

Supporting Information-2:

Antiviral New Limonoids Including Khayanolides from the Trang Mangrove Plant, *Xylocarpus moluccensis*

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Copies of HR-ESIMS, 1-D and 2D-NMR spectra for compounds 7-12

Content:

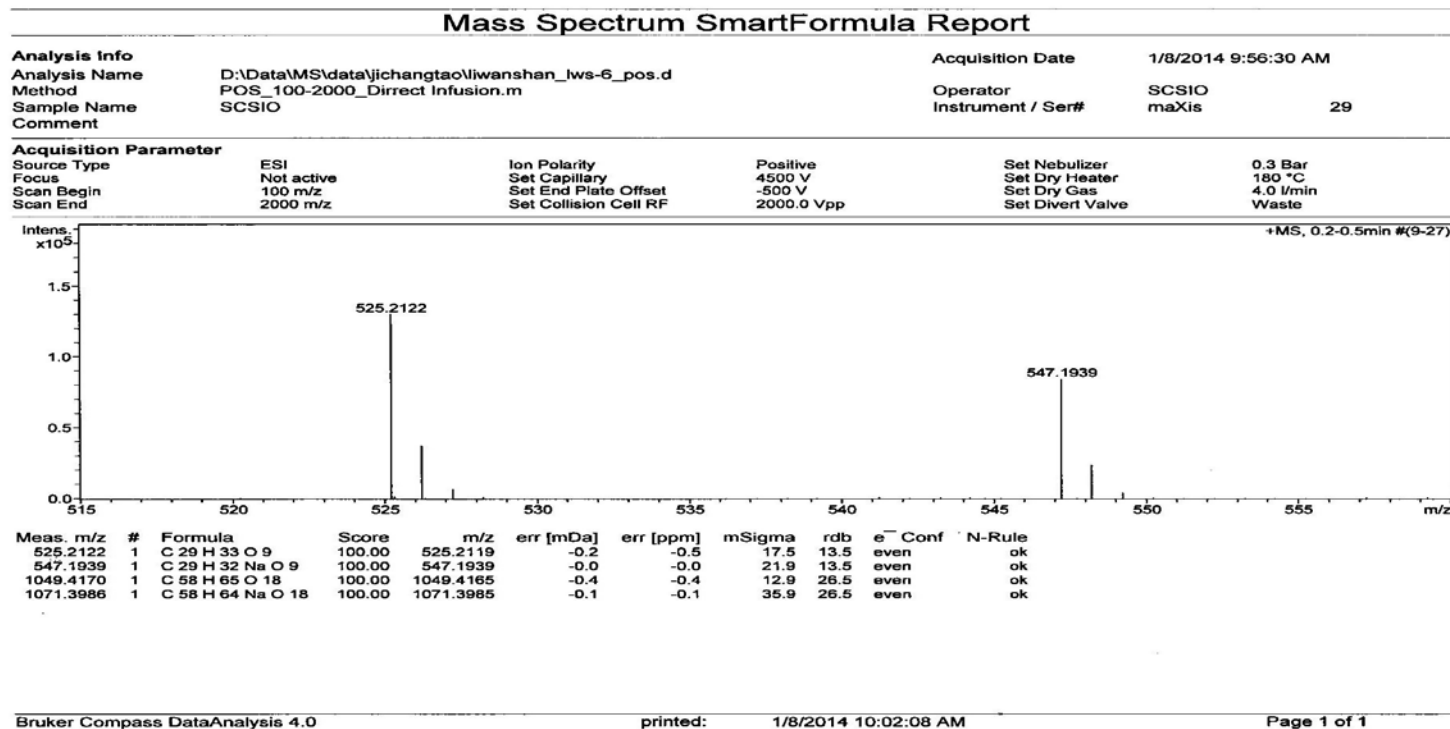
HR-ESIMS of Thaixylomolin M (7).....	S6
¹ H NMR (400 MHz) spectrum of Thaixylomolin M (7) in CDCl ₃	S8
¹³ C NMR (100 MHz) spectrum of Thaixylomolin M (7) in CDCl ₃	S10
DEPT135° (100 MHz) spectrum of Thaixylomolin M (7) in CDCl ₃	S12
¹ H- ¹ H COSY (400 MHz) spectrum of Thaixylomolin M (7) in CDCl ₃	S15
HSQC (400 MHz) spectrum of Thaixylomolin M (7) in CDCl ₃	S19
HMBC (400 MHz) spectrum of Thaixylomolin M (7) in CDCl ₃	S21
NOESY (400 MHz) spectrum of Thaixylomolin M (7) in CDCl ₃	S27
HR-ESIMS of Thaixylomolin N (8).....	S31
¹ H NMR (400 MHz) spectrum of Thaixylomolin N (8) in CDCl ₃	S33
¹³ C NMR (100 MHz) spectrum of Thaixylomolin N (8) in CDCl ₃	S37
DEPT135° (100 MHz) spectrum of Thaixylomolin N (8) in CDCl ₃	S40

¹ H- ¹ H COSY (400 MHz) spectrum of Thaixylomolin N (8) in CDCl ₃	S44
HSQC (400 MHz) spectrum of Thaixylomolin N (8) in CDCl ₃	S46
HMBC (400 MHz) spectrum of Thaixylomolin N (8) in CDCl ₃	S49
NOESY (400 MHz) spectrum of Thaixylomolin N (8) in CDCl ₃	S57
HR-ESIMS of Compound 9	S61
¹ H NMR (400 MHz) spectrum of Compound 9 in CDCl ₃	S63
¹³ C NMR (100 MHz) spectrum of Compound 9 in CDCl ₃	S67
DEPT135° (100 MHz) spectrum of Compound 9 in CDCl ₃	S71
¹ H- ¹ H COSY (400 MHz) spectrum of Compound 9 in CDCl ₃	S72
HSQC (400 MHz) spectrum of Compound 9 in CDCl ₃	S75
HMBC (400 MHz) spectrum of Compound 9 in CDCl ₃	S78
NOESY (400 MHz) spectrum of Compound 9 in CDCl ₃	S83
HR-ESIMS of Compound 10	S87

