

## **Supporting Information**

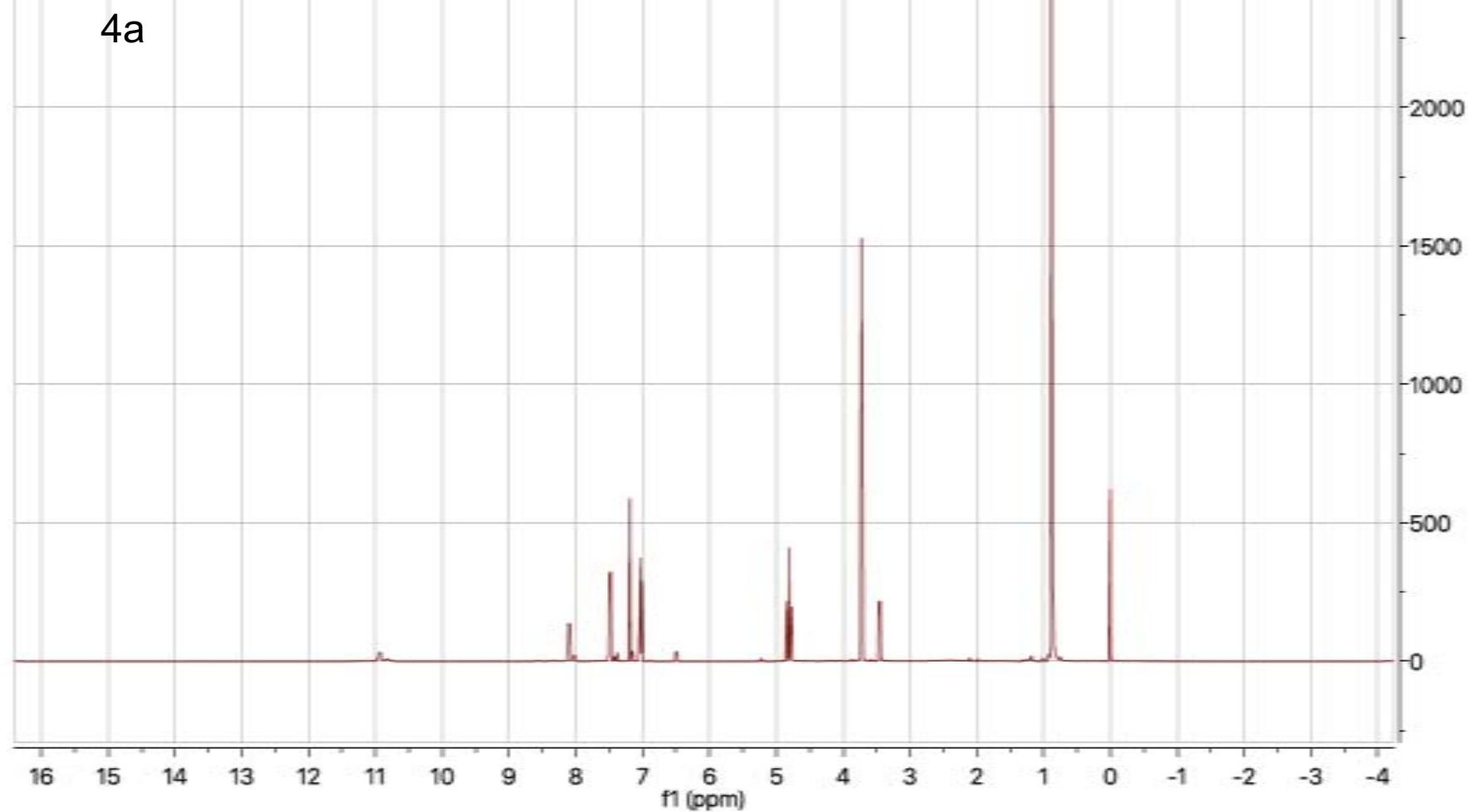
### **Fused Ring Oxazolopyrrolopyridopyrimidine Systems with Selective Gram Negative Activity**

Yiyuan Chen, Jonathan G. Moloney, Mark G. Moloney\* and Amber Thompson

Department of Chemistry, Chemistry Research Laboratory, The University of Oxford, 12  
Mansfield Road, Oxford. OX1 3TA.

[mark.moloney@chem.ox.ac.uk](mailto:mark.moloney@chem.ox.ac.uk)

yc48612705.1.fid  
Instrument AVC500  
Group MGM  
Project Account Code P2  
4861 Yiyuan Chen 27/5/16



YC016 CHARACT.4f12

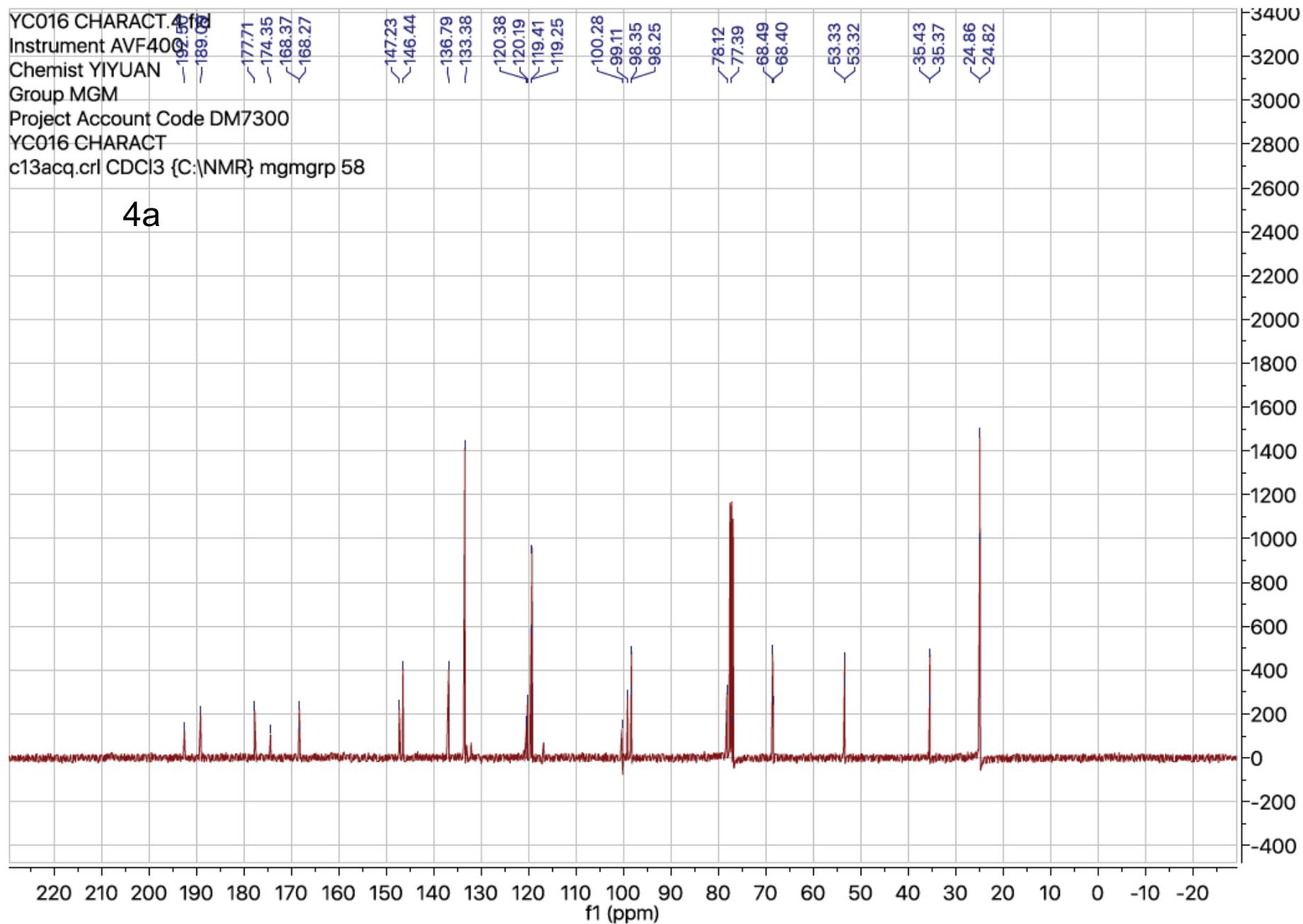
Instrument AVF400  
Chemist YIYUAN  
Group MGM

