

Supporting Information-I

**Copies of HR-ESIMS, and 1D and 2D NMR
spectra of compounds 1–5.**

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HR-ESIMS for compound 1

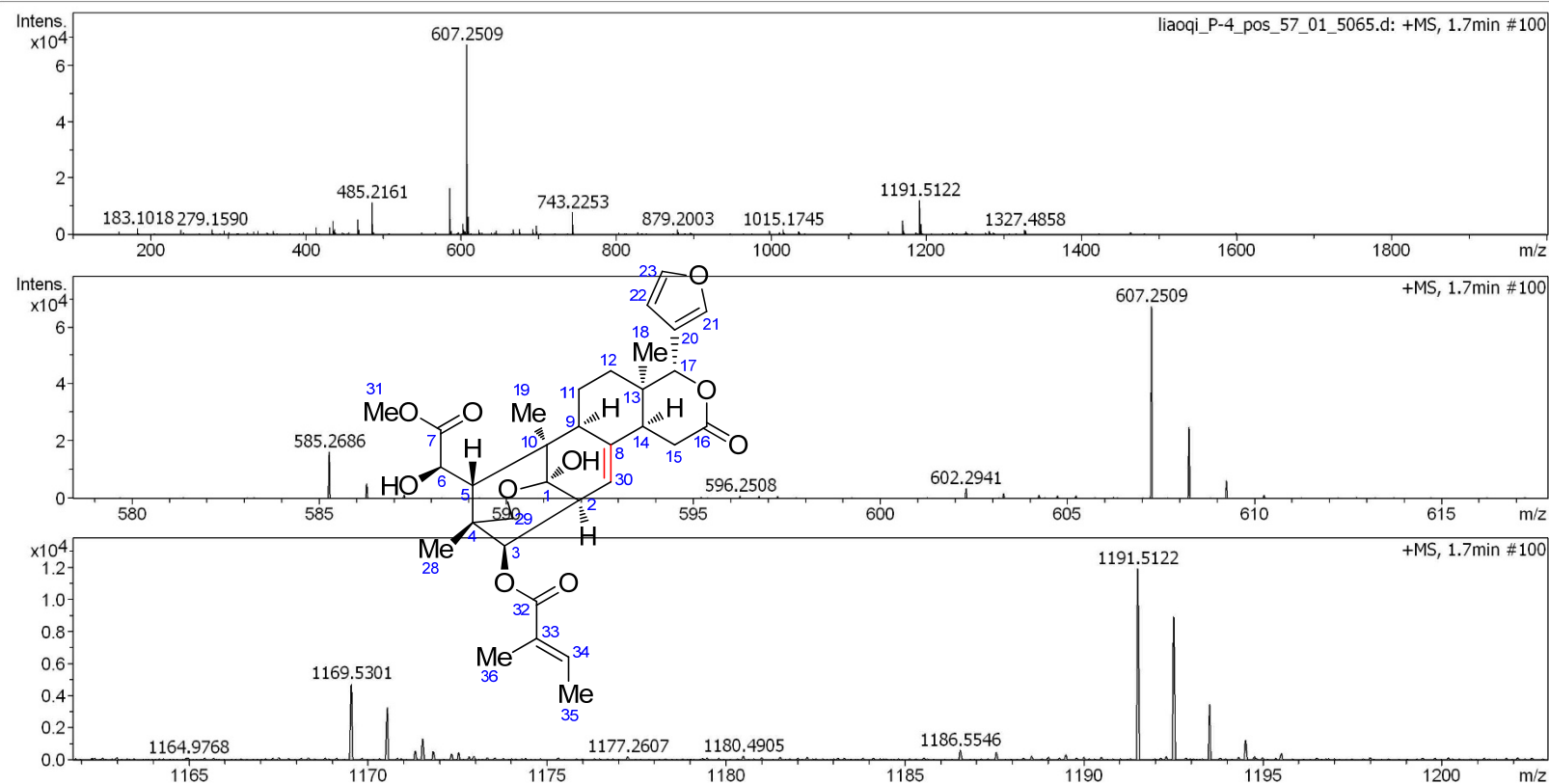
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Comment

Acquisition Date 7/3/2018 3:44:16 PM

Operator SCSIO
Instrument maXis



HR-ESIMS for compound 1

Mass Spectrum SmartFormula Report

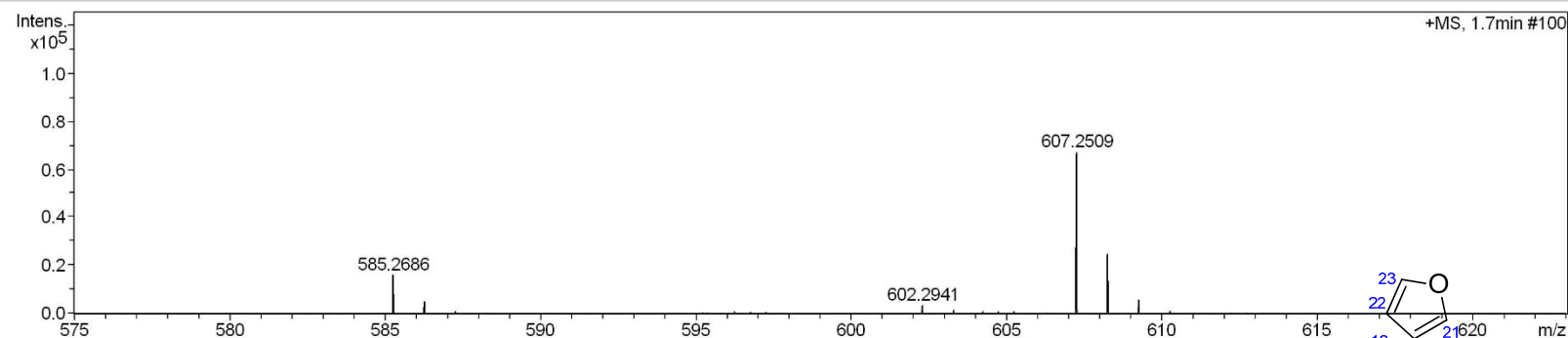
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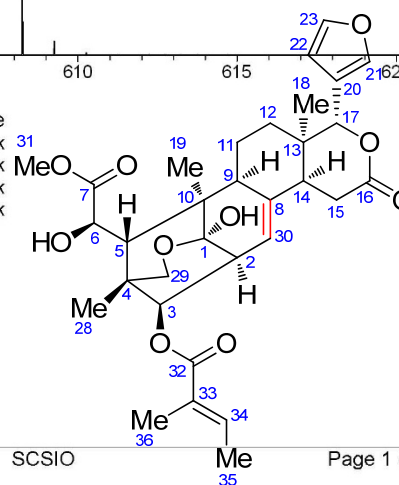
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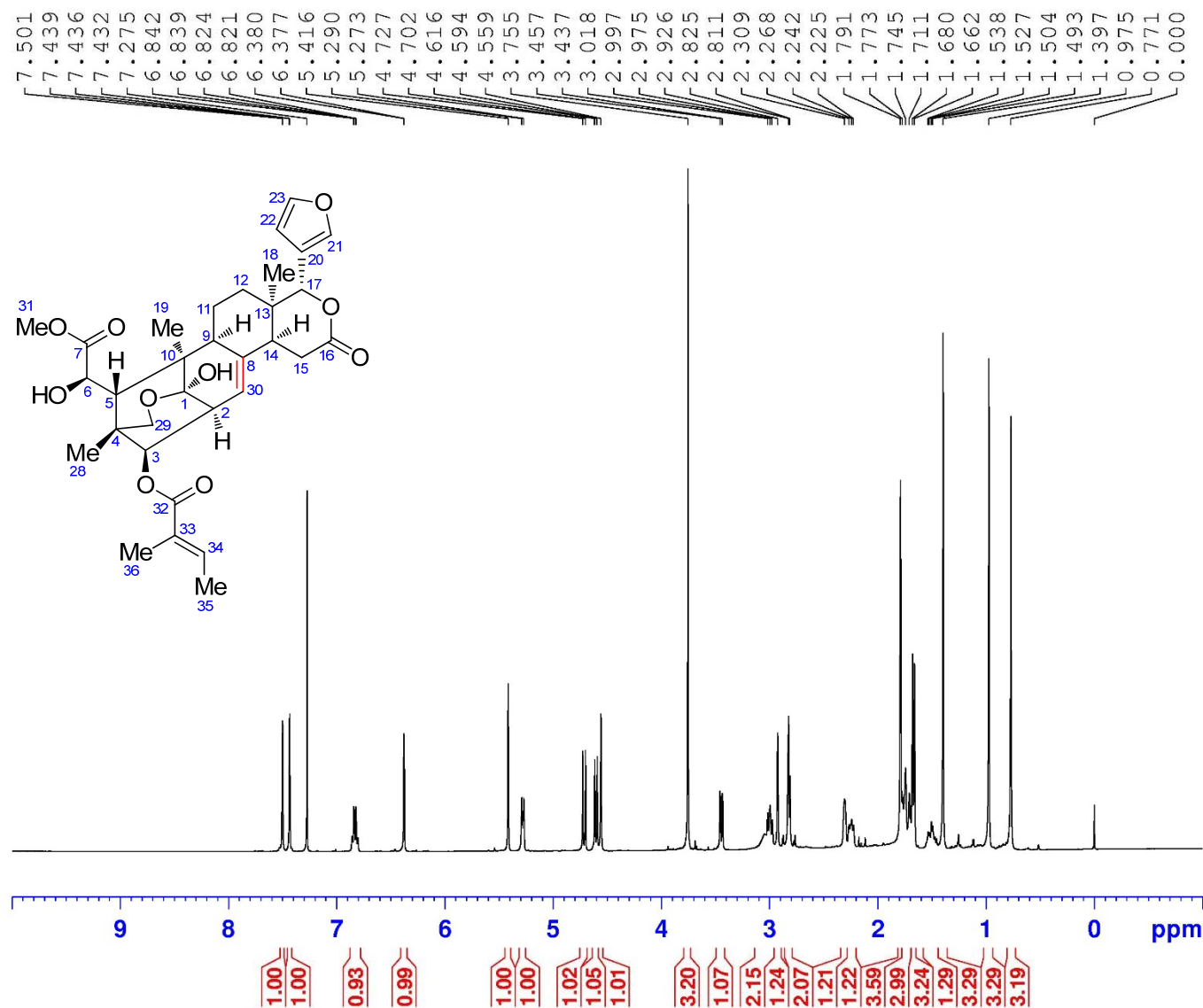
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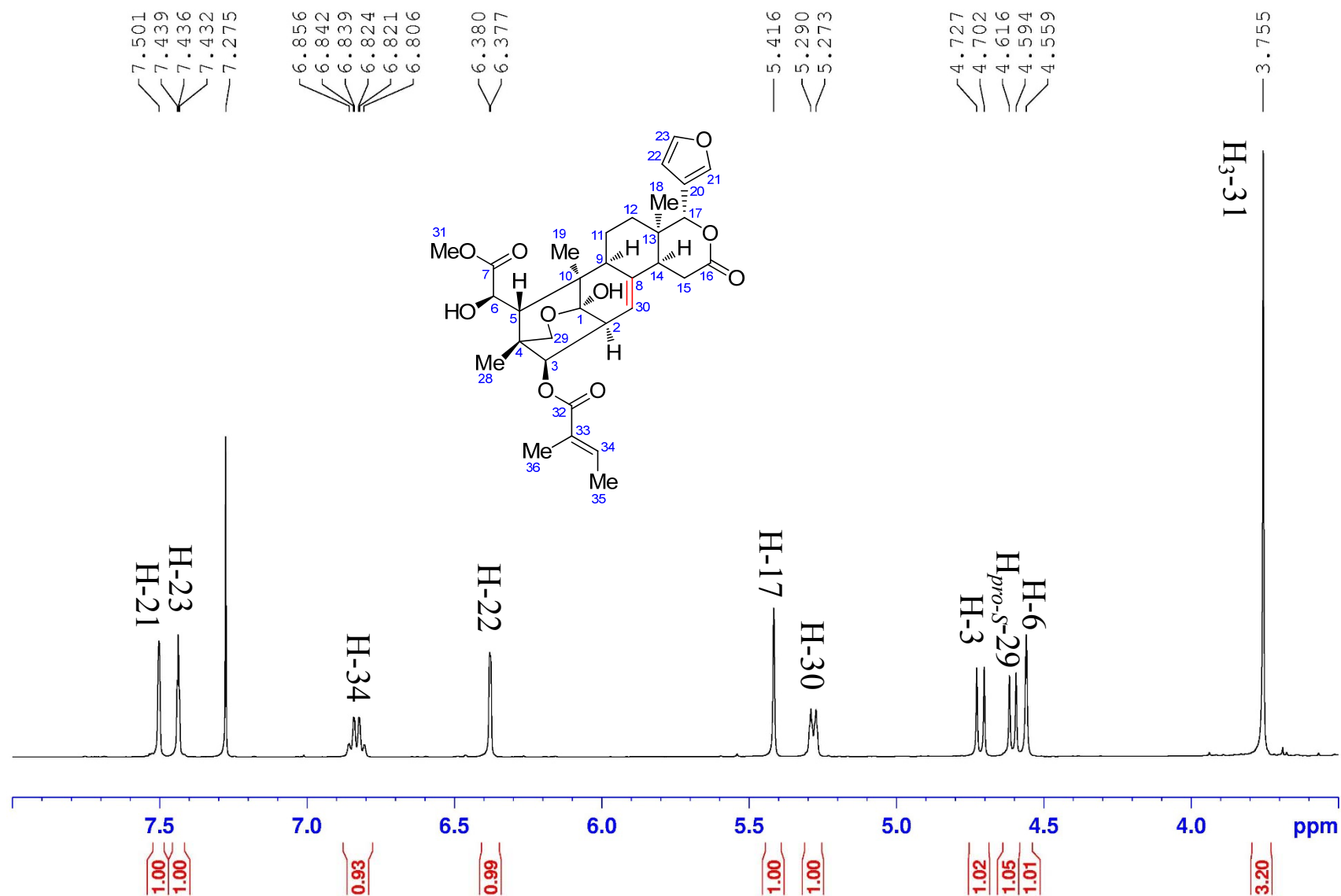
^1H NMR (400 MHz) spectrum of compound **1** in CDCl_3



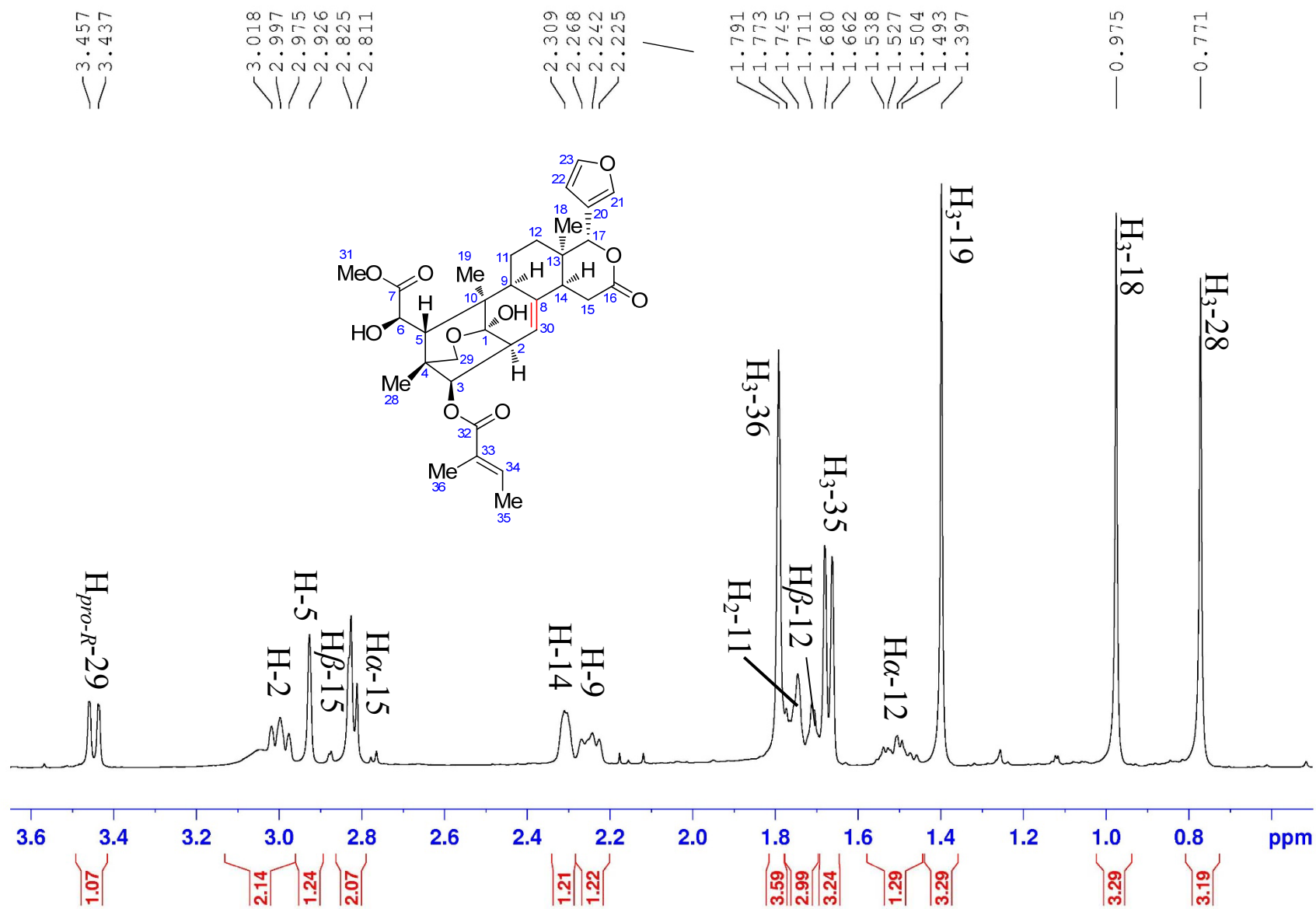
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 TD 65536
 SOLVENT CDCl_3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 44.55
 DW 60.800 usec
 DE 10.00 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

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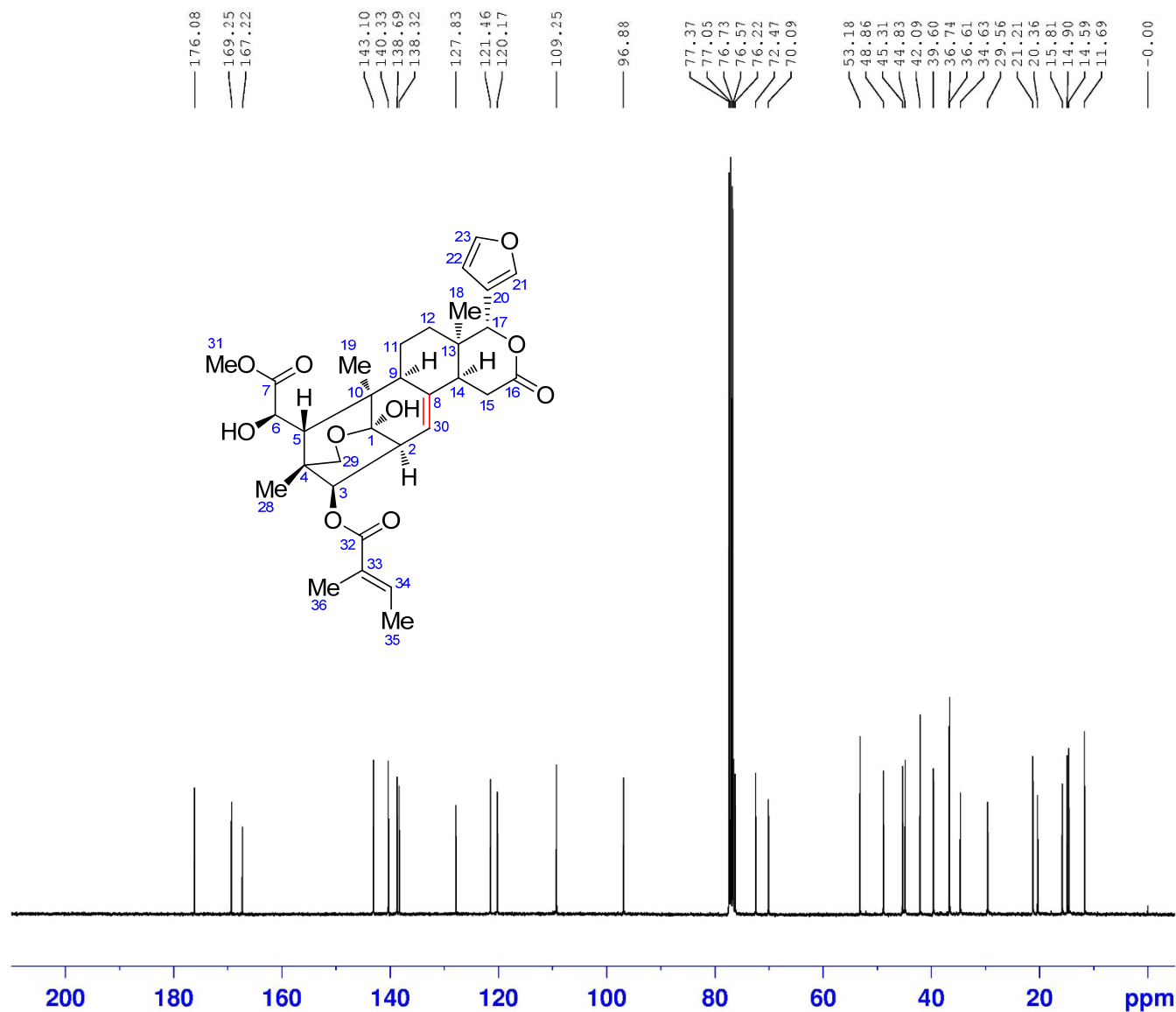
^1H NMR (400 MHz) spectrum of compound **1** in CDCl_3



^1H NMR (400 MHz) spectrum of compound **1** in CDCl_3



^{13}C NMR (100 MHz) spectrum of compound **1** in CDCl_3



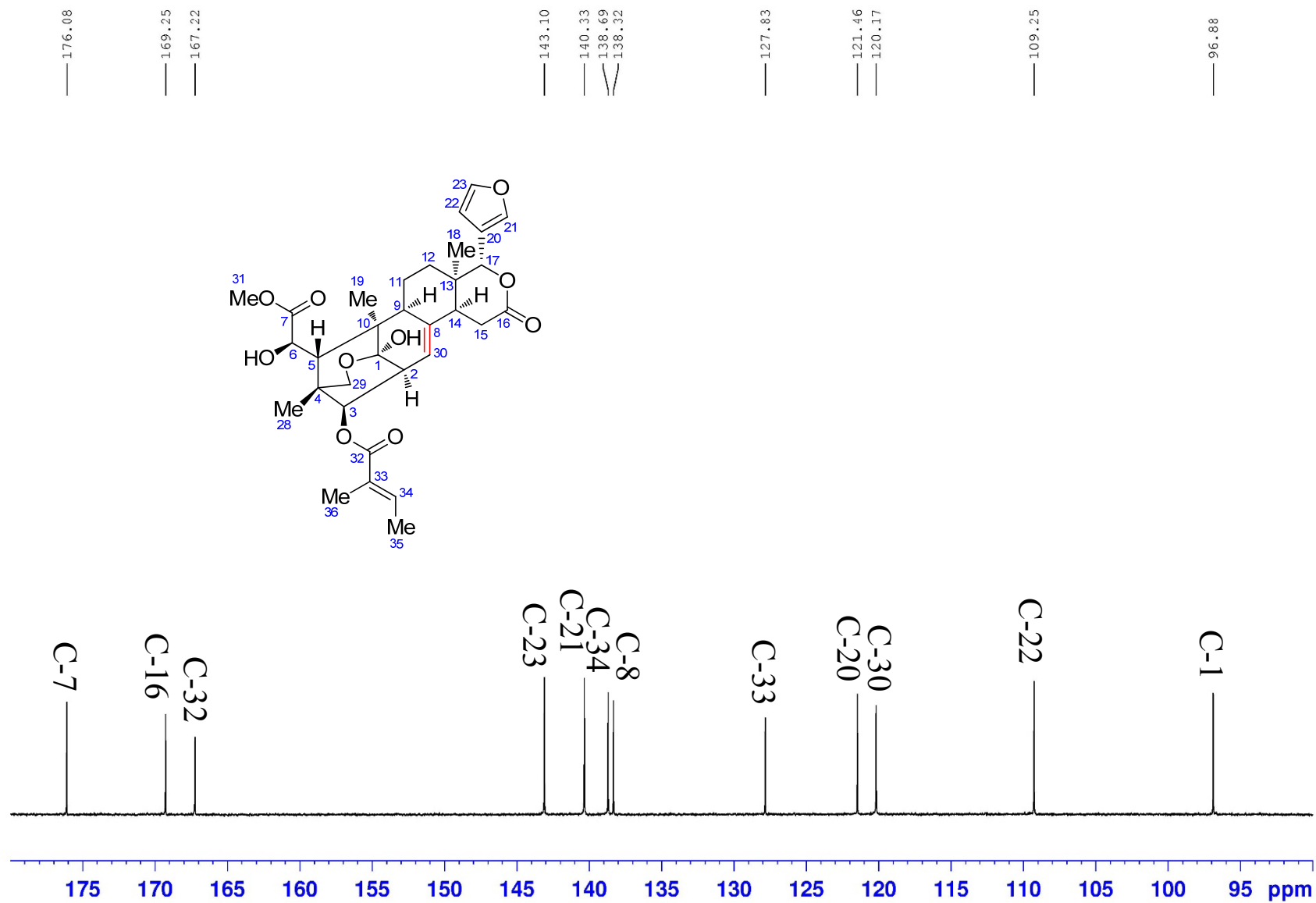
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PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
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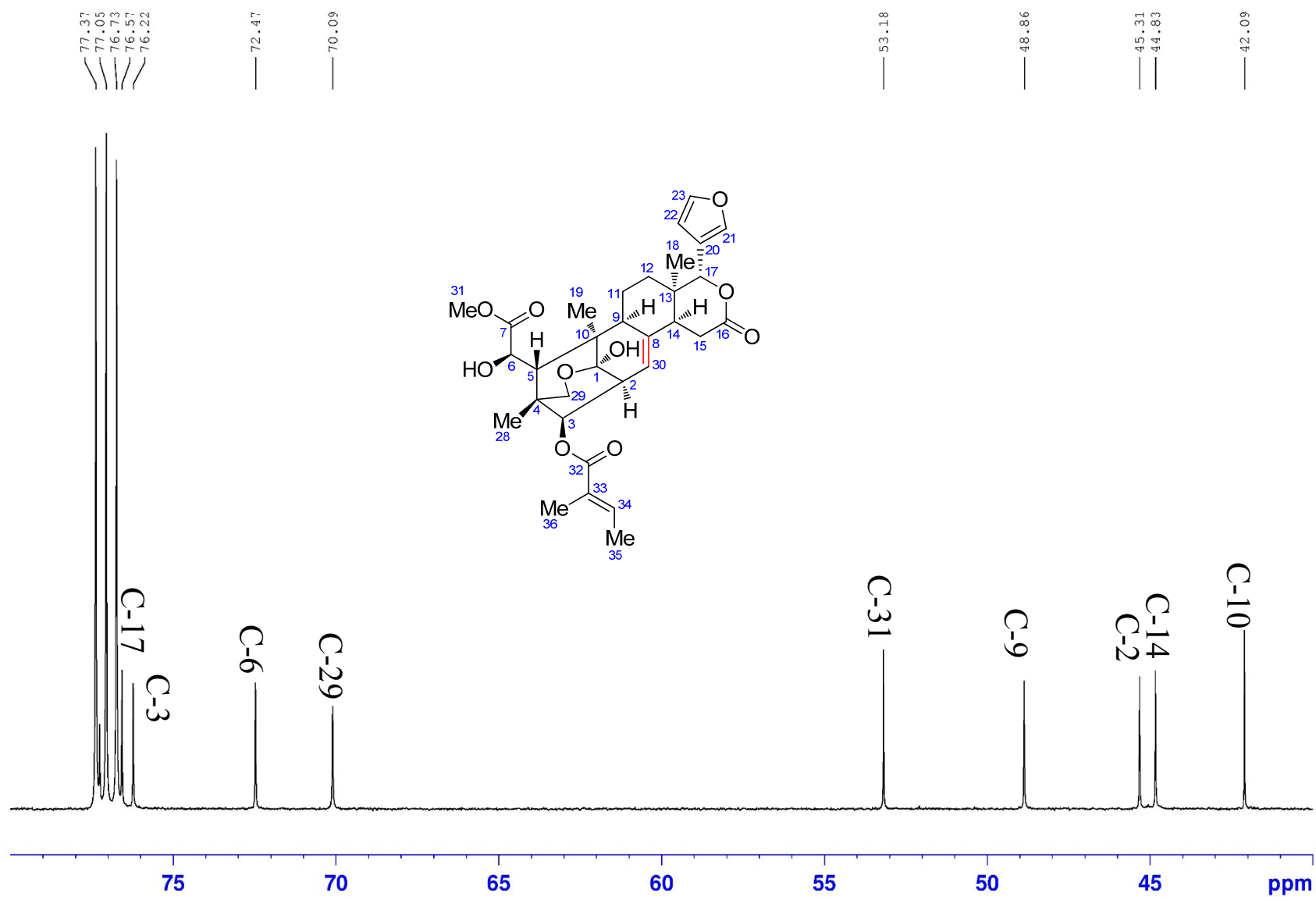
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LB       1.00 Hz
GB       0
PC       1.40
    
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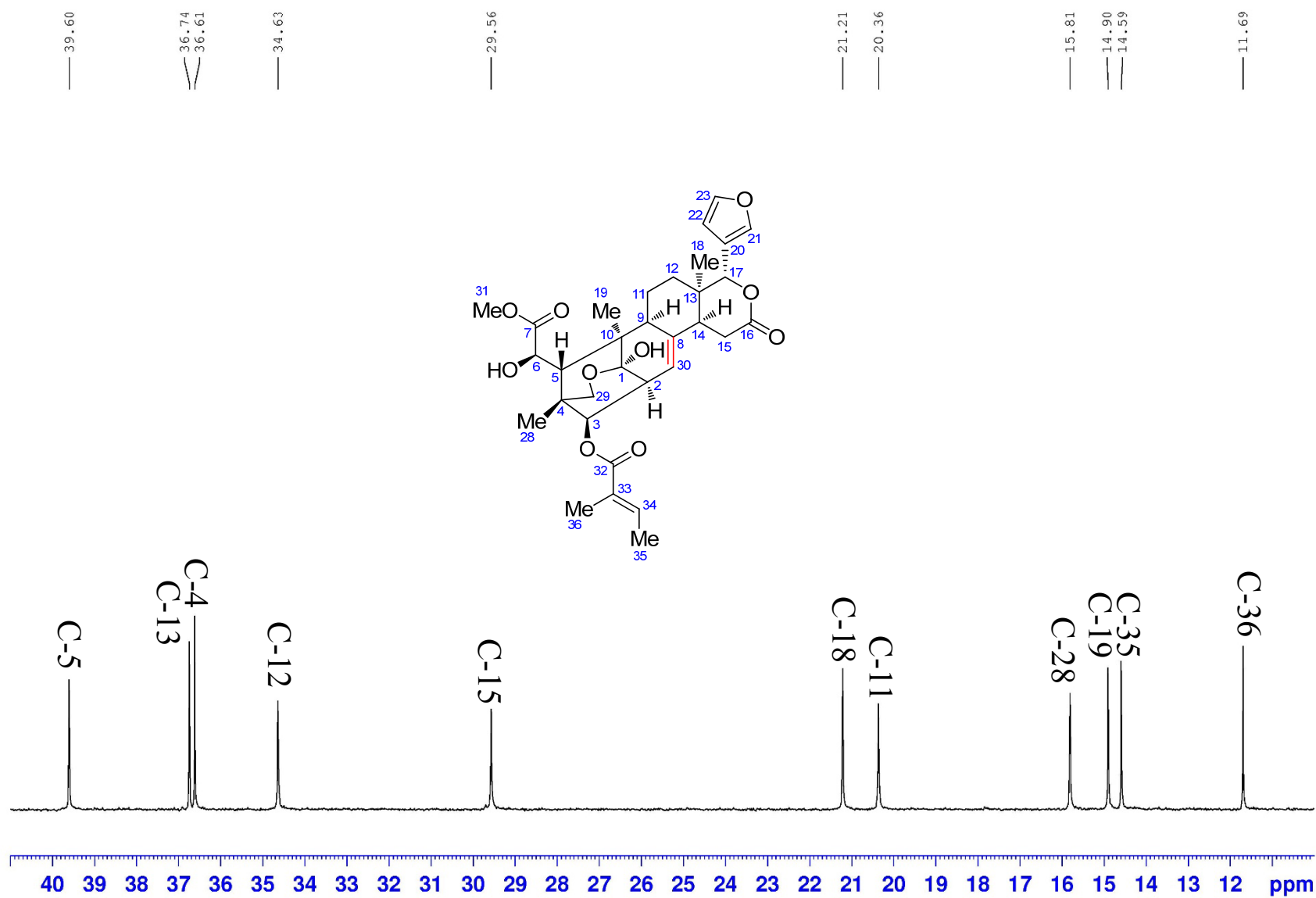
^{13}C NMR (100 MHz) spectrum of compound **1** in CDCl_3



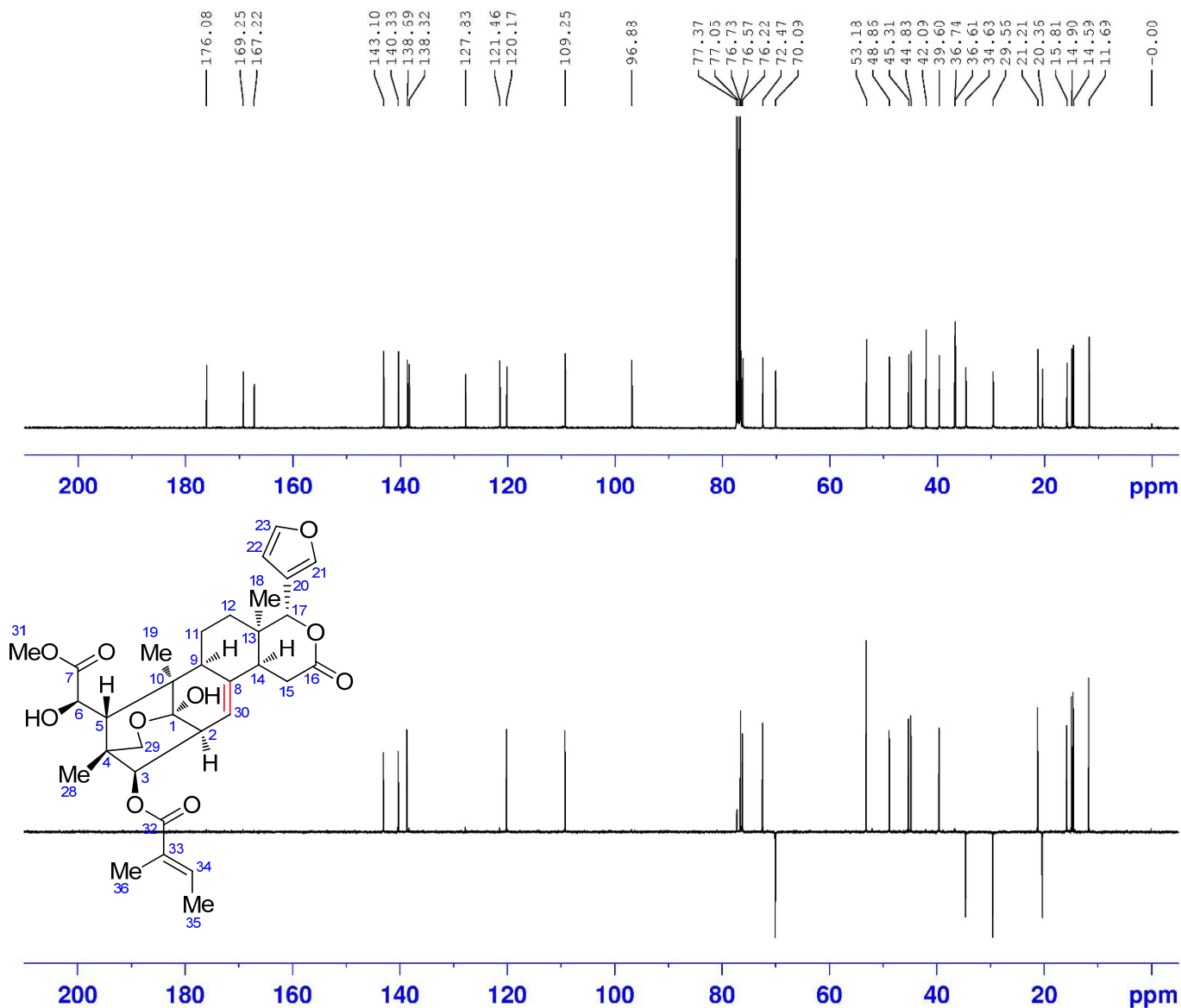
^{13}C NMR (100 MHz) spectrum of compound **1** in CDCl_3



^{13}C NMR (100 MHz) spectrum of compound **1** in CDCl_3



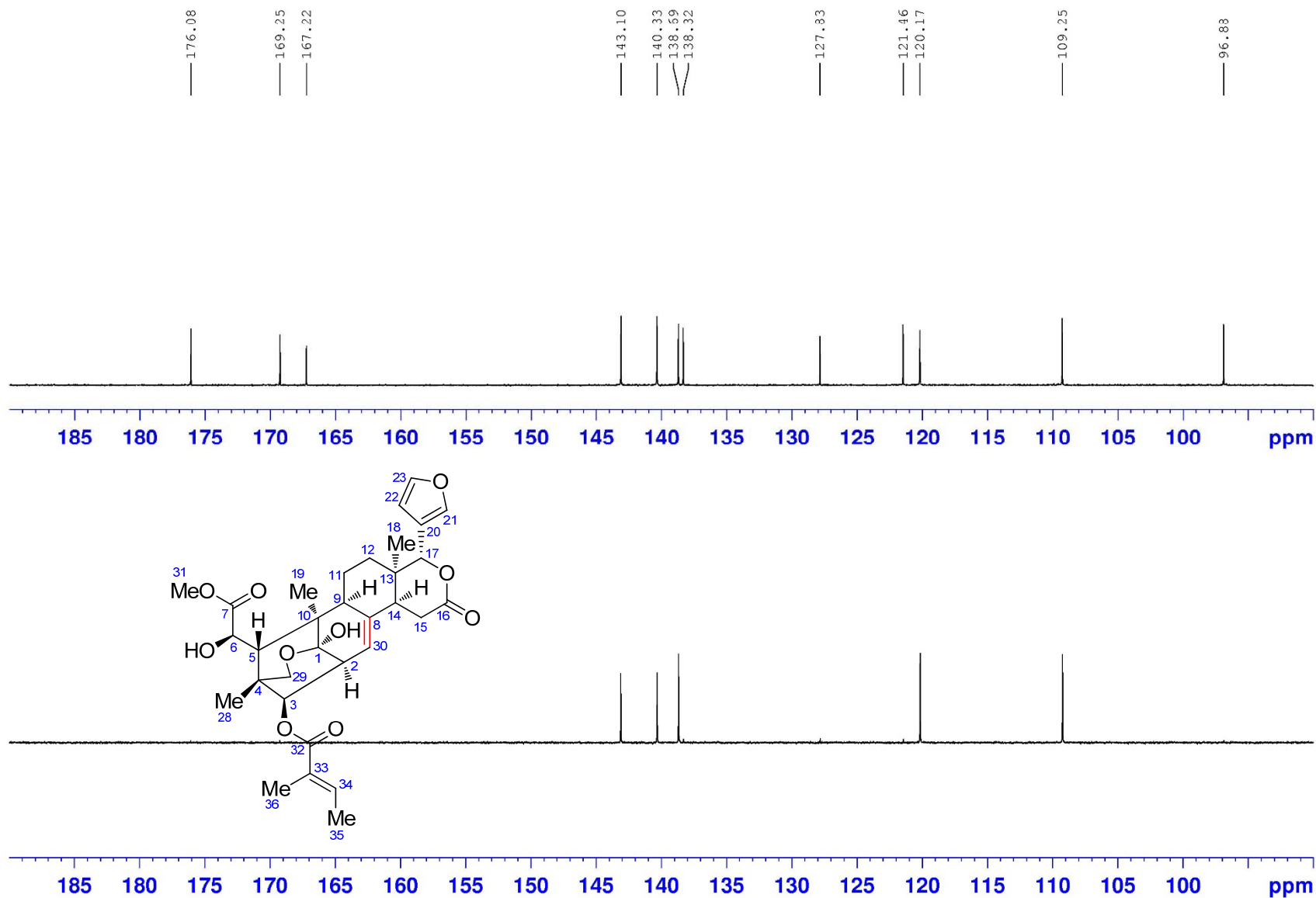
DEPT135 (100 MHz) spectrum of compound **1** in CDCl₃



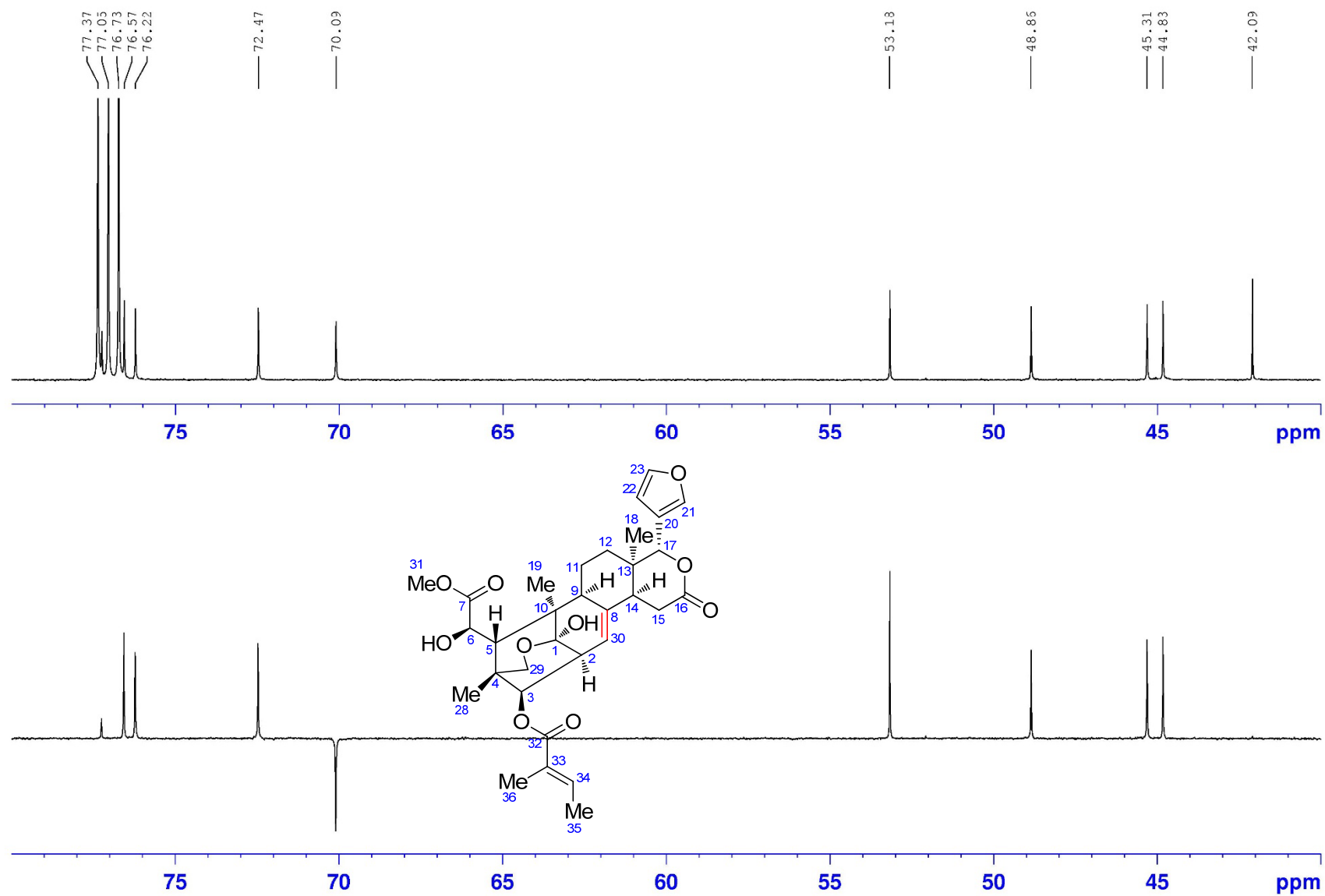
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 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 130.26
 DW 20.800 usec
 DE 18.00 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
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 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

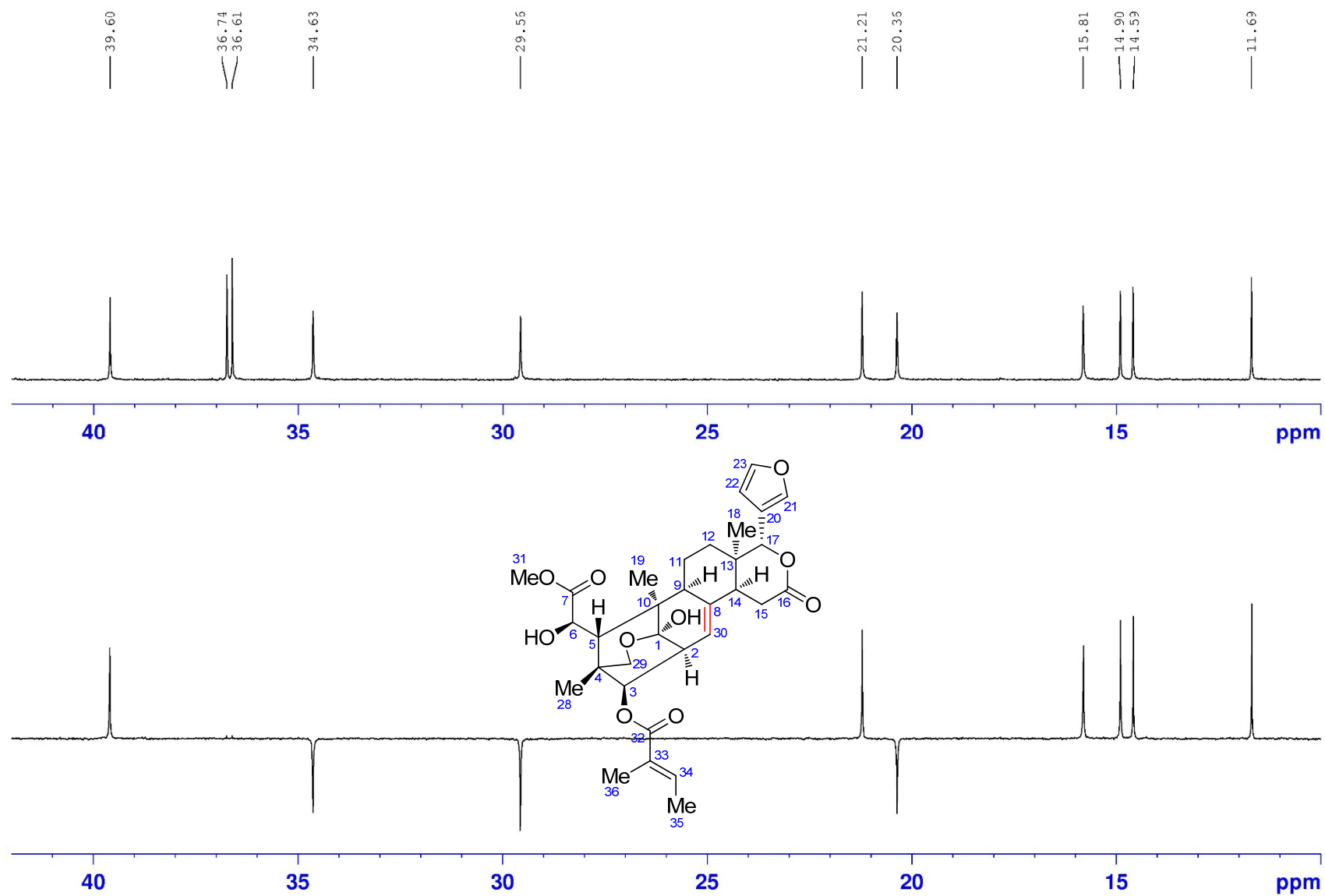
DEPT135 (100 MHz) spectrum of compound **1** in CDCl₃



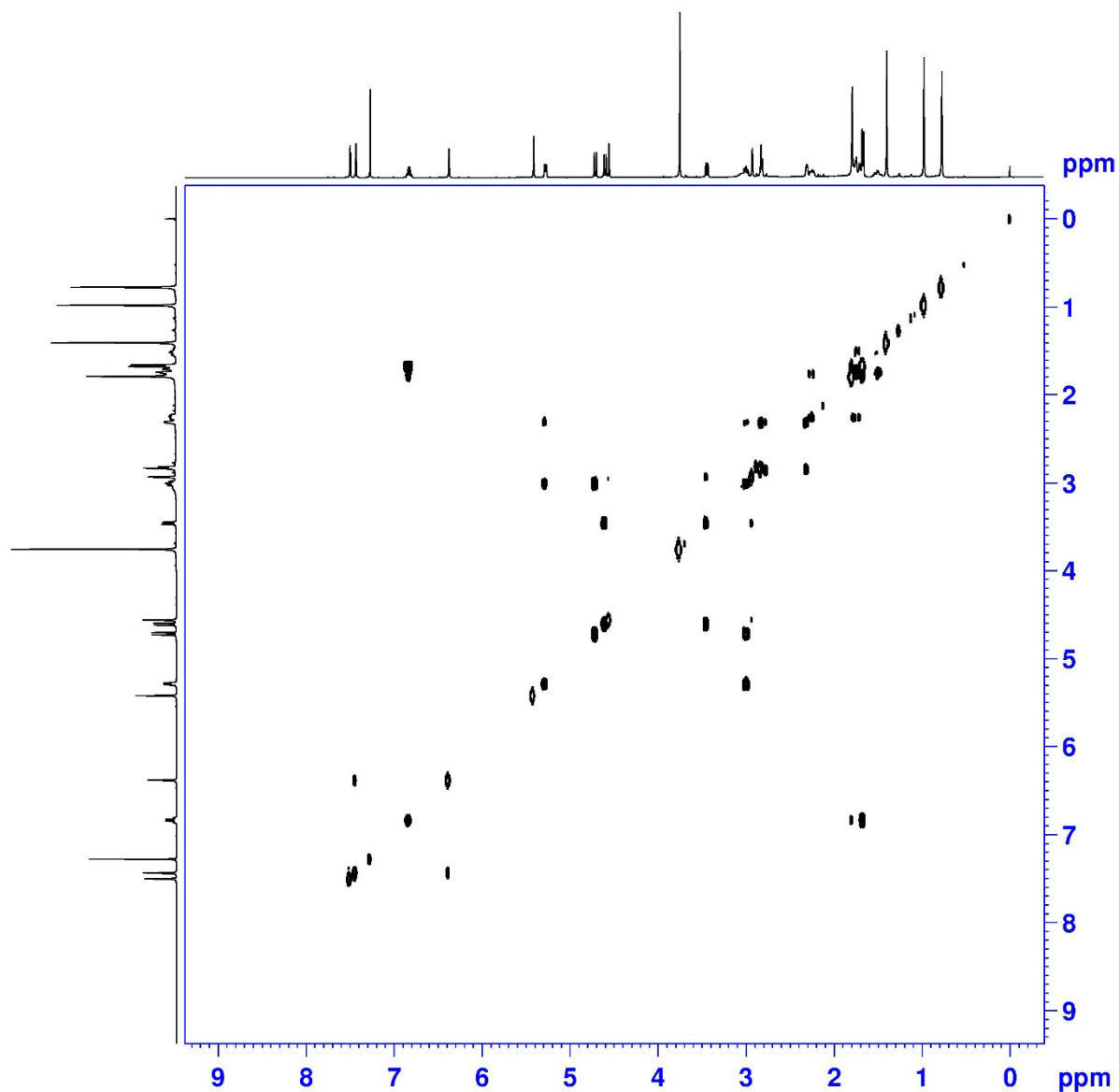
DEPT135 (100 MHz) spectrum of compound **1** in CDCl₃



DEPT135 (100 MHz) spectrum of compound **1** in CDCl₃



^1H - ^1H COSY (400 MHz) spectrum of compound **1** in CDCl_3



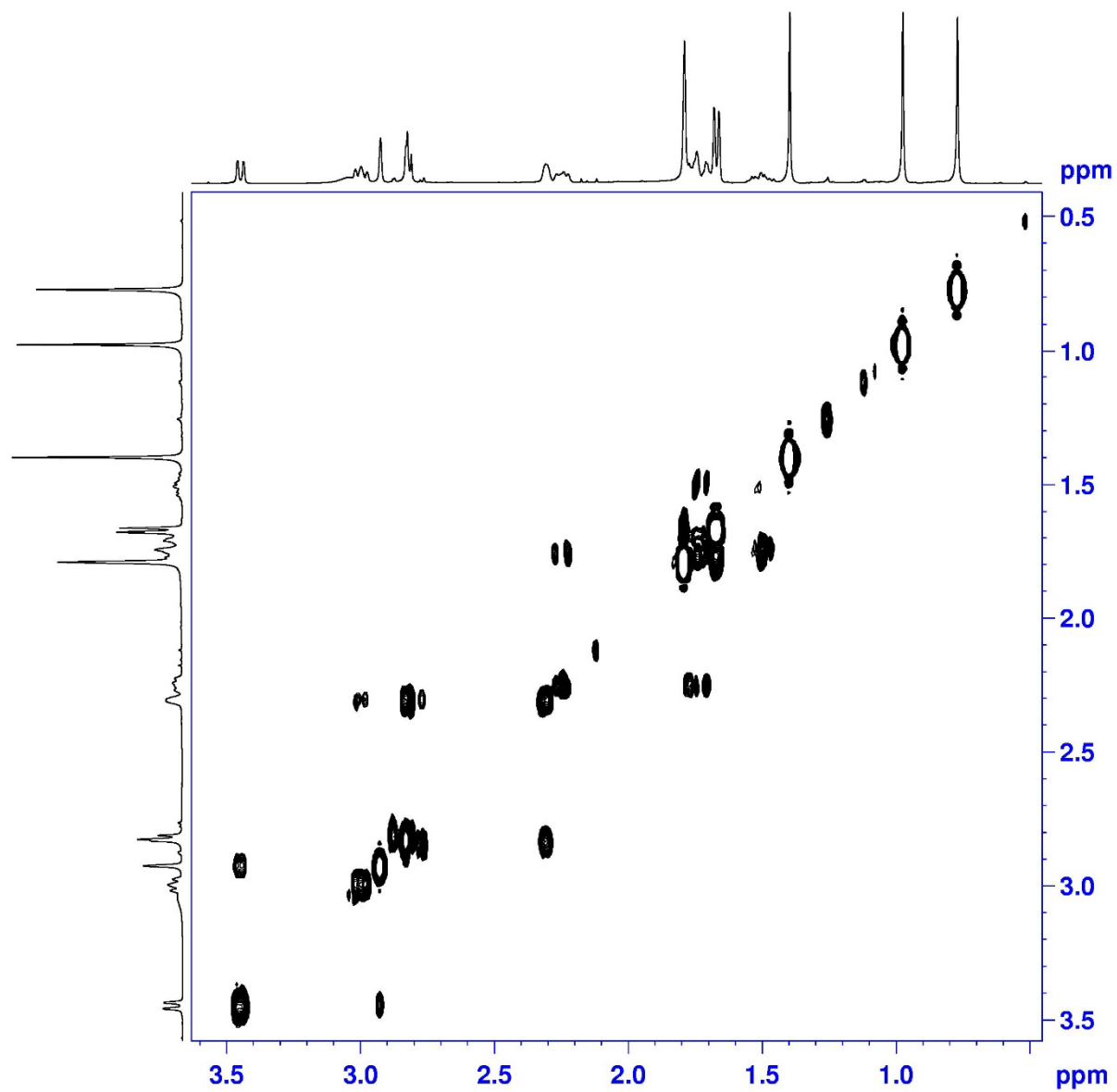
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SOLVENT   CDCl3
NS         8
DS         8
SWH        3906.250 Hz
FIDRES     1.907349 Hz
AQ         0.2621940 sec
RG         91.64
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DE         10.00 usec
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D1         1.89678097 sec
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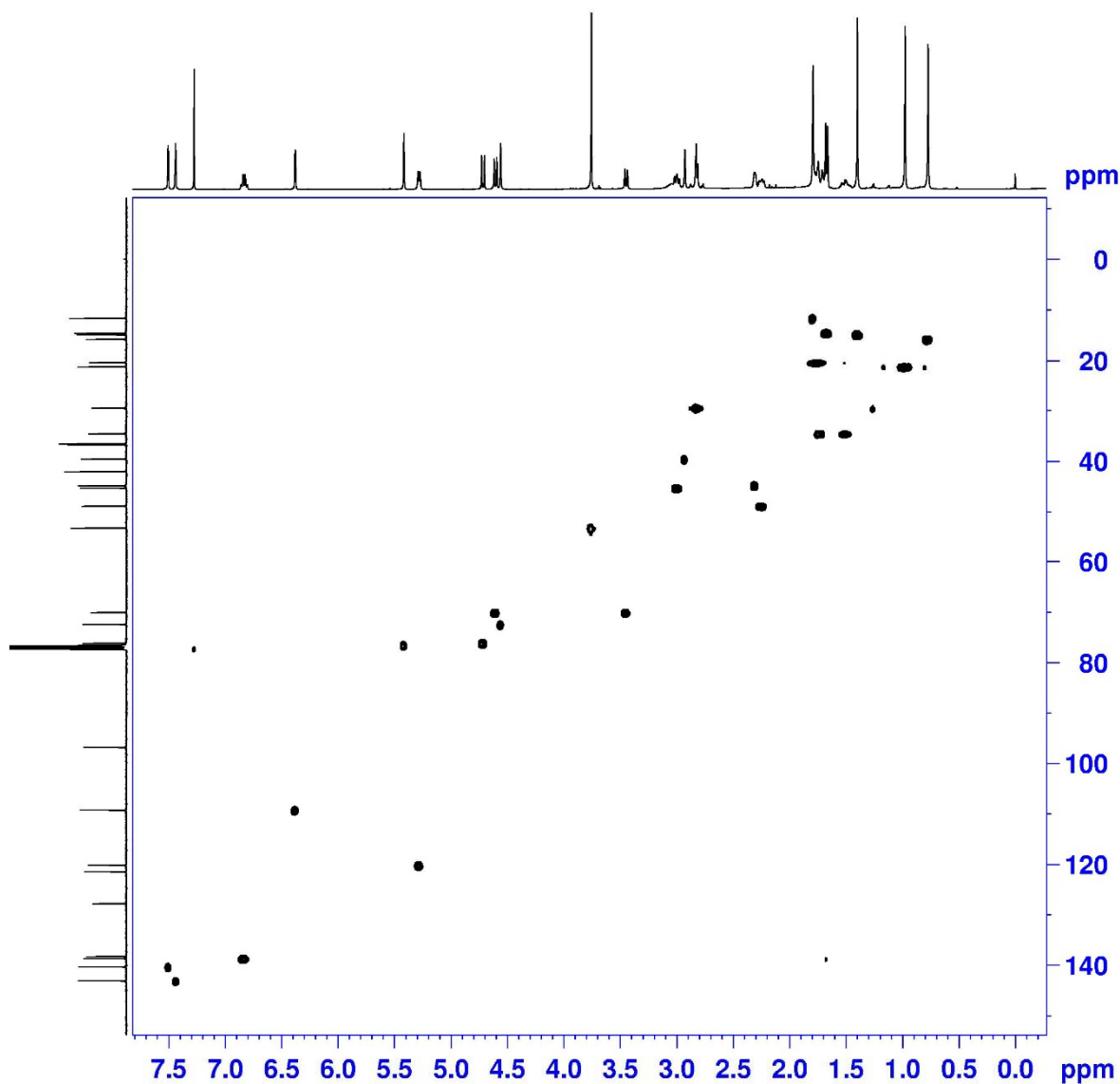
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P1         11.50 usec
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TD         128
SFO1      400.1318 MHz
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WDW        QSINE
SSB         0
LB         0.00 Hz
GB         0
PC         1.40
SI         1024
MC2        QF
SF         400.1300017 MHz
WDW        QSINE
SSB         0
LB         0.00 Hz
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^1H - ^1H COSY (400 MHz) spectrum of compound **1** in CDCl_3



HSQC (400 MHz) spectrum of compound **1** in CDCl₃



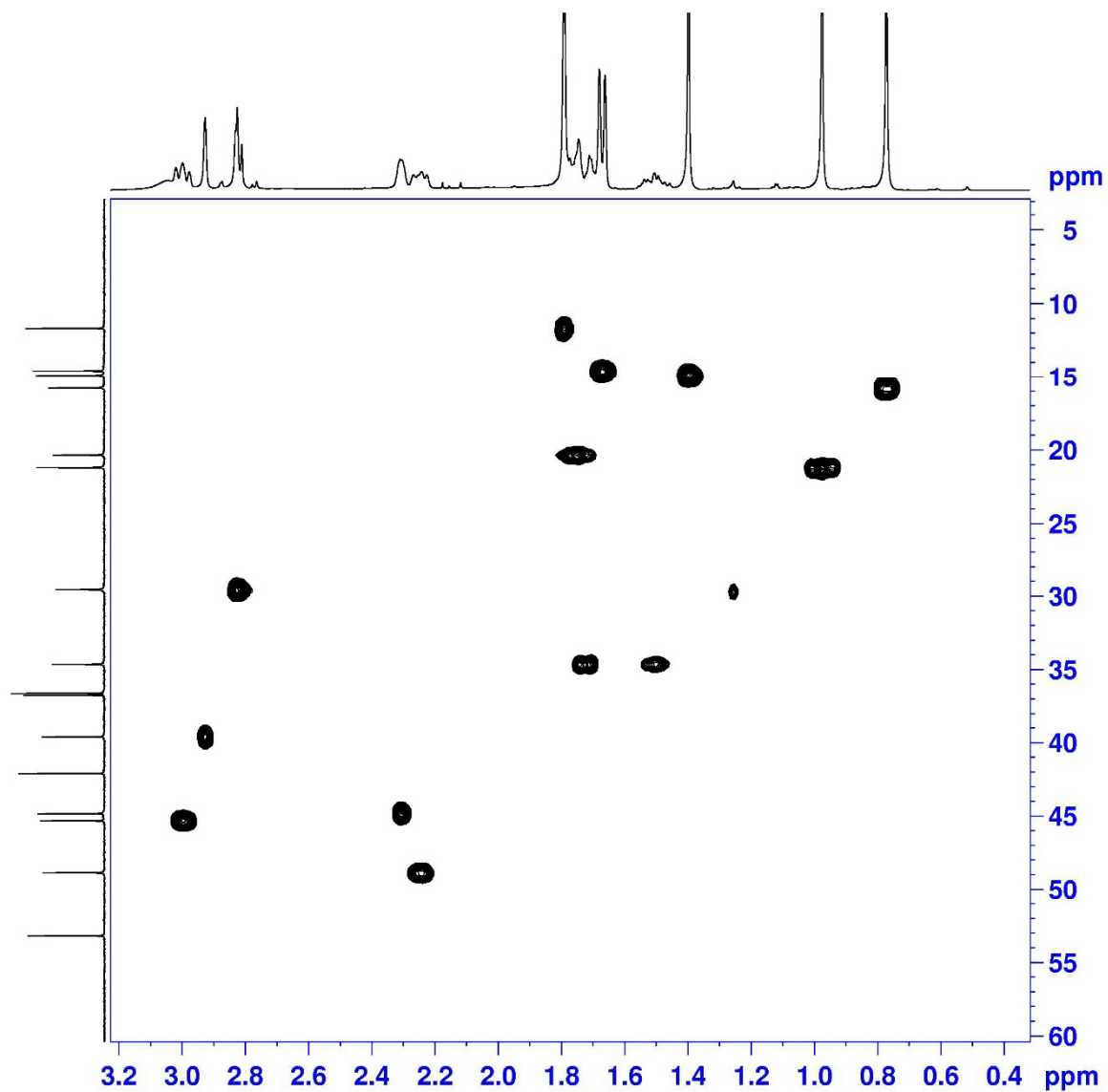
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SOLVENT   CDCl3
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FIDRES     4.202076 Hz
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CNST2     145.0000000
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D4         0.00172414 sec
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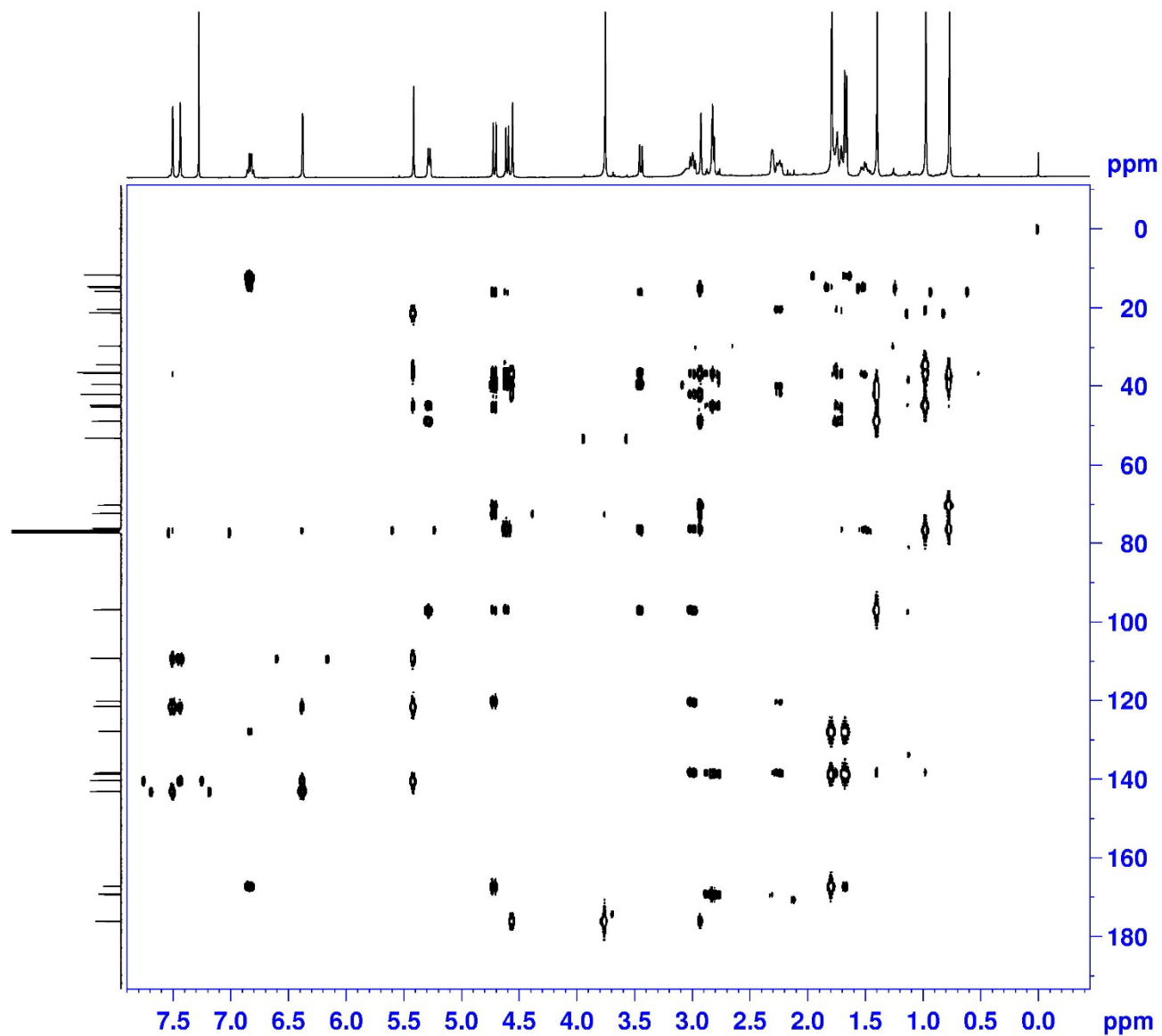
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P2         23.00 usec
P28        0.00 usec
ND0        2
TD         256
SFO1      100.6233 MHz
FIDRES     93.900238 Hz
SW         238.896 ppm
FqMODE     Echo-Antiecho
SI         1024
SF         400.1300023 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.40
SI         1024
MC2        echo-antiecho
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SSB        2
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HSQC (400 MHz) spectrum of compound **1** in CDCl₃