¹ H NMR (400 MHz) spectrum of Compound 10 in CDCl ₃	S89
¹³ C NMR (100 MHz) spectrum of Compound 10 in CDCl ₃	S93
DEPT135° (100 MHz) spectrum of Compound 10 in CDCl ₃	S97
¹ H- ¹ H COSY (400 MHz) spectrum of Compound 10 in CDCl ₃	S101
HSQC (400 MHz) spectrum of Compound 10 in CDCl ₃	S103
HMBC (400 MHz) spectrum of Compound 10 in CDCl ₃	S106
NOESY (400 MHz) spectrum of Compound 10 in CDCl ₃	S113
HR-ESIMS of Compound 11	S117
¹ H NMR (400 MHz) spectrum of Compound 11 in CDCl ₃	S119
¹³ C NMR (100 MHz) spectrum of Compound 11 in CDCl ₃	S123
DEPT135° (100 MHz) spectrum of Compound 11 in CDCl ₃	S126
¹ H- ¹ H COSY (400 MHz) spectrum of Compound 11 in CDCl ₃	S130
HSQC (400 MHz) spectrum of Compound 11 in CDCl ₃	S133

HMBC (400 MHz) spectrum of Compound 11 in CDCl ₃	S136
NOESY (400 MHz) spectrum of Compound 11 in CDCl ₃	S142
HR-ESIMS of Compound 12	S146
¹ H NMR (500 MHz) spectrum of Compound 12 in CDCl ₃	S148
¹³ C NMR (125 MHz) spectrum of Compound 12 in CDCl ₃	S152
DEPT135° (125 MHz) spectrum of Compound 12 in CDCl ₃	S154
¹ H- ¹ H COSY (500 MHz) spectrum of Compound 12 in CDCl ₃	S159
HSQC (500 MHz) spectrum of Compound 12 in CDCl ₃	S162
HMBC (500 MHz) spectrum of Compound 12 in CDCl ₃	S165
NOESY (500 MHz) spectrum of Compound 12 in CDCl ₃	S173

HR-ESIMS of Thaixylomolin M (7)



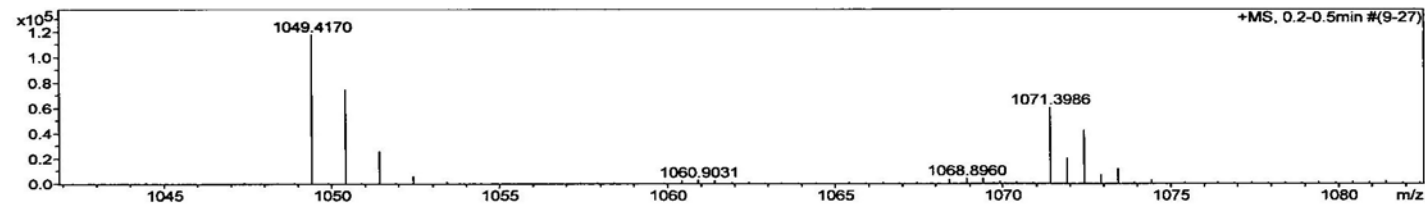
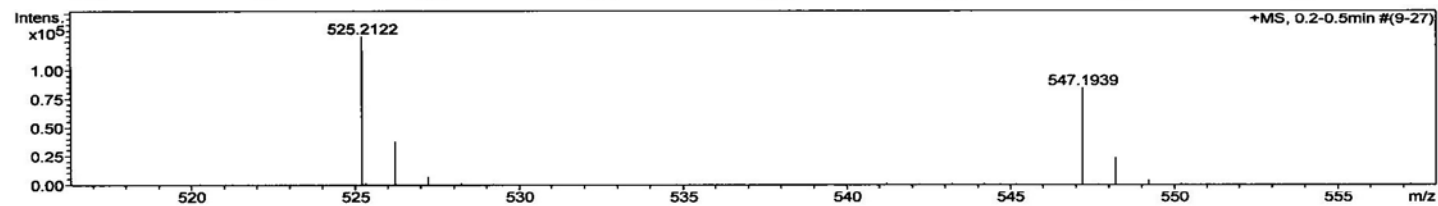
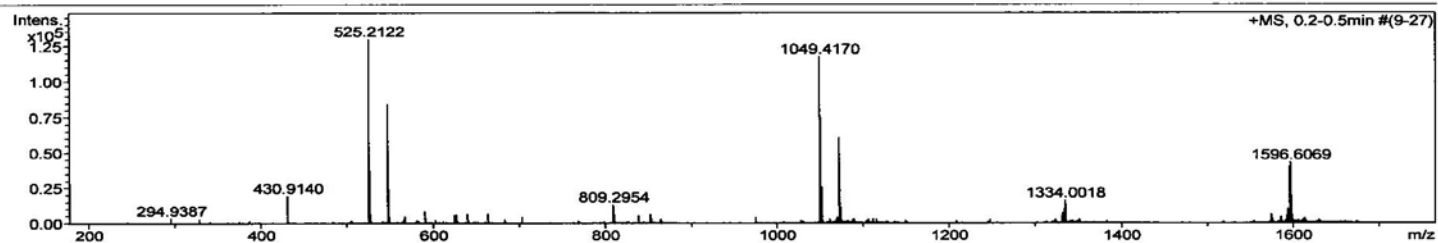
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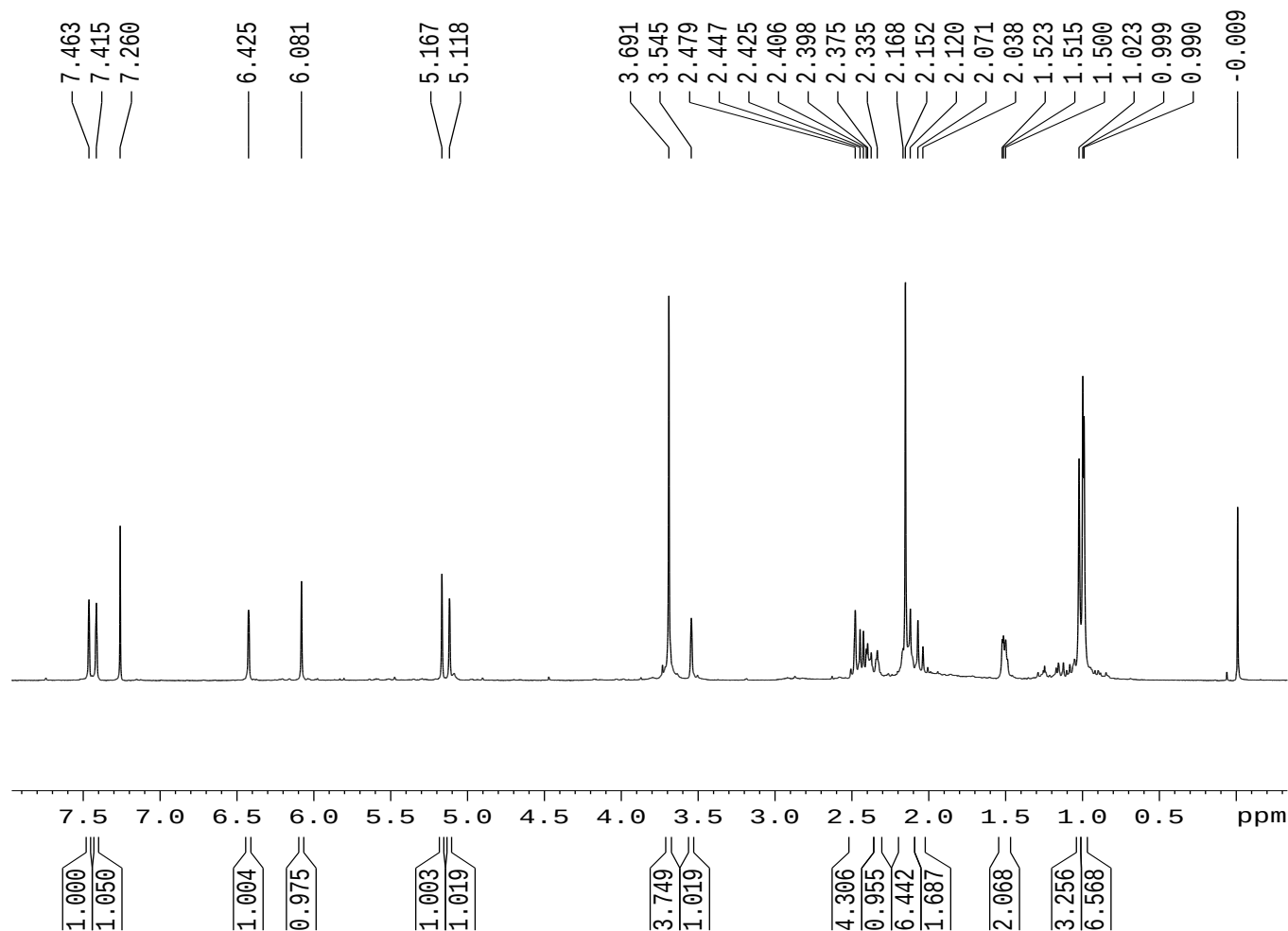
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Instrument maXis



