

Supporting Information-2:

Scaffold diversity-oriented synthesis of limonoid dimers: discovery of an axially chiral agent with *in vivo* anti-breast cancer activity

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Copies of HRESIMS, UV, IR, 1D and 2D NMR spectra of compounds 1, 2, and 2'.

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HR-ESIMS for compound 1

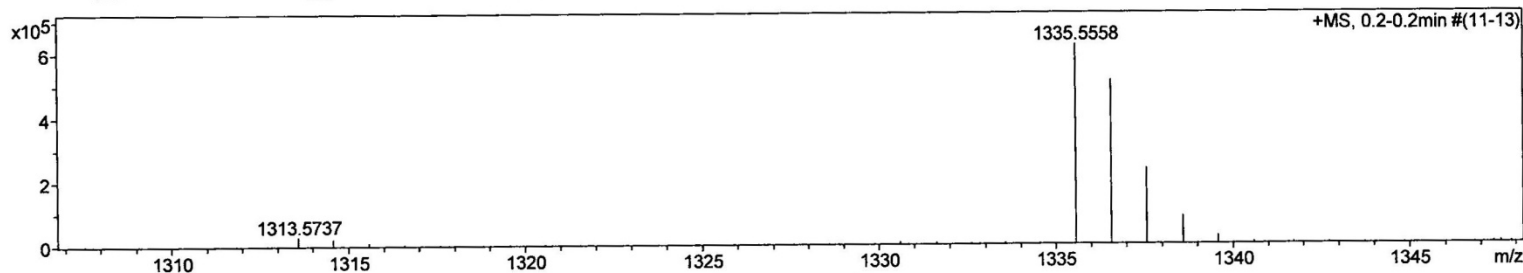
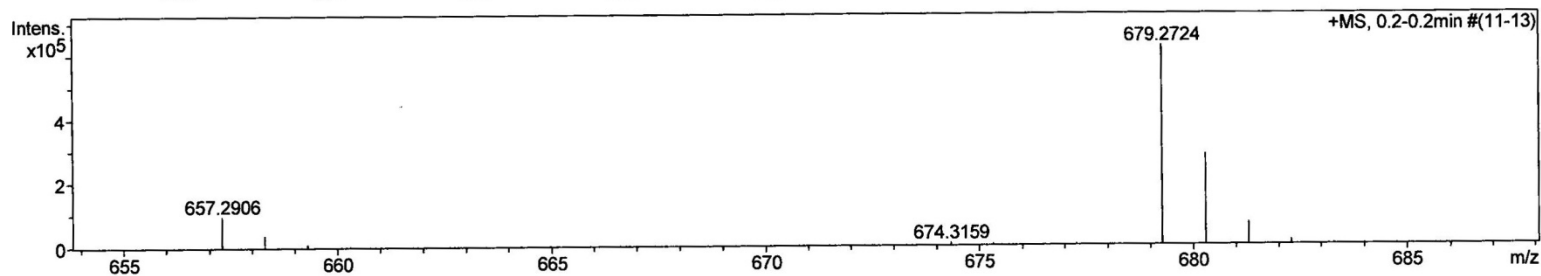
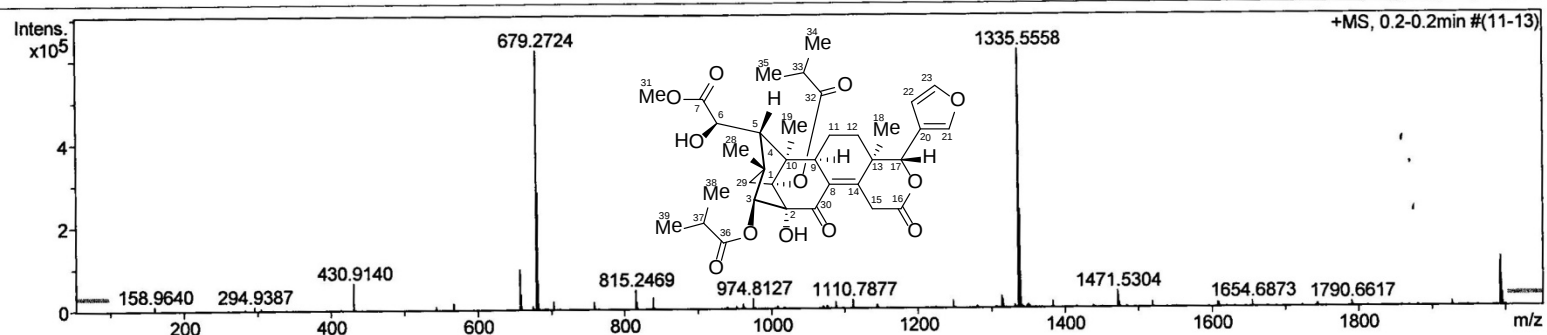
Generic Display Report

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Sample Name SCSIO
Comment

Acquisition Date 4/27/2015 10:34:48 AM

Operator SCSIO
Instrument maXis



HR-ESIMS for compound 1

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\MS\data\201504\liwanshan_LWS-42_pos.d
 Method POS_100-2000_Direct Infusion.m
 Sample Name SCSIO
 Comment

Acquisition Date 4/27/2015 10:34:48 AM

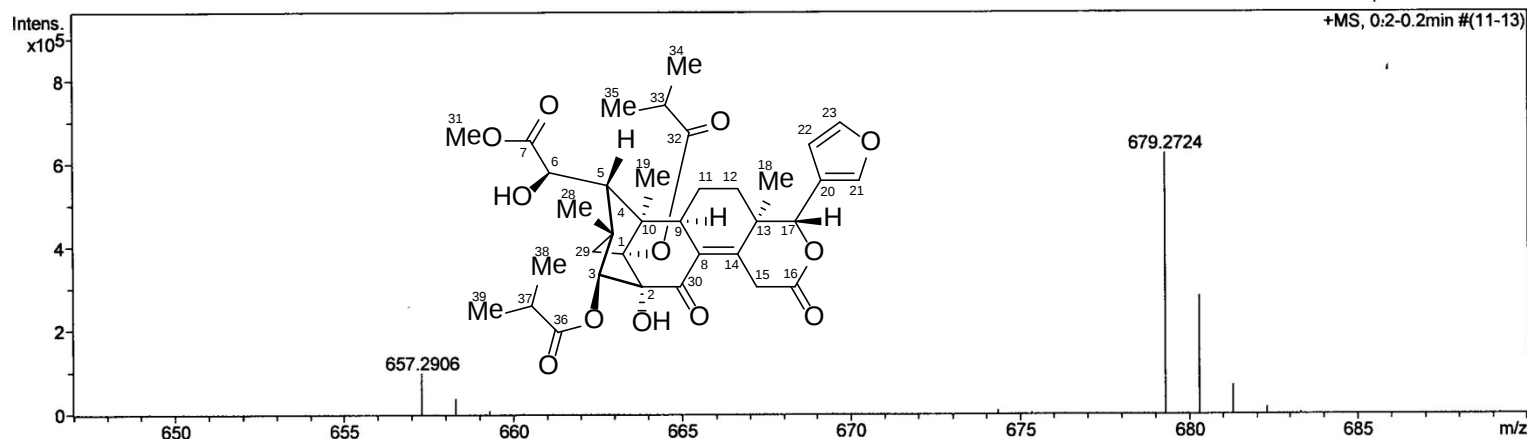
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 Instrument / Ser# maXis 29

Acquisition Parameter

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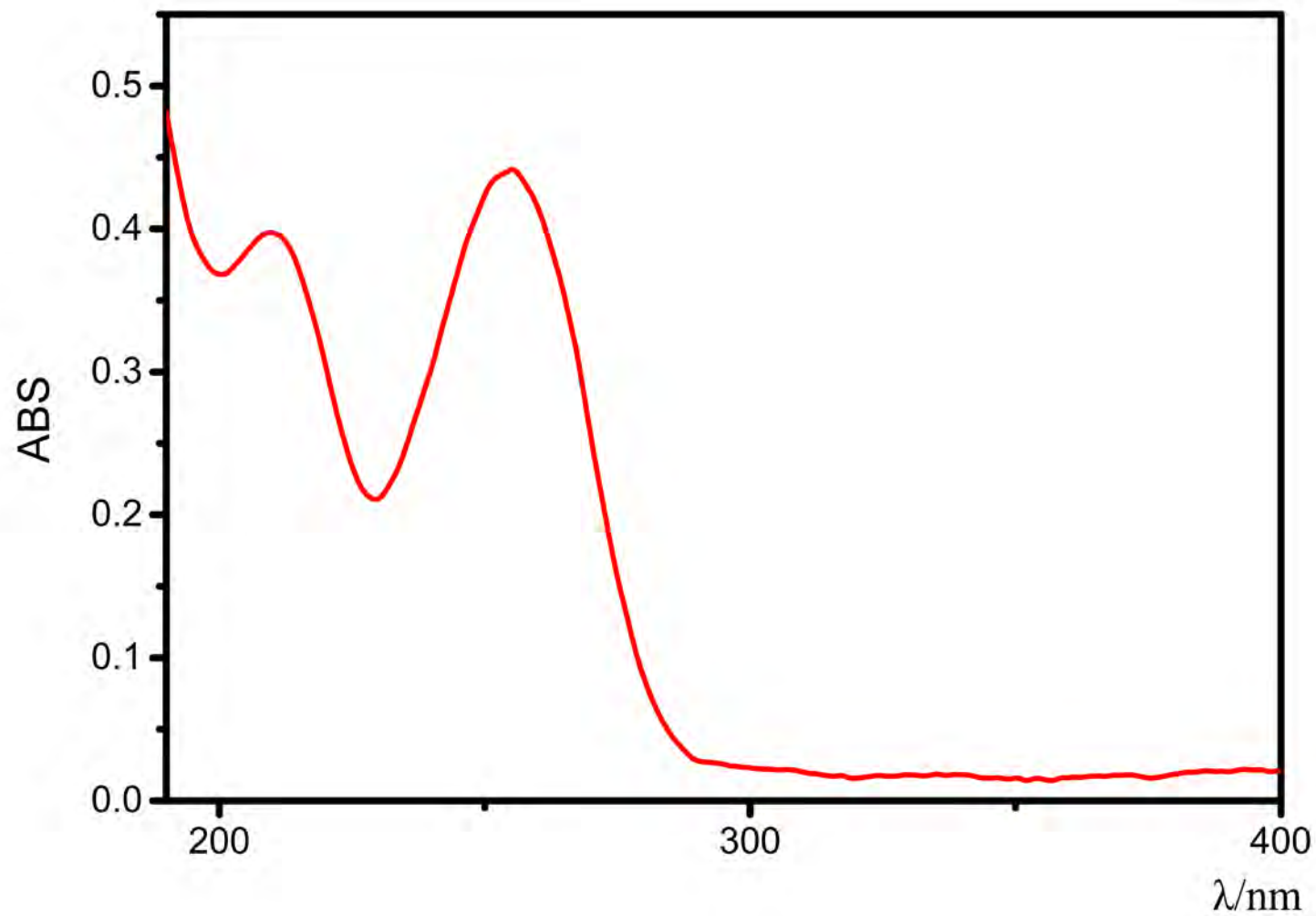
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 Set Divert Valve Waste



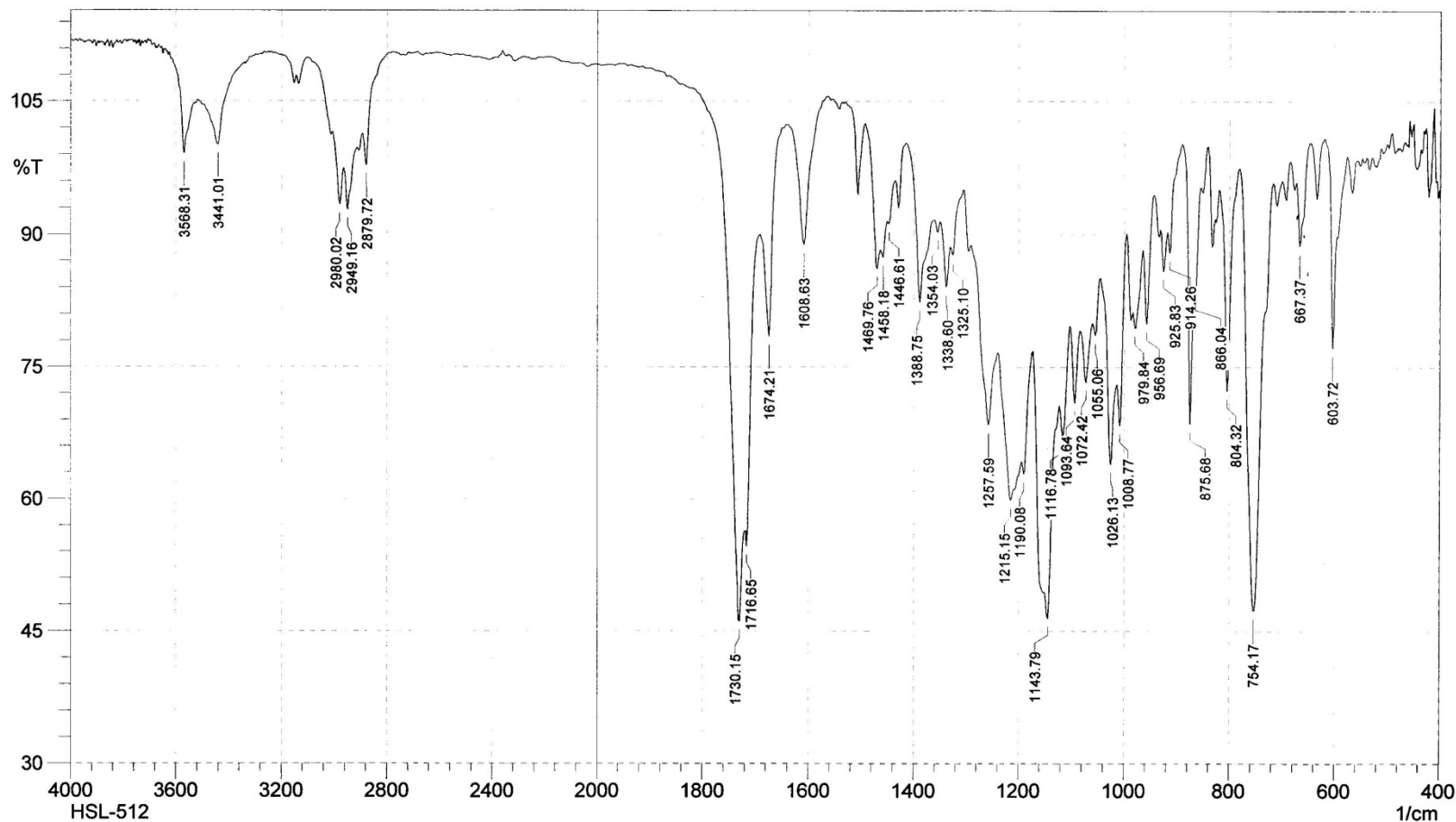
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UV spectrum for compound **1** in CH₃CN



IR spectrum for compound 1

SHIMADZU

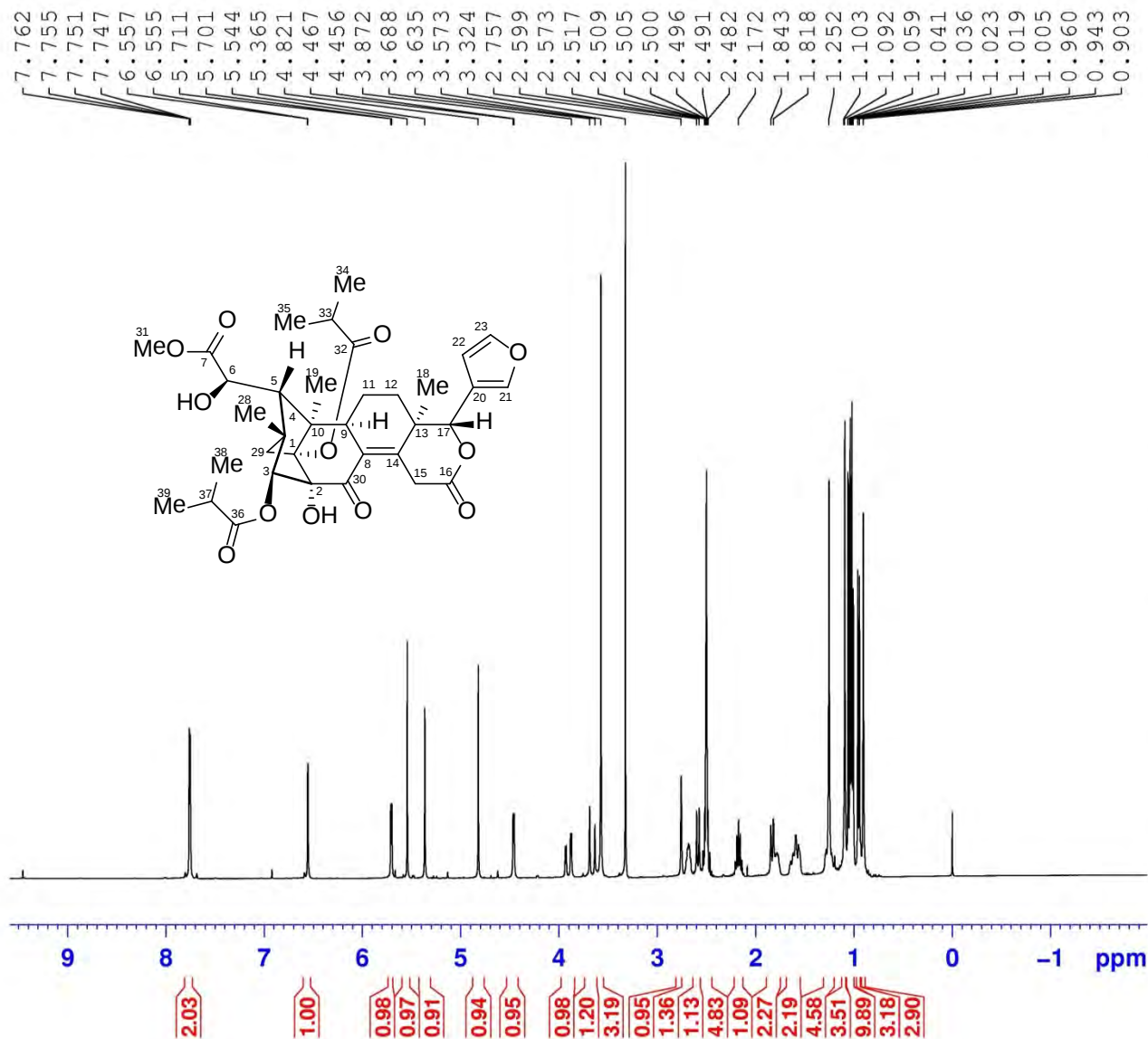


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F:\liwanshan\20180226\42
(4)1.smf

Scan number: 25
Resolution: 4 [1/cm]

Data: 2018-2-28 14:16:40
Operator: SCSIO

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



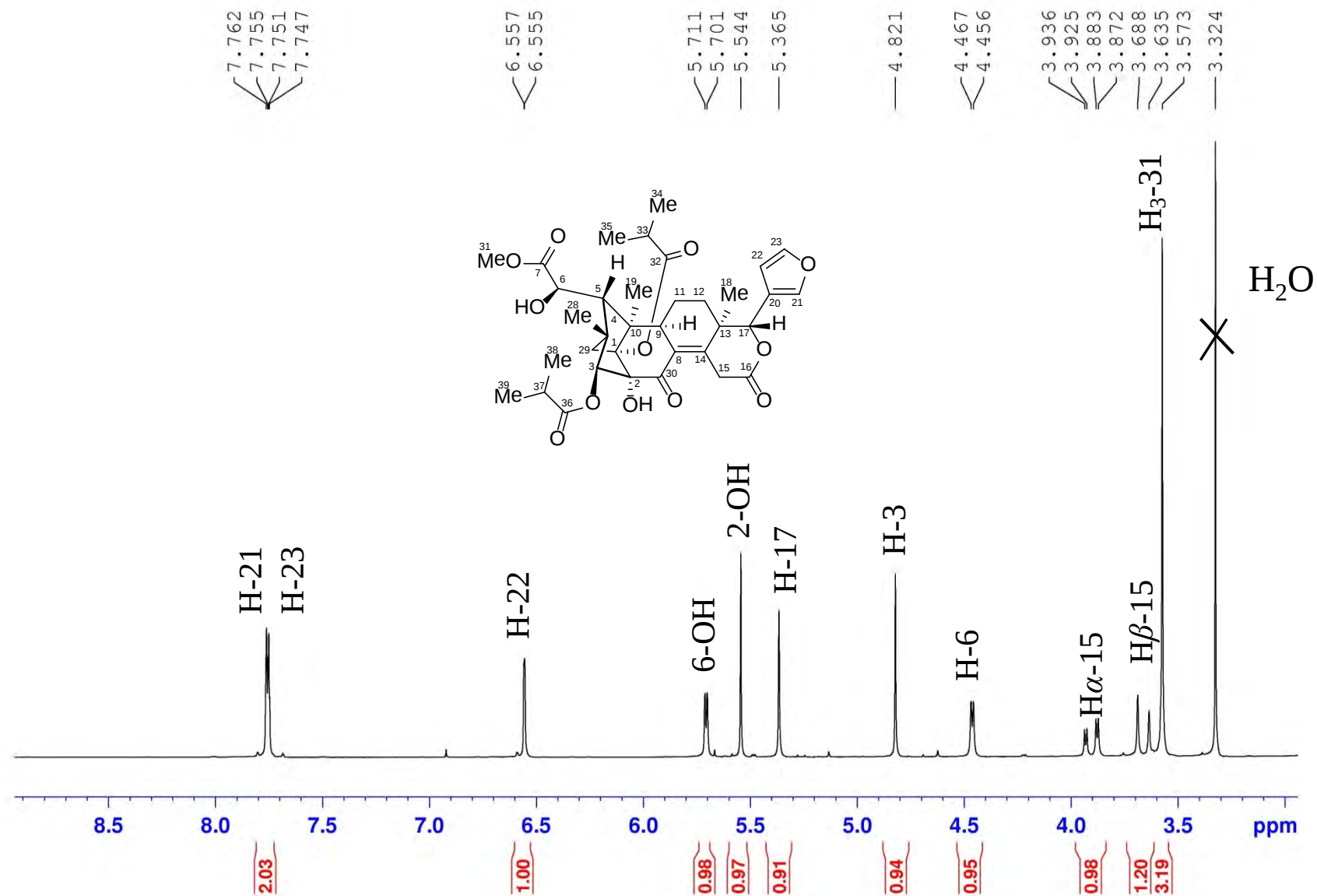
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EXPNO      10
PROCNO      1
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Time       19.46
INSTRUM     spect
PROBHD      5 mm CPPBBO BB
PULPROG     zg30
TD          65536
SOLVENT     DMSO
NS          16
DS          2
SWH         8223.685
FIDRES      0.125483
AQ          3.9846387
RG          85.34
DW          60.800
DE          10.00
TE          297.0
D1          1.00000000
TD0         1
    
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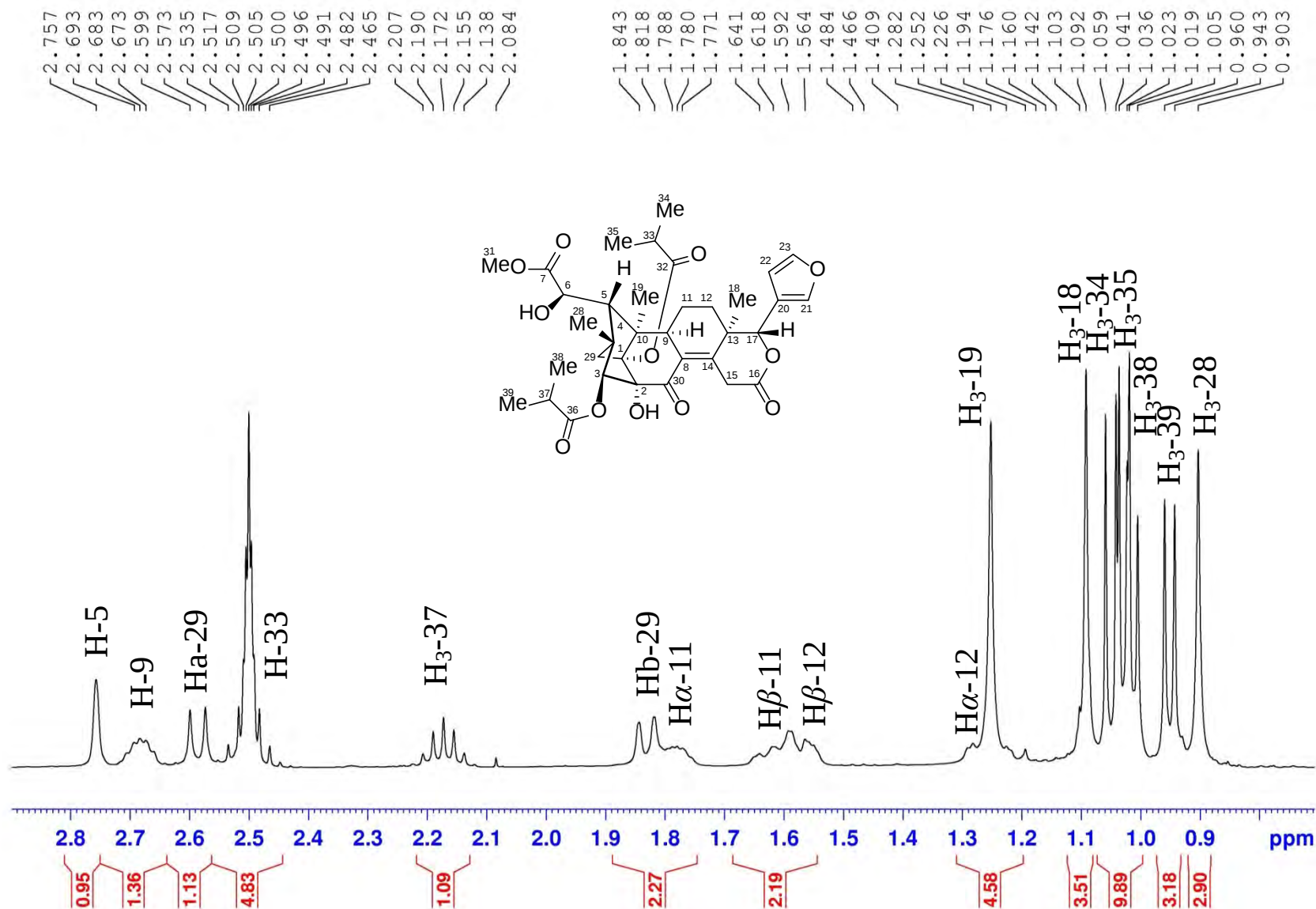
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NUC1       1H
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SI         65536
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WDW        EM
SSB        0
LB         0.30
GB         0
PC         1.00
    
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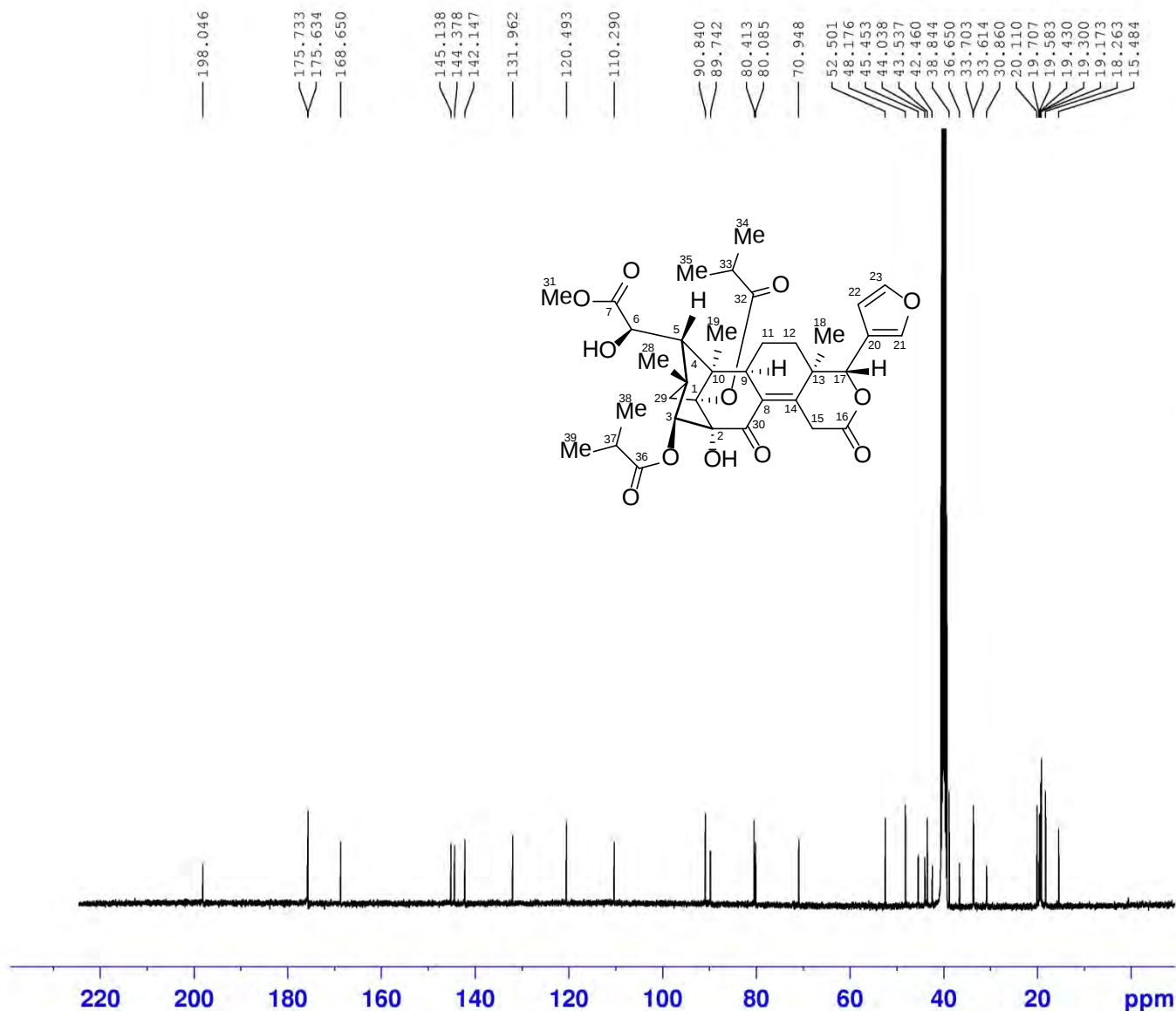
^1H NMR (400 MHz) spectrum of compound **1** in $\text{DMSO-}d_6$



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



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



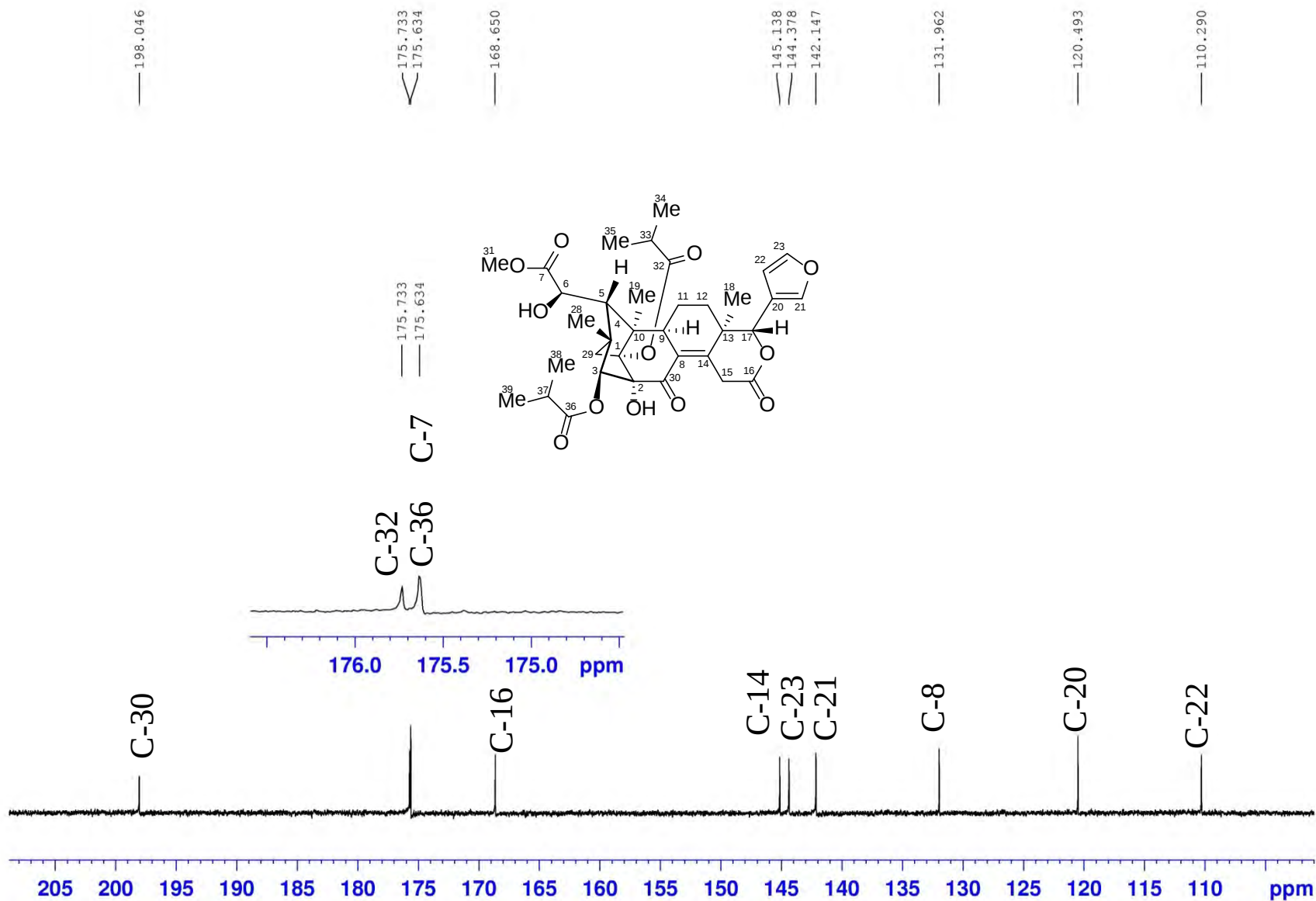
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EXPNO     11
PROCNO    1
Date_     20160411
Time      20.46
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
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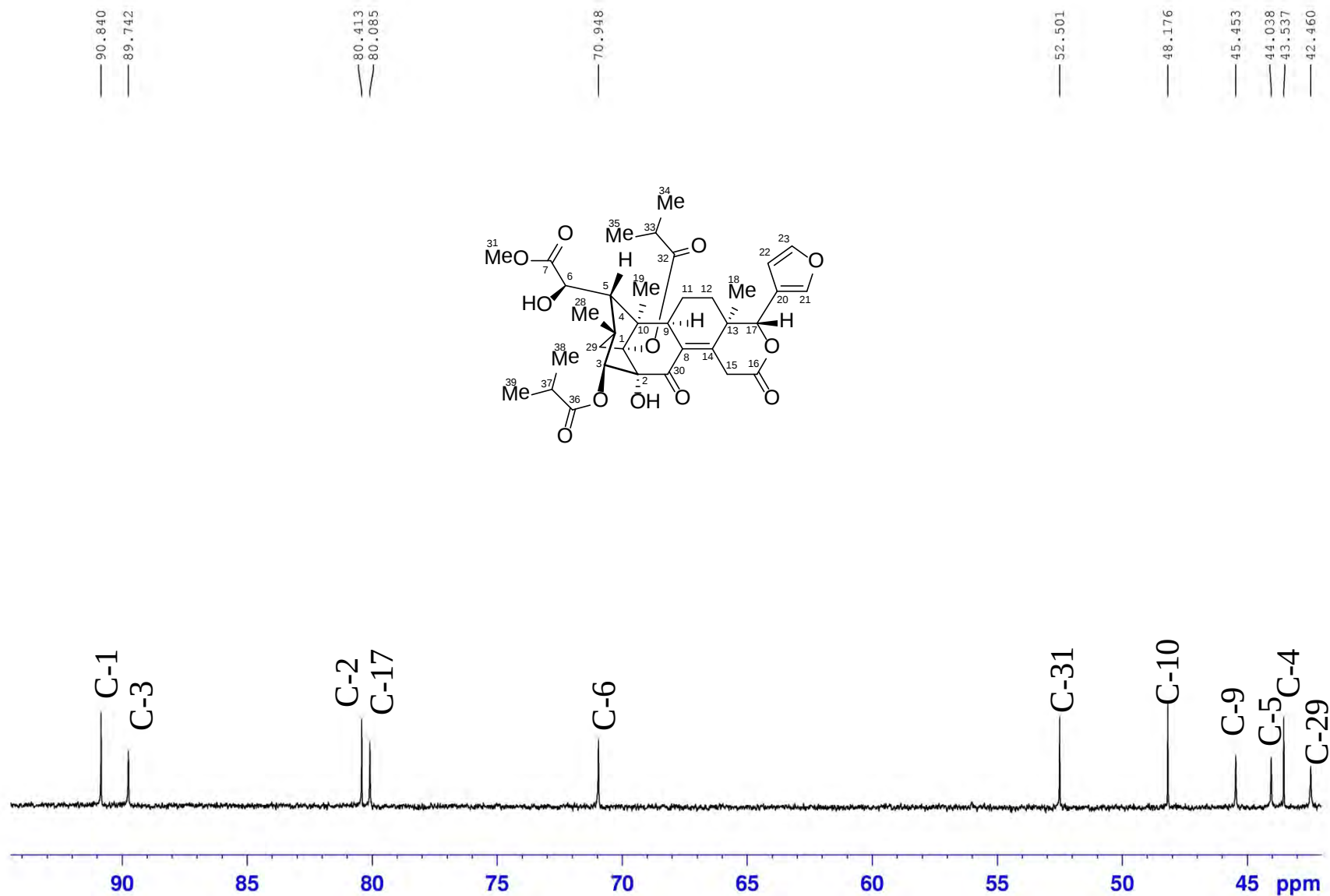
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SSB       0
LB        1.00 Hz
GB        0
PC        1.40
    
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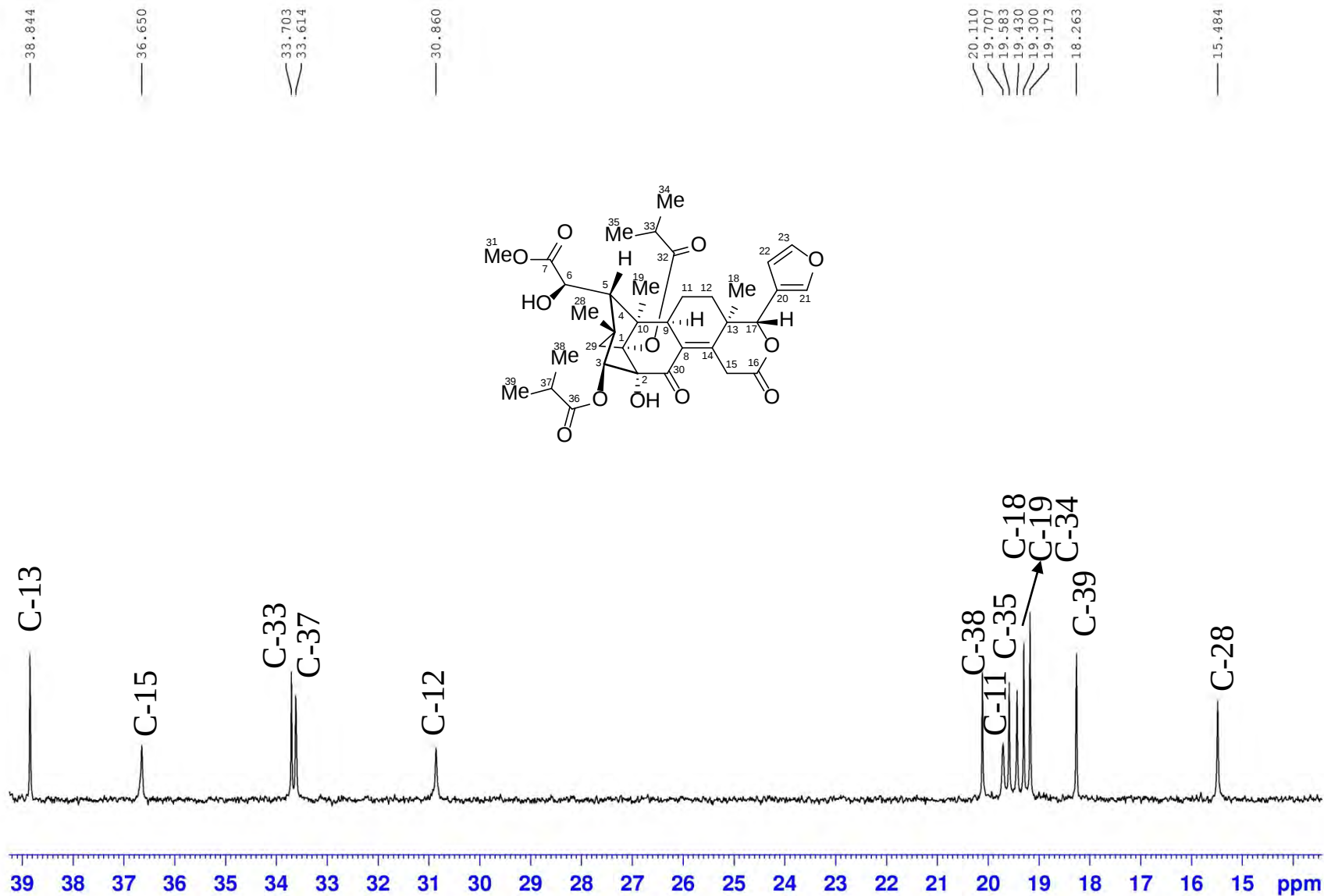
^{13}C NMR (100 MHz) spectrum of compound **1** in $\text{DMSO-}d_6$



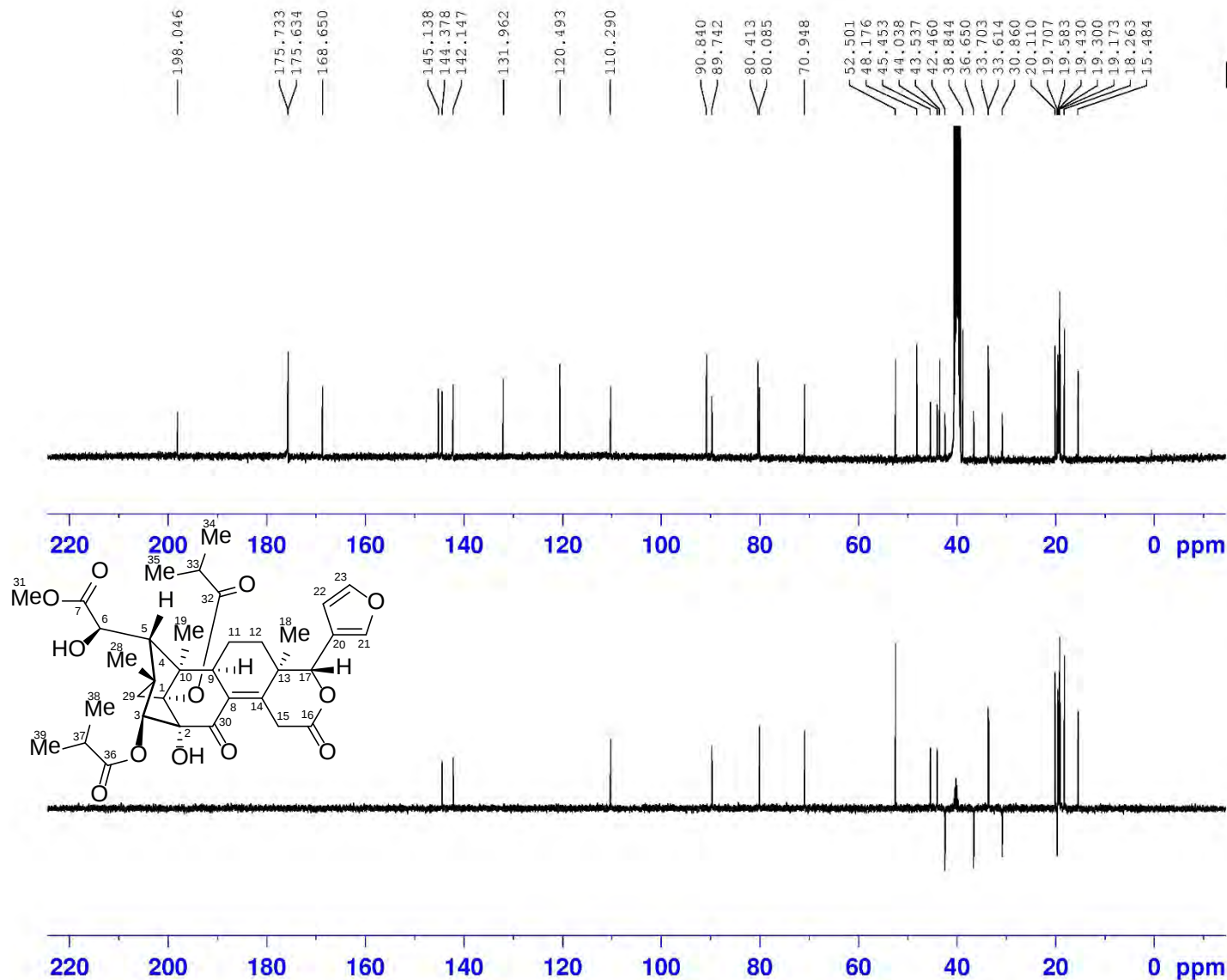
^{13}C NMR (100 MHz) spectrum of compound **1** in $\text{DMSO-}d_6$



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



DEPT135 (100 MHz) spectrum of compound **1** in DMSO-*d*₆

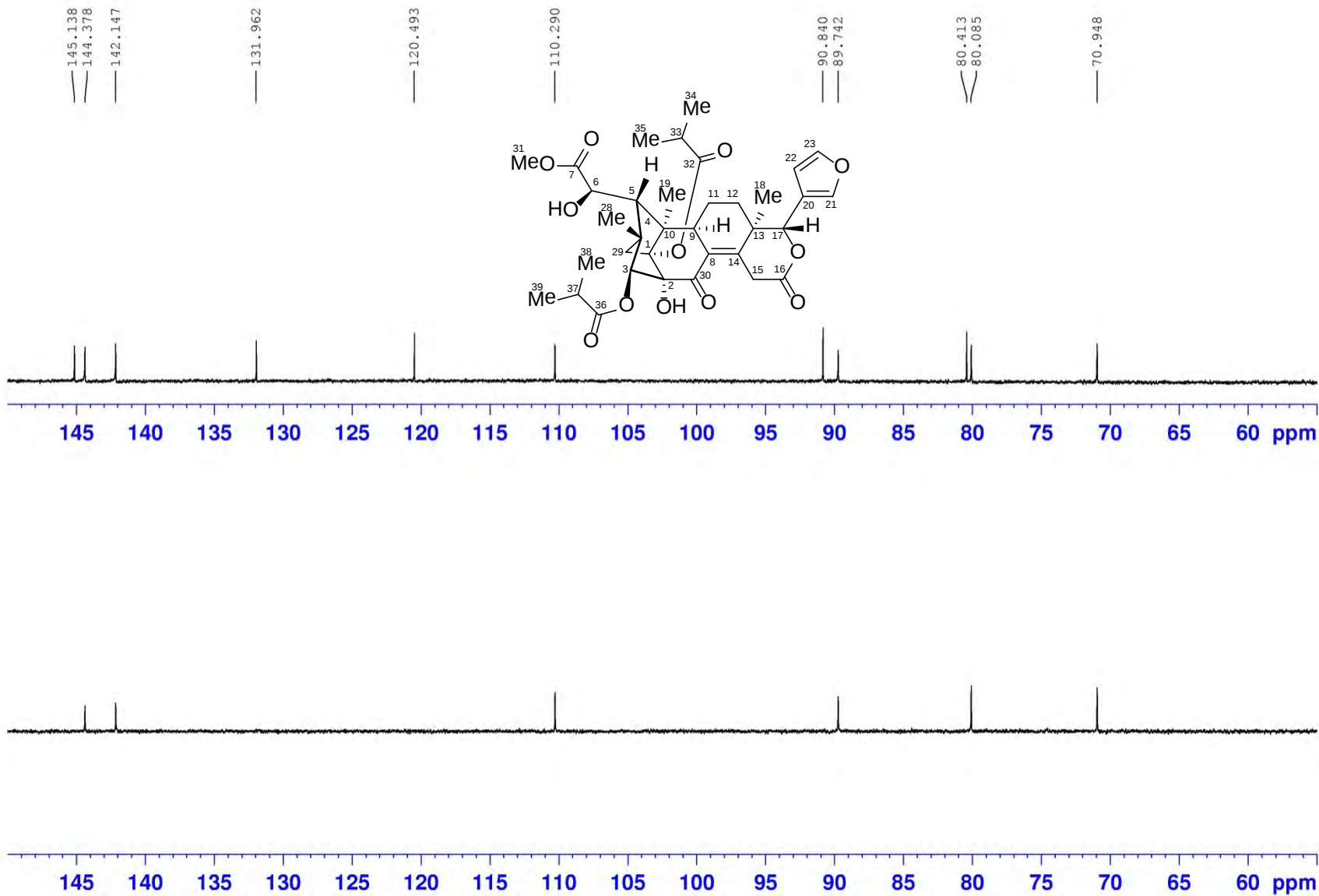


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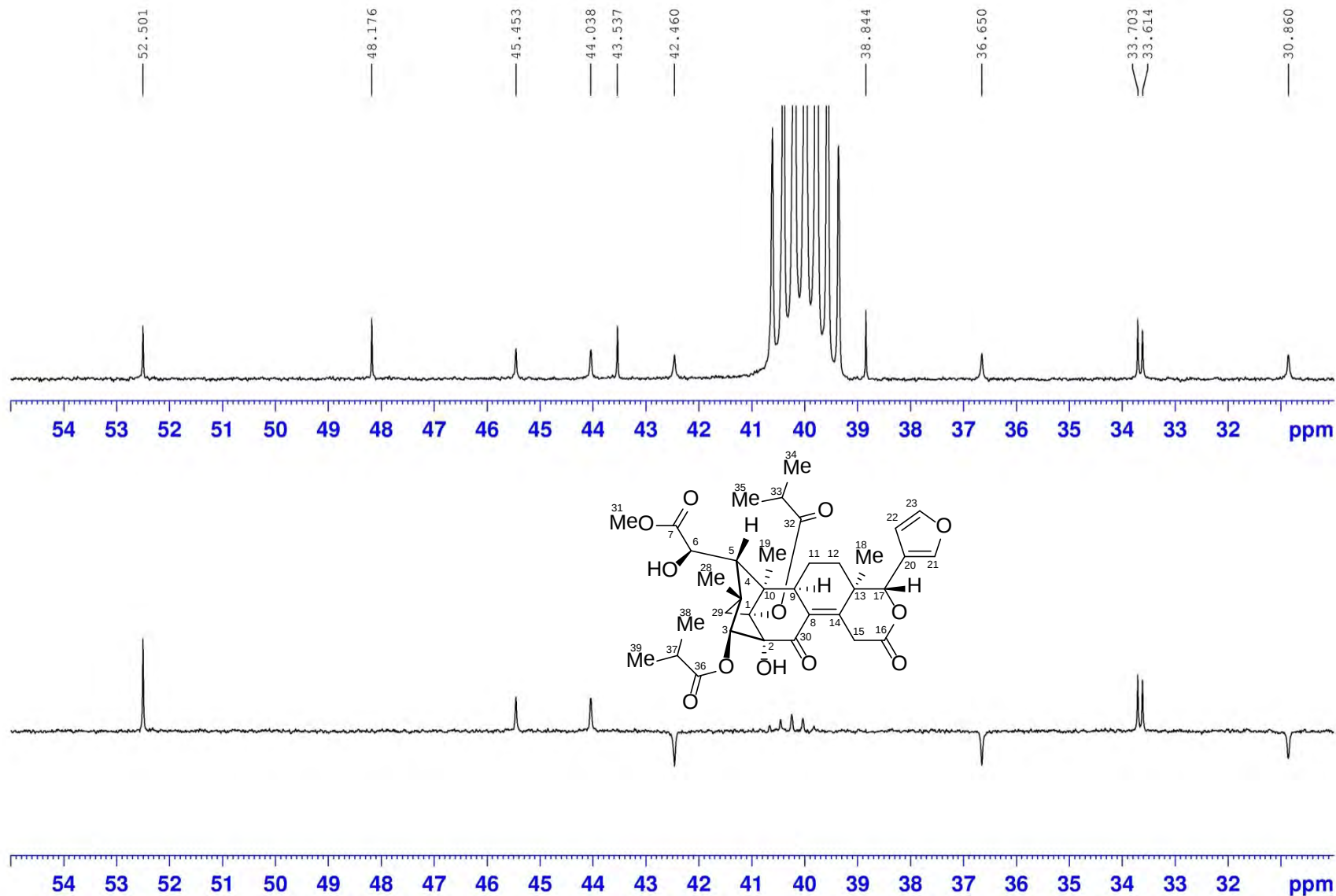
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PROCNO    1
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Time      21.04
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PULPROG   deptsp135
TD        65536
SOLVENT   DMSO
NS        300
DS        4
SWH       24038.461
FIDRES    0.366798
AQ        1.3631988
RG        91.64
DW        20.800
DE        18.00
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D12       0.00002000
TD0       1
    
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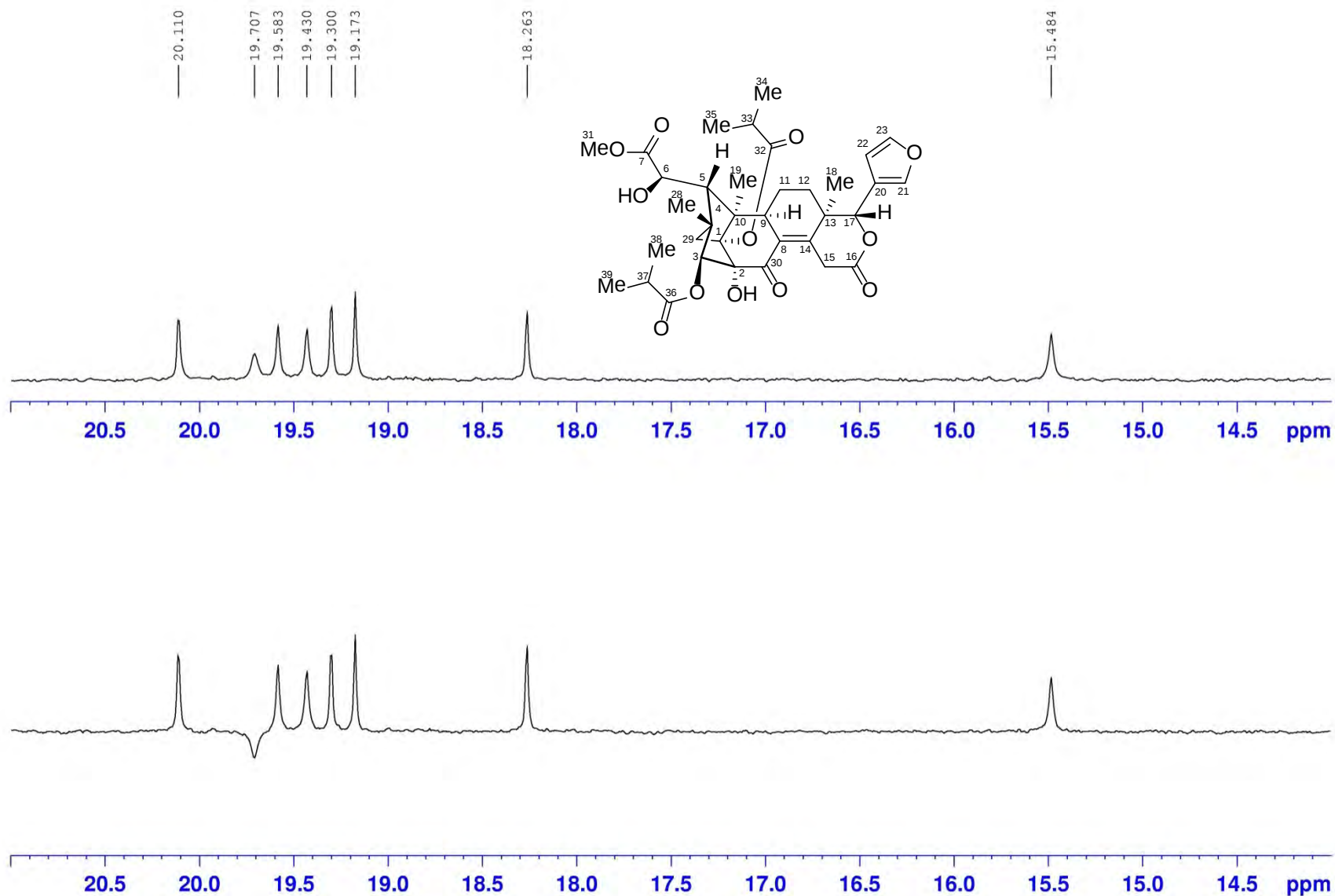
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P13       2000.00
SI        32768
SF        100.6127685
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LB        1.00
GB        0
PC        1.40
    
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DEPT135 (100 MHz) spectrum of compound **1** in DMSO-*d*₆

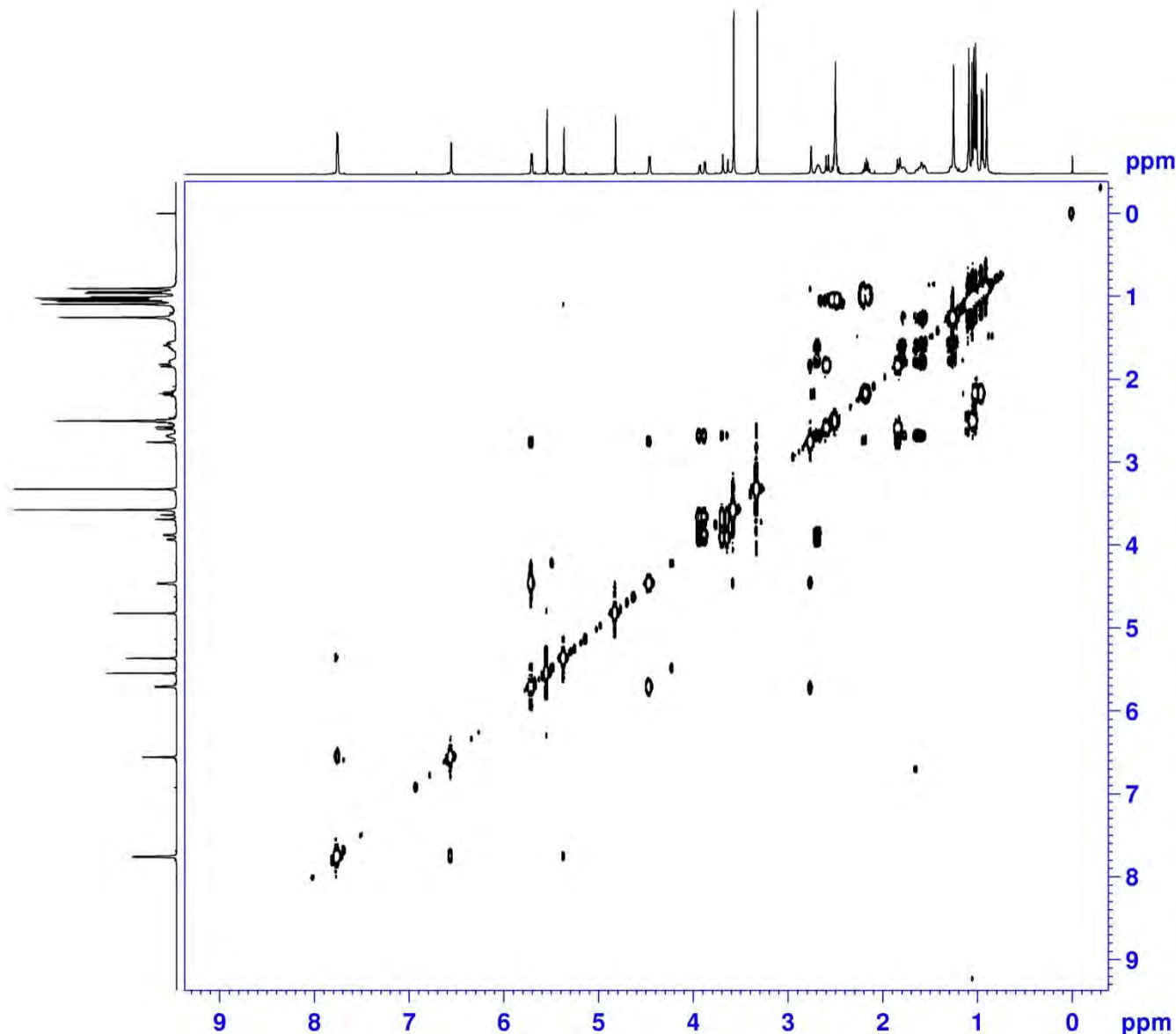
DEPT135 (100 MHz) spectrum of compound **1** in DMSO-*d*₆



