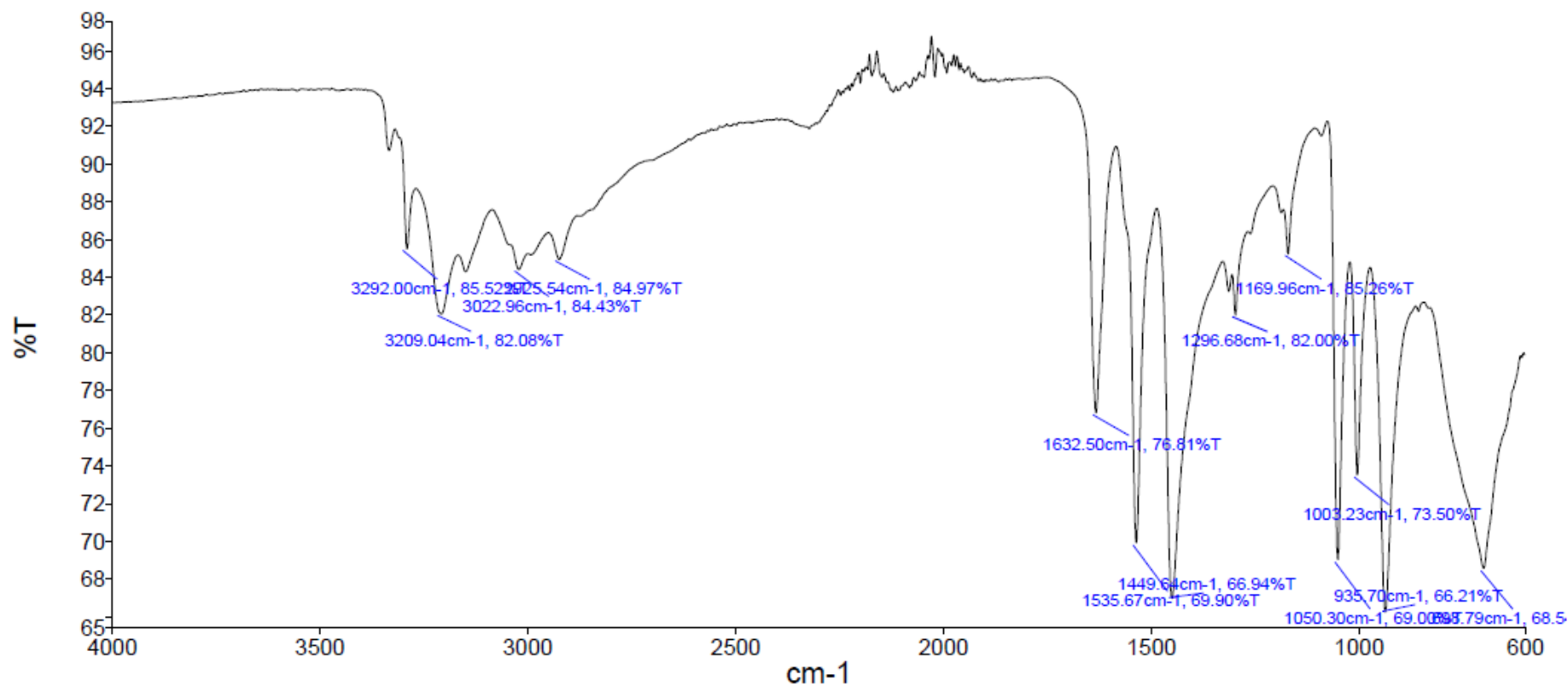
F2 - Processing parameters
SI 32768
SF 150.9028798 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

79 IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Tuesday, 7 January 2020 1:46 PM

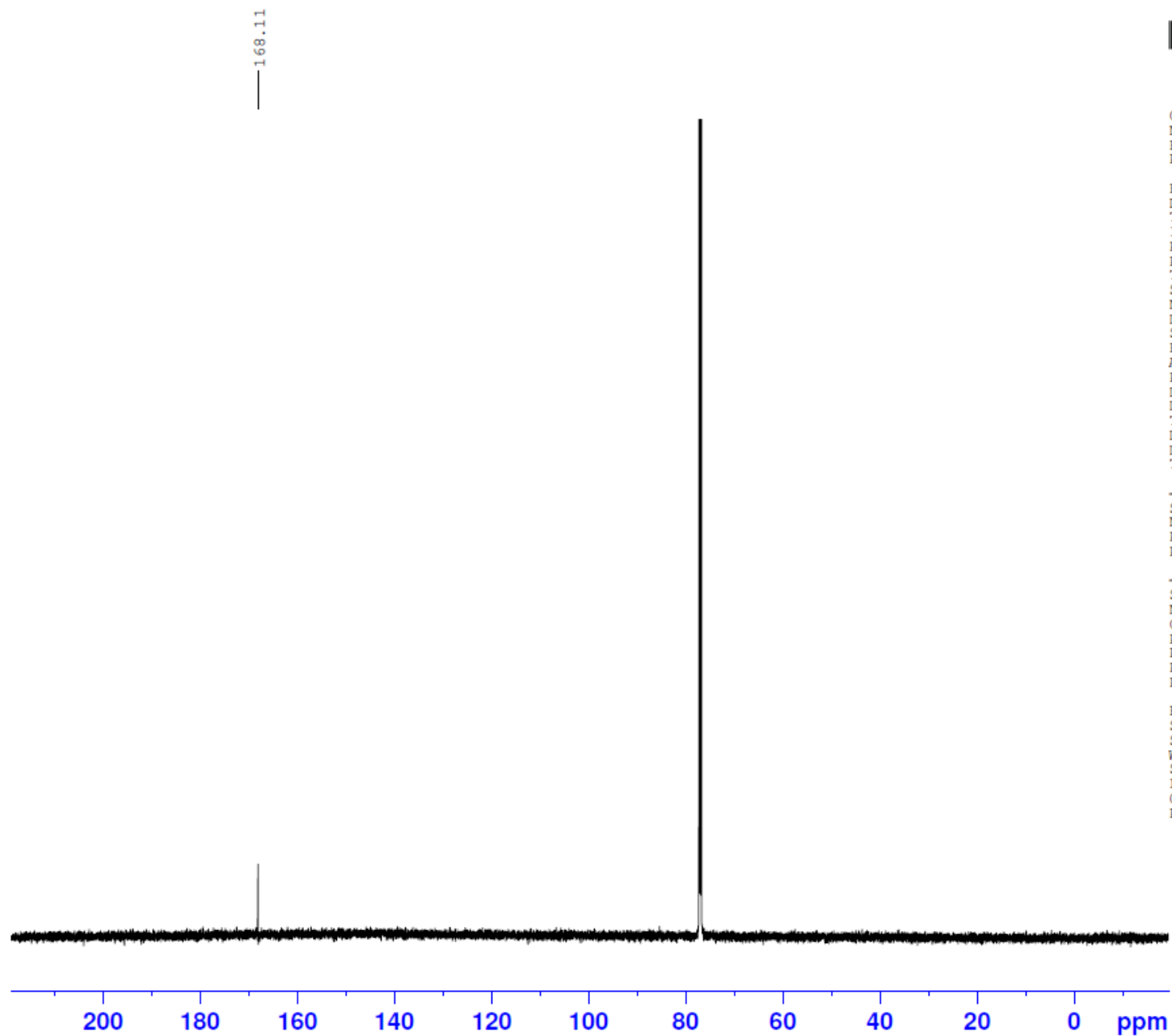
Analyst
Date

Analyst
Tuesday, 7 January 2020 1:46 PM



Hydrazinyttet Sample

80 NMR Characterisation



Current Data Parameters
 NAME 20200109 Dichlorotetrazine
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200109
 Time_ 21.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 4096
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

----- CHANNEL f2 -----
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

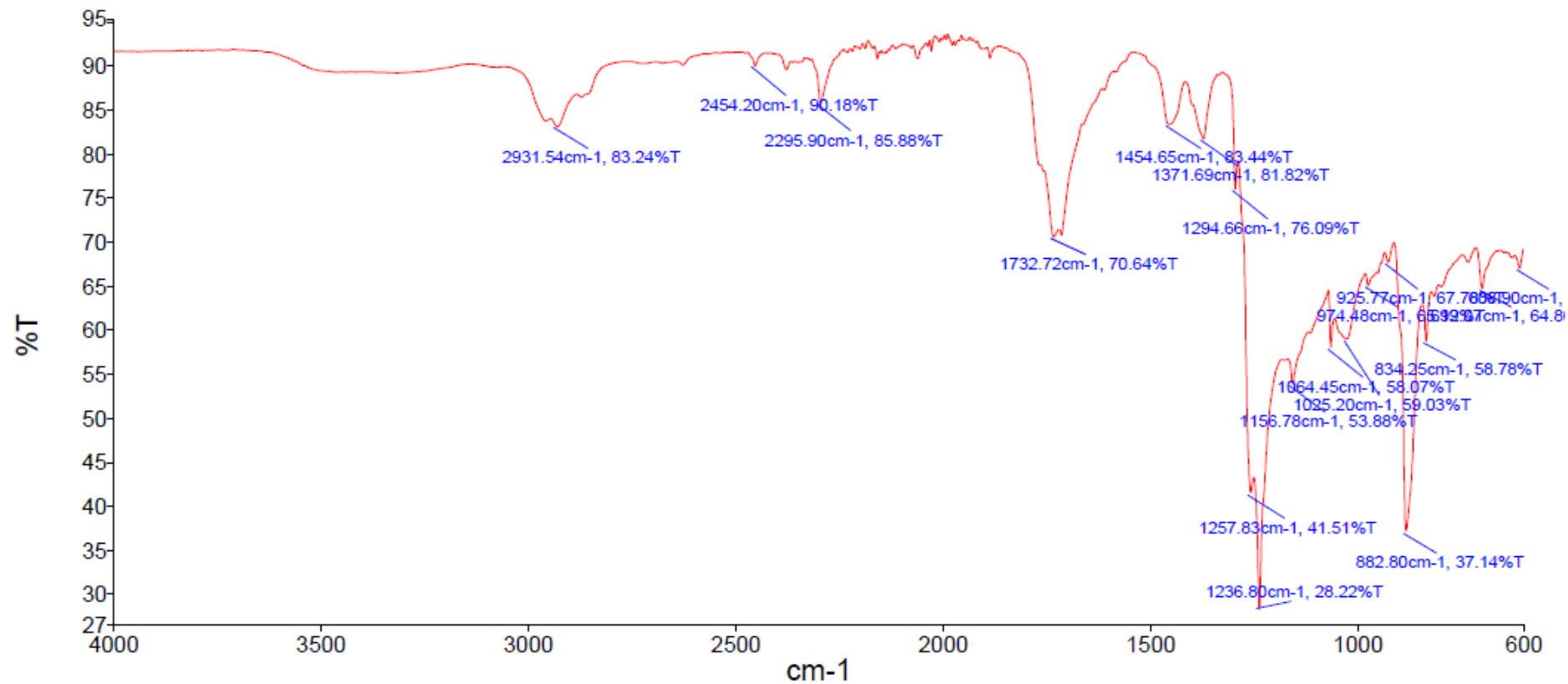
F2 - Processing parameters
 SI 32768
 SF 150.9028132 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

80 IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Wednesday, 8 January 2020 9:22 AM

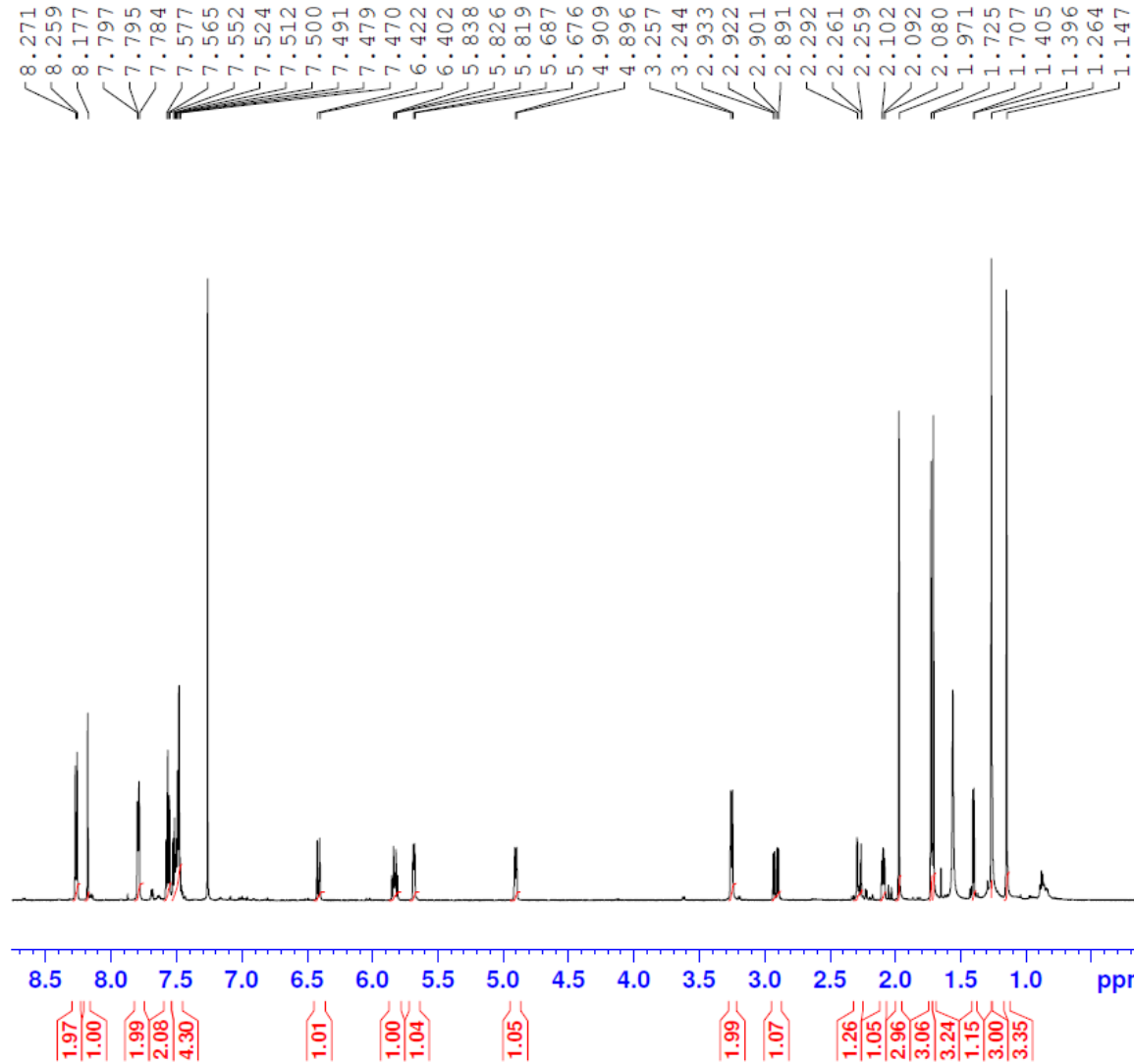
Analyst
Date

Analyst
Wednesday, 8 January 2020 9:22 AM



Dichlorotet Sample

88a NMR Characterisation

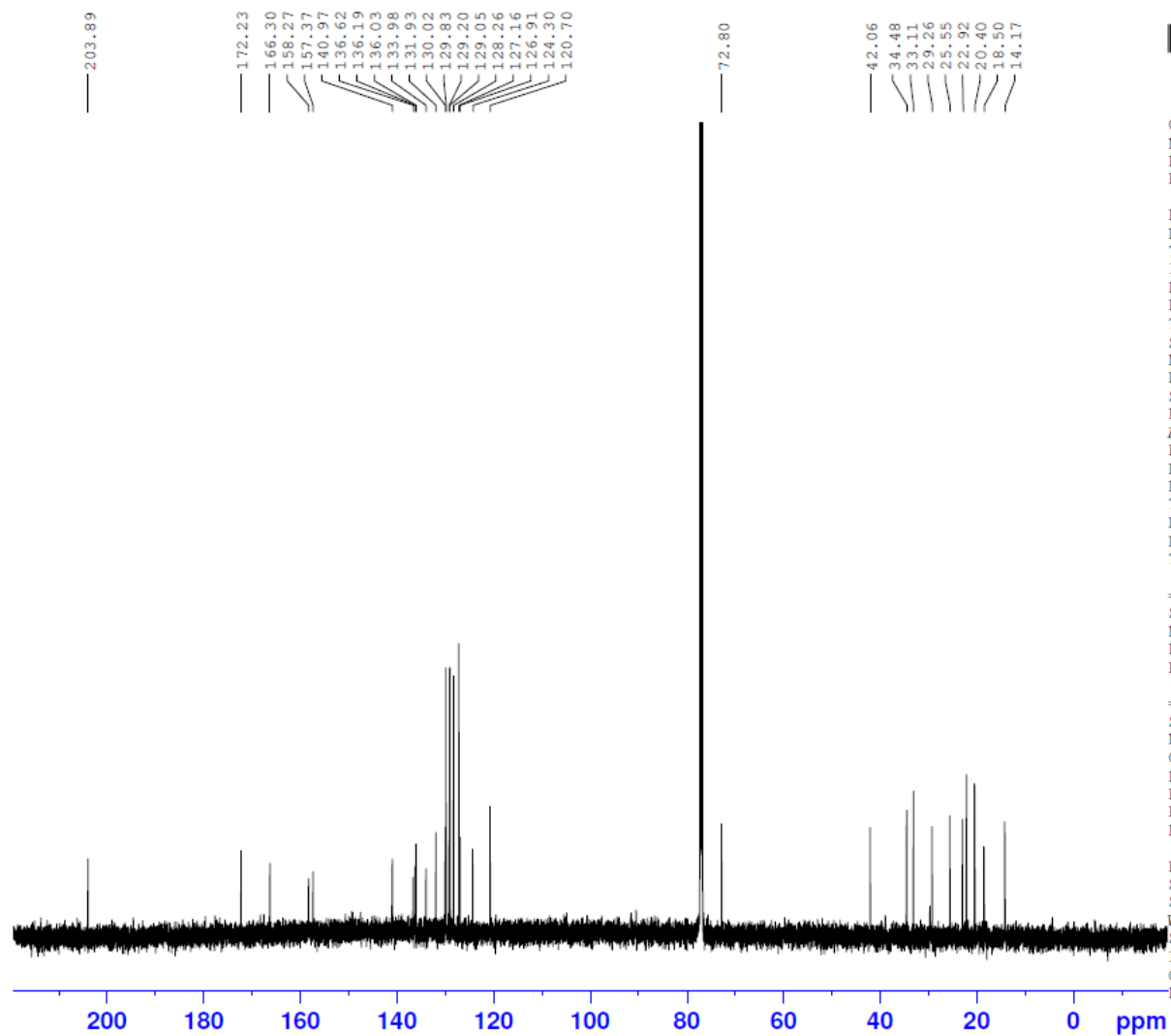


Current Data Parameters
 NAME 20200109 Phen I
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200109
 Time 21.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 322
 DW 41.600 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300261 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20200109 Phen I
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200109
 Time 23.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 2048
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028130 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200109 Phen I
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200109
Time 21.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppgf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 5263.158 Hz
FIDRES 2.569901 Hz
AQ 0.1945600 sec
RG 361
DW 95.000 usec
DE 6.50 usec
TE 298.3 K
D0 0.00000300 sec
D1 1.93323505 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00019000 sec

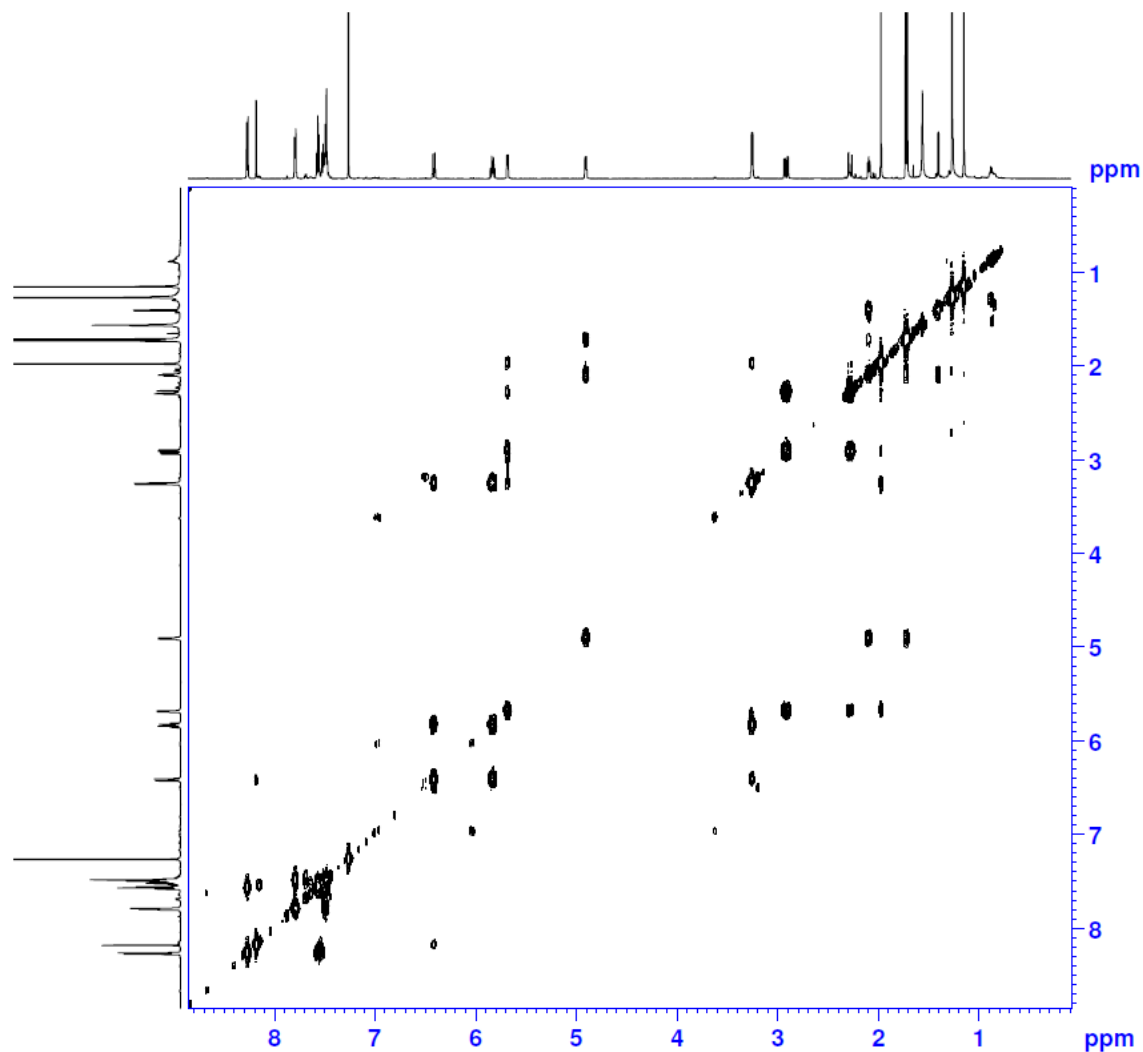
----- CHANNEL f1 -----
SFO1 600.1327082 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1327 MHz
FIDRES 41.118420 Hz
SW 8.770 ppm
FhMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300260 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300248 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200109 Phen I
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200110
Time 0
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 5208.333 Hz
FIDRES 9.086363 Hz
AQ 0.9983040 sec
RG 2050
DW 96.000 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46723199 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
INO 0.00082000 sec
ZGPGPINS

===== CHANNEL f1 =====
SFO1 600.1327198 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

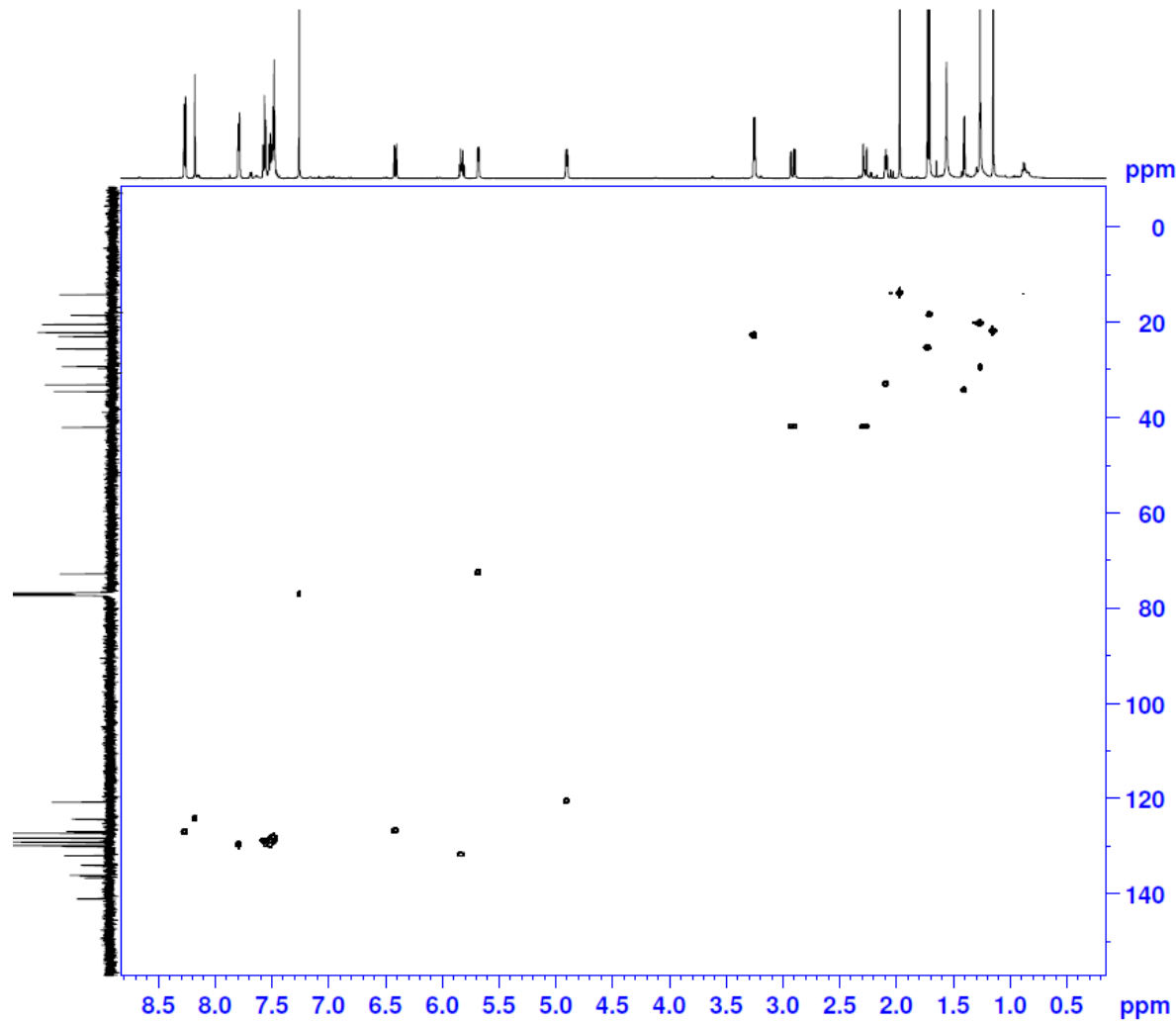
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 80.00000000 W
PLW12 3.20000005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
PRMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300253 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028473 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200109 Phen 1
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200110
Time 5:40
INSTRUM spect
PROBHD 5 mm FASBO BB/
PULPROG hmbcgpndgf
TD 4096
SOLVENT cdcl3
NS 70
DS 16
SWH 5208.333 Hz
FIDRES 1.271566 Hz
AQ 0.3932160 sec
RG 2050
DW 96.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.36237395 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1327198 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

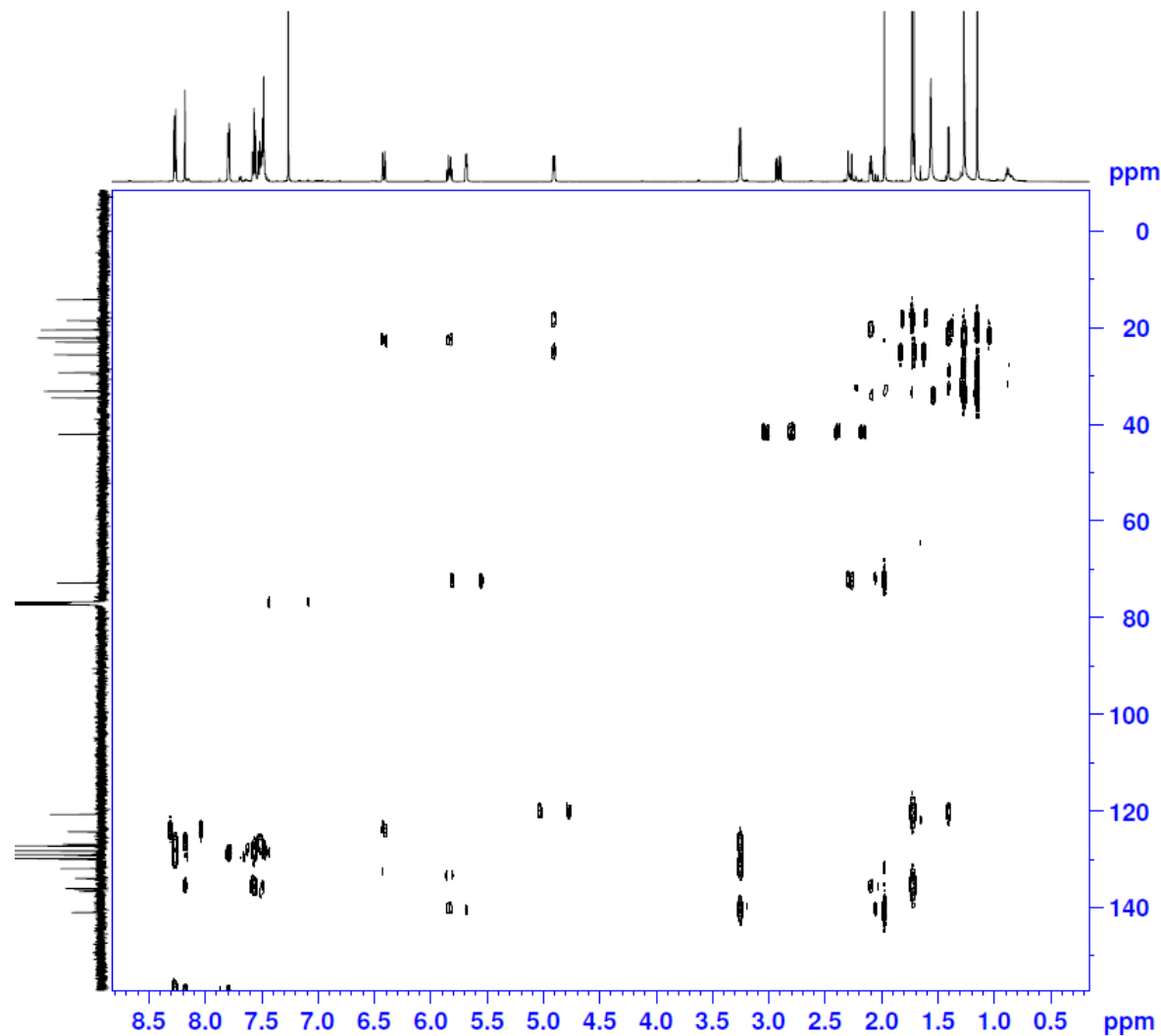
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 80.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 79
SFO1 150.9179 MHz
FIDRES 424.772736 Hz
SW 222.353 ppm
FAMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300269 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028645 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

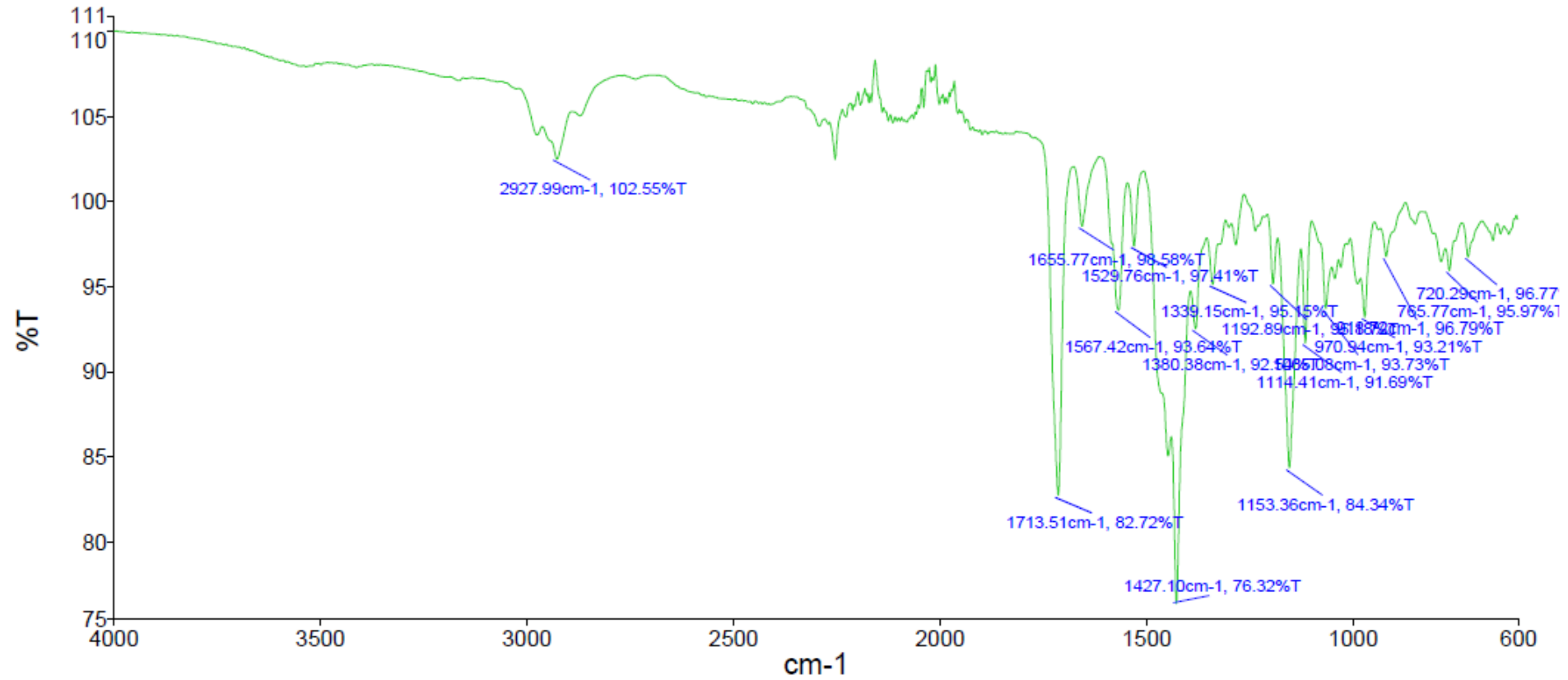


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PerkinElmer Spectrum Version 10.4.00
Friday, 3 January 2020 11:57 AM

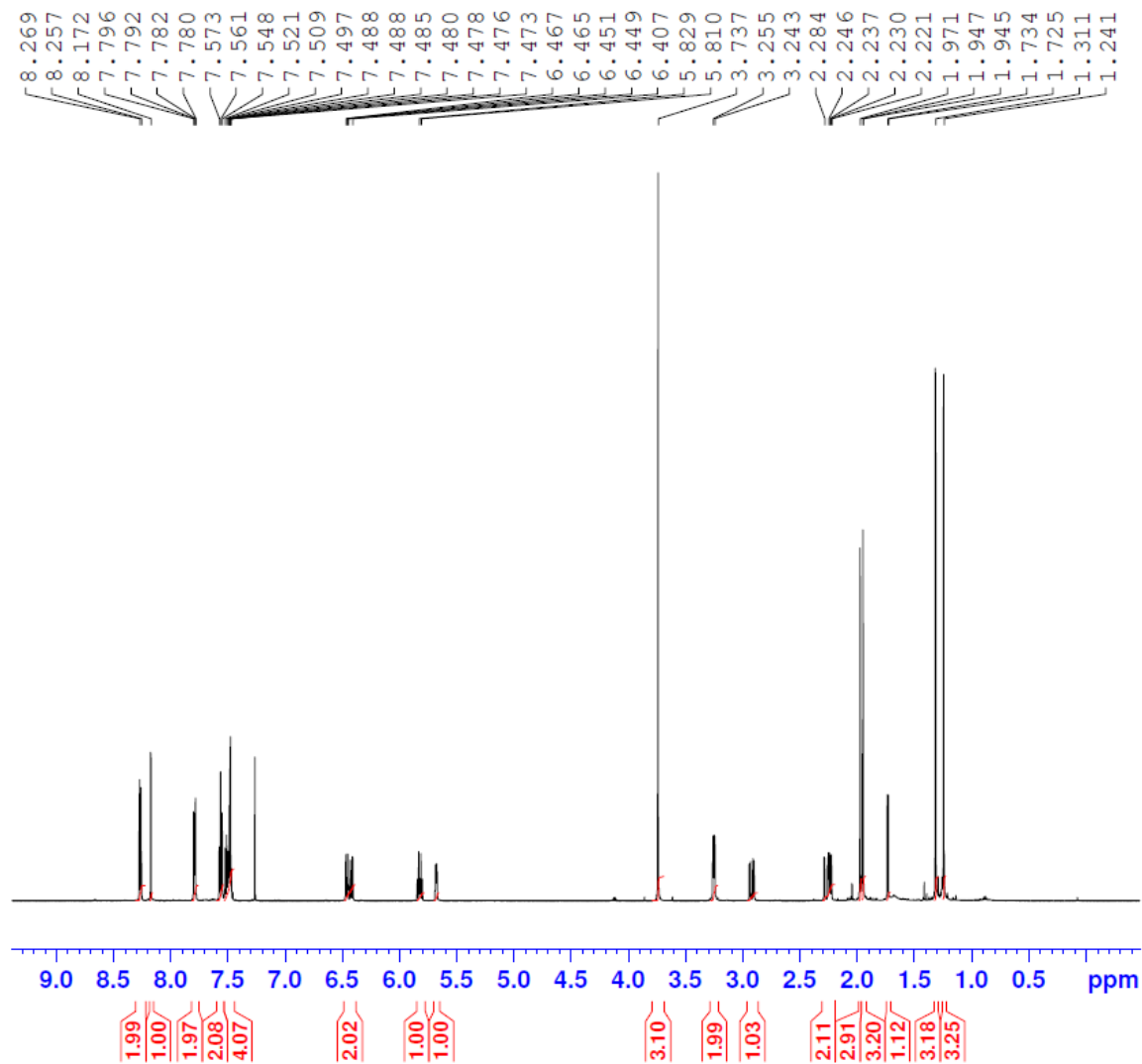
Analyst
Date

Analyst
Friday, 3 January 2020 11:57 AM



Phen I Sample

88b NMR Characterisation

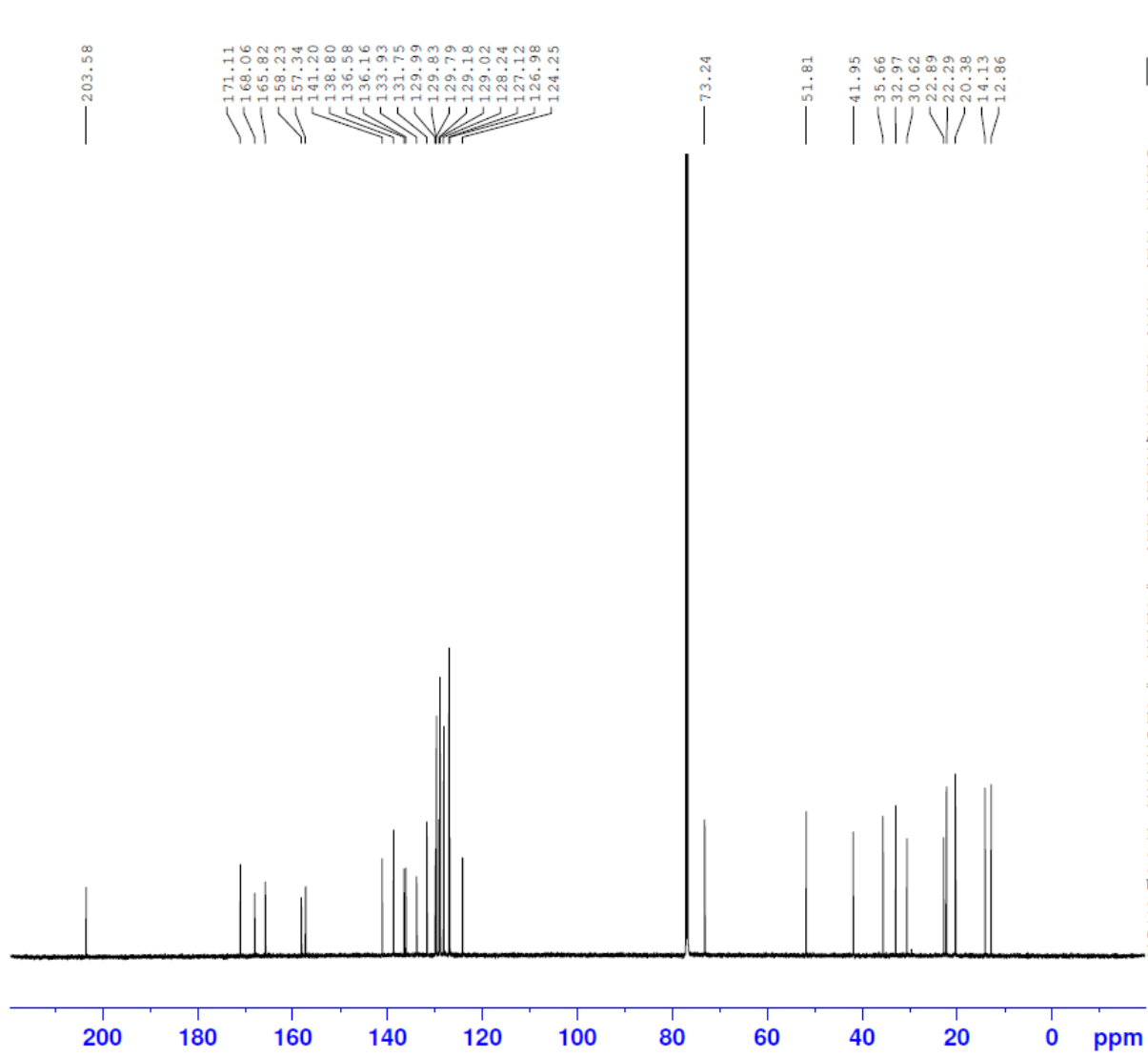


Current Data Parameters
 NAME 20190929 InvDa PhenII
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190929
 Time 13.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 144
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300252 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20190929 InvDa PhenII
 EXPNO 22
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190929
 Time 16.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 3072
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028172 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20190929 InvDa PhenII
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190929
Time 13.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpgpgf
TD 2048
SOLVENT CDCl3
NS 5
DS 8
SWH 5208.333 Hz
FIDRES 2.543132 Hz
AQ 0.1966080 sec
RG 64
DW 96.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.93118703 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
INO 0.00019200 sec

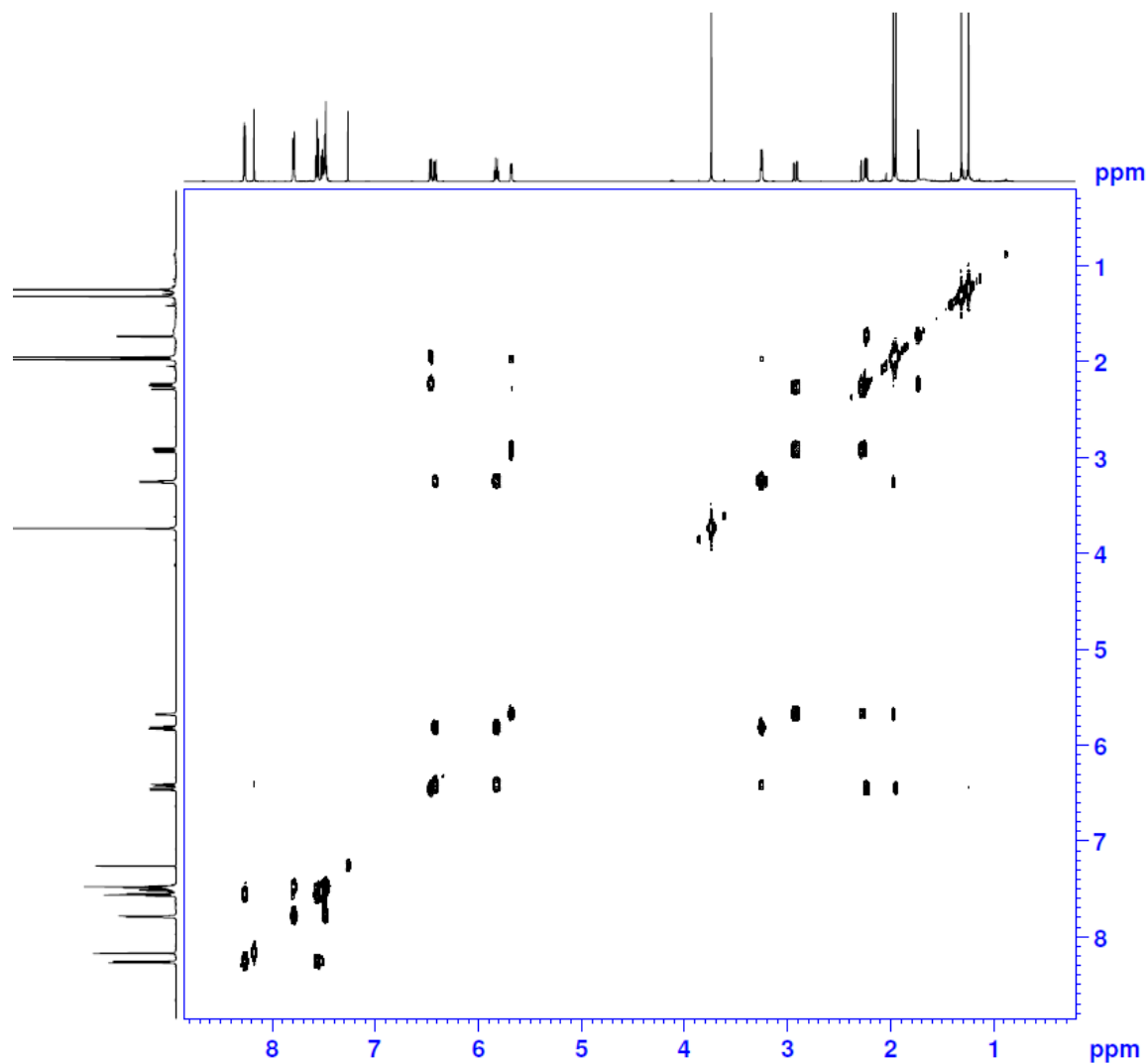
----- CHANNEL f1 -----
SFO1 600.1327516 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 328
SFO1 600.1328 MHz
FIDRES 40.690105 Hz
SW 8.679 ppm
FhMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300257 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300258 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190929 InvDa PhenII
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190929
Time 16:19
INSTRUM spect
PROBHD 5 mm PARBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 30
DS 16
SWH 5319.149 Hz
FIDRES 5.194481 Hz
AQ 0.0962560 sec
RG 2050
RW 94.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.000000
D0 0.00000300 sec
D1 1.46928000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPTNS

===== CHANNEL f1 =====
SFO1 600.1327458 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
P1M1 17.00000000 W

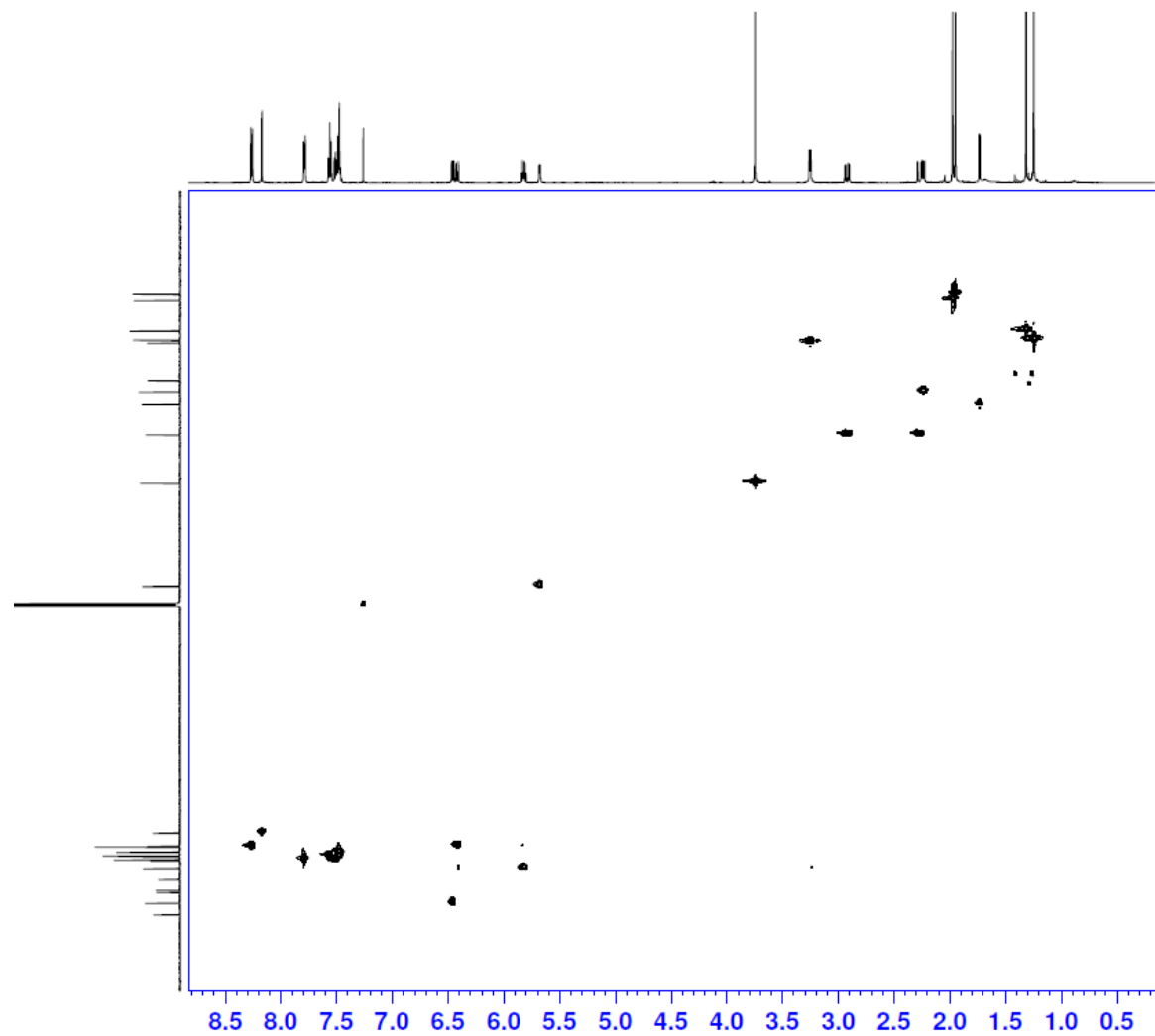
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPOPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
P1M2 80.00000000 W
P1M12 3.20000005 W

===== GRADIENT CHANNEL =====
CPNAM[1] SMSQ10.100
CPNAM[2] SMSQ10.100
GPE1 80.00 %
GPE2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
PRMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300253 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028617 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190929 InvDa PhenII
EXPNO 25
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190929
Time 19.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmcgpnzgqf
TD 4096
SOLVENT CDCl3
NS 50
DS 16
SWH 5319.149 Hz
FIDRES 1.298620 Hz
AQ 0.3850240 sec
RG 2050
DW 94.000 usec
DE 6.50 usec
TE 298.2 K
CNS113 8.0000000
D0 0.00000300 sec
D1 1.37056601 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1327458 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

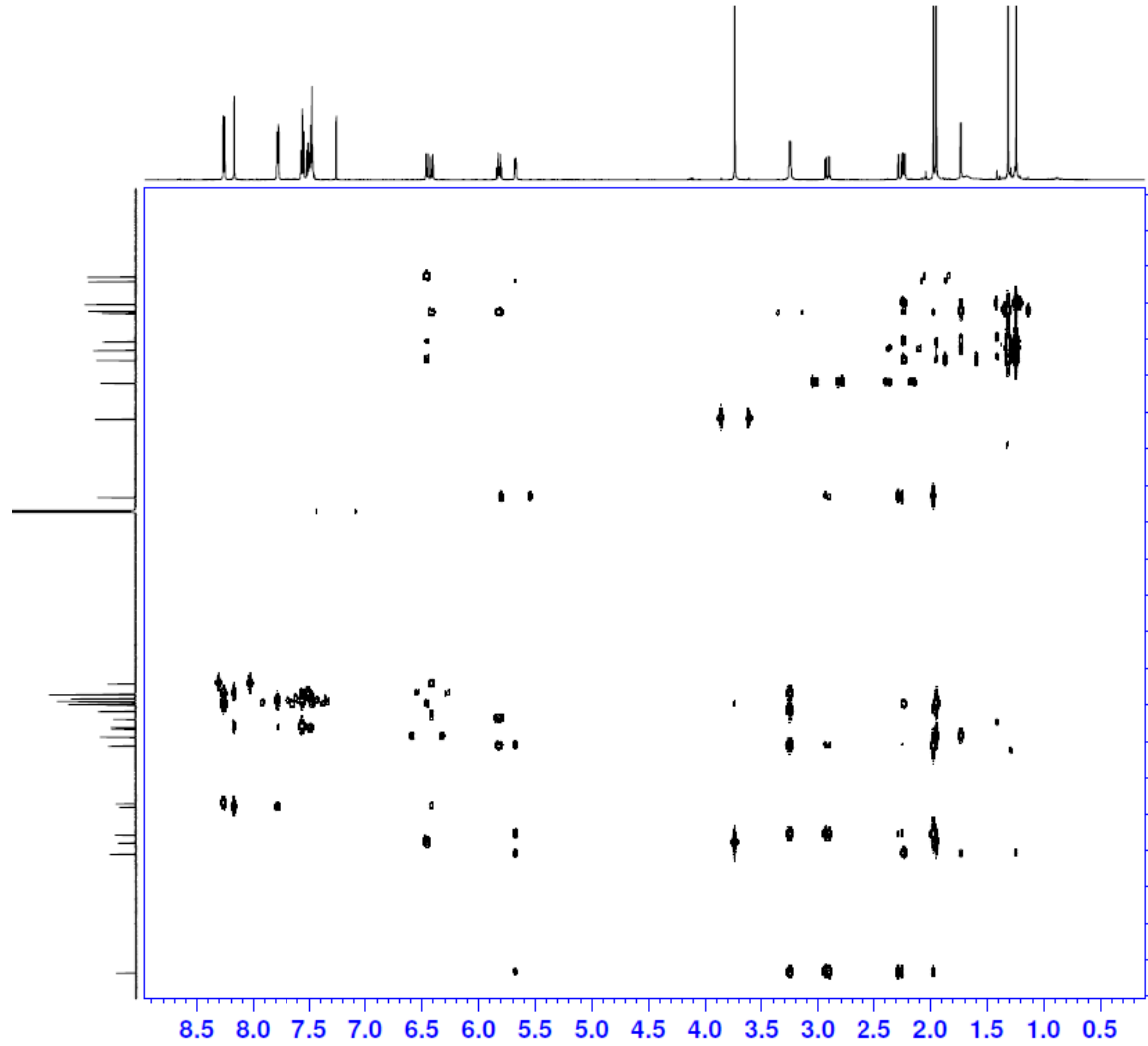
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 80.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300254 MHz
WDW SINC
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028627 MHz
WDW SINC
SSB 0
LB 0 Hz
GB 0

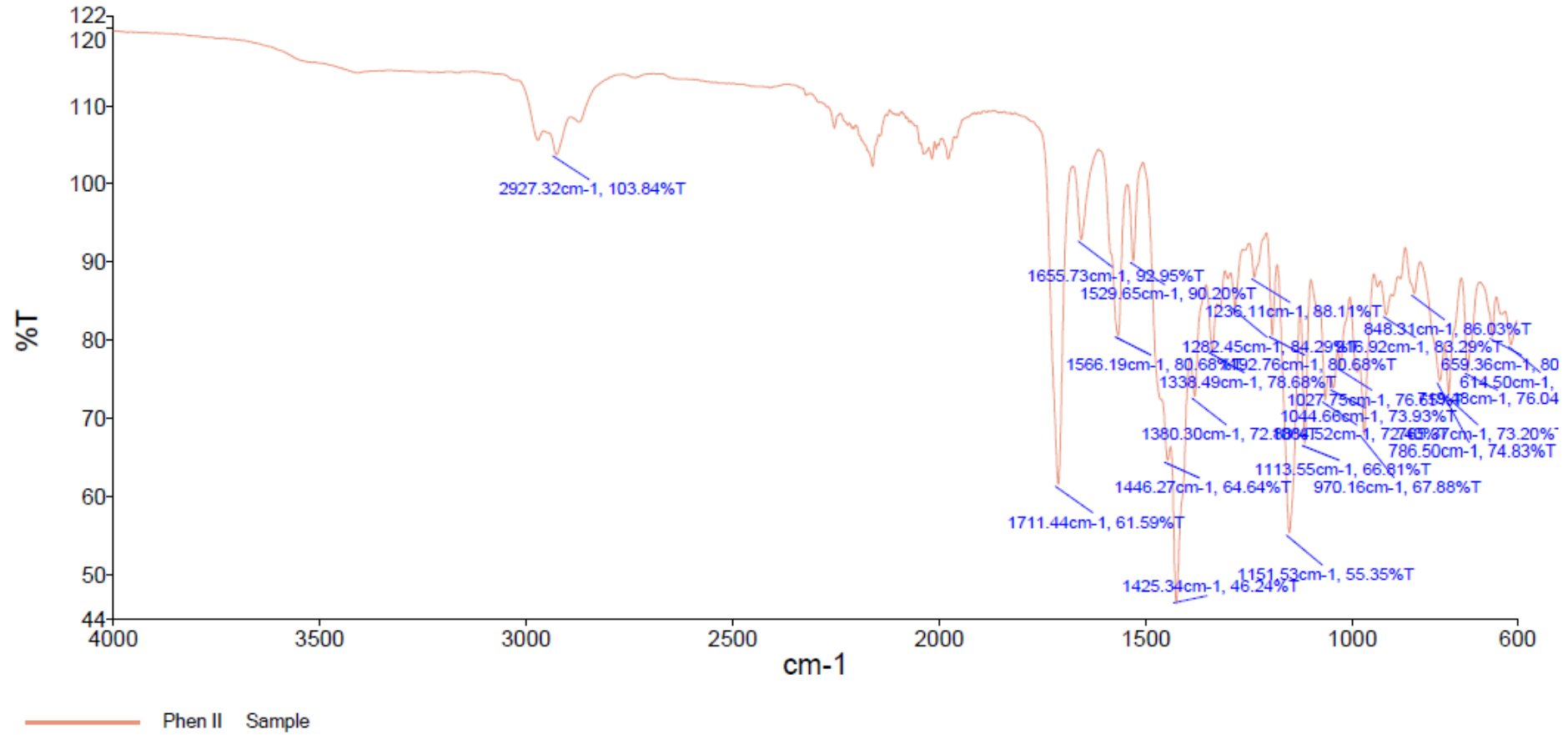


88b IR Spectrum

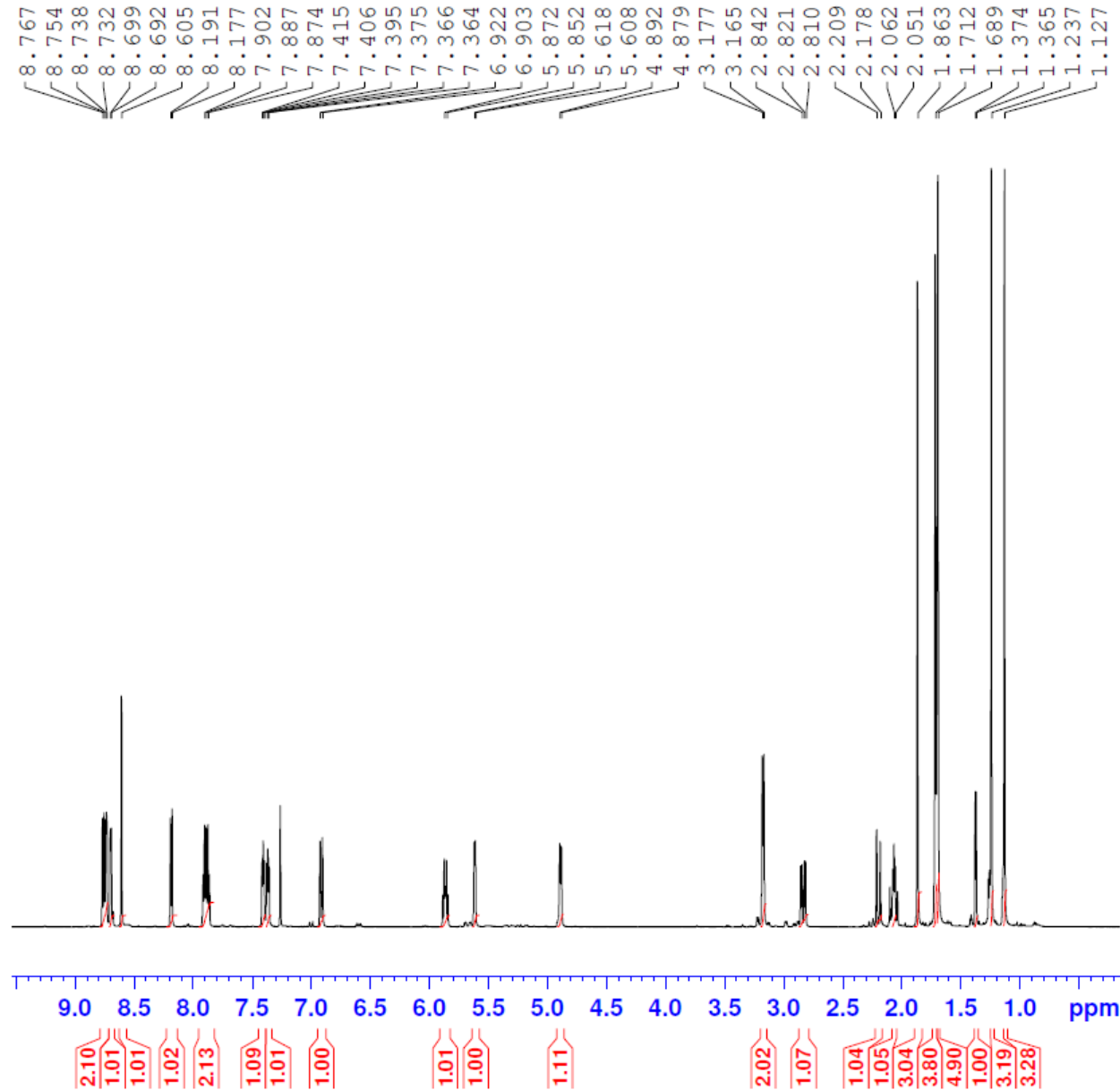
PerkinElmer Spectrum Version 10.4.00
Friday, 3 January 2020 12:02 PM

Analyst
Date

Analyst
Friday, 3 January 2020 12:02 PM



87a NMR Characterisation

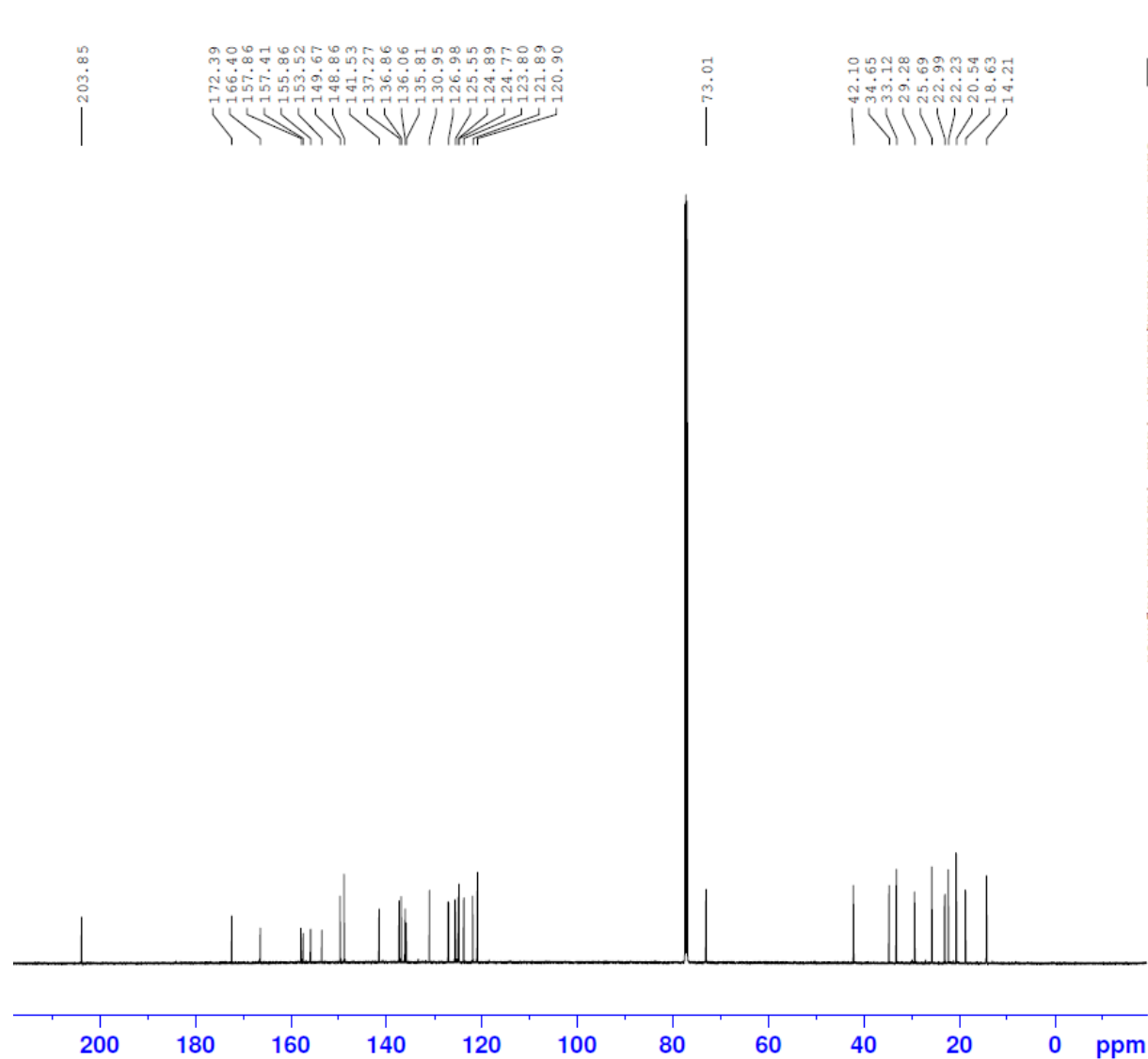


Current Data Parameters
NAME 20190527 Inv DA P1 2Py Terminal Isomer
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190527
Time 17.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 161
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 600.137060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300261 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 20190527 Inv DA PI 2py Terminal Isomer
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190527
 Time_ 22.27
 INSTRUM spect
 PRCMD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 5120
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

----- CHANNEL f2 -----
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9027918 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20190527 Inv DA PI 2Py Terminal Isom
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Data_ 20190527
Time 17.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosypppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 5681.818 Hz
FIDRES 2.774325 Hz
AQ 0.1802240 sec
RG 64
DW 88.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.94757104 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D14 0.00000000 sec
IN0 0.00017600 sec

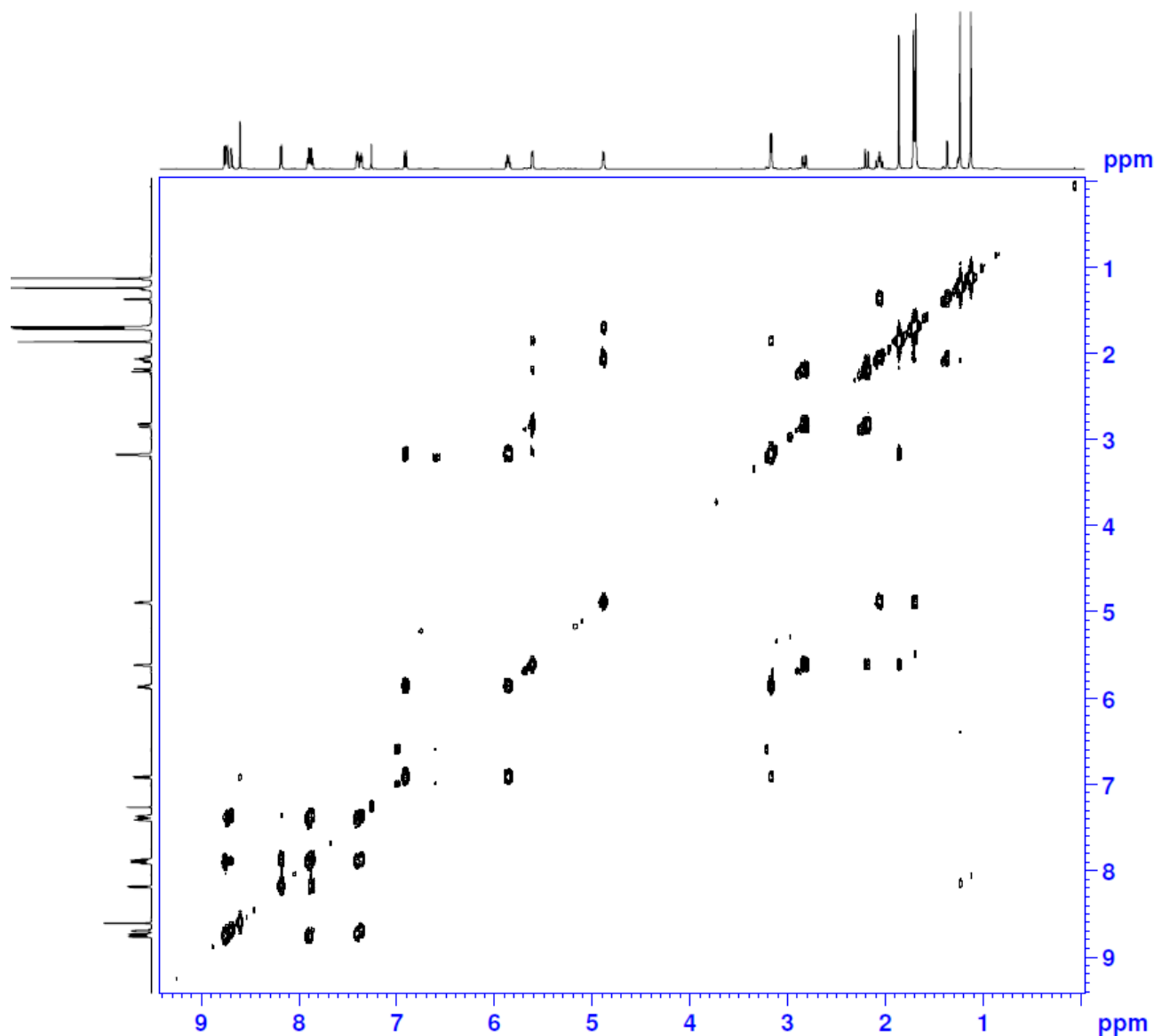
----- CHANNEL f1 -----
SF01 600.1328416 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPMAM[1] SMSQ10.100
CPE1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.1328 MHz
FIDRES 44.389206 Hz
SW 9.468 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300255 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300270 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190527 Inv DA PI 2Py Terminal Isomer
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters

Date_ 20190527
Time 22.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcztgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 5681.818 Hz
FIDRES 5.548651 Hz
AQ 0.0901120 sec
RG 2050
RW 88.000 usec
DE 6.50 usec
TE 298.3 K
CNS2 145.0000000
DO 0.00000300 sec
D1 1.47542405 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
INO 0.00002000 sec
RGOWNS

----- CHANNEL f1 -----
SFO1 600.1328390 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

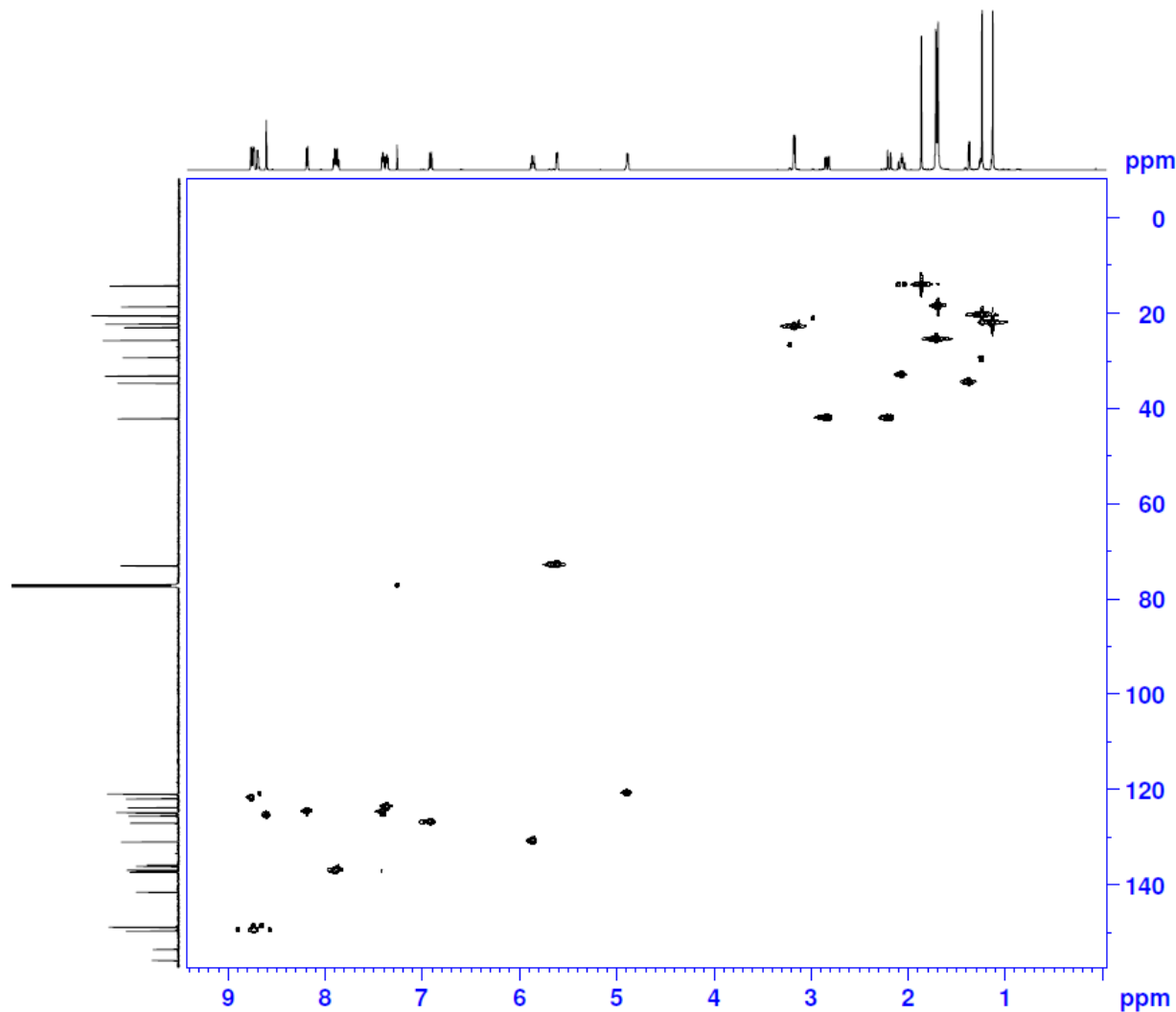
----- CHANNEL f2 -----
SFO2 150.9140636 MHz
NUC2 13C
CPOPRG[2] gcp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 80.00000000 W
PLW12 3.20000005 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
CPE1 80.00 %
CPE2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FNAME Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300259 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028227 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190527 Inv DA P1 2Py Terminal Isomer
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190528
Time 4.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hbmgppdgdg
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 5681.818 Hz
FIDRES 1.387163 Hz
AQ 0.3604480 sec
RG 2050
DQ 88.000 usec
DE 6.50 usec
TE 298.1 K
CNS113 8.0000000
D0 0.00000300 sec
D1 1.39514196 sec
D5 0.04250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

----- CHANNEL f1 -----
SFO1 600.1328390 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

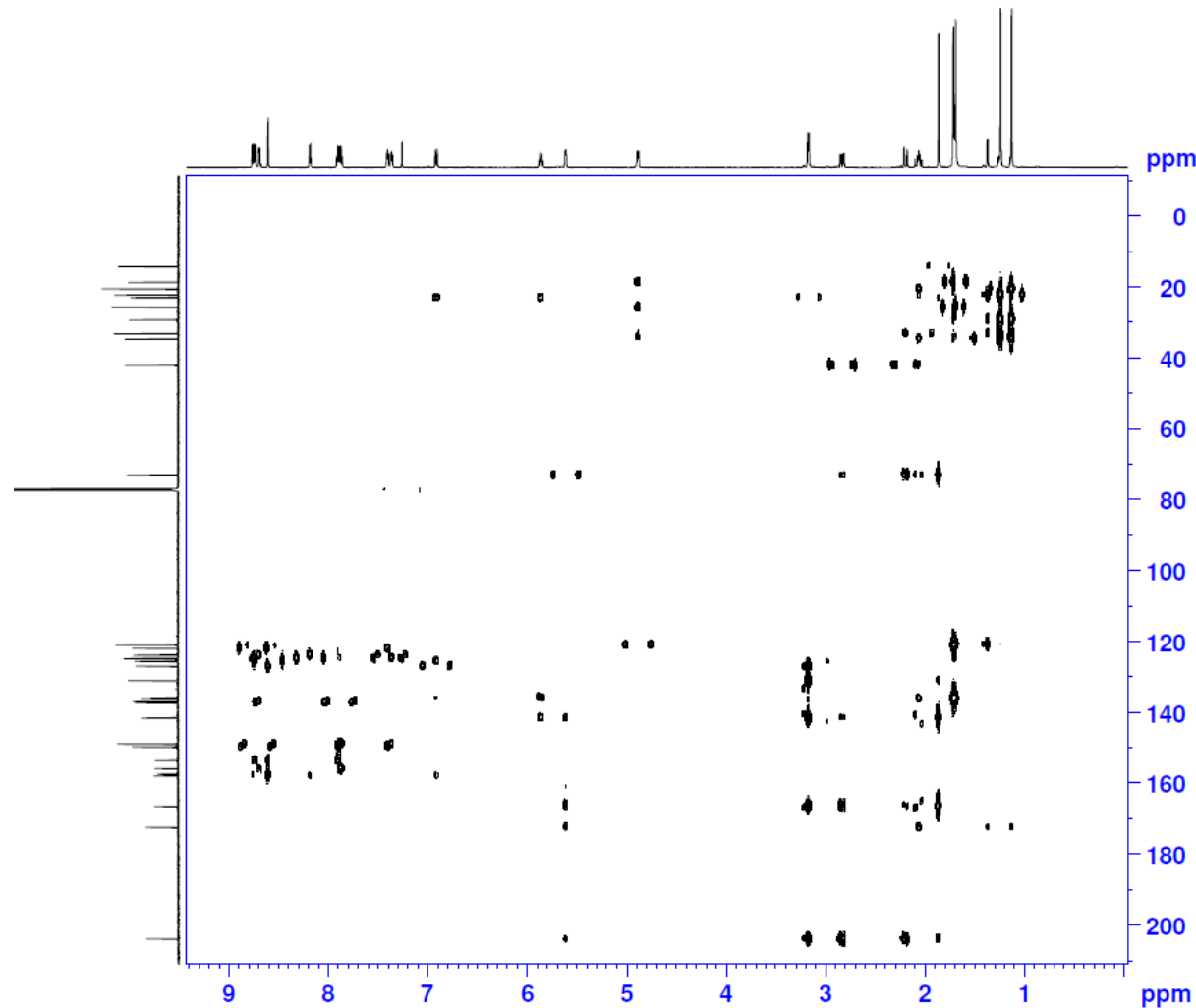
----- CHANNEL f2 -----
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 80.00000000 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPE1 50.00 %
GPE2 30.00 %
GPE3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FNAME QF

F2 - Processing parameters
SI 1024
SF 600.1300232 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028154 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

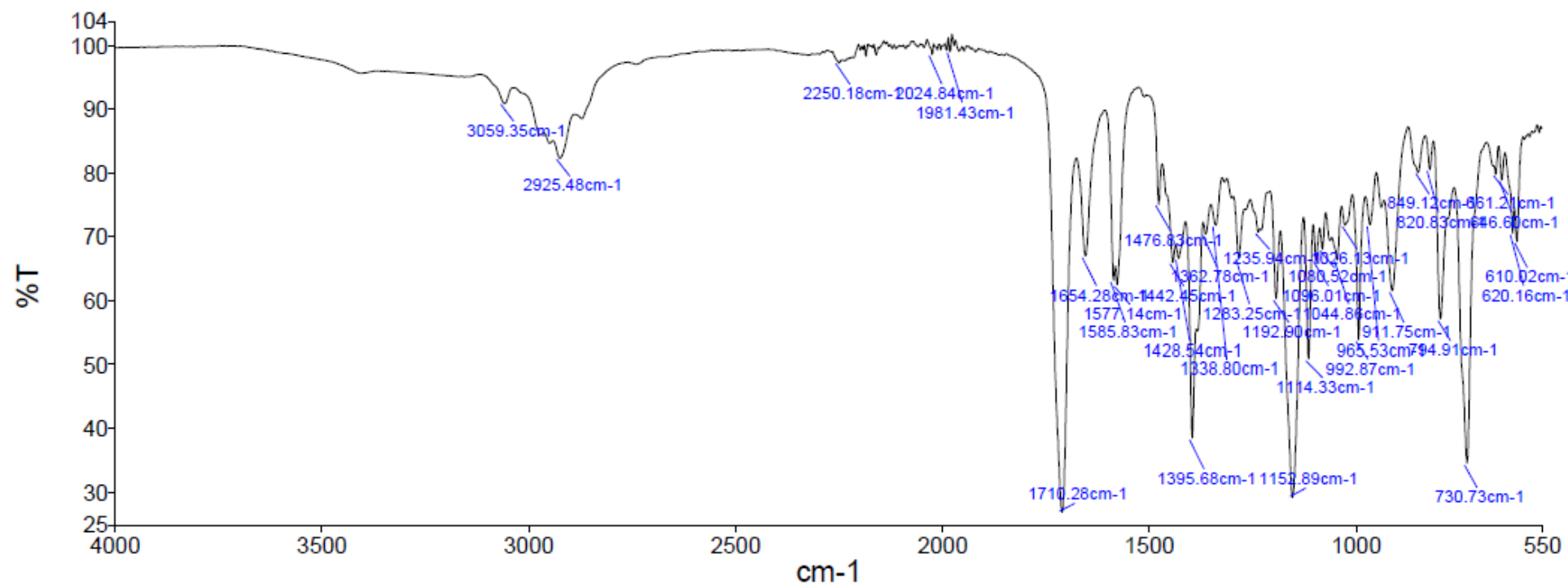


87a IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Tuesday, 18 June 2019 10:43 AM

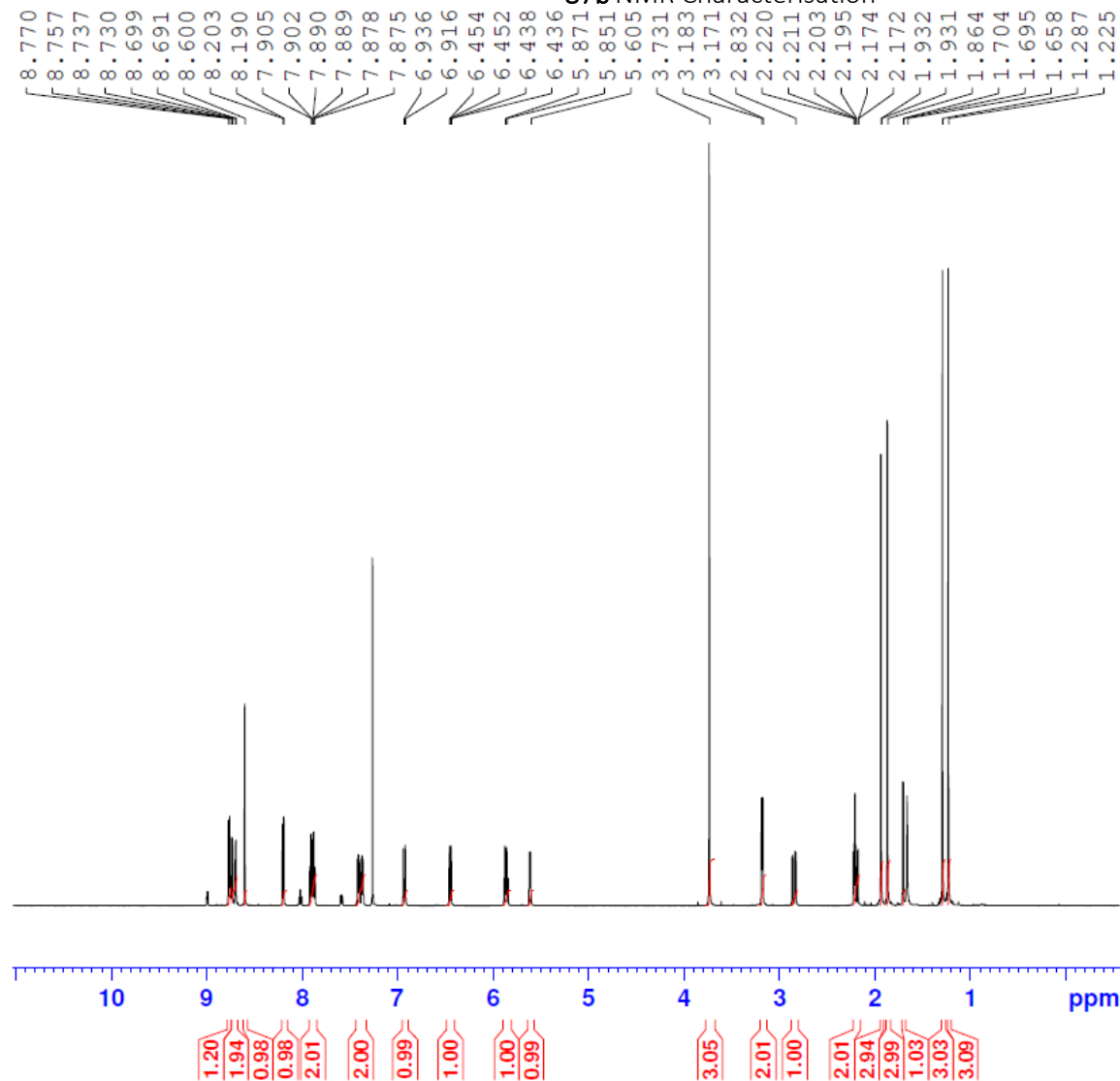
Analyst
Date

Analyst
Tuesday, 18 June 2019 10:43 AM



Sample Name	Description	Quality Checks
PI 2Py Cis	Sample 007 By Analyst Date Tuesday, June 18 2019	The Quality Checks do not report any warnings for the sample.

87b NMR Characterisation

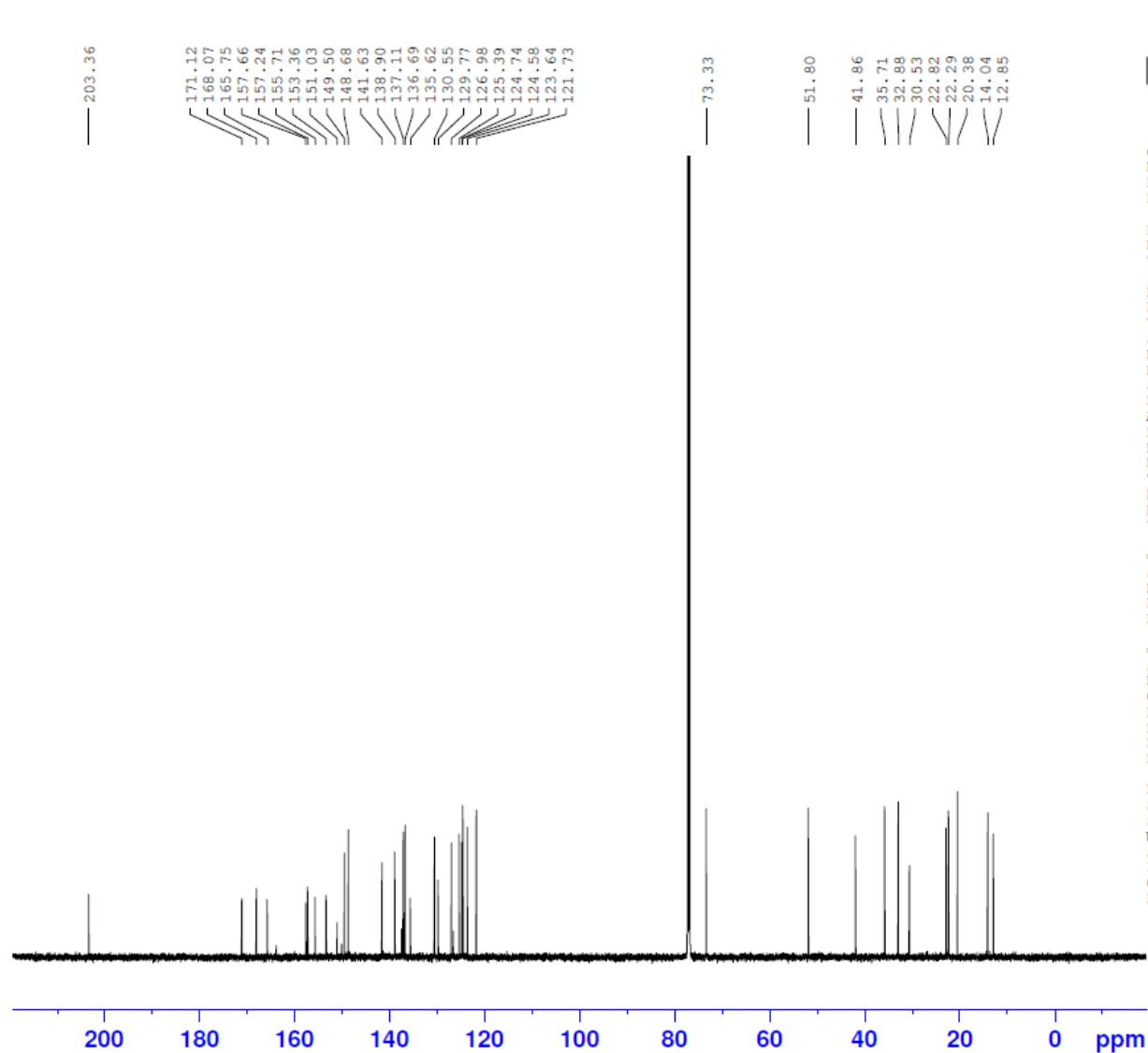


Current Data Parameters
NAME 20190806 Inv DA PII 2Py
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190806
Time 18.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 203
DW 41.600 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
D10 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300260 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 20190806 Inv DA PII 2Py
 EXPNO 32
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190806
 Time 20.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028162 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20190806 Inv DA PII 2Py
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190806
Time 18.09
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 5747.126 Hz
FIDRES 2.806214 Hz
AQ 0.1781760 sec
RG 64
DW 87.000 usec
DE 6.50 usec
TE 297.8 K
D0 0.00000300 sec
D1 1.94961905 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00017400 sec

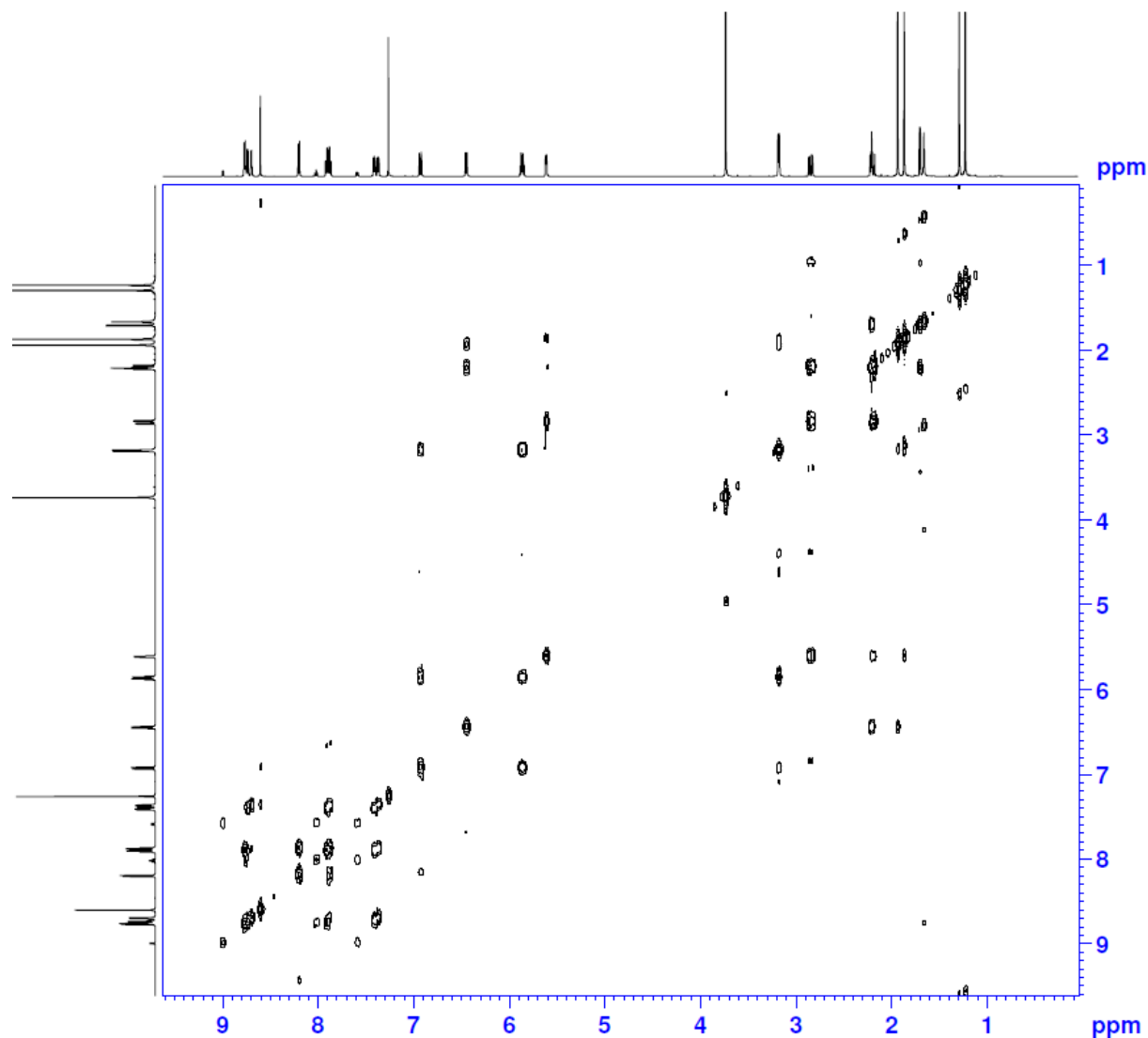
----- CHANNEL f1 -----
SFO1 600.1329257 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1329 MHz
FIDRES 44.899426 Hz
SW 9.576 ppm
FhMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300262 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300278 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190806 Inv DA P11 2py
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190806
Time 20.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 5681.818 Hz
FIDRES 5.548651 Hz
AQ 0.0901120 sec
RG 2050
CW 88.000 usec
DE 6.50 usec
TE 298.7 K
CNS12 145.0000000
D0 0.00000300 sec
D1 1.47542405 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1330024 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

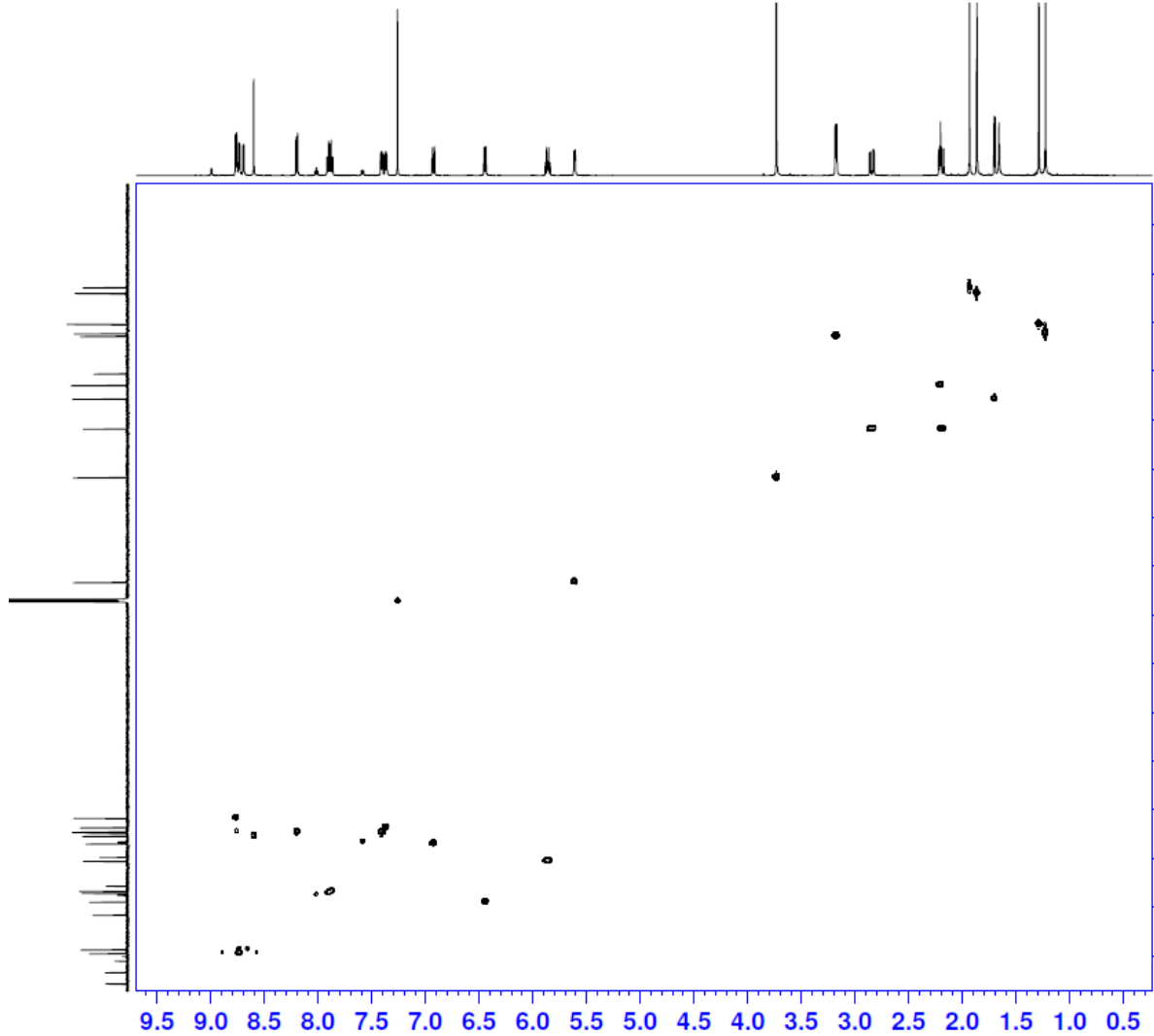
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
PCPDPRG2 garrp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 80.00000000 W
PLW12 3.20000005 W

===== GRADIENT CHANNEL =====
GPMAM[1] SMSG10.100
GPMAM[2] SMSG10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.627 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300246 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028455 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190806 Inv DA PII 2Py
EXPNO 35
PROCNO 1

F2 - Acquisition Parameters
Data_ 20190807
Time 2.24

INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 5681.818 Hz
FIDRES 1.387163 Hz
AQ 0.3604480 sec
RG 2050
DW 88.000 usec
DE 6.50 usec
TE 298.6 K
CNS113 8.0000000
D0 0.00000300 sec
D1 1.39514196 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.130024 MHz
NUC1 1H
P1 13.50 usec
F2 27.00 usec
PLW1 17.00000000 W

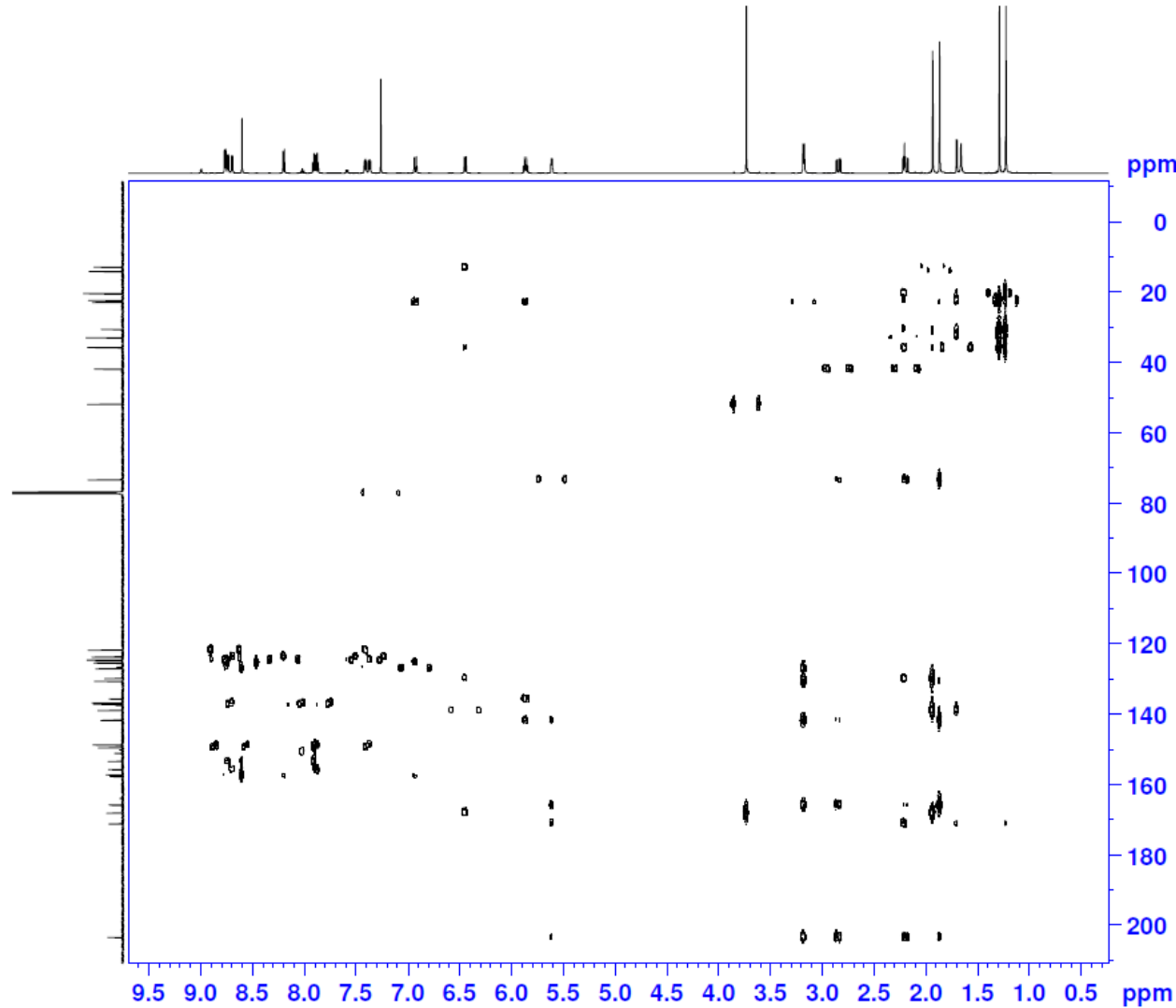
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
F3 12.00 usec
PLW2 80.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
F1MODE QF

F2 - Processing parameters
SI 1024
SF 600.1300222 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028408 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

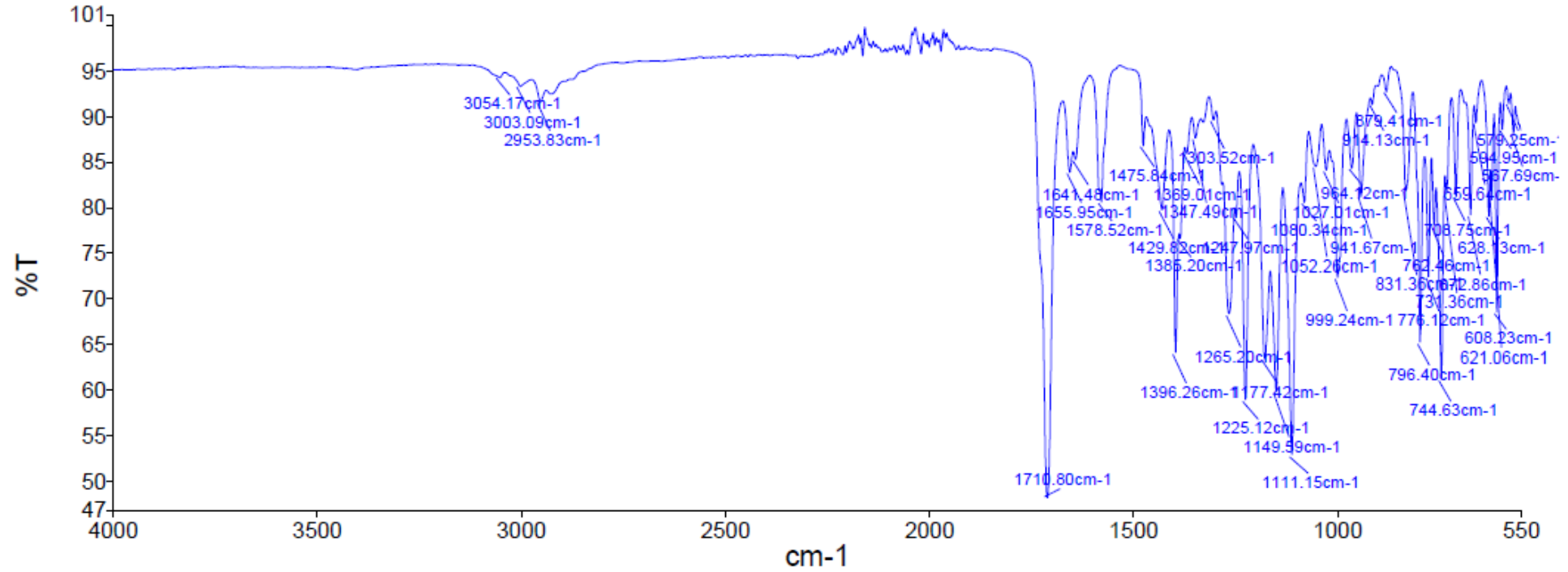


87b IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Tuesday, 18 June 2019 10:45 AM

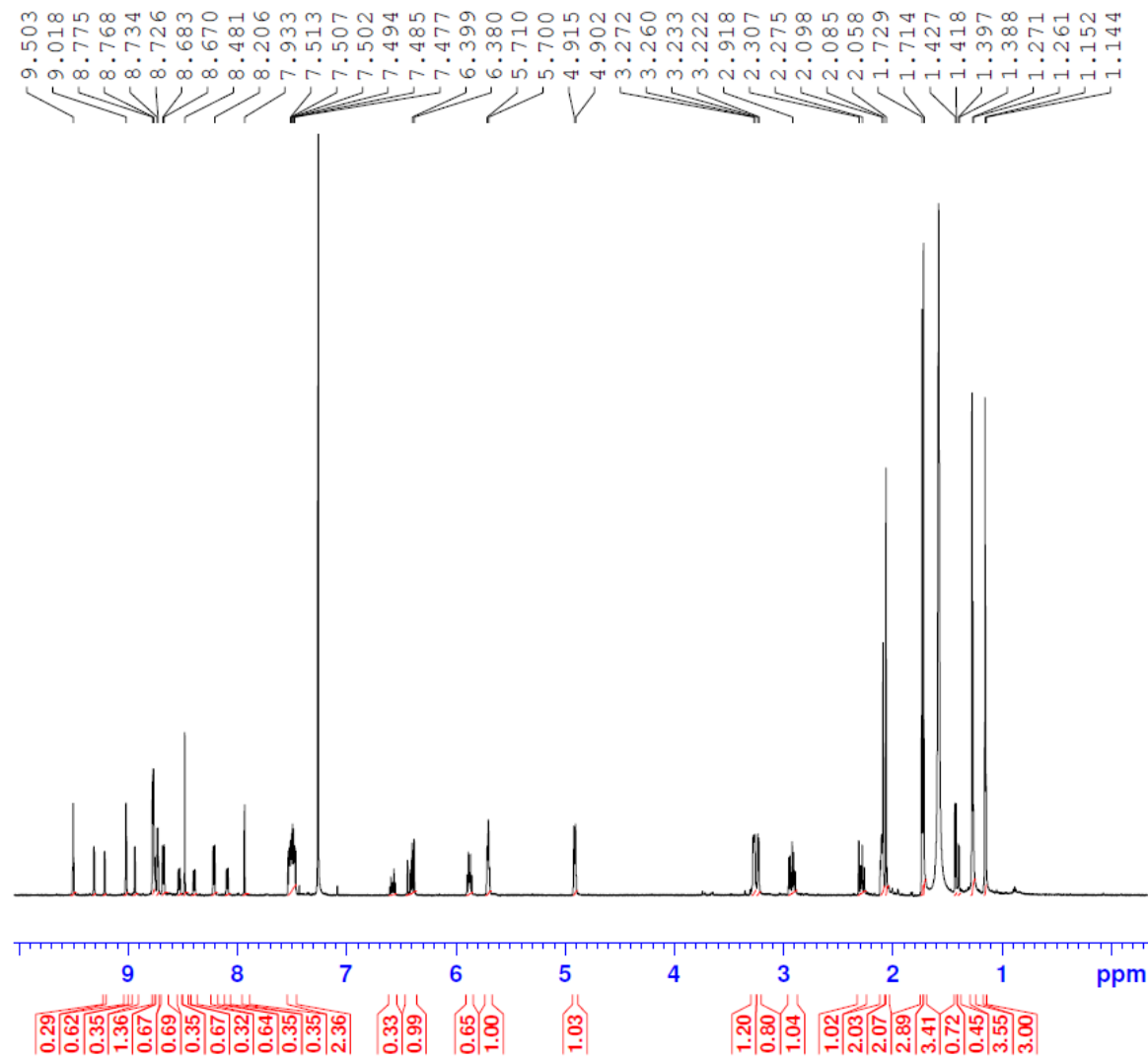
Analyst
Date

Analyst
Tuesday, 18 June 2019 10:45 AM



Sample Name	Description	Quality Checks
PII @Py cis	Sample 009 By Analyst Date Tuesday, June 18 2019	The Quality Checks do not report any warnings for the sample.