¹H NMR (400 MHz) spectrum of Thaixylomolin M (7) in CDCl₃



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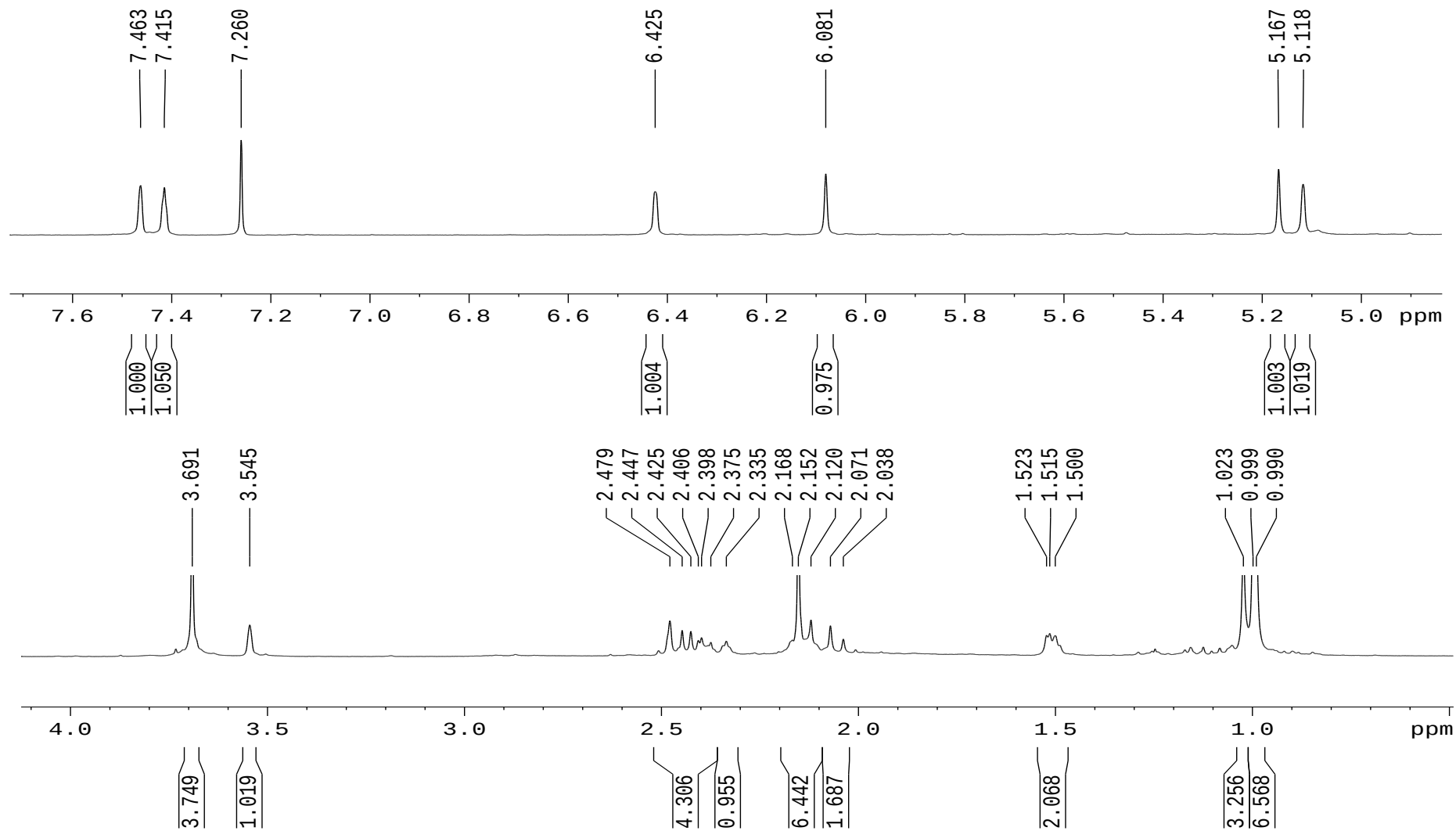
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