DEPT135 (100 MHz) spectrum of compound **1** in DMSO-*d*₆



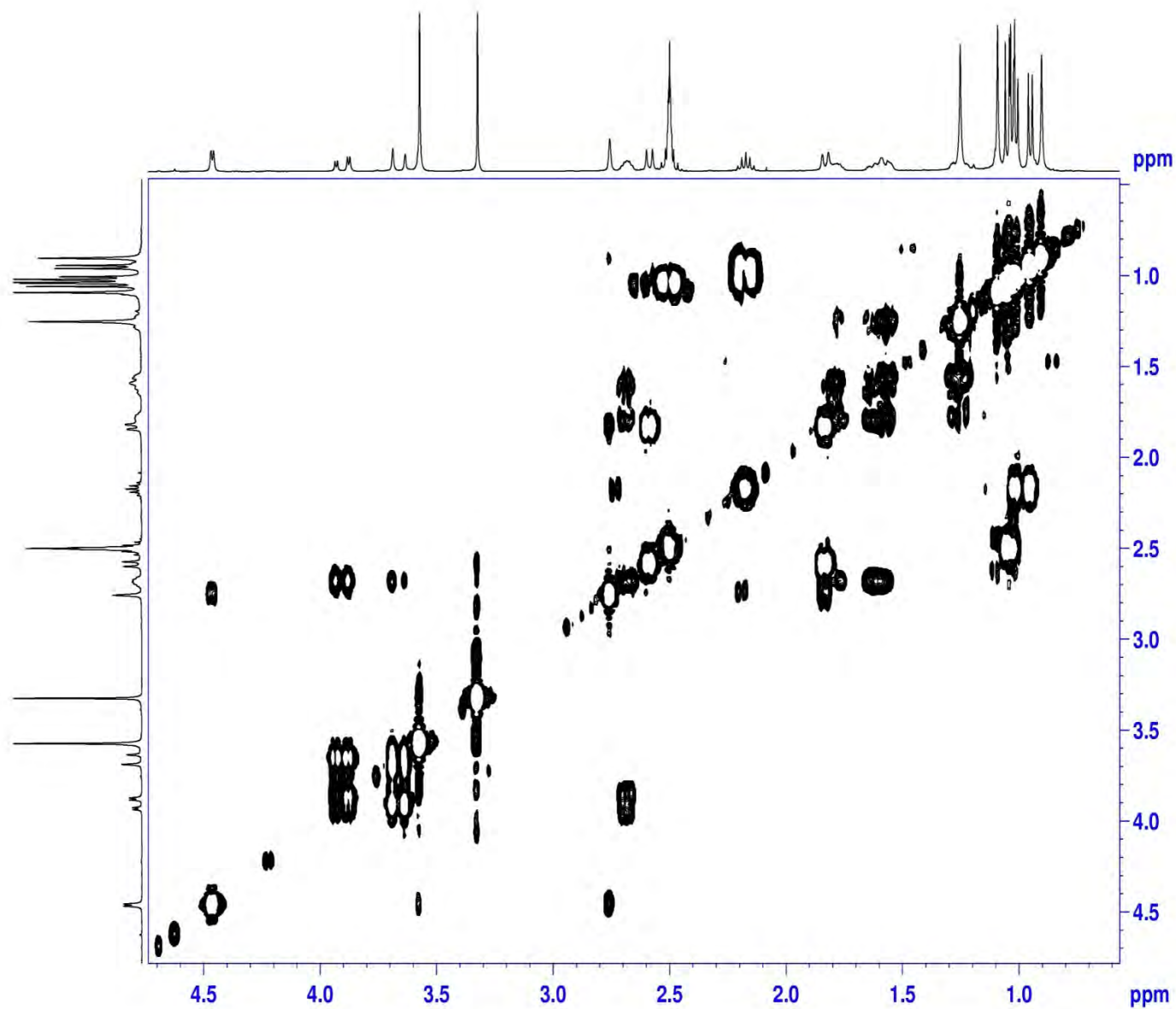
^1H - ^1H COSY (400 MHz) spectrum of compound **1** in $\text{DMSO-}d_6$



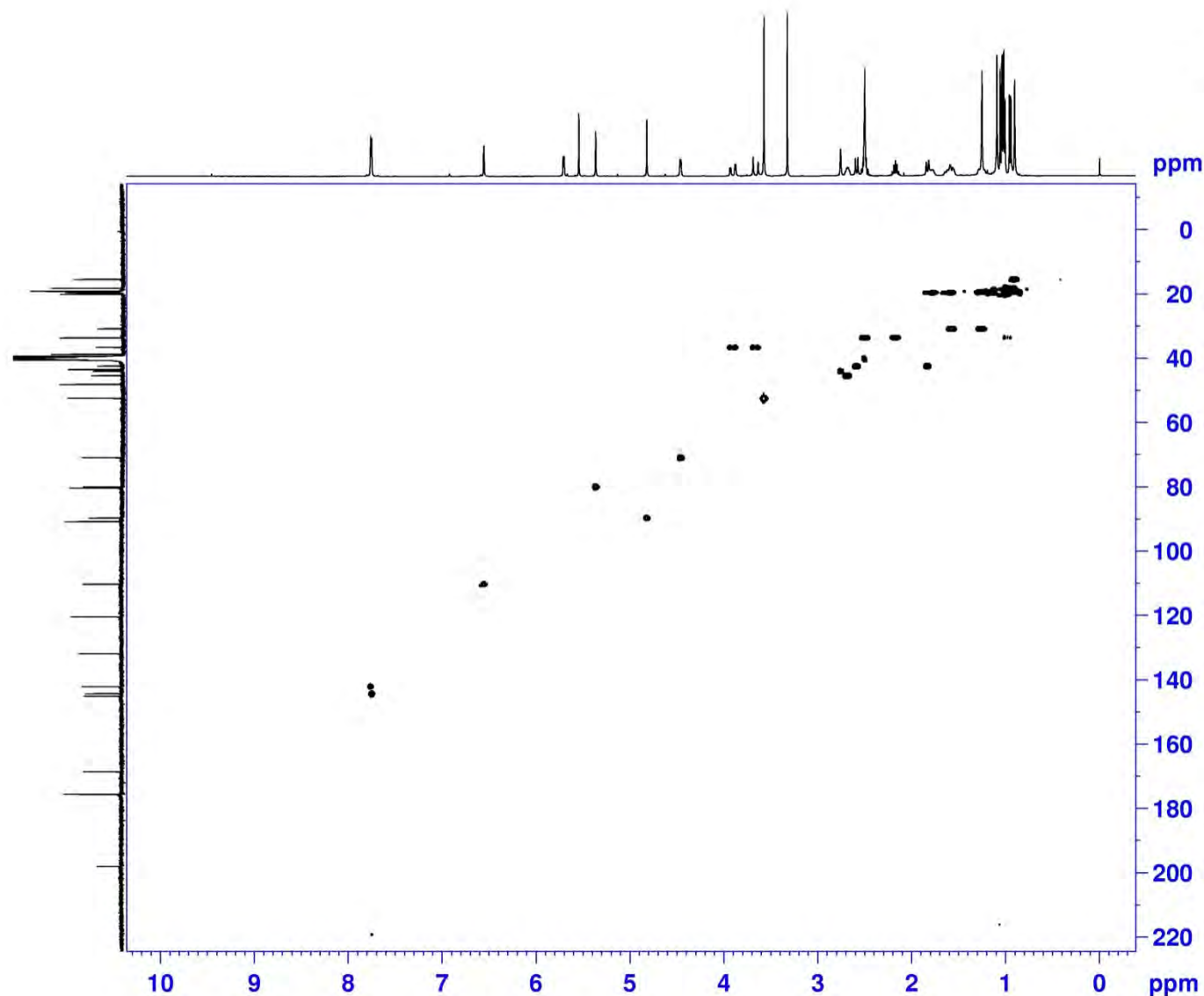
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PROCNO    1
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PULPROG   cosygpppgf
TD        2048
SOLVENT   DMSO
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DS        8
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FIDRES    1.907349 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
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```
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NUC1      1H
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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        400.1300037 MHz
WDW       QSINE
SSB       0
LB        0.00 Hz
GB        0
PC        1.40
SI        1024
MC2       QF
SF        400.1300037 MHz
WDW       QSINE
SSB       0
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^1H - ^1H COSY (400 MHz) spectrum of compound **1** in $\text{DMSO-}d_6$



HSQC (400 MHz) spectrum of compound **1** in DMSO- d_6



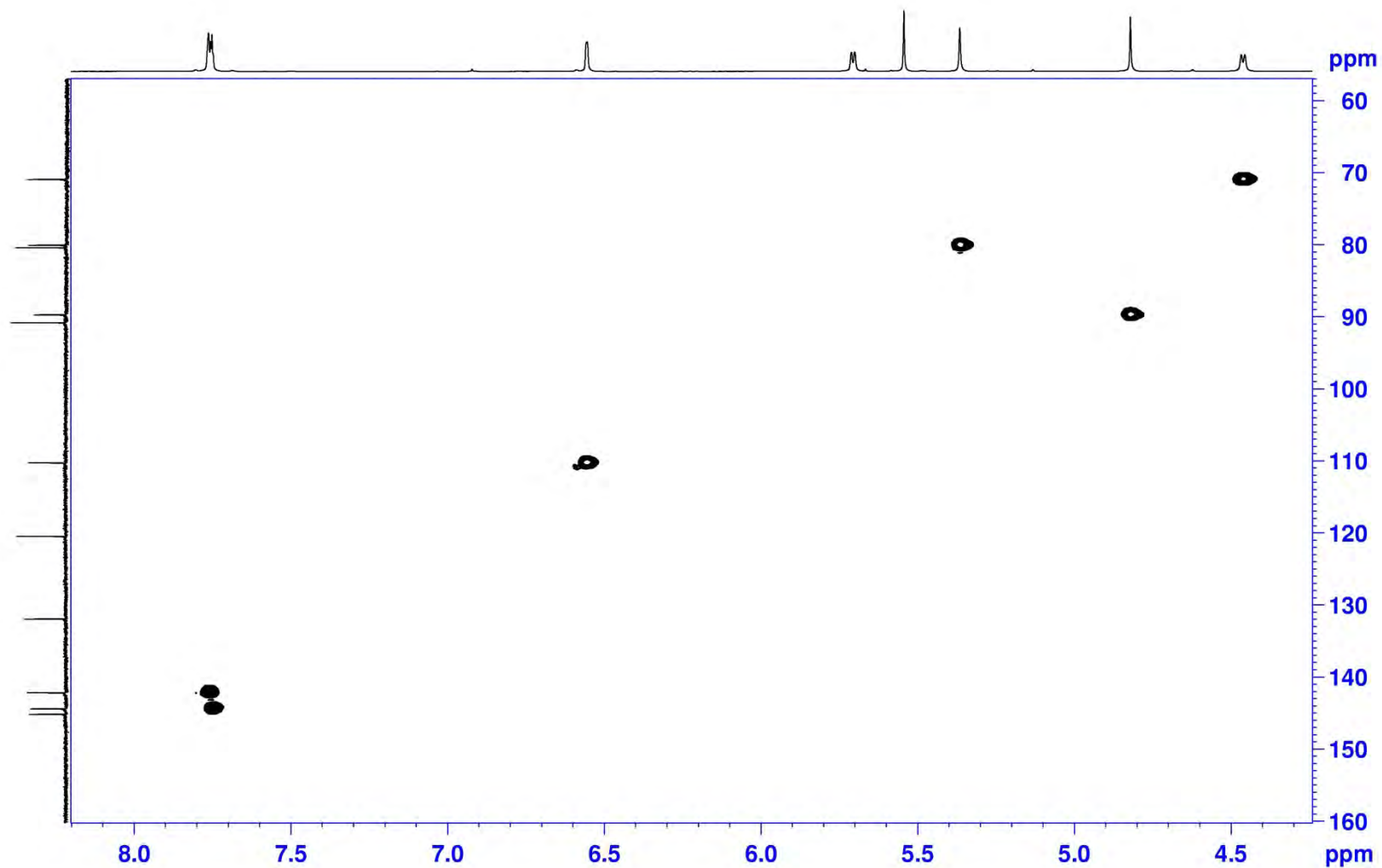
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PROCNO    1
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TD        1024
SOLVENT   DMSO
NS        16
DS        16
SWH       4302.926 Hz
FIDRES    4.202076 Hz
AQ        0.1190388 sec
RG        208.5
DW        116.200 usec
DE        10.00 usec
TE        297.0 K
CNST2     145.0000000
D0        0.00000300 sec
D1        1.46497905 sec
D4        0.00172414 sec
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IN0       0.00002080 sec
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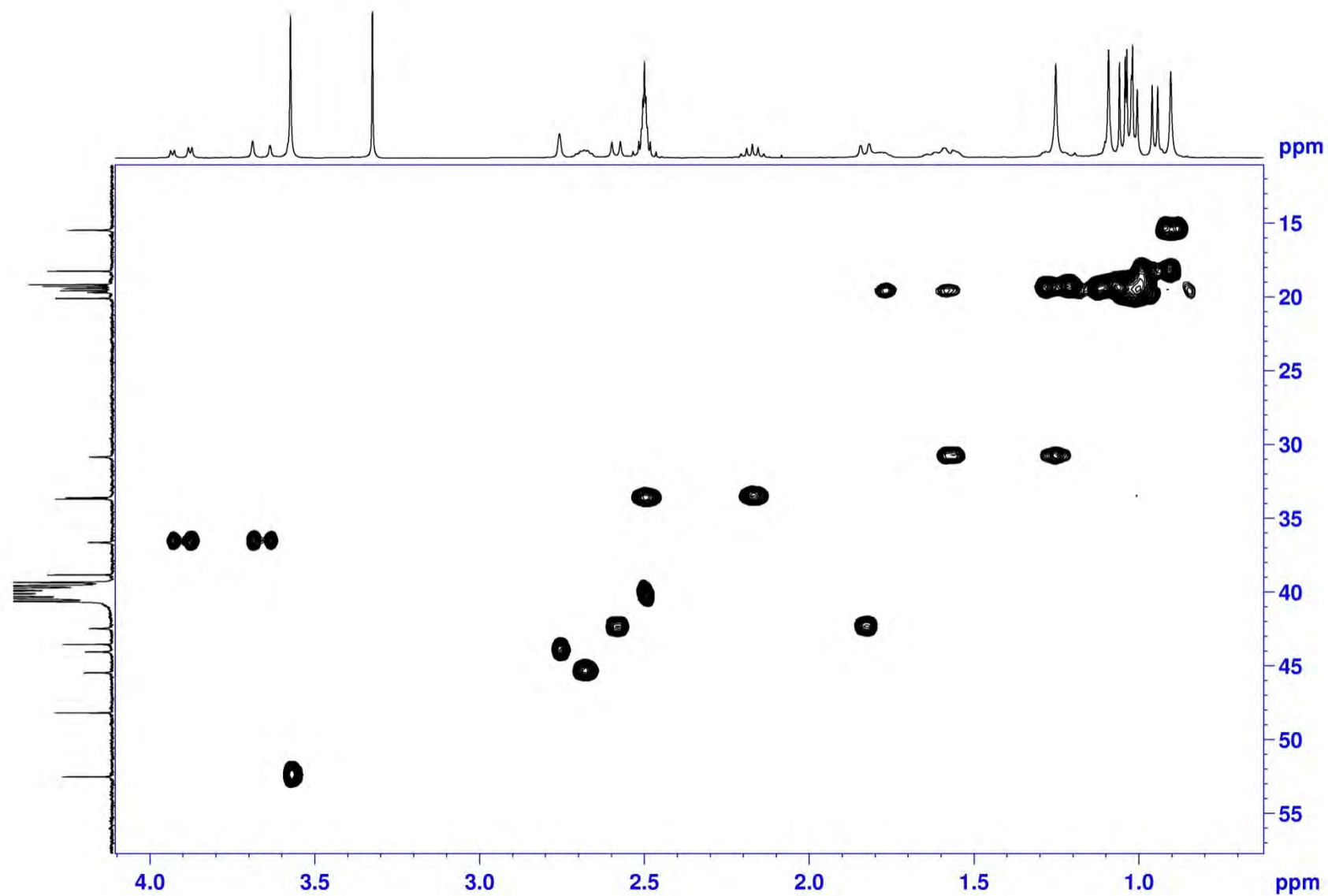
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P2        23.00 usec
P28       0.00 usec
ND0       2
TD        256
SFO1      100.6233 MHz
FIDRES    93.900238 Hz
SW        238.896 MHz
FnMODE    Echo-Antiecho
SI        1024
SF        400.1300037 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
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PC        1.40
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MC2       echo-antiecho
SF        100.6127685 MHz
    
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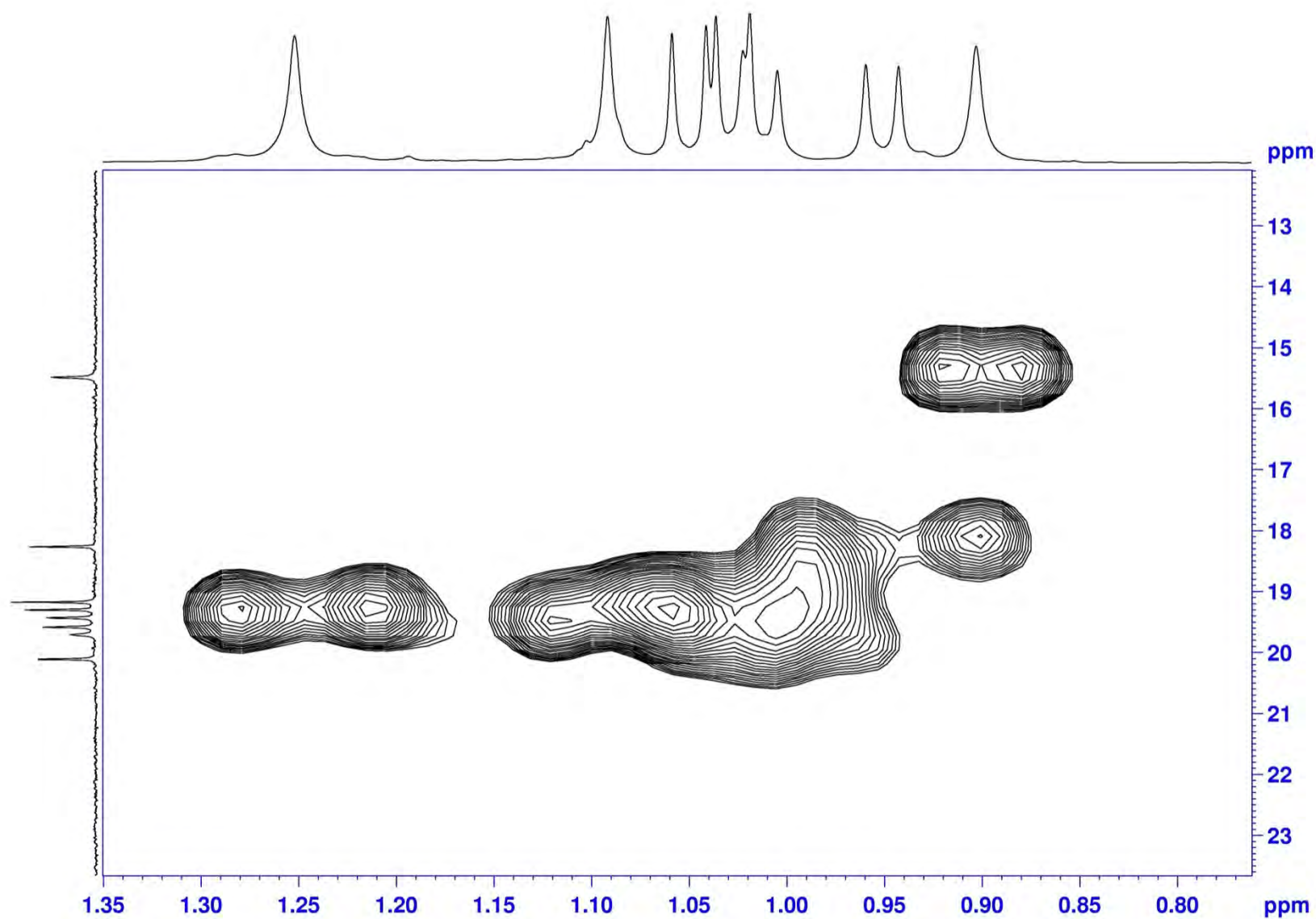
HSQC (400 MHz) spectrum of compound **1** in DMSO- d_6



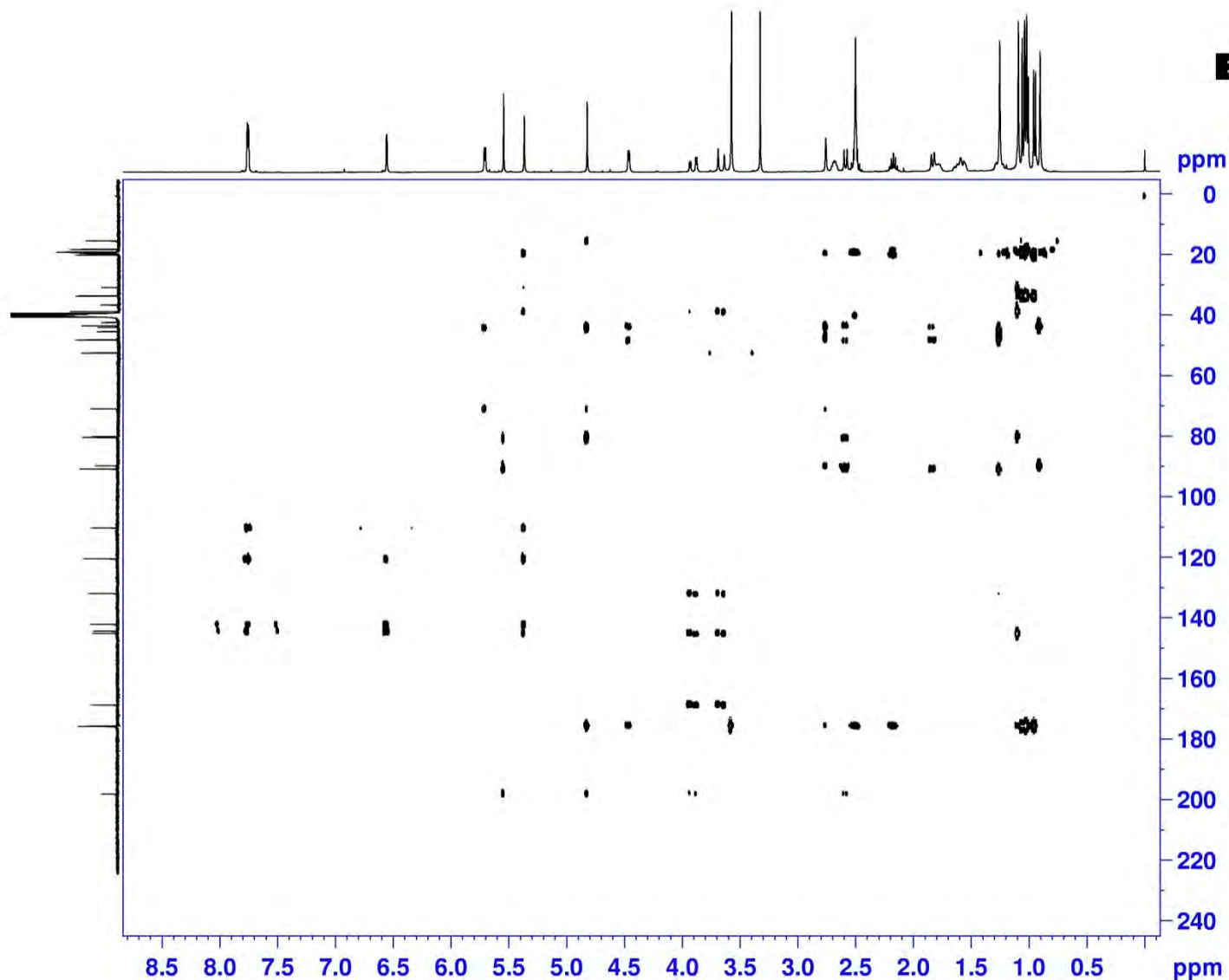
HSQC (400 MHz) spectrum of compound **1** in DMSO- d_6



HSQC (400 MHz) spectrum of compound **1** in DMSO- d_6



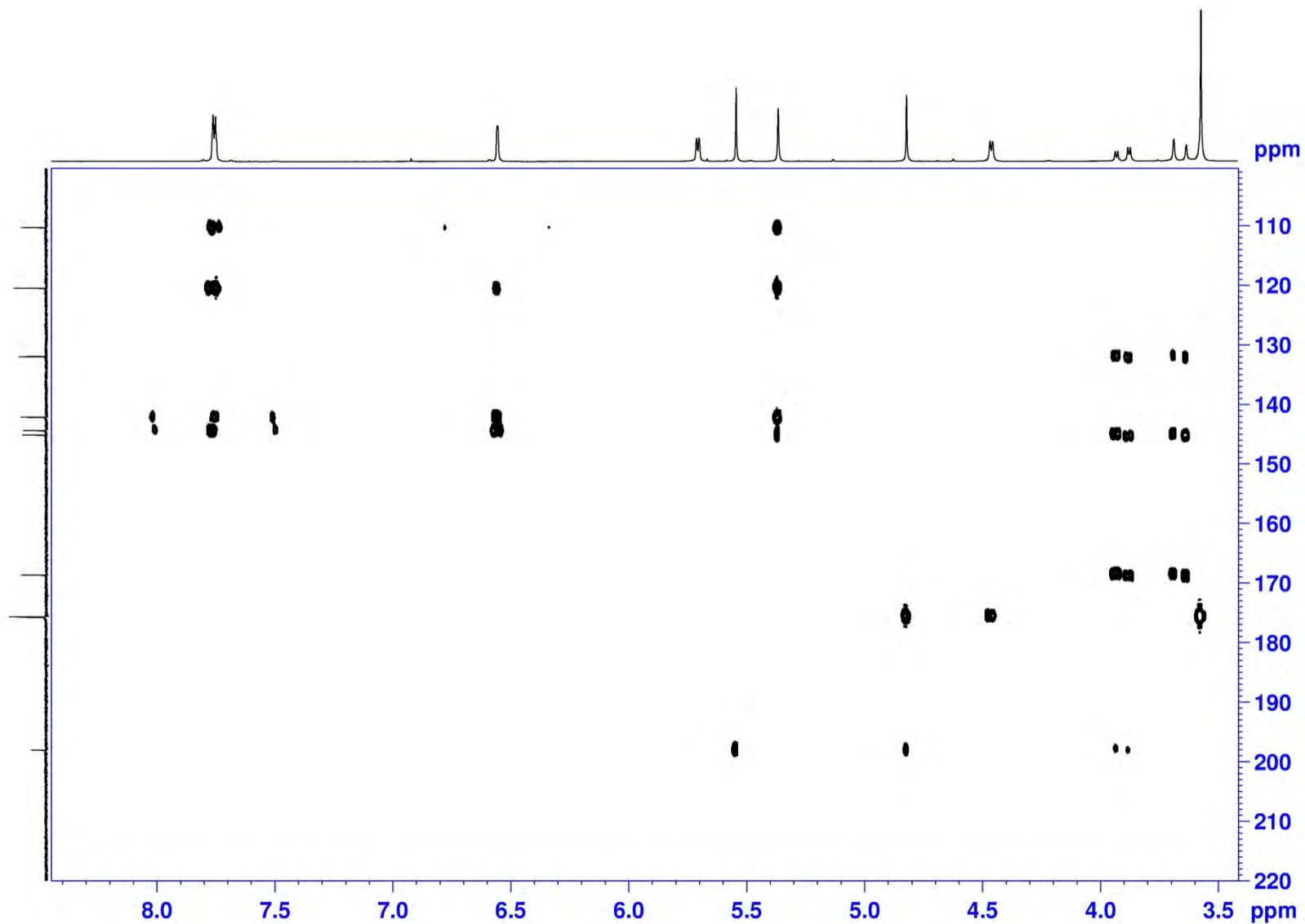
HMBC (400 MHz) spectrum of compound **1** in DMSO- d_6



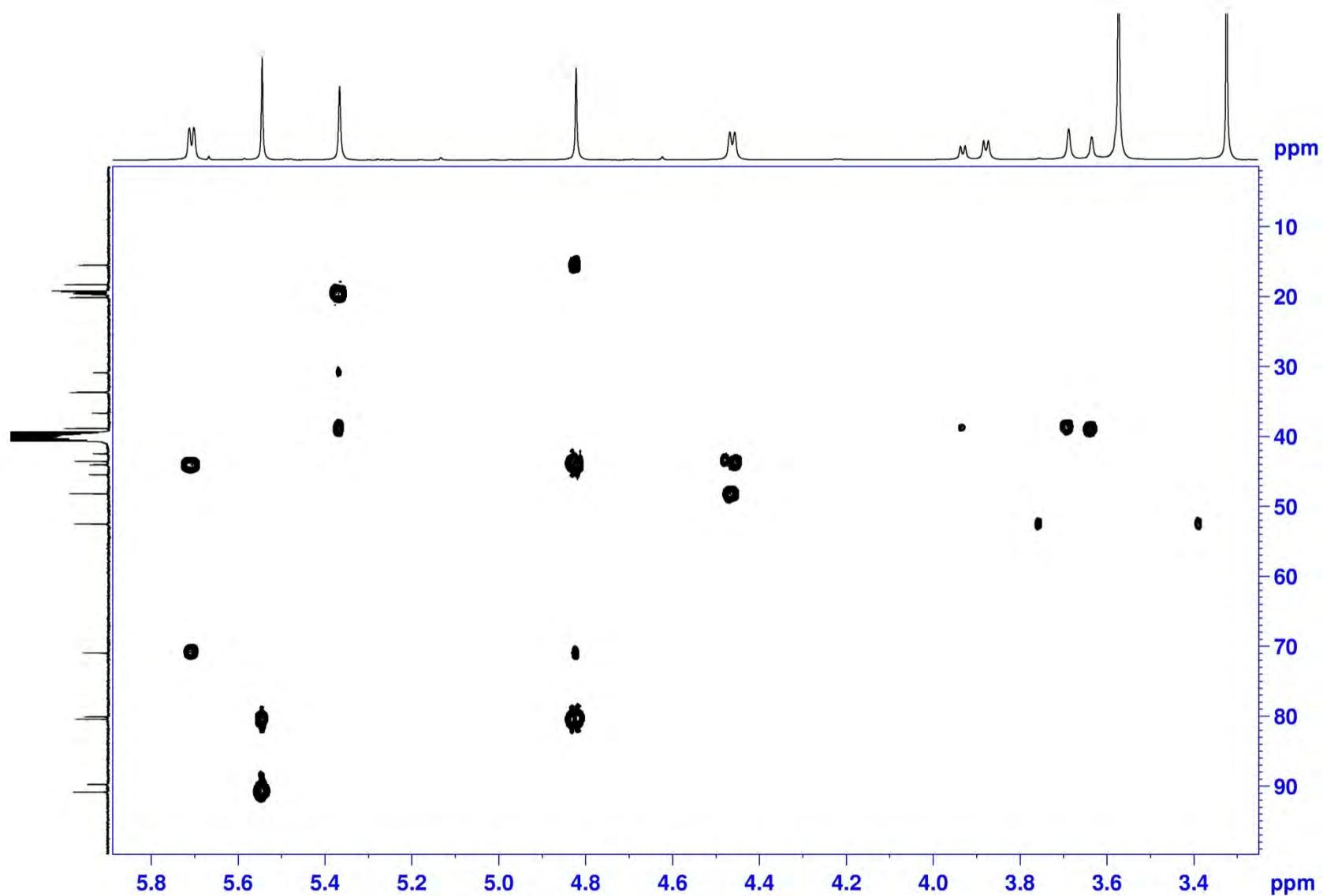
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 INSTRUM spect
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 PULPROG hmbegplndqf
 TD 4096
 SOLVENT DMSO
 NS 128
 DS 16
 SWH 5197.505 Hz
 FIDRES 1.268922 Hz
 AQ 0.3940852 sec
 RG 208.5
 DW 96.200 usec
 DE 10.00 usec
 TE 297.0 K
 CNST2 145.0000000
 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
 FhMODE QF
 SI 2048
 SF 400.1300037 MHz
 WDW SINE
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 SI 1024
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 WDW SINE
 SSB 0
 LB 0.00 Hz

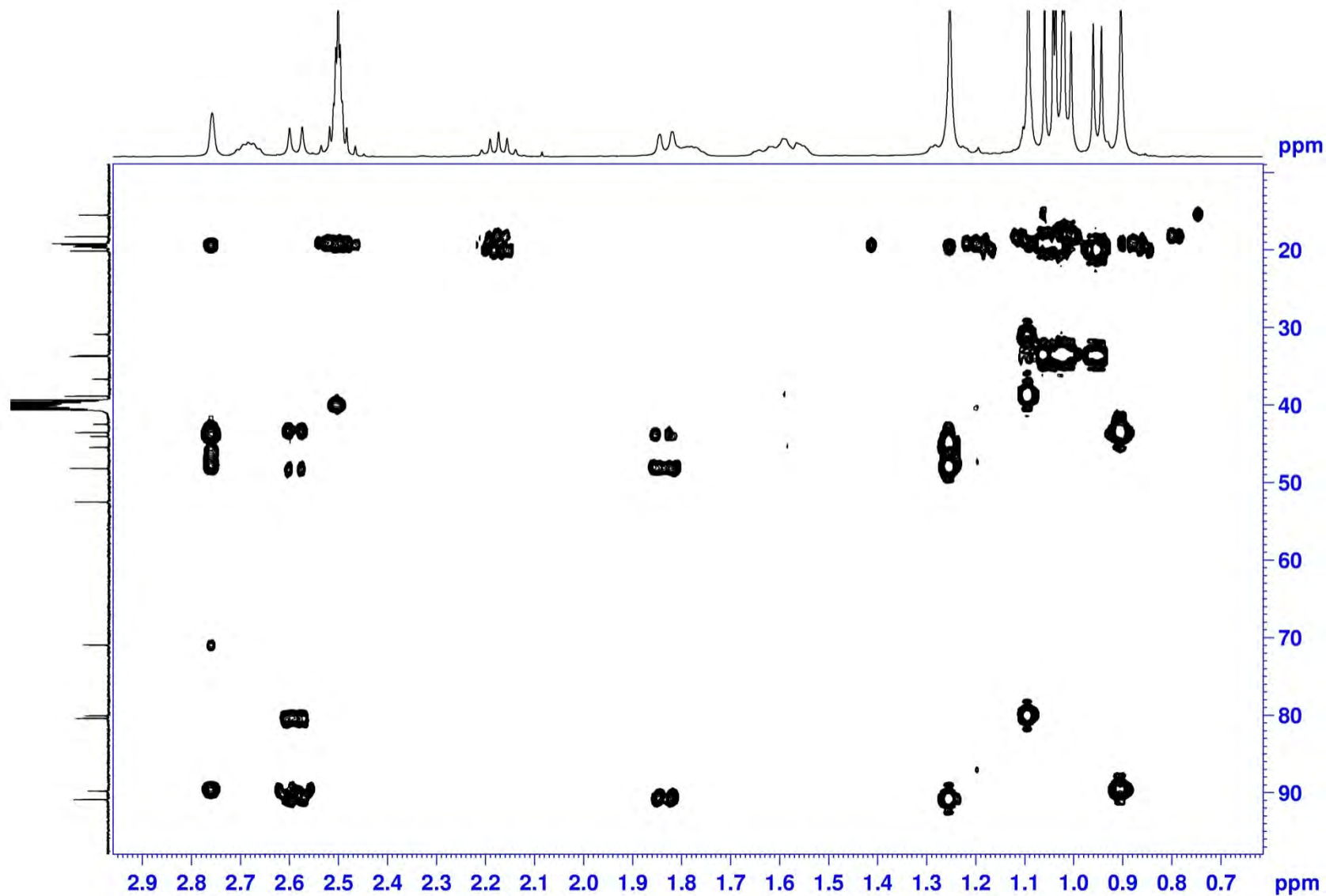
HMBC (400 MHz) spectrum of compound **1** in DMSO- d_6



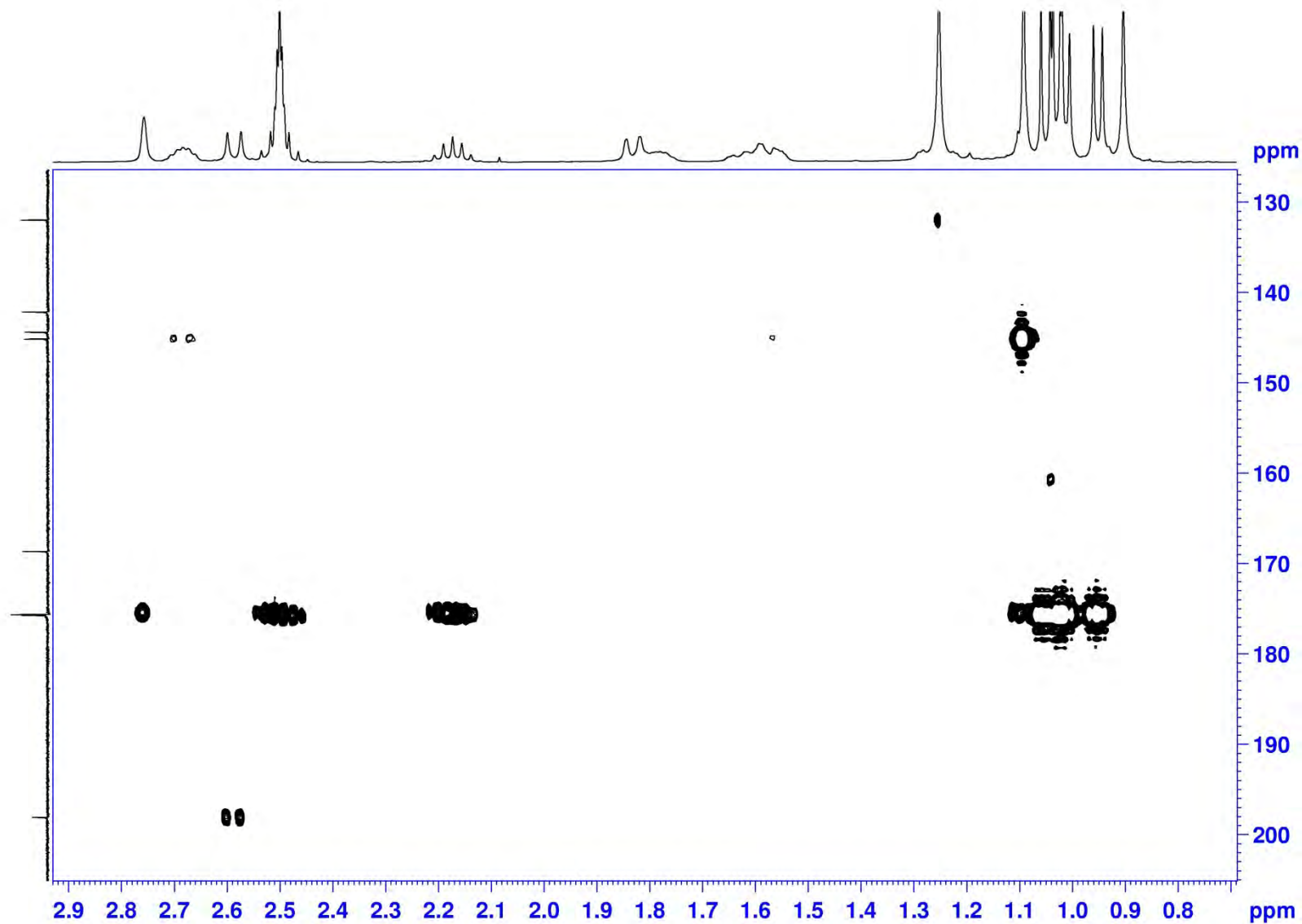
HMBC (400 MHz) spectrum of compound **1** in DMSO- d_6



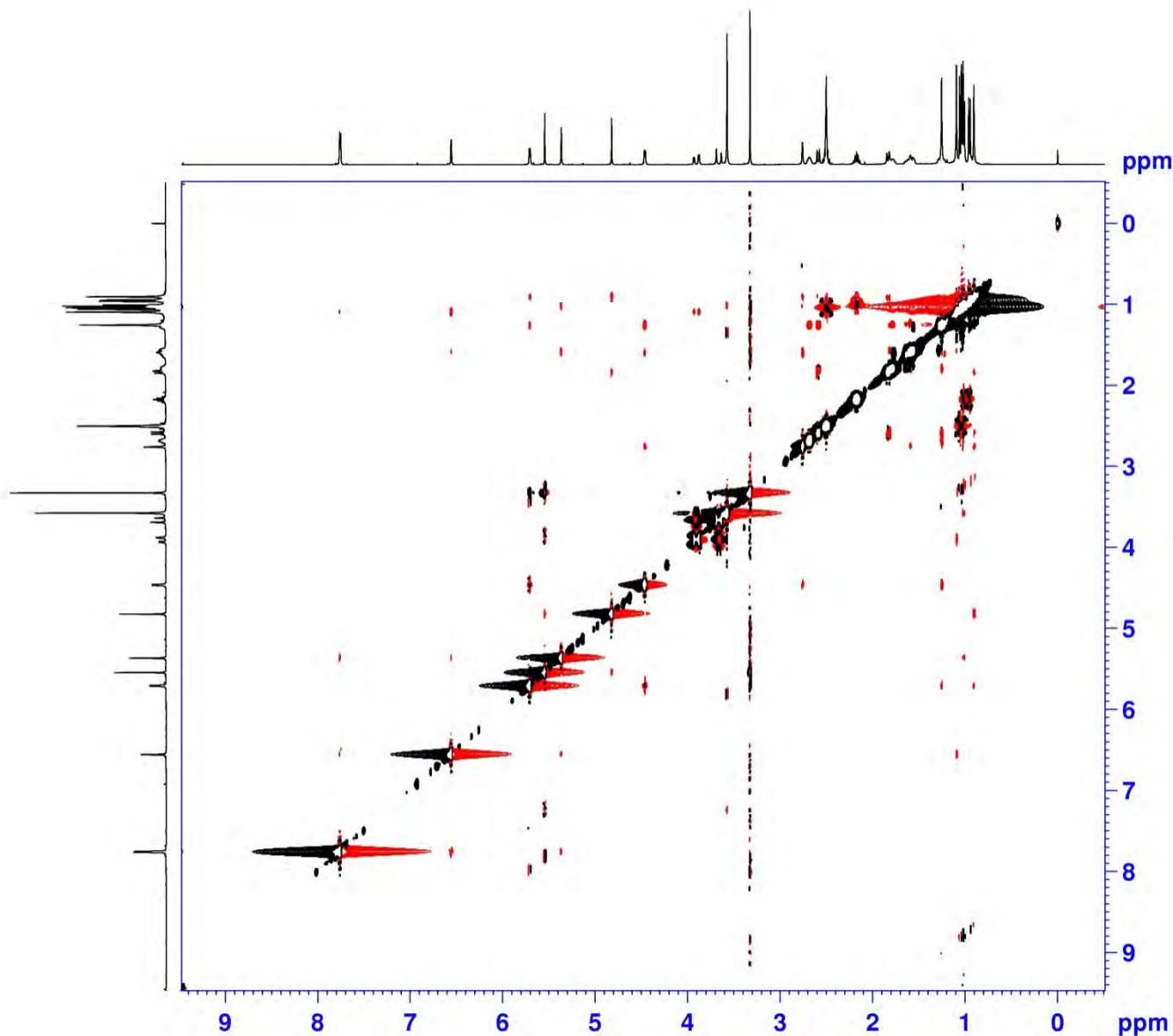
HMBC (400 MHz) spectrum of compound **1** in DMSO- d_6



HMBC (400 MHz) spectrum of compound **1** in DMSO- d_6



NOESY (400 MHz) spectrum of compound **1** in DMSO- d_6



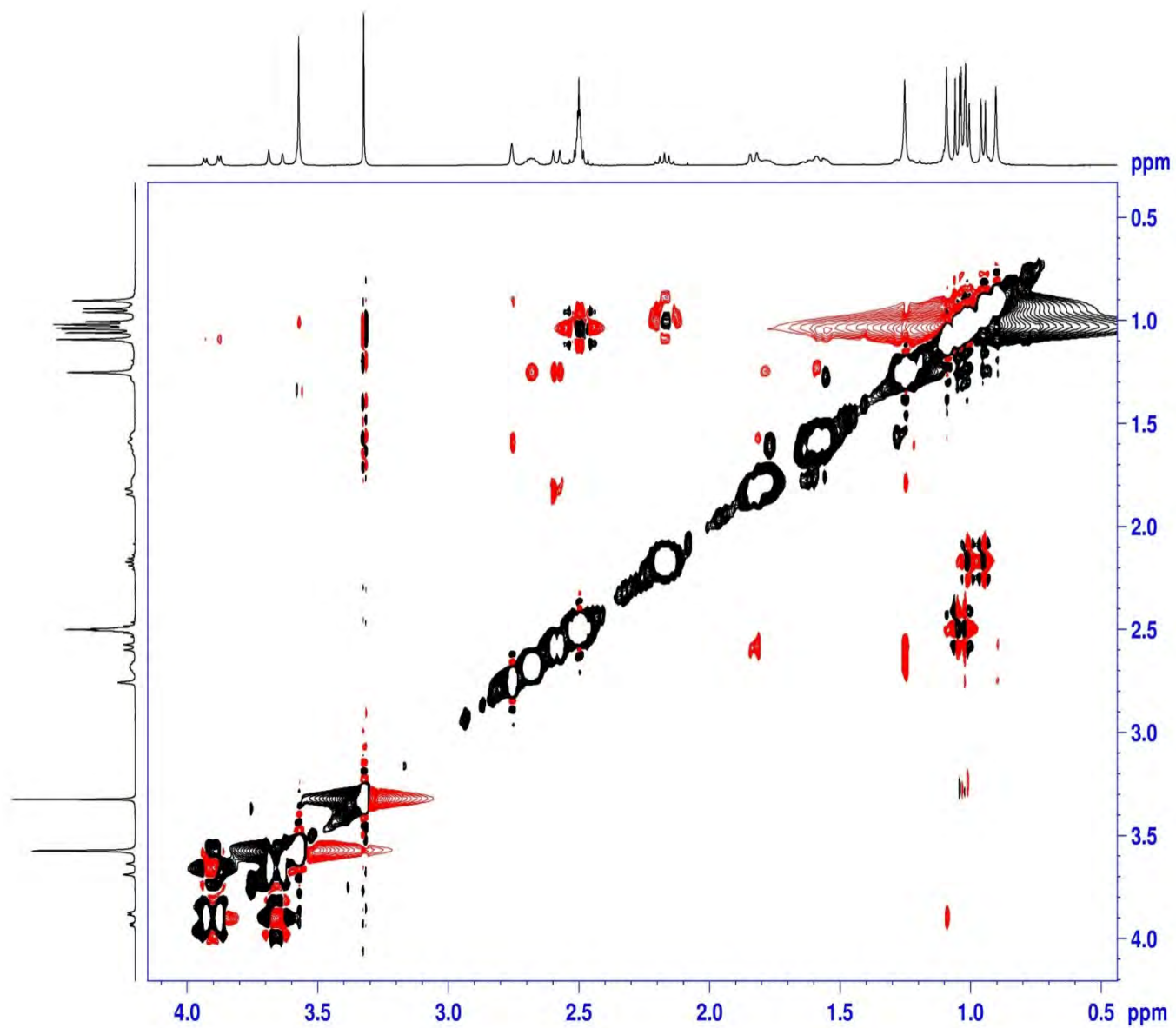
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PROCNO    1
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PULPROG   noesygpph
TD        2048
SOLVENT   DMSO
NS        32
DS        32
SWH       4000.000 Hz
FIDRES    1.953125 Hz
AQ        0.2560500 sec
RG        208.5
DW        125.000 usec
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
    
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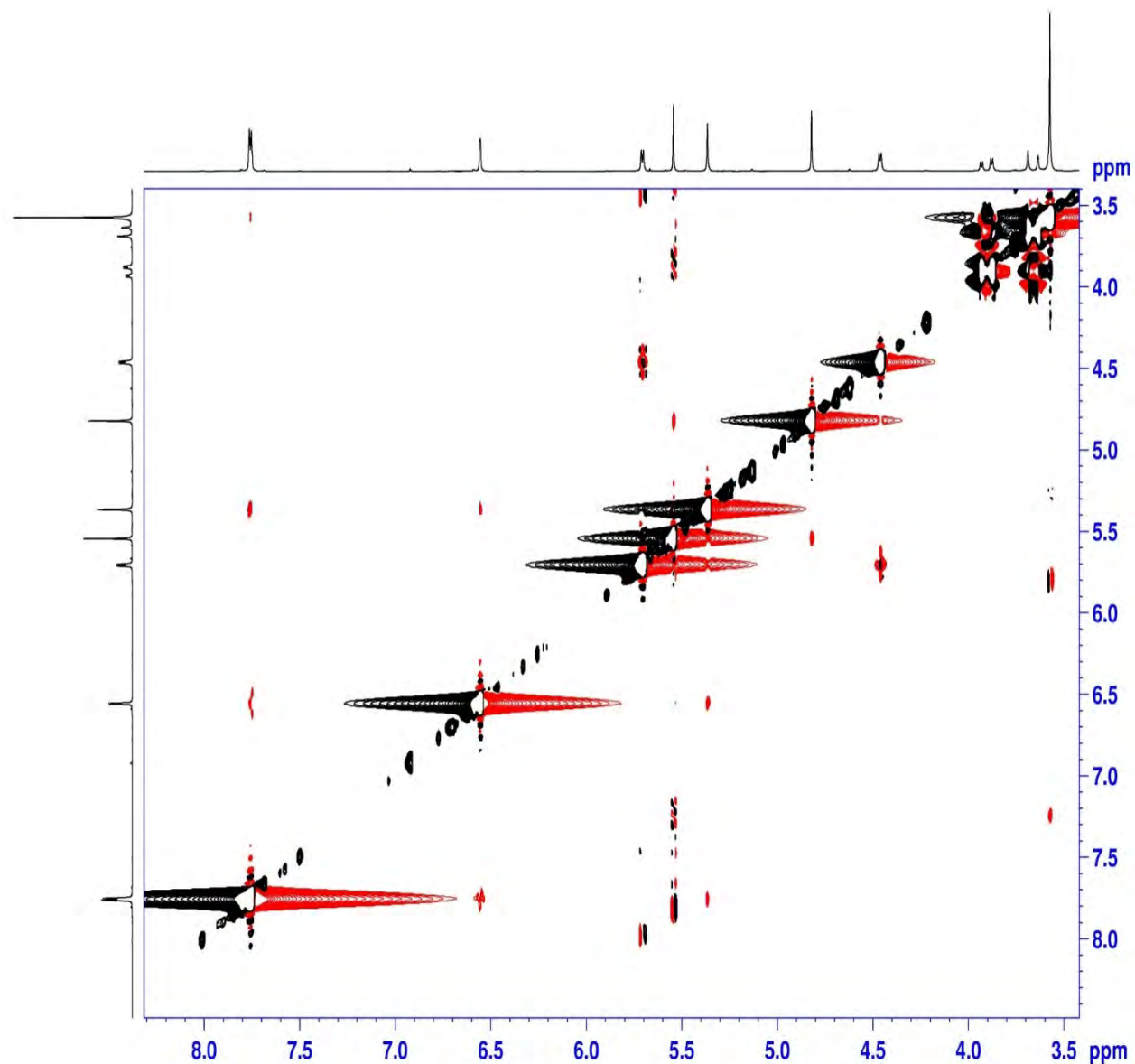
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SFO1      400.1318006 MHz
NUC1      1H
P1        11.50 usec
P2        23.00 usec
P17       2500.00 usec
ND0       1
TD        256
SFO1      400.1318 MHz
FIDRES    15.625000 Hz
SW        9.997 ppm
FnMODE    States-TPPI
SI        1024
SF        400.1300037 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
PC        1.00
SI        1024
MC2       States-TPPI
SF        400.1300037 MHz
WDW       QSINE
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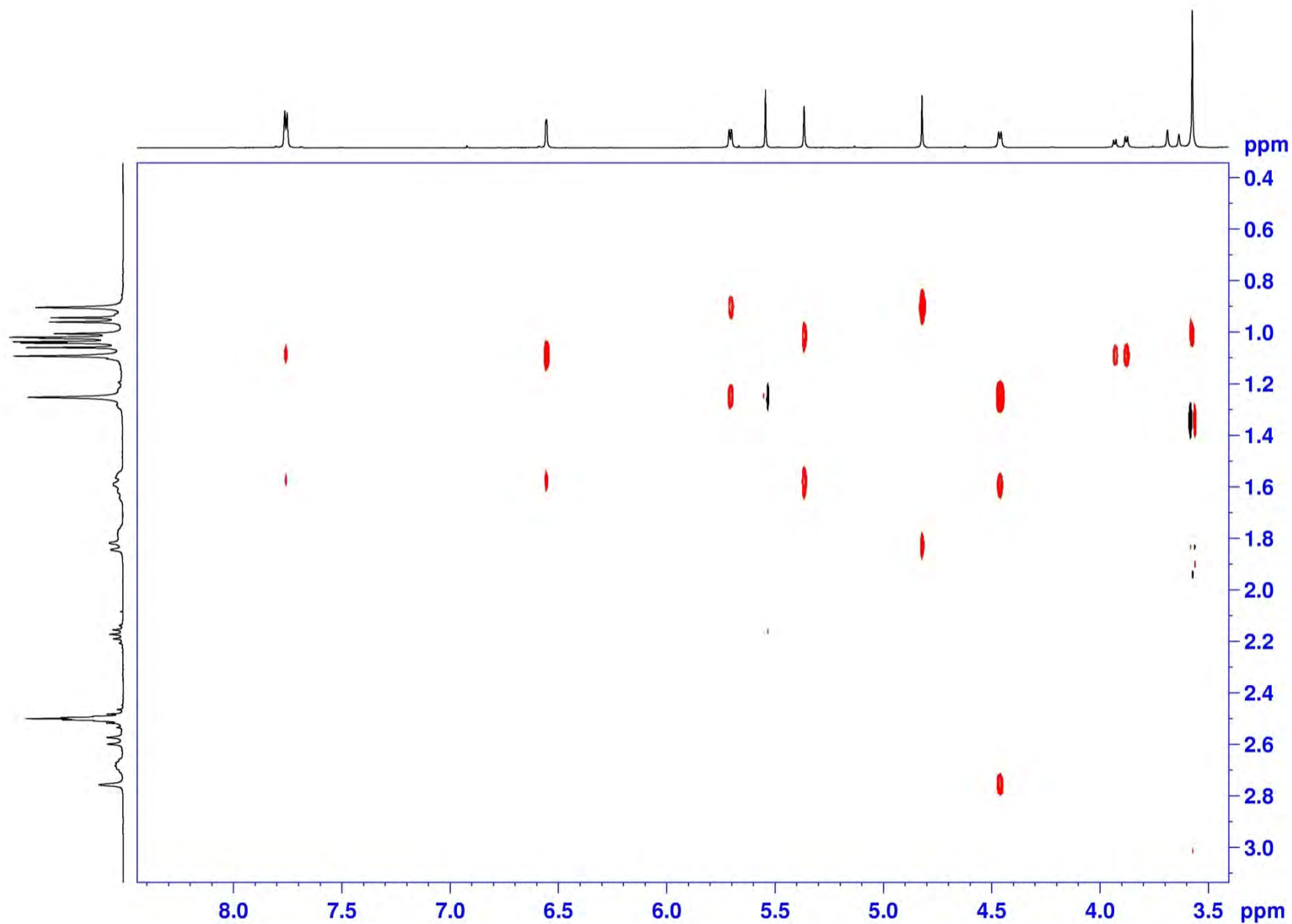
NOESY (400 MHz) spectrum of compound **1** in DMSO- d_6



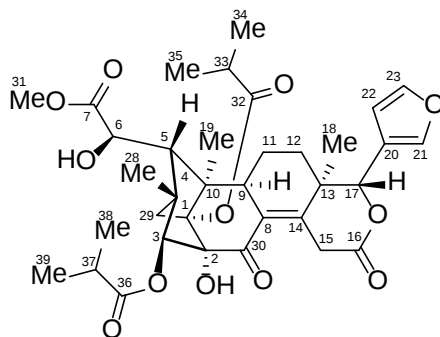
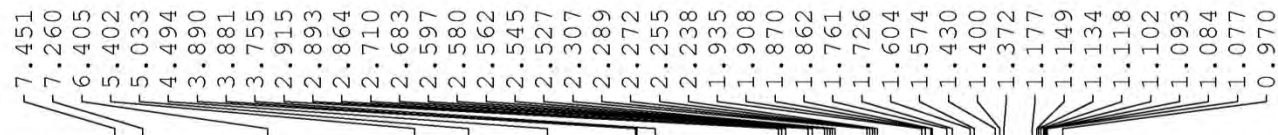
NOESY (400 MHz) spectrum of compound **1** in DMSO- d_6



NOESY (400 MHz) spectrum of compound **1** in DMSO- d_6



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

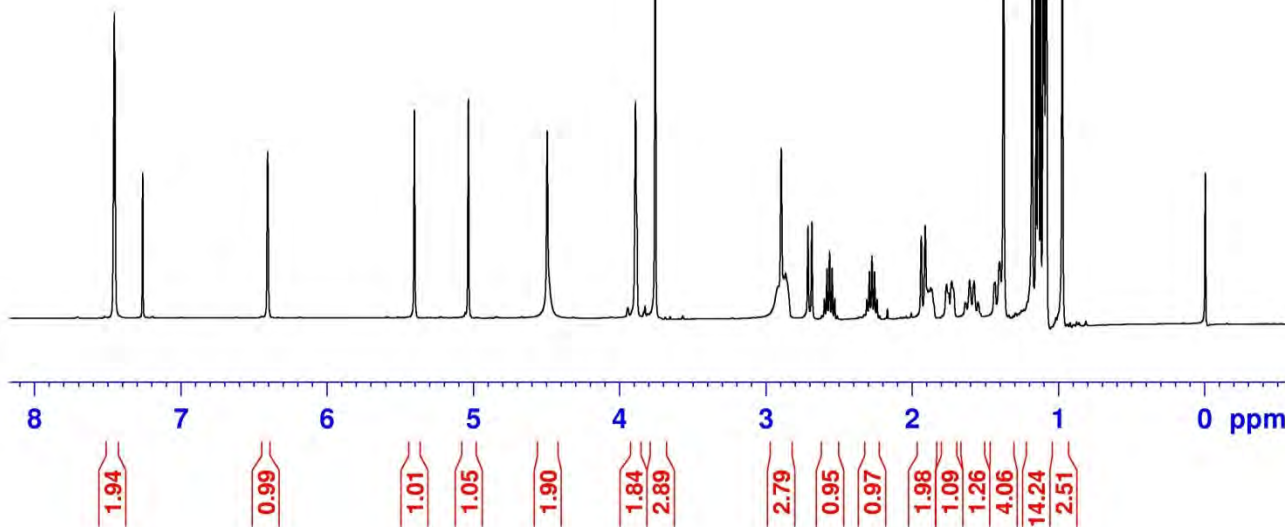


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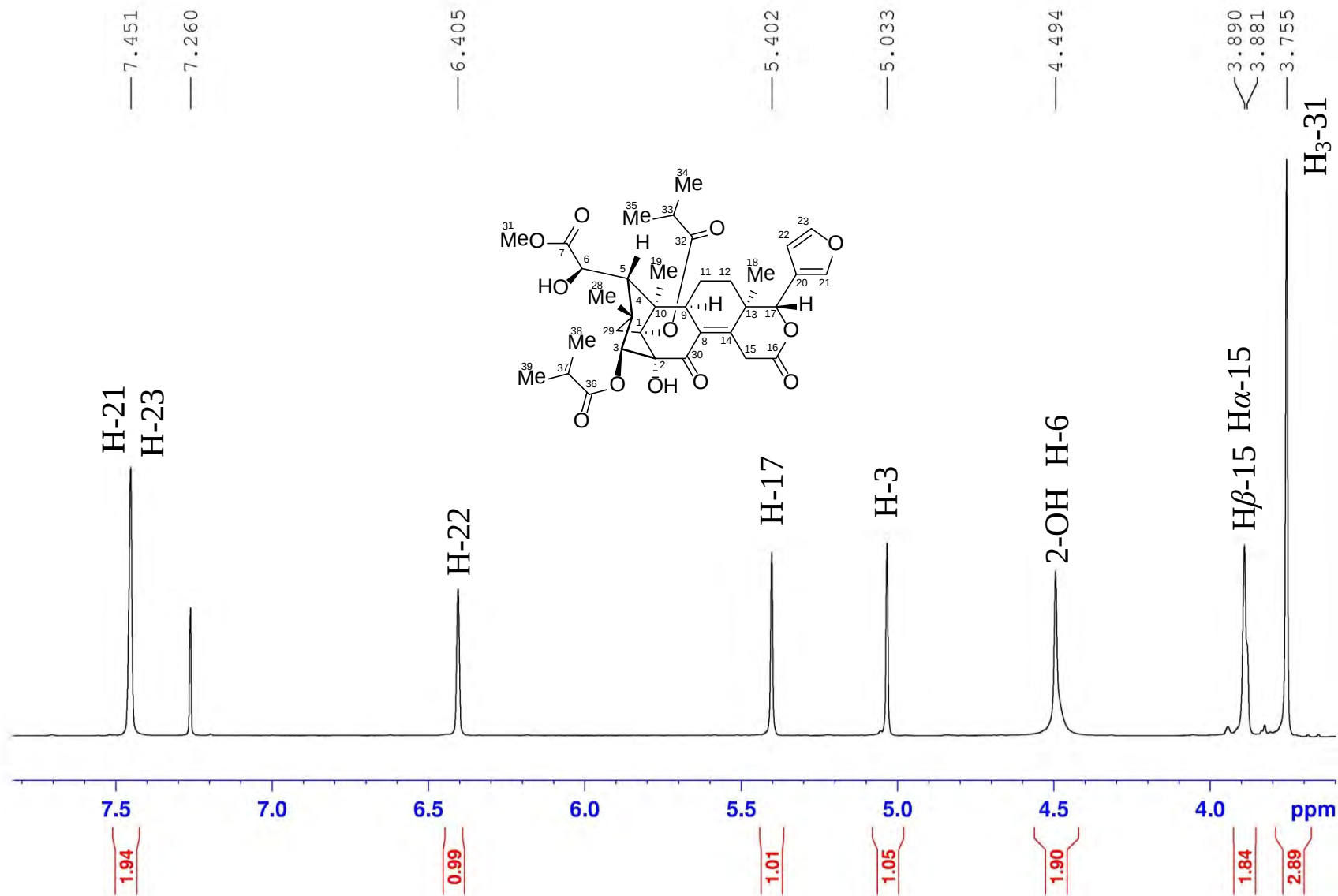
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EXPNO                1
PROCNO               1
Date_                20141107
Time                20.09
INSTRUM              spect
PROBHD               5 mm CPPBBO BB
PULPROG              zg30
TD                   65536
SOLVENT              CDC13
NS                    16
DS                     2
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                   4.0894966 sec
RG                     73.92
DW                   62.400 usec
DE                    10.00 usec
TE                   297.0 K
D1                   1.00000000 sec
TD0                   1
    