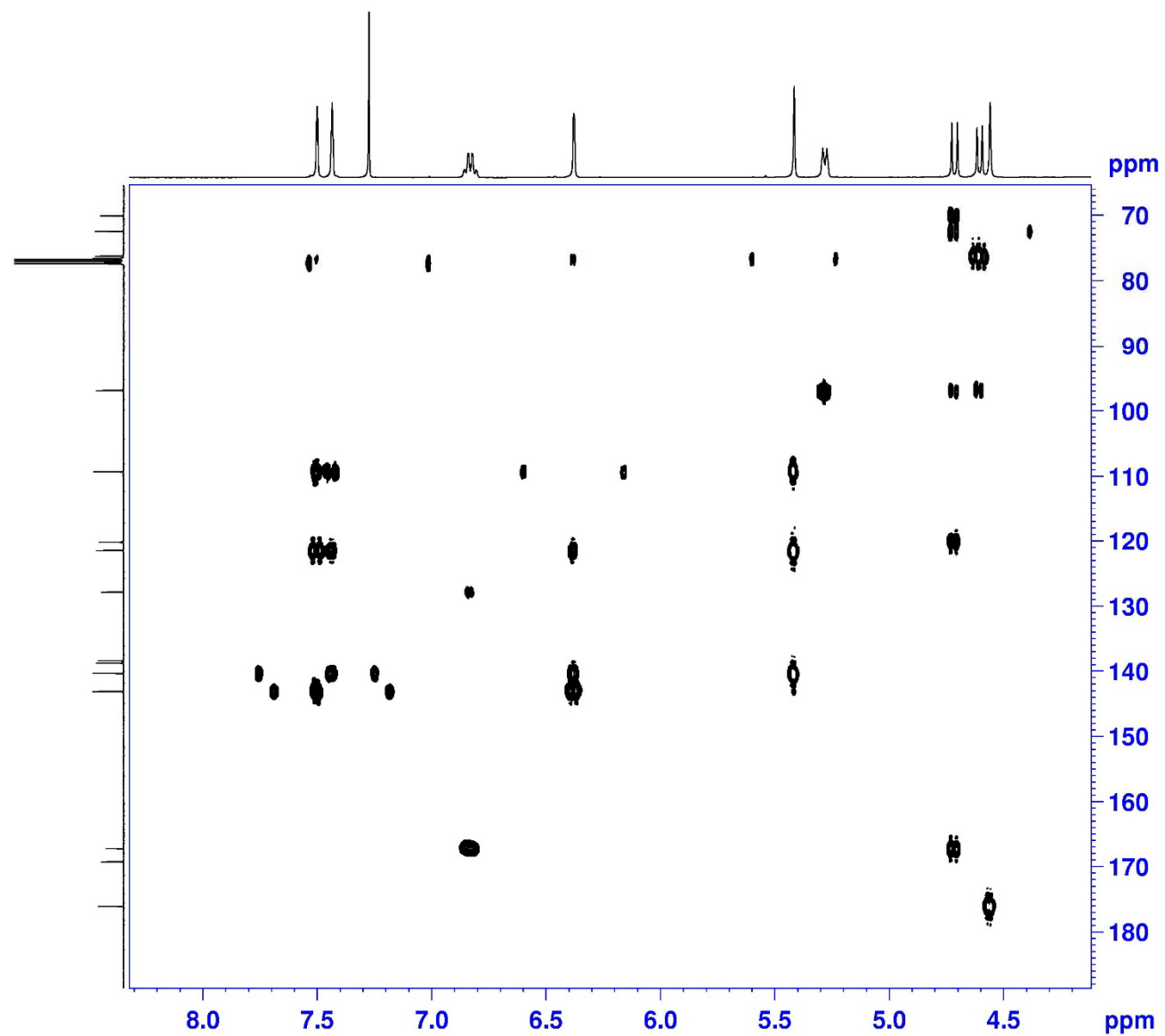
HMBC (400 MHz) spectrum of compound **1** in CDCl₃



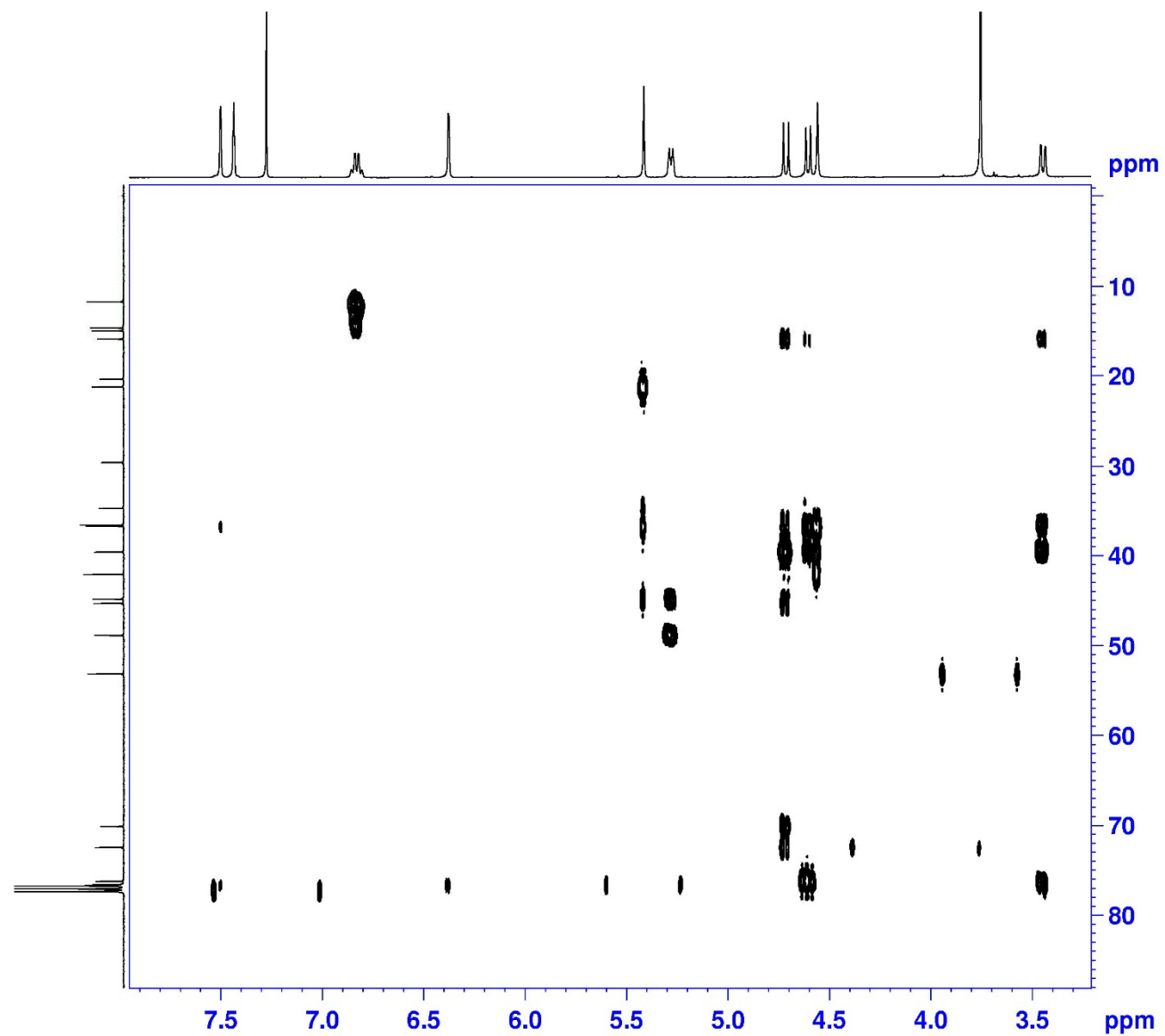
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PROCNO 1
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TD 4096
SOLVENT CDCl3
NS 32
DS 16
SWH 5197.505 Hz
FIDRES 1.268922 Hz
AQ 0.3940852 sec
RG 208.5
DW 96.200 usec
DE 10.00 usec
TE 297.0 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00344828 sec
D6 0.05000000 sec
D16 0.00020000 sec
IN0 0.00002080 sec

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P2 23.00 usec
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SFO1 100.6233 MHz
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SW 238.896 ppm
FMODE QF
SI 2048
SF 400.1300026 MHz
WDW SINE
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PC 1.40
SI 1024
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GB 0

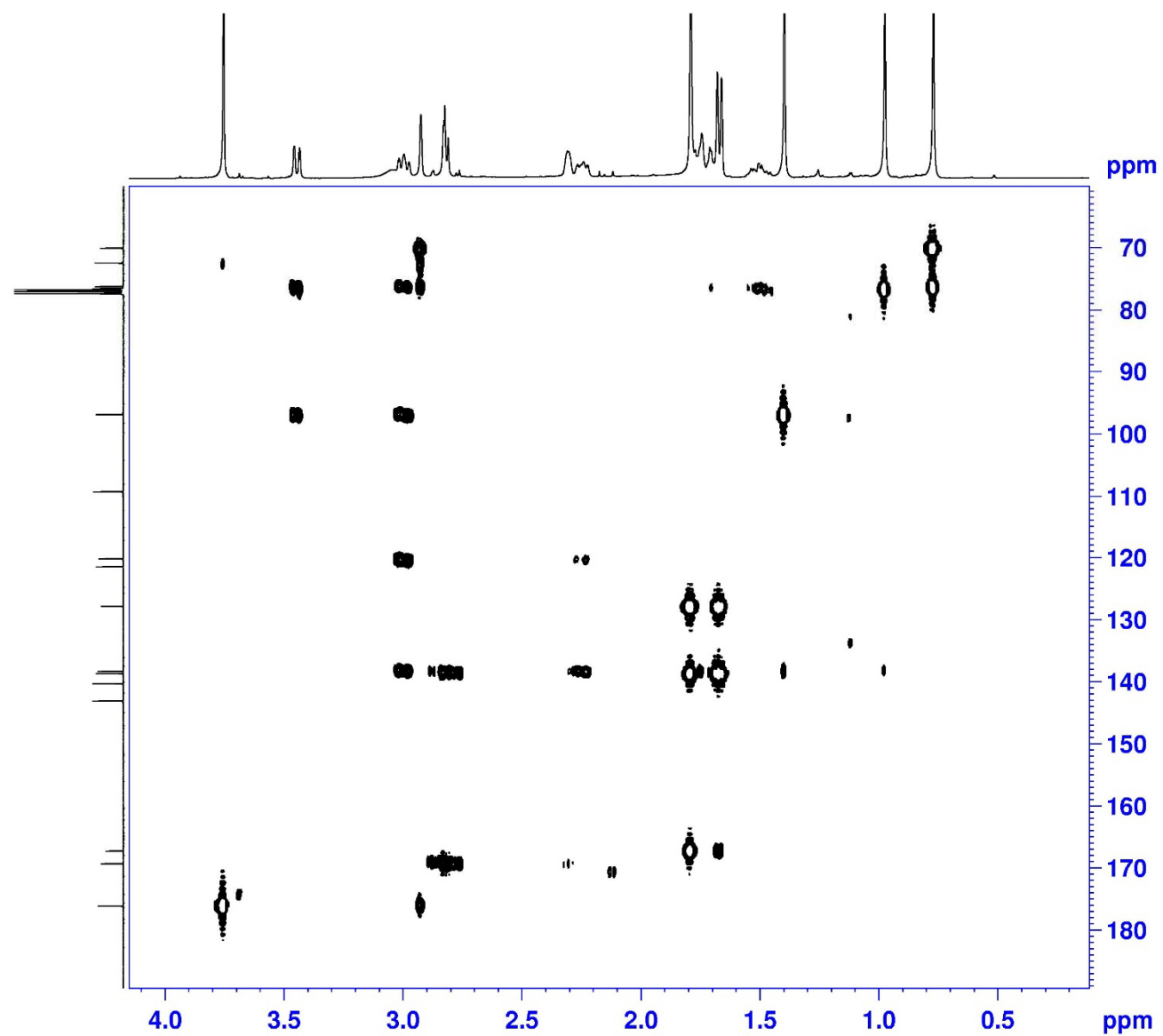
HMBC (400 MHz) spectrum of compound **1** in CDCl₃



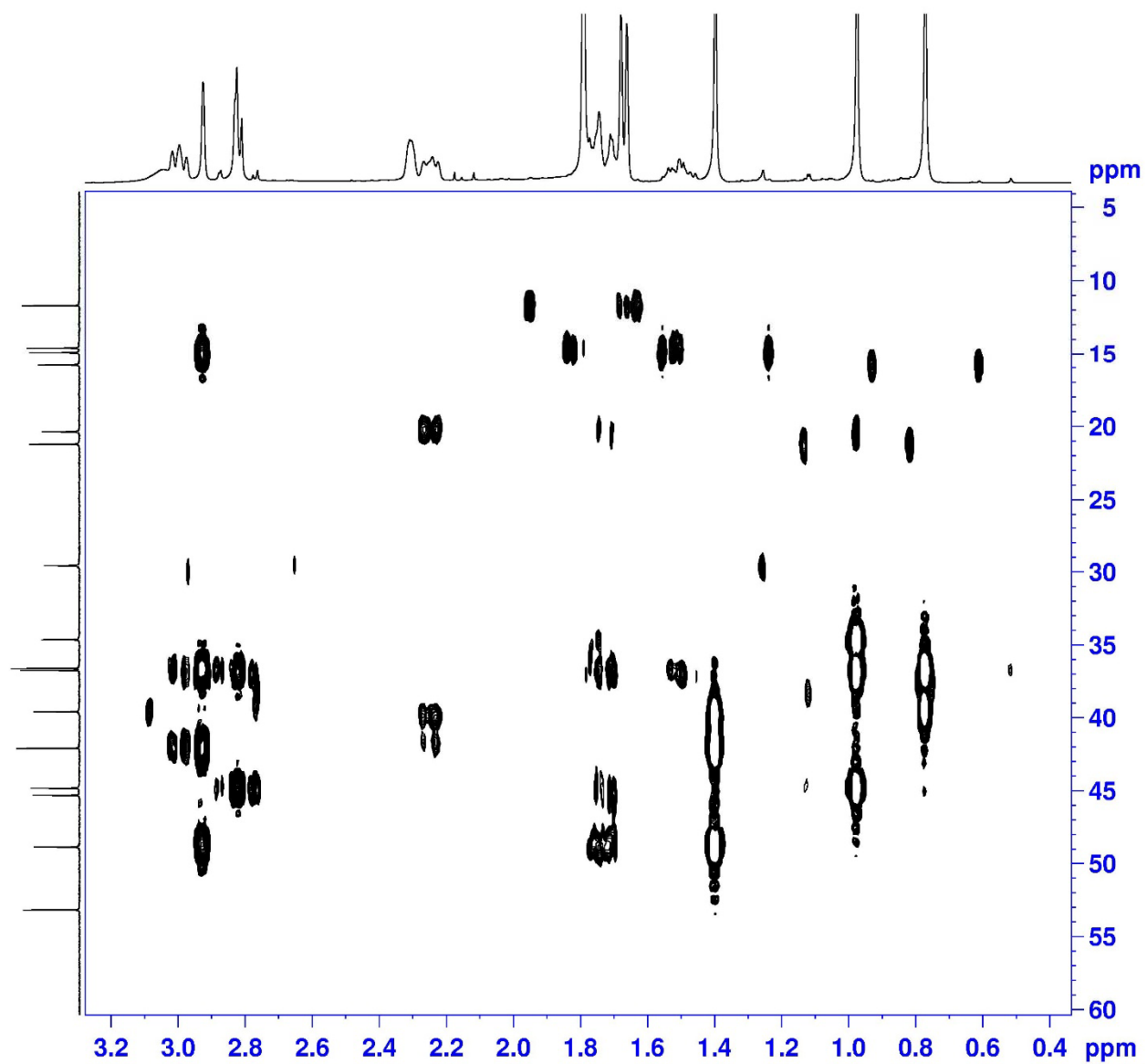
HMBC (400 MHz) spectrum of compound **1** in CDCl₃



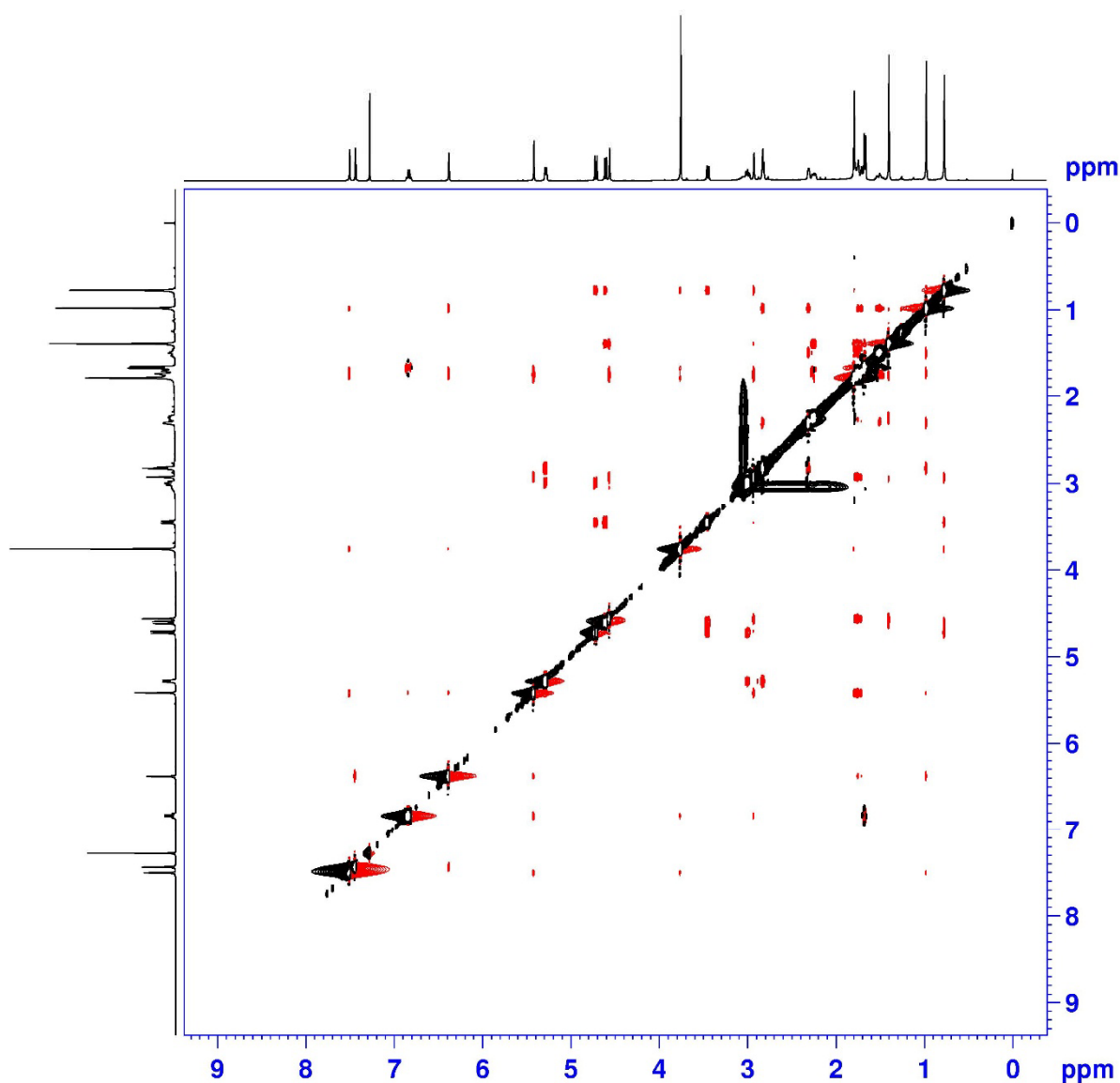
HMBC (400 MHz) spectrum of compound **1** in CDCl₃



HMBC (400 MHz) spectrum of compound **1** in CDCl₃



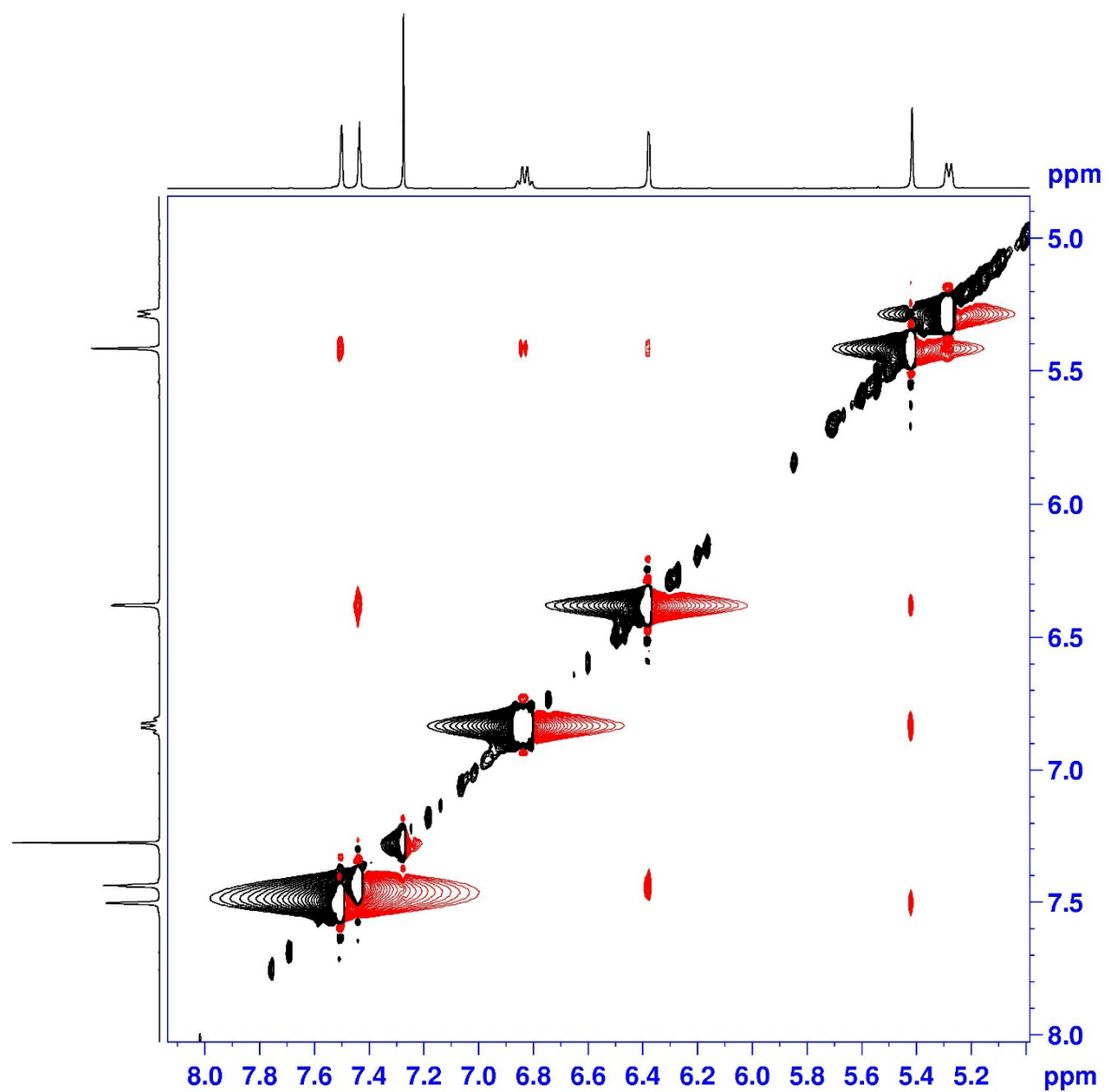
NOESY (400 MHz) spectrum of compound **1** in CDCl₃



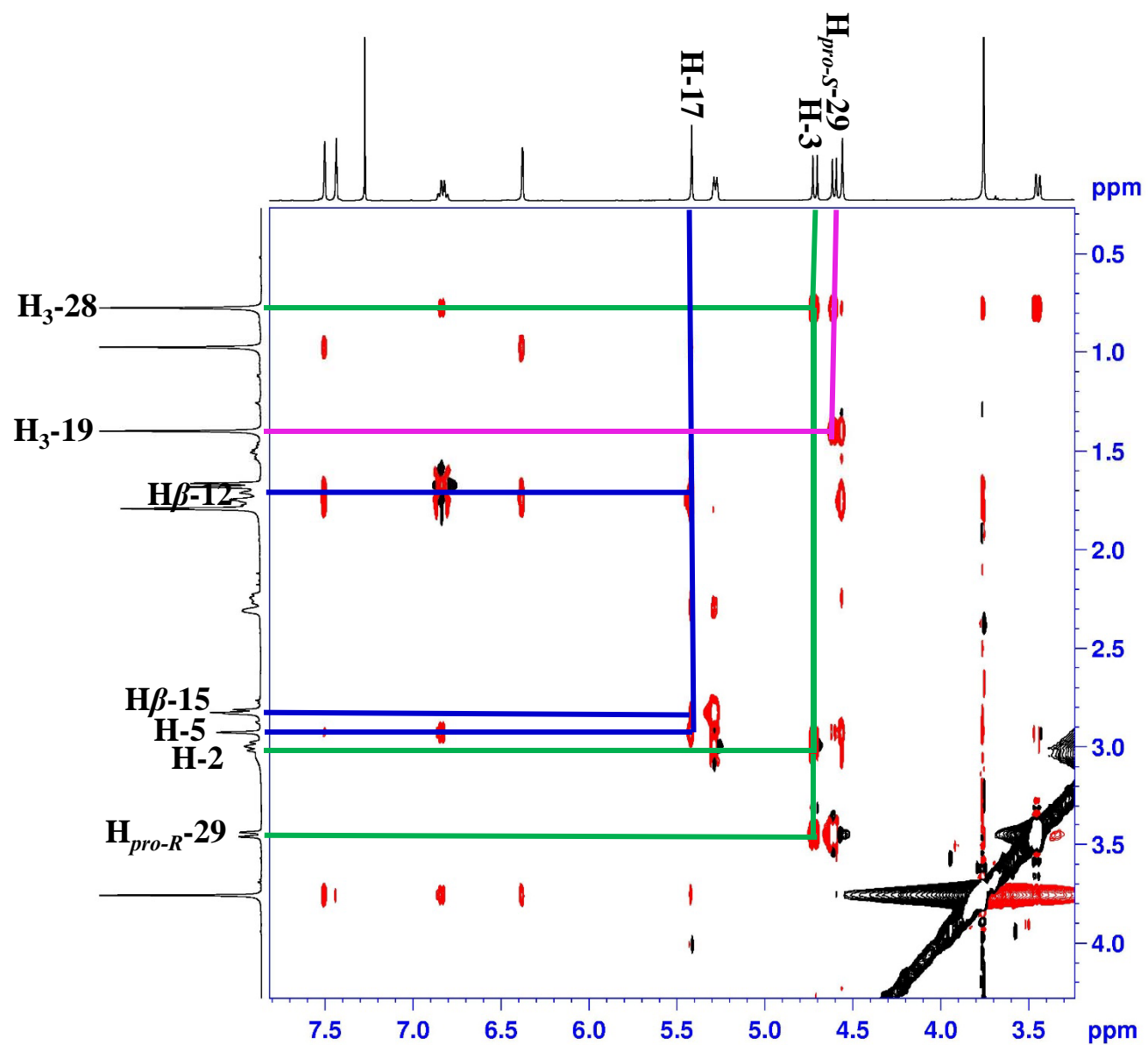
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TD         2048
SOLVENT    CDCl3
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DS         32
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FIDRES     1.953125 Hz
AQ         0.2560500 sec
RG         65.23
DW         125.000 usec
DE         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
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NUC1      1H
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P2        23.00 usec
P17       2500.00 usec
ND0       1
TD        256
SFO1      400.1318 MHz
FIDRES    15.625000 Hz
SW        9.997 ppm
FnMODE    States-TPPI
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SF        400.1300018 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
PC        1.00
SI        1024
MC2       States-TPPI
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SSB       2
LB        0.00 Hz
GB        0
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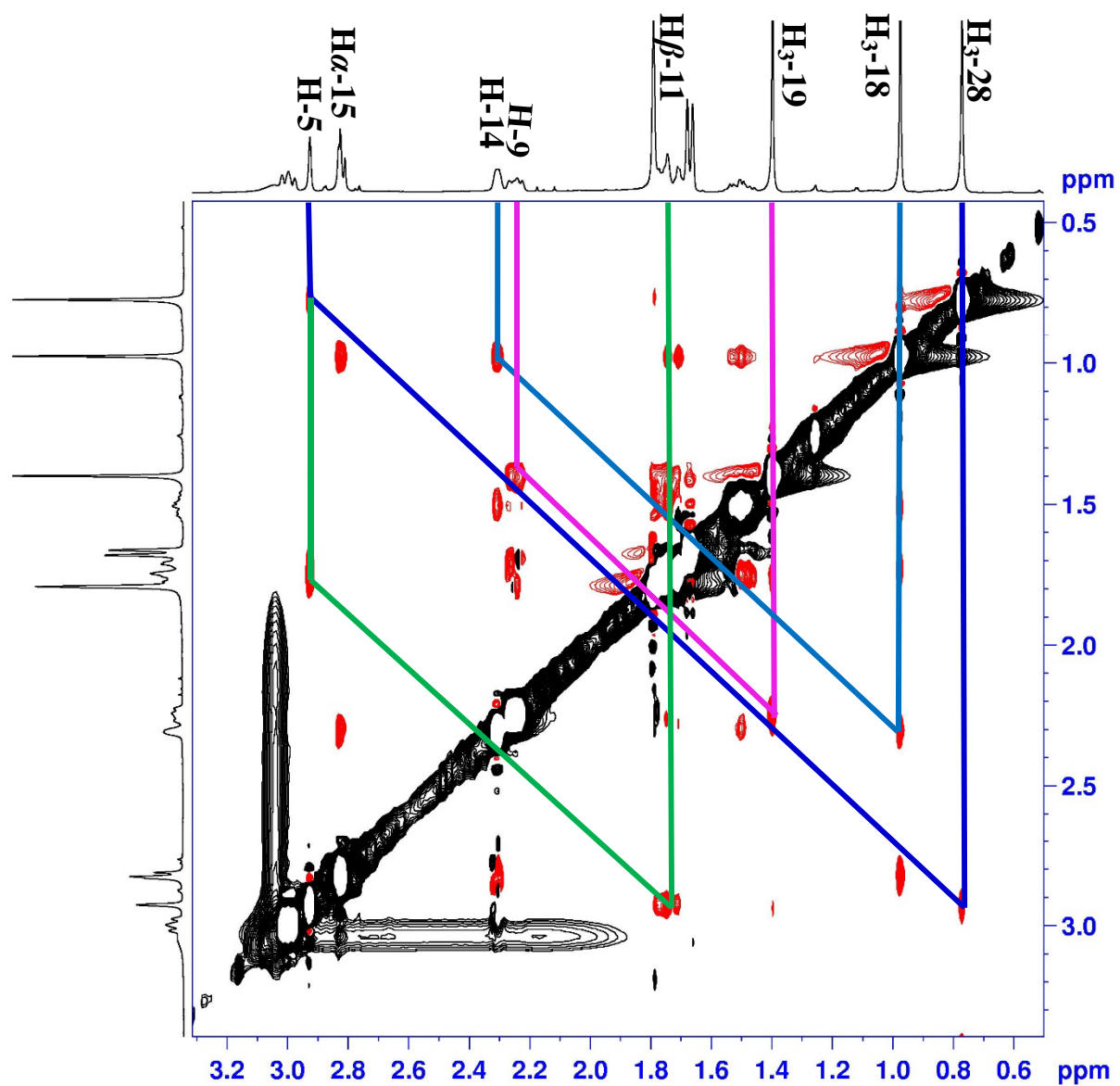

NOESY (400 MHz) spectrum of compound **1** in CDCl_3



NOESY (400 MHz) spectrum of compound **1** in CDCl_3



NOESY (400 MHz) spectrum of compound **1** in CDCl_3



HR-ESIMS for compound 2

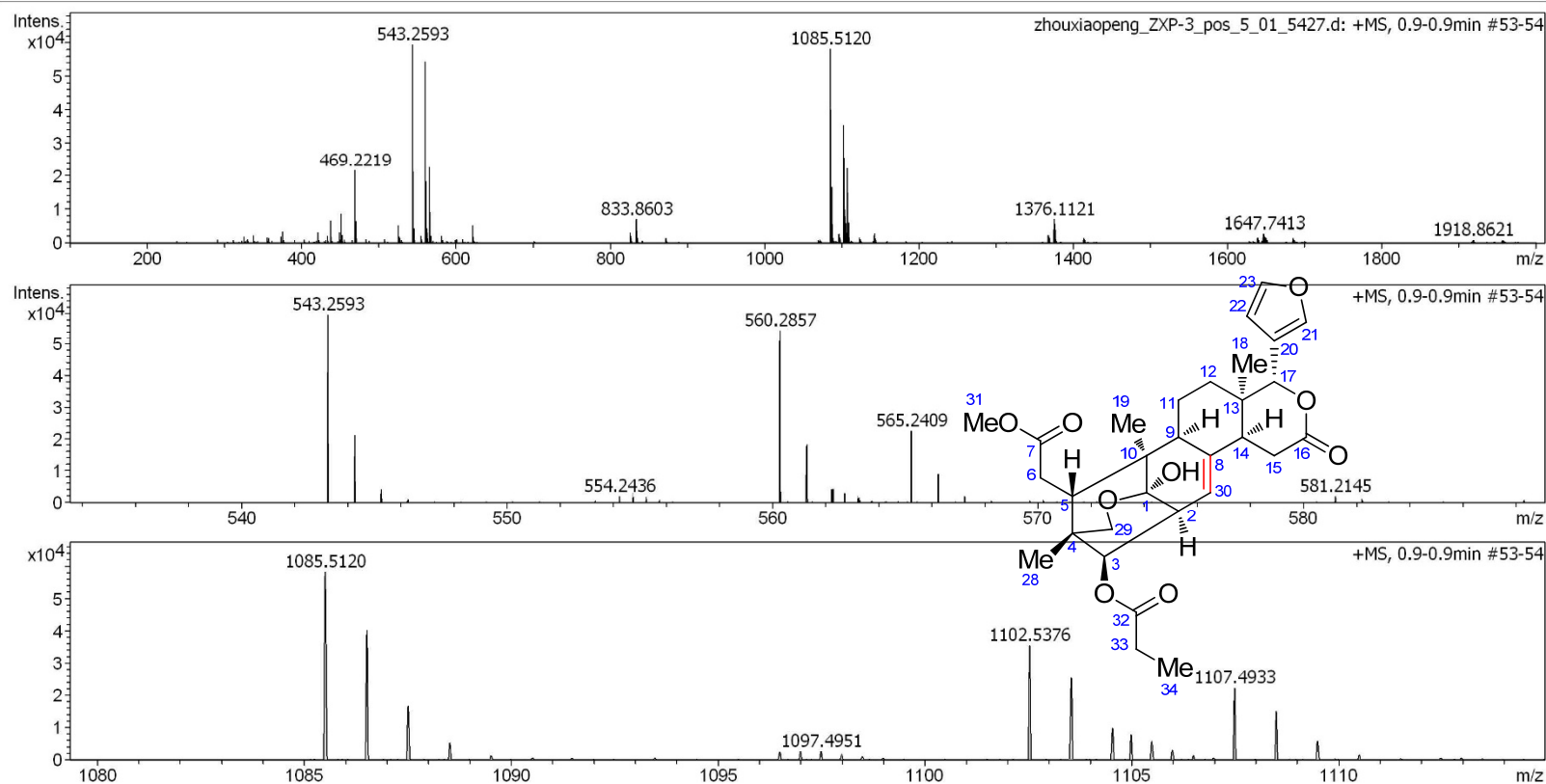
Generic Display Report

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Sample Name zhouxiaopeng_ZXP-3_pos
Comment

Acquisition Date 9/7/2018 5:05:23 PM

Operator SCSIO
Instrument maXis



HR-ESIMS for compound 2

Mass Spectrum SmartFormula Report

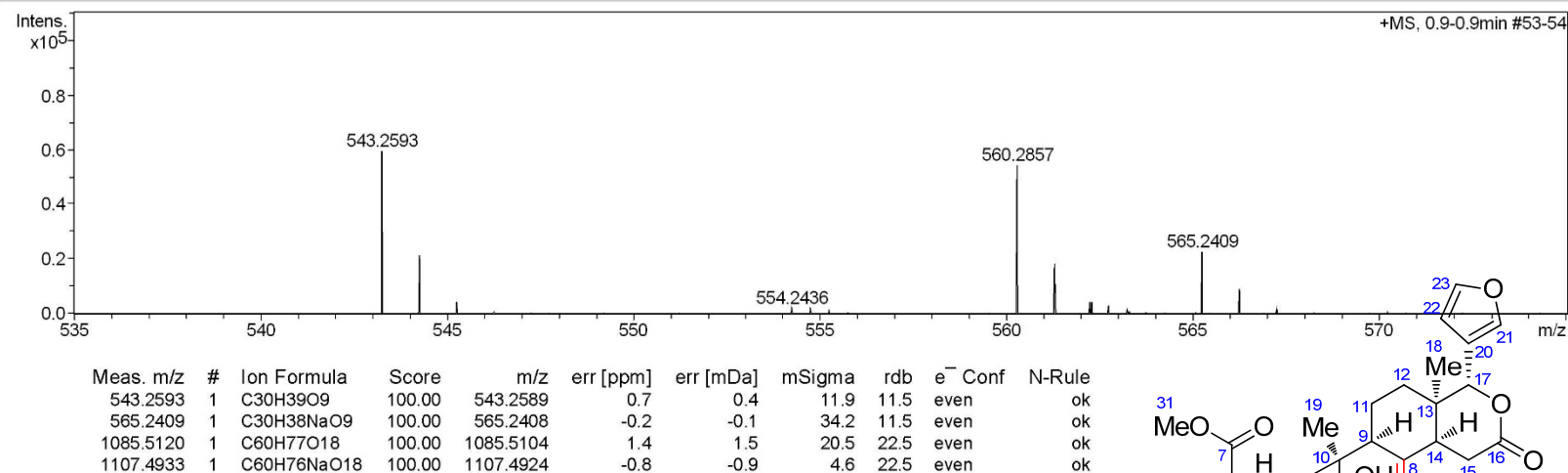
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 Comment

Acquisition Date 9/7/2018 5:05:23 PM
 Operator SCSIO
 Instrument maXis 255552.00029

Acquisition Parameter

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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



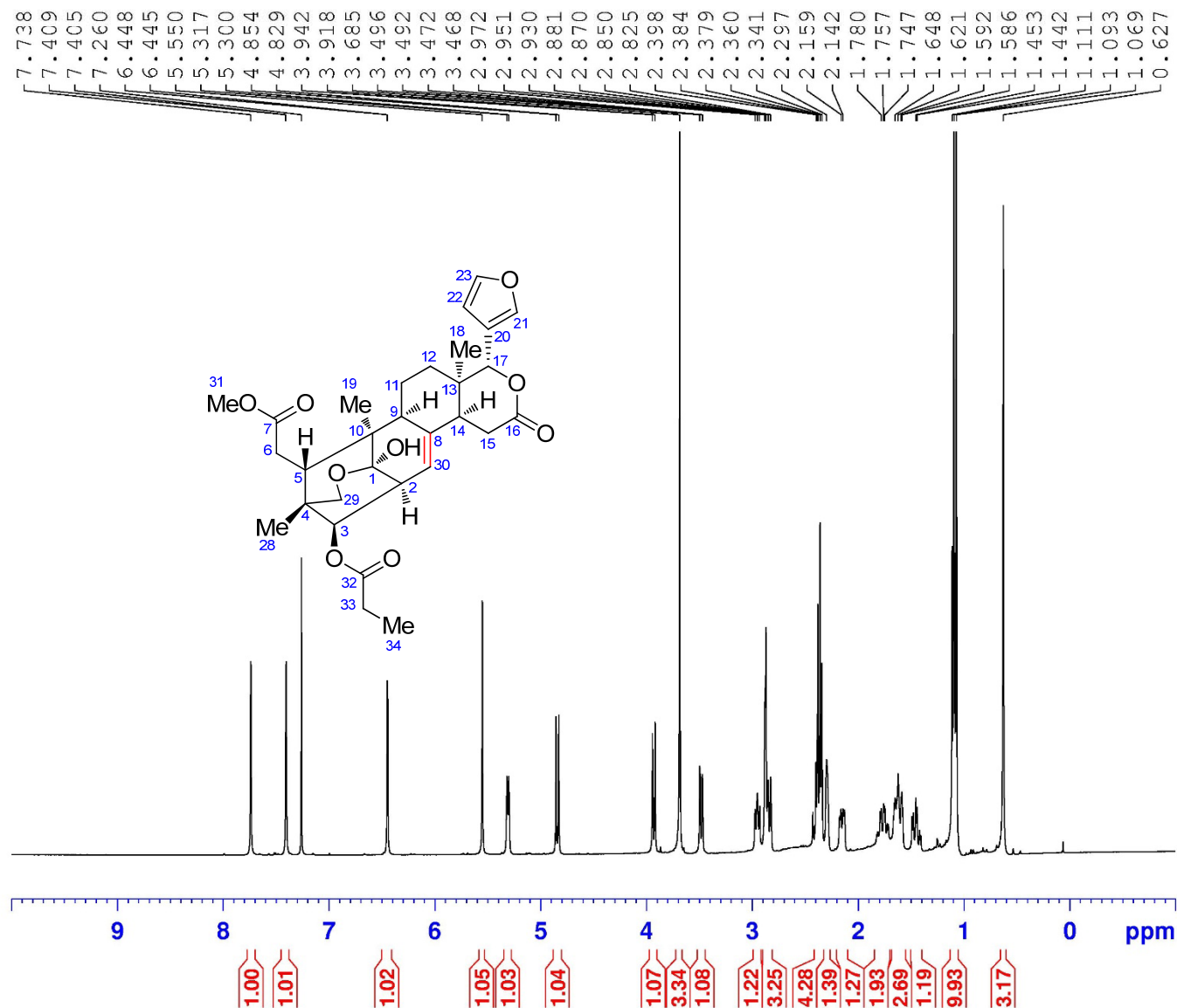
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printed: 9/7/2018 5:08:48 PM

by: SCSIO

Page 1 of 1

^1H NMR (400 MHz) spectrum of compound **2** in CDCl_3

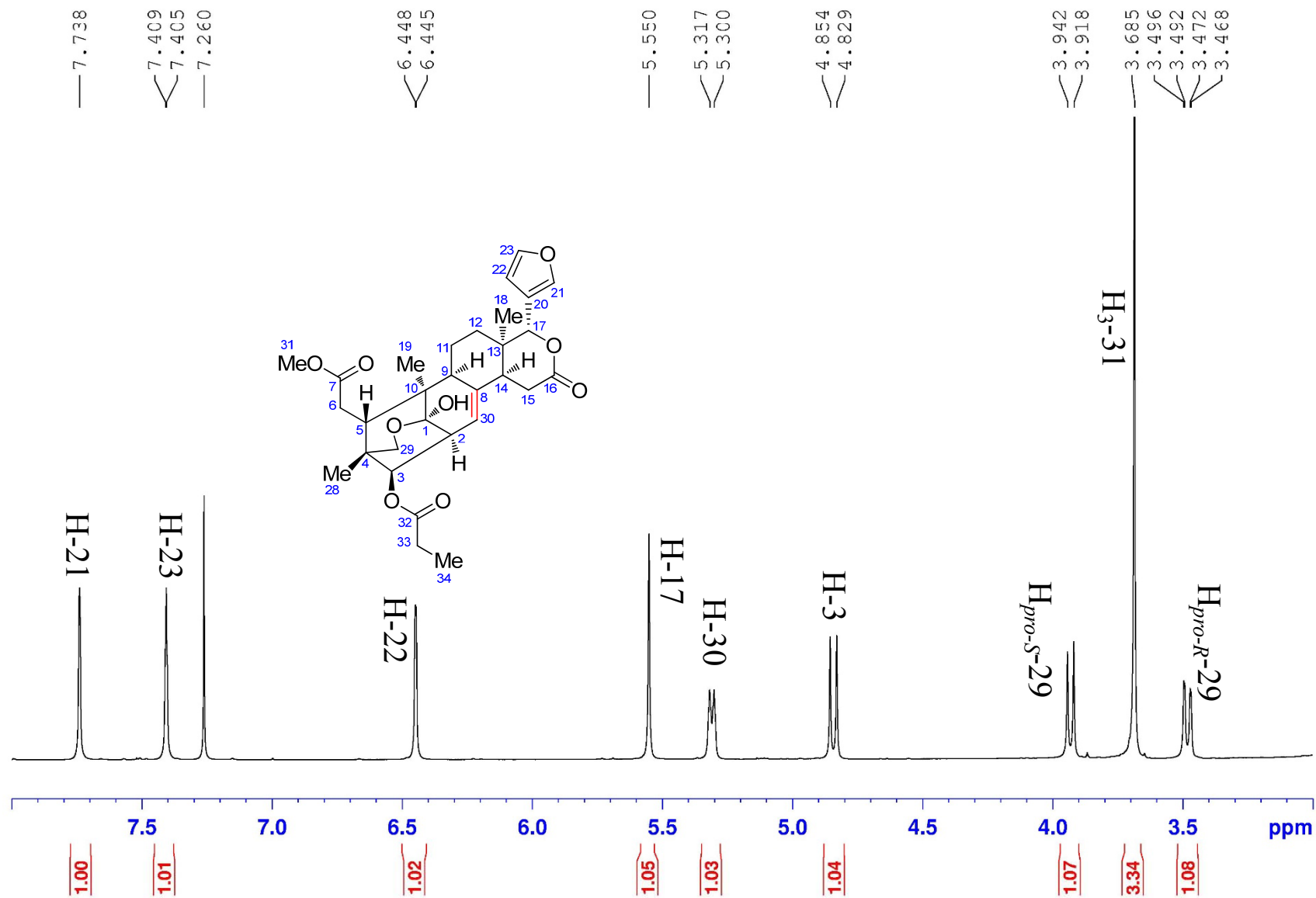


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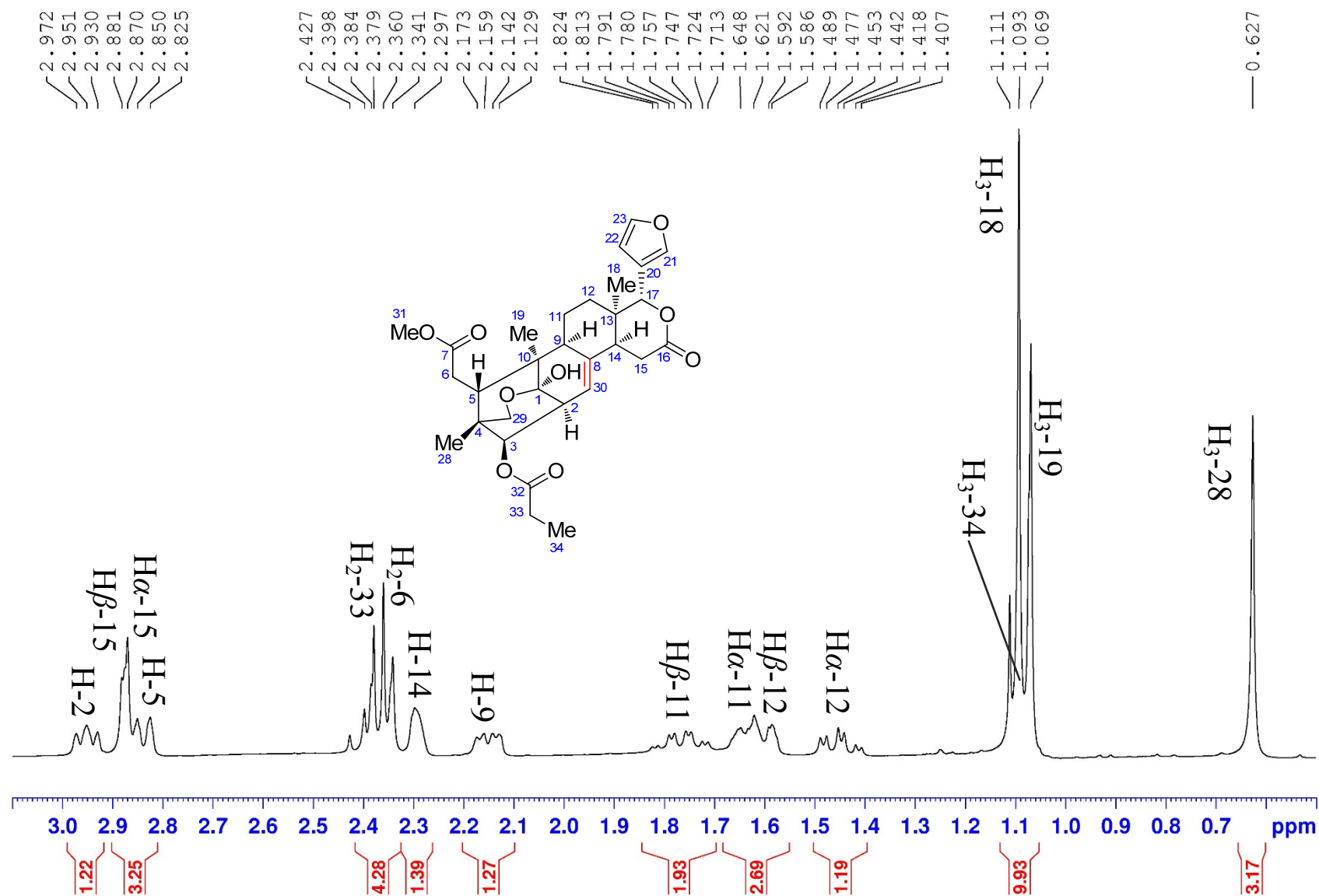
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PROCNO    1
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PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         117.37
DW         60.800 usec
DE         10.00 usec
TE         297.0 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
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NUC1       1H
P1         11.50 usec
SI         65536
SF         400.1300095 MHz
WDW        EM
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LB         0.30 Hz
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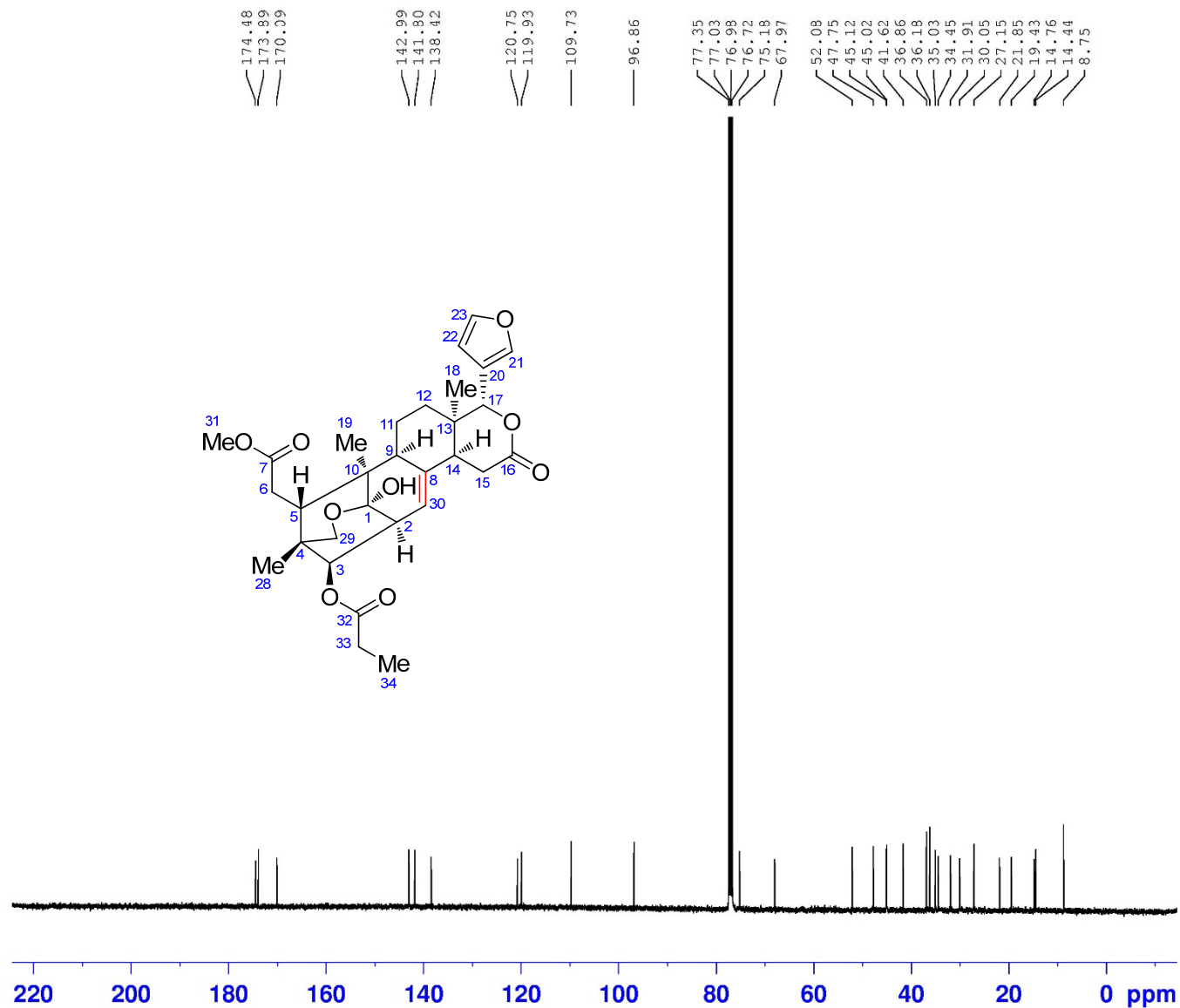
^1H NMR (400 MHz) spectrum of compound **2** in CDCl_3



^1H NMR (400 MHz) spectrum of compound **2** in CDCl_3



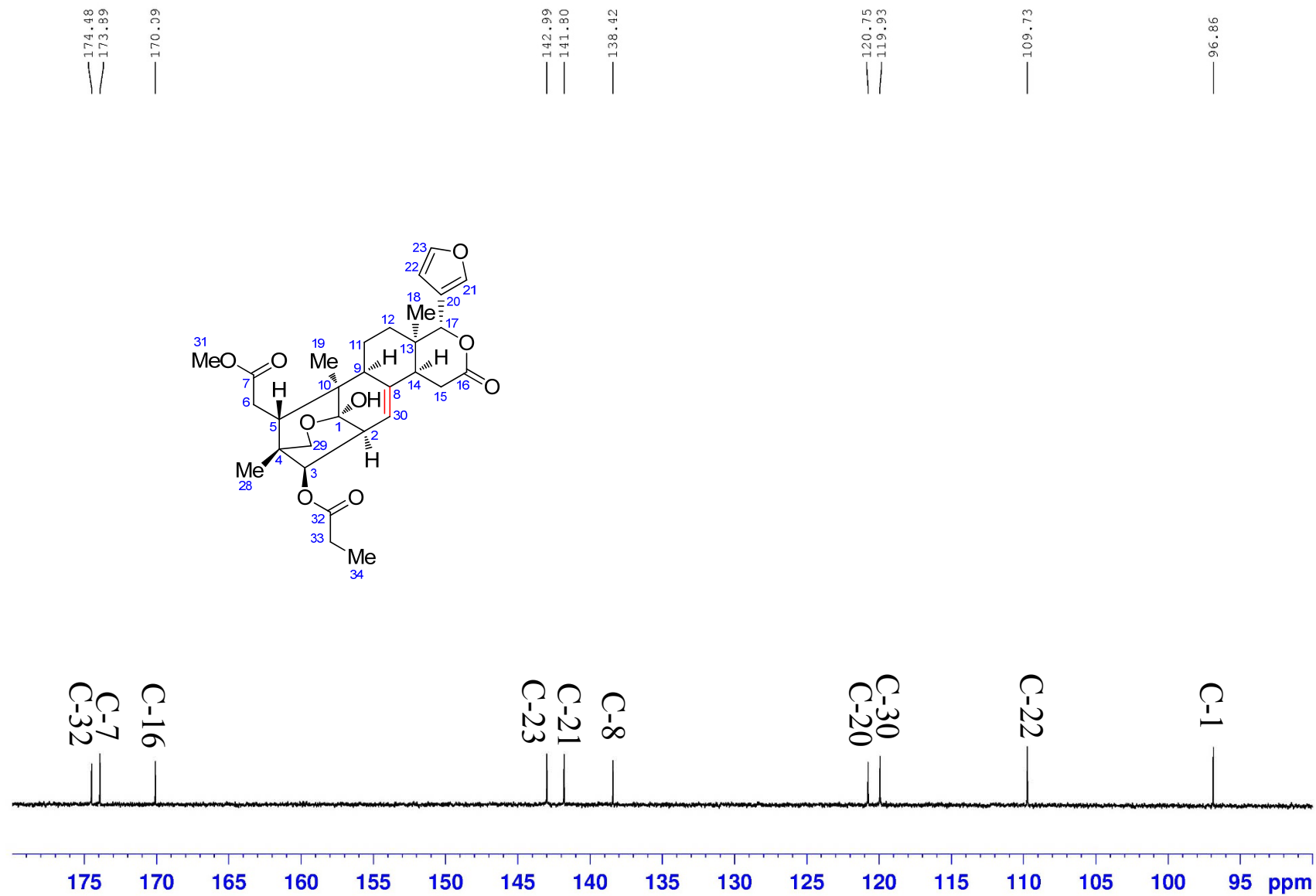
^{13}C NMR (100 MHz) spectrum of compound **2** in CDCl_3



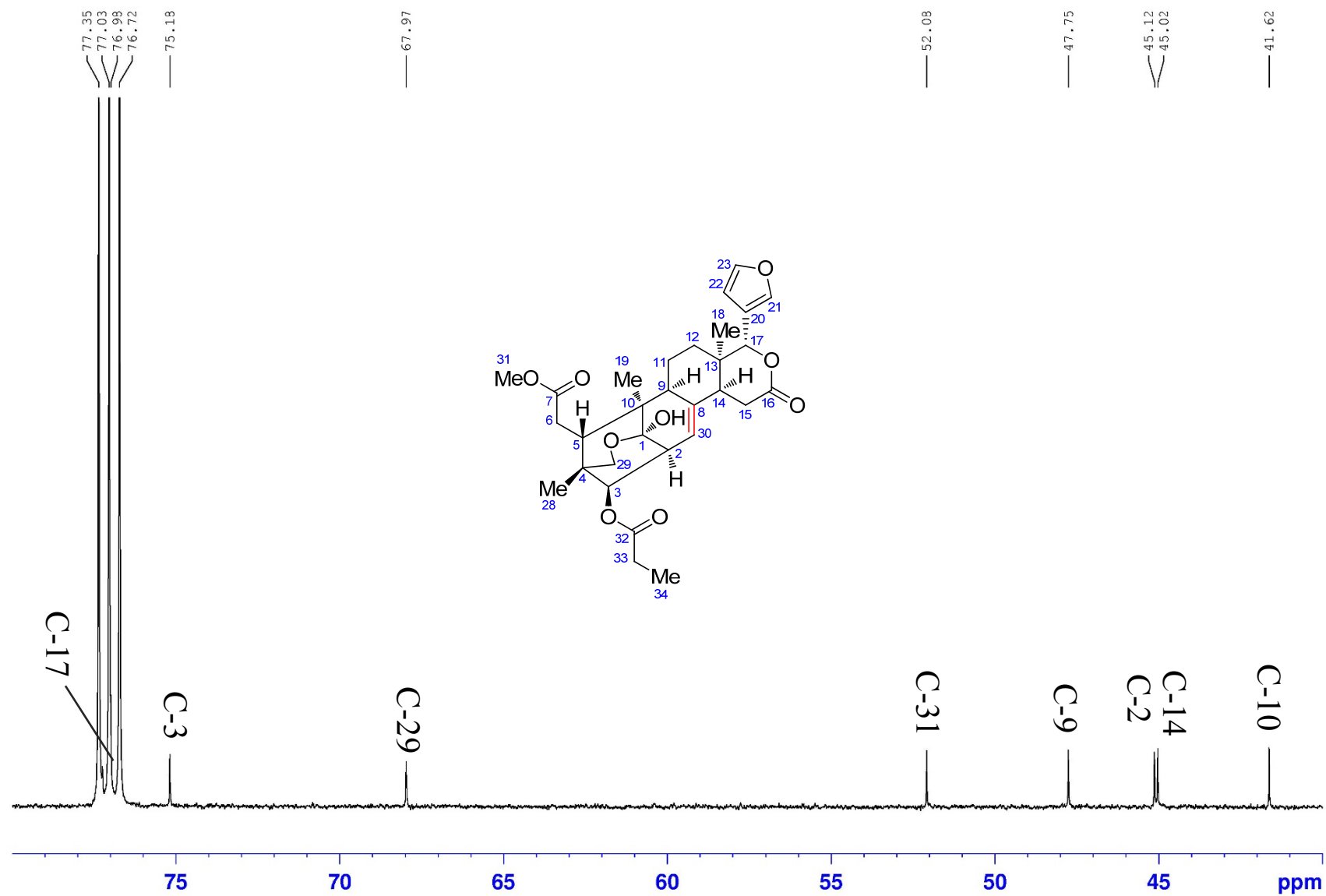
NAME ZXP-R-17-4-2-2-2
 EXPNO 2
 PROCNO 1
 Date_ 20180818
 Time 14.44
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 130.26
 DW 20.800 usec
 DE 18.00 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6233324 MHz
 NUC1 13C
 P1 10.00 usec
 SI 32768
 SF 100.6127692 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

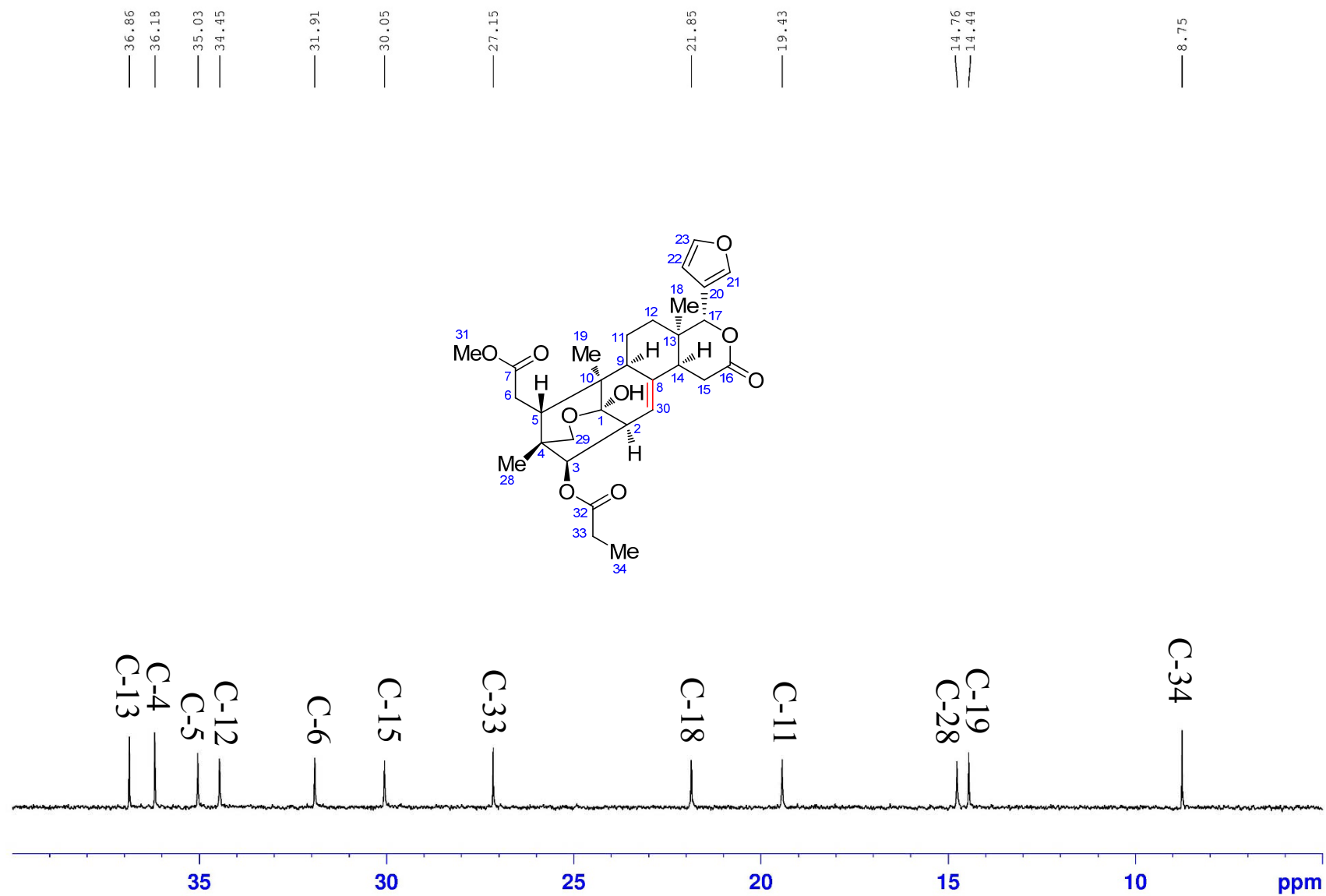
^{13}C NMR (100 MHz) spectrum of compound **2** in CDCl_3