89a NMR Characterisation

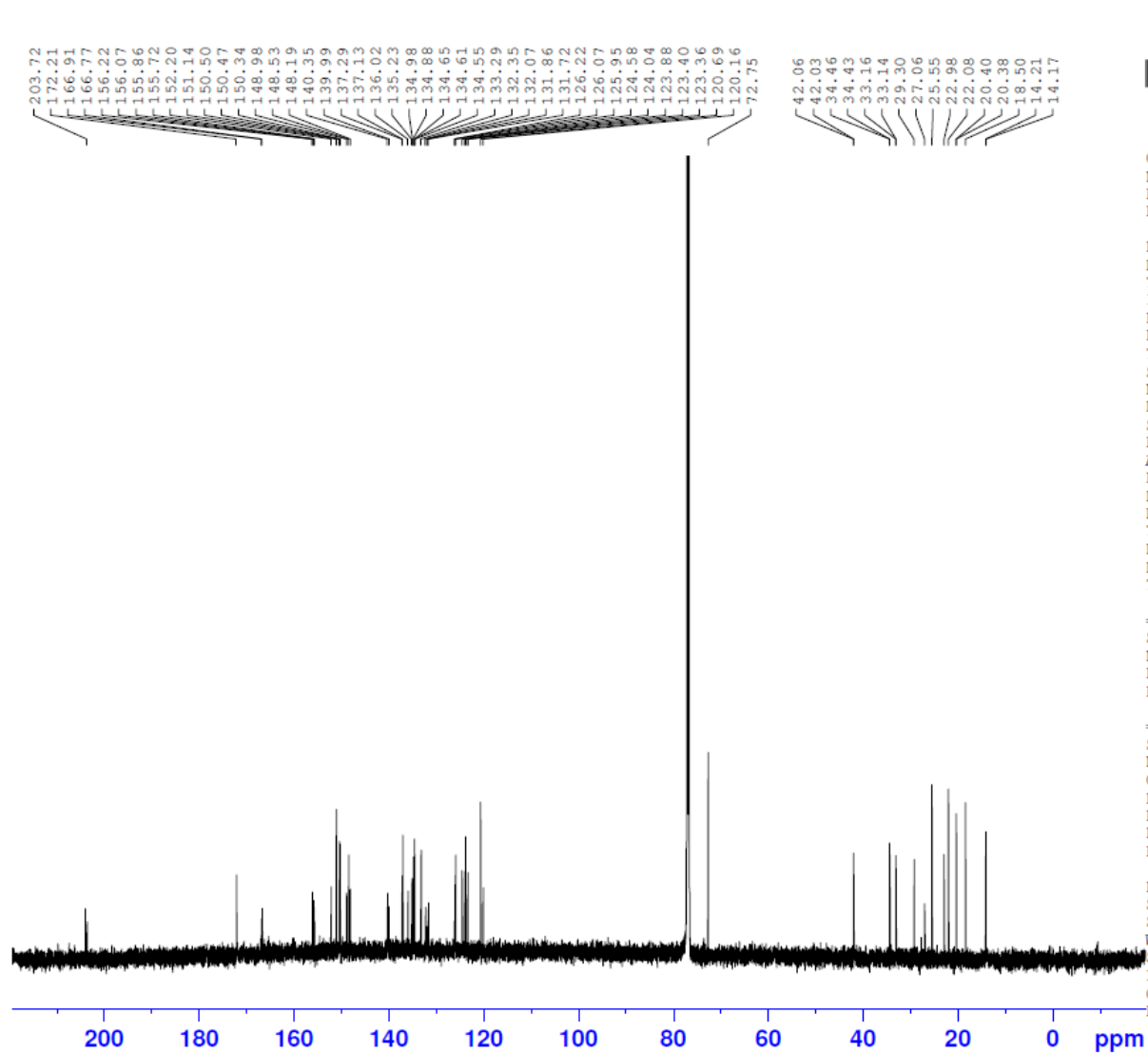


Current Data Parameters
 NAME 20200227 3Py 1 (PURIFIED)
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200227
 Time 17.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 362
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SF01 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300262 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20200401 3Py I
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200401
 Time 21.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 5120
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028140 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200227 3py 1 (PURIFIED)
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200227
Time 17.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 6024.096 Hz
FIDRES 2.941453 Hz
AQ 0.1699840 sec
RG 181
SW 83.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.95781100 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
INO 0.00016600 sec

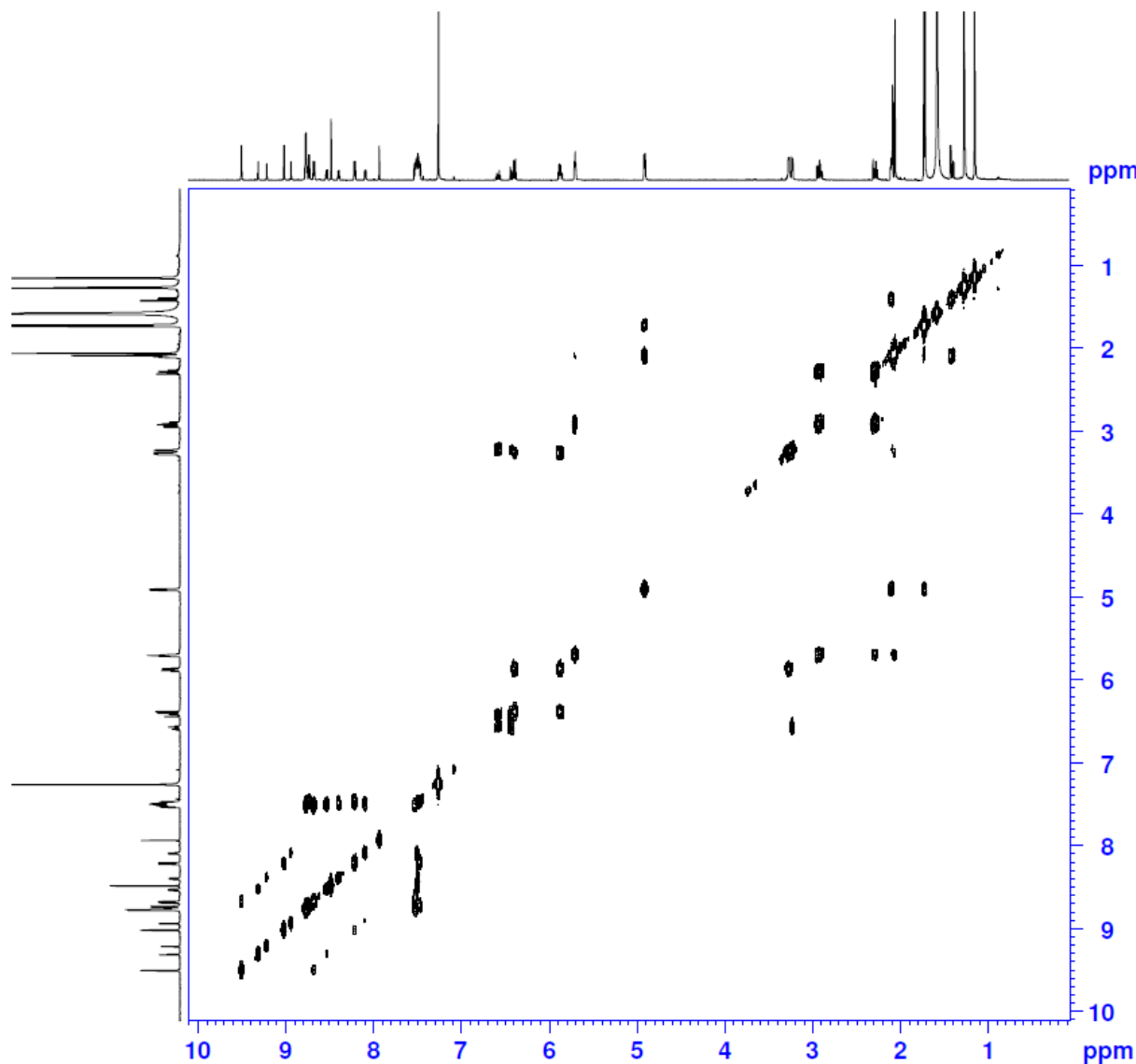
----- CHANNEL f1 -----
SFO1 600.1330829 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GF21 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1331 MHz
FIDRES 47.063251 Hz
SW 10.038 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300256 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300272 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200403 3py 1
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200404
Time 9.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcztgq
TD 1024
SOLVENT CDCl3
NS 60
DS 16
SWH 6097.561 Hz
FIDRES 5.954649 Hz
AQ 0.0839680 sec
RG 2050
LW 82.000 usec
DE 6.50 usec
TE 298.3 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.48156798 sec
D4 0.0012414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
RGOPHS

===== CHANNEL f1 =====
SFO1 600.1330546 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P2B 1000.00 usec
P1W1 17.00000000 W

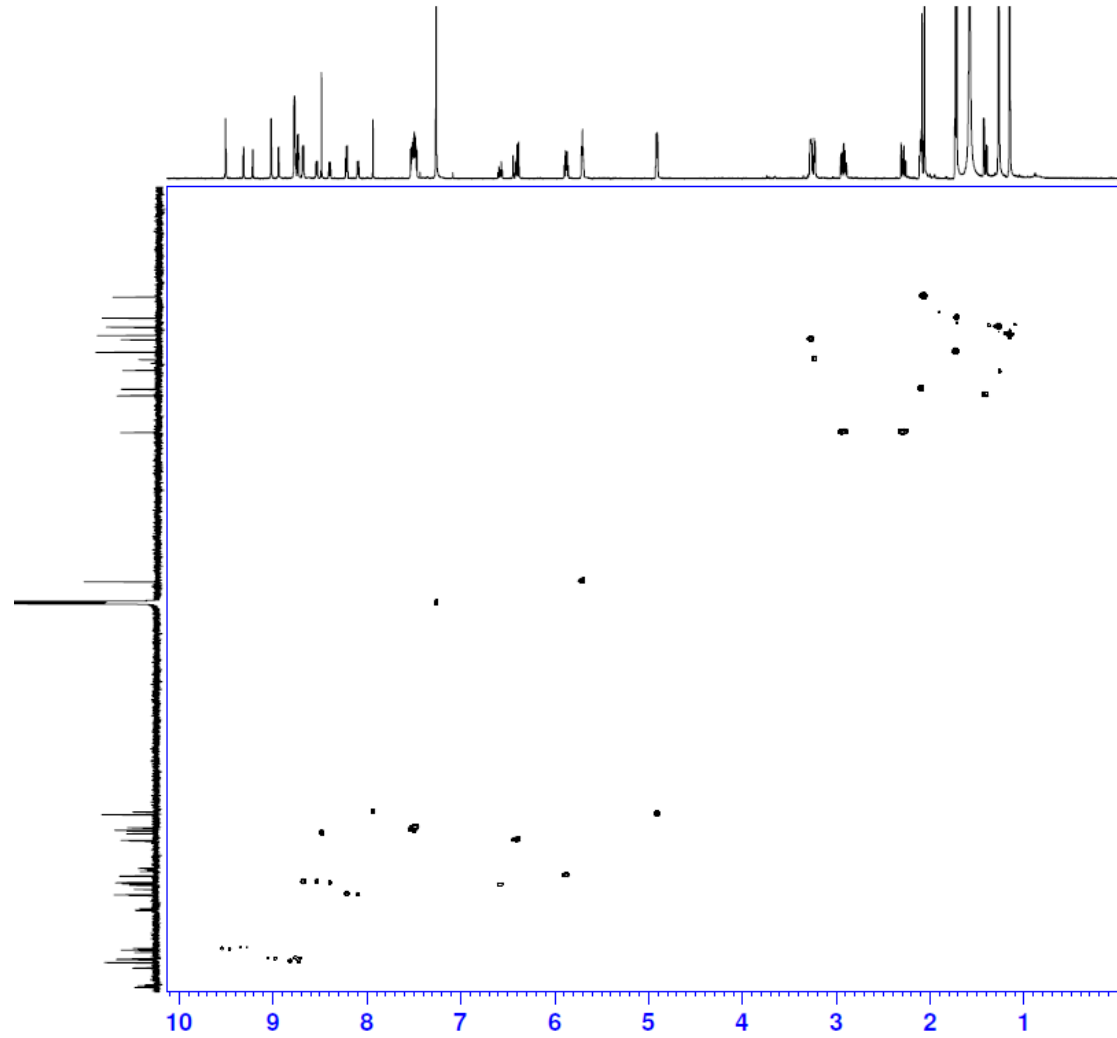
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
P1W2 79.98300171 W
P1W12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
CP1 80.00 %
CP2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.627 ppm
FnmODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300252 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

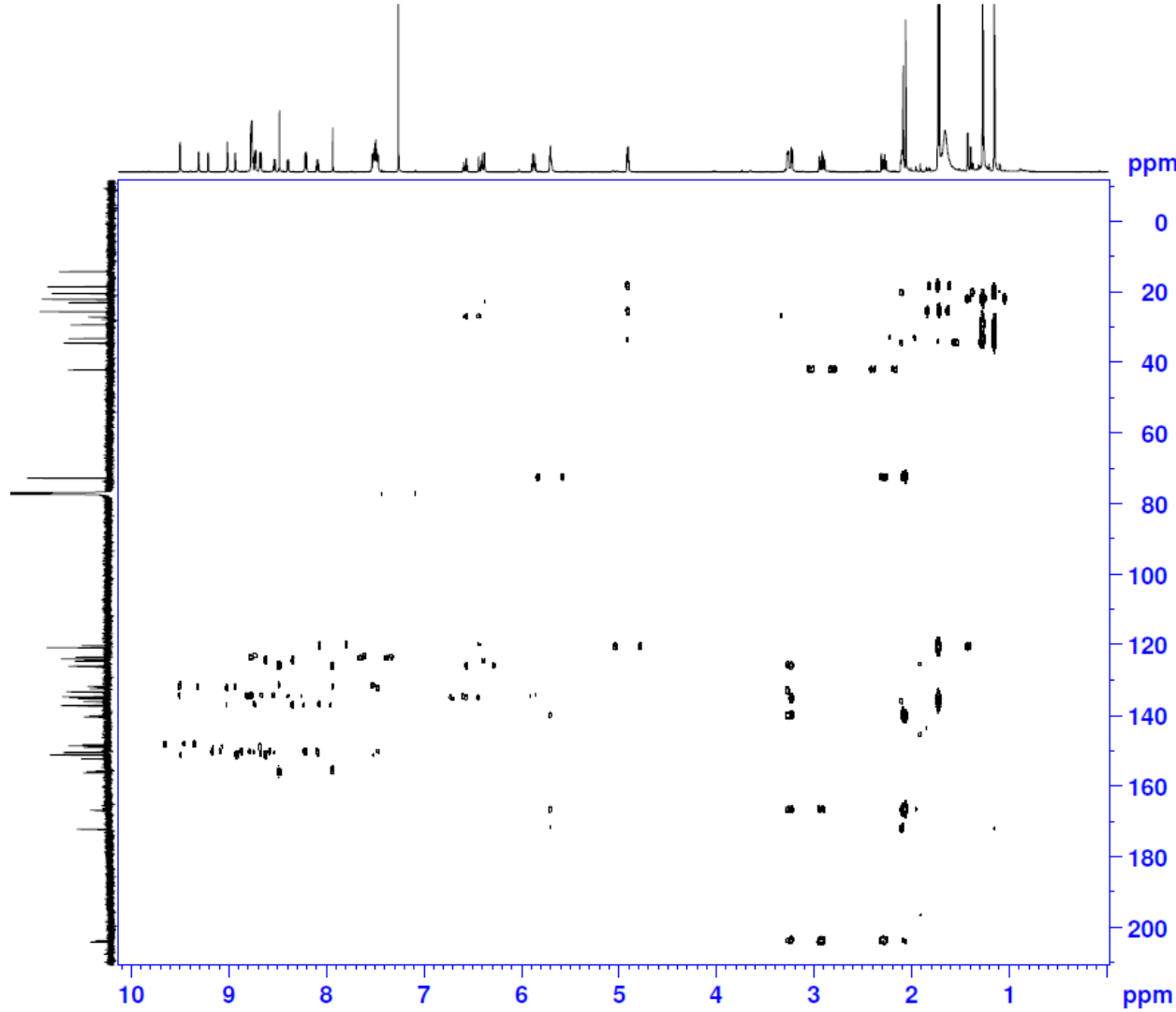
F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9026449 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200403 3py 1
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200404
Time 16.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 80
DS 16
SWH 6097.561 Hz
FIDRES 1.488662 Hz
AQ 0.3358720 sec
RG 2050
DM 82.000 usec
DE 6.50 usec
TE 298.3 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.41971803 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec
===== CHANNEL f1 =====
SFO1 600.1330546 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec
F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
F2 - Processing parameters
SI 1024
SF 600.1300246 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028548 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

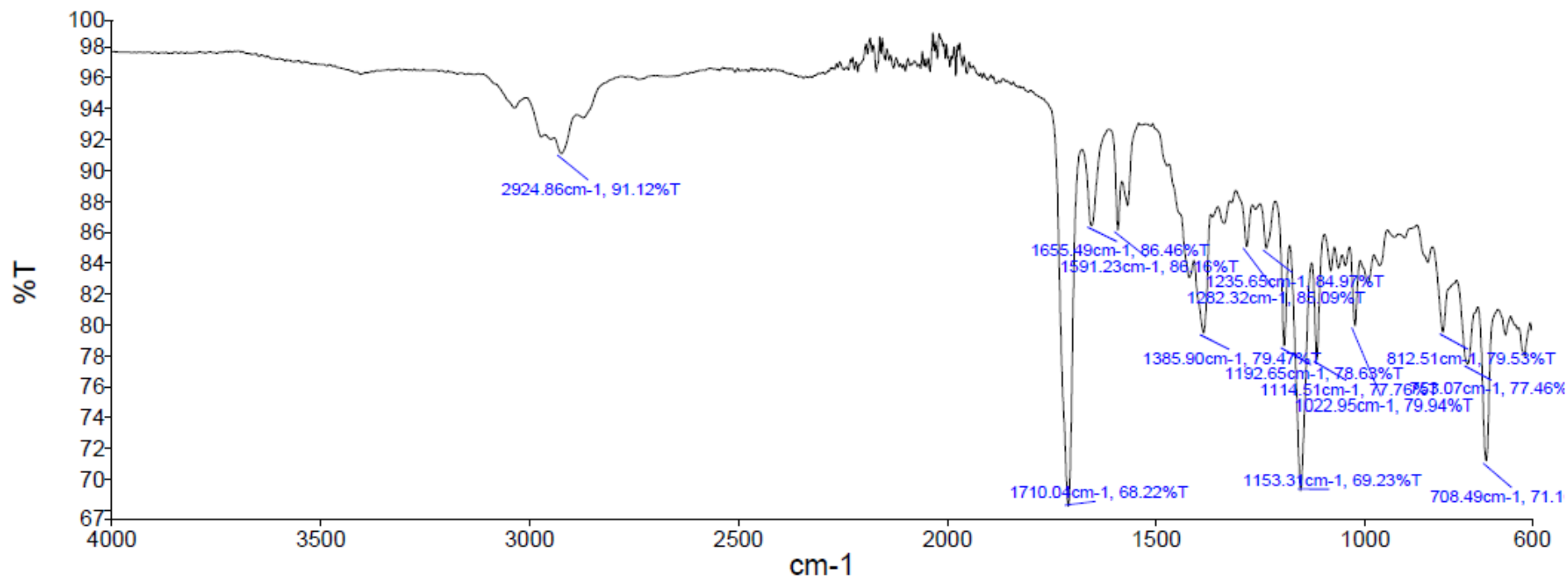


89a IR Spectrum

PerkinElmer Spectrum Version 10.4.2
Monday, 23 March 2020 10:18 AM

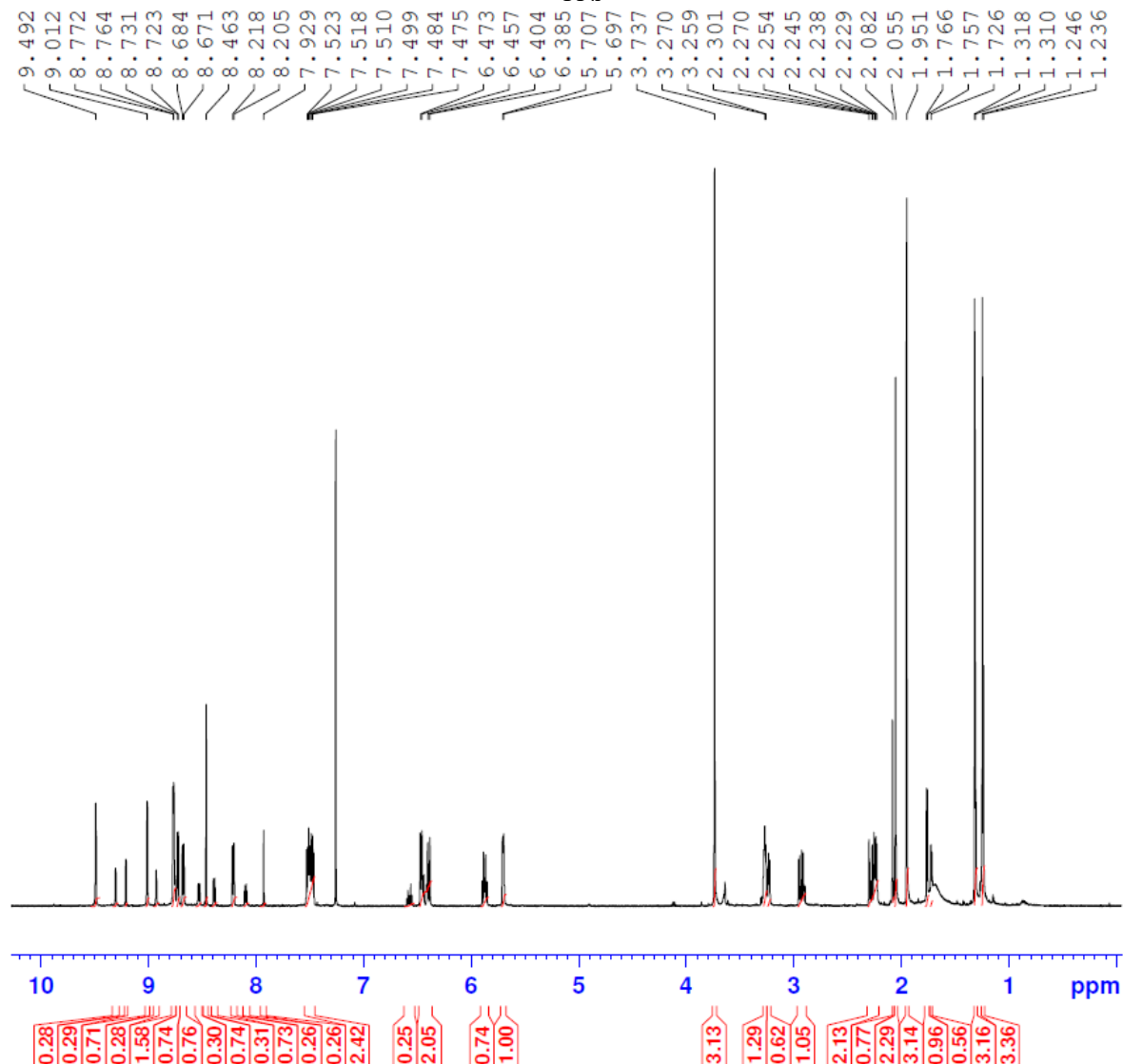
Analyst
Date

Analyst
Monday, 23 March 2020 10:18 AM



Sample Name	Description	Quality Checks
3Py I	Sample 110 By Analyst Date Wednesday, March 18 2020	The Quality Checks do not report any warnings for the sample.

89b NMR Characterisation

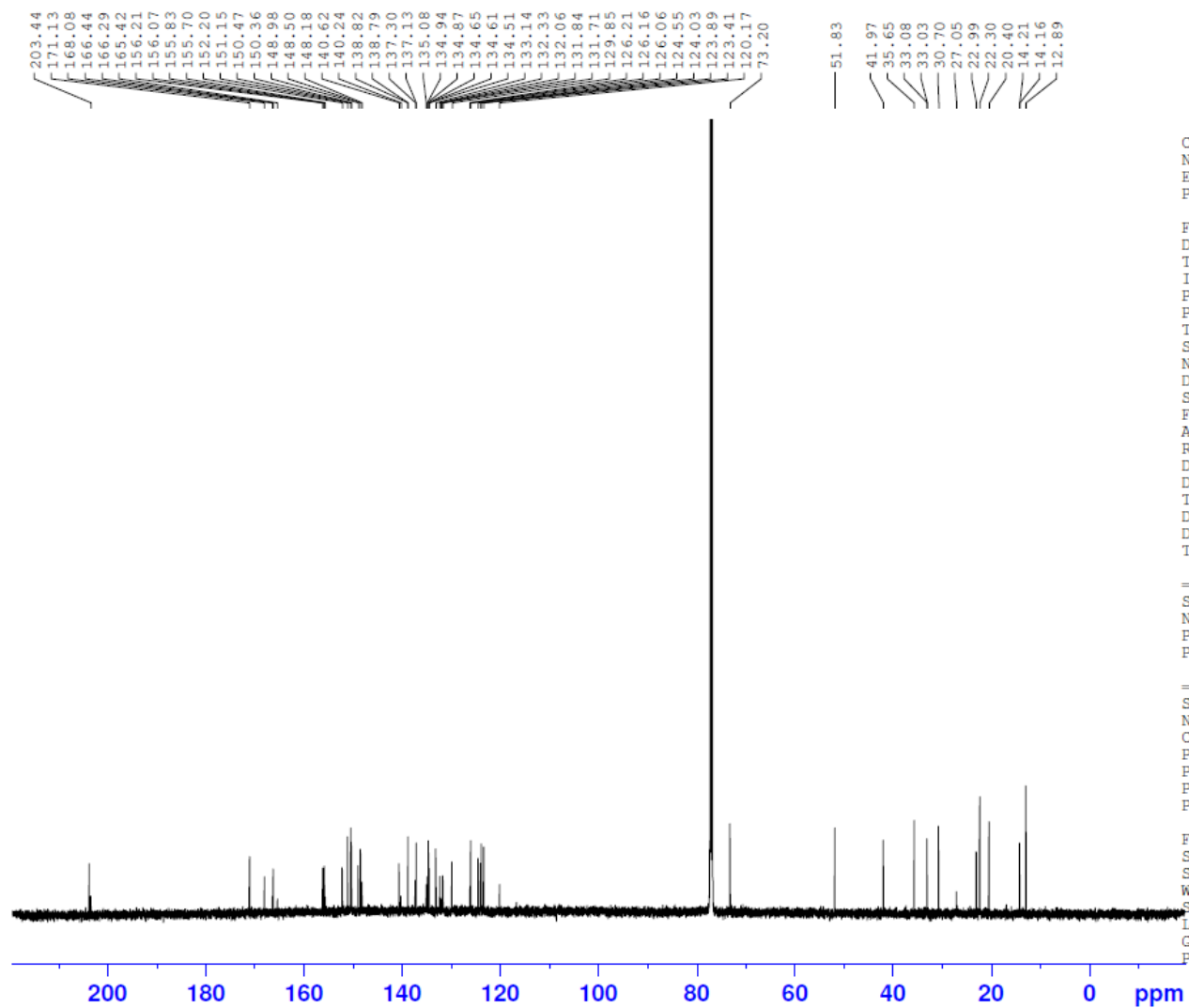


Current Data Parameters
NAME 20200310 3Py II CONC
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200310
Time 18.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 256
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300265 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 20200310 3Py II CONC
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200310
 Time 18.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4096
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028147 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200310 3py II CONC
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200310
Time 21.34
INSRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygmfphpp
ID 2048
SOLVENT CDCl3
NS 10
DS 4
SWH 5952.381 Hz
FIDRES 2.906436 Hz
AQ 0.1720320 sec
RG 2050
DW 84.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00006681 sec
D1 1.96641302 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00016800 sec

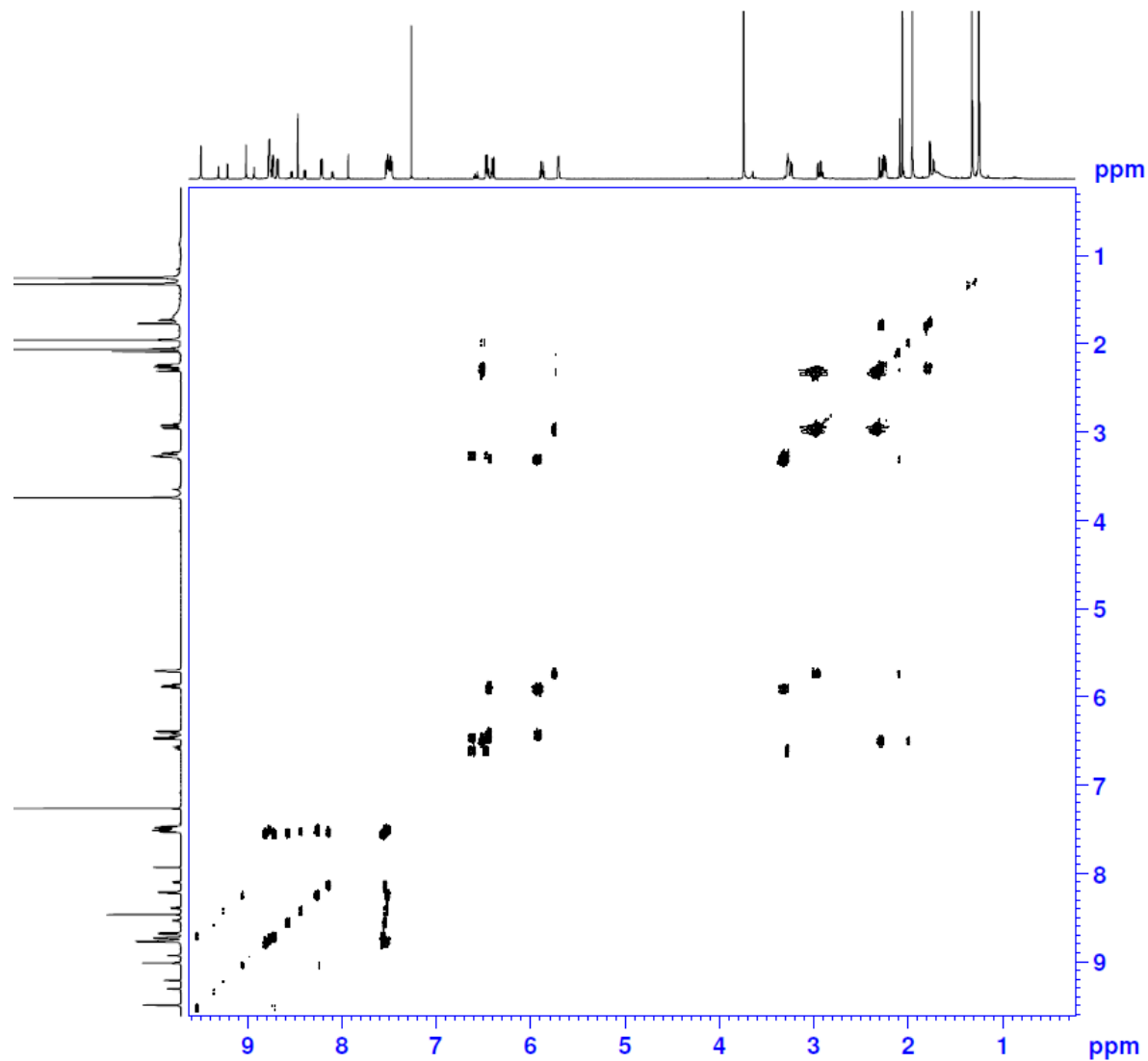
----- CHANNEL f1 -----
SFO1 600.1331104 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 256
SFO1 600.1331 MHz
FIDRES 23.251488 Hz
SW 9.918 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200310 3py 11 CCNC
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200310
Time 23.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 6024.096 Hz
FIDRES 5.882906 Hz
AQ 0.0849920 sec
RG 2050
DW 83.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.0000300 sec
D1 1.48054397 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS

===== CHANNEL f1 =====
SFO1 600.1330875 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

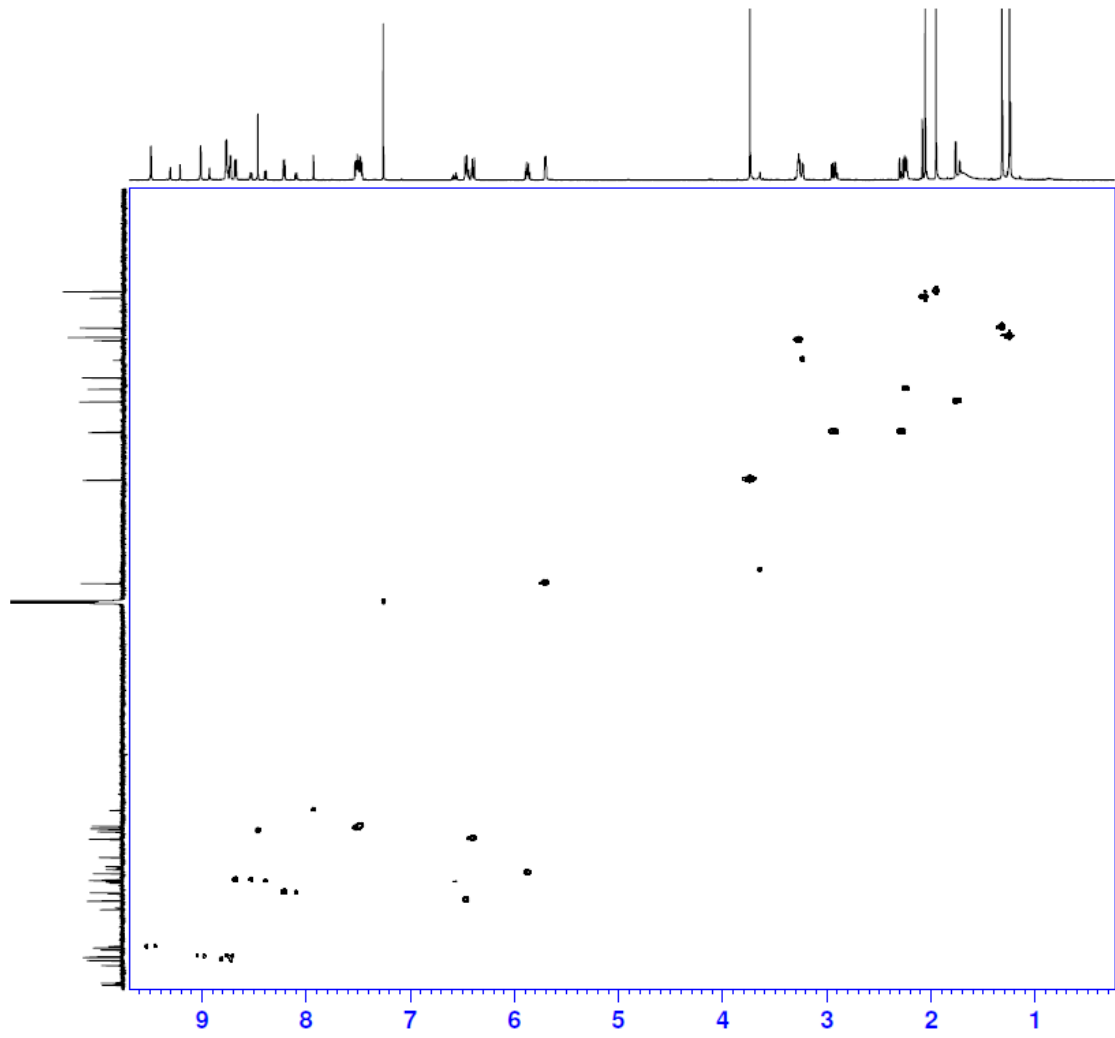
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPOPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
CPZ1 80.00 %
CPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300251 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028409 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200310 3py ii CONC
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200311
Time 4.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 6024.096 Hz
FIDRES 1.470727 Hz
AQ 0.3399680 sec
RG 2050
RW 83.000 usec
DE 6.50 usec
TE 298.2 K
CNS113 8.0000000
D0 0.0000000 sec
D1 1.41562200 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL F1 =====
SFO1 600.1330875 MHz
NUC1 1H
P1 13.50 usec
F2 27.00 usec
PLW1 17.00000000 W

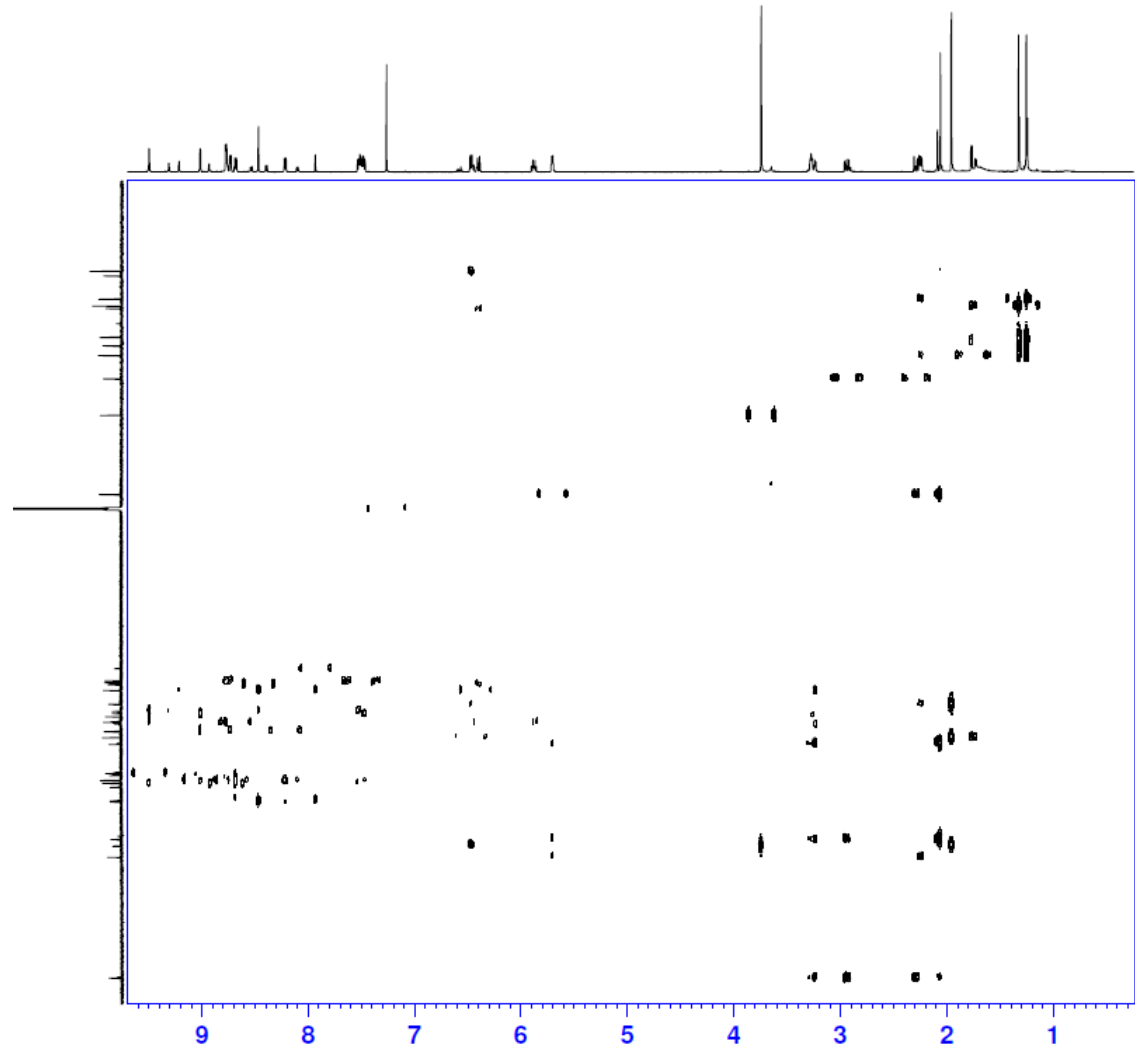
===== CHANNEL F2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 115
SFO1 150.9179 MHz
FIDRES 291.800415 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300254 MHz
WDW SINK
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028505 MHz
WDW SINK
SSB 0
LB 0 Hz
GB 0

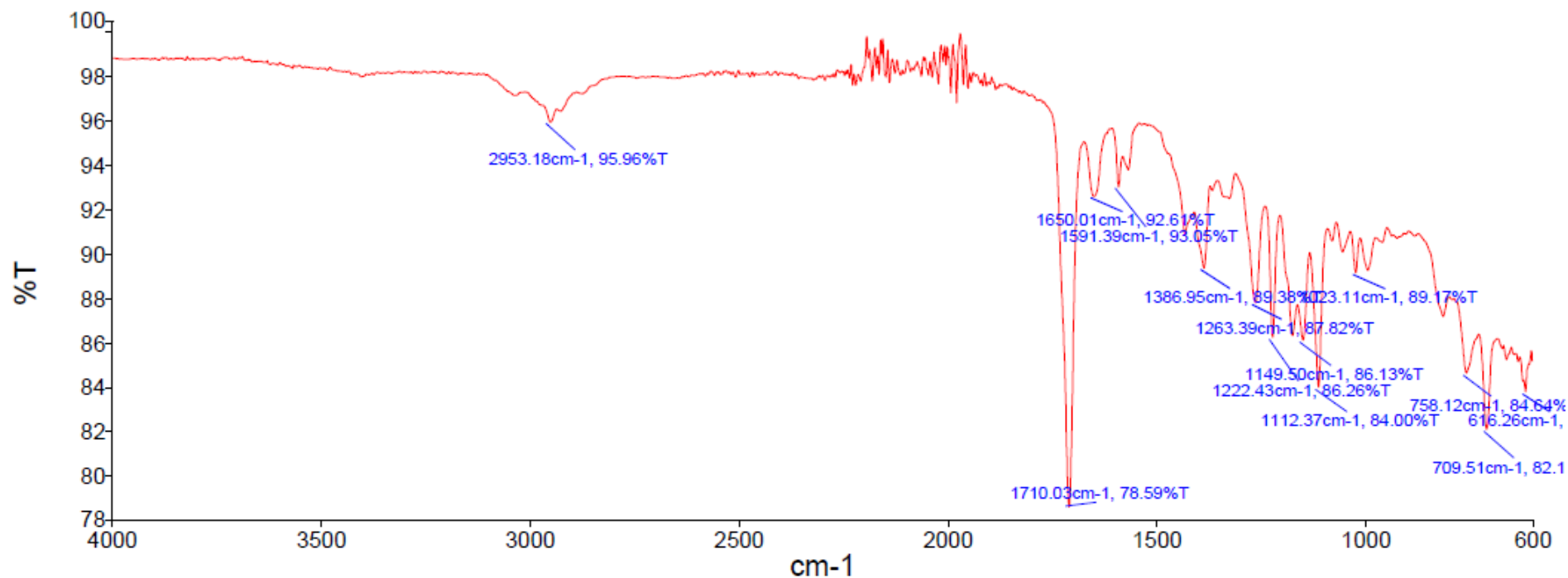


89b IR Spectrum

PerkinElmer Spectrum Version 10.4.2
Monday, 23 March 2020 10:17 AM

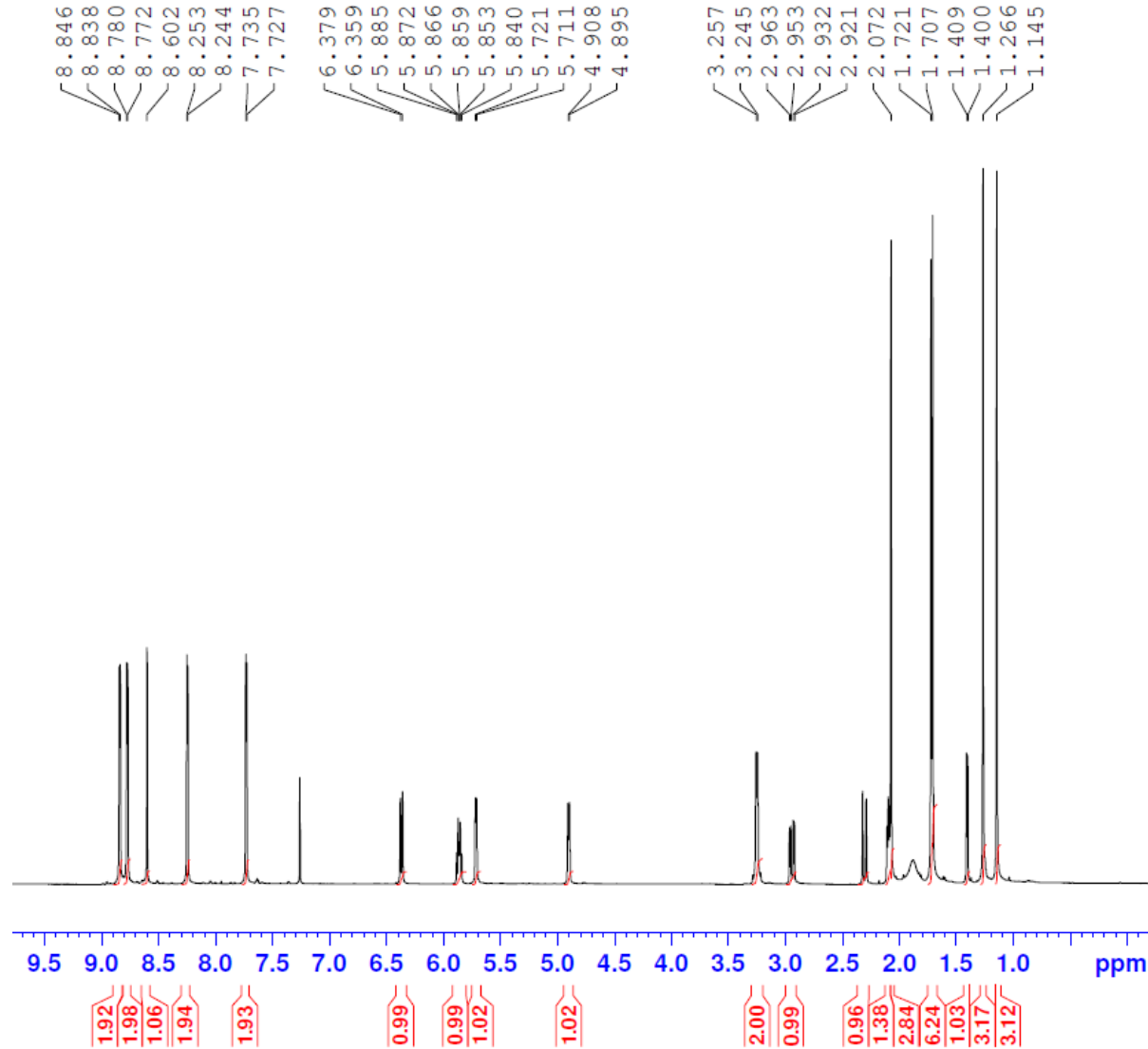
Analyst
Date

Analyst
Monday, 23 March 2020 10:17 AM



Sample Name	Description	Quality Checks
3Py II	Sample 111 By Analyst Date Monday, March 23 2020	The Quality Checks do not report any warnings for the sample.

90a NMR Characterisation

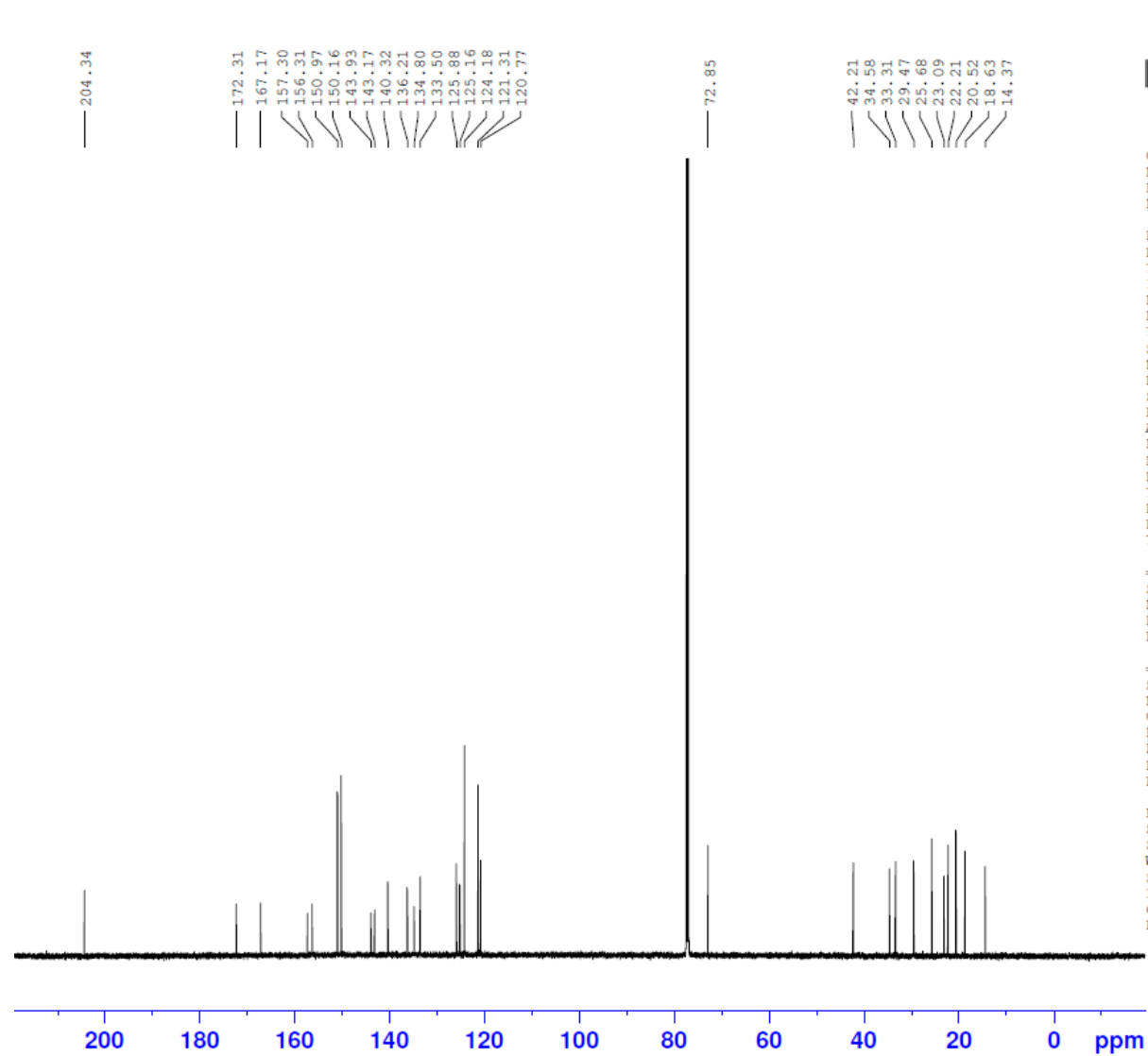


Current Data Parameters
 NAME 20190603 Inv DA PI 4Py
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190604
 Time 1.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 ID 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 161
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 ID0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300257 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20190603 Inv DA PI 4P
 EXPNO 22
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190604
 Time 3.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 ID 65536
 SOLVENT CDC13
 NS 1024
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9027942 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20190603 Inv DA PI 4py
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190604
Time 2.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 5
DS 8
SWH 6097.561 Hz
FIDRES 2.977325 Hz
AQ 0.1679360 sec
RG 64
DW 82.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.95985901 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00016400 sec

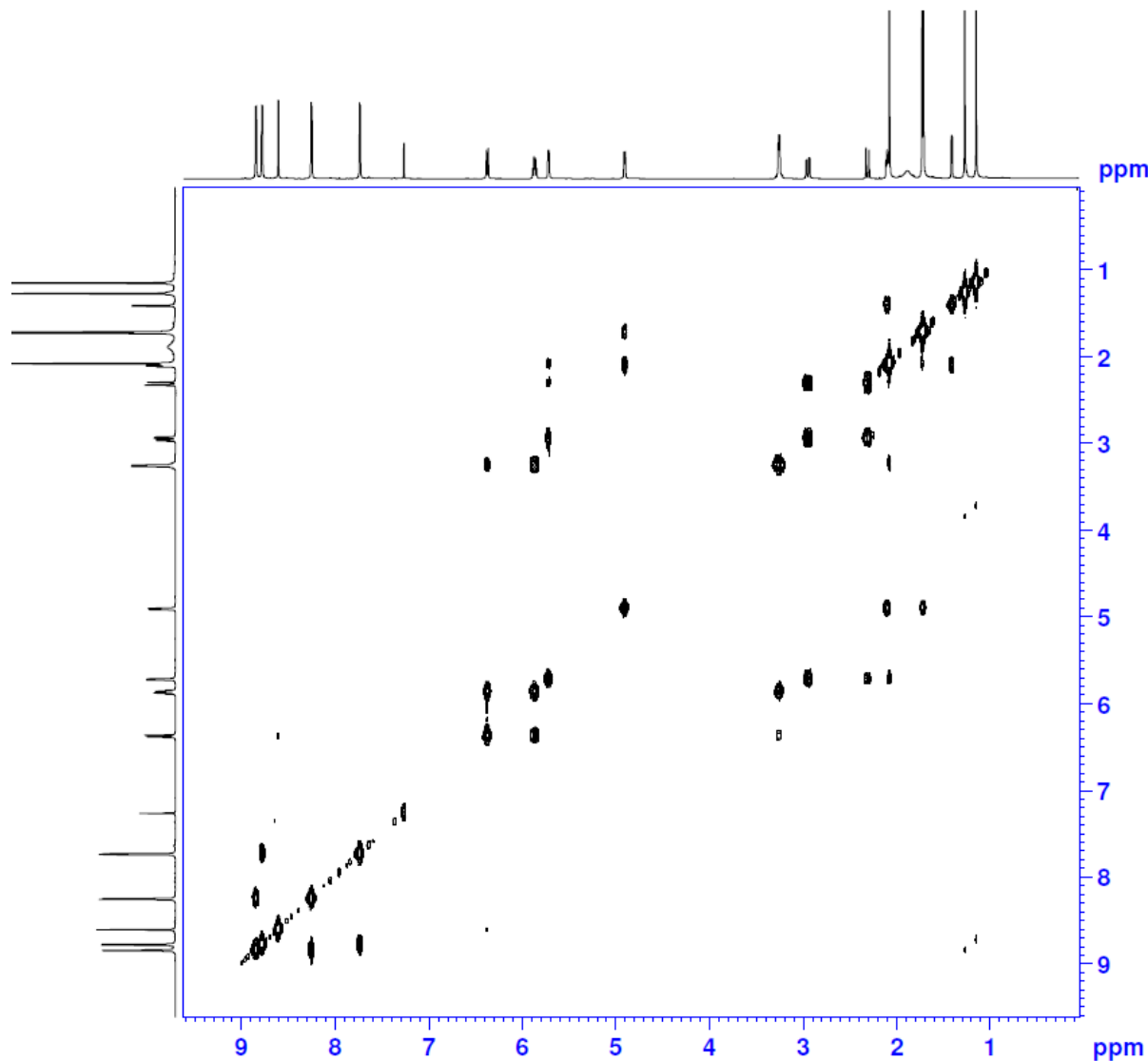
----- CHANNEL f1 -----
SF01 600.1329381 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 600.1329 MHz
FIDRES 47.637196 Hz
SW 10.160 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300248 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300238 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190603 Inv DA PI 4py
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190604
Time 3.20
INSTRUM spect
PROBHD 5 mm PARBO BB/
PULPROG hsqcztpp
TD 1024
SOLVENT CDCl3
DS 16
NS 16
SWH 5813.954 Hz
FIDRES 5.677689 Hz
AQ 0.0880640 sec
RG 2050
DW 86.000 usec
DE 6.50 usec
TE 298.3 K
CNS12 145.0000000
D0 0.00000300 sec
D1 1.47747195 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGFINS

===== CHANNEL f1 =====
SFO1 600.1329676 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PZ8 1000.00 usec
PIW1 17.00000000 W

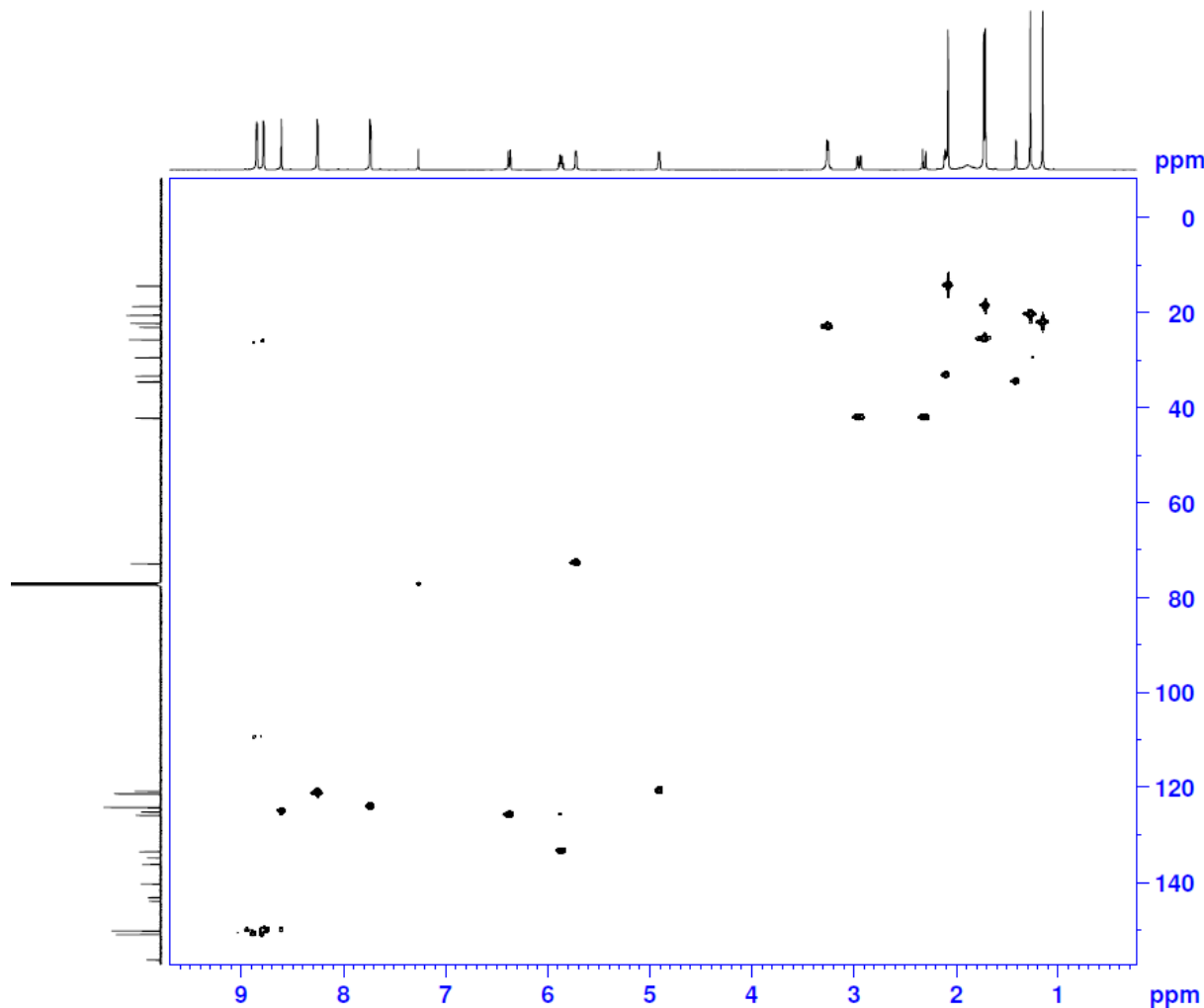
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PIW2 80.00000000 W
PIW12 3.20000005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
CPE1 80.00 %
CPE2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FhMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300256 MHz
WDW QSHINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
WC2 echo-antiecho
SF 150.9028304 MHz
WDW QSHINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190603 Inv DA PI 4py
EXPNO 25
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190604
Time 6.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 30
DS 16
SWH 5813.954 Hz
FIDRES 1.419422 Hz
AQ 0.3522560 sec
RG 2050
DW 86.000 usec
DE 6.50 usec
TE 298.3 K
CNS113 8.0000000
D0 0.0000000 sec
D1 1.40333402 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1329676 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

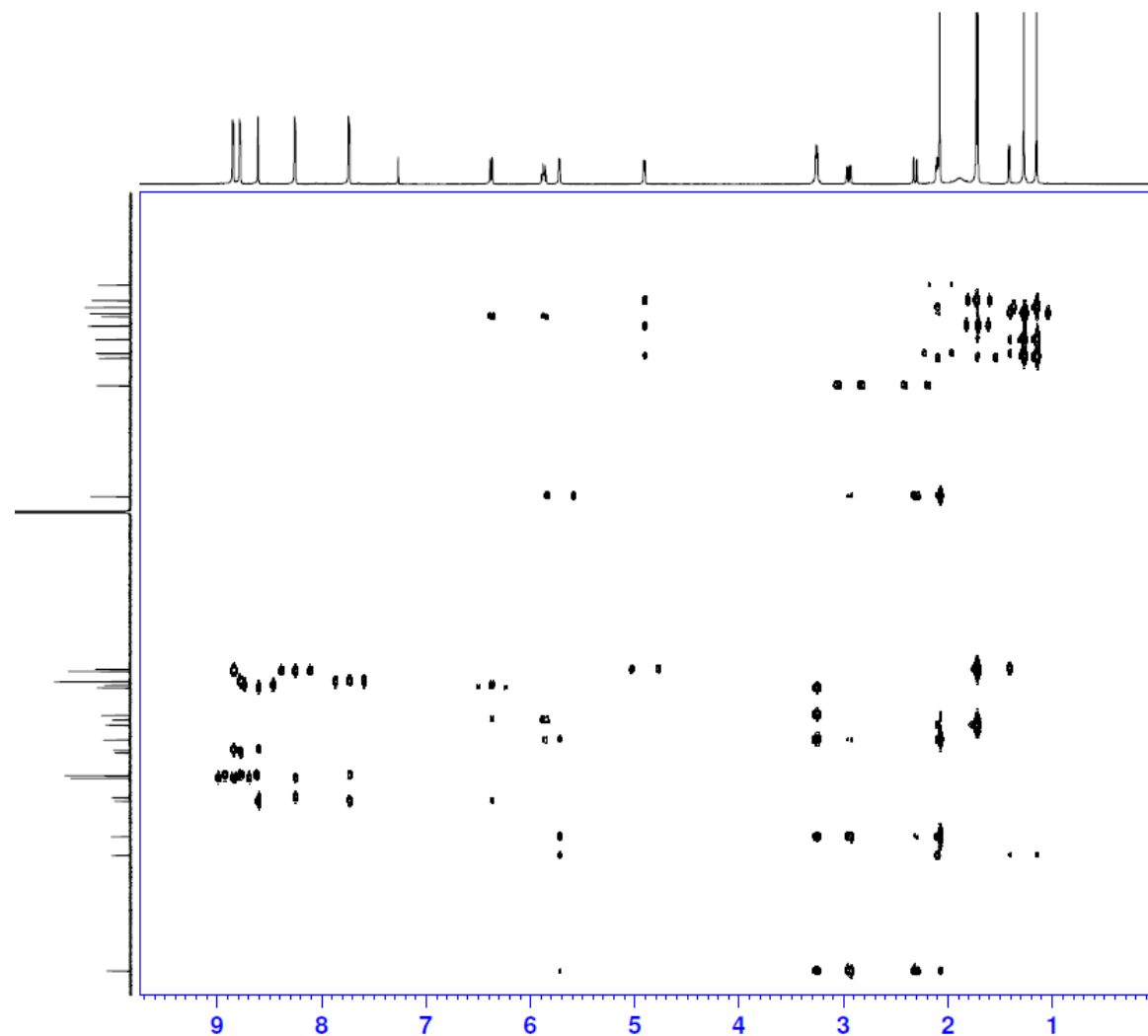
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 80.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FhMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300257 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028052 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

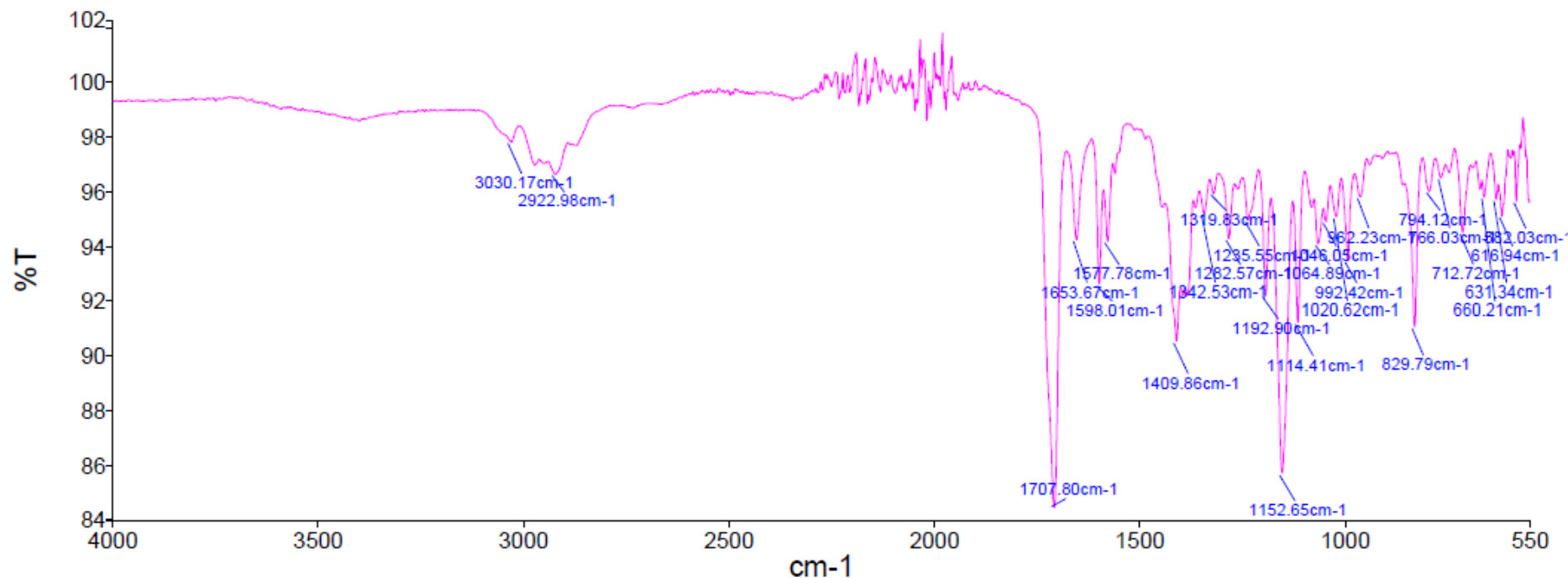


90a IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Tuesday, 18 June 2019 10:46 AM

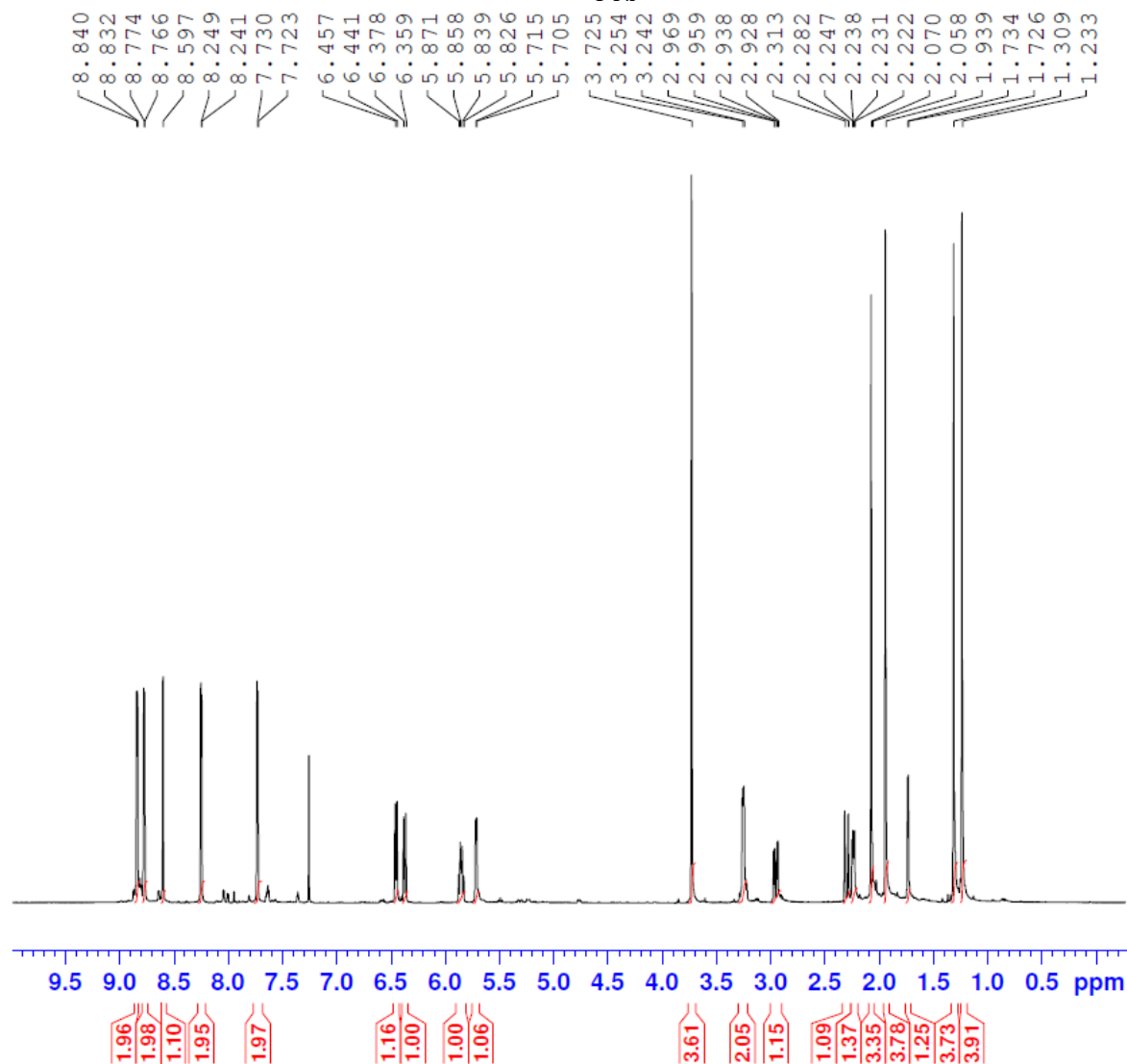
Analyst
Date

Analyst
Tuesday, 18 June 2019 10:46 AM



Sample Name	Description	Quality Checks
PI 4Py	Sample 010 By Analyst Date Tuesday, June 18 2019	The Quality Checks do not report any warnings for the sample.

90b NMR Characterisation

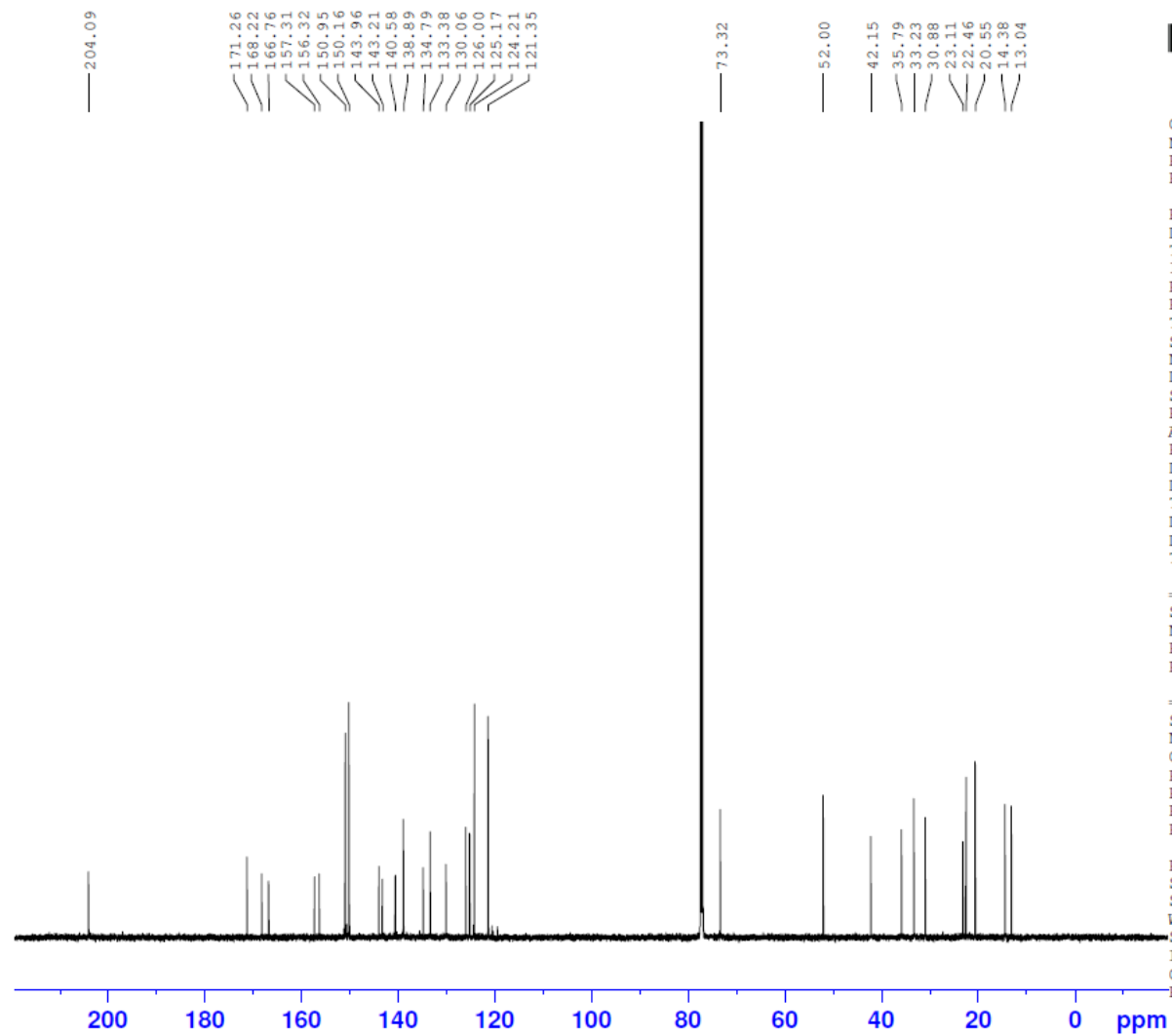


Current Data Parameters
 NAME 20190617 PII 4Py
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190617
 Time 20.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 203
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300310 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20190617 PII 4Py
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190618
 Time 0.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 3096
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9027914 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20190617 P11 4Py
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190617
Time 20.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygmfphpp
ID 2048
SOLVENT CDC13
NS 10
DS 4
SWH 6172.839 Hz
FIDRES 3.014082 Hz
AQ 0.1658880 sec
RG 2050
DW 81.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00006381 sec
D1 1.97255695 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00016200 sec

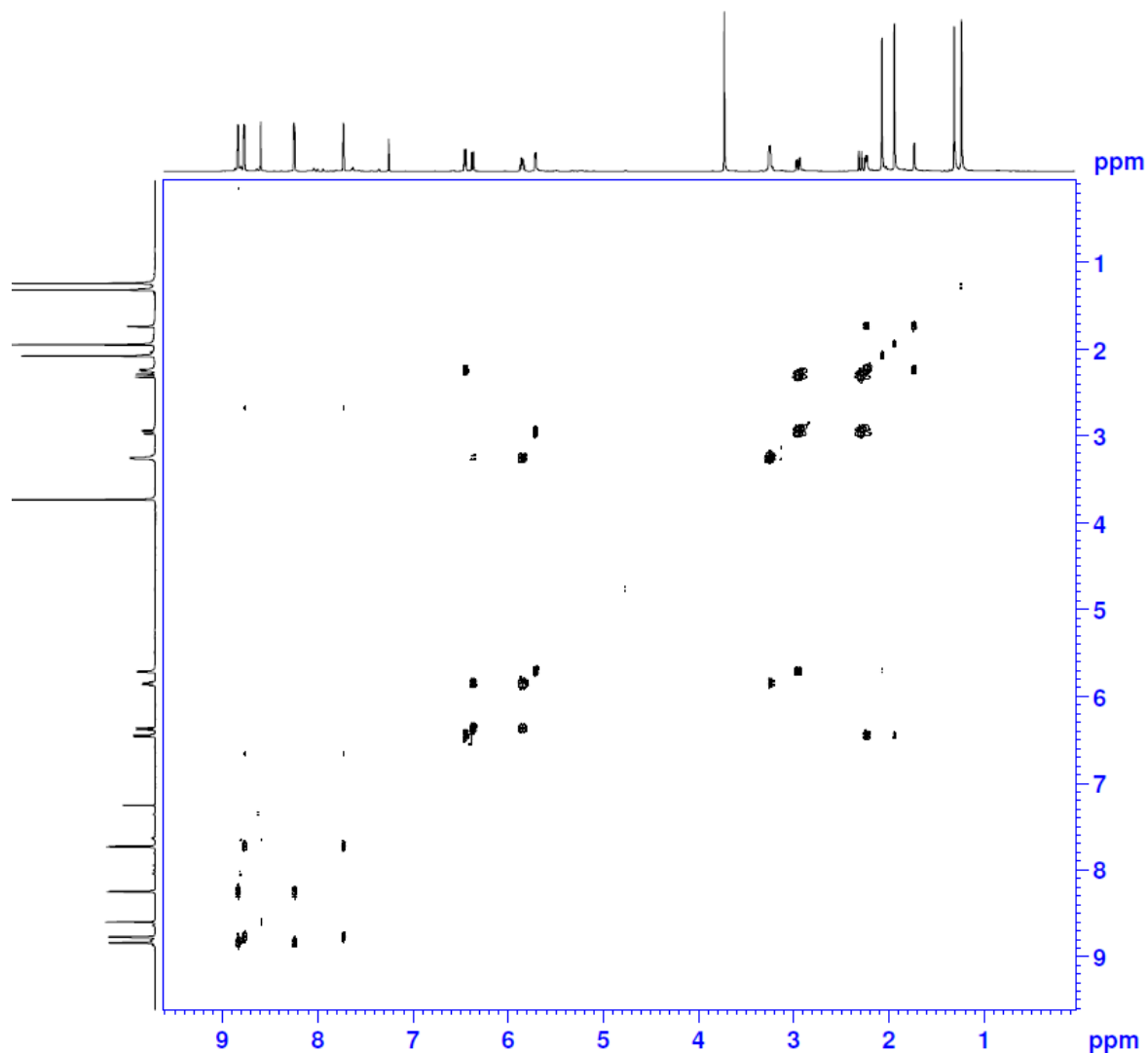
----- CHANNEL f1 -----
SFO1 600.1328399 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 256
SFO1 600.1328 MHz
FIDRES 24.112654 Hz
SW 10.286 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.1300298 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300301 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190617 P11 4py
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190618
Time 0.19
INSTRUM spect
PROBHD 5 mm FANNO BB/
PULPROG hsqcztgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 6024.096 Hz
FIDRES 5.882906 Hz
AQ 0.0849920 sec
RG 2050
RW 83.000 usec
DE 6.50 usec
TE 298.3 K
CNS12 145.0000000
D0 0.00000300 sec
D1 1.48054397 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGPINS

===== CHANNEL F1 =====
SFO1 600.1328696 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

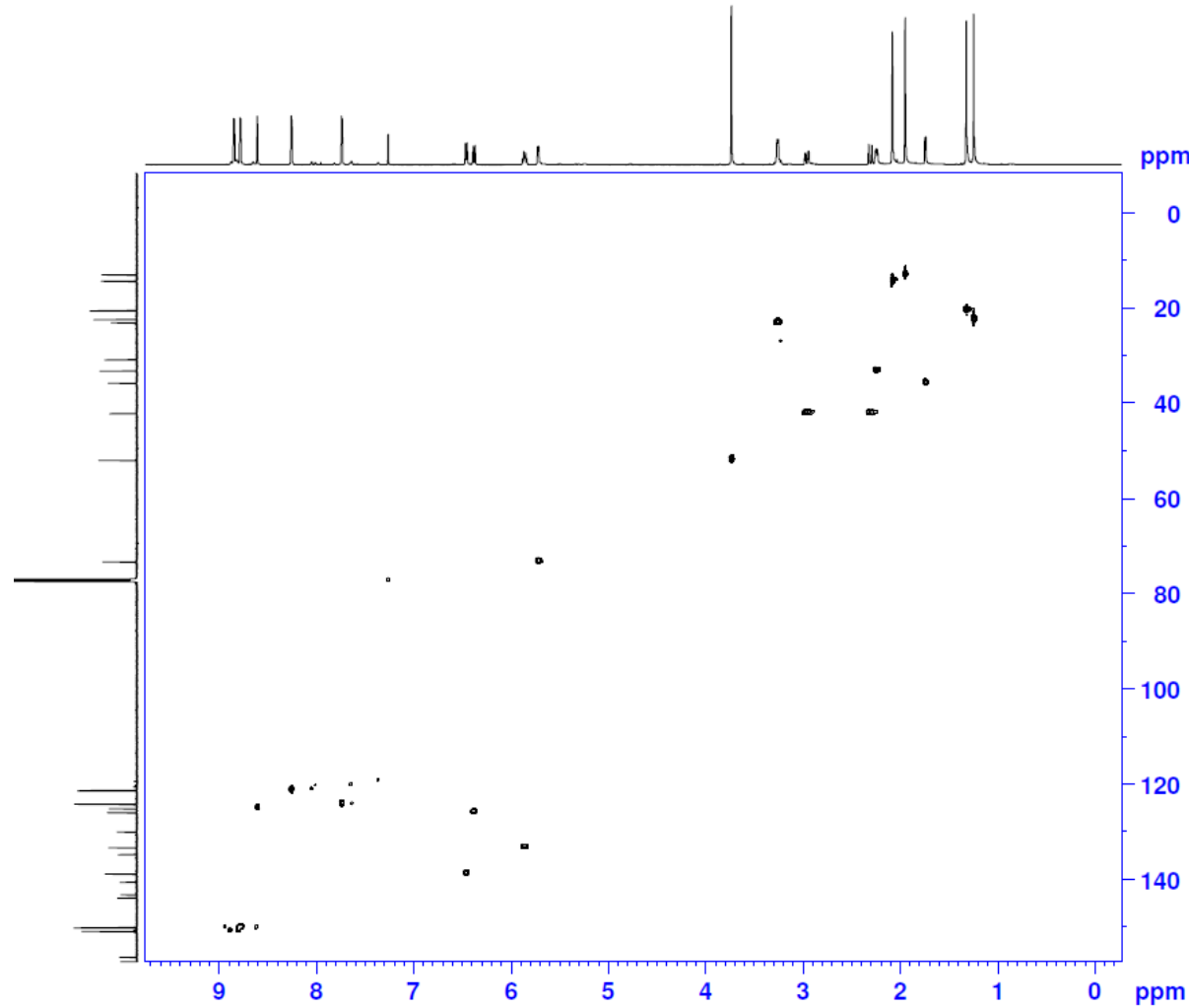
===== CHANNEL F2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 80.00000000 W
PLW12 3.20000005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300249 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028254 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190617 P11 4py
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190618
Time 5.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 6024.096 Hz
FIDRES 1.470727 Hz
AQ 0.3399680 sec
RG 2050
DW 83.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.41562200 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1328696 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

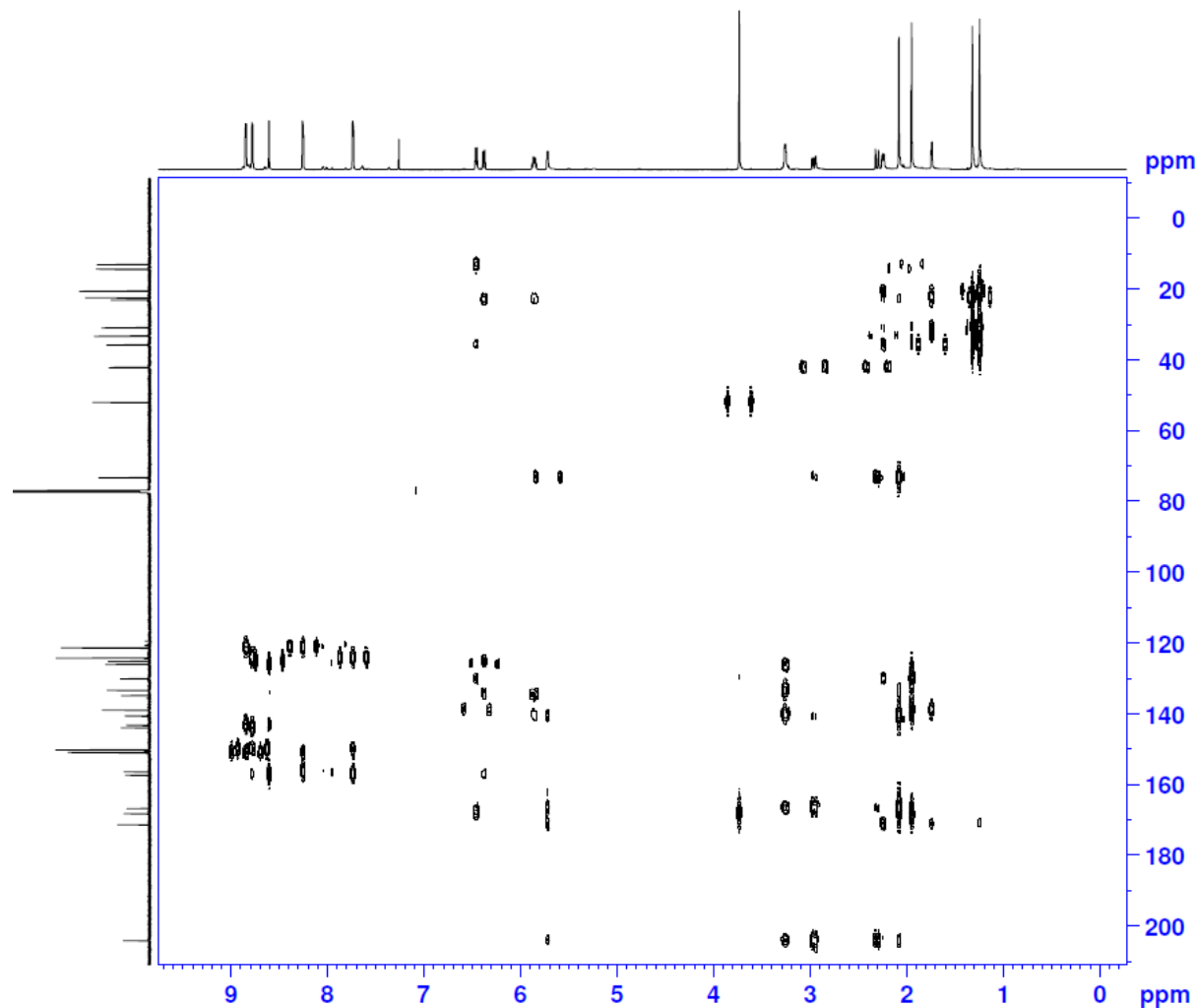
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 80.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSq10.100
GPNAM[2] SMSq10.100
GPNAM[3] SMSq10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 81
SFO1 150.9179 MHz
FIDRES 414.284515 Hz
SW 222.353 ppm
Fnm00E QF

F2 - Processing parameters
SI 1024
SF 600.1300256 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
WC2 QF
SF 150.9028202 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

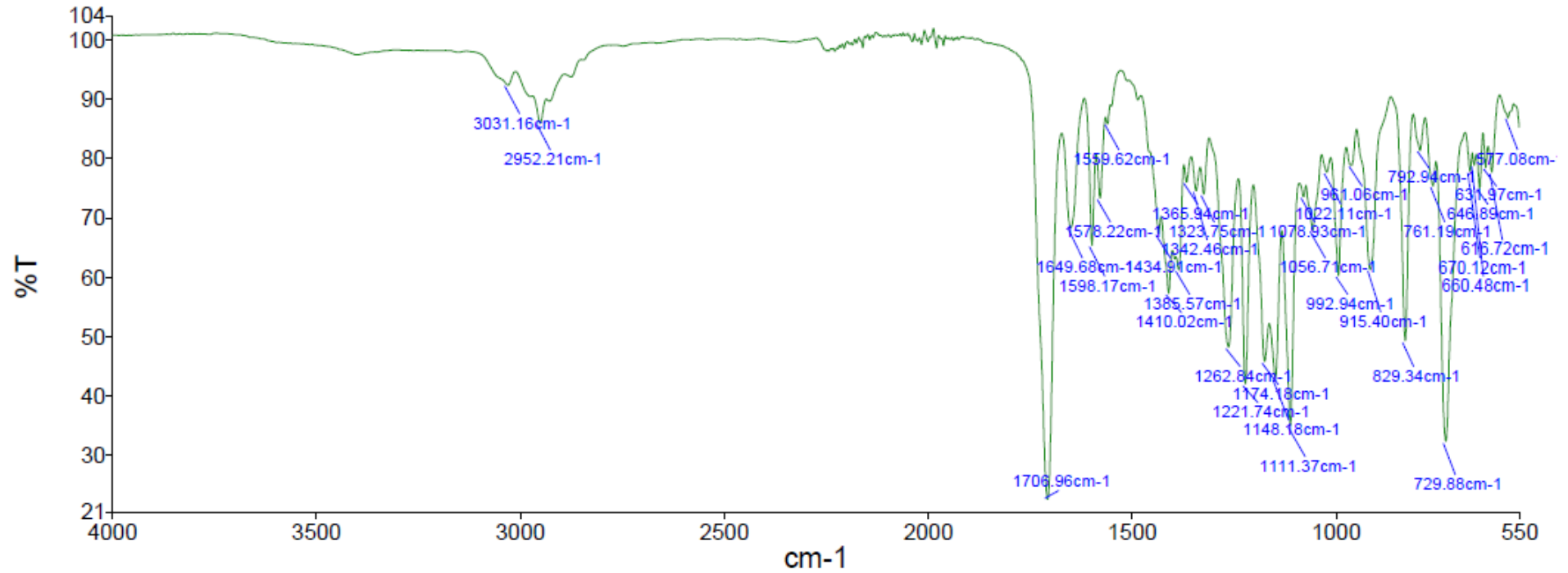


90b IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Tuesday, 18 June 2019 10:46 AM

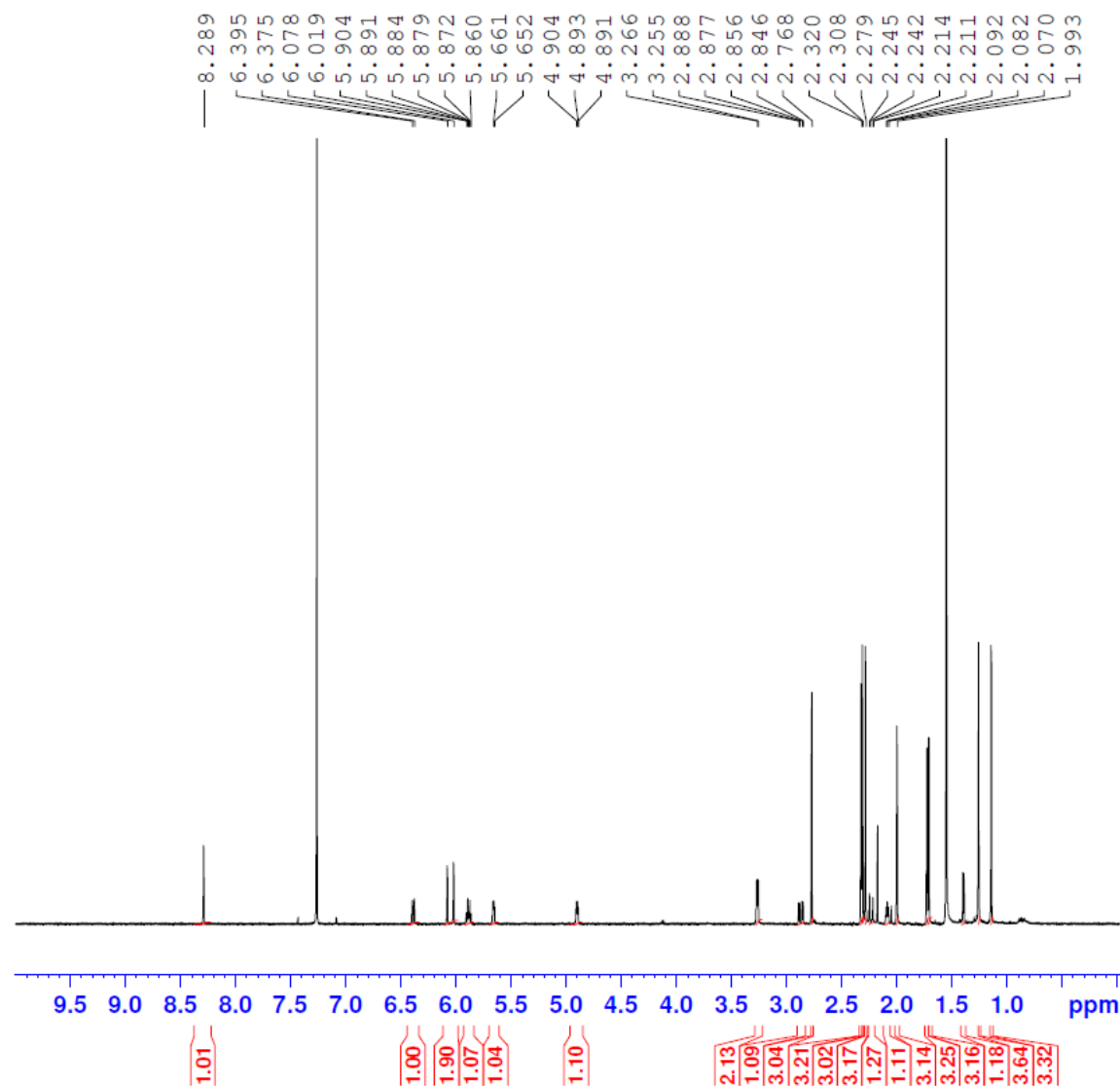
Analyst
Date

Analyst
Tuesday, 18 June 2019 10:46 AM



Sample Name	Description	Quality Checks
PII 4Py	Sample 011 By Analyst Date Tuesday, June 18 2019	The Quality Checks do not report any warnings for the sample.

91a NMR Characterisation



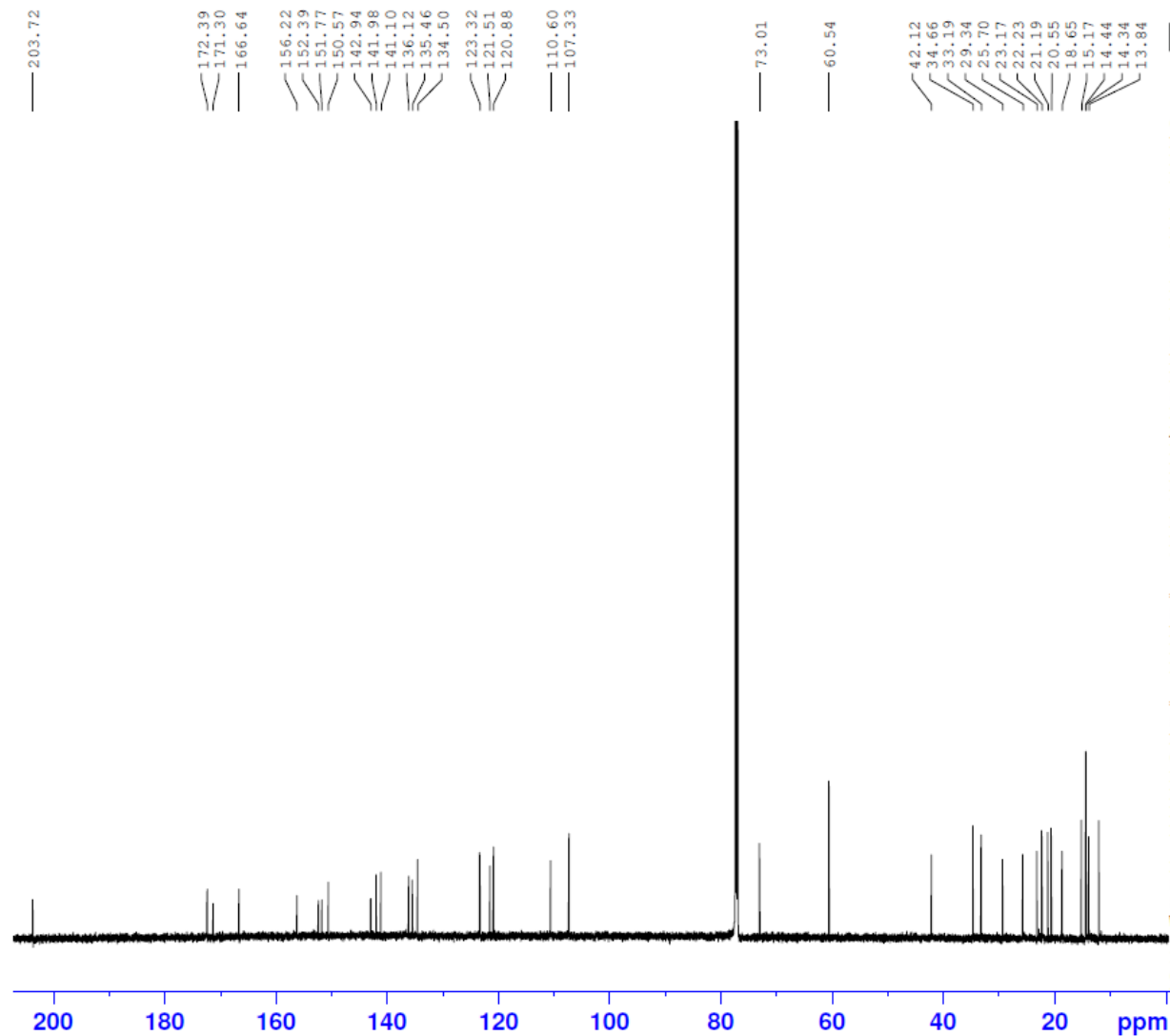
```

Current Data Parameters
NAME      20190924 Pyr PI
EXPNO     12
PROCNO    1

F2 - Acquisition Parameters
Date_     20190924
Time      22.47
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        12019.230 Hz
FIDRES     0.183399 Hz
AQ         2.7262976 sec
RG         406
DW         41.600 usec
DE         6.50 usec
TE         297.9 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      600.1337060 MHz
NUC1       1H
P1         13.50 usec
PLW1      17.00000000 W

F2 - Processing parameters
SI         65536
SF         600.1300257 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```



Current Data Parameters
 NAME 20190920 PI Pyr
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190921
 Time 11.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4096
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9027898 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20190924 Pyr PI
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190924
Time 22.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 5154.639 Hz
FIDRES 2.516914 Hz
AQ 0.1986560 sec
RG 228
DW 97.000 usec
DE 6.50 usec
TE 298.1 K
D0 0.00000300 sec
D1 1.92913902 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00019400 sec

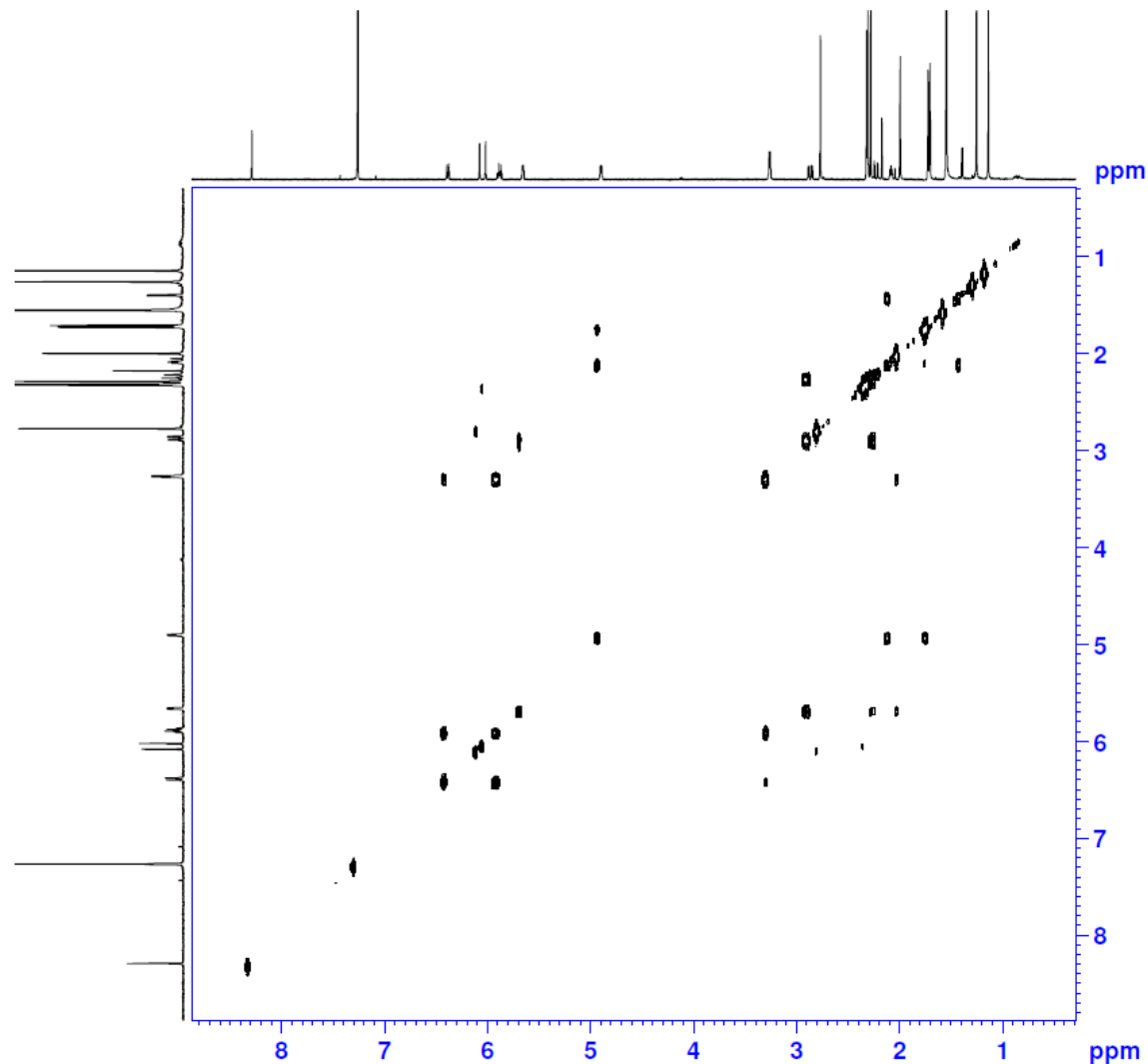
----- CHANNEL f1 -----
SFO1 600.1327497 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1327 MHz
FIDRES 40.270618 Hz
SW 8.589 ppm
FIRMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190920 F1 Pyr
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190921
Time 11.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT cdc13
NS 50
DS 16
SWH 5154.639 Hz
FIDRES 5.033027 Hz
AQ 0.0993280 sec
RG 2050
DW 97.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46620798 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1327389 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
P1W1 17.00000000 W

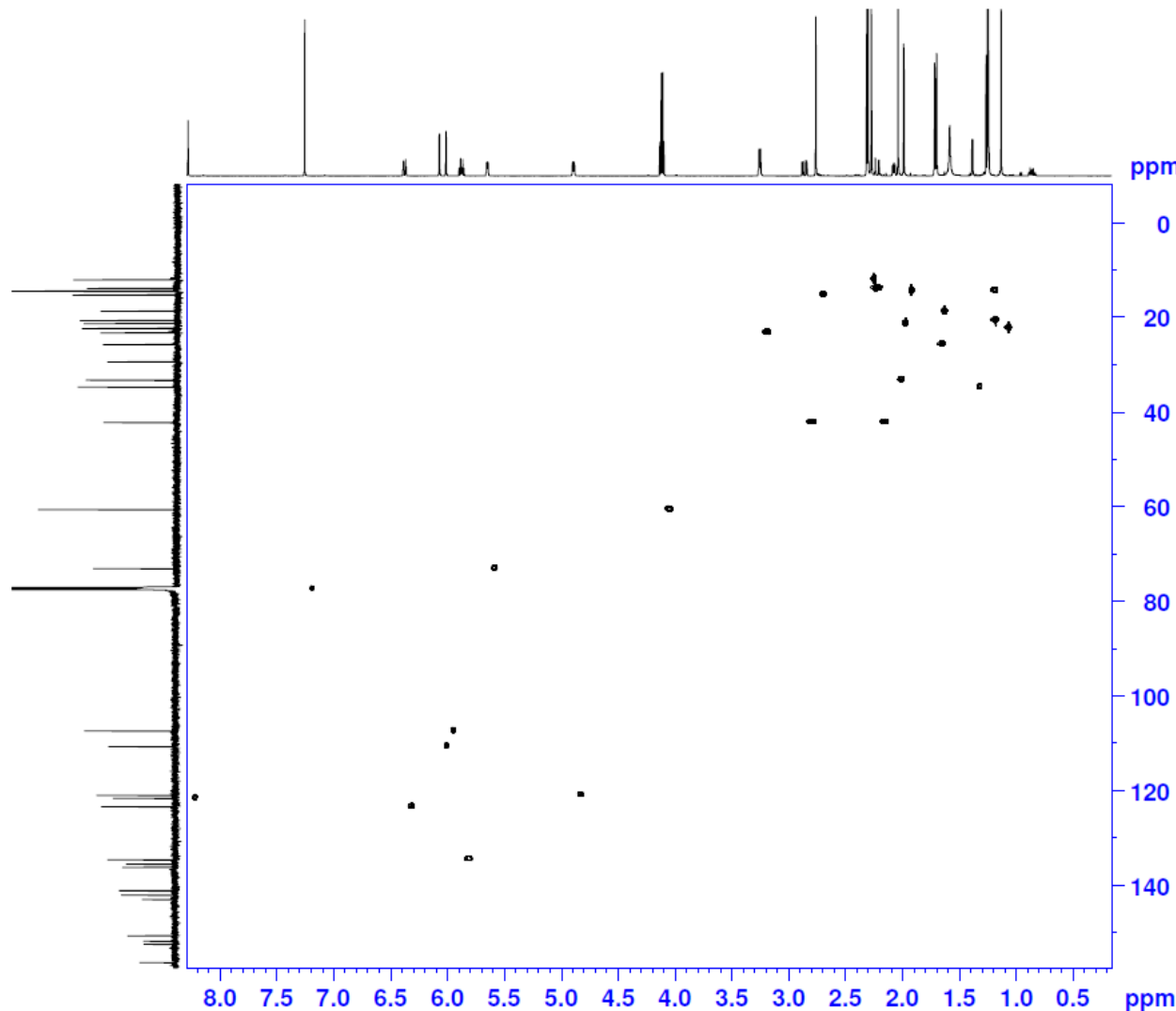
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPOPRG[2] garrp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
P1W2 80.00000000 W
P1W12 3.20000005 W

===== GRADIENT CHANNEL =====
CPN1[1] SMSQ10.100
CPN1[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
PnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300667 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190920 PI Pyr
EXPNO 25
PROCNO 1

ppm

0

20

40

60

80

100

120

140

ppm

```
F2 - Acquisition Parameters
Date_      20190921
Time       17.27
INSTRUM    spect
PROBHD     5 mm PABBO BB/
PULPROG    hmbcgpndqf
TD          4096
SOLVENT    CDCl3
NS          70
DS          16
SWH         5154.639 Hz
FIDRES      1.258457 Hz
AQ          0.3973120 sec
RG          2050
DW          97.000 usec
DE          6.50 usec
TE          298.2 K
CST13       8.0000000
D0          0.00000300 sec
D1          1.35827804 sec
D6          0.06250000 sec
D16         0.00020000 sec
IN0         0.00001490 sec

===== CHANNEL f1 =====
SFO1       600.1327389 MHz
NUC1        1H
P1         13.50 usec
P2          27.00 usec
PLW1       17.00000000 W

===== CHANNEL f2 =====
SFO2       150.9178748 MHz
NUC2        13C
P3          12.00 usec
PLW2       80.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1]   SMSQ10.100
GPNAM[2]   SMSQ10.100
GPNAM[3]   SMSQ10.100
GP21       50.00 %
GP22       30.00 %
GP23       40.10 %
P16        1000.00 usec

F1 - Acquisition parameters
TD          50
SFO1       150.9179 MHz
FIDRES      671.140930 Hz
SW          222.353 ppm
F2MODE      QF

F2 - Processing parameters
SI          1024
SF          600.1300667 MHz
WDW         SINE
SSB         0
LB          0 Hz
GB          0
PC          1.40