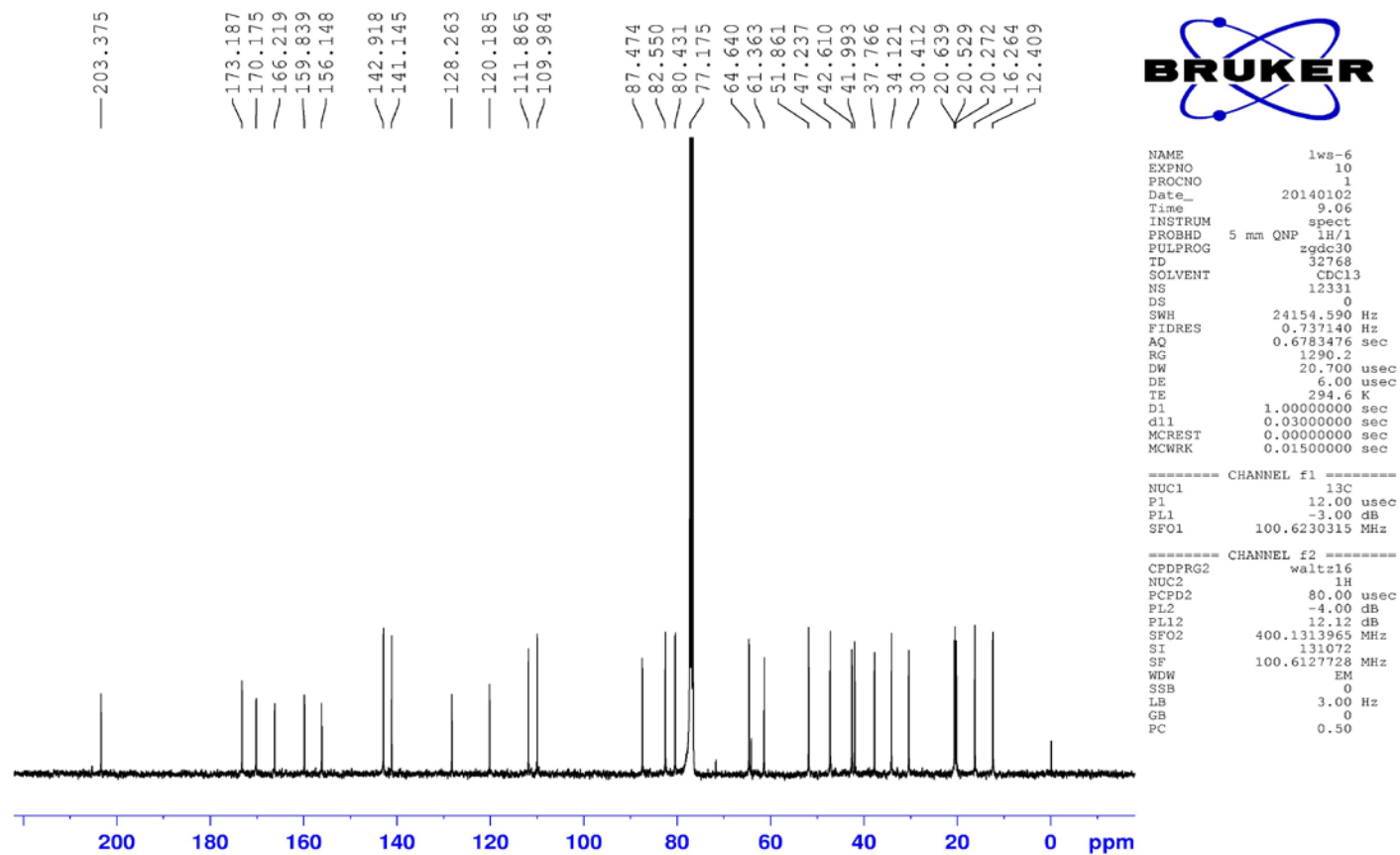
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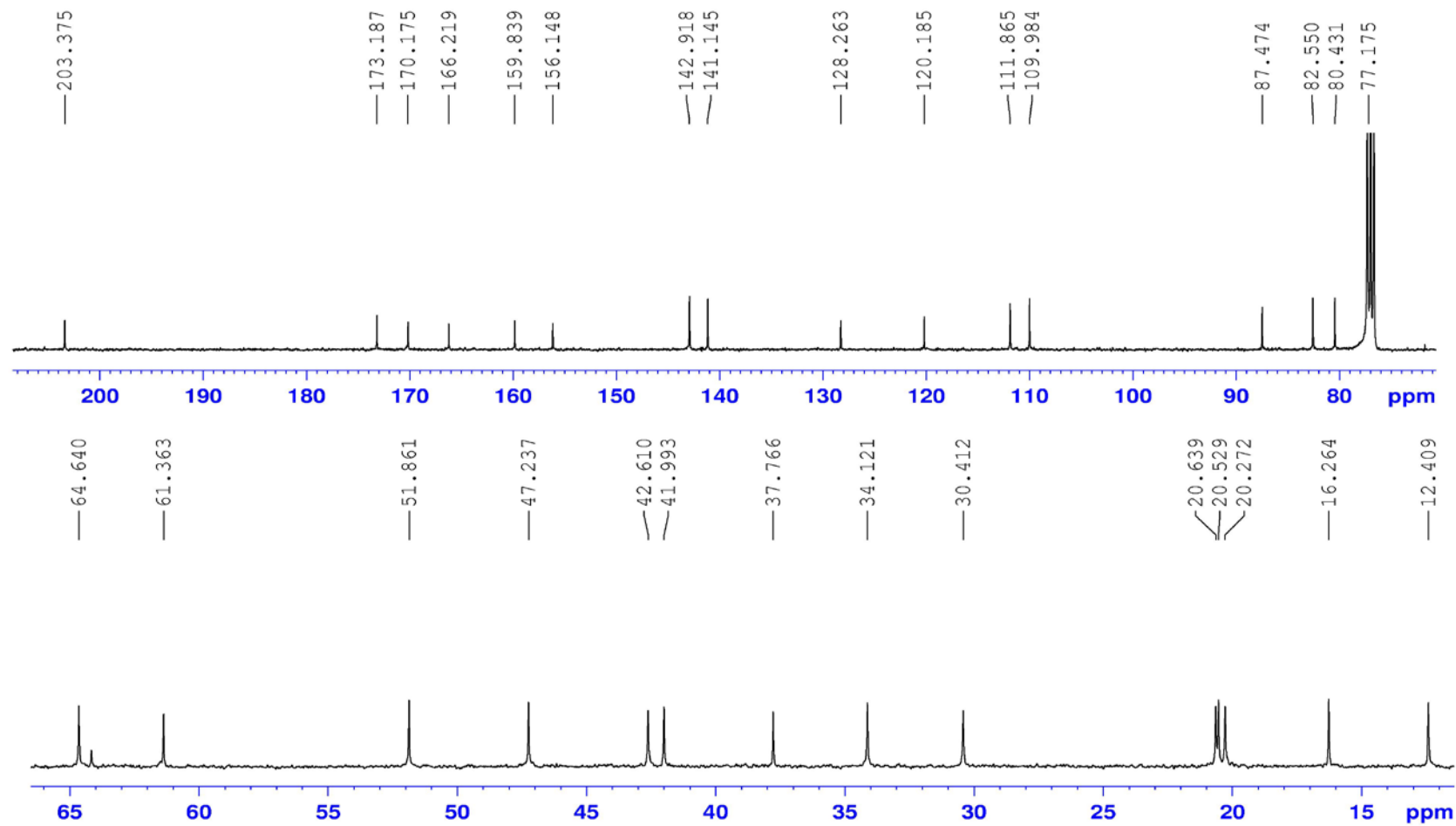
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lws-6-1H