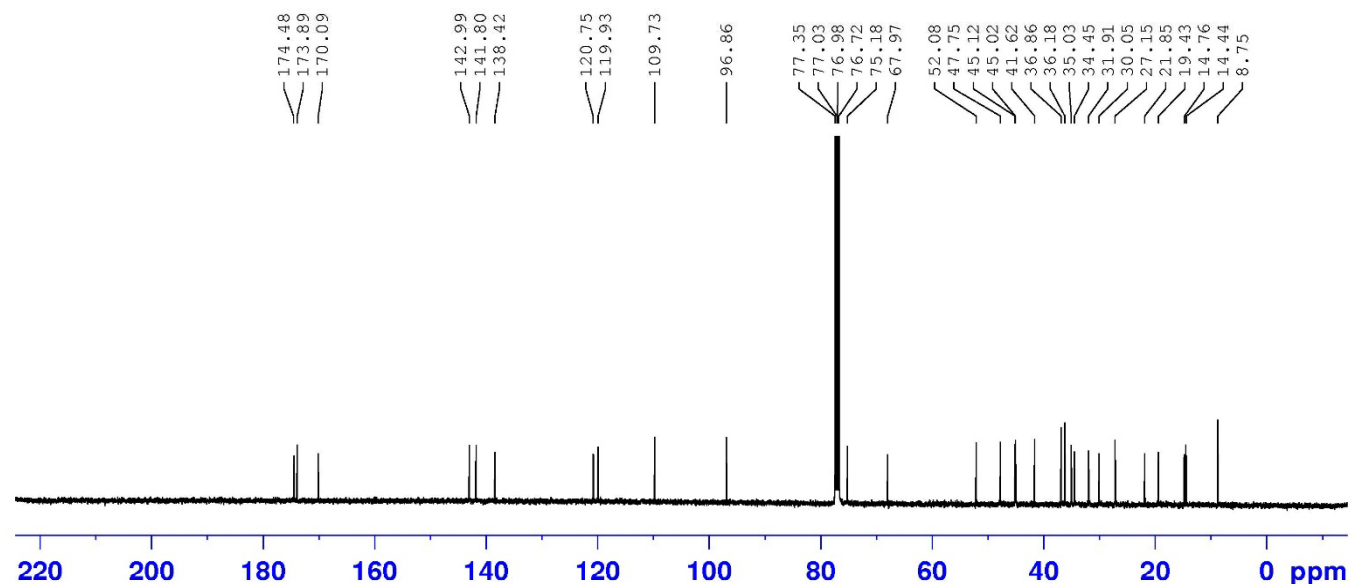
^{13}C NMR (100 MHz) spectrum of compound **2** in CDCl_3



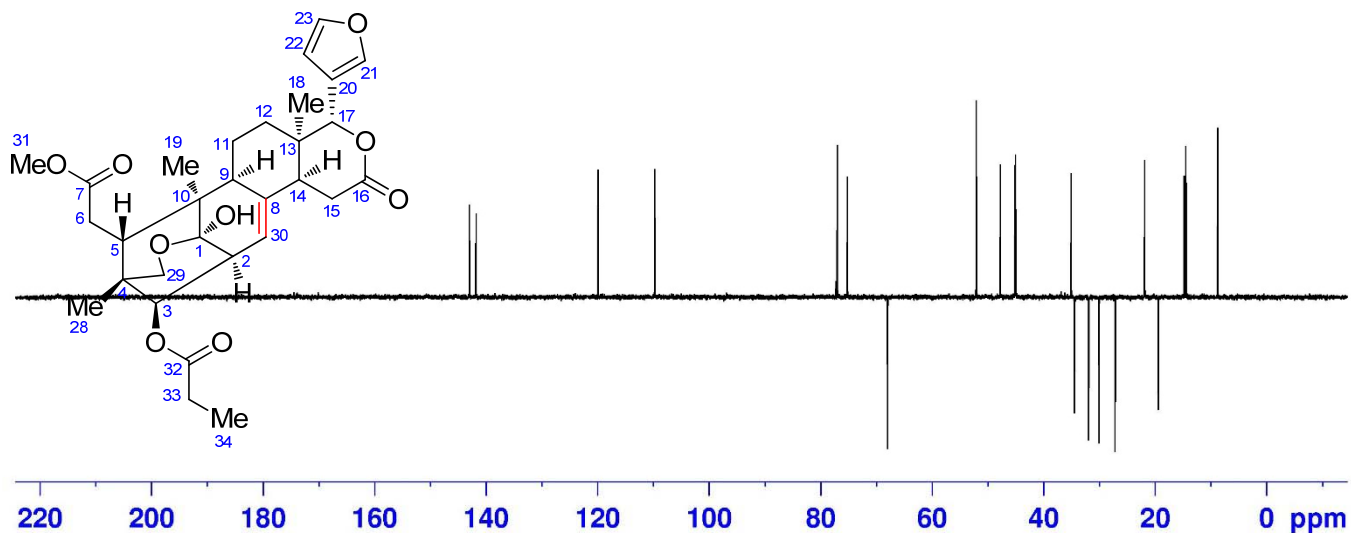
^{13}C NMR (100 MHz) spectrum of compound **2** in CDCl_3



DEPT135 (100 MHz) spectrum of compound **2** in CDCl₃

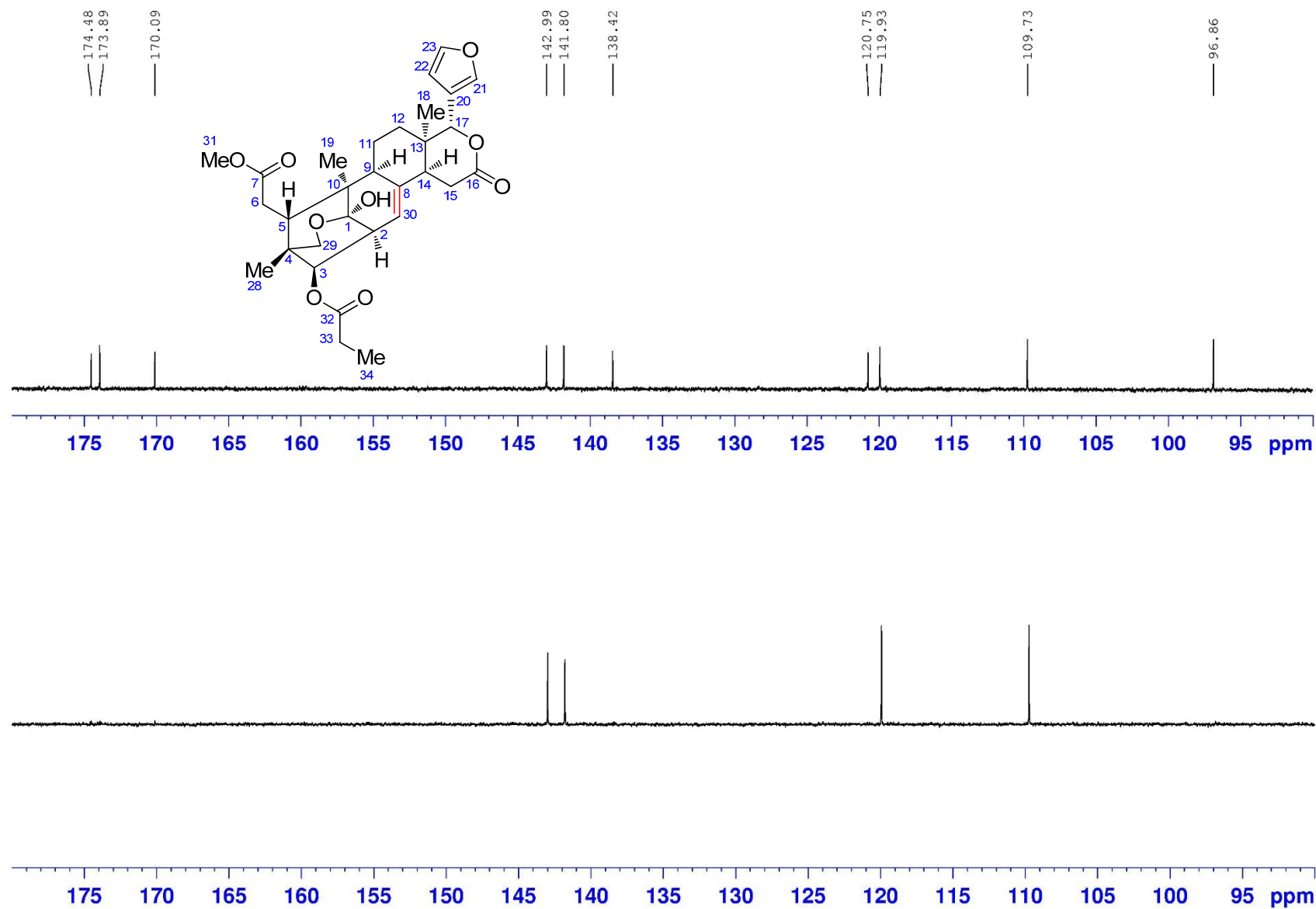


NAME 7XP-R-17-4-2-2-2
 EXPNO 2
 PROCNO 1
 Date_ 20180818
 Time 14.44
 INSTRUM spect
 PROBHD 5 mm CPMBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 130.26
 DW 20.800 usec
 DE 18.00 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

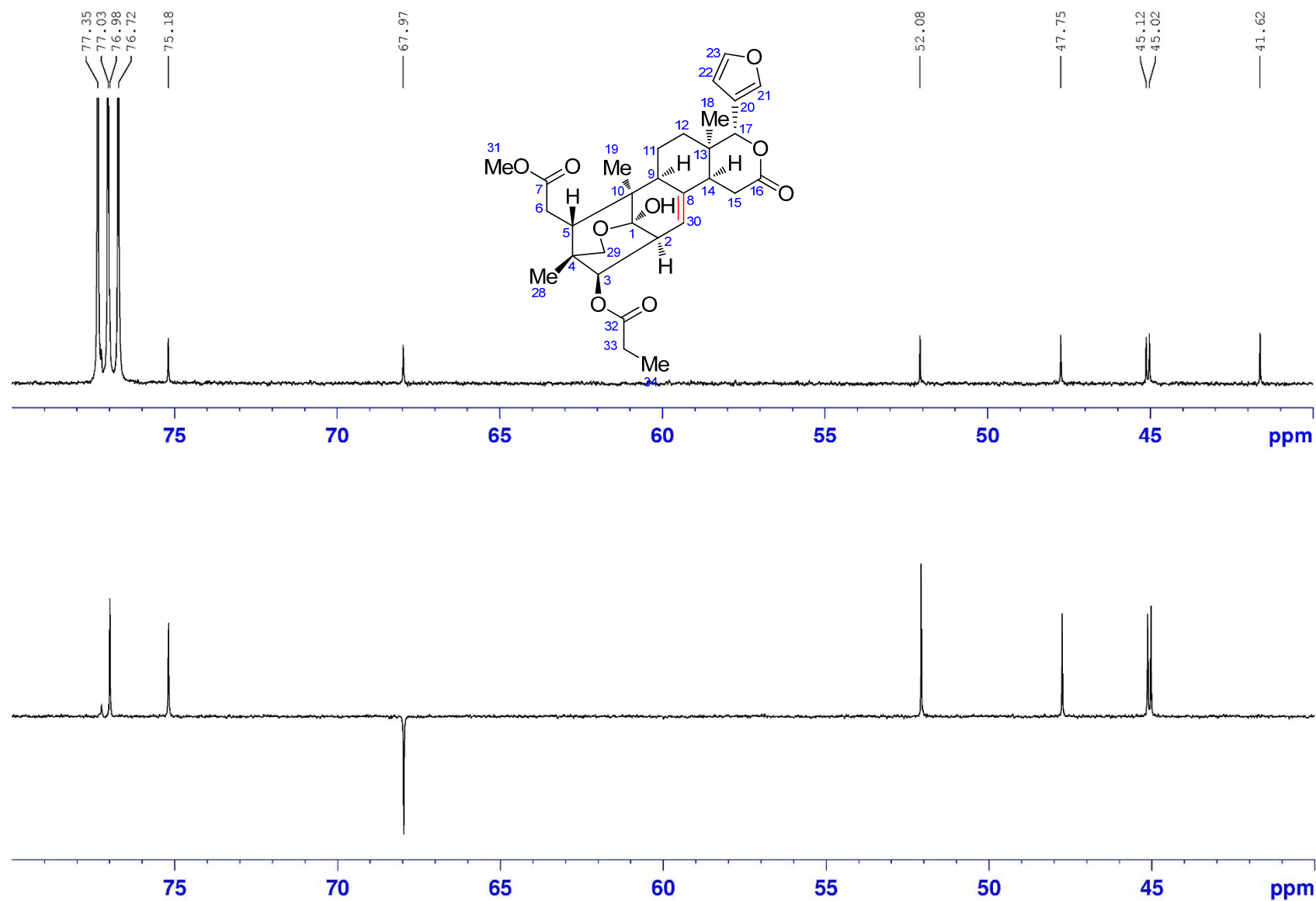


===== CHANNEL f1 =====
 SFO1 100.6233324 MHz
 NUC1 13C
 P1 10.00 usec
 SI 32768
 SF 100.6127692 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

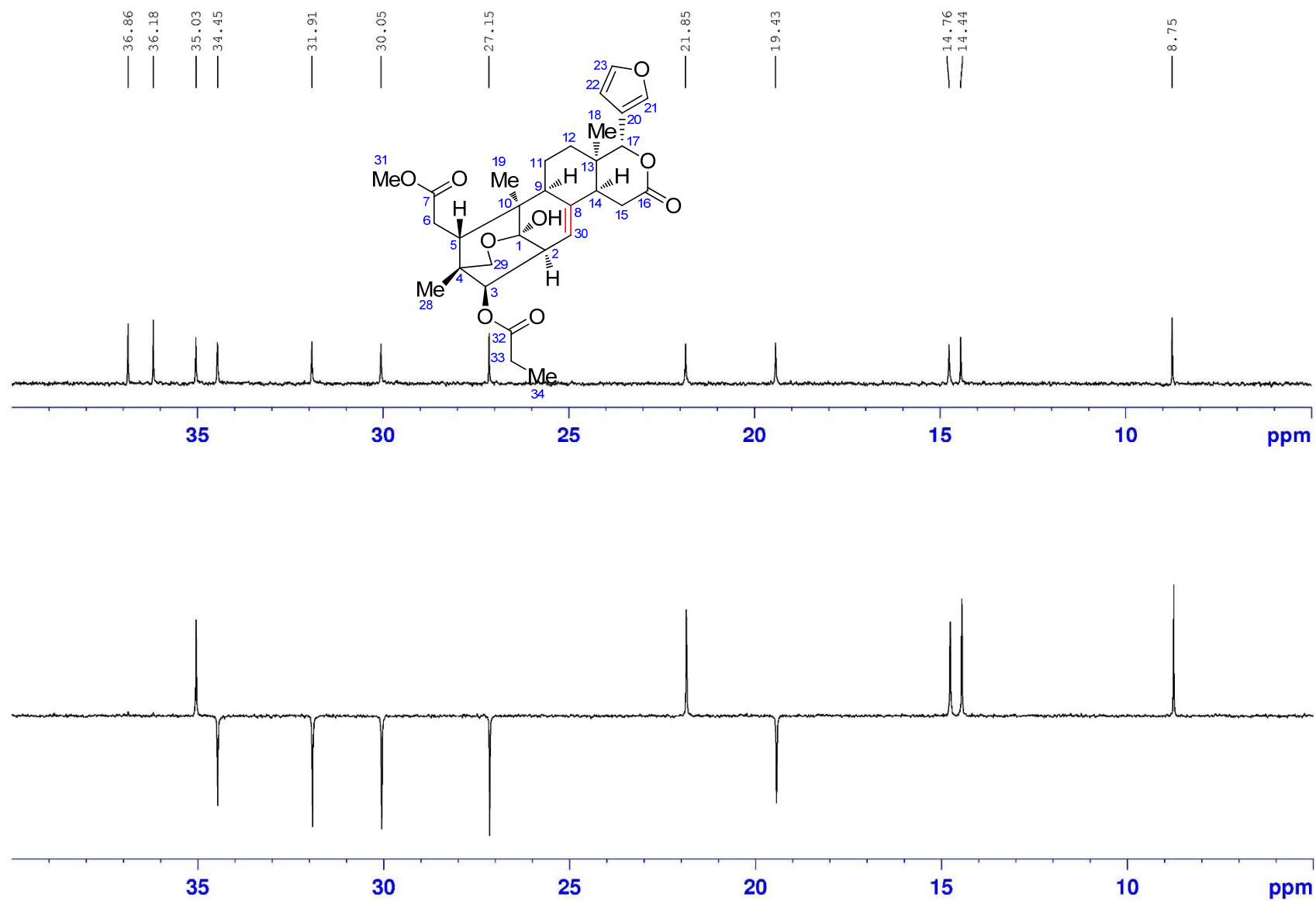
DEPT135 (100 MHz) spectrum of compound **2** in CDCl₃



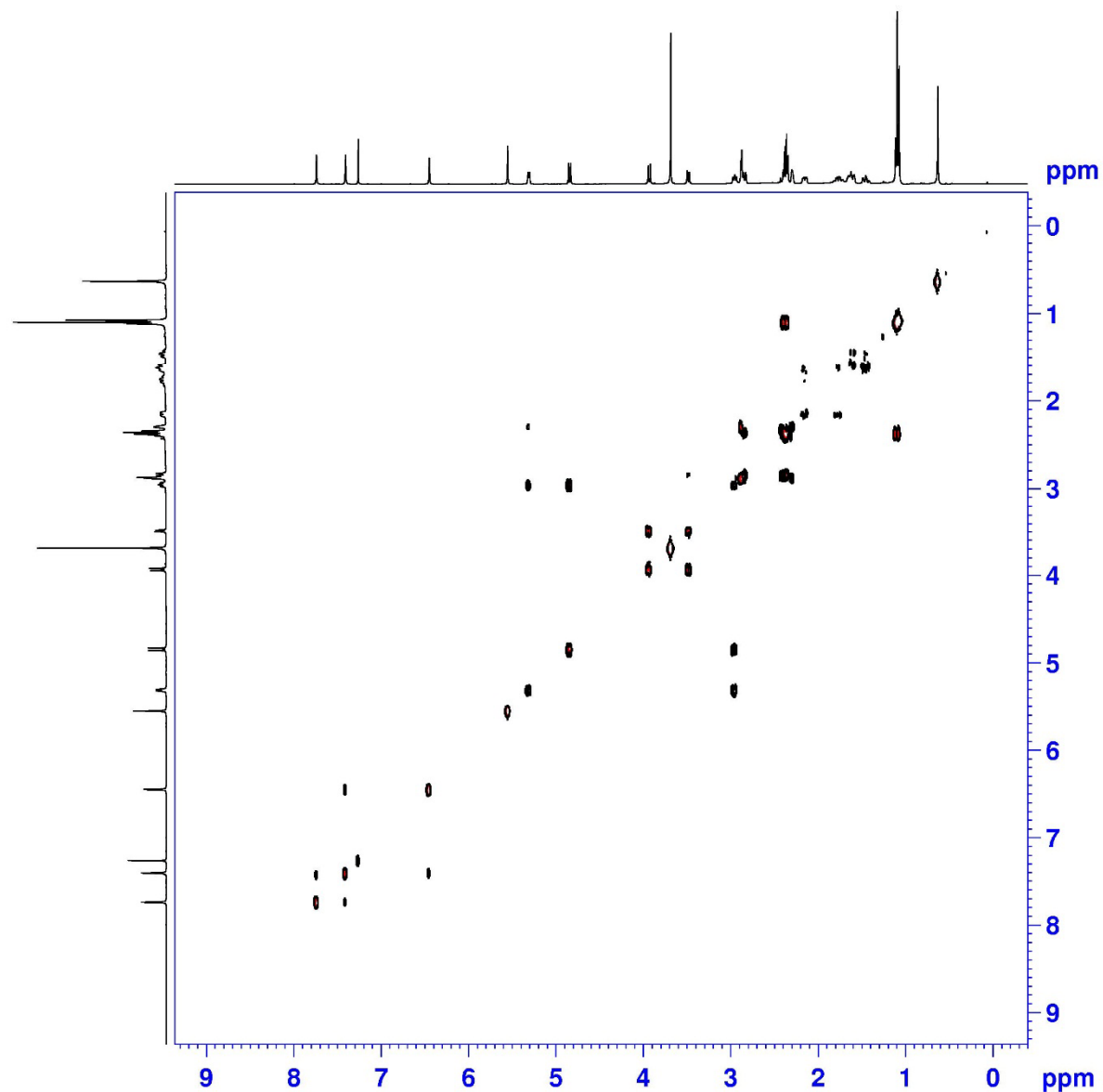
DEPT135 (100 MHz) spectrum of compound **2** in CDCl₃



DEPT135 (100 MHz) spectrum of compound **2** in CDCl₃



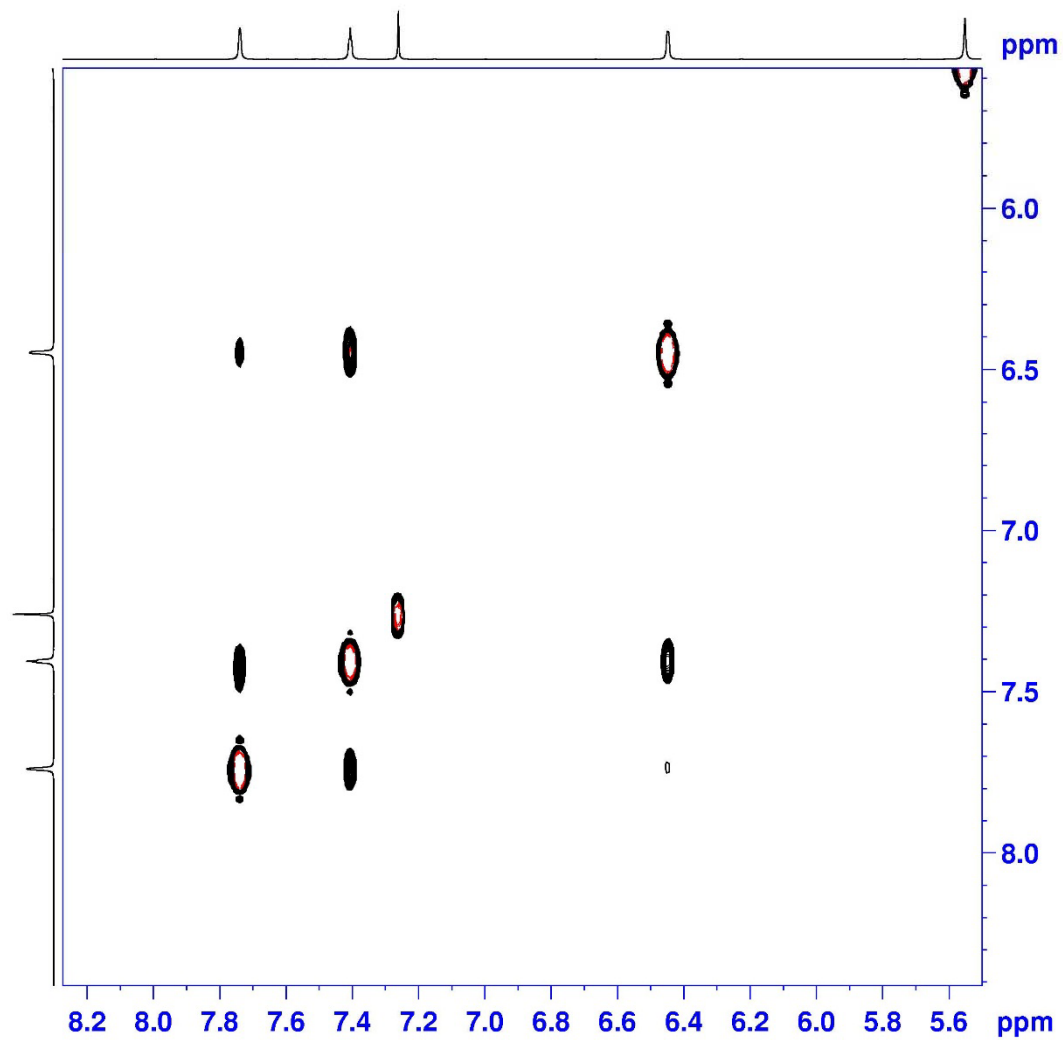
^1H - ^1H COSY (400 MHz) spectrum of compound **2** in CDCl_3



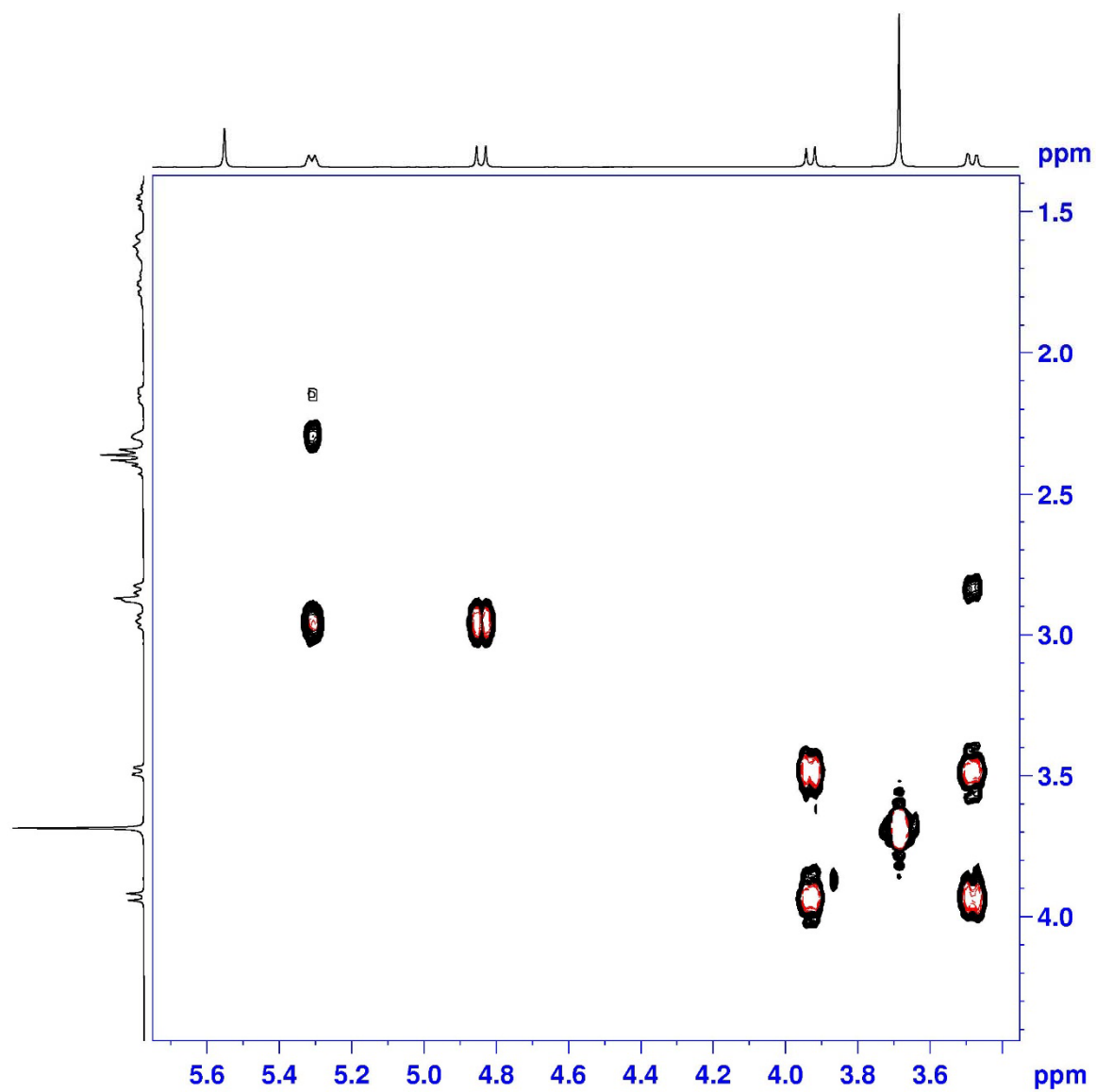
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NAME      ZXP-R-17-4-2-2-2
EXPNO     4
PROCNO    1
Date_     20180821
Time      4.42
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   cosygpppqf
TD        2048
SOLVENT   CDC13
NS        8
DS        8
SWH       3906.250 Hz
FIDRES    1.907349 Hz
AQ        0.2621940 sec
RG        147.94
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 =====
SF01    400.1318006 MHz
NUC1     1H
P0       11.50 usec
P1       11.50 usec
P17      2500.00 usec
ND0      1
TD       128
SF01    400.1318 MHz
FIDRES   30.517578 Hz
SW       9.762 ppm
FMODE    QF
SI       1024
SF       400.1300076 MHz
WDW      QSINE
SSB      0
LB       0.00 Hz
GB       0
PC       1.40
SI       1024
MC2      QF
SF       400.1300060 MHz
WDW      QSINE
SSB      0
LB       0.00 Hz
GB       0
```

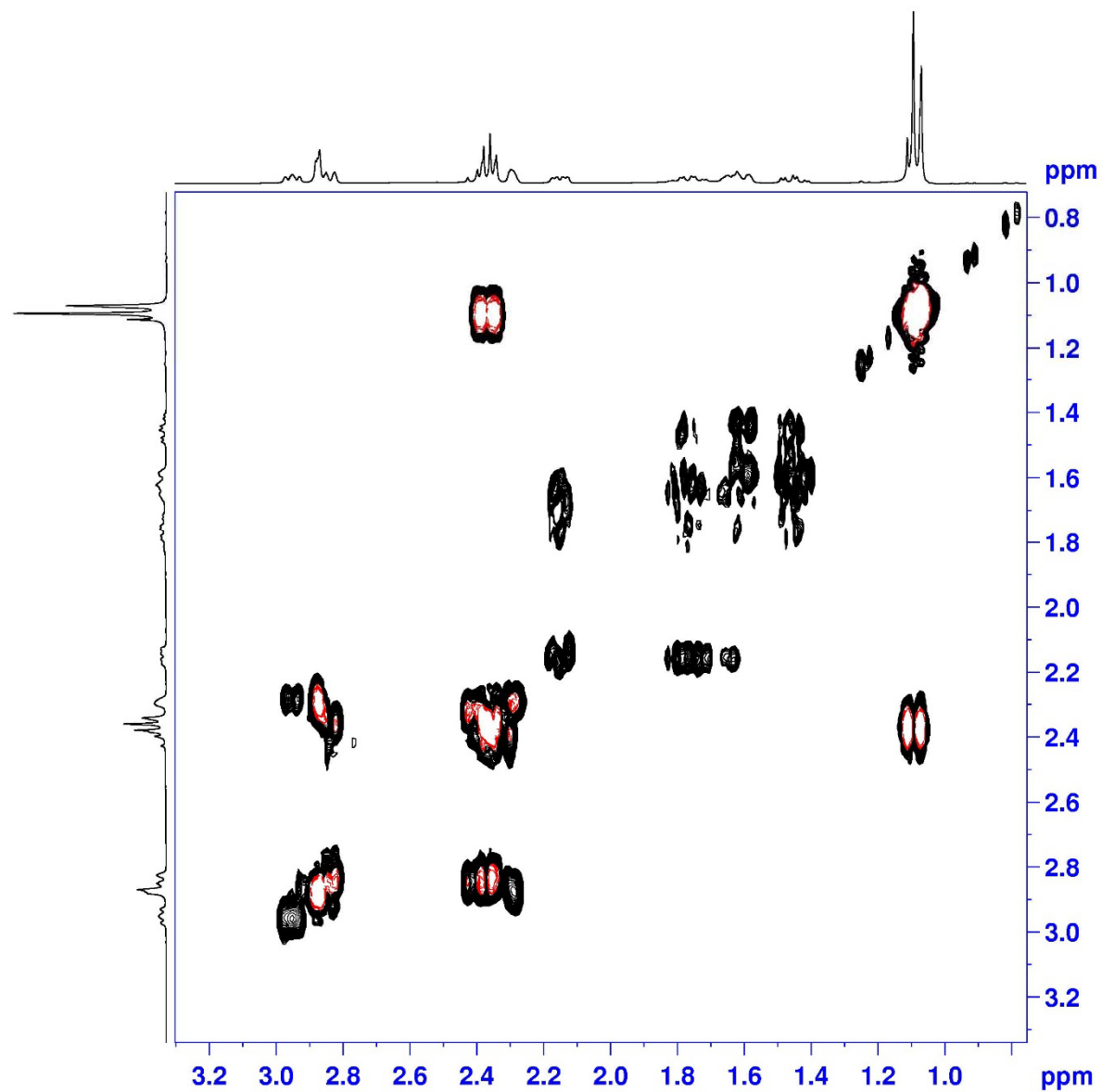
^1H - ^1H COSY (400 MHz) spectrum of compound **2** in CDCl_3



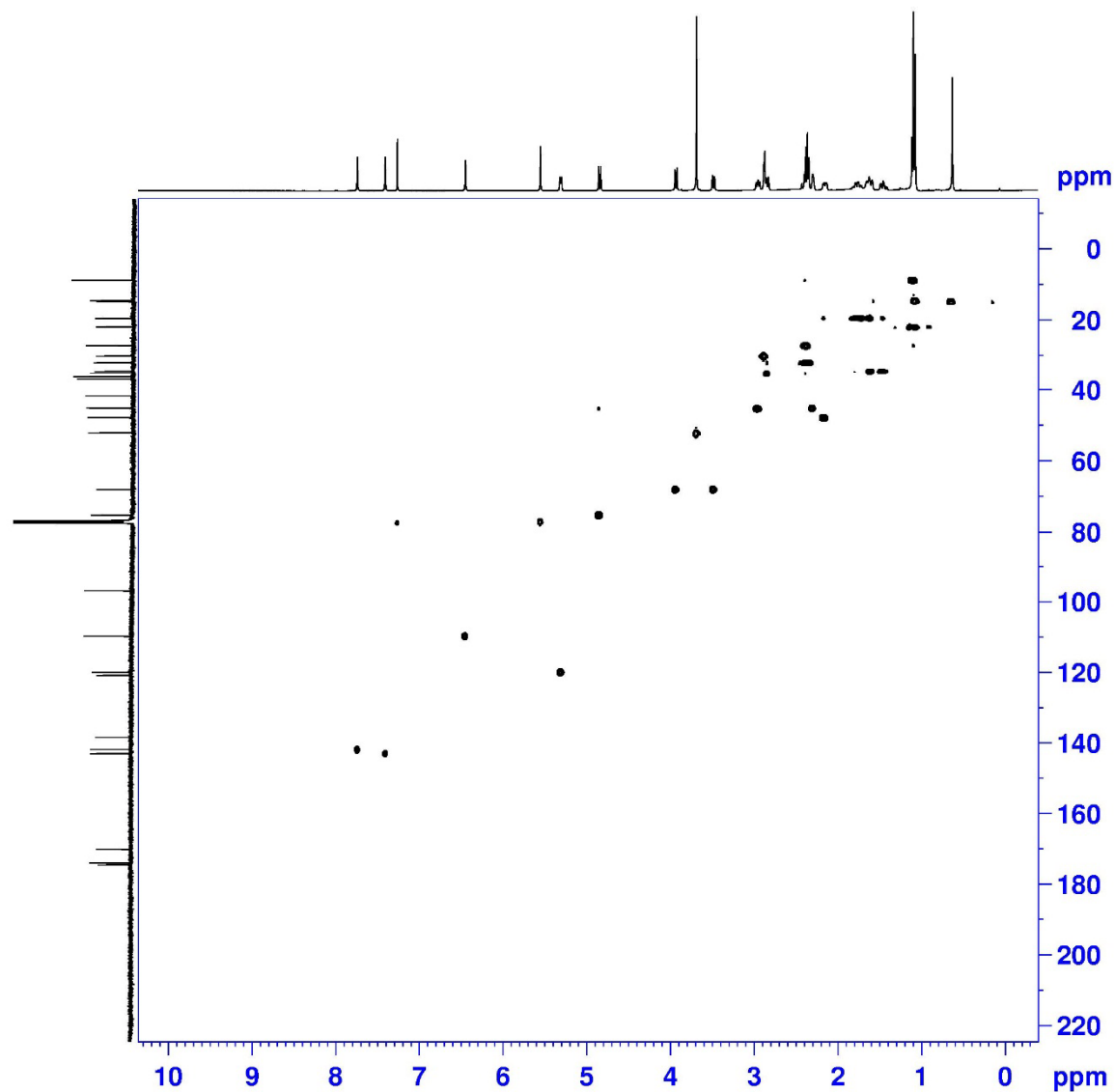
^1H - ^1H COSY (400 MHz) spectrum of compound **2** in CDCl_3



^1H - ^1H COSY (400 MHz) spectrum of compound **2** in CDCl_3



HSQC (400 MHz) spectrum of compound **2** in CDCl₃

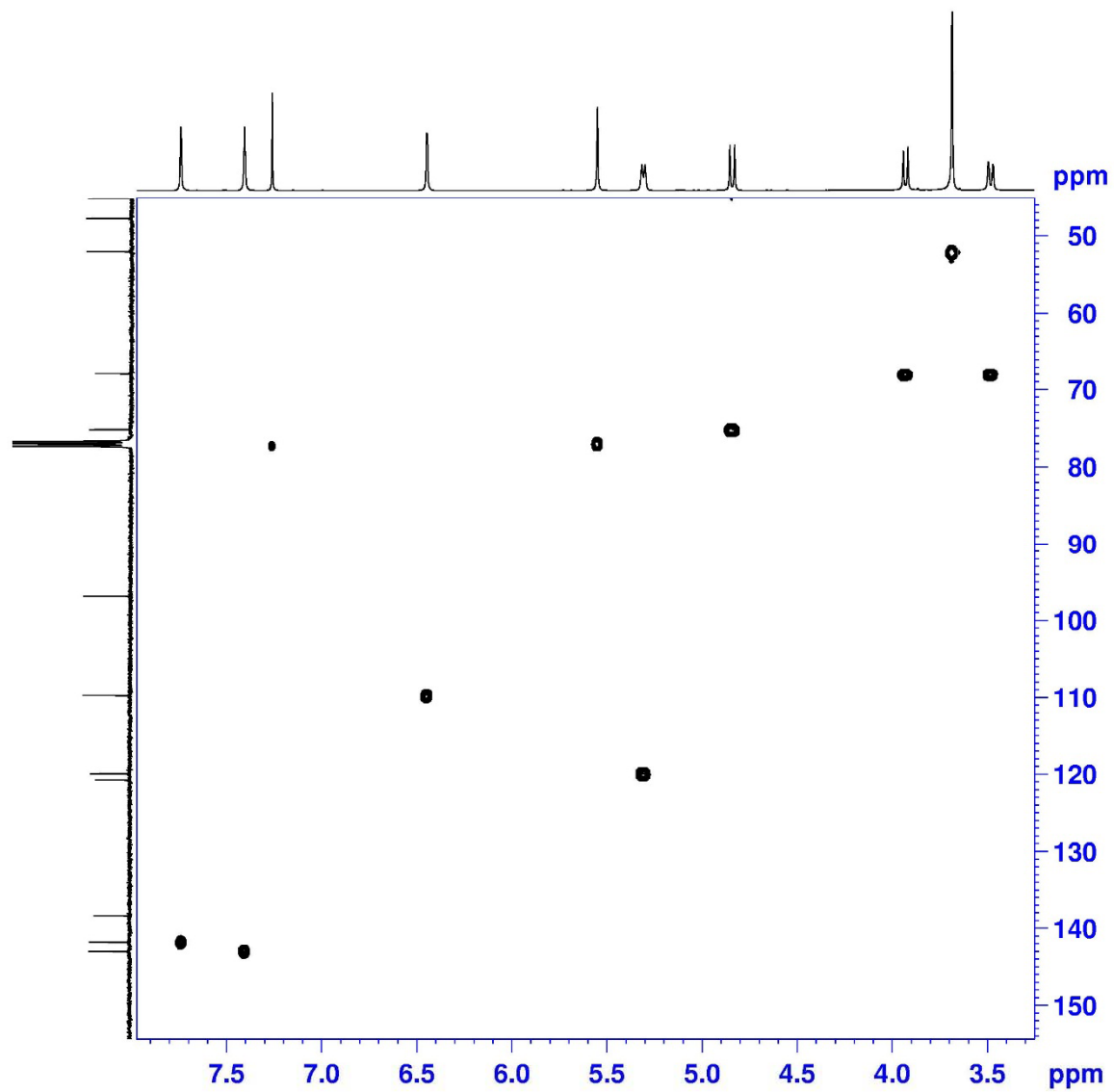


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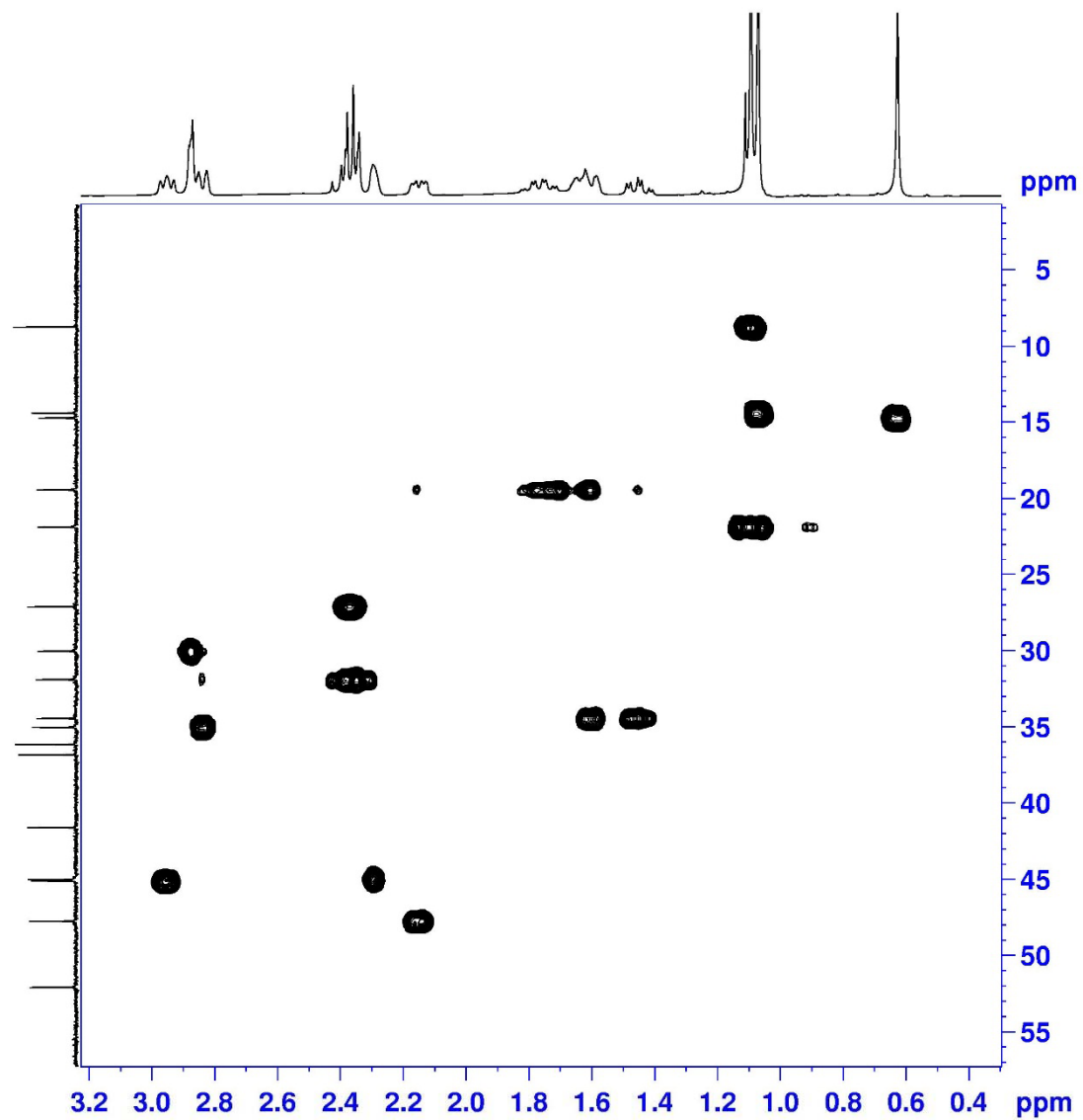
NAME      ZXP-R-17-4-2-2-2
EXPNO     5
PROCNO    1
Date_     20180821
Time      5.21
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   hsqcetgps12
TD        1024
SOLVENT   CDCl3
NS        16
DS        16
SWH       4302.926 Hz
FIDRES    4.202076 Hz
AQ        0.1190388 sec
RG        208.5
DW        116.200 usec
DE        10.00 usec
TE        297.0 K
CNST2     145.0000000
D0        0.00000300 sec
D1        1.46497905 sec
D4        0.00172414 sec
D11       0.03000000 sec
D16       0.00020000 sec
D24       0.00086207 sec
IN0       0.00002080 sec
ZGPTINS

===== CHANNEL f1 =====
SFO1      400.1320007 MHz
NUC1      1H
P1        11.50 usec
P2        23.00 usec
P28       0.00 usec
ND0       2
TD        256
SFO1      100.6233 MHz
FIDRES    93.900238 Hz
SW        238.896 ppm
FnMODE    Echo-Antiecho
SI        1024
SF        400.1300074 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
PC        1.40
SI        1024
MC2       echo-antiecho
SF        100.6127538 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
    
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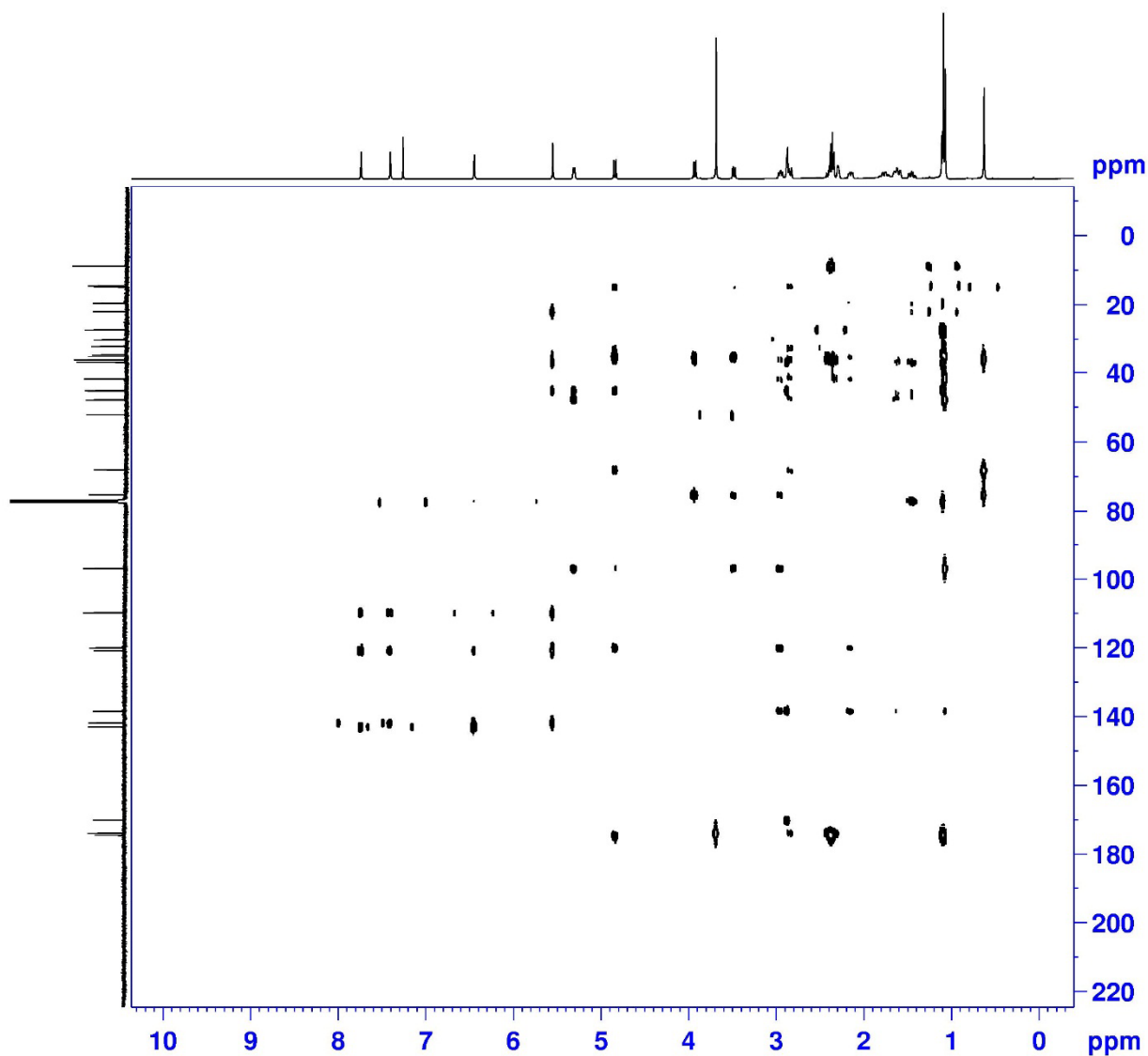
HSQC (400 MHz) spectrum of compound **2** in CDCl₃



HSQC (400 MHz) spectrum of compound **2** in CDCl₃



HMBC (400 MHz) spectrum of compound **2** in CDCl₃



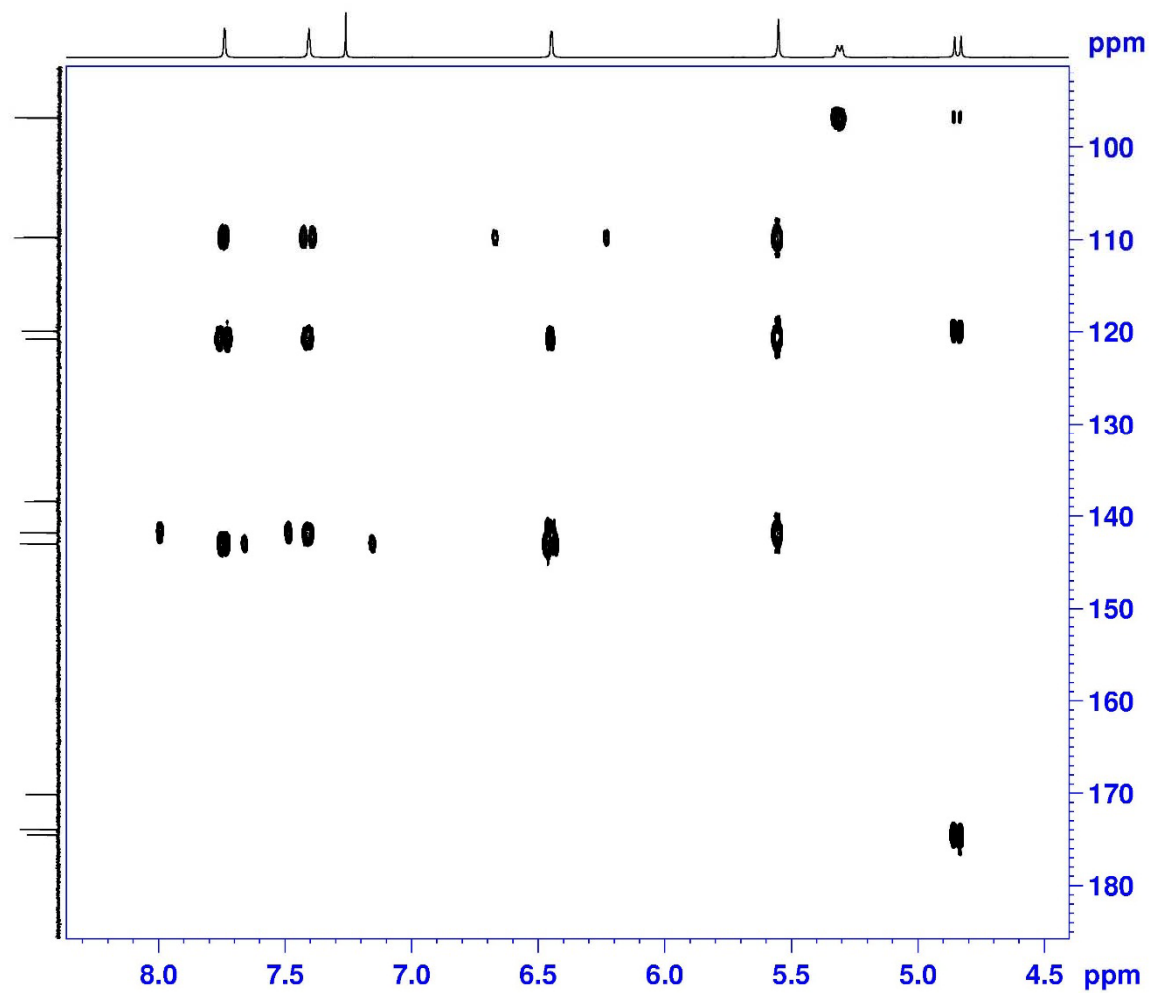
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NAME      ZXP-R-17-4-2-2-2
EXPNO     6
PROCNO    1
Date_     20180821
Time      7.13
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   hmbcgp1pndqf
TD         4096
SOLVENT   CDCl3
NS         32
DS         16
SWH        5197.505 Hz
FIDRES     1.268922 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
    
```

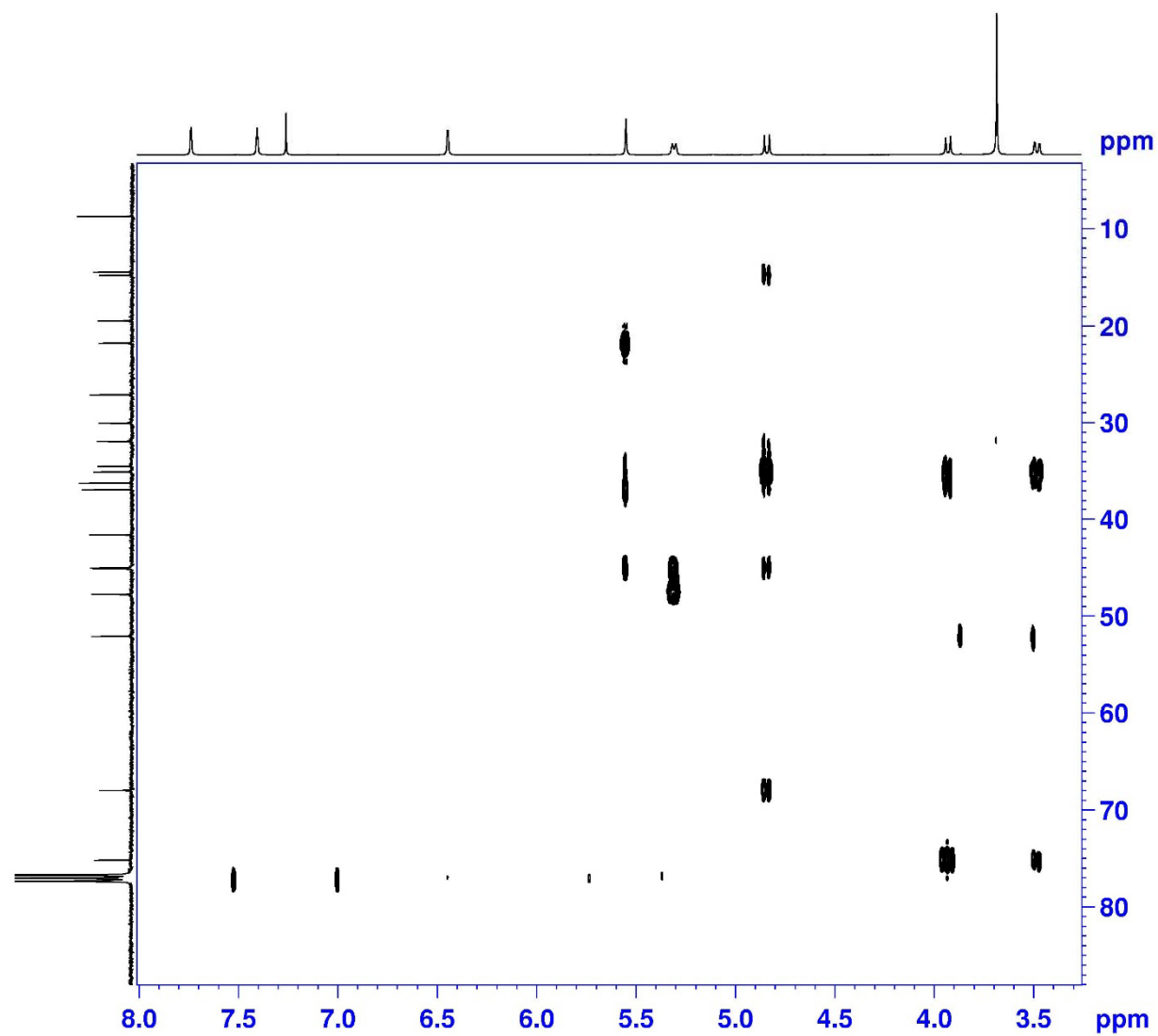
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===== CHANNEL f1 =====
SF01      400.1323208 MHz
NUC1       1H
P1         11.50 usec
P2         23.00 usec
ND0        2
TD         119
SF01      100.6233 MHz
FIDRES     202.003876 Hz
SW         238.896 ppm
FnMODE     QF
SI         2048
SF         400.1300072 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40
SI         1024
MC2        QF
SF         100.6127637 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
    