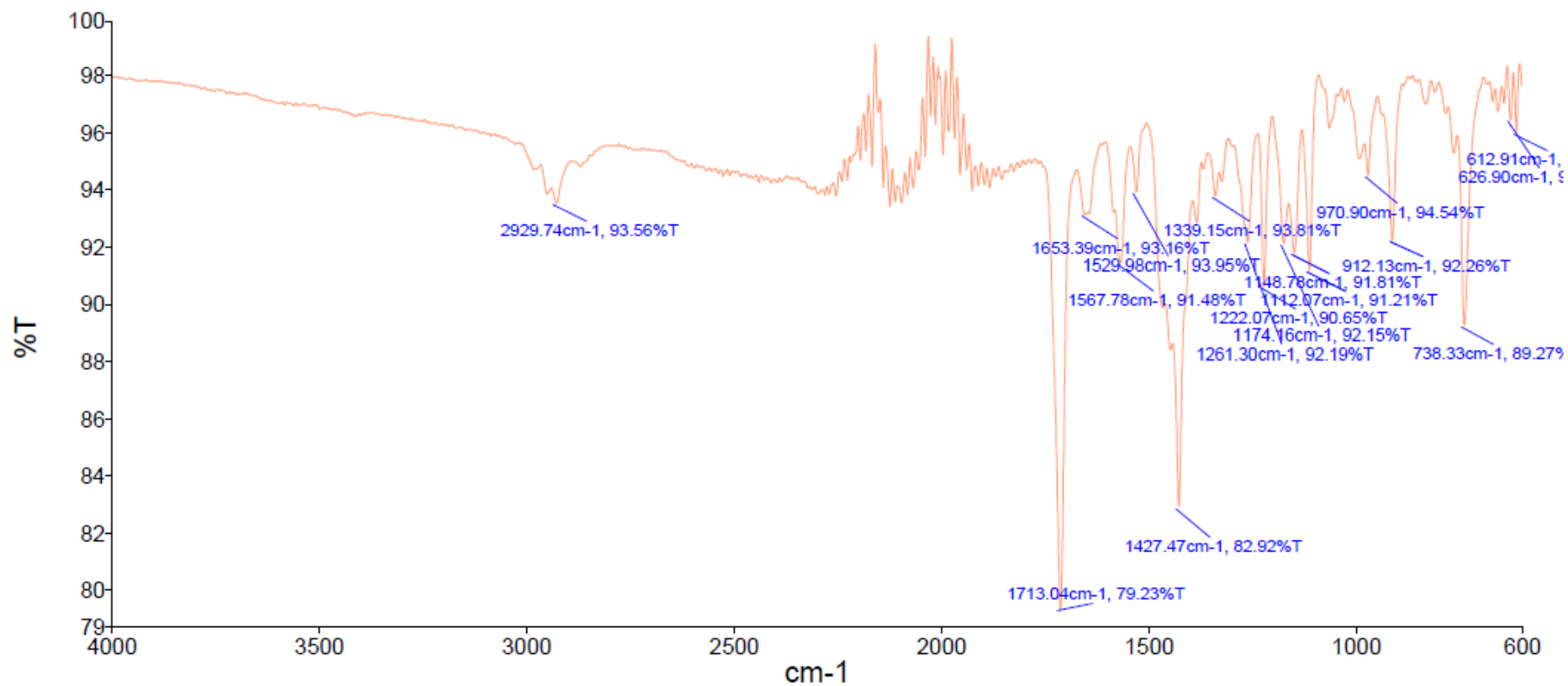
F1 - Processing parameters
SI          1024
MC2         QF
SF          150.9028085 MHz
WDW         SINE
SSB         0
LB          0 Hz
GB          0
```

91a IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 3 January 2020 11:38 AM

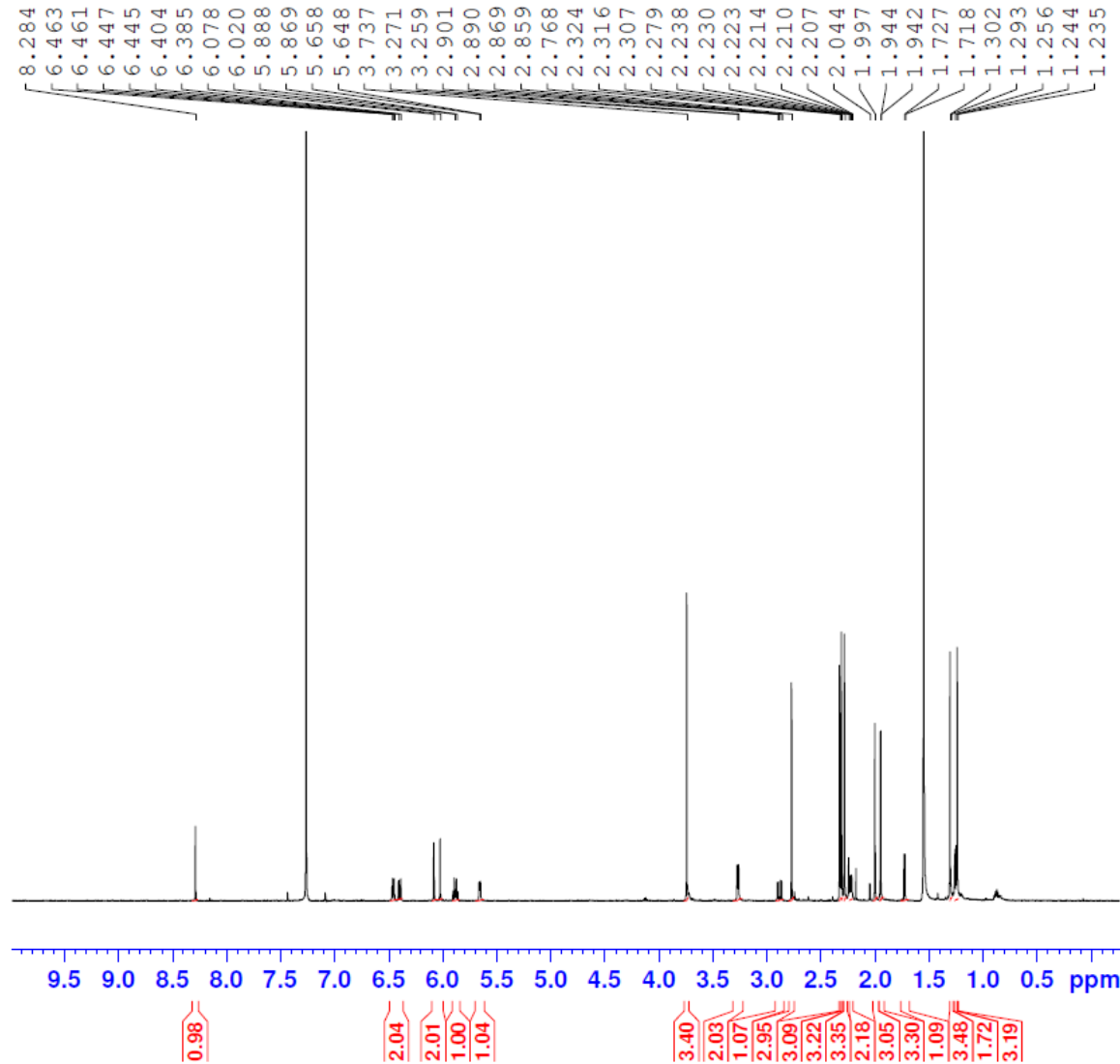
Analyst
Date

Analyst
Friday, 3 January 2020 11:38 AM



— Pyr I_001_1 Sample

91b NMR Characterisation

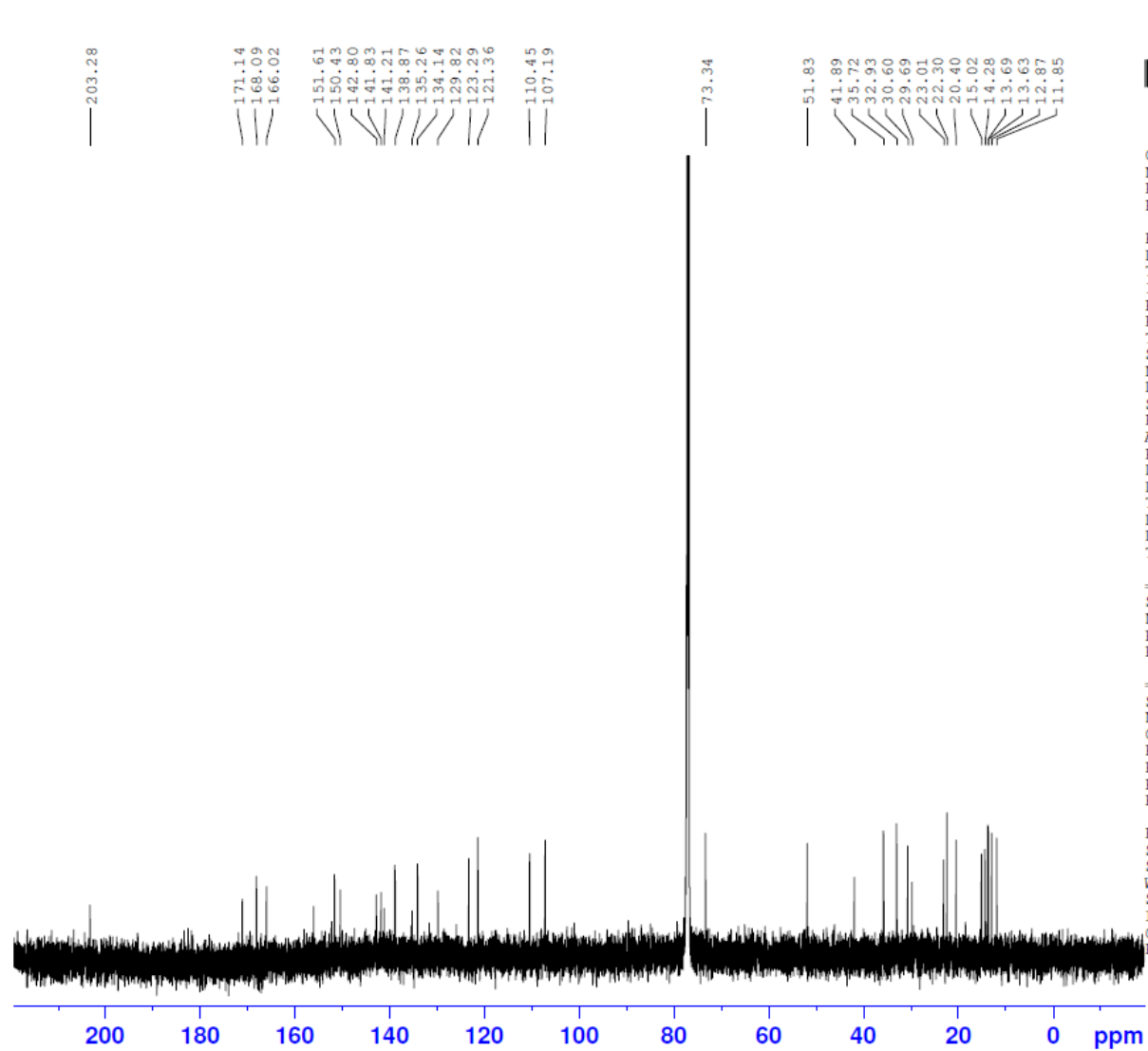


Current Data Parameters
 NAME 20191011 InvDA Pyr II
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191011
 Time 19.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 362
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300261 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20191011 InvDA Pyr II
 EXPNO 17
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191013
 Time 13.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 4096
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028135 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20191011 InvDA Pyr II
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191011
Time 19.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
ID 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 5208.333 Hz
FIDRES 2.543132 Hz
AQ 0.1966080 sec
RG 203
DW 96.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.0000300 sec
D1 1.93118703 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00019200 sec

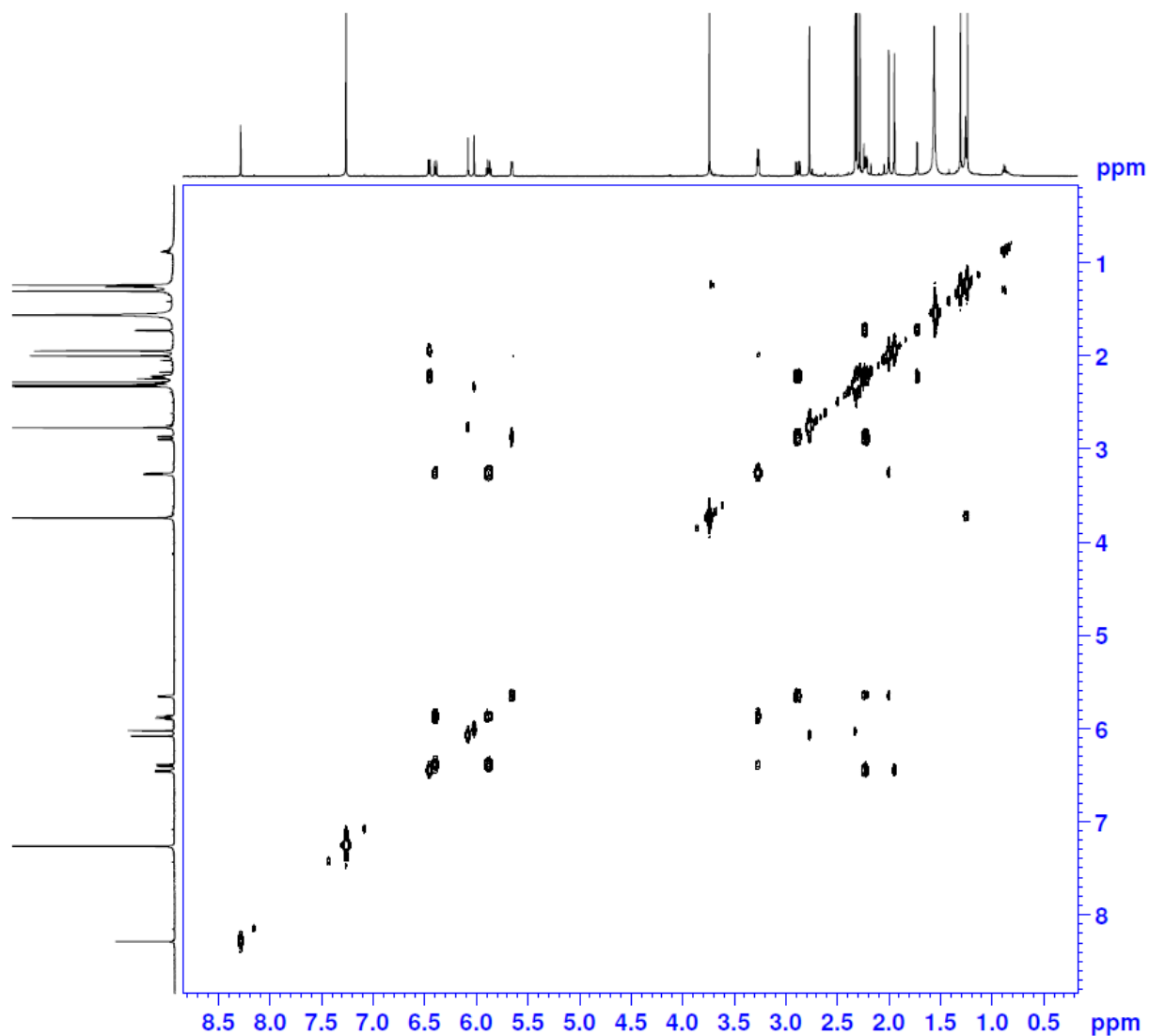
----- CHANNEL f1 -----
SFO1 600.1327298 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 128
SFO1 600.1327 MHz
FIDRES 40.690105 Hz
SW 8.679 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300262 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300266 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20191011 InvDA Pyr II
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters

Date_ 20191012
Time 0.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 5102.041 Hz
FIDRES 4.982462 Hz
AQ 0.1003520 sec
RG 2050
DW 98.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.0000300 sec
D1 1.46518397 sec
D4 0.0012414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
RGOPIN

===== CHANNEL f1 =====
SFO1 600.1327539 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P2B 1000.00 usec
P1W1 17.00000000 W

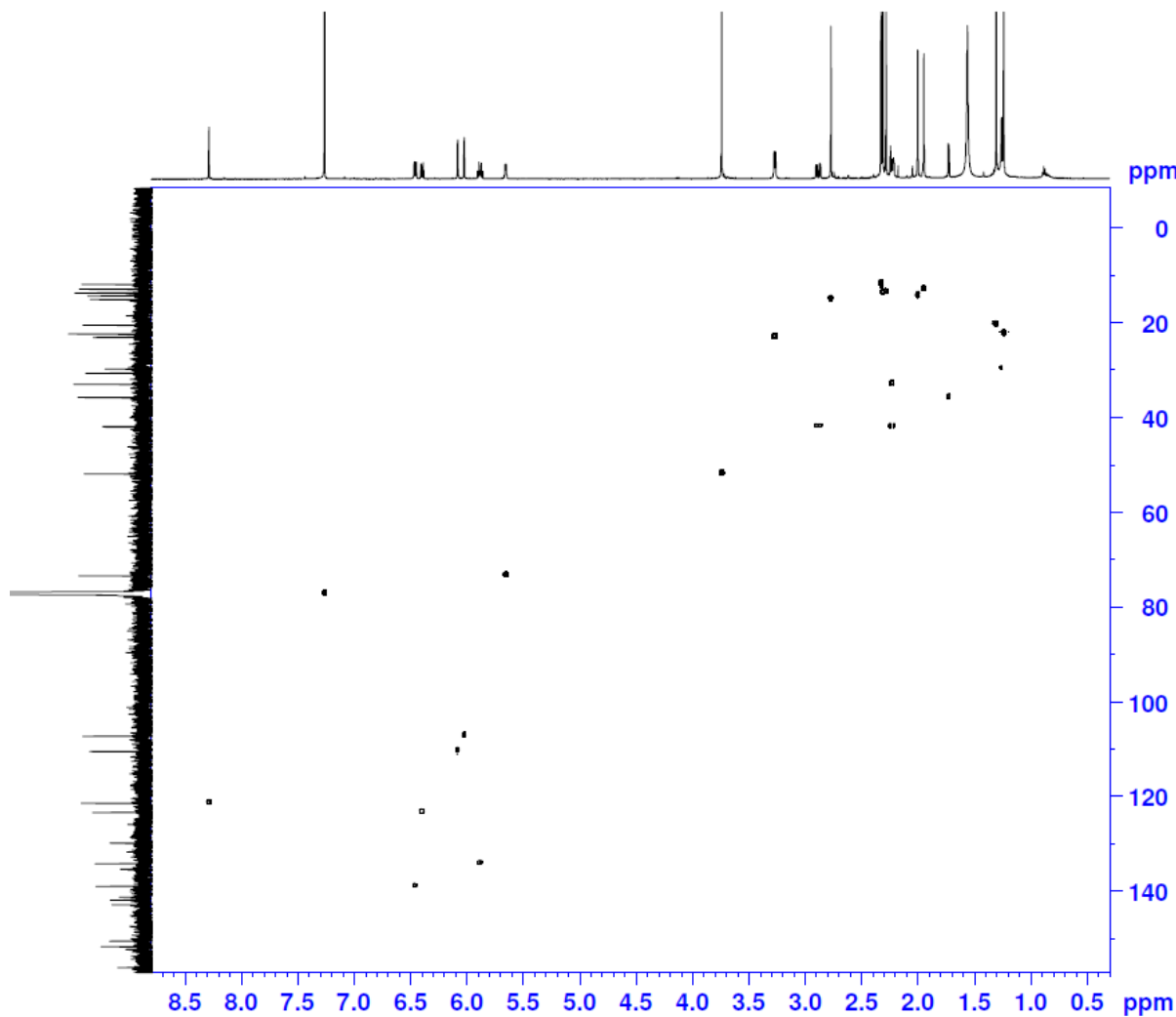
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
P1W2 80.00000000 W
P1W12 3.20000005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GP1 80.00 %
GP2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
F1MODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300252 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028485 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20191011 InvDA Pyr II
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Data_ 20191012
Time 5.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcpgndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 5102.041 Hz
FIDRES 1.245615 Hz
AQ 0.4014080 sec
RG 2050
DW 98.000 usec
DE 6.50 usec
TE 298.2 K
CNS113 8.0000000
D0 0.00000300 sec
D1 1.35418200 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1327539 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

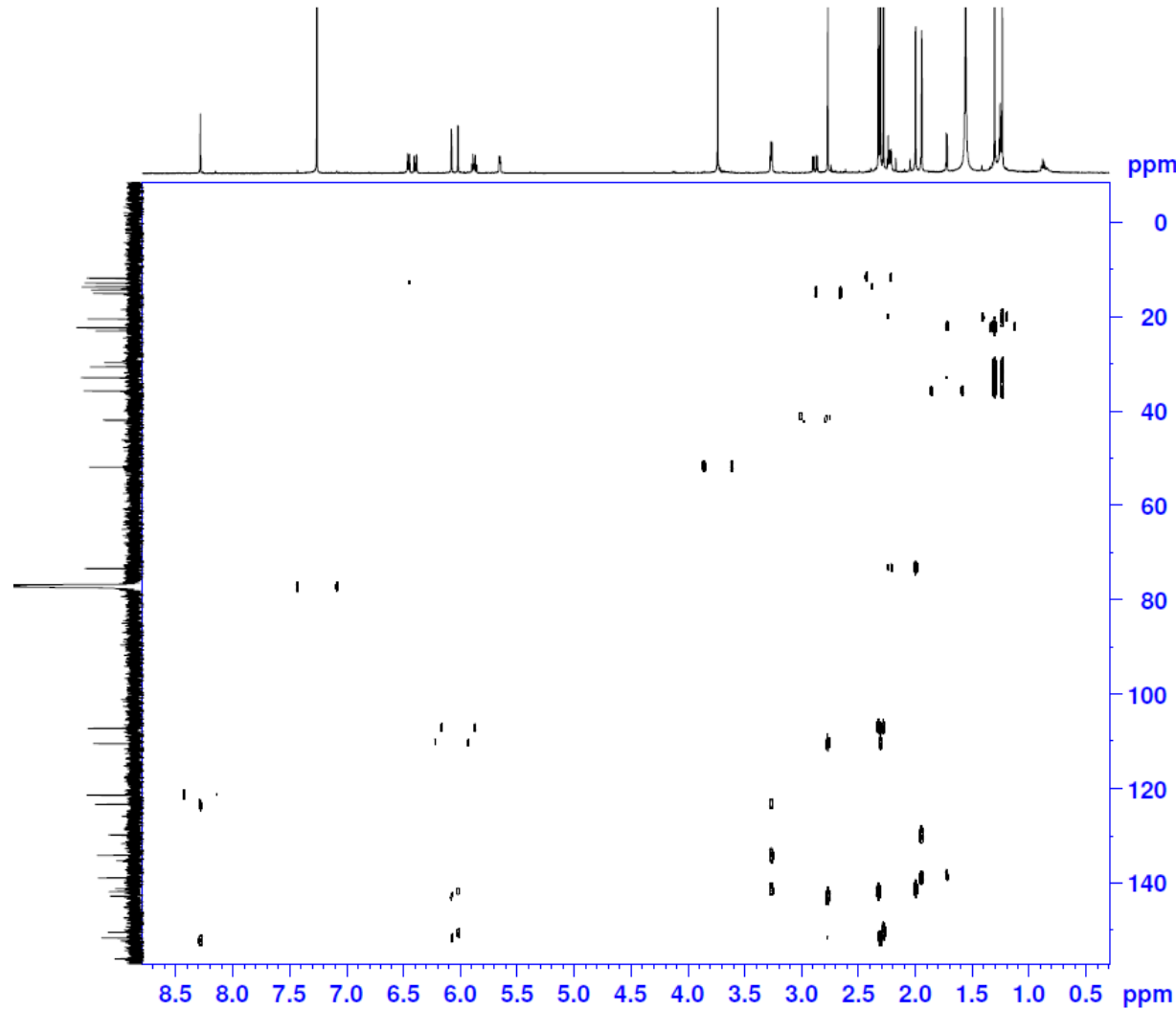
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 80.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GP21 50.00 %
GP22 30.00 %
GP23 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300265 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028263 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

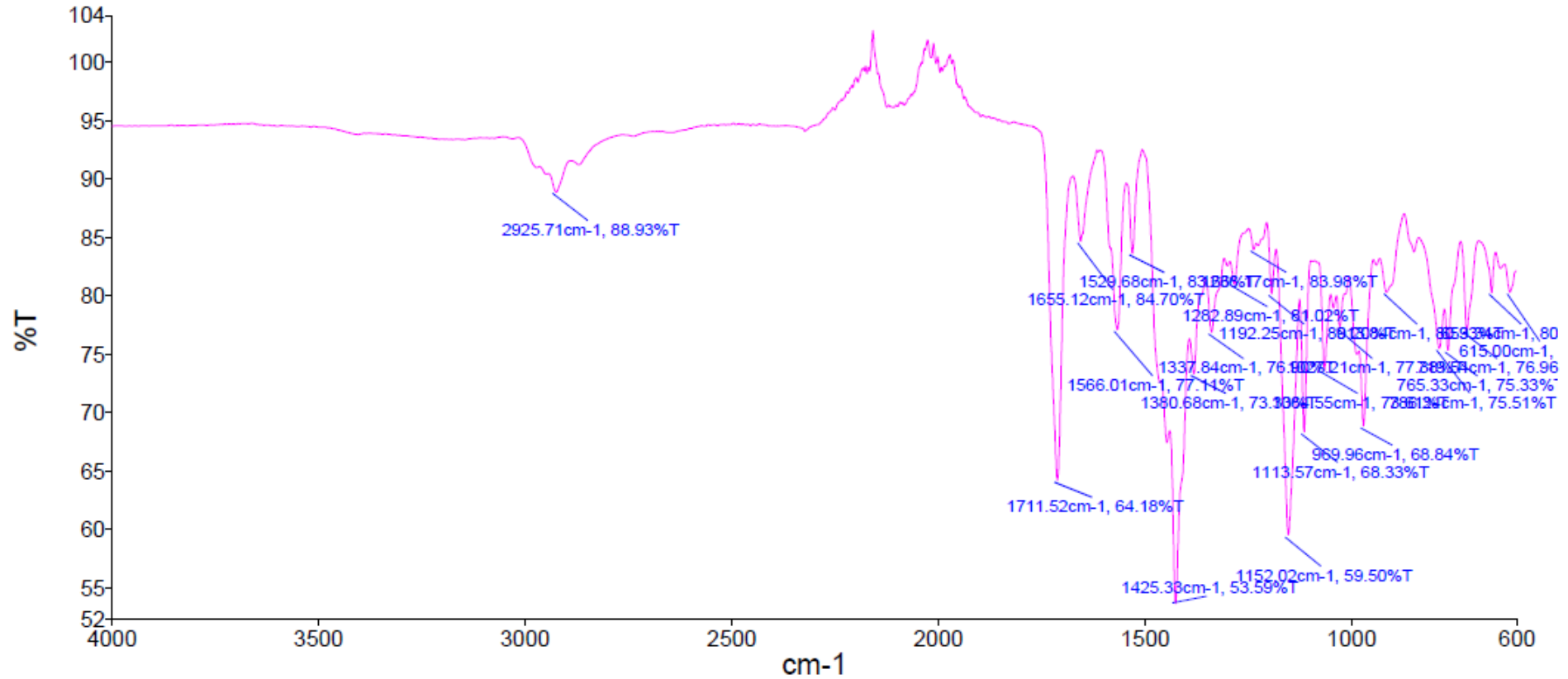


91b IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 3 January 2020 11:50 AM

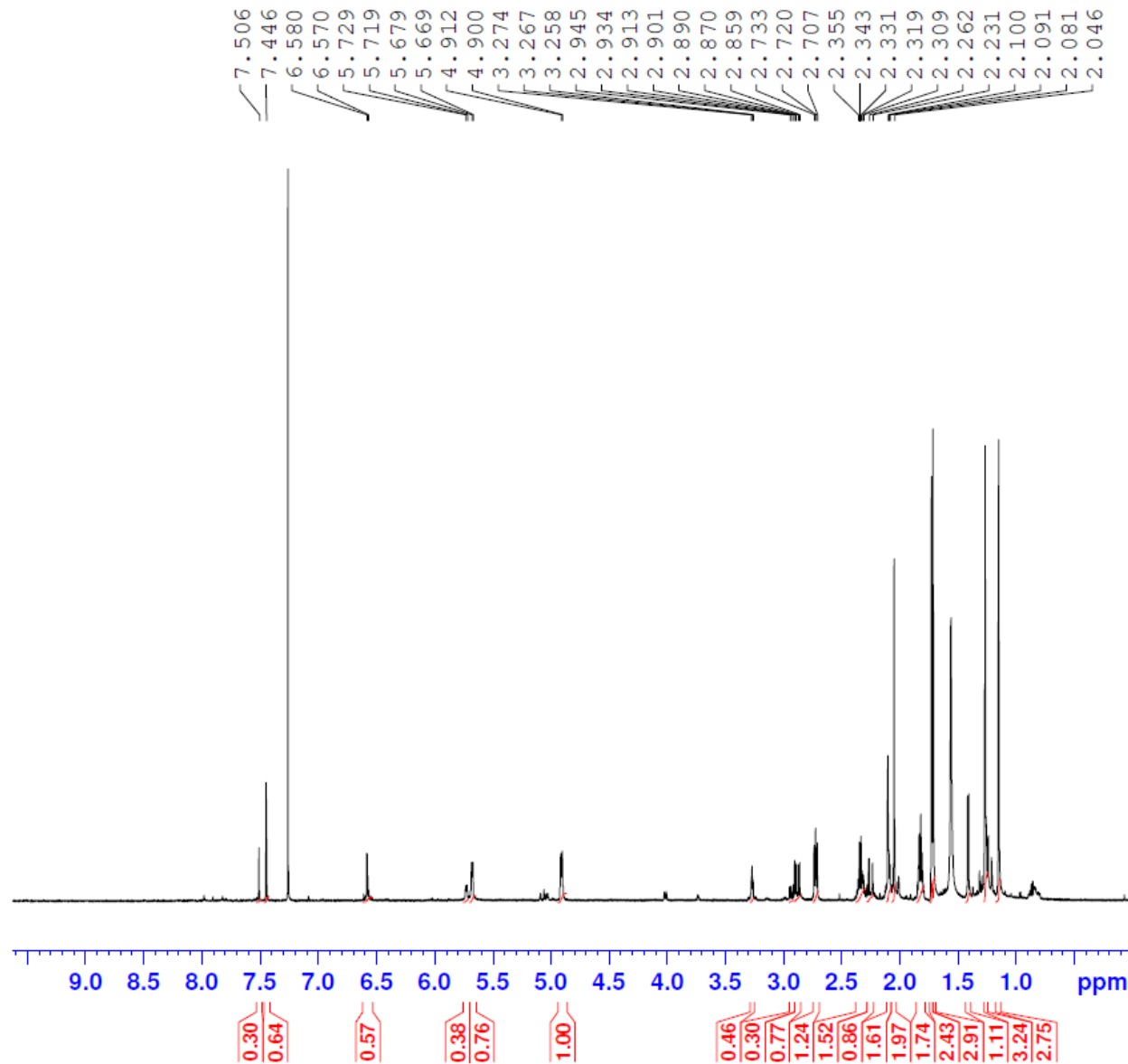
Analyst
Date

Analyst
Friday, 3 January 2020 11:50 AM



Pyr II_001 Sample

92a + 93a NMR Characterisation

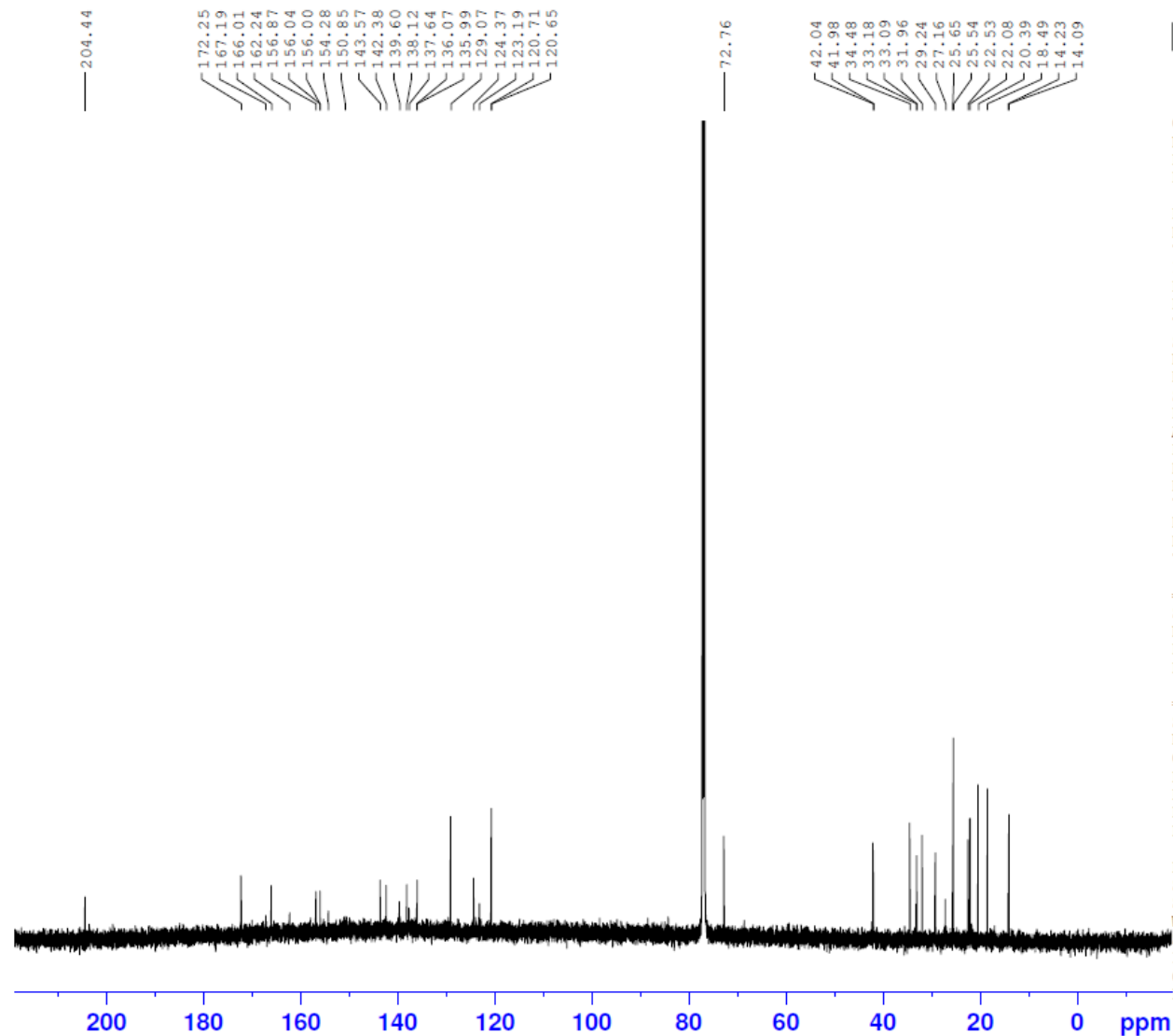


Current Data Parameters
 NAME 20200911 C12 I
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200911
 Time 17.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 322
 DW 41.600 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300272 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20200911 C12 I
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200912
 Time 0.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 7168
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028153 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200911 c12_1
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200911
Time 17.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 4672.897 Hz
FIDRES 2.281688 Hz
AQ 0.2191360 sec
RG 2050
DW 107.000 usec
DE 6.50 usec
TE 298.1 K
D0 0.00008981 sec
D1 1.91930902 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021400 sec

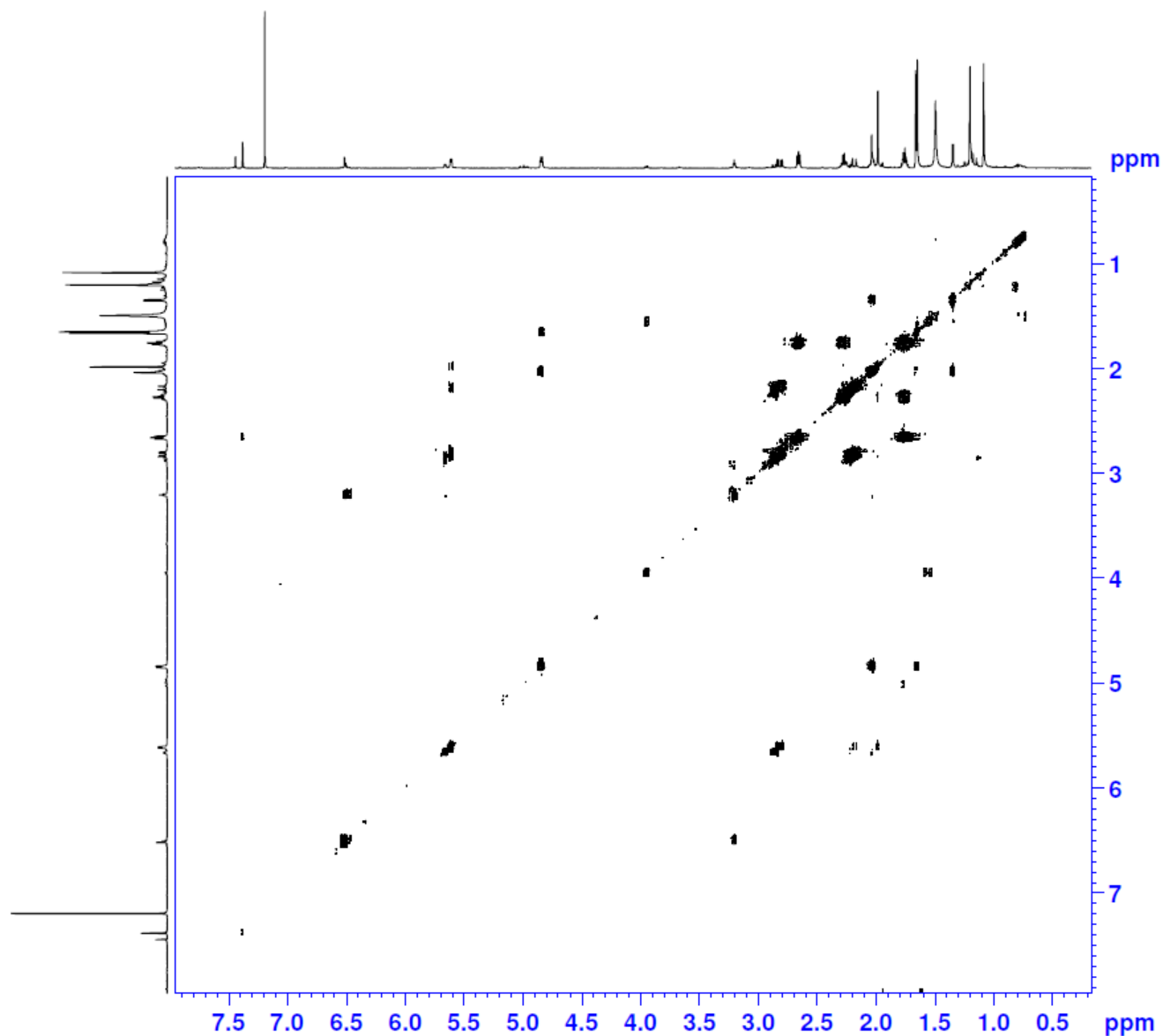
----- CHANNEL f1 -----
SFO1 600.1325037 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1325 MHz
FIDRES 18.253504 Hz
SW 7.786 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300668 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300668 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200911 c12 1
EXFNO 14
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200912
Time 0.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 4672.897 Hz
FIDRES 4.563376 Hz
AQ 0.1095680 sec
RG 2050
RW 107.000 usec
DE 6.50 usec
TE 298.3 K
CNST2 145.0000000
D0 0.0000300 sec
D1 1.45596802 sec
D4 0.0012414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1325037 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P2B 1000.00 usec
PLW1 17.00000000 W

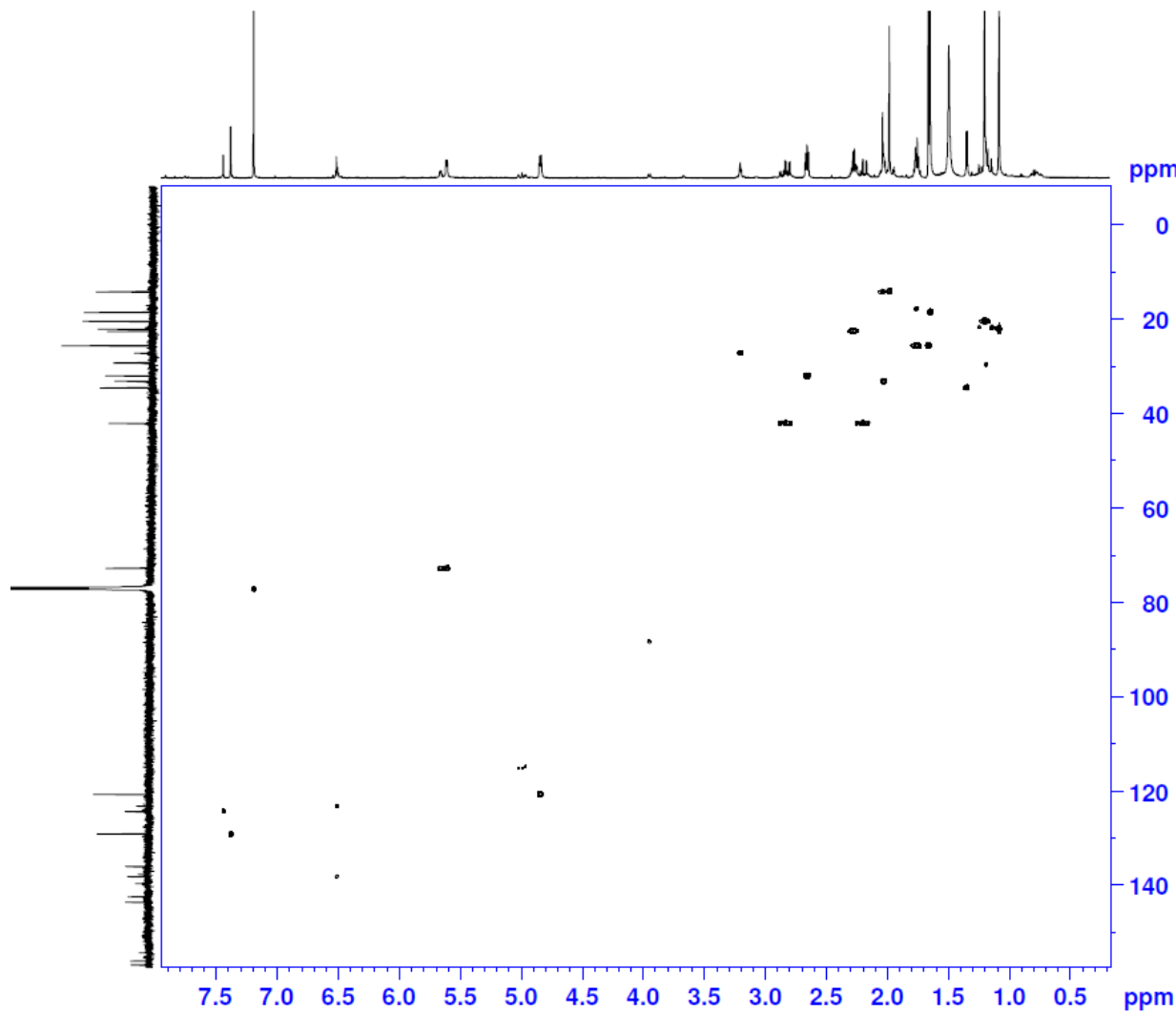
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
PL6 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
F1MODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300668 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200911 C12 i
EXENO 15
PROCNO 1

F2 - Acquisition Parameters
Data_ 20200912
Time 6.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 4672.897 Hz
FIDRES 1.140844 Hz
AQ 0.4382720 sec
RG 2050
DW 107.000 usec
DE 6.50 usec
TE 298.2 K
CNS113 8.0000000
D0 0.00000300 sec
D1 1.31731796 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1325037 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

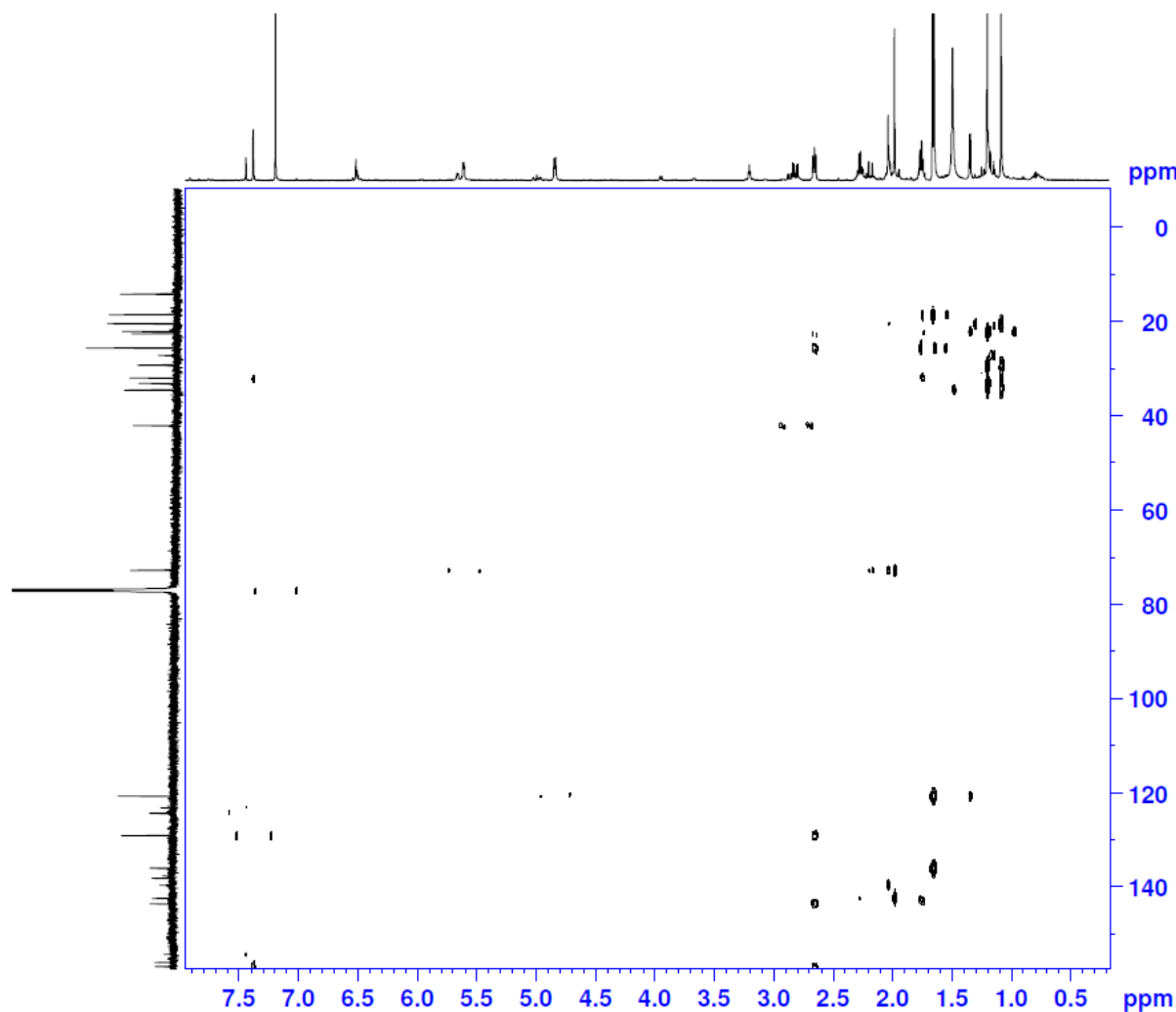
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPMAM[1] SMSQ10.100
GPMAM[2] SMSQ10.100
GPMAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

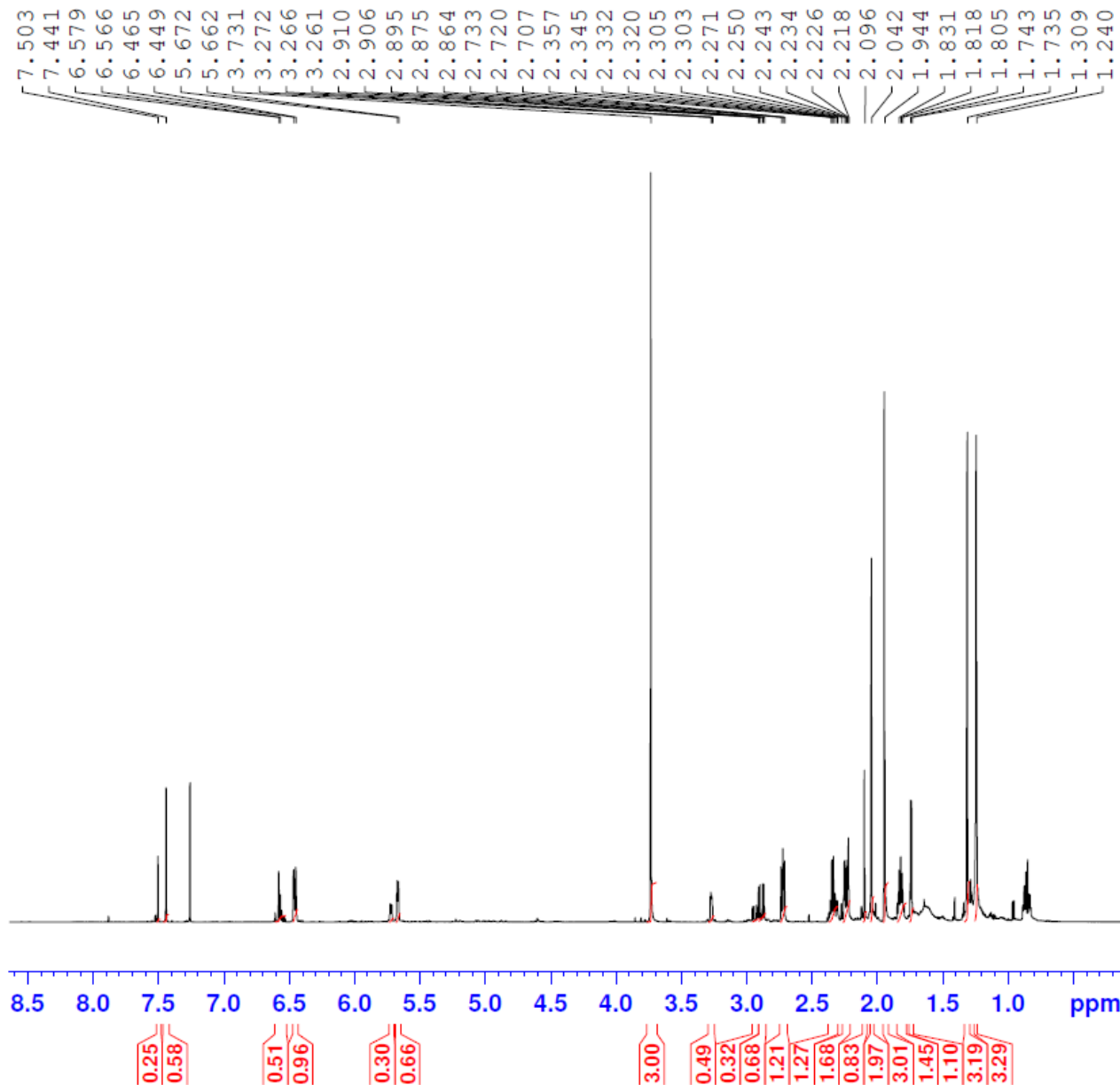
F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FhMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300668 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



92b + 93b NMR Characterisation

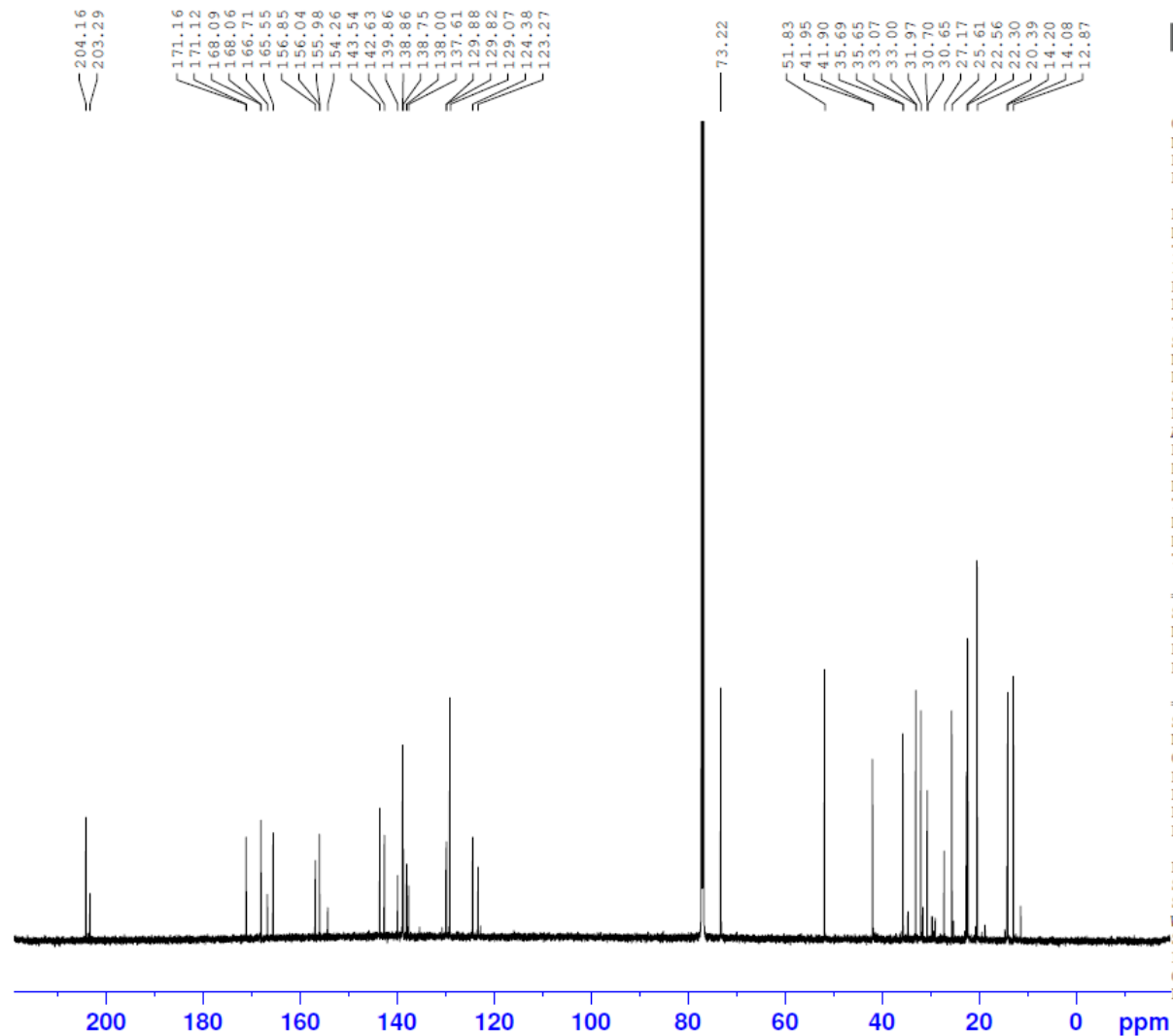


Current Data Parameters
 NAME 20200911 C12 II
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200912
 Time 10.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 181
 DW 41.600 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300274 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20200911 C12 II
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200912
Time 17.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7168
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028157 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20200911 CL2 II
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200912
Time 10.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 5263.158 Hz
FIDRES 2.569901 Hz
AQ 0.1945600 sec
RG 2050
DW 95.000 usec
DE 6.50 usec
TE 298.1 K
D0 0.00007781 sec
D1 1.94388497 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00019000 sec

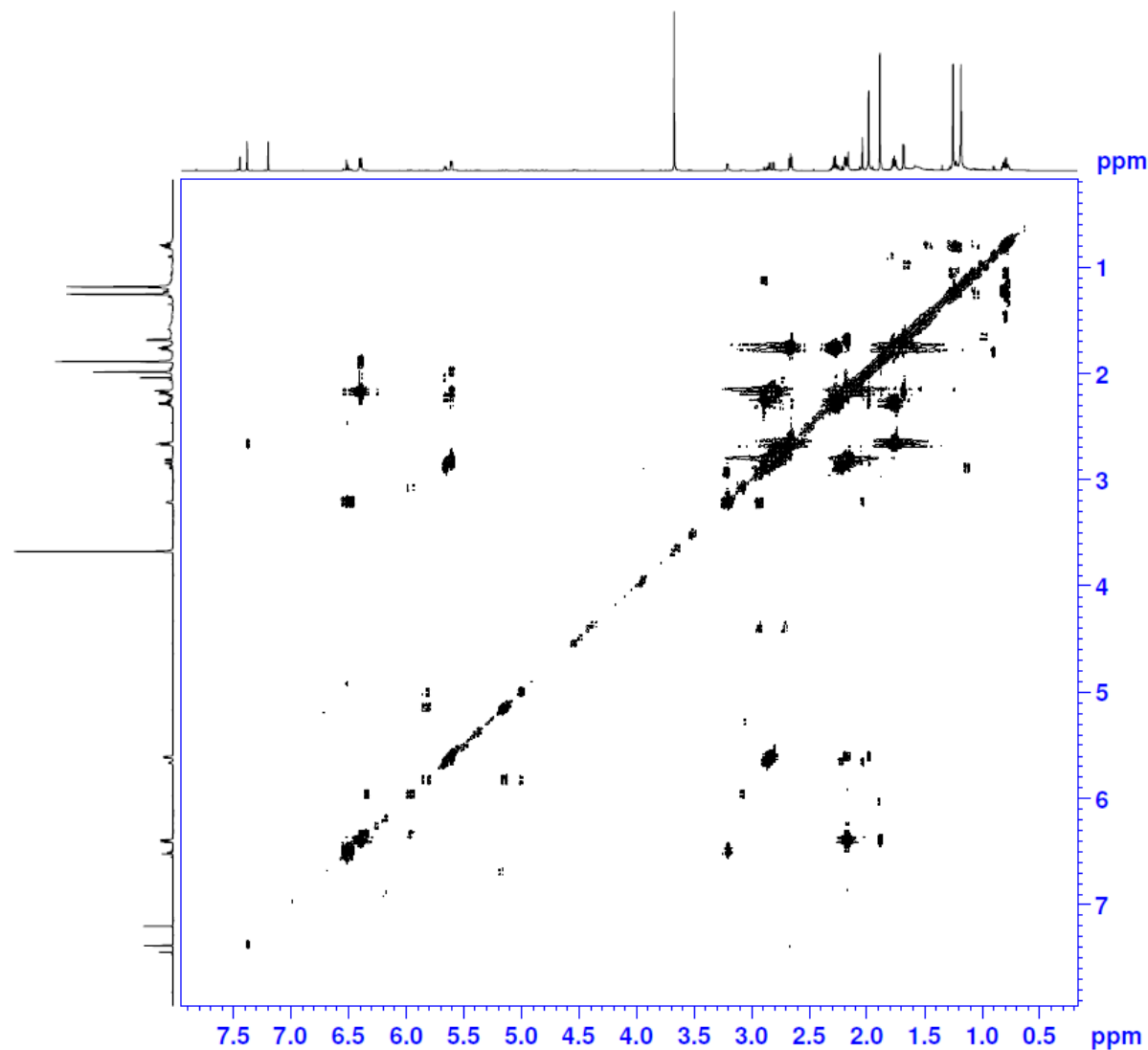
----- CHANNEL f1 -----
SFO1 600.1322896 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 256
SFO1 600.1323 MHz
FIDRES 20.559210 Hz
SW 8.770 ppm
FnmODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300638 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300638 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200911_C12_I1
EXFNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200912
Time 17.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 5263.158 Hz
FIDRES 5.139802 Hz
AQ 0.0972800 sec
RG 2050
RW 95.000 usec
DE 6.50 usec
TE 298.2 K
CNS12 145.0000000
D0 0.00000300 sec
D1 1.46825600 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGPNS

===== CHANNEL f1 =====
SFO1 600.1322896 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

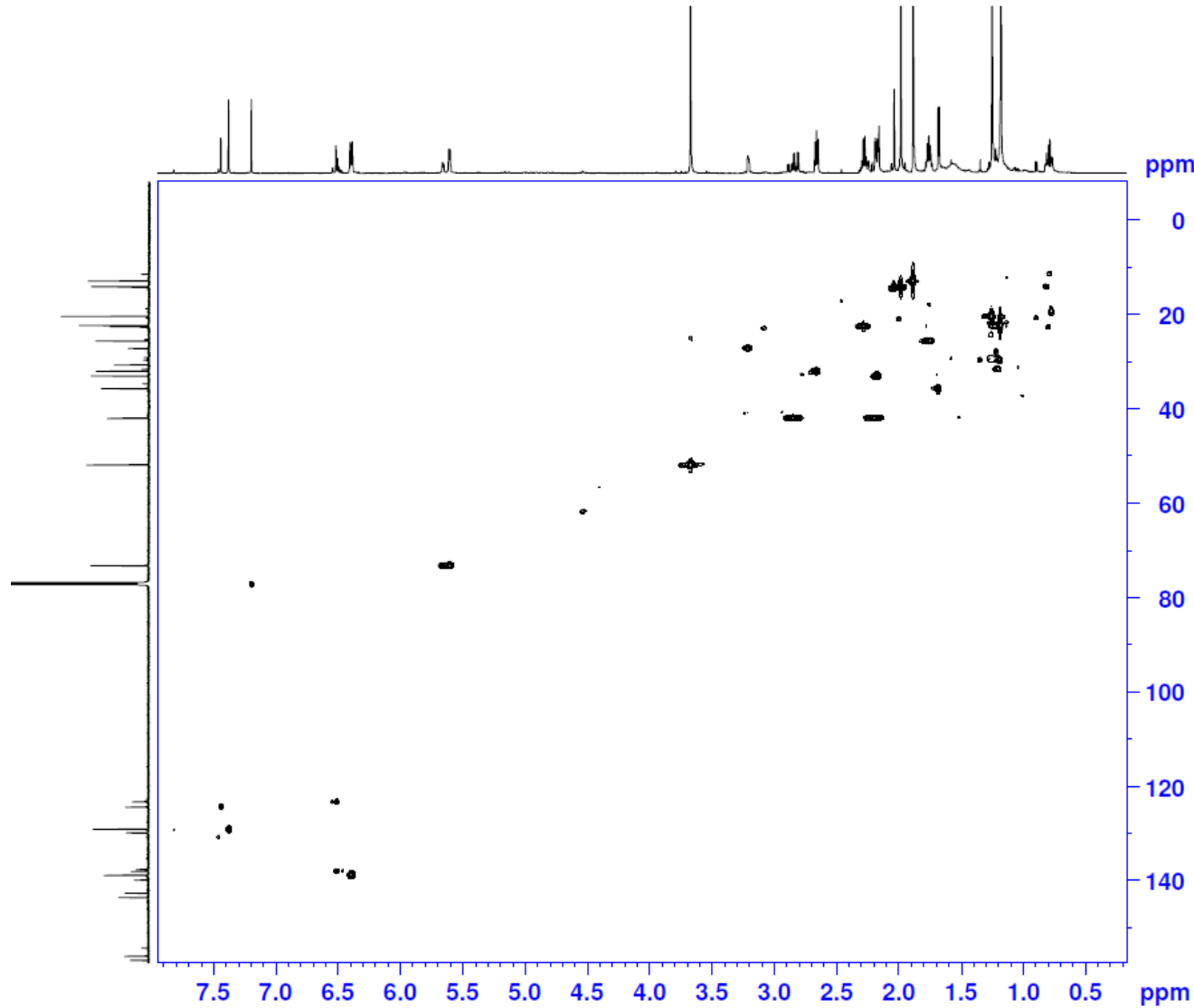
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
CPZ1 80.00 %
CPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
F2MODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300638 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200911 C12 i1
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Data_ 20200912
Time 23.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcpgndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 5263.158 Hz
FIDRES 1.284951 Hz
AQ 0.3891200 sec
RG 2050
DW 95.000 usec
DE 6.50 usec
TE 298.2 K
CNS113 8.0000000
D0 0.00000300 sec
D1 1.36646998 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1322896 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

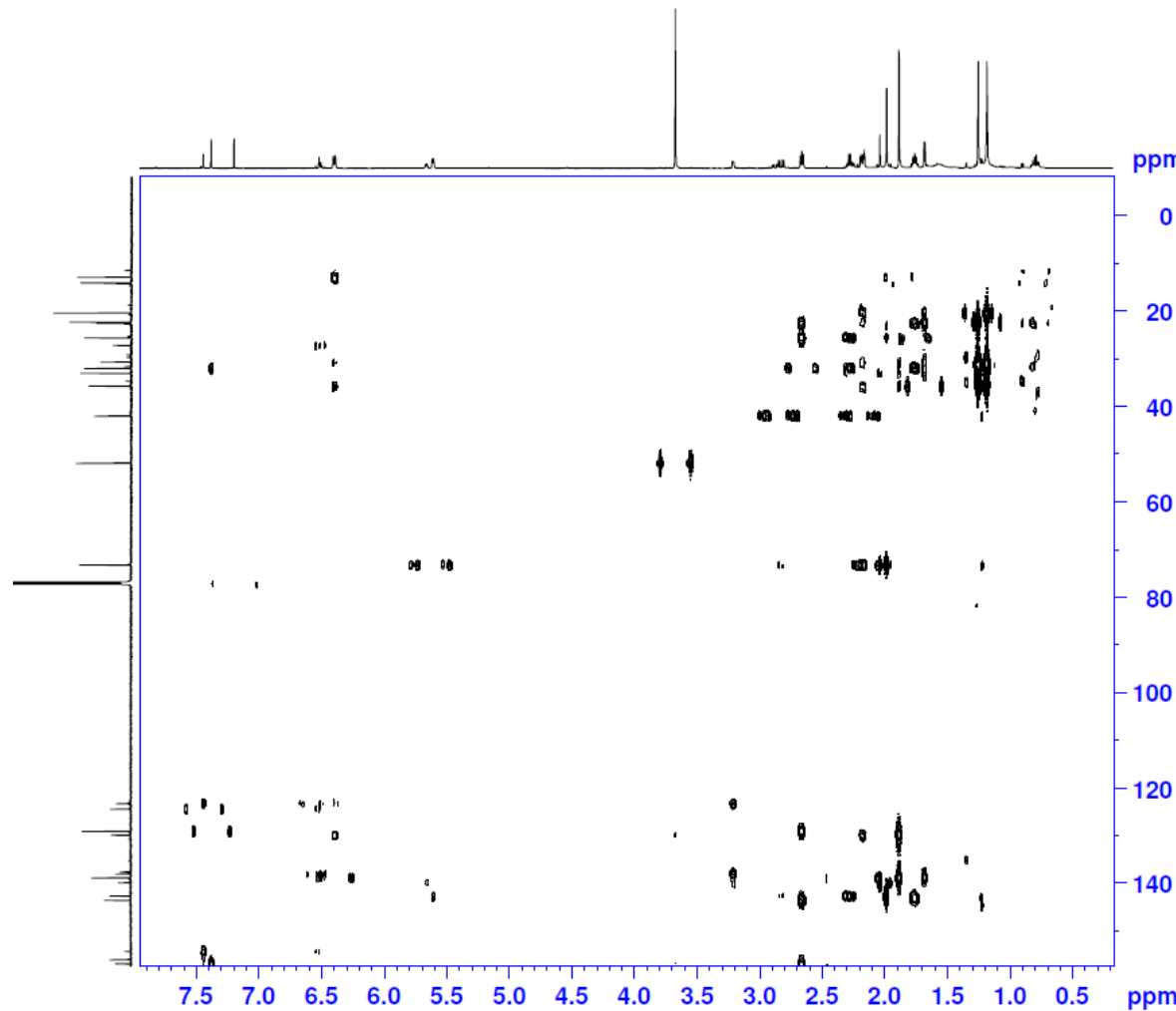
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
F1MODE QF

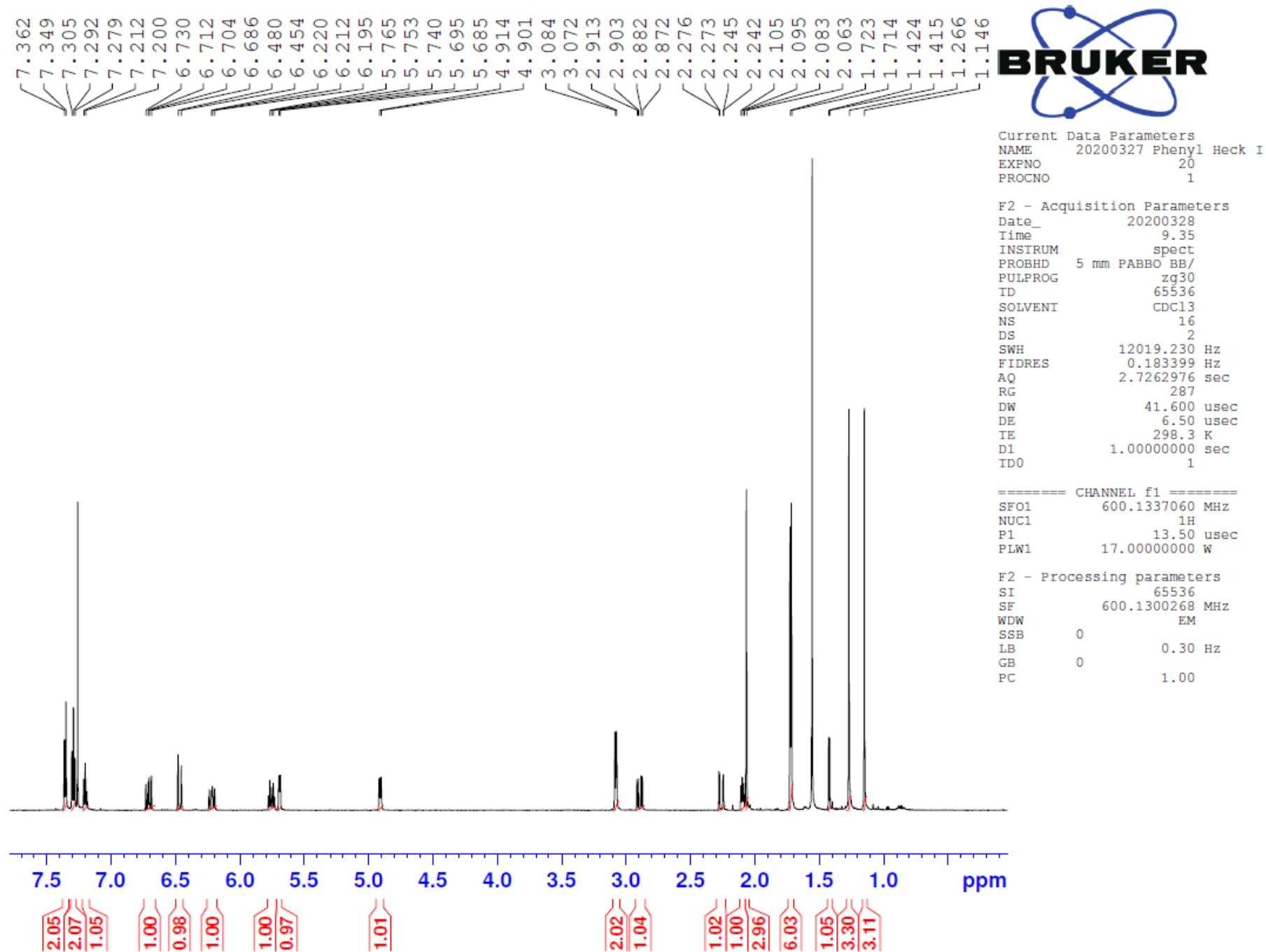
F2 - Processing parameters
SI 1024
SF 600.1300638 MHz
WDW SINK
SSB 0
LB 0 Hz
GB 0
PC 1.40

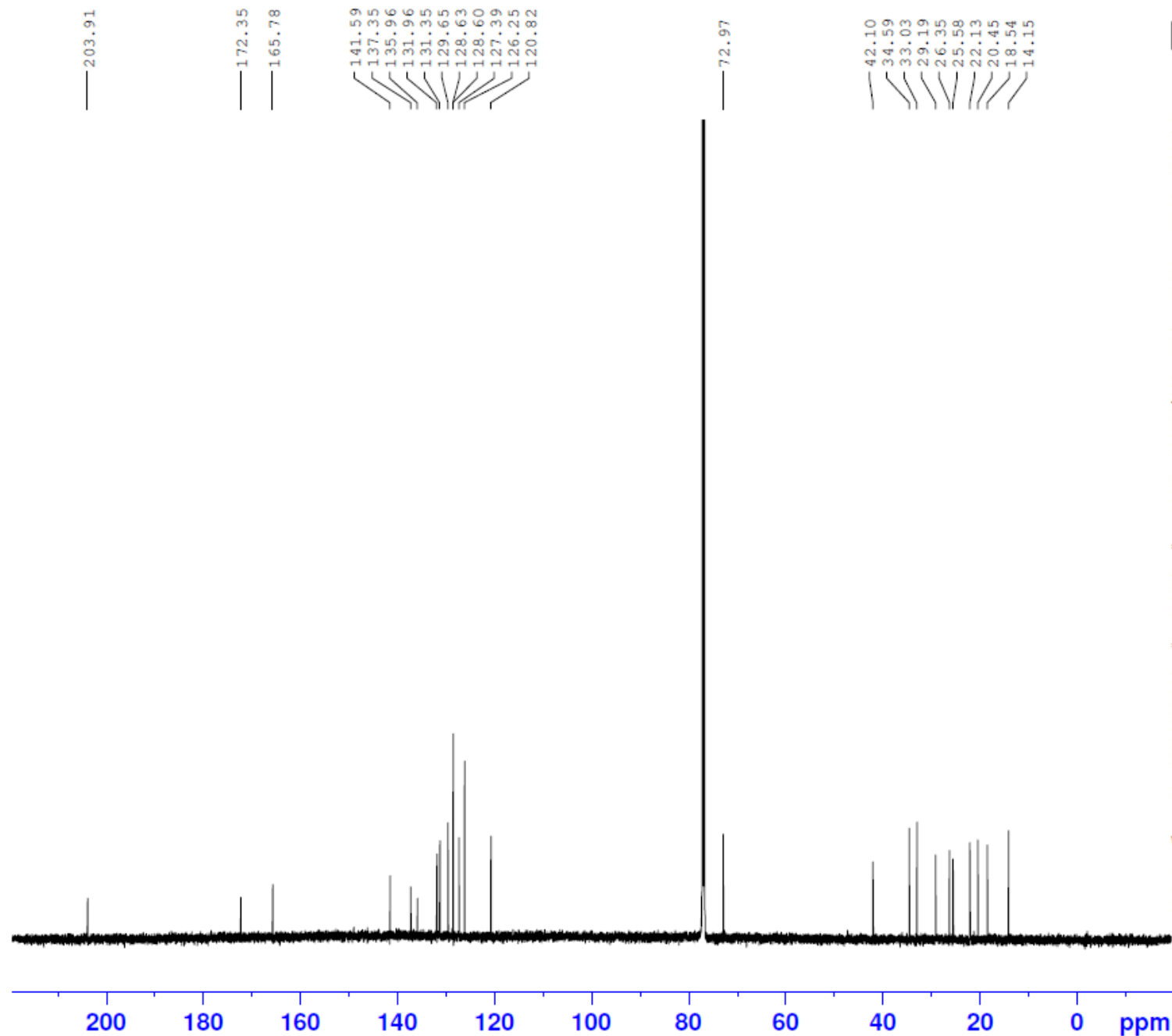
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINK
SSB 0
LB 0 Hz
GB 0



Mizoroki-Heck Chemistry Characterisation Data

111a NMR Characterisation





Current Data Parameters
NAME 20200327 Phenyl Heck I
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200328
Time 13.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
ID 65536
SOLVENT CDCl3
NS 4096
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20200327 Phenyl Heck I
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200328
Time 9.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 4629.629 Hz
FIDRES 2.260561 Hz
AQ 0.2211840 sec
RG 161
DW 108.000 usec
DE 6.50 usec
TE 298.3 K
D0 0.00000300 sec
D1 1.90661097 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00021600 sec

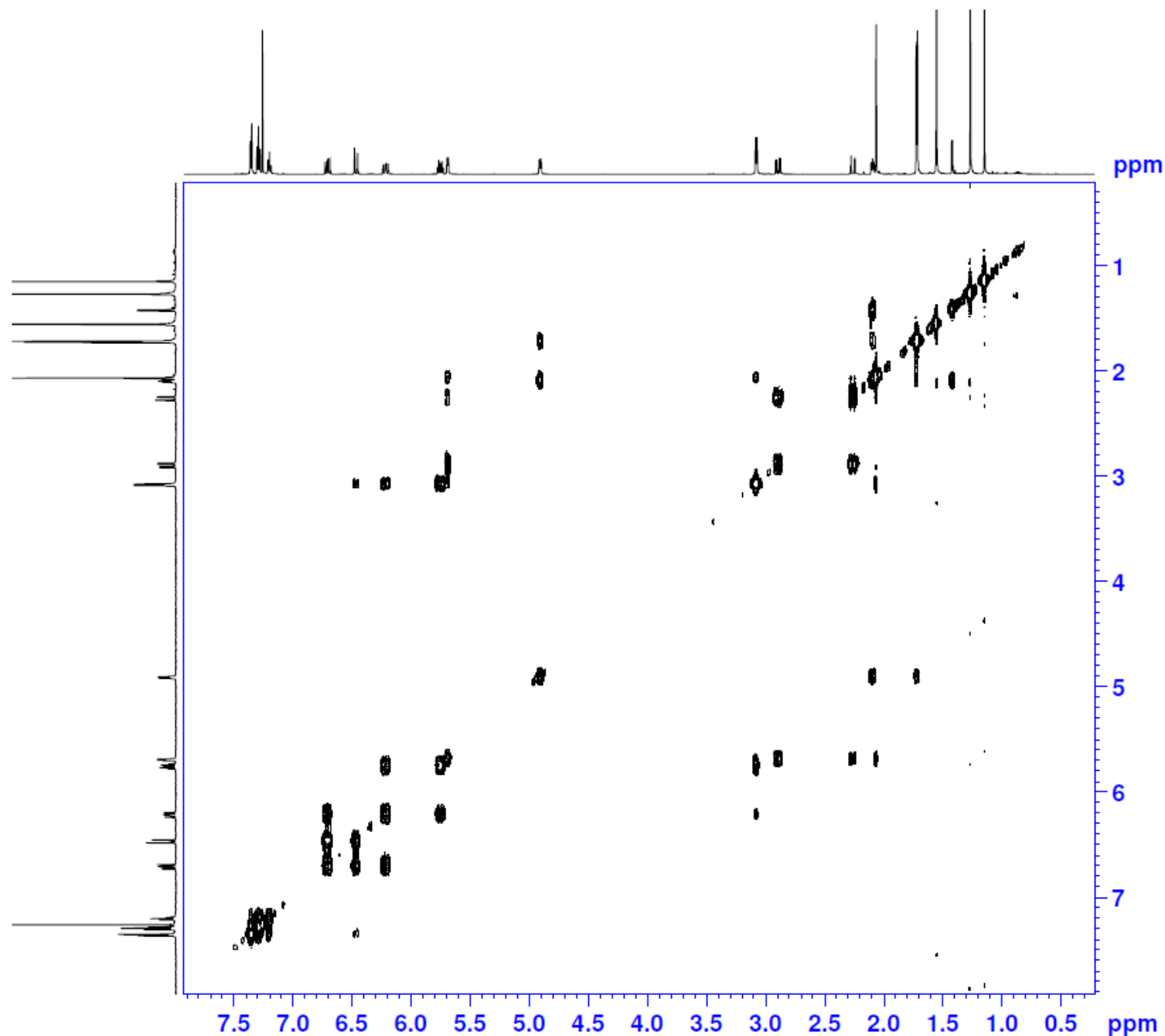
----- CHANNEL f1 -----
SFO1 600.1324672 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1325 MHz
FIDRES 36.168980 Hz
SW 7.714 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300257 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300283 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200327 Phenyl Heck I
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200328
Time 13.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
ID 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 4629.629 Hz
FIDRES 4.521122 Hz
AQ 0.1105920 sec
RG 2050
DW 108.000 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45494401 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS

===== CHANNEL f1 =====

SFO1 600.1324760 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

===== CHANNEL f2 =====

SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====

GNAM[1] SMSQ10.100
GNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters

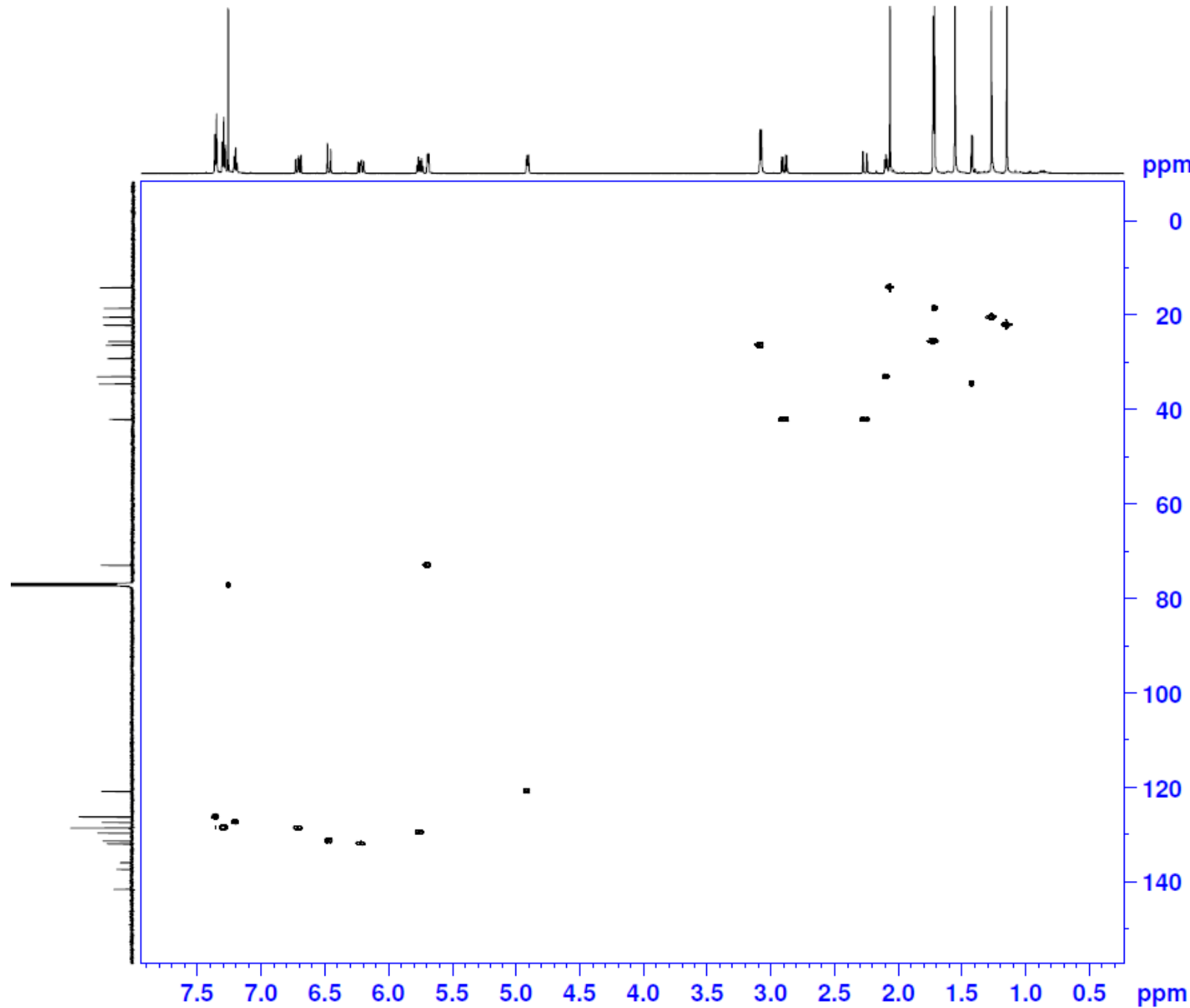
ID 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FmMODE Echo-Antiecho

F2 - Processing parameters

SI 1024
SF 600.1300248 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

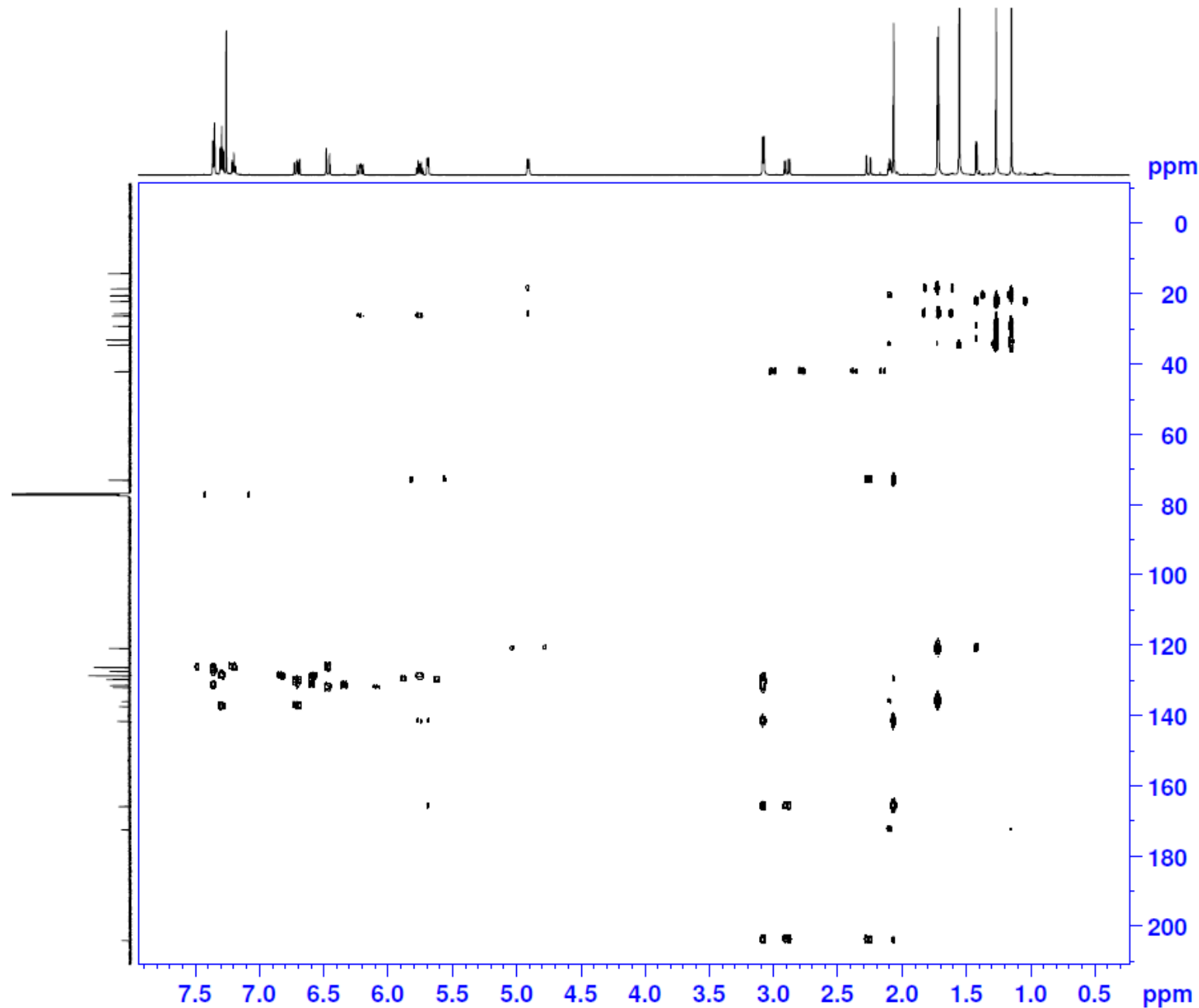
F1 - Processing parameters

SI 1024
MC2 echo-antiecho
SF 150.9028163 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200327 Phenyl Heck I
EXPNO 25
PROCNO 1



F2 - Acquisition Parameters
Data_ 20200328
Time 19.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 4629.629 Hz
FIDRES 1.130281 Hz
AQ 0.4423680 sec
RG 2050
DW 108.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.31322205 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec
===== CHANNEL F1 =====
SFO1 600.1324760 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W
===== CHANNEL F2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec
F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF
F2 - Processing parameters
SI 1024
SF 600.1300243 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028380 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

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Analyst
Date

Analyst
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100
98
96
94
92
90
88
86
84
82
80
78
76
75

4000 3500 3000 2500 2000 1500 1000 600

cm-1

3024.09cm-1, 92.99%T
2925.32cm-1, 91.79%T
1714.06cm-1, 75.97%T
1596.89cm-1, 93.07%T
1495.16cm-1, 91.41%T
1656.08cm-1, 89.63%T
1421.53cm-1, 88.74%T
1380.88cm-1, 87.74%T
1282.36cm-1, 88.43%T
1447.66cm-1, 88.90%T
1193.33cm-1, 85.72%T
1235.30cm-1, 88.46%T
1362.83cm-1, 89.82%T
1152.70cm-1, 79.11%T
1043.22cm-1, 88.87%T
1014.54cm-1, 85.68%T
990.57cm-1, 83.40%T
848.20cm-1, 87.75%T
814.97cm-1, 88.72%T
799.08cm-1, 89.56%T
692.48cm-1, 84.05%T
603.93cm-1, 85.53%T

Sample Name	Description	Quality Checks
Phenyl I E	Sample	The Quality Checks do not report any warnings for the sample.

125a NMR Characterisation

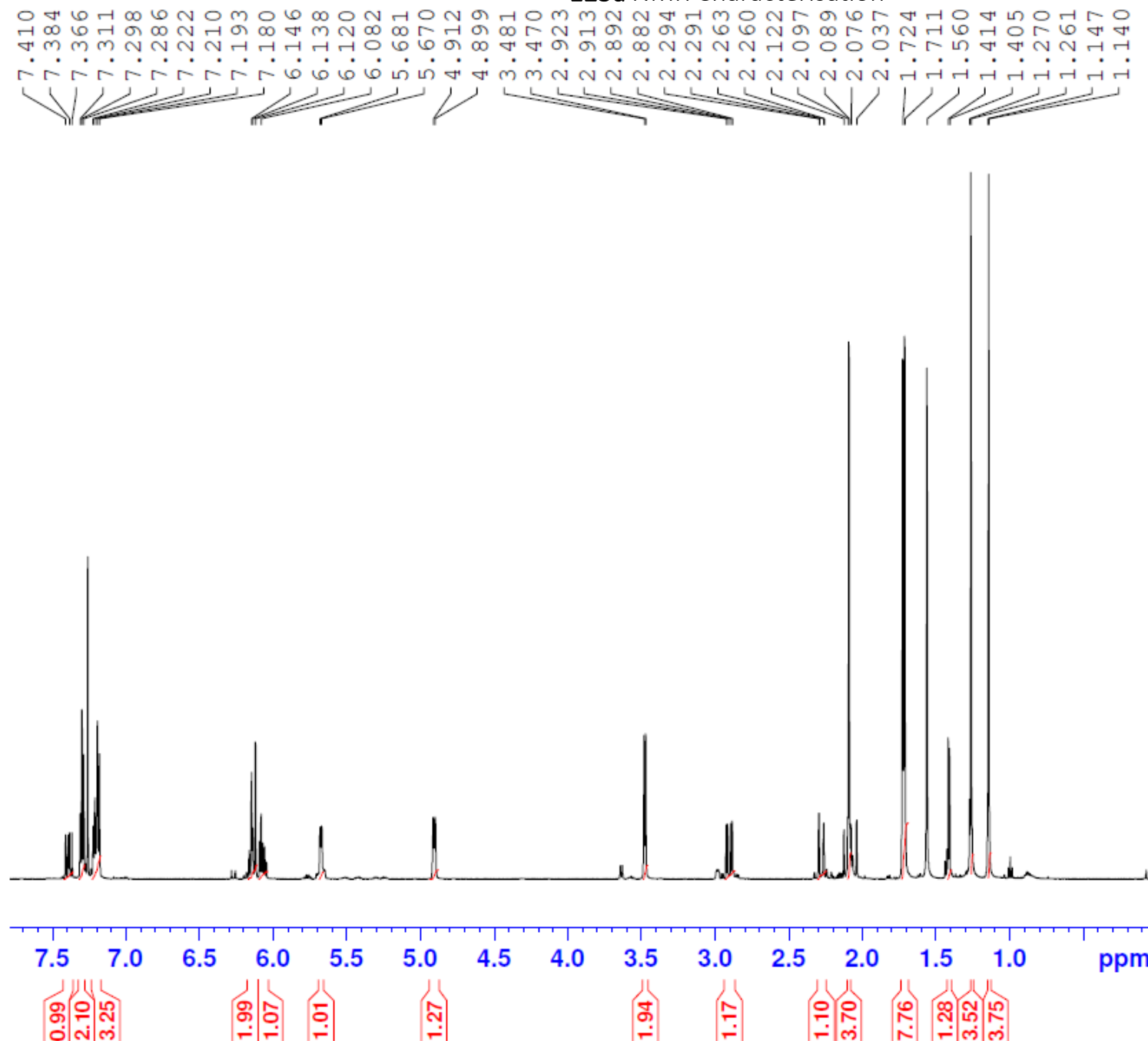


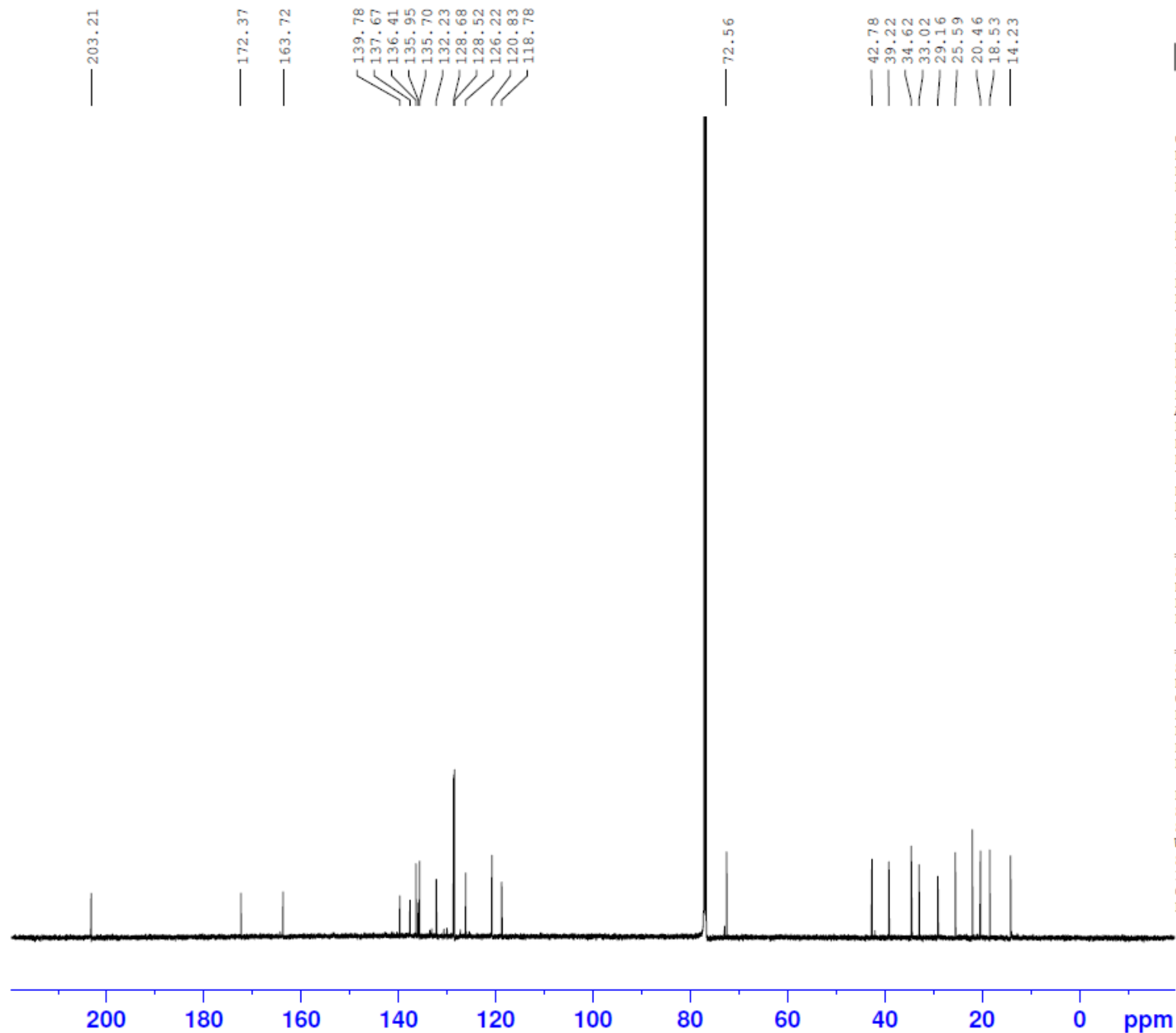
Current Data Parameters
 NAME 20200327 Phenyl Heck I
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200327
 Time 18.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 ID 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 256
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300265 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
NAME 20200327 Phenyl Heck 1
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200327
Time 22.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
ID 65536
SOLVENT CDCl3
NS 4096
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20200327 Phenyl Heck I
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200327
Time 18.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppgf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 4672.897 Hz
FIDRES 2.281688 Hz
AQ 0.2191360 sec
RG 128
DW 107.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.90865898 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00021400 sec

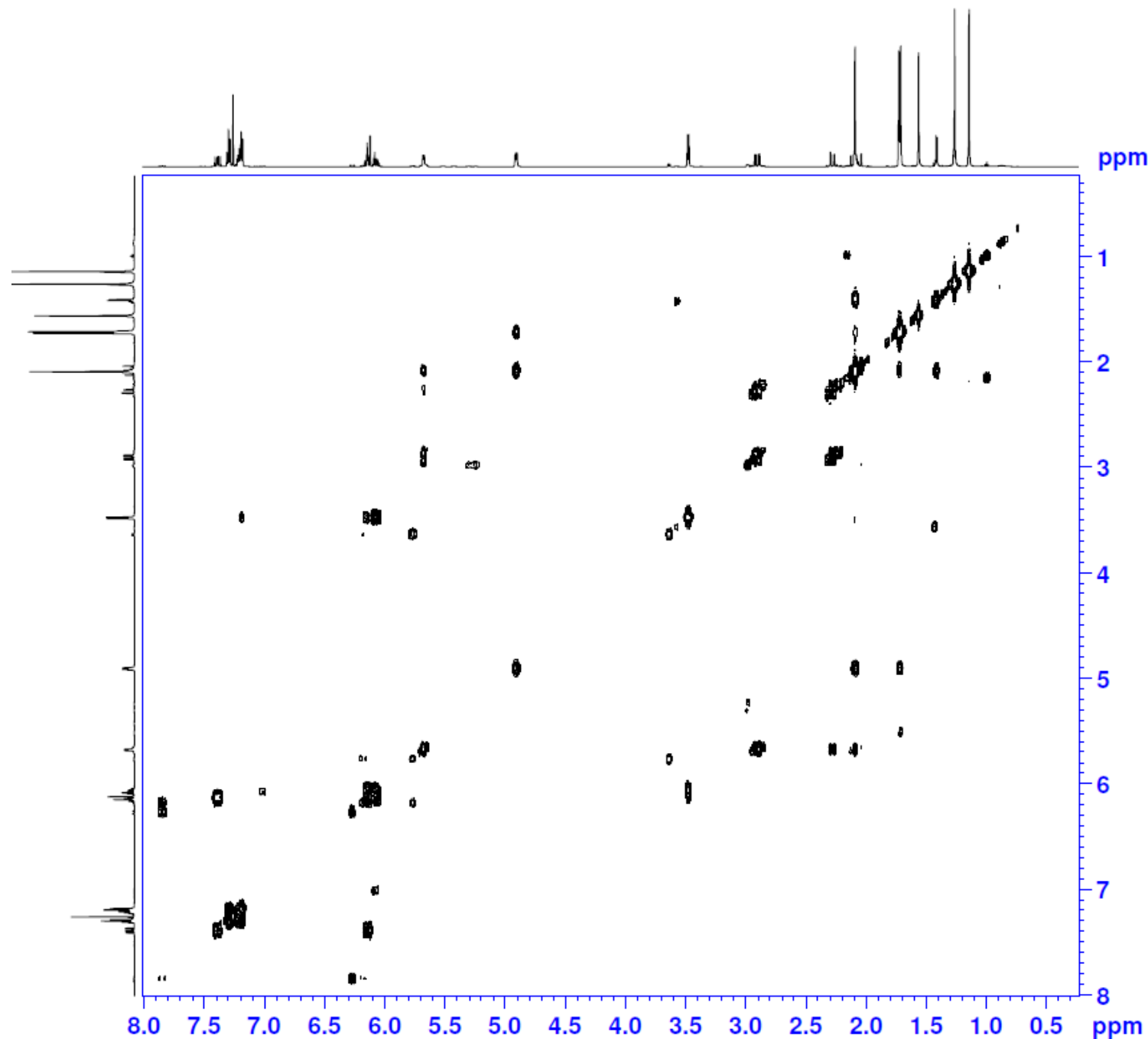
----- CHANNEL f1 -----
SFO1 600.1324992 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1325 MHz
FIDRES 36.507008 Hz
SW 7.786 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300259 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300258 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200327 Phenyl Hack 1
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200327
Time 22.23
INSTRUM spect
PROBHD 5 mm F400 BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 70
DS 16
SWH 4629.629 Hz
FIDRES 4.521122 Hz
AQ 0.1105920 sec
RG 2050
DW 108.000 usec
DE 6.50 usec
TE 298.3 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45494401 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS

===== CHANNEL f1 =====
SFO1 600.1324664 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

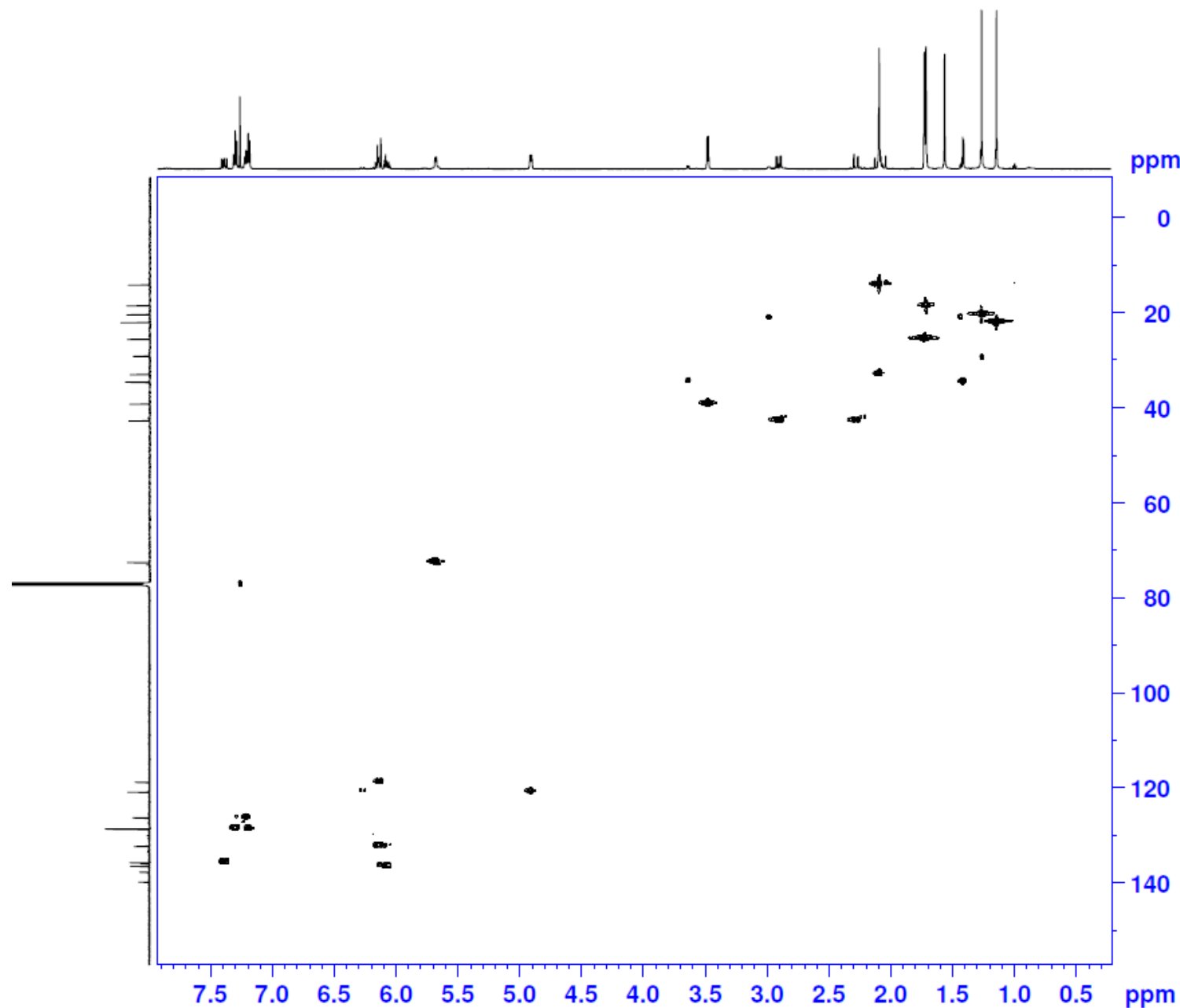
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GFNAM[1] SMSQ10.100
GFNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
PL6 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300255 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028464 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200327 Phenyl Hack I
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Data_ 20200328
Time 6.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT cdcl3
NS 50
DS 16
SWH 4629.629 Hz
FIDRES 1.130281 Hz
AQ 0.4423680 sec
RG 2050
DW 108.000 usec
DE 6.50 usec
TE 298.1 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.31322205 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1324664 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

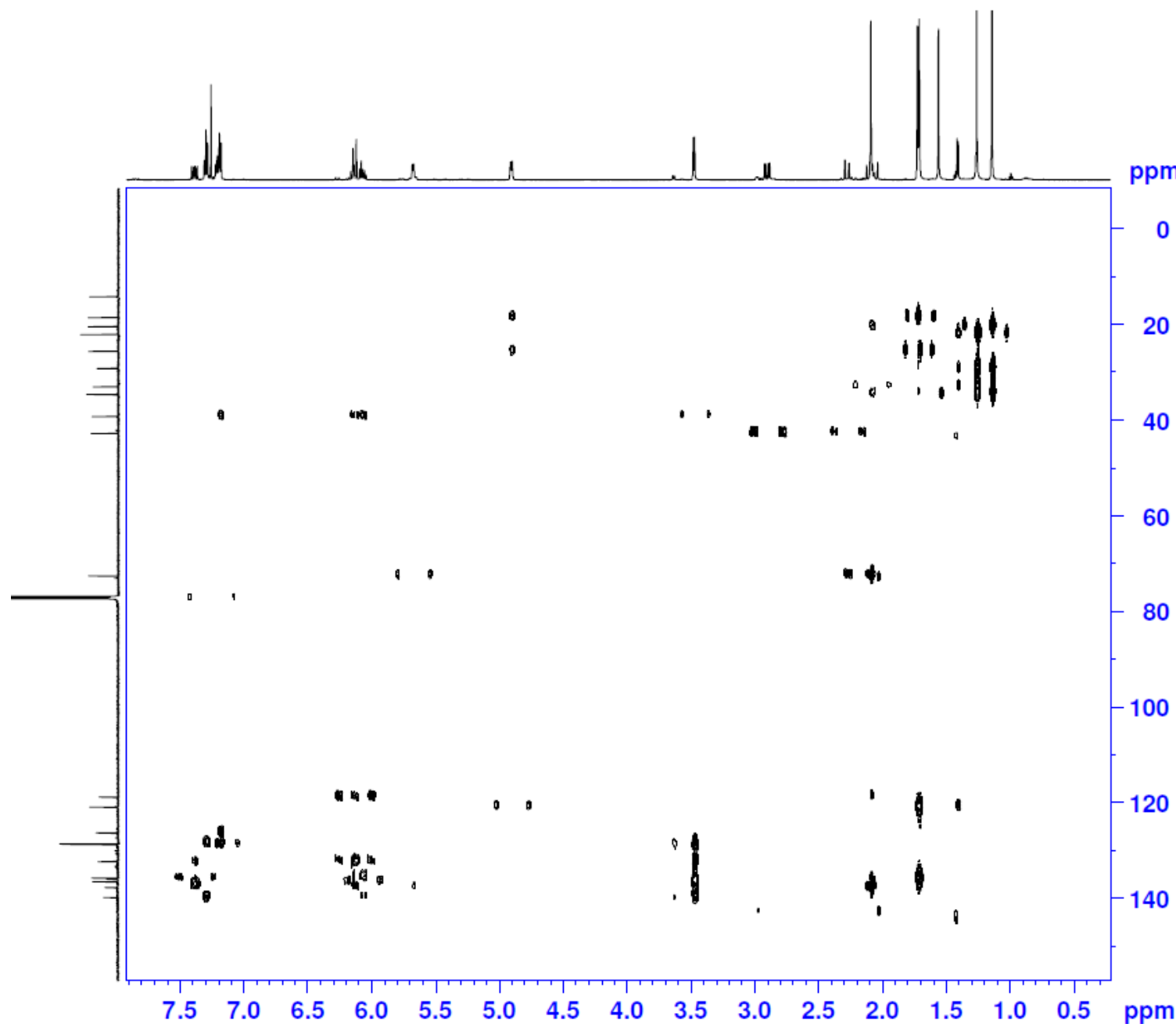
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FmMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300285 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028550 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

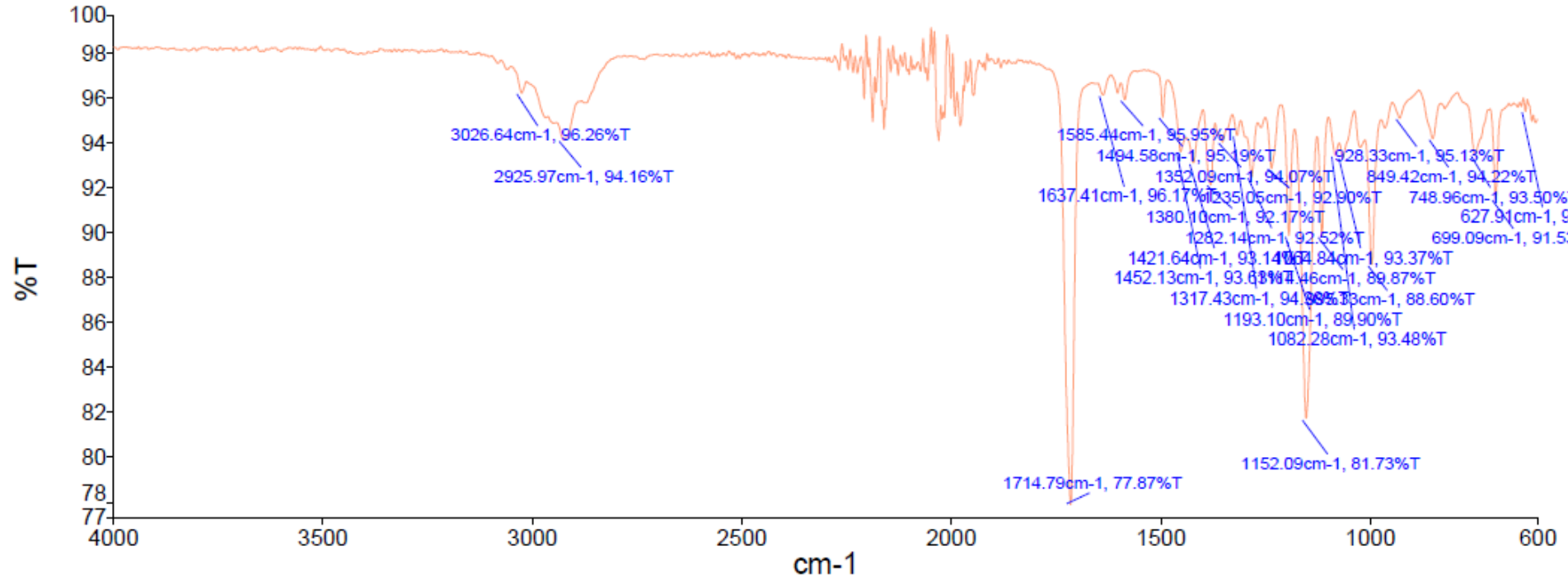


125a IR Spectrum

PerkinElmer Spectrum Version 10.4.00
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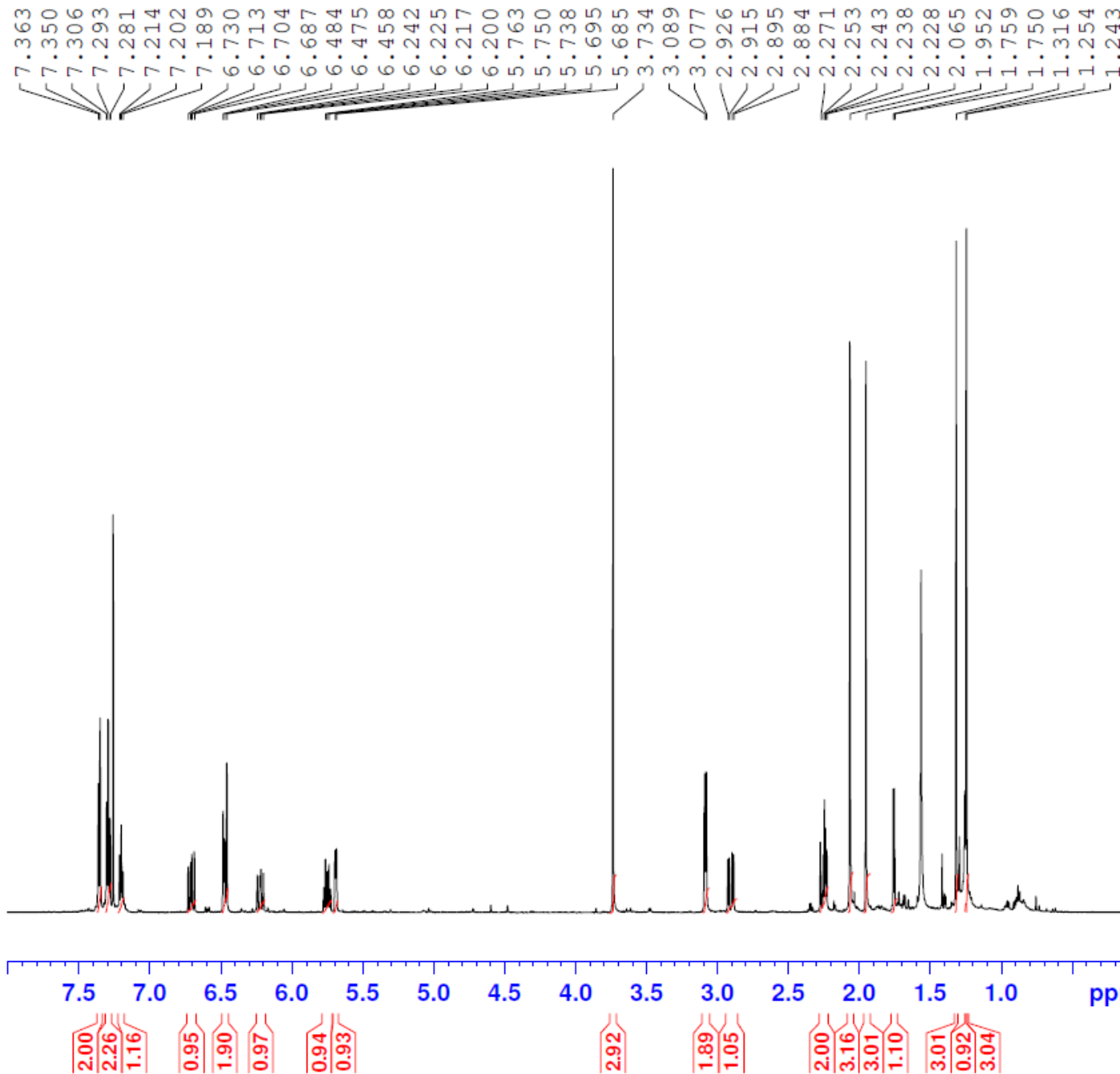
Analyst
Date

Analyst
Friday, 12 June 2020 9:54 AM



Sample Name	Description	Quality Checks
Phenyl I Migration	Sample	The Quality Checks do not report any warnings for the sample.

111b NMR Characterisation

