

Supporting Information

Copies of HR-ESIMS, and 1D and 2D NMR spectra of Compounds 24-29.

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HR-ESIMS for compound 24

Mass Spectrum SmartFormula Report

Analysis Info

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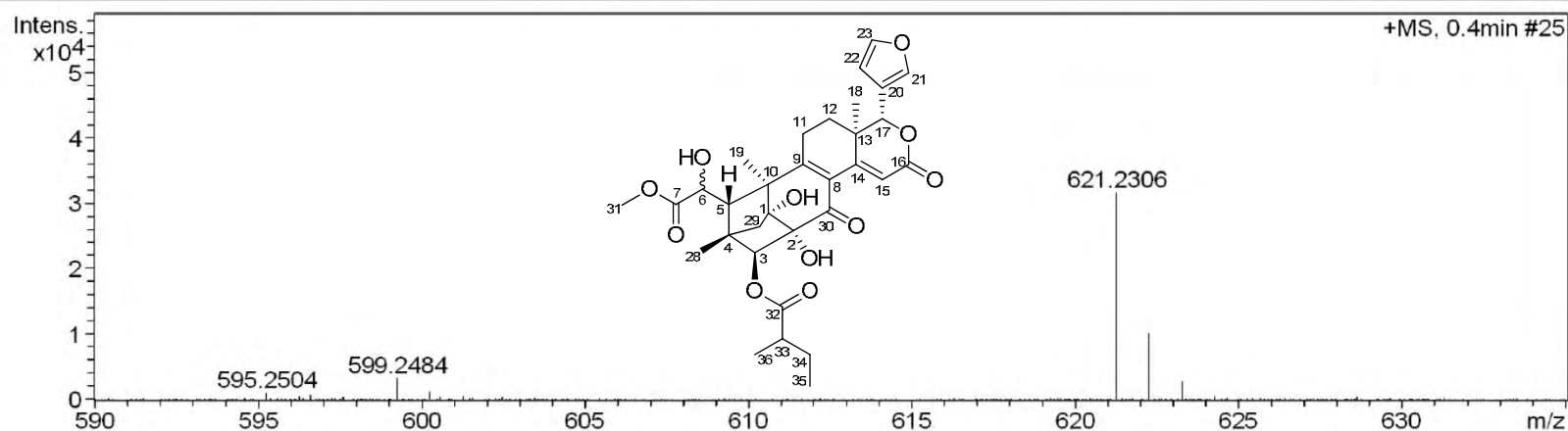
Acquisition Date 5/19/2016 8:48:09 AM

Operator SCSIO

Instrument / Ser# maXis 29

Acquisition Parameter

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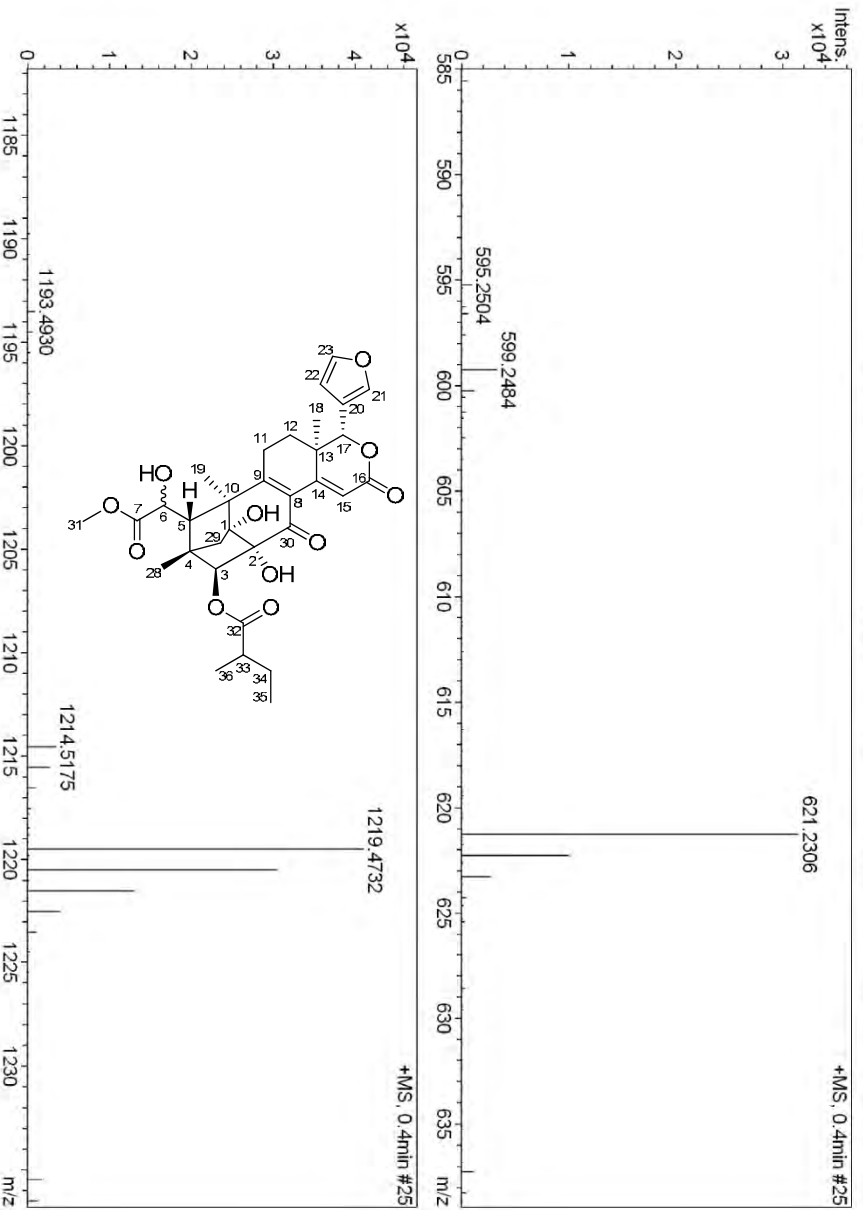
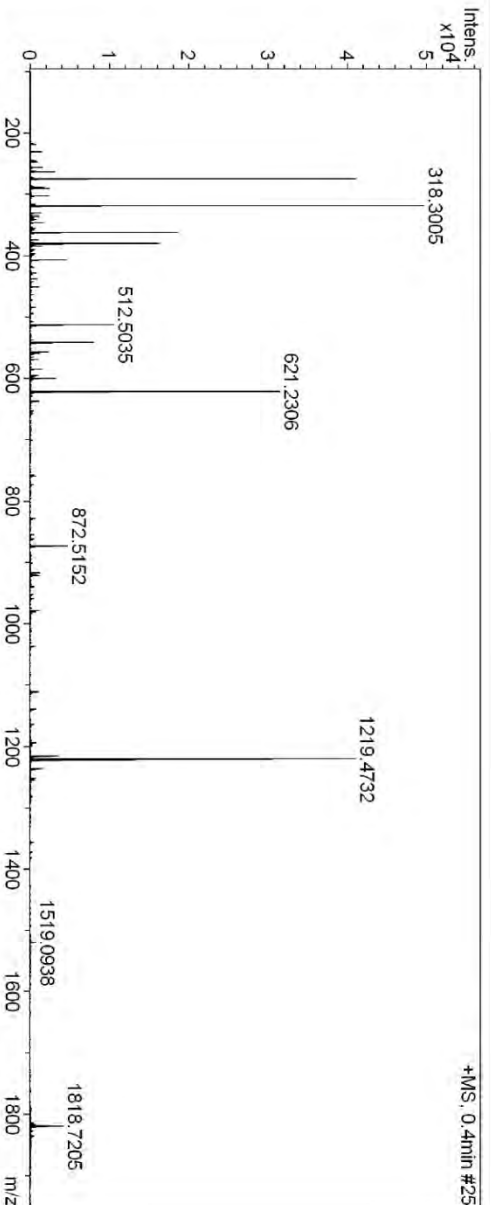
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Generic Display Report

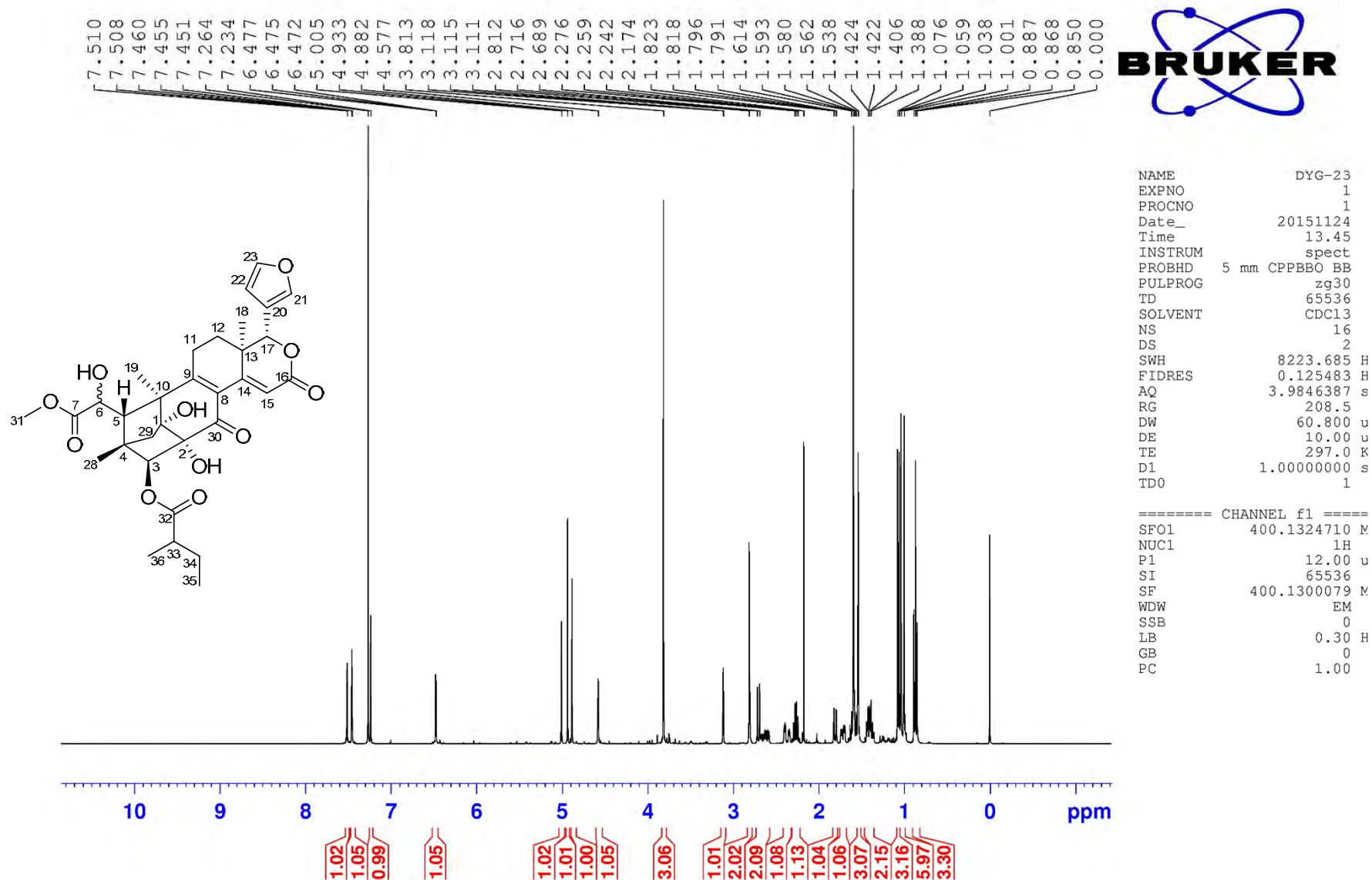
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Analysis Info

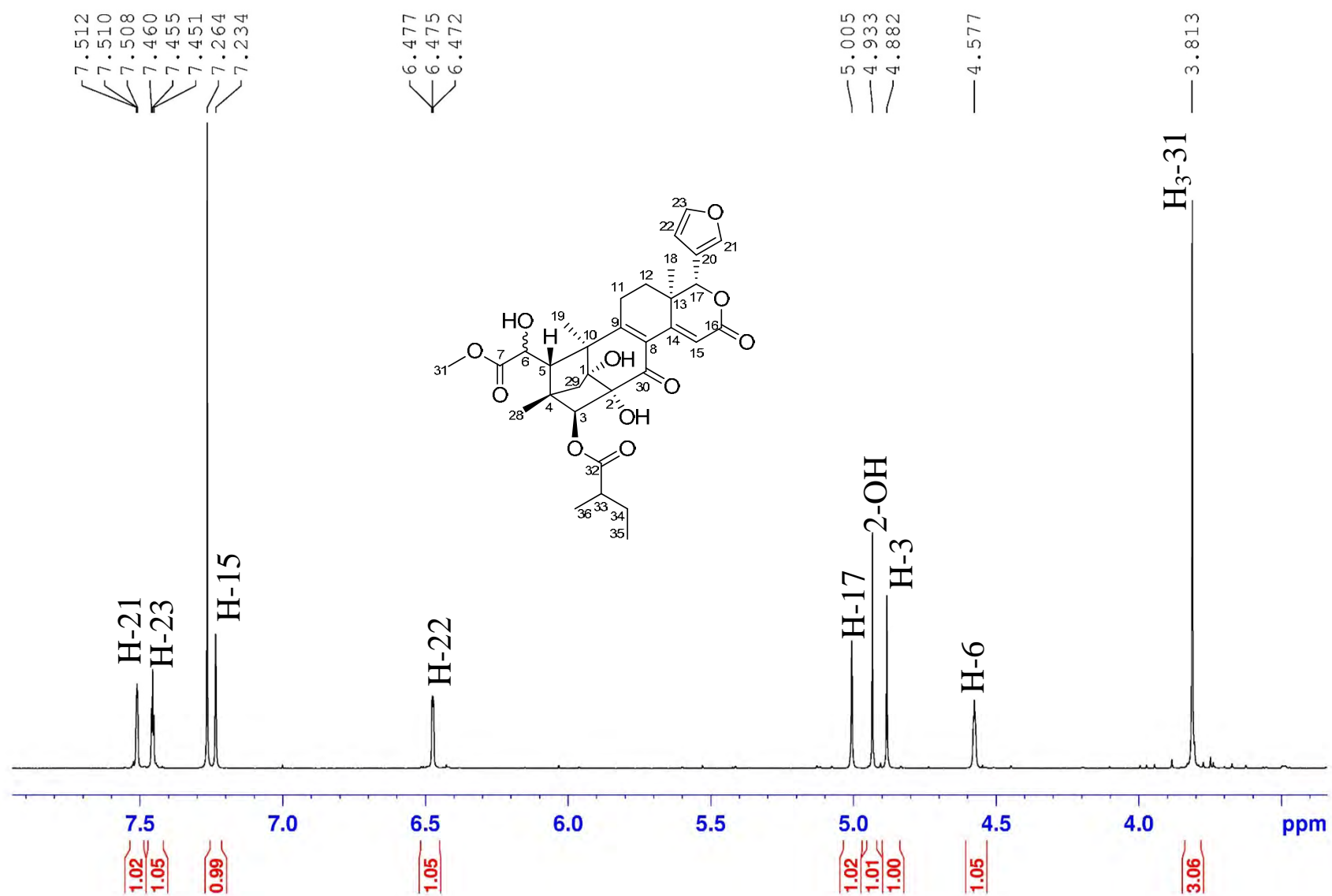
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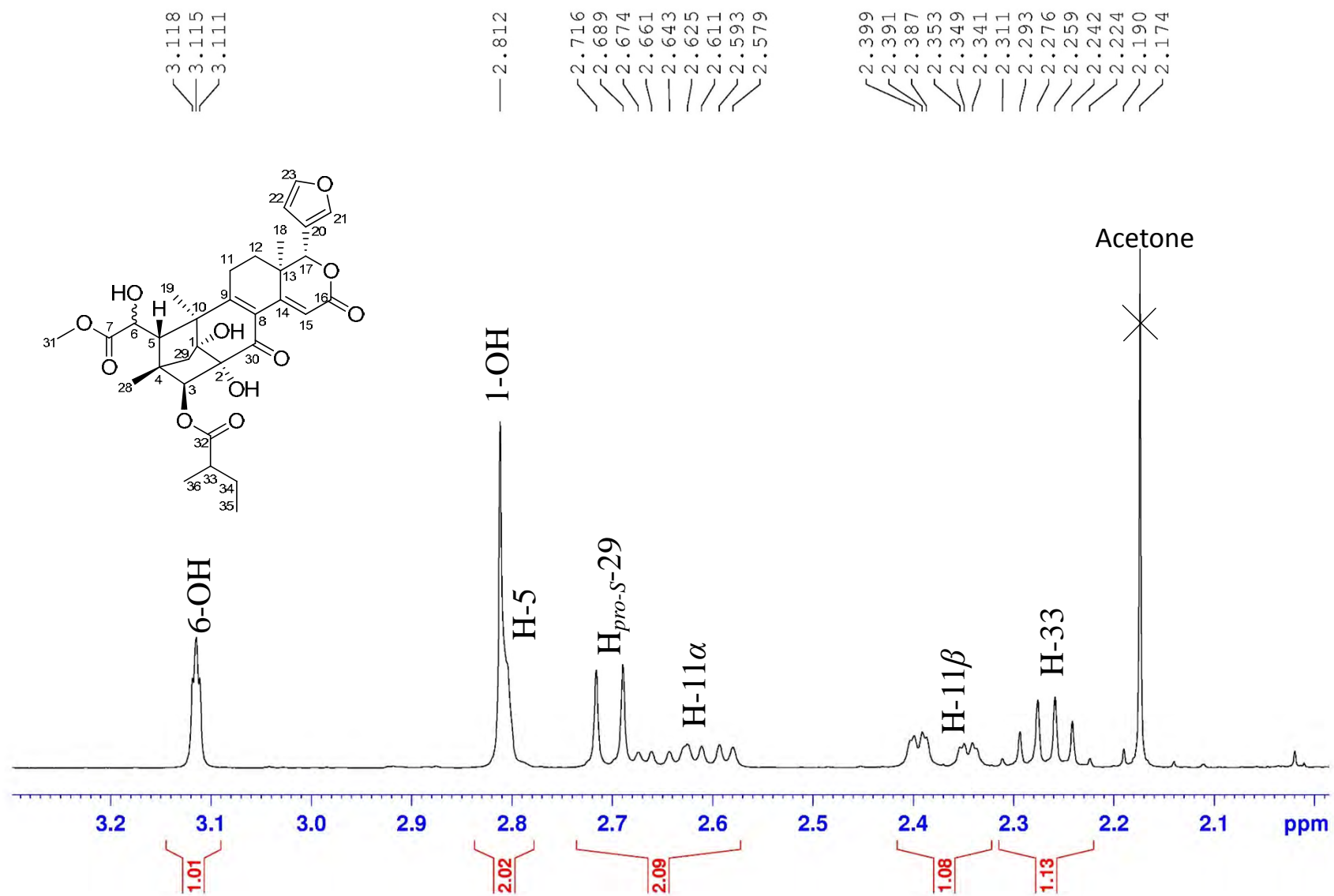
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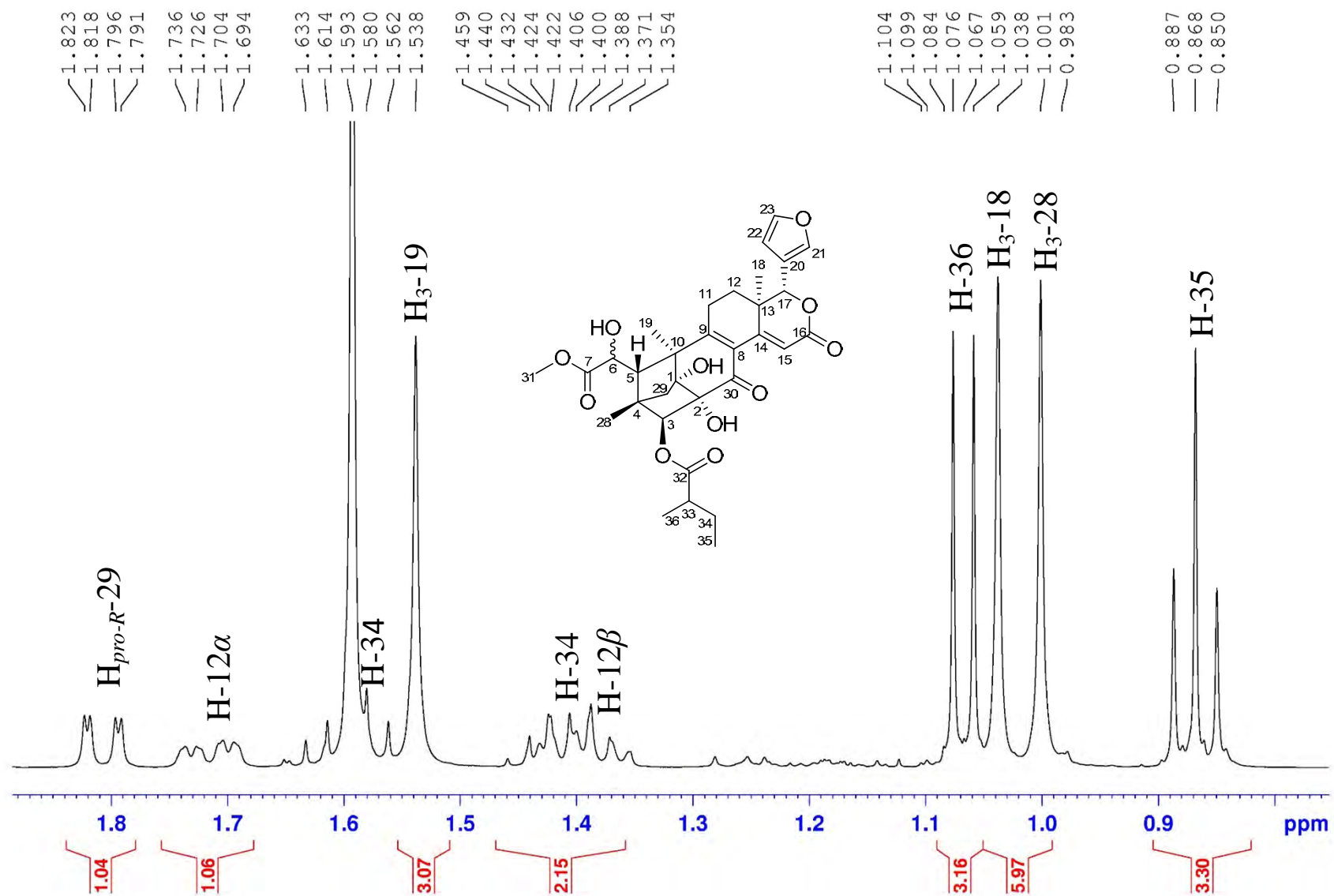
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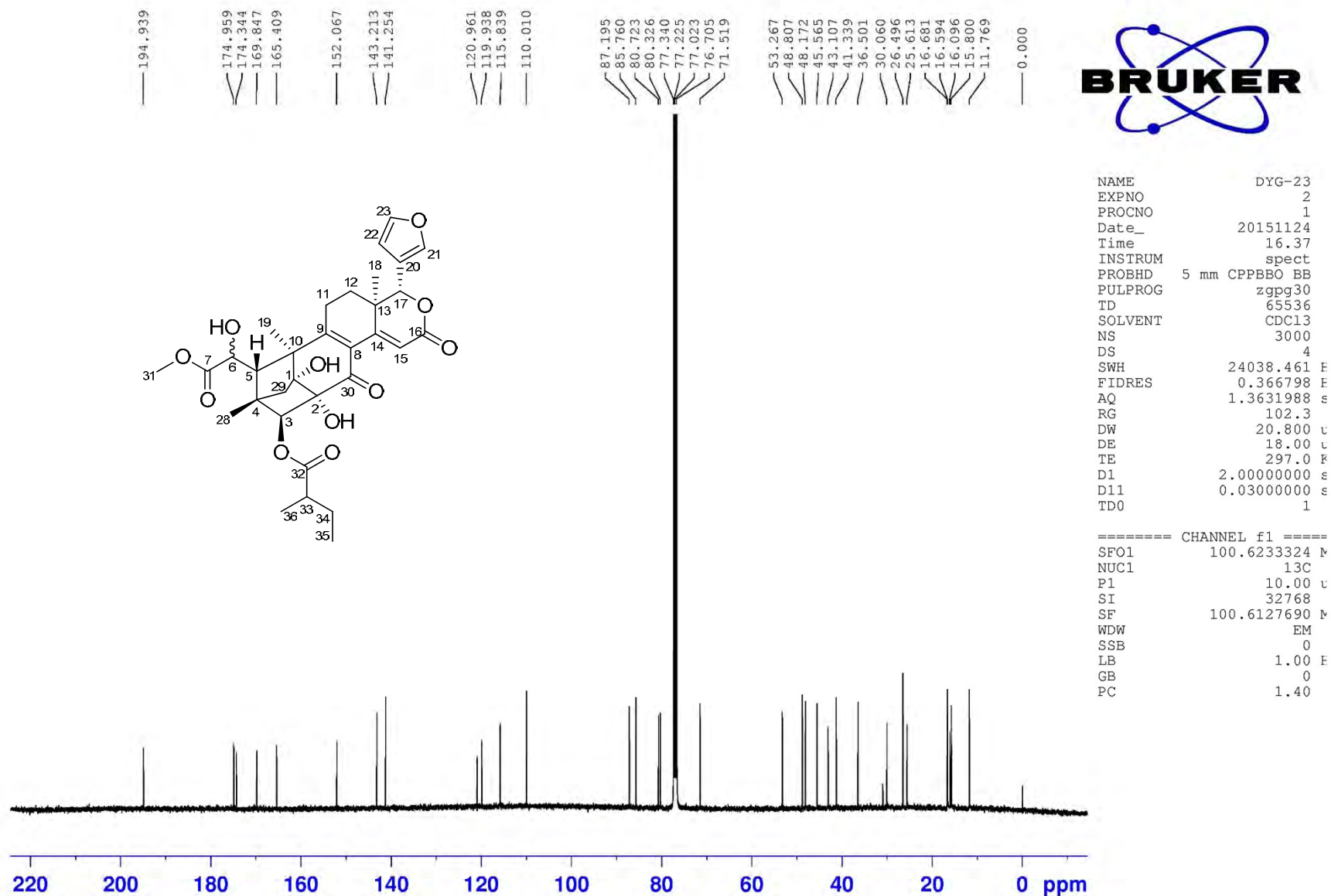
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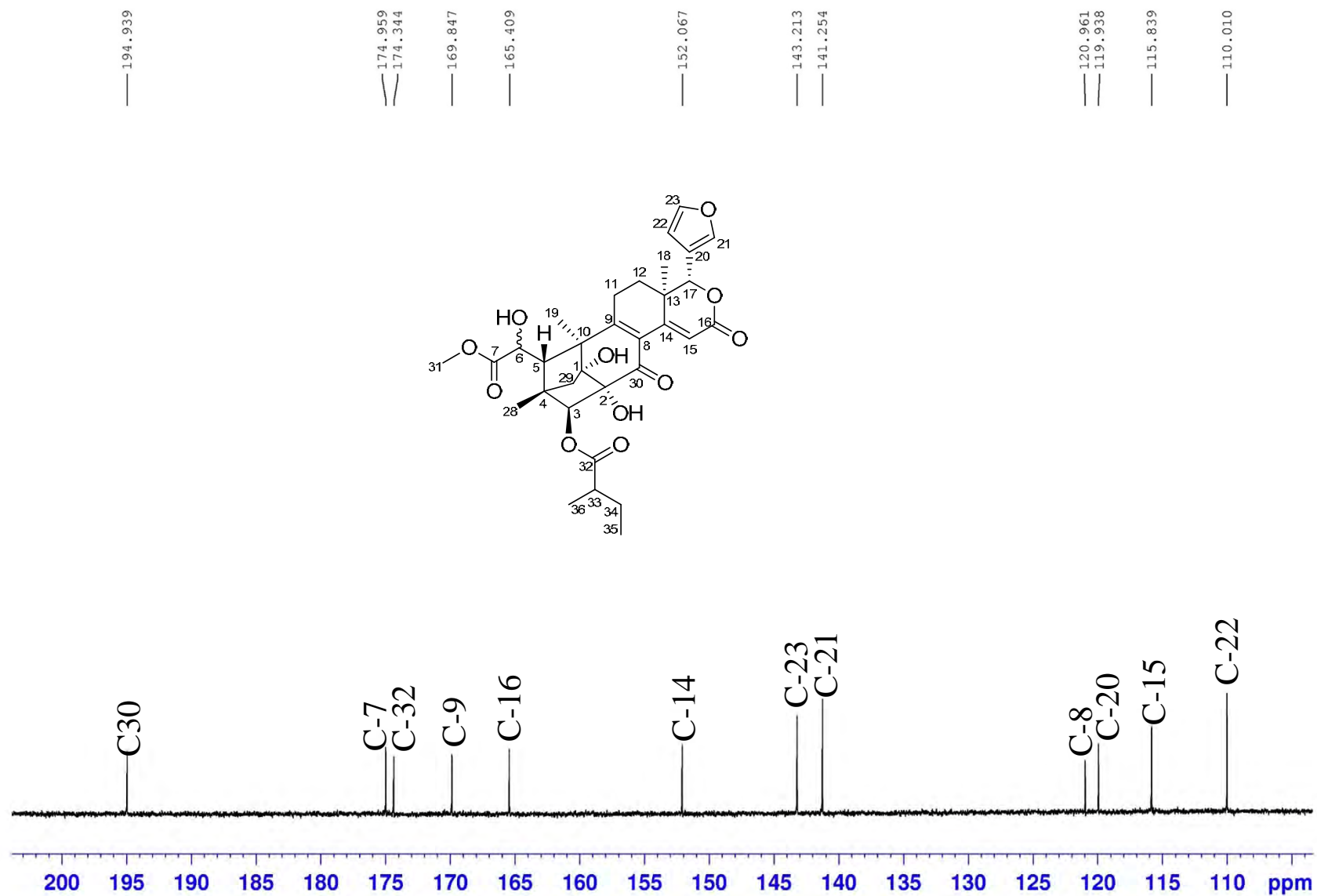
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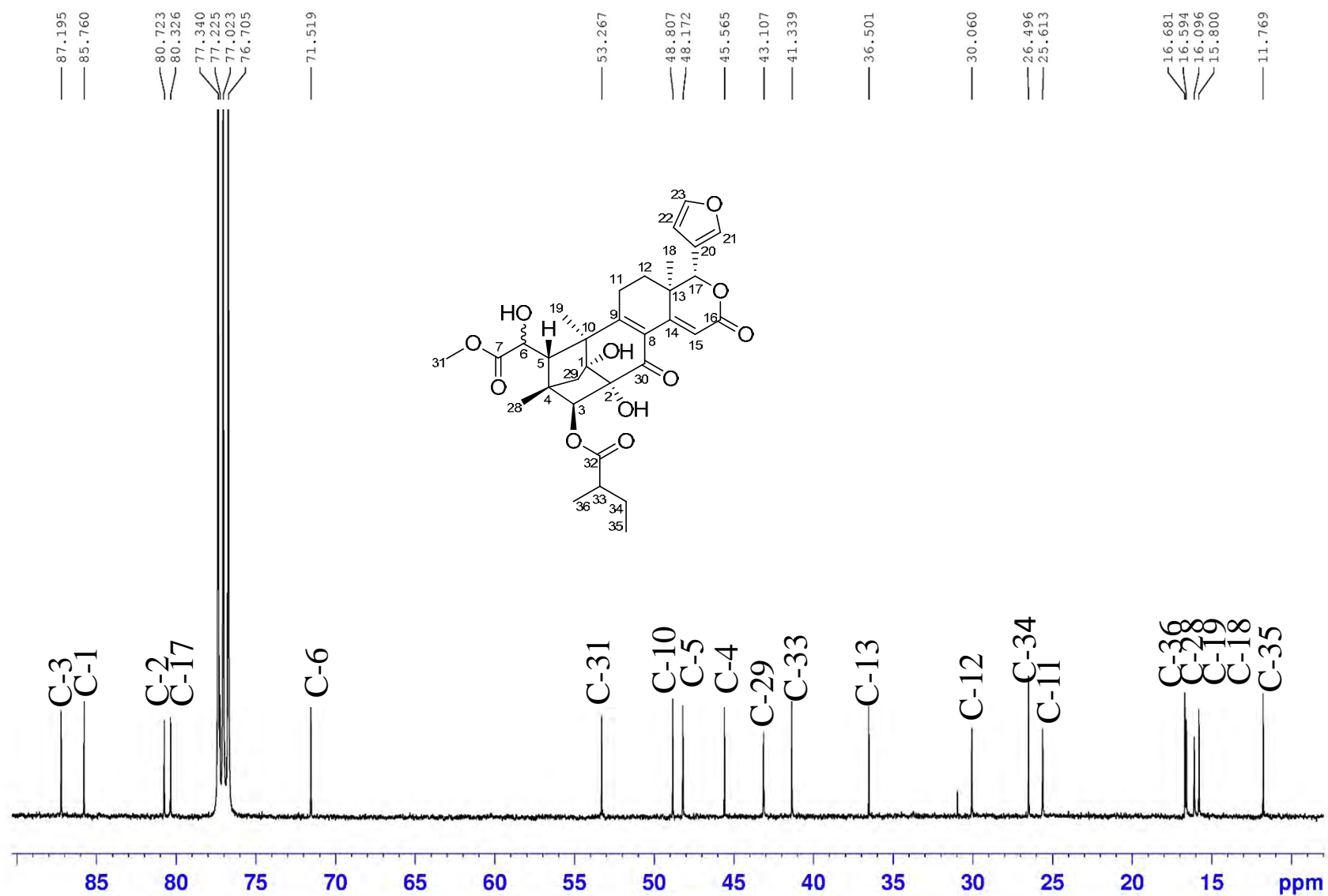
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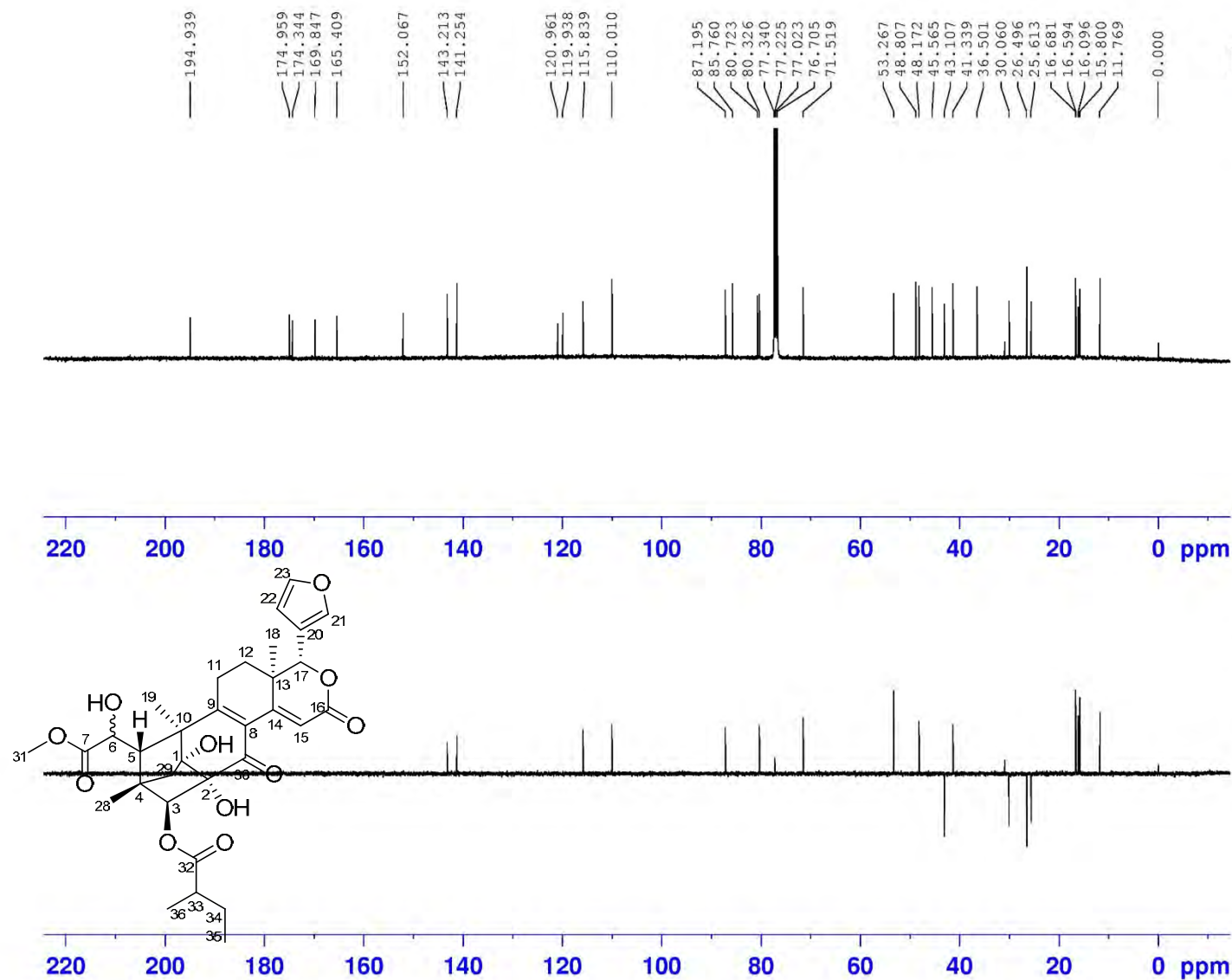
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^{13}C NMR (100 MHz) spectrum of compound **24** in CDCl_3



DEPT135 (100 MHz) spectrum of compound **24** in CDCl₃



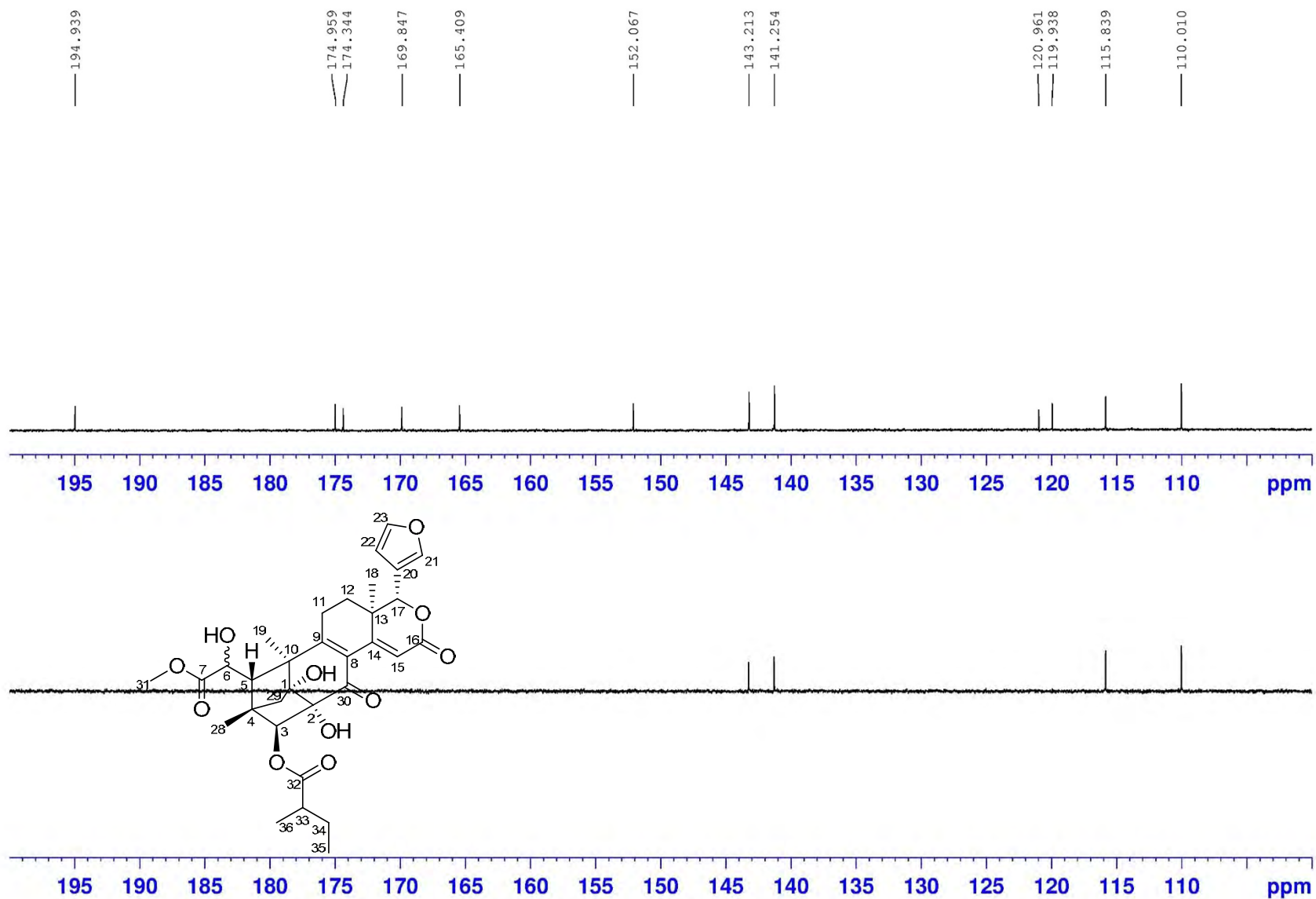
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FIDRES         0.366798 F
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RG             91.64
DW            20.800 s
DE            18.00 s
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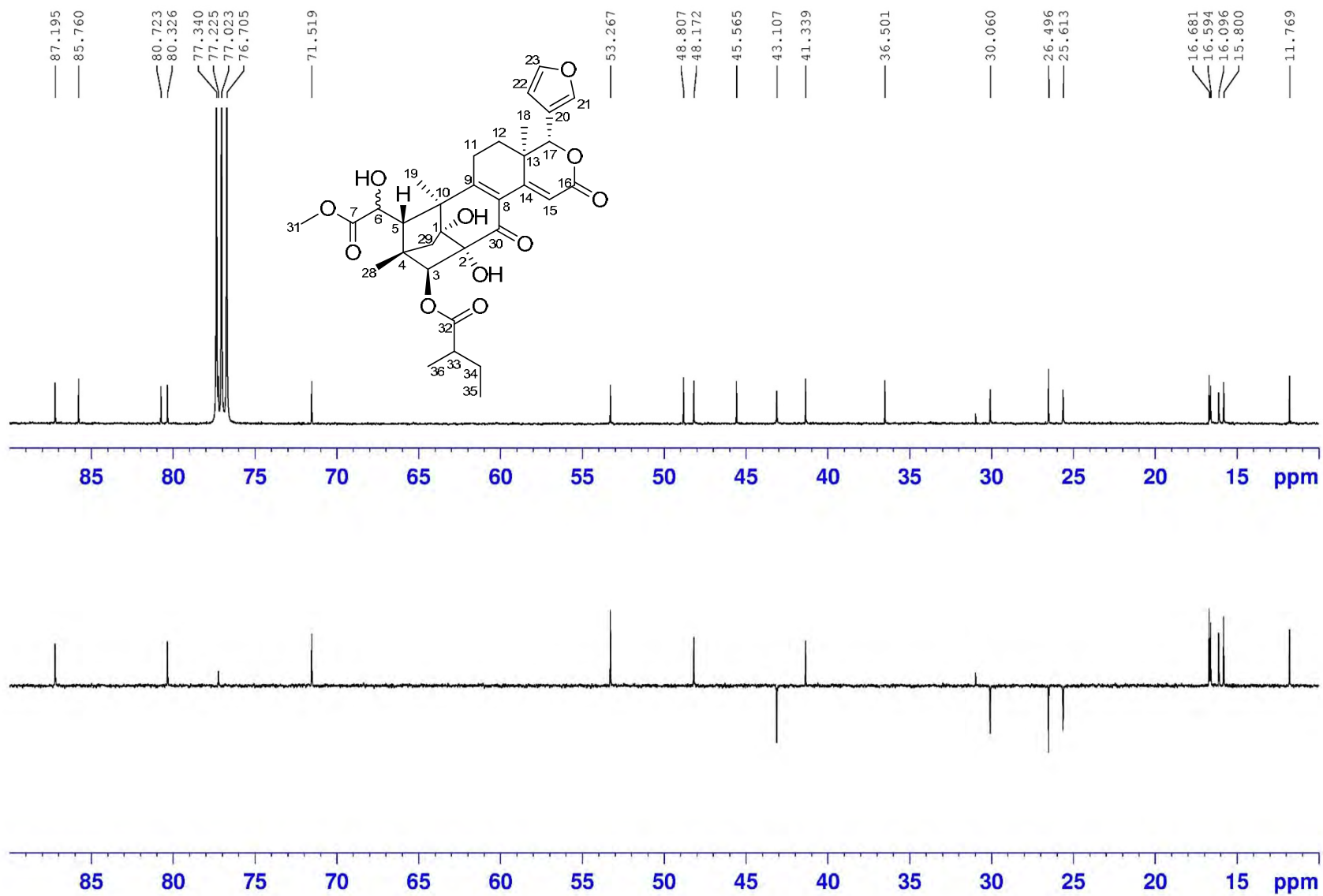
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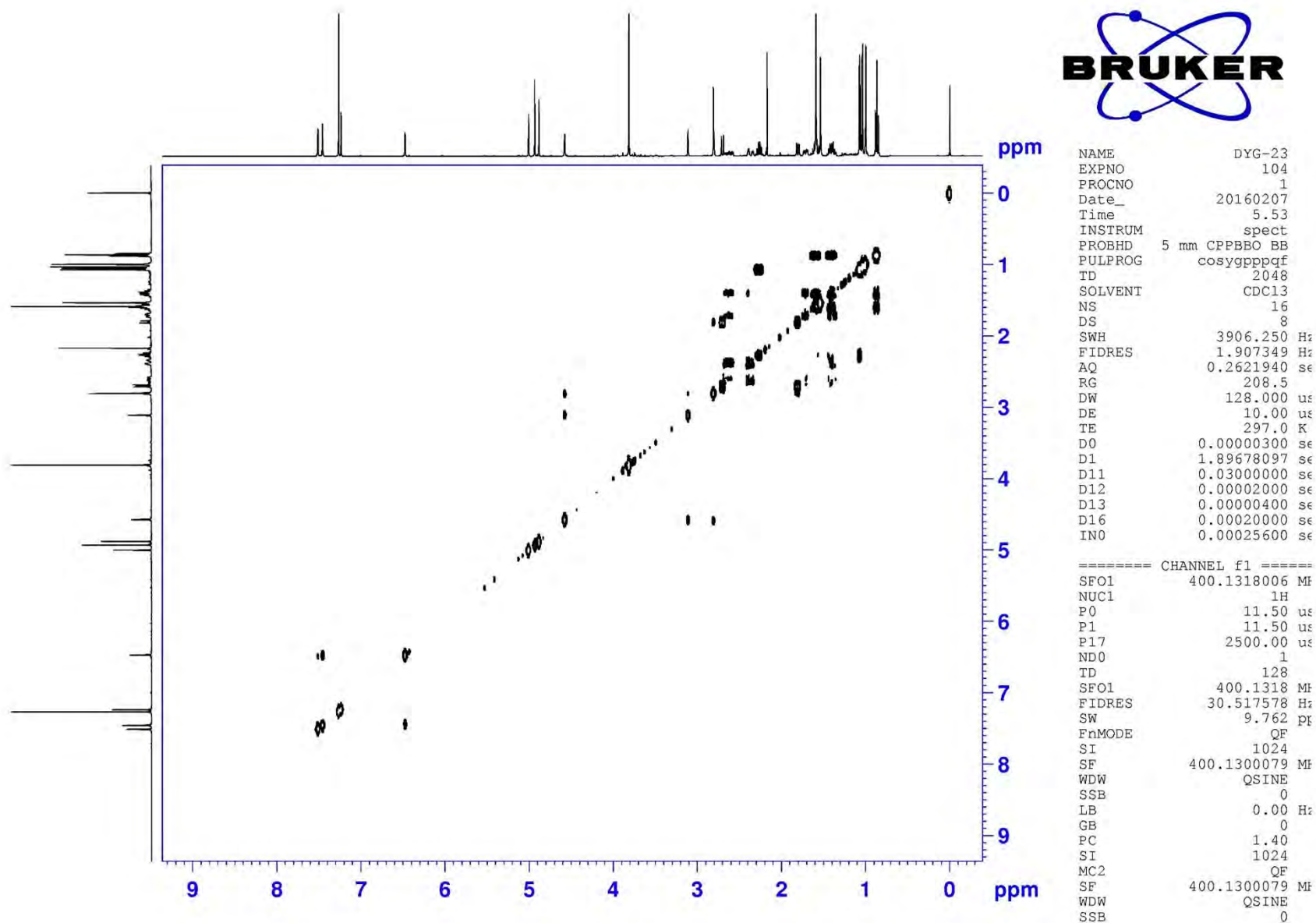
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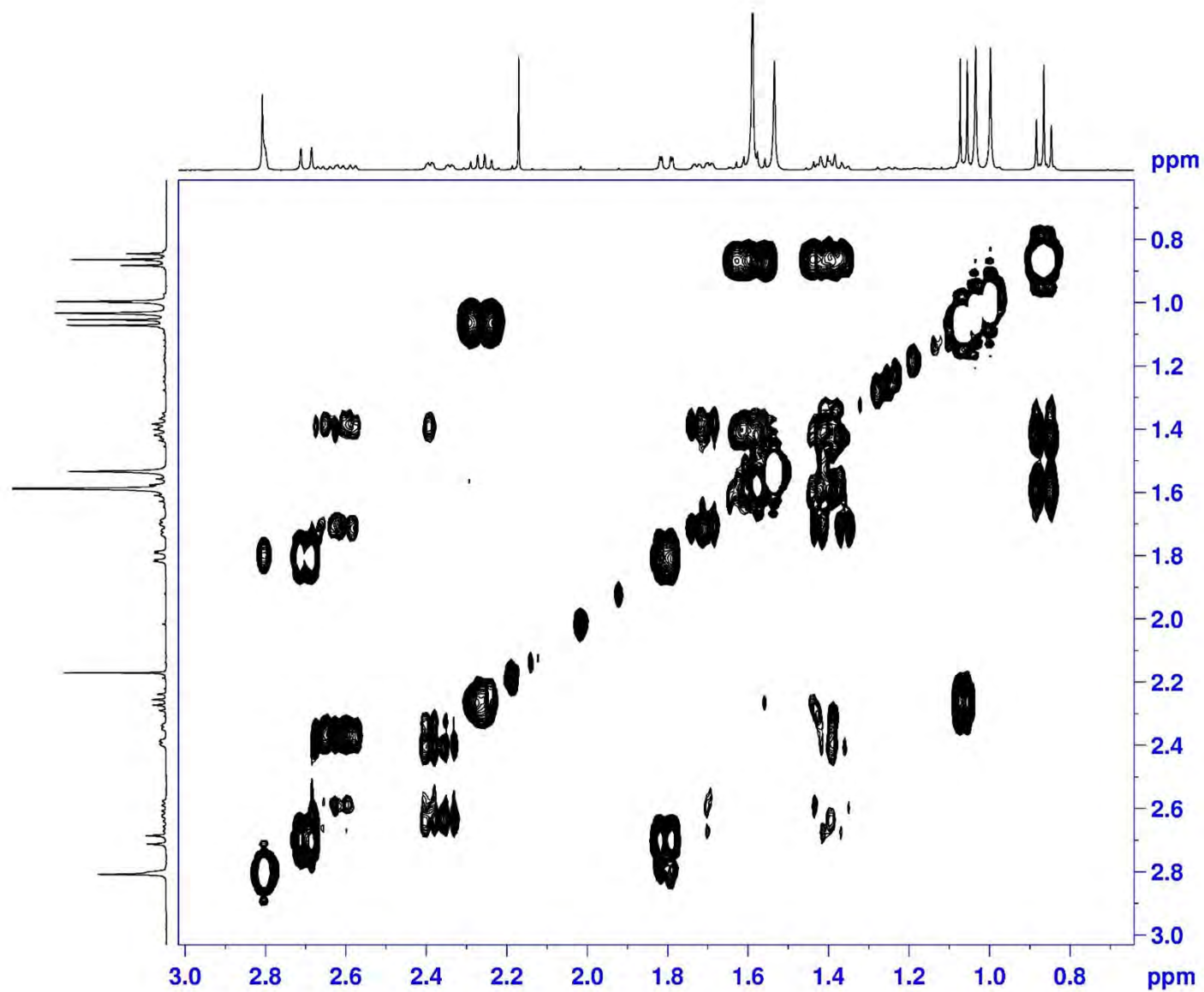
DEPT135 (100 MHz) spectrum of compound **24** in CDCl₃



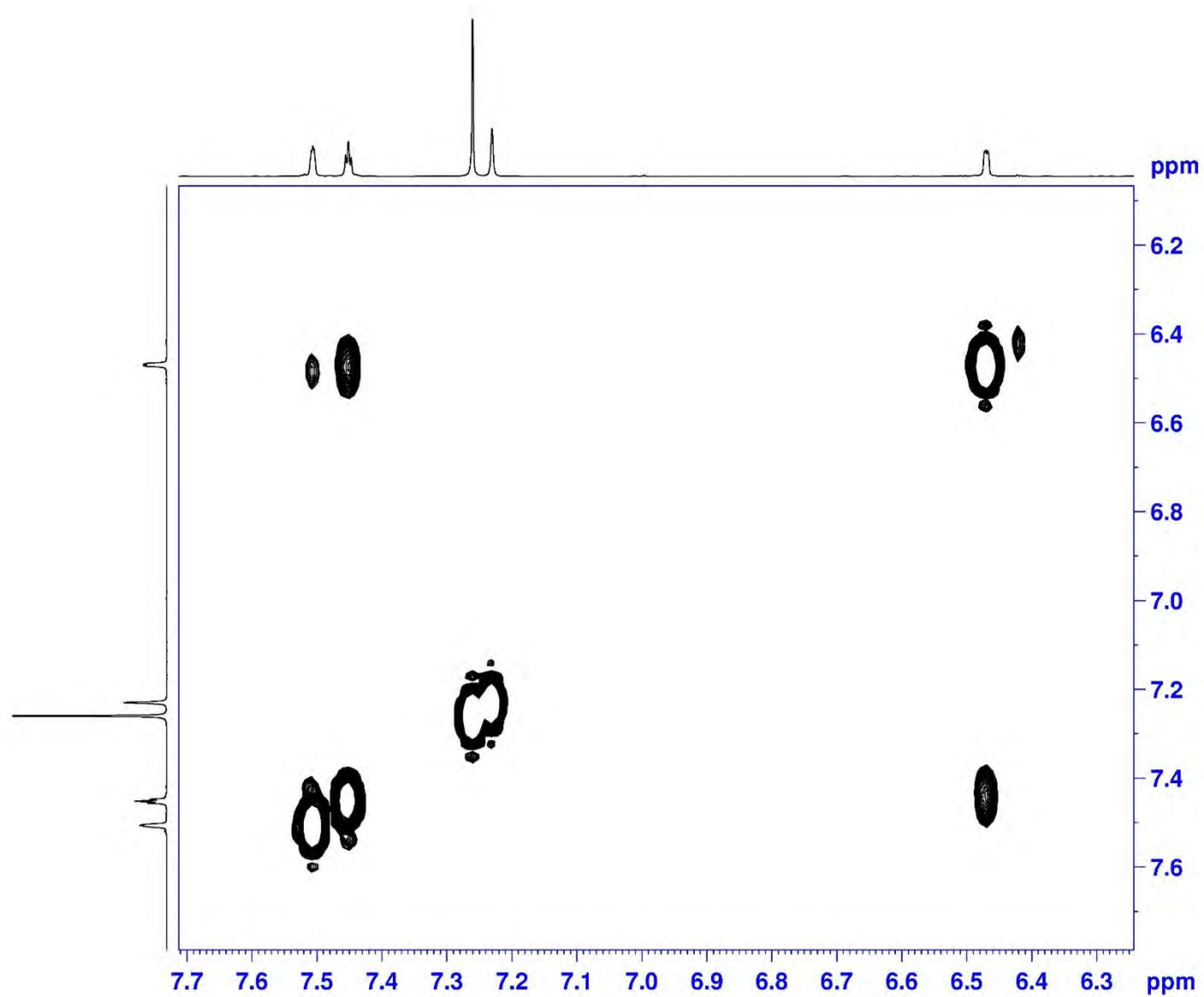
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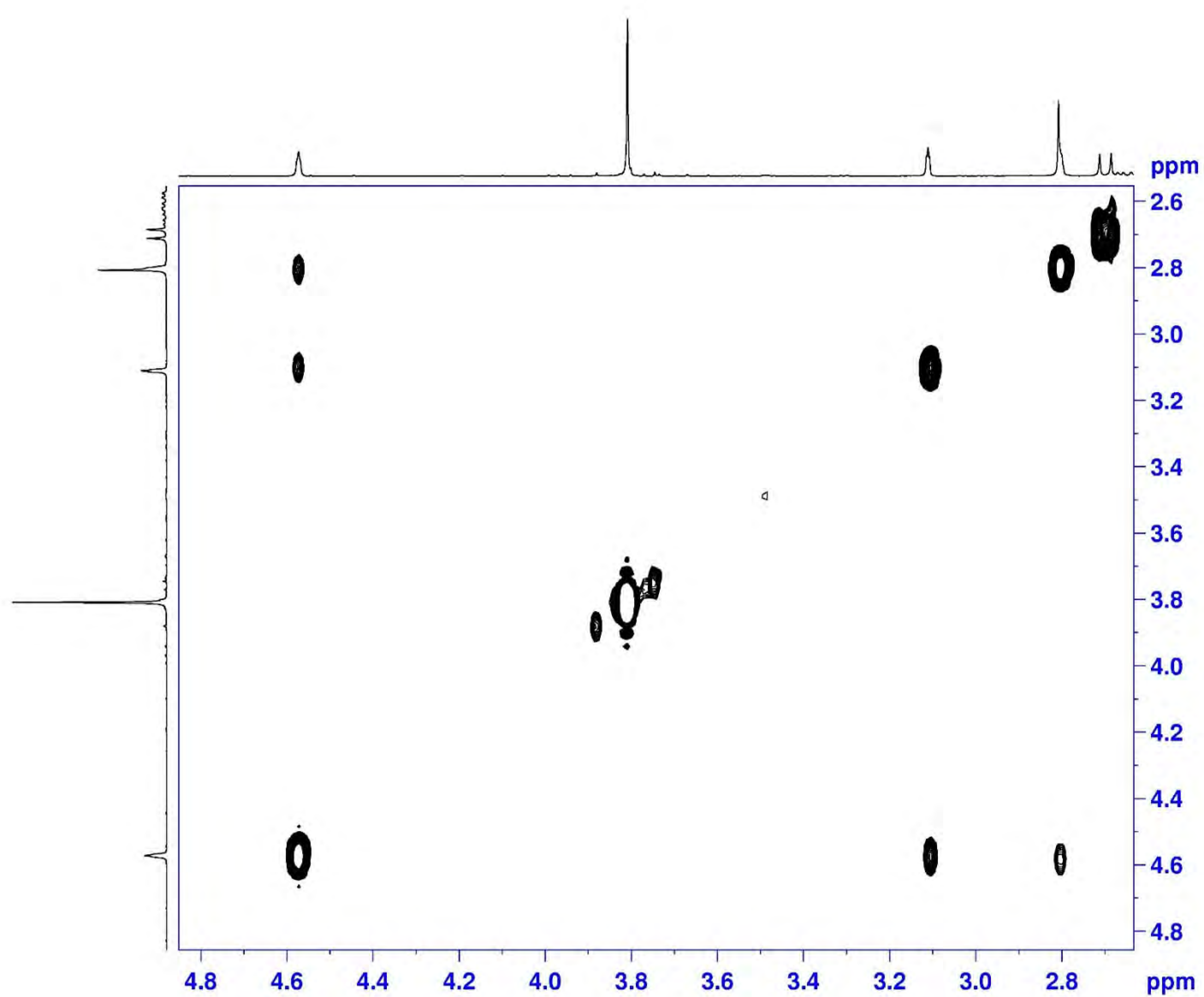
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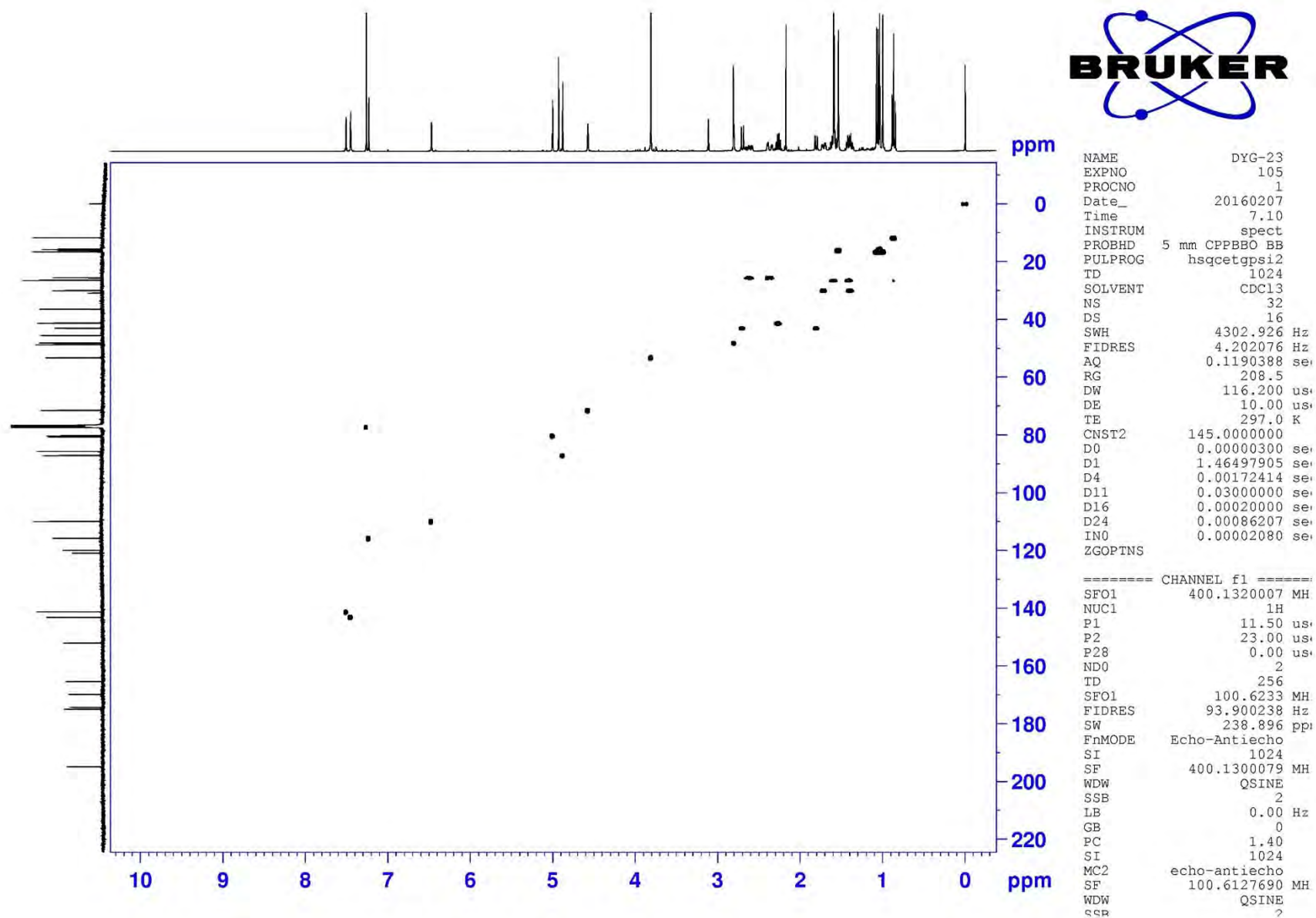
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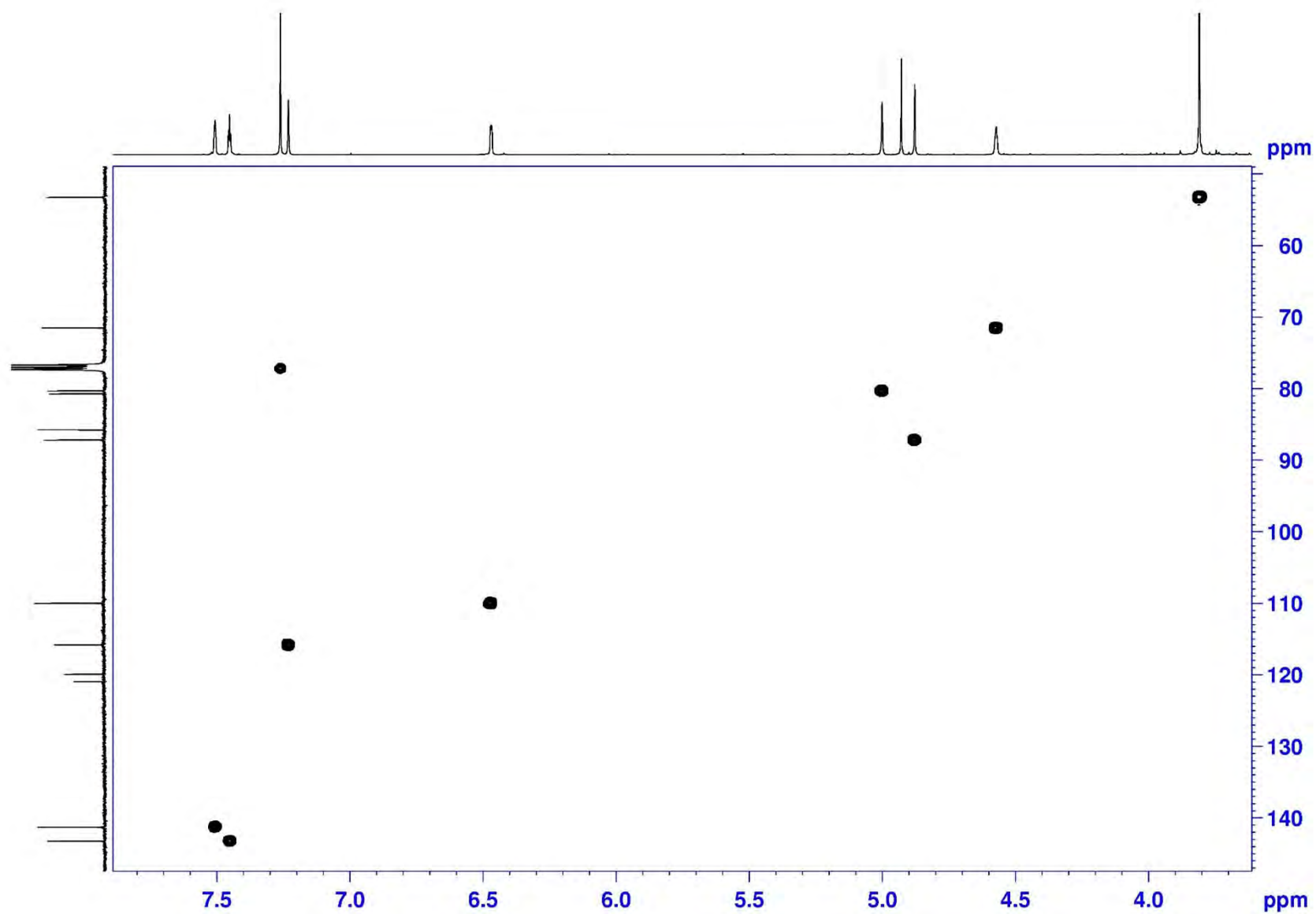
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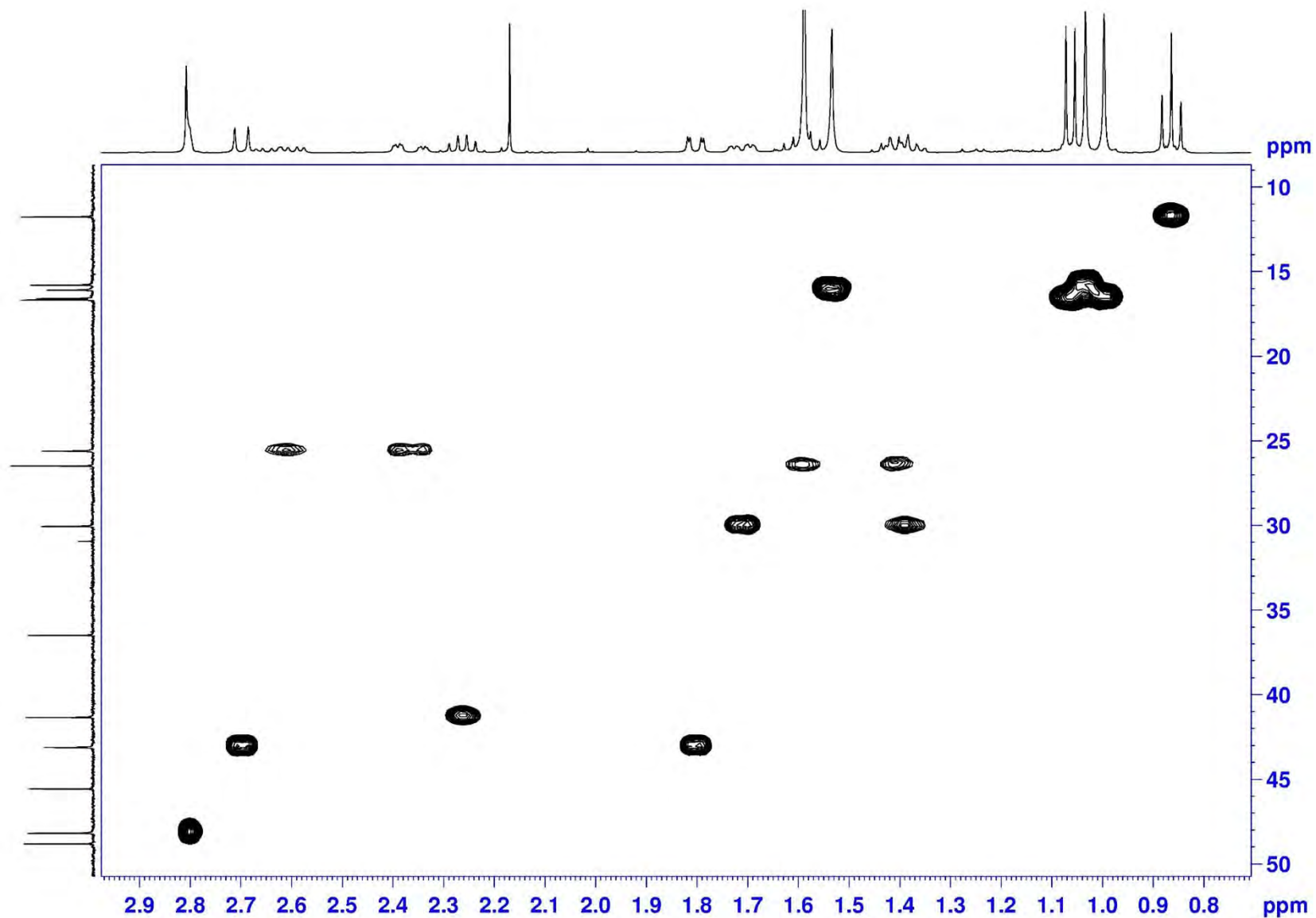
HSQC (400 MHz) spectrum of compound **24** in CDCl₃



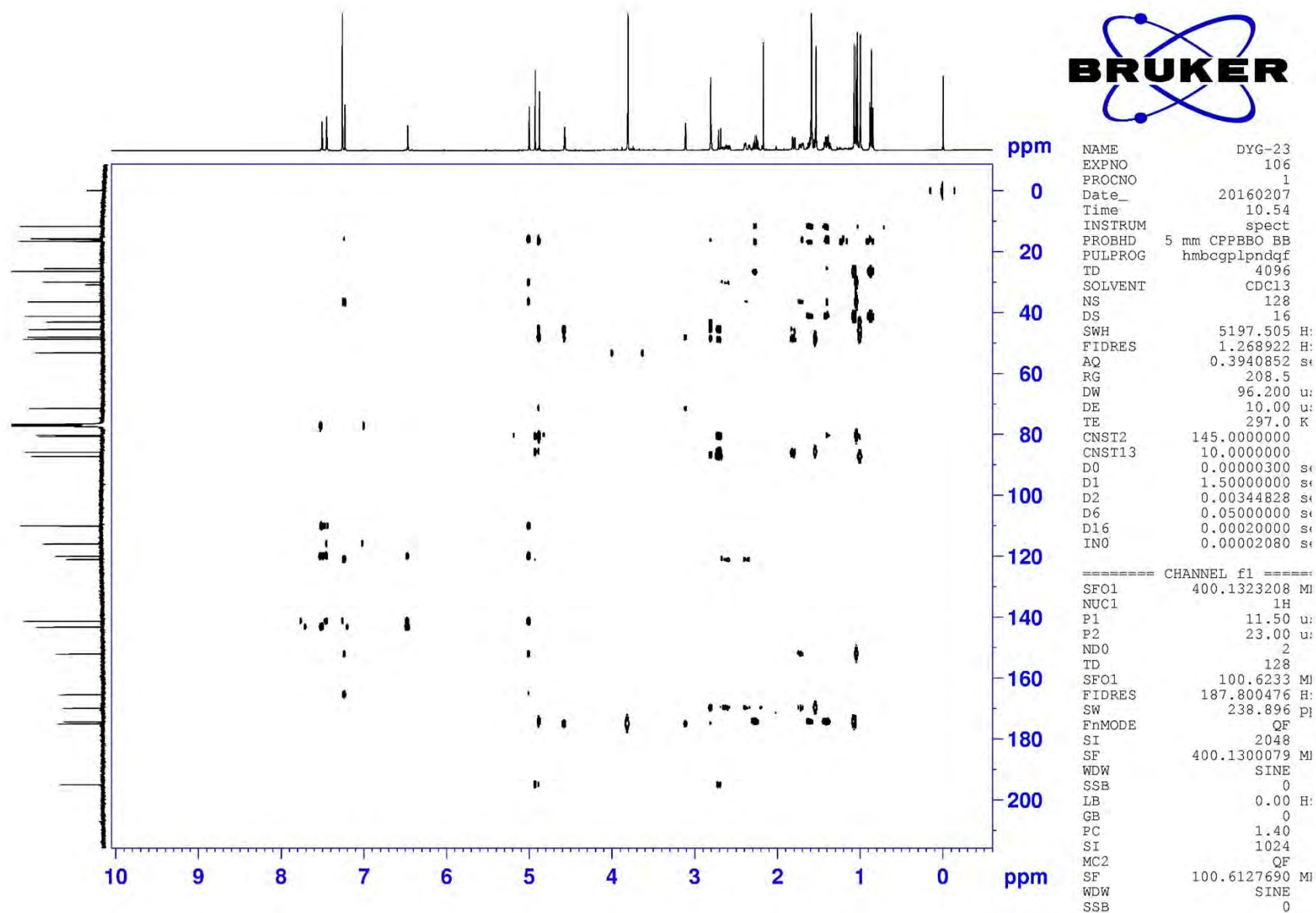
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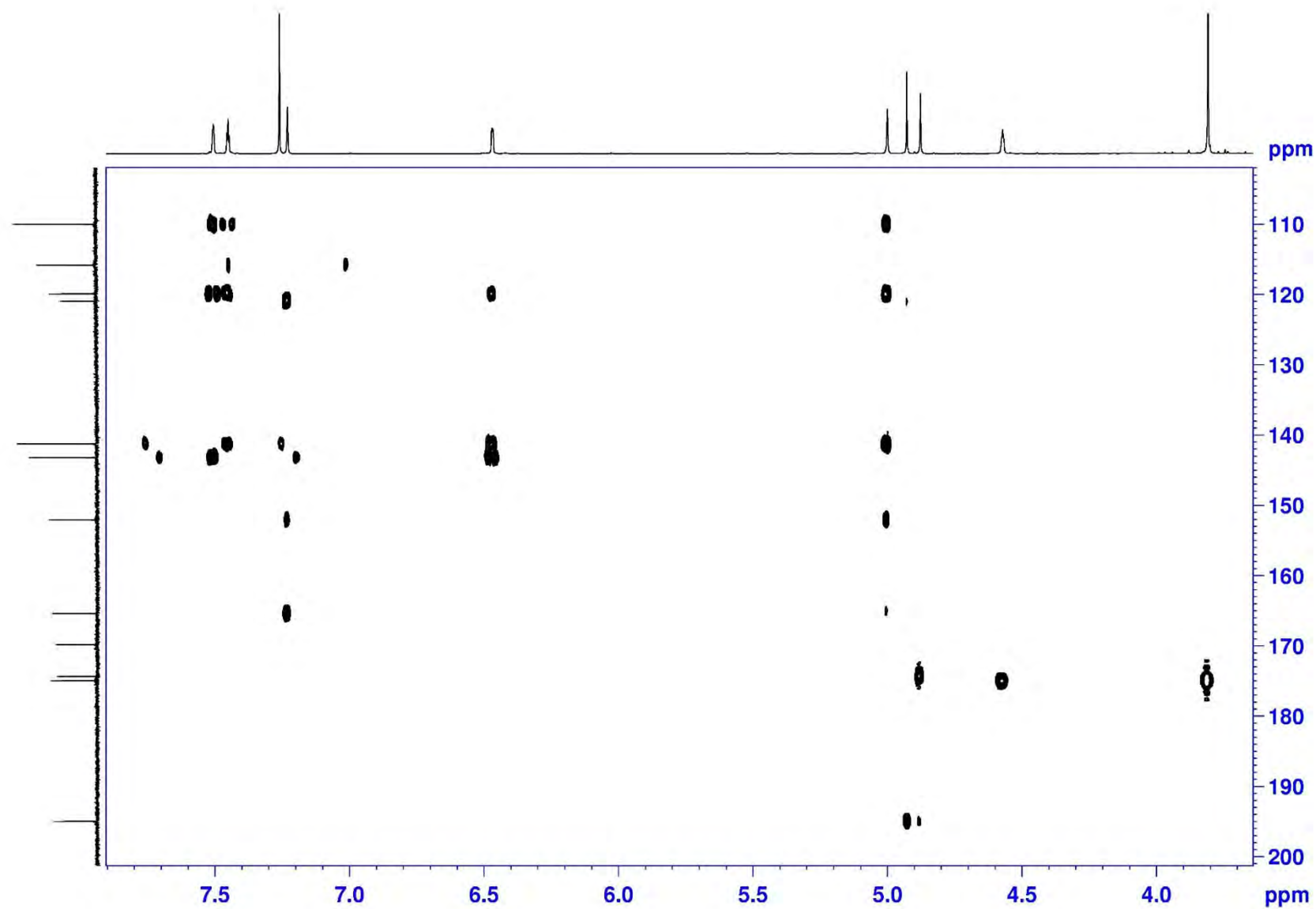
HSQC (400 MHz) spectrum of compound **24** in CDCl_3



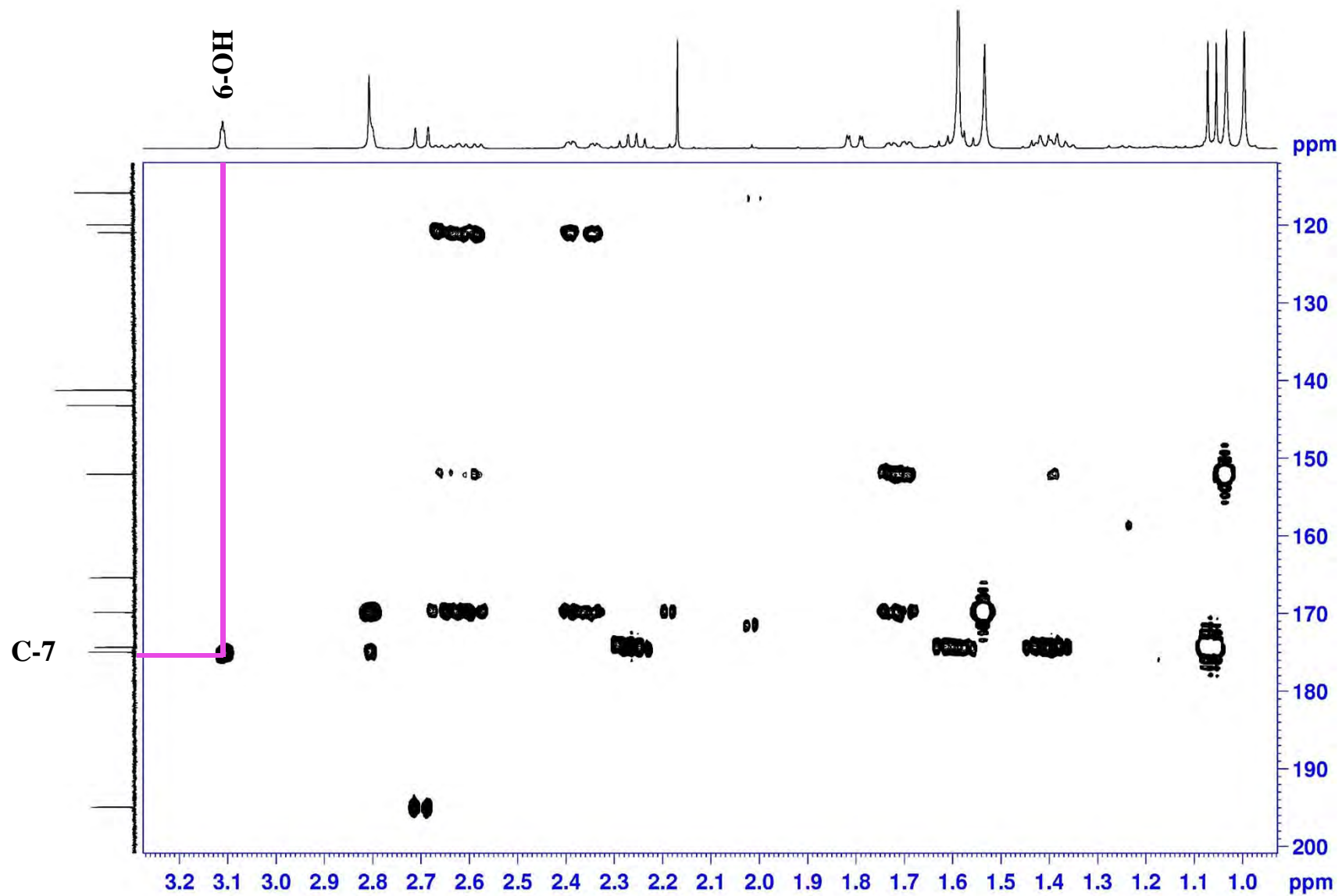
HMBC (400 MHz) spectrum of compound **24** in CDCl₃