```

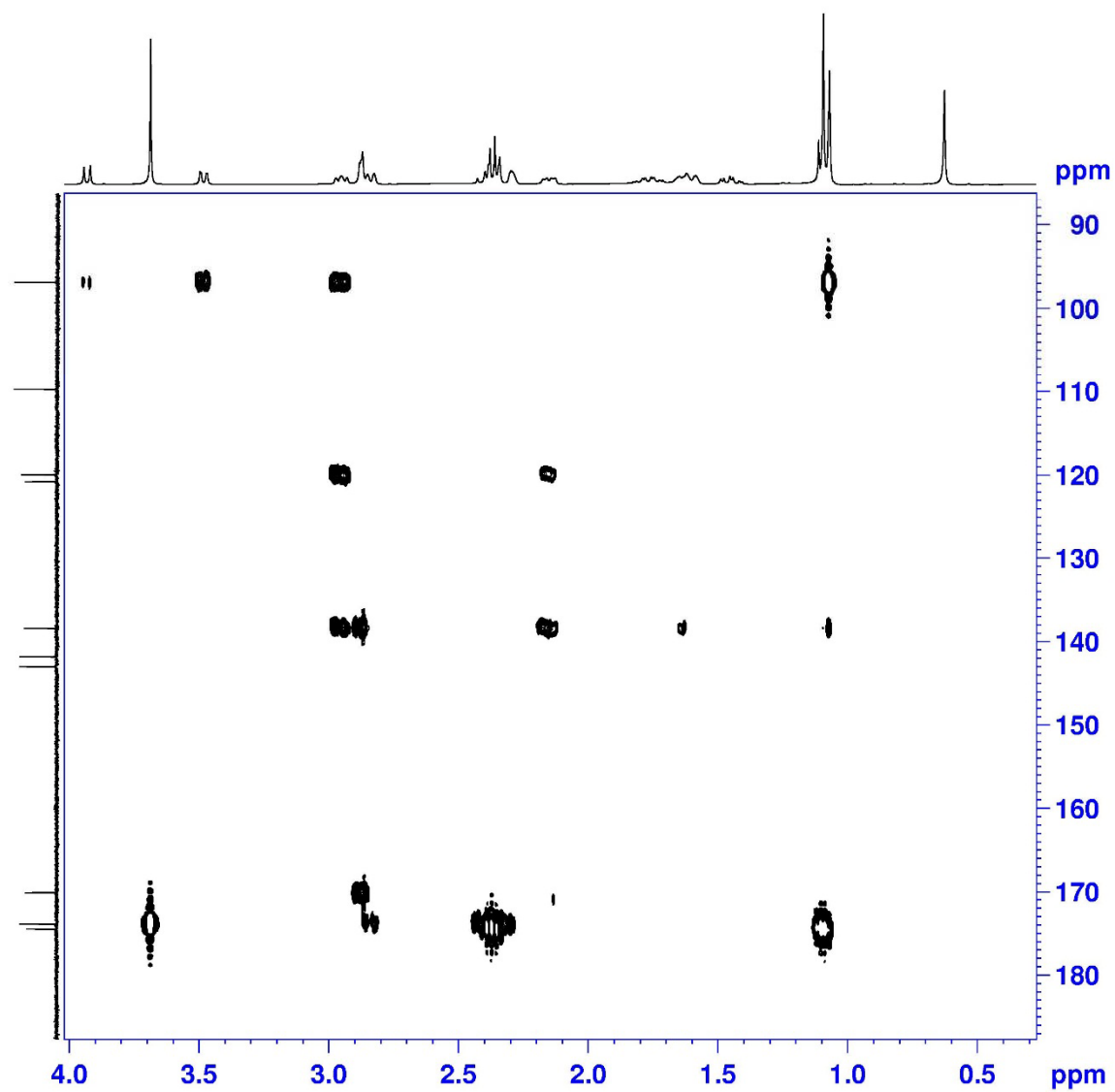

HMBC (400 MHz) spectrum of compound **2** in CDCl_3



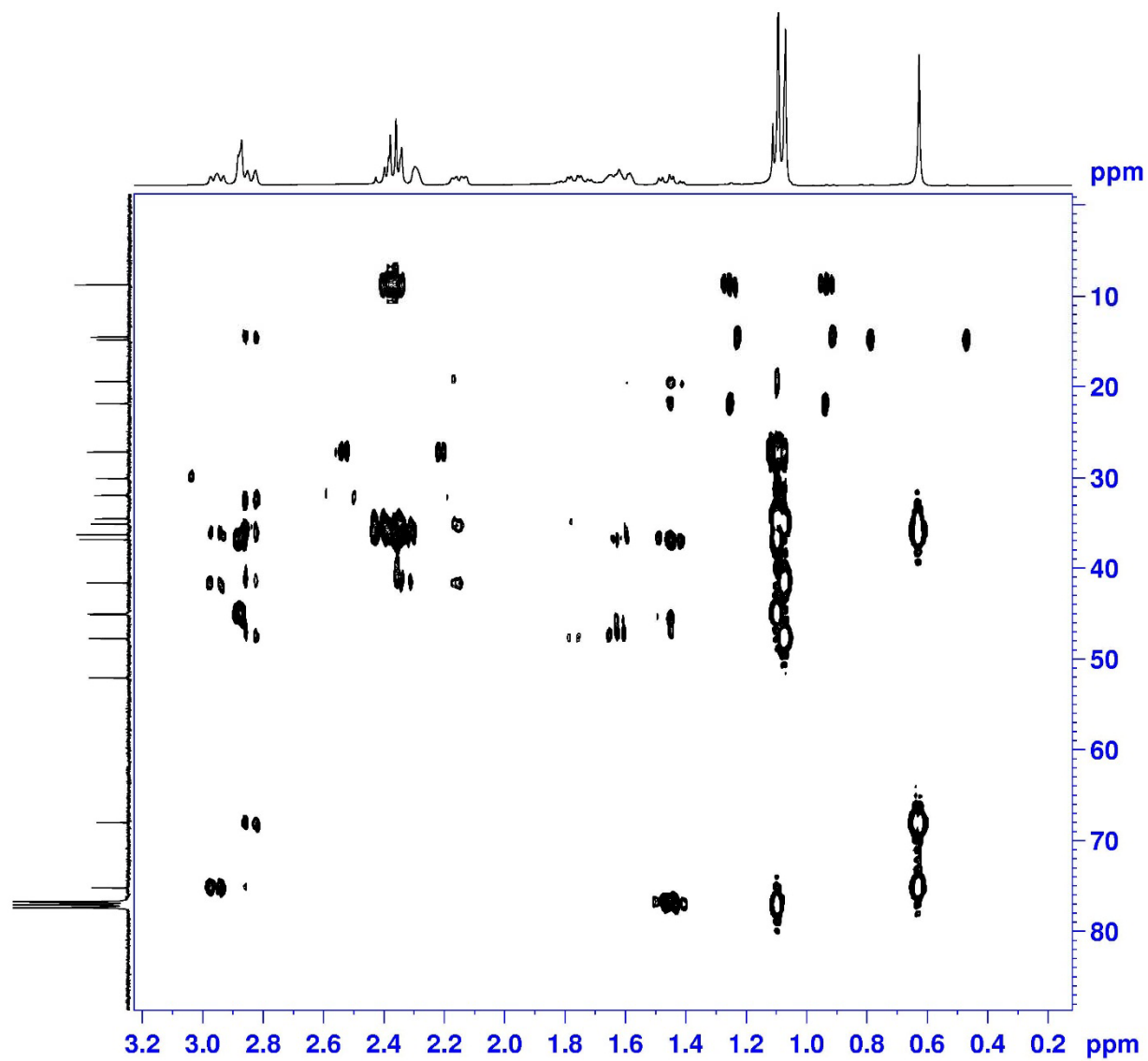
HMBC (400 MHz) spectrum of compound **2** in CDCl₃



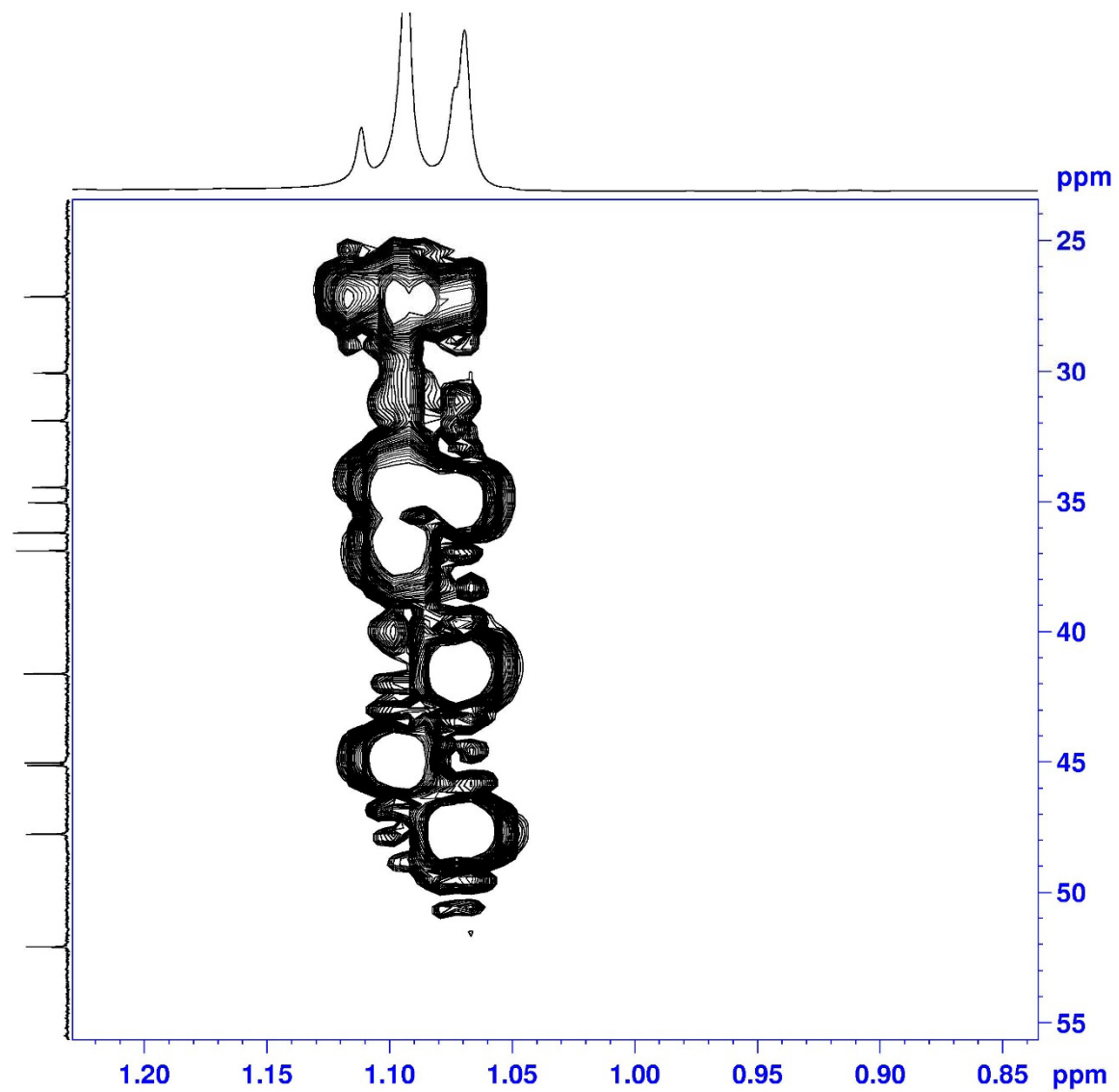
HMBC (400 MHz) spectrum of compound **2** in CDCl₃



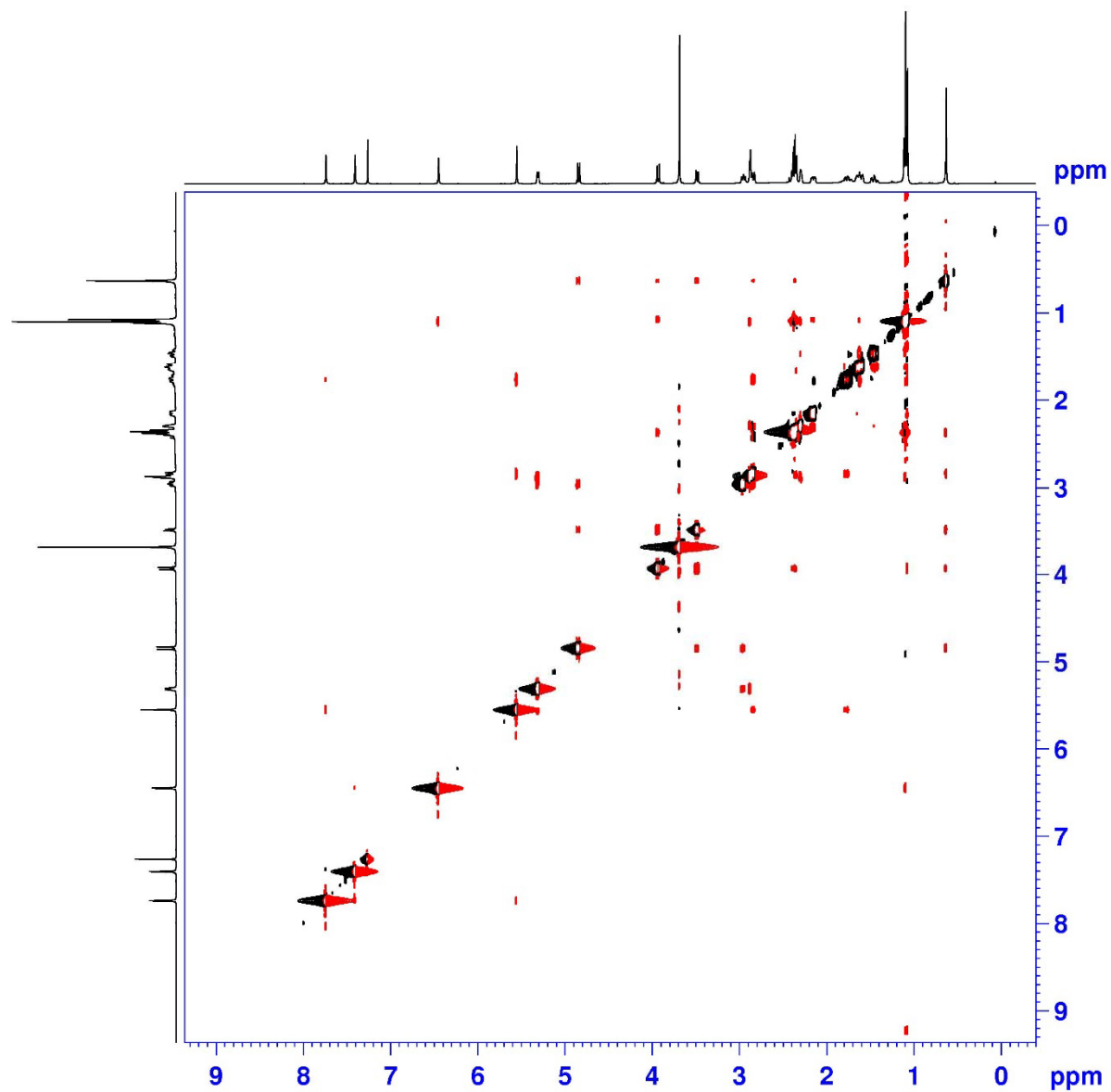
HMBC (400 MHz) spectrum of compound **2** in CDCl₃



HMBC (400 MHz) spectrum of compound **2** in CDCl₃



NOESY (400 MHz) spectrum of compound **2** in CDCl₃



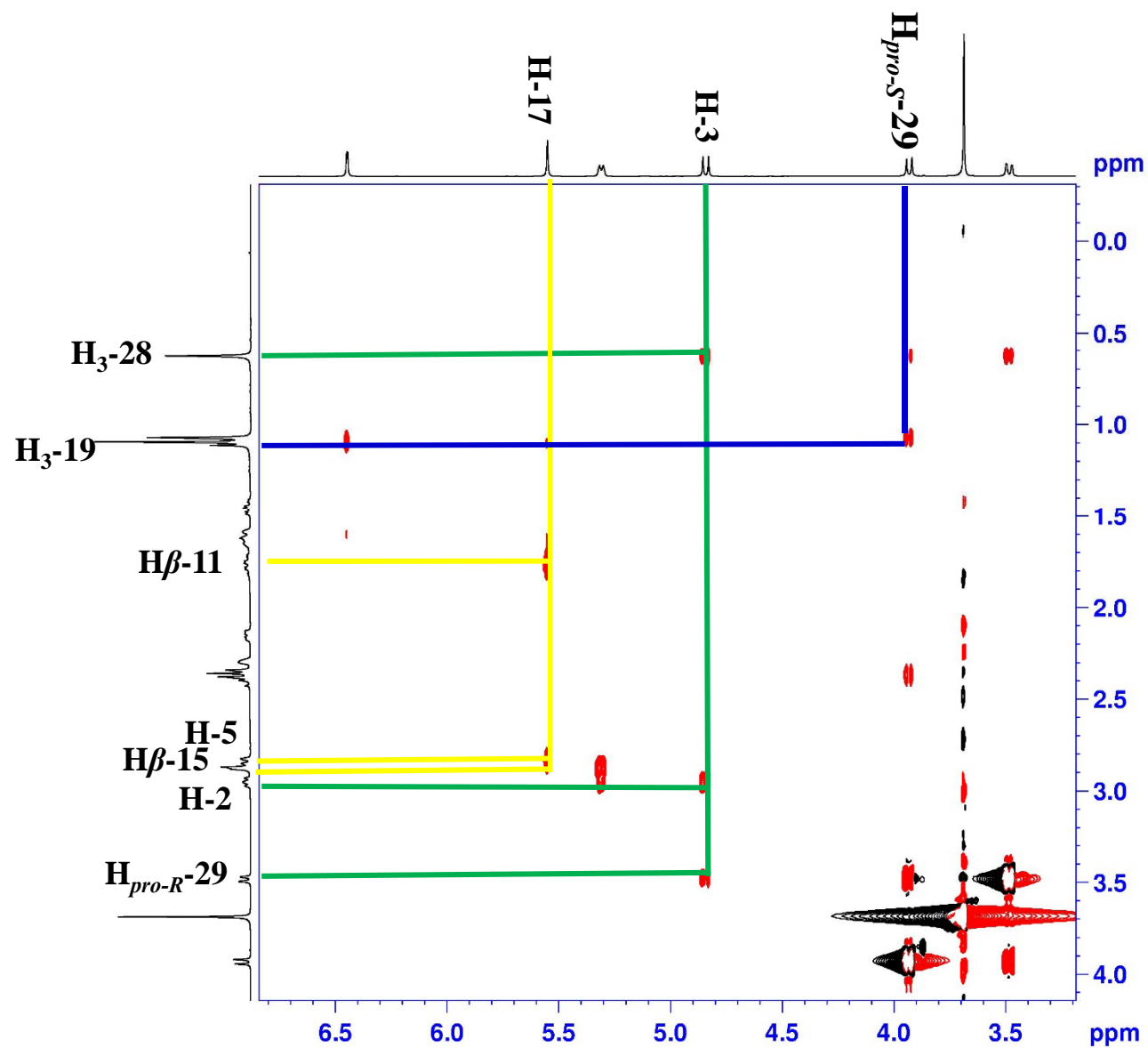
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NAME      ZXP-R-17-4-2-2-2
EXPNO     7
PROCNO    1
Date_     20180823
Time      4.30
INSTRUM   spect
PROBHD    5 mm CFPBBO BB
PULPROG   noesygpphph
TD        2048
SOLVENT   CDCl3
NS        16
DS        32
SWH       4000.000 Hz
FIDRES    1.953125 Hz
AQ        0.2560500 sec
RG        117.37
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
    
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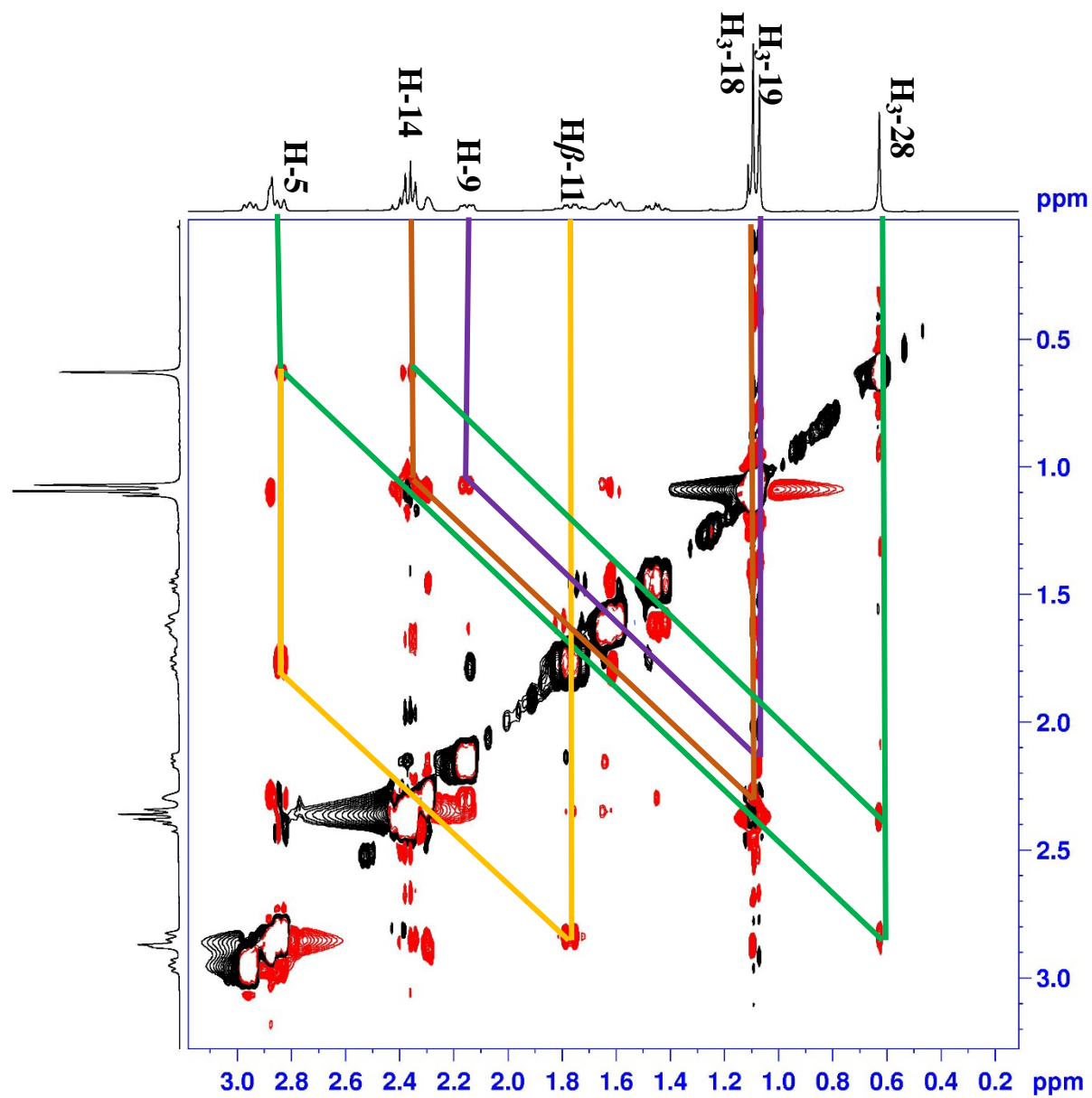
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===== CHANNEL f1 =====
SFO1    400.1318006 MHz
NUC1     1H
P1       11.50 usec
P2       23.00 usec
P17      2500.00 usec
ND0       1
TD       256
SFO1    400.1318 MHz
FIDRES   15.625000 Hz
SW       9.997 ppm
FnMODE   States-TPPI
SI       1024
SF       400.1300072 MHz
WDW      QSINE
SSB      2
LB       0.00 Hz
GB       0
PC       1.00
SI       1024
MC2      States-TPPI
SF       400.1300076 MHz
WDW      QSINE
SSB      2
LB       0.00 Hz
GB       0
    
```

NOESY (400 MHz) spectrum of compound **2** in CDCl₃



NOESY (400 MHz) spectrum of compound **2** in CDCl_3



HR-ESIMS for compound 3

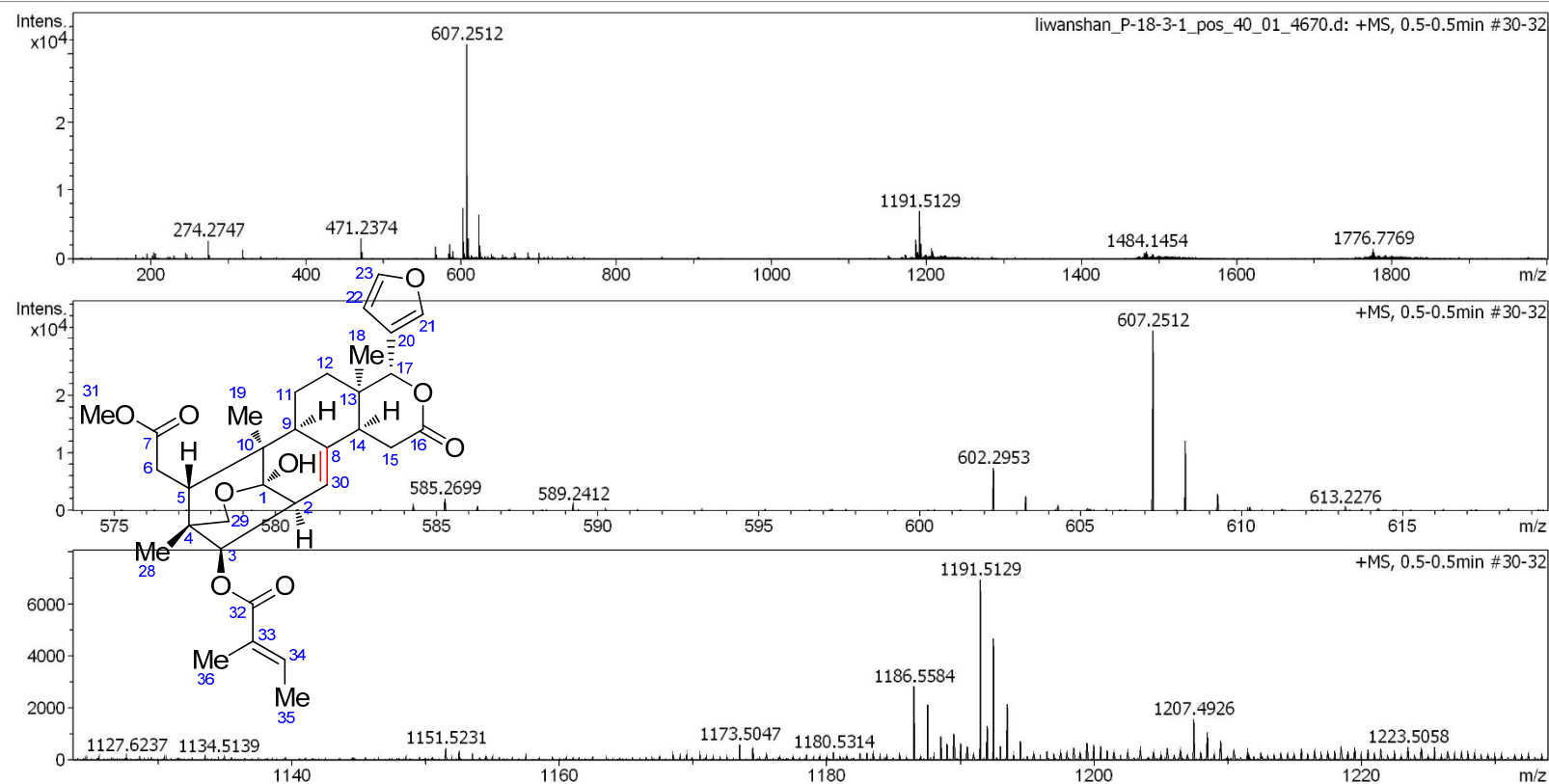
Generic Display Report

Analysis Info

Analysis Name D:\Data\MS\data\201805\liwanshan_P-18-3-1_pos_40_01_4670.d
Method LC_Direct Infusion_pos_100-1000mz.m
Sample Name liwanshan_P-18-3-1_pos
Comment

Acquisition Date 5/4/2018 11:54:44 AM

Operator SCSIO
Instrument maXis



HR-ESIMS for compound 3

Mass Spectrum SmartFormula Report

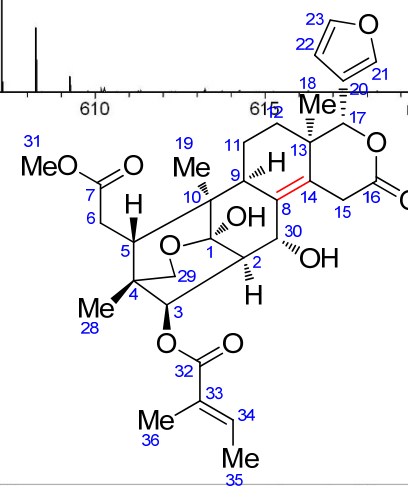
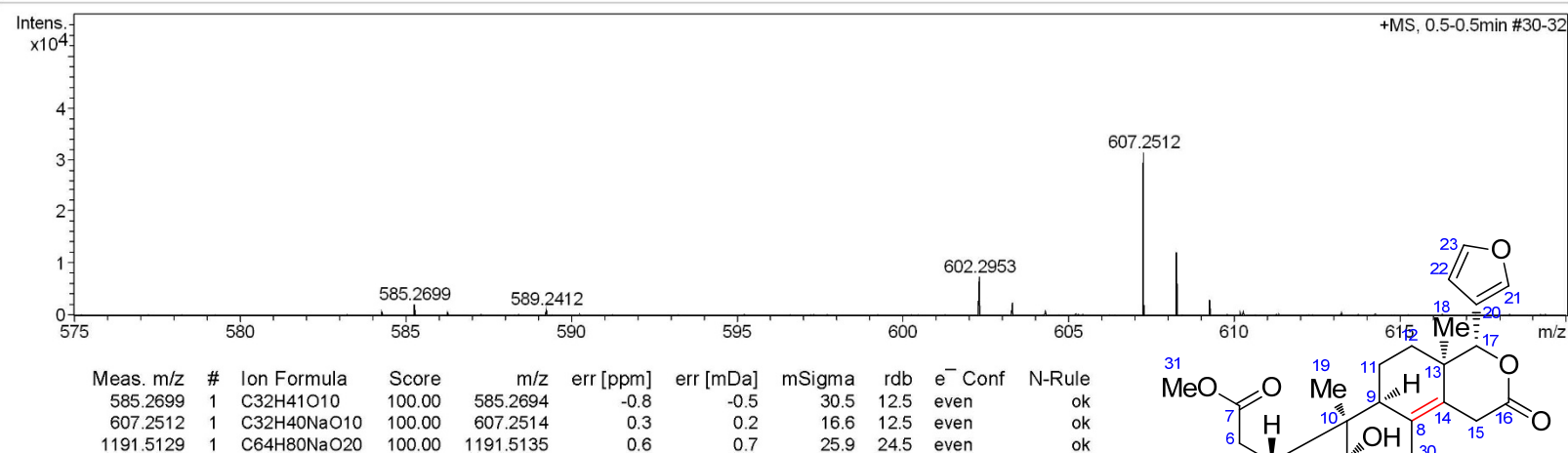
Analysis Info

Analysis Name D:\Data\MS\data\201805\liwanshan_P-18-3-1_pos_40_01_4670.d
Method LC_Direct Infusion_pos_100-1000mz.m
Sample Name liwanshan_P-18-3-1_pos
Comment

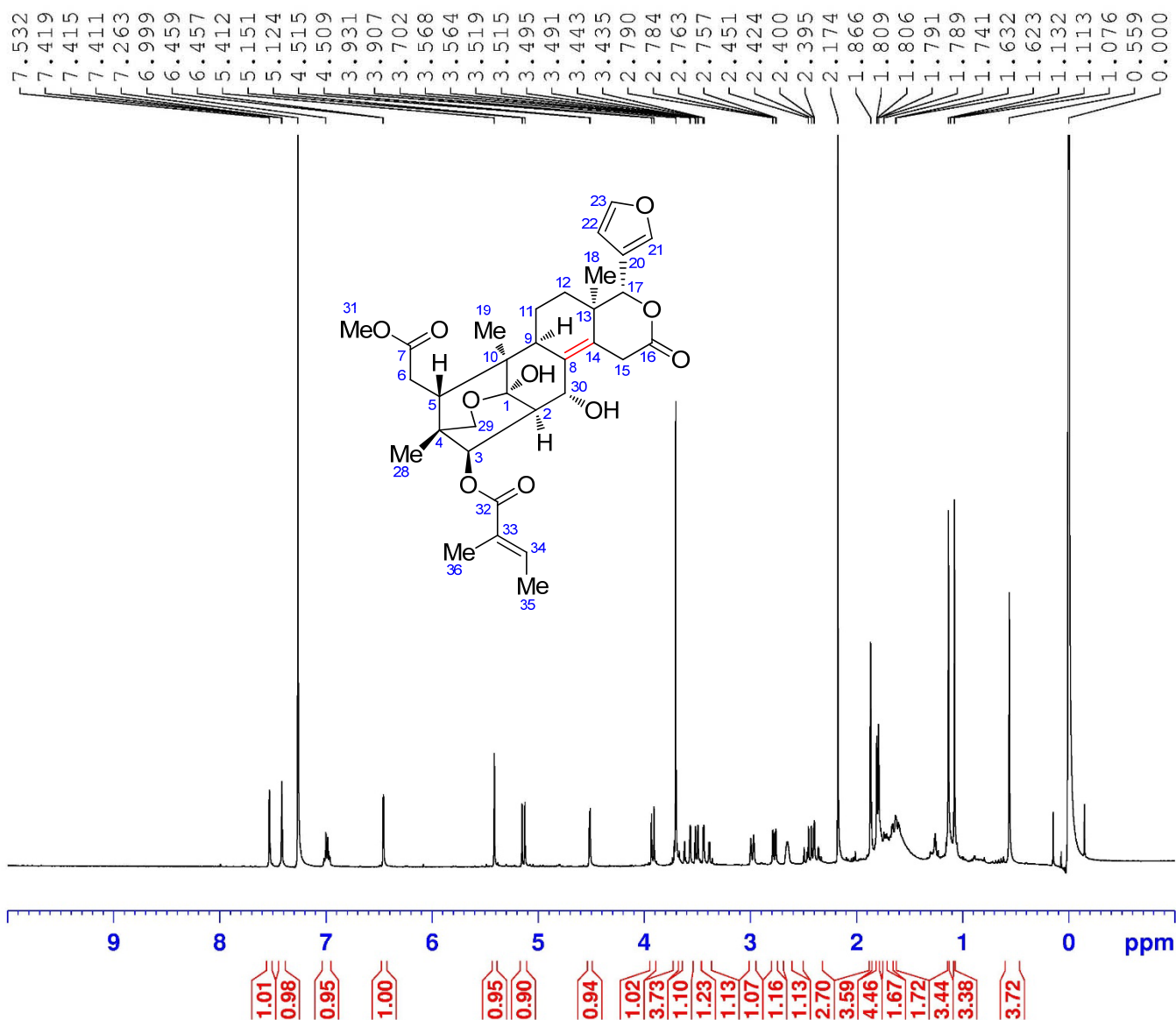
Acquisition Date 5/4/2018 11:54:44 AM
Operator SCSIO
Instrument maXis 255552.00029

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	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



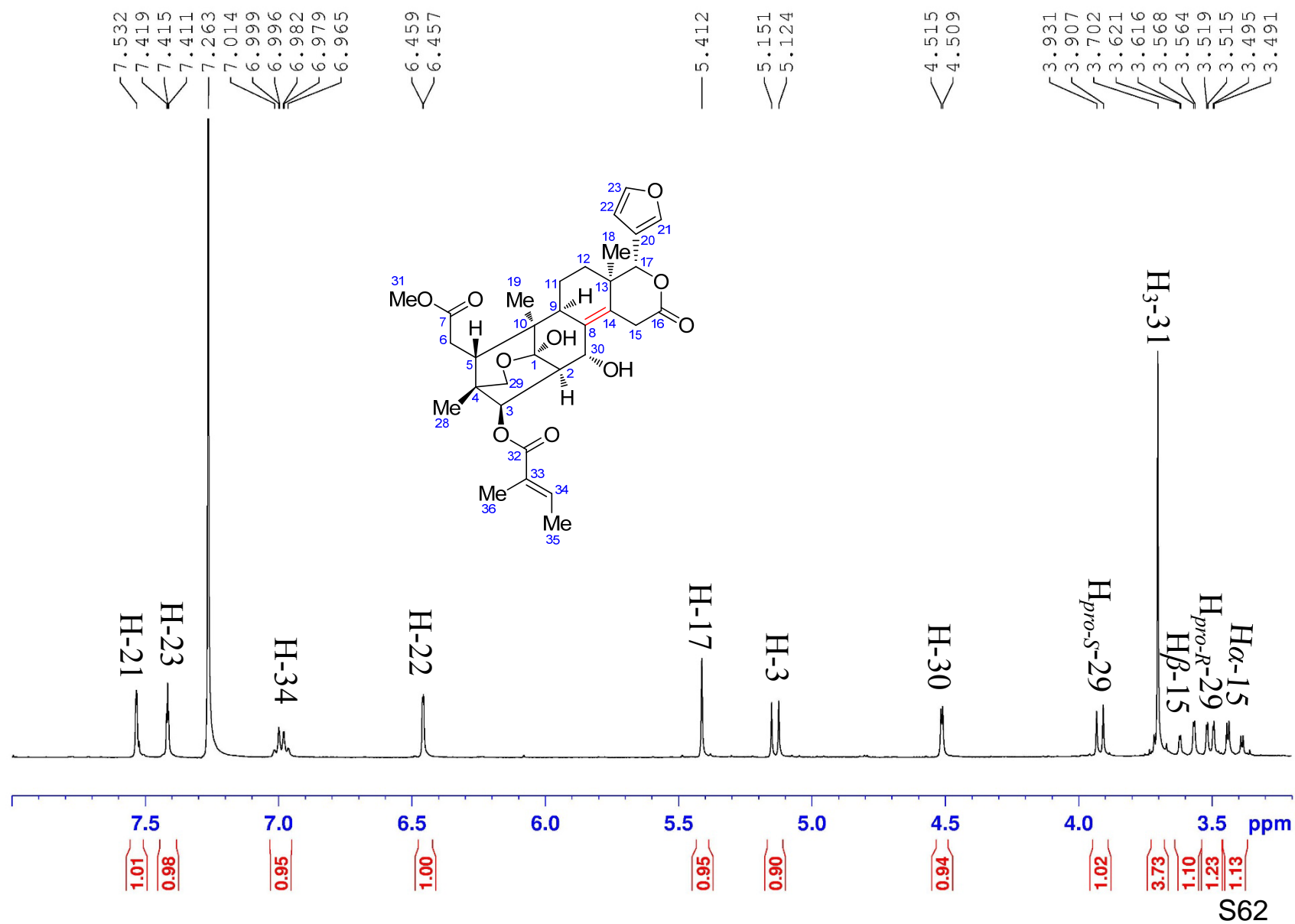
^1H NMR (400 MHz) spectrum of compound **3** in CDCl_3



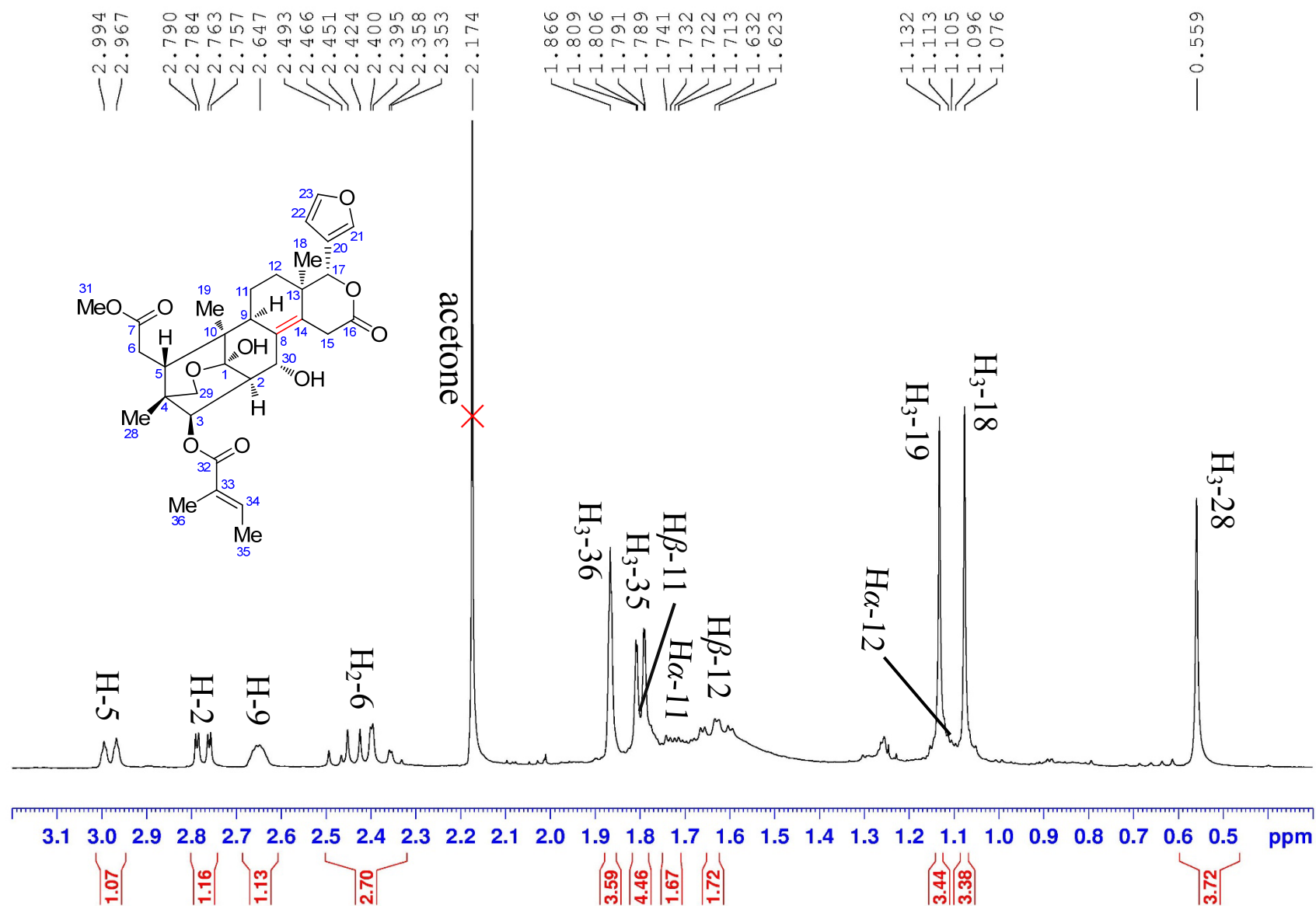
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 EXPNO 1
 PROCNO 1
 Date_ 20180109
 Time 8.01
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl_3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 208.5
 DW 60.800 usec
 DE 10.00 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 ^1H
 P1 11.50 usec
 SI 65536
 SF 400.1300087 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

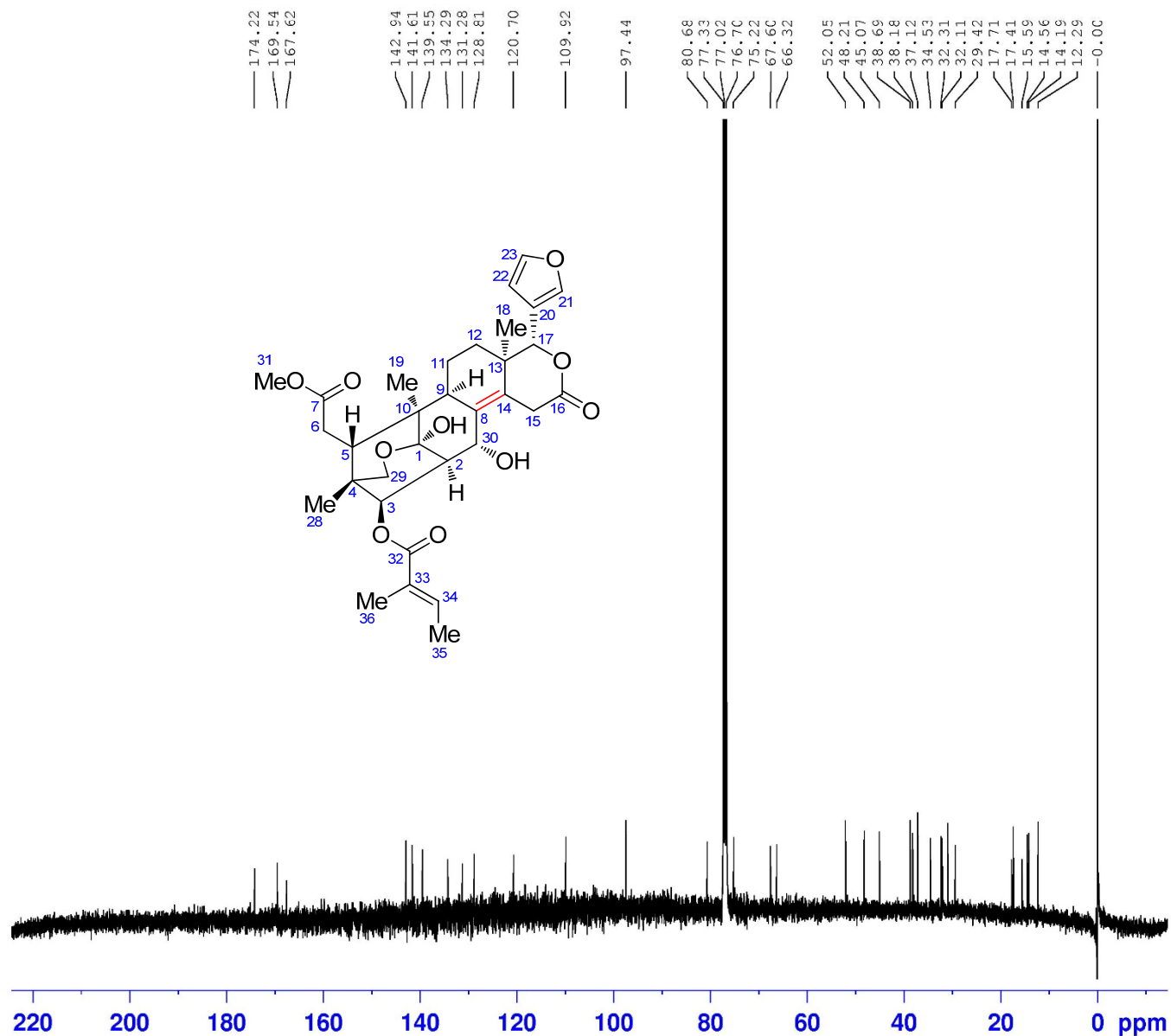
^1H NMR (400 MHz) spectrum of compound **3** in CDCl_3



^1H NMR (400 MHz) spectrum of compound **3** in CDCl_3



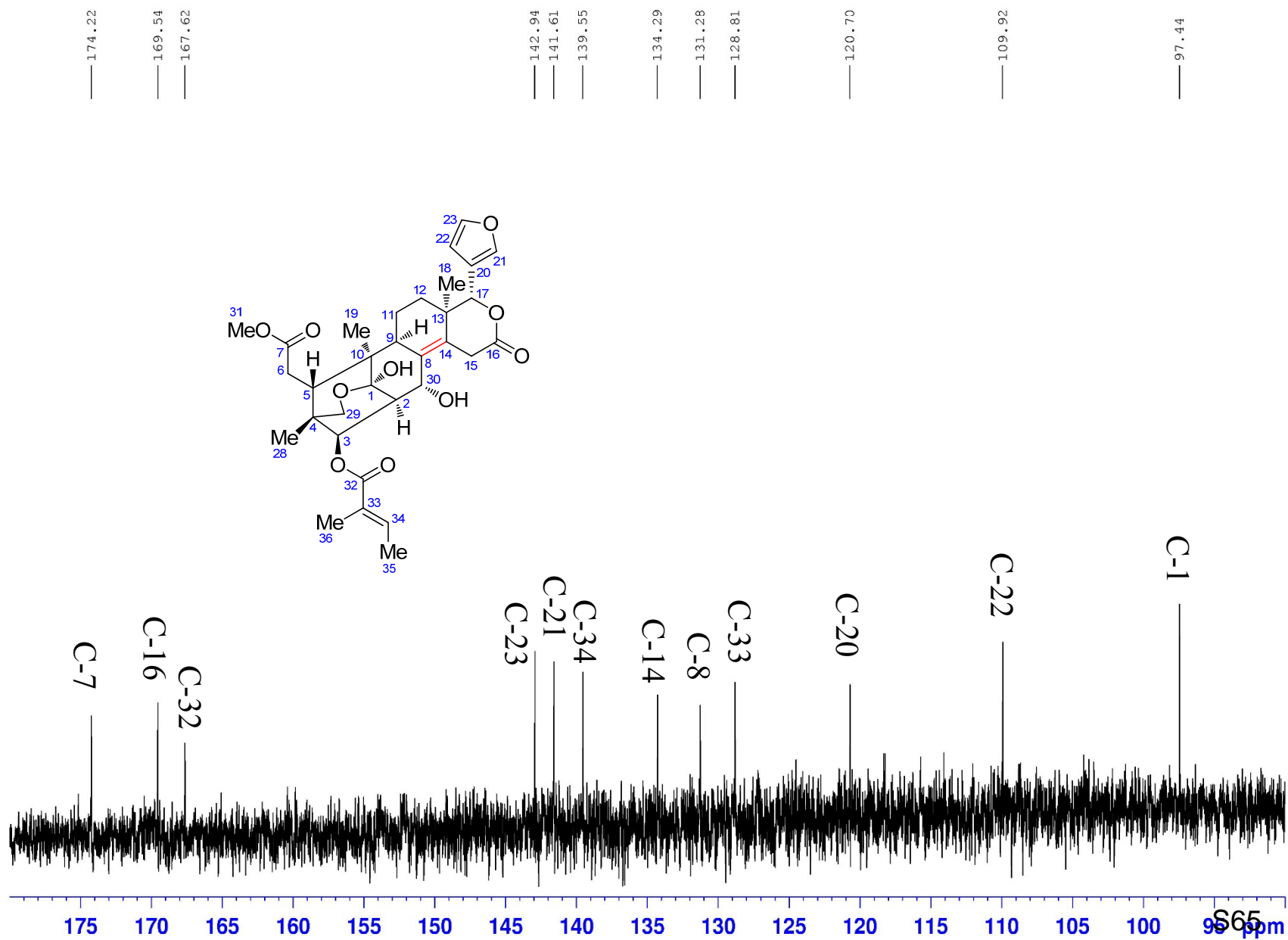
^{13}C NMR (100 MHz) spectrum of compound **3** in CDCl_3



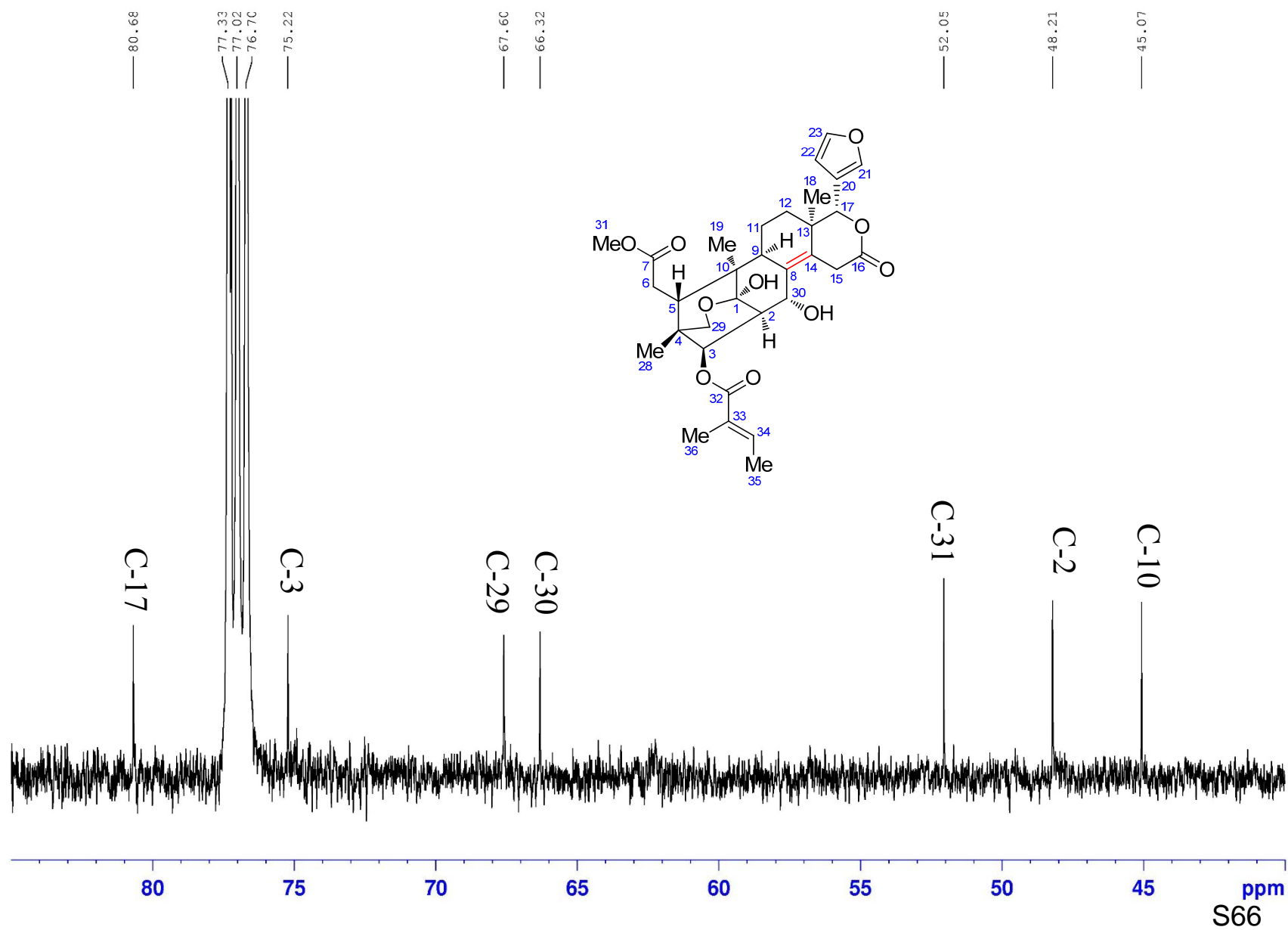
NAME ZXP-R-18-3-1-3-3 new
 EXPNO 2
 PROCNO 1
 Date_ 20180109
 Time 9.01
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 73.92
 DW 20.800 usec
 DE 18.00 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6233324 MHz
 NUC1 ^{13}C
 P1 10.00 usec
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

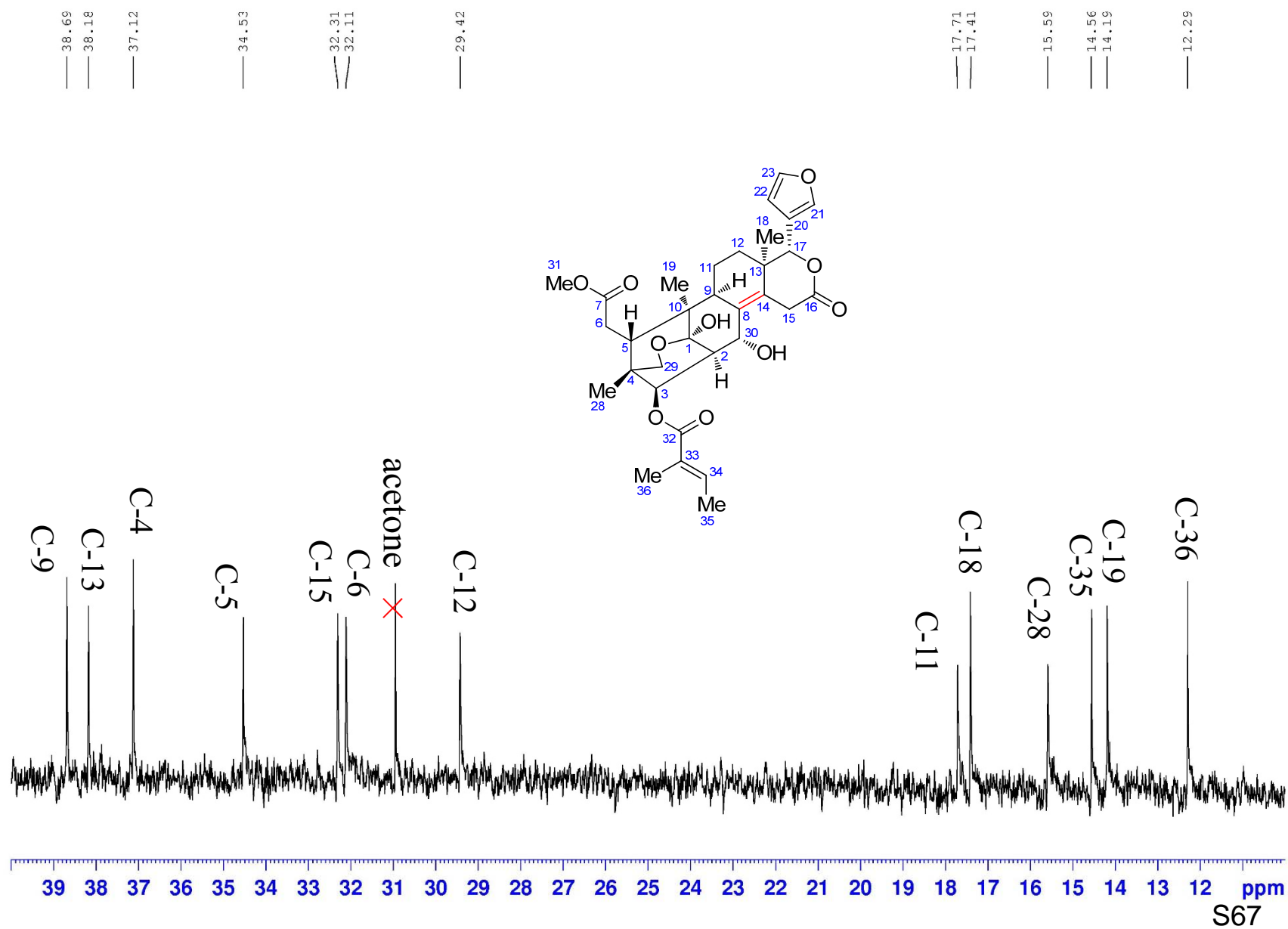
^{13}C NMR (100 MHz) spectrum of compound **3** in CDCl_3



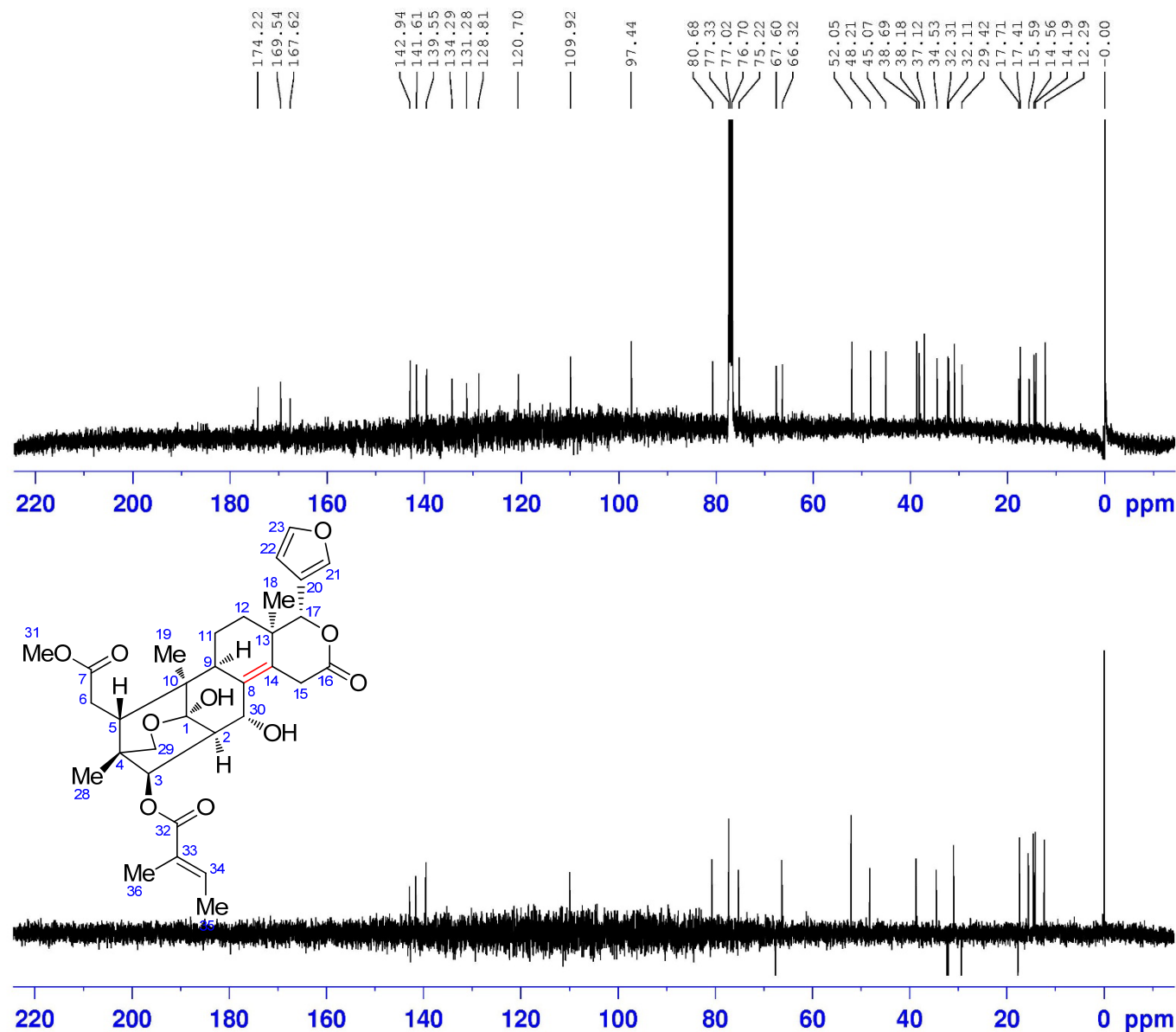
^{13}C NMR (100 MHz) spectrum of compound **3** in CDCl_3



^{13}C NMR (100 MHz) spectrum of compound **3** in CDCl_3



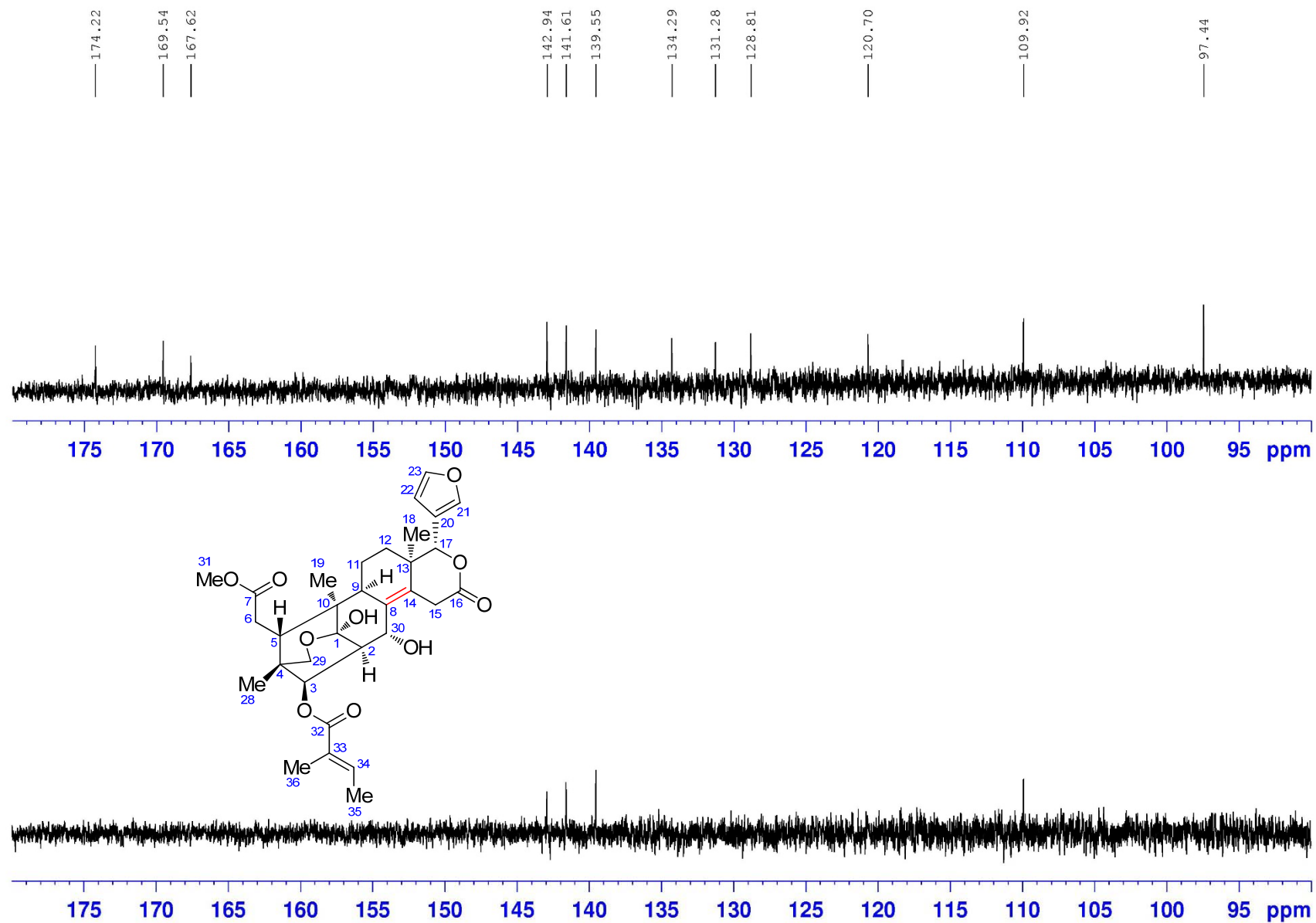
DEPT135 (100 MHz) spectrum of compound **3** in CDCl₃



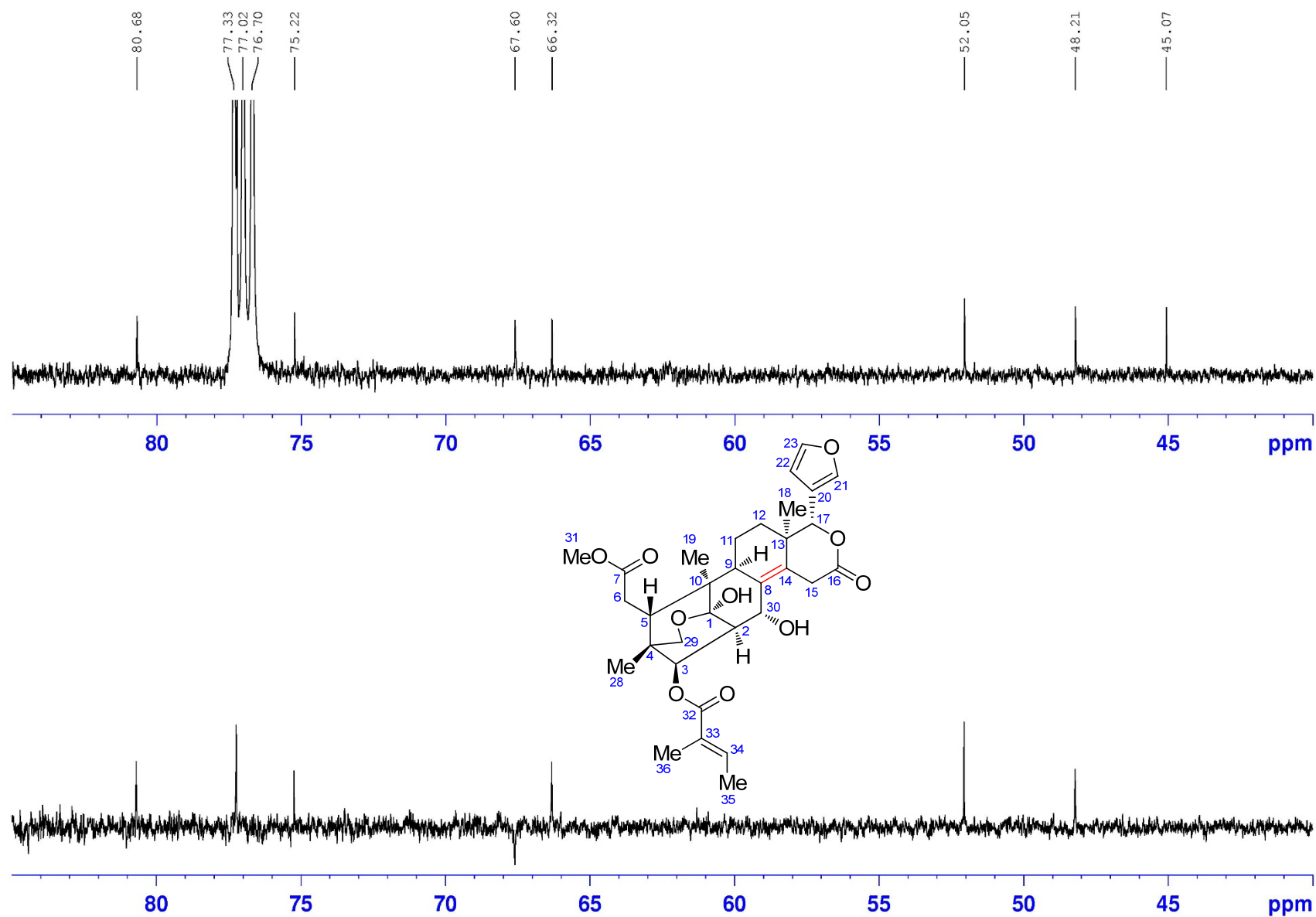
NAME ZXP-R-18-3-1-3-3 new
 EXPNO 2
 PROCNO 1
 Date_ 20180109
 Time 9.01
 INSTRUM spect
 PROBHD 5 mm CPMBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 73.92
 DW 20.800 usec
 DE 18.00 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.623324 MHz
 NUC1 13C
 P1 10.00 usec
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

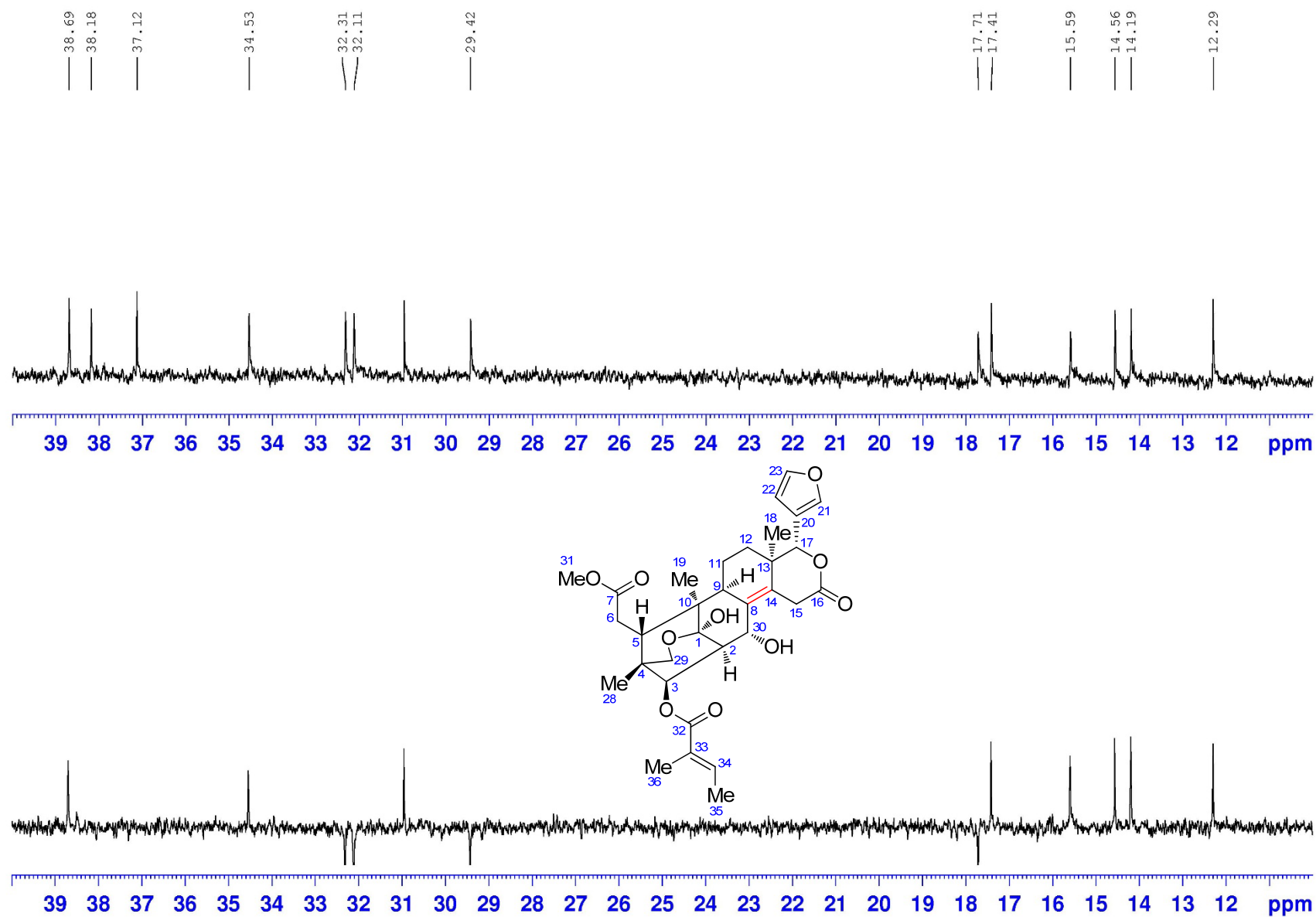
DEPT135 (100 MHz) spectrum of compound **3** in CDCl₃



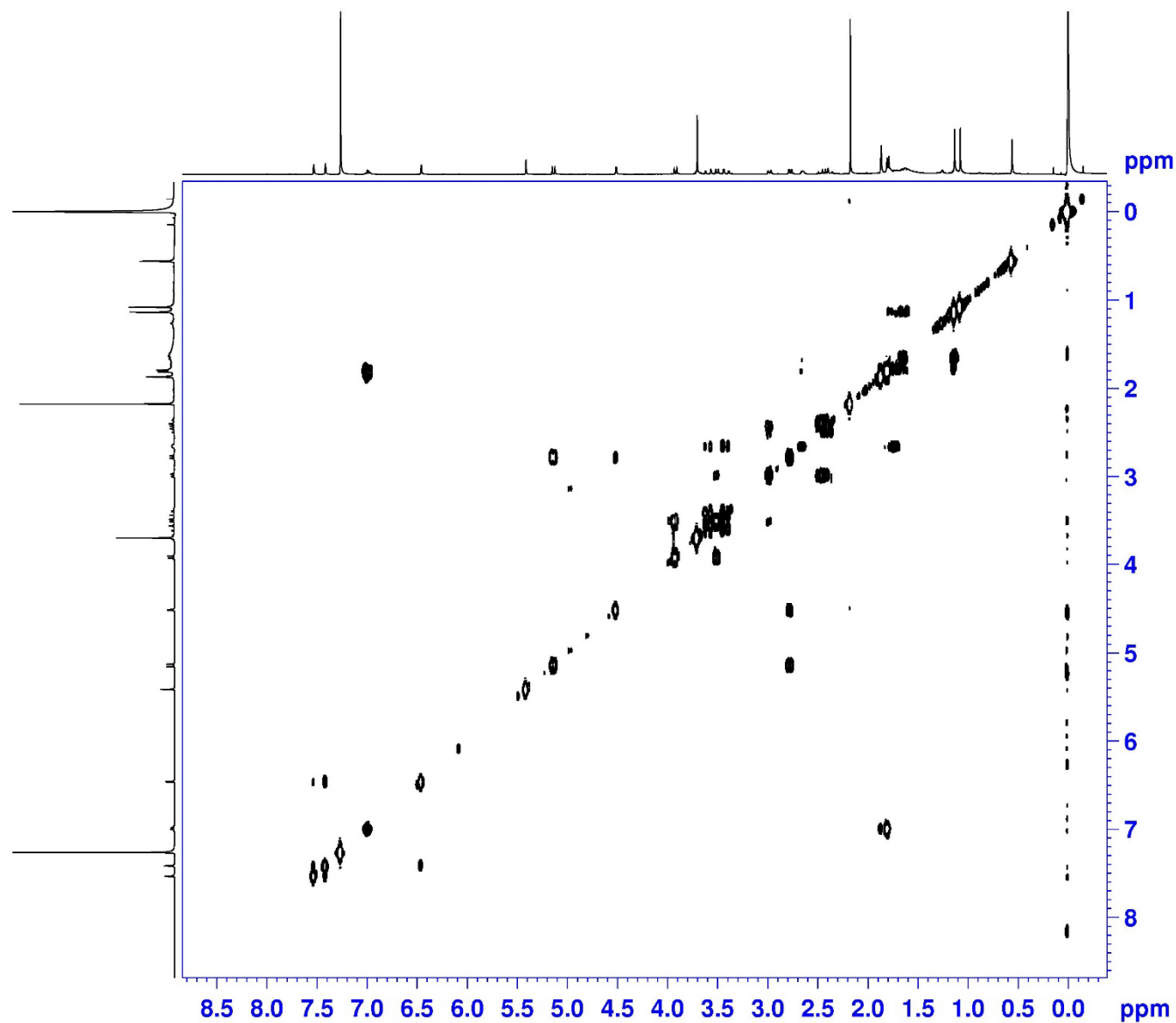
DEPT135 (100 MHz) spectrum of compound **3** in CDCl₃