```

```

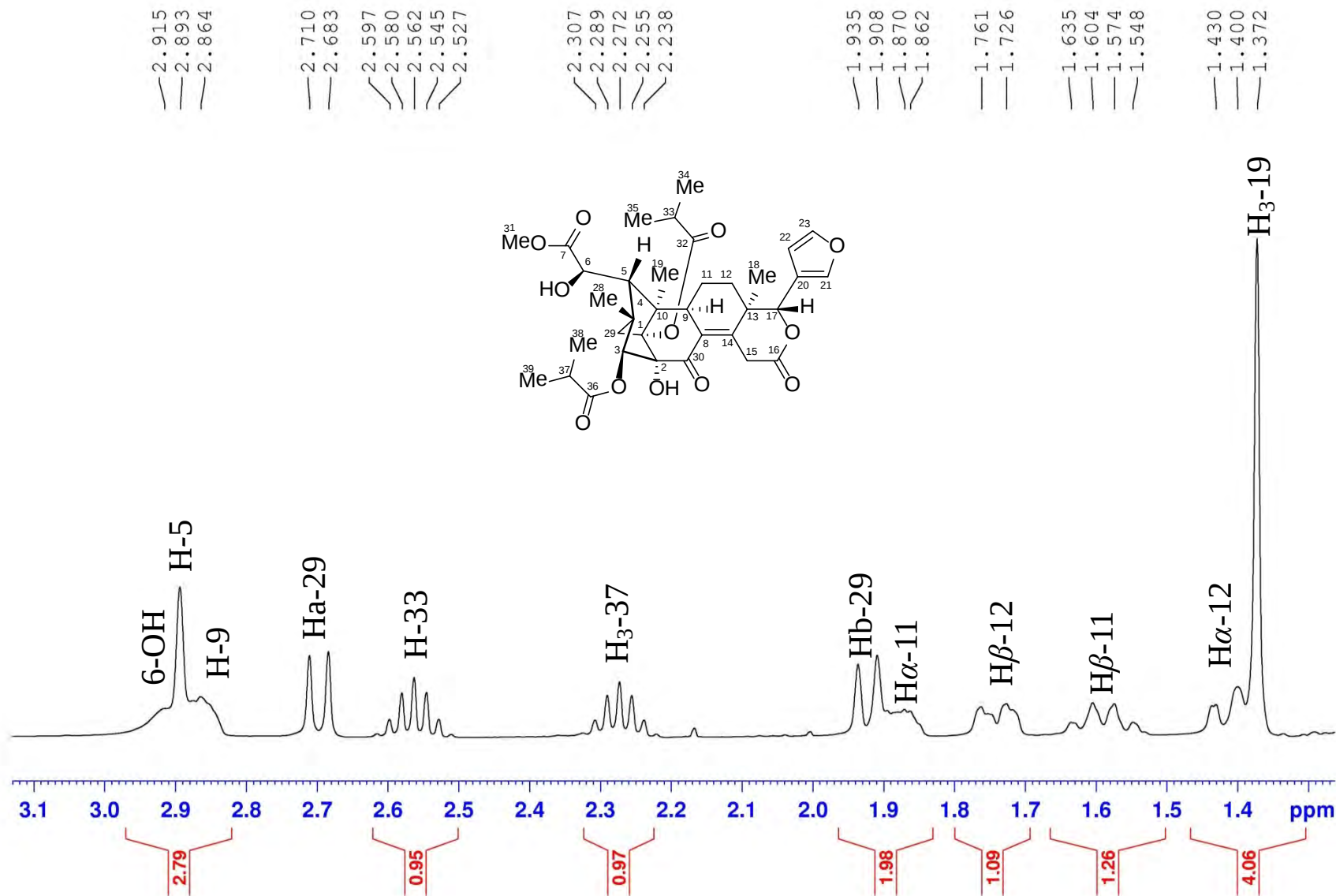
===== CHANNEL f1 =====
SF01                 400.1324710 MHz
NUC1                  1H
P1                    12.00 usec
SI                    65536
SF                   400.1300097 MHz
WDW                   EM
SSB                    0
LB                    0.30 Hz
GB                     0
PC                     1.00
    
```



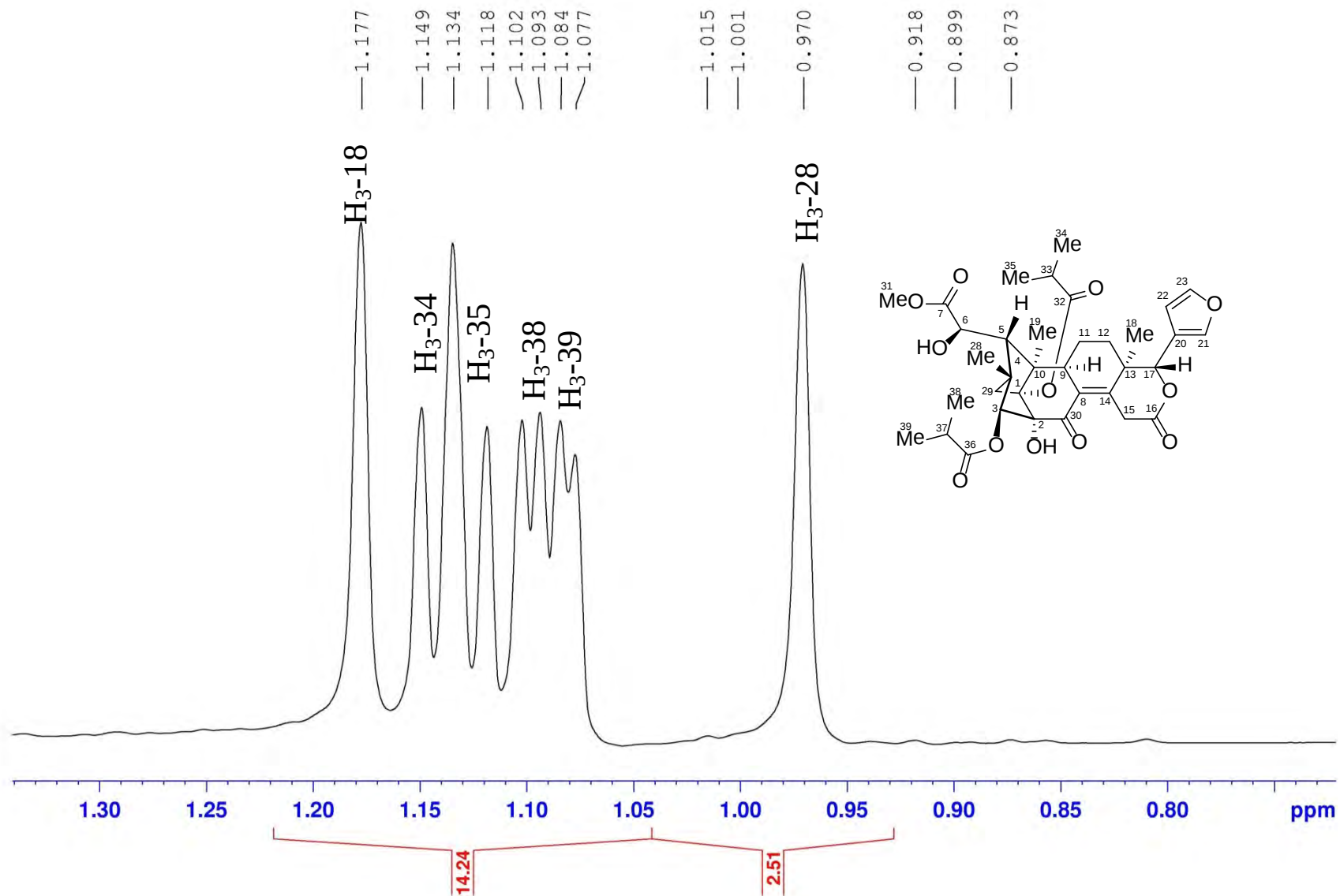
^1H NMR (400 MHz) spectrum of compound **1** in CDCl_3



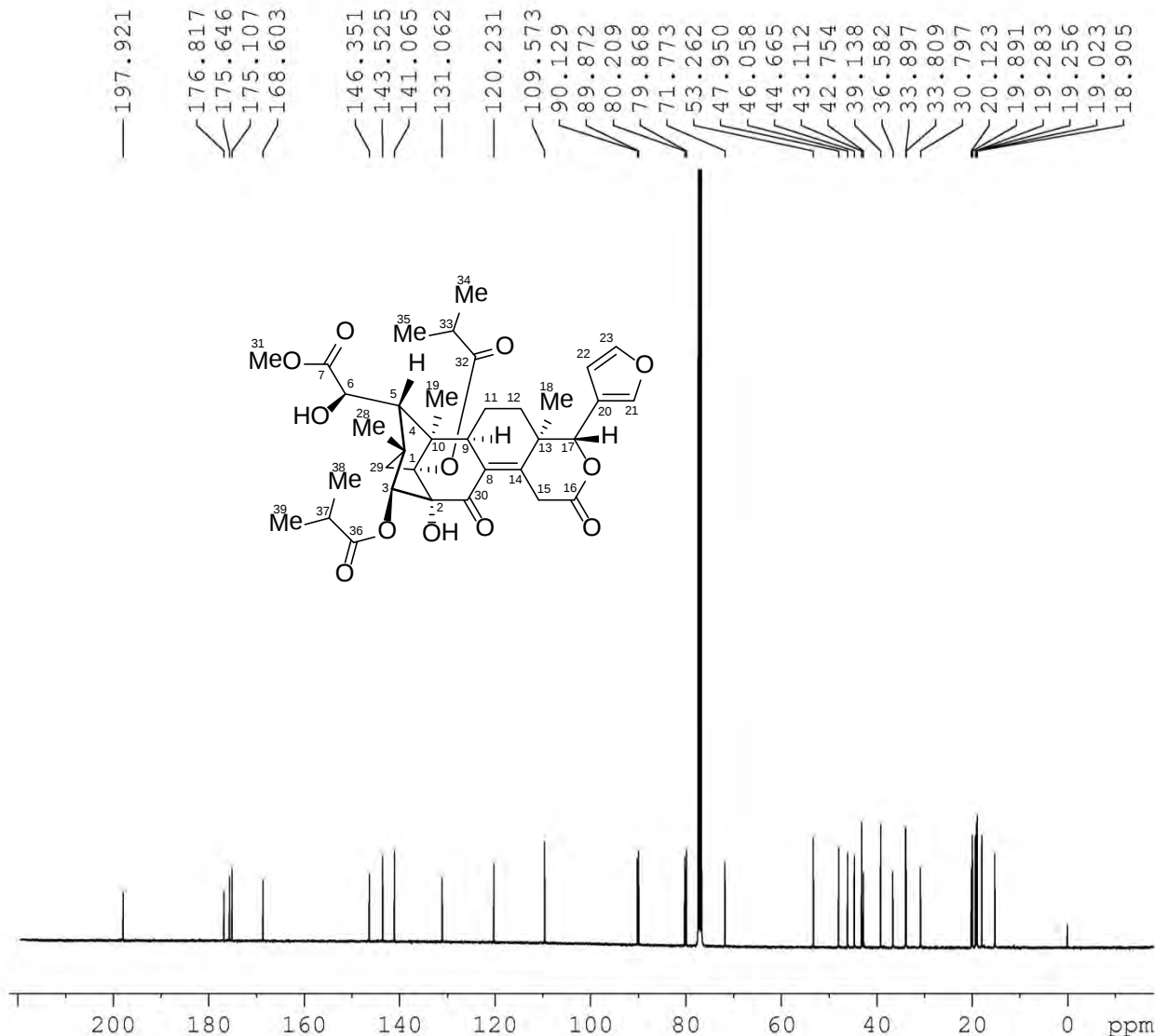
^1H NMR (400 MHz) spectrum of compound **1** in CDCl_3



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



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



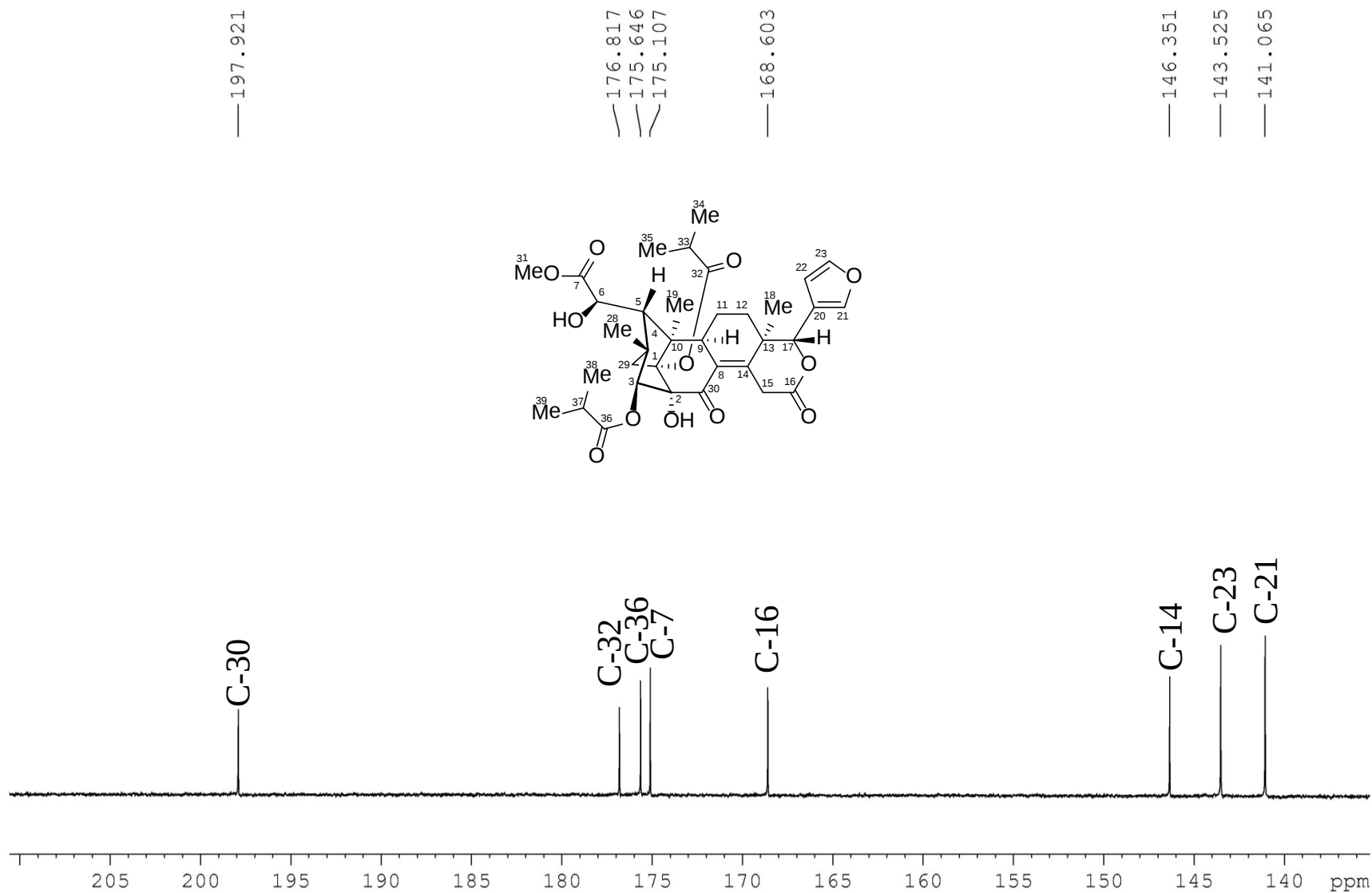
```

NAME                lws-42
EXPNO                2
PROCNO               1
Date_                20141108
Time                 1.01
INSTRUM              spect
PROBHD               5 mm CPPBBO BB
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                   5000
DS                   4
SWH                  24038.461
FIDRES               0.366798
AQ                   1.3631988
RG                   130.26
DW                   20.800
DE                   18.00
TE                   297.0
D1                   2.00000000
D11                  0.03000000
TD0                  1
  
```

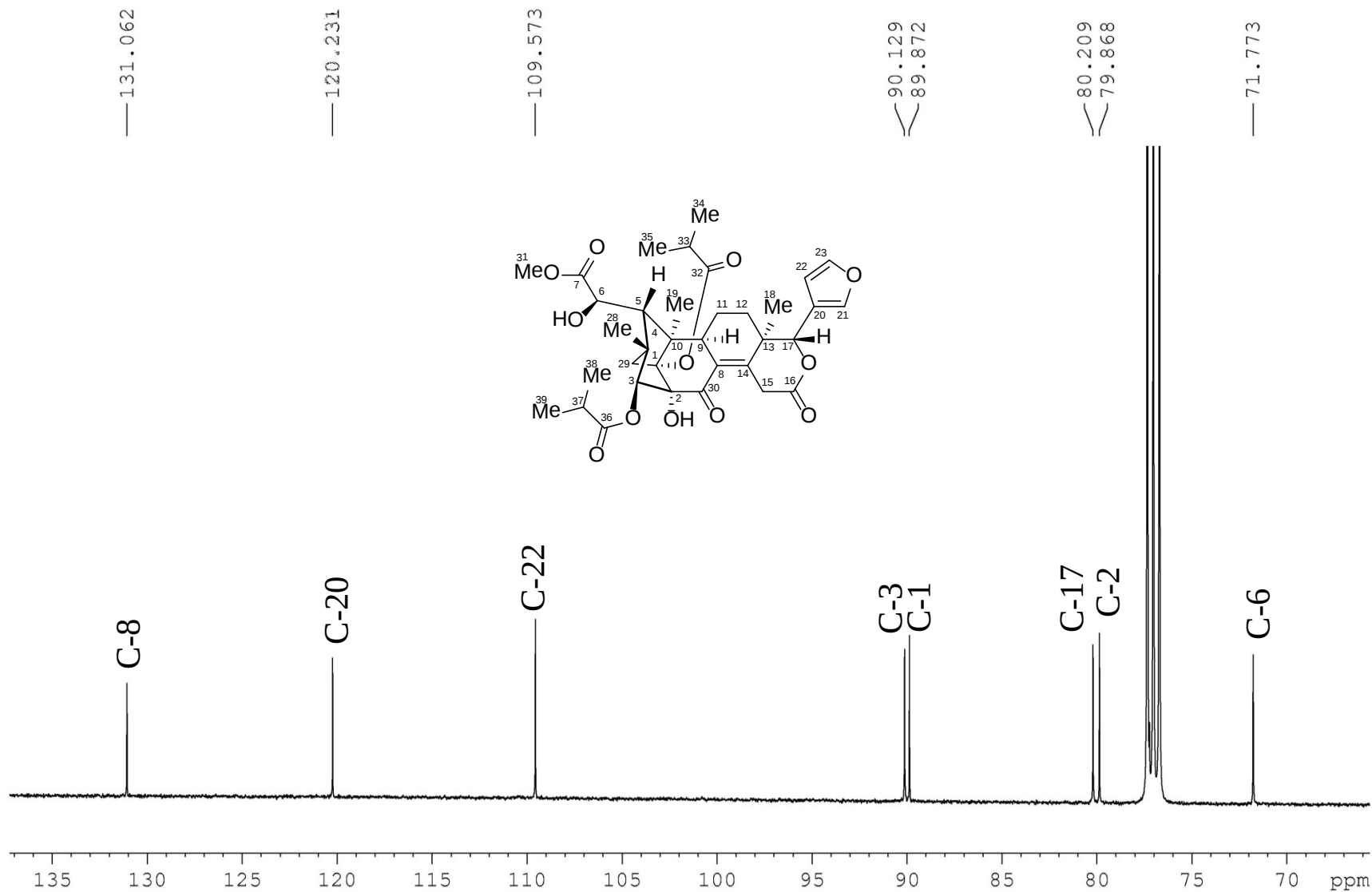
```

===== CHANNEL f1 =====
SFO1                100.6228293
NUC1                 13C
P1                   10.00
SI                   32768
SF                  100.6127693
WDW                  EM
SSB                  0
LB                   1.00
GB                   0
PC                   1.00
  
```

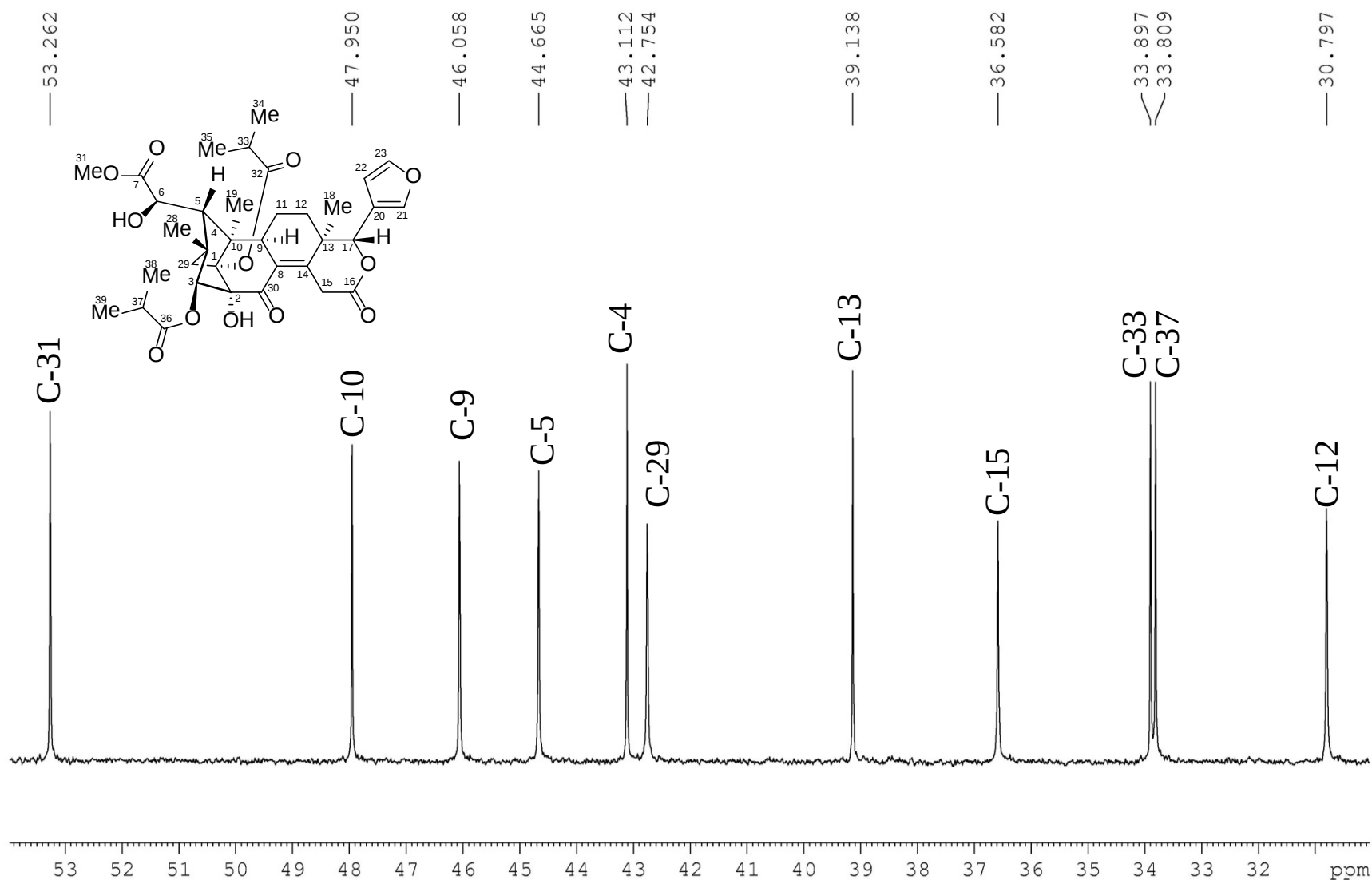
^{13}C NMR (100 MHz) spectrum of compound **1** in CDCl_3



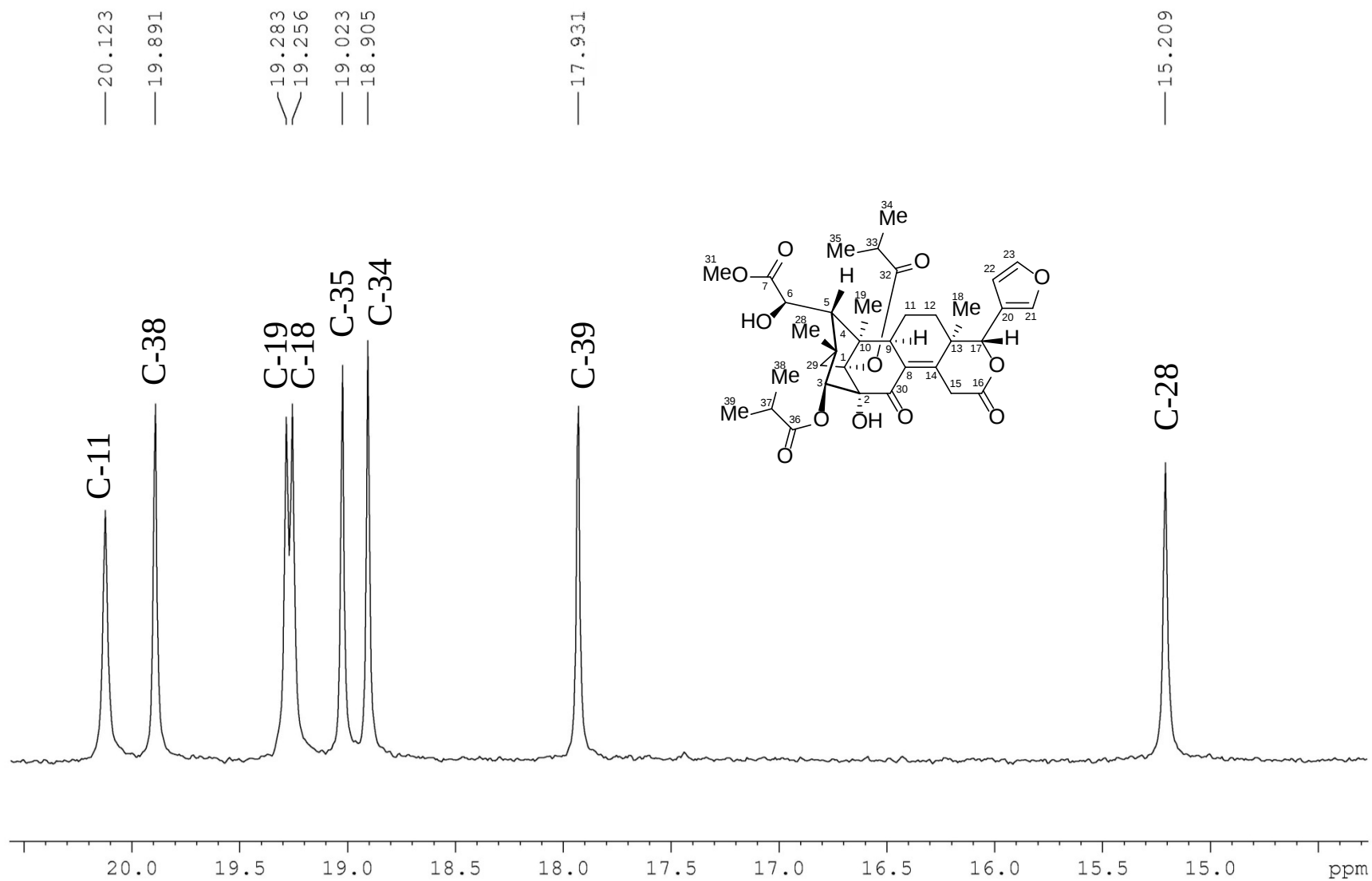
^{13}C NMR (100 MHz) spectrum of compound **1** in CDCl_3



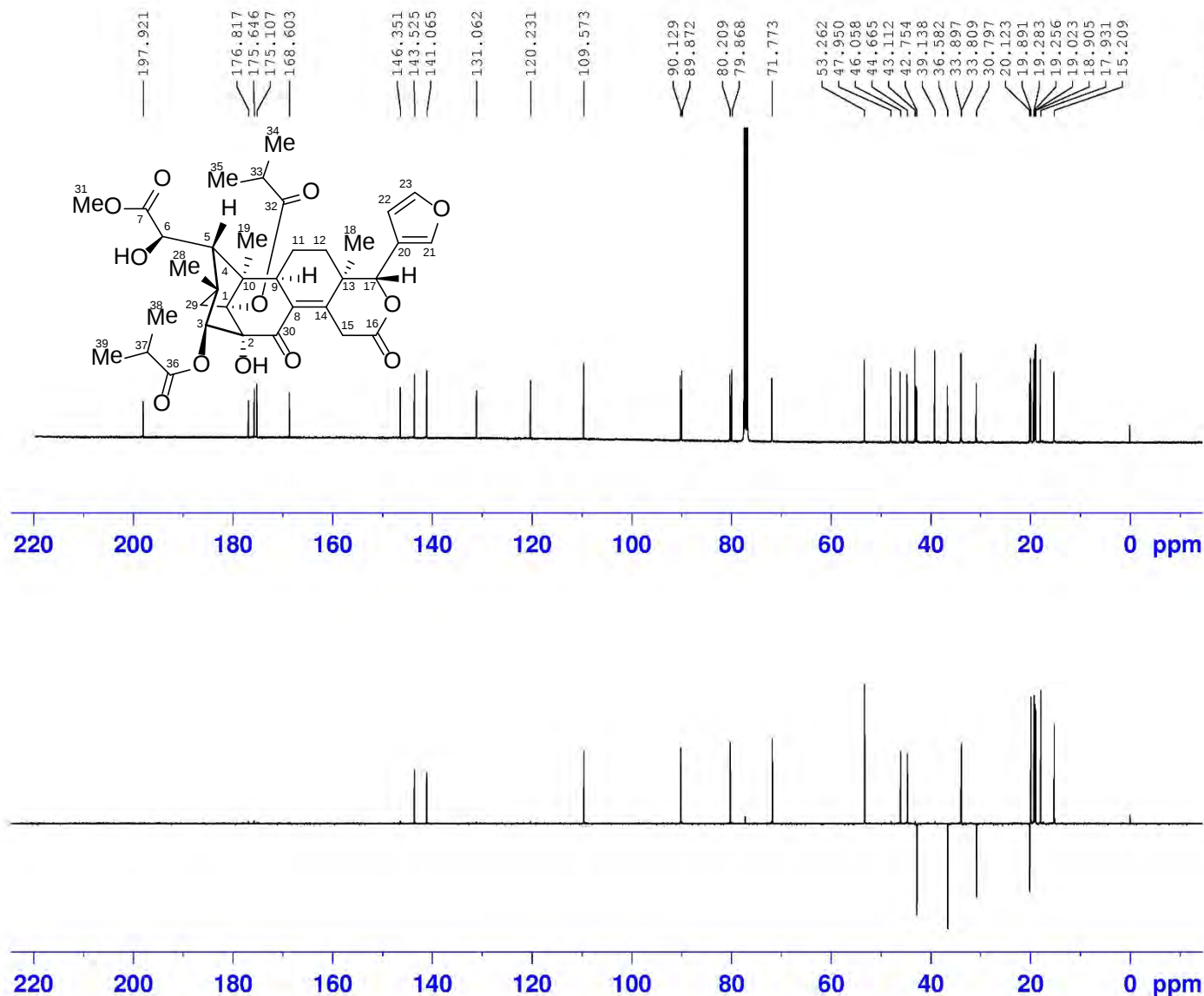
^{13}C NMR (100 MHz) spectrum of compound **1** in CDCl_3



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



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



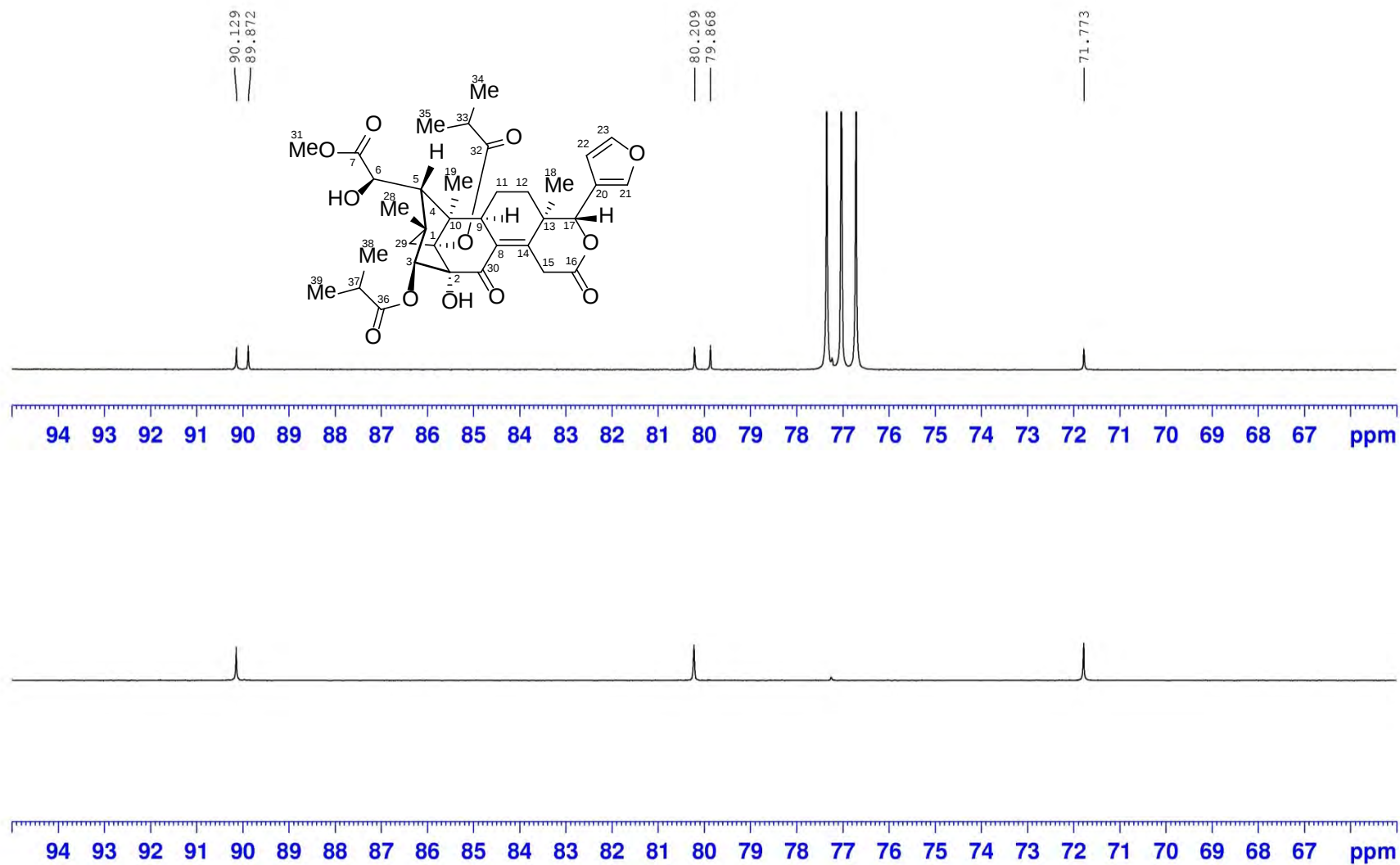
```

NAME                lws-42
EXPNO                3
PROCNO               1
Date_                20141108
Time                 3.24
INSTRUM              spect
PROBHD               5 mm CFPBBO BB
PULPROG              deptspl35
TD                   65536
SOLVENT              CDC13
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
    
```

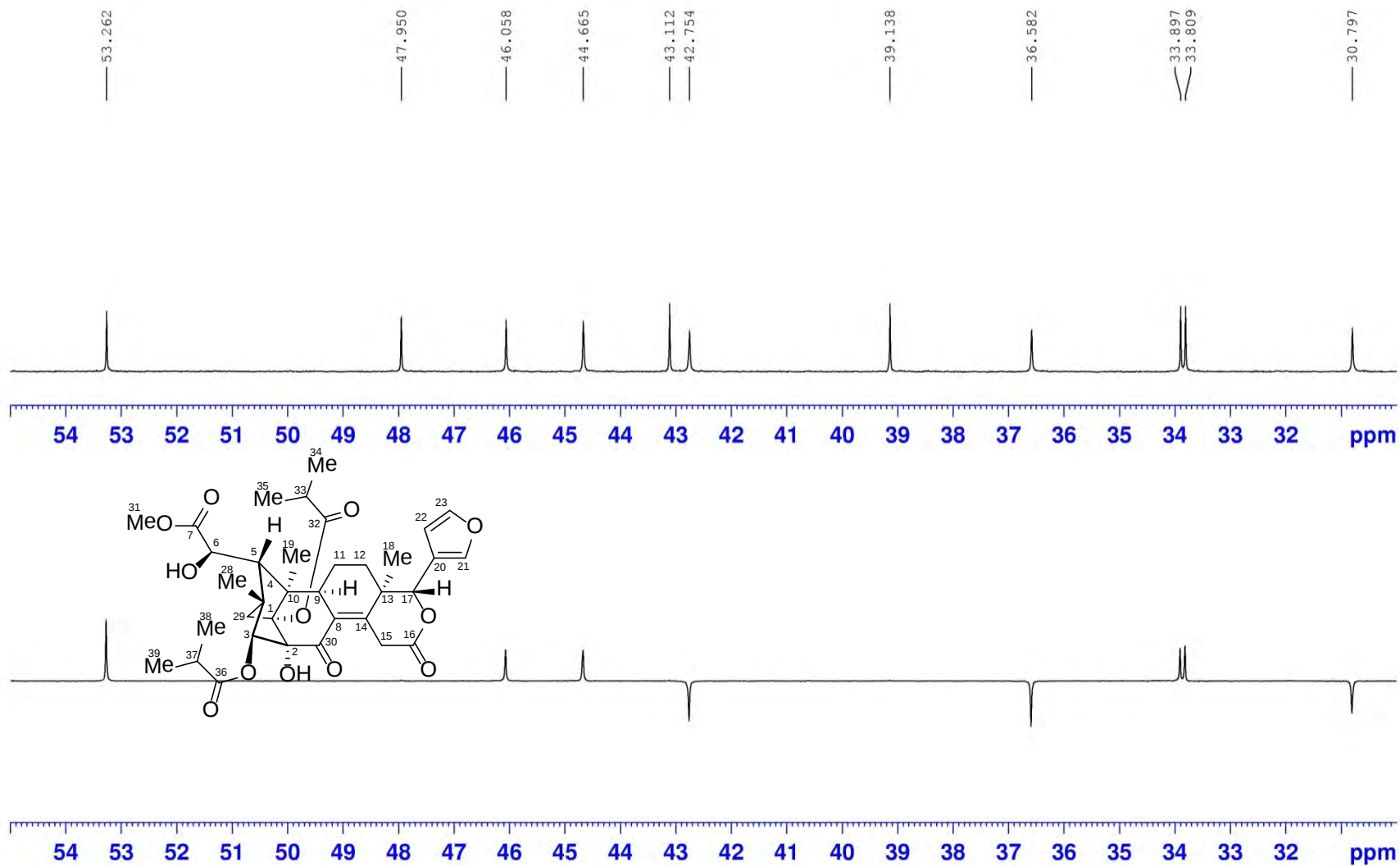
```

===== CHANNEL f1 =====
SFO1                100.6233324
NUC1                 13C
P1                   10.00
P13                  2000.00
SI                   32768
SF                   100.6127685
WDW                  EM
SSB                   0
LB                   1.00
GB                    0
PC                   1.40
    
```

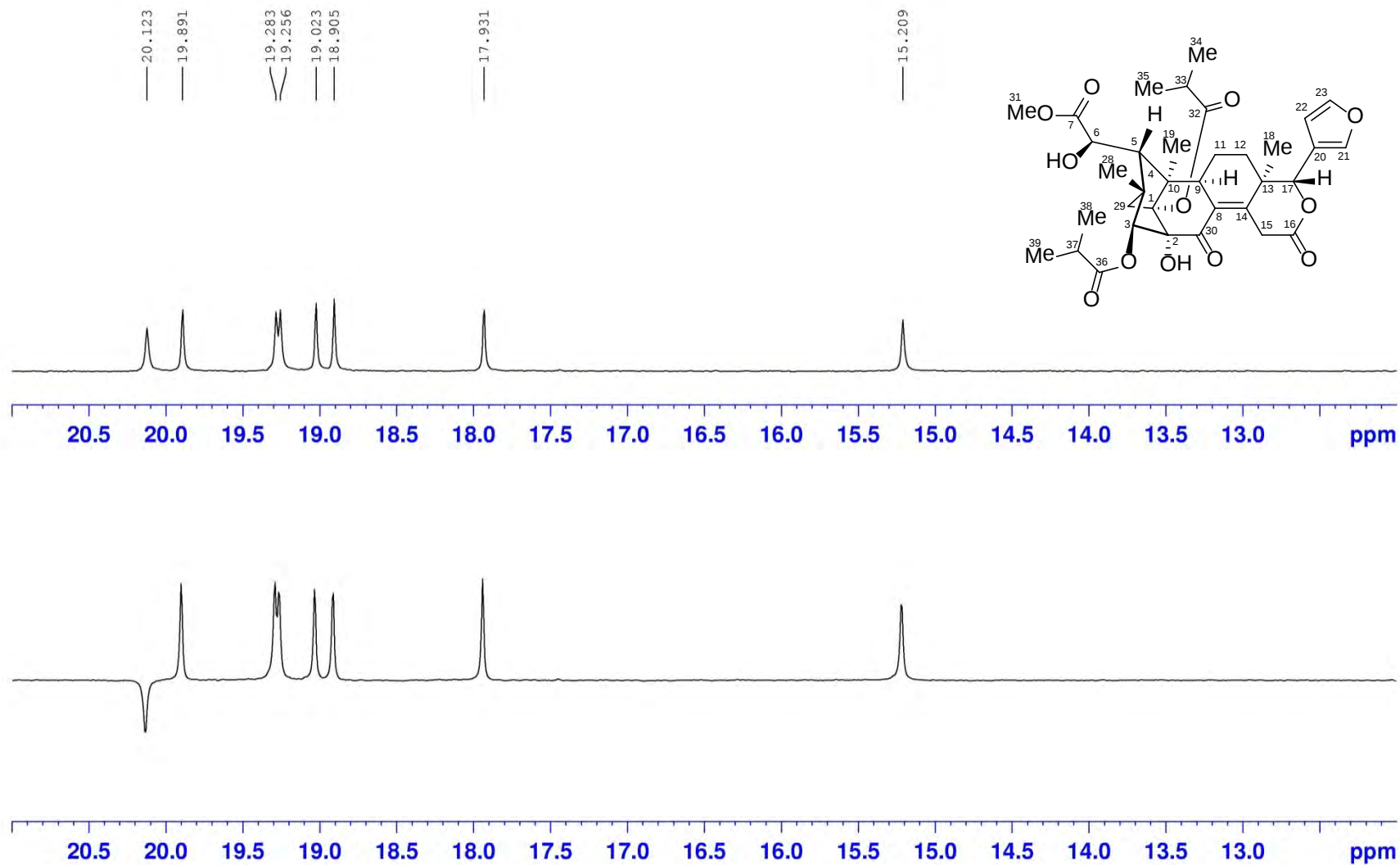
DEPT135 (100 MHz) spectrum of compound **1** in CDCl₃



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



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

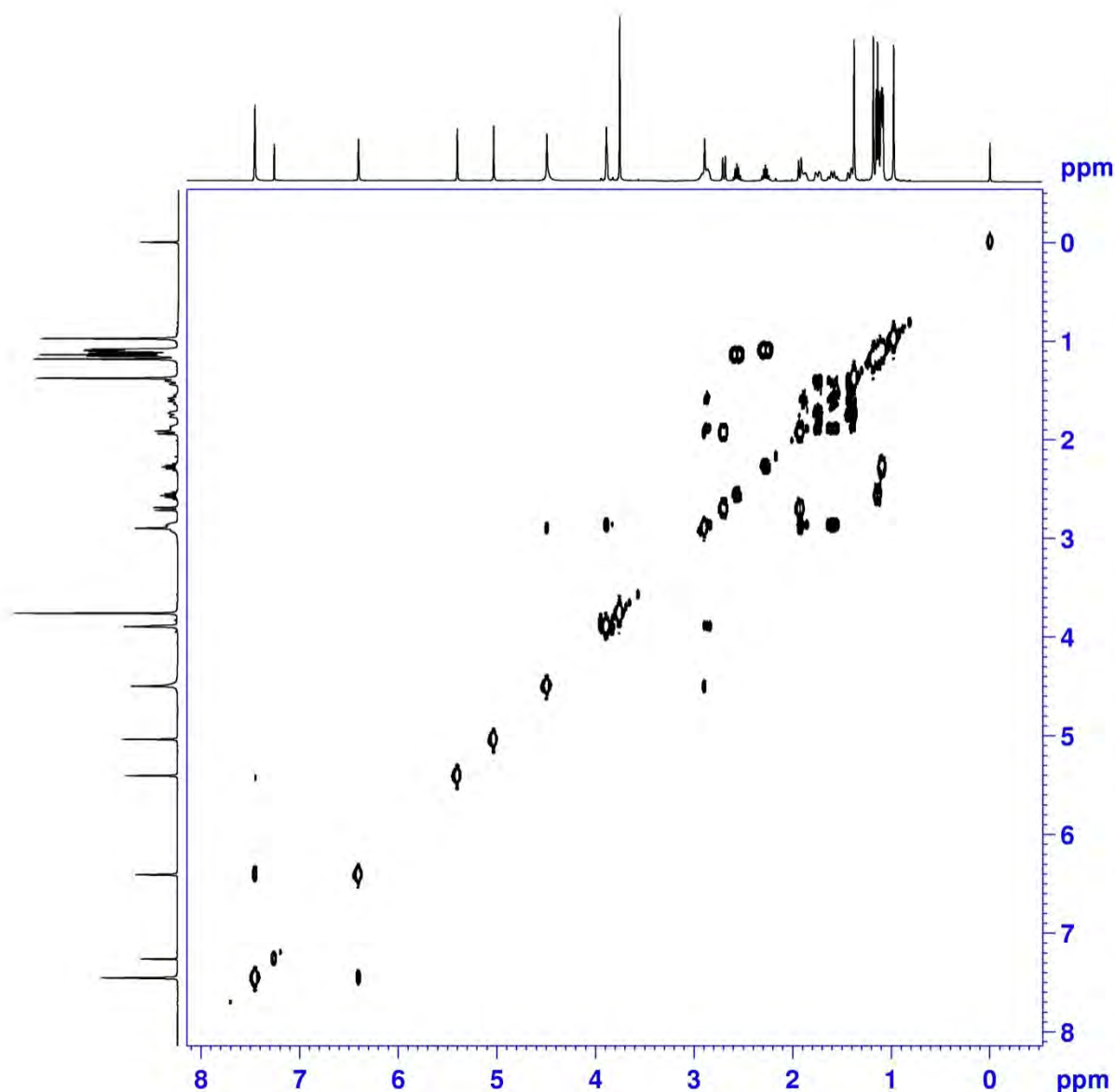


^1H - ^1H COSY (400 MHz) spectrum of compound **1** in CDCl_3



NAME lws-42
EXPNO 4
PROCNO 1
Date_ 20141108
Time 3.25
INSTRUM spect
PROBHD 5 mm CPMBBO 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 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 =====
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 400.1300098 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 400.1300098 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0



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

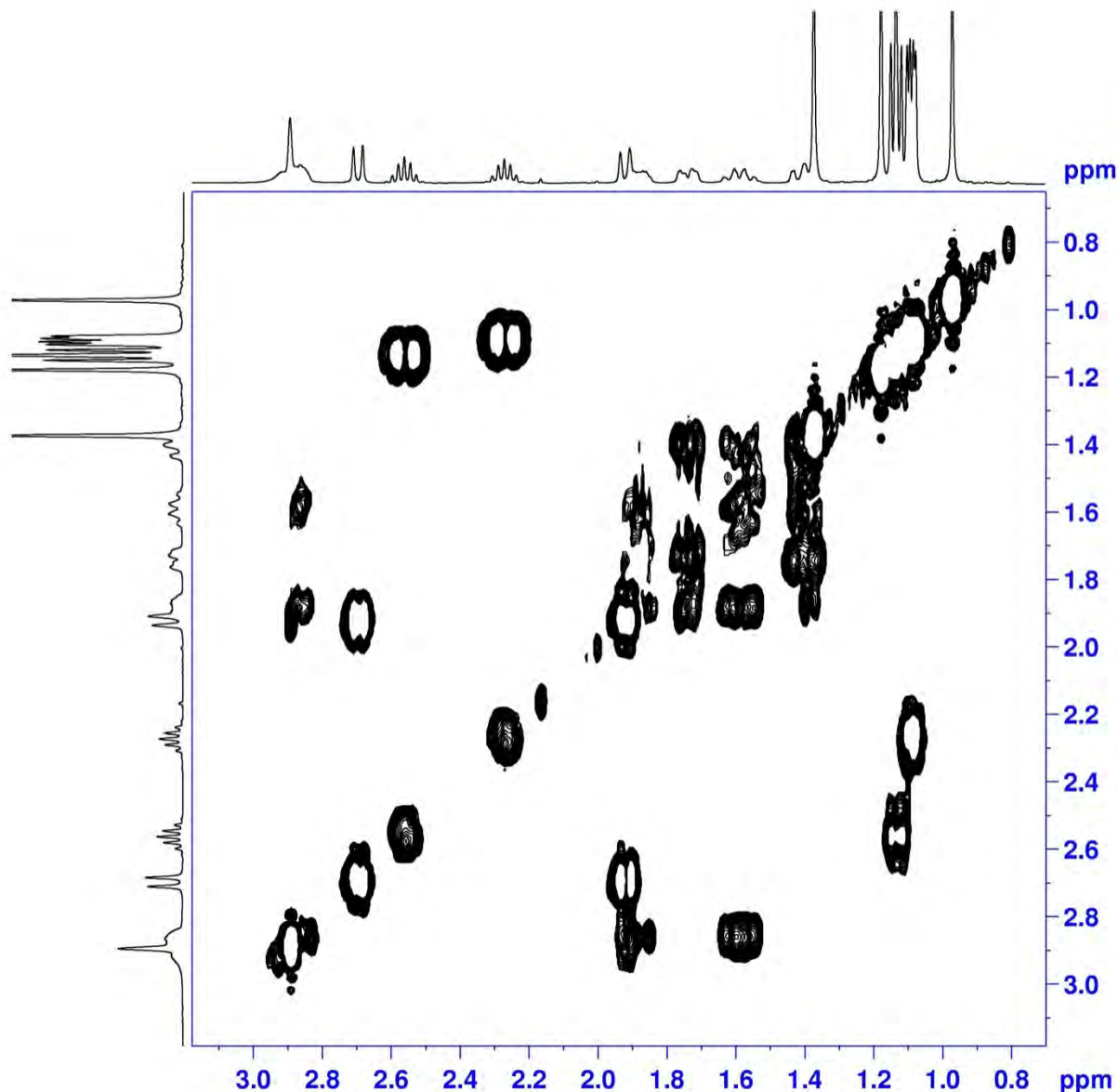


```

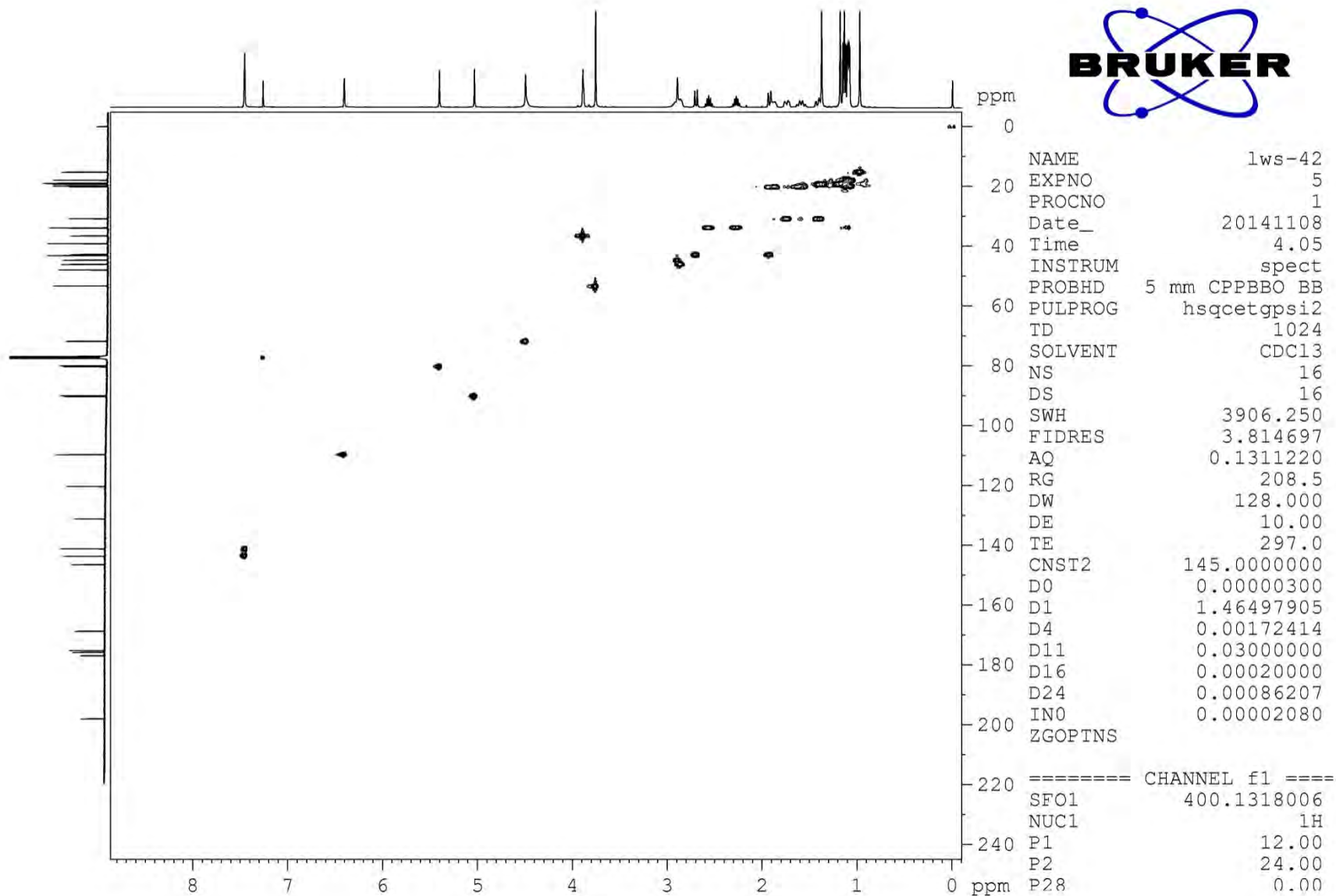
NAME          lws-42
EXPNO         4
PROCNO        1
Date_         20141108
Time          3.25
INSTRUM       spect
PROBHD        5 mm CPMBO BB
PULPROG       cosygpppqf
TD            2048
SOLVENT       CDCl3
NS            8
DS            8
SWH           3906.250 Hz
FIDRES        1.907349 Hz
AQ            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
  
```