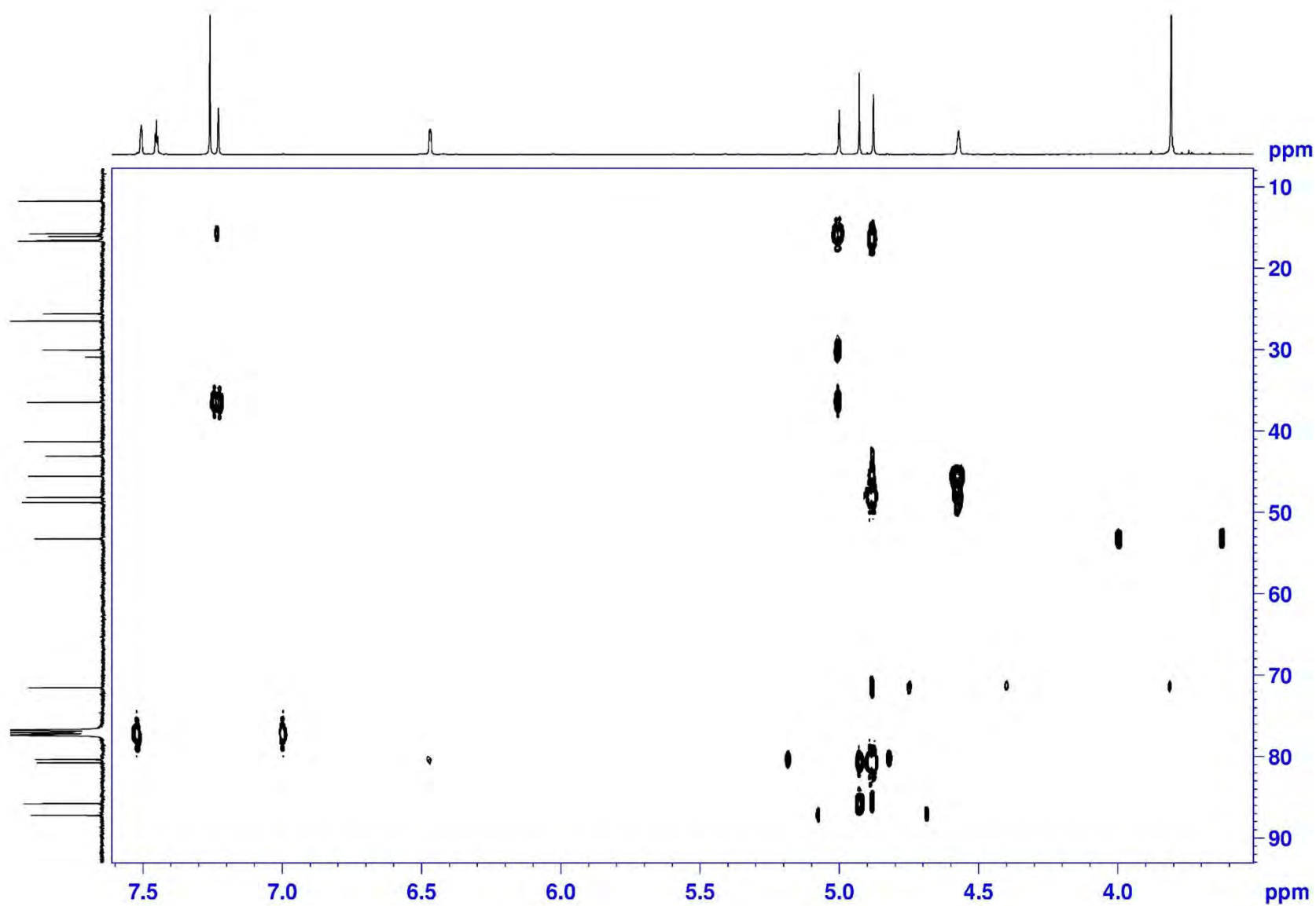
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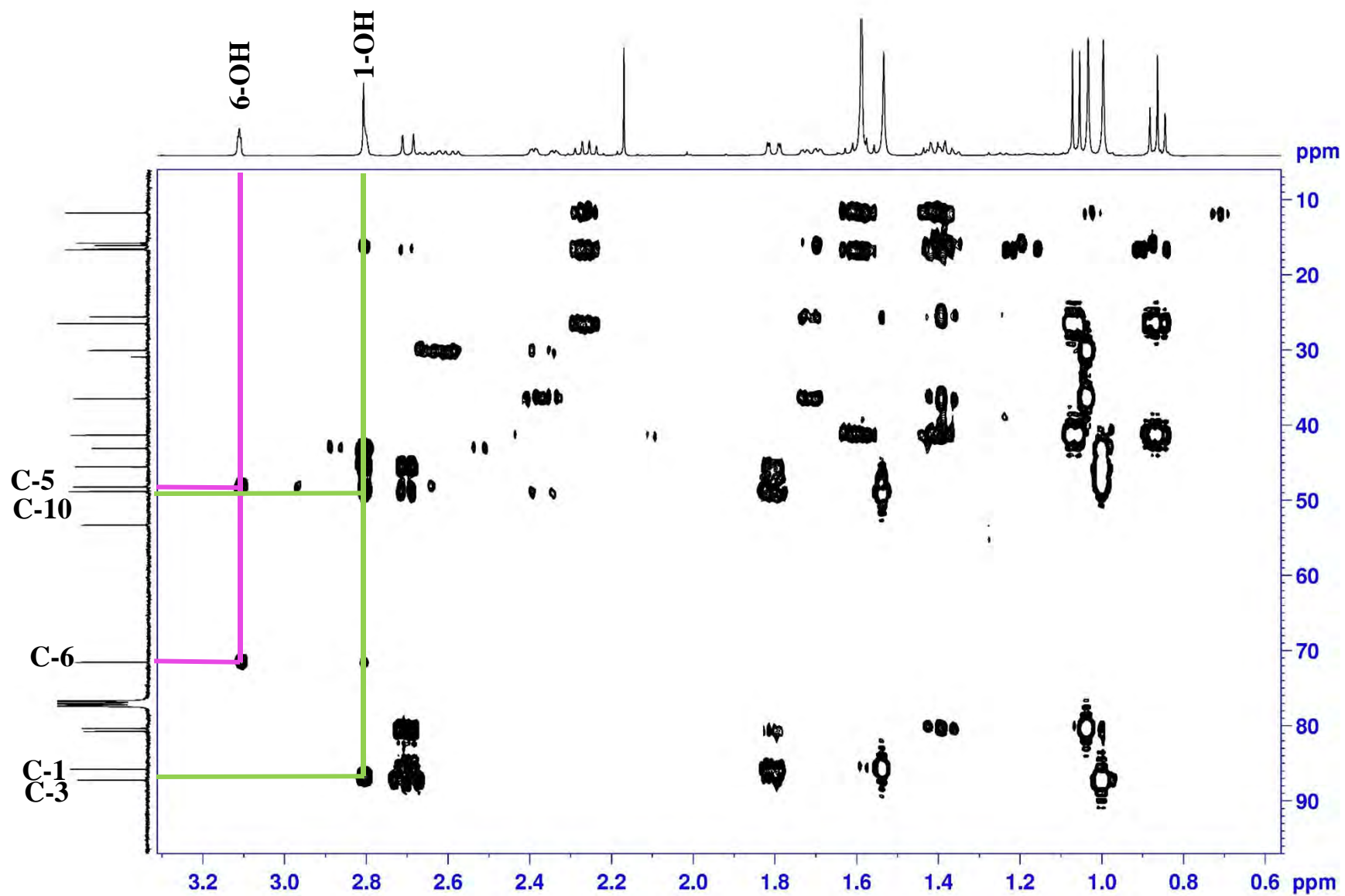
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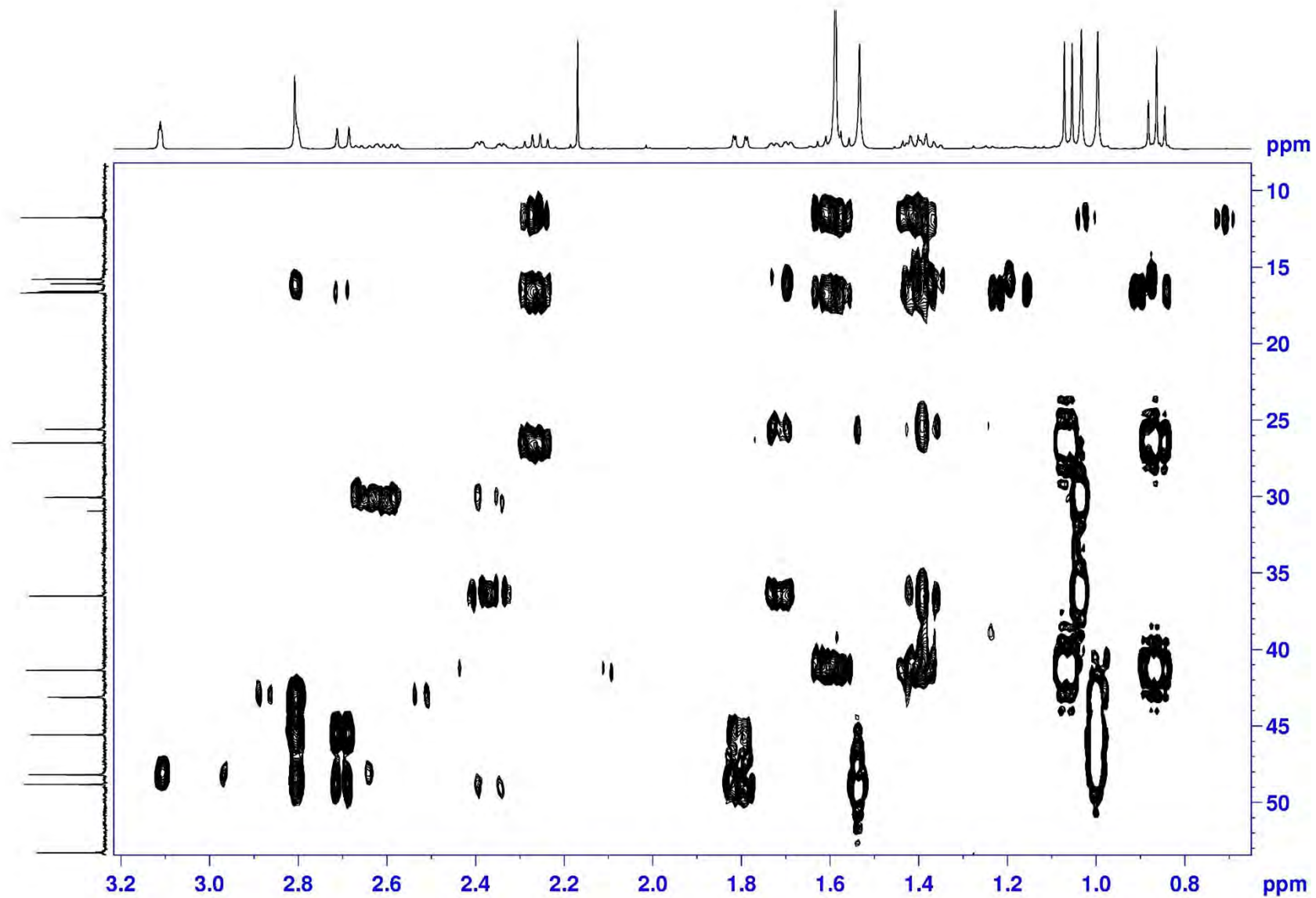
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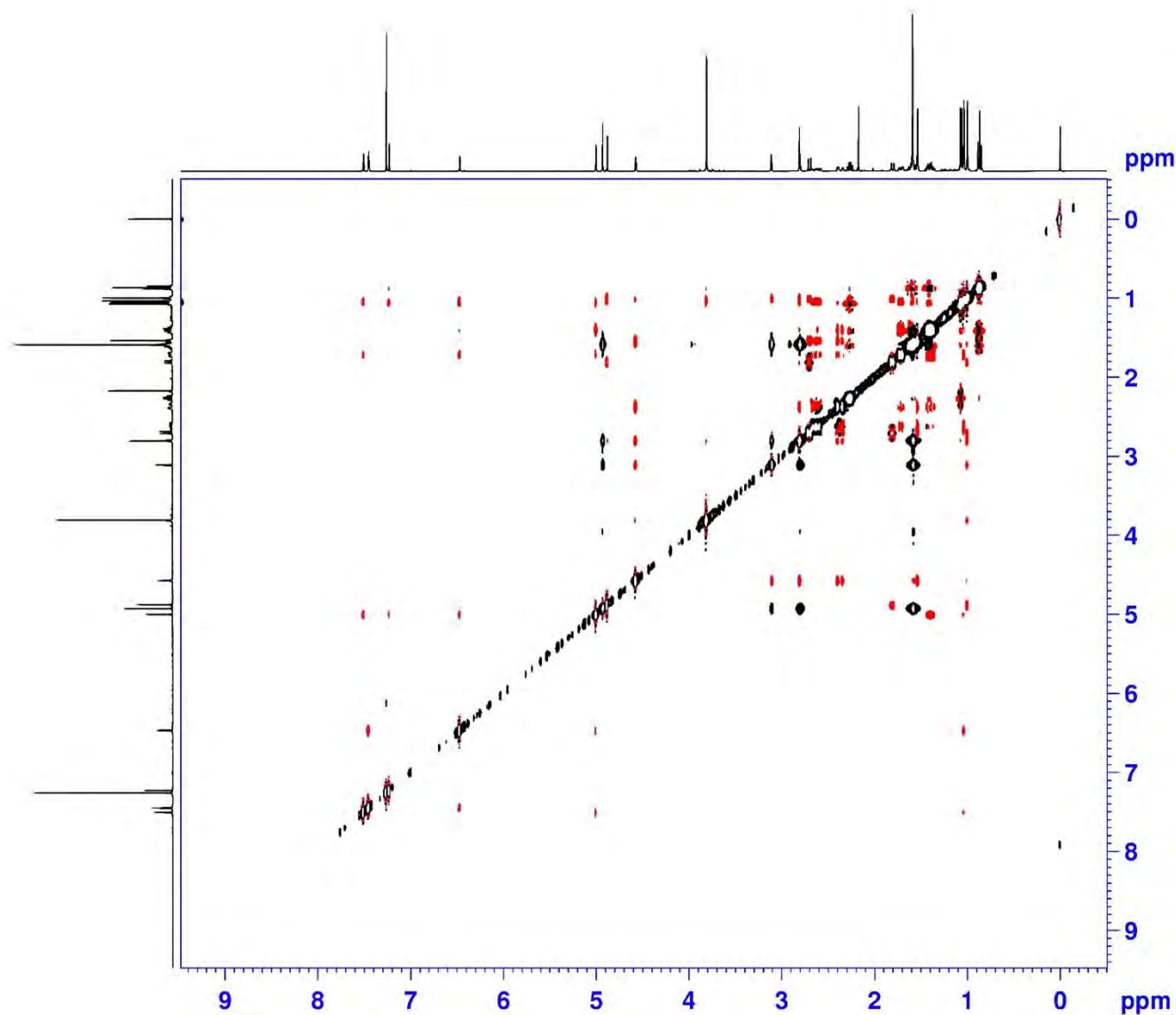
HMBC (400 MHz) spectrum of compound **24** in CDCl_3



HMBC (400 MHz) spectrum of compound **24** in CDCl₃



NOESY (400 MHz) spectrum of compound **24** in CDCl₃



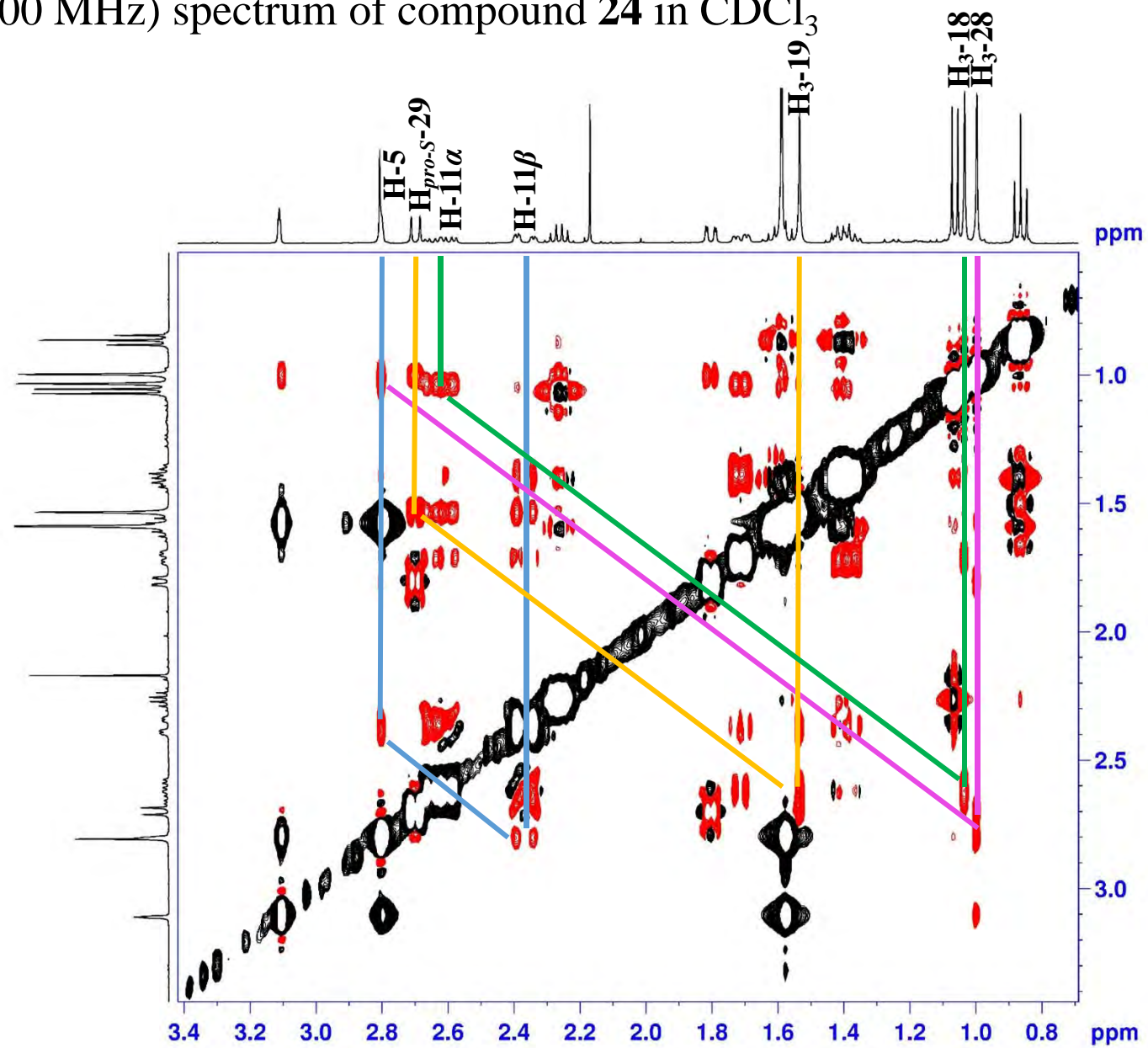
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FIDRES        1.953125 H
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RG            208.5
DW            125.000 u
DE            10.00 u
TE            297.0 K
D0            0.00011036 s
D1            1.99385595 s
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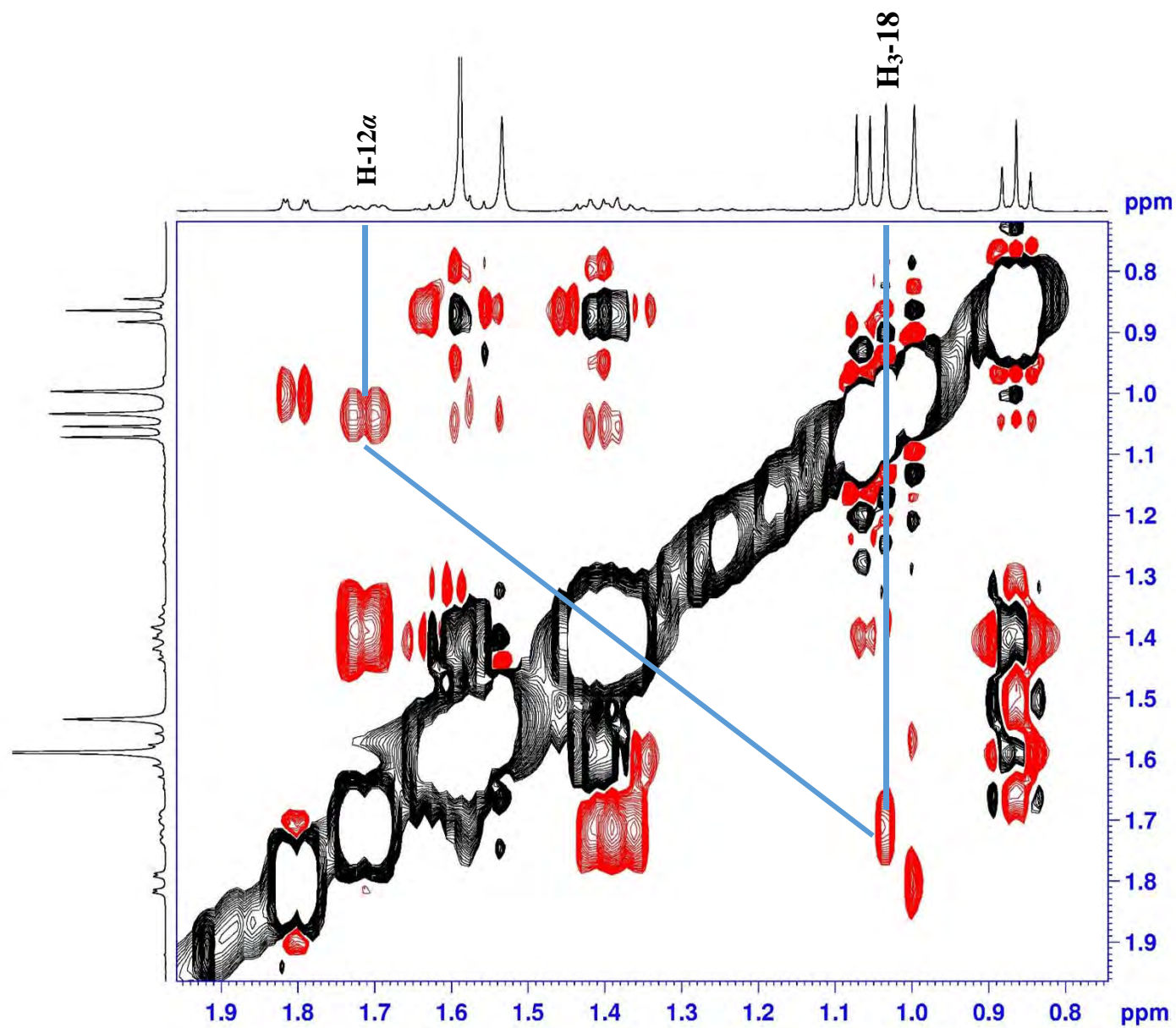
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SW          9.997 p
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SI         1024
SF         400.1300079 M
WDW         QSINE
SSB         2
LB          0.00 H
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WDW         QSINE
    
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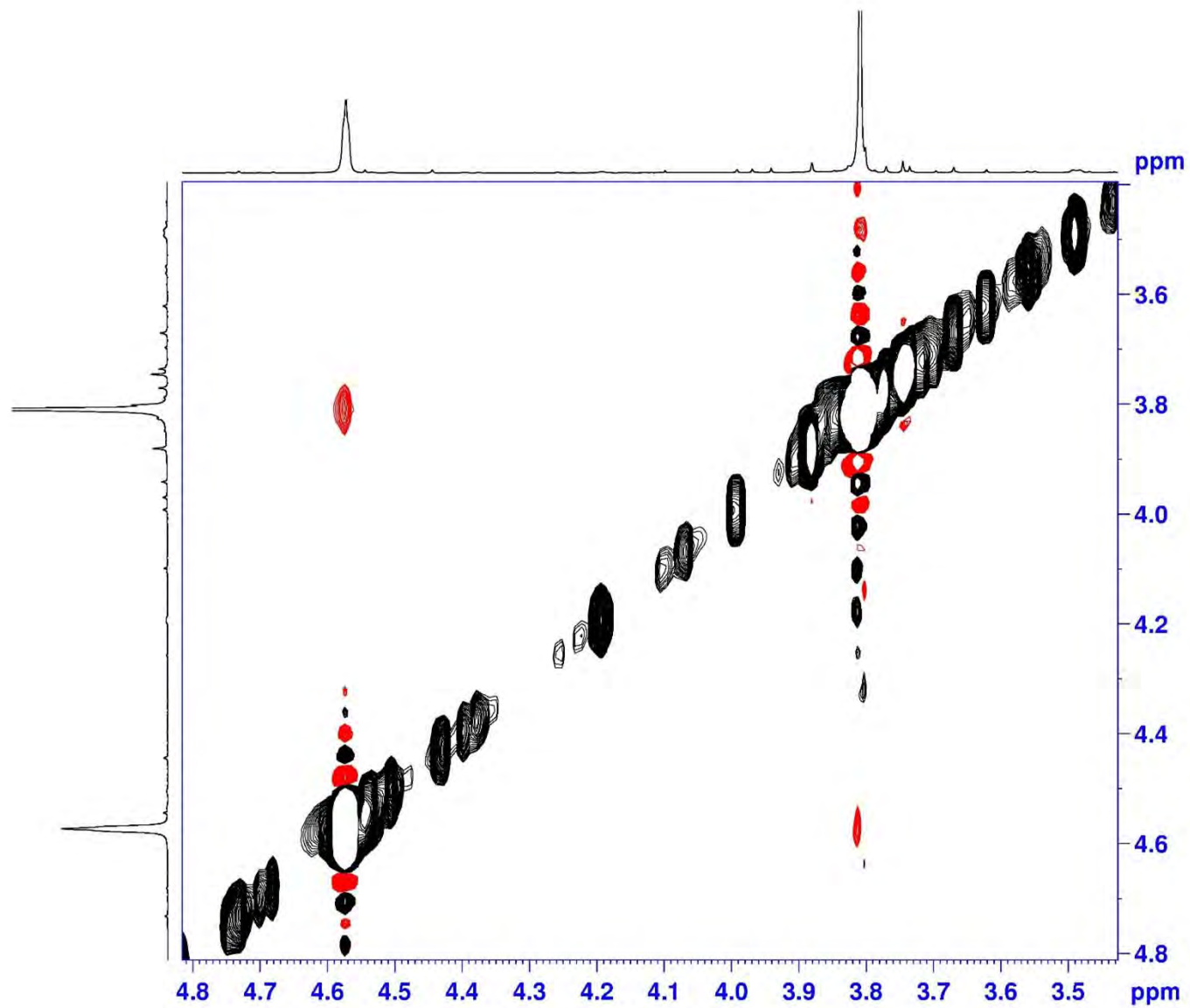
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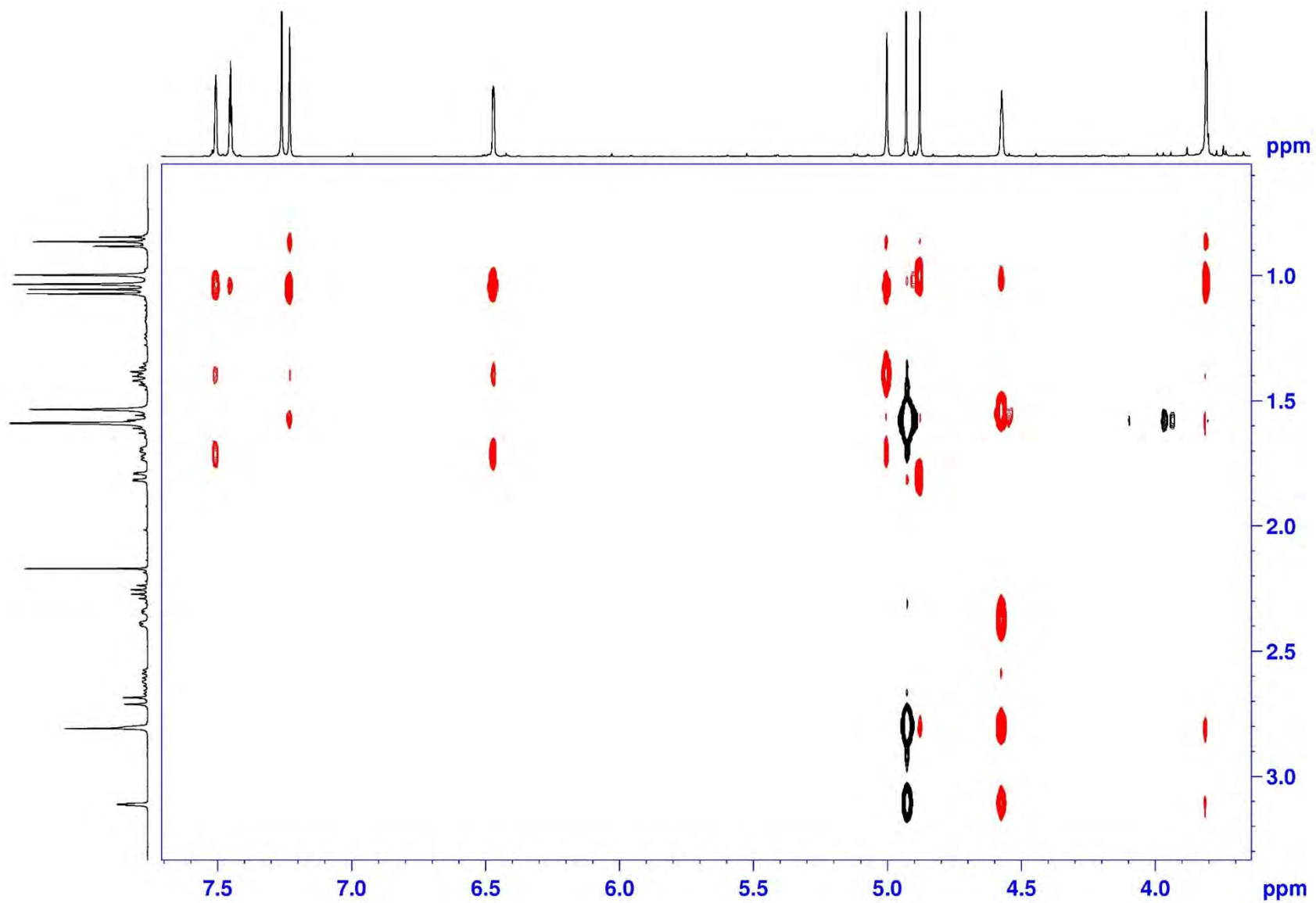
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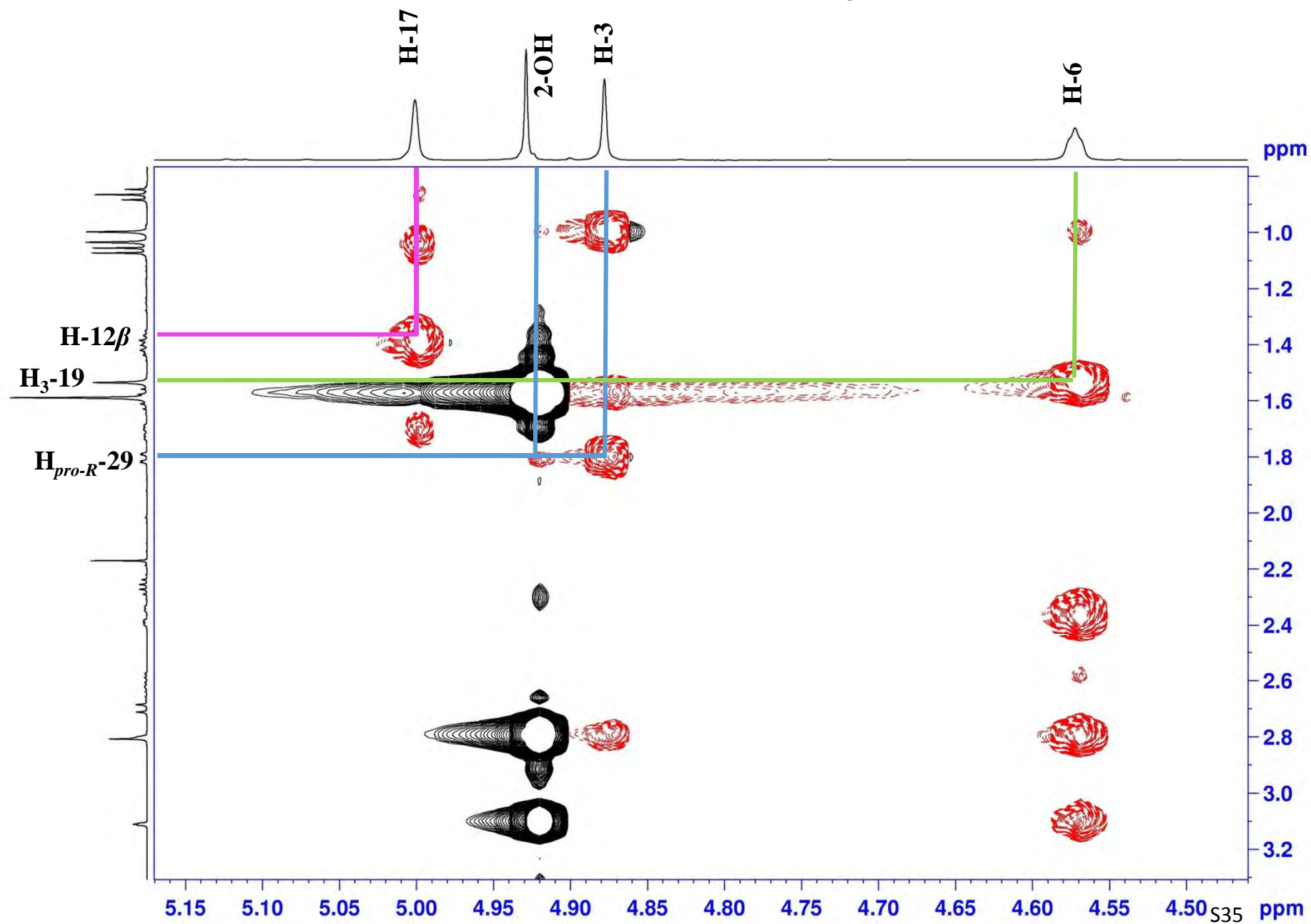
NOESY (400 MHz) spectrum of compound **24** in CDCl₃



NOESY (400 MHz) spectrum of compound **24** in CDCl₃



NOESY (400 MHz) spectrum of compound **24** in CDCl₃



HRESIMS for compound 25

Mass Spectrum SmartFormula Report

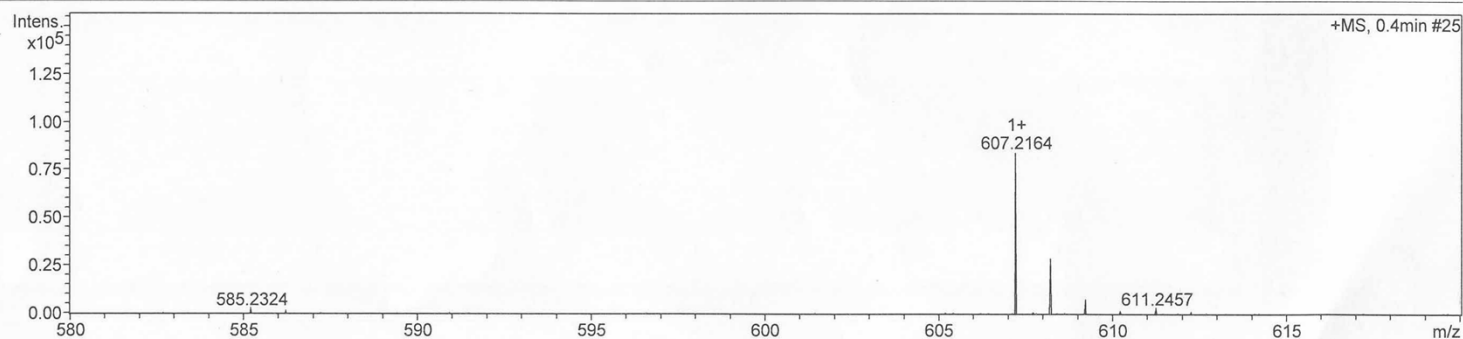
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 Sample Name zhangjianzhi_zjz-16_pos
 Comment

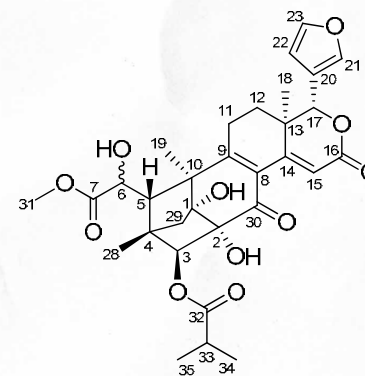
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 Operator SCSIO
 Instrument maXis 255552.00029

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 |



| Meas. m/z | # | Ion Formula | Score | m/z | err [ppm] | err [mDa] | mSigma | rdB | e ⁻ Conf | N-Rule |
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| 607.216367 | 1 | C31H36NaO11 | 100.00 | 607.214983 | -2.3 | -1.4 | 5.6 | 13.5 | even | ok |
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HRESIMS for compound **25**

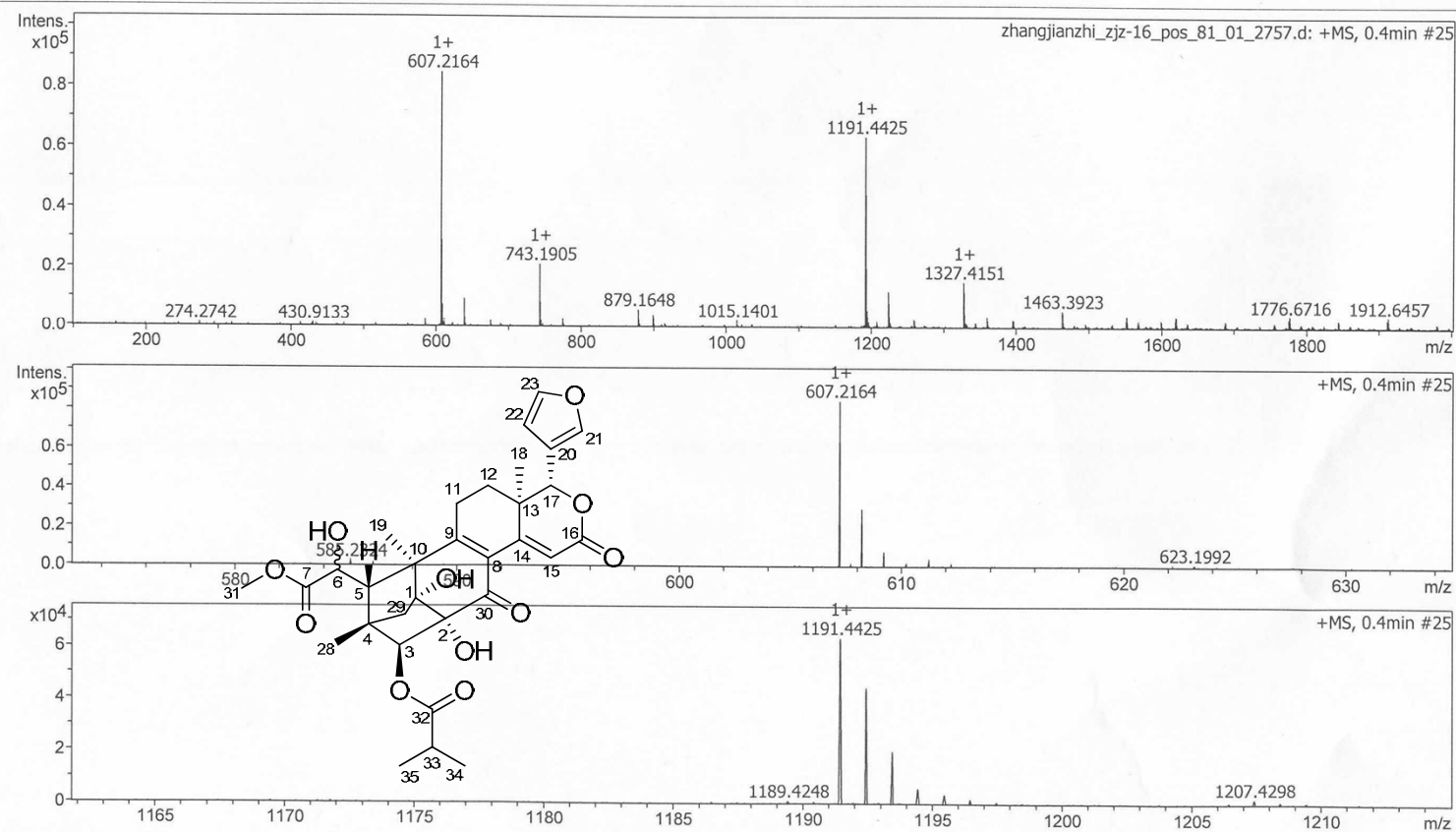
Generic Display Report

Analysis Info

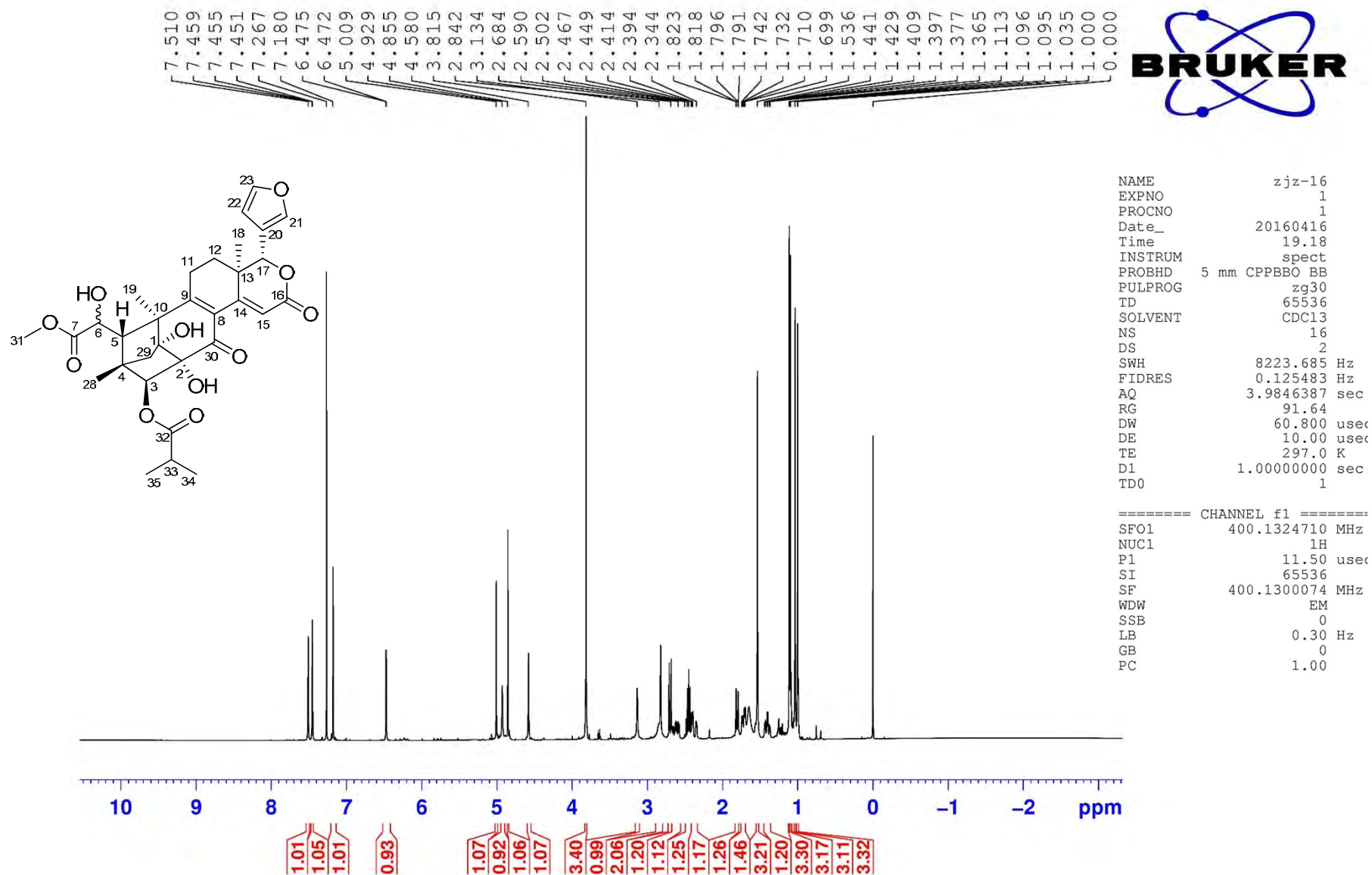
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Comment

Acquisition Date 12/14/2016 2:45:12 PM

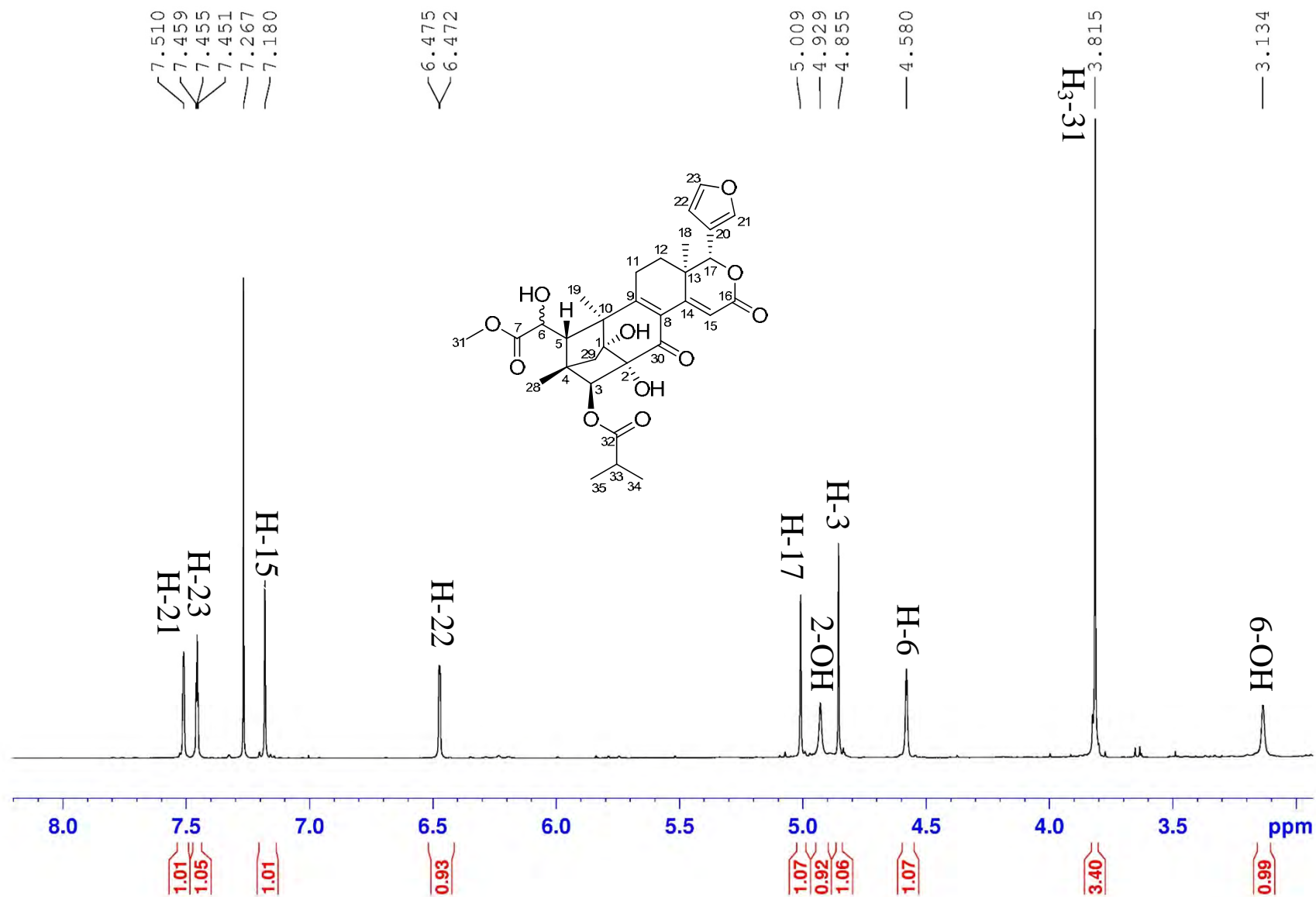
Operator SCSIO
Instrument maXis



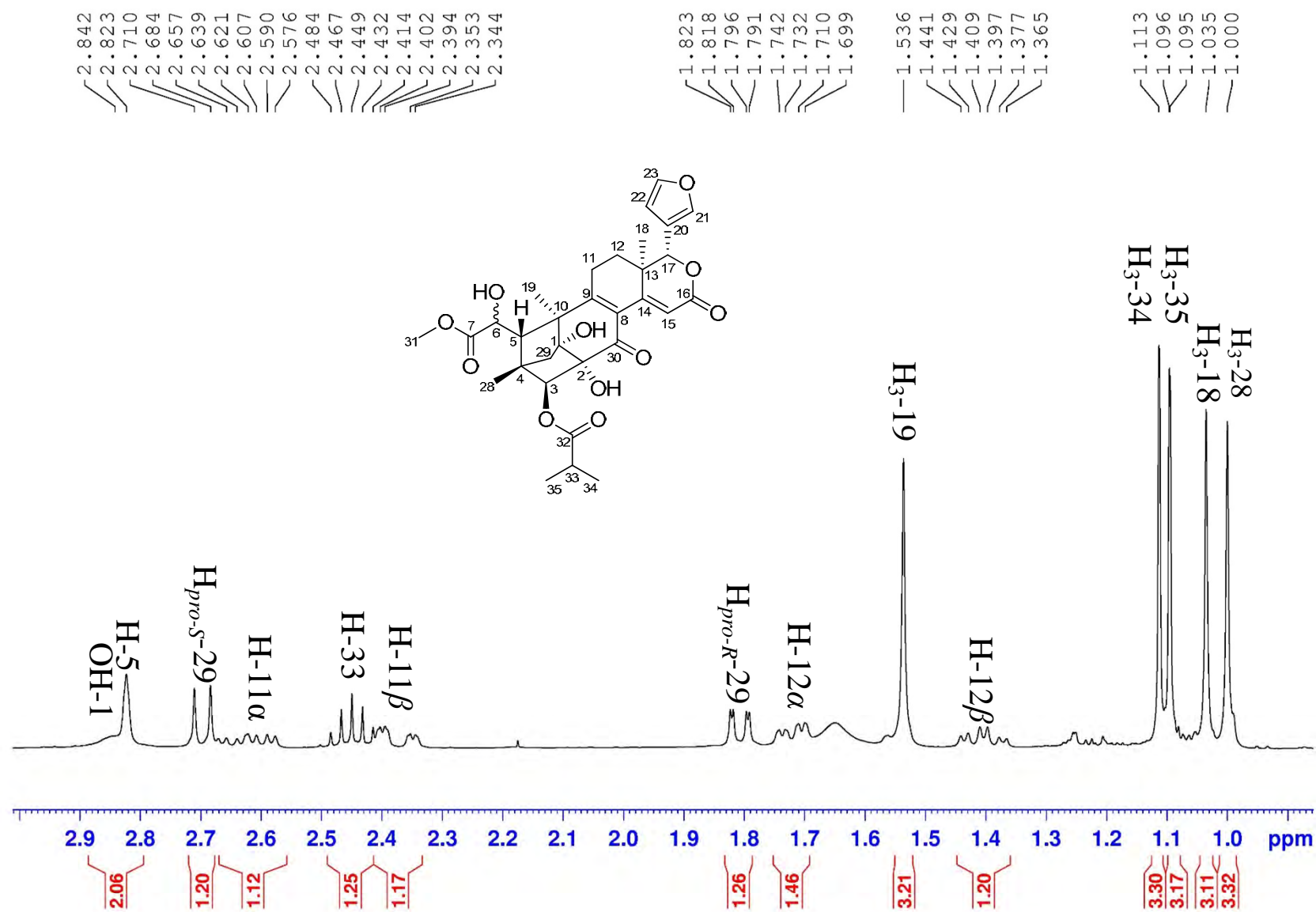
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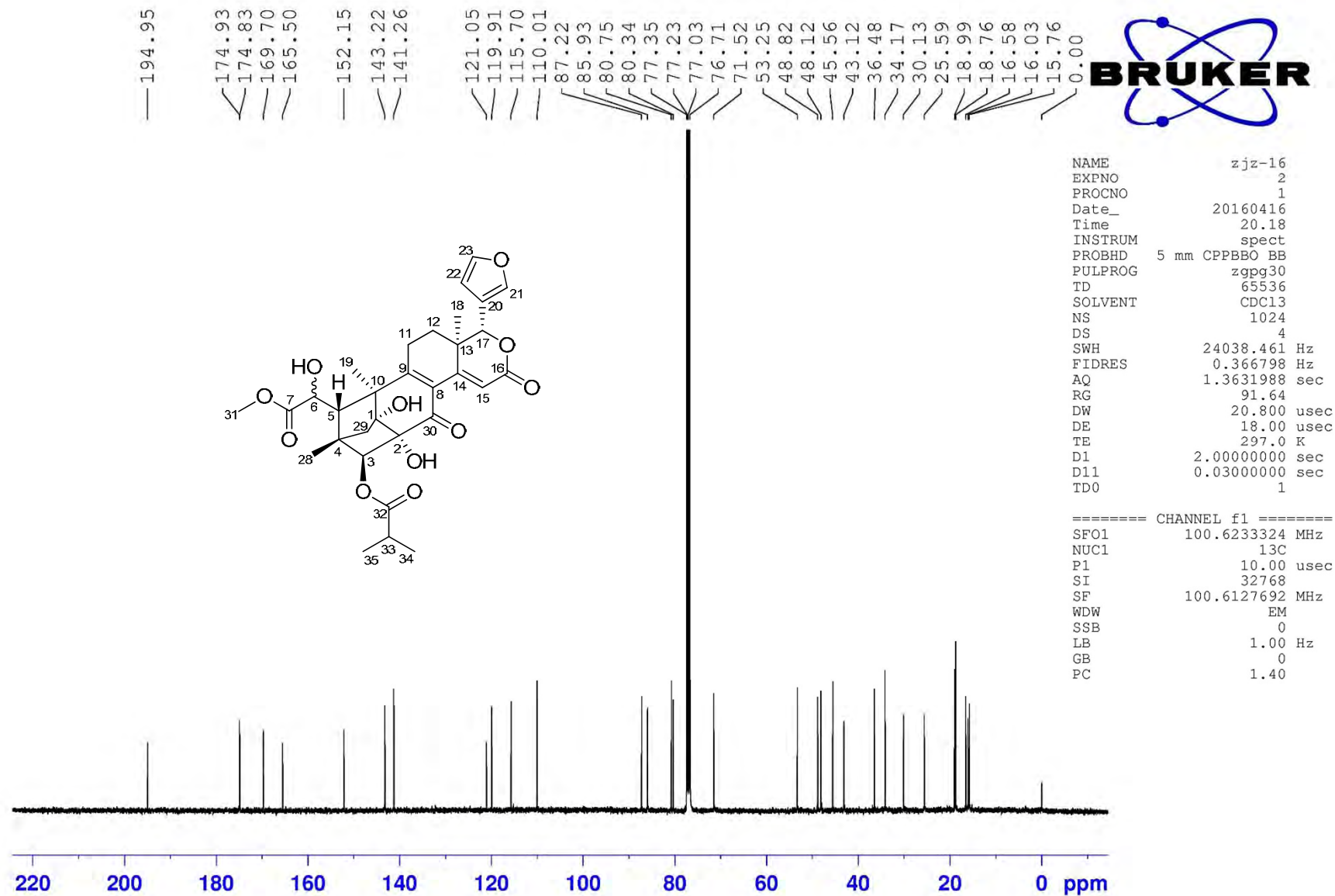
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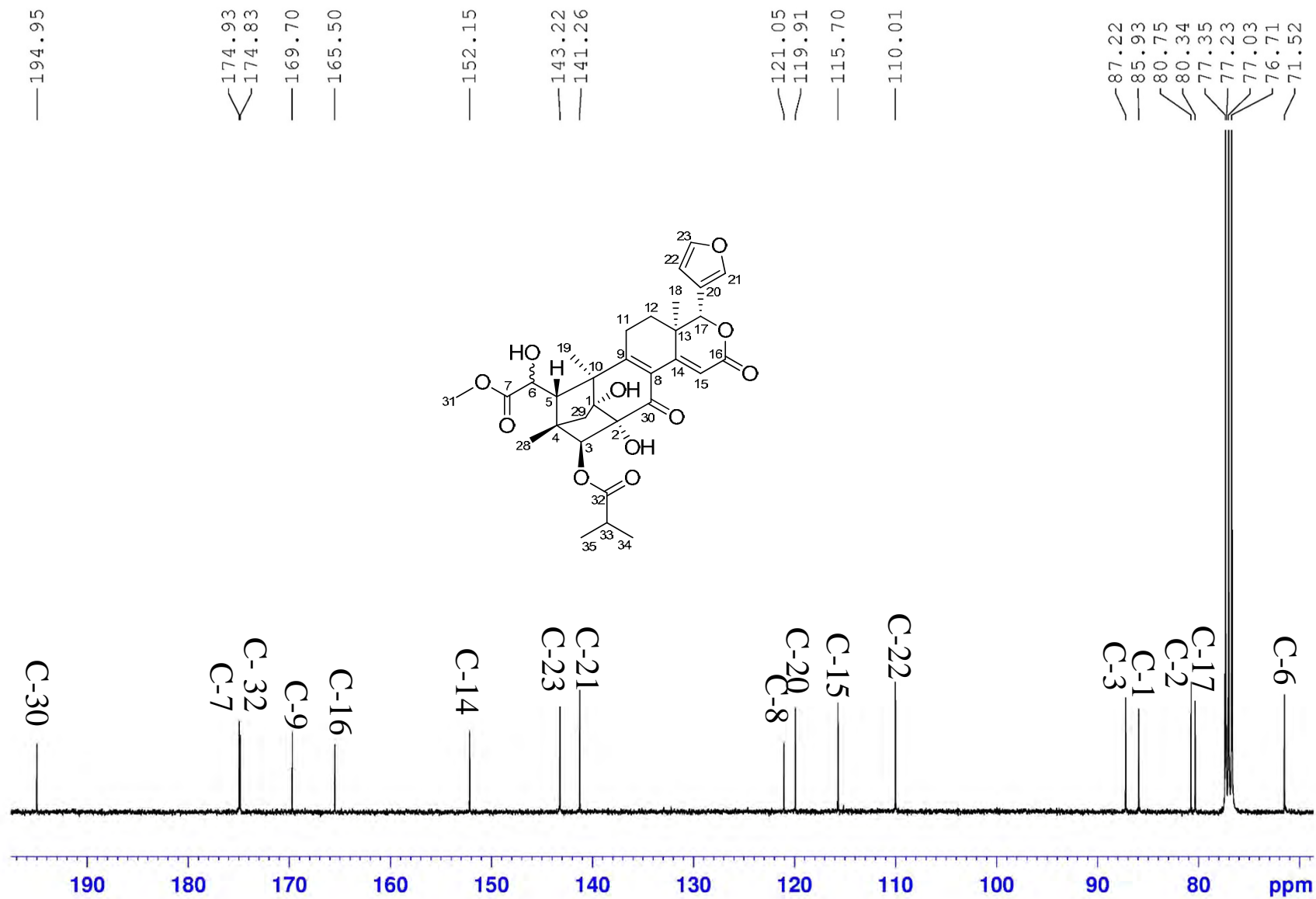
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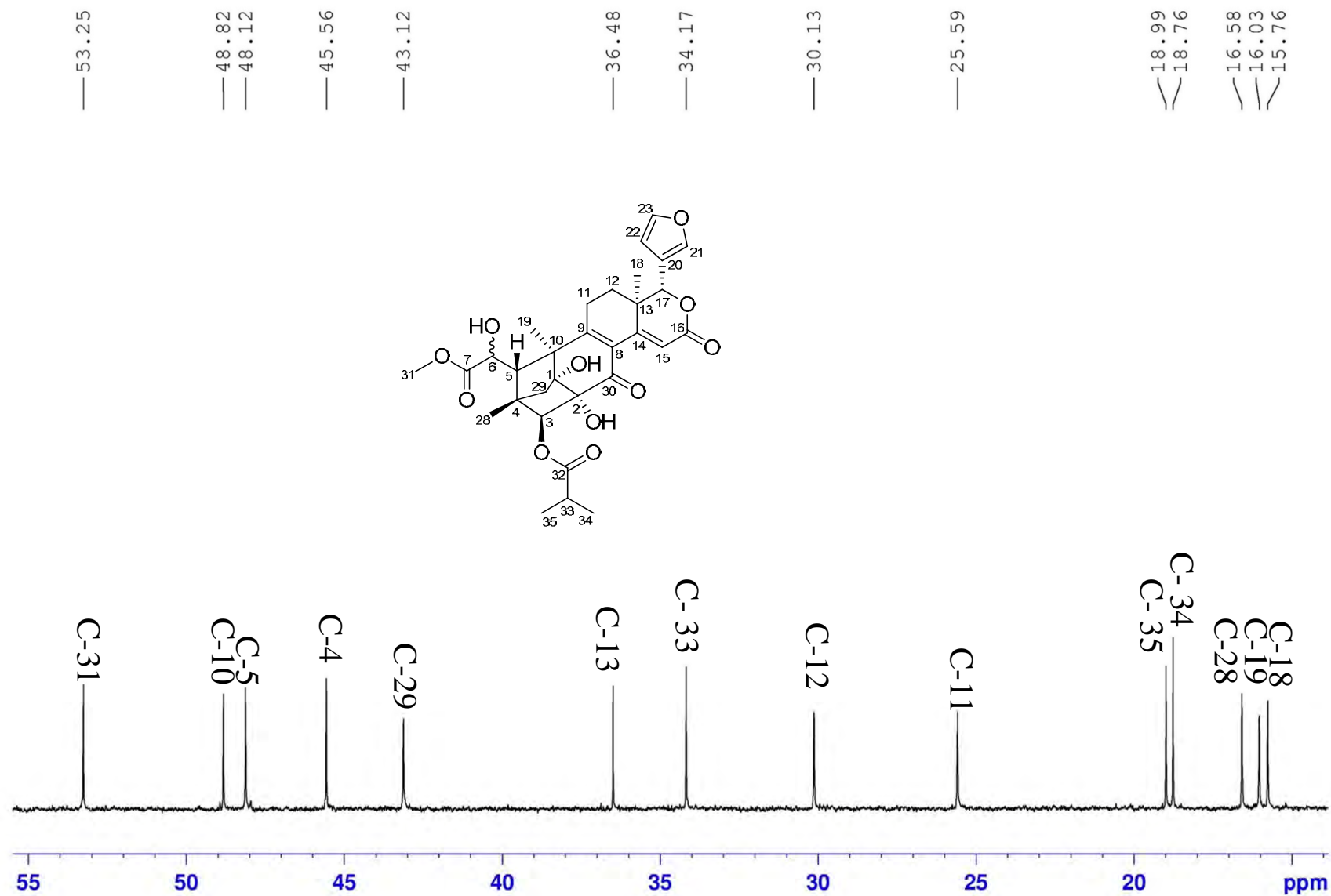
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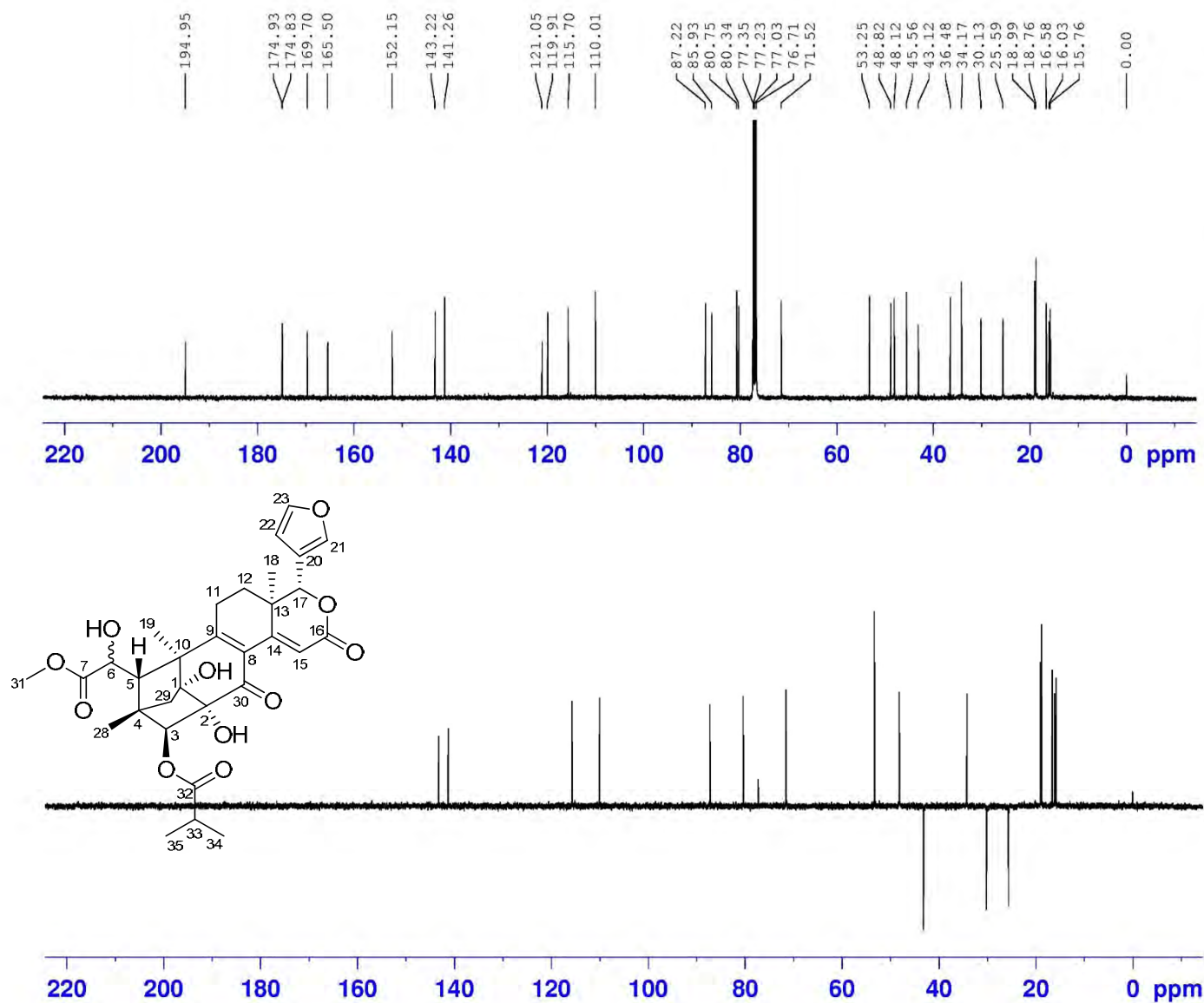
^{13}C NMR (100 MHz) spectrum of compound **25** in CDCl_3



^{13}C NMR (100 MHz) spectrum of compound **25** in CDCl_3



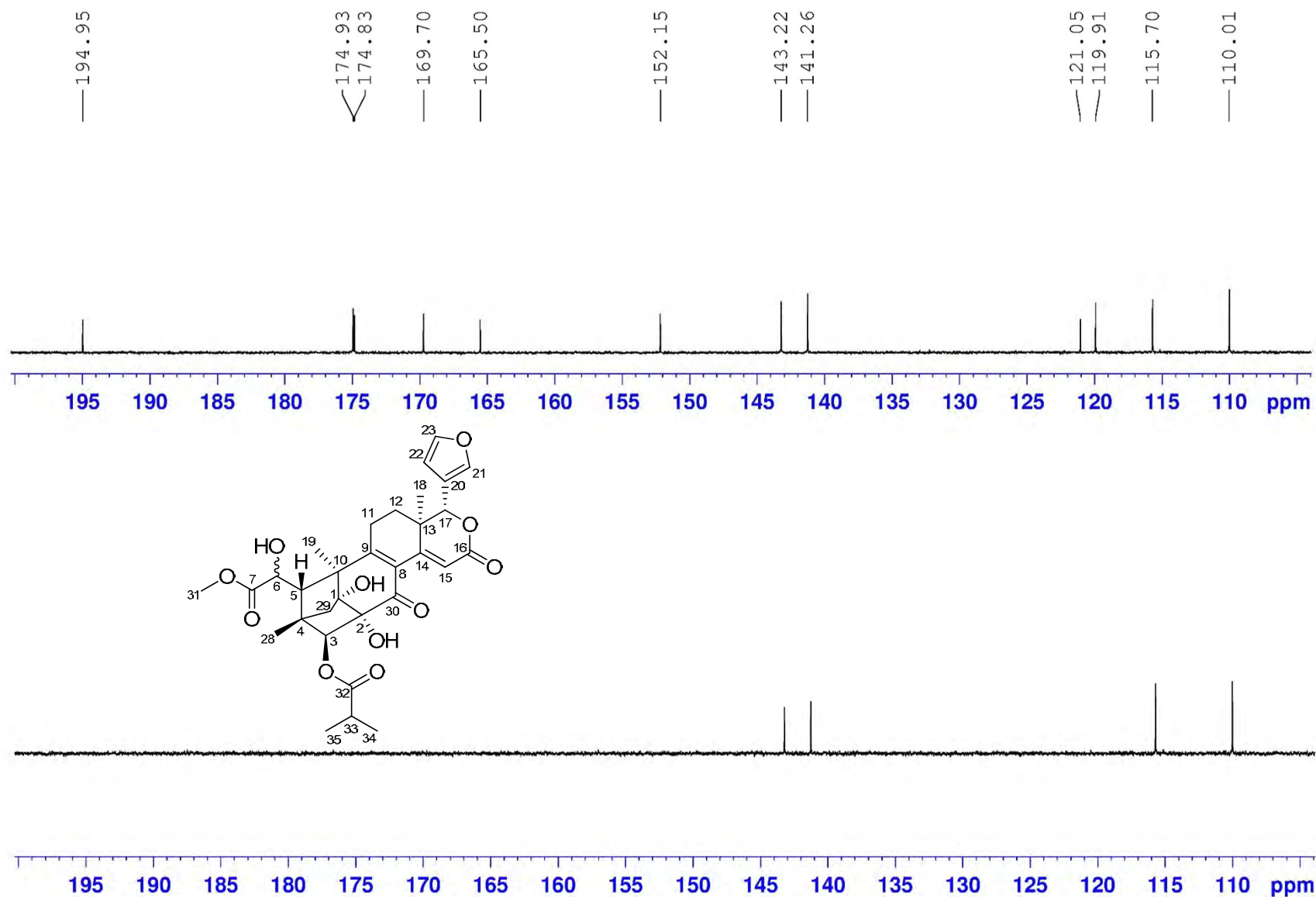
DEPT135 (100 MHz) spectrum of compound **25** in CDCl₃



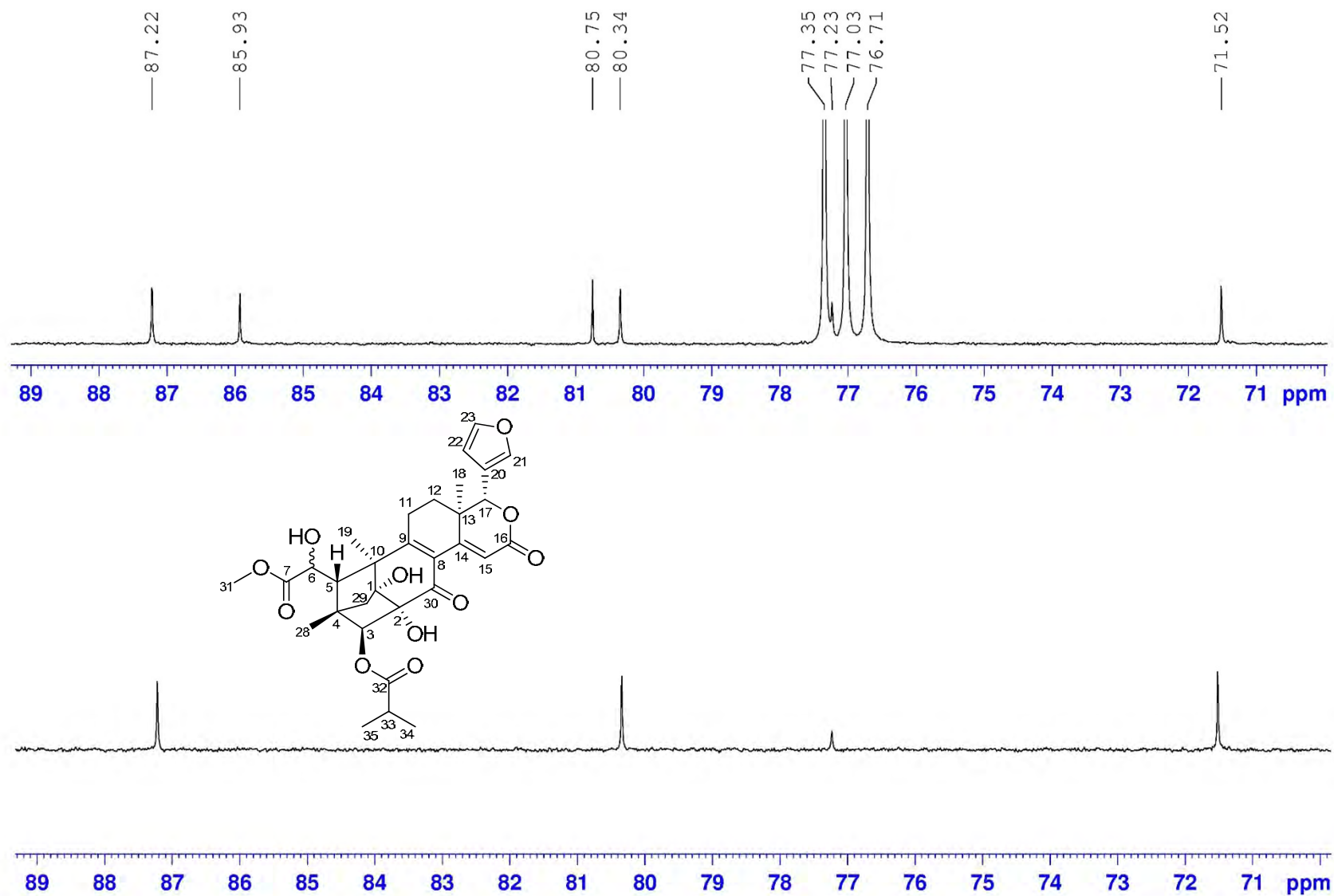
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 PROCNO 1
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 INSTRUM spect
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 PULPROG deptsp135
 TD 65536
 SOLVENT CDCl3
 NS 300
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 130.26
 DW 20.800 usec
 DE 18.00 usec
 TE 297.0 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1

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 NUC1 13C
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 SF 100.6127692 MHz
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 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

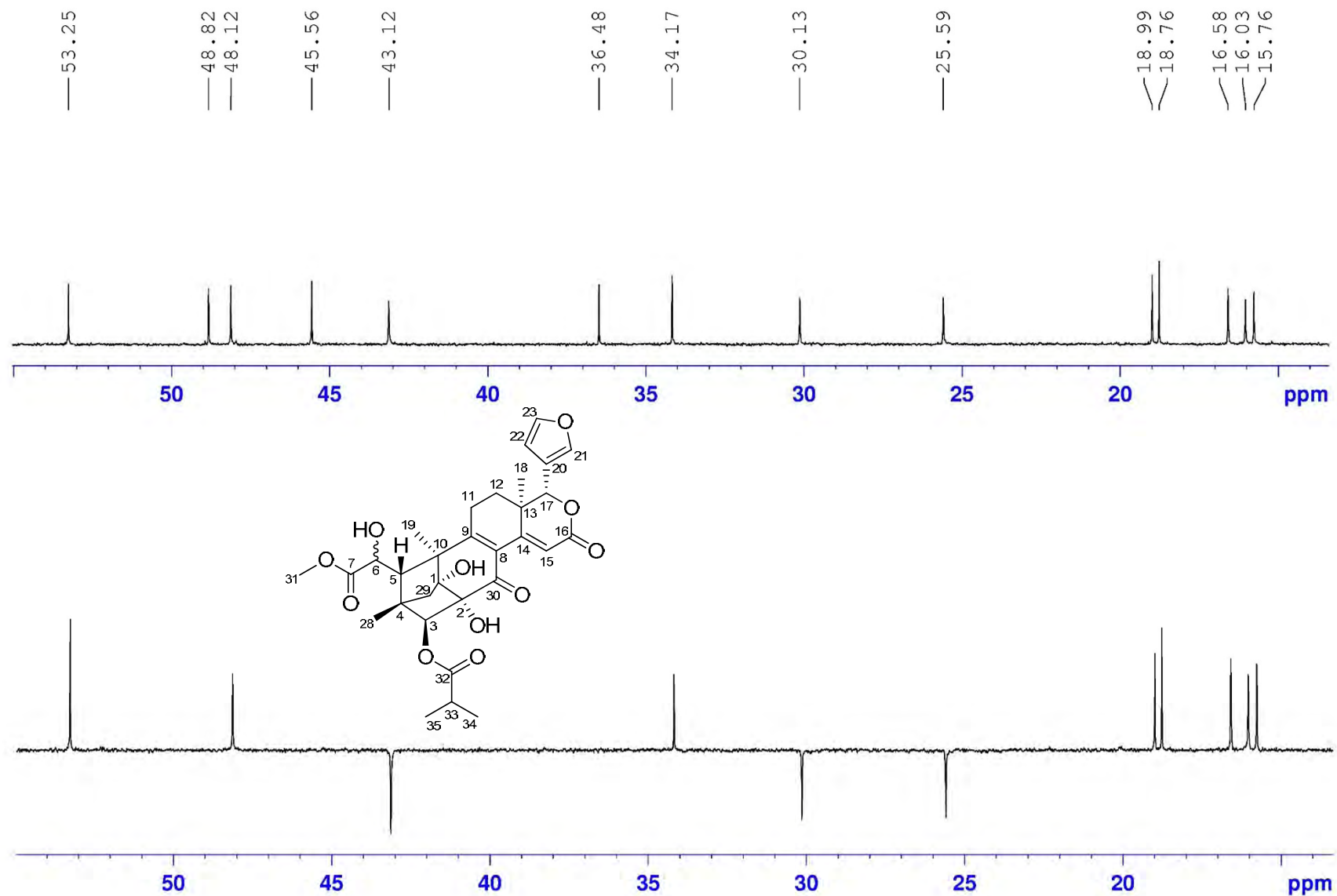
DEPT135 (100 MHz) spectrum of compound **25** in CDCl₃



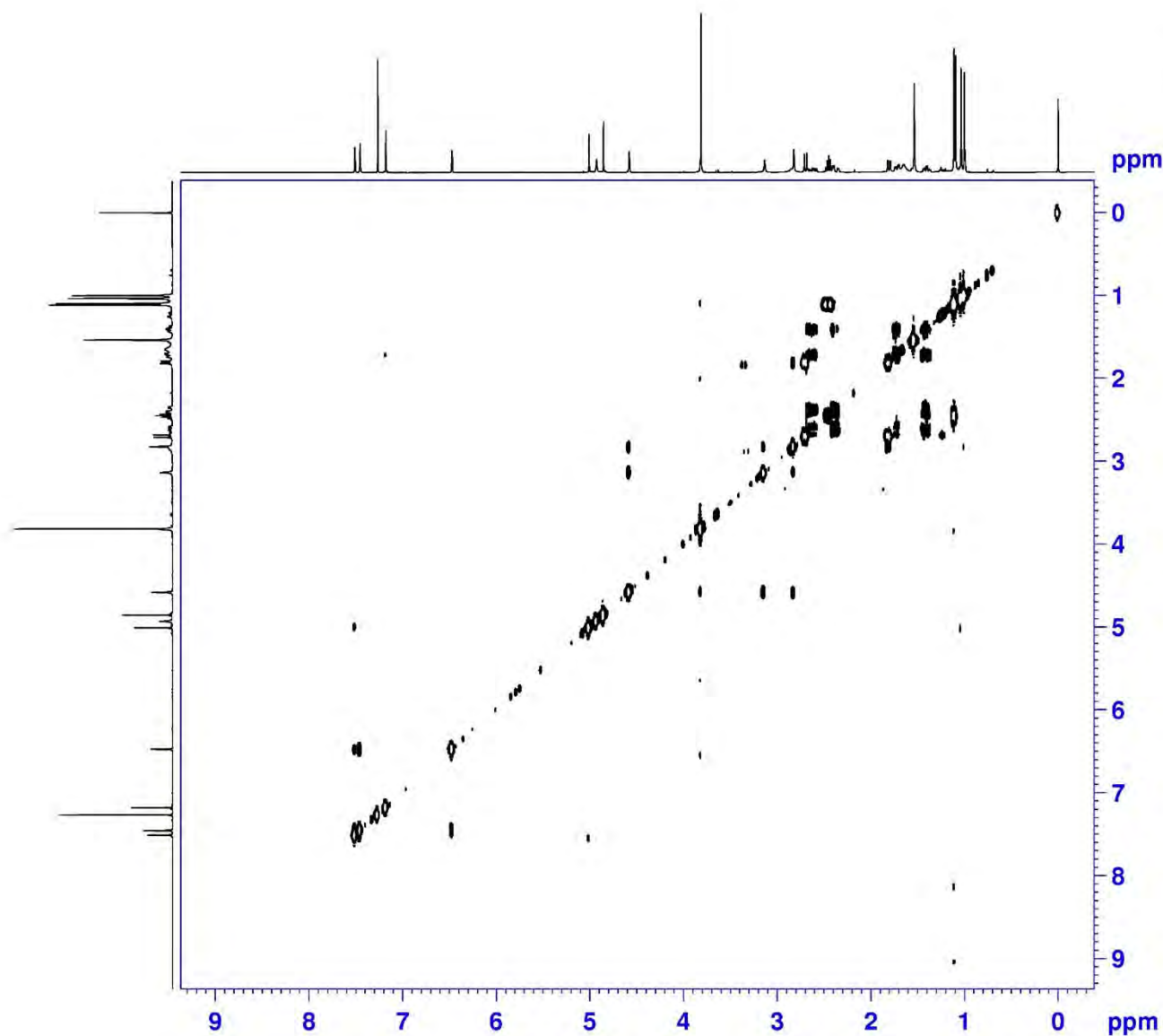
DEPT135 (100 MHz) spectrum of compound **25** in CDCl₃



DEPT135 (100 MHz) spectrum of compound **25** in CDCl₃



^1H - ^1H COSY (400 MHz) spectrum of compound **25** in CDCl_3



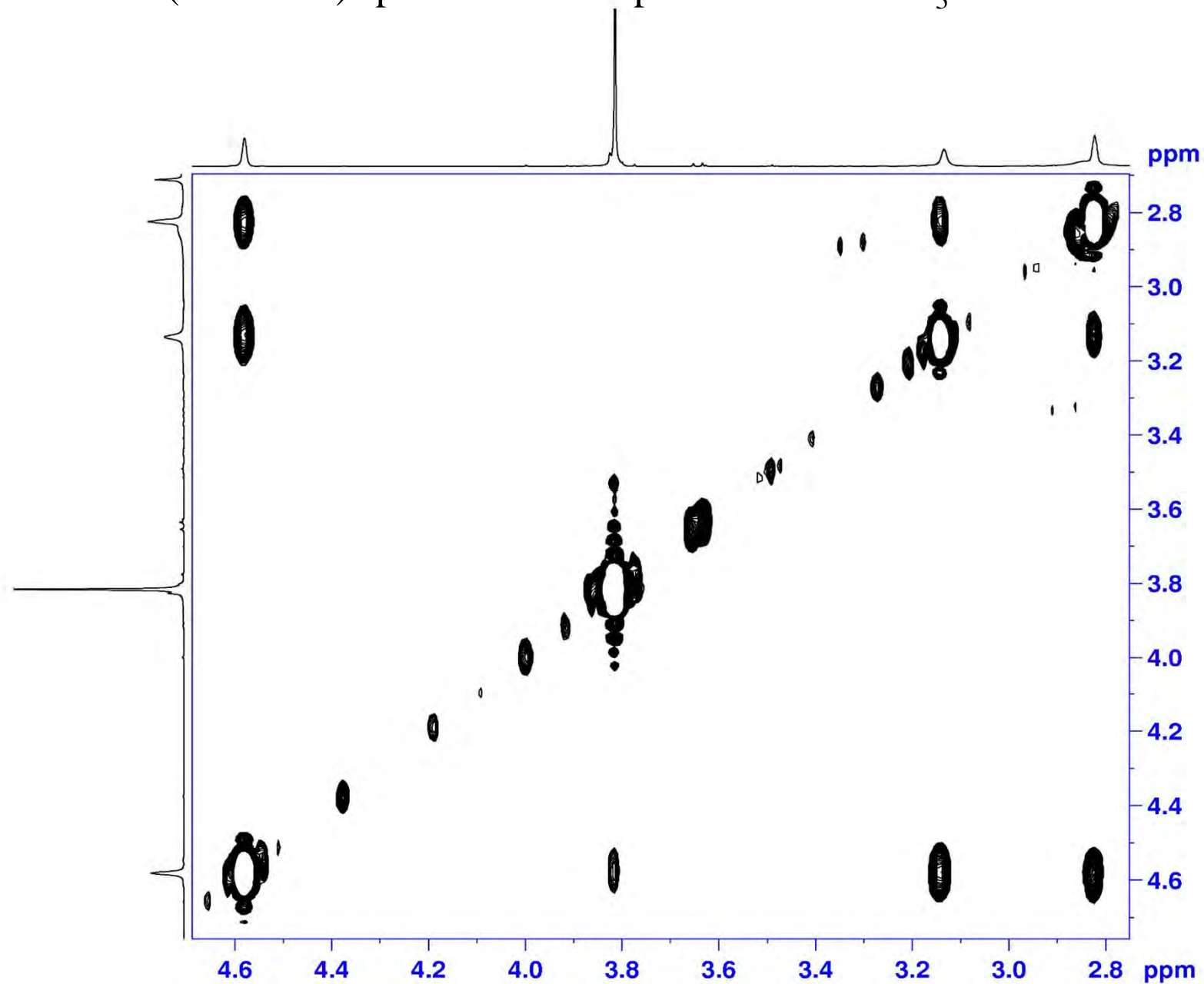
```

NAME           zjz-16
EXPNO           4
PROCNO          1
Date_           20160426
Time            18.41
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
    
```

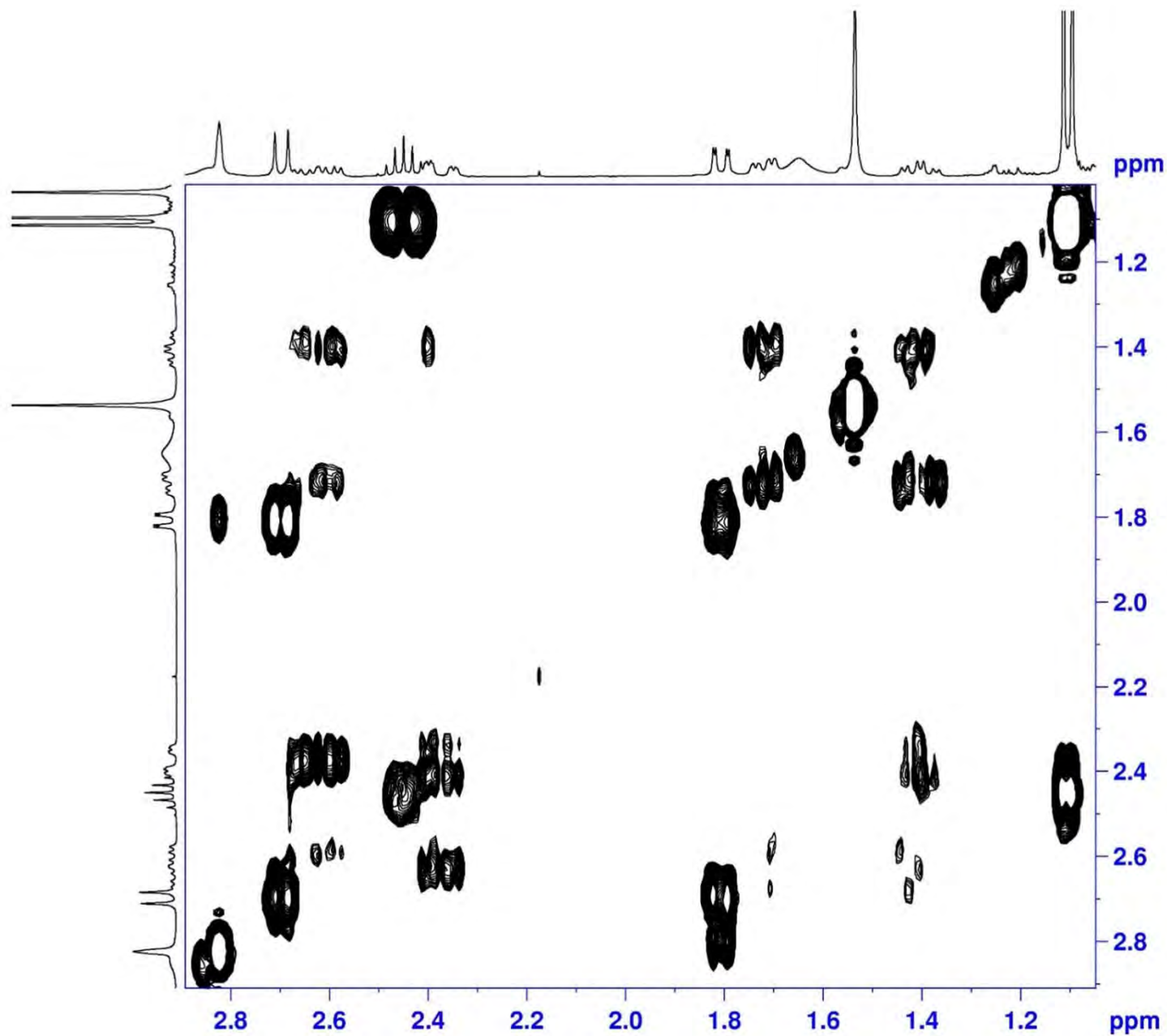
```

===== 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            400.1300055 MHz
WDW            QSINE
SSB            0
LB              0.00 Hz
GB              0
PC              1.40
SI             1024
MC2            QF
SF            400.1300054 MHz
WDW            QSINE
SSB            0
LB              0.00 Hz
GB              0
    
```

