

# Supporting Information-II

Copies of HR-ESIMS, 1D and 2D NMR spectra of compounds **1–4**.

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# HR-ESIMS for compound 1

## Mass Spectrum SmartFormula Report

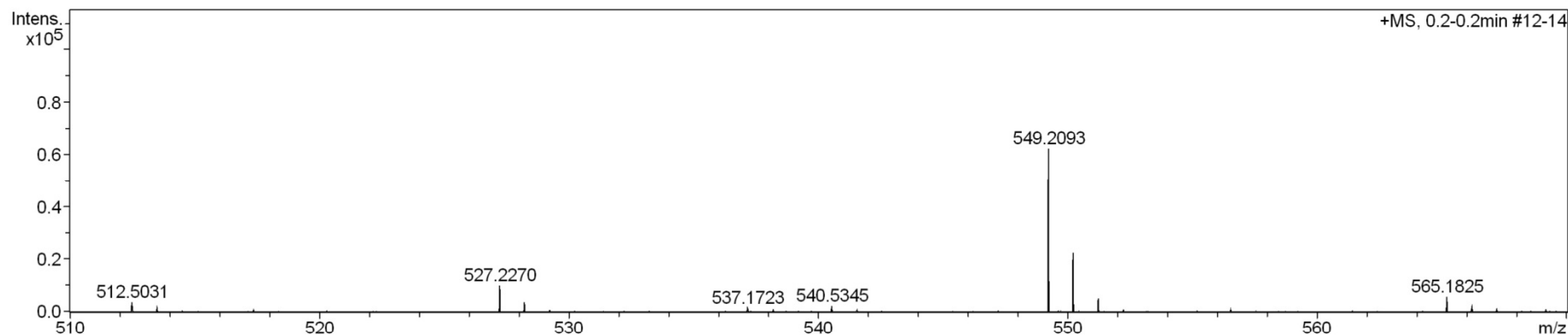
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 Sample Name liwanshan\_23-6\_pos  
 Comment

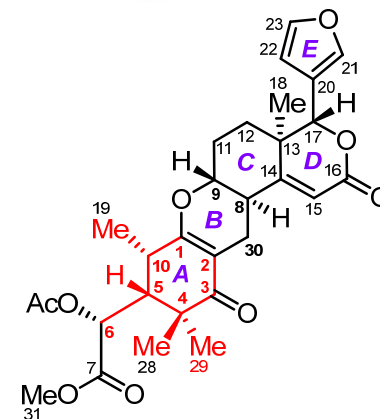
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 Operator SCSIO  
 Instrument maXis 255552.00029

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Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
527.2270	1	C29H35O9	100.00	527.2276	-1.1	-0.6	24.2	12.5	even	ok
549.2093	1	C29H34NaO9	100.00	549.2095	0.4	0.2	22.7	12.5	even	ok
1053.4473	1	C58H69O18	100.00	1053.4478	0.5	0.5	60.3	24.5	even	ok
1075.4289	1	C58H68NaO18	100.00	1075.4298	-0.9	-0.9	68.6	24.5	even	ok



# HR-ESIMS for compound 1

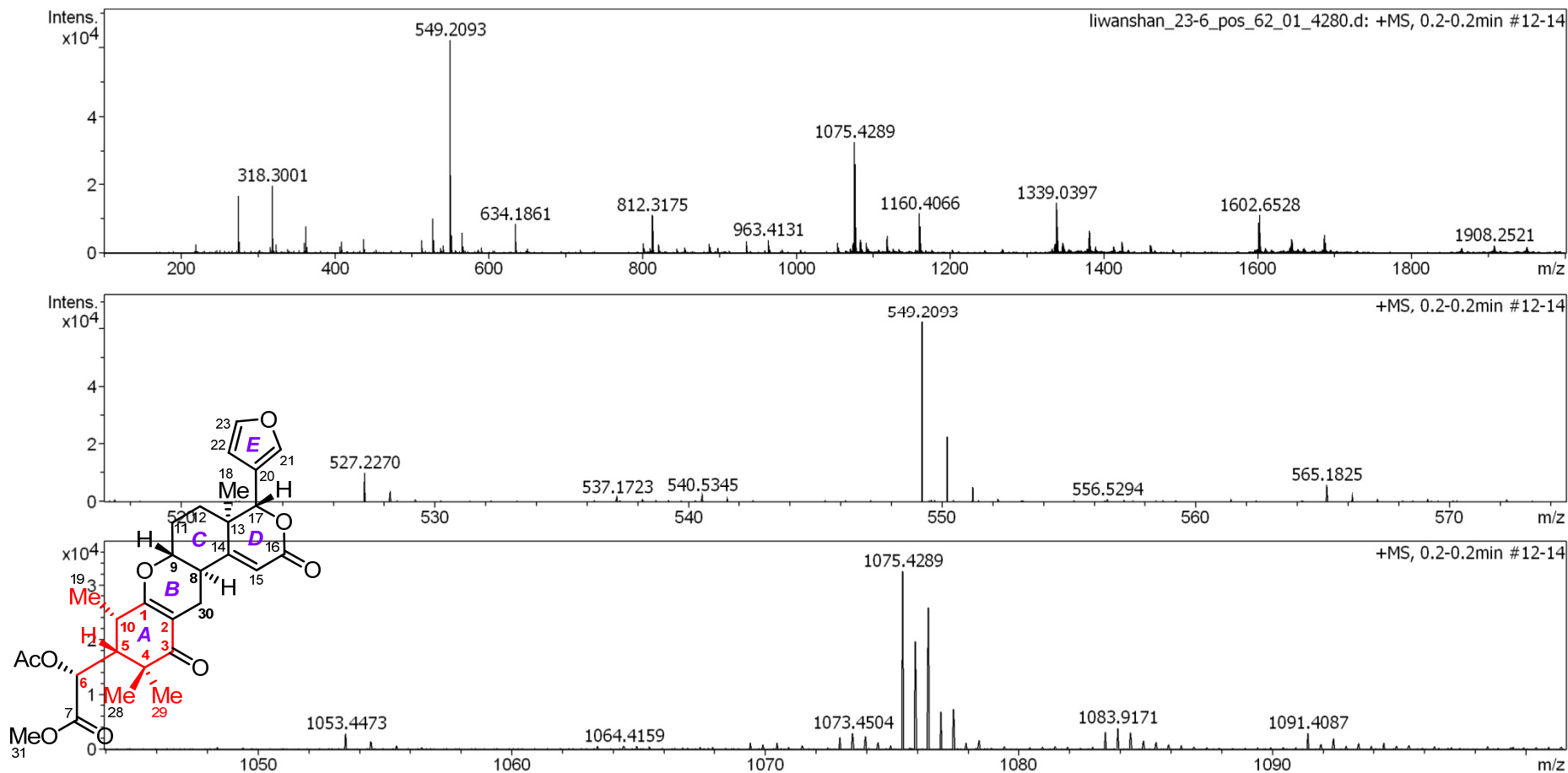
## Generic Display Report

### Analysis Info

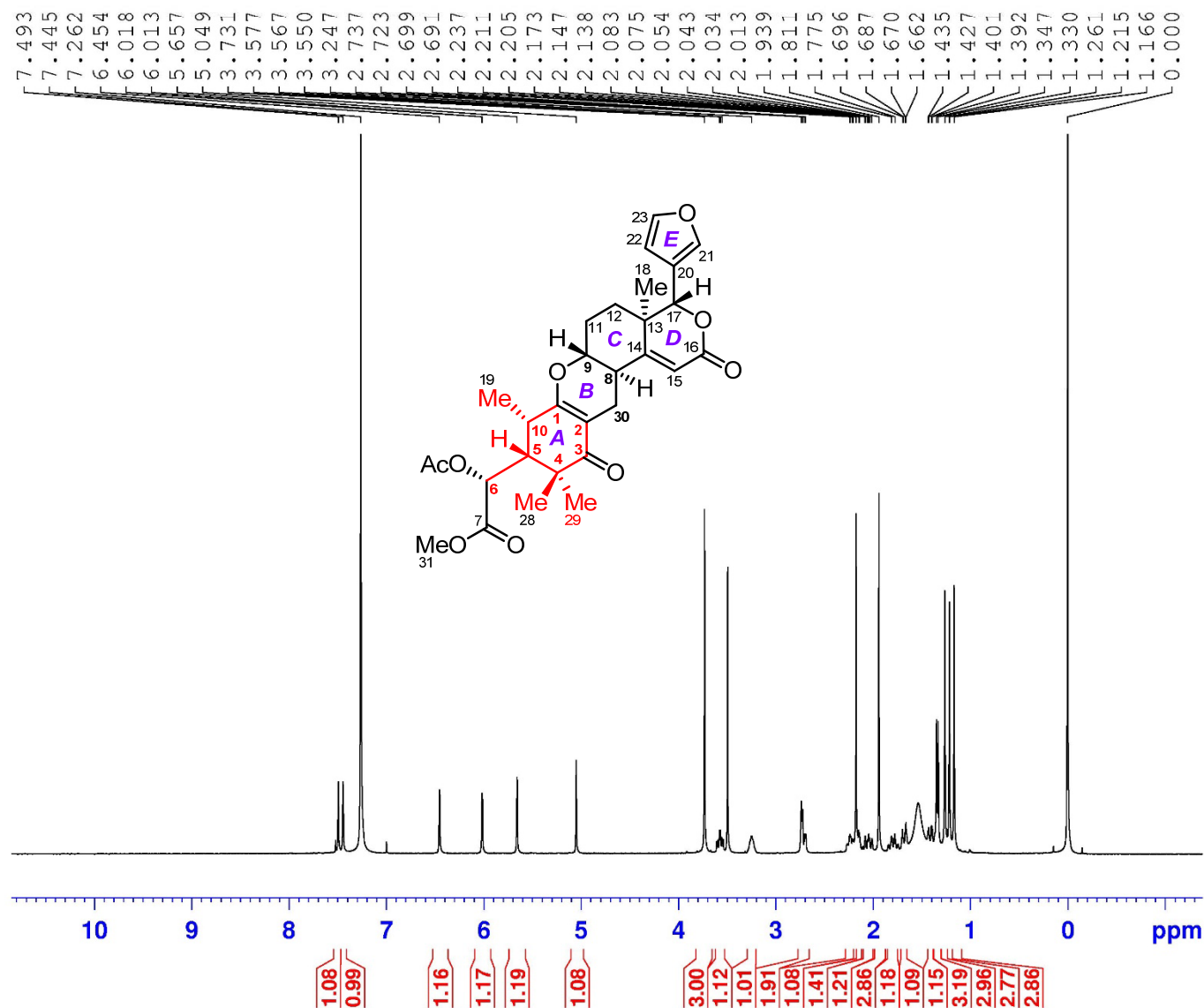
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Sample Name liwanshan\_23-6\_pos  
Comment

Acquisition Date 2/8/2018 5:34:27 PM

Operator SCSIO  
Instrument maXis



# $^1\text{H}$ NMR (400 MHz) spectrum of compound **1** in $\text{CDCl}_3$



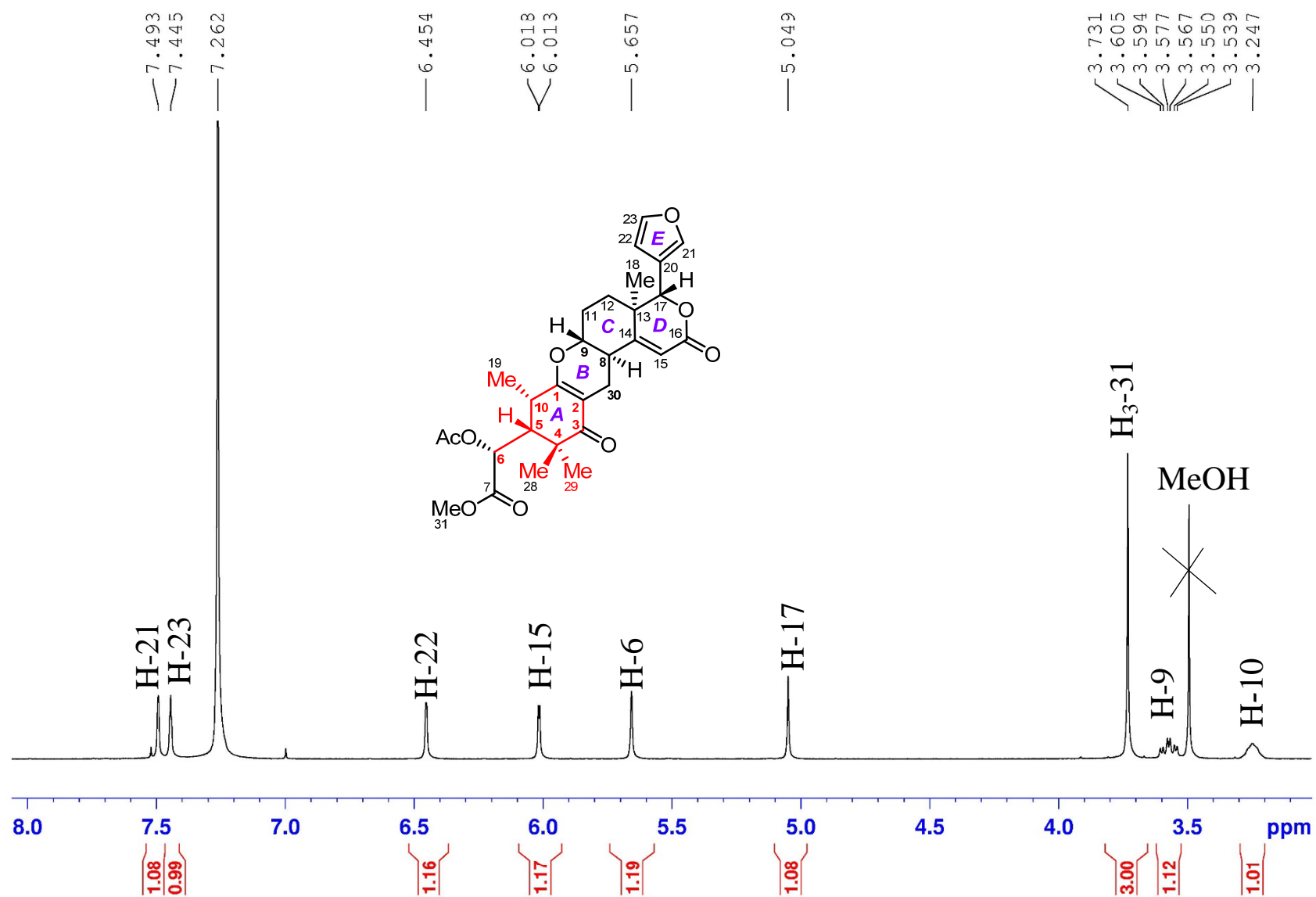
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PROCNO         1
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Time           17.47
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PULPROG        zg30
TD             65536
SOLVENT        CDCl3
NS             32
DS             2
SWH            8223.685 H
FIDRES         0.125483 H
AQ            3.9846387 s
RG            208.5
DW            60.800 u
DE            10.00 u
TE            297.0 K
D1            1.00000000 s
TD0           1
  
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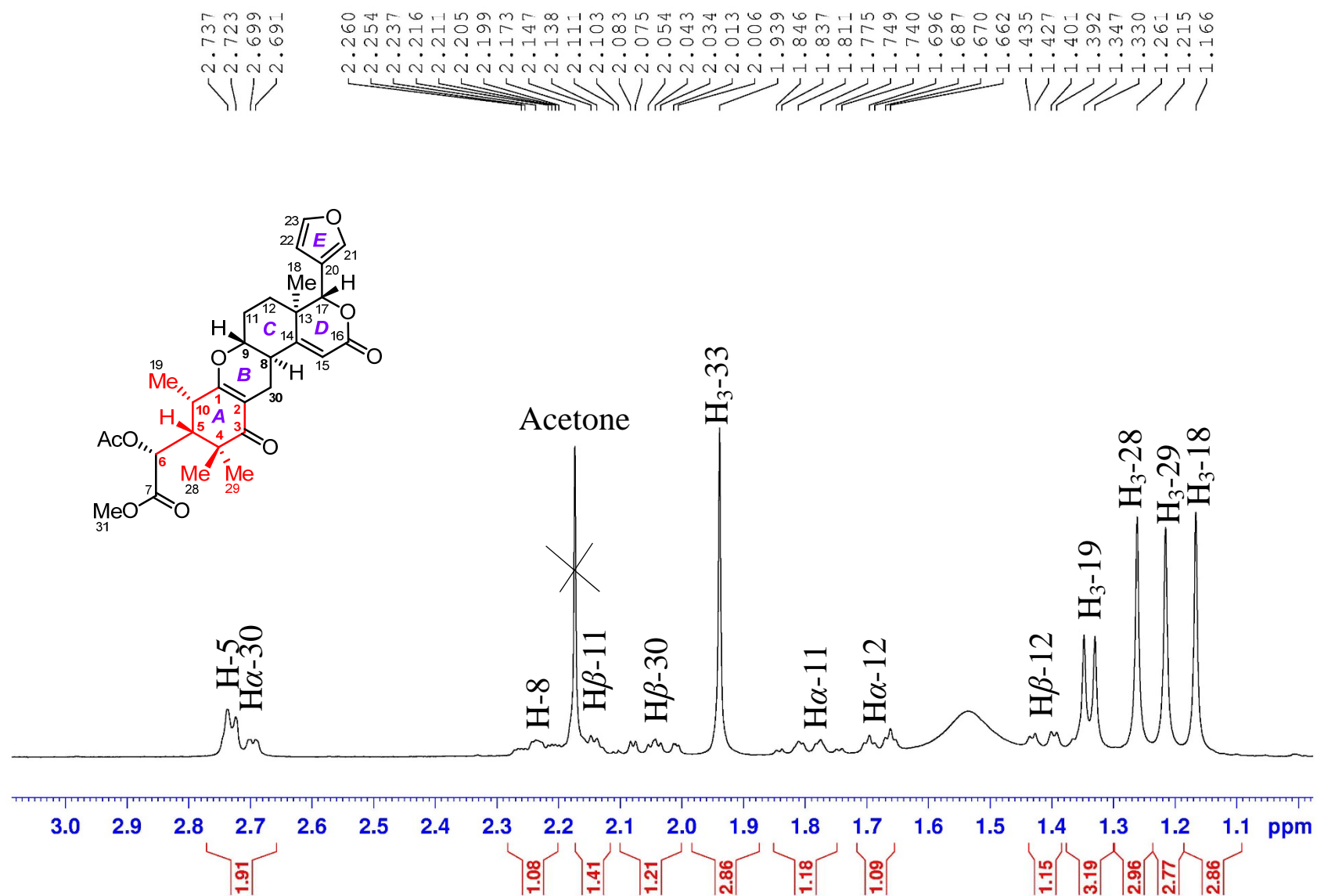
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===== CHANNEL f1 =====
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NUC1           1H
P1            11.50 u
SI            65536
SF            400.1300089 M
WDW            EM
SSB            0
LB            0.30 H
GB            0
PC            1.00
  
```

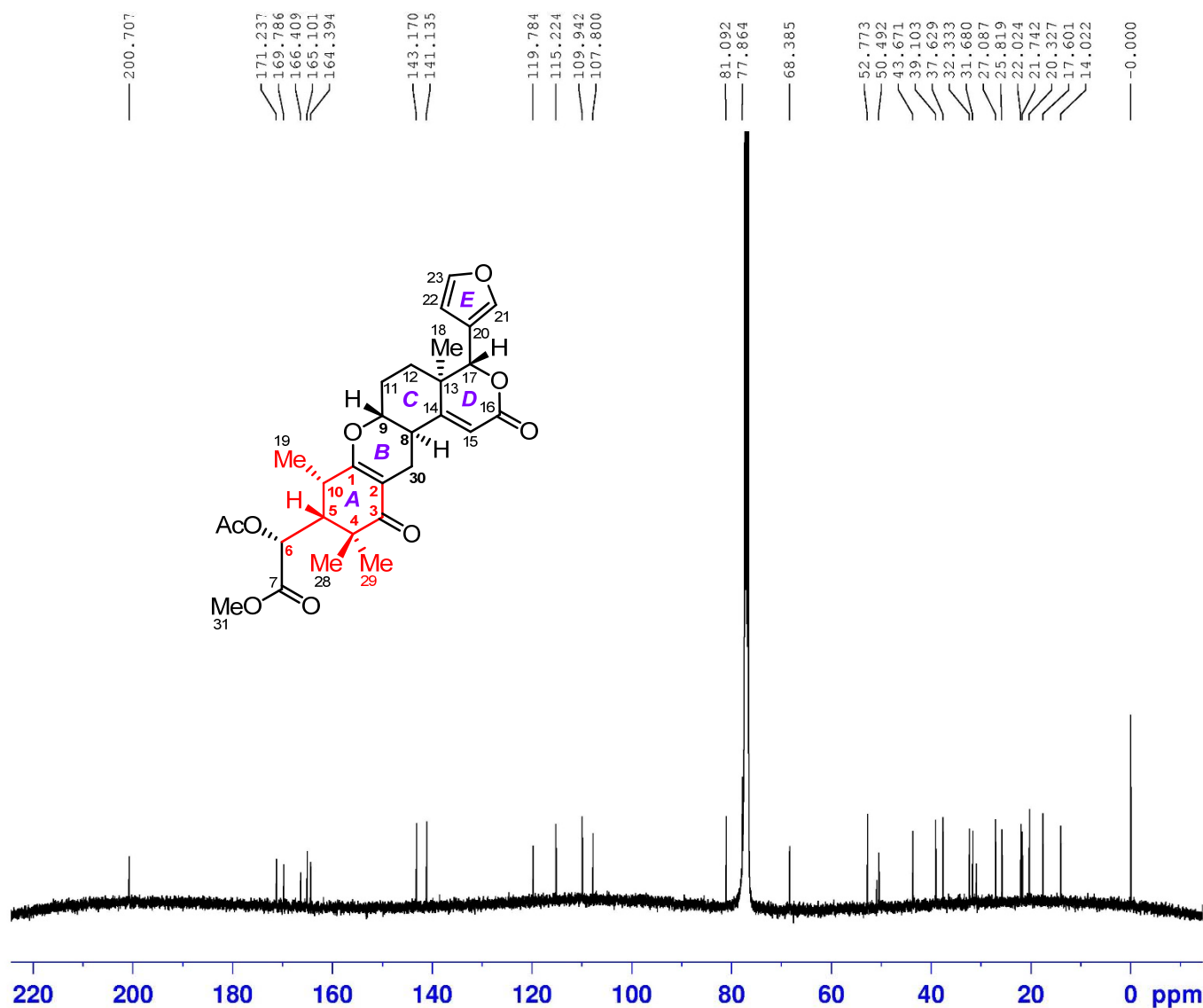
$^1\text{H}$  NMR (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$



$^1\text{H}$  NMR (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$



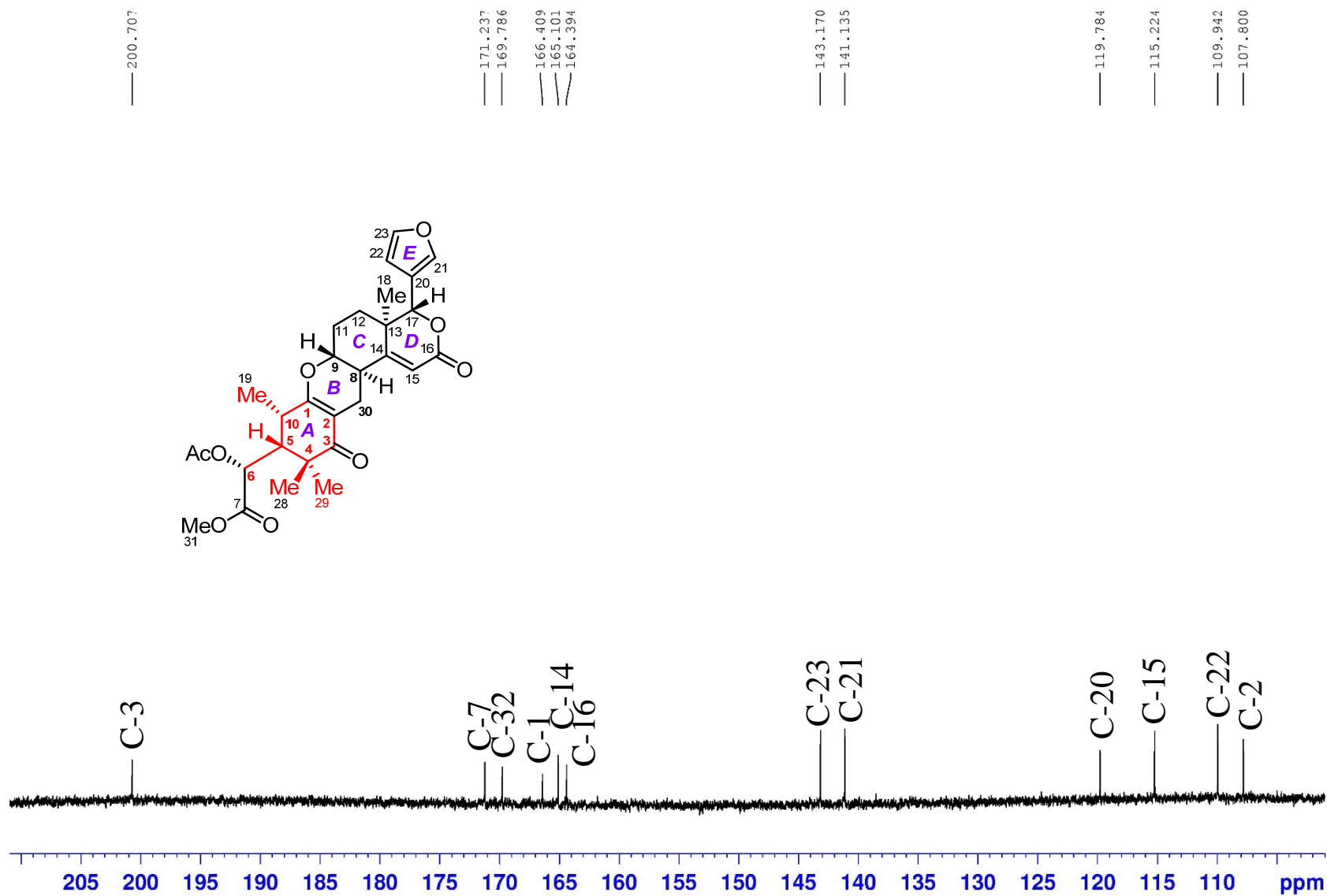
# $^{13}\text{C}$ NMR (100 MHz) spectrum of compound **1** in $\text{CDCl}_3$



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 PROCNO 1  
 Date\_ 20180114  
 Time 3.24  
 INSTRUM spect  
 PROBHD 5 mm CPPBBO BB  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT  $\text{CDCl}_3$   
 NS 10000  
 DS 4  
 SWH 24038.461 H:  
 FIDRES 0.366798 H:  
 AQ 1.3631988 s:  
 RG 73.92  
 DW 20.800 u:  
 DE 18.00 u:  
 TE 297.0 K  
 D1 2.00000000 s:  
 D11 0.03000000 s:  
 TD0 1

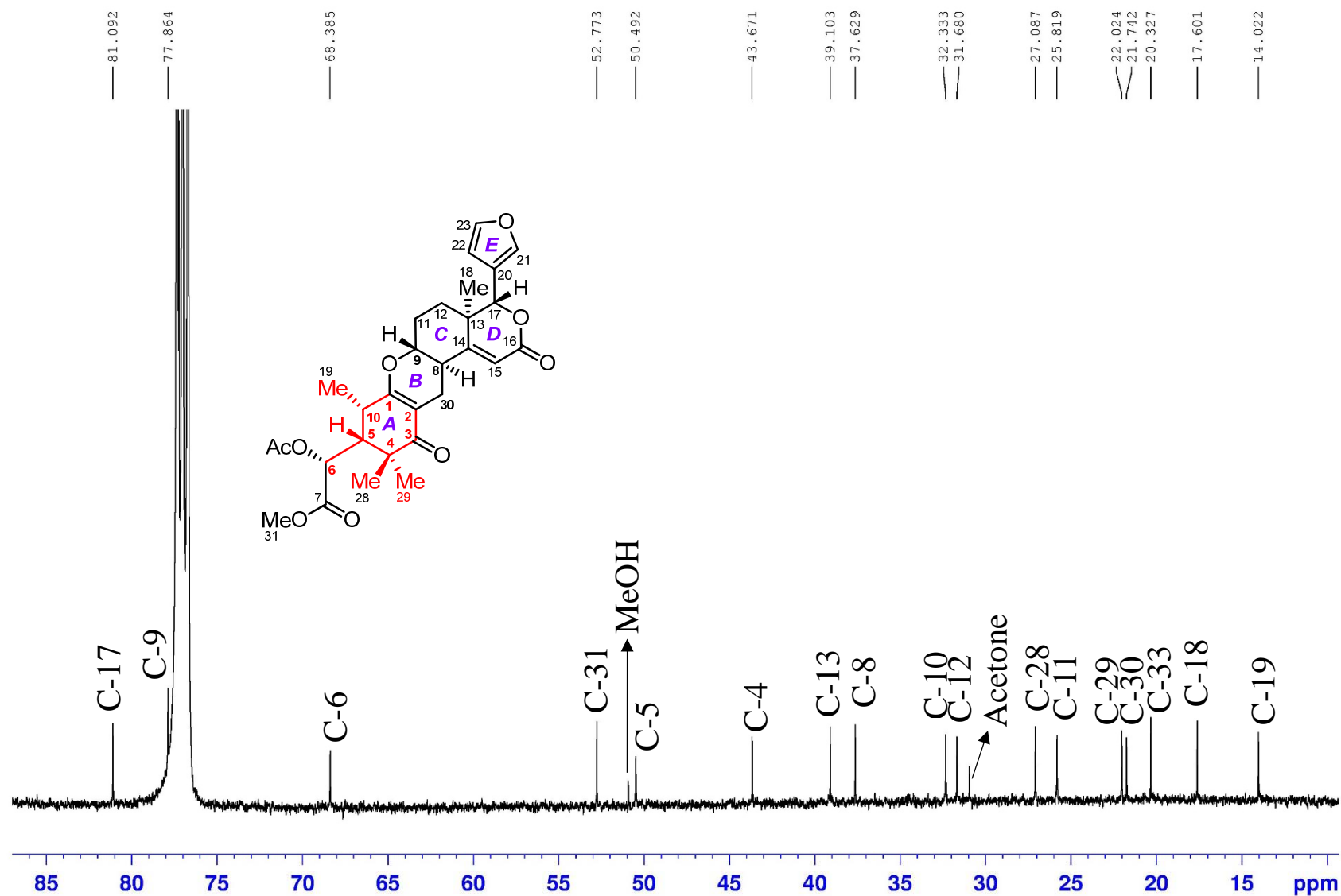
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 SF01 100.6233324 M  
 NUC1  $^{13}\text{C}$   
 P1 10.00 u:  
 SI 32768  
 SF 100.6127691 M  
 WDW EM  
 SSB 0  
 LB 1.00 H:  
 GB 0  
 PC 1.40

$^{13}\text{C}$  NMR (100 MHz) spectrum of compound **1** in  $\text{CDCl}_3$

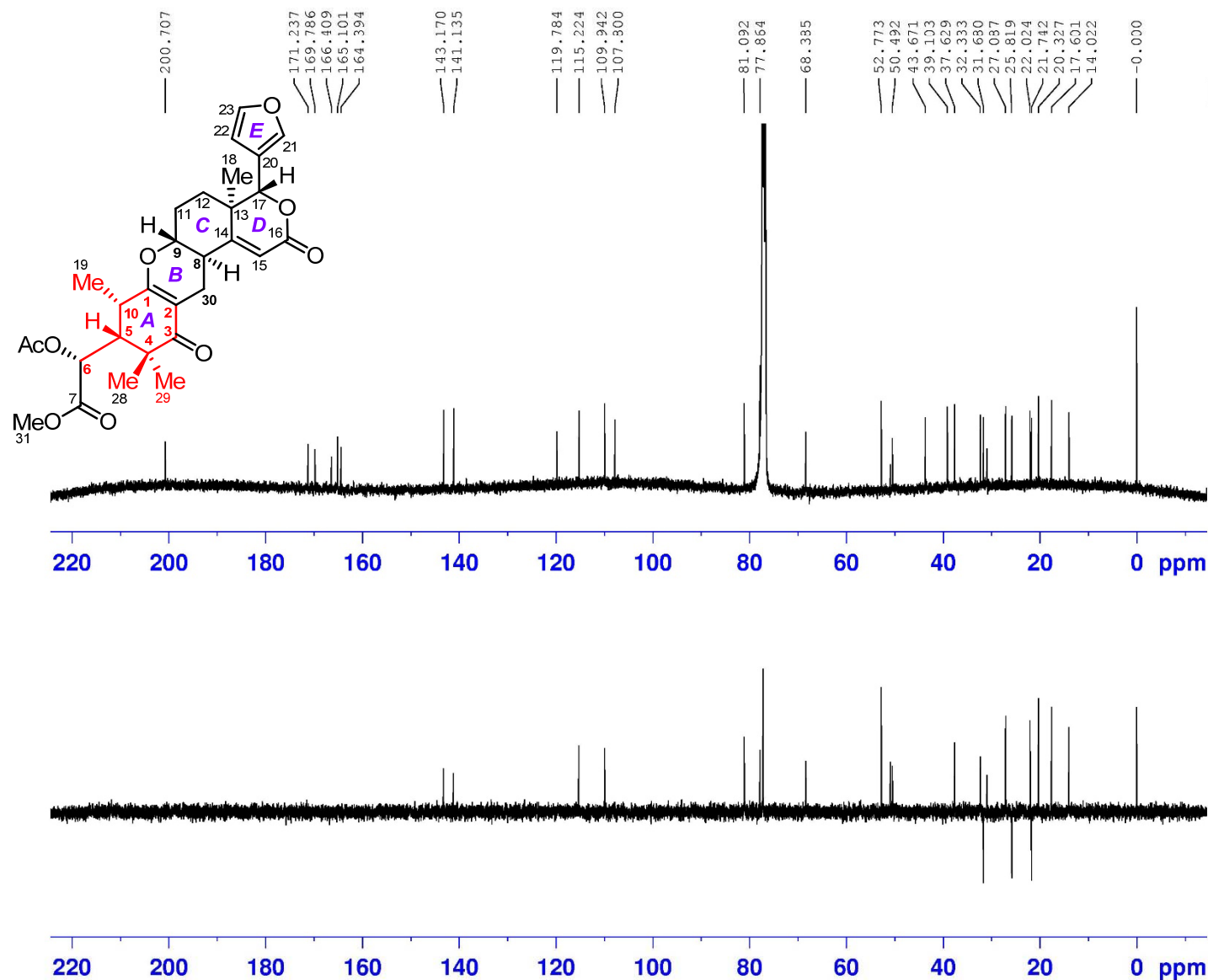




$^{13}\text{C}$  NMR (100 MHz) spectrum of compound **1** in  $\text{CDCl}_3$



# DEPT135 (100 MHz) spectrum of compound **1** in CDCl<sub>3</sub>



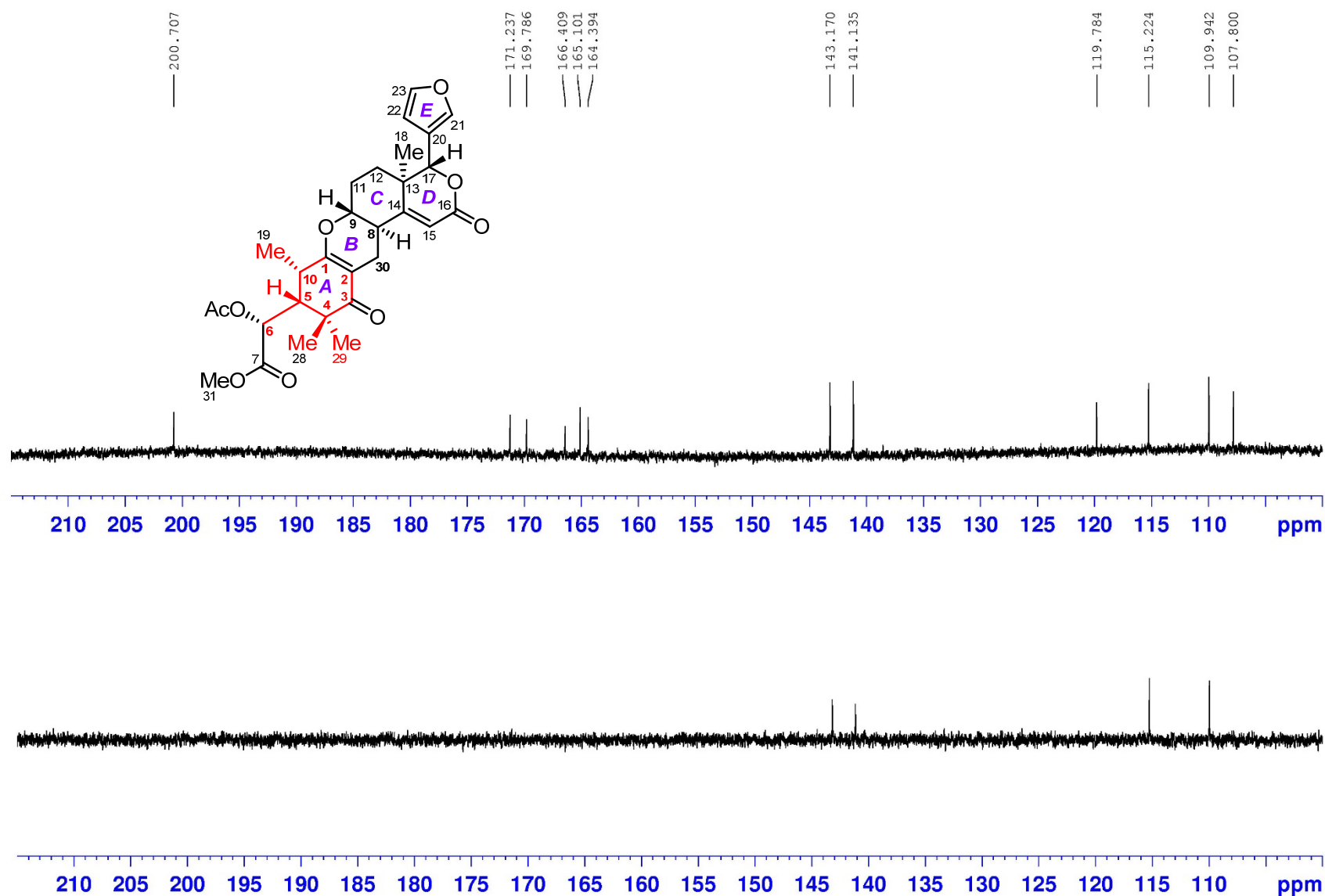
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PROCNO     1
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PULPROG    deptsp135
TD         65536
SOLVENT    CDCl3
NS         2500
DS         4
SWH        24038.461
FIDRES     0.366798
AQ         1.3631988
RG         130.26
DW         20.800
DE         18.00
TE         297.0
CNST2      145.0000000
D1         2.000000000
D2         0.00344828
D12        0.00002000
TD0        1
    
```

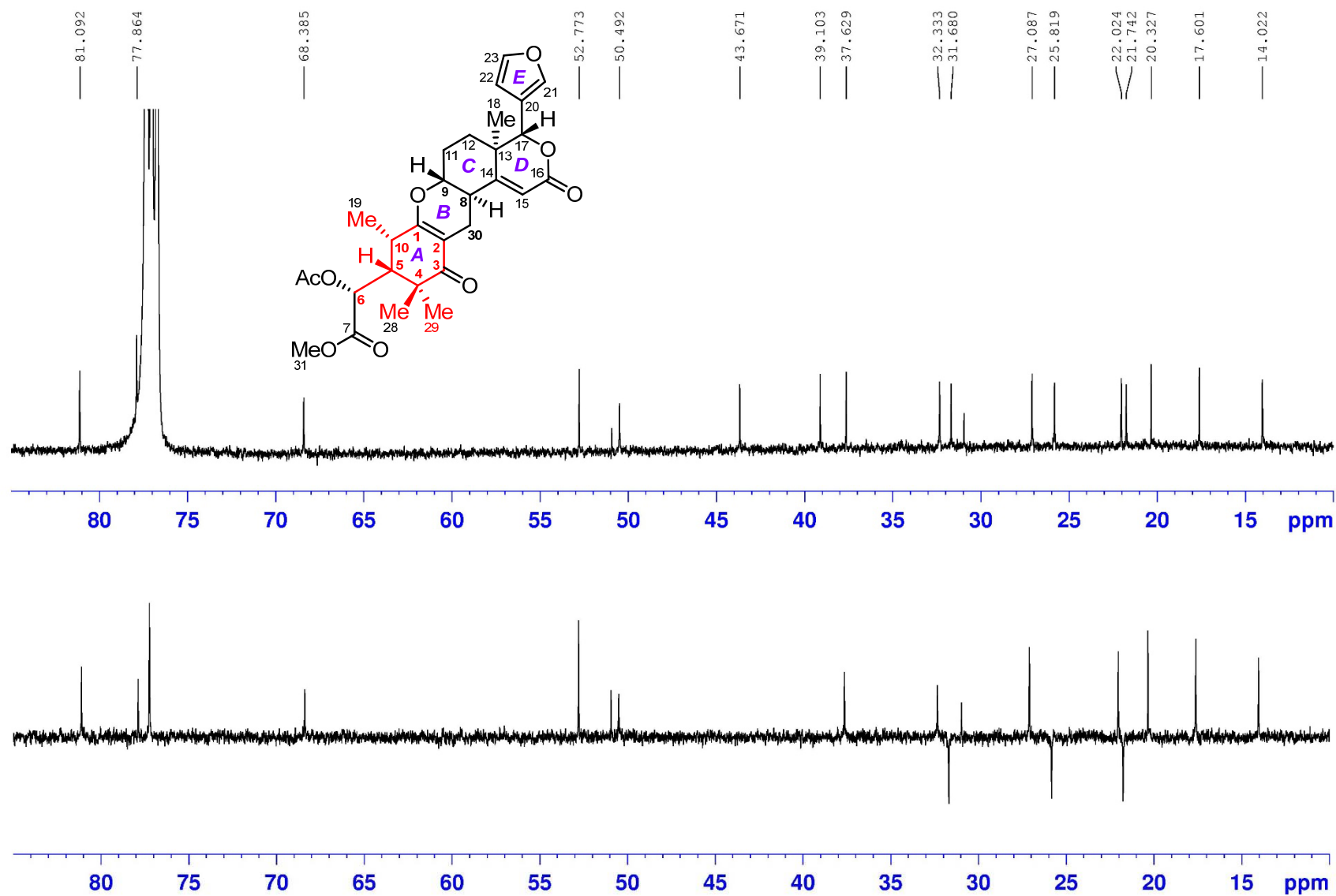
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NUC1       13C
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P13        2000.00
SI         32768
SF         100.6127685
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SSB        0
LB         1.00
GB         0
PC         1.40
    
