

# Novel Vulgarin Derivatives: Chemical Transformation, *In Silico* and *In Vitro* Studies

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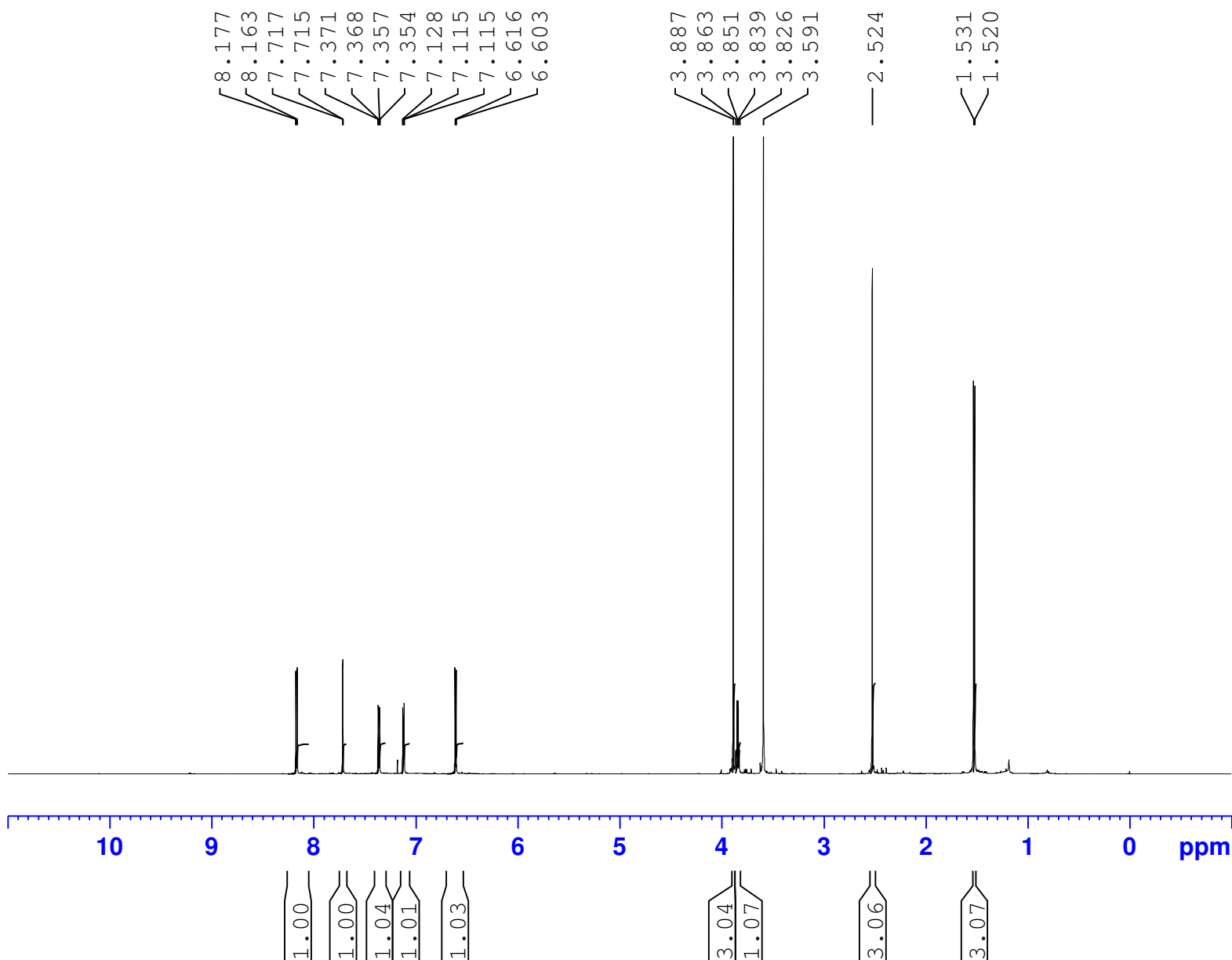
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S1. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of derivative 1

<sup>1</sup>H spectra Dr.Orabi Vul 2 in CDCL3



Current Data Parameters  
NAME Vul2-2D  
EXPNO 1  
PROCNO 1

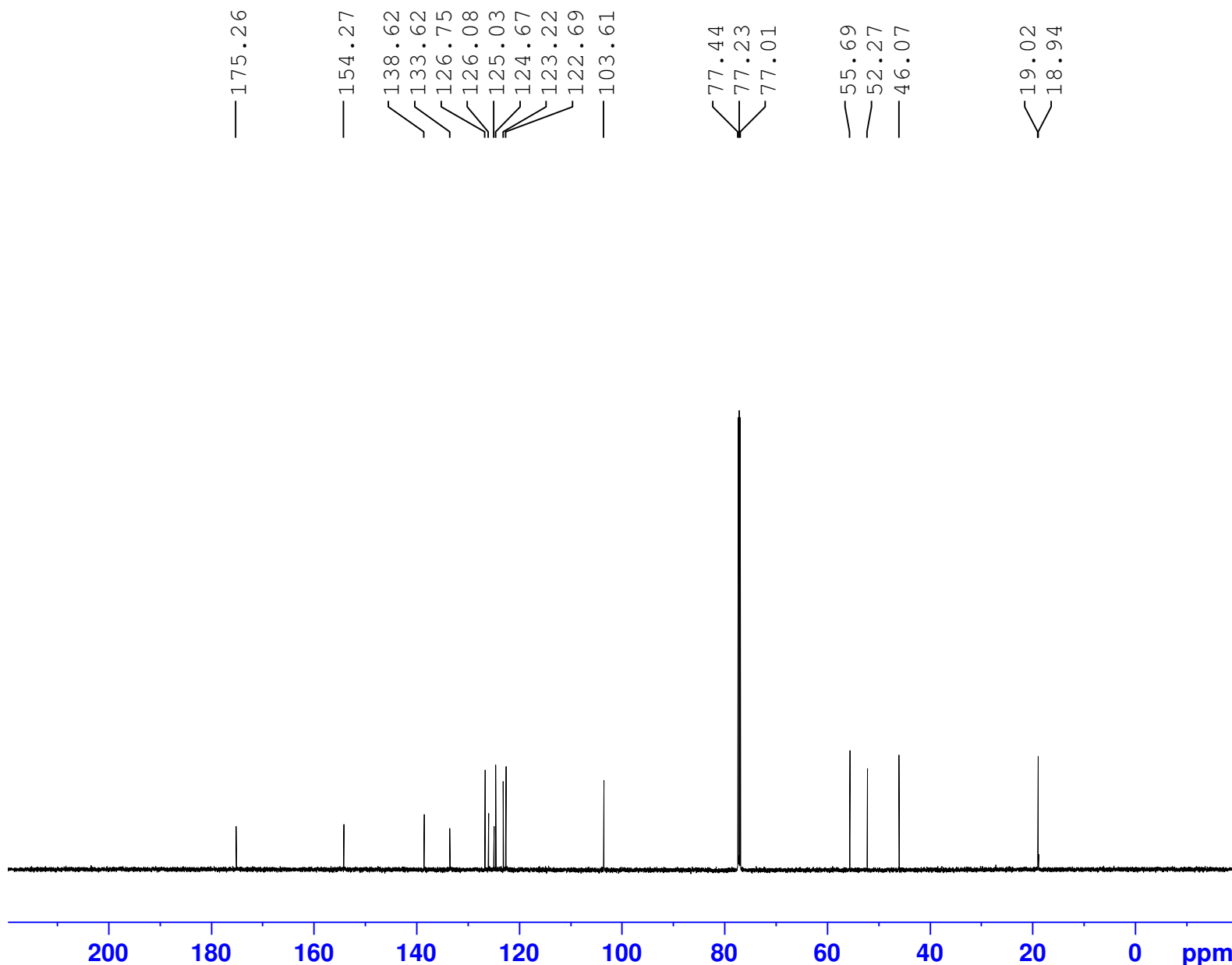
F2 - Acquisition Parameters  
Date\_ 20211025  
Time 10.17  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12335.526 Hz  
FIDRES 0.188225 Hz  
AQ 2.6563926 sec  
RG 203  
DW 40.533 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 600.1337060 MHz  
NUC1 1H  
P1 10.60 usec  
PLW1 27.82500076 W

F2 - Processing parameters  
SI 32768  
SF 600.1300654 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

S2.  $^{13}\text{C}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of derivative 1

$^{13}\text{C}$  decoupled spectra Dr.Orabi Vul-2 in  $\text{CDCl}_3$



Current Data Parameters  
NAME Vul2-2D  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211025  
Time 10.30  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT  $\text{CDCl}_3$   
NS 520  
DS 4  
SWH 36057.691 Hz  
FIDRES 0.550197 Hz  
AQ 0.9087659 sec  
RG 203  
DW 13.867 usec  
DE 50.00 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