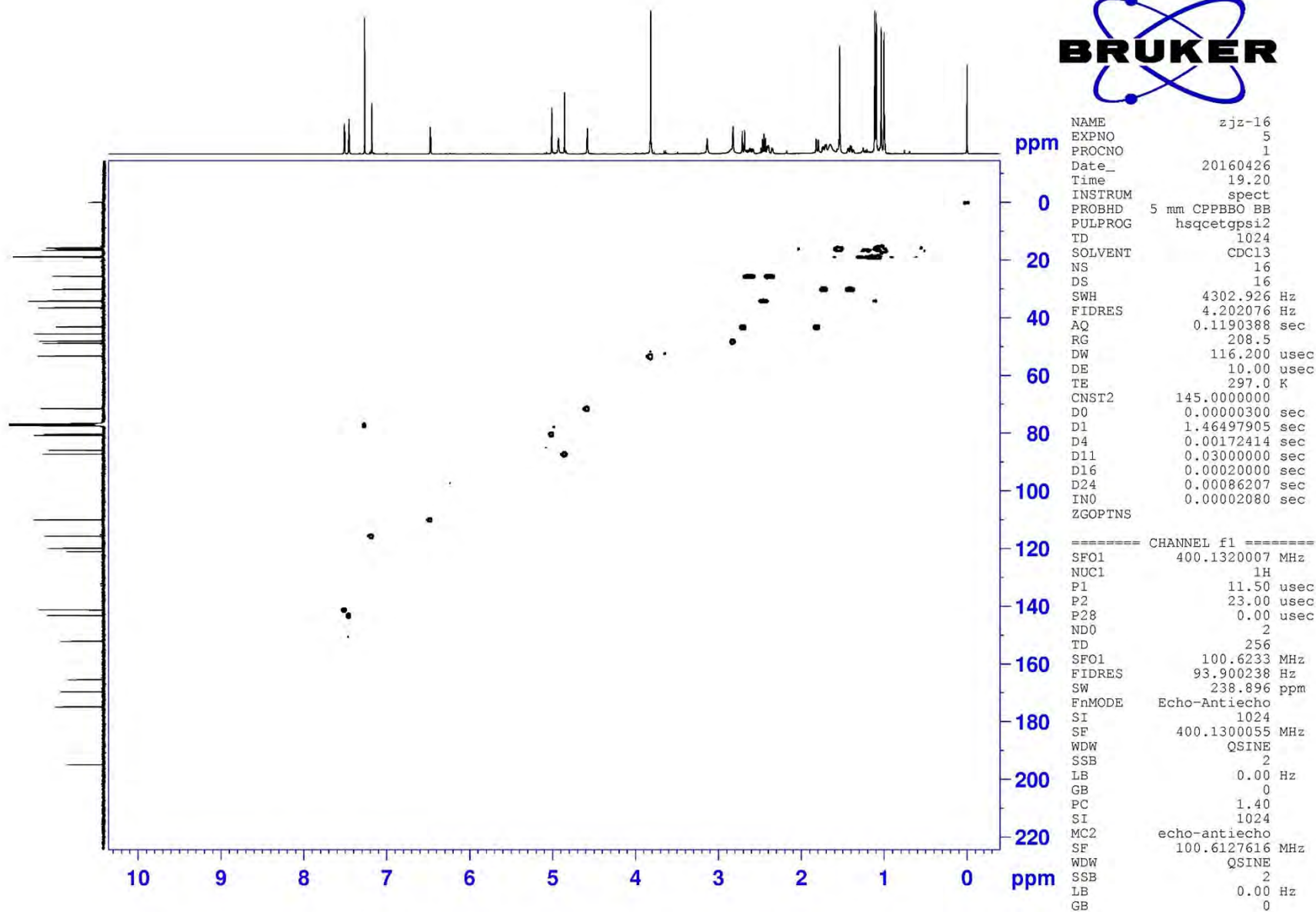
^1H - ^1H COSY (400 MHz) spectrum of compound **25** in CDCl_3



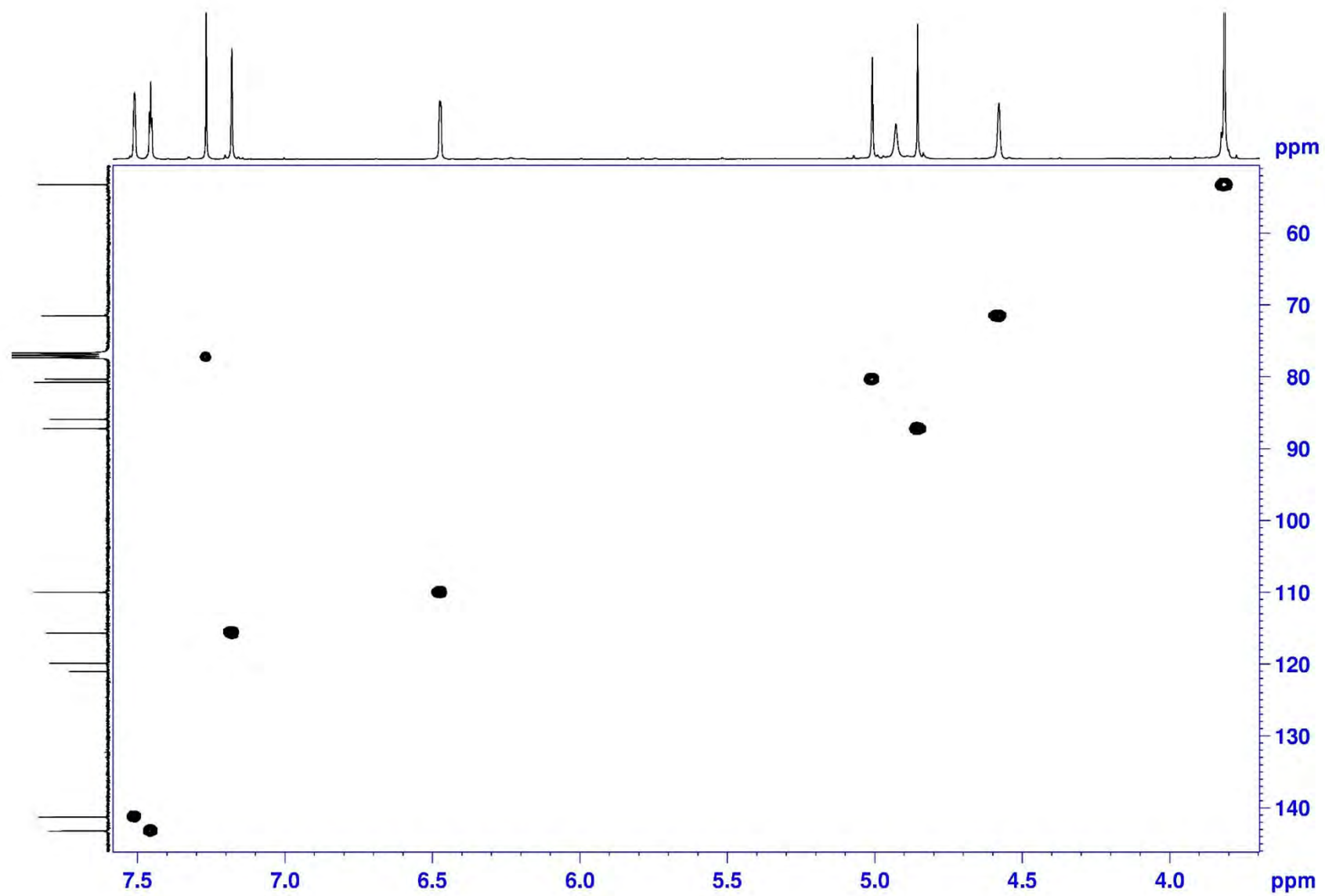
^1H - ^1H COSY (400 MHz) spectrum of compound **25** in CDCl_3



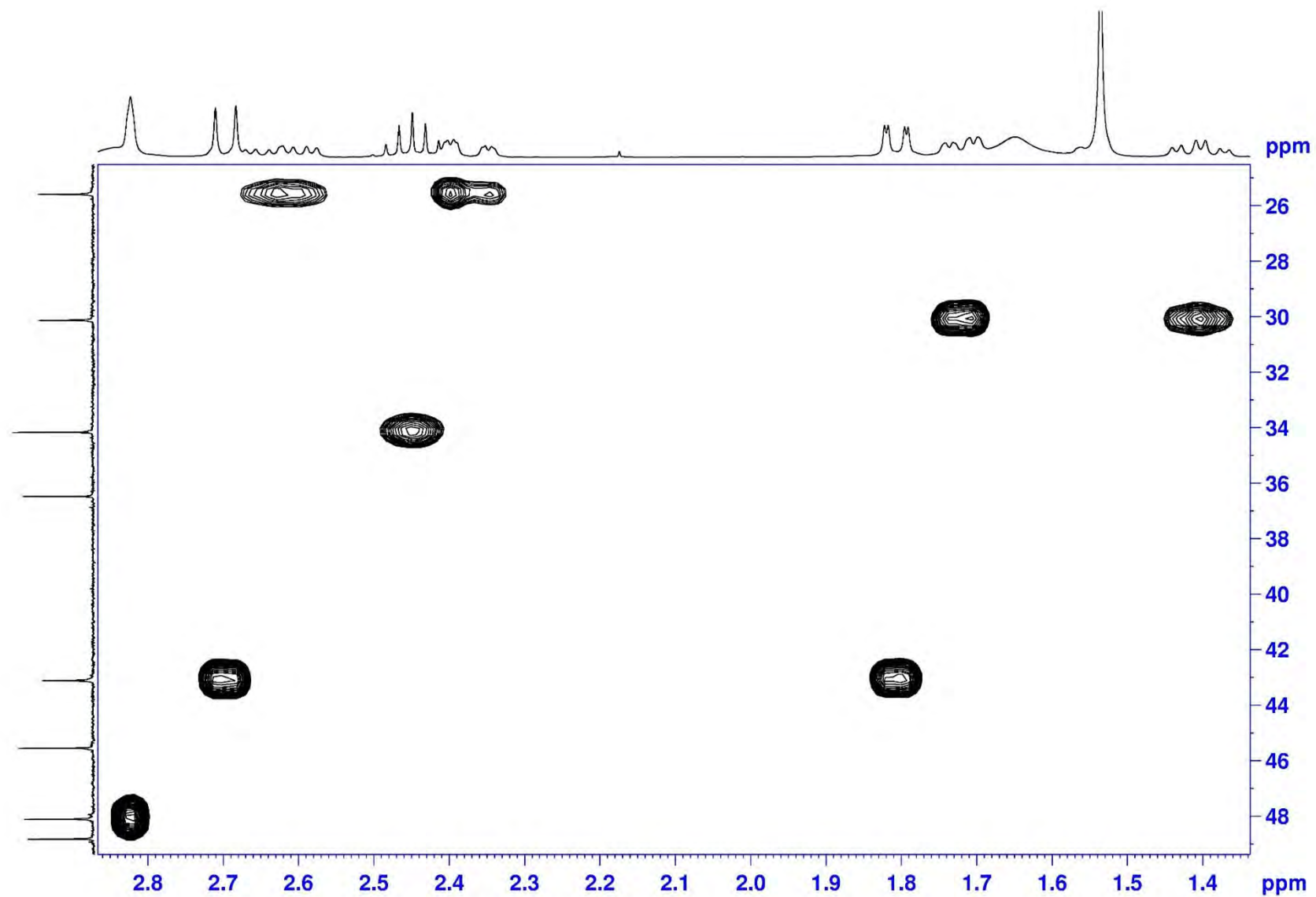
HSQC (400 MHz) spectrum of compound **25** in CDCl₃



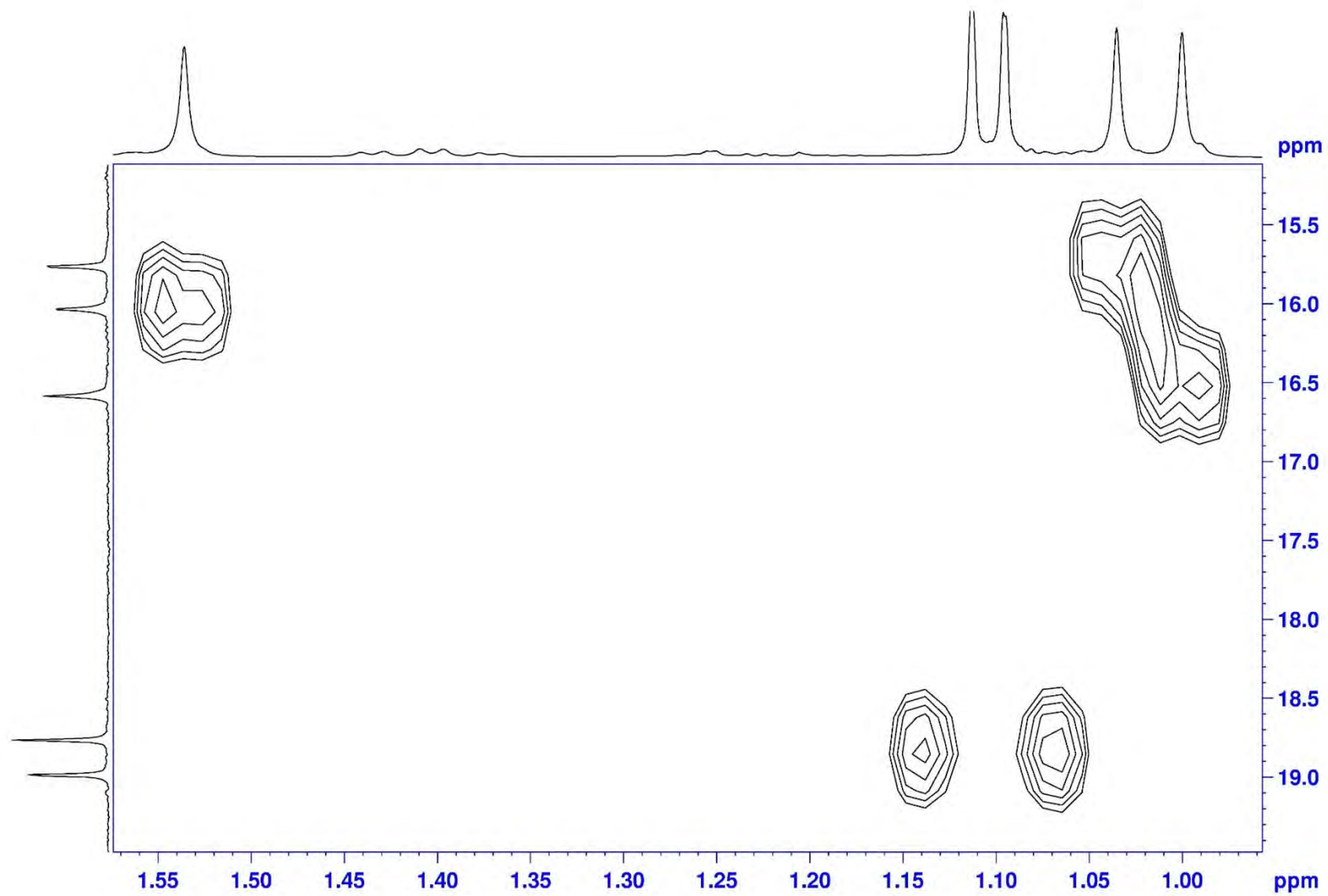
HSQC (400 MHz) spectrum of compound **25** in CDCl₃



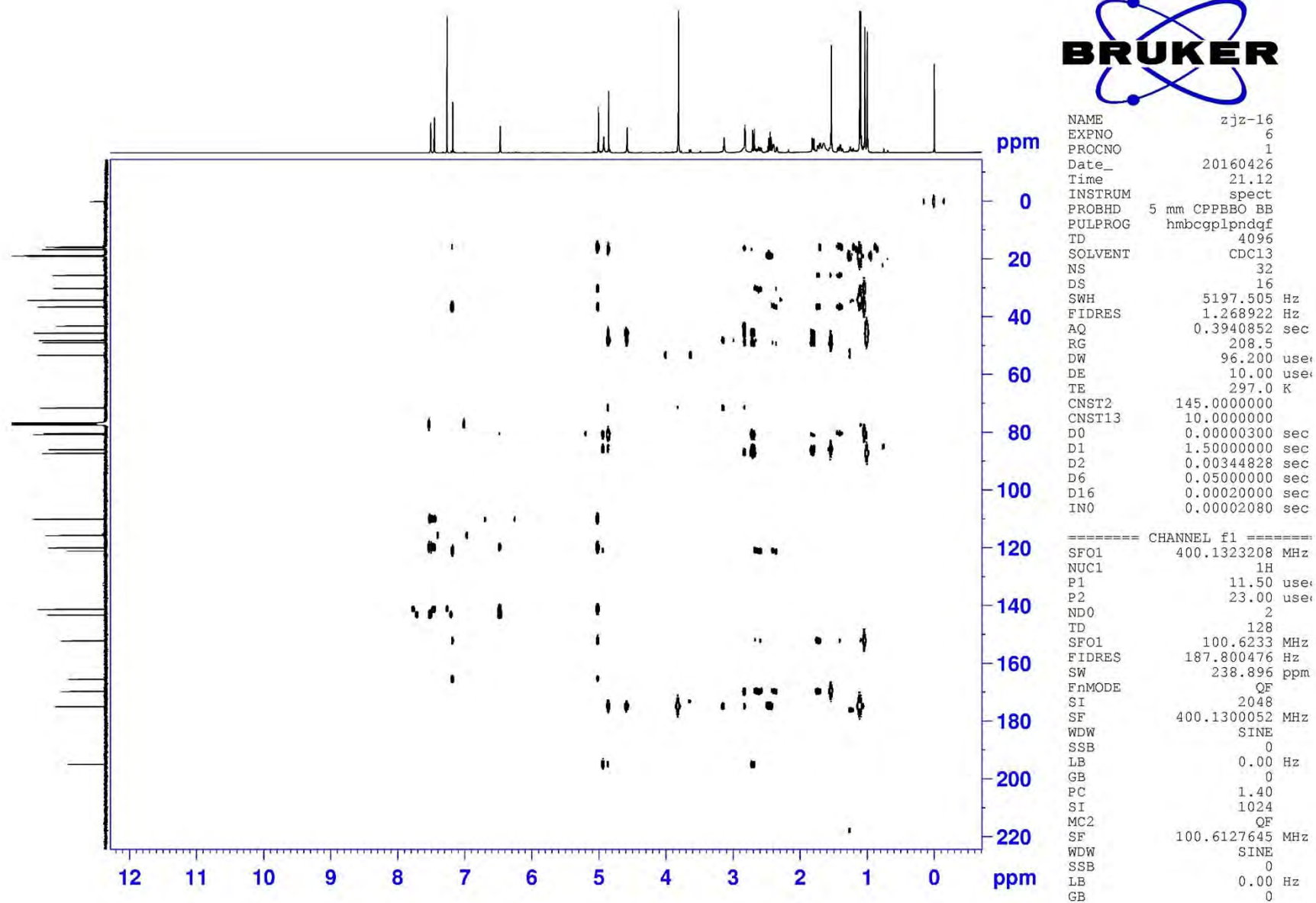
HSQC (400 MHz) spectrum of compound **25** in CDCl₃



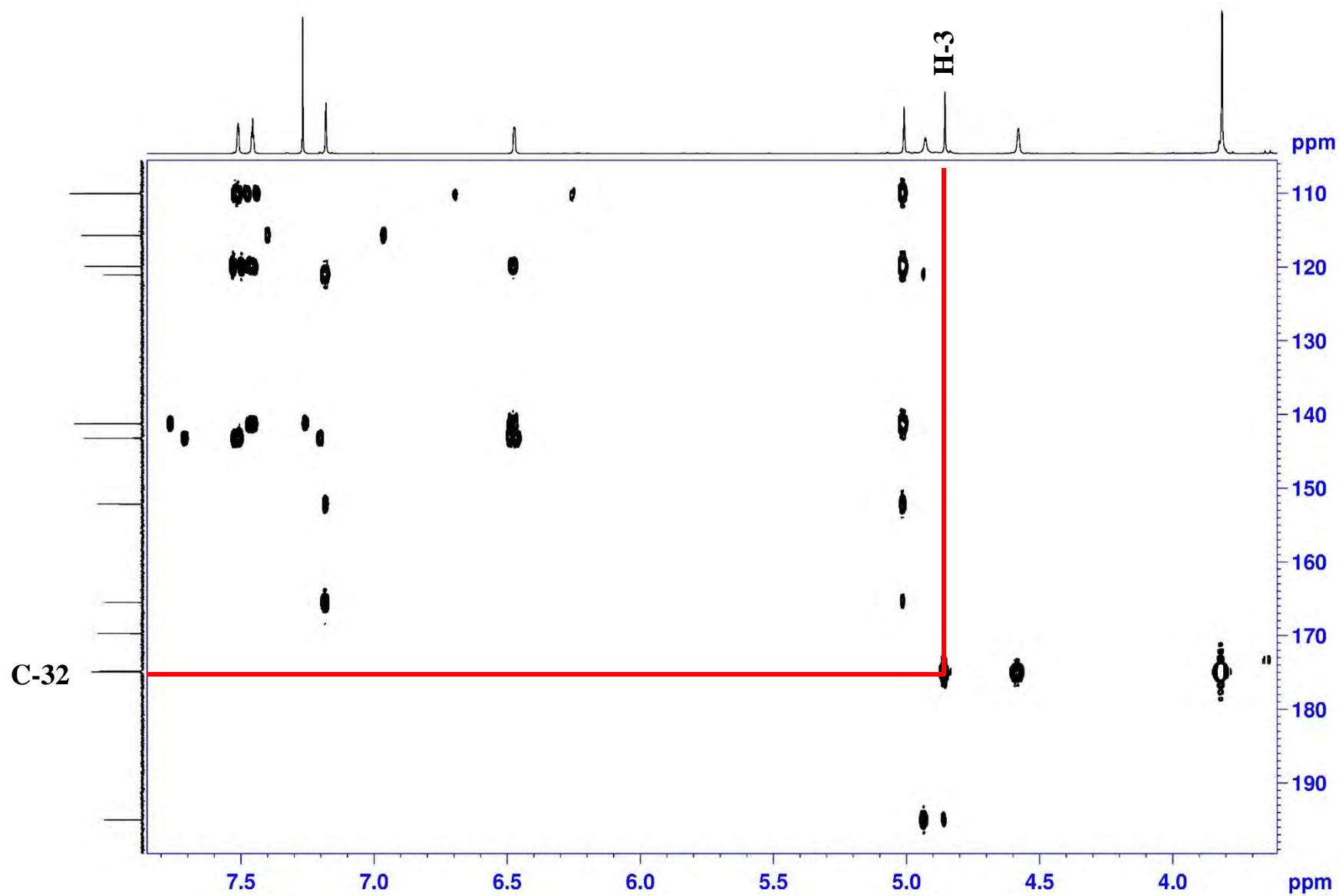
HSQC (400 MHz) spectrum of compound **25** in CDCl₃



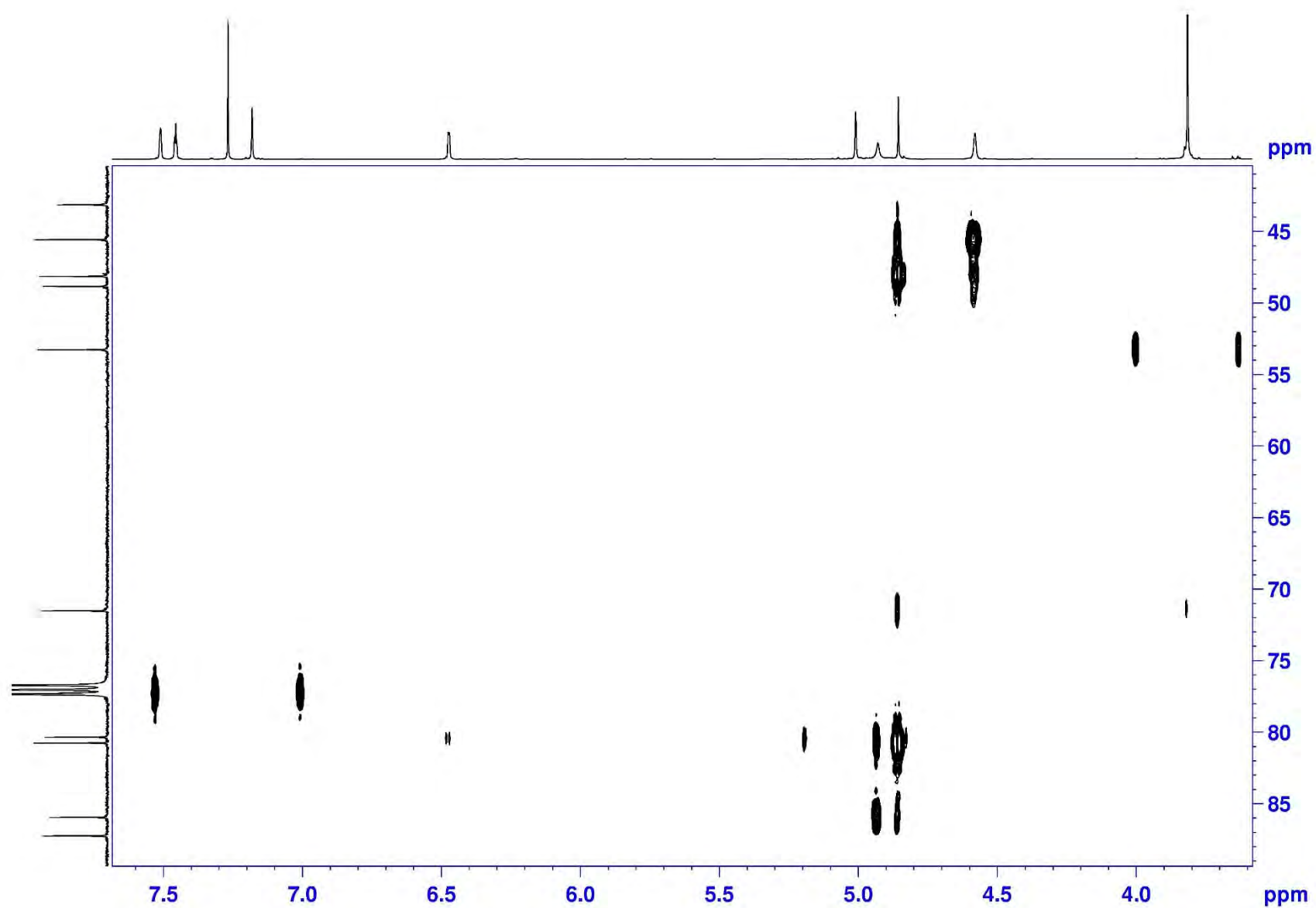
HMBC (400 MHz) spectrum of compound **25** in CDCl₃



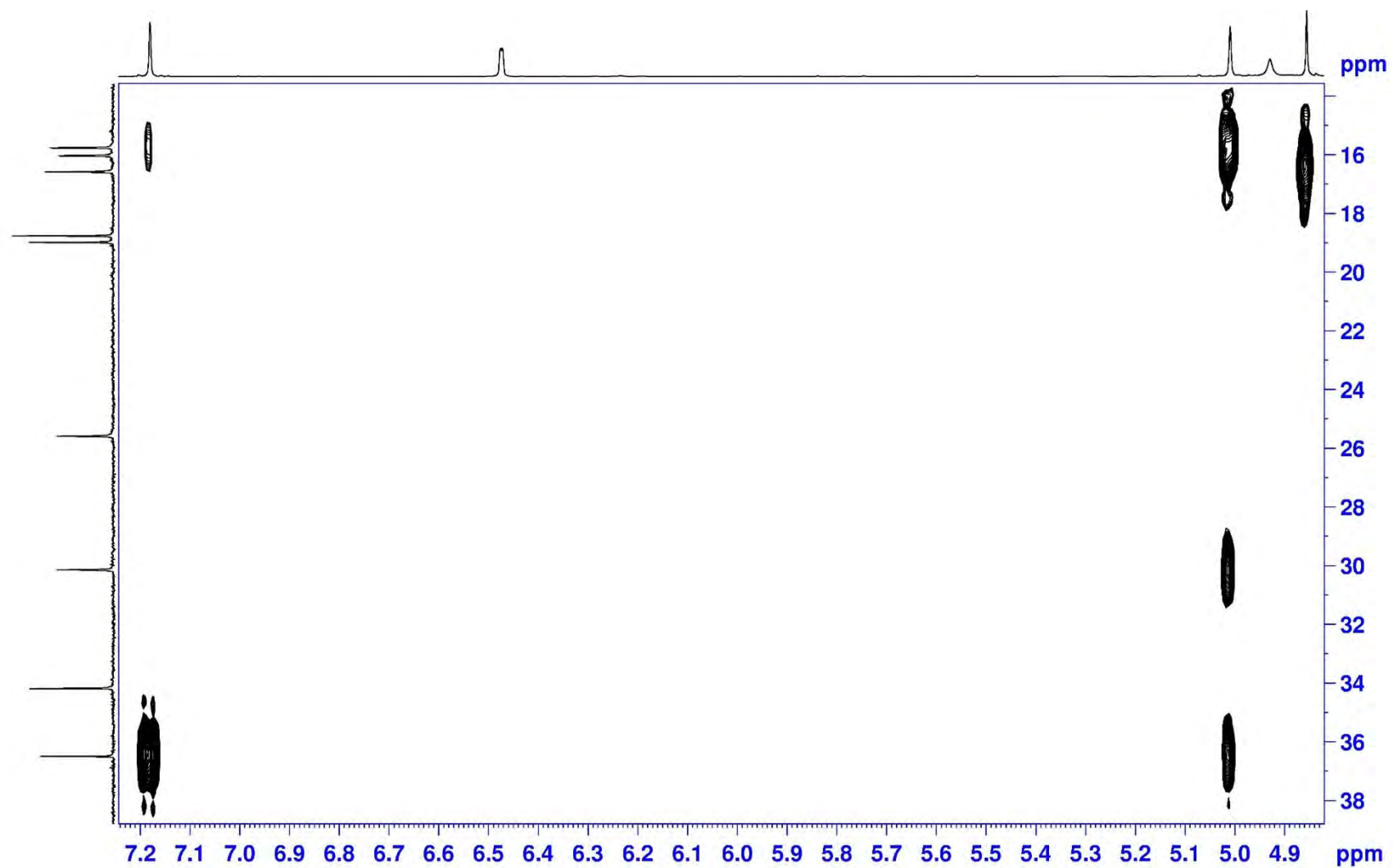
HMBC (400 MHz) spectrum of compound **25** in CDCl_3



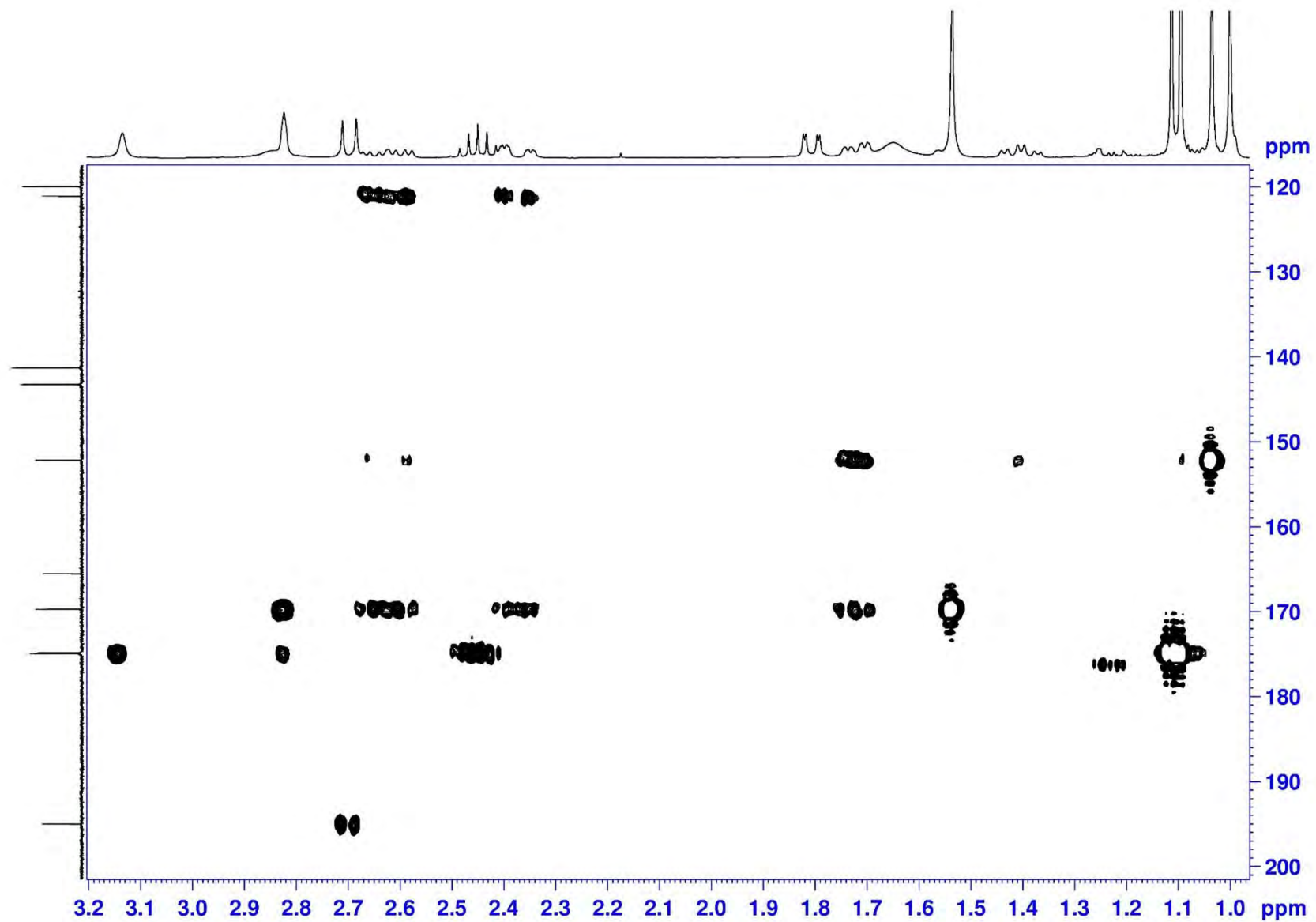
HMBC (400 MHz) spectrum of compound **25** in CDCl₃



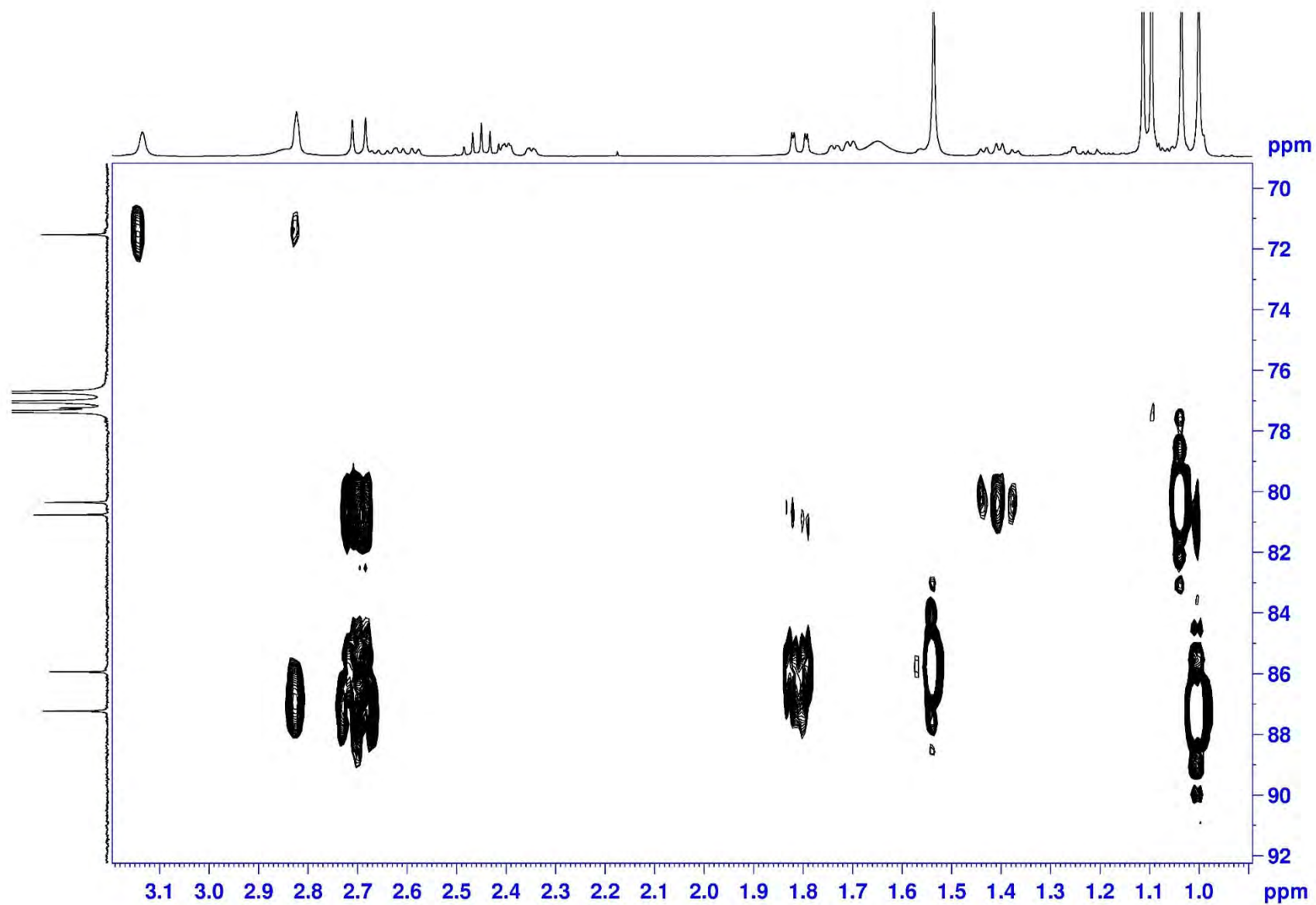
HMBC (400 MHz) spectrum of compound **25** in CDCl_3



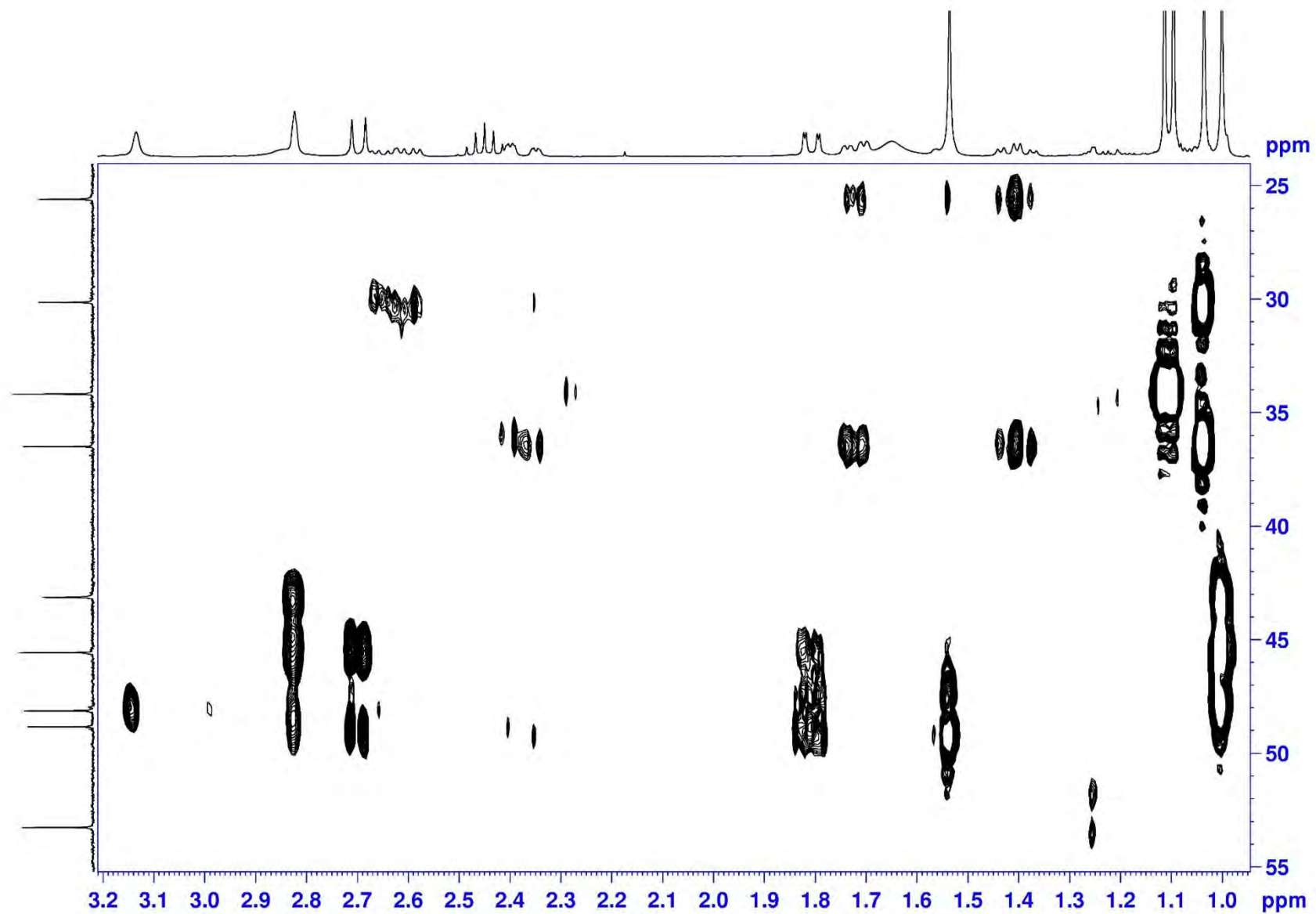
HMBC (400 MHz) spectrum of compound **25** in CDCl_3



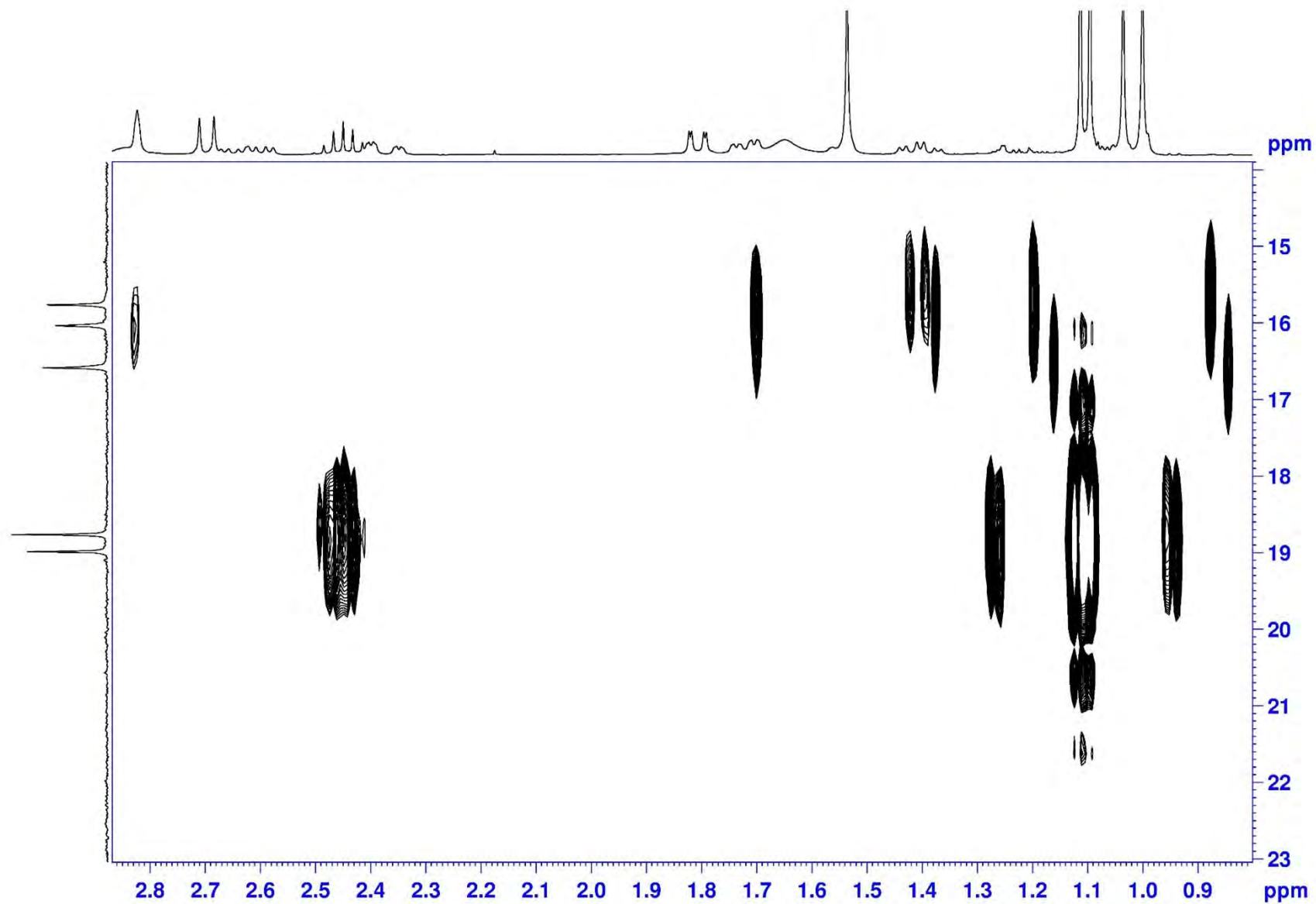
HMBC (400 MHz) spectrum of compound **25** in CDCl_3



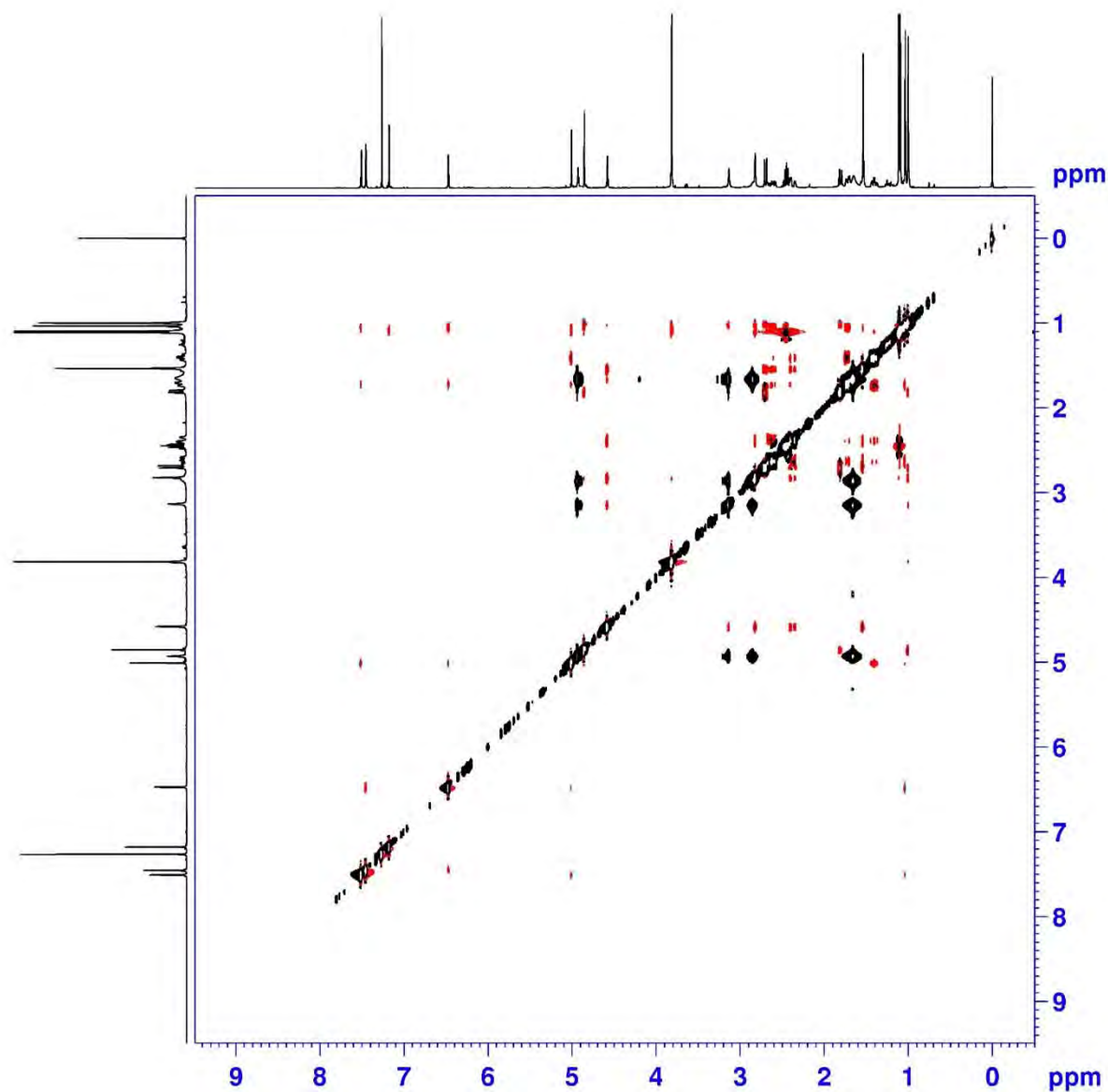
HMBC (400 MHz) spectrum of compound **25** in CDCl_3



HMBC (400 MHz) spectrum of compound **25** in CDCl_3



NOESY (400 MHz) spectrum of compound **25** in CDCl₃



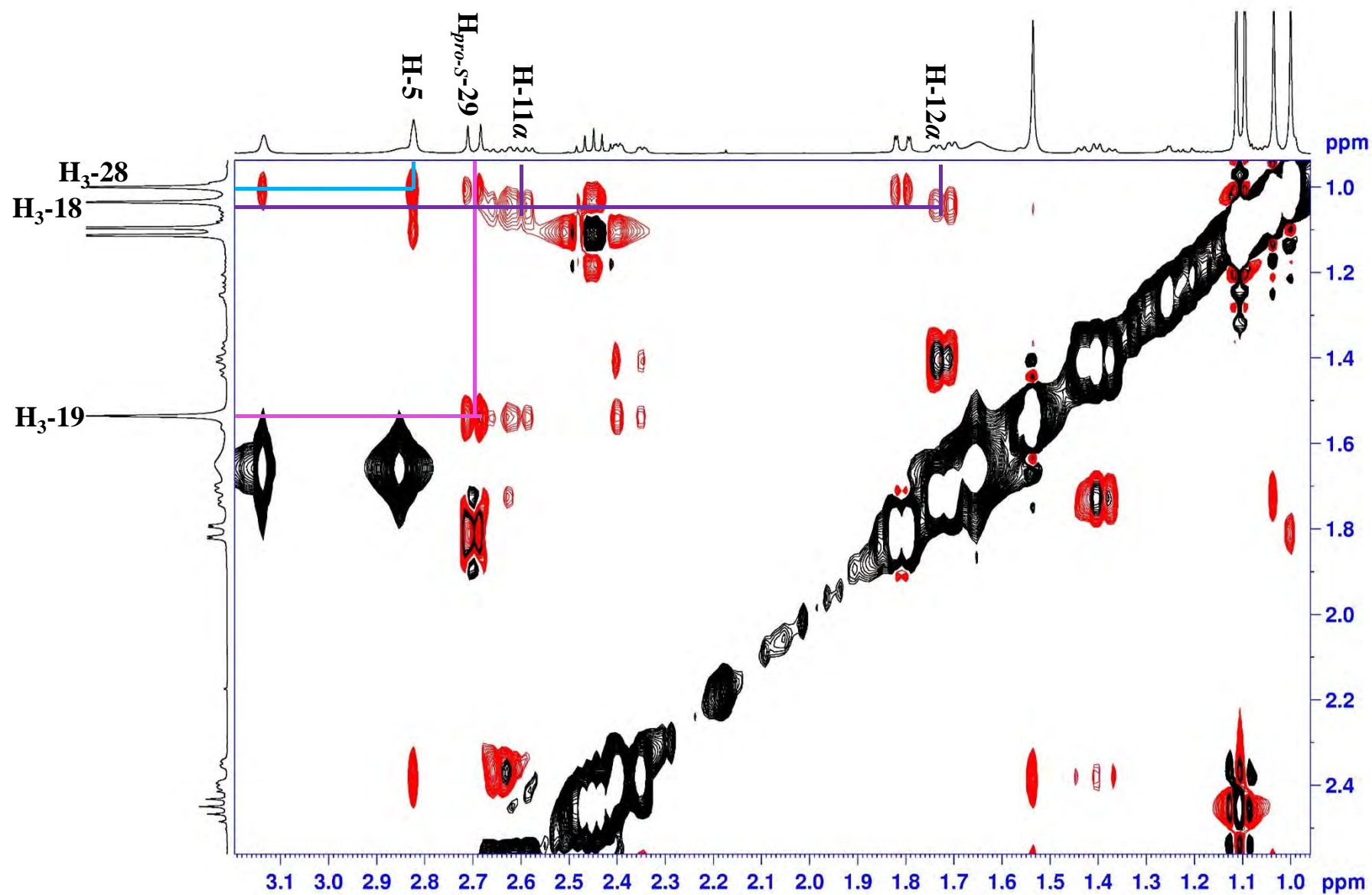
```

NAME          zjz-16
EXPNO          7
PROCNO         1
Date_          20160514
Time           19.55
INSTRUM        spect
PROBHD         5 mm CFPBBO 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             0.00011036 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
    
```

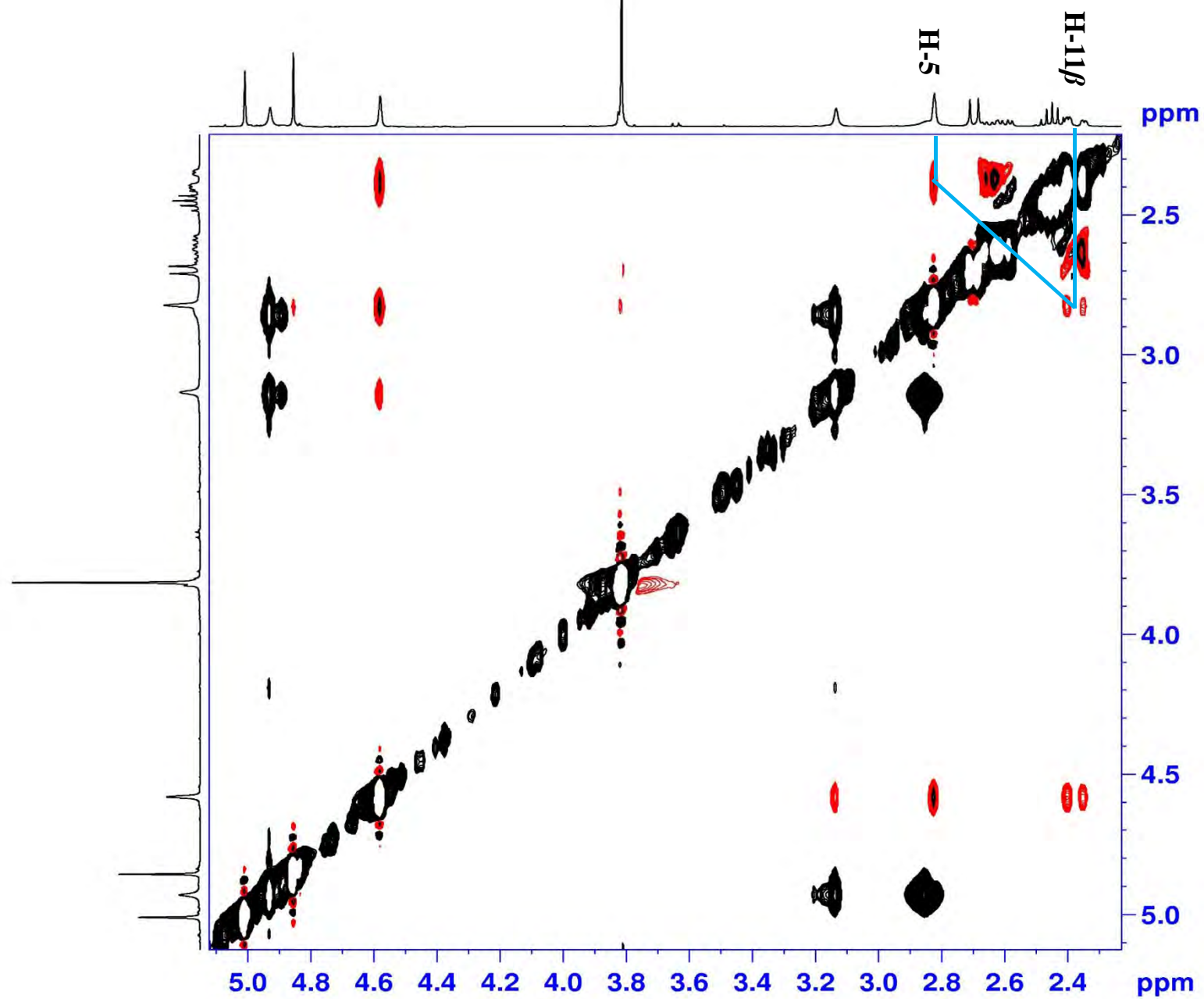
```

===== 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            400.1300051 MHz
WDW            QSINE
SSB            2
LB             0.00 Hz
GB             0
PC             1.00
SI             1024
MC2            States-TPPI
SF            400.1300043 MHz
WDW            QSINE
SSB            2
LB             0.00 Hz
GB             0
    
```

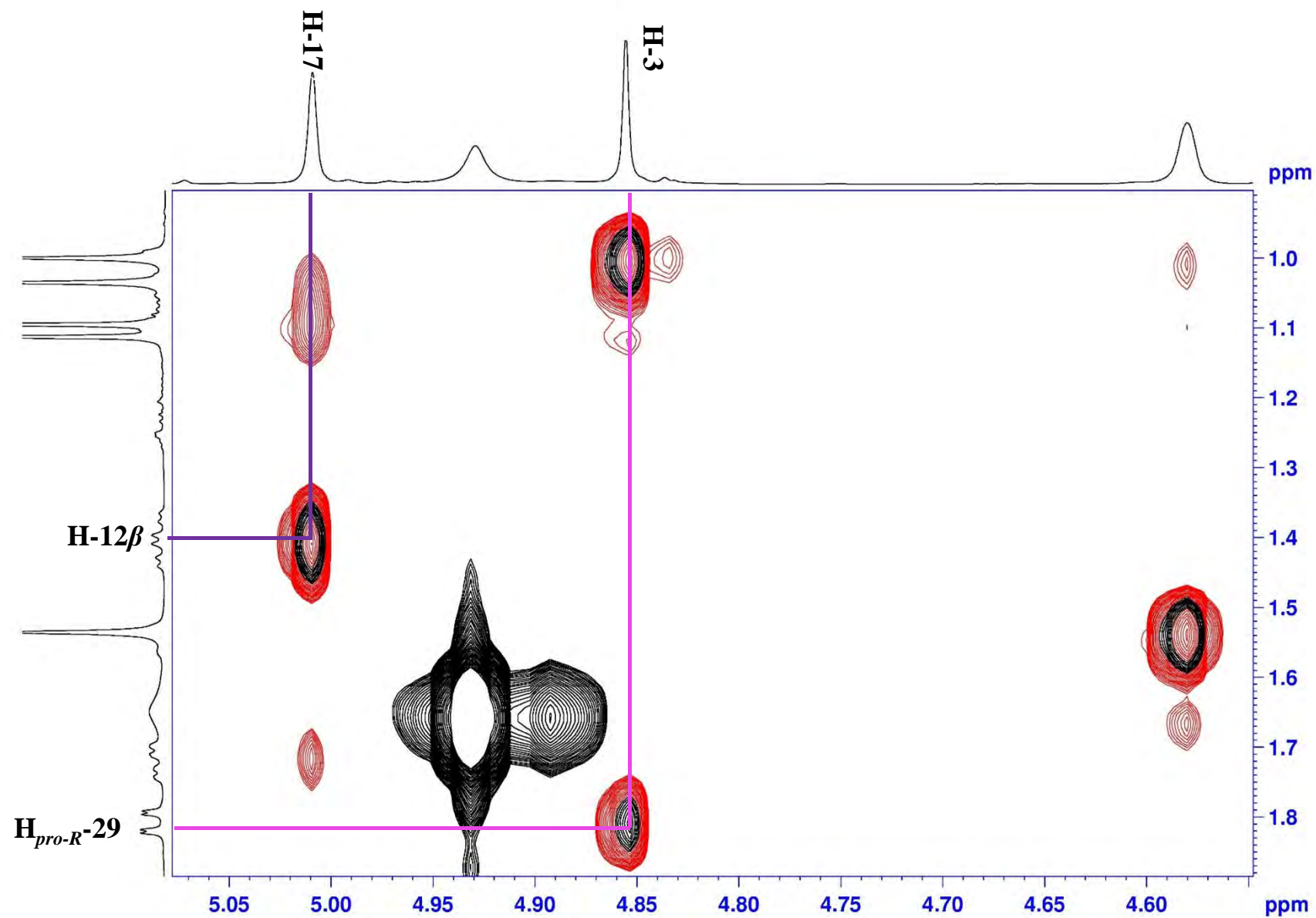

NOESY (400 MHz) spectrum of compound **25** in CDCl_3



NOESY (400 MHz) spectrum of compound **25** in CDCl₃



NOESY (400 MHz) spectrum of compound **25** in CDCl_3



HR-ESIMS for compound **26**

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\MS\data\201605\liwanshan_dgy-10_pos_4_01_1852.d
 Method LC_Direct Infusion_pos_100-1000mz.m
 Sample Name liwanshan_dgy-10_pos
 Comment

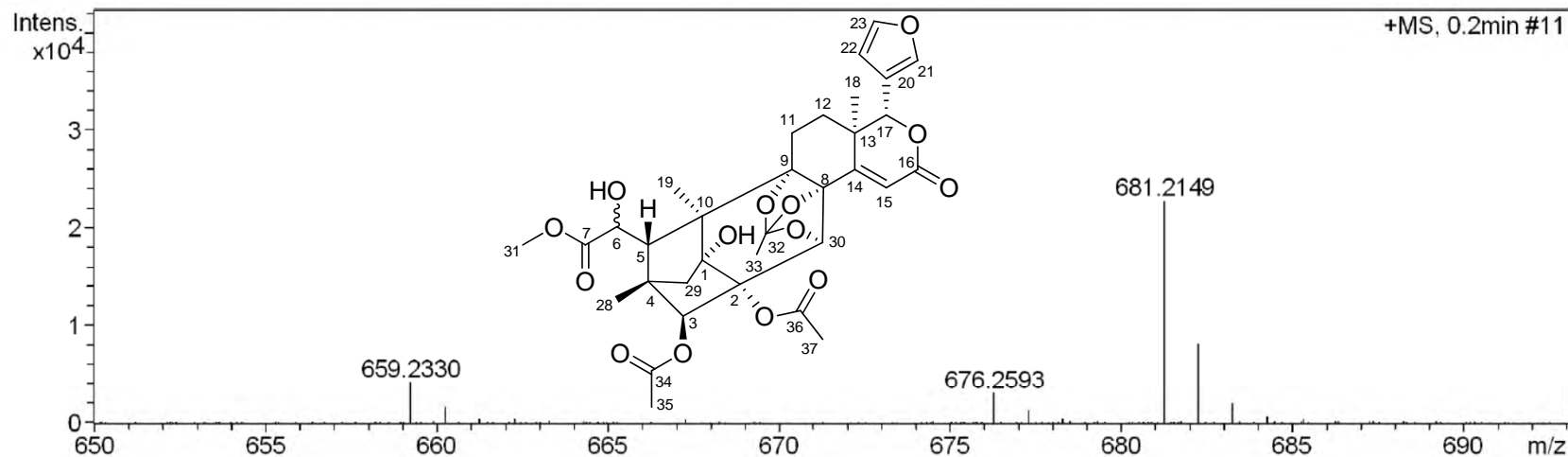
Acquisition Date 5/19/2016 8:30:55 AM

Operator SCSIO

Instrument / Ser# maXis 29

Acquisition Parameter

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



| Meas. m/z | # | Formula | Score | m/z | err [ppm] | err [mDa] | mSigma | rdB | e ⁻ Conf | N-Rule |
|-----------|---|-------------------|--------|-----------|-----------|-----------|--------|------|---------------------|--------|
| 659.2330 | 1 | C 33 H 39 O 14 | 100.00 | 659.2334 | 0.6 | 0.4 | 11.2 | 14.5 | even | ok |
| 681.2149 | 1 | C 33 H 38 Na O 14 | 100.00 | 681.2154 | 0.7 | 0.5 | 5.7 | 14.5 | even | ok |
| 1339.4422 | 1 | C 66 H 76 Na O 28 | 100.00 | 1339.4415 | -0.5 | -0.6 | 44.9 | 28.5 | even | ok |

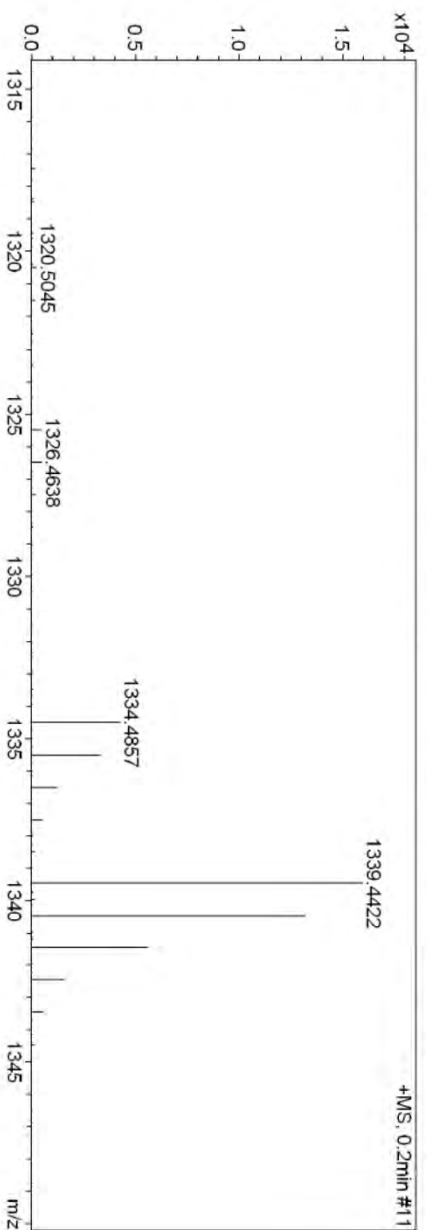
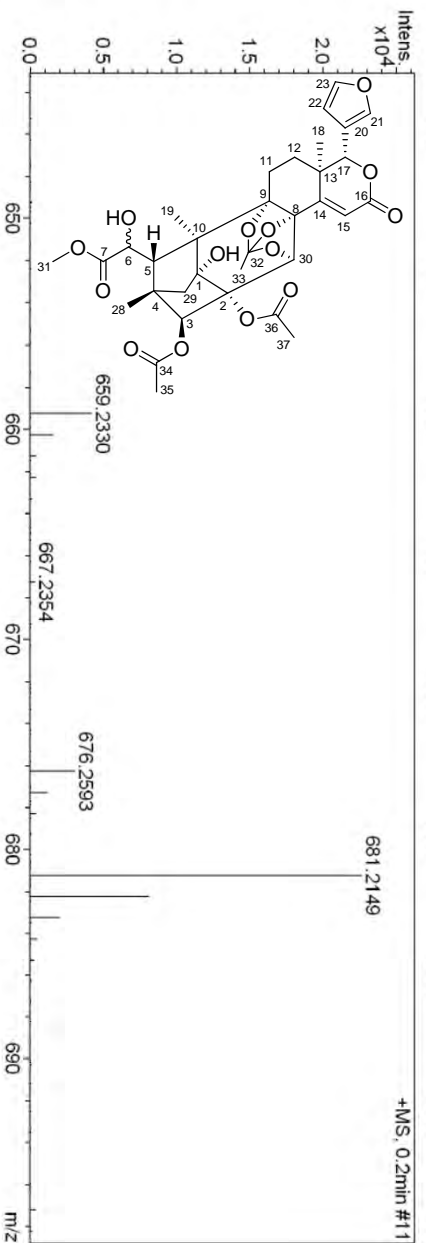
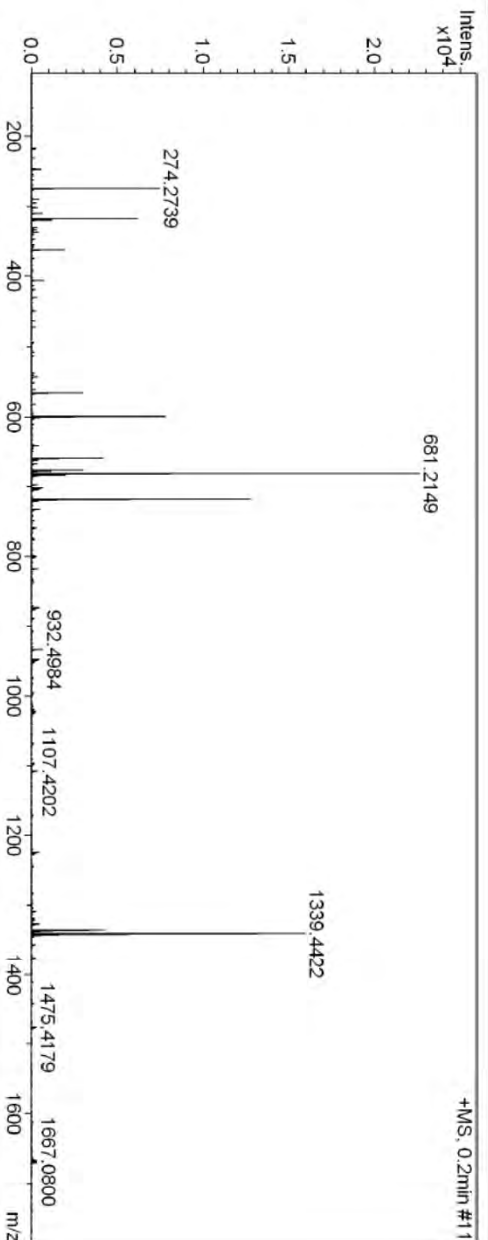
Generic Display Report

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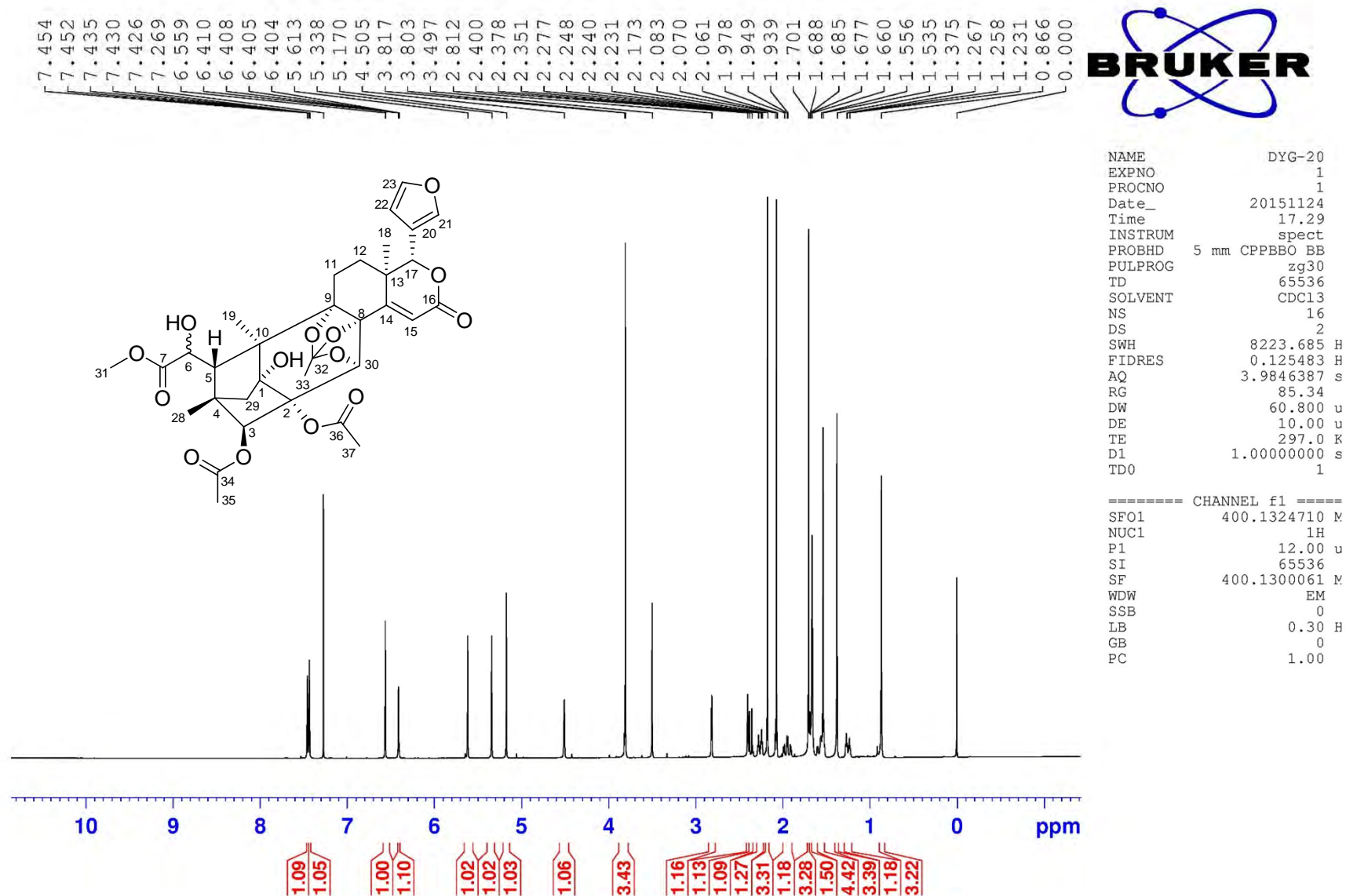
Analysis Info
Analysis Name
Method
Sample Name
Comment

D:\Data\MS\data\201605\llwanshan_dgy-10_pos_4_01_1852.d
LC_Direct Infusion_pos_100-1000mz.m
llwanshan_dgy-10_pos

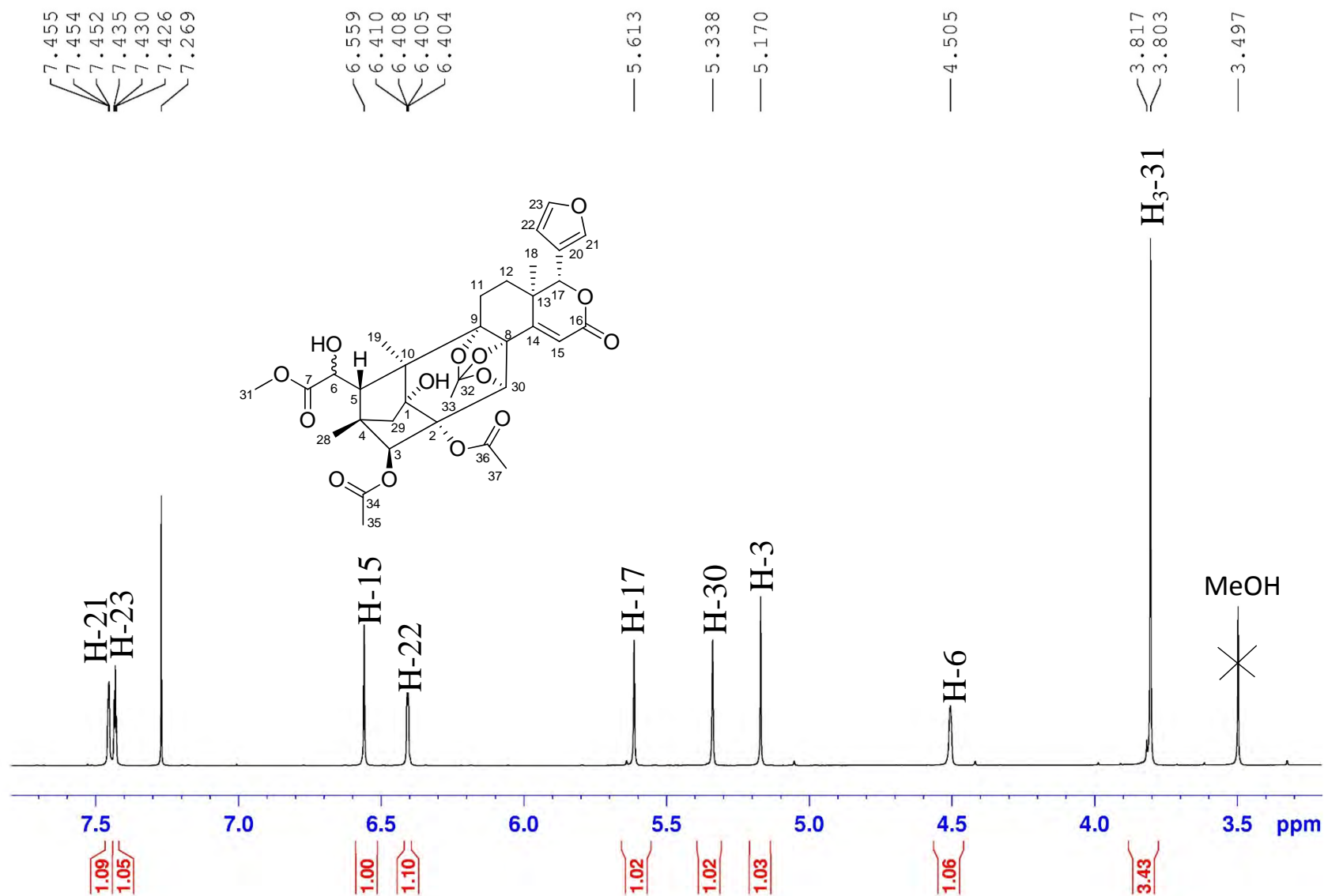
Acquisition Date 5/19/2016 8:30:55 AM
Operator
Instrument
SCSIO
maxis



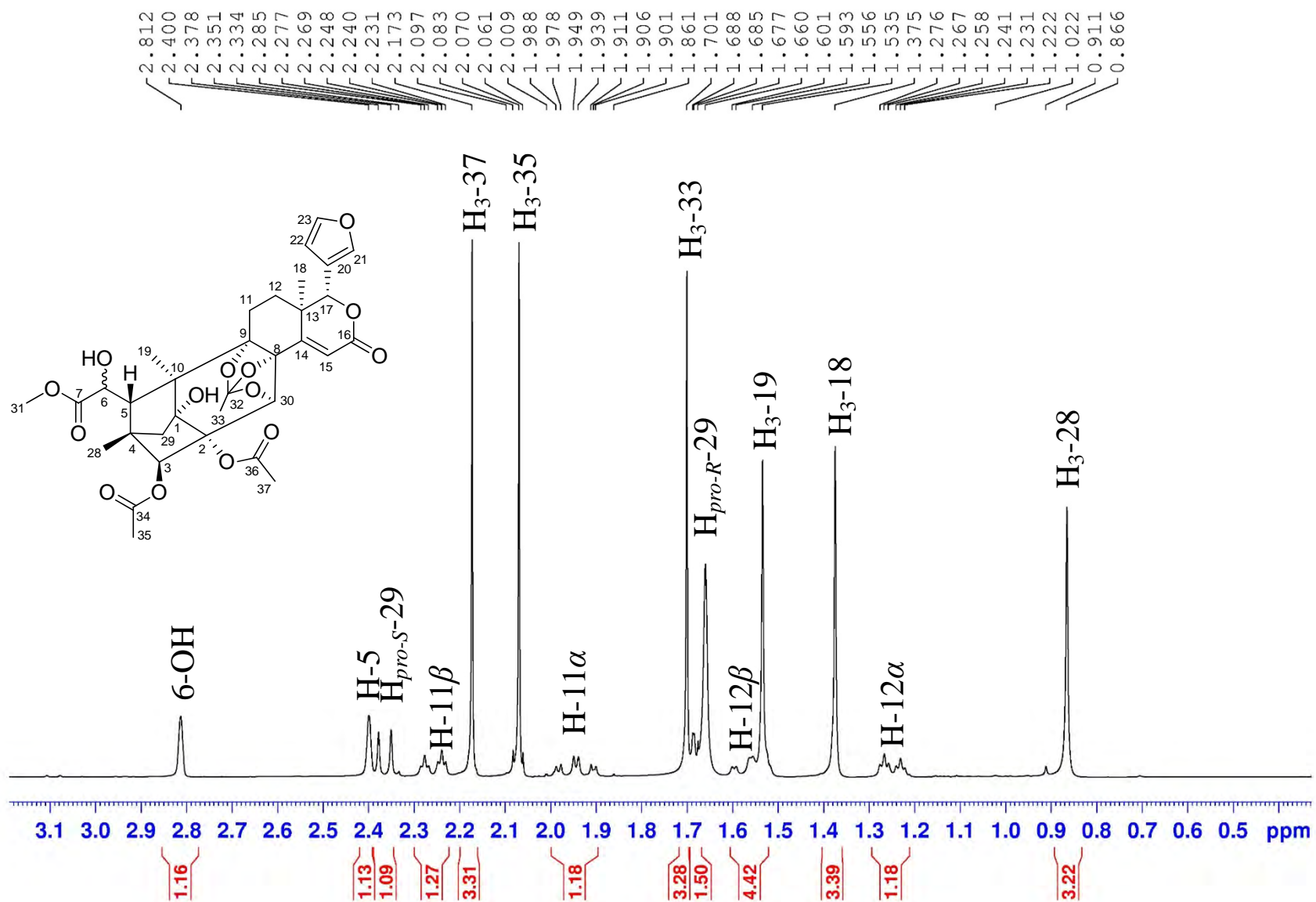
^1H NMR (400 MHz) spectrum of compound **26** in CDCl_3



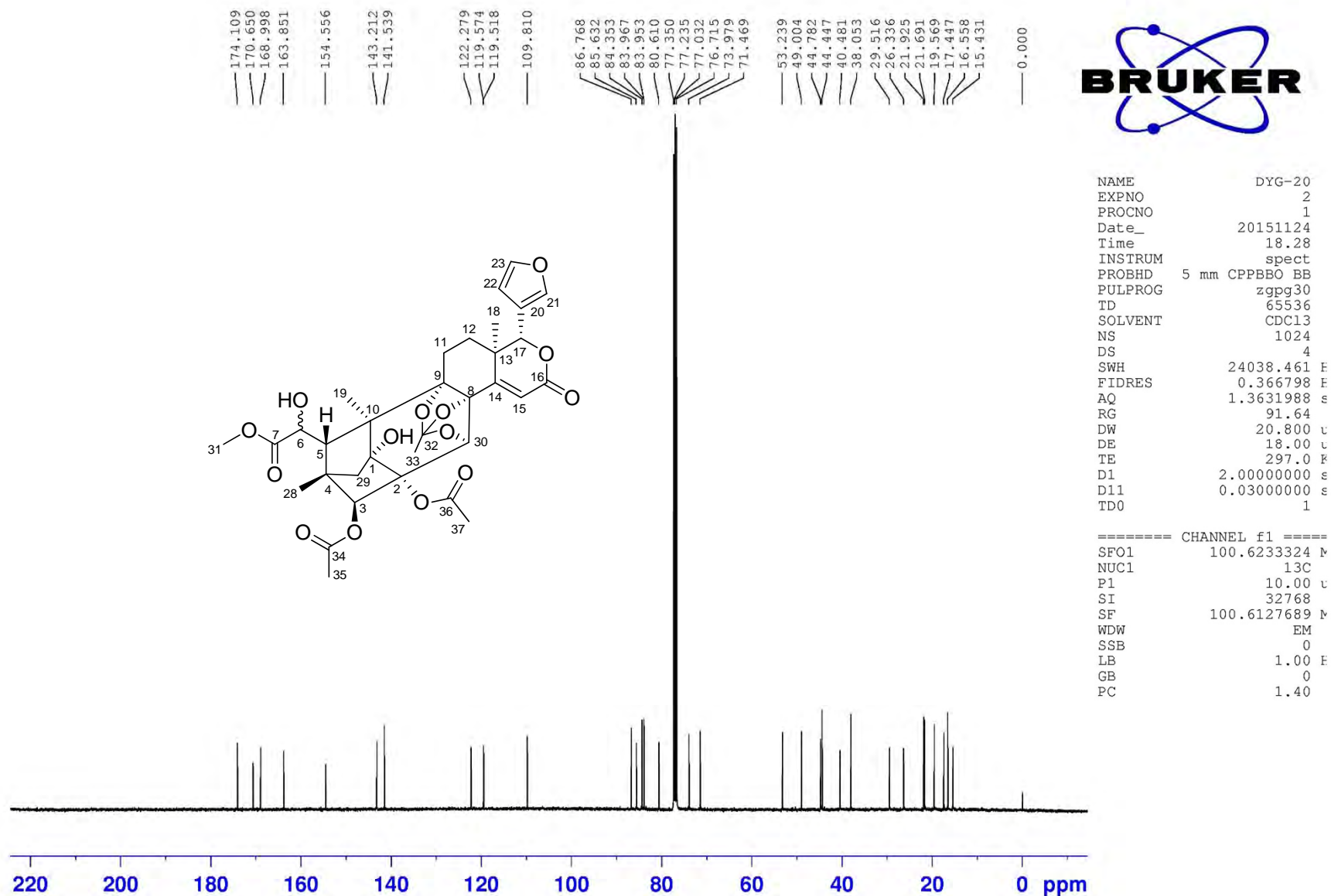
^1H NMR (400 MHz) spectrum of compound **26** in CDCl_3