DEPT135 (100 MHz) spectrum of compound **3** in CDCl₃



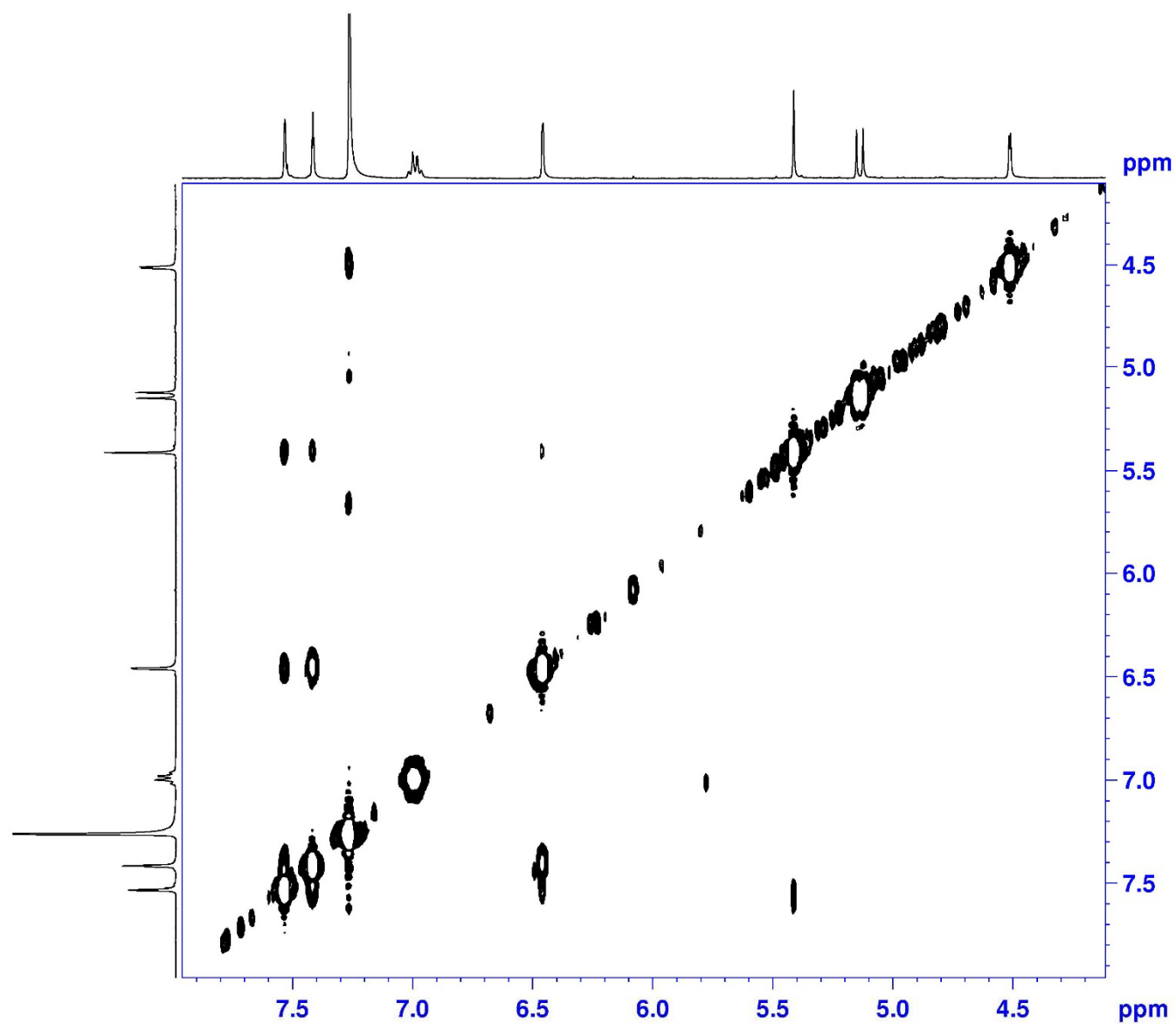
^1H - ^1H COSY (400 MHz) spectrum of compound **3** in CDCl_3



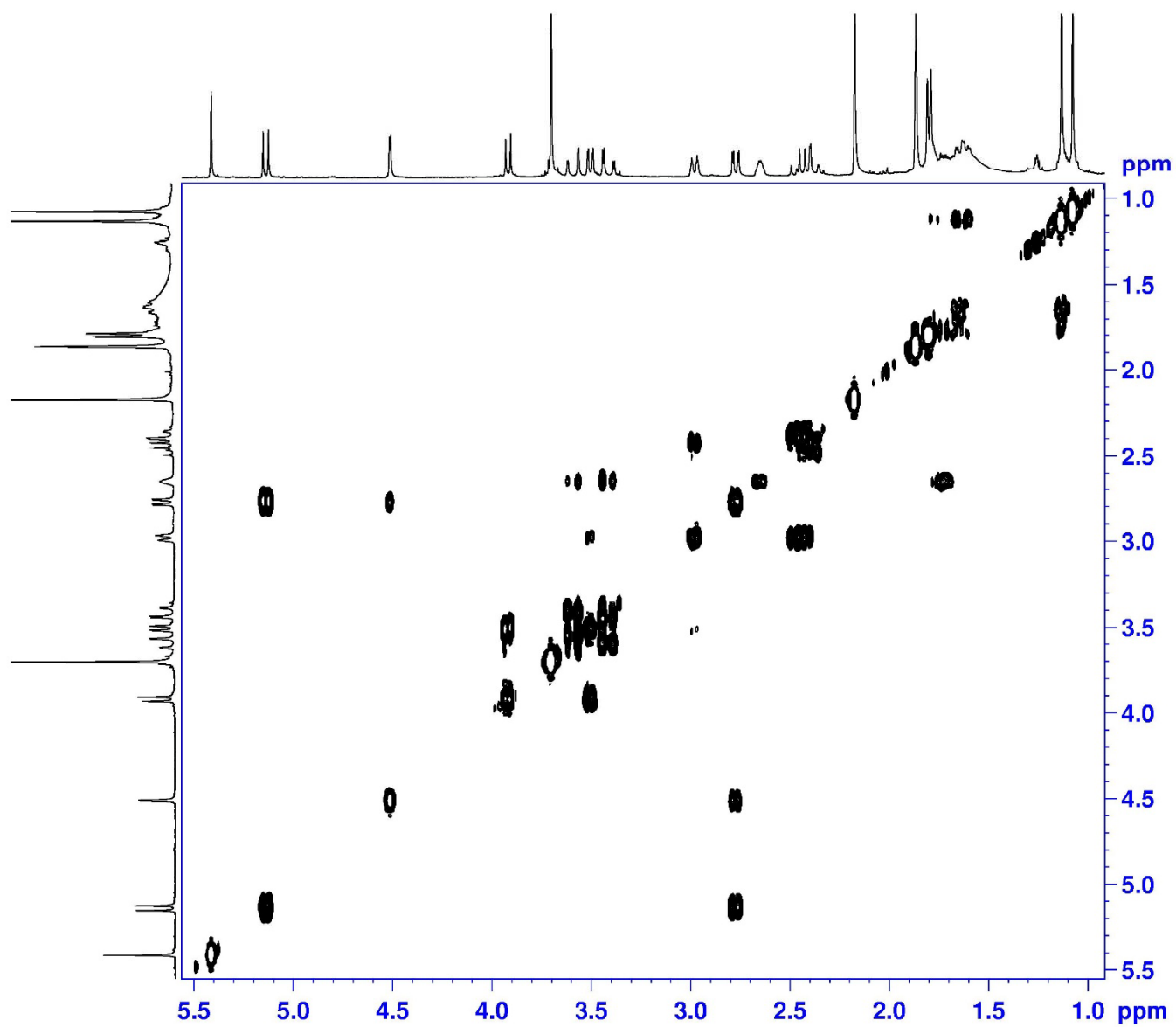
NAME ZXP-R-18-3-1-3-3 new
EXPNO 4
PROCNO 1
Date_ 20180122
Time 23.49
INSTRUM spect
PROBHD 5 mm CPMBO BB
PULPROG cosygpppgf
TD 2048
SOLVENT CDCl_3
NS 8
DS 8
SWH 3906.250 Hz
FIDRES 1.907349 Hz
AQ 0.2621940 sec
RG 208.5
DW 128.000 usec
DE 10.00 usec
TE 297.0 K
D0 0.00000300 sec
D1 1.89678097 sec
D11 0.03000000 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 400.1300064 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 400.1300071 MHz
WDW QSINE
SSB 0
LB 0.00 Hz

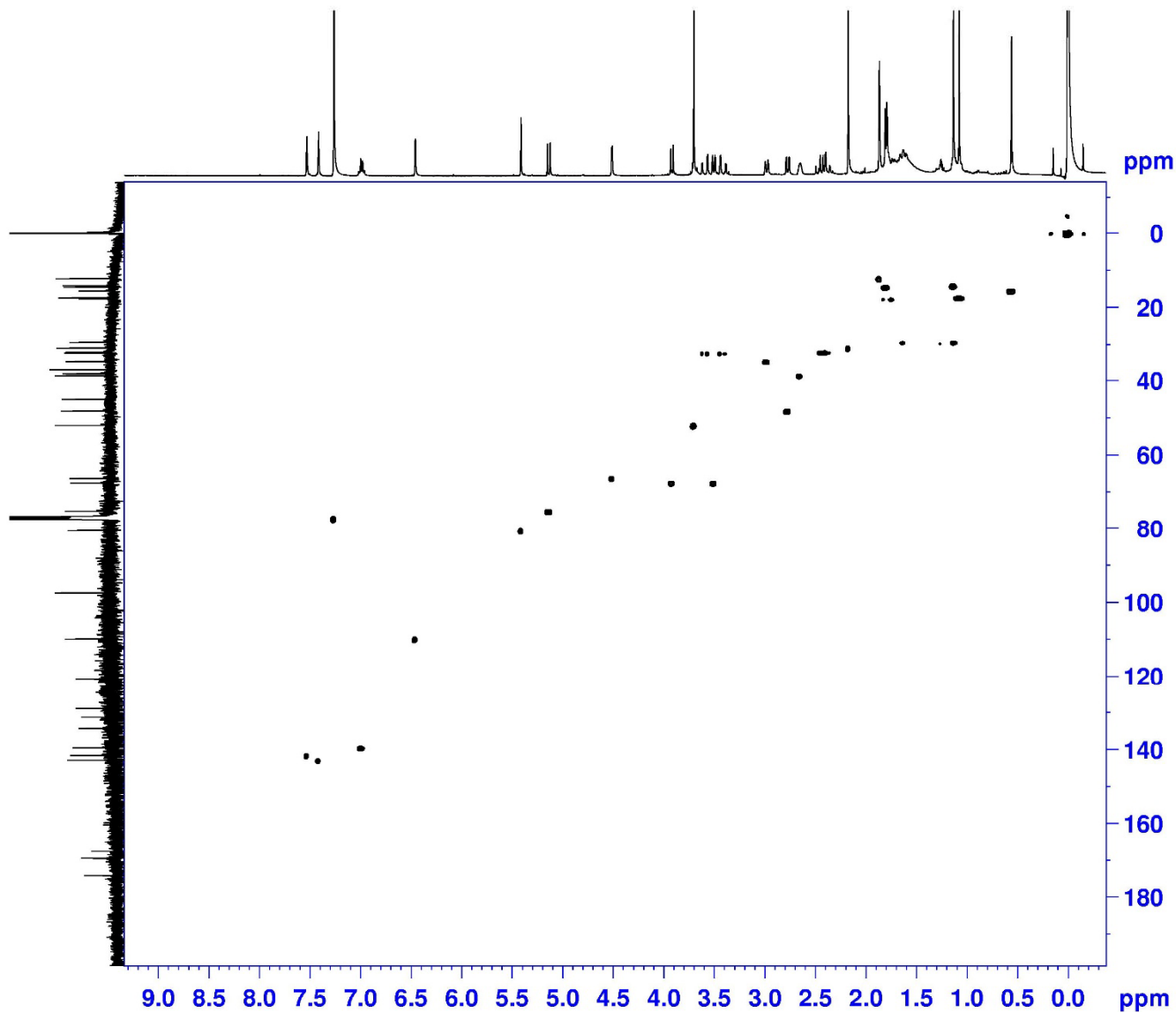
^1H - ^1H COSY (400 MHz) spectrum of compound **3** in CDCl_3



^1H - ^1H COSY (400 MHz) spectrum of compound **3** in CDCl_3



HSQC (400 MHz) spectrum of compound **3** in CDCl₃



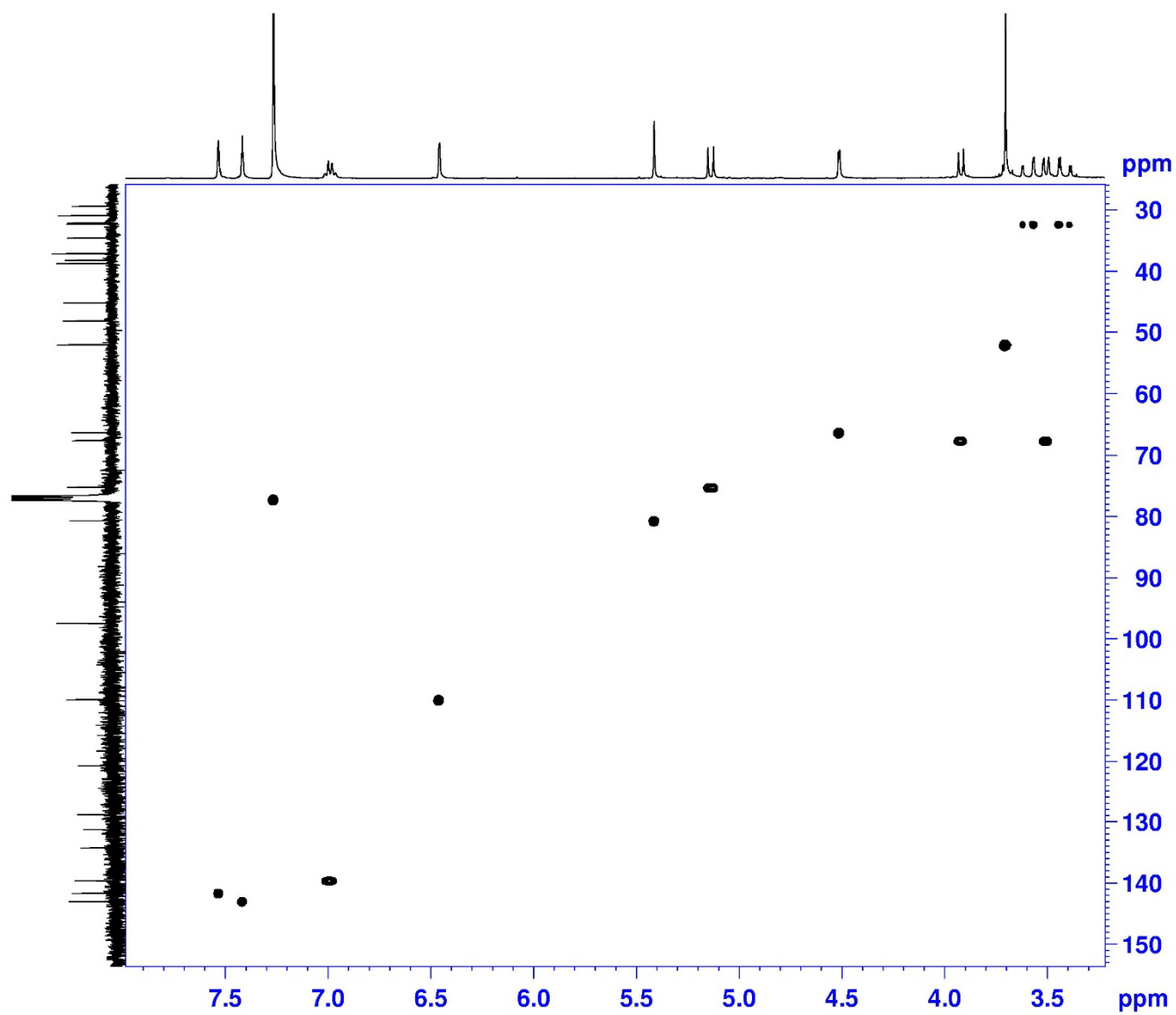
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NAME      ZXP-R-18-3-1-3-3 new
EXPNO     5
PROCNO    1
Date_     20180123
Time      0.28
INSTRUM    spect
PROBHD     5 mm CPPBBO BB
PULPROG    hsqcetgpsi2
TD         1024
SOLVENT    CDCl3
NS         16
DS         16
SWH        4302.926 Hz
FIDRES     4.202076 Hz
AQ         0.1190388 sec
RG         208.5
DW         116.200 usec
DE         10.00 usec
TE         297.0 K
CNST2      145.0000000
D0         0.00000300 sec
D1         1.46497905 sec
D4         0.00172414 sec
D11        0.03000000 sec
D16        0.00020000 sec
D24        0.00086207 sec
IN0        0.00002080 sec
ZGPTNS
  
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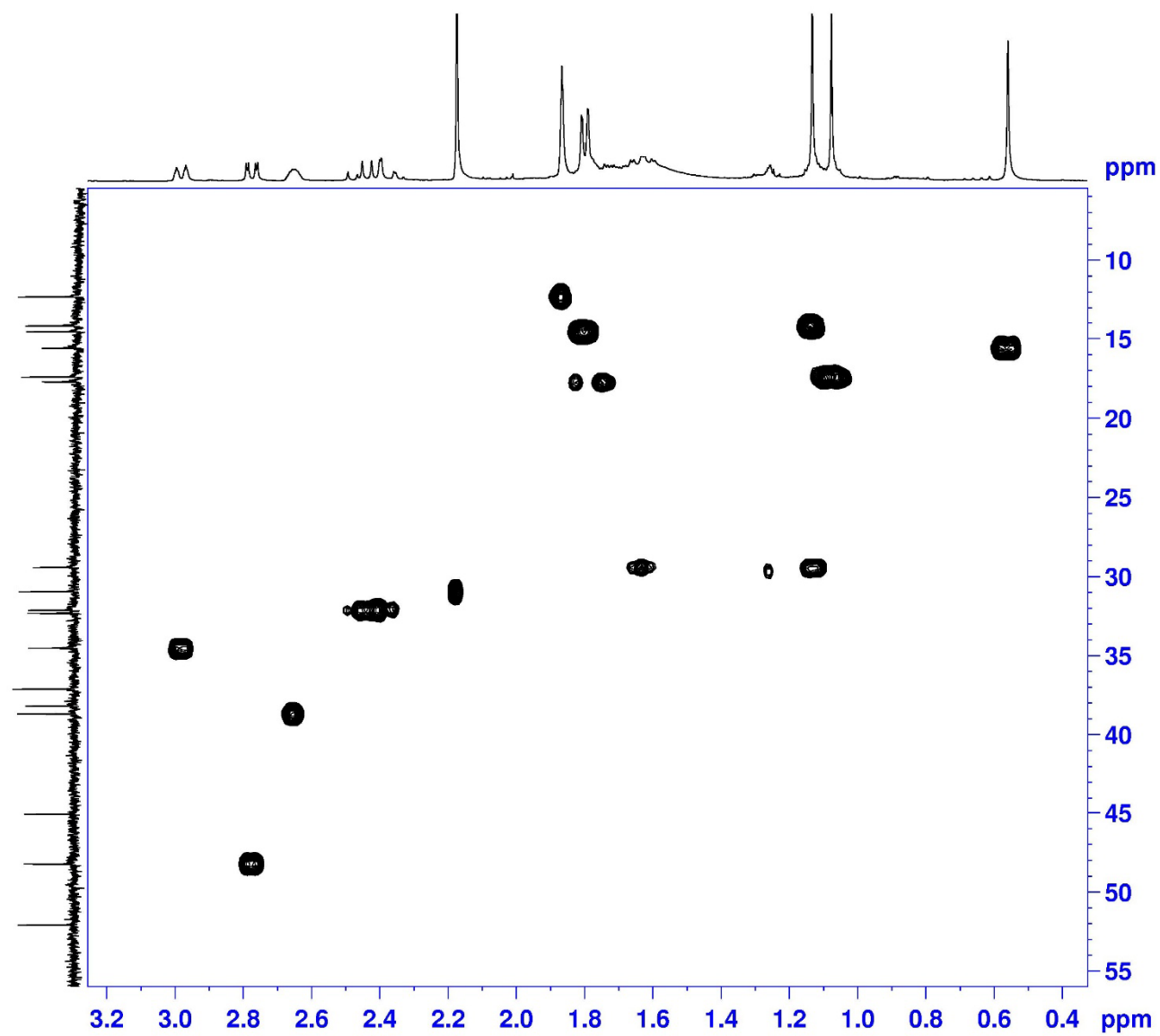
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===== CHANNEL f1 =====
SFO1      400.1320007 MHz
NUC1       1H
P1         11.50 usec
P2         23.00 usec
P28        0.00 usec
ND0        2
TD         256
SFO1      100.6233 MHz
FIDRES     93.900238 Hz
SW         238.896 ppm
FnMODE     Echo-Antiecho
SI         1024
SF         400.1300055 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.40
SI         1024
MC2        echo-antiecho
SF         100.6127548 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
  
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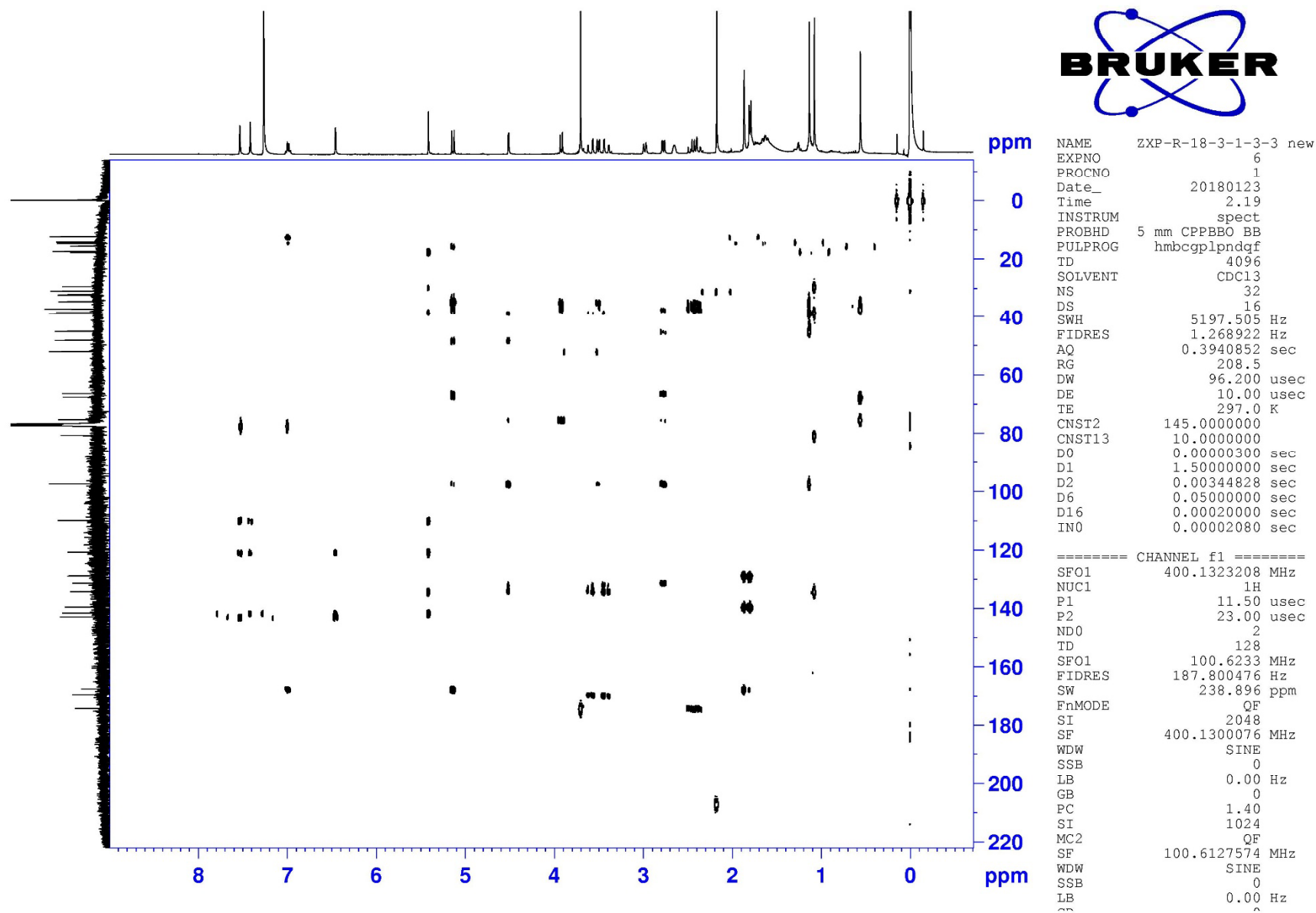
HSQC (400 MHz) spectrum of compound **3** in CDCl₃



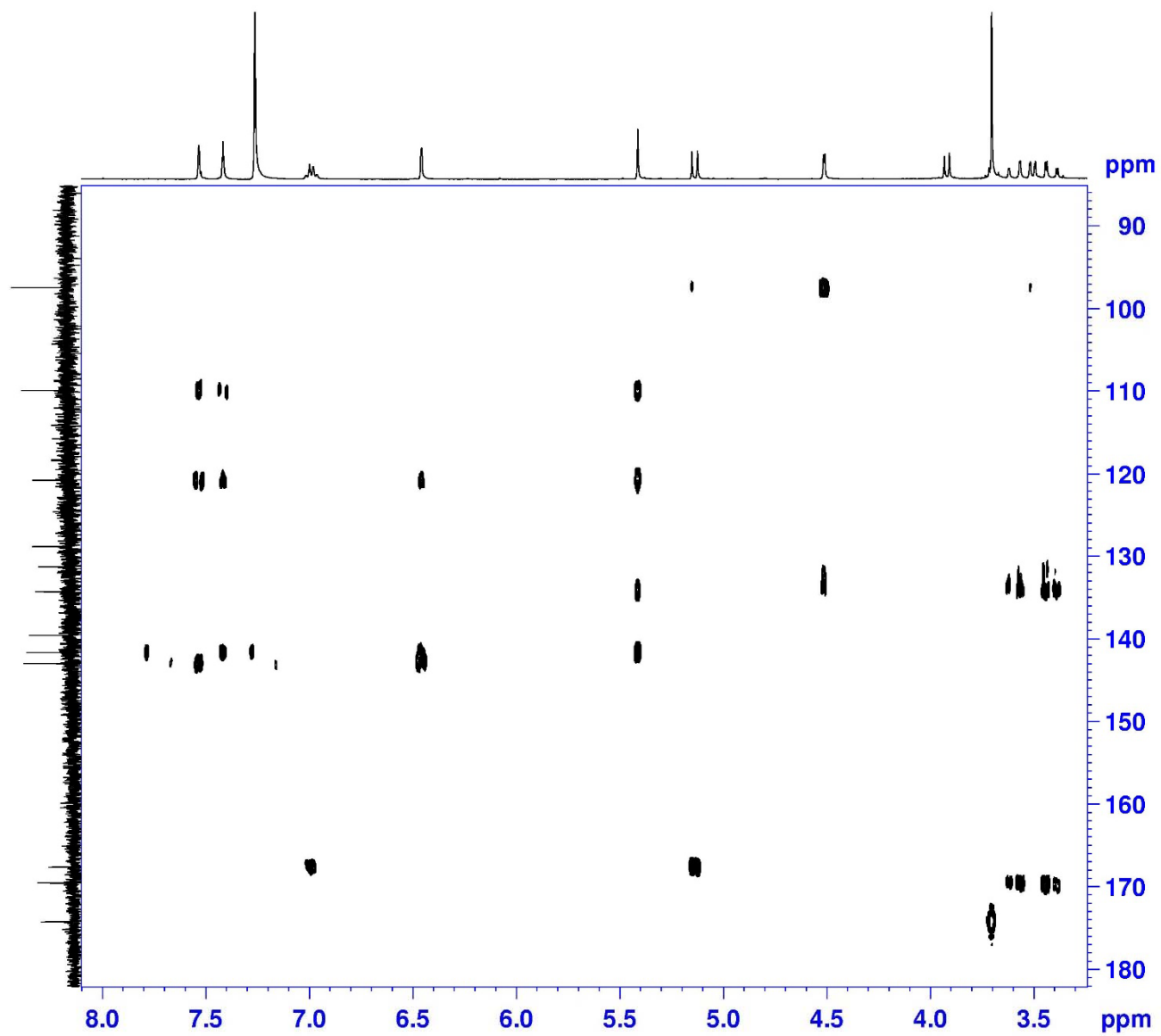
HSQC (400 MHz) spectrum of compound **3** in CDCl₃



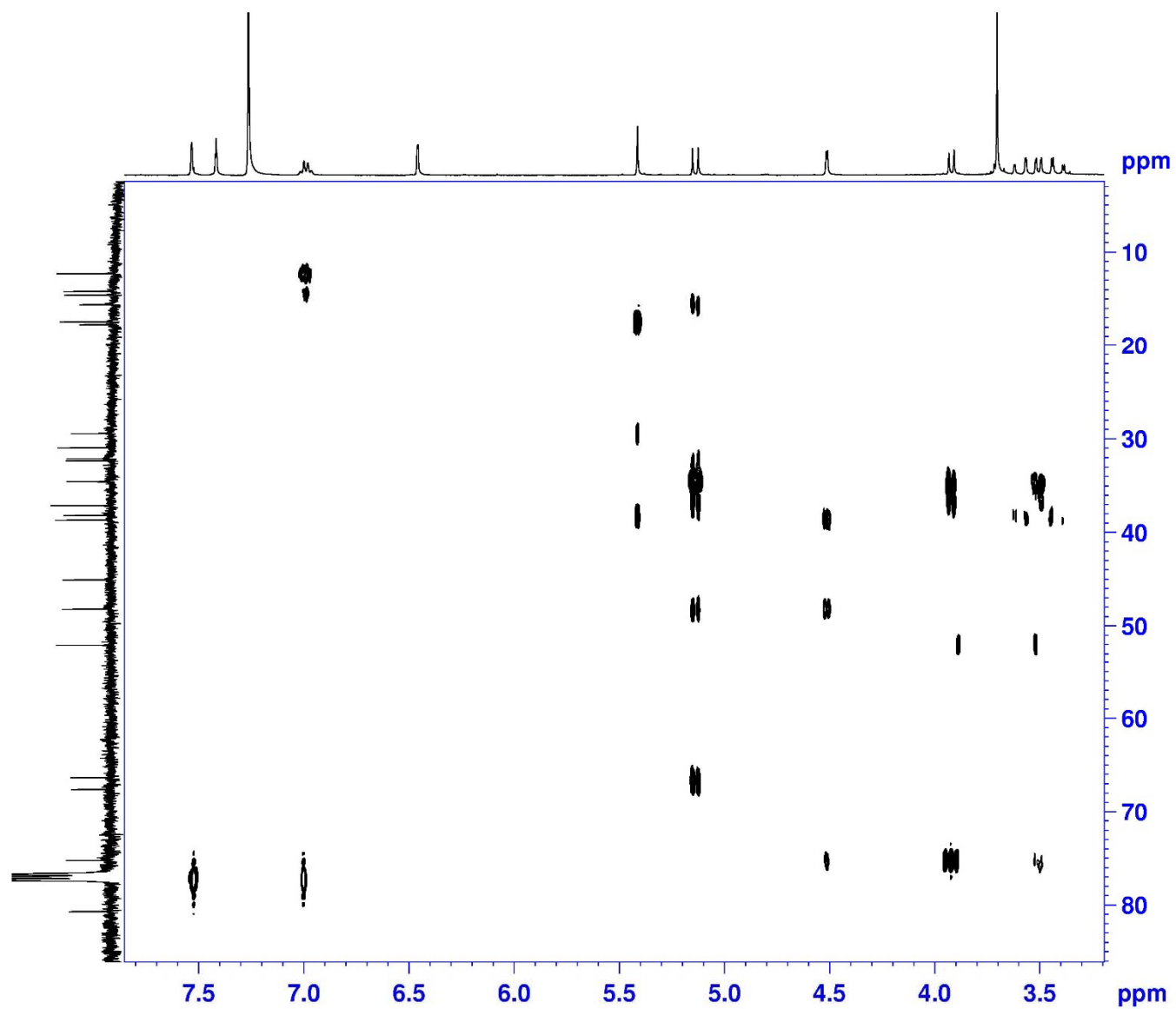
HMBC (400 MHz) spectrum of compound **3** in CDCl₃



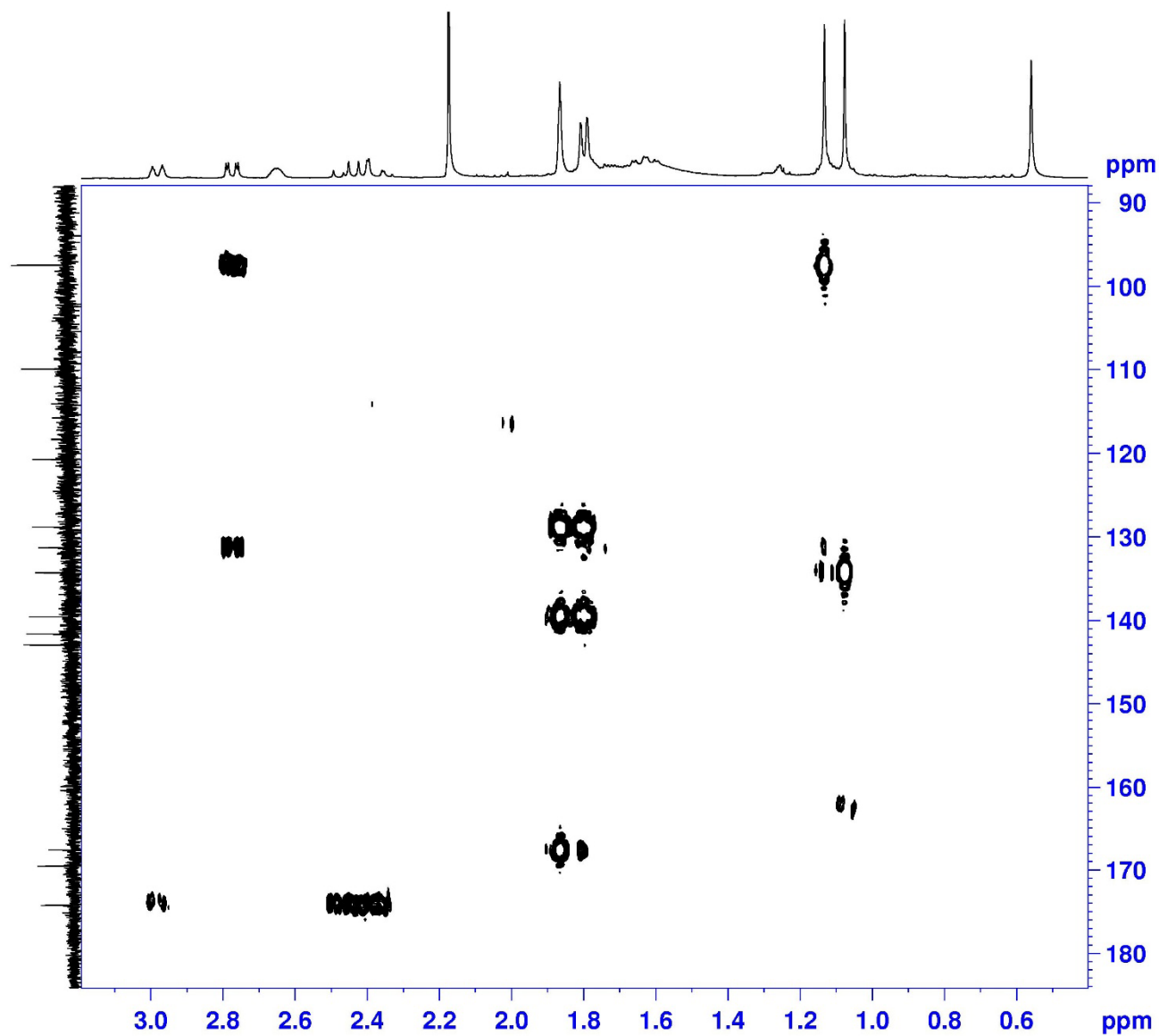
HMBC (400 MHz) spectrum of compound **3** in CDCl_3



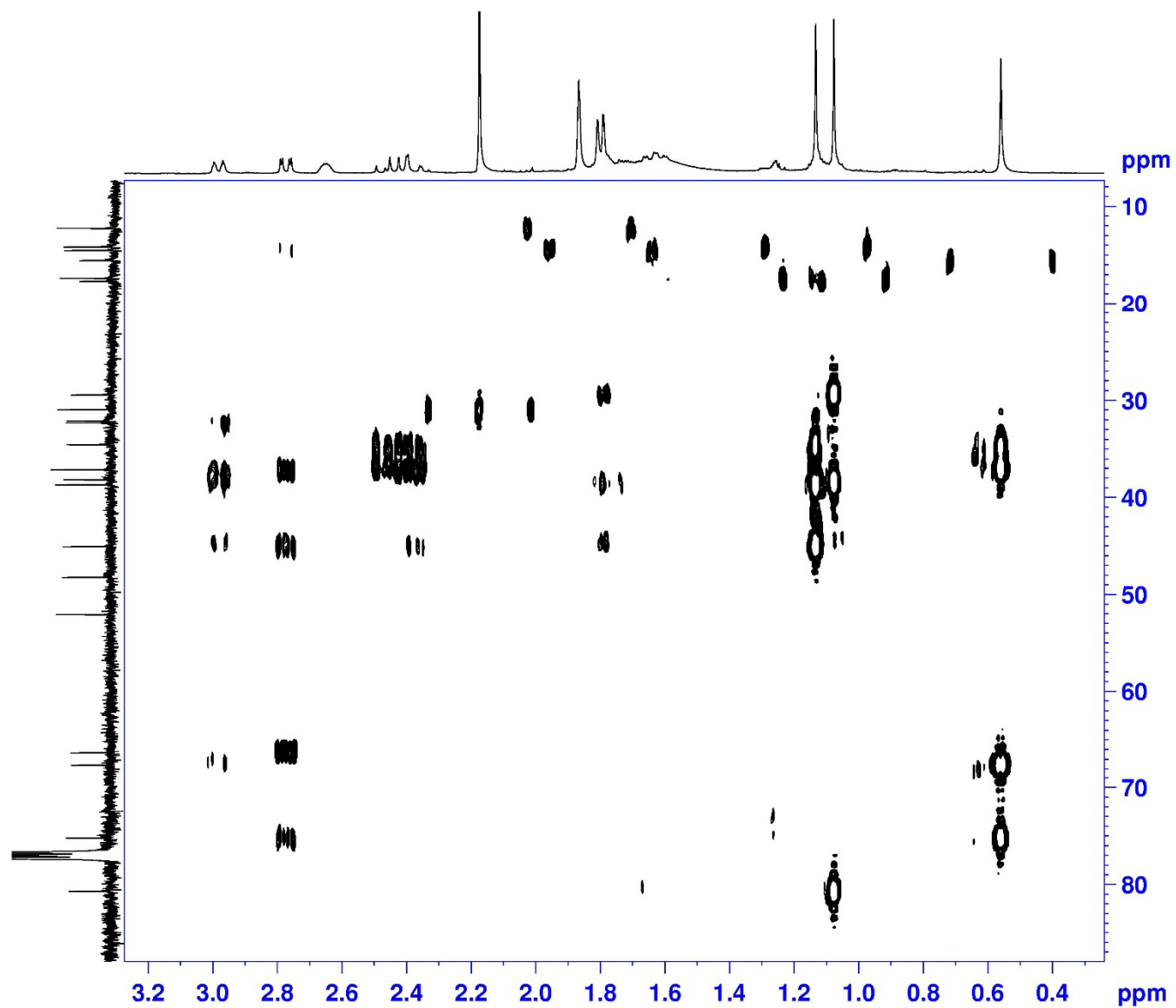
HMBC (400 MHz) spectrum of compound **3** in CDCl₃



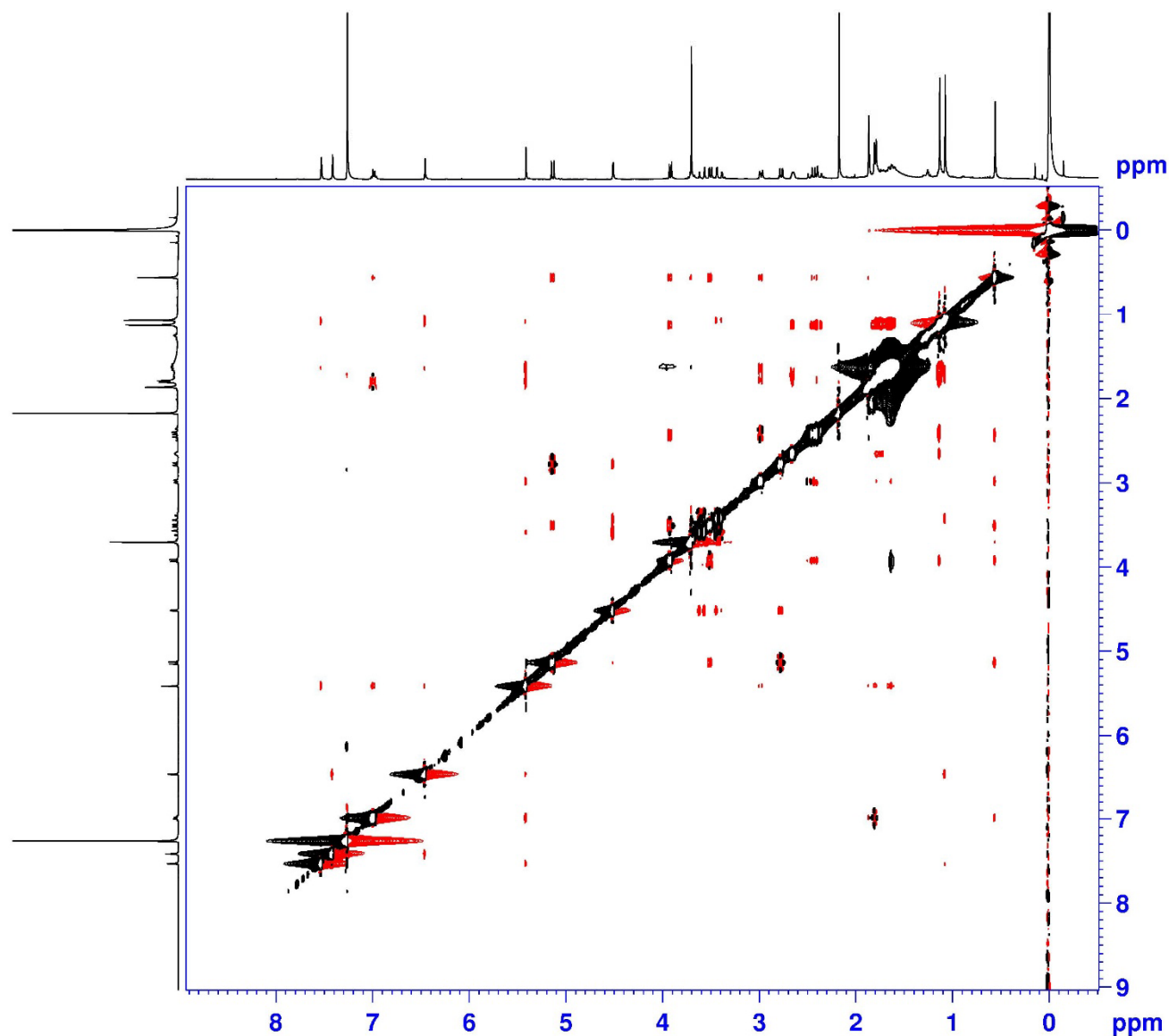
HMBC (400 MHz) spectrum of compound **3** in CDCl₃



HMBC (400 MHz) spectrum of compound **3** in CDCl_3



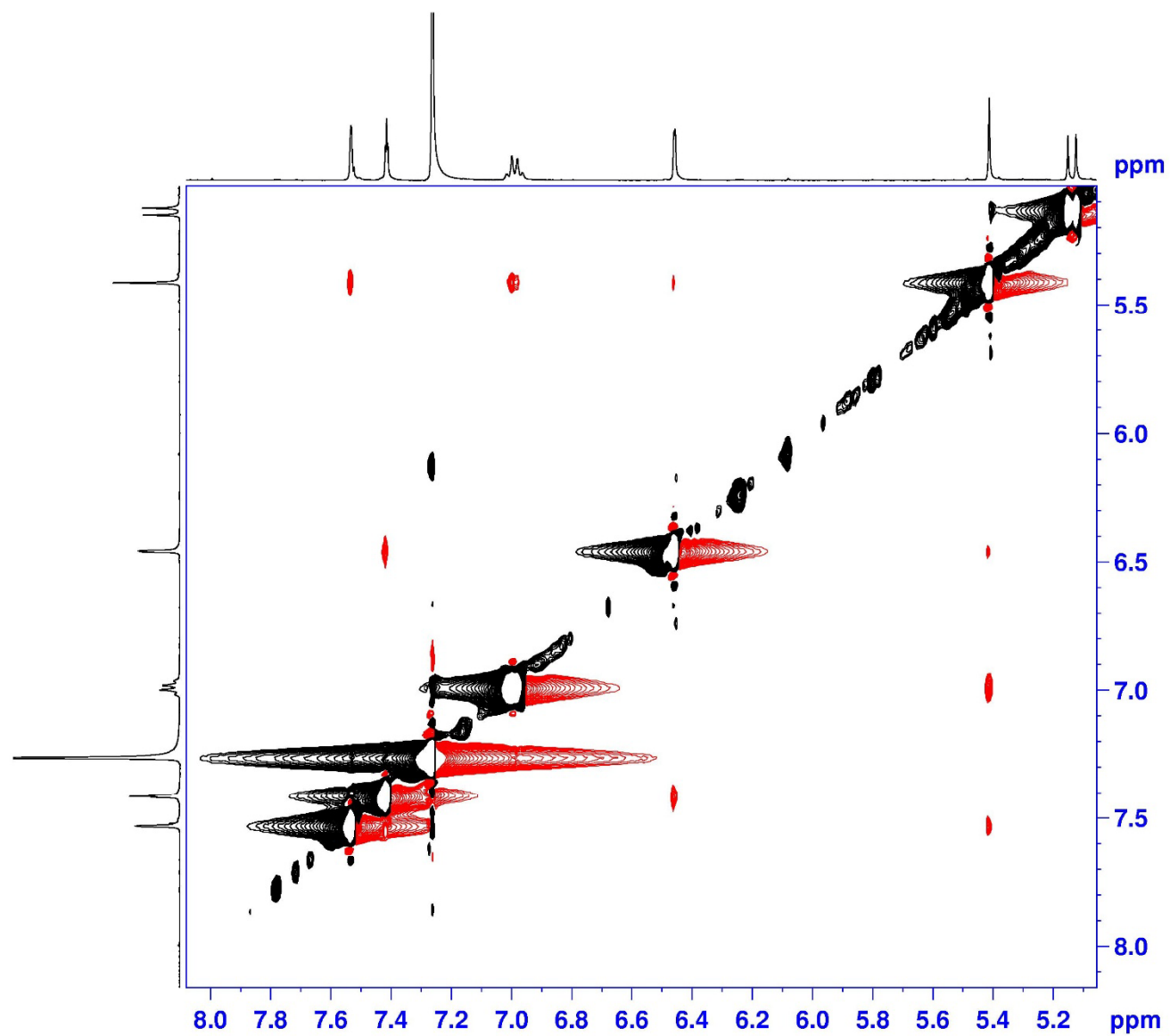
NOESY (400 MHz) spectrum of compound **3** in CDCl₃



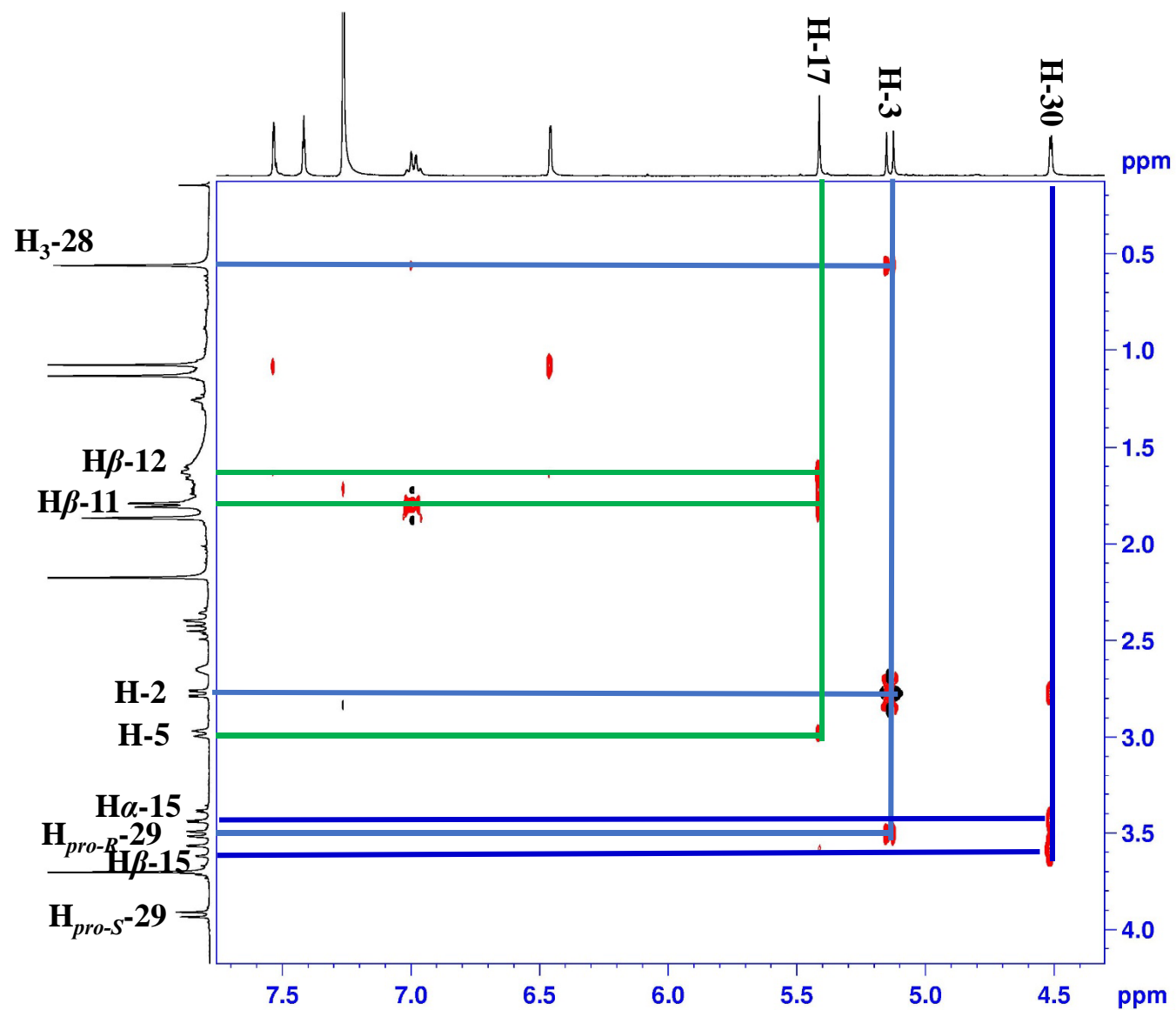
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EXPNO      7
PROCNO     1
Date_      20180123
Time       4.35
INSTRUM     spect
PROBHD      5 mm CPPBBO BB
PULPROG     noesygpphph
TD          2048
SOLVENT     CDCl3
NS          16
DS          32
SWH         4000.000 Hz
FIDRES      1.953125 Hz
AQ          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 ppm
FnMODE     States-TPPI
SI         1024
SF         400.1300062 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
LB         0.00 Hz
GB         0
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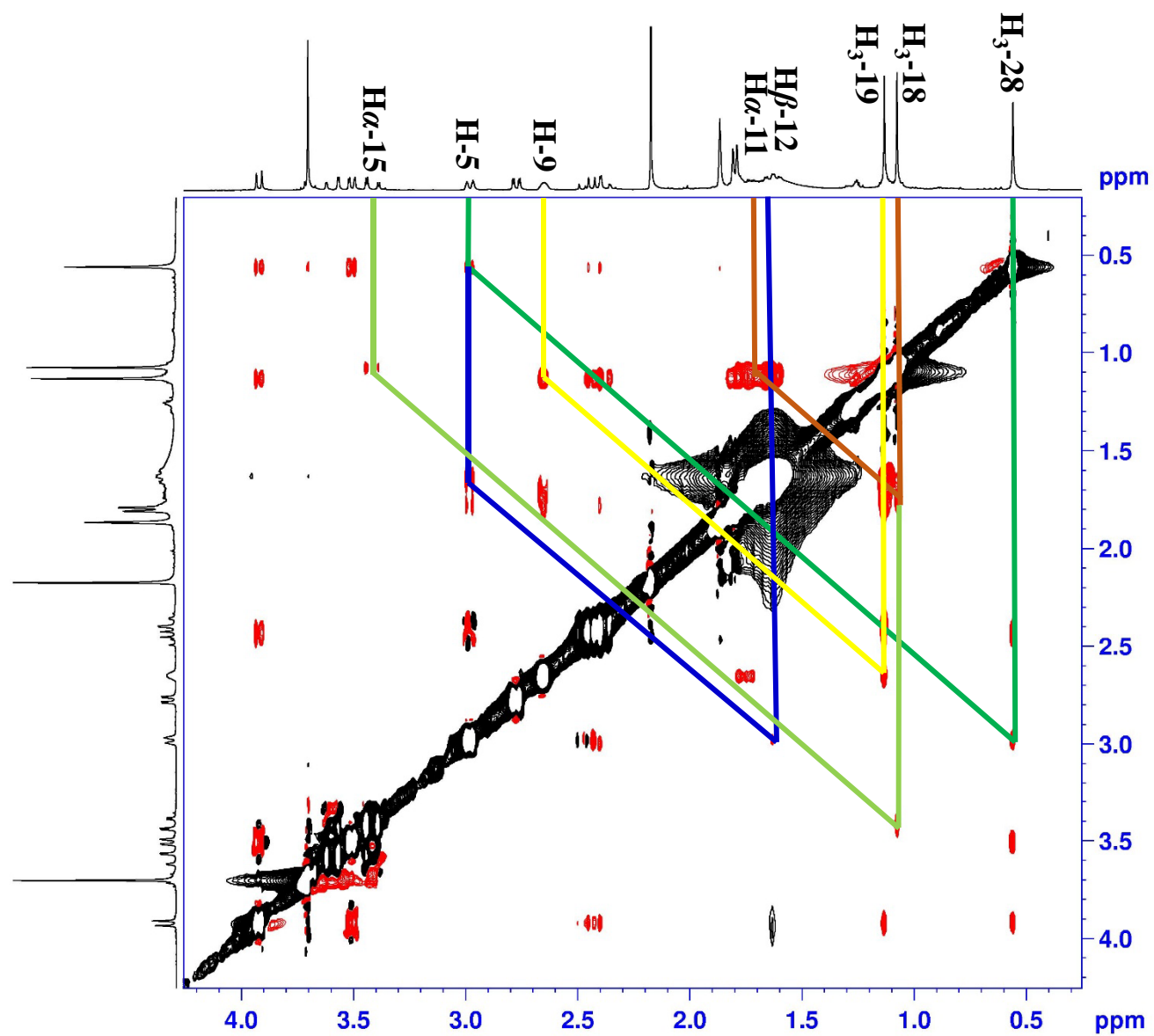
NOESY (400 MHz) spectrum of compound **3** in CDCl_3



NOESY (400 MHz) spectrum of compound **3** in CDCl₃



NOESY (400 MHz) spectrum of compound **3** in CDCl_3



HR-ESIMS for compound 4

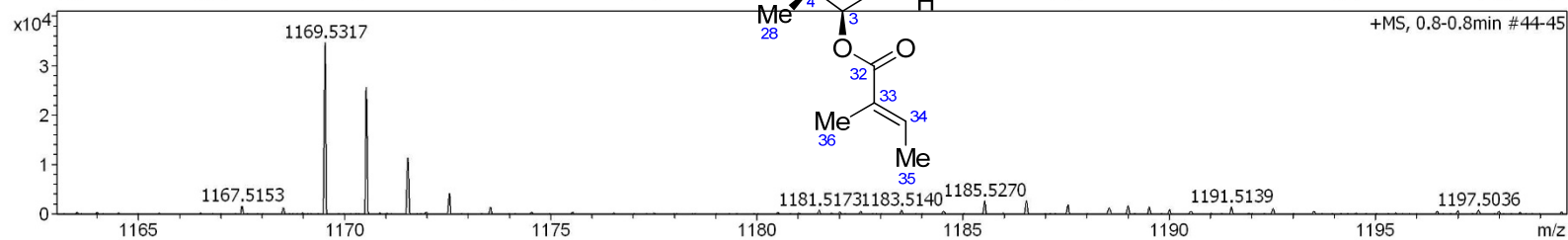
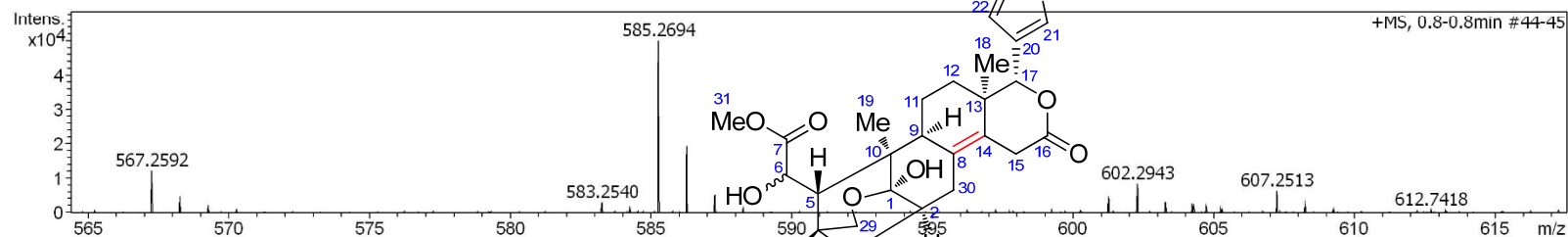
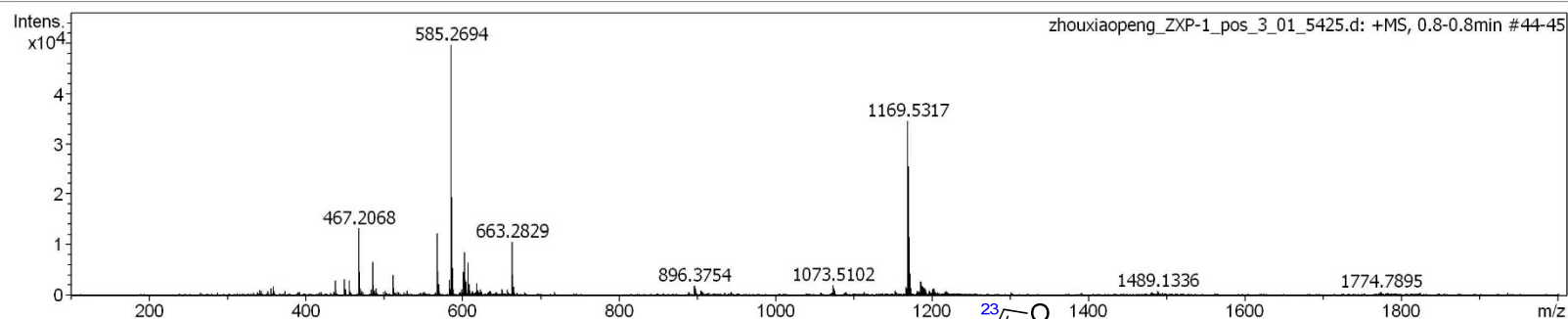
Generic Display Report

Analysis Info

Analysis Name D:\Data\MS\data\201809\zhouxiaopeng_ZXP-1_pos_3_01_5425.d
Method LC_Direct Infusion_pos_100-1000mz.m
Sample Name zhouxiaopeng_ZXP-1_pos
Comment

Acquisition Date 9/7/2018 4:58:32 PM

Operator SCSIO
Instrument maXis



HR-ESIMS for compound 4

Mass Spectrum SmartFormula Report

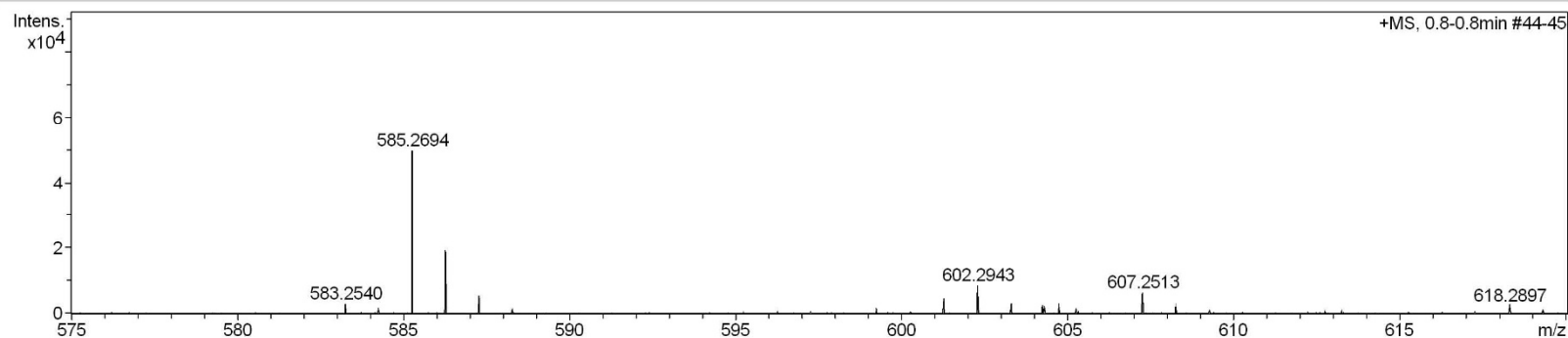
Analysis Info

Analysis Name D:\Data\MS\data\201809\zhouxiaopeng_ZXP-1_pos_3_01_5425.d
 Method LC_Direct Infusion_pos_100-1000mz.m
 Sample Name zhouxiaopeng_ZXP-1_pos
 Comment

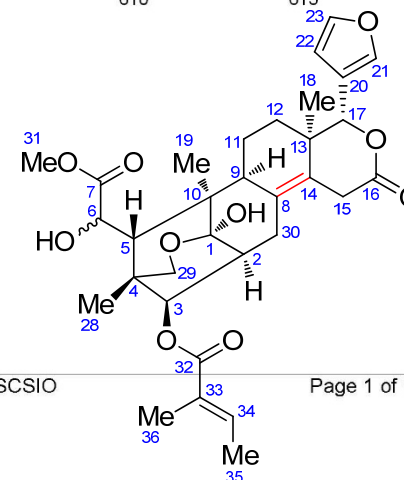
Acquisition Date 9/7/2018 4:58:32 PM
 Operator SCSIO
 Instrument maXis 255552.00029

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	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
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 ⁻ Conf	N-Rule
585.2694	1	C32H41O10	100.00	585.2694	-0.1	-0.1	22.1	12.5	even	ok
607.2513	1	C32H40NaO10	100.00	607.2514	-0.1	-0.0	38.7	12.5	even	ok
1169.5317	1	C64H81O20	100.00	1169.5316	-0.1	-0.1	26.9	24.5	even	ok



zhouxiaopeng_ZXP-1_pos_3_01_5425.d
 Bruker Compass DataAnalysis 4.1

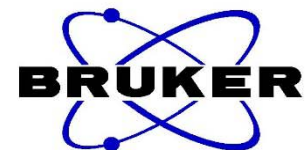
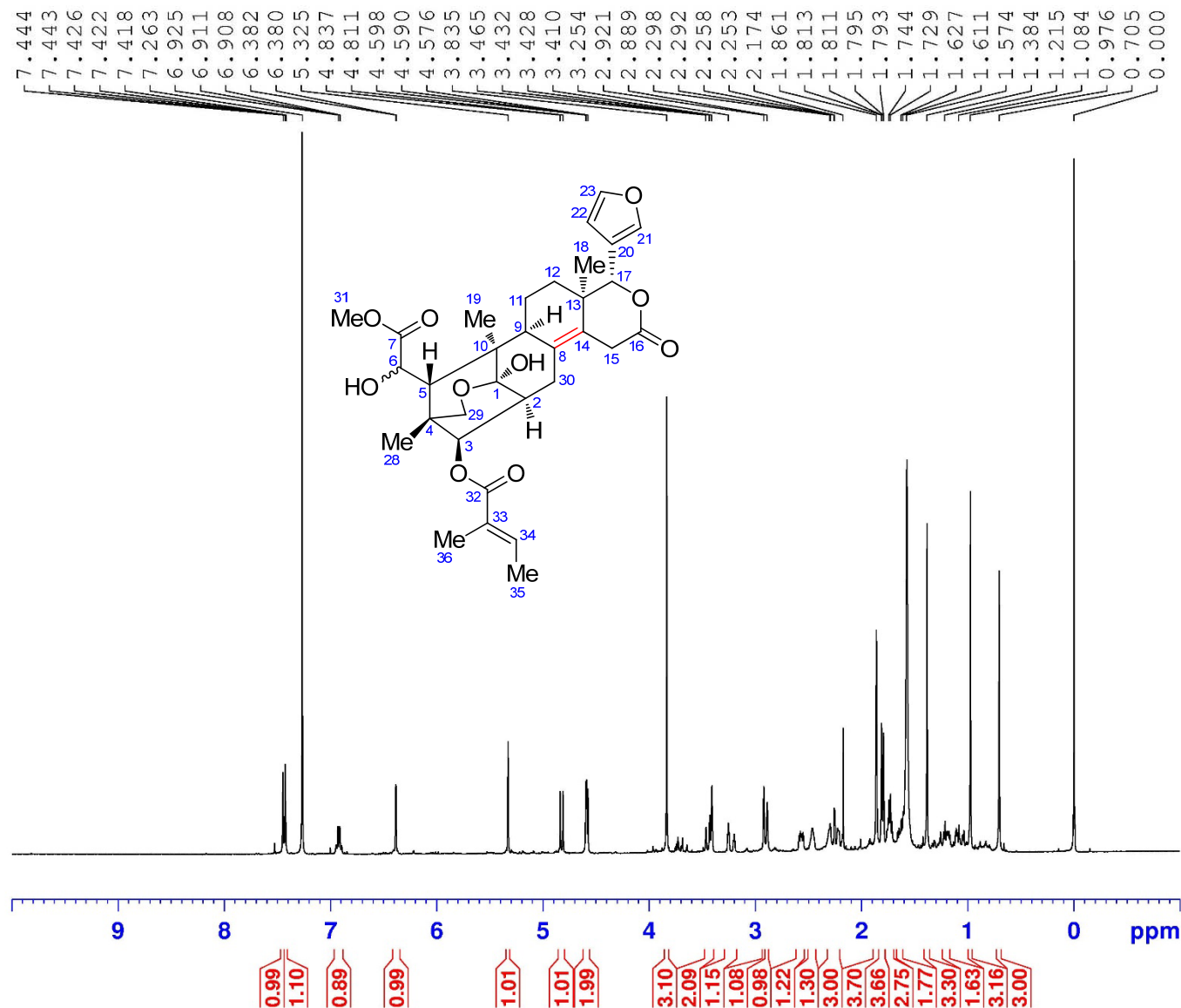
printed: 9/7/2018 5:03:16 PM

by: SCSIO

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¹H NMR (400 MHz) spectrum of compound **4** in CDCl₃