```

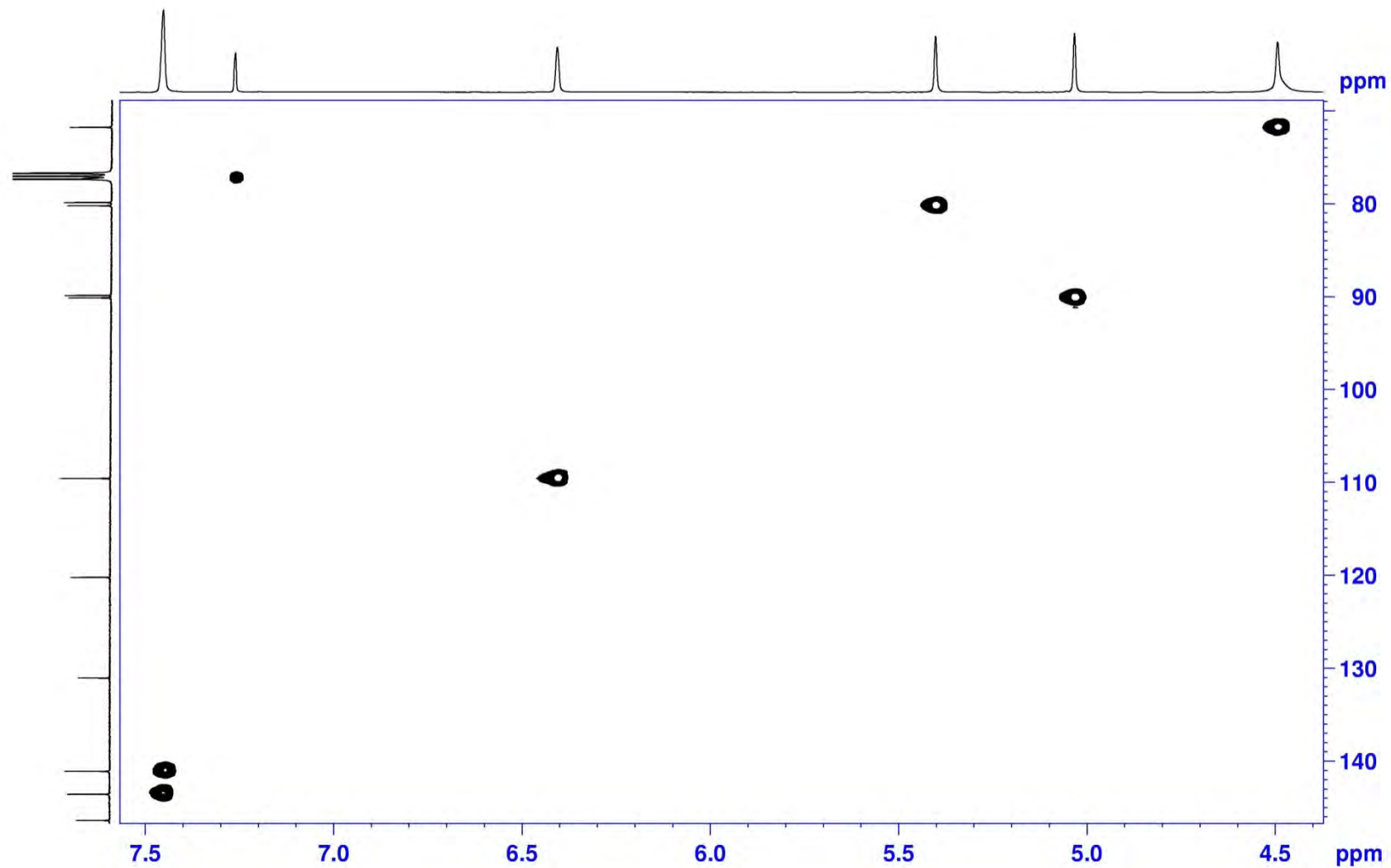
===== CHANNEL f1 =====
SFO1          400.1318006 MHz
NUC1           1H
P0             12.00 usec
P1             12.00 usec
P17            2500.00 usec
ND0            1
TD             128
SFO1          400.1318 MHz
FIDRES        30.517578 Hz
SW             9.762 ppm
FnMODE        QF
SI             1024
SF            400.1300098 MHz
WDW            QSINE
SSB            0
LB             0.00 Hz
GB             0
PC             1.40
SI             1024
MC2           QF
SF            400.1300098 MHz
WDW            QSINE
SSB            0
LB             0.00 Hz
GB             0
  
```



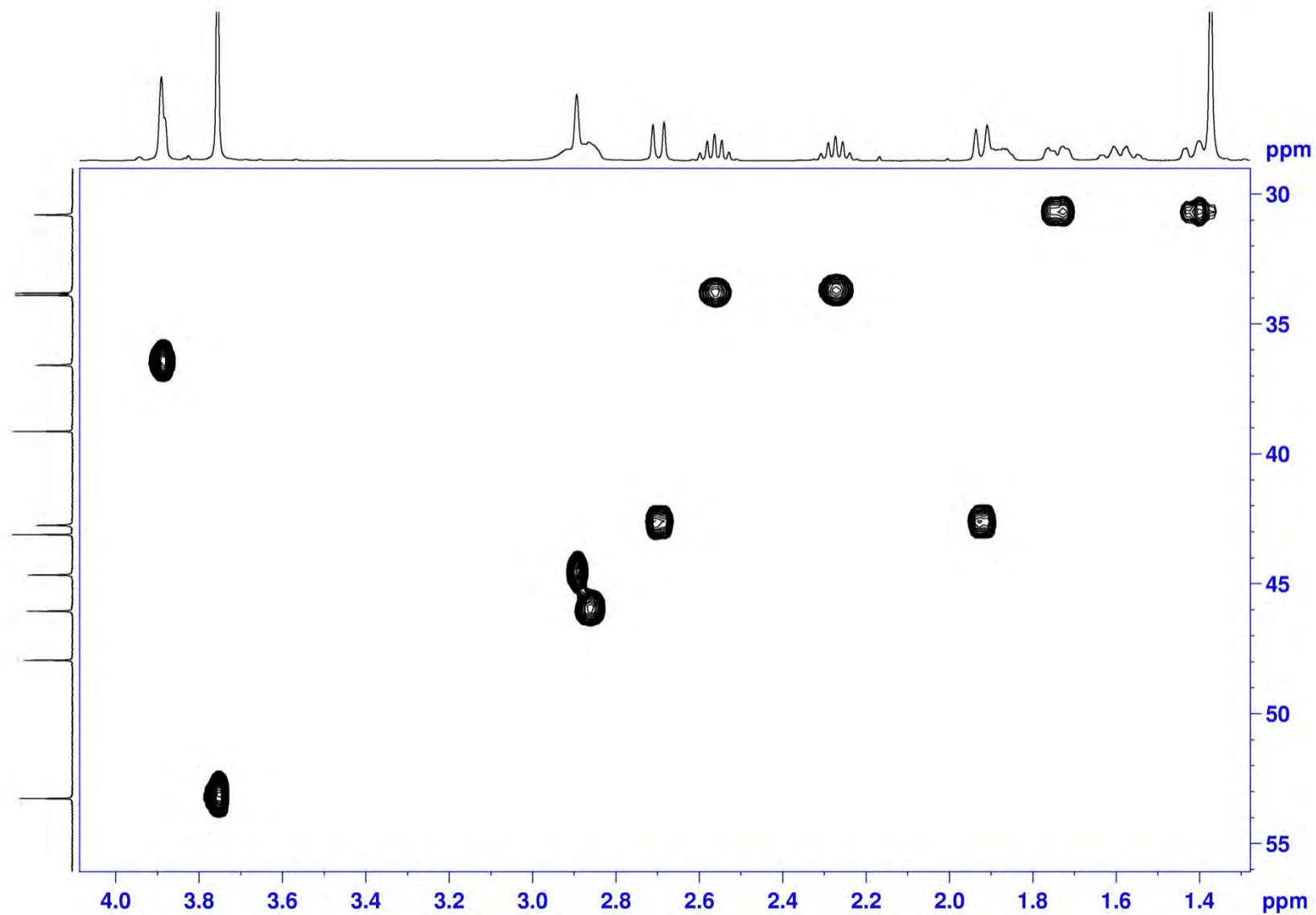
HSQC (400 MHz) spectrum of compound **1** in CDCl₃



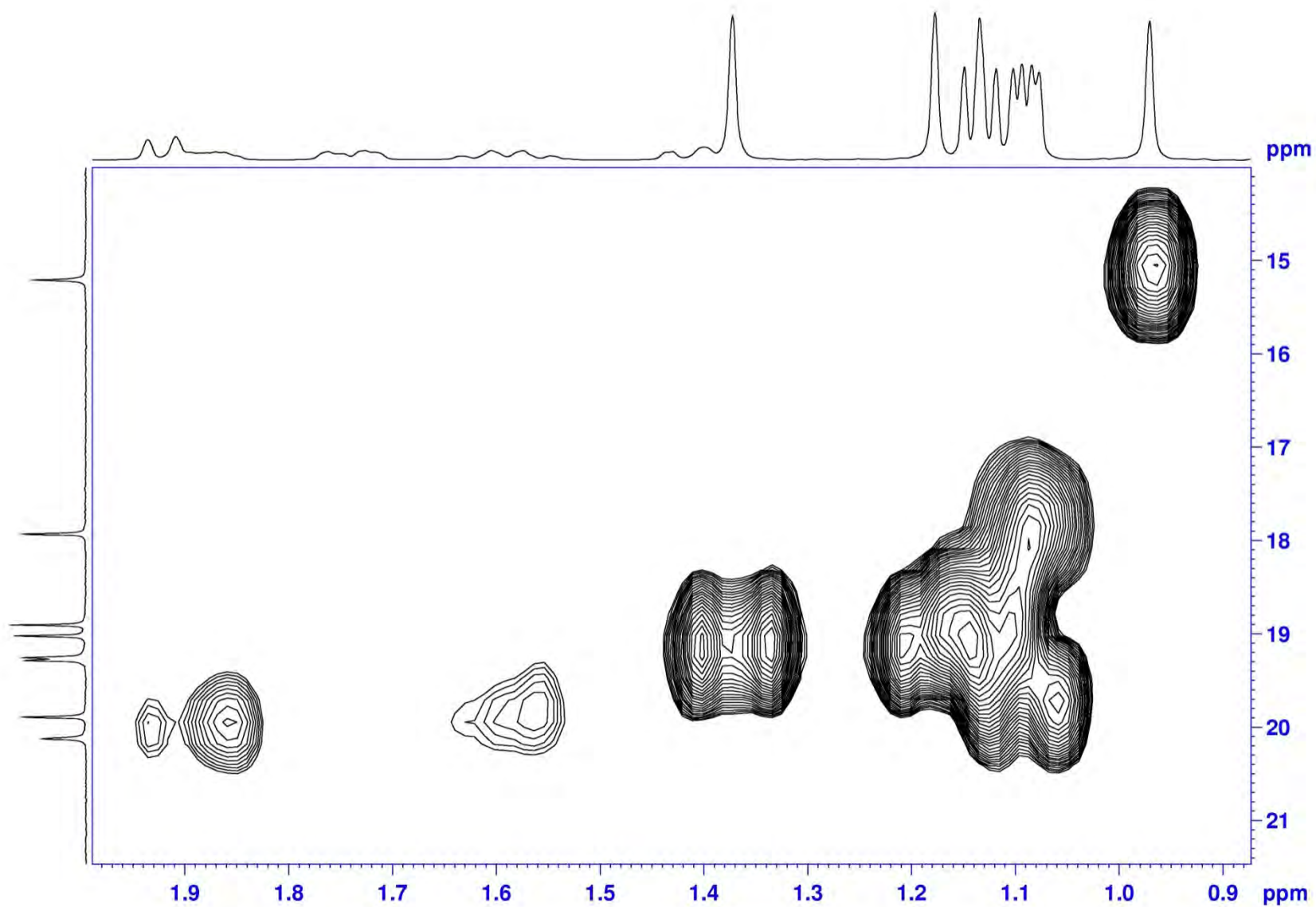
HSQC (400 MHz) spectrum of compound **1** in CDCl₃



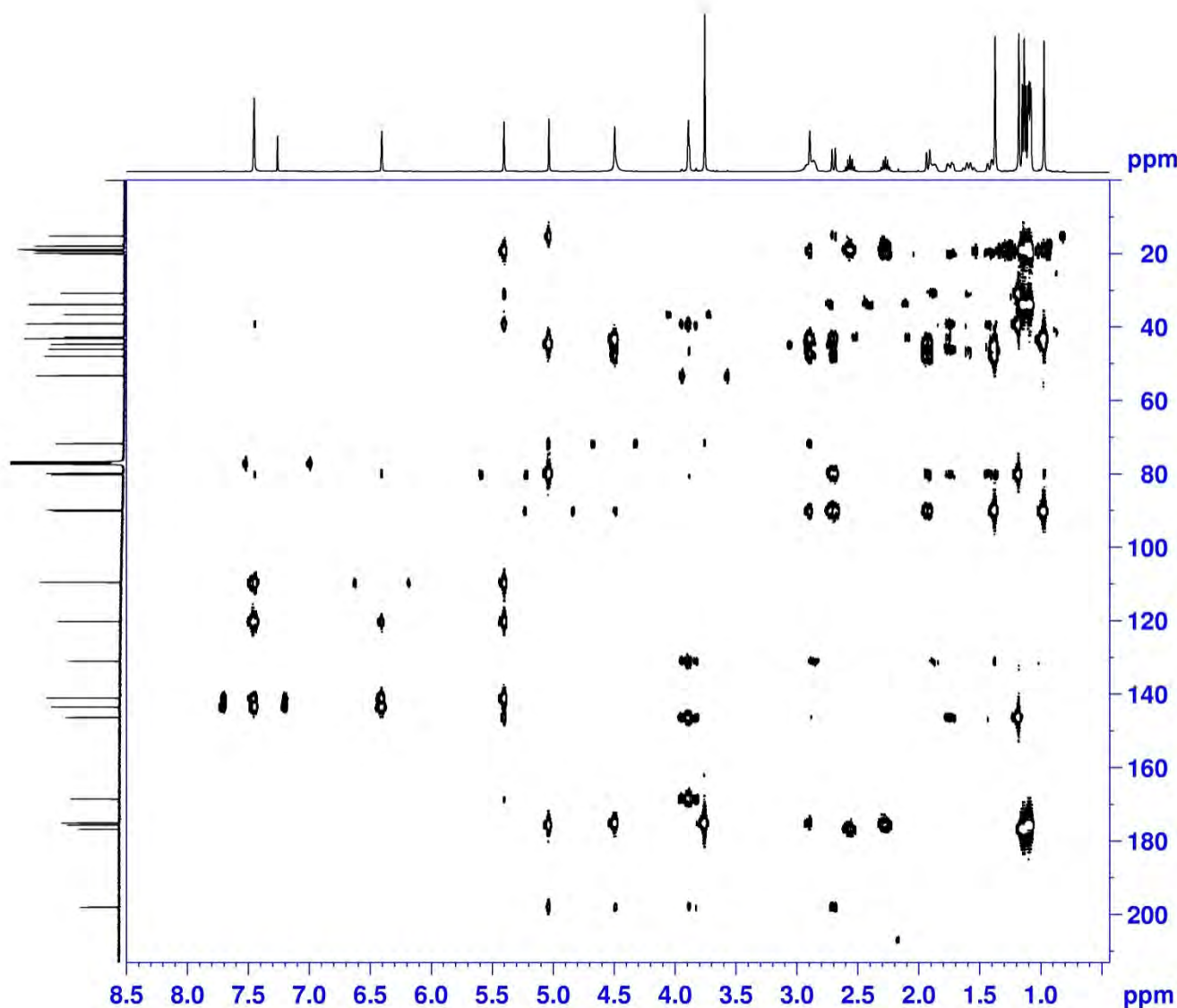
HSQC (400 MHz) spectrum of compound **1** in CDCl₃



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



HMBC (400 MHz) spectrum of compound 1 in CDCl₃

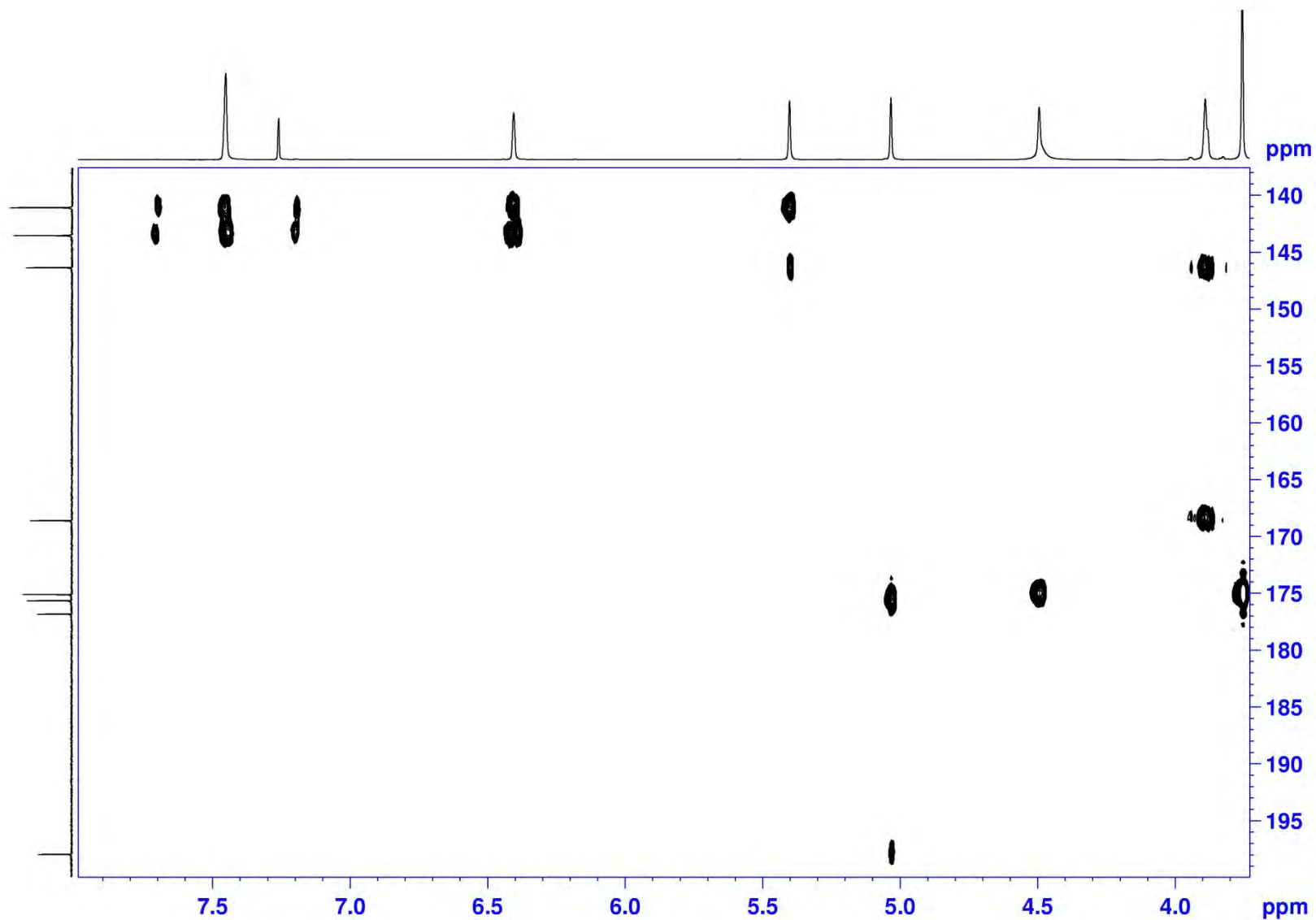


```

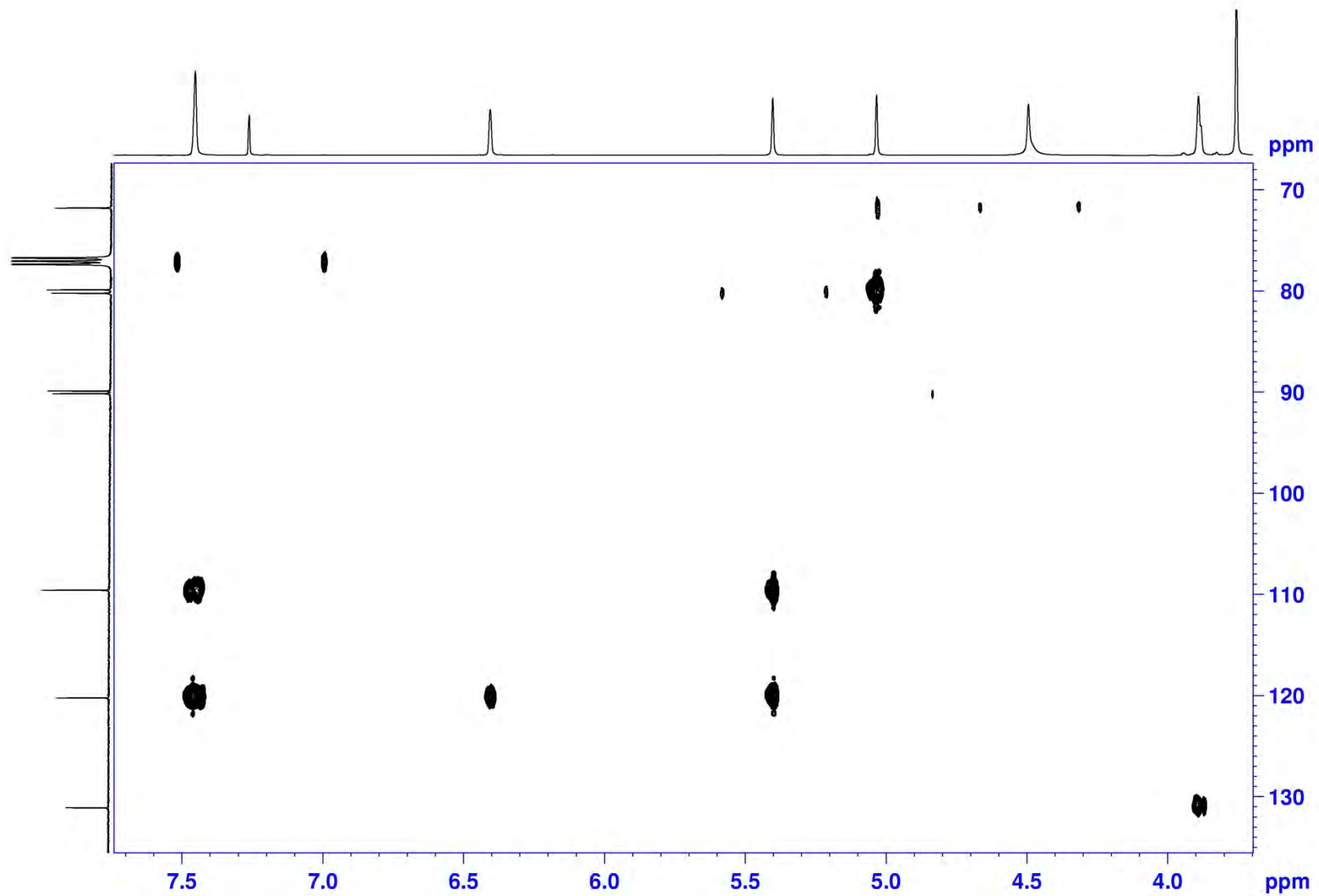
NAME                lws-42
EXPNO                6
PROCNO              1
Date_               20141108
Time                5.57
INSTRUM             spect
PROBHD              5 mm CPPBBO BB
PULPROG             hmbcgp1pndqf
TD                  4096
SOLVENT             CDCl3
NS                   32
DS                   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               145.000000
CNST13              10.000000
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                   12.00 usec
P2                   24.00 usec
ND0                   2
TD                   128
SFO1                100.6233 MHz
FIDRES              187.800476 Hz
SW                   238.896 ppm
FMODE                QF
SI                   2048
SF                   400.1300097 MHz
WDW                  SINE
SSB                   0
LB                   0.00 Hz
GB                   0
PC                   1.40
SI                   1024
MC2                  QF
SF                   100.6127693 MHz
WDW                  SINE
SSB                   0
LB                   0.00 Hz
GB                   0
    
```

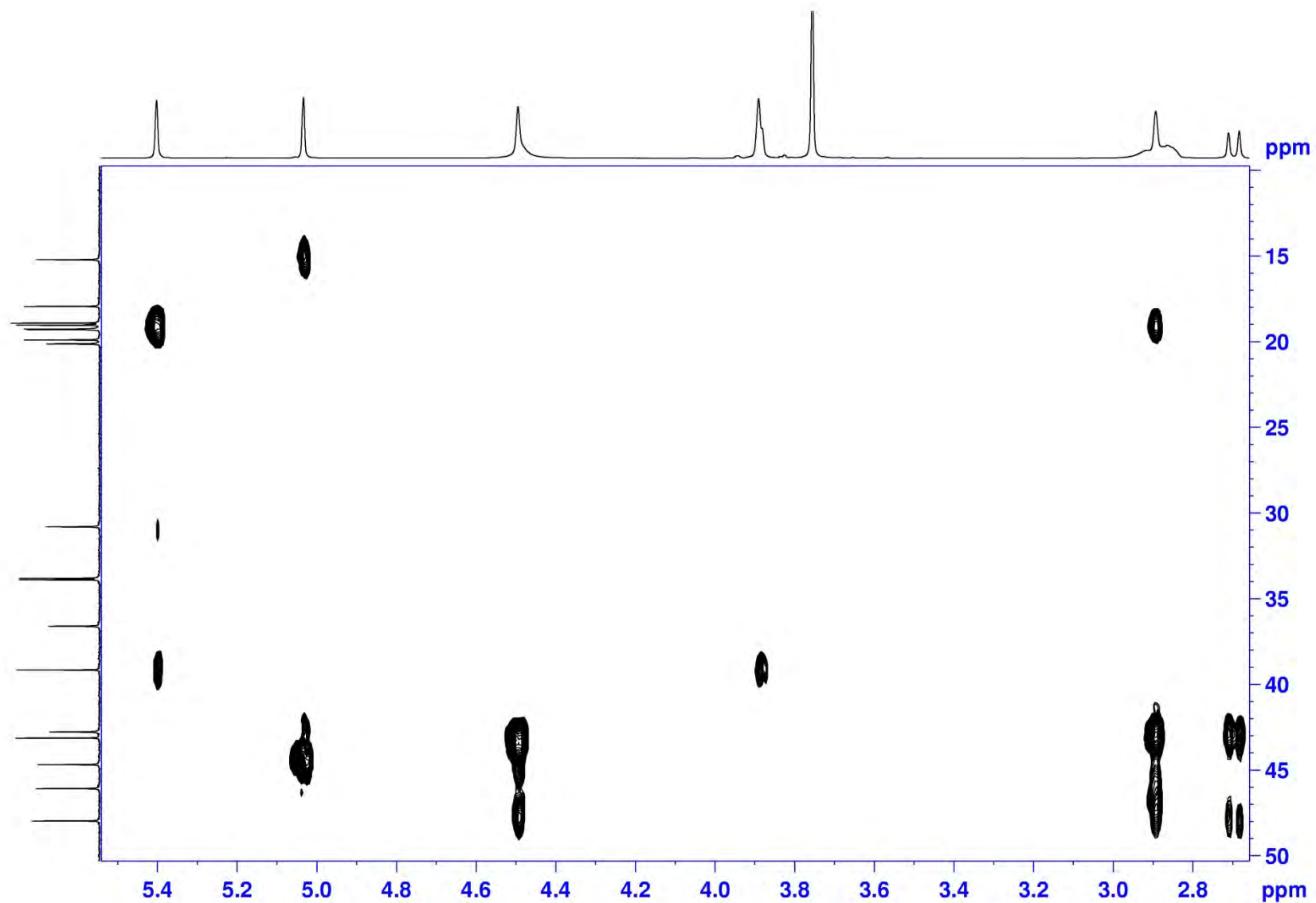
HMBC (400 MHz) spectrum of compound **1** in CDCl₃



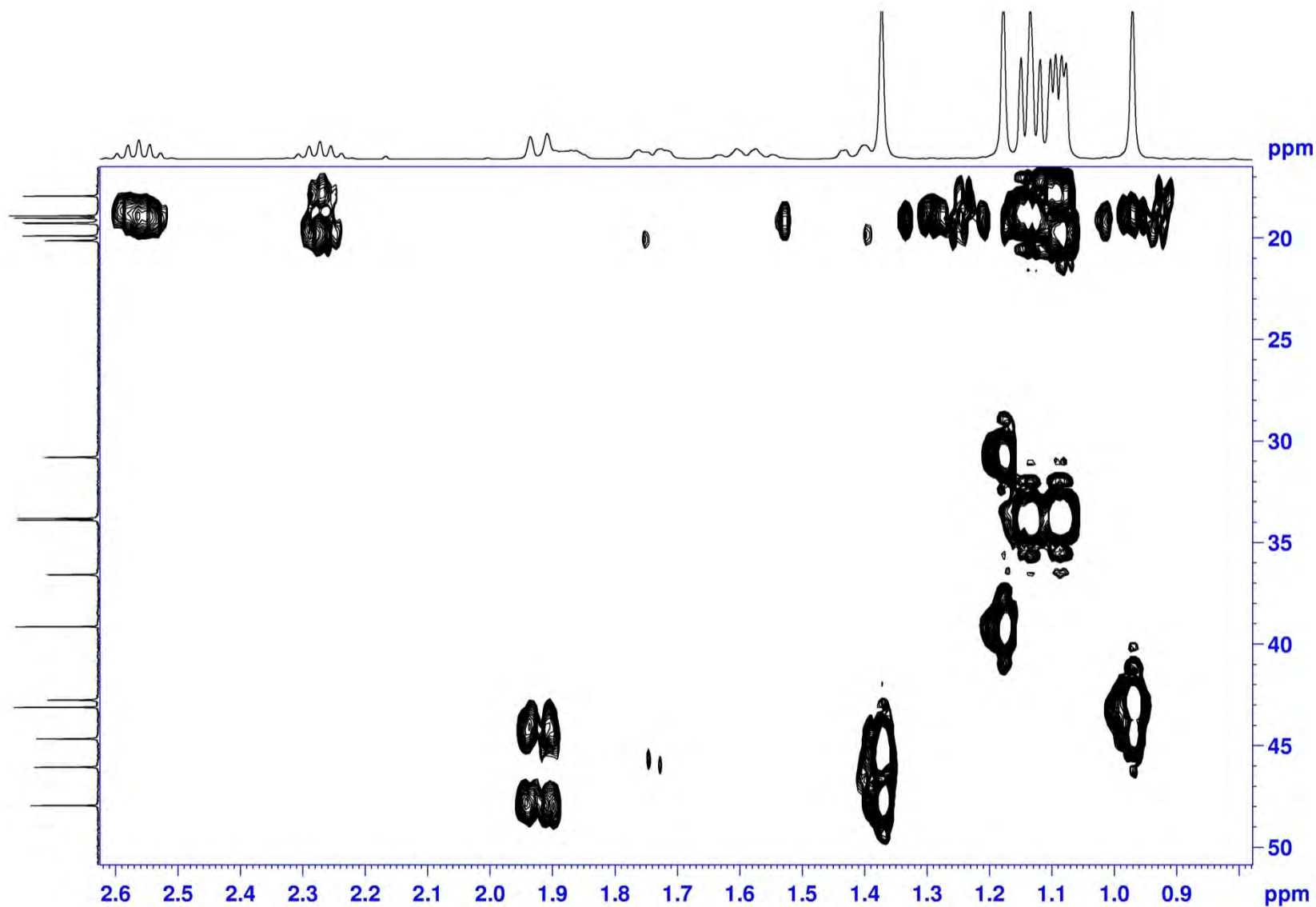
HMBC (400 MHz) spectrum of compound **1** in CDCl₃



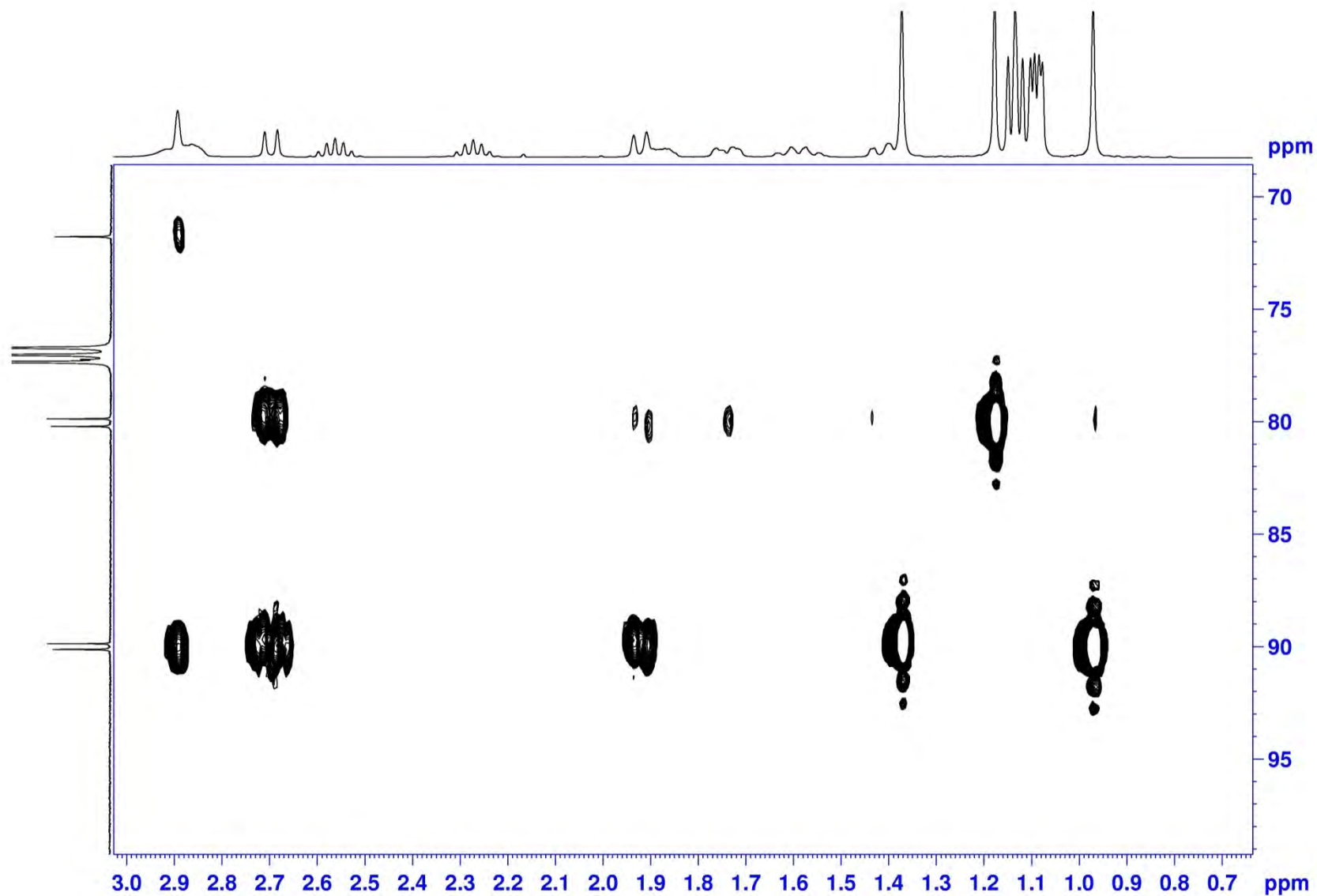
HMBC (400 MHz) spectrum of compound **1** in CDCl₃



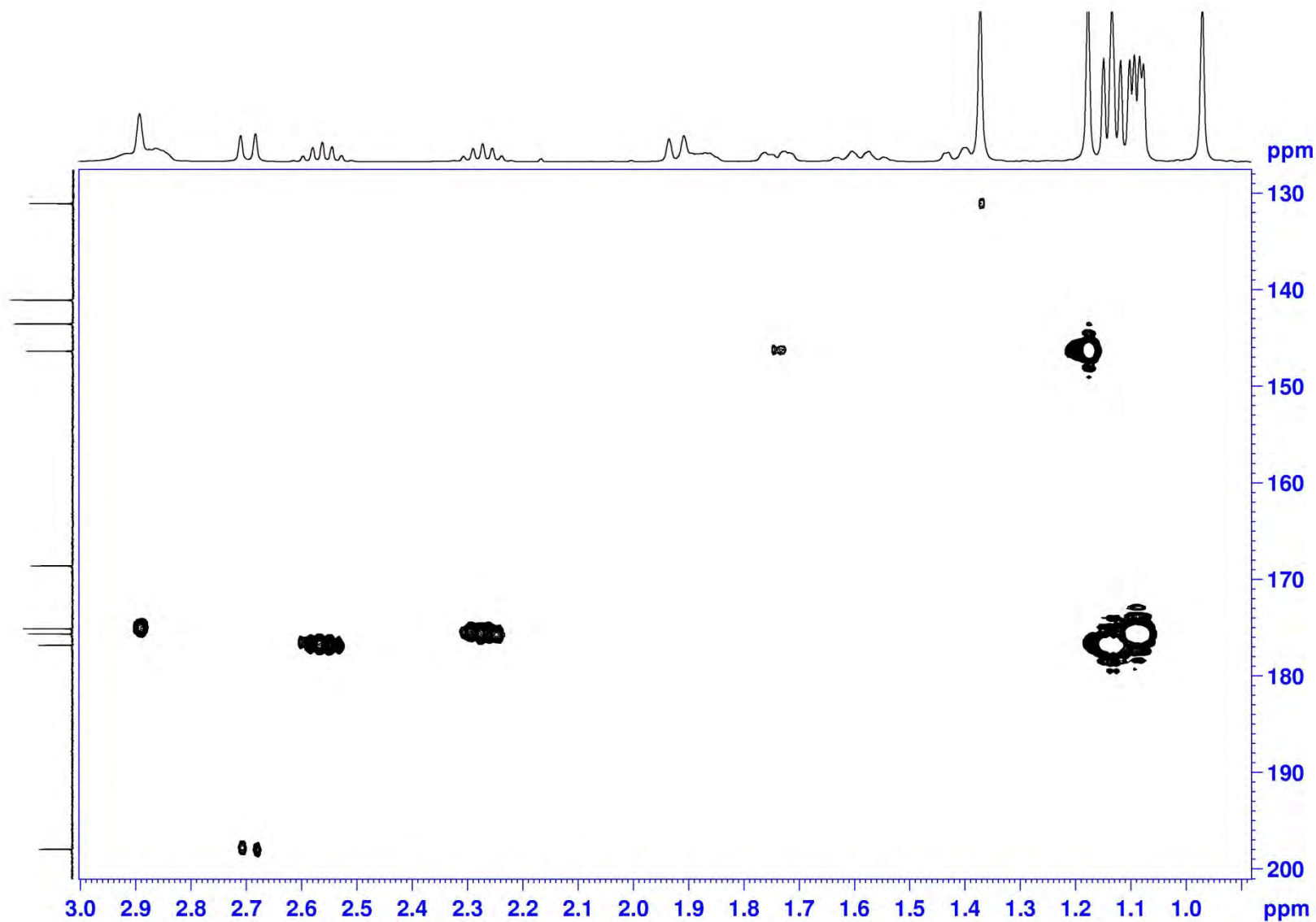
HMBC (400 MHz) spectrum of compound **1** in CDCl₃



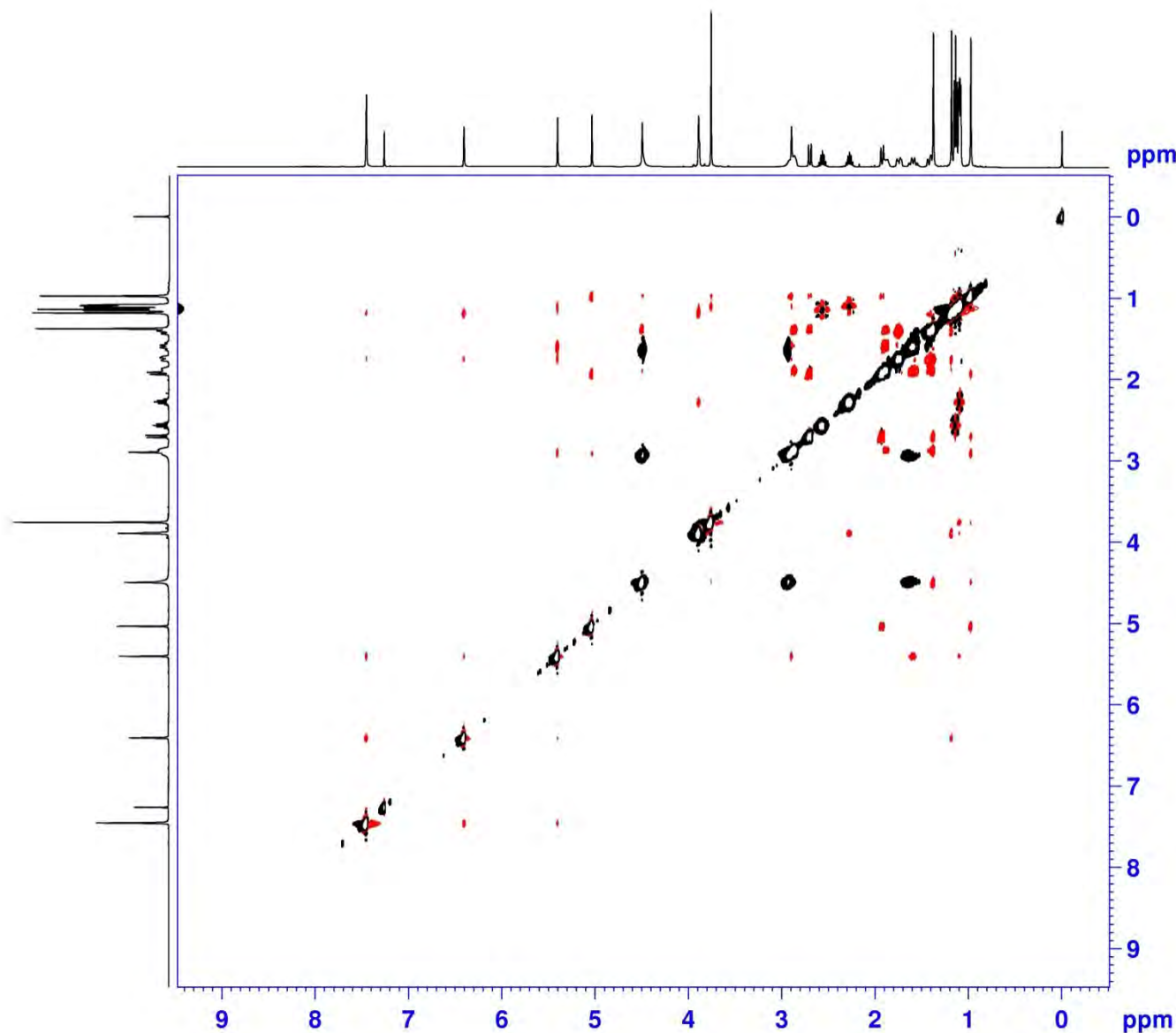
HMBC (400 MHz) spectrum of compound **1** in CDCl₃



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



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



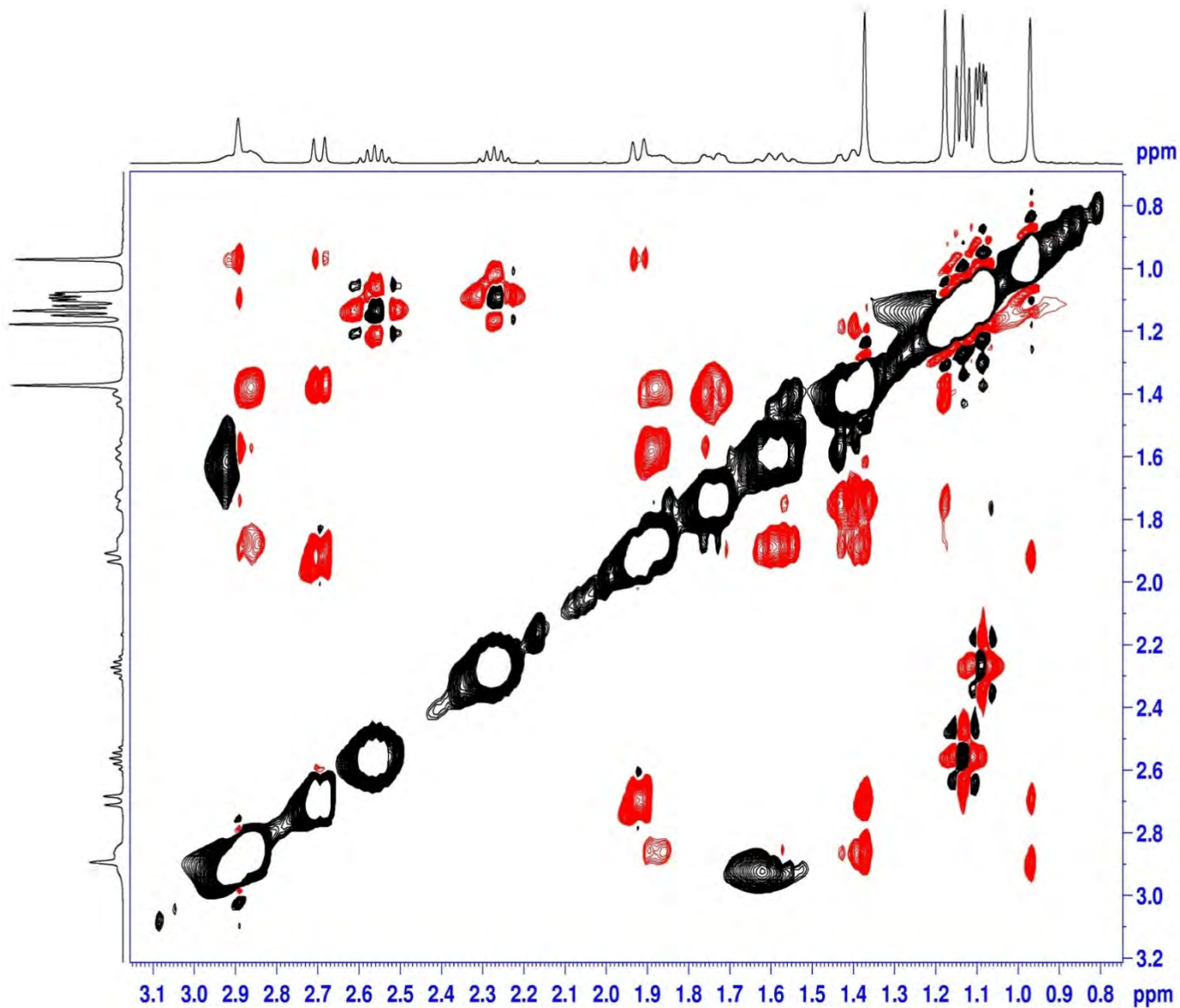
```

NAME                lws-42
EXPNO                7
PROCNO               1
Date_                20141108
Time                8.13
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                   117.37
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
    
```

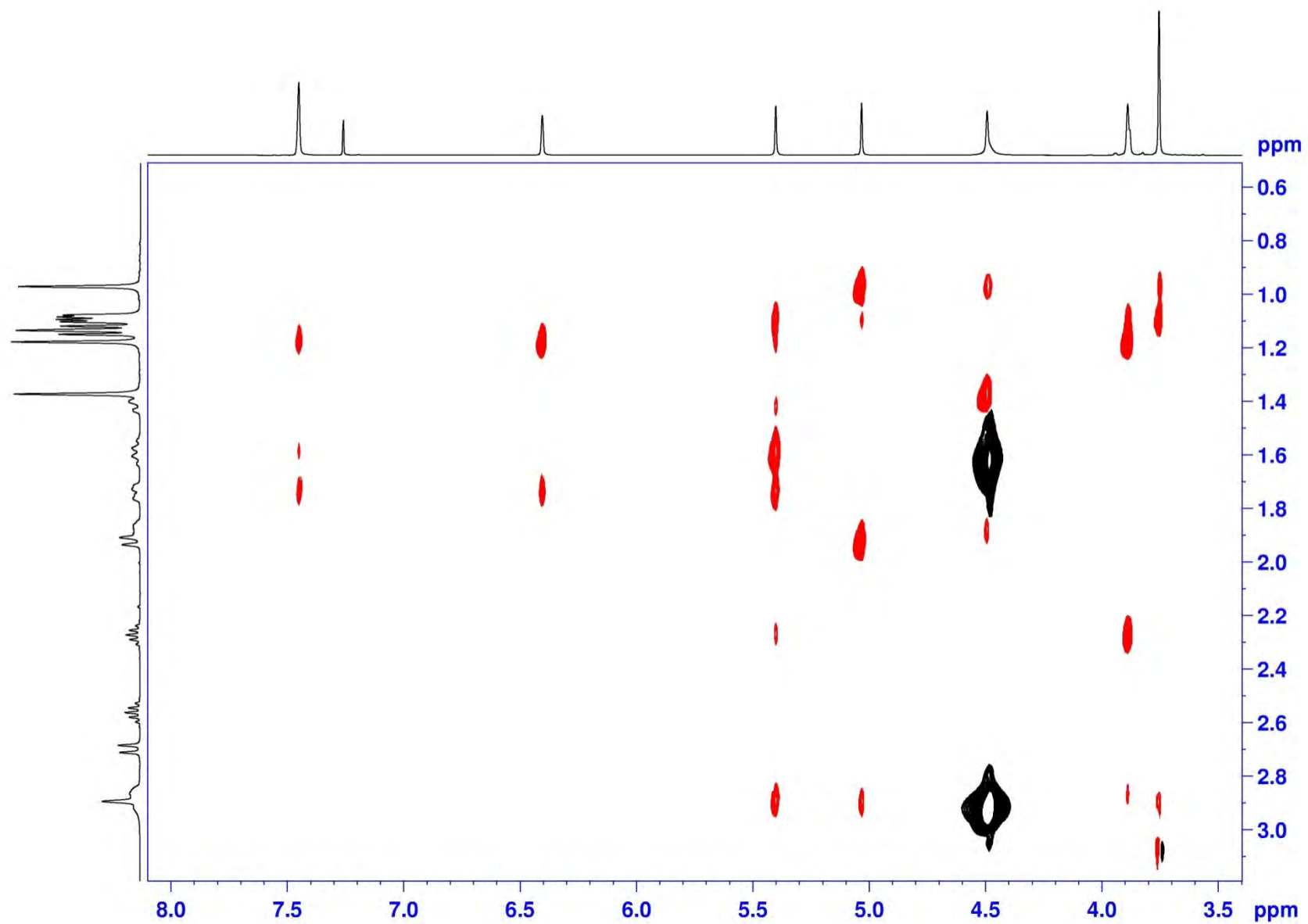
```

===== 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                   400.1300098 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
LB                   0.00 Hz
    
```

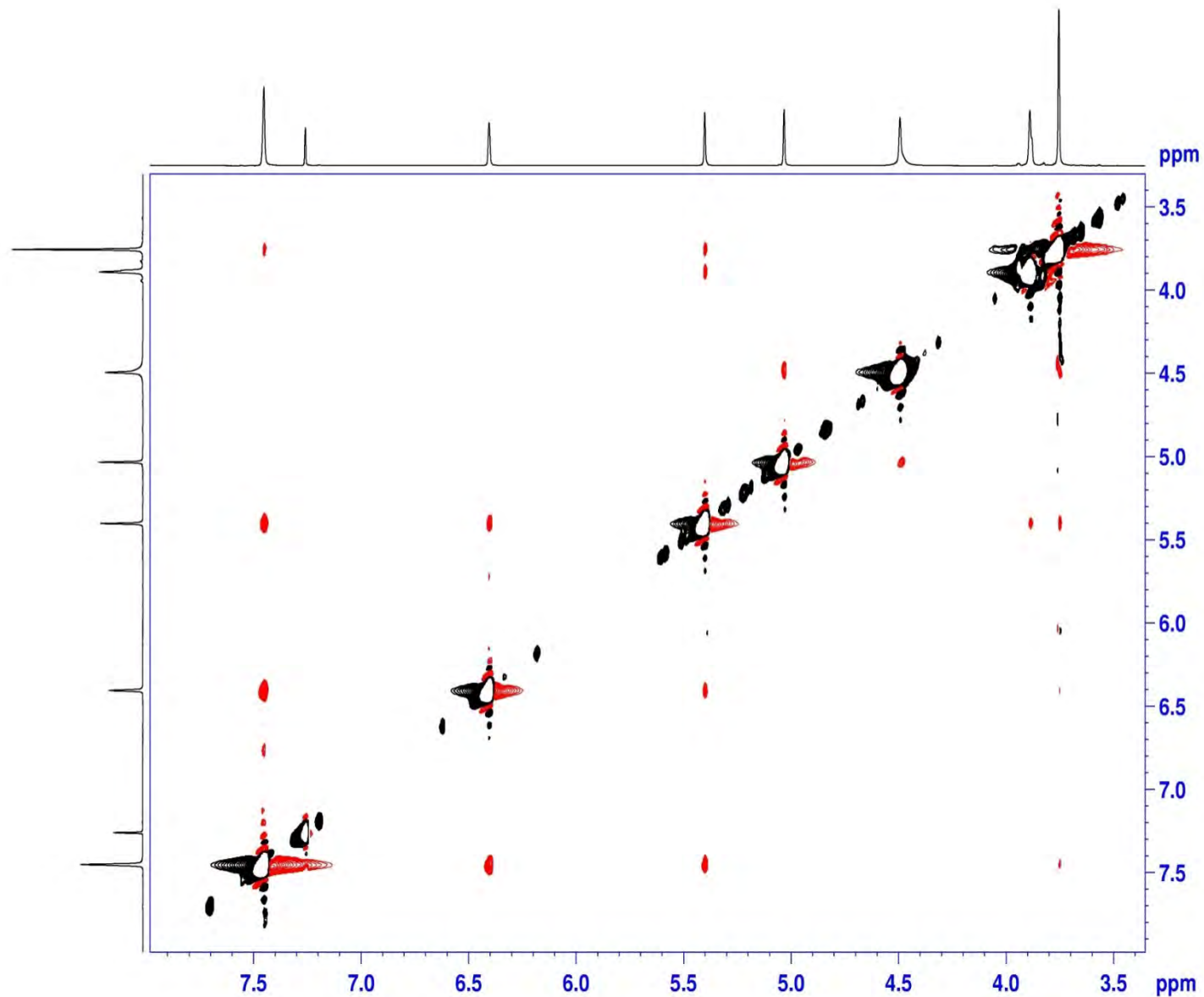
NOESY (400 MHz) spectrum of compound **1** in CDCl₃



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



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



HR-ESIMS for compound 2

Generic Display Report

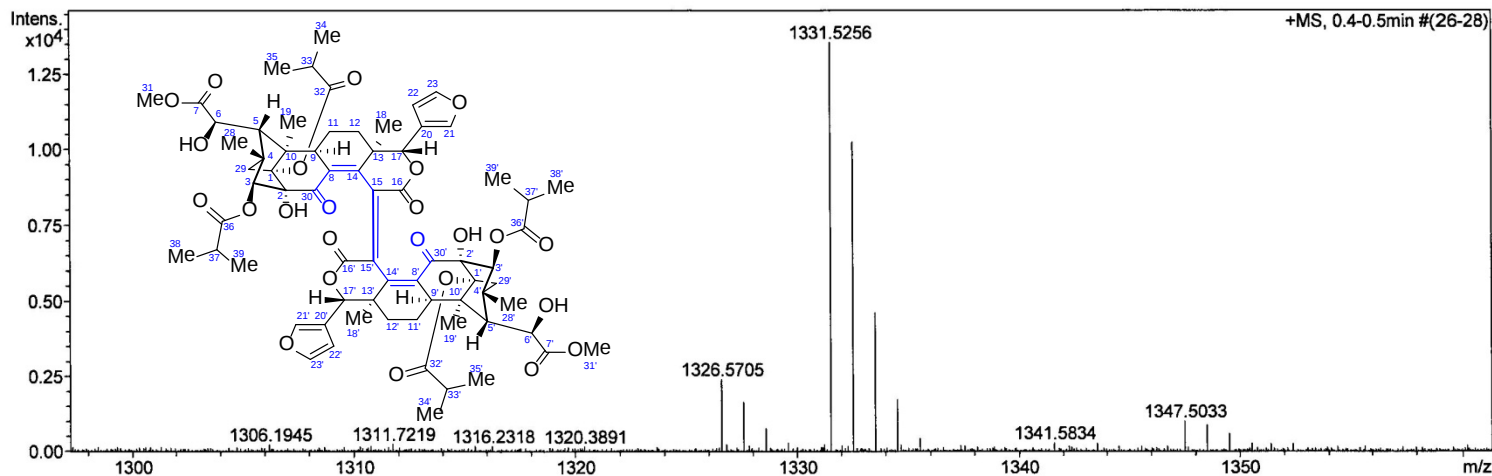
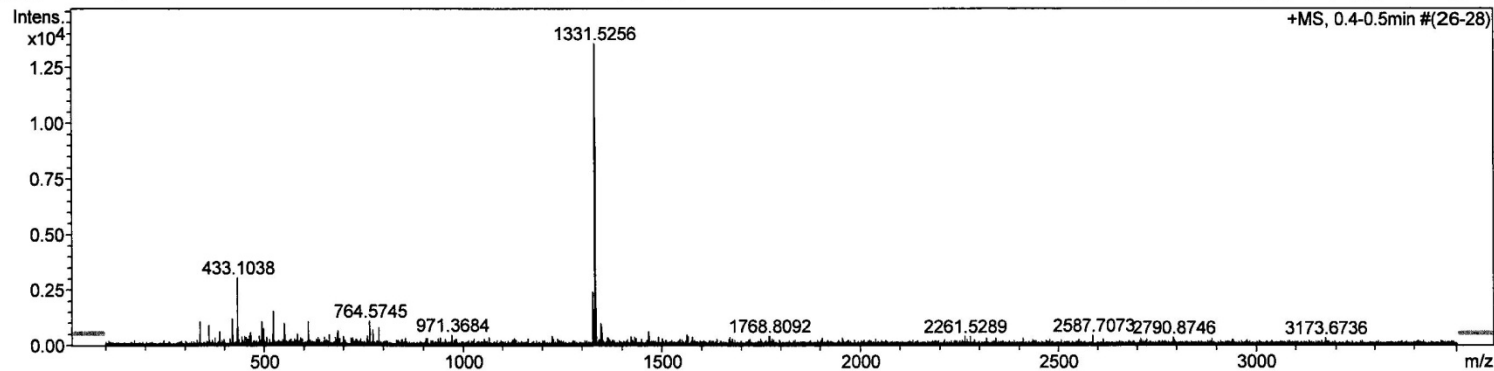
Analysis Info

Analysis Name D:\Data\MS\data\201509\liwanshan_lws-42-0_pos_1_01_344.d
Method LC_Direct Infusion_pos_100-3000mz.m
Sample Name liwanshan_lws-42-0_pos
Comment

Acquisition Date 9/7/2015 11:42:33 PM

Operator SCSIO

Instrument maXis



HR-ESIMS for compound 2

Mass Spectrum SmartFormula Report

Analysis Info

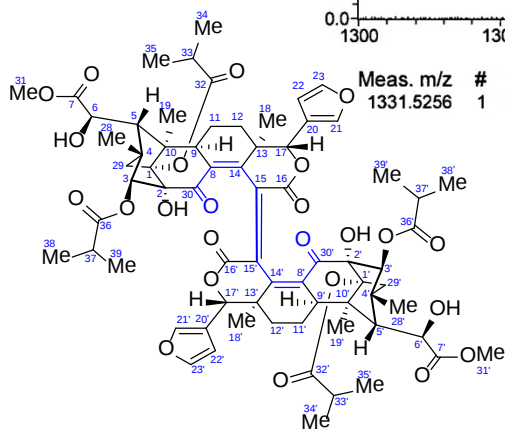
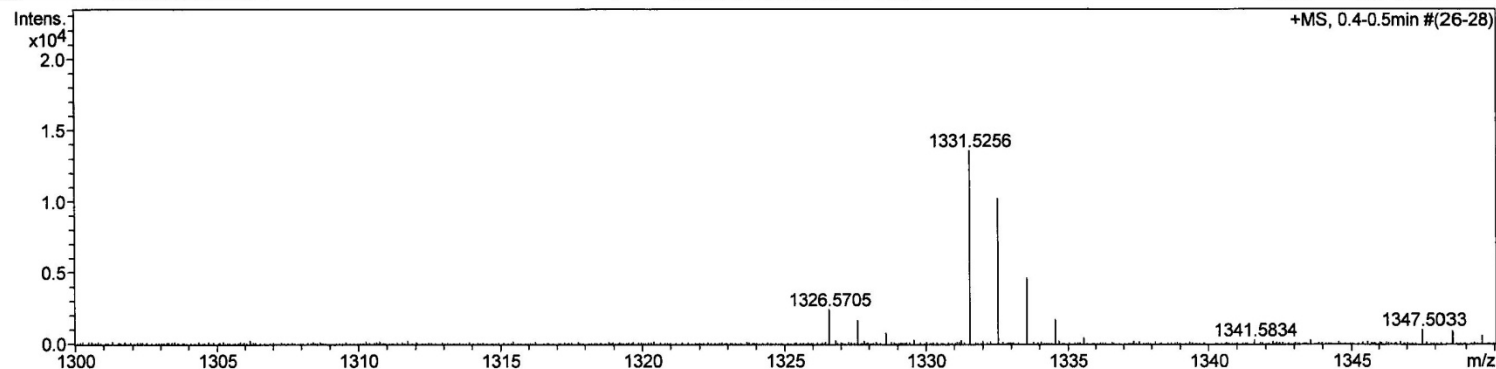
Analysis Name D:\Data\MS\data\201509\liwanshan_lws-42-0_pos_1_01_344.d
 Method LC_Direct Infusion_pos_100-3000mz.m
 Sample Name liwanshan_lws-42-0_pos
 Comment

Acquisition Date 9/7/2015 11:42:33 PM

Operator SCSIO
 Instrument / Ser# maXis 29

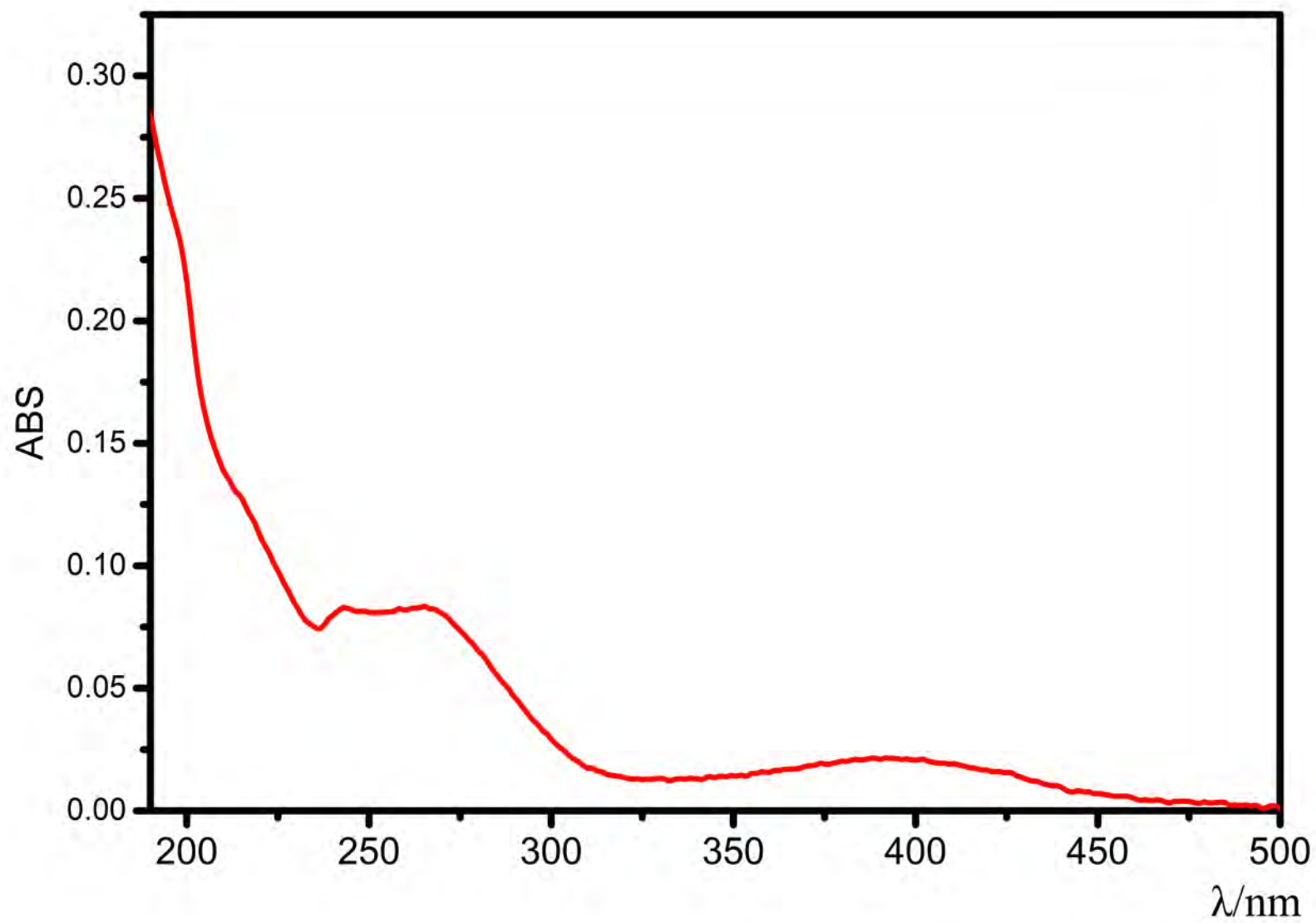
Acquisition Parameter

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	3500 m/z	Set Collision Cell RF	1800.0 Vpp	Set Divert Valve	Waste



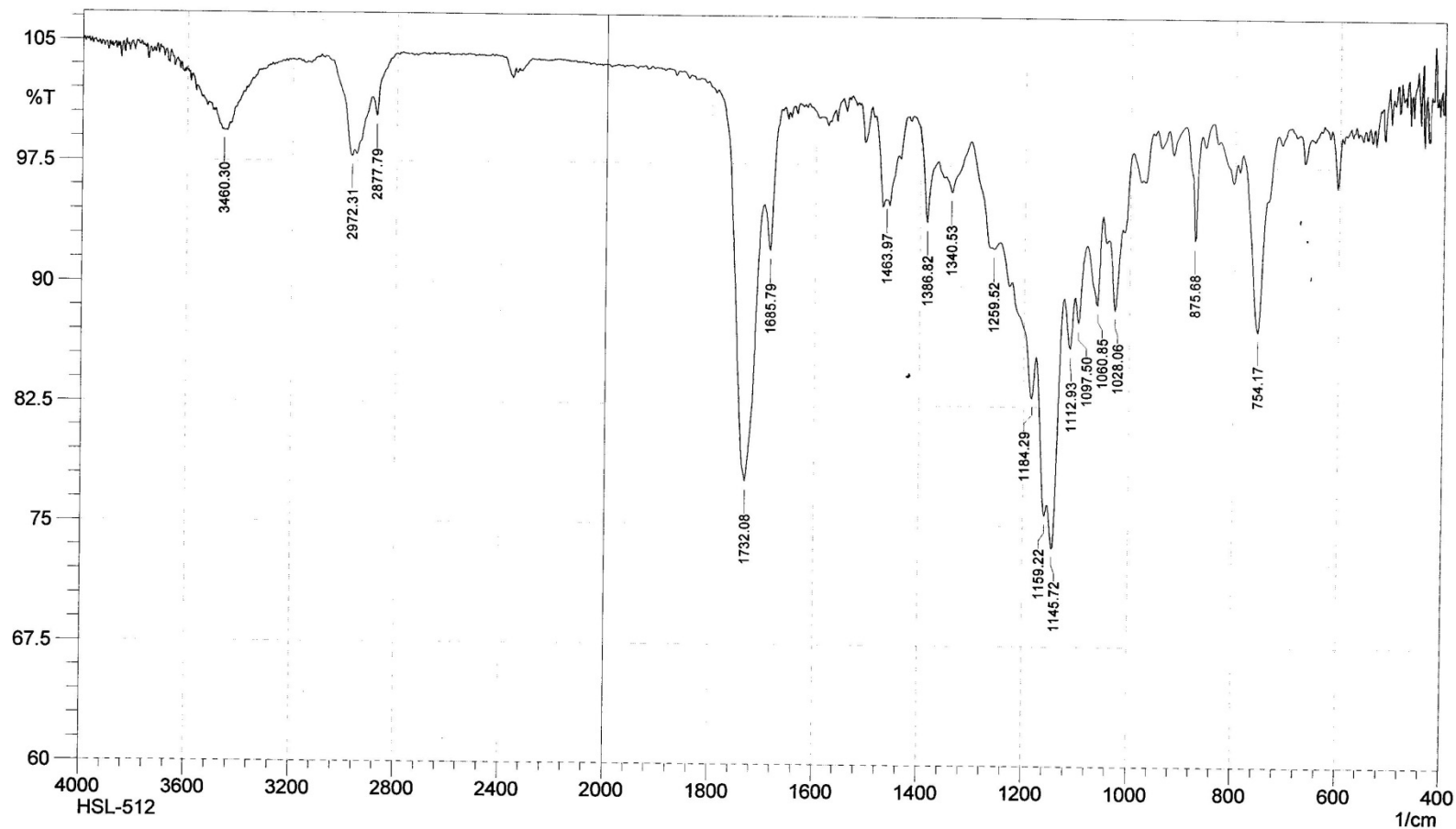
Meas. m/z	#	Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
1331.5256	1	C 70 H 84 Na O 24	100.00	1331.5245	-0.8	-1.1	11.5	28.5	even	ok

UV spectrum for compound **2** in CHCl_3



IR spectrum for compound 2

SHIMADZU



Sample name: 42-0-21 (2)
F:\liwanshan\20180226\42-
0-21.smf

Scan number: 25
Resolution: 4 [1/cm]

Data: 2018-2-26 13:48:42
Operator: SCSIO

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

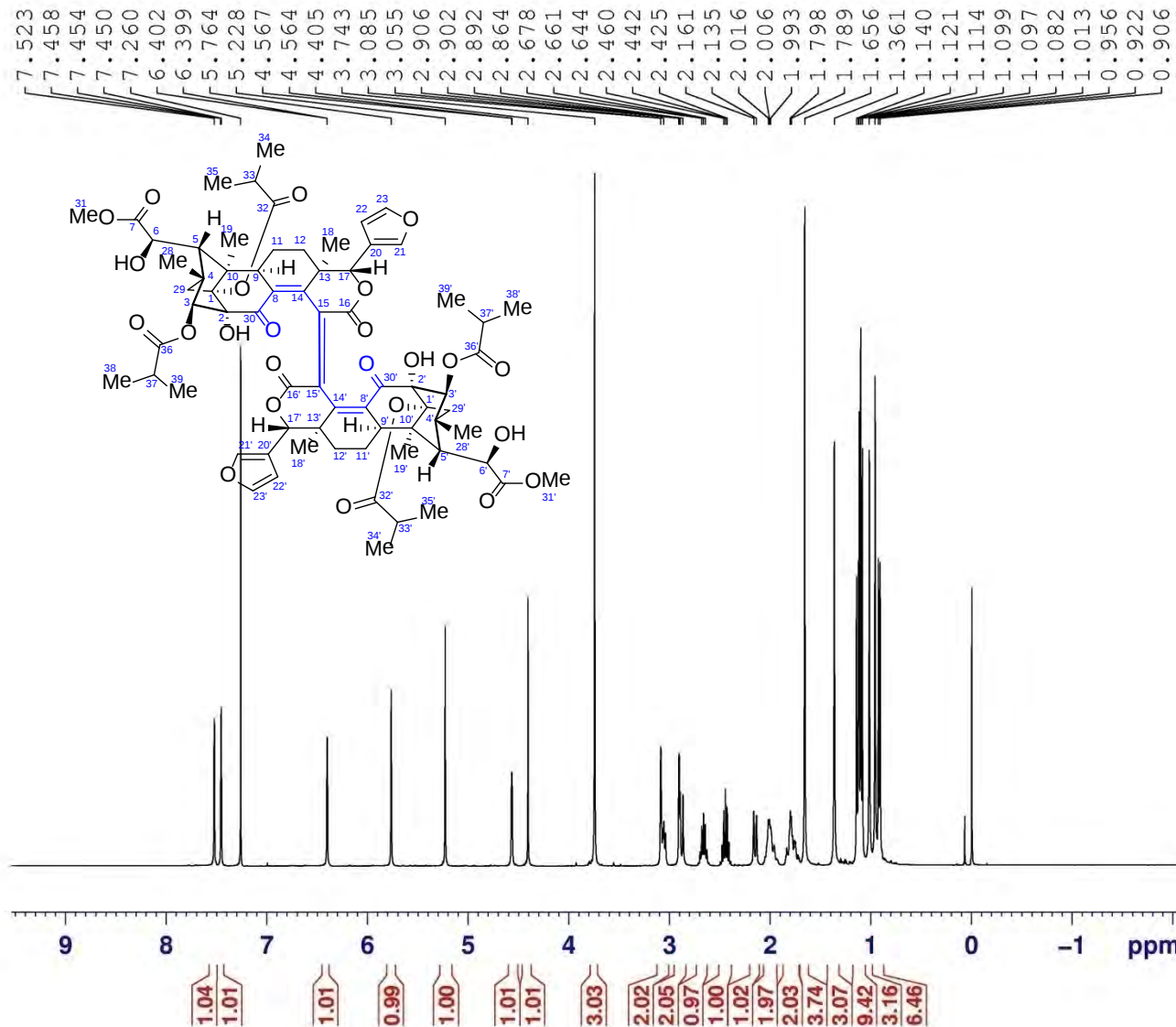