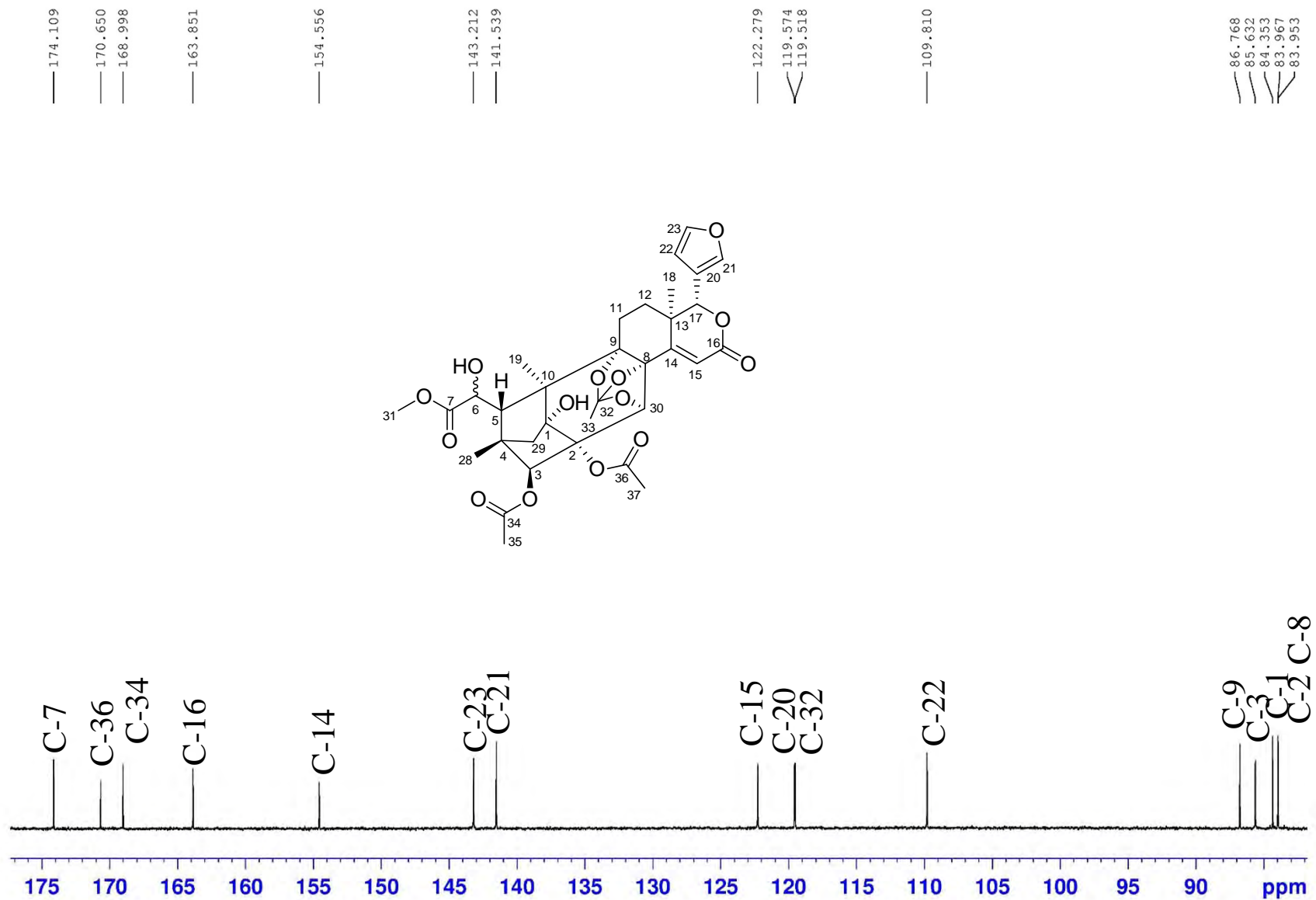
^1H NMR (400 MHz) spectrum of compound **26** in CDCl_3



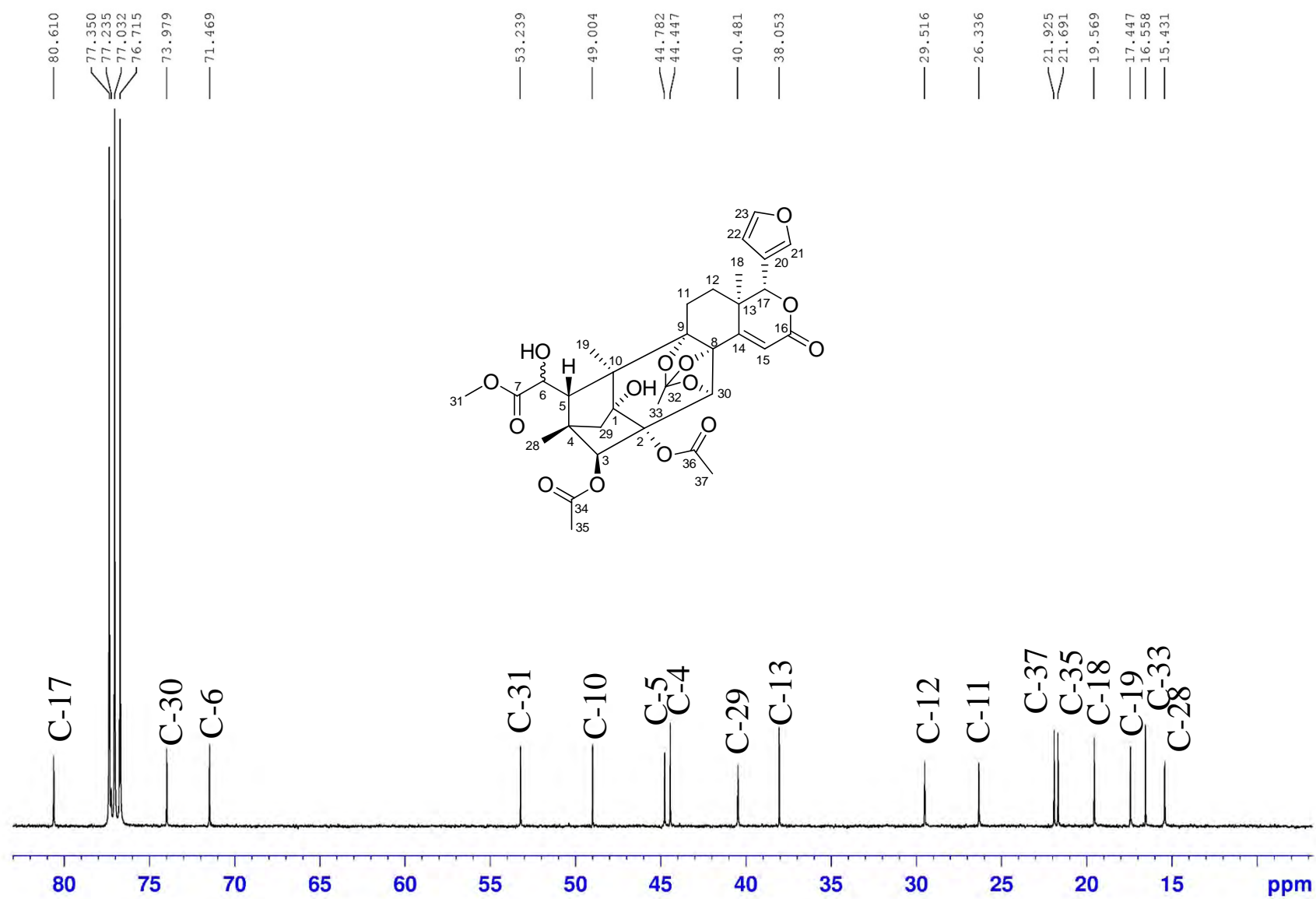
^{13}C NMR (100 MHz) spectrum of compound **26** in CDCl_3



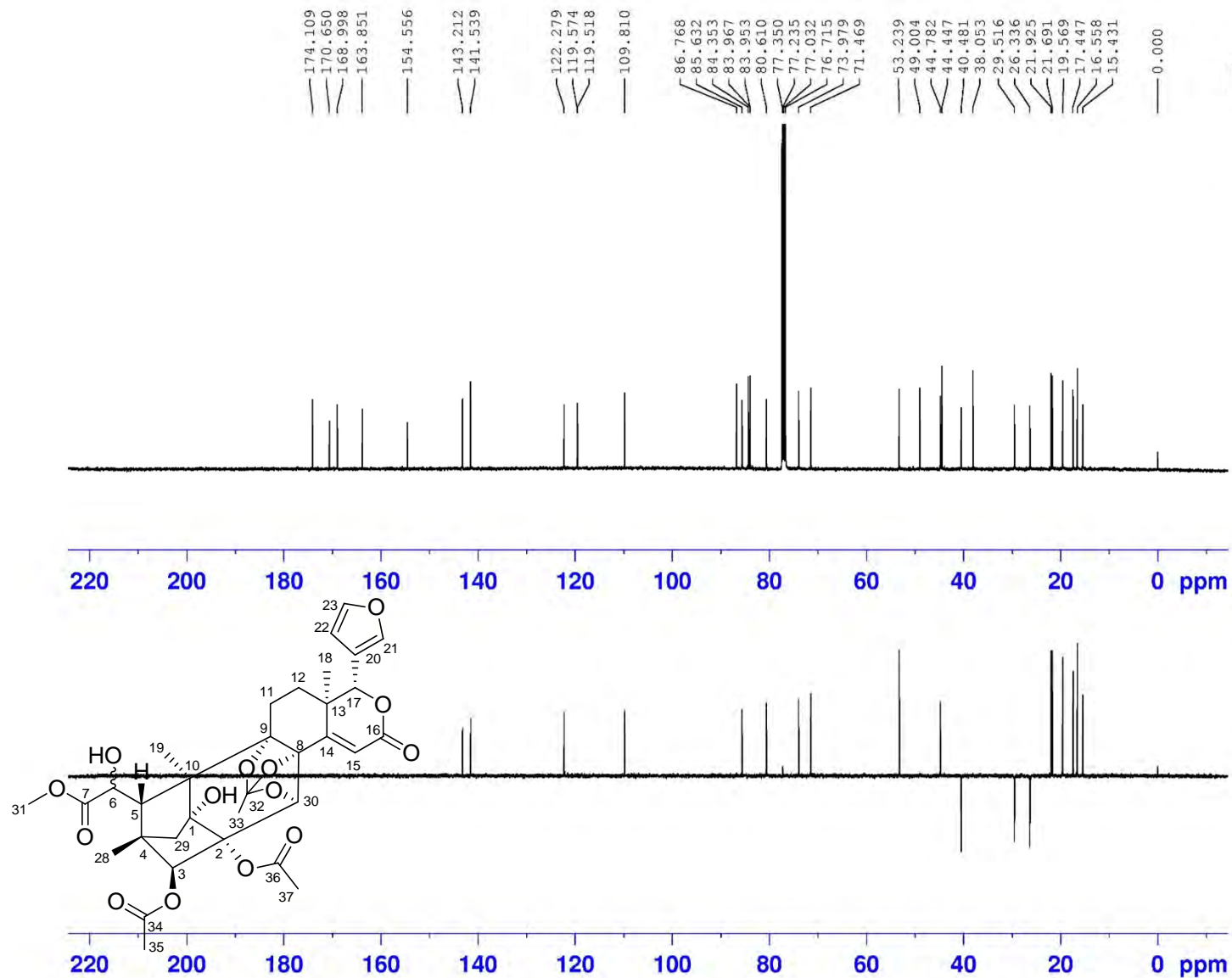
^{13}C NMR (100 MHz) spectrum of compound **26** in CDCl_3



^{13}C NMR (100 MHz) spectrum of compound **26** in CDCl_3



DEPT135 (100 MHz) spectrum of compound **26** in CDCl₃



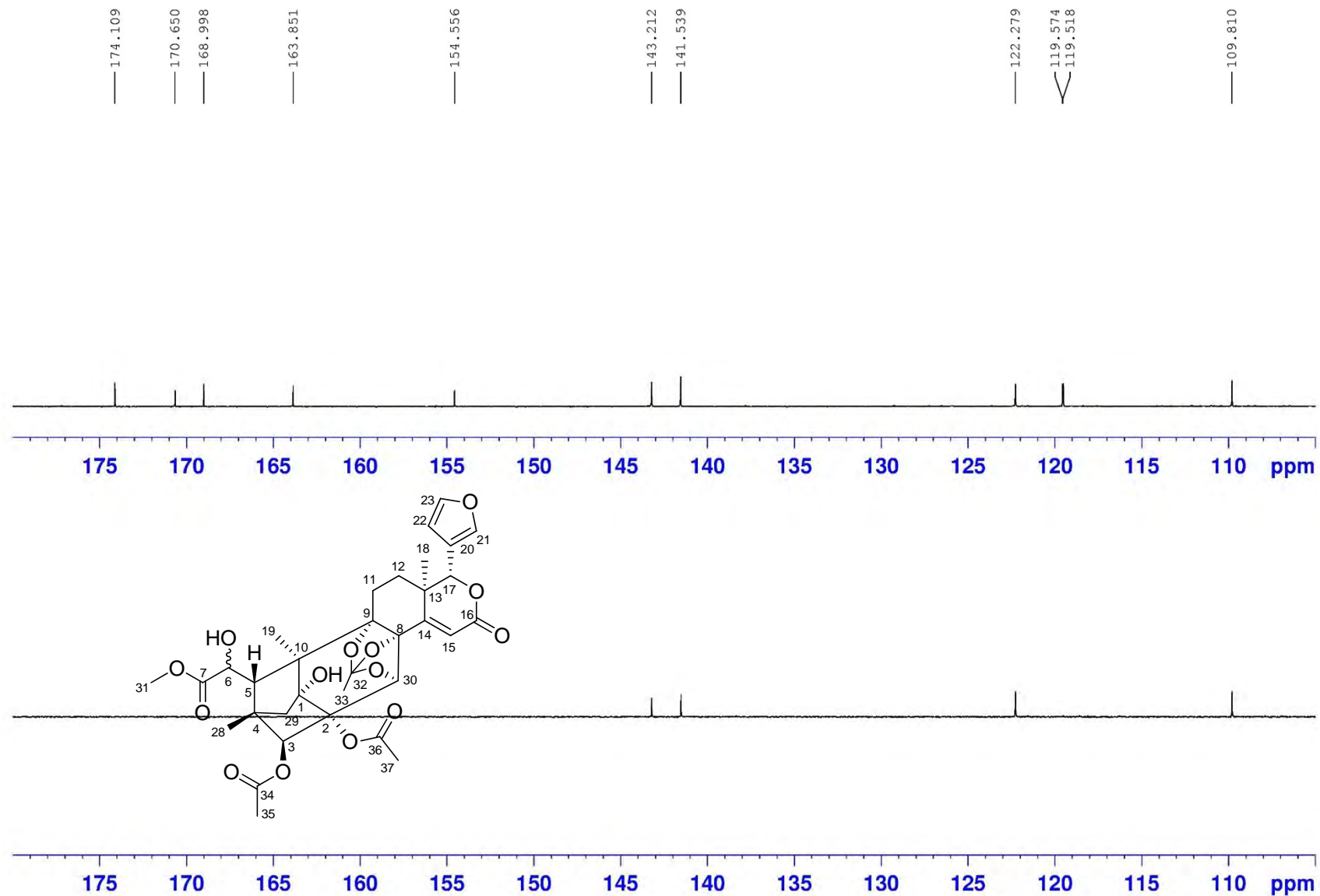
```

NAME          DYG-20
EXPNO         3
PROCNO        1
Date_         20151124
Time          18.47
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       deptsp135
TD            65536
SOLVENT       CDCl3
NS            300
DS            4
SWH           24038.461 F
FIDRES        0.366798 F
AQ            1.3631988 s
RG            130.26
DW            20.800 s
DE            18.00 s
TE            297.0 F
CNST2         145.0000000
D1            2.00000000 s
D2            0.00344828 s
D12           0.00002000 s
TD0           1
    
```

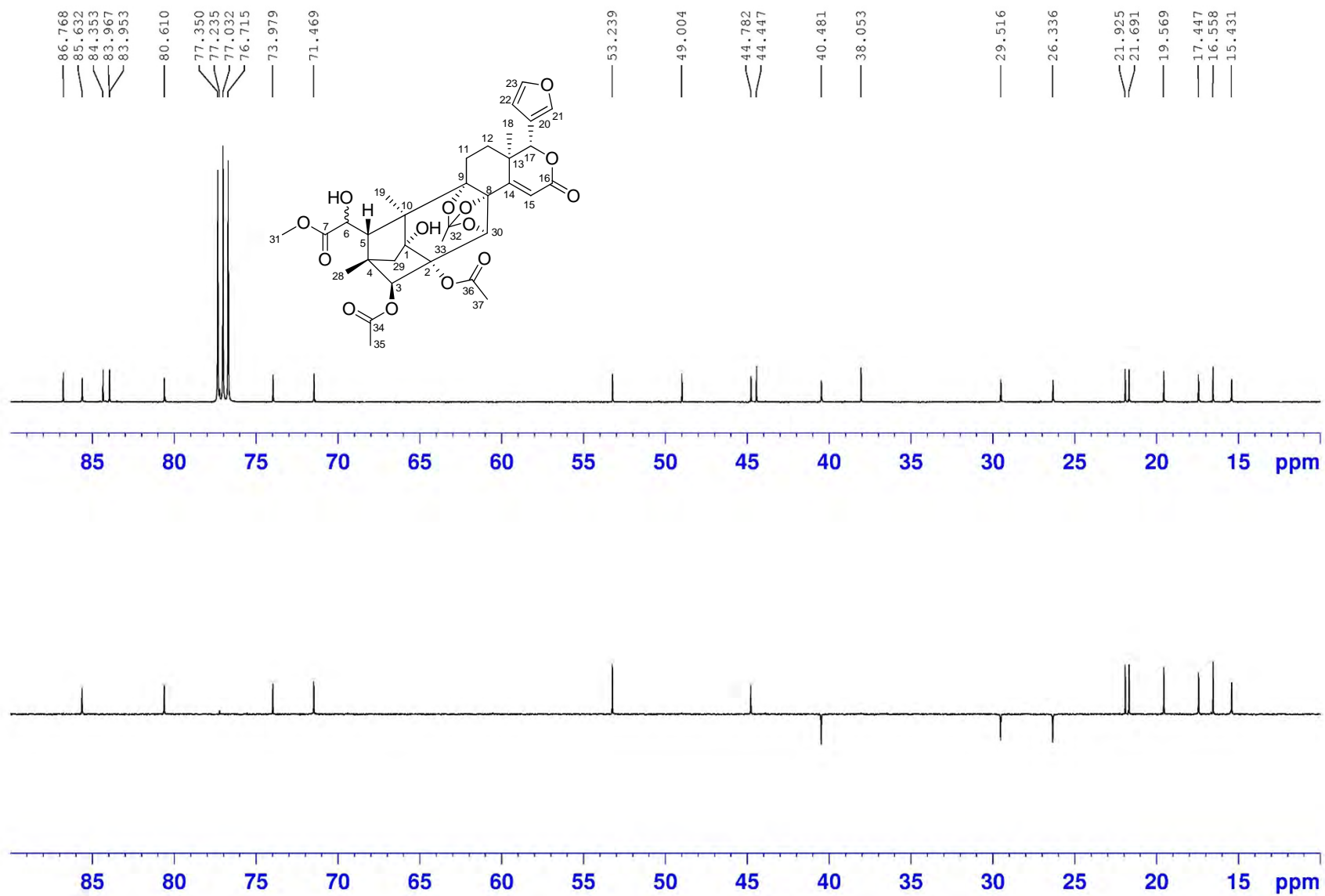
```

===== CHANNEL f1 =====
SFO1         100.623324 M
NUC1          13C
P1            10.00 s
P13           2000.00 s
SI            32768
SF            100.6127690 M
WDW           EM
SSB           0
LB            1.00 F
GB            0
PC            1.40
    
```

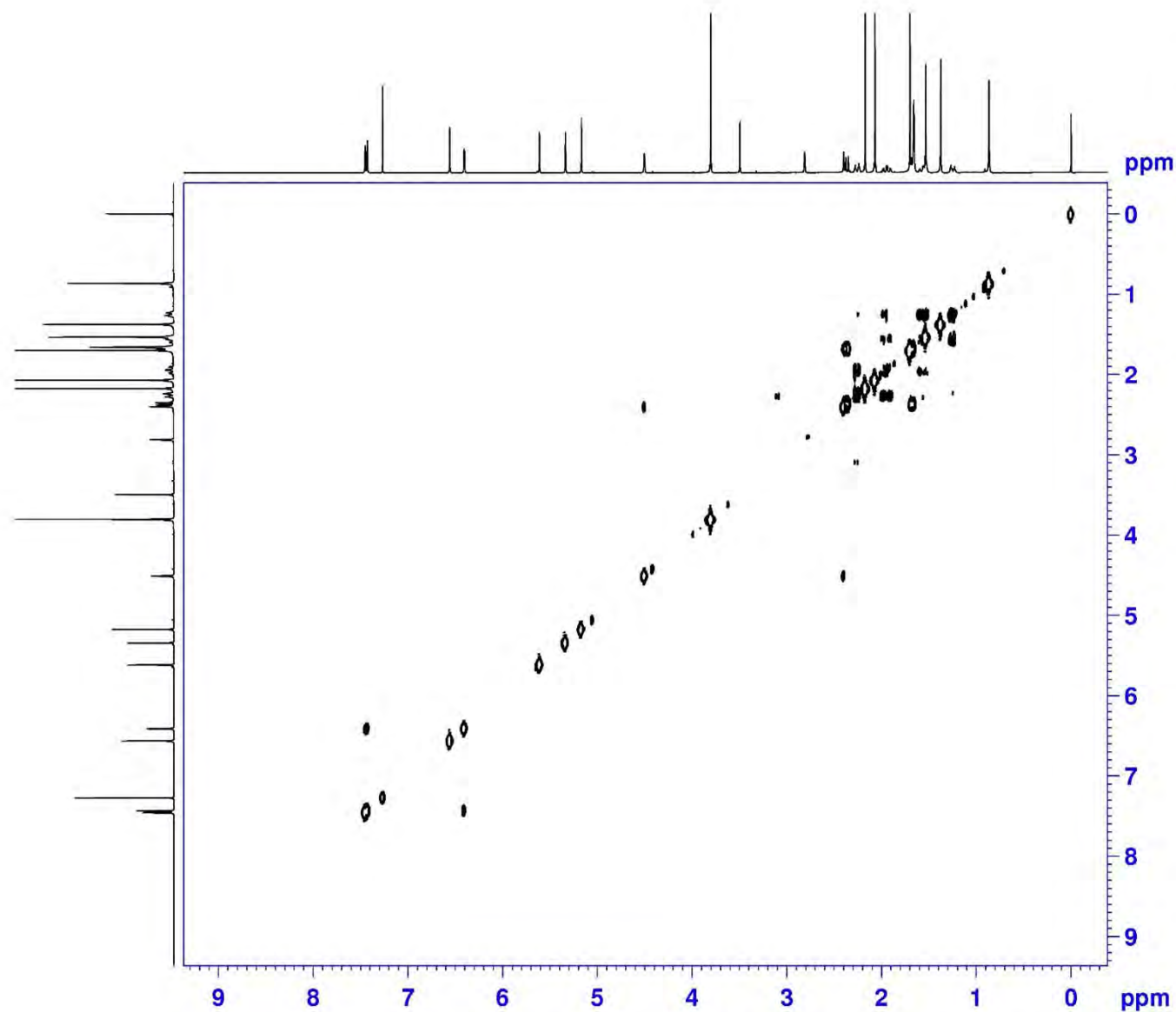
DEPT135 (100 MHz) spectrum of compound **26** in CDCl₃



DEPT135 (100 MHz) spectrum of compound **26** in CDCl₃



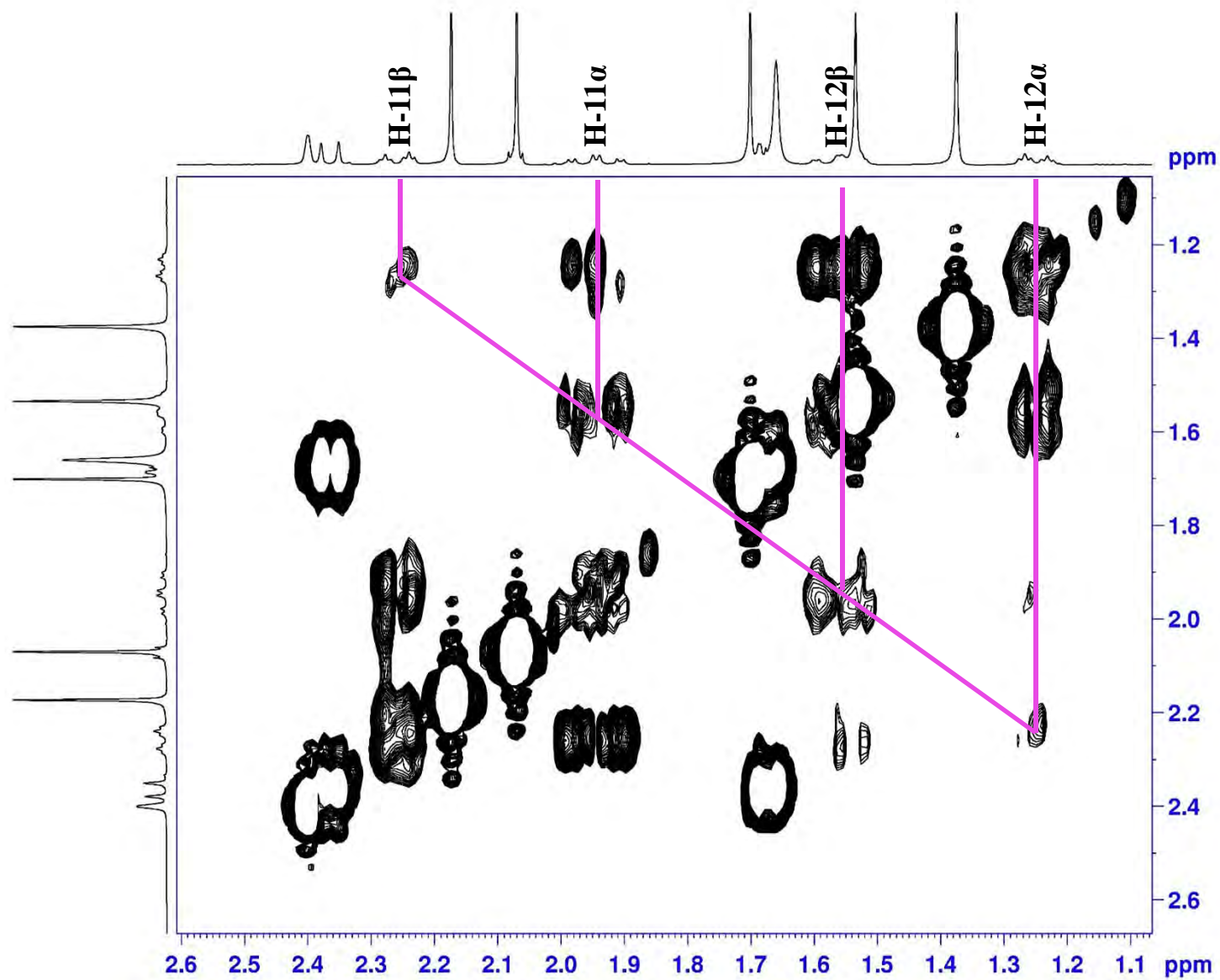
^1H - ^1H COSY (400 MHz) spectrum of compound **26** in CDCl_3



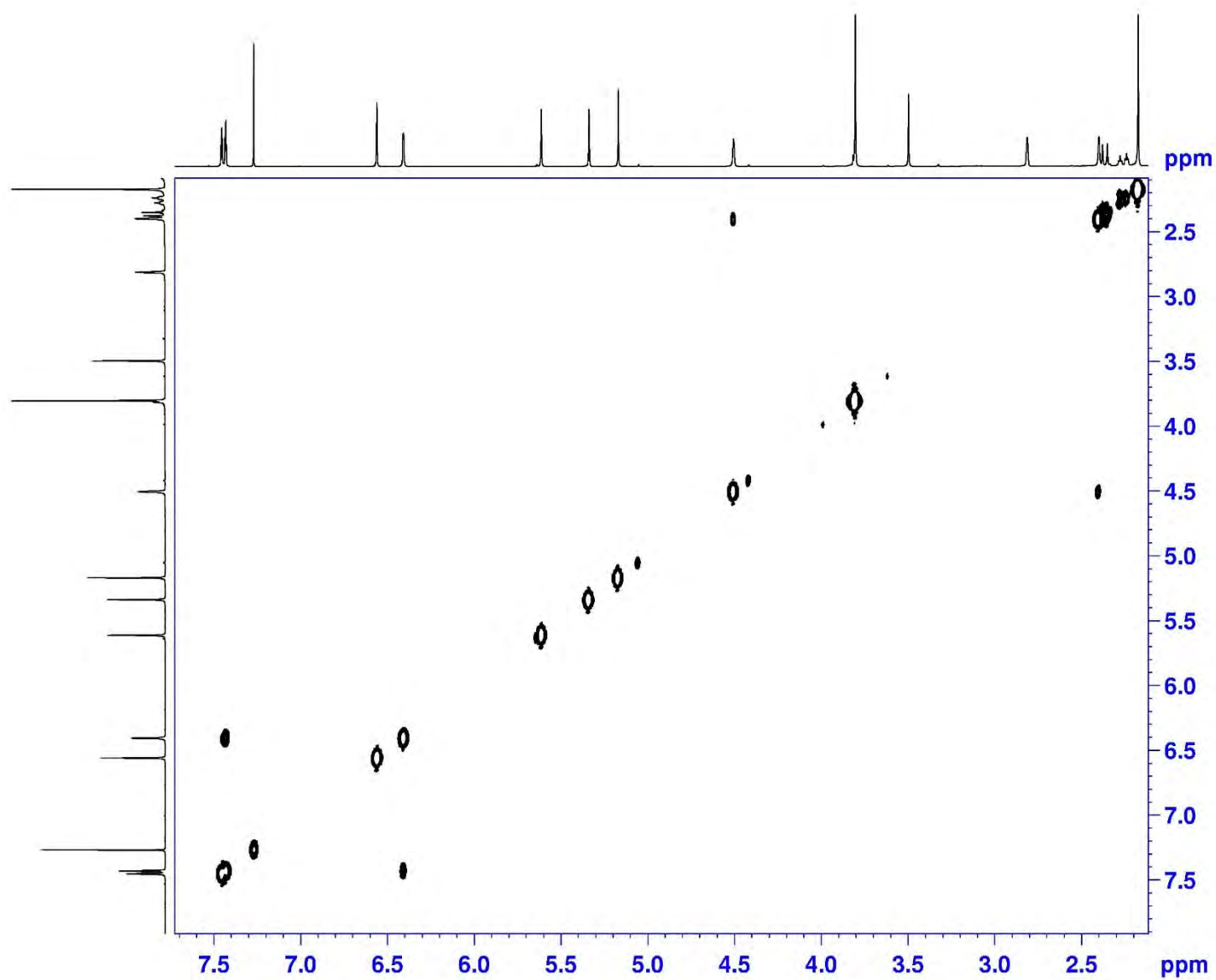
NAME DYG-20
EXPNO 4
PROCNO 1
Date_ 20160313
Time 22.36
INSTRUM spect
PROBHD 5 mm CFPBBO BB
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl_3
NS 8
DS 8
SWH 3906.250 H
FIDRES 1.907349 H
AQ 0.2621940 s
RG 208.5
DW 128.000 u
DE 10.00 u
TE 297.0 K
D0 0.00000300 s
D1 1.89678097 s
D11 0.03000000 s
D12 0.00002000 s
D13 0.00000400 s
D16 0.00020000 s
IN0 0.00025600 s

===== CHANNEL f1 =====
SFO1 400.1318006 M
NUC1 ^1H
P0 11.50 u
P1 11.50 u
P17 2500.00 u
ND0 1
TD 128
SFO1 400.1318 M
FIDRES 30.517578 H
SW 9.762 p
FnMODE QF
SI 1024
SF 400.1300061 M
WDW QSINE
SSB 0
LB 0.00 H
GB 0
PC 1.40
SI 1024
MC2 QF
SF 400.1300061 M
WDW QSINE
SSB 0

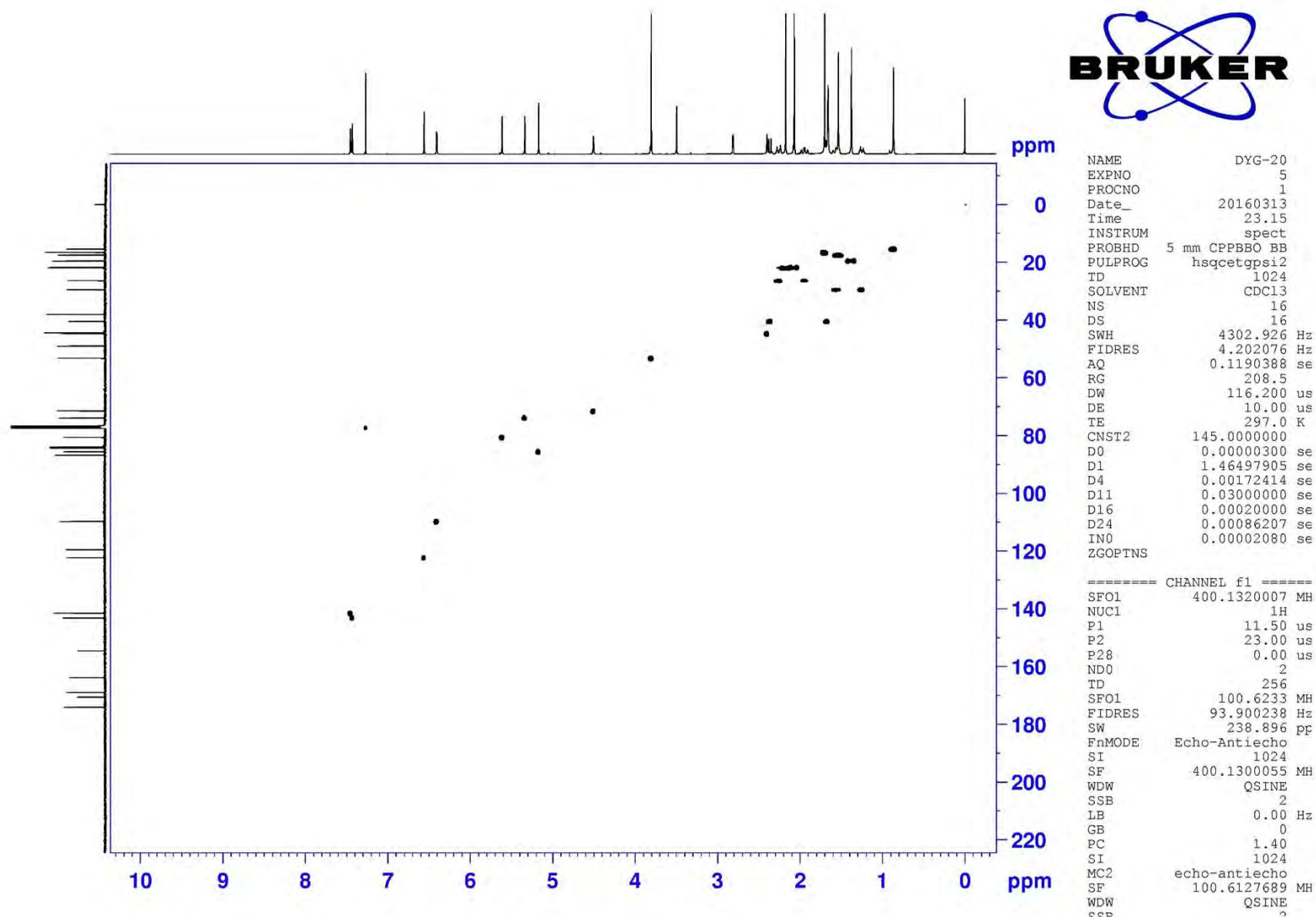
^1H - ^1H COSY (400 MHz) spectrum of compound **26** in CDCl_3



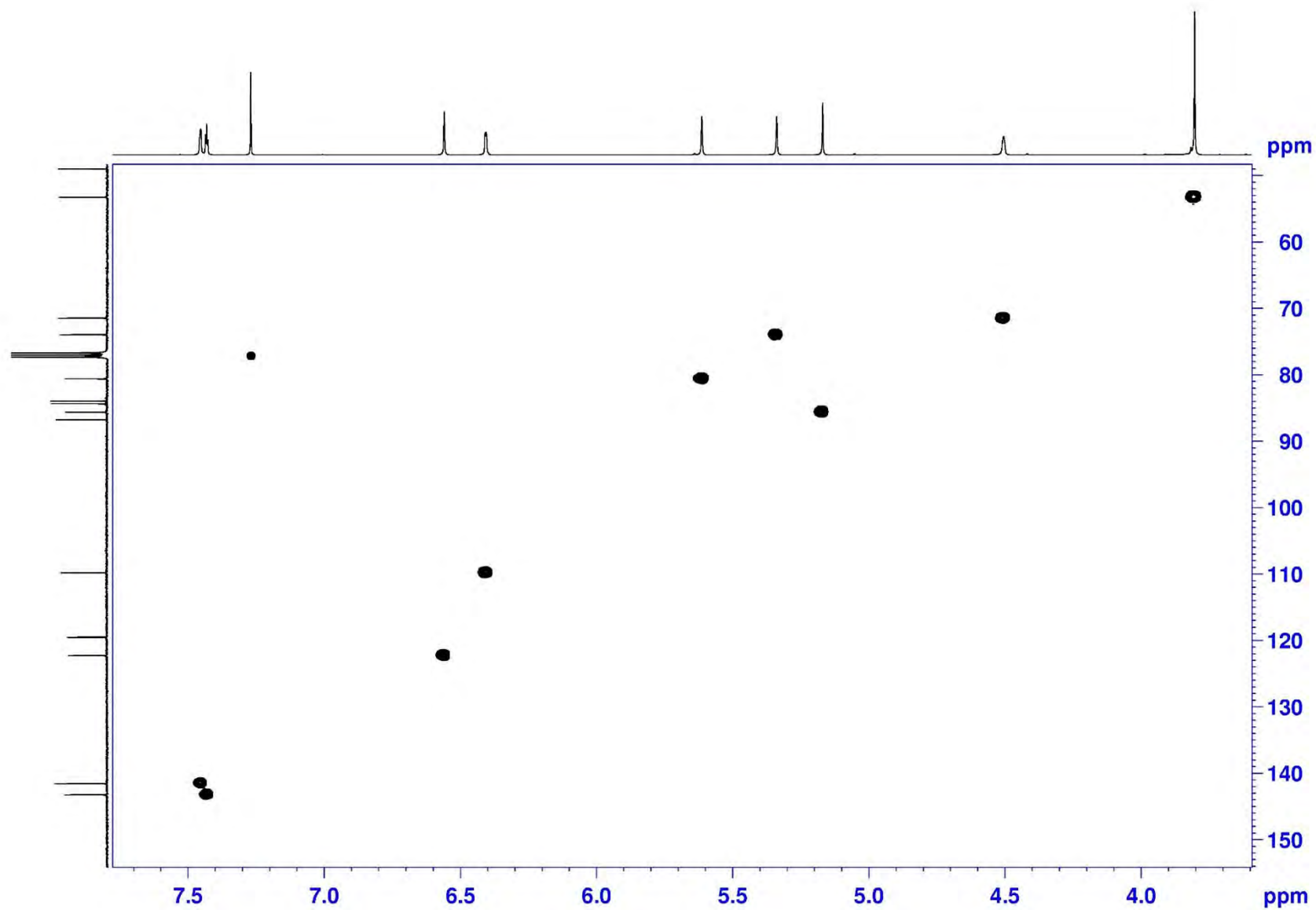
^1H - ^1H COSY (400 MHz) spectrum of compound **26** in CDCl_3



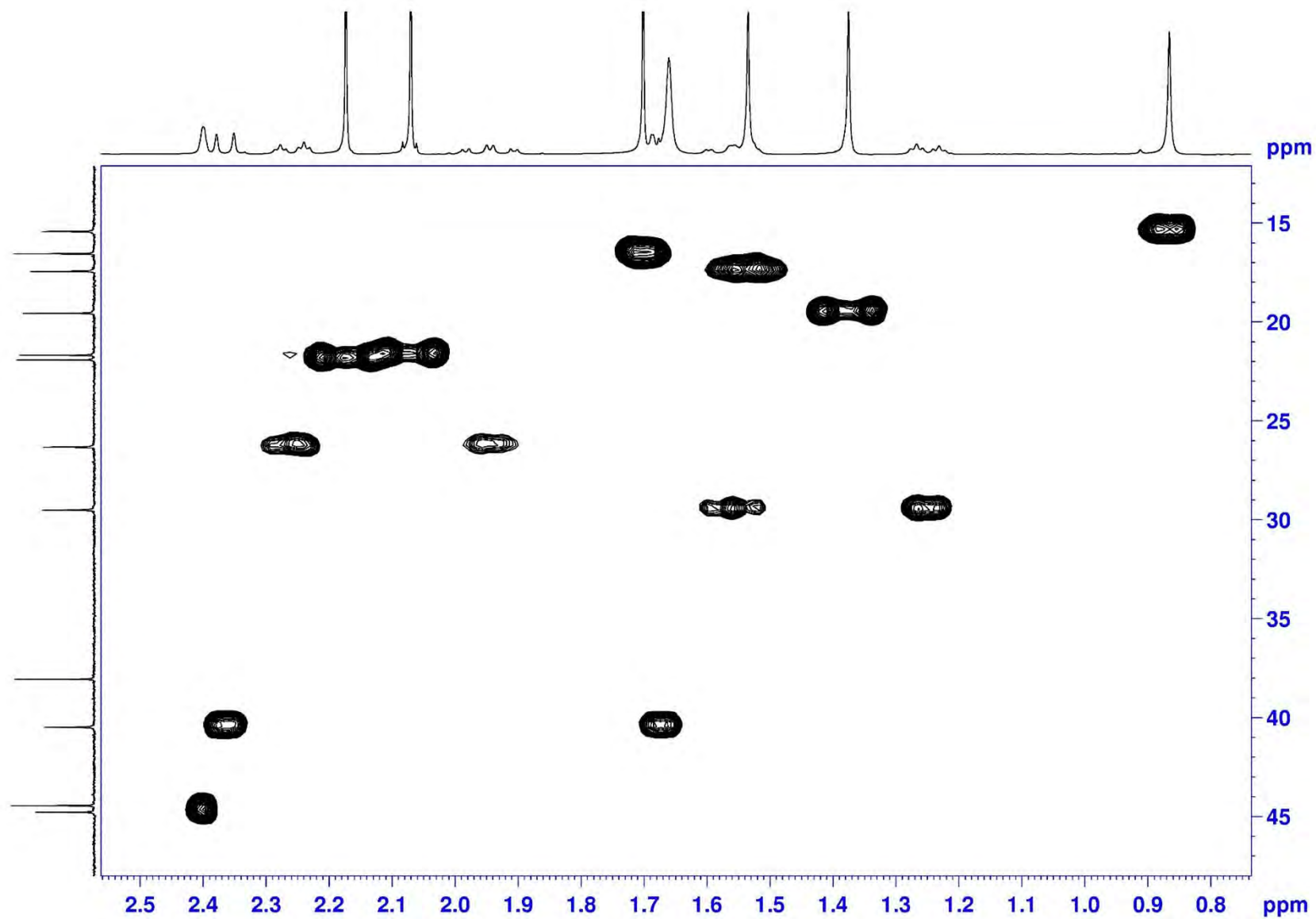
HSQC (400 MHz) spectrum of compound **26** in CDCl₃



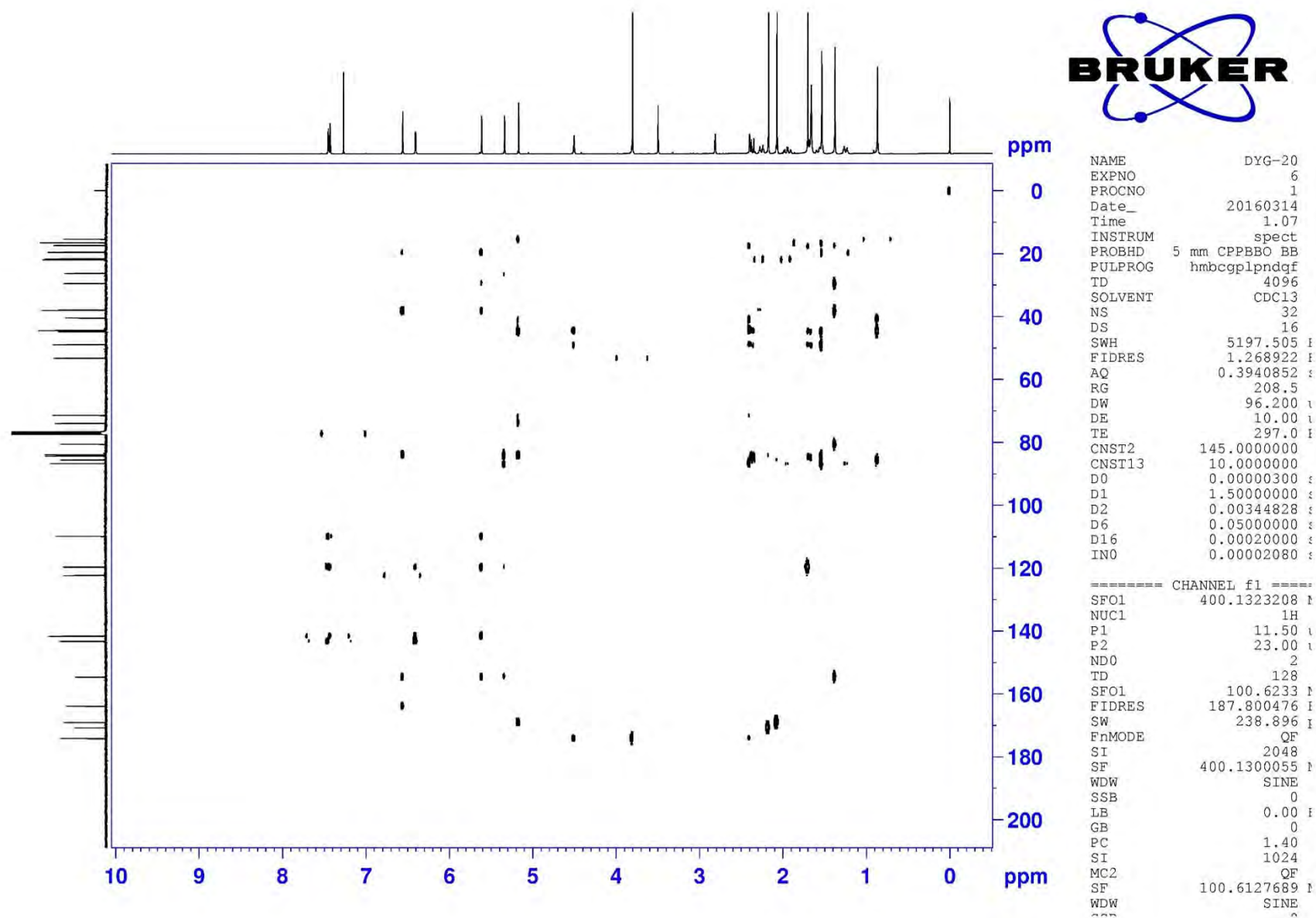
HSQC (400 MHz) spectrum of compound **26** in CDCl₃



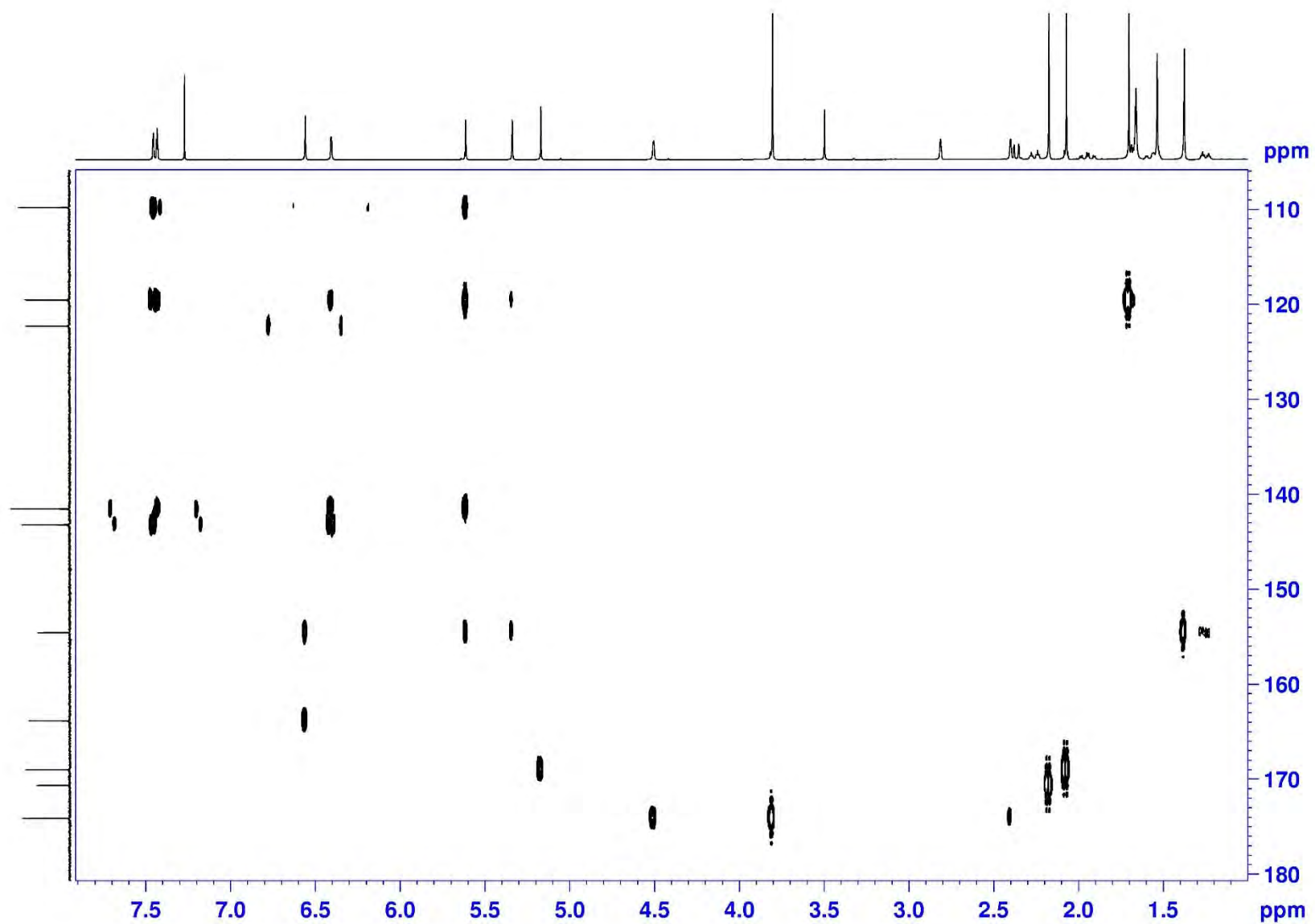
HSQC (400 MHz) spectrum of compound **26** in CDCl₃



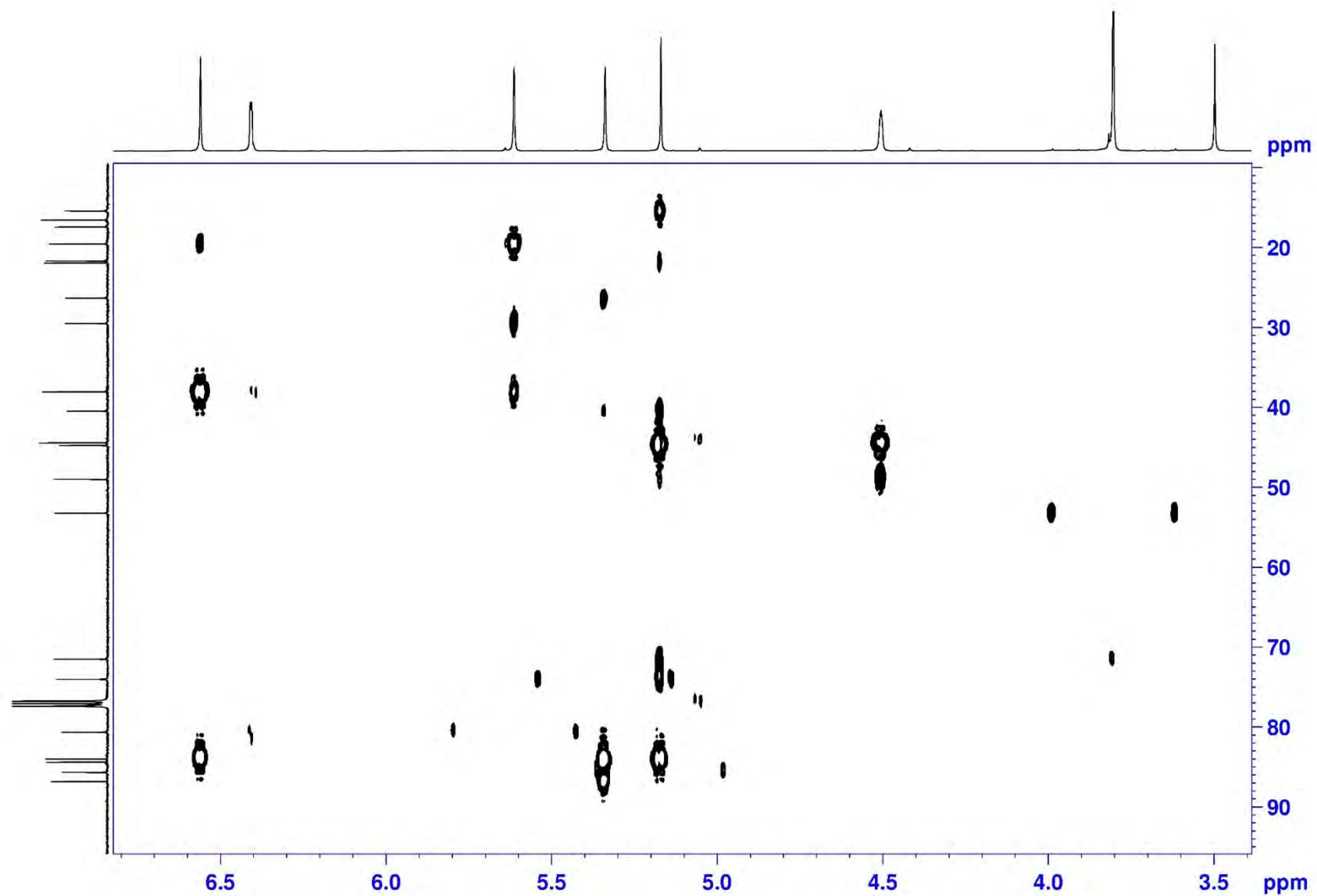
HMBC (400 MHz) spectrum of compound **26** in CDCl₃



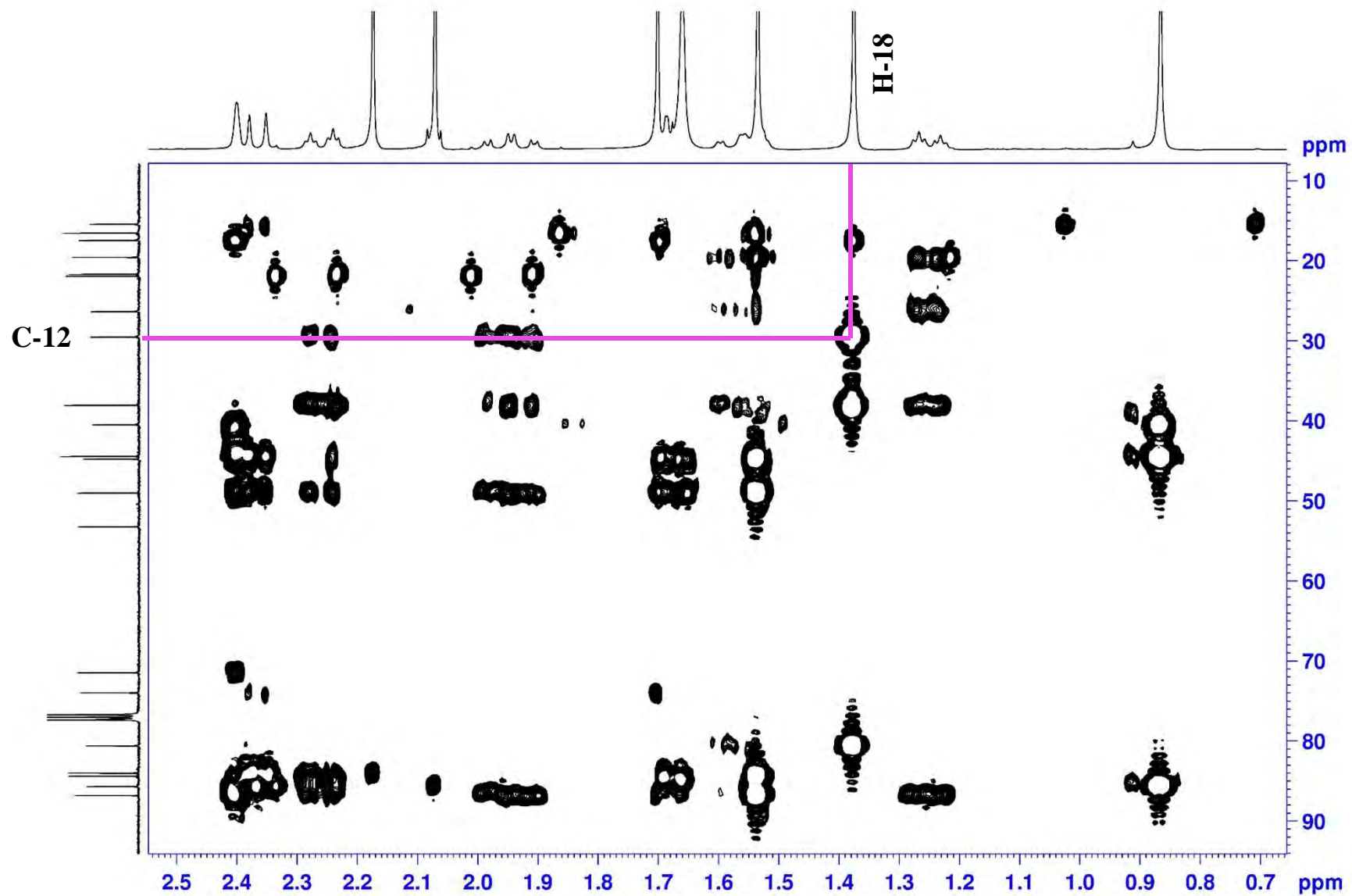
HMBC (400 MHz) spectrum of compound **26** in CDCl_3



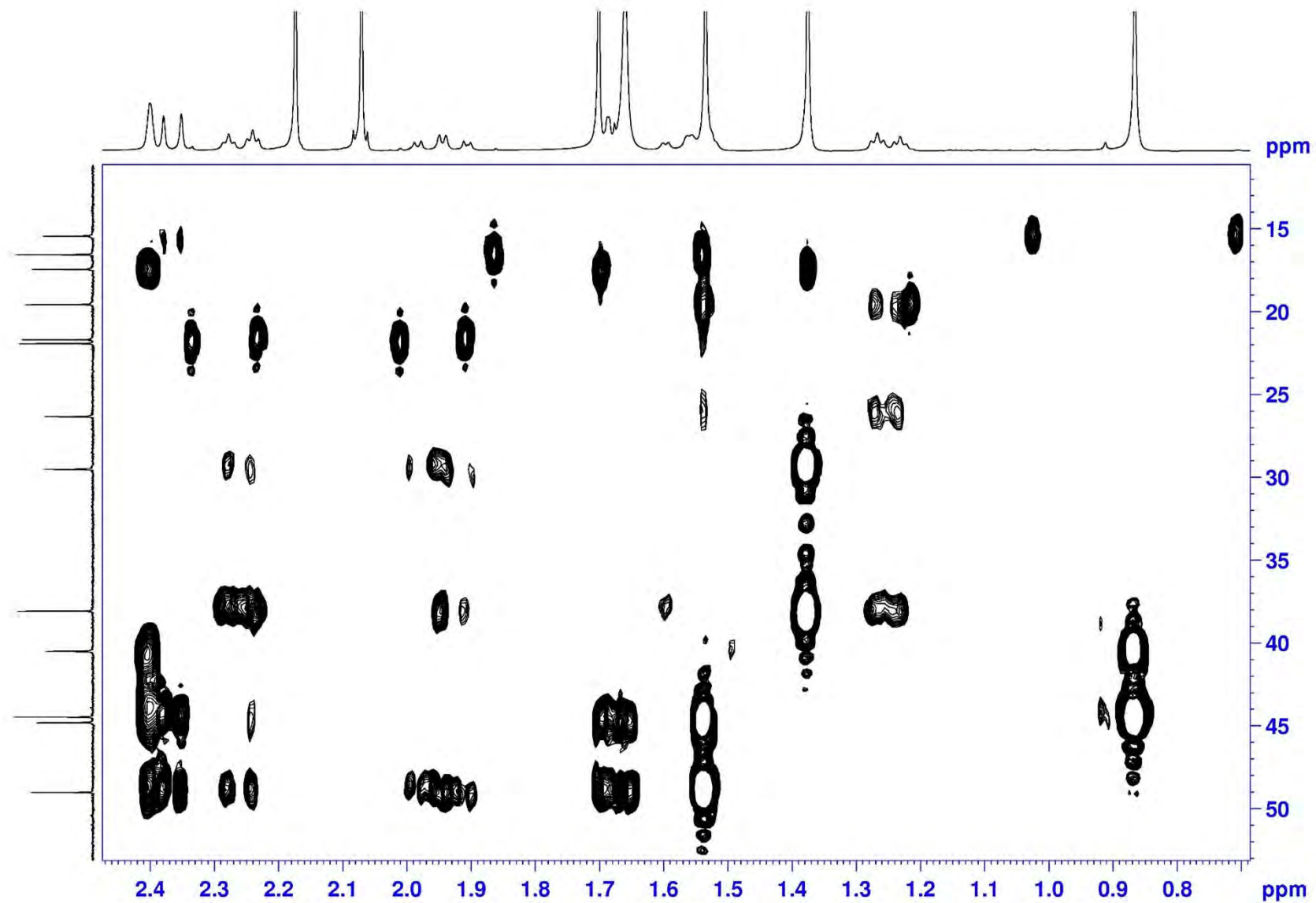
HMBC (400 MHz) spectrum of compound **26** in CDCl₃



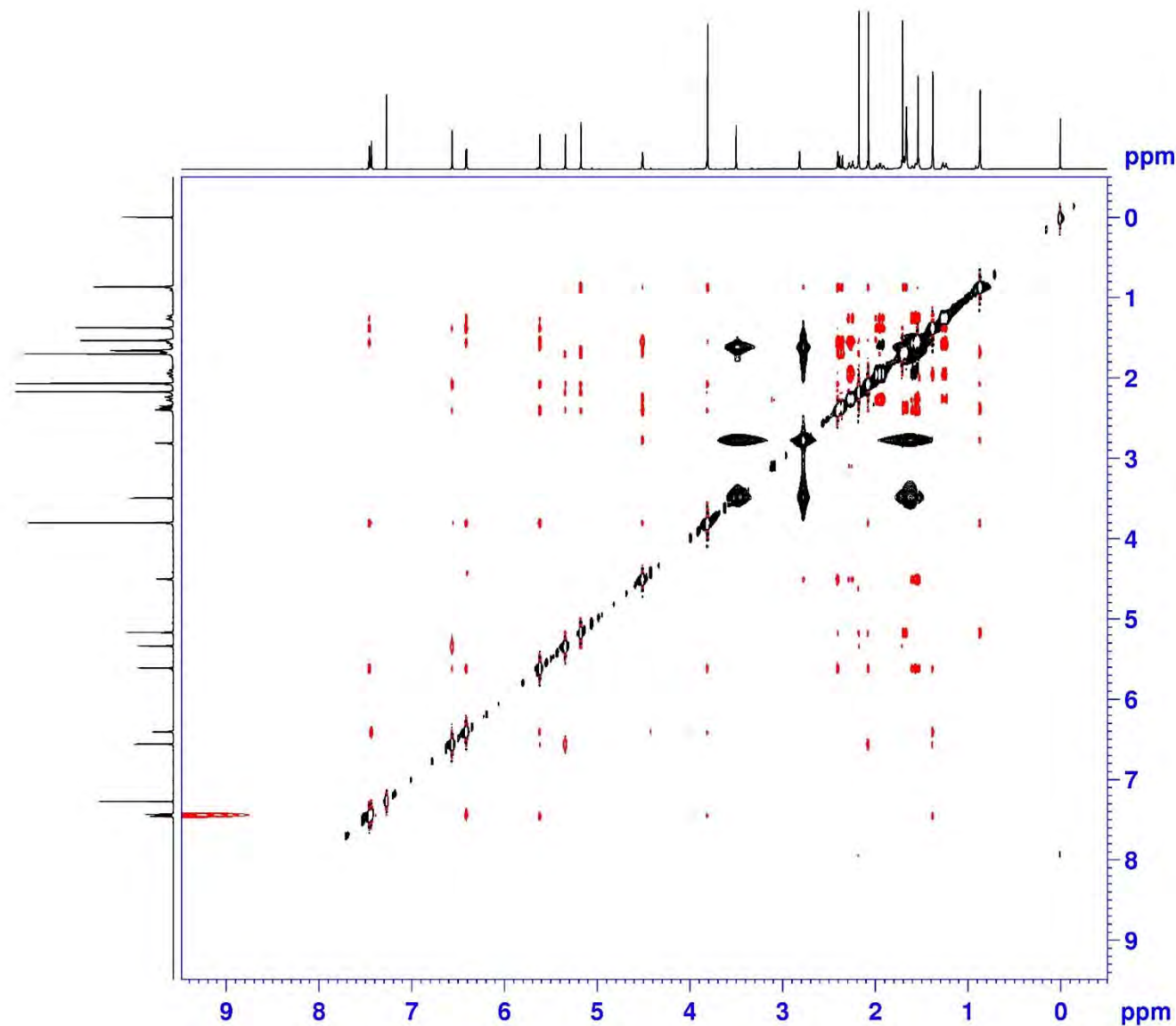
HMBC (400 MHz) spectrum of compound **26** in CDCl_3



HMBC (400 MHz) spectrum of compound **26** in CDCl_3



NOESY (400 MHz) spectrum of compound **26** in CDCl₃



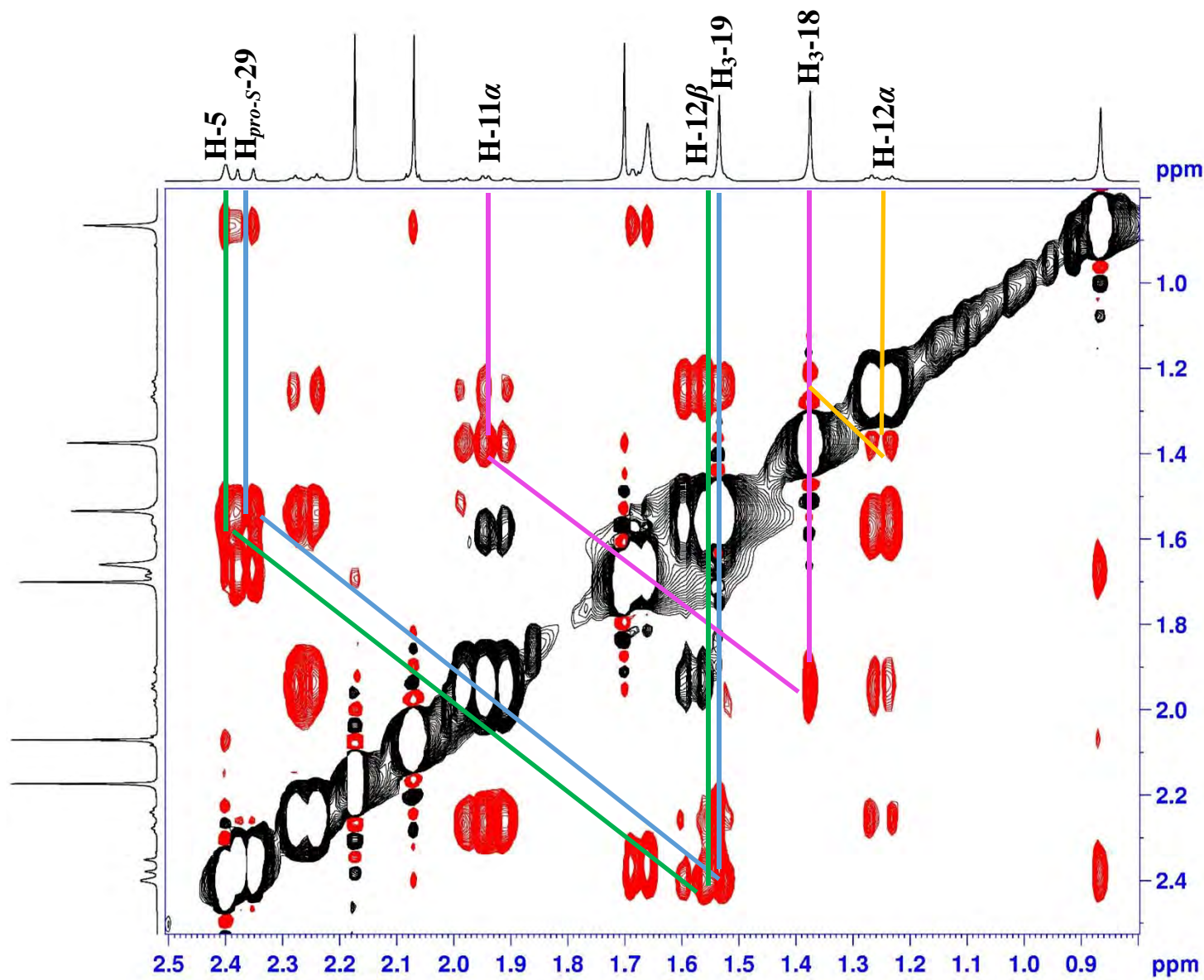
```

NAME          DYG-20
EXPNO          7
PROCNO         1
Date_         20160314
Time          3.22
INSTRUM        spect
PROBHD         5 mm CPPBBO BB
PULPROG        noesygpphph
TD            2048
SOLVENT        CDCl3
NS             16
DS             32
SWH            4000.000 H:
FIDRES         1.953125 H:
AQ             0.2560500 s:
RG             208.5
DW            125.000 u:
DE             10.00 u:
TE             297.0 K
D0             0.00011036 s:
D1             1.99385595 s:
D8             0.30000001 s:
D11            0.03000000 s:
D12            0.00002000 s:
D16            0.00020000 s:
IN0            0.00025000 s:
    
```

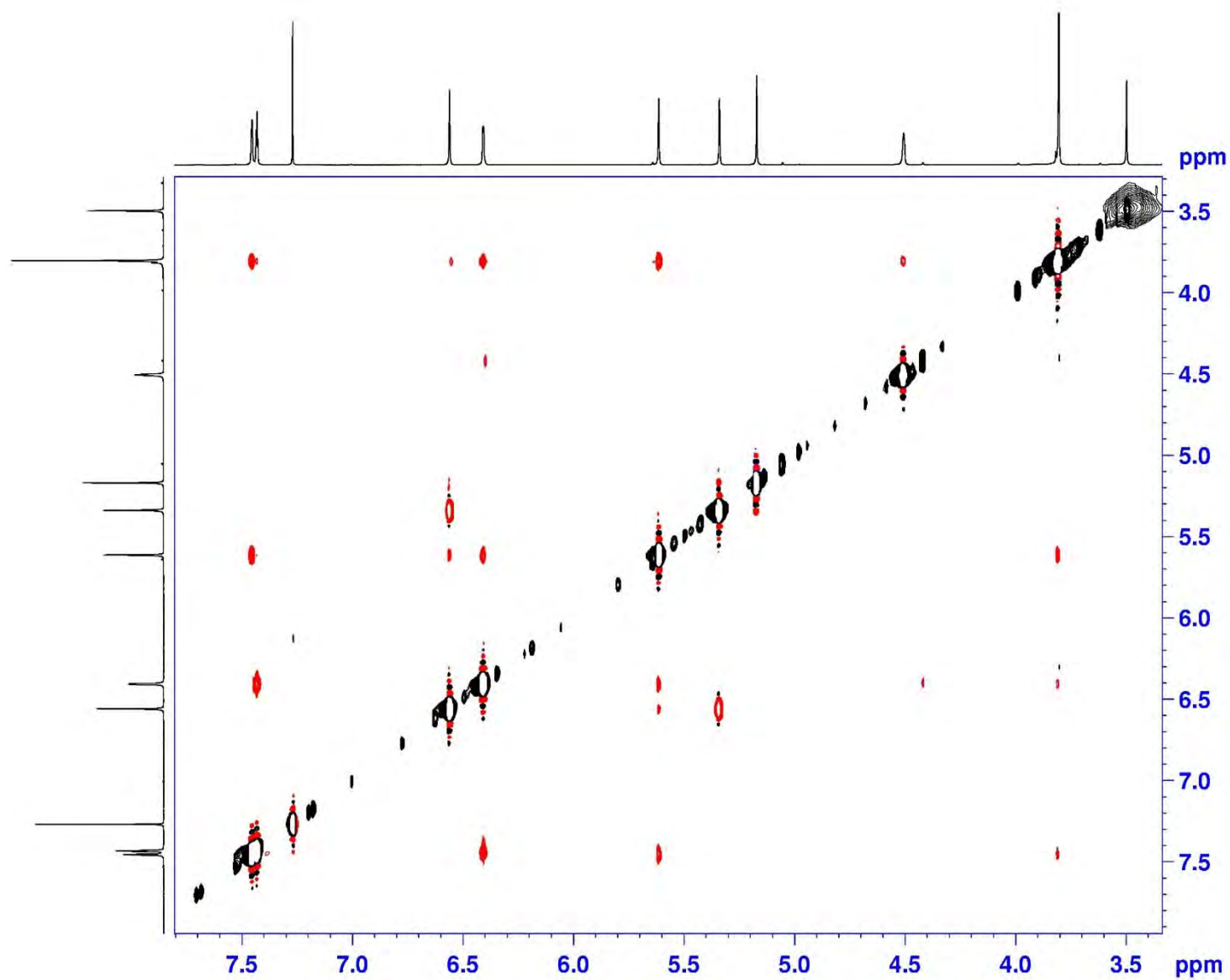
```

===== CHANNEL f1 =====
SFO1         400.1318006 M:
NUC1          1H
P1            11.50 u:
P2            23.00 u:
P17           2500.00 u:
ND0           1
TD            256
SFO1         400.1318 M:
FIDRES        15.625000 H:
SW            9.997 P:
FnMODE        States-TPPI
SI            1024
SF           400.1300055 M:
WDW           QSINE
SSB           2
LB            0.00 H:
GB            0
PC            1.00
SI            1024
MC2           States-TPPI
SF           400.1300055 M:
WDW           QSINE
    
```

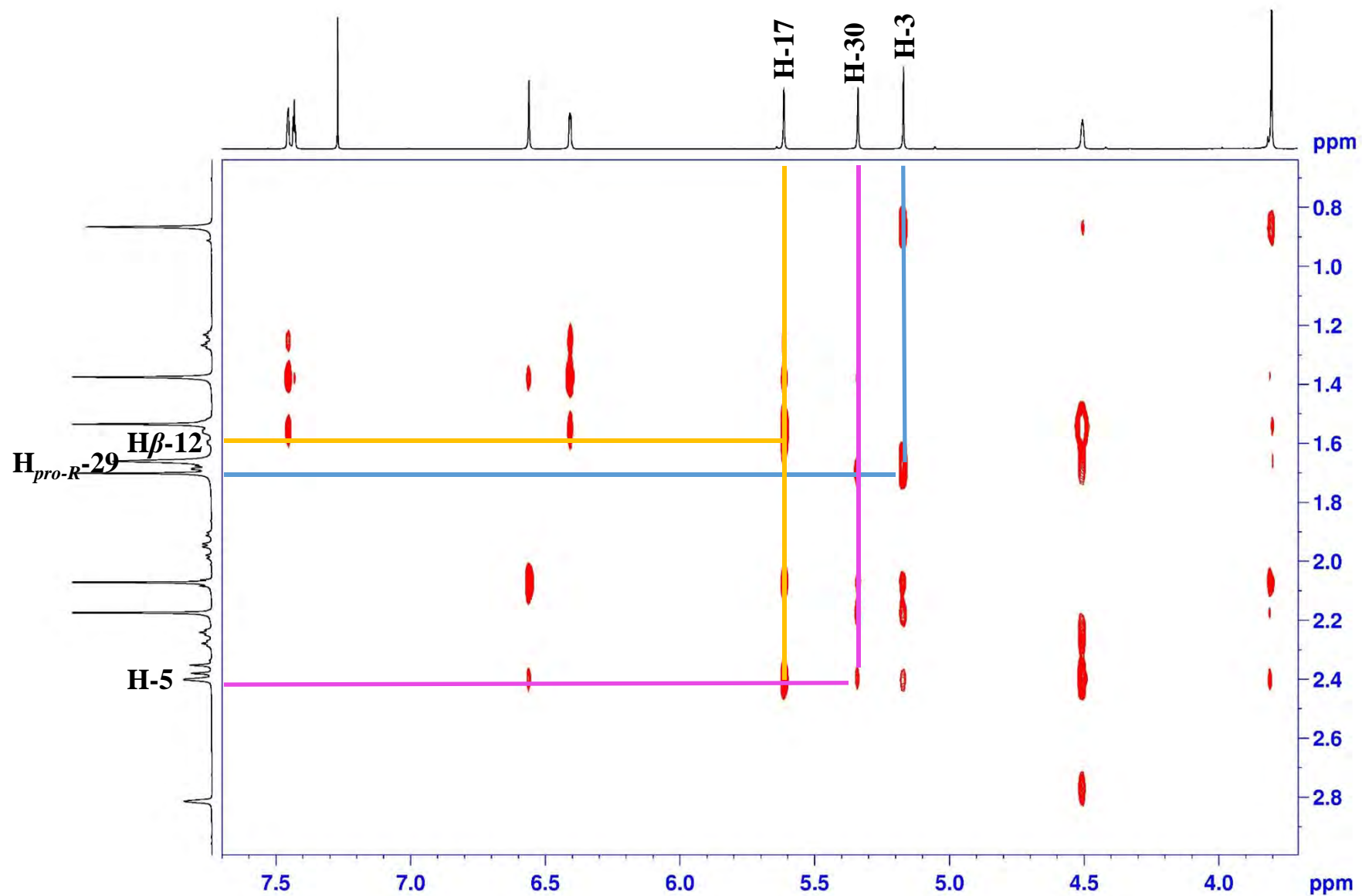
NOESY (400 MHz) spectrum of compound **26** in CDCl₃



NOESY (400 MHz) spectrum of compound **26** in CDCl₃



NOESY (400 MHz) spectrum of compound **26** in CDCl₃



HR-ESIMS for compound 27

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\MS\data\201605\liwanshan_dgy-12_pos_5_01_1853.d
 Method LC_Direct Infusion_pos_100-1000mz.m
 Sample Name liwanshan_dgy-12_pos
 Comment

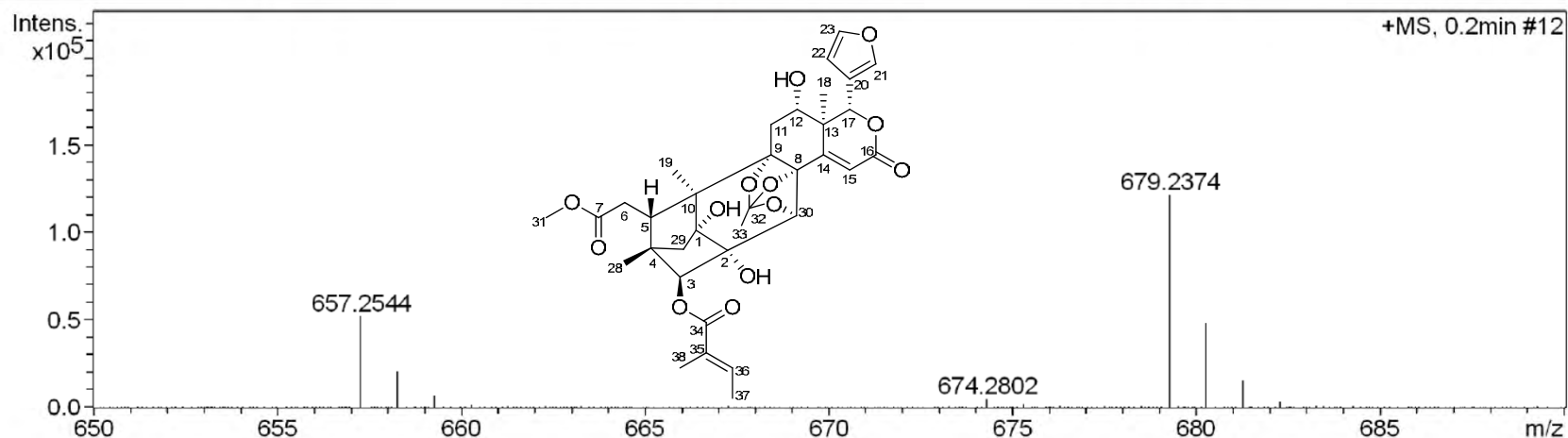
Acquisition Date 5/19/2016 8:34:21 AM

Operator SCSIO

Instrument / Ser# maXis 29

Acquisition Parameter

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

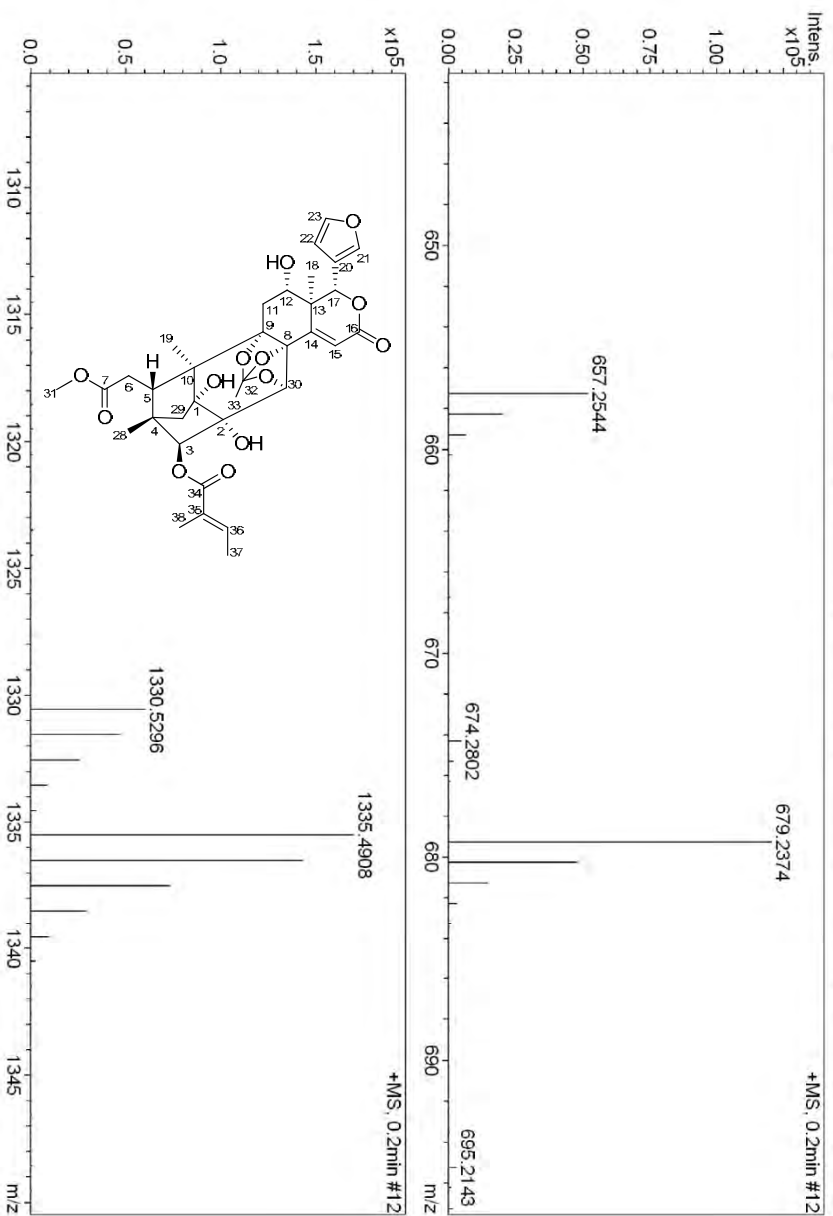
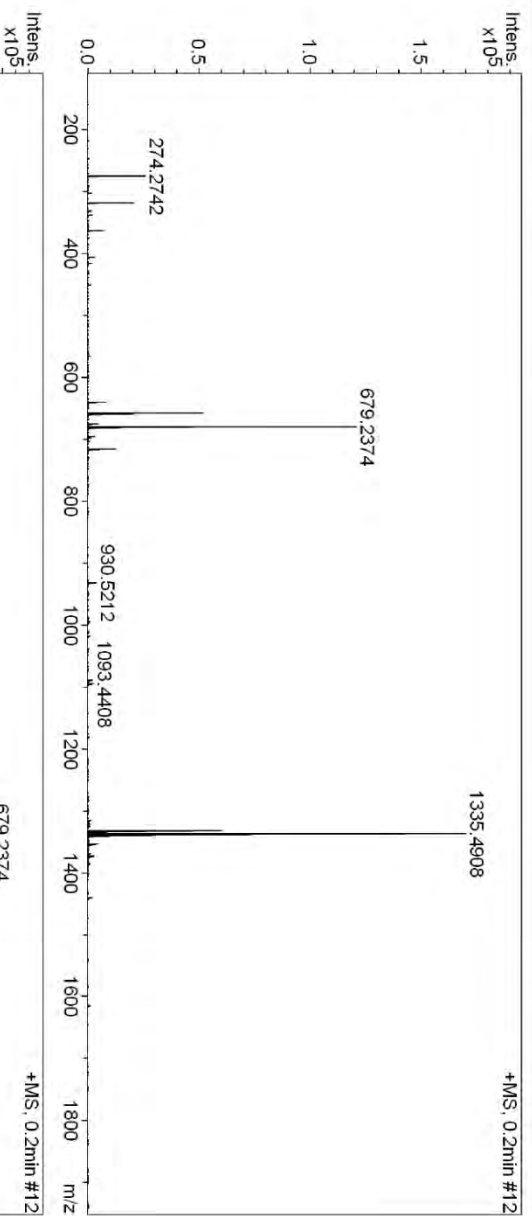


| Meas. m/z | # | Formula | Score | m/z | err [ppm] | err [mDa] | mSigma | rdb | e ⁻ Conf | N-Rule |
|-----------|---|-------------------|--------|----------|-----------|-----------|--------|------|---------------------|--------|
| 657.2544 | 1 | C 34 H 41 O 13 | 100.00 | 657.2542 | -0.4 | -0.3 | 15.3 | 14.5 | even | ok |
| 679.2374 | 1 | C 34 H 40 Na O 13 | 79.62 | 679.2361 | -1.9 | -1.3 | 16.6 | 14.5 | even | ok |