Project Account Code DM7300

YC016 CHARACT

c13acq.crl CDC|3 {C:\NMR} mgmgrp 58

4a



YC020 CHARACT 41d

Instrument AVG400

Group MGM

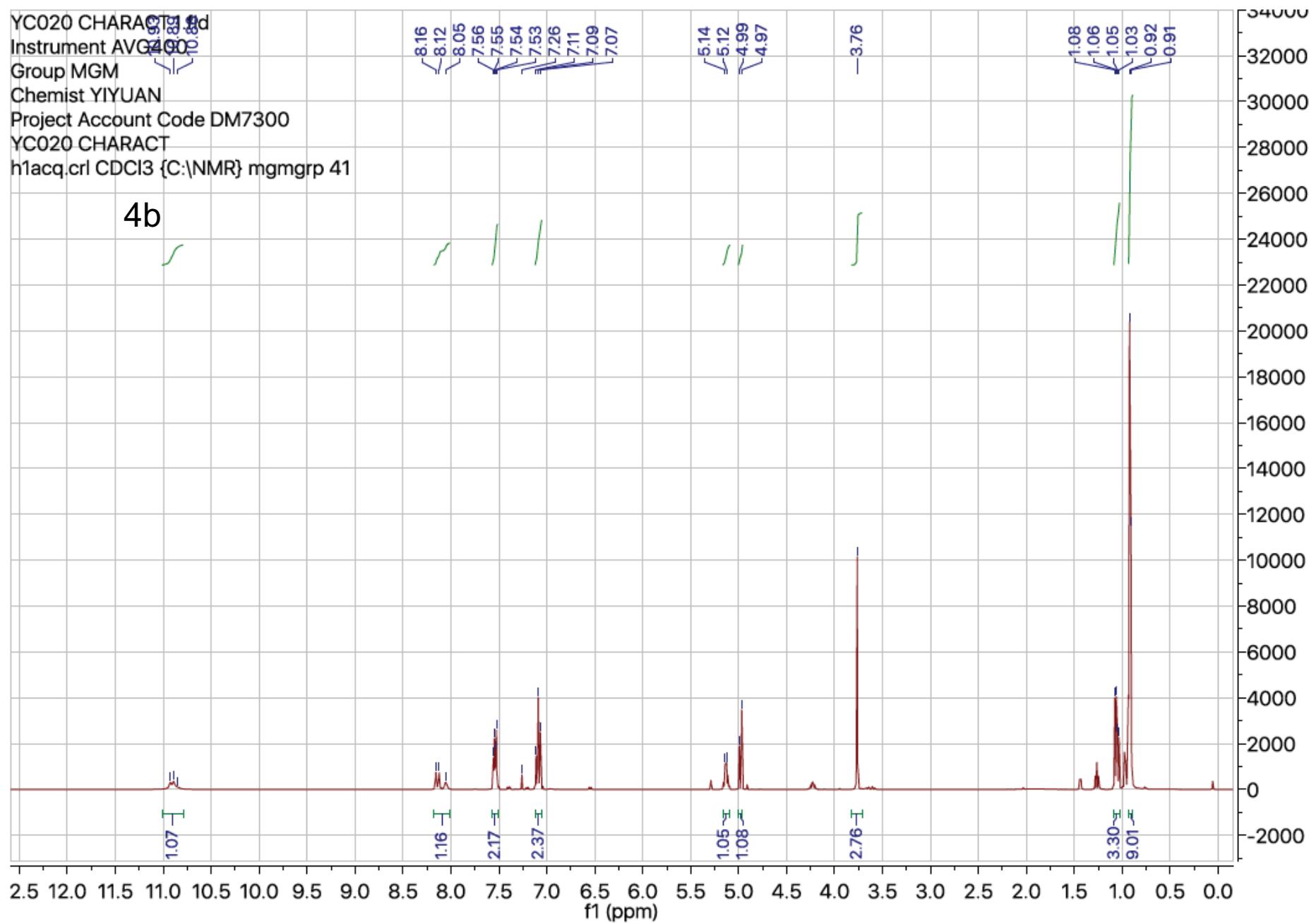
Chemist YIYUAN

Project Account Code DM7300

YC020 CHARACT

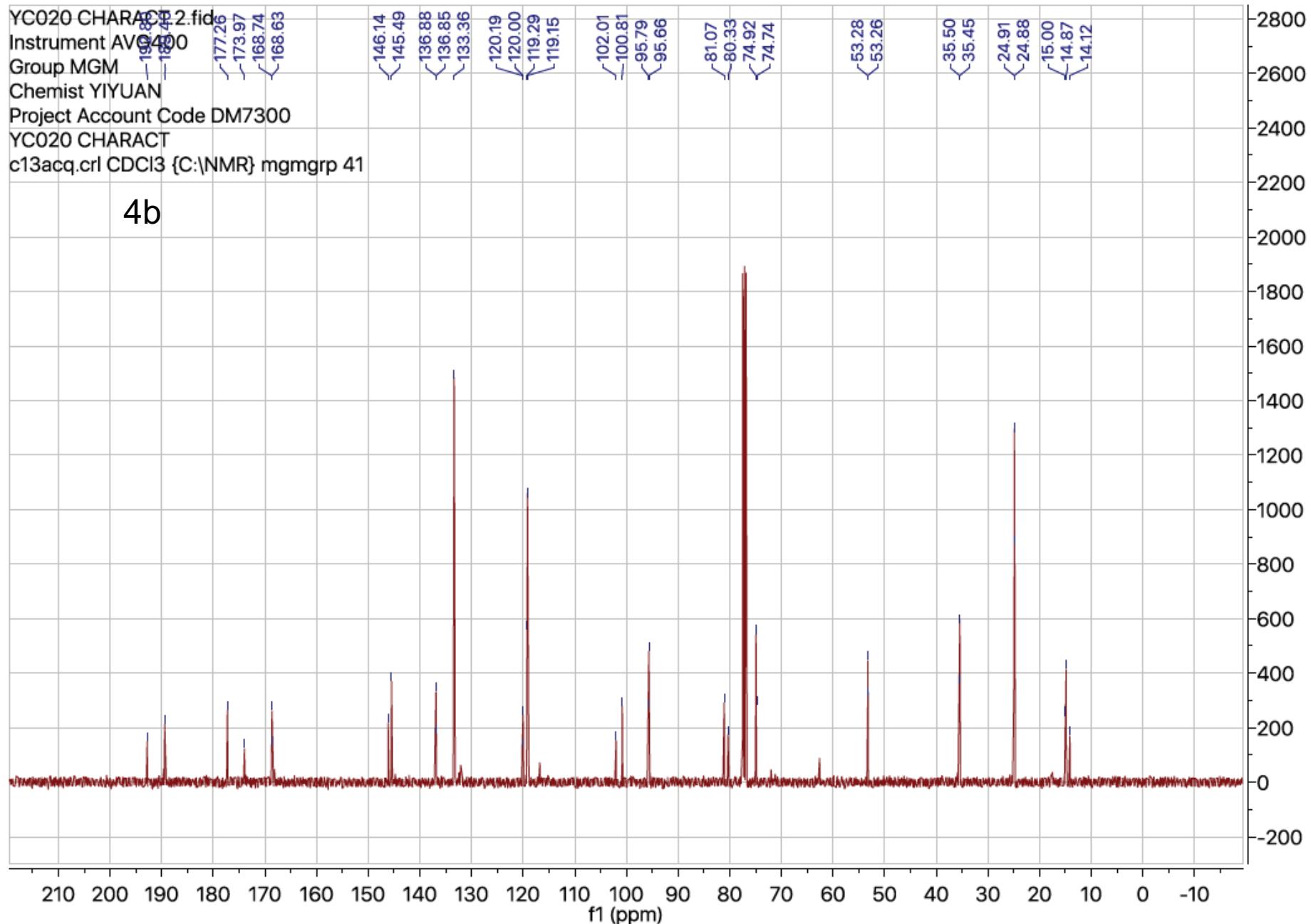
h1acq.crl CDCl3 {C:\NMR} mgmgrp 41

4b



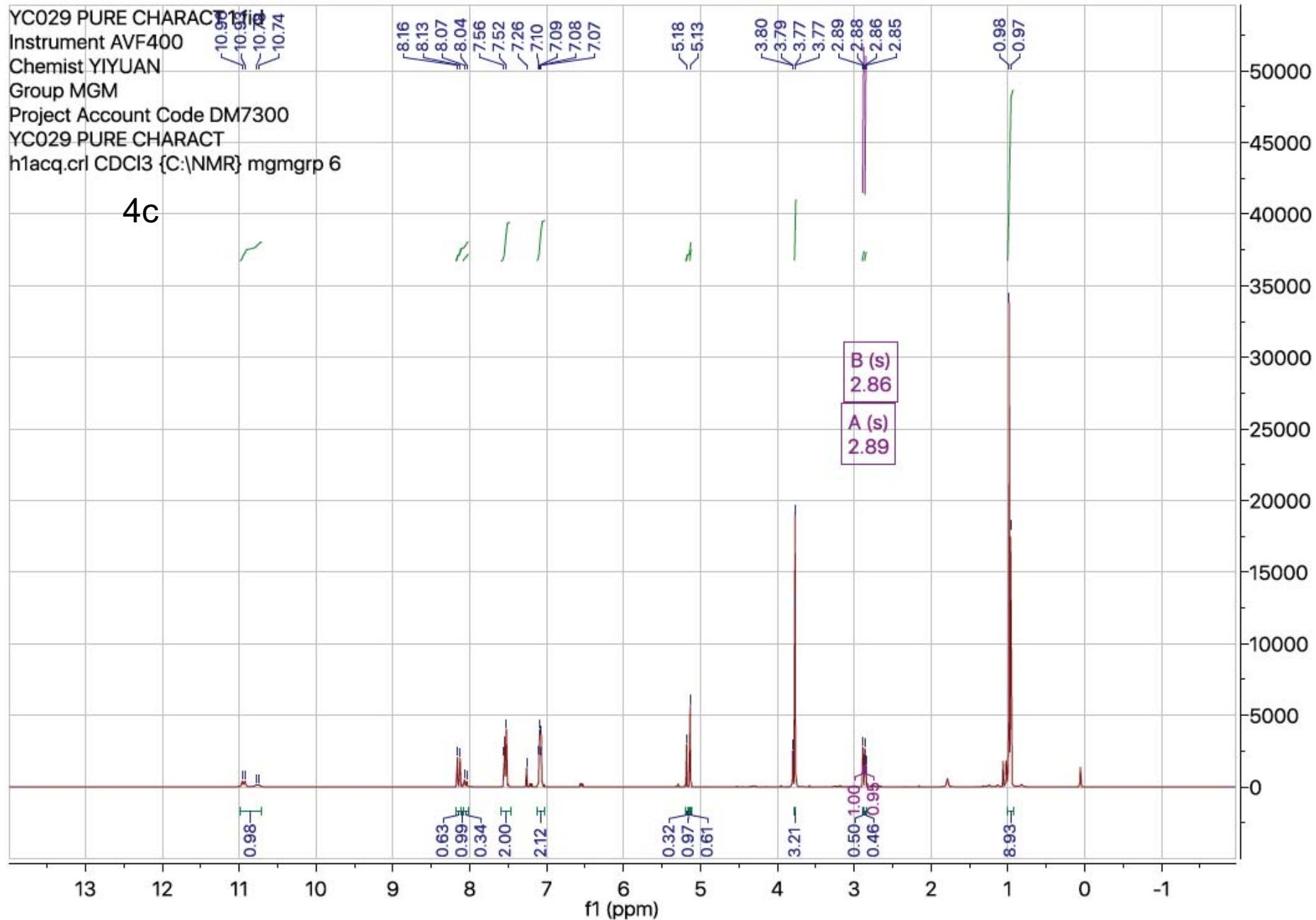
YC020 CHARACT.2.fid  
Instrument AVA400  
Group MGM  
Chemist YIYUAN  
Project Account Code DM7300  
YC020 CHARACT  
c13acq.crl CDCl3 {C:\NMR} mgmgrp 41

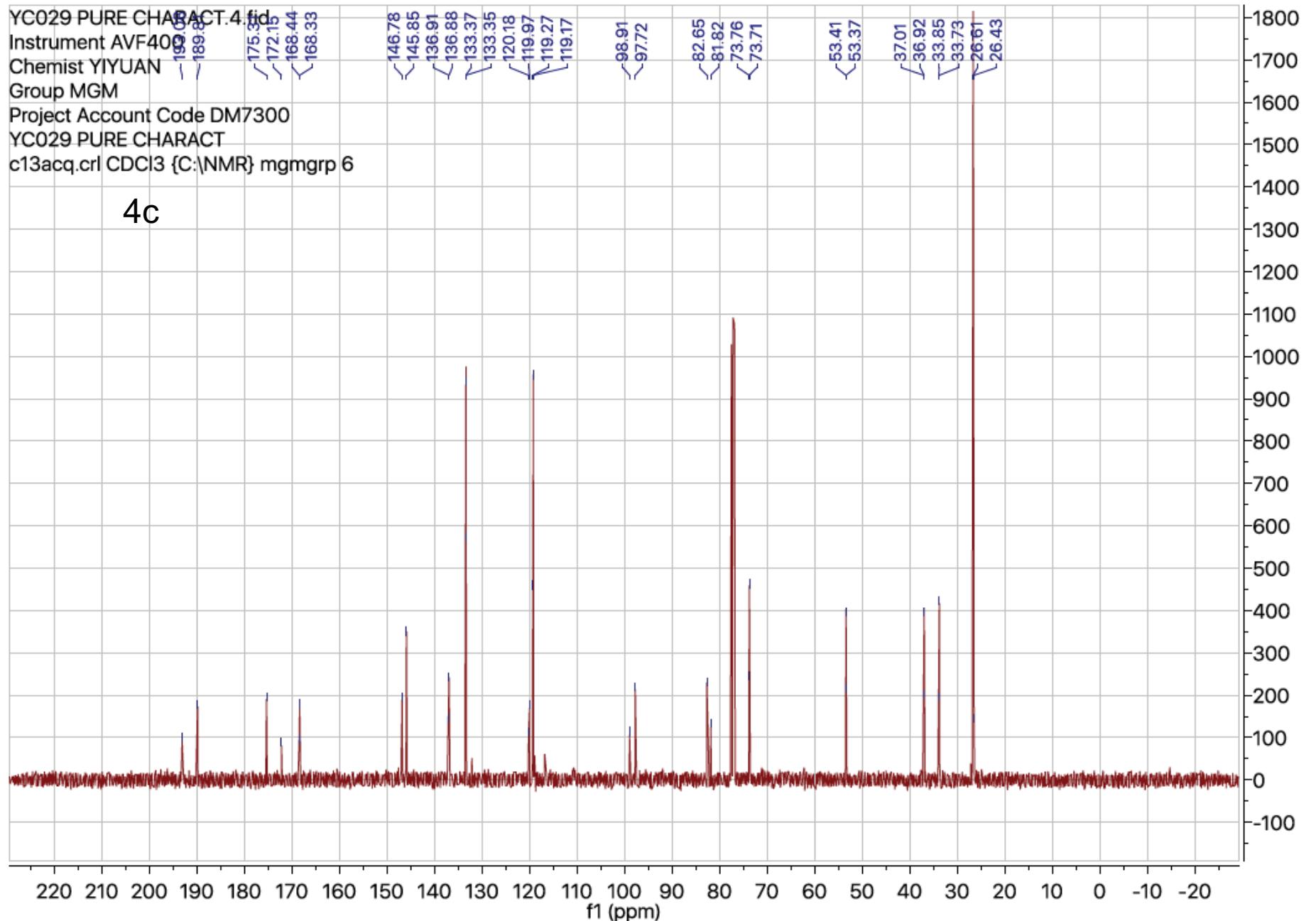
4b



YC029 PURE CHARACT  
Instrument AVF400  
Chemist YIYUAN  
Group MGM  
Project Account Code DM7300  
YC029 PURE CHARACT  
h1acq.crl CDCl3 {C:\NMR} mgmgrp 6

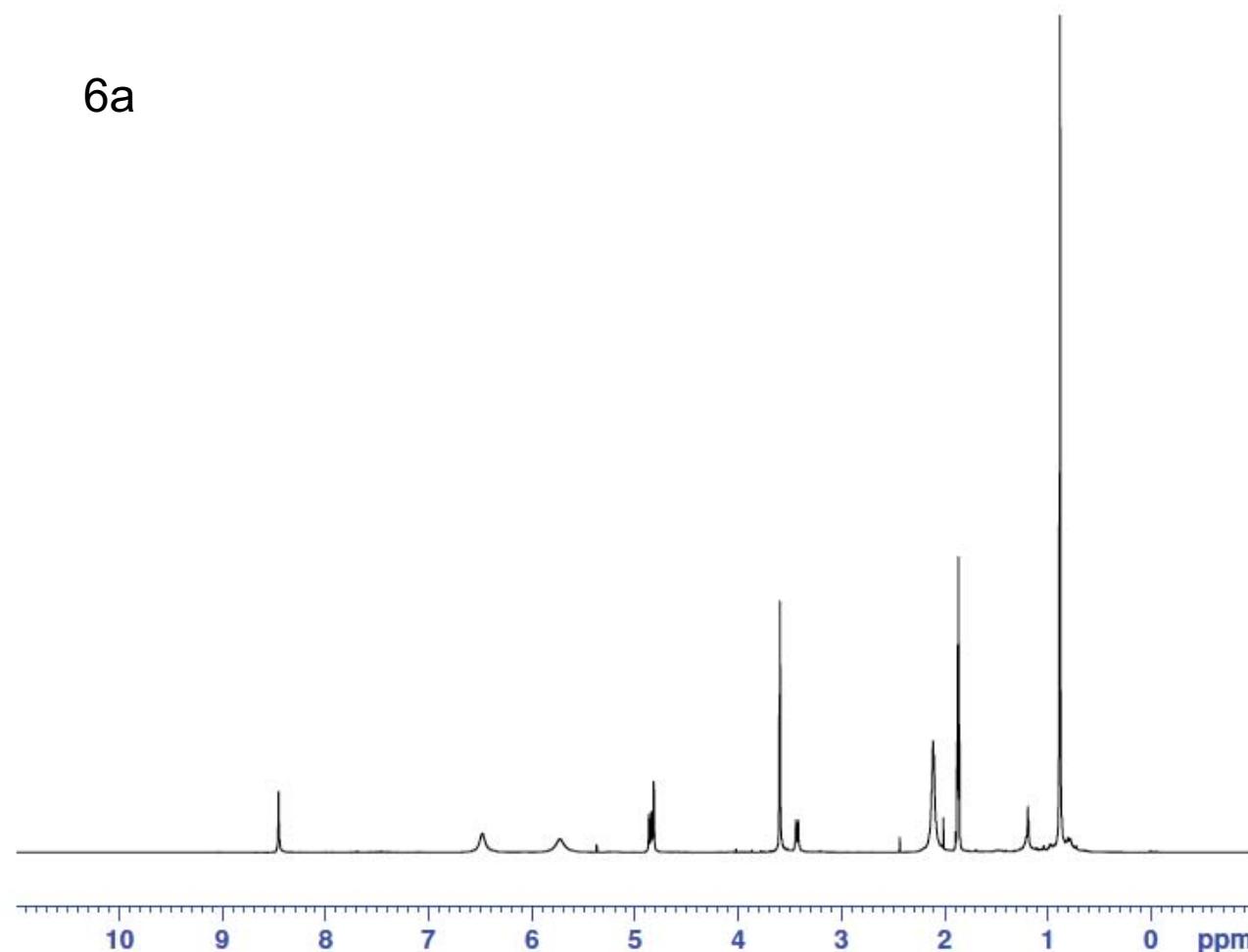
4c





Instrument AVF400  
Chemist YIYUAN CHEN  
Group MGM  
Project Account Code DM7300  
YC046 CHARACT CD3CN  
h1acq.crl CD3CN {C:\NMR\} mqmrap 46