```

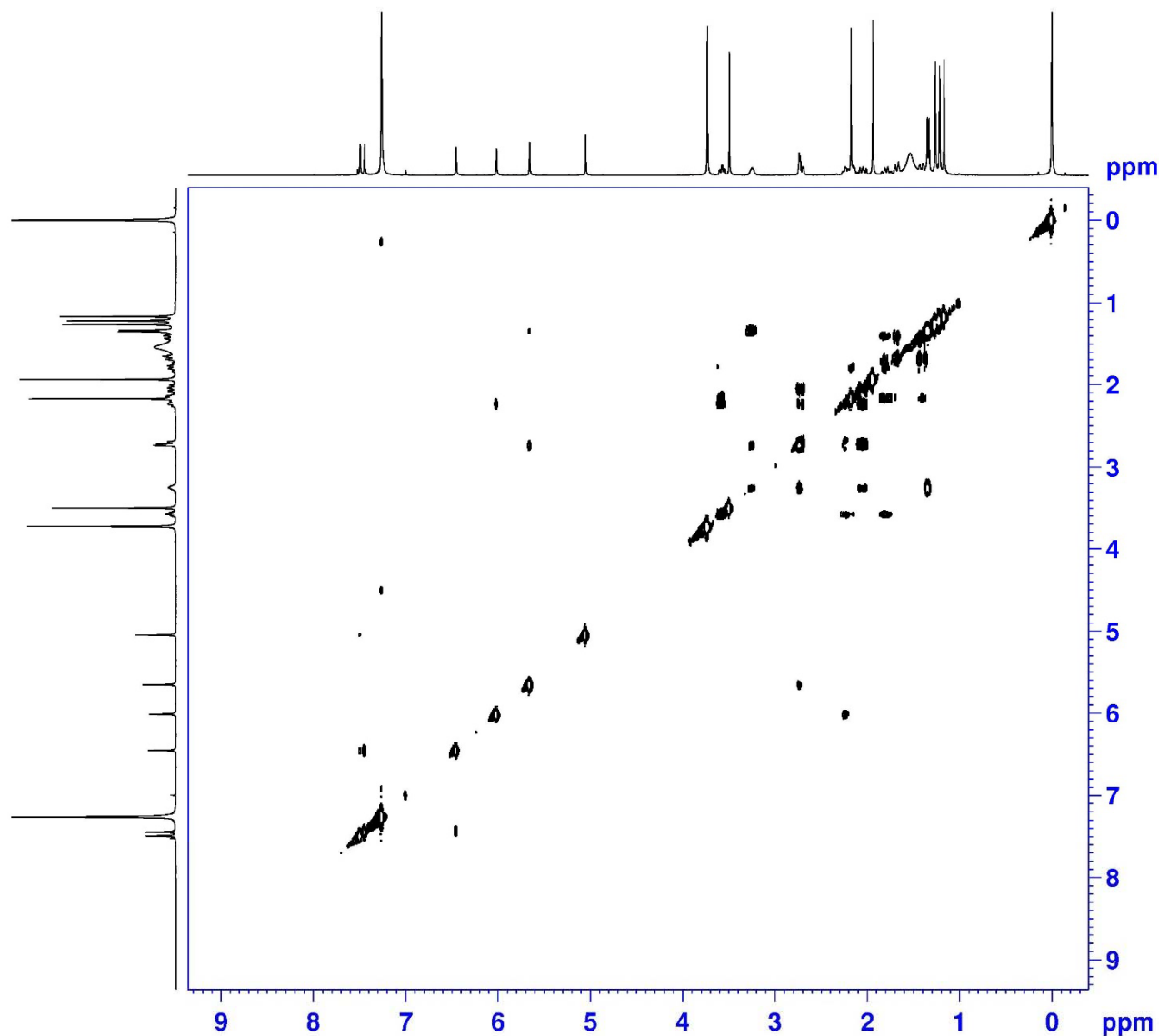
# DEPT135 (100 MHz) spectrum of compound **1** in CDCl<sub>3</sub>



# DEPT135 (100 MHz) spectrum of compound **1** in CDCl<sub>3</sub>



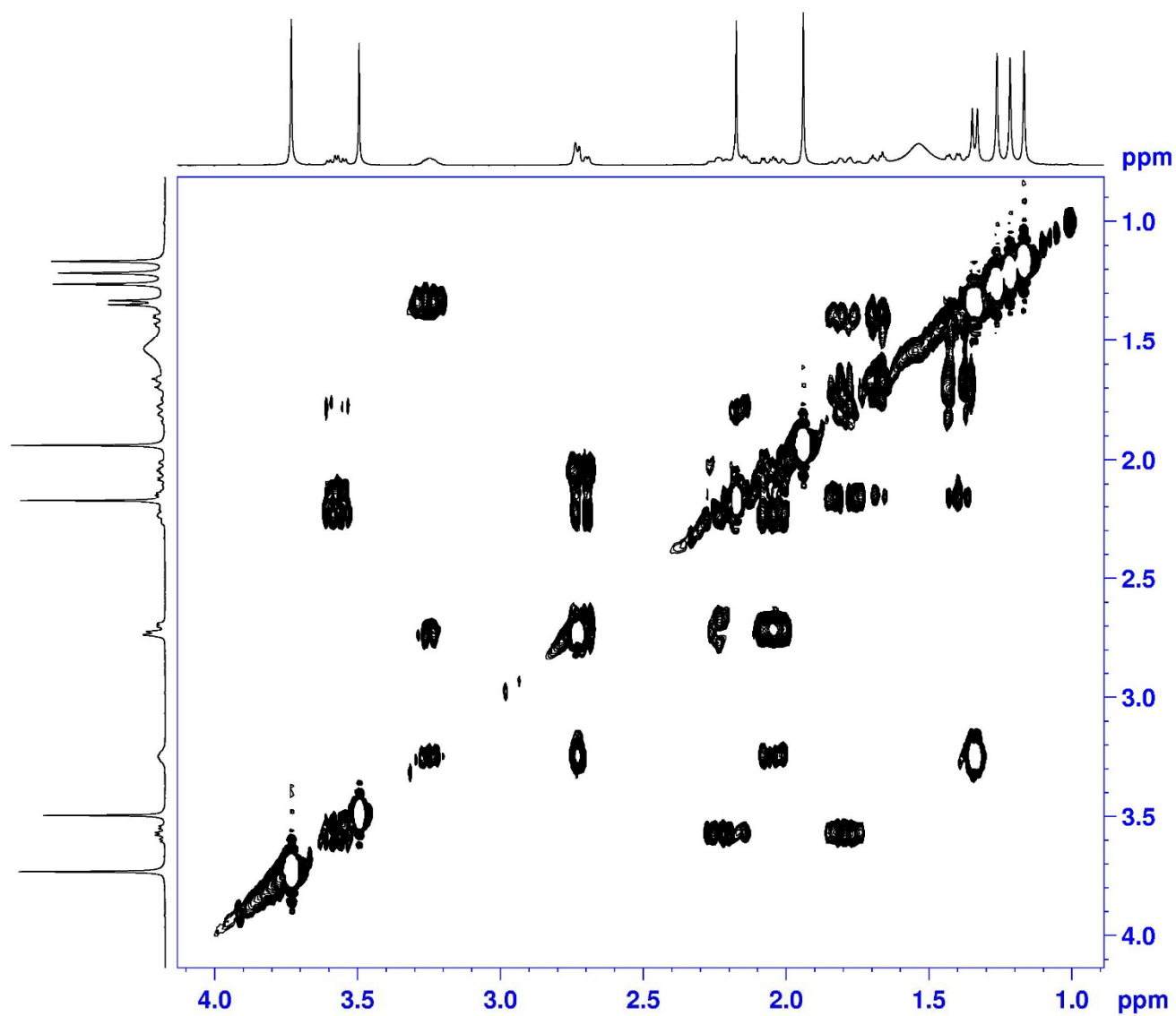
# $^1\text{H}$ - $^1\text{H}$ COSY (400 MHz) spectrum of compound **1** in $\text{CDCl}_3$



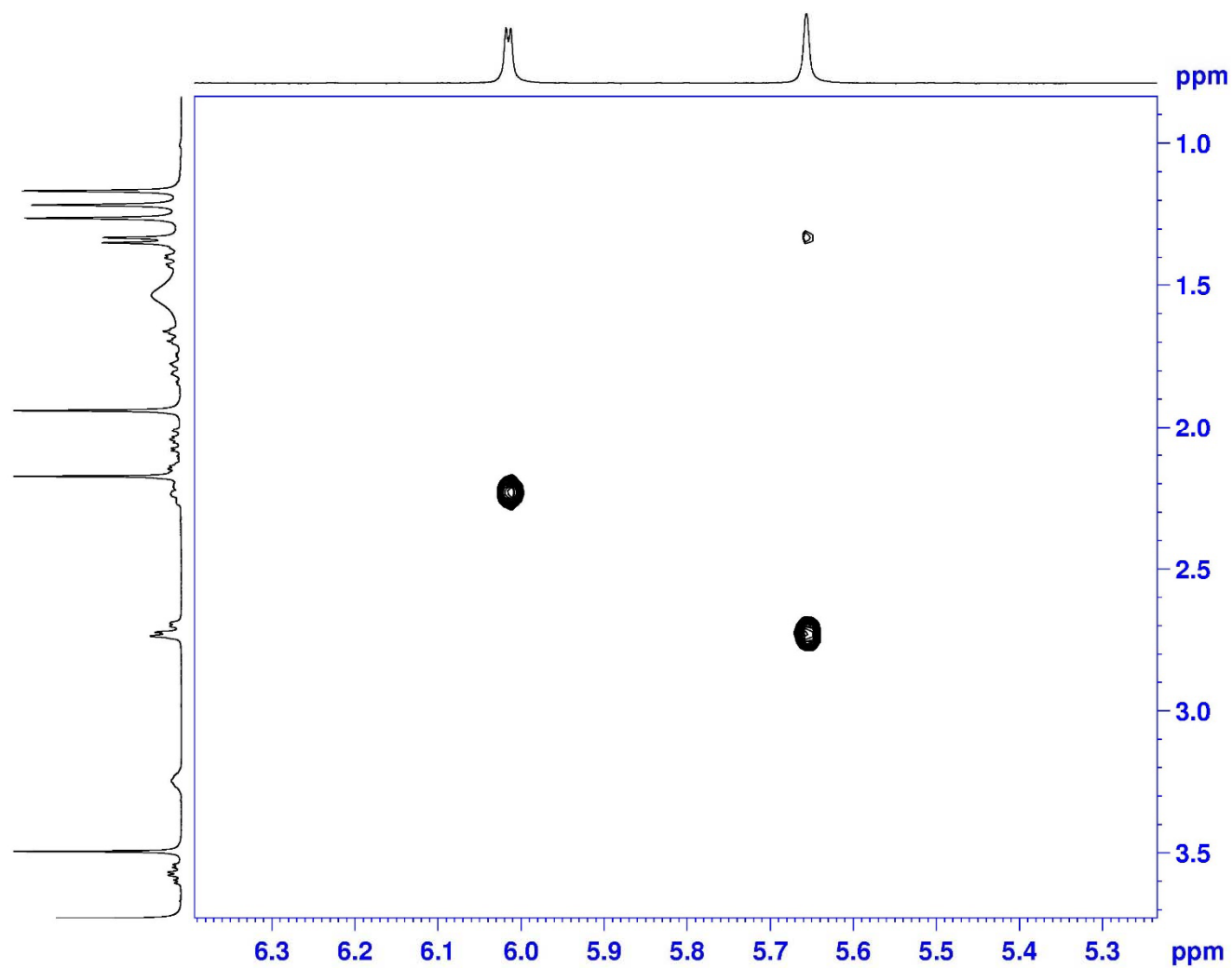
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EXPNO          4
PROCNO         1
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Time           5.49
INSTRUM        spect
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PULPROG        cosygpppqf
TD             2048
SOLVENT        CDCl3
NS             32
DS             8
SWH            3906.250 Hz
FIDRES         1.907349 Hz
AQ             0.2621940 sec
RG             208.5
DW             128.000 use
DE             10.00 use
TE             297.0 K
D0             0.00000300 sec
D1             1.89678097 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00025600 sec
```

```
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SFO1          400.1318006 MHz
NUC1           1H
P0            11.50 use
P1            11.50 use
P17           2500.00 use
ND0           1
TD            128
SFO1          400.1318 MHz
FIDRES        30.517578 Hz
SW            9.762 ppm
FnMODE        QF
SI            1024
SF            400.1300080 MHz
WDW           QSINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF            400.1300080 MHz
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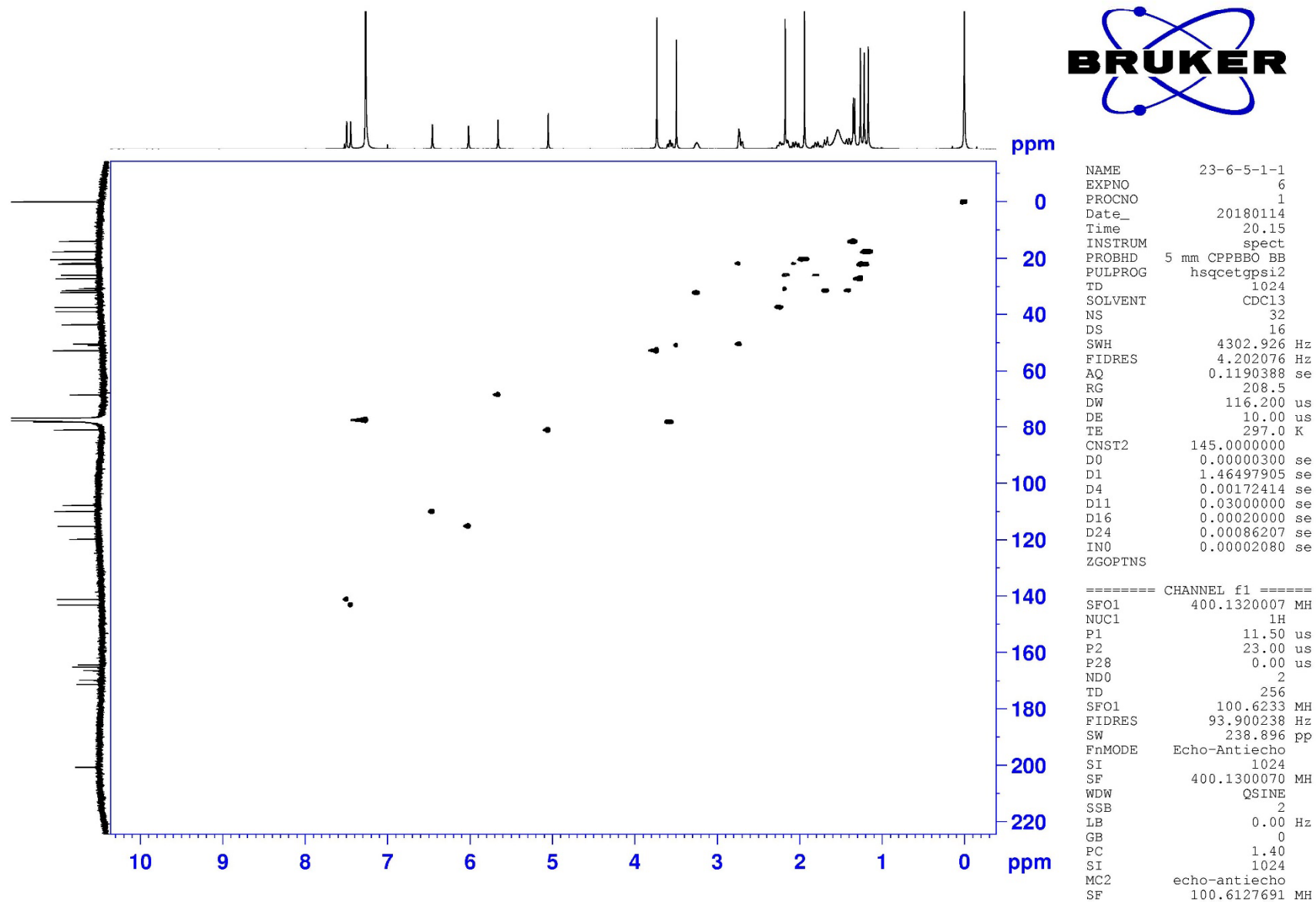
$^1\text{H}$ - $^1\text{H}$  COSY (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$



$^1\text{H}$ - $^1\text{H}$  COSY (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$

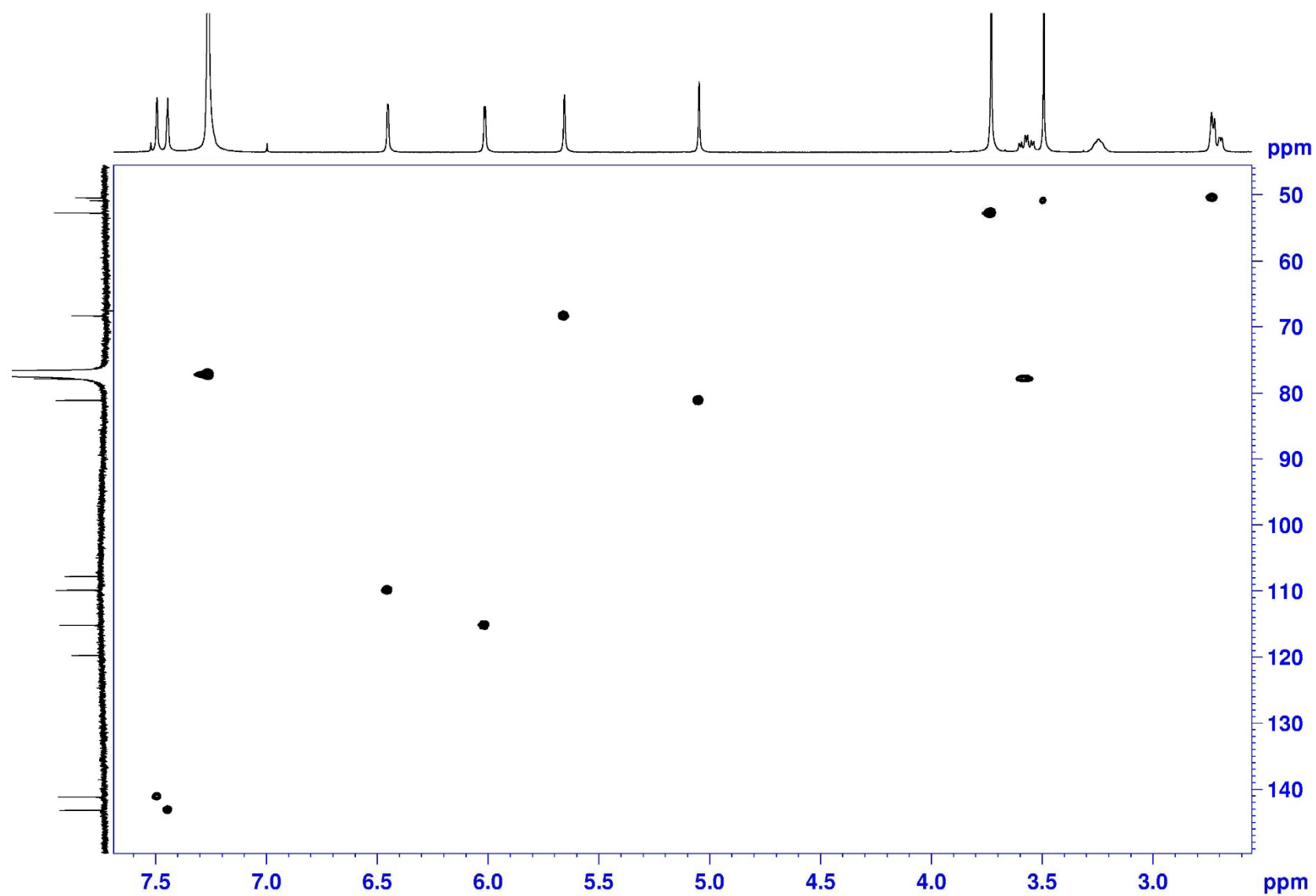


# HSQC (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>

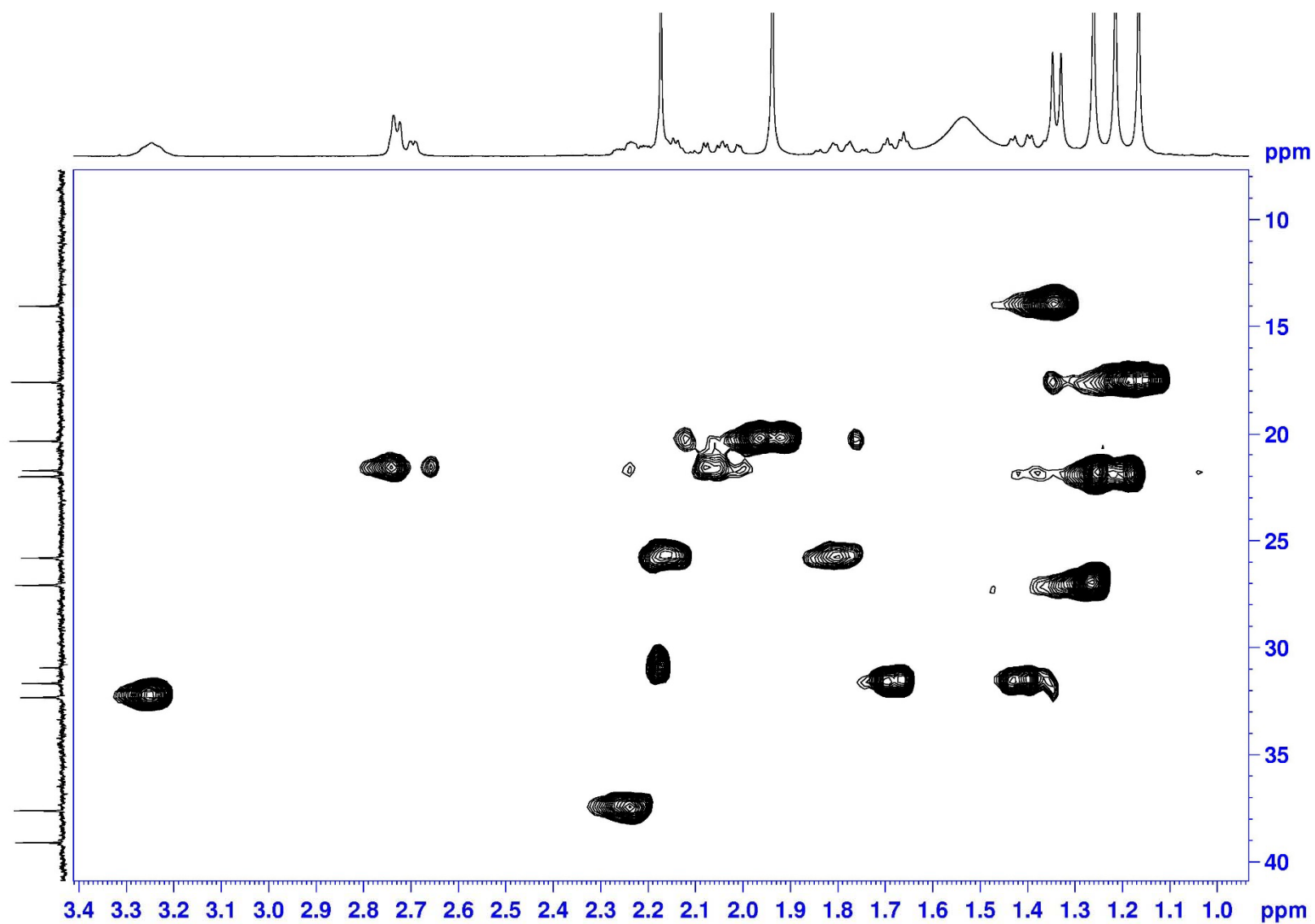




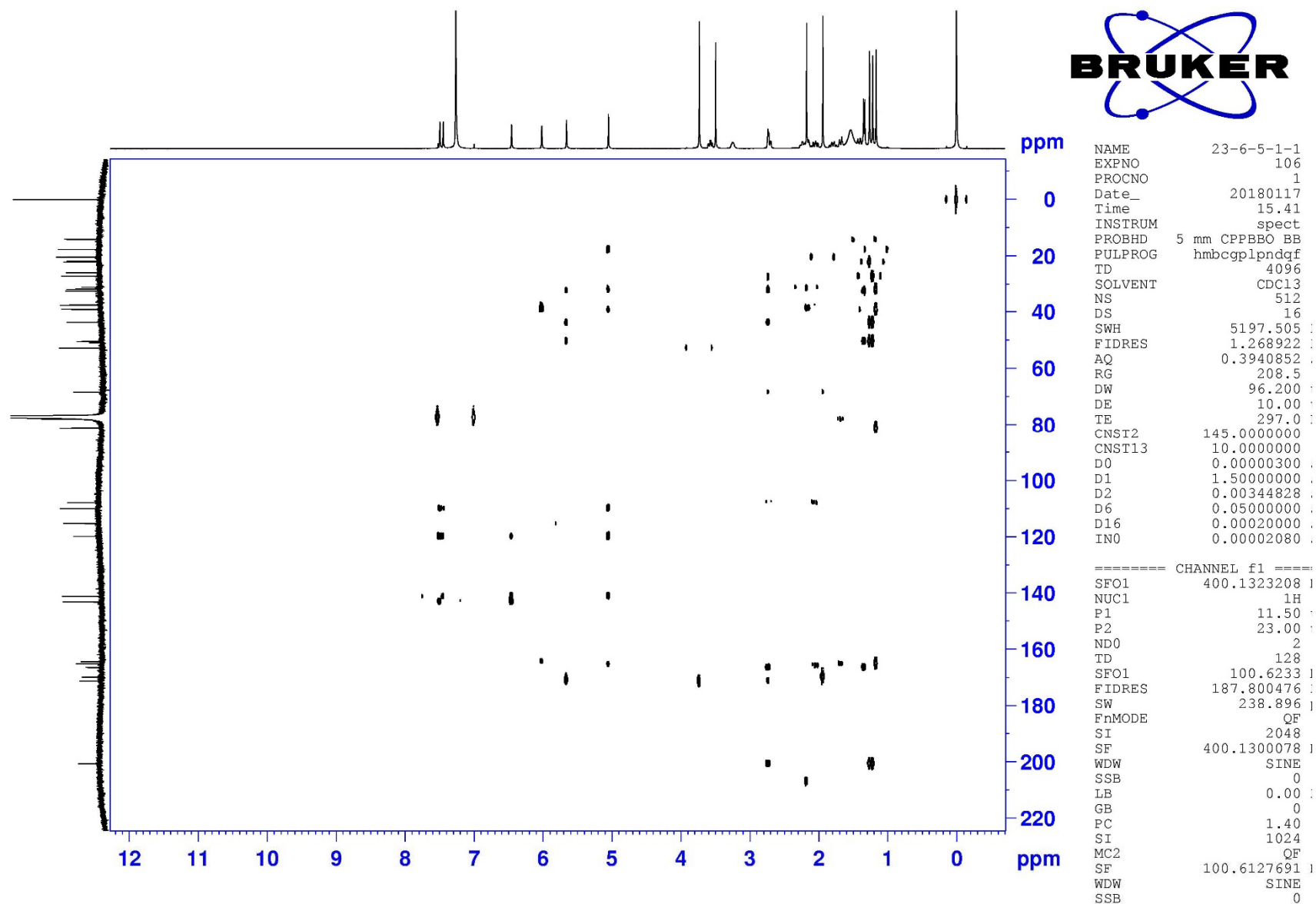
HSQC (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>



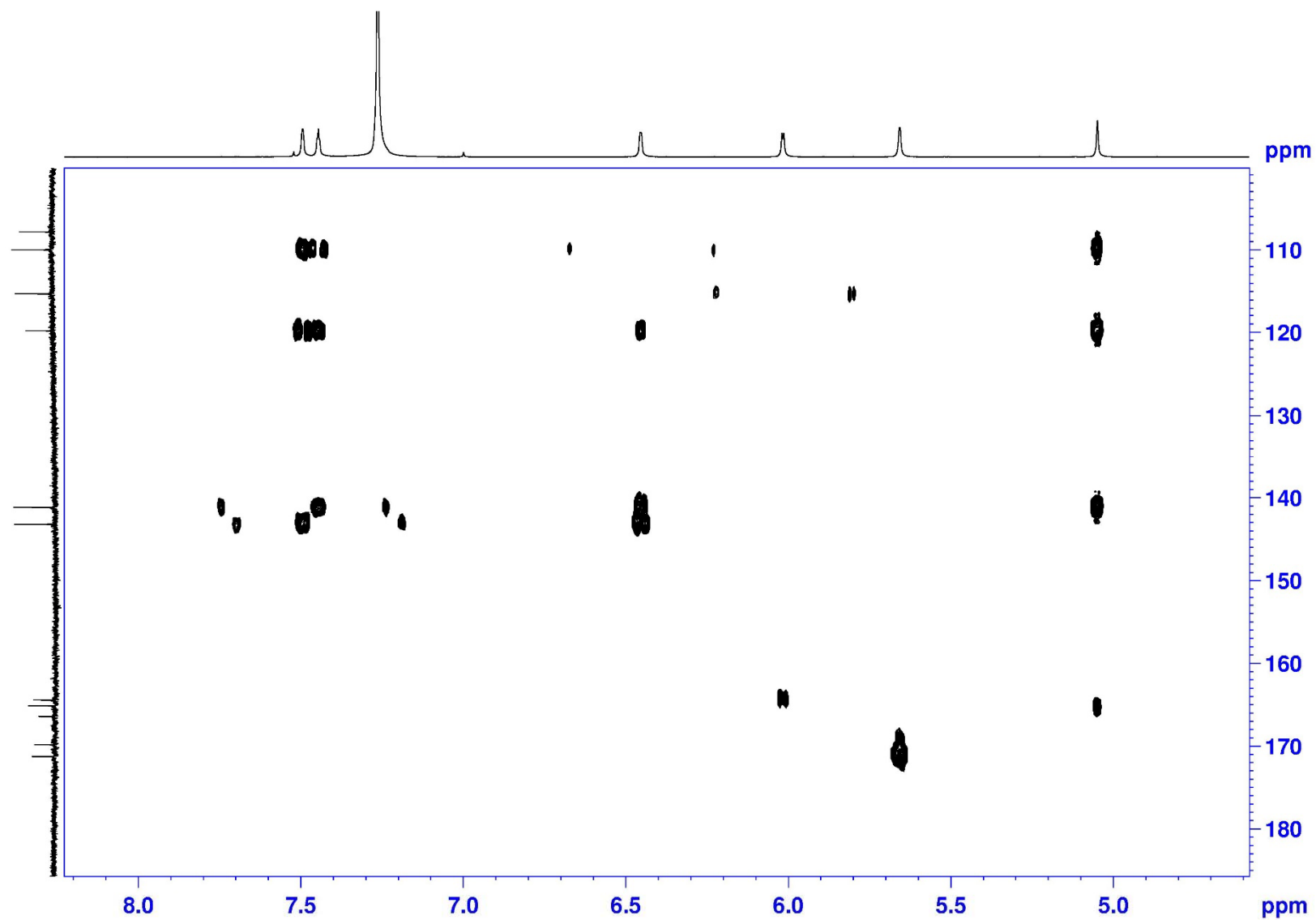
HSQC (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>



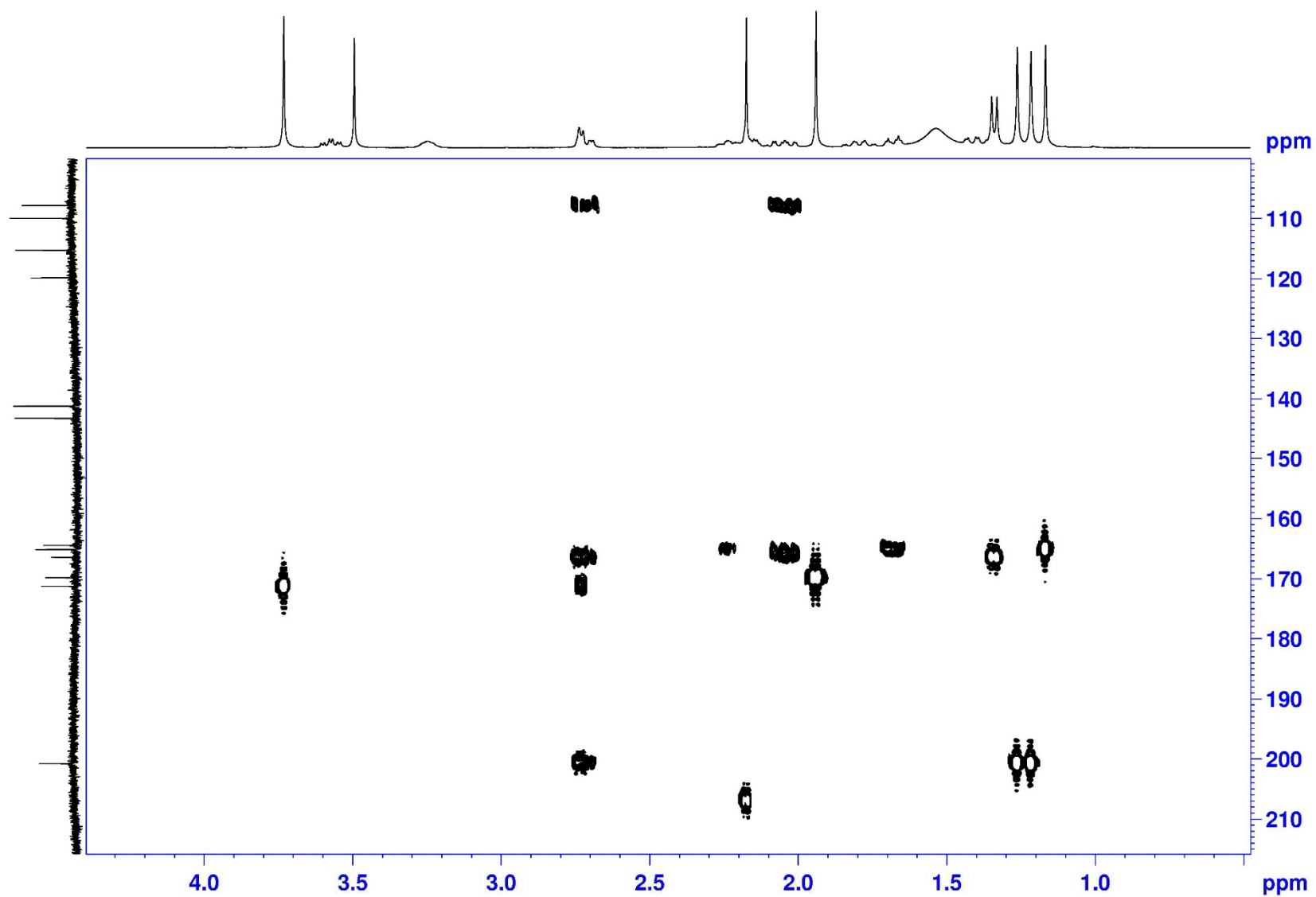
# HMBC (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>



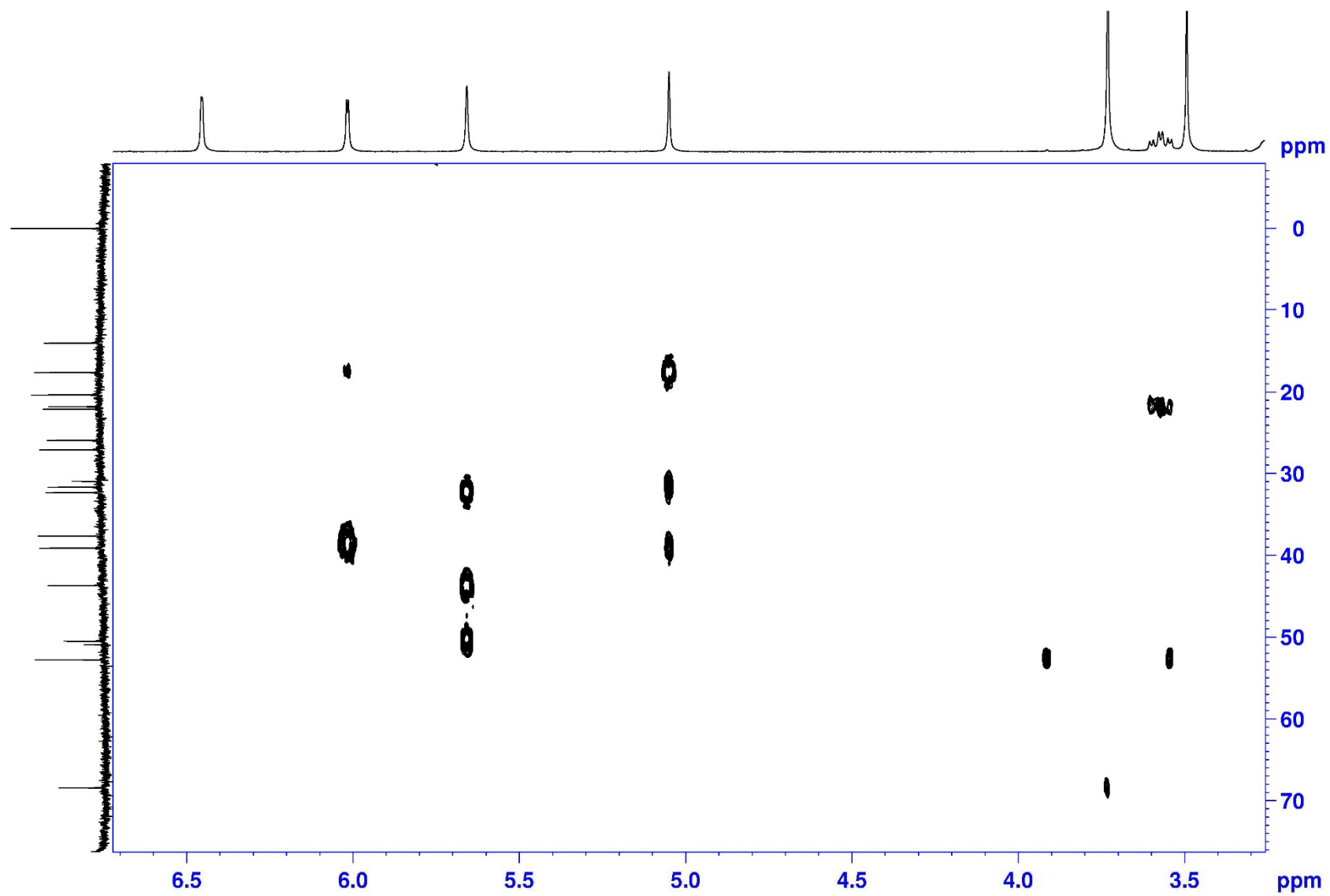
HMBC (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$



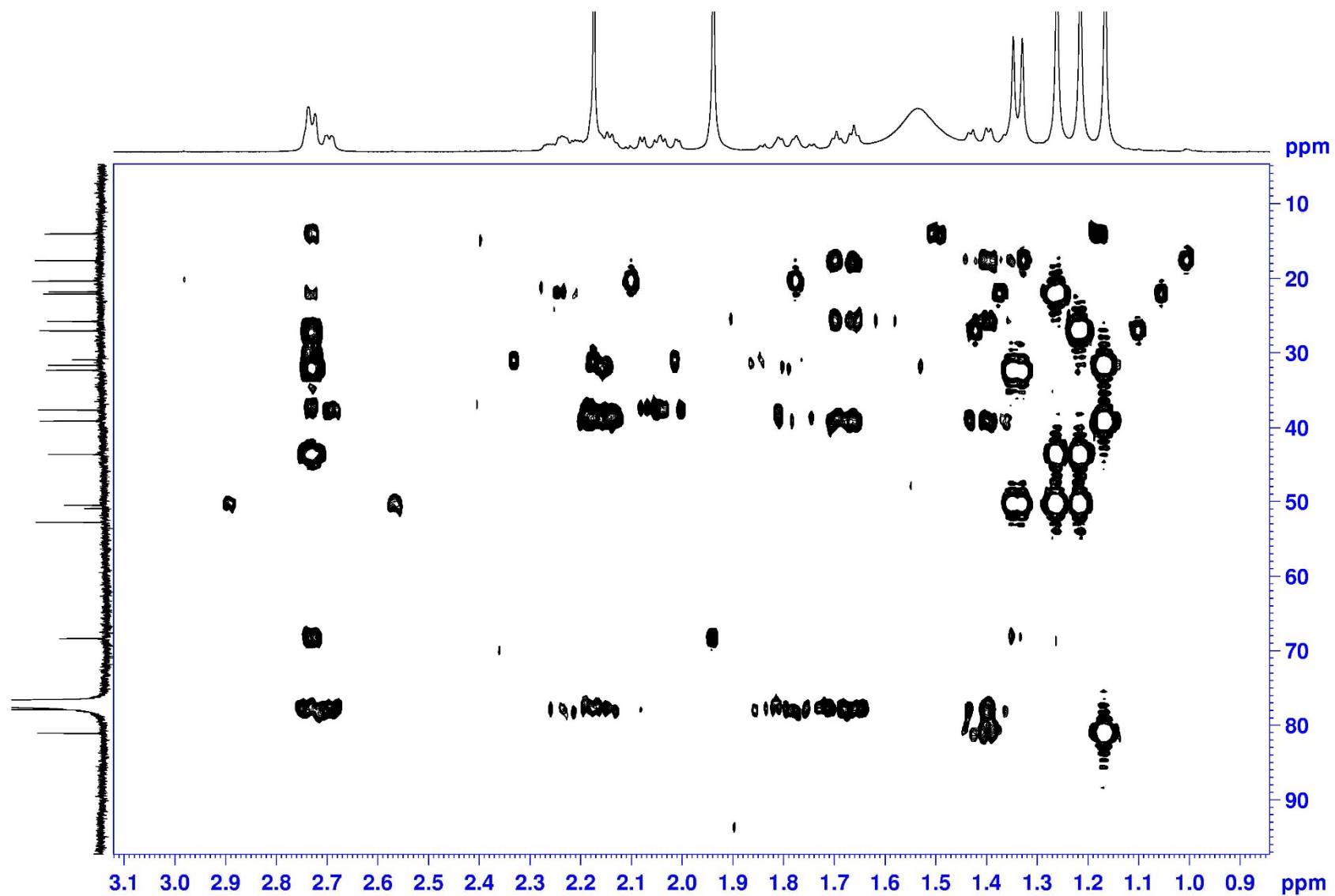
HMBC (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>



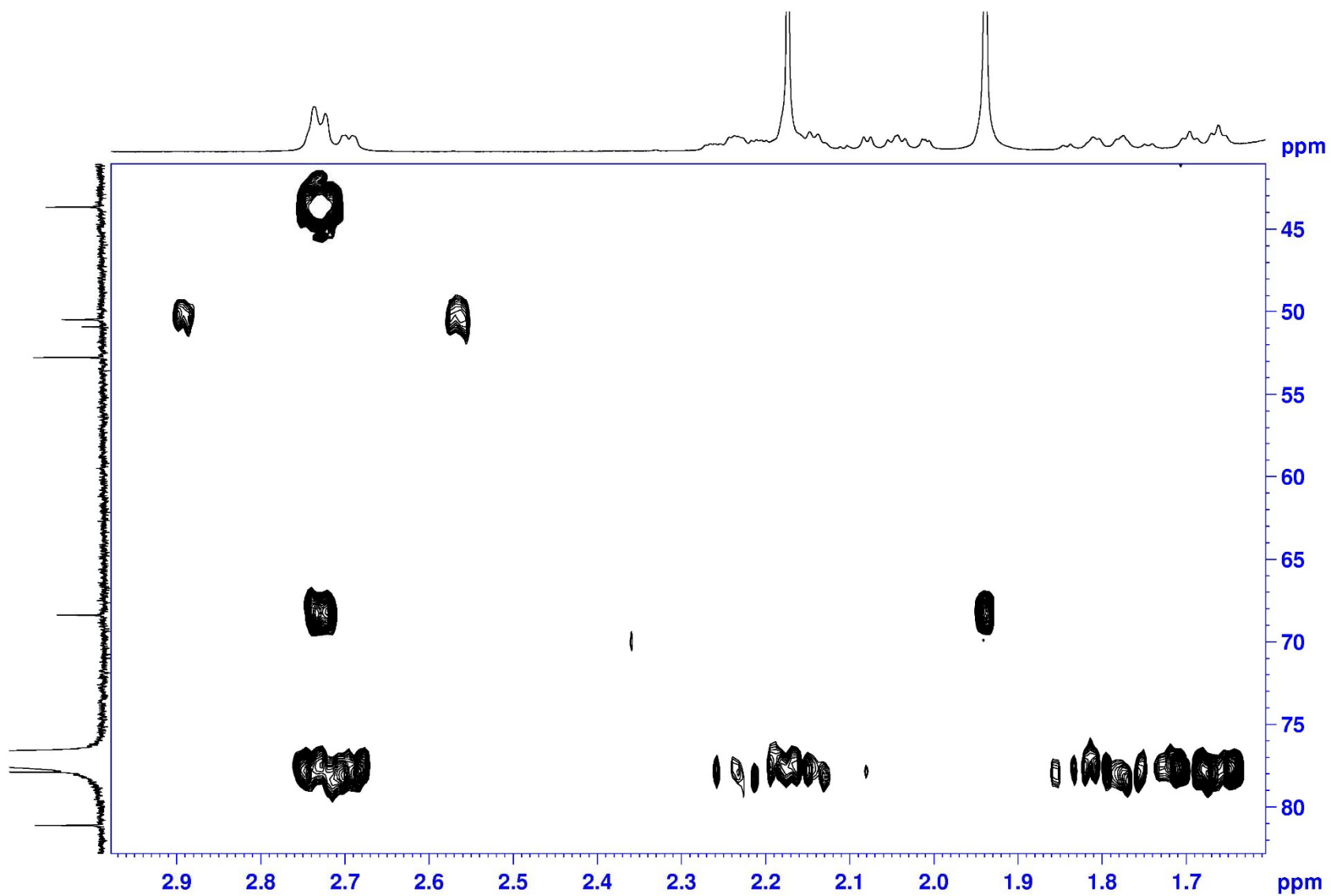
HMBC (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$



HMBC (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$

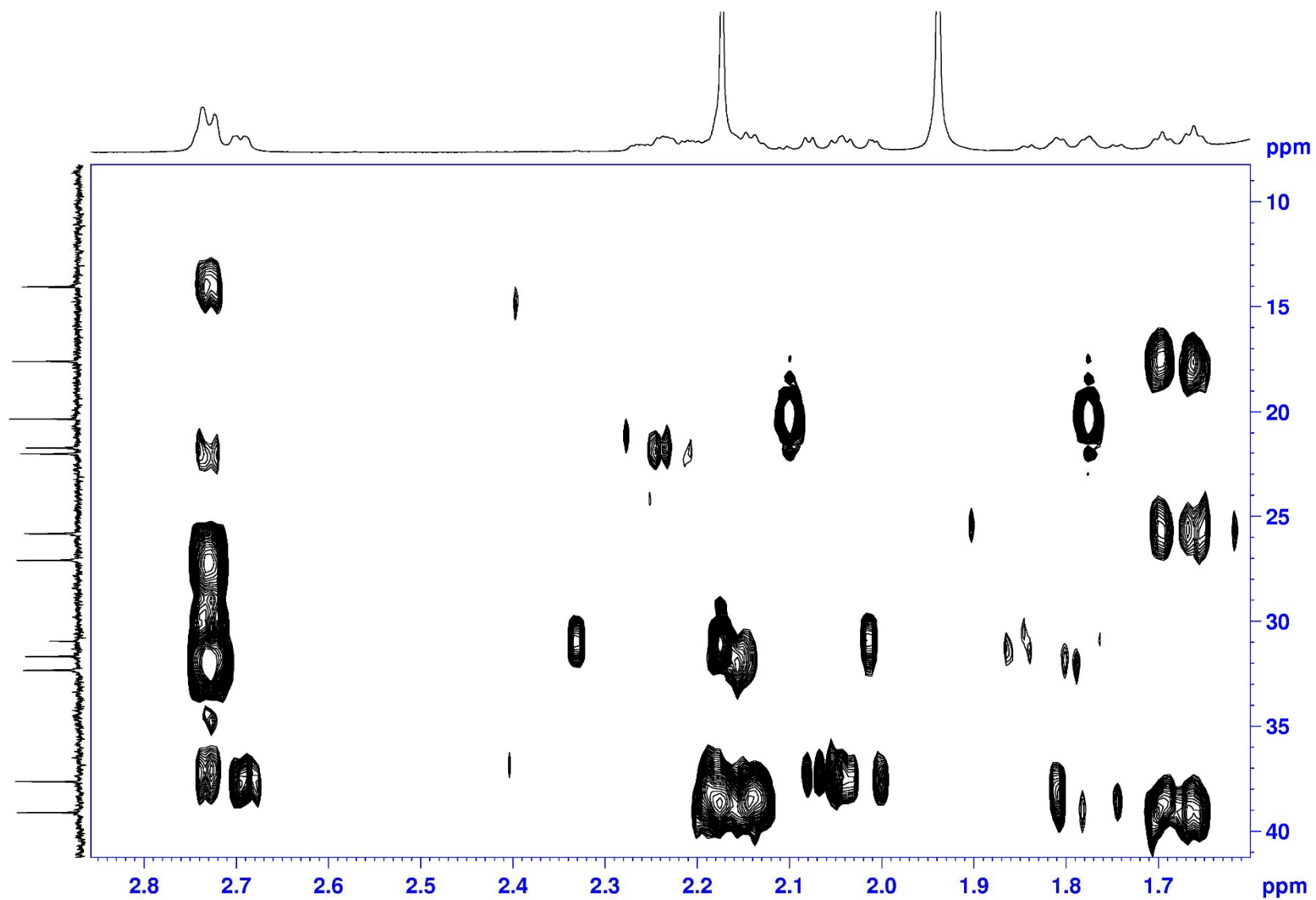


HMBC (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>

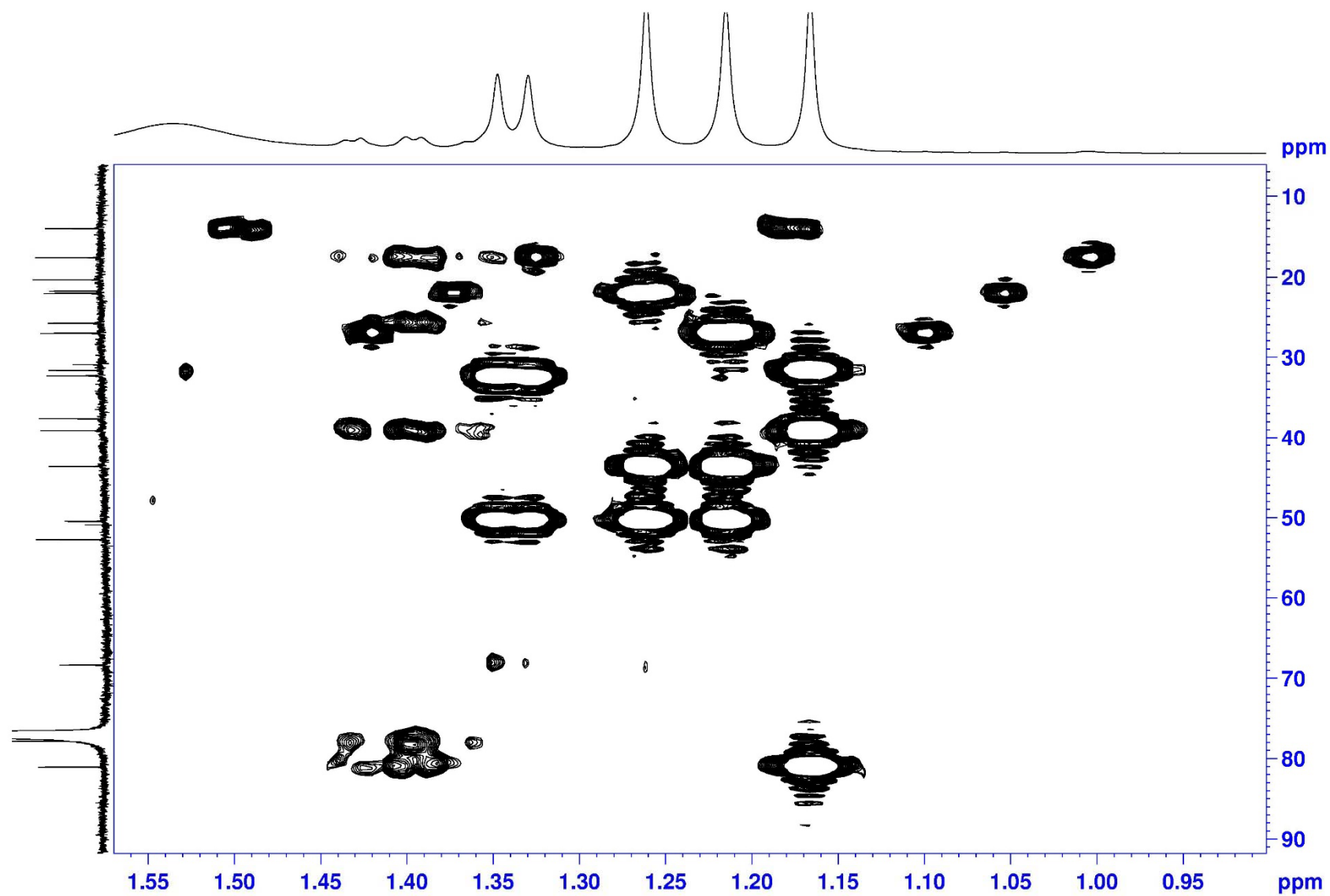




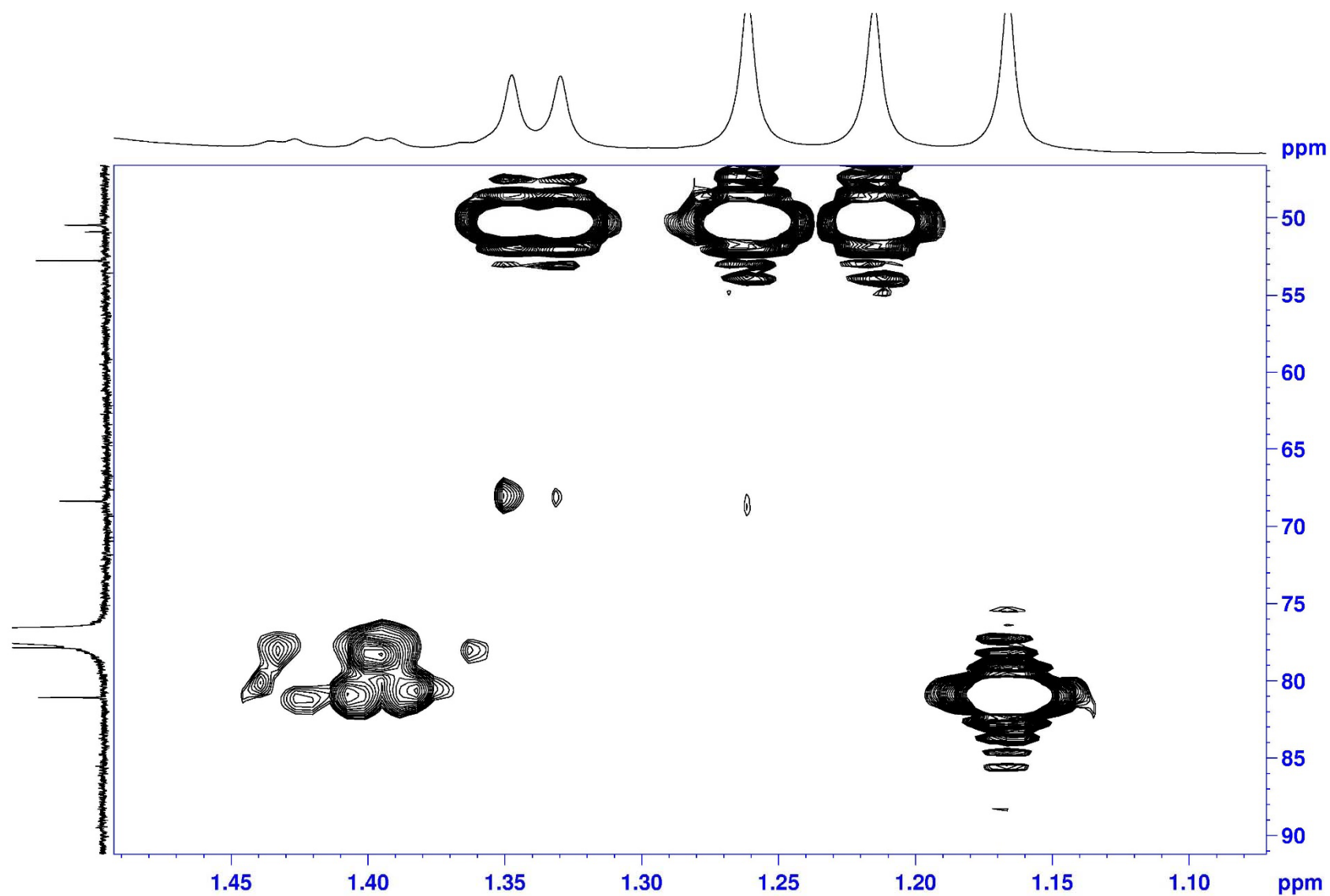
HMBC (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$



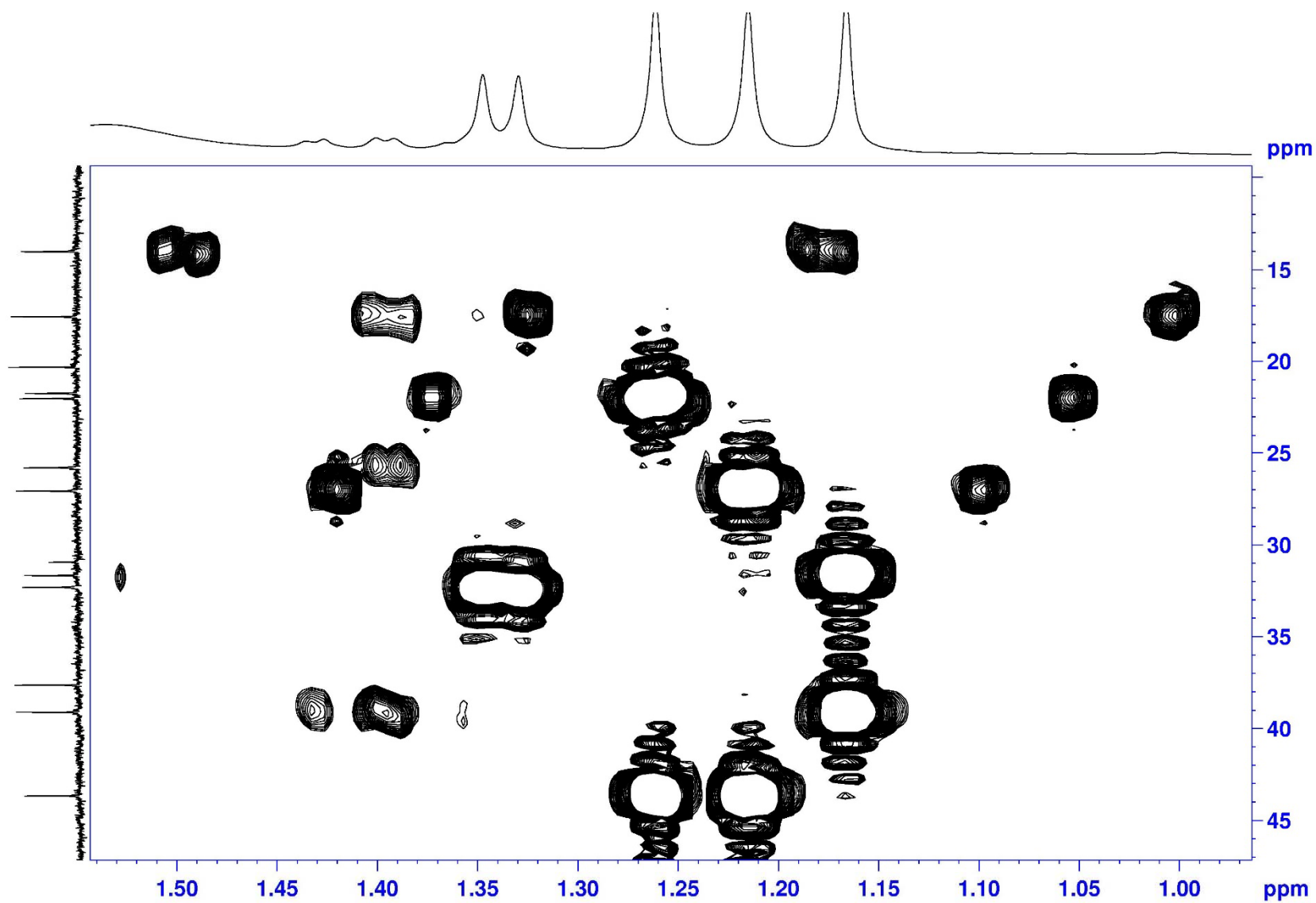
HMBC (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>



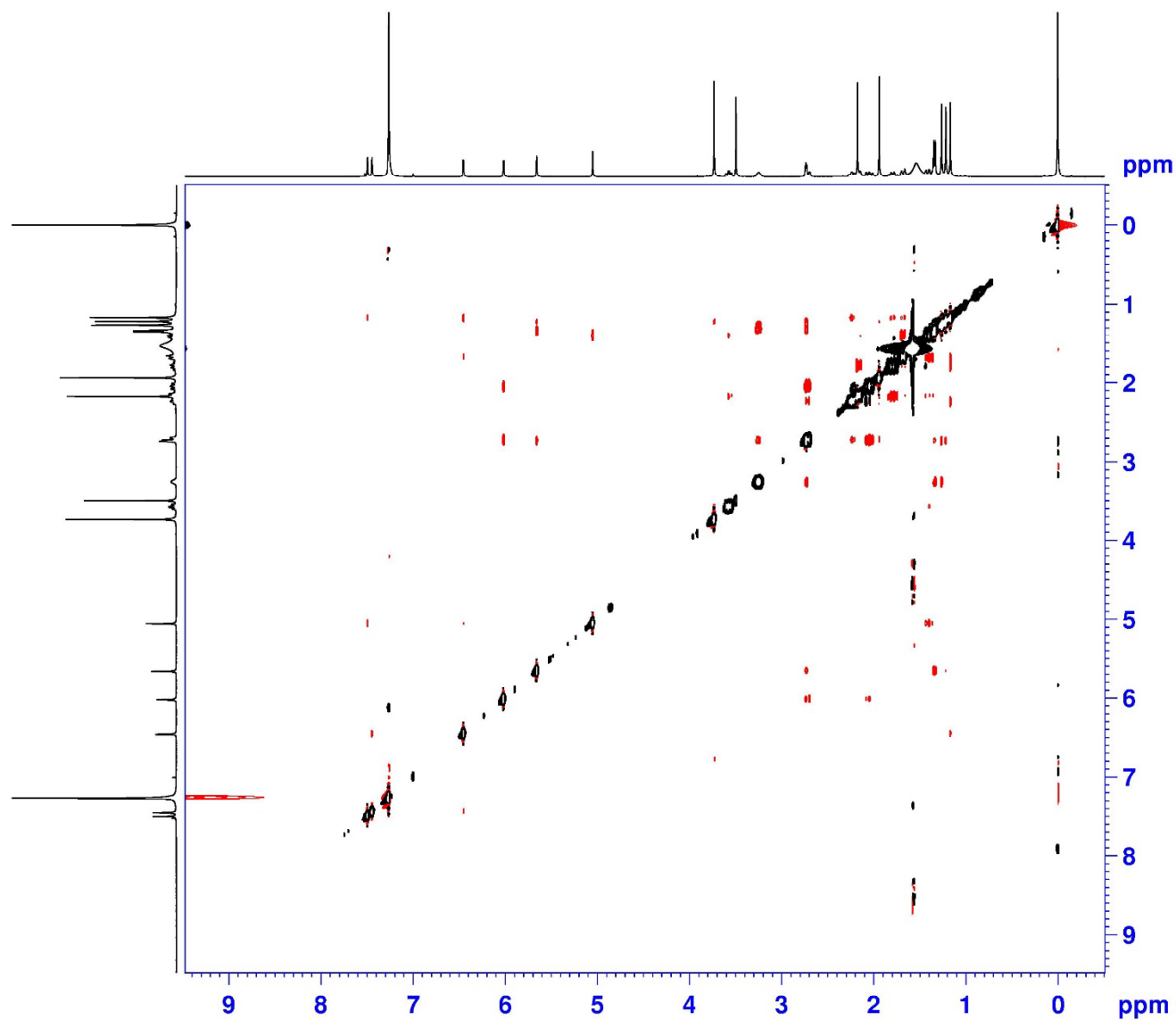
HMBC (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>



HMBC (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$



# NOESY (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>



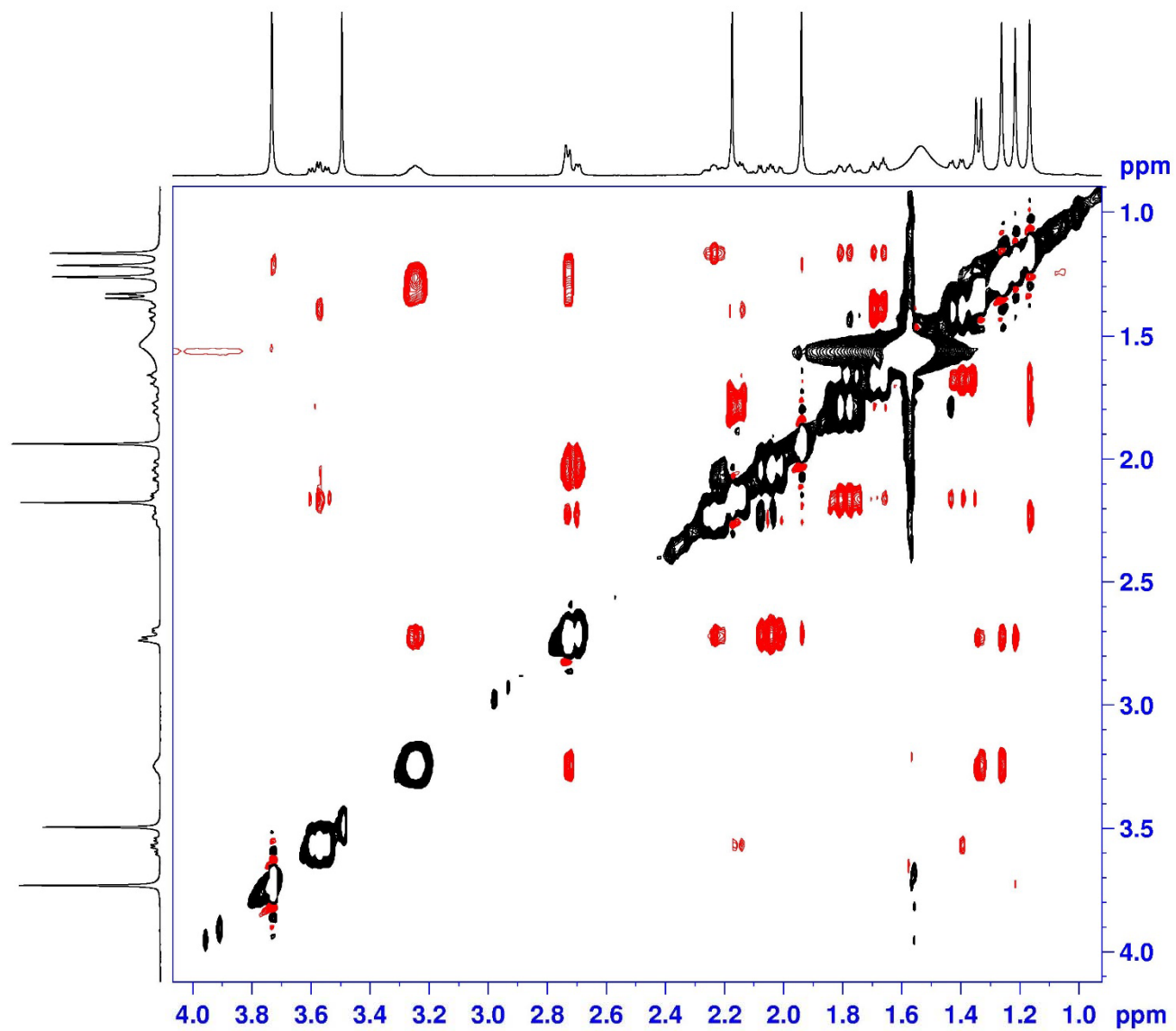
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PROCNO          1
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PULPROG         noesygpphpp
TD              2048
SOLVENT         CDC13
NS              128
DS              32
SWH             4000.000 H
FIDRES          1.953125 H
AQ              0.2560500 s
RG              208.5
DW              125.000 u
DE              10.00 u
TE              297.0 K
D0              0.00011036 s
D1              1.99385595 s
D8              0.30000001 s
D11             0.03000000 s
D12             0.00002000 s
D16             0.00020000 s
IN0             0.00025000 s
    
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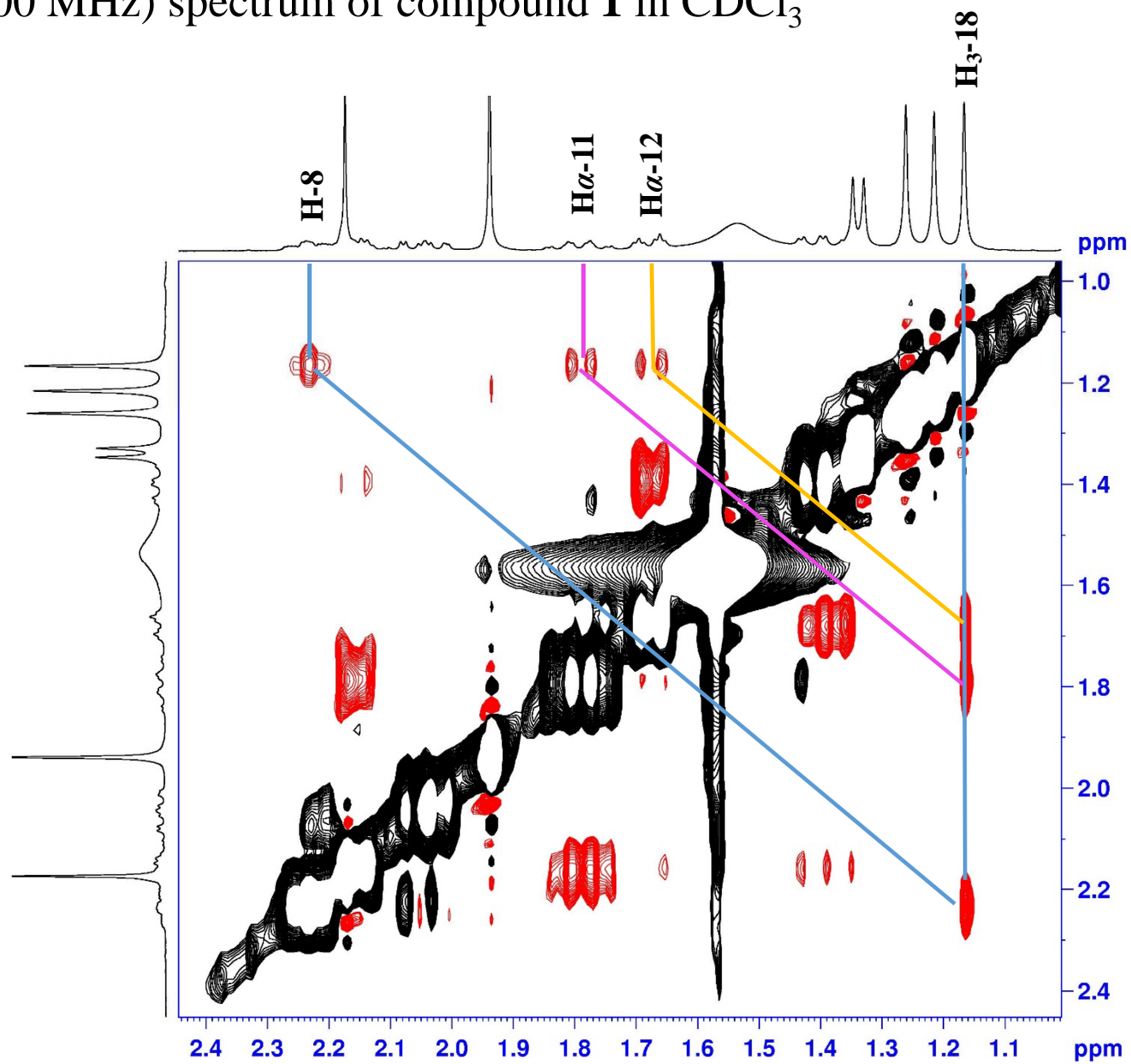
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P17            2500.00 u
ND0             1
TD             256
SFO1          400.1318 M
FIDRES         15.625000 H
SW              9.997 p
FnMODE         States-TPPI
SI             1024
SF            400.1300089 M
WDW            QSINE
SSB             2
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WDW            QSINE
SSB             2
    
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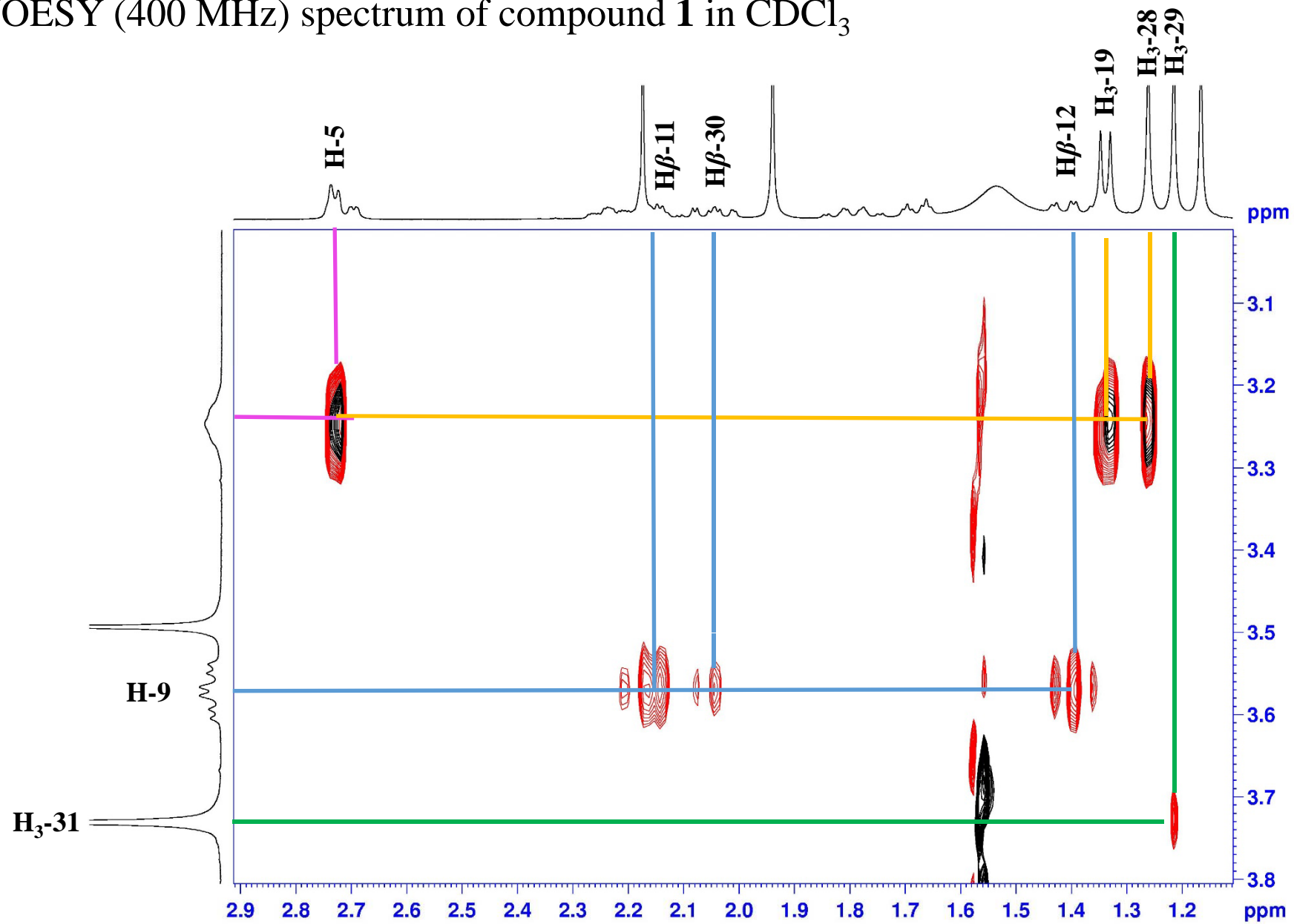
NOESY (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$



NOESY (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$

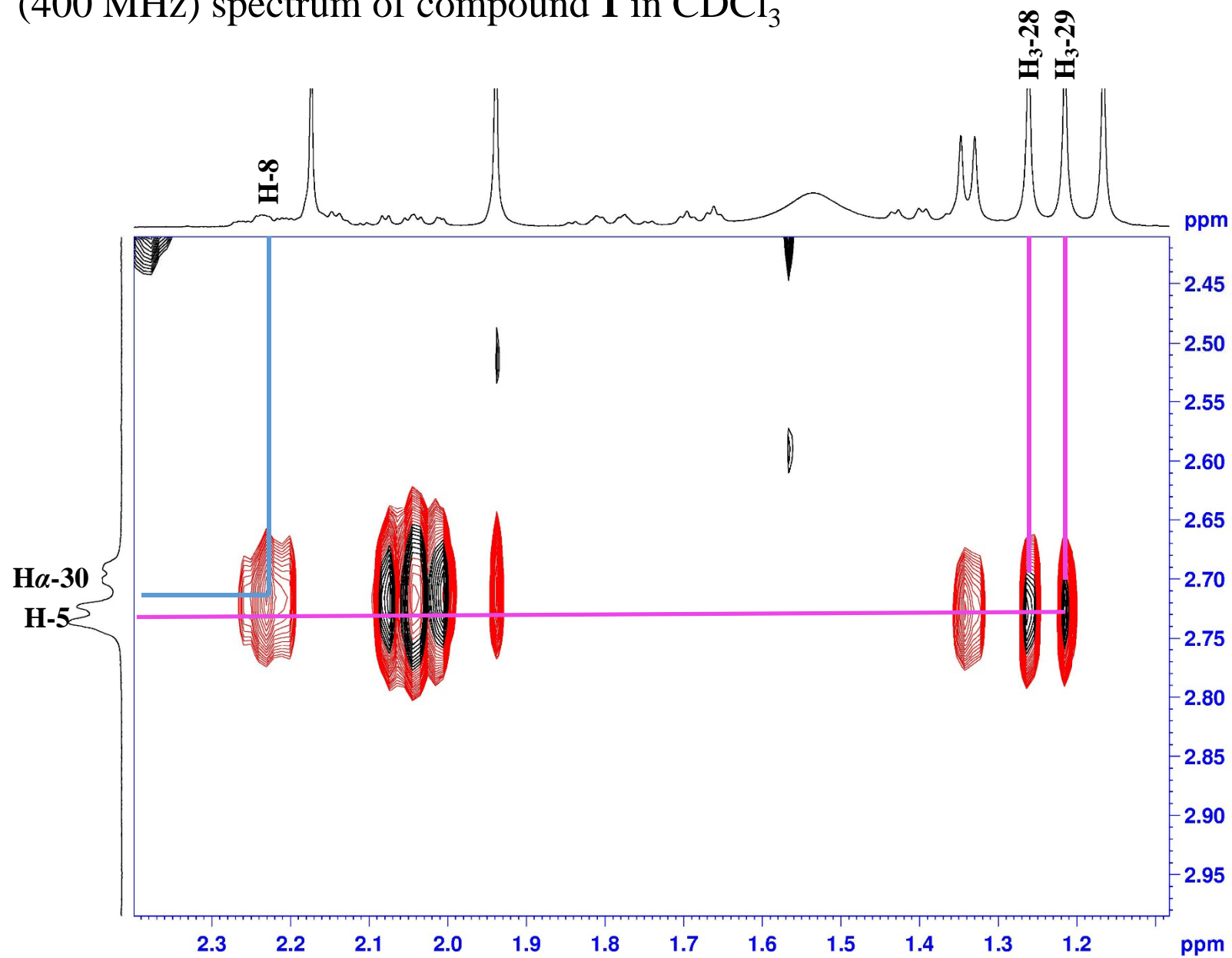


NOESY (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$

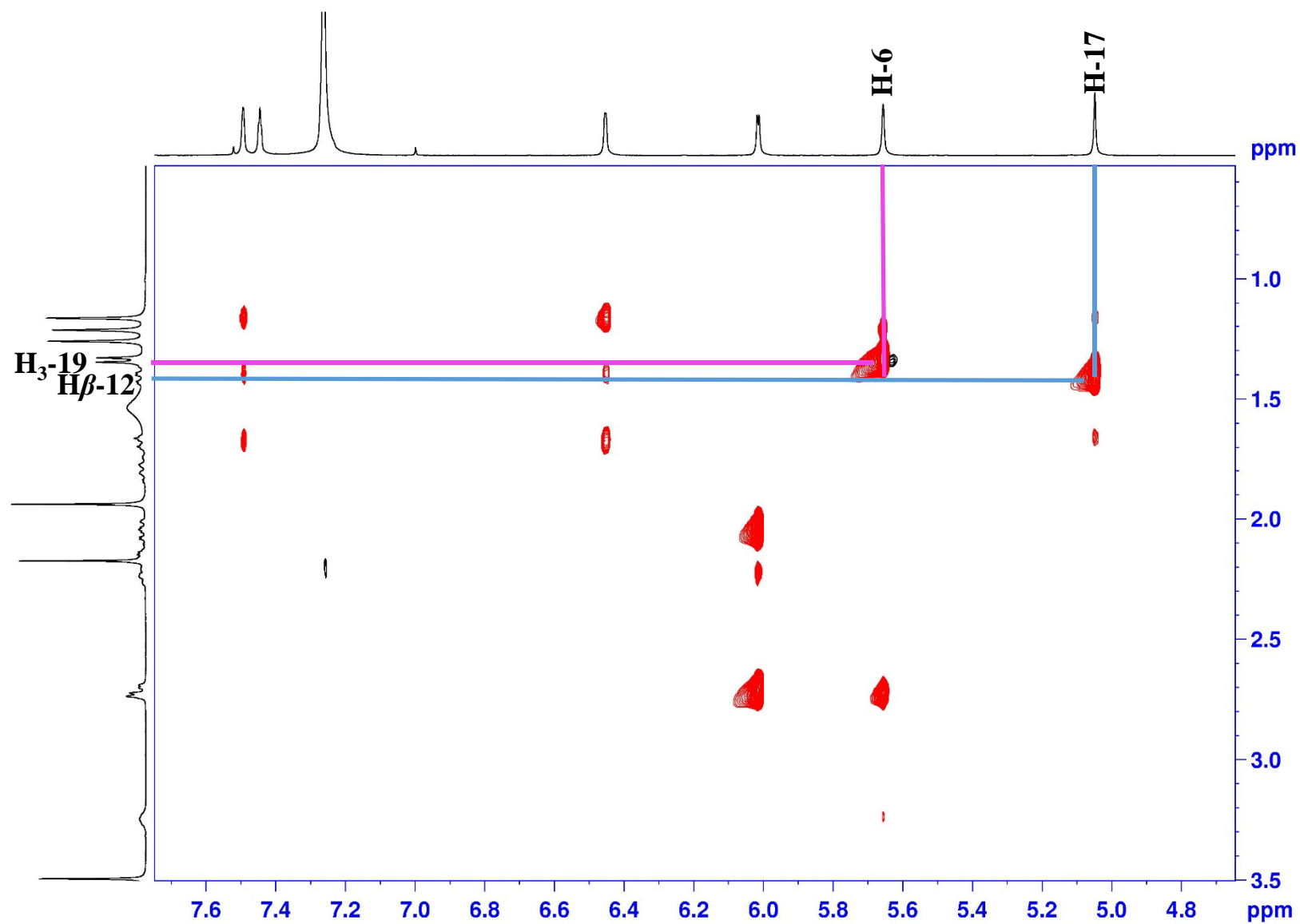




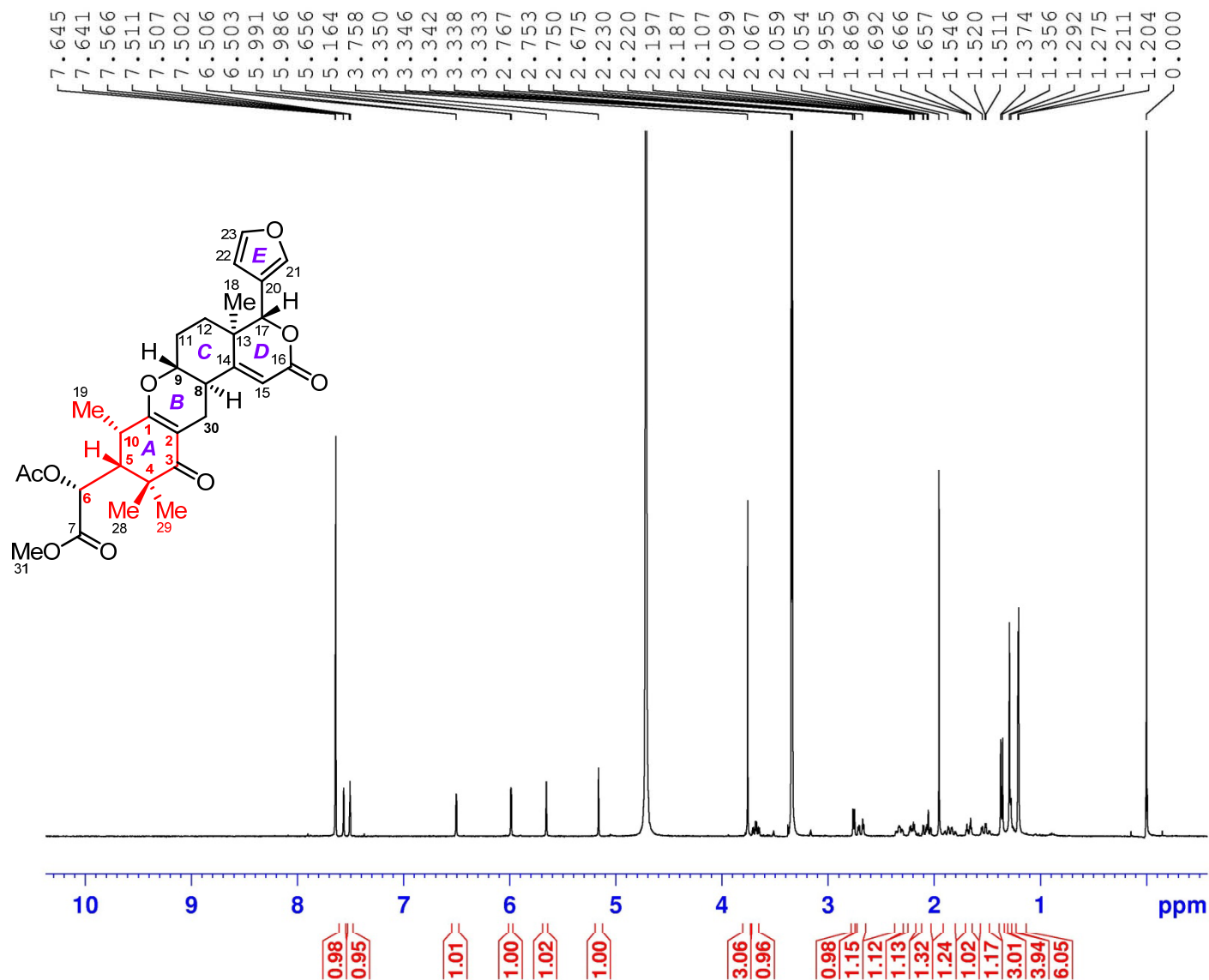
NOESY (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$



NOESY (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3$



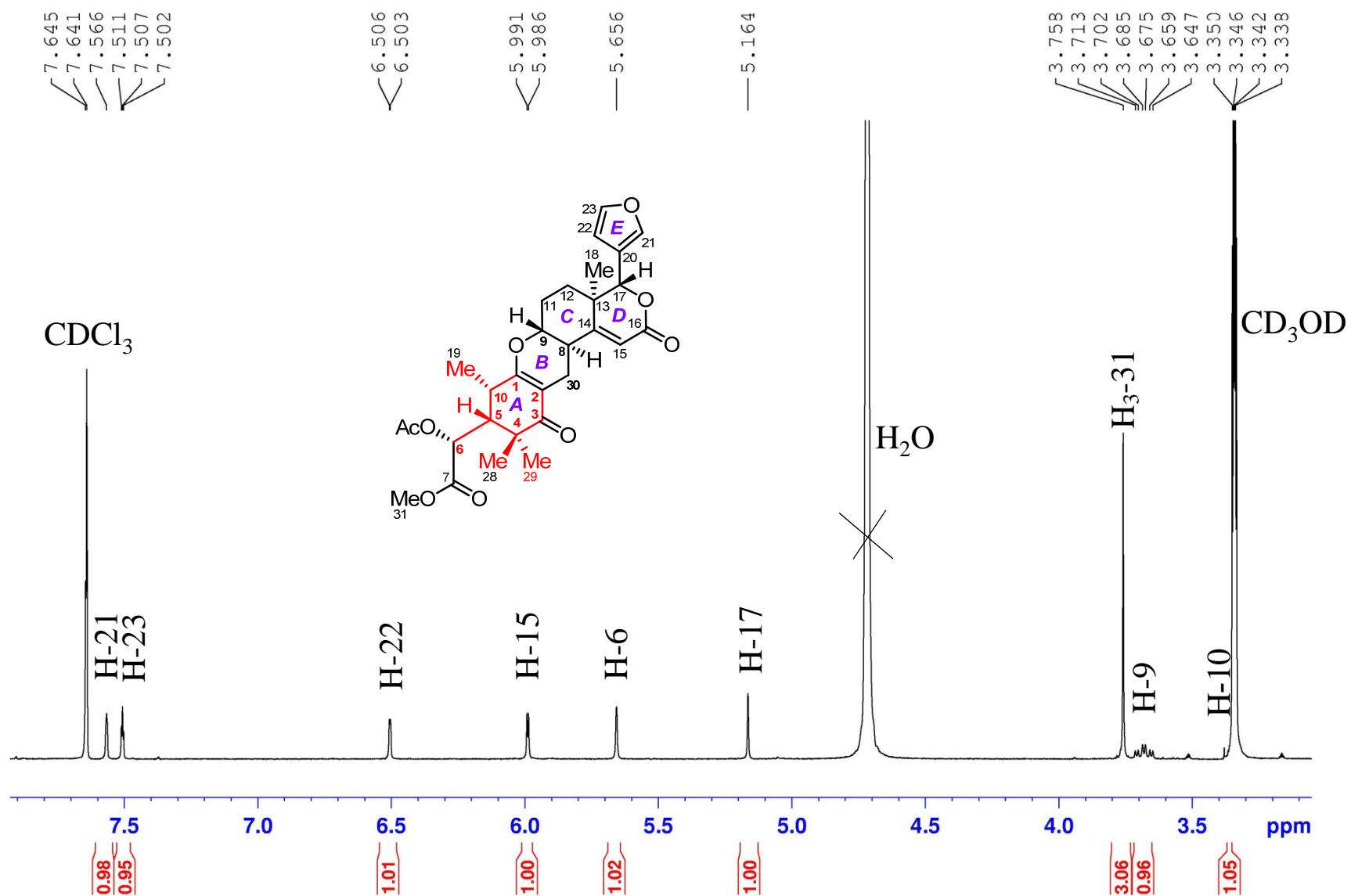
$^1\text{H}$  NMR (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3/\text{CD}_3\text{OD}$  (1:1)



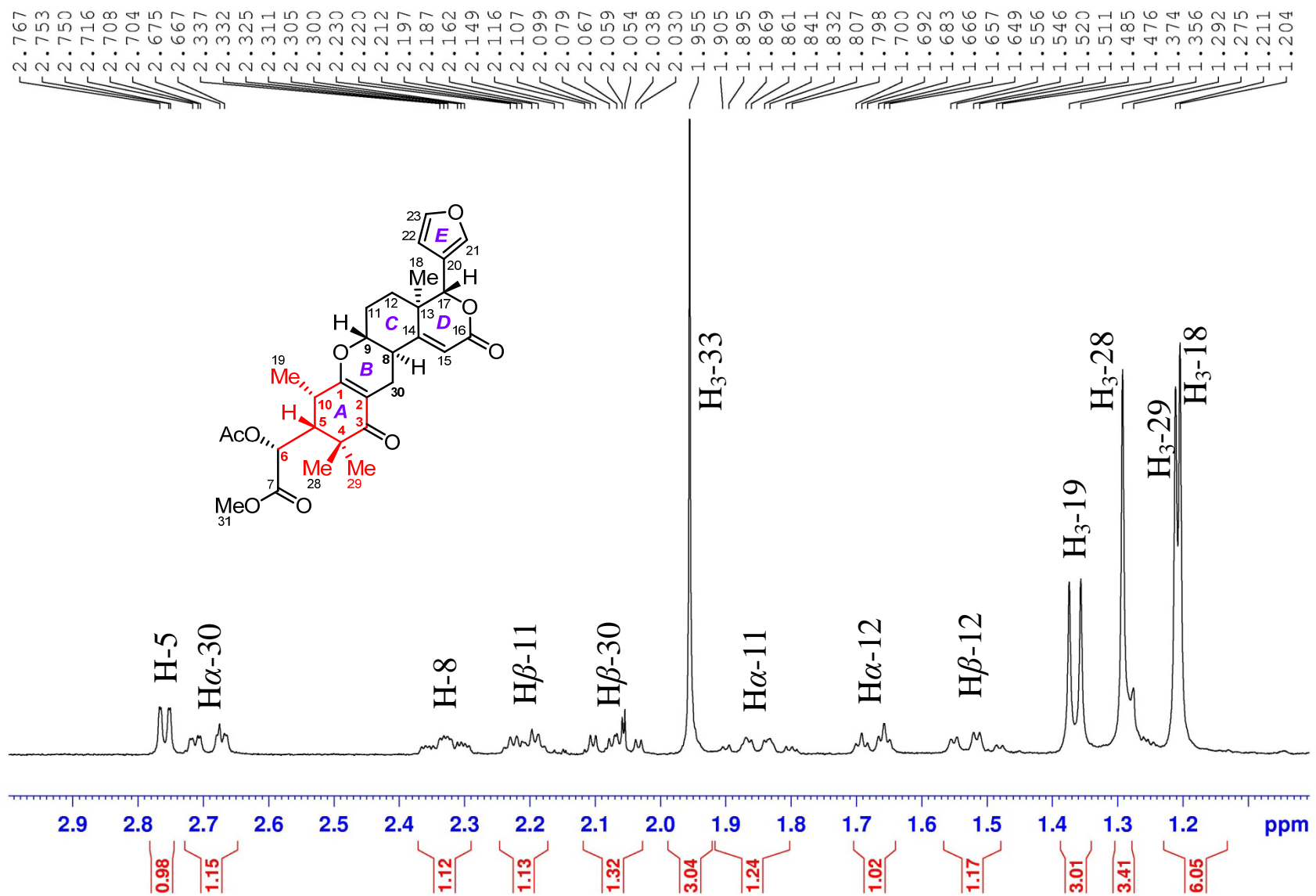
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 PROCNO 1  
 Date\_ 20180629  
 Time 20.14  
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 PROBHD 5 mm CPPBBO BB  
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 TD 65536  
 SOLVENT MeOD  
 NS 16  
 DS 2  
 SWH 8223.685 I  
 FIDRES 0.125483 I  
 AQ 3.9846387 I  
 RG 208.5  
 DW 60.800 I  
 DE 10.00 I  
 TE 297.0 I  
 D1 1.00000000 I  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 400.1324710 I  
 NUC1 1H  
 P1 11.50 I  
 SI 65536  
 SF 400.1299953 I  
 WDW EM  
 SSB 0  
 LB 0.30 I  
 GB 0  
 PC 1.00

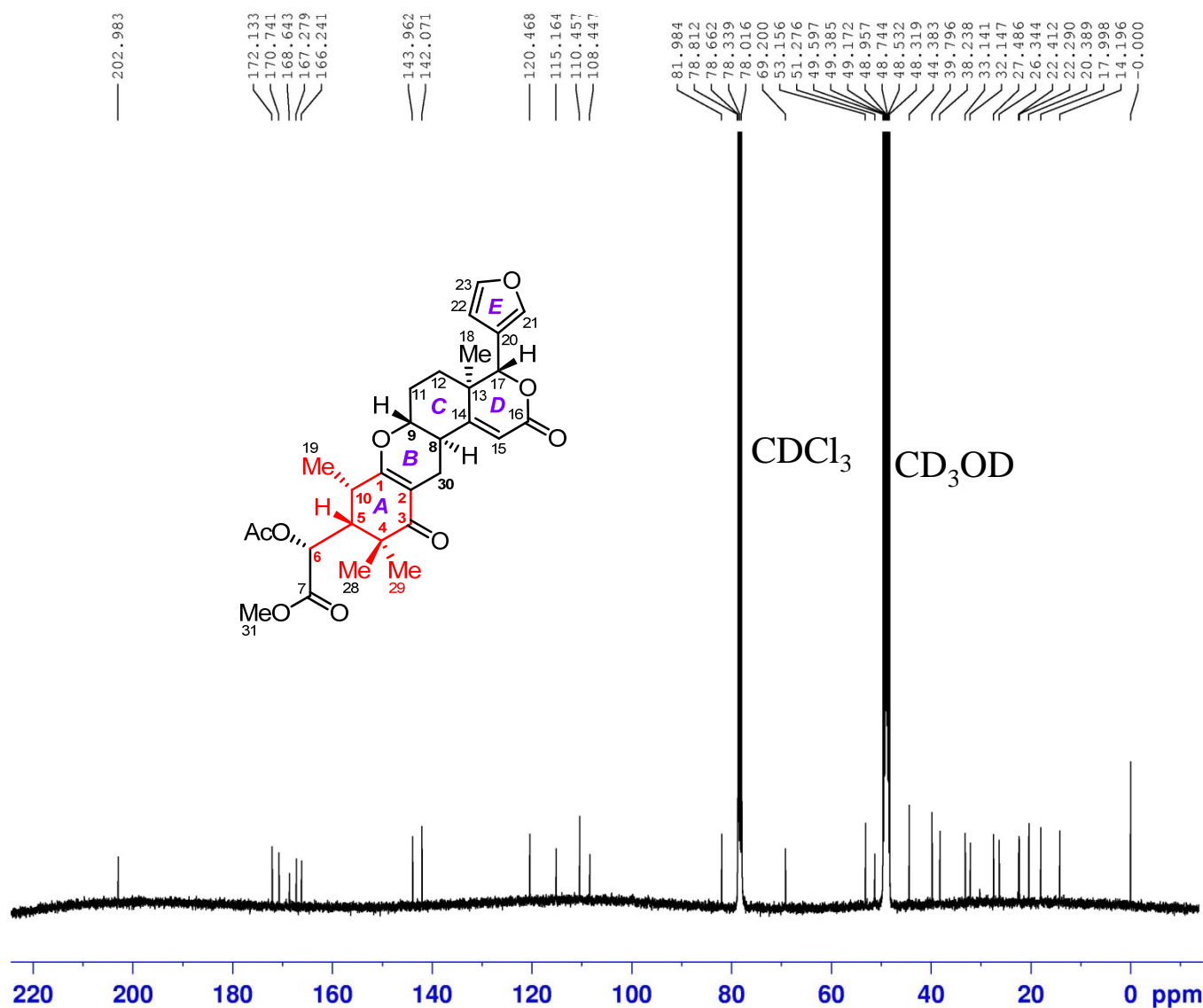
$^1\text{H}$  NMR (400 MHz) spectrum of compound **1** in  $\text{CDCl}_3/\text{CD}_3\text{OD}$  (1:1)



<sup>1</sup>H NMR (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>/CD<sub>3</sub>OD (1:1)



$^{13}\text{C}$  NMR (100 MHz) spectrum of compound **1** in  $\text{CDCl}_3/\text{CD}_3\text{OD}$  (1:1)



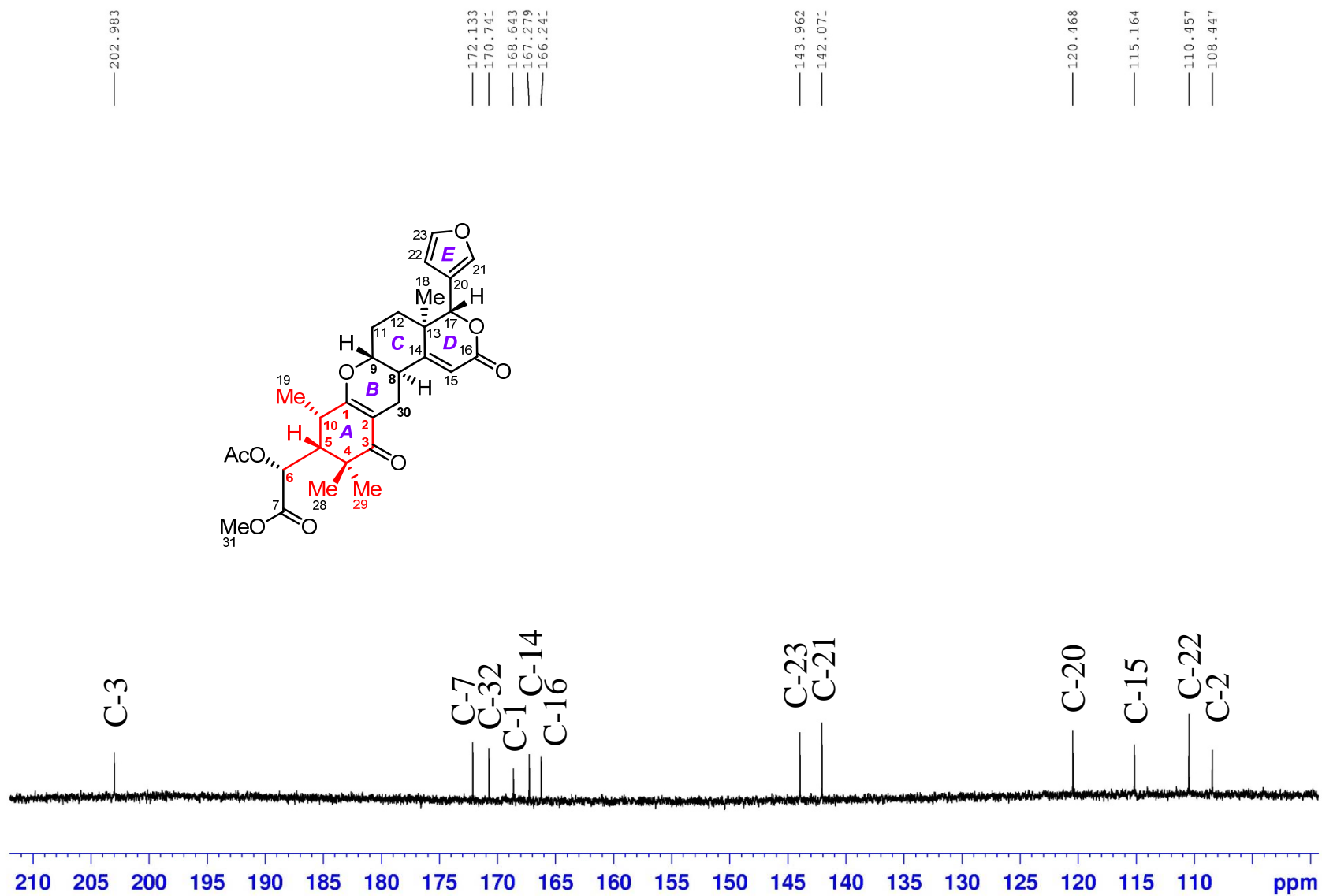
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NAME          lws-23-6
EXPNO          10
PROCNO         1
Date_          20180706
Time           10.18
INSTRUM        spect
PROBHD         5 mm CPPBBO BB
PULPROG        zgpg30
TD             65536
SOLVENT         MeOD
NS             20500
DS              4
SWH            24038.461 H:
FIDRES         0.366798 H:
AQ            1.3631988 s:
RG             85.34
DW            20.800 u:
DE            18.00 u:
TE            297.0 K
D1            2.00000000 s:
D11           0.03000000 s:
TD0            1
    
```