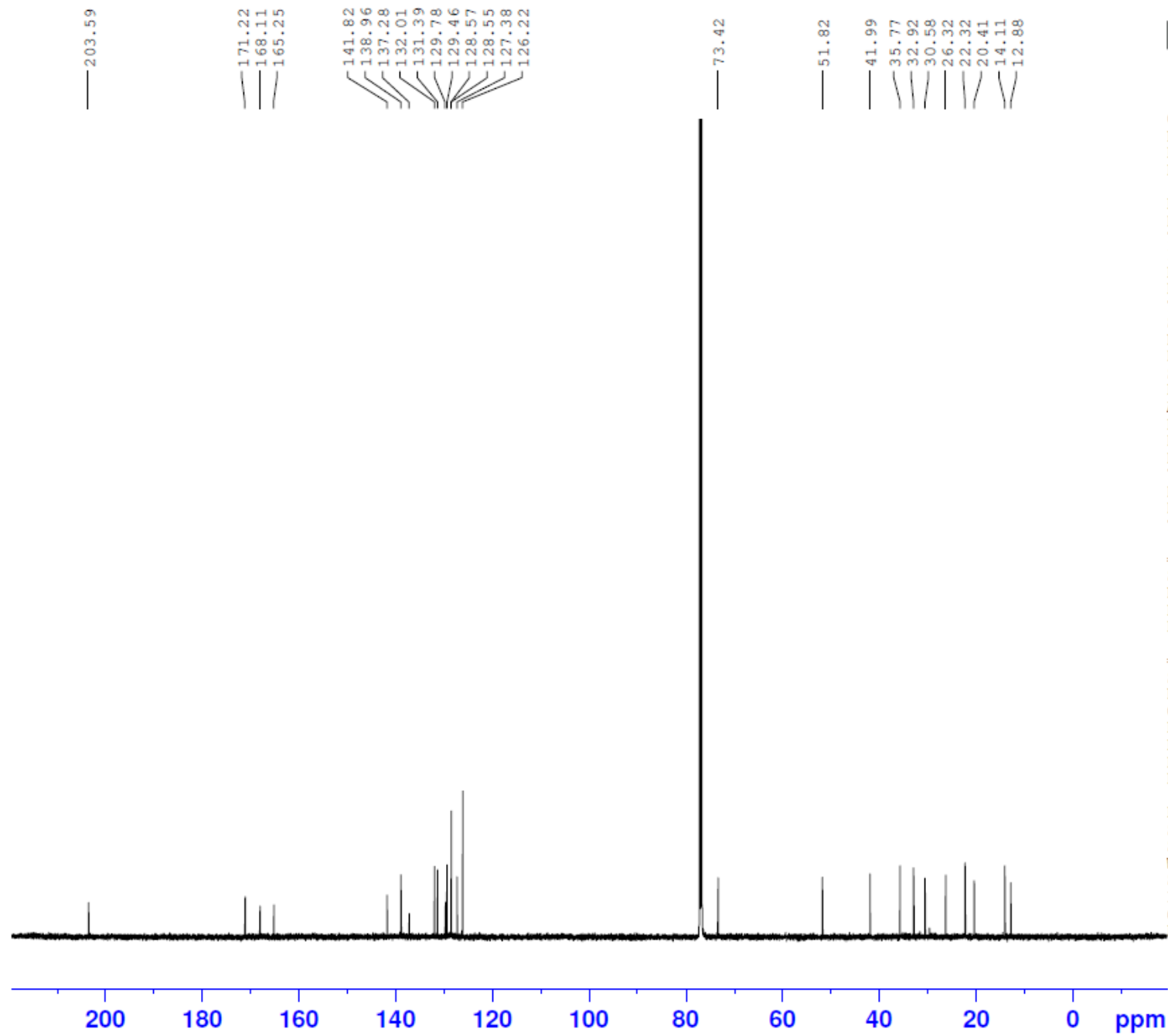


Current Data Parameters
NAME 20200417 PII Phenyl E
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200418
Time 7.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 256
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20200417 PII Phenyl E
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200418
Time 10.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028141 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20200417 P11 Phenyl E
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200418
Time 7.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 4807.692 Hz
FIDRES 2.347506 Hz
AQ 0.2129920 sec
RG 2050
DW 104.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00008681 sec
D1 1.92545295 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00020800 sec

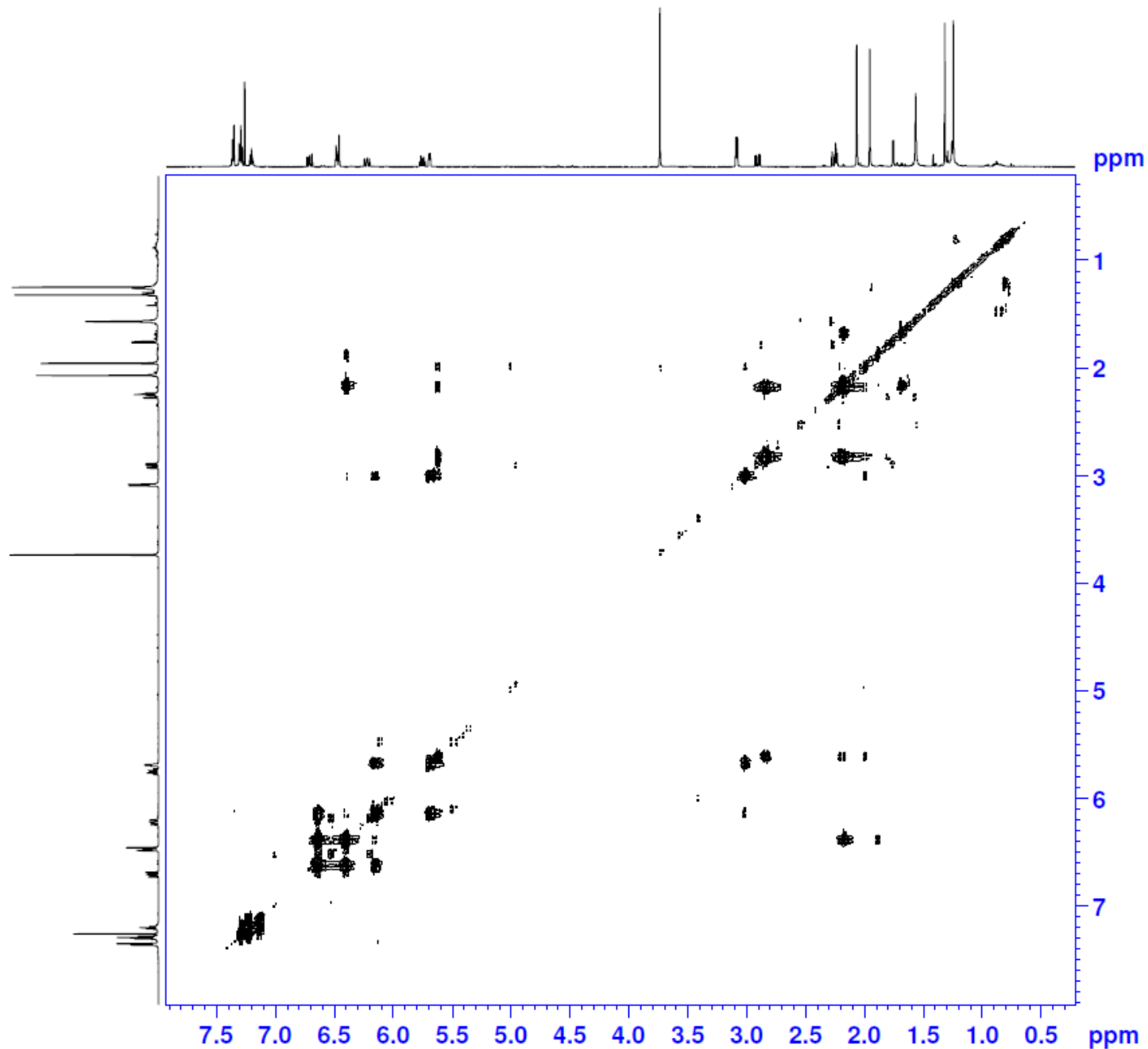
----- CHANNEL f1 -----
SFO1 600.1324848 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW0 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1325 MHz
FIDRES 18.780048 Hz
SW 8.011 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300677 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300677 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200417 P11 Phenyl E
EXPNO 25
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200418
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 4854.369 Hz
FIDRES 4.740595 Hz
AQ 0.1054720 sec
RG 2050
DW 103.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46006405 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.0002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1324493 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PIN1 17.00000000 W

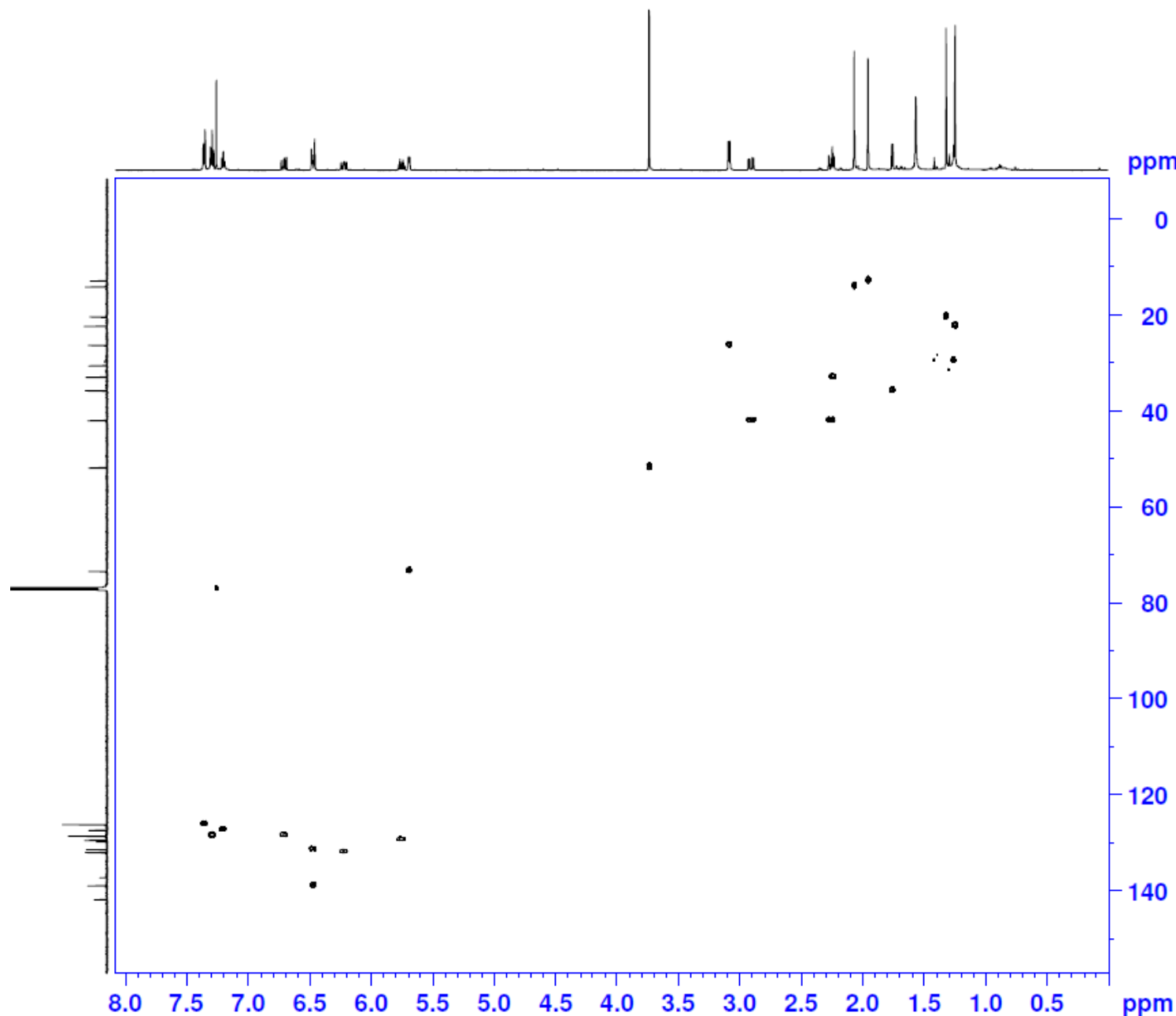
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PIN2 79.98300171 W
PIN12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GFZ1 80.00 %
GFZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

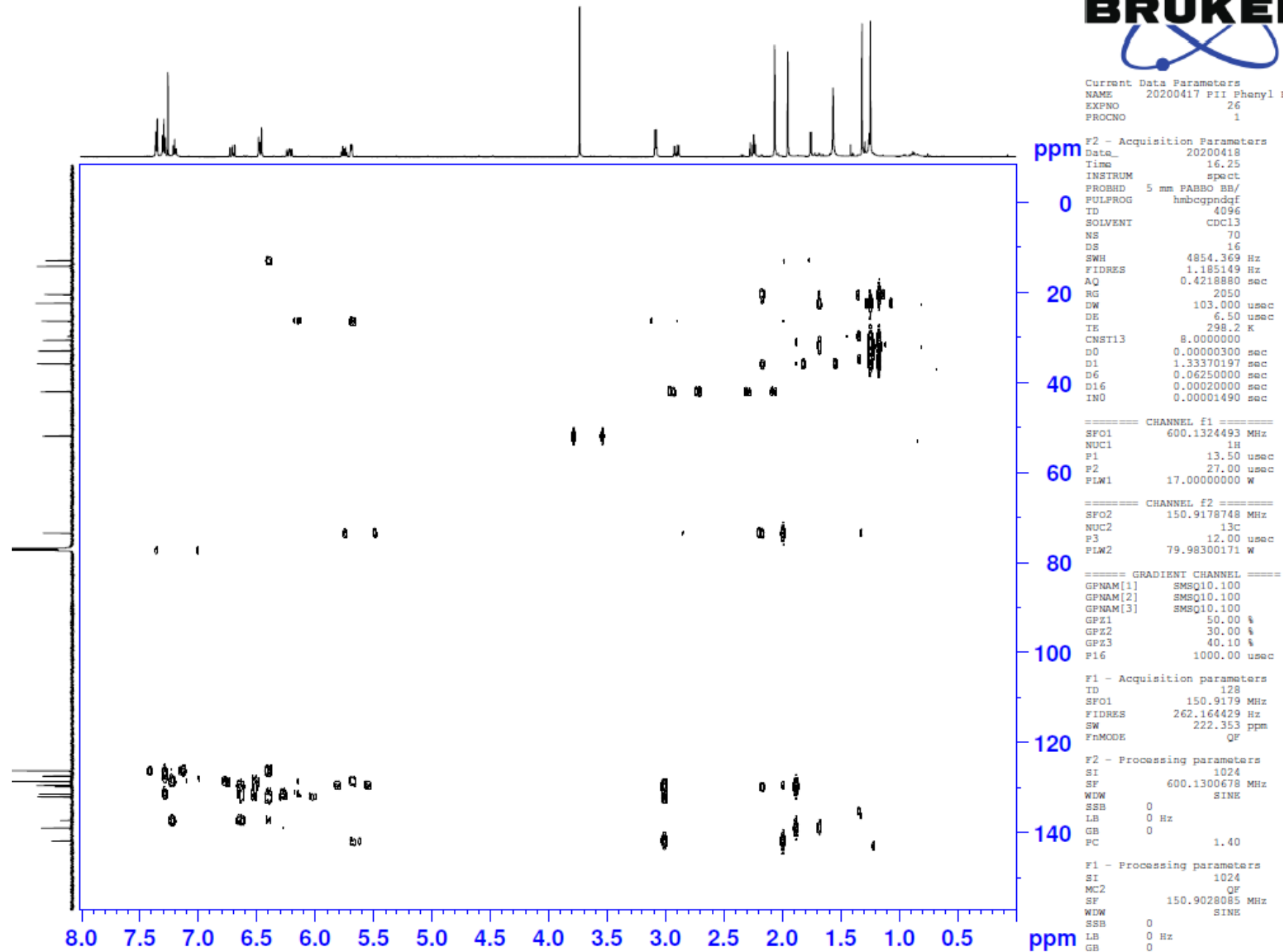
F2 - Processing parameters
SI 1024
SF 600.1300249 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028409 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200417 P11 Phenyl E
EXPNO 26
PROCNO 1

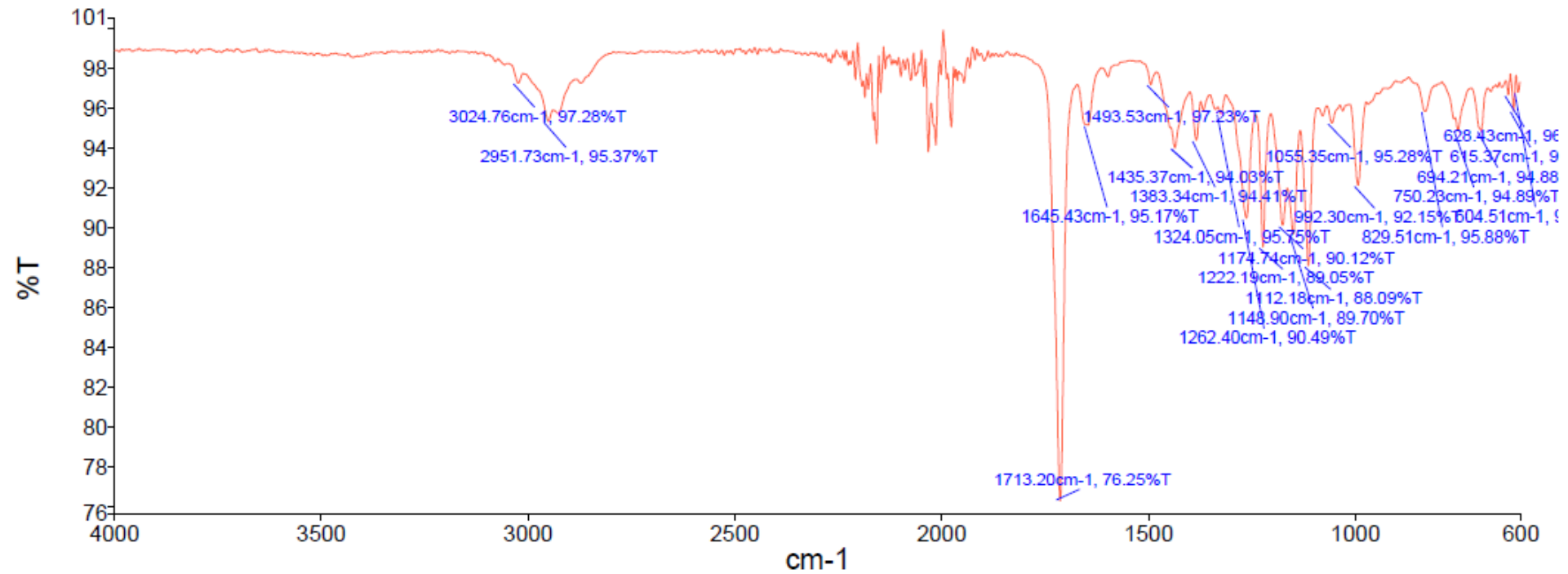


111b IR Spectrum

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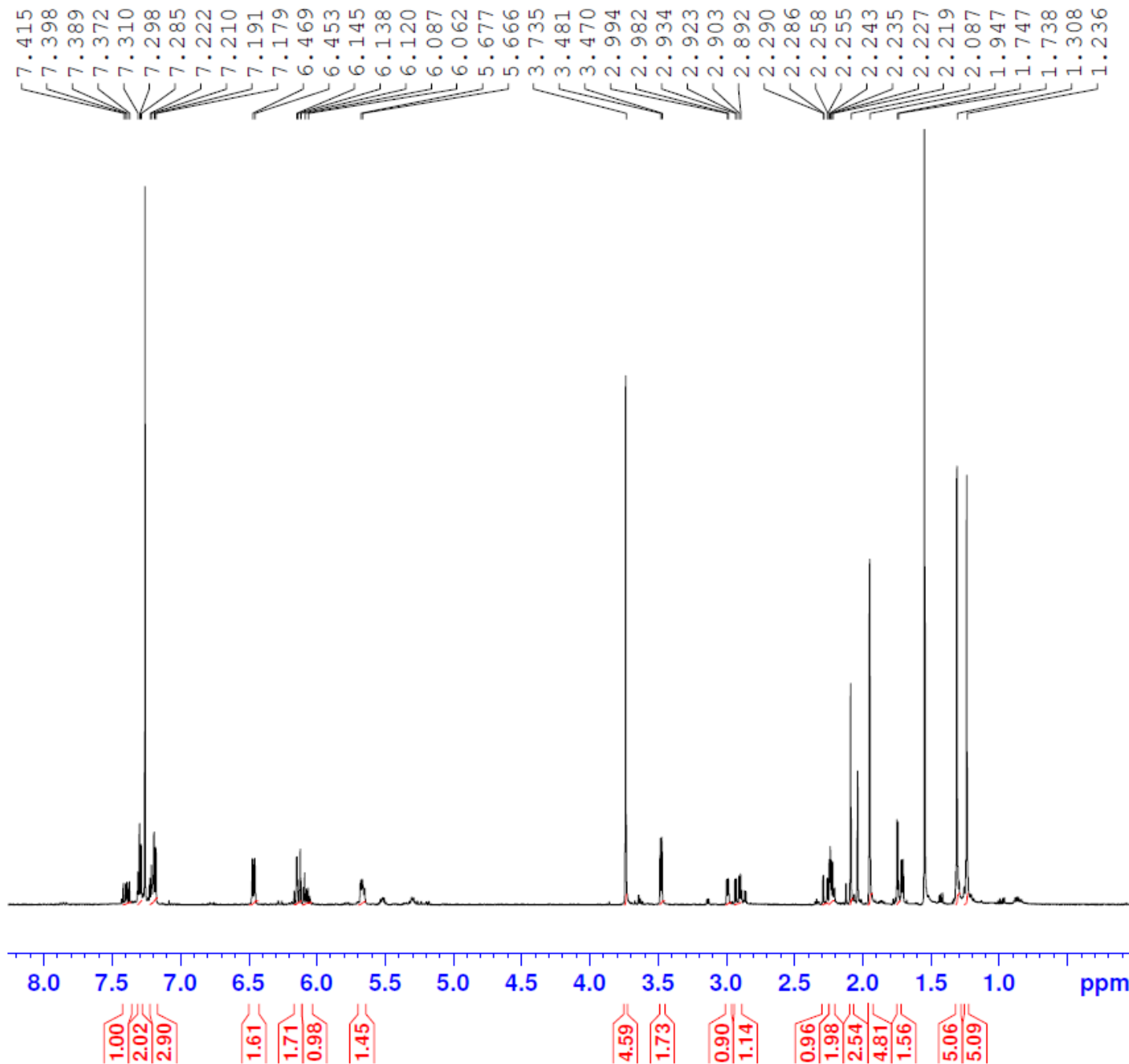
Analyst
Date

Analyst
Friday, 12 June 2020 10:05 AM



Sample Name	Description	Quality Checks
Phenyl II E	Sample	The Quality Checks do not report any warnings for the sample.

125b NMR Characterisation

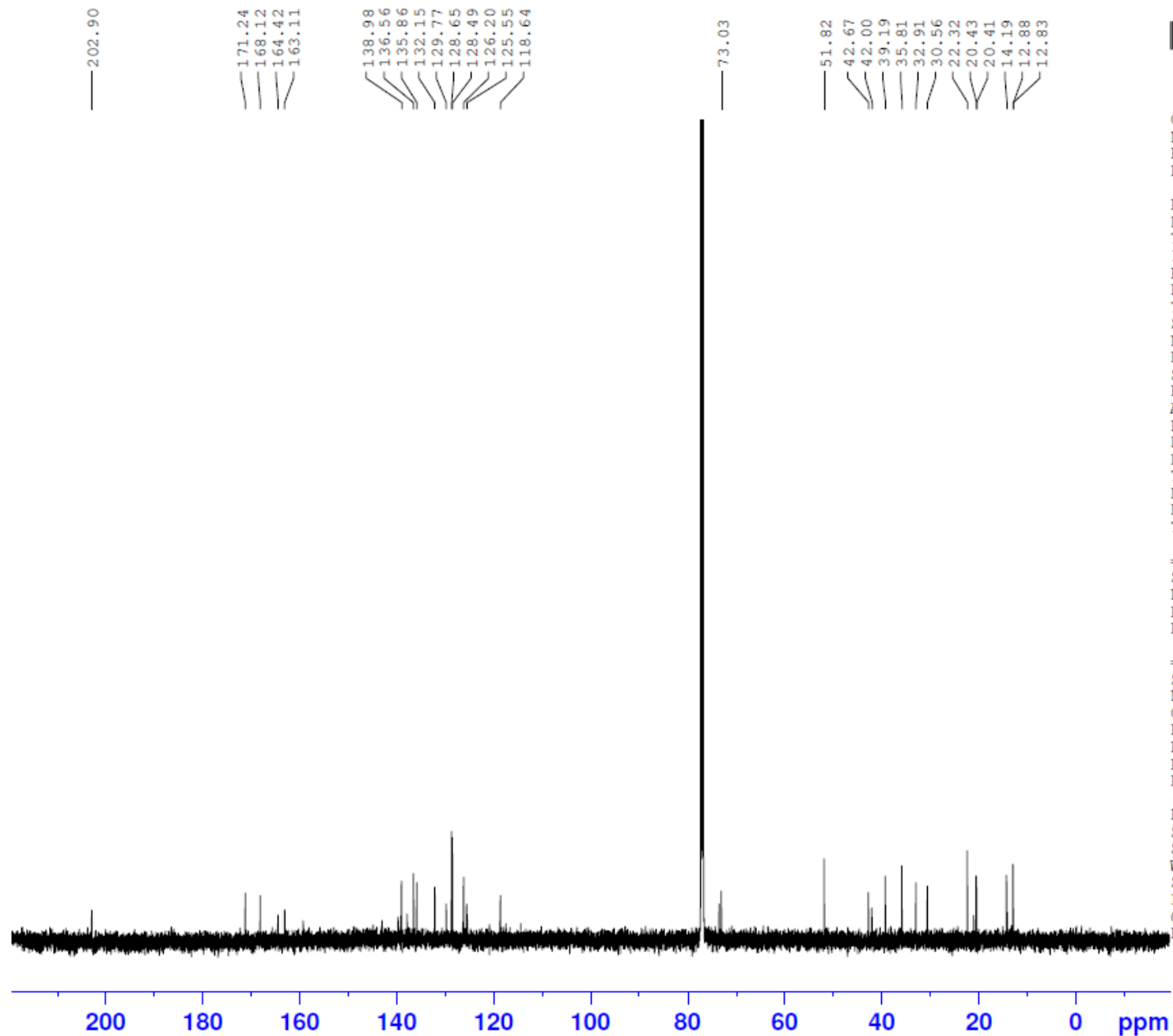


Current Data Parameters
NAME 20200417 PII Phenyl Z
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200417
Time 17.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 322
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300277 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20200417 PII Phenyl Z
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200417
Time 20.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028129 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20200417 P11 Phenyl Z
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200417
Time 17.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 4672.897 Hz
FIDRES 2.281688 Hz
AQ 0.2191360 sec
RG 2050
DW 107.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00008981 sec
D1 1.91930902 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021400 sec

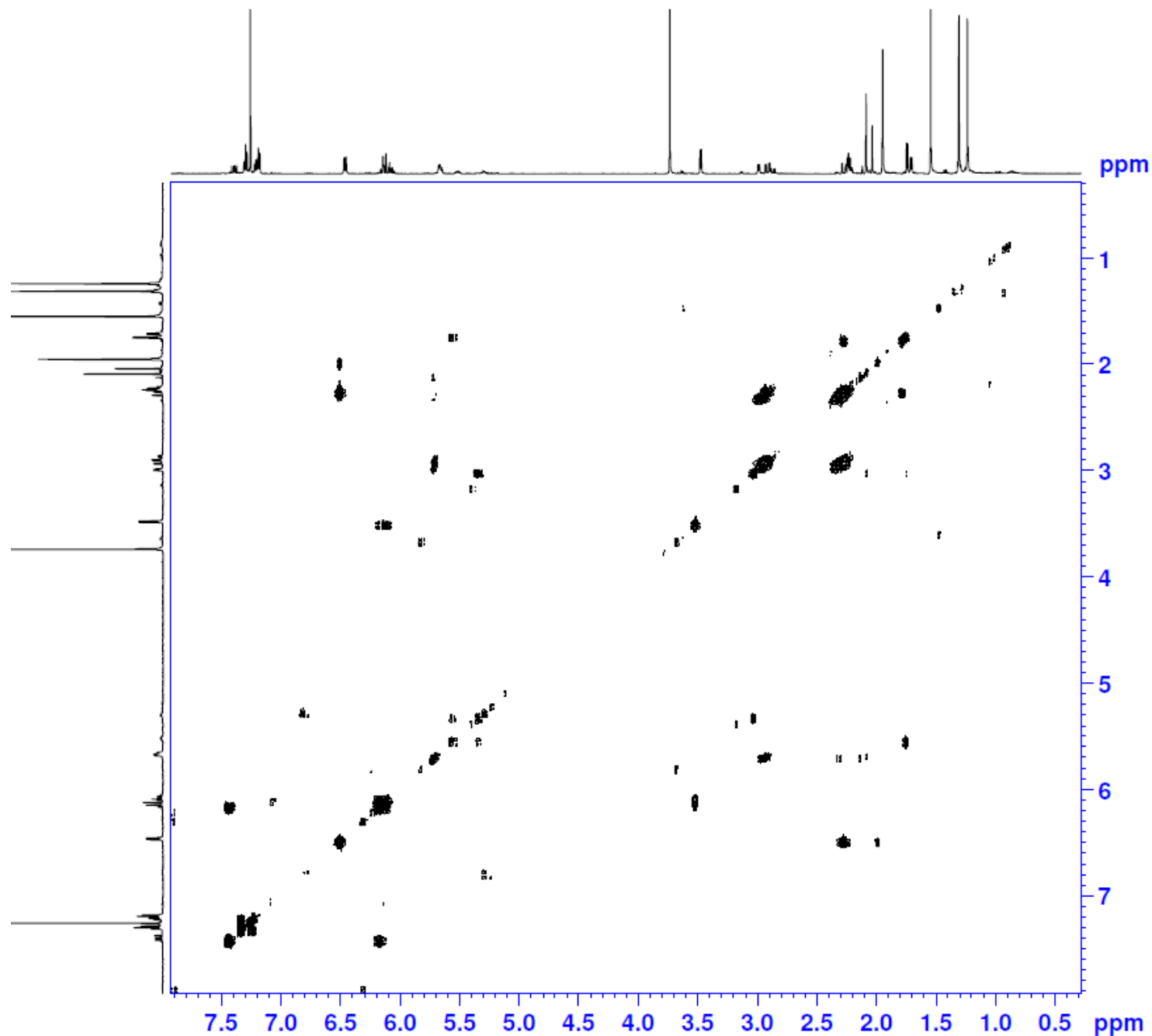
----- CHANNEL f1 -----
SFO1 600.1325048 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1325 MHz
FIDRES 18.253504 Hz
SW 7.786 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200417 P11 Phenyl Z
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200417
Time 21.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetqp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 4587.156 Hz
FIDRES 4.479644 Hz
AQ 0.1116160 sec
RG 2050
DW 109.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.0000300 sec
D1 1.45392001 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPTNS

===== CHANNEL f1 =====
SFO1 600.1324790 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
P1W1 17.00000000 W

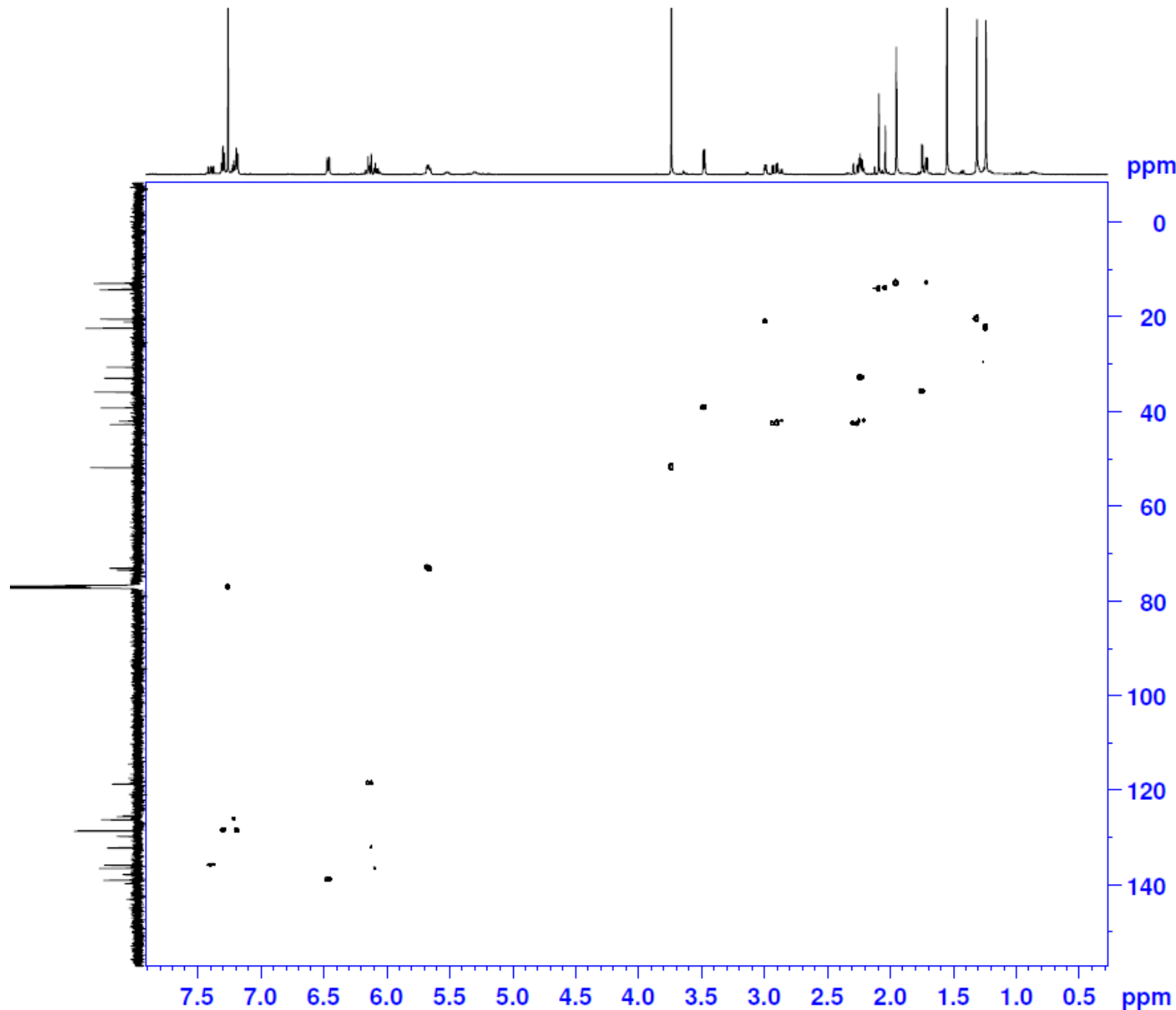
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
P1W2 79.98300171 W
P1W12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPE1 80.00 %
GPE2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300242 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028372 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200417 F11 Phenyl Z
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200418
Time 2.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 4587.156 Hz
FIDRES 1.119911 Hz
AQ 0.4464640 sec
RG 2050
DW 109.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.30912602 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1324790 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

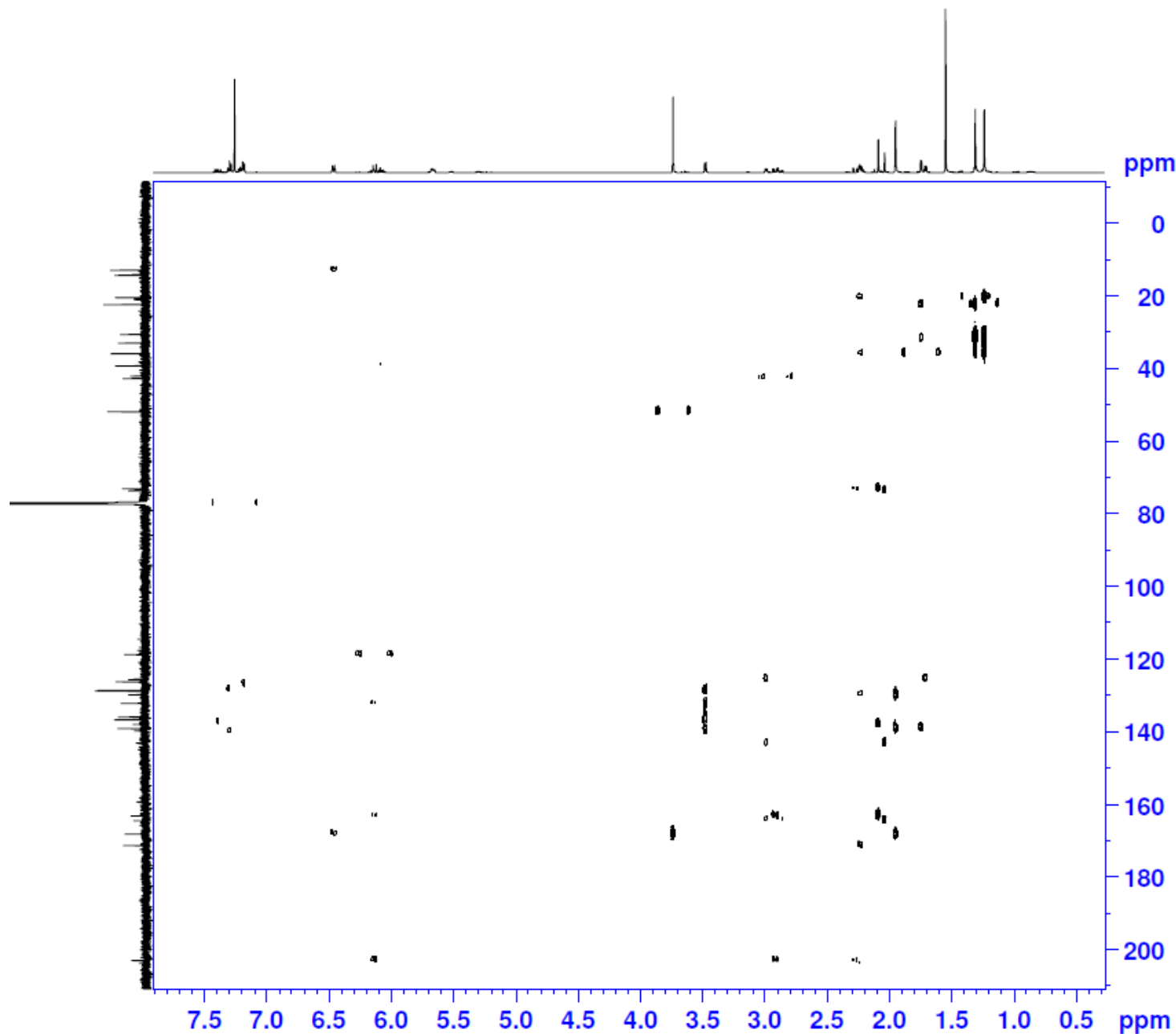
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

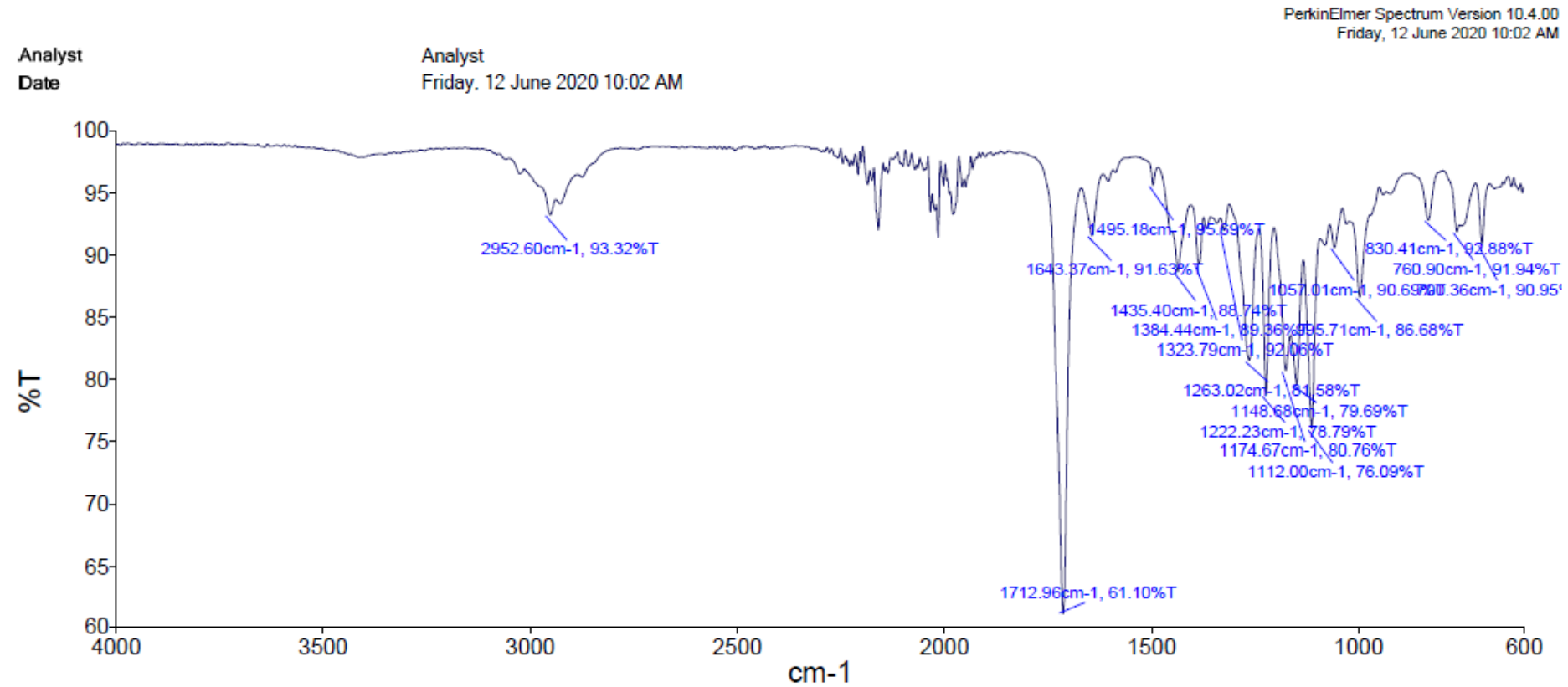
F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300245 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028501 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



125b IR Spectrum



Sample Name	Description	Quality Checks
Phenyl II Mig	Sample	The Quality Checks do not report any warnings for the sample.

129a NMR Characterisation

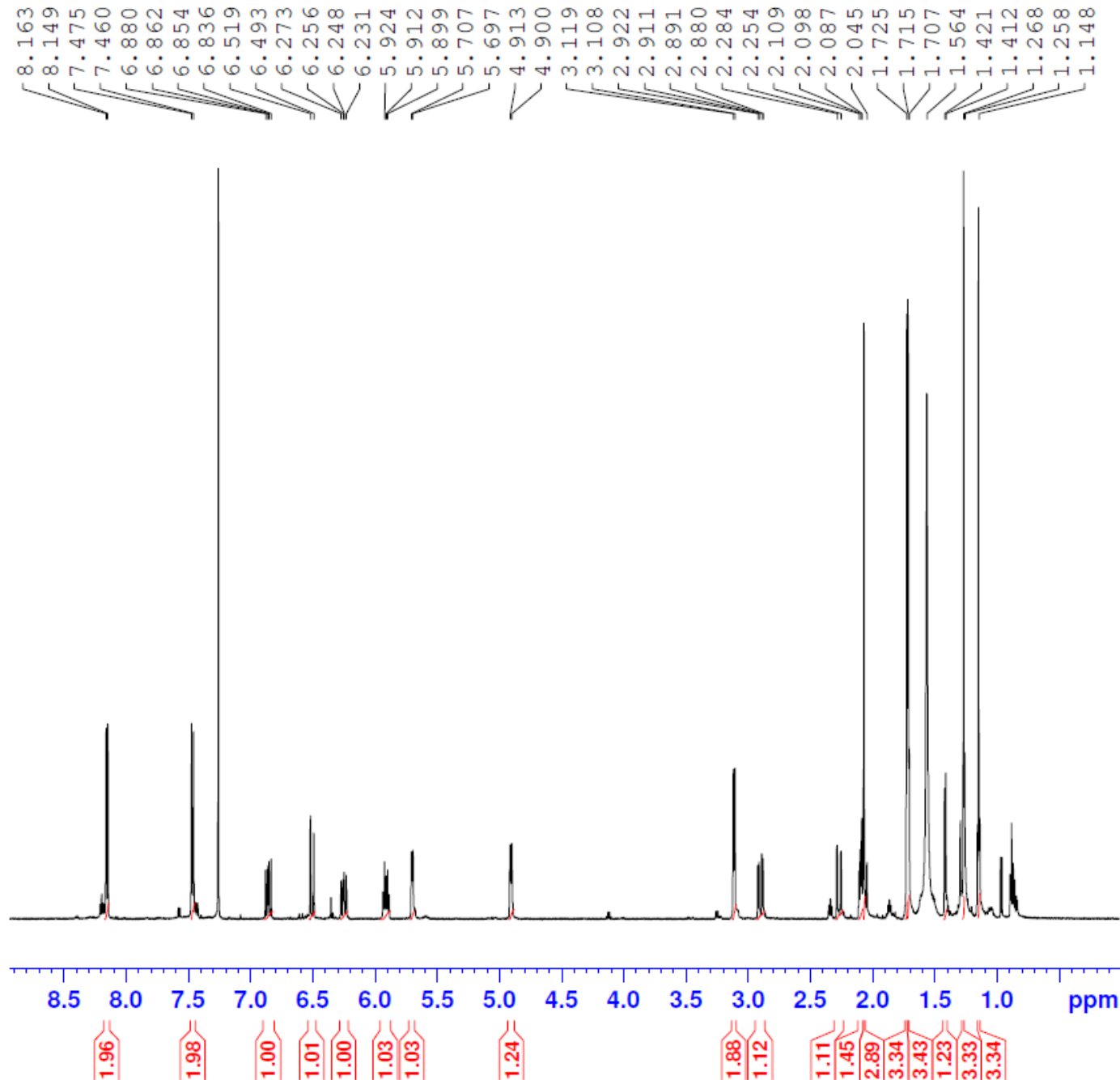


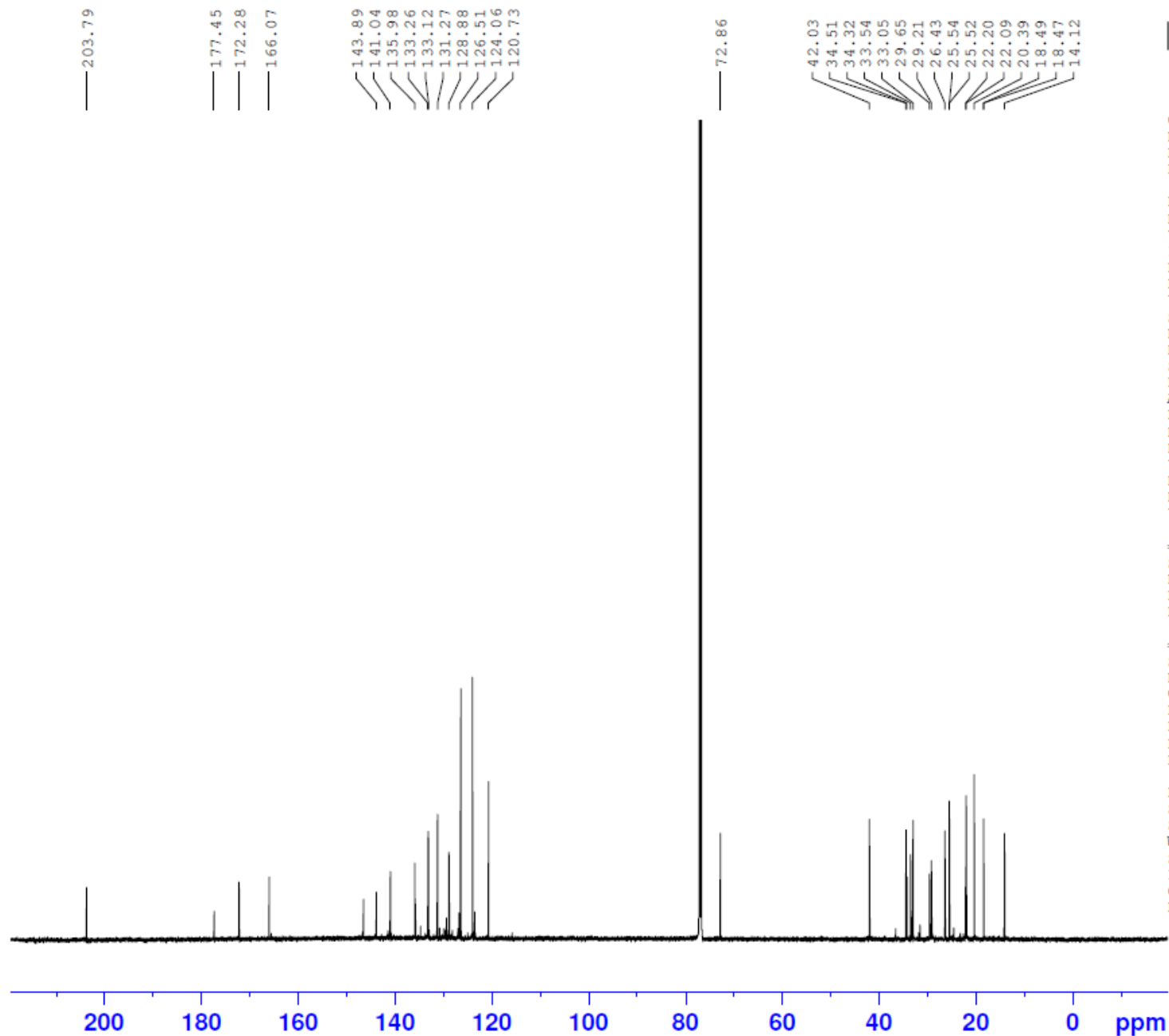
Current Data Parameters
 NAME 20200402 p-NO2 PI
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200402
 Time_ 17.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 322
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300261 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





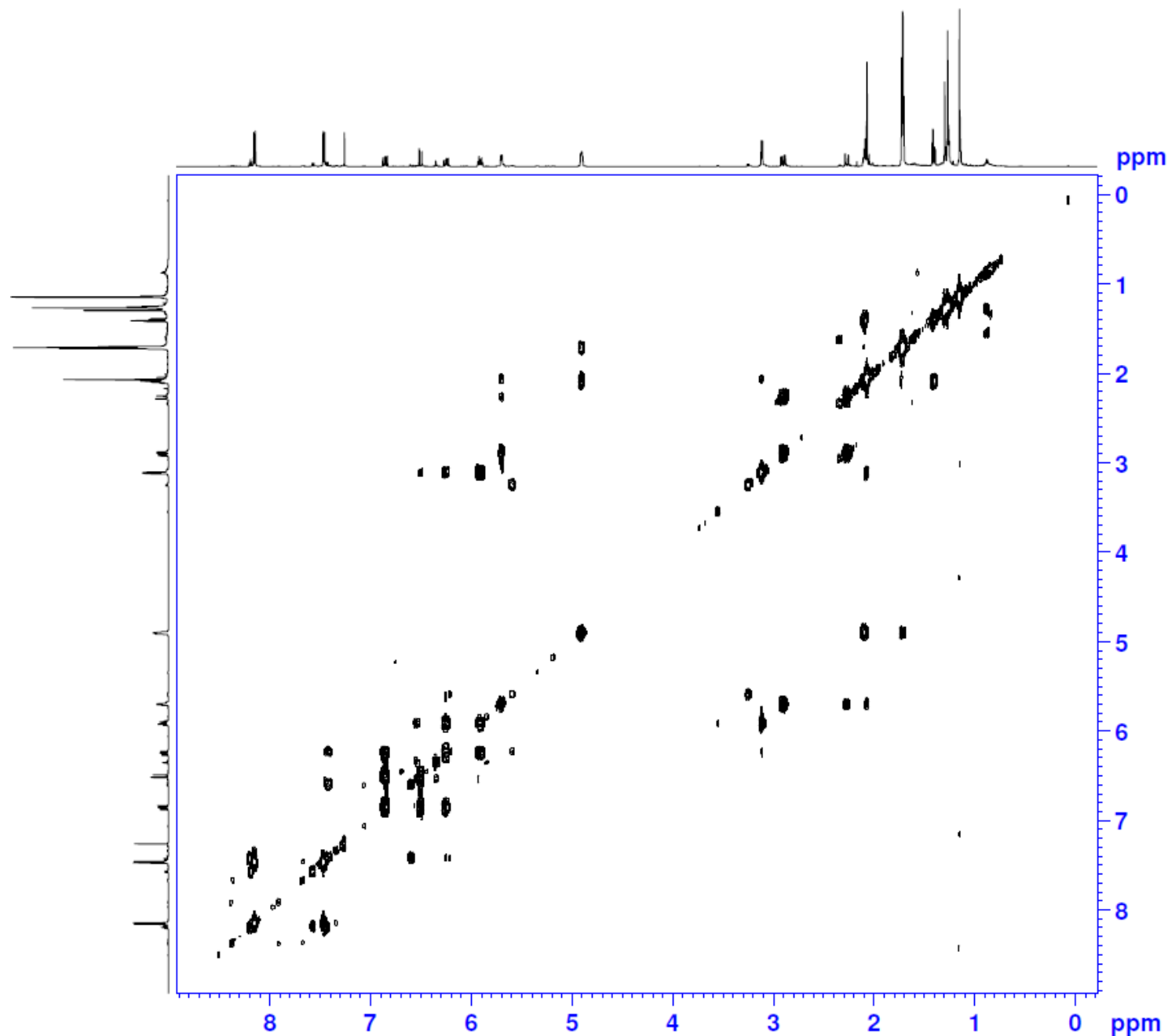
Current Data Parameters
 NAME 20200324 PI p-NO2 Hec
 EXPNO 62
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200324
 Time 21.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 ID 65536
 SOLVENT CDCl3
 NS 4096
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028151 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200324 PI p-NO2 Heck
EXPNO 61
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200324
Time 17.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 5494.505 Hz
FIDRES 2.682864 Hz
AQ 0.1863680 sec
RG 64
DW 91.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.94142699 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00018200 sec

----- CHANNEL f1 -----
SFO1 600.1326379 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1326 MHz
FIDRES 42.925823 Hz
SW 9.155 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300253 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300233 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0



Current Data Parameters
NAME 20200324 F1 p-NO2 Heck
EXPNO 64
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200324
Time 21.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 5494.505 Hz
FIDRES 5.365728 Hz
AQ 0.0931840 sec
RG 2050
DW 91.000 usec
DE 6.50 usec
TE 298.4 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.47235203 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1326379 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PIN1 17.00000000 W

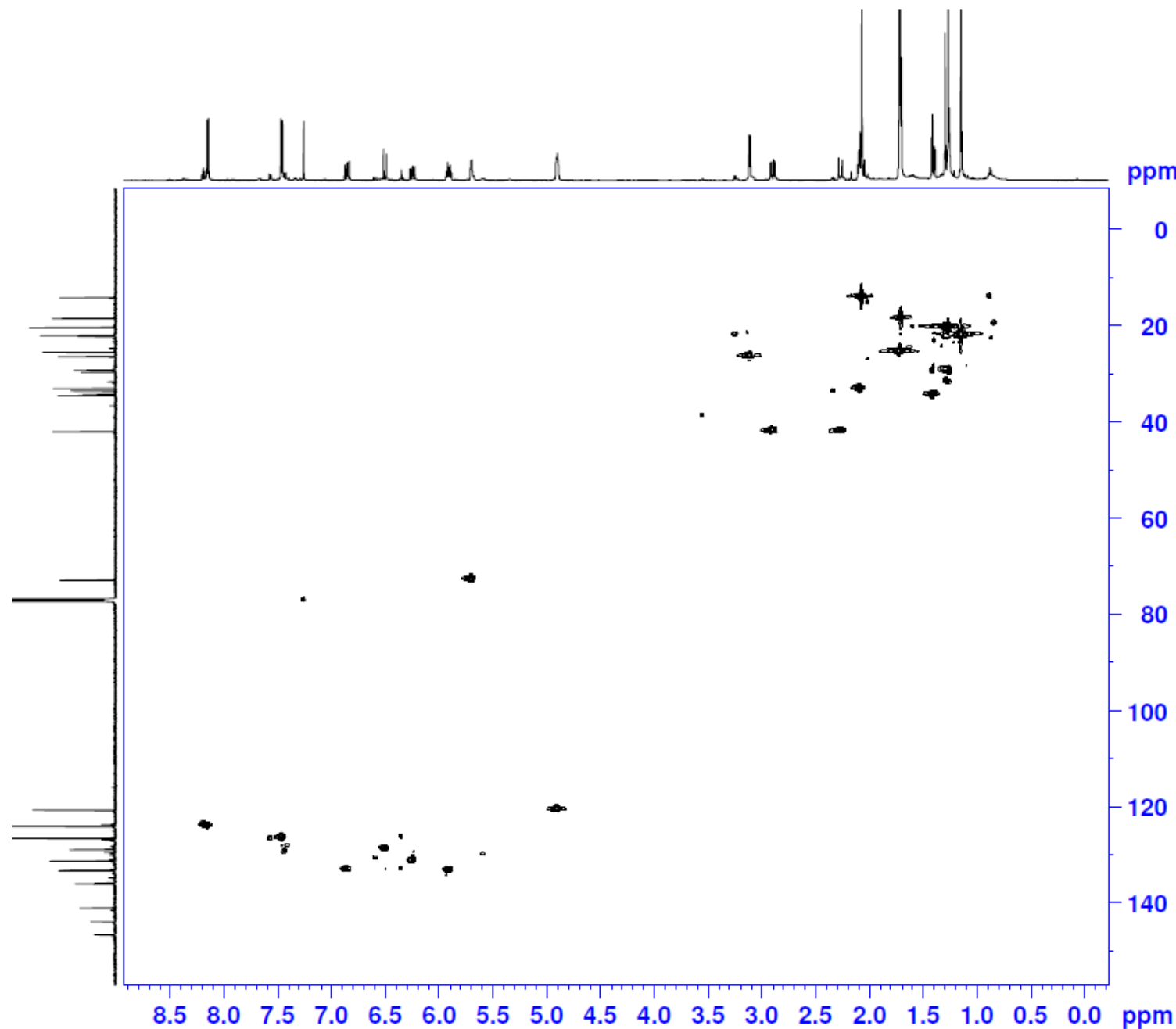
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PIN2 79.98300171 W
PIN12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GFZ1 80.00 %
GFZ2 20.10 %
F16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

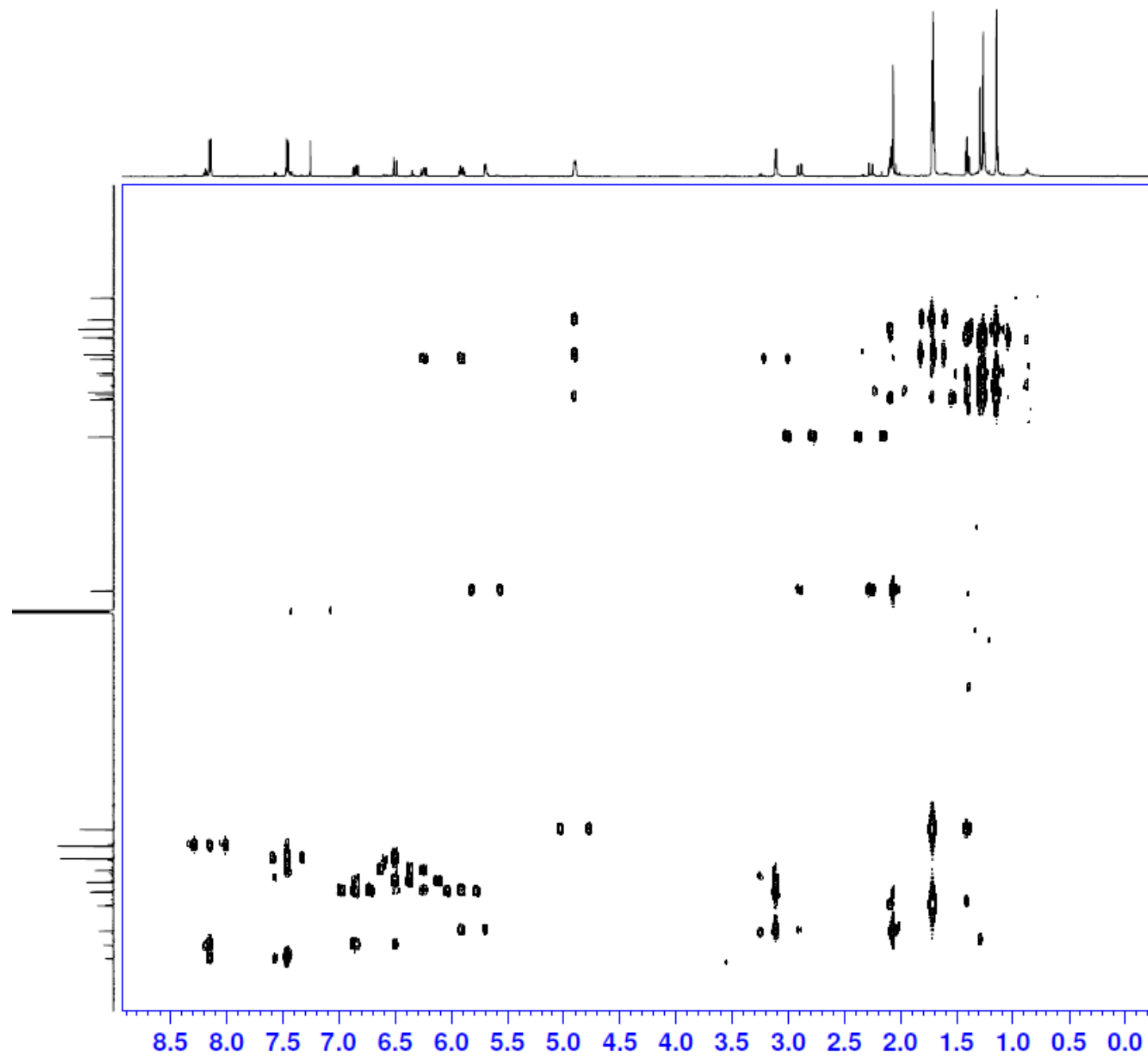
F2 - Processing parameters
SI 1024
SF 600.1300252 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028521 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200324 F1 p-NO2 Heck
EXPNO 65
PROCNO 1



F2 - Acquisition Parameters
Data_ 20200325
Time 3.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 5494.505 Hz
FIDRES 1.341432 Hz
AQ 0.3727360 sec
RG 2050
DW 91.000 usec
DE 6.50 usec
TE 298.2 K
CNS113 8.0000000
D0 0.00000300 sec
D1 1.38285398 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

==== CHANNEL F1 =====
SFO1 600.1326379 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

==== CHANNEL F2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

==== GRADIENT CHANNEL =====
GPNAM[1] SMSq10.100
GPNAM[2] SMSq10.100
GPNAM[3] SMSq10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300240 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

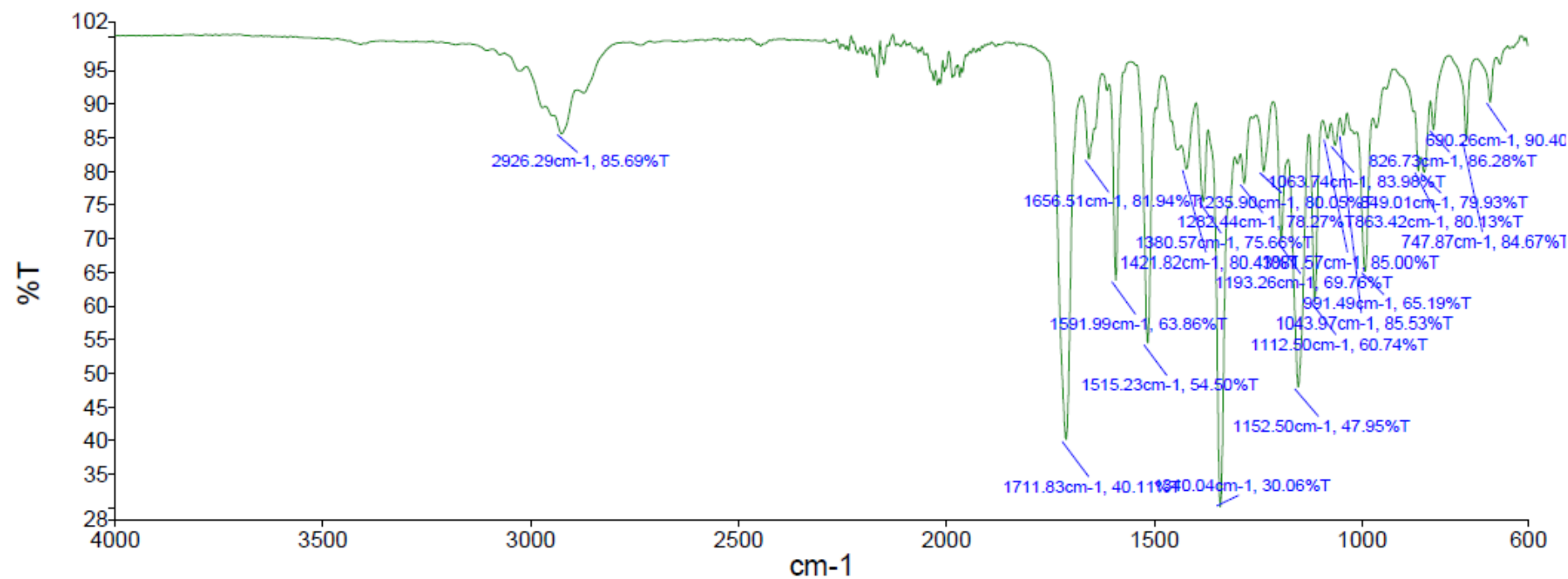
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028362 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

129a IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Thursday, 11 June 2020 5:10 PM

Analyst
Date

Analyst
Thursday, 11 June 2020 5:10 PM



Sample Name	Description	Quality Checks
4NO2 I E	Sample	The Quality Checks do not report any warnings for the sample.

129b NMR Characterisation

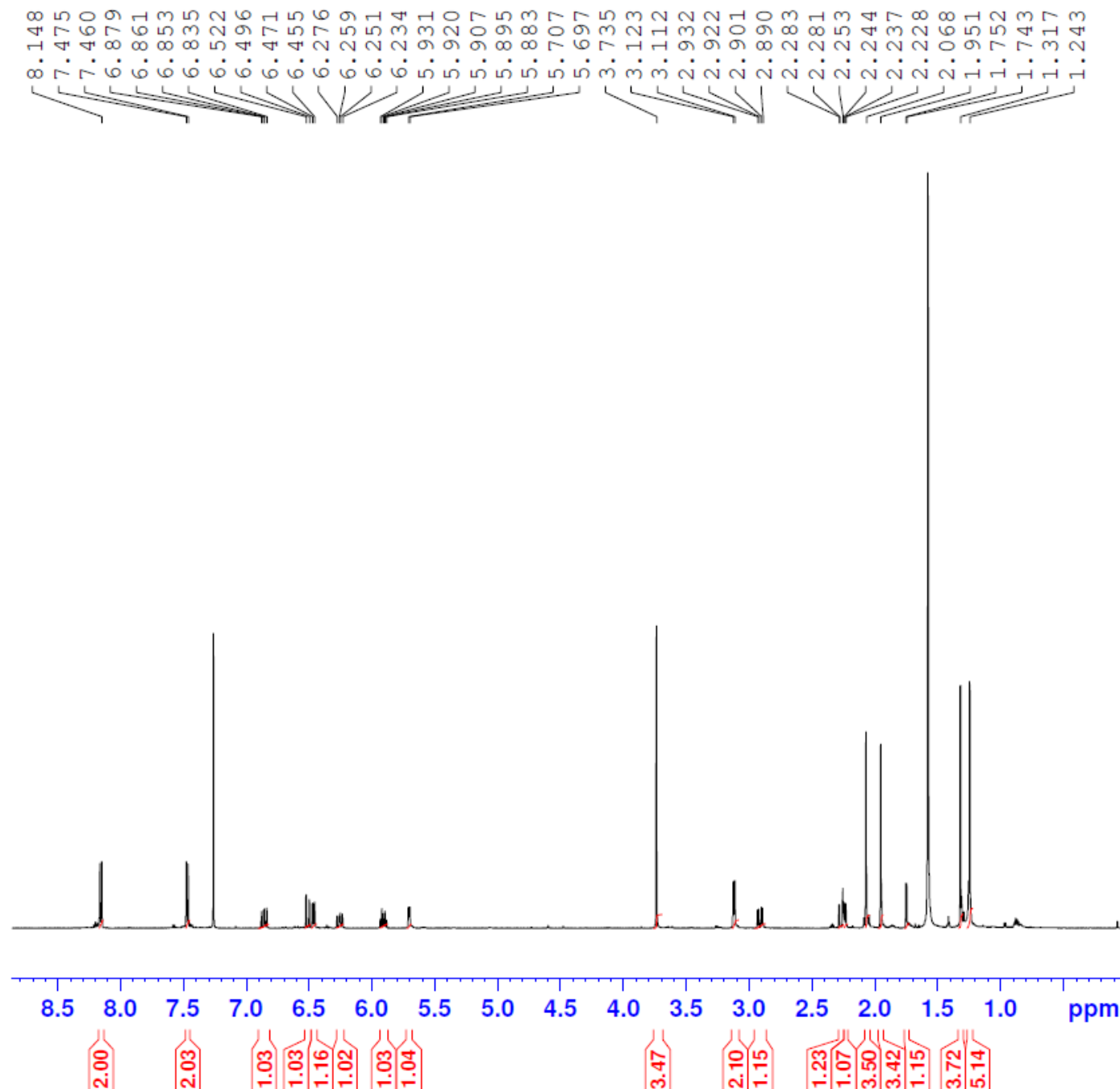


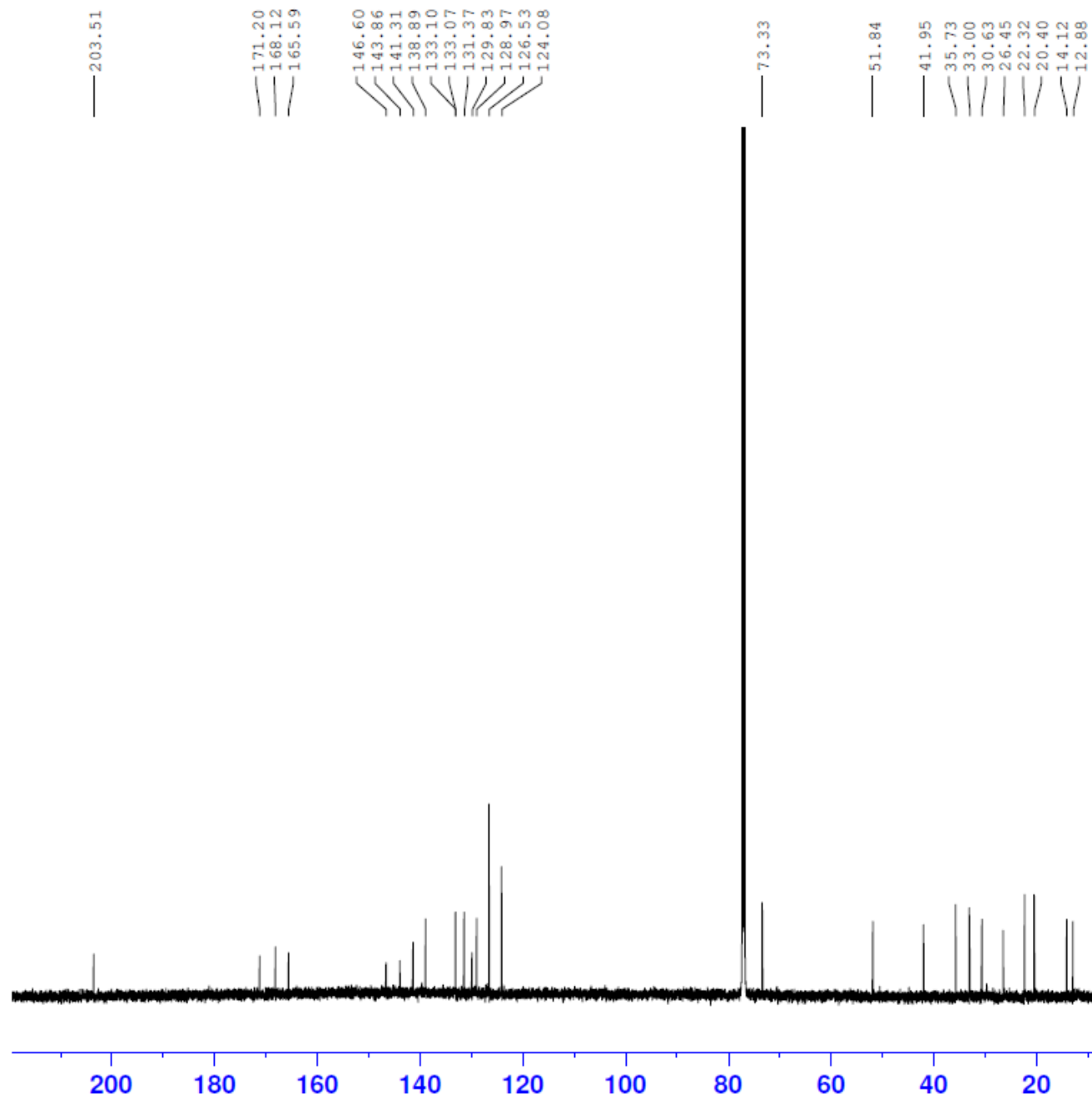
Current Data Parameters
NAME 20200403 p-NO2 II
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200405
Time 10.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 322
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
 NAME 20200403 p-NO2 II
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200405
 Time 15.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 5120
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028140 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200403 p-NO2 II
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200405
Time 10.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppgf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 5319.149 Hz
FIDRES 2.597241 Hz
AQ 0.1925120 sec
RG 161
DW 94.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.93528295 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00018800 sec

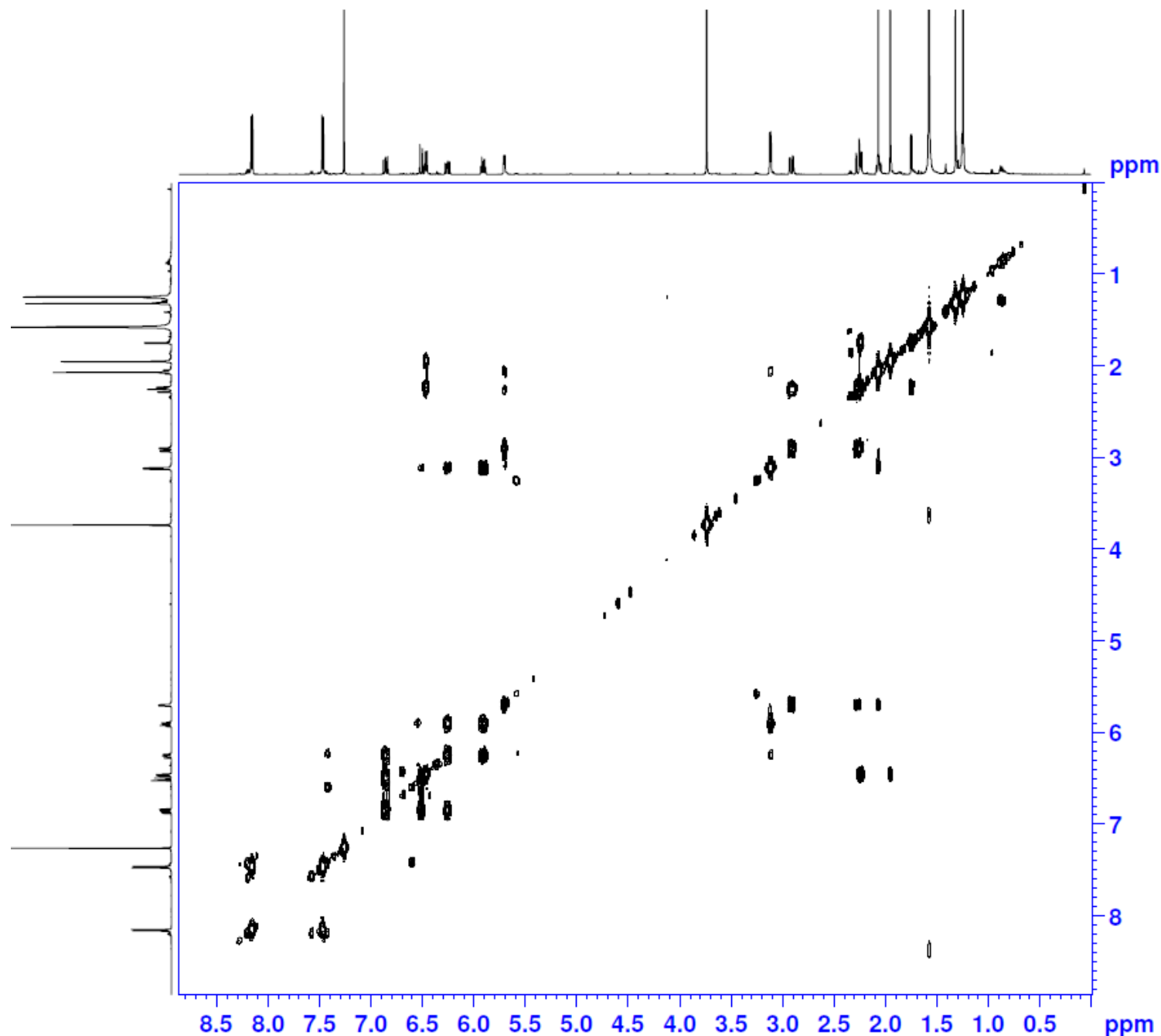
----- CHANNEL f1 -----
SFO1 600.1326853 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1327 MHz
FIDRES 41.555851 Hz
SW 8.863 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300260 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300259 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200403 p-No2 11
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200405
Time 15.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 5263.158 Hz
FIDRES 5.139802 Hz
AQ 0.0972800 sec
RG 2050
LW 95.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46825600 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS

===== CHANNEL f1 =====
SFO1 600.1327035 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

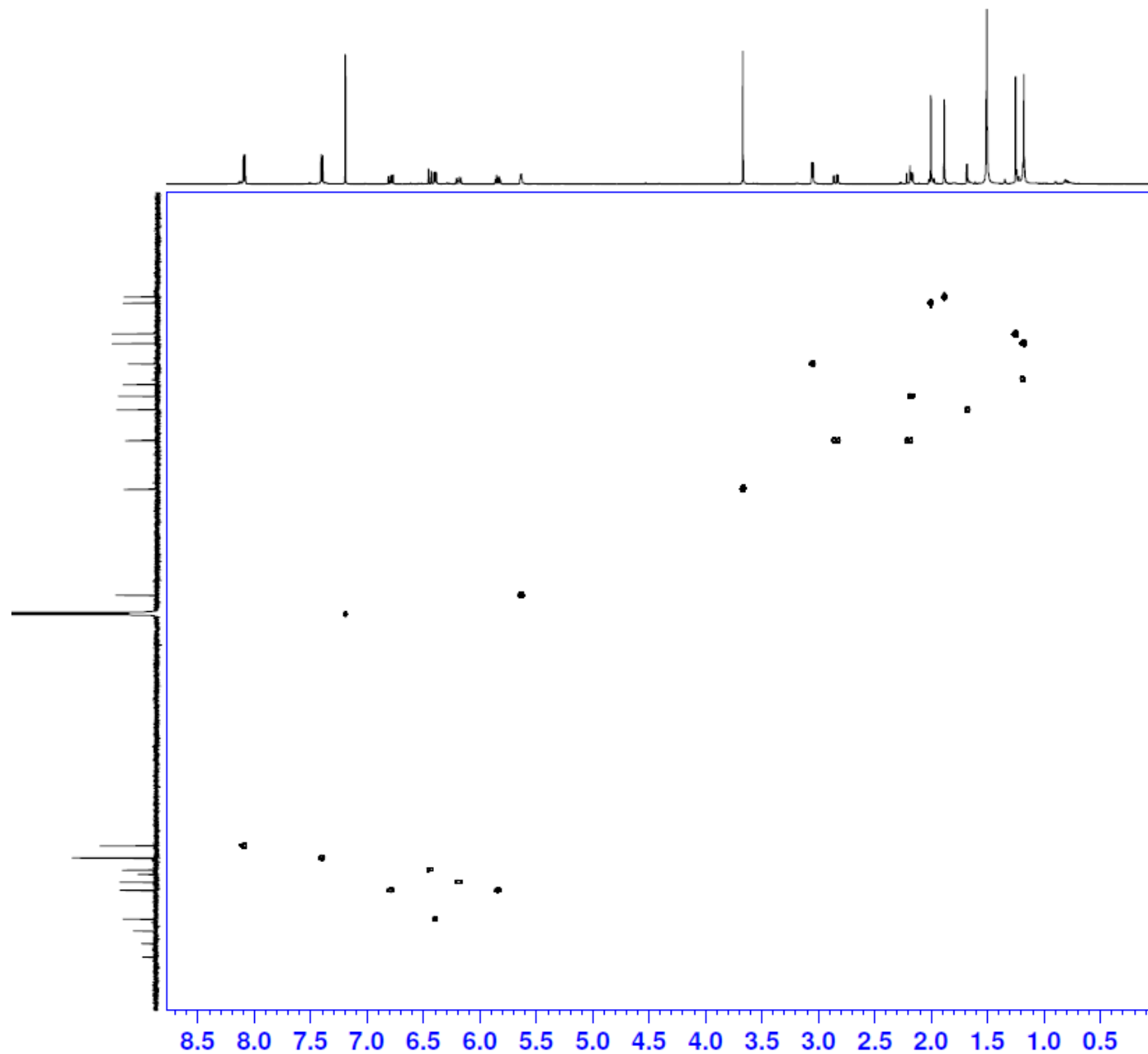
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPE1 80.00 %
GPE2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300667 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200403 p-NO2 II
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Data_ 20200405
Time 21.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmcgpnqf
TD 4096
SOLVENT CDCl3
NS 50
DS 16
SWH 5263.158 Hz
FIDRES 1.284951 Hz
AQ 0.3891200 sec
RG 2050
DW 95.000 usec
DE 6.50 usec
TE 298.1 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.36646998 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

==== CHANNEL f1 =====
SFO1 600.1327035 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

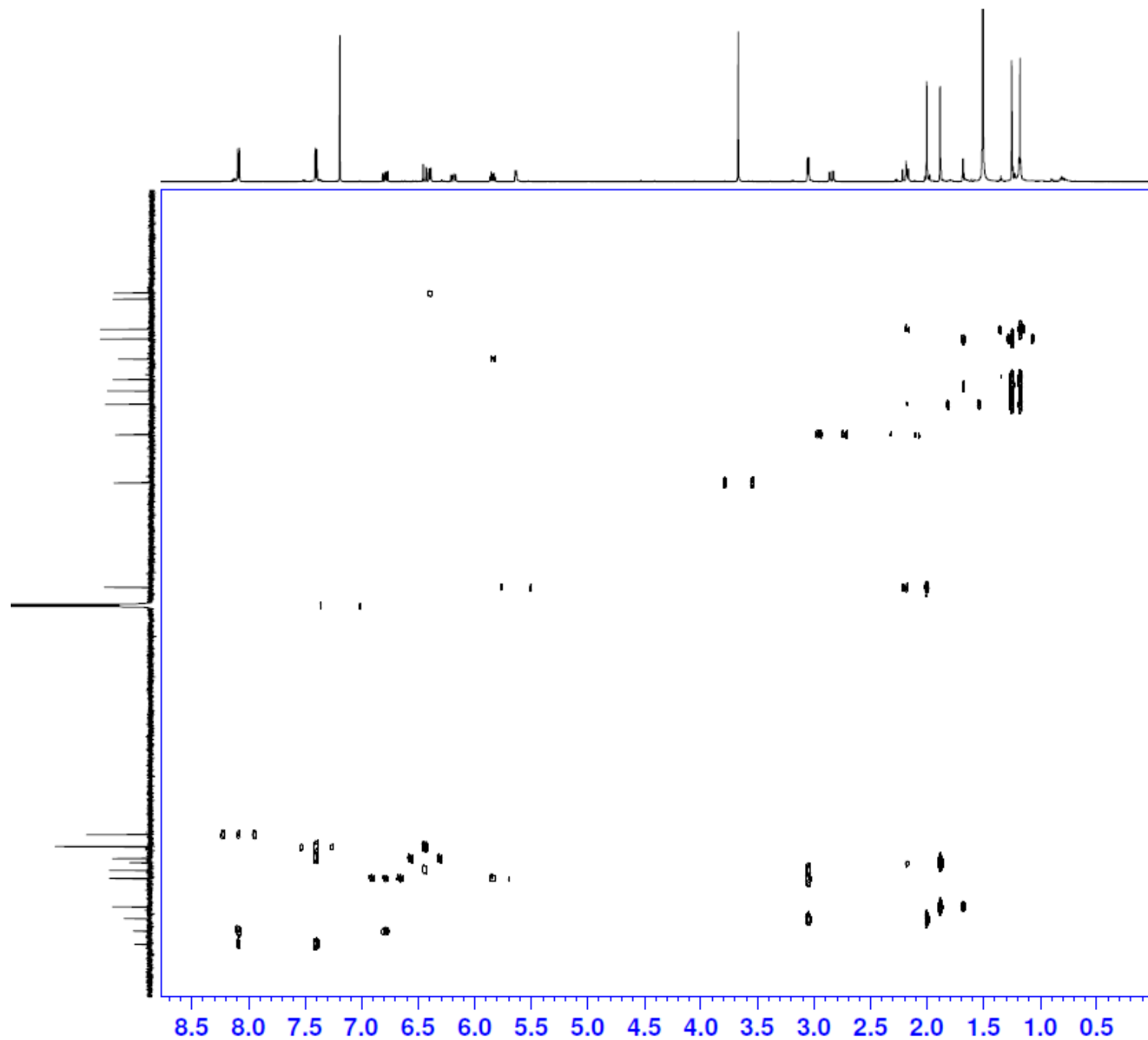
==== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

==== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300667 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

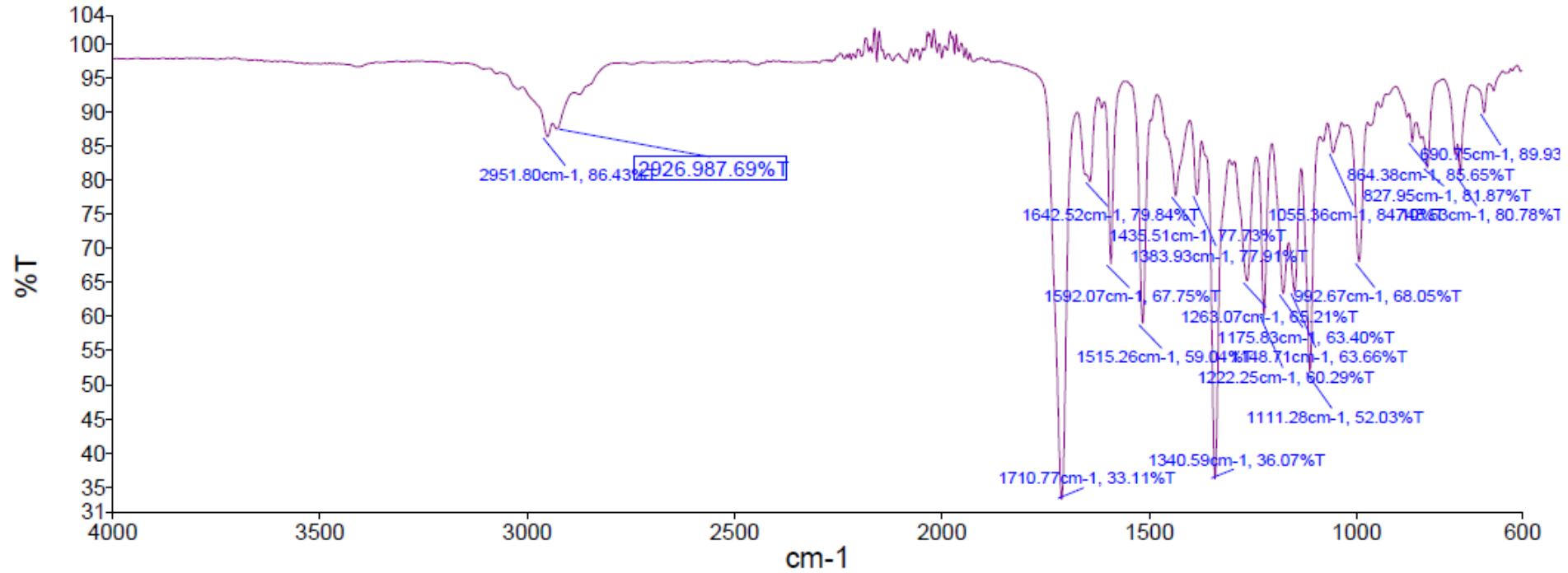


129b IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Thursday, 11 June 2020 5:16 PM

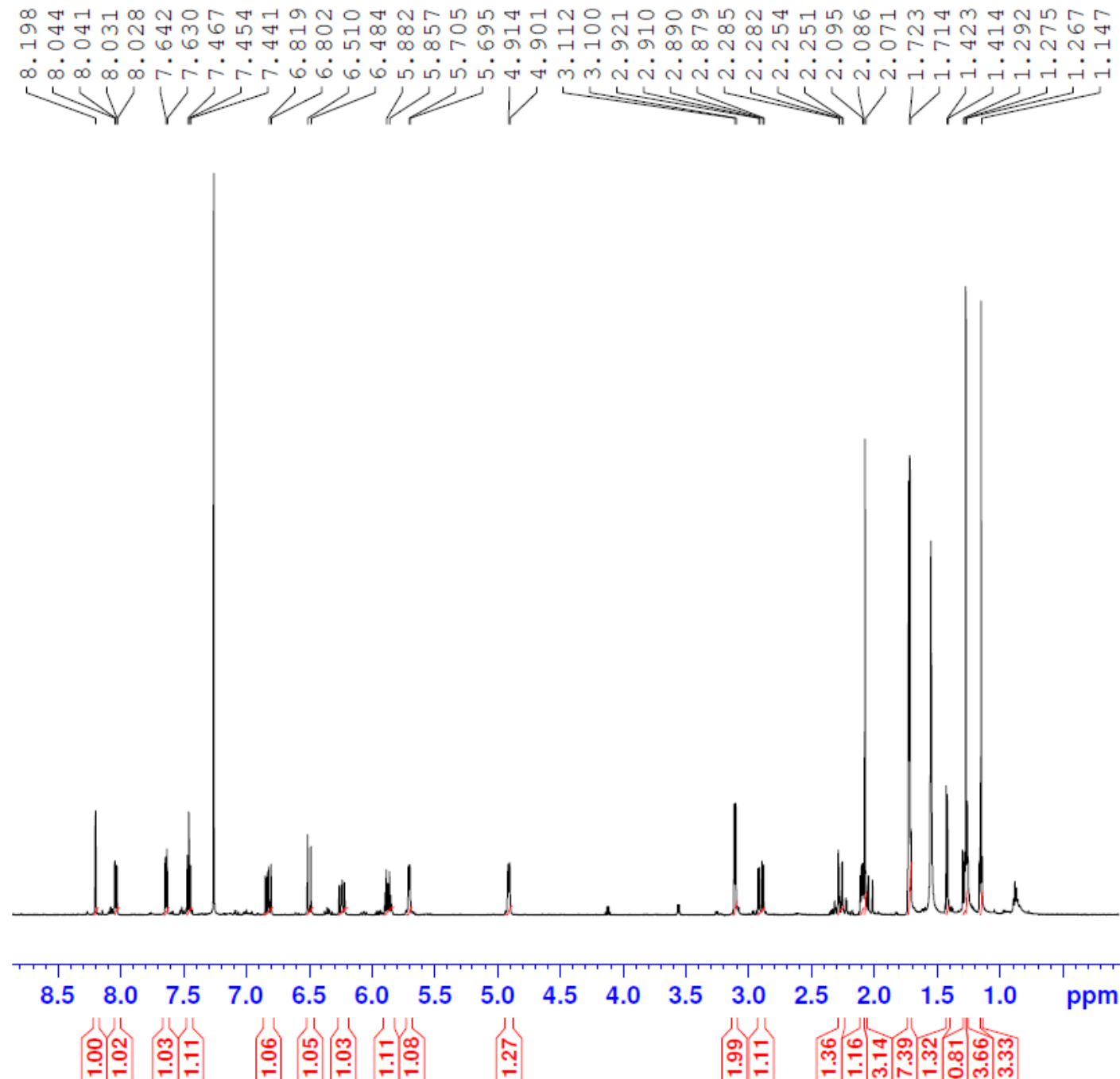
Analyst
Date

Analyst
Thursday, 11 June 2020 5:16 PM



Sample Name	Description	Quality Checks
4NO2 II E	Sample	The Quality Checks do not report any warnings for the sample.

¹³0a NMR Characterisation

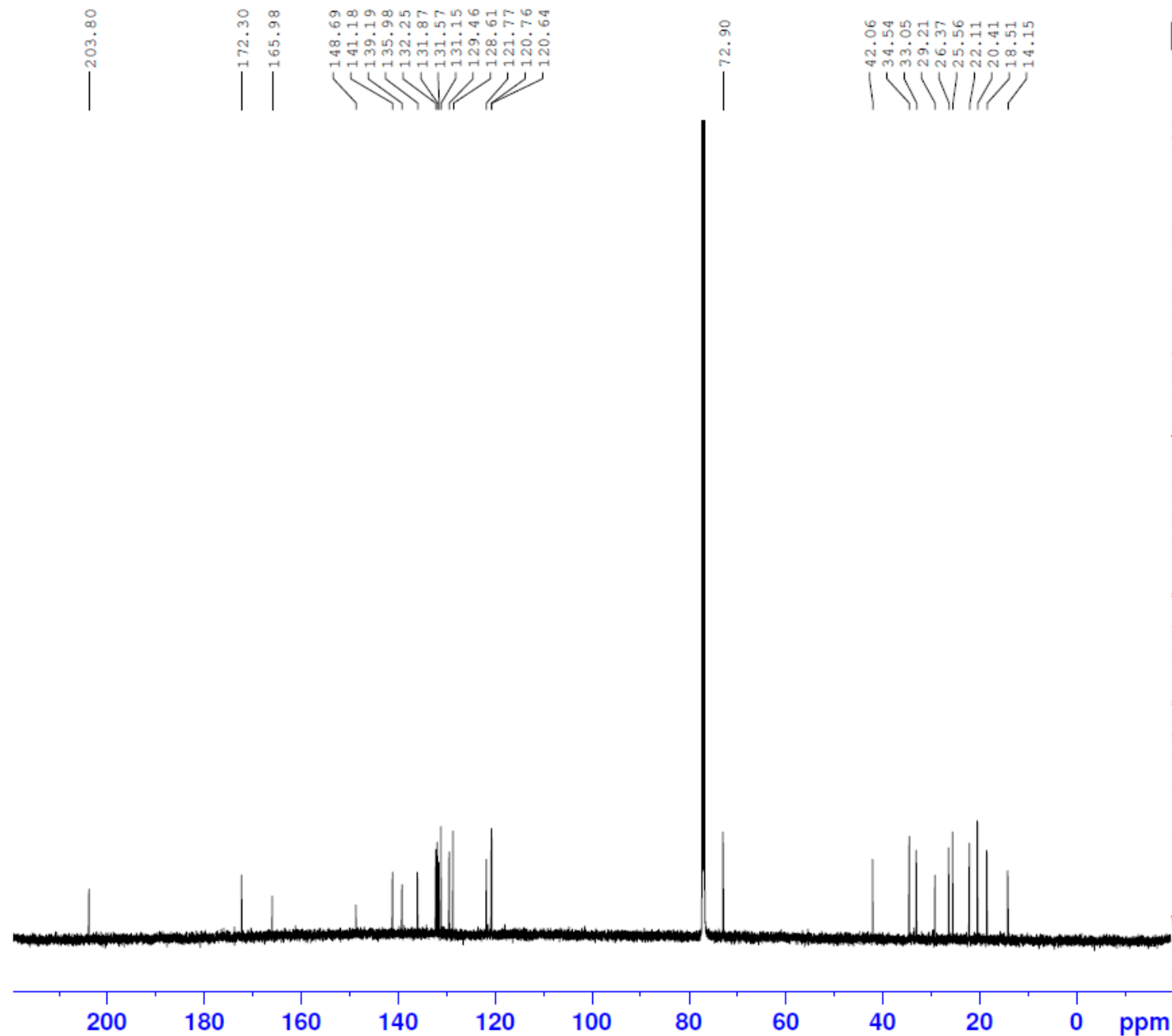


Current Data Parameters
NAME 20200608 3NO2 I E
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200608
Time 14.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 322
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300278 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



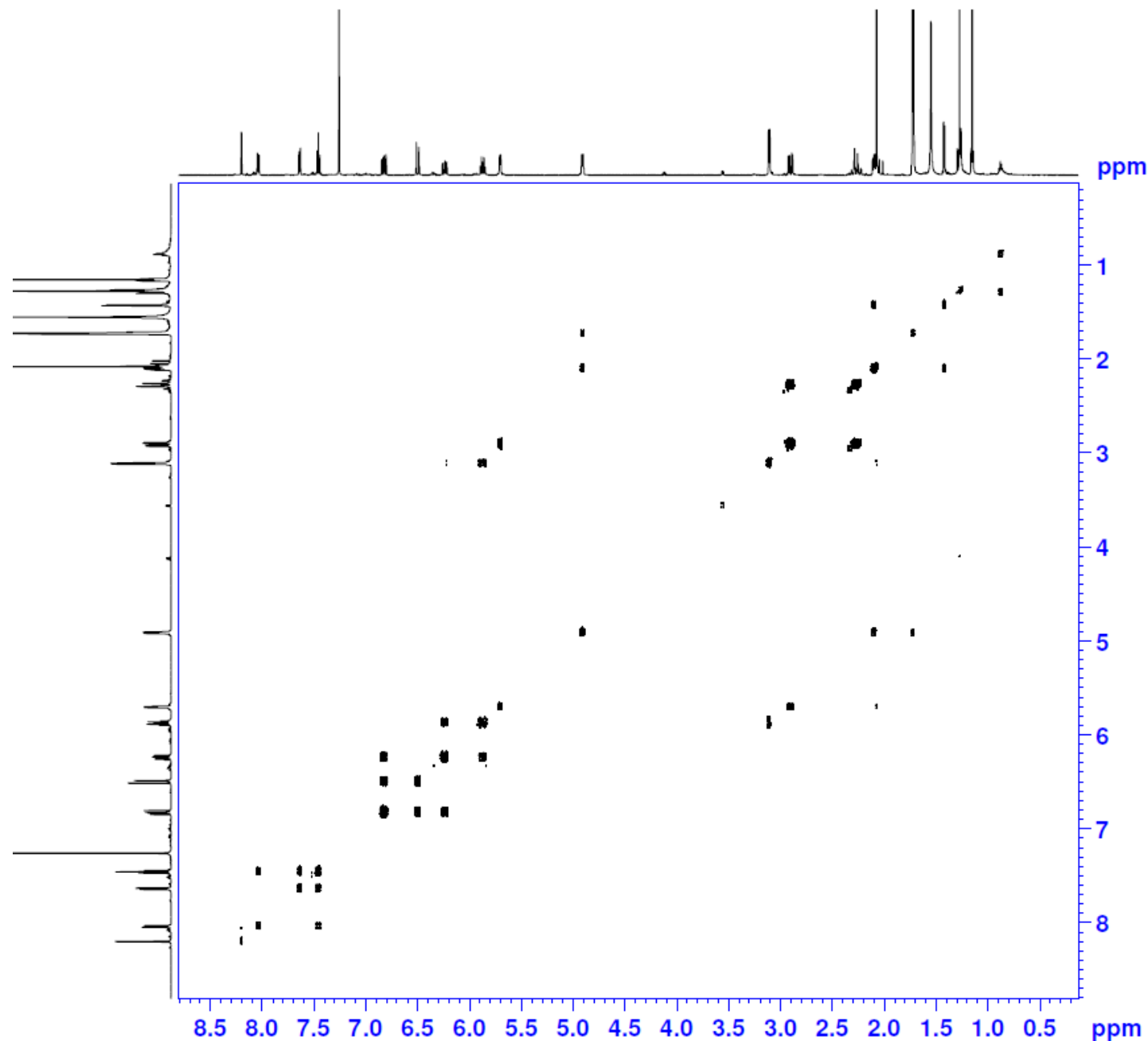
Current Data Parameters
 NAME 20200608 3NO2 I E
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200608
 Time 21.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8000
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028123 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200608 3NO2 I E
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200608
Time 14.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 3
DS 4
SWH 5208.333 Hz
FIDRES 2.543132 Hz
AQ 0.1966080 sec
RG 2050
DW 96.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00007881 sec
D1 1.94183695 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
INO 0.00019200 sec

----- CHANNEL f1 -----
SFO1 600.1327068 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1327 MHz
FIDRES 20.345053 Hz
SW 8.679 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300282 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300273 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



Current Data Parameters
NAME 20200608 3no2 1 E
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200608
Time 21.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 5154.639 Hz
FIDRES 5.033827 Hz
AQ 0.0993280 sec
RG 2050
DW 97.000 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46620798 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1326998 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

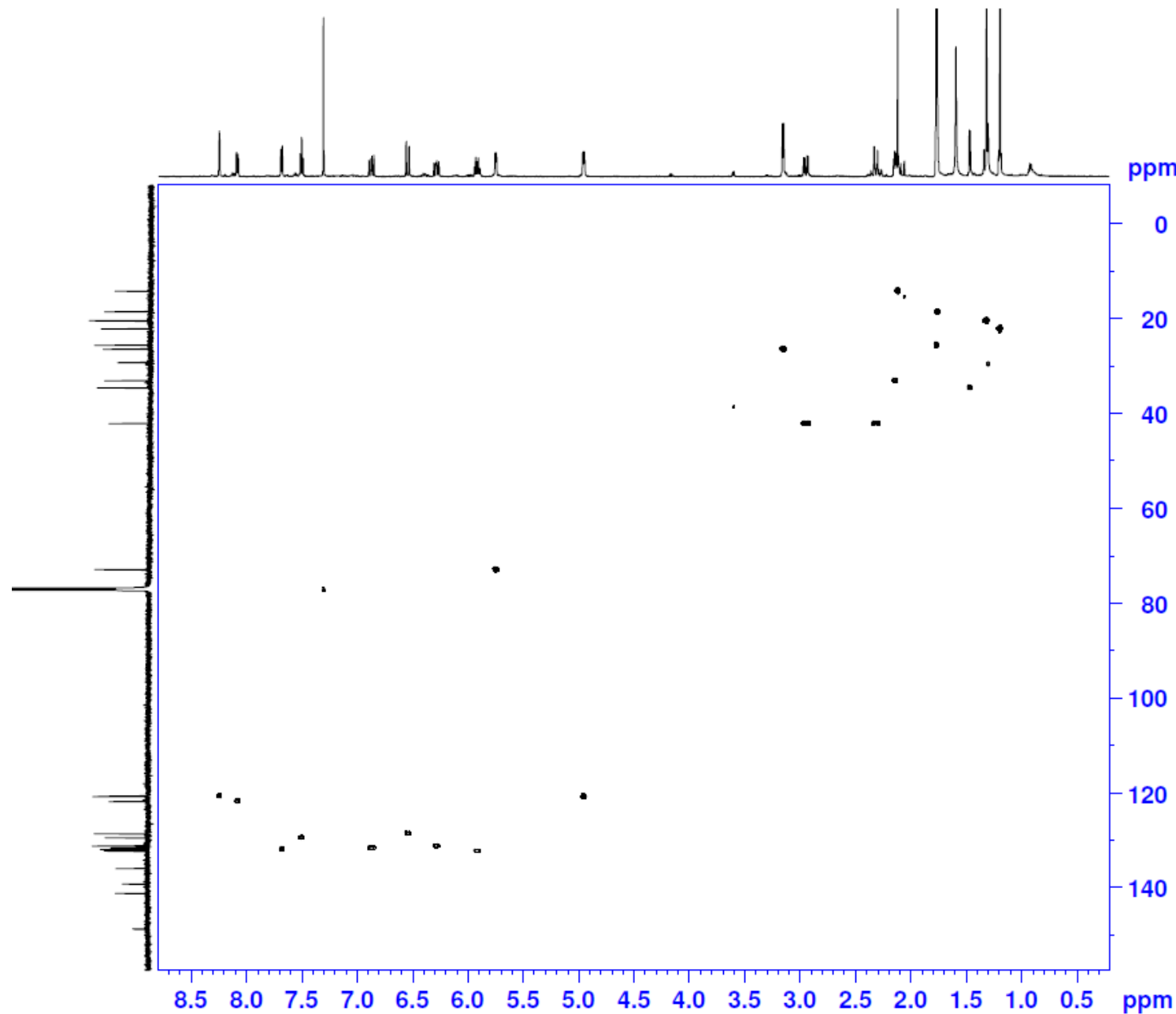
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FMODE Echo-Antiecho

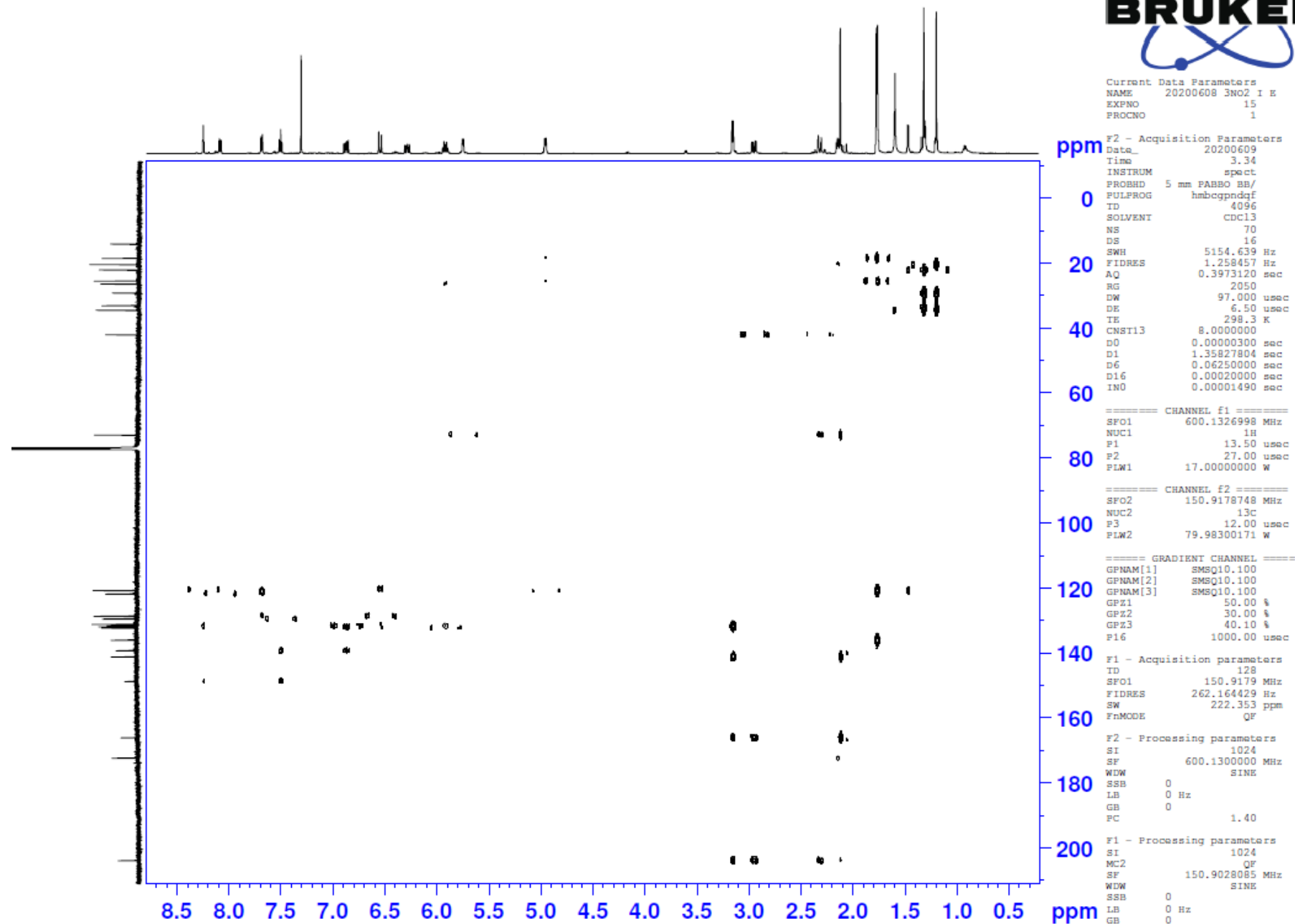
F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200608 3NO2 I E
EXPNO 15
PROCNO 1

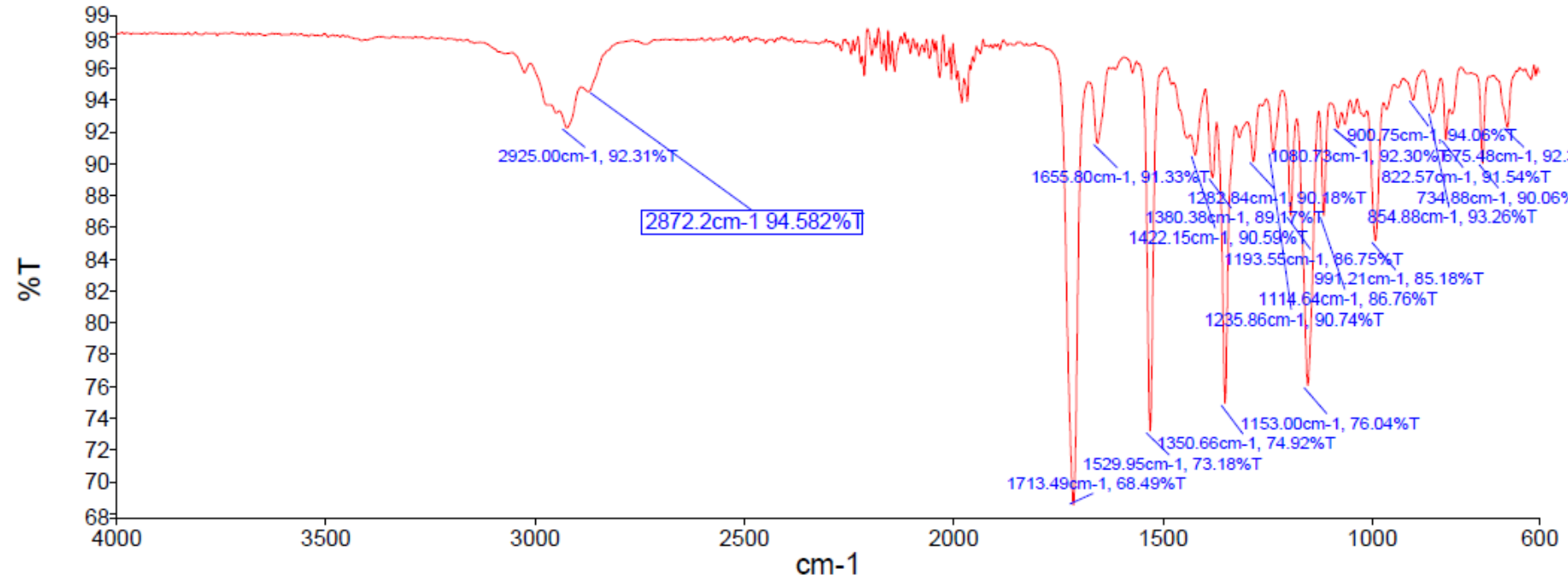


130a IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 12 June 2020 10:59 AM

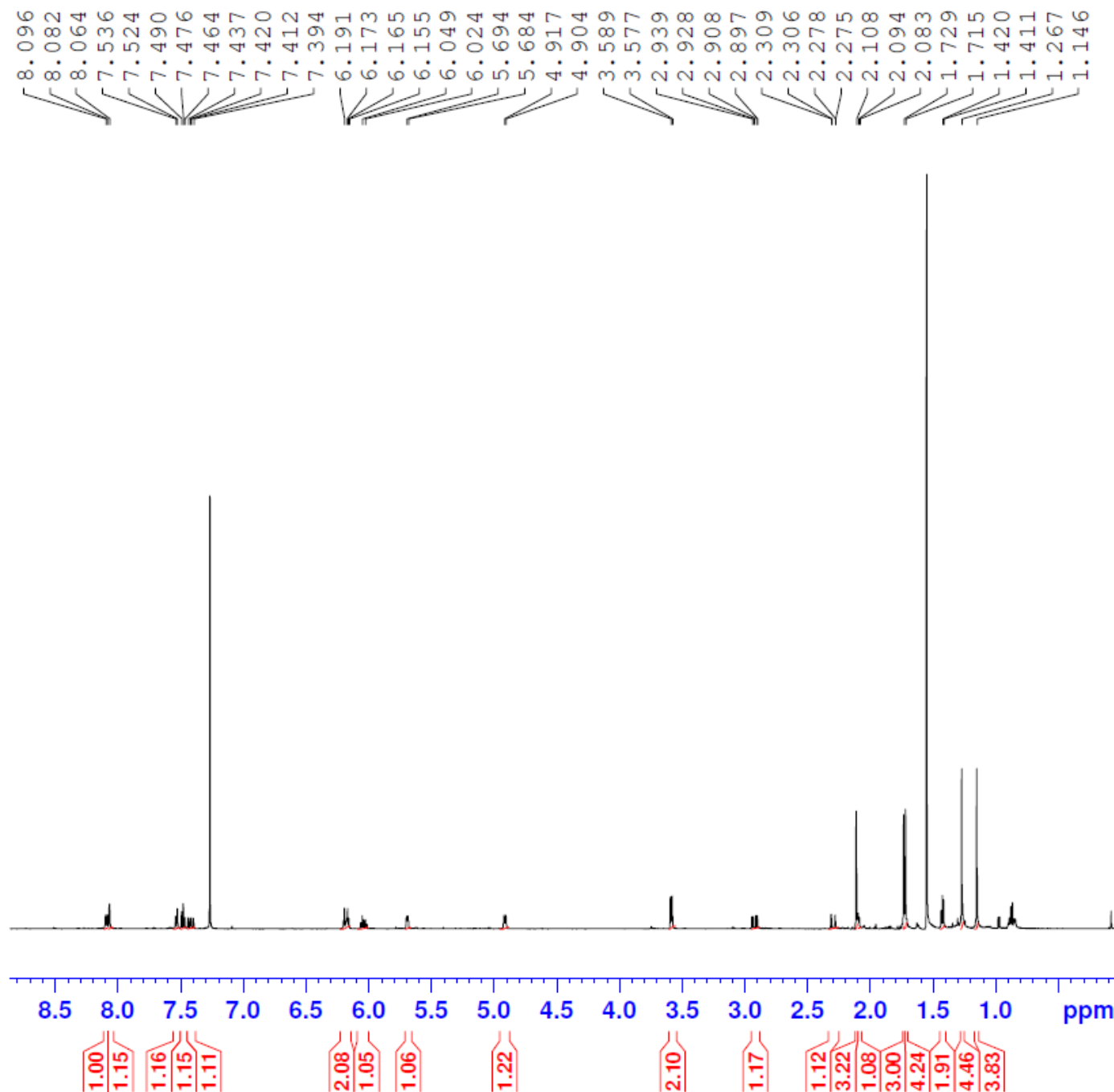
Analyst
Date

Analyst
Friday, 12 June 2020 10:59 AM



Sample Name	Description	Quality Checks
3NO2 I E	Sample	The Quality Checks do not report any warnings for the sample.

¹³⁵a NMR Characterisation

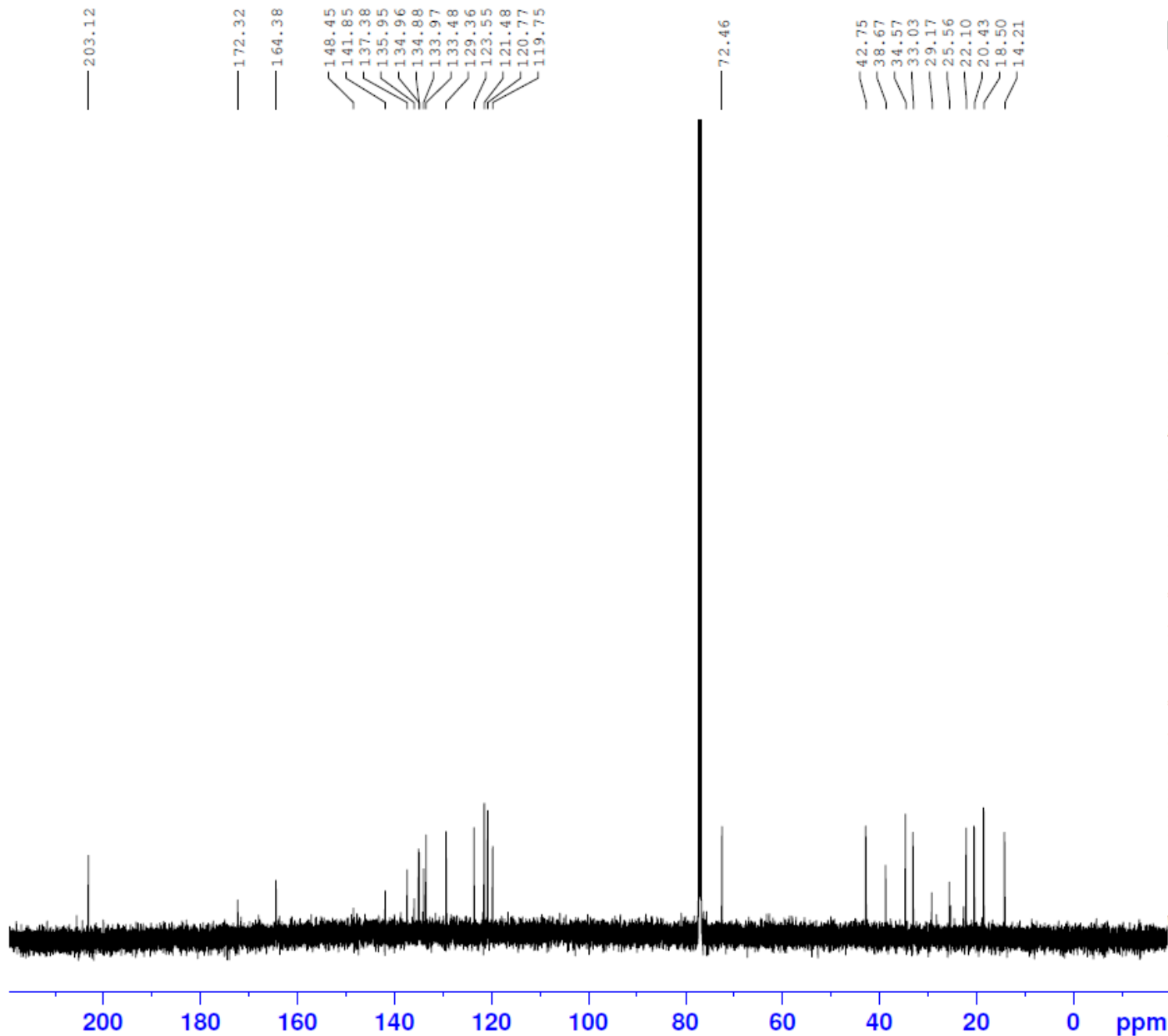


Current Data Parameters
NAME 20200605 3NO2 I mig
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200605
Time 17.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 362
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300236 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



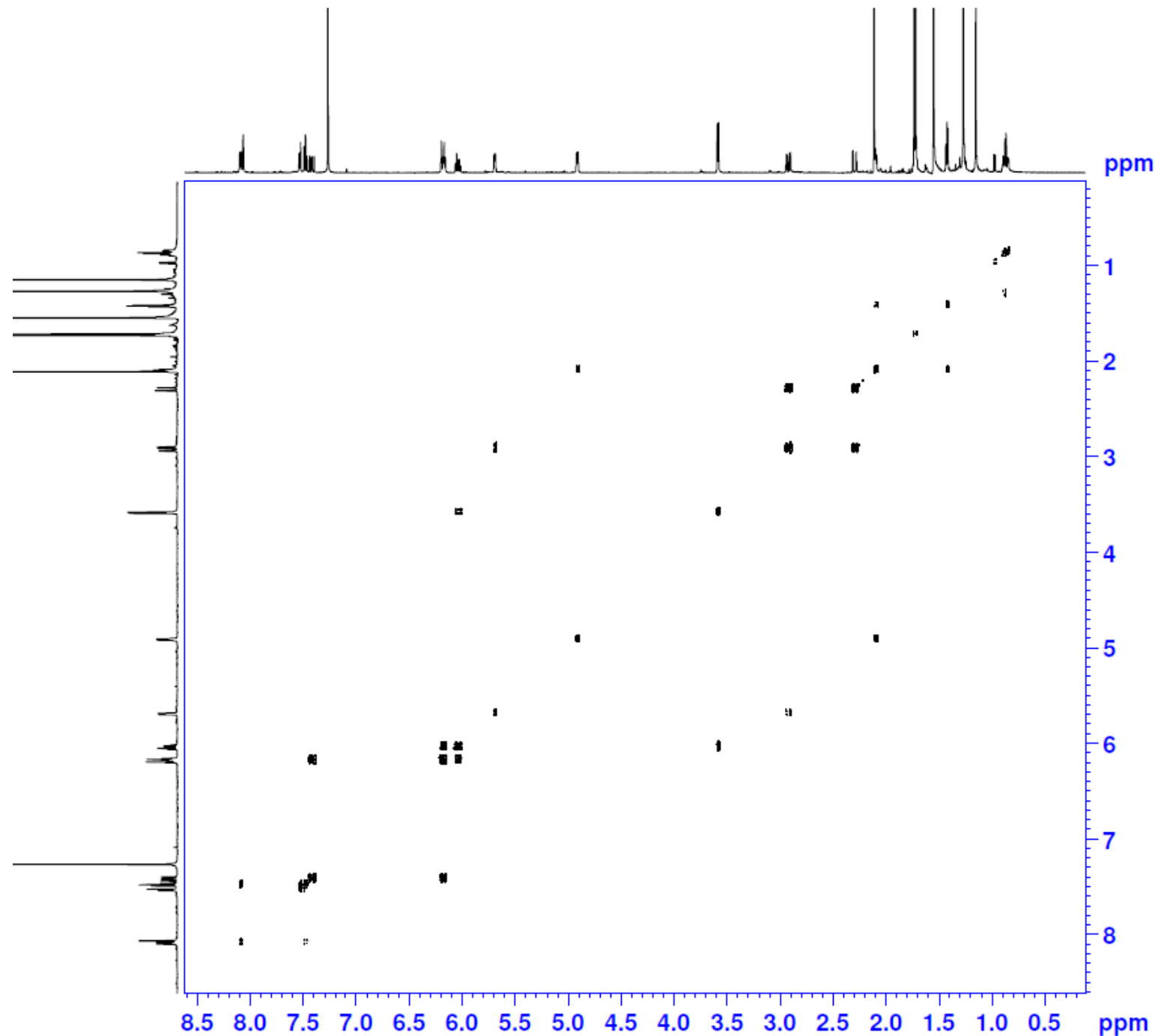
Current Data Parameters
 NAME 20200605 3NO2 I mig
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200606
 Time 1.02
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8000
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028128 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40



ppm

1

2

3

4

5

6

7

8

ppm

Current Data Parameters
NAME 20200605 3No2 I mig
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200605
Time 17.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
ID 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 5102.041 Hz
FIDRES 2.491231 Hz
AQ 0.2007040 sec
RG 2050
RW 98.000 usec
DE 6.50 usec
TE 298.1 K
D0 0.00008081 sec
D1 1.93774104 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00019600 sec

----- CHANNEL f1 -----
SFO1 600.1326455 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 256
SFO1 600.1326 MHz
FIDRES 19.929848 Hz
SW 8.502 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300264 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300254 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



Current Data Parameters
NAME 20200605 3no2 1 mig
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200606
Time 1.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDC13
NS 40
DS 16
SWH 5102.041 Hz
FIDRES 4.982462 Hz
AQ 0.1003520 sec
RG 2050
DW 98.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46518397 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPTNS

===== CHANNEL f1 =====
SFO1 600.1326455 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

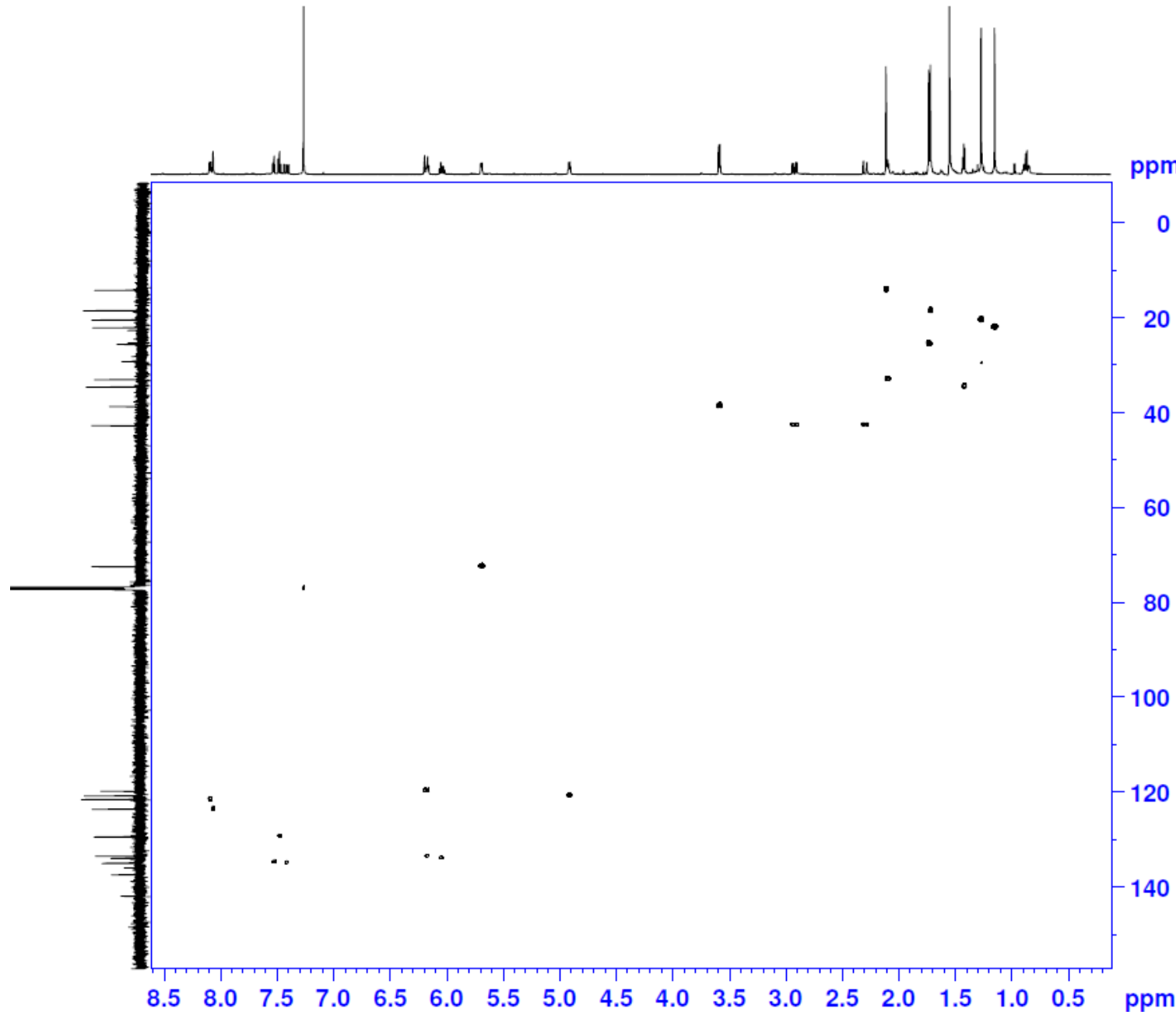
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300256 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028423 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200605 3NO2 1 mig
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Data_ 20200606