Generic Display Report

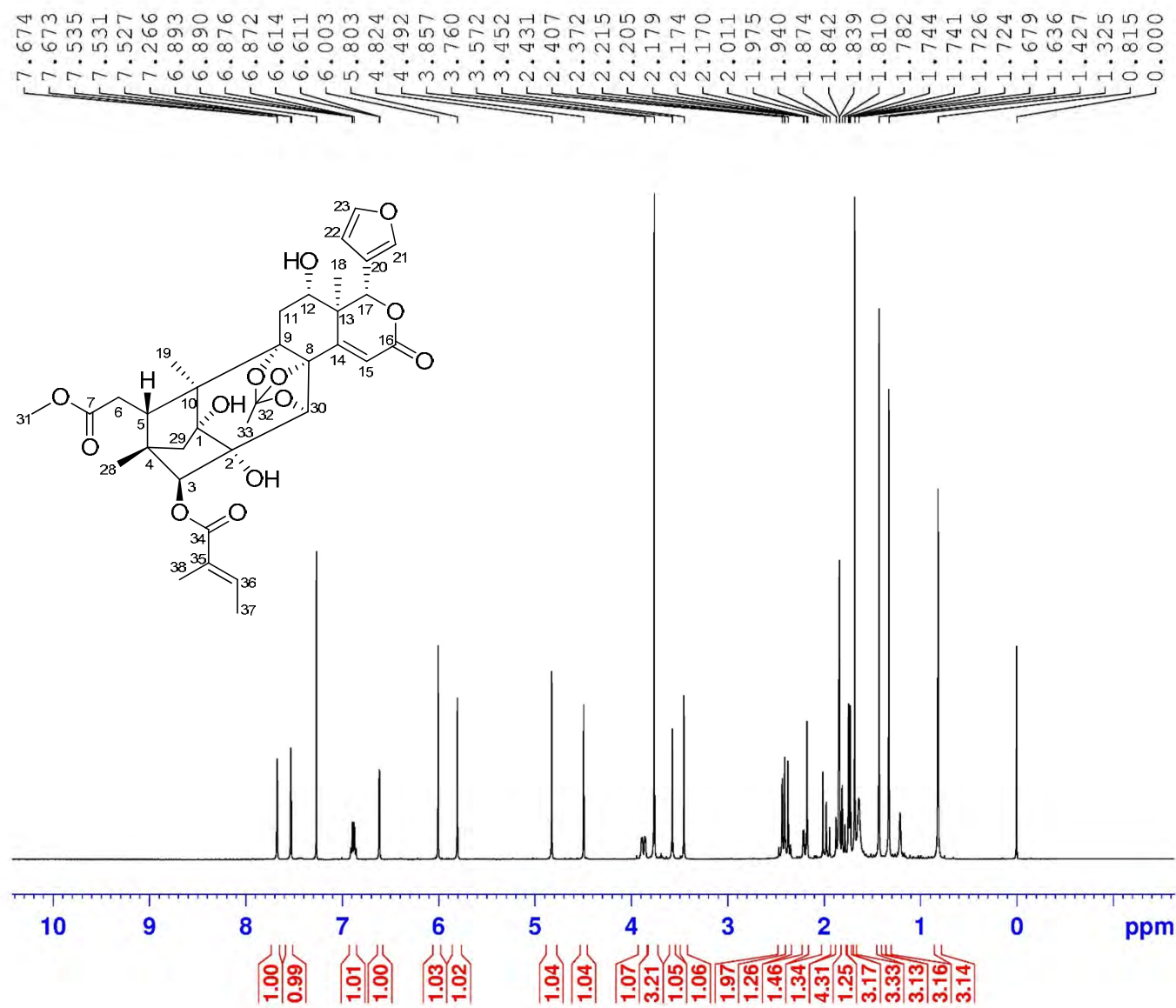
Analysis Info

| | | | |
|---------------|---|------------------|----------------------|
| Analysis Name | D:\Data\MS\data\201605\liwanshan_dgy-12_pos_5_01_1853.d | Acquisition Date | 5/19/2016 8:34:21 AM |
| Method | LC_Direct Infusion_pos_100-1000mz.m | Operator | SCSIO |
| Sample Name | liwanshan_dgy-12_pos | Instrument | maxis |
| Comment | | | |



HR-ESIMS for compound 27

^1H NMR (400 MHz) spectrum of compound **27** in CDCl_3



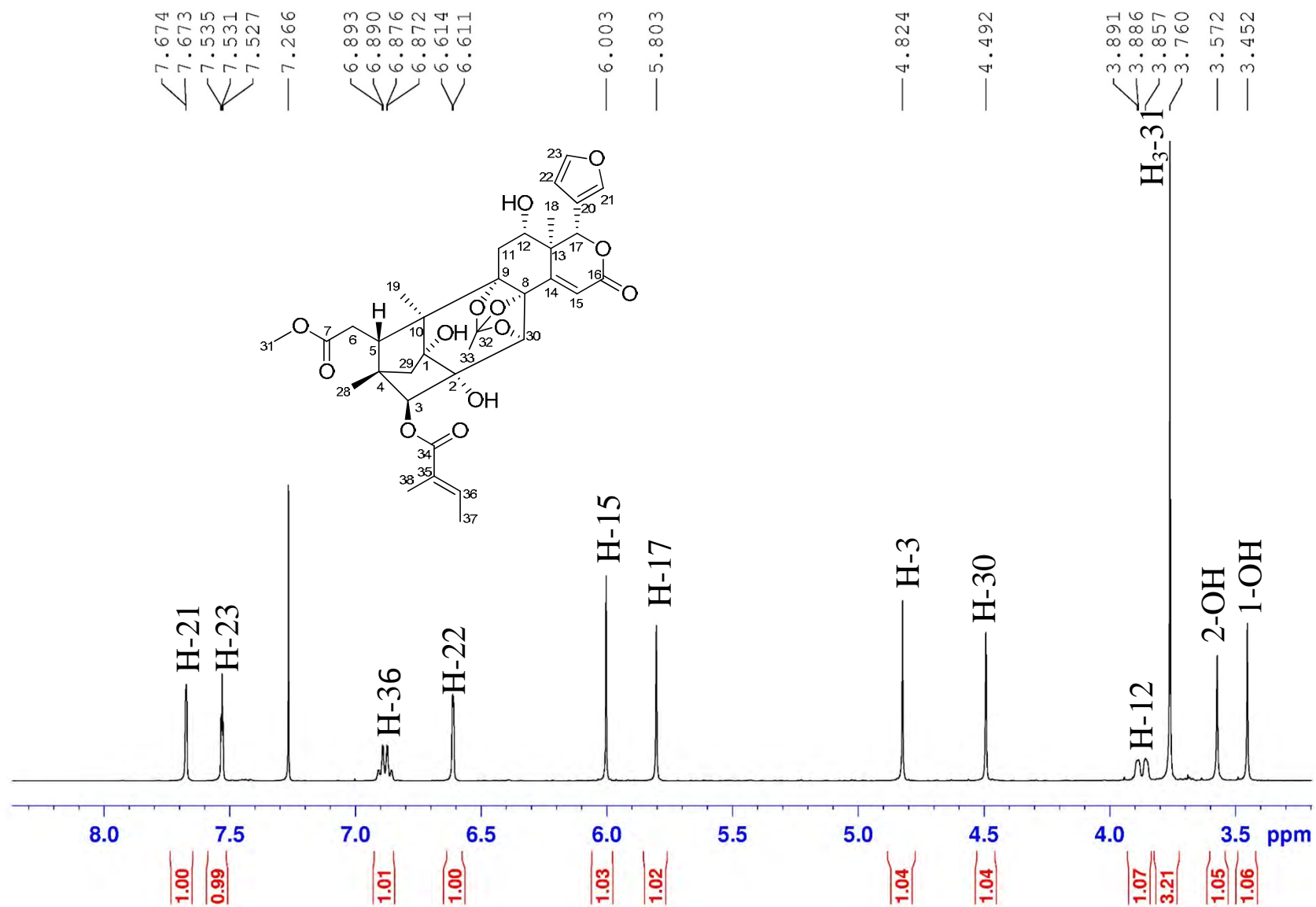
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NAME          dyg-12
EXPNO          1
PROCNO         1
Date_          20151016
Time           16.26
INSTRUM        spect
PROBHD          5 mm CPPBBO BB
PULPROG         zg30
TD             65536
SOLVENT         CDCl3
NS              16
DS              2
SWH            8223.685 F
FIDRES         0.125483 F
AQ             3.9846387 s
RG              91.64
DW             60.800 u
DE             10.00 u
TE             297.0 K
D1             1.00000000 s
TD0            1
  
```

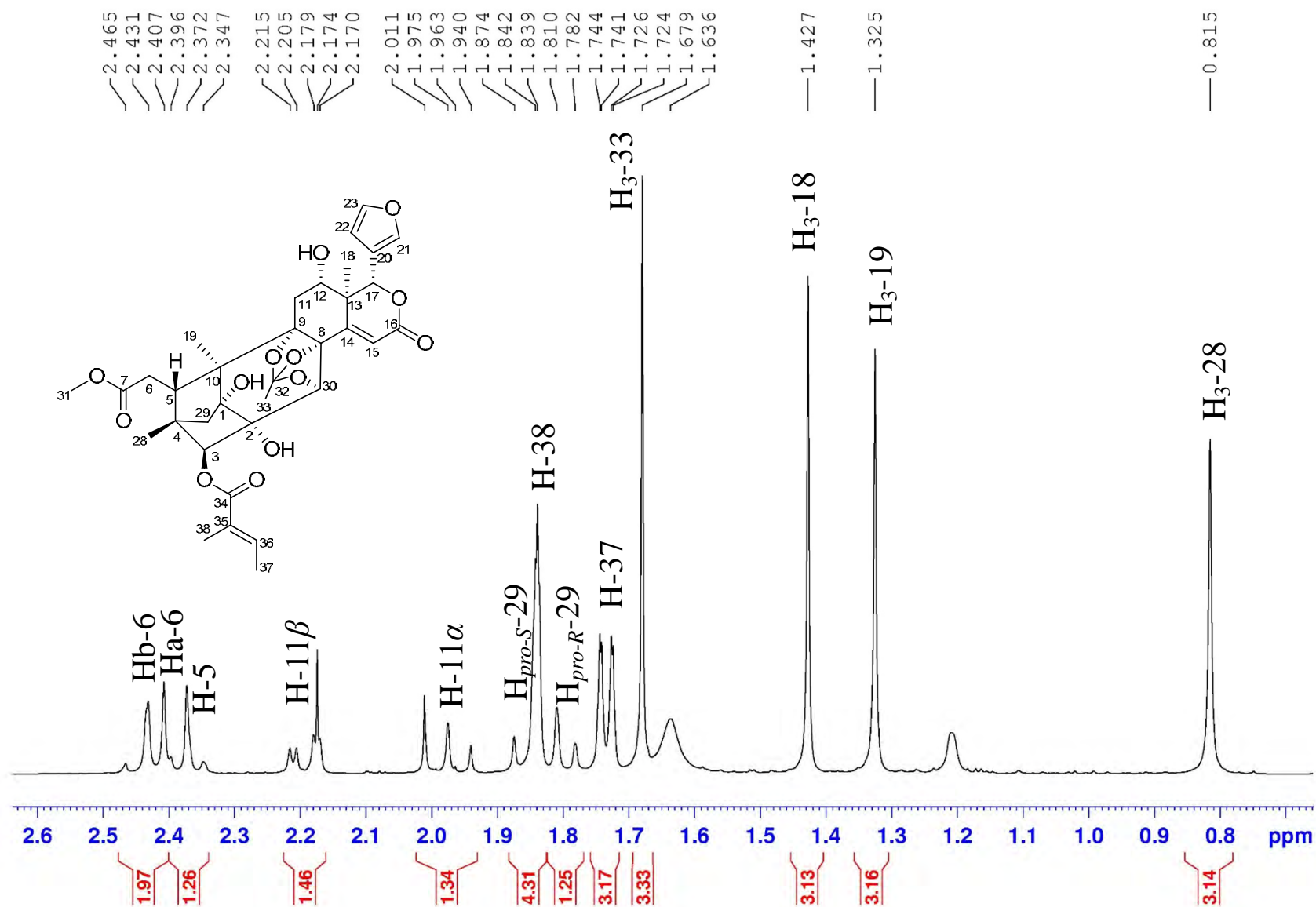
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===== CHANNEL f1 =====
SFO1          400.1324710 M
NUC1           1H
P1            12.00 u
SI            65536
SF            400.1300072 M
WDW            EM
SSB            0
LB            0.30 F
GB            0
PC            1.00
  
```

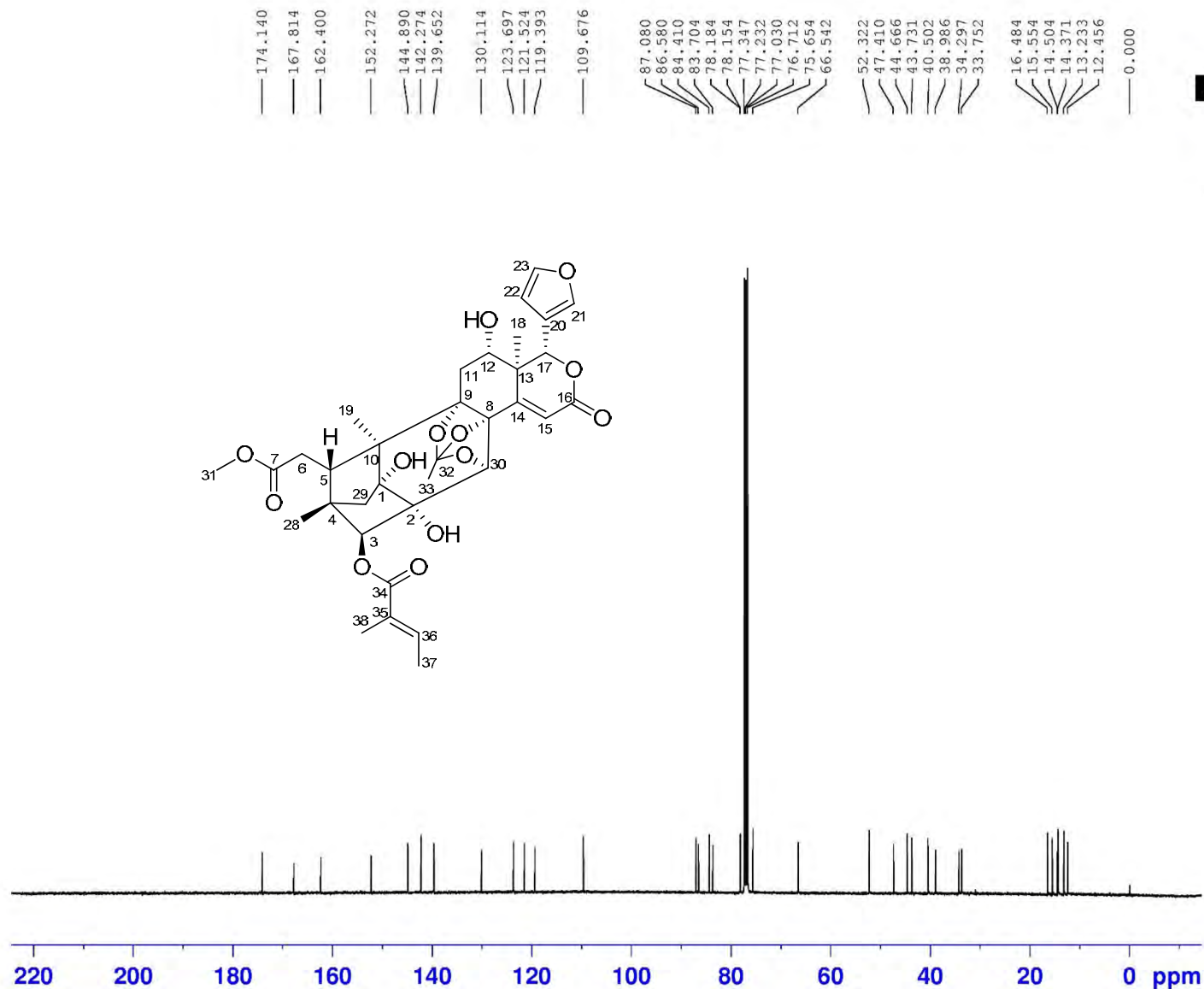
^1H NMR (400 MHz) spectrum of compound **27** in CDCl_3



^1H NMR (400 MHz) spectrum of compound **27** in CDCl_3



^{13}C NMR (100 MHz) spectrum of compound **27** in CDCl_3



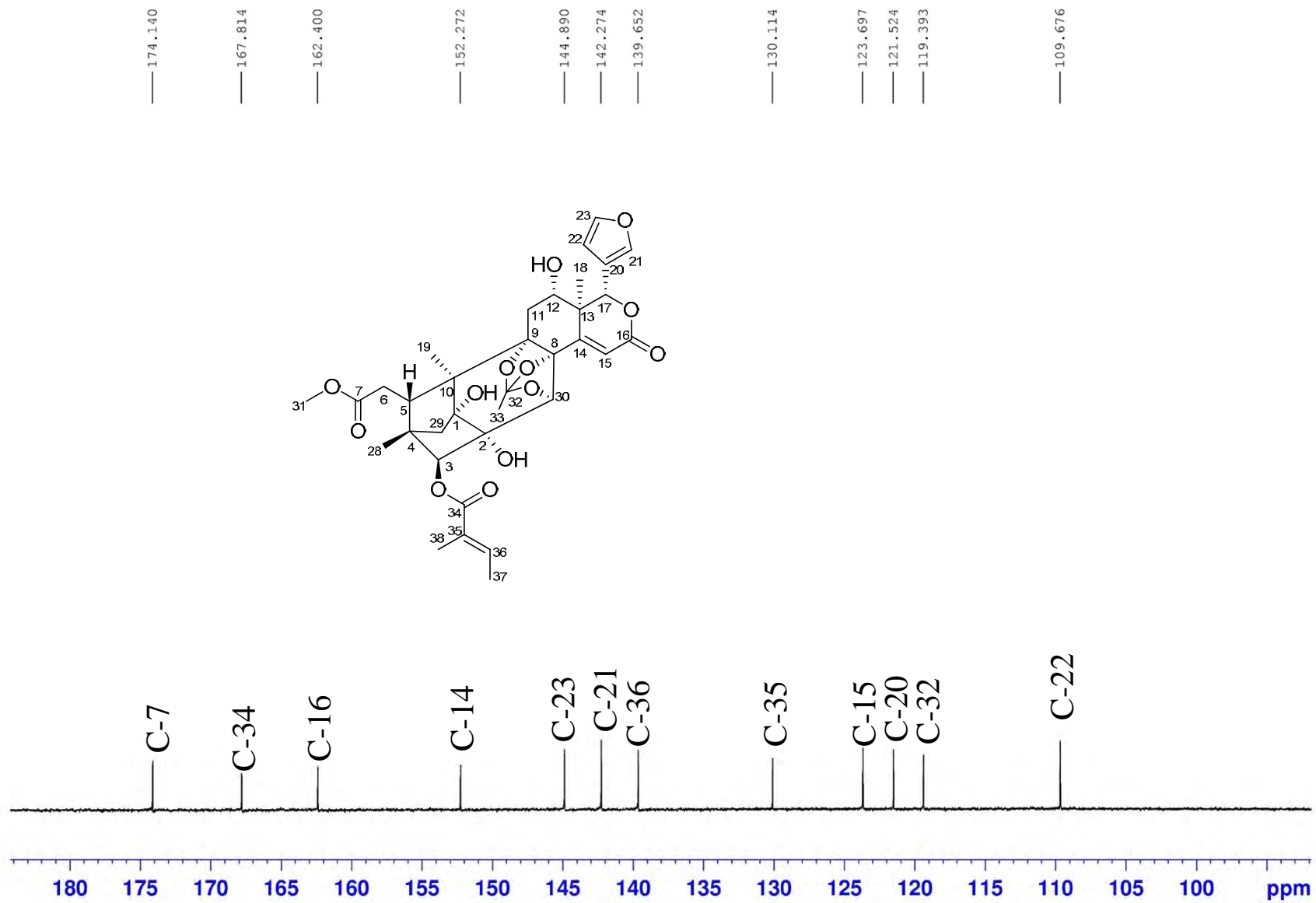
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NAME          dyg-12
EXPNO         2
PROCNO        1
Date_         20151016
Time          17.26
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            1024
DS            4
SWH           24038.461 F
FIDRES        0.366798 F
AQ            1.3631988 s
RG            73.92
DW            20.800 u
DE            18.00 u
TE            297.0 K
D1            2.00000000 s
D11           0.03000000 s
TD0           1
  
```

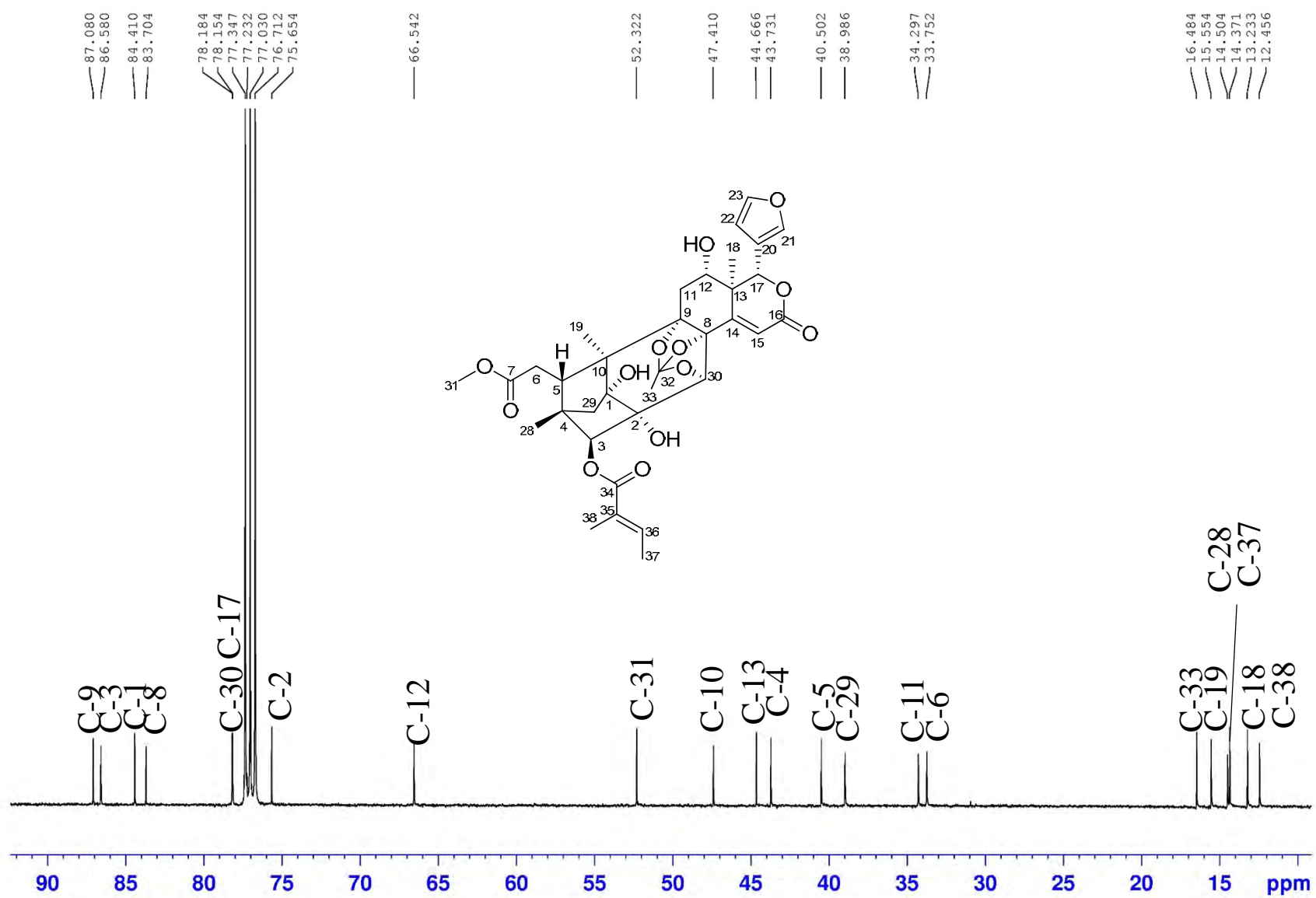
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===== CHANNEL f1 =====
SFO1          100.6233324 M
NUC1          13C
P1            10.00 u
SI            32768
SF            100.6127690 M
WDW           EM
SSB           0
LB            1.00 F
GB            0
PC            1.40
  
```

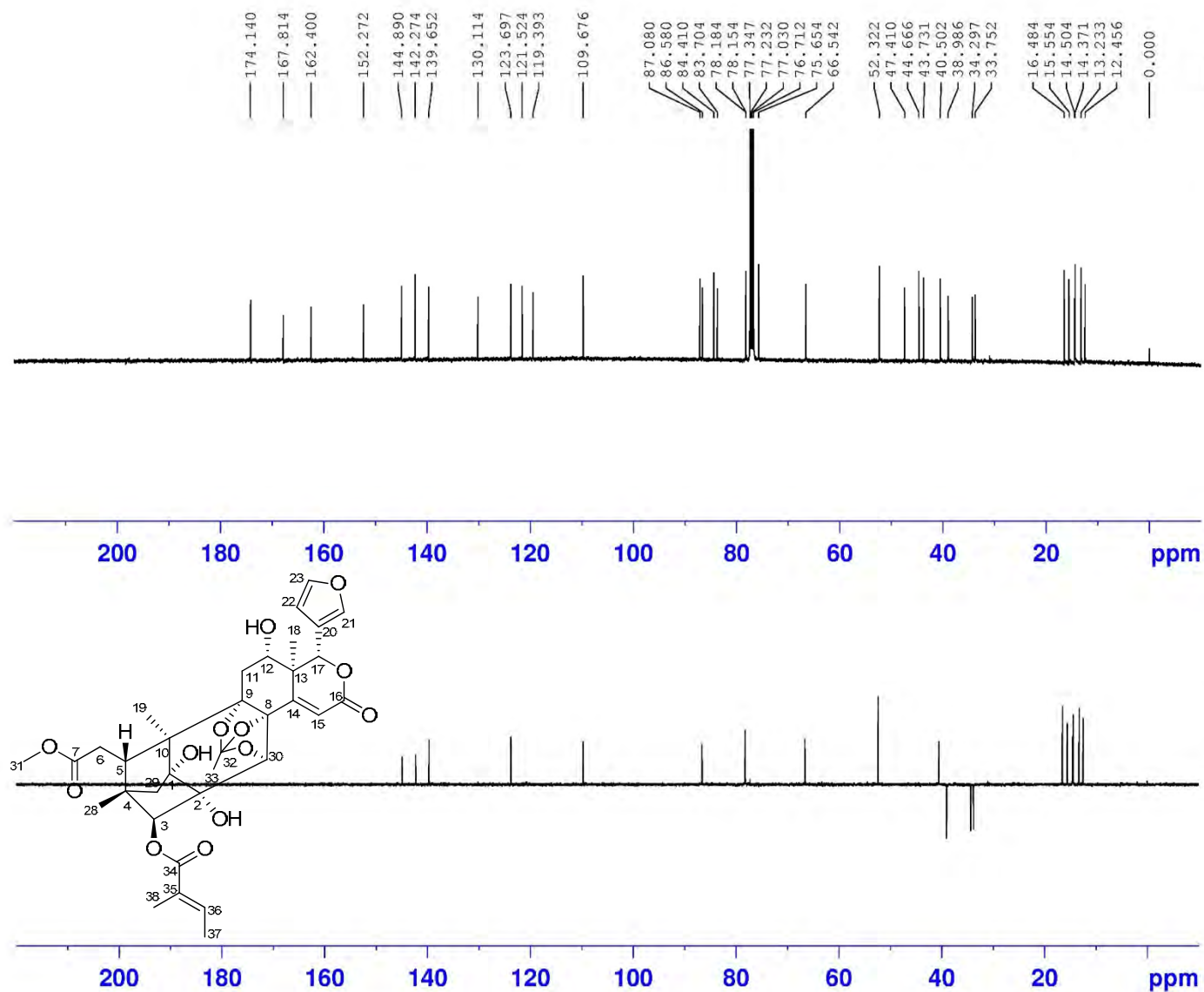
^{13}C NMR (100 MHz) spectrum of compound **27** in CDCl_3



^{13}C NMR (100 MHz) spectrum of compound **27** in CDCl_3



DEPT135 (100 MHz) spectrum of compound **27** in CDCl₃



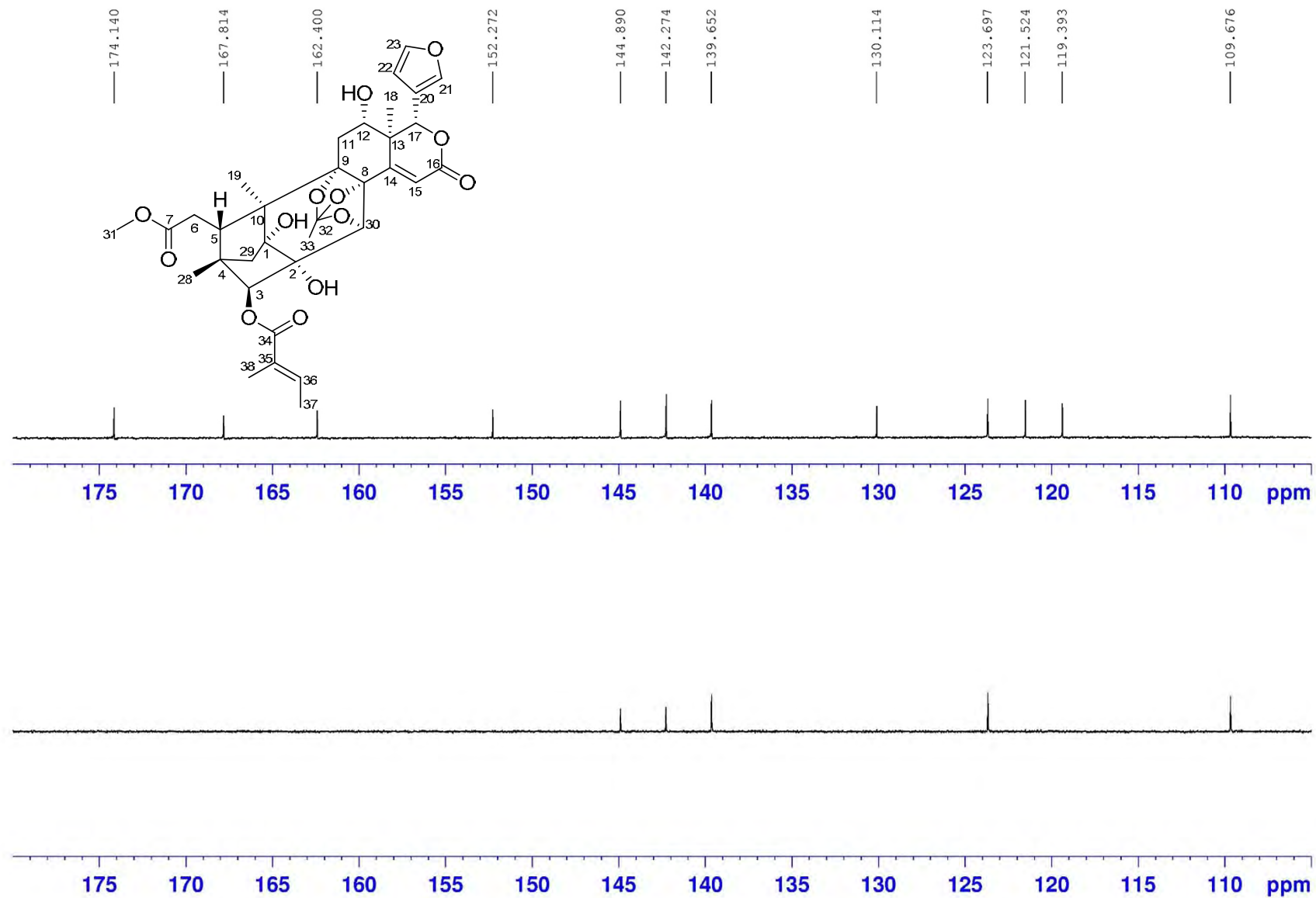
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NAME          dyg-12
EXPNO          3
PROCNO         1
Date_          20151016
Time           17.44
INSTRUM        spect
PROBHD         5 mm CPBBO BB
PULPROG        deptspl35
TD             65536
SOLVENT        CDCl3
NS             300
DS             4
SWH            24038.461 F
FIDRES         0.366798 F
AQ            1.3631988 s
RG            102.3
DW            20.800 u
DE            18.00 u
TE            297.0 F
CNST2          145.0000000
D1            2.0000000 s
D2            0.00344828 s
D12           0.00002000 s
TD0           1
  
```

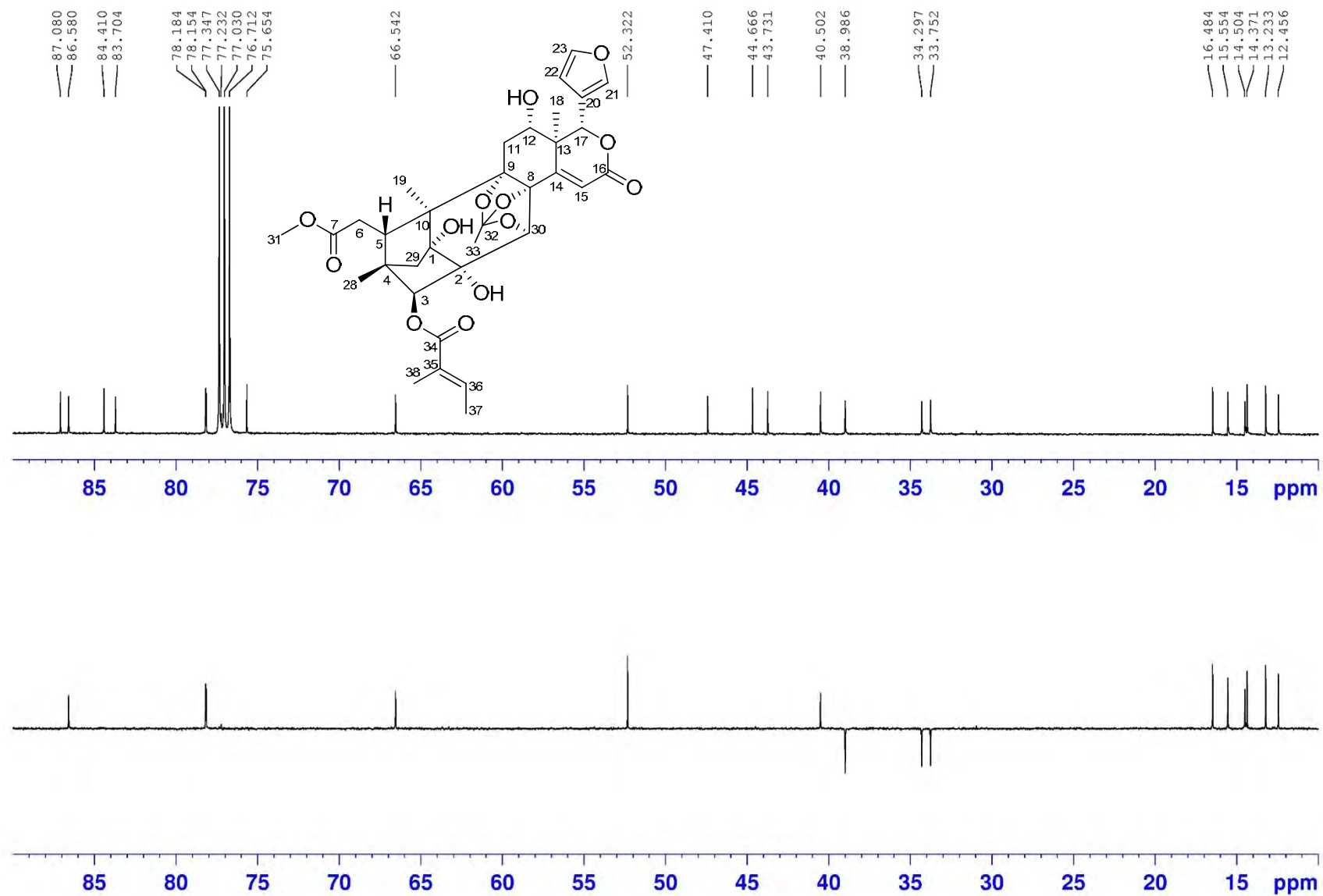
```

===== CHANNEL f1 =====
SFO1          100.6233324 M
NUC1           13C
P1            10.00 u
P13           2000.00 u
SI            32768
SF            100.6127690 M
WDW           EM
SSB           0
LB            1.00 F
GB            0
PC            1.40
  
```

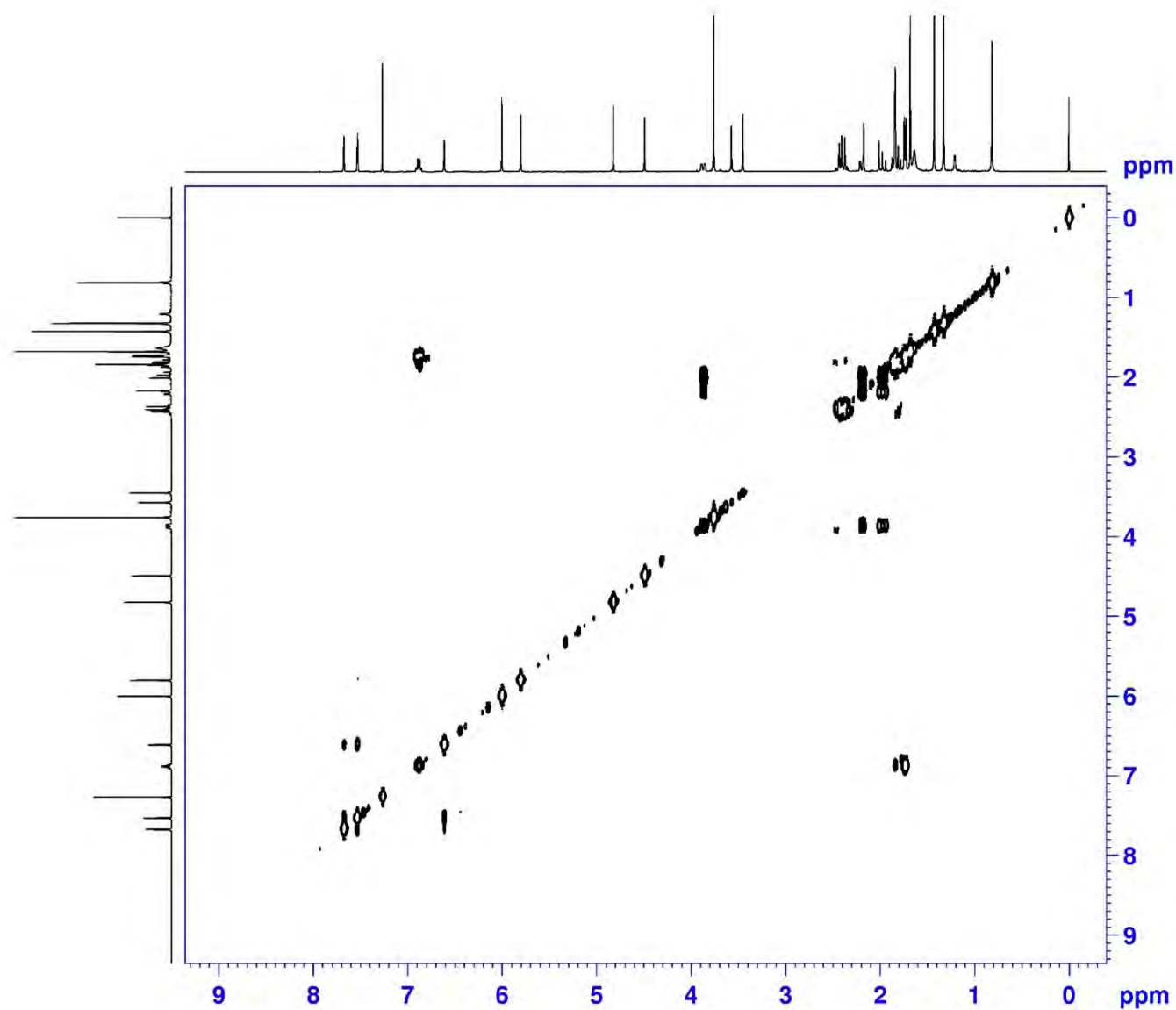
DEPT135 (100 MHz) spectrum of compound **27** in CDCl₃



DEPT135 (100 MHz) spectrum of compound **27** in CDCl₃



^1H - ^1H COSY (400 MHz) spectrum of compound **27** in CDCl_3



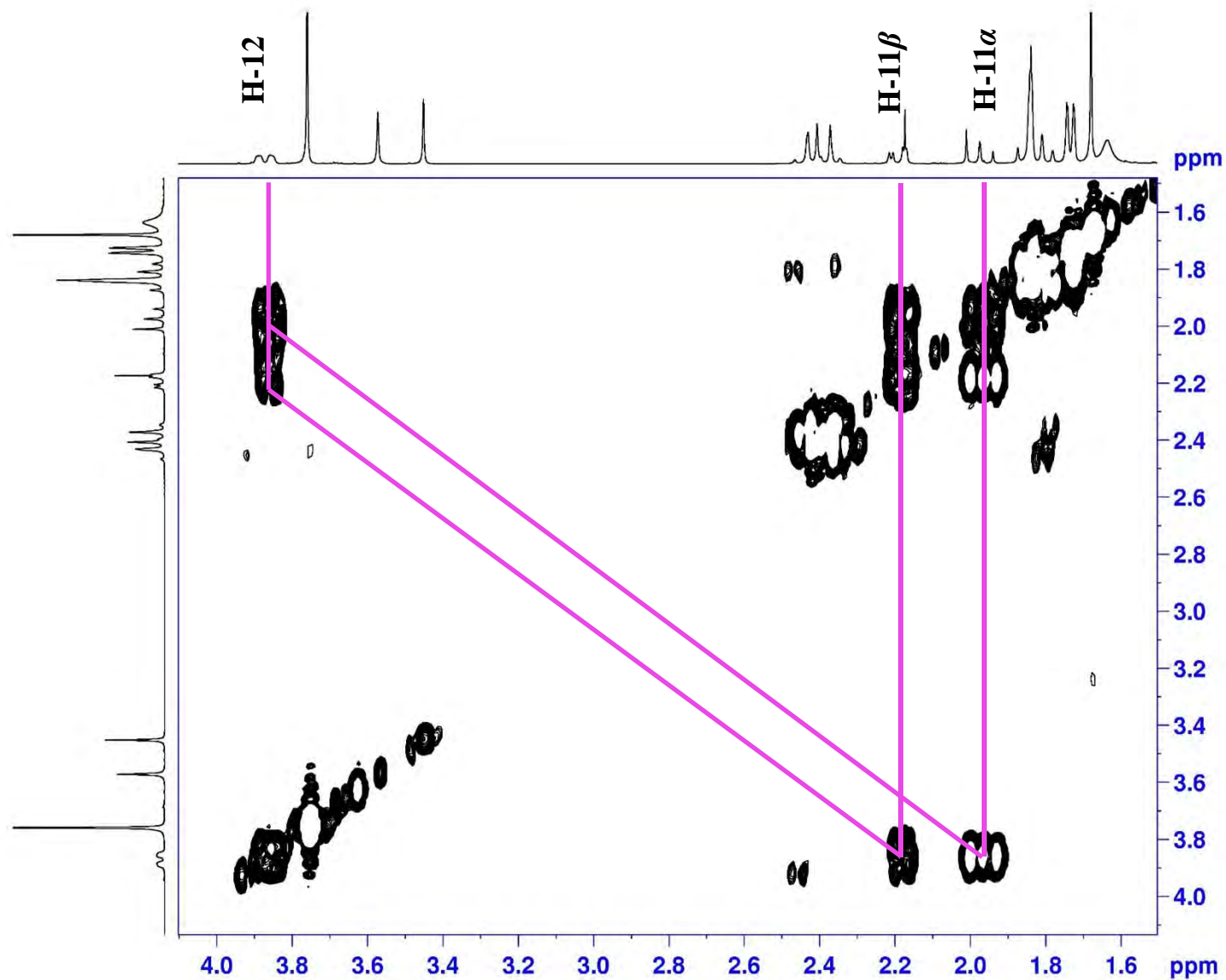
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NAME          dyg-12
EXPNO         4
PROCNO        1
Date_         20160313
Time          13.17
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       cosygpppqf
TD            2048
SOLVENT       CDCl3
NS            8
DS            8
SWH           3906.250 H
FIDRES        1.907349 H
AQ            0.2621940 s
RG            208.5
DW            128.000 u
DE            10.00 u
TE            291.0 K
D0            0.00000300 s
D1            1.89678097 s
D11           0.03000000 s
D12           0.00002000 s
D13           0.00000400 s
D16           0.00020000 s
IN0           0.00025600 s
    
```

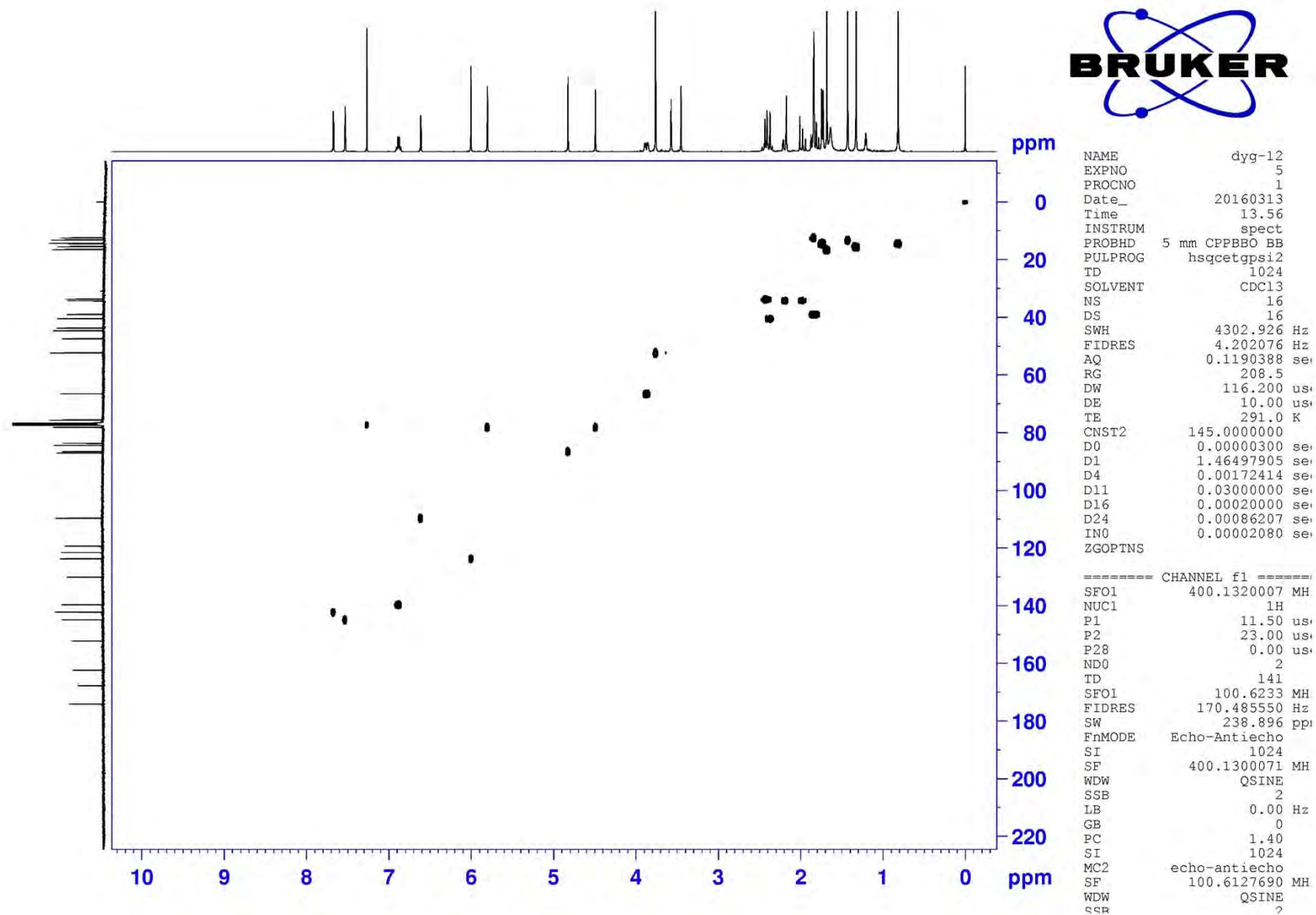
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===== CHANNEL f1 =====
SFO1      400.1318006 M
NUC1       1H
P0         11.50 u
P1         11.50 u
P17        2500.00 u
ND0         1
TD          128
SFO1      400.1318 M
FIDRES     30.517578 H
SW          9.762 p
FnMODE     QF
SI          1024
SF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

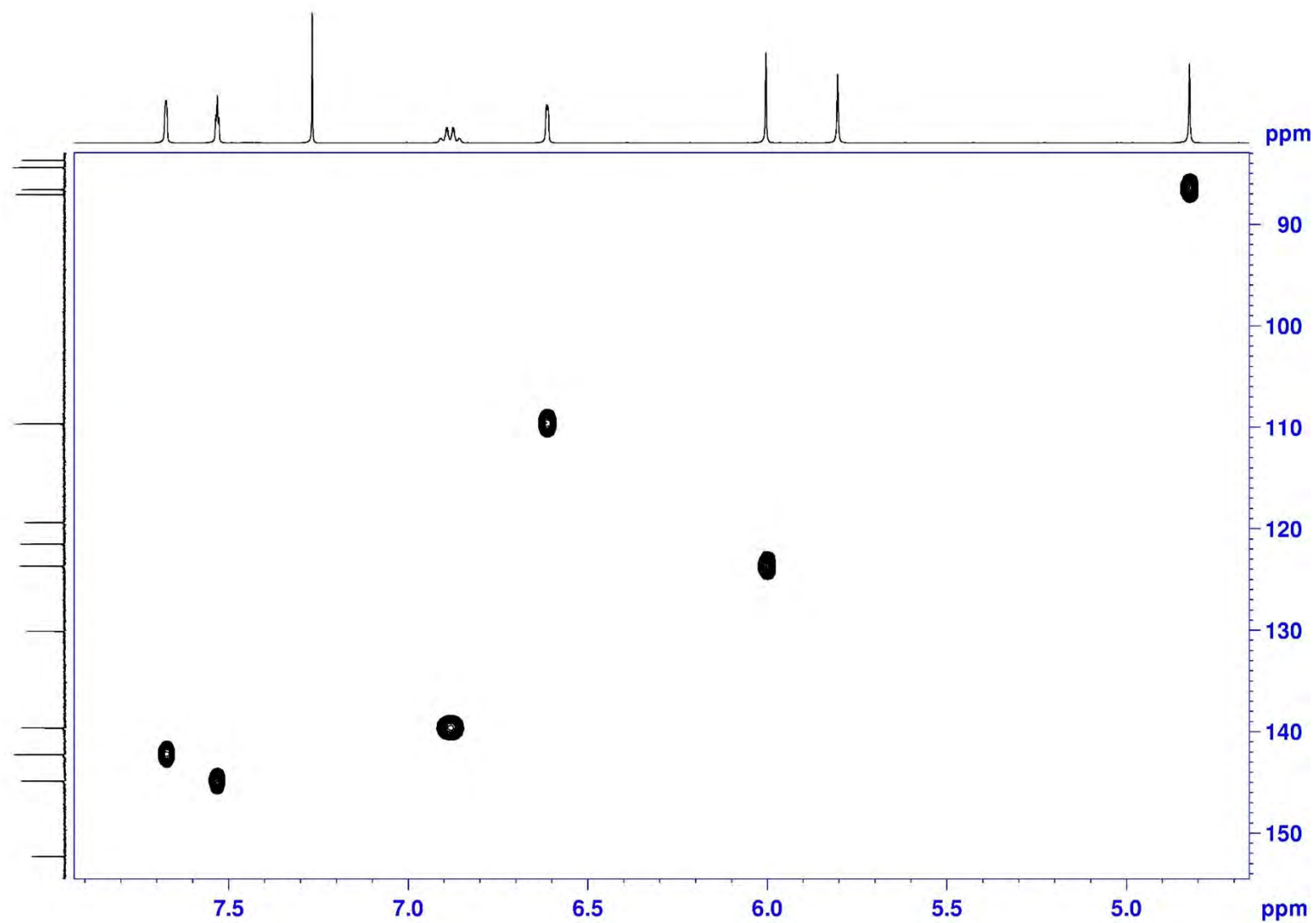
^1H - ^1H COSY (400 MHz) spectrum of compound **27** in CDCl_3



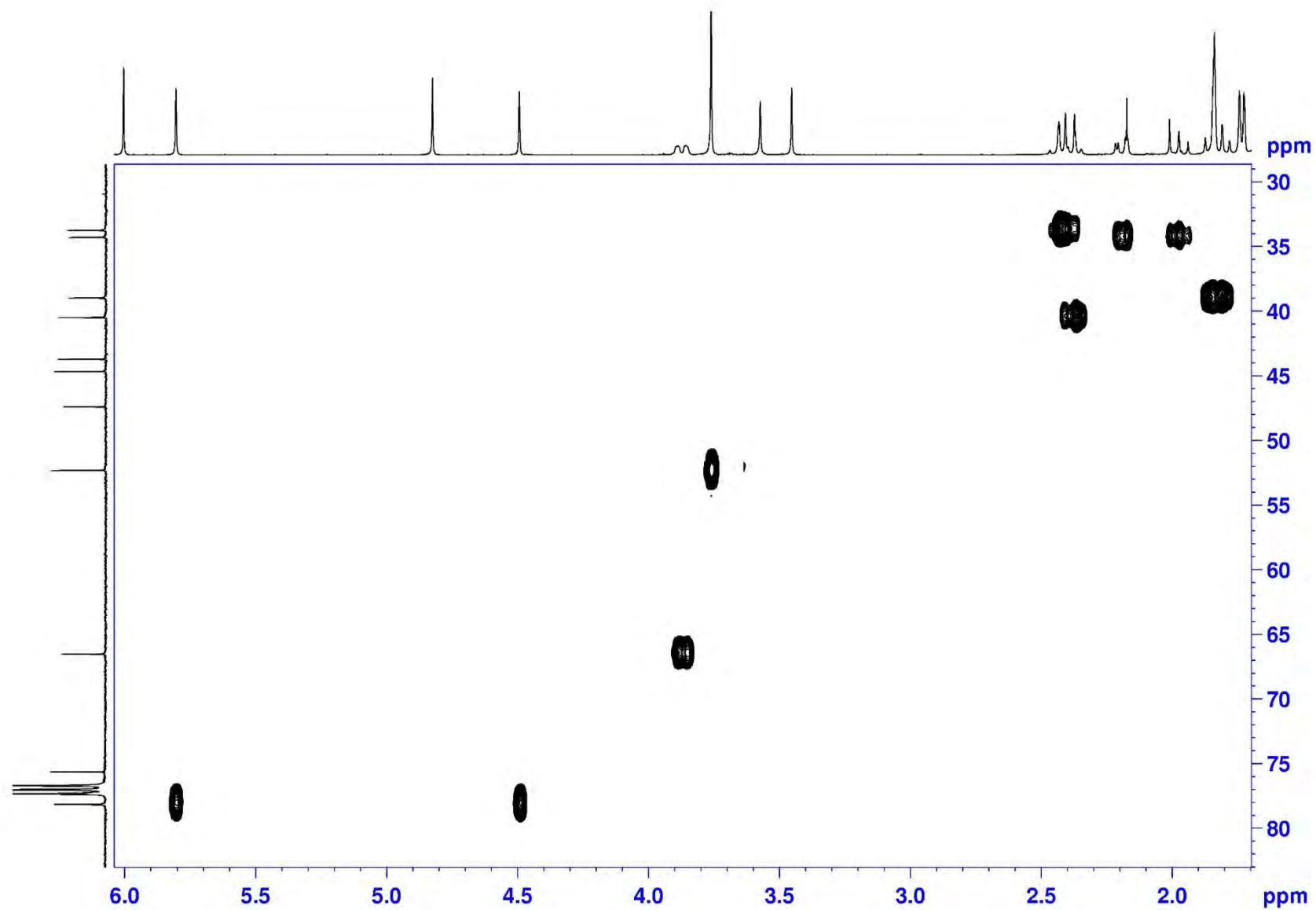
HSQC (400 MHz) spectrum of compound **27** in CDCl₃



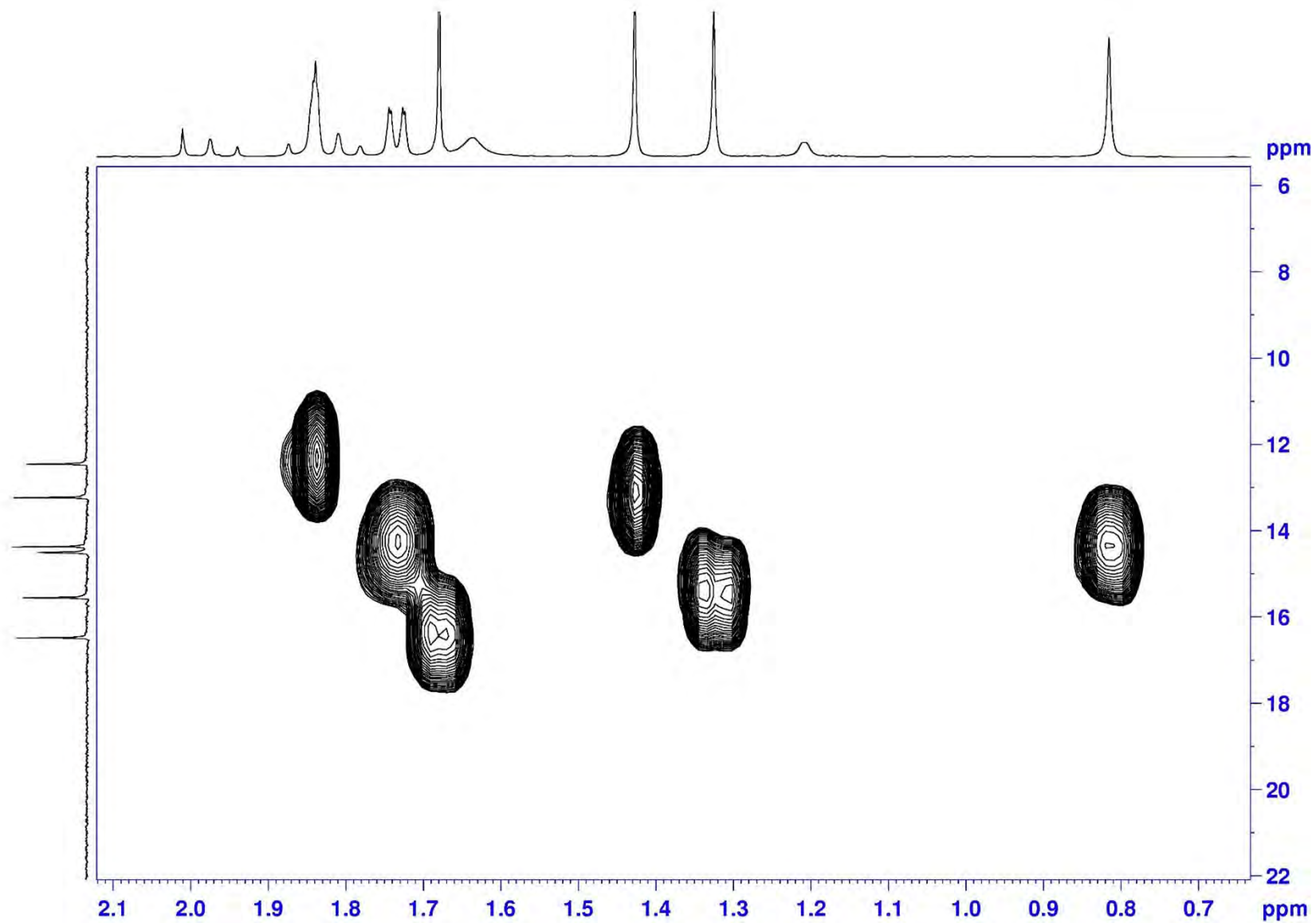
HSQC (400 MHz) spectrum of compound **27** in CDCl₃



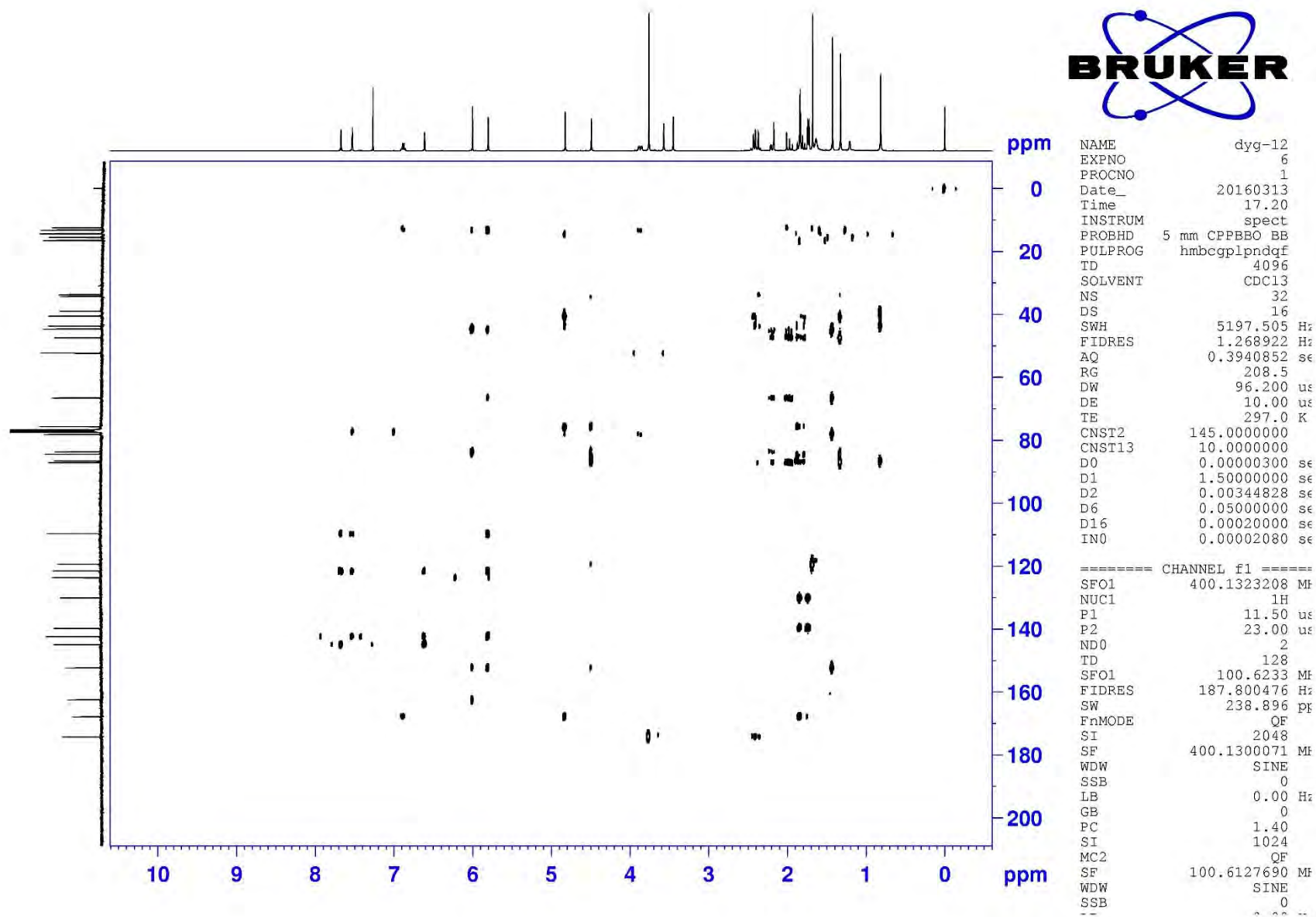
HSQC (400 MHz) spectrum of compound **27** in CDCl₃



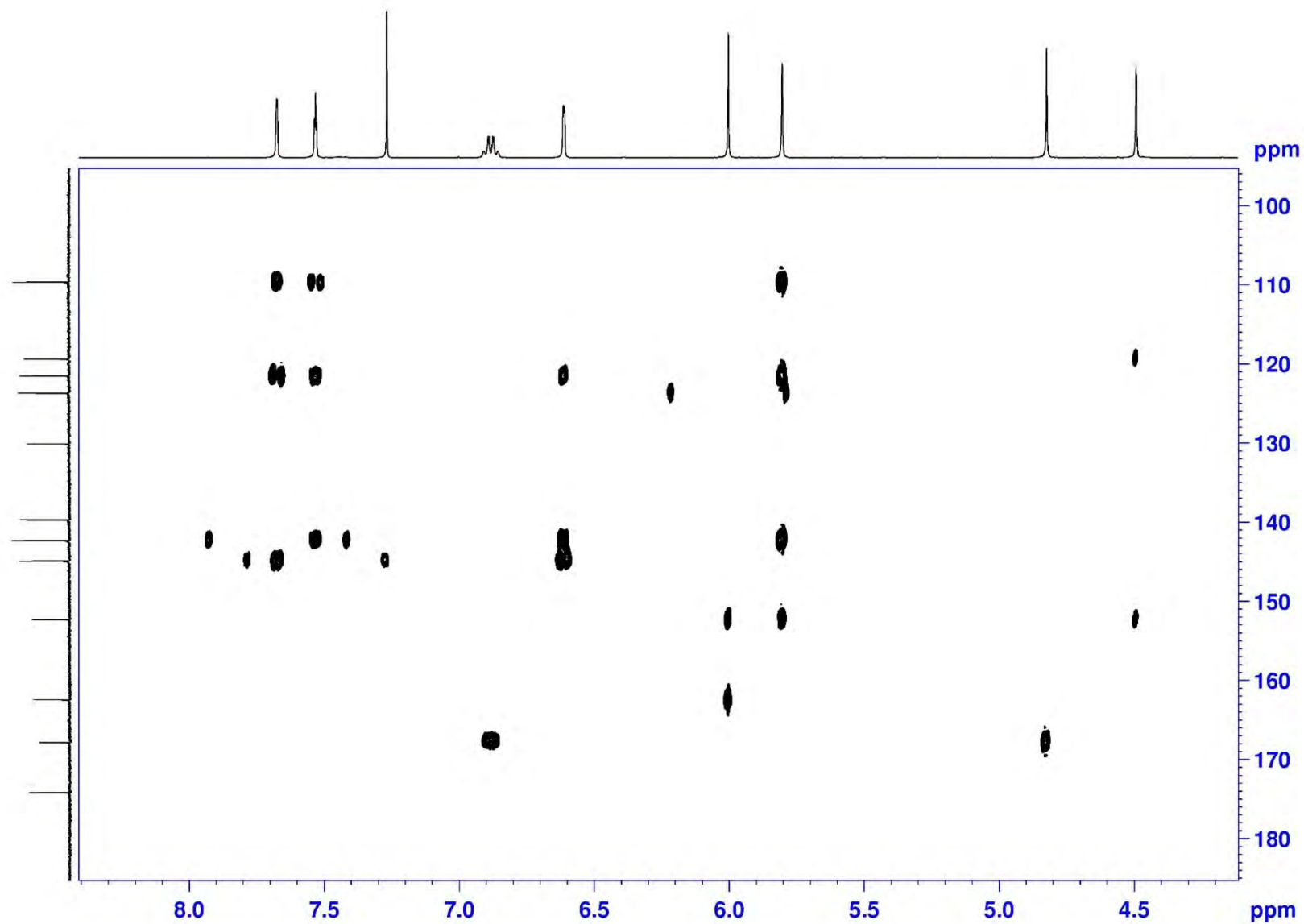
HSQC (400 MHz) spectrum of compound **27** in CDCl₃



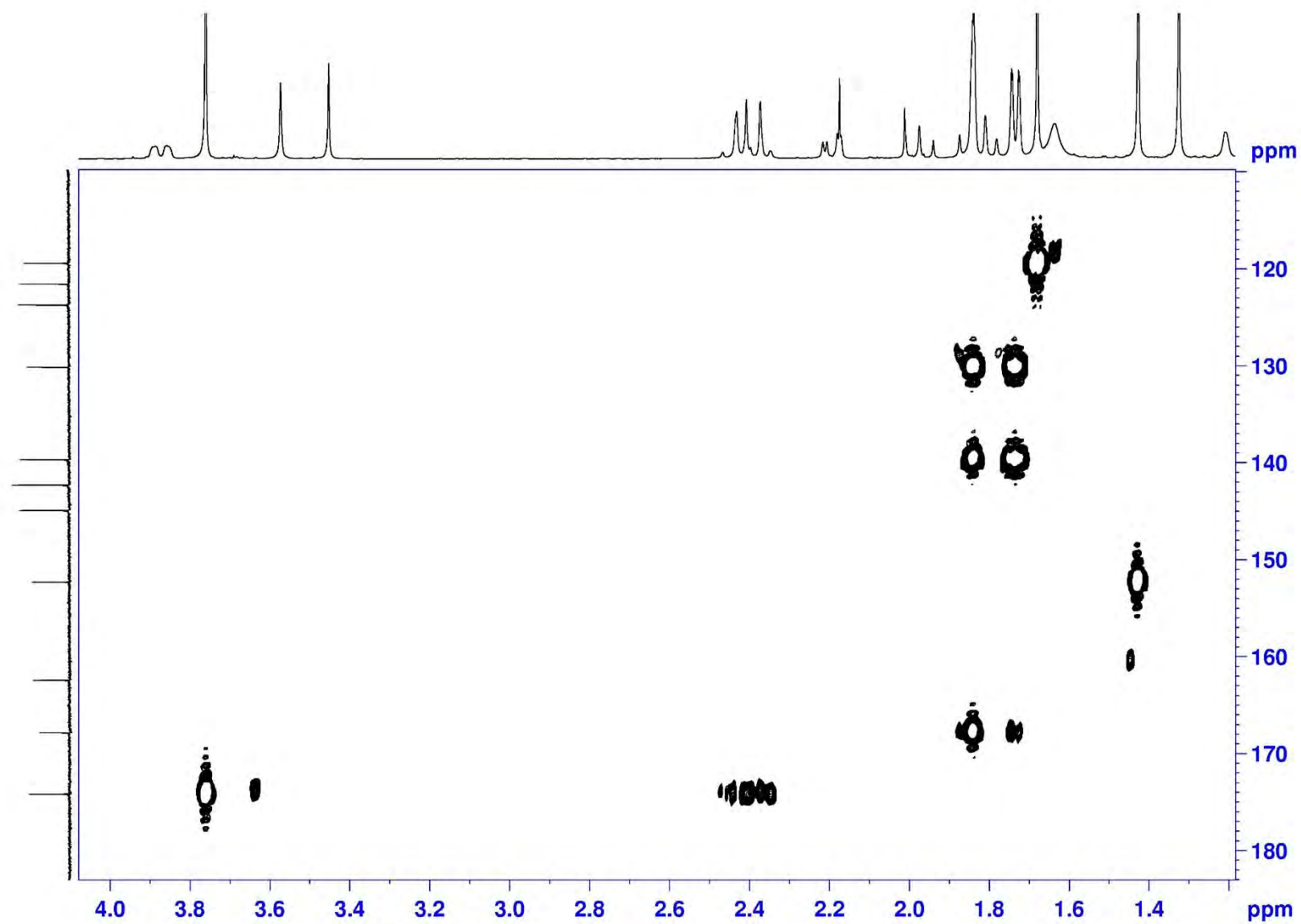
HMBC (400 MHz) spectrum of compound **27** in CDCl₃



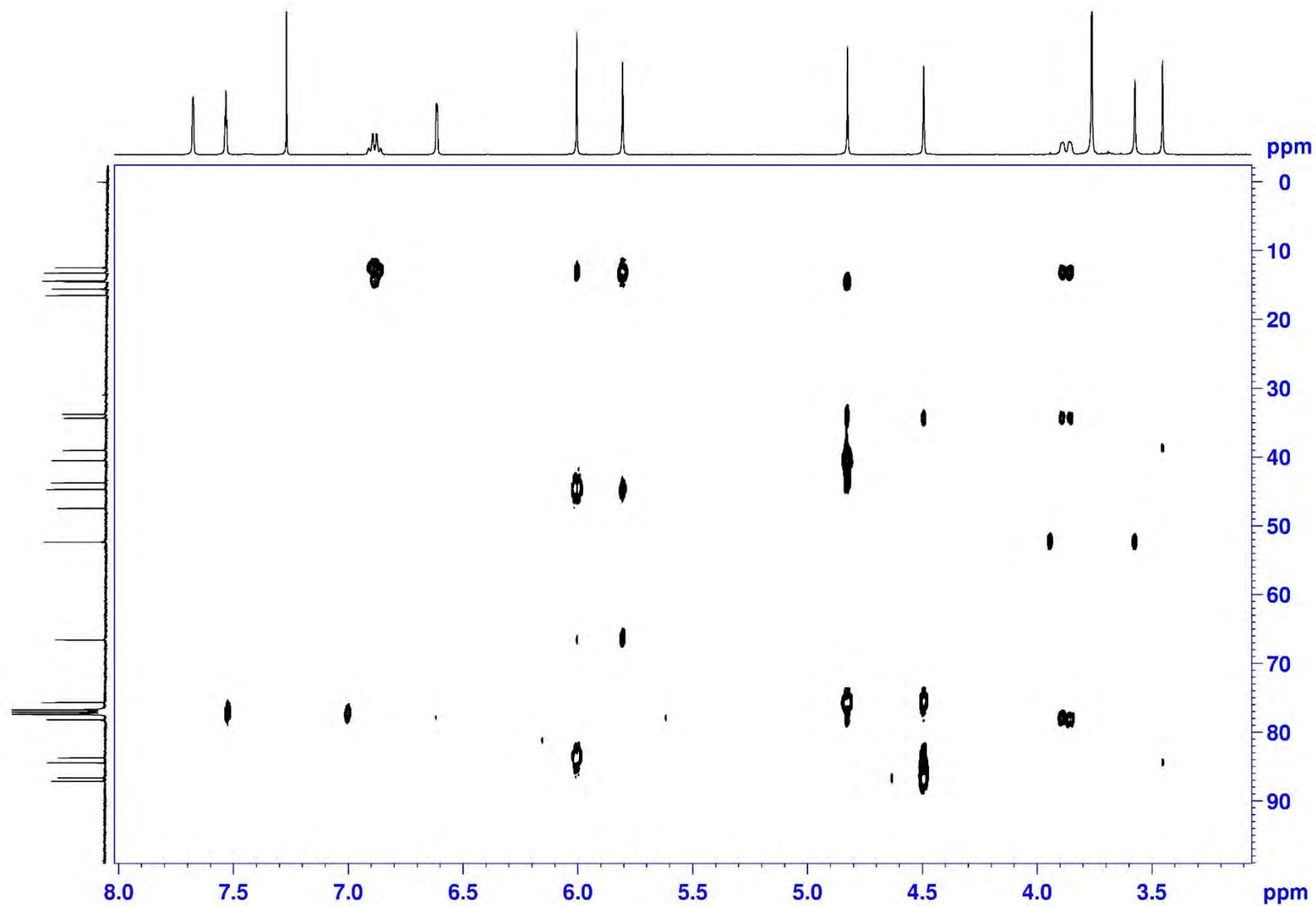
HMBC (400 MHz) spectrum of compound **27** in CDCl₃



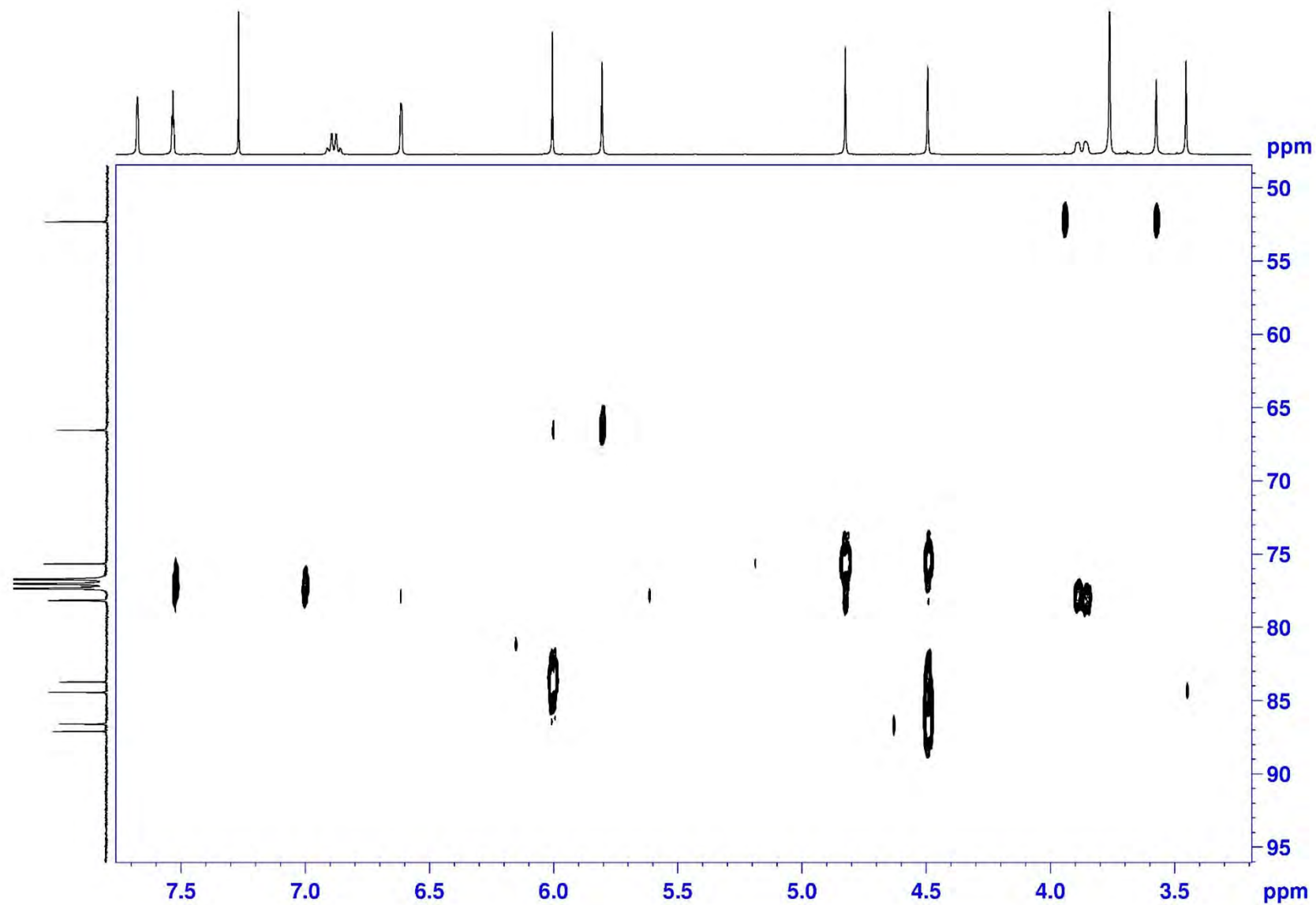
HMBC (400 MHz) spectrum of compound **27** in CDCl_3



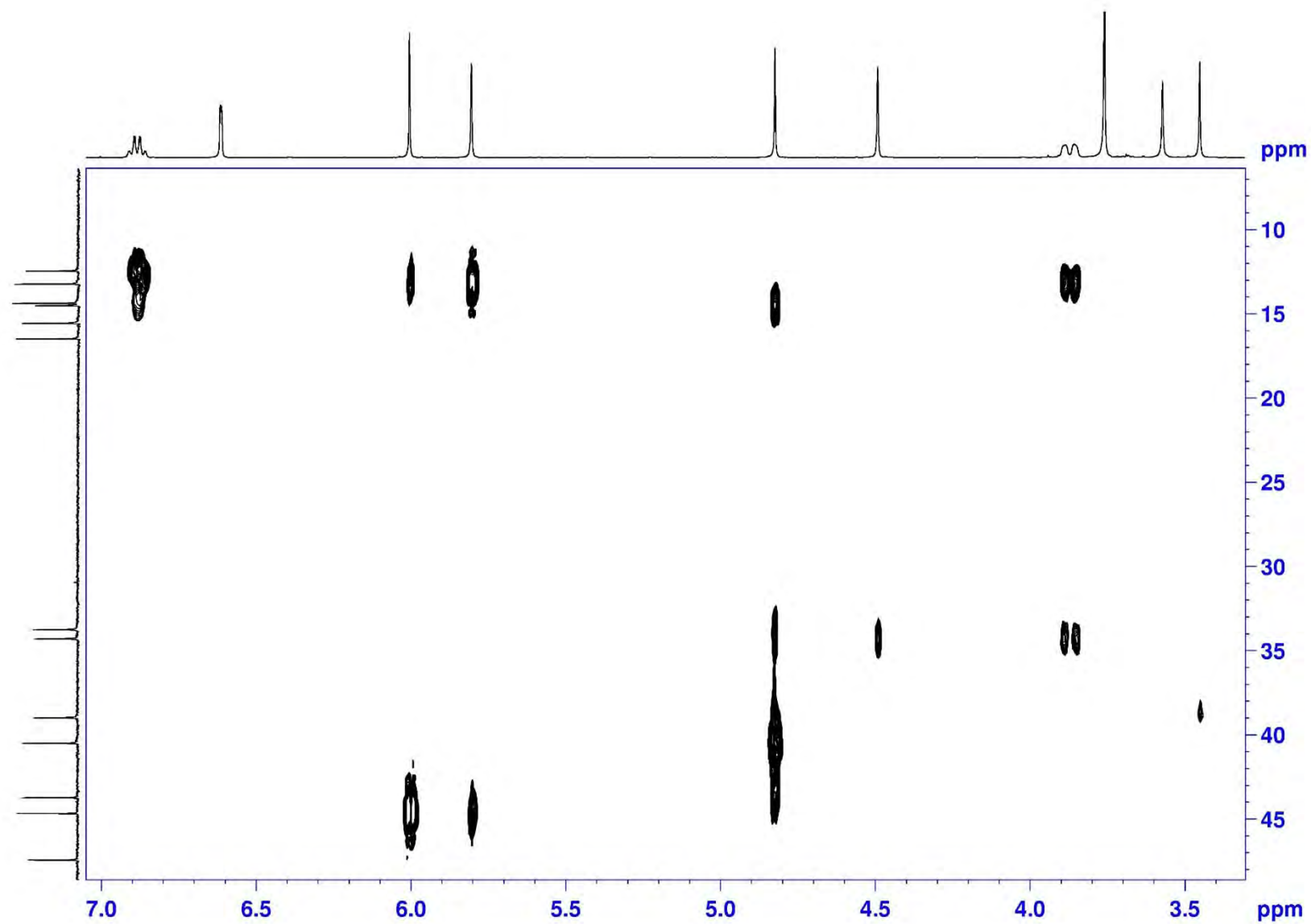
HMBC (400 MHz) spectrum of compound **27** in CDCl₃