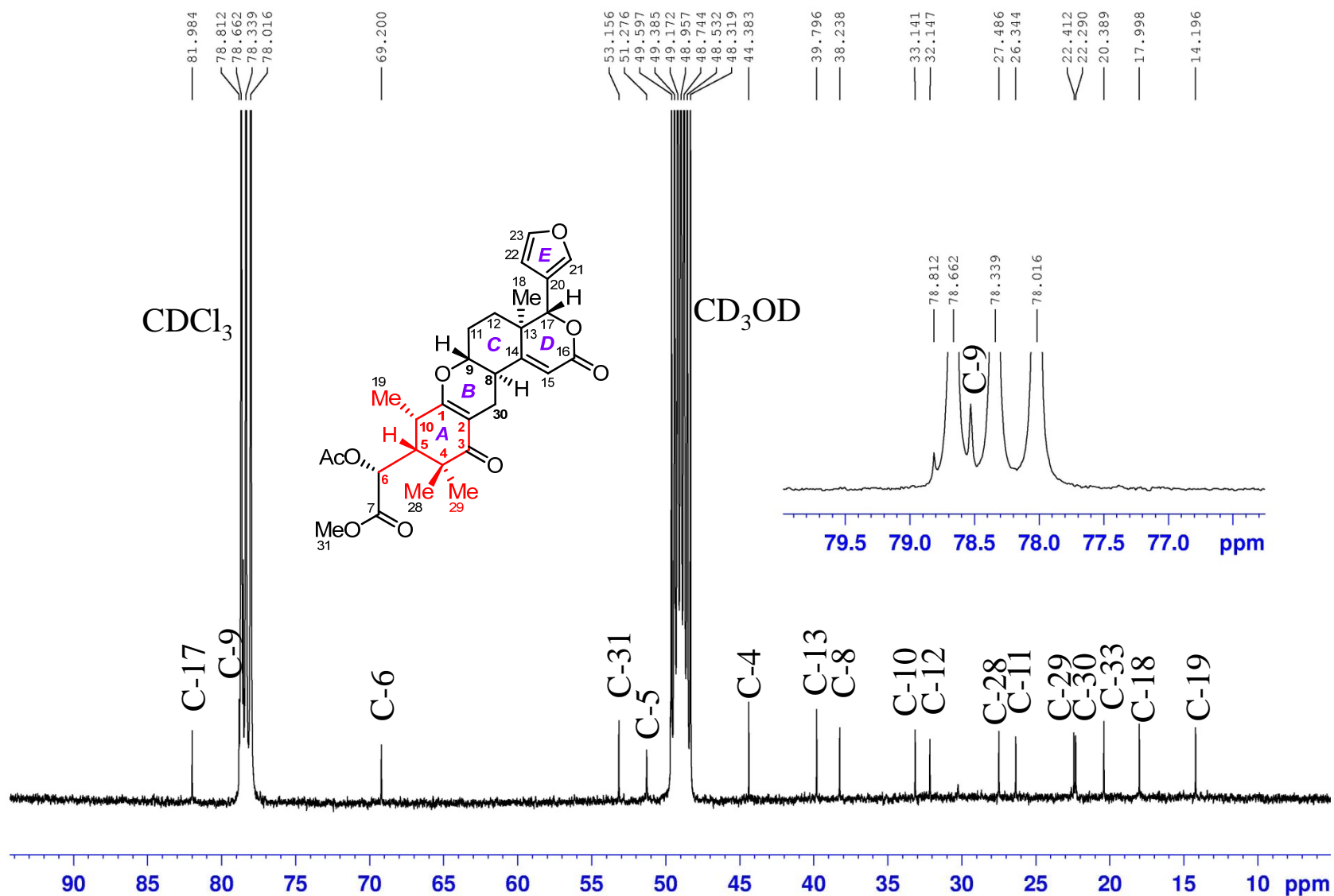
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===== CHANNEL f1 =====
SF01          100.6233324 MI
NUC1           13C
P1            10.00 u:
SI            32768
SF            100.6126911 MI
WDW            EM
SSB            0
LB            1.00 H:
GB            0
PC            1.40
    
```

$^{13}\text{C}$  NMR (100 MHz) spectrum of compound **1** in  $\text{CDCl}_3/\text{CD}_3\text{OD}$  (1:1)

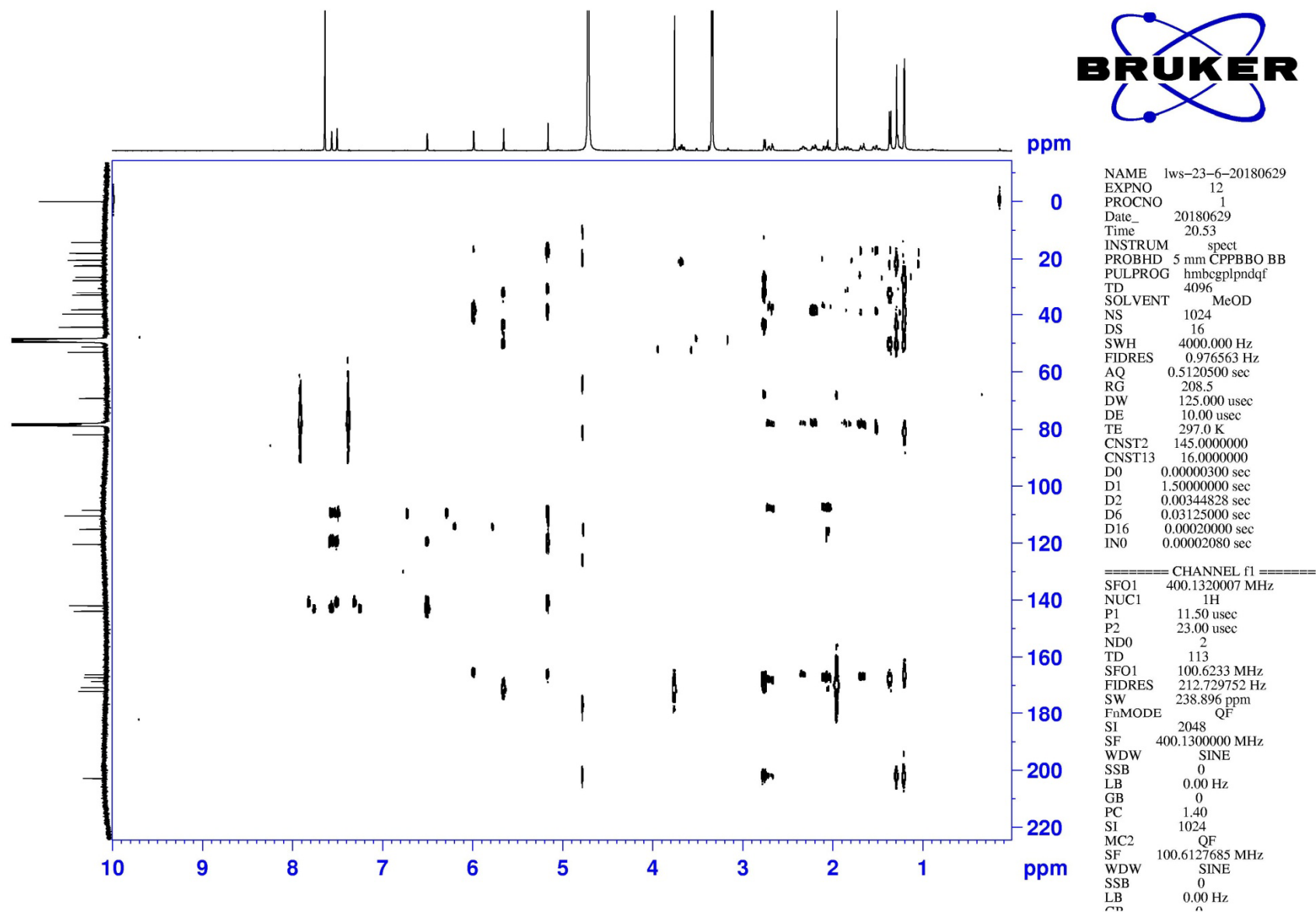


$^{13}\text{C}$  NMR (100 MHz) spectrum of compound **1** in  $\text{CDCl}_3/\text{CD}_3\text{OD}$  (1:1)

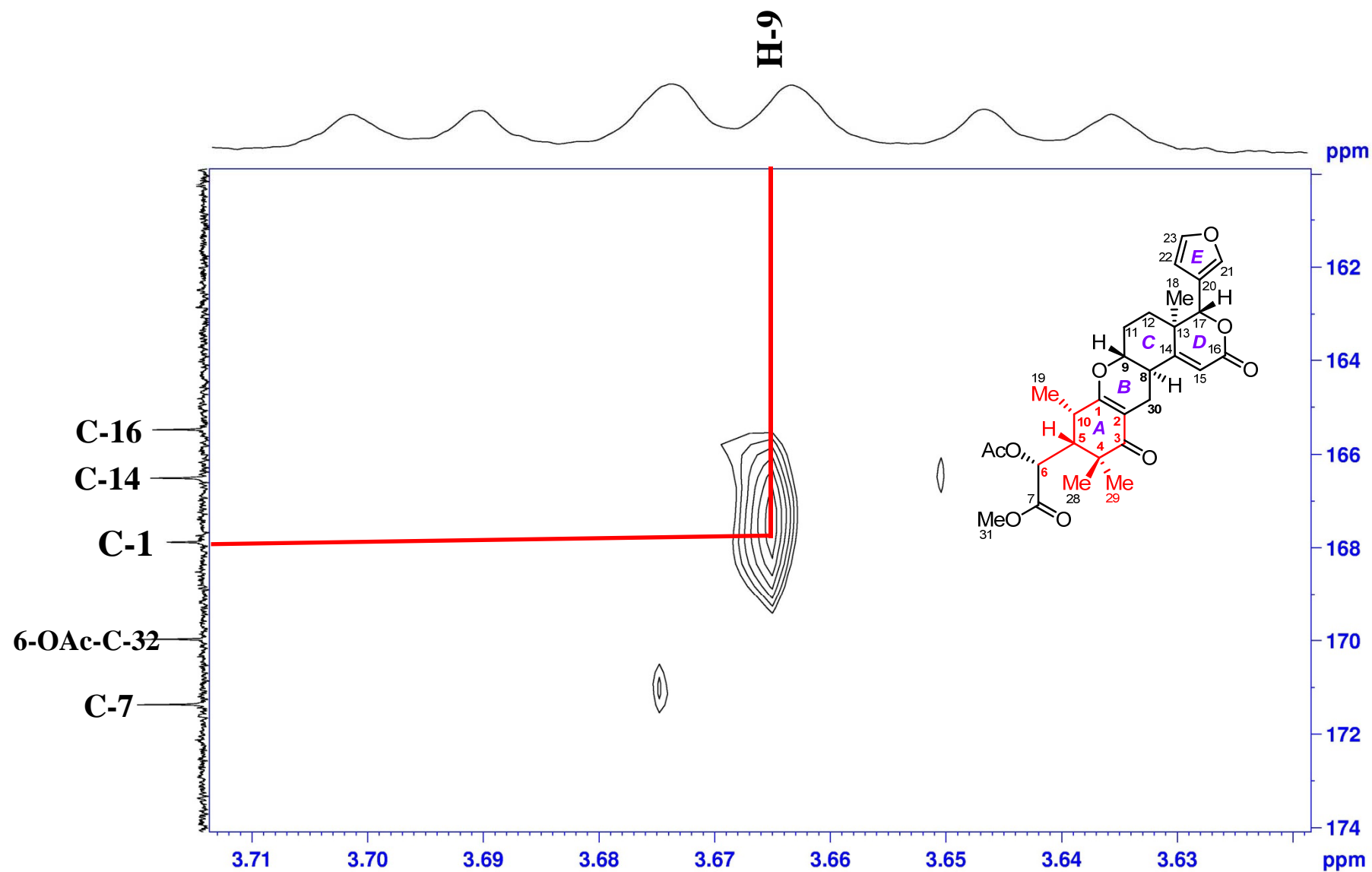




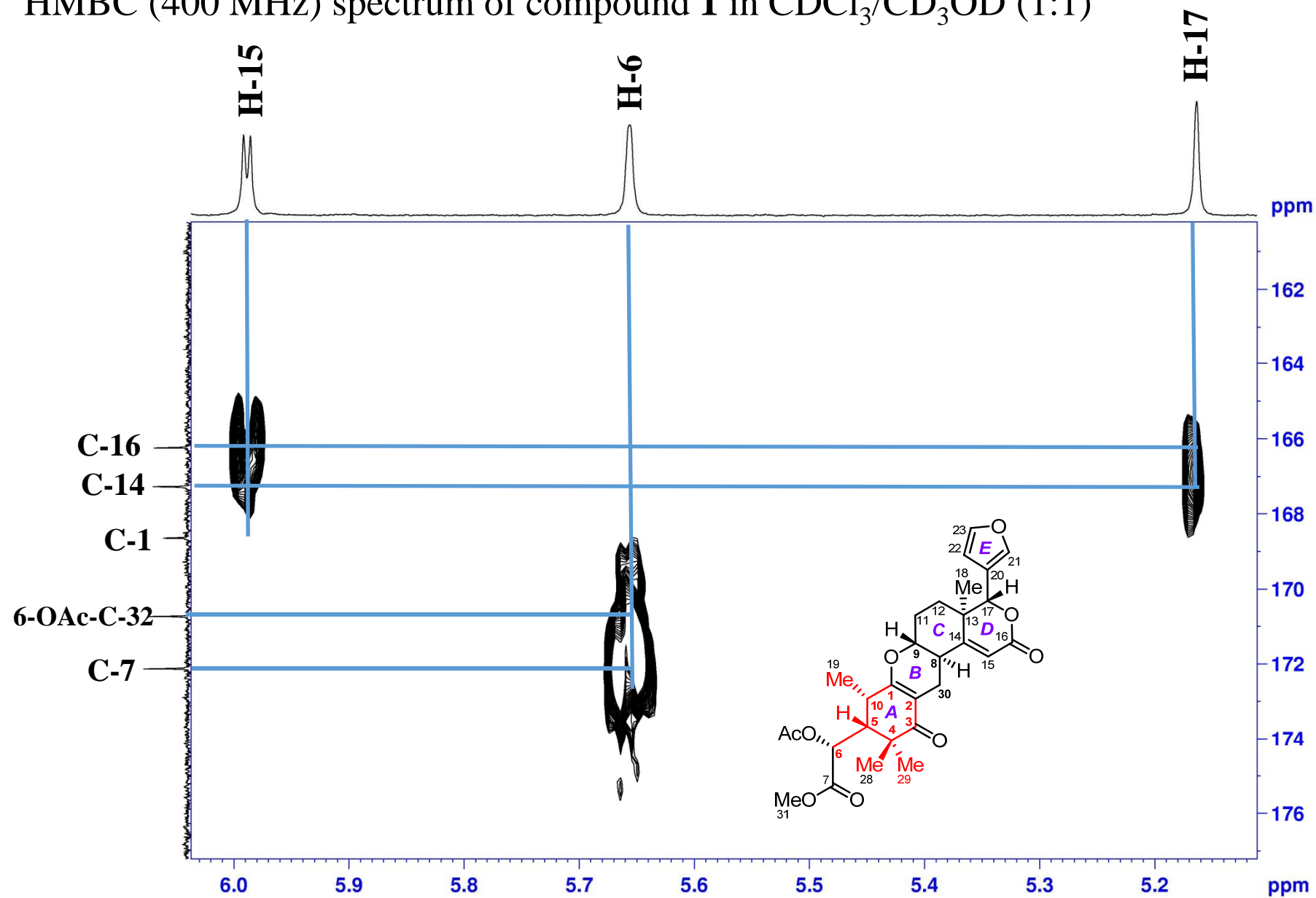
# HMBC (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>/CD<sub>3</sub>OD (1:1)



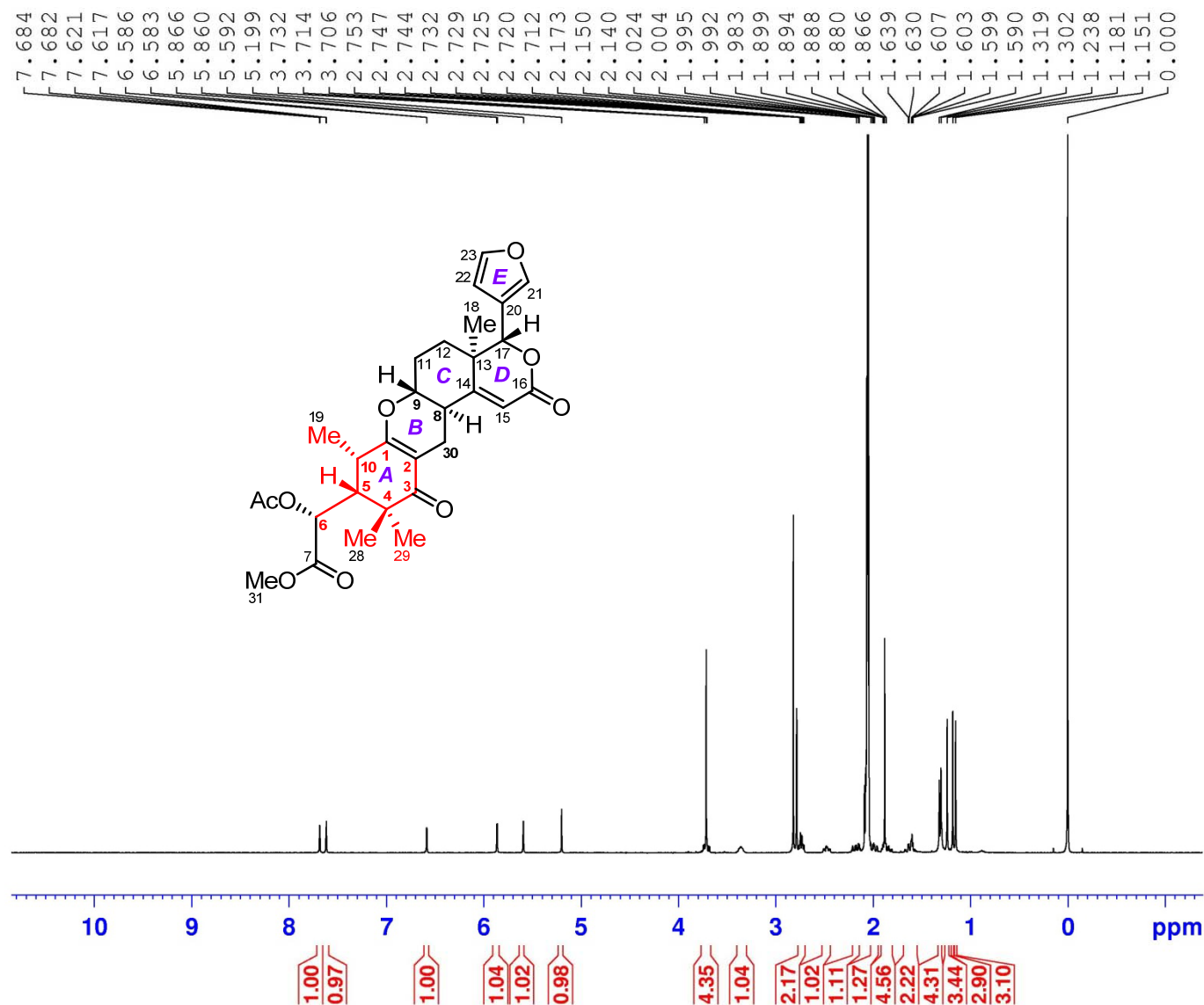
HMBC (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>/CD<sub>3</sub>OD (1:1)



HMBC (400 MHz) spectrum of compound **1** in CDCl<sub>3</sub>/CD<sub>3</sub>OD (1:1)



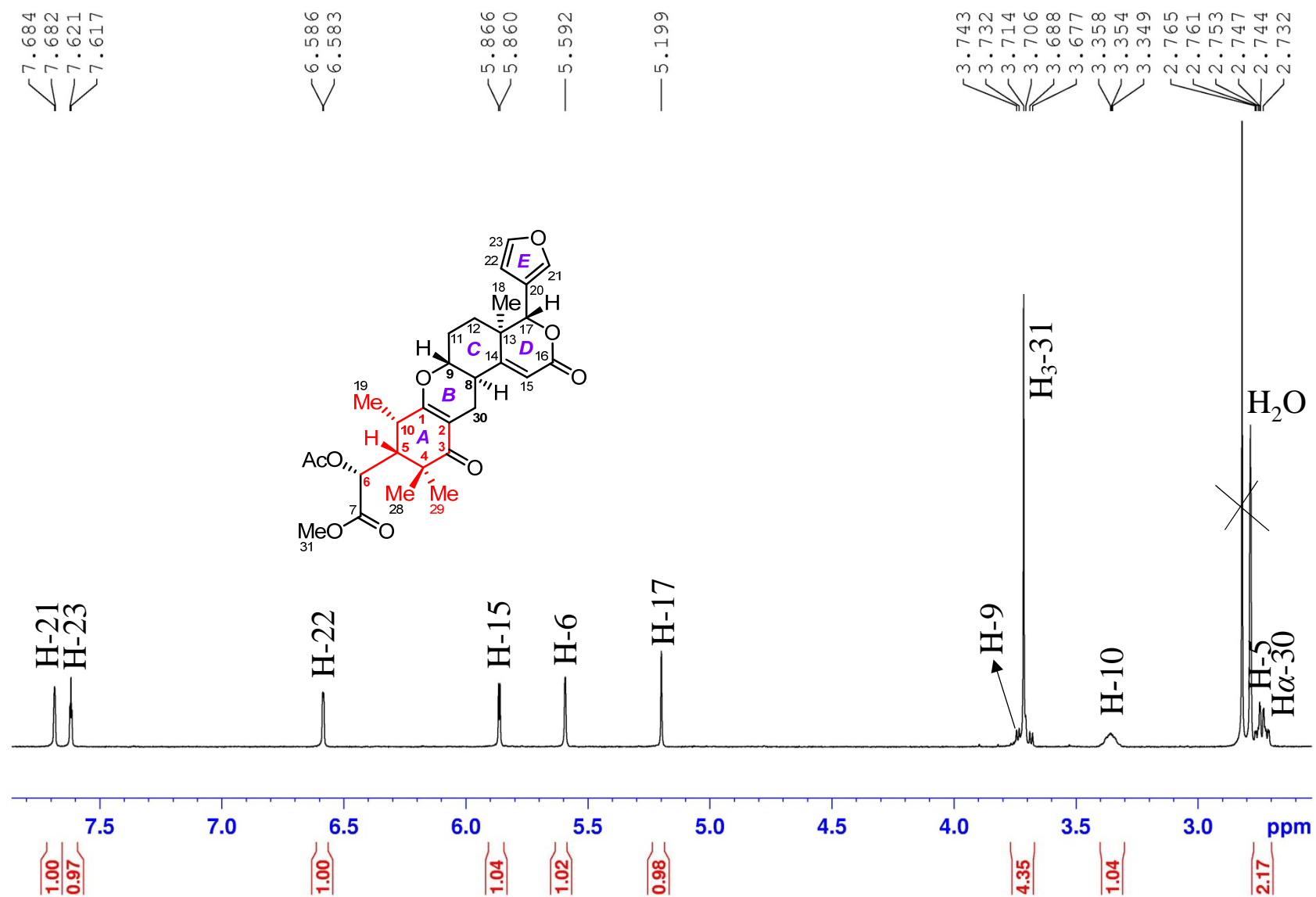
# $^1\text{H}$ NMR (400 MHz) spectrum of compound **1** in Acetone- $d_6$



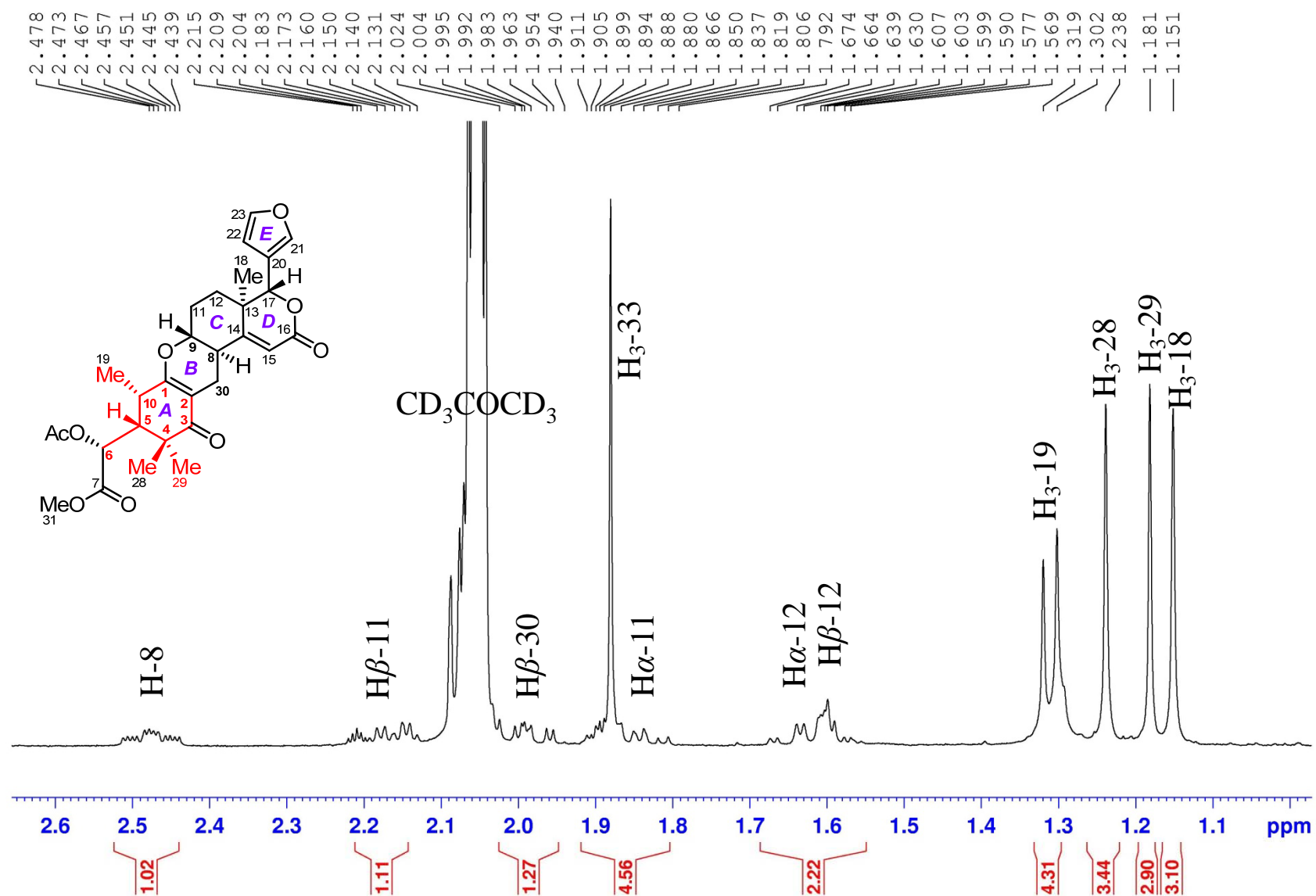
NAME 23-6-5-1-1-Acetc  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20180316  
 Time 19.16  
 INSTRUM spect  
 PROBHD 5 mm CPPBBO BB  
 PULPROG zg30  
 TD 65536  
 SOLVENT Acetone  
 NS 16  
 DS 2  
 SWH 8223.685 E  
 FIDRES 0.125483 E  
 AQ 3.9846387 s  
 RG 208.5  
 DW 60.800  $\mu$   
 DE 10.00  $\mu$   
 TE 297.0 K  
 D1 1.00000000 s  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 400.1324710 M  
 NUC1  $^1\text{H}$   
 P1 11.50  $\mu$   
 SI 65536  
 SF 400.1300055 M  
 WDW EM  
 SSB 0  
 LB 0.30 E  
 GB 0  
 PC 1.00

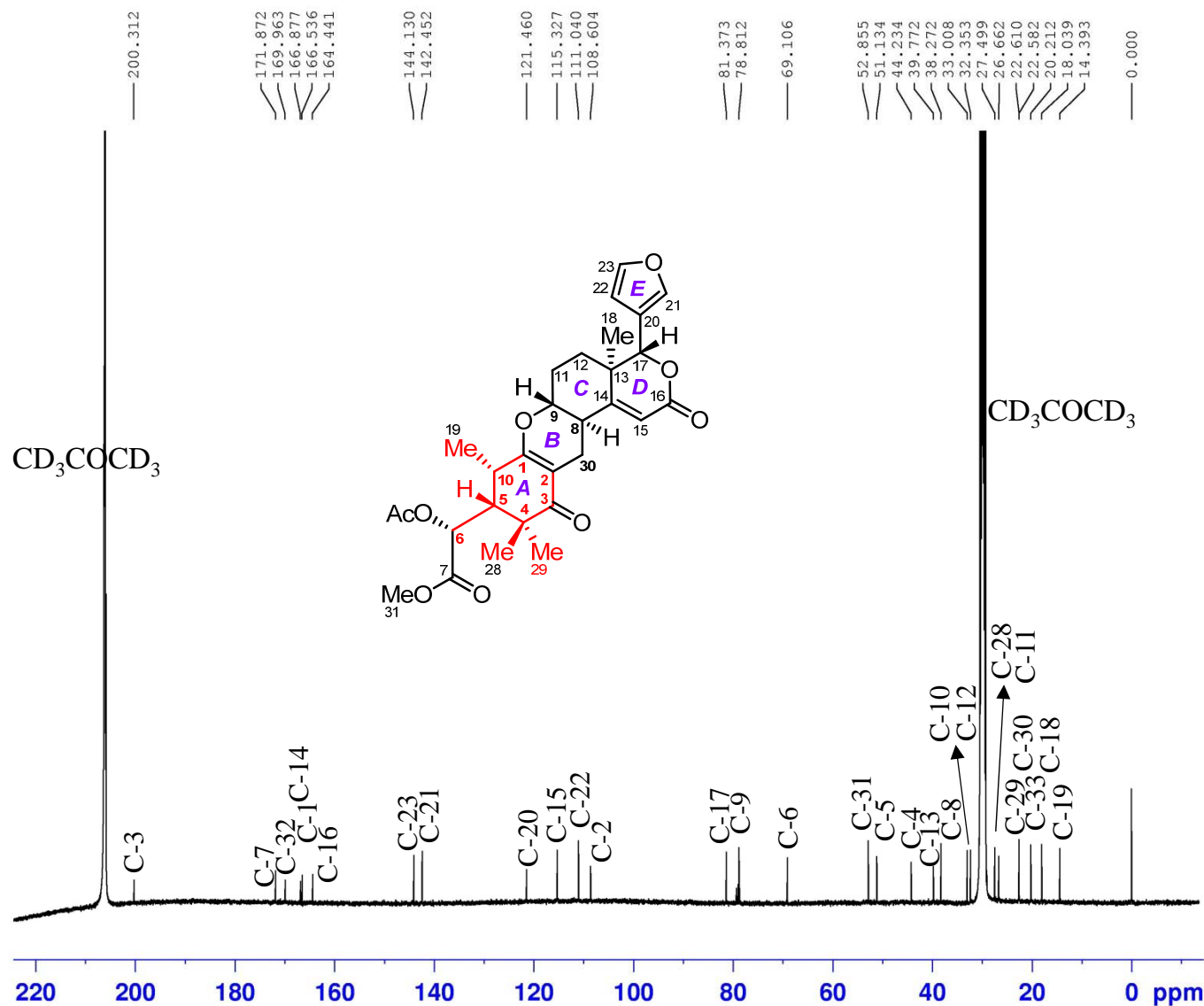
$^1\text{H}$  NMR (400 MHz) spectrum of compound **1** in Acetone- $d_6$



$^1\text{H}$  NMR (400 MHz) spectrum of compound **1** in Acetone- $d_6$



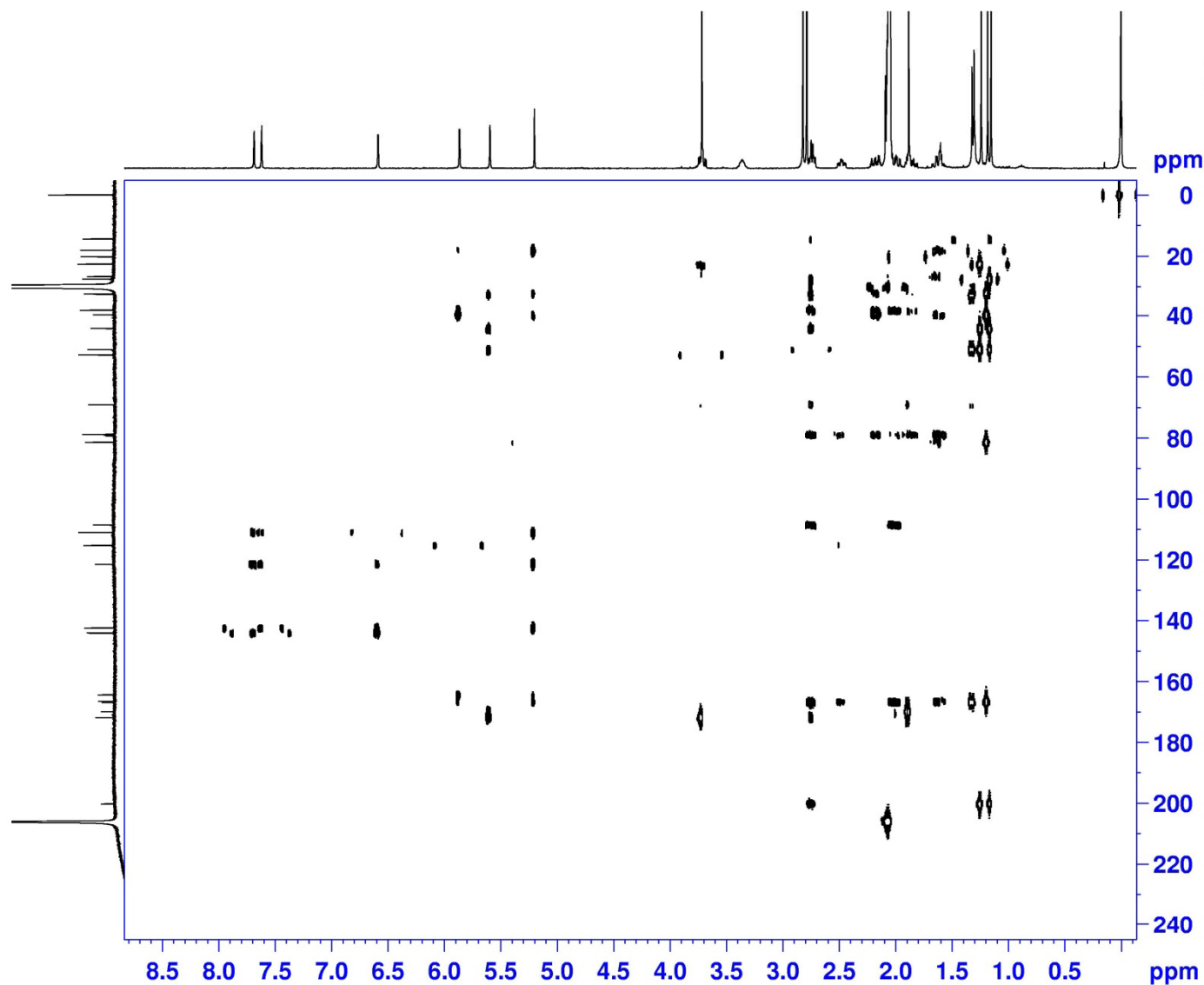
$^{13}\text{C}$  NMR (100 MHz) spectrum of compound **1** in Acetone- $d_6$



NAME 23-6-5-1-1-Aceto  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20180714  
 Time 21.52  
 INSTRUM spect  
 PROBHD 5 mm CPPBBO BB  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 30000  
 DS 4  
 SWH 24038.461 H:  
 FIDRES 0.366798 H:  
 AQ 1.3631988 s:  
 RG 117.37  
 DW 20.800 u:  
 DE 18.00 u:  
 TE 297.0 K  
 D1 2.00000000 s:  
 D11 0.03000000 s:  
 TD0 1

===== CHANNEL f1 =====  
 SF01 100.6233324 MI  
 NUC1 13C  
 P1 10.00 u:  
 SI 32768  
 SF 100.6126779 MI  
 WDW EM  
 SSB 0  
 LB 1.00 H:  
 GB 0  
 PC 1.40

# HMBC (400 MHz) spectrum of compound **1** in Acetone- $d_6$

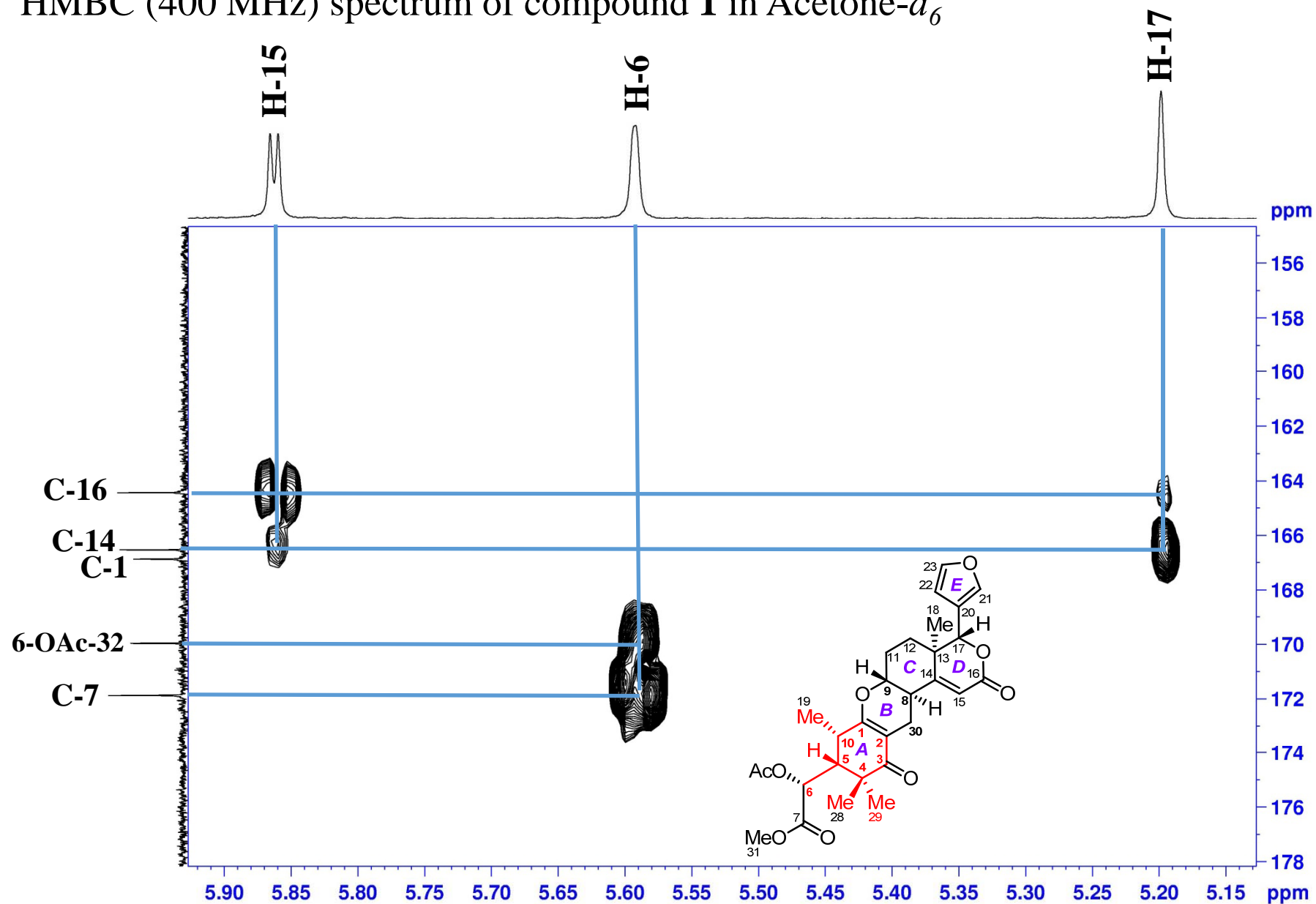


NAME 23-6-5-1-1-Acetone  
 EXPNO 6  
 PROCNO 1  
 Date\_ 20180316  
 Time 19.36  
 INSTRUM spect  
 PROBHD 5 mm CPBBO BB  
 PULPROG hmbcgp1pdqf  
 TD 4096  
 SOLVENT Acetone  
 NS 512  
 DS 16  
 SWH 5197.505 Hz  
 FIDRES 1.268922 Hz  
 AQ 0.3940852 sec  
 RG 208.5  
 DW 96.200 usec  
 DE 10.00 usec  
 TE 297.0 K  
 CNST2 145.0000000  
 CNST13 10.0000000  
 D0 0.00000300 sec  
 D1 1.50000000 sec  
 D2 0.00344828 sec  
 D6 0.05000000 sec  
 D16 0.00020000 sec  
 IN0 0.00002080 sec

===== CHANNEL f1 =====  
 SFO1 400.1323208 MHz  
 NUC1 1H  
 P1 11.50 usec  
 P2 23.00 usec  
 ND0 2  
 TD 128  
 SFO1 100.6233 MHz  
 FIDRES 187.800476 Hz  
 SW 238.896 ppm  
 F0MODE QF  
 SI 2048  
 SF 400.1300000 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40  
 SI 1024  
 MC2 QF  
 SF 100.6126779 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0



# HMBC (400 MHz) spectrum of compound **1** in Acetone- $d_6$



# HR-ESIMS for compound 2

## Mass Spectrum SmartFormula Report

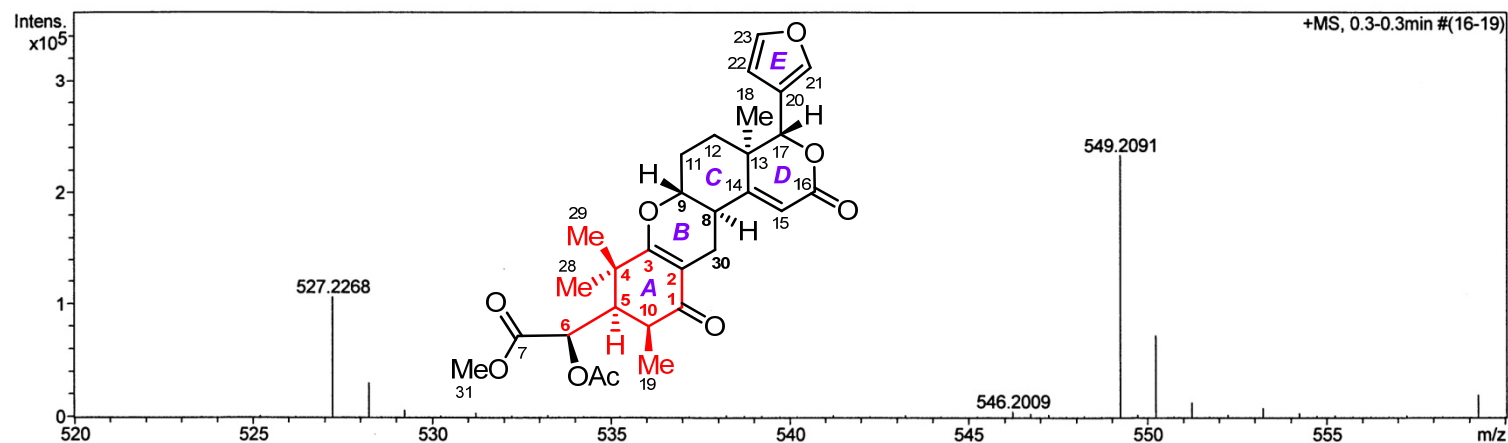
### Analysis Info

Analysis Name D:\Data\MS\data\201412\liwanshan\_lws-43\_pos.d  
Method POS\_100-2000\_Direct Infusion.m  
Sample Name SCSIO  
Comment

Acquisition Date 12/2/2014 4:04:24 PM  
Operator SCSIO  
Instrument / Ser# maXis 29

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e <sup>-</sup> Conf	mSigma	Std I	Std Mean m/z	Std VarNor m	Std m/z Diff	Std Comb Dev
527.2268	1	C <sub>29</sub> H <sub>35</sub> O <sub>9</sub>	527.2276	1.4	1.7	12.5	ok	even	19.1	33.1	1.0	10.5	1.2	842.7
549.2091	1	C <sub>29</sub> H <sub>34</sub> NaO <sub>9</sub>	549.2095	0.8	1.0	12.5	ok	even	7.2	13.9	0.6	5.2	0.8	842.7
1053.4471	1	C <sub>58</sub> H <sub>69</sub> O <sub>18</sub>	1053.4478	0.7	1.4	24.5	ok	even	33.3	35.7	3.1	19.3	1.8	842.7
1075.4308	1	C <sub>58</sub> H <sub>68</sub> NaO <sub>18</sub>	1075.4298	-1.0	-0.5	24.5	ok	even	20.2	21.9	1.8	10.8	1.2	842.7

# HR-ESIMS for compound 2

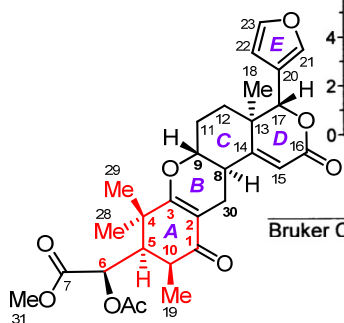
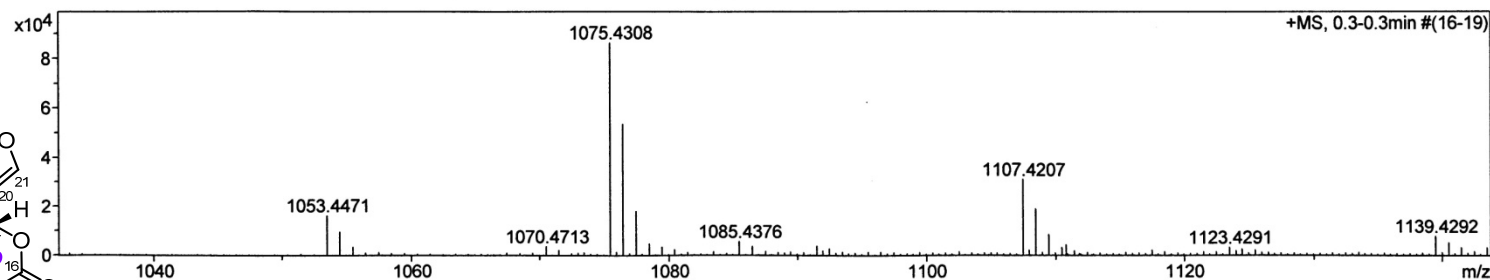
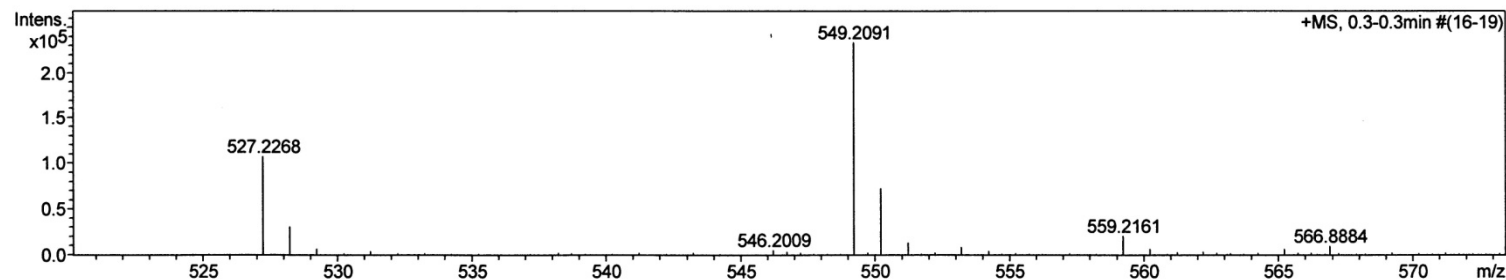
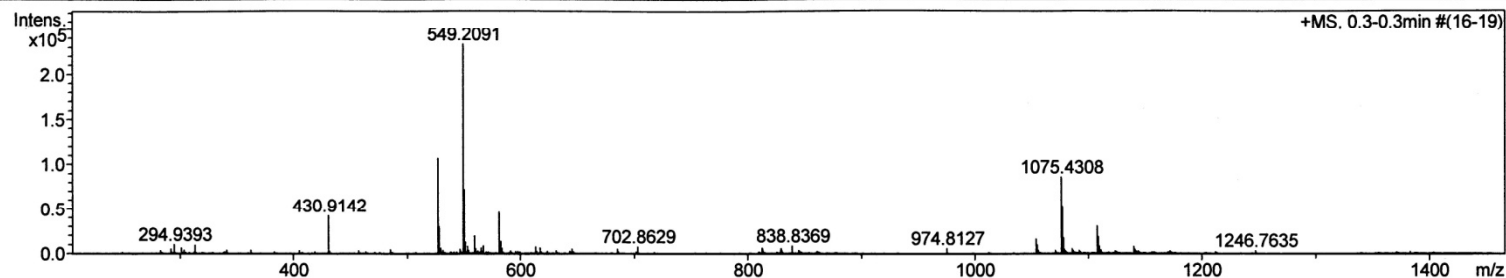
## Generic Display Report

### Analysis Info

Analysis Name D:\Data\MS\data\201412\liwanshan\_lws-43\_pos.d  
Method POS\_100-2000\_Dirrect Infusion.m  
Sample Name SCSIO  
Comment

Acquisition Date 12/2/2014 4:04:24 PM

Operator SCSIO  
Instrument maXis

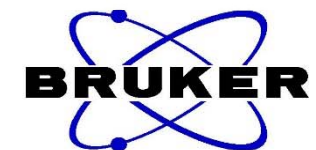
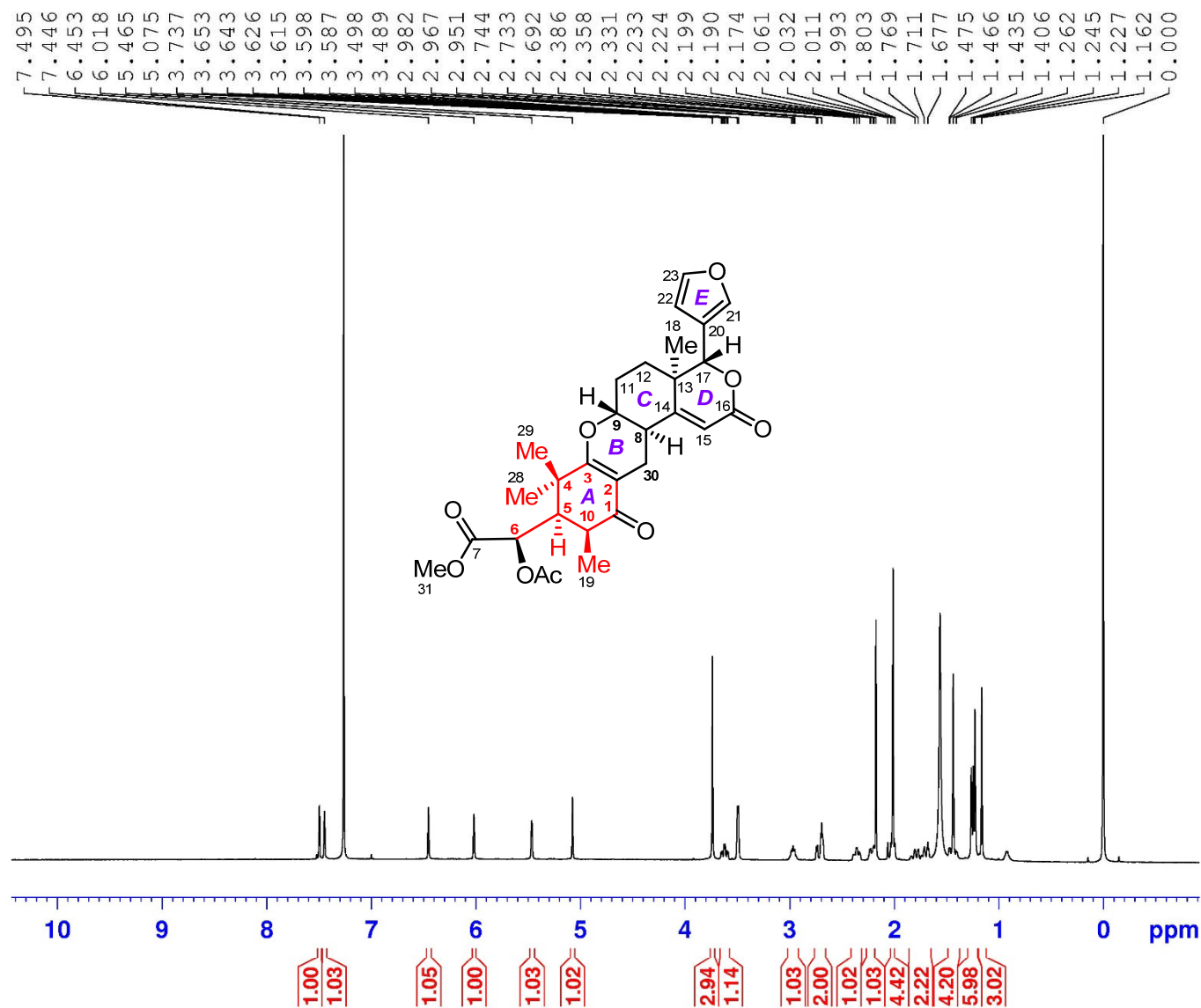


Bruker Compass DataAnalysis 4.0

printed: 12/2/2014 4:11:35 PM

Page 1 of 1

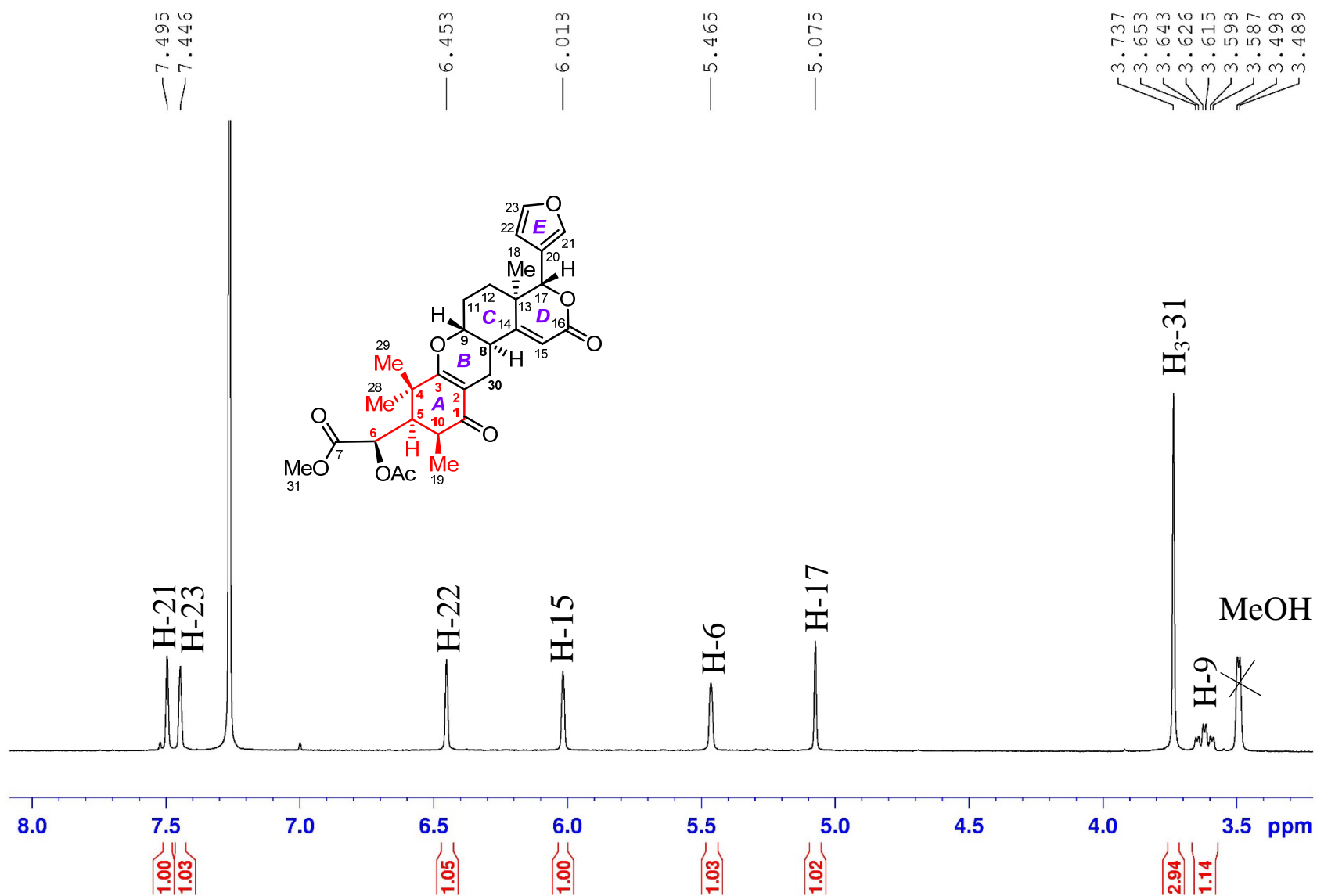
$^1\text{H}$  NMR (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



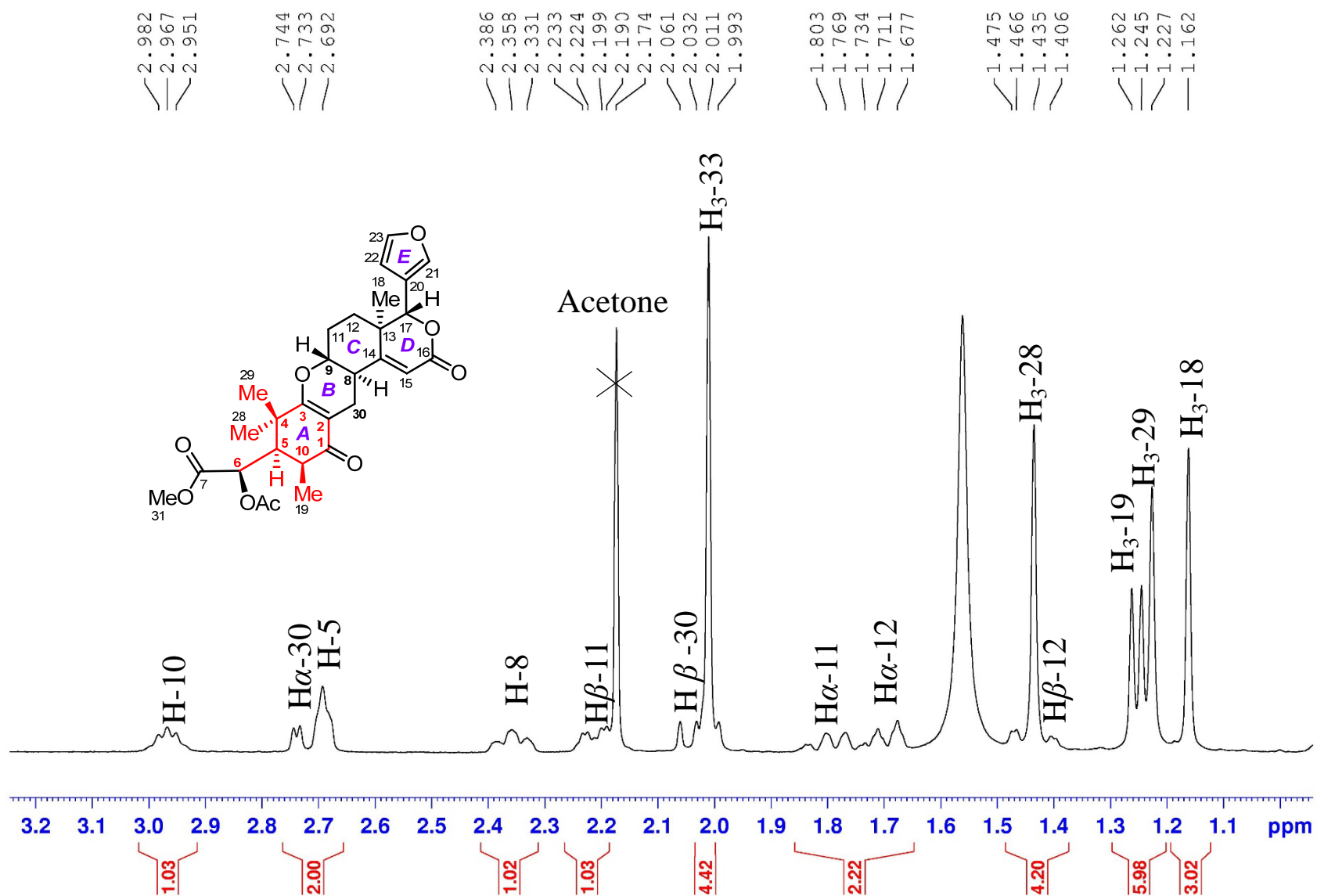
NAME lws-43  
EXPNO 101  
PROCNO 1  
Date\_ 20141118  
Time 11.19  
INSTRUM spect  
PROBHD 5 mm CPPBBO BB  
PULPROG zg30  
TD 65536  
SOLVENT  $\text{CDCl}_3$   
NS 32  
DS 2  
SWH 8012.820 H  
FIDRES 0.122266 H  
AQ 4.0894966 s  
RG 208.5  
DW 62.400 u  
DE 10.00 u  
TE 297.0 K  
D1 1.00000000 s  
TD0 1

===== CHANNEL f1 =====  
SF01 400.1324710 M  
NUC1  $^1\text{H}$   
P1 12.00 u  
SI 65536  
SF 400.1300088 M  
WDW EM  
SSB 0  
LB 0.30 H  
GB 0  
PC 1.00

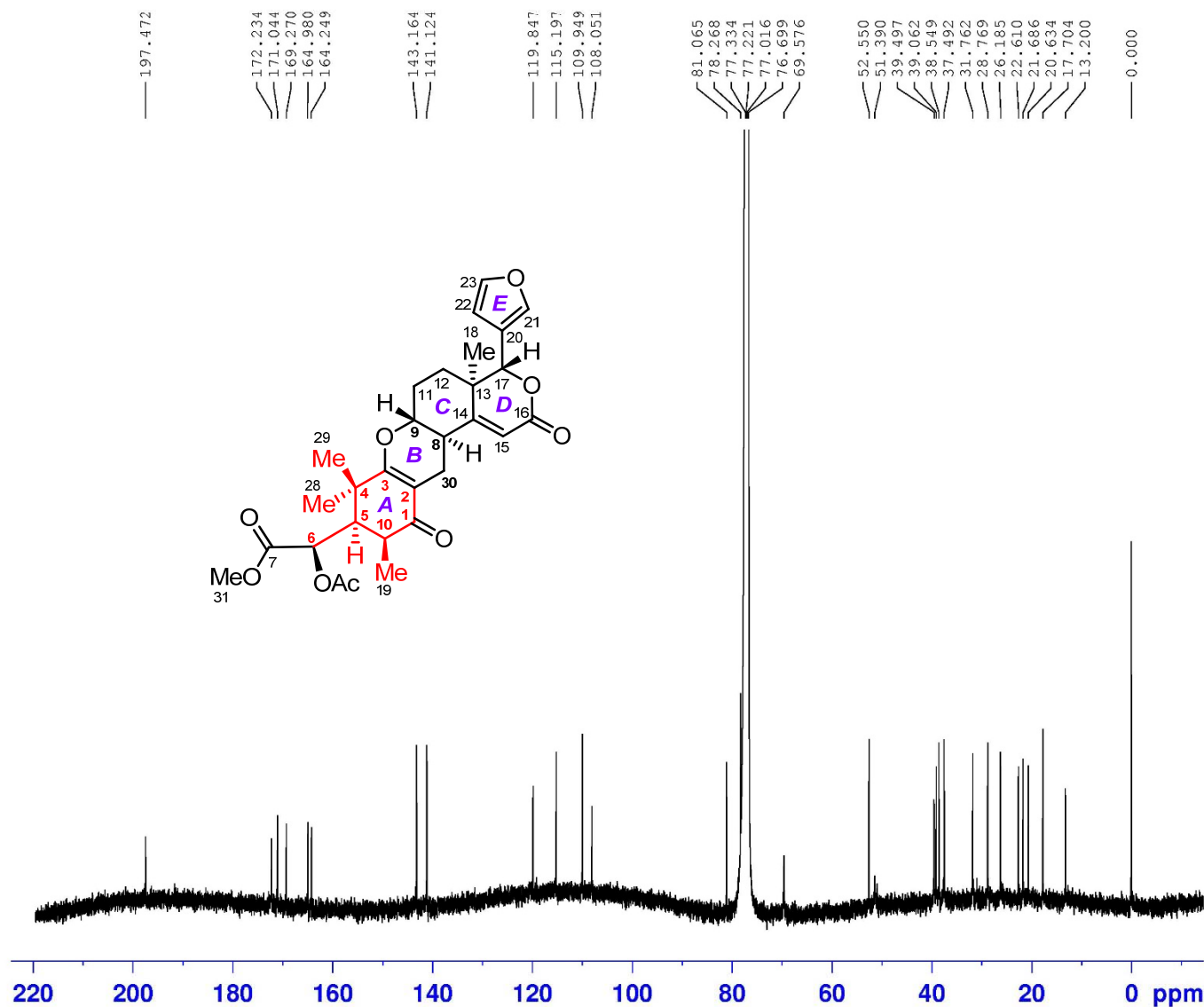
$^1\text{H}$  NMR (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



$^1\text{H}$  NMR (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



# $^{13}\text{C}$ NMR (100 MHz) spectrum of compound **2** in $\text{CDCl}_3$



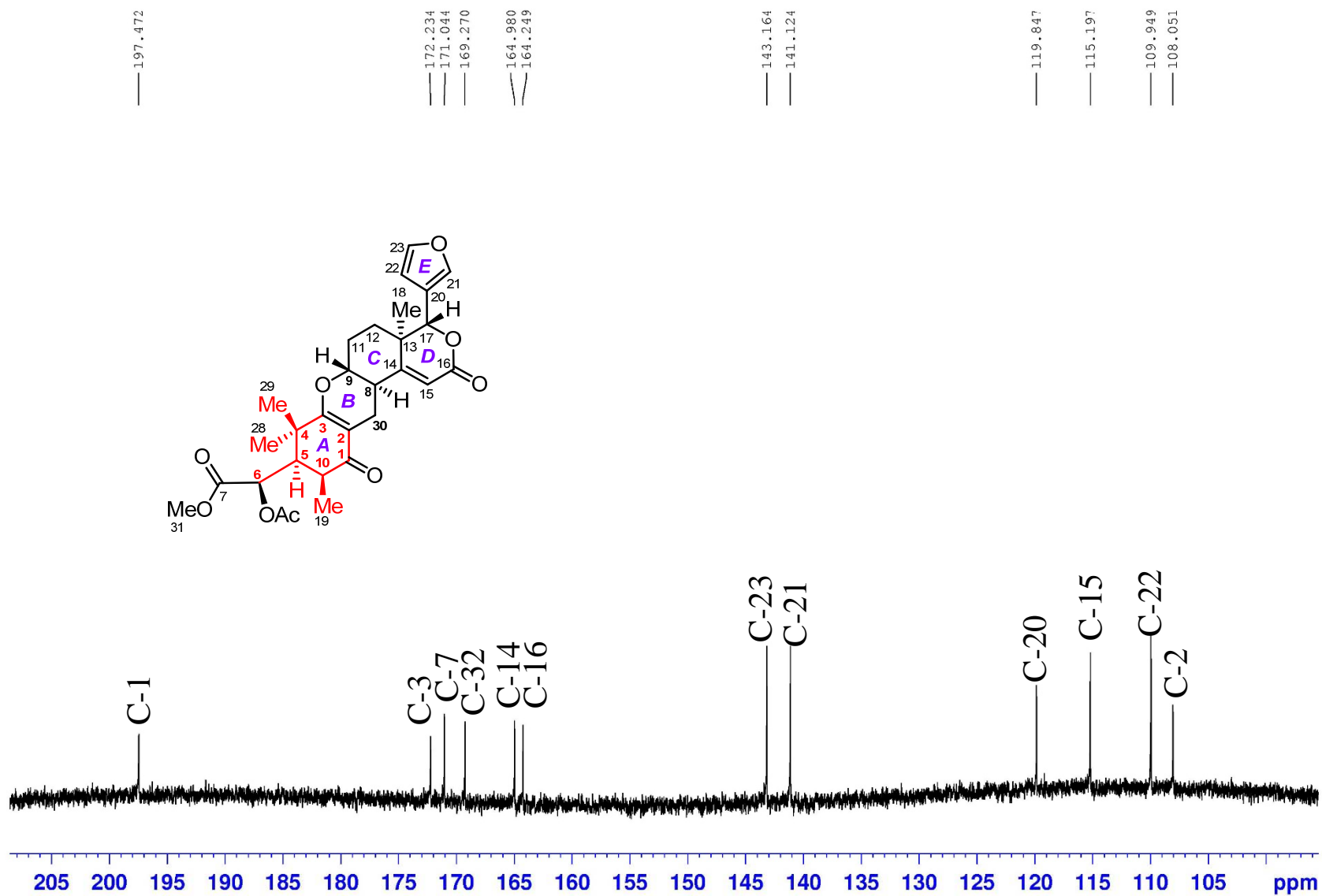
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NAME          lws-43
EXPNO         102
PROCNO        1
Date_         20141124
Time          22.05
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            37286
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 s
RG            117.37
DW            20.800 us
DE            18.00 us
TE            297.0 K
D1            2.00000000 s
D11           0.03000000 s
TD0           1
  