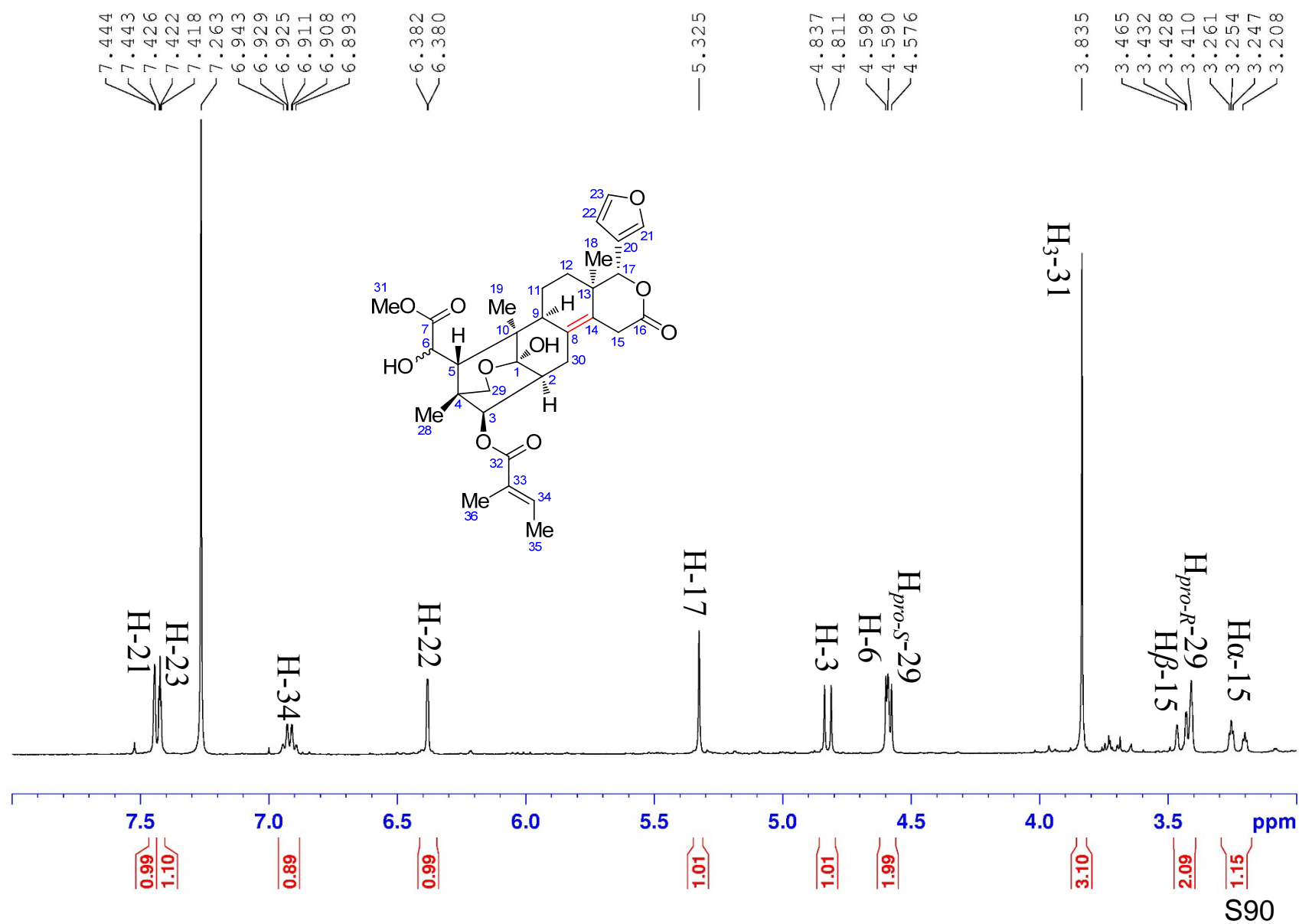


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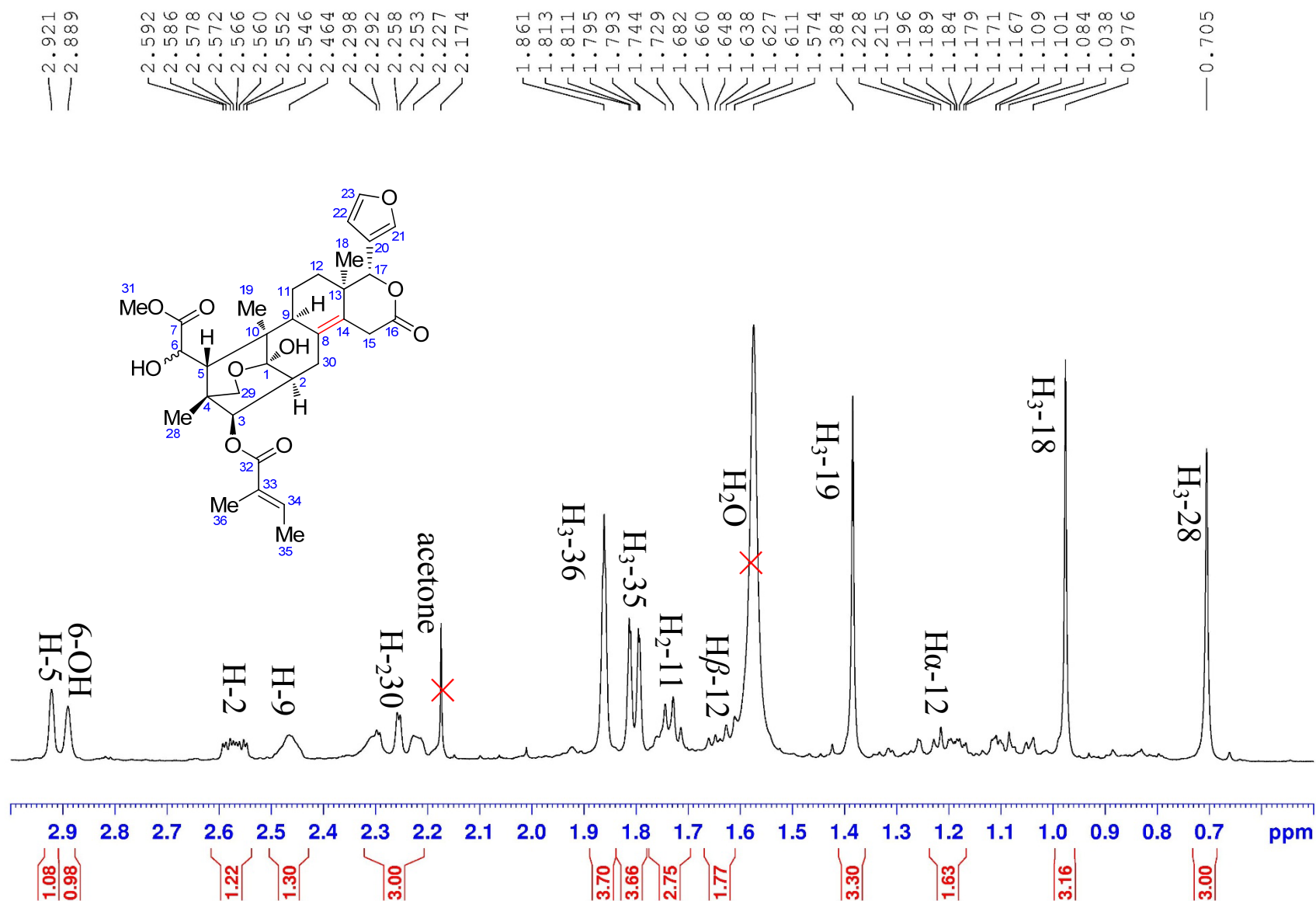
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EXPNO     1
PROCNO    1
Date_     20180704
Time      6.26
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS        16
DS        2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ        3.9846387 sec
RG        208.5
DW        60.800 usec
DE        10.00 usec
TE        297.0 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1      400.1324710 MHz
NUC1      1H
P1        11.50 usec
SI        65536
SF        400.1300088 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

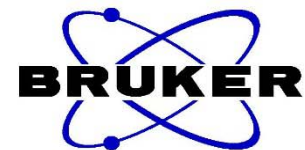
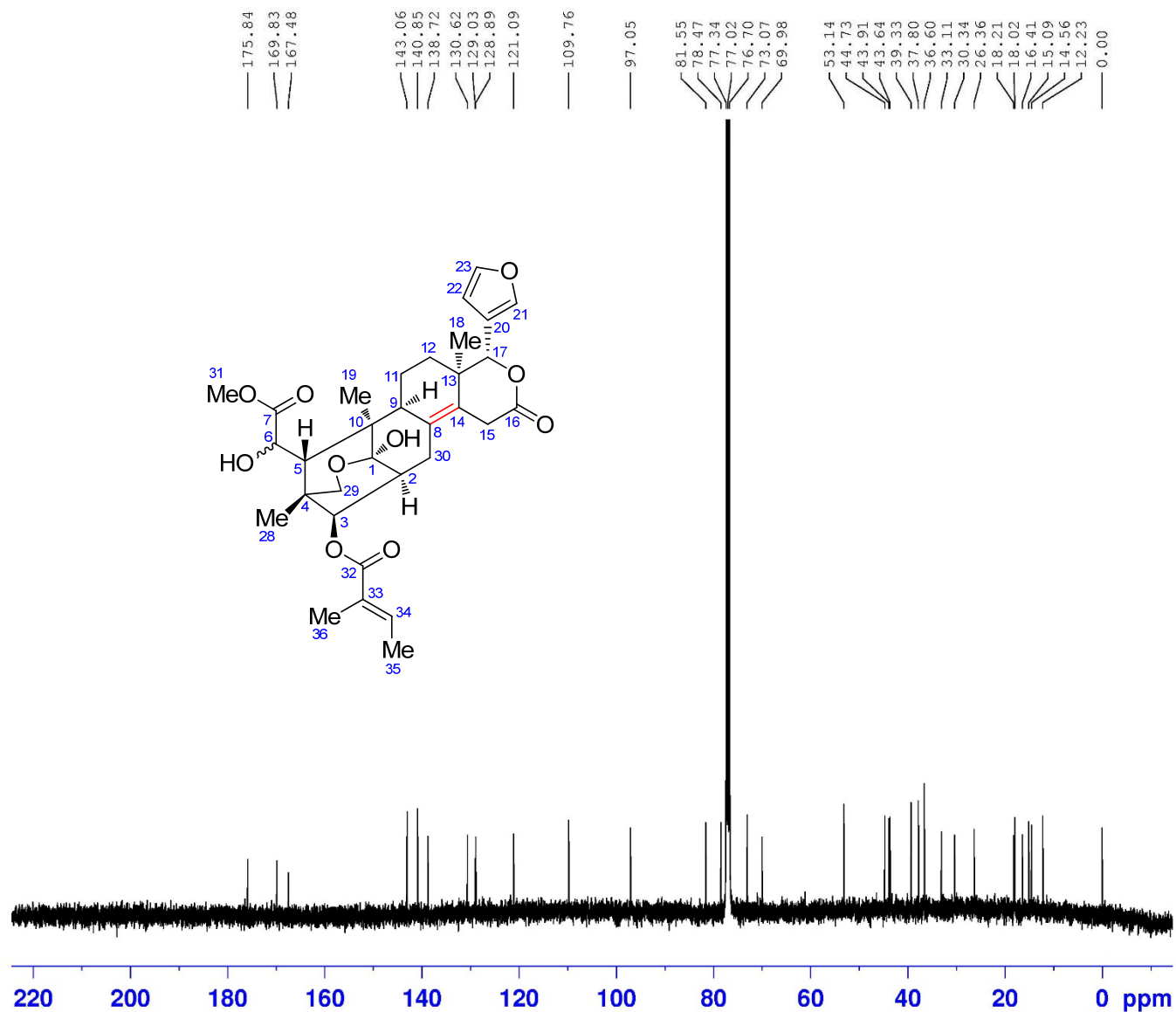
^1H NMR (400 MHz) spectrum of compound **4** in CDCl_3



^1H NMR (400 MHz) spectrum of compound **4** in CDCl_3



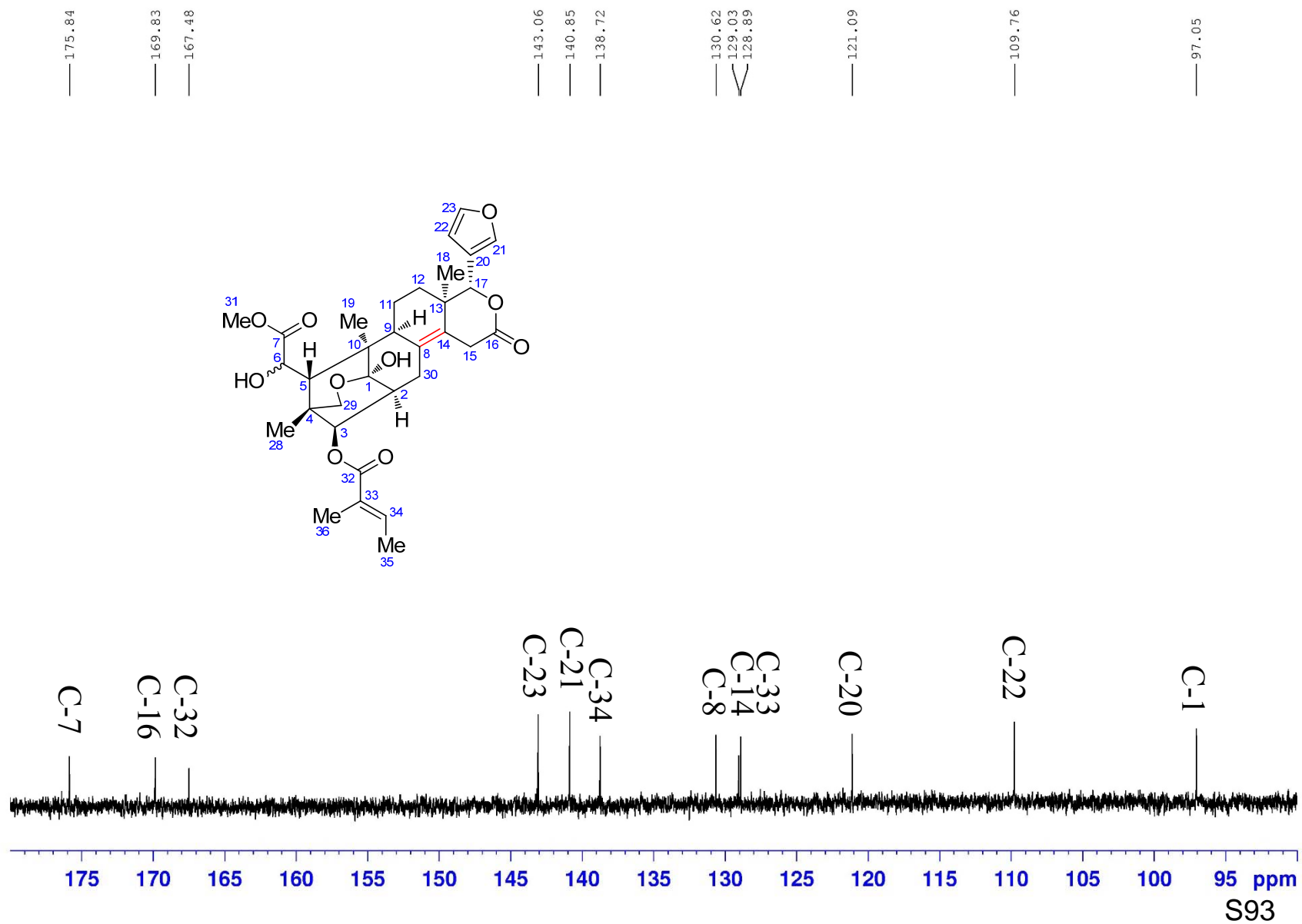
^{13}C NMR (100 MHz) spectrum of compound **4** in CDCl_3



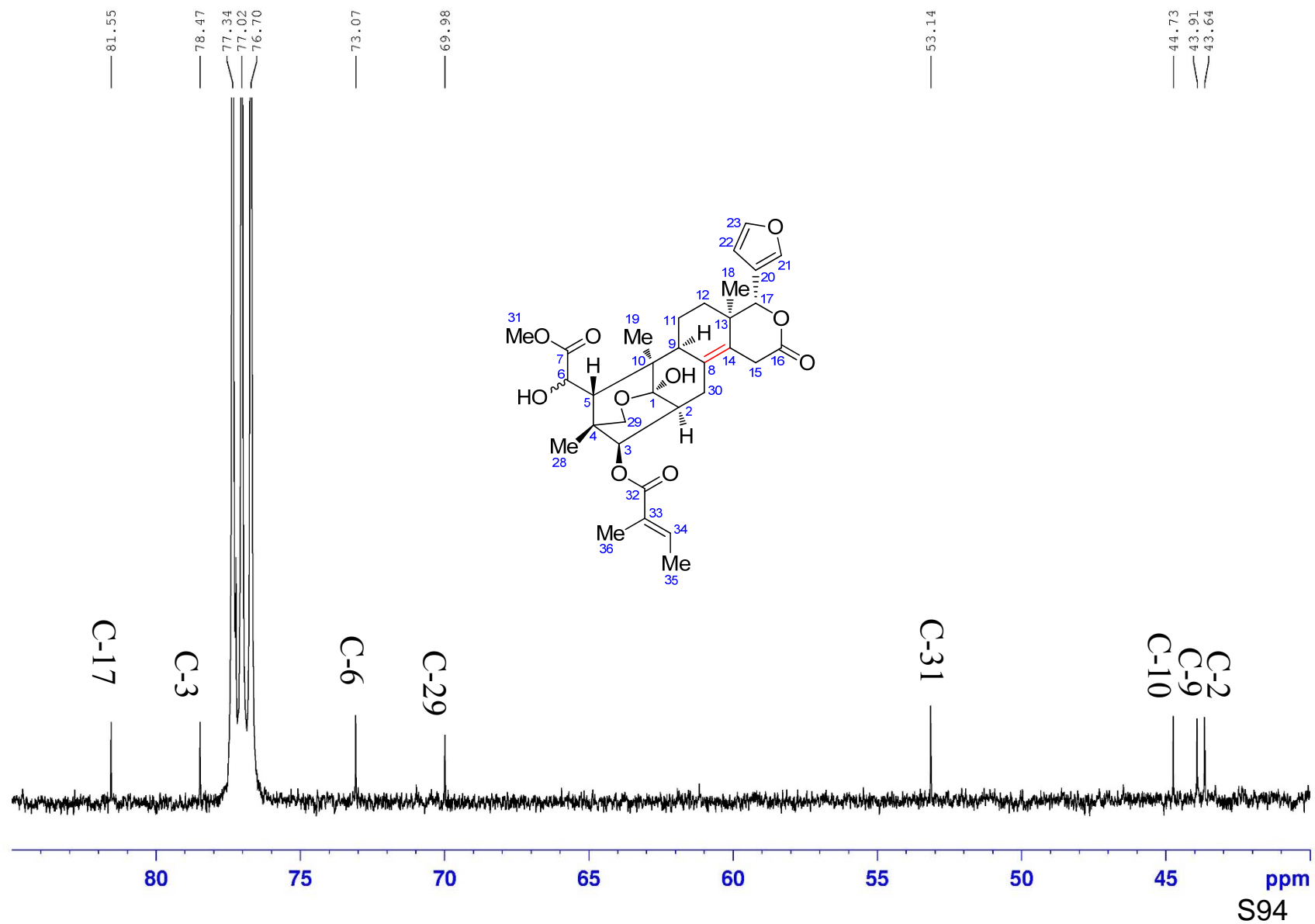
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 EXPNO 2
 PROCNO 1
 Date_ 20180704
 Time 7.26
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 147.94
 DW 20.800 usec
 DE 18.00 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6233324 MHz
 NUC1 ^{13}C
 P1 10.00 usec
 SI 32768
 SF 100.6127689 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

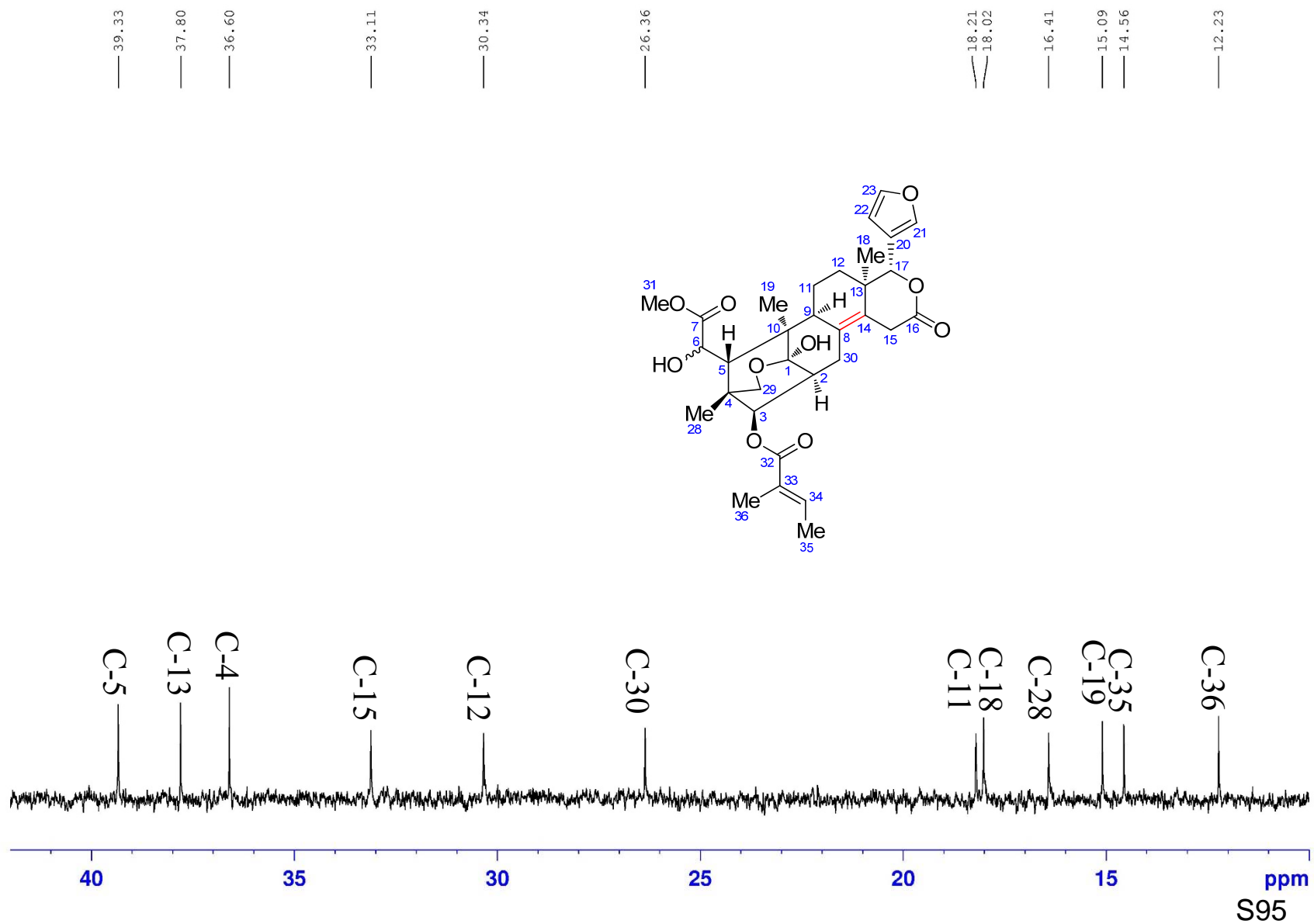
^{13}C NMR (100 MHz) spectrum of compound **4** in CDCl_3



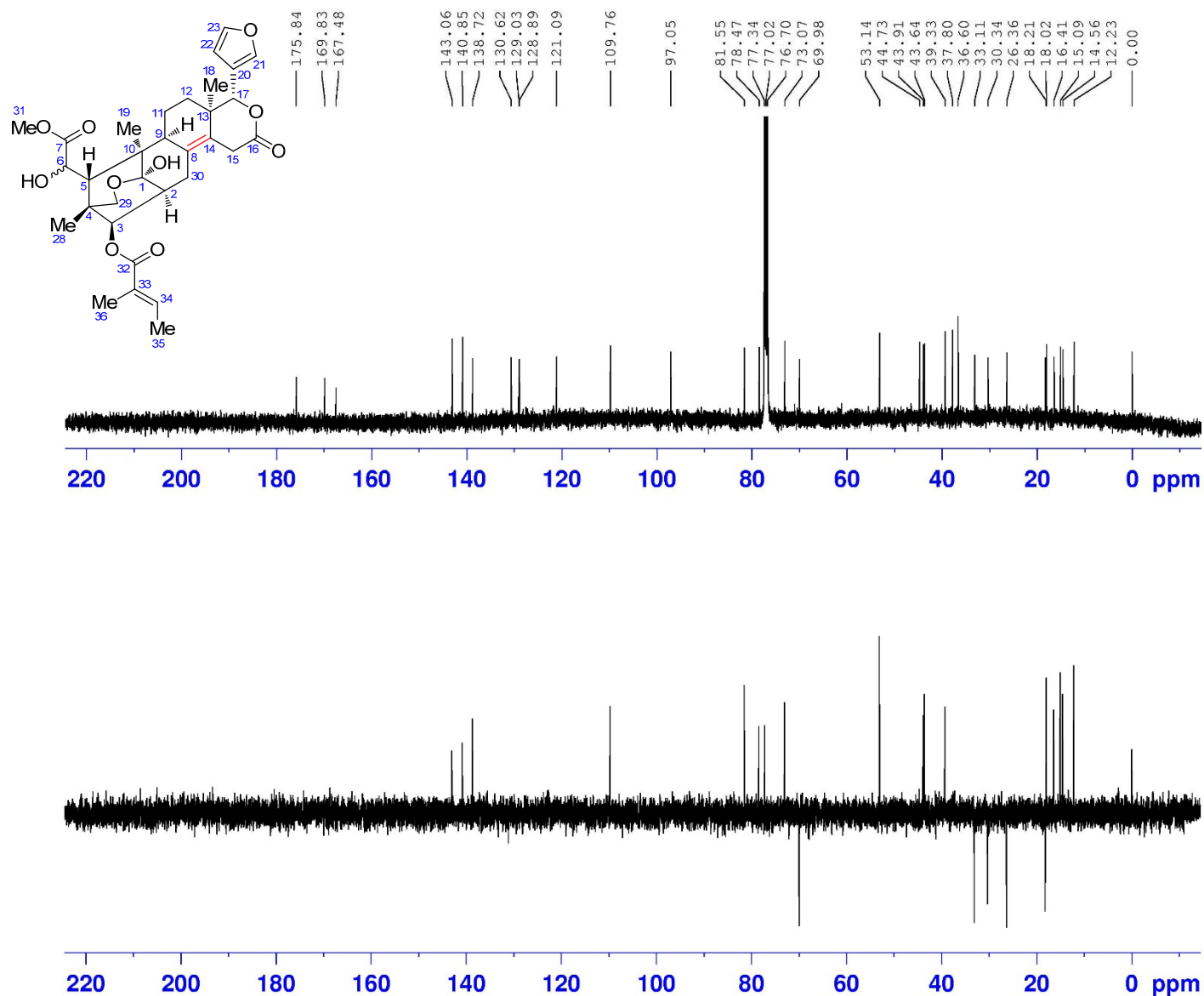
^{13}C NMR (100 MHz) spectrum of compound **4** in CDCl_3



^{13}C NMR (100 MHz) spectrum of compound **4** in CDCl_3



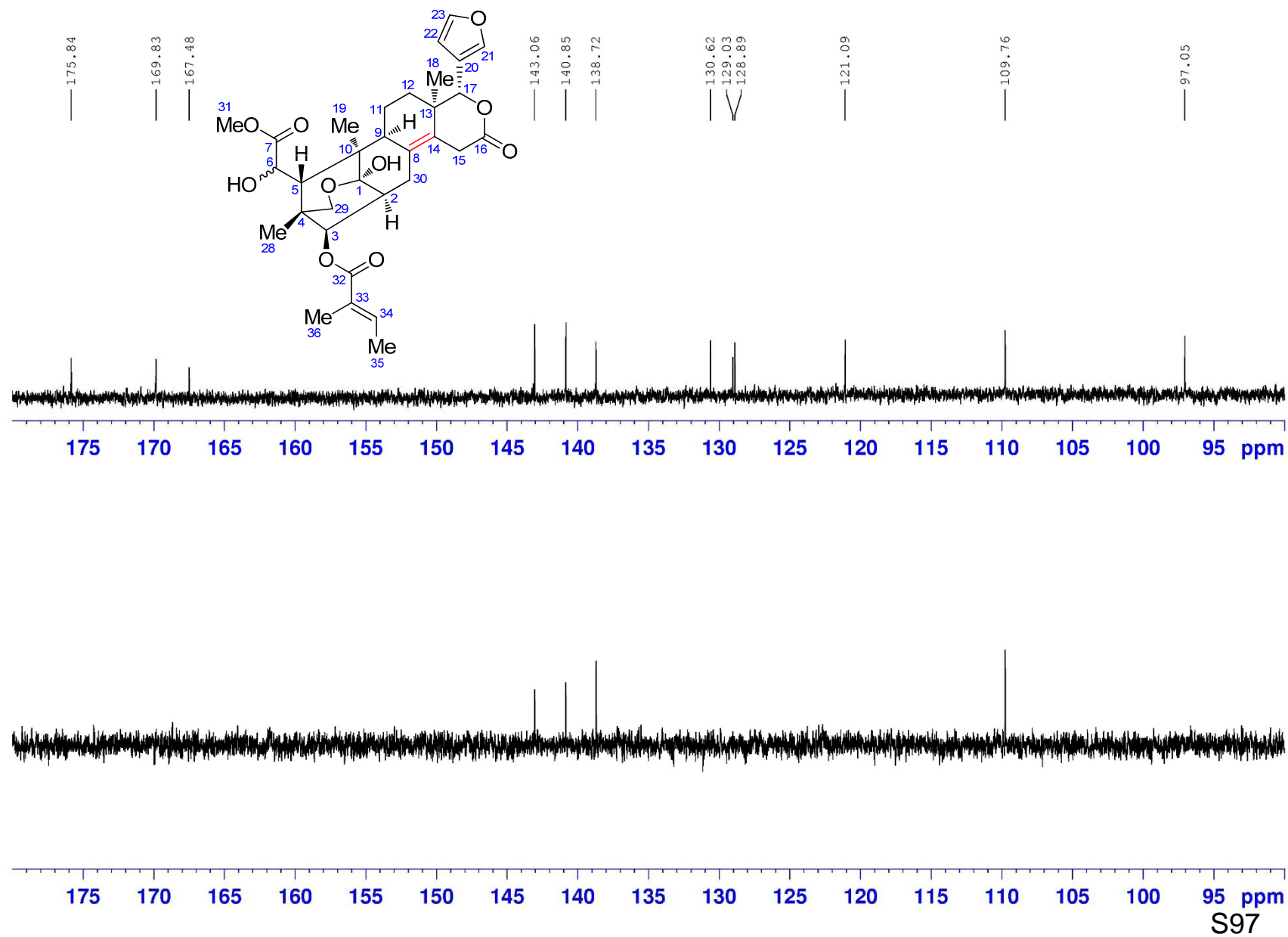
DEPT135 (100 MHz) spectrum of compound **4** in CDCl₃



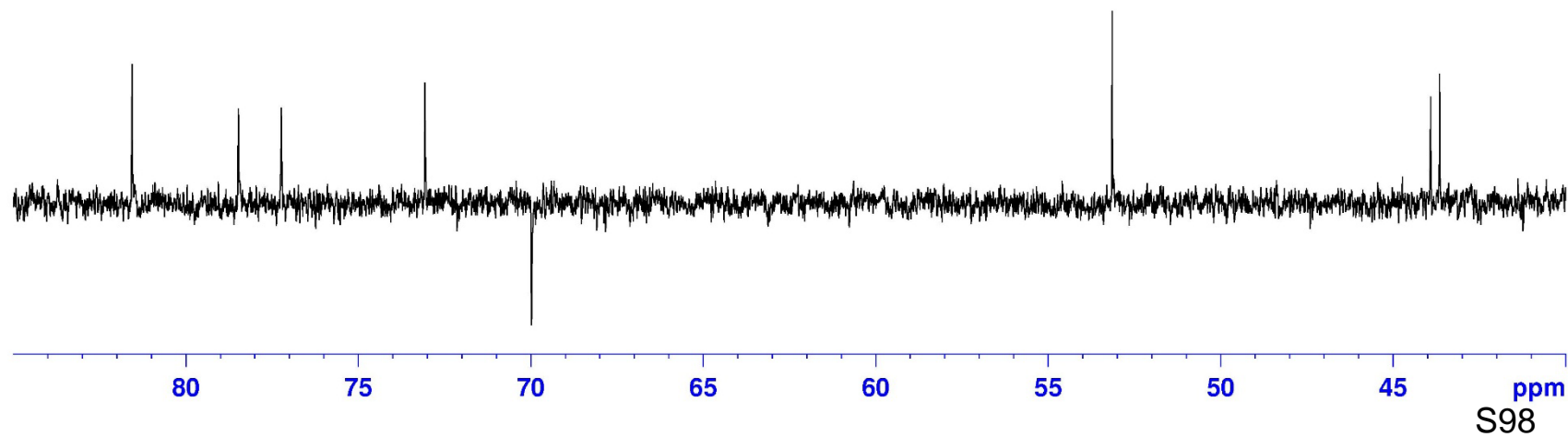
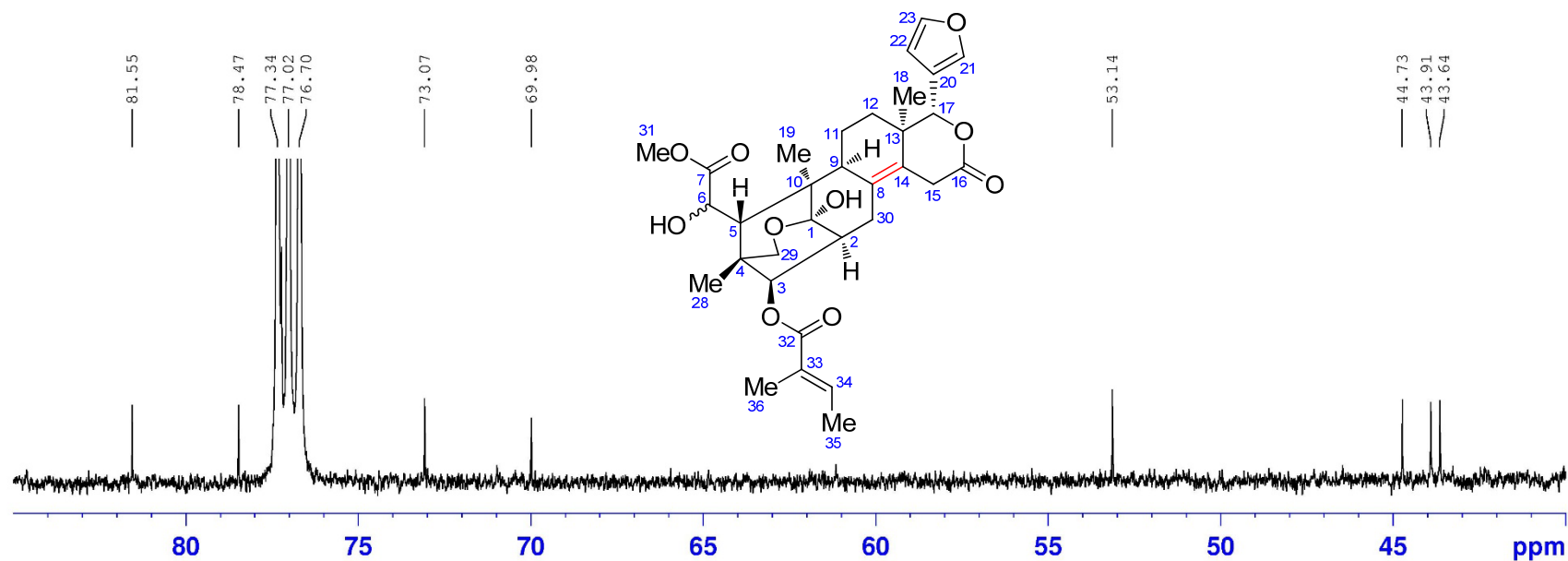
NAME ZXP-R-17-2-1-2
 EXPNO 2
 PROCNO 1
 Date_ 20180704
 Time 7.26
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 147.94
 DW 20.800 usec
 DE 18.00 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6233324 MHz
 NUC1 13C
 P1 10.00 usec
 SI 32768
 SF 100.6127689 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

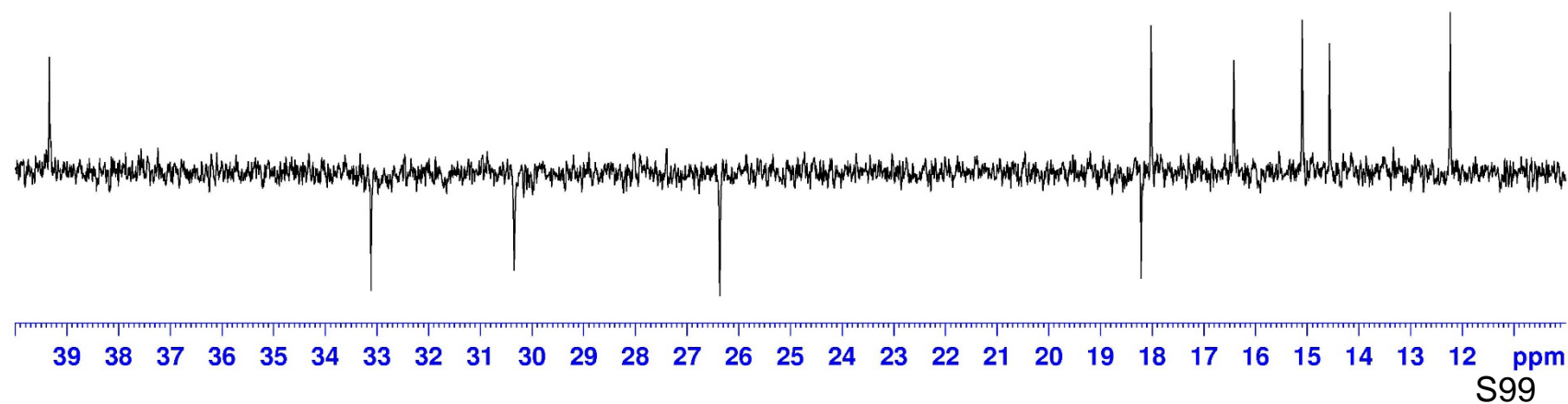
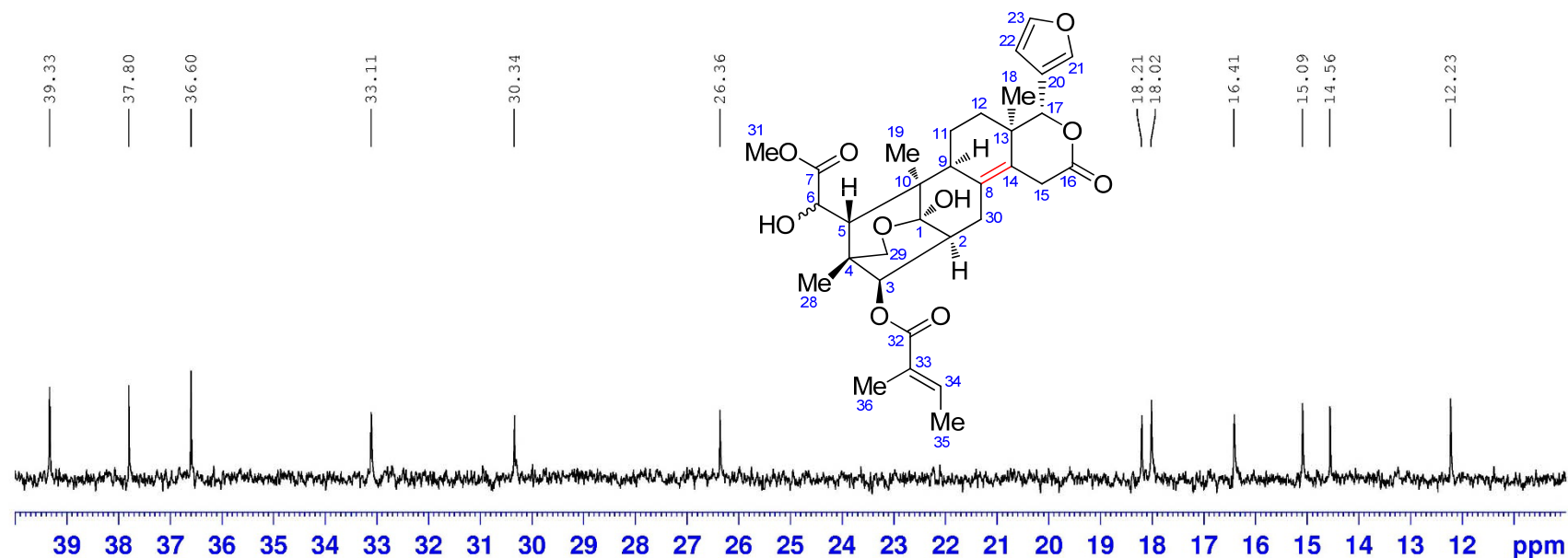
DEPT135 (100 MHz) spectrum of compound **4** in CDCl₃



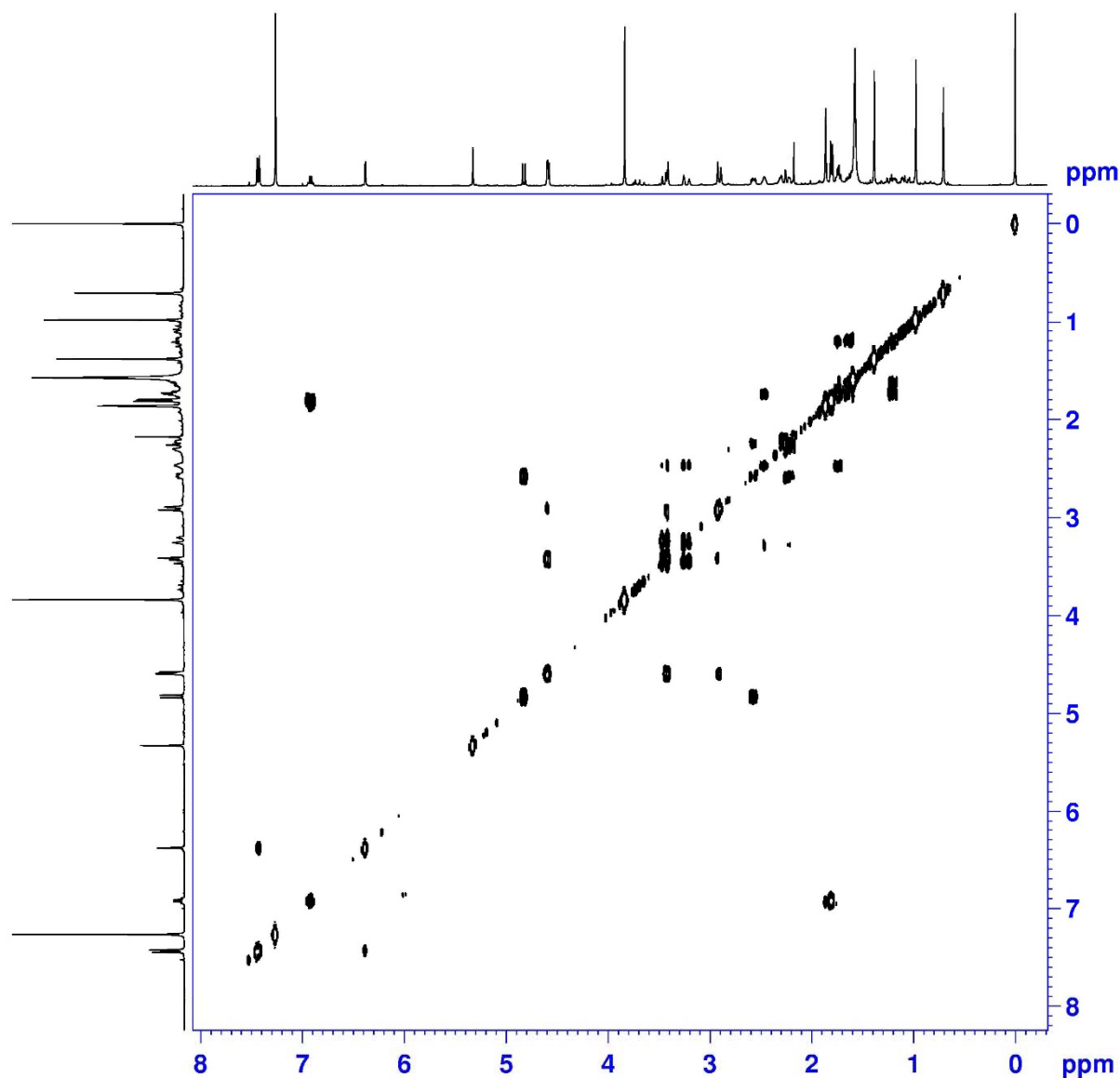
DEPT135 (100 MHz) spectrum of compound **4** in CDCl₃



DEPT135 (100 MHz) spectrum of compound **4** in CDCl₃



^1H - ^1H COSY (400 MHz) spectrum of compound **4** in CDCl_3

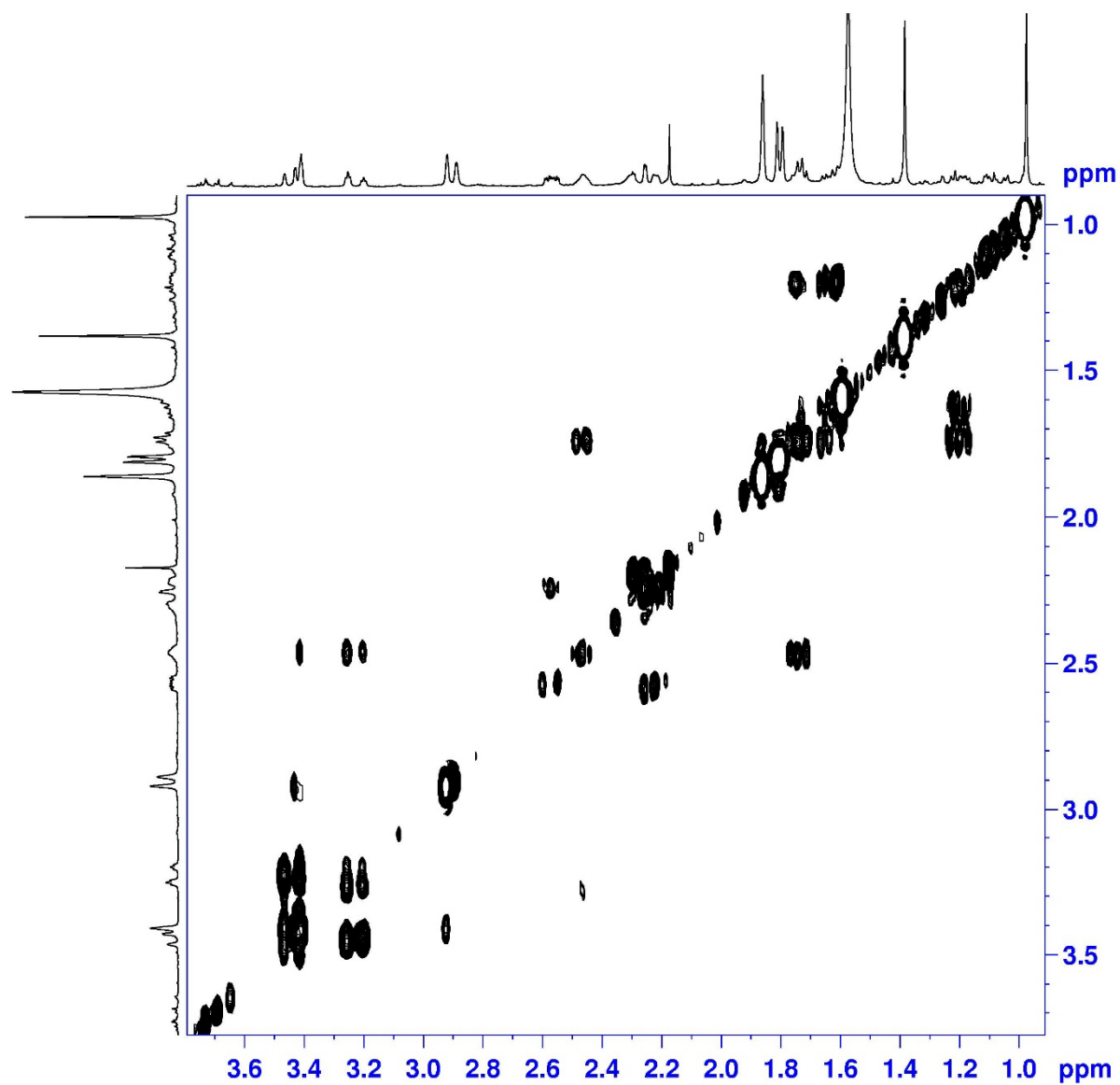


NAME ZXP-R-17-2-1-2
EXPNO 4
PROCNO 1
Date_ 20180707
Time 17.34
INSTRUM spect
PROBHD 5 mm CFPBBO BB
PULPROG cosygppqf
TD 2048
SOLVENT CDCl_3
NS 8
DS 8
SWH 3906.250 Hz
FIDRES 1.907349 Hz
AQ 0.2621940 sec
RG 208.5
DW 128.000 usec
DE 10.00 usec
TE 297.0 K
D0 0.00000300 sec
D1 1.89678097 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00025600 sec

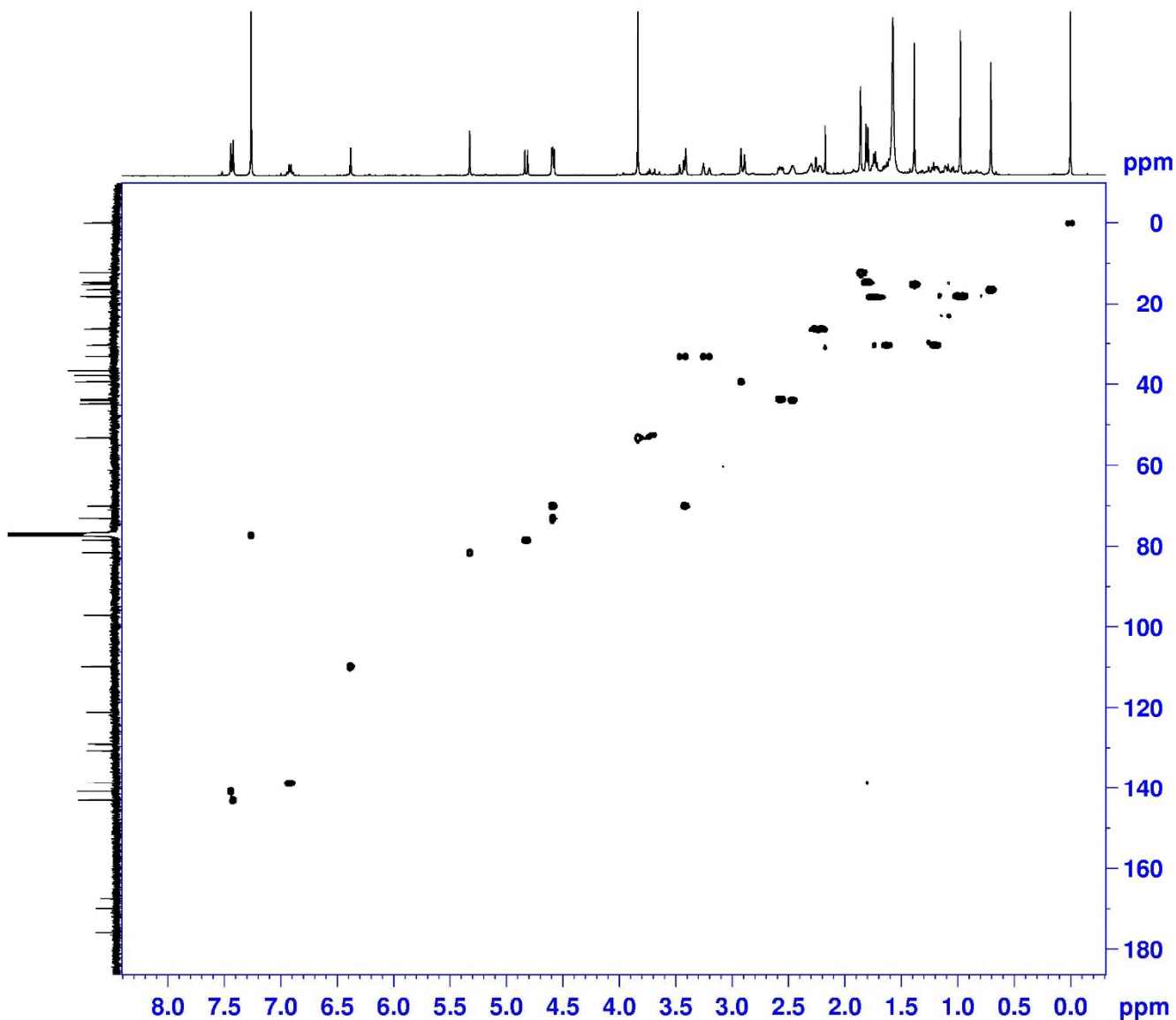
===== CHANNEL f1 =====
SFO1 400.1318006 MHz
NUC1 ^1H
P0 11.50 usec
P1 11.50 usec
P17 2500.00 usec
ND0 1
TD 128
SFO1 400.1318 MHz
FIDRES 30.517578 Hz
SW 9.762 ppm
FrMODE QF
SI 1024
SF 400.1300060 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 400.1300049 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0

S100

^1H - ^1H COSY (400 MHz) spectrum of compound **4** in CDCl_3



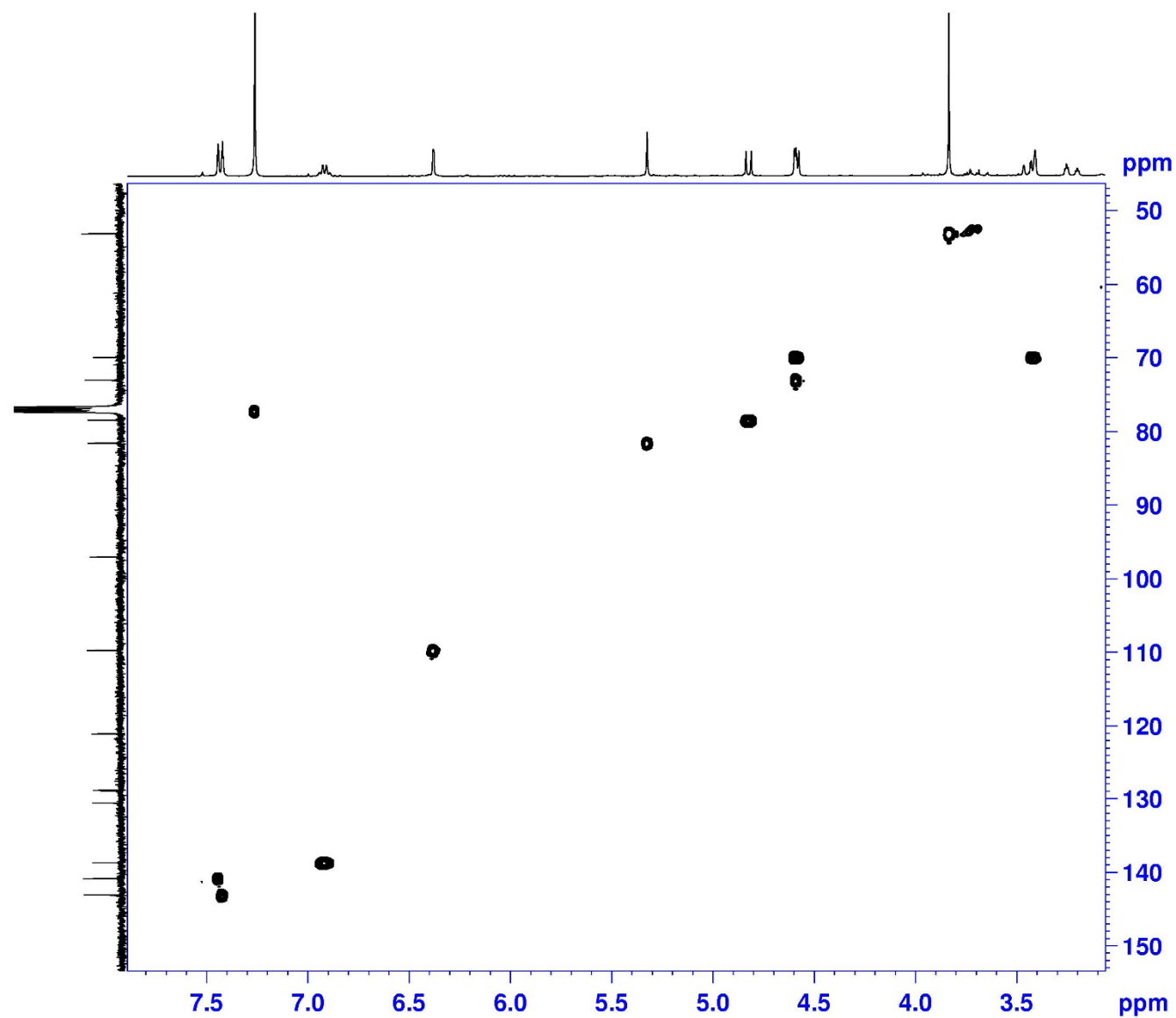
HSQC (400 MHz) spectrum of compound **4** in CDCl₃



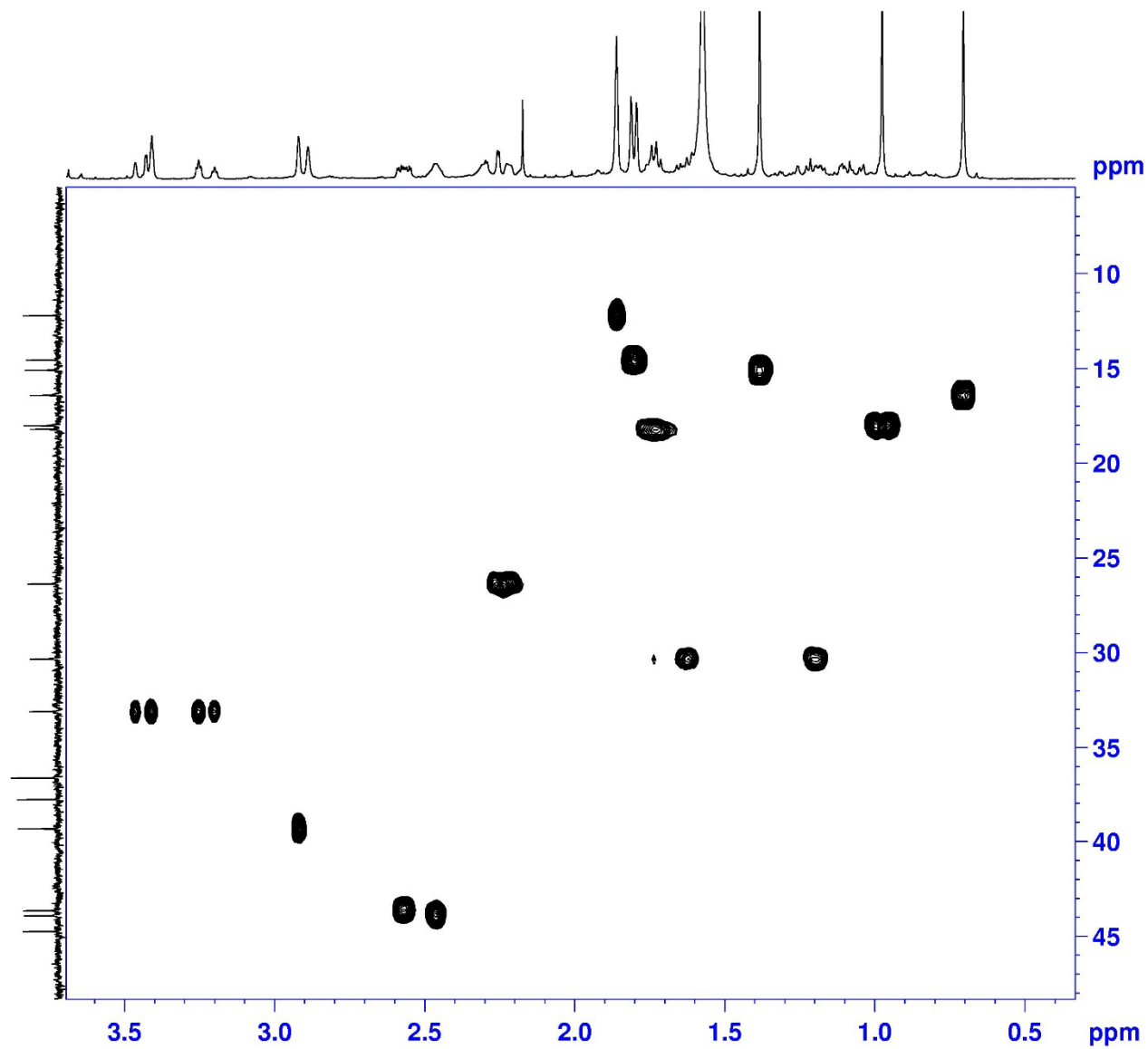
NAME ZXP-R-17-2-1-2
EXPNO 5
PROCNO 1
Date_ 20180707
Time 18.14
INSTRUM spect
PROBHD 5 mm CFPBBO BB
PULPROG hsqcetgpsi2
TD 1024
SOLVENT CDCl₃
NS 16
DS 16
SWH 4302.926 Hz
FIDRES 4.202076 Hz
AQ 0.1190388 sec
RG 208.5
DW 116.200 usec
DE 10.00 usec
TE 297.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46497905 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
IN0 0.00002080 sec
ZGPTNS

===== CHANNEL f1 =====
SF01 400.1320007 MHz
NUC1 ¹H
P1 11.50 usec
P2 23.00 usec
P28 0.00 usec
ND0 2
TD 256
SF01 100.6233 MHz
FIDRES 93.900238 Hz
SW 238.896 ppm
FnMODE Echo-Antiecho
SI 1024
SF 400.1300068 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 100.6127562 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

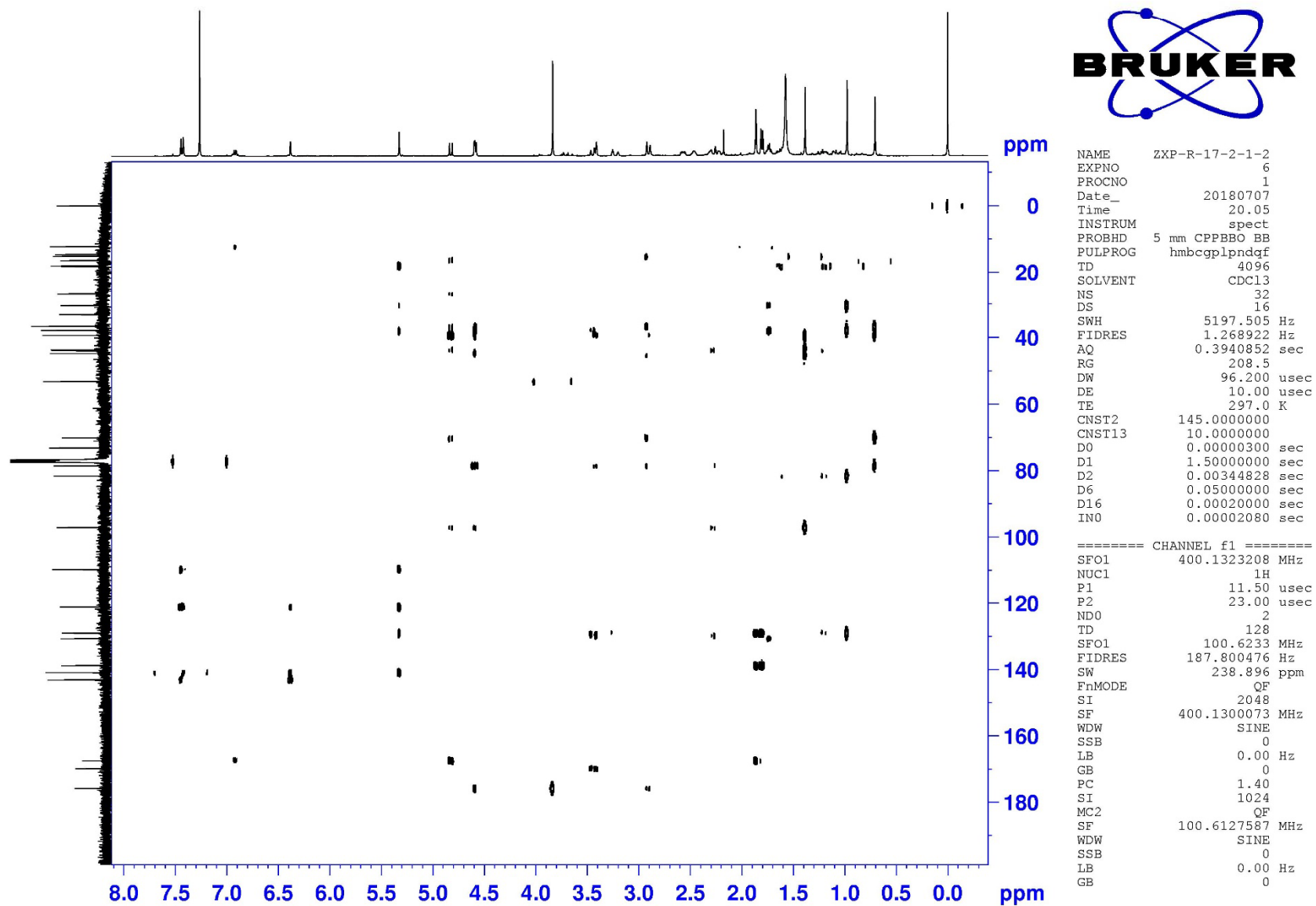
HSQC (400 MHz) spectrum of compound **4** in CDCl_3