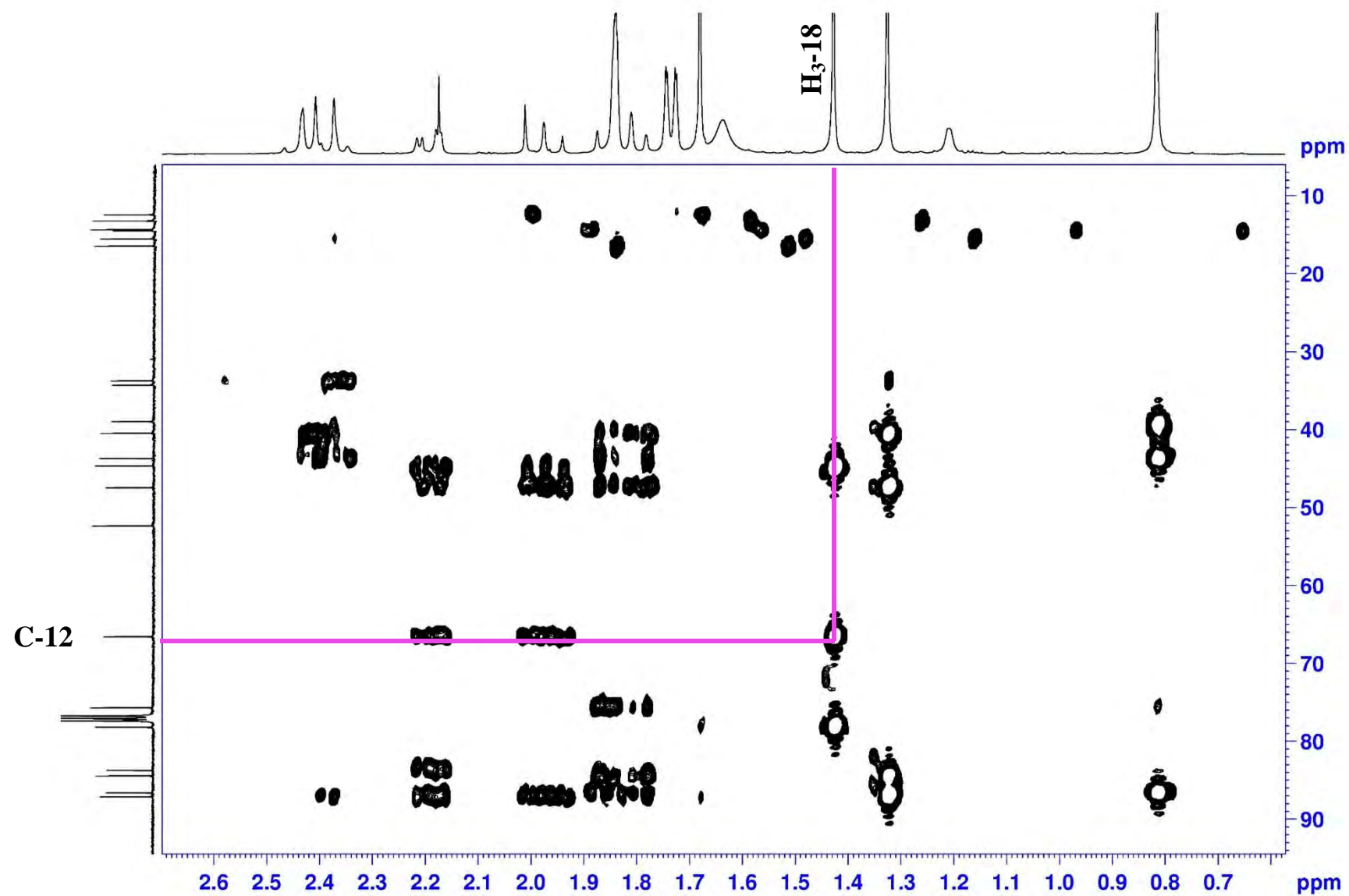
HMBC (400 MHz) spectrum of compound **27** in CDCl₃



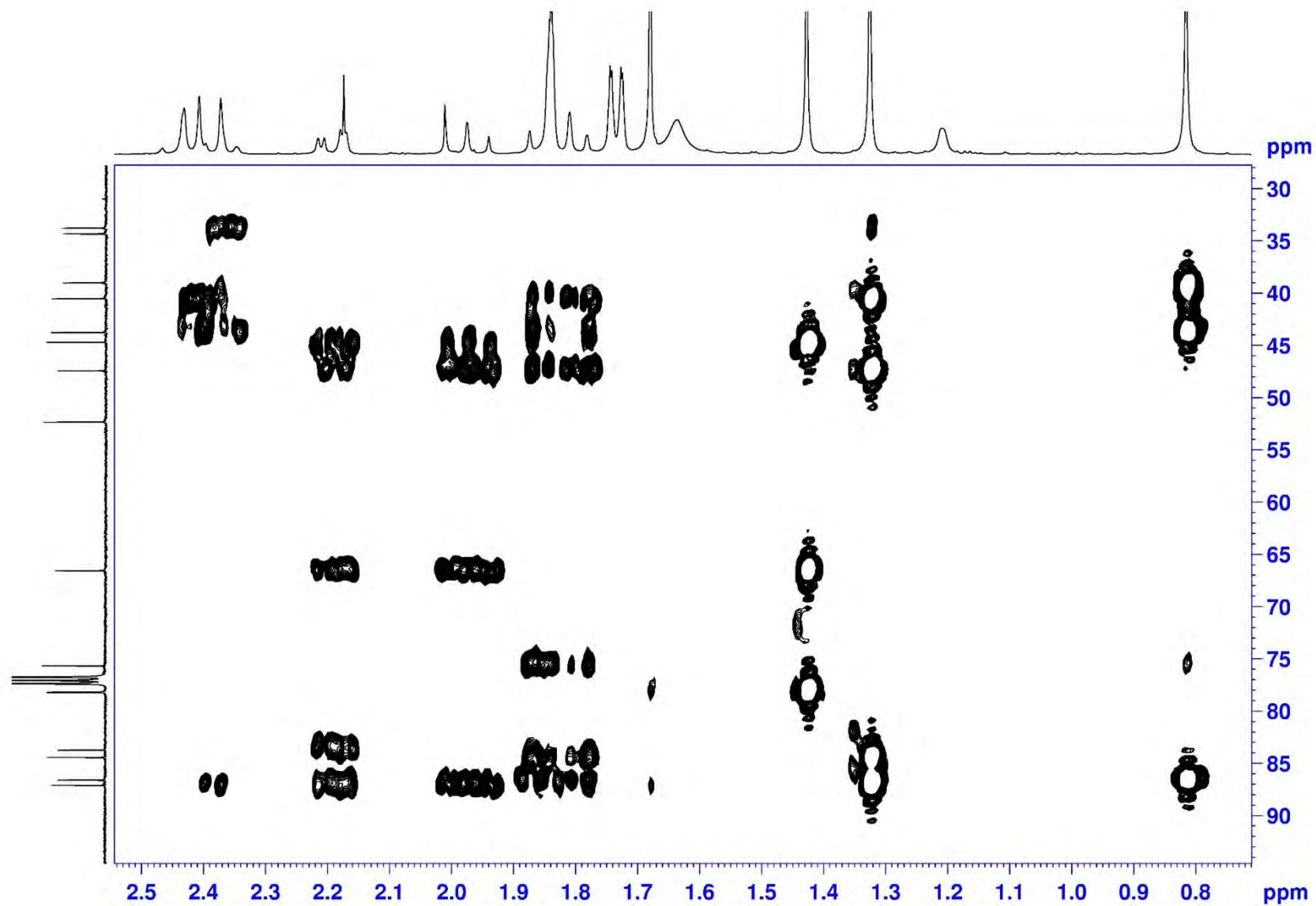
HMBC (400 MHz) spectrum of compound **27** in CDCl₃



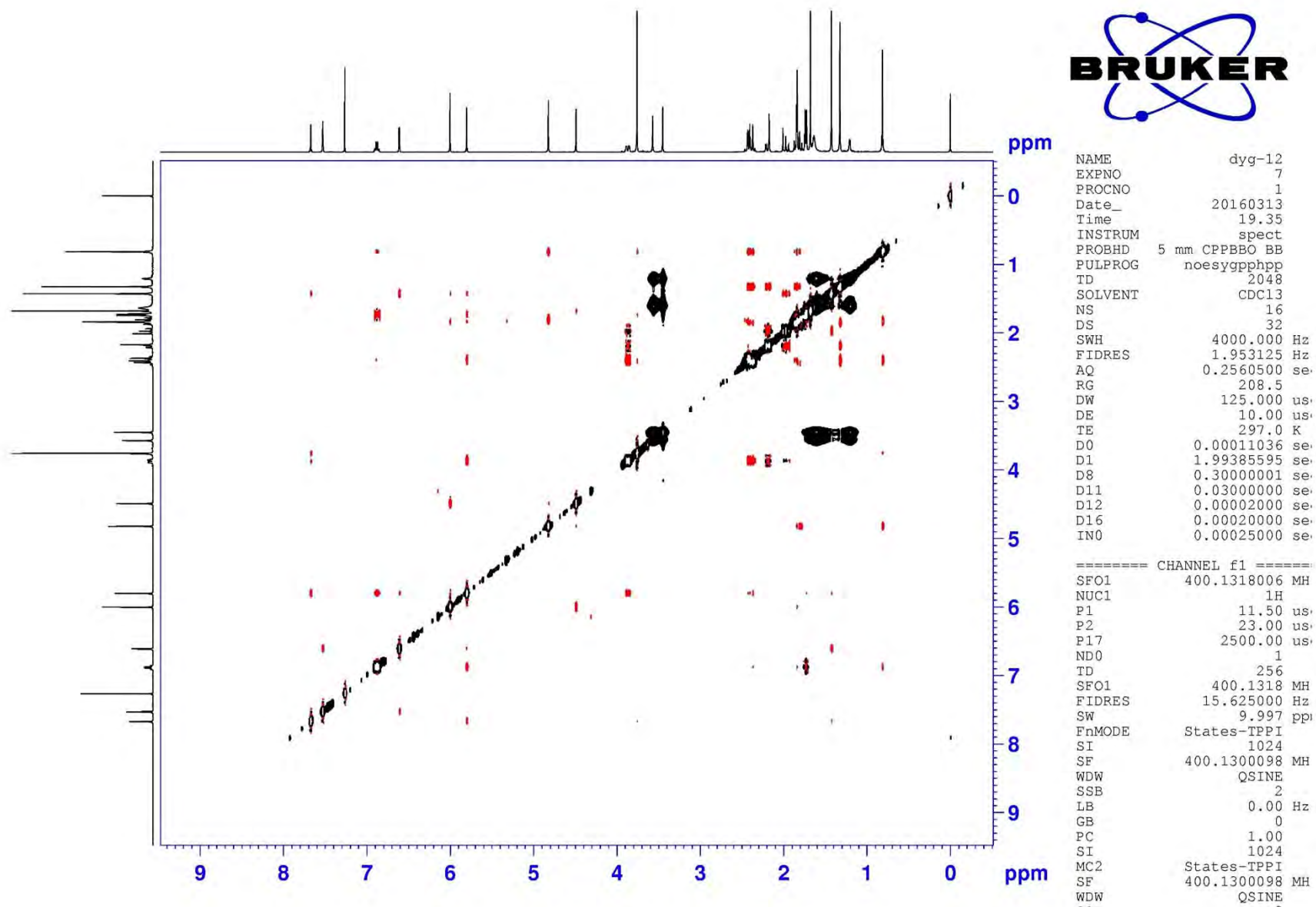
HMBC (400 MHz) spectrum of compound **27** in CDCl₃



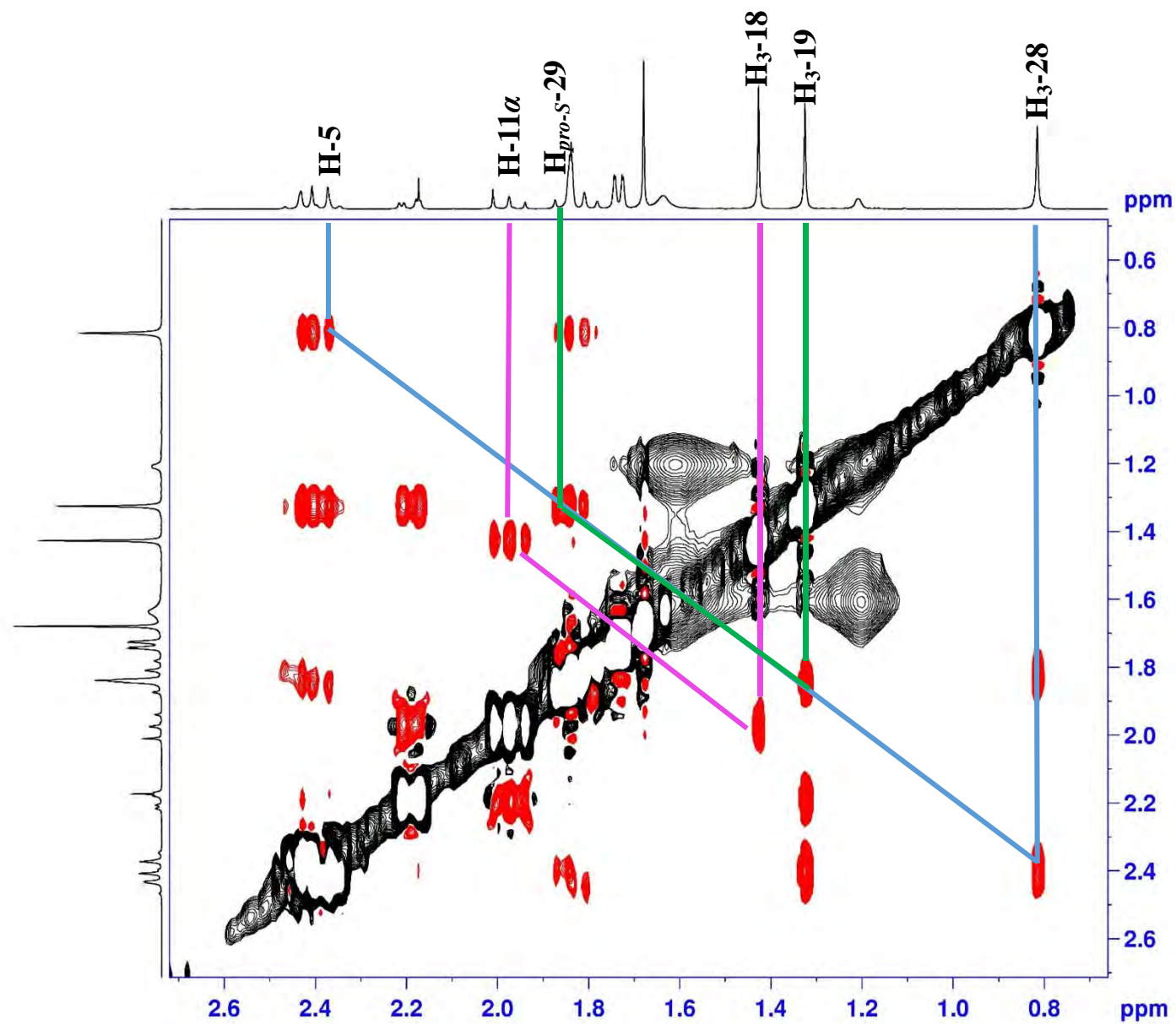
HMBC (400 MHz) spectrum of compound **27** in CDCl₃



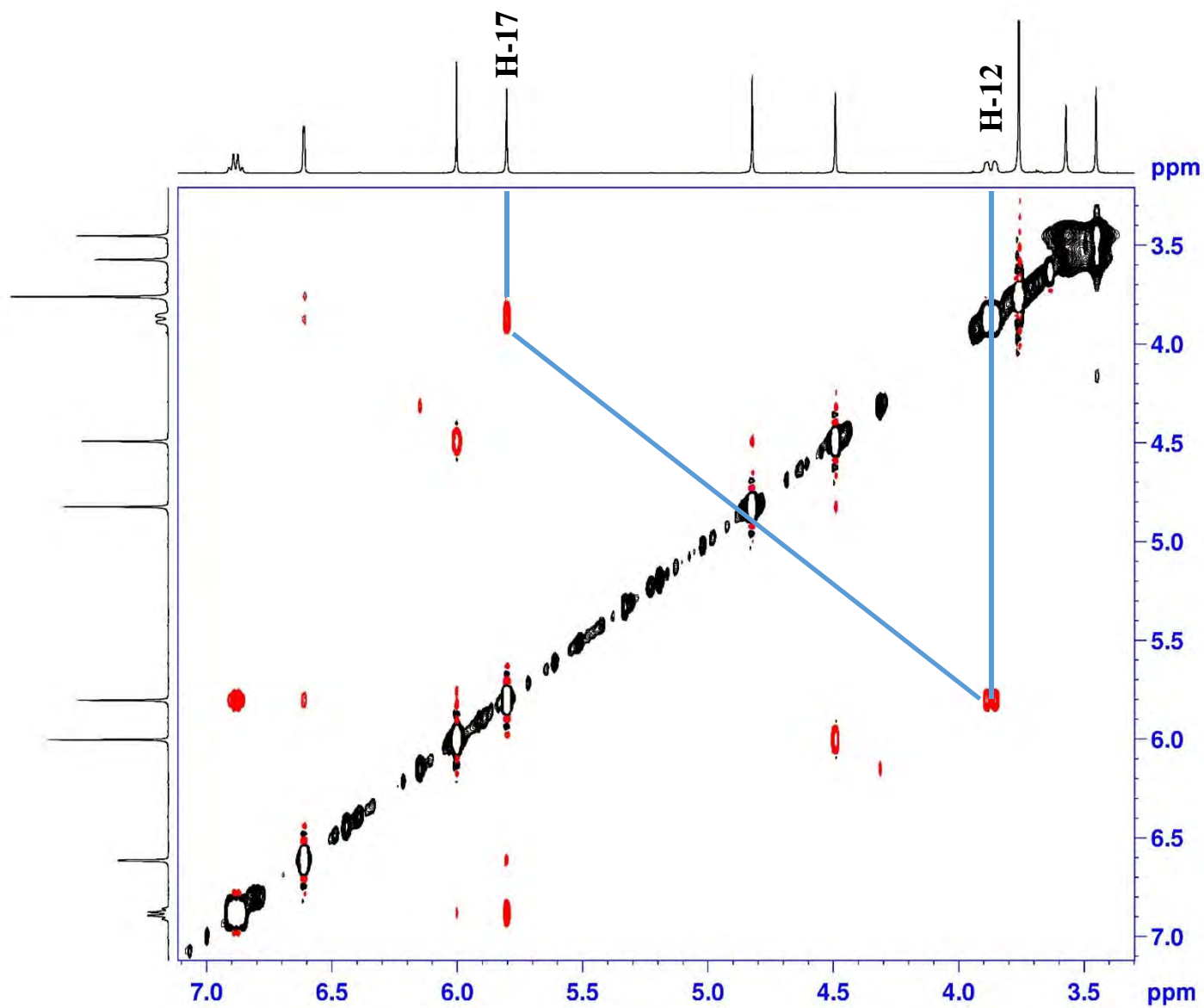
NOESY (400 MHz) spectrum of compound **27** in CDCl₃



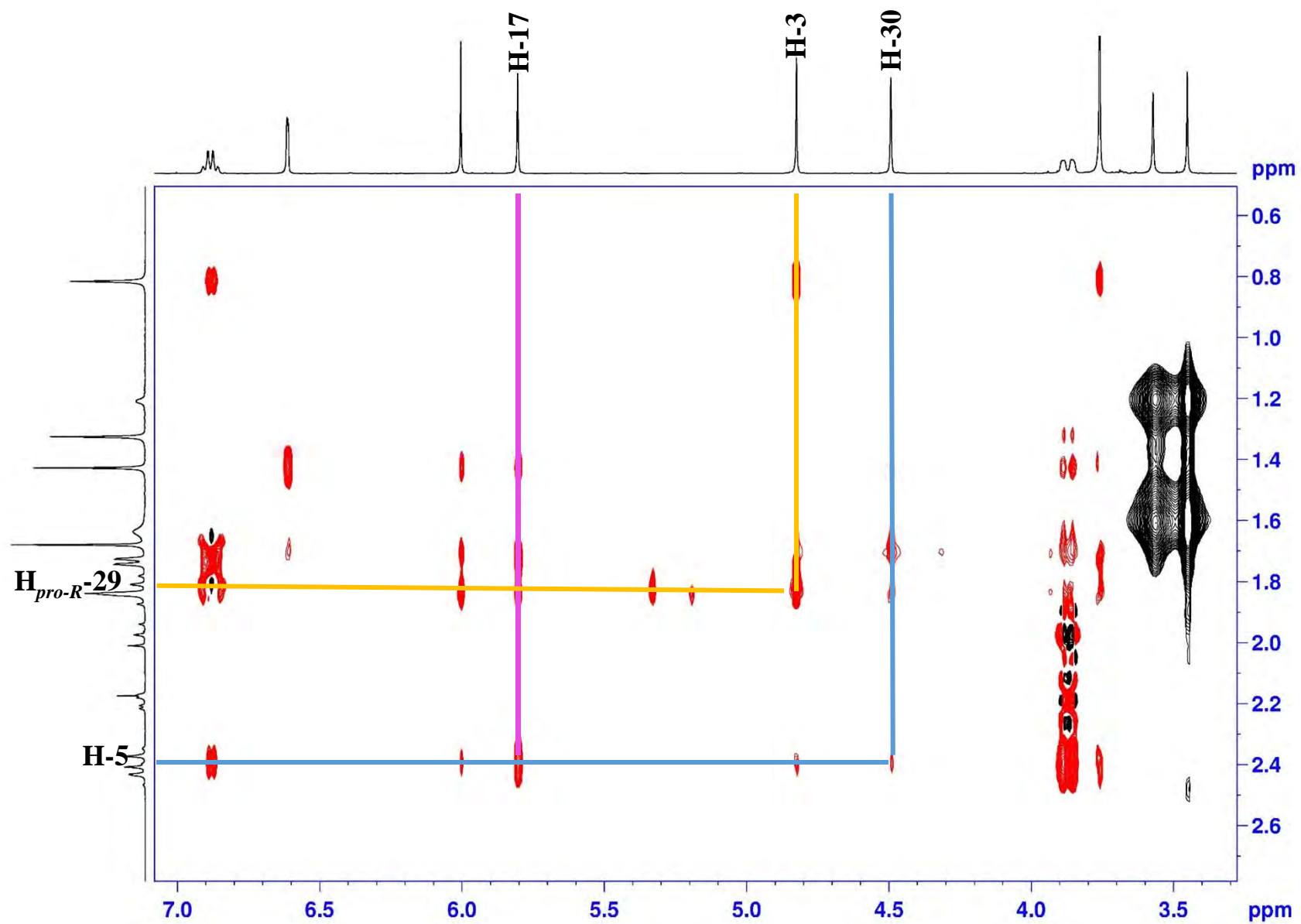
NOESY (400 MHz) spectrum of compound **27** in CDCl_3



NOESY (400 MHz) spectrum of compound **27** in CDCl₃



NOESY (400 MHz) spectrum of compound **27** in CDCl₃



HRESIMS for compound 28

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\MS\data\201612\zhangjianzhi_zjz-23_pos_81_01_2734.d
Method LC MS_Direct Infusion_pos_100-1000mz.m
Sample Name zhangjianzhi_zjz-23_pos
Comment

Acquisition Date

12/12/2016 3:08:24 PM

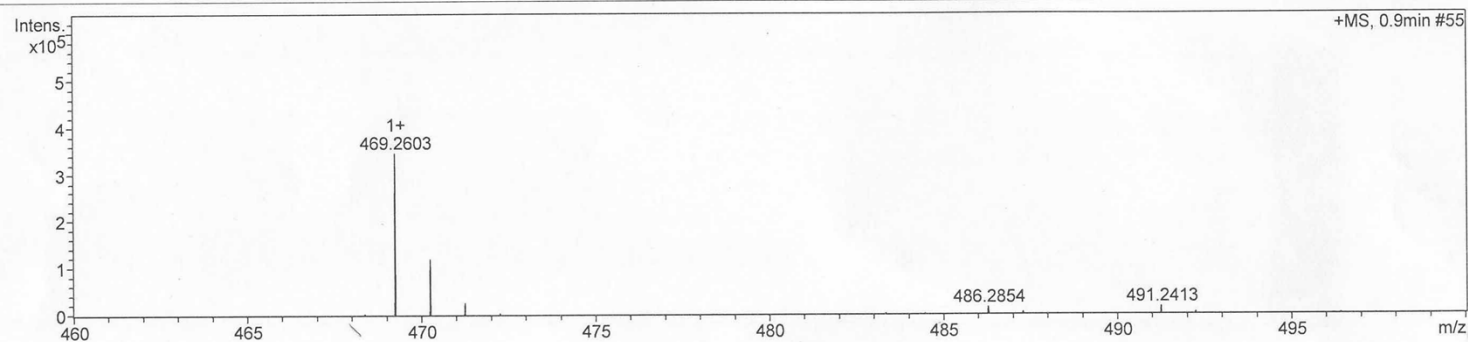
Operator
Instrument

SCSIO
maXis

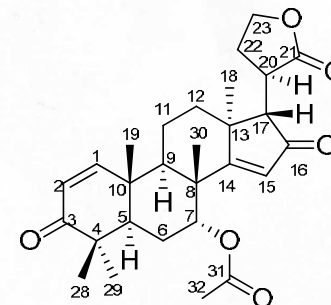
255552.00029

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 |
|------------|---|-------------|--------|------------|-----------|-----------|--------|------|---------------------|--------|
| 469.260338 | 1 | C28H37O6 | 100.00 | 469.258465 | 4.0 | 1.9 | 19.5 | 10.5 | even | ok |
| 491.241289 | 1 | C28H36NaO6 | 100.00 | 491.240410 | 1.8 | 0.9 | 7.2 | 10.5 | even | ok |
| 937.510657 | 1 | C56H73O12 | 100.00 | 937.509654 | -1.1 | -1.0 | 31.6 | 20.5 | even | ok |
| 959.493824 | 1 | C56H72NaO12 | 100.00 | 959.491598 | -2.3 | -2.2 | 42.8 | 20.5 | even | ok |



HRESIMS for compound 28

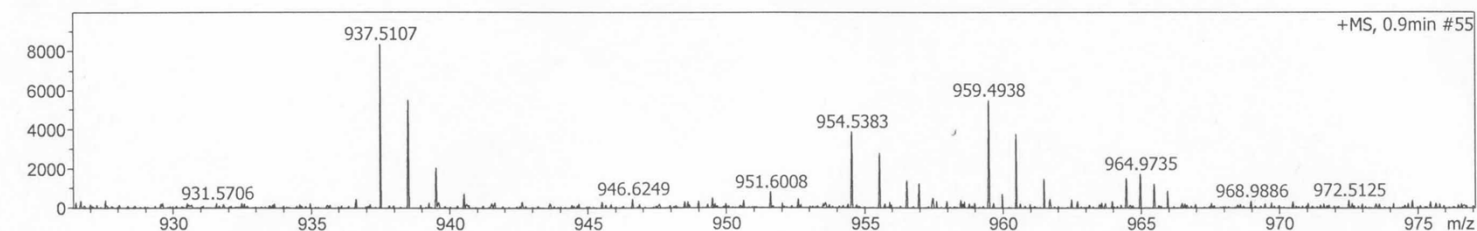
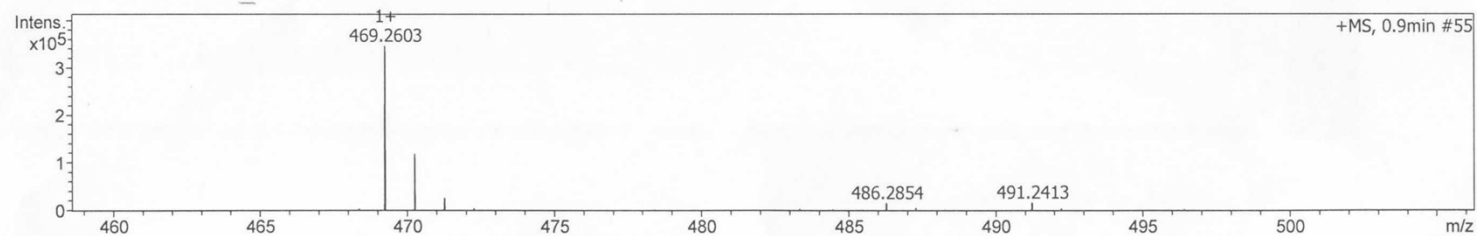
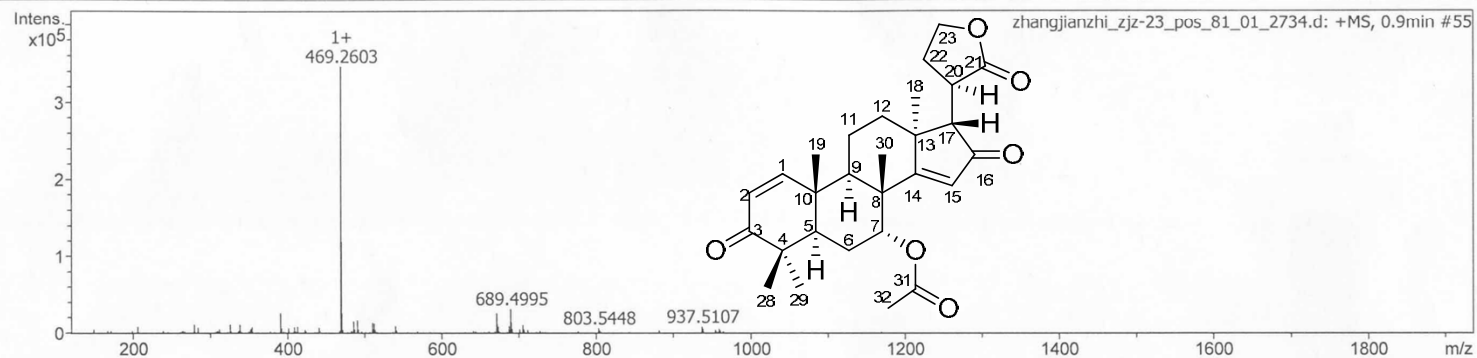
Generic Display Report

Analysis Info

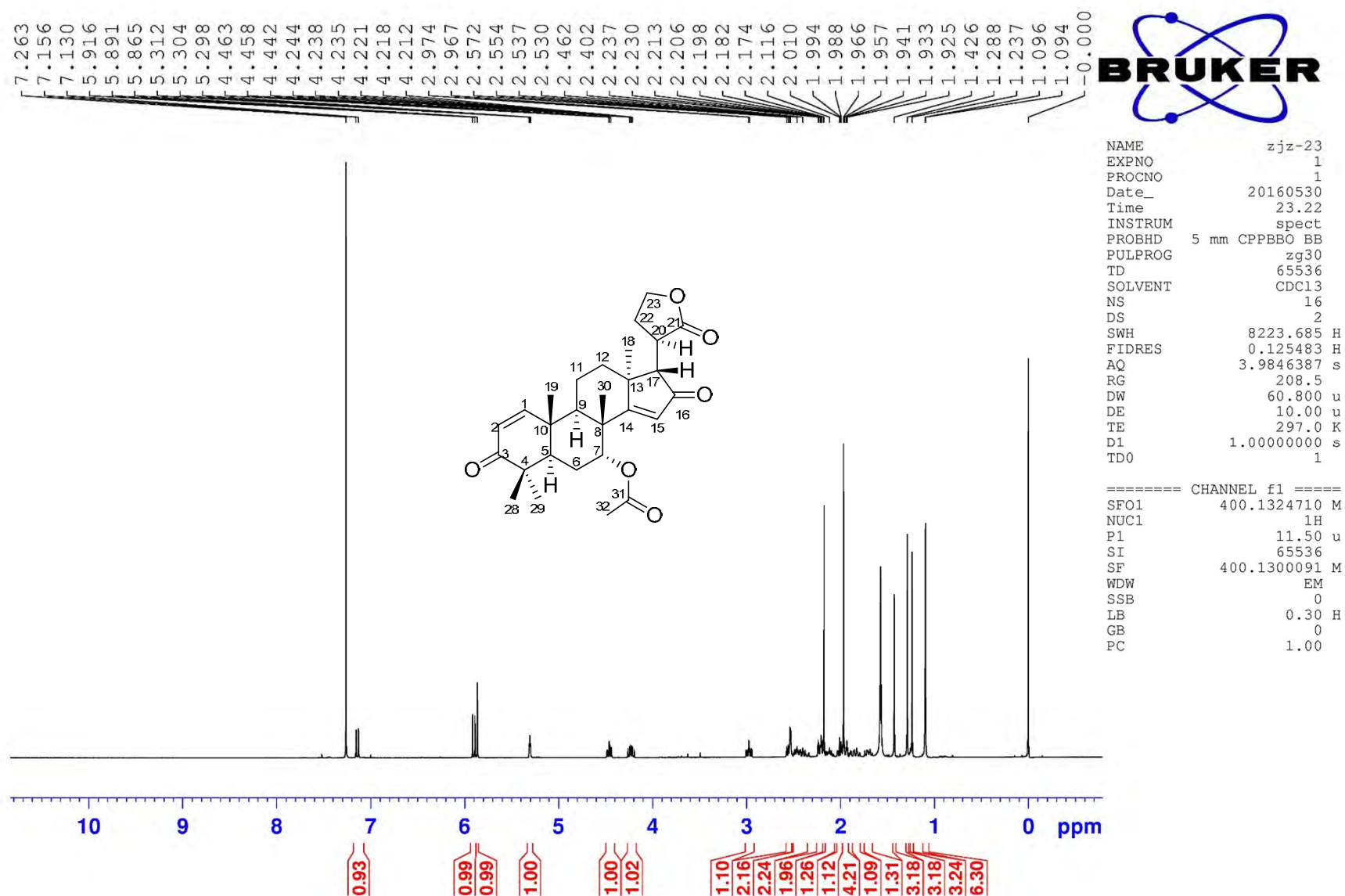
Analysis Name D:\Data\MS\data\201612\zhangjianzhi_zjz-23_pos_81_01_2734.d
Method LC MS_Direct Infusion_pos_100-1000mz.m
Sample Name zhangjianzhi_zjz-23_pos
Comment

Acquisition Date 12/12/2016 3:08:24 PM

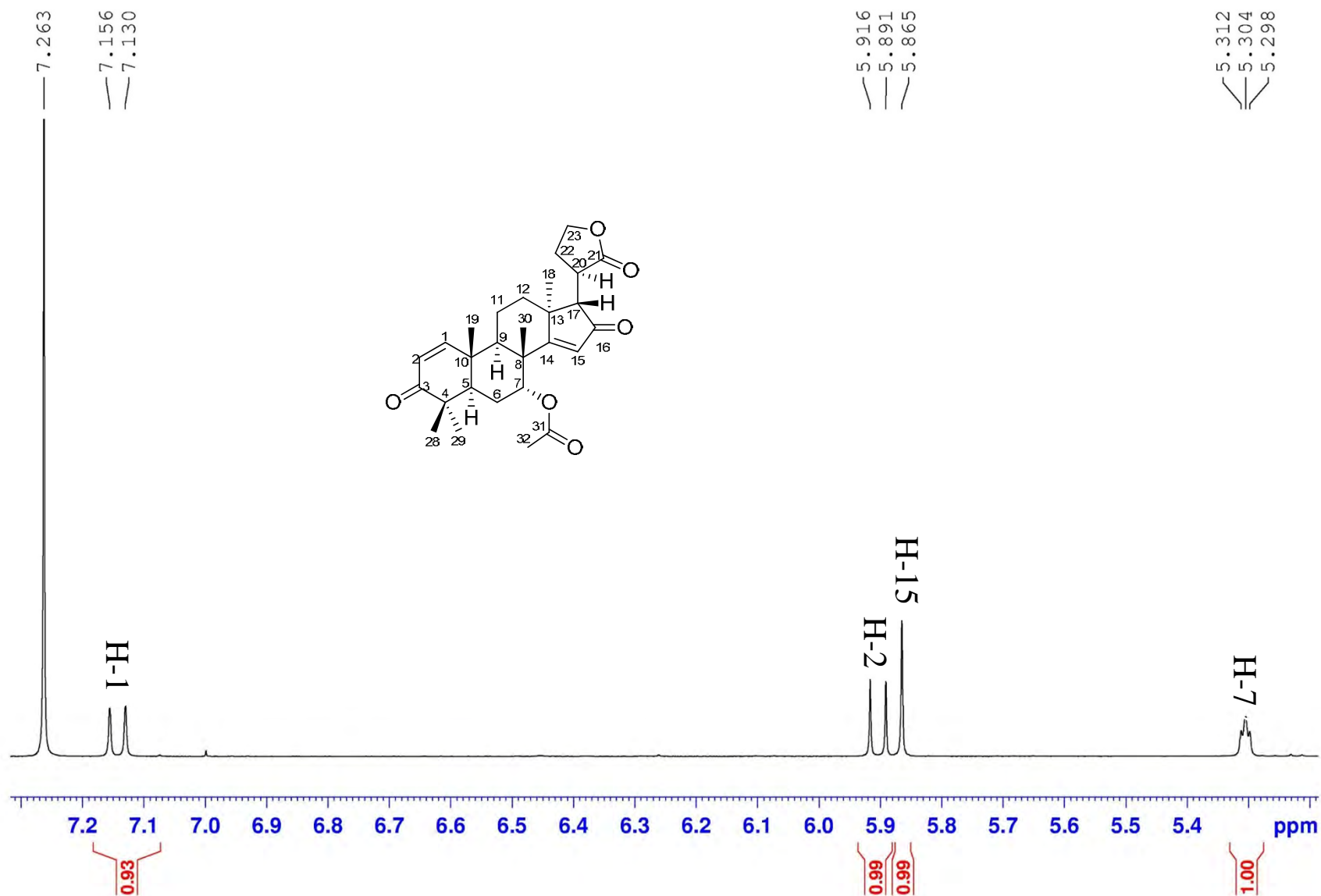
Operator SCSIO
Instrument maXis



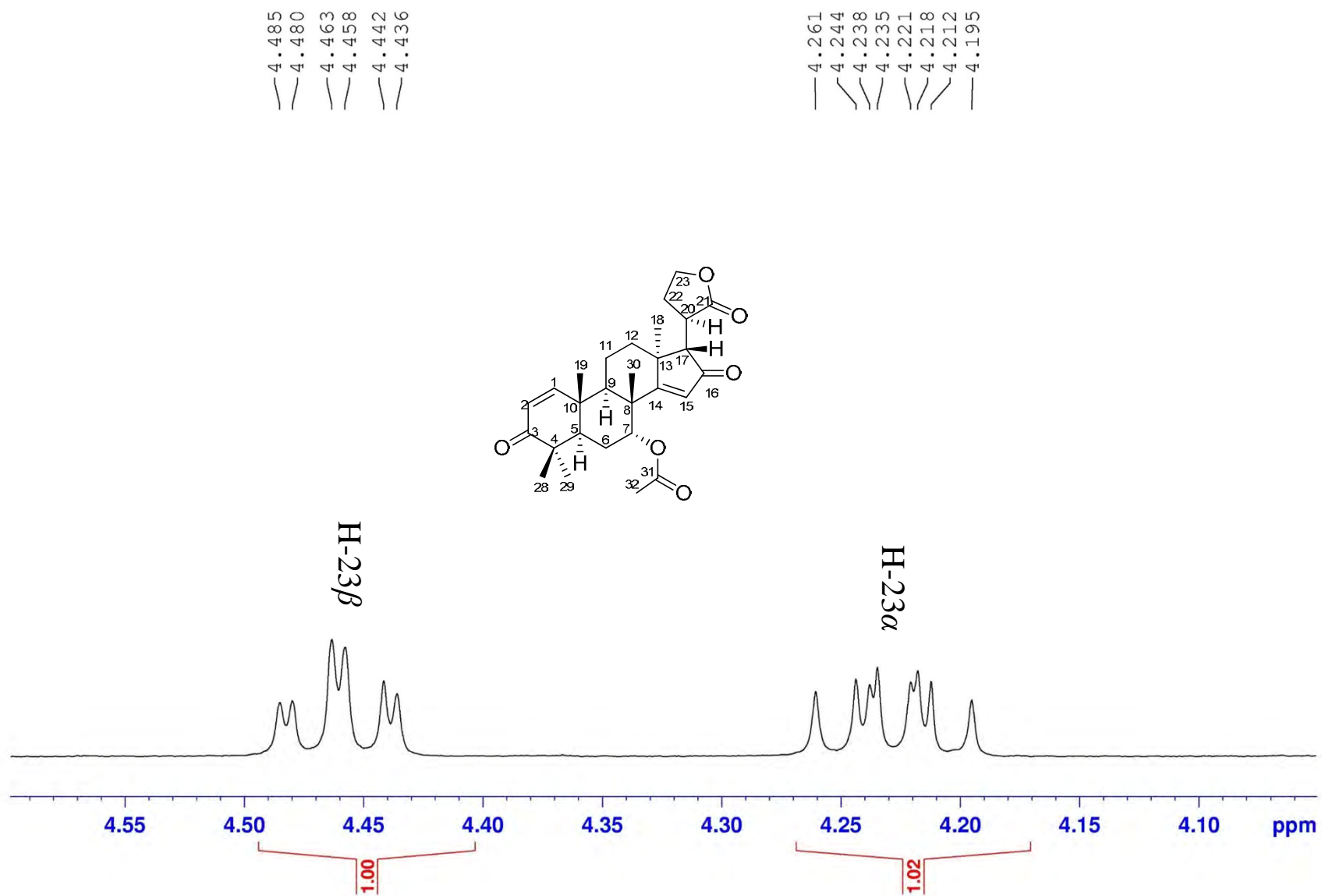
^1H NMR (400 MHz) spectrum of compound **28** in CDCl_3



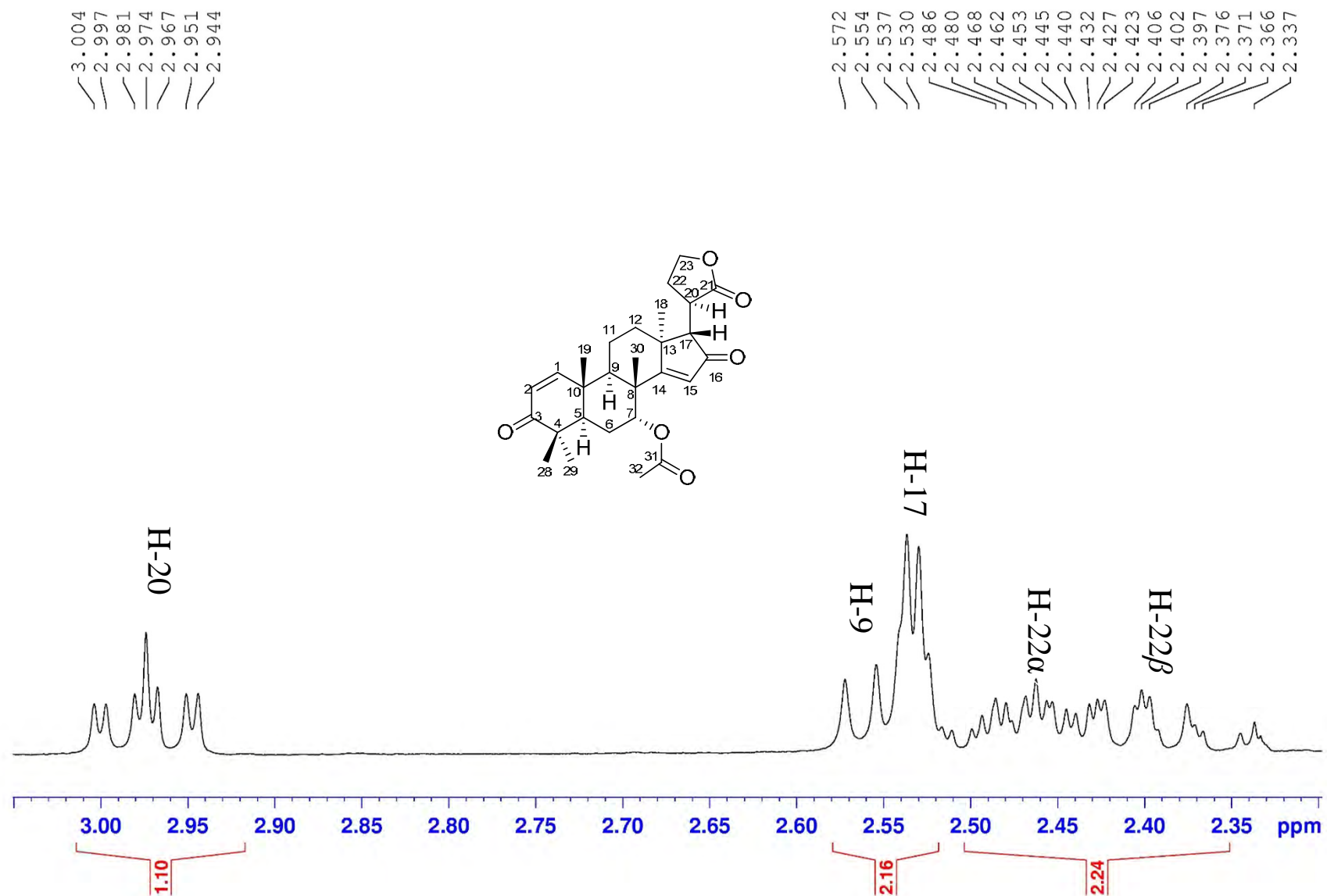
^1H NMR (400 MHz) spectrum of compound **28** in CDCl_3



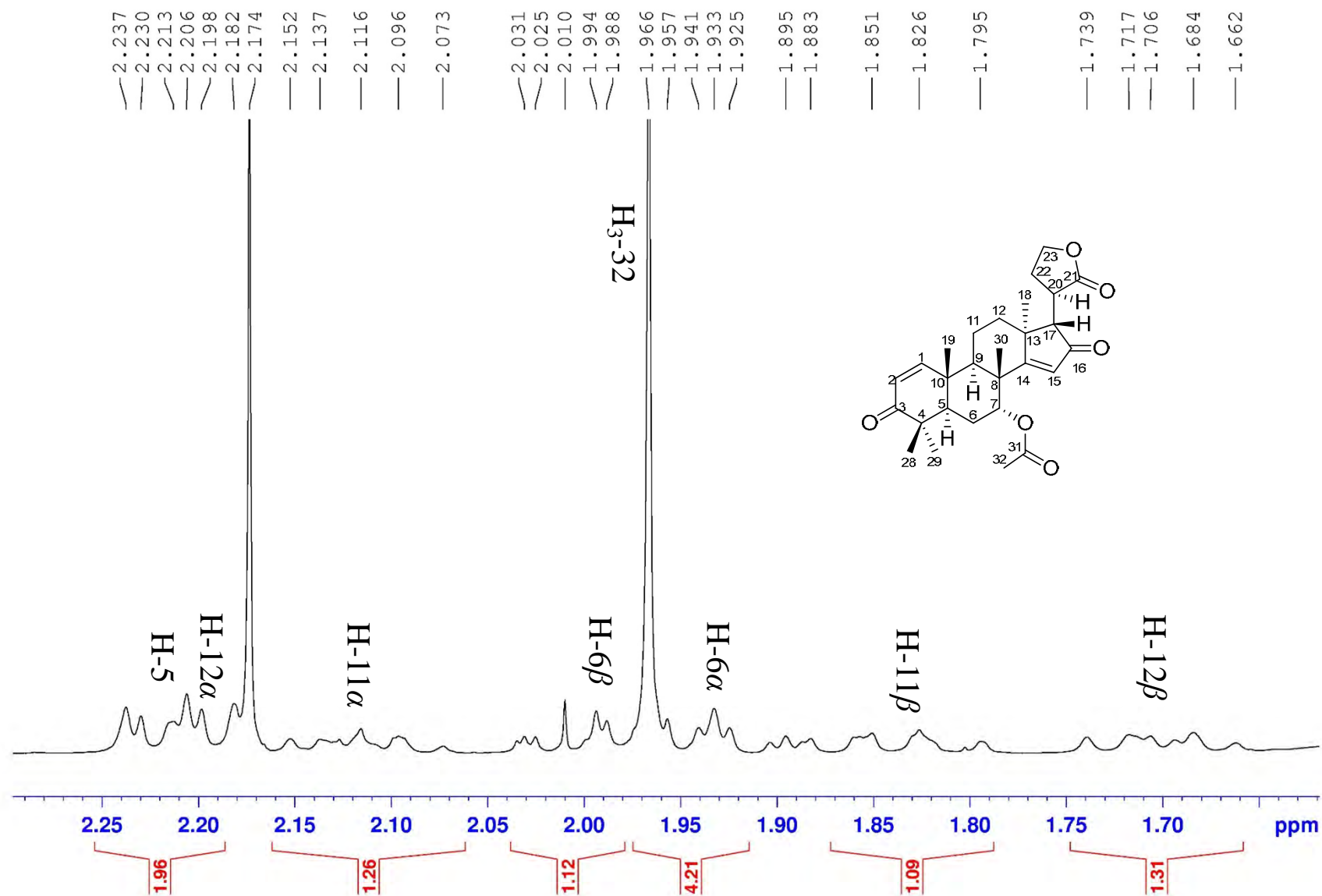
^1H NMR (400 MHz) spectrum of compound **28** in CDCl_3



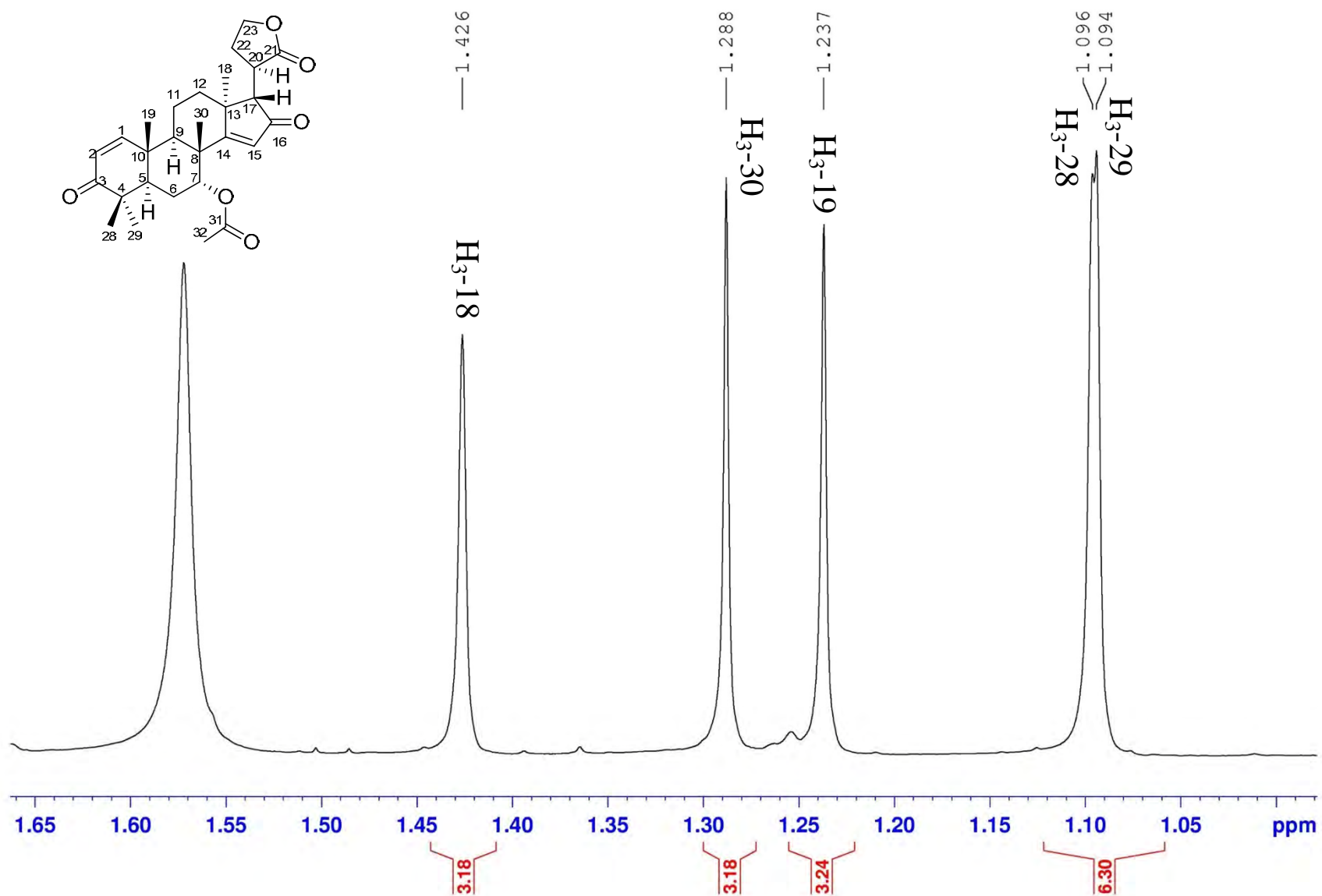
^1H NMR (400 MHz) spectrum of compound **28** in CDCl_3



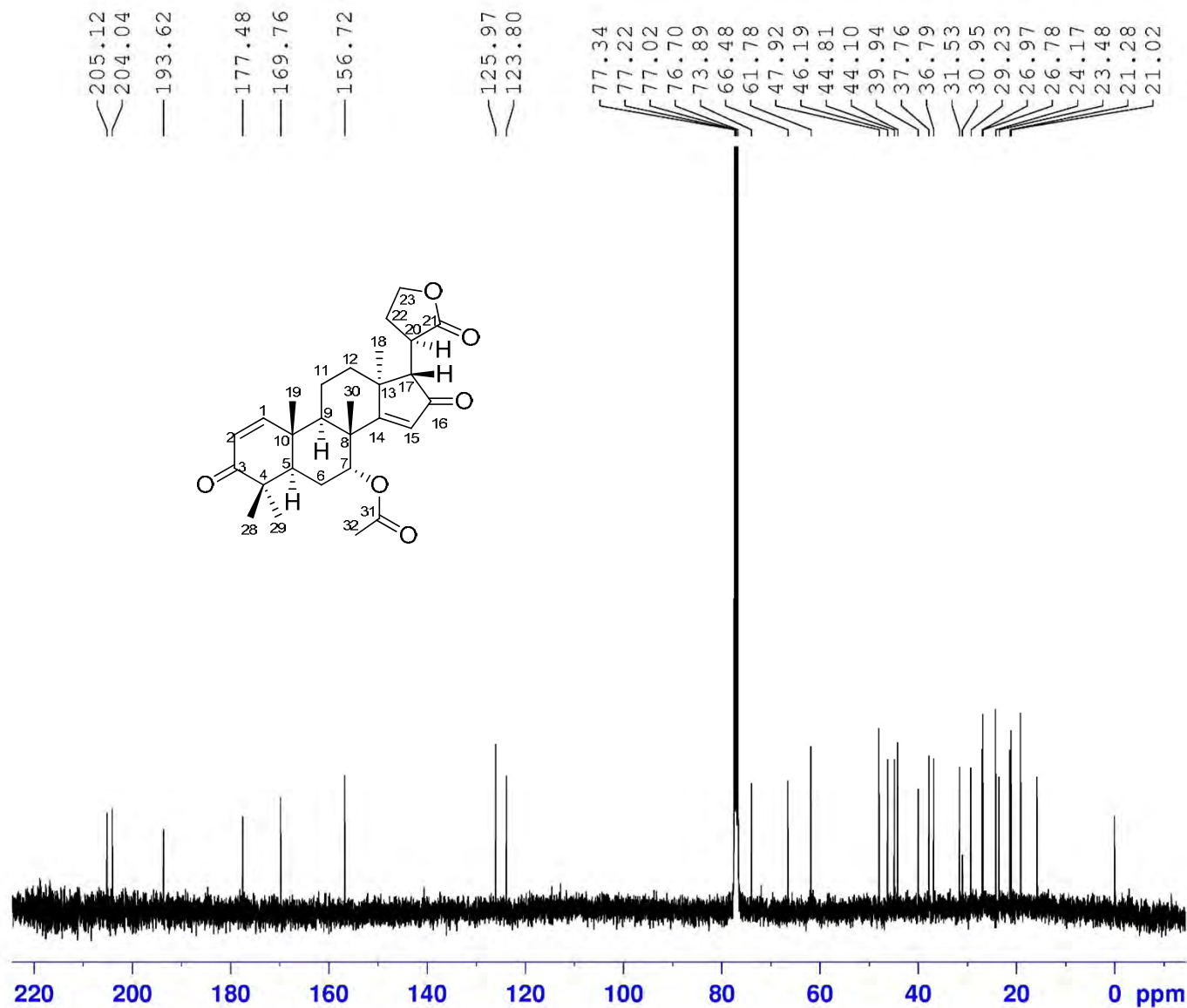
^1H NMR (400 MHz) spectrum of compound **28** in CDCl_3



^1H NMR (400 MHz) spectrum of compound **28** in CDCl_3



^{13}C NMR (100 MHz) spectrum of compound **28** in CDCl_3



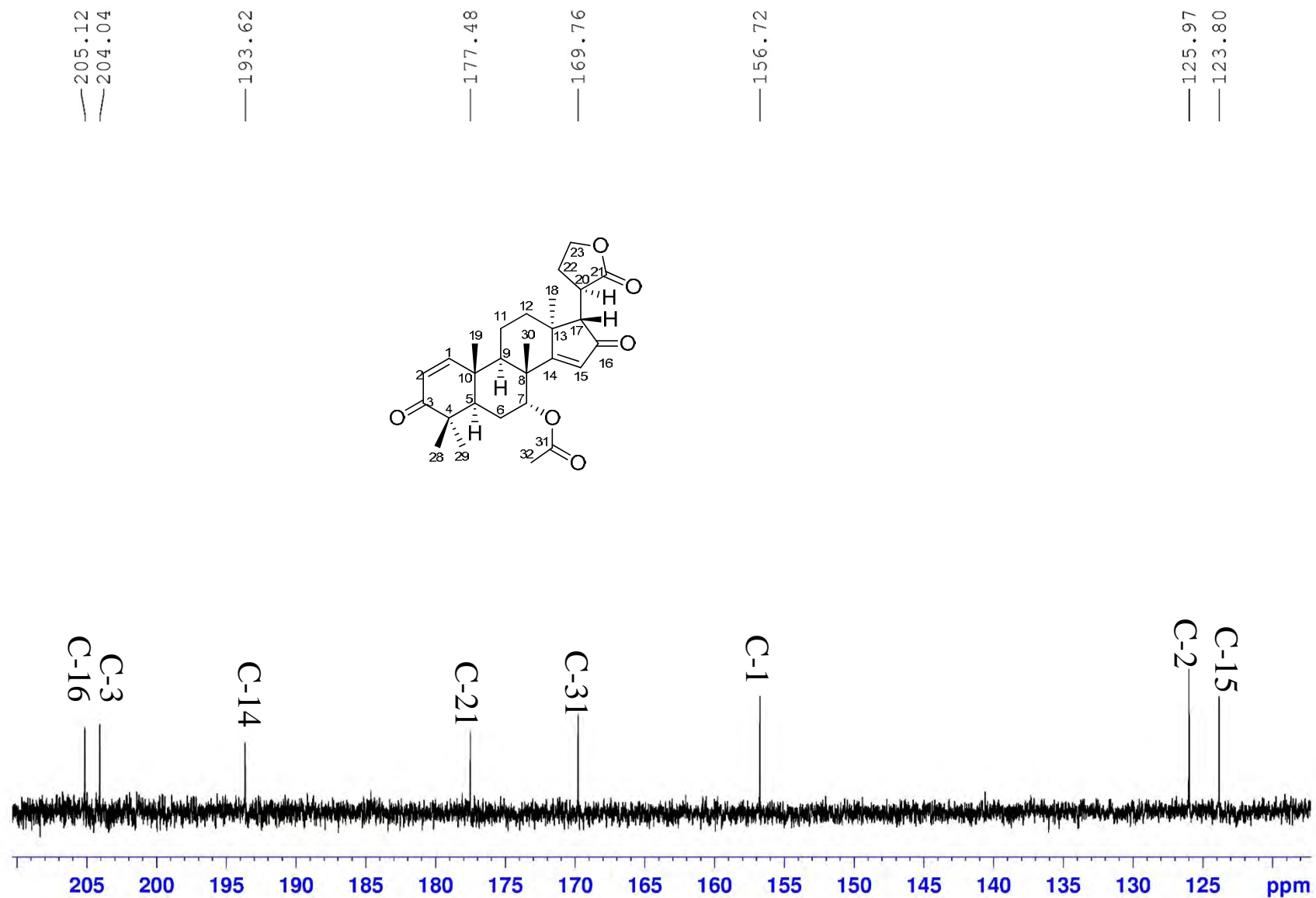
```

NAME           zjz-23
EXPNO           2
PROCNO          1
Date_           20160531
Time            0.21
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 s
RG              117.37
DW              20.800 us
DE              18.00 us
TE              297.0 K
D1              2.00000000 s
D11             0.03000000 s
TD0             1
    
```

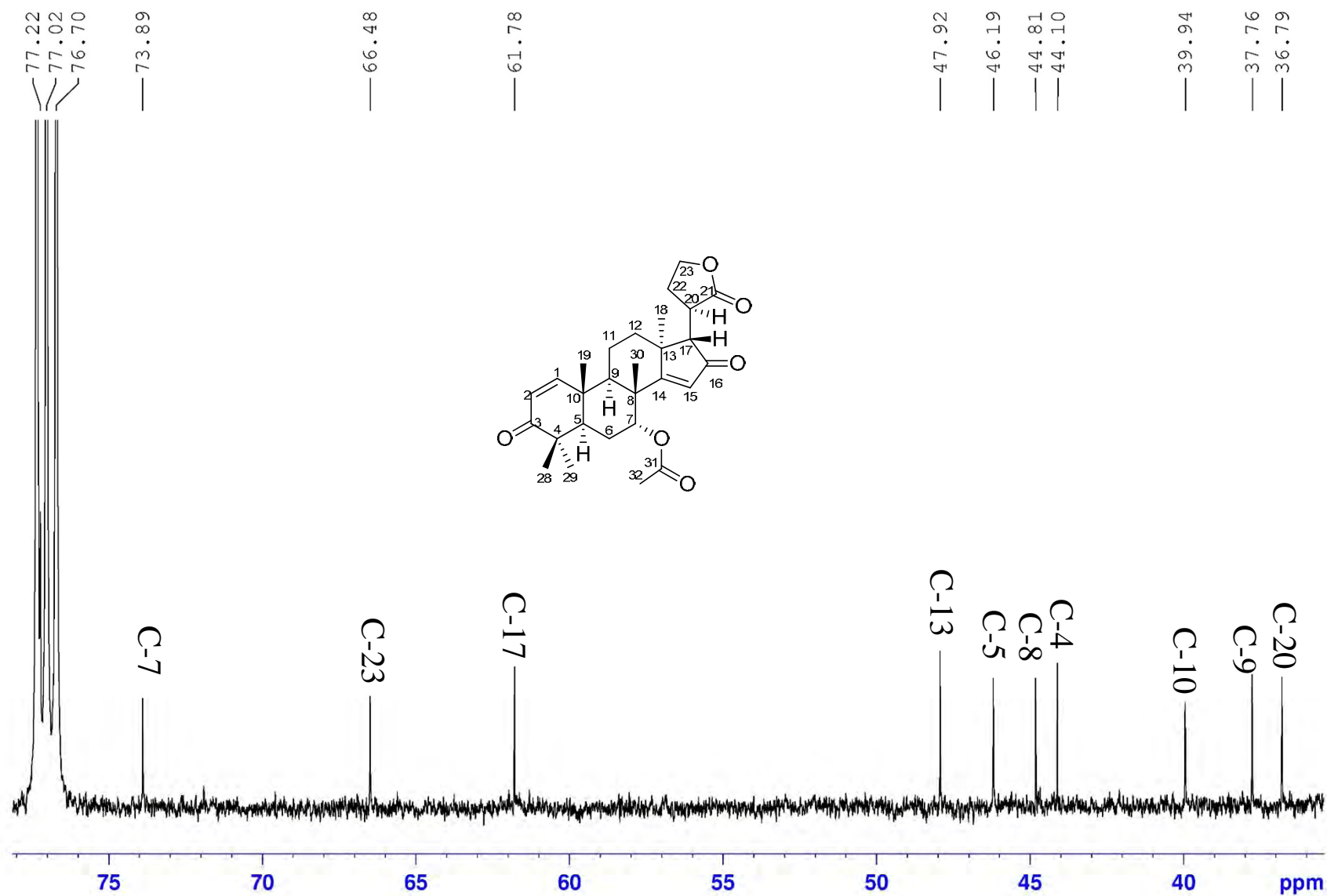
```

===== CHANNEL f1 =====
SF01          100.6233324 MHz
NUC1           13C
P1             10.00 us
SI             32768
SF            100.6127694 MHz
WDW            EM
SSB            0
LB             1.00 Hz
GB             0
PC             1.40
    
```

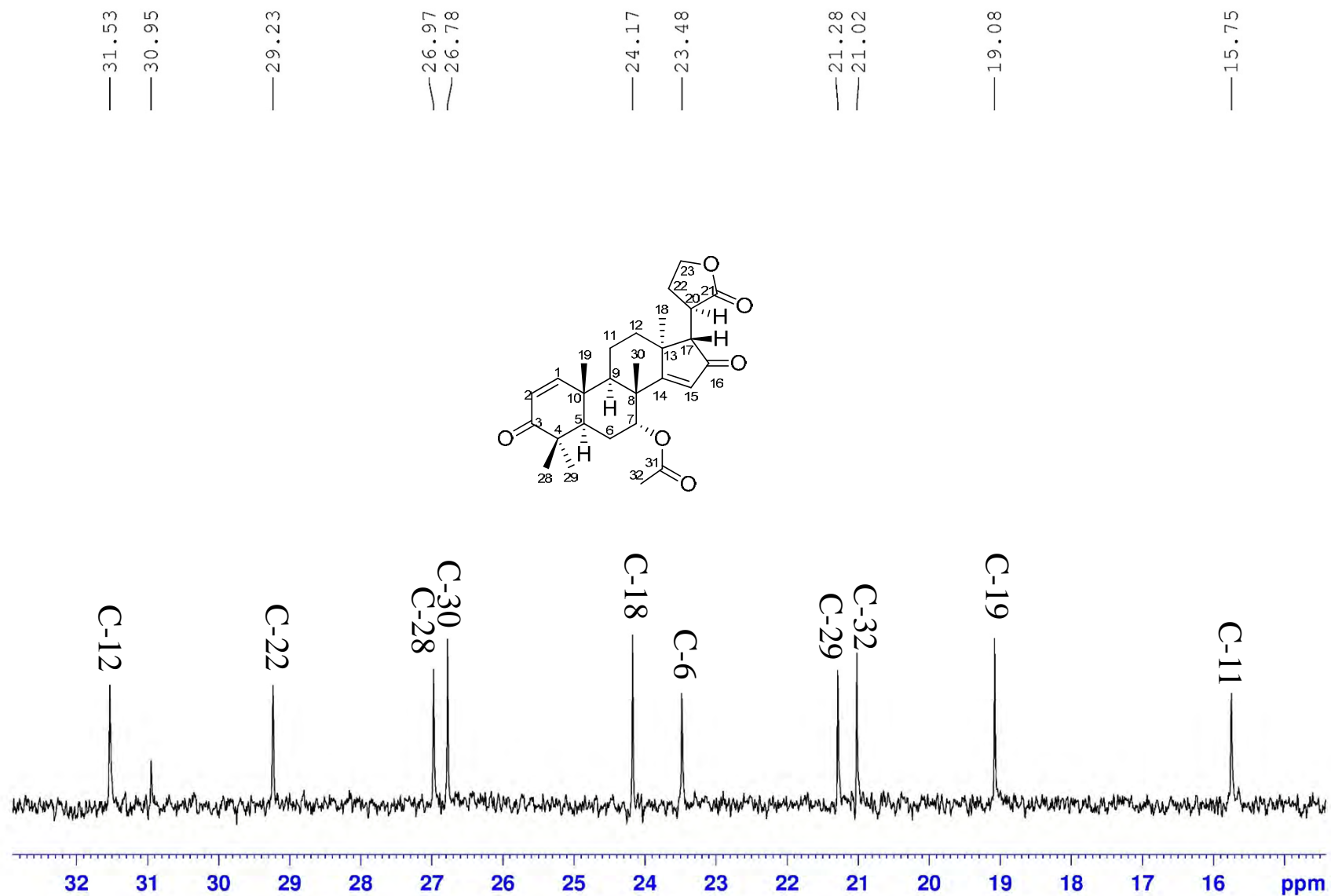
^{13}C NMR (100 MHz) spectrum of compound **28** in CDCl_3



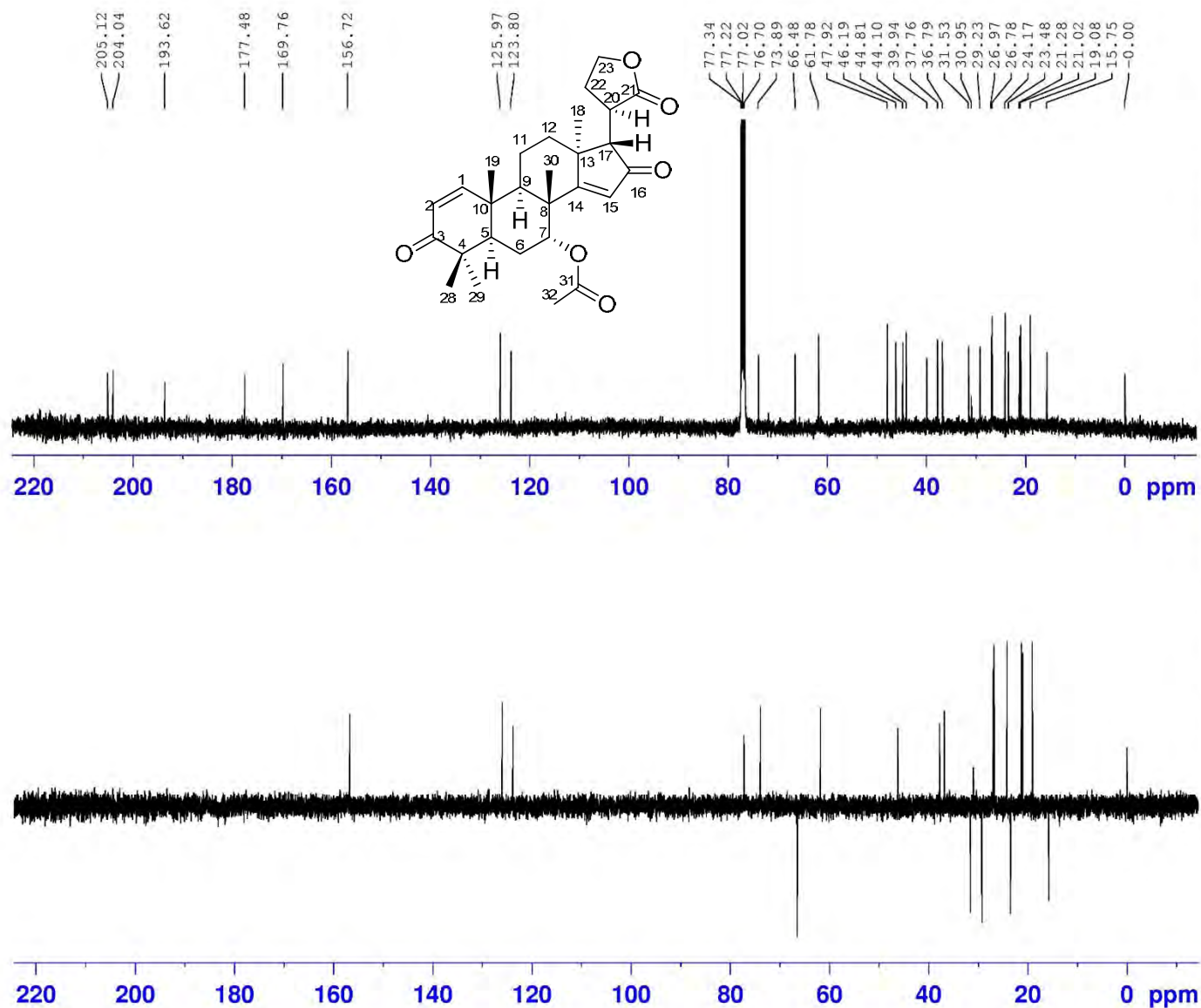
^{13}C NMR (100 MHz) spectrum of compound **28** in CDCl_3



^{13}C NMR (100 MHz) spectrum of compound **28** in CDCl_3



DEPT135 (100 MHz) spectrum of compound **28** in CDCl₃



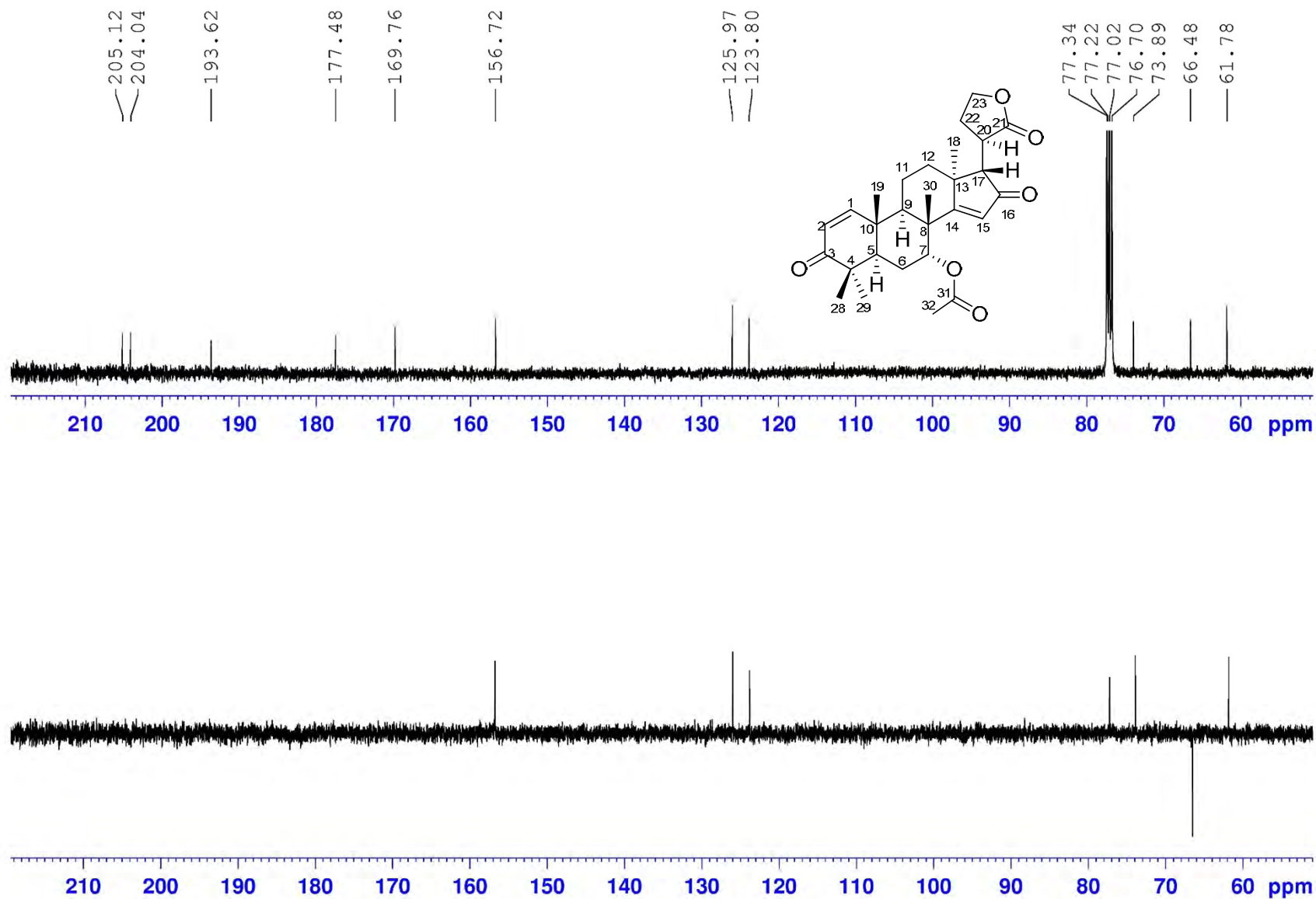
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NAME          zjz-23
EXPNO         3
PROCNO        1
Date_         20160531
Time          0.40
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       deptspl35
TD            65536
SOLVENT       CDC13
NS            300
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 se
RG            130.26
DW            20.800 us
DE            18.00 us
TE            297.0 K
CNST2         145.0000000
D1            2.00000000 se
D2            0.00344828 se
D12           0.00002000 se
TD0           1
    
```

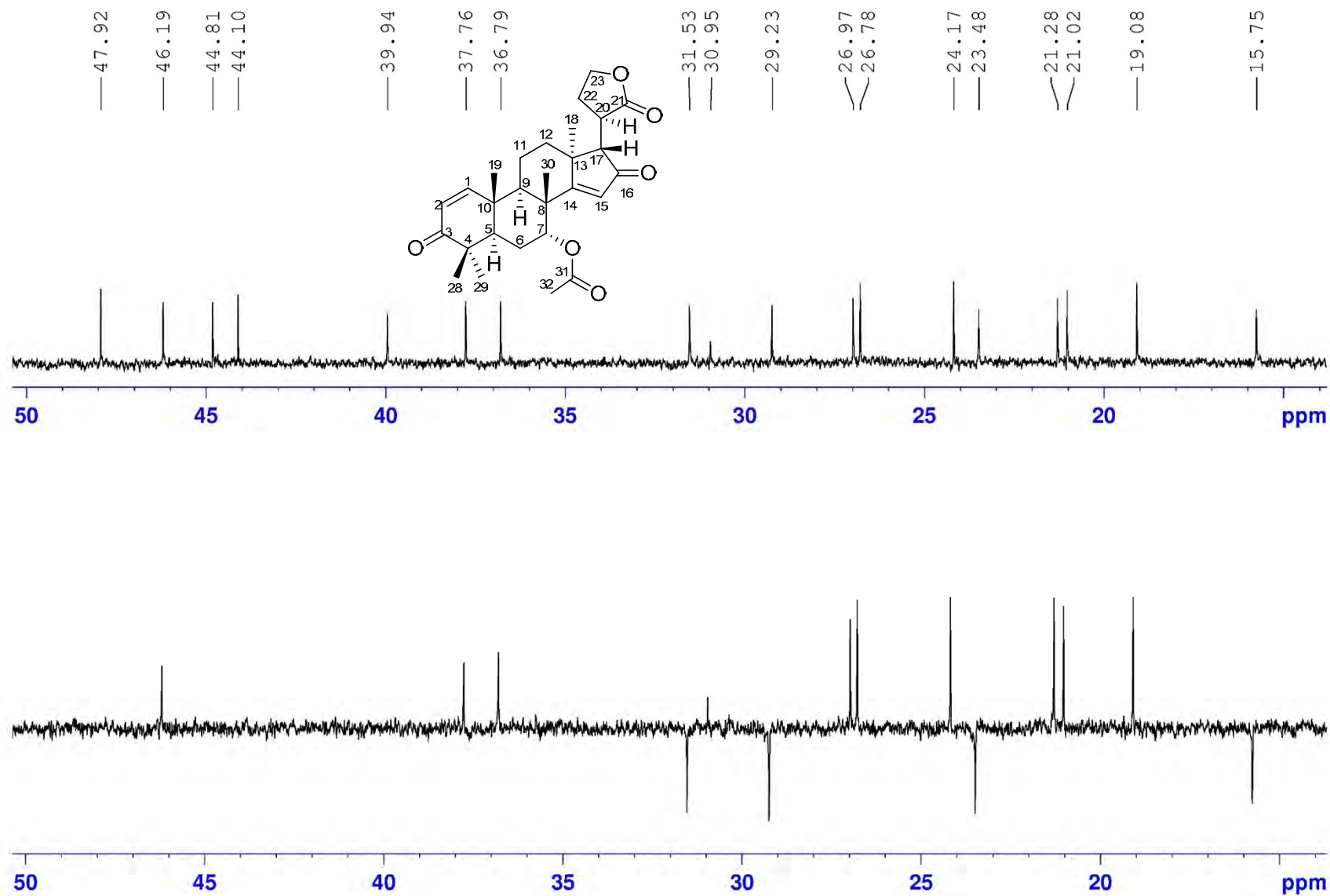
```

===== CHANNEL f1 =====
SFO1         100.6233324 MH
NUC1          13C
P1            10.00 us
P13           2000.00 us
SI            32768
SF            100.6127694 MH
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

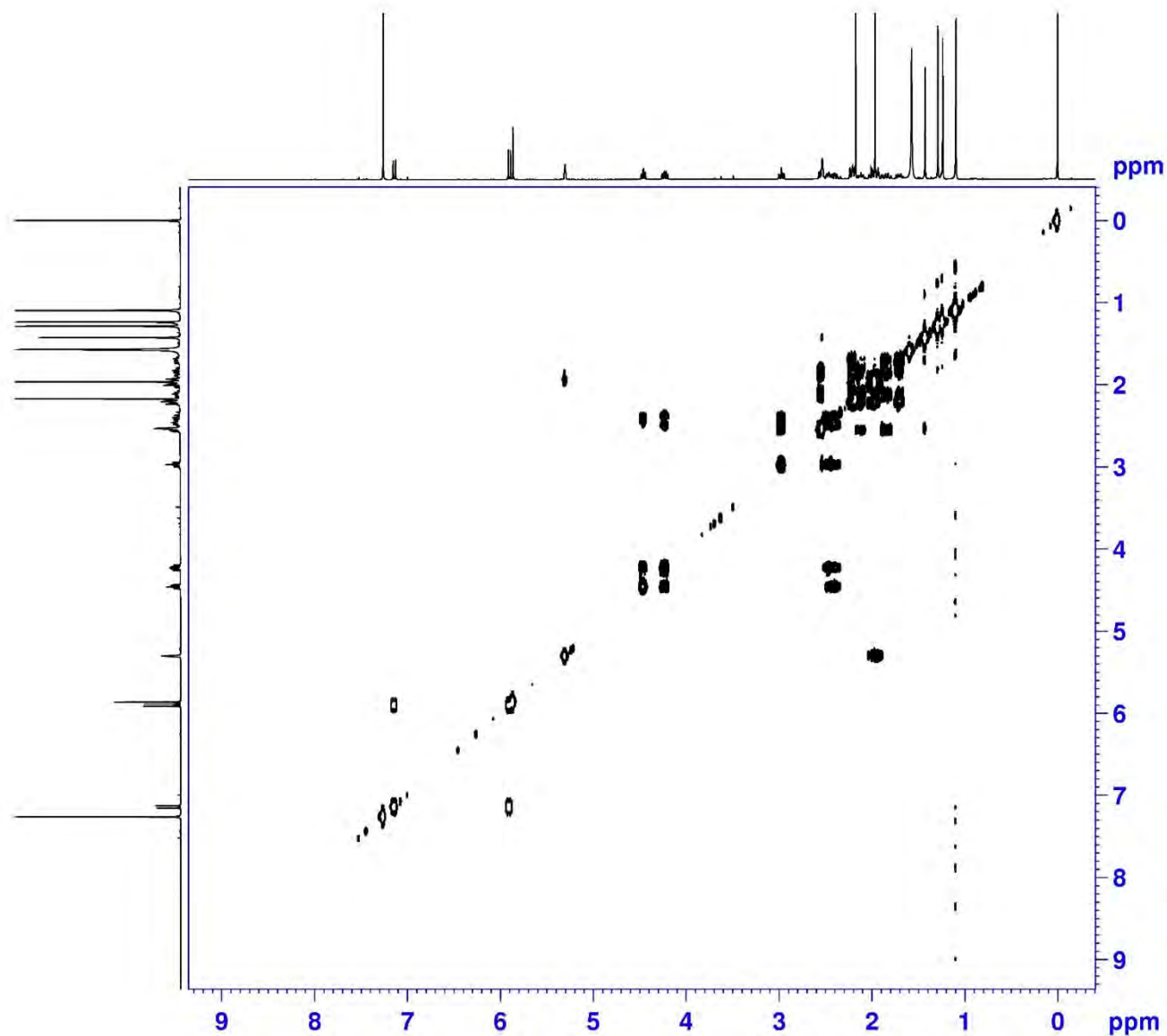
DEPT135 (100 MHz) spectrum of compound **28** in CDCl₃



DEPT135 (100 MHz) spectrum of compound **28** in CDCl₃



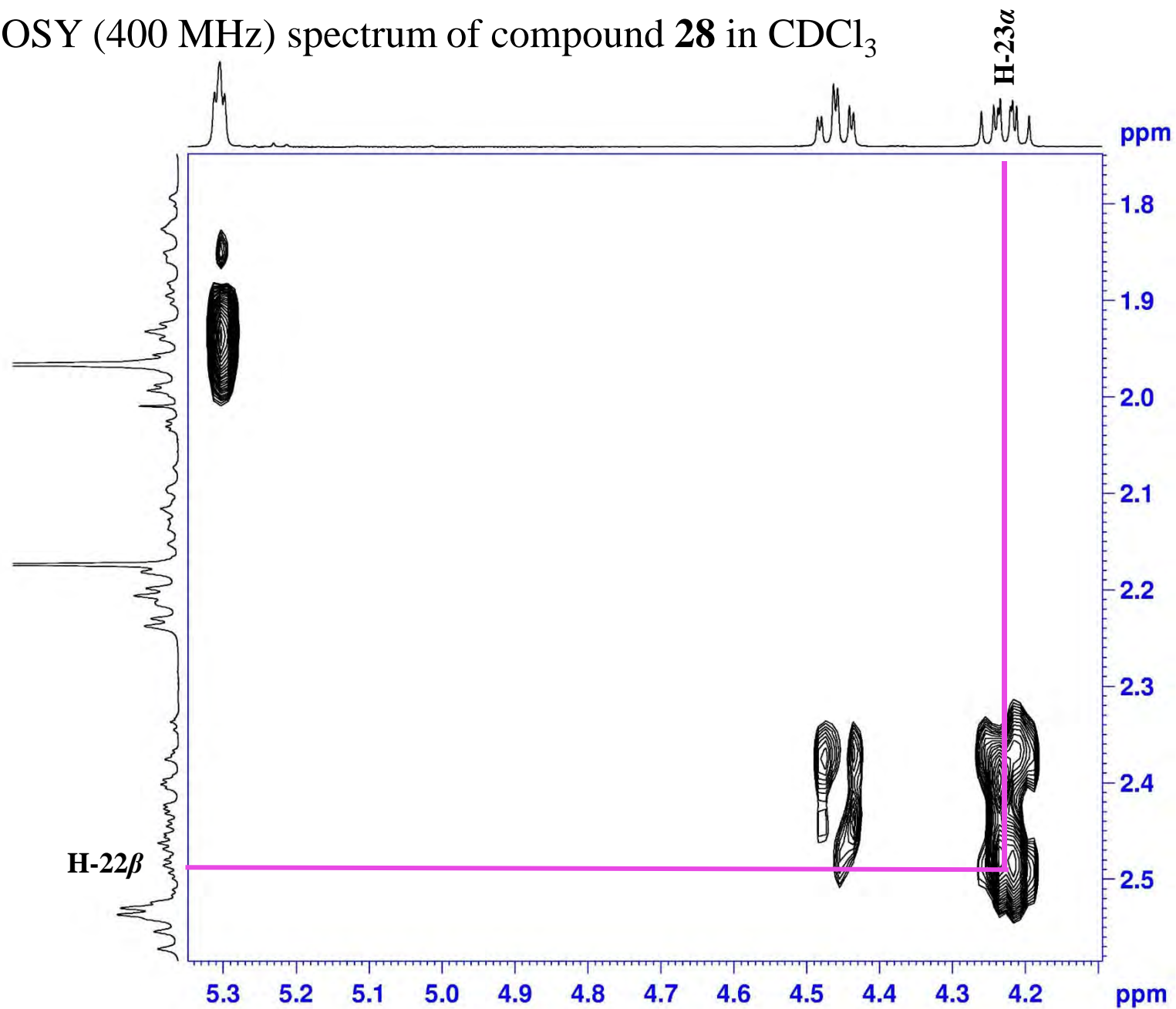
^1H - ^1H COSY (400 MHz) spectrum of compound **28** in CDCl_3