```

```

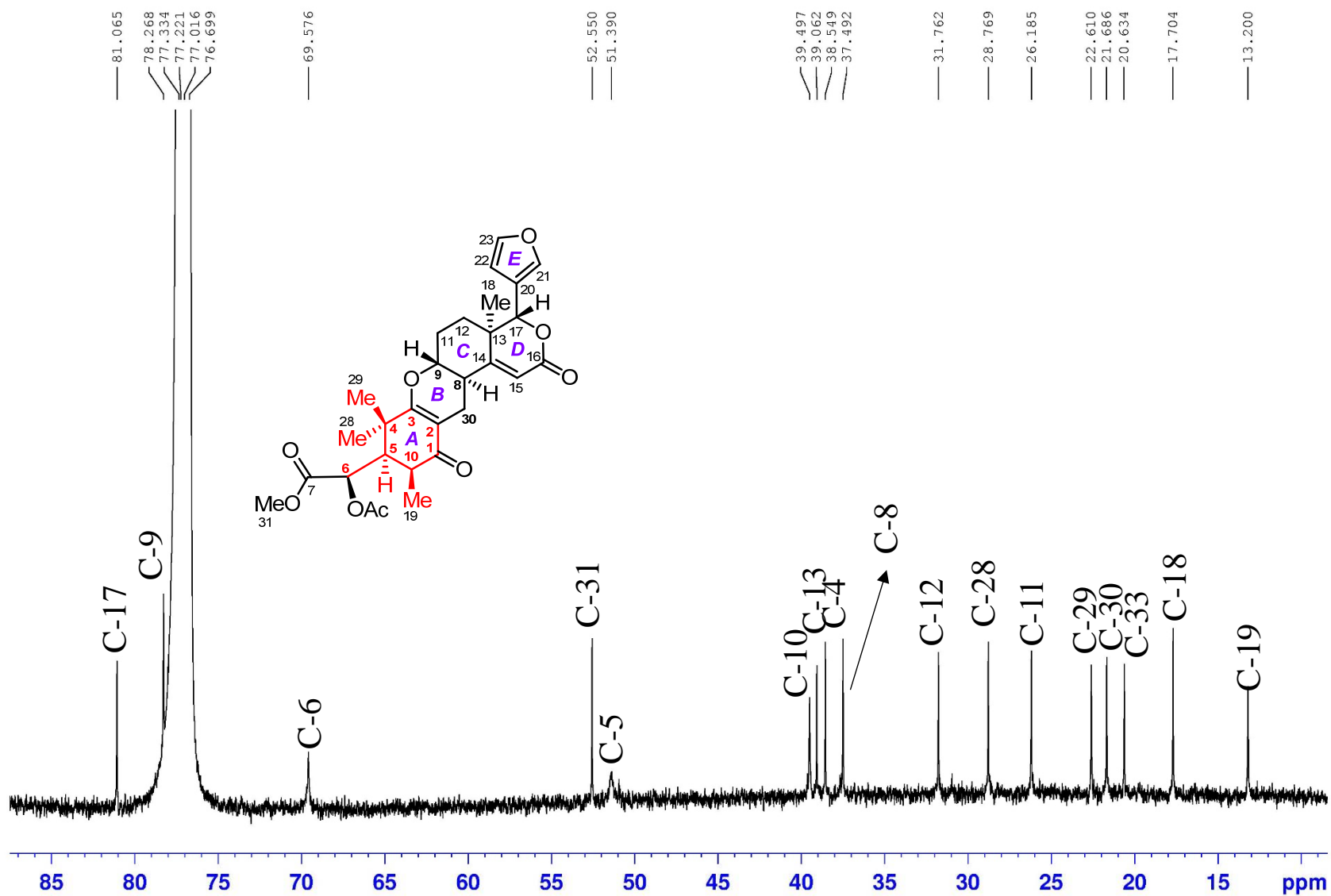
===== CHANNEL f1 =====
SFO1         100.6228293 MHz
NUC1          13C
P1           10.00 us
SI           32768
SF           100.6127692 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

$^{13}\text{C}$  NMR (100 MHz) spectrum of compound **2** in  $\text{CDCl}_3$

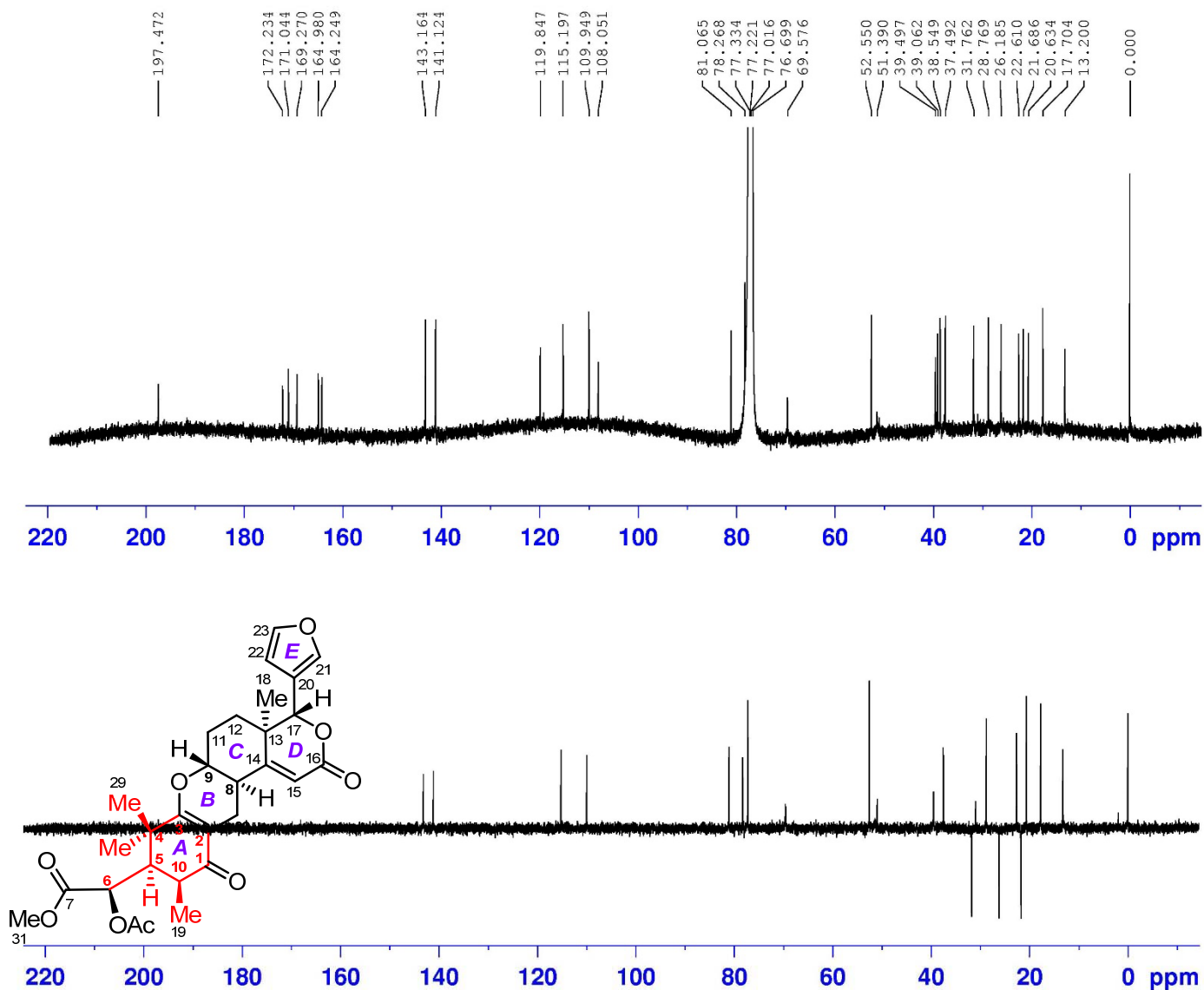




$^{13}\text{C}$  NMR (100 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



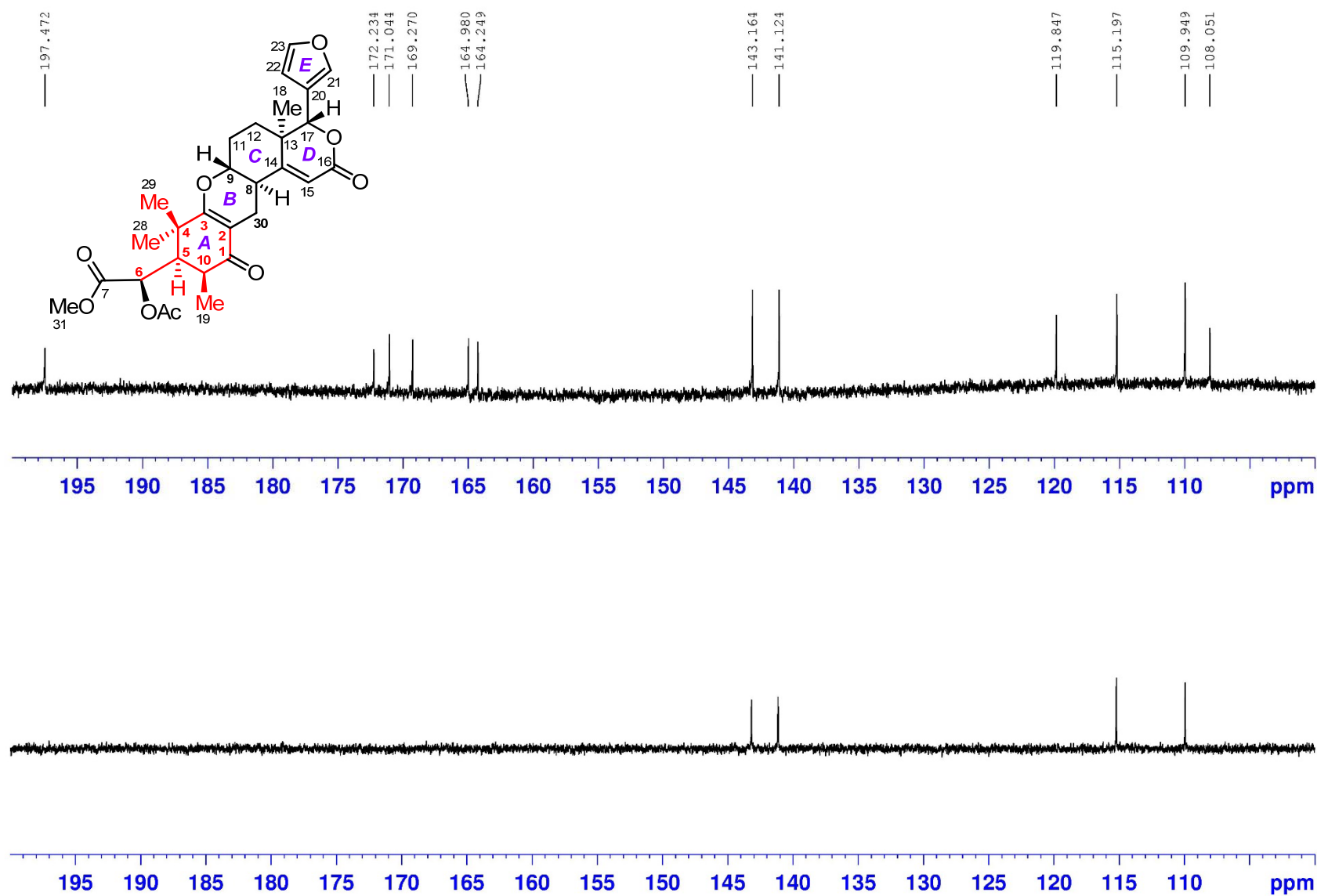
# DEPT135 (100 MHz) spectrum of compound **2** in CDCl<sub>3</sub>



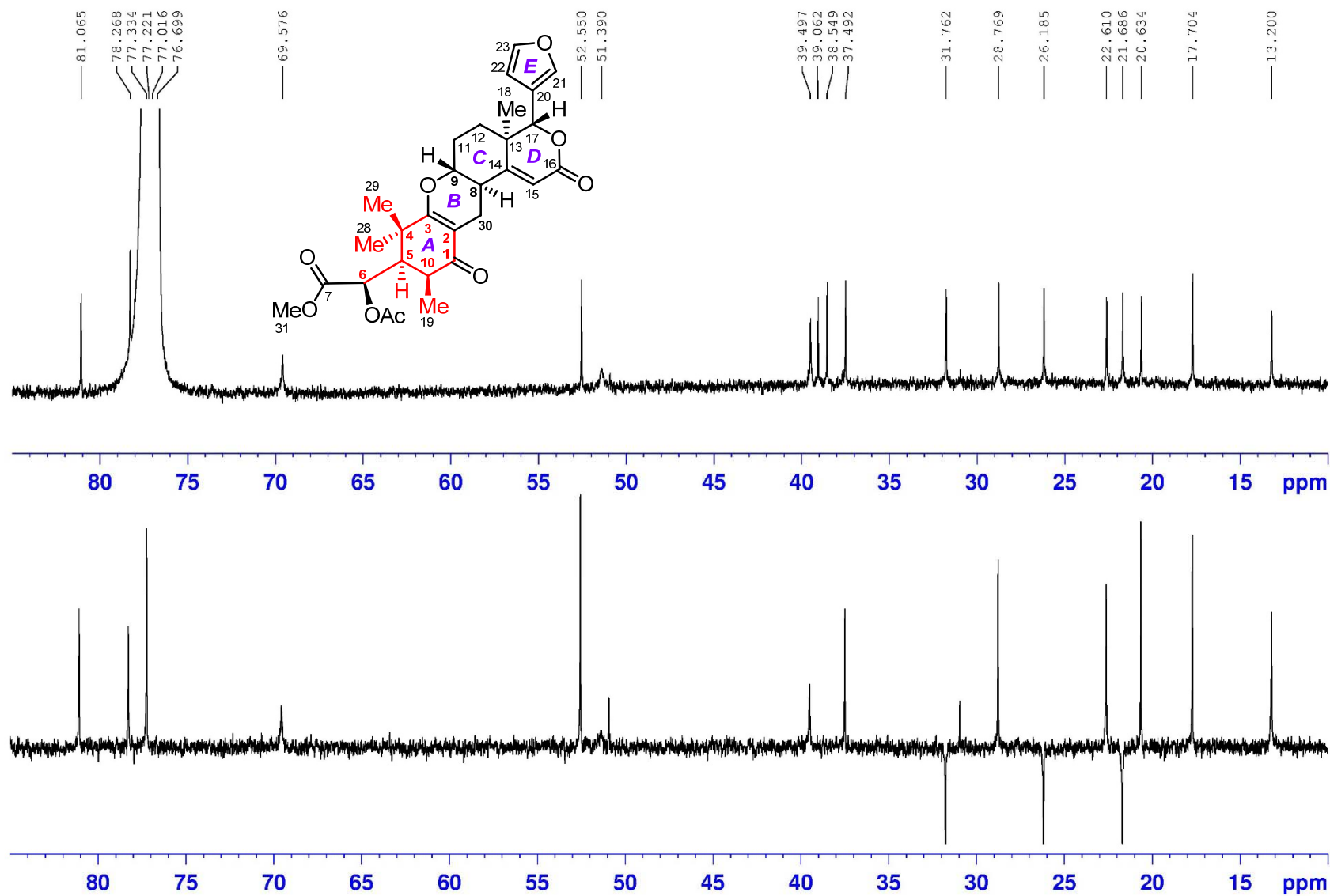
NAME lws-43  
 EXPNO 3  
 PROCNO 1  
 Date\_ 20141125  
 Time 16.56  
 INSTRUM spect  
 PROBHD 5 mm CPPBBO BB  
 PULPROG deptsp135  
 TD 65536  
 SOLVENT CDCl3  
 NS 15000  
 DS 4  
 SWH 24038.461 H  
 FIDRES 0.366798 H  
 AQ 1.3631988 s  
 RG 130.26  
 DW 20.800 u  
 DE 18.00 u  
 TE 297.0 K  
 CNST2 145.0000000  
 D1 2.00000000 s  
 D2 0.00344828 s  
 D12 0.00002000 s  
 TD0 1

===== CHANNEL f1 =====  
 SF01 100.6233324 M  
 NUC1 13C  
 P1 10.00 u  
 P13 2000.00 u  
 SI 32768  
 SF 100.6127694 M  
 WDW EM  
 SSB 0  
 LB 1.00 H  
 GB 0  
 PC 1.40

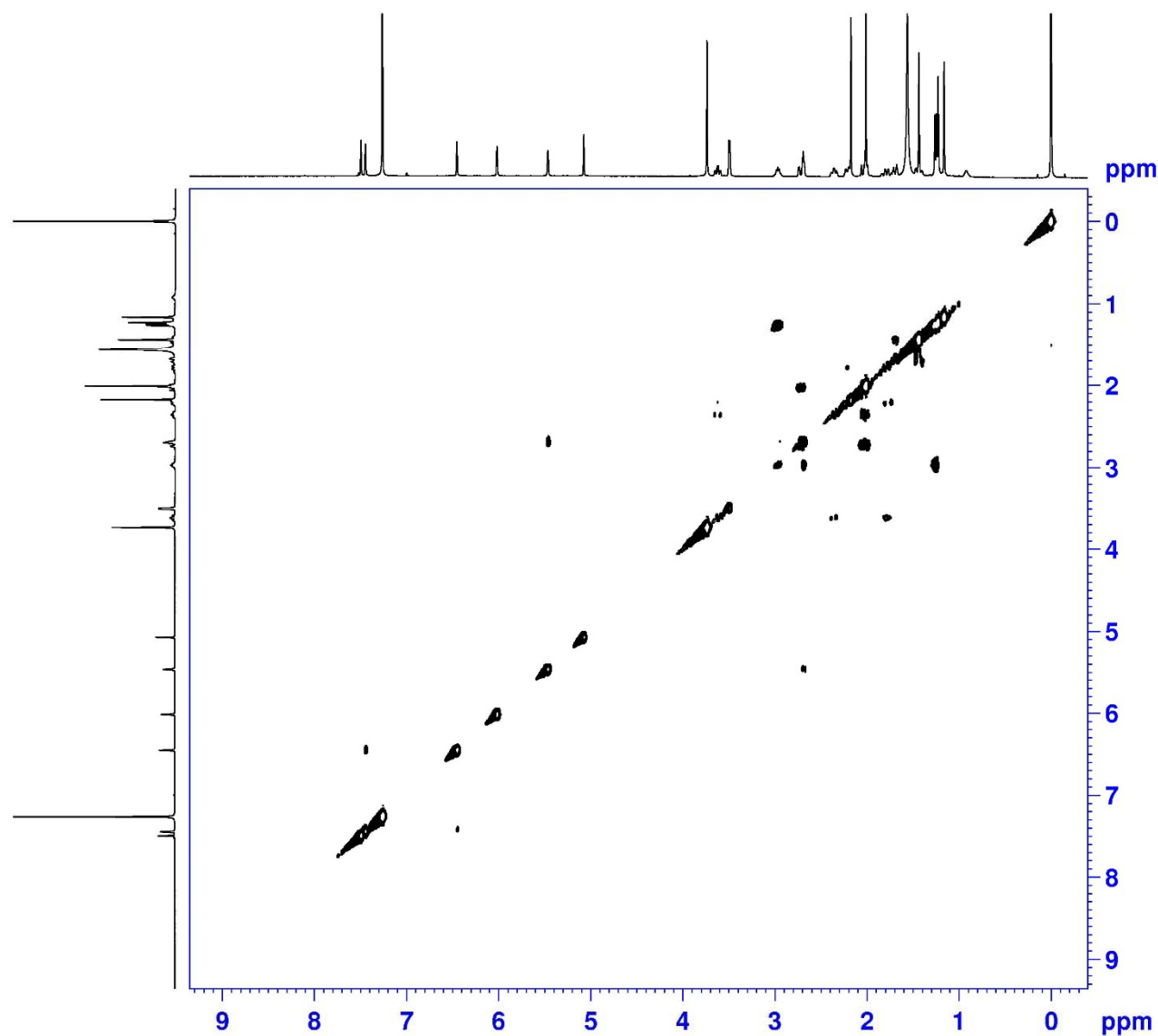
# DEPT135 (100 MHz) spectrum of compound **2** in CDCl<sub>3</sub>



# DEPT135 (100 MHz) spectrum of compound **2** in CDCl<sub>3</sub>



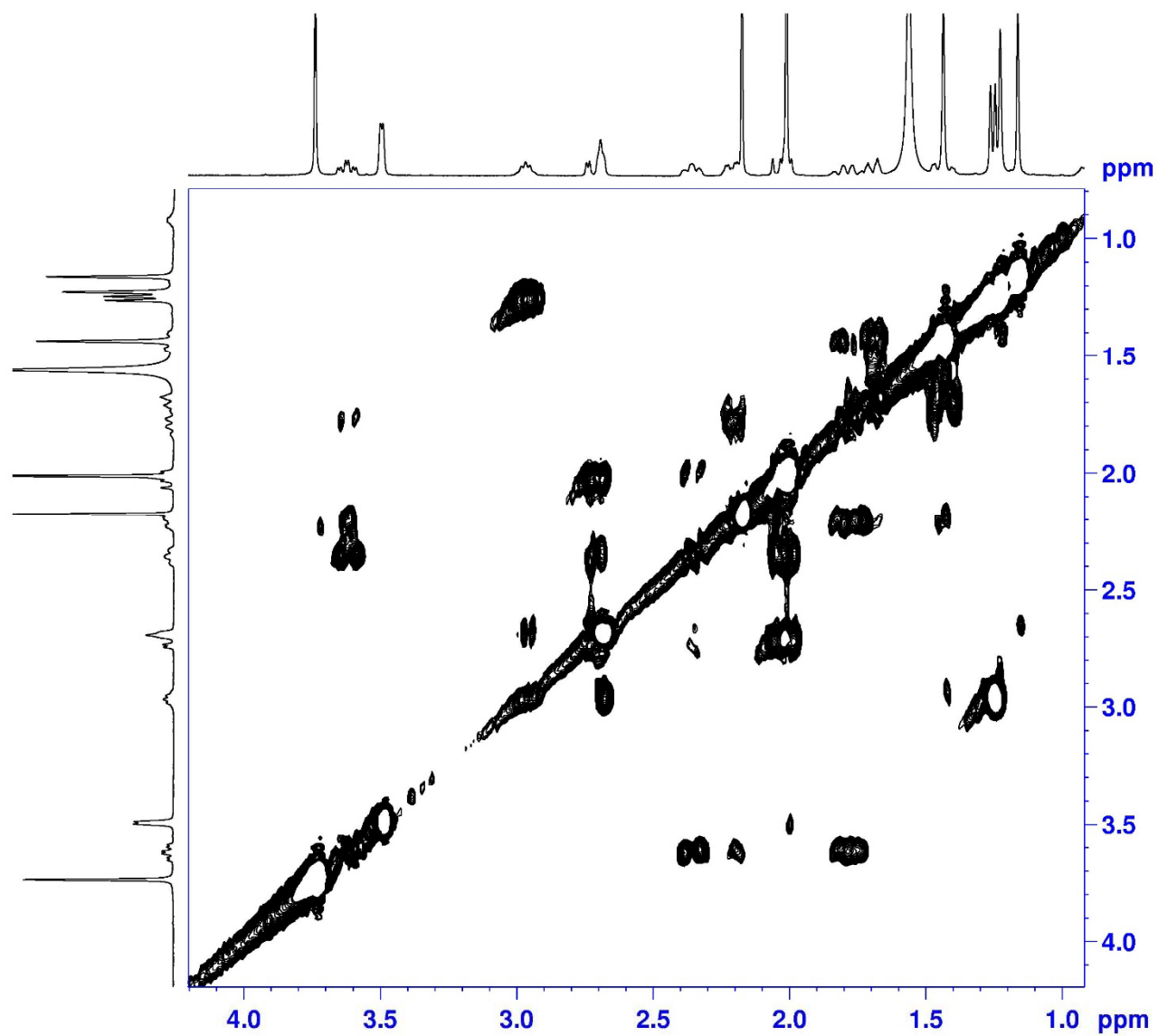
# $^1\text{H}$ - $^1\text{H}$ COSY (400 MHz) spectrum of compound **2** in $\text{CDCl}_3$



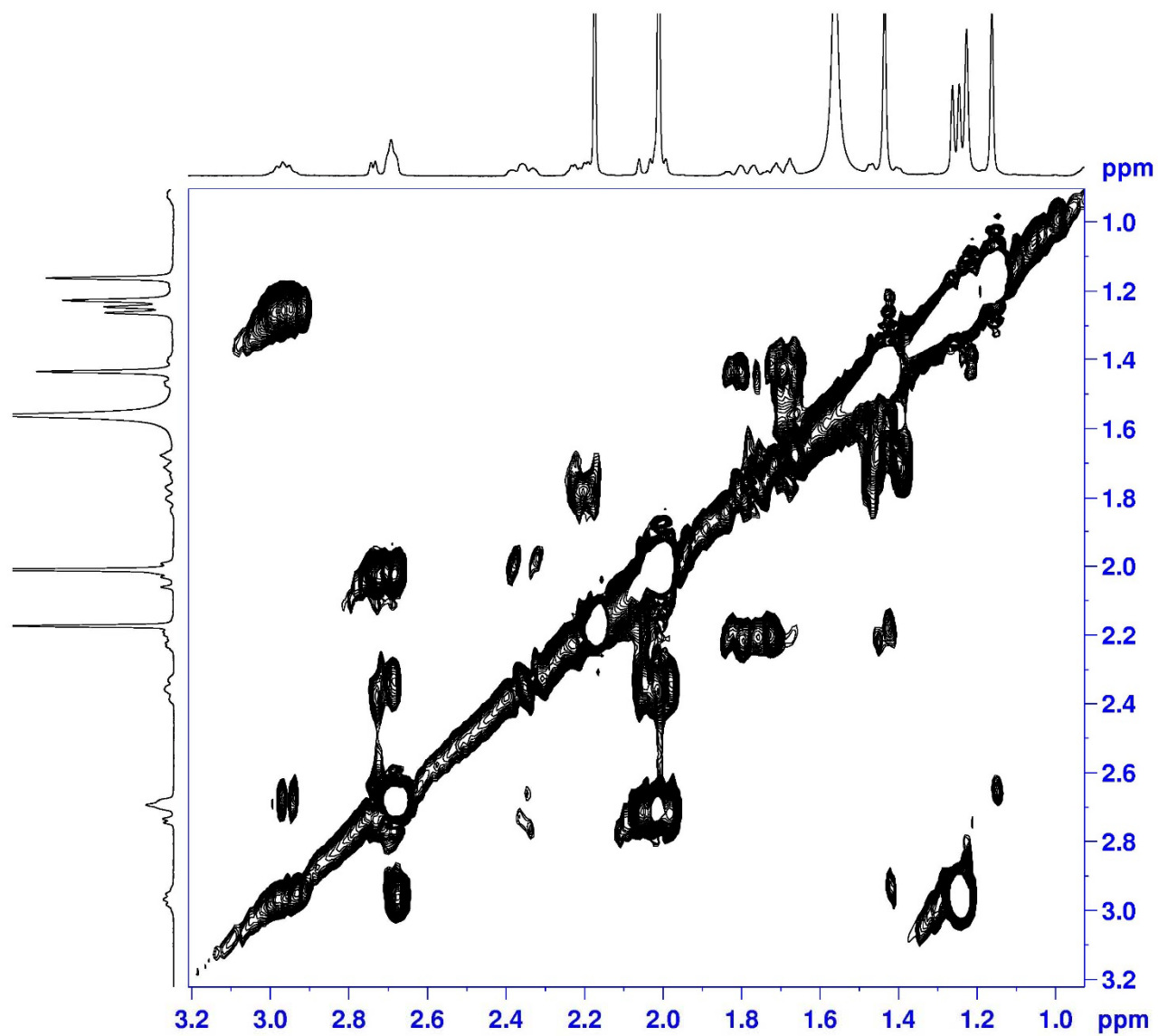
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NAME          lws-43
EXPNO          4
PROCNO         1
Date_         20141126
Time           2.00
INSTRUM        spect
PROBHD         5 mm CPPBBO BB
PULPROG        cosygpppqf
TD             2048
SOLVENT        CDCl3
NS             64
DS             8
SWH            3906.250 Hz
FIDRES         1.907349 Hz
AQ             0.2621940 sec
RG             208.5
DW            128.000 usec
DE             10.00 usec
TE             297.0 K
D0             0.00000300 sec
D1             1.89678097 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00025600 sec
```

```
===== CHANNEL f1 =====
SFO1          400.1318006 MHz
NUC1           1H
P0             12.00 usec
P1             12.00 usec
P17            2500.00 usec
ND0            1
TD             128
SFO1          400.1318 MHz
FIDRES         30.517578 Hz
SW             9.762 ppm
FnMODE         QF
SI             1024
SF            400.1300097 MHz
WDW            QSINE
SSB            0
LB             0.00 Hz
GB             0
PC             1.40
SI             1024
MC2            QF
SF            400.1300097 MHz
WDW            QSINE
```

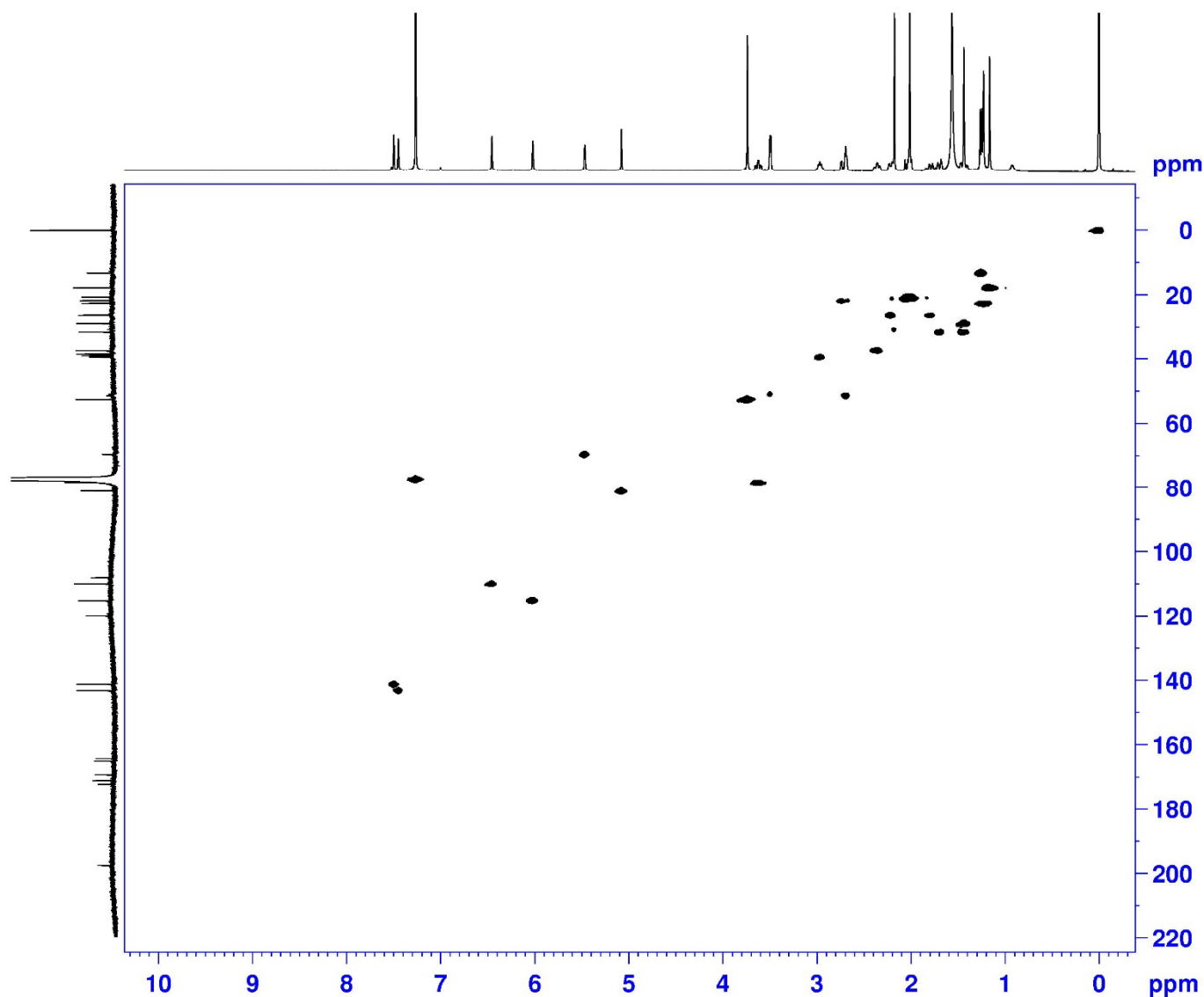
$^1\text{H}$ - $^1\text{H}$  COSY (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



$^1\text{H}$ - $^1\text{H}$  COSY (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



# HSQC (400 MHz) spectrum of compound **2** in CDCl<sub>3</sub>



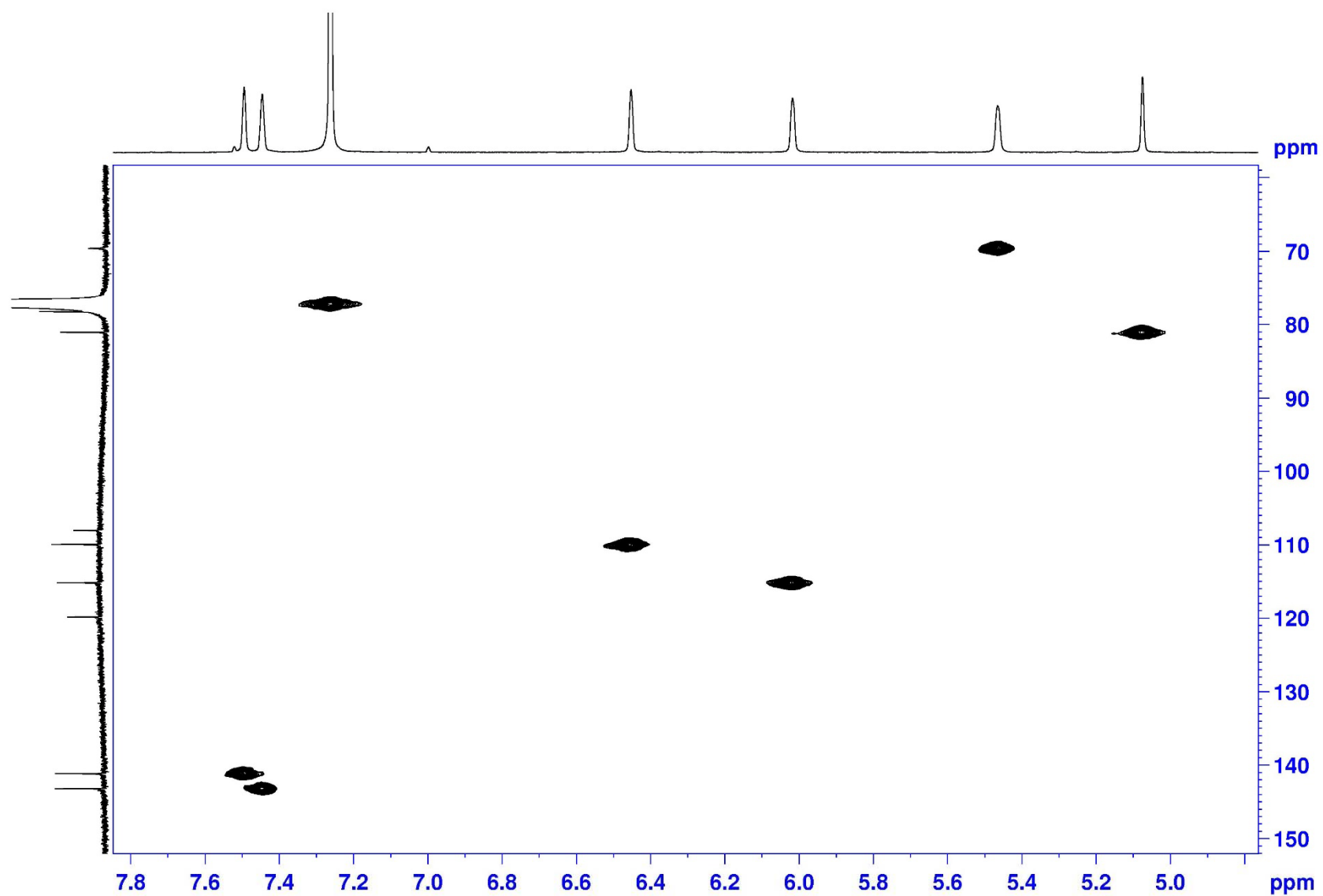
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NAME                lws-43
EXPNO                5
PROCNO               1
Date_                20141126
Time                7.04
INSTRUM              spect
PROBHD               5 mm CPPBBO BB
PULPROG              hsqcetgpsi2
TD                   1024
SOLVENT              CDCl3
NS                    64
DS                     16
SWH                  3906.250 Hz
FIDRES               3.814697 Hz
AQ                   0.1311220 se
RG                    208.5
DW                   128.000 us
DE                    10.00 us
TE                   297.0 K
CNST2                145.0000000
D0                   0.00000300 se
D1                   1.46497905 se
D4                   0.00172414 se
D11                  0.03000000 se
D16                  0.00020000 se
D24                  0.00086207 se
IN0                  0.00002080 se
ZGPTNS