```

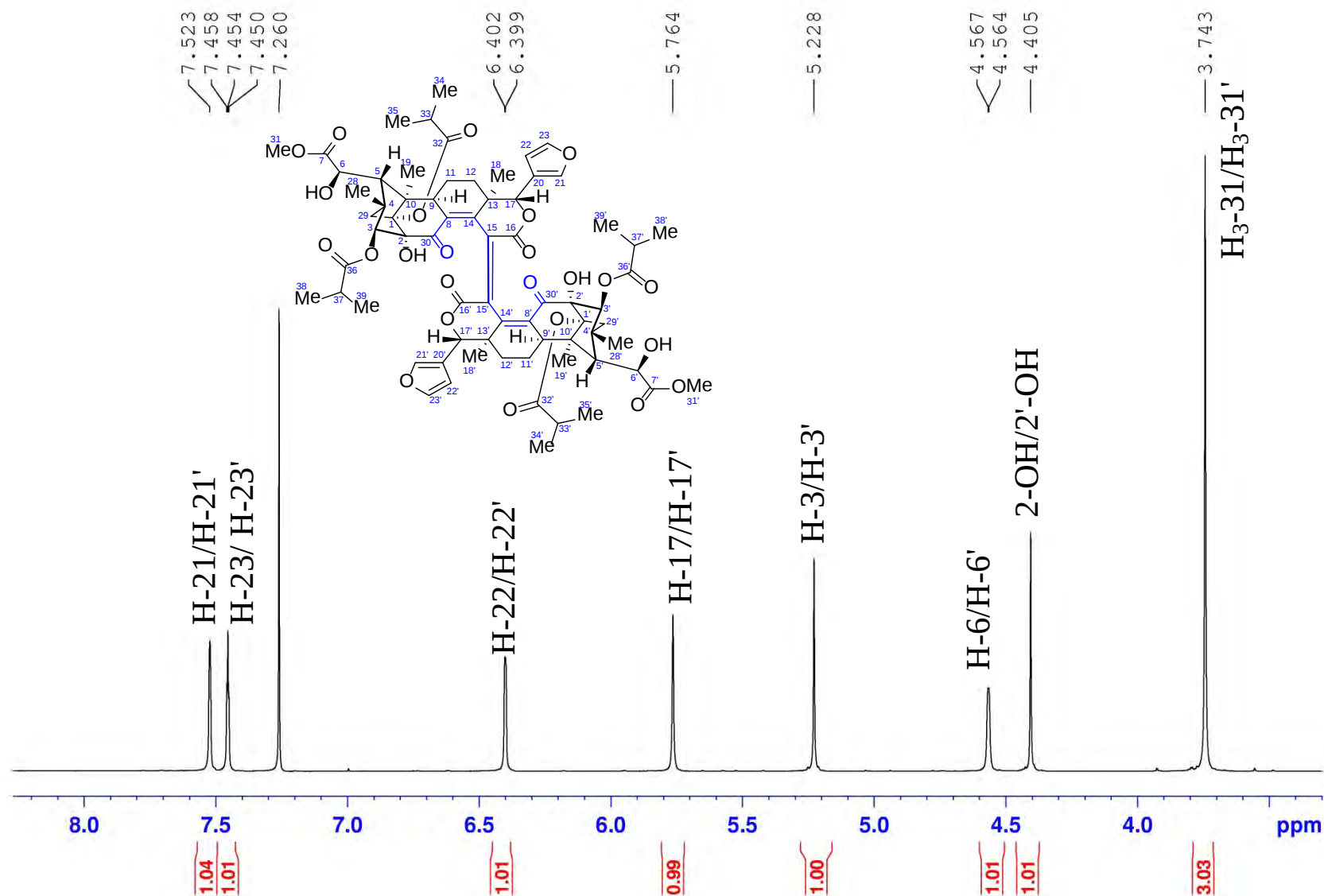
NAME          LWS-42-0
EXPNO          1
PROCNO         1
Date_          20150727
Time           11.07
INSTRUM        spect
PROBHD         5 mm CPPBBO BB
PULPROG        zg30
TD             65536
SOLVENT        CDCl3
NS             16
DS             2
SWH            8223.685 Hz
FIDRES         0.125483 Hz
AQ             3.9846387 sec
RG             102.3
DW             60.800 usec
DE             10.00 usec
TE             297.0 K
D1             1.00000000 sec
TD0            1
    
```

```

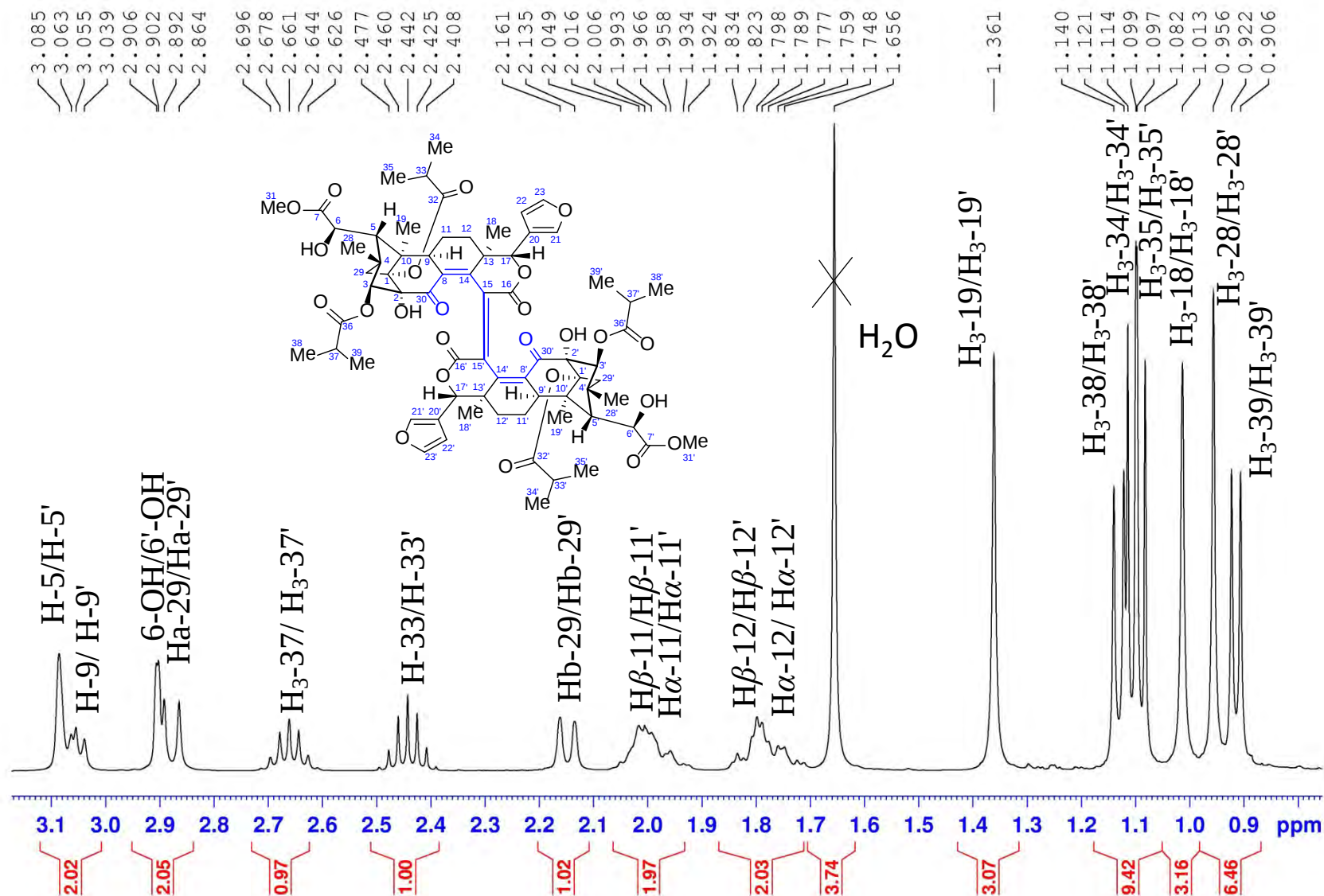
===== CHANNEL f1 =====
SF01          400.1324710 MHz
NUC1           1H
P1             12.00 usec
SI            65536
SF            400.1300094 MHz
WDW            EM
SSB            0
LB             0.30 Hz
GB            0
PC            1.00
    
```



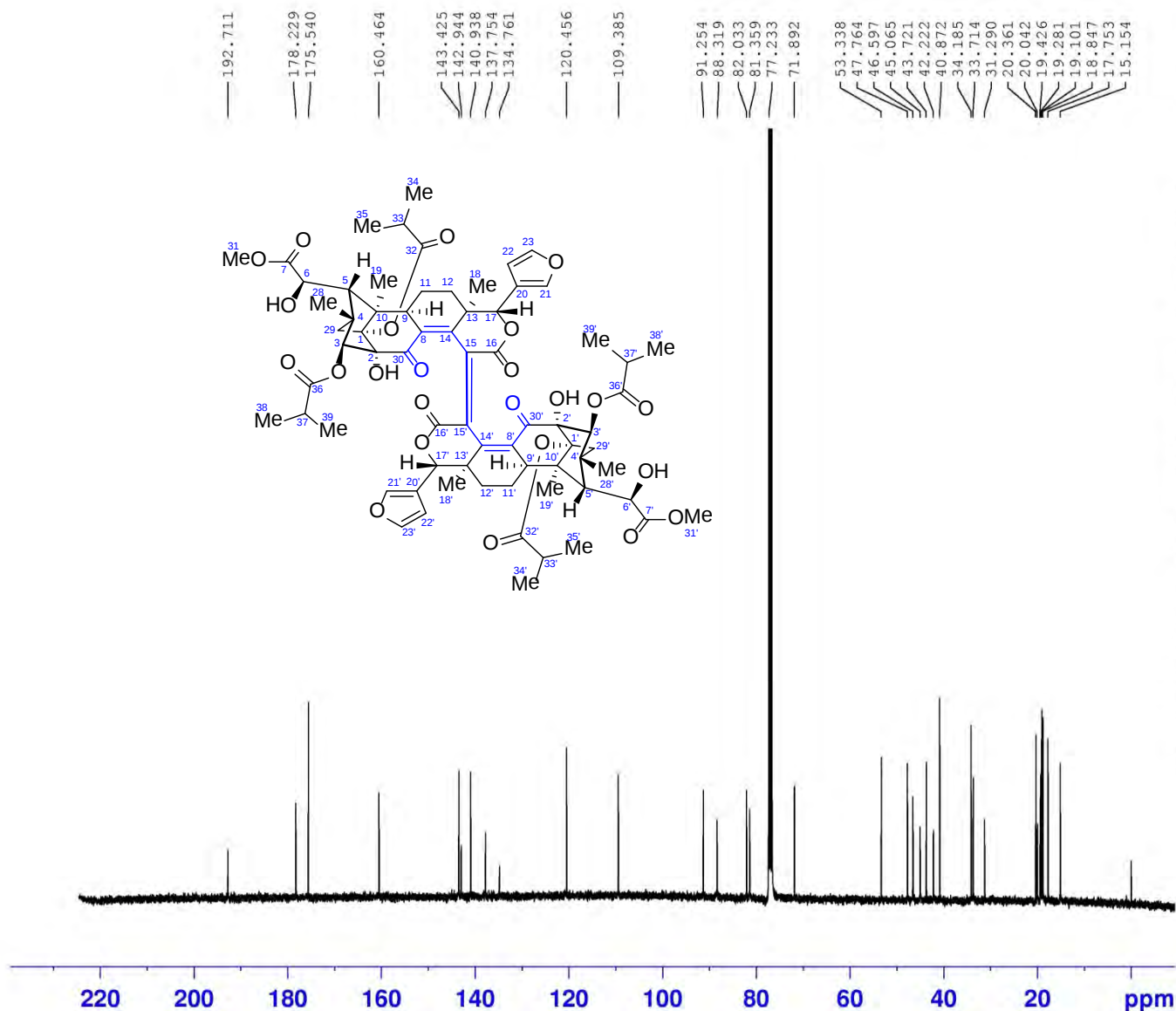
^1H NMR (400 MHz) spectrum of compound **2** in CDCl_3



¹H NMR (400 MHz) spectrum of compound **2** in CDCl₃



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



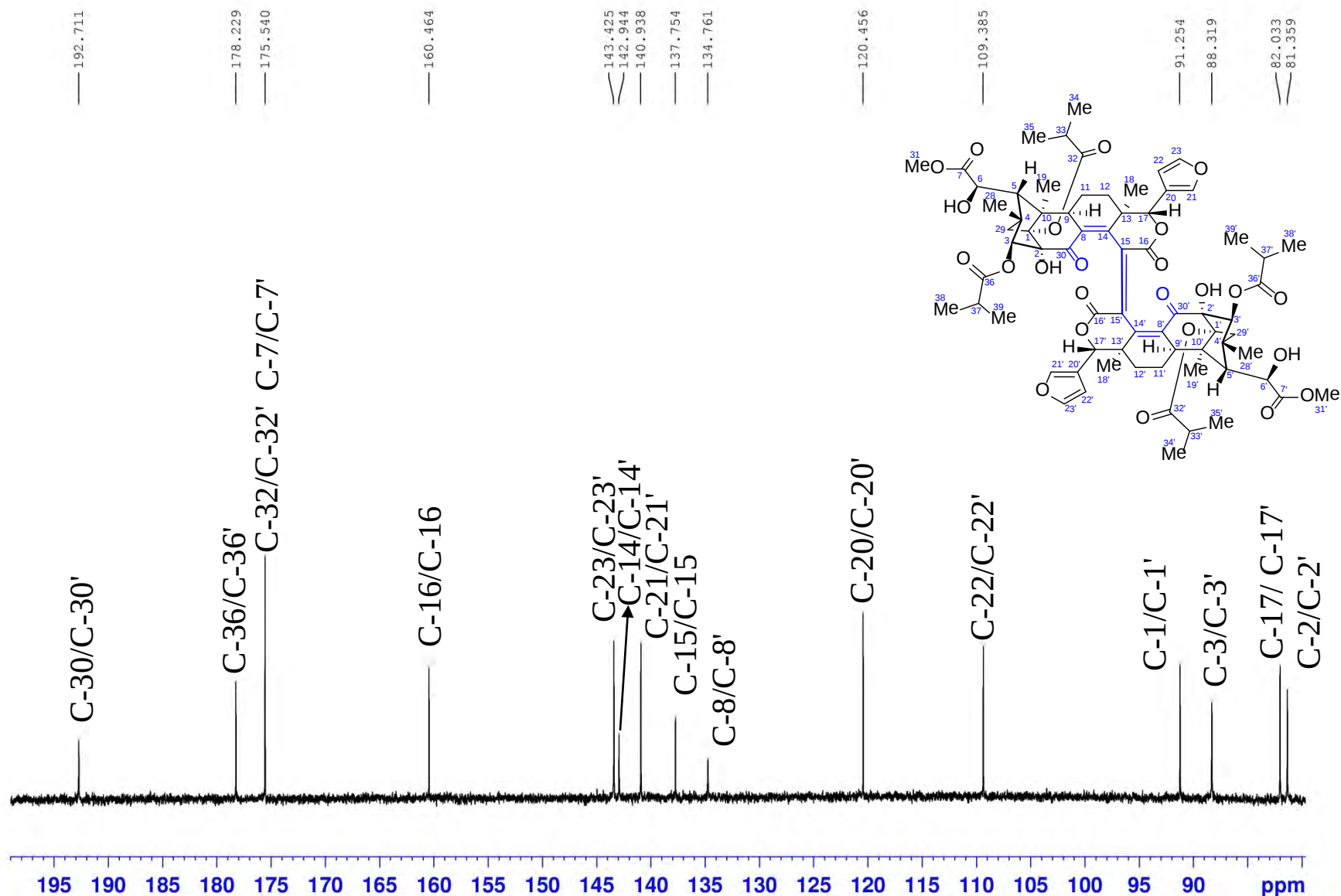
```

NAME          LWS-42-0
EXPNO         2
PROCNO        1
Date_         20150727
Time          12.11
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            85.34
DW            20.800 usec
DE            18.00 usec
TE            297.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
    
```

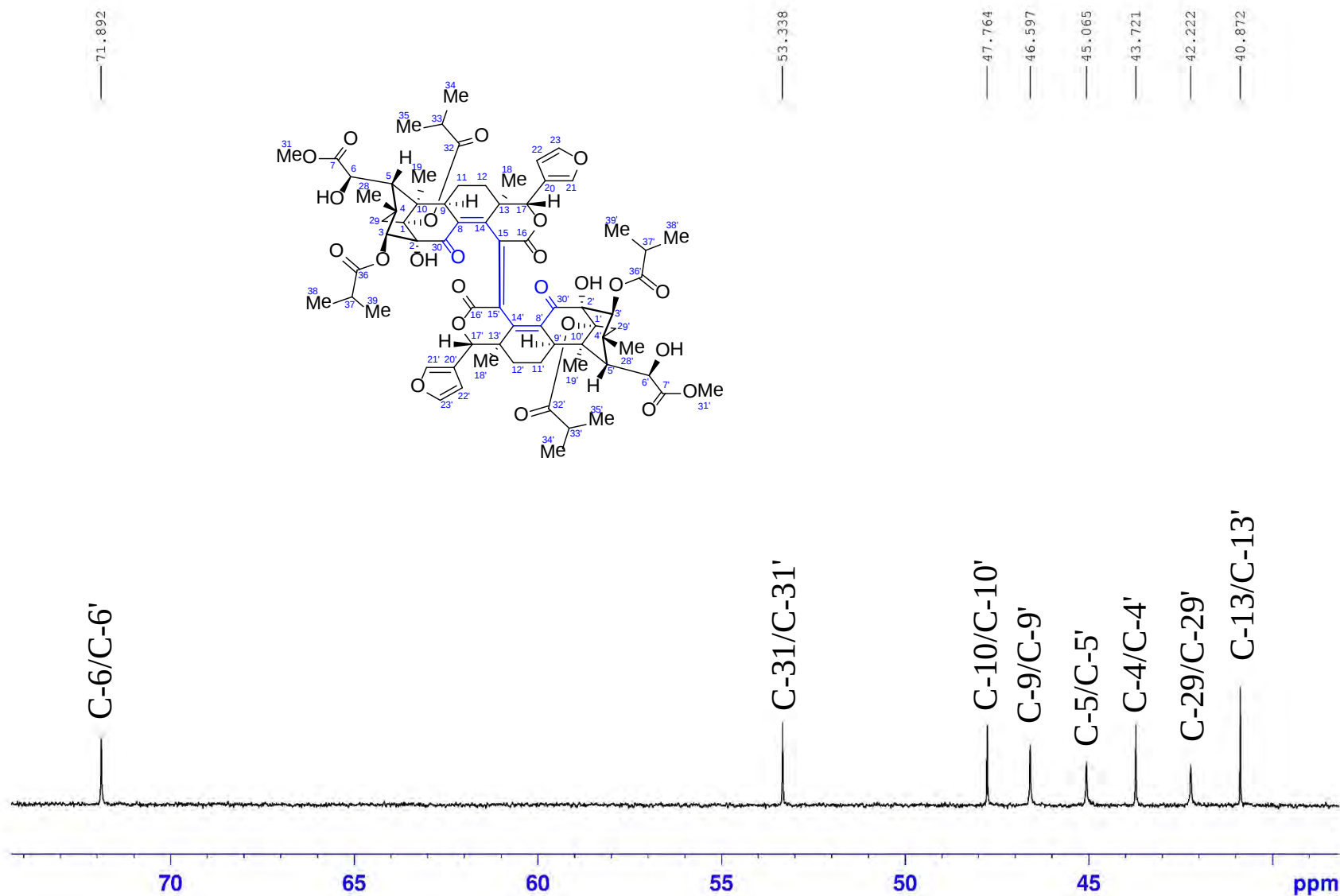
```

===== CHANNEL f1 =====
SFO1          100.6233324 MHz
NUC1          13C
P1            10.00 usec
SI            32768
SF            100.6127686 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

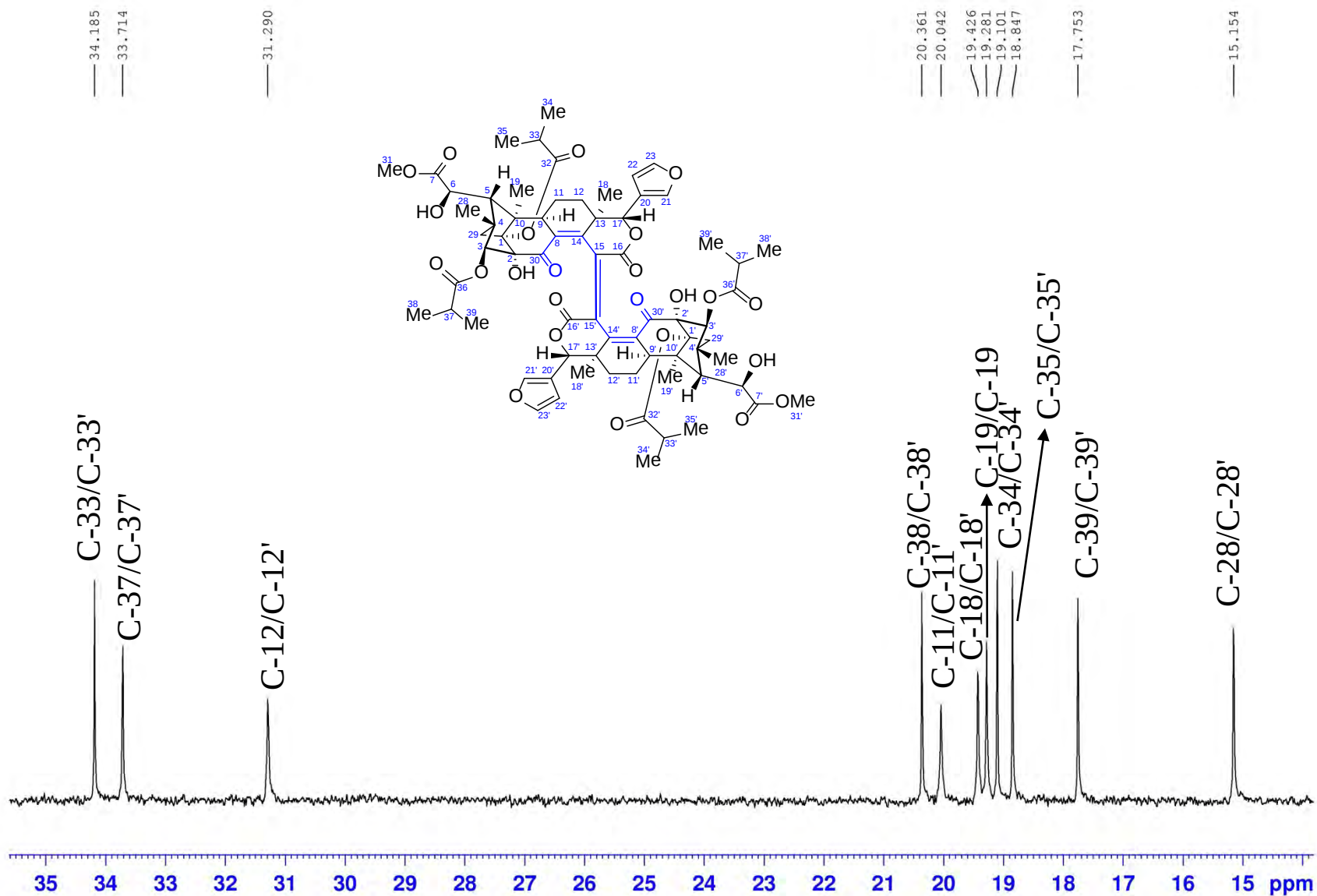
^{13}C NMR (100 MHz) spectrum of compound **2** in CDCl_3



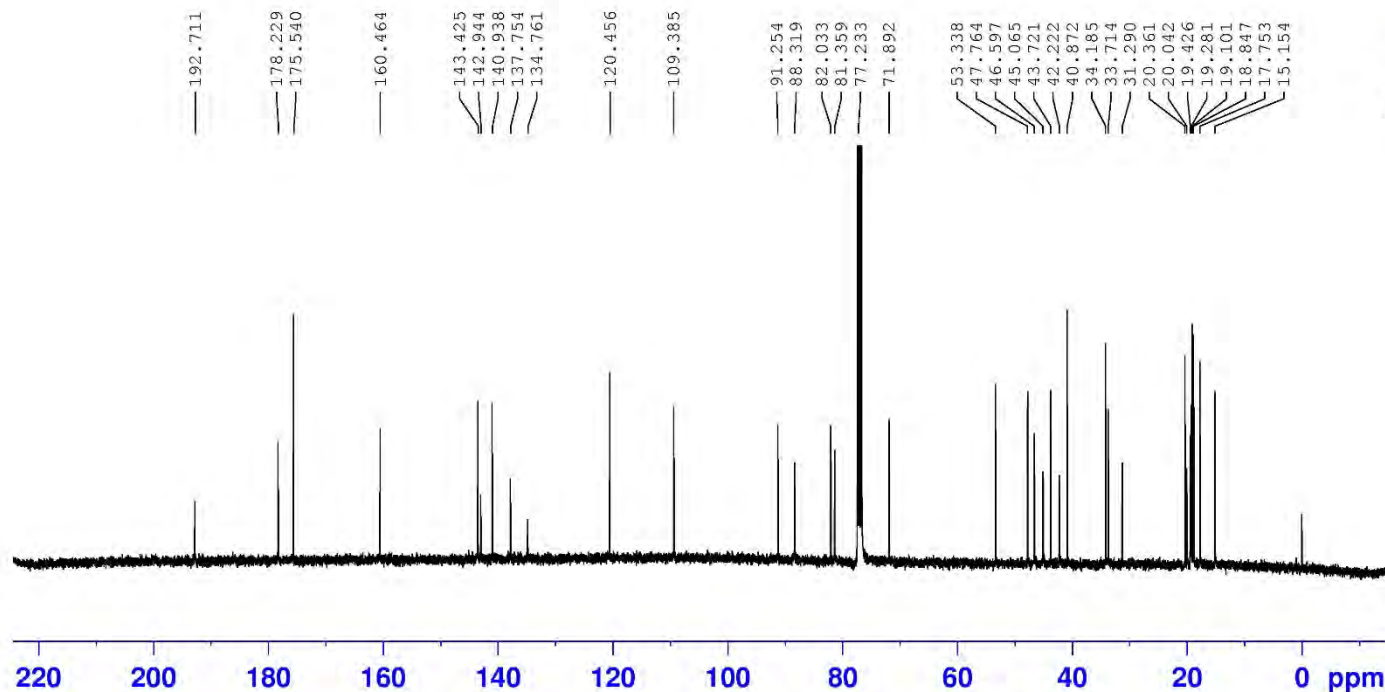
^{13}C NMR (100 MHz) spectrum of compound **2** in CDCl_3



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

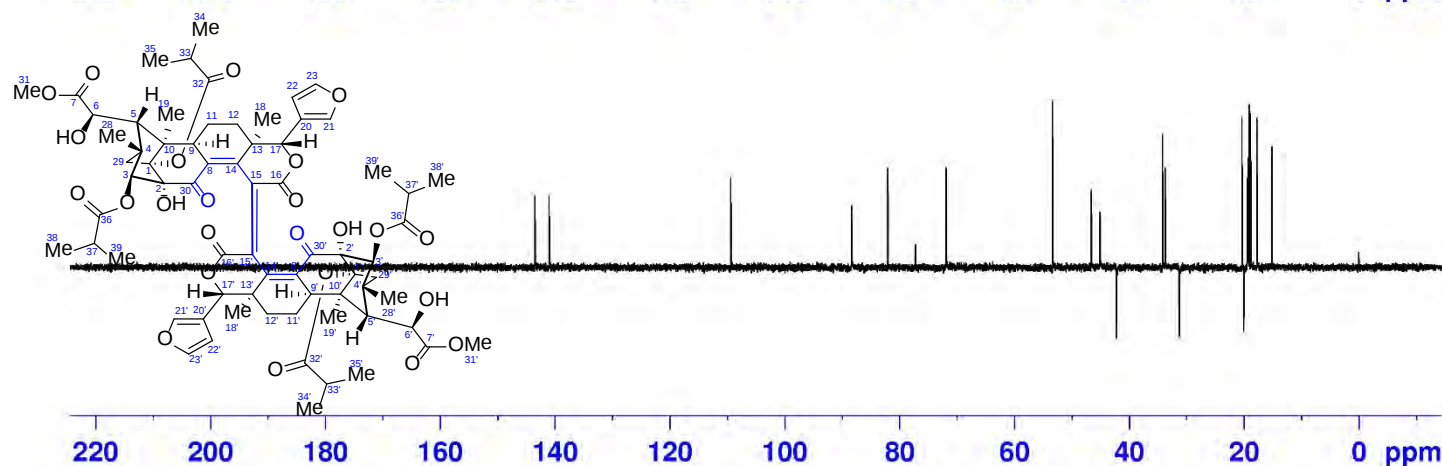


DEPT135 (100 MHz) spectrum of compound **2** in CDCl₃



```

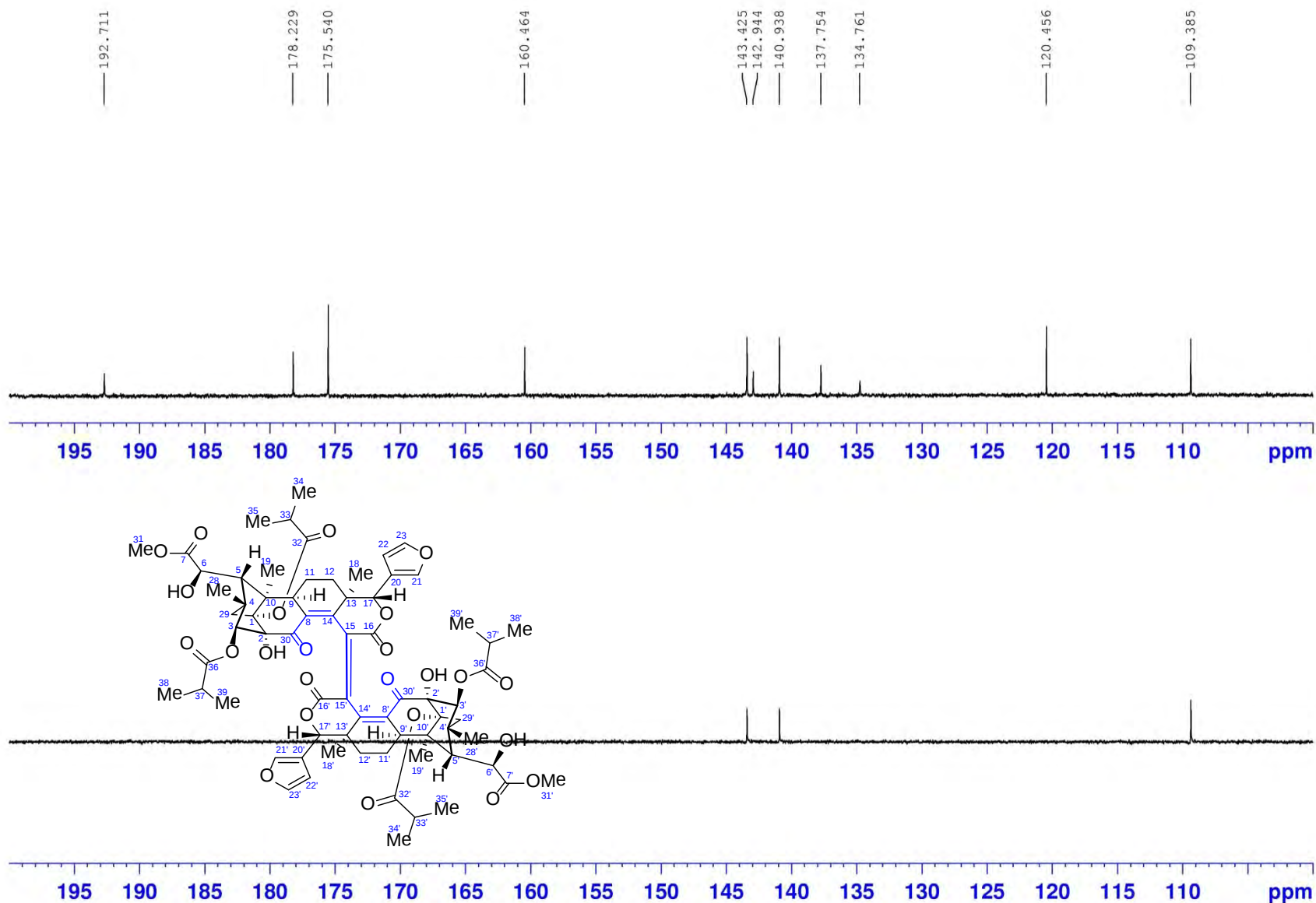
NAME          LWS-42-0
EXPNO         3
PROCNO        1
Date_         20150727
Time          12.29
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       deptsp135
TD            65536
SOLVENT       CDC13
NS            300
DS            4
SWH           24038.461
FIDRES        0.366798
AQ            1.3631988
RG            130.26
DW            20.800
DE            18.00
TE            297.0
CNST2         145.0000000
D1            2.00000000
D2            0.00344828
D12           0.00002000
TD0           1
    
```



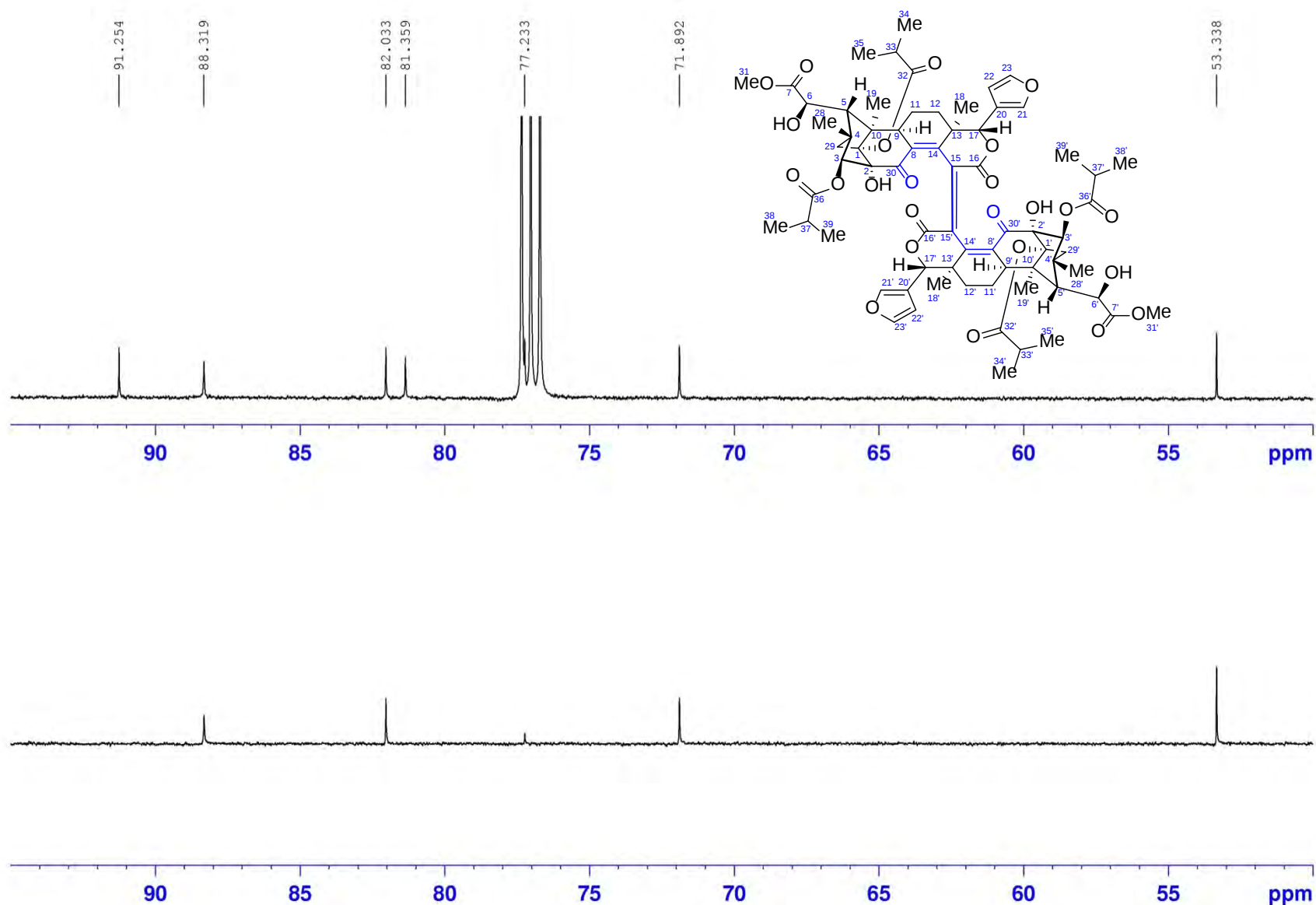
```

===== CHANNEL f1 =====
SF01          100.6233324
NUC1           13C
P1            10.00
P13           2000.00
SI            32768
SF            100.6127685
WDW           EM
SSB           0
LB            1.00
GB            0
PC            1.40
    
```

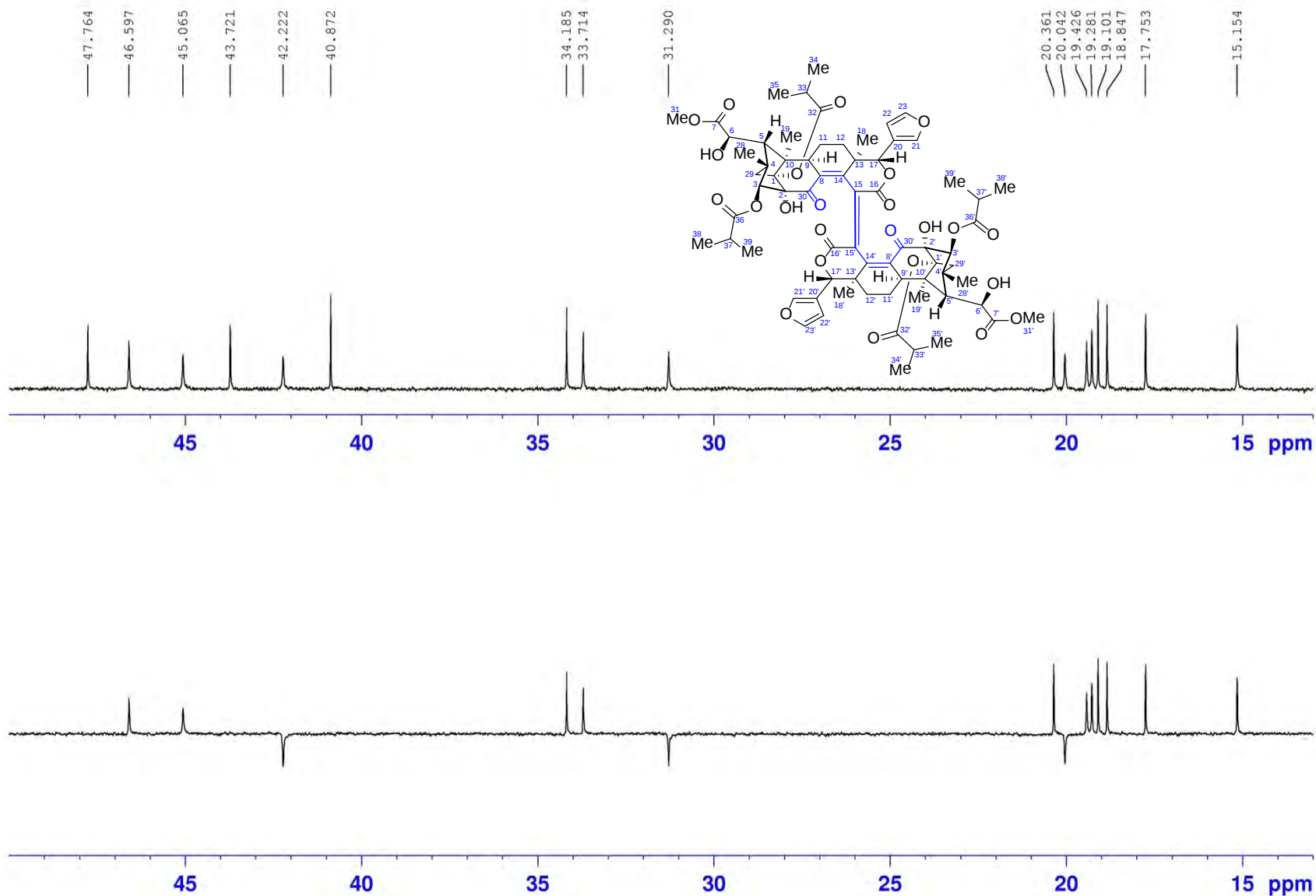
DEPT135 (100 MHz) spectrum of compound **2** in CDCl₃



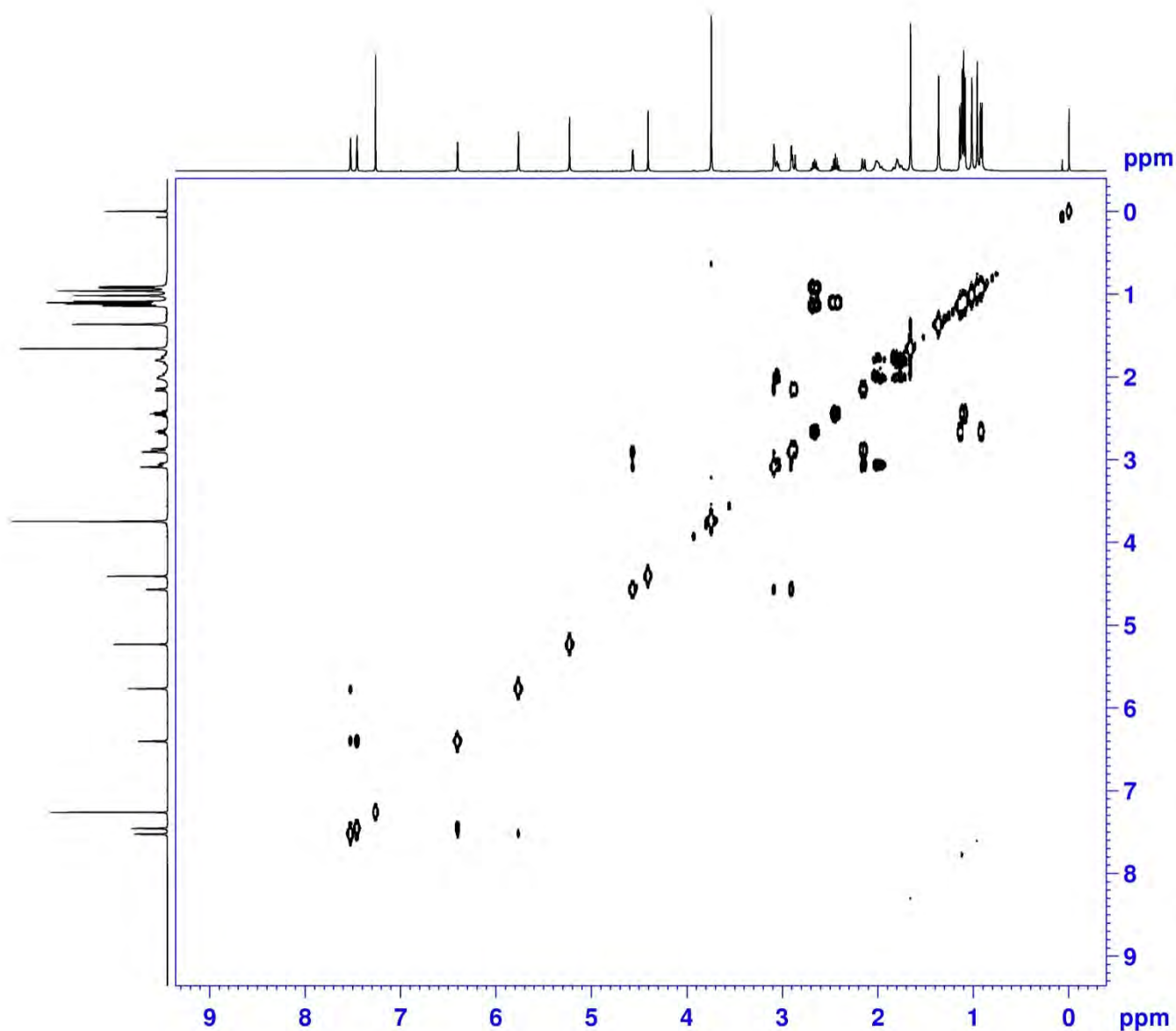
DEPT135 (100 MHz) spectrum of compound **2** in CDCl₃



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



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



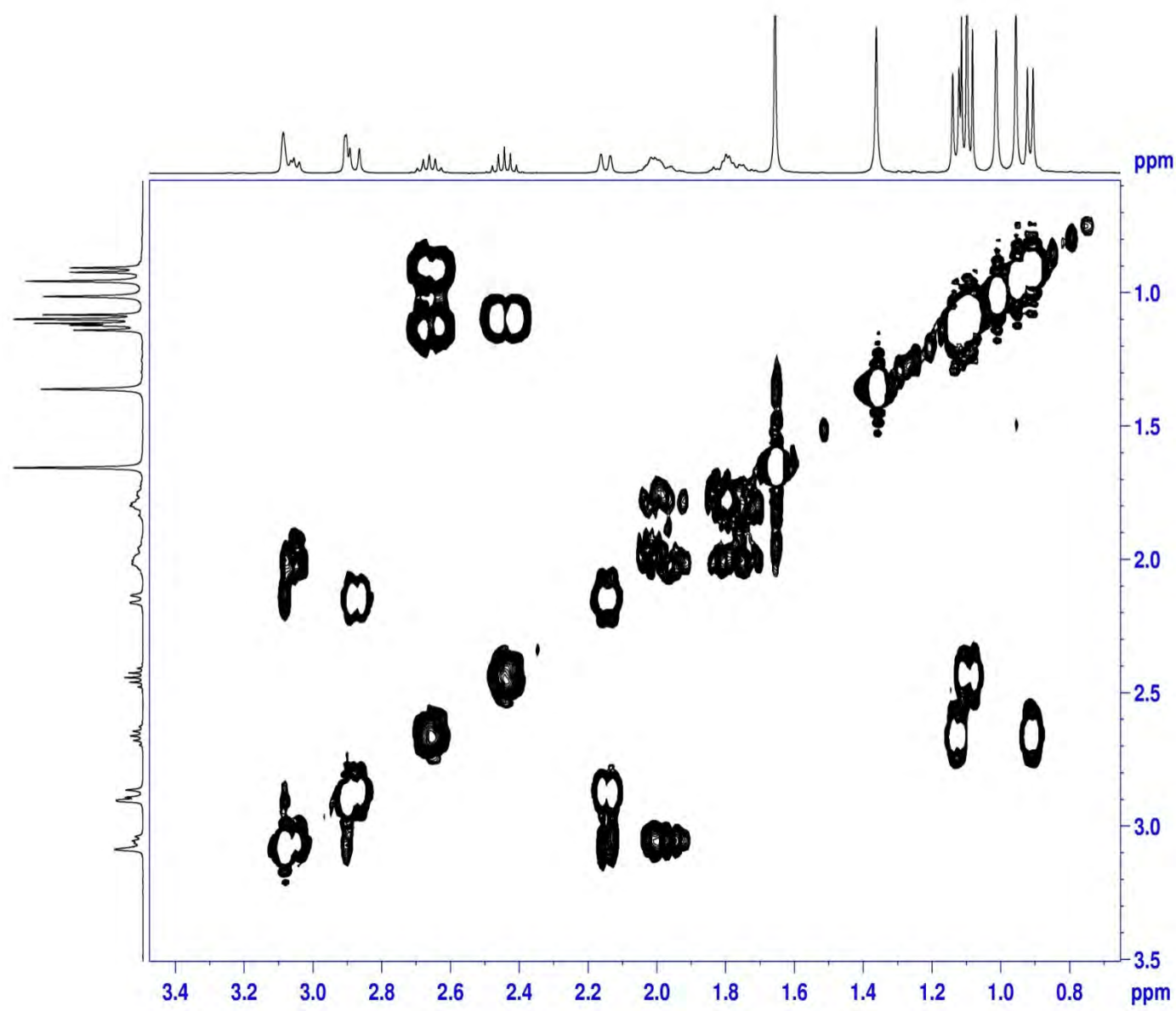
```

NAME                LWS-42-0
EXPNO                4
PROCNO               1
Date_                20150727
Time                 12.30
INSTRUM              spect
PROBHD               5 mm CFPBBO BB
PULPROG              cosygpppgf
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
  
```

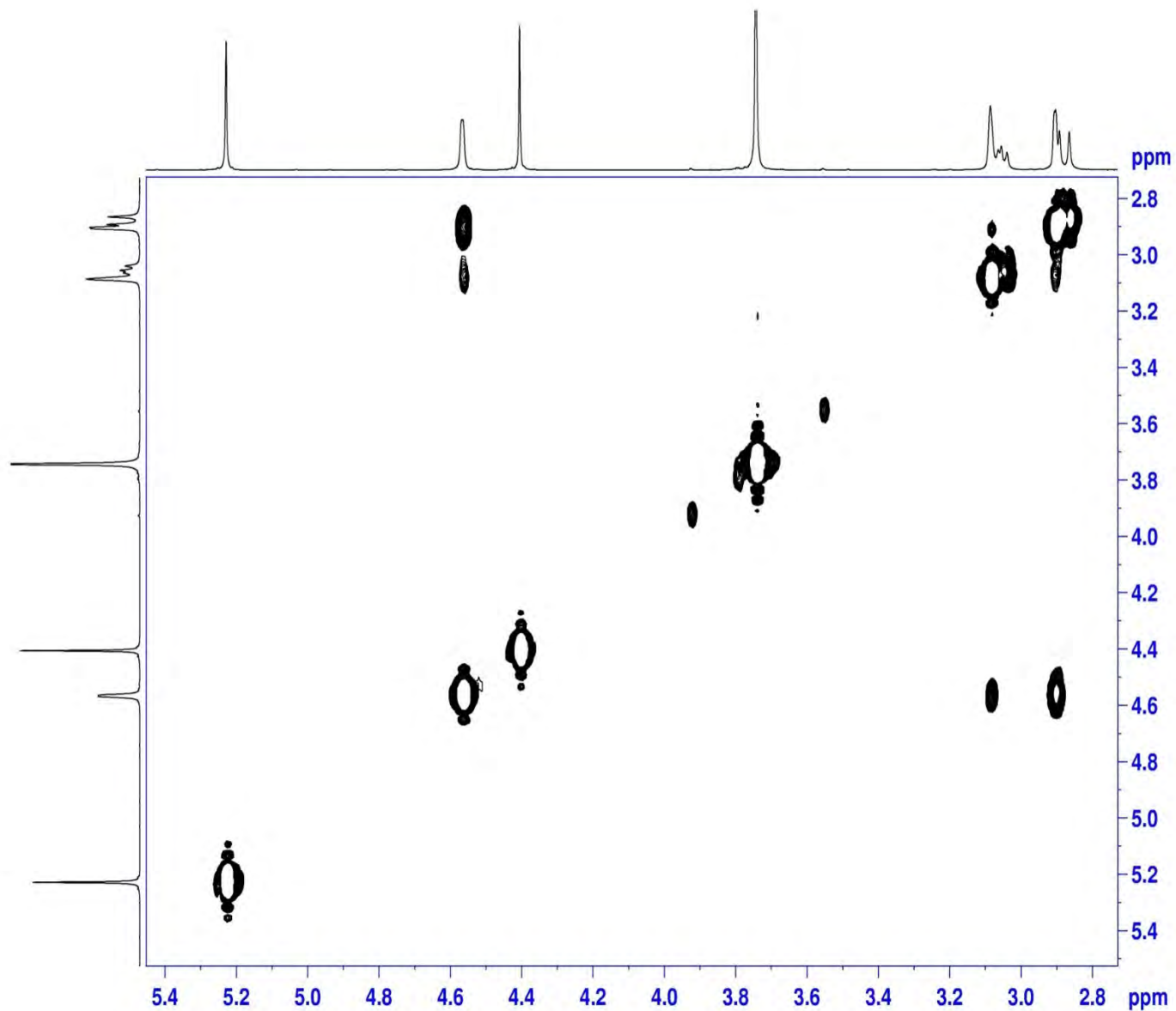
```

===== CHANNEL f1 =====
SFO1                400.1318006 MHz
NUC1                 1H
P0                   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                   400.1300094 MHz
WDW                  QSINE
SSB                   0
LB                   0.00 Hz
GB                   0
PC                   1.40
SI                   1024
MC2                  QF
SF                   400.1300094 MHz
WDW                  QSINE
  