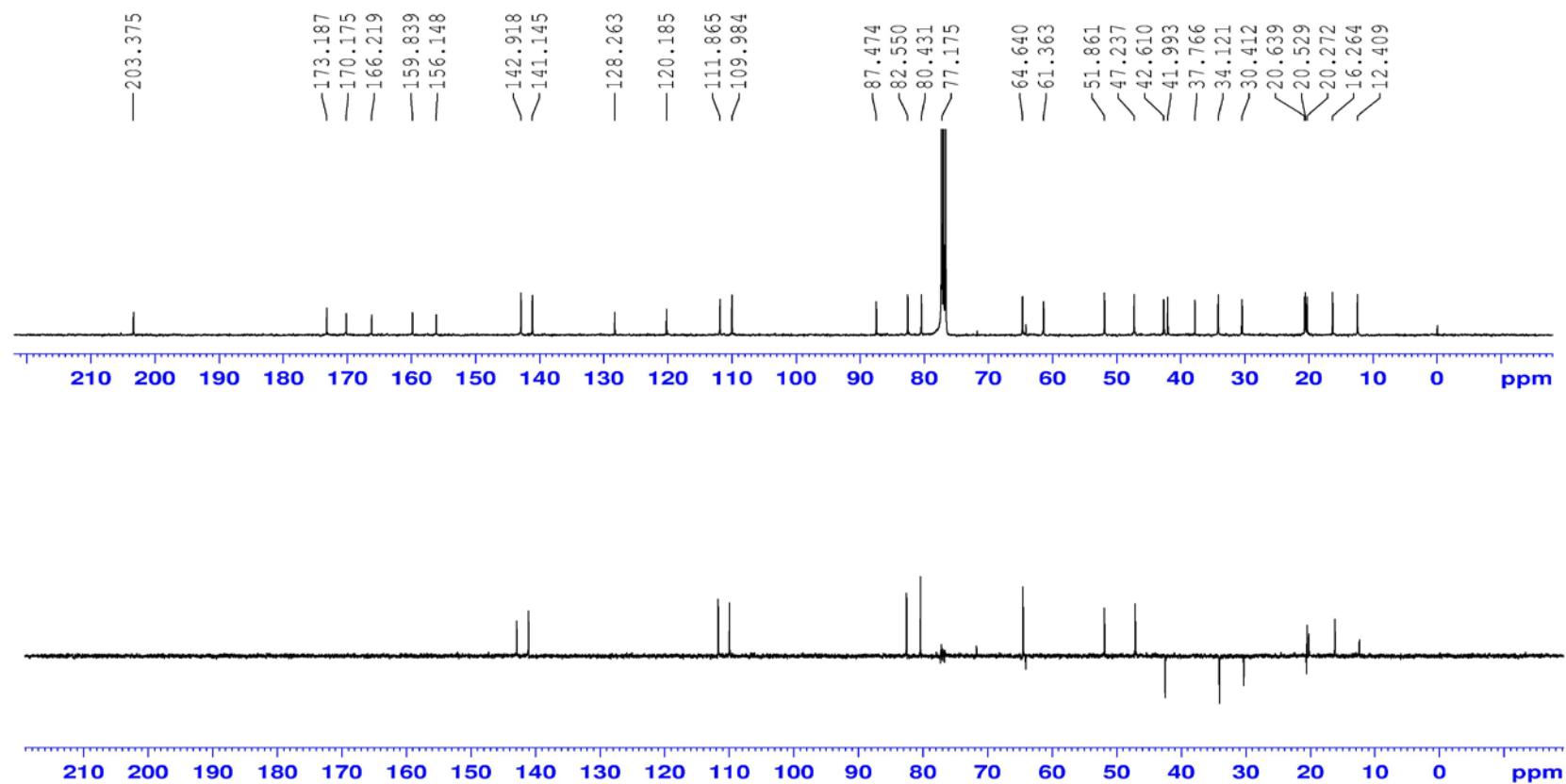


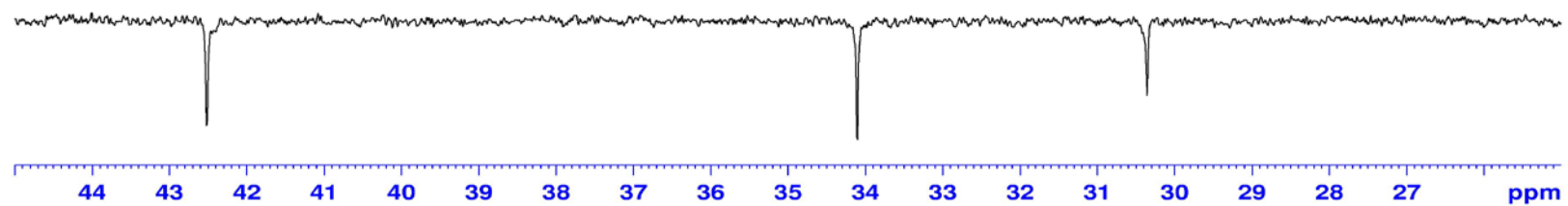
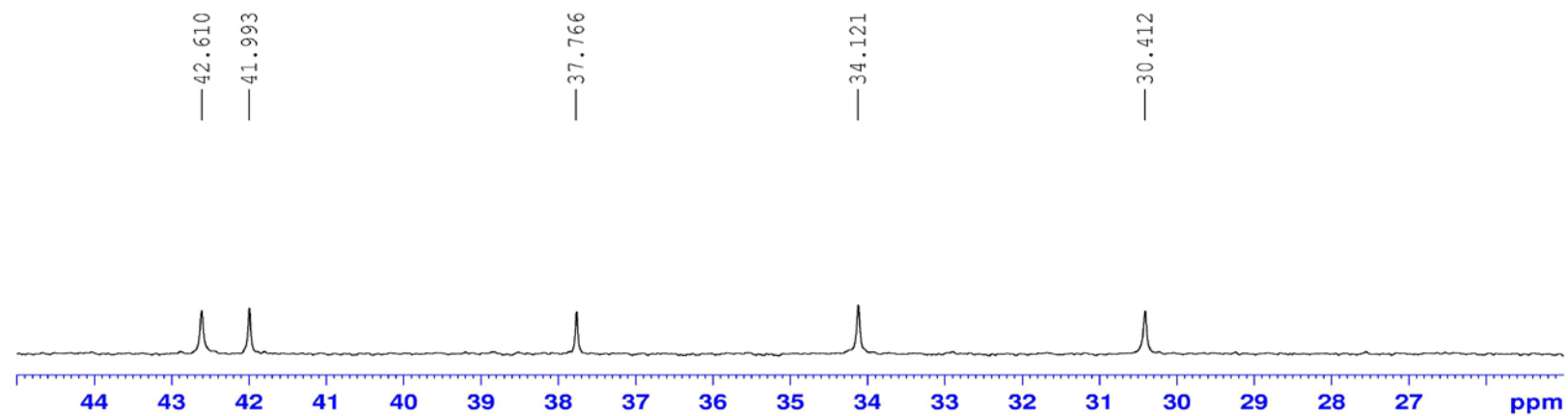