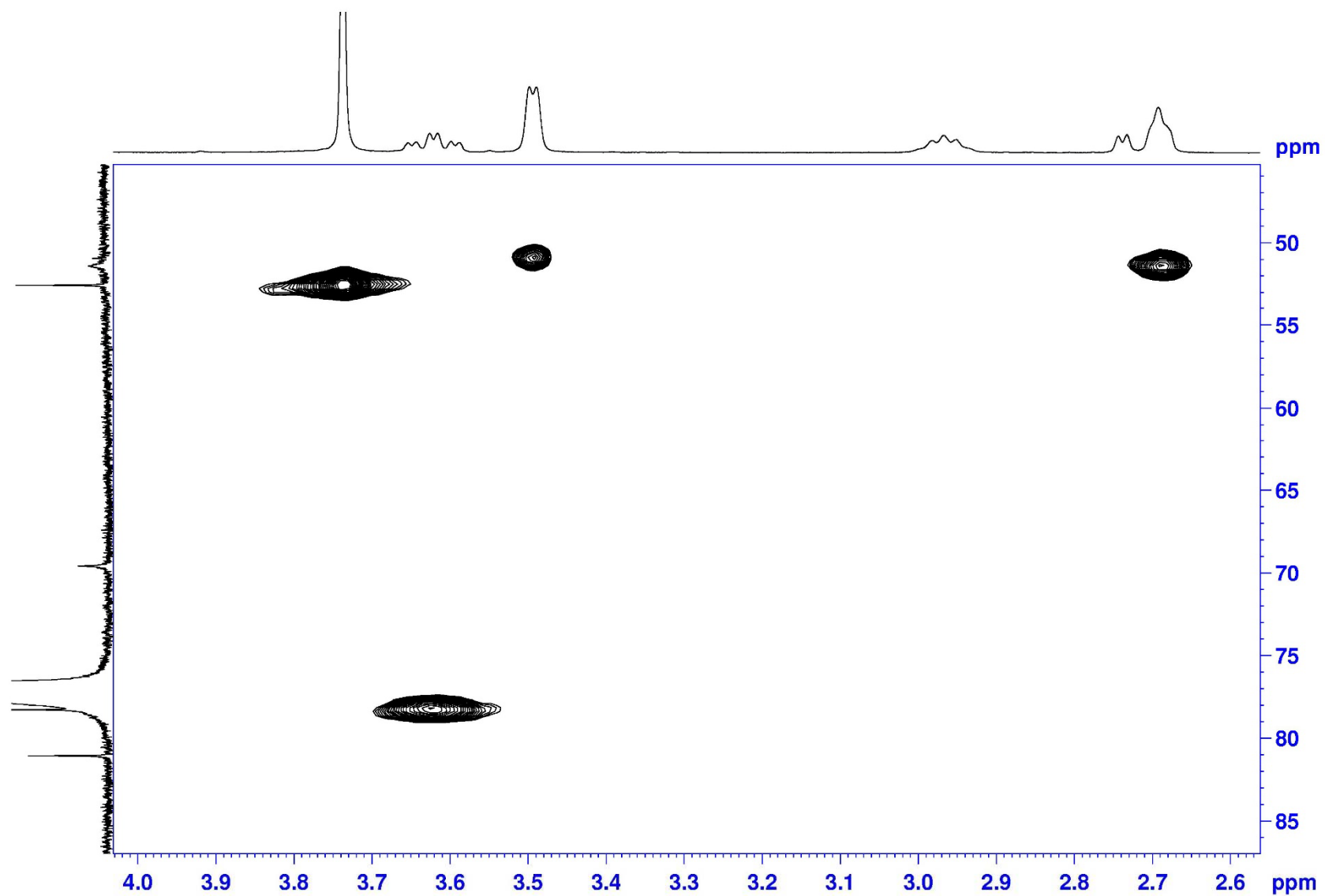
===== CHANNEL f1 =====
SFO1                 400.1318006 MH
NUC1                  1H
P1                    12.00 us
P2                    24.00 us
P28                   0.00 us
ND0                   2
TD                    256
SFO1                 100.6233 MH
FIDRES               93.900238 Hz
SW                   238.896 pp
FnMODE               Echo-Antiecho
SI                    1024
SF                   400.1300050 MH
WDW                   QSINE
SSB                   2
LB                    0.00 Hz
GB                    0
PC                    1.40
SI                    1024
MC2                  echo-antiecho
SF                   100.6127585 MH
    
```



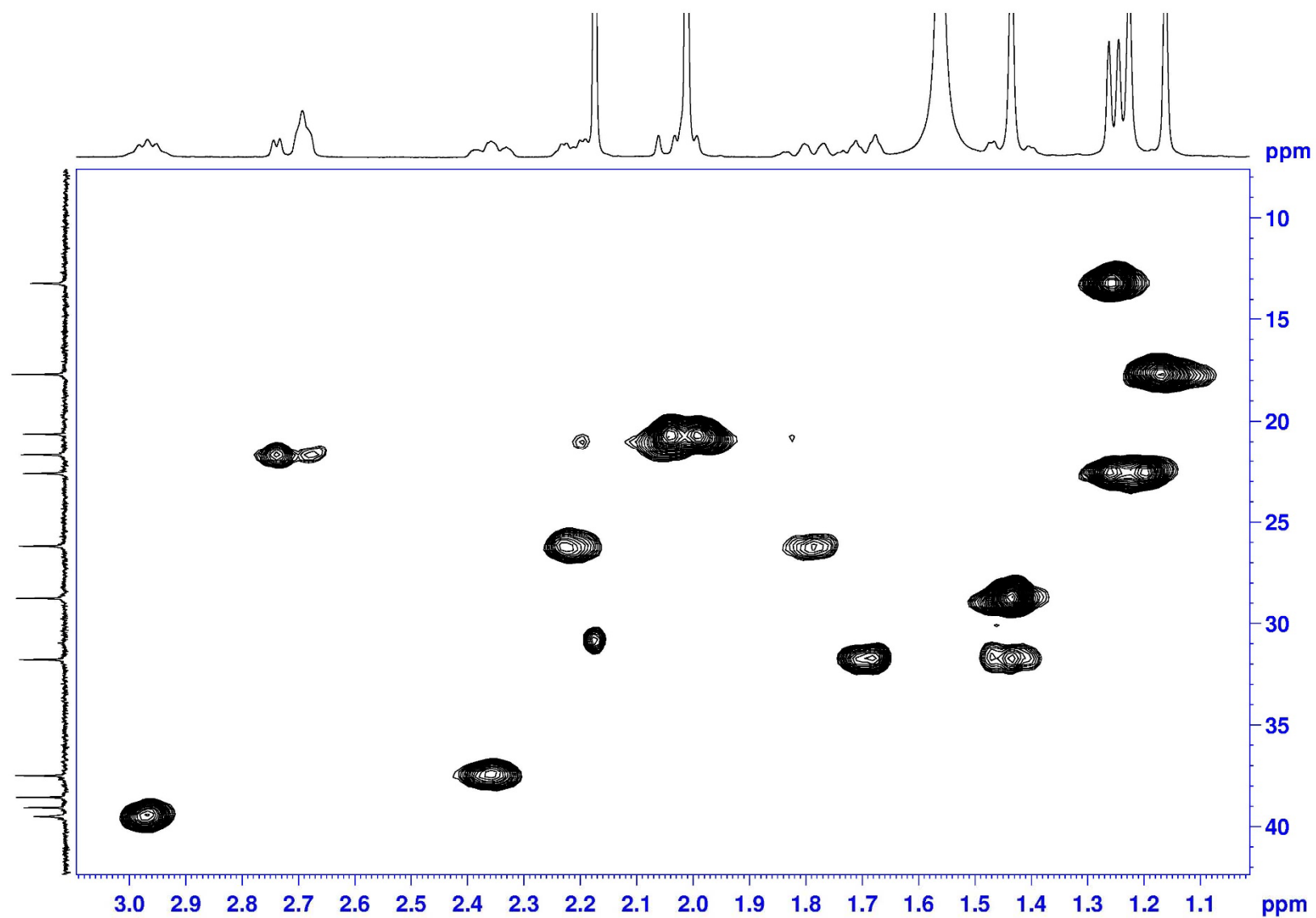
HSQC (400 MHz) spectrum of compound **2** in CDCl<sub>3</sub>



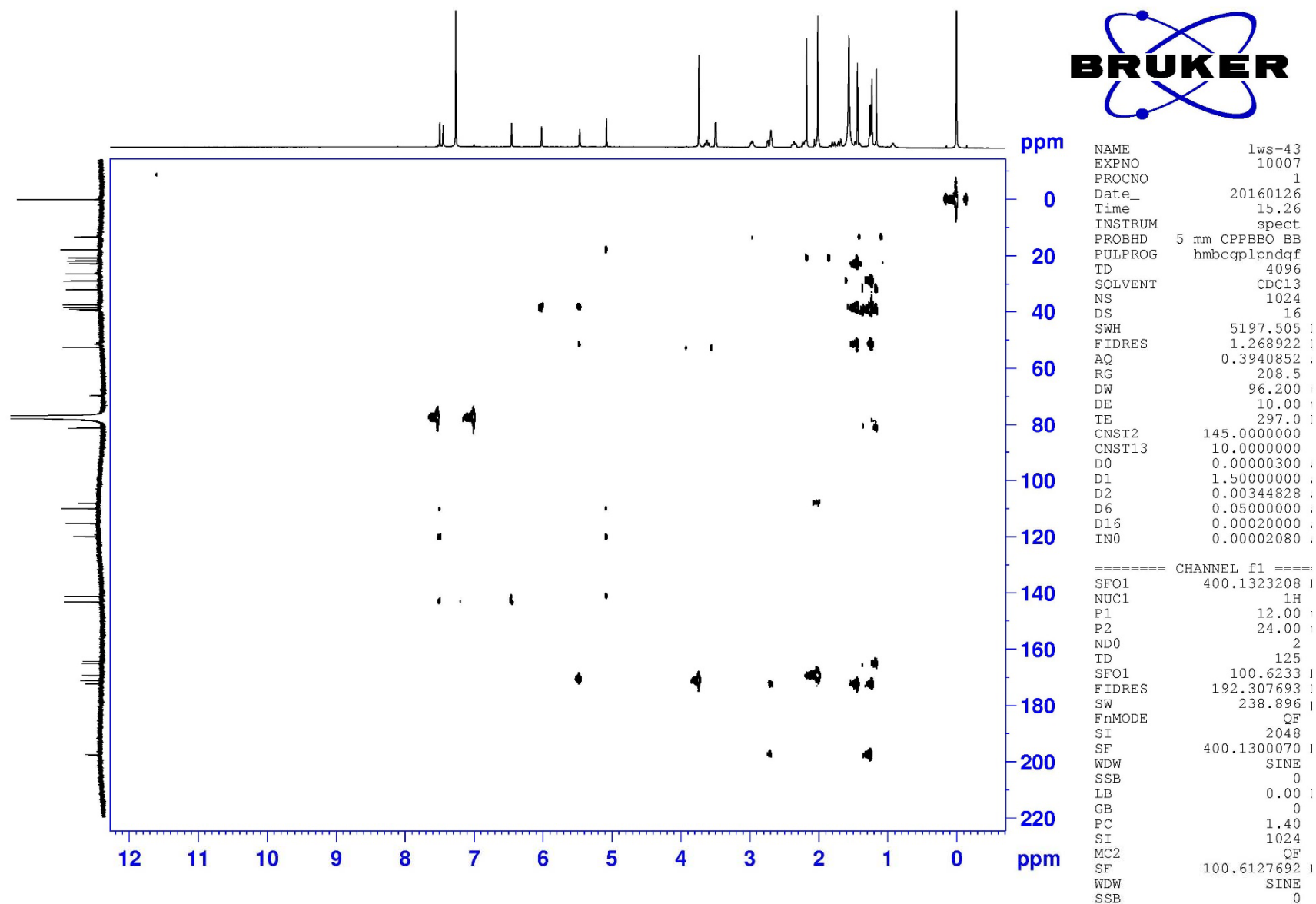
HSQC (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



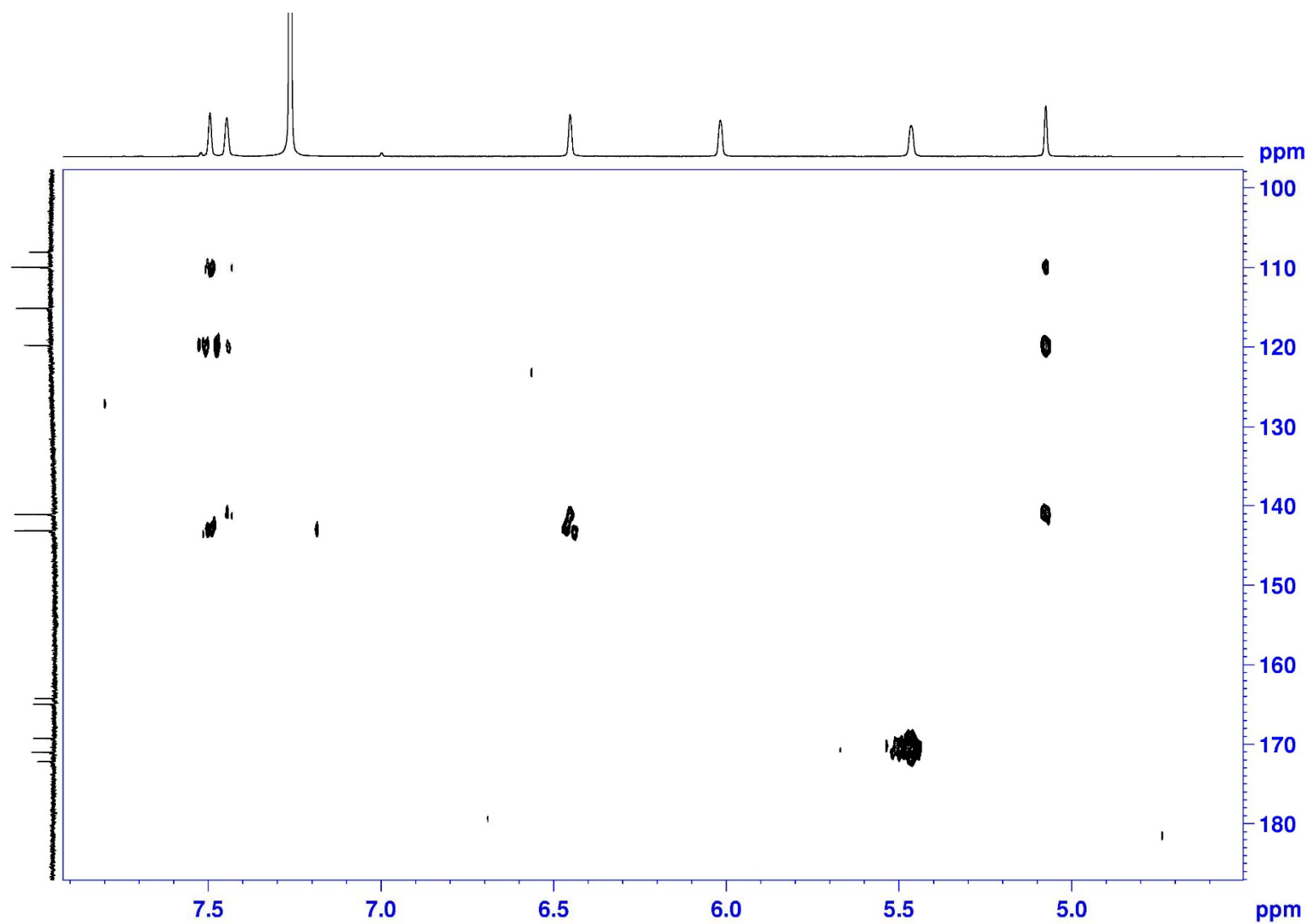
HSQC (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



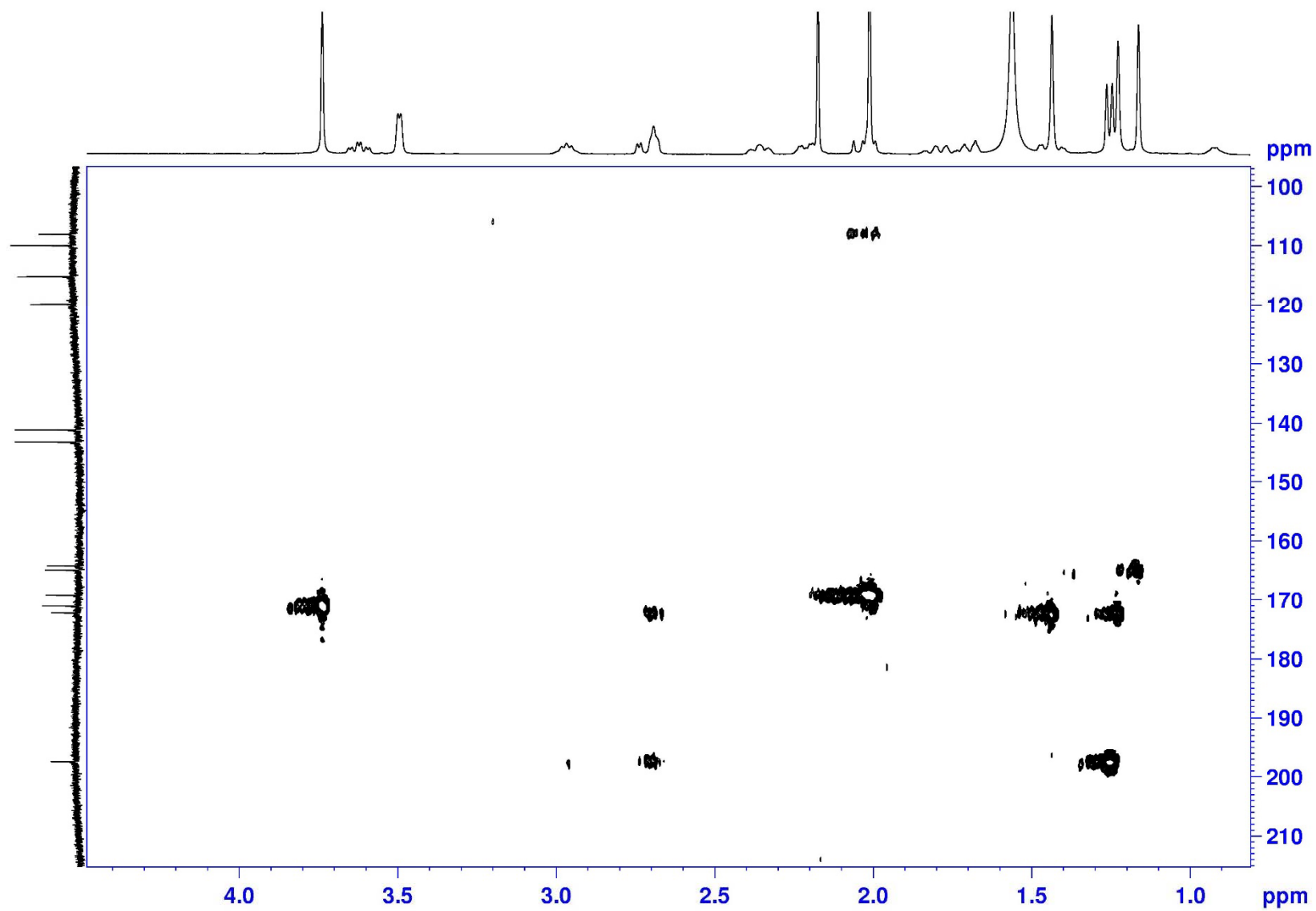
# HMBC (400 MHz) spectrum of compound **2** in CDCl<sub>3</sub>



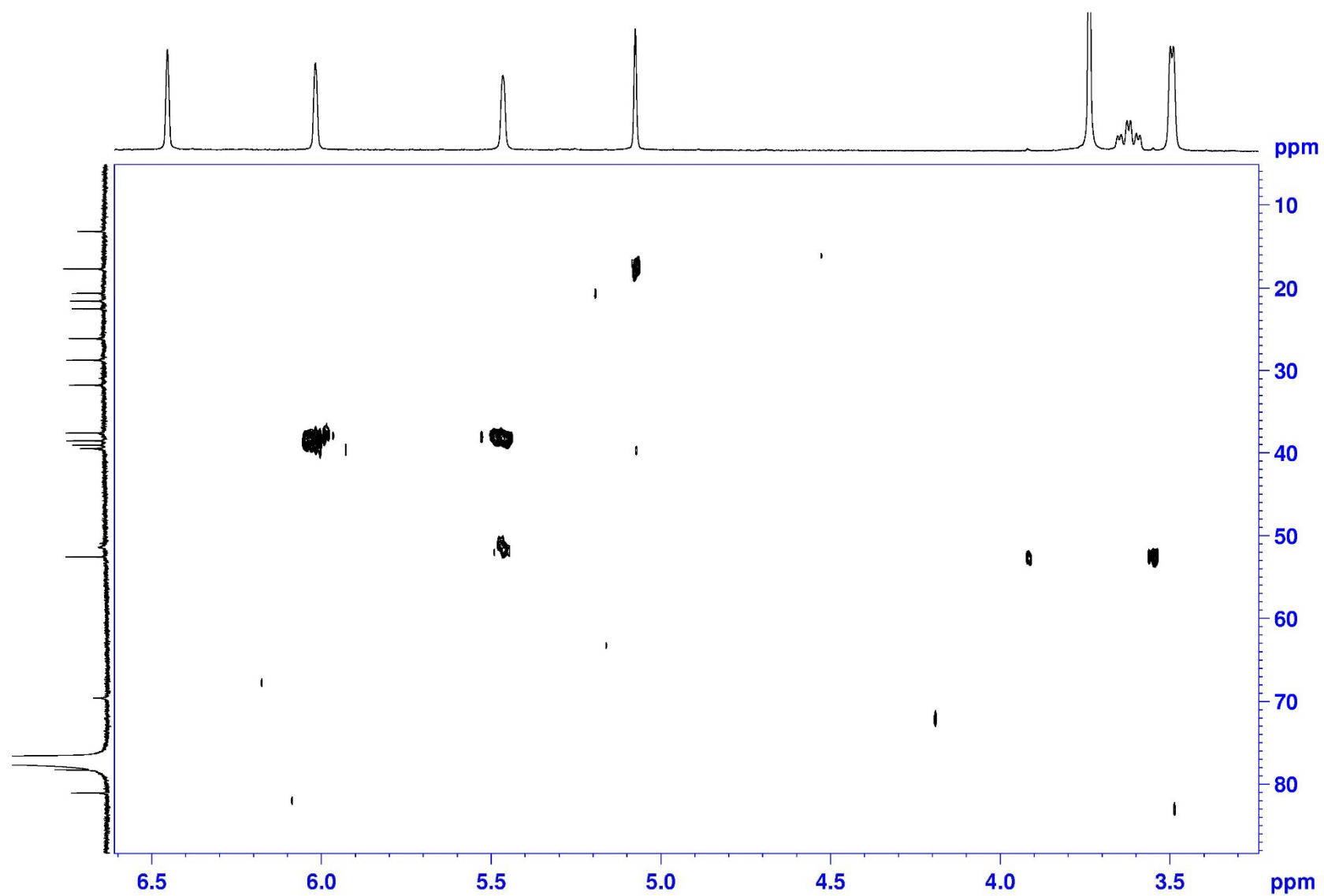
HMBC (400 MHz) spectrum of compound **2** in CDCl<sub>3</sub>



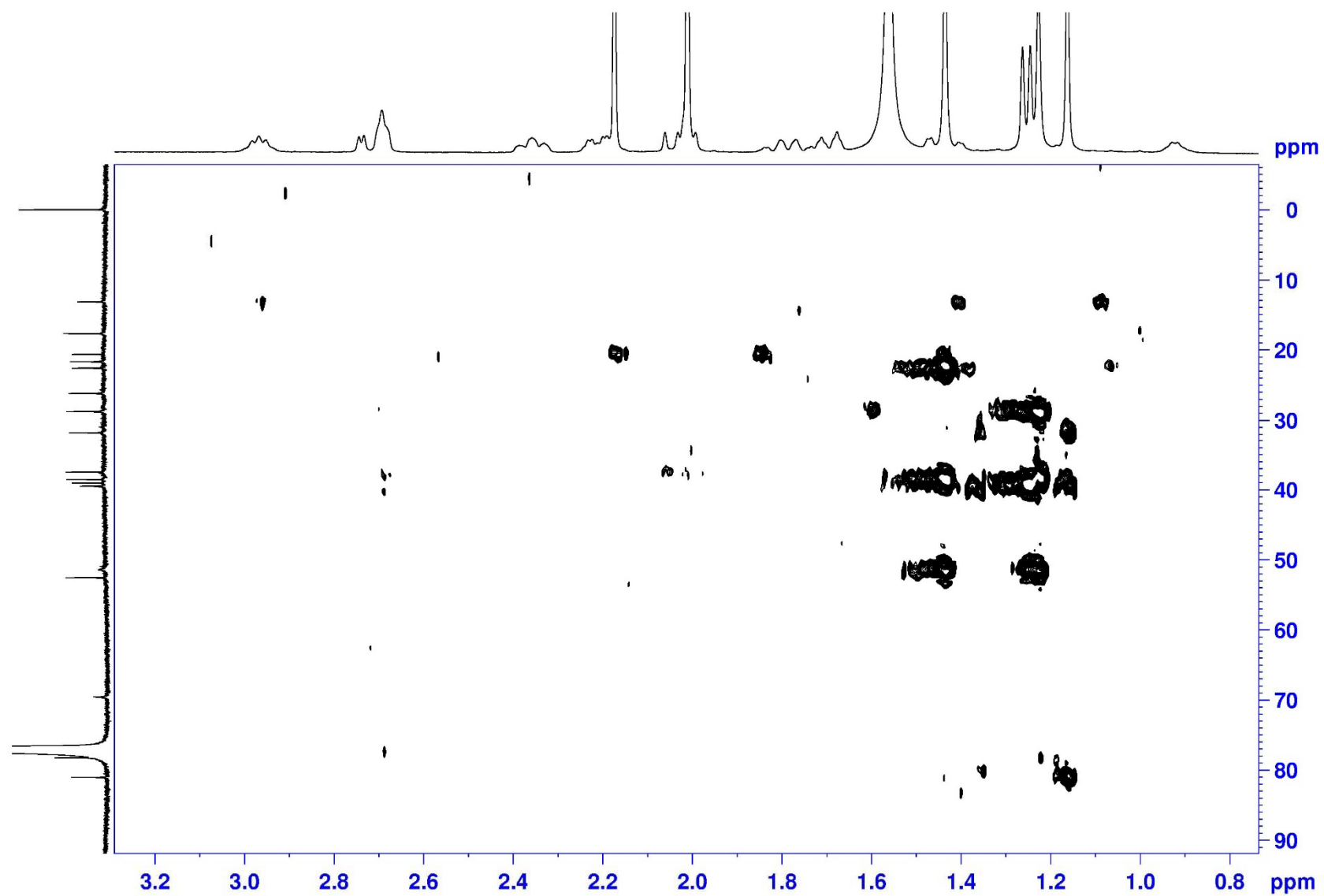
HMBC (400 MHz) spectrum of compound **2** in CDCl<sub>3</sub>



HMBC (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$

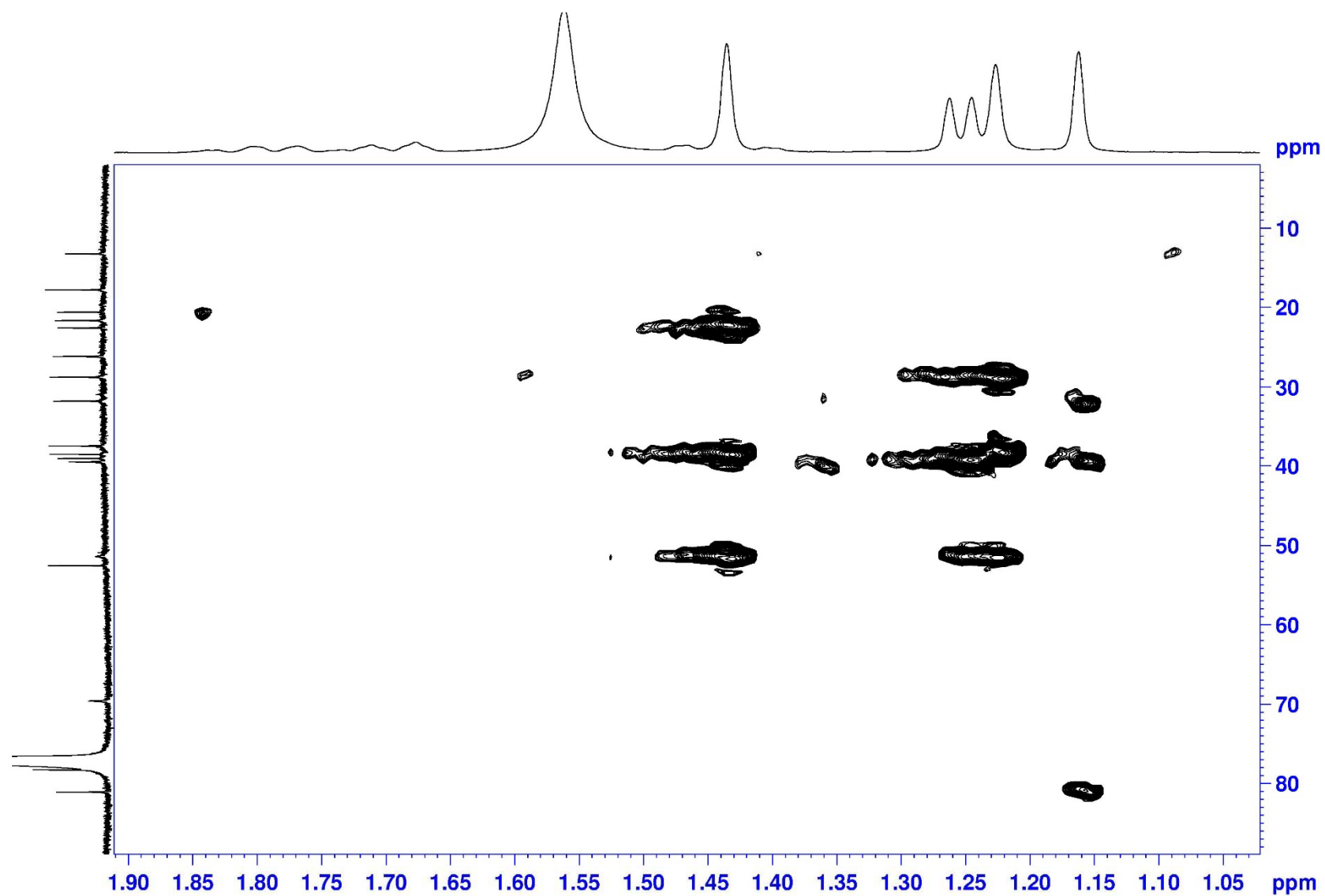


HMBC (400 MHz) spectrum of compound **2** in CDCl<sub>3</sub>

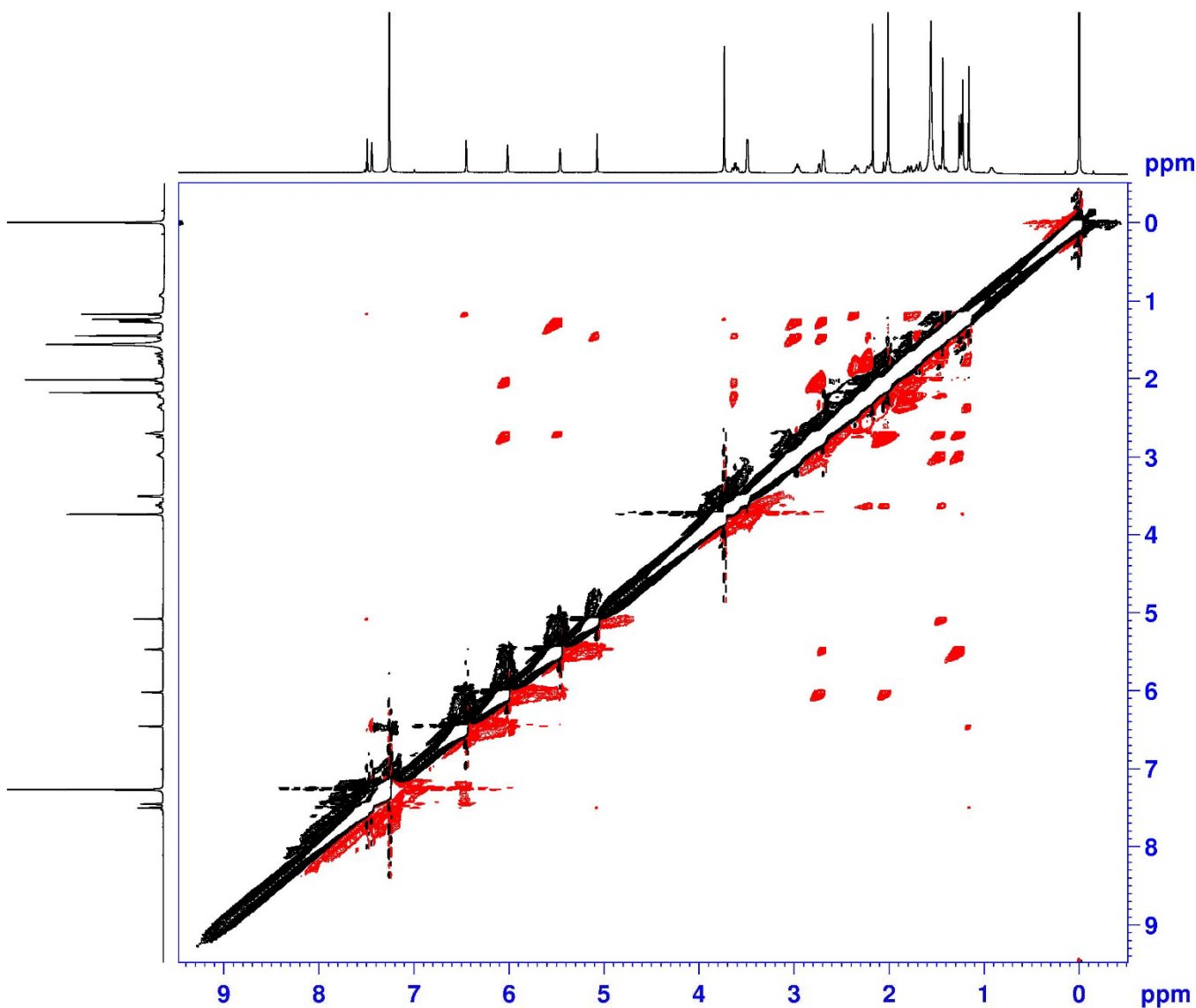




HMBC (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



# NOESY (400 MHz) spectrum of compound **2** in CDCl<sub>3</sub>



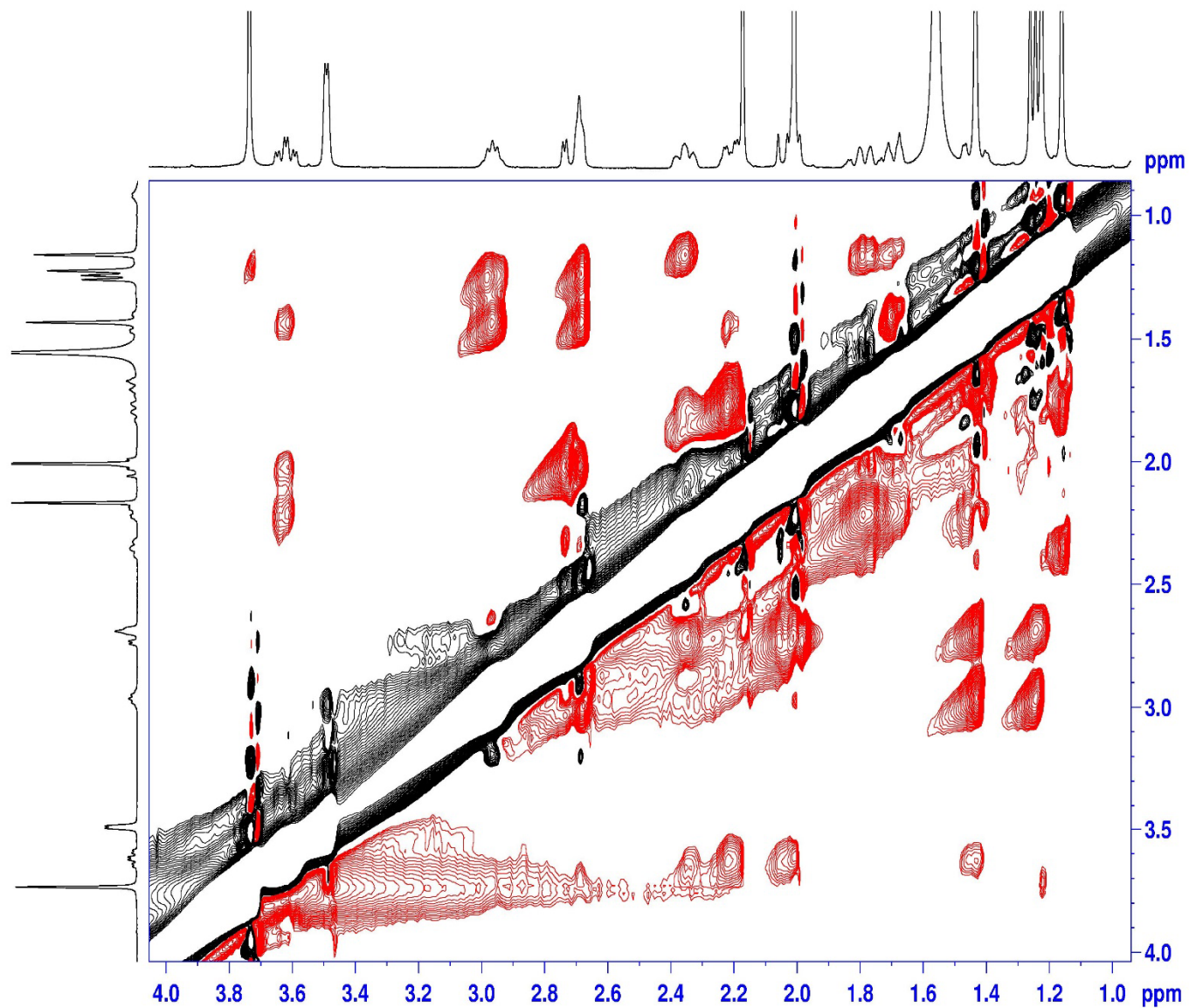
```

NAME                lws-43
EXPNO                7
PROCNO               1
Date_                20141127
Time                 8.27
INSTRUM              spect
PROBHD               5 mm CPPBBO BB
PULPROG              noesygpphpp
TD                   2048
SOLVENT              CDCl3
NS                   256
DS                   32
SWH                  4000.000 Hz
FIDRES               1.953125 Hz
AQ                   0.2560500 se
RG                   208.5
DW                   125.000 us
DE                   10.00 us
TE                   297.0 K
D0                   0.00010972 se
D1                   1.99385595 se
D8                   0.30000001 se
D11                  0.03000000 se
D12                  0.00002000 se
D16                  0.00020000 se
IN0                  0.00025000 se
  
```

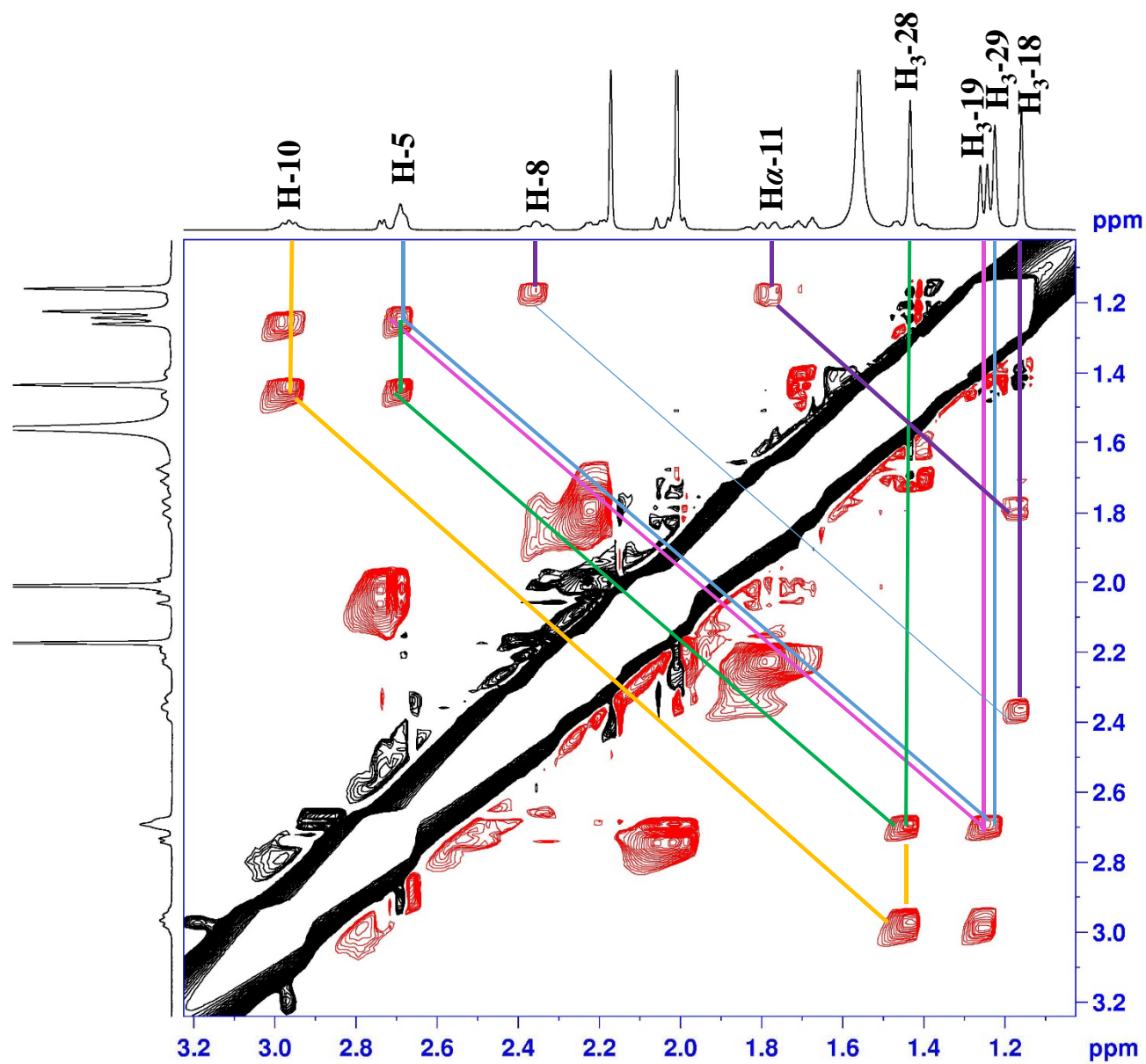
```