Time 5.38

INSTRUM spect
PROBHD 5 mm PABBO BB/
FULPROG hmbcgpndqf
TD 4096
SOLVENT cdcl3
NS 60
DS 16
SWH 5102.041 Hz
FIDRES 1.245615 Hz
AQ 0.4014080 sec
RG 2050
DW 98.000 usec
DE 6.50 usec
TE 298.0 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.35418200 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1326455 MHz
NUC1 1H
P1 13.50 usec
F2 27.00 usec
PLW1 17.00000000 W

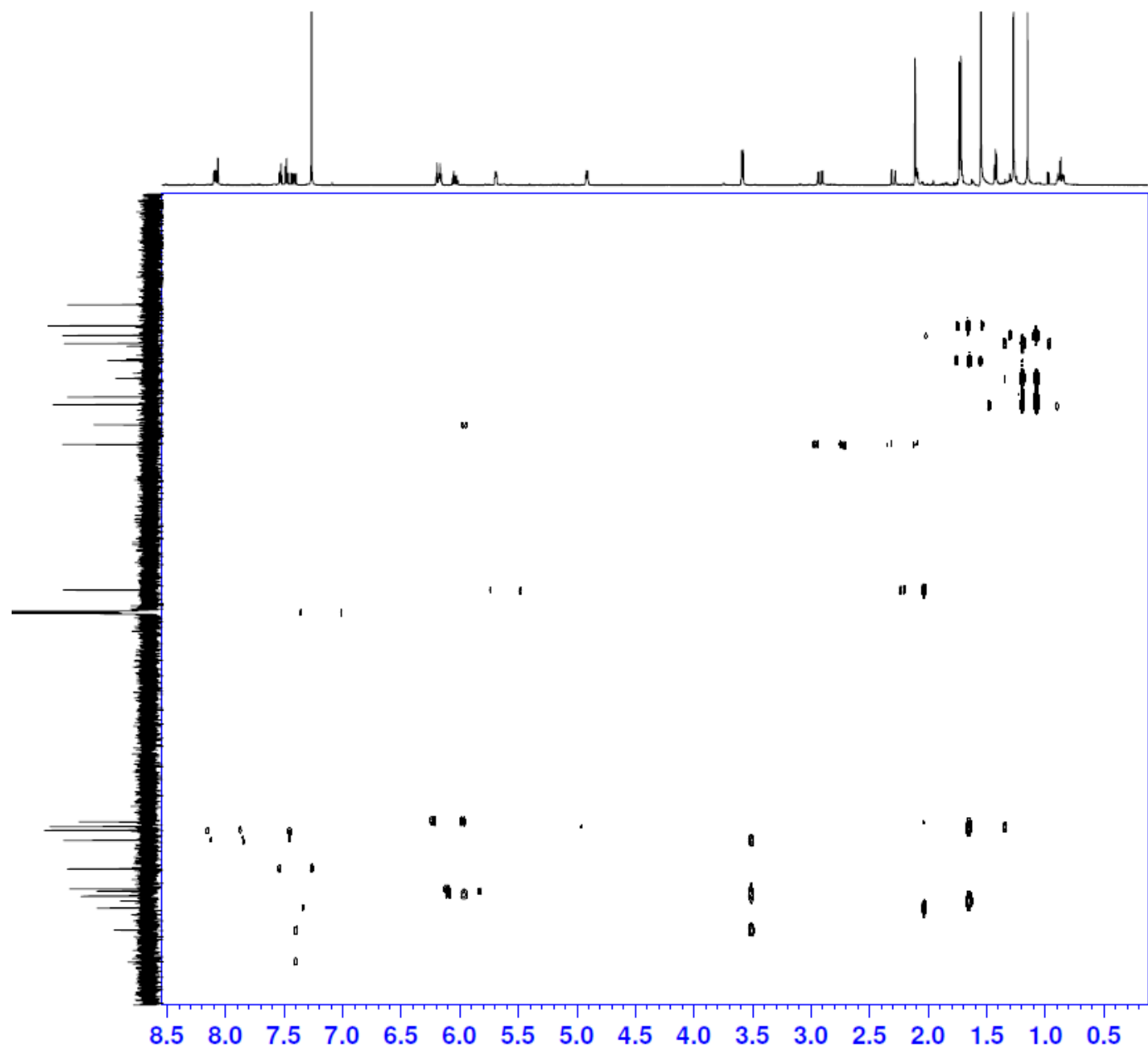
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300676 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

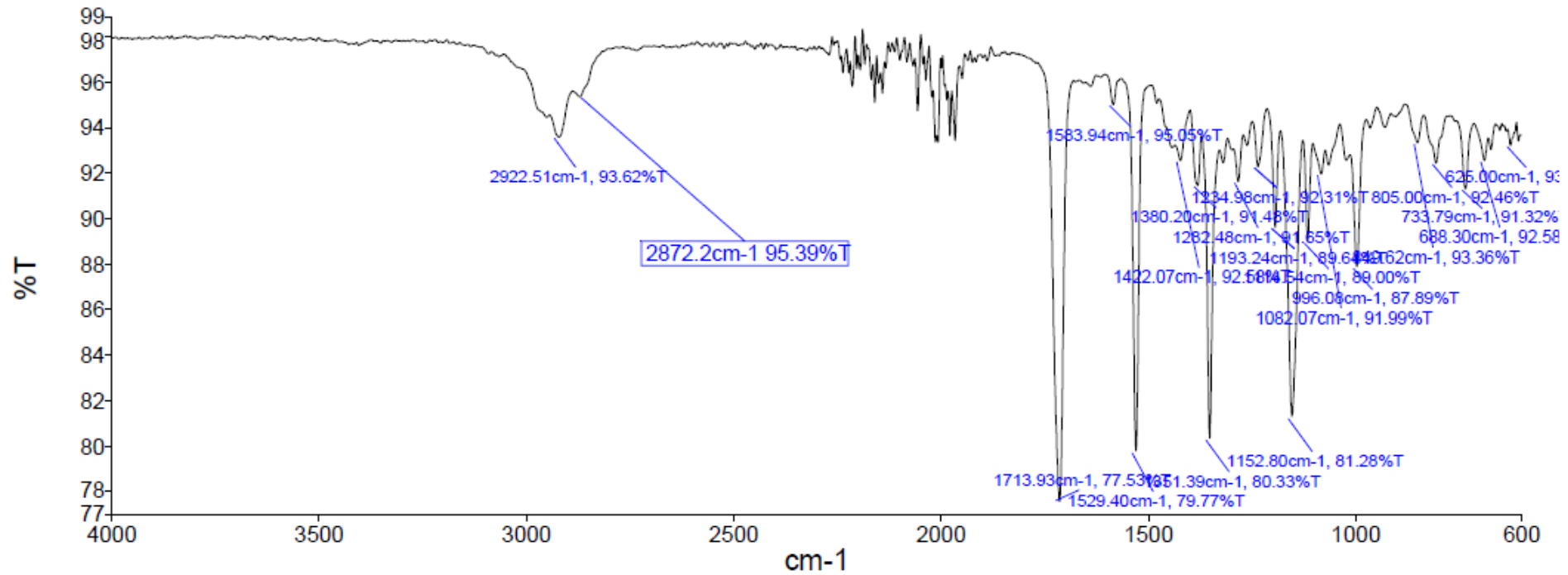


135a IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 12 June 2020 10:57 AM

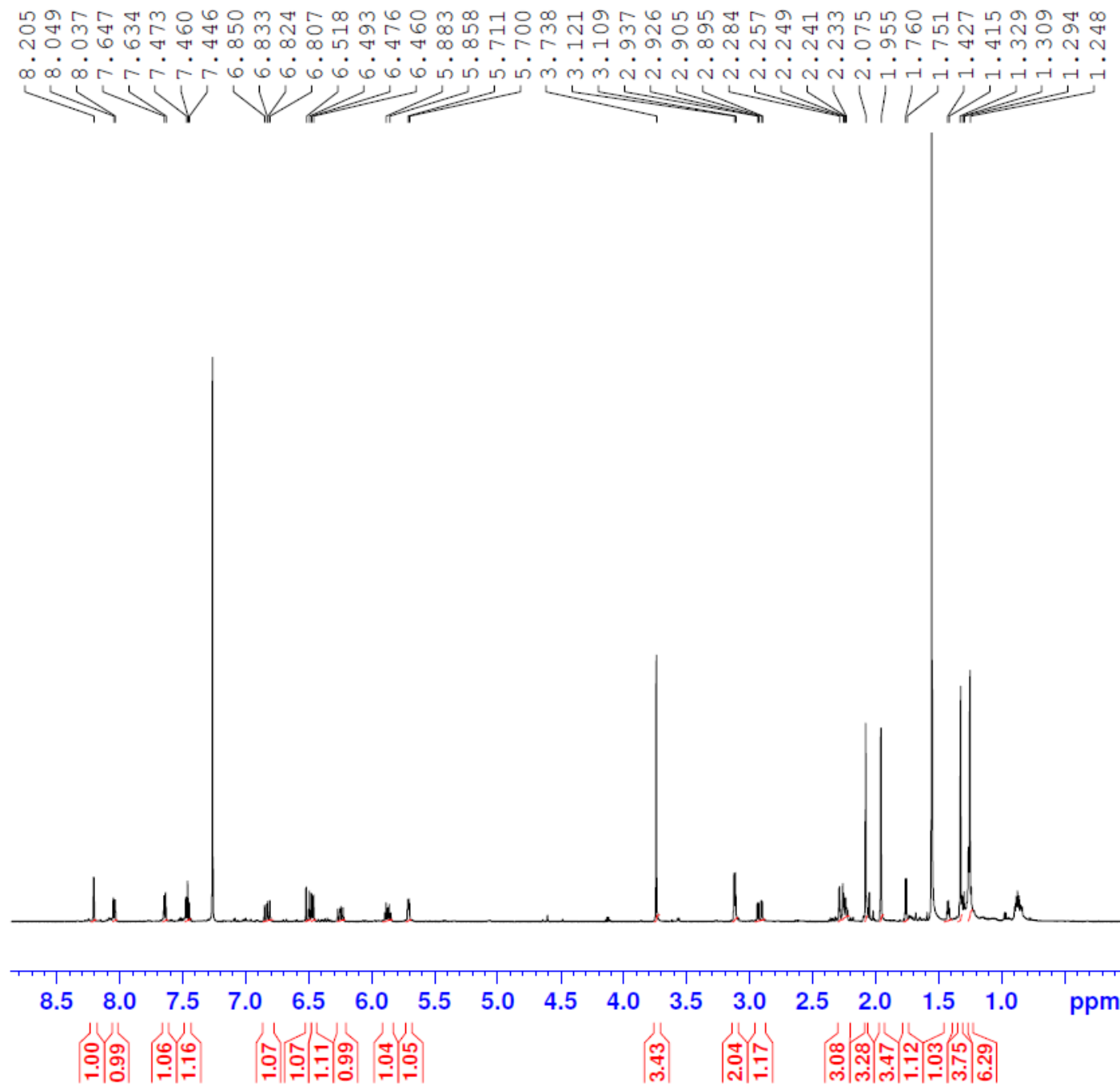
Analyst
Date

Analyst
Friday, 12 June 2020 10:57 AM



Sample Name	Description	Quality Checks
3NO2 I Mig	Sample	The Quality Checks do not report any warnings for the sample.

¹³C NMR Characterisation

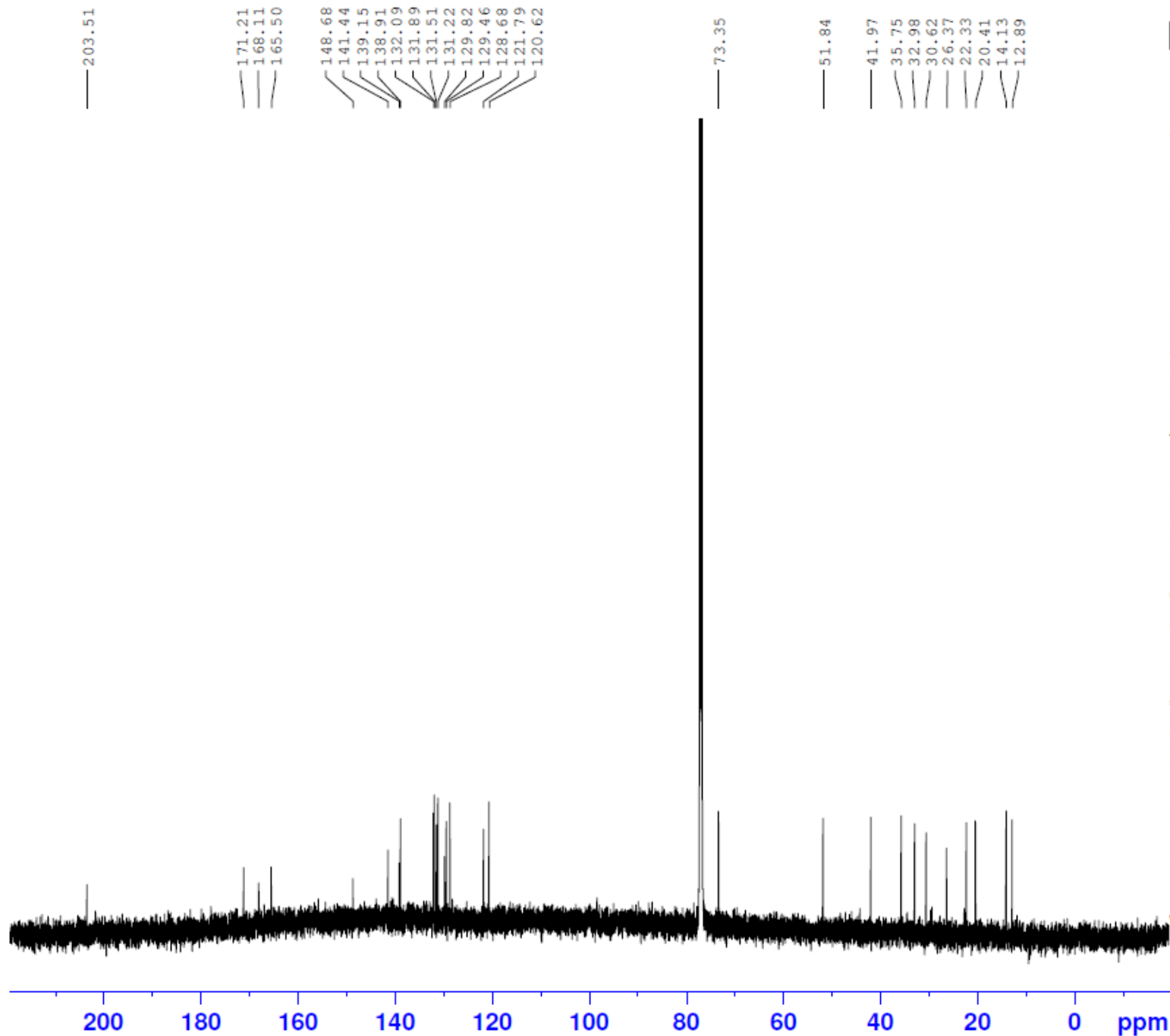


Current Data Parameters
NAME 20200612 3NO2 II E
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200613
Time 8.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 362
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300254 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 20200612 3NO2 II E
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200613
 Time 16.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8000
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028137 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200612 3NO2 II E
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200613
Time 8.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 5208.333 Hz
FIDRES 2.543132 Hz
AQ 0.1966080 sec
RG 2050
DW 96.000 usec
DE 6.50 usec
TE 298.1 K
D0 0.00007881 sec
D1 1.94183695 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00019200 sec

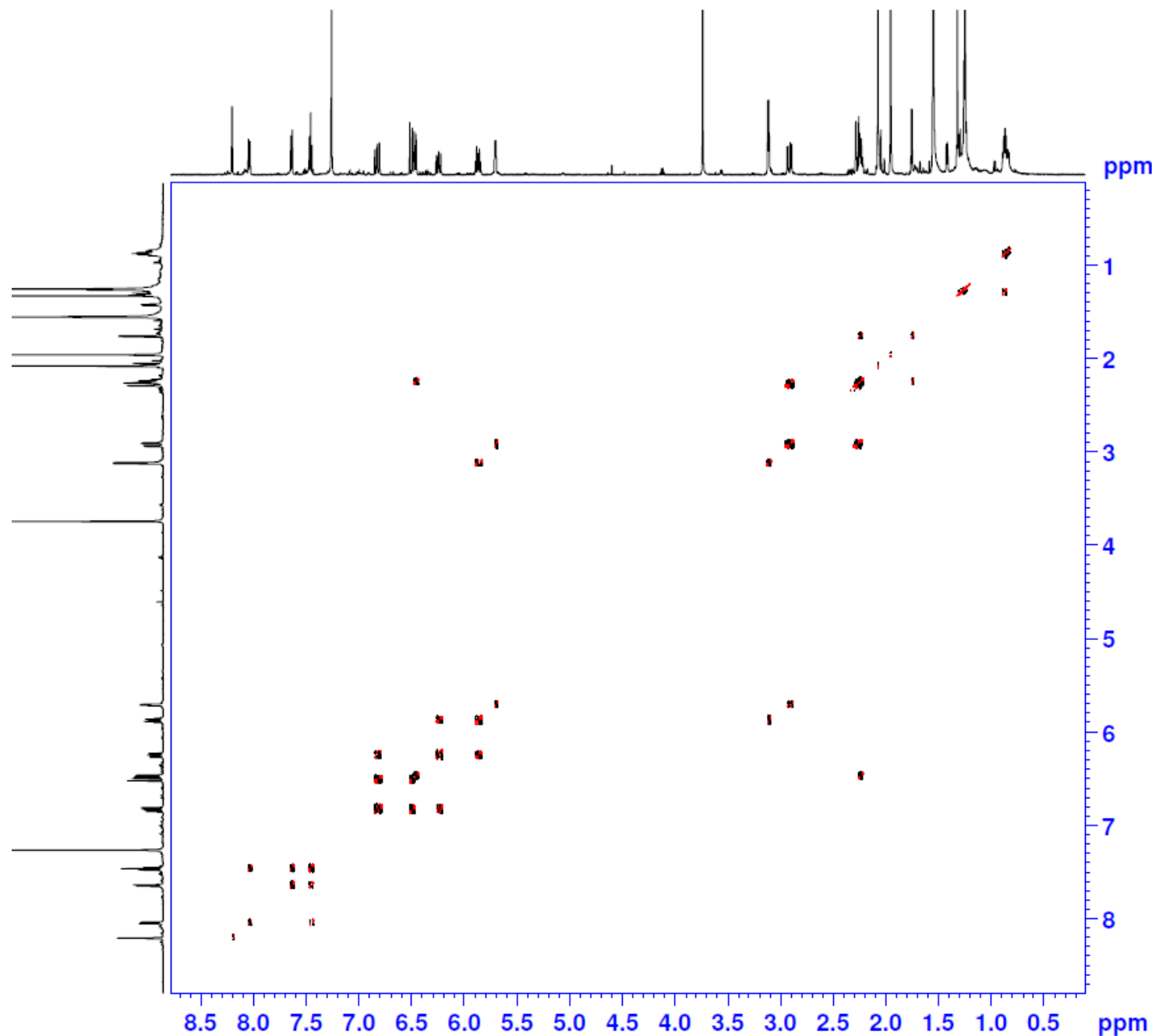
----- CHANNEL f1 -----
SFO1 600.1326981 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1327 MHz
FIDRES 20.345053 Hz
SW 8.679 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.1300292 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300245 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200612 3NO2 II E
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200613
Time 16.10
INSTRUM spect
PROBHD 5 mm FASBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 40
DS 16
SWH 5154.639 Hz
FIDRES 5.033827 Hz
AQ 0.0993280 sec
RG 2050
RW 97.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46620798 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1327104 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

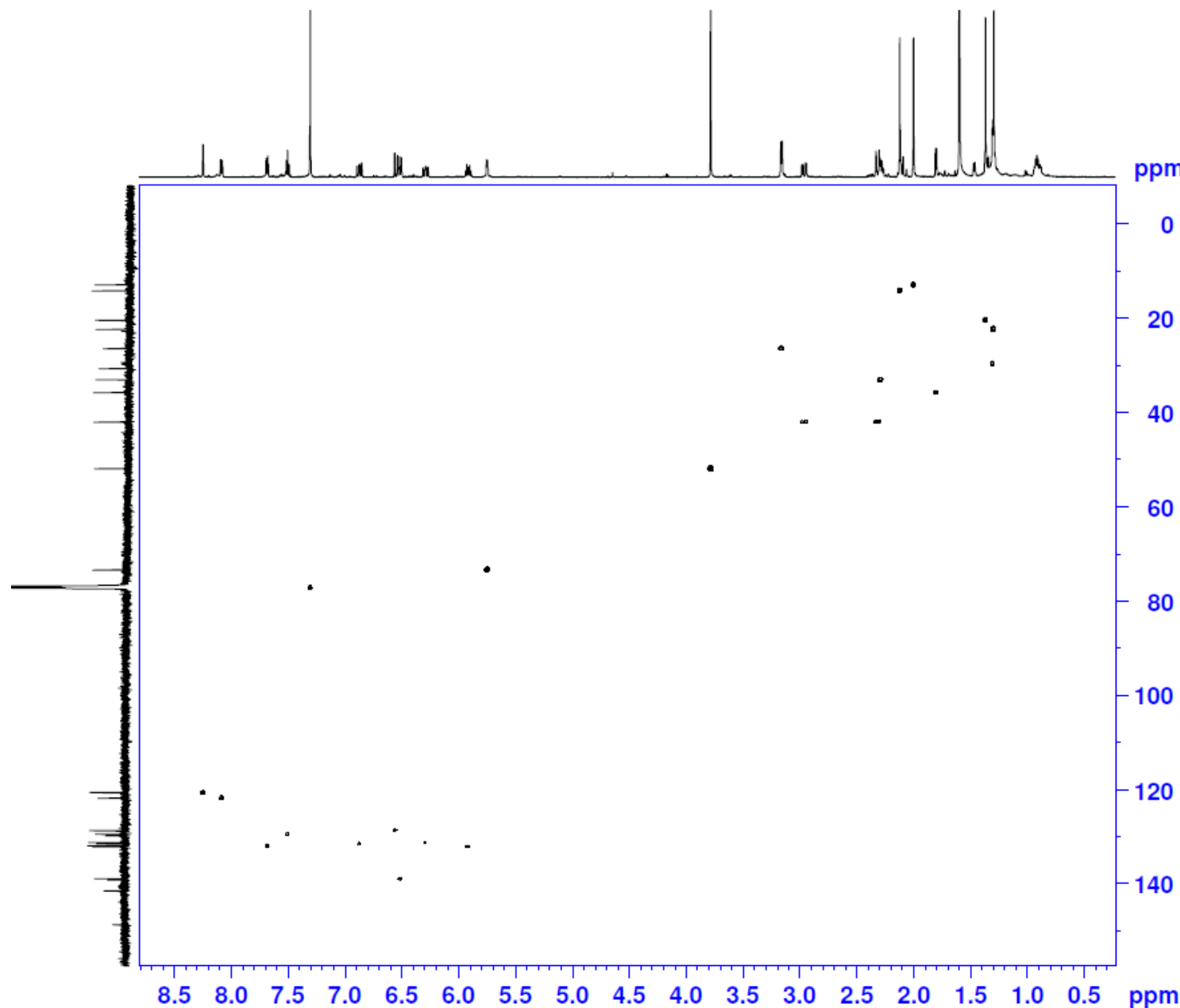
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
CPNAM[1] SMSQ10.100
CPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FMODE Echo-Antiecho

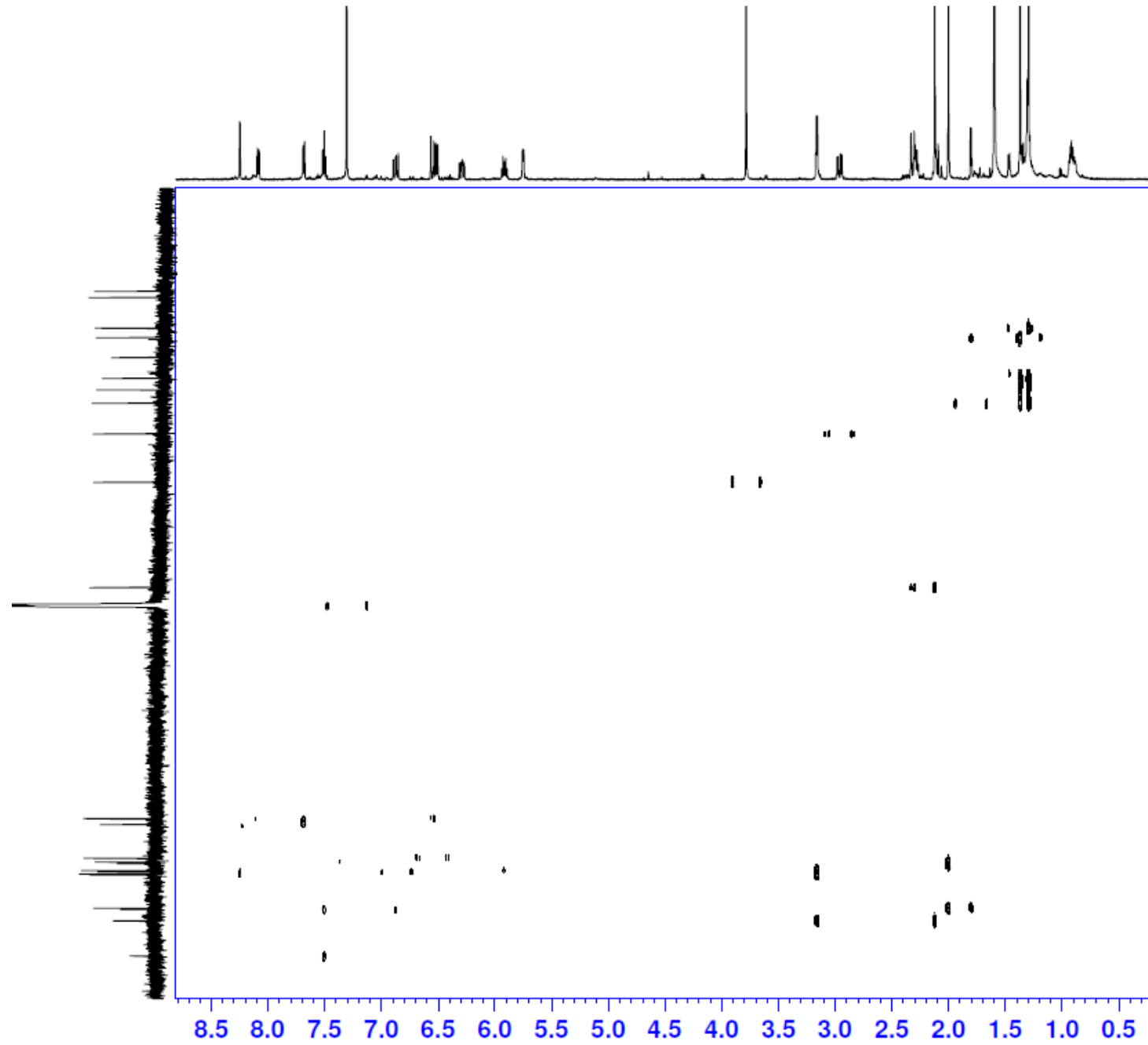
F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200612 3NO2 II E
EXPNO 15
PROCNO 1



ppm

0

20

40

60

80

100

120

140

ppm

F2 - Acquisition Parameters
Data_ 20200613
Time 20.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 50
DS 16
SWH 5154.639 Hz
FIDRES 1.258457 Hz
AQ 0.3973120 sec
RG 2050
RW 97.000 usec
DE 6.50 usec
TE 298.1 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.35827804 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1327104 MHz
NUC1 1H
P1 13.50 usec
F2 27.00 usec
PLW1 17.00000000 W

===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

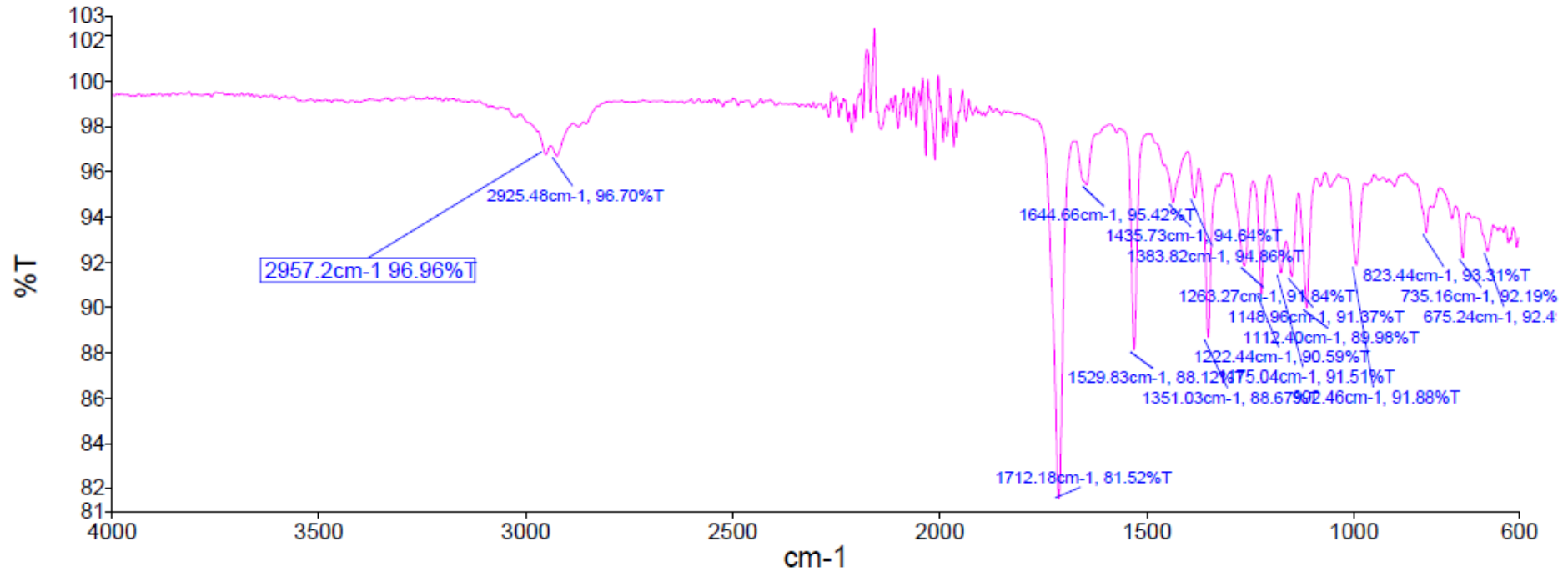
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

130b IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 12 June 2020 11:04 AM

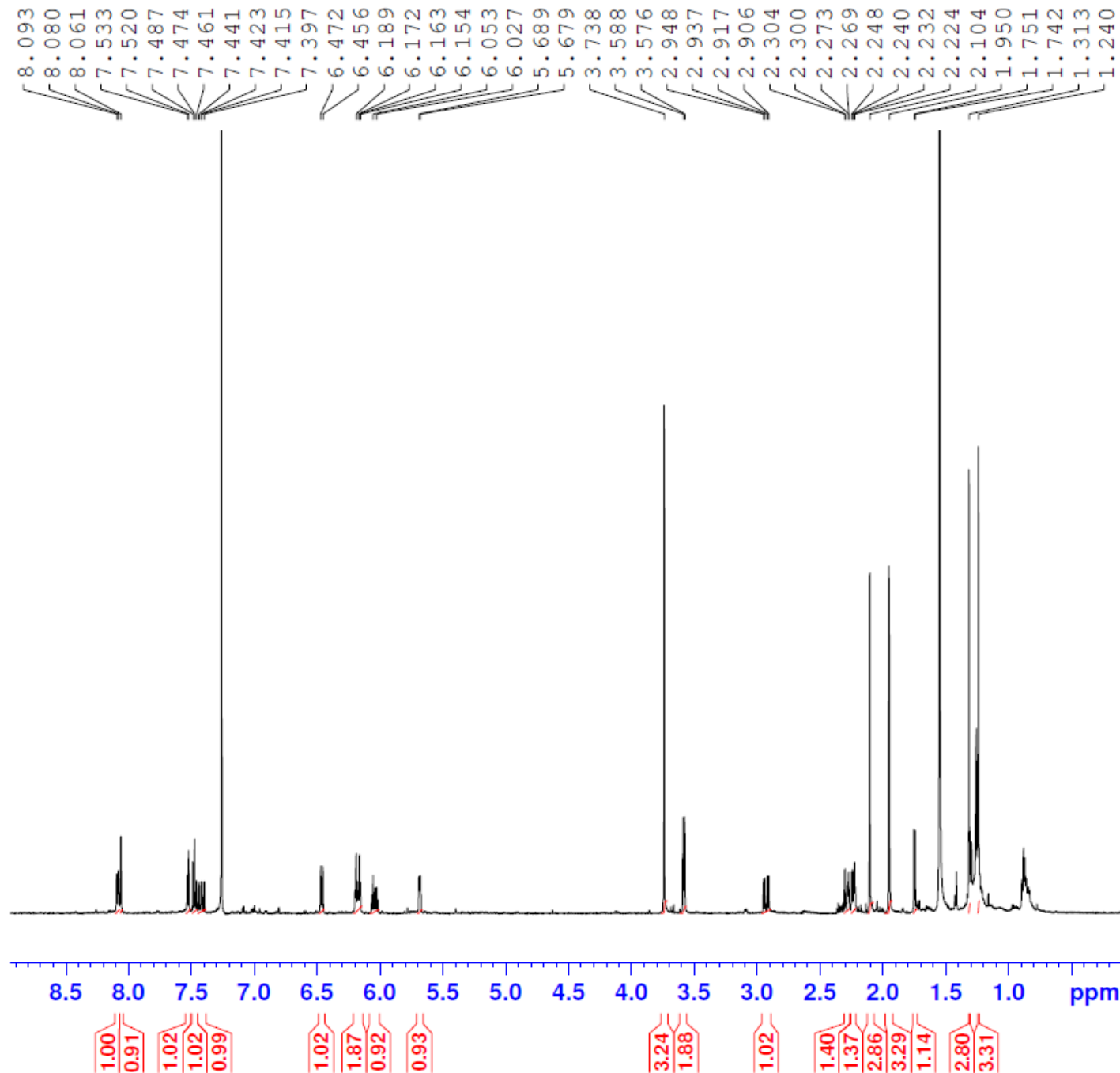
Analyst
Date

Analyst
Friday, 12 June 2020 11:04 AM



Sample Name	Description	Quality Checks
3NO2 II E	Sample	The Quality Checks do not report any warnings for the sample.

135b NMR Characterisation

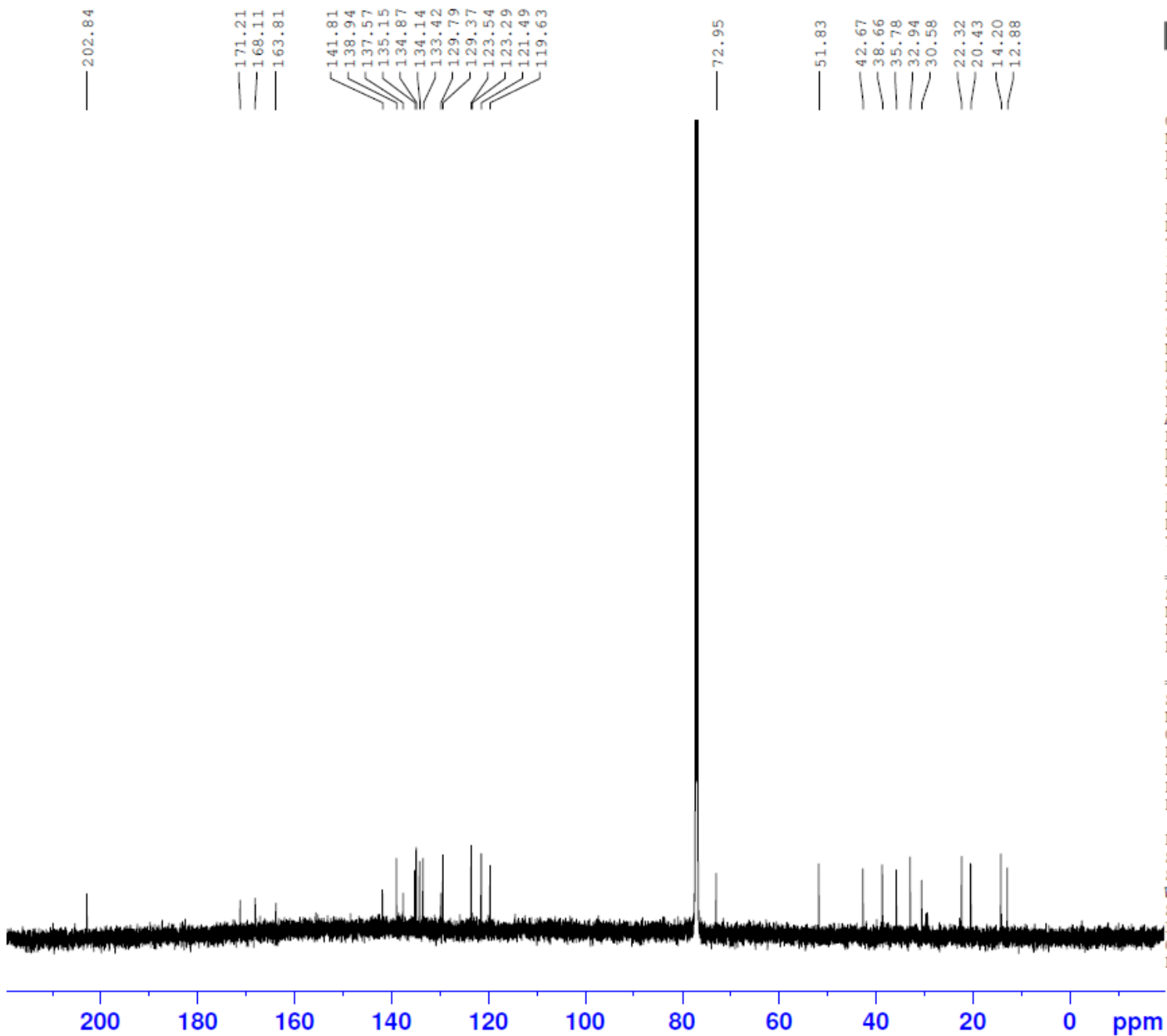


Current Data Parameters
NAME 20200612 3NO2 II Mig
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200612
Time 17.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 362
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300259 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20200612 3NO2 II Mig
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200613
Time 0.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8000
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028141 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20200612 3NO2 II Mig
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200612
Time 17.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 5208.333 Hz
FIDRES 2.543132 Hz
AQ 0.1966080 sec
RG 2050
DW 96.000 usec
DE 6.50 usec
TE 298.1 K
D0 0.00007881 sec
D1 1.94183695 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00019200 sec

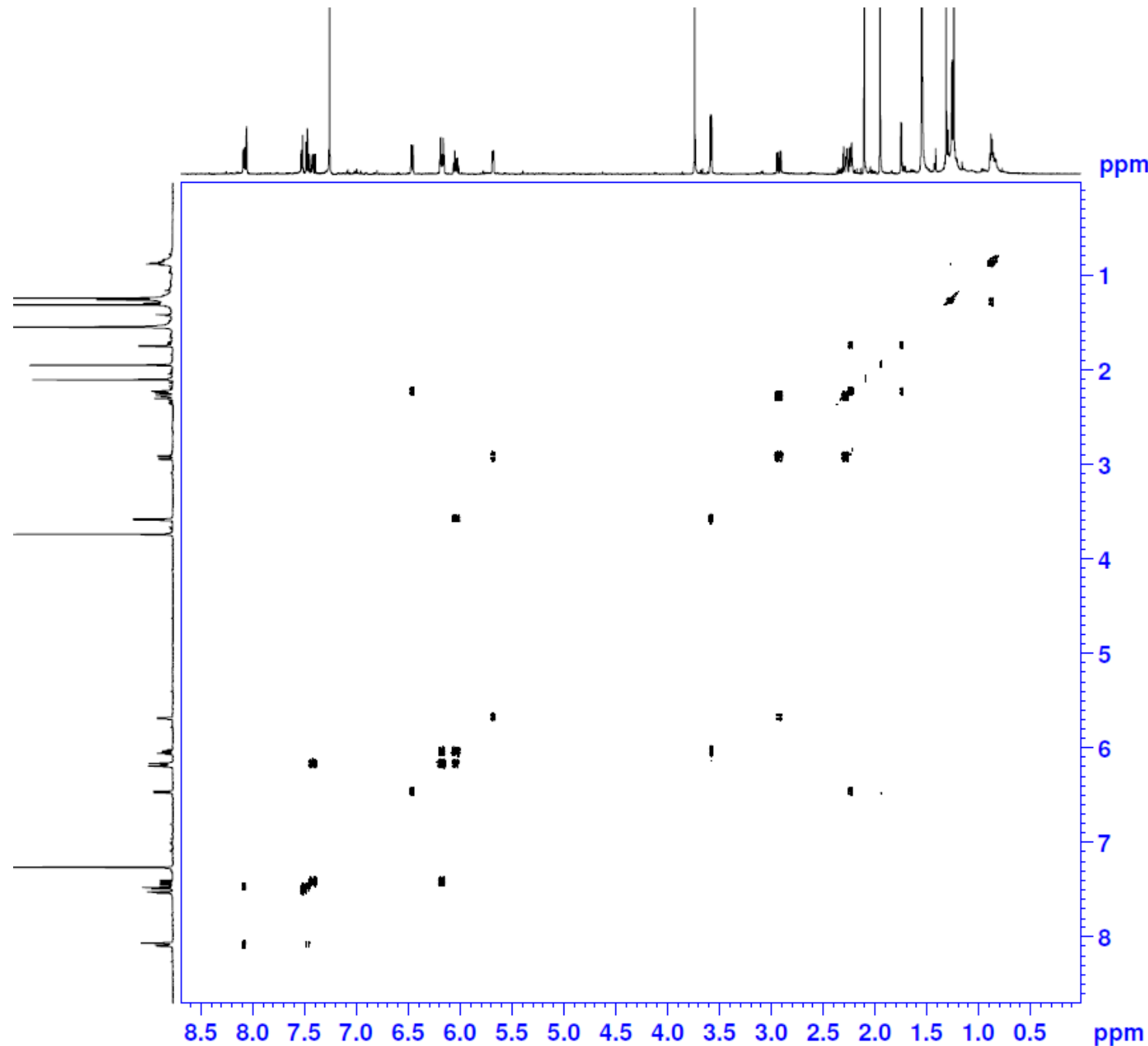
----- CHANNEL f1 -----
SFO1 600.1326417 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1326 MHz
FIDRES 20.345053 Hz
SW 8.679 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300279 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300264 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200612 3NO2 II Mig
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200613
Time 0.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 40
DS 16
SWH 5102.041 Hz
FIDRES 4.982462 Hz
AQ 0.1003520 sec
RG 2050
DW 98.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46518397 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1326605 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

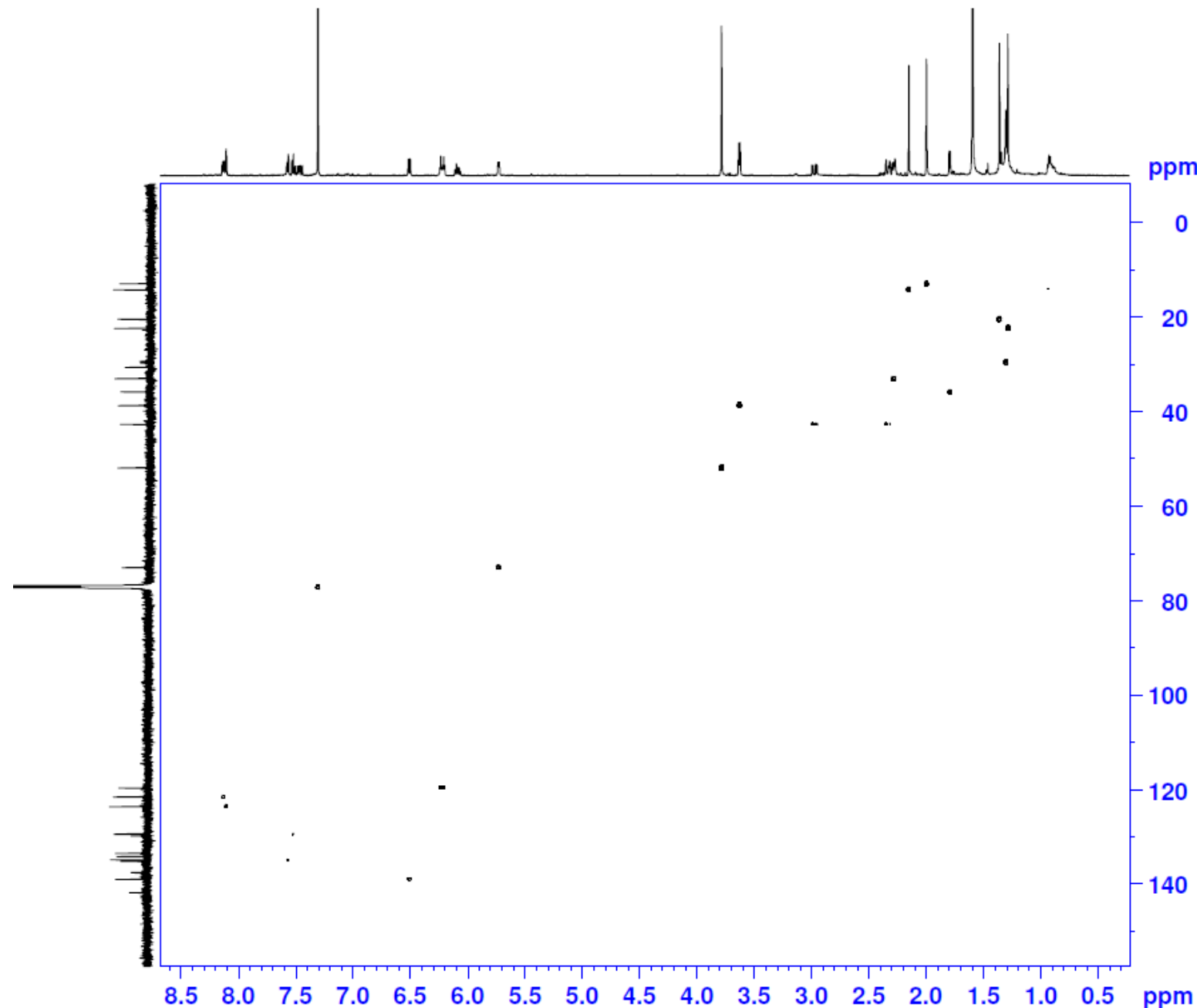
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

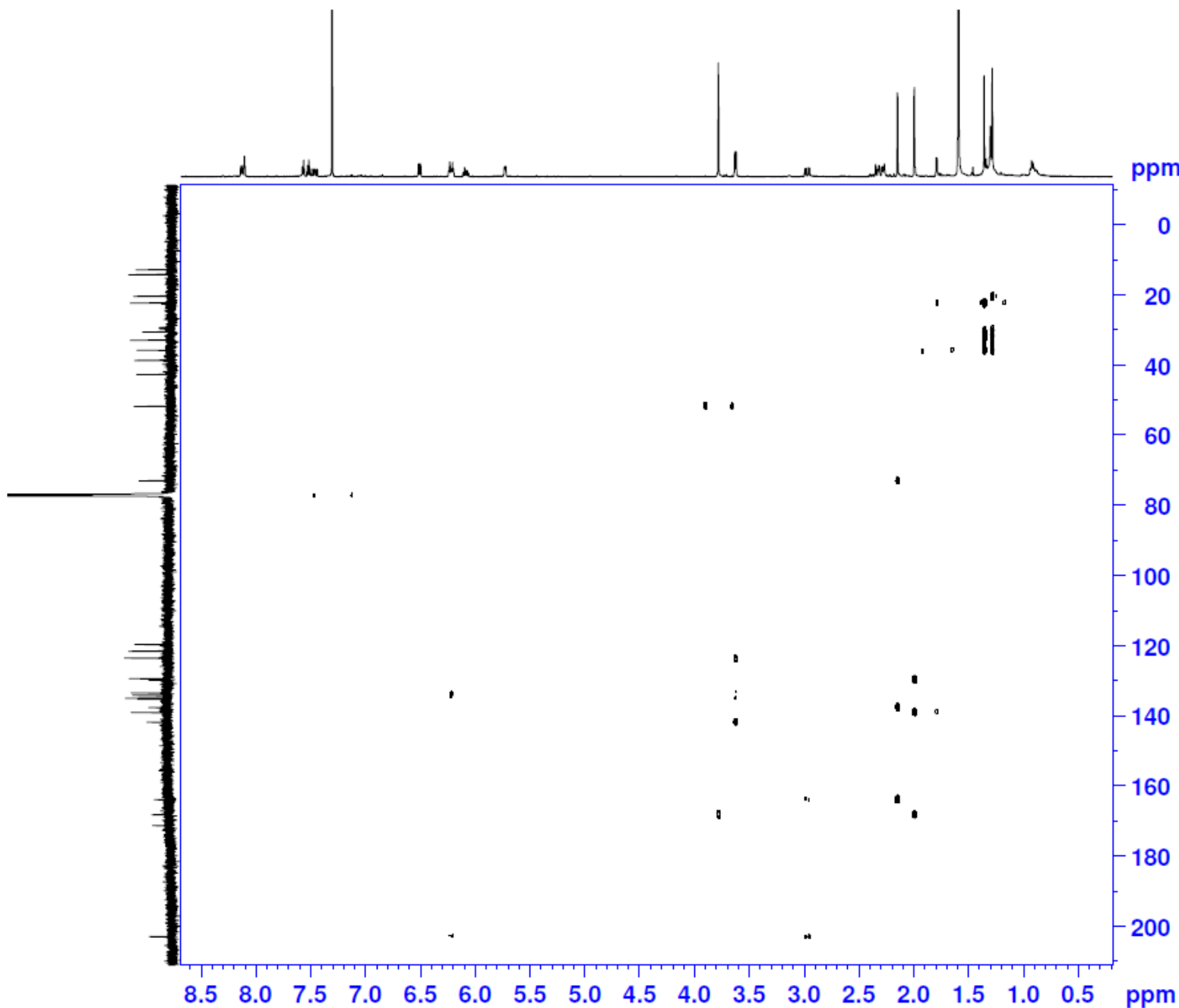
F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200612 3NO2 11 Mig
EXPNO 15
PROCNO 1



F2 - Acquisition Parameters
Date_ 20200613
Time 5.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 50
DS 16
SWH 5102.041 Hz
FIDRES 1.245615 Hz
AQ 0.4014080 sec
RG 2050
DW 98.000 usec
DE 6.50 usec
TE 298.1 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.35418200 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1326605 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

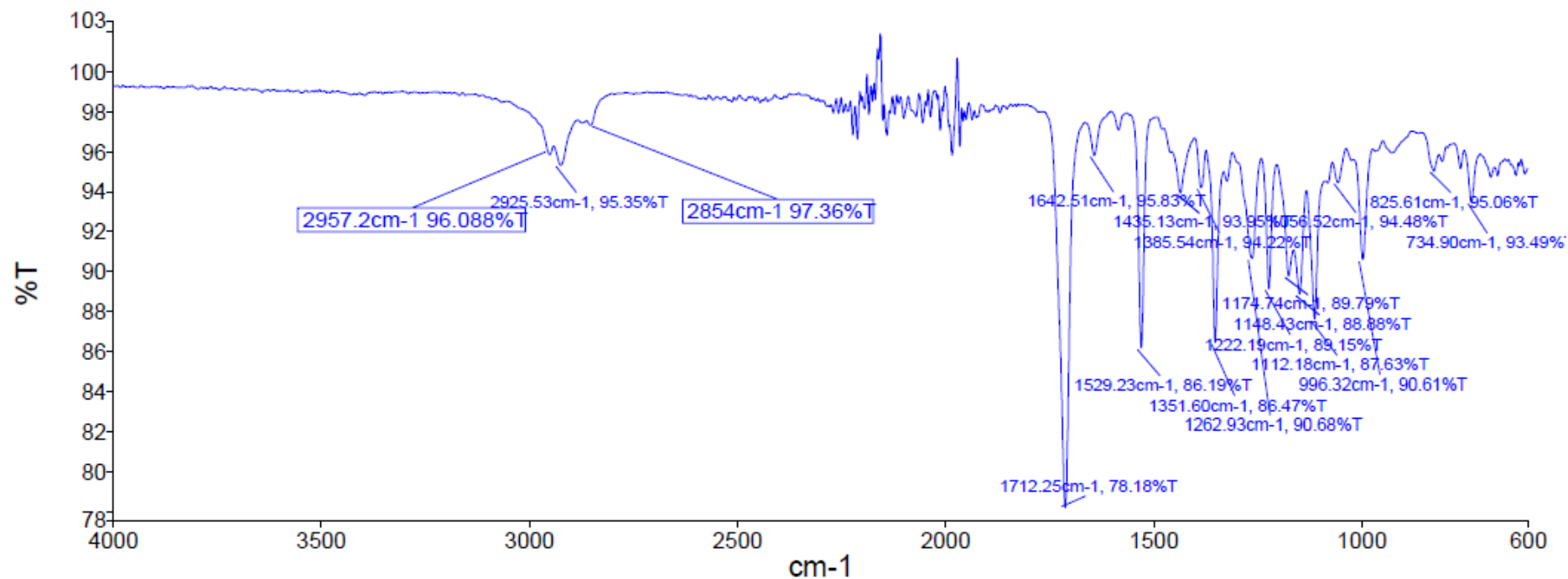
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

135b IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 12 June 2020 11:01 AM

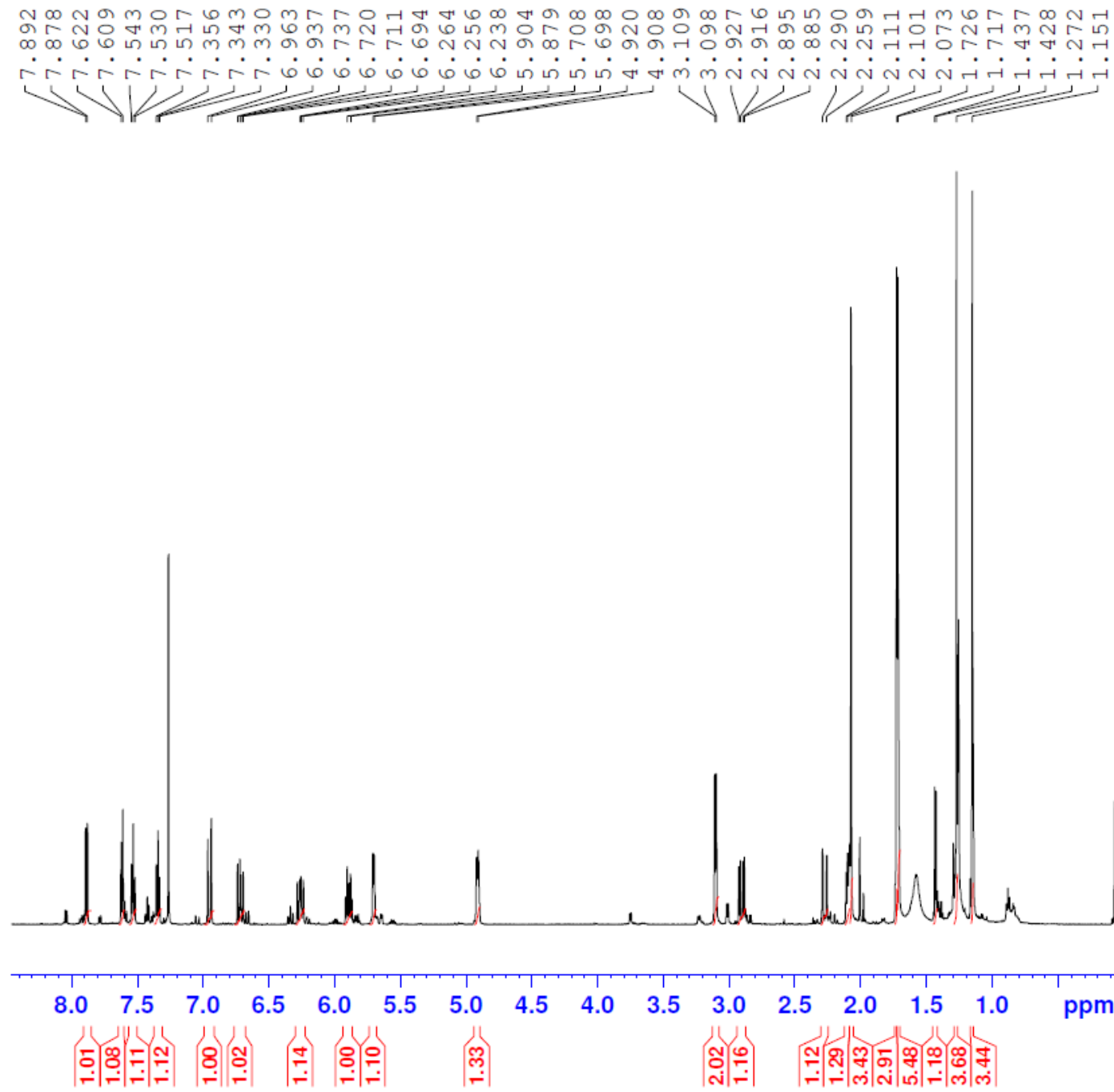
Analyst
Date

Analyst
Friday, 12 June 2020 11:01 AM



Sample Name	Description	Quality Checks
3NO2 II Mig	Sample	The Quality Checks do not report any warnings for the sample.

¹³1a NMR Characterisation

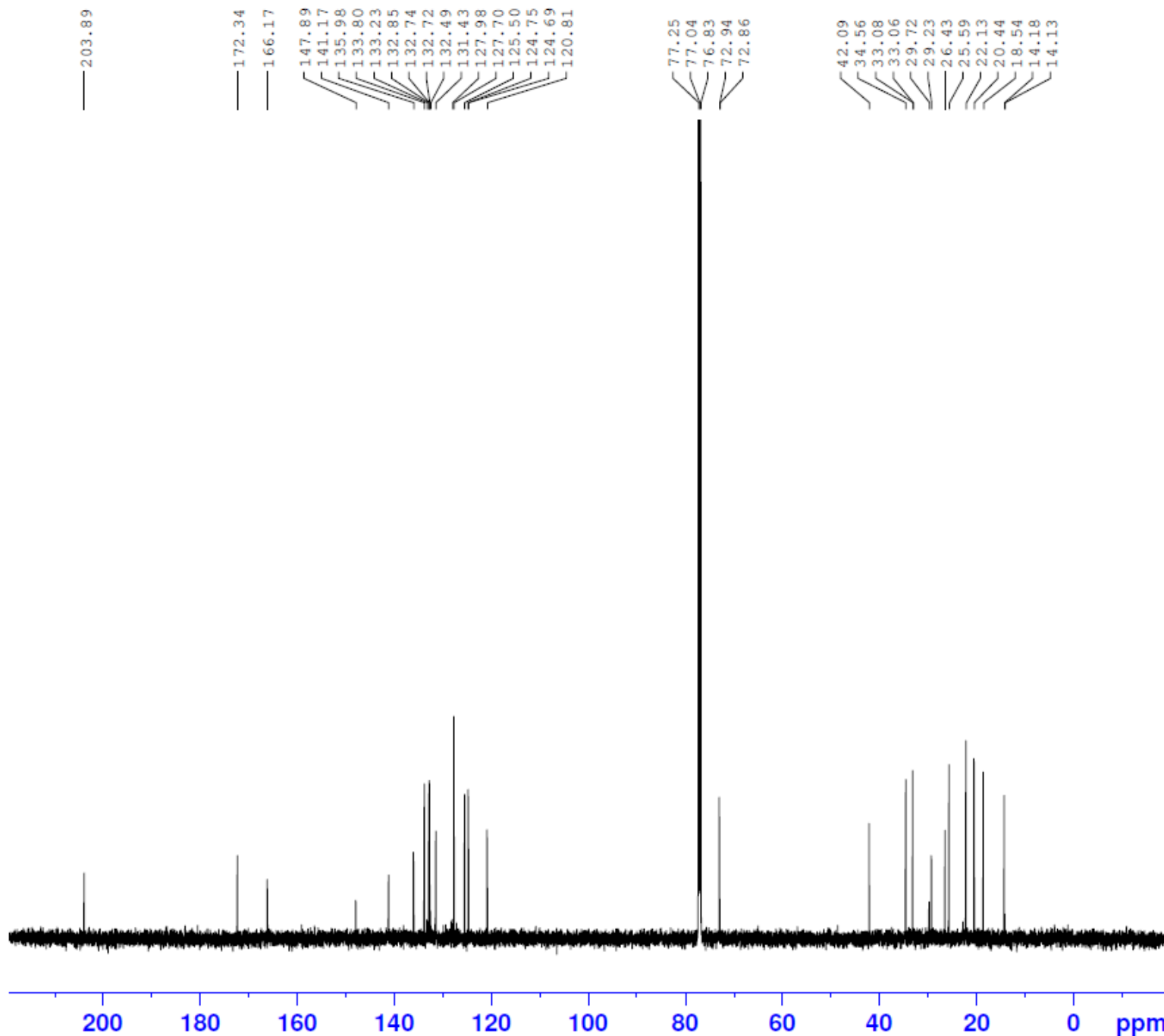


Current Data Parameters
NAME 20200803 2NO2 I E
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200803
Time 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 228
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300245 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20200803 2NO2 I E
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200803
Time 16.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20200424 2NO2 I E
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200424
Time 17.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphp
TD 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 5000.000 Hz
FIDRES 2.441406 Hz
AQ 0.2048000 sec
RG 2050
DW 100.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00008281 sec
D1 1.93364501 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00020000 sec

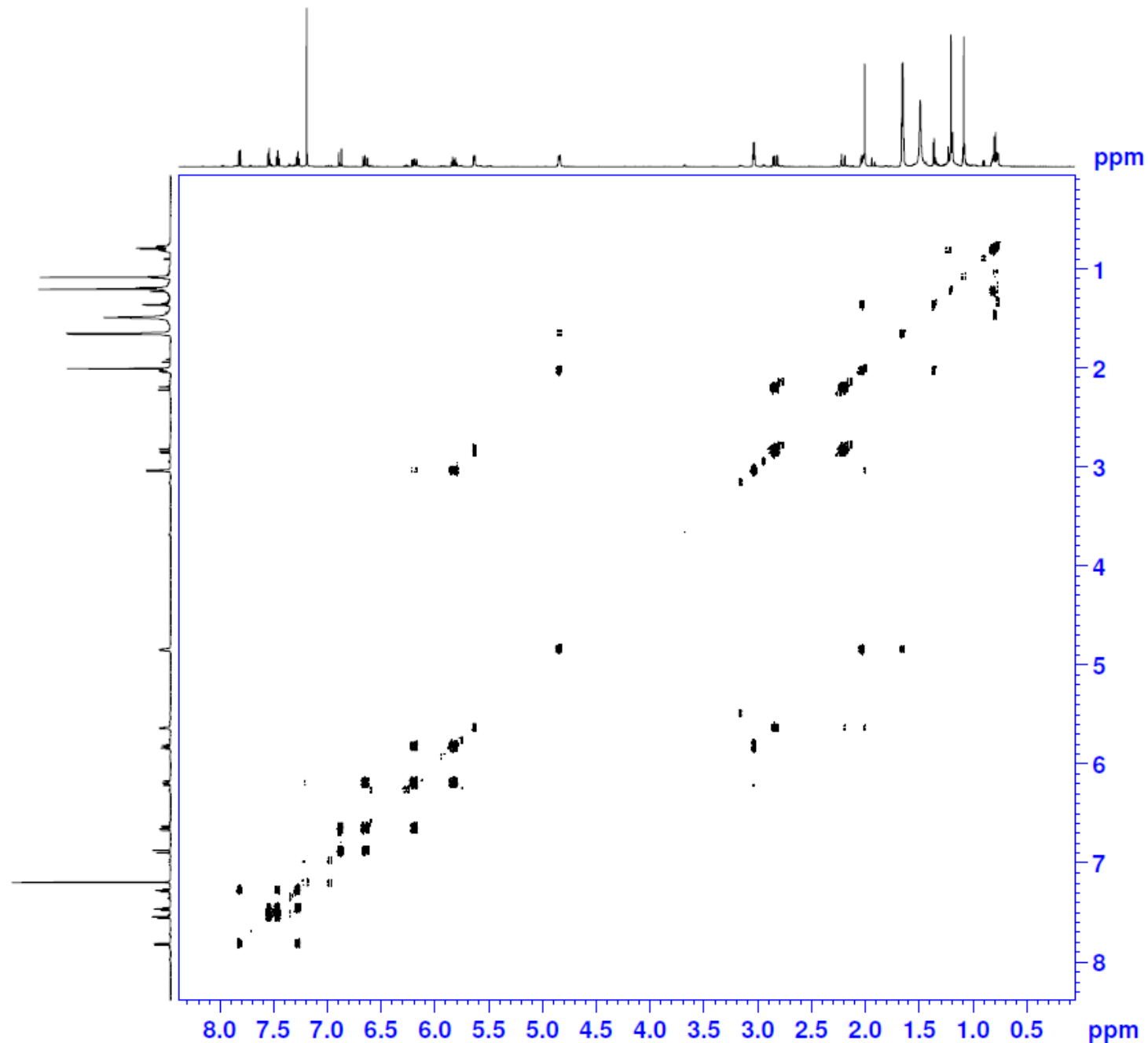
----- CHANNEL f1 -----
SFO1 600.1325984 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1326 MHz
FIDRES 19.531250 Hz
SW 8.331 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.1300674 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300674 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200424 2NO2 I K
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200424
Time 22.15
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 5434.783 Hz
FIDRES 5.307405 Hz
AQ 0.0942080 sec
RG 2050
DW 92.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.47132802 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1324025 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

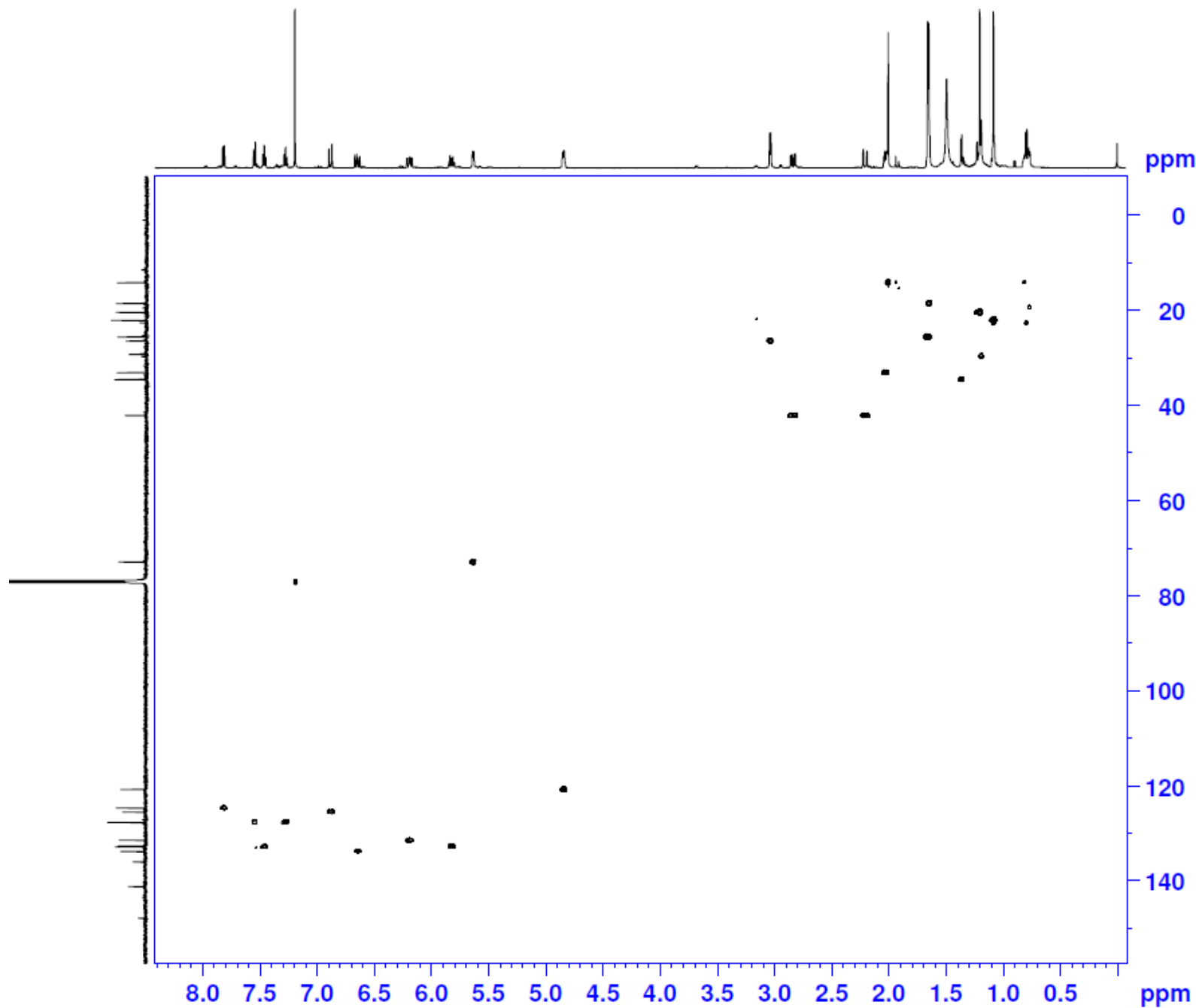
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPX1 80.00 %
GPX2 20.10 %
PI6 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300675 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200424 2NO2 1 E
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Data_ 20200425
Time 3.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 5434.783 Hz
FIDRES 1.326951 Hz
AQ 0.3768320 sec
RG 2050
DW 92.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.37875795 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

==== CHANNEL f1 =====
SFO1 600.1324025 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

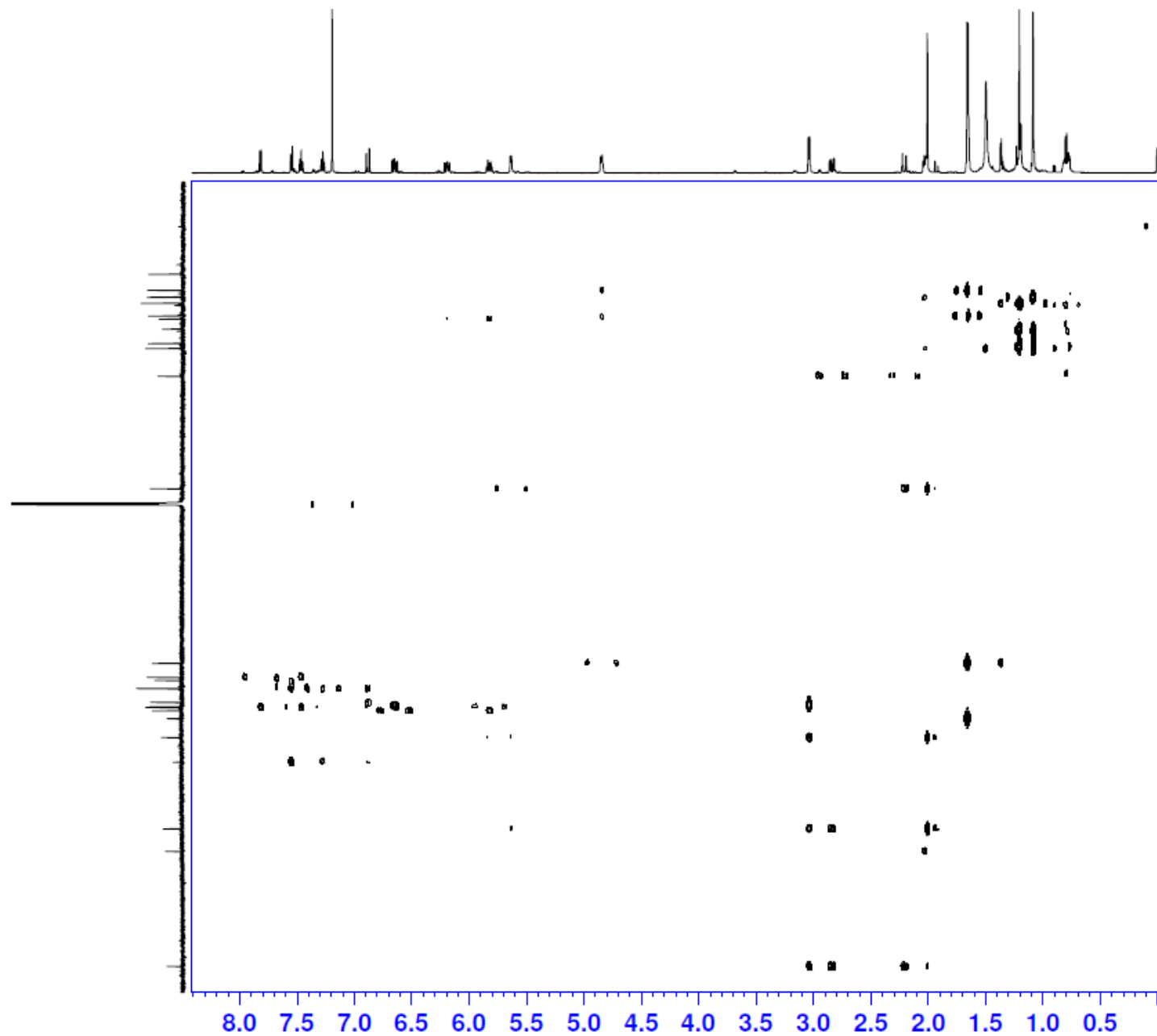
==== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

==== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

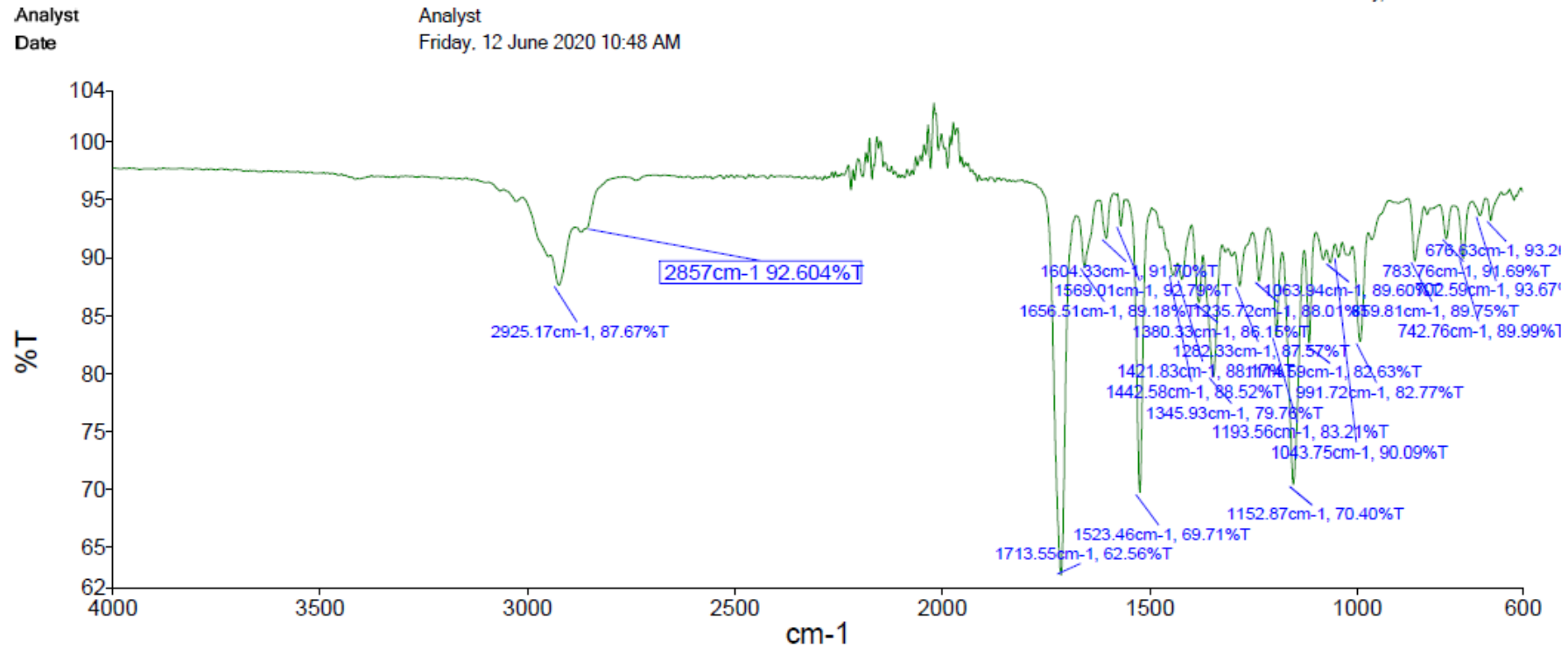
F2 - Processing parameters
SI 1024
SF 600.1300675 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



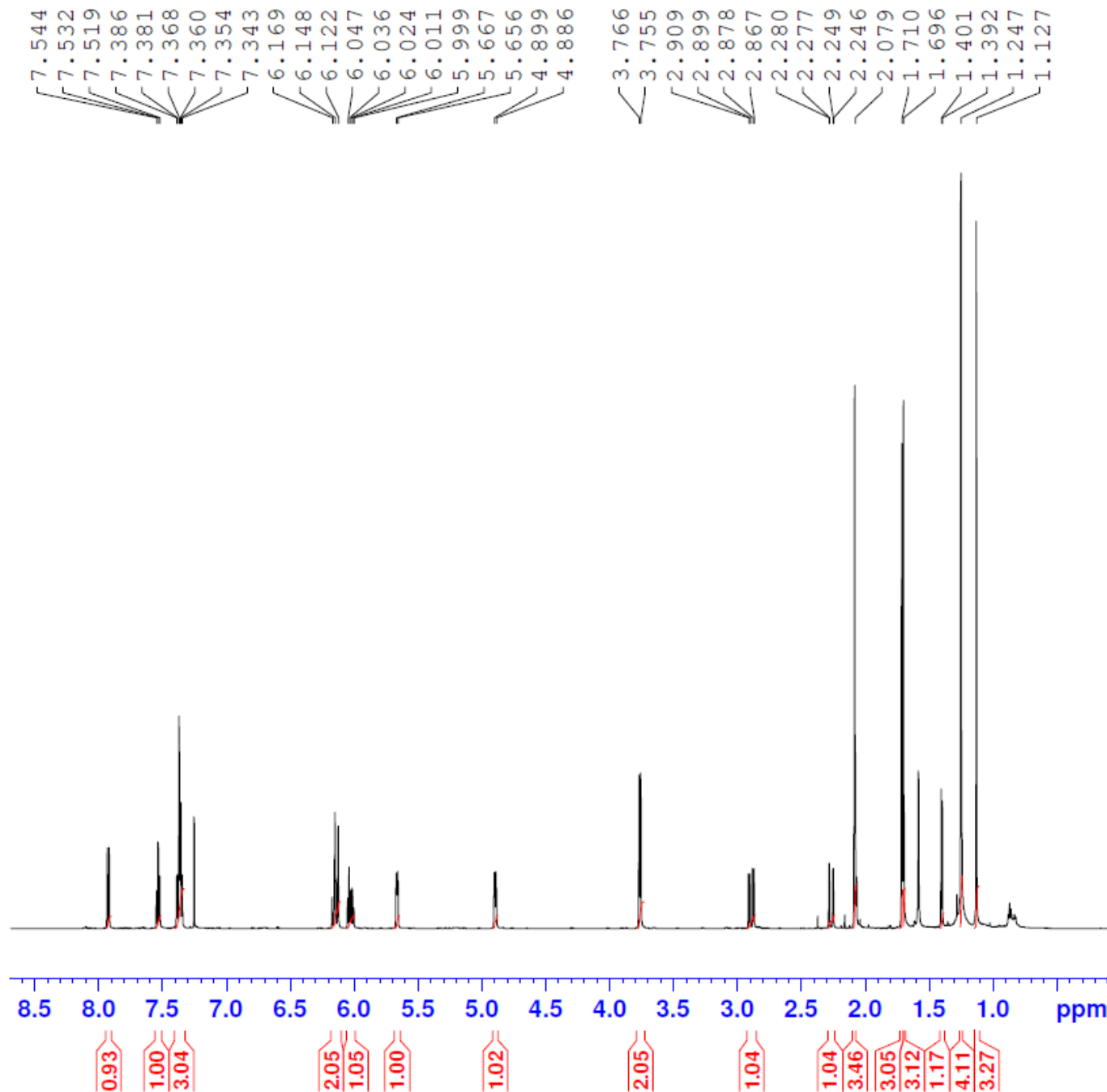
131a IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 12 June 2020 10:48 AM



Sample Name	Description	Quality Checks
2NO2 IE	Sample	The Quality Checks do not report any warnings for the sample.

¹³⁶a NMR Characterisation

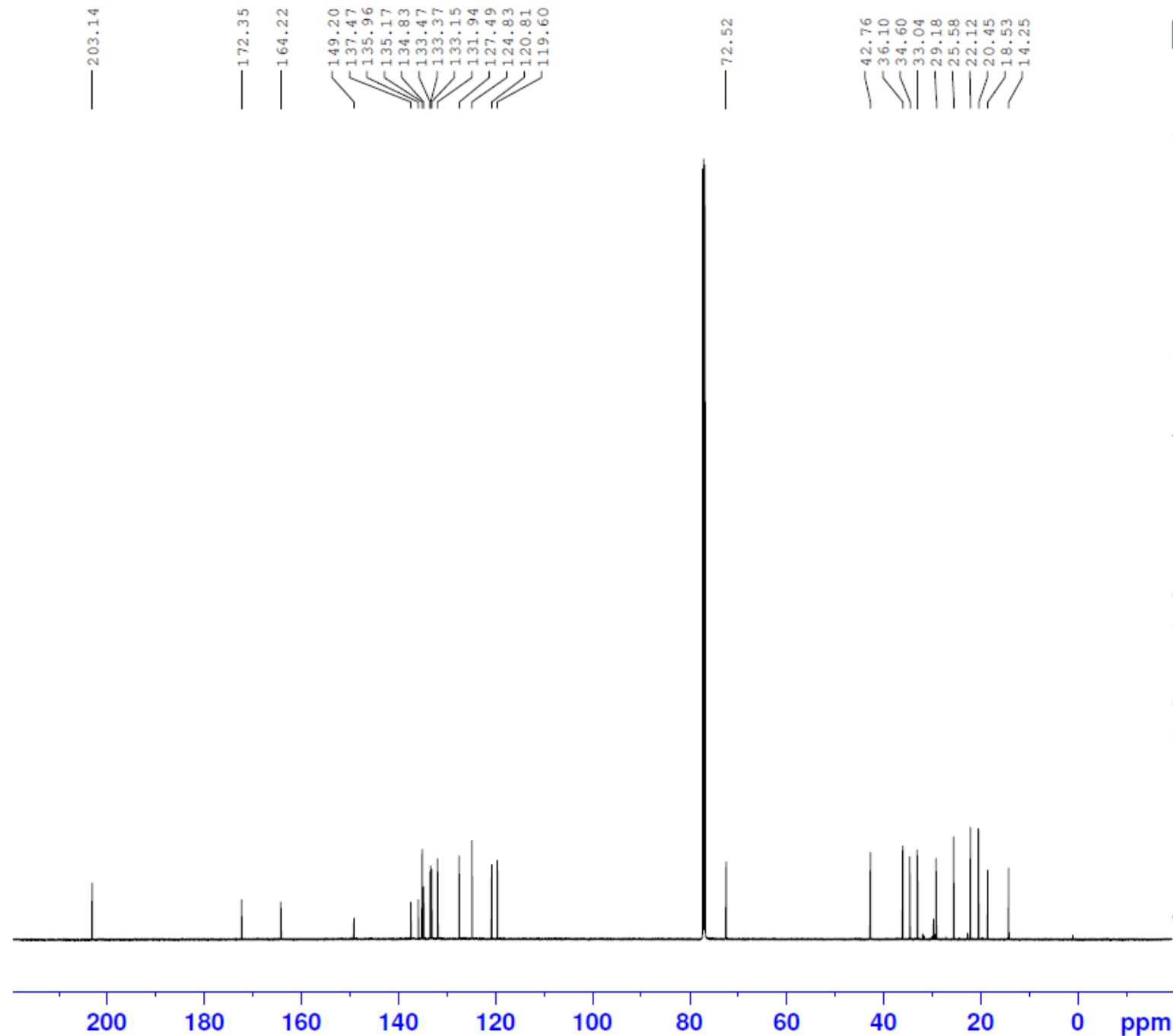


Current Data Parameters
 NAME 20200423 2NO2 I Z
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200423
 Time 17.36
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 161
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300322 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters

NAME 20200423 2NO2 I Z
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200423
Time 22.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5120
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028154 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20200423 2NO2 I Z
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200423
Time 17.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 5208.333 Hz
FIDRES 2.543132 Hz
AQ 0.1966080 sec
RG 2050
DW 96.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00007881 sec
D1 1.94183695 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00019200 sec

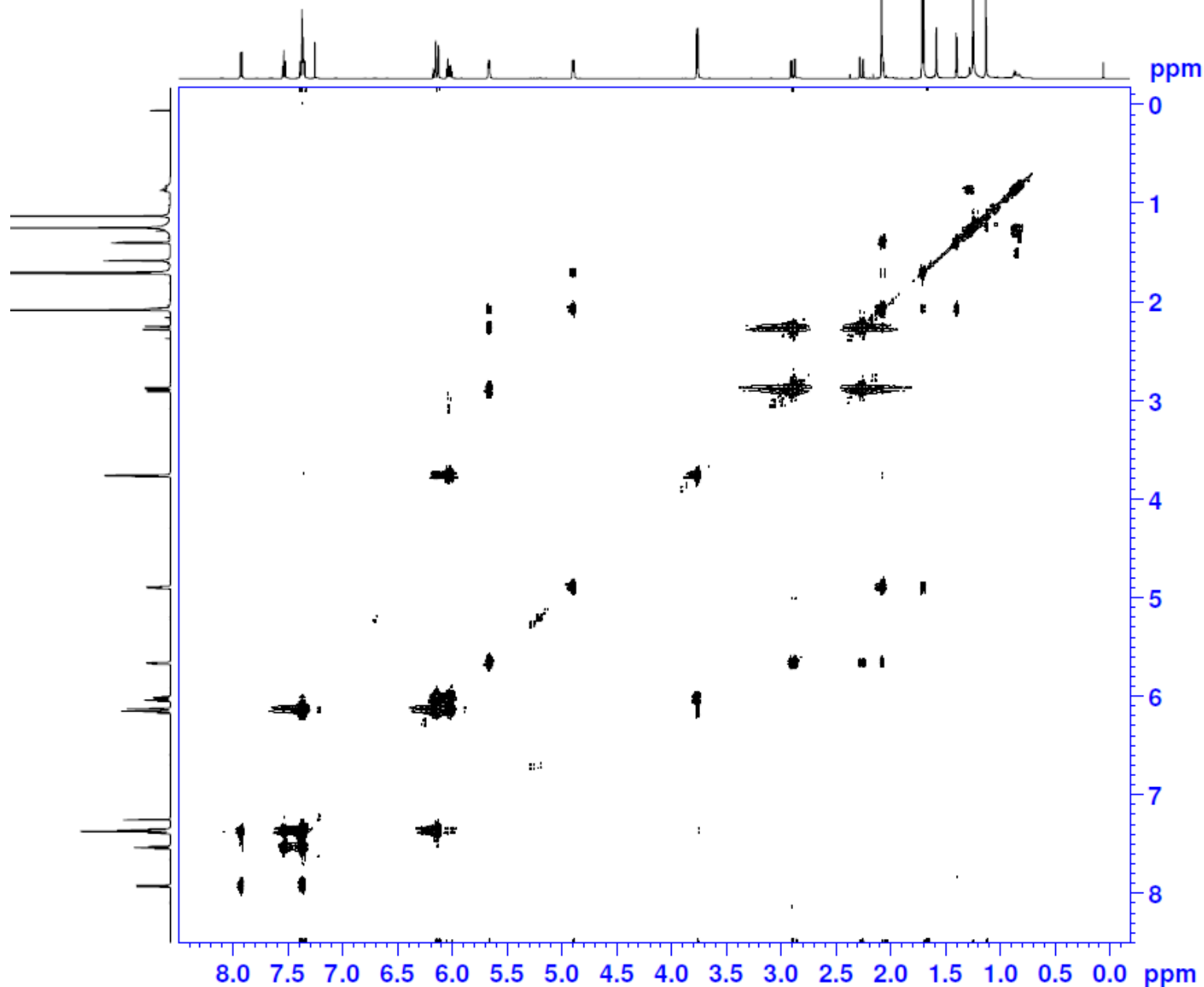
----- CHANNEL f1 -----
SFO1 600.1325270 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1325 MHz
FIDRES 20.345053 Hz
SW 8.679 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300341 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300290 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200423 2NO2 I Z
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200423
Time 22.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 5102.041 Hz
FIDRES 4.982462 Hz
AQ 0.1003520 sec
RG 2050
DW 98.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46518397 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1325706 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

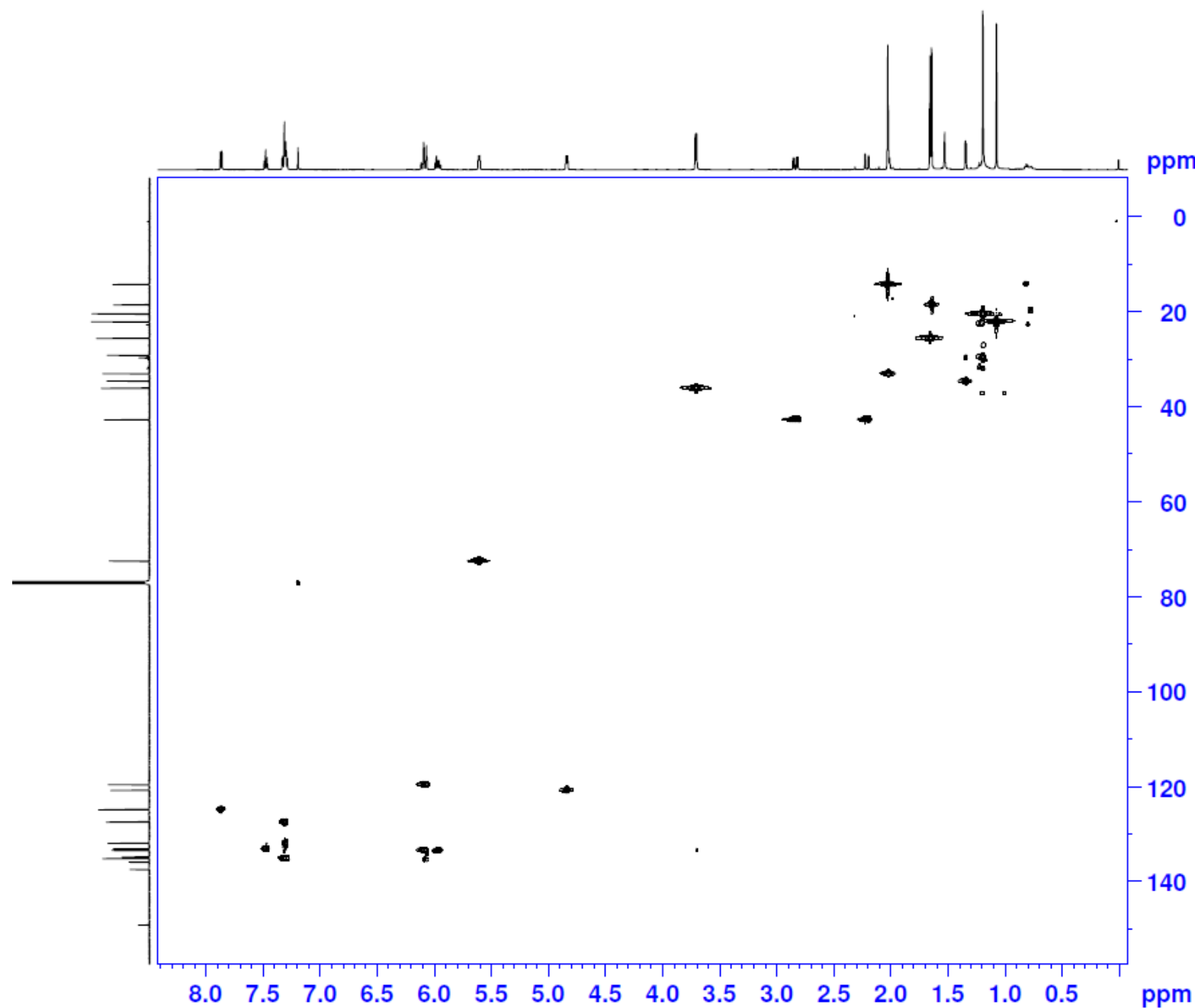
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300665 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200423 2NO2 1 Z
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200424
Time 4.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 5102.041 Hz
FIDRES 1.245615 Hz
AQ 0.4014080 sec
RG 2050
DW 98.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.35418200 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1325706 MHz
NUC1 1H
P1 13.50 usec
F2 27.00 usec
PLW1 17.00000000 W

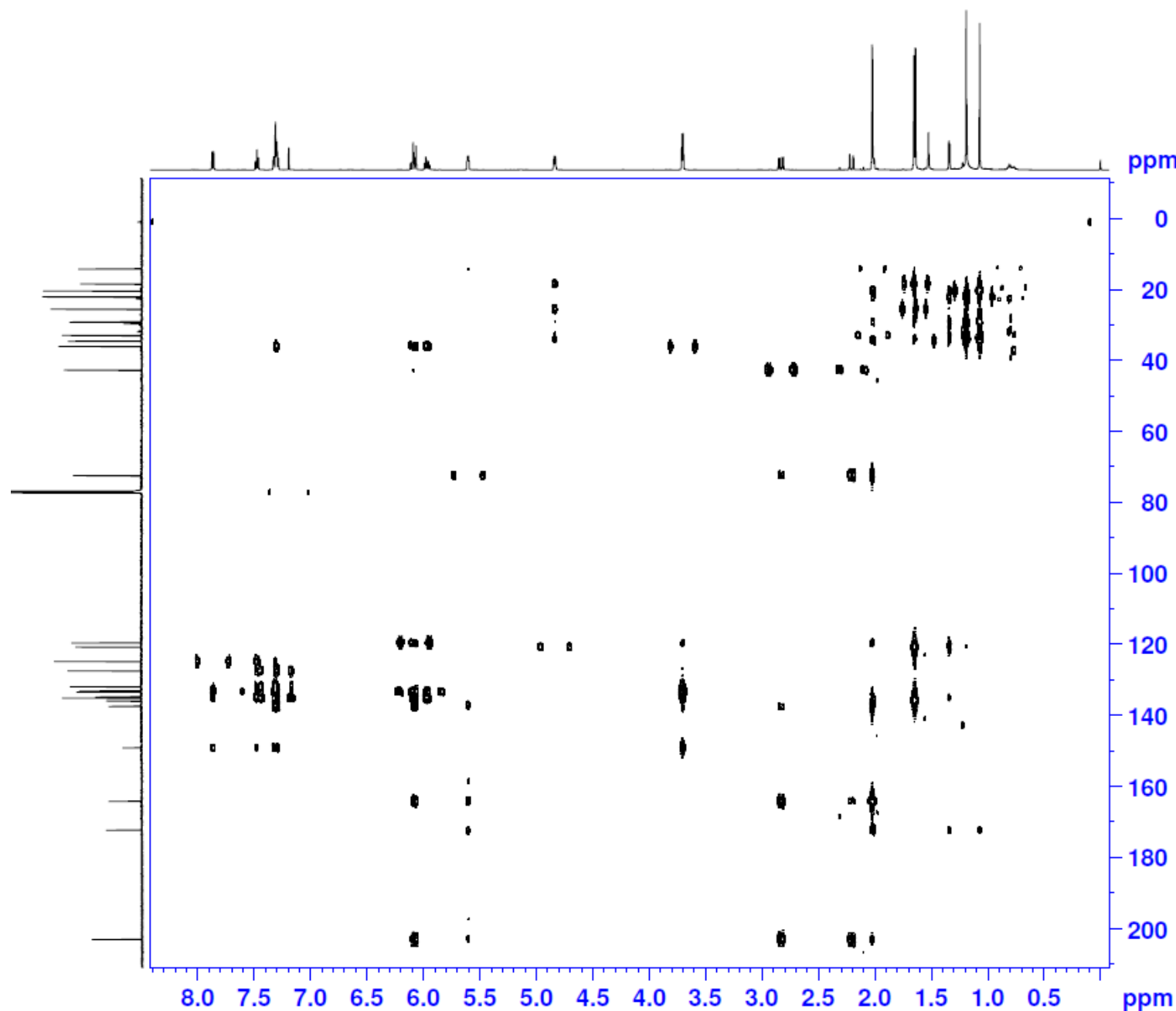
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPX1 50.00 %
GPX2 30.00 %
GPX3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300665 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

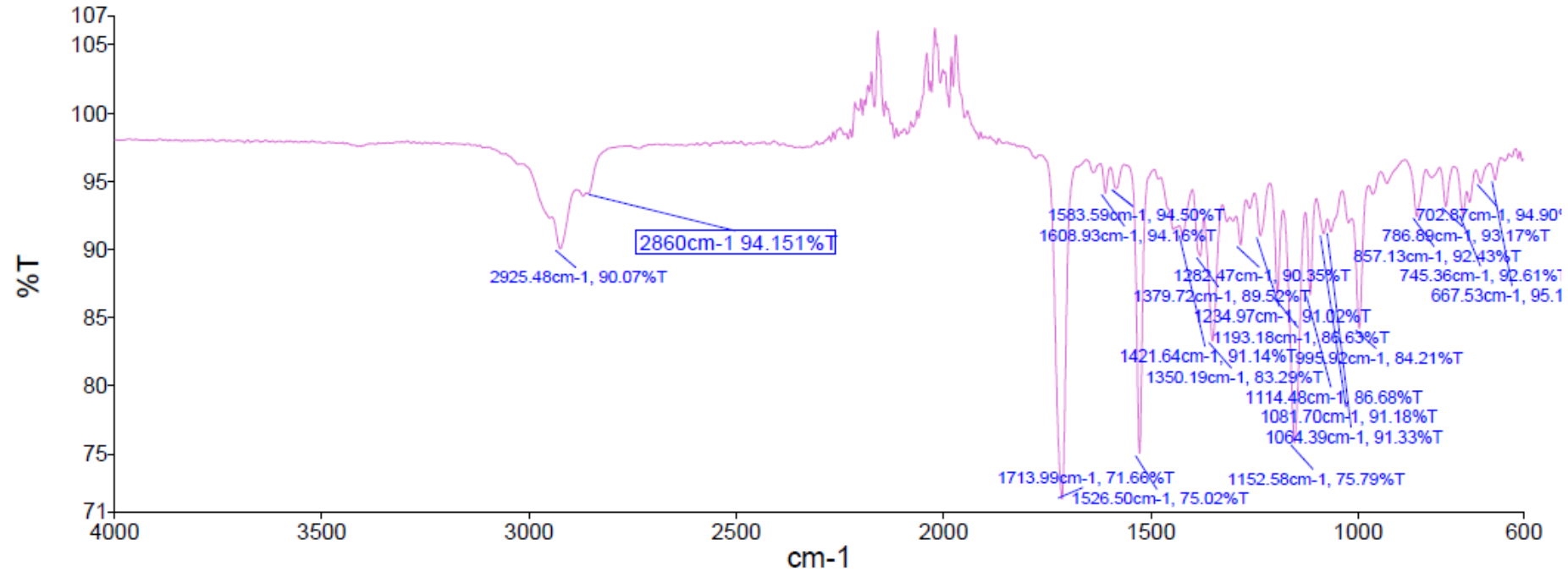


136a IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 12 June 2020 10:46 AM

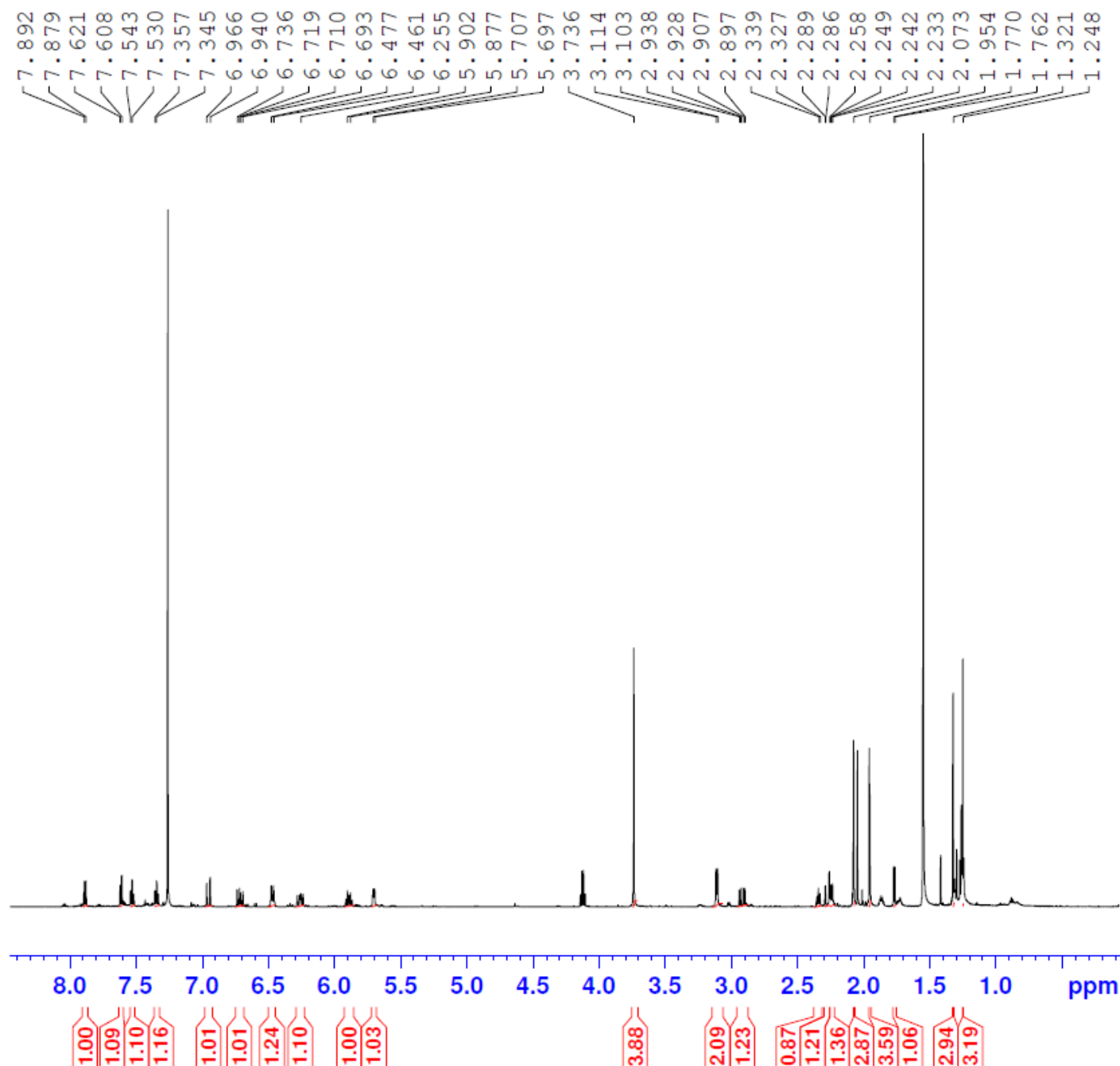
Analyst
Date

Analyst
Friday, 12 June 2020 10:46 AM



Sample Name	Description	Quality Checks
2NO2 I Mig	Sample	The Quality Checks do not report any warnings for the sample.

131b NMR Characterisation

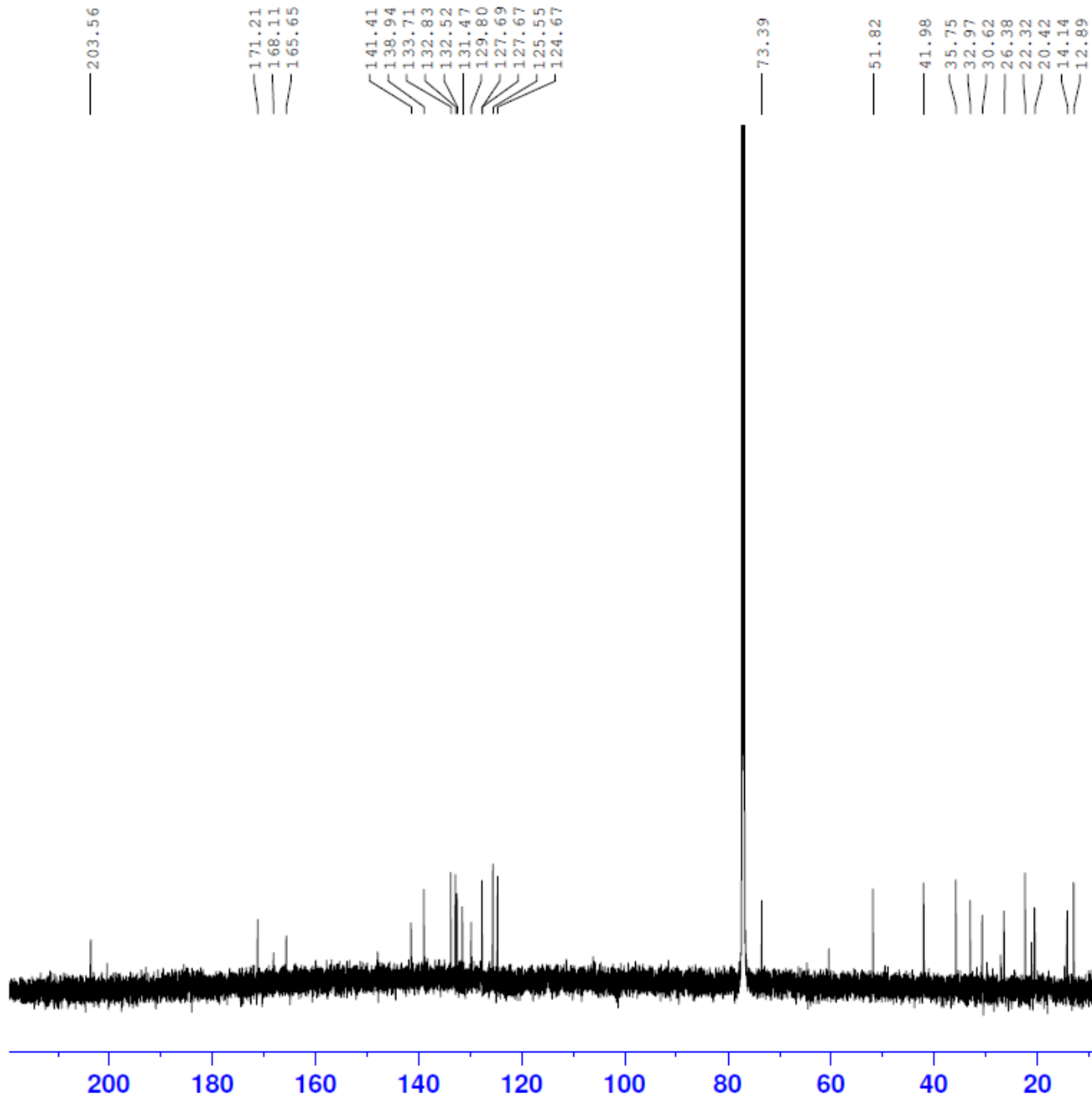


Current Data Parameters
 NAME 20200508 2NO2 II E
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200510
 Time 22.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 362
 DW 41.600 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300260 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20200508 2NO2 II E
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200511
 Time 4.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 6144
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028135 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200508 2NO2 II E
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200510
Time 22.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 5
DS 8
SWH 4950.495 Hz
FIDRES 2.417234 Hz
AQ 0.2068480 sec
RG 203
DW 101.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.92094696 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00020200 sec

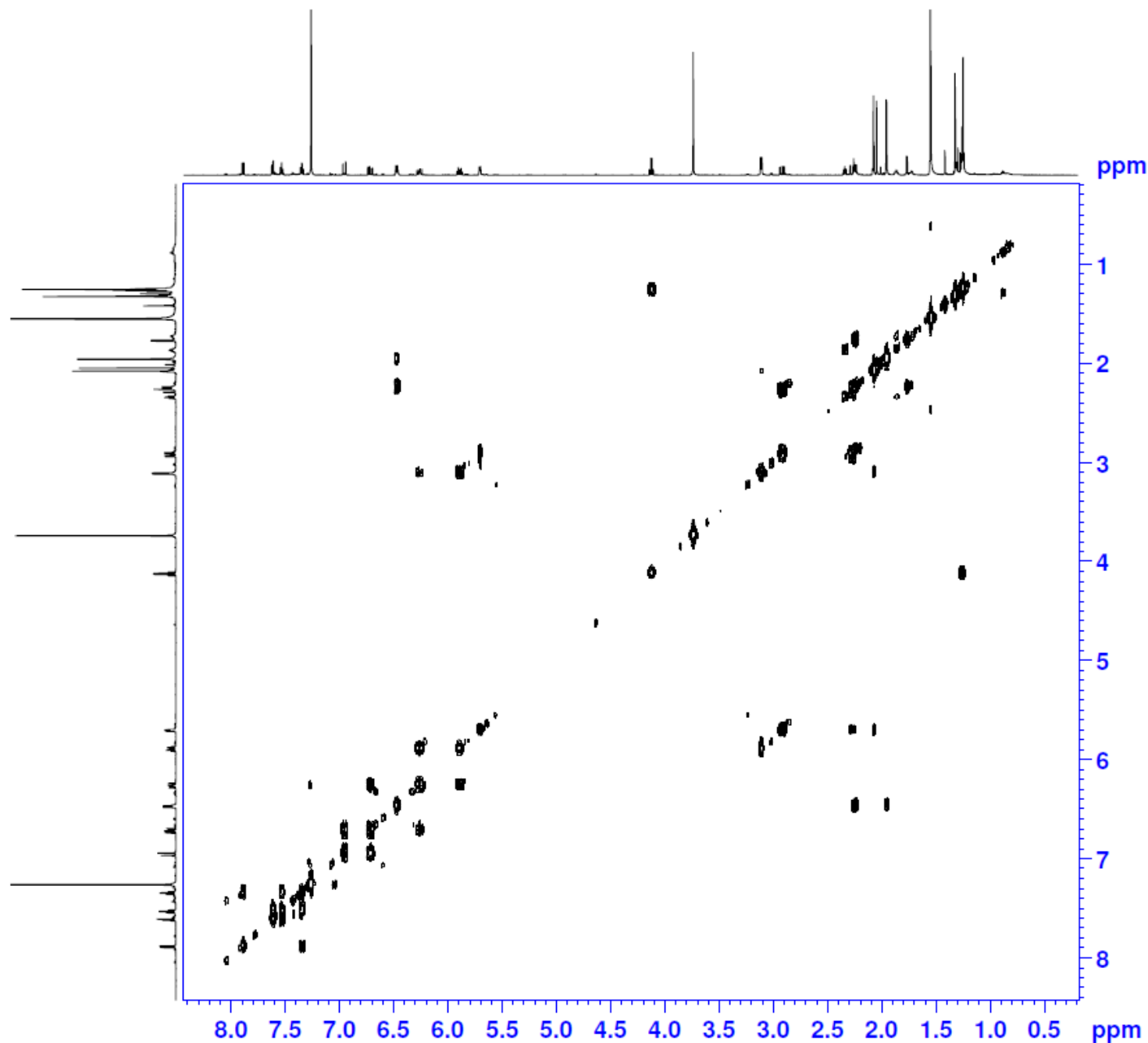
----- CHANNEL f1 -----
SFO1 600.1326129 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1326 MHz
FIDRES 38.675743 Hz
SW 8.249 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300254 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300285 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200508 2NO2 II E
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200511
Time 4.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDC13
NS 40
DS 16
SWH 5000.000 Hz
FIDRES 4.882813 Hz
AQ 0.1024000 sec
RG 2050
DW 100.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46313596 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1326057 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

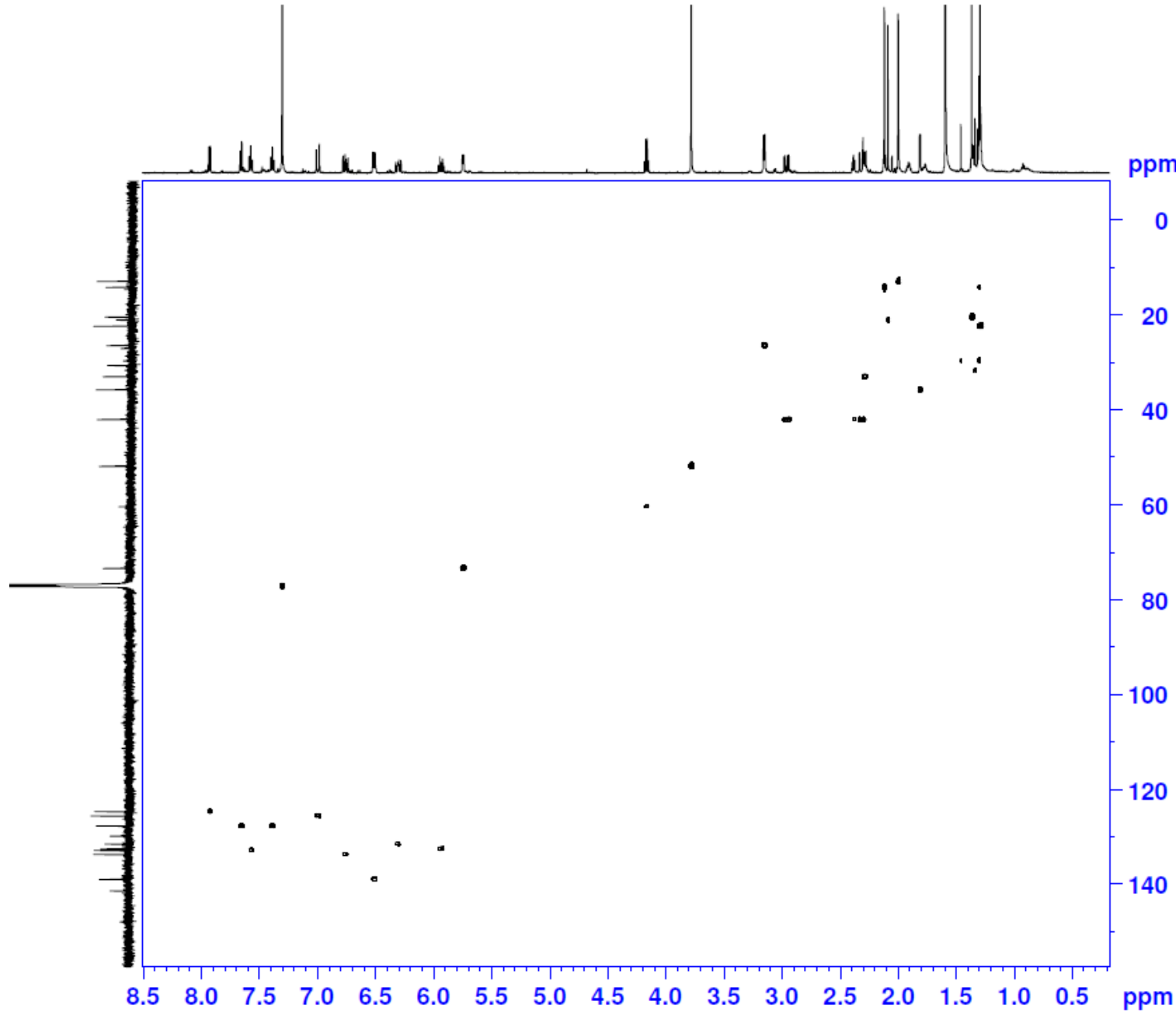
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 238
SFO1 150.9141 MHz
FIDRES 105.042015 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200511_2NO2_11_E
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200512
Time 6.08
INSTRUM spect
PROBHD 5 mm FASBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 50
DS 16
SWH 4950.495 Hz
FIDRES 1.208617 Hz
AQ 0.4136960 sec
RG 2050
DW 101.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.34189403 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1326199 MHz
NUC1 1H
P1 13.50 usec
F2 27.00 usec
PLW1 17.00000000 W

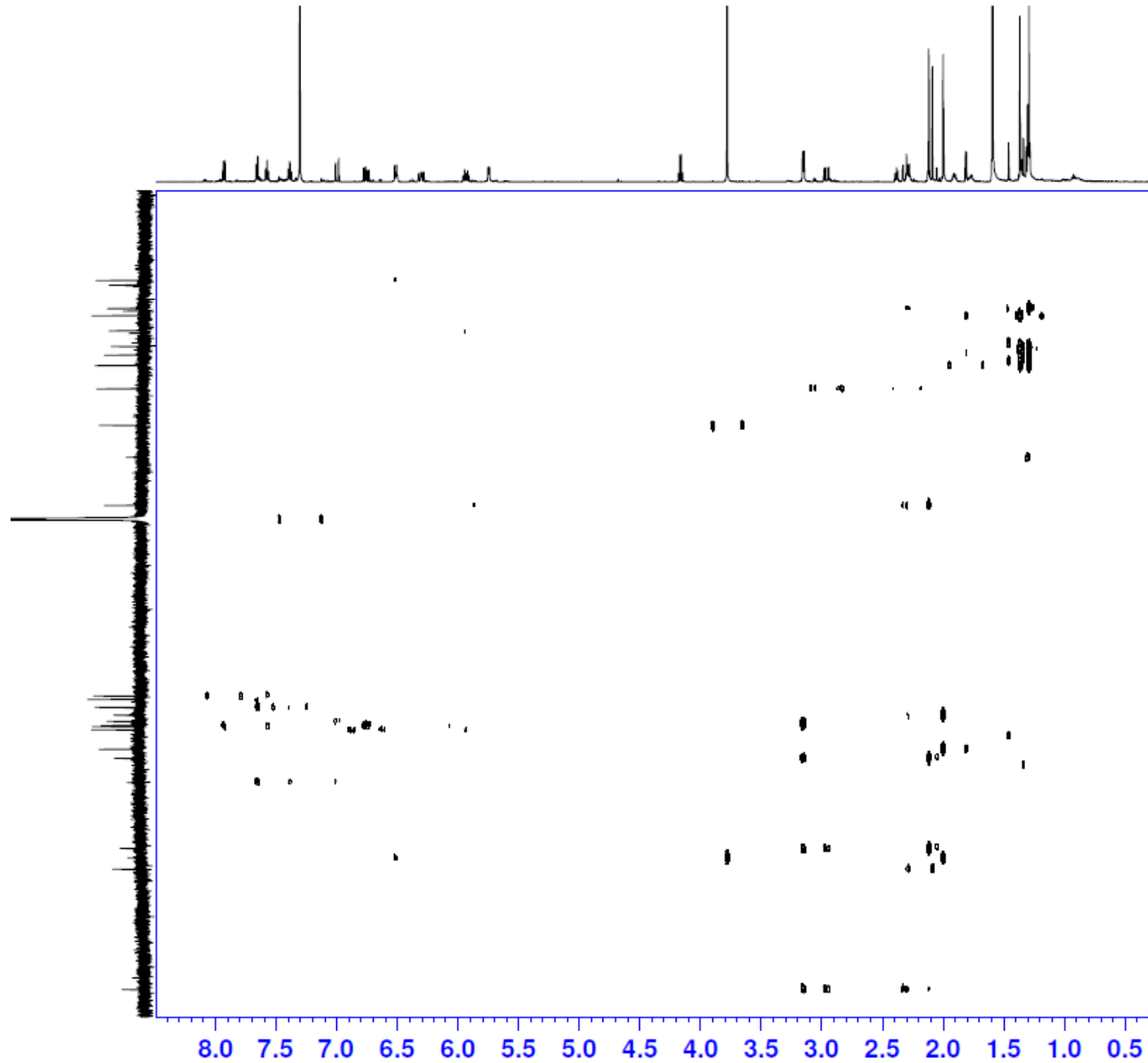
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

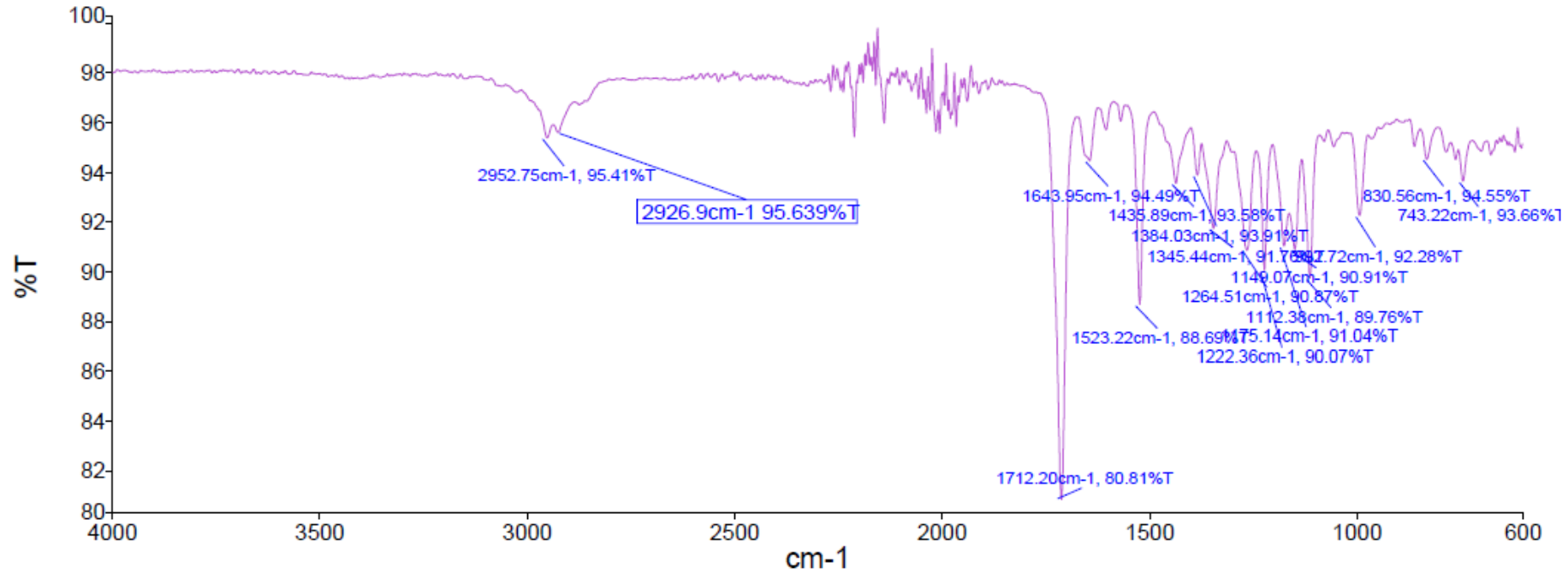


131b IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 12 June 2020 10:55 AM

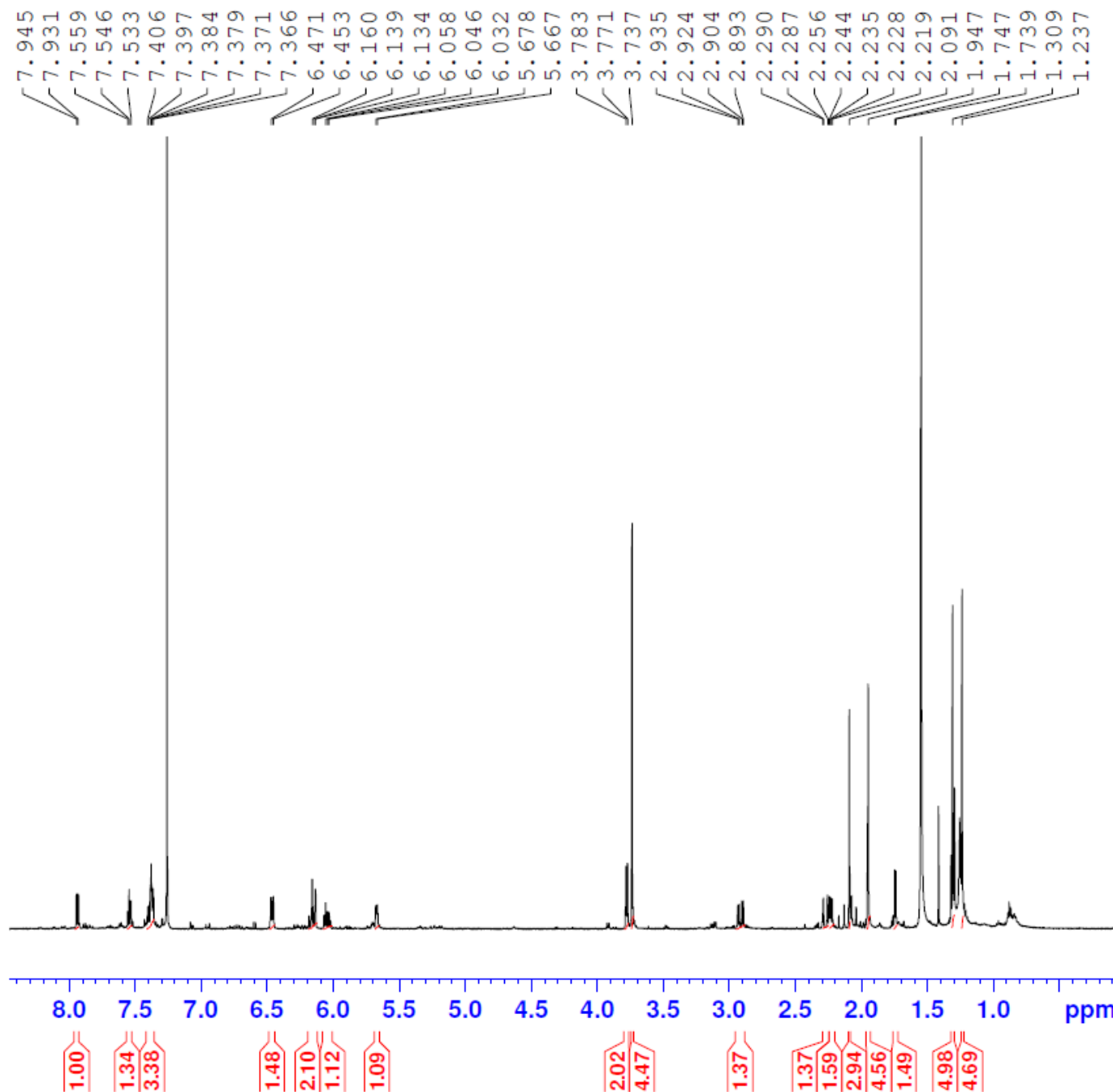
Analyst
Date

Analyst
Friday, 12 June 2020 10:55 AM



Sample Name	Description	Quality Checks
2NO2 II E	Sample	The Quality Checks do not report any warnings for the sample.

136b NMR Characterisation

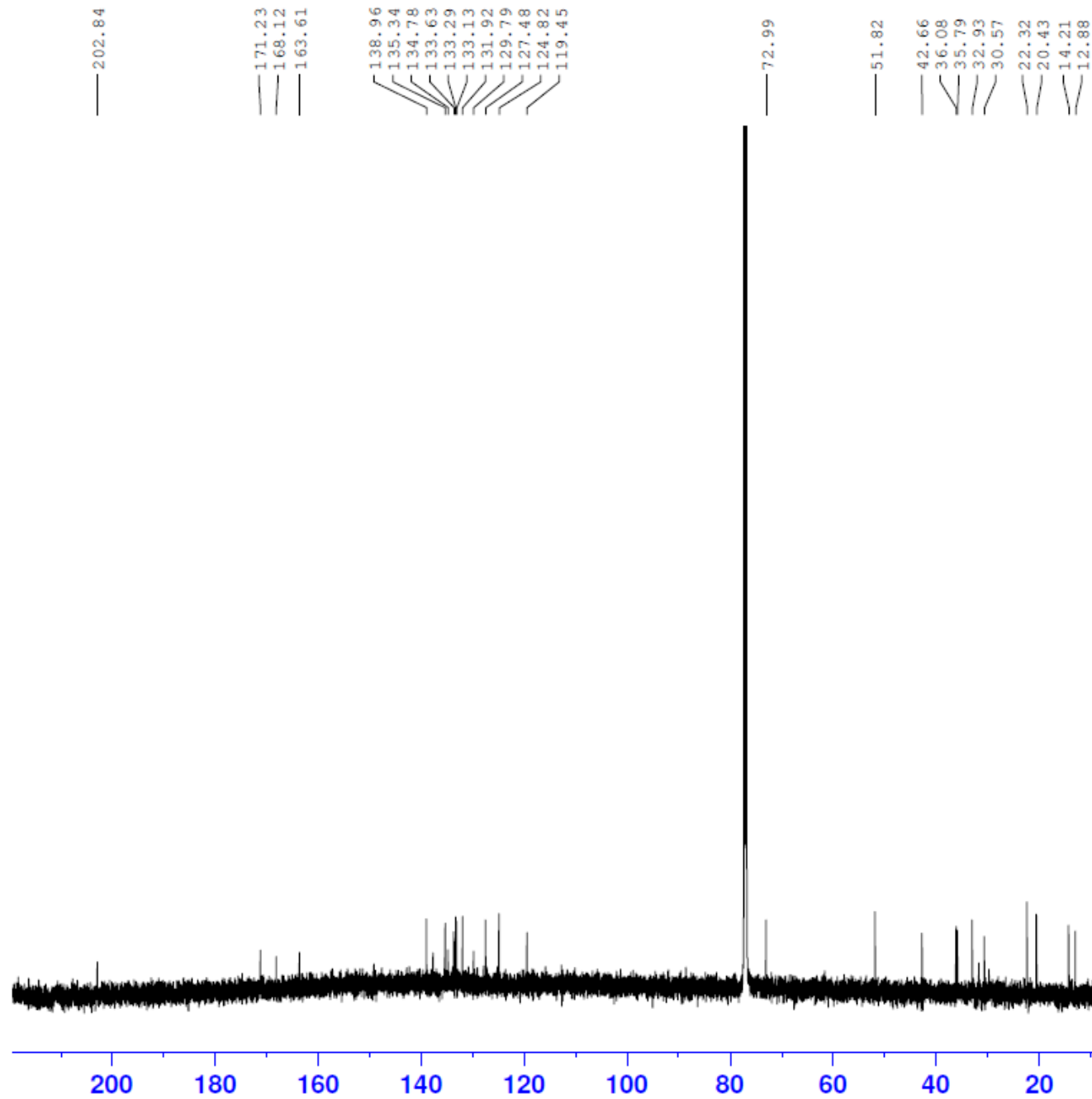


Current Data Parameters
 NAME 20200508 2NO2 II Z
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200510
 Time 8.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 362
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300265 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20200508 2NO2 II Z
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200510
 Time 13.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 6144
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028125 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200508 2NO2 II Z
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200510
Time 8.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
ID 2048
SOLVENT CDCl3
NS 5
DS 8
SWH 5050.505 Hz
FIDRES 2.466067 Hz
AQ 0.2027520 sec
RG 203
DW 99.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.92504299 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00019800 sec

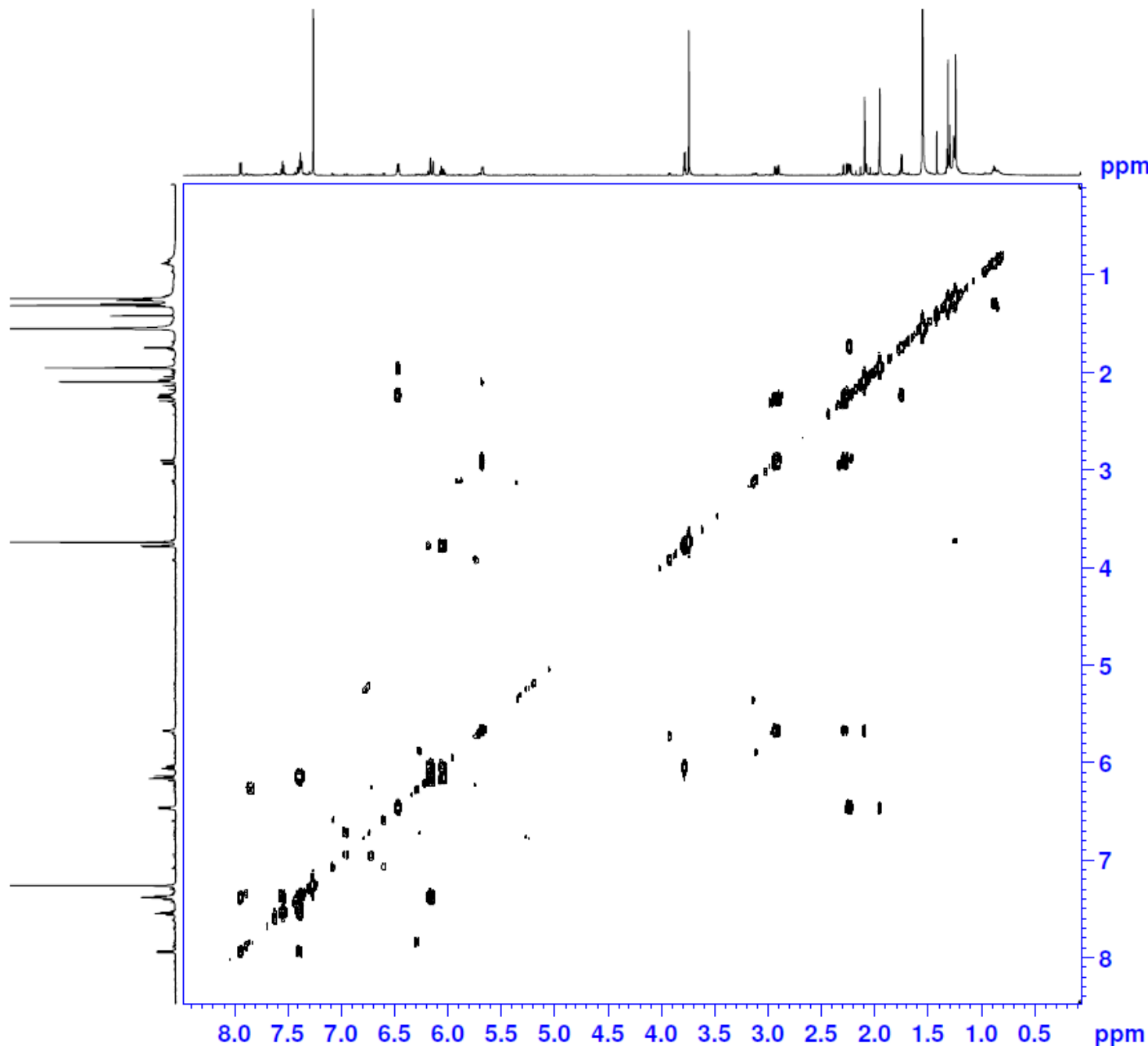
----- CHANNEL f1 -----
SFO1 600.1325881 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 128
SFO1 600.1326 MHz
FIDRES 39.457069 Hz
SW 8.416 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300258 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300253 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200508 2NO2 II Z
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200510
Time 14.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 40
DS 16