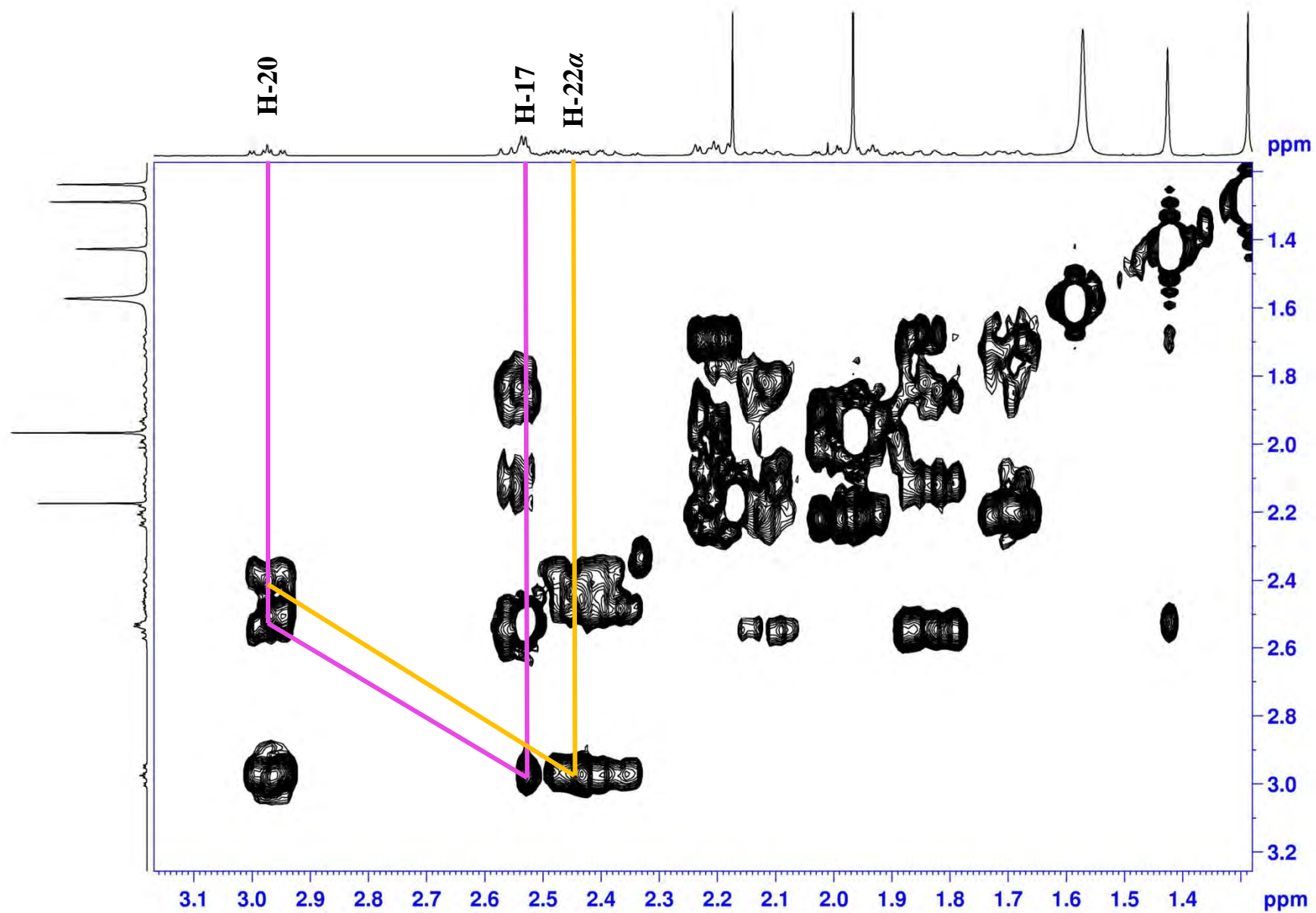
NAME zjz-23
EXPNO 4
PROCNO 1
Date_ 20160618
Time 0.02
INSTRUM spect
PROBHD 5 mm CPMBO BB
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl_3
NS 16
DS 8
SWH 3906.250 Hz
FIDRES 1.907349 Hz
AQ 0.2621940 sec
RG 208.5
DW 128.000 usec
DE 10.00 usec
TE 297.0 K
D0 0.00000300 sec
D1 1.89678097 sec
D11 0.03000000 sec
D12 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 400.1300089 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 400.1300089 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0

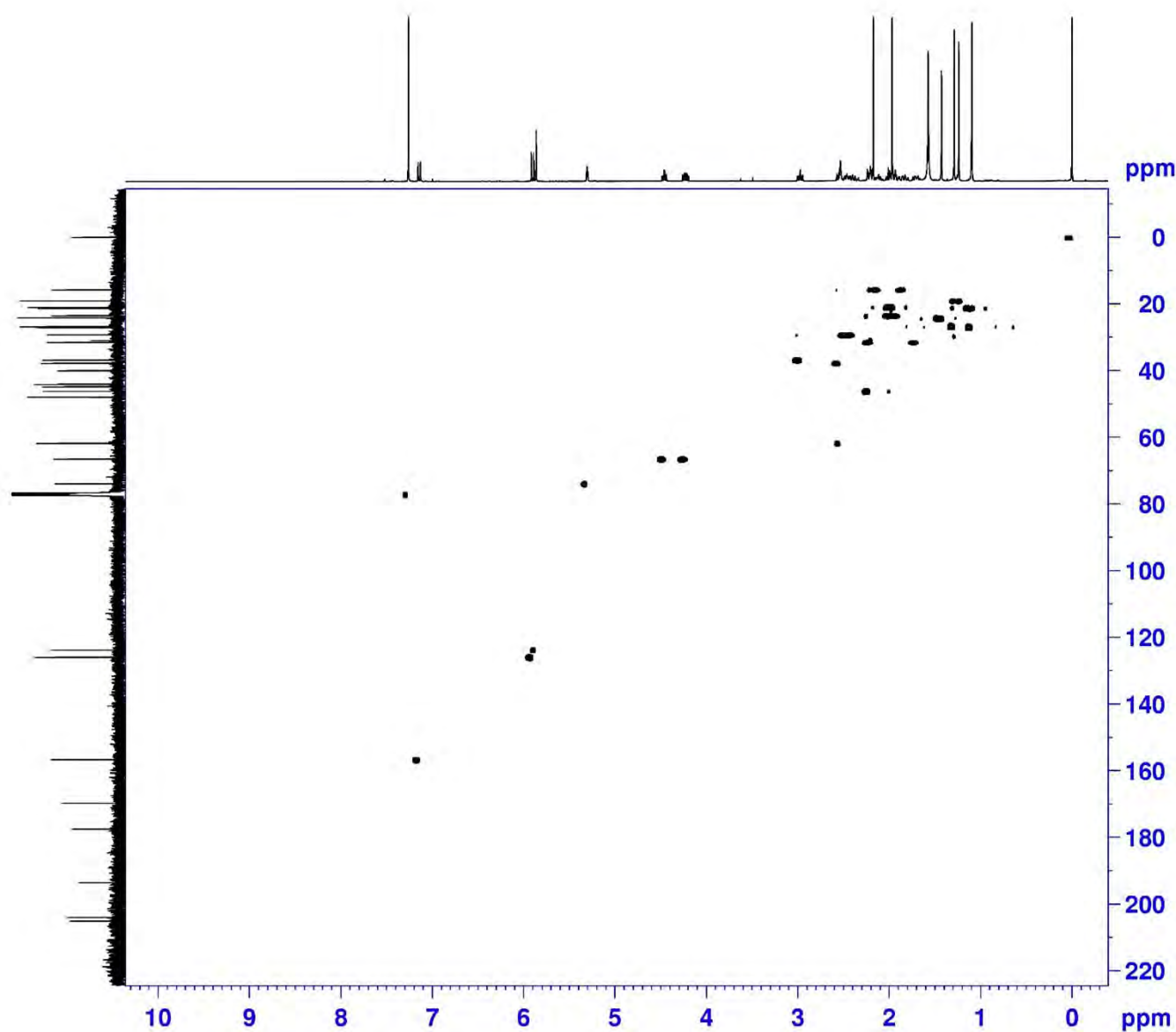
^1H - ^1H COSY (400 MHz) spectrum of compound **28** in CDCl_3



^1H - ^1H COSY (400 MHz) spectrum of compound **28** in CDCl_3



HSQC (400 MHz) spectrum of compound **28** in CDCl₃



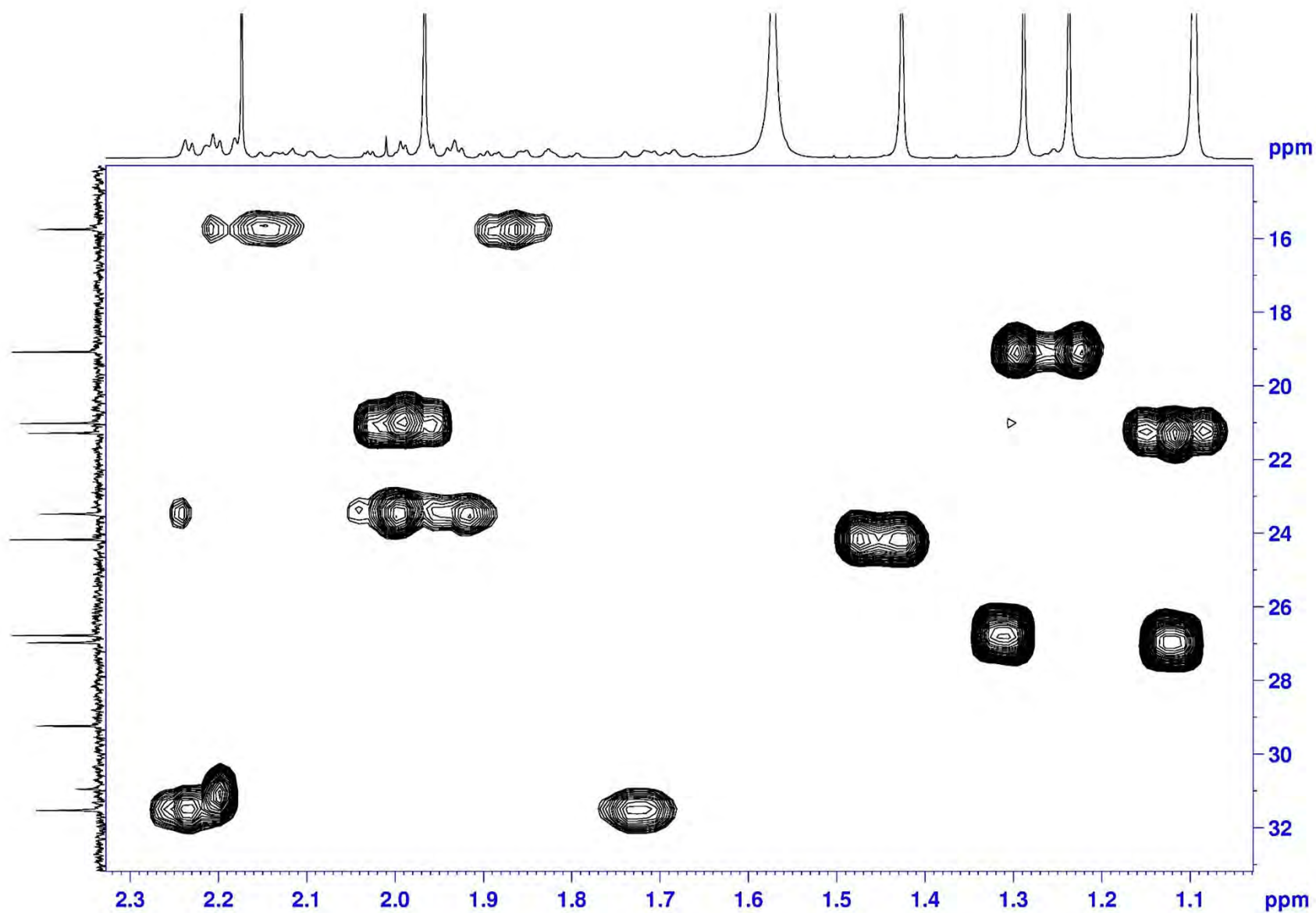
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NAME          zjz-23
EXPNO         5
PROCNO        1
Date_         20160618
Time          1.19
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       hsqcetgpsi2
TD            1024
SOLVENT       CDCl3
NS            16
DS            16
SWH           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
    
```

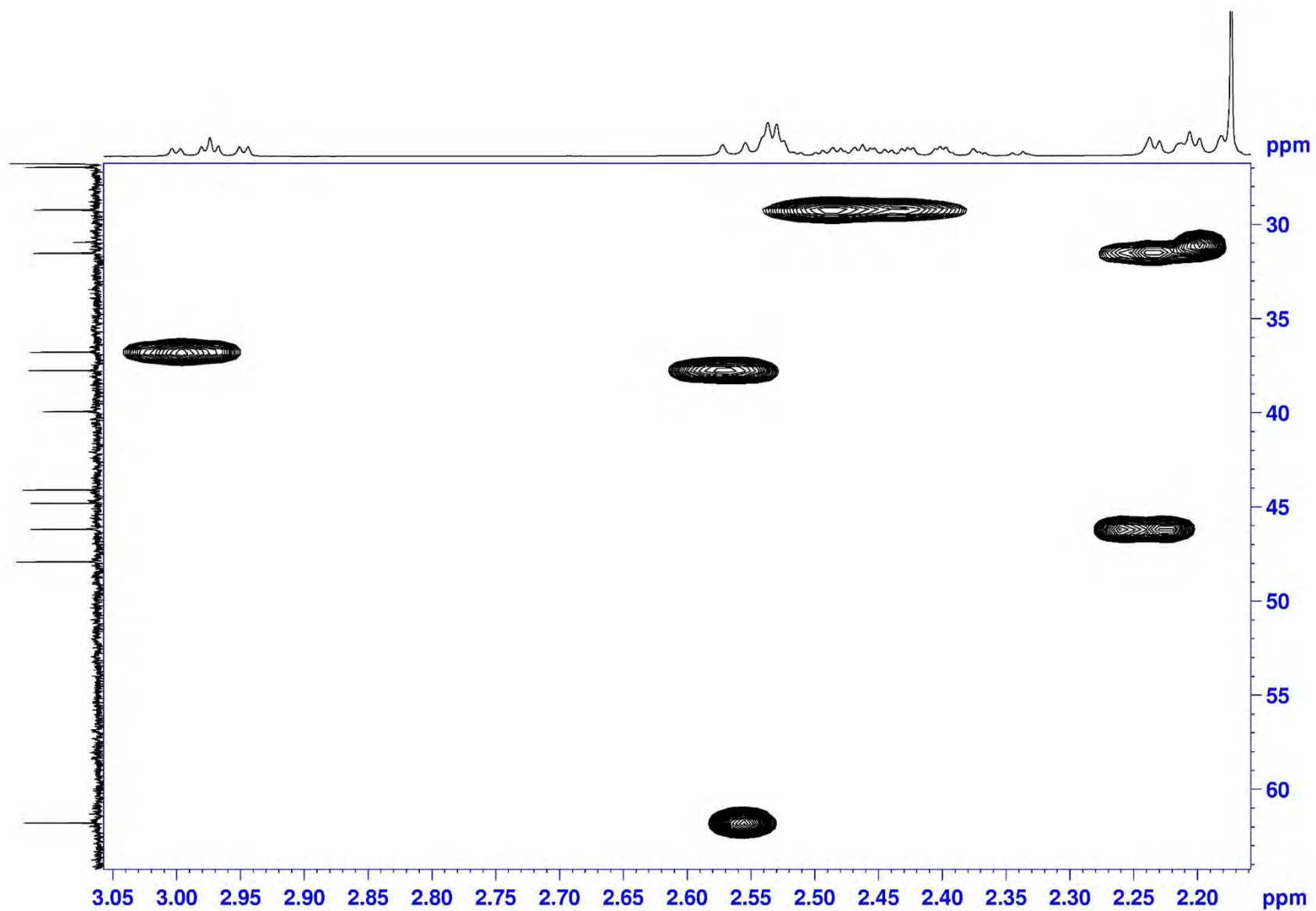
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===== CHANNEL f1 =====
SFO1         400.1320007 MHz
NUC1          1H
P1            11.50 usec
P2            23.00 usec
P28           0.00 usec
ND0           2
TD            256
SFO1         100.6233 MHz
FIDRES        93.900238 Hz
SW            238.896 ppm
FnMODE       Echo-Antiecho
SI            1024
SF            400.1299972 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2          echo-antiecho
SF            100.6127578 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
    
```

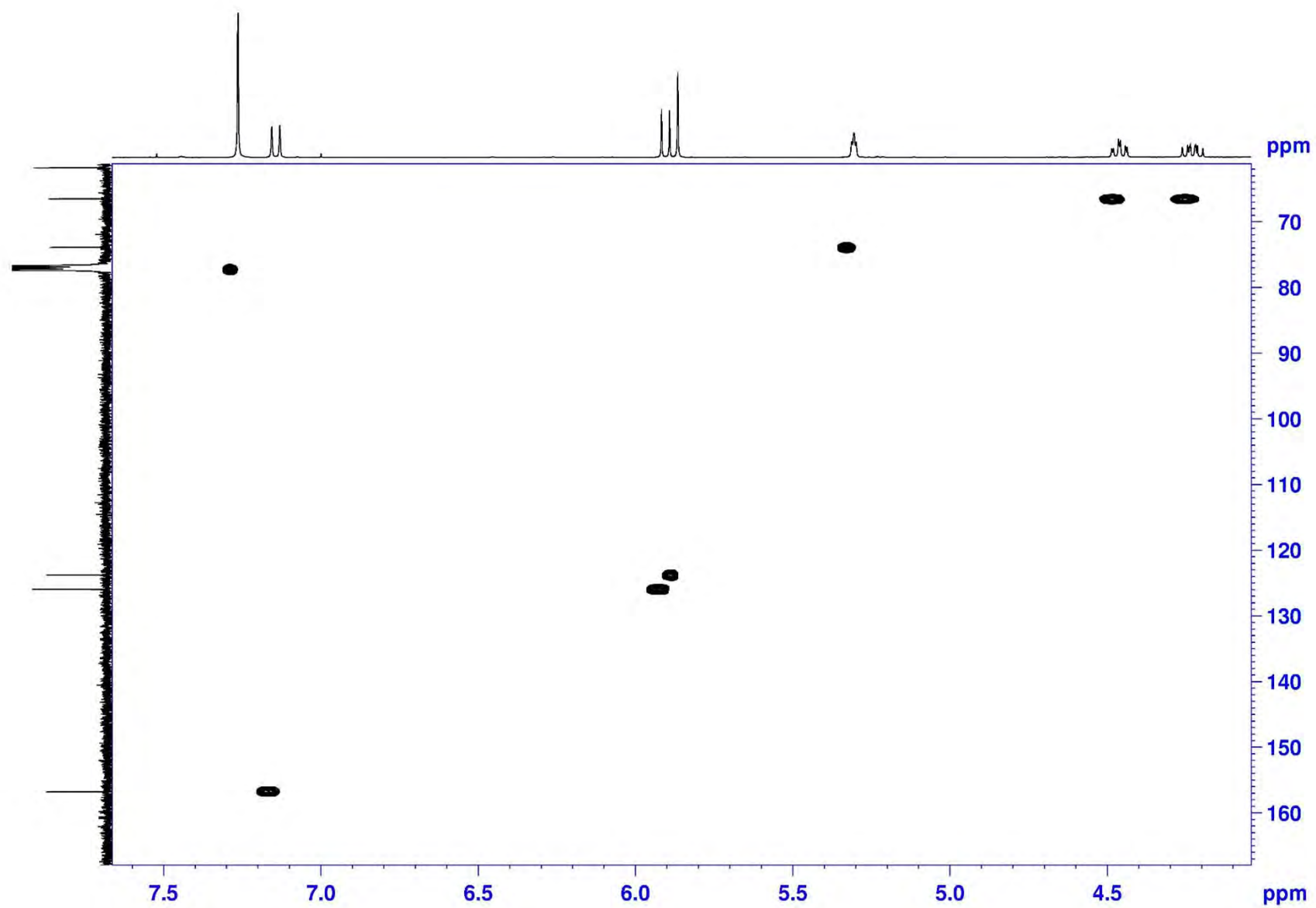
HSQC (400 MHz) spectrum of compound **28** in CDCl₃



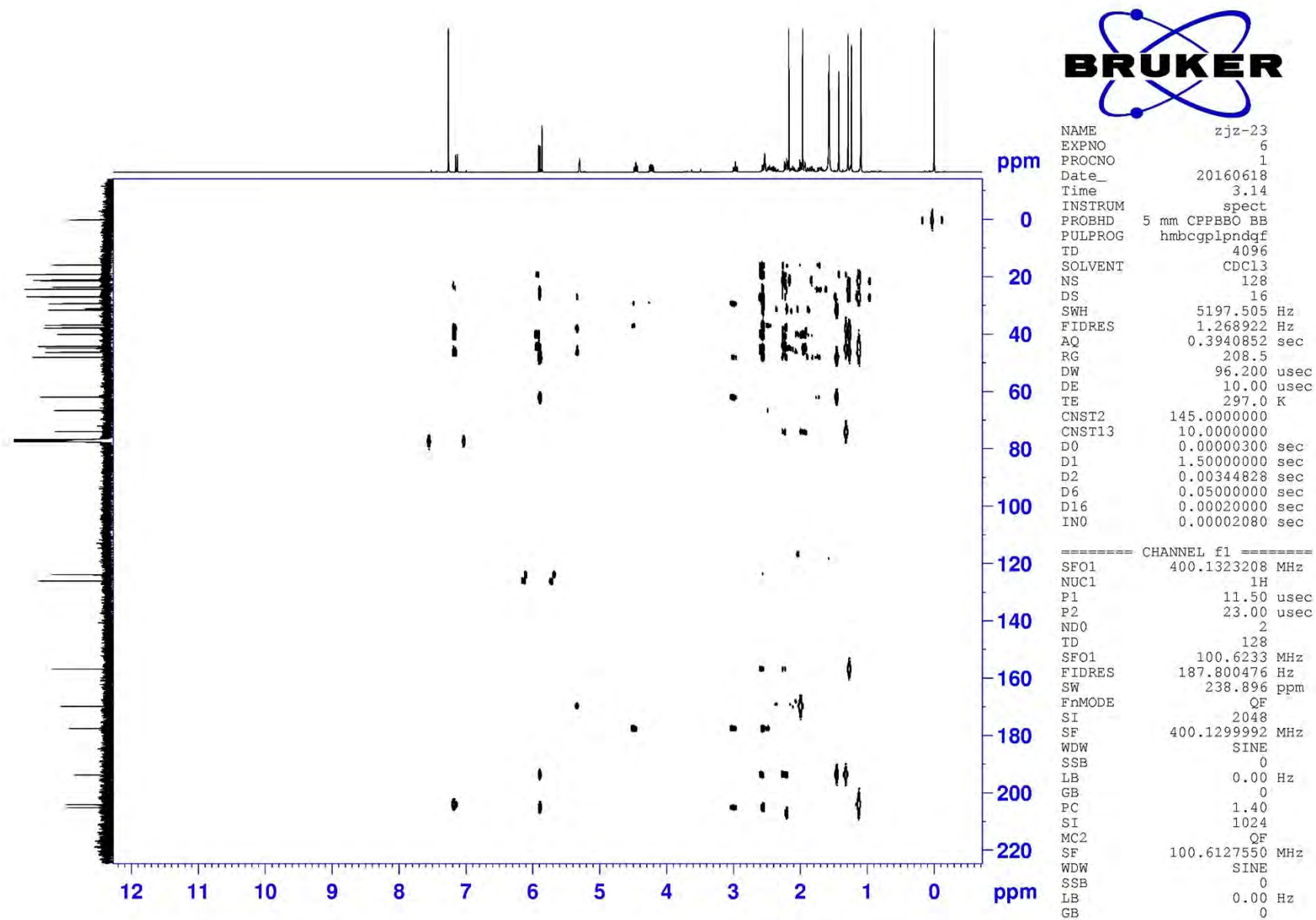
HSQC (400 MHz) spectrum of compound **28** in CDCl₃



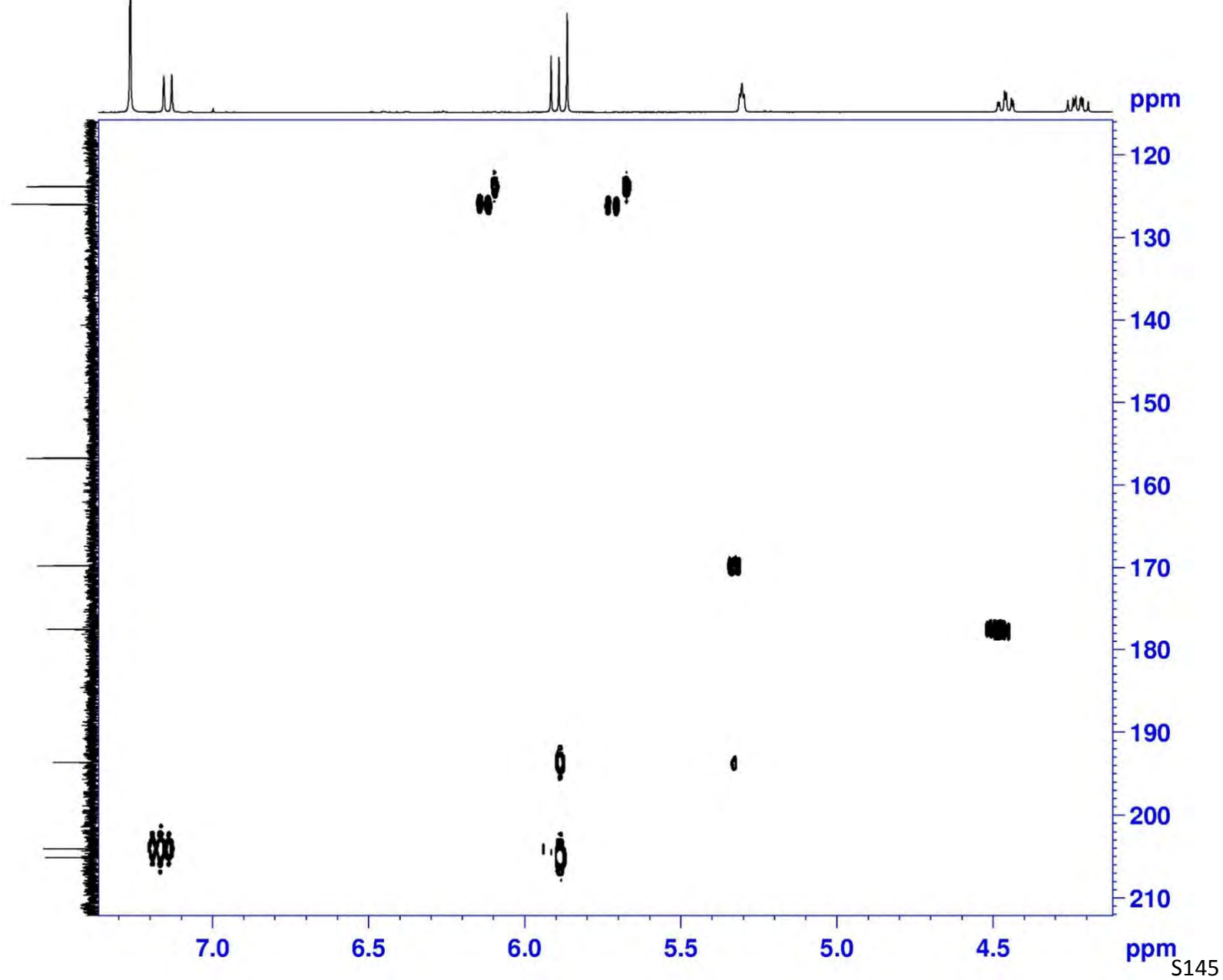
HSQC (400 MHz) spectrum of compound **28** in CDCl₃



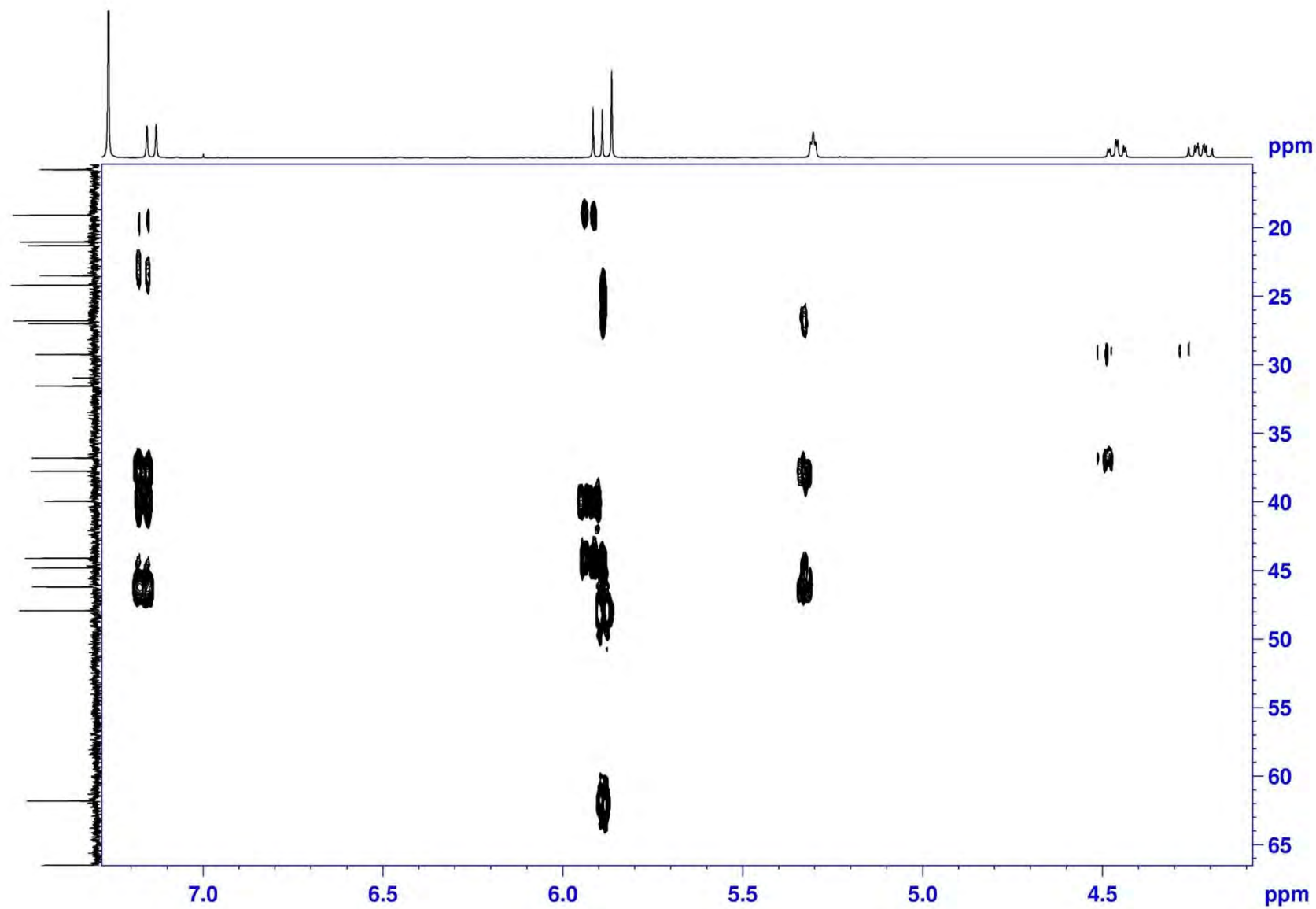
HMBC (400 MHz) spectrum of compound **28** in CDCl₃



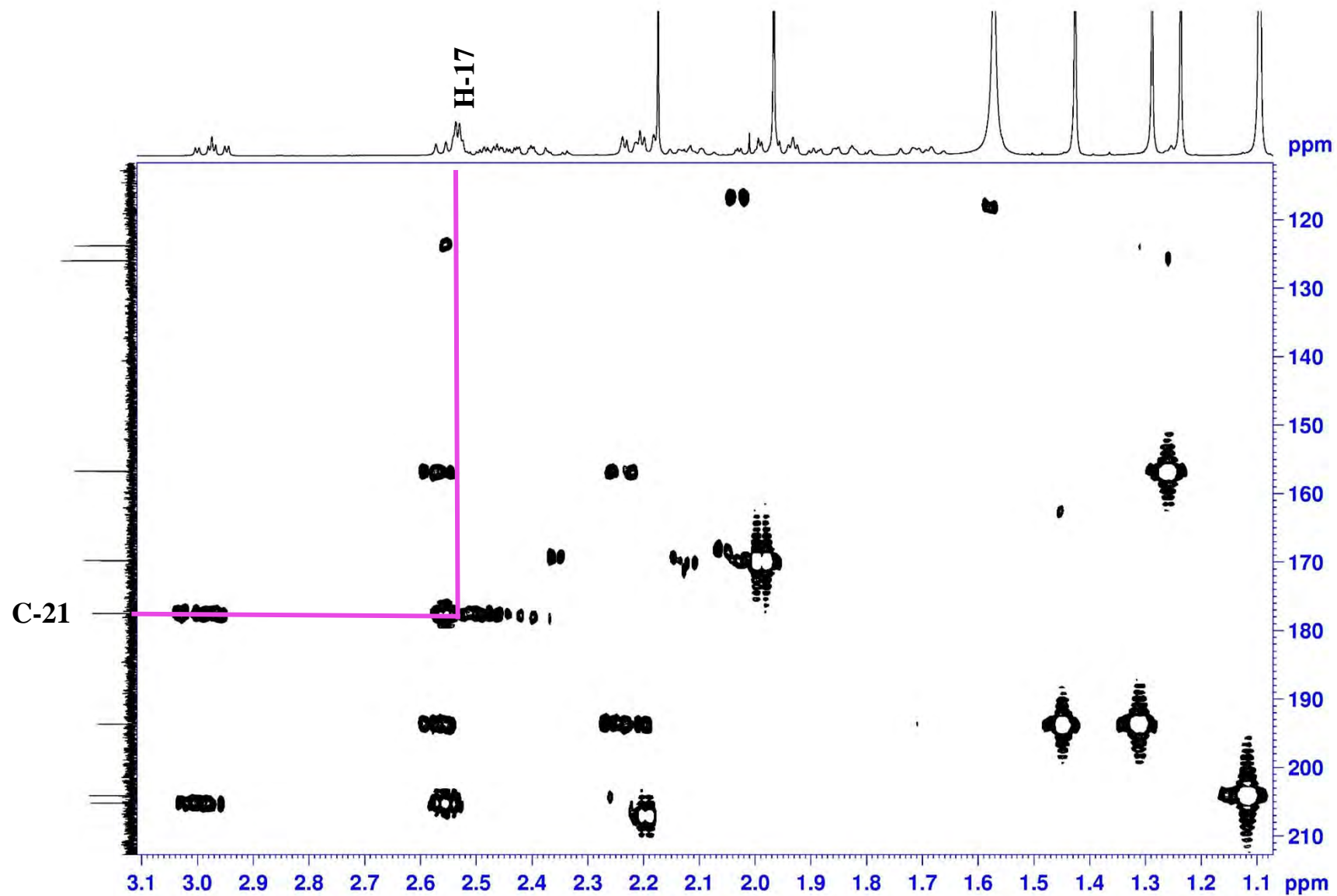
HMBC (400 MHz) spectrum of compound **28** in CDCl_3



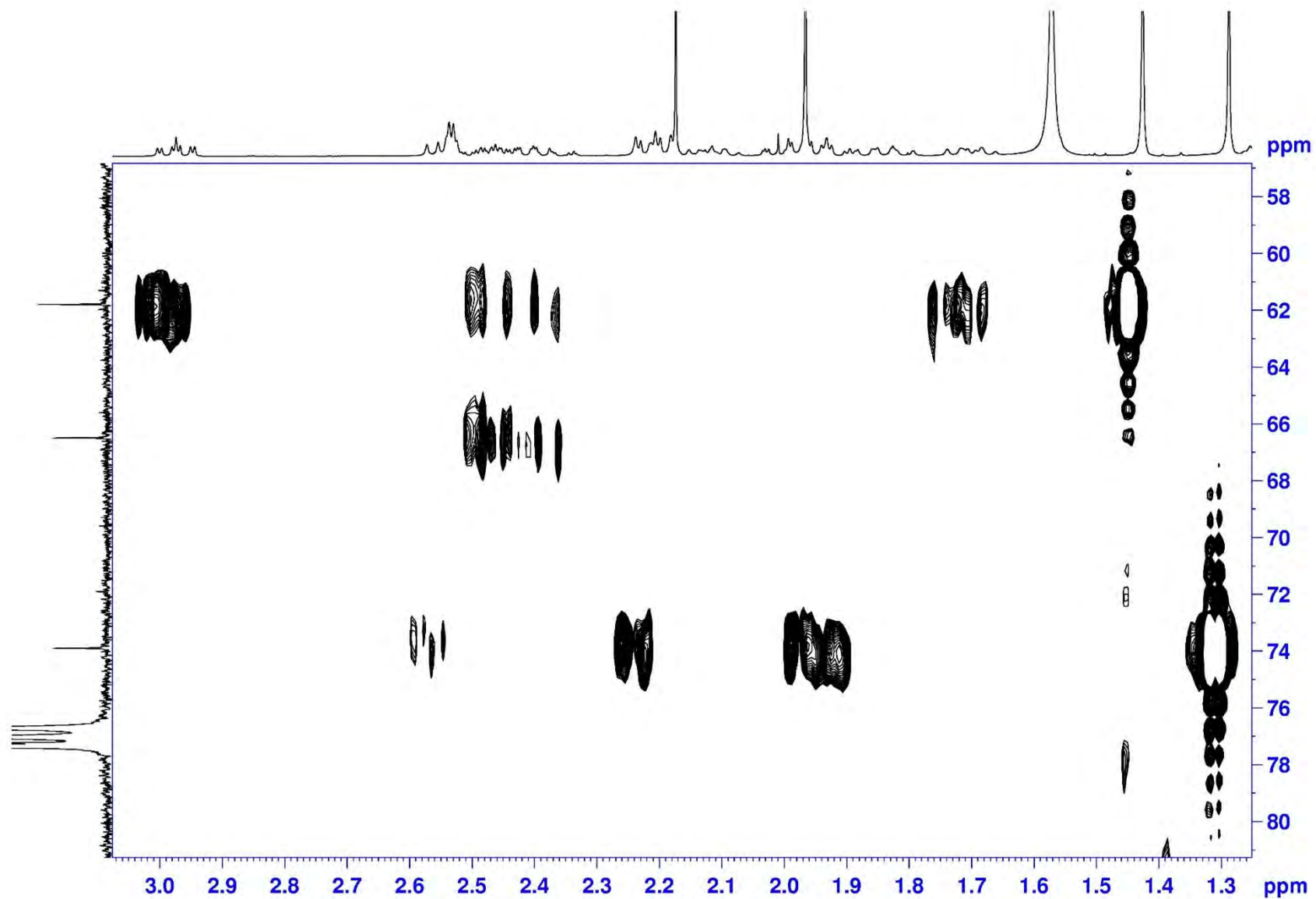
HMBC (400 MHz) spectrum of compound **28** in CDCl_3



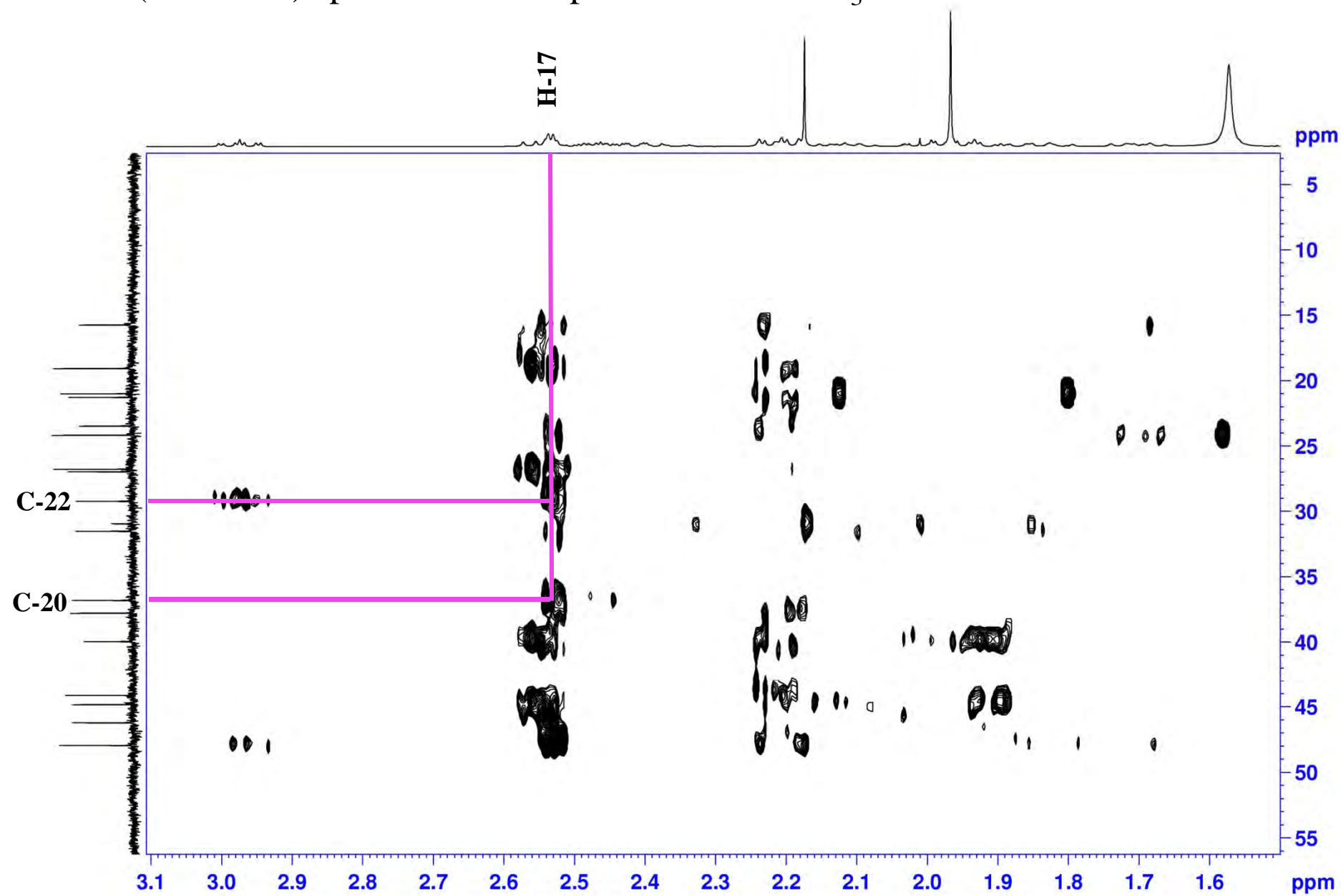
HMBC (400 MHz) spectrum of compound **28** in CDCl_3



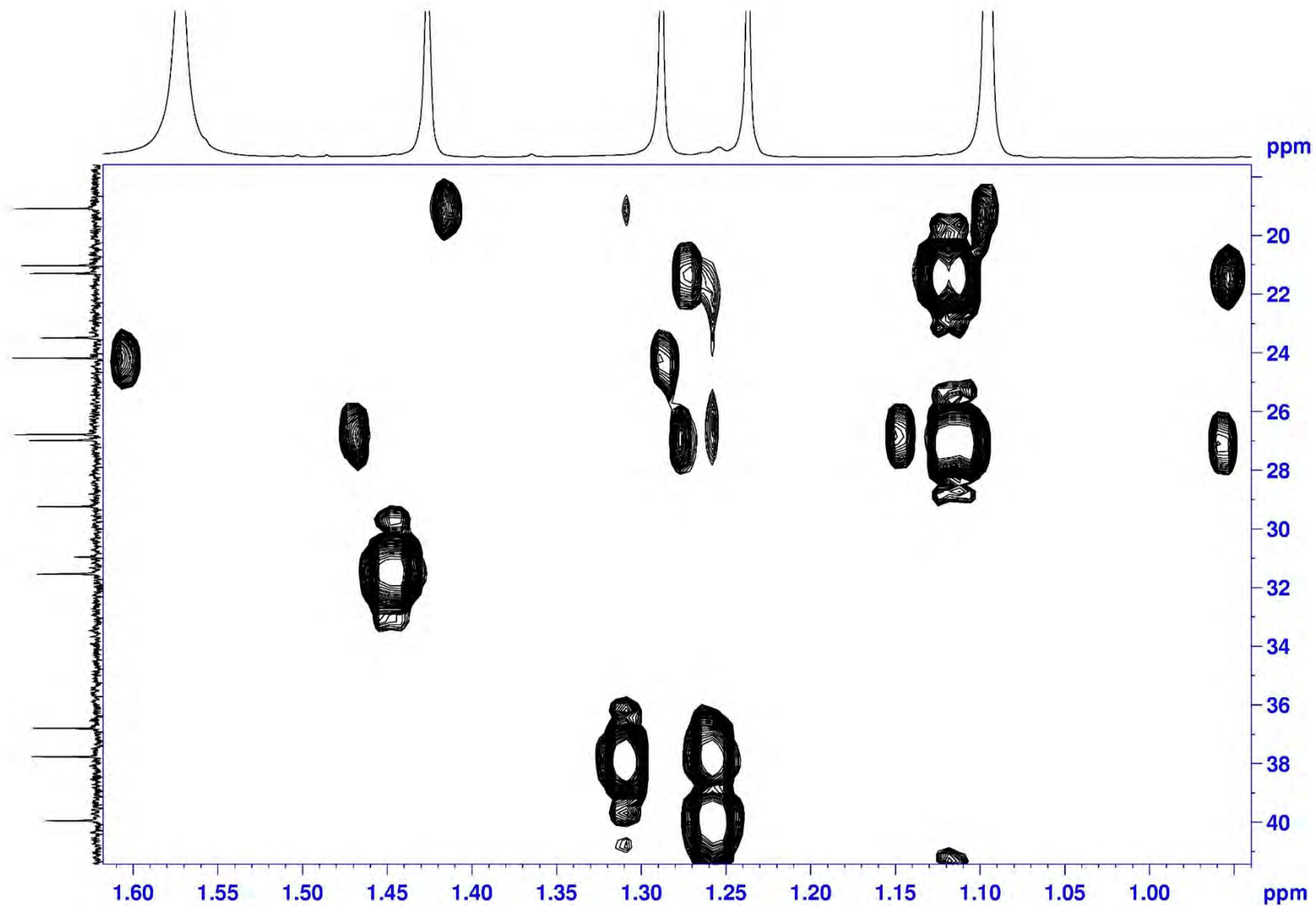
HMBC (400 MHz) spectrum of compound **28** in CDCl_3



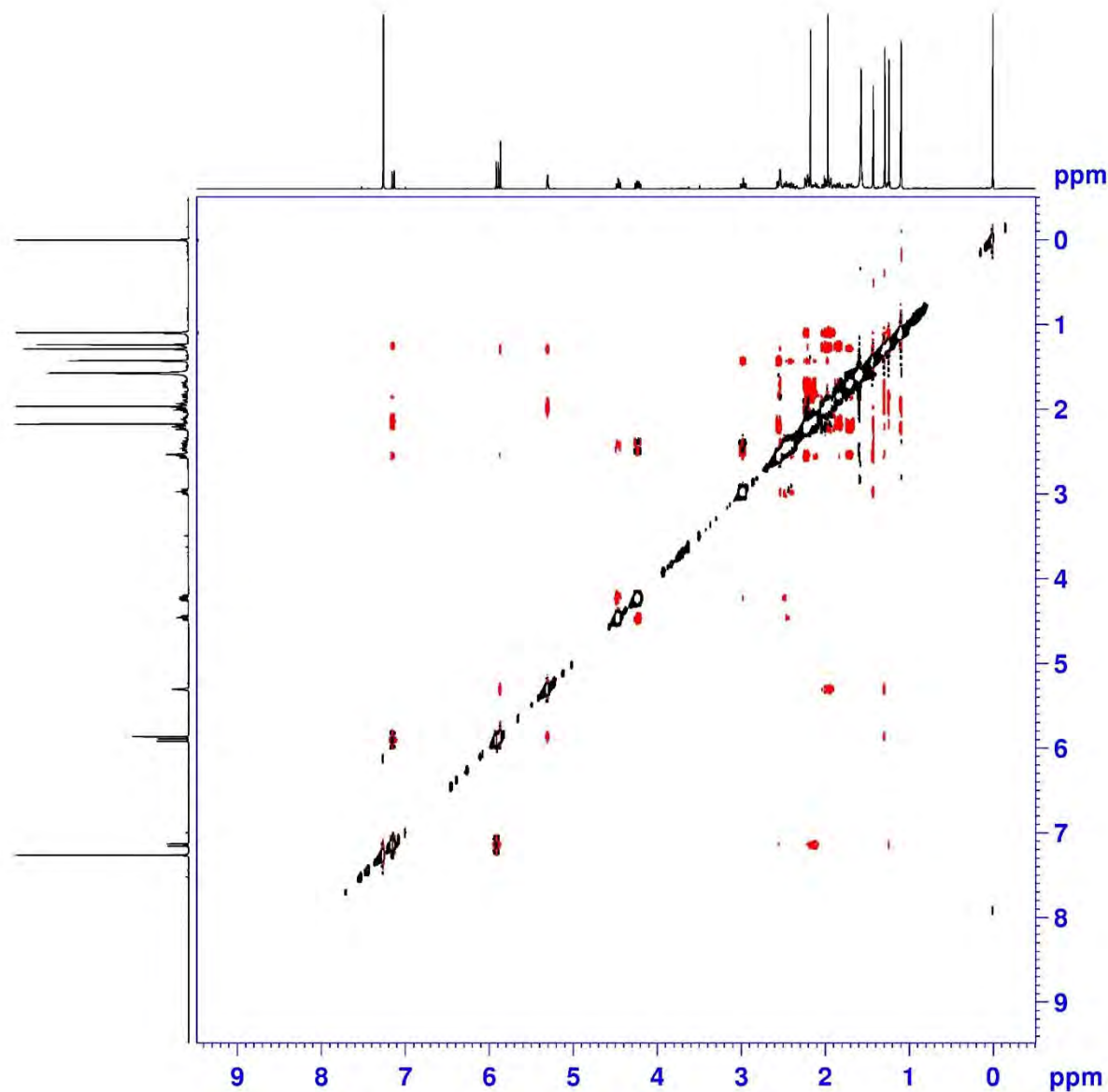
HMBC (400 MHz) spectrum of compound **28** in CDCl_3



HMBC (400 MHz) spectrum of compound **28** in CDCl_3



NOESY (400 MHz) spectrum of compound **28** in CDCl₃



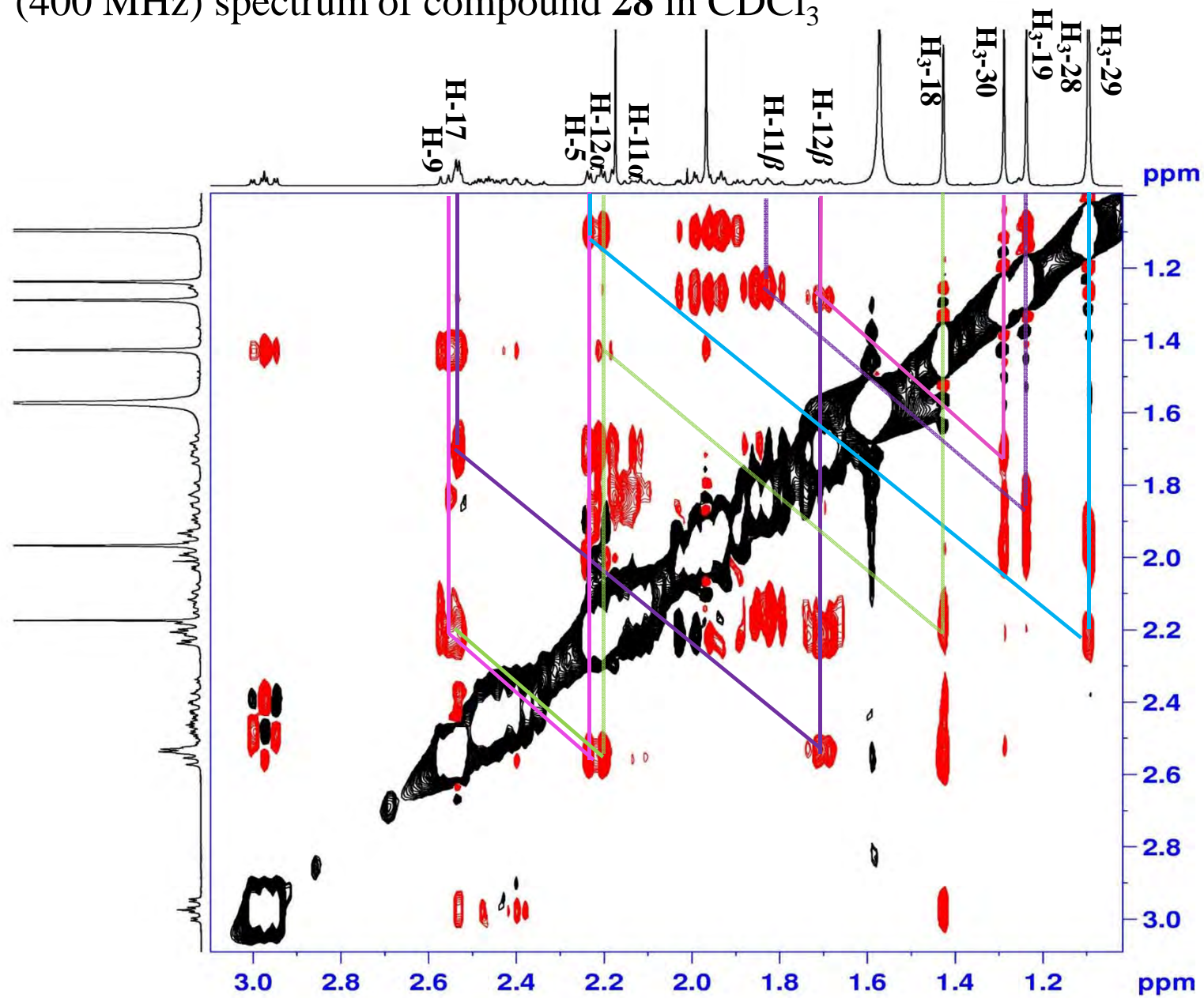
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EXPNO          7
PROCNO         1
Date_         20160618
Time          12.07
INSTRUM        spect
PROBHD         5 mm CFPBBO BB
PULPROG        noesygpphpp
TD            2048
SOLVENT        CDCl3
NS             32
DS             32
SWH            4000.000 Hz
FIDRES         1.953125 Hz
AQ            0.2560500 sec
RG             208.5
DW            125.000 usec
DE             10.00 usec
TE            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
    
```

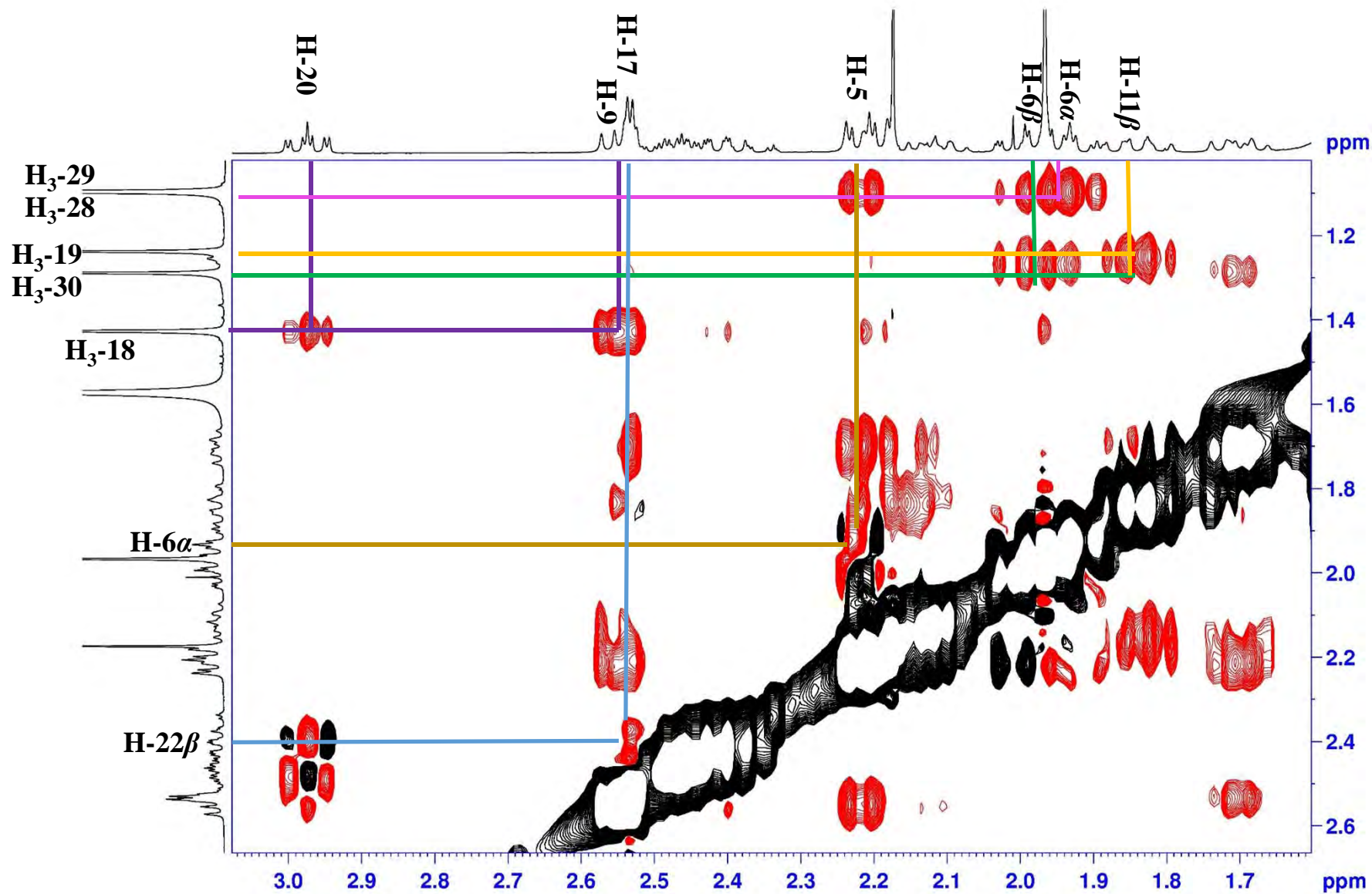
```

===== 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            400.1300070 MHz
WDW            QSINE
SSB            2
LB             0.00 Hz
GB             0
PC             1.00
SI            1024
MC2            States-TPPI
SF            400.1300065 MHz
WDW            QSINE
SSB            2
LB             0.00 Hz
GB             0
    
```

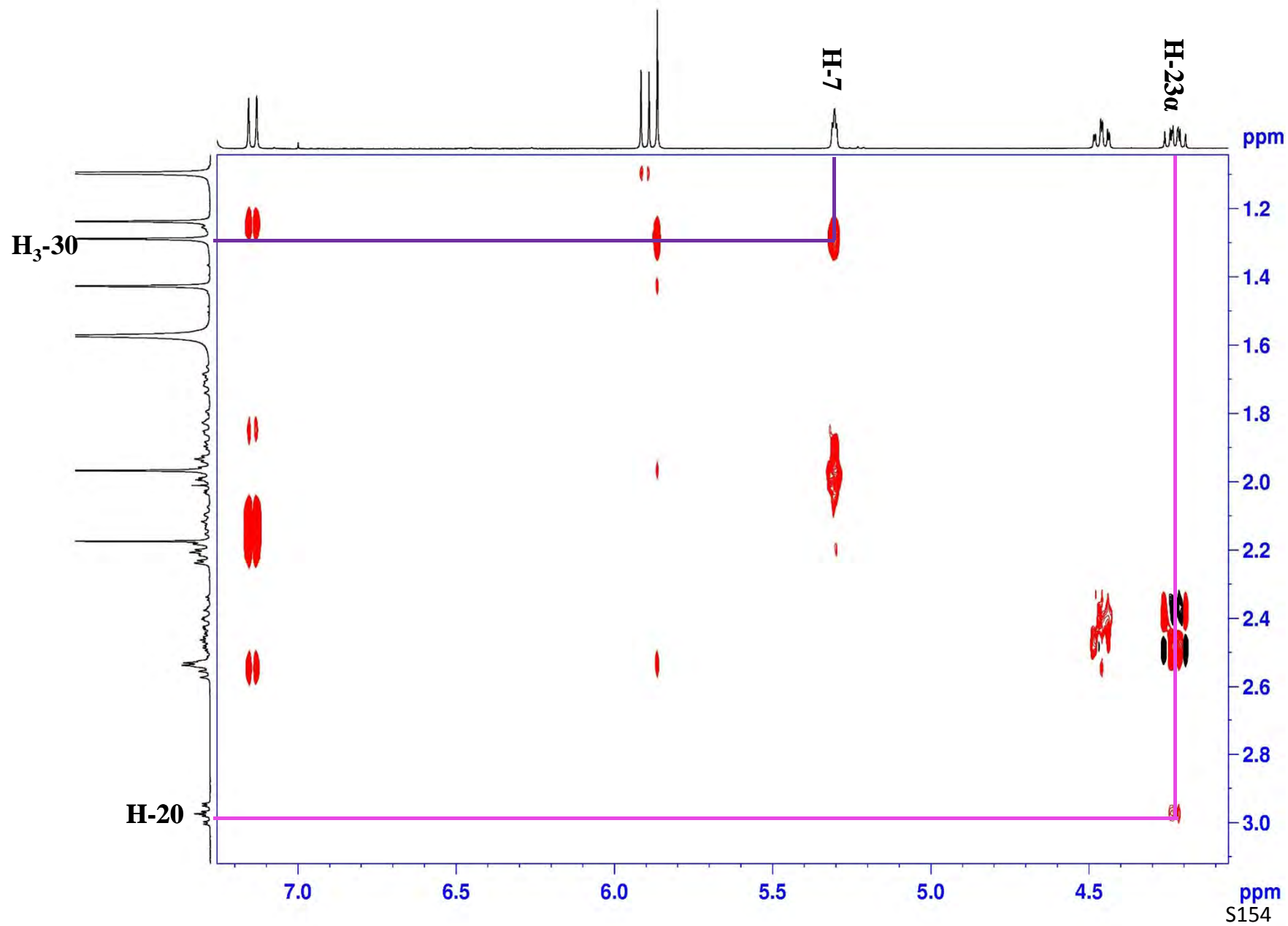

NOESY (400 MHz) spectrum of compound **28** in CDCl₃



NOESY (400 MHz) spectrum of compound **28** in CDCl_3



NOESY (400 MHz) spectrum of compound **28** in CDCl₃



HR-ESIMS for compound 29

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\MS\data\201605\liwanshan_dgy-17_pos_6_01_1854.d
 Method LC_Direct Infusion_pos_100-1000mz.m
 Sample Name liwanshan_dgy-17_pos
 Comment

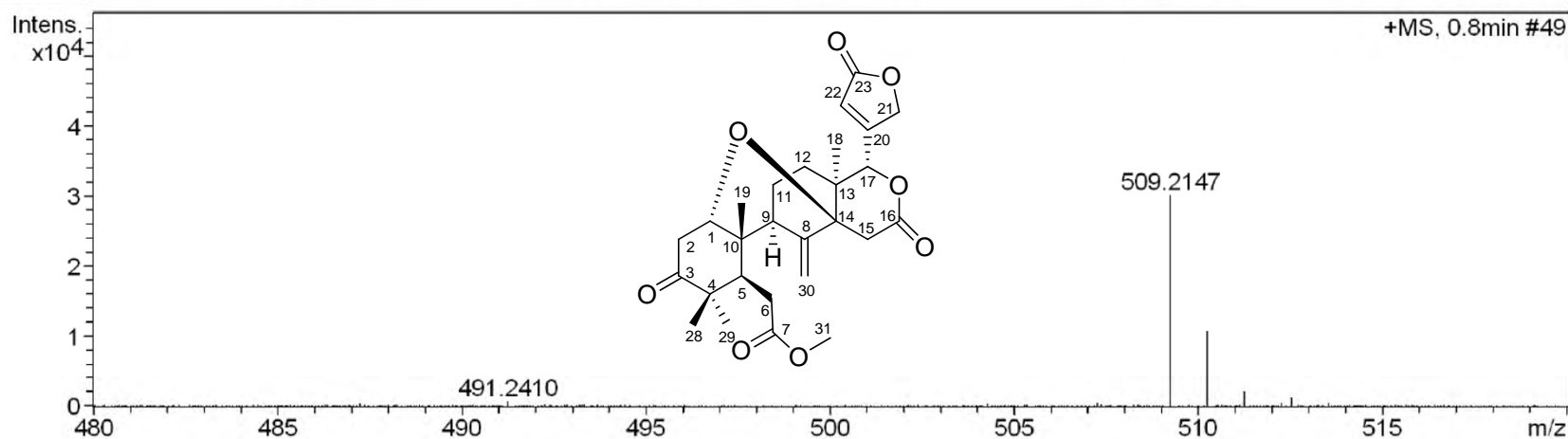
Acquisition Date 5/19/2016 8:37:47 AM

Operator SCSIO

Instrument / Ser# maXis 29

Acquisition Parameter

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



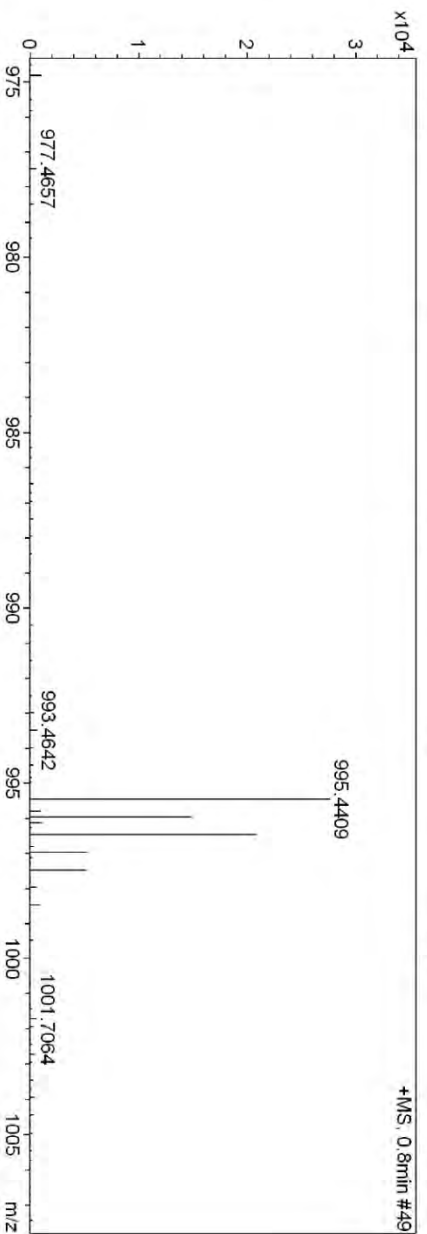
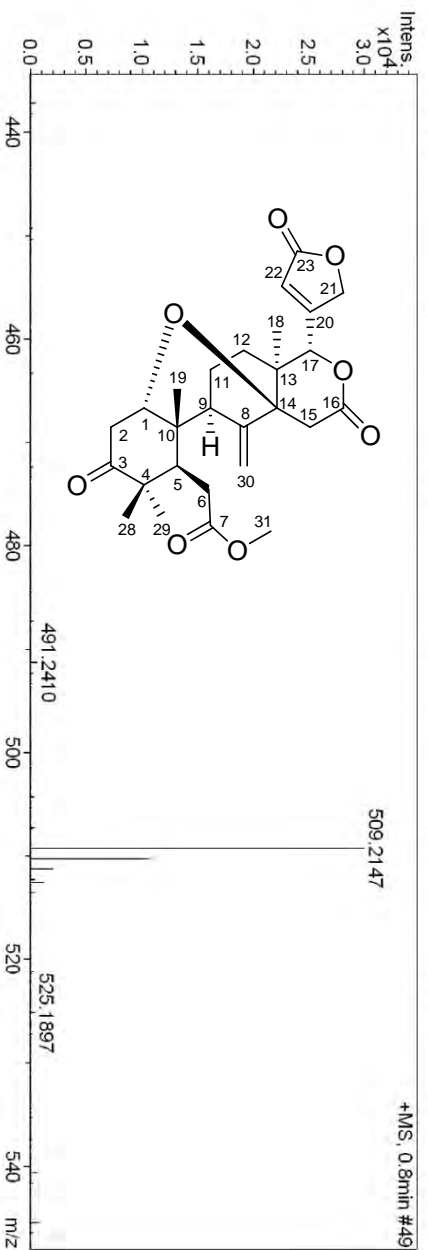
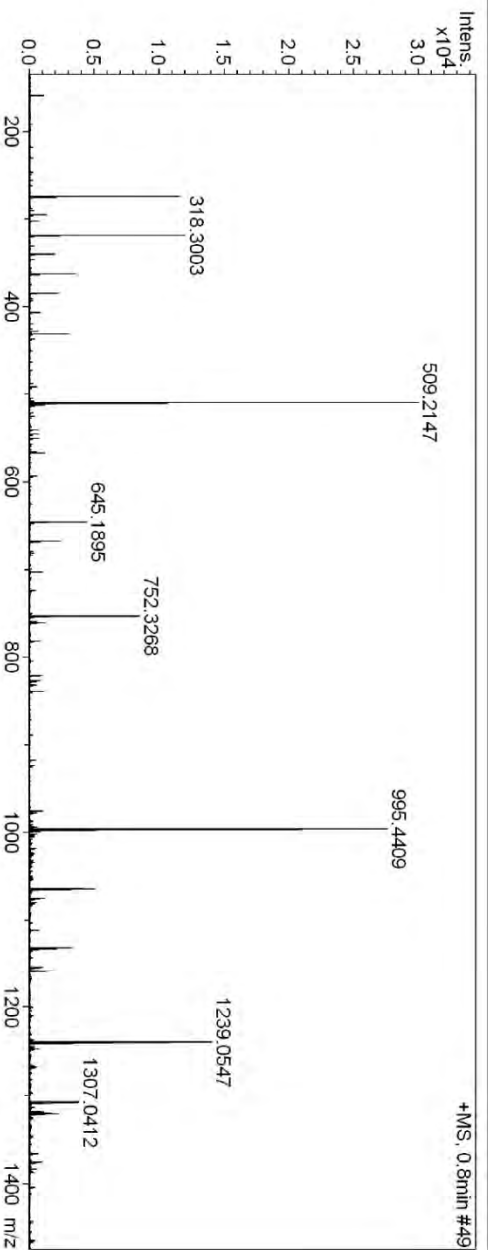
| Meas. m/z | # | Formula | Score | m/z | err [ppm] | err [mDa] | mSigma | rdb | e ⁻ Conf | N-Rule |
|-----------|---|-------------------|--------|----------|-----------|-----------|--------|------|---------------------|--------|
| 487.2327 | 1 | C 27 H 35 O 8 | 100.00 | 487.2326 | -0.0 | -0.0 | 85.1 | 10.5 | even | ok |
| 509.2147 | 1 | C 27 H 34 Na O 8 | 100.00 | 509.2146 | -0.2 | -0.1 | 29.9 | 10.5 | even | ok |
| 995.4409 | 1 | C 54 H 68 Na O 16 | 100.00 | 995.4400 | -0.9 | -0.9 | 71.3 | 20.5 | even | ok |

Generic Display Report

S156

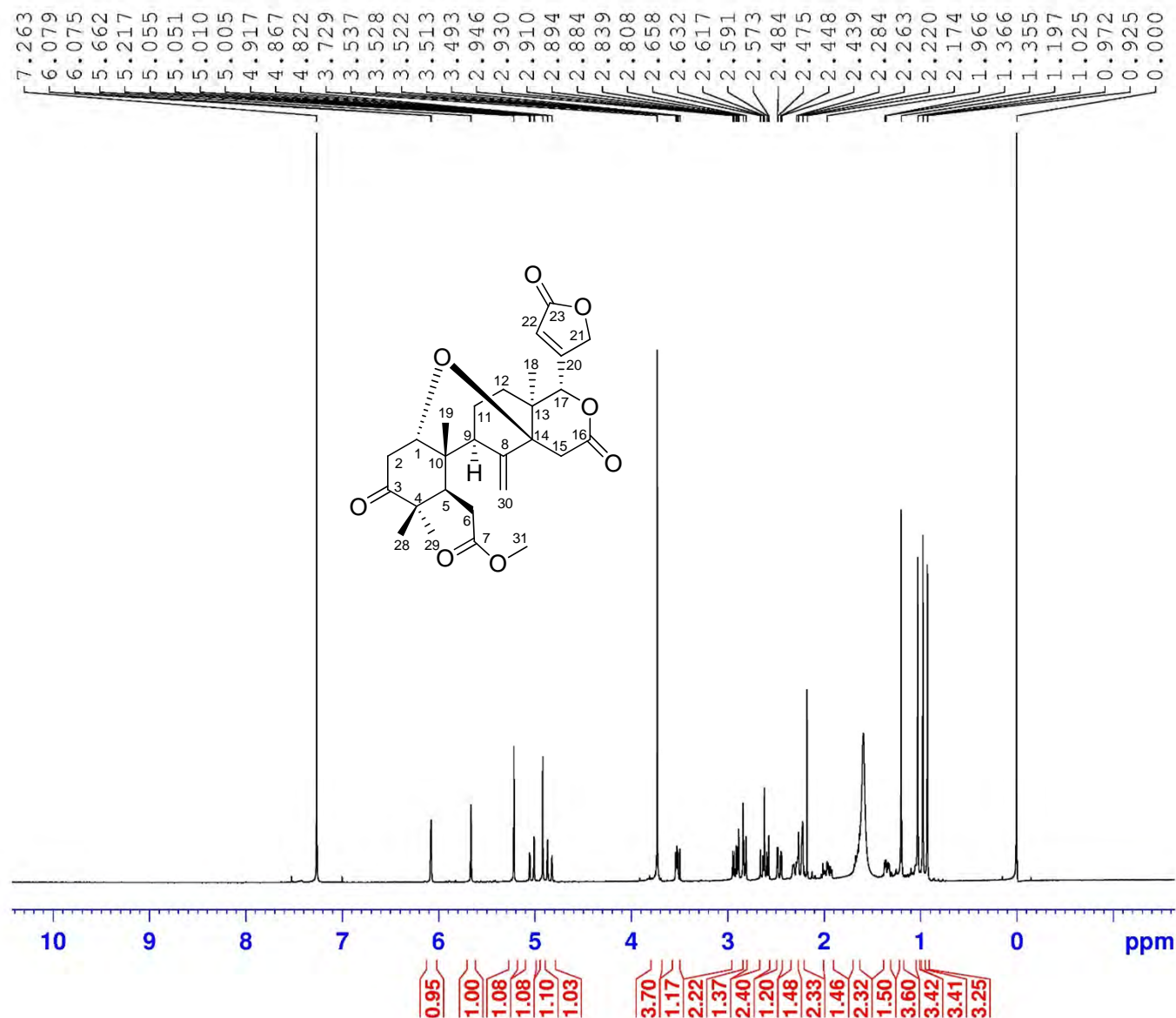
Analysis Info

| | | | |
|---------------|---|------------------|----------------------|
| Analysis Name | D:\Data\MS\data\201605\liwanshan_dgy-17_pos_6_01_1854.d | Acquisition Date | 5/19/2016 8:37:47 AM |
| Method | LC_Direct Infusion_pos_100-1000mz.m | Operator | SCSIO |
| Sample Name | liwanshan_dgy-17_pos | Instrument | maxis |
| Comment | | | |



HR-ESIMS for compound 29

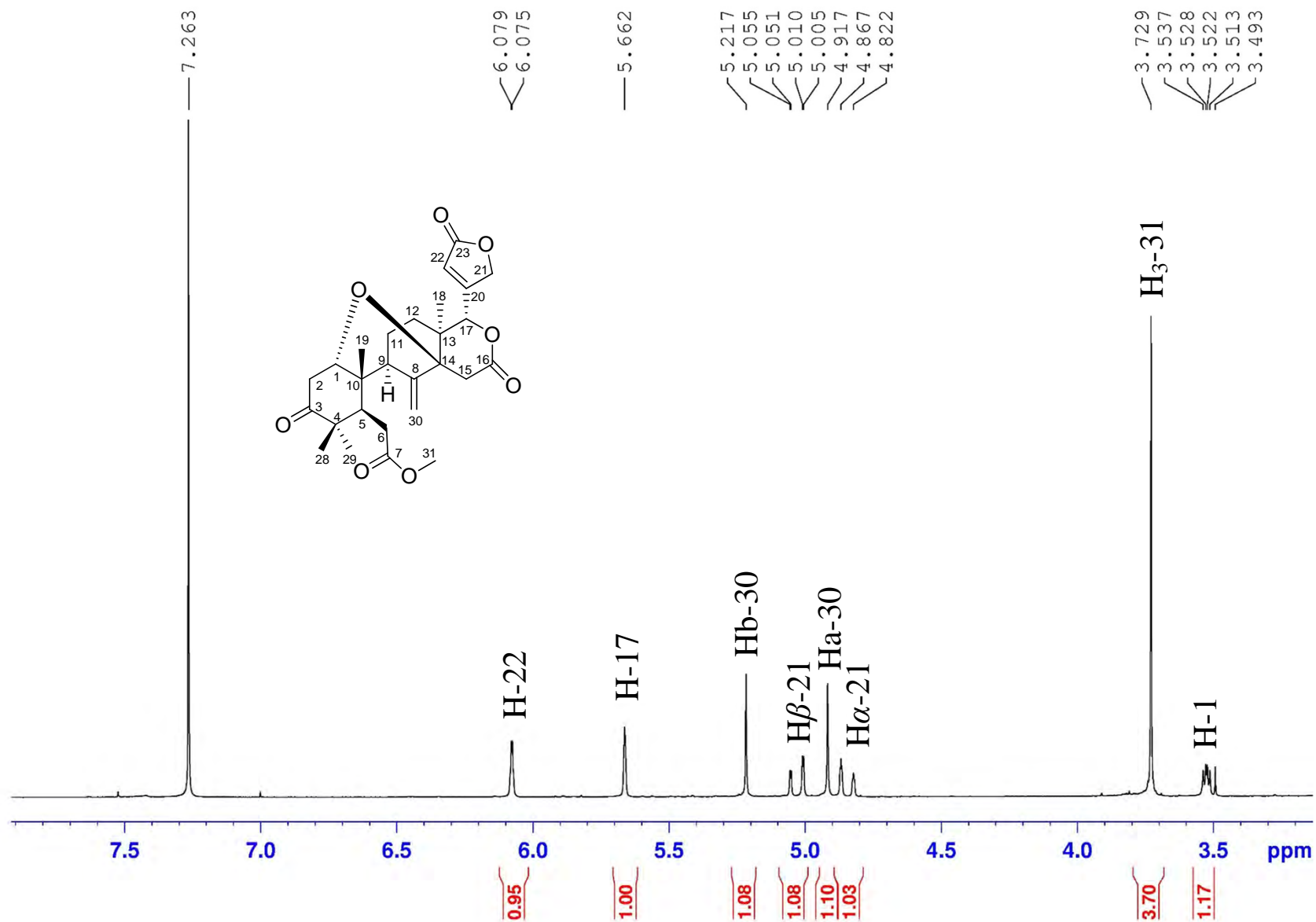
^1H NMR (400 MHz) spectrum of compound **29** in CDCl_3



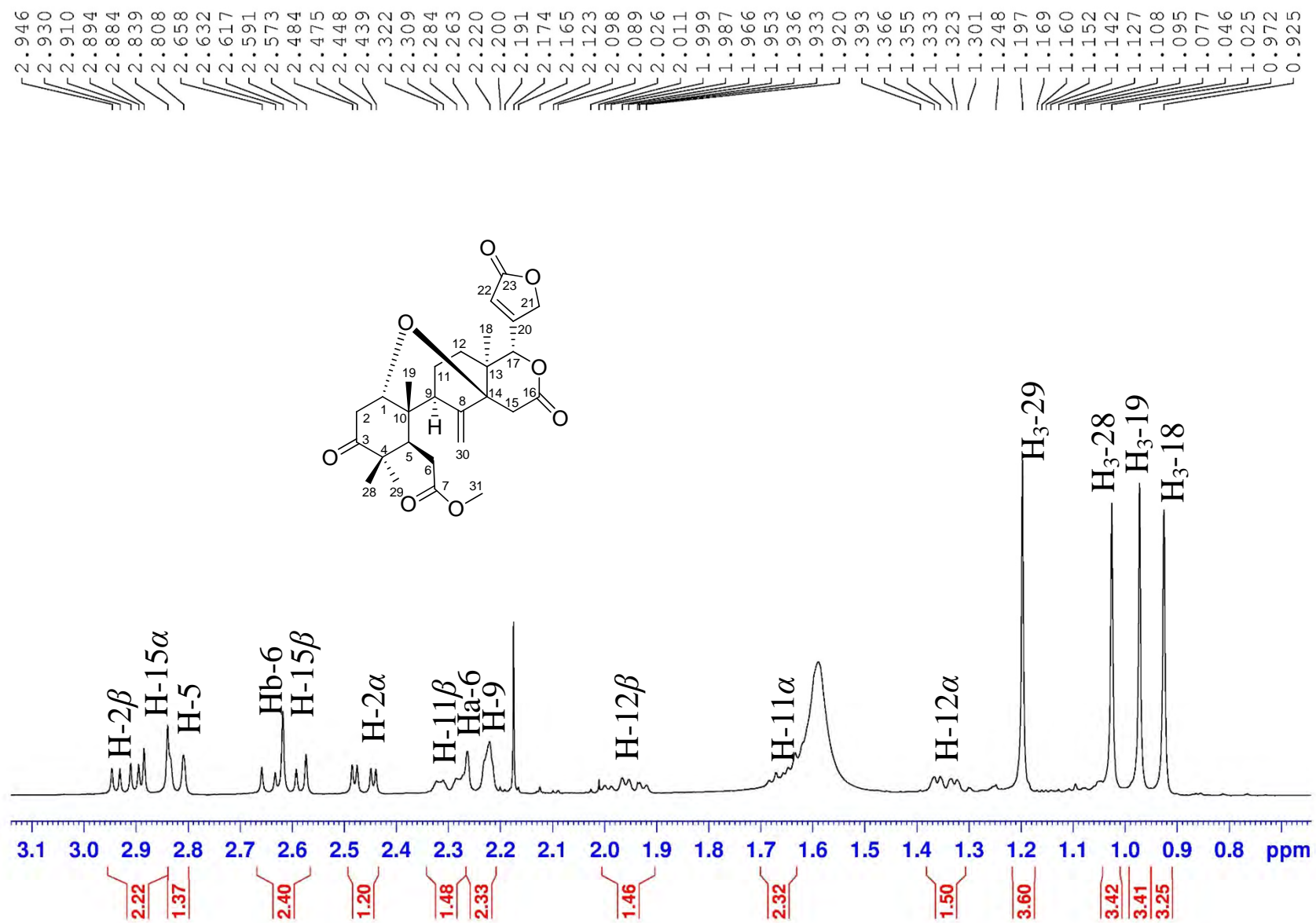
NAME dyg-17
 EXPNO 1
 PROCNO 1
 Date_ 20151105
 Time 4.00
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl_3
 NS 16
 DS 2
 SWH 8223.685 F
 FIDRES 0.125483 F
 AQ 3.9846387 s
 RG 208.5
 DW 60.800 μ
 DE 10.00 μ
 TE 297.0 K
 D1 1.00000000 s
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 M
 NUC1 ^1H
 P1 12.00 μ
 SI 65536
 SF 400.1300083 M
 WDW EM
 SSB 0
 LB 0.30 F
 GB 0
 PC 1.00

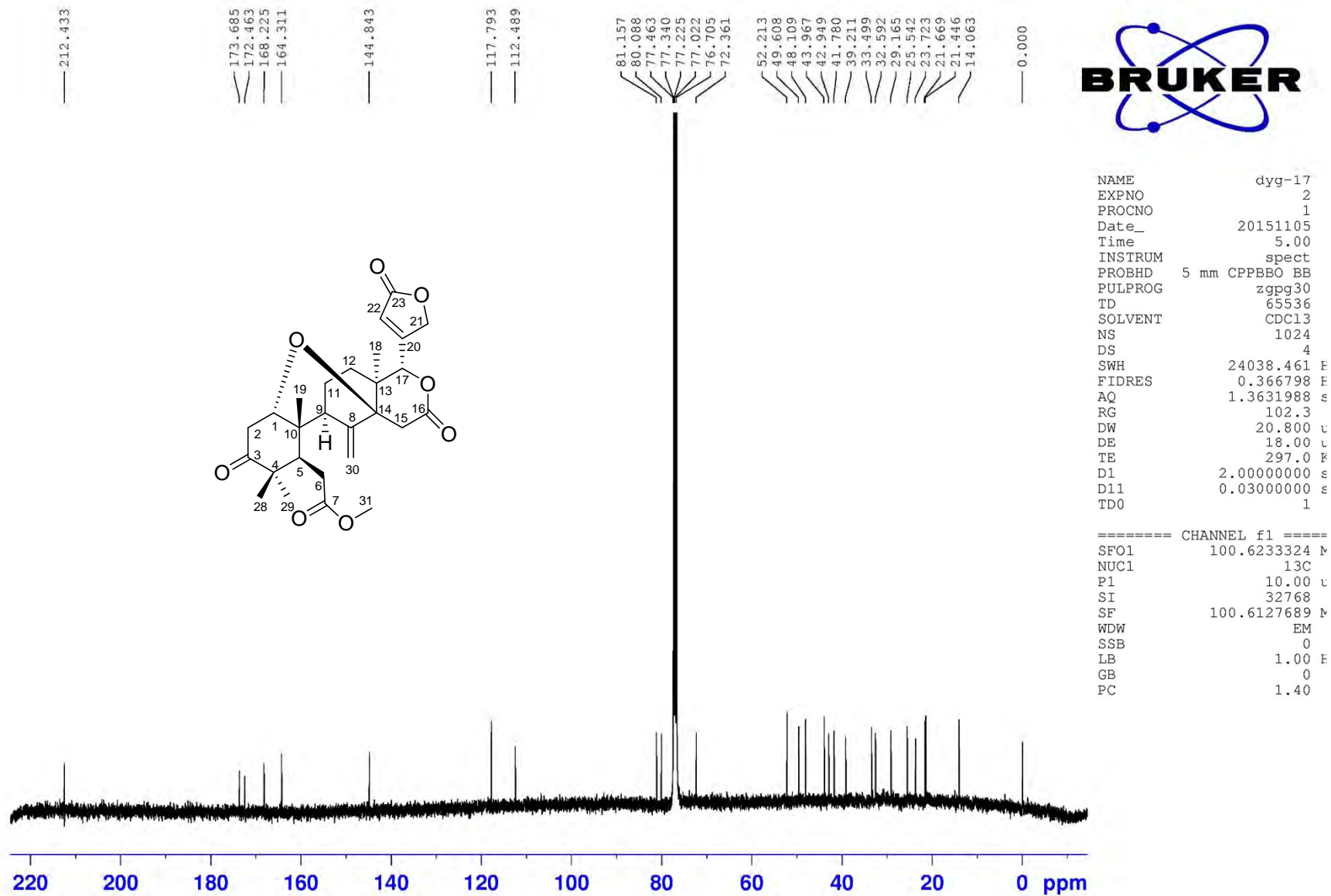
^1H NMR (400 MHz) spectrum of compound **29** in CDCl_3



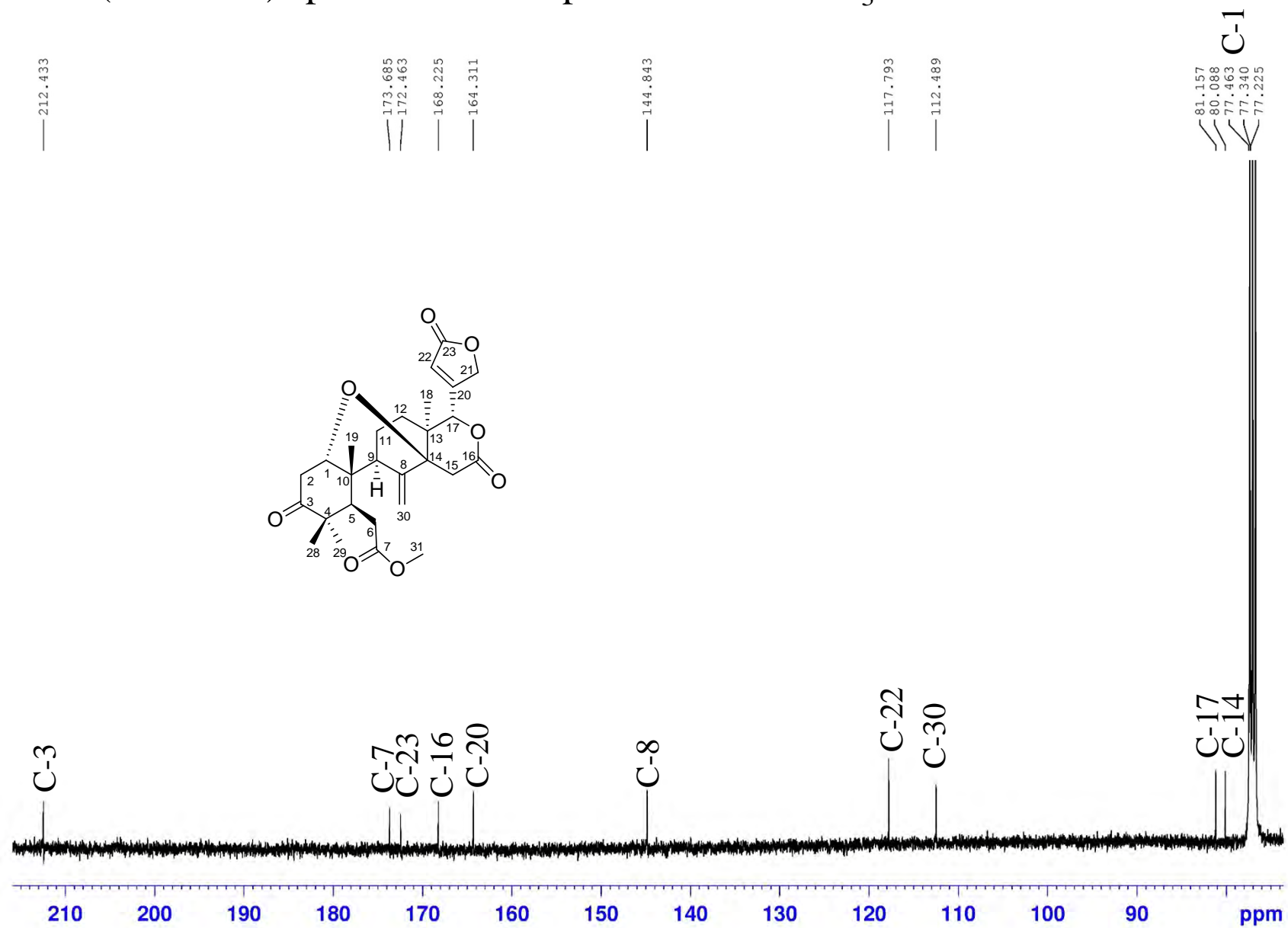
^1H NMR (400 MHz) spectrum of compound **29** in CDCl_3



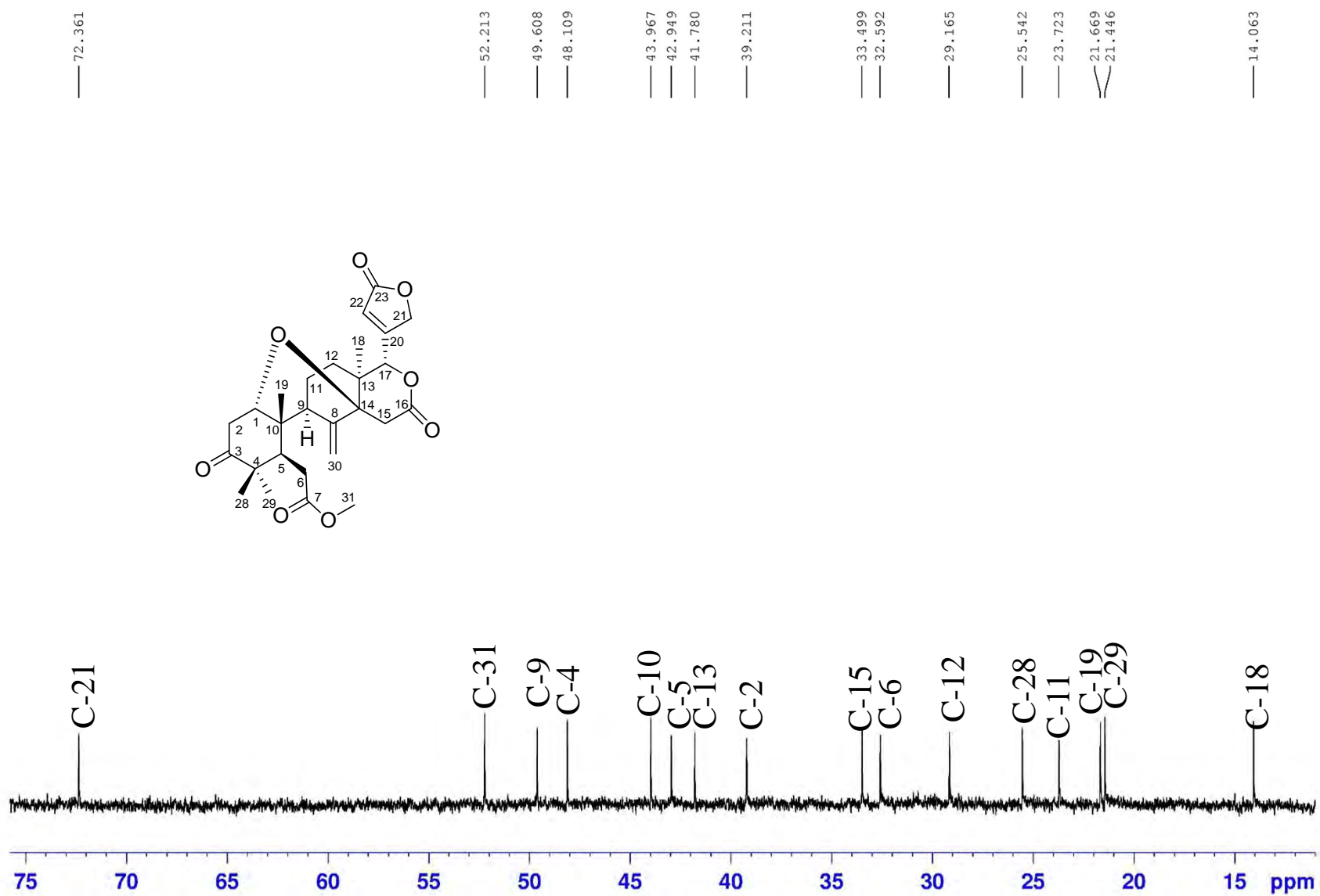
^{13}C NMR (100 MHz) spectrum of compound **29** in CDCl_3



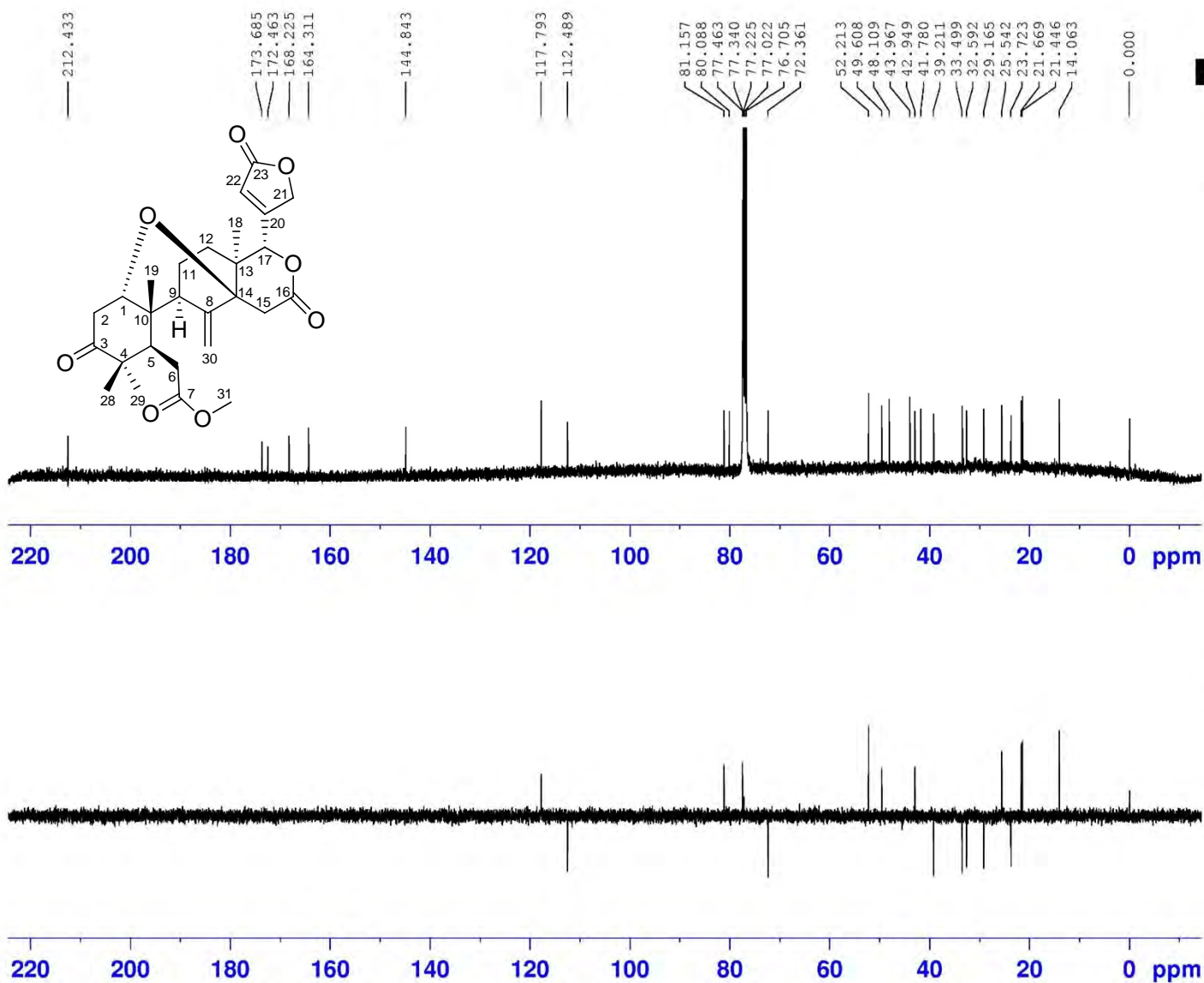
^{13}C NMR (100 MHz) spectrum of compound **29** in CDCl_3



^{13}C NMR (100 MHz) spectrum of compound **29** in CDCl_3



DEPT135 (100 MHz) spectrum of compound **29** in CDCl₃



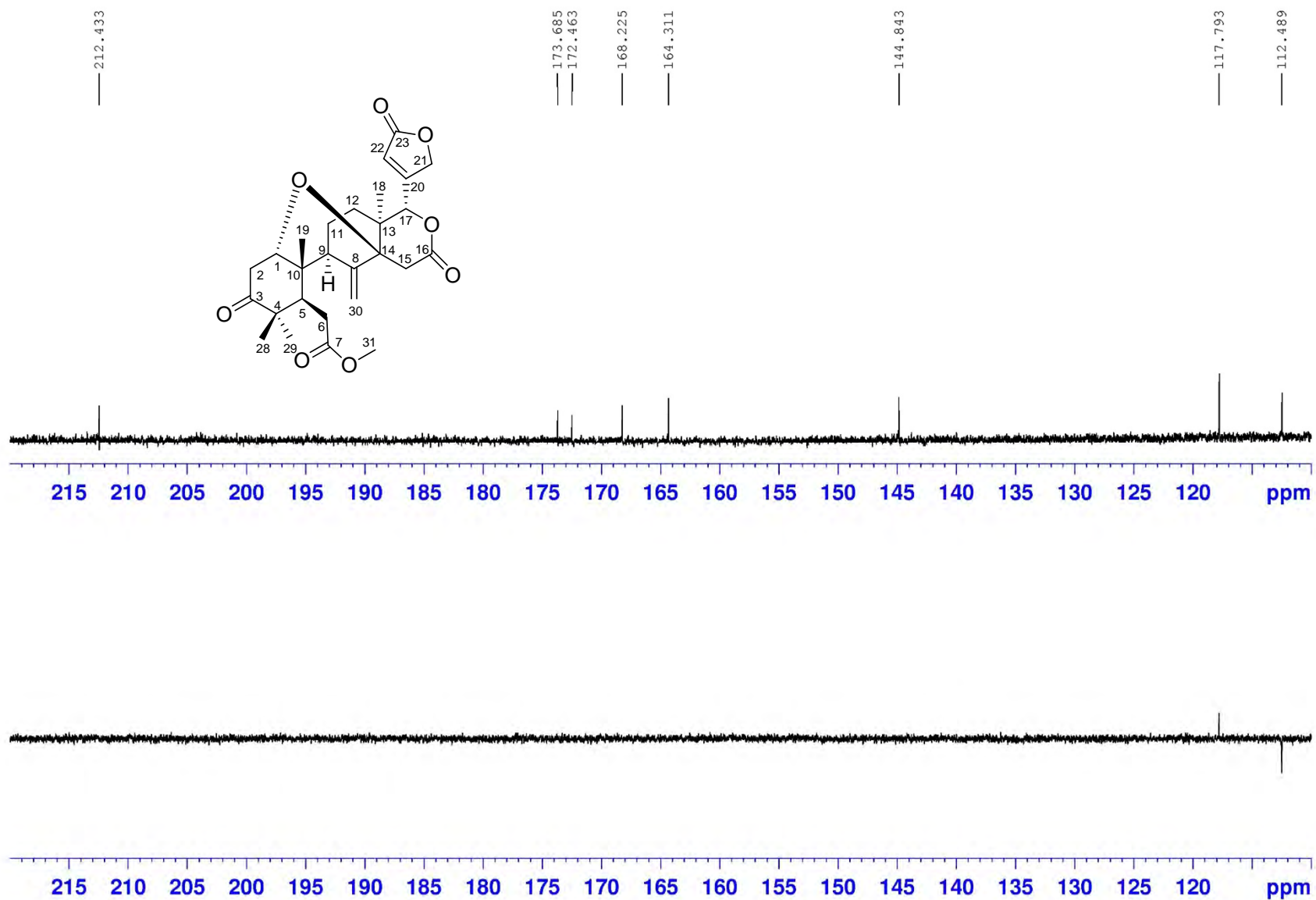
```