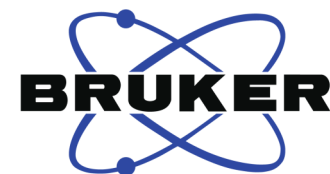
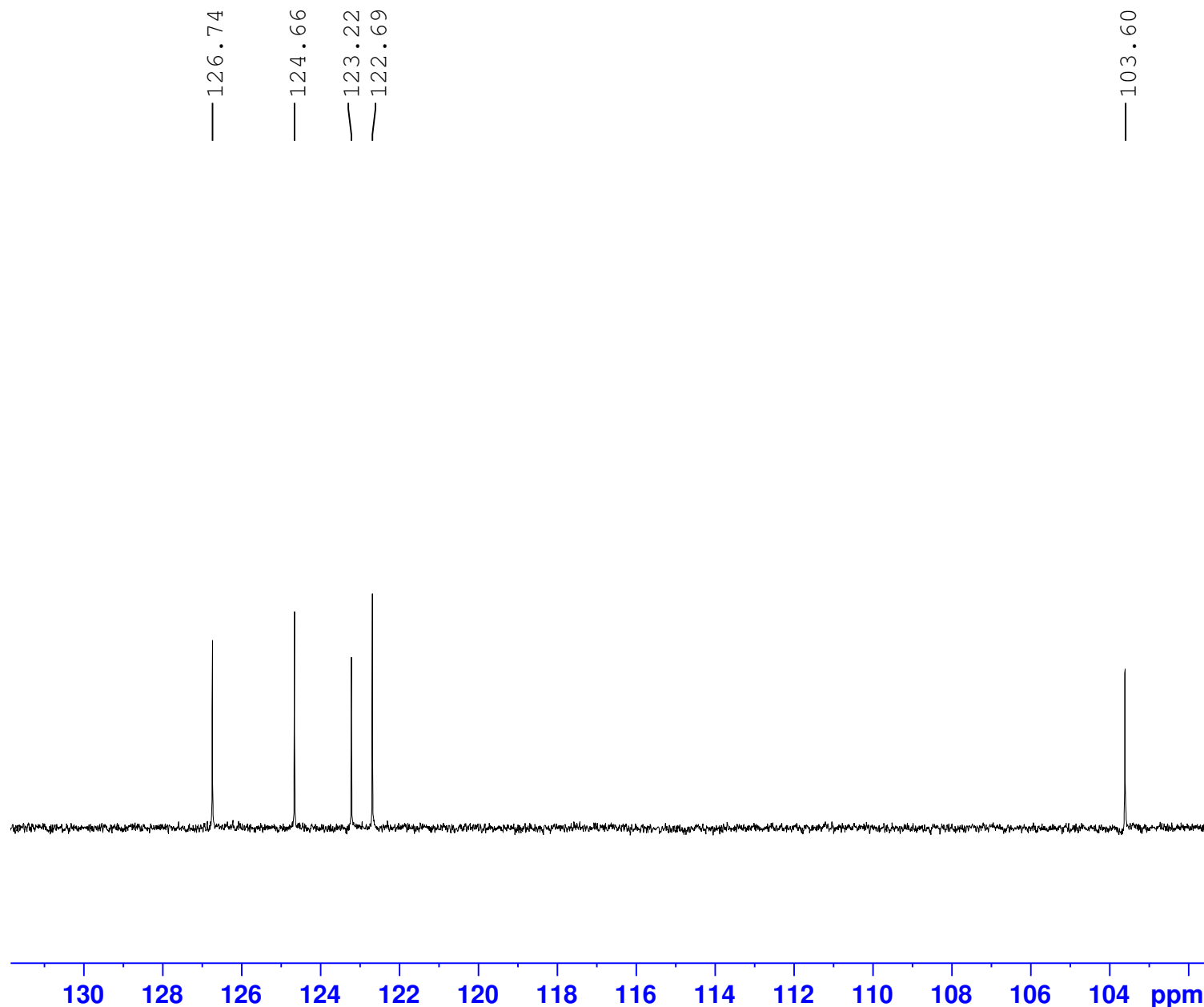
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SFO1 150.9178979 MHz  
NUC1  $^{13}\text{C}$   
P1 8.80 usec  
PLW1 78.13500214 W

===== CHANNEL f2 =====  
SFO2 600.1324005 MHz  
NUC2  $^1\text{H}$   
CPDPRG[2] waltz65  
PCPD2 70.00 usec  
PLW2 27.82500076 W  
PLW12 0.63804001 W  
PLW13 0.32093000 W

F2 - Processing parameters  
SI 32768  
SF 150.9027796 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

# S3. DEPT-135 (600 MHz, CDCl<sub>3</sub>) spectrum of derivative 1

DEPT 135 spectra Dr.Orabi Vul-2 in CDCL3



## Current Data Parameters

NAME Vul2-2D  
EXPNO 5  
PROCNO 1

## F2 - Acquisition Parameters

Date\_ 20211025  
Time 11.45  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG deptsp135  
TD 65536  
SOLVENT CDCL3  
NS 169  
DS 4  
SWH 36057.691 Hz  
FIDRES 0.550197 Hz  
AQ 0.9087659 sec  
RG 203  
DW 13.867 usec  
DE 50.00 usec  
TE 298.0 K  
CNST2 145.0000000  
D1 2.00000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
TD0 1

## ===== CHANNEL f1 =====

SFO1 150.9178979 MHz  
NUC1 13C  
P1 8.80 usec  
P13 2000.00 usec  
PLW0 0 W  
PLW1 78.13500214 W  
SPNAM[5] Crp60comp.4  
SPOAL5 0.500  
SPOFFS5 0 Hz  
SPW5 9.24489975 W

## ===== CHANNEL f2 =====

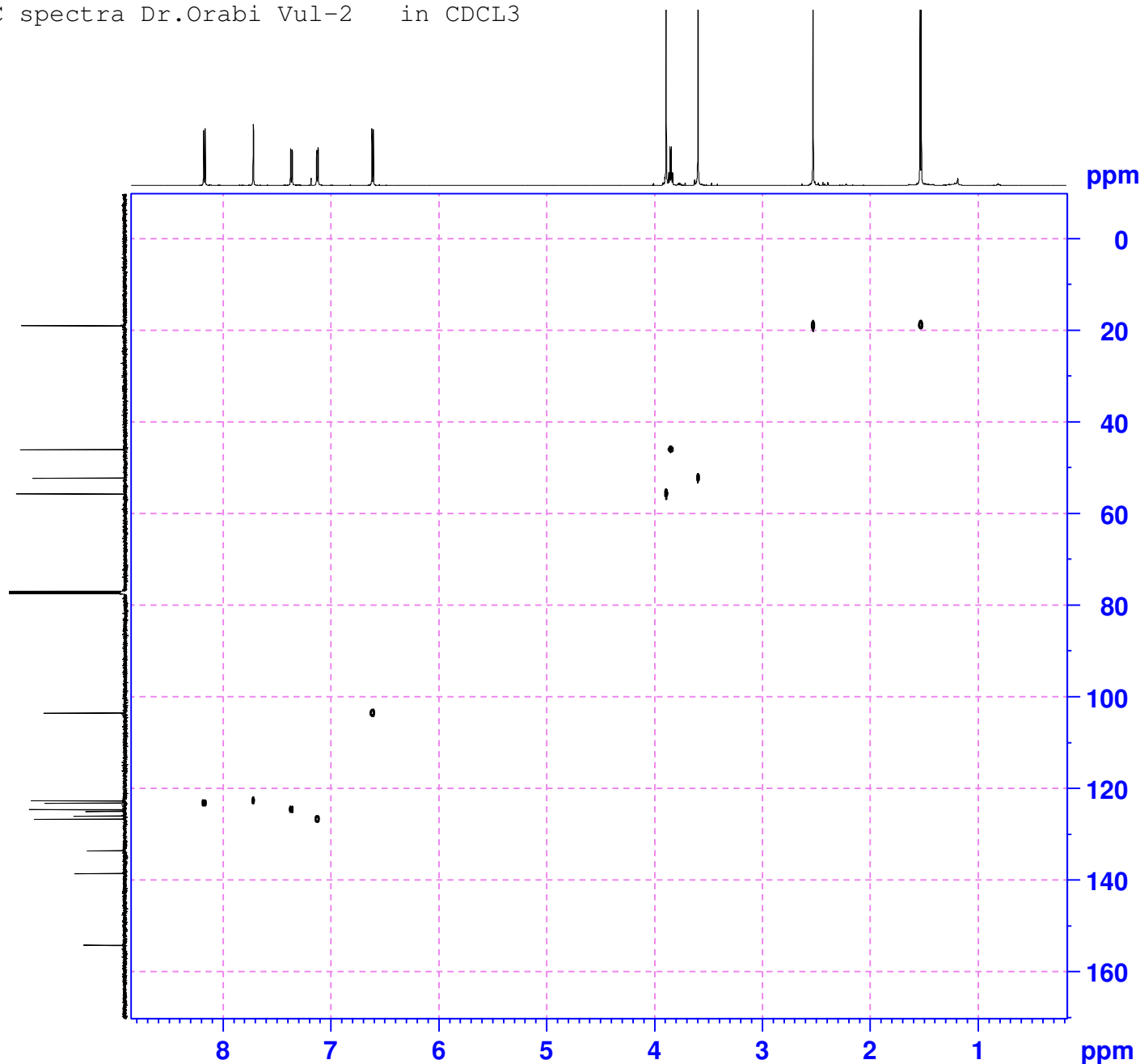
SFO2 600.1324005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
P3 10.60 usec  
P4 21.20 usec  
PCPD2 70.00 usec  
PLW2 27.82500076 W  
PLW12 0.63804001 W