SWH 5050.505 Hz
FIDRES 4.932134 Hz
AQ 0.1013760 sec
RG 2050
DM 99.000 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D0 0.0000300 sec
D1 1.4641597 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1325968 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

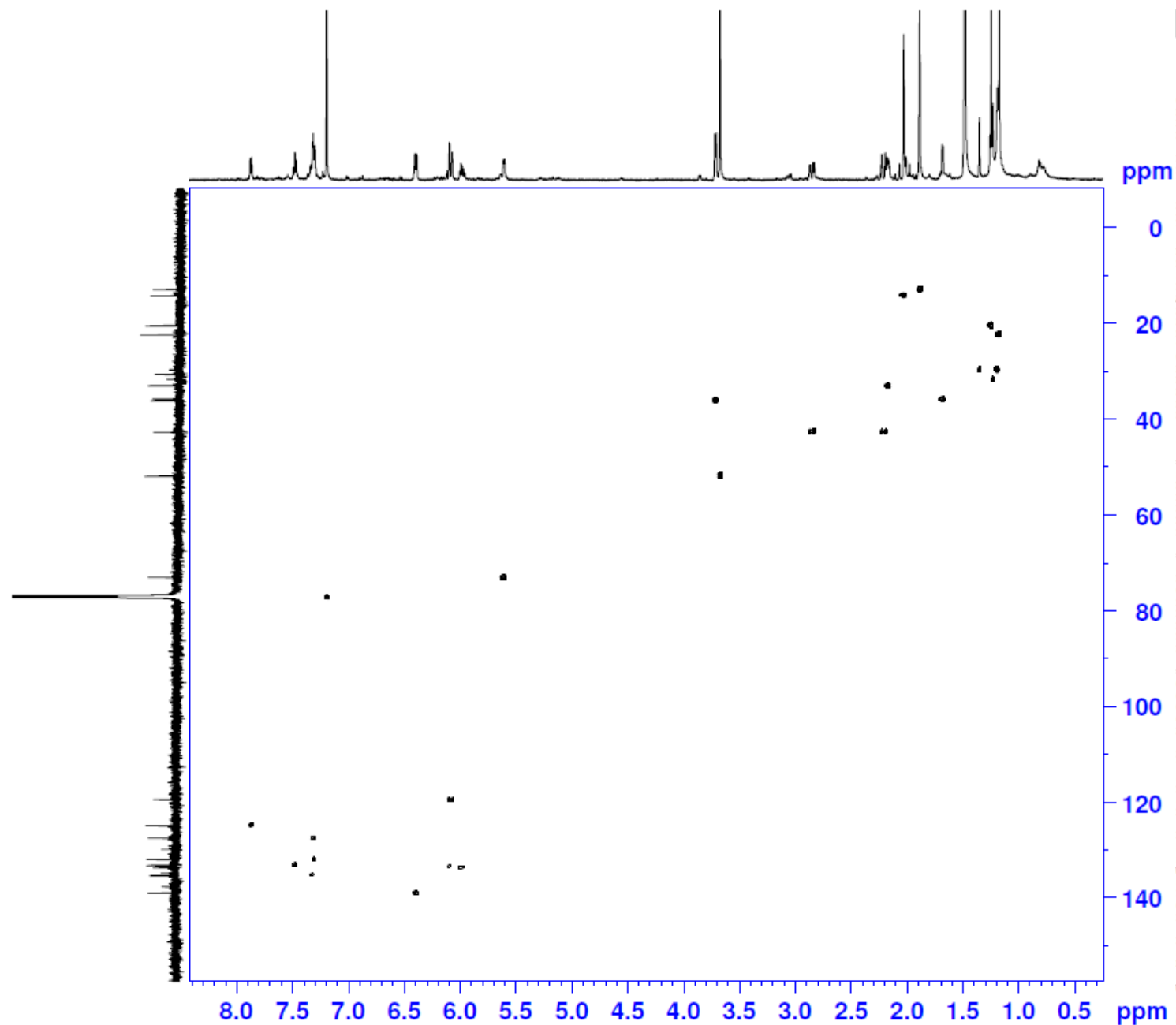
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300668 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200508 2NO2 II Z
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200510
Time 18.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 60
DS 16
SWH 5050.505 Hz
FIDRES 1.233033 Hz
AQ 0.4055040 sec
RG 2050
DW 99.000 usec
DE 6.50 usec
TE 298.1 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.35008597 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

==== CHANNEL f1 =====

SFO1 600.1325968 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

==== CHANNEL f2 =====

SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====

GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters

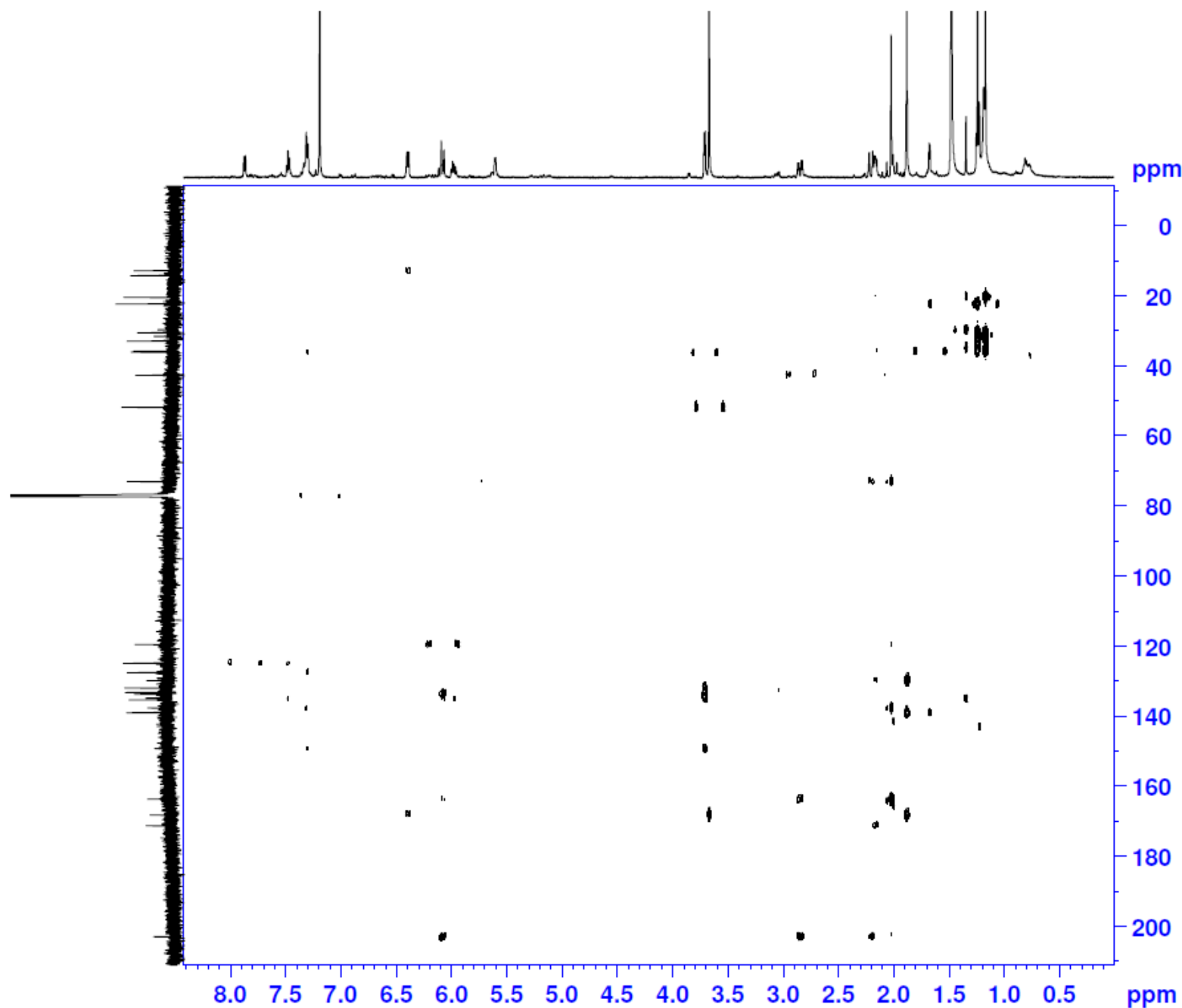
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters

SI 1024
SF 600.1300668 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

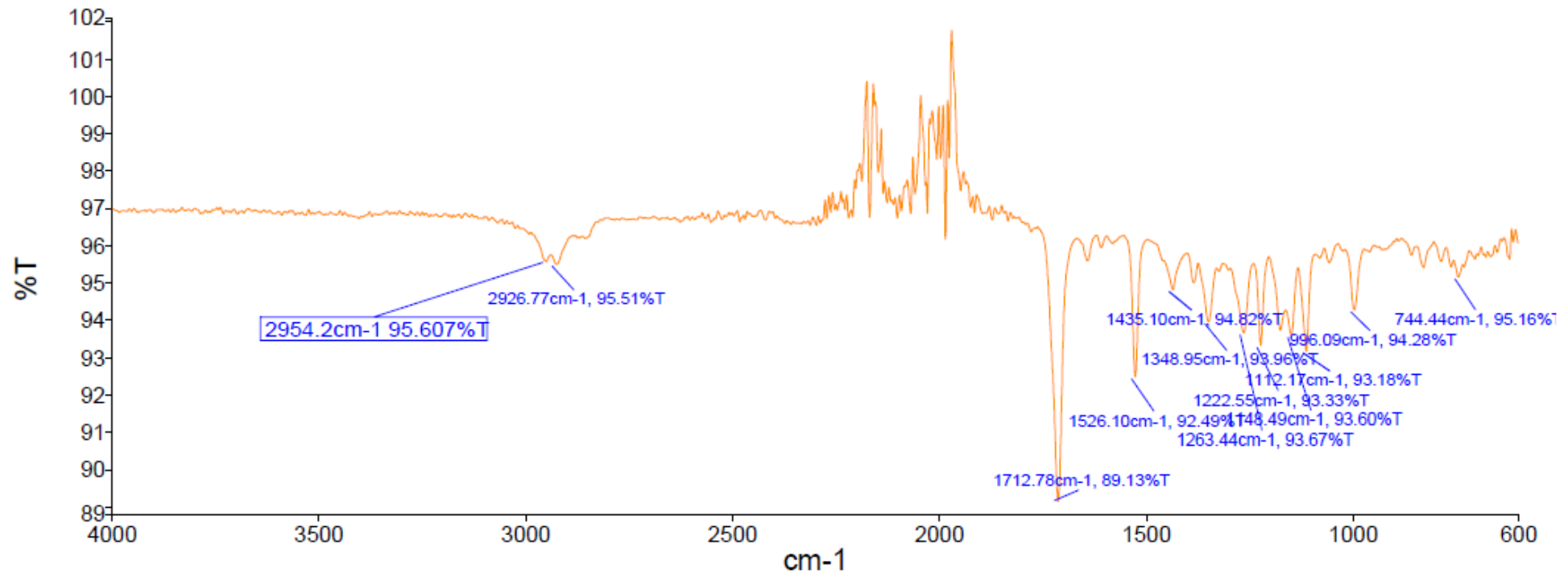


136b IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 12 June 2020 10:52 AM

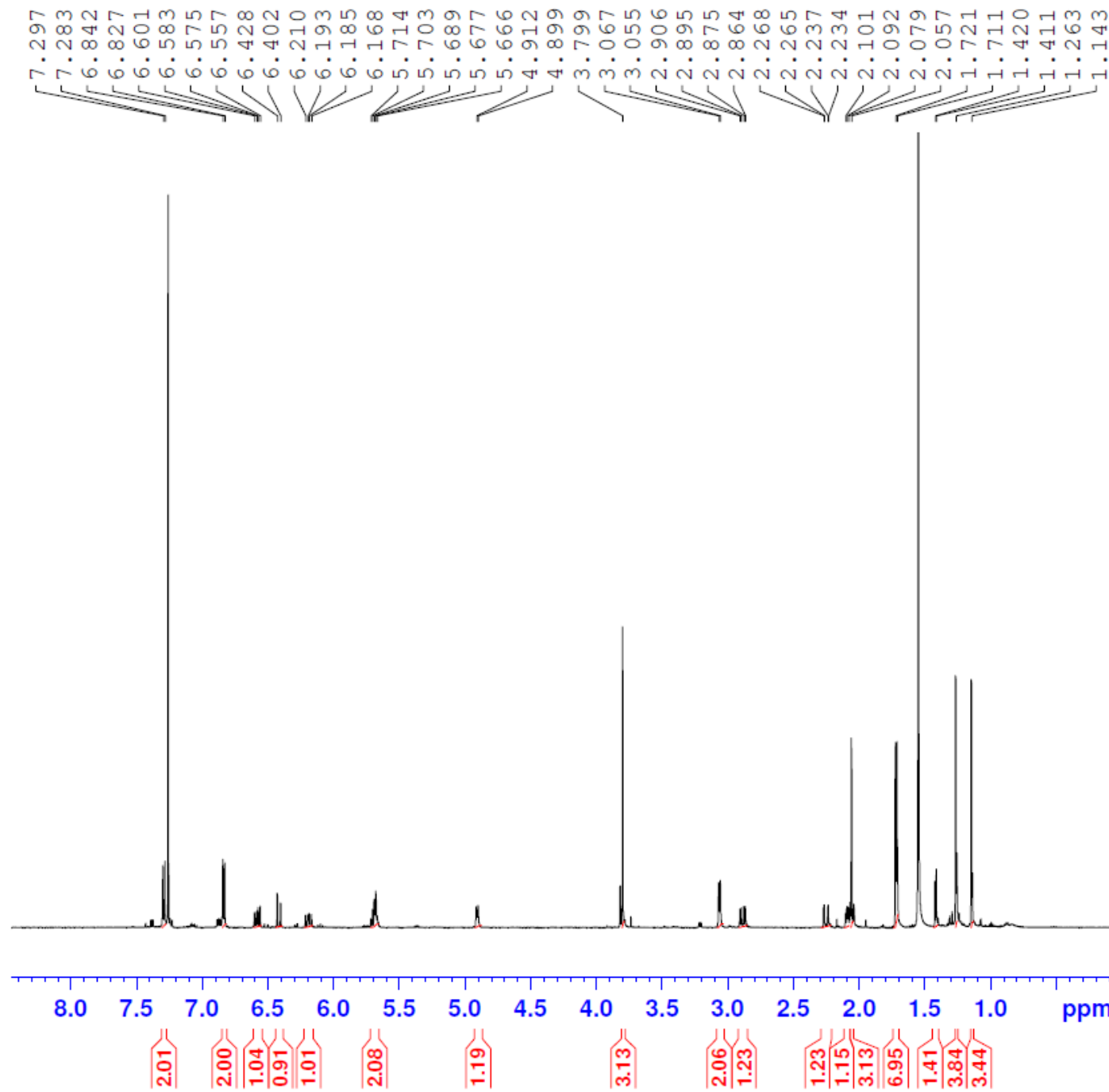
Analyst
Date

Analyst
Friday, 12 June 2020 10:52 AM



Sample Name	Description	Quality Checks
2NO2 II Mig	Sample	The Quality Checks do not report any warnings for the sample.

¹³2a NMR Characterisation

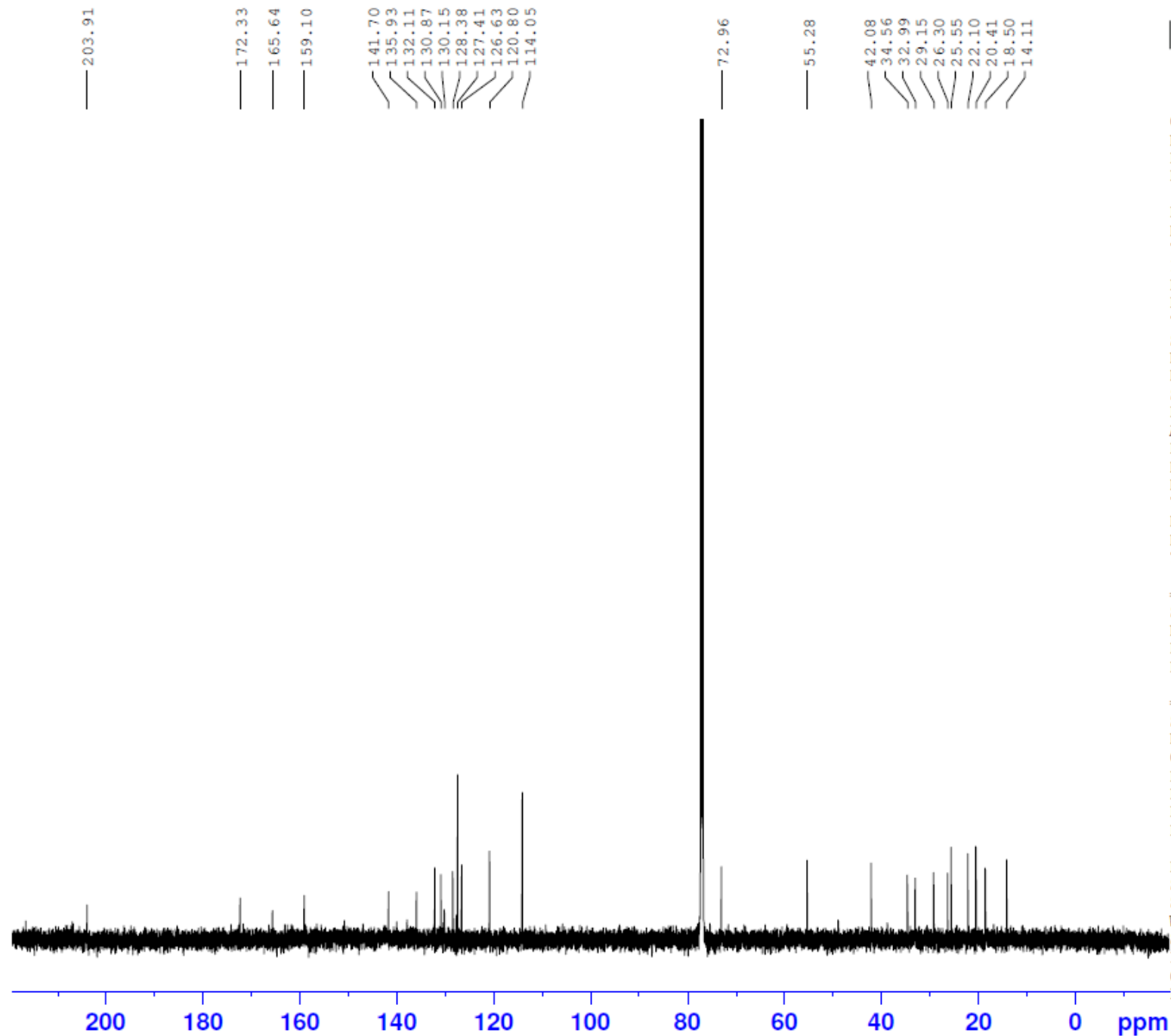


Current Data Parameters
NAME 20200522 40Me I E
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200524
Time 7.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 362
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300279 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters

NAME 20200522 40Me I E
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200524
Time 12.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6144
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====

SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====

SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters

SI 32768
SF 150.9028126 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20200522 40Me I E
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200524
Time 7.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 3
DS 4
SWH 4629.629 Hz
FIDRES 2.260561 Hz
AQ 0.2211840 sec
RG 2050
DW 108.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00009081 sec
D1 1.91726100 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021600 sec

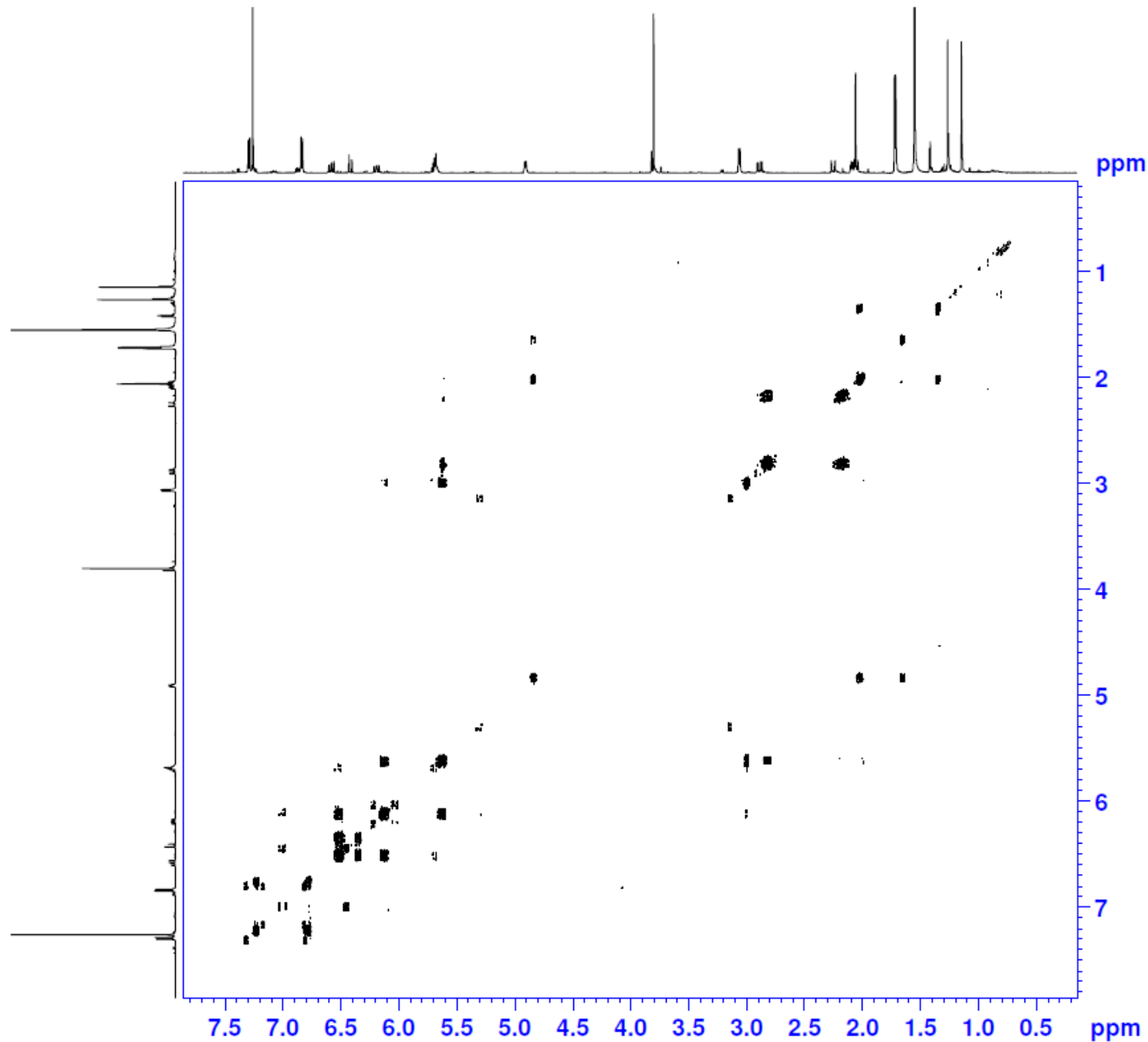
----- CHANNEL f1 -----
SFO1 600.1324690 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1325 MHz
FIDRES 18.084490 Hz
SW 7.714 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300673 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300673 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200522 40ms 1 K
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200524
Time 12.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 40
DS 16
SWH 4629.629 Hz
FIDRES 4.521122 Hz
AQ 0.1105920 sec
RG 2050
DW 108.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45494401 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1324690 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

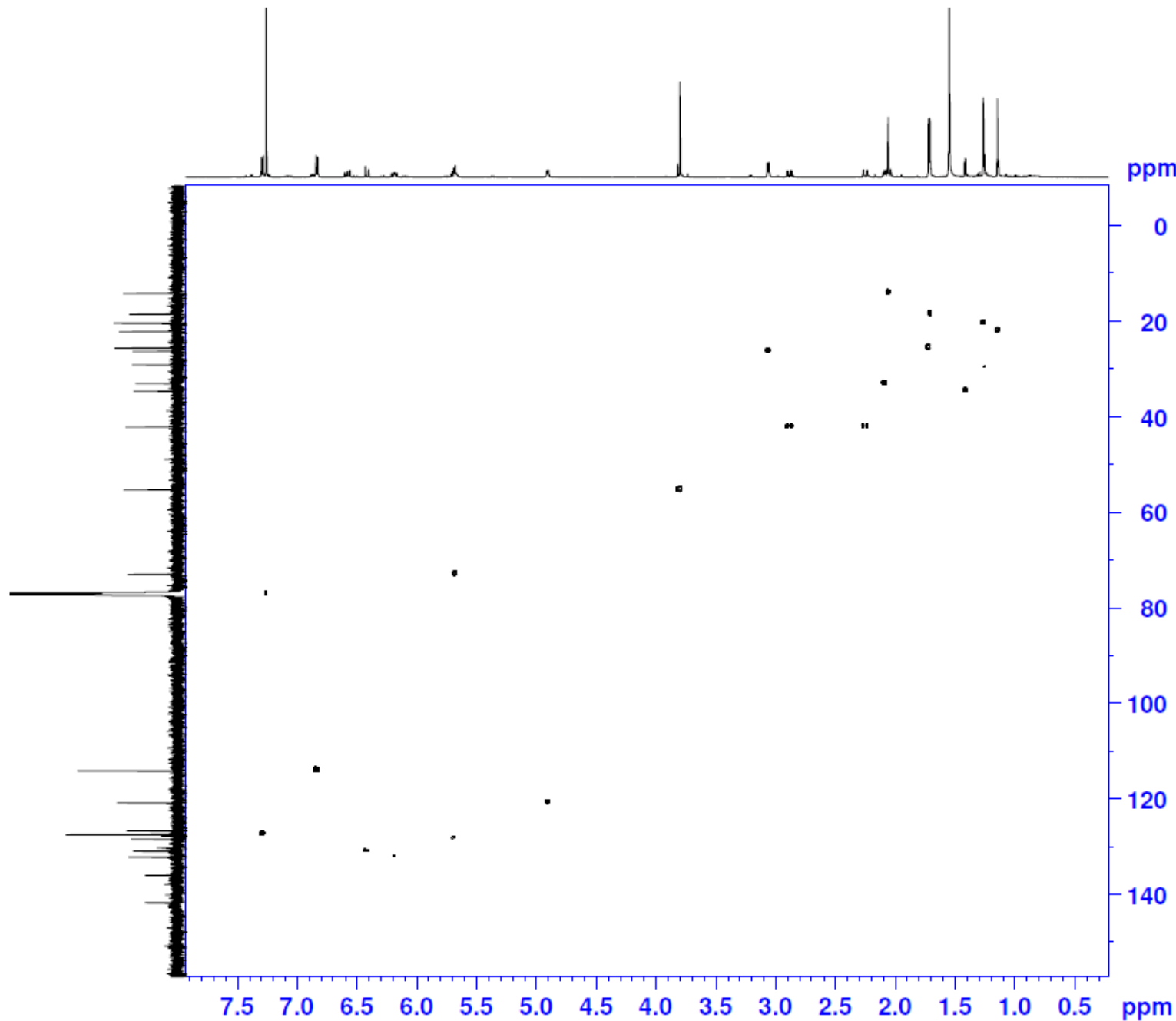
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300246 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028395 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200522 40mg 1 E
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200524
Time 17.27

INSTRUM spect
PROBHD 5 mm PABBO BB/
FULPROG hmbcgpndqf
ID 4096
SOLVENT CDCl3
NS 60
DS 16
SWH 4629.629 Hz
FIDRES 1.130281 Hz
AQ 0.4423680 sec
RG 2050
DW 108.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.31322205 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL F1 =====
SFO1 600.1324690 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

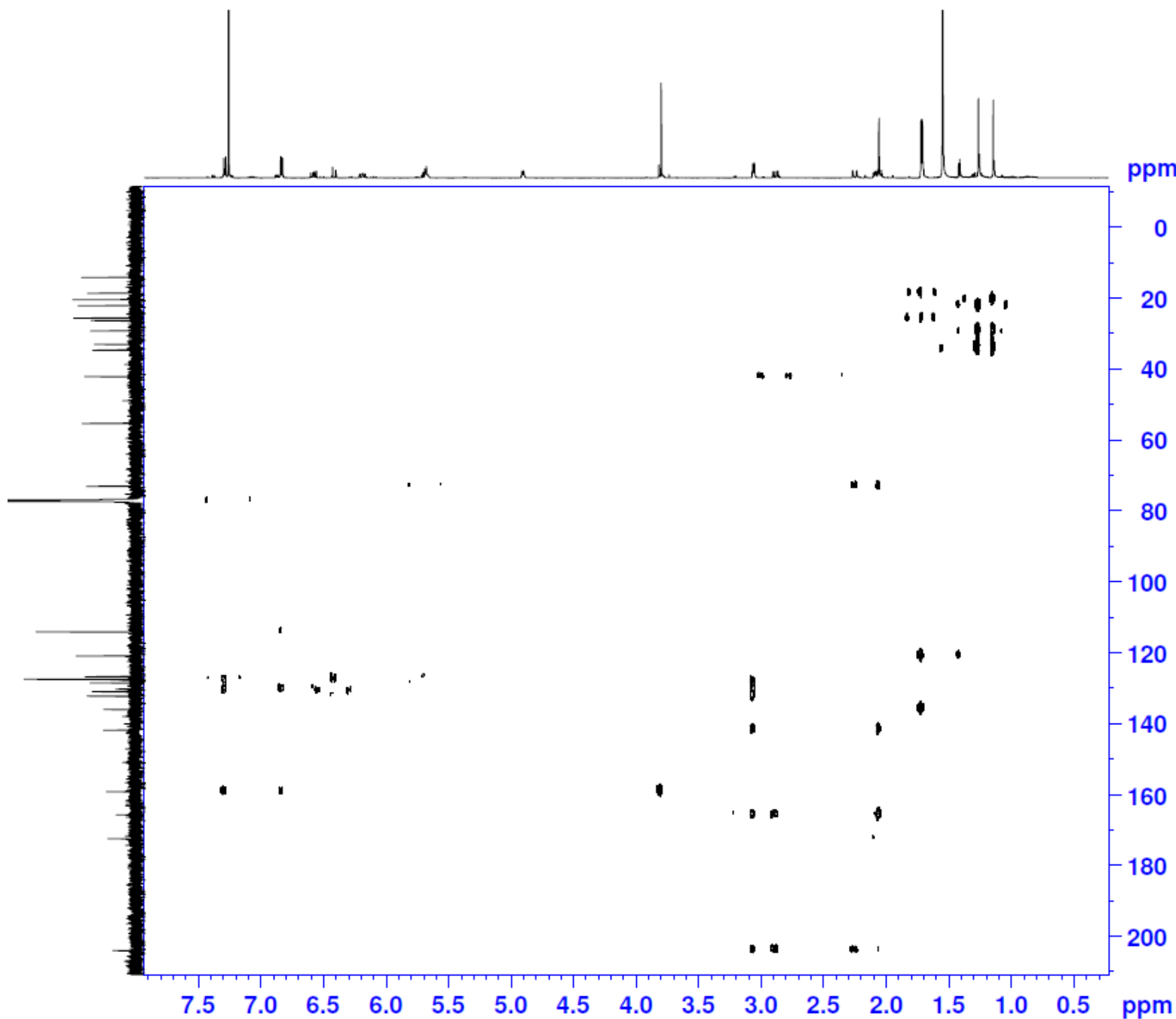
===== CHANNEL F2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

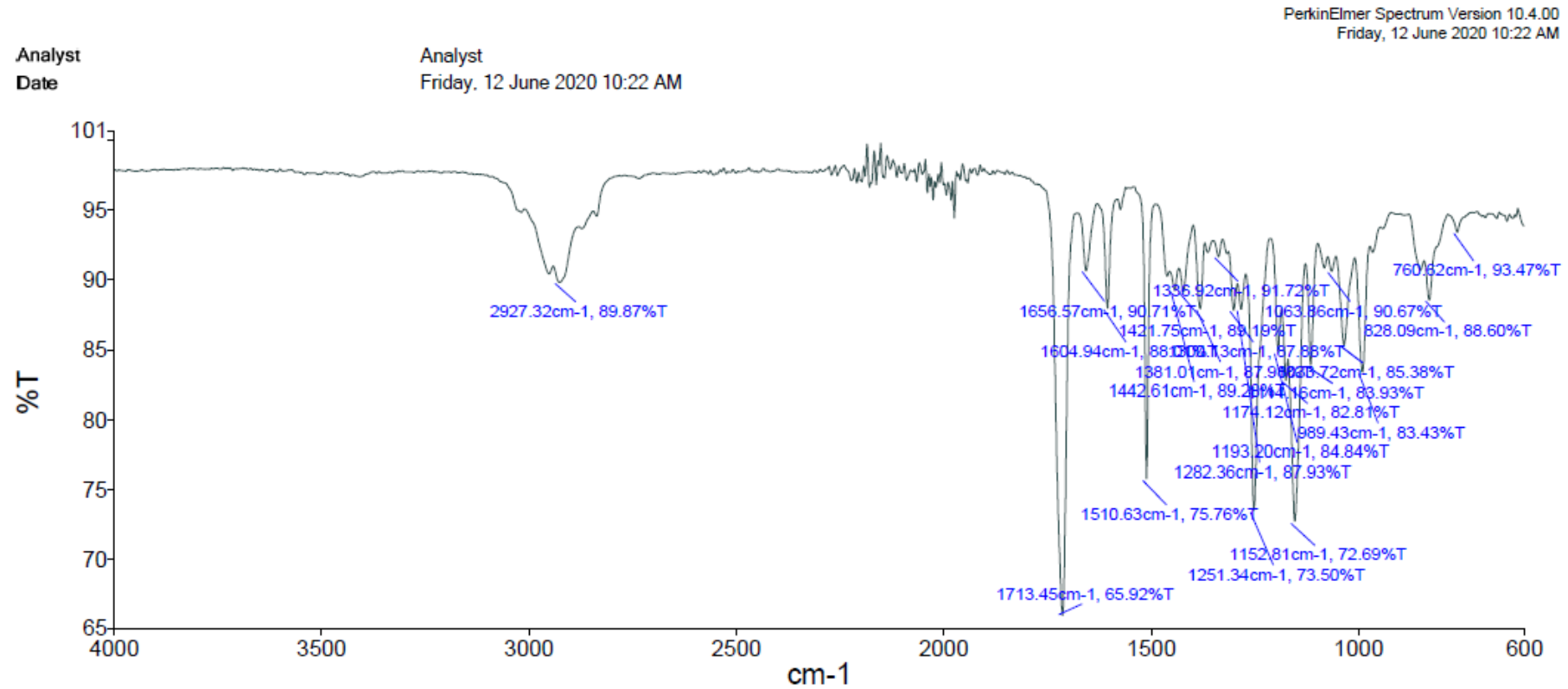
F1 - Acquisition parameters
ID 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300226 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028515 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

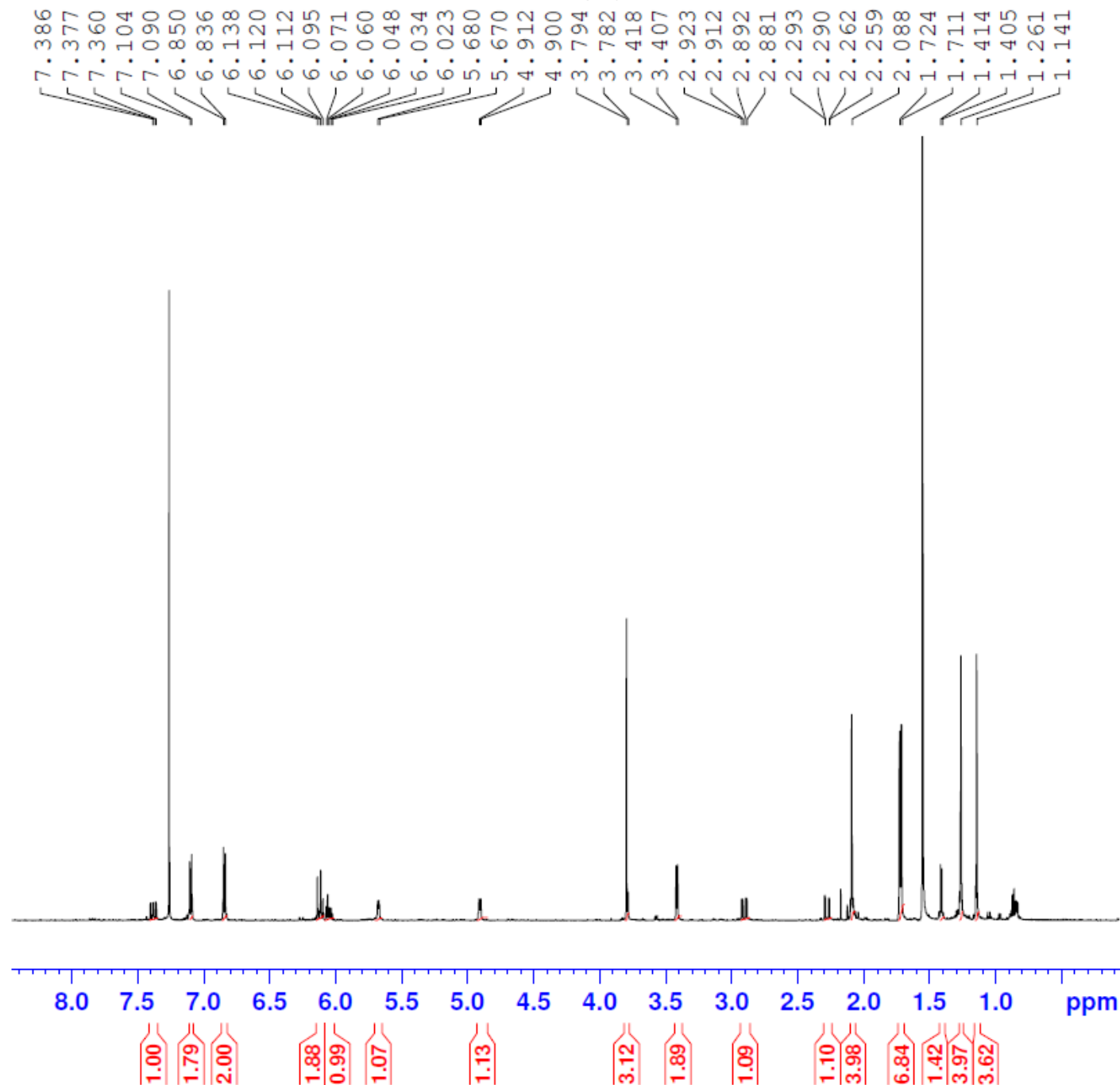


132a IR Spectrum



Sample Name	Description	Quality Checks
4OMe I E	Sample	The Quality Checks do not report any warnings for the sample.

¹³⁷a NMR Characterisation

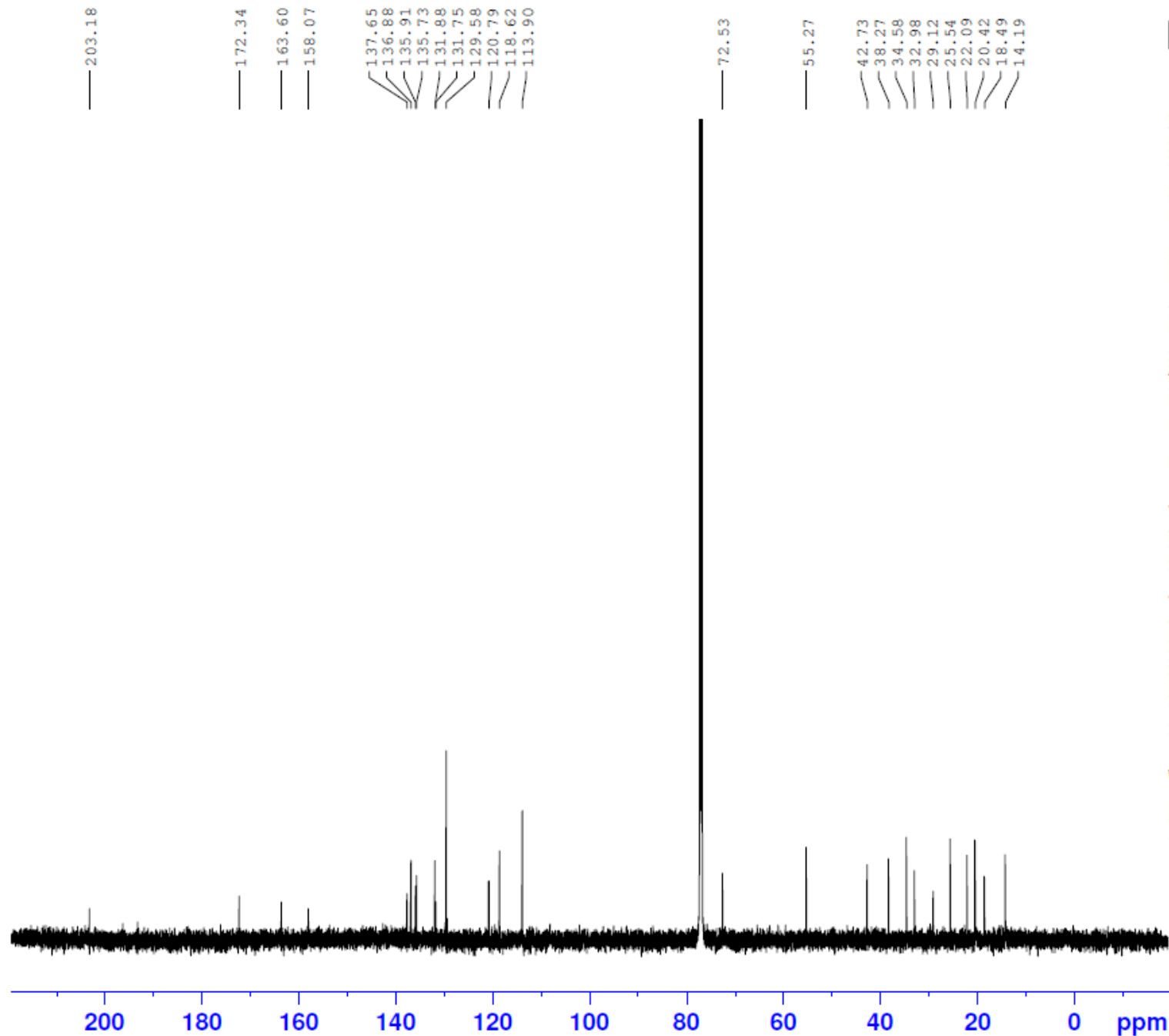


Current Data Parameters
 NAME 20200522 40Me I migration
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200523
 Time 18.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 362
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300259 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20200522 40Me I migration
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200523
 Time 23.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 6144
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

----- CHANNEL f2 -----
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028144 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200522 40Me 1 migration
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200523
Time 18.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphp
TD 2048
SOLVENT CDCl3
NS 3
DS 4
SWH 4629.629 Hz
FIDRES 2.260561 Hz
AQ 0.2211840 sec
RG 2050
DW 108.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00009081 sec
D1 1.91726100 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021600 sec

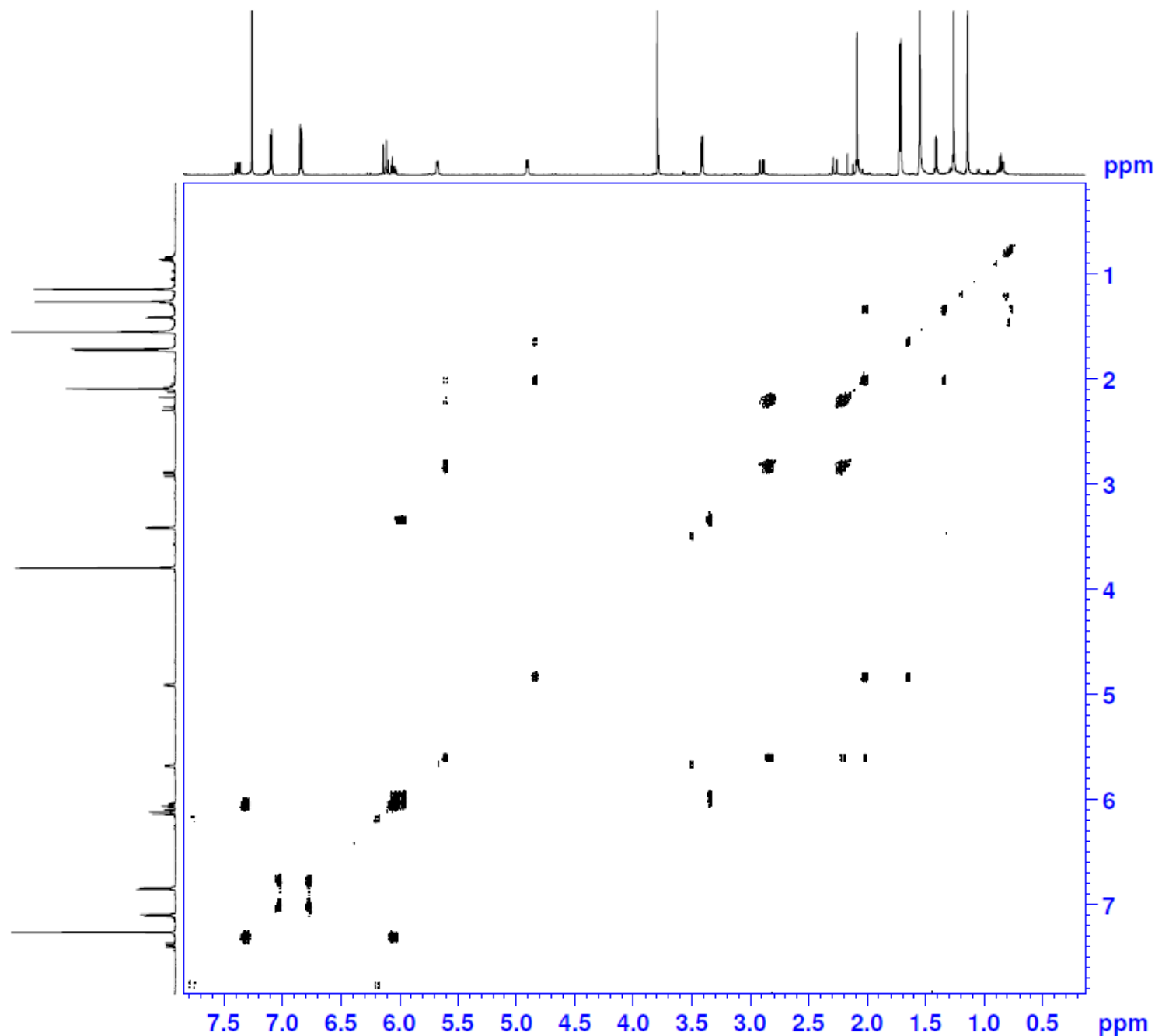
----- CHANNEL f1 -----
SFO1 600.1324621 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1325 MHz
FIDRES 18.084490 Hz
SW 7.714 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.1300673 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300673 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200522 40Ma 1 migration
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200523
Time 23.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcaltq
TD 1024
SOLVENT CDCl3
NS 35
DS 16
SWH 4629.629 Hz
FIDRES 4.521122 Hz
AQ 0.1105920 sec
RG 2050
DW 108.000 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45494401 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS

===== CHANNEL f1 =====
SFO1 600.1324621 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
P1W1 17.00000000 W

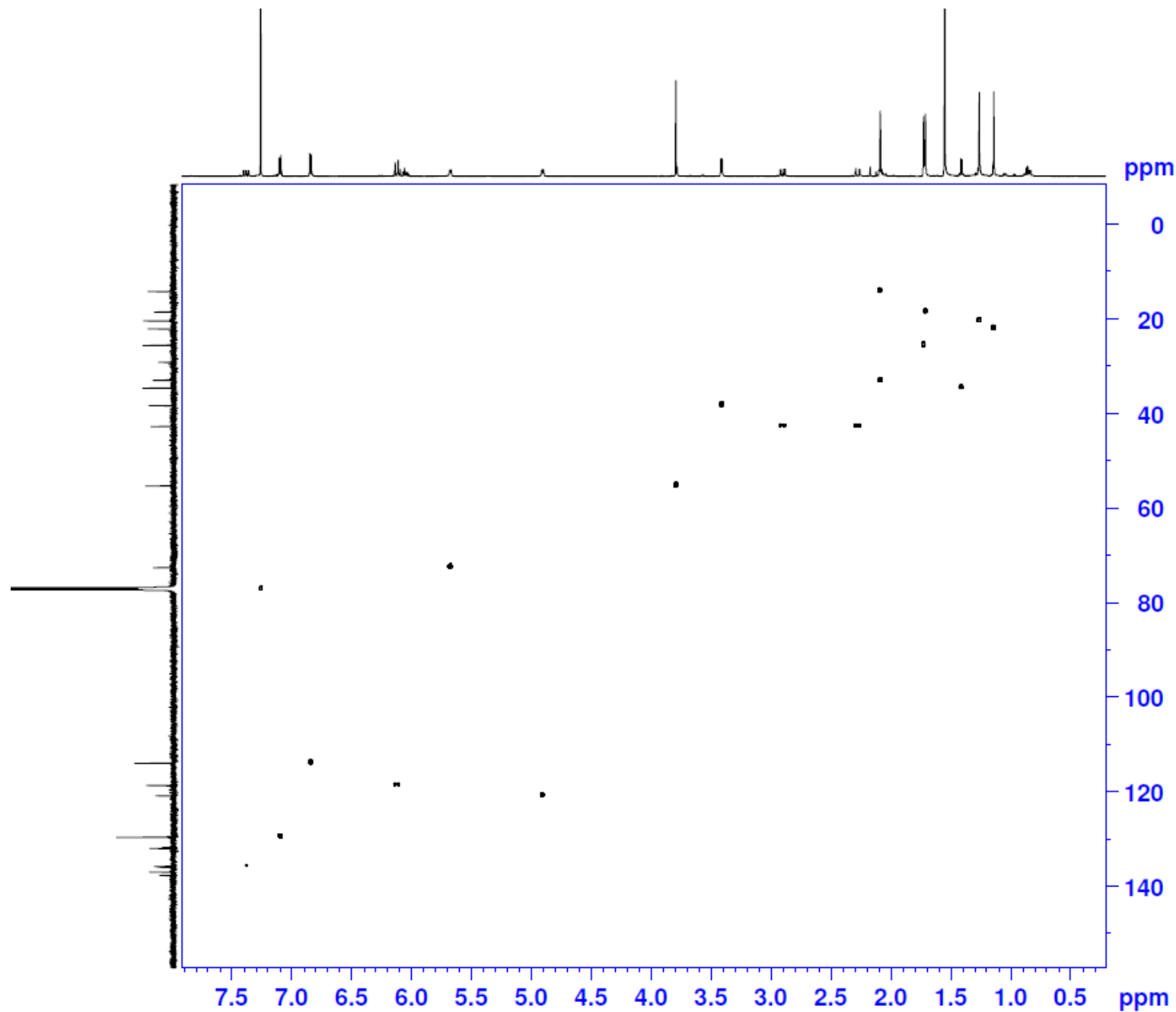
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
P1W2 79.98300171 W
P1W12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300243 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028395 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200522 40Me 1 migration
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200524
Time 3.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmcgpnqf
TD 4096
SOLVENT CDCl3
NS 50
DS 16
SWH 4629.629 Hz
FIDRES 1.130281 Hz
AQ 0.4423680 sec
RG 2050
DW 108.000 usec
DE 6.50 usec
TE 298.2 K
CNS113 8.0000000
D0 0.00000300 sec
D1 1.31322205 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1324621 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

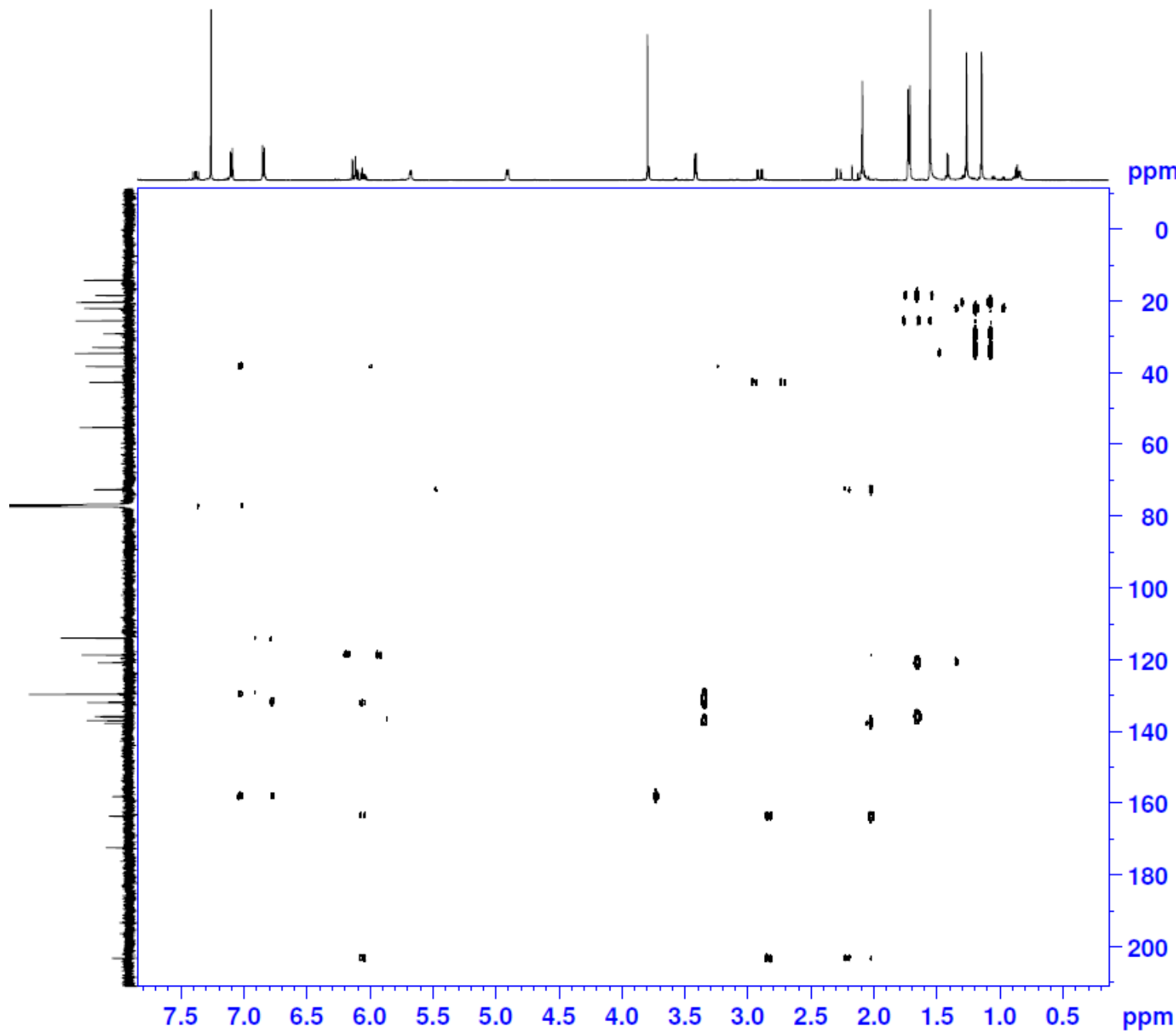
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300673 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

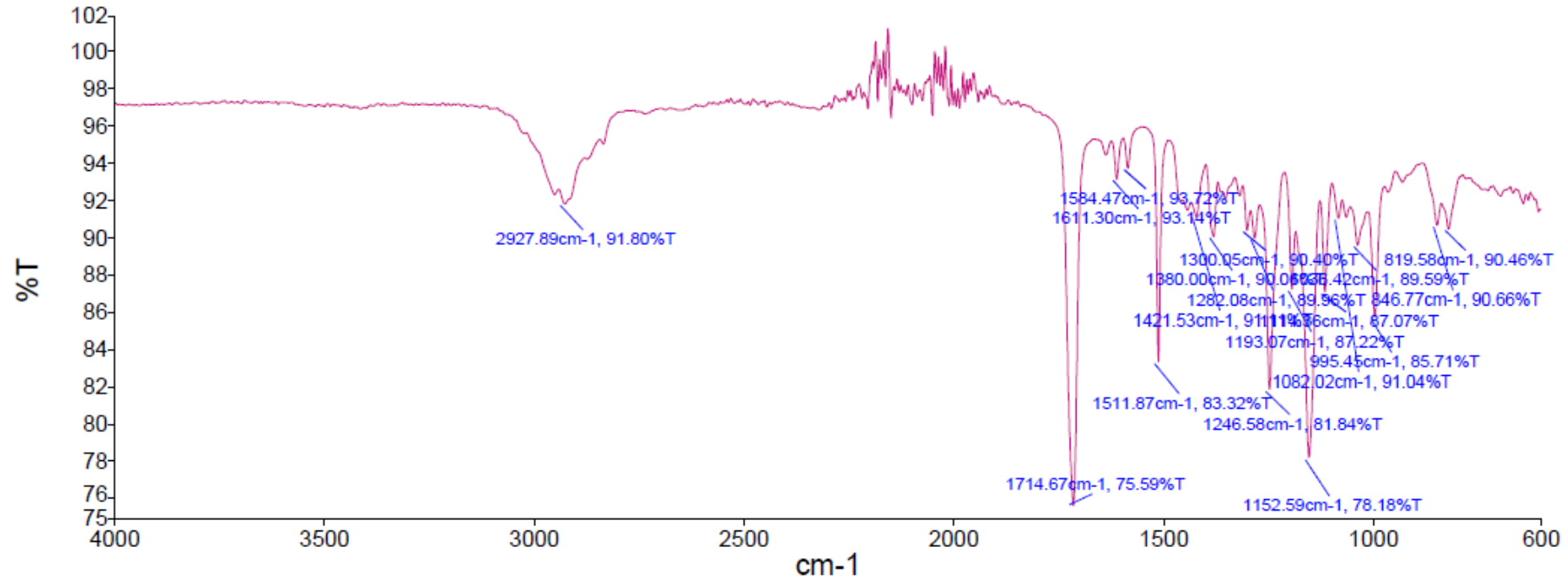


137a IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 12 June 2020 10:20 AM

Analyst
Date

Analyst
Friday, 12 June 2020 10:20 AM



Sample Name	Description	Quality Checks
4OMe I Mig	Sample	The Quality Checks do not report any warnings for the sample.

132b NMR Characterisation

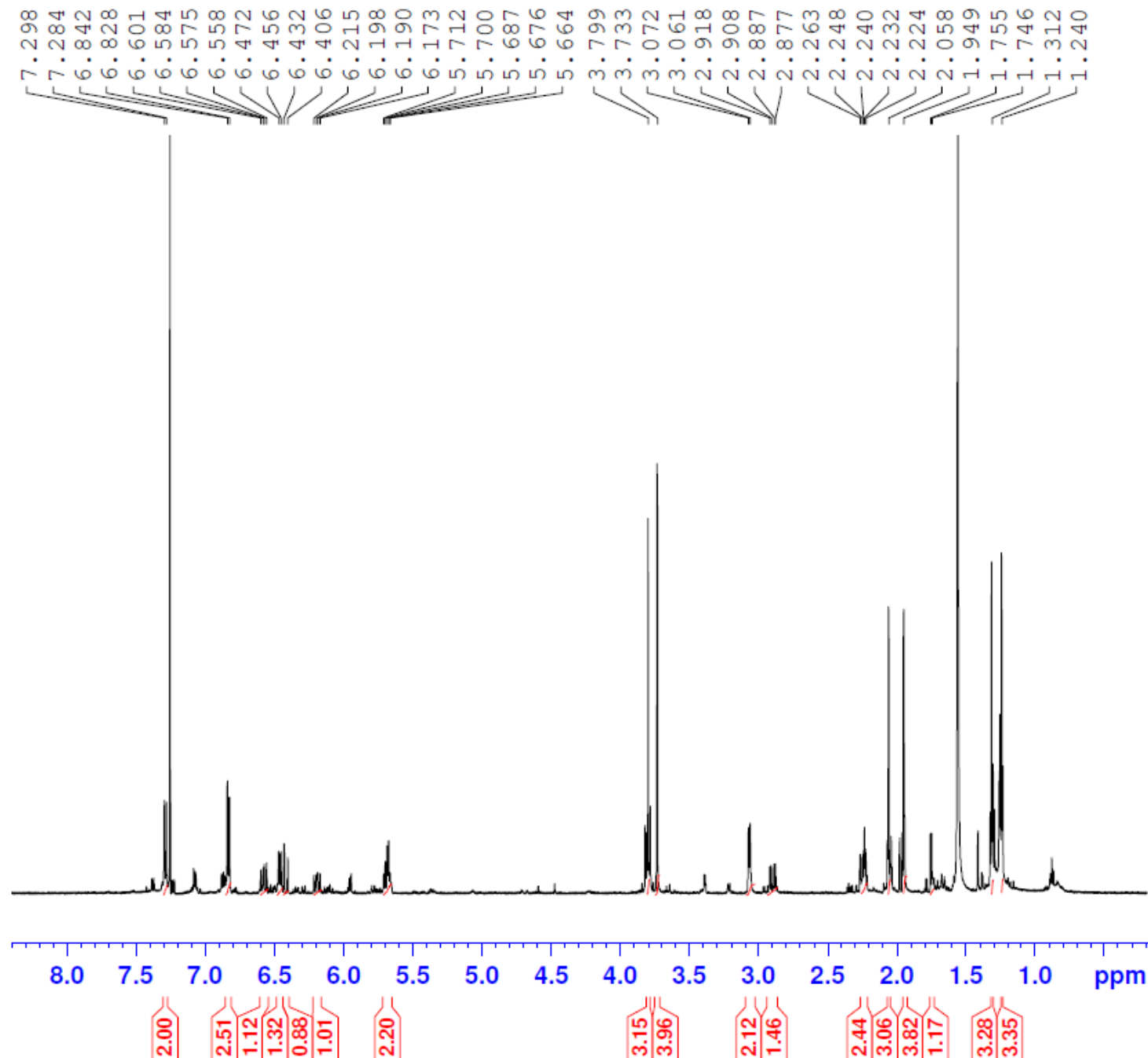


Current Data Parameters
 NAME 20200807 40Me II E
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200808
 Time 12.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 322
 DW 41.600 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300277 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00





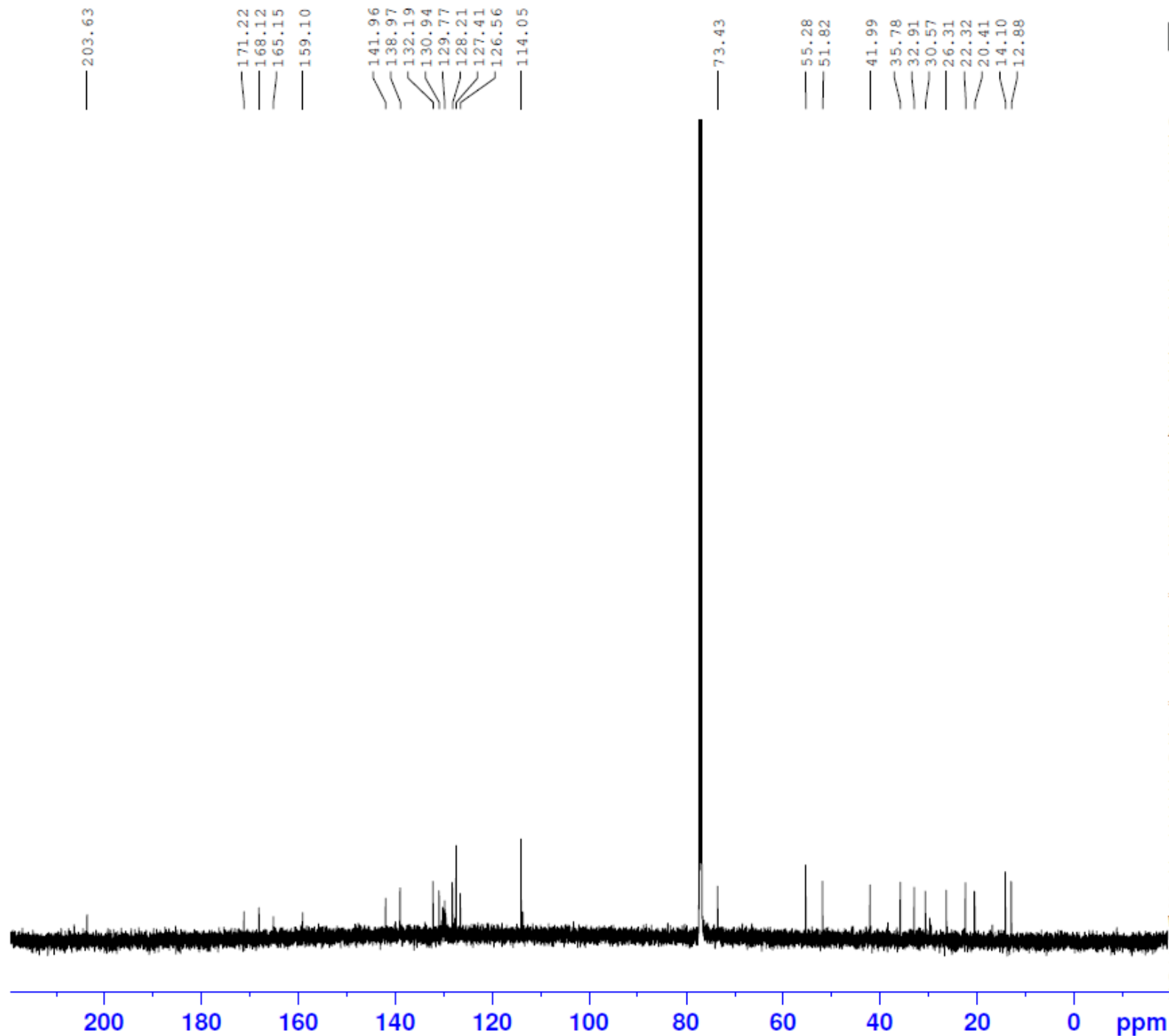
Current Data Parameters
NAME 20200807 4OMe II E
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200808
Time 14.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028145 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
NAME 20200807 40Me II E
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200808
Time 12.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 3
DS 4
SWH 4672.897 Hz
FIDRES 2.281688 Hz
AQ 0.2191360 sec
RG 2050
DW 107.000 usec
DE 6.50 usec
TE 298.1 K
D0 0.00008981 sec
D1 1.91930902 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021400 sec

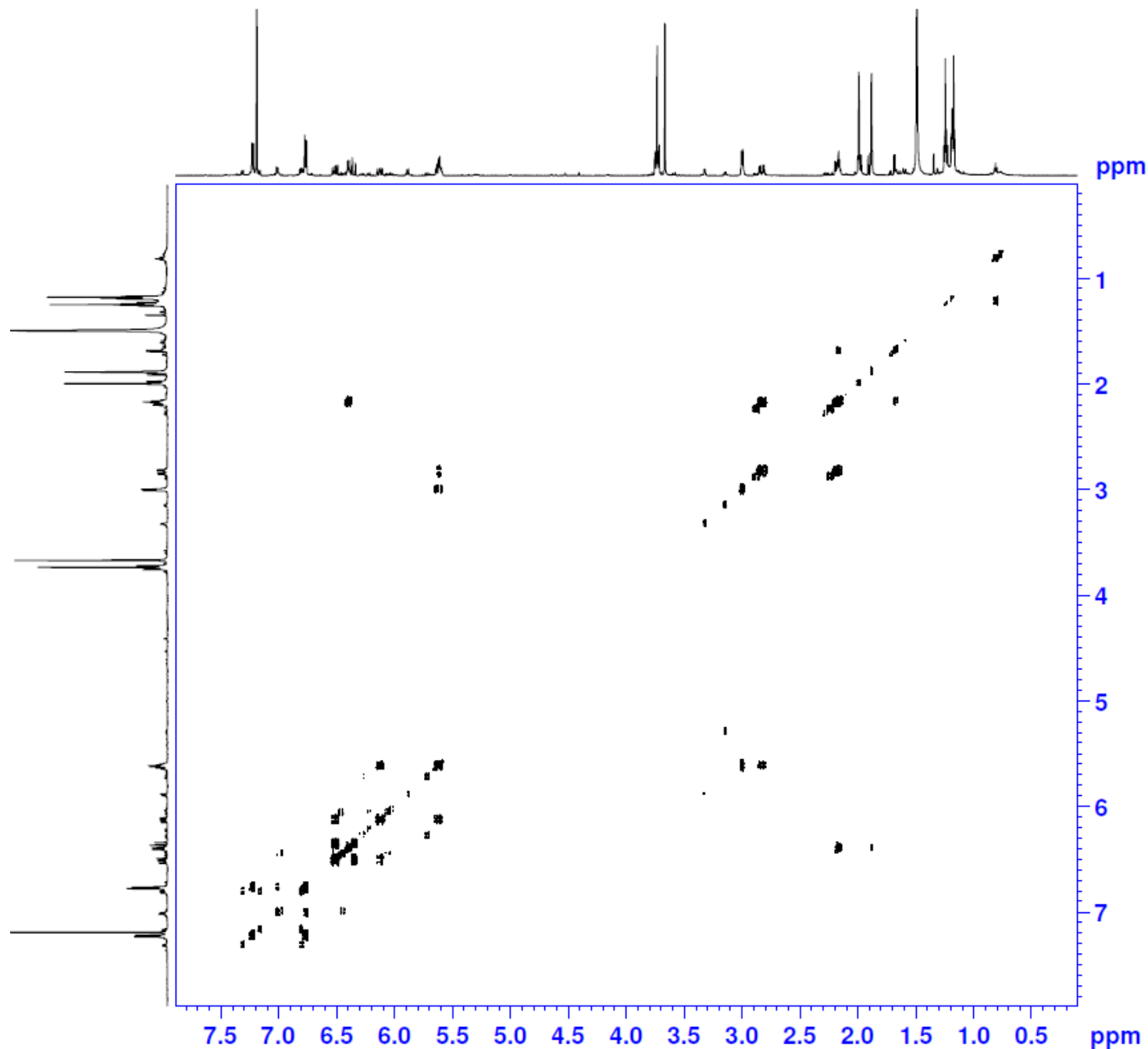
----- CHANNEL f1 -----
SFO1 600.1324671 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1325 MHz
FIDRES 18.253504 Hz
SW 7.786 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300675 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300675 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200807 4cMe II K
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200808
Time 14.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 25
DS 16
SWH 4672.897 Hz
FIDRES 4.563376 Hz
AQ 0.1095680 sec
RG 2050
DW 107.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45596802 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1324671 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
P1W1 17.00000000 W

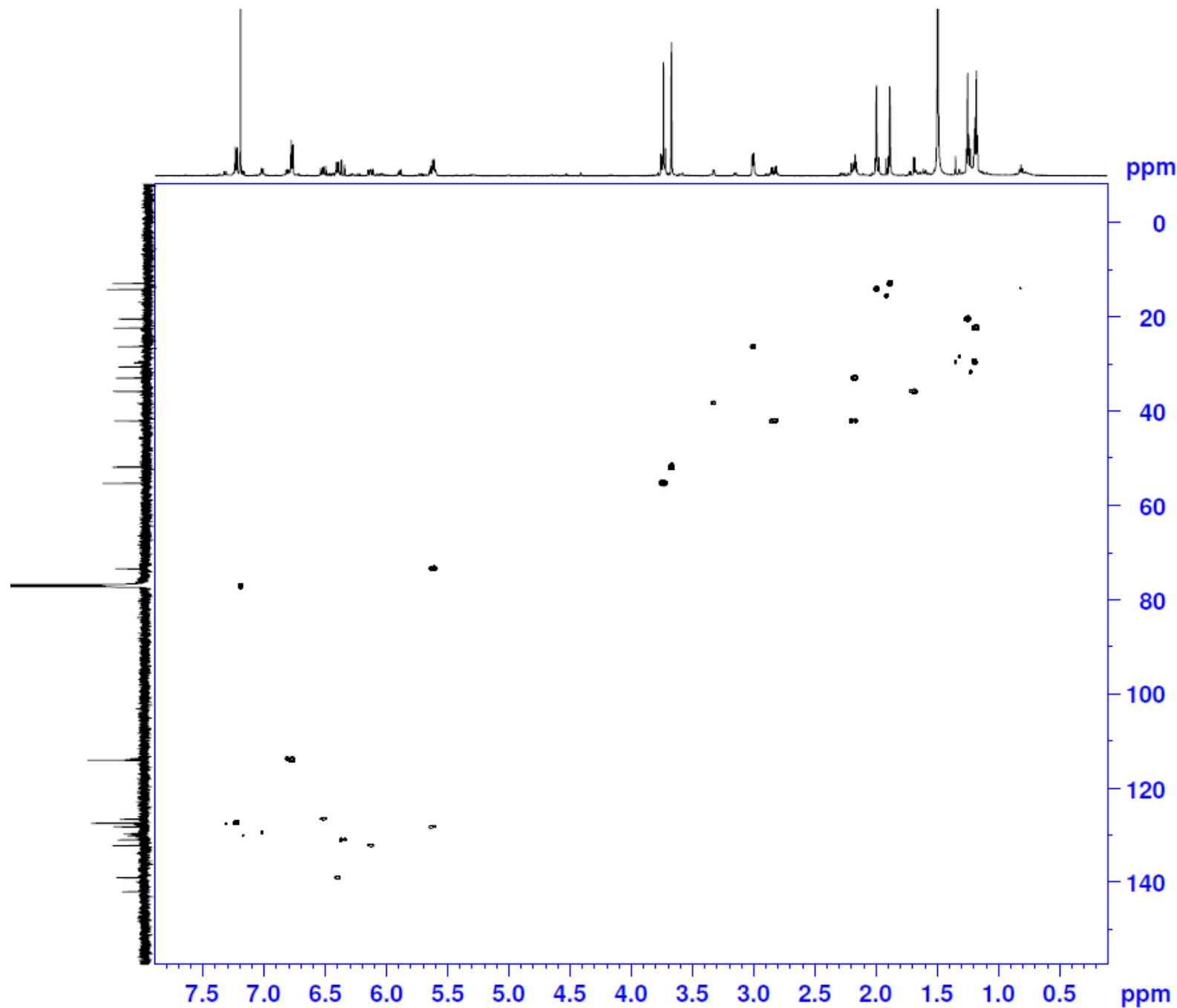
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
P1W2 79.98300171 W
P1W12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

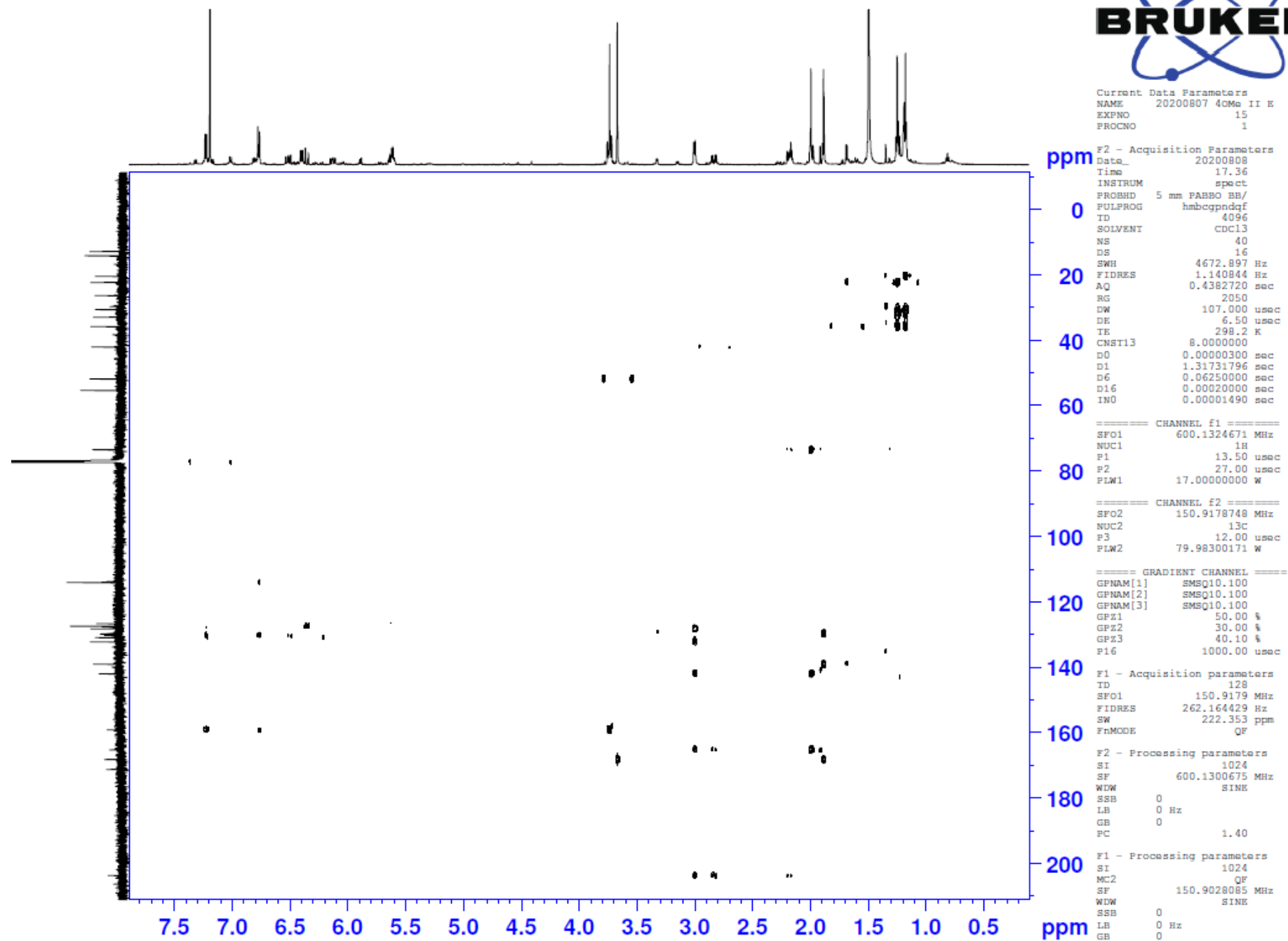
F2 - Processing parameters
SI 1024
SF 600.1300675 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200807 40Ma II E
EXPNO 15
PROCNO 1

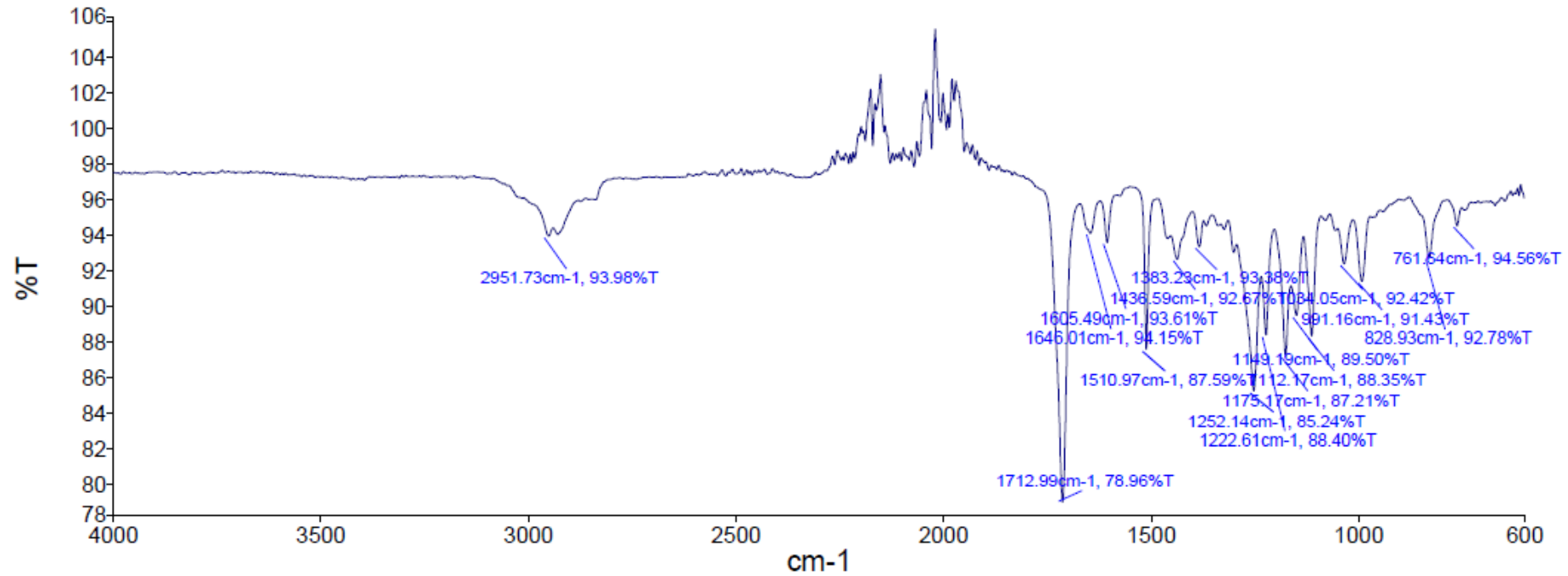


132b IR Spectrum

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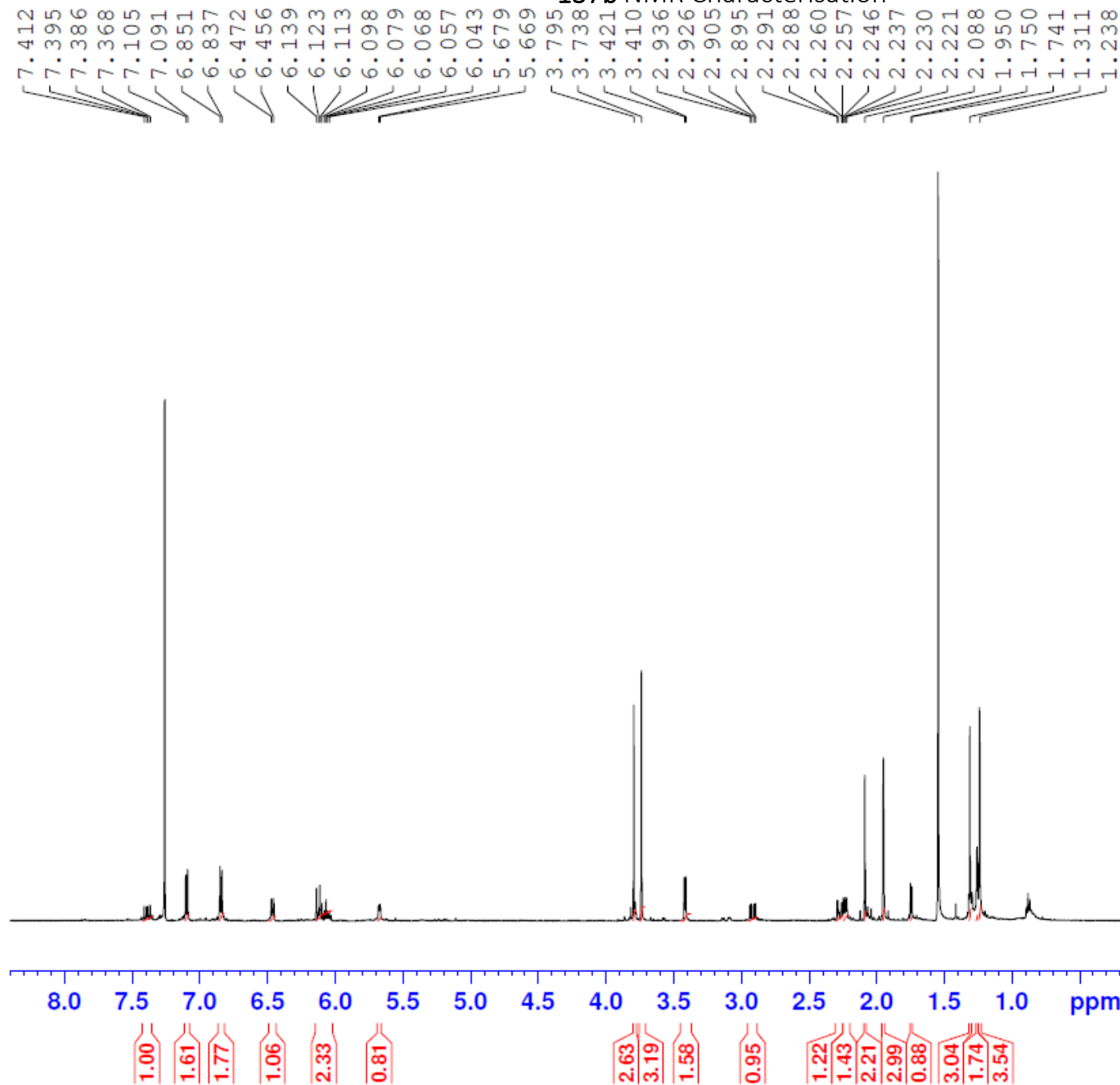
Analyst
Date

Analyst
Friday, 12 June 2020 10:43 AM



Sample Name	Description	Quality Checks
4OMe II E	Sample	The Quality Checks do not report any warnings for the sample.

¹³⁷b NMR Characterisation

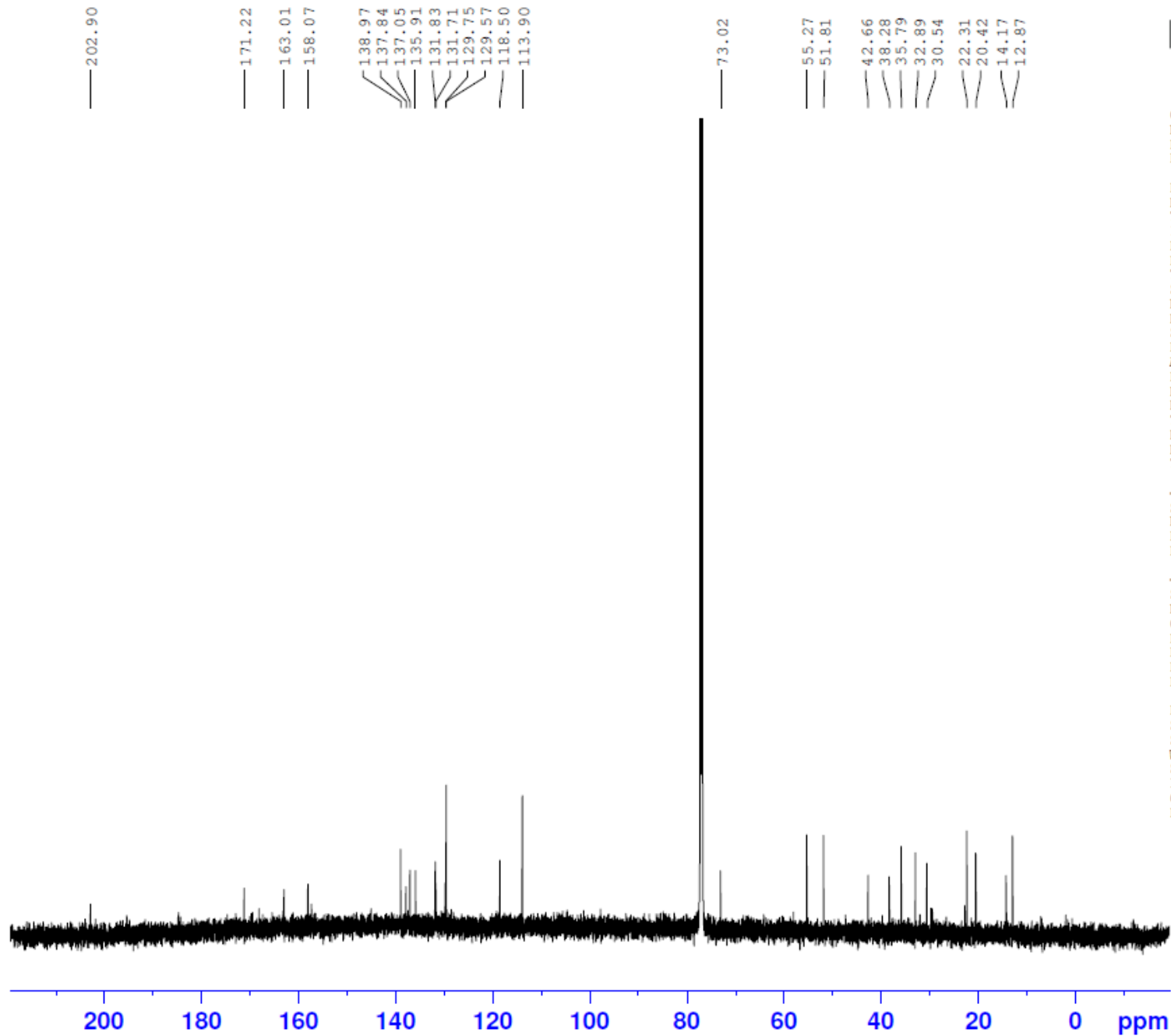


Current Data Parameters
 NAME 20200529 40Me II migration
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200531
 Time 1.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 362
 DW 41.600 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300258 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20200529 40Me II migration
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200531
 Time 8.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 6144
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

----- CHANNEL f2 -----
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028155 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200529 40Me II migration
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200531
Time 1.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygmfphpp
TD 2048
SOLVENT CDCl3
NS 10
DS 4
SWH 4761.905 Hz
FIDRES 2.325149 Hz
AQ 0.2150400 sec
RG 2050
DW 105.000 usec
DE 6.50 usec
TE 298.1 K
DO 0.00008781 sec
D1 1.92340505 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021000 sec

----- CHANNEL f1 -----

SFO1 600.1324450 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----

GP1AM[1] SMSQ10.100
GP1AM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters

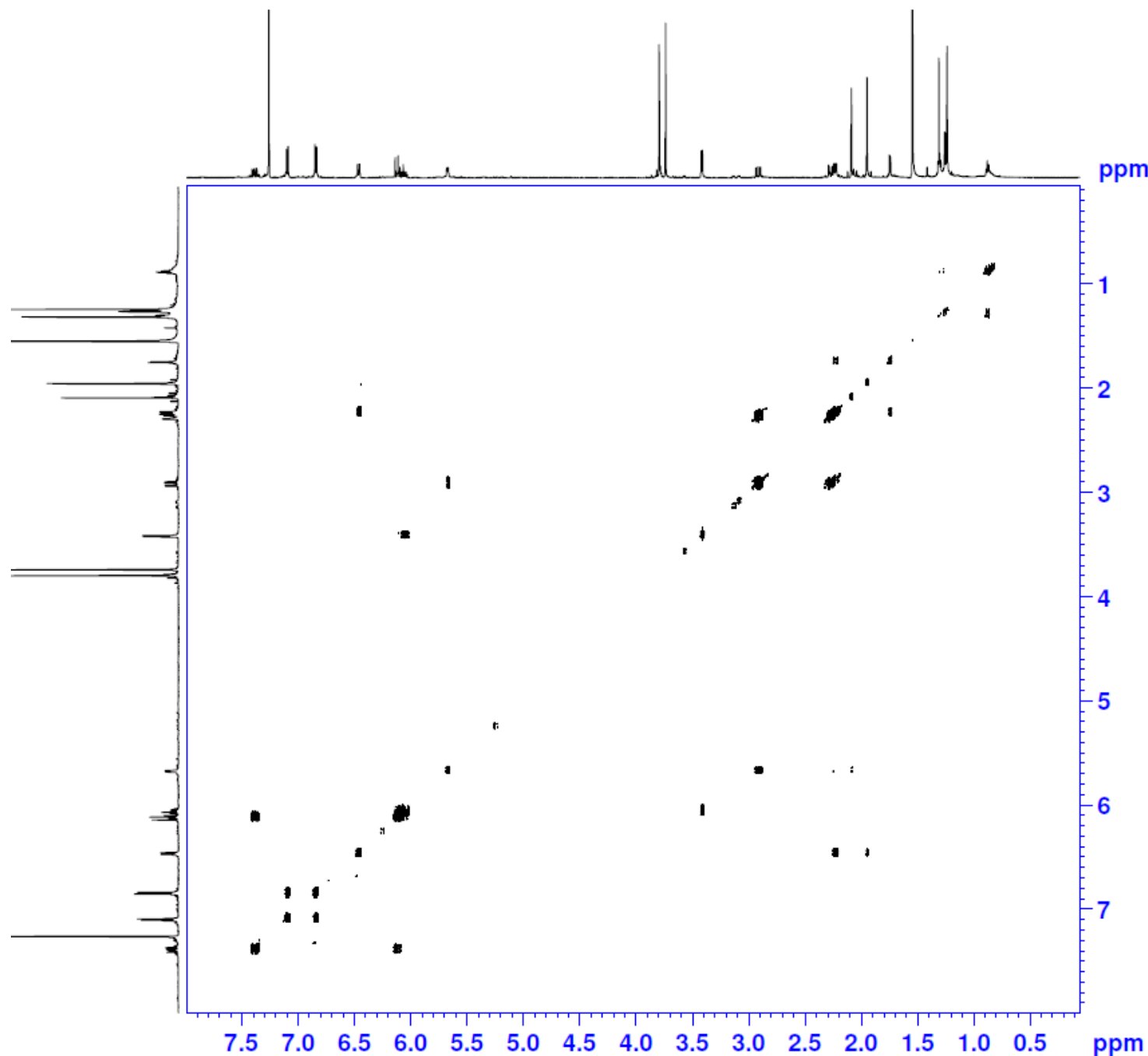
ID 256
SFO1 600.1324 MHz
FIDRES 18.601191 Hz
SW 7.935 ppm
FnMODE States-TPPI

F2 - Processing parameters

SI 1024
SF 600.1300293 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 States-TPPI
SF 600.1300296 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200529 40ms II migration
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200531
Time 8.33

INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetqp
TD 1024
SOLVENT CDCl3
NS 45
DS 16
SWH 4716.981 Hz
FIDRES 4.606427 Hz
AQ 0.1085440 sec
RG 2050
DW 106.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45699203 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPTNS

===== CHANNEL f1 =====
SFO1 600.1324337 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

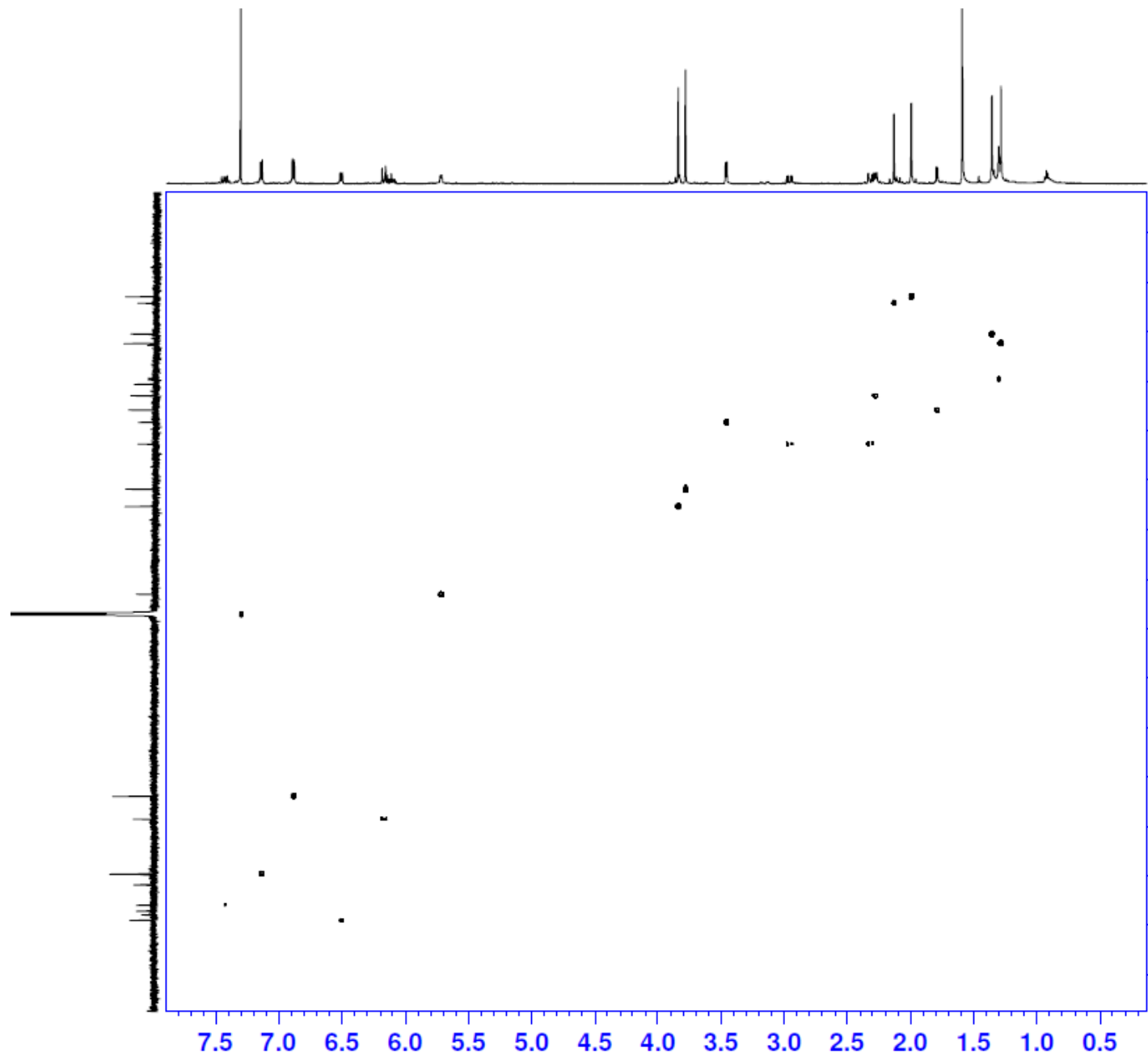
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

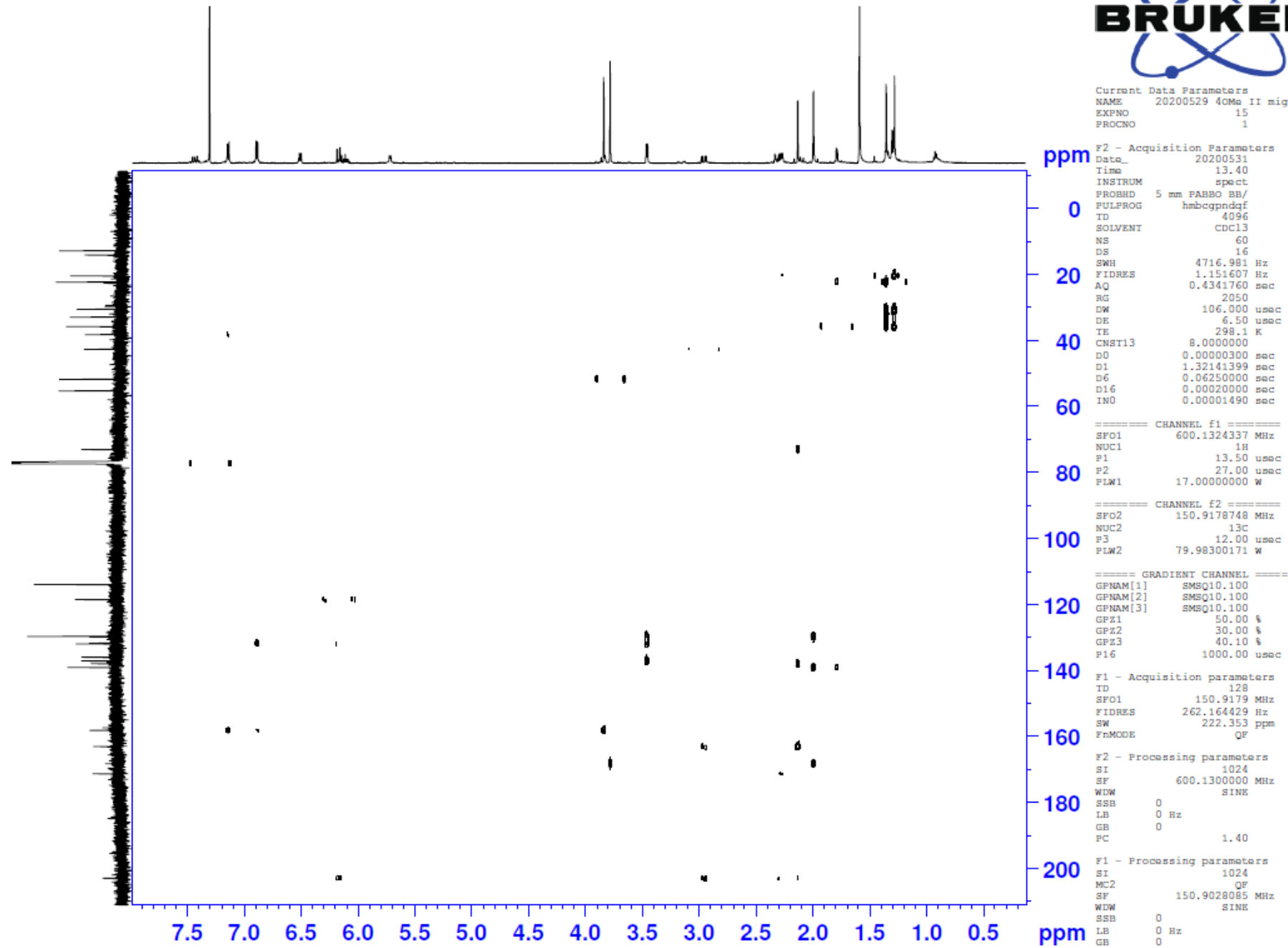
F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200529 40Me II migration
EXPNO 15
PROCNO 1

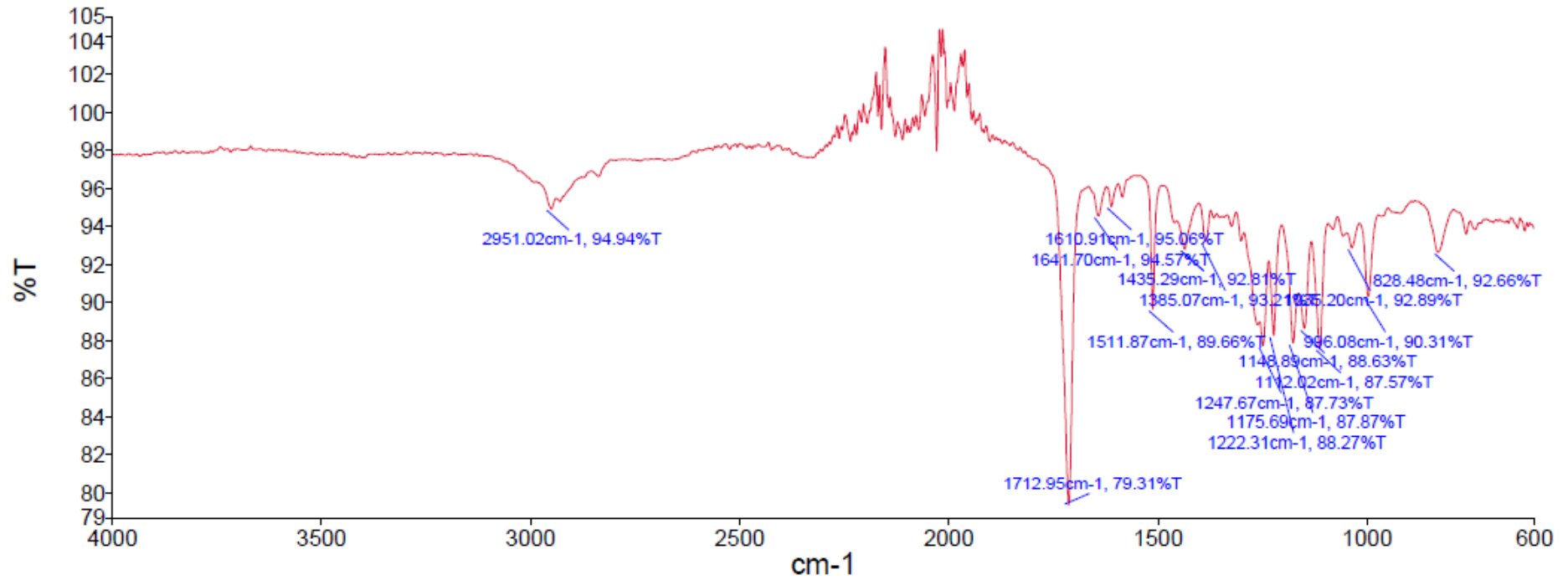


137b IR Spectrum

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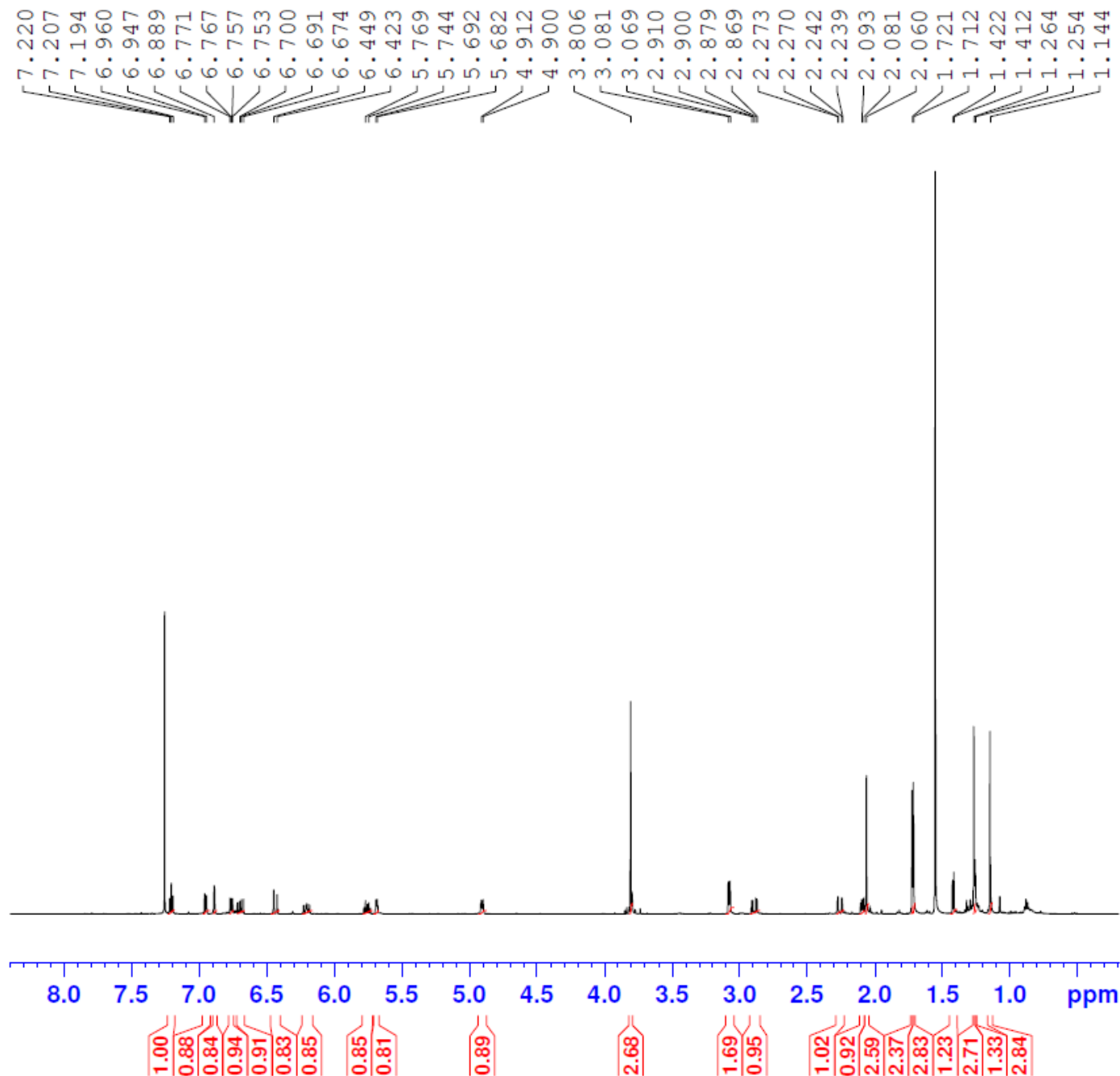
Analyst
Date

Analyst
Friday, 12 June 2020 10:40 AM



Sample Name	Description	Quality Checks
4OMe II Mig	Sample	The Quality Checks do not report any warnings for the sample.

¹³C NMR Characterisation

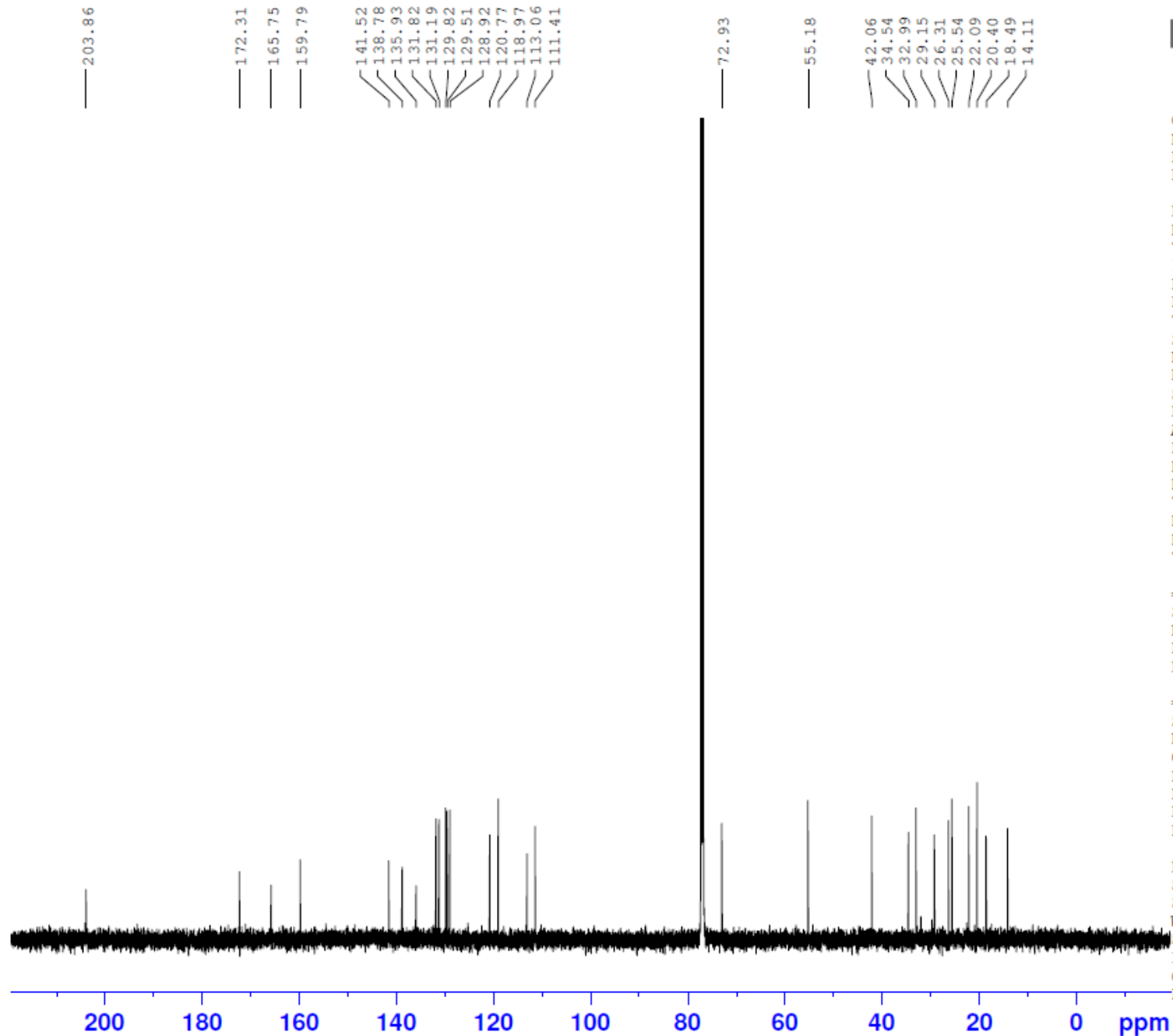


Current Data Parameters
NAME 20200522 30Me I E
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200523
Time 5.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 362
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300279 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20200522 30Me I E
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200523
Time 10.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6144
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9028146 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20200522 30Me I E
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200523
Time 5.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 3
DS 4
SWH 4716.981 Hz
FIDRES 2.303213 Hz
AQ 0.2170880 sec
RG 2050
DW 106.000 usec
DE 6.50 usec
TE 298.2 K
DO 0.00008881 sec
D1 1.92135704 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021200 sec

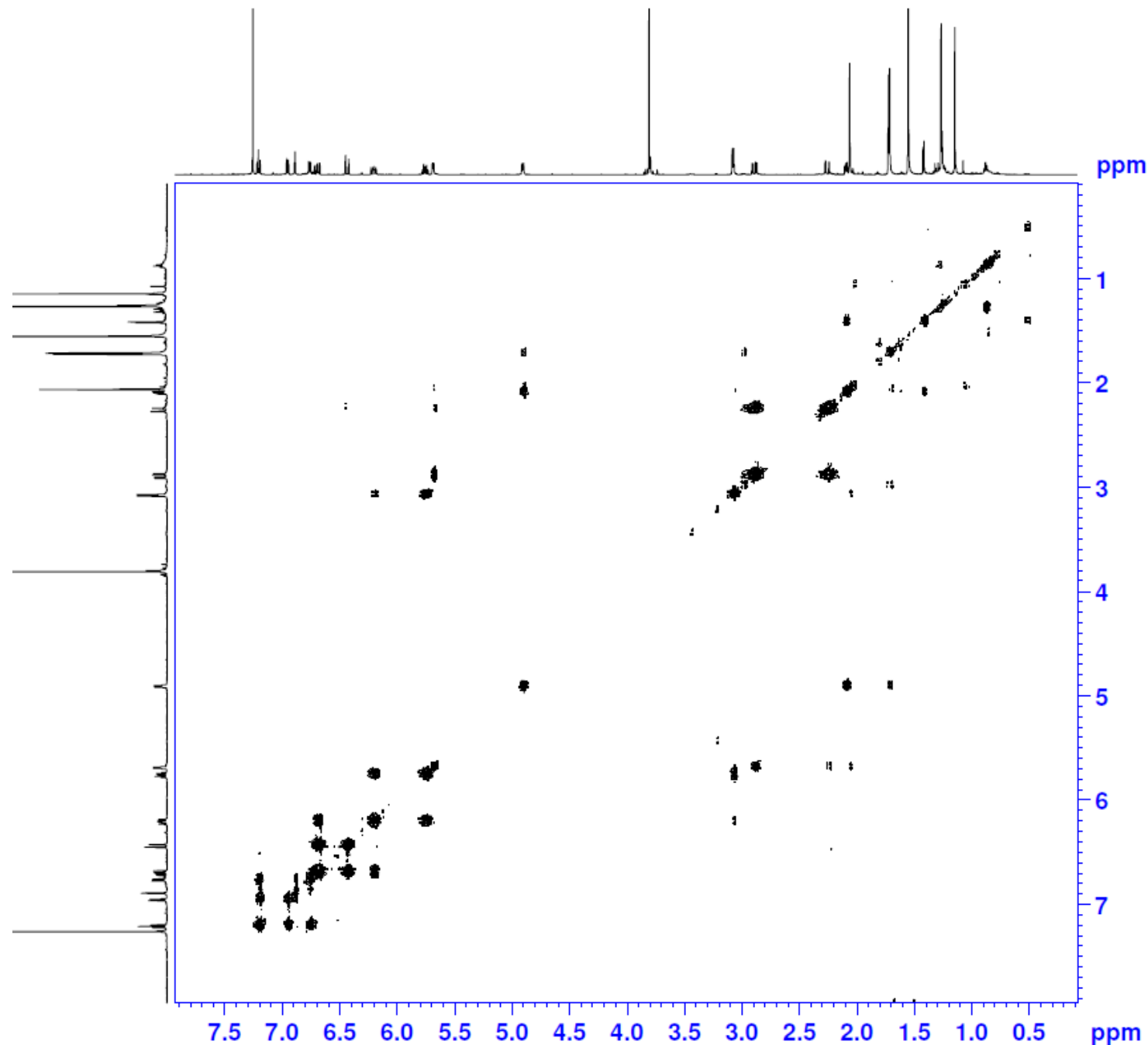
----- CHANNEL f1 -----
SFO1 600.1324392 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1324 MHz
FIDRES 18.425707 Hz
SW 7.860 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300347 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300311 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200522 30Me I E
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200523
Time 11.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 35
DS 16
SWH 4716.981 Hz
FIDRES 4.606427 Hz
AQ 0.1085440 sec
RG 2050
DW 106.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45699203 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPTNS

===== CHANNEL f1 =====
SFO1 600.1324392 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
P1W1 17.00000000 W

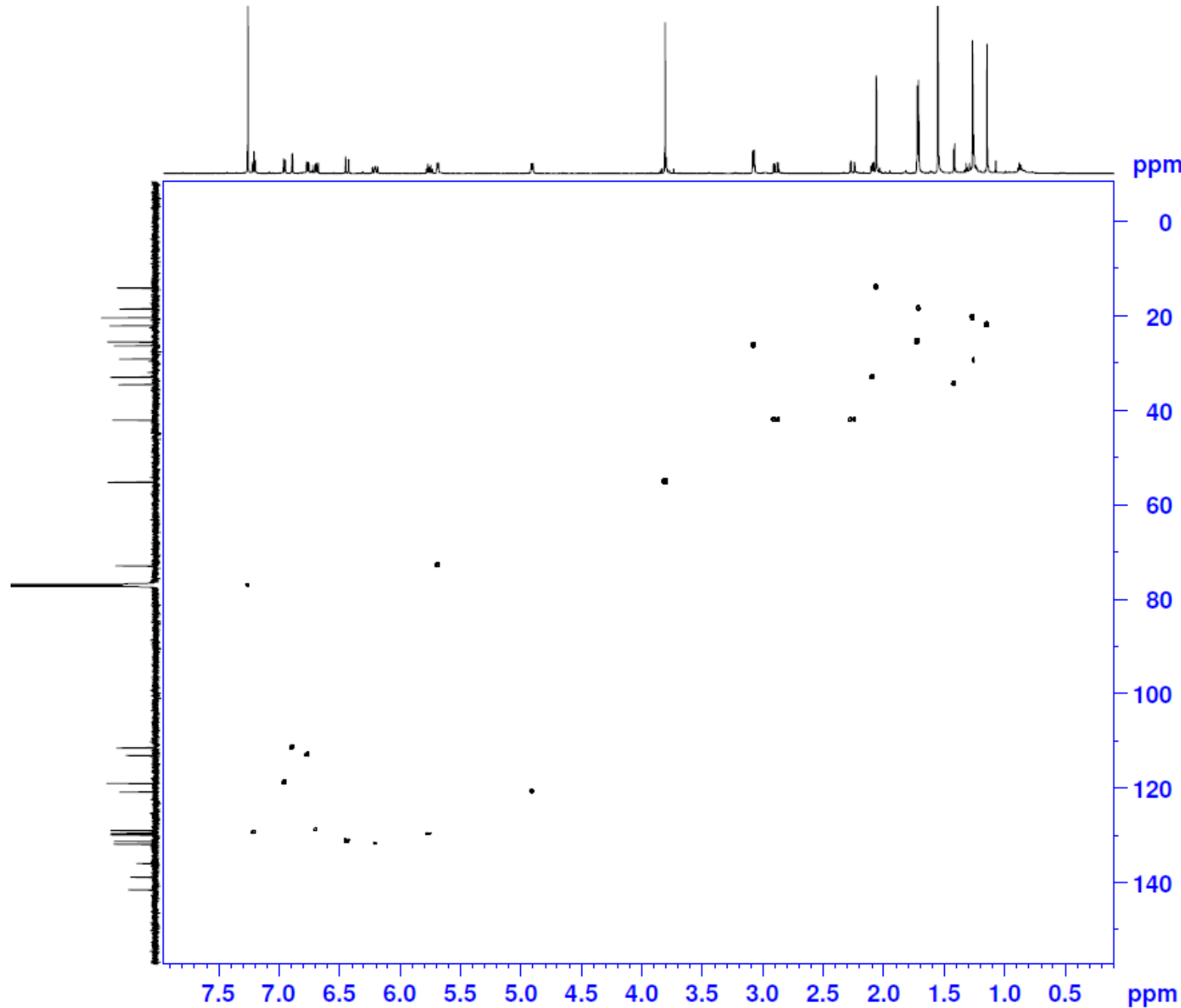
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
P1W2 79.98300171 W
P1W12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300245 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028365 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200522 30Me I E
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200523
Time 15.00
INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 50
DS 16
SWH 4716.981 Hz
FIDRES 1.151607 Hz
AQ 0.4341760 sec
RG 2050
DW 106.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.32141399 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1324392 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

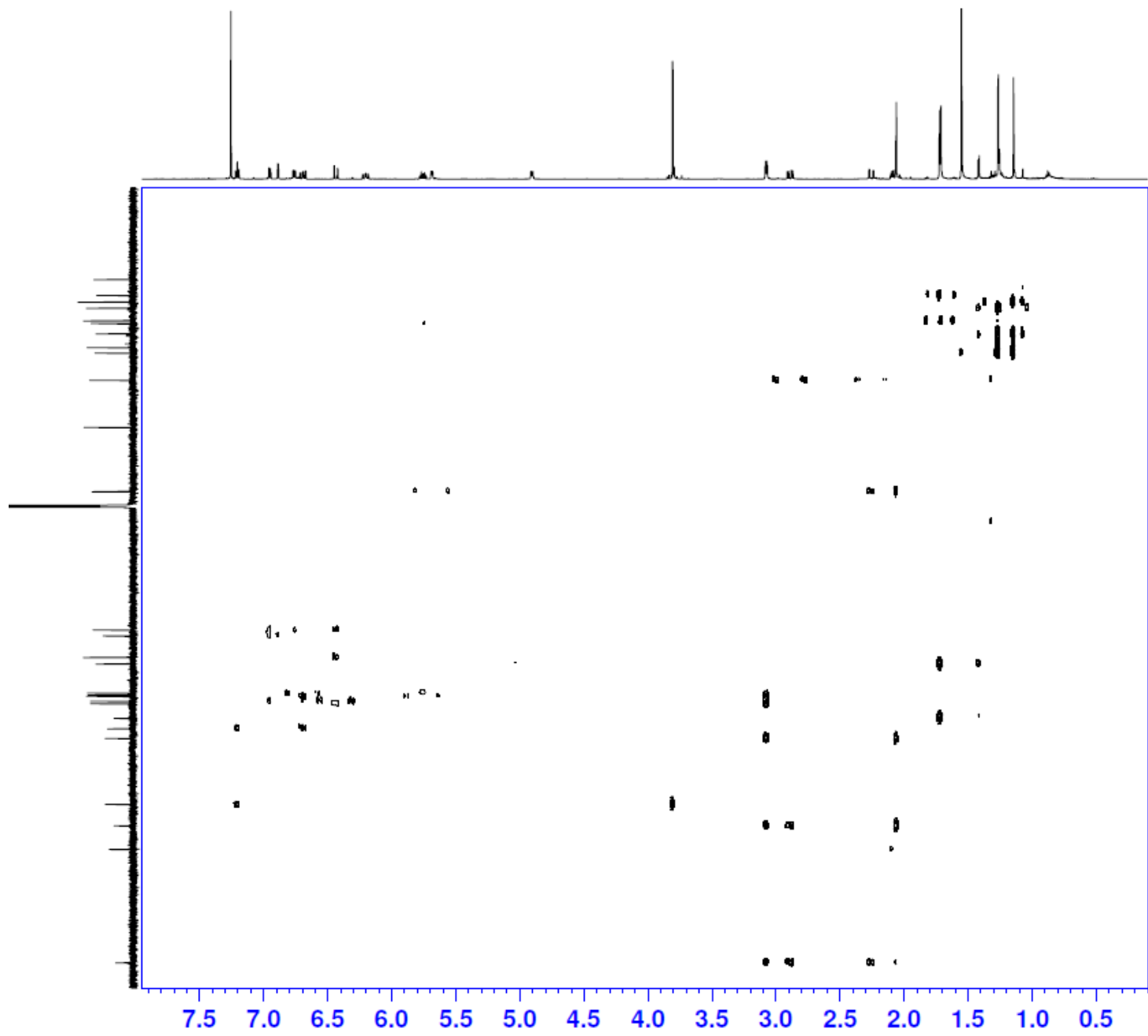
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300244 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028297 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

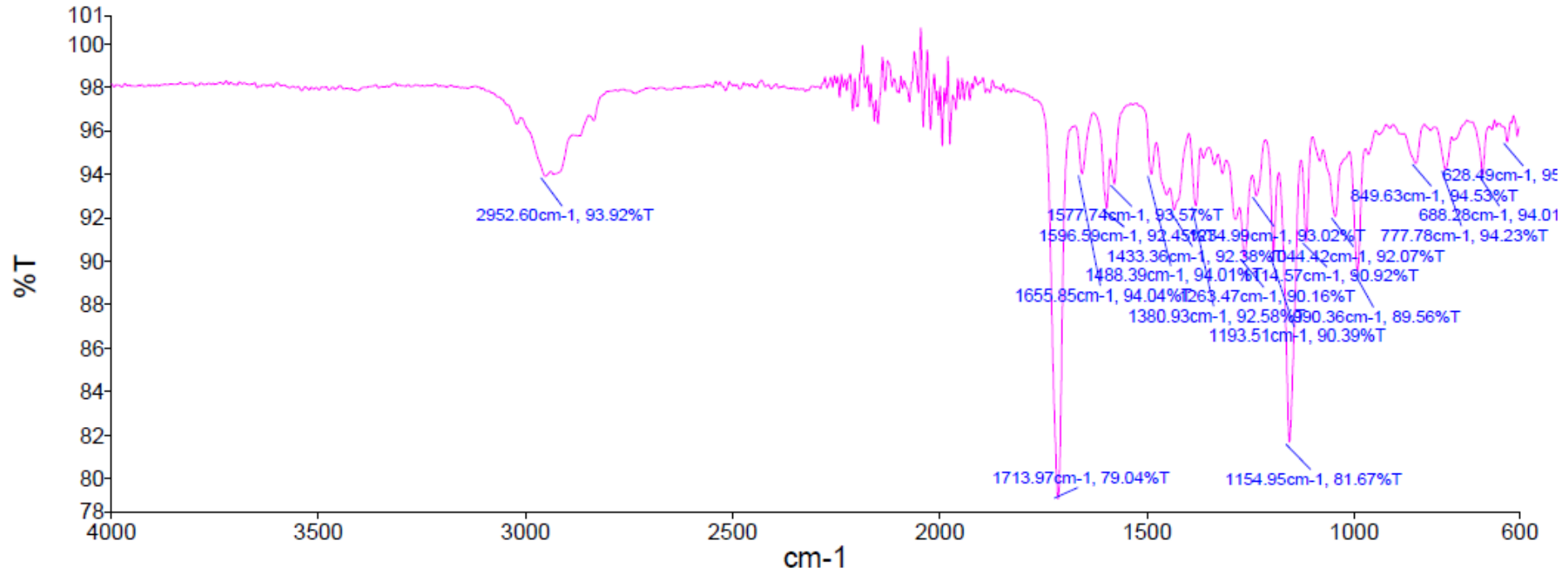


133a IR Spectrum

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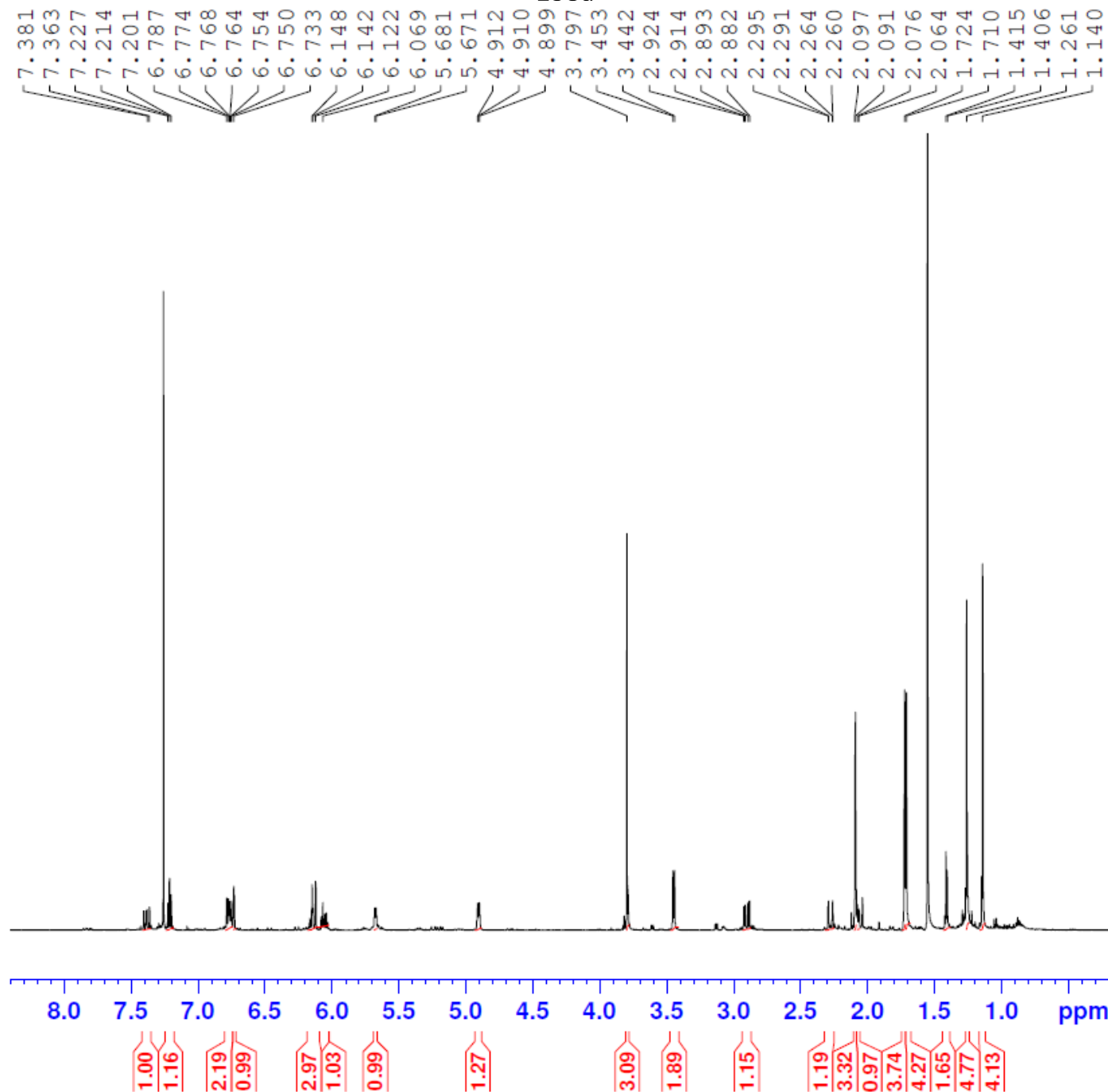
Analyst
Date

Analyst
Friday, 12 June 2020 10:11 AM



Sample Name	Description	Quality Checks
3OMe I E	Sample	The Quality Checks do not report any warnings for the sample.

¹³⁸a NMR Characterisation

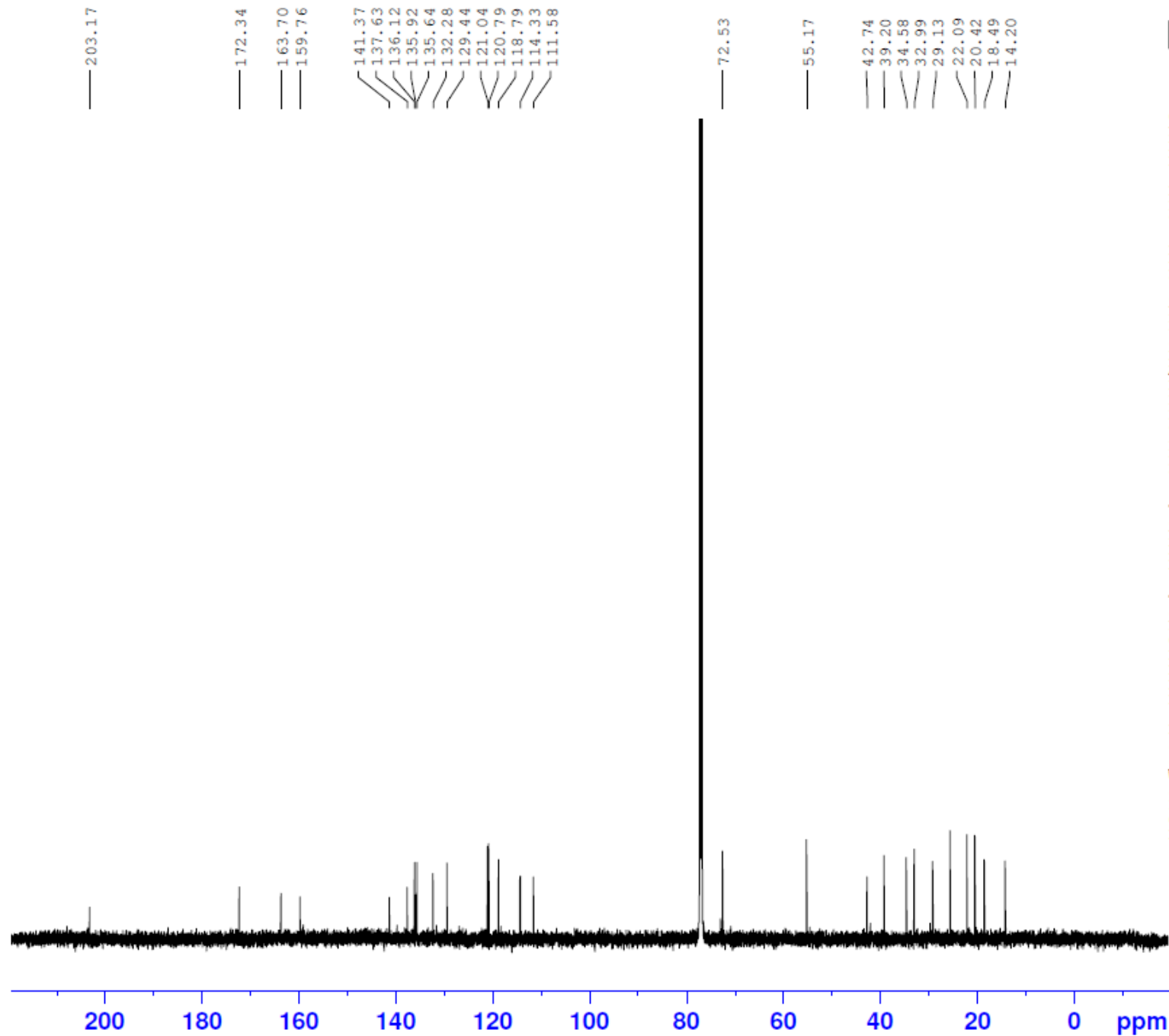


Current Data Parameters
NAME 20200522 30Me I migration
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200524
Time 21.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 362
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300263 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 20200522 30Me I migration
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200525
 Time 3.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 6144
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

----- CHANNEL f2 -----
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028135 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200522 30Me I migration