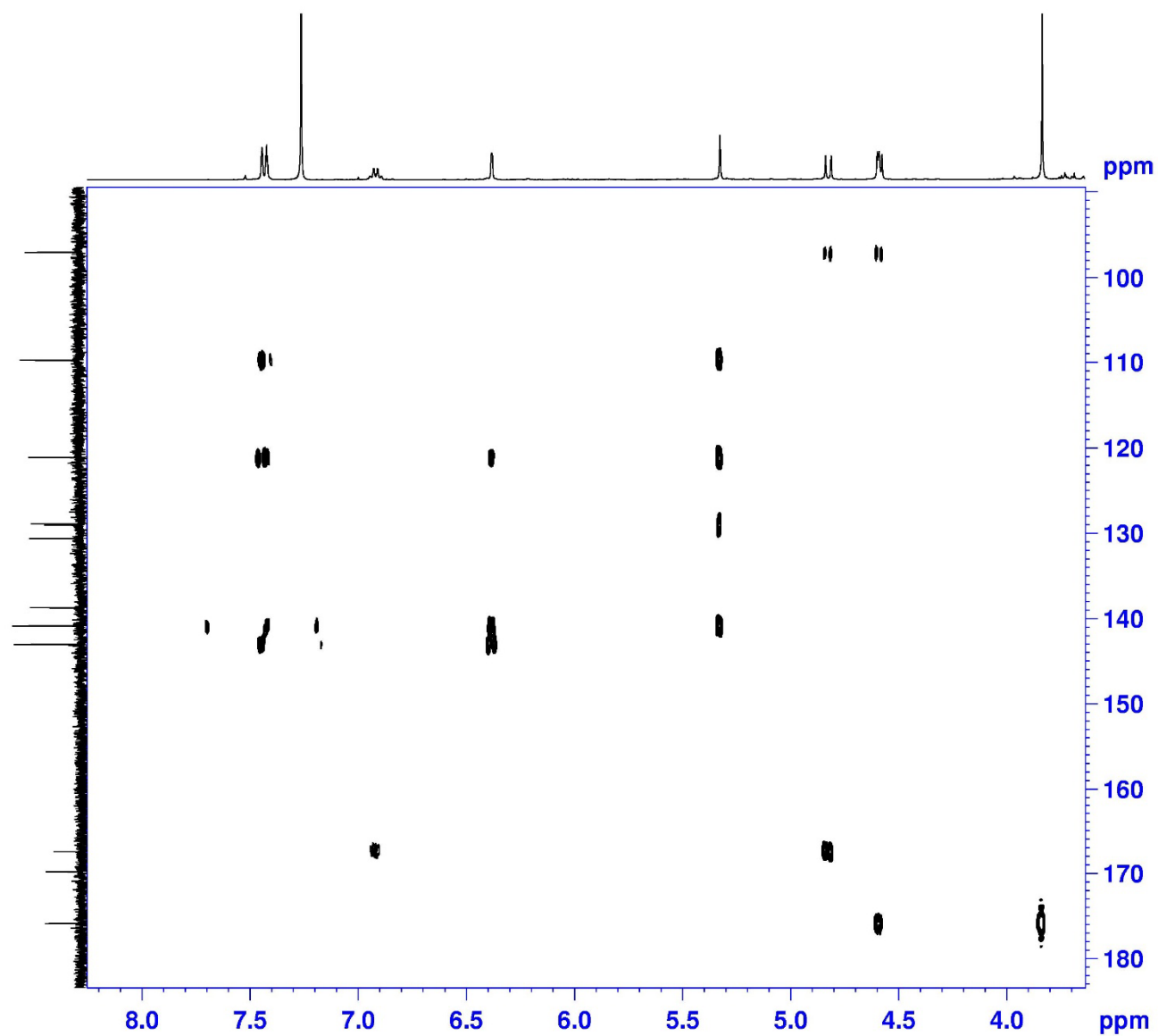
HSQC (400 MHz) spectrum of compound **4** in CDCl_3



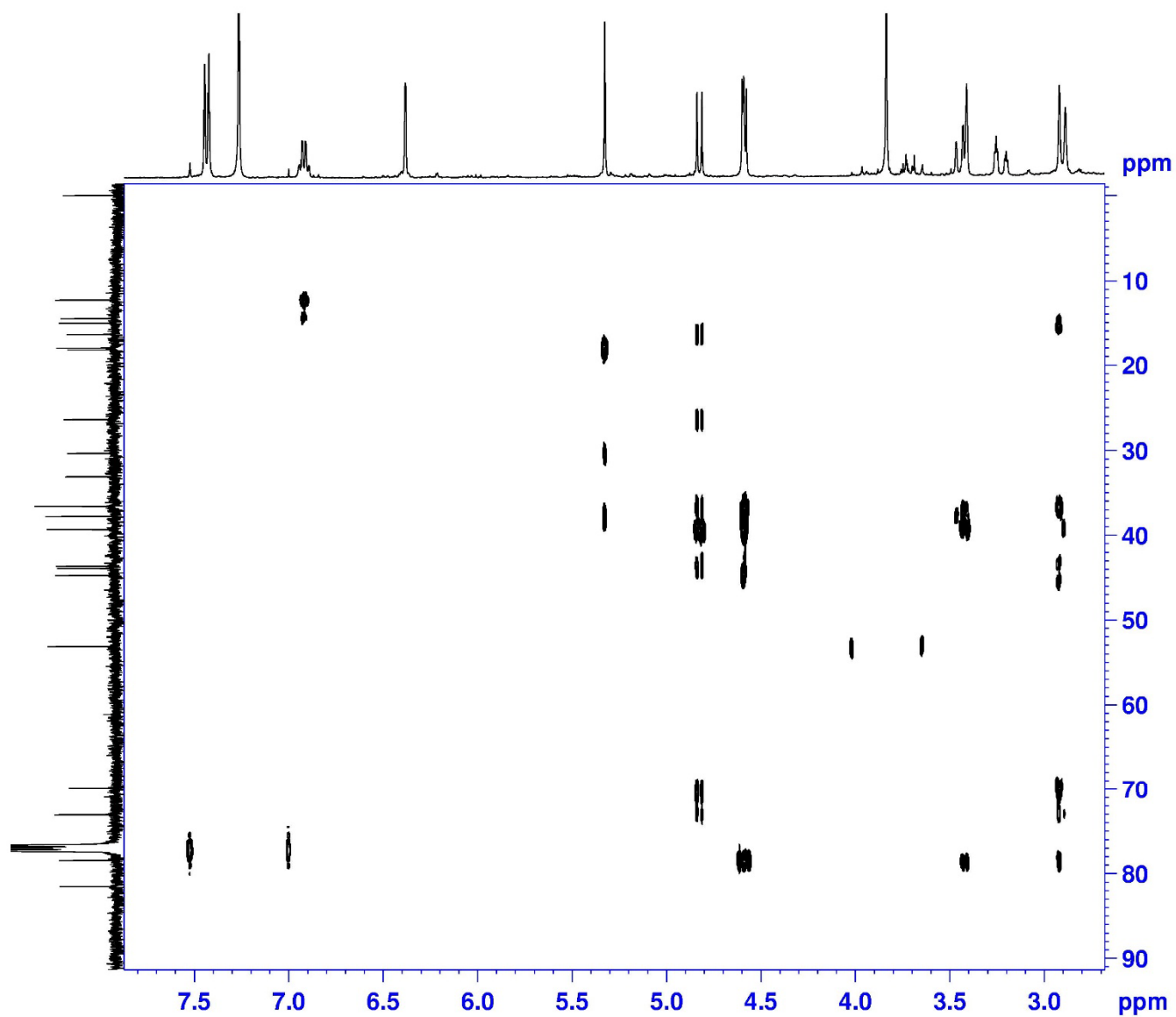
HMBC (400 MHz) spectrum of compound **4** in CDCl₃



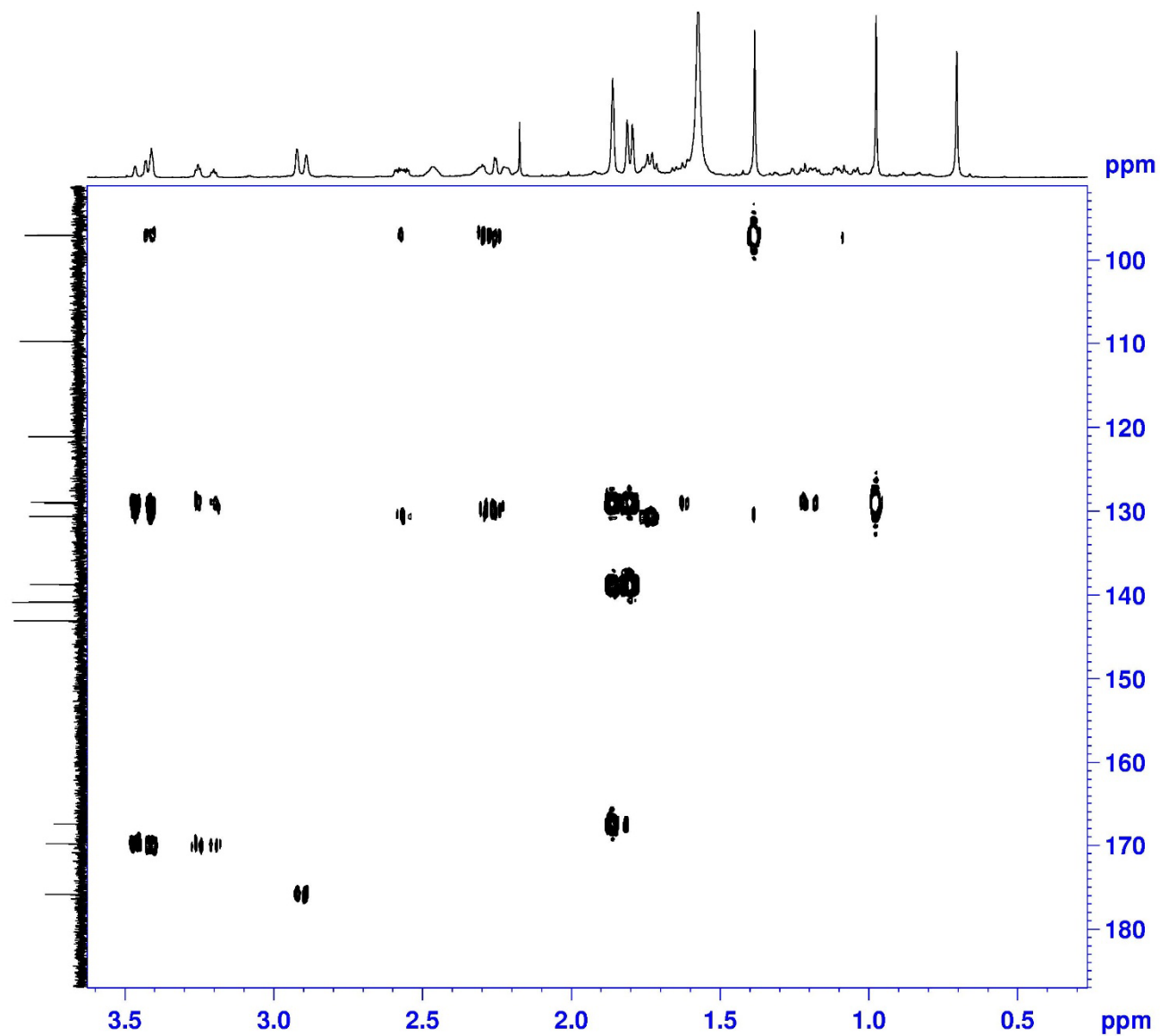
HMBC (400 MHz) spectrum of compound **4** in CDCl₃



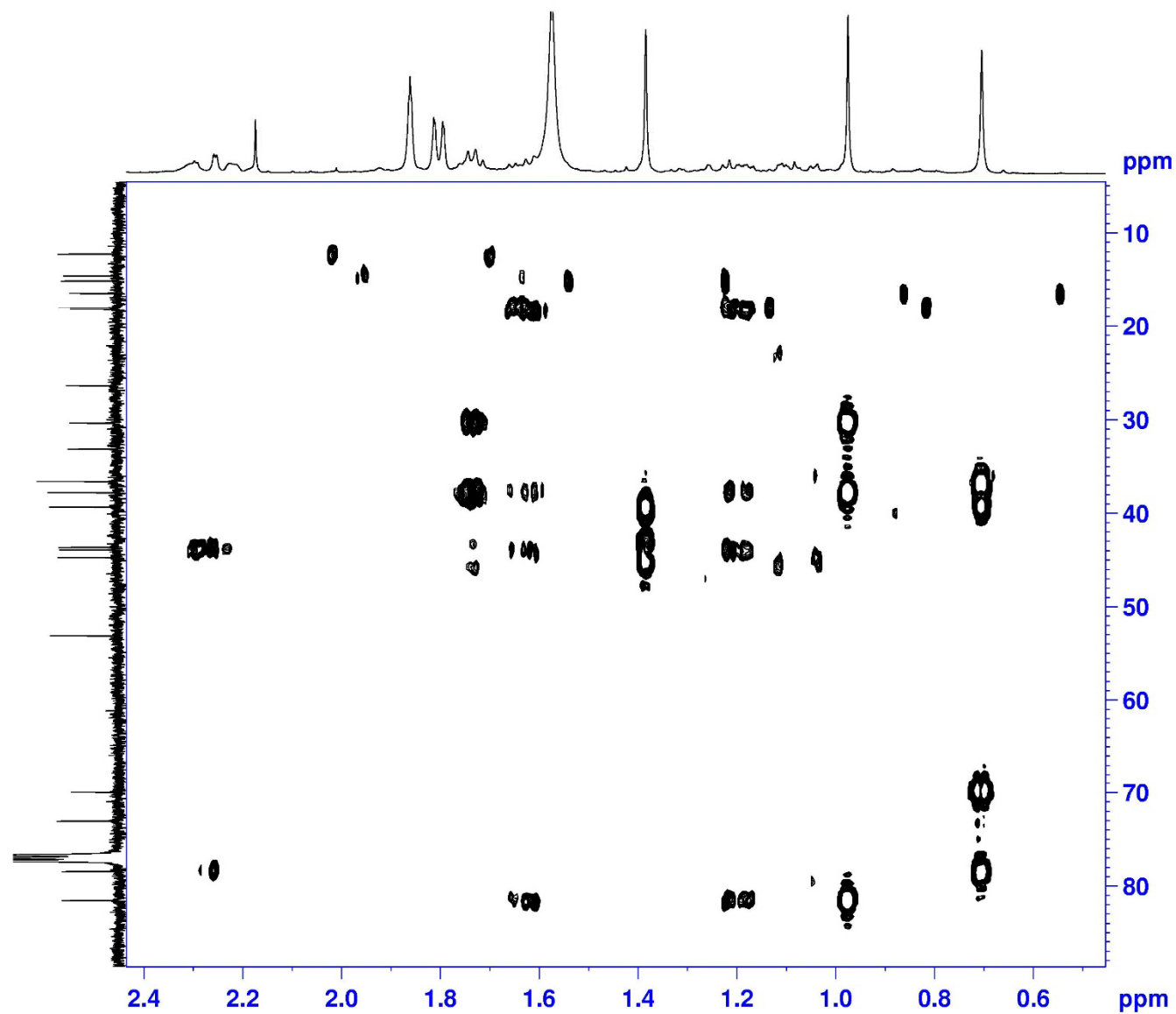
HMBC (400 MHz) spectrum of compound **4** in CDCl₃



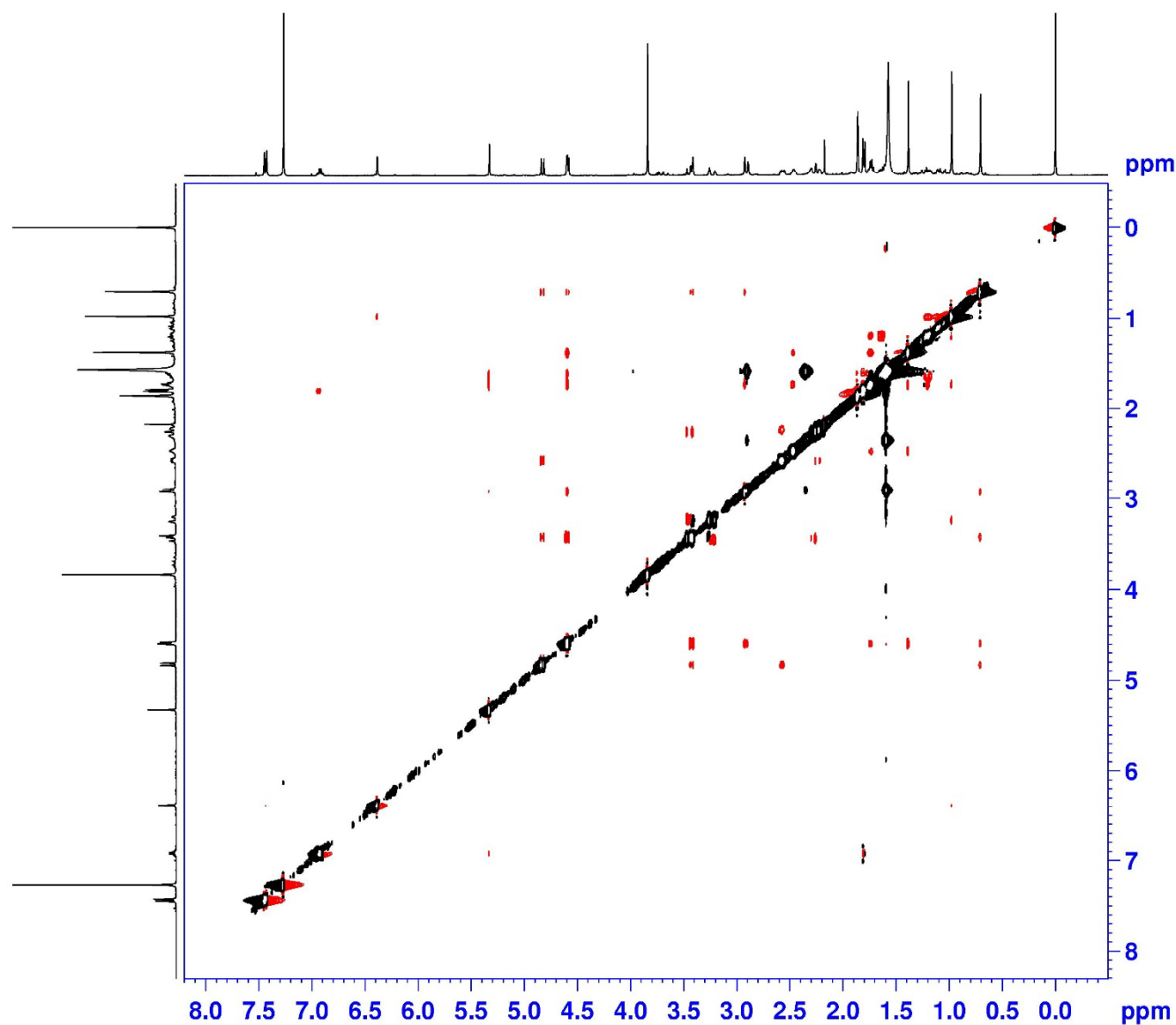
HMBC (400 MHz) spectrum of compound **4** in CDCl_3



HMBC (400 MHz) spectrum of compound **4** in CDCl₃



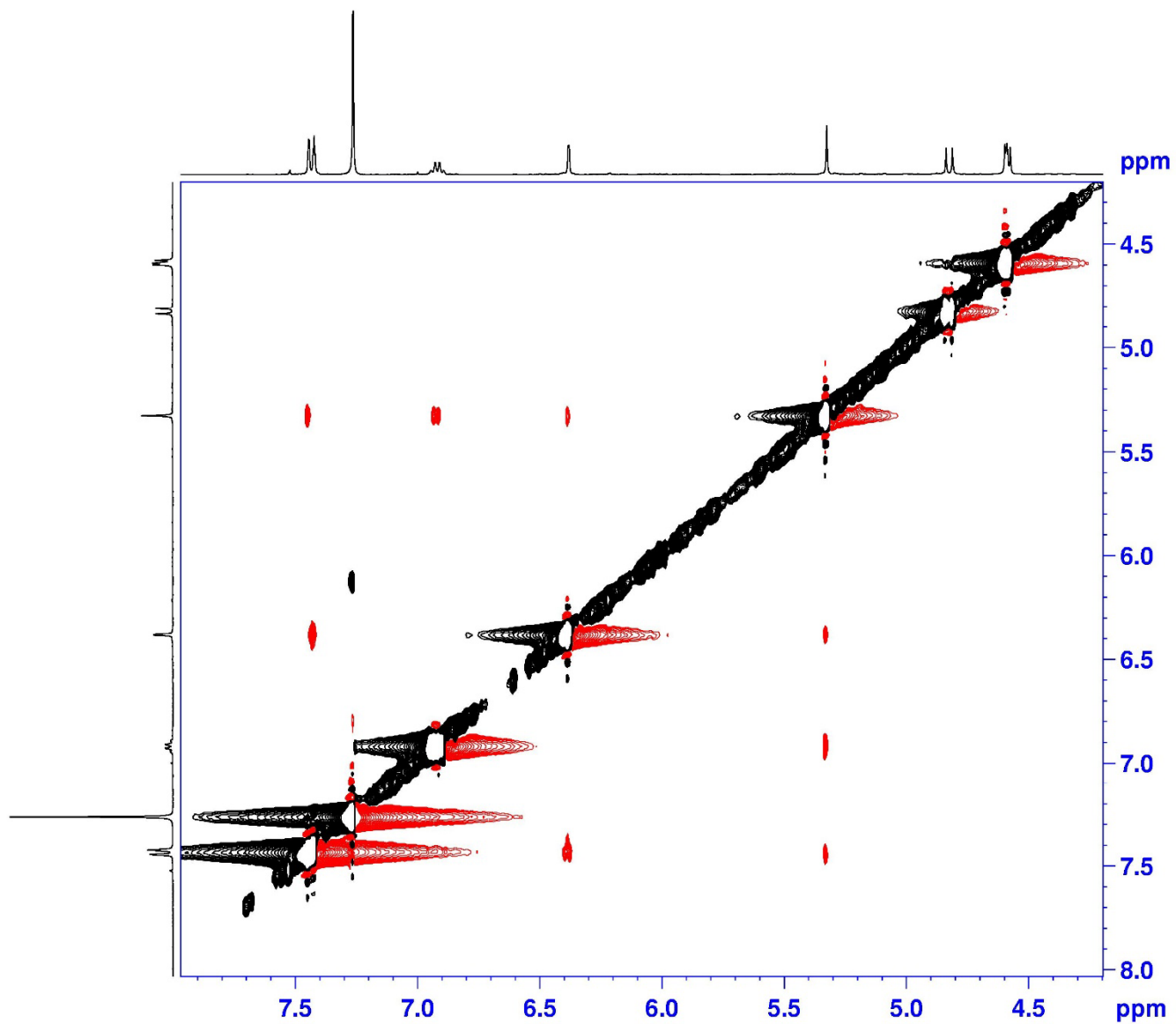
NOESY (400 MHz) spectrum of compound **4** in CDCl_3



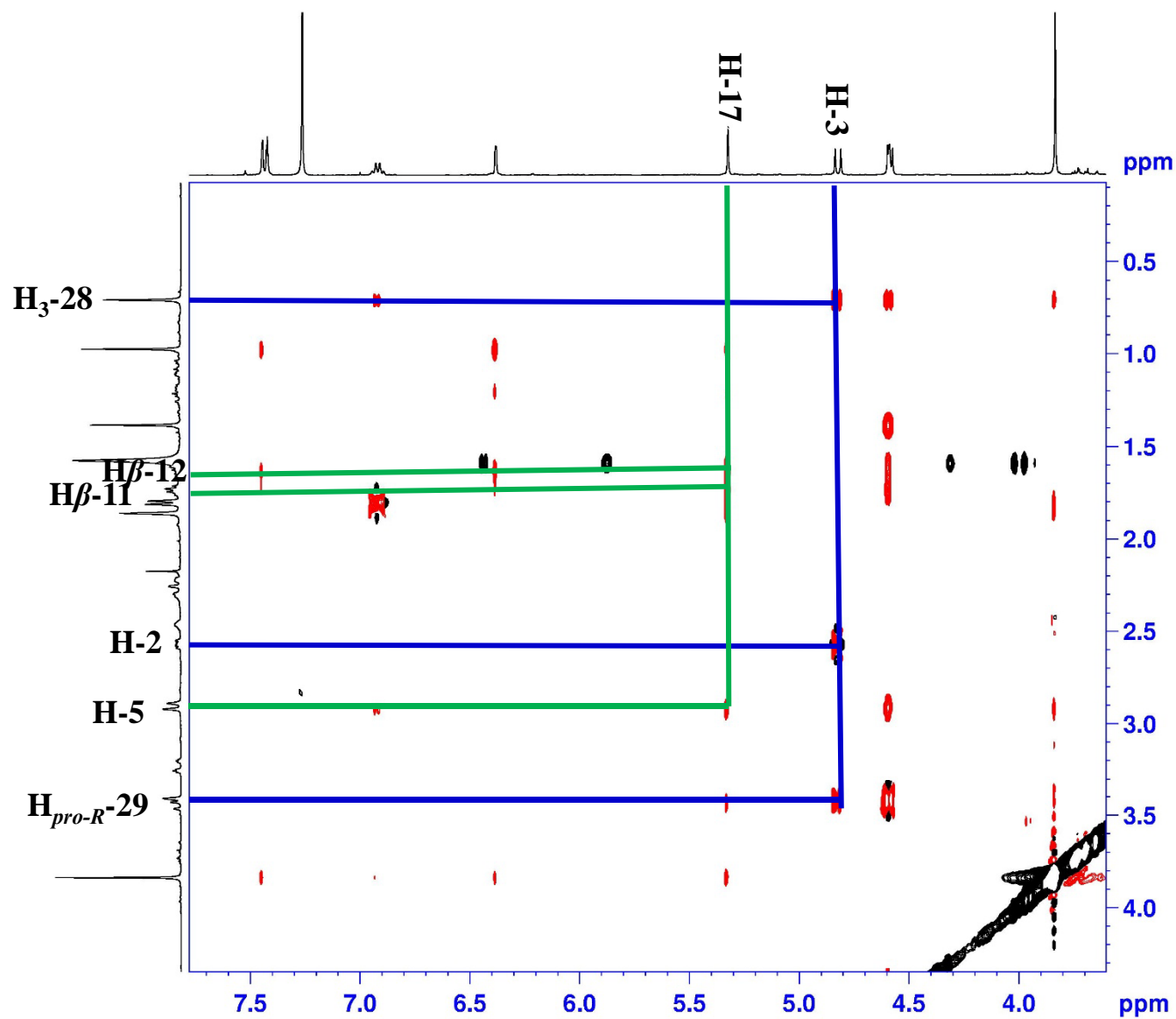
NAME ZXP-R-17-2-1-2
EXPNO 7
PROCNO 1
Date_ 20180707
Time 22.21
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG noesygpphpp
TD 2048
SOLVENT CDCl_3
NS 16
DS 32
SWH 4000.000 Hz
FIDRES 1.953125 Hz
AQ 0.2560500 sec
RG 208.5
DW 125.000 usec
DE 10.00 usec
TE 297.0 K
D0 0.00011036 sec
D1 1.99385595 sec
D8 0.30000001 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
INO 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 ppm
FnMODE States-TPPI
SI 1024
SF 400.1300057 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 States-TPPI
SF 400.1300066 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

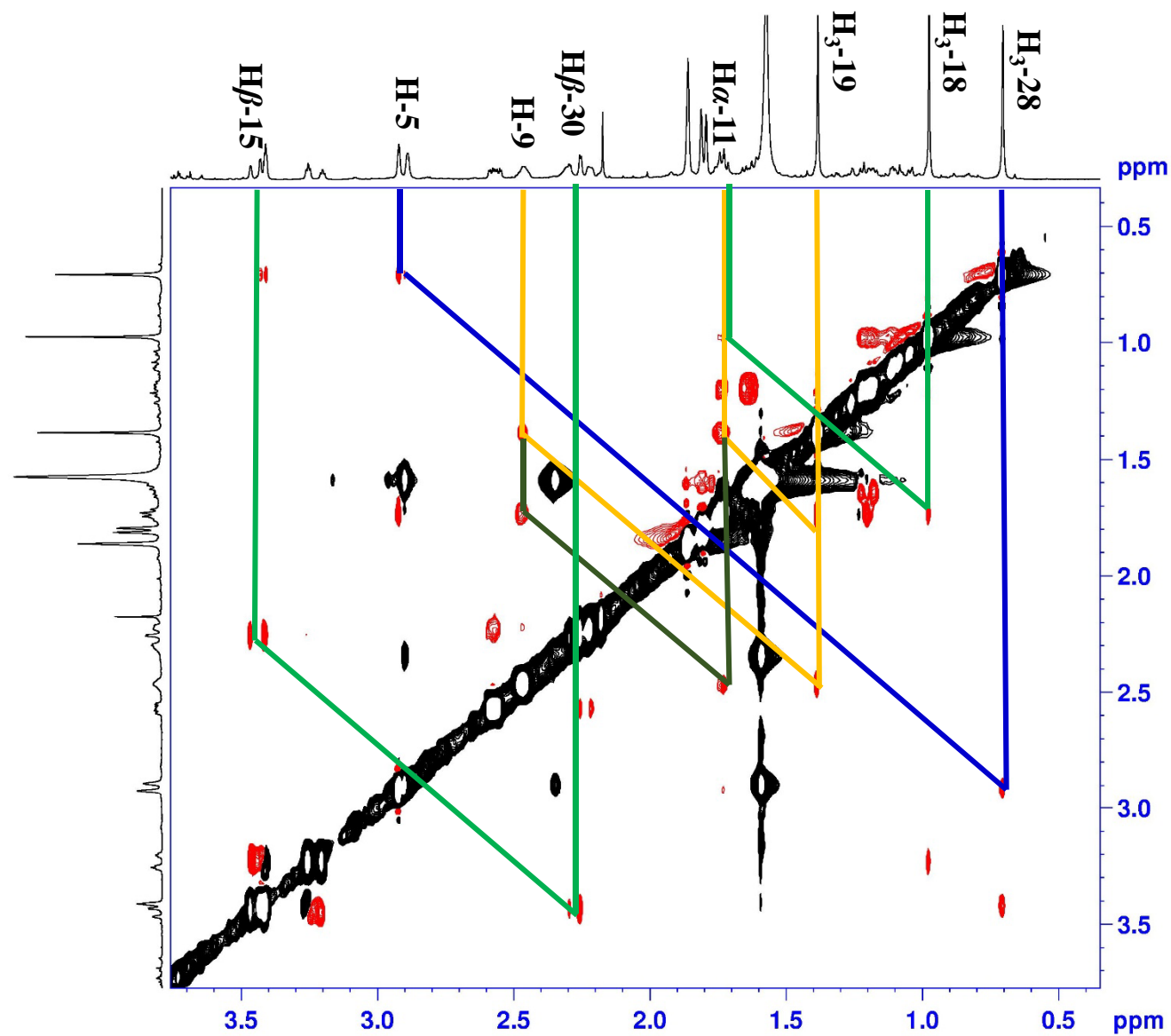
NOESY (400 MHz) spectrum of compound **4** in CDCl_3



NOESY (400 MHz) spectrum of compound **4** in CDCl_3



NOESY (400 MHz) spectrum of compound **4** in CDCl_3



HR-ESIMS for compound 5

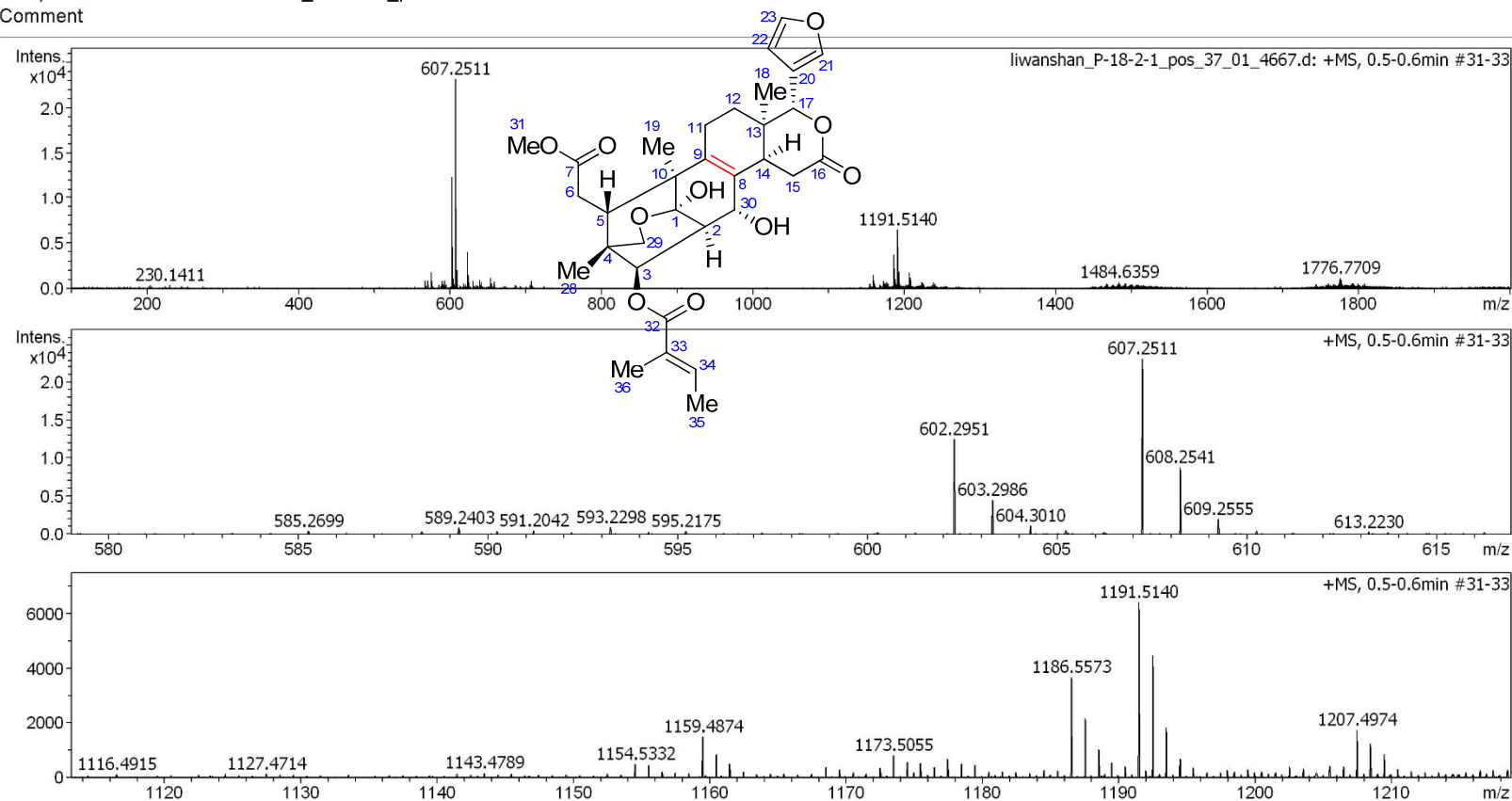
Generic Display Report

Analysis Info

Analysis Name D:\Data\MS\data\201805\liwanshan_P-18-2-1_pos_37_01_4667.d
Method LC_Direct Infusion_pos_100-1000mz.m
Sample Name liwanshan_P-18-2-1_pos
Comment

Acquisition Date 5/4/2018 11:44:10 AM

Operator SCSIO
Instrument maXis



HR-ESIMS for compound 5

Mass Spectrum SmartFormula Report

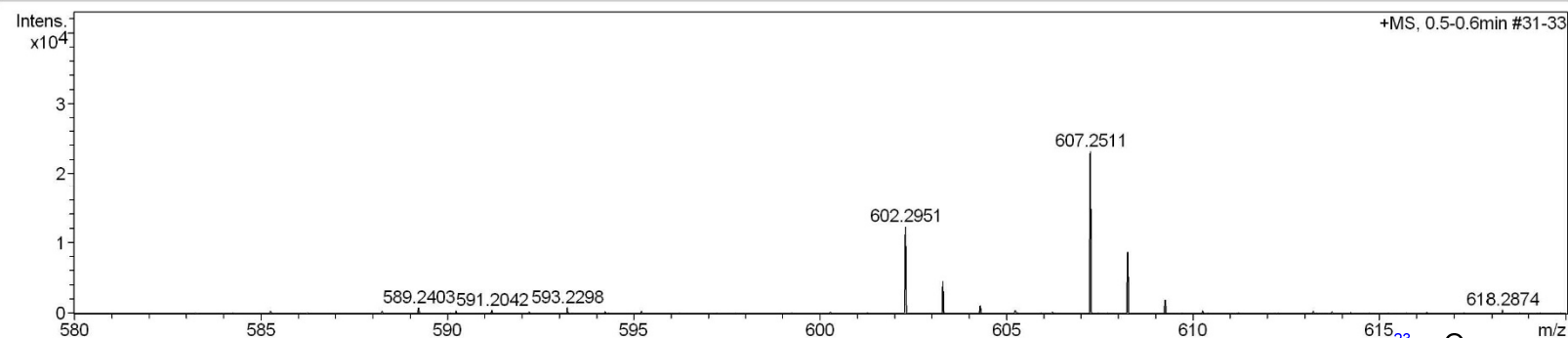
Analysis Info

Analysis Name D:\Data\MS\data\201805\liwanshan_P-18-2-1_pos_37_01_4667.d
 Method LC_Direct Infusion_pos_100-1000mz.m
 Sample Name liwanshan_P-18-2-1_pos
 Comment

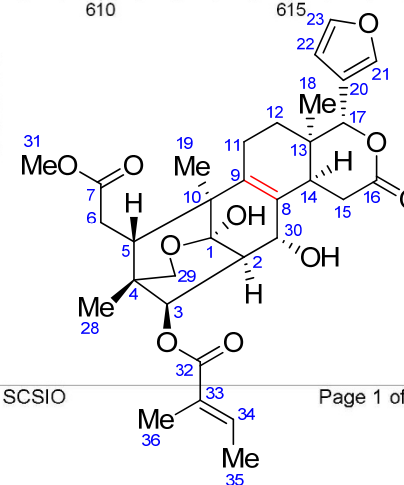
Acquisition Date 5/4/2018 11:44:10 AM
 Operator SCSIO
 Instrument maXis 255552.00029

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	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
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 ⁻ Conf	N-Rule
585.2699	1	C32H41O10	100.00	585.2694	-0.9	-0.5	371.8	12.5	even	ok
602.2951	1	C32H44NO10	100.00	602.2960	-1.4	-0.9	4.6	11.5	even	ok
607.2511	1	C32H40NaO10	100.00	607.2514	0.4	0.2	12.7	12.5	even	ok
1191.5140	1	C64H80NaO20	100.00	1191.5135	0.4	0.5	13.9	24.5	even	ok



liwanshan_P-18-2-1_pos_37_01_4667.d
 Bruker Compass DataAnalysis 4.1

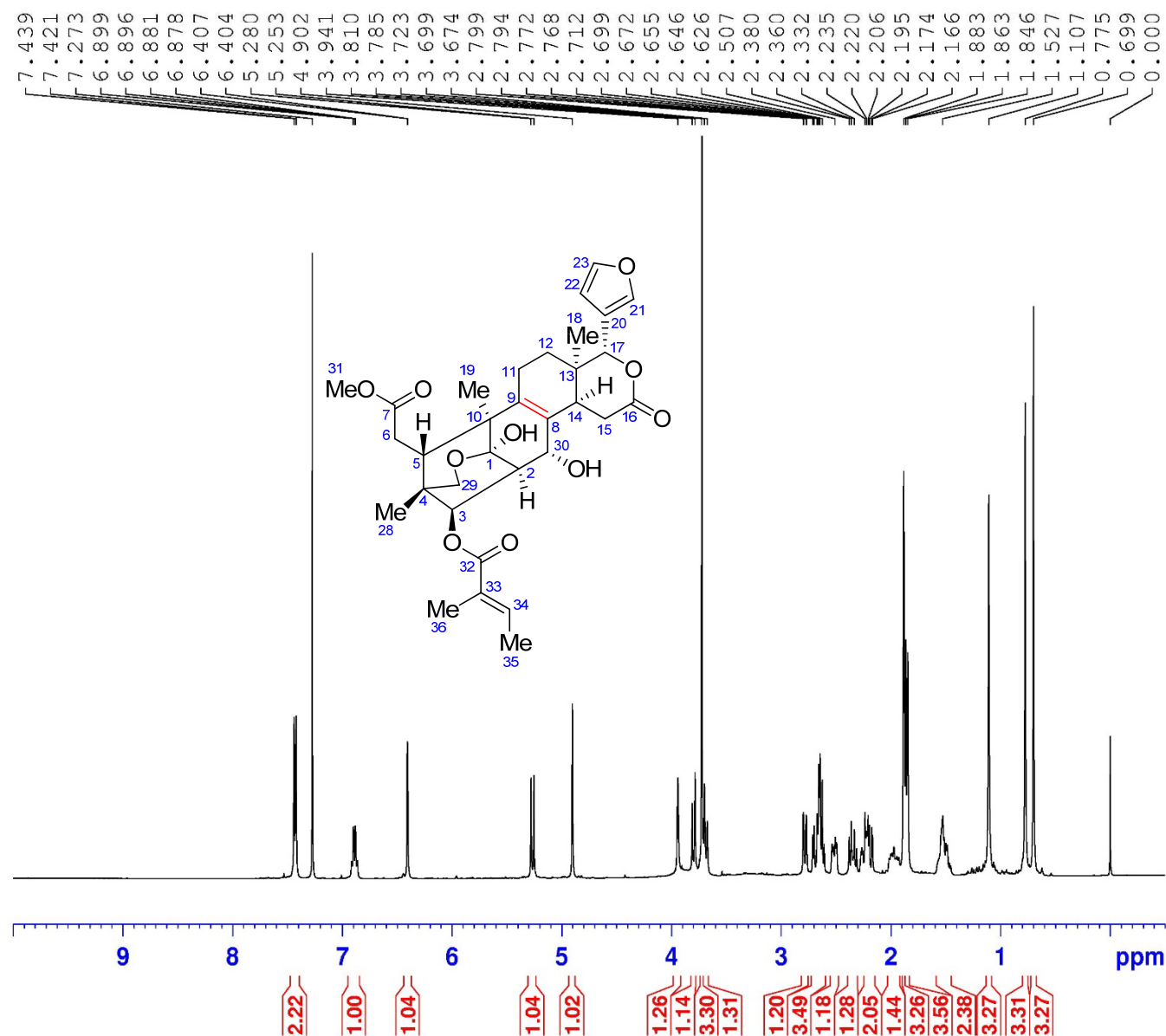
printed: 5/4/2018 3:39:17 PM

by: SCSIO

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^1H NMR (400 MHz) spectrum of compound **5** in CDCl_3



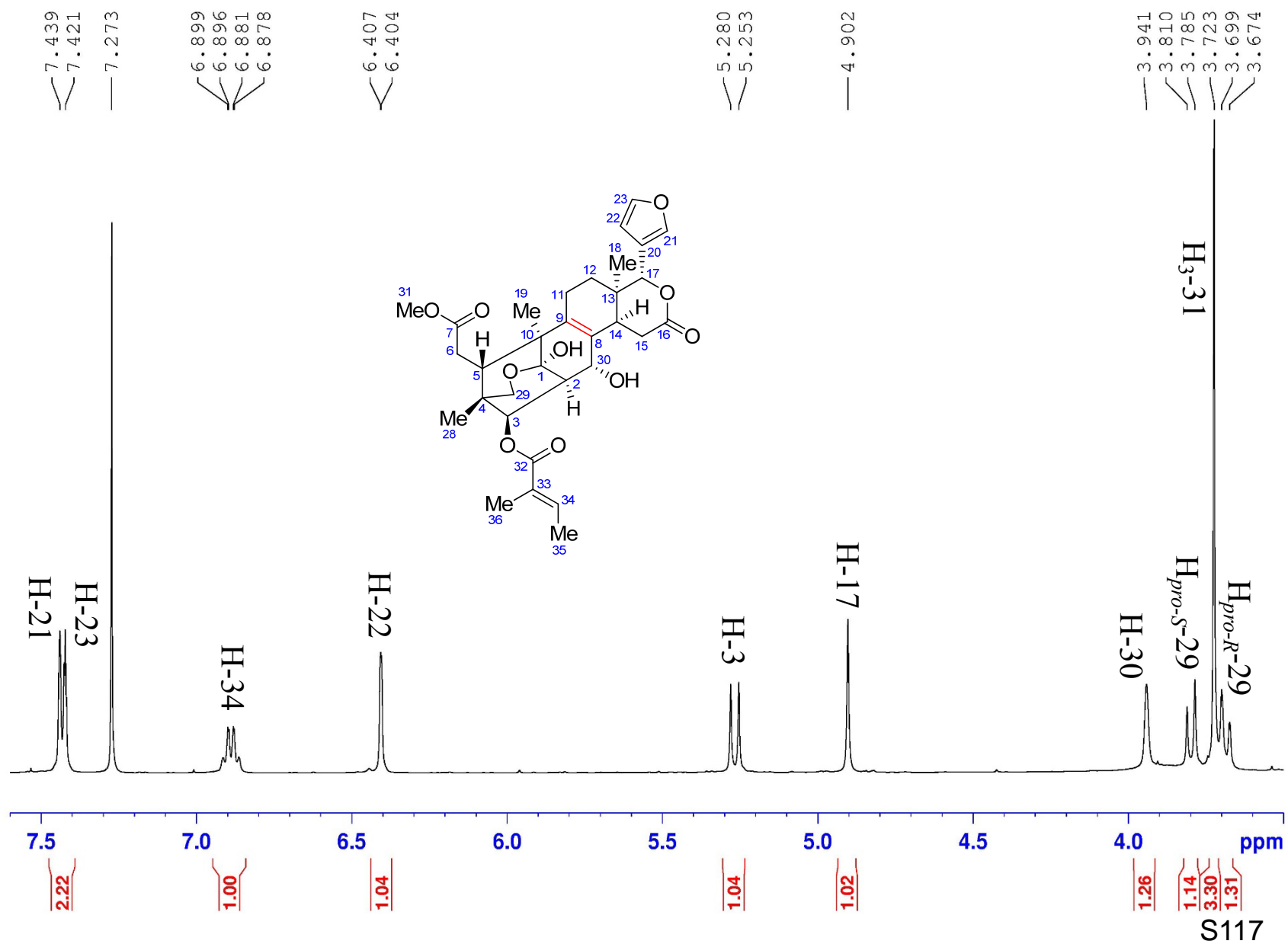
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NAME      ZXP-R-18-2-2-2  new
EXPNO     1
PROCNO    1
Date_     20171206
Time      22.34
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         85.34
DW         60.800 usec
DE         10.00 usec
TE         297.0 K
D1         1.00000000 sec
TD0        1
    