## F2 - Processing parameters

SI 32768  
SF 150.9027803 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

# S4. HSQC (600 MHz, CDCl<sub>3</sub>) spectrum of derivative 1

<sup>13</sup>C HSQC spectra Dr.Orabi Vul-2 in CDCl<sub>3</sub>



Current Data Parameters  
NAME Vul2-2D  
EXPNO 7  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211025  
Time 12.11  
INSTRUM spect  
PROBHD 5 mm FABBO BB-  
PULPROG hsqcetgpgp2  
TD 2048  
SOLVENT CDCl<sub>3</sub>  
NS 4  
DS 16  
SWH 5208.333 Hz  
FIDRES 2.543132 Hz  
AQ 0.1966080 sec  
RG 203  
DW 96.000 usec  
DE 6.50 usec  
TE 298.1 K  
CNST2 145.0000000  
D0 0.00000300 sec  
D1 1.90988803 sec  
D4 0.00172414 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
INO 0.00001840 sec  
ZGPGTNS

===== CHANNEL f1 =====  
SFO1 600.1327722 MHz  
NUC1 1H  
P1 10.60 usec  
P2 21.20 usec  
P28 1000.00 usec  
PLW1 27.82500076 W

===== CHANNEL f2 =====  
SFO2 150.9148803 MHz  
NUC2 13C  
CPDPRG2 gartp4  
P3 8.80 usec  
P14 500.00 usec  
P24 2000.00 usec  
PCPD2 60.00 usec  
PLW0 0 W  
PLW2 78.13500214 W  
PLW12 1.68079996 W  
SPNAM[3] Crp60,0.5,20.1  
SFOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 9.24489975 W  
SPNAM[7] Crp60comp.4  
SFOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 9.24489975 W

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

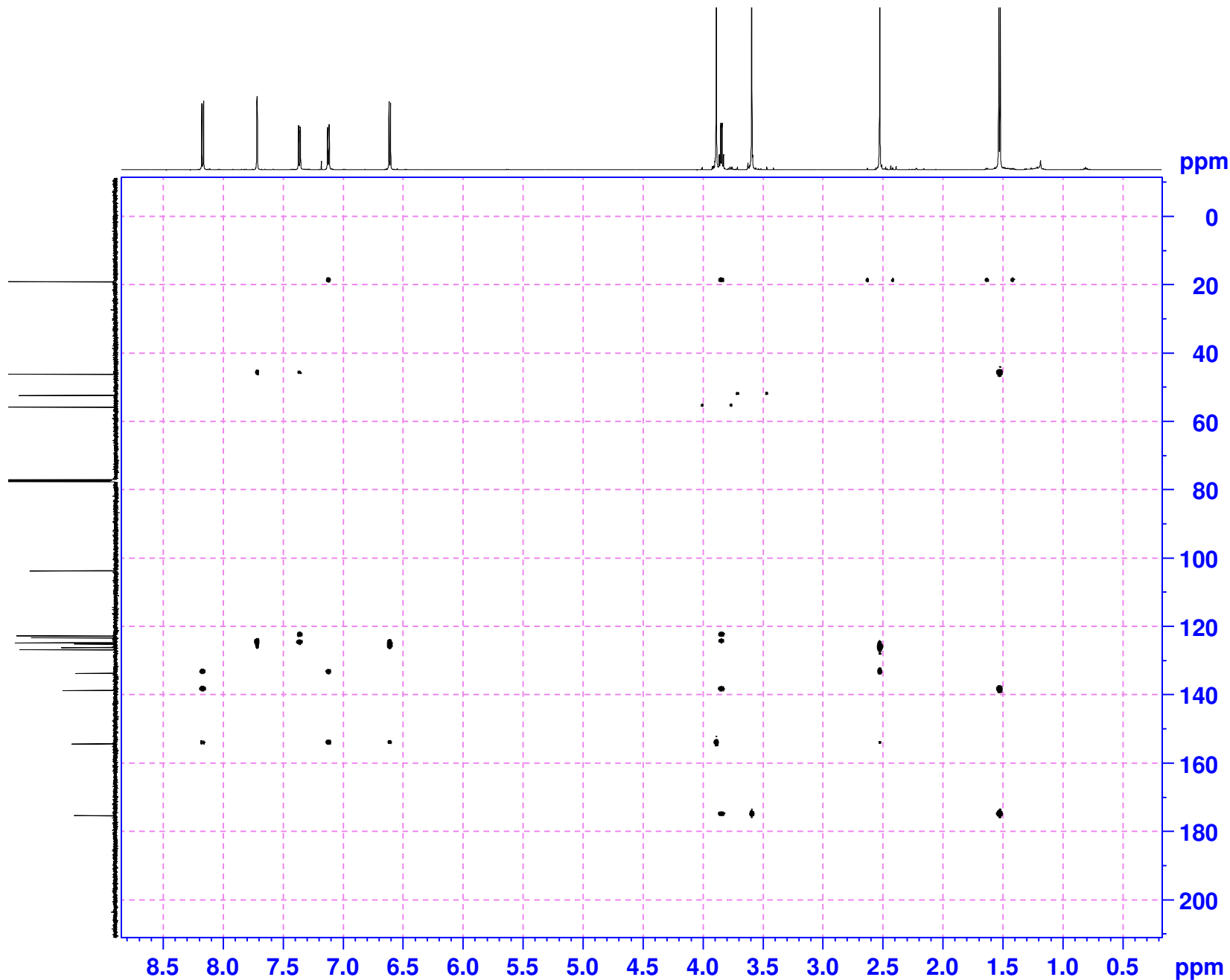
F1 - Acquisition parameters  
TD 187  
SFO1 150.9149 MHz  
FIDRES 145.315048 Hz  
SW 180.061 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 2048  
SF 600.1300640 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 echo-antiecho  
SF 150.9027671 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0

# S5. HMBC (600 MHz, CDCl<sub>3</sub>) spectrum of derivative 1

<sup>13</sup>C HMBC spectra Dr.Orabi Vul-2 in CDCl<sub>3</sub>



Current Data Parameters  
NAME Vul2-2D  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211025  
Time 12.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hmbcetgp12nd  
TD 2048  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 16  
SWH 5208.333 Hz  
FIDRES 2.543132 Hz  
AQ 0.1966080 sec  
RG 203  
DW 96.000 usec  
DE 6.50 usec  
TE 297.9 K  
CNST6 125.0000000  
CNST7 165.0000000  
CNST13 10.0000000  
CNST30 0.5981153  
D0 0.00000300 sec  
D1 1.43446398 sec  
D6 0.05000000 sec  
D16 0.00020000 sec  
INO 0.00001490 sec

===== CHANNEL f1 =====  
SFO1 600.1327722 MHz  
NUC1 1H  
P1 10.60 usec  
P2 21.20 usec  
PLW1 27.82500076 W

===== CHANNEL f2 =====  
SFO2 150.9178738 MHz  
NUC2 13C  
P3 8.80 usec  
P24 2000.00 usec  
PLW2 78.13500214 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 9.24489975 W

===== GRADIENT CHANNEL =====  
GPNAM[1] SINE.100  
GPNAM[3] SINE.100  
GPNAM[4] SINE.100  
GPNAM[5] SINE.100  
GPZ1 80.00 %  
GPZ3 15.00 %  
GPZ4 -10.00 %  
GPZ5 -5.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SFO1 150.9179 MHz  
FIDRES 131.082214 Hz  
SW 222.353 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 2048  
SF 600.1300654 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 512  
MC2 echo-antiecho  
SF 150.9028990 MHz  
WDW SINE  
SSB 2  
LB 0 Hz  
GB 0