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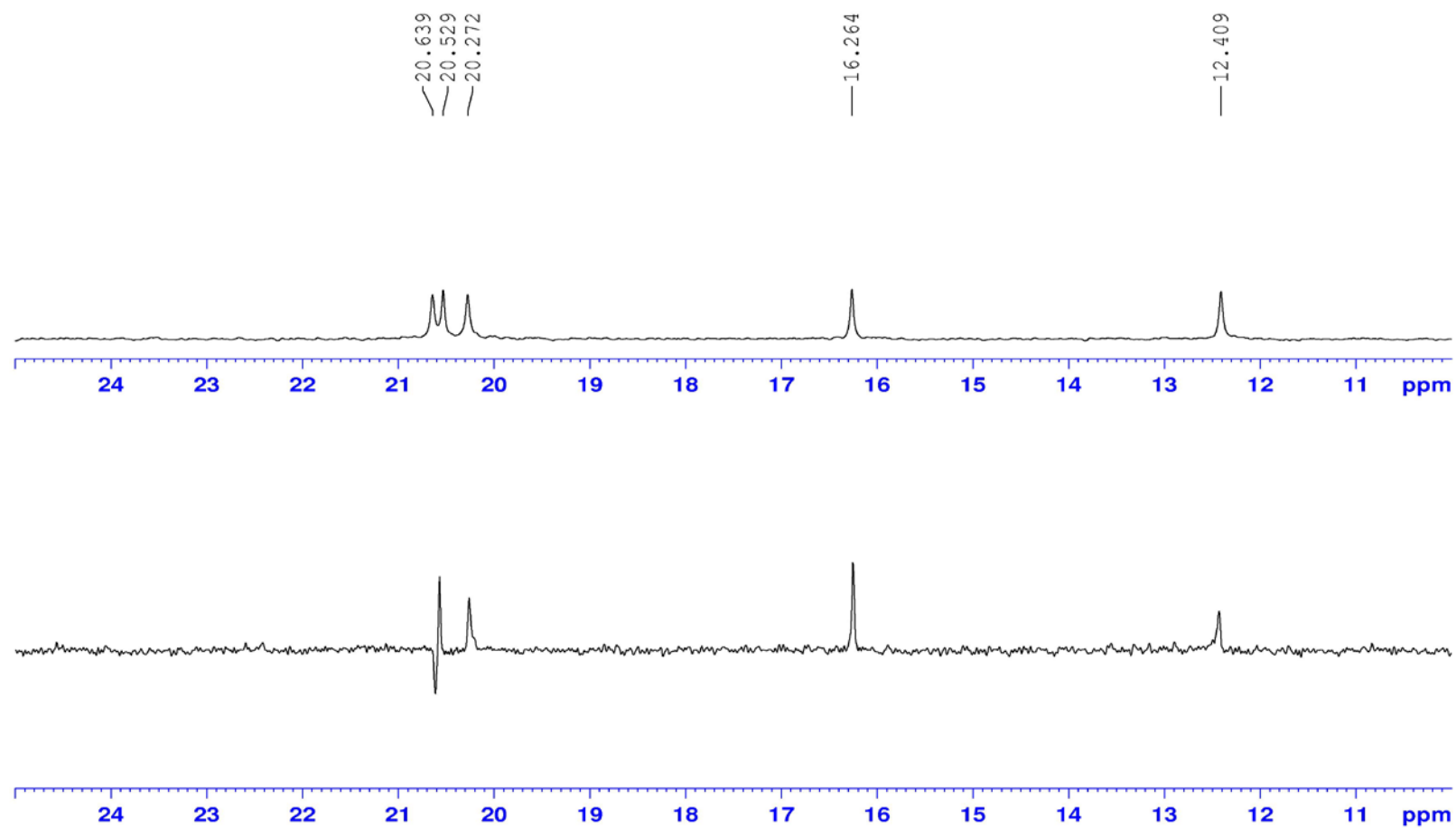