NAME          dyg-17
EXPNO          3
PROCNO         1
Date_          20151105
Time           5.18
INSTRUM        spect
PROBHD         5 mm CPPBBO BB
PULPROG        deptsp135
TD             65536
SOLVENT        CDCl3
NS             300
DS             4
SWH            24038.461
FIDRES         0.366798
AQ             1.3631988
RG             91.64
DW             20.800
DE             18.00
TE             297.0
CNST2          145.0000000
D1             2.00000000
D2             0.00344828
D12            0.00002000
TD0            1
    
```

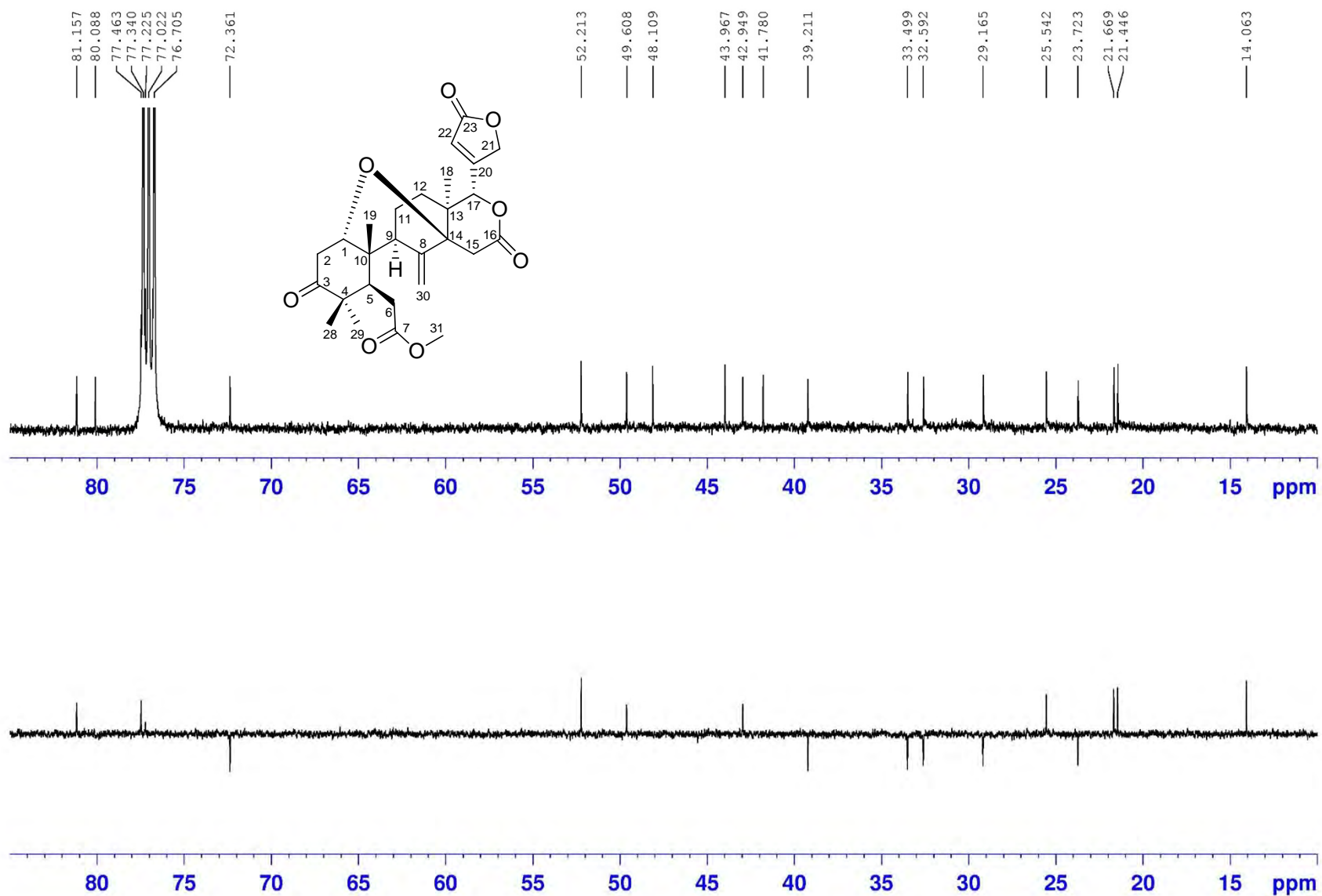
```

===== CHANNEL f1 =====
SFO1          100.6233324
NUC1           13C
P1             10.00
P13            2000.00
SI             32768
SF            100.6127690
WDW            EM
SSB            0
LB             1.00
GB             0
PC             1.40
    
```

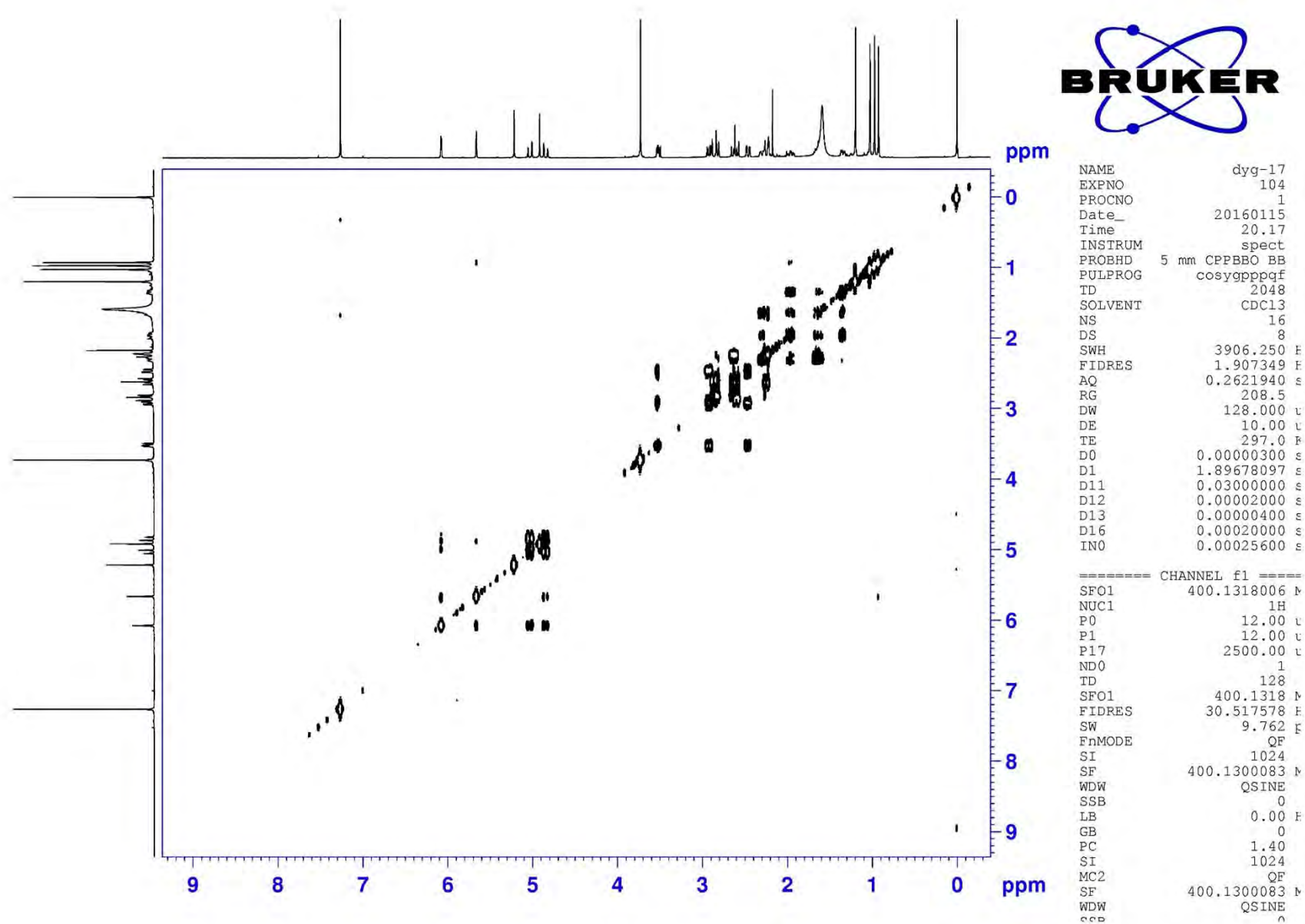

DEPT135 (100 MHz) spectrum of compound **29** in CDCl_3



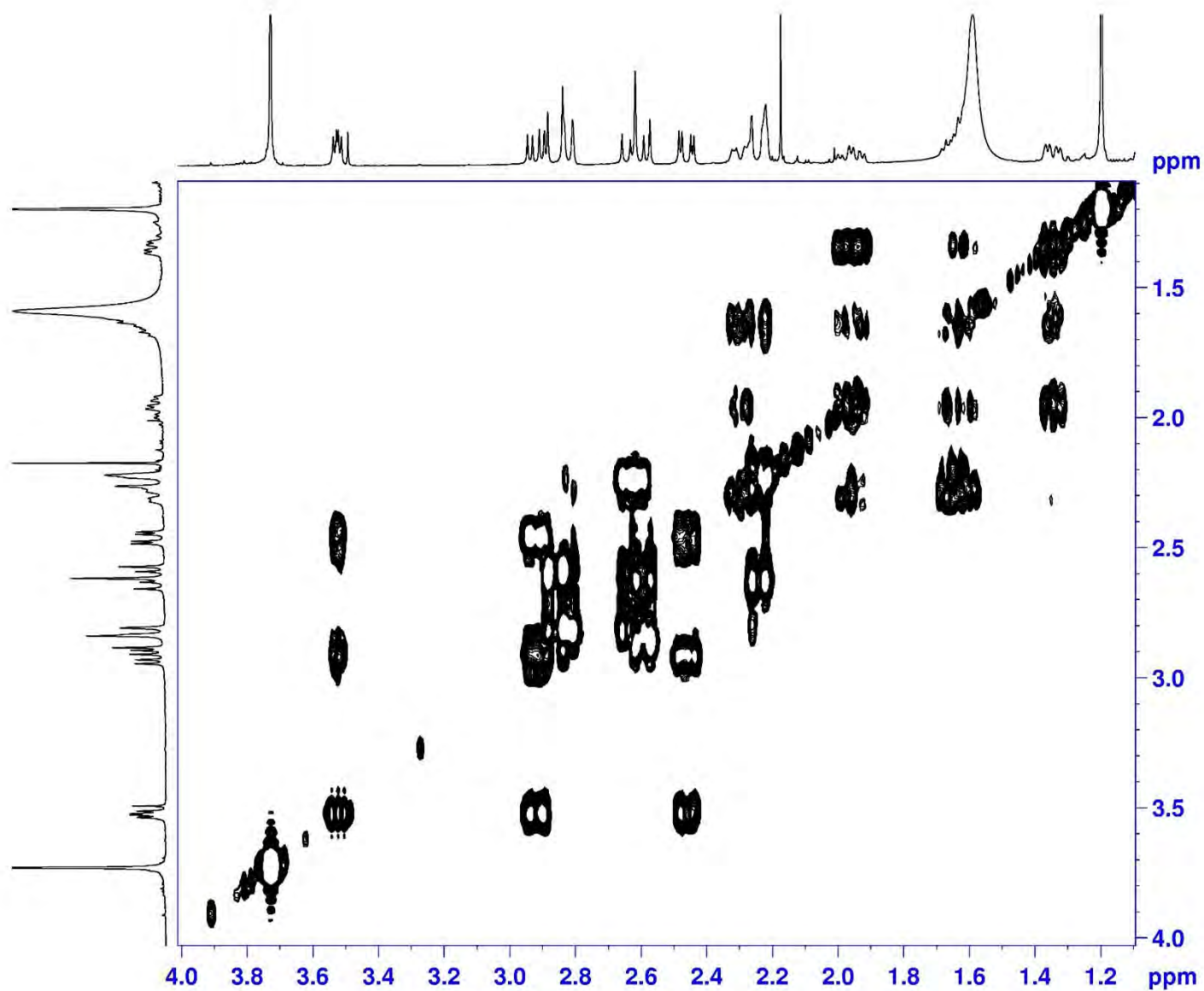
DEPT135 (100 MHz) spectrum of compound **29** in CDCl₃



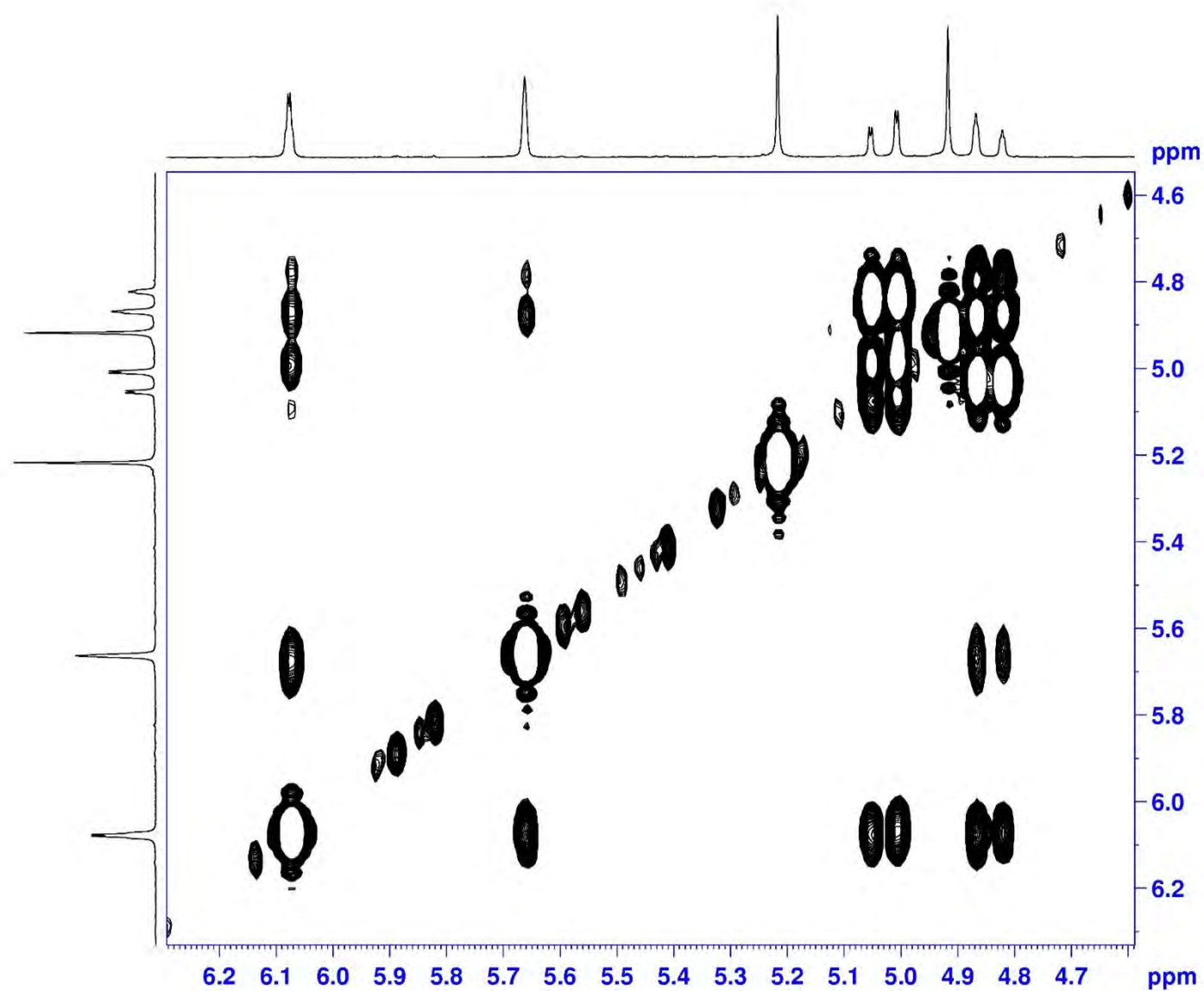
^1H - ^1H COSY (400 MHz) spectrum of compound **29** in CDCl_3



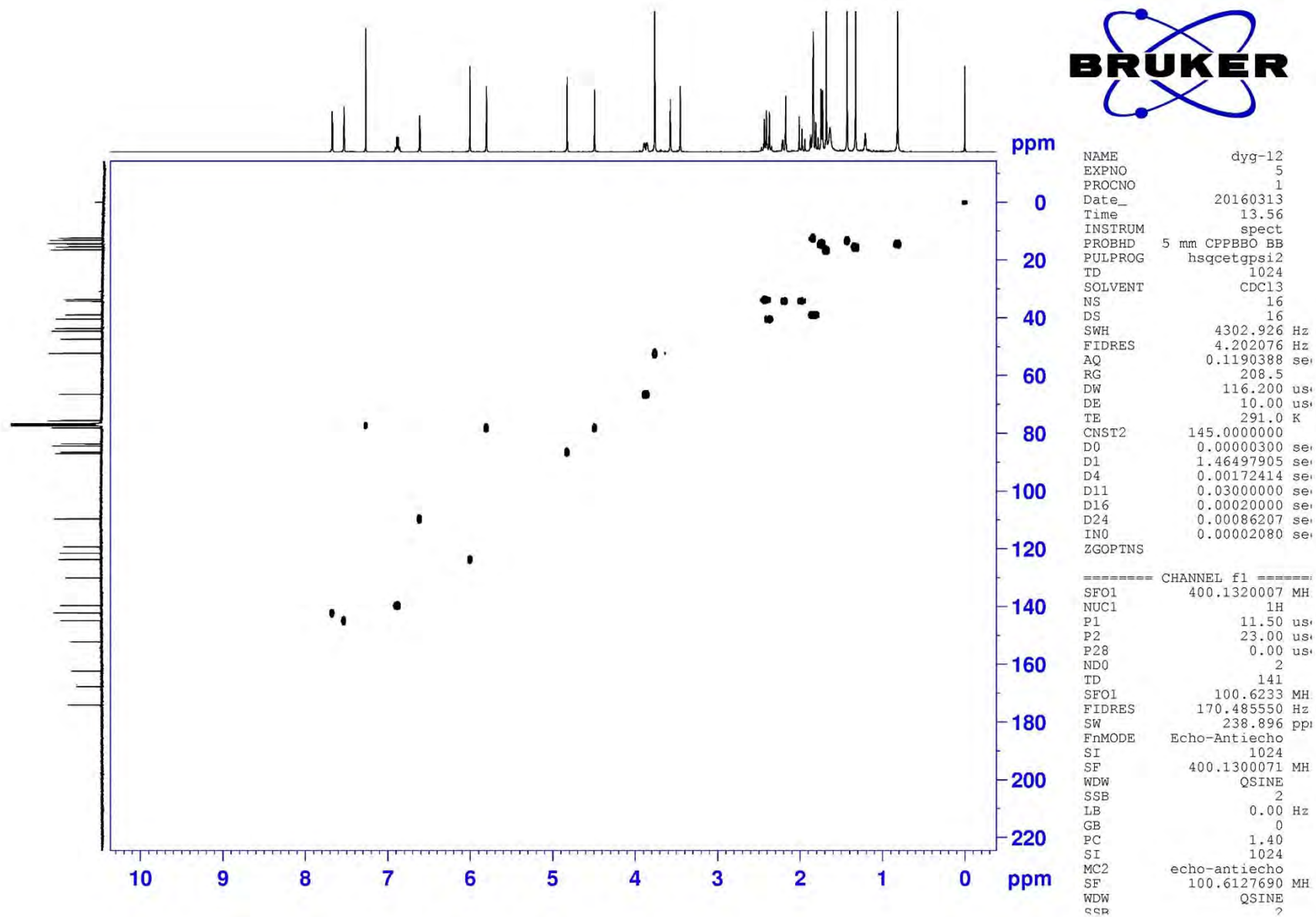
^1H - ^1H COSY (400 MHz) spectrum of compound **29** in CDCl_3



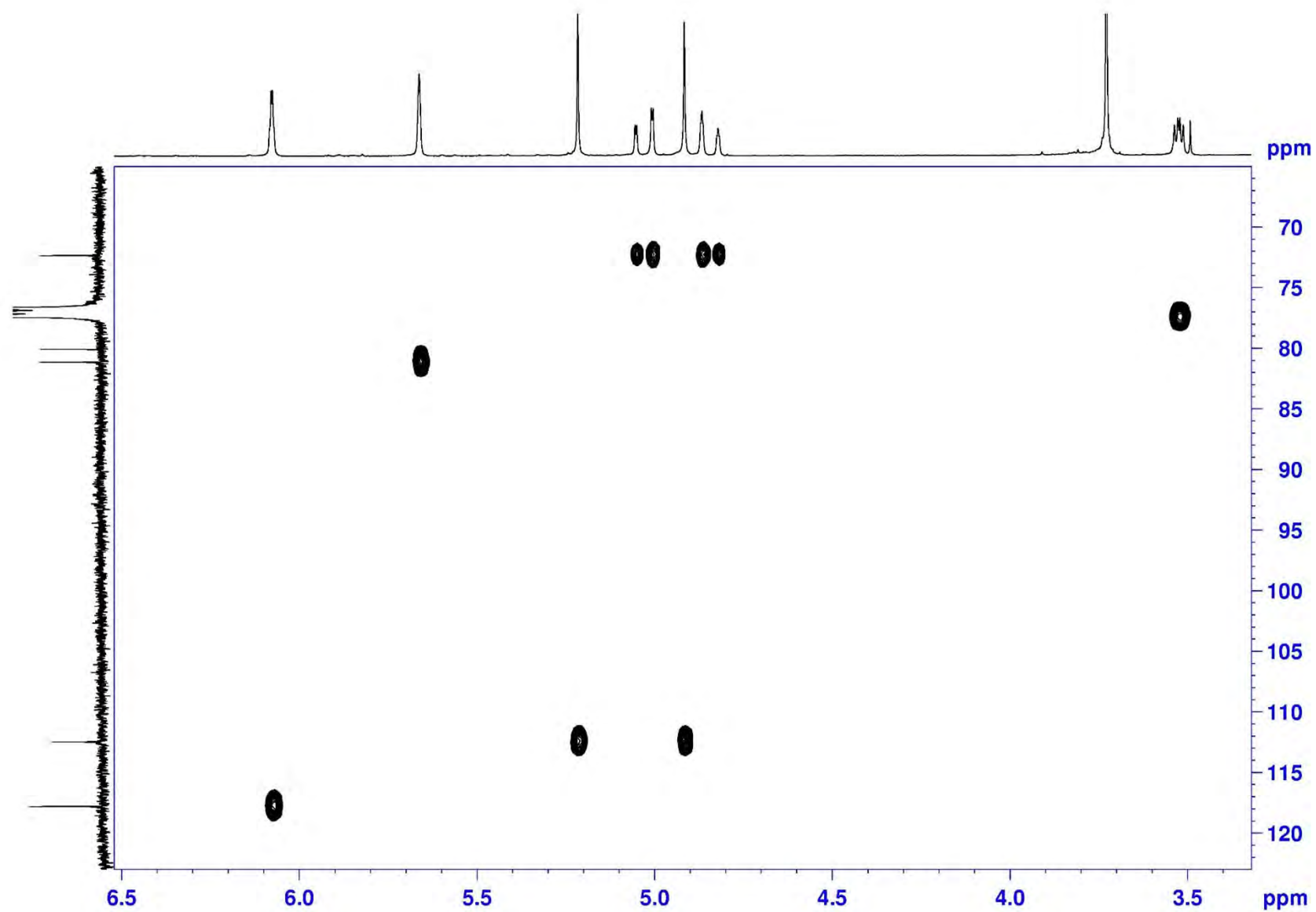
^1H - ^1H COSY (400 MHz) spectrum of compound **29** in CDCl_3



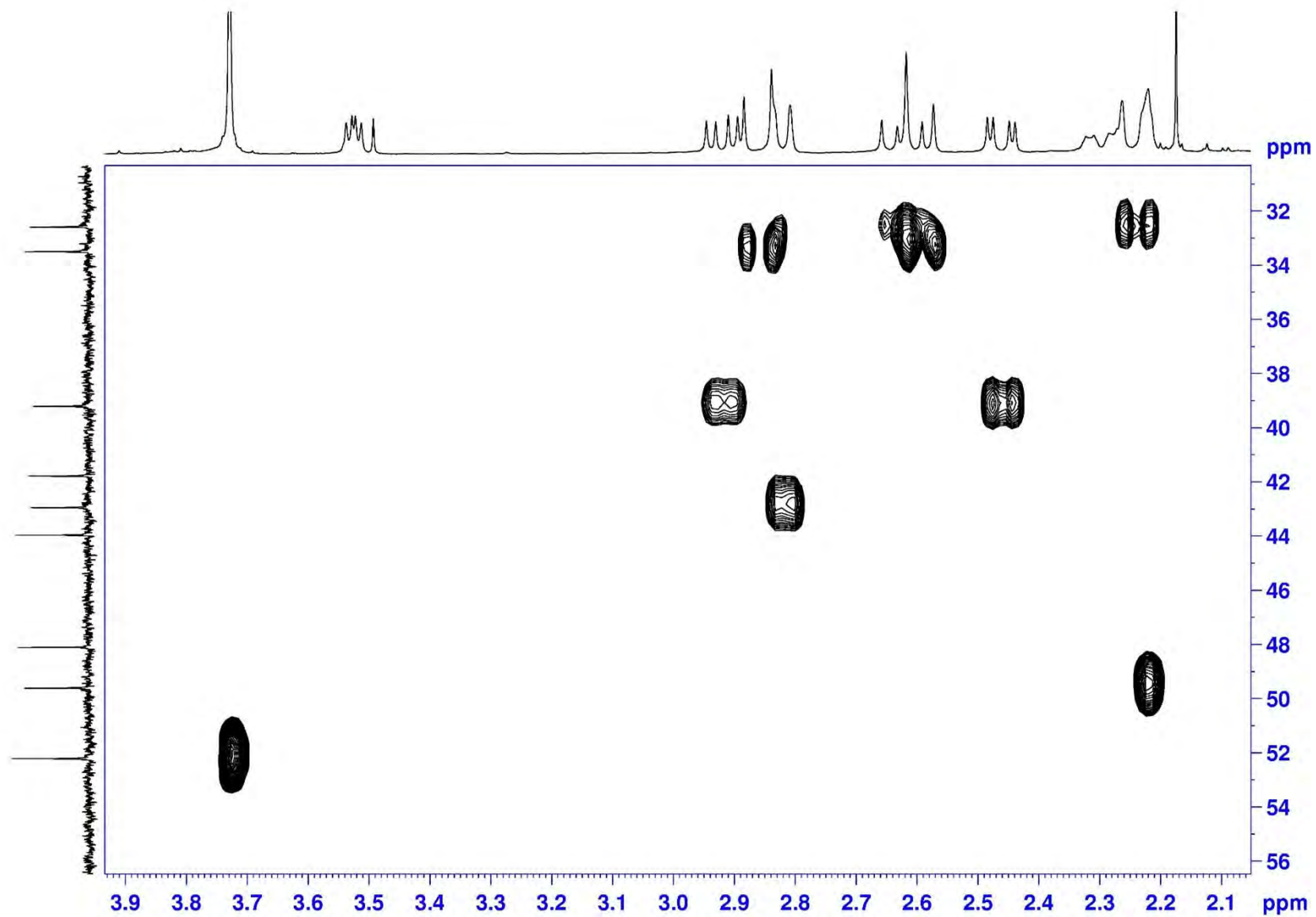
HSQC (400 MHz) spectrum of compound **29** in CDCl₃



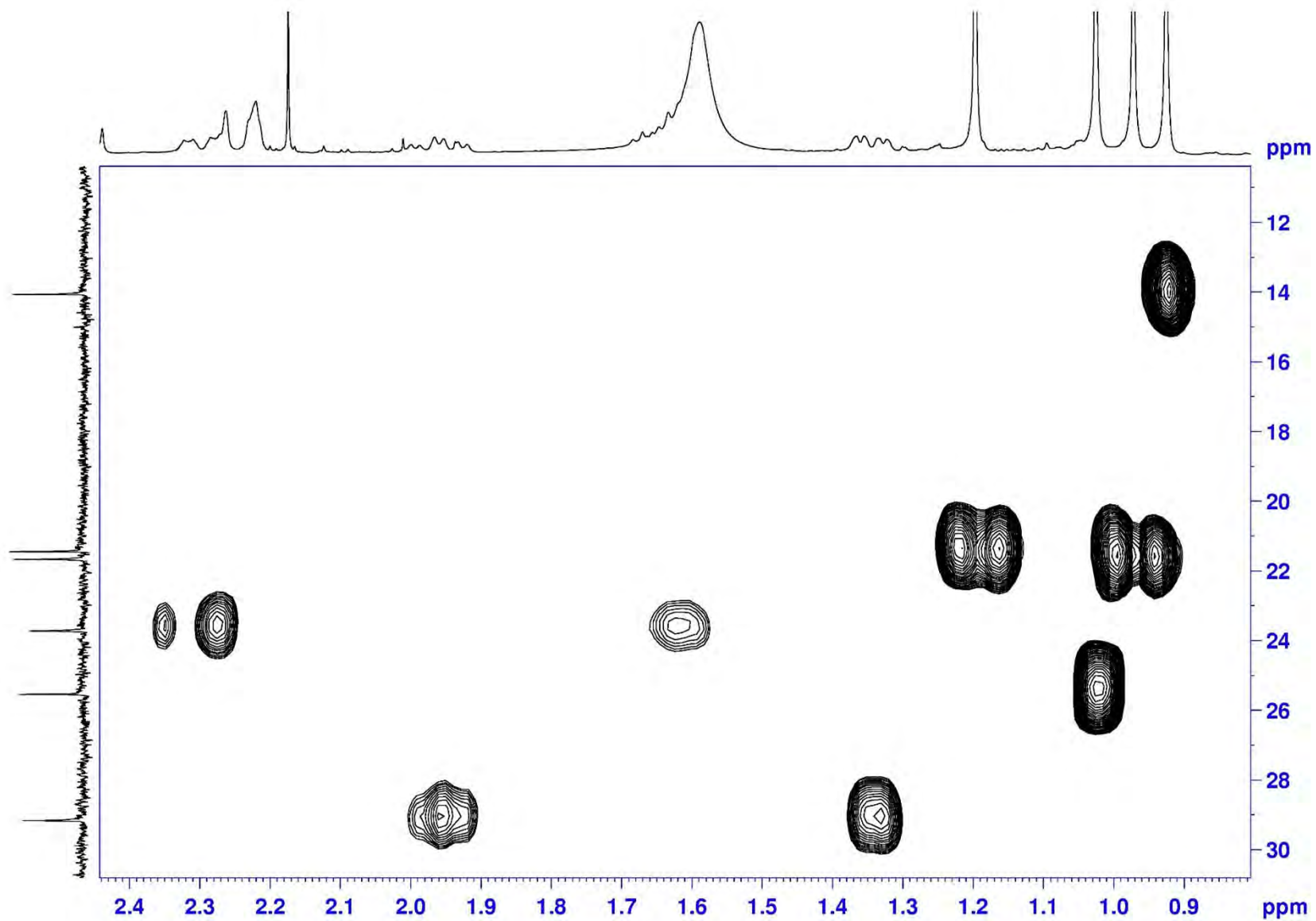
HSQC (400 MHz) spectrum of compound **29** in CDCl₃



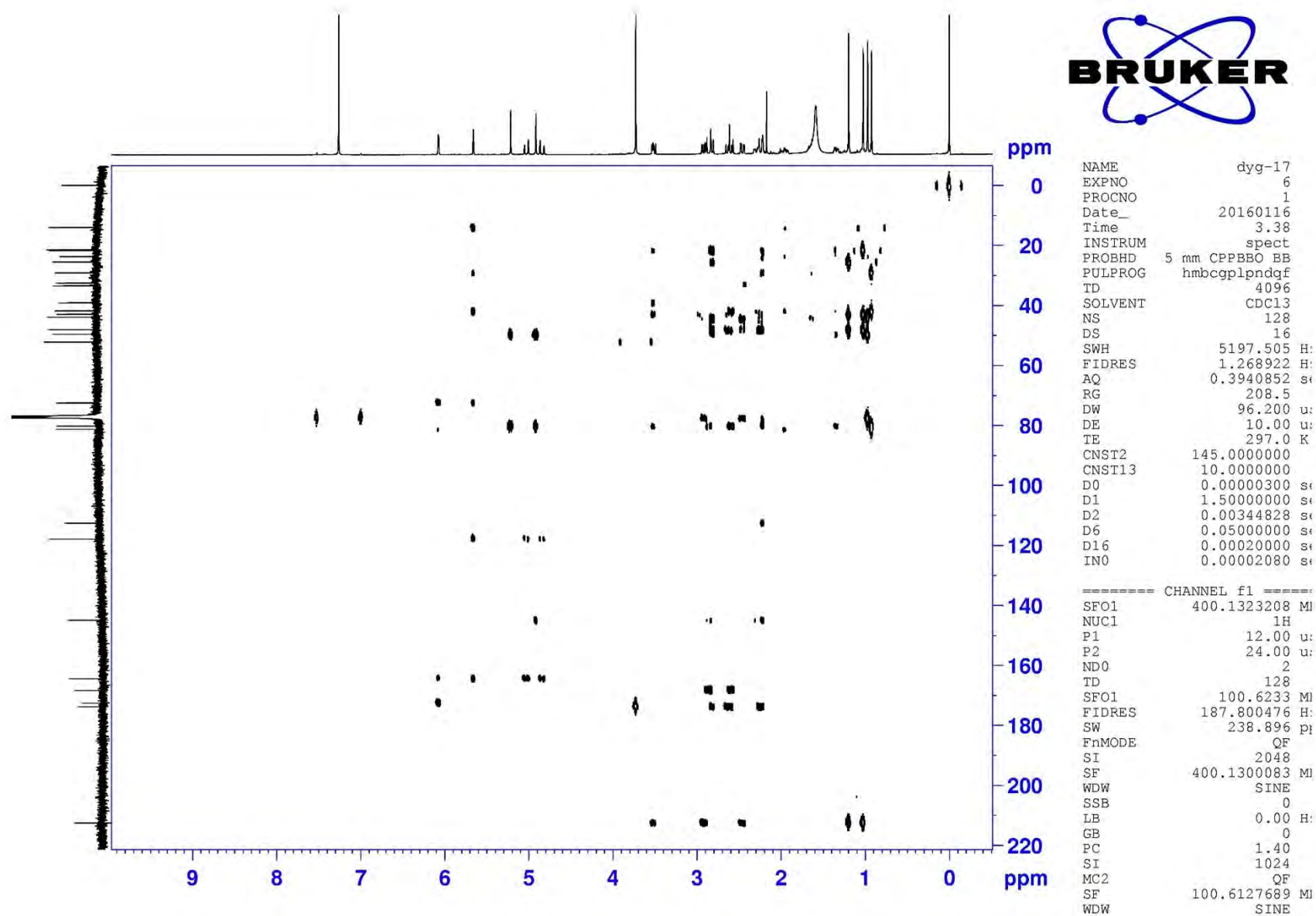
HSQC (400 MHz) spectrum of compound **29** in CDCl₃



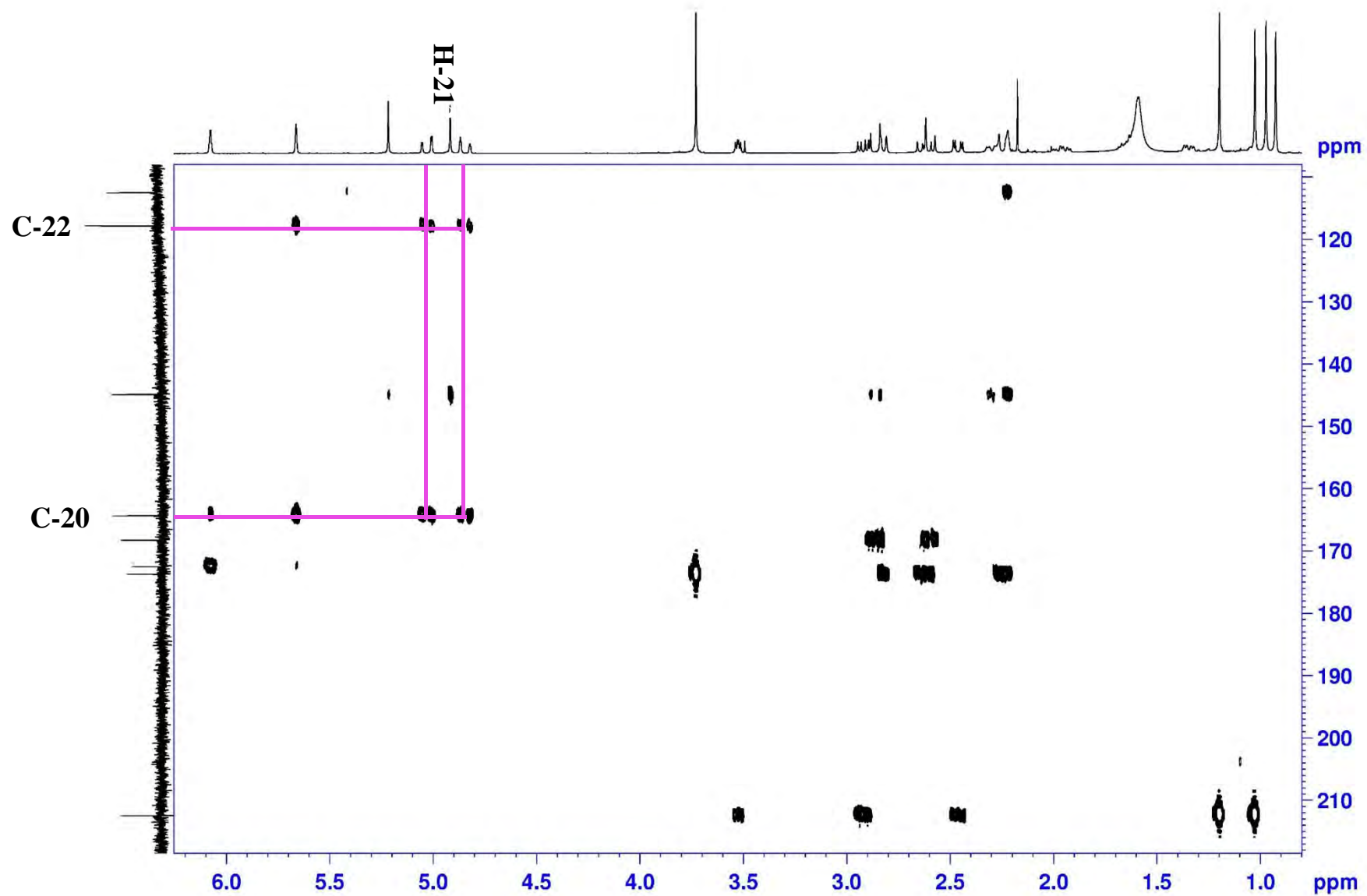
HSQC (400 MHz) spectrum of compound **29** in CDCl₃



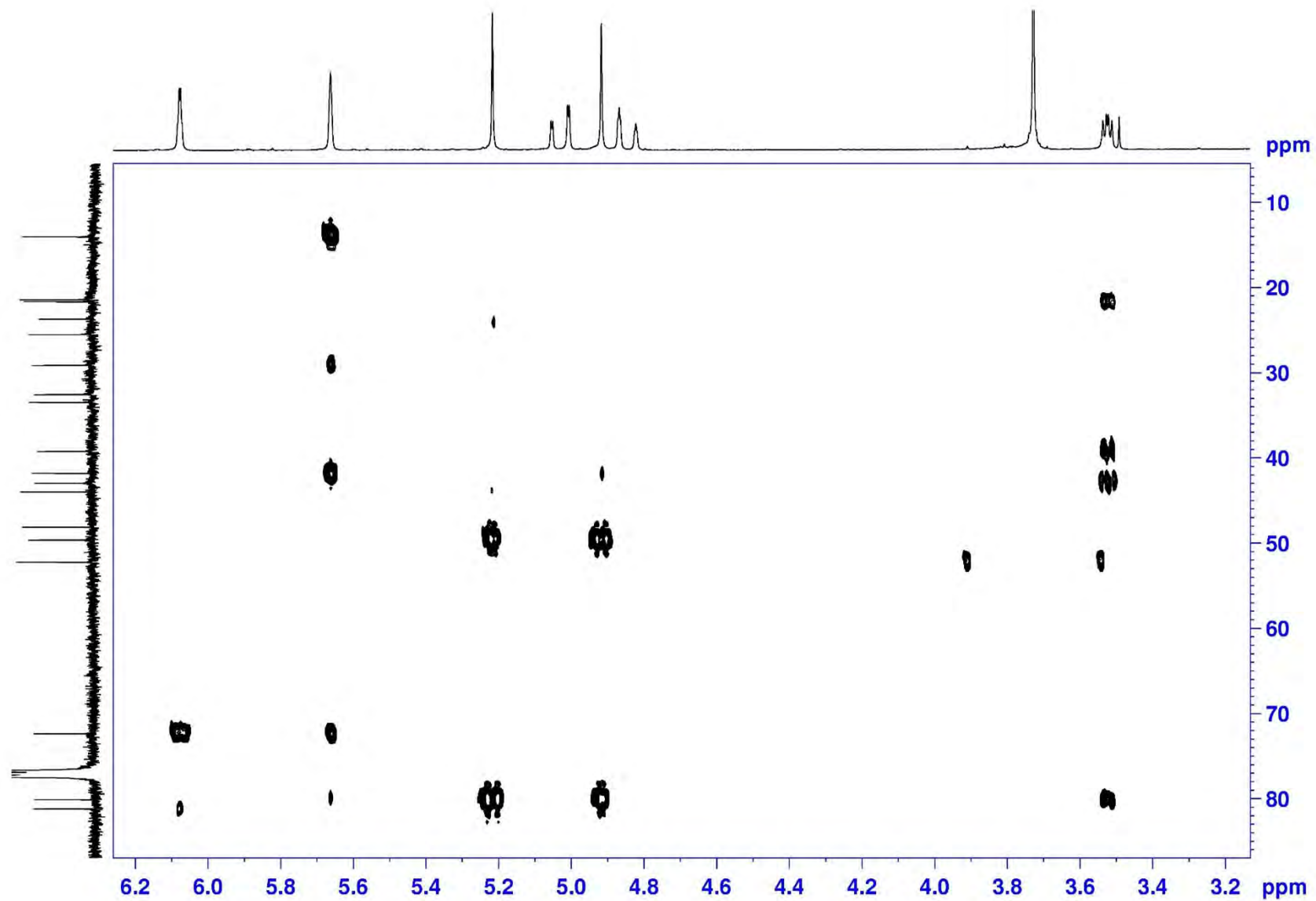
HMBC (400 MHz) spectrum of compound **29** in CDCl₃



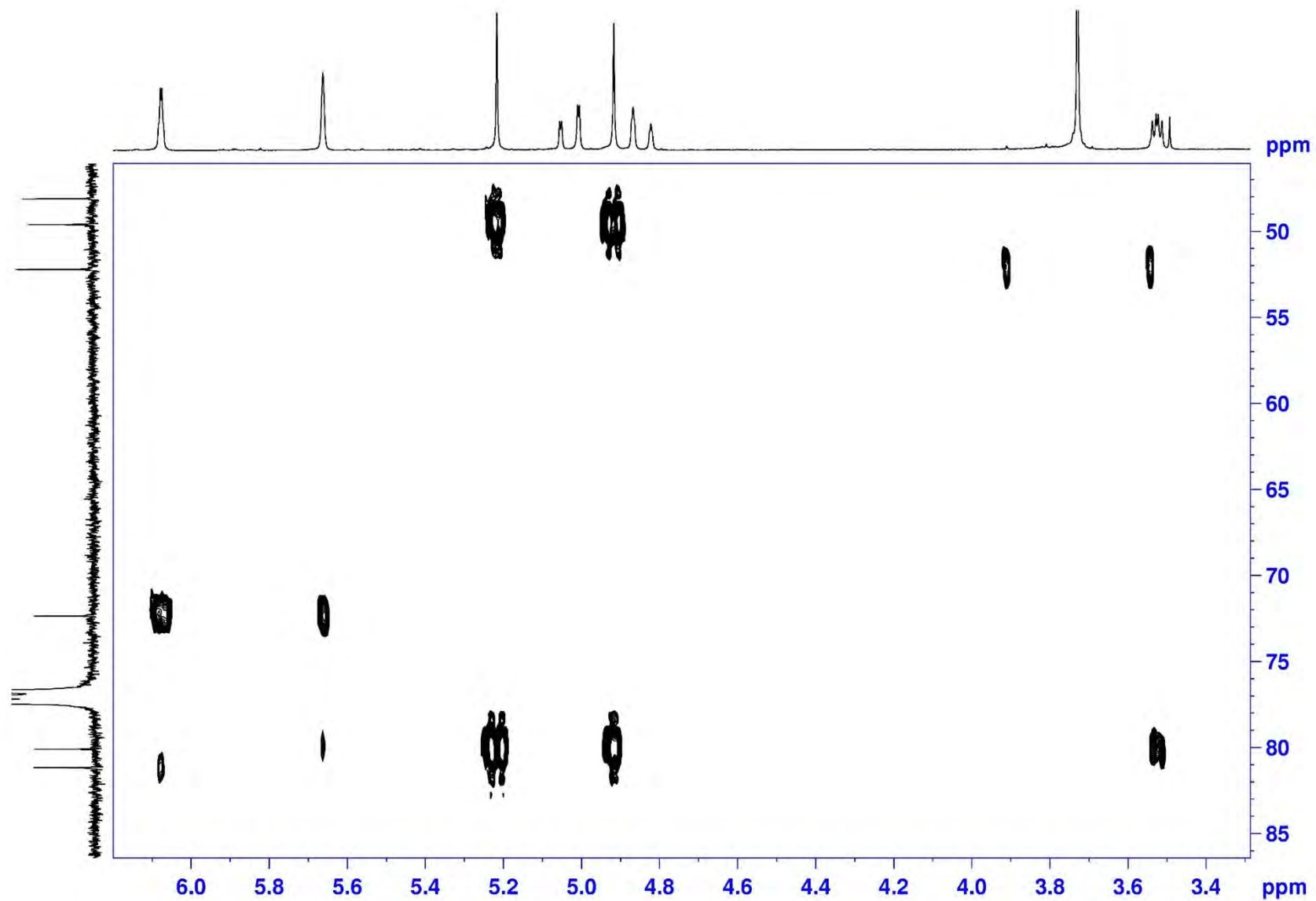
HMBC (400 MHz) spectrum of compound **29** in CDCl₃



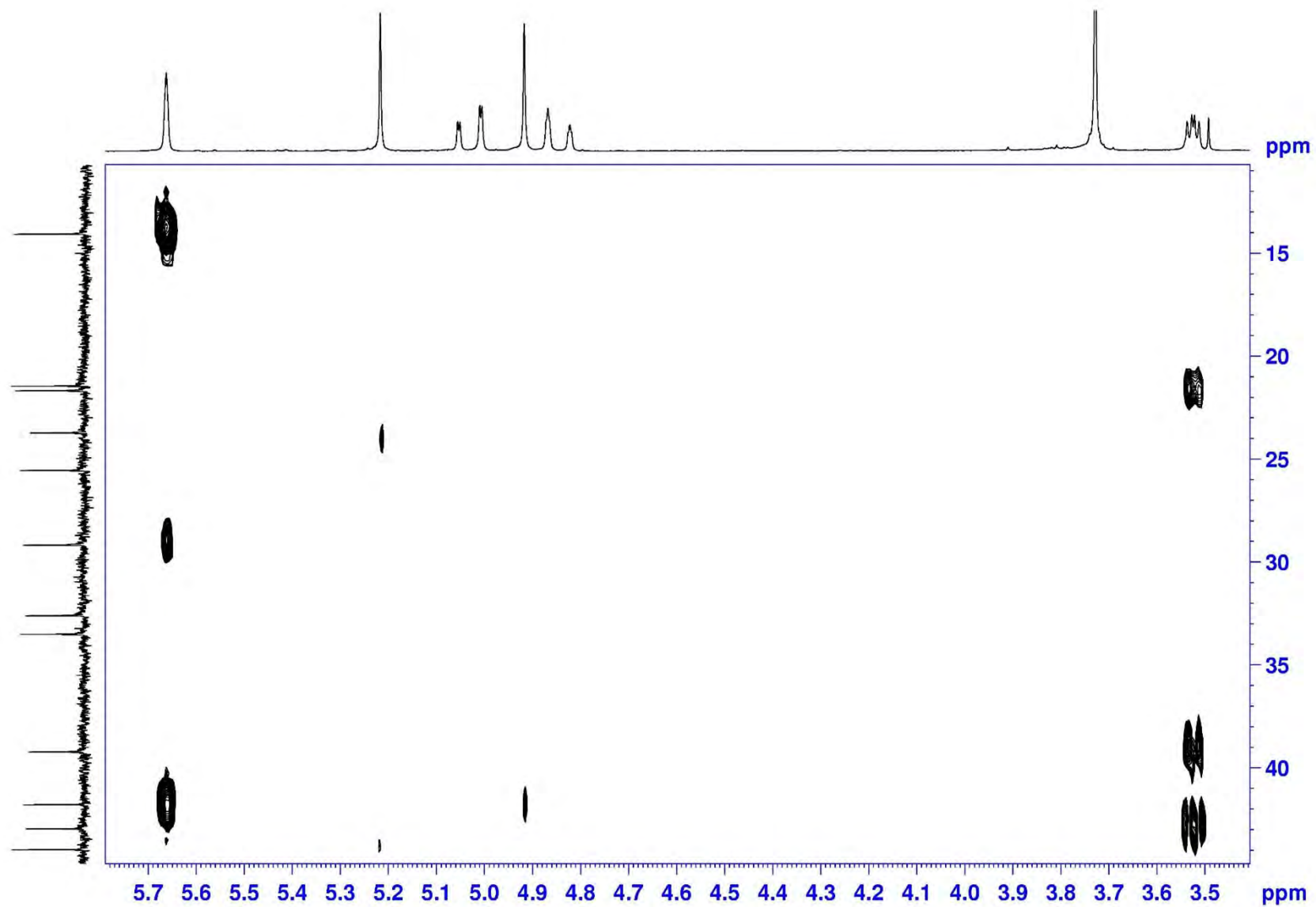
HMBC (400 MHz) spectrum of compound **29** in CDCl_3



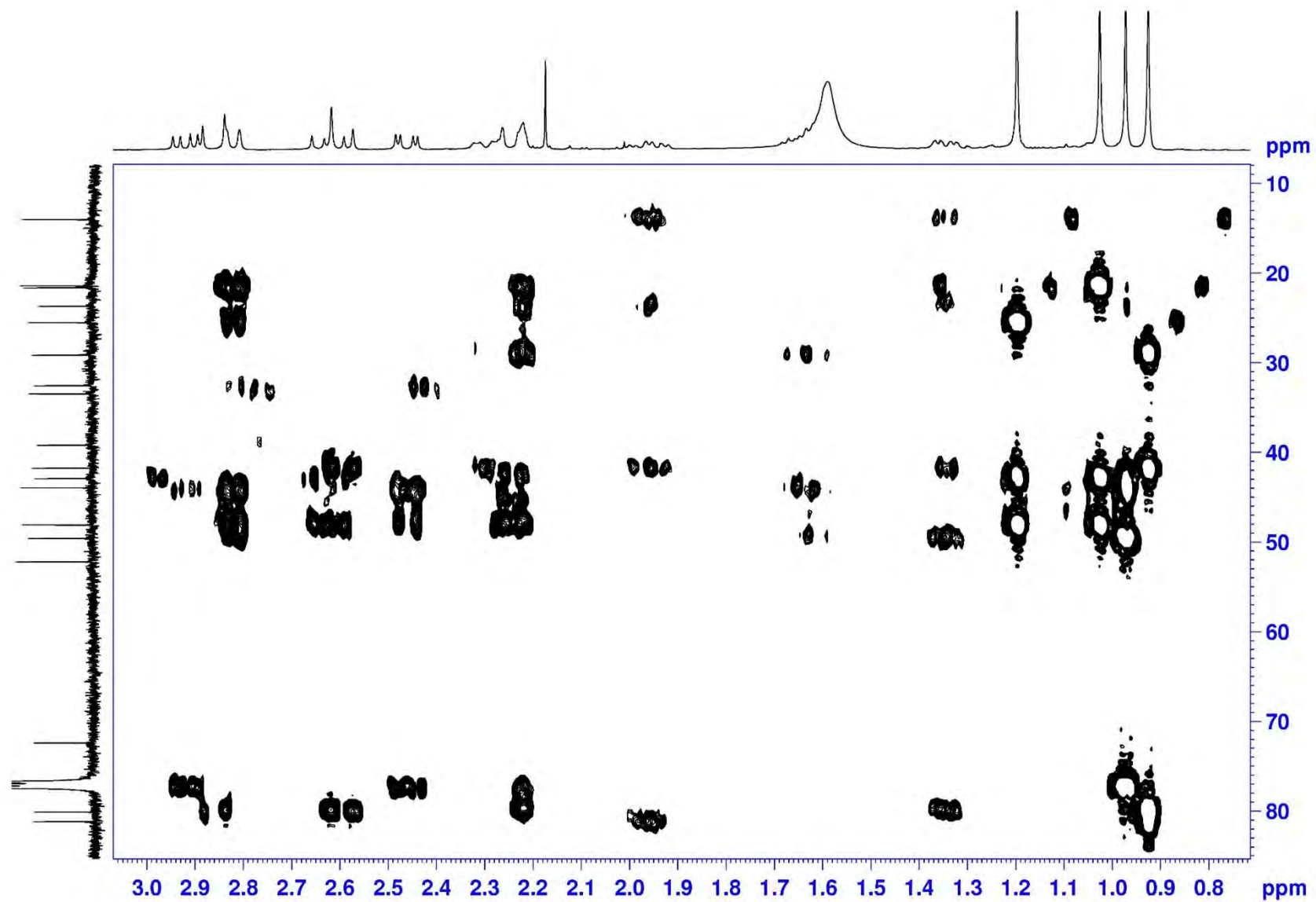
HMBC (400 MHz) spectrum of compound **29** in CDCl₃



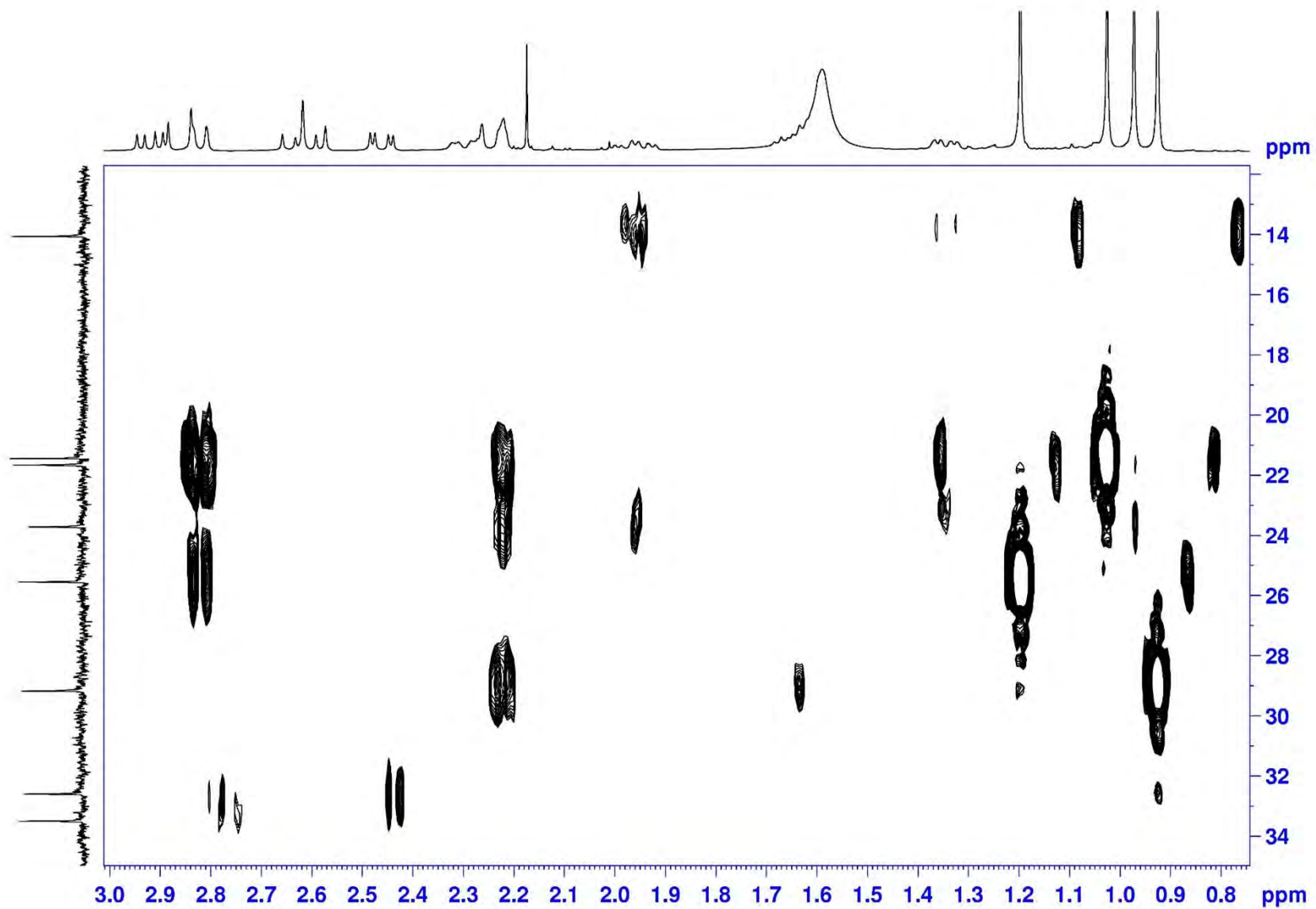
HMBC (400 MHz) spectrum of compound **29** in CDCl_3



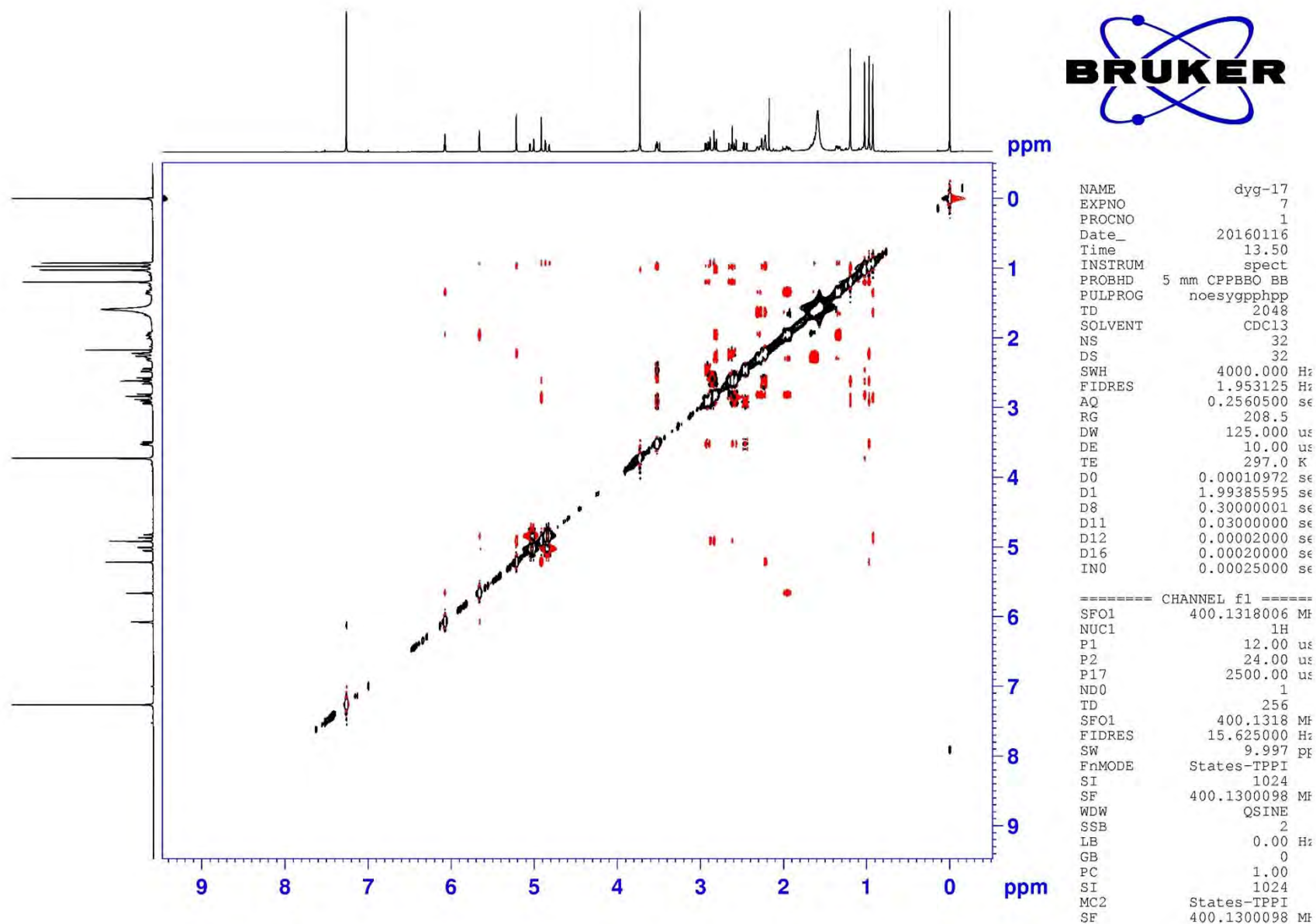
HMBC (400 MHz) spectrum of compound **29** in CDCl_3



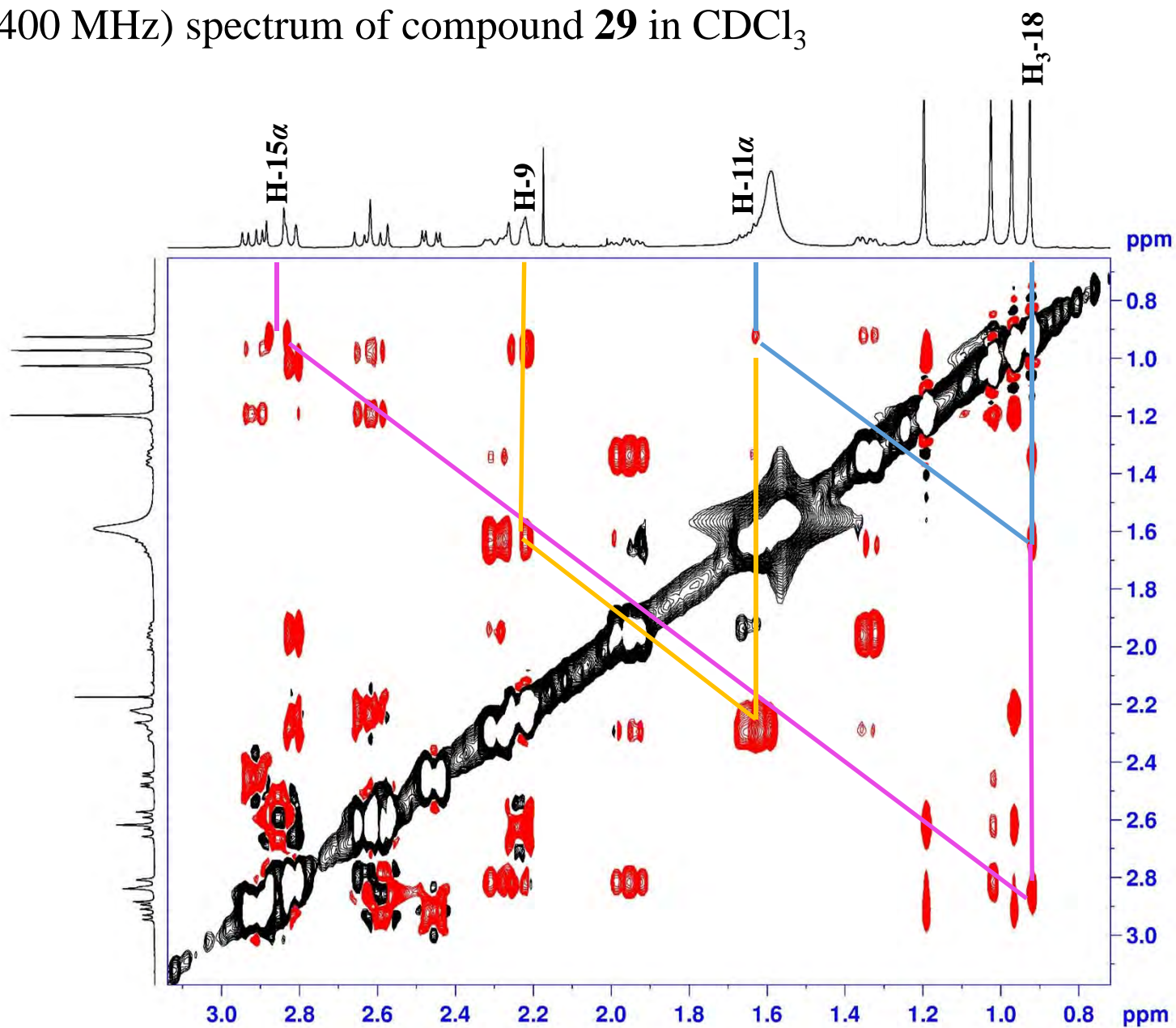
HMBC (400 MHz) spectrum of compound **29** in CDCl_3



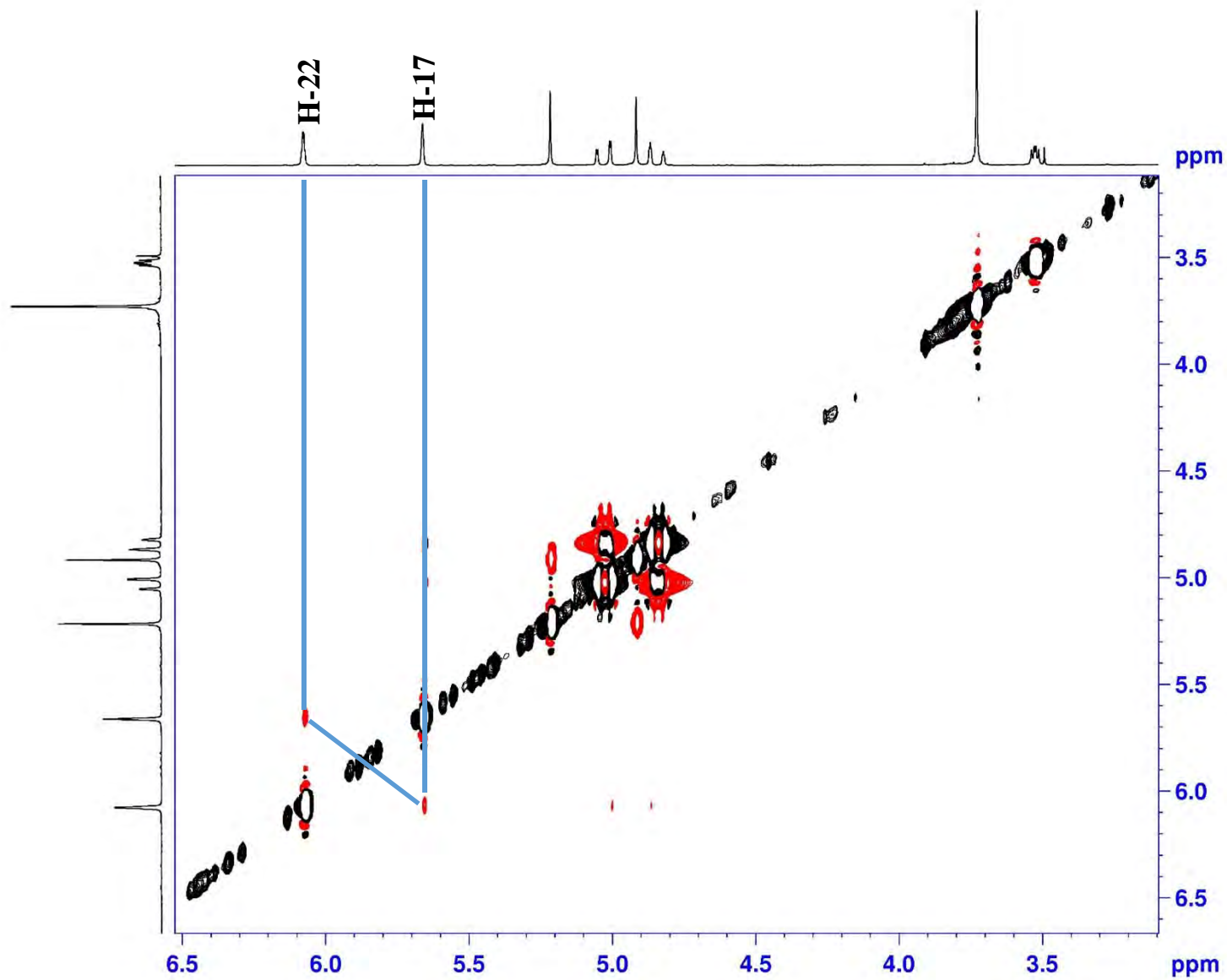
NOESY (400 MHz) spectrum of compound **29** in CDCl₃



NOESY (400 MHz) spectrum of compound **29** in CDCl₃



NOESY (400 MHz) spectrum of compound **29** in CDCl₃



NOESY (400 MHz) spectrum of compound **29** in CDCl₃