===== CHANNEL f1 =====
SFO1                400.1318006 MHz
NUC1                 1H
P1                   12.00 us
P2                   24.00 us
P17                  2500.00 us
ND0                  1
TD                   143
SFO1                400.1318 MHz
FIDRES               27.972029 Hz
SW                   9.997 MHz
FnMODE               States-TPPI
SI                   1024
SF                   400.1300090 MHz
WDW                  QSINE
SSB                   2
LB                   0.00 Hz
GB                   0
PC                   1.00
SI                   1024
MC2                  States-TPPI
SF                   400.1300070 MHz
WDW                  QSINE
SSB                   2
  
```

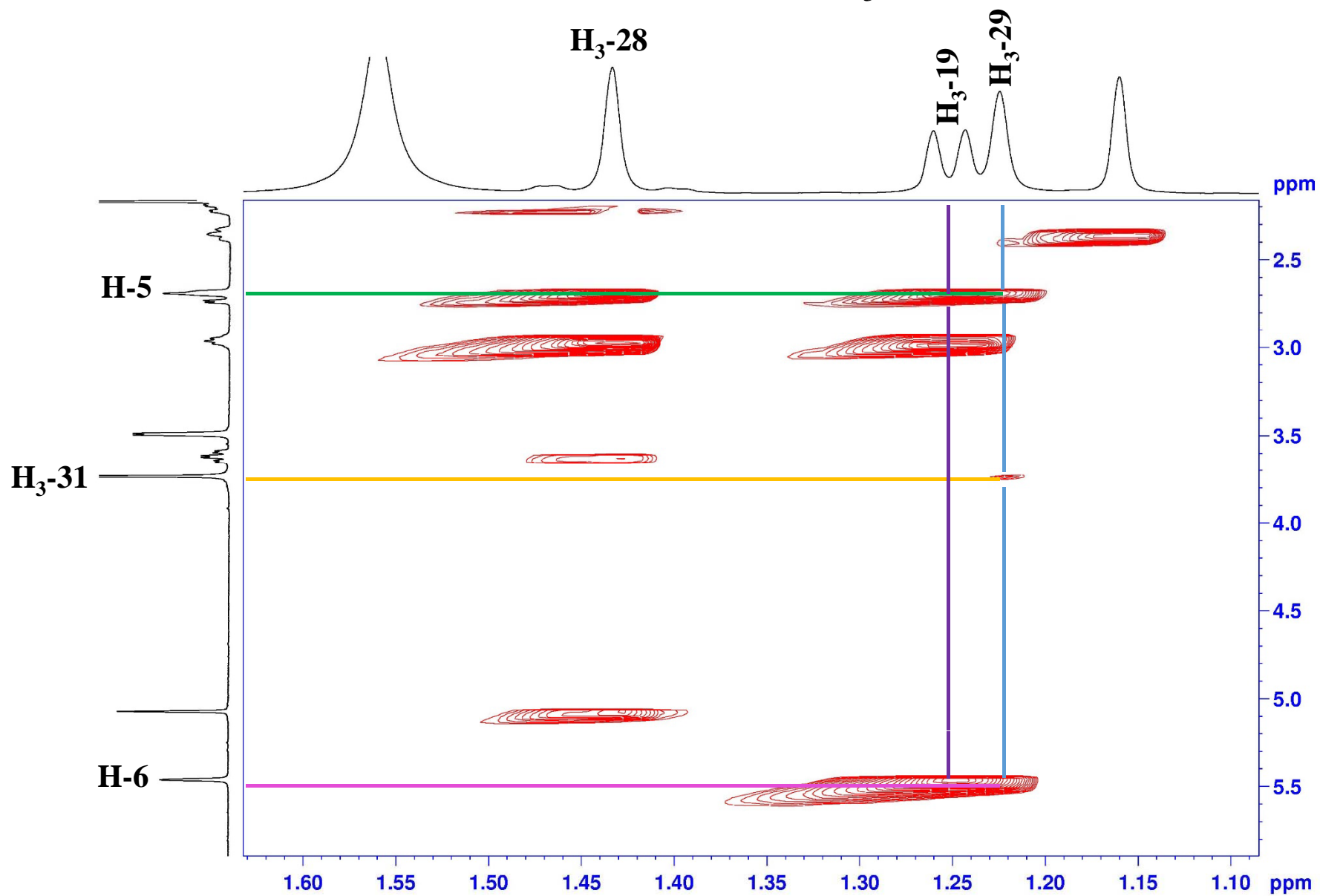
NOESY (400 MHz) spectrum of compound **2** in CDCl<sub>3</sub>



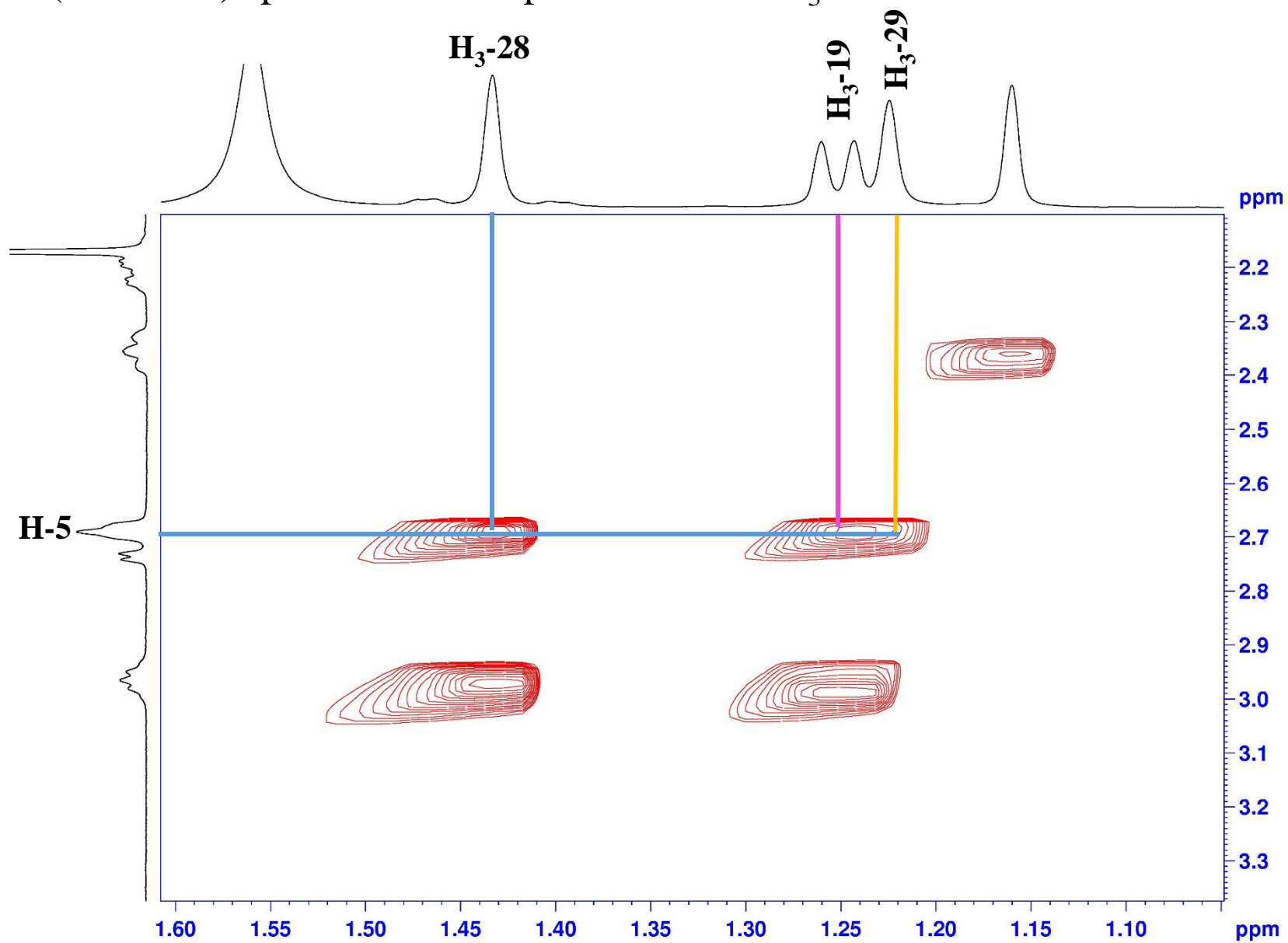
NOESY (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



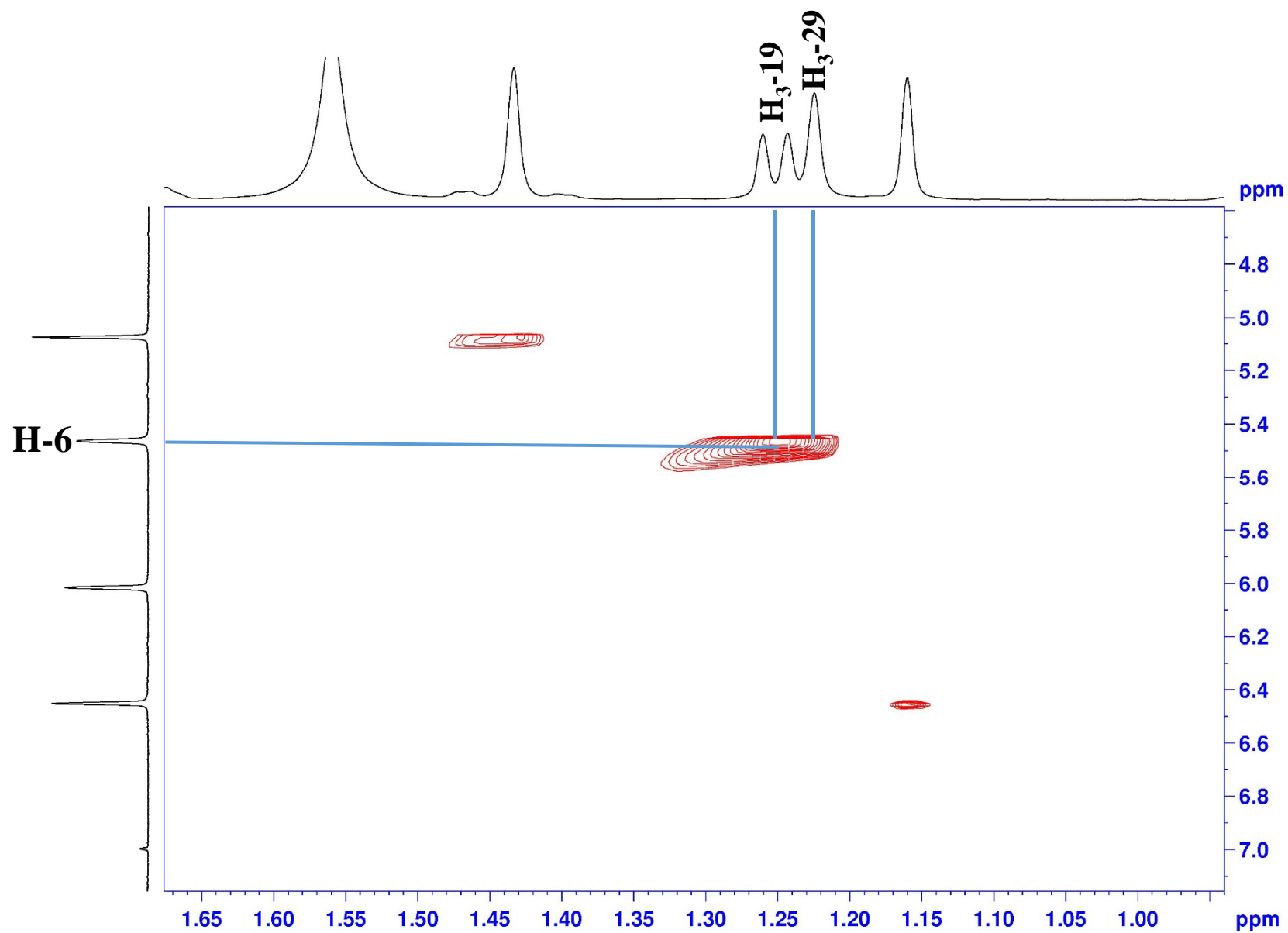
NOESY (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



NOESY (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$

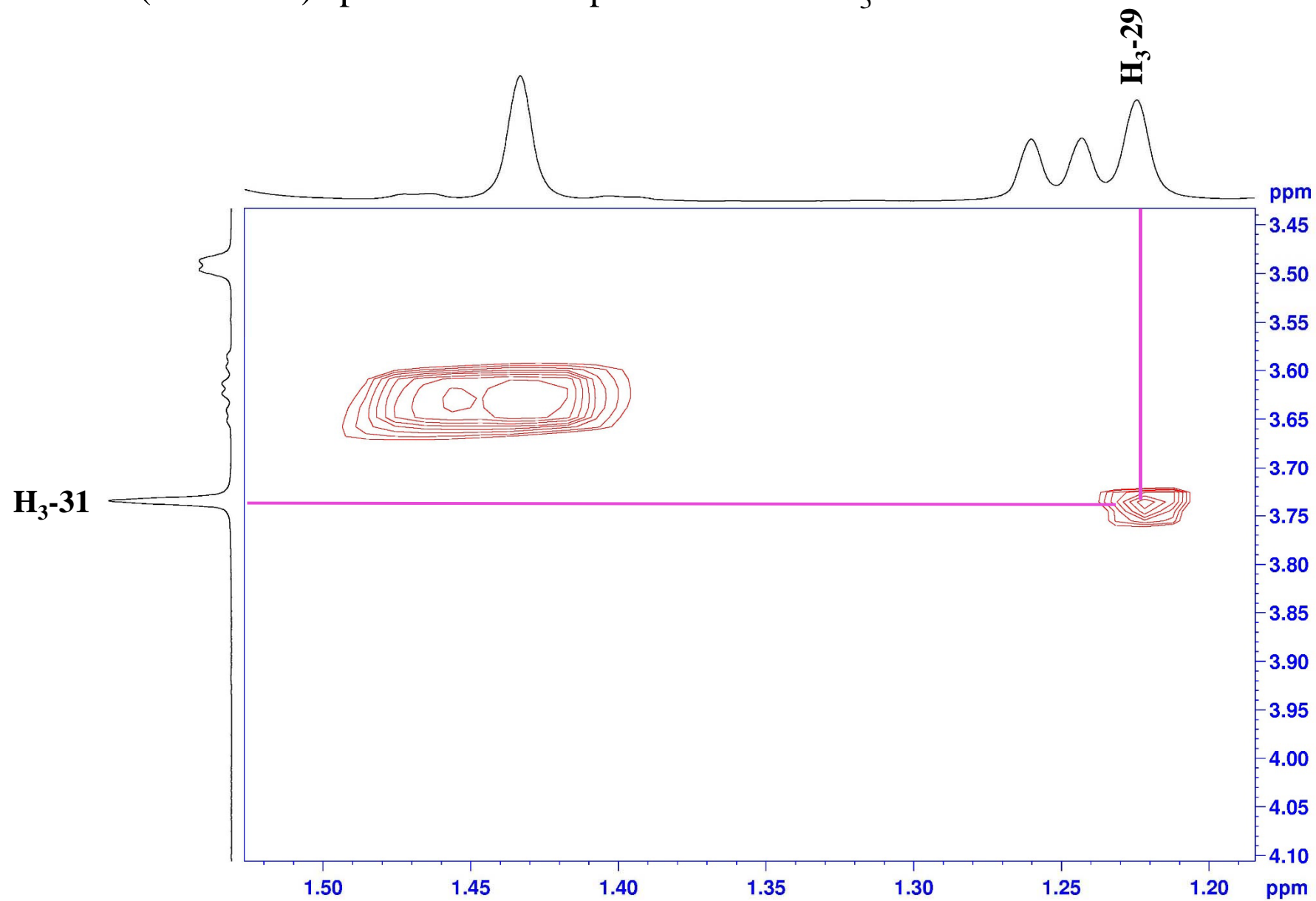


NOESY (400 MHz) spectrum of compound **2** in CDCl<sub>3</sub>



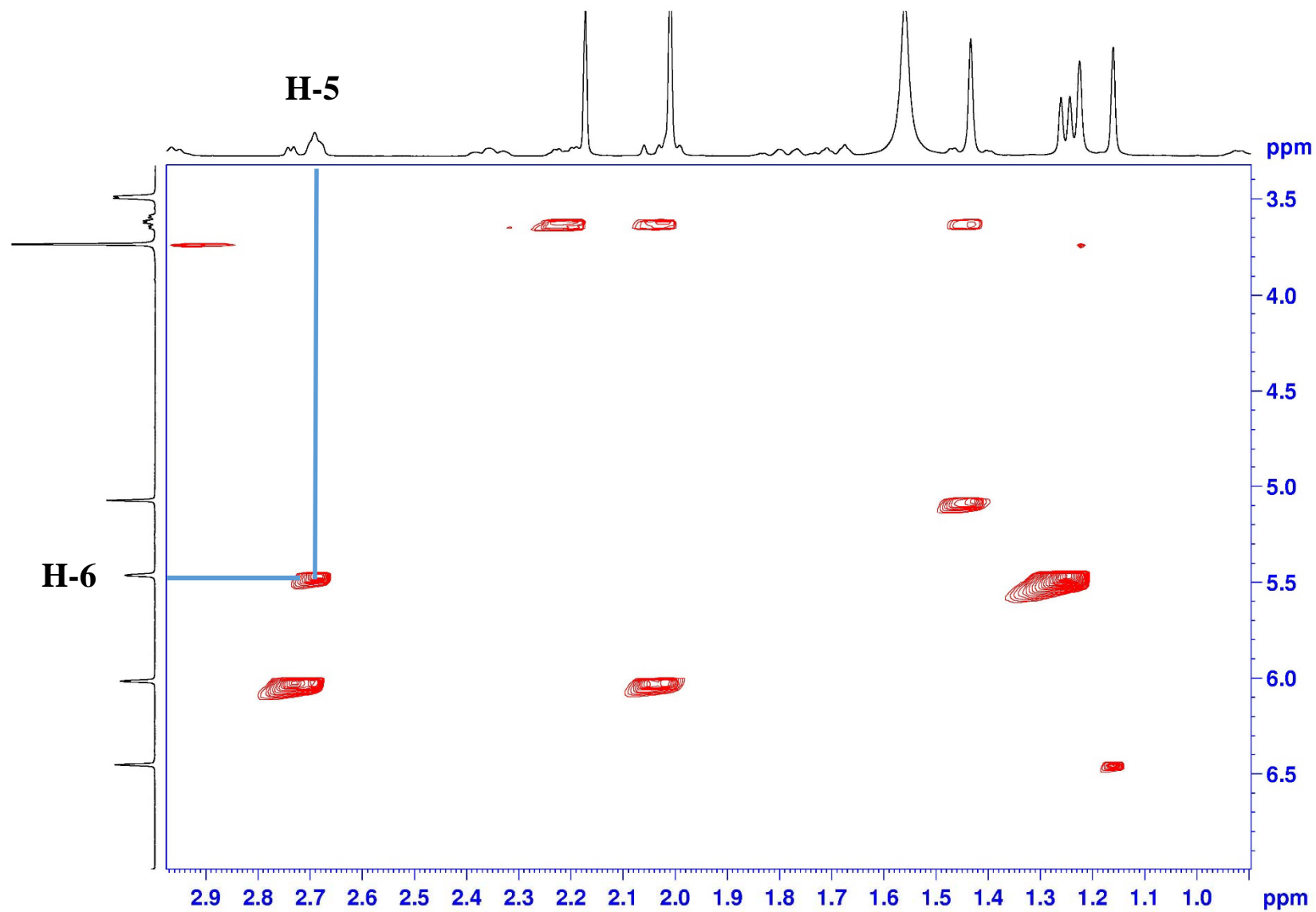


NOESY (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$

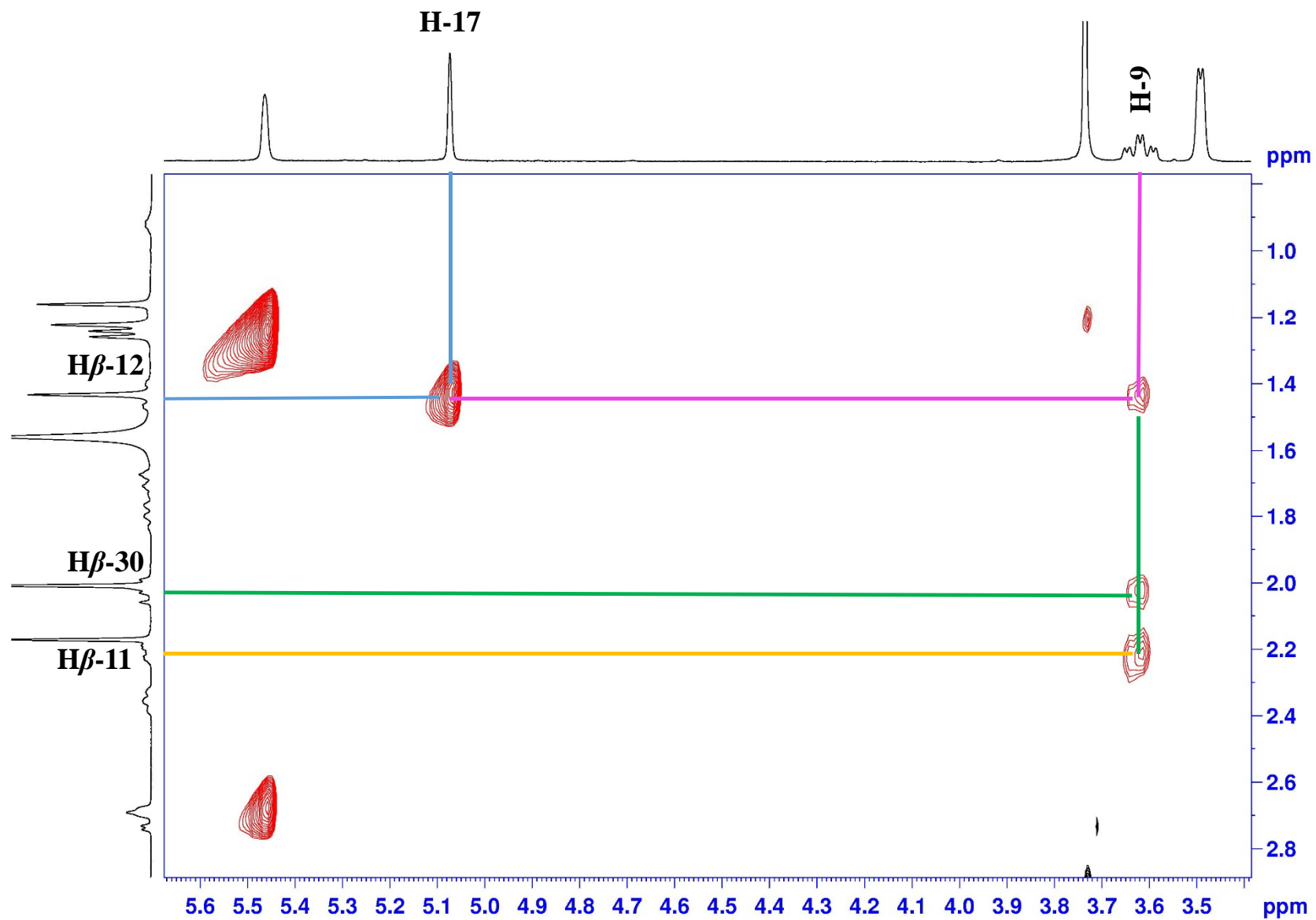




NOESY (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



NOESY (400 MHz) spectrum of compound **2** in  $\text{CDCl}_3$



# HR-ESIMS for compound 3

## Mass Spectrum SmartFormula Report

### Analysis Info

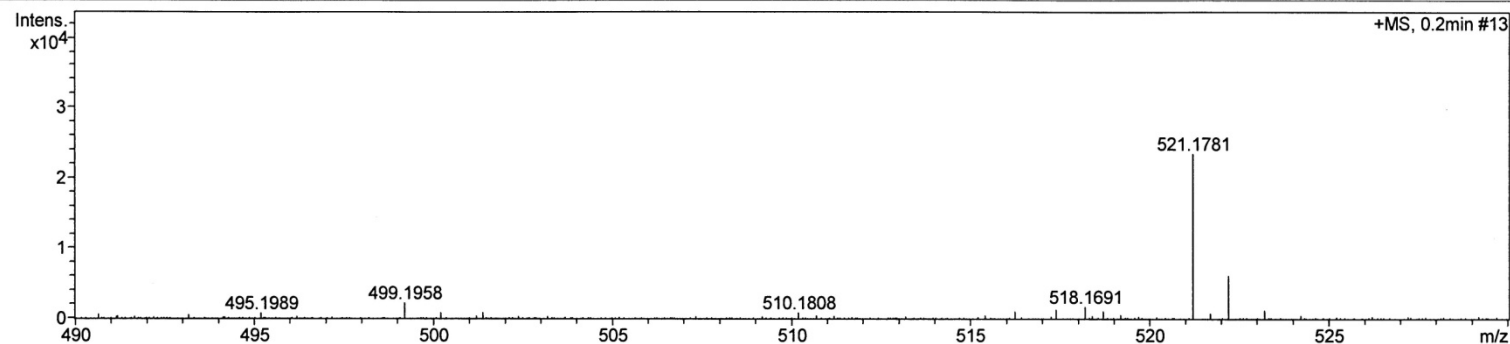
Analysis Name D:\Data\MS\data\201512\liwanshan\_lws-82\_pos\_11\_01\_1015.d  
 Method LC\_Direct Infusion\_pos\_100-1000mz.m  
 Sample Name liwanshan\_lws-82\_pos  
 Comment

Acquisition Date 12/18/2015 5:35:56 AM

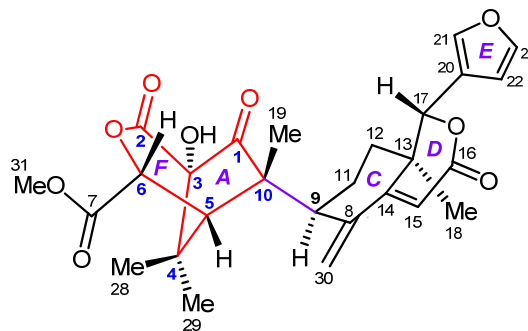
Operator SCSIO  
 Instrument / Ser# maXis 29

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
499.1958	1	C 27 H 31 O 9	100.00	499.1963	0.8	0.4	53.9	12.5	even	ok
521.1781	1	C 27 H 30 Na O 9	100.00	521.1782	0.3	0.1	16.6	12.5	even	ok



# HR-ESIMS for compound 3

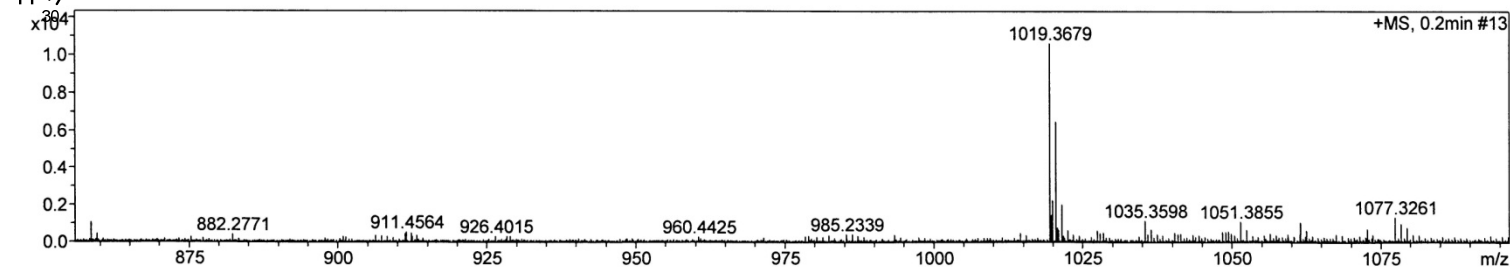
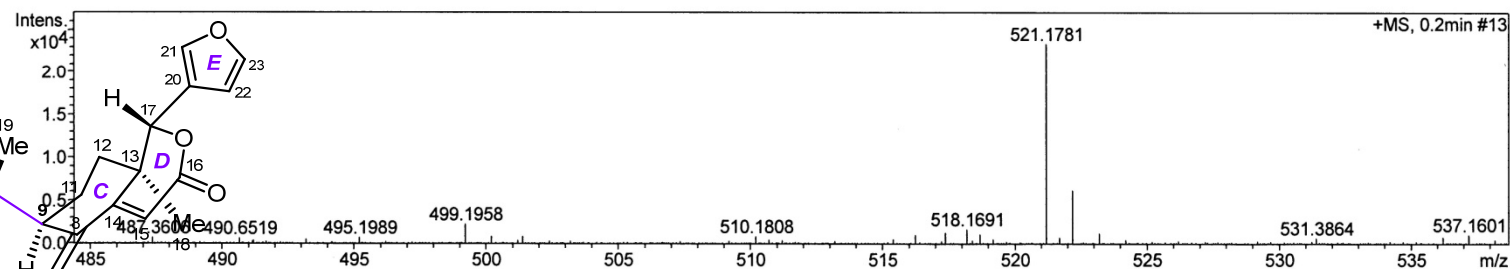
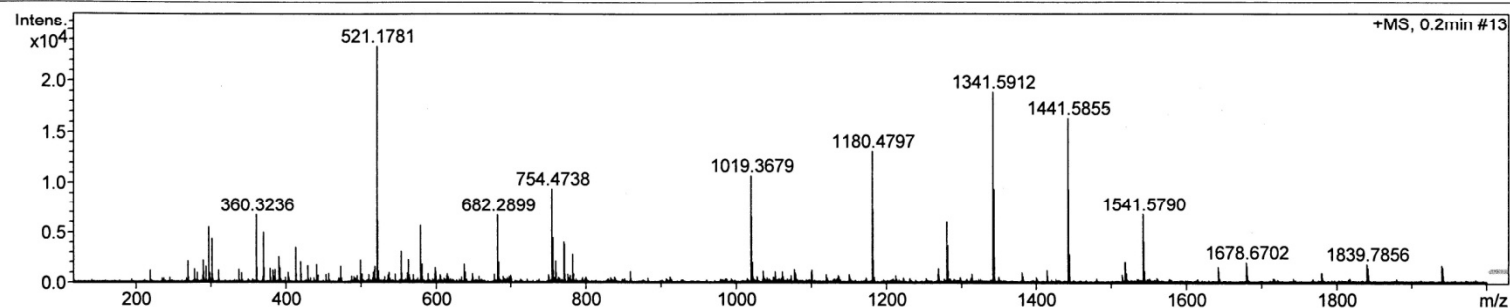
## Generic Display Report

### Analysis Info

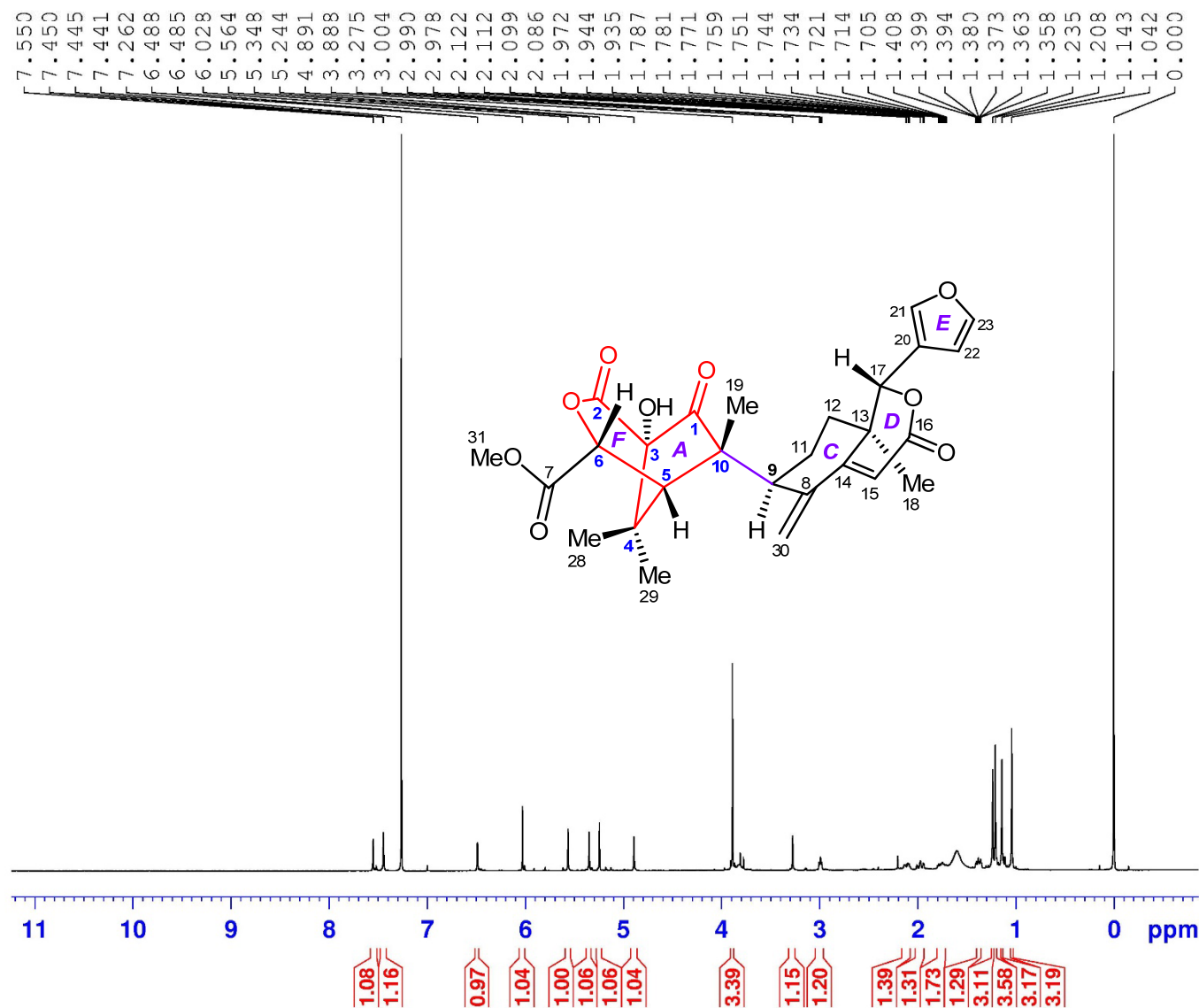
Analysis Name D:\Data\MS\data\201512\liwanshan\_lws-82\_pos\_11\_01\_1015.d  
Method LC\_Direct Infusion\_pos\_100-1000mz.m  
Sample Name liwanshan\_lws-82\_pos  
Comment

Acquisition Date 12/18/2015 5:35:56 AM

Operator SCSIO  
Instrument maXis



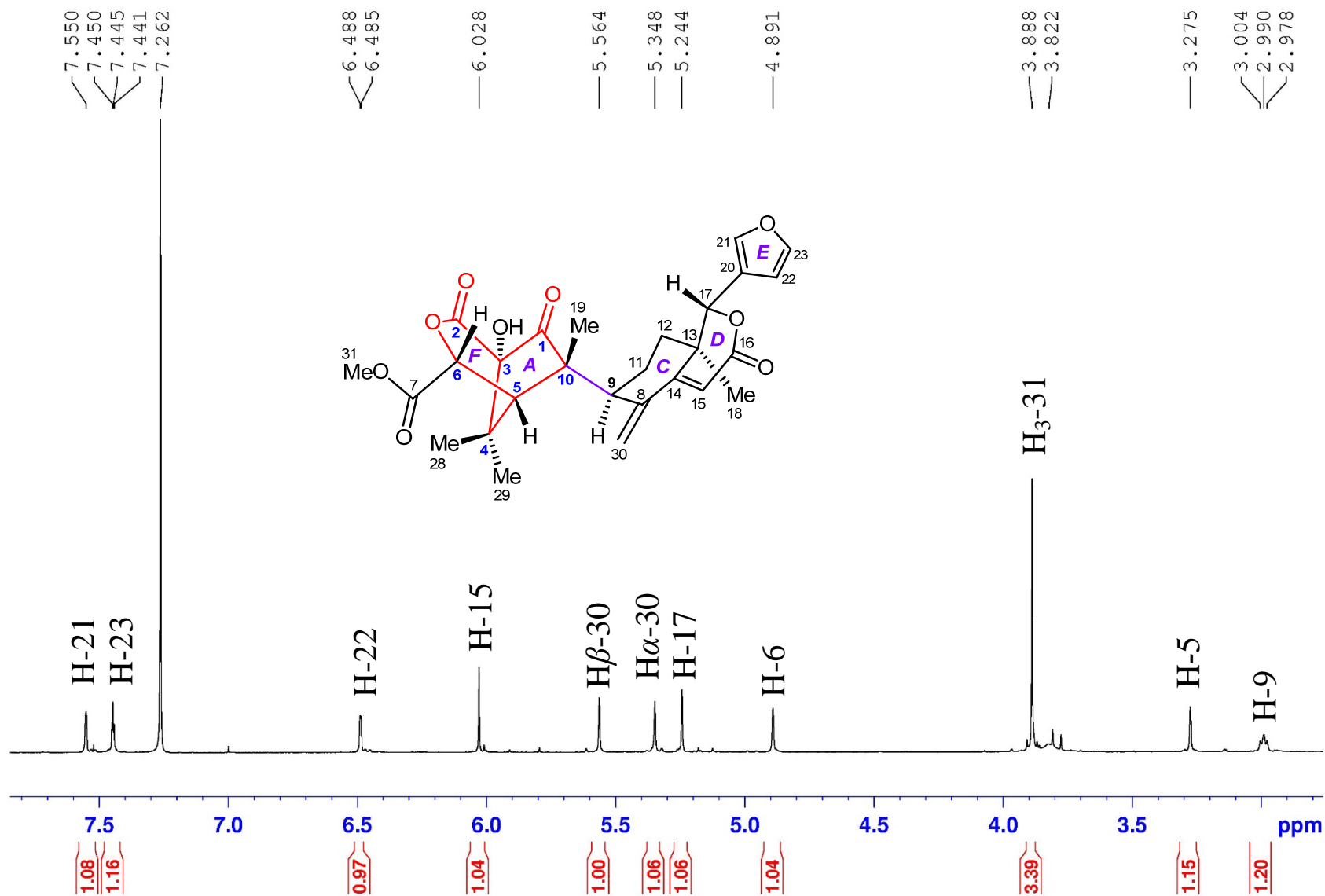
$^1\text{H}$  NMR (400 MHz) spectrum of compound **3** in  $\text{CDCl}_3$



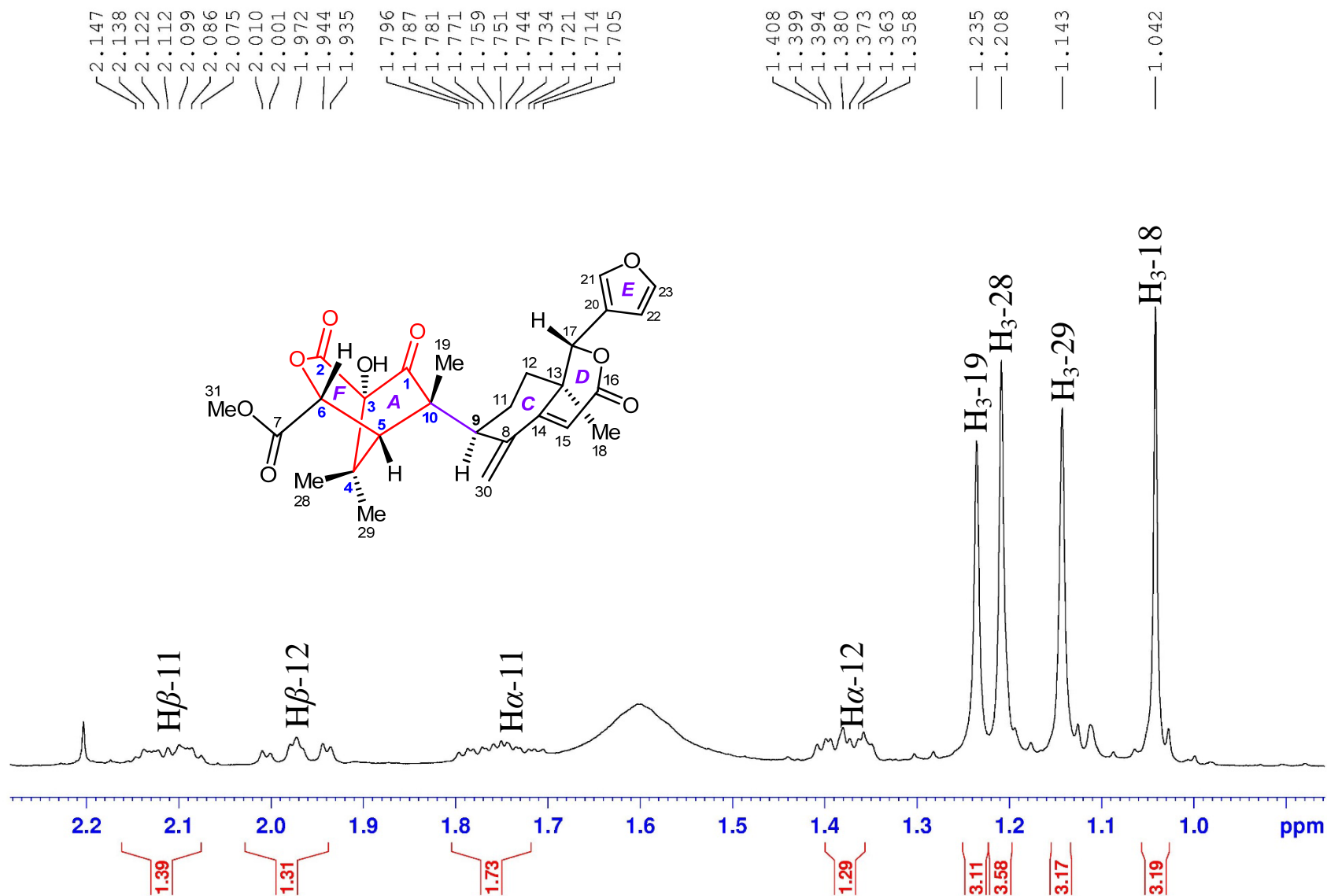
NAME lws-82-2017  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20171004  
 Time 14.29  
 INSTRUM spect  
 PROBHD 5 mm CPPBBO BB  
 PULPROG zg30  
 TD 65536  
 SOLVENT  $\text{CDCl}_3$   
 NS 32  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9846387 s  
 RG 208.5  
 DW 60.800  $\mu\text{s}$   
 DE 10.00  $\mu\text{s}$   
 TE 297.0 K  
 D1 1.00000000 s  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 400.1324710 MHz  
 NUC1  $^1\text{H}$   
 P1 11.50  $\mu\text{s}$   
 SI 65536  
 SF 400.1300091 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

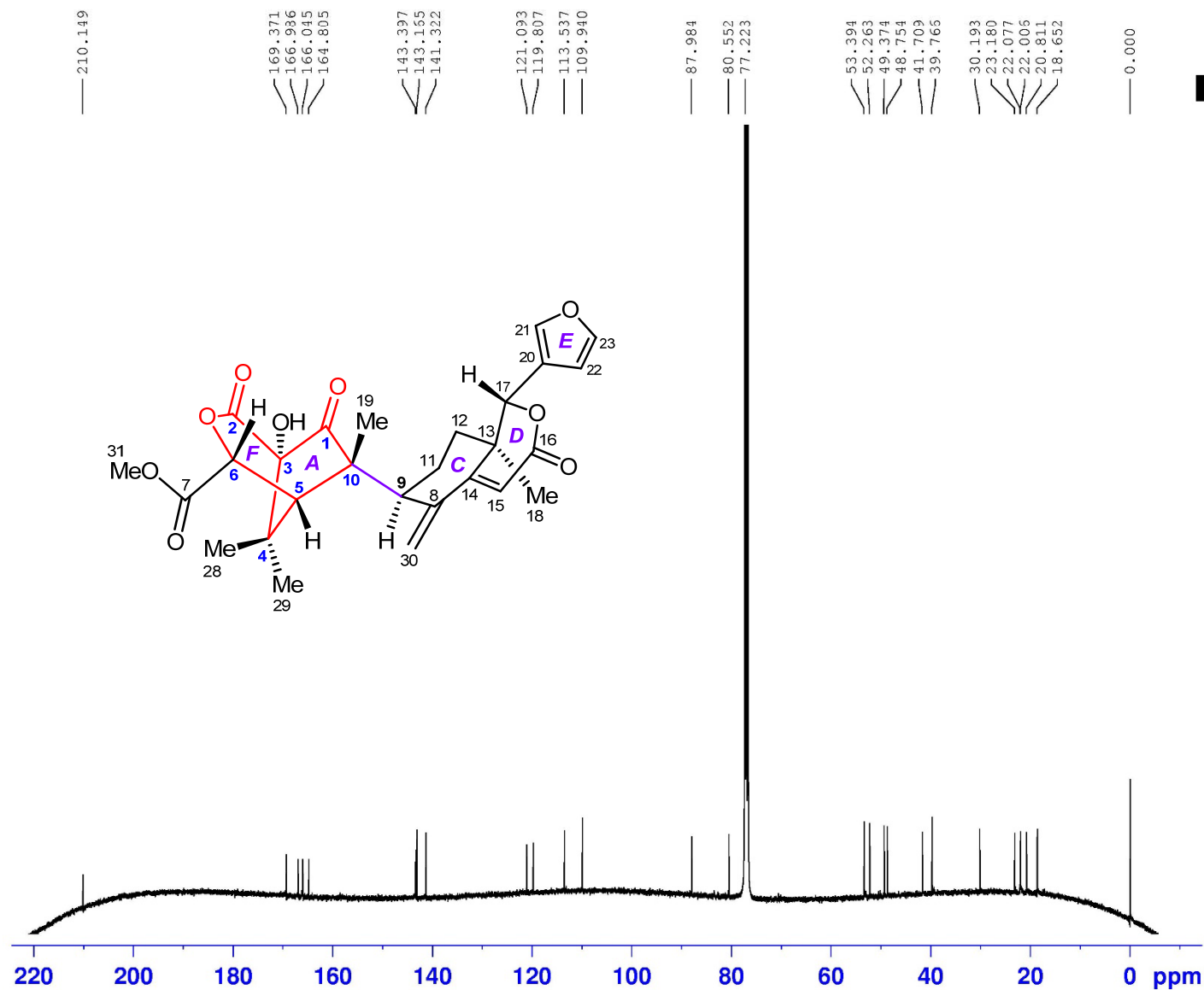
$^1\text{H}$  NMR (400 MHz) spectrum of compound **3** in  $\text{CDCl}_3$



$^1\text{H}$  NMR (400 MHz) spectrum of compound **3** in  $\text{CDCl}_3$



# $^{13}\text{C}$ NMR (100 MHz) spectrum of compound **3** in $\text{CDCl}_3$



```

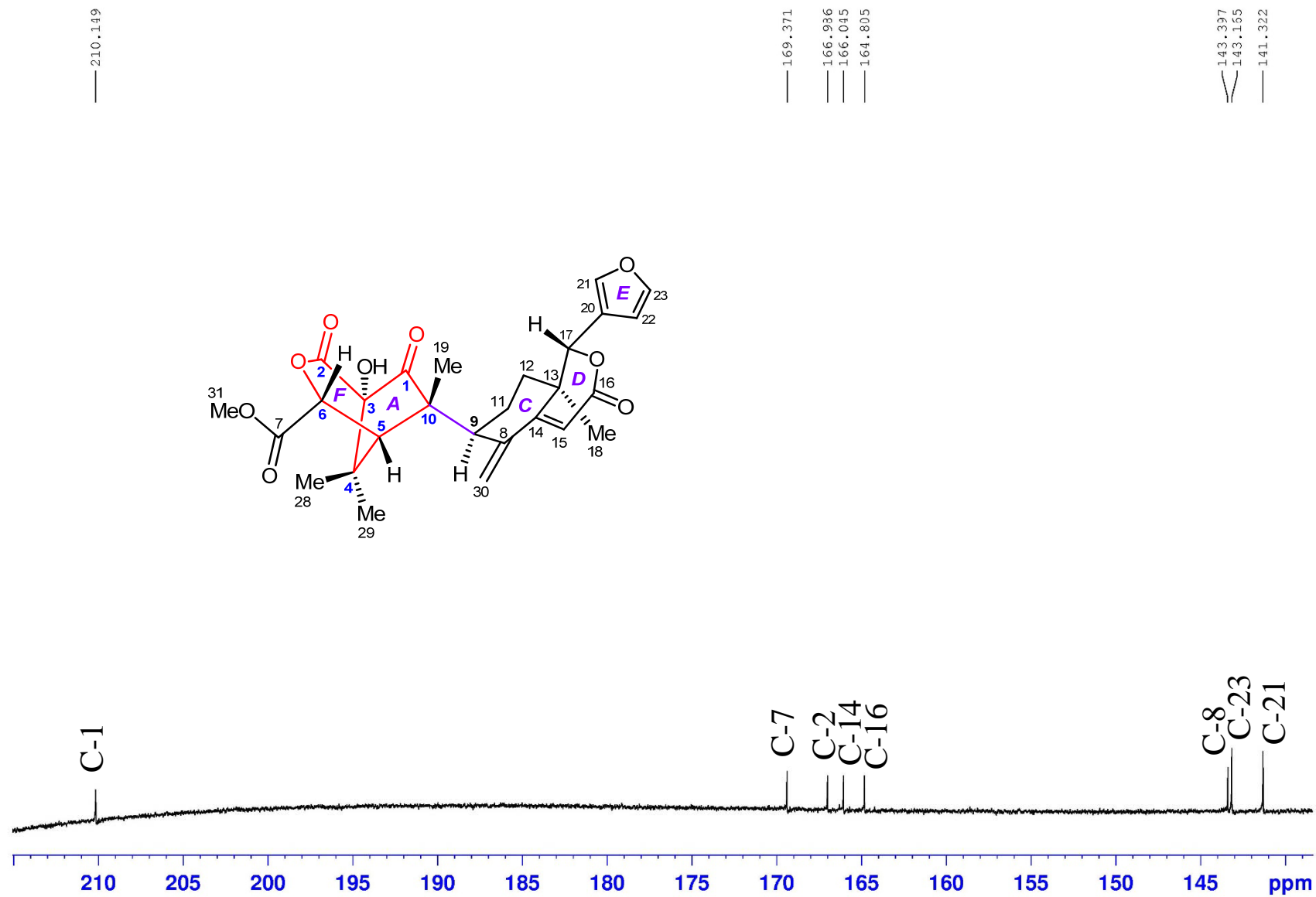
NAME                lws-82
EXPNO                2
PROCNO              1
Date_               20151007
Time                23.08
INSTRUM             spect
PROBHD             5 mm CPPBBO BB
PULPROG             zgpg30
TD                 65536
SOLVENT             CDCl3
NS                  40000
DS                   4
SWH                 24038.461 F
FIDRES              0.366798 F
AQ                  1.3631988 s
RG                  102.3
DW                  20.800 u
DE                   18.00 u
TE                   297.0 K
D1                   2.00000000 s
D11                  0.03000000 s
TD0                  1
  
```

```

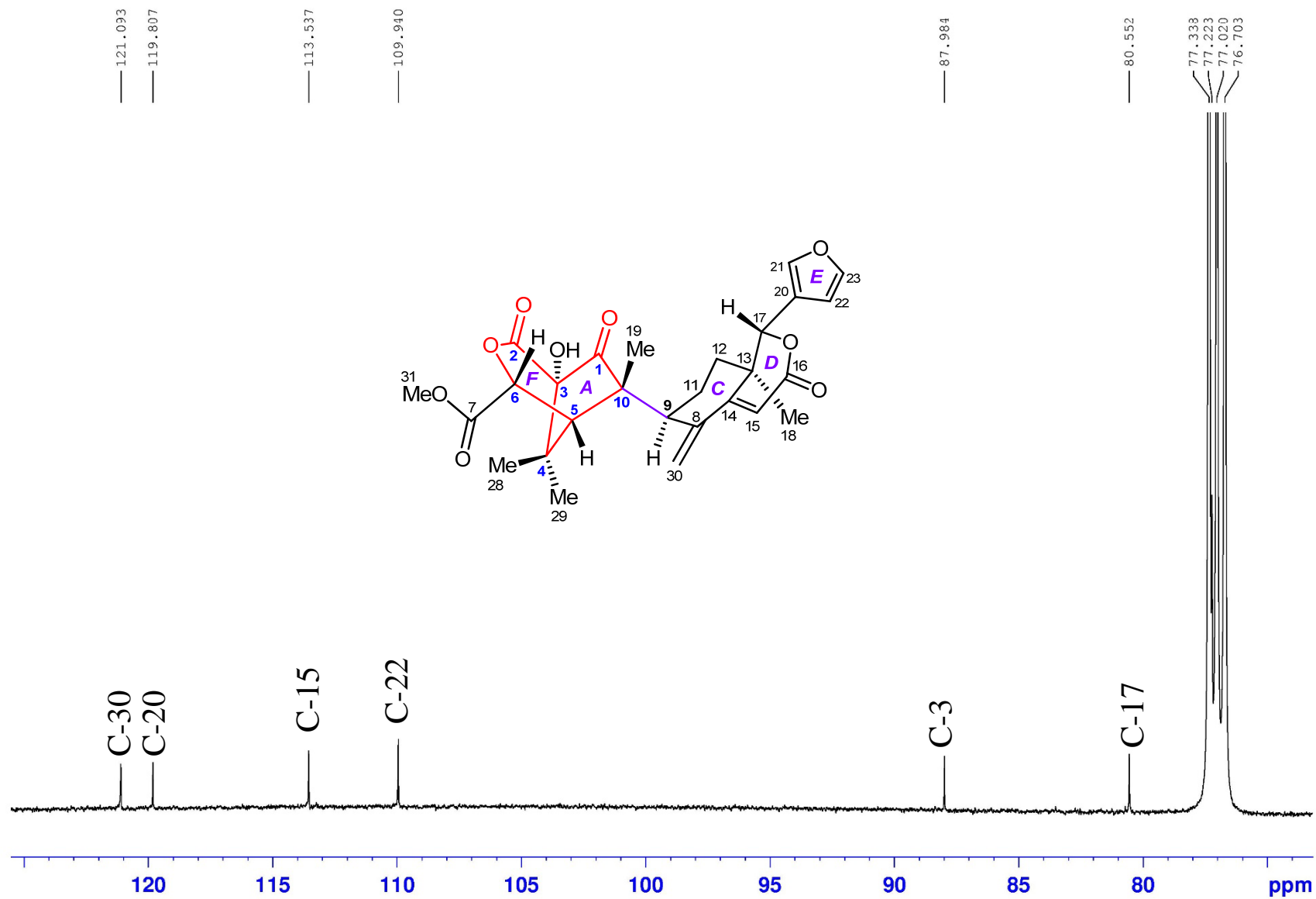
===== CHANNEL f1 =====
SFO1             100.6233324 M
NUC1              13C
P1                 10.00 u
SI                 32768
SF                100.6127690 M
WDW                EM
SSB                 0
LB                  1.00 F
GB                   0
PC                  1.40
  
```



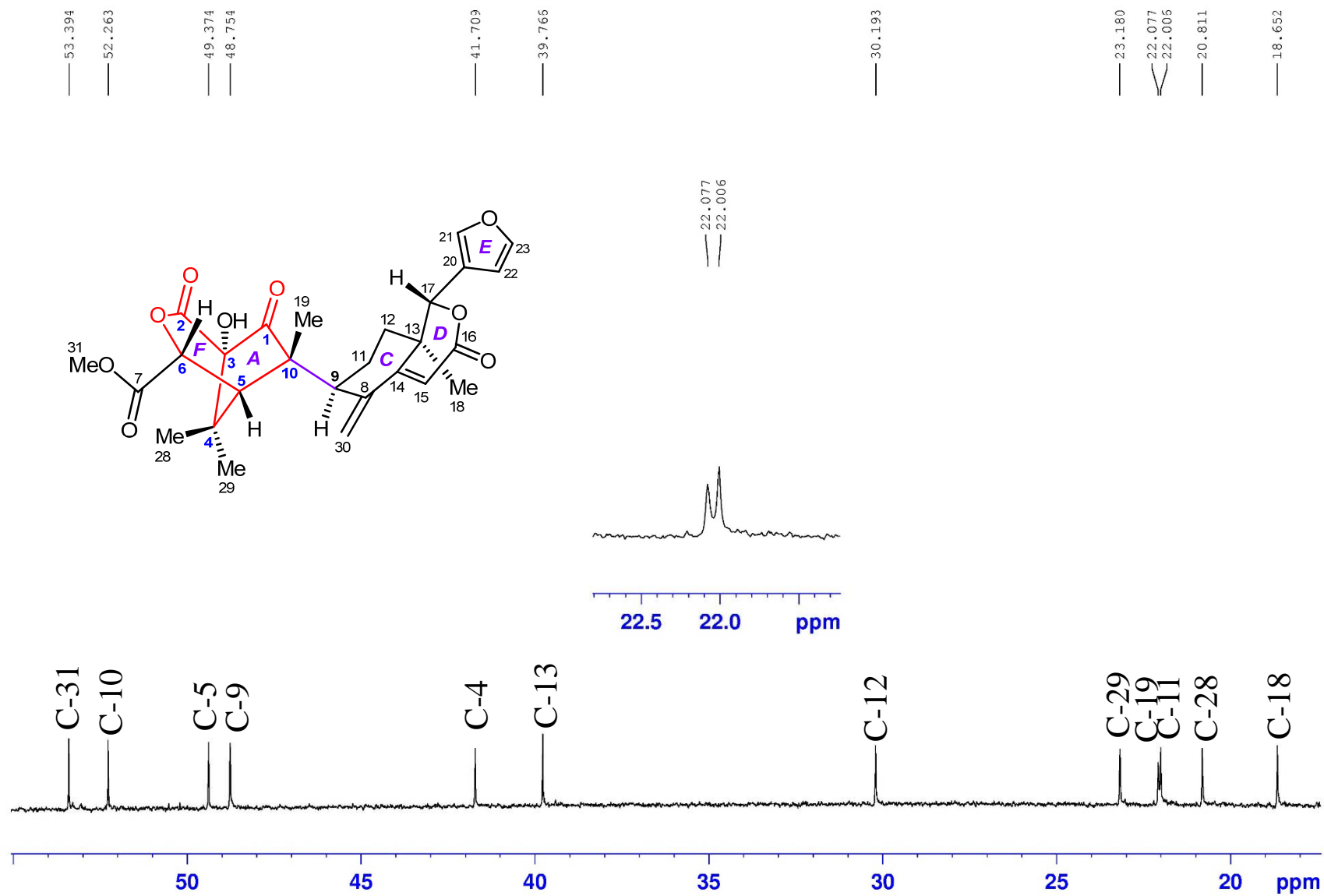
$^{13}\text{C}$  NMR (100 MHz) spectrum of compound **3** in  $\text{CDCl}_3$



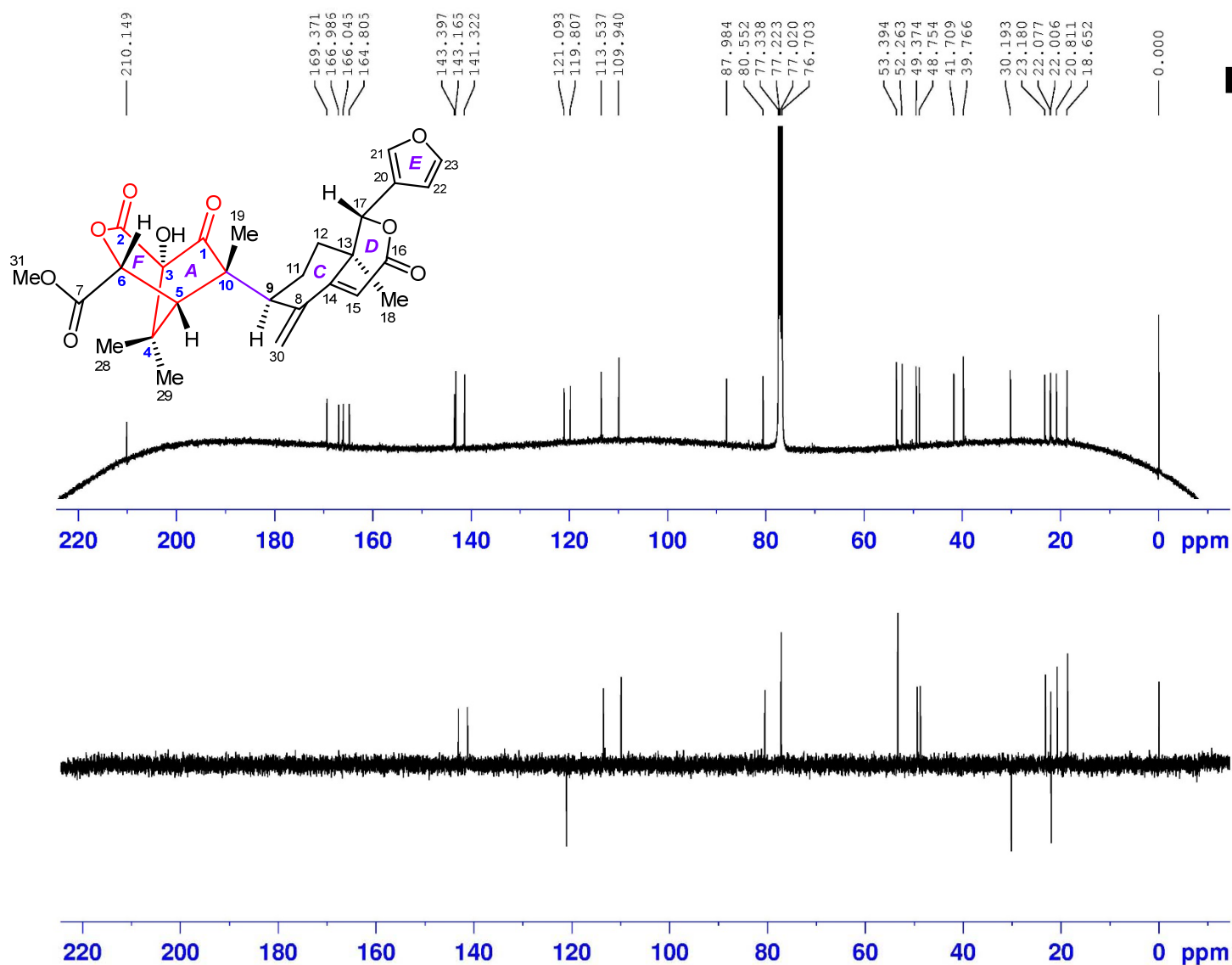
$^{13}\text{C}$  NMR (100 MHz) spectrum of compound **3** in  $\text{CDCl}_3$



$^{13}\text{C}$  NMR (100 MHz) spectrum of compound **3** in  $\text{CDCl}_3$



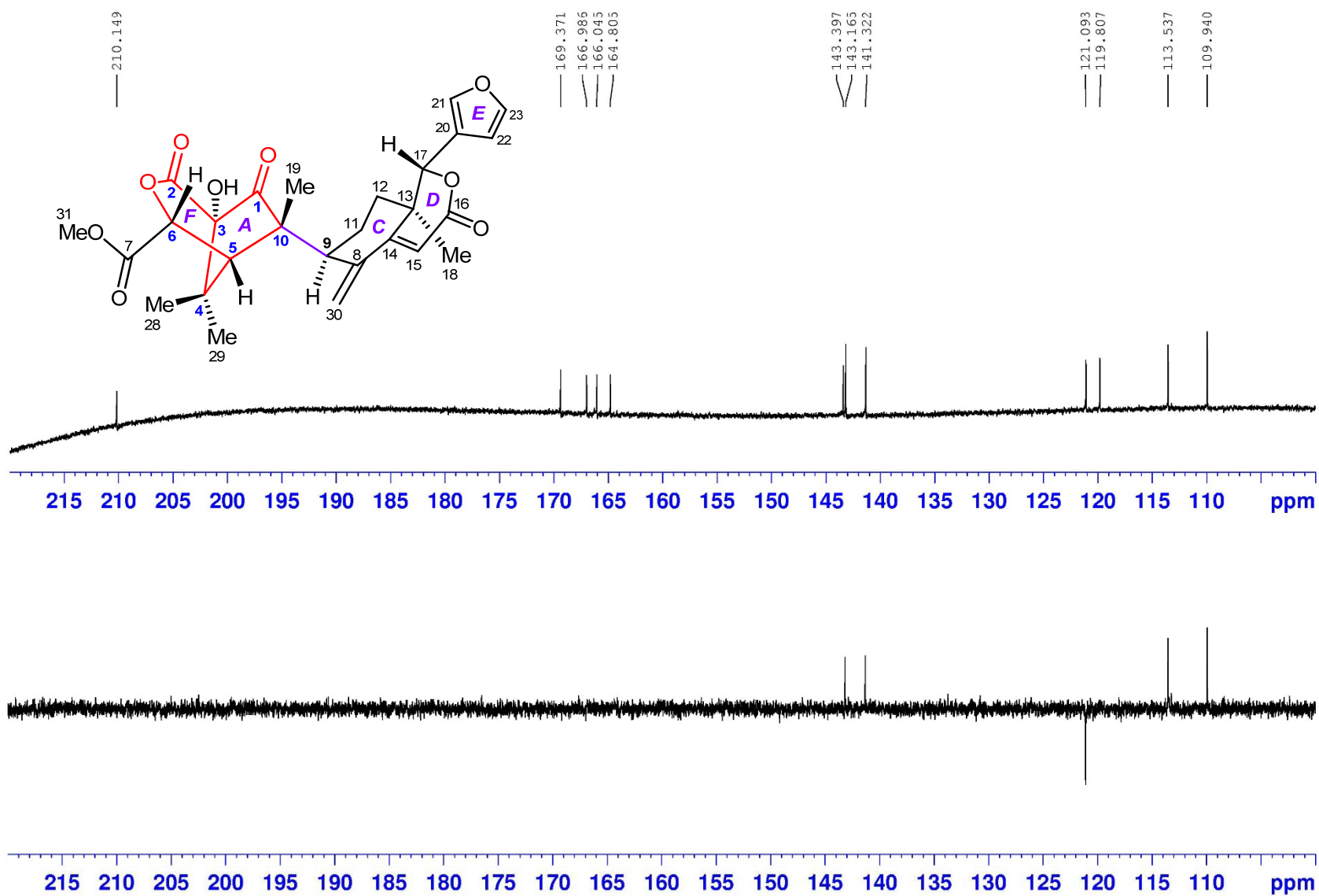
# DEPT135 (100 MHz) spectrum of compound **3** in CDCl<sub>3</sub>



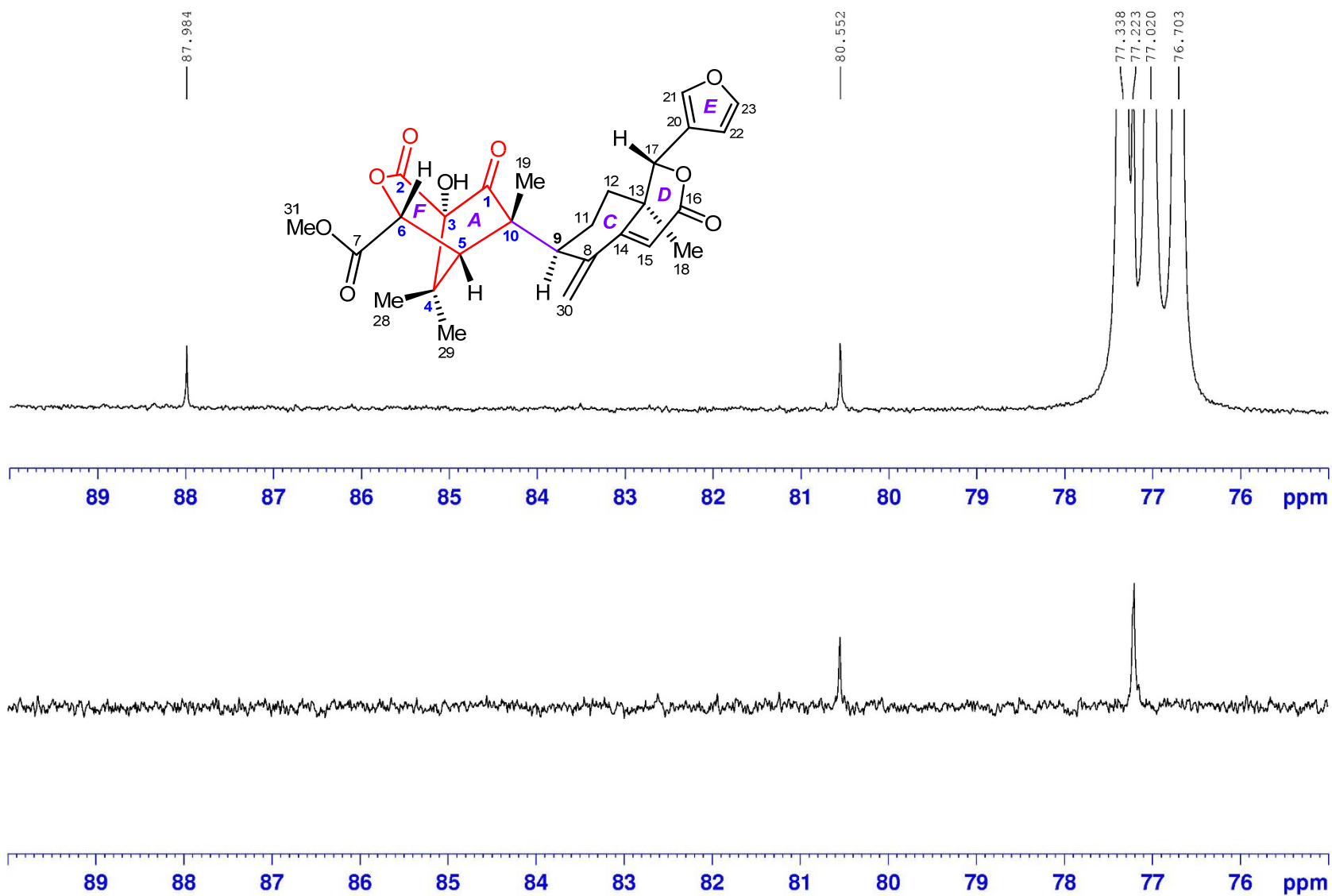
NAME lws-82  
 EXPNO 3  
 PROCNO 1  
 Date\_ 20151010  
 Time 16.58  
 INSTRUM spect  
 PROBHD 5 mm CPPBBO BB  
 PULPROG deptspl35  
 TD 65536  
 SOLVENT CDCl3  
 NS 1246  
 DS 4  
 SWH 24038.461 F  
 FIDRES 0.366798 F  
 AQ 1.3631988 s  
 RG 130.26  
 DW 20.800 u  
 DE 18.00 u  
 TE 297.0 F  
 CNST2 145.0000000  
 D1 2.00000000 s  
 D2 0.00344828 s  
 D12 0.00002000 s  
 TD0 1

===== CHANNEL f1 =====  
 SF01 100.6233324 M  
 NUC1 13C  
 P1 10.00 u  
 P13 2000.00 u  
 SI 32768  
 SF 100.6127690 M  
 WDW EM  
 SSB 0  
 LB 1.00 F  
 GB 0  
 PC 1.40

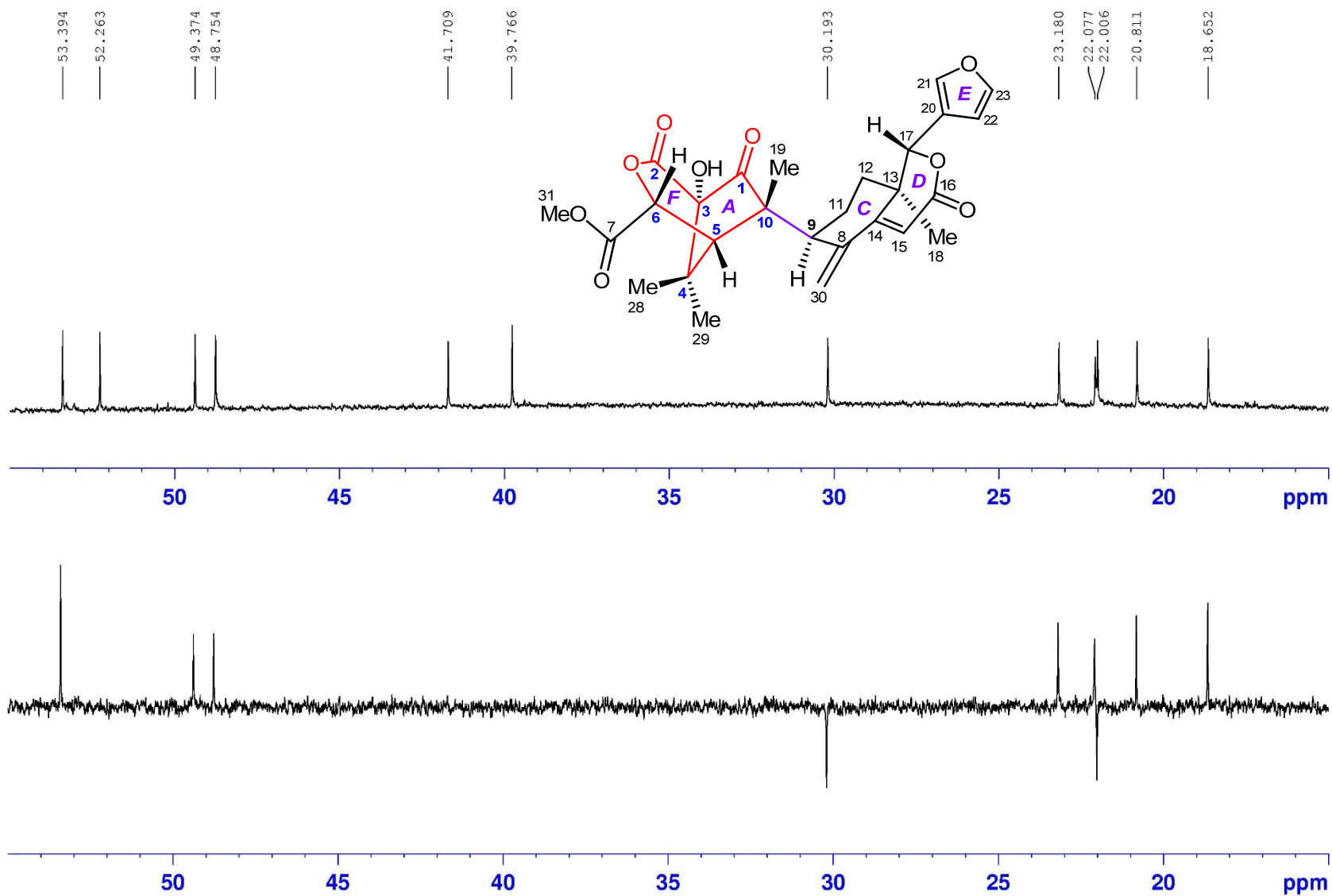
# DEPT135 (100 MHz) spectrum of compound **3** in CDCl<sub>3</sub>



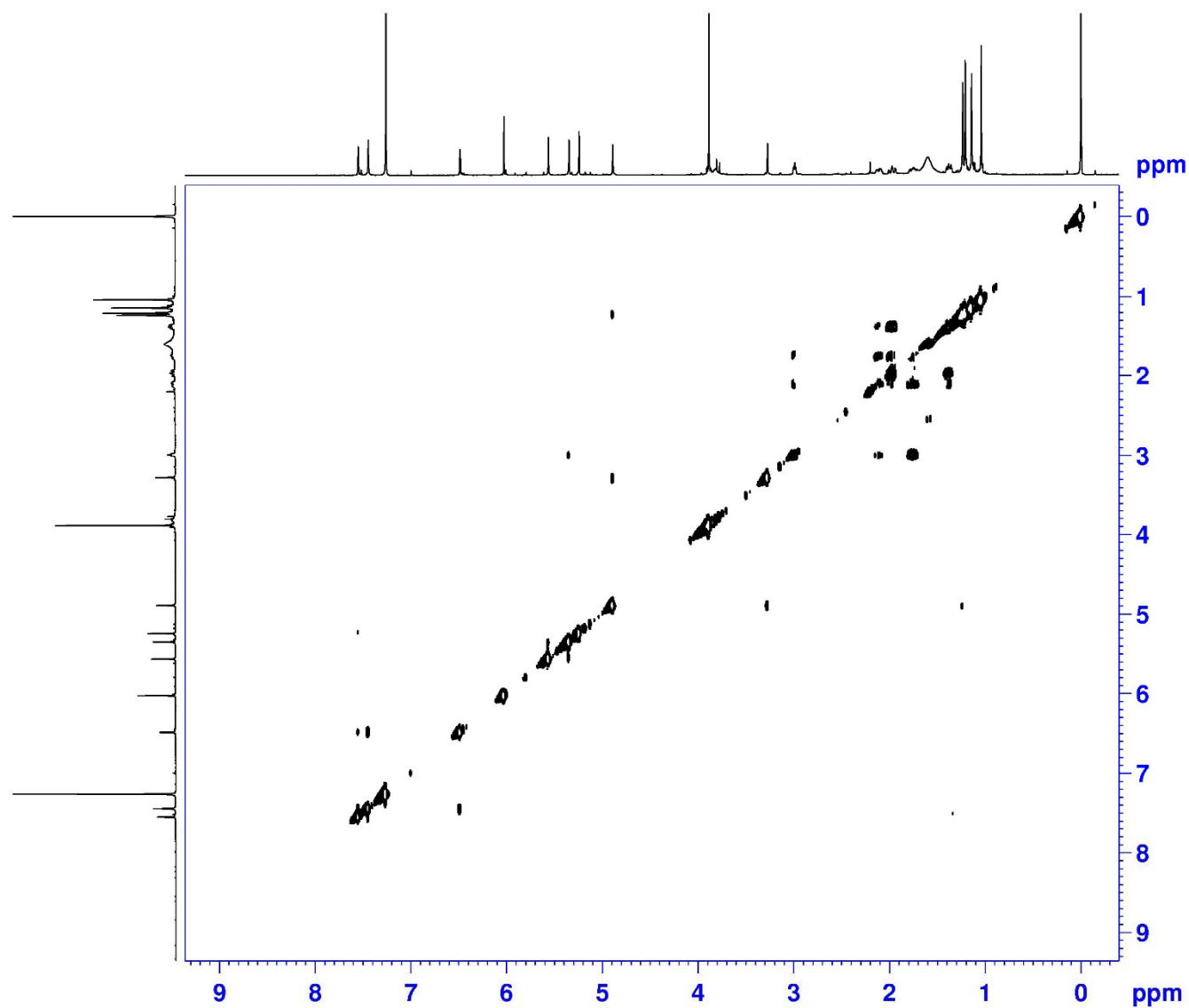
# DEPT135 (100 MHz) spectrum of compound **3** in CDCl<sub>3</sub>



$^1\text{H}$ - $^1\text{H}$  COSY (400 MHz) spectrum of compound **3** in  $\text{CDCl}_3$



# $^1\text{H}$ - $^1\text{H}$ COSY (400 MHz) spectrum of compound **3** in $\text{CDCl}_3$

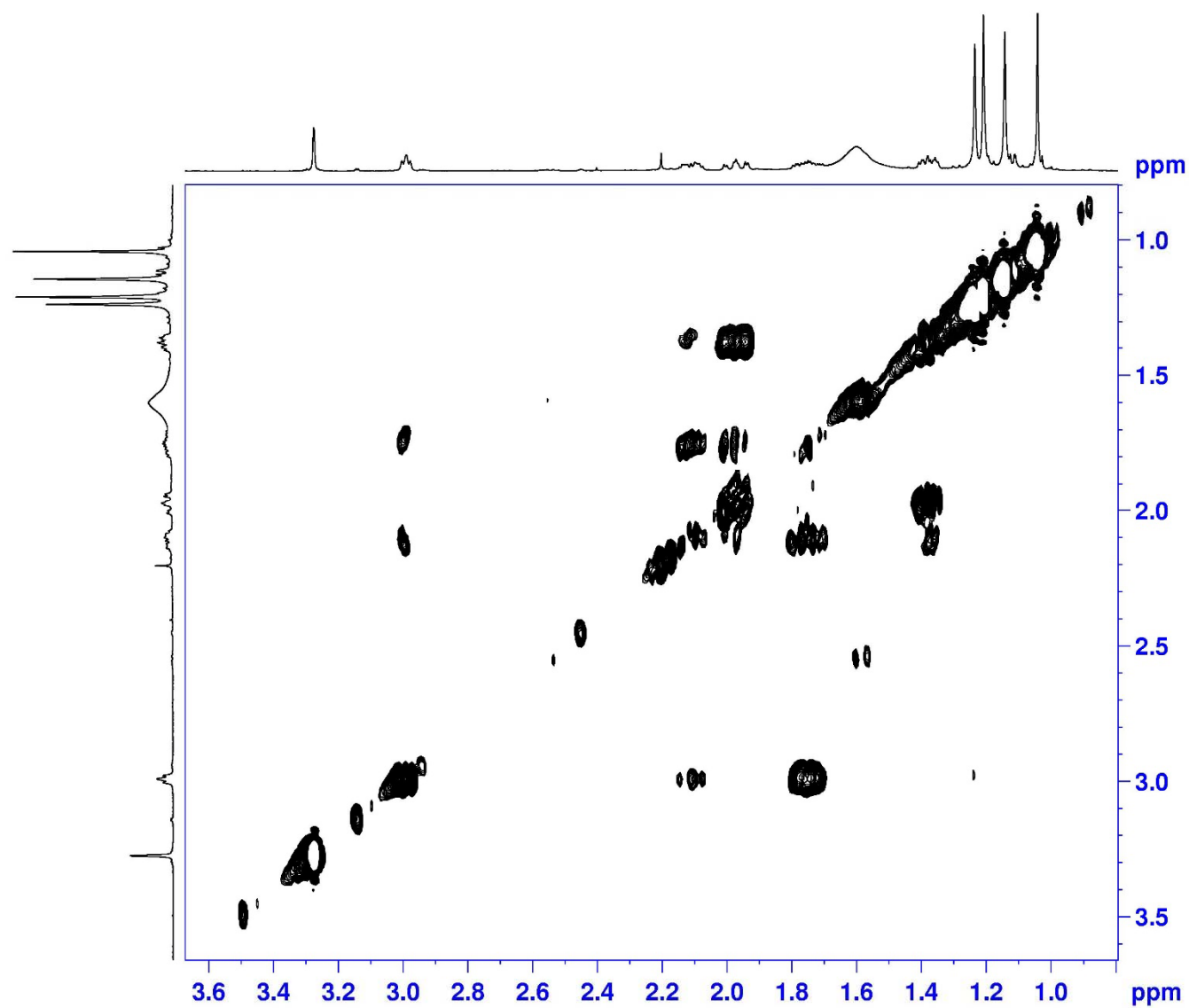