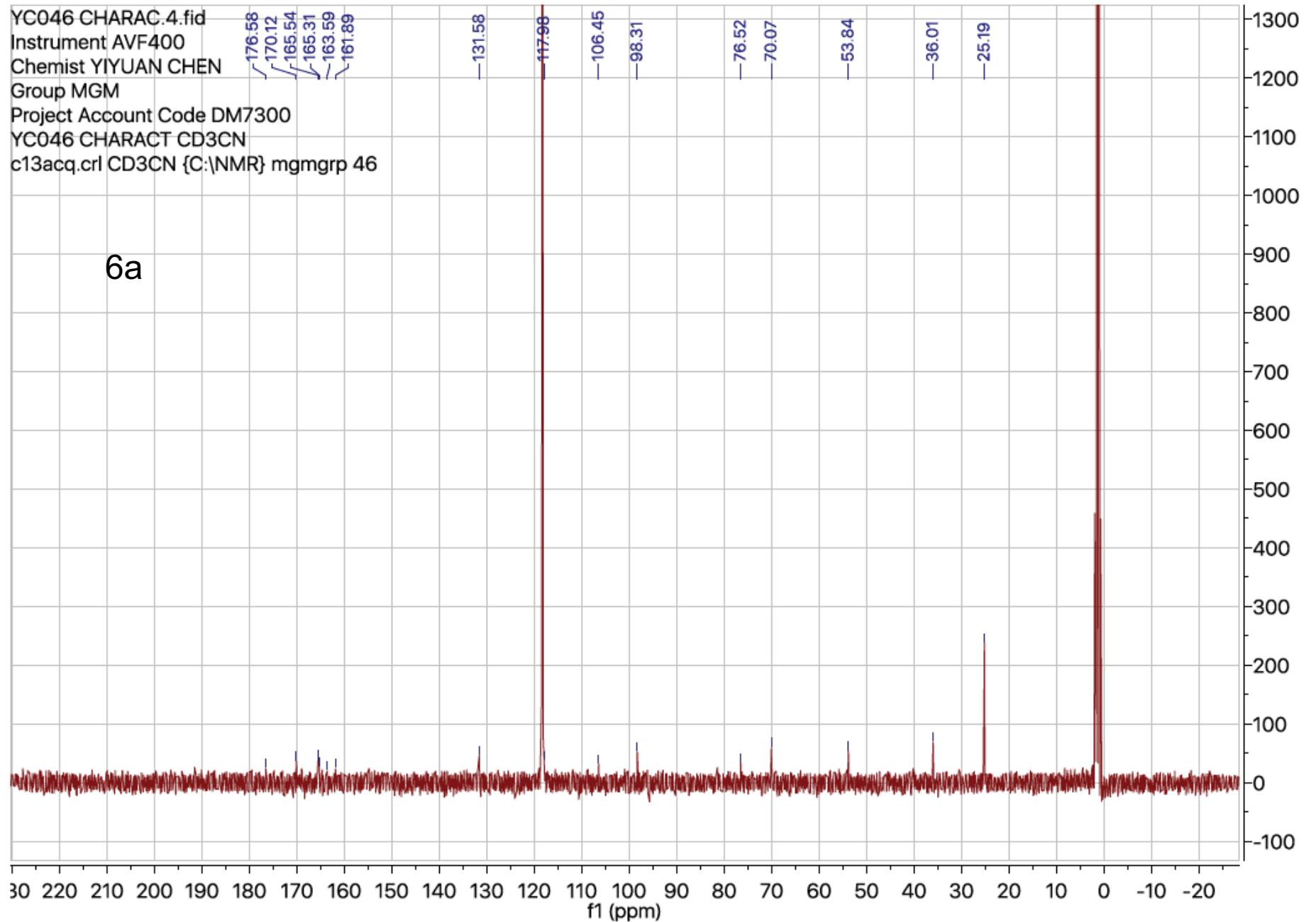
NMR@CHEM.OX



Current Data Parameters  
NAME YC046 CHARAC  
EXPNO 1  
PROCNO 1

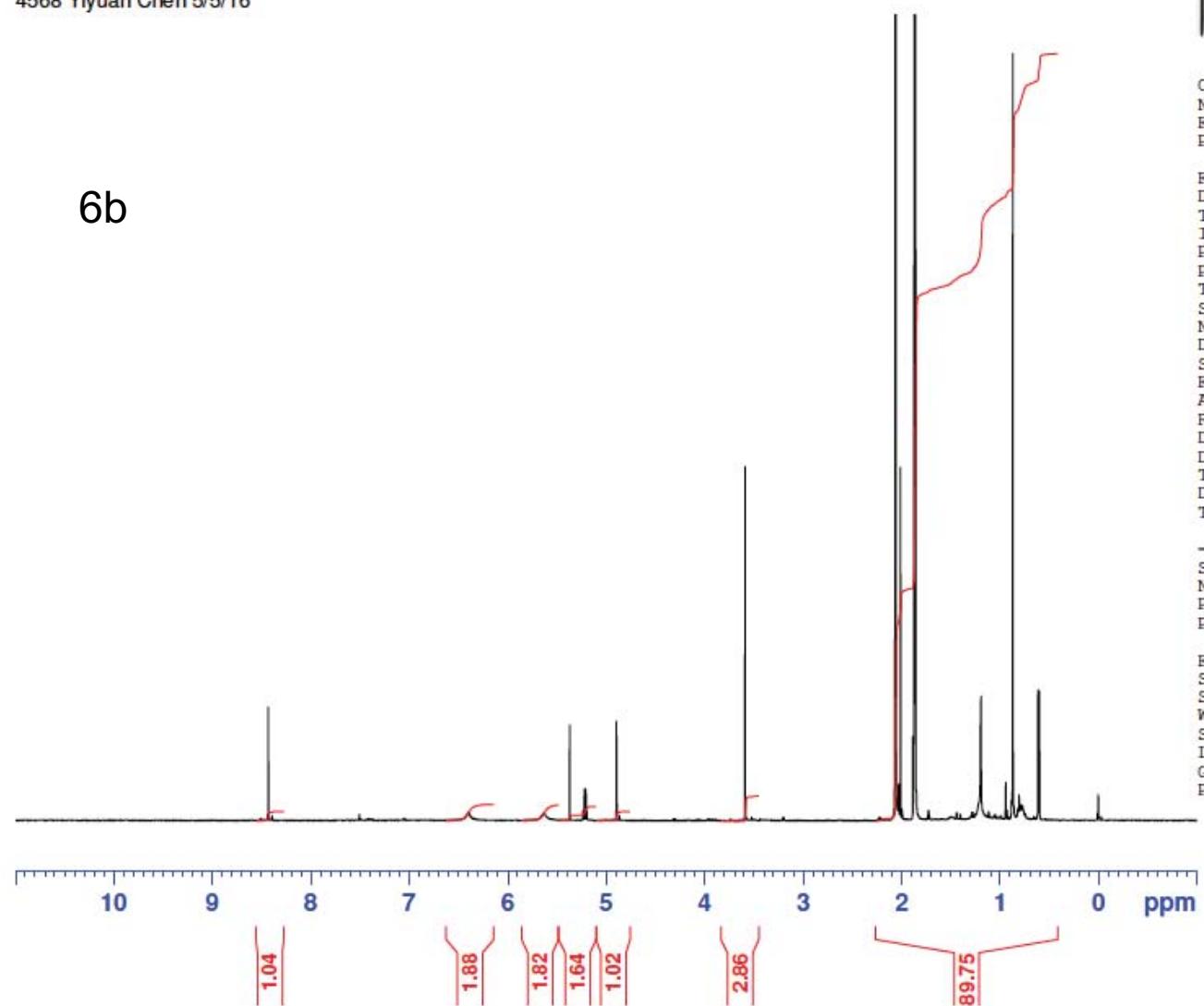
F2 - Acquisition Parameters  
Date\_ 20160505  
Time 3.50 h  
INSTRUM avf400  
PROBHD Z108618\_0533 (   
PULPROG zg60  
TD 65536  
SOLVENT CD3CN  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 93  
DW 62.400 usec  
DE 6.50 usec  
TE 294.9 K  
D1 1.0000000 sec  
TDO 1  
SFO1 400.2524015 MHz  
NUC1 1H  
P1 19.50 usec  
PLW1 16.70000076 W

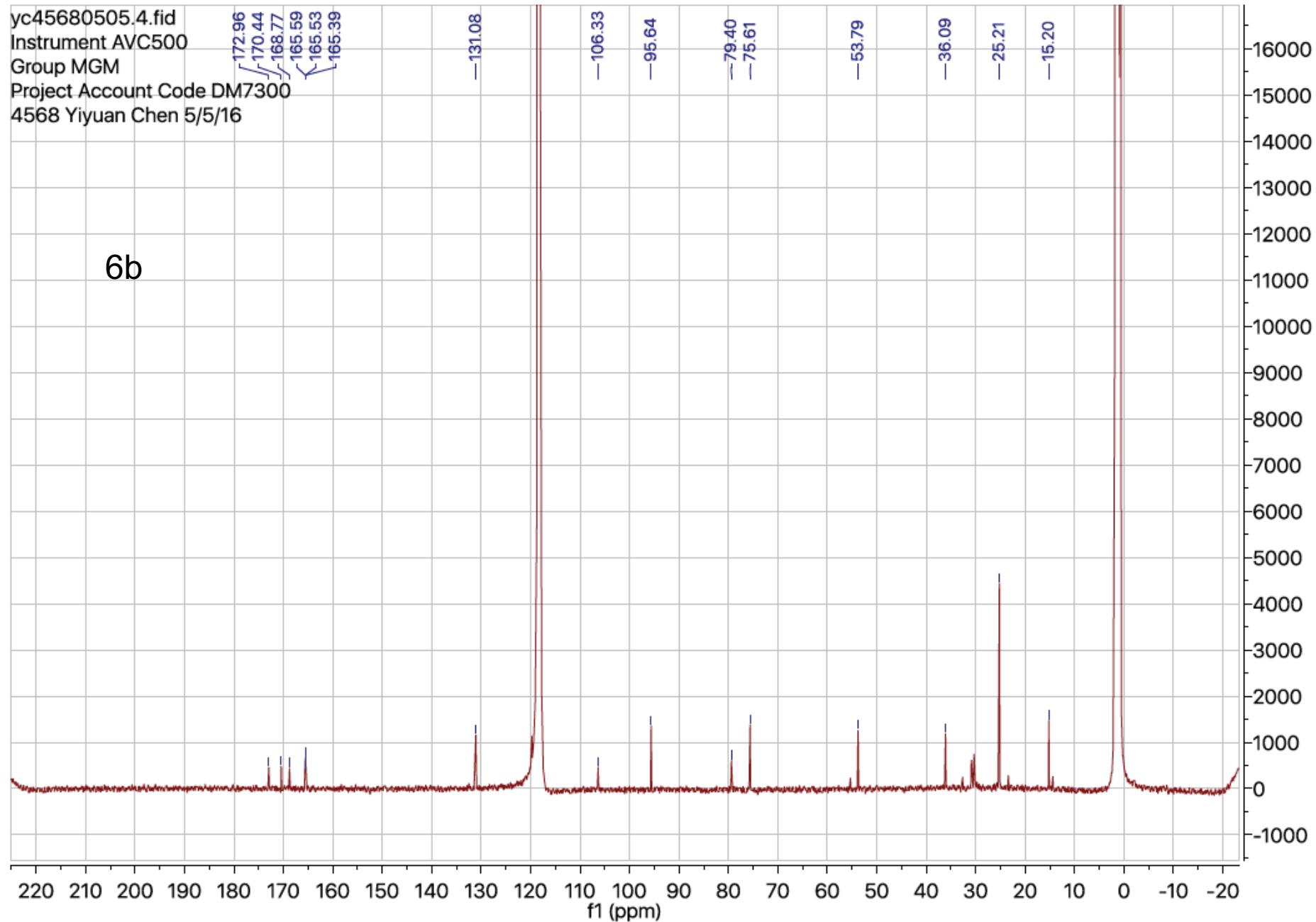
F2 - Processing parameters  
SI 32768  
SF 400.2500418 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

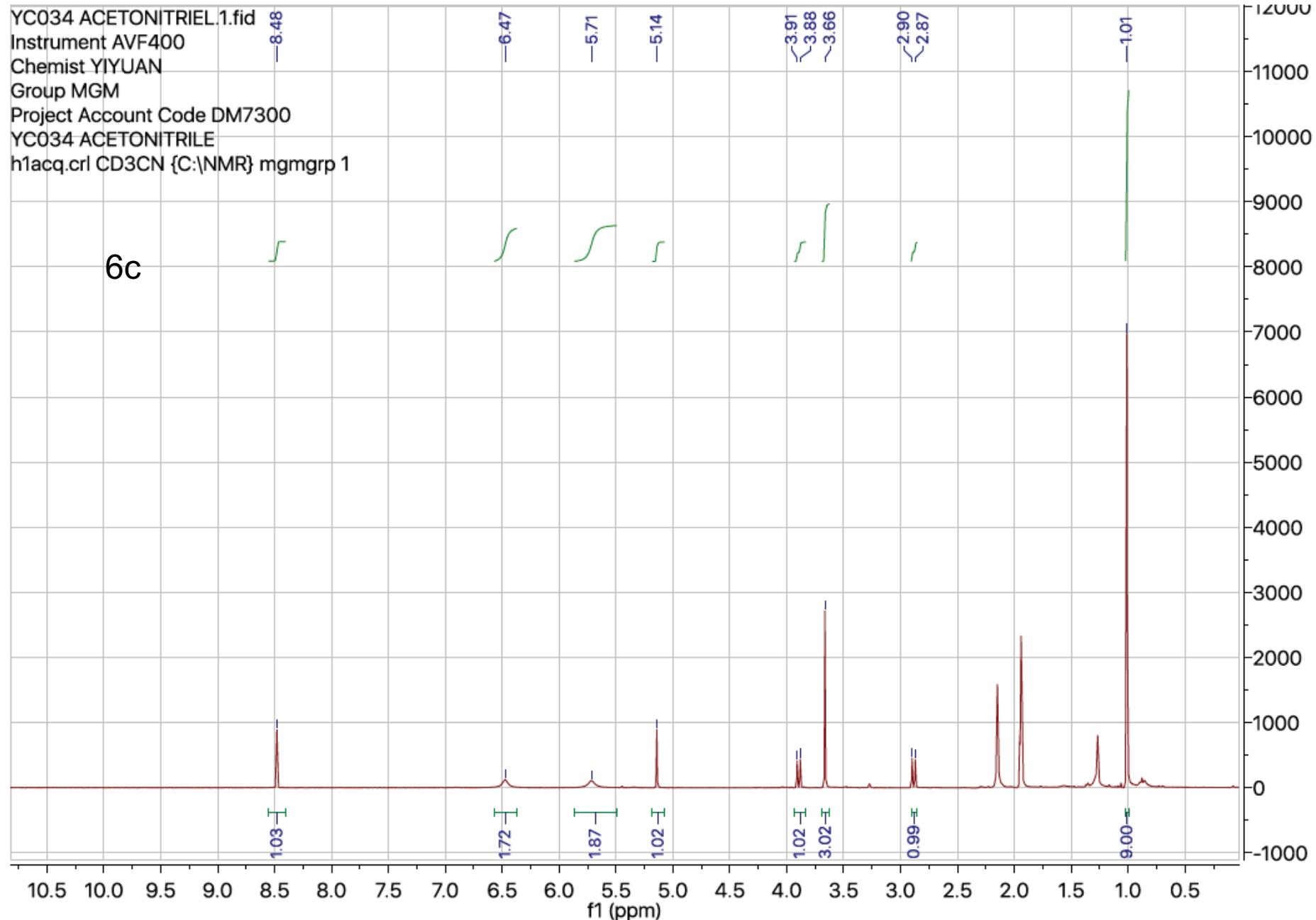


Instrument AVC500  
Group MGM  
Project Account Code DM7300  
4568 Yiyuan Chen 5/5/16