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200524
Time 21.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
ID 2048
SOLVENT CDCl3
NS 3
DS 4
SWH 4716.981 Hz
FIDRES 2.303213 Hz
AQ 0.2170880 sec
RG 2050
DW 106.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00008881 sec
D1 1.92135704 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021200 sec

----- CHANNEL f1 -----

SFO1 600.1324773 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----

GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters

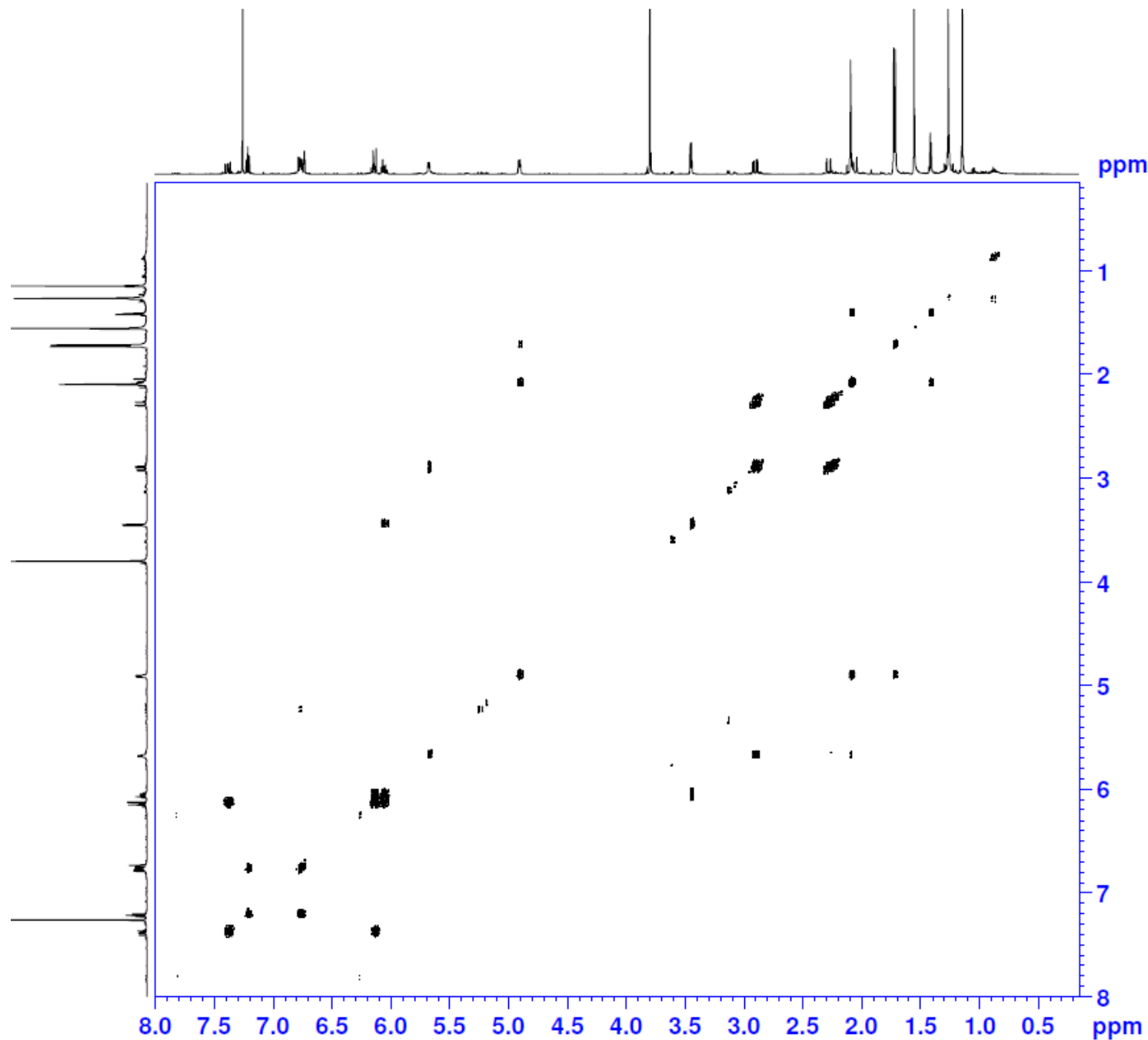
ID 256
SFO1 600.1325 MHz
FIDRES 18.425707 Hz
SW 7.860 ppm
FnMODE States-IPPI

F2 - Processing parameters

SI 1024
SF 600.1300295 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 States-IPPI
SF 600.1300330 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200522 30Me 1 migration
EXFNO 13
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200525
Time 3.03
INSTRUM spect
PROBHD 5 mm FASBO BB/
PULPROG hsqcetgp
ID 1024
SOLVENT CDCl3
NS 35
DS 16
SWH 4716.981 Hz
FIDRES 4.606427 Hz
AQ 0.1085440 sec
RG 2050
DW 106.000 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45699203 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1324773 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

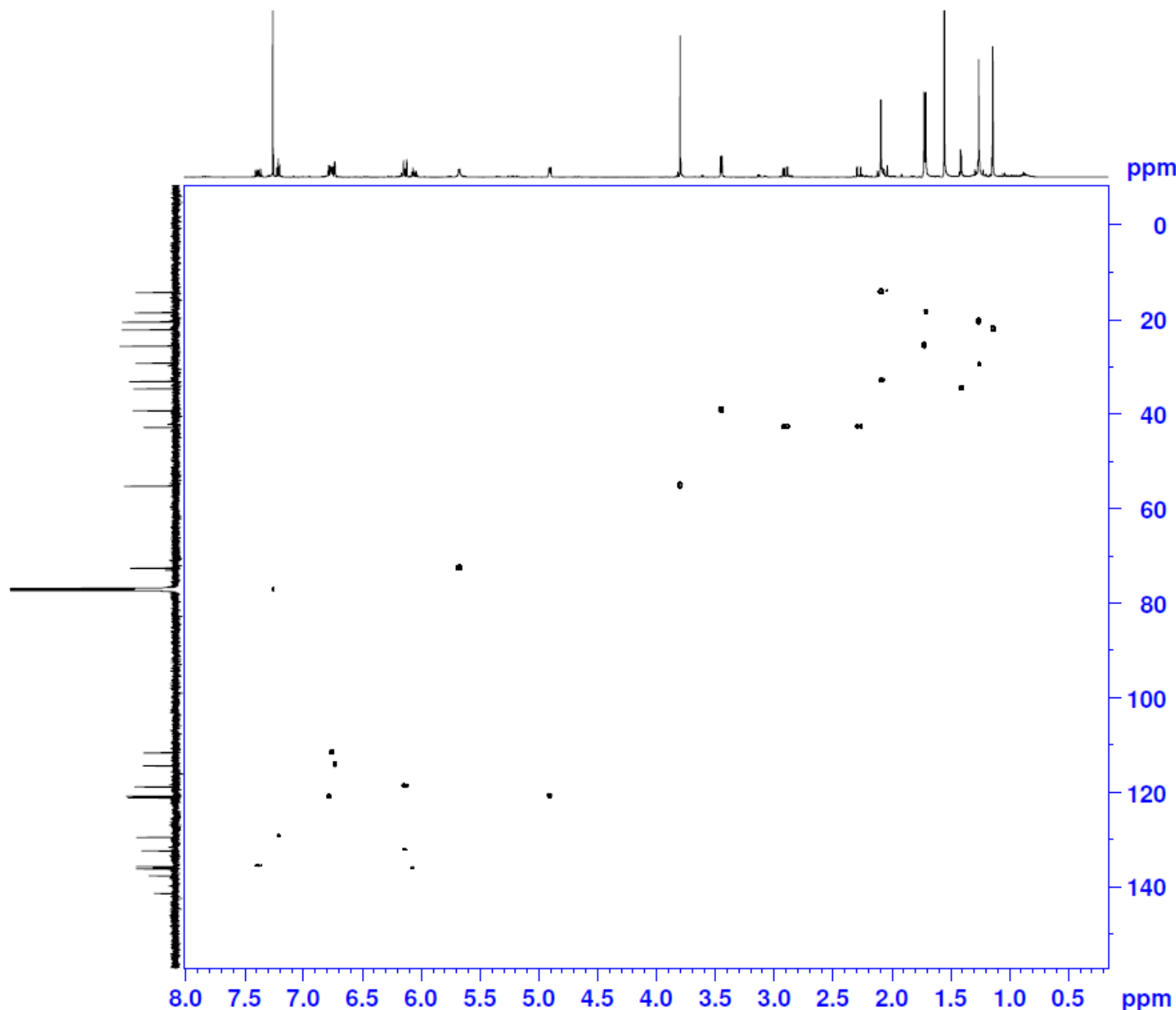
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
F1MODE Echo-Antiecho

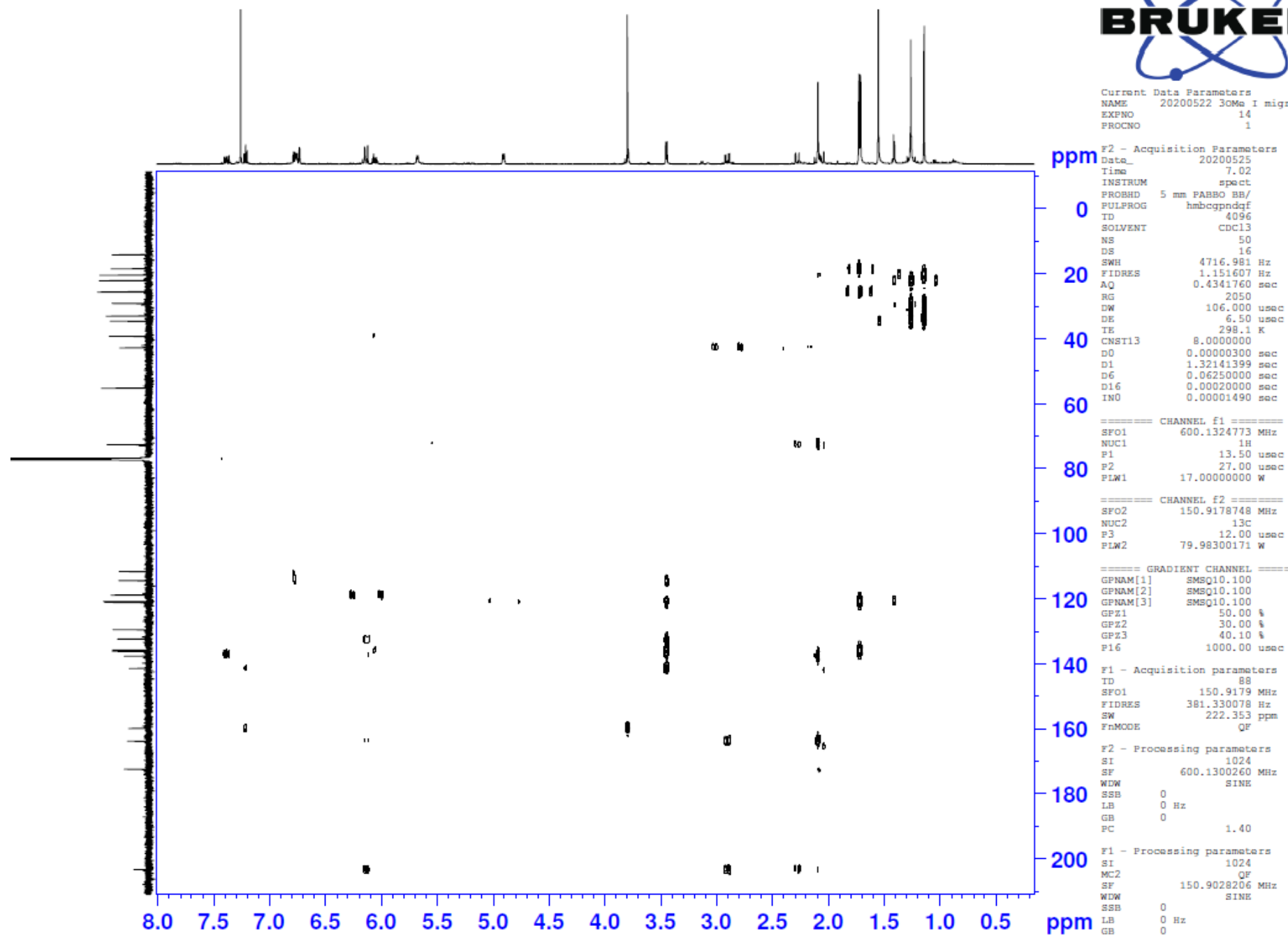
F2 - Processing parameters
SI 1024
SF 600.1300246 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028465 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200522 30Ma I migration
EXPNO 14
PROCNO 1

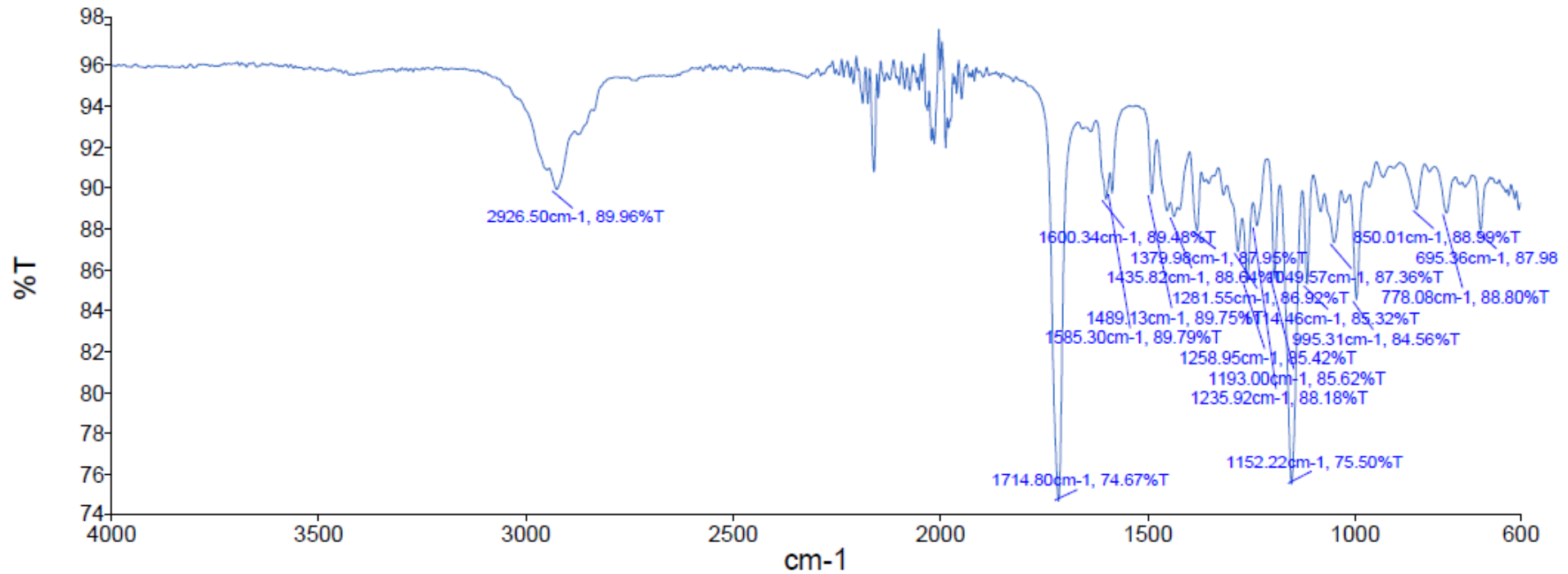


138a IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Friday, 12 June 2020 10:07 AM

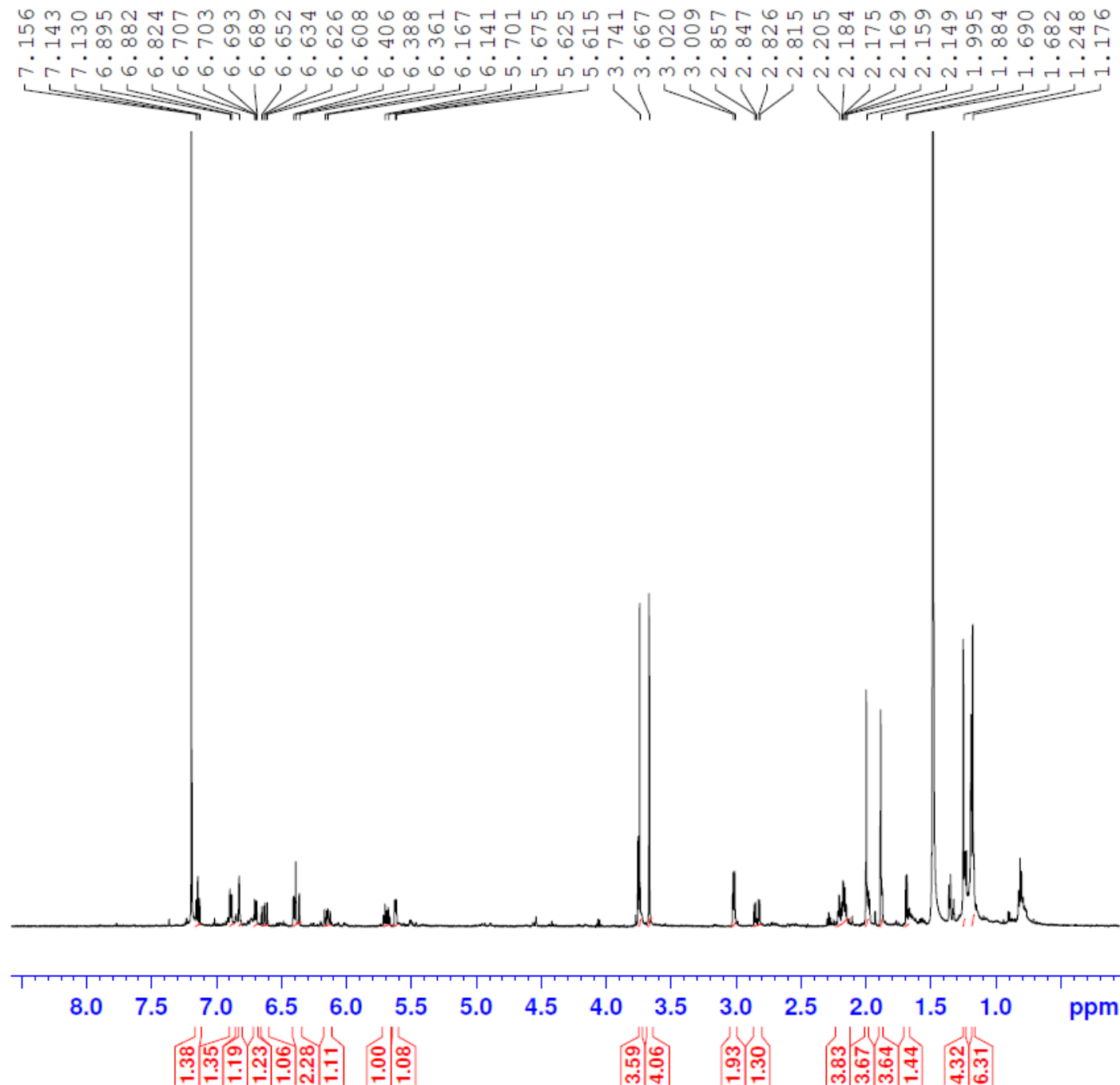
Analyst
Date

Analyst
Friday, 12 June 2020 10:07 AM



Sample Name	Description	Quality Checks
3OMe I Mig	Sample	The Quality Checks do not report any warnings for the sample.

¹³³b NMR Characterisation

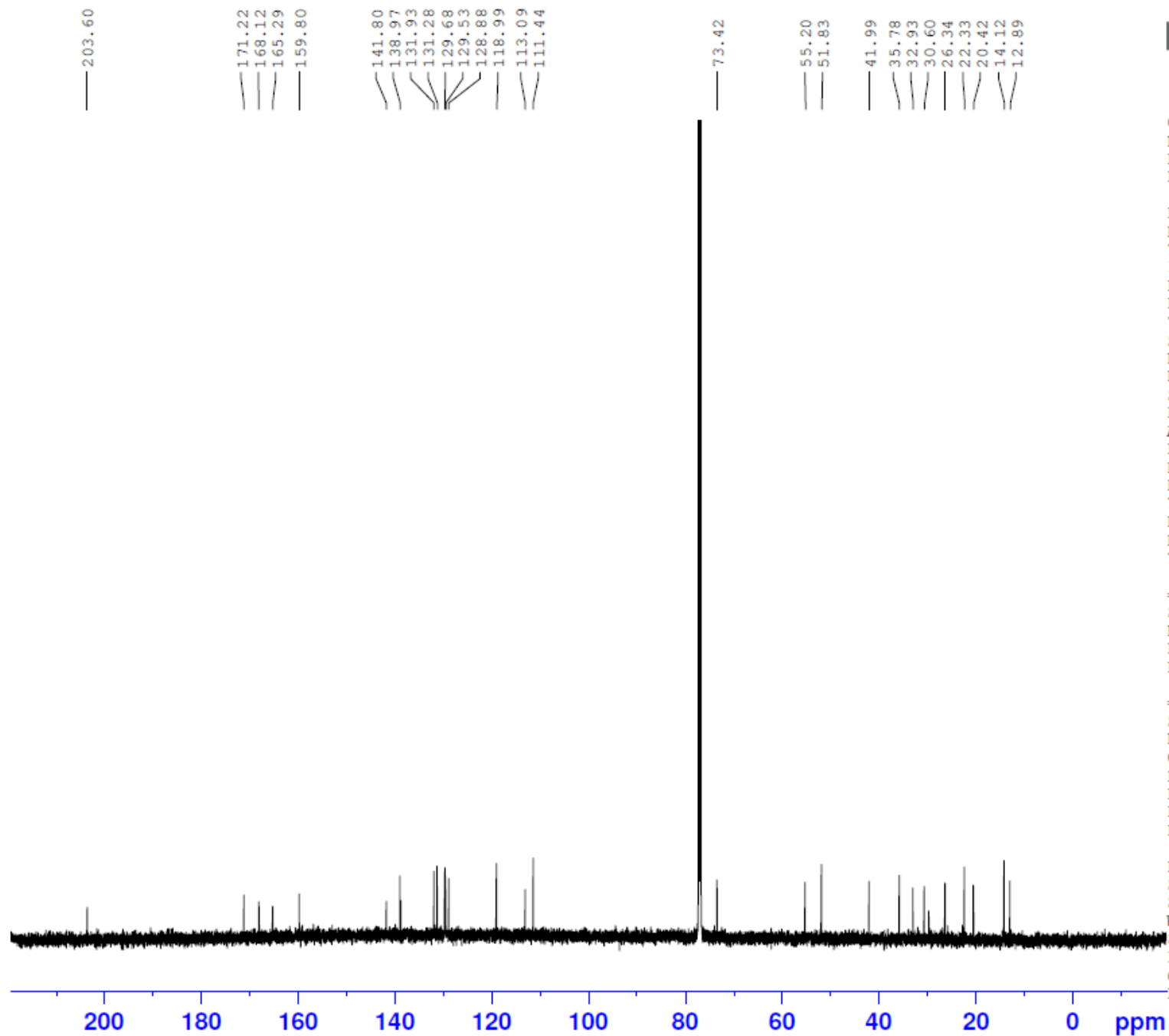


Current Data Parameters
NAME 20200529 30Me II E
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200530
Time 9.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 362
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300672 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 20200807 30Me II E
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200807
 Time 22.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028131 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200807 30Me II E
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200807
Time 22.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
ID 2048
SOLVENT CDCl3
NS 3
DS 4
SWH 4761.905 Hz
FIDRES 2.325149 Hz
AQ 0.2150400 sec
RG 2050
DW 105.000 usec
DE 6.50 usec
TE 298.1 K
D0 0.00008781 sec
D1 1.92340505 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021000 sec

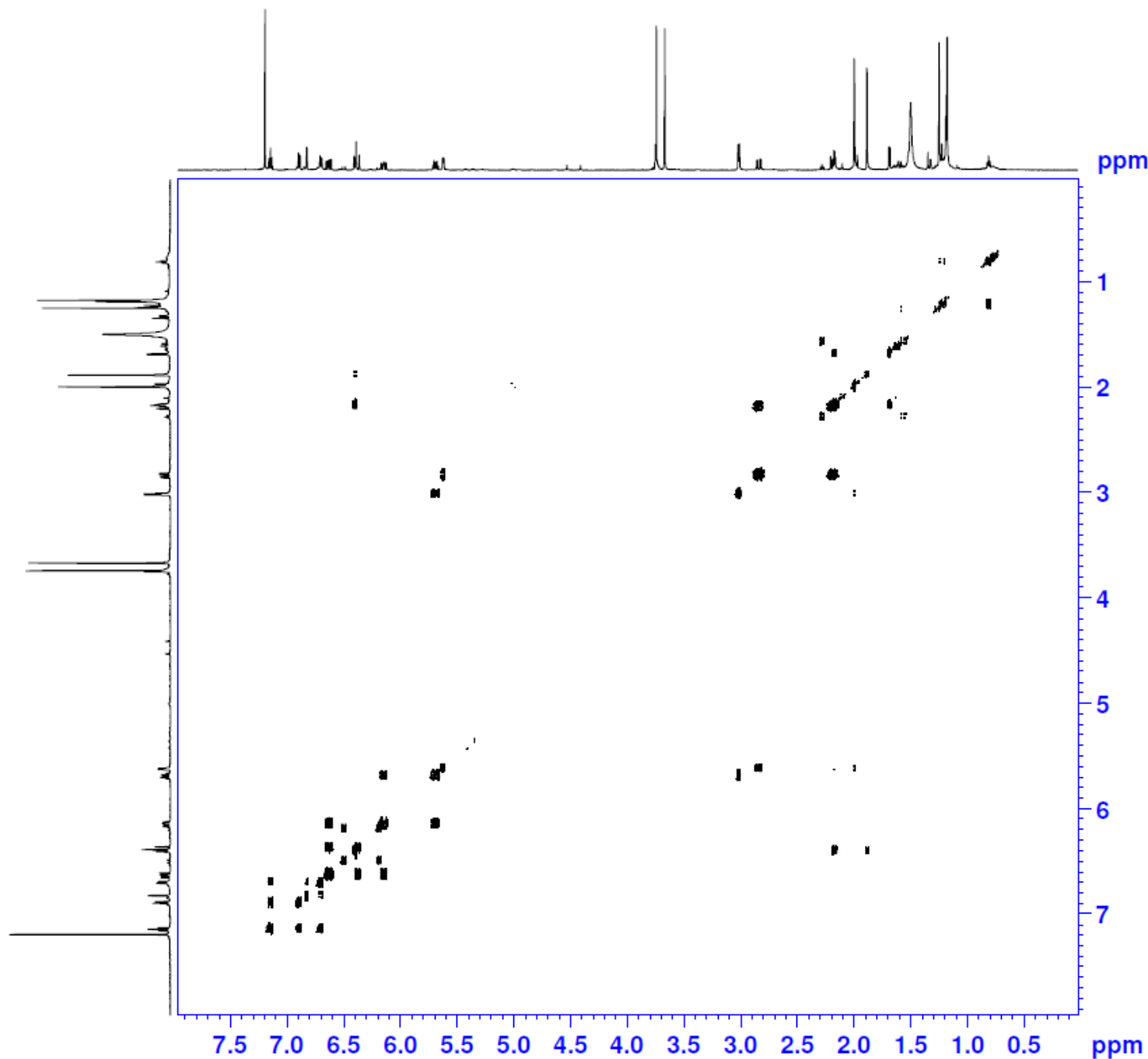
----- CHANNEL f1 -----
SFO1 600.1324618 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 256
SFO1 600.1325 MHz
FIDRES 18.601191 Hz
SW 7.935 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300672 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300672 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200807 30Ma 11 E
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200807
Time 23.06

INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDC13
NS 25
DS 16
SWH 4761.905 Hz
FIDRES 4.650298 Hz
AQ 0.1075200 sec
RG 2050
DW 105.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45801604 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGTNS

===== CHANNEL f1 =====
SFO1 600.1324618 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

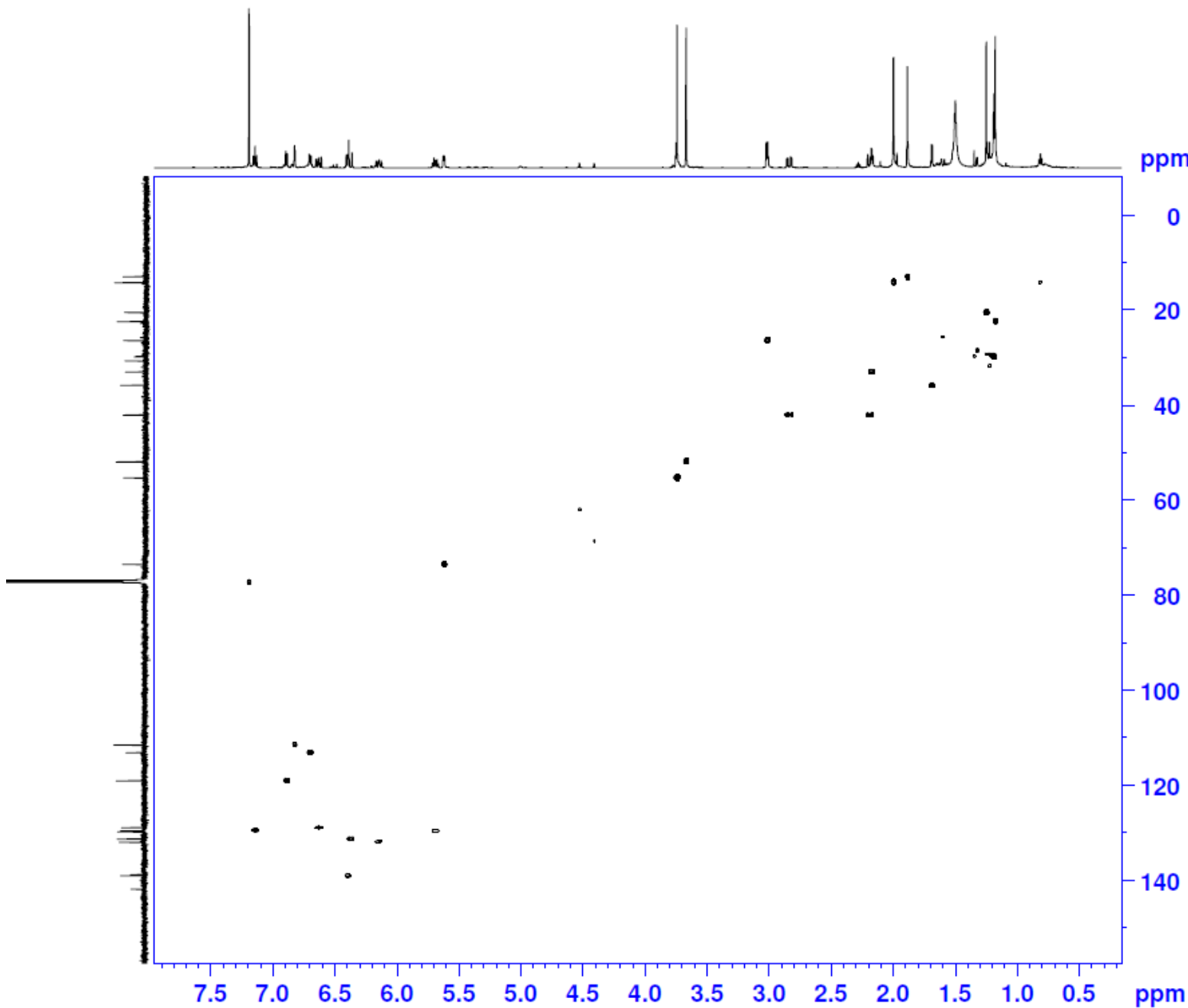
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300672 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200807 30Ma II E
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200808

Time 1.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDC13
NS 40
DS 16
SWH 4761.905 Hz
FIDRES 1.162574 Hz
AQ 0.4300800 sec
RG 2050
DW 105.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.32551003 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1324618 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

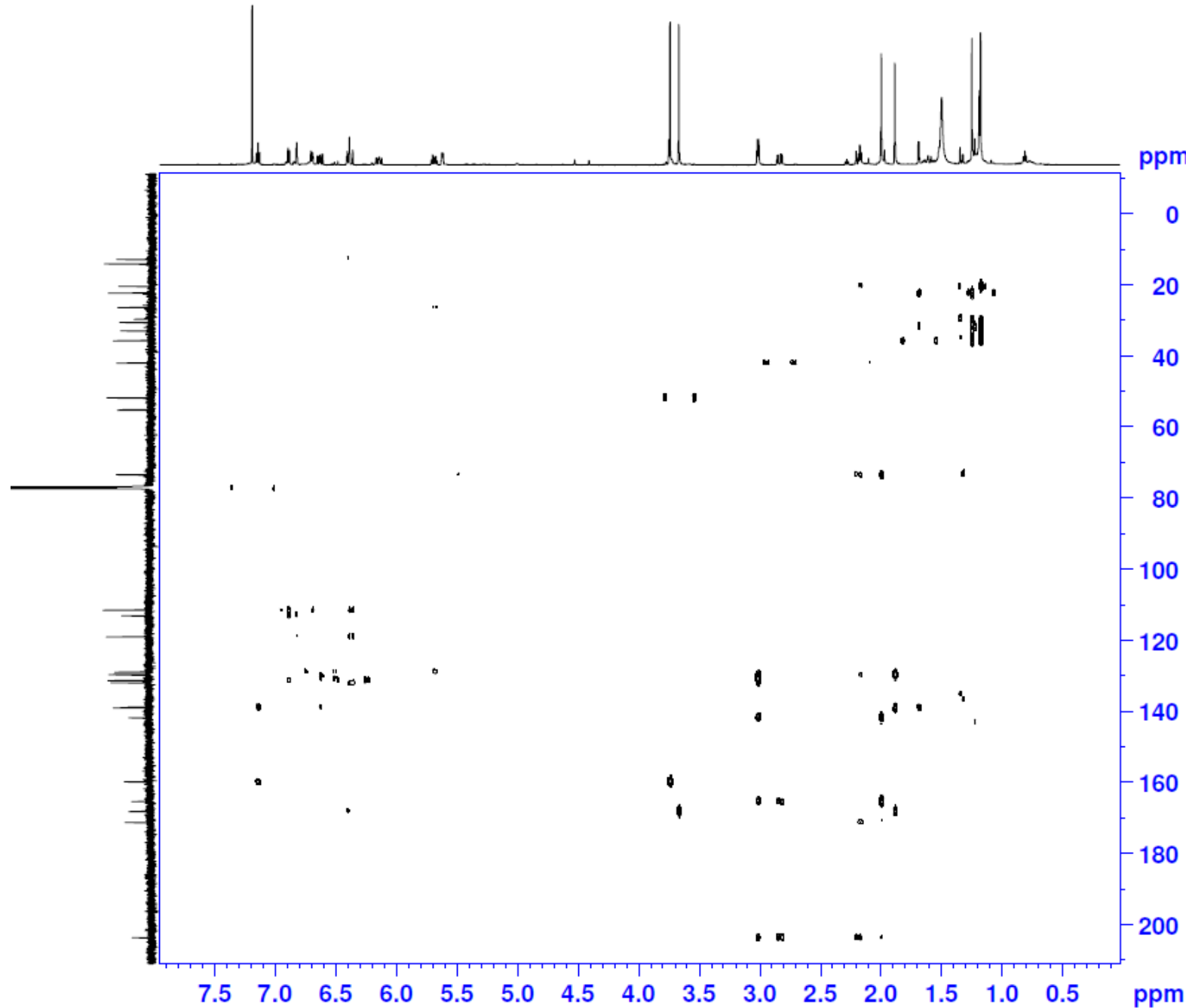
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300672 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

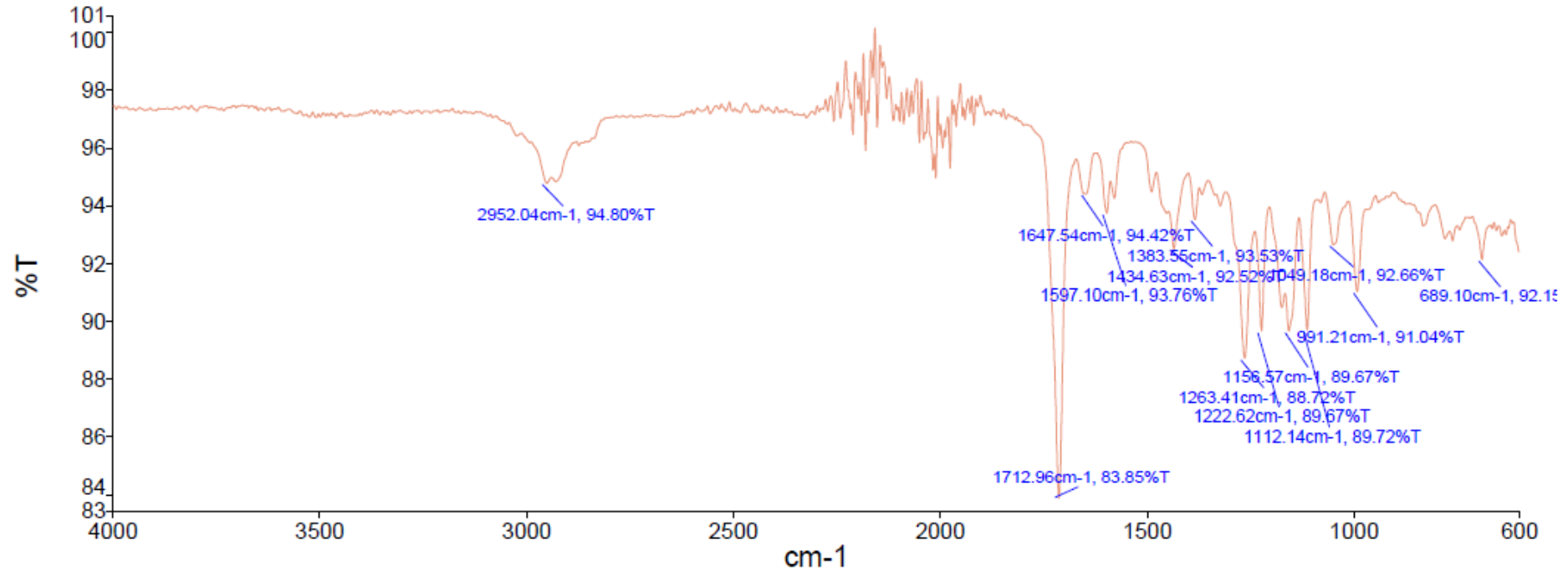


133b IR Spectrum

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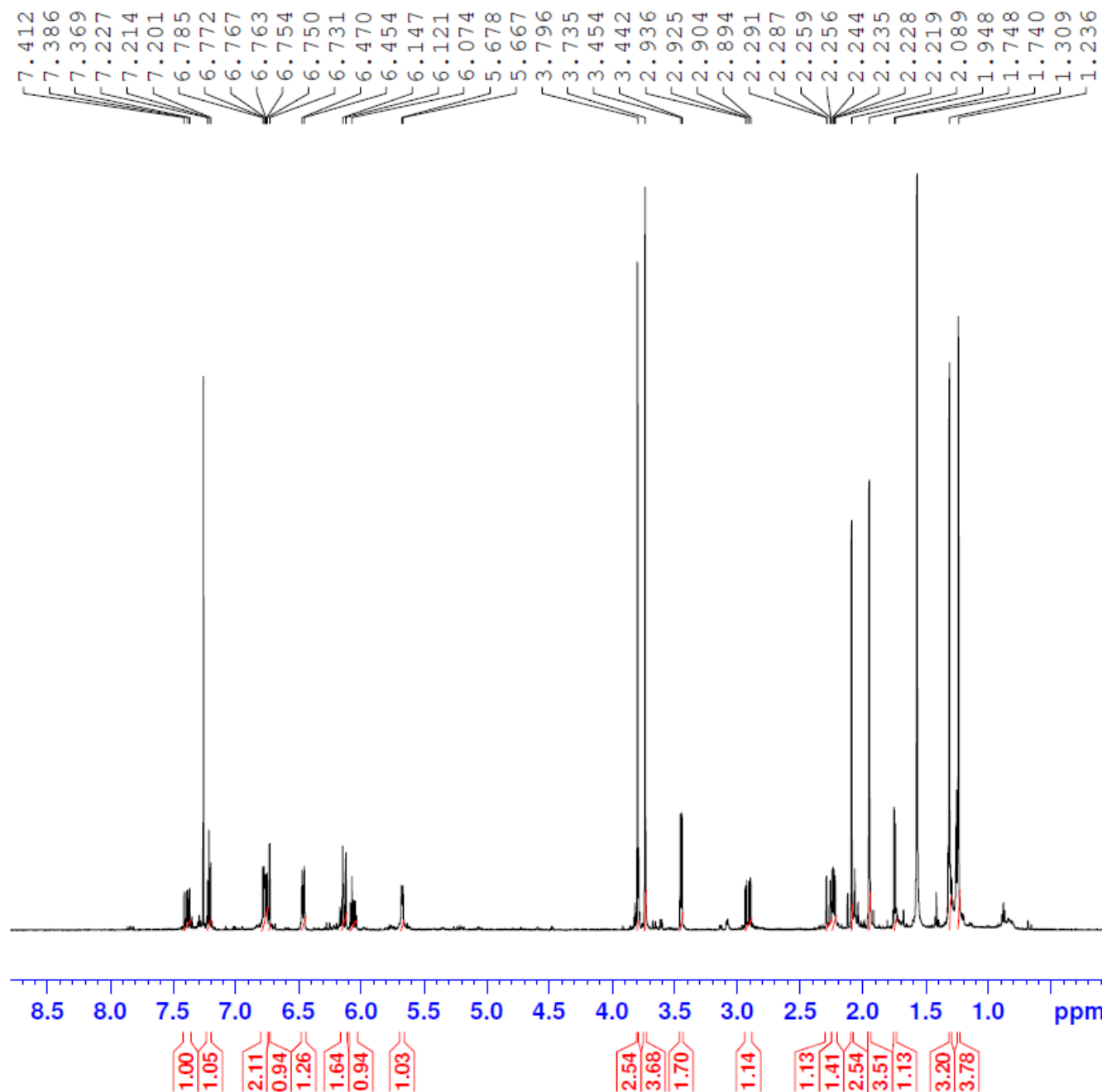
Analyst
Date

Analyst
Friday, 12 June 2020 10:17 AM



Sample Name	Description	Quality Checks
3OMe II E	Sample	The Quality Checks do not report any warnings for the sample.

138b NMR Characterisation

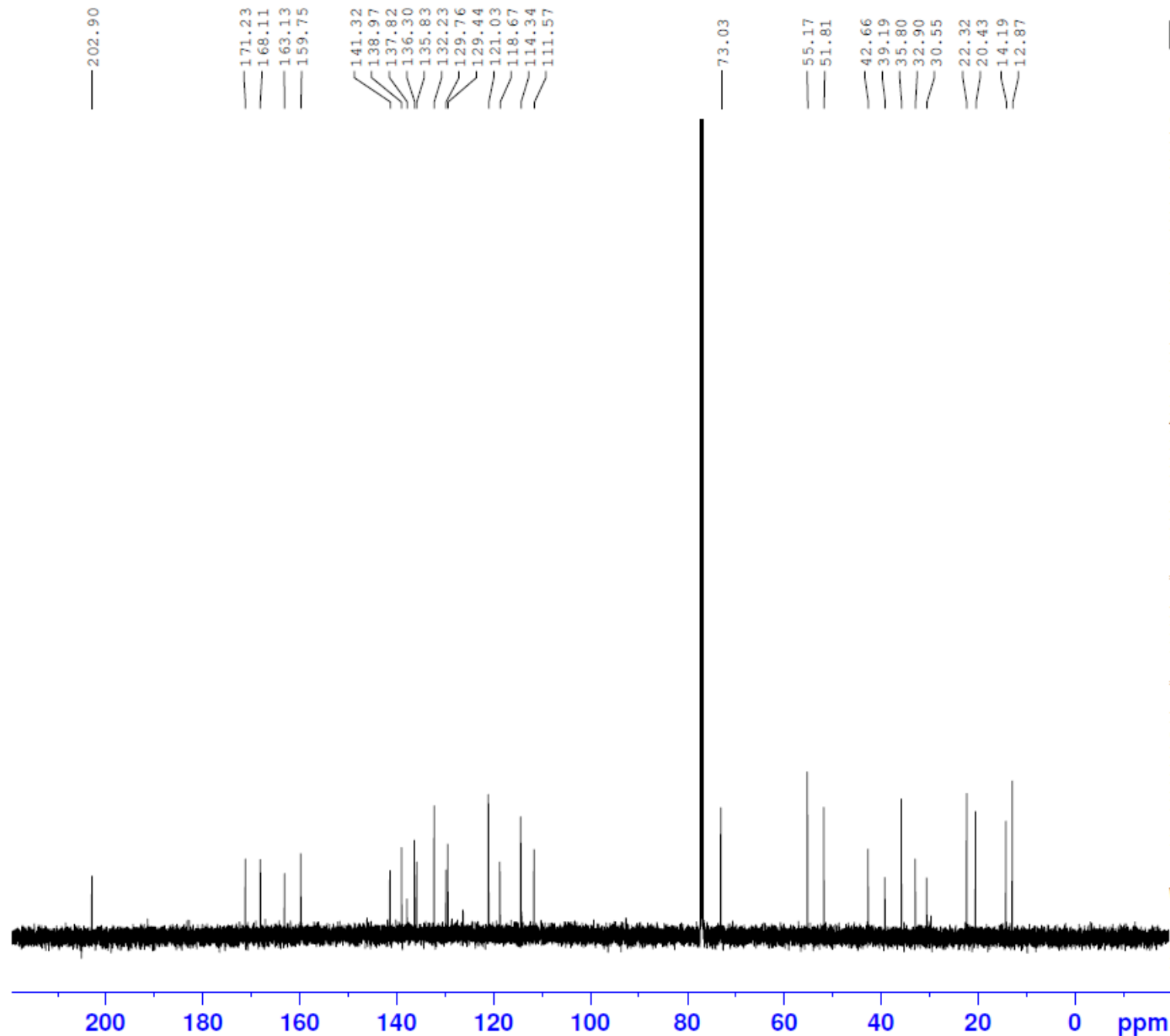


Current Data Parameters
NAME 20200807 30Me II Mig
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200808
Time 4.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 287
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300269 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 20200807 30Me II Mig
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200808
 Time 6.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028148 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20200807 30Me II Mig
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200808
Time 4.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 3
DS 4
SWH 4761.905 Hz
FIDRES 2.325149 Hz
AQ 0.2150400 sec
RG 2050
DW 105.000 usec
DE 6.50 usec
TE 298.1 K
D0 0.00008781 sec
D1 1.92340505 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021000 sec

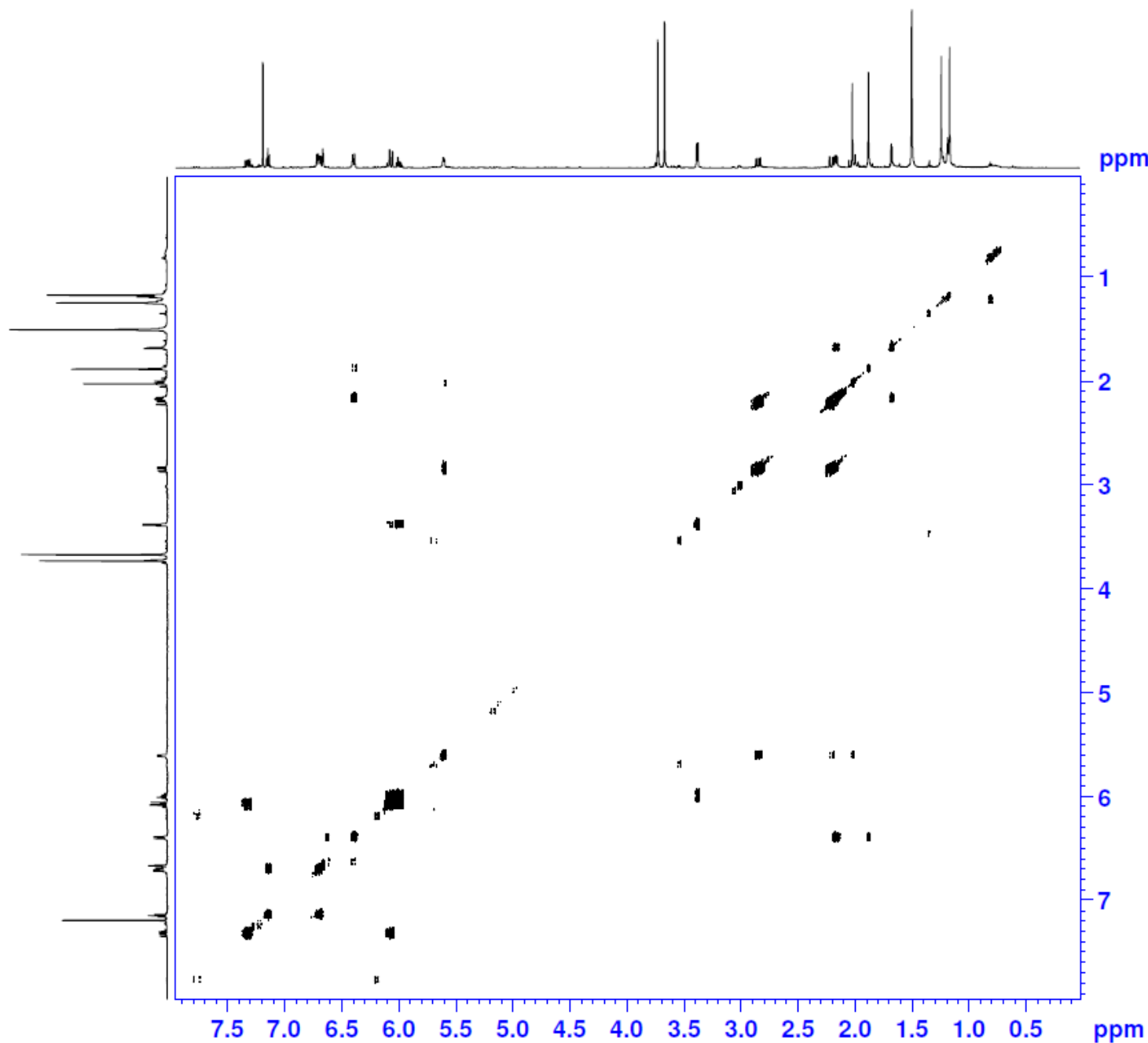
----- CHANNEL f1 -----
SFO1 600.1324627 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.1325 MHz
FIDRES 18.601191 Hz
SW 7.935 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 600.1300672 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.1300672 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200807 30Me II Mig
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200808
Time 6.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcctqd
TD 1024
SOLVENT cdc13
NS 25
DS 16
SWH 4761.905 Hz
FIDRES 4.650298 Hz
AQ 0.1075200 sec
RG 2050
DW 105.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.0000300 sec
D1 1.45801604 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPTNS

===== CHANNEL f1 =====
SFO1 600.1324627 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P2S 1000.00 usec
PIW1 17.00000000 W

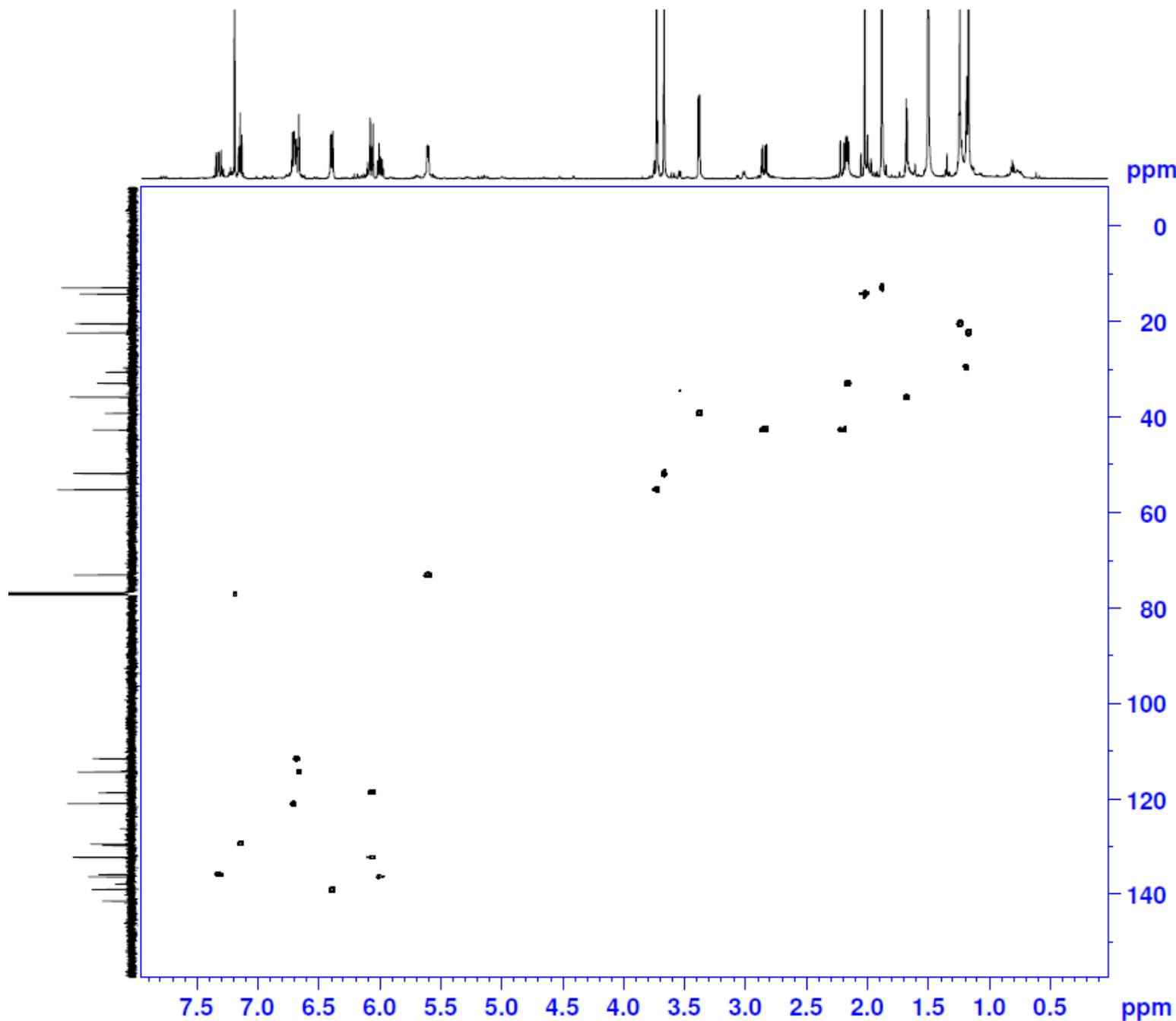
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PIW2 79.98300171 W
PIW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300672 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200807 30Ma II Mig
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200808
Time 9.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 40
DS 16
SWH 4761.905 Hz
FIDRES 1.162574 Hz
AQ 0.4300800 sec
RG 2050
DW 105.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.32551003 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1324627 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

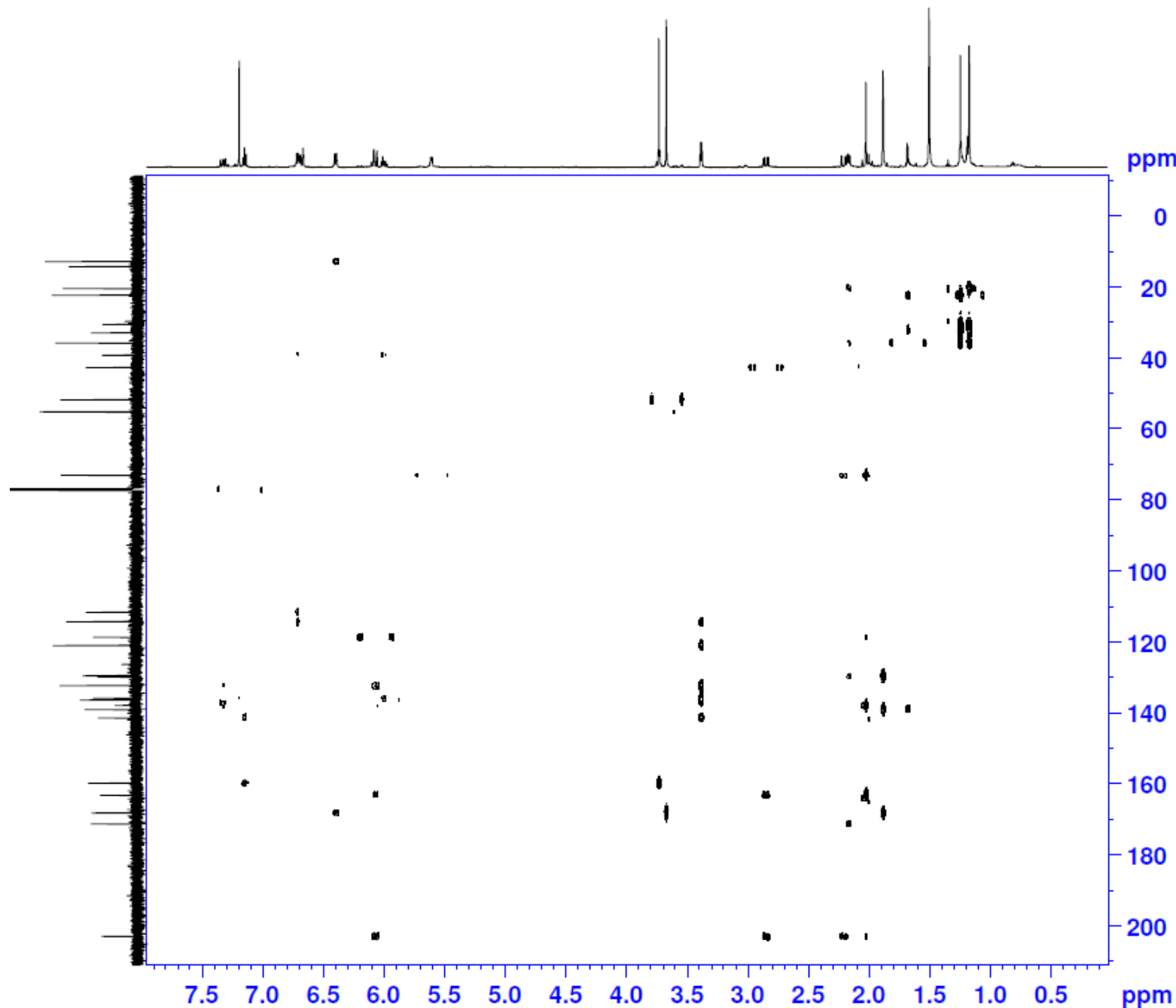
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300672 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

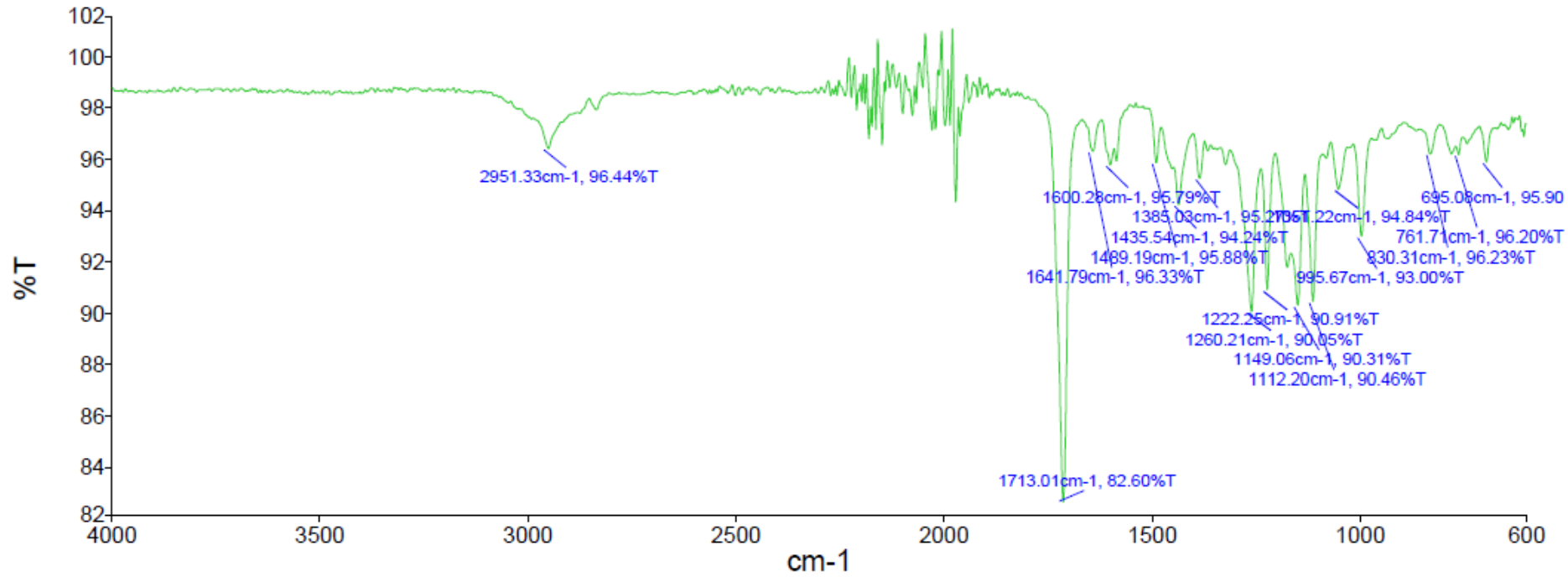


138b IR Spectrum

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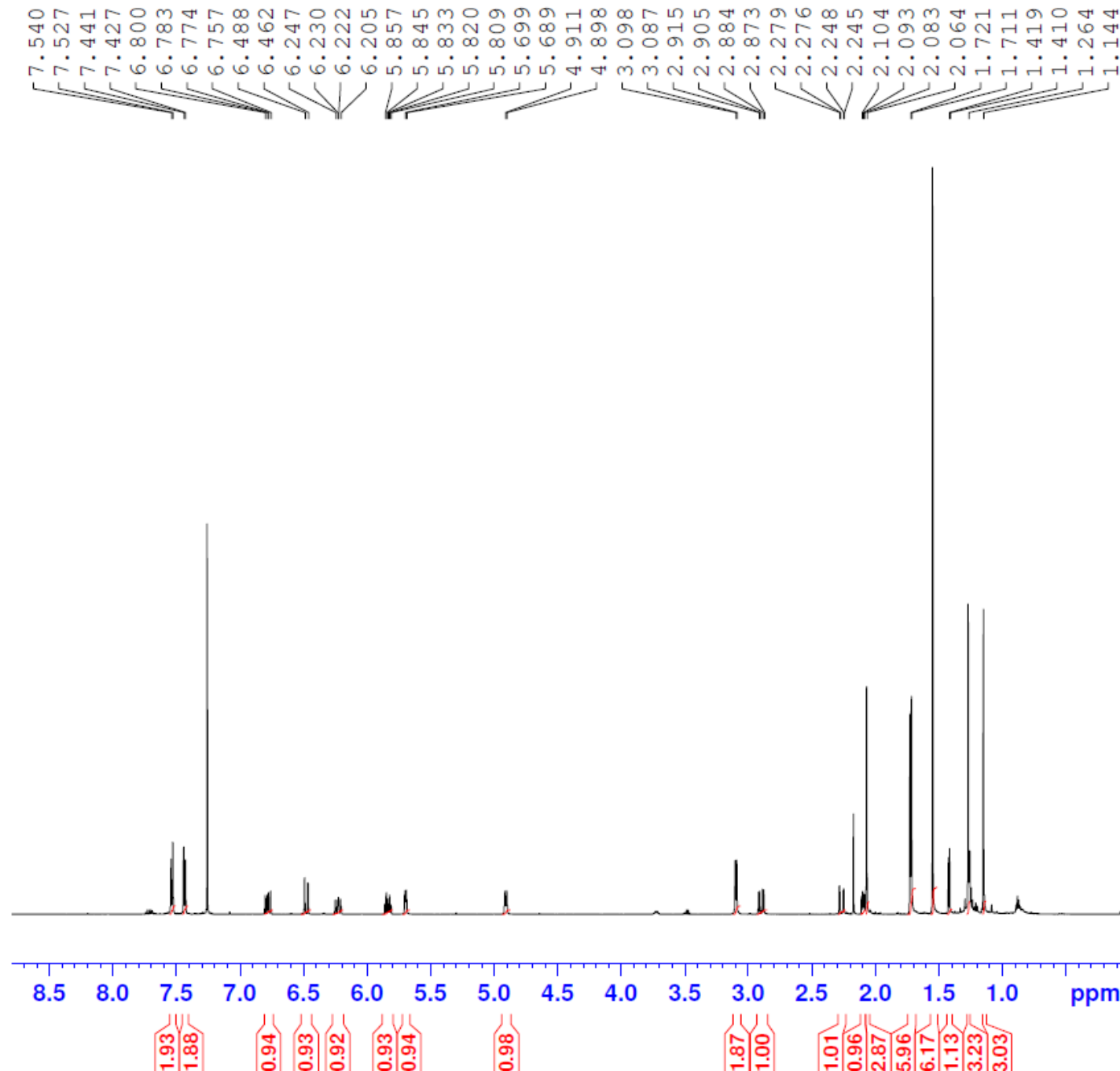
Analyst
Date

Analyst
Friday, 12 June 2020 10:15 AM



Sample Name	Description	Quality Checks
3OMe II Mig	Sample	The Quality Checks do not report any warnings for the sample.

¹³C NMR Characterisation

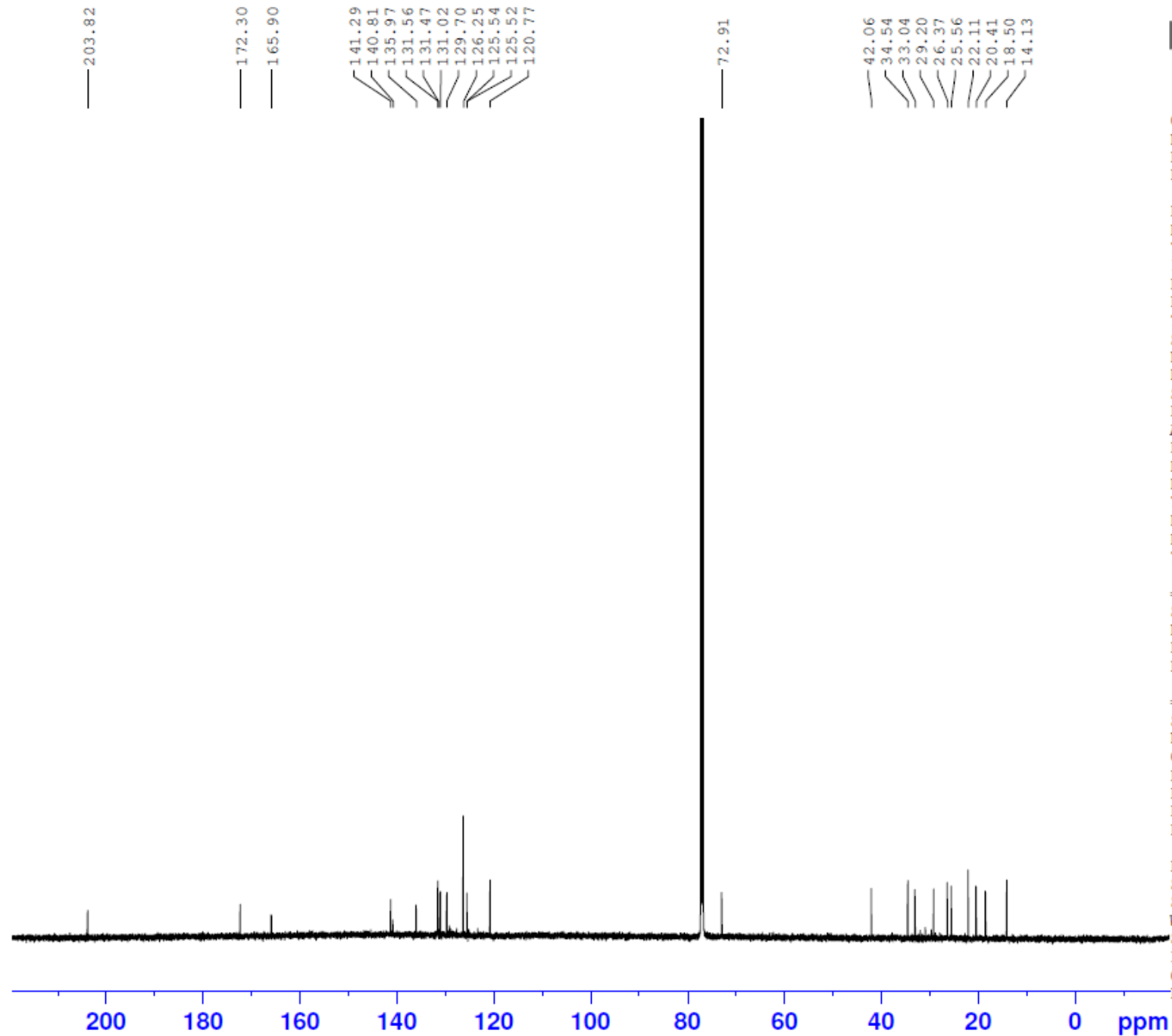


Current Data Parameters
NAME 20200612 4CF3 I E
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200614
Time_ 0.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 362
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300285 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters

NAME 20200612 4CF3 I E
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200614
Time 7.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8000
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====

SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====

SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters

SI 32768
SF 150.9028123 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20200612 4cf3 i e
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200614
Time 0.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
ID 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 4901.961 Hz
FIDRES 2.393536 Hz
AQ 0.2088960 sec
RG 2050
DW 102.000 usec
DE 6.50 usec
TE 298.1 K
D0 0.00008481 sec
D1 1.92954898 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00020400 sec

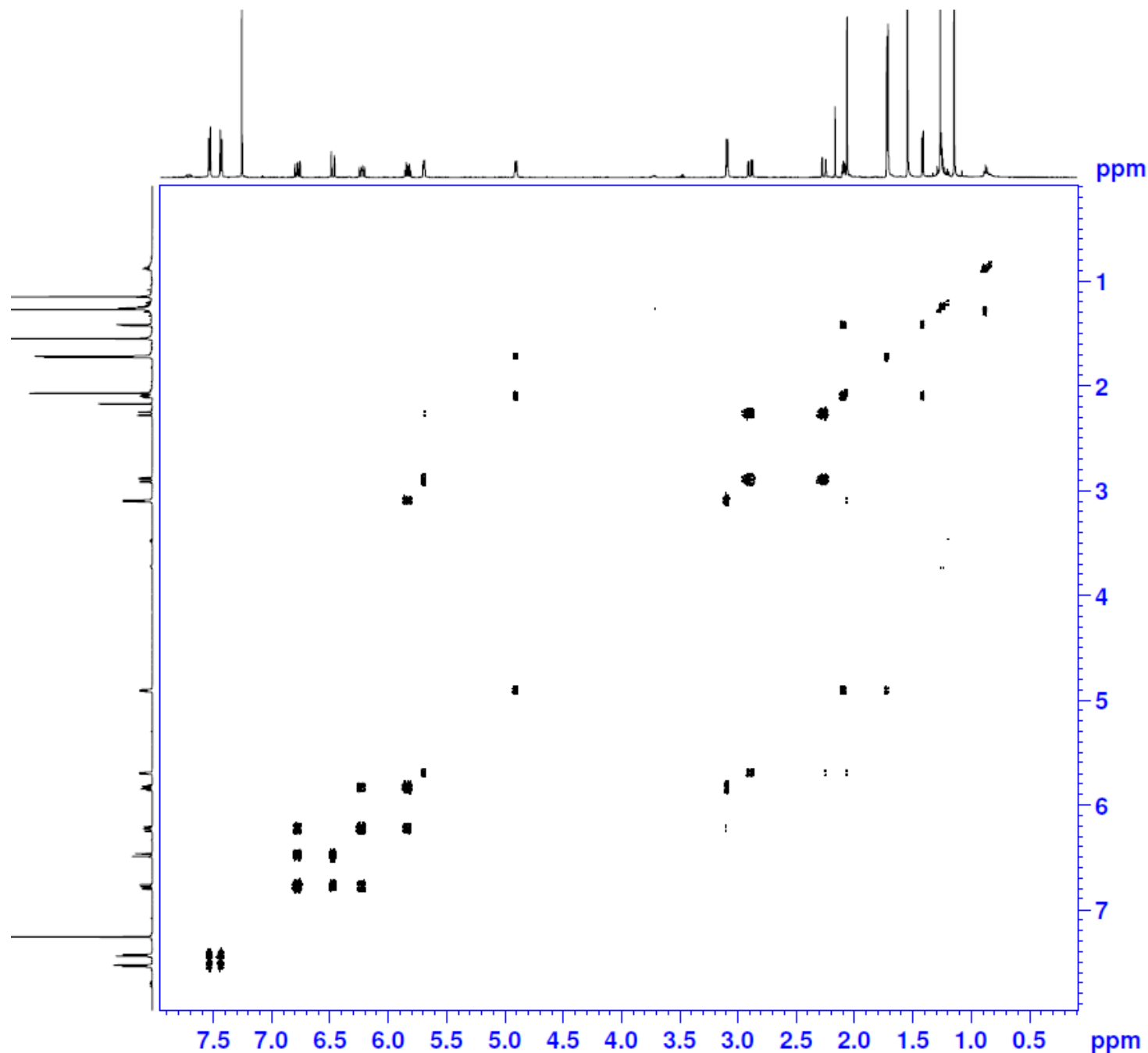
----- CHANNEL f1 -----
SFO1 600.1325295 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 256
SFO1 600.1325 MHz
FIDRES 19.148285 Hz
SW 8.168 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300267 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300267 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200612 4CF3 1 K
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200614
Time 7.33
INSTRUM spect
PROBHD 5 mm FASBO BB/
PULPROG hsqcetop
TD 1024
SOLVENT CDCl3
NS 40
DS 16
SWH 4807.692 Hz
FIDRES 4.695012 Hz
AQ 0.1064960 sec
RG 2050
DW 104.000 usec
DE 6.50 usec
TE 297.9 K
CNST2 145.000000
D0 0.00000300 sec
D1 1.45904005 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1325643 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

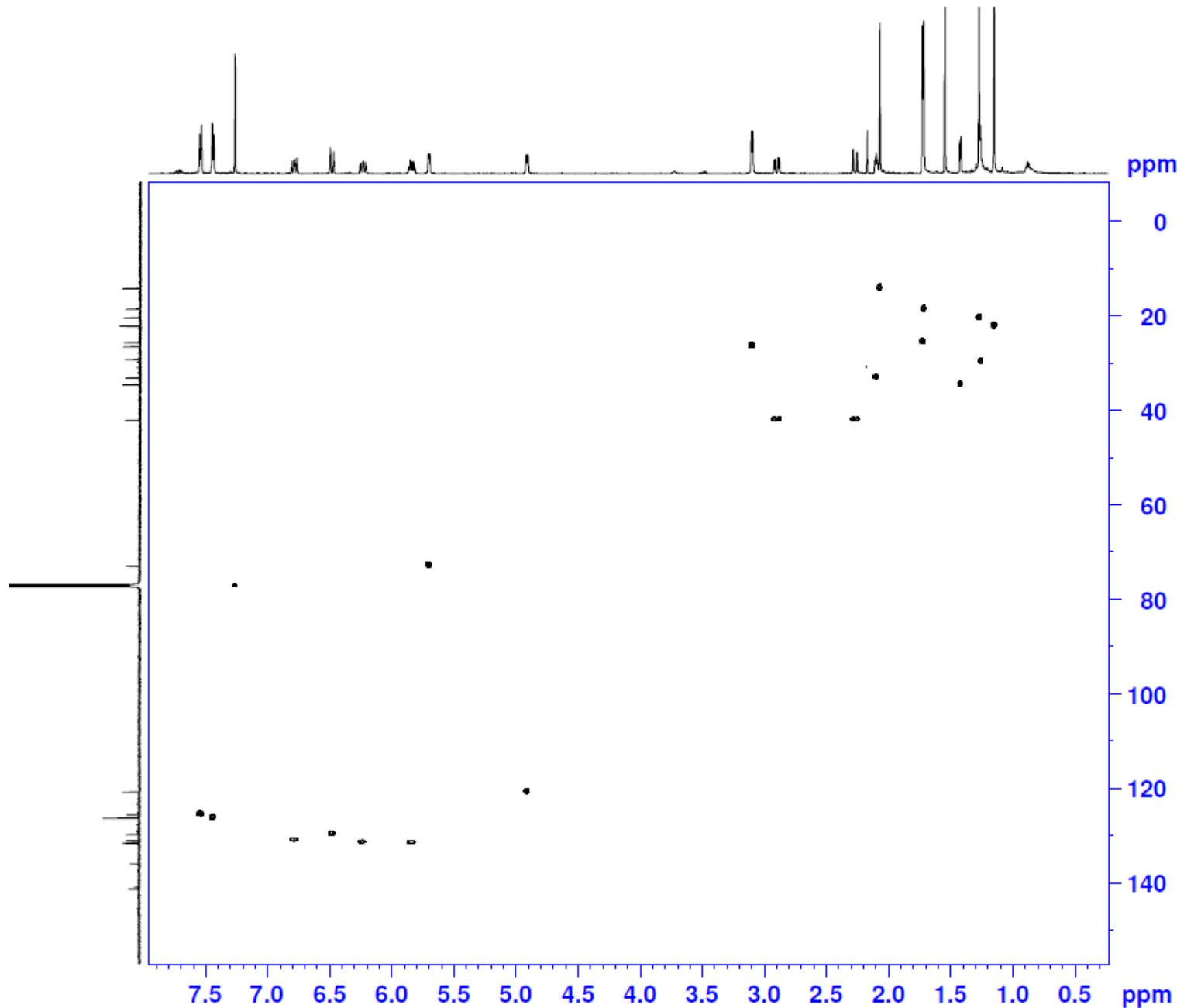
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GFNAM[1] SMSQ10.100
GFNAM[2] SMSQ10.100
GFE1 80.00 %
GFE2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

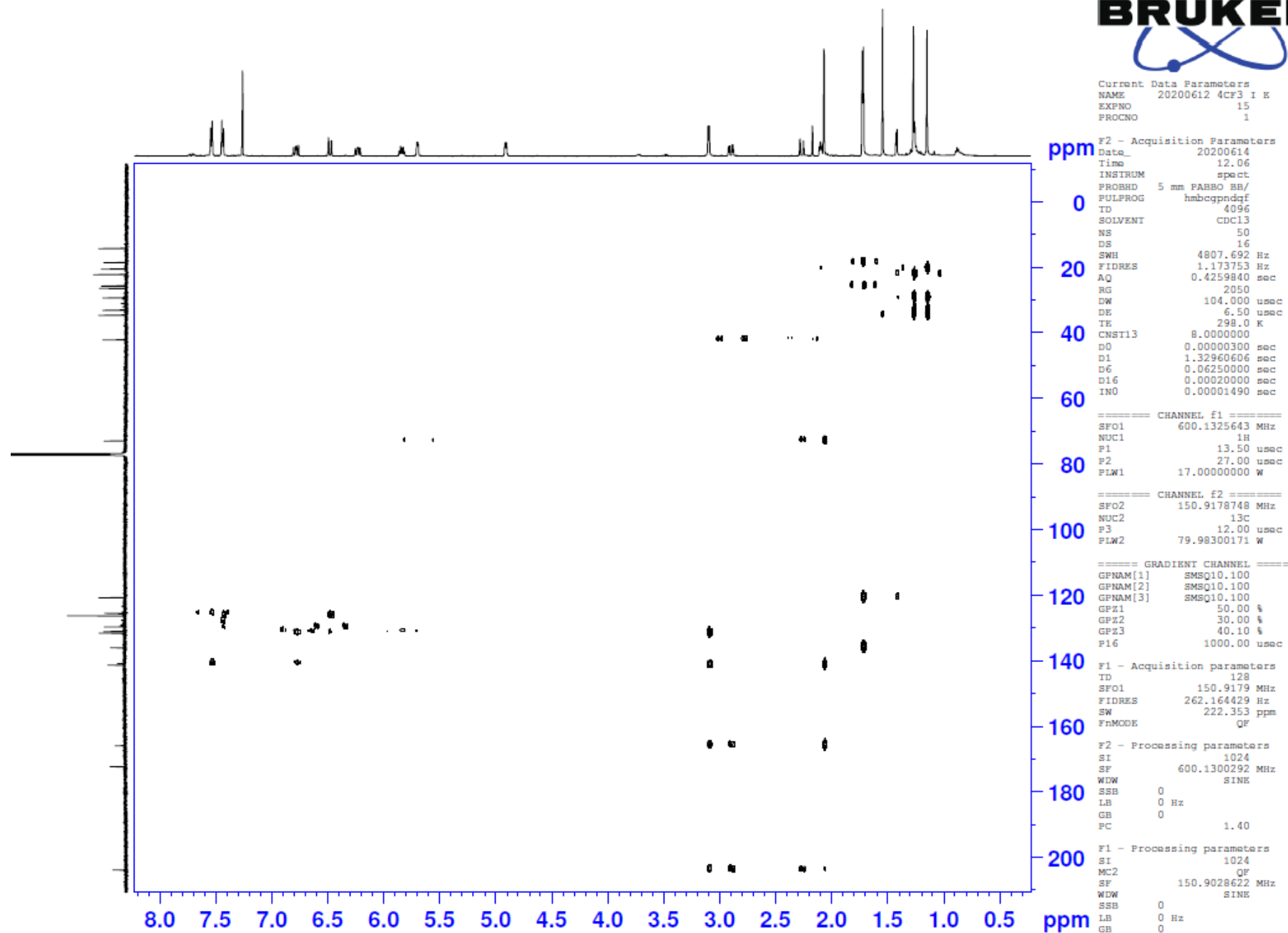
F2 - Processing parameters
SI 1024
SF 600.1300249 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028385 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200612 4cf3 1 E
EXPNO 15
PROCNO 1

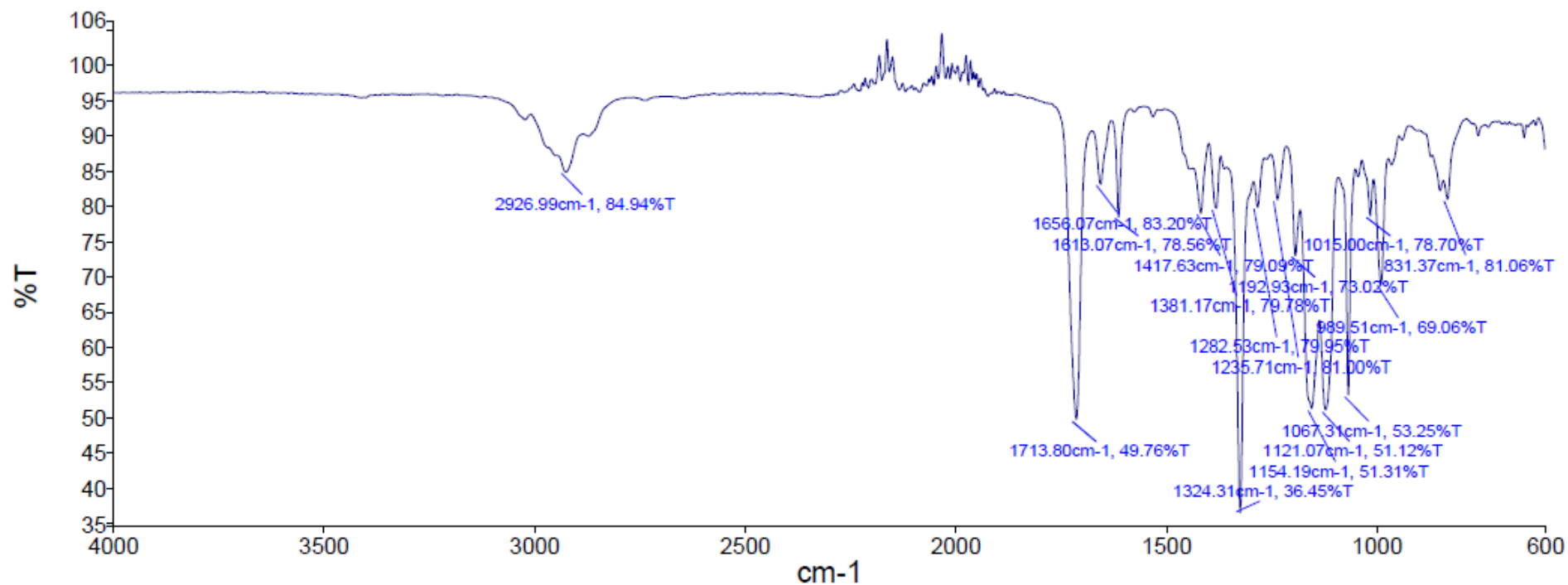


134a IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Thursday, 11 June 2020 5:25 PM

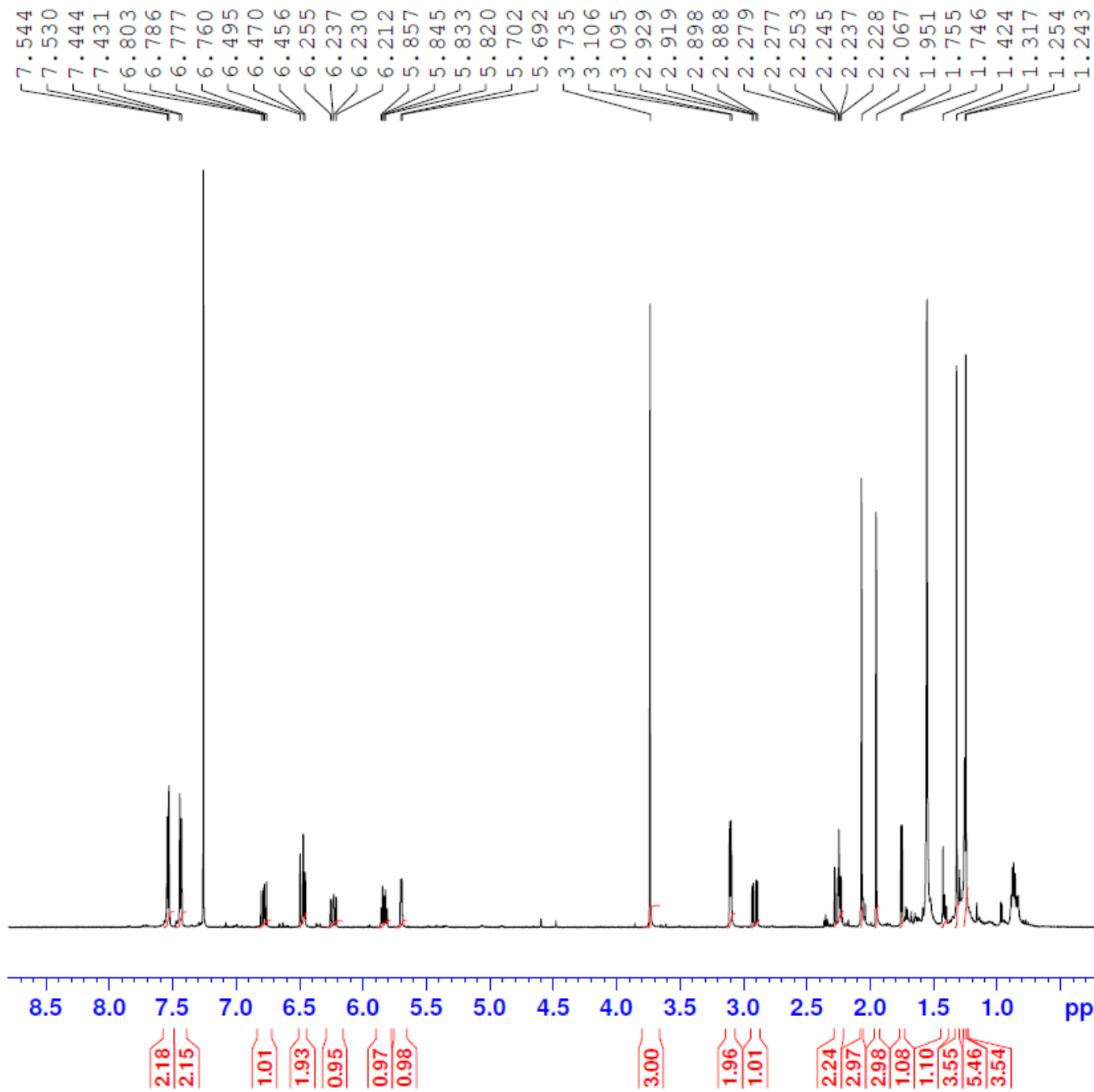
Analyst
Date

Analyst
Thursday, 11 June 2020 5:25 PM



Sample Name	Description	Quality Checks
4CF3 IE	Sample	The Quality Checks do not report any warnings for the sample.

¹³b NMR Characterisation

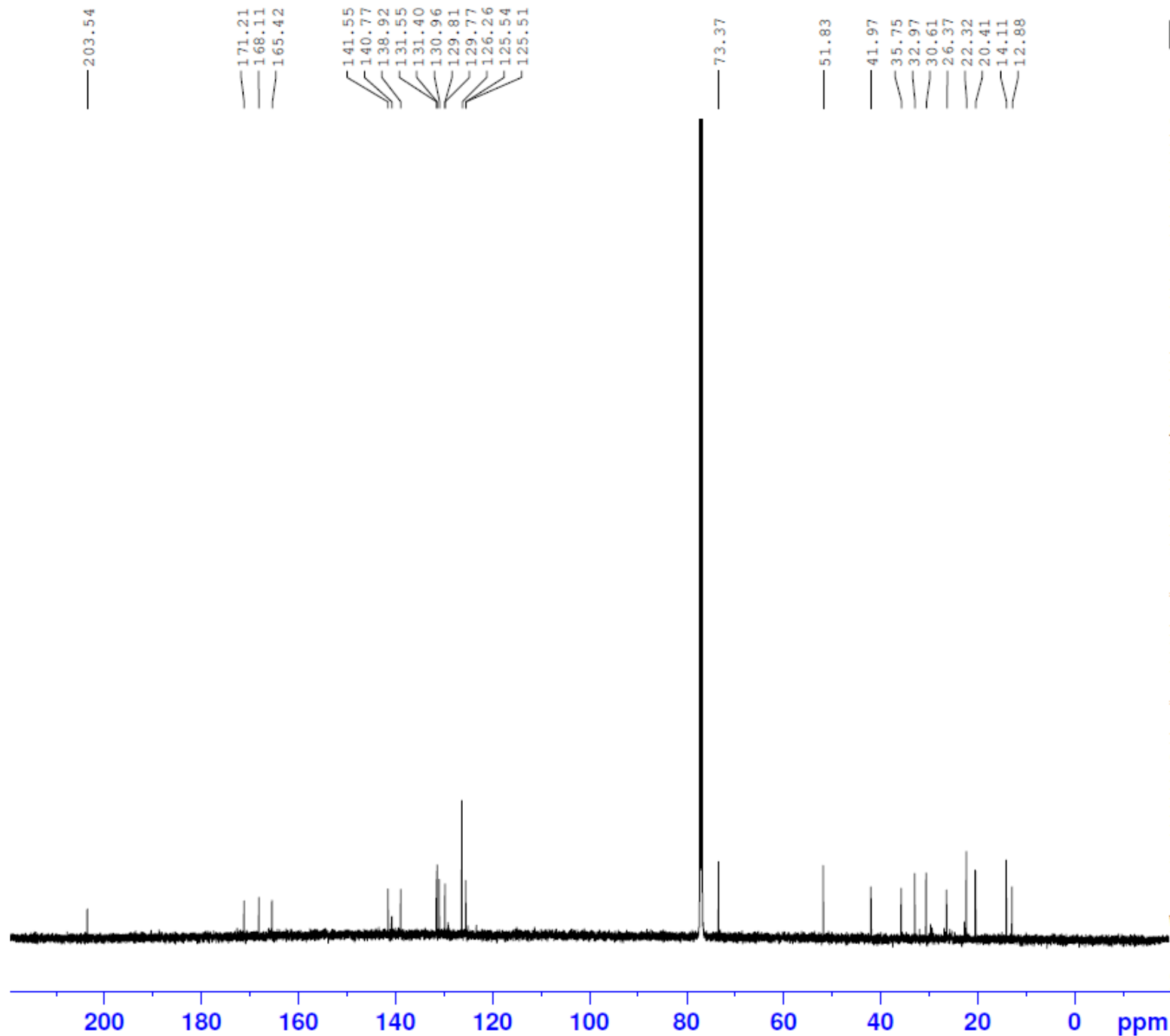


Current Data Parameters
NAME 20200612 4CF3 II E
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200614
Time 15.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 362
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 13.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300269 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters

NAME 20200612 4CF3 II E
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters

Date_ 20200614
Time 22.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8000
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====

SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====

SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters

SI 32768
SF 150.9028138 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20200612 4CF3 II E
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200614
Time 15.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpmfphpp
ID 2048
SOLVENT CDCl3
NS 5
DS 4
SWH 4901.961 Hz
FIDRES 2.393536 Hz
AQ 0.2088960 sec
RG 2050
DW 102.000 usec
DE 6.50 usec
TE 298.2 K
DO 0.00008481 sec
D1 1.92954898 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00020400 sec

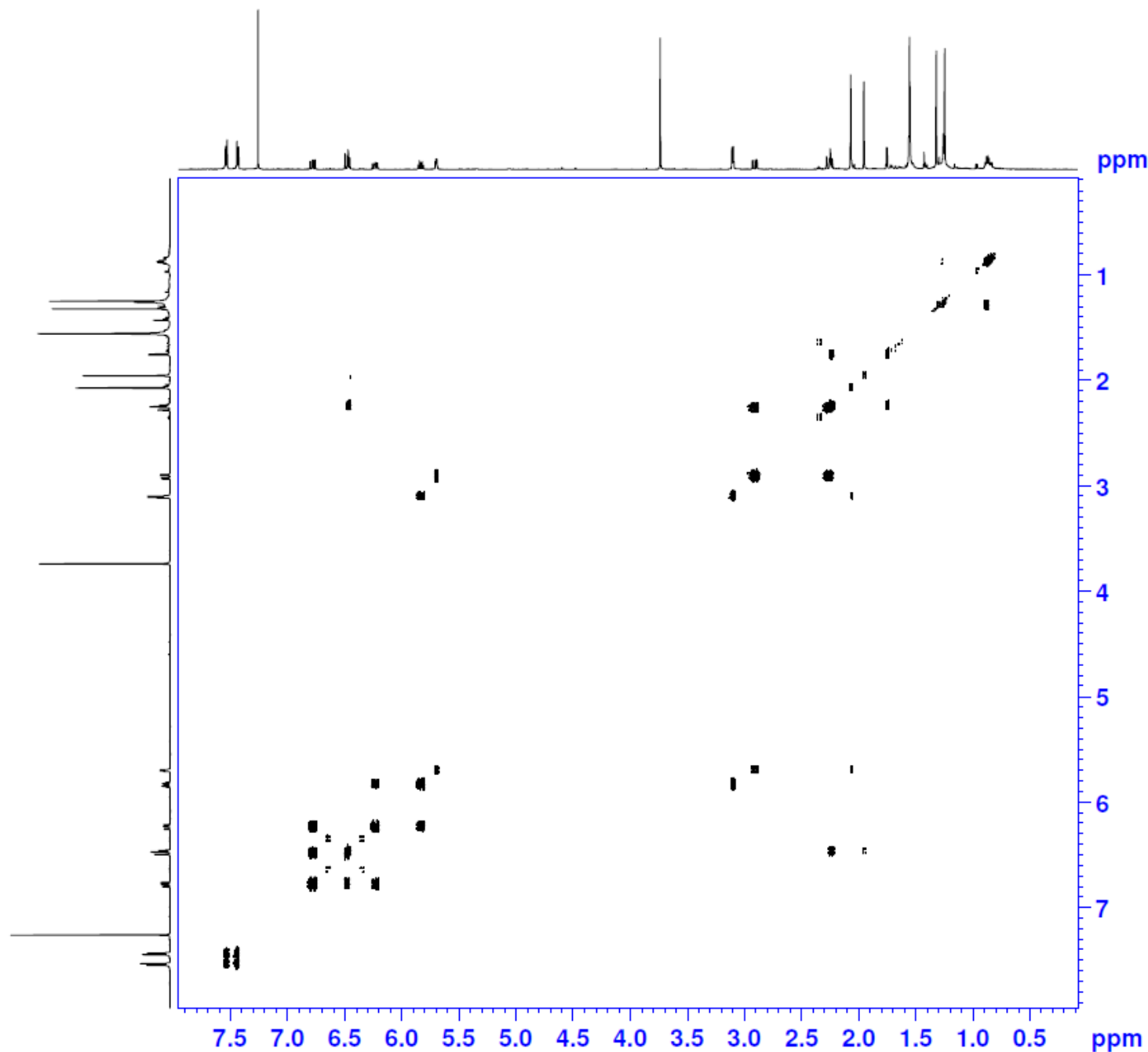
----- CHANNEL f1 -----
SFO1 600.1325235 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 256
SFO1 600.1325 MHz
FIDRES 19.148285 Hz
SW 8.168 ppm
FnMODE States-IPPI

F2 - Processing parameters
SI 1024
SF 600.1300263 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-IPPI
SF 600.1300270 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200612 4cf3 ii E
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200614
Time 22.57

INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetqp
TD 1024
SOLVENT CDCl3
NS 40
DS 16
SWH 4807.692 Hz
FIDRES 4.695012 Hz
AQ 0.1064960 sec
RG 2050
DW 104.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45904005 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPTNS

===== CHANNEL f1 =====
SFO1 600.1324890 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

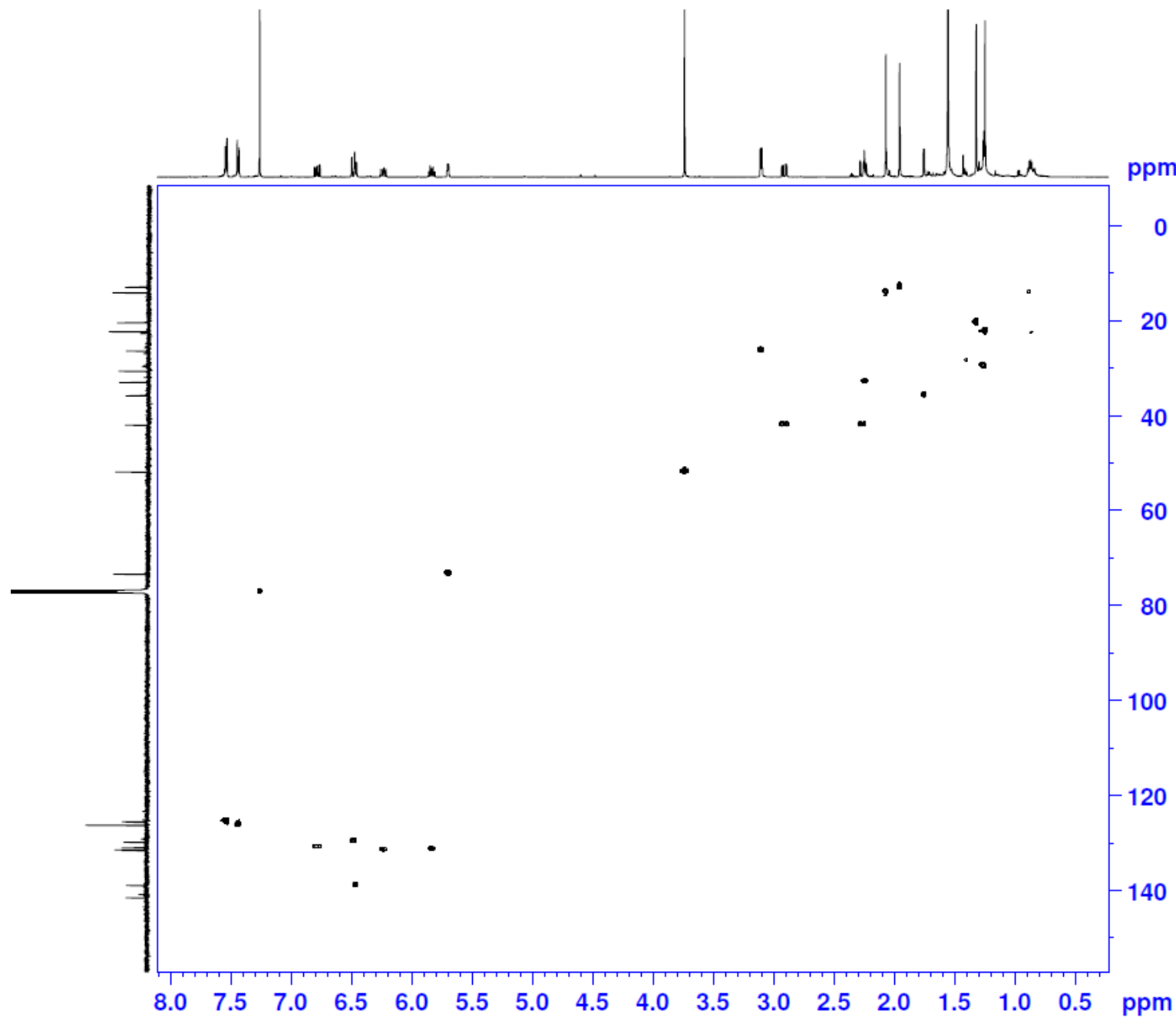
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 79.98300171 W
PLW12 3.19930005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPX1 80.00 %
GPX2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnmODE Echo-Antiecho

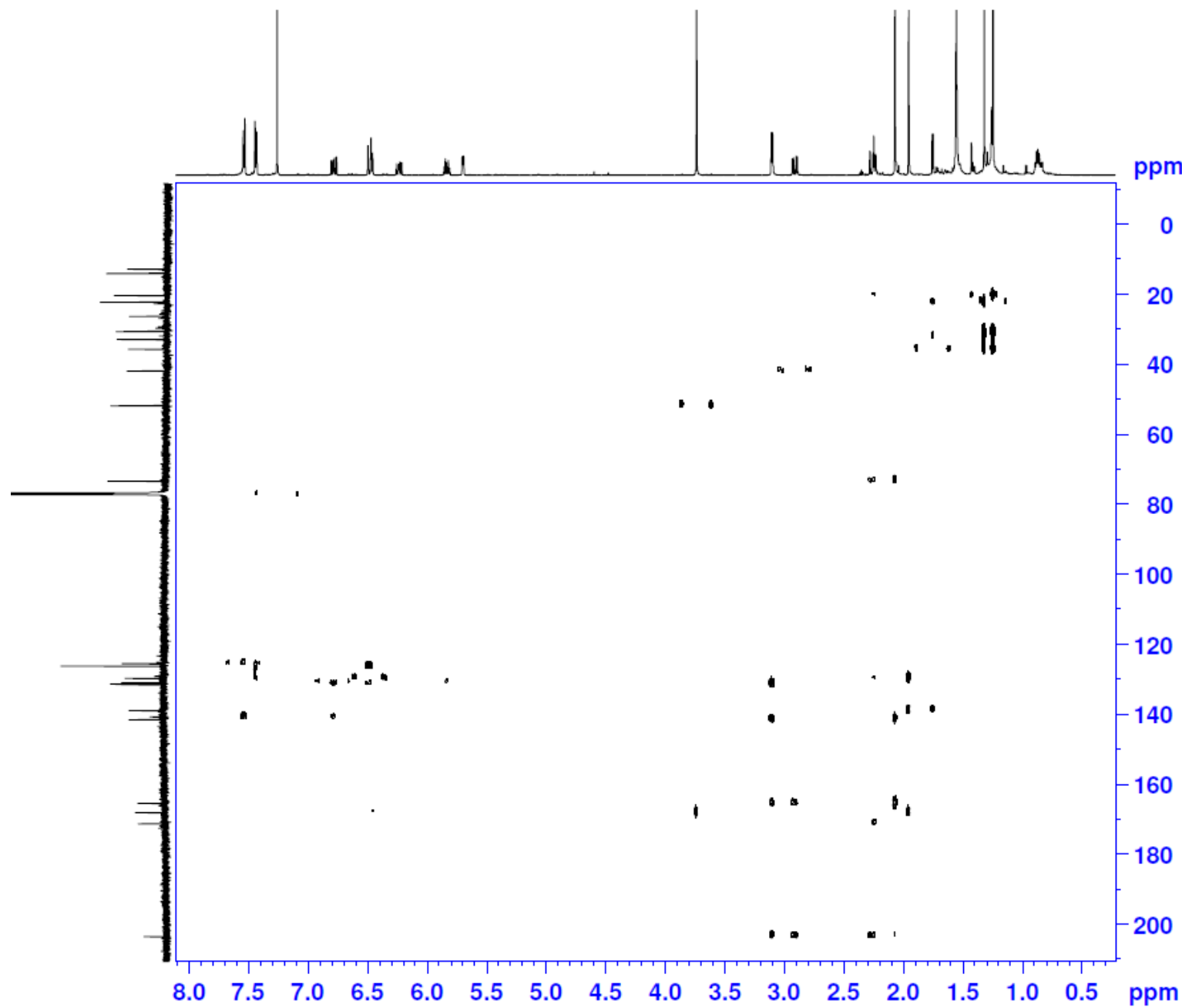
F2 - Processing parameters
SI 1024
SF 600.1300259 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028509 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20200612 4CP3 II E
EXPNO 15
PROCNO 1



F2 - Acquisition Parameters
Date_ 20200615
Time 3.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
ID 4096
SOLVENT CDCl3
NS 50
DS 16
SWH 4807.692 Hz
FIDRES 1.173753 Hz
AQ 0.4259840 sec
RG 2050
DW 104.000 usec
DE 6.50 usec
TE 298.0 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.32960606 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1324890 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 79.98300171 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSq10.100
GPNAM[2] SMSq10.100
GPNAM[3] SMSq10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300239 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

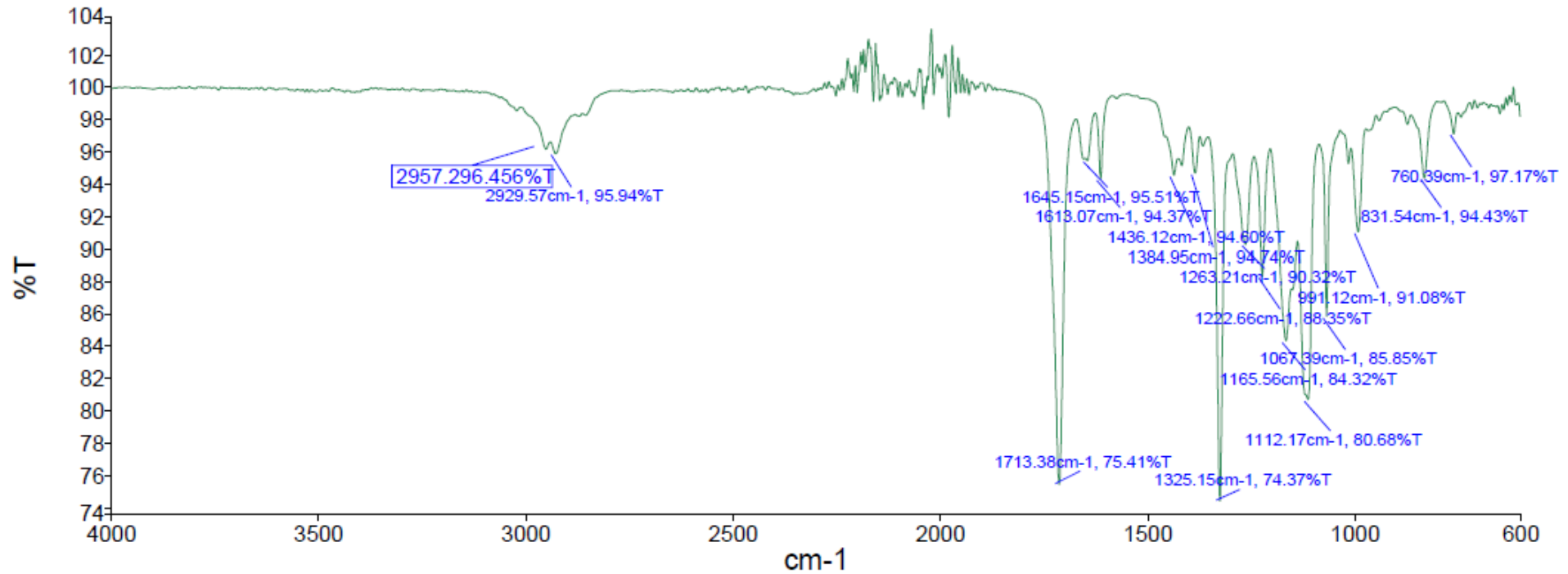
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028536 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

134b IR Spectrum

PerkinElmer Spectrum Version 10.4.00
Thursday, 11 June 2020 5:31 PM

Analyst
Date

Analyst
Thursday, 11 June 2020 5:31 PM



Sample Name	Description	Quality Checks
4CF3 II E	Sample	The Quality Checks do not report any warnings for the sample.

Model Compound Characterisation Data

NMR Characterisation 188

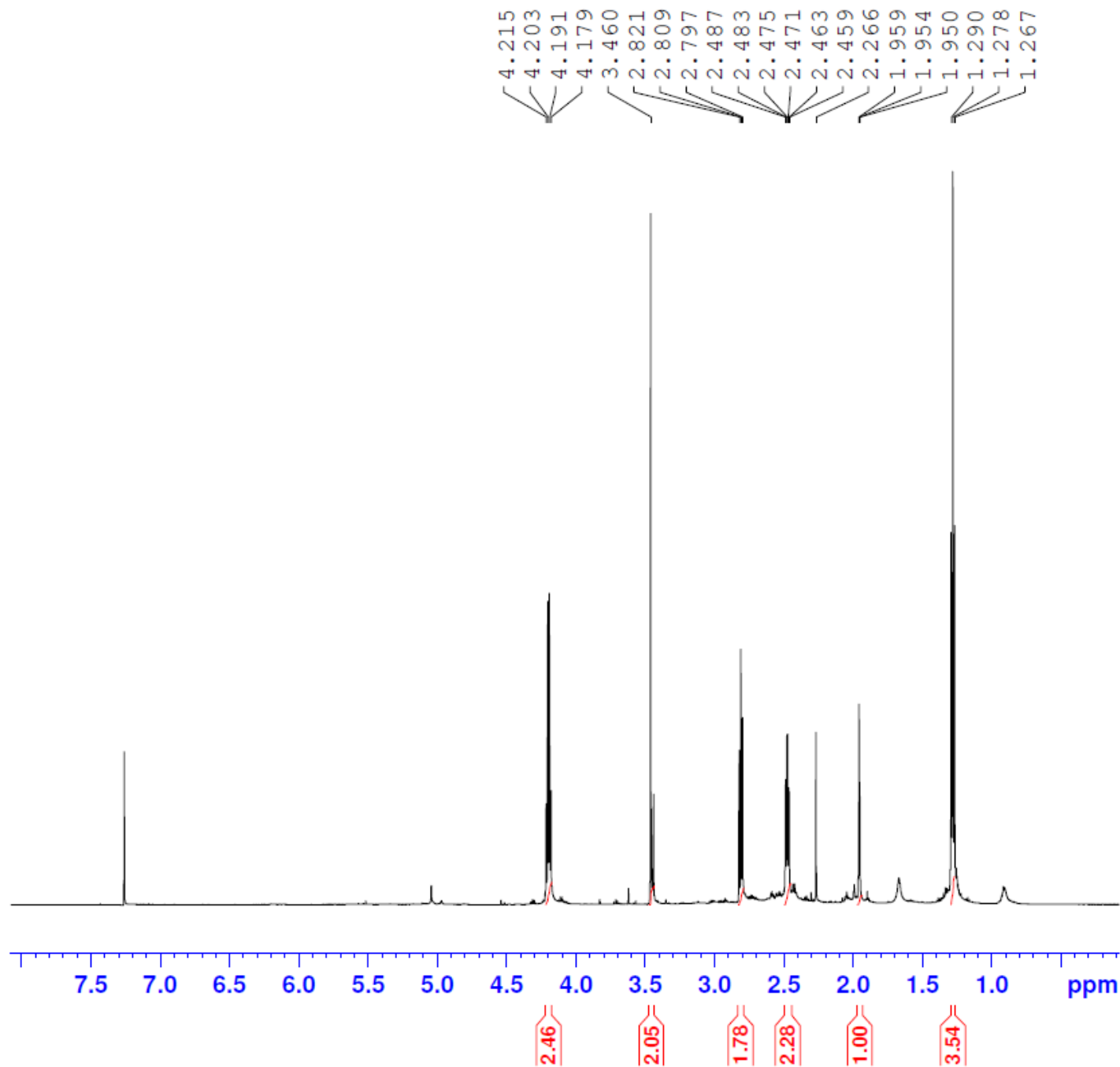


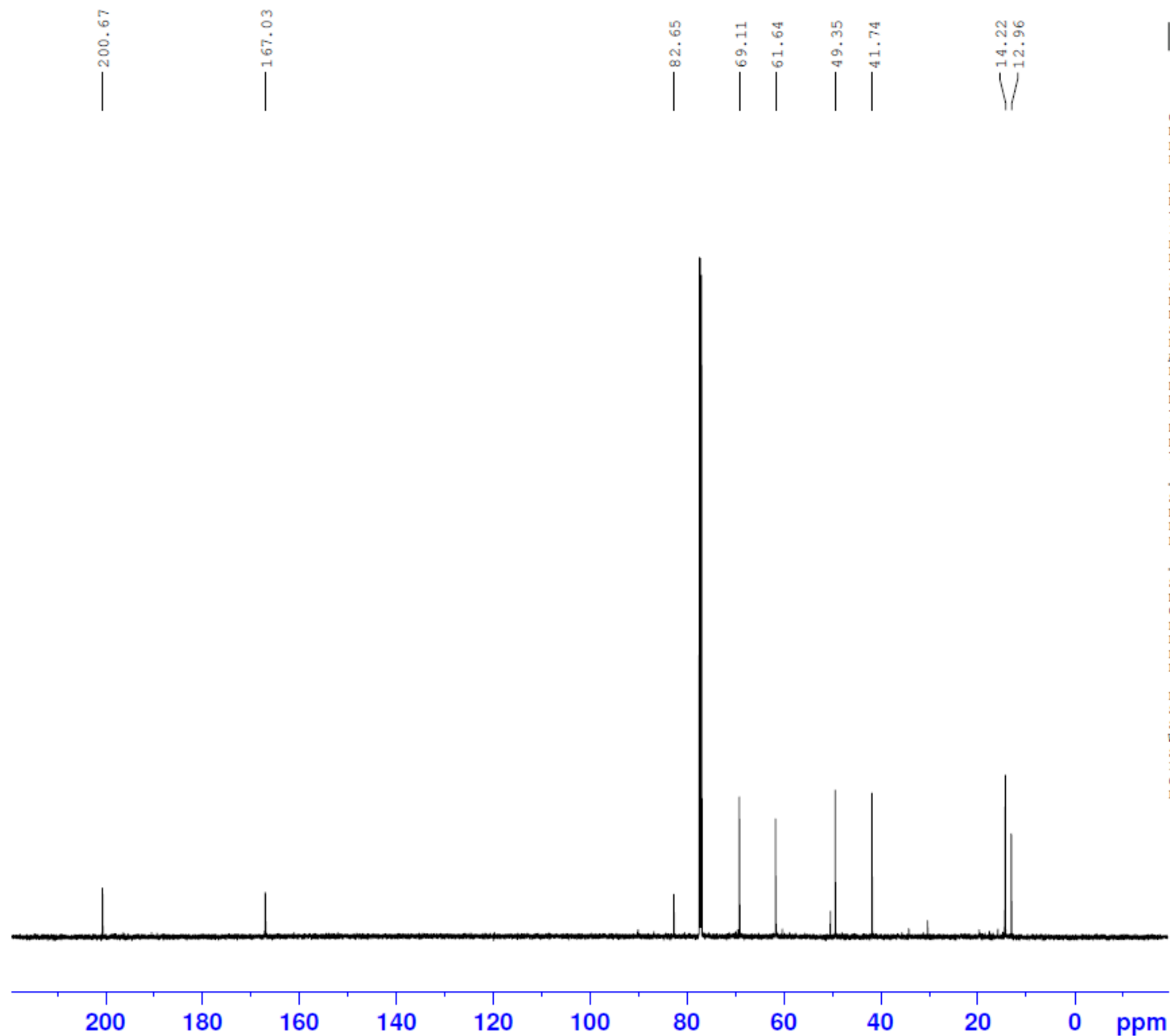
Current Data Parameters
NAME 20180227 Dianion alkylation
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180227
Time 17.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 228
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 600.1337060 MHz
NUC1 1H
P1 14.00 usec
PLW1 17.79999924 W

F2 - Processing parameters
SI 65536
SF 600.1300263 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
 NAME 20180227 Dianion alkylation
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180227
 Time 19.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 90.00000000 W

----- CHANNEL f2 -----
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.79999924 W
 PLW12 0.71200001 W
 PLW13 0.34887999 W

F2 - Processing parameters
 SI 32768
 SF 150.9027924 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20180227 Dianion alkylation
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180227
Time 17.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 4000.000 Hz
FIDRES 1.953125 Hz
AQ 0.2560000 sec
RG 64
DW 125.000 usec
DE 6.50 usec
TE 298.3 K
D0 0.00000300 sec
D1 1.87179506 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00025000 sec

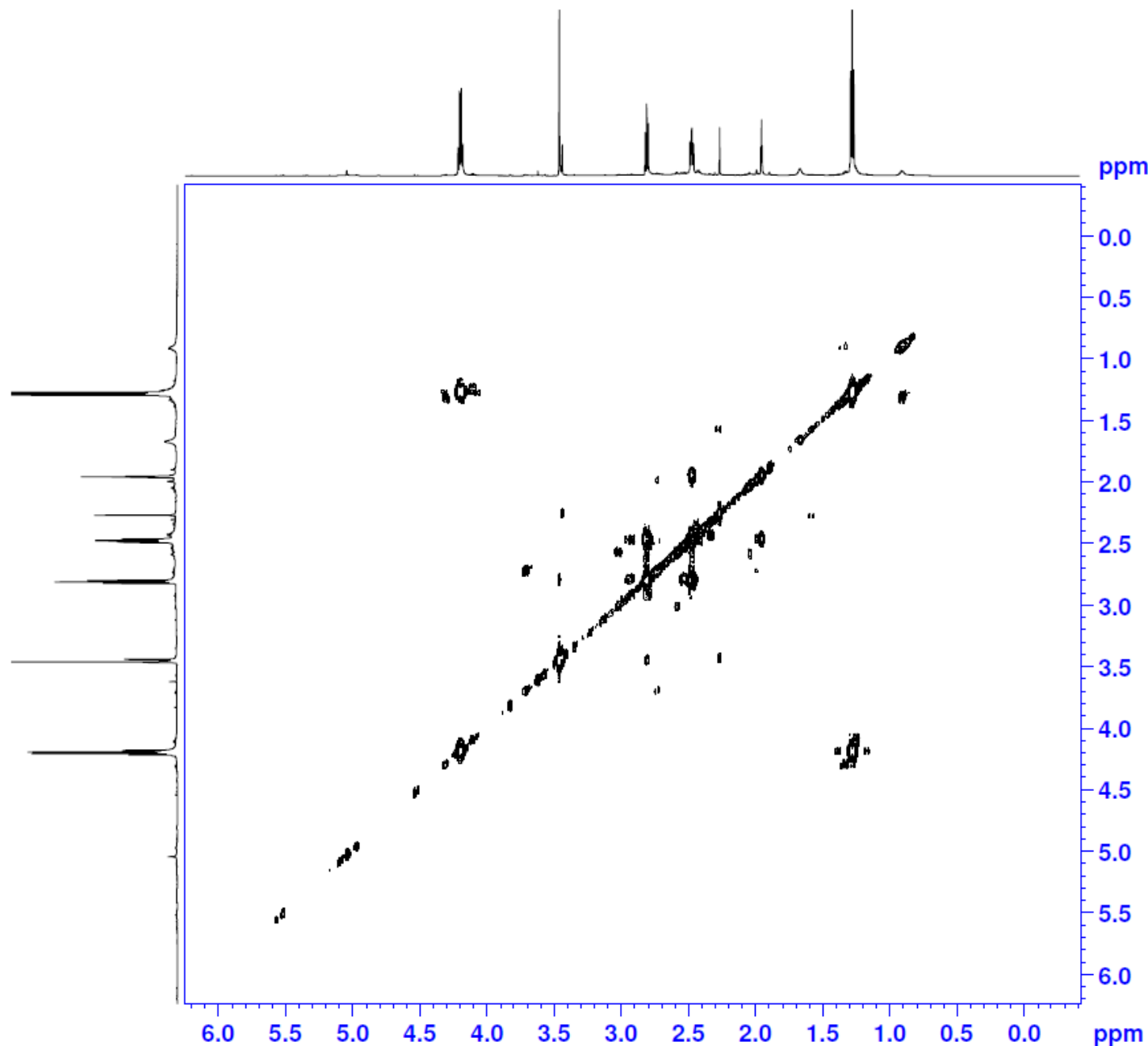
----- CHANNEL f1 -----
SFO1 600.1317763 MHz
NUC1 1H
P0 14.00 usec
P1 14.00 usec
P17 2500.00 usec
PLW1 17.79999924 W
PLW10 5.16090012 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1318 MHz
FIDRES 31.250000 Hz
SW 6.665 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300264 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300300 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20180227 Dianion alkylation
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180227
Time 19.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcqtgps12
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 3205.128 Hz
FIDRES 3.130008 Hz
AQ 0.1597440 sec
RG 2050
DW 156.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.40415394 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
INO 0.00002000 sec
ZCOPTNS

CHANNEL f1
SFO1 600.1317643 MHz
NUC1 1H
P1 14.00 usec
P2 28.00 usec
P28 1000.00 usec
PLW1 17.79999924 W

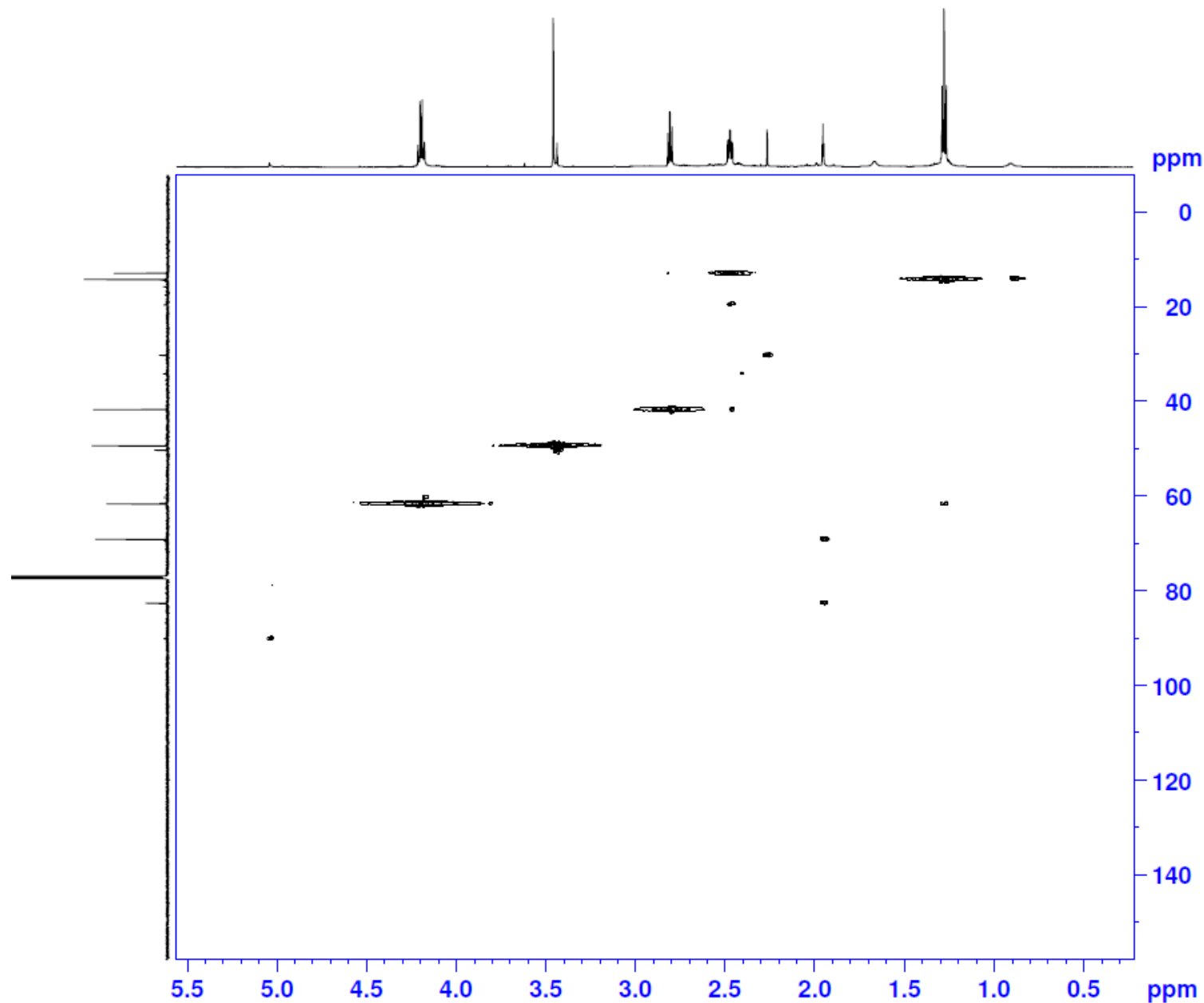
CHANNEL f2
SFO2 150.9141231 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 90.00000000 W