```

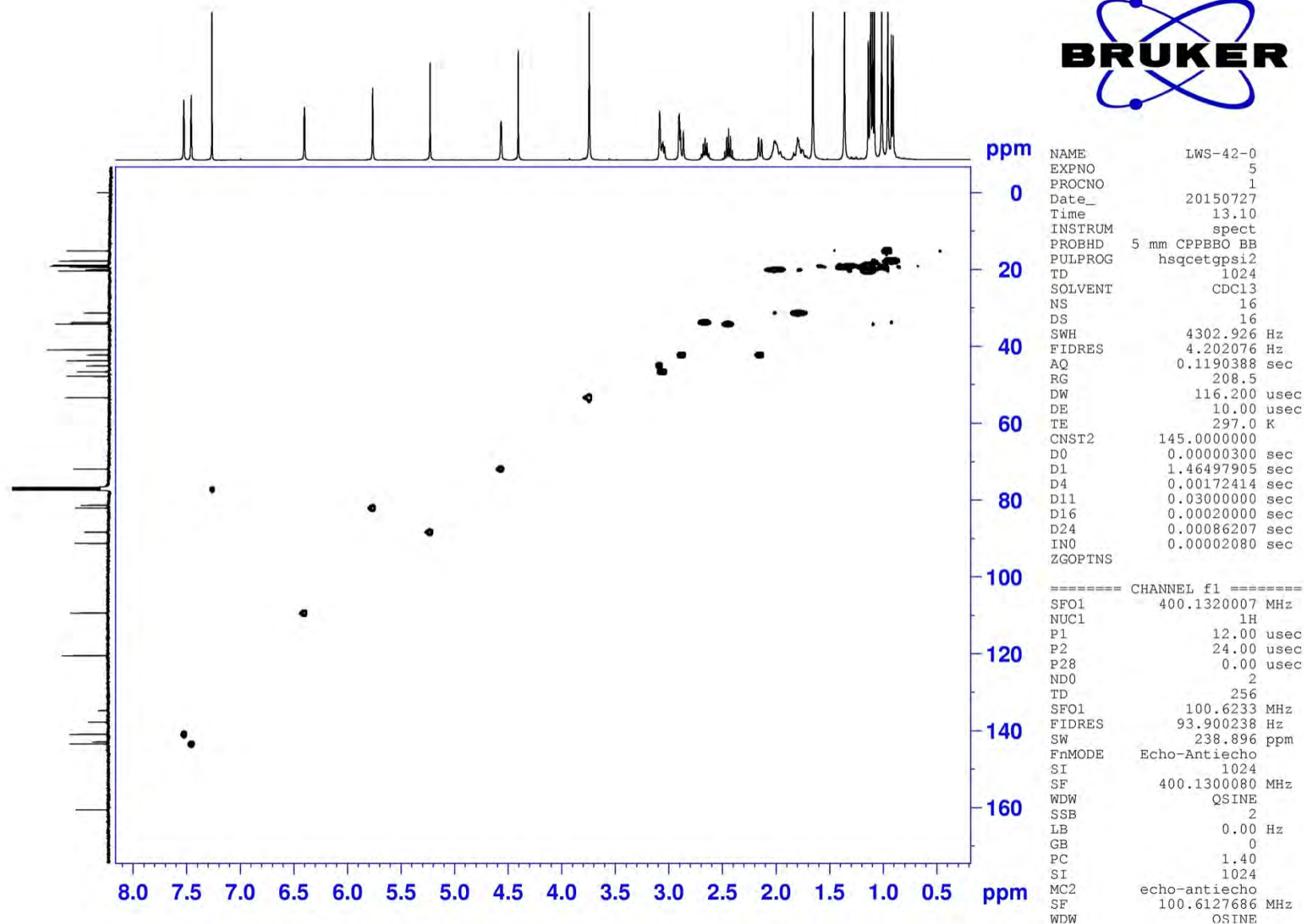
^1H - ^1H COSY (400 MHz) spectrum of compound **2** in CDCl_3



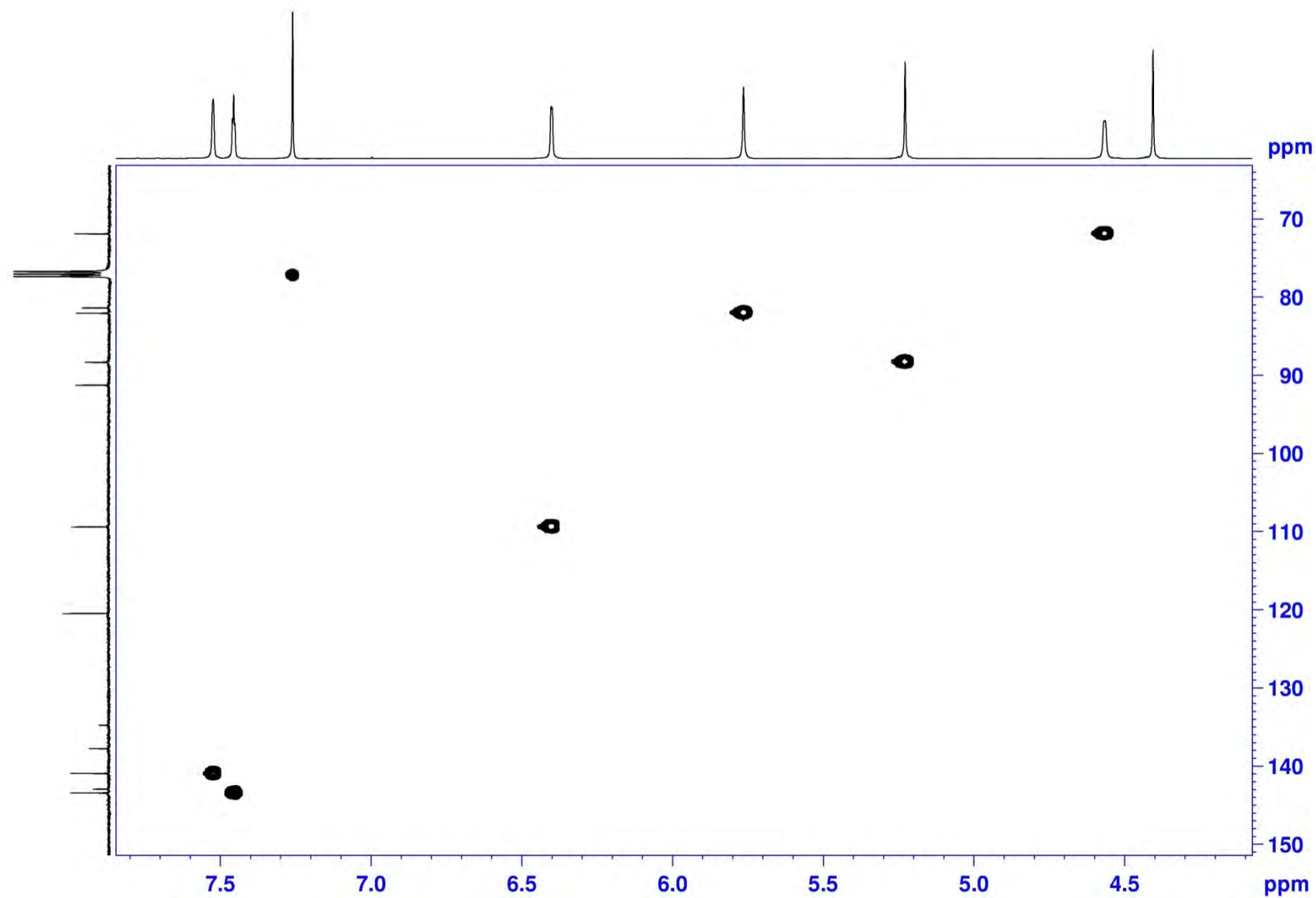
^1H - ^1H COSY (400 MHz) spectrum of compound **2** in CDCl_3



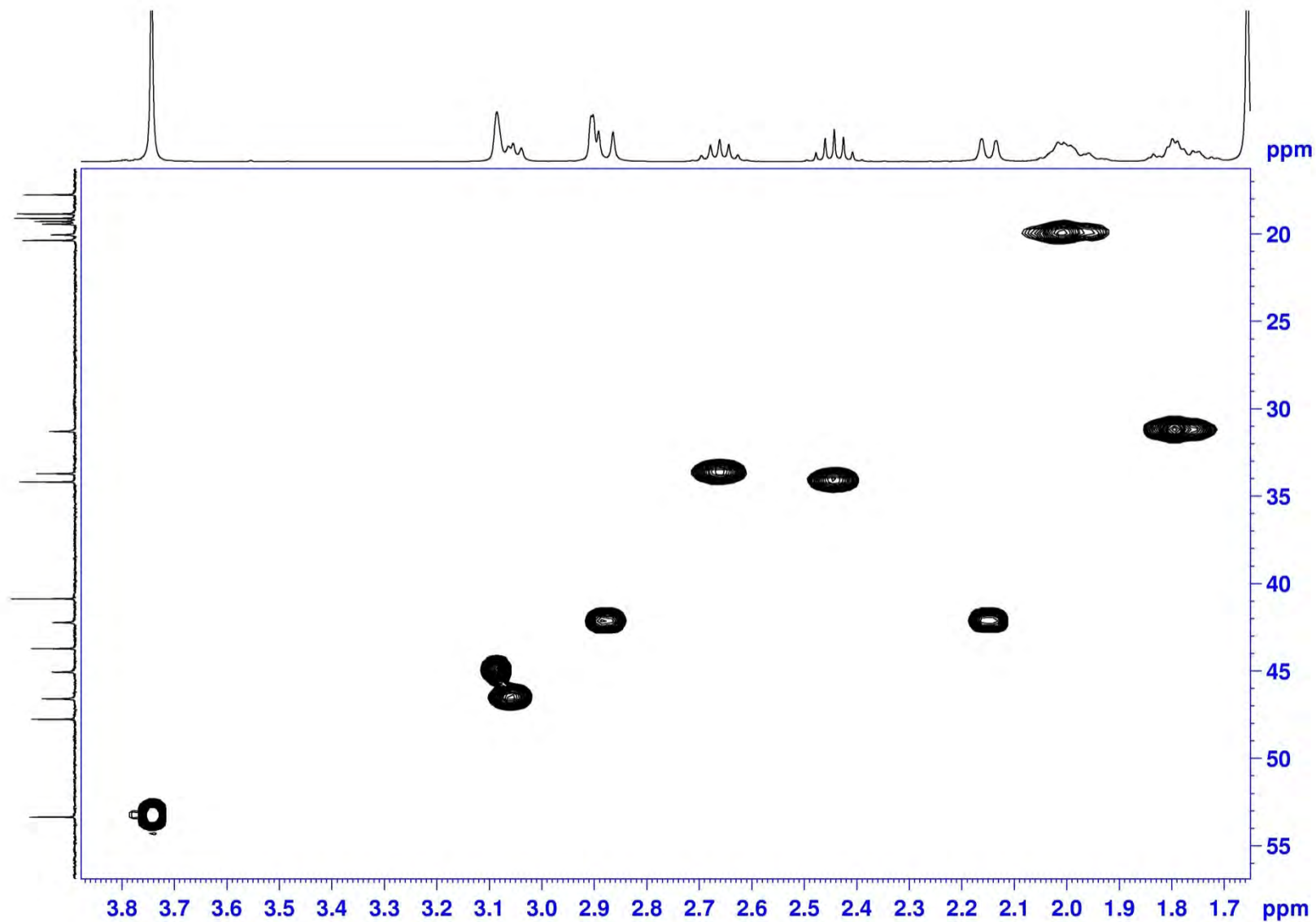
HSQC (400 MHz) spectrum of compound **2** in CDCl₃



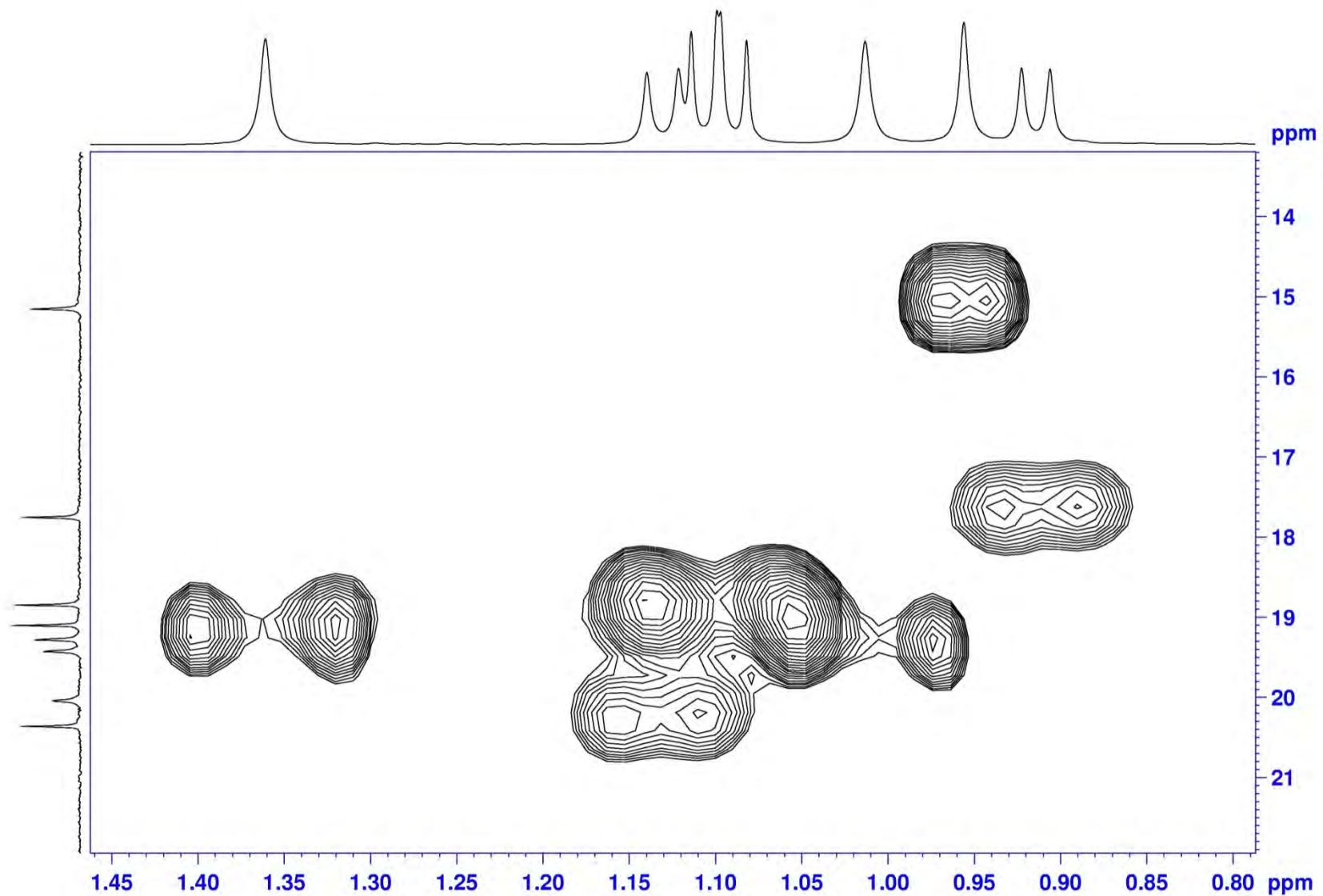
HSQC (400 MHz) spectrum of compound **2** in CDCl₃



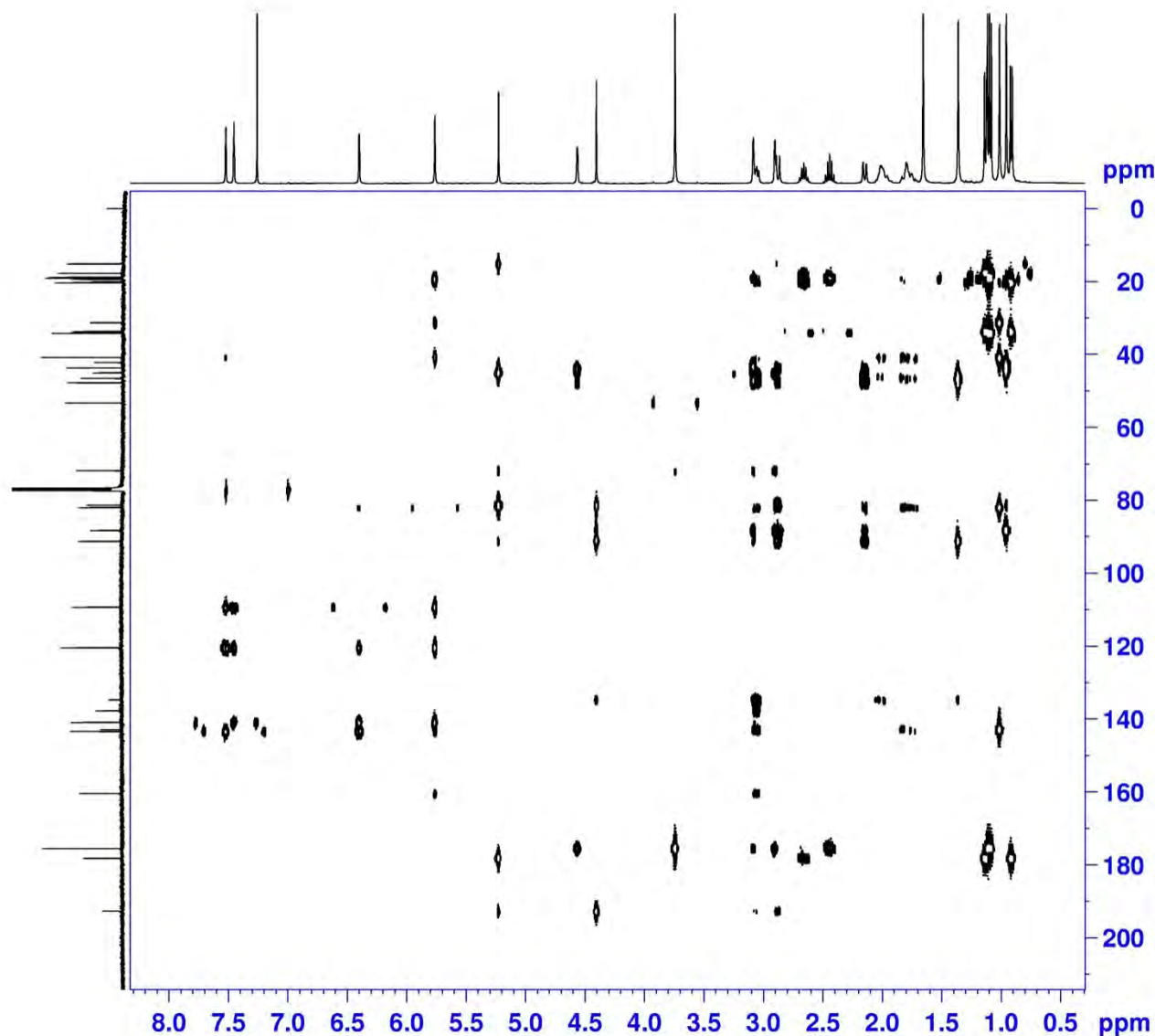
HSQC (400 MHz) spectrum of compound **2** in CDCl₃



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



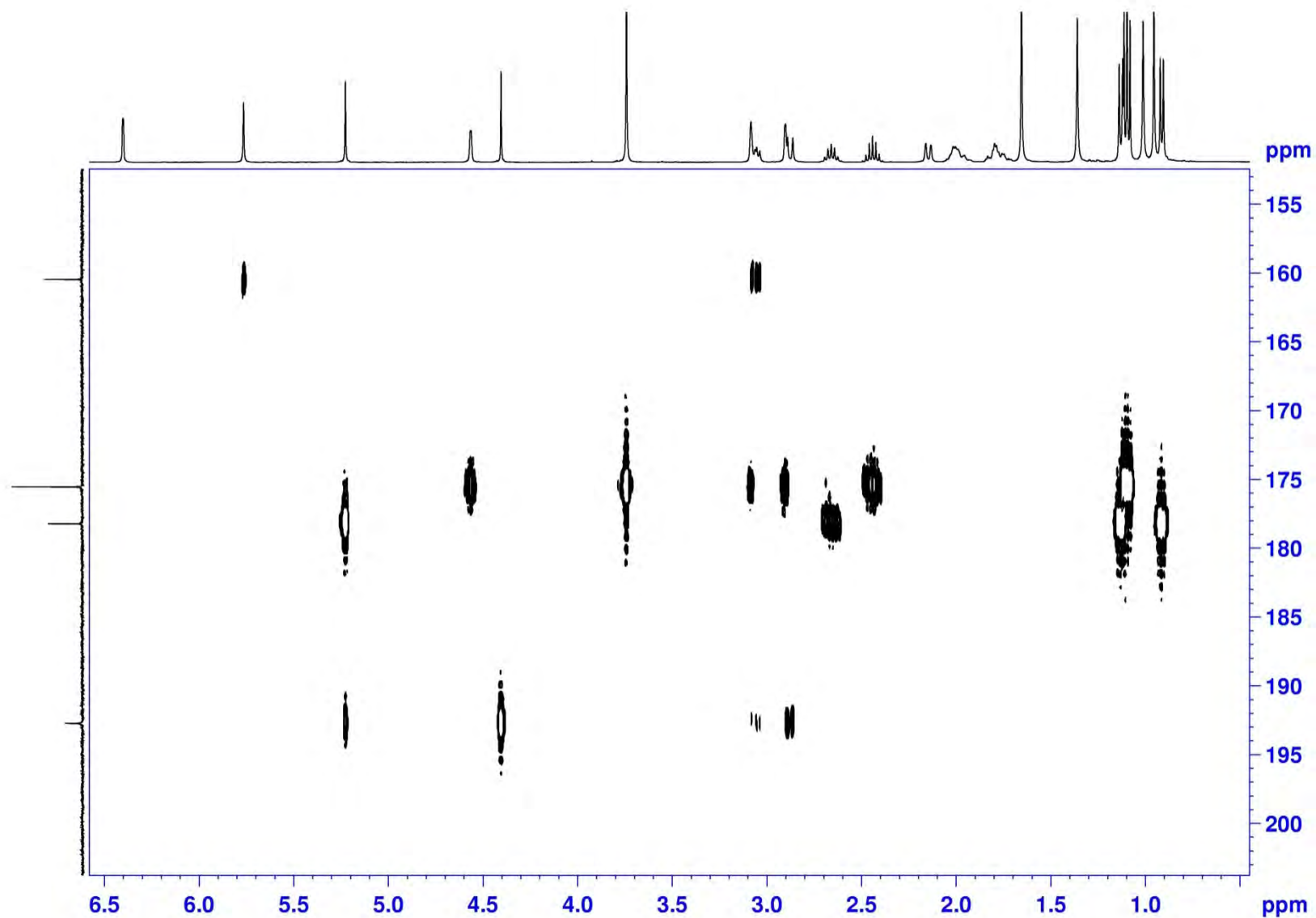
HMBC (400 MHz) spectrum of compound **2** in CDCl₃



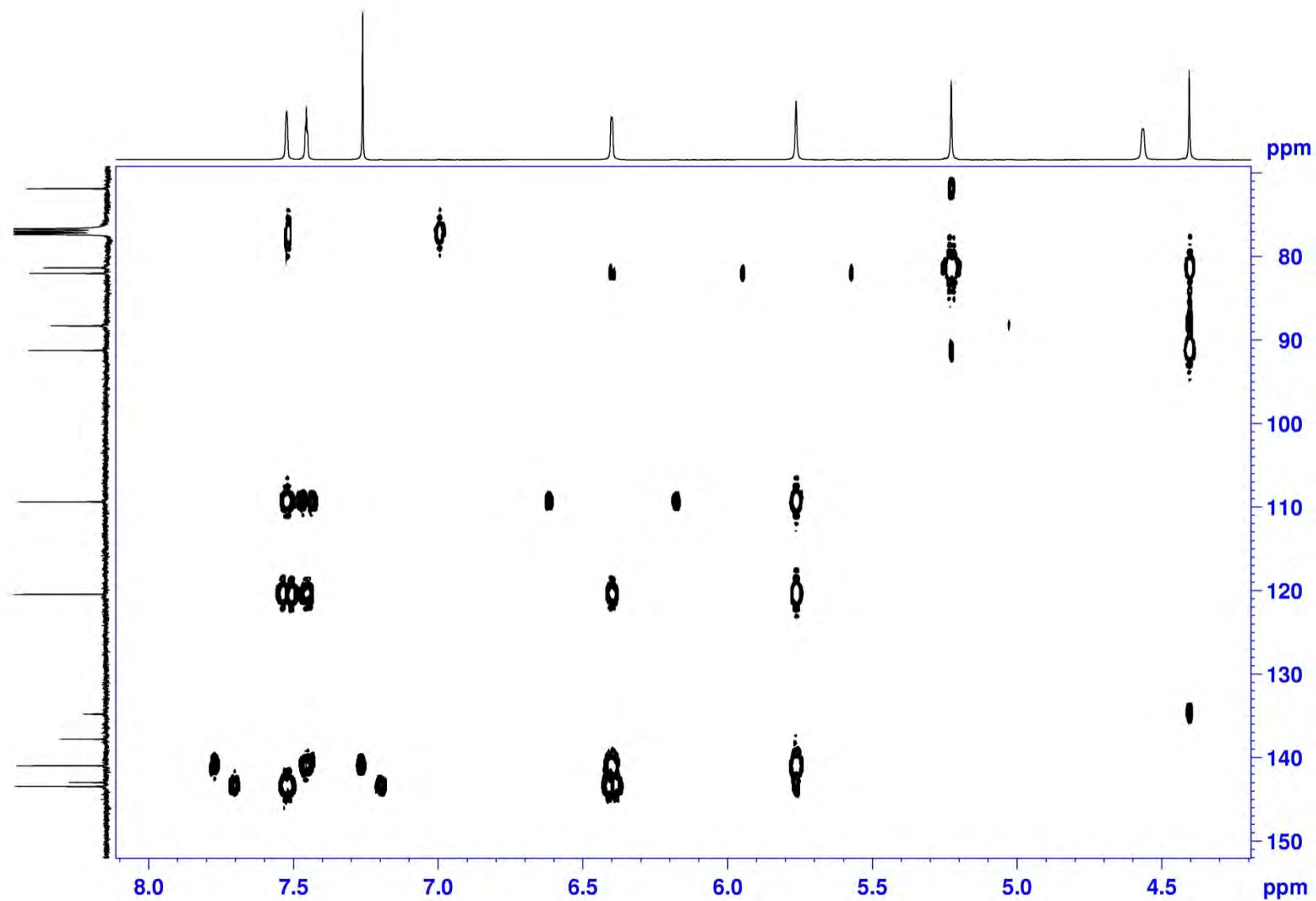
NAME LWS-42-0
 EXPNO 6
 PROCNO 1
 Date_ 20150727
 Time 15.01
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG hmbcgp1pndqf
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 16
 SWH 5197.505 Hz
 FIDRES 1.268922 Hz
 AQ 0.3940852 sec
 RG 208.5
 DW 96.200 usec
 DE 10.00 usec
 TE 297.0 K
 CNST2 145.0000000
 CNST13 10.0000000
 D0 0.00000300 sec
 D1 1.50000000 sec
 D2 0.00344828 sec
 D6 0.05000000 sec
 D16 0.00020000 sec
 IN0 0.00002080 sec

===== CHANNEL f1 =====
 SFO1 400.1323208 MHz
 NUC1 1H
 P1 12.00 usec
 P2 24.00 usec
 ND0 2
 TD 128
 SFO1 100.6233 MHz
 FIDRES 187.800476 Hz
 SW 238.896 ppm
 FnmODE QF
 SI 2048
 SF 400.1300094 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 QF
 SF 100.6127685 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

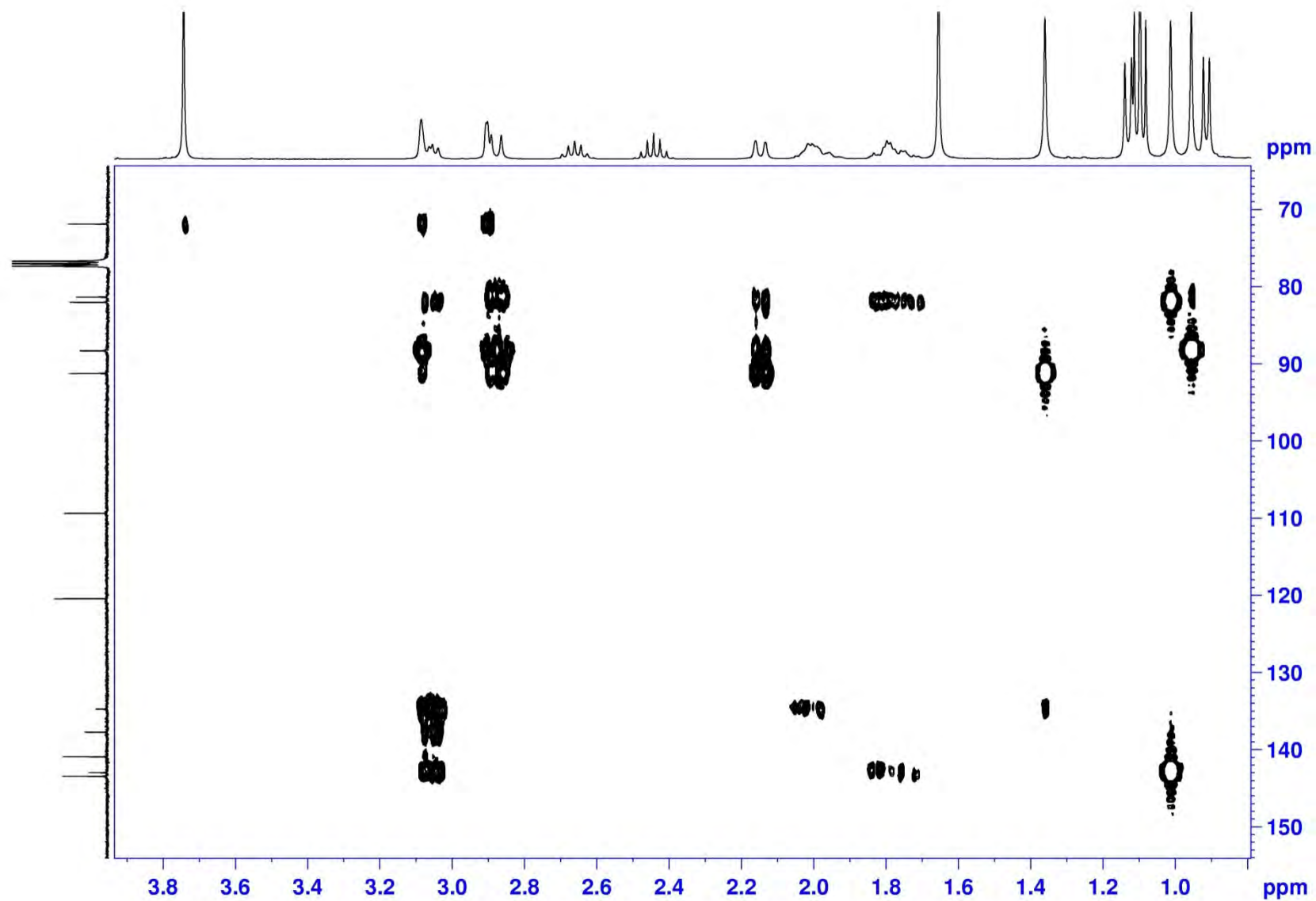
HMBC (400 MHz) spectrum of compound **2** in CDCl₃



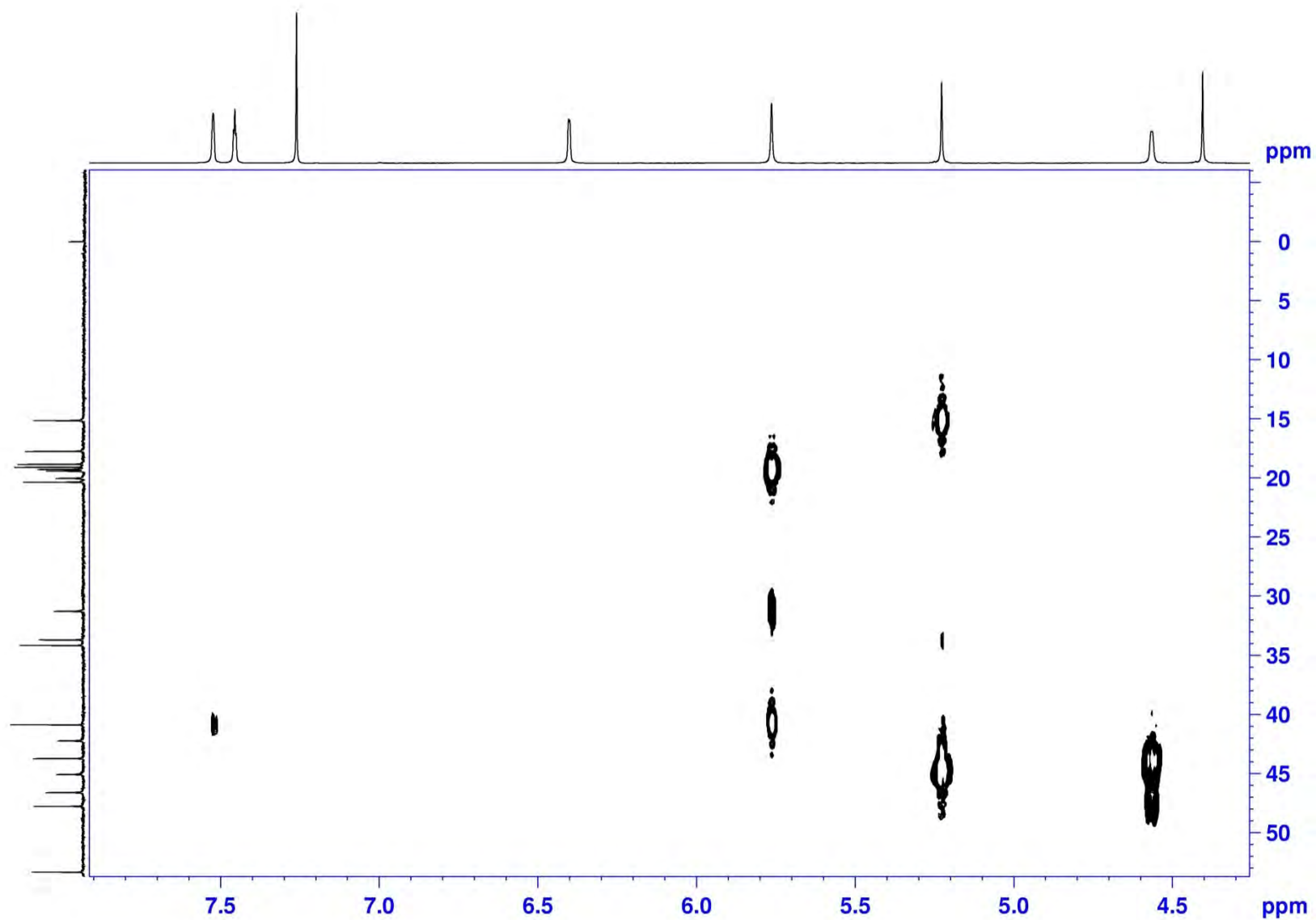
HMBC (400 MHz) spectrum of compound **2** in CDCl₃



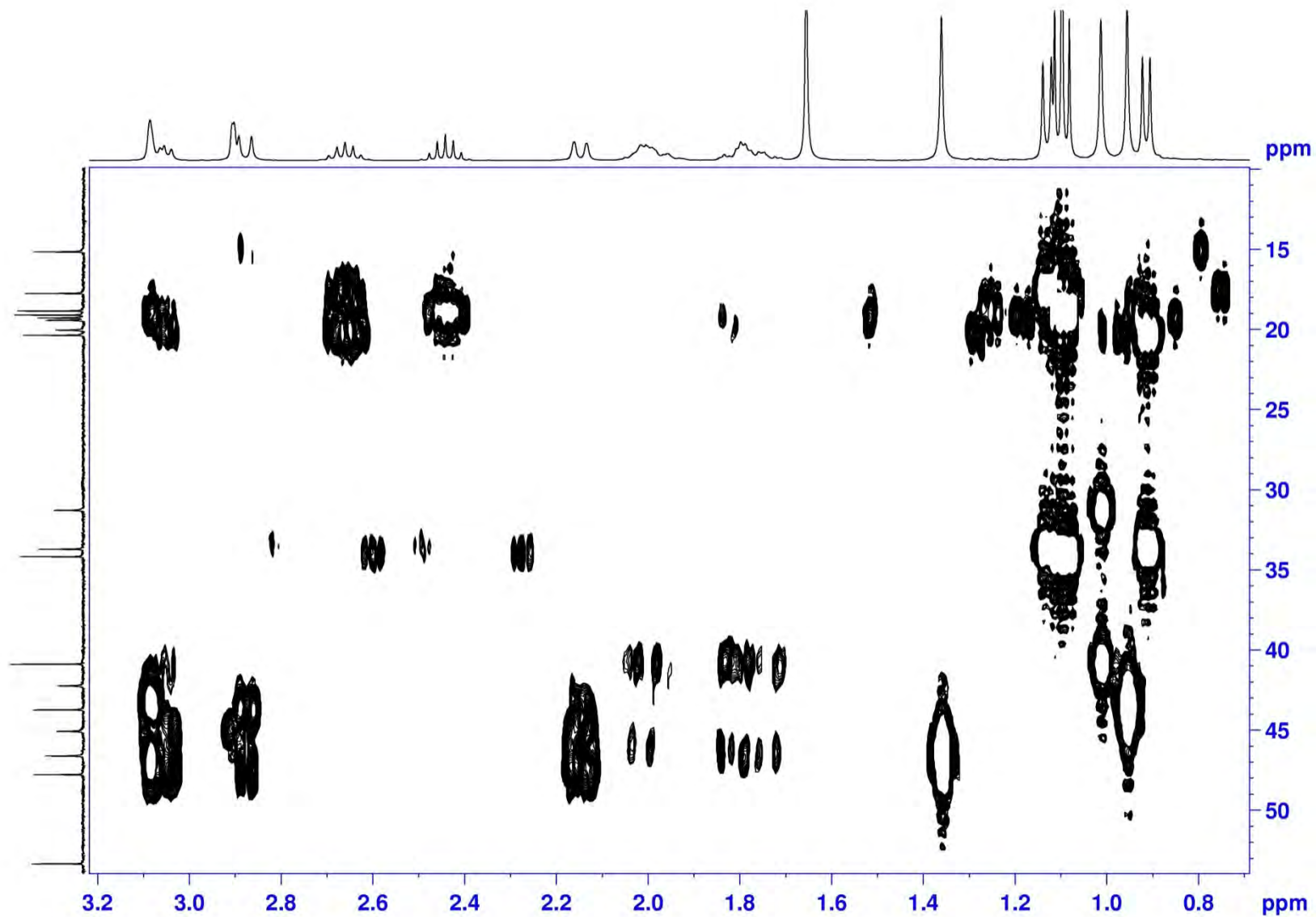
HMBC (400 MHz) spectrum of compound **2** in CDCl₃



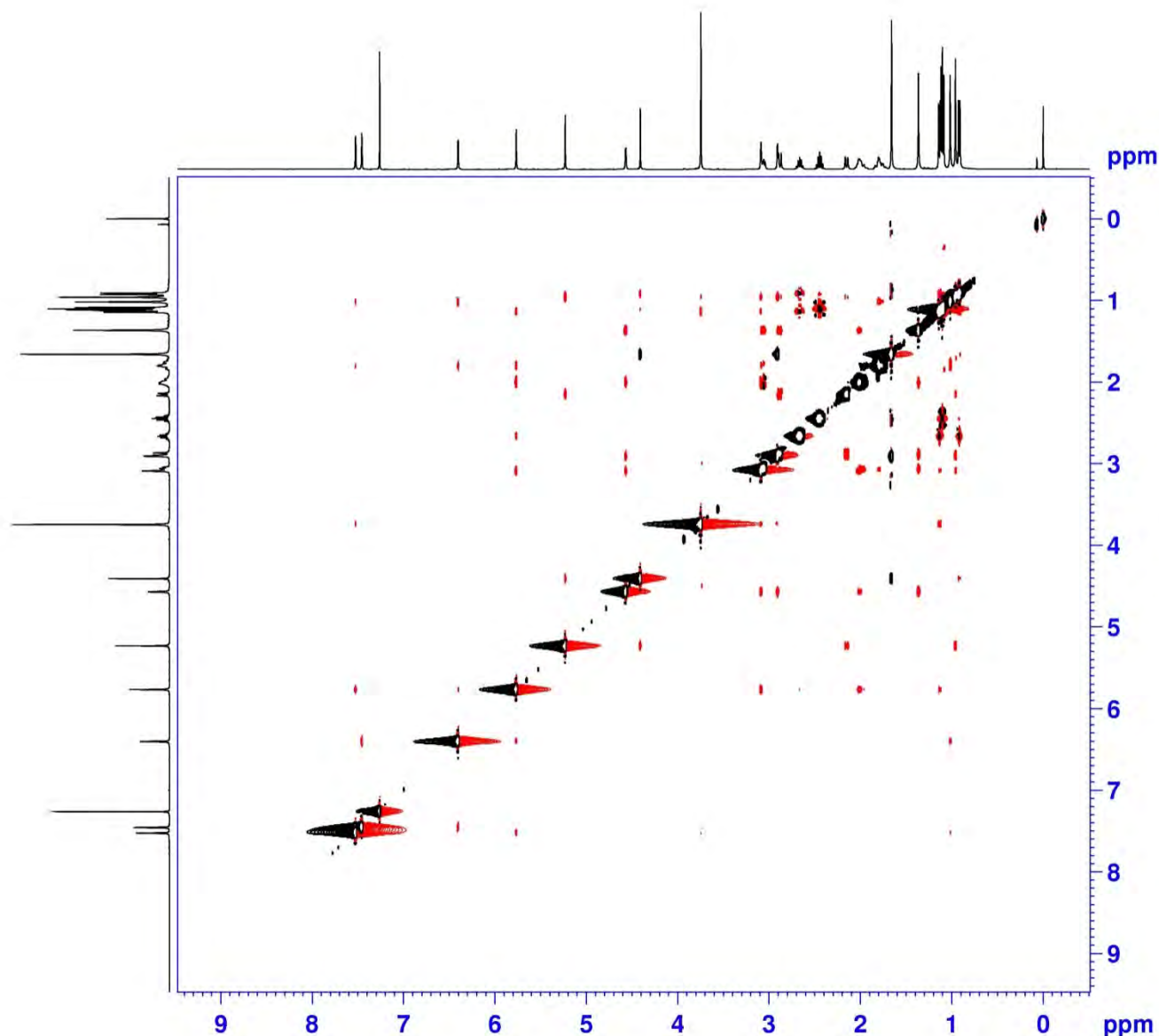
HMBC (400 MHz) spectrum of compound **2** in CDCl₃



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



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



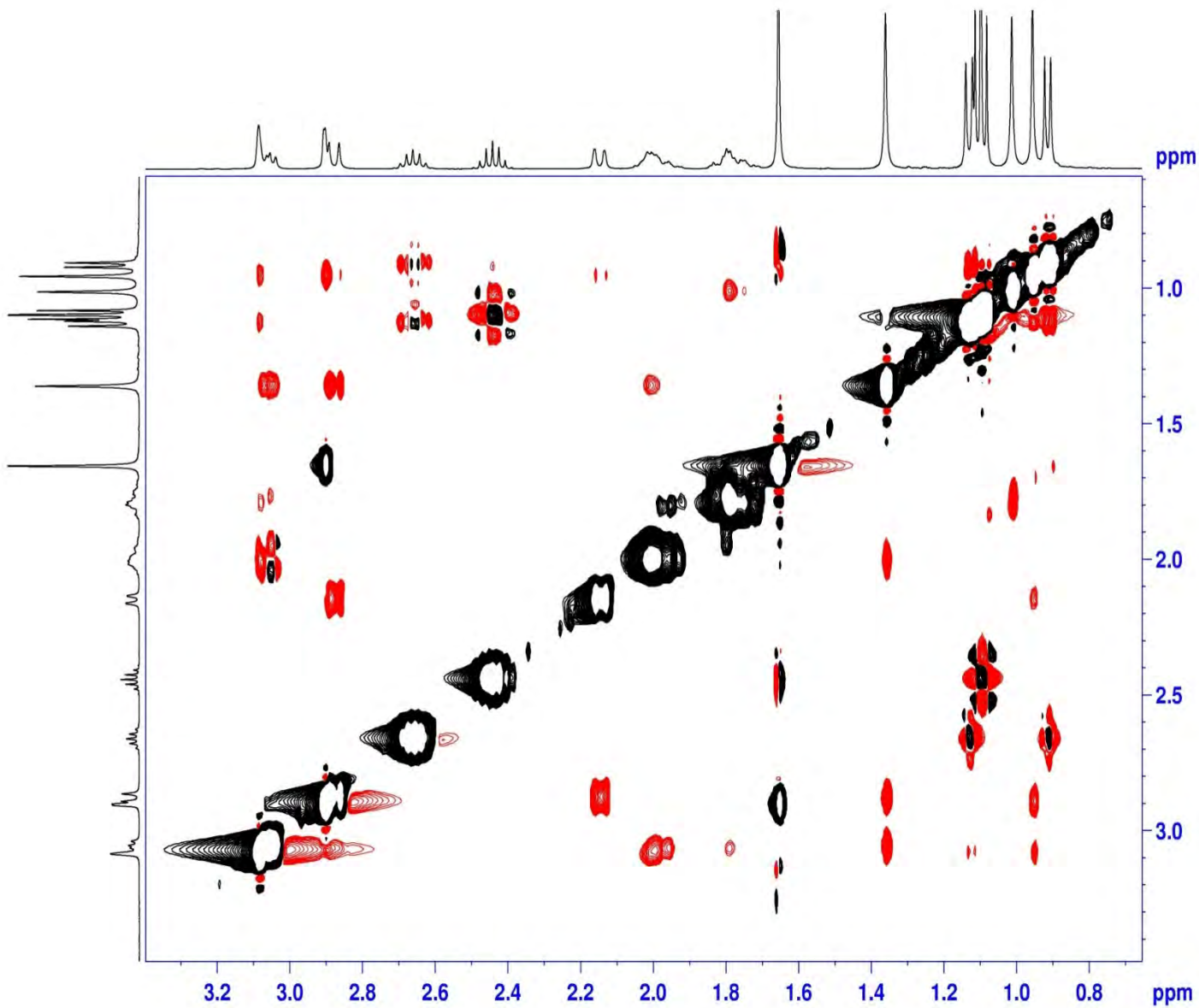
```

NAME           LWS-42-0
EXPNO           7
PROCNO          1
Date_           20150727
Time            17.16
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              0.00010972 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
    
```

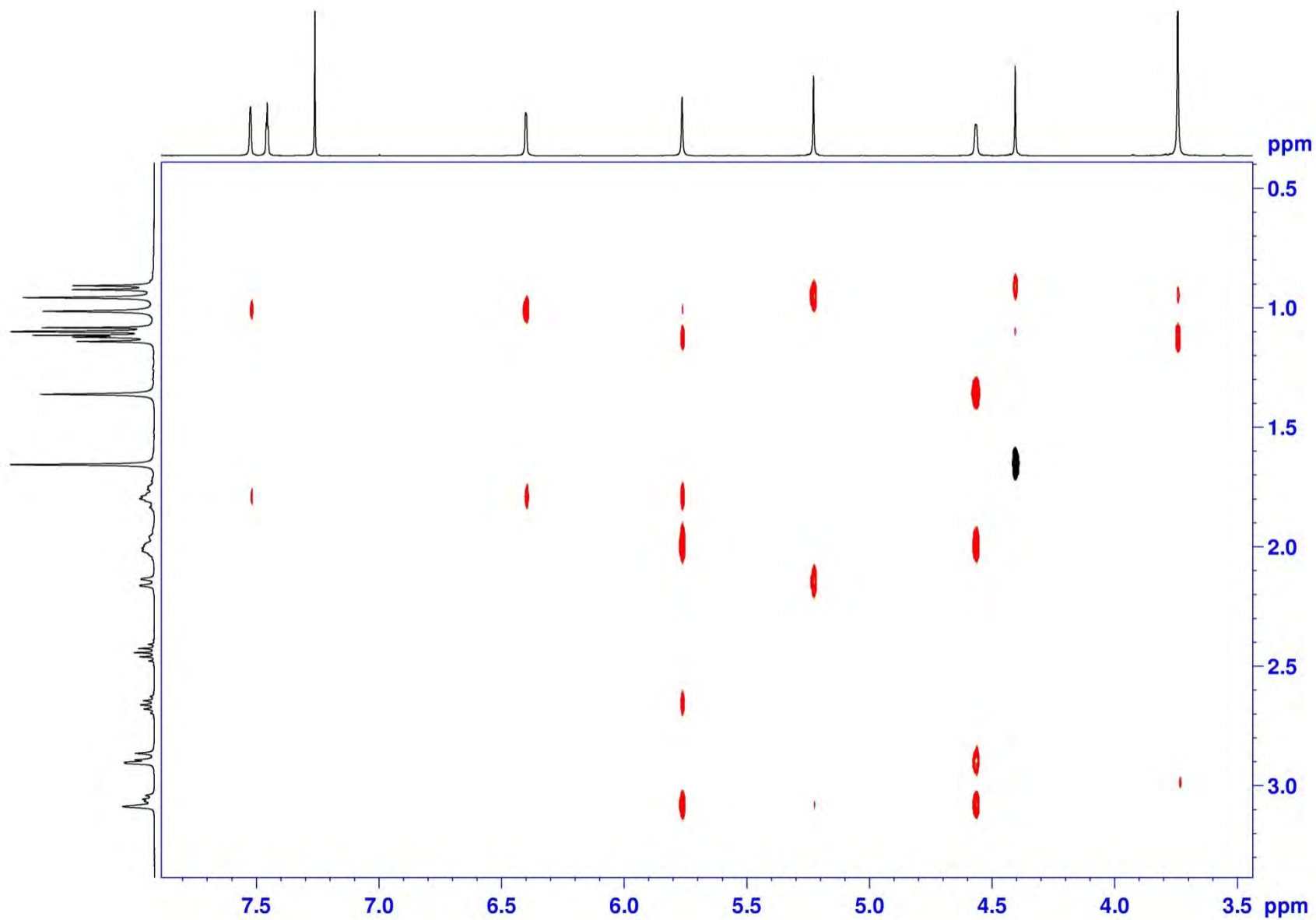
```

===== 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              400.1300098 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
    
```

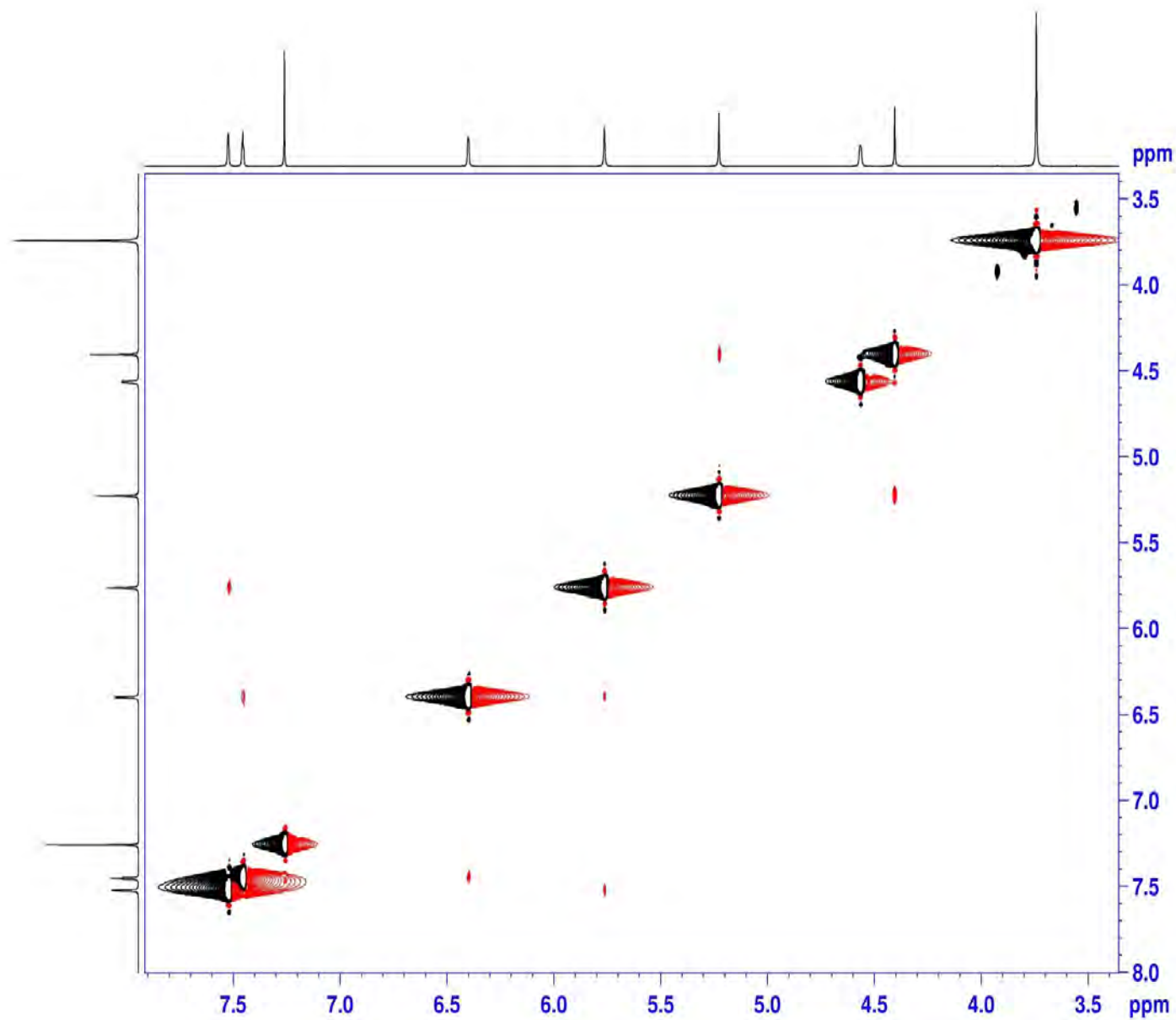
NOESY (400 MHz) spectrum of compound **2** in CDCl_3



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



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

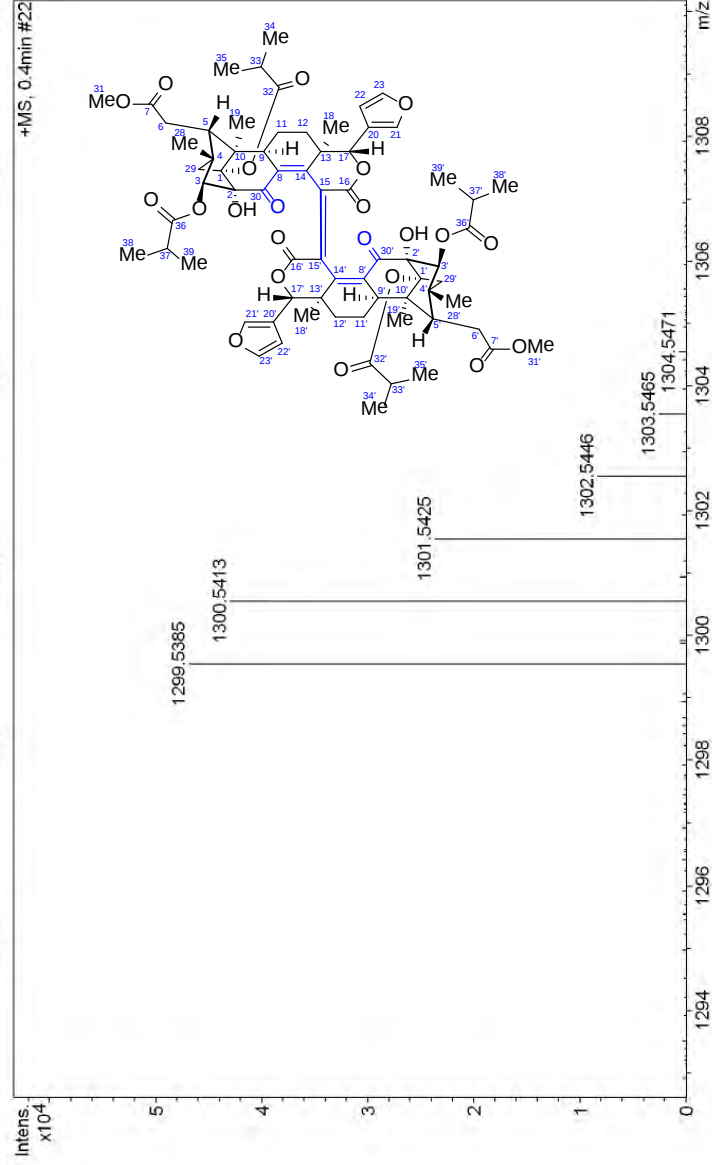
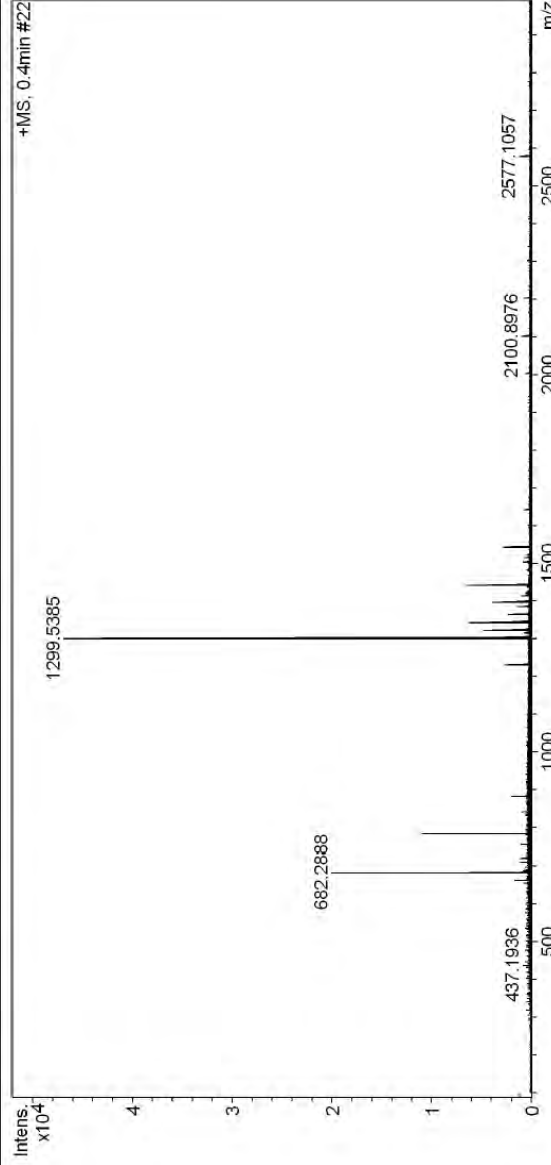


HR-ESIMS for compound 2'

Generic Display Report

Analysis Info

Analysis Name: D:\Data\MS\data\201607\liwanshan_37-0_pos_21_01_2190.d
 Method: LC_Direct Infusion_pos_100-3000mz.m
 Sample Name: liwanshan_37-0_pos
 Comment:
 Acquisition Date: 7/15/2016 5:04:35 PM
 Operator: SCSIO
 Instrument: maXis



HR-ESIMS for compound 2'

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\MS\data\201607\liwanshan_37-0_pos_21_01_2190.d
 Method LC_Direct Infusion_pos_100-3000mz.m
 Sample Name liwanshan_37-0_pos
 Comment