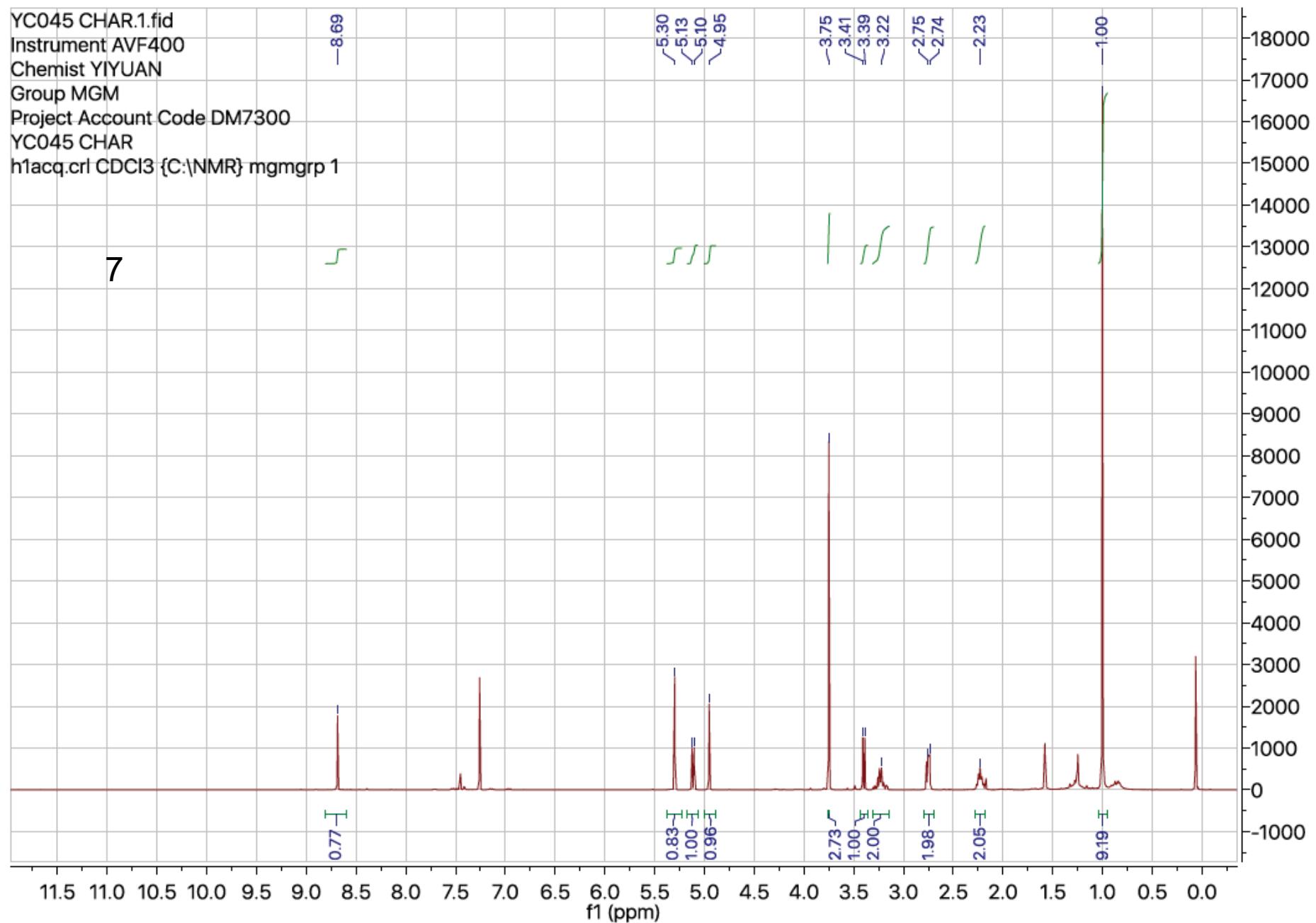
NMR@CHEM.OX

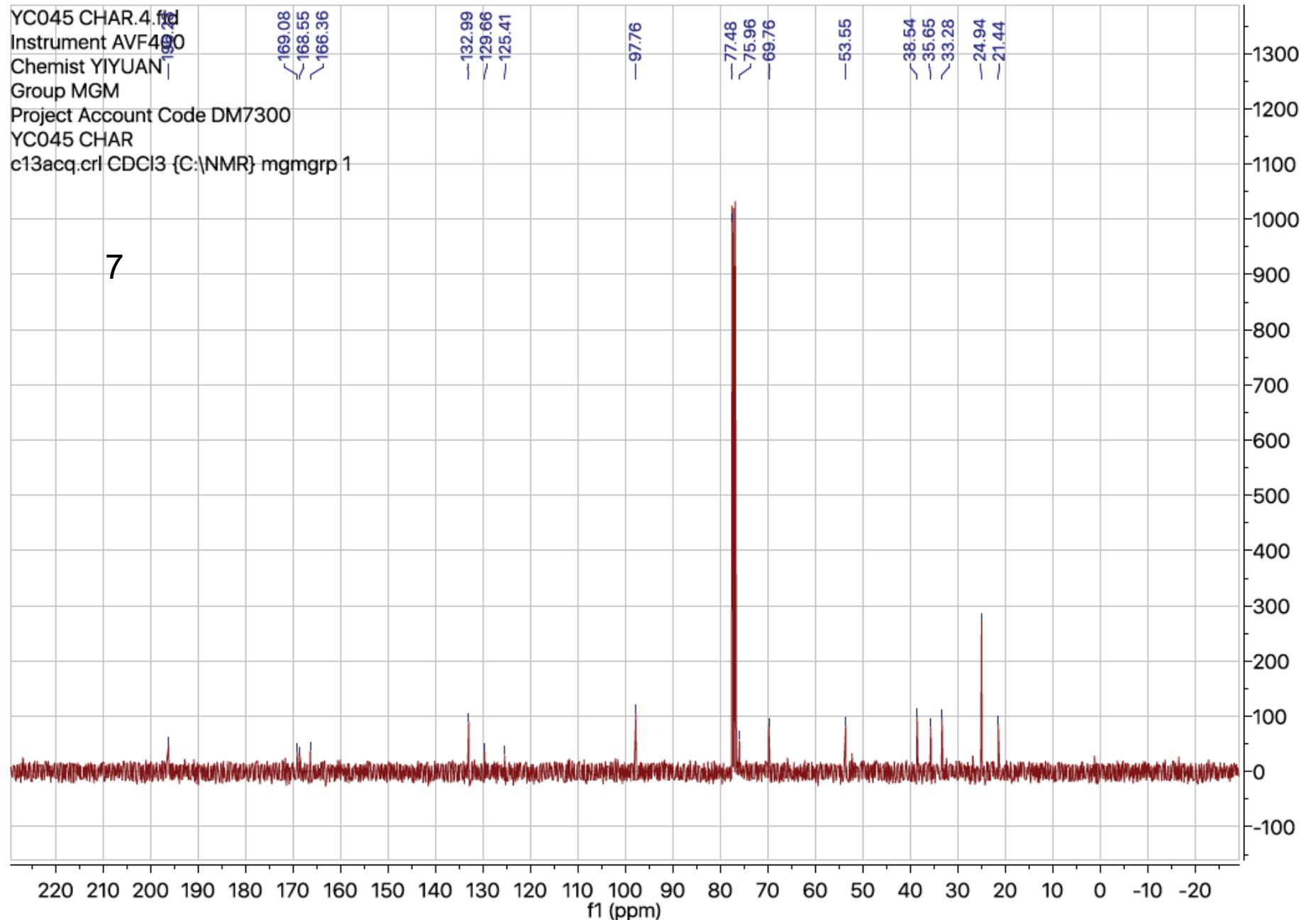






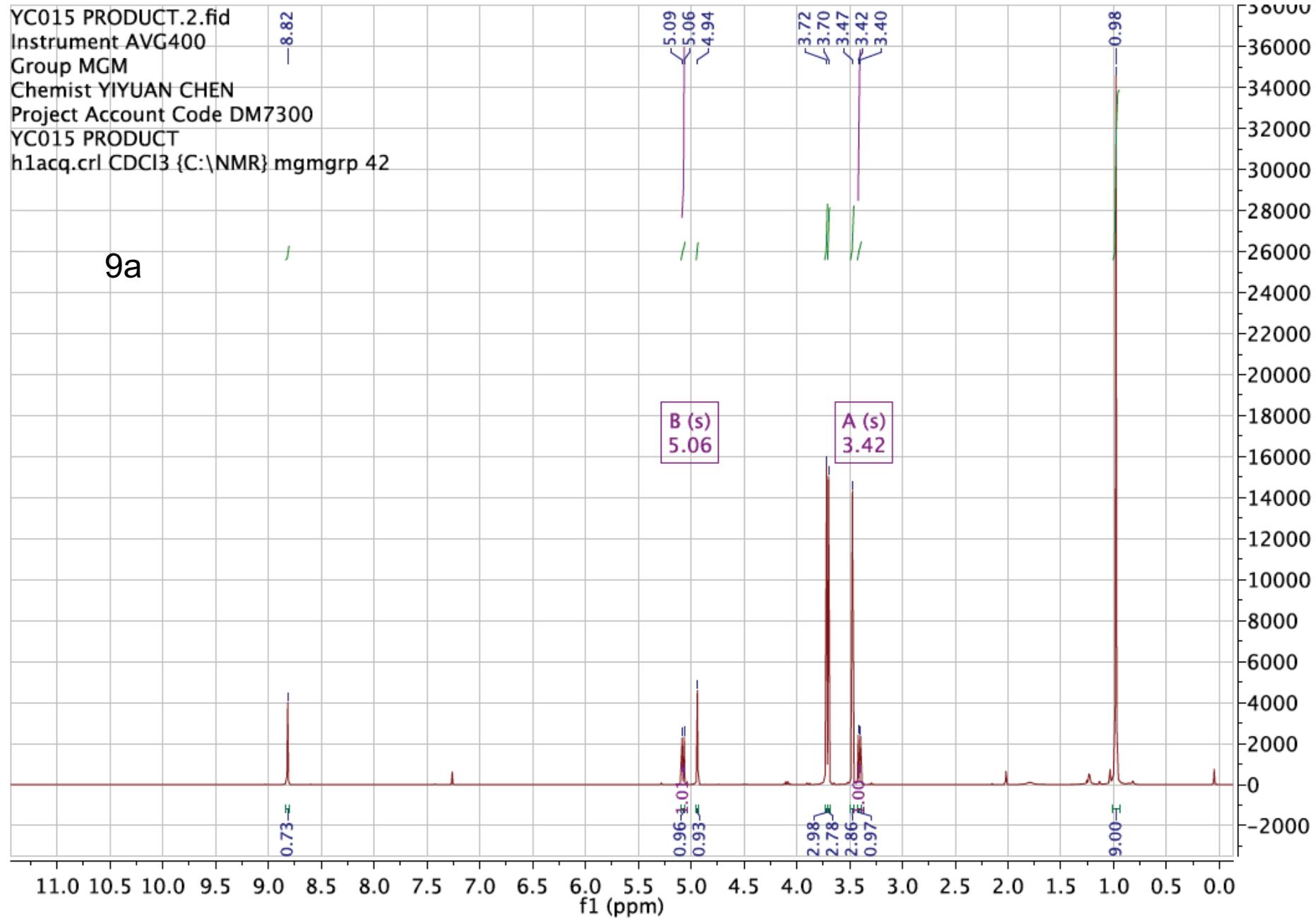
YC045 CHAR.1.fid  
Instrument AVF400  
Chemist YIYUAN  
Group MGM  
Project Account Code DM7300  
YC045 CHAR  
h1acq.crl CDCl3 {C:\NMR} mgmgrp 1

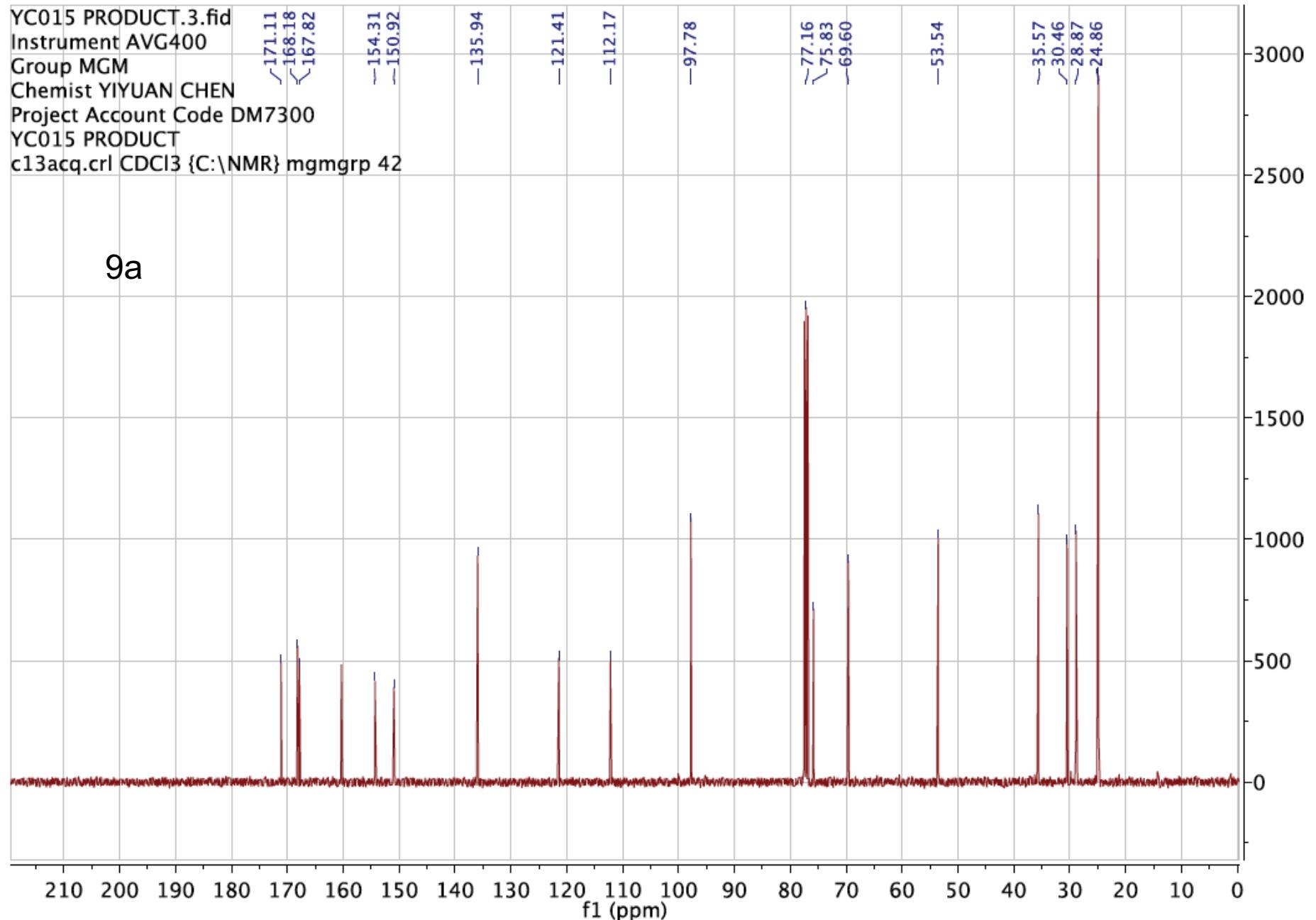


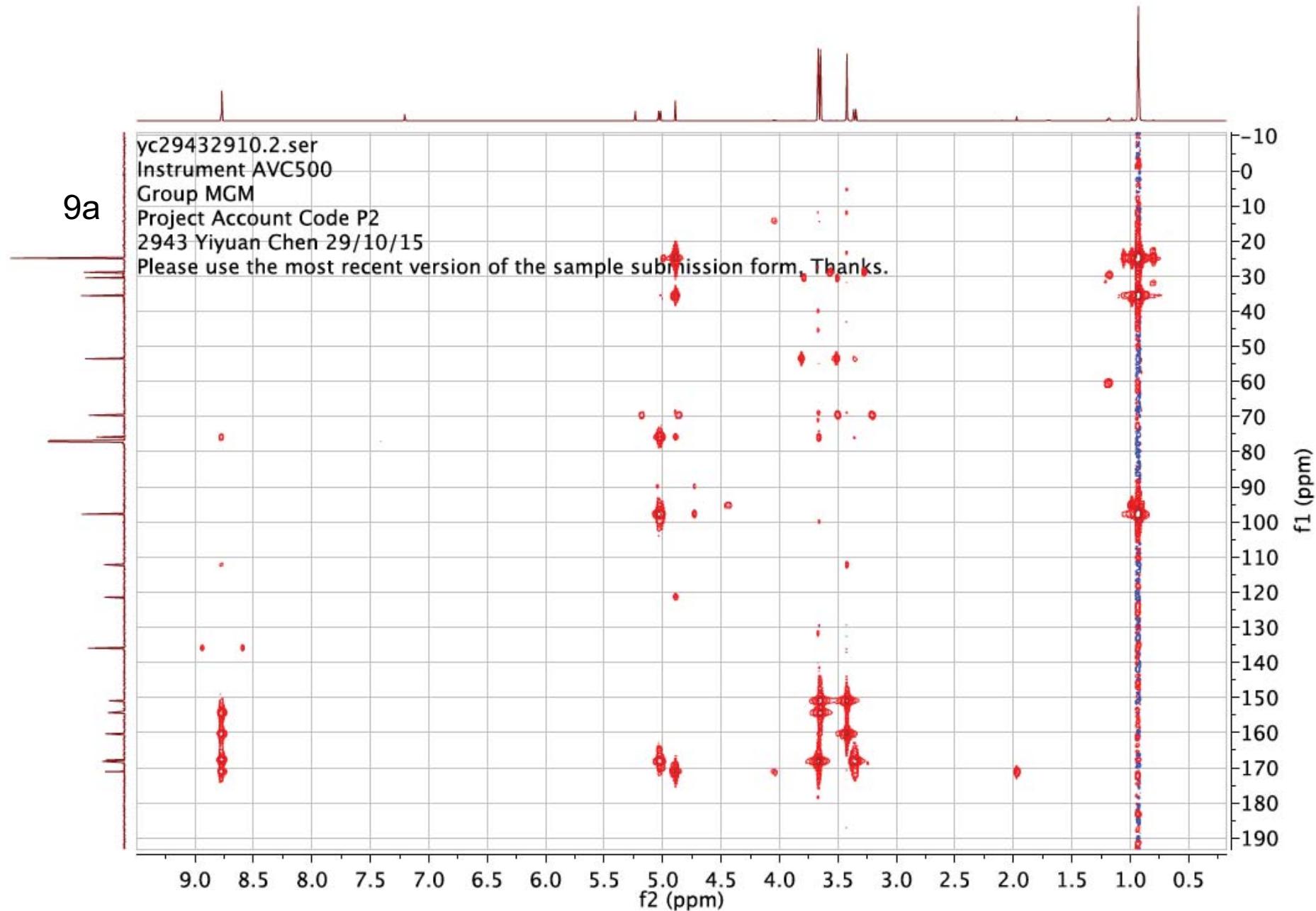


YC015 PRODUCT.2.fid  
Instrument AVG400  
Group MGM  
Chemist YIYUAN CHEN  
Project Account Code DM7300  
YC015 PRODUCT  
h1acq.crl CDCl3 {C:\NMR} mgmgrp 42

9a



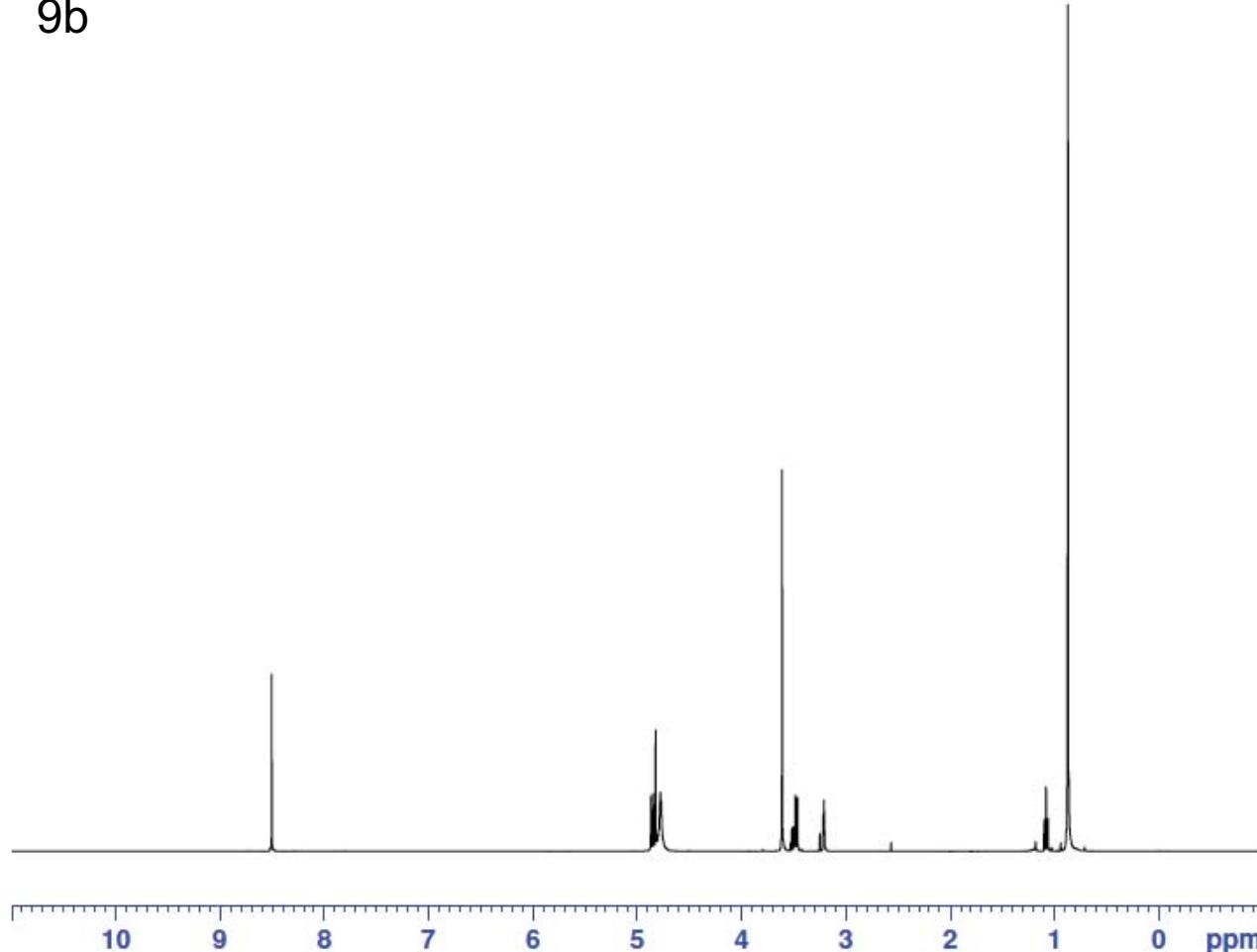




Instrument AVF400  
Chemist YIYUAN  
Group MGM  
Project Account Code DM7300  
YC070 MeOD  
h1acq.crl MeOD {C:\NMR} mqmrap 5