```
NAME          lws-82
EXPNO          5
PROCNO         1
Date_         20151011
Time          5.30
INSTRUM        spect
PROBHD         5 mm CPBBO BB
PULPROG        cosygpppgf
TD             2048
SOLVENT        CDCl3
NS             32
DS             8
SWH            3906.250 Hz
FIDRES         1.907349 Hz
AQ             0.2621940 se
RG             208.5
DW             128.000 us
DE             10.00 us
TE             297.0 K
D0             0.00000300 se
D1             1.89678097 se
D11            0.03000000 se
D12            0.00002000 se
D13            0.00000400 se
D16            0.00020000 se
IN0            0.00025600 se
```

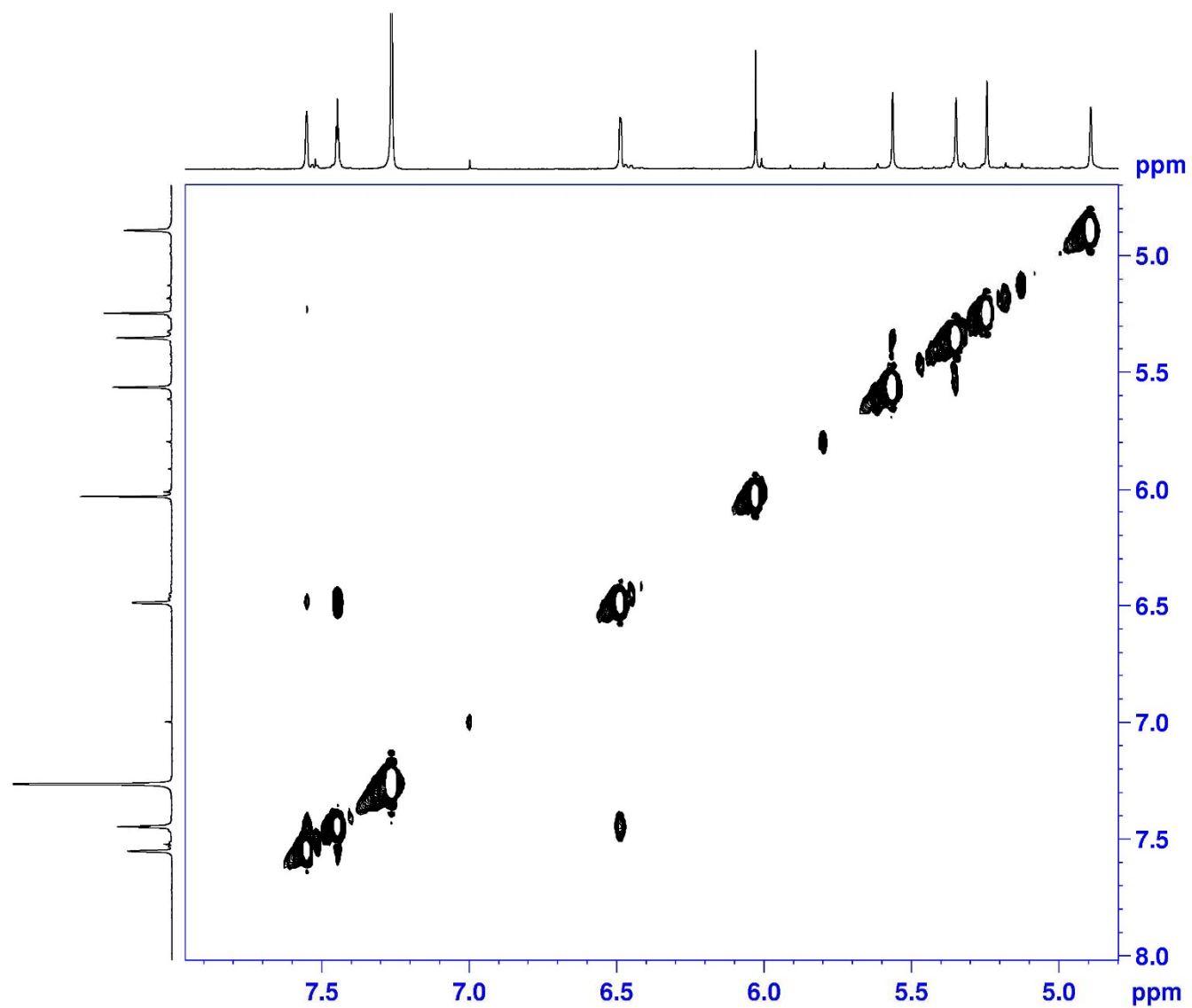
```
===== CHANNEL f1 =====
SFO1          400.1318006 MH
NUC1           1H
P0             12.00 us
P1             12.00 us
P17            2500.00 us
ND0            1
TD             128
SFO1          400.1318 MH
FIDRES         30.517578 Hz
SW             9.762 pp
FnmODE         QF
SI             1024
SF             400.1300070 MH
WDW            QSINE
SSB            0
LB             0.00 Hz
GB             0
PC             1.40
SI             1024
MC2            QF
SF             400.1300070 MH
```



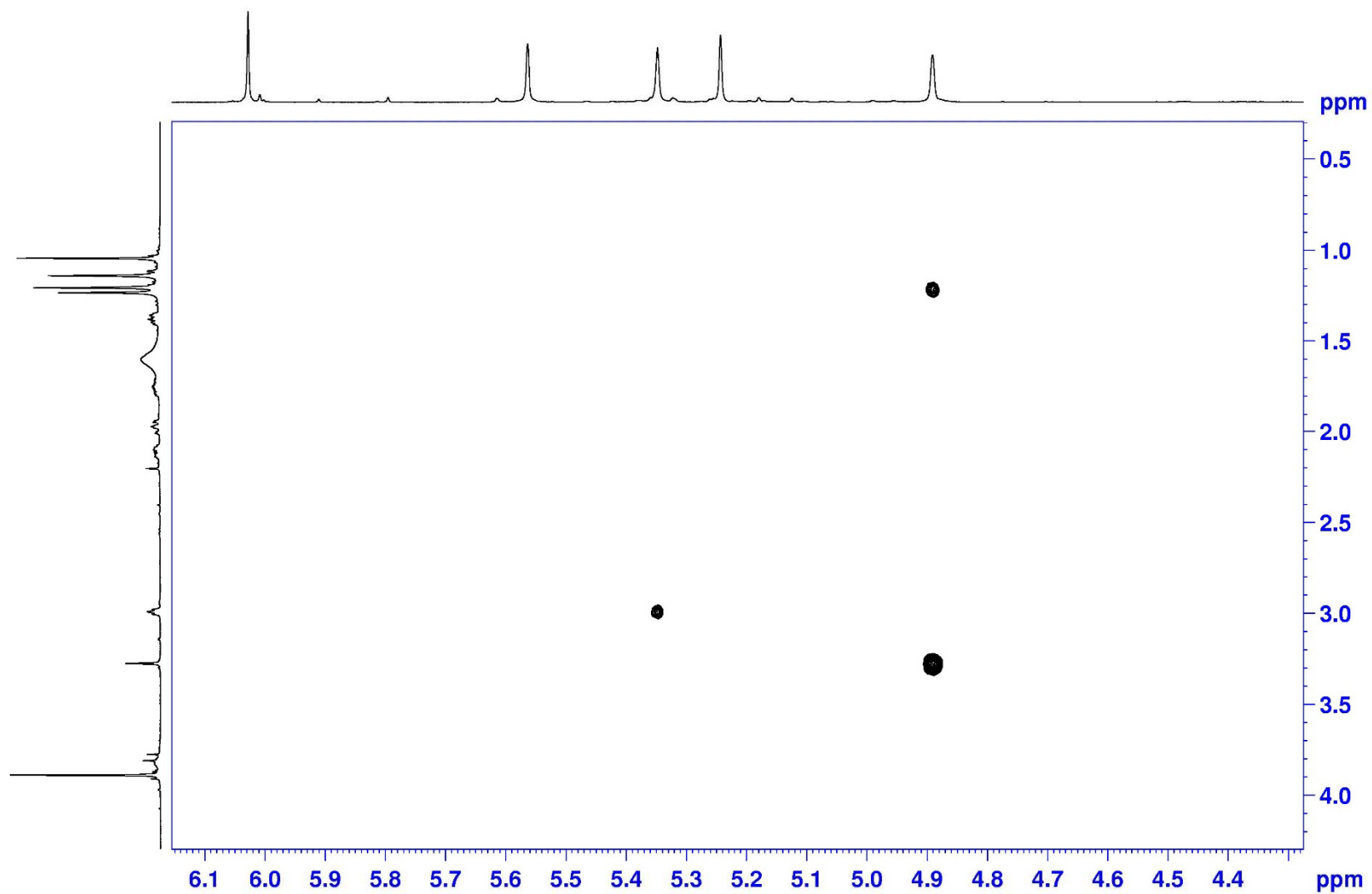
$^1\text{H}$ - $^1\text{H}$  COSY (400 MHz) spectrum of compound **3** in  $\text{CDCl}_3$



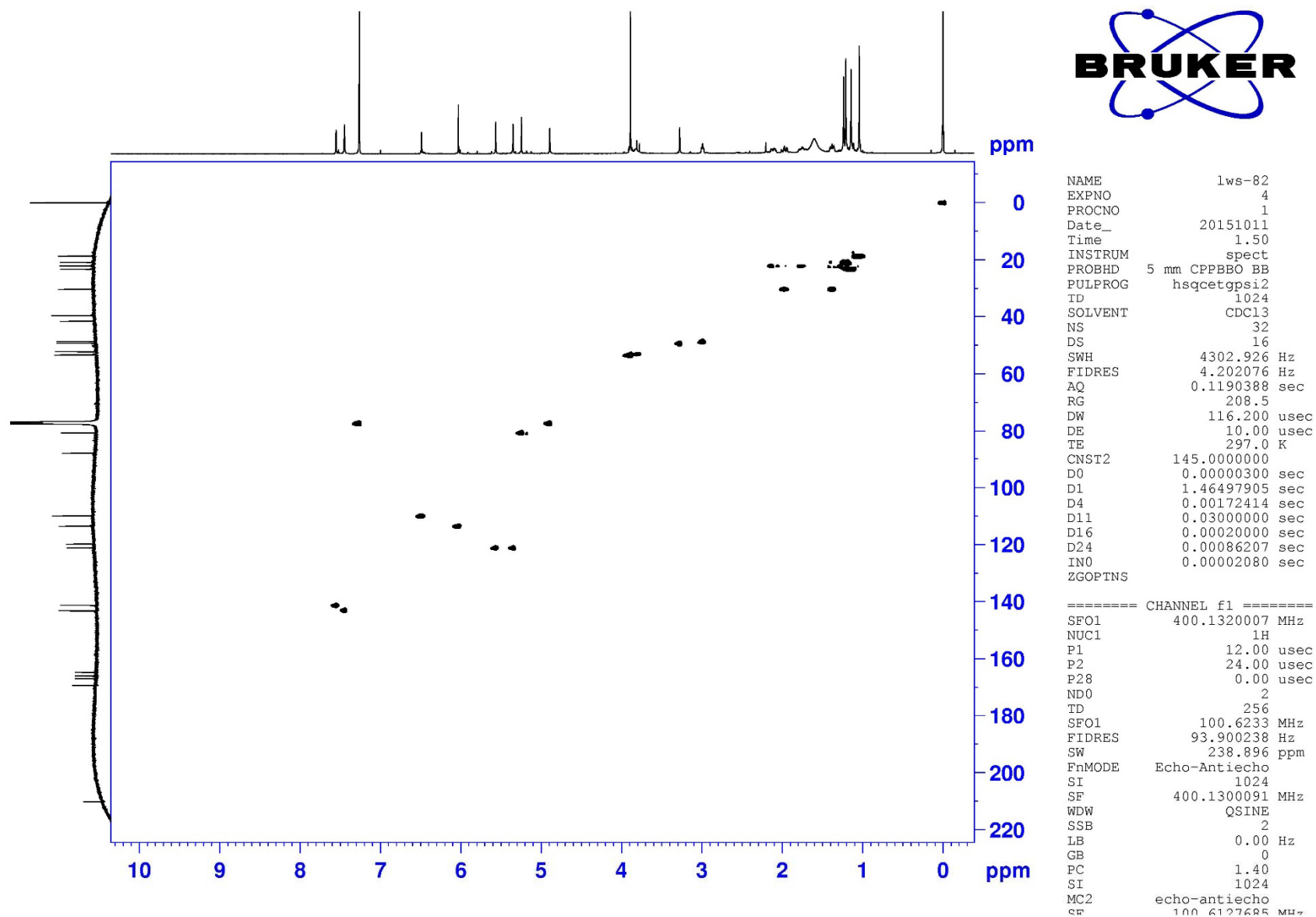
$^1\text{H}$ - $^1\text{H}$  COSY (400 MHz) spectrum of compound **3** in  $\text{CDCl}_3$



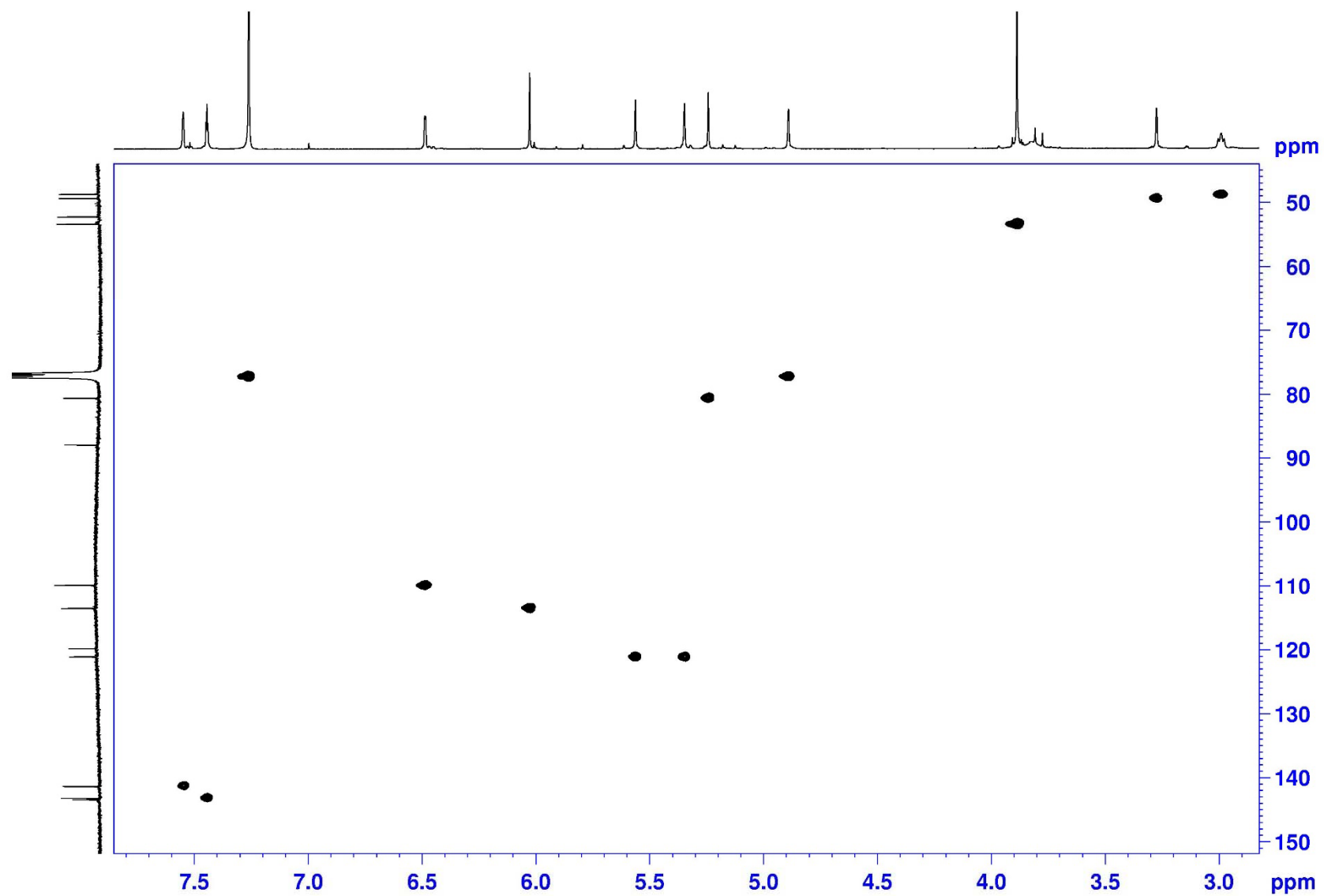
$^1\text{H}$ - $^1\text{H}$  COSY (400 MHz) spectrum of compound **3** in  $\text{CDCl}_3$



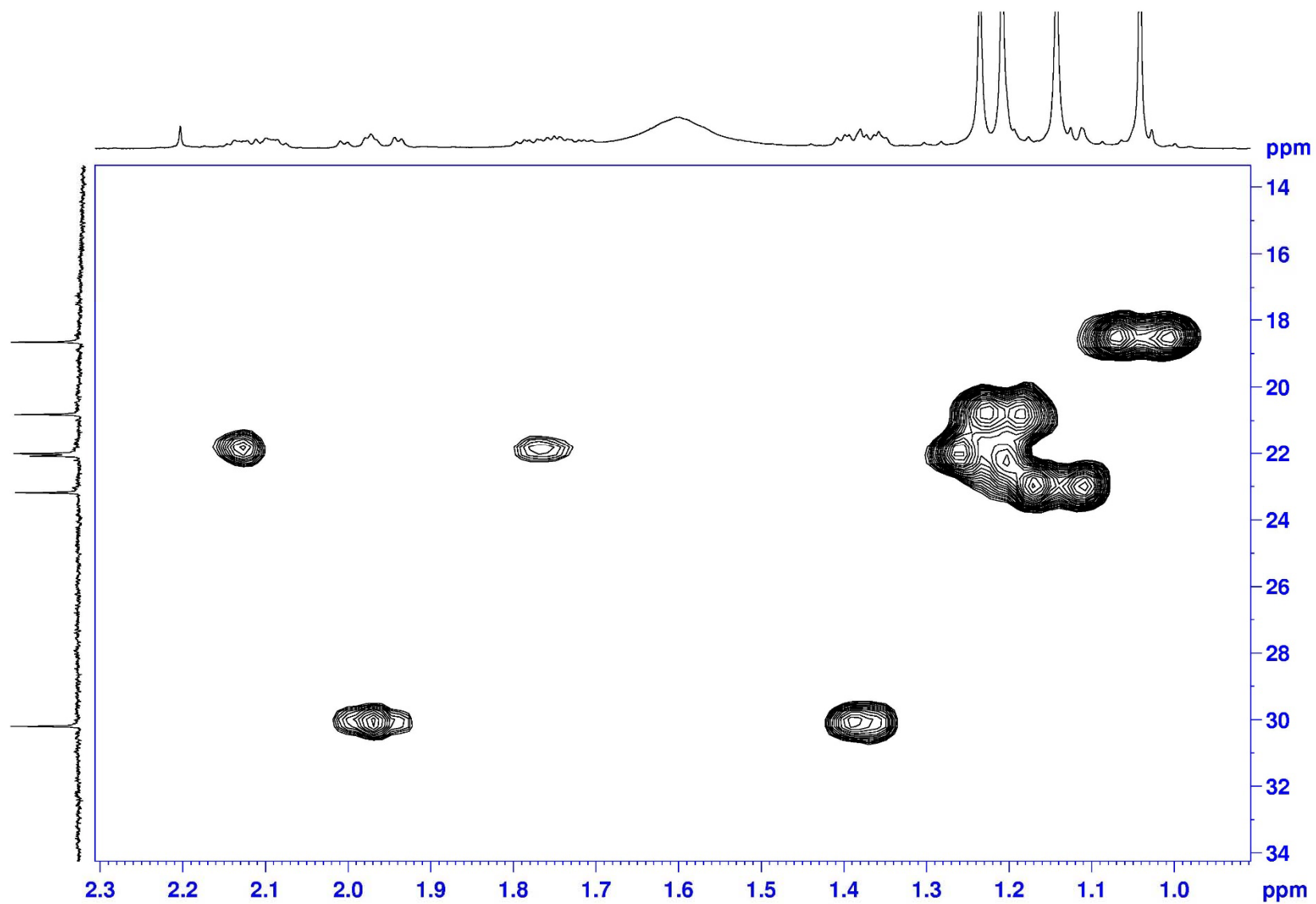
# HSQC (400 MHz) spectrum of compound **3** in CDCl<sub>3</sub>



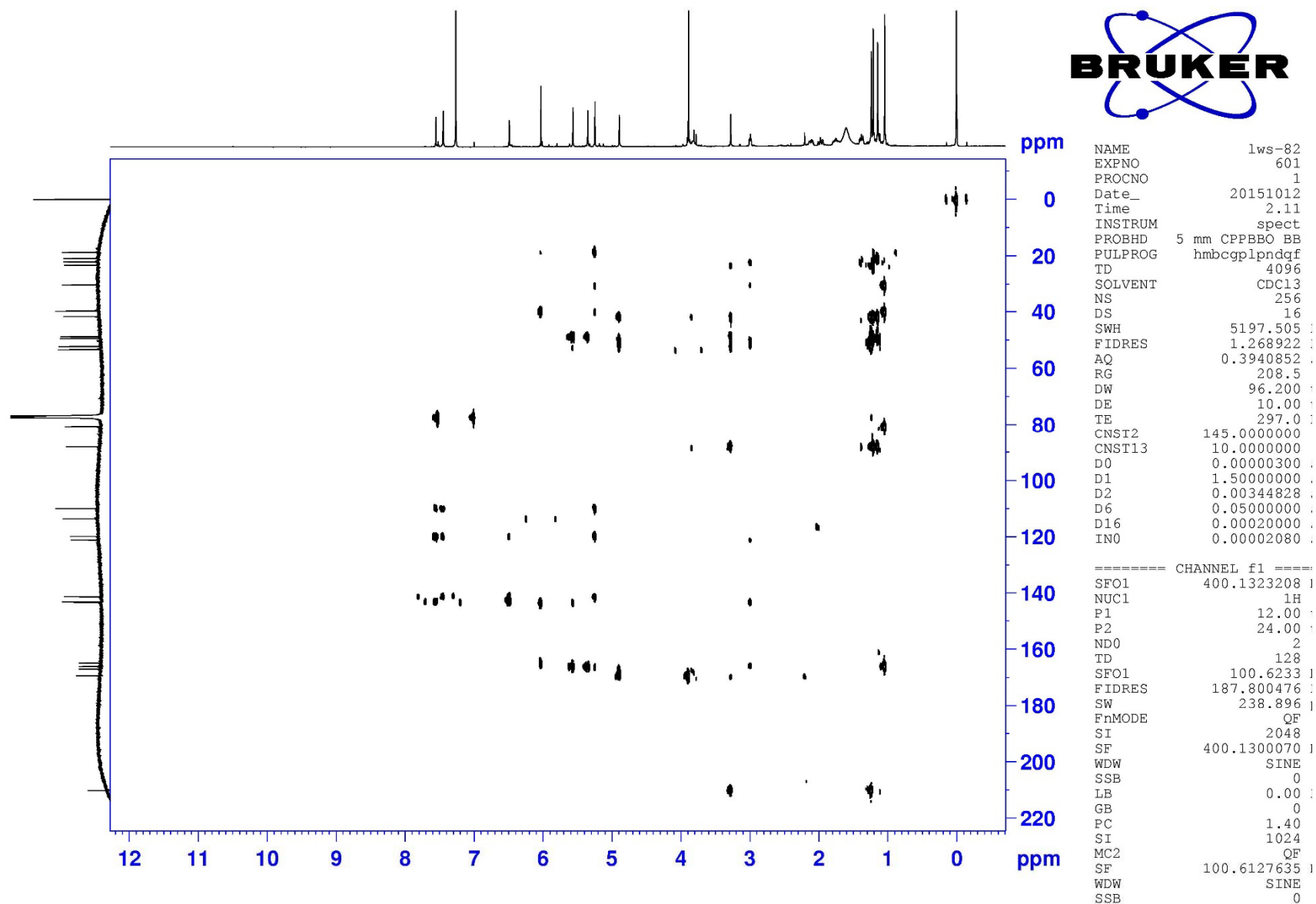
HSQC (400 MHz) spectrum of compound **3** in CDCl<sub>3</sub>



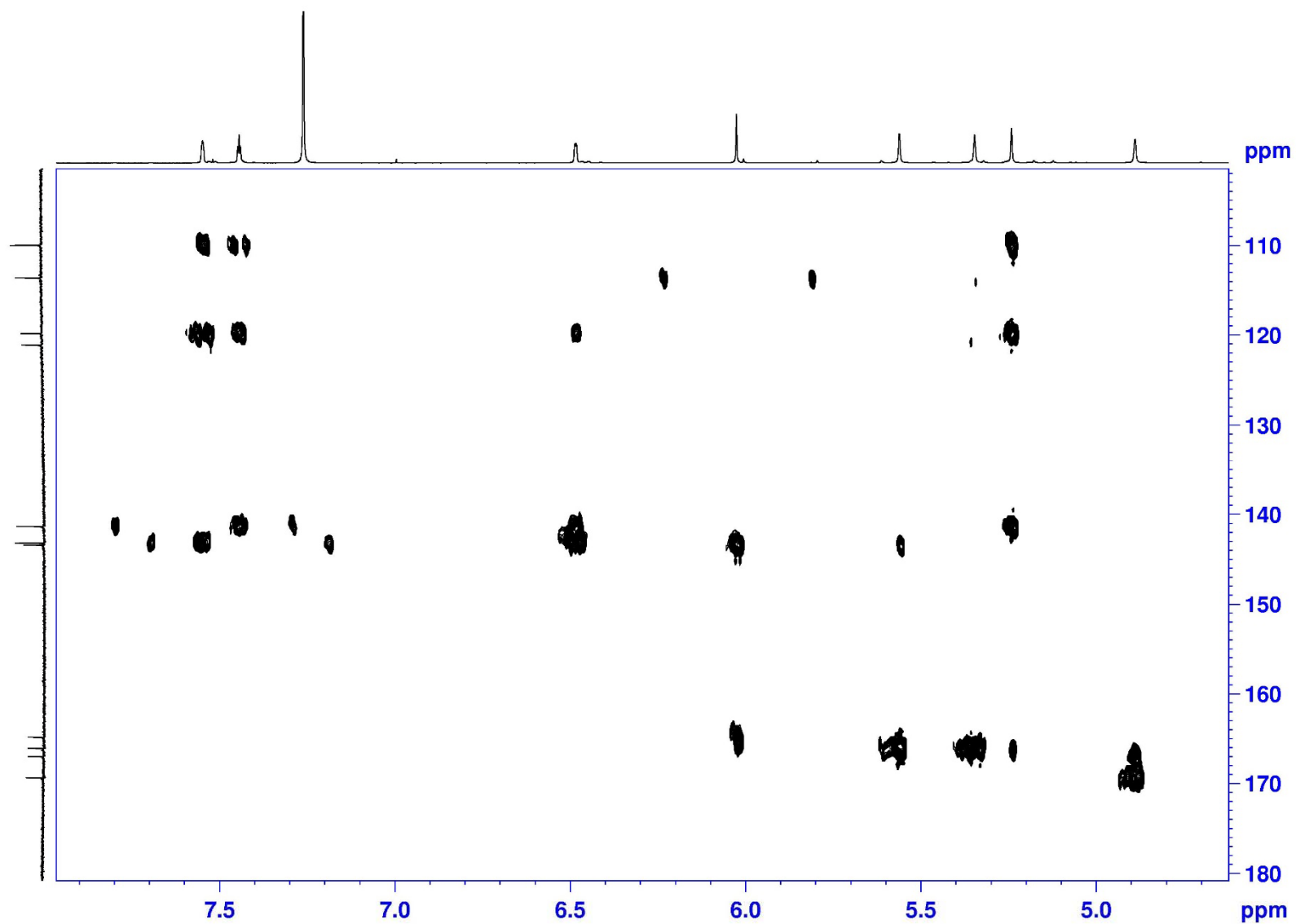
HSQC (400 MHz) spectrum of compound **3** in CDCl<sub>3</sub>



# HMBC (400 MHz) spectrum of compound **3** in CDCl<sub>3</sub>

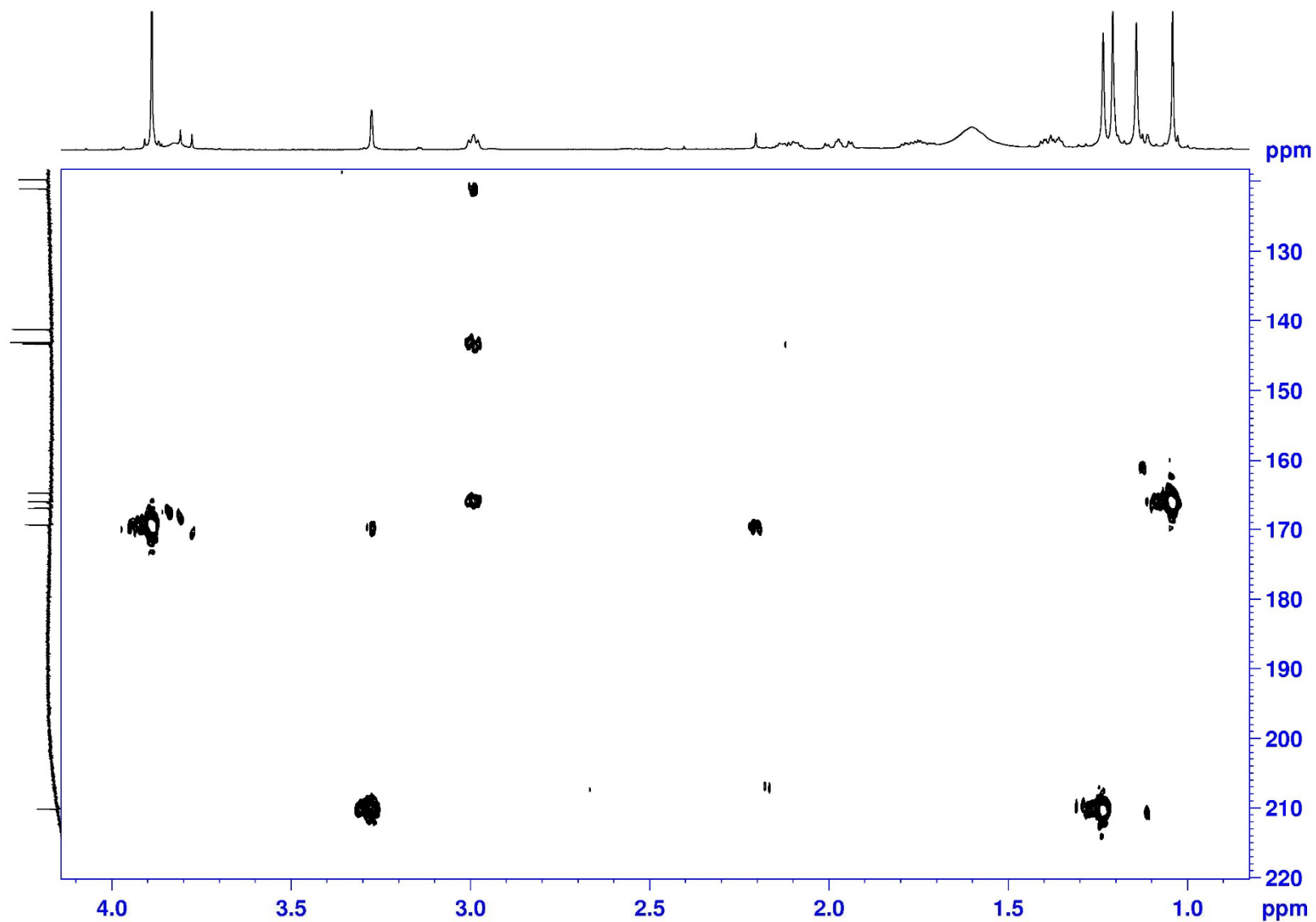


HMBC (400 MHz) spectrum of compound **3** in CDCl<sub>3</sub>

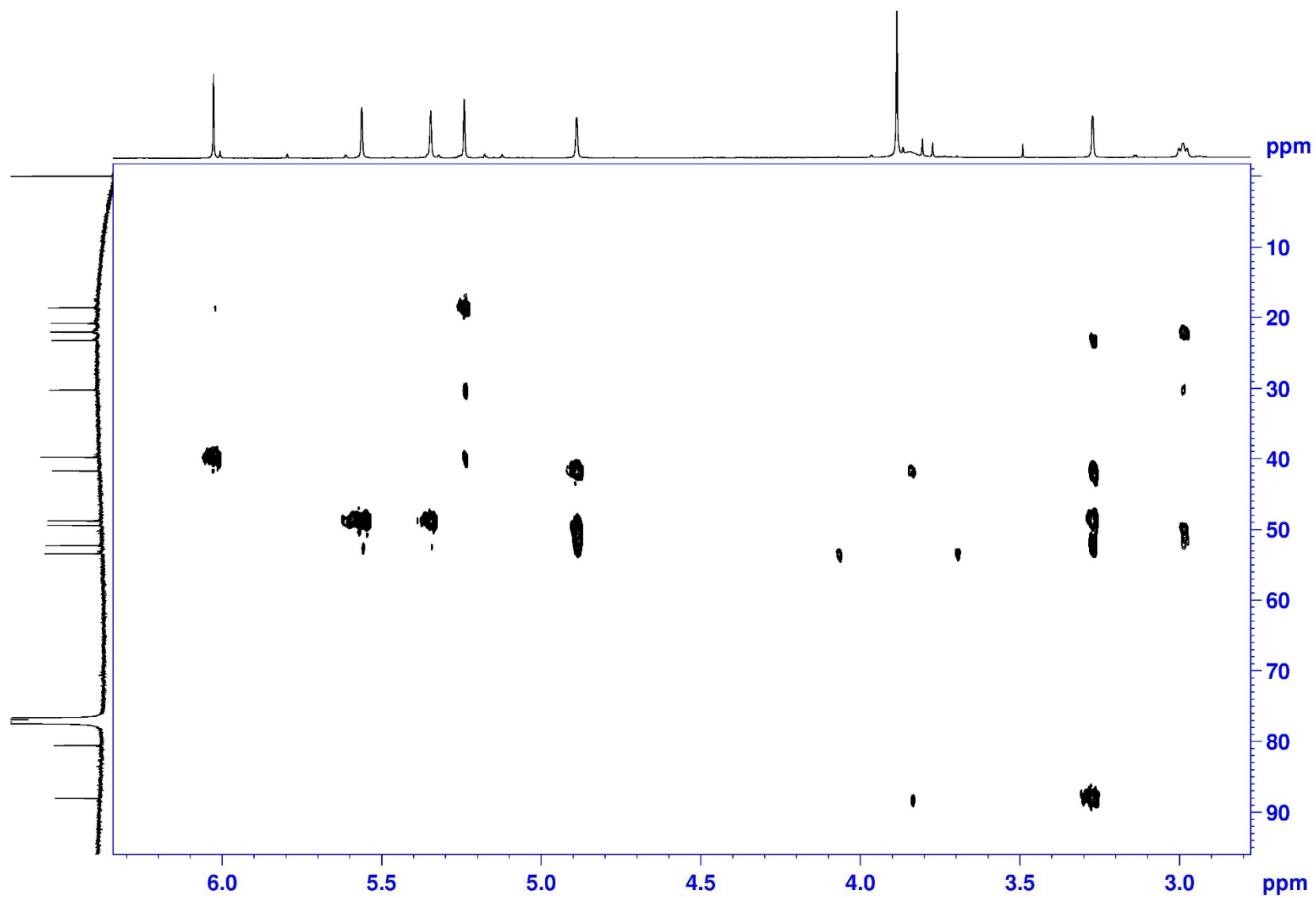




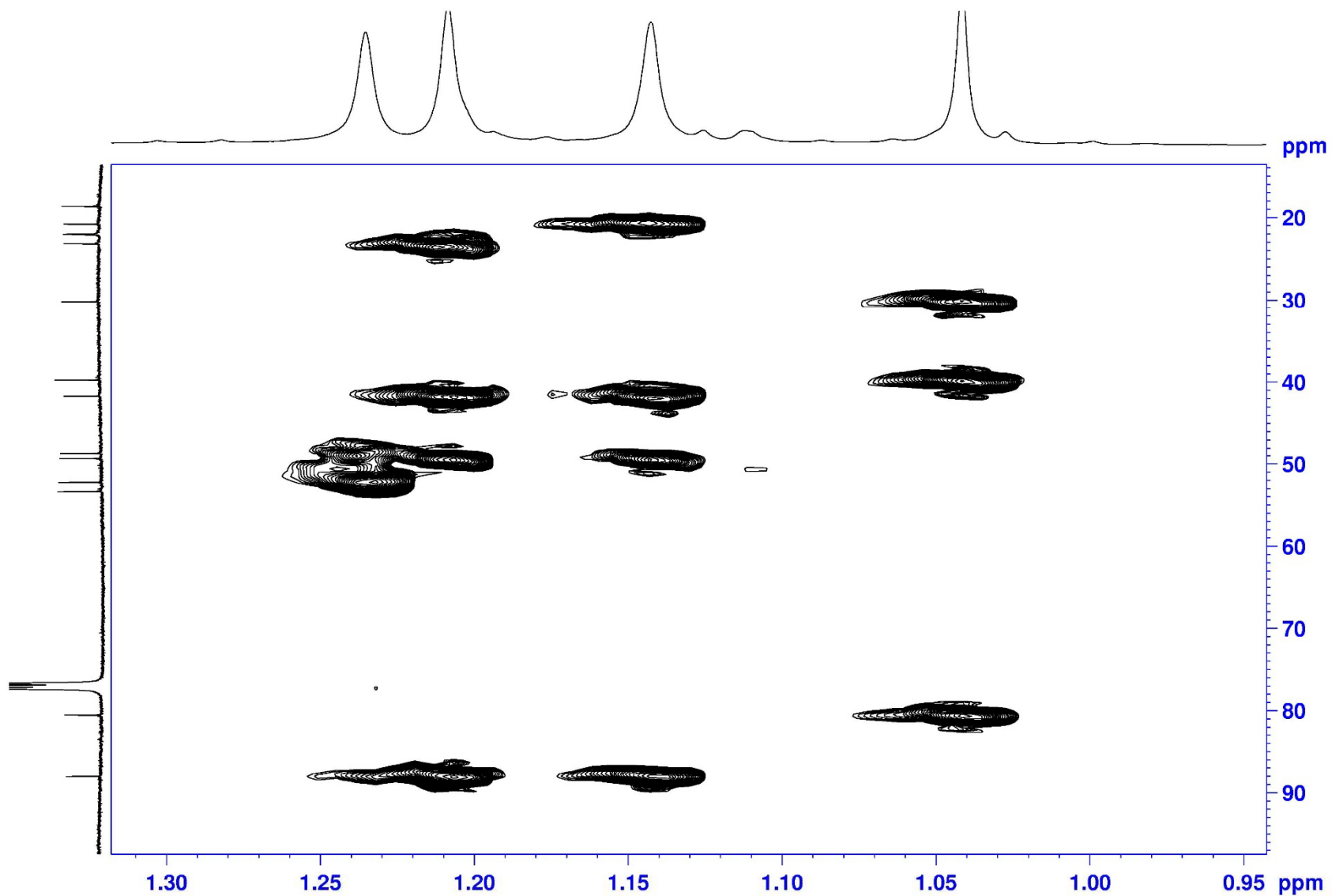
HMBC (400 MHz) spectrum of compound **3** in  $\text{CDCl}_3$



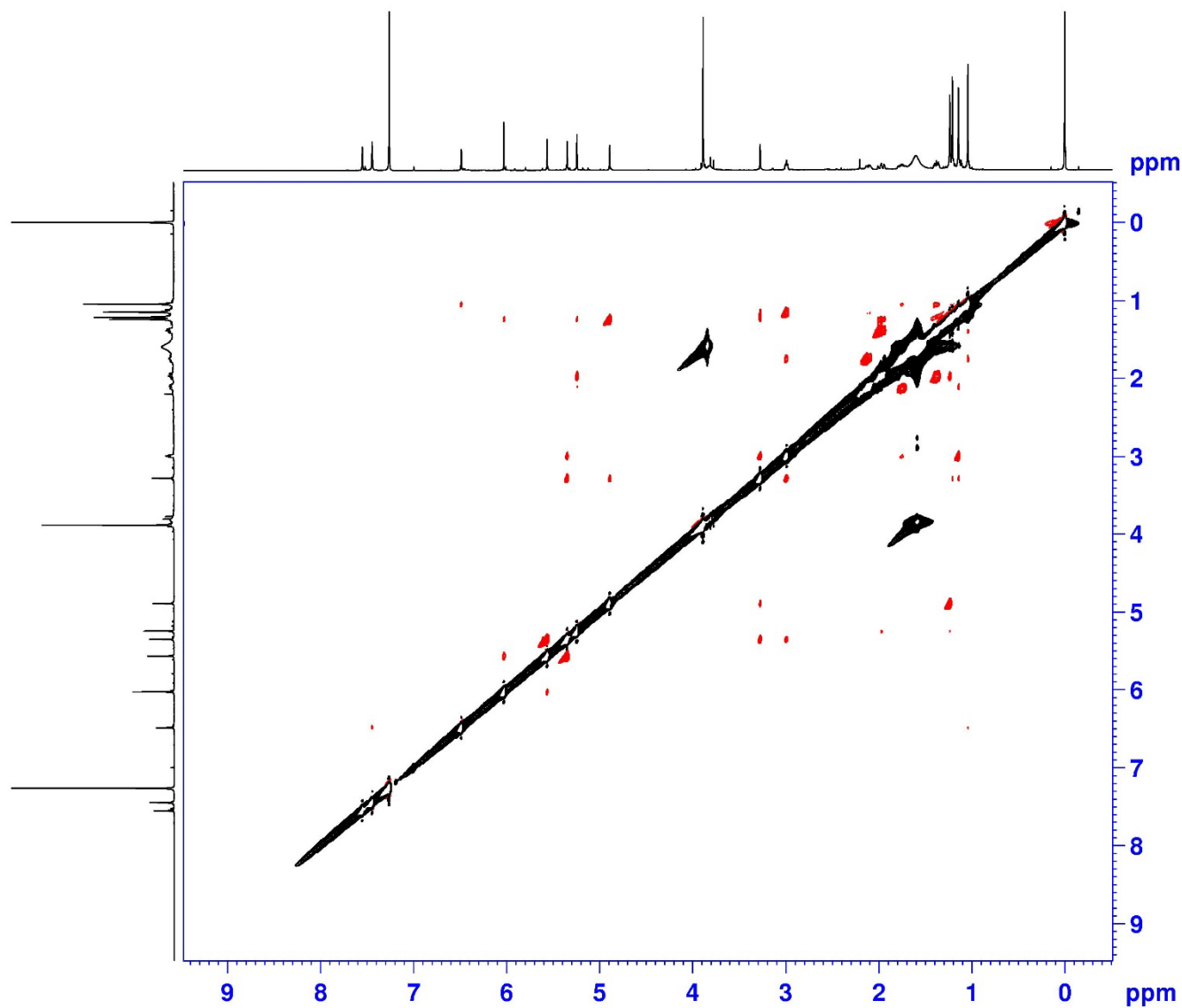
HMBC (400 MHz) spectrum of compound **3** in CDCl<sub>3</sub>



HMBC (400 MHz) spectrum of compound **3** in CDCl<sub>3</sub>



# NOESY (400 MHz) spectrum of compound **3** in CDCl<sub>3</sub>



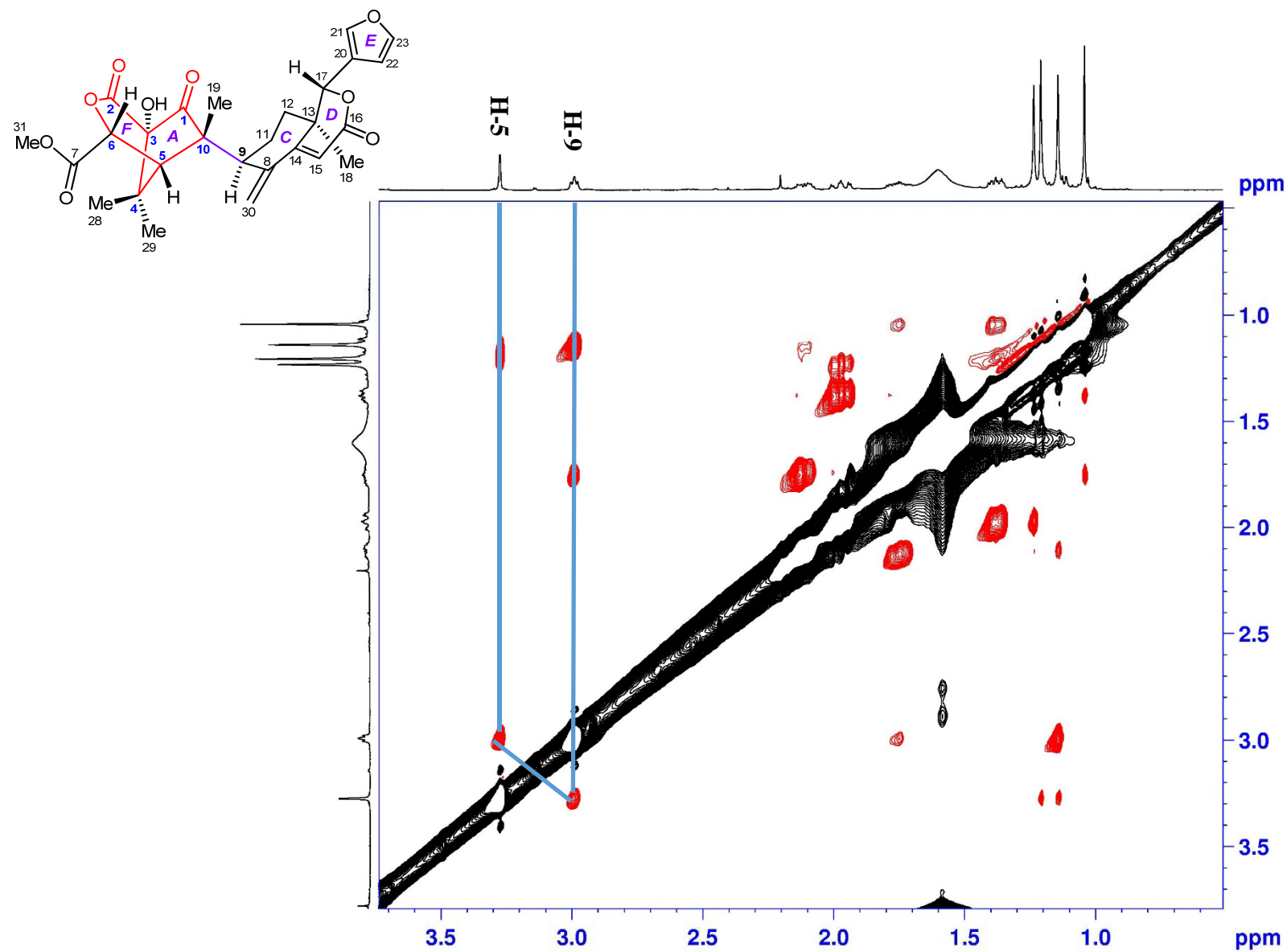
```

NAME          lws-82
EXPNO          7
PROCNO         1
Date_         20151012
Time          19.56
INSTRUM        spect
PROBHD         5 mm CPPBBO BB
PULPROG        noesygpphph
TD            2048
SOLVENT        CDCl3
NS             64
DS            32
SWH           4000.000 Hz
FIDRES        1.953125 Hz
AQ           0.2560500 sec
RG           208.5
DW           125.000 usec
DE           10.00 usec
TE           297.0 K
D0           0.00010972 sec
D1           1.99385595 sec
D8           0.30000001 sec
D11          0.03000000 sec
D12          0.00002000 sec
D16          0.00020000 sec
IN0          0.00025000 sec
  
```

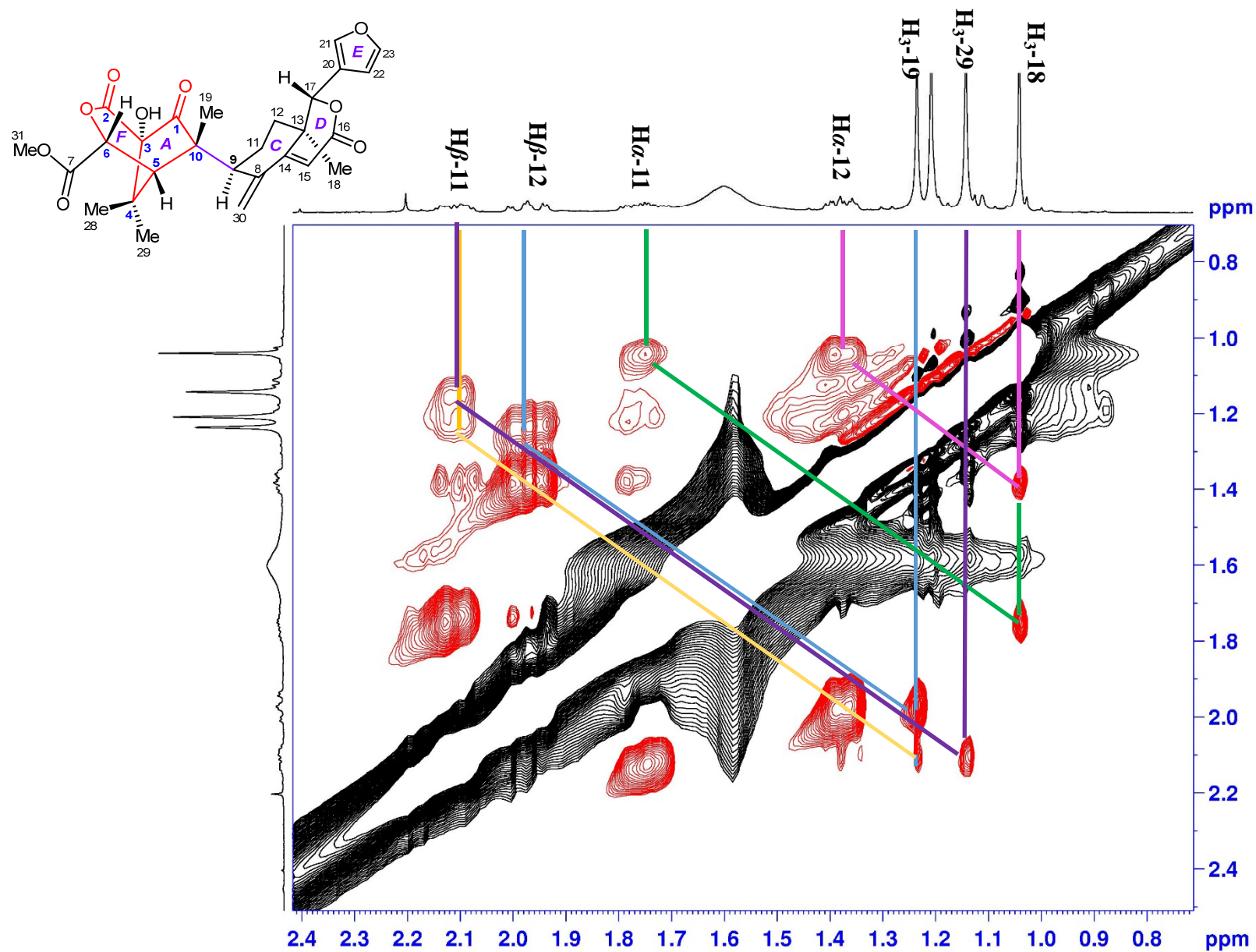
```