# S6. HMBC (600 MHz, CDCl<sub>3</sub>) spectrum of derivative 1

<sup>13</sup>C HMBC spectra Dr.Orabi Vul-2 in CDCl<sub>3</sub>



Current Data Parameters  
NAME Vul2-2D  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211025  
Time 12.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hmbcetgpl2nd  
TD 2048  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 16  
SWH 5208.333 Hz  
FIDRES 2.543132 Hz  
AQ 0.1966080 sec  
RG 203  
DW 96.000 usec  
DE 6.50 usec  
TE 297.9 K  
CNST6 125.0000000  
CNST7 165.0000000  
CNST13 10.0000000  
CNST30 0.5981153  
D0 0.00000300 sec  
D1 1.43446398 sec  
D6 0.05000000 sec  
D16 0.00020000 sec  
IN0 0.00001490 sec

===== CHANNEL f1 =====  
SFO1 600.1327722 MHz  
NUC1 1H  
P1 10.60 usec  
P2 21.20 usec  
PLW1 27.82500076 W

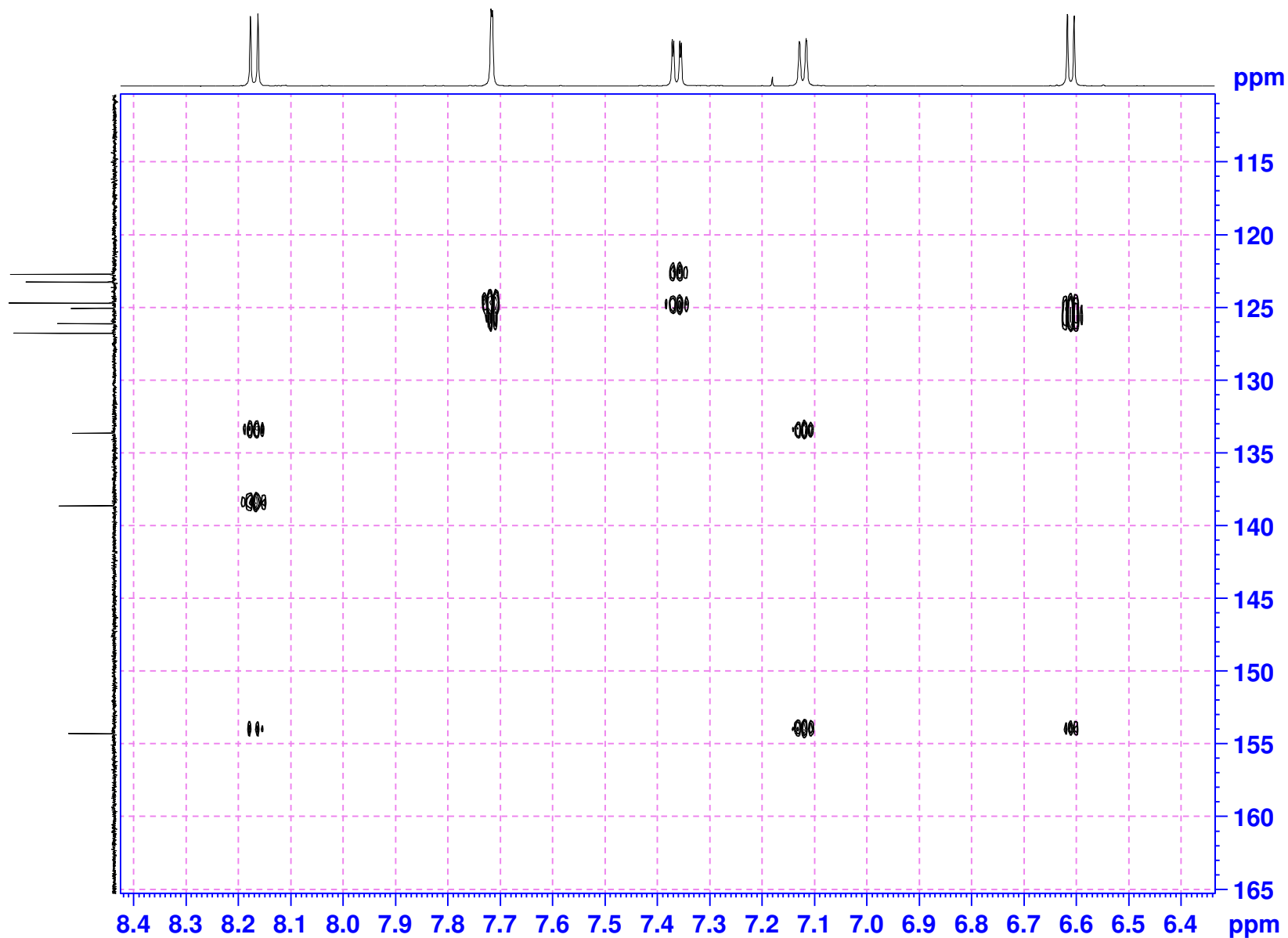
===== CHANNEL f2 =====  
SFO2 150.9178738 MHz  
NUC2 13C  
P3 8.80 usec  
P24 2000.00 usec  
PLW2 78.13500214 W  
SPNAM[7] Crp60comp.4  
SFOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 9.24489975 W

===== GRADIENT CHANNEL =====  
GPNAM[1] SINE.100  
GPNAM[3] SINE.100  
GPNAM[4] SINE.100  
GPNAM[5] SINE.100  
GPZ1 80.00 %  
GPZ3 15.00 %  
GPZ4 -10.00 %  
GPZ5 -5.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SFO1 150.9179 MHz  
FIDRES 131.082214 Hz  
SW 222.353 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 2048  
SF 600.1300654 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 512  
MC2 echo-antiecho  
SF 150.9028090 MHz  
WDW SINE  
SSB 2  
LB 0 Hz  
GB 0



# S7. COSY (600 MHz, CDCl<sub>3</sub>) spectrum of derivative 1

COSY spectra Dr.Orabi Vul-2 in CDCl<sub>3</sub>



Current Data Parameters  
NAME Vul2-2D  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211025  
Time 11.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG cosygpppgf  
TD 2048  
SOLVENT CDCl<sub>3</sub>  
NS 4  
DS 8  
SWH 5102.041 Hz  
FIDRES 2.491231 Hz  
AQ 0.2007040 sec  
RG 90.5  
DW 98.000 usec  
DE 6.50 usec  
TE 298.0 K  
D0 0.00000300 sec  
D1 0.67709088 sec  
D11 0.03000000 sec  
D12 0.00002000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00019600 sec

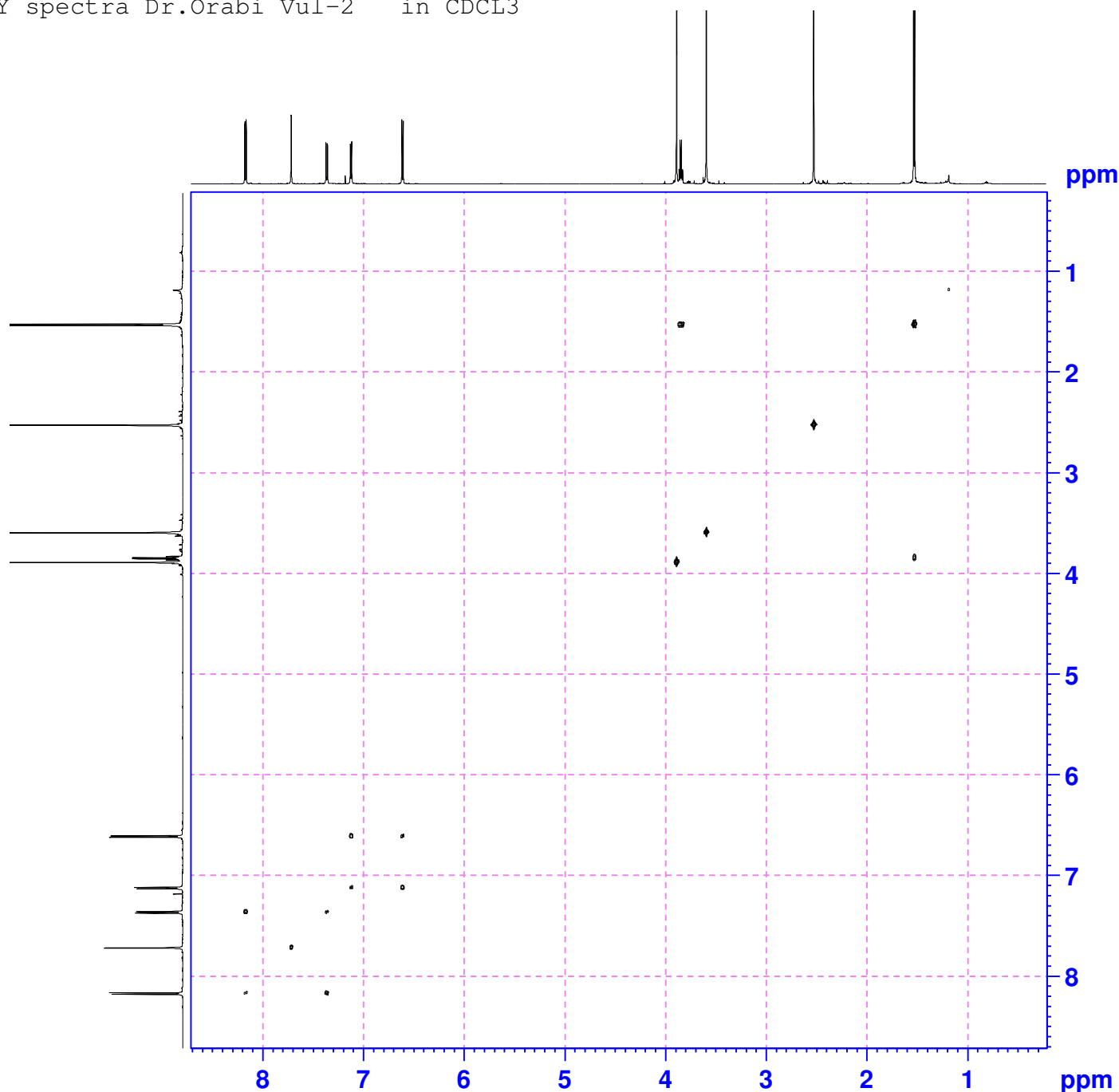
===== CHANNEL f1 =====  
SFO1 600.1327447 MHz  
NUC1 1H  
P0 10.60 usec  
P1 10.60 usec  
P17 2500.00 usec  
PLW1 27.82500076 W  
PLW10 5.00229979 W