```

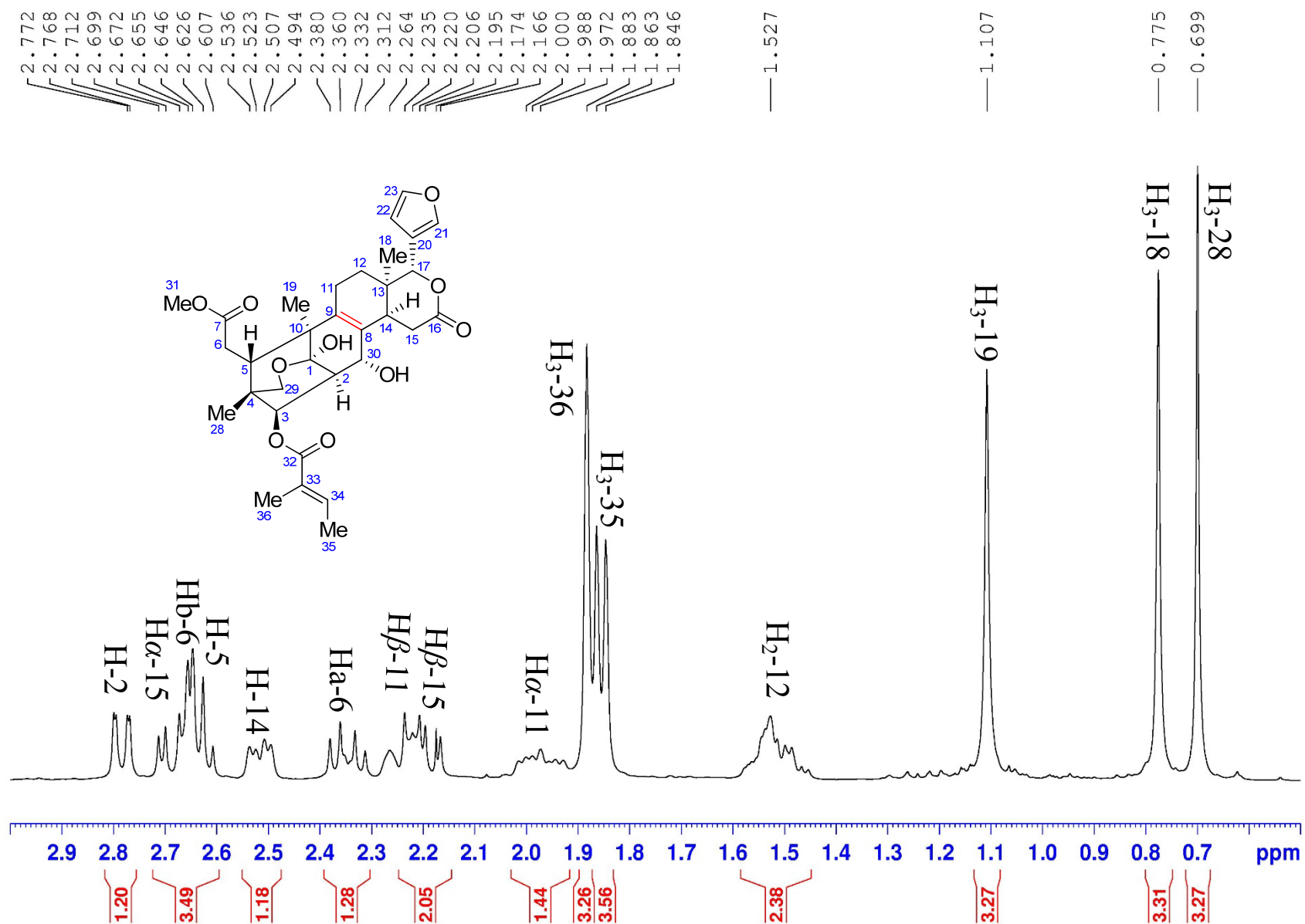
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===== CHANNEL f1 =====
SF01      400.1324710 MHz
NUC1       1H
P1         11.50 usec
SI         65536
SF         400.1300045 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

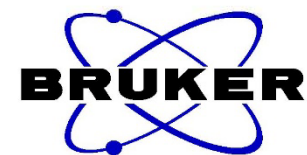
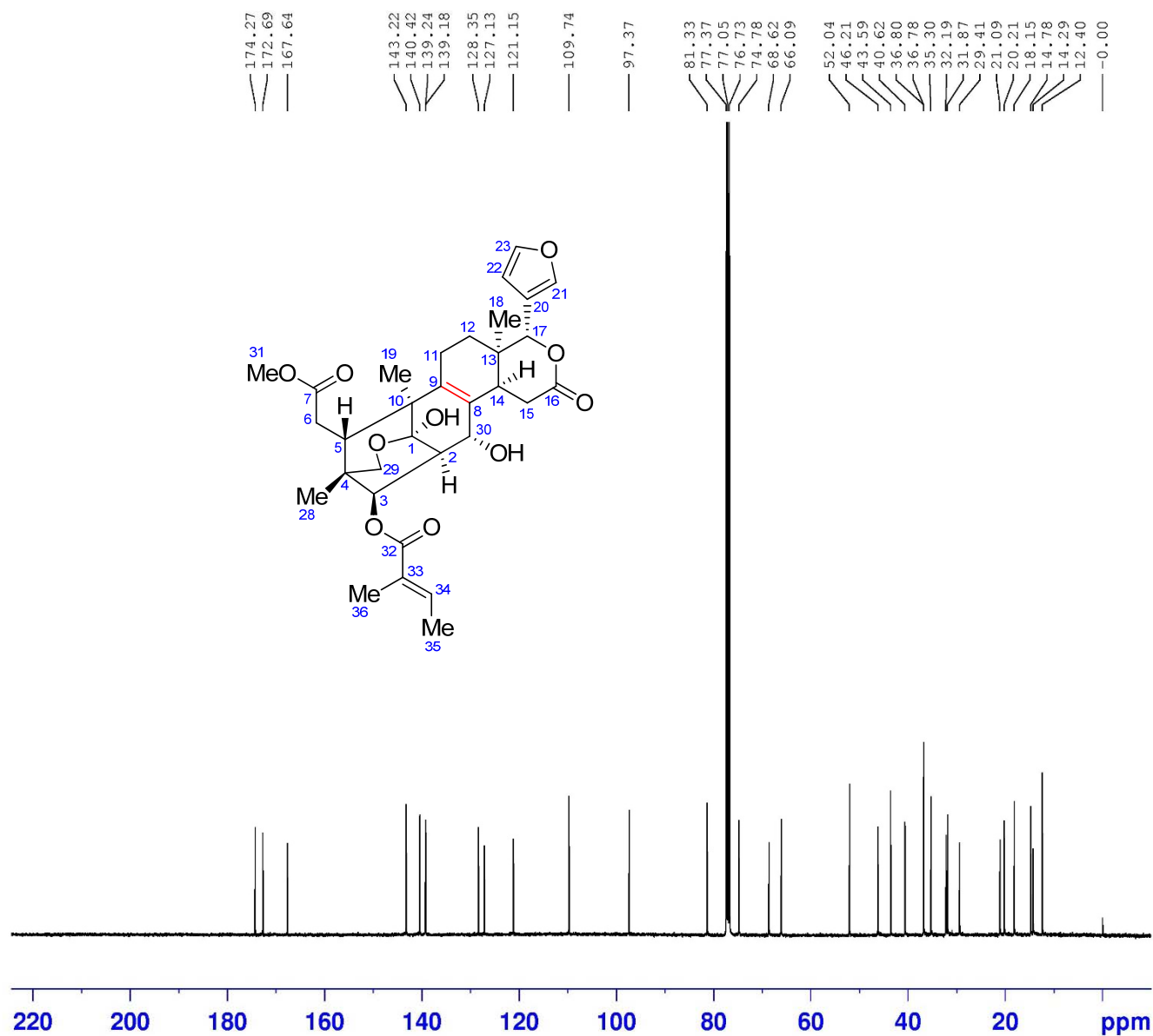
^1H NMR (400 MHz) spectrum of compound **5** in CDCl_3



^1H NMR (400 MHz) spectrum of compound **5** in CDCl_3



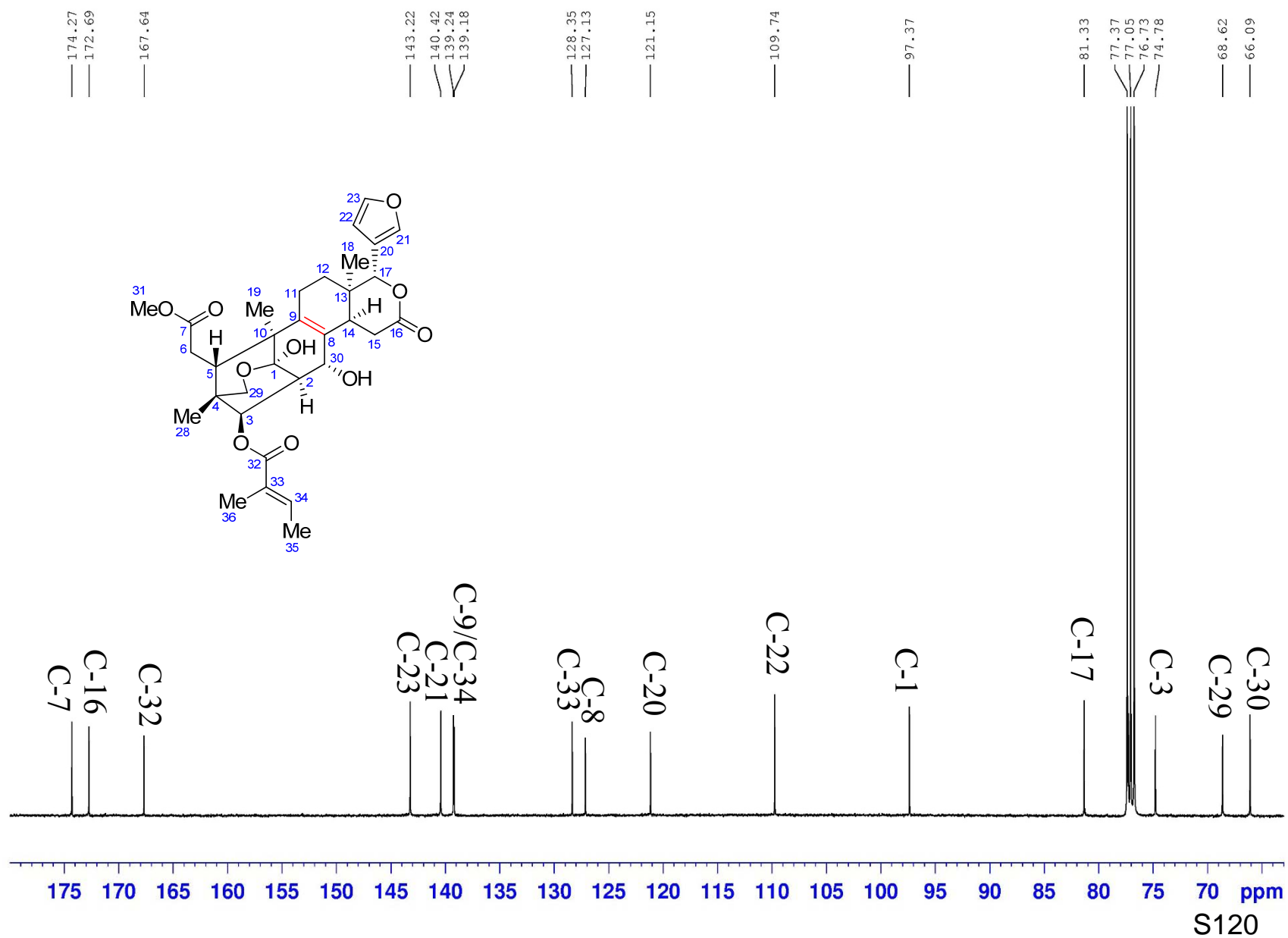
^{13}C NMR (100 MHz) spectrum of compound **5** in CDCl_3



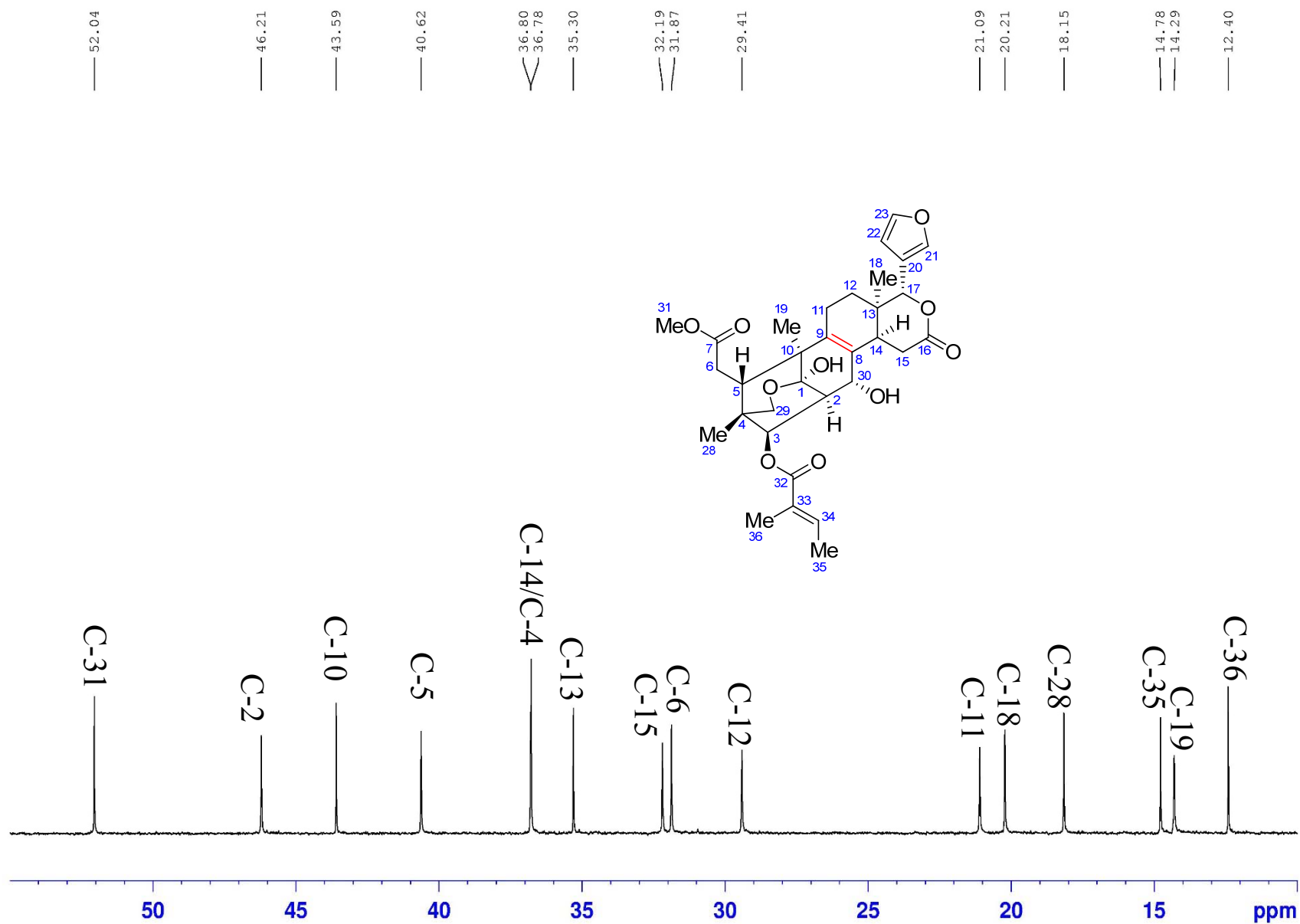
NAME ZXP-R-18-2-2-2 new
 EXPNO 2
 PROCNO 1
 Date_ 20171206
 Time 23.34
 INSTRUM spect
 PROBHD 5 mm CPMBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 117.37
 DW 20.800 usec
 DE 18.00 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6233324 MHz
 NUC1 ^{13}C
 P1 10.00 usec
 SI 32768
 SF 100.6127689 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

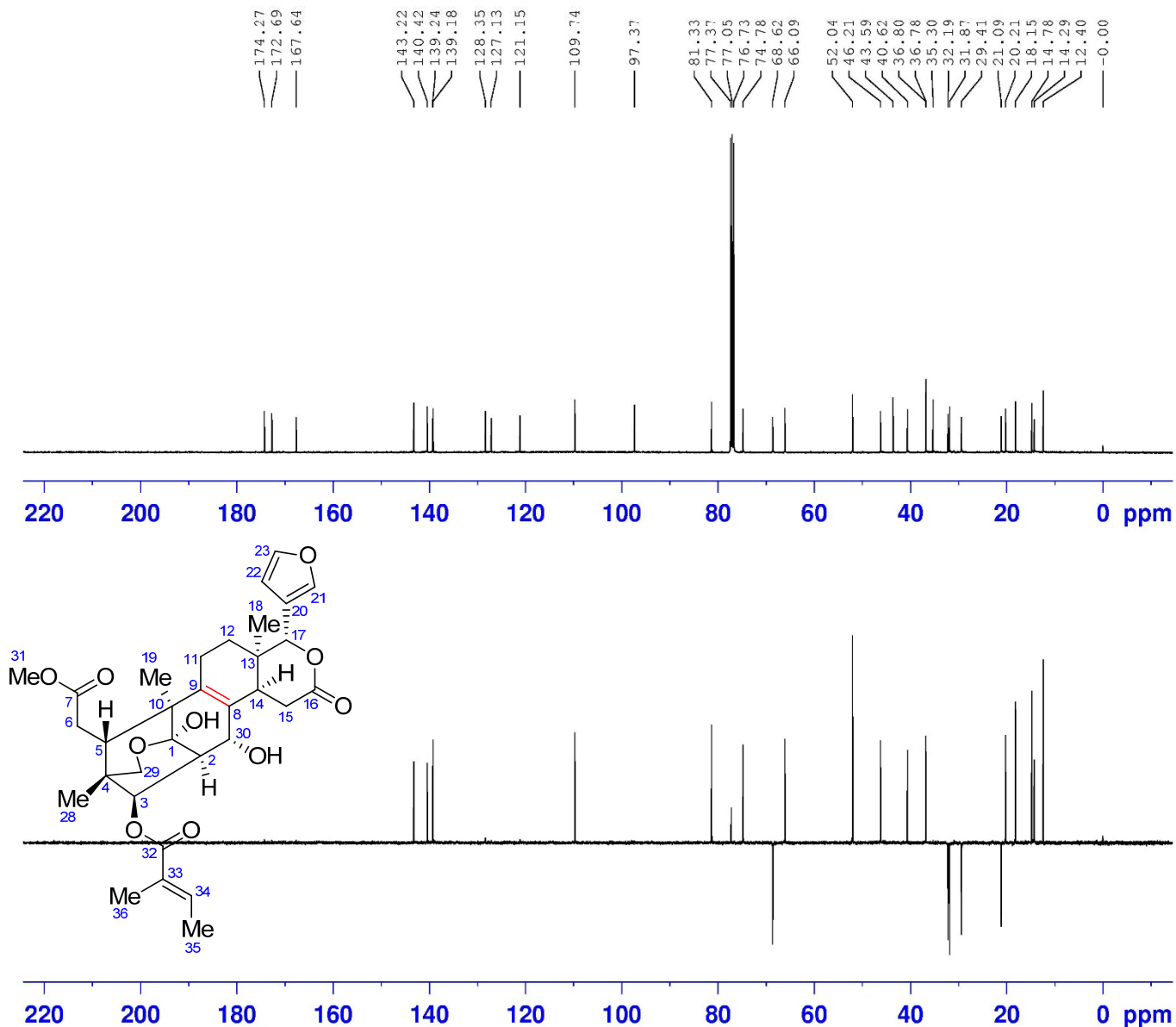
^{13}C NMR (100 MHz) spectrum of compound **5** in CDCl_3



^{13}C NMR (100 MHz) spectrum of compound **5** in CDCl_3



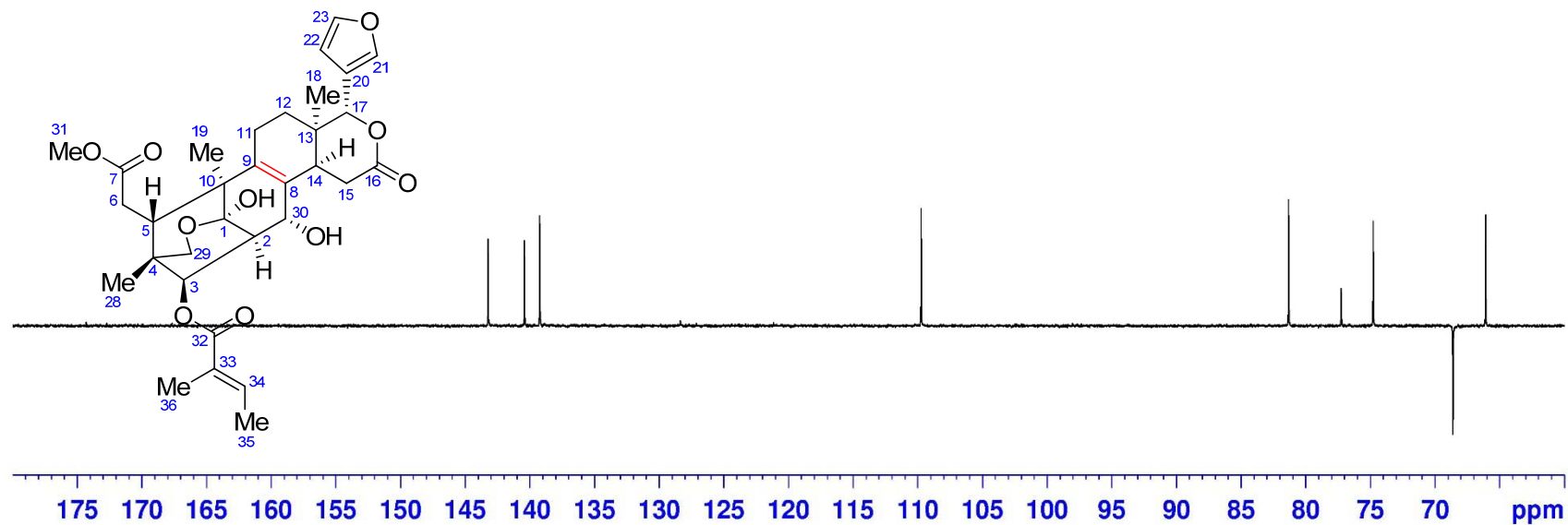
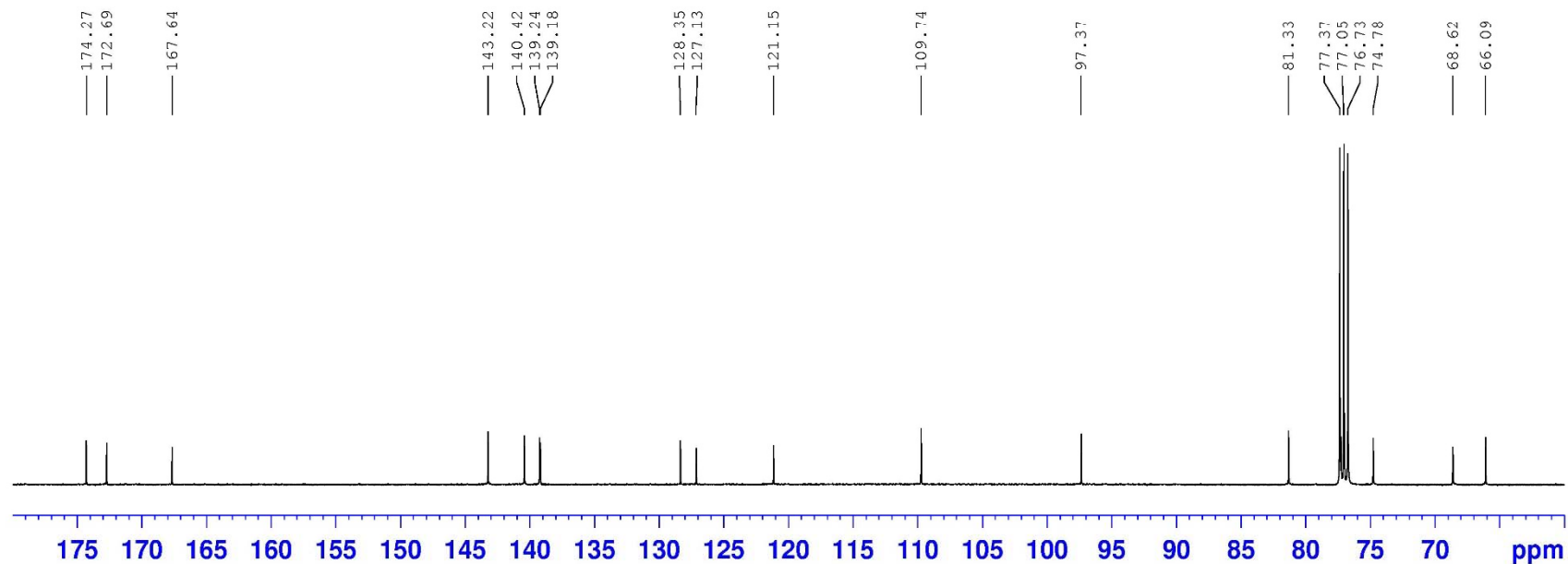
DEPT135 (100 MHz) spectrum of compound **5** in CDCl₃



NAME ZXP-R-18-2-2-2 new
 EXPNO 2
 PROCNO 1
 Date_ 20171206
 Time 23.34
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 117.37
 DW 20.800 usec
 DE 18.00 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6233324 MHz
 NUC1 13C
 P1 10.00 usec
 SI 32768
 SF 100.6127689 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

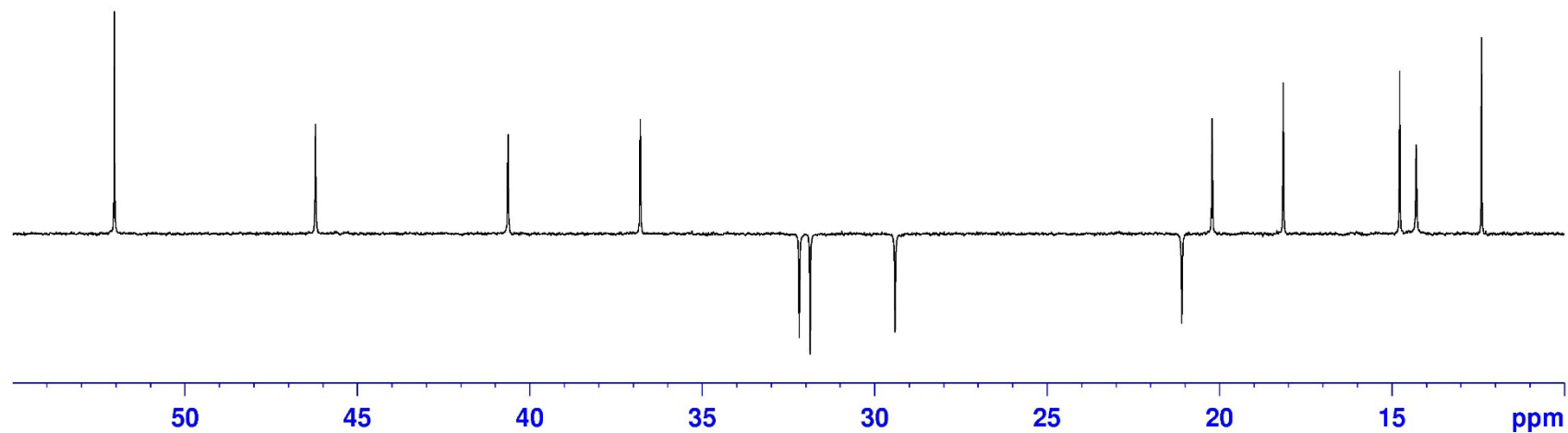
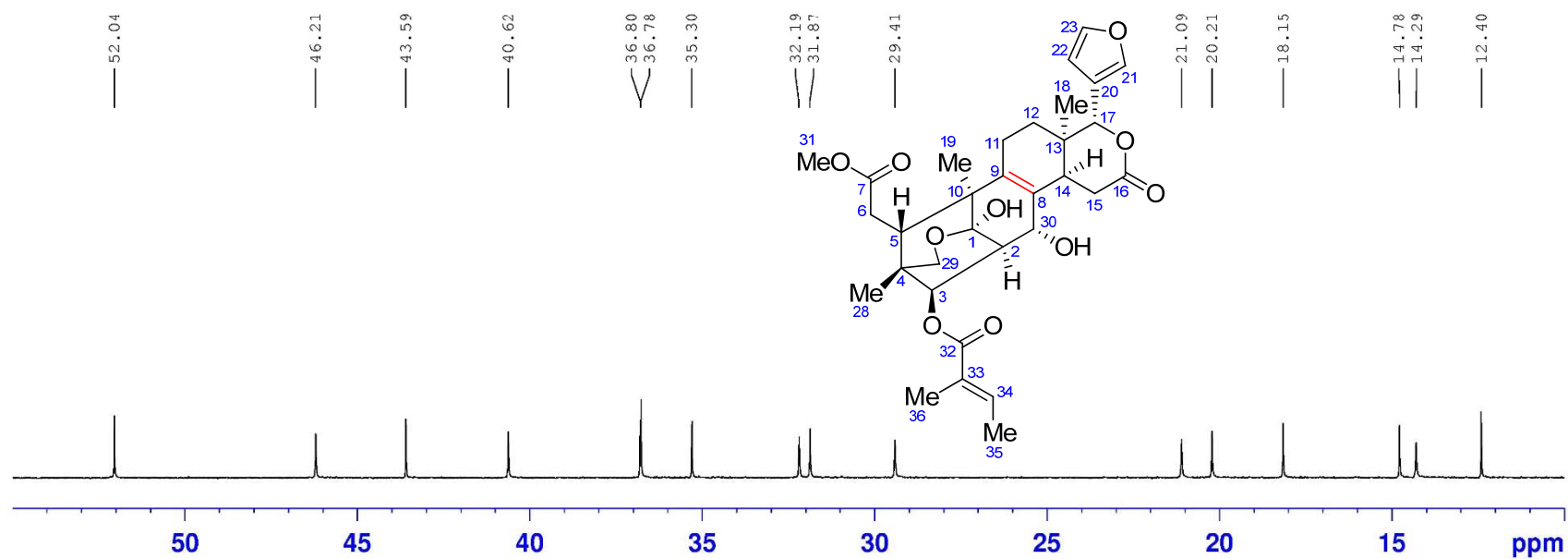
DEPT135 (100 MHz) spectrum of compound **5** in CDCl₃



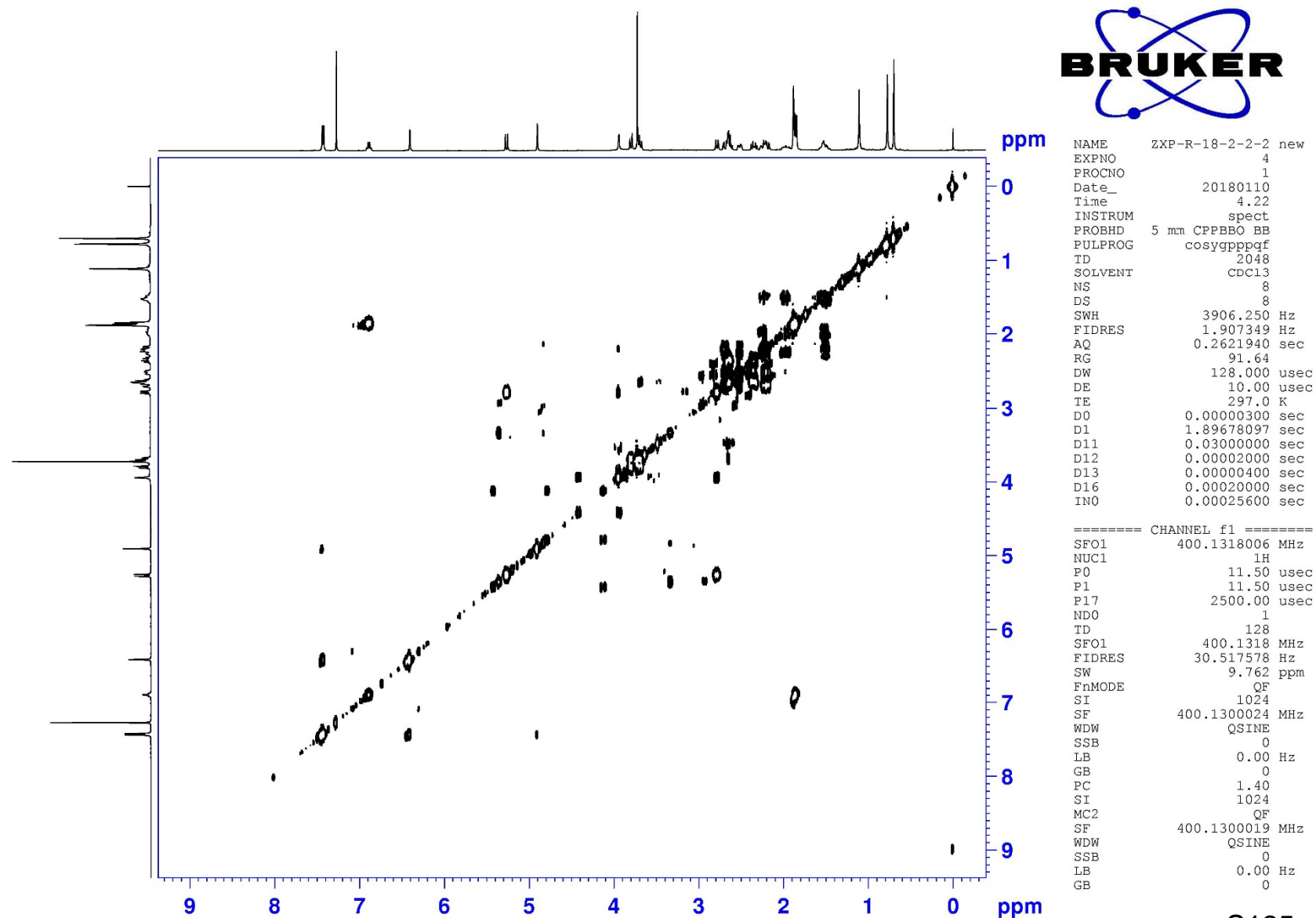
S123

S123

DEPT135 (100 MHz) spectrum of compound **5** in CDCl₃

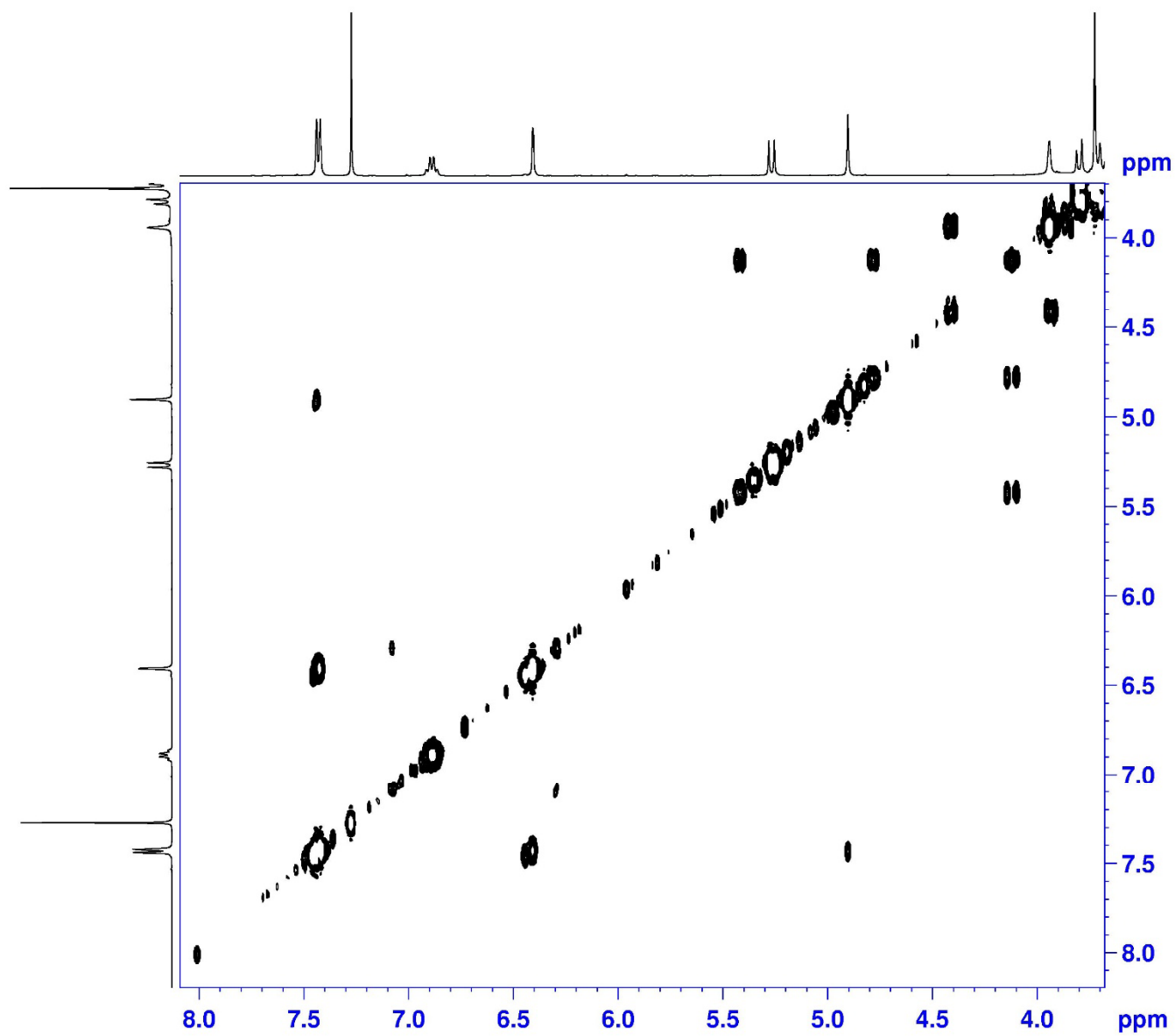


^1H - ^1H COSY (400 MHz) spectrum of compound **5** in CDCl_3

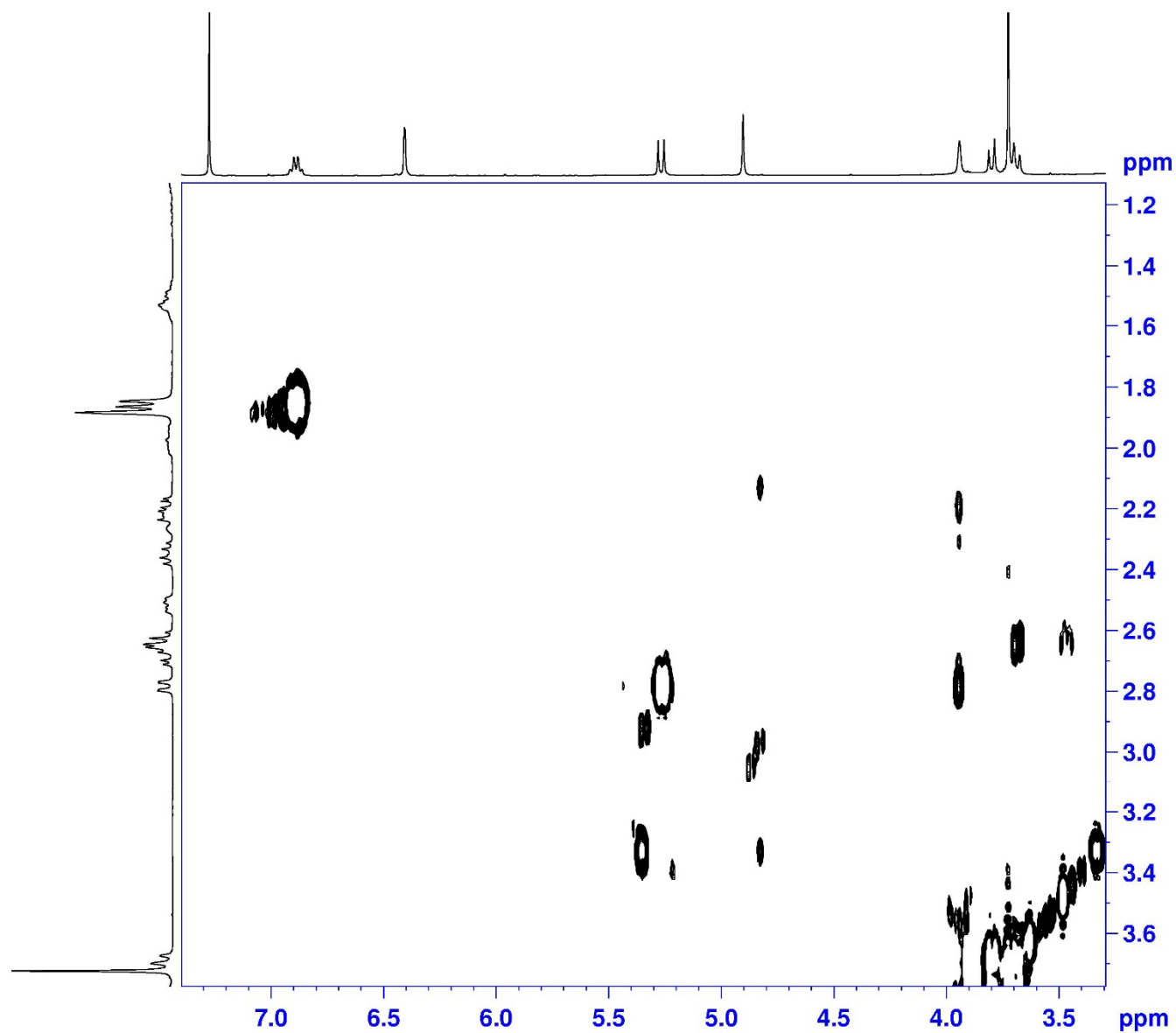


S125

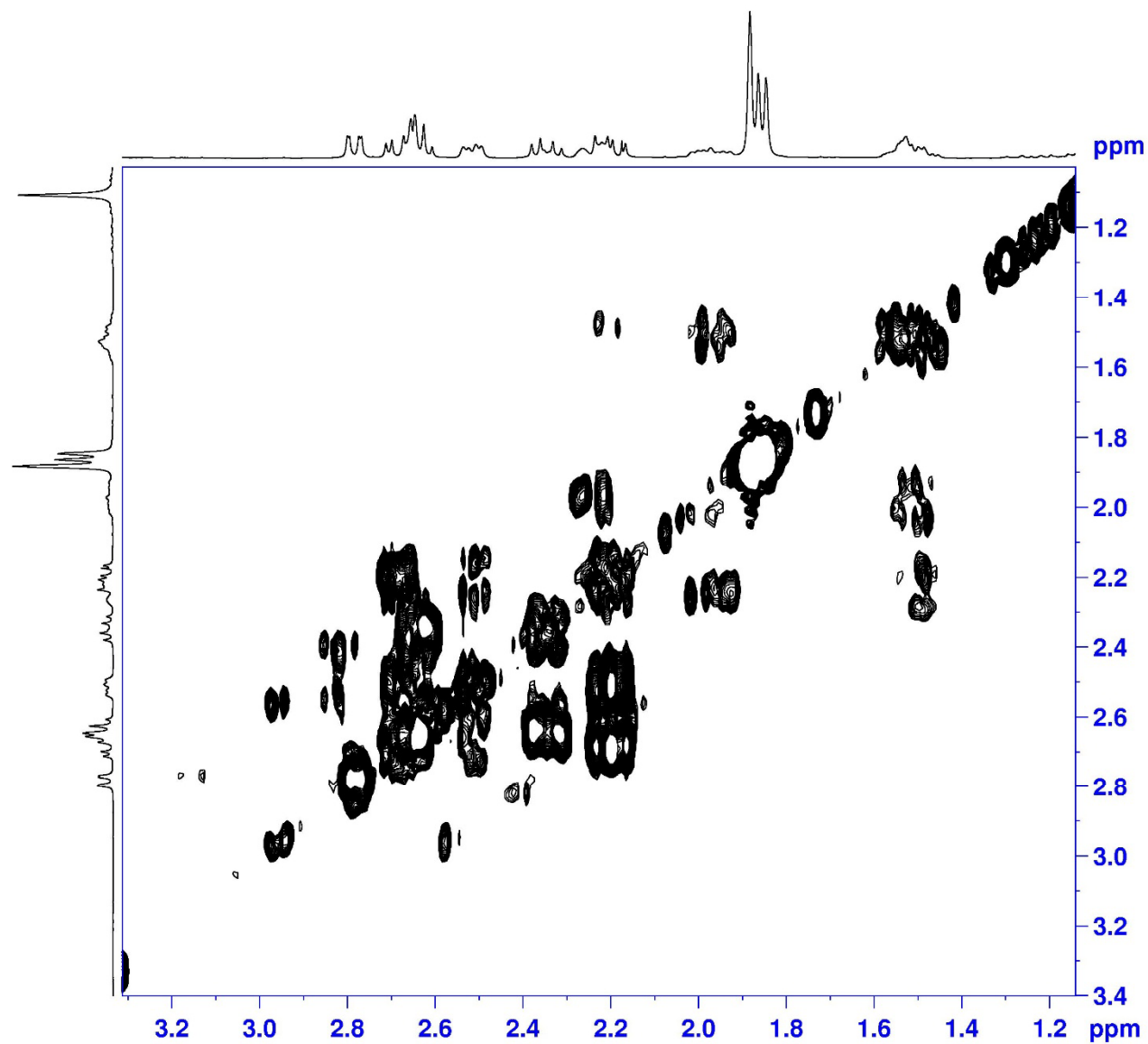
^1H - ^1H COSY (400 MHz) spectrum of compound **5** in CDCl_3



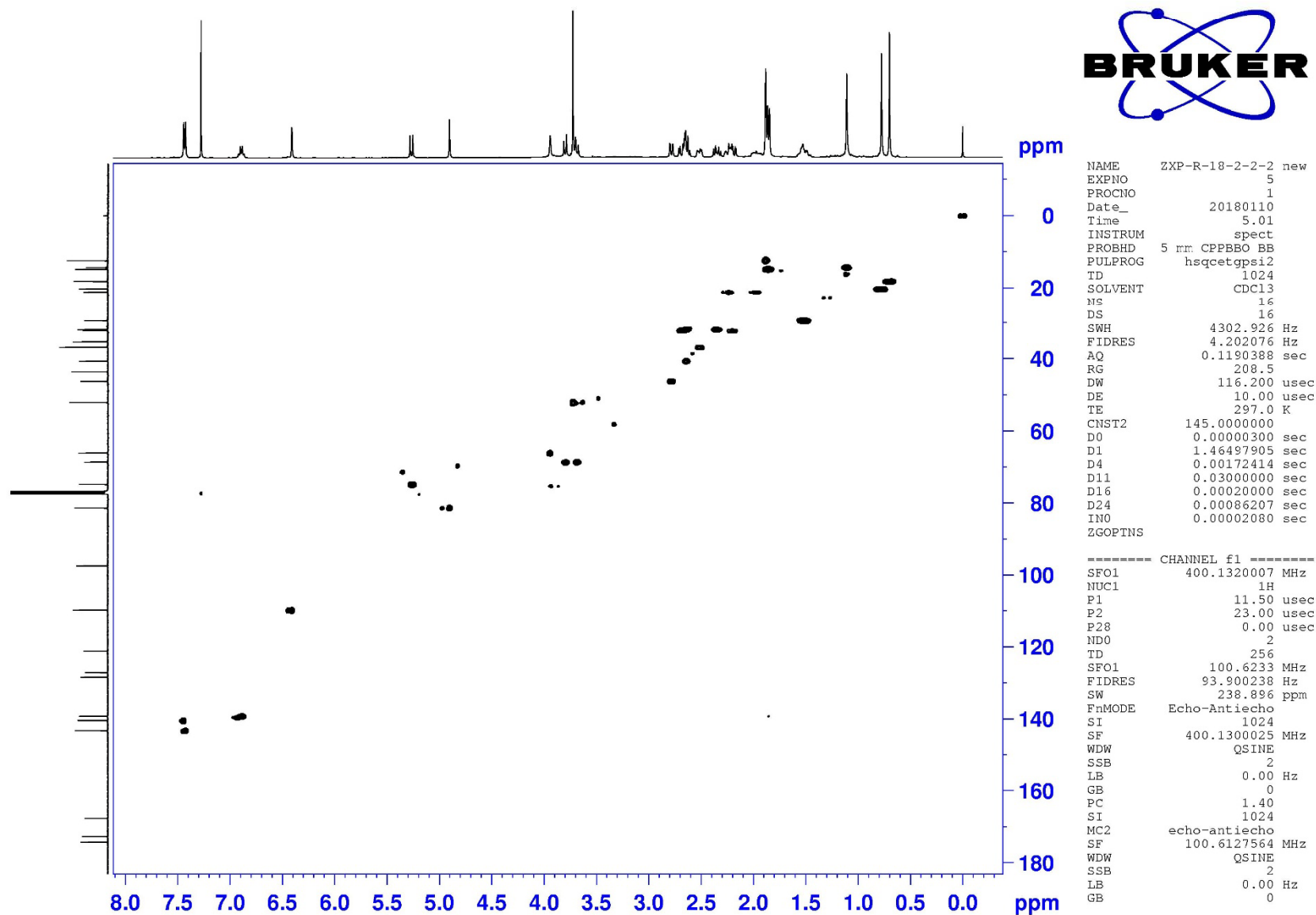
^1H - ^1H COSY (400 MHz) spectrum of compound **5** in CDCl_3



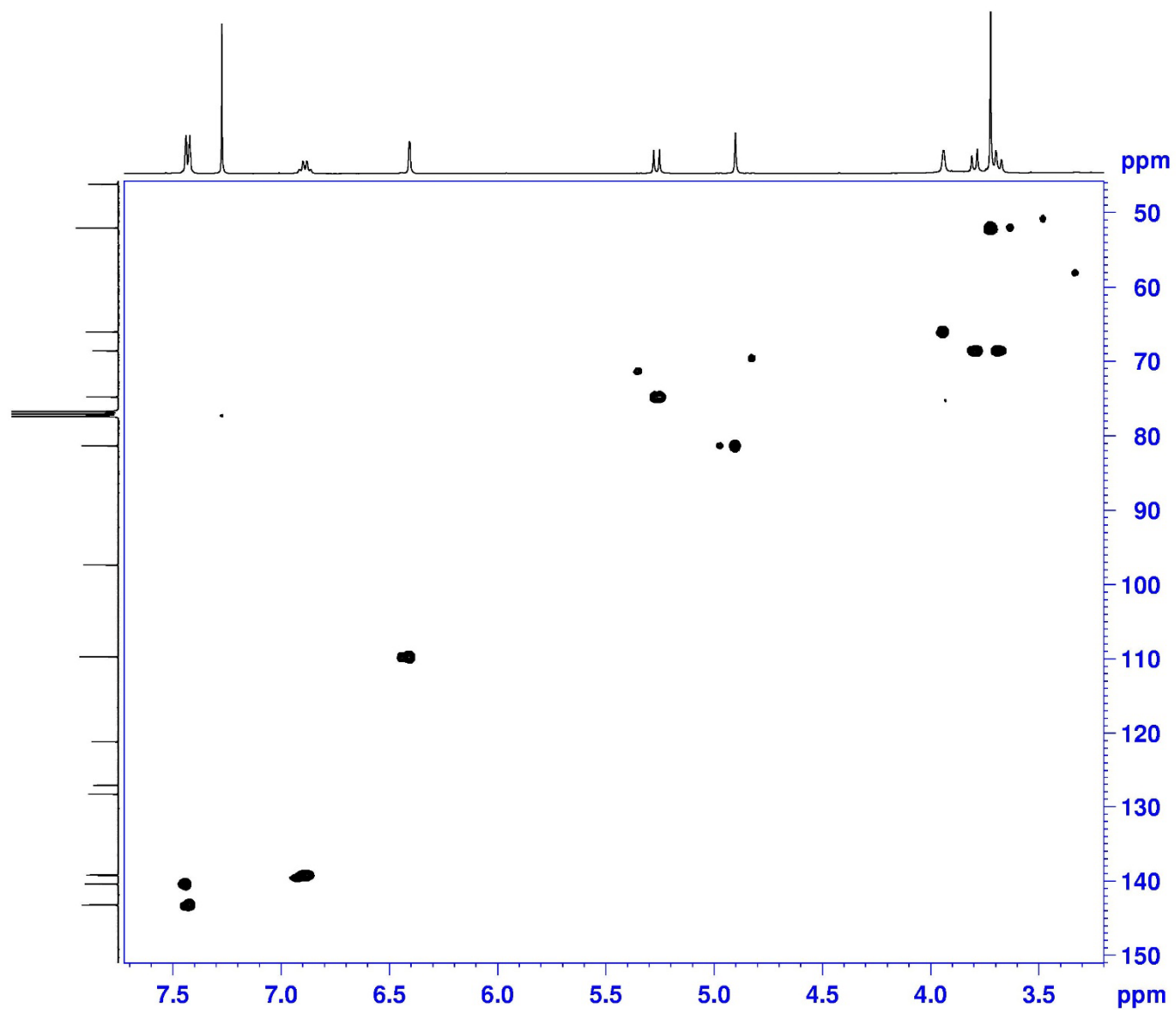
^1H - ^1H COSY (400 MHz) spectrum of compound **5** in CDCl_3



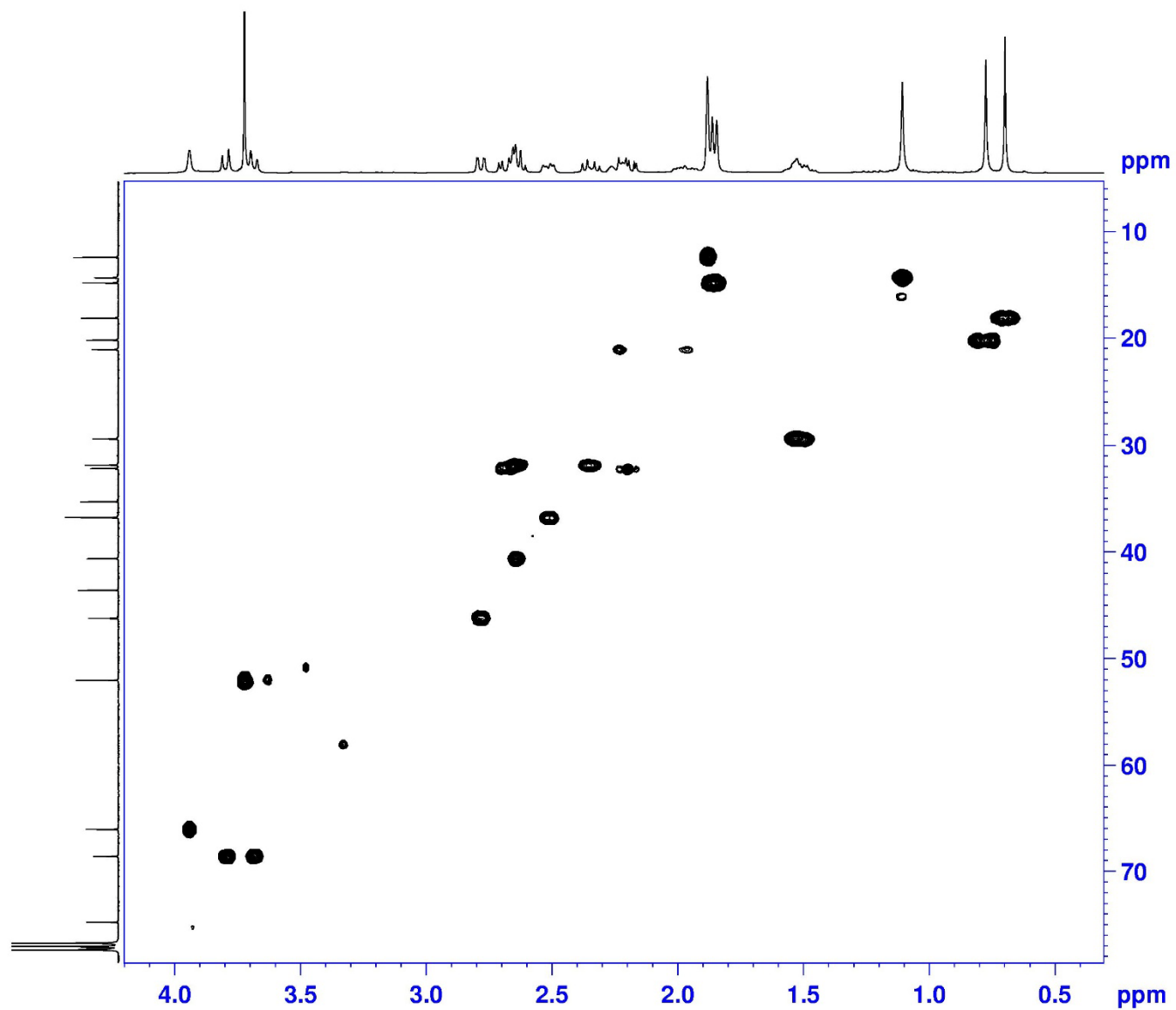
HSQC (400 MHz) spectrum of compound **5** in CDCl₃



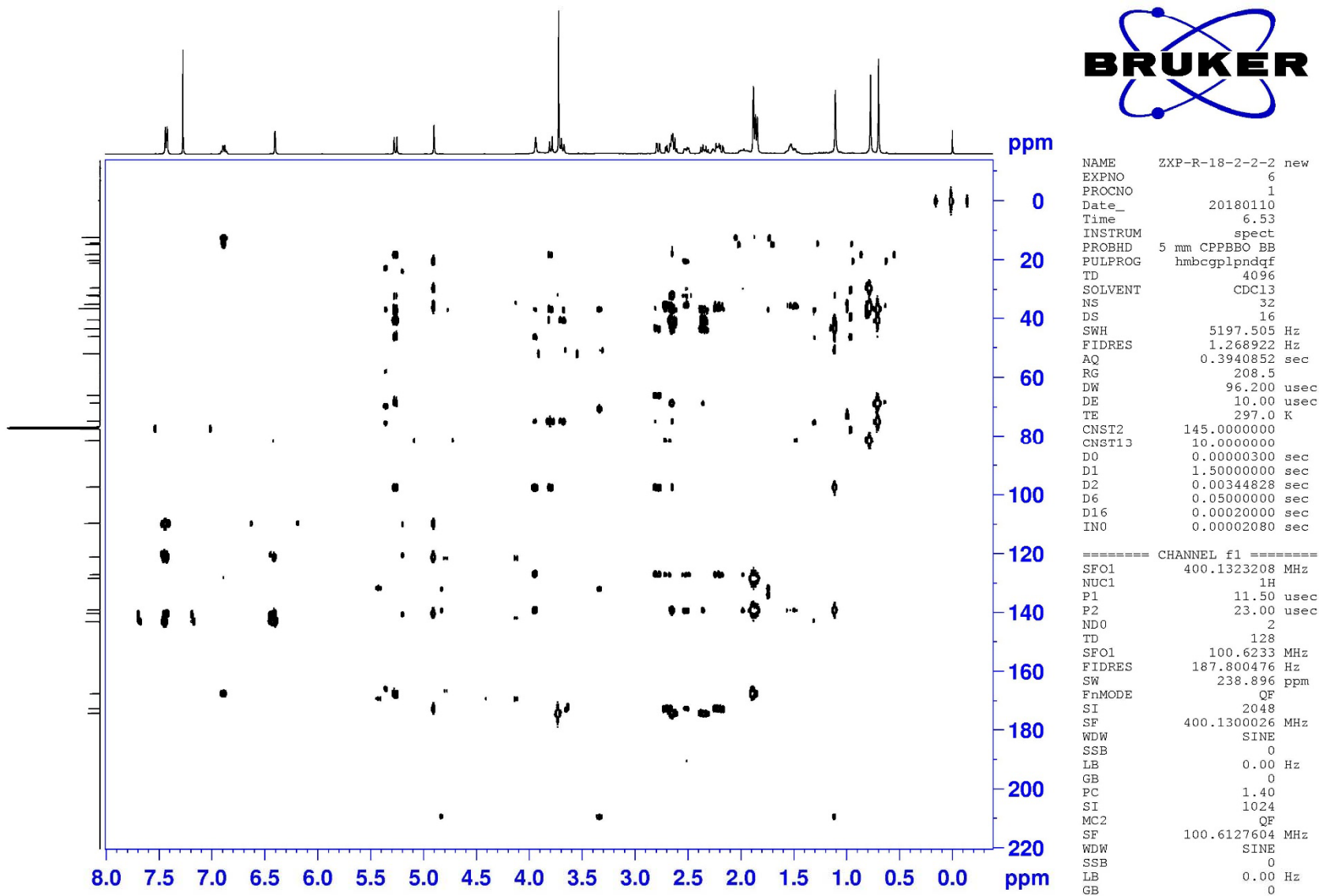
HSQC (400 MHz) spectrum of compound **5** in CDCl₃



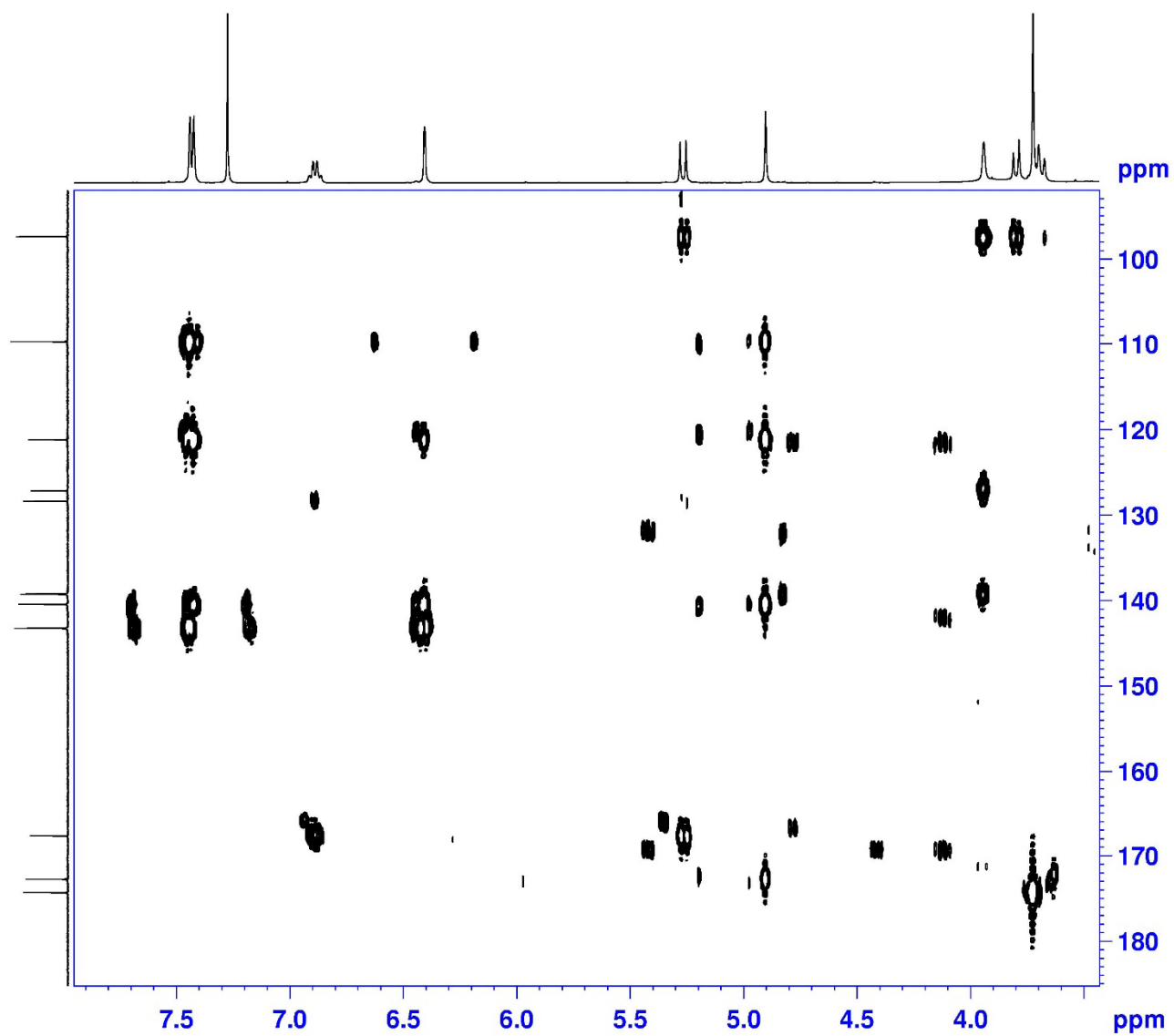
HSQC (400 MHz) spectrum of compound **5** in CDCl_3



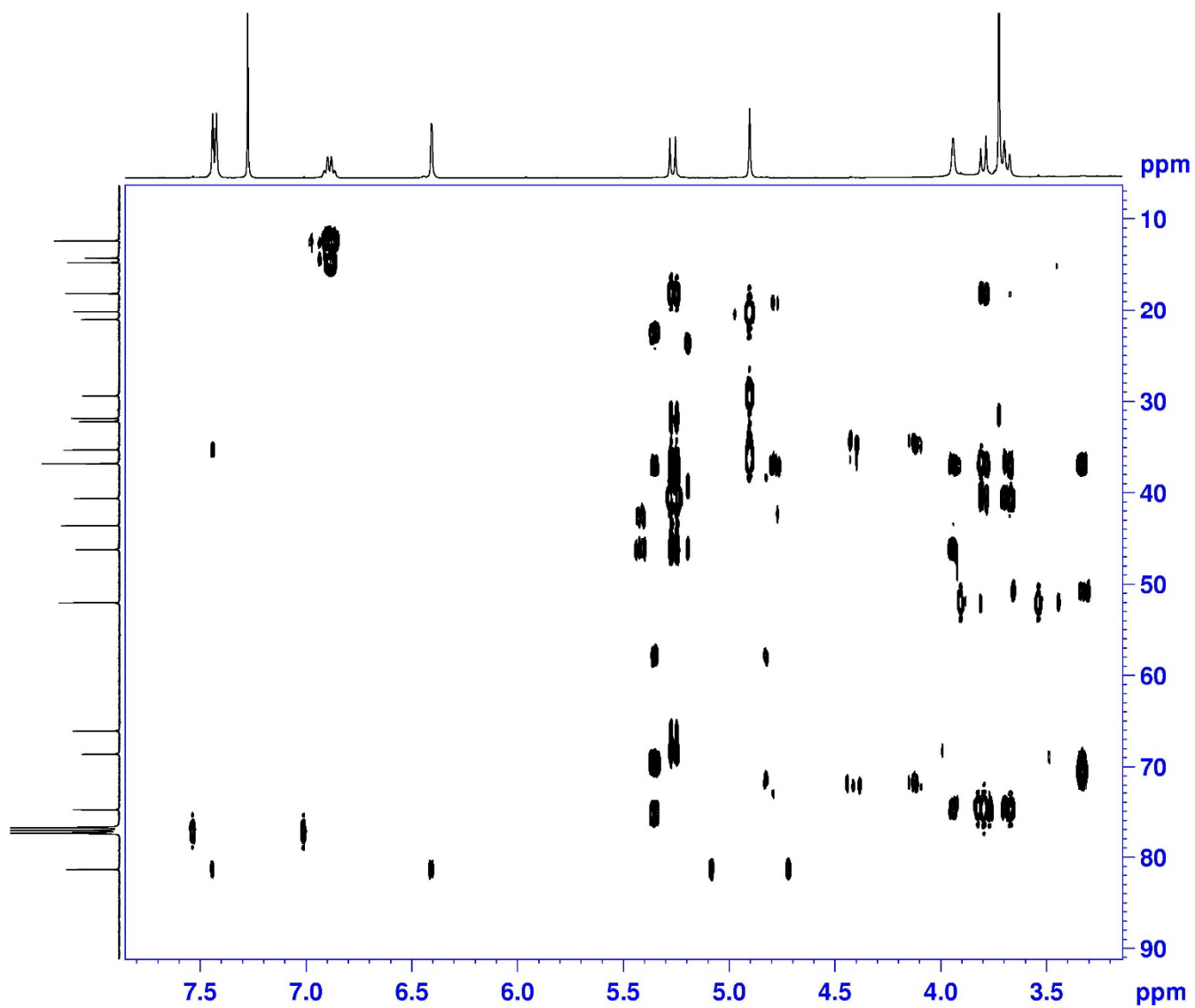
HMBC (400 MHz) spectrum of compound **5** in CDCl₃



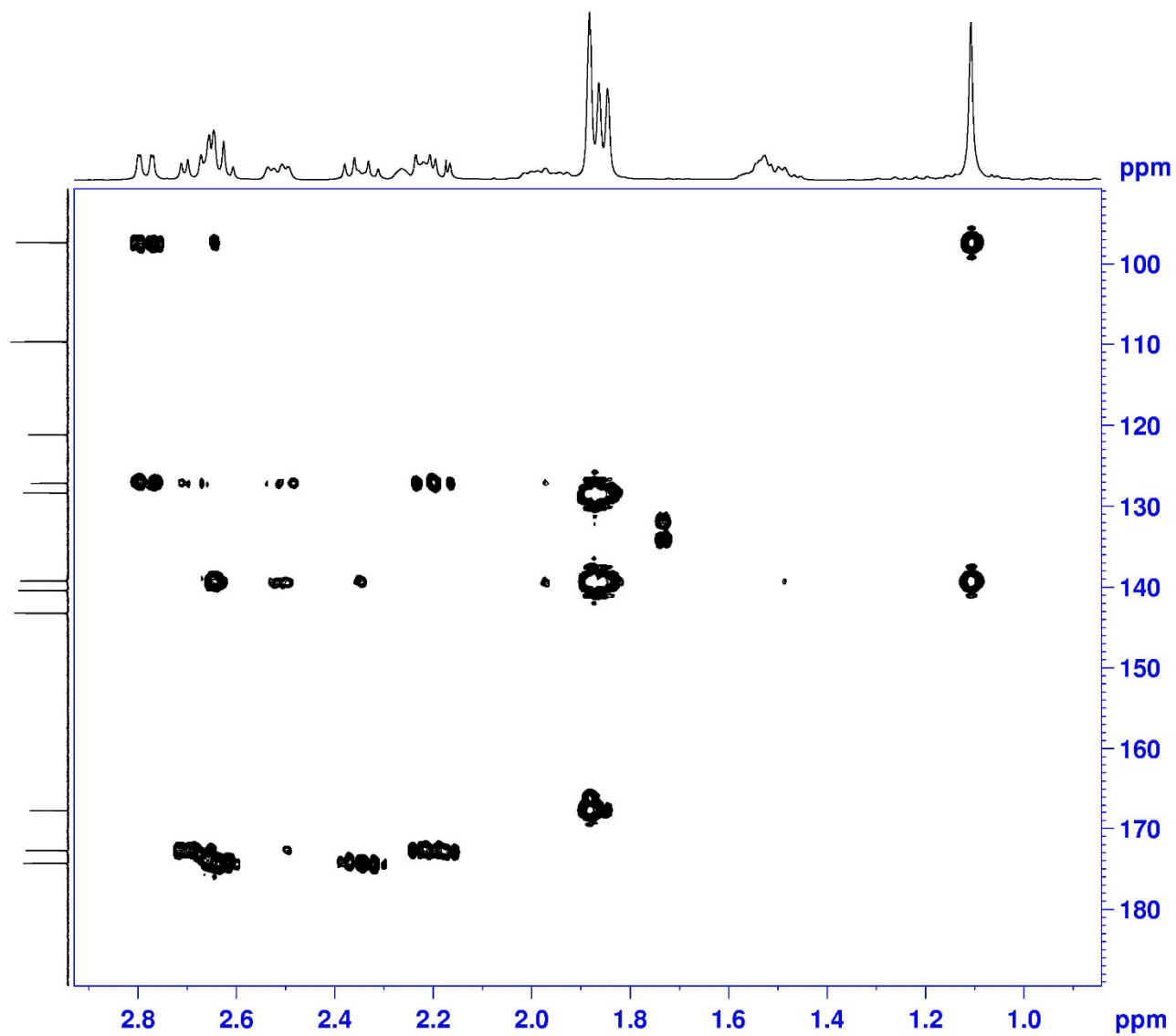
HMBC (400 MHz) spectrum of compound **5** in CDCl_3



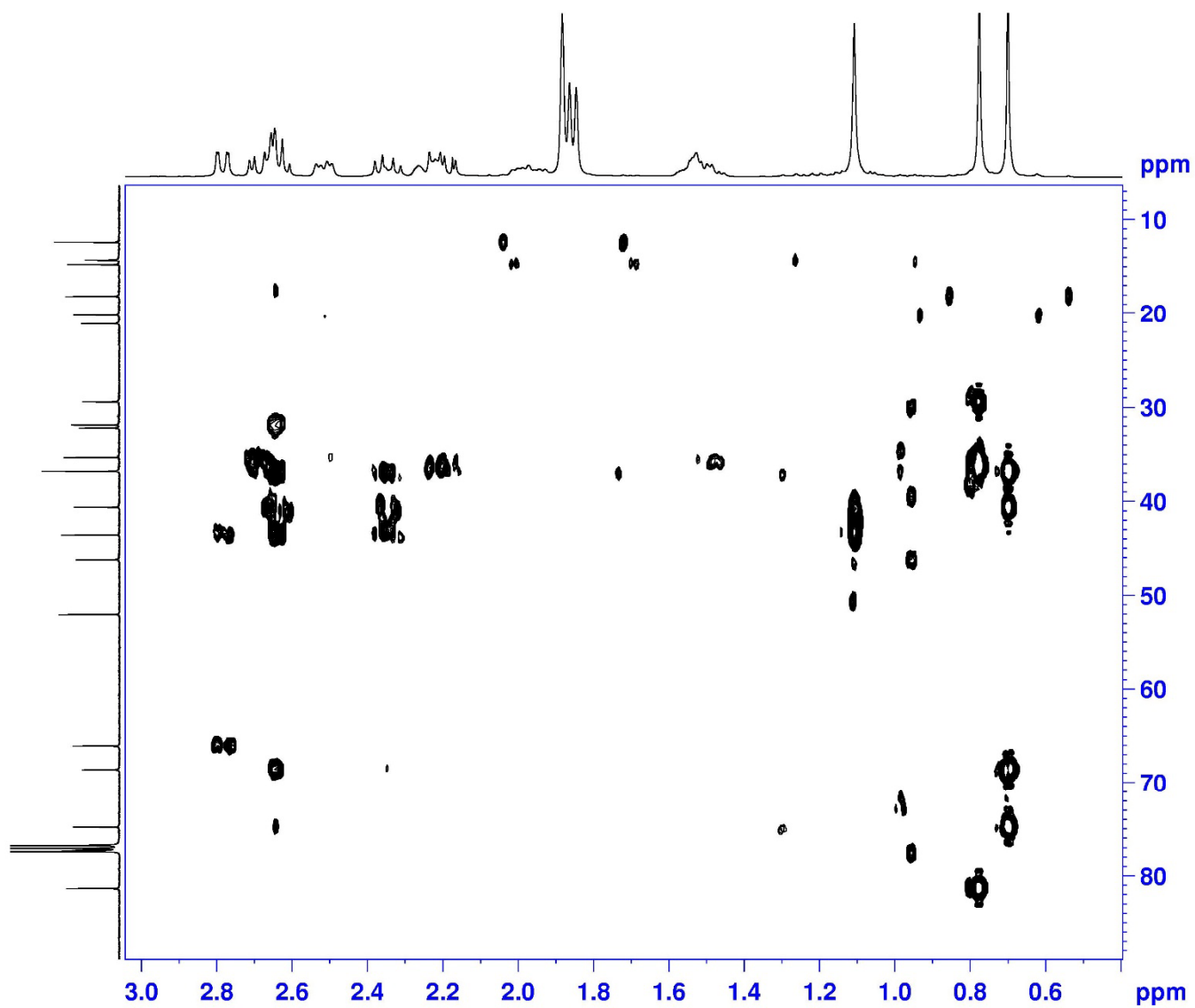
HMBC (400 MHz) spectrum of compound **5** in CDCl_3



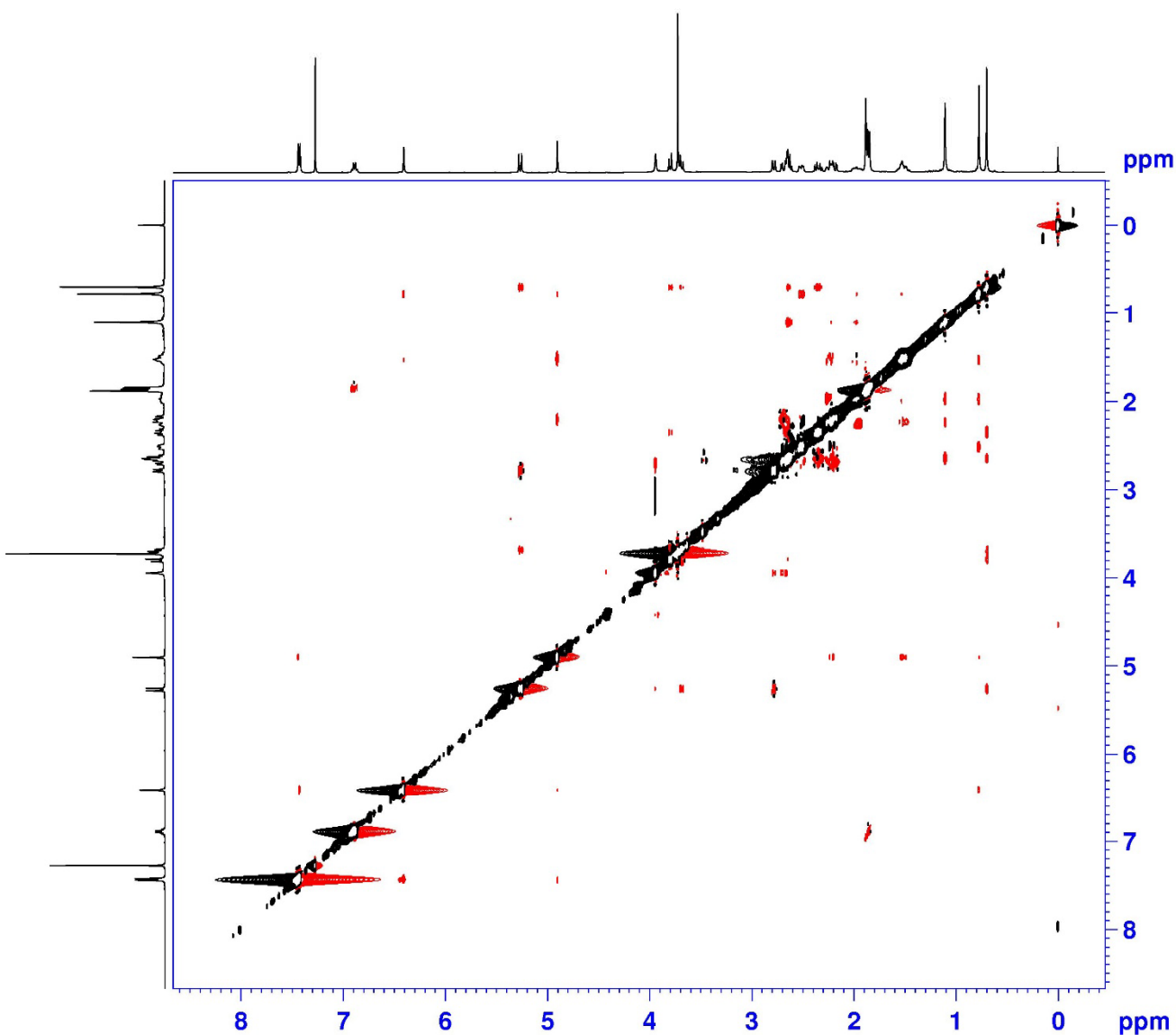
HMBC (400 MHz) spectrum of compound **5** in CDCl₃



HMBC (400 MHz) spectrum of compound **5** in CDCl_3



NOESY (400 MHz) spectrum of compound **5** in CDCl₃

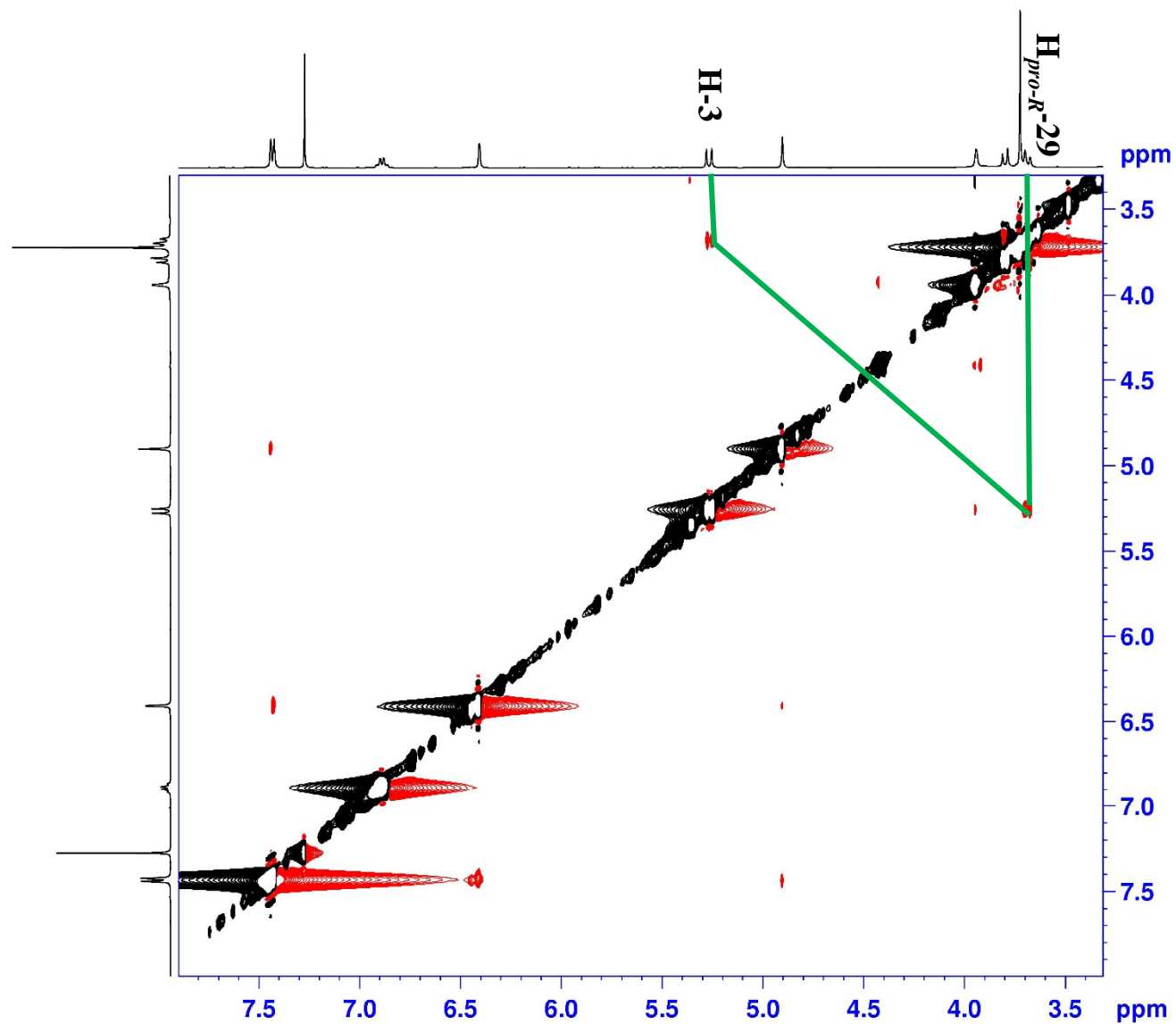


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EXPNO      7
PROCNO     1
Date_      20180110
Time       9.08
INSTRUM    spect
PROBHD     5 mm CPPBBO BB
PULPROG    noesygpphph
TD         2048
SOLVENT    CDCl3
NS         16
DS         32
SWH        4000.000 Hz
FIDRES     1.953125 Hz
AQ         0.2560500 sec
RG         85.34
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
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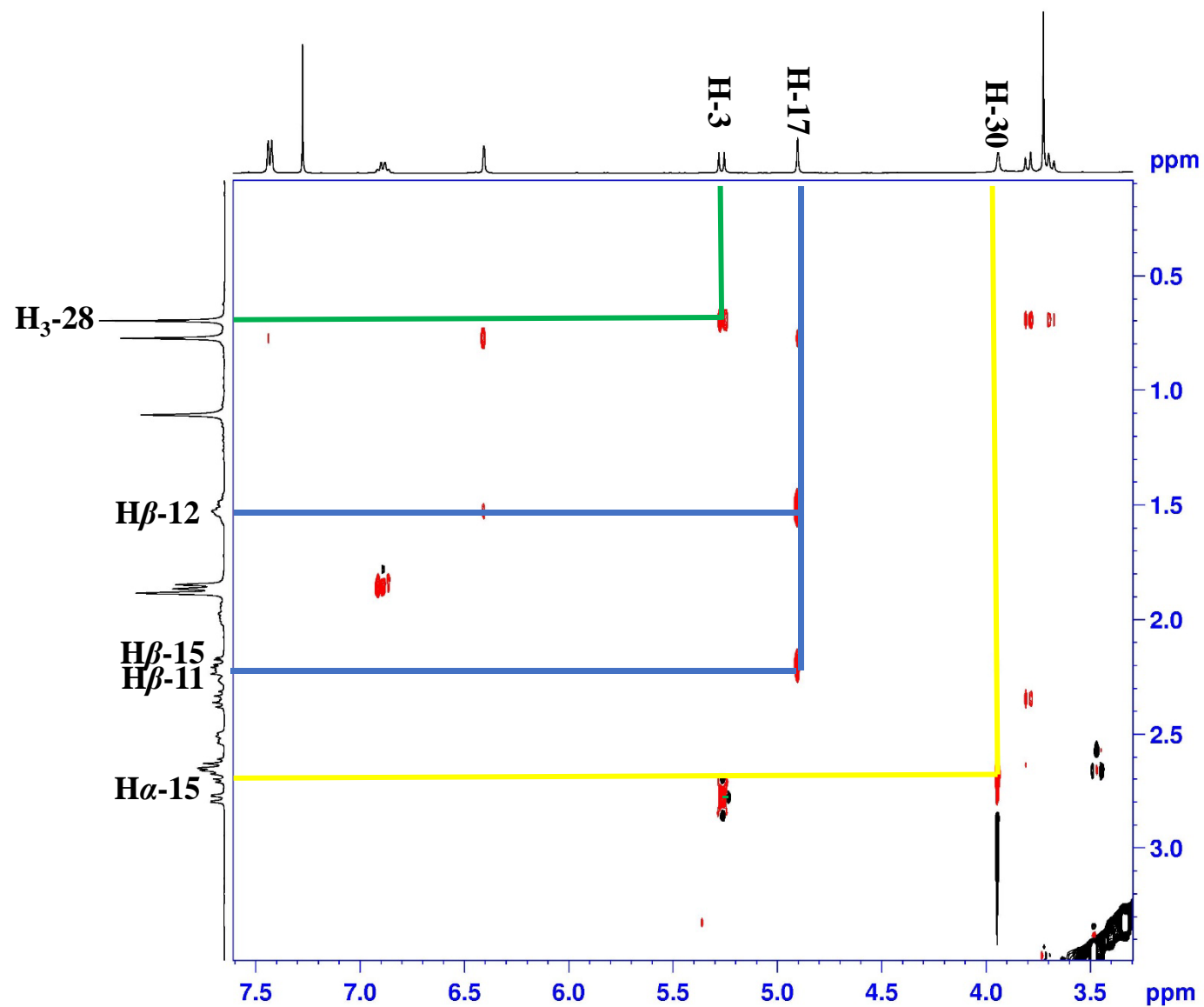
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===== CHANNEL f1 =====
SFO1      400.1318006 MHz
NUC1       1H
P1         11.50 usec
P2         23.00 usec
P17        2500.00 usec
ND0        1
TD         256
SFO1      400.1318 MHz
FIDRES     15.625000 Hz
SW         9.997 ppm
FnMODE     States-TPPI
SI         1024
SF         400.1300018 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.00
SI         1024
MC2        States-TPPI
SF         400.1300029 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
```

S137

NOESY (400 MHz) spectrum of compound **5** in CDCl_3



NOESY (400 MHz) spectrum of compound **5** in CDCl₃



NOESY (400 MHz) spectrum of compound **5** in CDCl_3