===== CHANNEL f1 =====
SFO1          400.1318006 MHz
NUC1           1H
P1            12.00 usec
P2            24.00 usec
P17           2500.00 usec
ND0            1
TD            256
SFO1          400.1318 MHz
FIDRES        15.625000 Hz
SW            9.997 ppm
FnMODE        States-TPPI
SI            1024
SF            400.1300091 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.00
SI            1024
MC2           States-TPPI
SF            400.1300091 MHz
WDW           QSINE
  
```

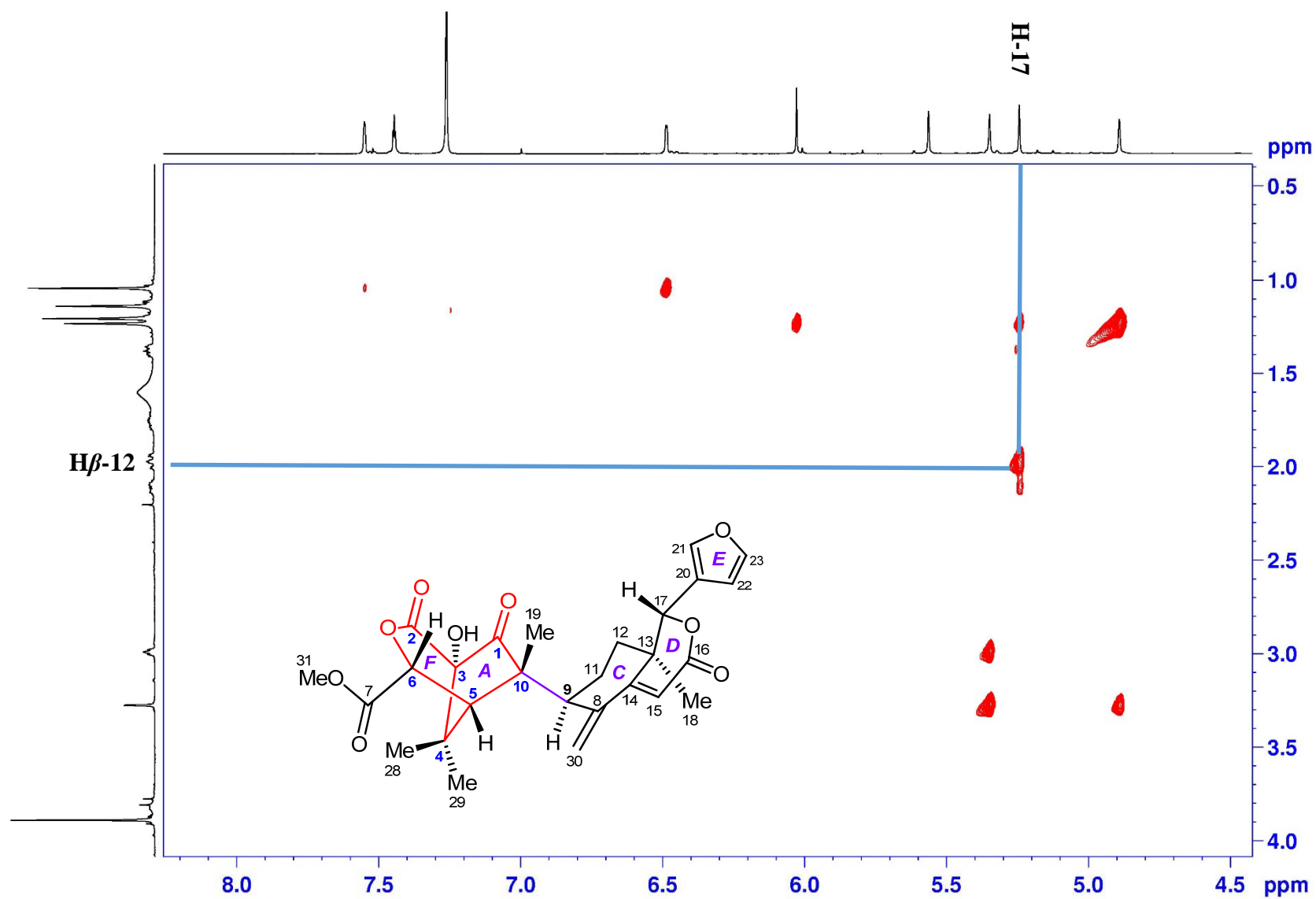
NOESY (400 MHz) spectrum of compound **3** in  $\text{CDCl}_3$



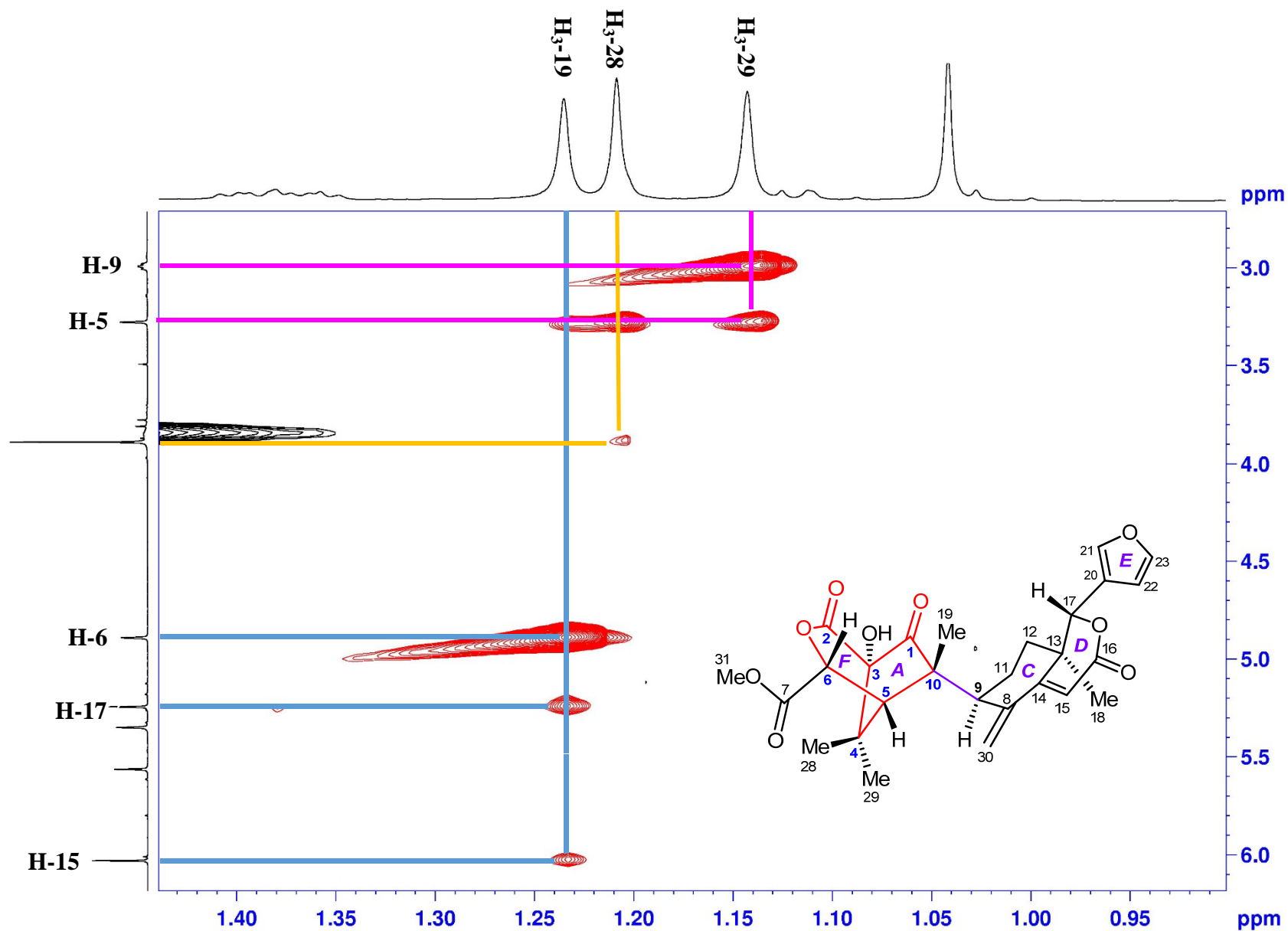
NOESY (400 MHz) spectrum of compound **3** in CDCl<sub>3</sub>



NOESY (400 MHz) spectrum of compound **3** in CDCl<sub>3</sub>

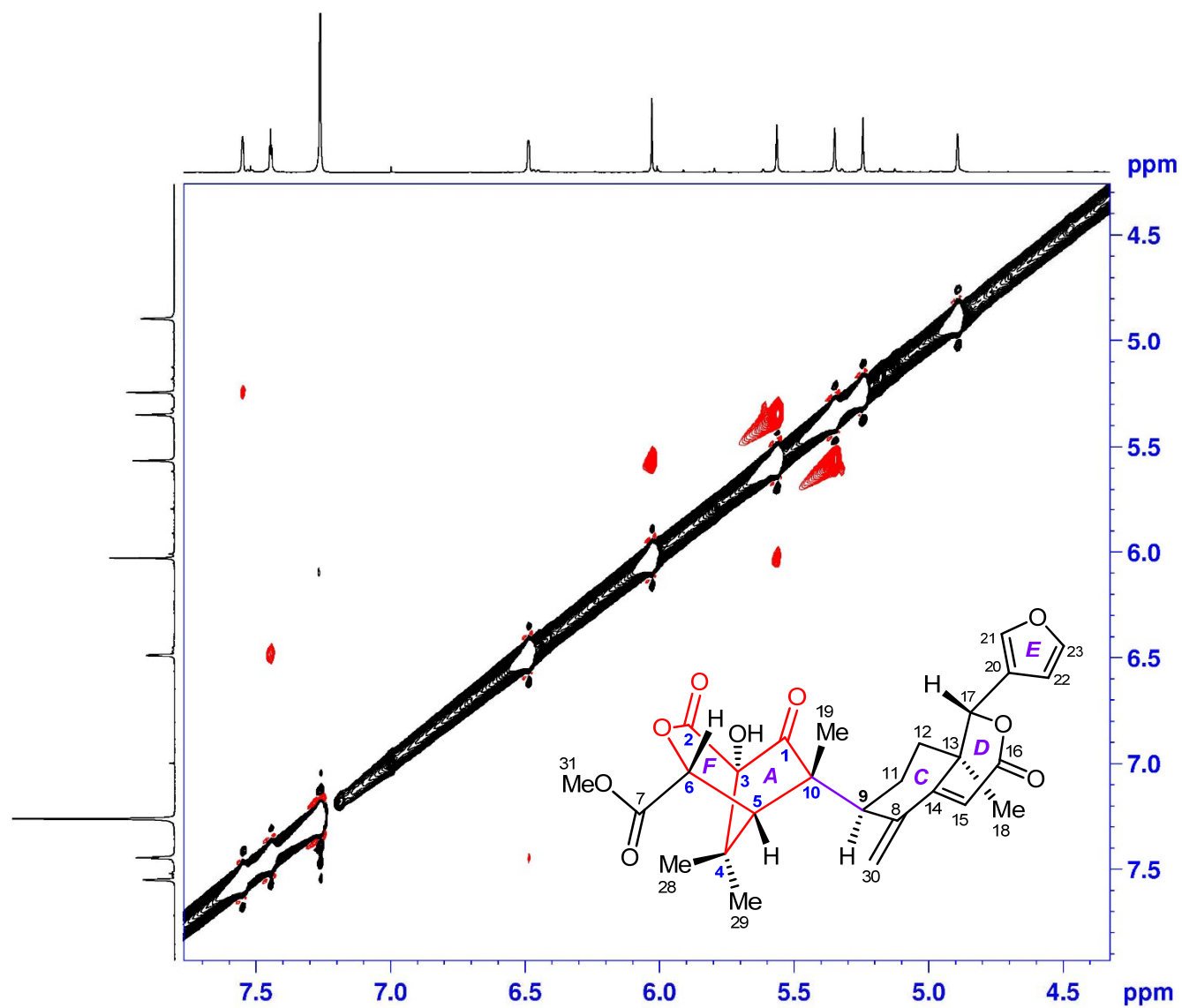


NOESY (400 MHz) spectrum of compound compound **3** in CDCl<sub>3</sub>





NOESY (400 MHz) spectrum of compound **3** in CDCl<sub>3</sub>



# HR-ESIMS for compound 4

## Mass Spectrum SmartFormula Report

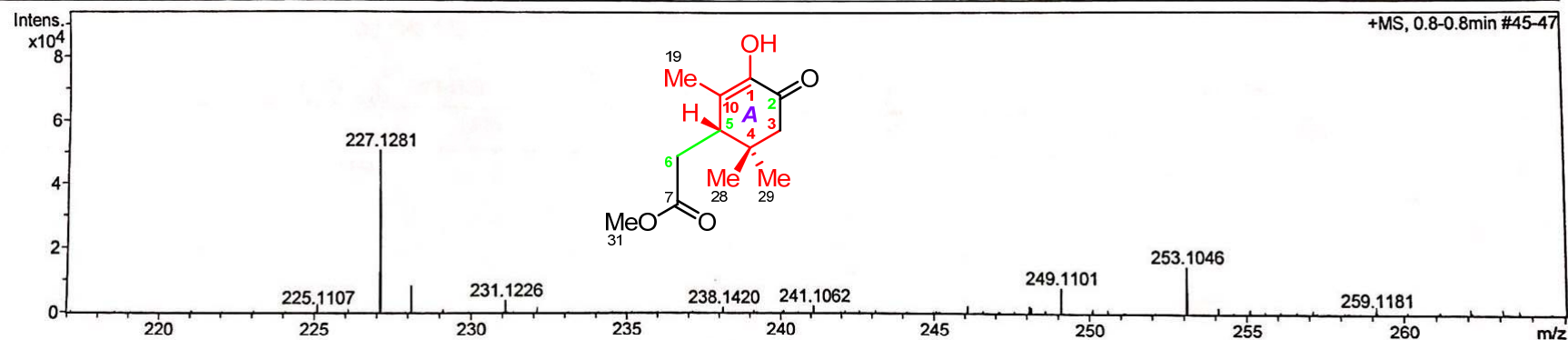
### Analysis Info

Analysis Name D:\Data\MS\data\201808\liwanshan\_lws-18\_pos\_31\_01\_5327.d  
Method LC\_Direct Infusion\_pos\_70-500mz.m  
Sample Name liwanshan\_lws-18\_pos  
Comment

Acquisition Date 8/20/2018 4:27:30 PM  
Operator SCSIO  
Instrument maXis 255552.00029

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
227.1281	1	C <sub>12</sub> H <sub>19</sub> O <sub>4</sub>	100.00	227.1278	1.4	0.3	19.2	3.5	even	ok
249.1101	1	C <sub>12</sub> H <sub>18</sub> NaO <sub>4</sub>	100.00	249.1097	1.3	0.3	9.8	3.5	even	ok

# HR-ESIMS for compound 4

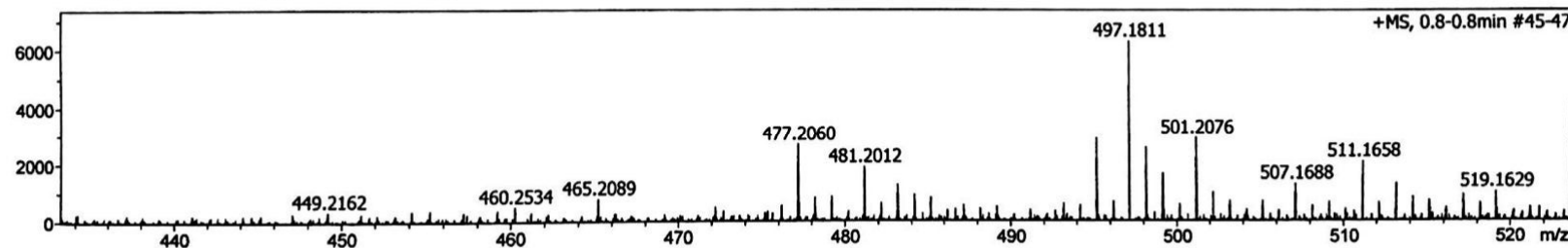
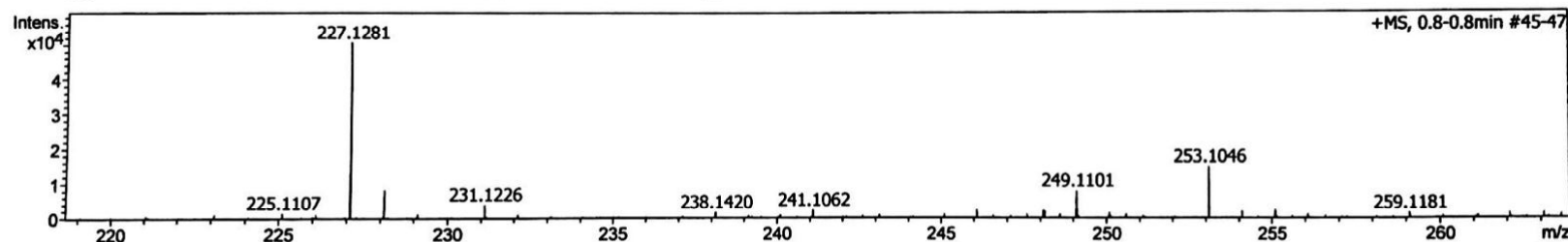
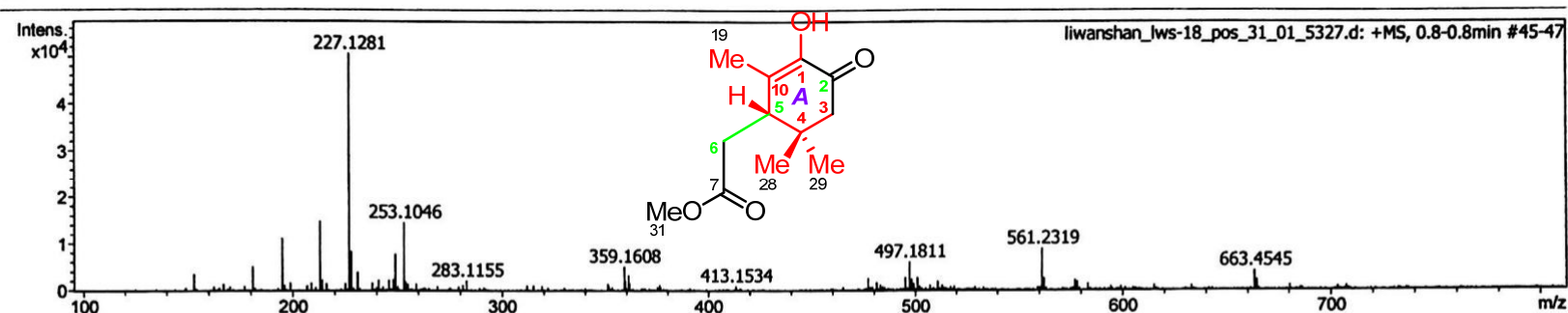
## Generic Display Report

### Analysis Info

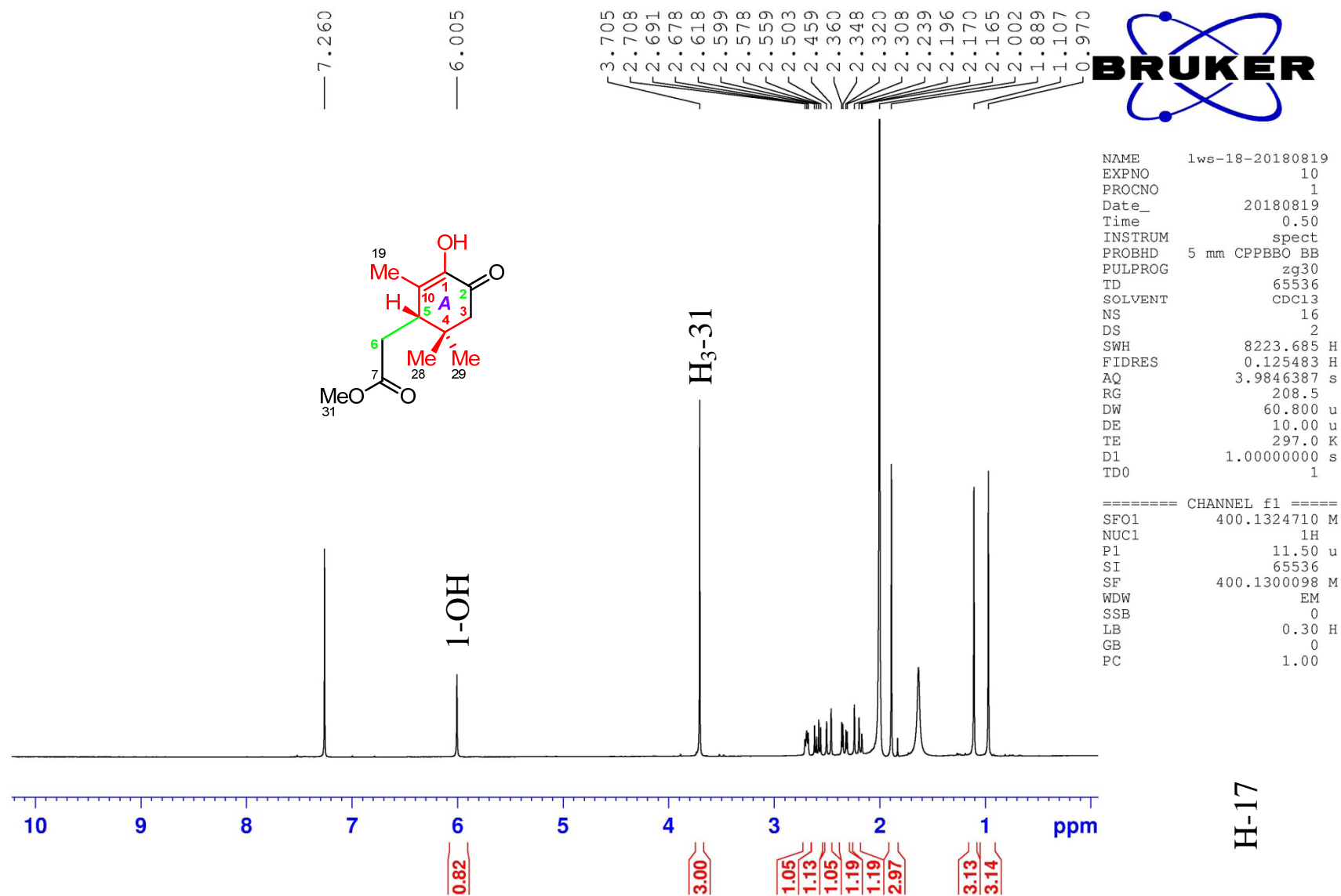
Analysis Name D:\Data\MS\data\201808\liwanshan\_lws-18\_pos\_31\_01\_5327.d  
Method LC\_Direct Infusion\_pos\_70-500mz.m  
Sample Name liwanshan\_lws-18\_pos  
Comment

Acquisition Date 8/20/2018 4:27:30 PM

Operator SCSIO  
Instrument maXis

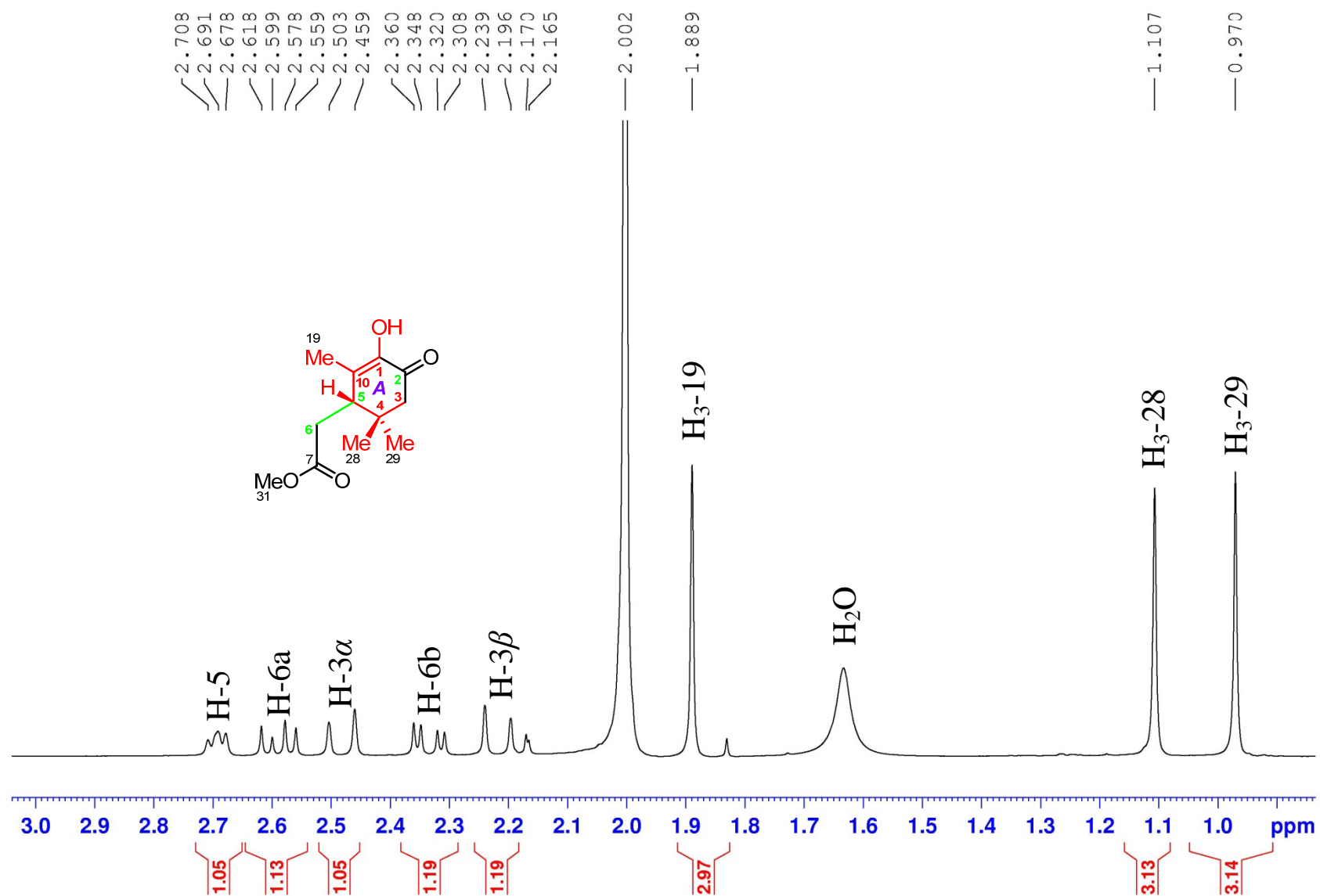


$^1\text{H}$  NMR (400 MHz) spectrum of compound **4** in  $\text{CDCl}_3$

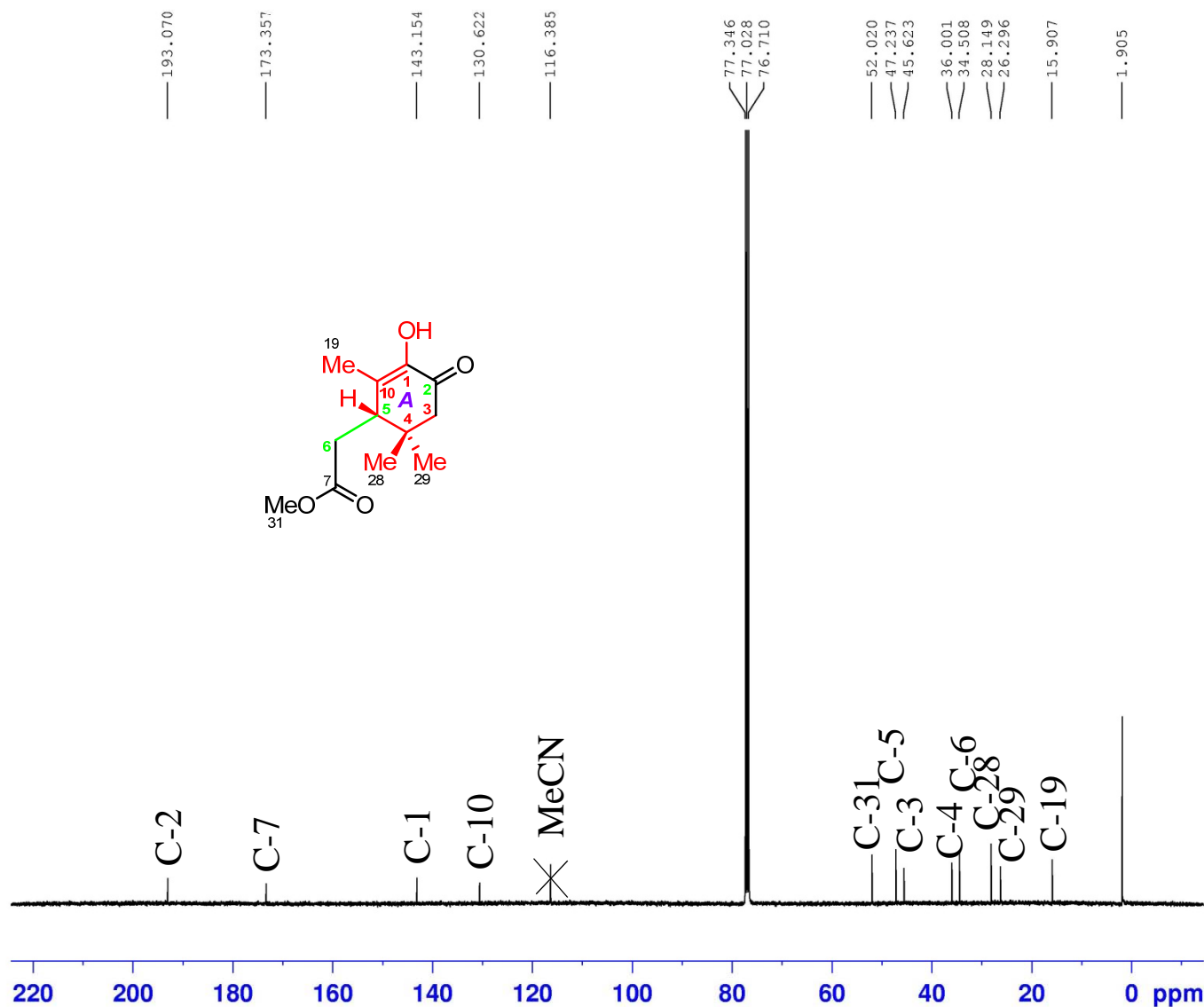


H-17

$^1\text{H}$  NMR (400 MHz) spectrum of compound **4** in  $\text{CDCl}_3$



$^{13}\text{C}$  NMR (100 MHz) spectrum of compound **4** in  $\text{CDCl}_3$



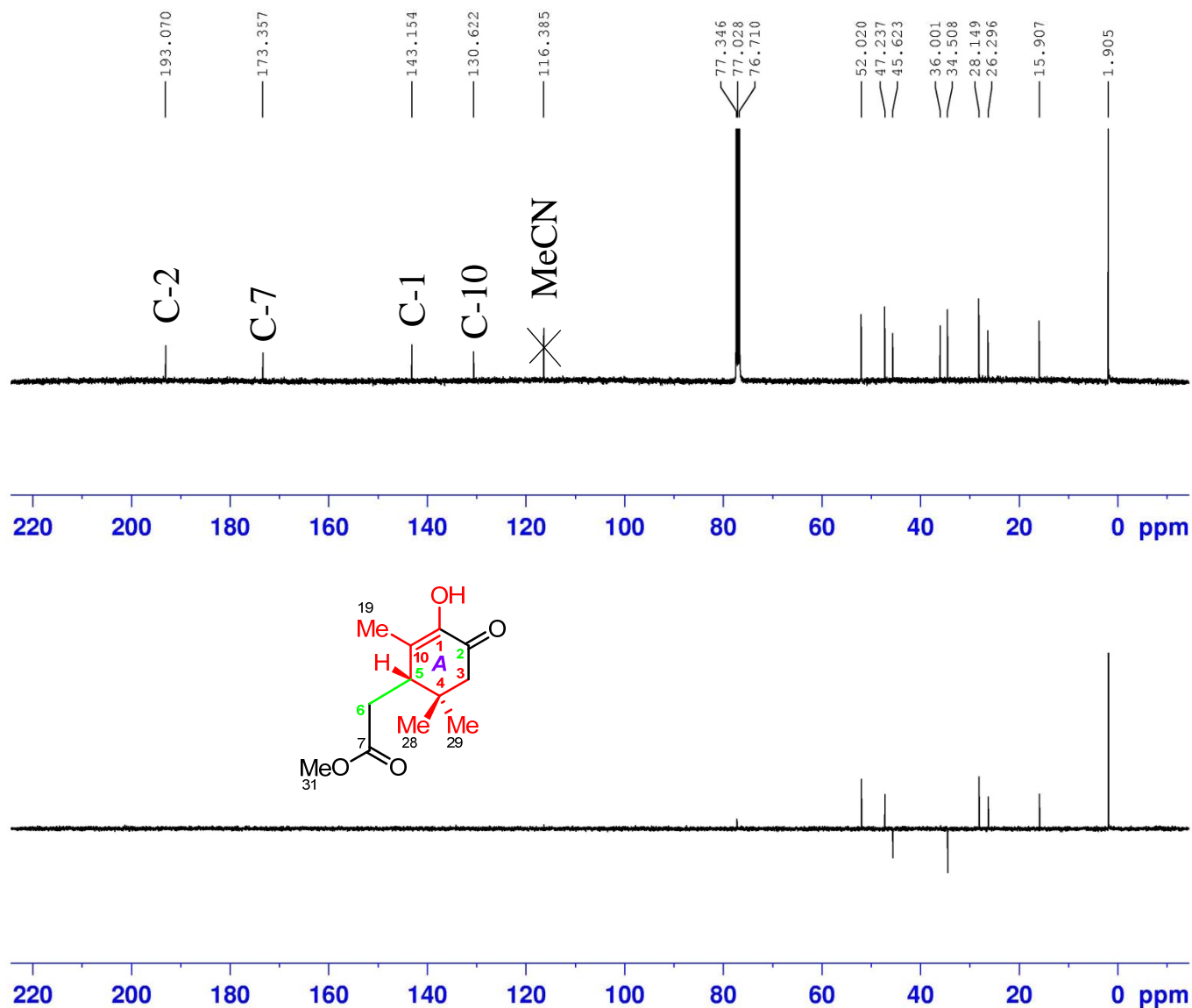
```

NAME      lws-18-20180819
EXPNO     11
PROCNO    1
Date_     20180819
Time      1.50
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        1024
DS        4
SWH       24038.461 H:
FIDRES    0.366798 H:
AQ        1.3631988 s:
RG        147.94
DW        20.800 u:
DE        18.00 u:
TE        297.0 K
D1        2.00000000 s:
D11       0.03000000 s:
TD0       1
    
```

```

===== CHANNEL f1 =====
SF01    100.6233324 MI
NUC1     13C
P1       10.00 u:
SI       32768
SF       100.6127700 MI
WDW      EM
SSB      0
LB       1.00 H:
GB       0
PC       1.40
    
```

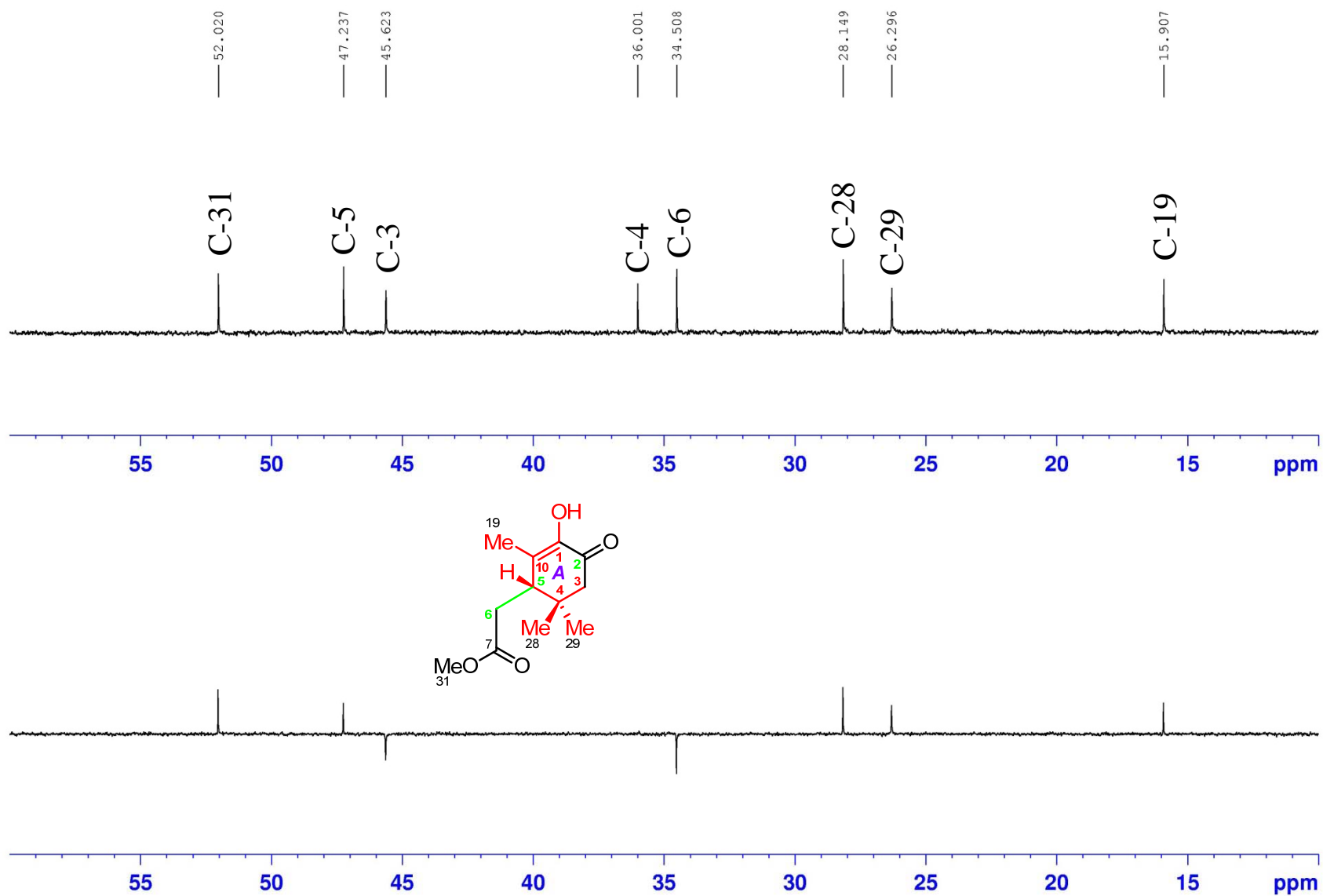
# DEPT135 (100 MHz) spectrum of compound **4** in CDCl<sub>3</sub>



NAME lws-18-20180819  
 EXPNO 12  
 PROCNO 1  
 Date\_ 20180819  
 Time 2.08  
 INSTRUM spect  
 PROBHD 5 mm CPPBBO BB  
 PULPROG deptsp135  
 TD 65536  
 SOLVENT CDCl3  
 NS 300  
 DS 4  
 SWH 24038.461 H  
 FIDRES 0.366798 H  
 AQ 1.3631988 s  
 RG 130.26  
 DW 20.800 u  
 DE 18.00 u  
 TE 297.0 K  
 CNST2 145.0000000  
 D1 2.00000000 s  
 D2 0.00344828 s  
 D12 0.00002000 s  
 TD0 1

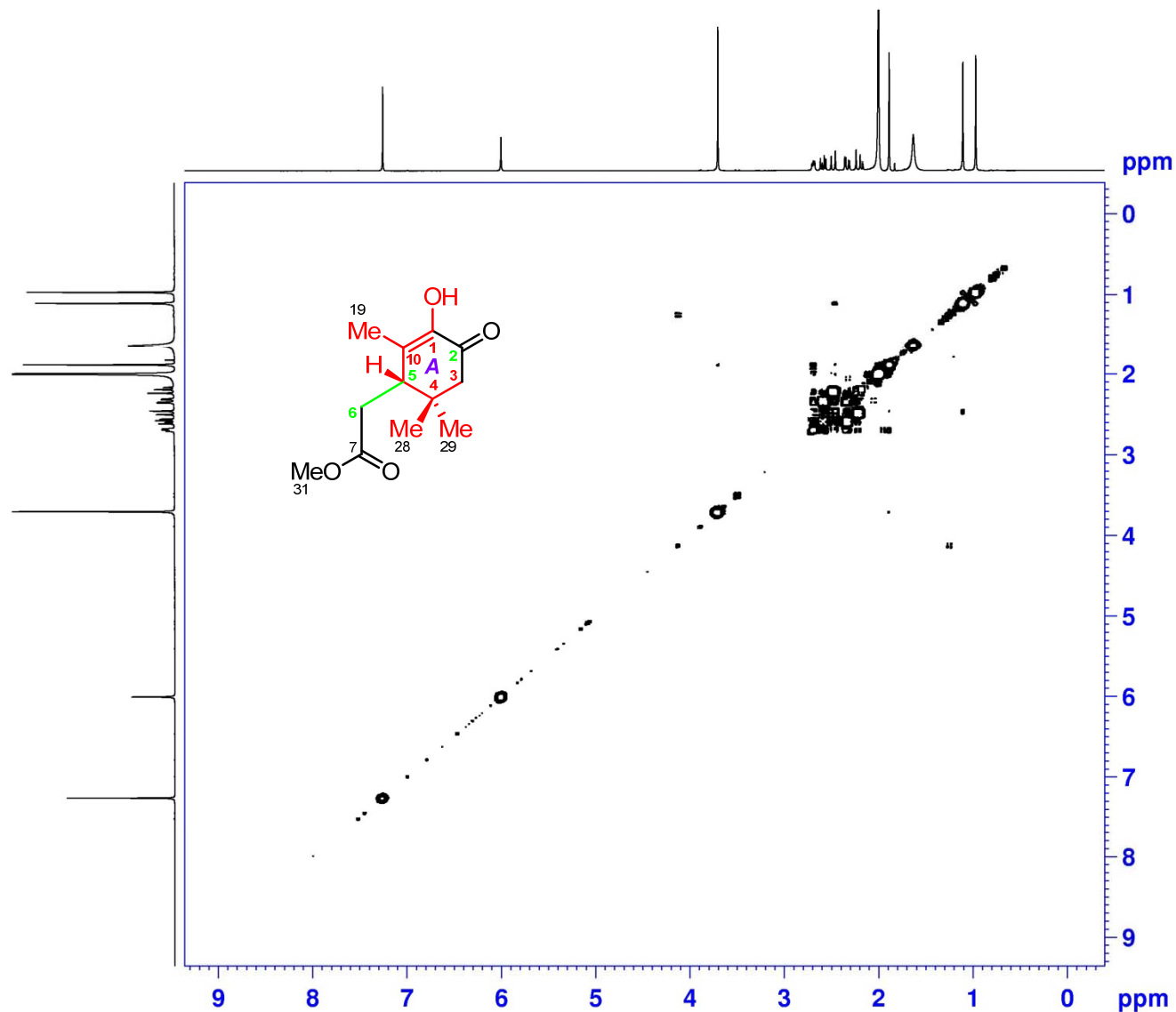
===== CHANNEL f1 =====  
 SFO1 100.623324 M  
 NUC1 13C  
 P1 10.00 u  
 P13 2000.00 u  
 SI 32768  
 SF 100.6127685 M  
 WDW EM  
 SSB 0  
 LB 1.00 H  
 GB 0  
 PC 1.40

DEPT135 (100 MHz) spectrum of compound **4** in CDCl<sub>3</sub>





# $^1\text{H}$ - $^1\text{H}$ COSY (400 MHz) spectrum of compound **4** in $\text{CDCl}_3$



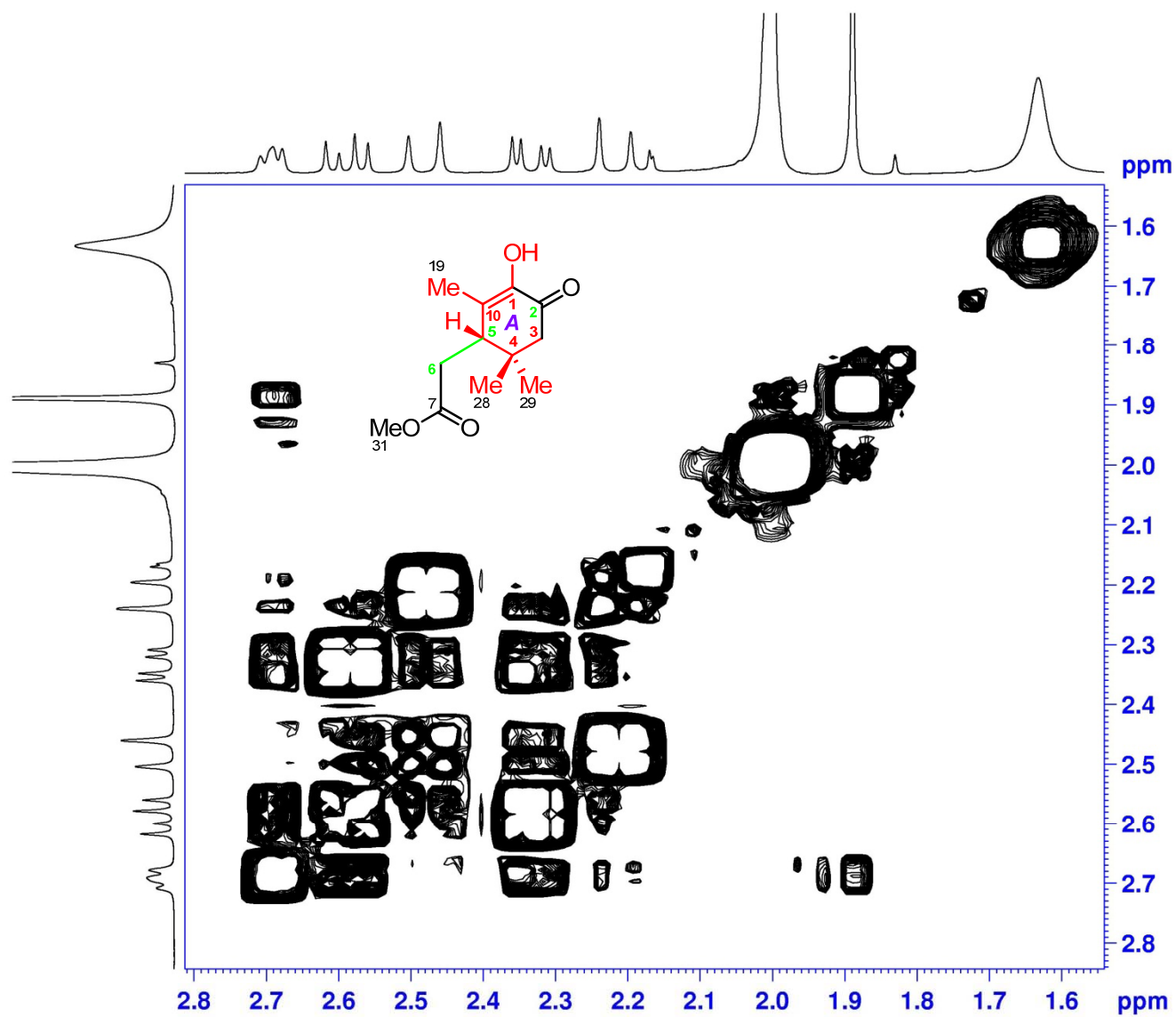
```

NAME      lws-18-20180819
EXPNO     13
PROCNO    1
Date_     20180819
Time      2.10
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   cosygpppqf
TD         2048
SOLVENT   CDCl3
NS         8
DS         8
SWH        3906.250 Hz
FIDRES     1.907349 Hz
AQ         0.2621940 sec
RG         208.5
DW         128.000 usec
DE         10.00 usec
TE         297.0 K
D0         0.00000300 sec
D1         1.89678097 sec
D11        0.03000000 sec
D12        0.00002000 sec
D13        0.00000400 sec
D16        0.00020000 sec
IN0        0.00025600 sec
    
```

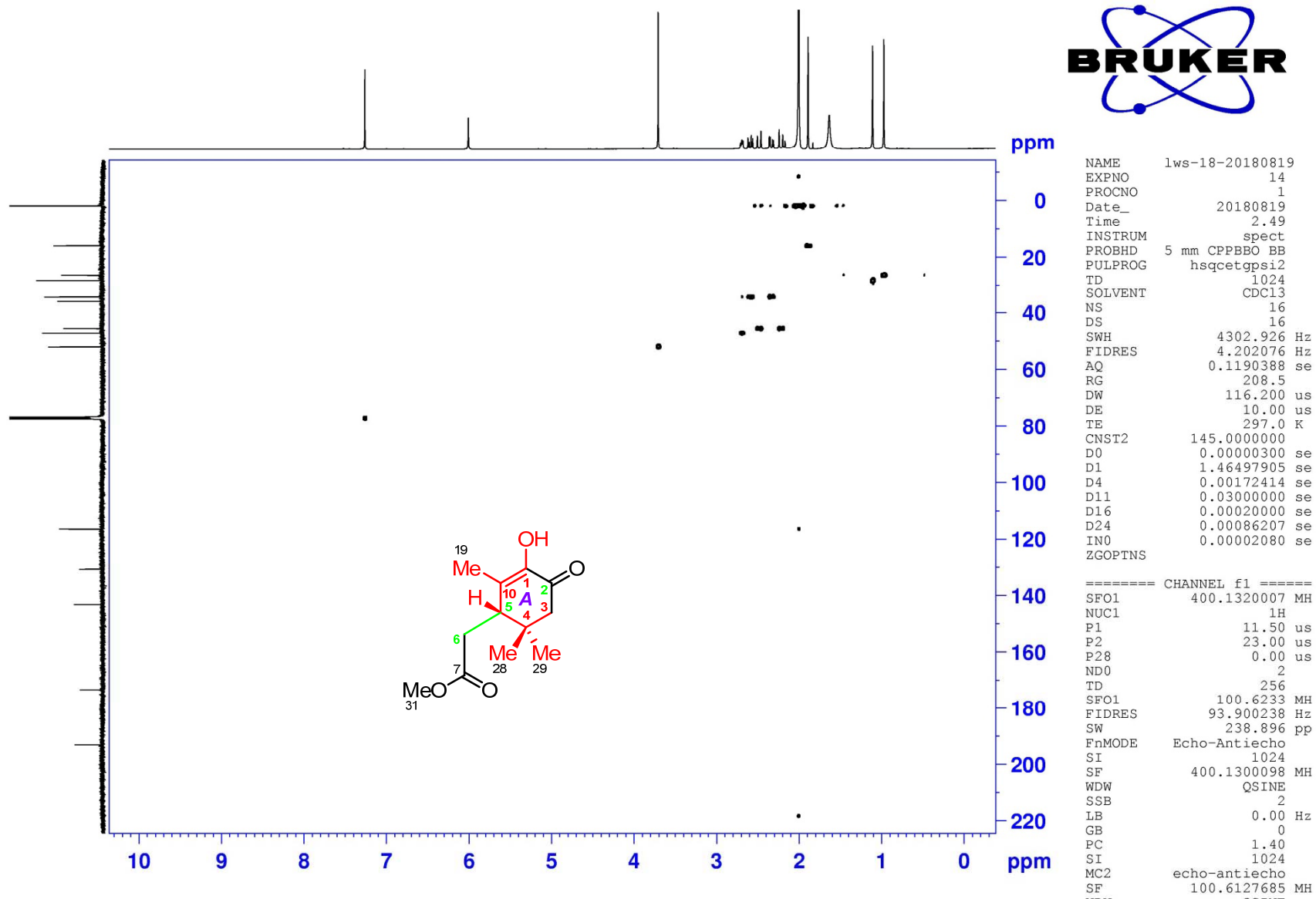
```

===== CHANNEL f1 =====
SFO1      400.1318006 MHz
NUC1       1H
P0         11.50 usec
P1         11.50 usec
P17        2500.00 usec
ND0         1
TD         128
SFO1      400.1318 MHz
FIDRES     30.517578 Hz
SW         9.762 ppm
FnMODE     QF
SI         1024
SF         400.1300098 MHz
WDW        QSINE
SSB         0
LB         0.00 Hz
GB         0
PC         1.40
SI         1024
MC2        QF
SF         400.1300098 MHz
    
```

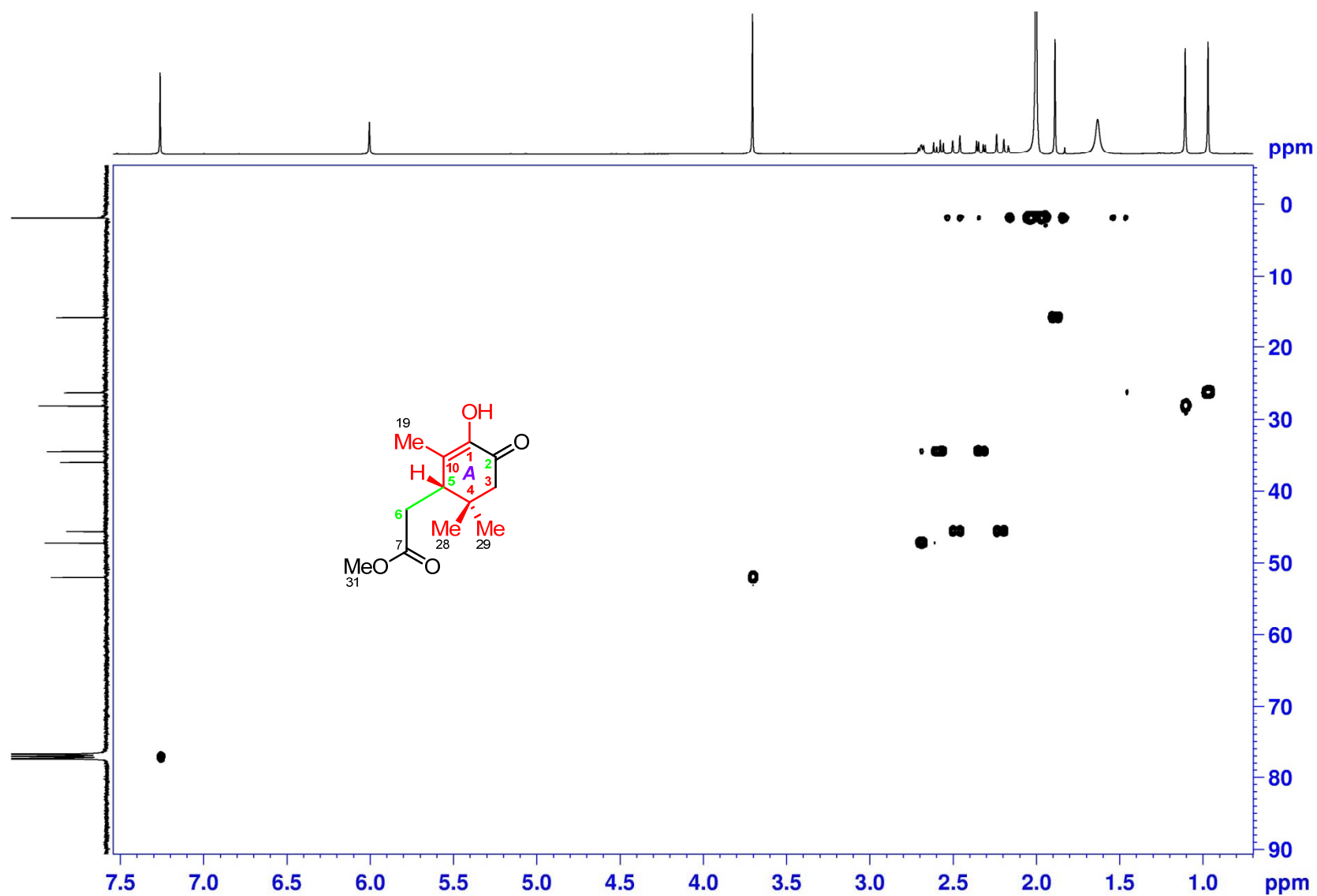
$^1\text{H}$ - $^1\text{H}$  COSY (400 MHz) spectrum of compound **4** in  $\text{CDCl}_3$



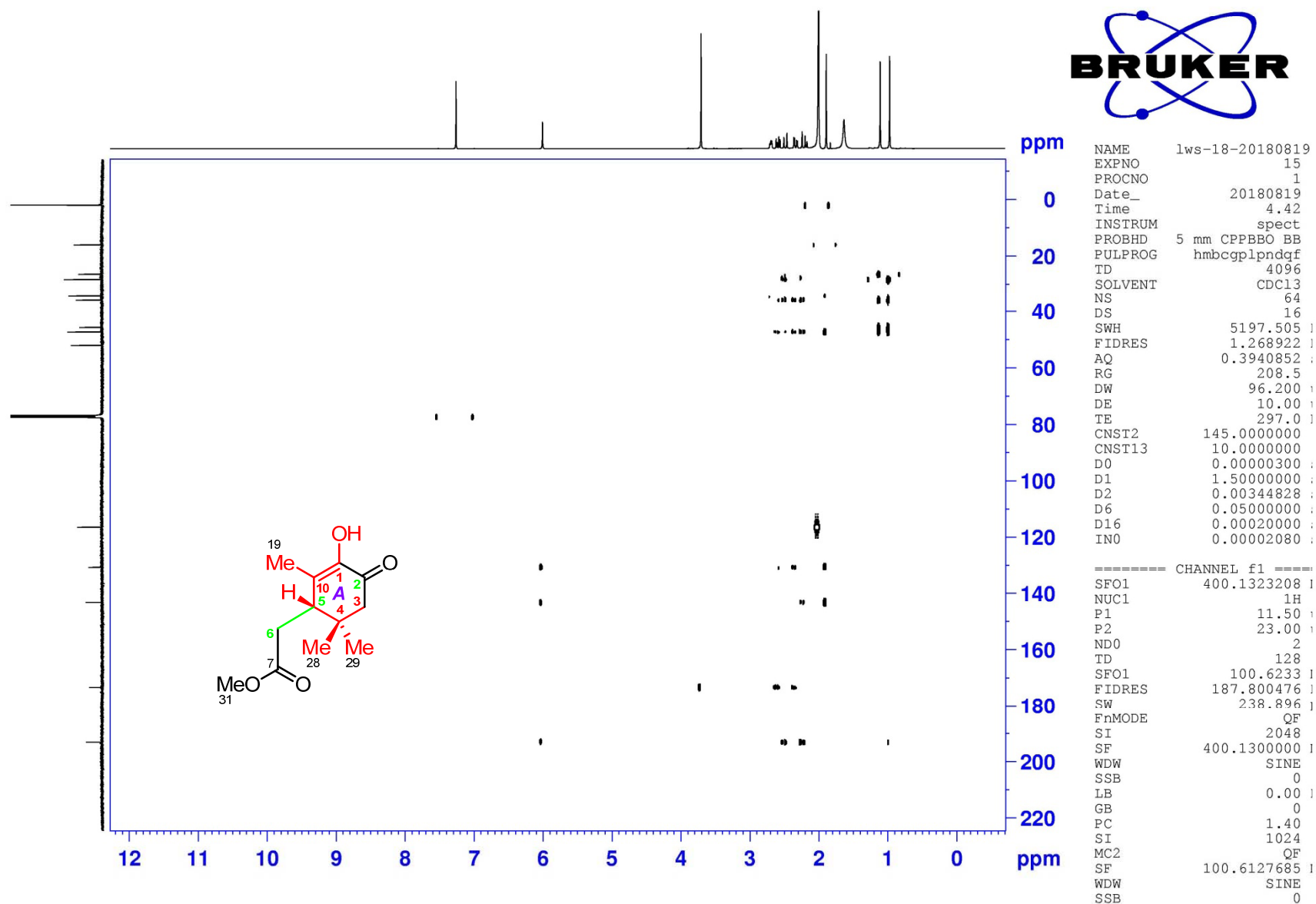
# HSQC (400 MHz) spectrum of compound **4** in CDCl<sub>3</sub>



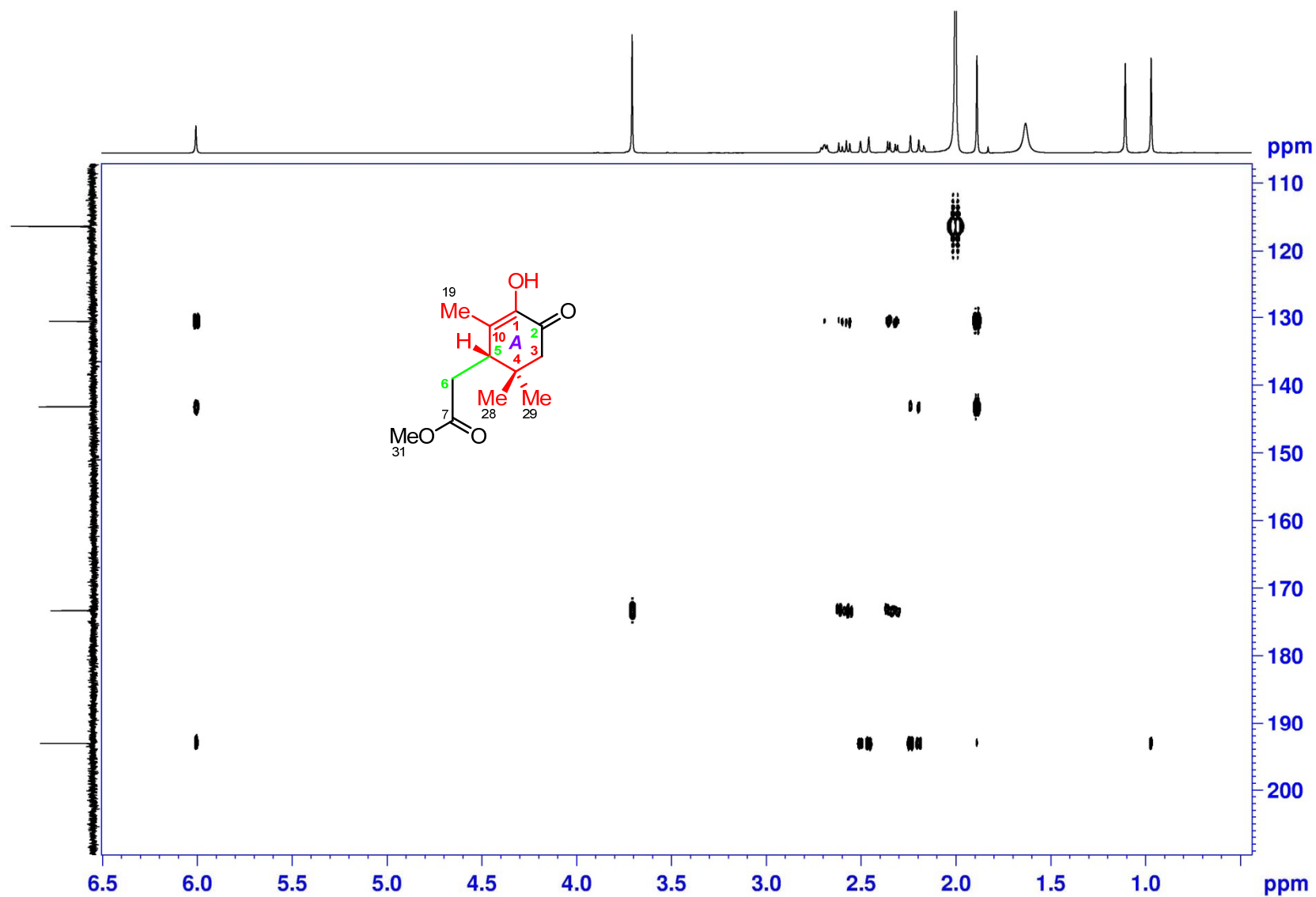
# HSQC (400 MHz) spectrum of compound **4** in CDCl<sub>3</sub>



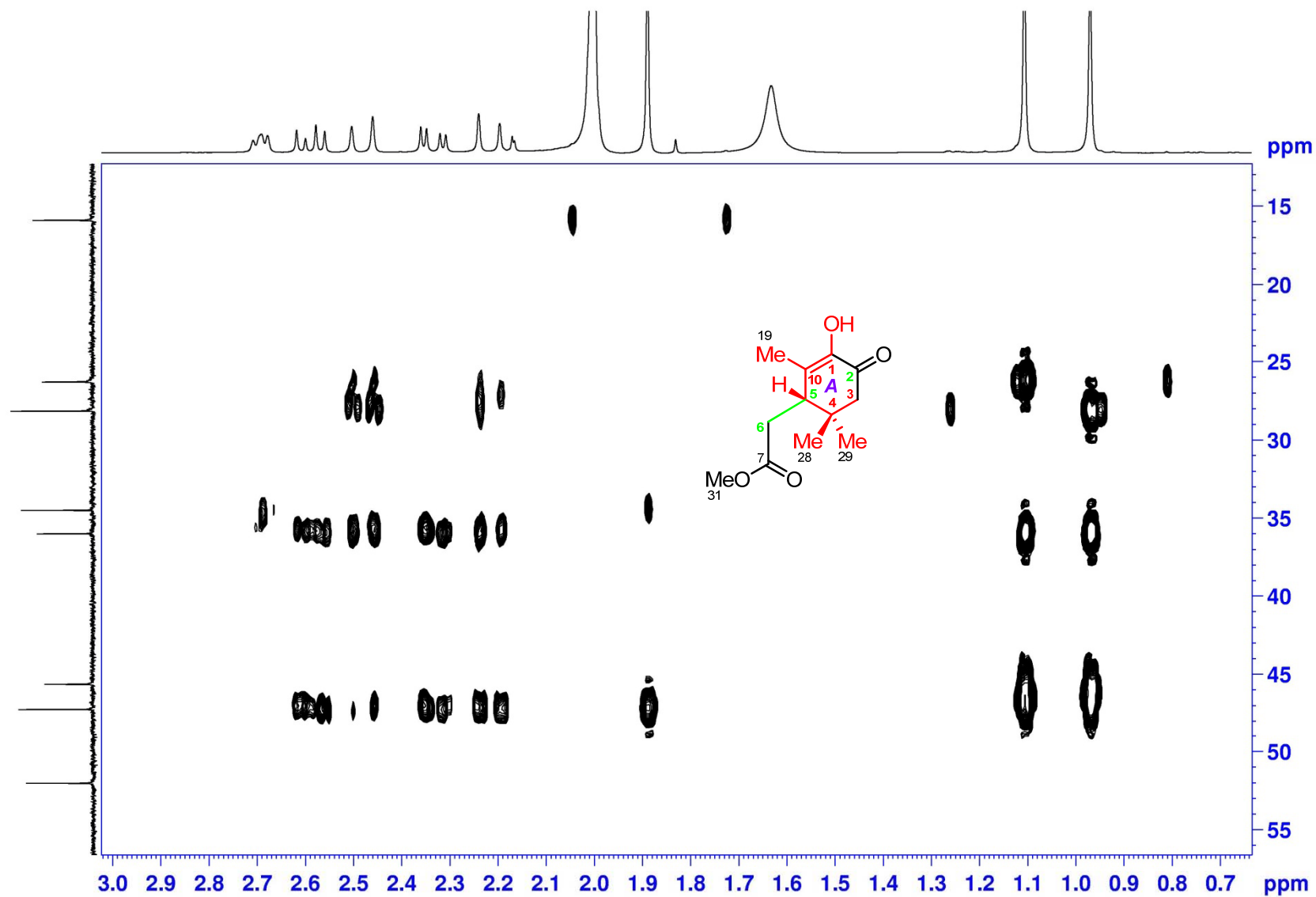
# HMBC (400 MHz) spectrum of compound **4** in CDCl<sub>3</sub>



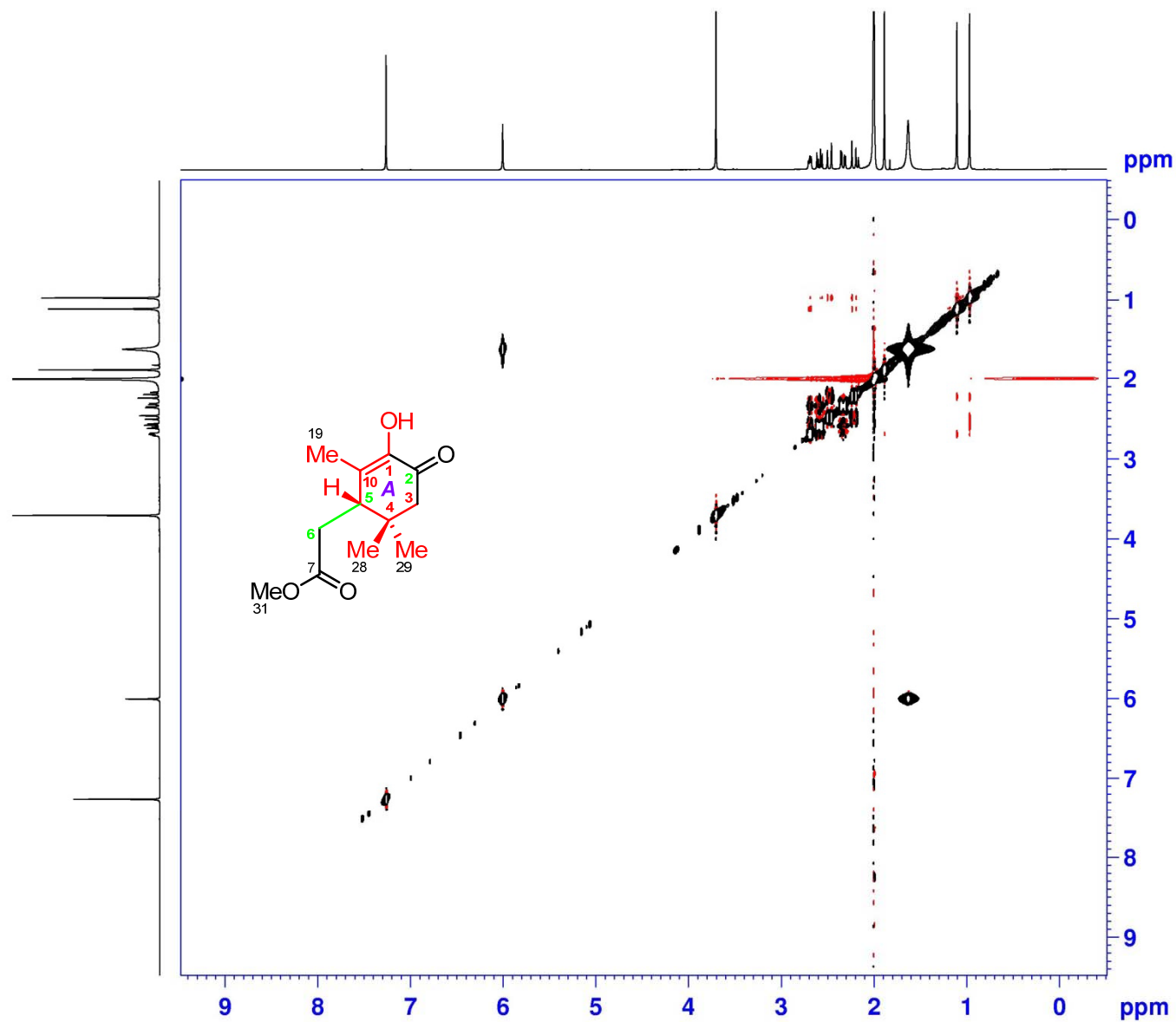
# HMBC (400 MHz) spectrum of compound **4** in CDCl<sub>3</sub>



HMBC (400 MHz) spectrum of compound **4** in CDCl<sub>3</sub>



# NOESY (400 MHz) spectrum of compound compound 4 in CDCl<sub>3</sub>



```

NAME      lws-18-20180819
EXPNO     16
PROCNO    1
Date_     20180819
Time      9.09
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   noesygpphpp
TD        2048
SOLVENT   CDCl3
NS        16
DS        32
SWH       4000.000 Hz
FIDRES    1.953125 Hz
AQ        0.2560500 sec
RG        208.5
DW        125.000 usec
DE        10.00 usec
TE        297.0 K
D0        0.00011036 sec
D1        1.99385595 sec
D8        0.30000001 sec
D11       0.03000000 sec
D12       0.00002000 sec
D16       0.00020000 sec
IN0       0.00025000 sec
    
```

```

===== CHANNEL f1 =====
SFO1    400.1318006 MHz
NUC1     1H
P1       11.50 usec
P2       23.00 usec
P17      2500.00 usec
ND0      1
TD       256
SFO1    400.1318 MHz
FIDRES   15.625000 Hz
SW       9.997 ppr
FnMODE   States-TPPI
SI       1024
SF       400.1300098 MHz
WDW      QSINE
SSB      2
LB       0.00 Hz
GB       0
PC       1.00
SI       1024
MC2      States-TPPI
SF       400.1300098 MHz
WDW      QSINE
SSB      2
    
```



# NOESY (400 MHz) spectrum of compound compound **4** in CDCl<sub>3</sub>