===== GRADIENT CHANNEL =====  
GPNAM[1] SINE.100  
GPZ1 20.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 320  
SFO1 600.1327 MHz  
FIDRES 15.943877 Hz  
SW 8.502 ppm  
FnMODE QF

F2 - Processing parameters  
SI 2048  
SF 600.1300658 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 2048  
MC2 QF  
SF 600.1300653 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



S8.  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of derivative 2

$^1\text{H}$  spectra Dr.Orabi Vul 3 in  $\text{CDCl}_3$

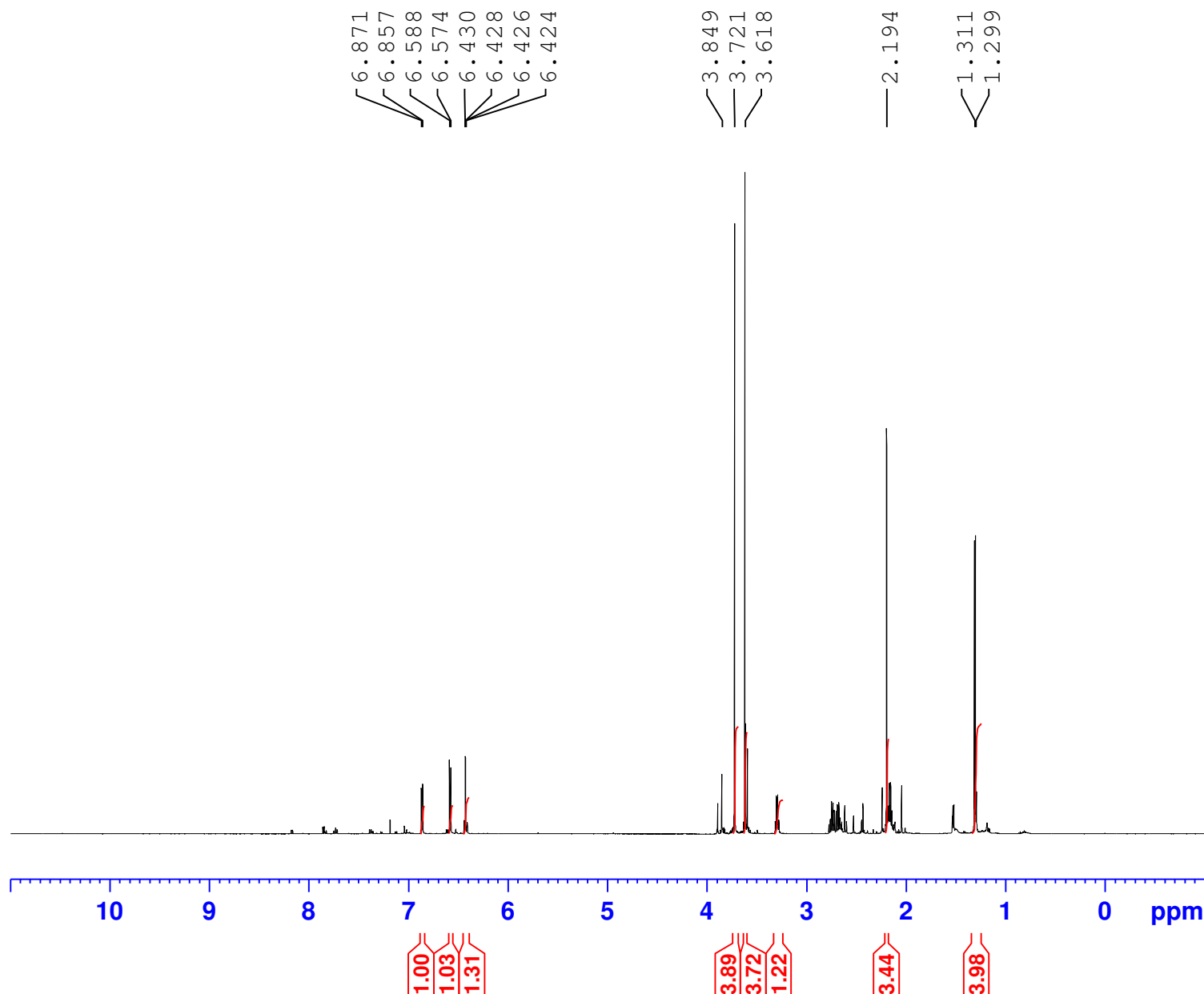


Current Data Parameters  
NAME Vul3-2D  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211025  
Time 14.42  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT  $\text{CDCl}_3$   
NS 16  
DS 2  
SWH 12335.526 Hz  
FIDRES 0.188225 Hz  
AQ 2.6563926 sec  
RG 203  
DW 40.533 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 600.1337060 MHz  
NUC1  $^1\text{H}$   
P1 10.60 usec  
PLW1 27.82500076 W

F2 - Processing parameters  
SI 32768  
SF 600.1300629 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



S9.  $^{13}\text{C}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of derivative 2