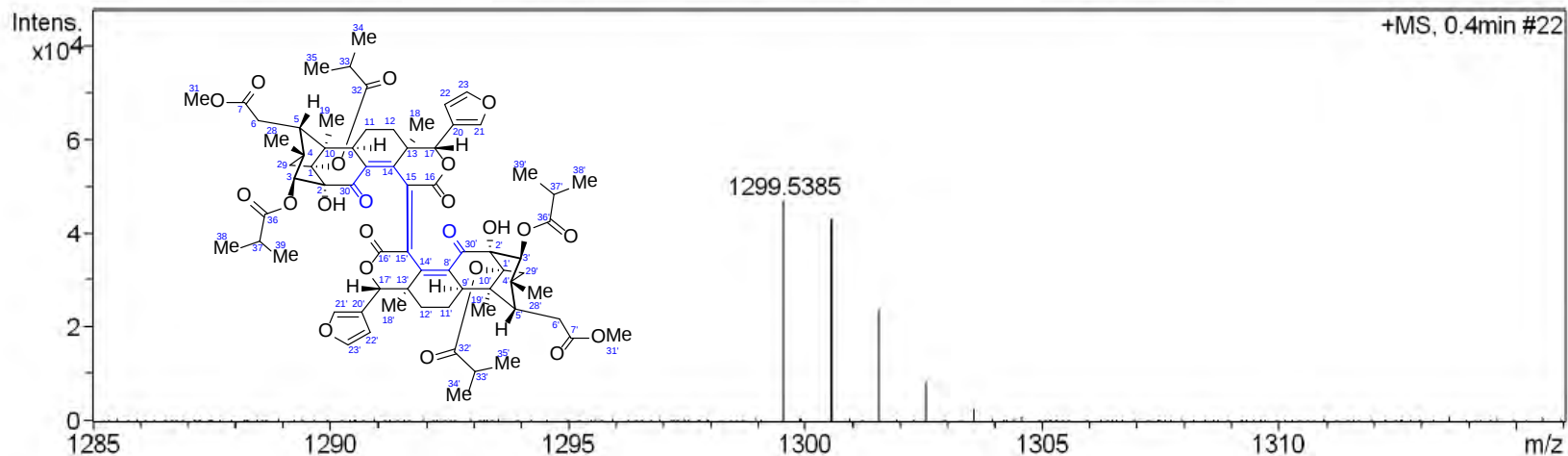
Acquisition Date 7/15/2016 5:04:35 PM

Operator SCSIO

Instrument / Ser# maXis 29

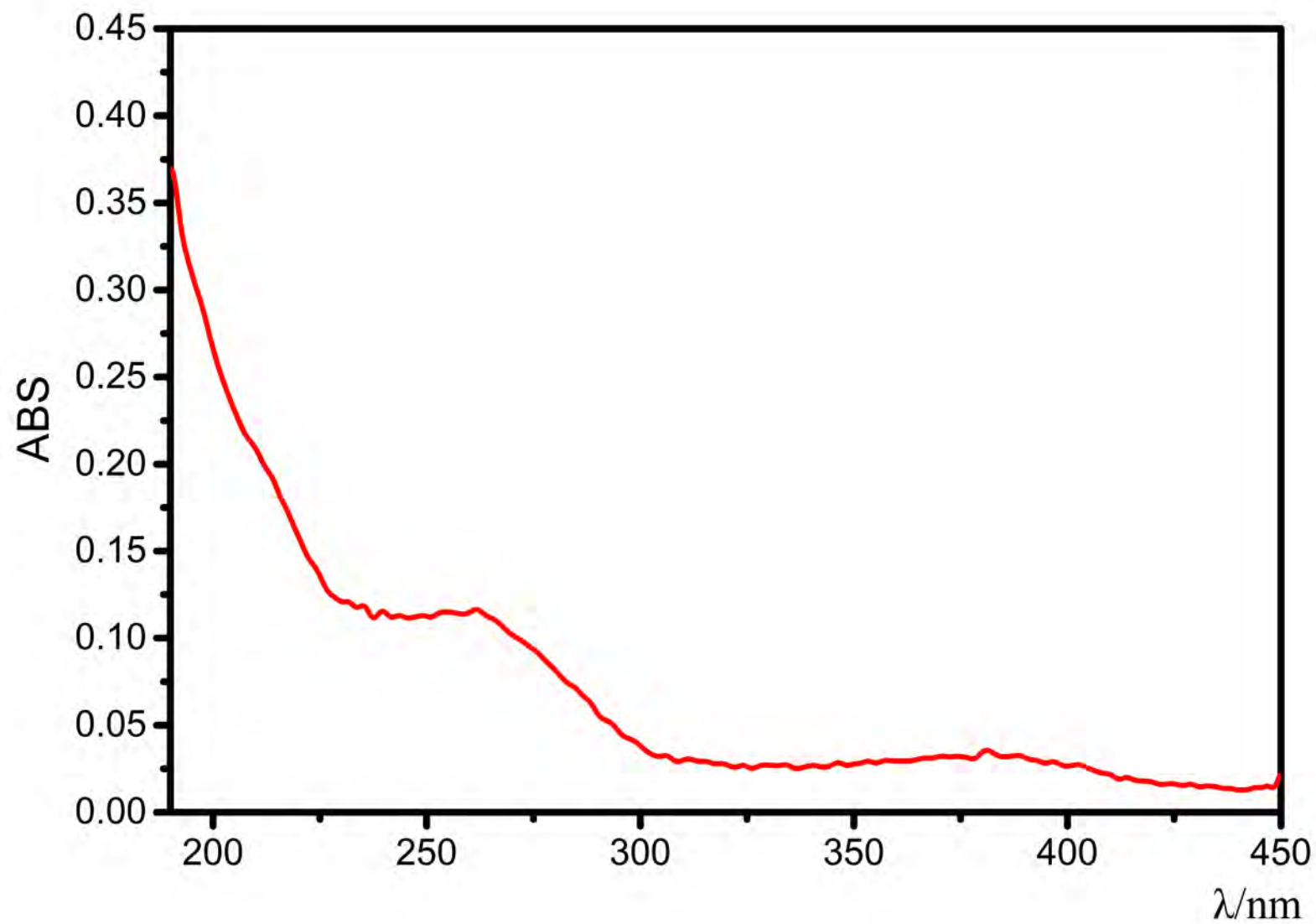
Acquisition Parameter

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	3000 m/z	Set Collision Cell RF	1800.0 Vpp	Set Divert Valve	Waste



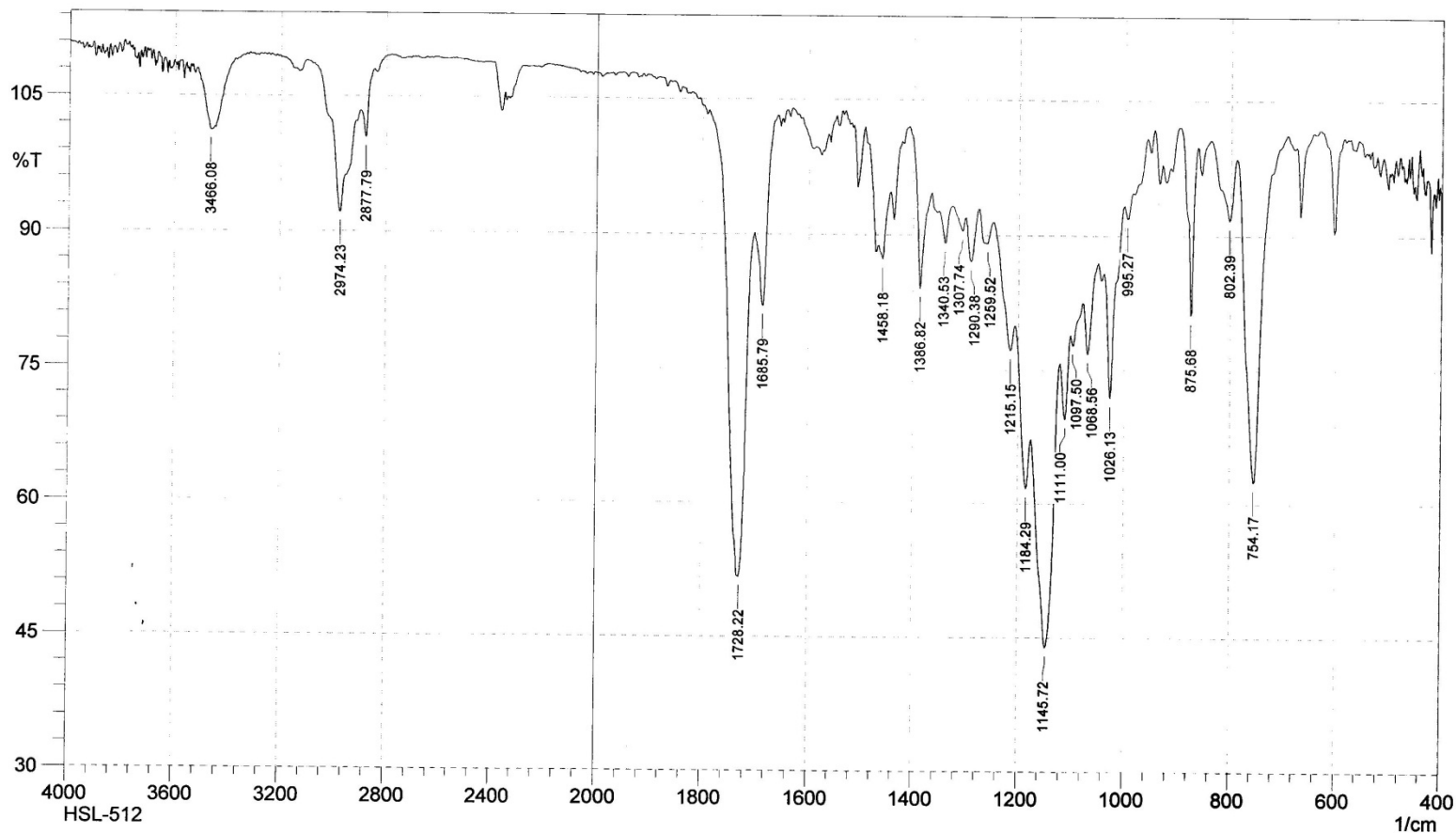
Meas. m/z	#	Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
1299.5385	1	C 70 H 84 Na O 22	100.00	1299.5346	-3.0	-3.9	102.5	28.5	even	ok

UV spectrum for compound **2'** in CHCl_3



IR spectrum for compound 2'

SHIMADZU

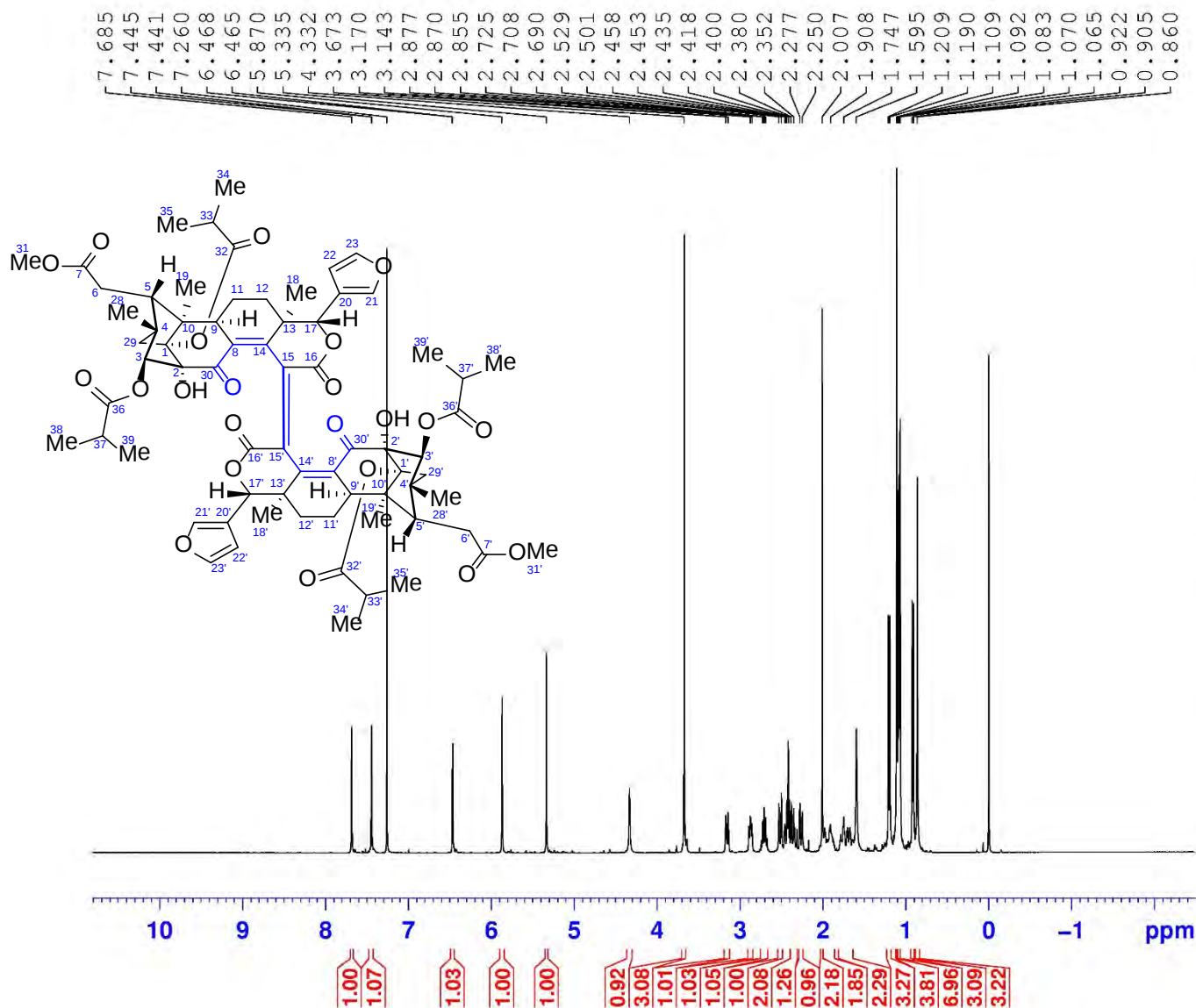


Sample name: 37-01 (2')
F:\liwanshan\20180226\37-
01.smf

Scan number: 25
Resolution: 4 [1/cm]

Data: 2018-2-26 13:35:13
Operator: SCSIO

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



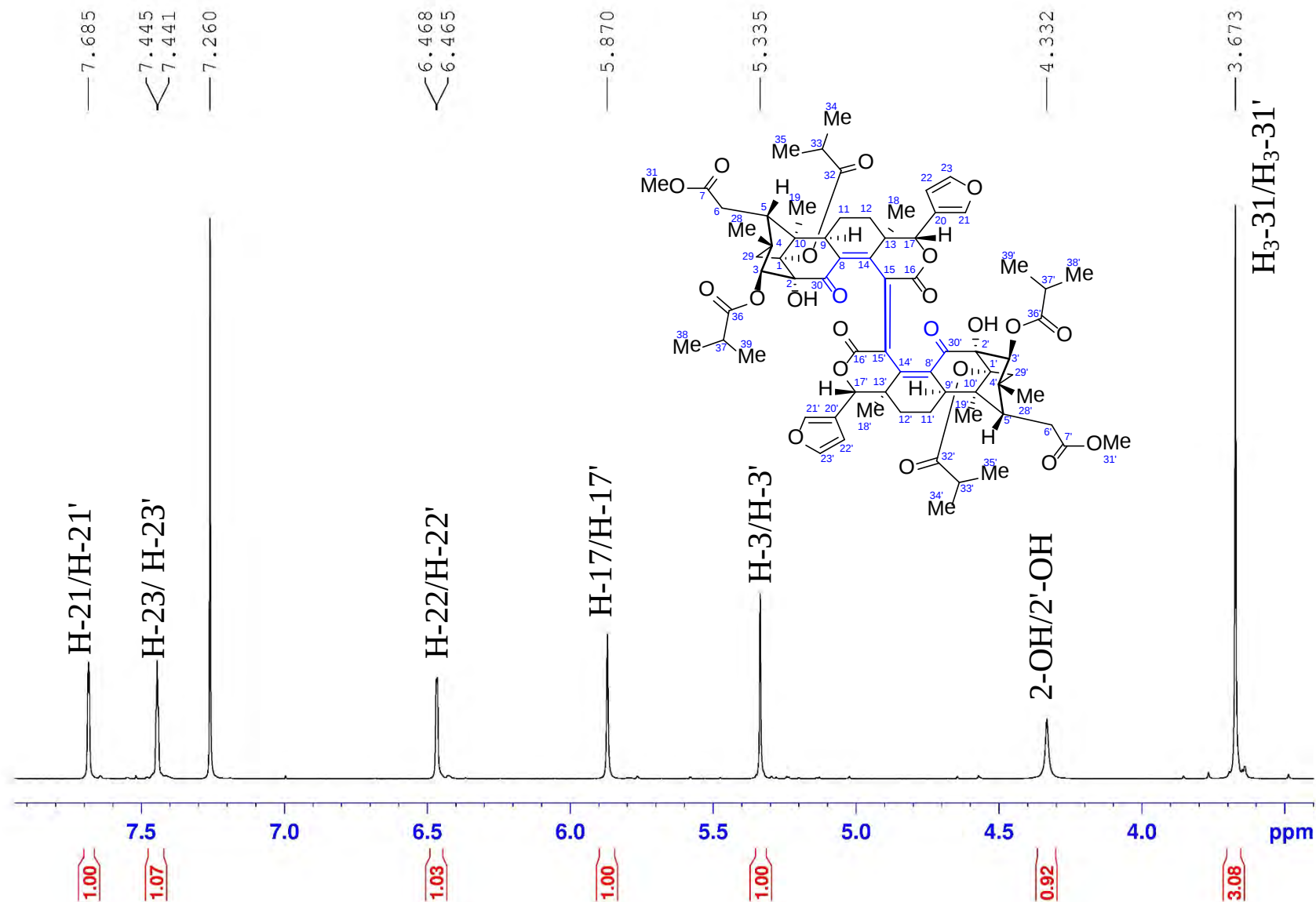
```

NAME                lws-37-0
EXPNO                1
PROCNO              1
Date_                20160519
Time                23.24
INSTRUM             spect
PROBHD              5 mm CPPBBO BB
PULPROG             zg30
TD                  65536
SOLVENT             CDC13
NS                   16
DS                   2
SWH                 8223.685
FIDRES              0.125483
AQ                  3.9846387
RG                  208.5
DW                  60.800
DE                   10.00
TE                   297.0
D1                  1.00000000
TD0                  1
    
```

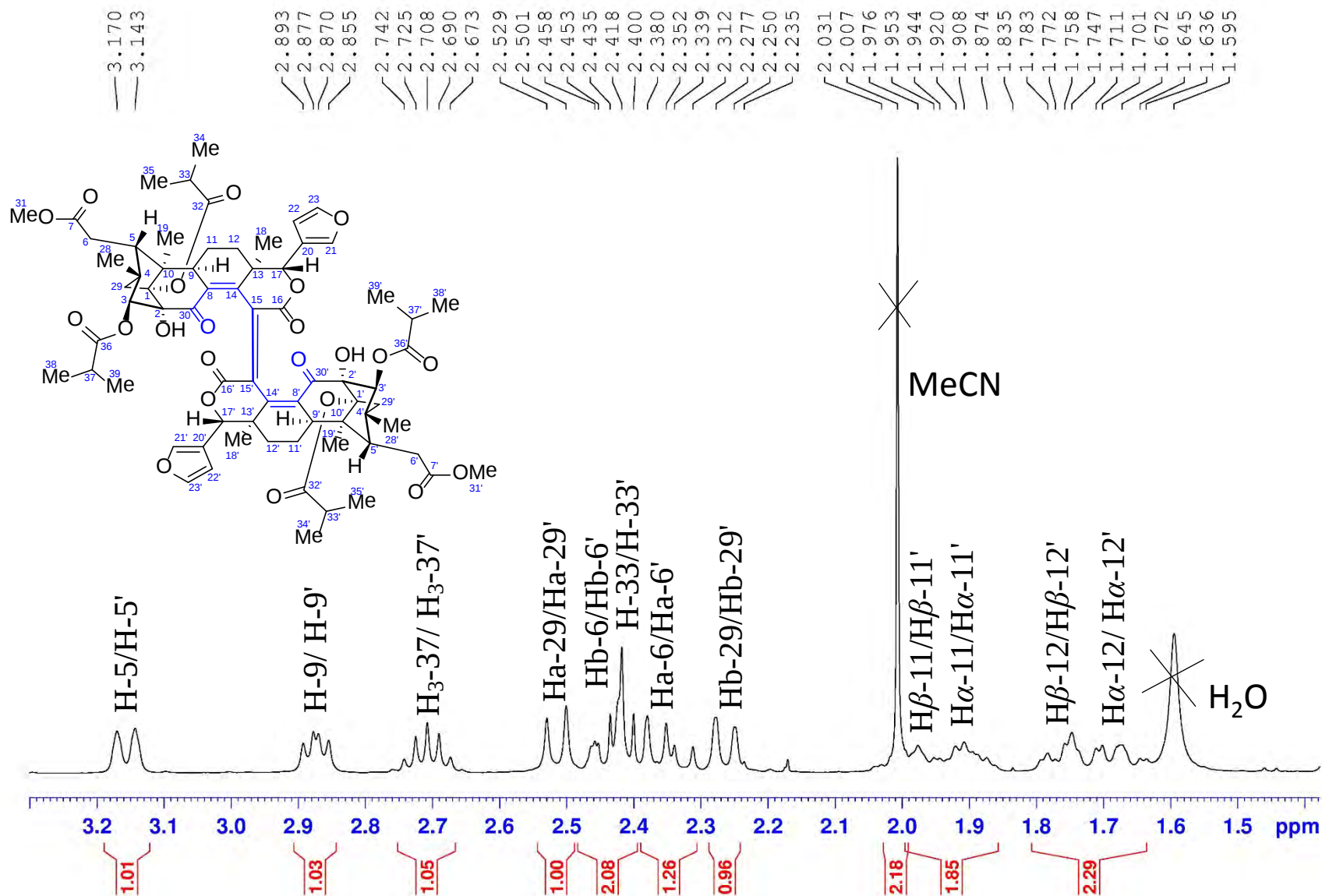
```

===== CHANNEL f1 =====
SFO1                400.1324710
NUC1                 1H
P1                   11.50
SI                   65536
SF                  400.1300100
WDW                  EM
SSB                   0
LB                   0.30
GB                   0
PC                   1.00
    
```

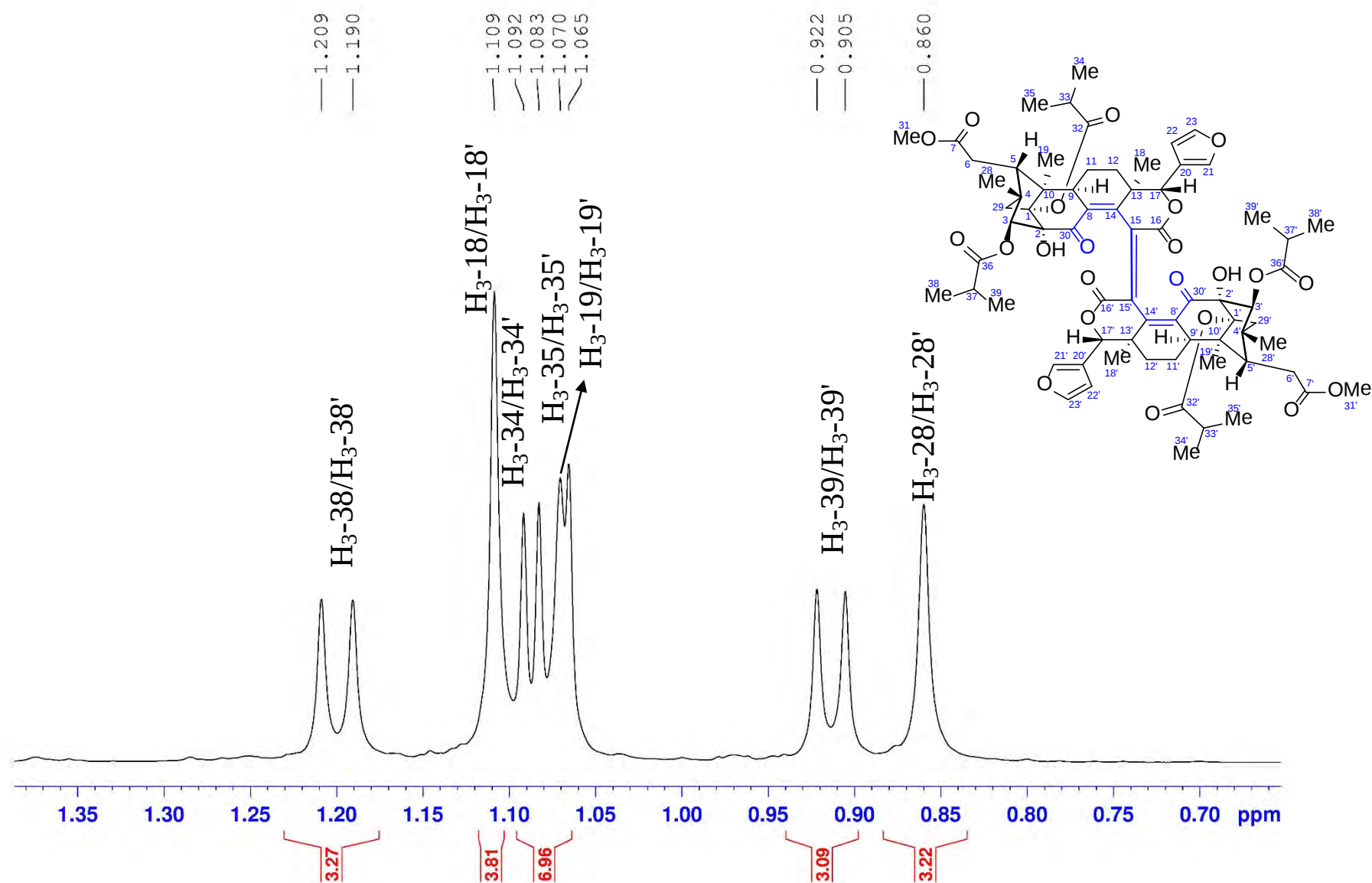
^1H NMR (400 MHz) spectrum of compound **2'** in CDCl_3



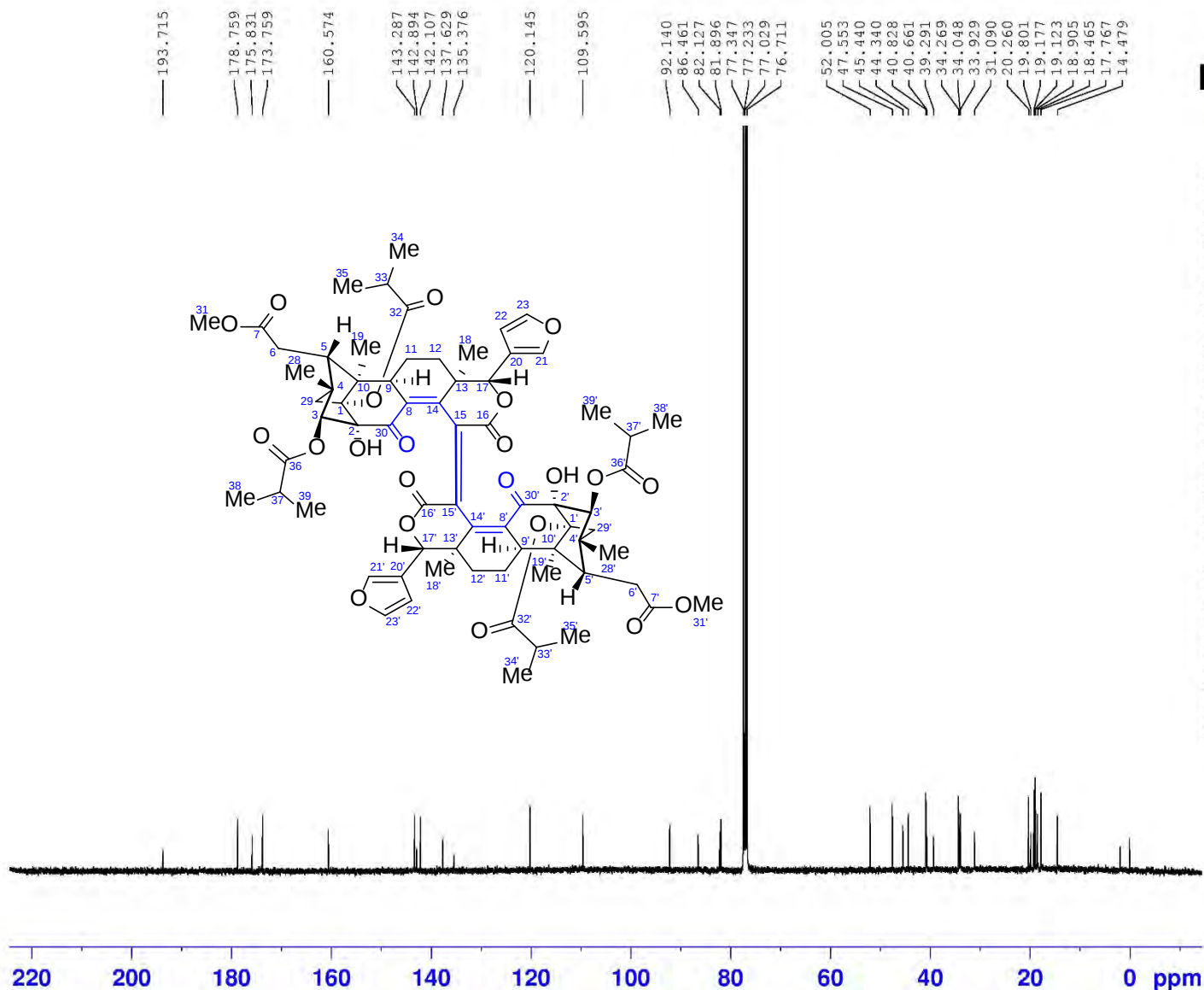
^1H NMR (400 MHz) spectrum of compound **2'** in CDCl_3



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



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



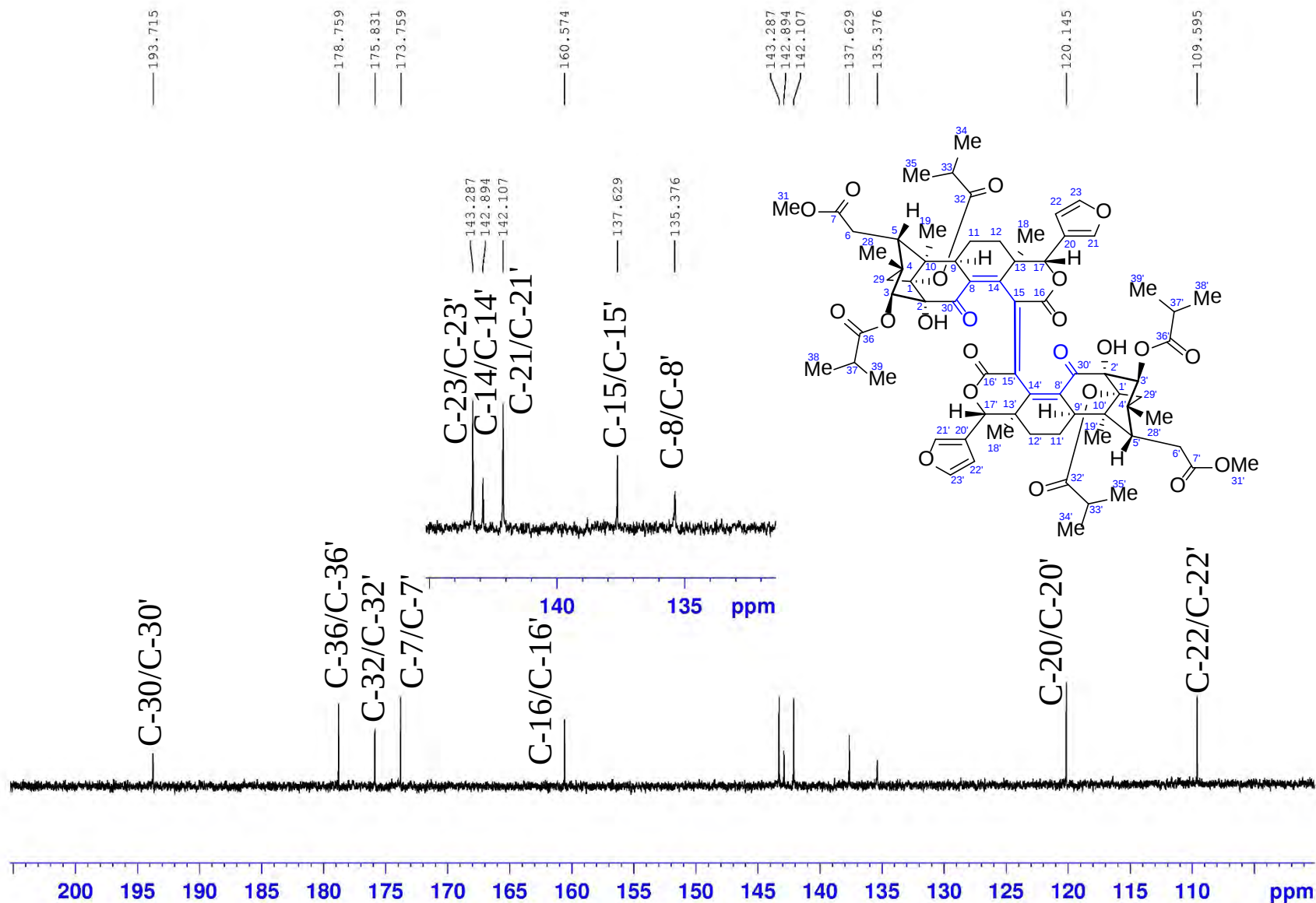
```

NAME          lws-37-0
EXPNO          2
PROCNO         1
Date_          20160521
Time           7.05
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            102.3
DW            20.800 usec
DE            18.00 usec
TE            297.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
  
```

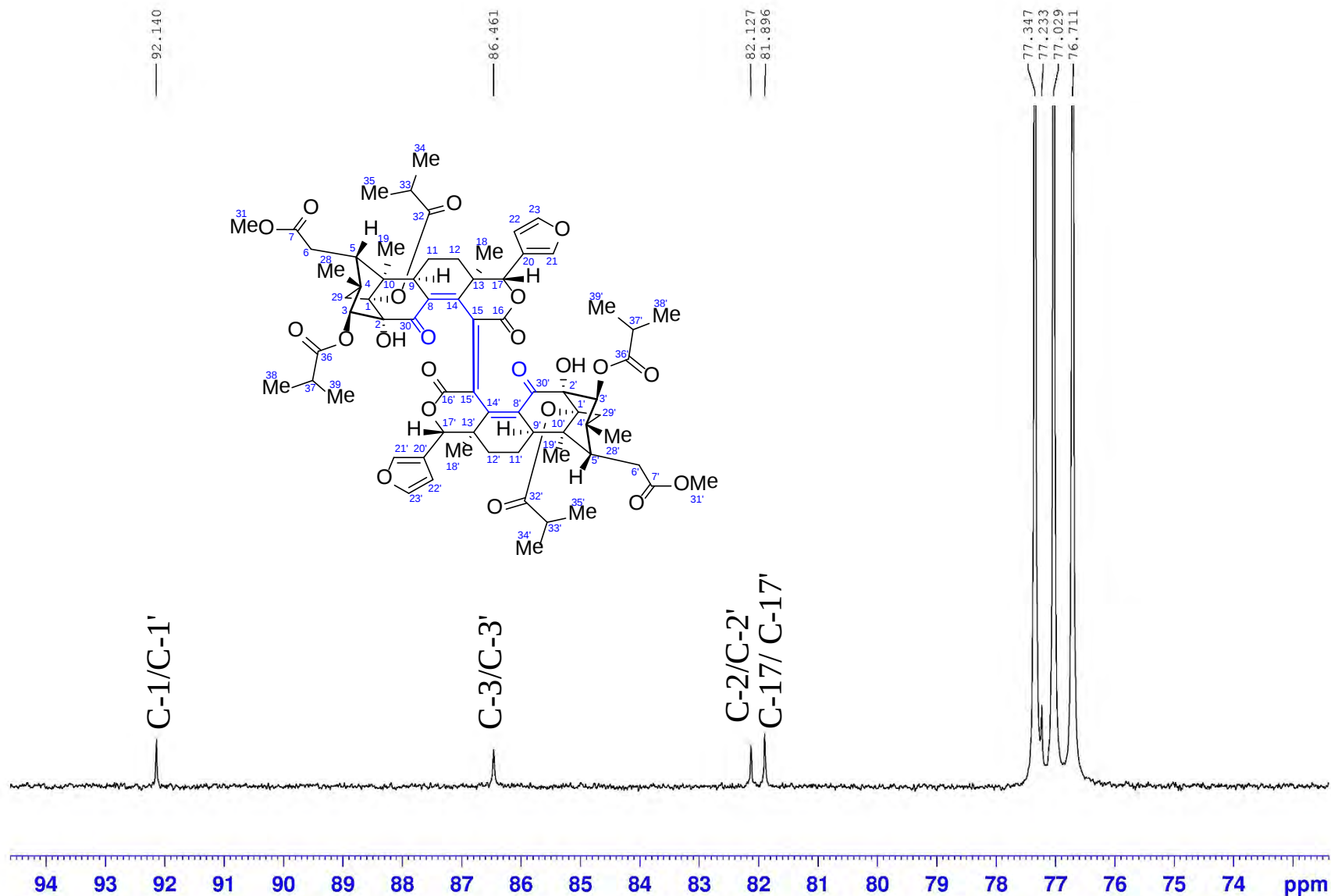
```

===== CHANNEL f1 =====
SF01          100.6233324 MHz
NUC1           13C
P1            10.00 usec
SI            32768
SF            100.6127684 MHz
WDW            EM
SSB            0
LB            1.00 Hz
GB            0
PC            1.40
  
```

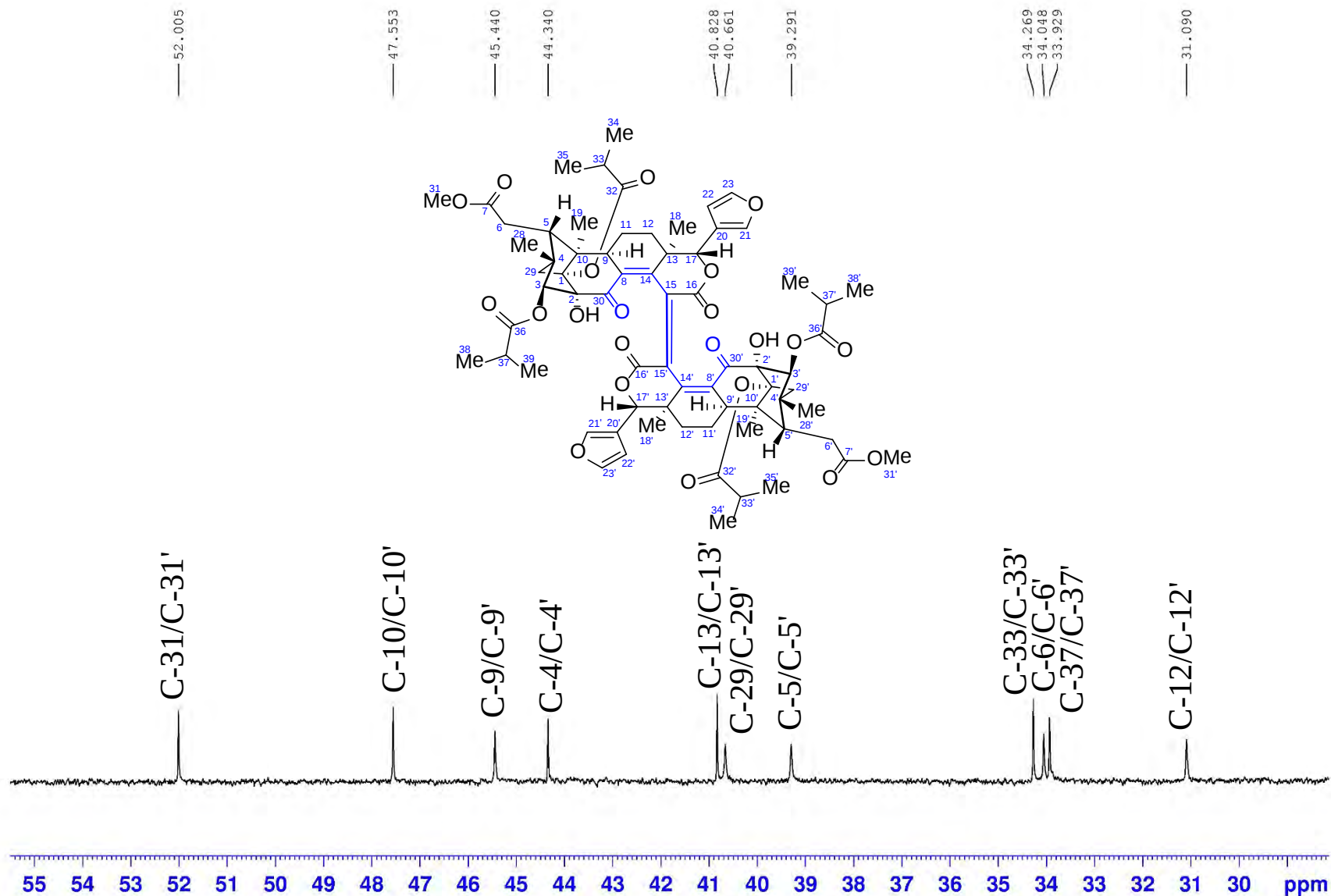
^{13}C NMR (100 MHz) spectrum of compound **2'** in CDCl_3



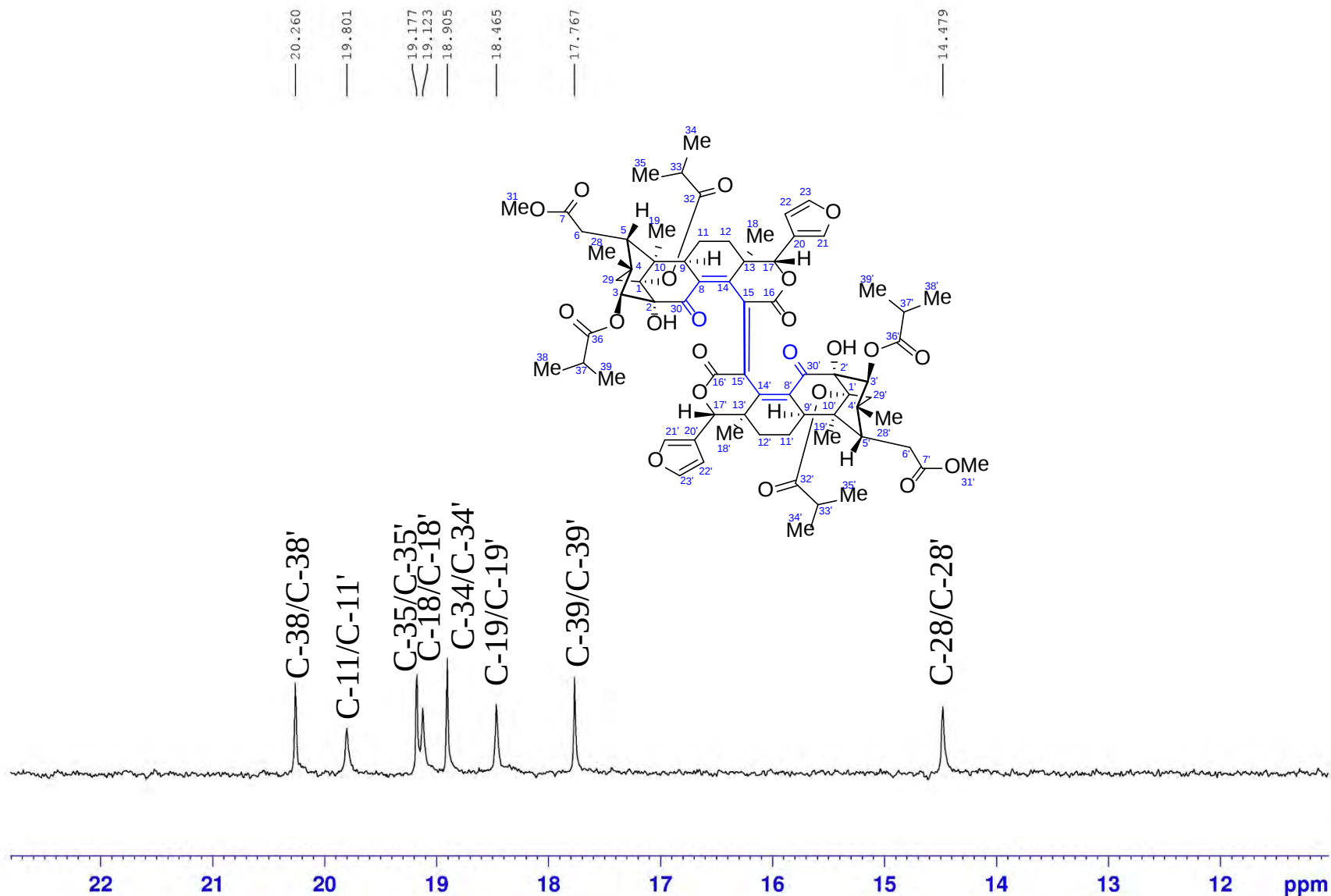
^{13}C NMR (100 MHz) spectrum of compound **2'** in CDCl_3



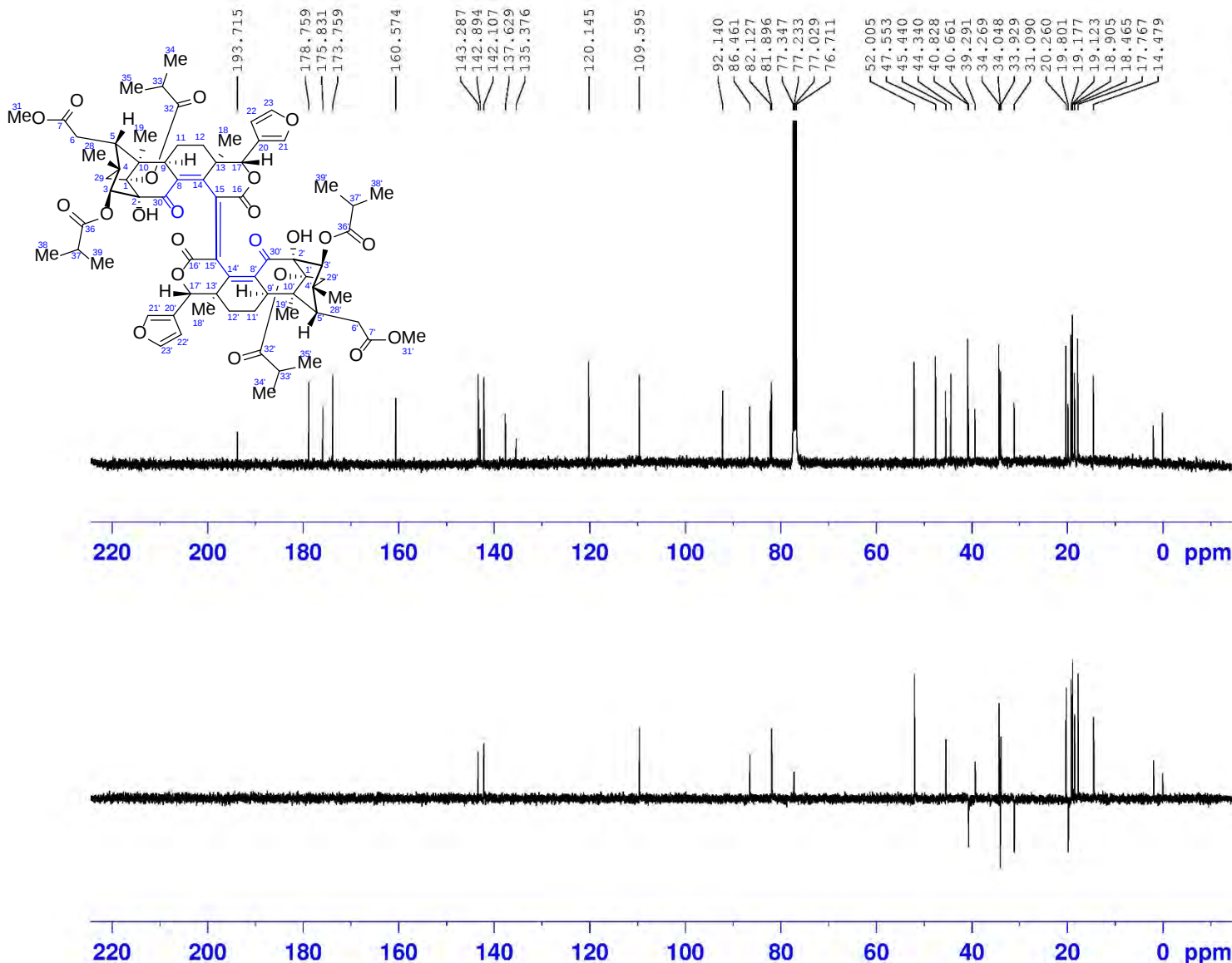
^{13}C NMR (100 MHz) spectrum of compound **2'** in CDCl_3



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



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



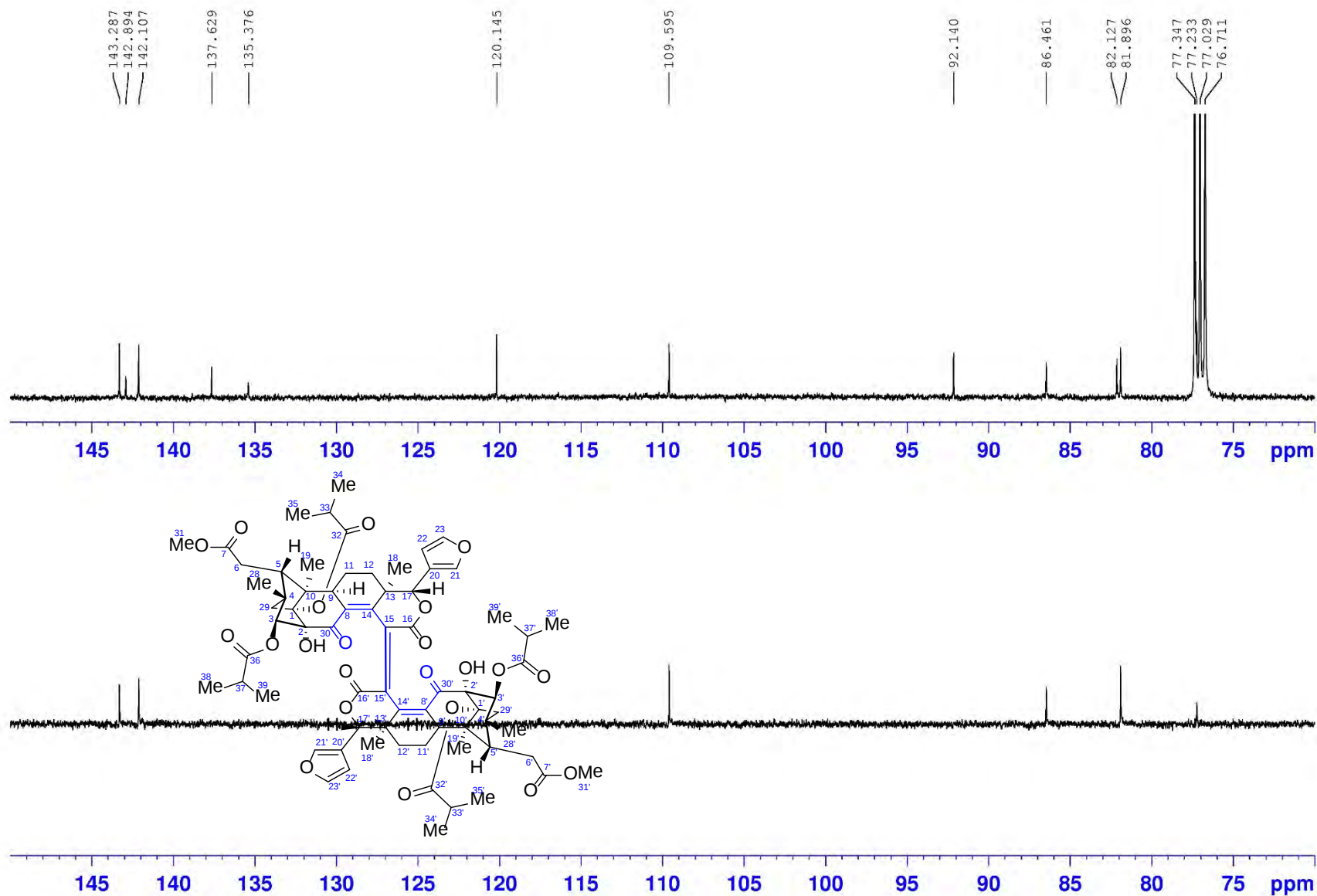
```

NAME          lws-37-0
EXPNO         3
PROCNO        1
Date_         20160521
Time          7.23
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       deptsp135
TD            65536
SOLVENT       CDC13
NS            300
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
    
```

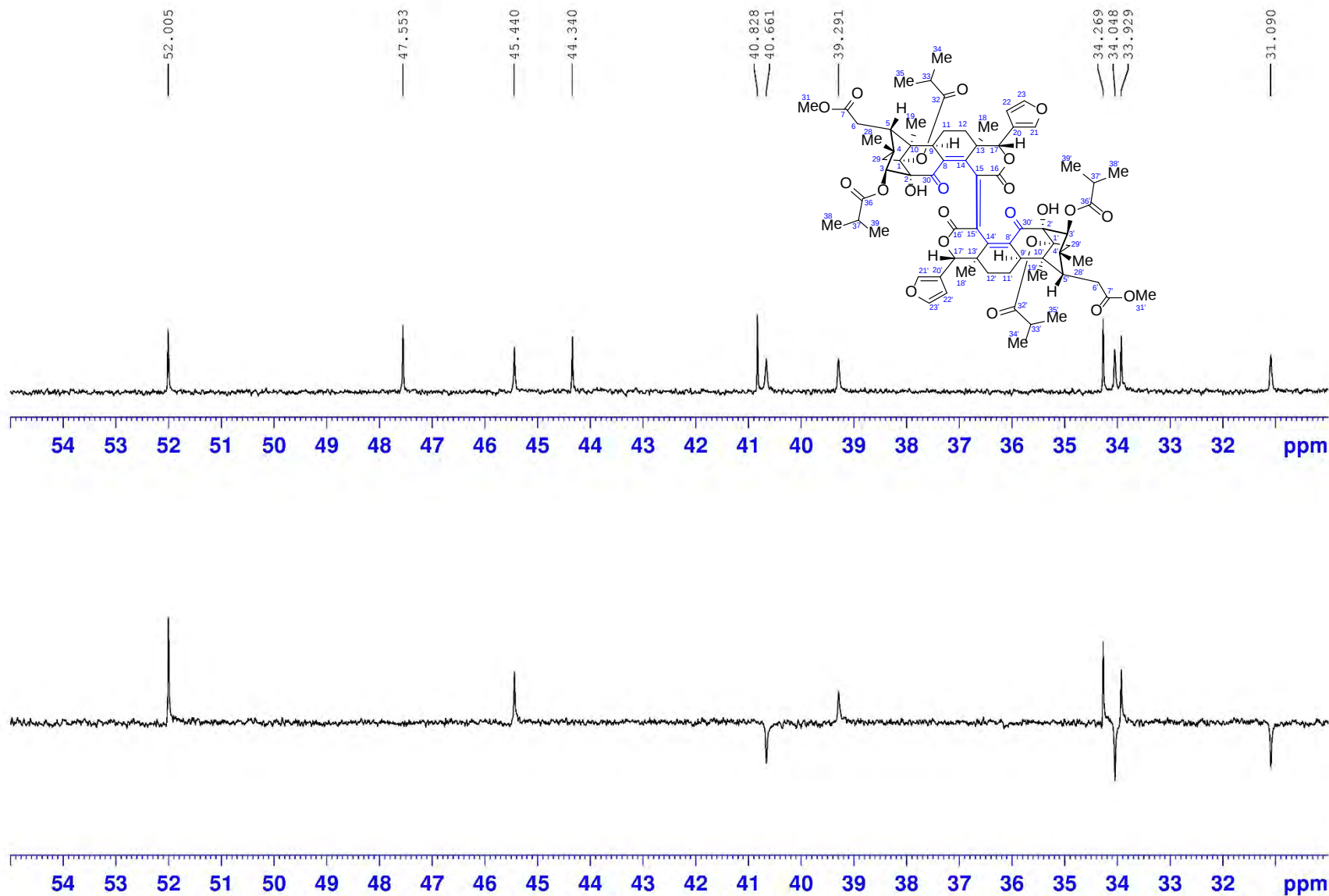
```

===== CHANNEL f1 =====
SF01         100.6233324
NUC1          13C
P1            10.00
P13           2000.00
SI            32768
SF            100.6127685
WDW           EM
SSB           0
LB            1.00
GB            0
PC            1.40
    
```

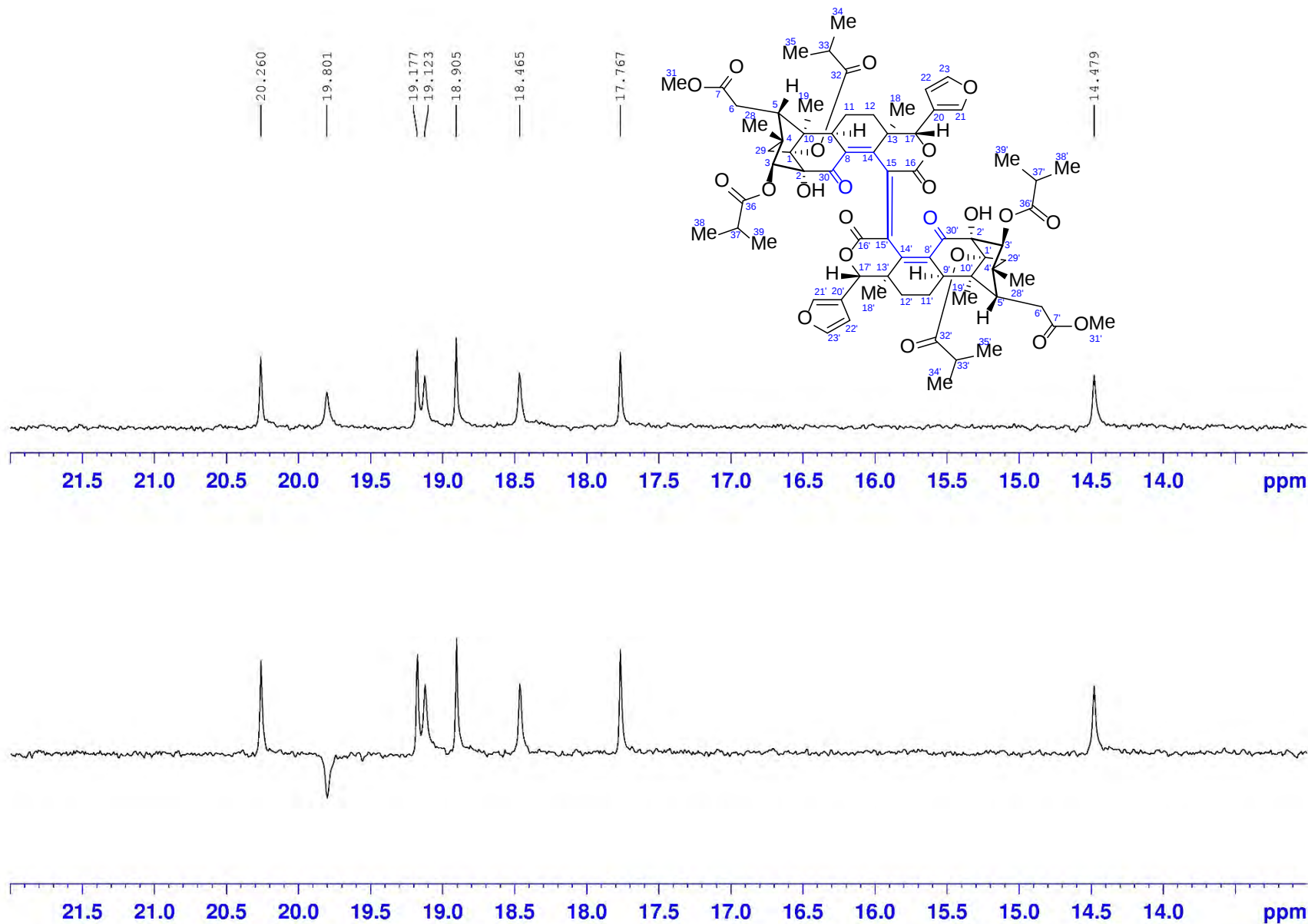
DEPT135 (100 MHz) spectrum of compound **2'** in CDCl₃



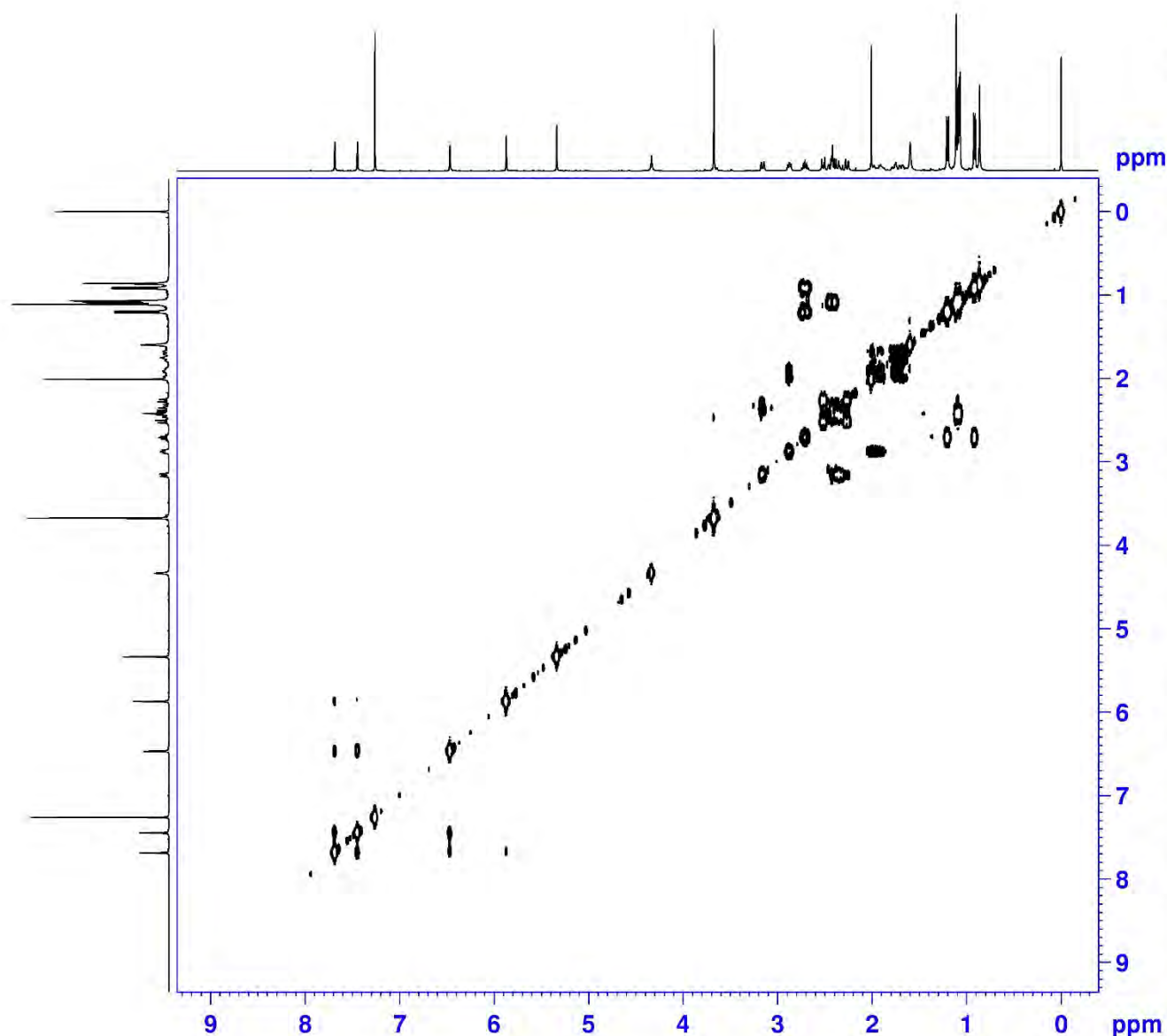
DEPT135 (100 MHz) spectrum of compound **2'** in CDCl₃