NMR@CHEM.OX

9b



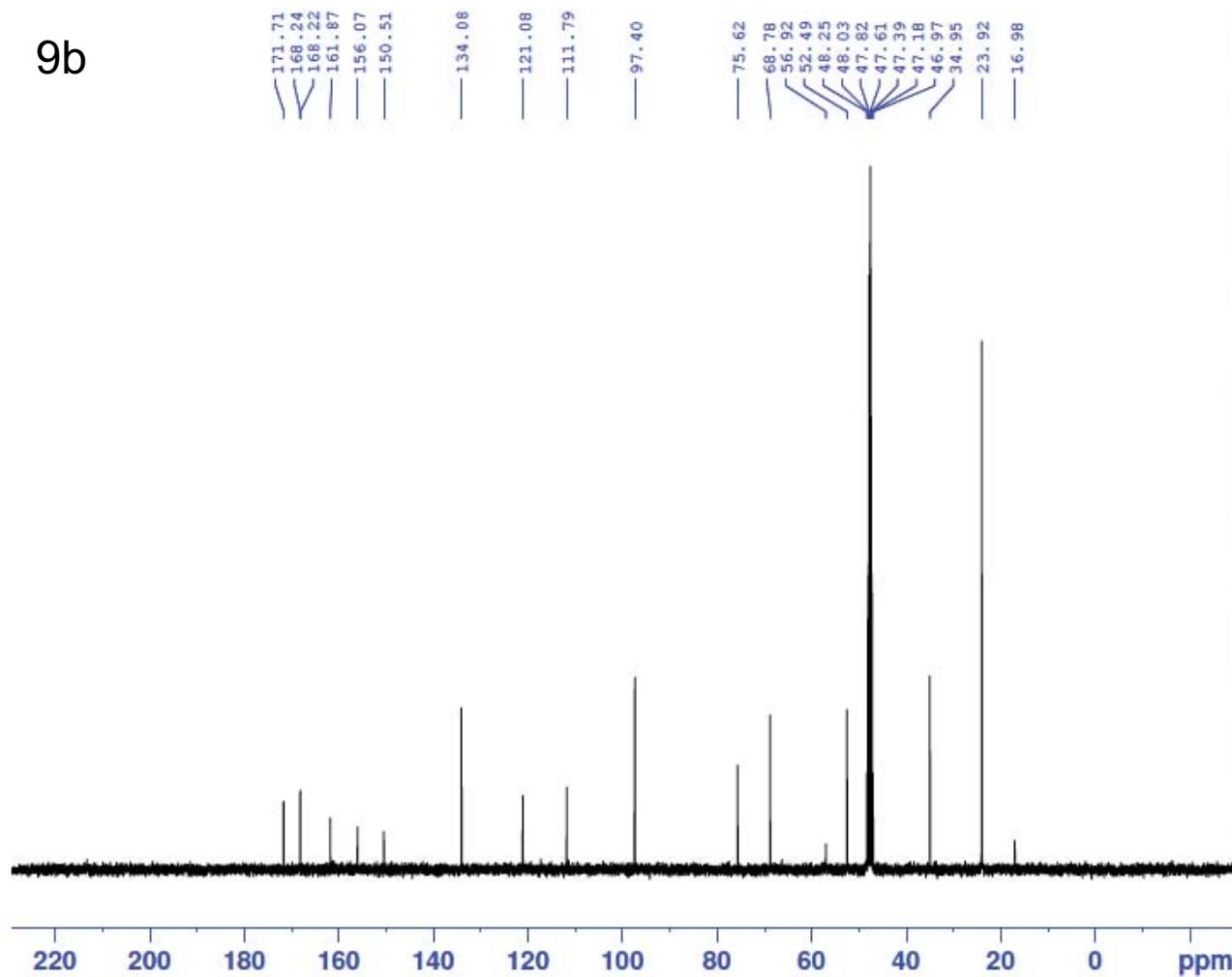
Current Data Parameters  
NAME YC070 MeOD  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160423  
Time 12.15 h  
INSTRUM avf400  
PROBHD Z108618\_0533 (   
PULPROG zg60  
TD 65536  
SOLVENT MeOD  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 65.71  
DW 62.400 usec  
DE 6.50 usec  
TE 295.0 K  
D1 1.0000000 sec  
TDO 1  
SFO1 400.2524015 MHz  
NUC1 1H  
P1 19.50 usec  
PLW1 16.70000076 W

F2 - Processing parameters  
SI 32768  
SF 400.2500484 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Instrument AVF400  
Chemist YIYUAN  
Group MGM  
Project Account Code DM7300  
YC070 MeOD  
c13acq.crl MeOD {C:NMR} mqmrap 5

9b



NMR@CHEM.OX

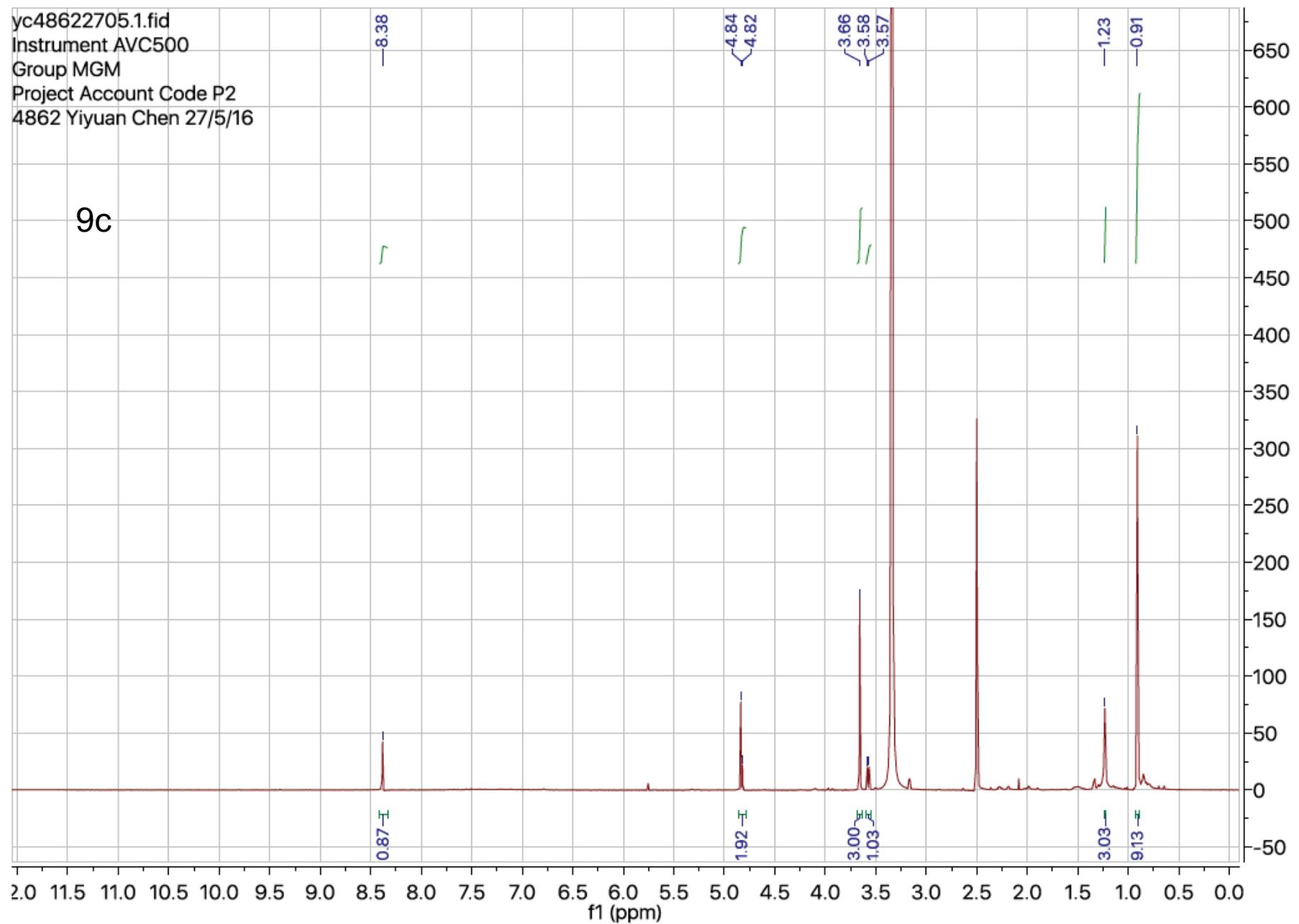
Current Data Parameters  
NAME YC070 MeOD  
EXPNO 4  
PROCNO 1

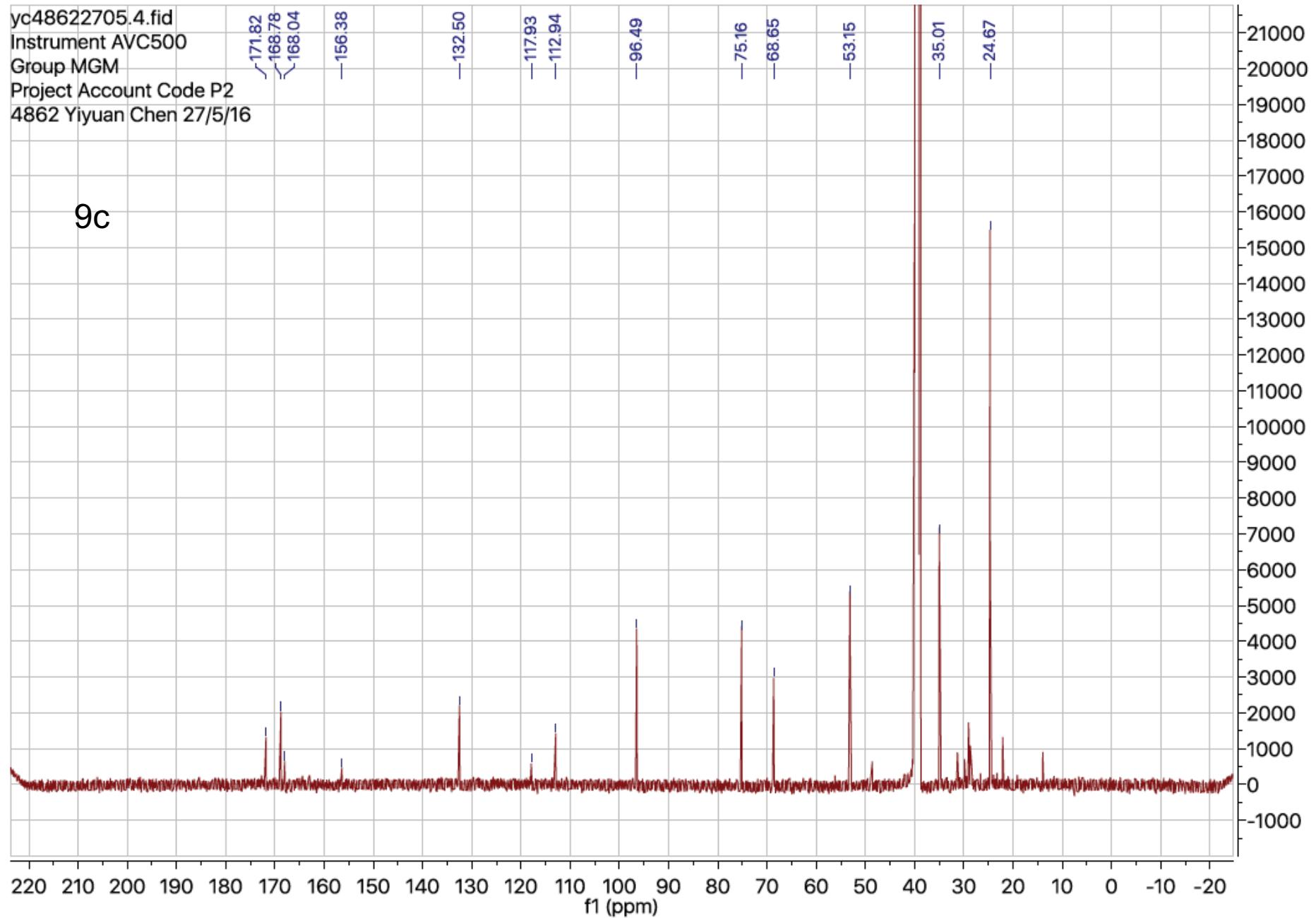
F2 - Acquisition Parameters  
Date\_ 20160423  
Time 12.39 h  
INSTRUM avf400  
PROBHD Z108618\_0533 (   
PULPROG zgpg30  
TD 32768  
SOLVENT MeOD  
NS 256  
DS 4  
SWH 26041.666 Hz  
FIDRES 1.589457 Hz  
AQ 0.6291456 sec  
RG 205.43  
DW 19.200 usec  
DE 6.50 usec  
TE 295.7 K  
D1 1.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SFO1 100.6530068 MHz  
NUC1 13C  
P1 9.00 usec  
PLW1 58.70000076 W  
SFO2 400.2516010 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 16.70000076 W  
PLW12 0.78397000 W  
PLW13 0.39432999 W

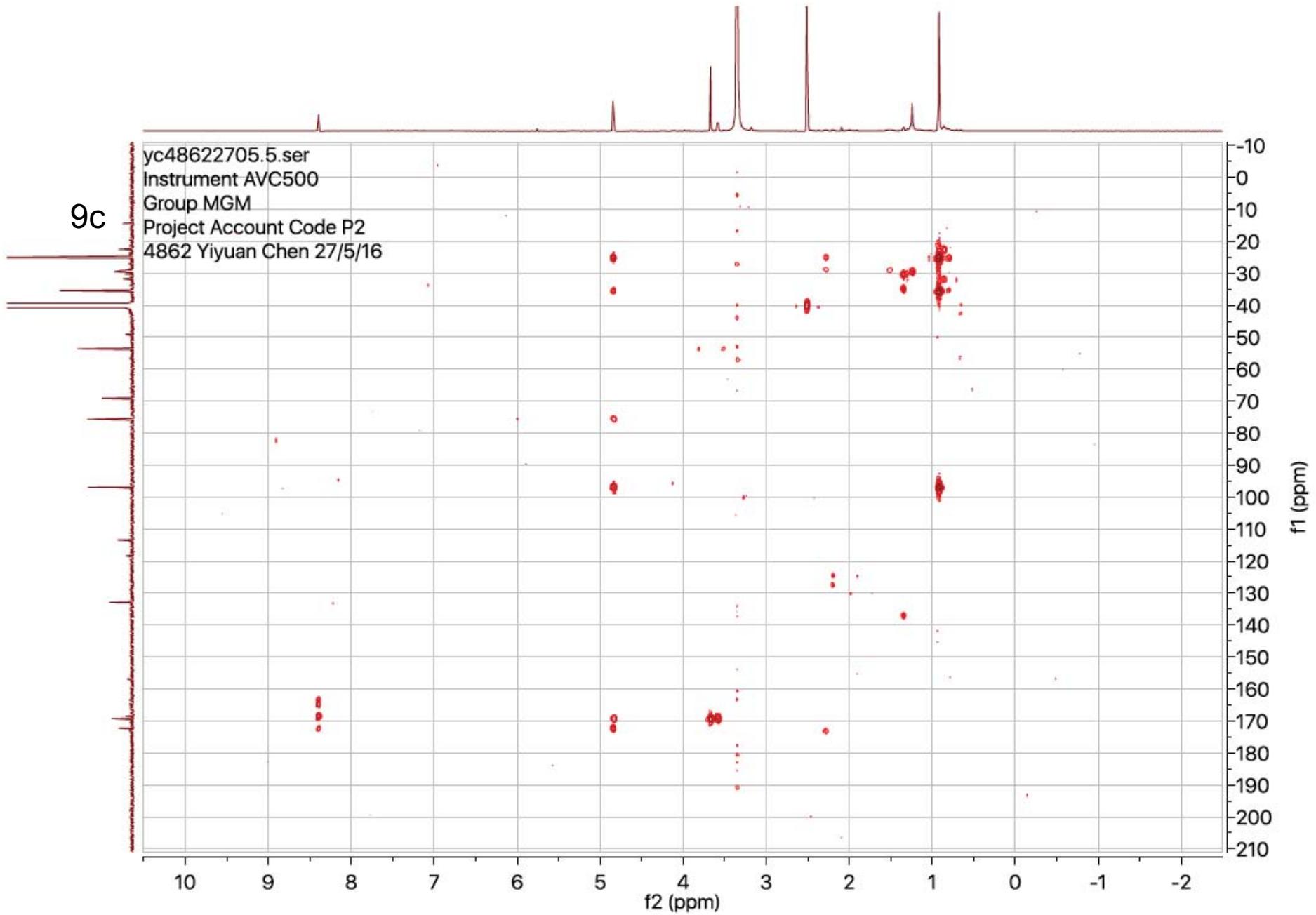
F2 - Processing parameters  
SI 32768  
SF 100.6429430 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

yc48622705.1.fid  
Instrument AVC500  
Group MGM  
Project Account Code P2  
4862 Yiyuan Chen 27/5/16