$^{13}\text{C}$  decoupled spectra Dr.Orabi Vul-3 in  $\text{CDCl}_3$



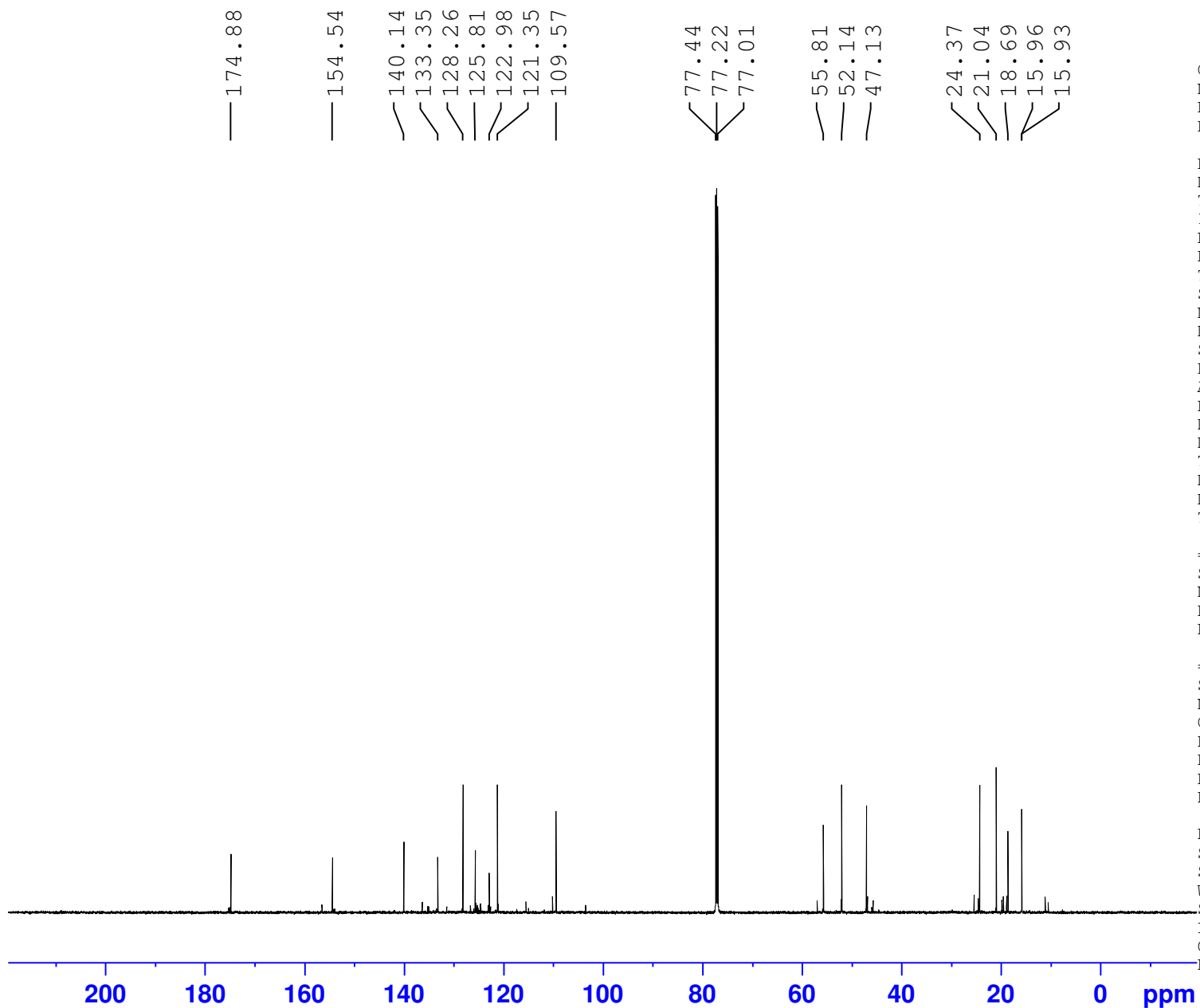
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NAME Vul3-2D  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211025  
Time 19.22  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT  $\text{CDCl}_3$   
NS 5120  
DS 4  
SWH 36057.691 Hz  
FIDRES 0.550197 Hz  
AQ 0.9087659 sec  
RG 203  
DW 13.867 usec  
DE 50.00 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 150.9178979 MHz  
NUC1  $^{13}\text{C}$   
P1 8.80 usec  
PLW1 78.13500214 W

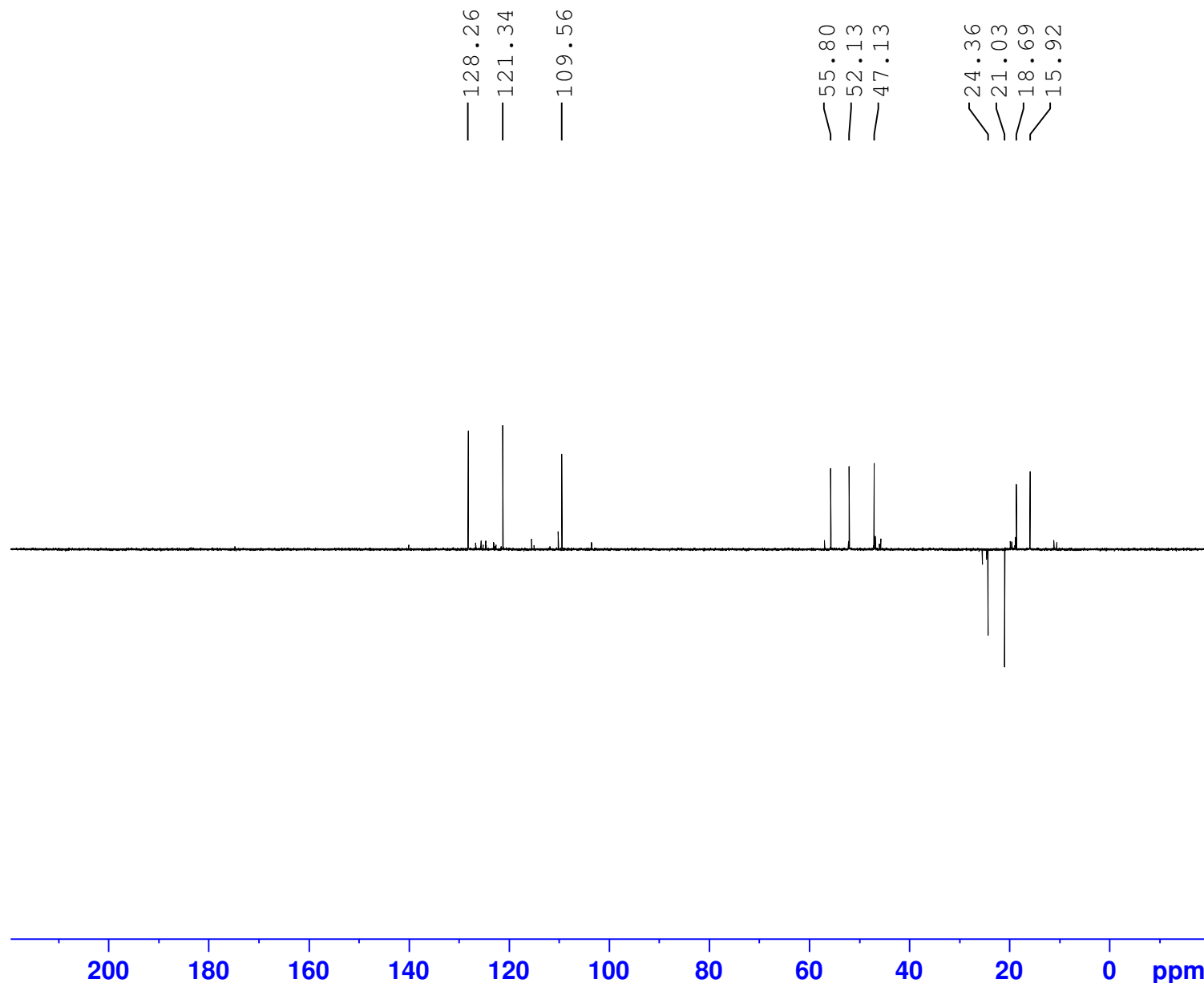
===== CHANNEL f2 =====  
SFO2 600.1324005 MHz  
NUC2  $^1\text{H}$   
CPDPRG[2] waltz65  
PCPD2 70.00 usec  
PLW2 27.82500076 W  
PLW12 0.63804001 W  
PLW13 0.32093000 W

F2 - Processing parameters  
SI 32768  
SF 150.9027795 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 2.00



# S10. DEPT-135 (600 MHz, CDCl<sub>3</sub>) spectrum of derivative 2

DEPT 135 spectra Dr.Orabi Vul-3 in CDCl<sub>3</sub>



Current Data Parameters  
NAME Vul3-2D  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211026  
Time 0.34  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG deptsp135  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 2048  
DS 4  
SWH 36057.691 Hz  
FIDRES 0.550197 Hz  
AQ 0.9087659 sec  
RG 203  
DW 13.867 usec  
DE 50.00 usec  
TE 298.0 K  
CNST2 145.0000000  
D1 2.00000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
TD0 1