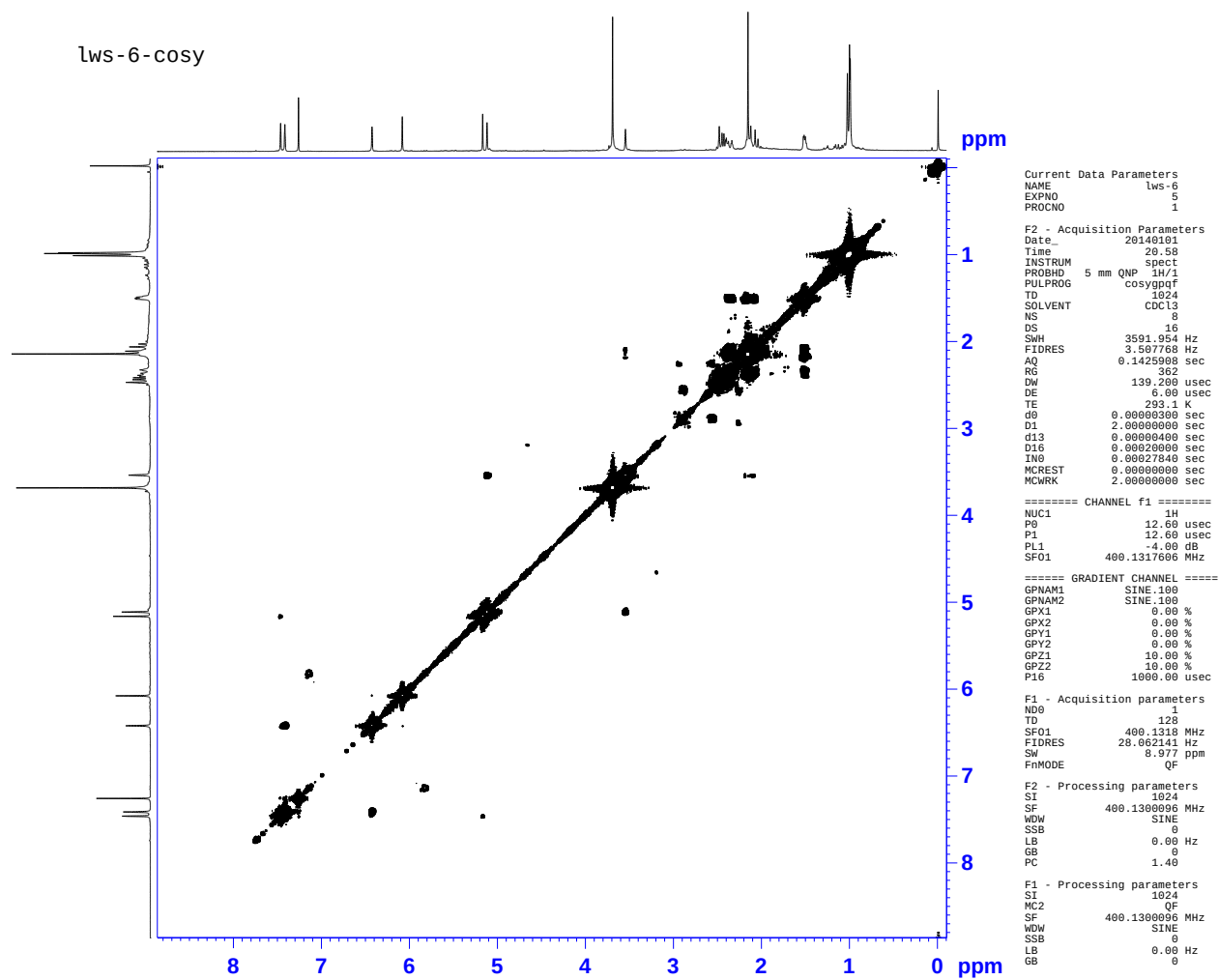
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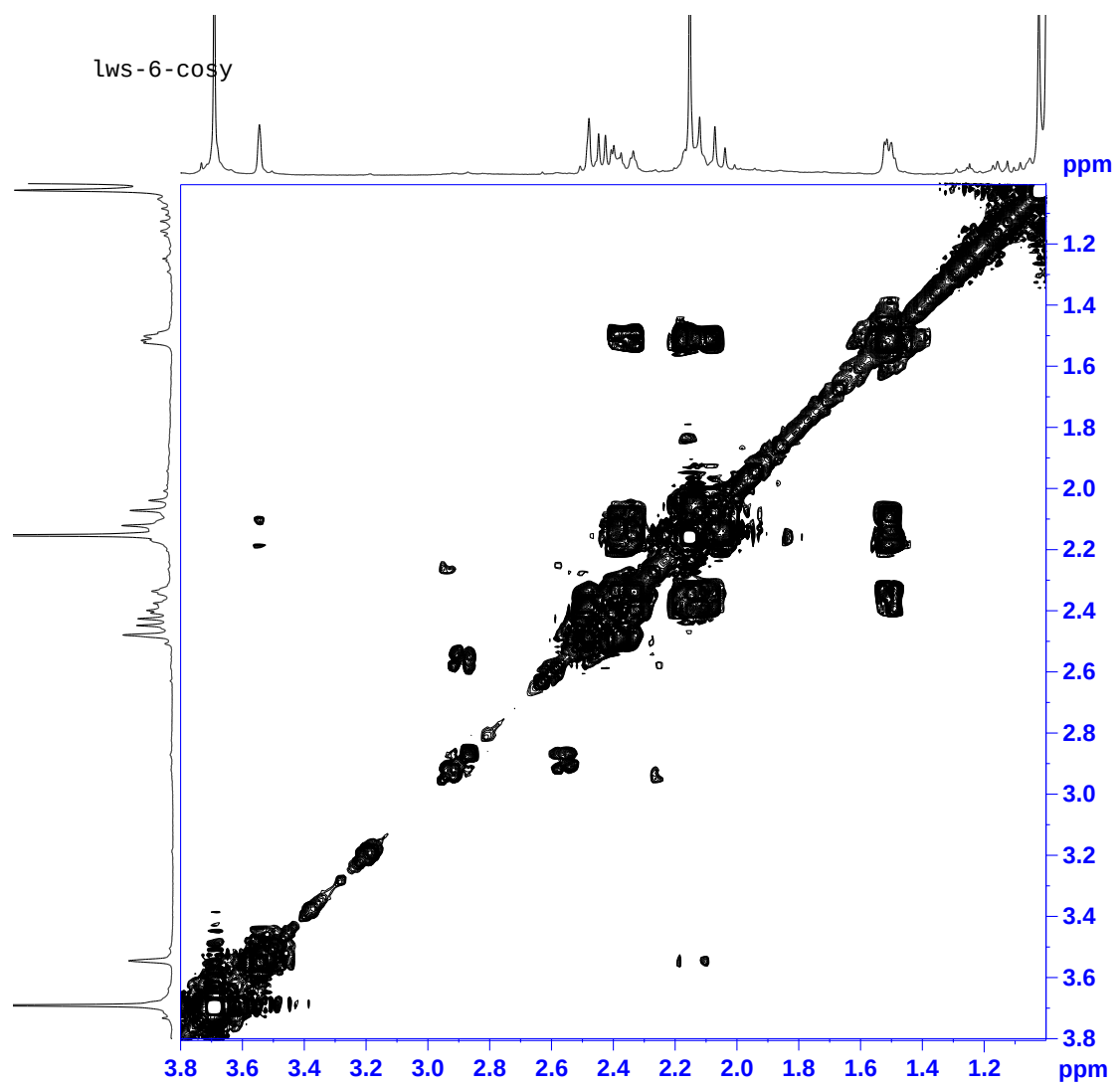