9c



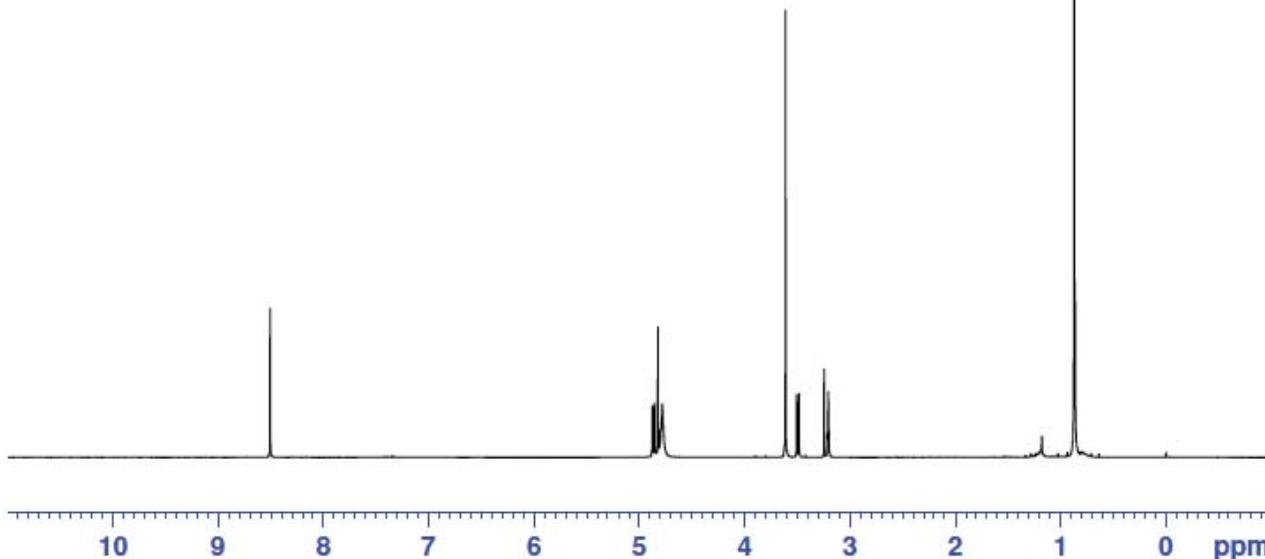




Instrument AVF400  
Chemist YIYUAN  
Group MGM  
Project Account Code DM7300  
YC071 AFTER COLUMN  
h1acq.crl MeOD {C:\NMR} mqmrap 1

NMR@CHEM.OX

9d



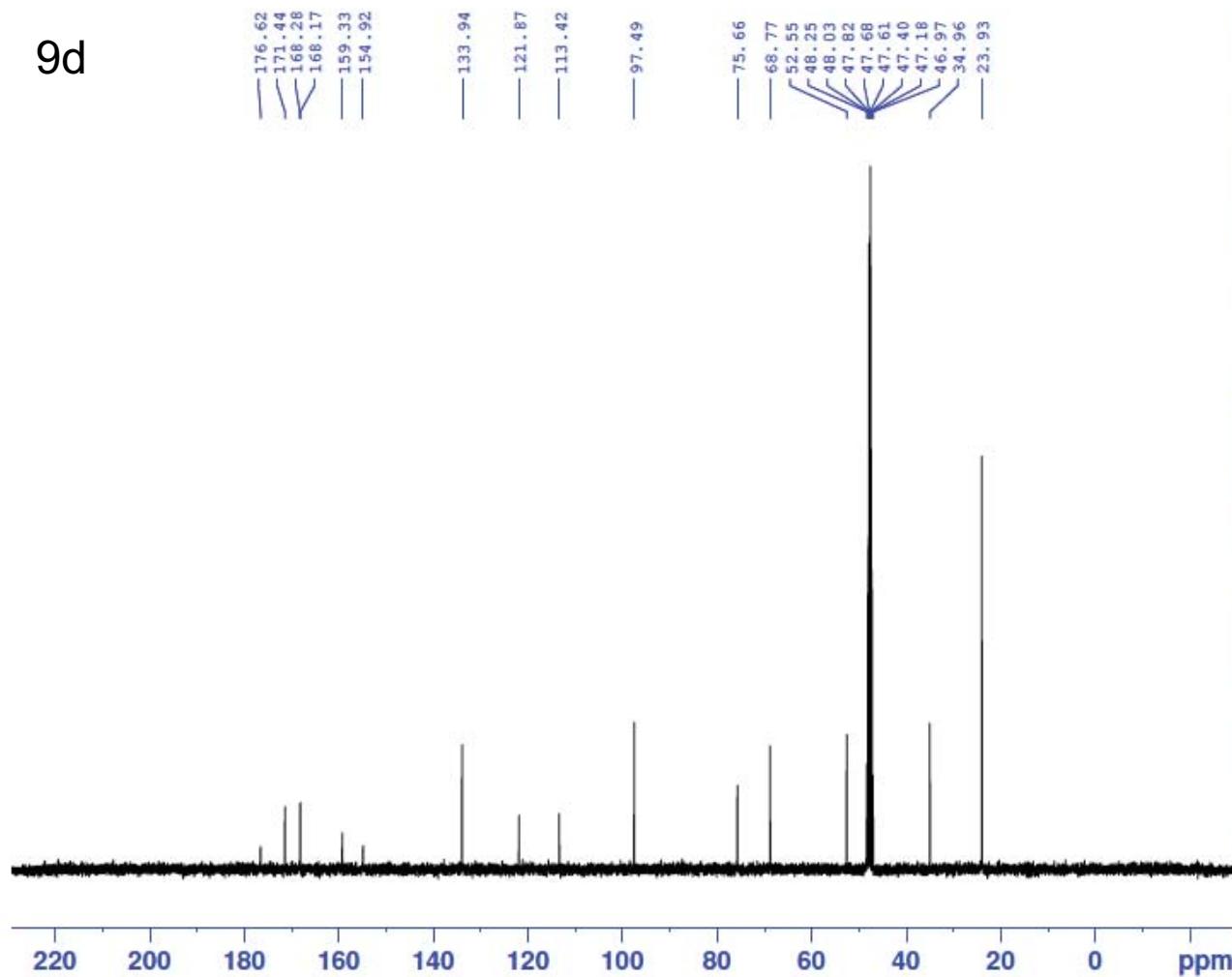
Current Data Parameters  
NAME YC071 Column  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160503  
Time 12.27 h  
INSTRUM avf400  
PROBHD Z108618\_0533 (   
PULPROG zg60  
TD 65536  
SOLVENT MeOD  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 65.71  
DW 62.400 usec  
DE 6.50 usec  
TE 294.4 K  
D1 1.0000000 sec  
TDO 1  
SFO1 400.2524015 MHz  
NUC1 1H  
P1 19.50 usec  
PLW1 16.70000076 W

F2 - Processing parameters  
SI 32768  
SF 400.2500482 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Instrument AVF400  
Chemist YIYUAN  
Group MGM  
Project Account Code DM7300  
YC071 AFTER COLUMN  
c13acq.crl MeOD {C:NMR} mqmrap 1

9d



NMR@CHEM.OX

Current Data Parameters  
NAME YC071 Column  
EXPN 4  
PROCNO 1

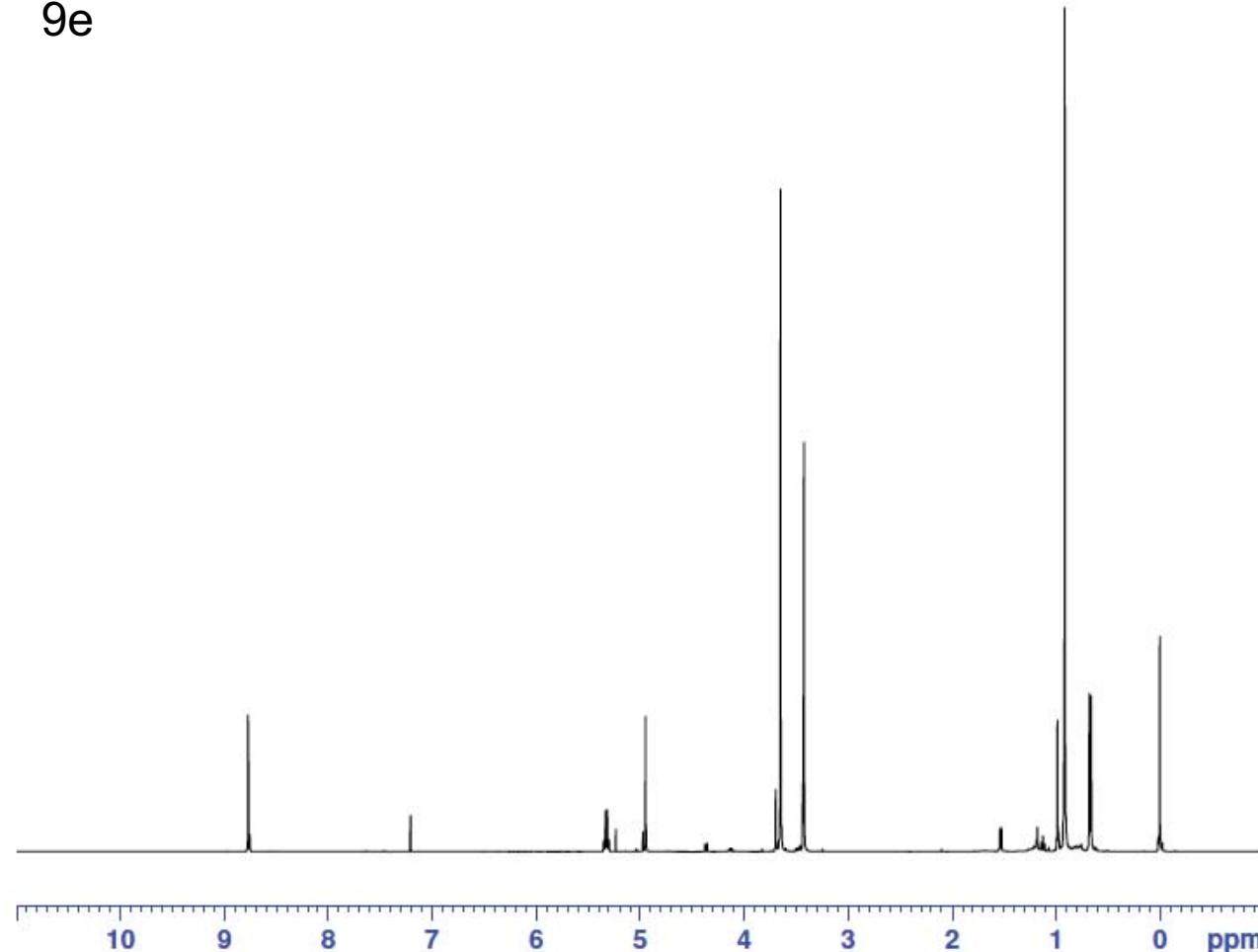
F2 - Acquisition Parameters  
Date\_ 20160503  
Time 12.51 h  
INSTRUM avf400  
PROBHD Z108618\_0533 (   
PULPROG zgpg30  
TD 32768  
SOLVENT MeOD  
NS 256  
DS 4  
SWH 26041.666 Hz  
FIDRES 1.589457 Hz  
AQ 0.6291456 sec  
RG 205.43  
DW 19.200 usec  
DE 6.50 usec  
TE 295.1 K  
D1 1.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SFO1 100.6530068 MHz  
NUC1 13C  
P1 9.00 usec  
PLW1 58.70000076 W  
SFO2 400.2516010 MHz  
NUC2 1H  
CPDPKG[2] waltz16  
PCPD2 90.00 usec  
PLW2 16.70000076 W  
PLW12 0.78397000 W  
PLW13 0.39432999 W

F2 - Processing parameters  
SI 32768  
SF 100.6429430 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Instrument AVF400  
Chemist YIYUAN CHEN  
Group MGM  
Project Account Code DM7300  
YC030 CHARACT CDCl<sub>3</sub>  
h1acq.crl CDCl<sub>3</sub> {C:NMR} mqmqrp 30

NMR@CHEM.OX

9e



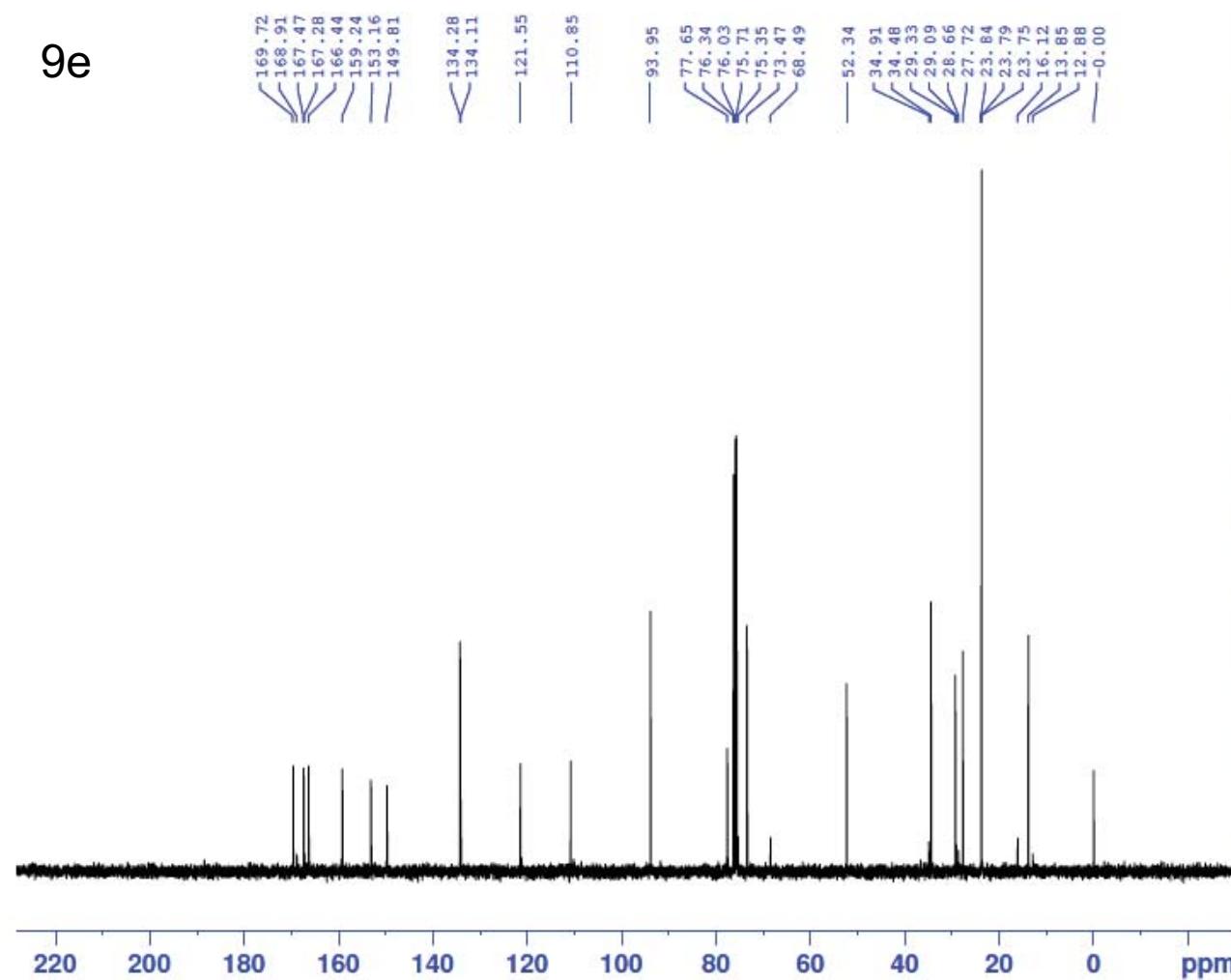
Current Data Parameters  
NAME YC030 CHAR  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160505  
Time 7.04 h  
INSTRUM avf400  
PROBHD Z108618\_0533 (   
PULPROG zg60  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 39.49  
DW 62.400 usec  
DE 6.50 usec  
TE 294.9 K  
D1 1.0000000 sec  
TDO 1  
SFO1 400.2524015 MHz  
NUC1 1H  
P1 19.50 usec  
PLW1 16.70000076 W