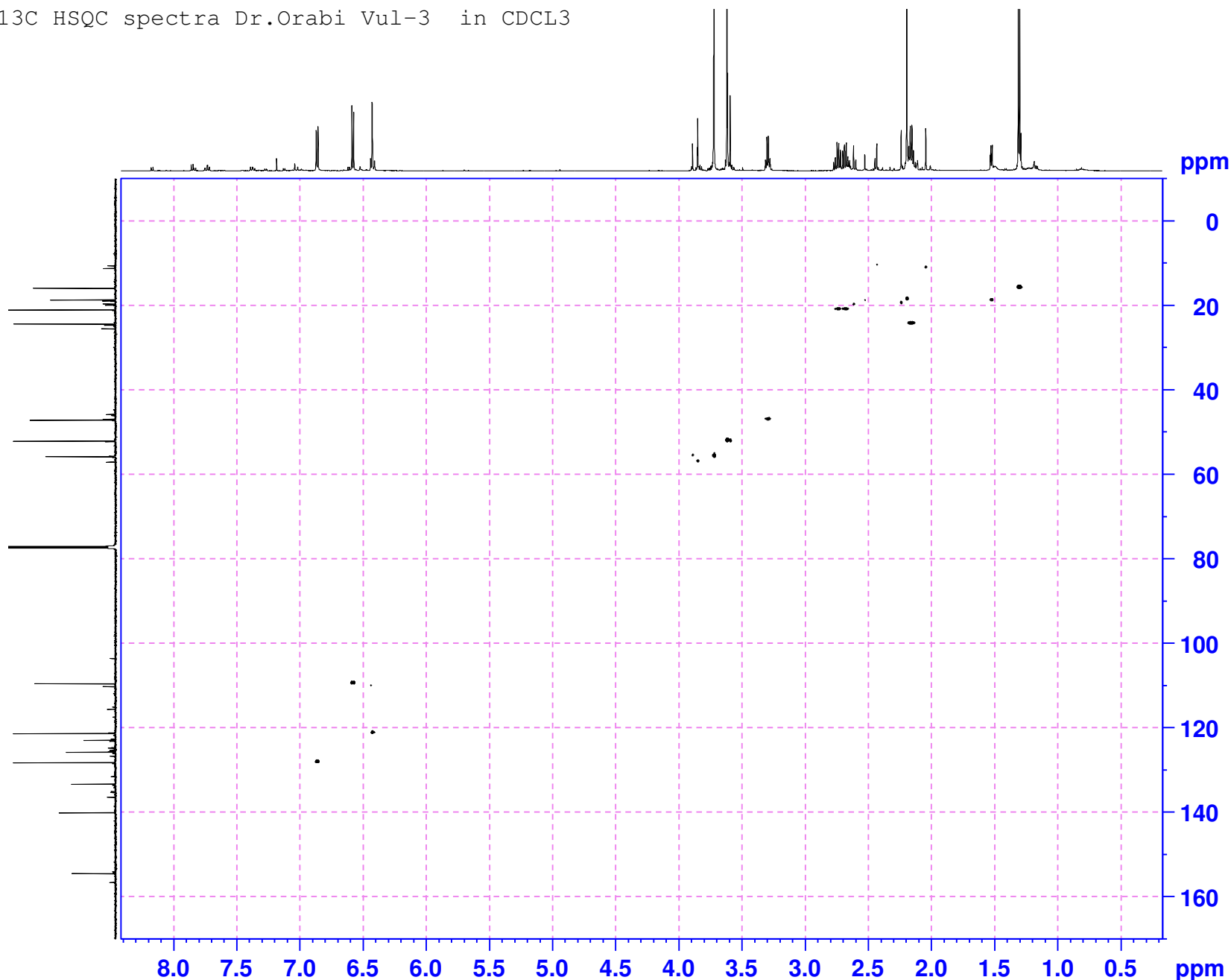
===== CHANNEL f1 =====  
SFO1 150.9178979 MHz  
NUC1 13C  
P1 8.80 usec  
P13 2000.00 usec  
PLW0 0 W  
PLW1 78.13500214 W  
SPNAM[5] Crp60comp.4  
SPOAL5 0.500  
SPOFFS5 0 Hz  
SPW5 9.24489975 W

===== CHANNEL f2 =====  
SFO2 600.1324005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
P3 10.60 usec  
P4 21.20 usec  
PCPD2 70.00 usec  
PLW2 27.82500076 W  
PLW12 0.63804001 W

F2 - Processing parameters  
SI 32768  
SF 150.9027805 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 3.00

# S11. HSQC (600 MHz, CDCl<sub>3</sub>) spectrum of derivative 2

<sup>13</sup>C HSQC spectra Dr.Orabi Vul-3 in CDCl<sub>3</sub>



Current Data Parameters  
NAME Vul3-2D  
EXPNO 7  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211026  
Time\_ 1.01  
INSTRUM spect  
PROBHD 5 mm FABBO BB-  
PULPROG hsqcetgpsp.2  
TD 2048  
SOLVENT CDCl<sub>3</sub>  
NS 8  
DS 16  
SWH 4950.495 Hz  
FIDRES 2.417234 Hz  
AQ 0.2068480 sec  
RG 203  
DW 101.000 usec  
DE 6.50 usec  
TE 298.1 K  
CNST2 145.0000000  
D0 0.00000300 sec  
D1 1.89964795 sec  
D4 0.00172414 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
IN0 0.00001840 sec  
ZGPTNS

===== CHANNEL f1 =====  
SFO1 600.1326395 MHz  
NUC1 1H  
P1 10.60 usec  
P2 21.20 usec  
P28 1000.00 usec  
PLW1 27.82500076 W

===== CHANNEL f2 =====  
SFO2 150.9148803 MHz  
NUC2 13C  
CPDPRG2 garp4  
P3 8.80 usec  
P14 500.00 usec  
P24 2000.00 usec  
PCPD2 60.00 usec  
PLW0 0 W  
PLW2 78.13500214 W  
PLW12 1.68079996 W  
SPNAM[3] Crp60,0.5,20.1  
SPOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 9.24489975 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 9.24489975 W

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

F1 - Acquisition parameters  
TD 512  
SFO1 150.9149 MHz  
FIDRES 53.074047 Hz  
SW 180.061 ppm  
FMODE Echo-Antiecho

F2 - Processing parameters  
SI 2048  
SF 600.1300629 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 echo-antiecho  
SF 150.9028090 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0

# S12. HMBC (600 MHz, CDCl<sub>3</sub>) spectrum of derivative 2

<sup>13</sup>C HMBC spectra Dr.Orabi Vul-3 in CDCl<sub>3</sub>



Current Data Parameters  
NAME Vul3-2D  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211026  
Time 3.30  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hmbcetgp12nd  
TD 2048  
SOLVENT CDCl<sub>3</sub>  
NS 32  
DS 16  
SWH 4950.495 Hz  
FIDRES 2.417234 Hz  
AQ 0.2068480 sec  
RG 203  
DW 101.000 usec  
DE 6.50 usec  
TE 298.0 K  
CNST6 125.0000000  
CNST7 165.0000000  
CNST13 10.0000000  
CNST30 0.5981153  
D0 0.00000300 sec  
D1 1.42422402 sec  
D6 0.05000000 sec  
D16 0.00020000 sec  
IN0 0.00001490 sec

===== CHANNEL f1 =====  
SFO1 600.1326395 MHz  
NUC1 1H  
P1 10.60 usec  
P2 21.20 usec  
PLW1 27.82500076 W

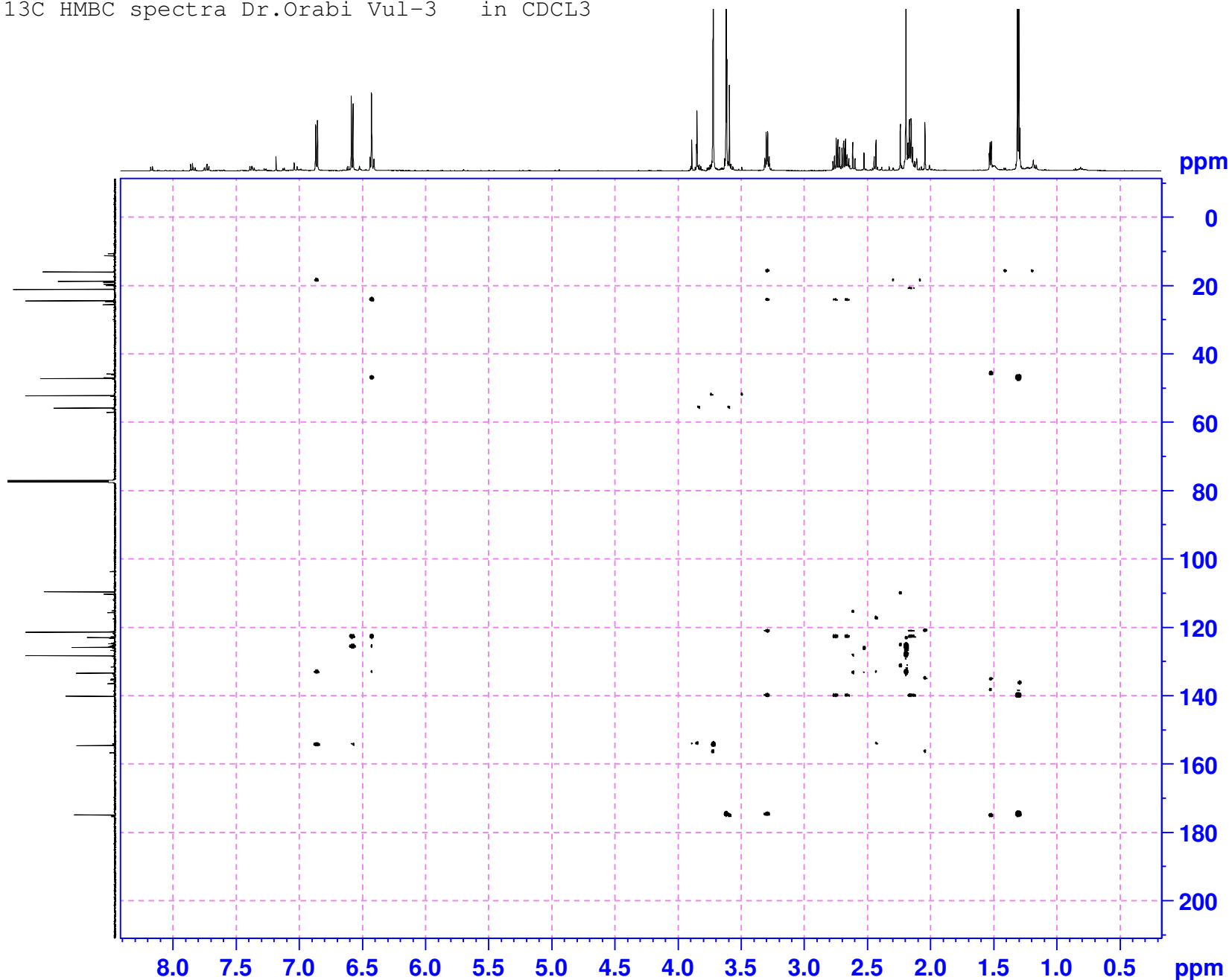
===== CHANNEL f2 =====  
SFO2 150.9178738 MHz  
NUC2 13C  
P3 8.80 usec  
P24 2000.00 usec  
PLW2 78.13500214 W  
SPNAM[7] Crp60comp.4  
SFOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 9.24489975 W