PLW12 3.59999990 W

GRADIENT CHANNEL
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPE1 80.00 %
GPE2 20.10 %
GPE3 11.00 %
GPE4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FrMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300292 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9027965 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20180227 Dianion alkylation
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180228
Time 0.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndgf
TD 4096
SOLVENT CDCl3
NS 65
DS 16
SWH 3205.128 Hz
FIDRES 0.782502 Hz
AQ 0.6389760 sec
RG 2050
DW 156.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.11661398 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1317643 MHz
NUC1 1H
P1 14.00 usec
P2 28.00 usec
PLW1 17.79999924 W

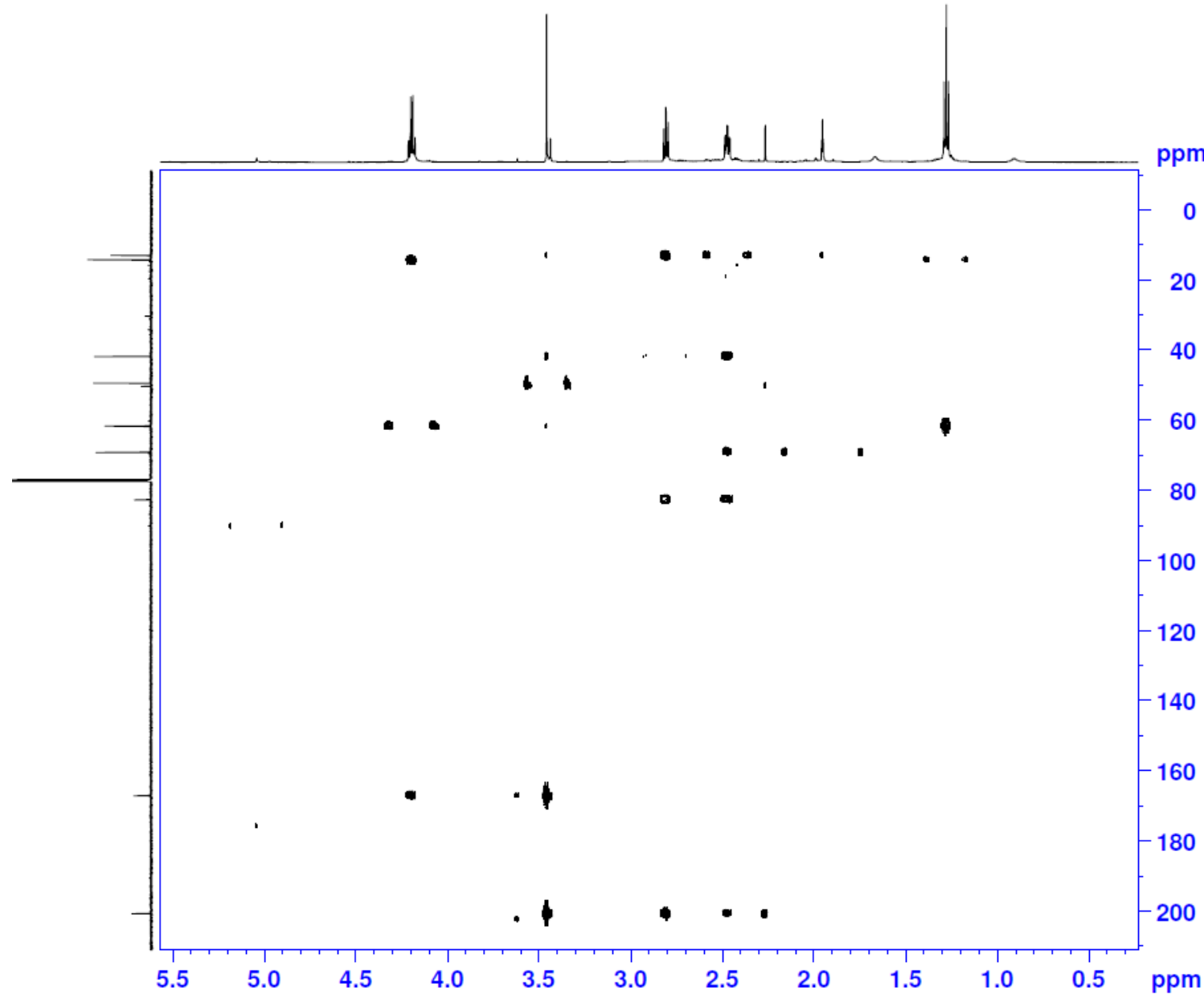
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 90.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

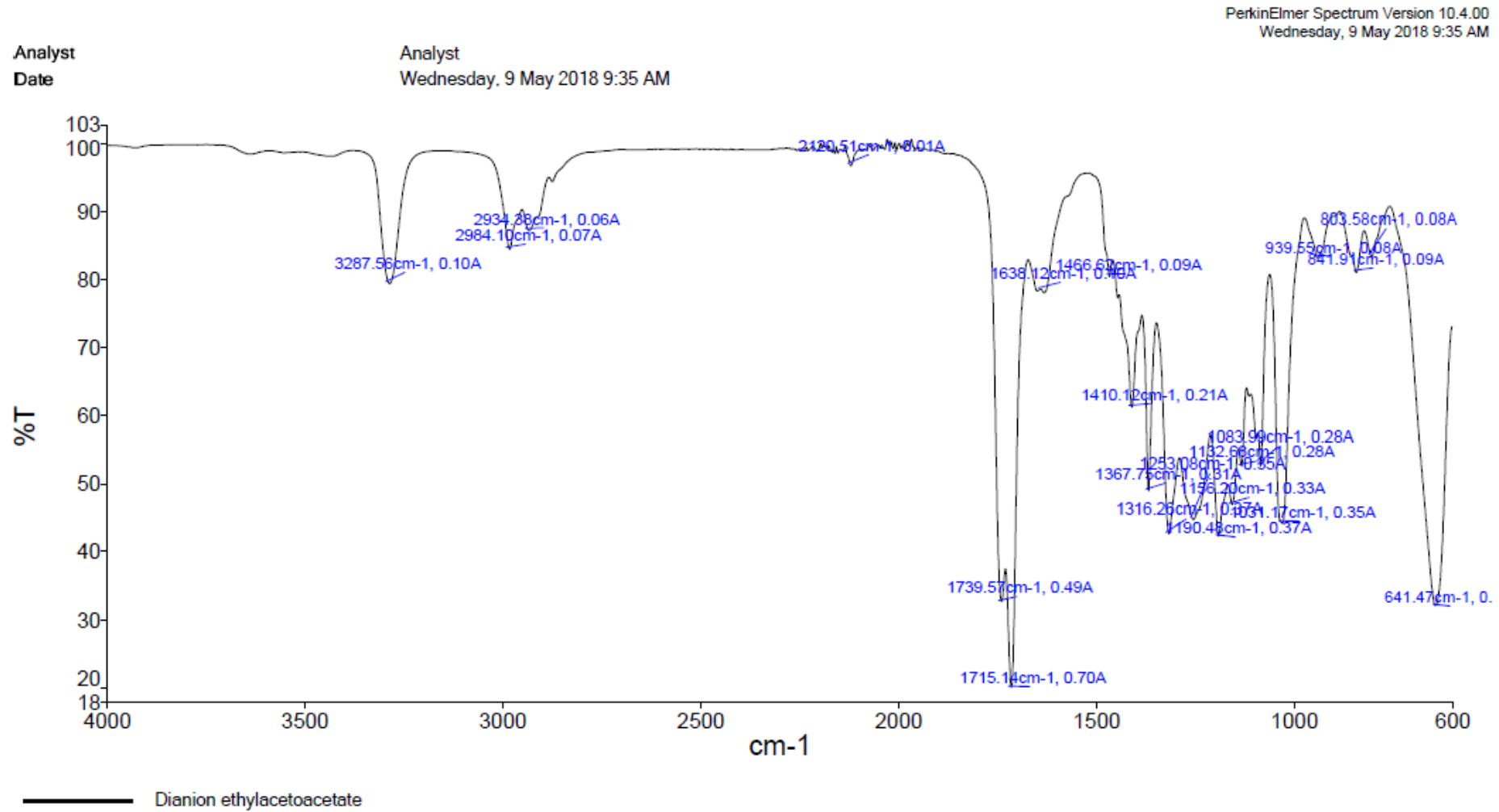
F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
F1MODE QF

F2 - Processing parameters
SI 1024
SF 600.1300243 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9027985 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



188 IR spectrum



NMR Characterisation 174

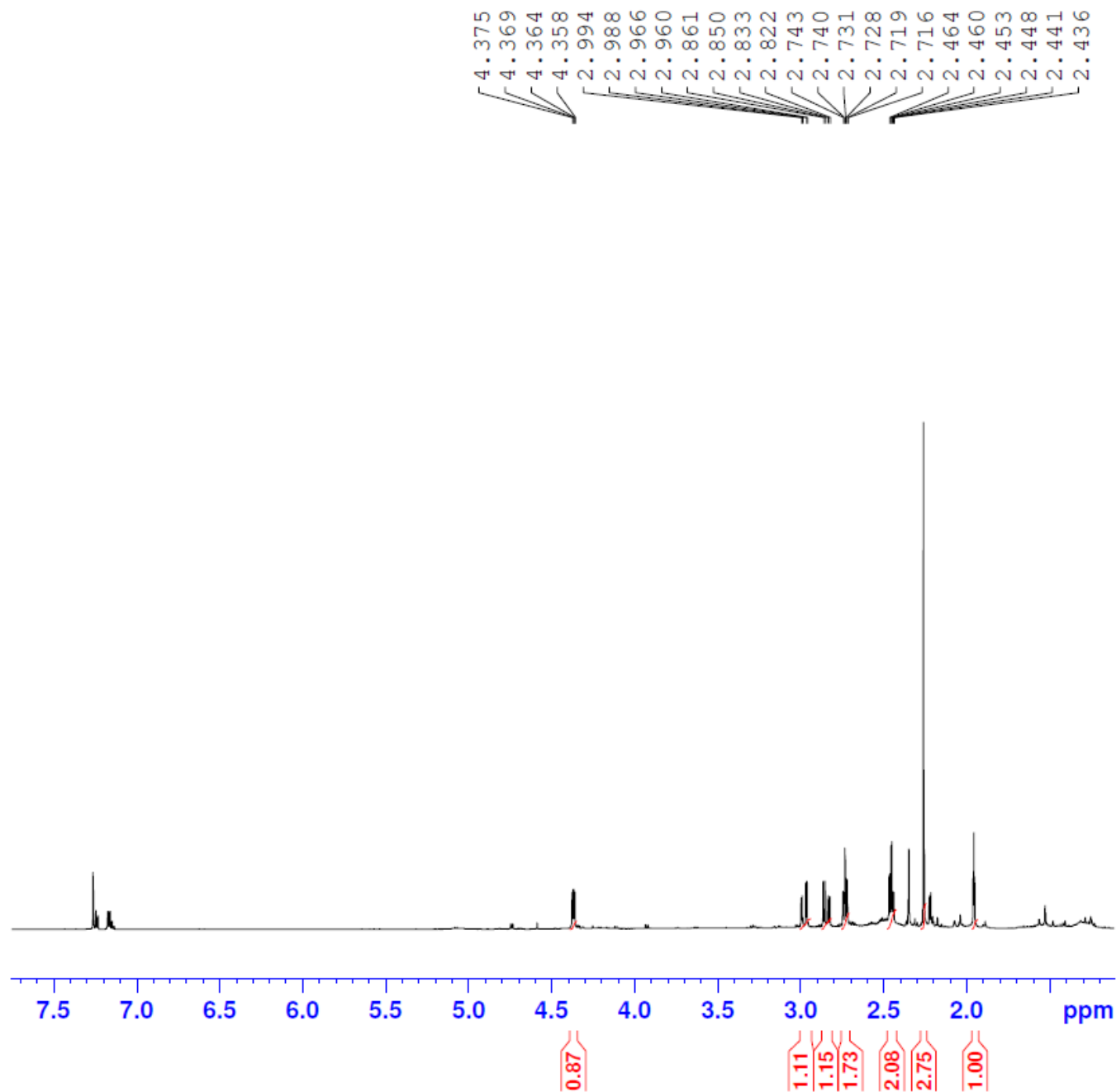


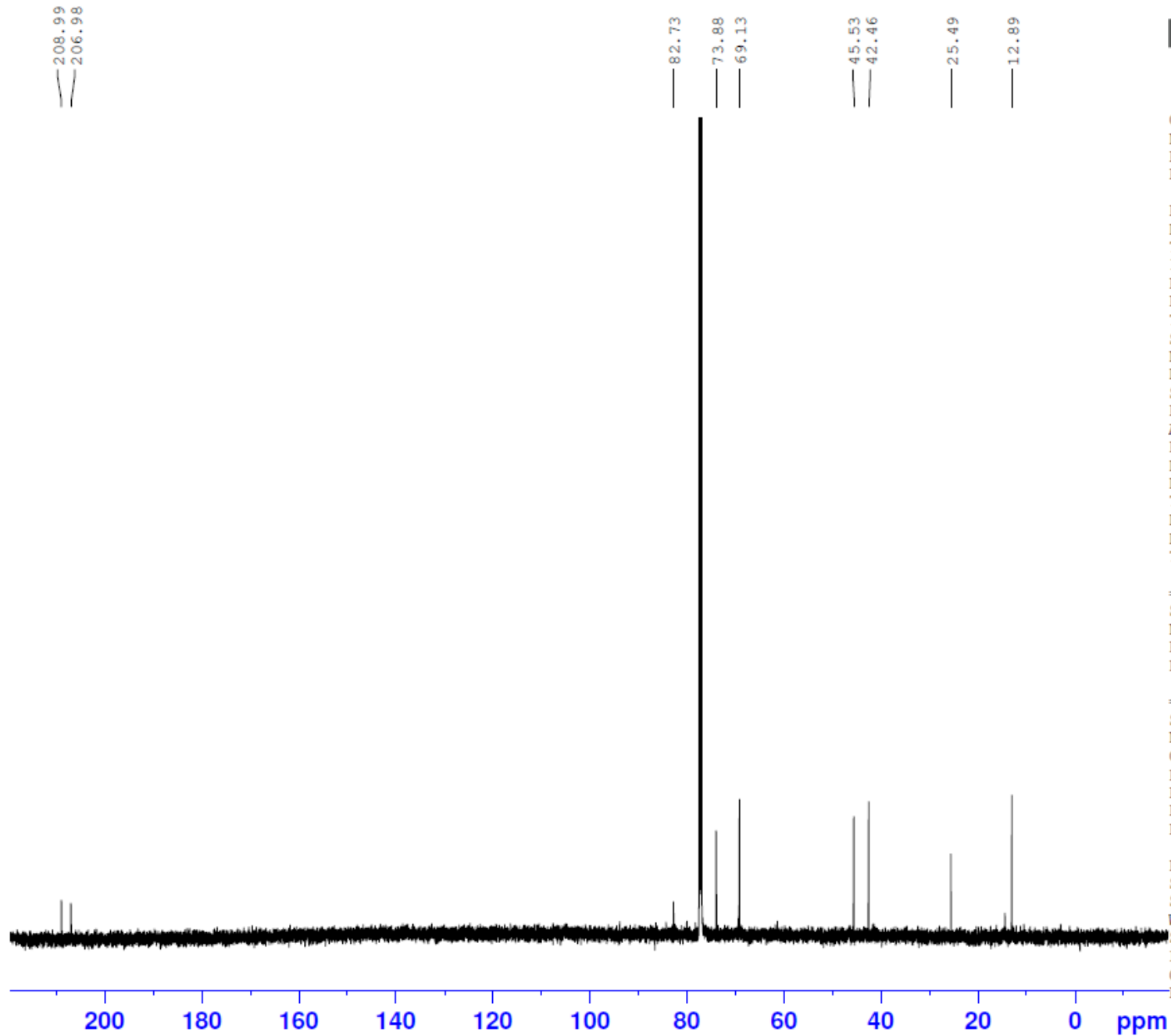
Current Data Parameters
 NAME 20180301 Decarb aldol
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180301
 Time 18.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 181
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 14.00 usec
 PLW1 17.79999924 W

F2 - Processing parameters
 SI 65536
 SF 600.1300261 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
NAME 20190628 MC2
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190628
Time 20.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 12.00 usec
PLW1 80.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 17.00000000 W
PLW12 0.63230002 W
PLW13 0.30983001 W

F2 - Processing parameters
SI 32768
SF 150.9027897 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20180301 Decarb aldol
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180301
Time 18.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppgf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 5952.381 Hz
FIDRES 2.906436 Hz
AQ 0.1720320 sec
RG 64
DW 84.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.95576298 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00016800 sec

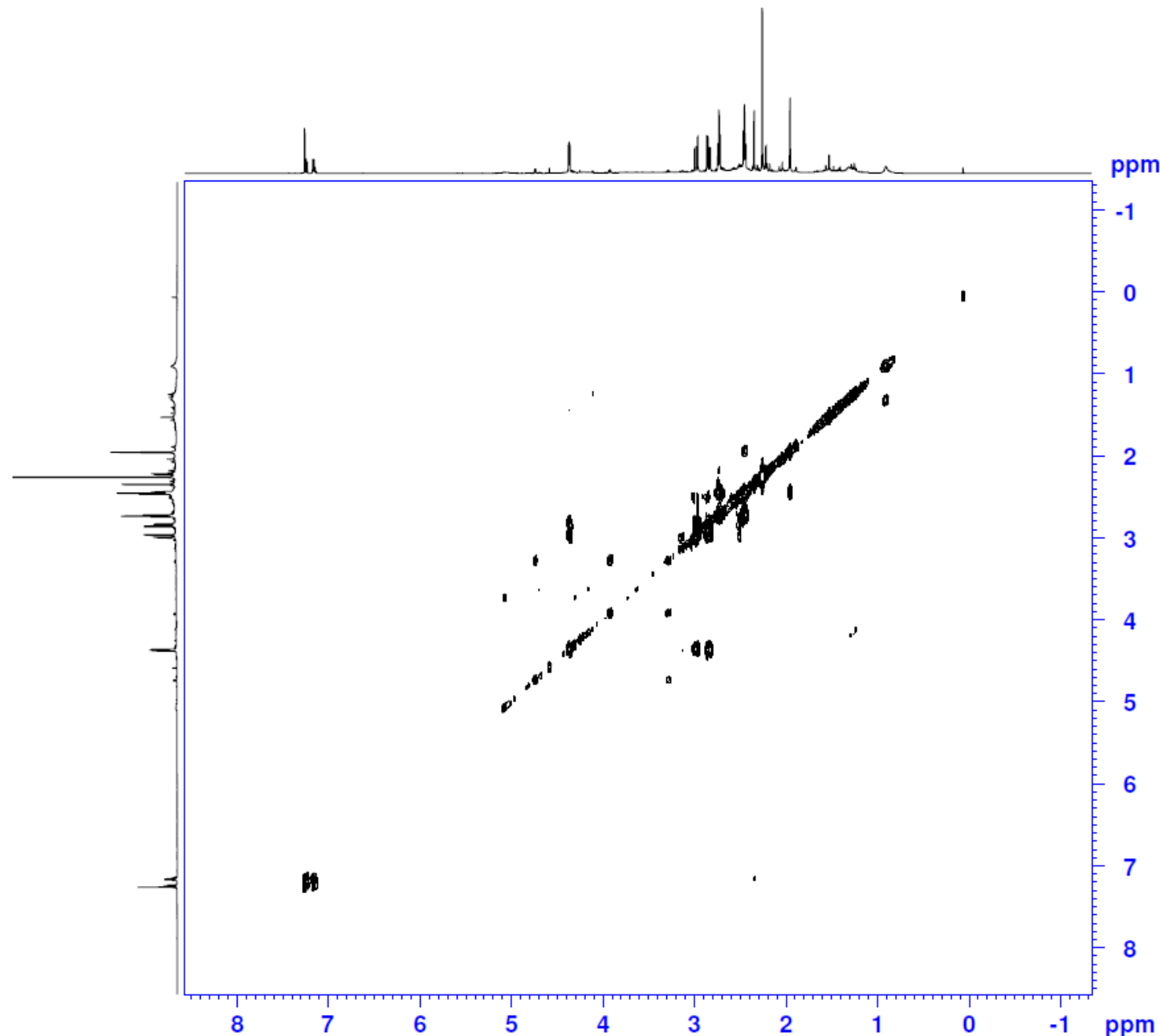
----- CHANNEL f1 -----
SFO1 600.1321951 MHz
NUC1 1H
P0 14.00 usec
P1 14.00 usec
P17 2500.00 usec
PLW1 17.79999924 W
PLW10 5.16090012 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 128
SFO1 600.1322 MHz
FIDRES 46.502975 Hz
SW 9.918 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300276 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300274 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190628 MC2
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190628
Time 20.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 2702.703 Hz
FIDRES 2.639358 Hz
AQ 0.1894400 sec
RG 2050
DW 185.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.0000300 sec
D1 1.37609601 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1315626 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
P1W1 17.00000000 W

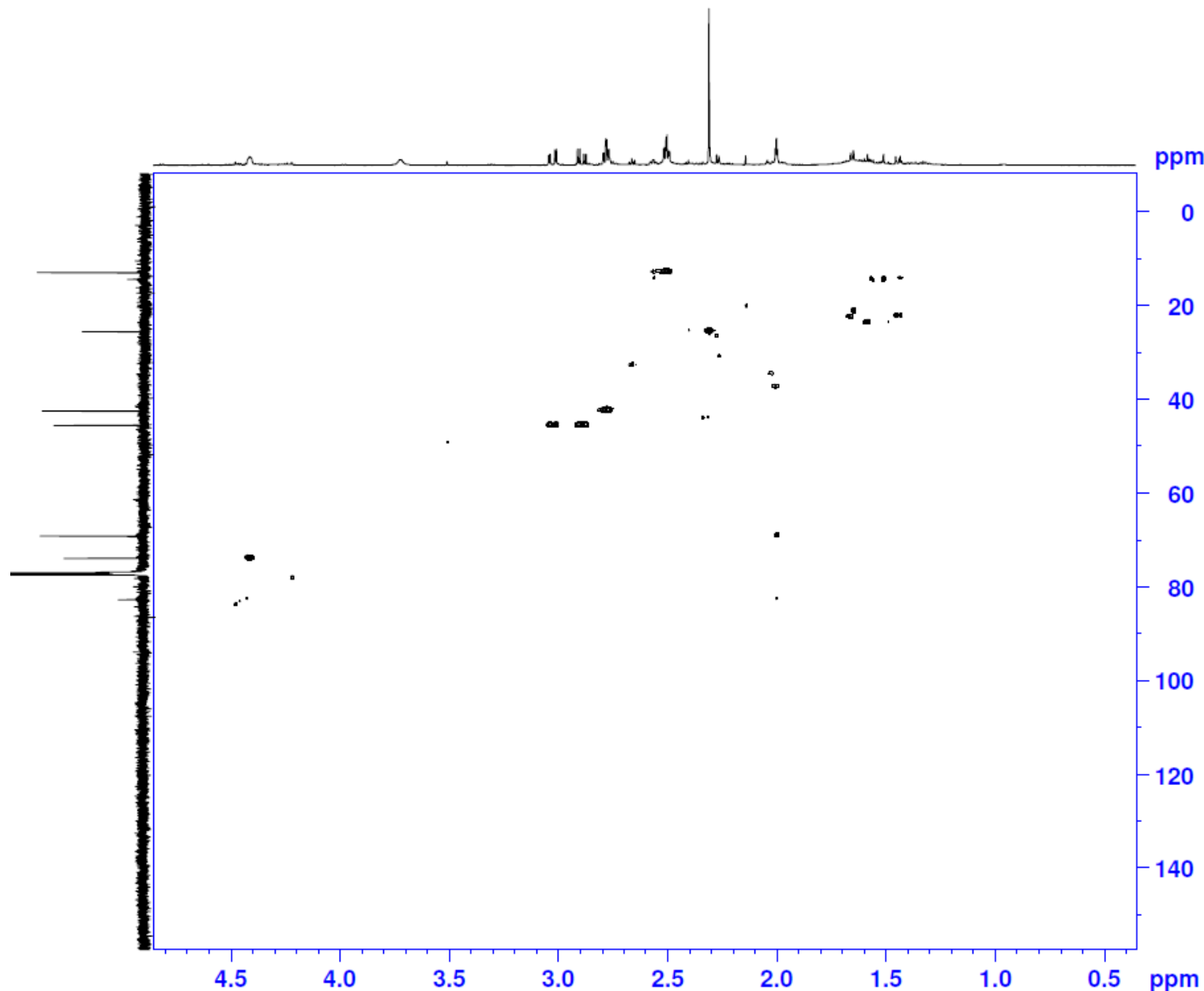
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
P1W2 80.00000000 W
P1W12 3.20000005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnmODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
CB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
CB 0





Current Data Parameters
NAME 20190628 MC2
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190629
Time 2.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcpgpdqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 2702.703 Hz
FIDRES 0.659840 Hz
AQ 0.7577600 sec
RG 2050
DW 185.000 usec
DE 6.50 usec
TE 298.1 K
CNST13 8.0000000
D0 0.00000300 sec
D1 0.99783027 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

==== CHANNEL f1 =====
SFO1 600.1315626 MHz
NUC1 1H
P1 13.50 usec
F2 27.00 usec
PLW1 17.00000000 W

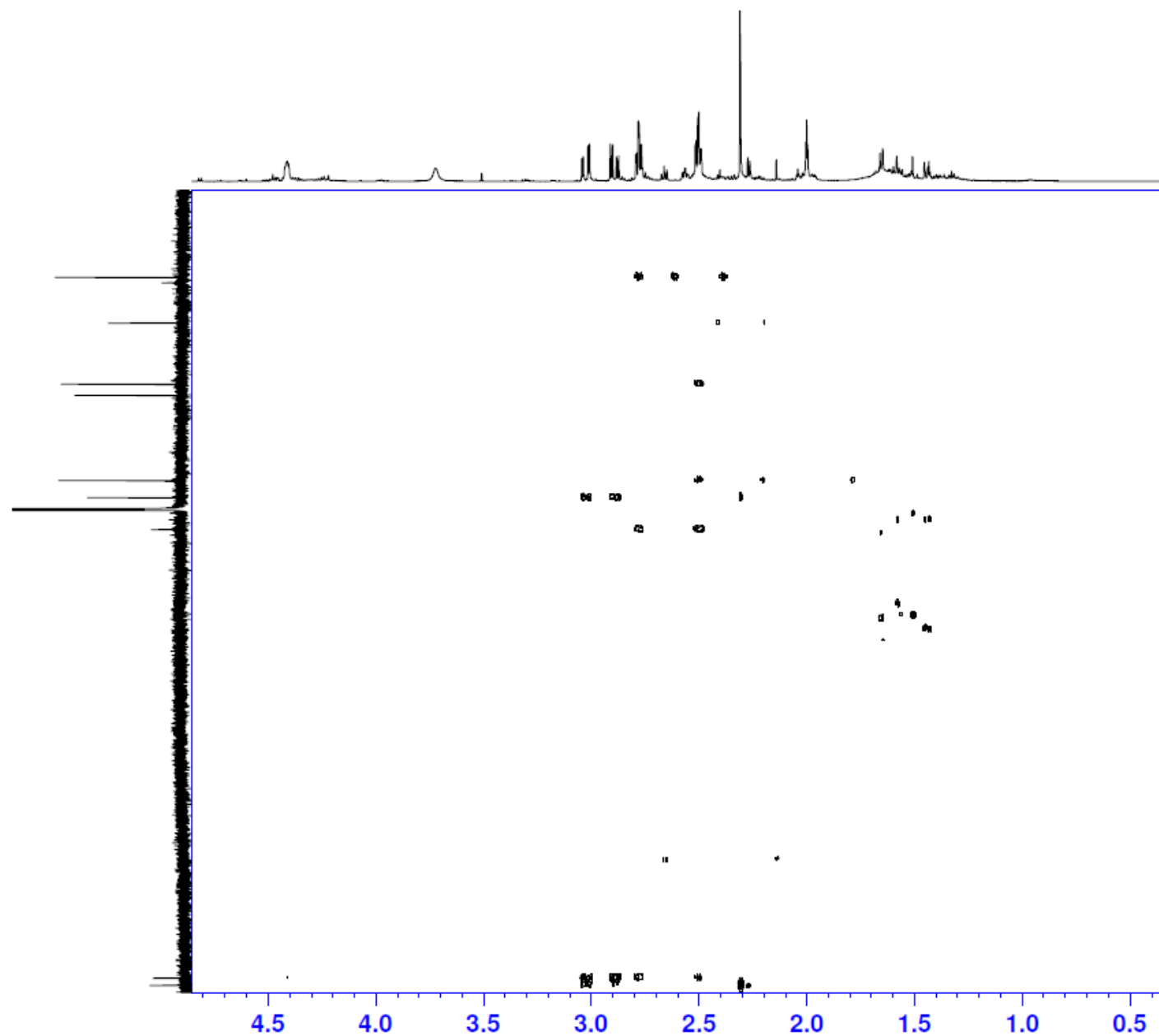
==== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 80.00000000 W

==== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

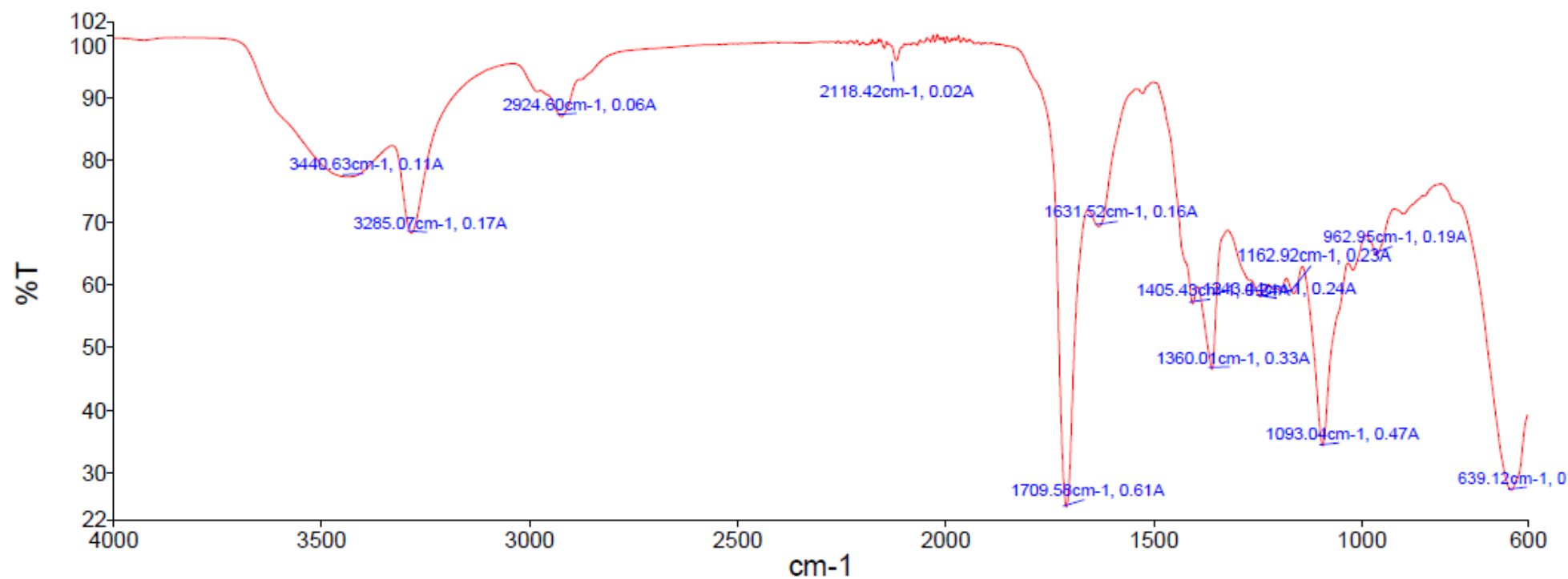


174 IR spectrum

PerkinElmer Spectrum Version 10.4.00
Wednesday, 9 May 2018 9:40 AM

Analyst
Date

Analyst
Wednesday, 9 May 2018 9:40 AM



Sample Name	Description	Quality Checks
Decarboxylative aldol		The Quality Checks give rise to a Zero Transmission warning for the sample.

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4.750
4.740
3.151
3.147
3.121
3.117
3.109
3.105
3.079
3.076
2.831
2.820
2.800
2.790
2.322
2.319
2.292
2.288
2.220
1.967
1.963
1.958

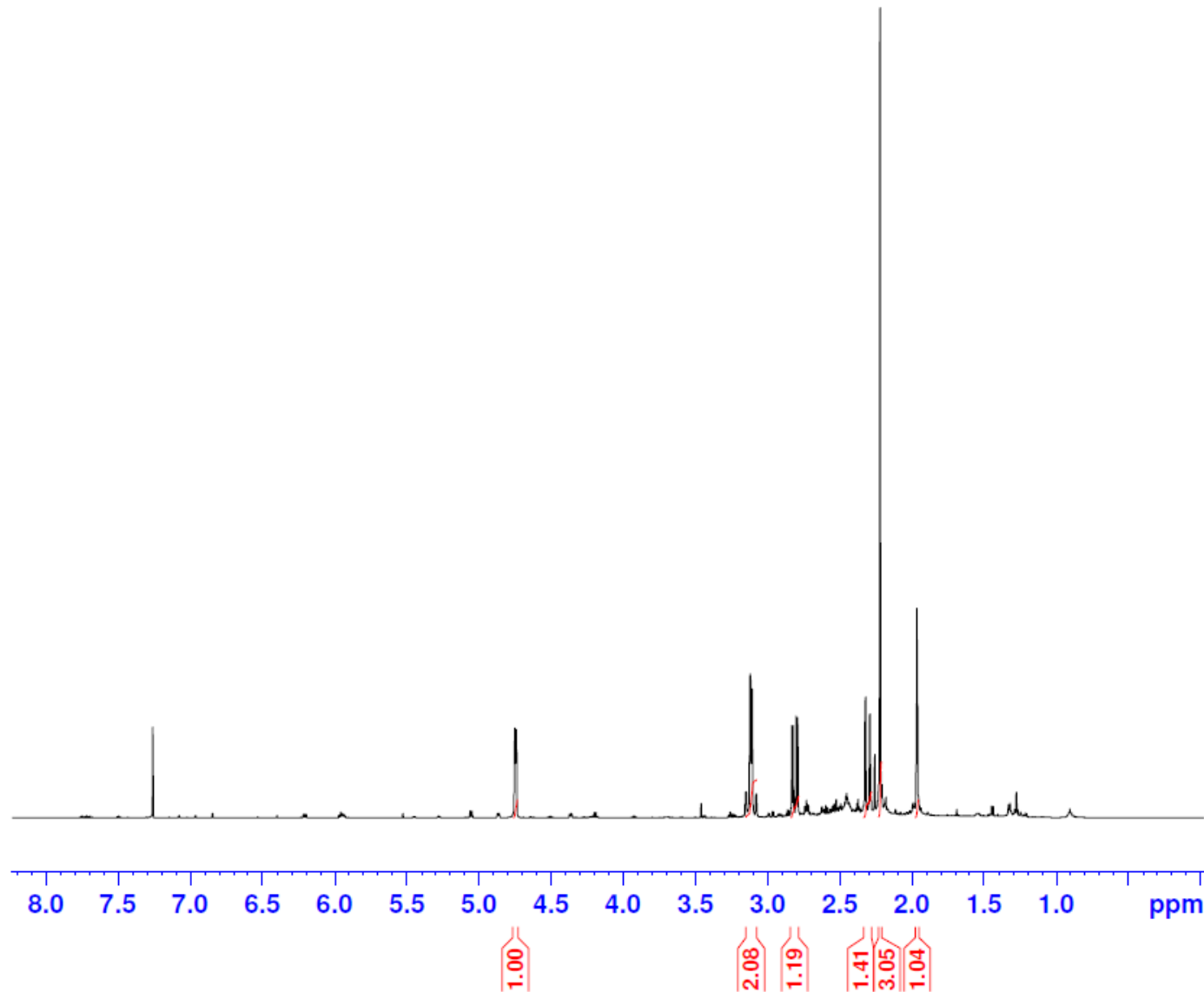


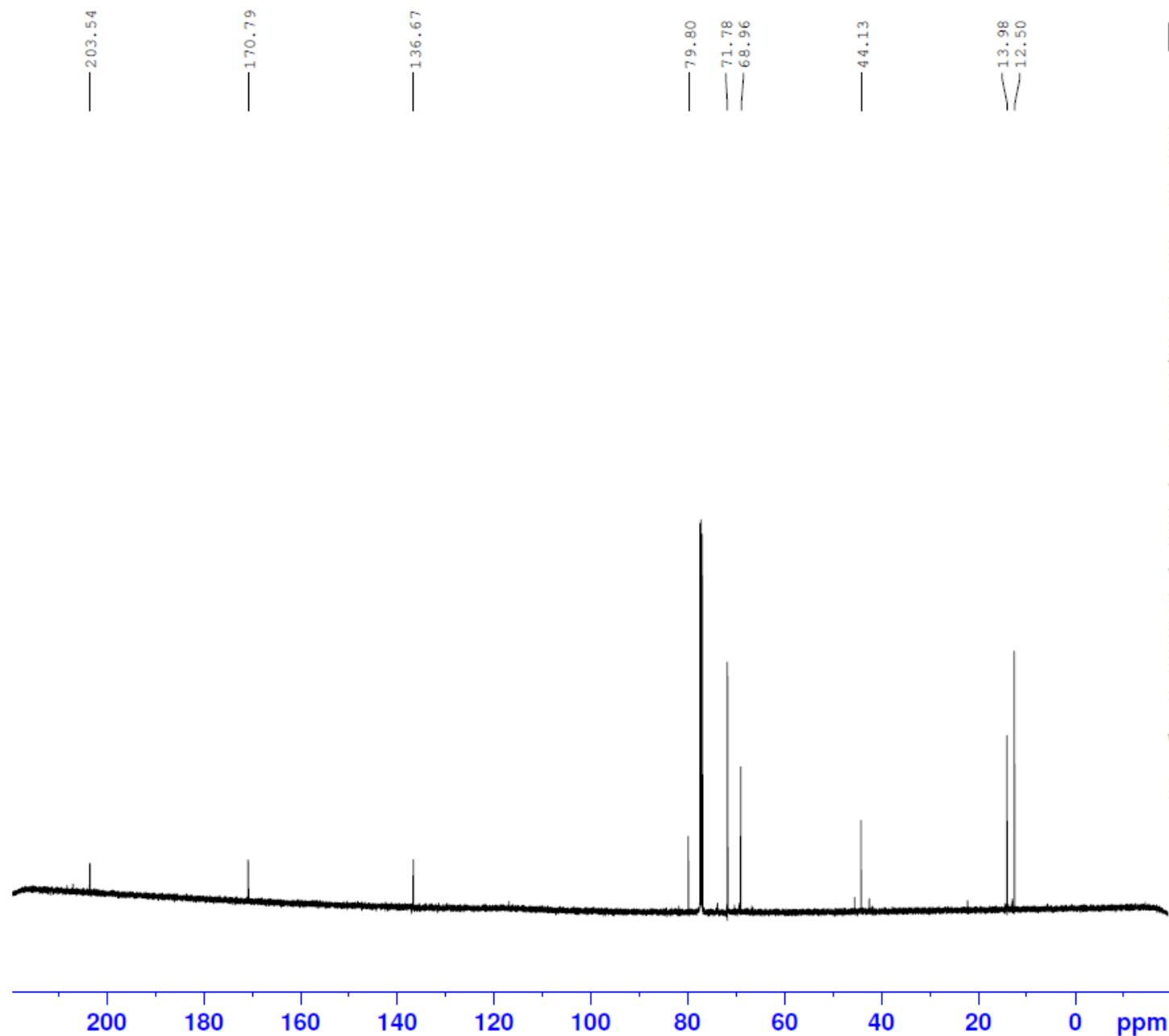
Current Data Parameters
NAME 20180514 Cyclisation (pure)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180514
Time 17.23
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 114
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 600.1337060 MHz
NUC1 1H
P1 8.40 usec
PLW1 12.55000019 W

F2 - Processing parameters
SI 65536
SF 600.1300251 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





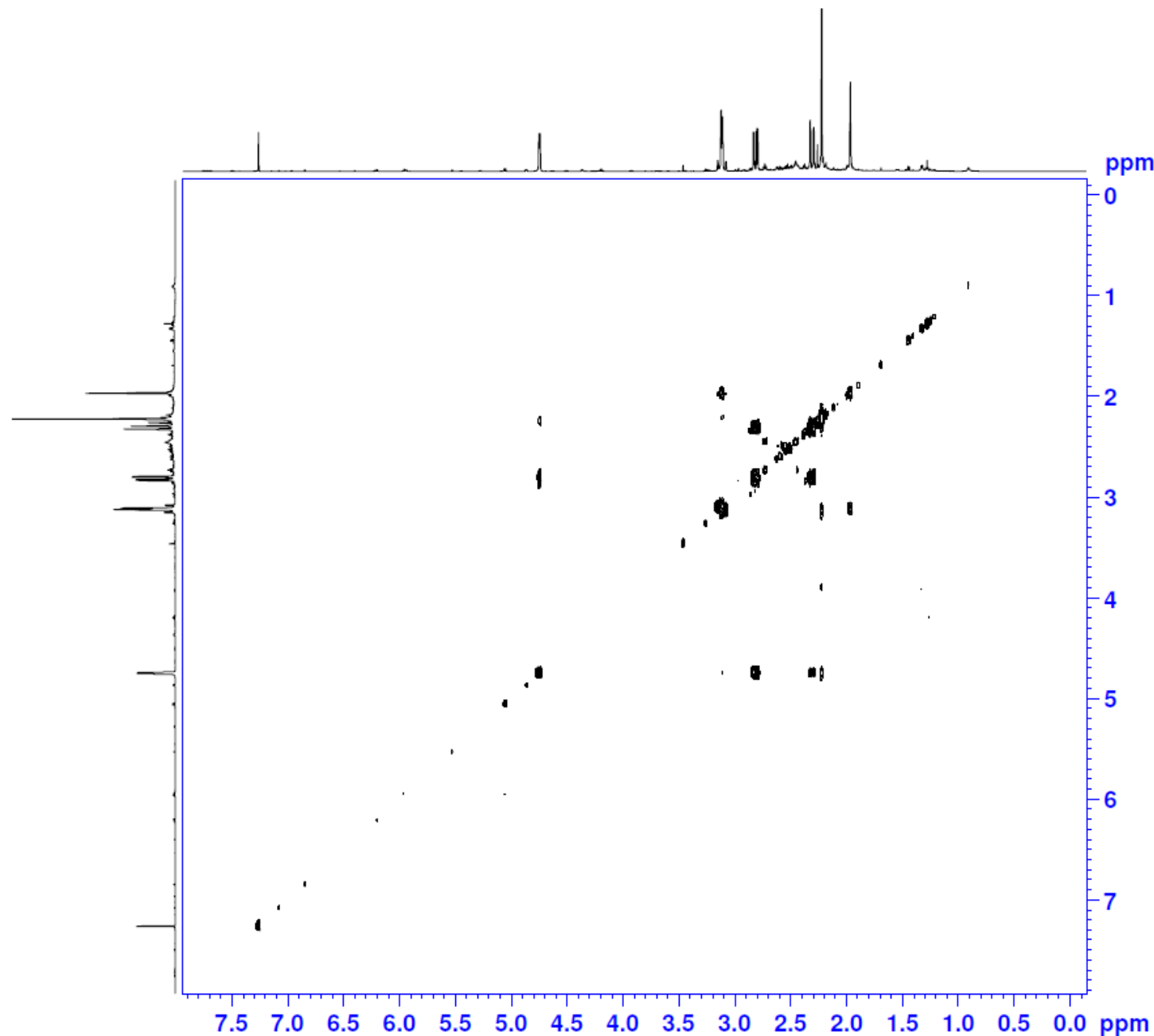
Current Data Parameters
 NAME 20180514 Cyclisation (pure)
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180514
 Time 19.13
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 2048
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 912
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 110.76000214 W

----- CHANNEL f2 -----
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 12.55000019 W
 PLW12 0.18072000 W
 PLW13 0.08855400 W

F2 - Processing parameters
 SI 32768
 SF 150.9027922 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20180514 Cyclisation (pure)
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180514
Time 17.24
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG cosygpppgf
TD 2048
SOLVENT CDCl3
NS 1
DS 8
SWH 4854.369 Hz
FIDRES 2.370297 Hz
AQ 0.2109440 sec
RG 64
DW 103.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.91685104 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00020600 sec

----- CHANNEL f1 -----
SFO1 600.1323570 MHz
NUC1 1H
P0 8.40 usec
P1 8.40 usec
P17 2500.00 usec
PLW1 12.55000019 W
PLW10 1.309999994 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1324 MHz
FIDRES 37.924759 Hz
SW 8.089 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300207 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300235 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0



Current Data Parameters
NAME 20180514 Cyclisation (pure)
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters

Data_ 20180514
Time 19.19
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG hsqcetgps12
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 4950.495 Hz
FIDRES 4.834468 Hz
AQ 0.1034240 sec
RG 2050
LW 101.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46047401 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
IN0 0.00002000 sec
ZGPGTNS

CHANNEL f1

SFO1 600.1323102 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P2B 1000.00 usec
PLW1 12.55000019 W

CHANNEL f2

SFO2 150.9141231 MHz
NUC2 13C
CPDPRG2 garrp
P3 16.00 usec
P4 32.00 usec
PCPD2 60.00 usec
PLW2 110.76000214 W
PLW12 7.87610006 W

GRADIENT CHANNEL

GP1AM[1] SMSQ10.100
GP1AM[2] SMSQ10.100
GP1AM[3] SMSQ10.100
GP1AM[4] SMSQ10.100
GPE1 80.00 %
GPE2 20.10 %
GPE3 11.00 %
GPE4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters

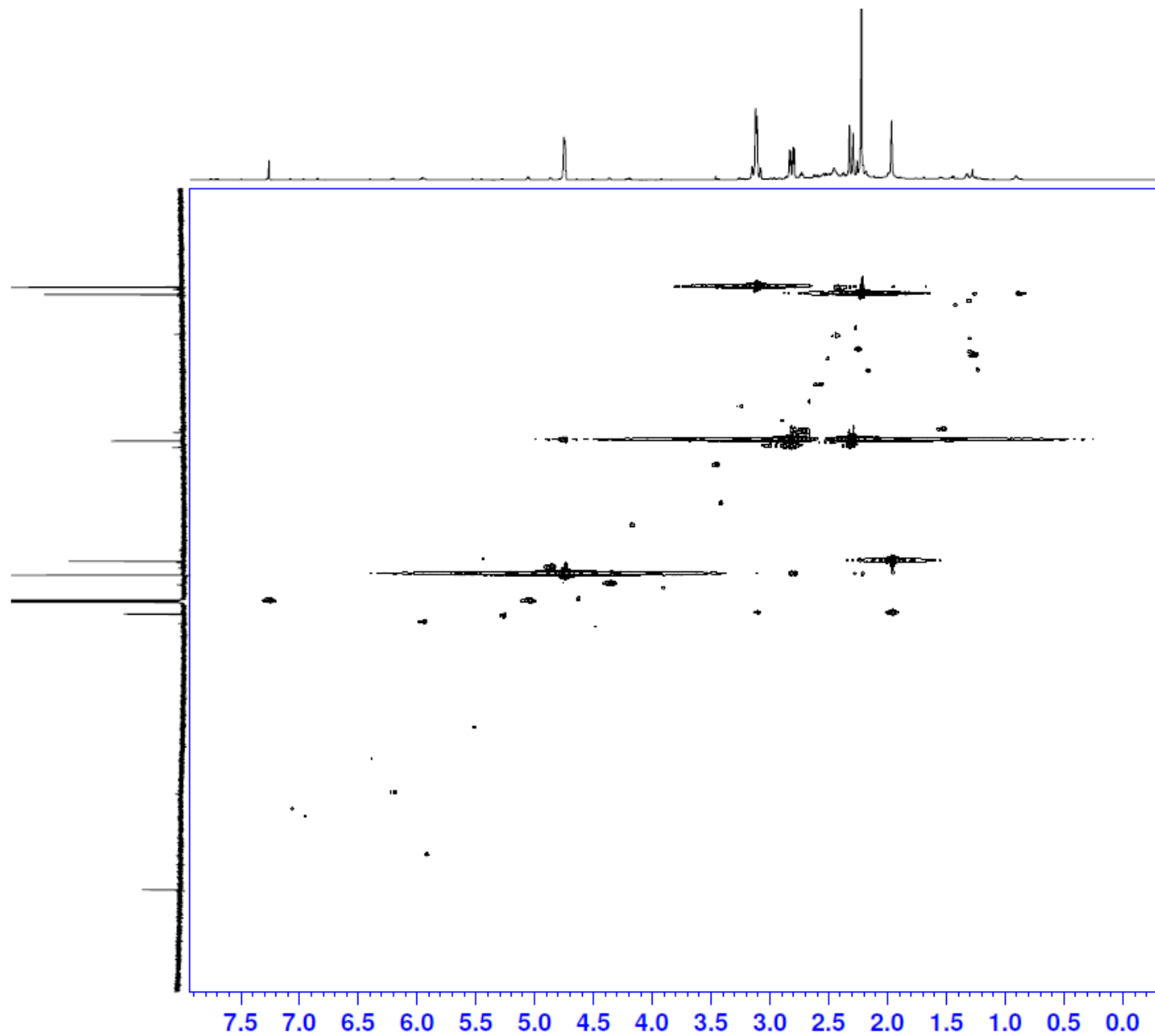
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiacho

F2 - Processing parameters

SI 1024
SF 600.1300247 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 echo-antiacho
SF 150.9028211 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20180514 Cyclisation (pure)
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180515
Time 1.00
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 4950.495 Hz
FIDRES 1.208617 Hz
AQ 0.4136960 sec
RG 2050
DW 101.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.34189403 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1323102 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
PLW1 12.55000019 W

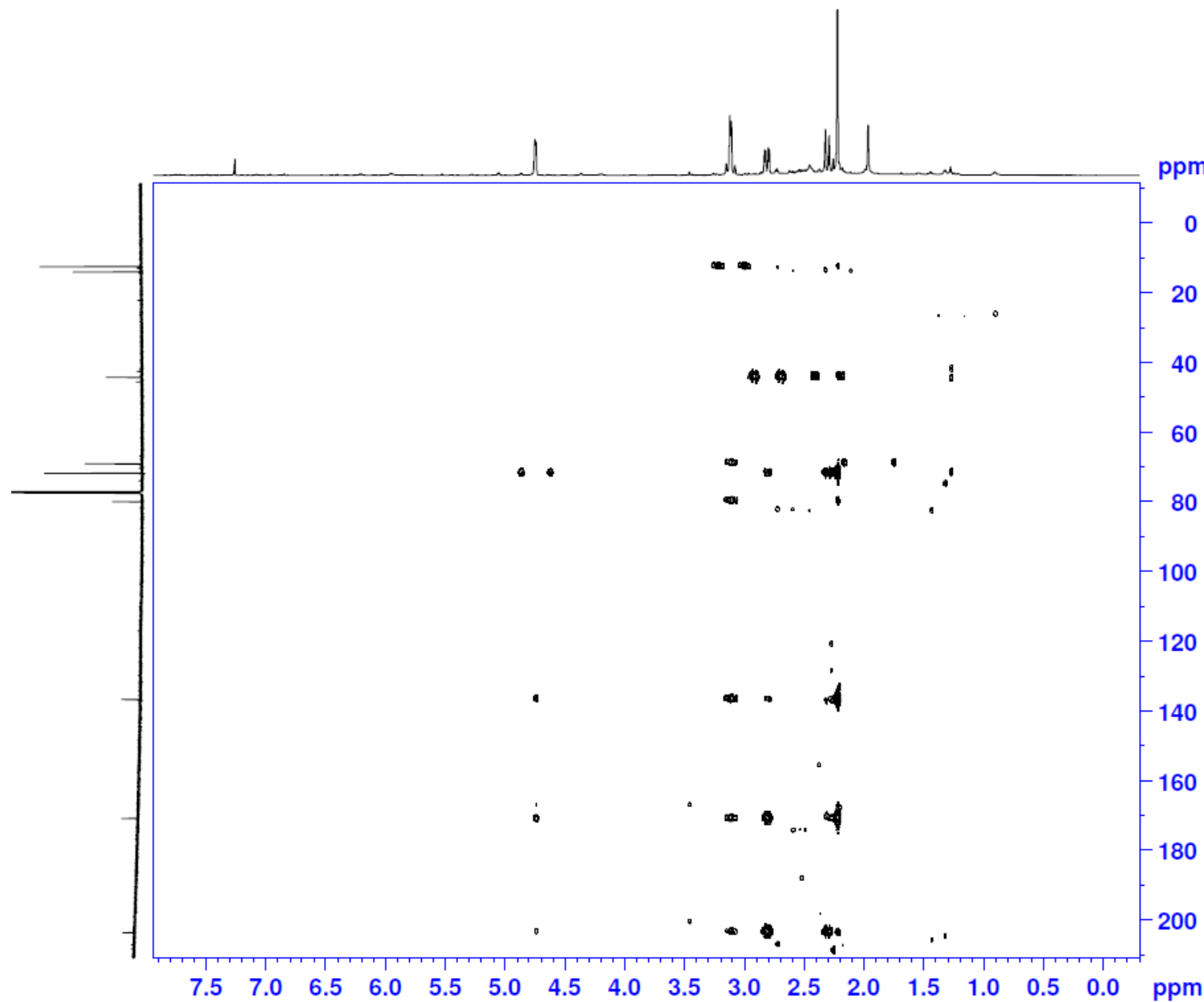
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 16.00 usec
PLW2 110.76000214 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

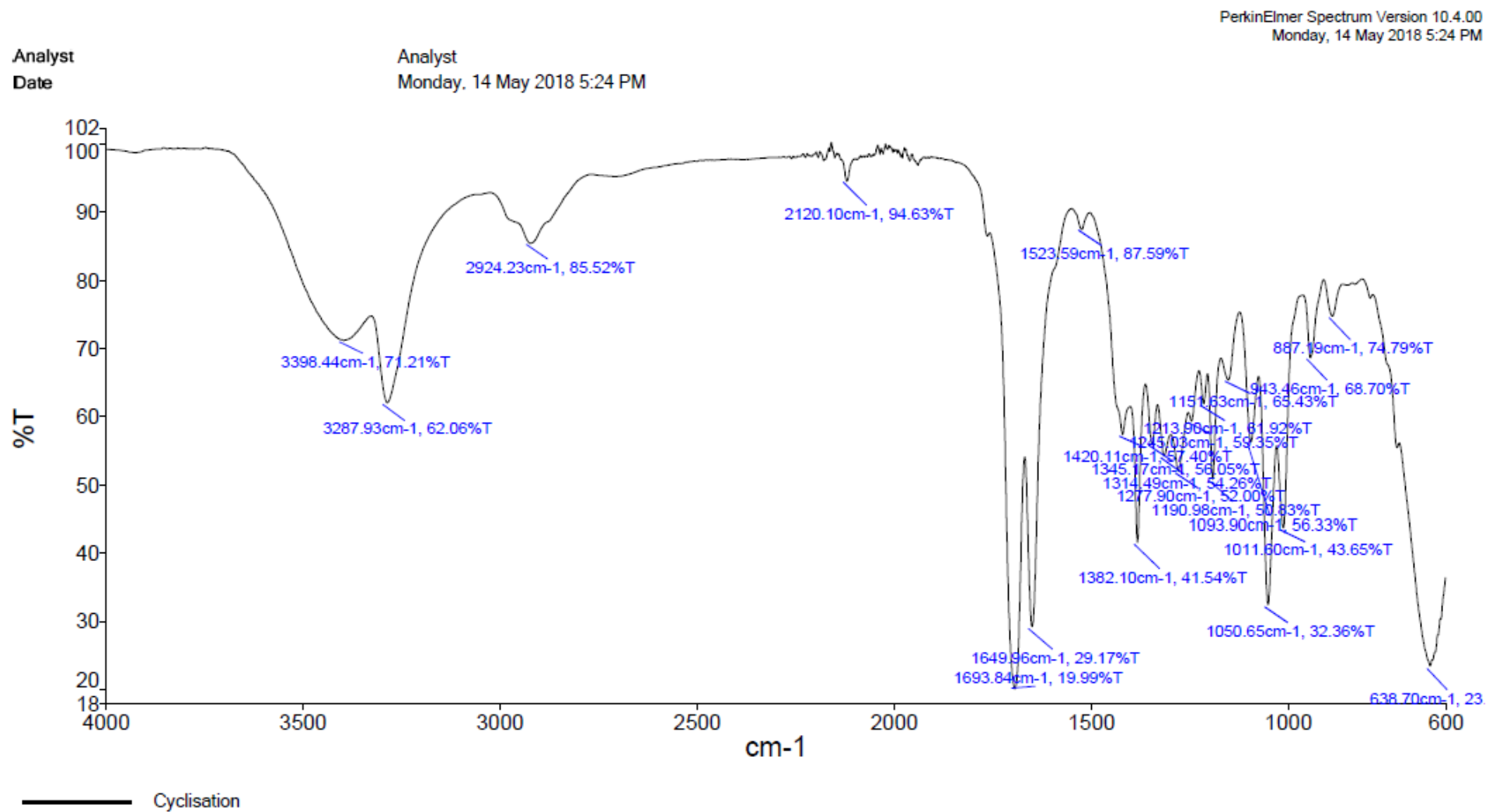
F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300188 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

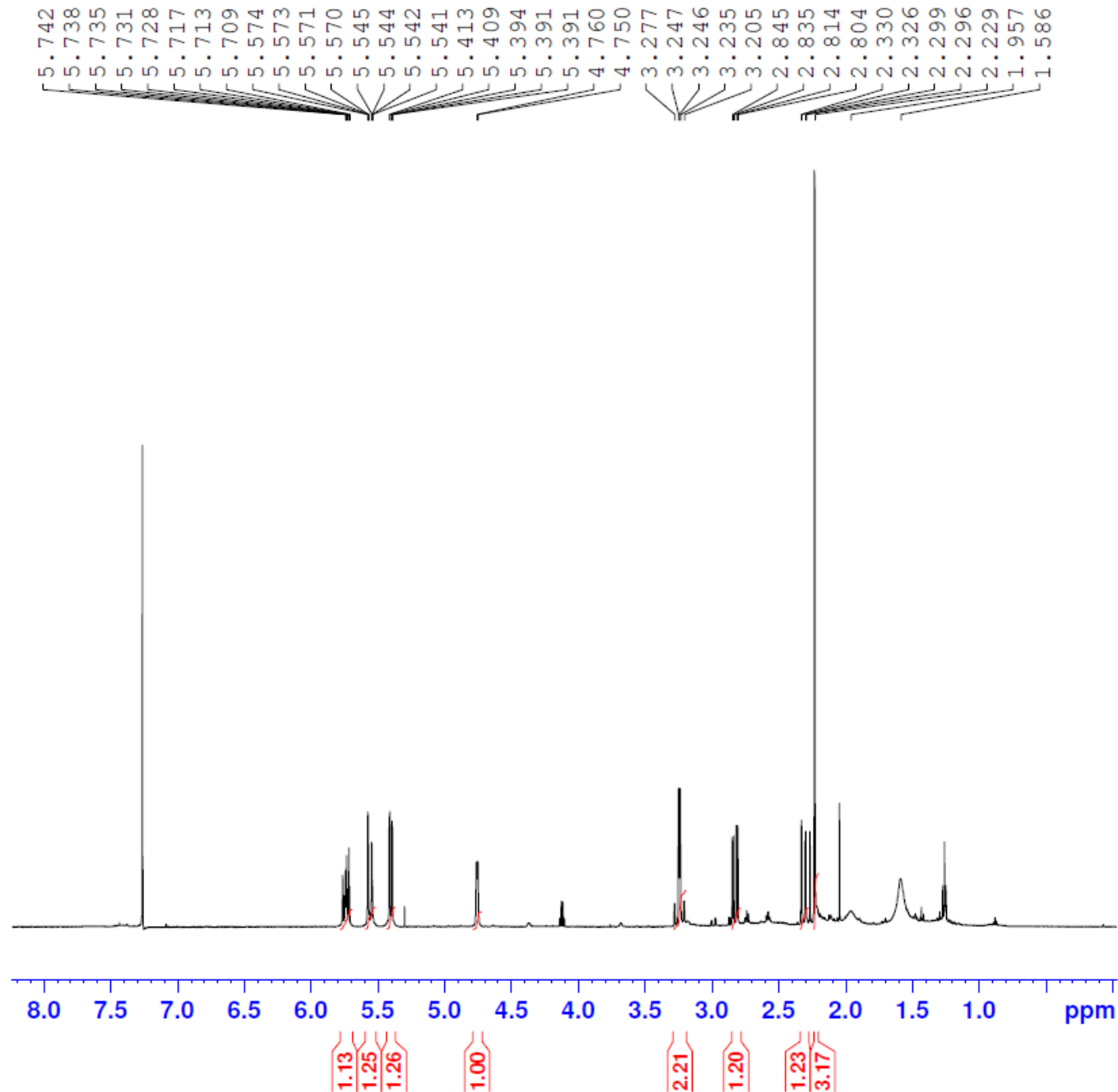
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028281 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



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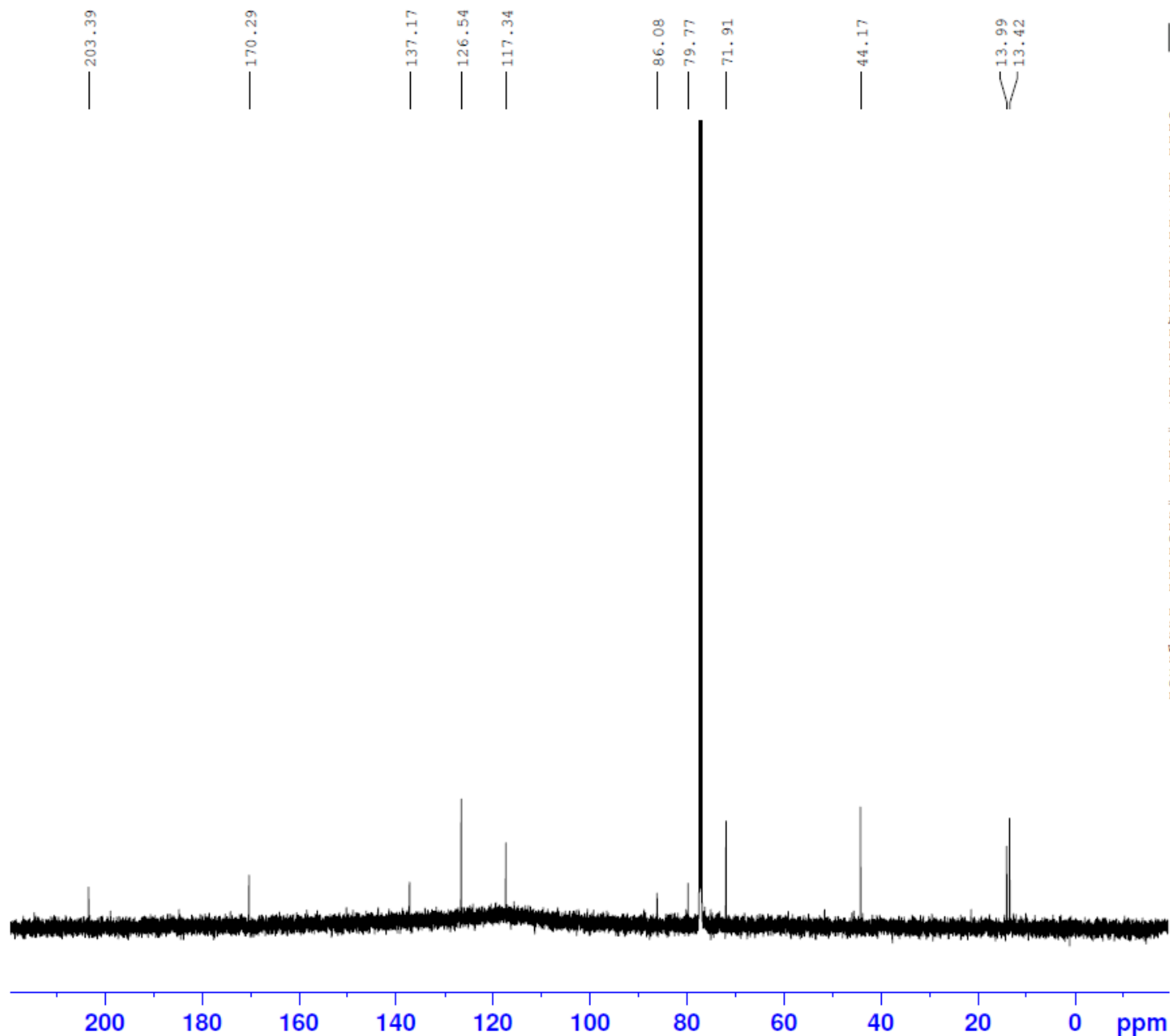


Current Data Parameters
 NAME 20180710 Sonagashira Cross Couple
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180710
 Time 17.21
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 256
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 8.40 usec
 PLW1 12.55000019 W

F2 - Processing parameters
 SI 65536
 SF 600.1300240 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 20180710 Sonagashira Cross Couple
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180710
Time 19.01
INSTRUM spect
PROBHD 5 mm PABBI 1H/
FULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 1820
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178988 MHz
NUC1 13C
P1 16.00 usec
PLW1 110.76000214 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 70.00 usec
PLW2 12.55000019 W
PLW12 0.18072000 W
PLW13 0.08855400 W

F2 - Processing parameters
SI 32768
SF 150.9027891 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 20180710 Sonagashira Cross Couple
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180710
Time 17.23
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 5050.505 Hz
FIDRES 2.466067 Hz
AQ 0.2027520 sec
RG 203
DW 99.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.92504299 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00019800 sec

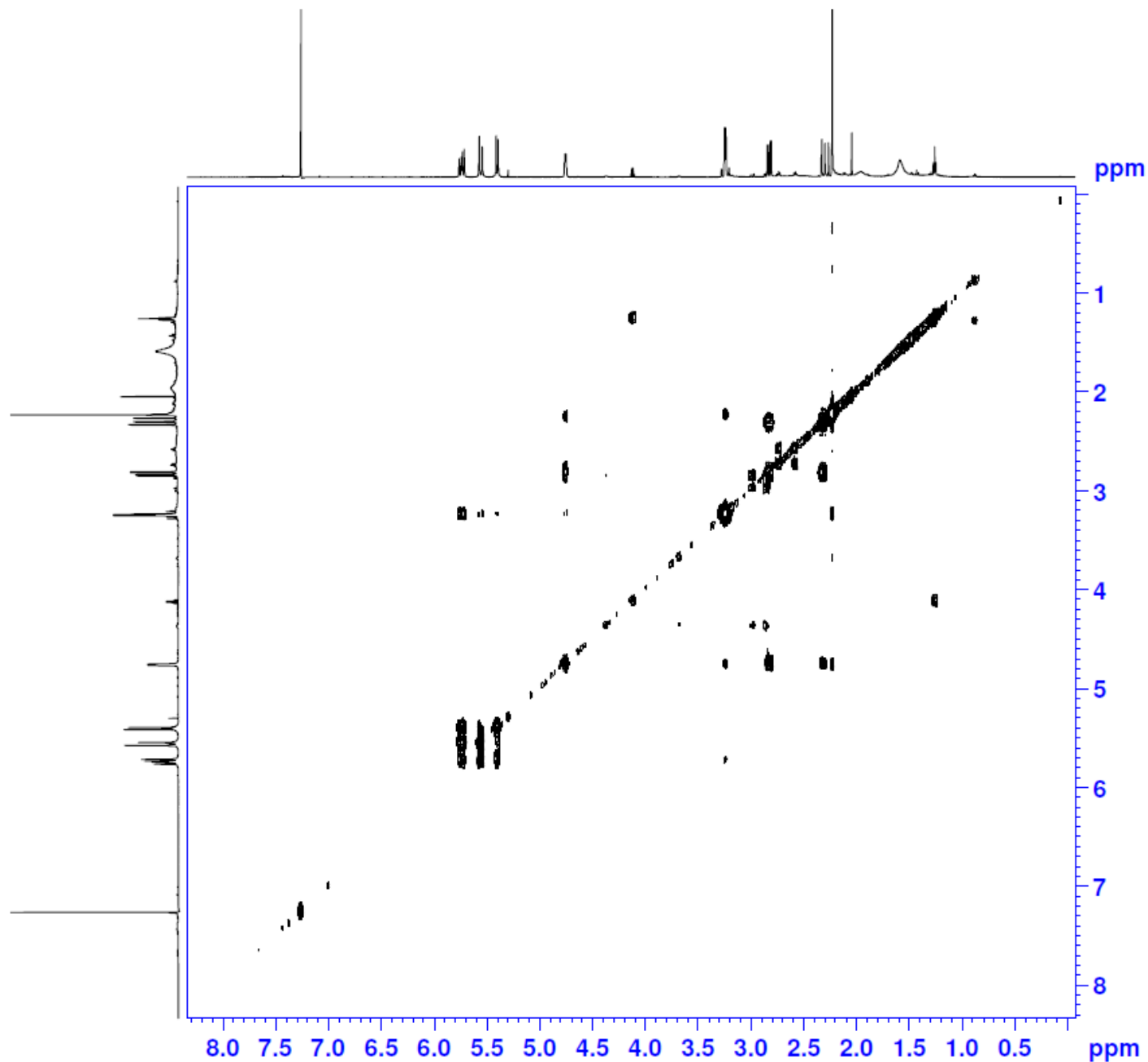
===== CHANNEL f1 =====
SFO1 600.1325023 MHz
NUC1 1H
P0 8.40 usec
P1 8.40 usec
P17 2500.00 usec
PLW1 12.55000019 W
PLW10 1.309999994 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 600.1325 MHz
FIDRES 39.457069 Hz
SW 8.416 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.1300210 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300262 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20180710 Sonagashira Cross Couple
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters

Date_ 20180710
Time 19.07
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG hsqcctop
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 5000.000 Hz
FIDRES 4.882813 Hz
AQ 0.1024000 sec
RG 2050
RW 100.000 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46313596 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGFNS

===== CHANNEL f1 =====
SFO1 600.1325359 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
P28 1000.00 usec
PLW1 12.55000019 W

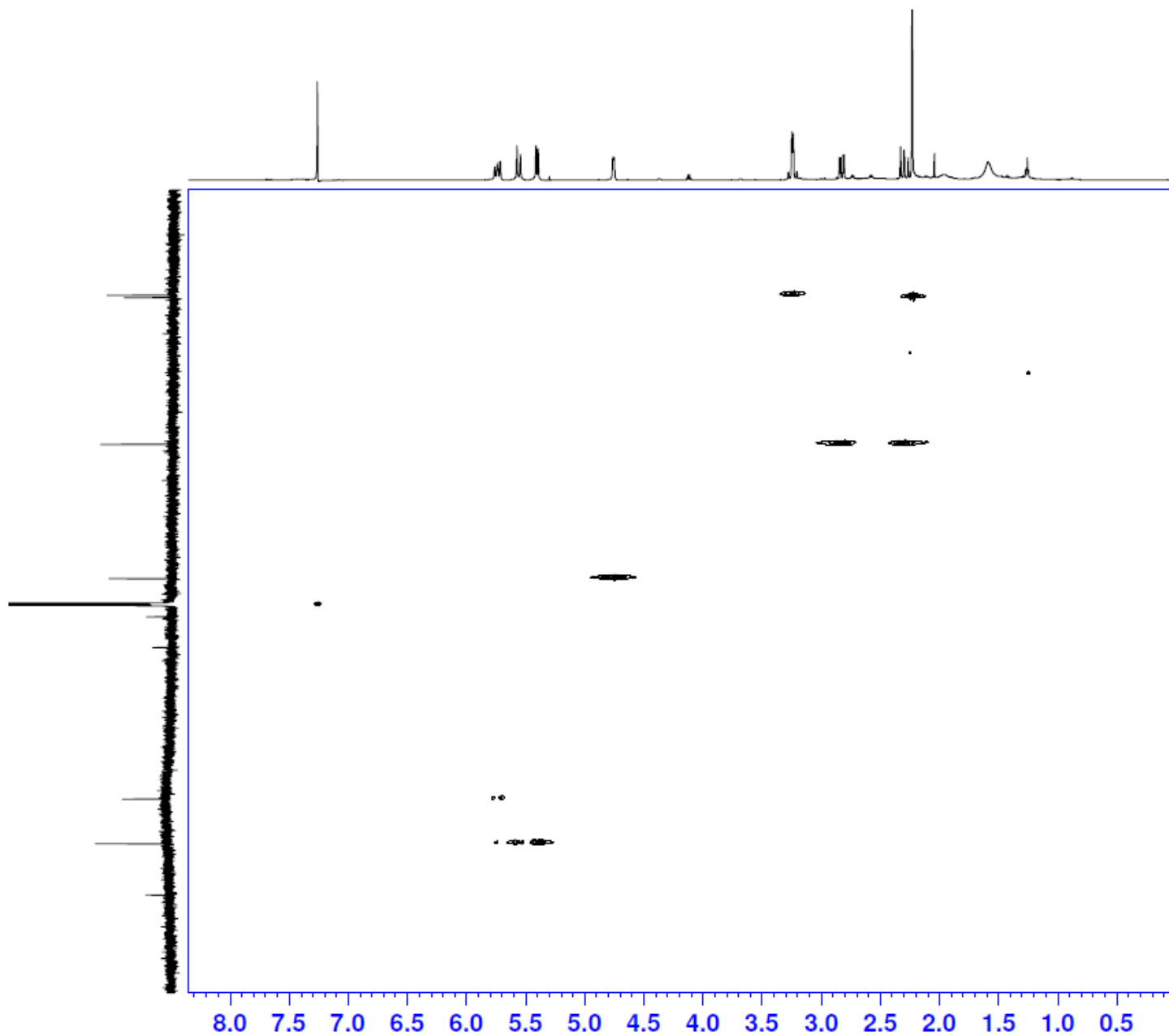
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 gsp
P3 16.00 usec
P4 32.00 usec
PCPD2 60.00 usec
PLW2 110.76000214 W
PLW12 7.87610006 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
F1MODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300225 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028180 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20180710 Sonagashira Cross Couple
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Data_ 20180711
Time 0.47

INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 5000.000 Hz
FIDRES 1.220703 Hz
AQ 0.4096000 sec
RG 2050
DW 100.000 usec
DE 6.50 usec
TE 298.2 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.34598994 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====
SFO1 600.1325359 MHz
NUC1 1H
P1 8.40 usec
P2 16.80 usec
PLW1 12.55000019 W

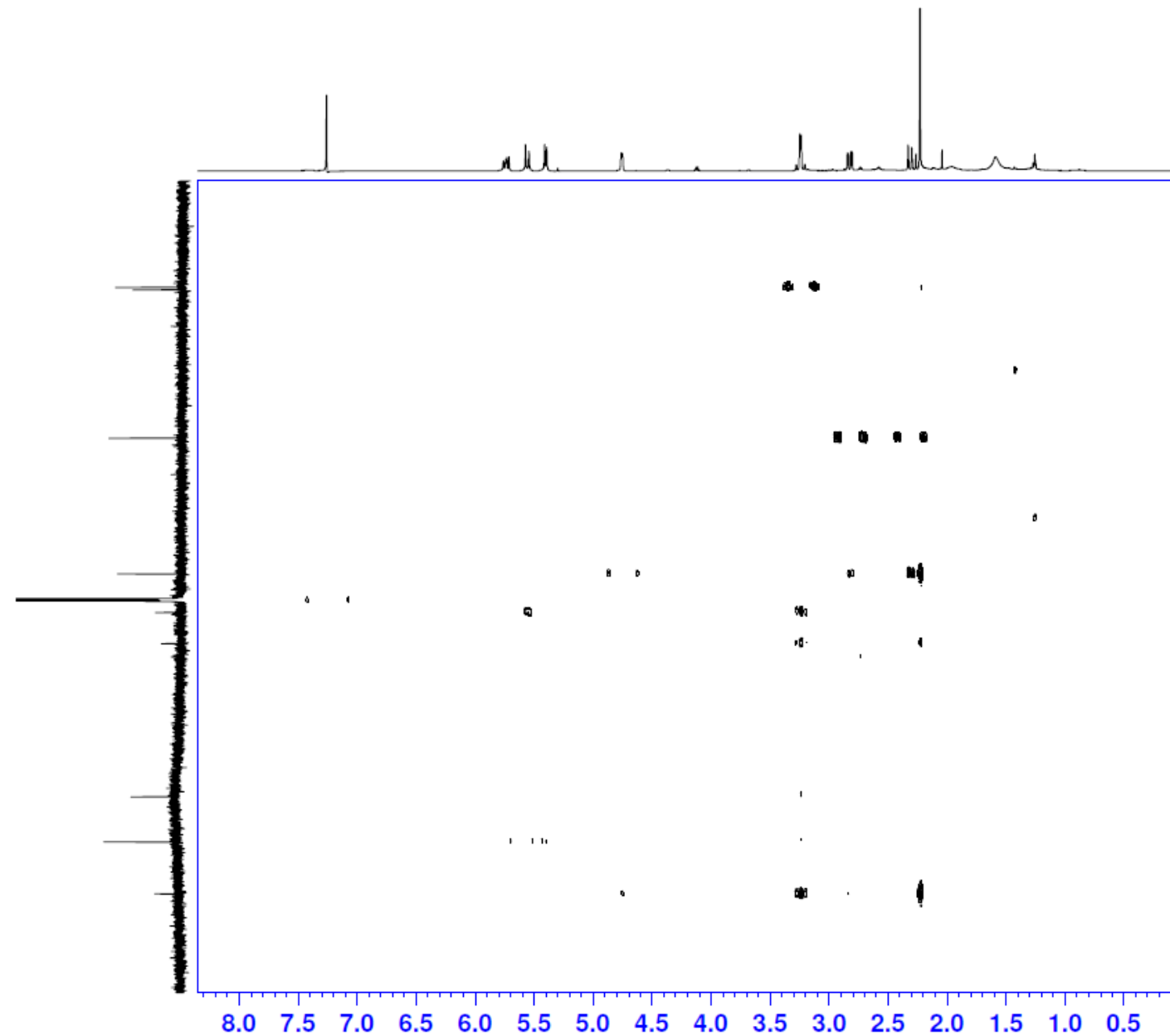
===== CHANNEL f2 =====
SFO2 150.9178748 MHz
NUC2 13C
P3 16.00 usec
PLW2 110.76000214 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnmODE QF

F2 - Processing parameters
SI 1024
SF 600.1300211 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028241 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

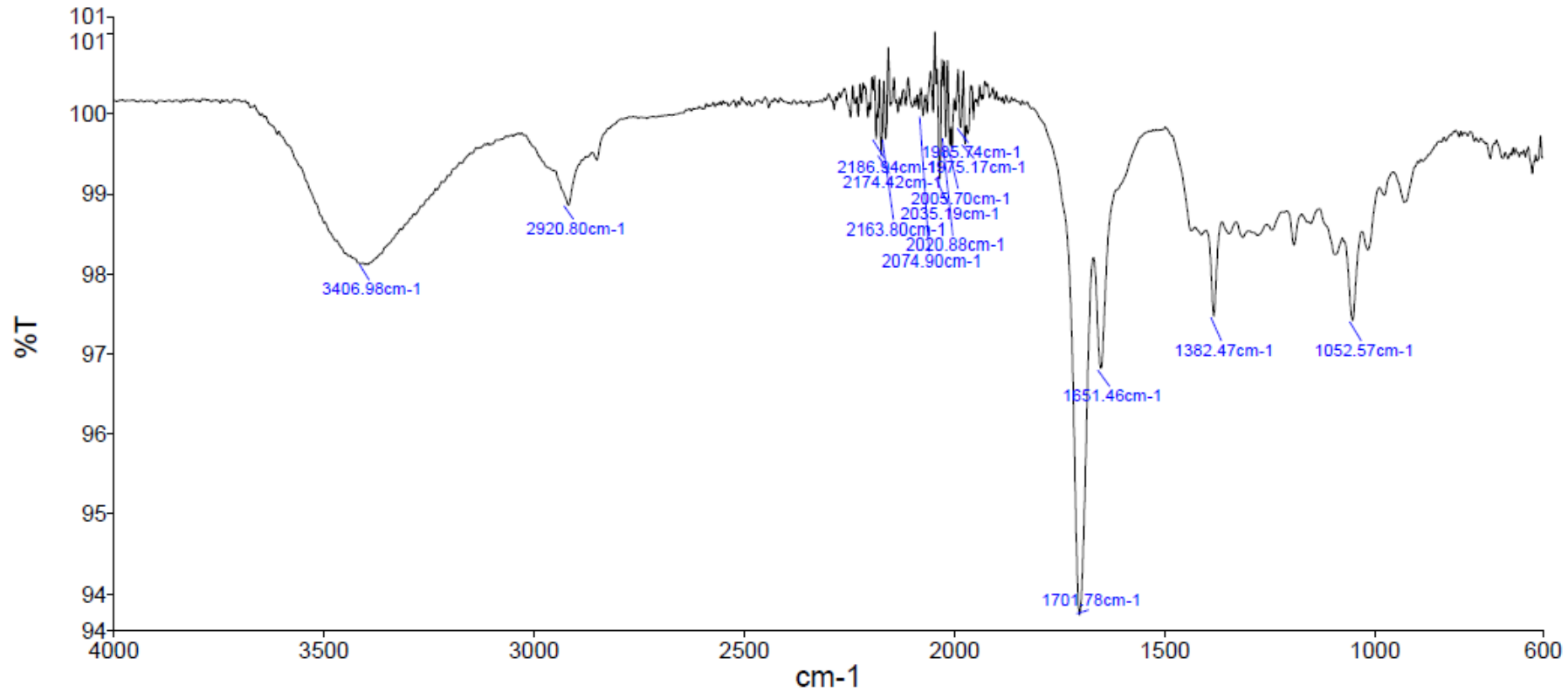


155 IR spectrum

PerkinElmer Spectrum Version 10.4.00
Monday, 5 November 2018 2:25 PM

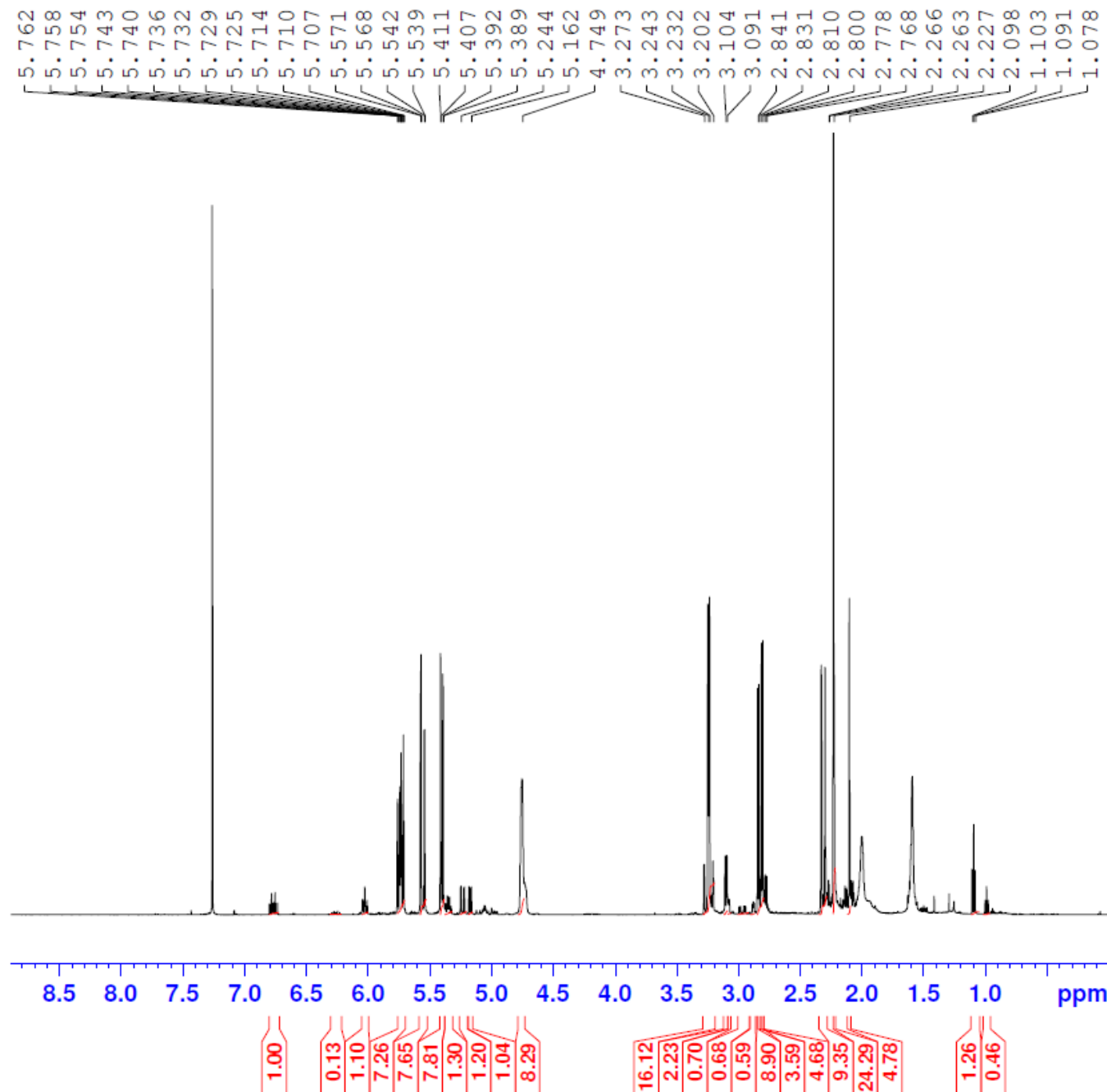
Analyst
Date

Analyst
Monday, 5 November 2018 2:25 PM



— Cross Couple GOOD

NMR Characterisation 21 mixture

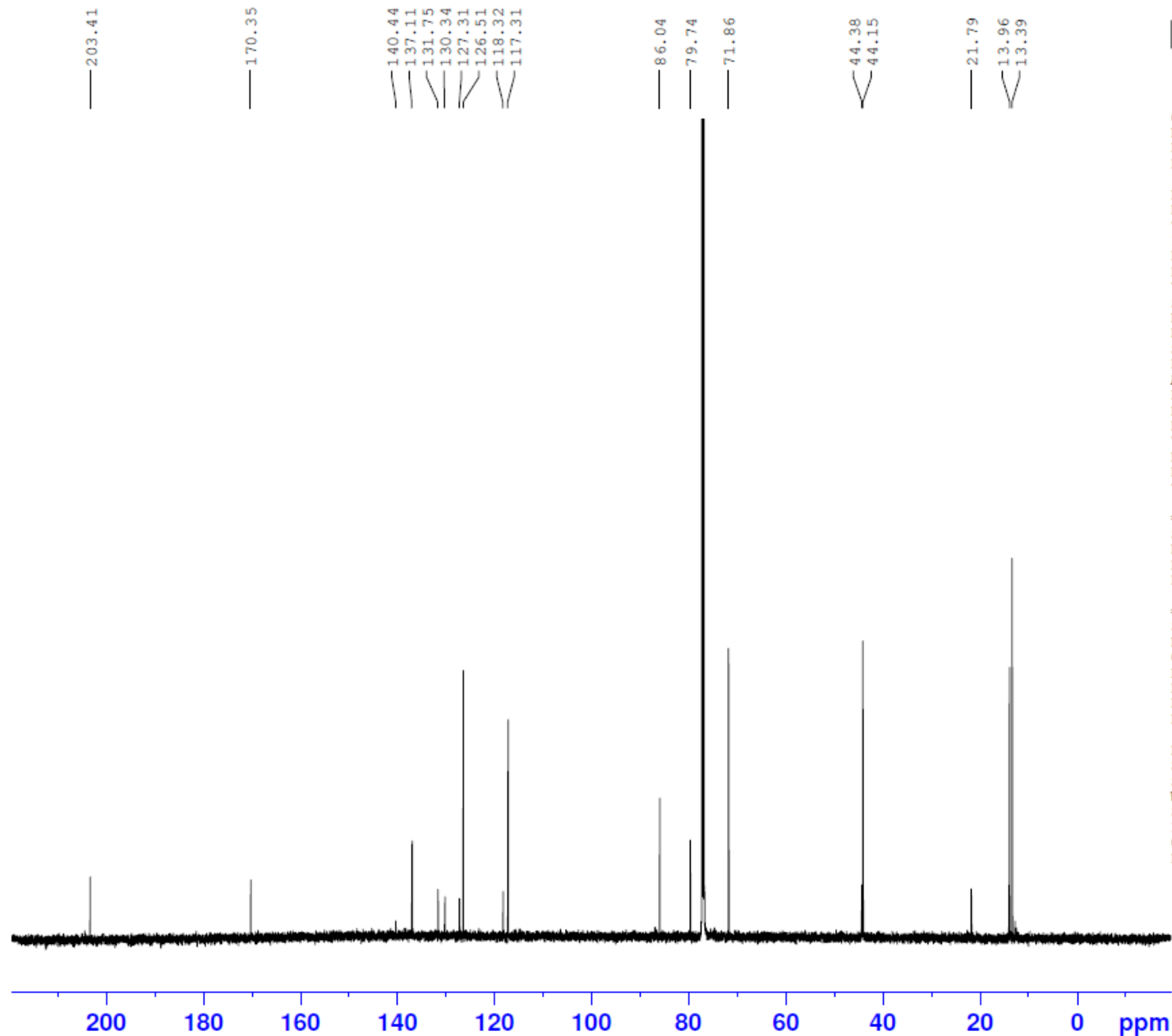


Current Data Parameters
 NAME 20190627 MC5 FINAL CRUDE
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190627
 Time 19.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7262976 sec
 RG 256
 DW 41.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 17.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1300267 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20190627 MC5 FINAL CRUDE
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190627
 Time 22.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 3096
 DS 2
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178988 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 80.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 17.00000000 W
 PLW12 0.63230002 W
 PLW13 0.30983001 W

F2 - Processing parameters
 SI 32768
 SF 150.9027946 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 20190627 MC5 FINAL CRUDE
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters

Date_ 20190627
Time 19.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
ID 2048
SOLVENT CDCl3
NS 10
DS 8
SWH 4201.681 Hz
FIDRES 2.051602 Hz
AQ 0.2437120 sec
RG 144
DW 119.000 usec
DE 6.50 usec
TE 298.2 K
D0 0.00000300 sec
D1 1.88408303 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00023800 sec

CHANNEL f1

SFO1 600.1322736 MHz
NUC1 1H
P0 13.50 usec
P1 13.50 usec
P17 2500.00 usec
PLW1 17.00000000 W
PLW10 4.58319998 W

GRADIENT CHANNEL

GP1AM[1] SMSQ10.100
GP21 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters

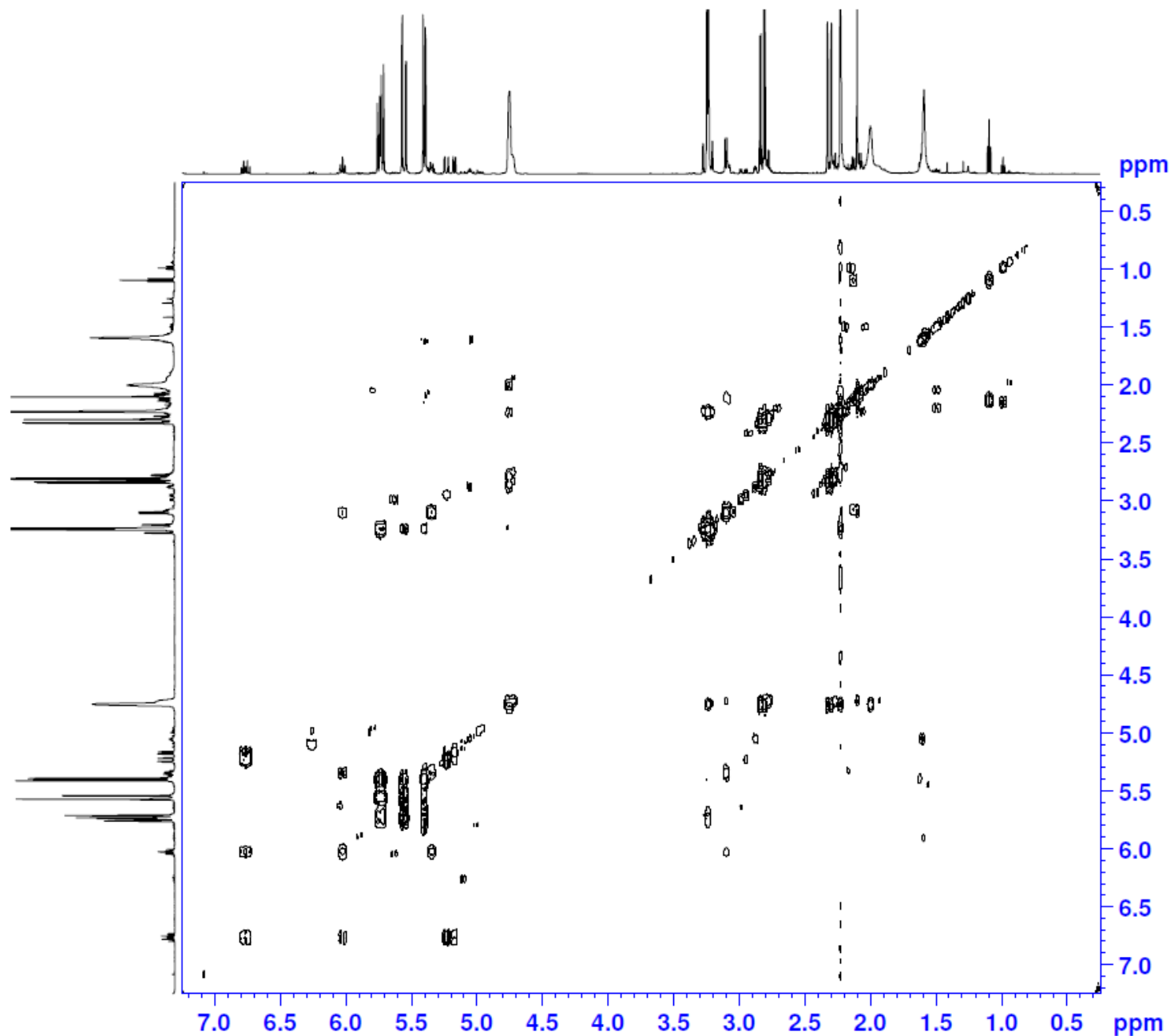
ID 128
SFO1 600.1323 MHz
FIDRES 32.825630 Hz
SW 7.001 ppm
FnMODE QF

F2 - Processing parameters

SI 1024
SF 600.1300266 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 QF
SF 600.1300242 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190627 MC5 FINAL CRUDE
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190627
Time 22.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcstg
TD 1024
SOLVENT CDCl3
NS 50
DS 16
SWH 4132.231 Hz
FIDRES 4.035382 Hz
AQ 0.1239040 sec
RG 2050
DW 121.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D0 0.0000300 sec
D1 1.44163203 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
IN0 0.00002000 sec
ZGPGINS

===== CHANNEL f1 =====
SFO1 600.1323015 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
P28 1000.00 usec
PLW1 17.00000000 W

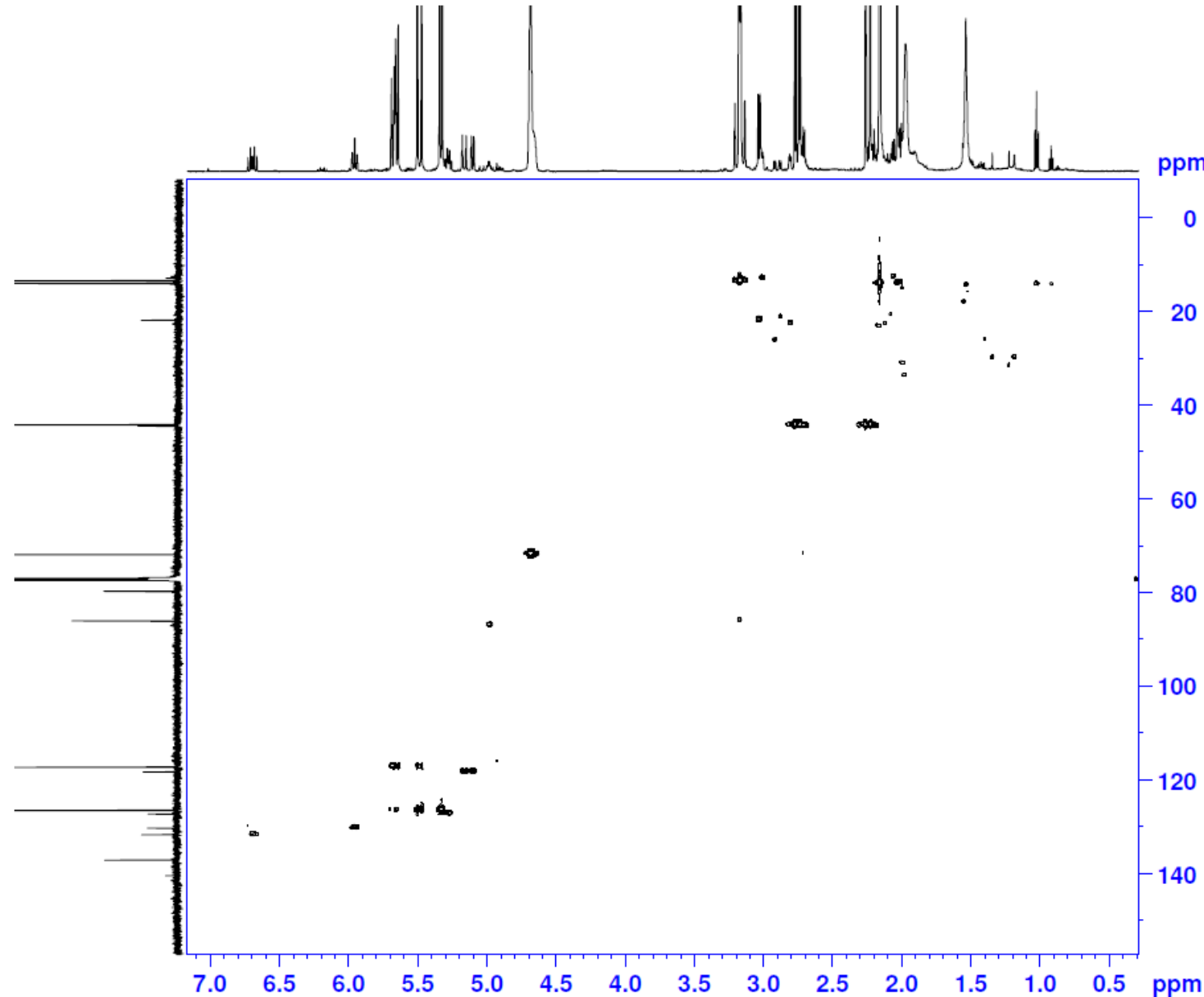
===== CHANNEL f2 =====
SFO2 150.9140636 MHz
NUC2 13C
CPDPRG2 garp
P3 12.00 usec
P4 24.00 usec
PCPD2 60.00 usec
PLW2 80.00000000 W
PLW12 3.20000005 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.9141 MHz
FIDRES 97.656250 Hz
SW 165.657 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.1300655 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028085 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0





Current Data Parameters
NAME 20190627 MC5 FINAL CRUDE
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters

Date_ 20190628
Time 4.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 70
DS 16
SWH 4132.231 Hz
FIDRES 1.008846 Hz
AQ 0.4956160 sec
RG 2050
DW 121.000 usec
DE 6.50 usec
TE 298.1 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.25997400 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001490 sec

===== CHANNEL f1 =====

SFO1 600.1323015 MHz
NUC1 1H
P1 13.50 usec
P2 27.00 usec
PLW1 17.00000000 W

===== CHANNEL f2 =====

SFO2 150.9178748 MHz
NUC2 13C
P3 12.00 usec
PLW2 80.00000000 W

===== GRADIENT CHANNEL =====

GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters

TD 128
SFO1 150.9179 MHz
FIDRES 262.164429 Hz
SW 222.353 ppm
FnMODE QF

F2 - Processing parameters

SI 1024
SF 600.1300655 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