F2 - Processing parameters  
SI 32768  
SF 400.2500300 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Instrument AVF400  
Chemist YIYUAN CHEN  
Group MGM  
Project Account Code DM7300  
YC030 CHARACT CDCl<sub>3</sub>  
c13acq.crl CDCl<sub>3</sub> {C:NMR} mqmrap 30

9e



NMR@CHEM.OX

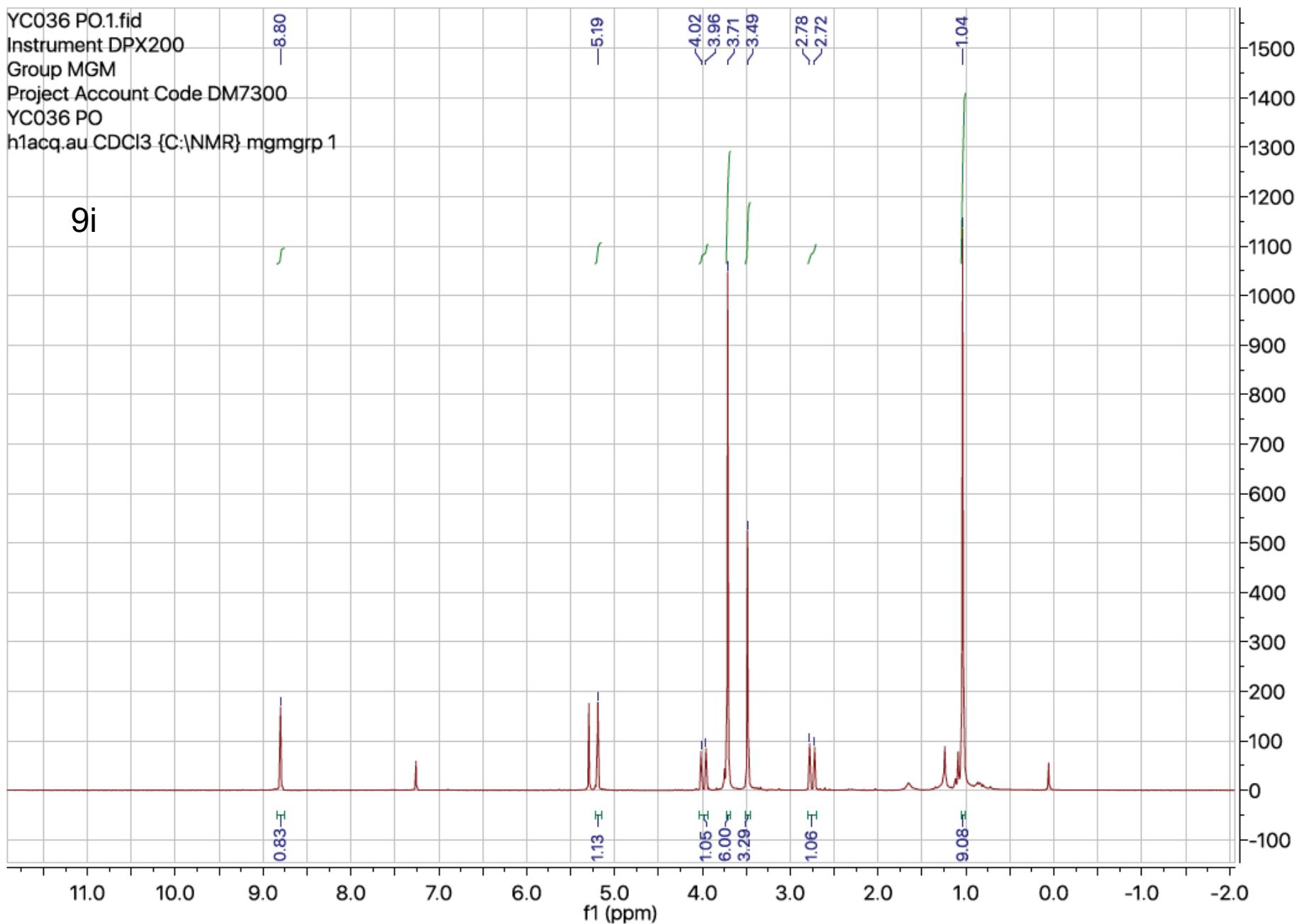
Current Data Parameters  
NAME YC030 CHAR  
EXPN 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160505  
Time 7.27 h  
INSTRUM avf400  
PROBHD Z108618\_0533 (zgpg30  
PULPROG 32768  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 256  
DS 4  
SWH 26041.666 Hz  
FIDRES 1.589457 Hz  
AQ 0.6291456 sec  
RG 205.43  
DW 19.200 usec  
DE 6.50 usec  
TE 295.5 K  
D1 1.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SFO1 100.6530068 MHz  
NUC1 13C  
P1 9.00 usec  
PLW1 58.70000076 W  
SFO2 400.2516010 MHz  
NUC2 1H  
CPDPKG[2] waltz16  
PCPD2 90.00 usec  
PLW2 16.70000076 W  
PLW12 0.78397000 W  
PLW13 0.39432999 W

F2 - Processing parameters  
SI 32768  
SF 100.6430464 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

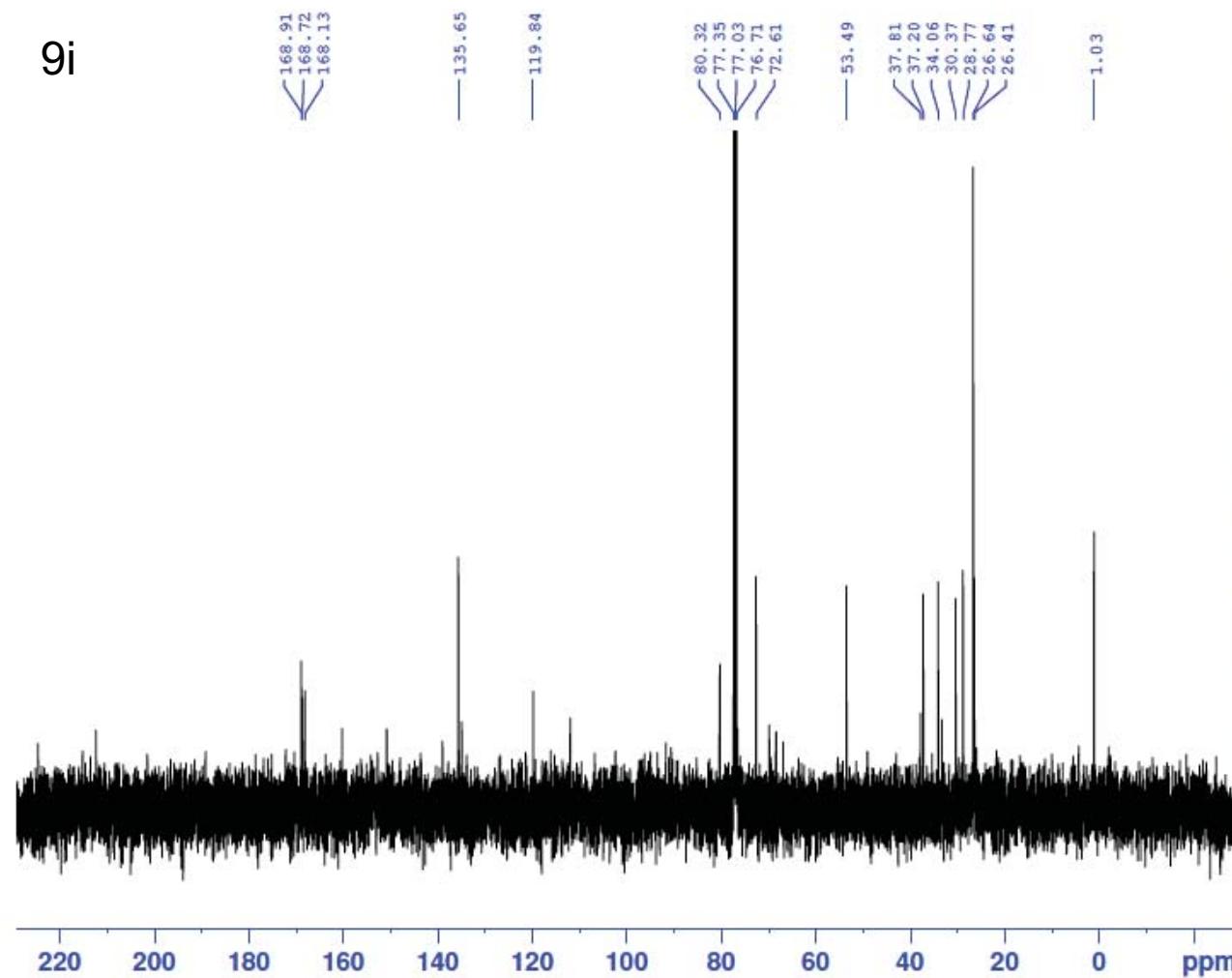
YC036 PO1.fid  
Instrument DPX200  
Group MGM  
Project Account Code DM7300  
YC036 PO  
h1acq.au CDCl3 {C:\NMR} mgmgrp 1

9i



Instrument AVF400  
Chemist YIYUAN CHEN  
Group MGM  
Project Account Code DM7300  
YC033 BIO CHAR  
c13acq.crl CDCl<sub>3</sub> (C:NMR) mqmrap 33

9i



NMR@CHEM.OX

Current Data Parameters  
NAME YC033 BIO CHAR  
EXPN 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160505  
Time 6.54 h  
INSTRUM avf400  
PROBHD Z108618\_0533 (   
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 256  
DS 4  
SWH 26041.666 Hz  
FIDRES 1.589457 Hz  
AQ 0.6291456 sec  
RG 205.43  
DW 19.200 usec  
DE 6.50 usec  
TE 295.5 K  
D1 1.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SFO1 100.6530068 MHz  
NUC1 <sup>13</sup>C  
P1 9.00 usec  
PLW1 58.70000076 W  
SFO2 400.2516010 MHz  
NUC2 <sup>1</sup>H  
CPDPG[2] waltz16  
PCPD2 90.00 usec  
PLW2 16.70000076 W  
PLW12 0.78397000 W  
PLW13 0.39432999 W

F2 - Processing parameters  
SI 32768  
SF 100.6429430 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Aug12-2016-6-JM027.1.fid