===== GRADIENT CHANNEL =====  
GPNAM[1] SINE.100  
GPNAM[3] SINE.100  
GPNAM[4] SINE.100  
GPNAM[5] SINE.100  
GPZ1 80.00 %  
GPZ3 15.00 %  
GPZ4 -10.00 %  
GPZ5 -5.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SFO1 150.9179 MHz  
FIDRES 131.082214 Hz  
SW 222.353 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 2048  
SF 600.1300629 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 512  
MC2 echo-antiecho  
SF 150.9028090 MHz  
WDW SINE  
SSB 2  
LB 0 Hz  
GB 0



# S13. HMBC (600 MHz, CDCl<sub>3</sub>) spectrum of derivative 2

<sup>13</sup>C HMBC spectra Dr.Orabi Vul-3 in CDCl<sub>3</sub>



Current Data Parameters  
NAME Vul3-2D  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211026  
Time 3.30  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hmbcetgp12nd  
TD 2048  
SOLVENT CDCl<sub>3</sub>  
NS 32  
DS 16  
SWH 4950.495 Hz  
FIDRES 2.417234 Hz  
AQ 0.2068480 sec  
RG 203  
DW 101.000 usec  
DE 6.50 usec  
TE 298.0 K  
CNST6 125.0000000  
CNST7 165.0000000  
CNST13 10.0000000  
CNST30 0.5981153  
D0 0.00000300 sec  
D1 1.42422402 sec  
D6 0.05000000 sec  
D16 0.00020000 sec  
IN0 0.00001490 sec

===== CHANNEL f1 =====  
SFO1 600.1326395 MHz  
NUC1 1H  
P1 10.60 usec  
P2 21.20 usec  
PLW1 27.82500076 W

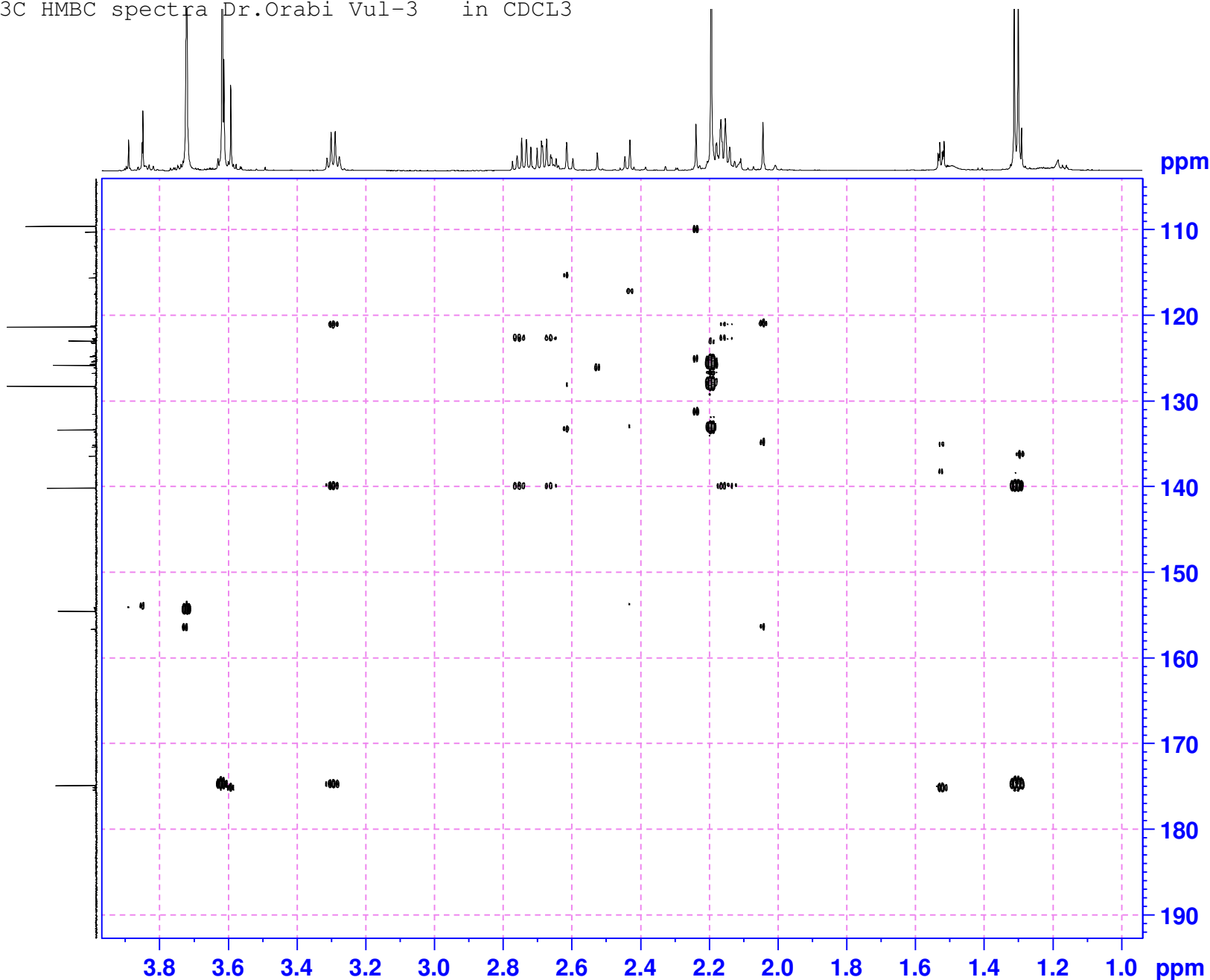
===== CHANNEL f2 =====  
SFO2 150.9178738 MHz  
NUC2 13C  
P3 8.80 usec  
P24 2000.00 usec  
PLW2 78.13500214 W  
SPNAM[7] Crp60comp.4  
SFOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 9.24489975 W

===== GRADIENT CHANNEL =====  
GPNAM[1] SINE.100  
GPNAM[3] SINE.100  
GPNAM[4] SINE.100  
GPNAM[5] SINE.100  
GPZ1 80.00 %  
GPZ3 15.00 %  
GPZ4 -10.00 %  
GPZ5 -5.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SFO1 150.9179 MHz  
FIDRES 131.082214 Hz  
SW 222.353 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 2048  
SF 600.1300629 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 512  
MC2 echo-antiecho  
SF 150.9028090 MHz  
WDW SINE  
SSB 2  
LB 0 Hz  
GB 0



# S14. COSY (600 MHz, CDCl<sub>3</sub>) spectrum of derivative 2

COSY spectra Dr.Orabi Vul-3 in CDCl<sub>3</sub>



Current Data Parameters  
NAME Vul3-2D  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211026  
Time 0.36  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG cosygpppgf  
TD 2048  
SOLVENT CDCl<sub>3</sub>  
NS 4  
DS 8  
SWH 4950.495 Hz  
FIDRES 2.417234 Hz  
AQ 0.2068480 sec  
RG 90.5  
DW 101.000 usec  
DE 6.50 usec  
TE 297.9 K  
D0 0.00000300 sec  
D1 0.67094702 sec  
D11 0.03000000 sec  
D12 0.00002000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
INO 0.00020200 sec

===== CHANNEL f1 =====  
SF01 600.1326237 MHz  
NUC1 1H  
P0 10.60 usec  
P1 10.60 usec  
P17 2500.00 usec  
PLW1 27.82500076 W  
PLW10 5.00229979 W

===== GRADIENT CHANNEL =====  
GPNAM[1] SINE.100  
GPZ1 20.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 320  
SF01 600.1326 MHz  
FIDRES 15.470297 Hz  
SW 8.249 ppm  
FnMODE QF

F2 - Processing parameters  
SI 2048  
SF 600.1300618 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 2048  
MC2 QF  
SF 600.1300594 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