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



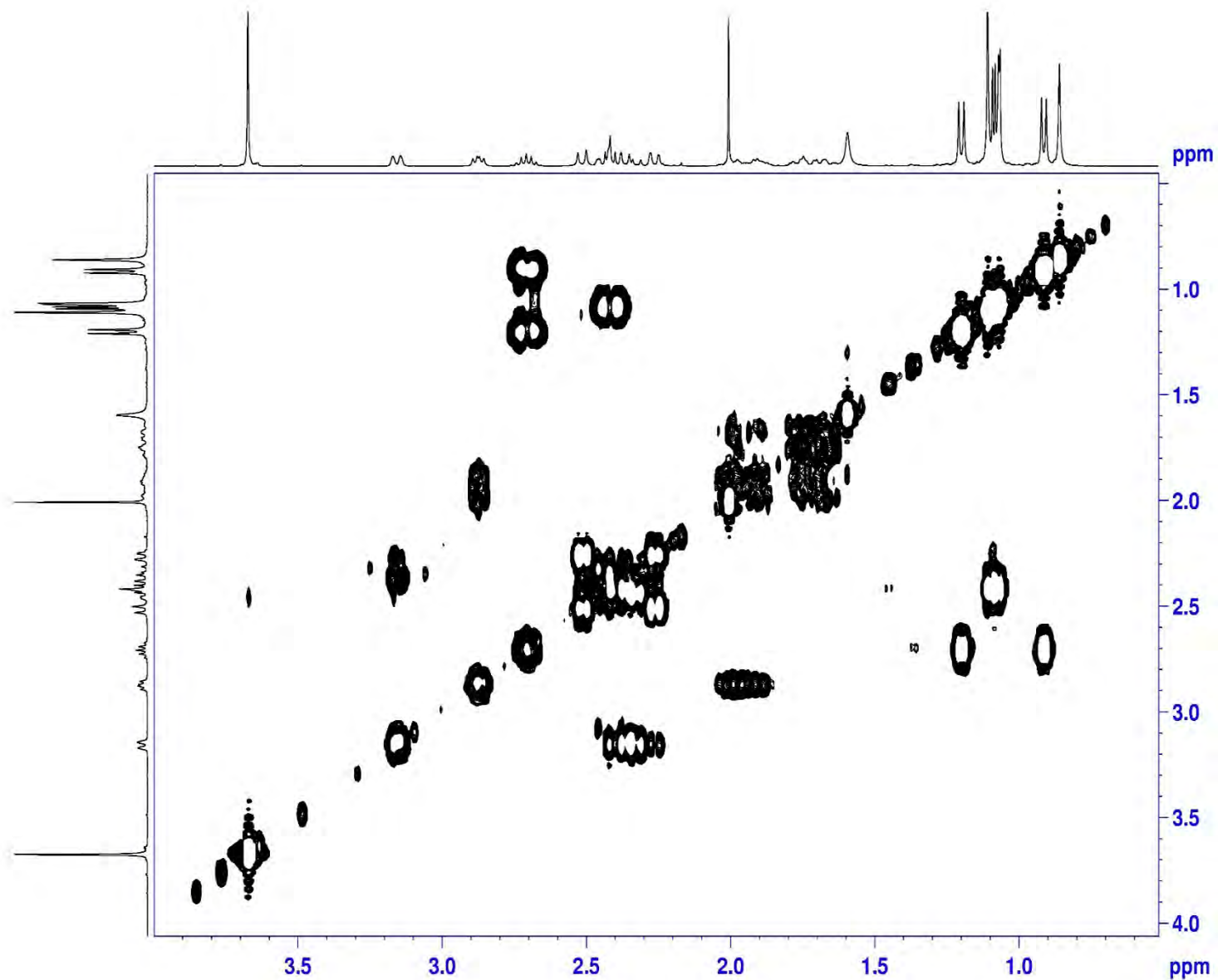
^1H - ^1H COSY (400 MHz) spectrum of compound **2'** in CDCl_3



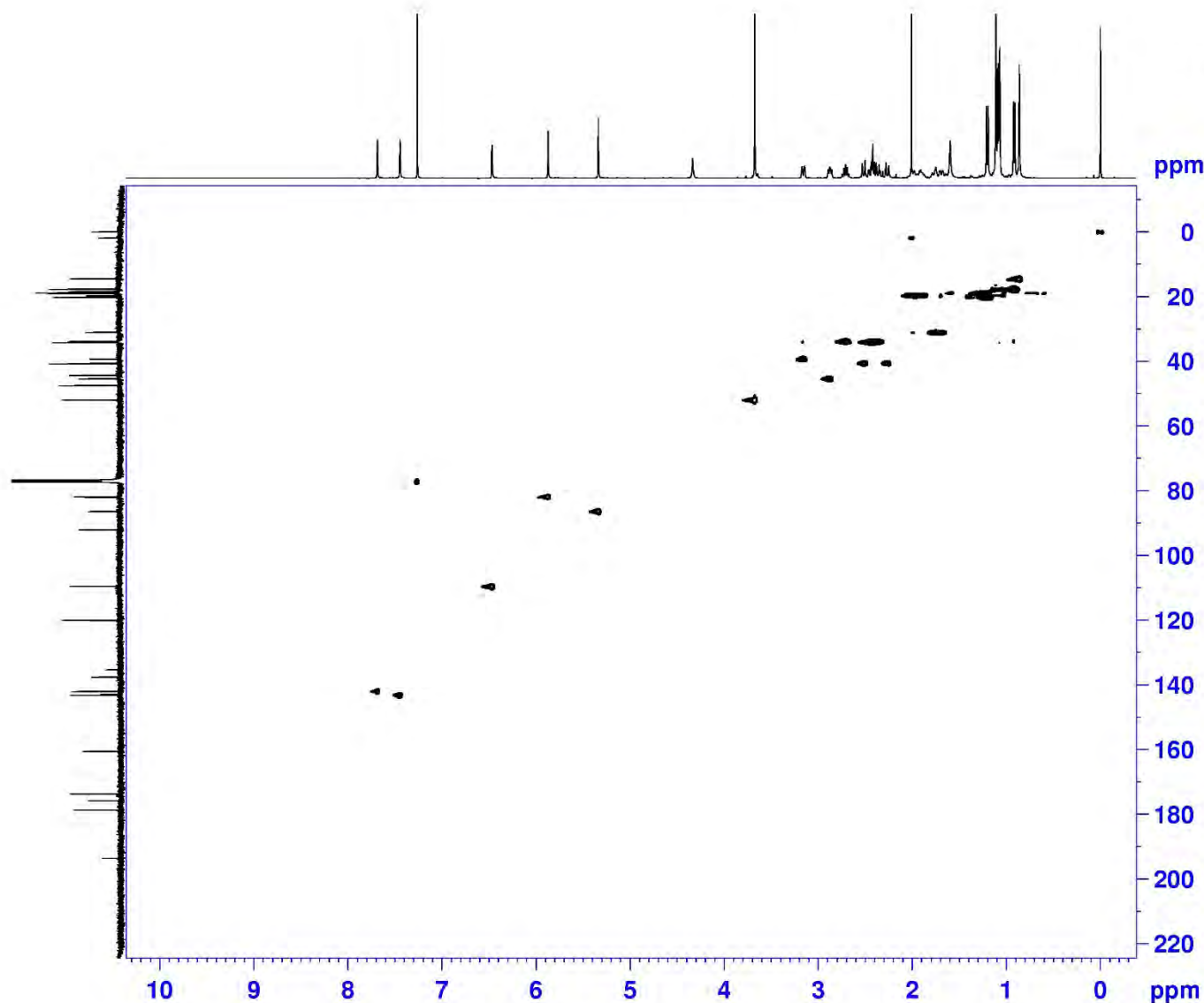
```
NAME          lws-37-0
EXPNO          4
PROCNO         1
Date_         20160521
Time           7.24
INSTRUM        spect
PROBHD         5 mm CPPBBO BB
PULPROG        cosygpppqf
TD             2048
SOLVENT        CDCl3
NS              8
DS              8
SWH            3906.250 Hz
FIDRES         1.907349 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
WDW            QSINE
---
```

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

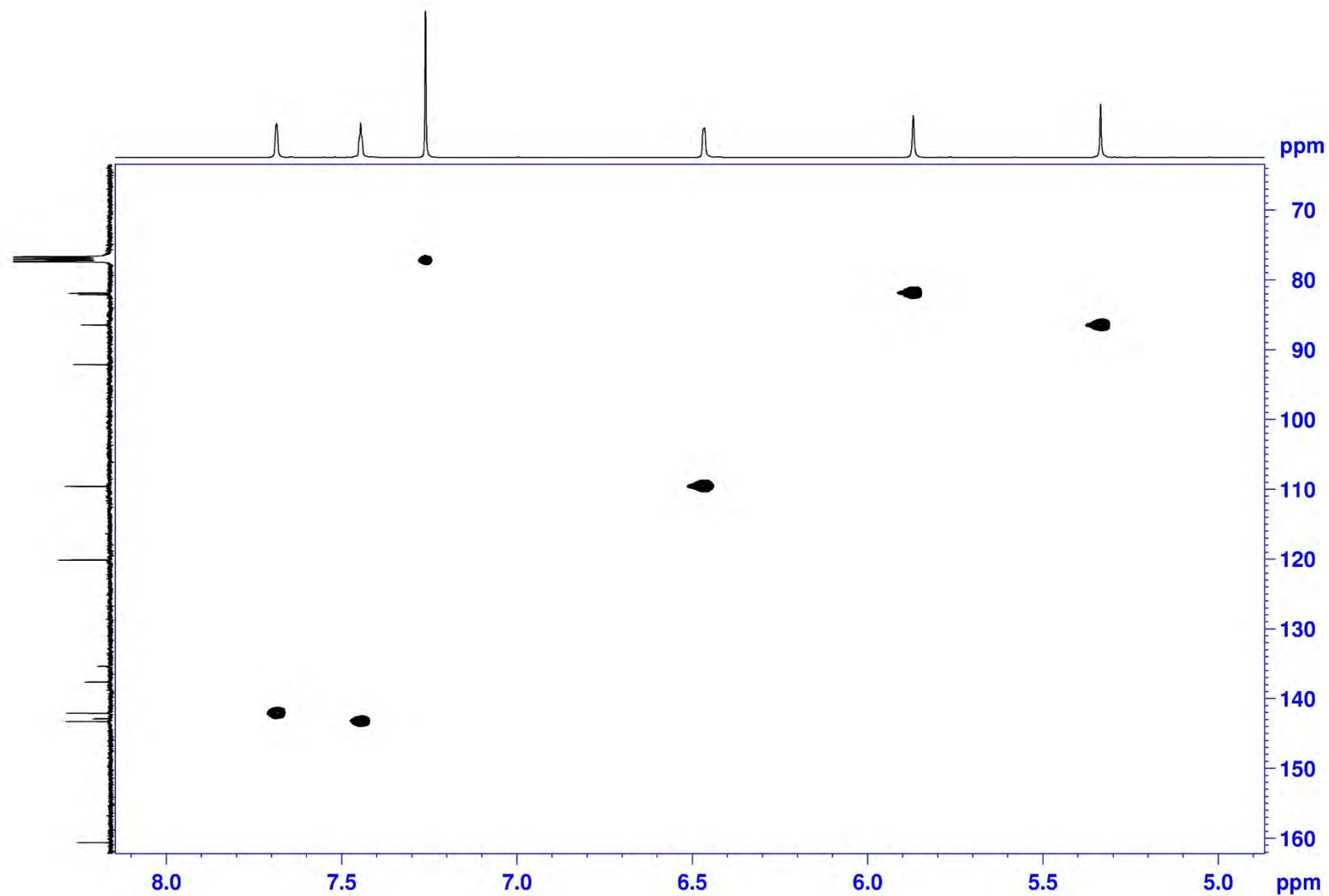


HSQC (400 MHz) spectrum of compound **2'** in CDCl₃

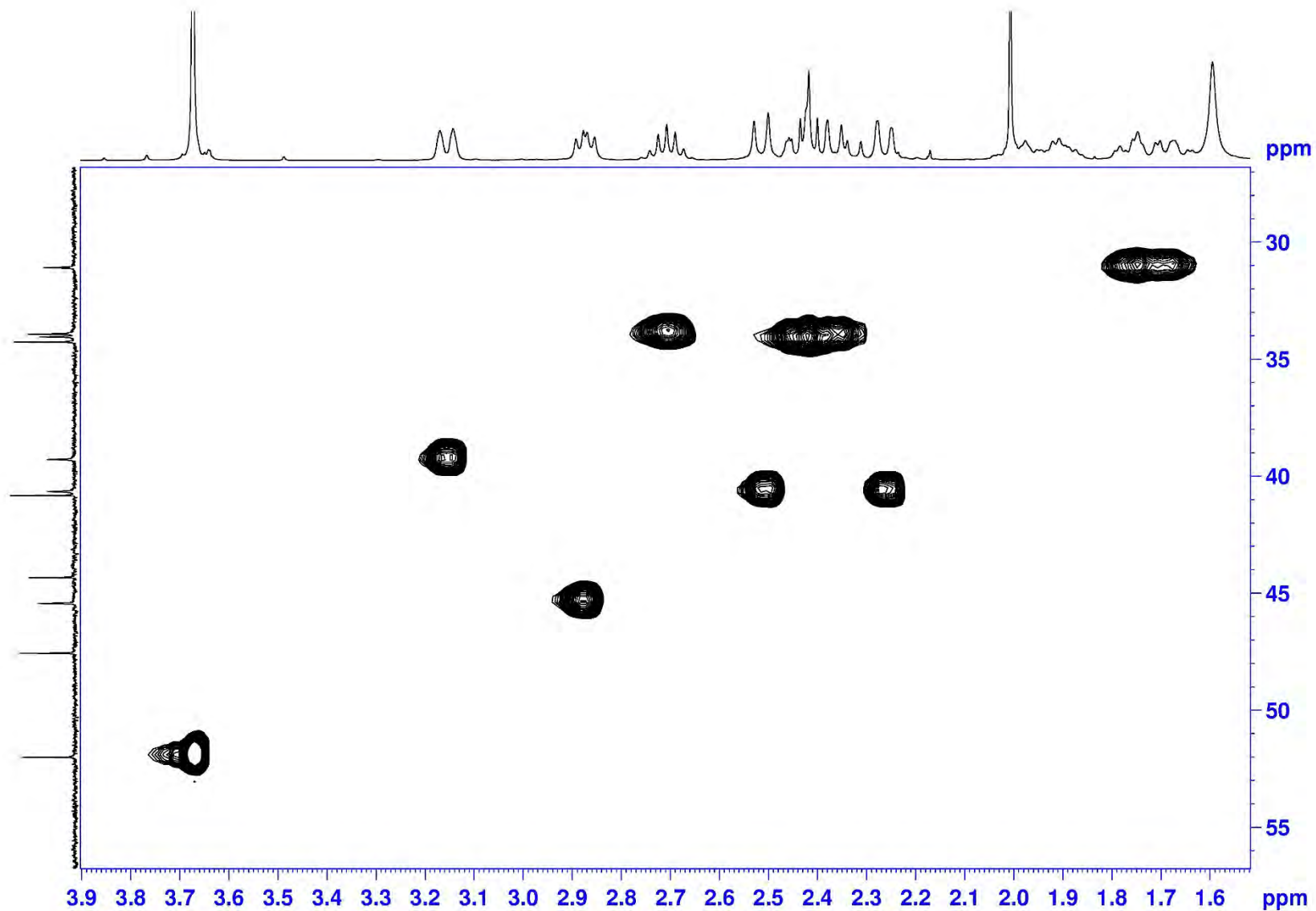


NAME	lws-37-0
EXPNO	104
PROCNO	1
Date_	20160527
Time	16.21
INSTRUM	spect
PROBHD	5 mm CPPBBO BB
PULPROG	hsqcetgpsi2
TD	1024
SOLVENT	CDCl3
NS	16
DS	16
SWH	4302.926 Hz
FIDRES	4.202076 Hz
AQ	0.1190388 sec
RG	208.5
DW	116.200 use
DE	10.00 use
TE	297.0 K
CNST2	145.0000000
D0	0.00000300 sec
D1	1.46497905 sec
D4	0.00172414 sec
D11	0.03000000 sec
D16	0.00020000 sec
D24	0.00086207 sec
IN0	0.00002080 sec
ZGPTNS	
===== CHANNEL f1 =====	
SFO1	400.1320007 MHz
NUC1	1H
P1	11.50 use
P2	23.00 use
P28	0.00 use
ND0	2
TD	256
SFO1	100.6233 MHz
FIDRES	93.900238 Hz
SW	238.896 ppm
FnMODE	Echo-Antiecho
SI	1024
SF	400.1300090 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	100.6127684 MHz
WDW	QSINE
SSB	2

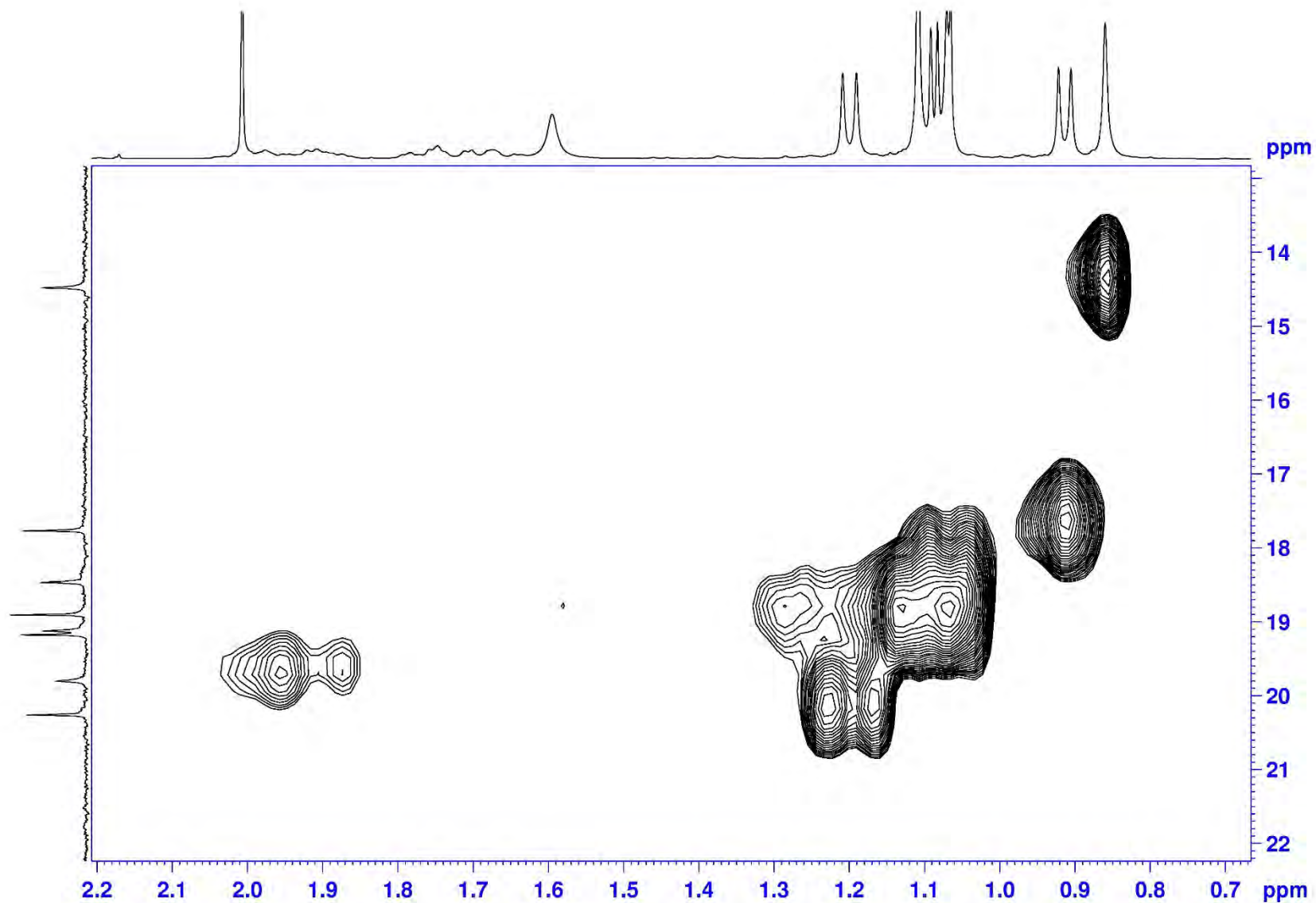
HSQC (400 MHz) spectrum of compound **2'** in CDCl₃



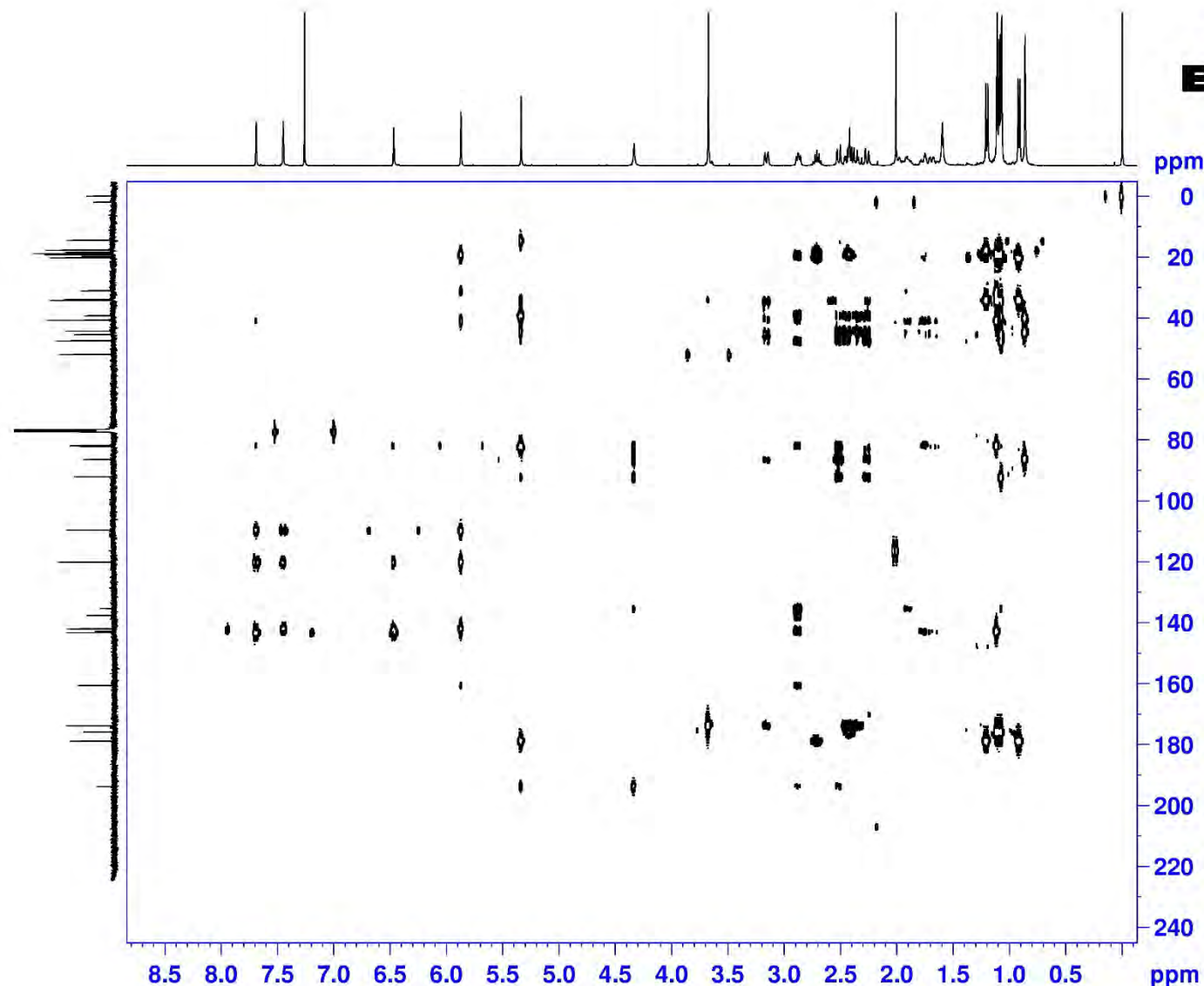
HSQC (400 MHz) spectrum of compound **2'** in CDCl₃



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



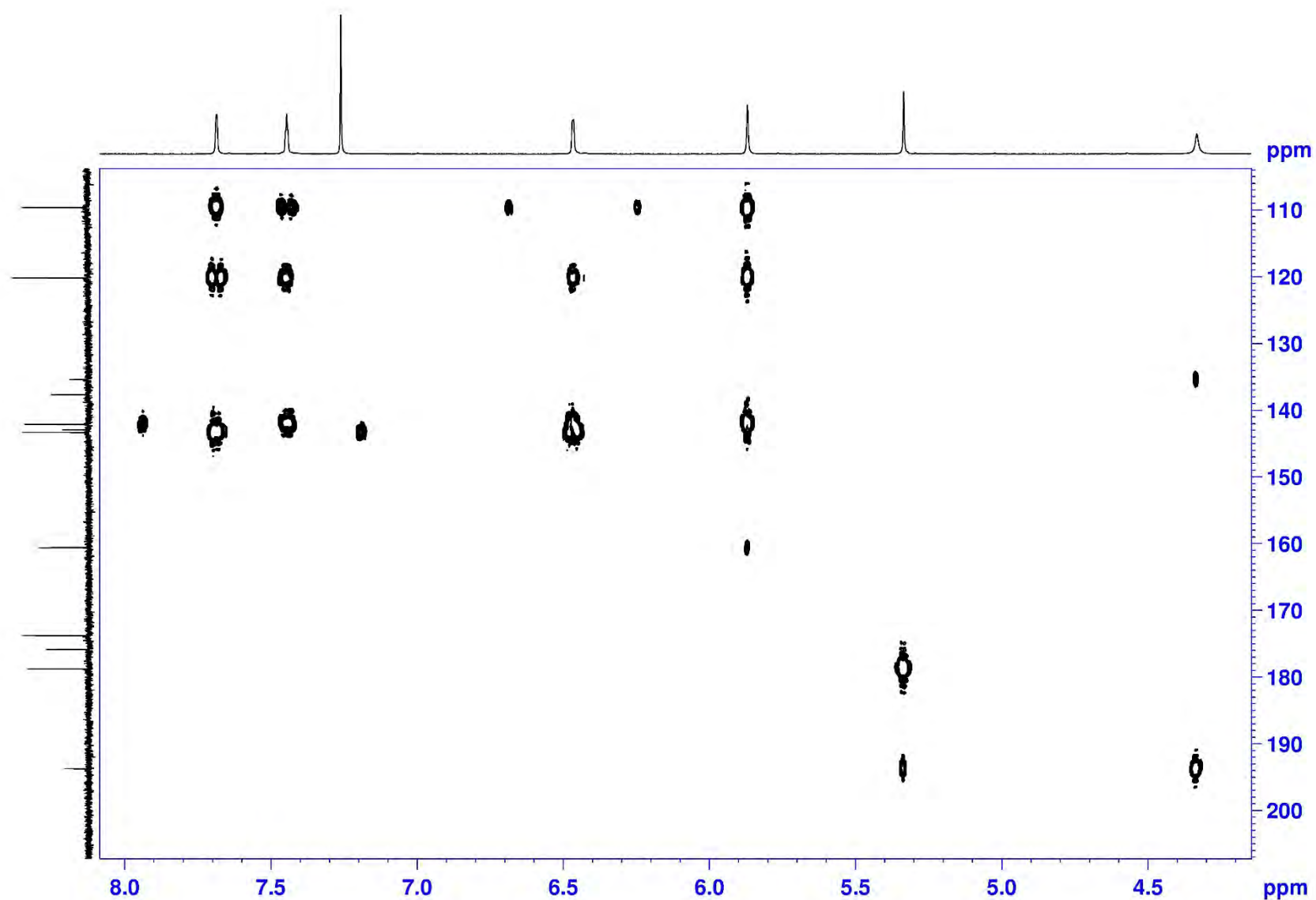
HMBC (400 MHz) spectrum of compound 2' in CDCl₃



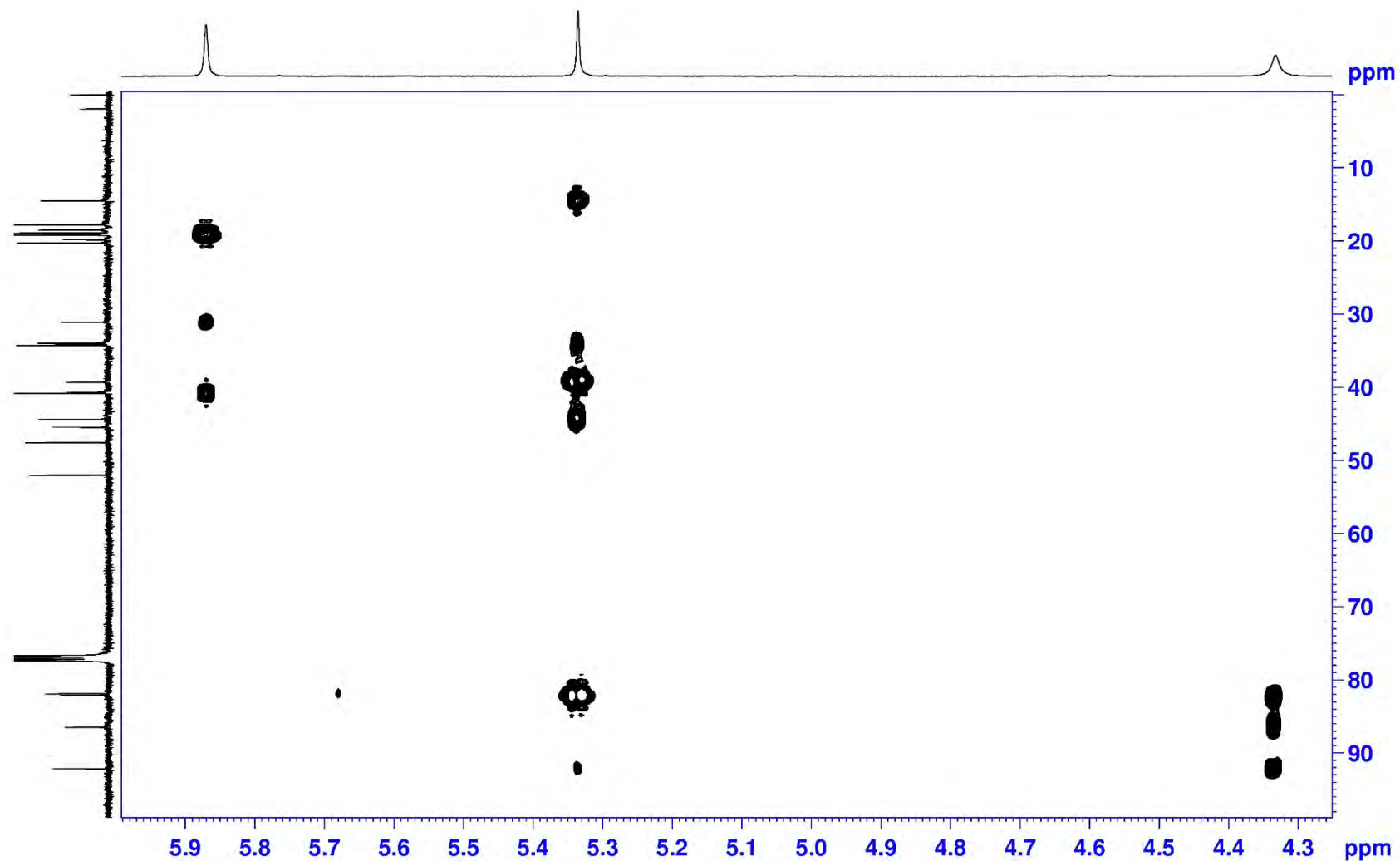
NAME lws-37-0
 EXPNO 6
 PROCNO 1
 Date_ 20160521
 Time 9.58
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG hmbcpglpndqf
 TD 4096
 SOLVENT CDCl3
 NS 128
 DS 16
 SWH 5197.505 Hz
 FIDRES 1.268922 Hz
 AQ 0.3940852 sec
 RG 208.5
 DW 96.200 usec
 DE 10.00 usec
 TE 293.1 K
 CNST2 145.0000000
 CNST13 10.0000000
 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
 FnmODE QF
 SI 2048
 SF 400.1300090 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 QF
 SF 100.6127685 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz

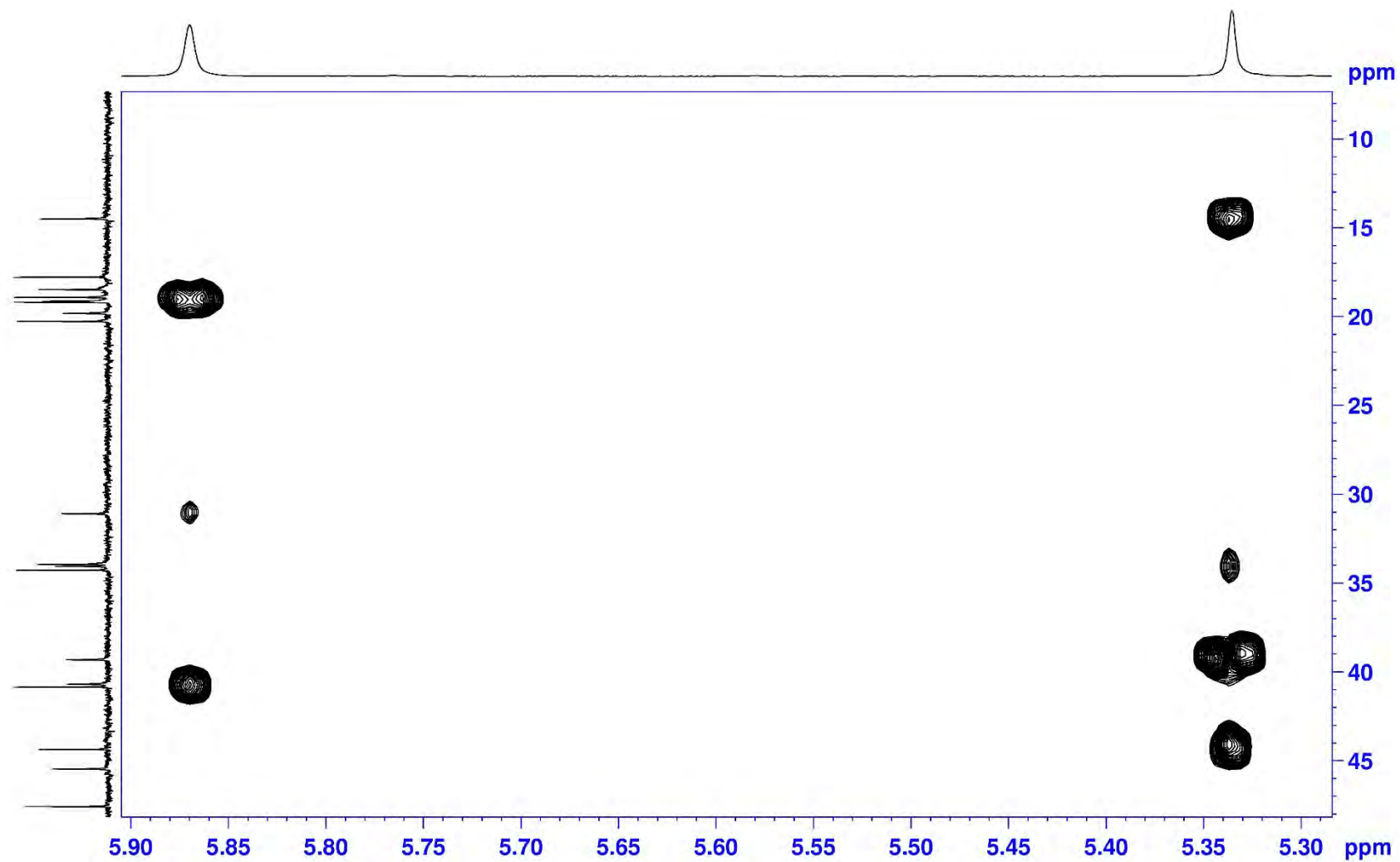
HMBC (400 MHz) spectrum of compound **2'** in CDCl₃



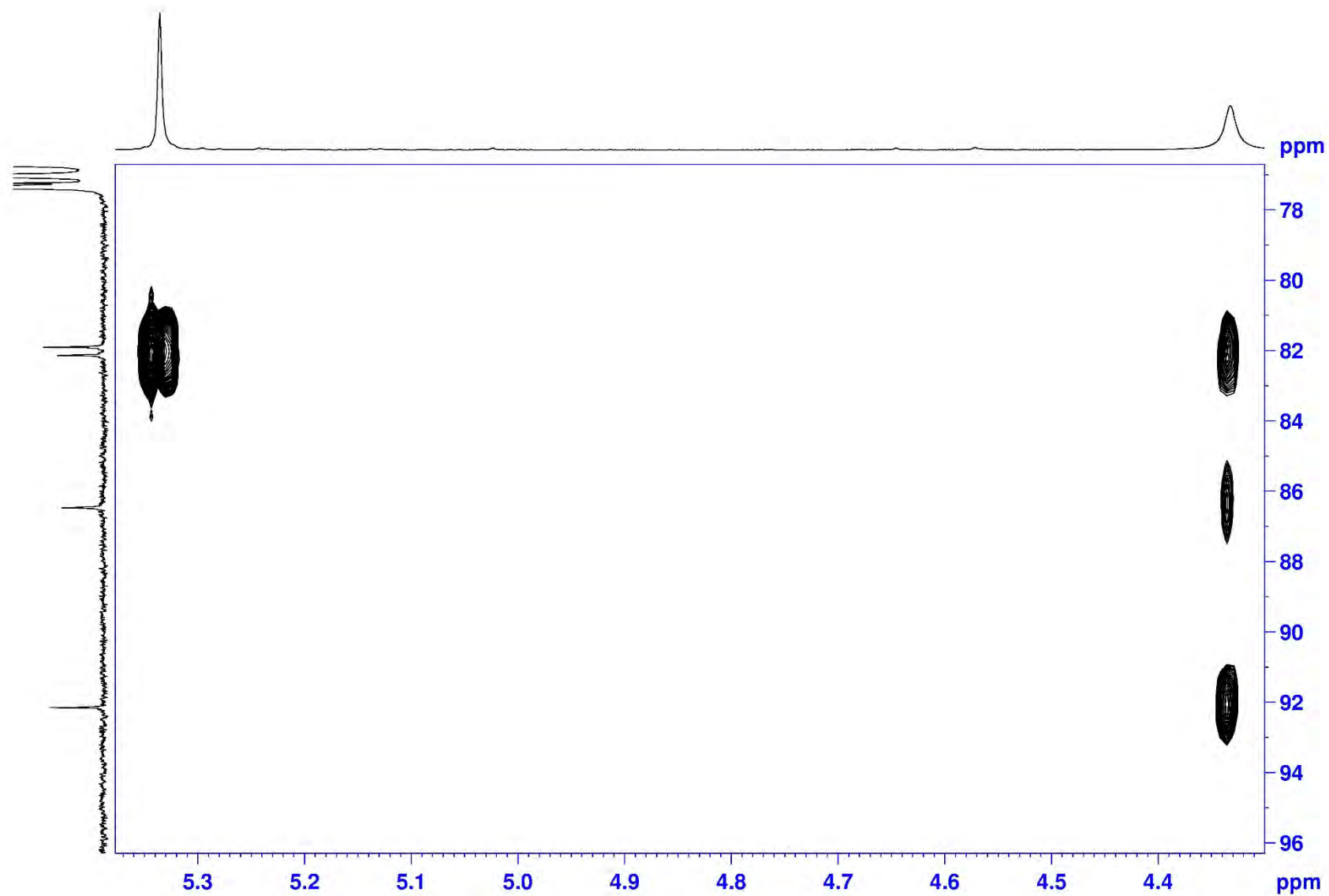
HMBC (400 MHz) spectrum of compound **2'** in CDCl₃



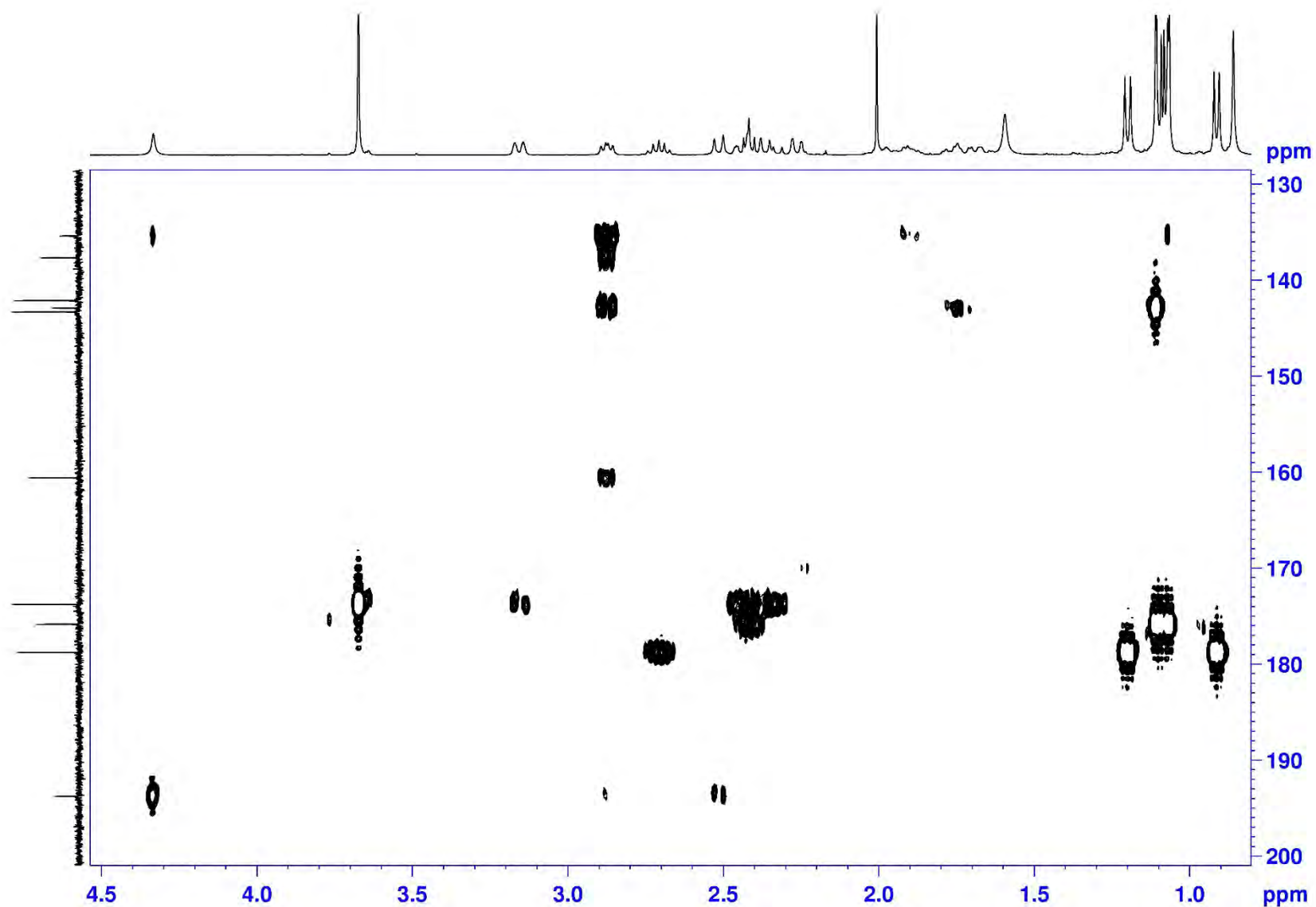
HMBC (400 MHz) spectrum of compound **2'** in CDCl₃



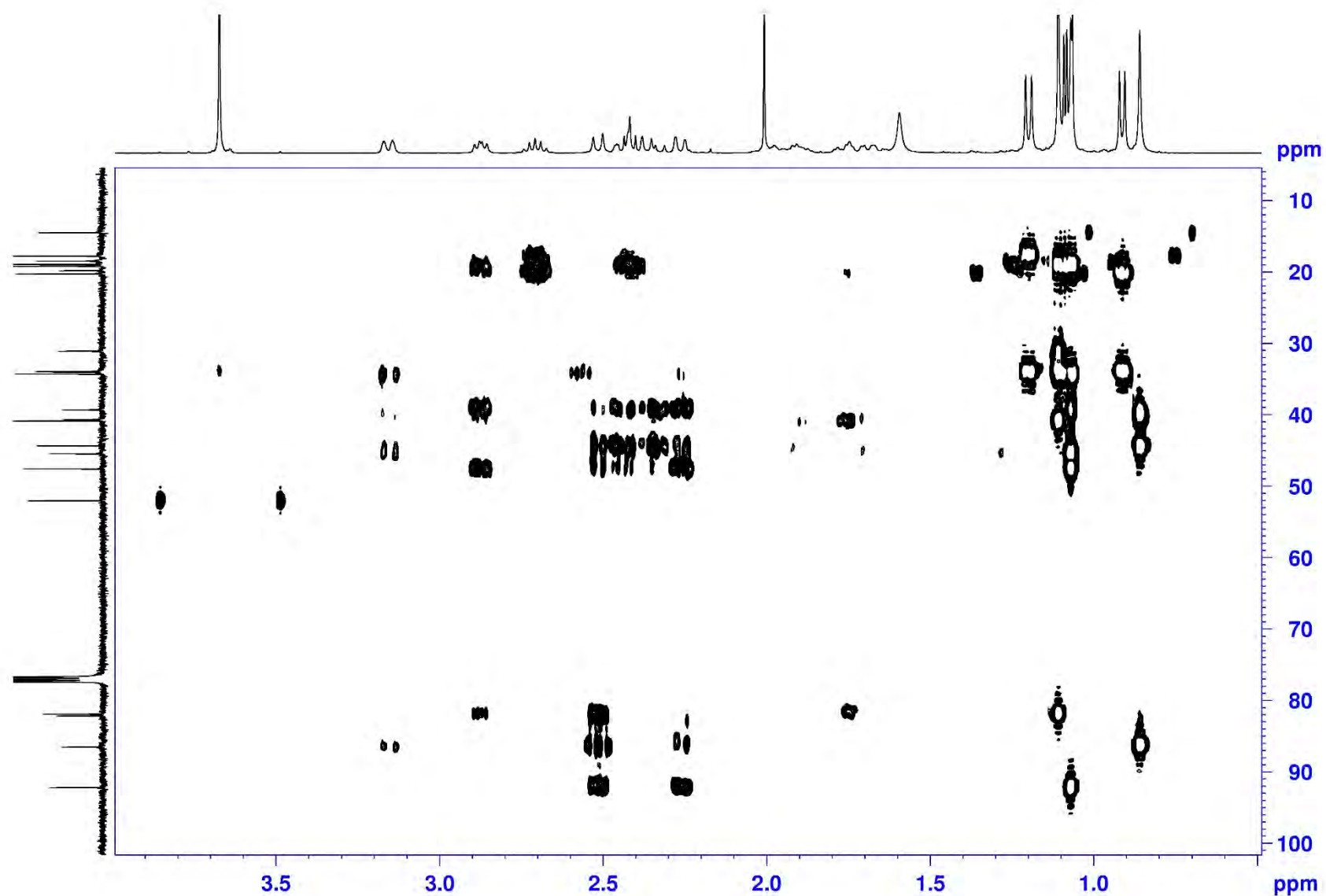
HMBC (400 MHz) spectrum of compound **2'** in CDCl₃



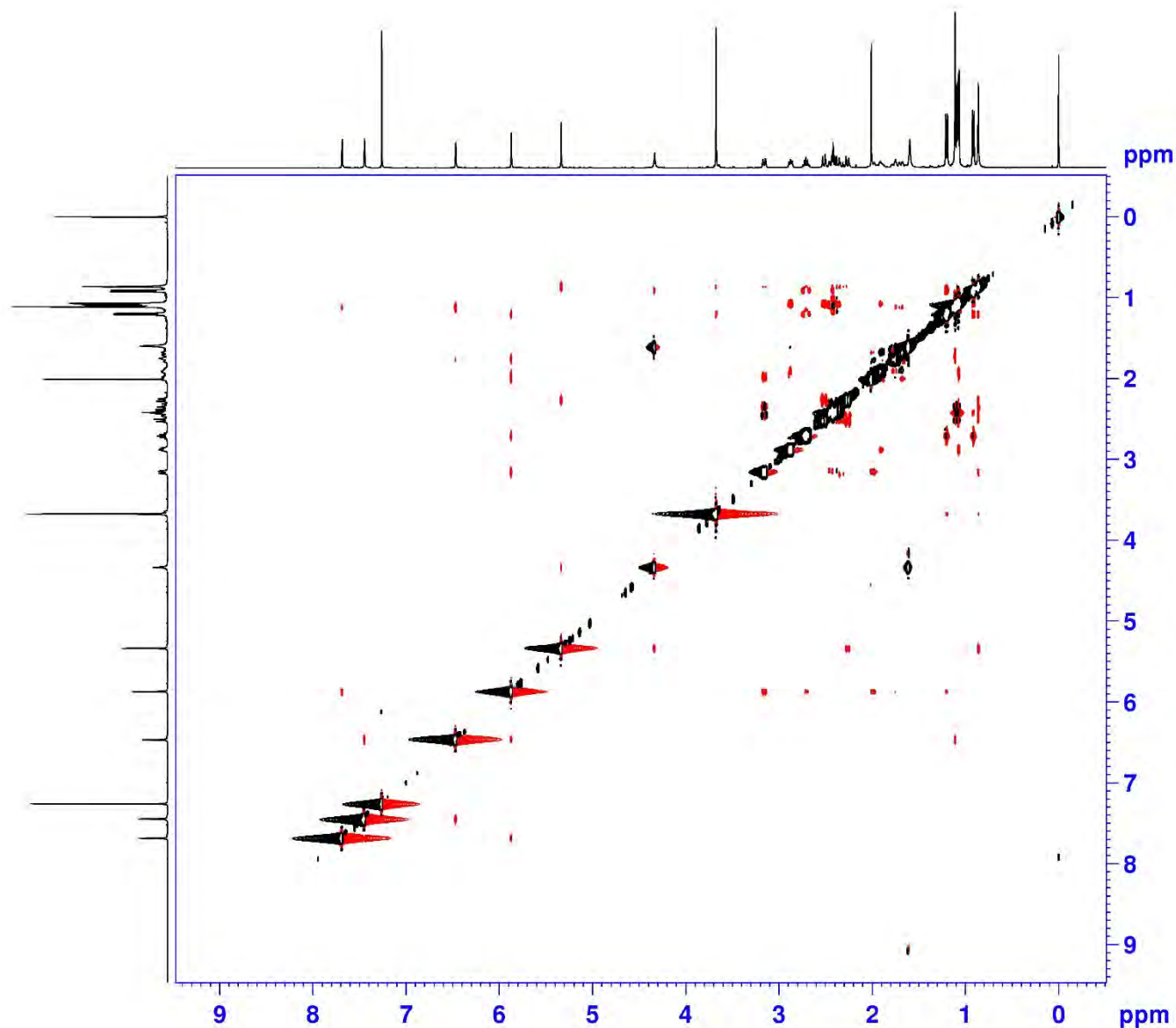
HMBC (400 MHz) spectrum of compound **2'** in CDCl₃



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



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



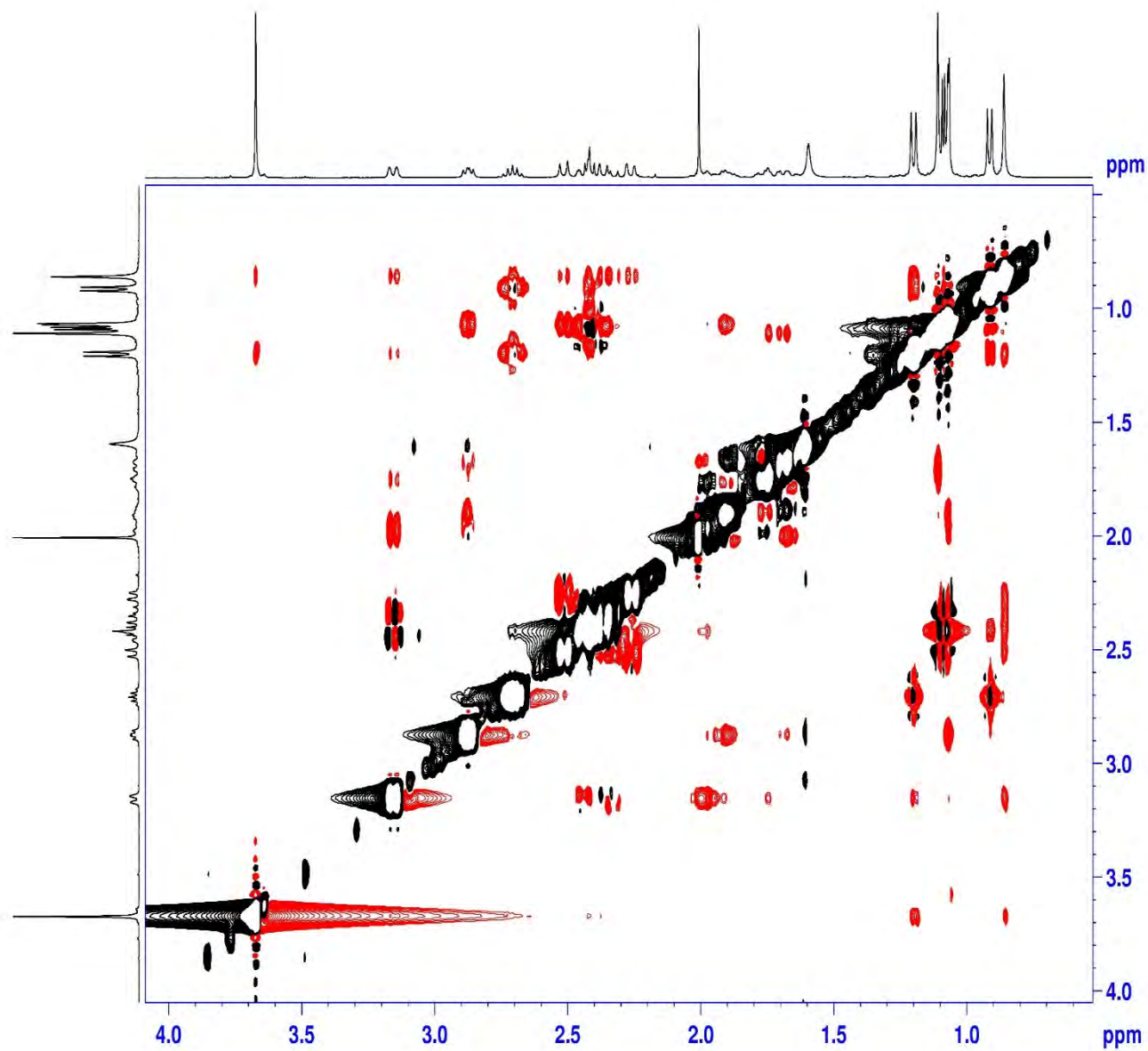
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NAME                lws-37-0
EXPNO                7
PROCNO              1
Date_               20160521
Time                18.52
INSTRUM             spect
PROBHD              5 mm CPPBBO BB
PULPROG             noesygpphpp
TD                  2048
SOLVENT             CDCl3
NS                   32
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                   293.1 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
  
```

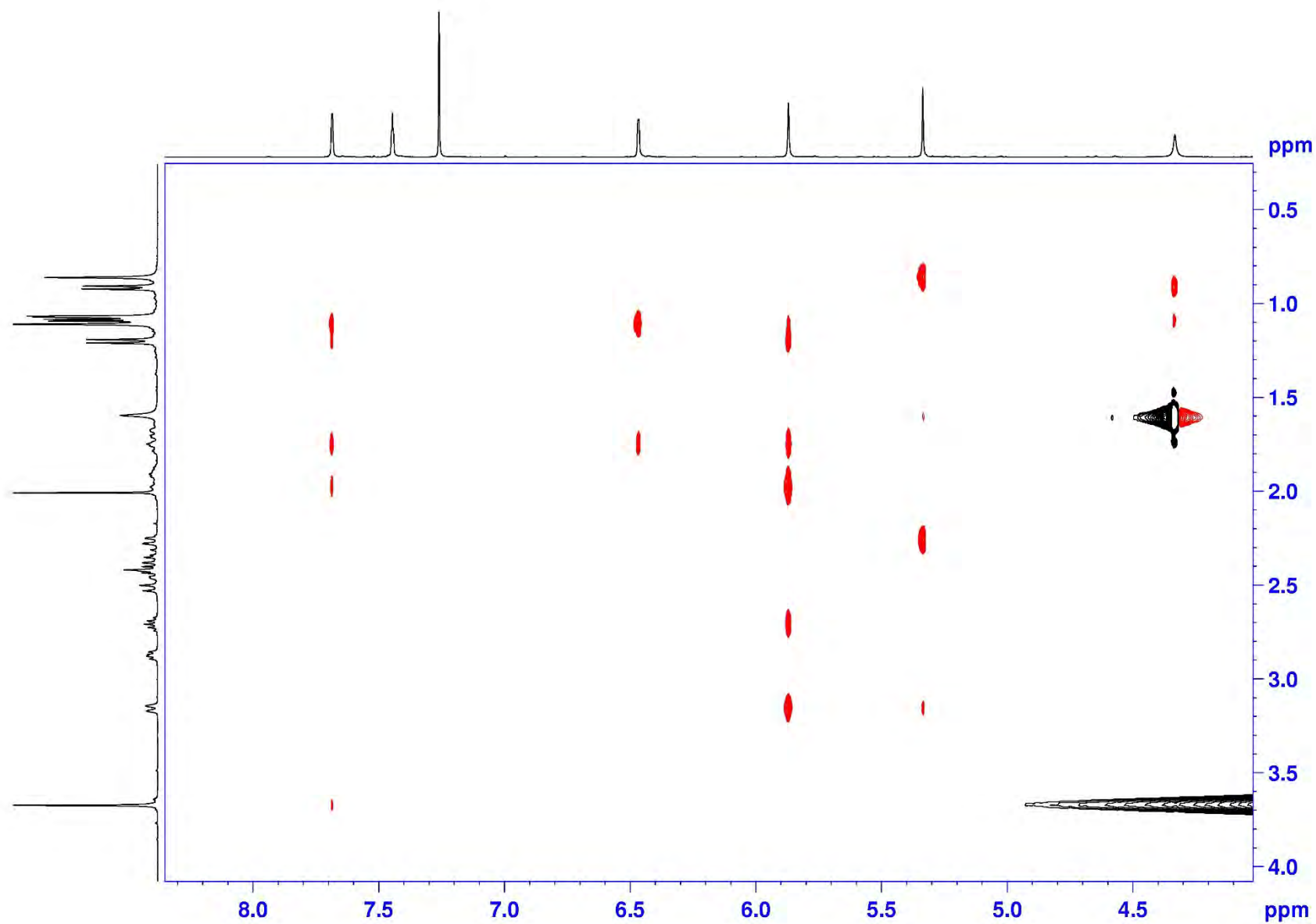
```

===== 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                   400.1300090 MHz
WDW                  QSINE
SSB                  2
LB                   0.00 Hz
GB                   0
PC                   1.00
SI                   1024
MC2                  States-TPPI
SF                   400.1300090 MHz
WDW                  QSINE
  
```

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



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



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