Instrument AVF400

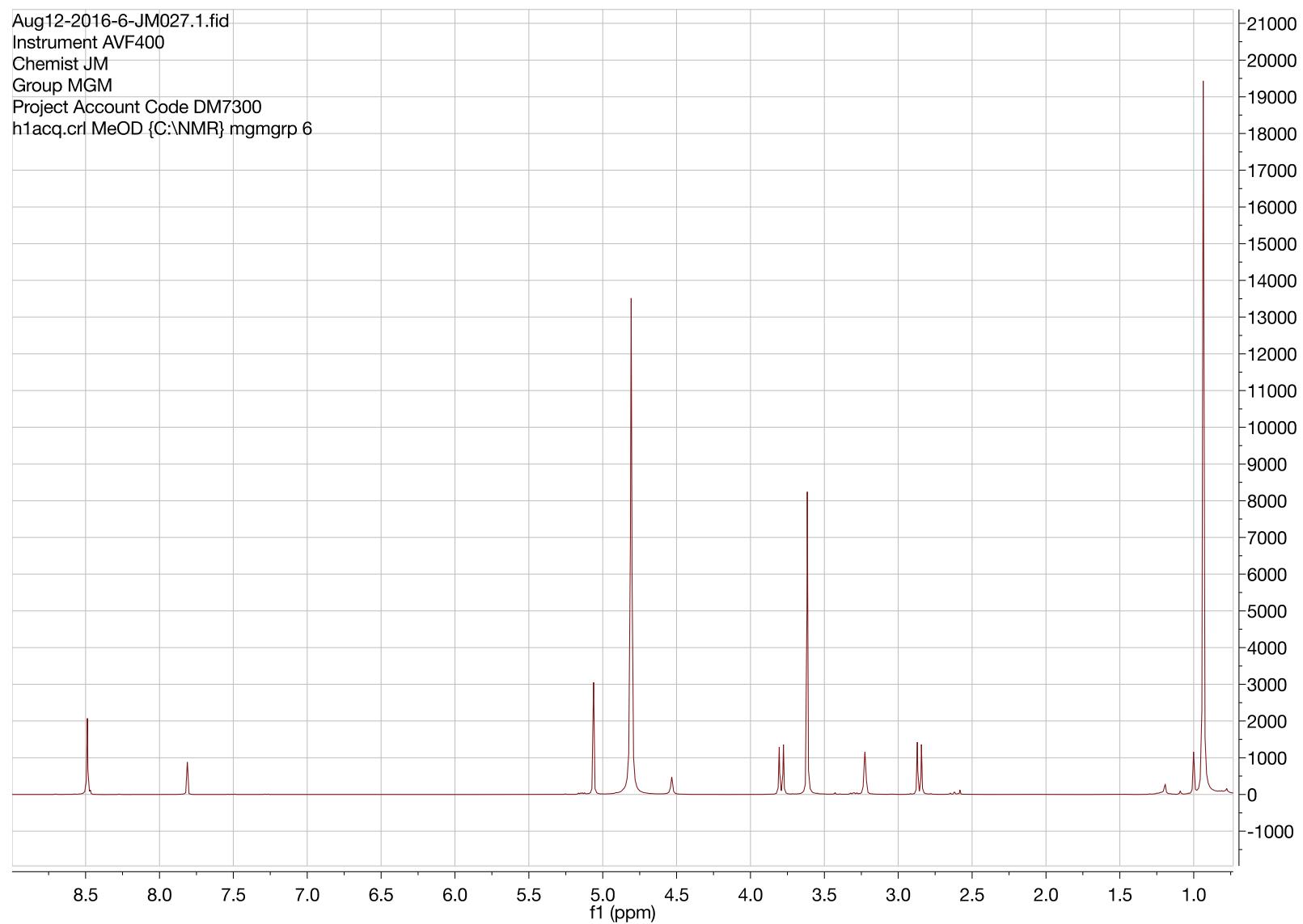
Chemist JM

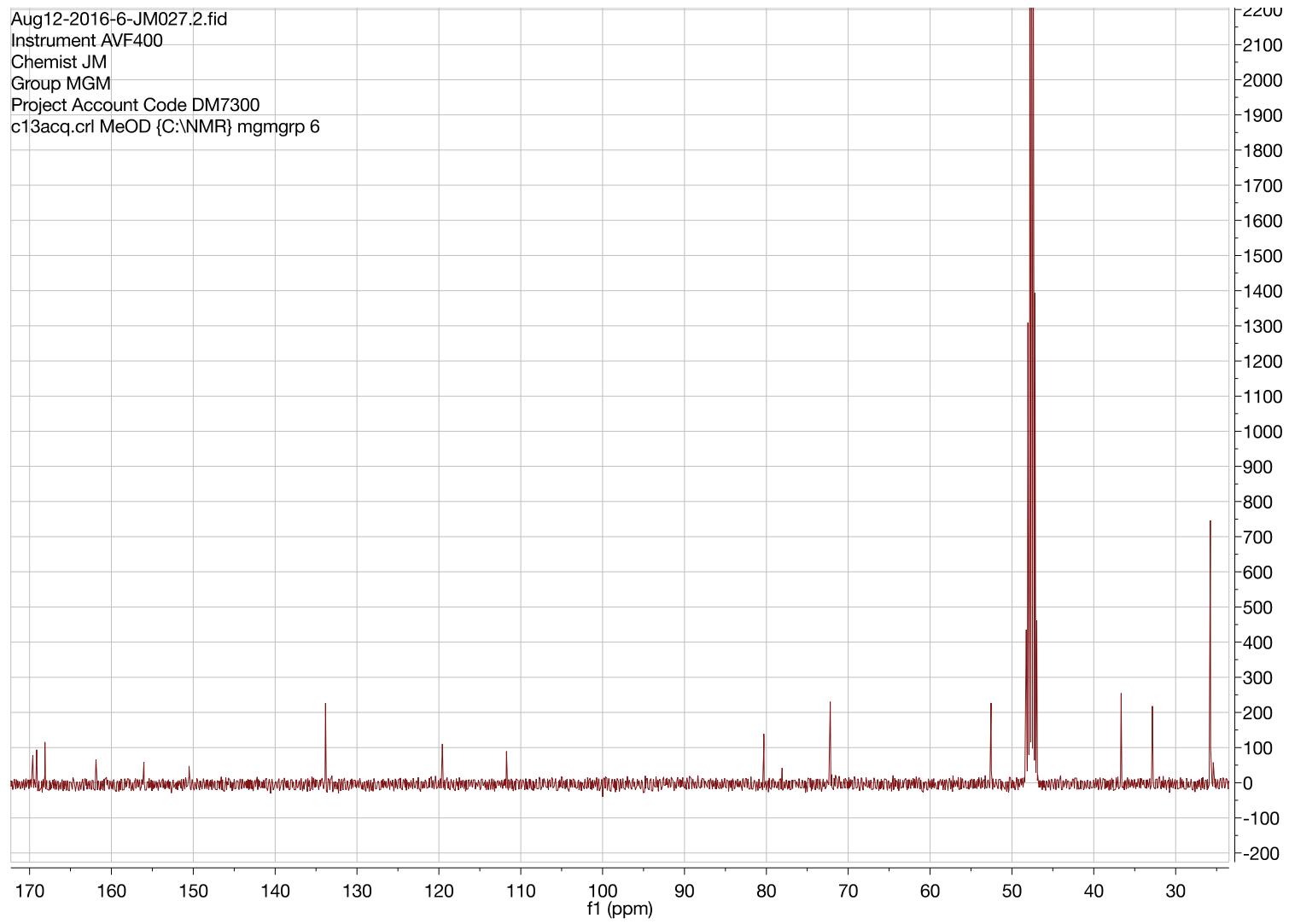
Group MGM

Project Account Code DM7300

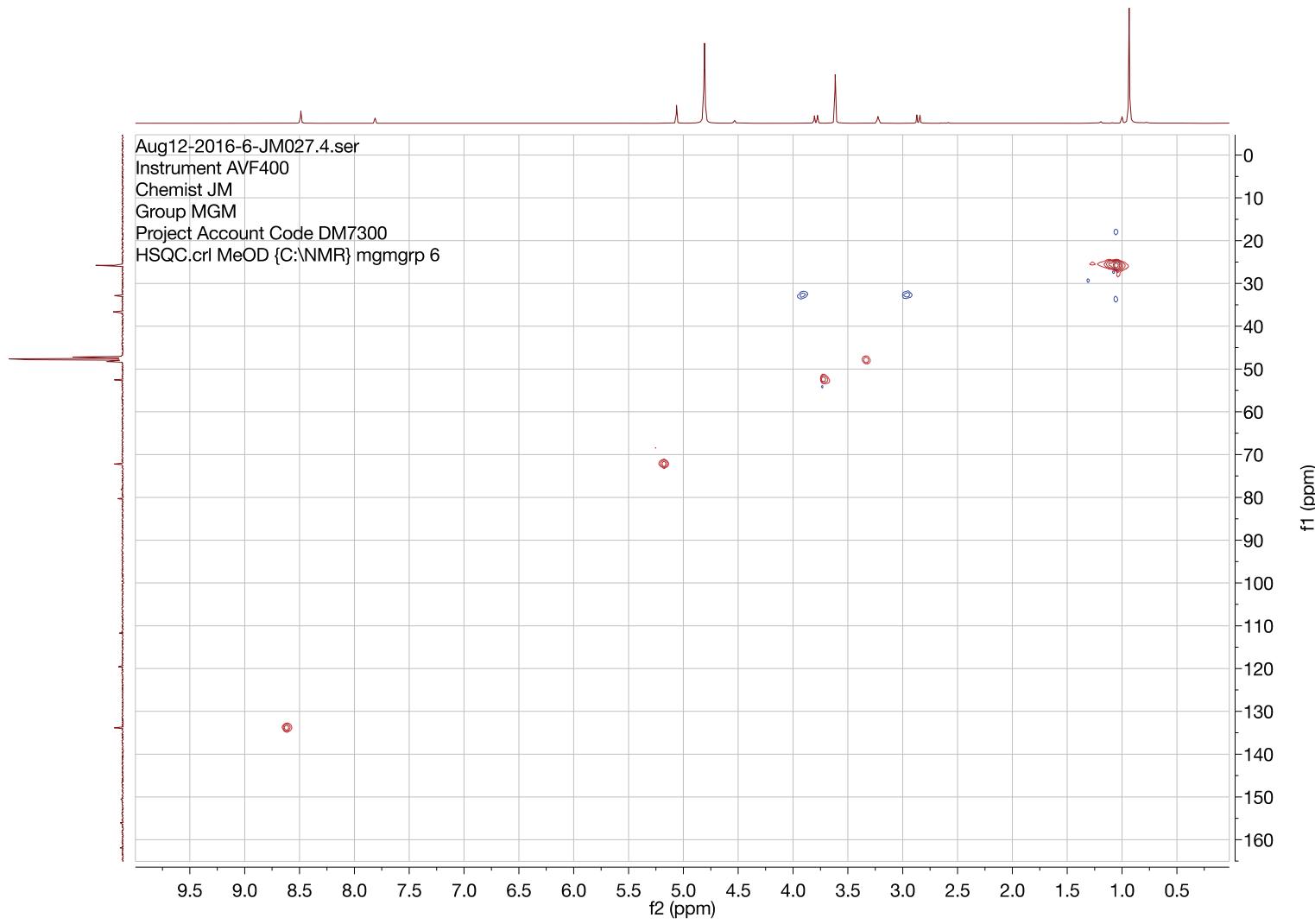
h1acq.crl MeOD {C:\NMR} mgmgrp 6

9j



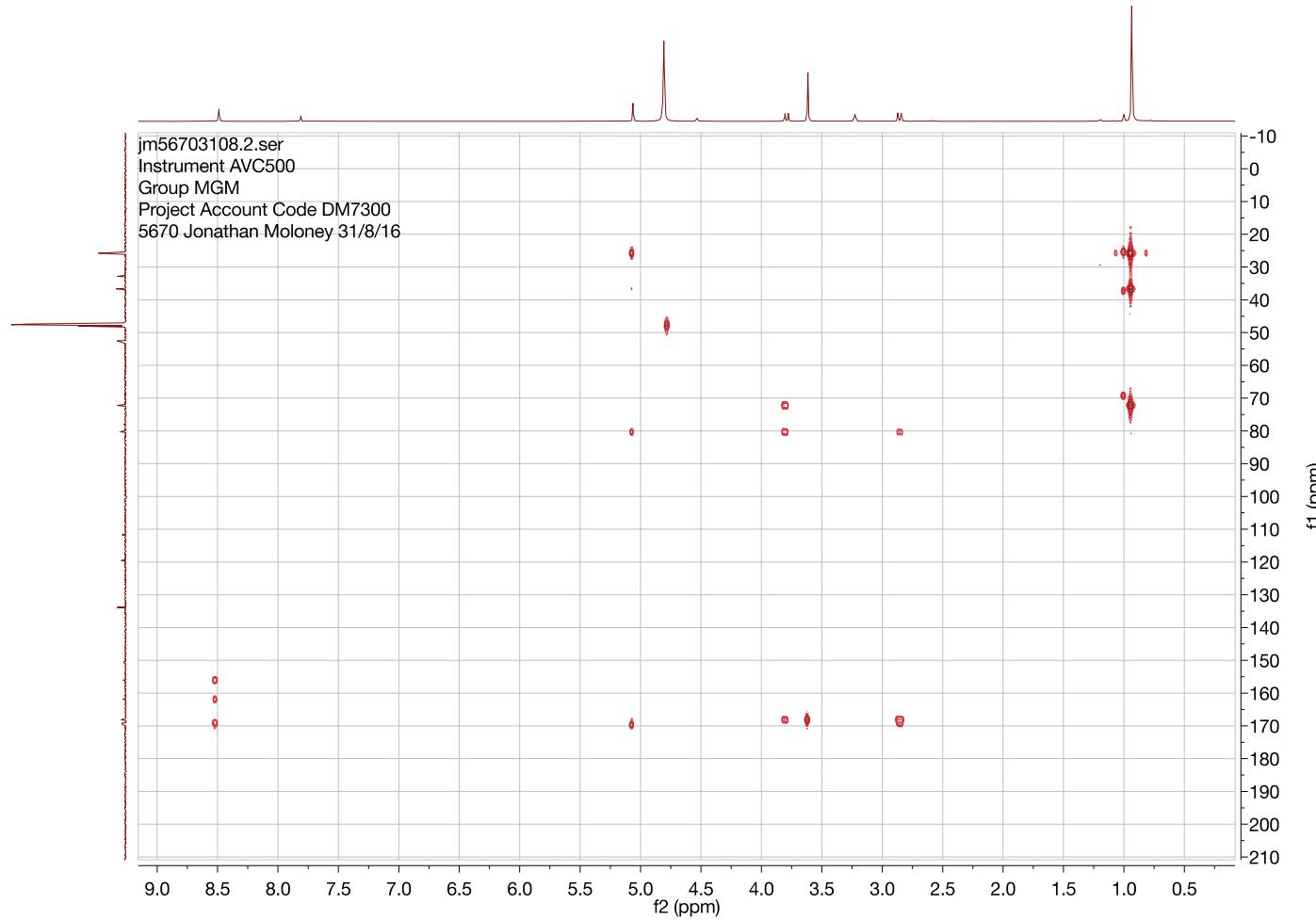


9j



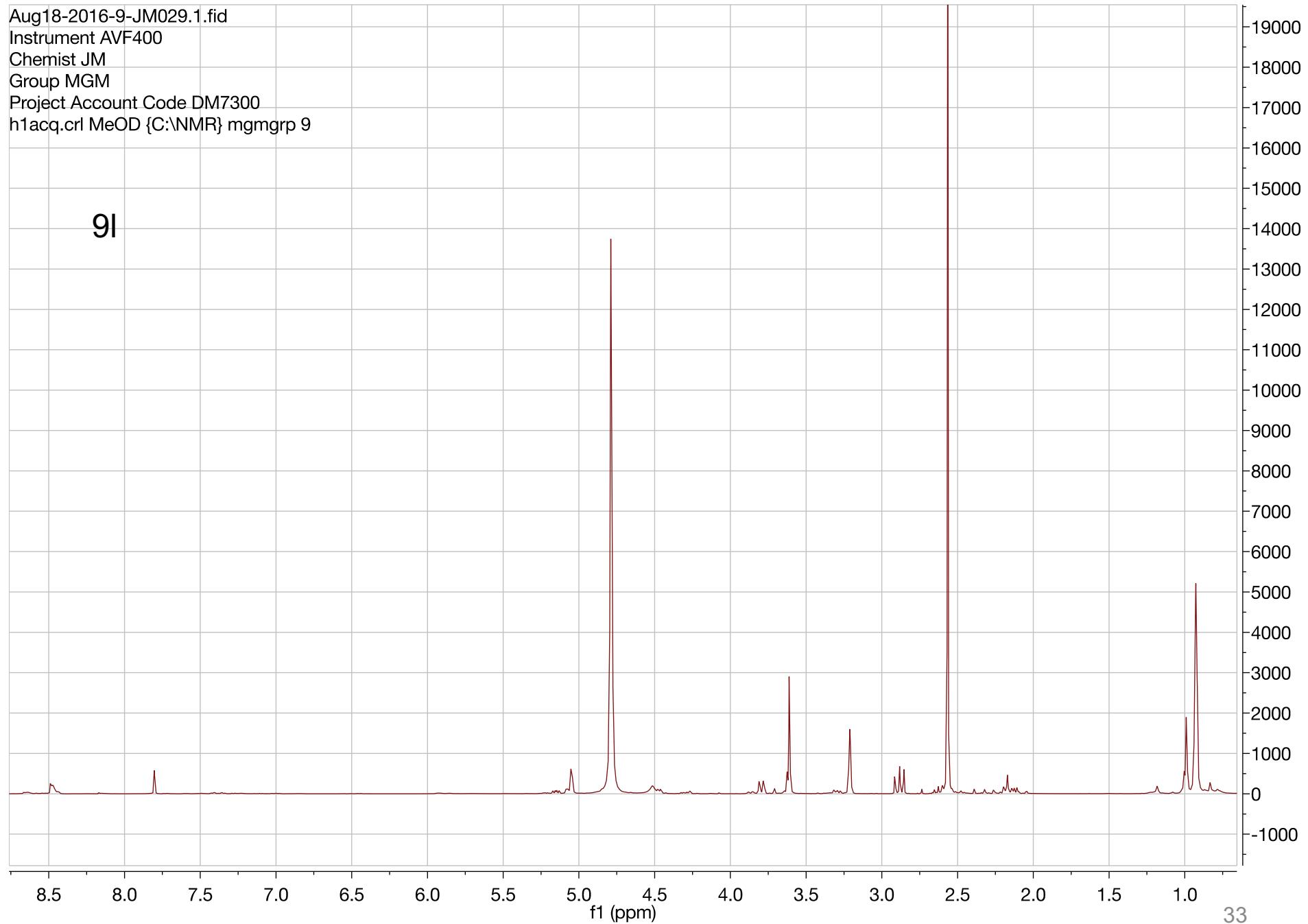
# HMBC

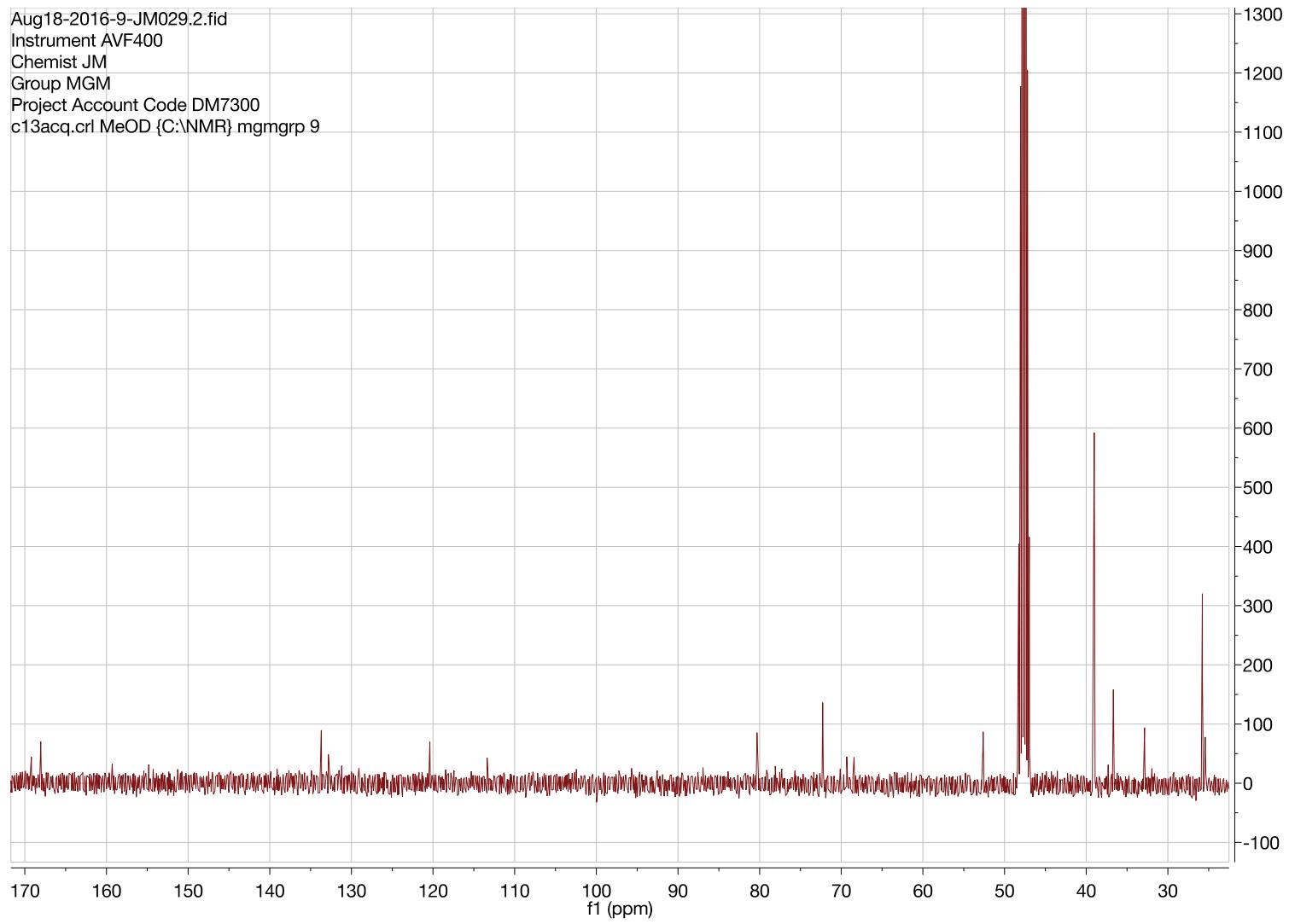
9j



Aug18-2016-9-JM029.1.fid  
Instrument AVF400  
Chemist JM  
Group MGM  
Project Account Code DM7300  
h1acc.crl MeOD {C:\NMR} mgmgrp 9

91





9I