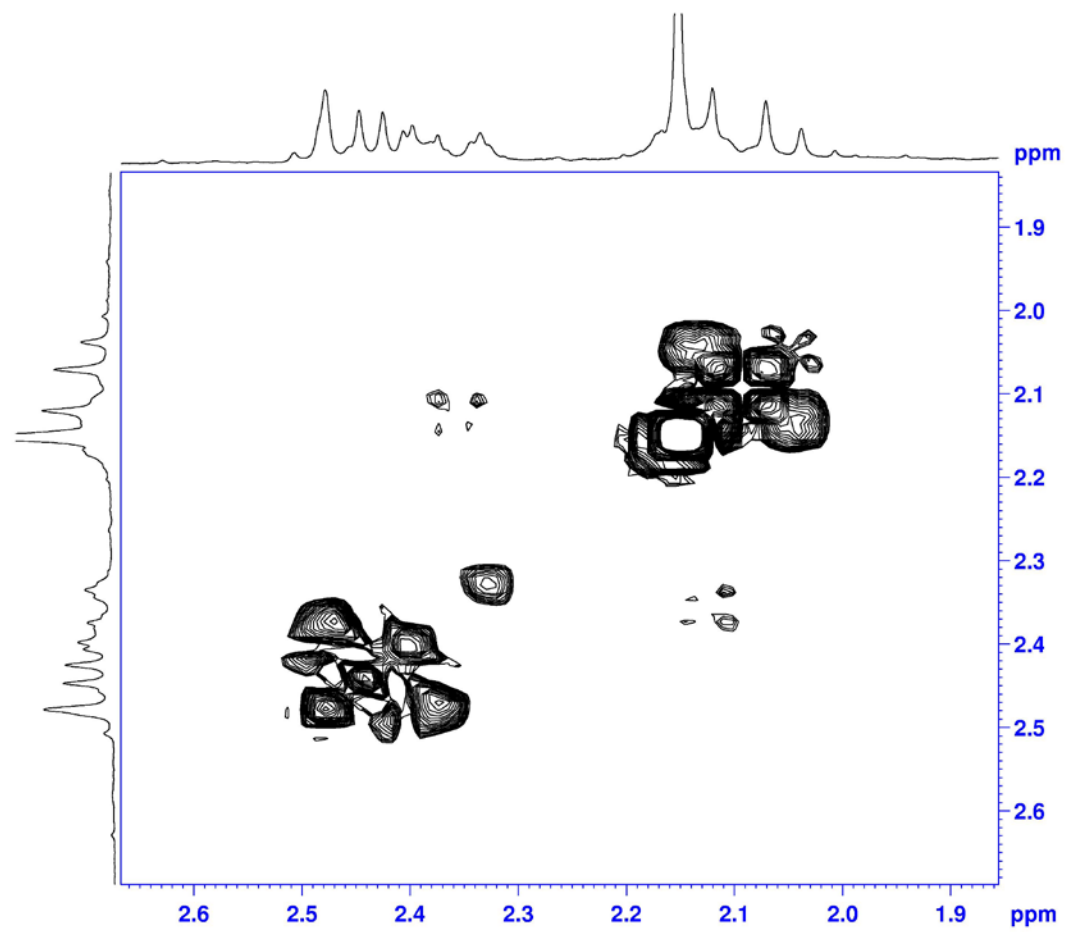


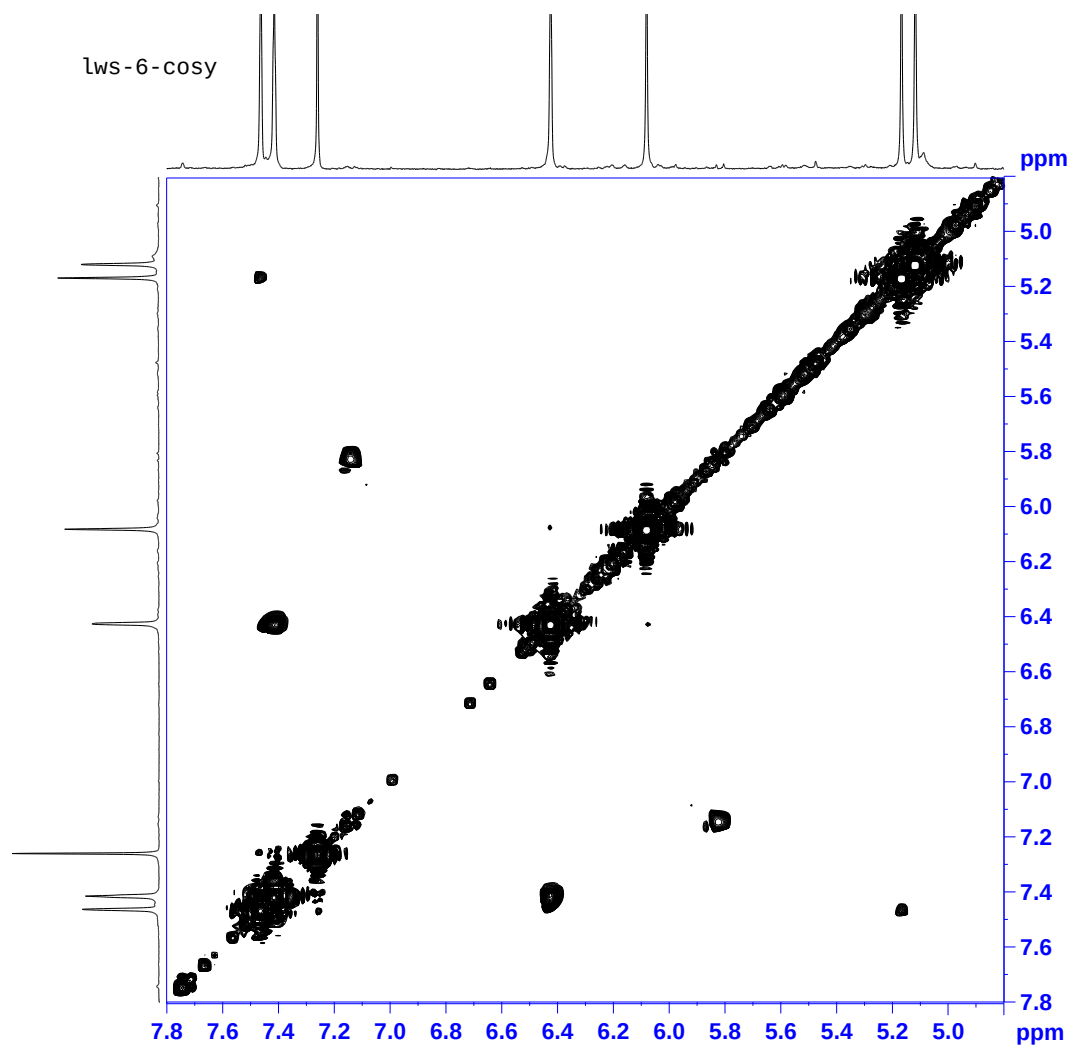
^1H - ^1H COSY (400 MHz) spectrum of Thaixylomolin M (7) in CDCl_3





S16

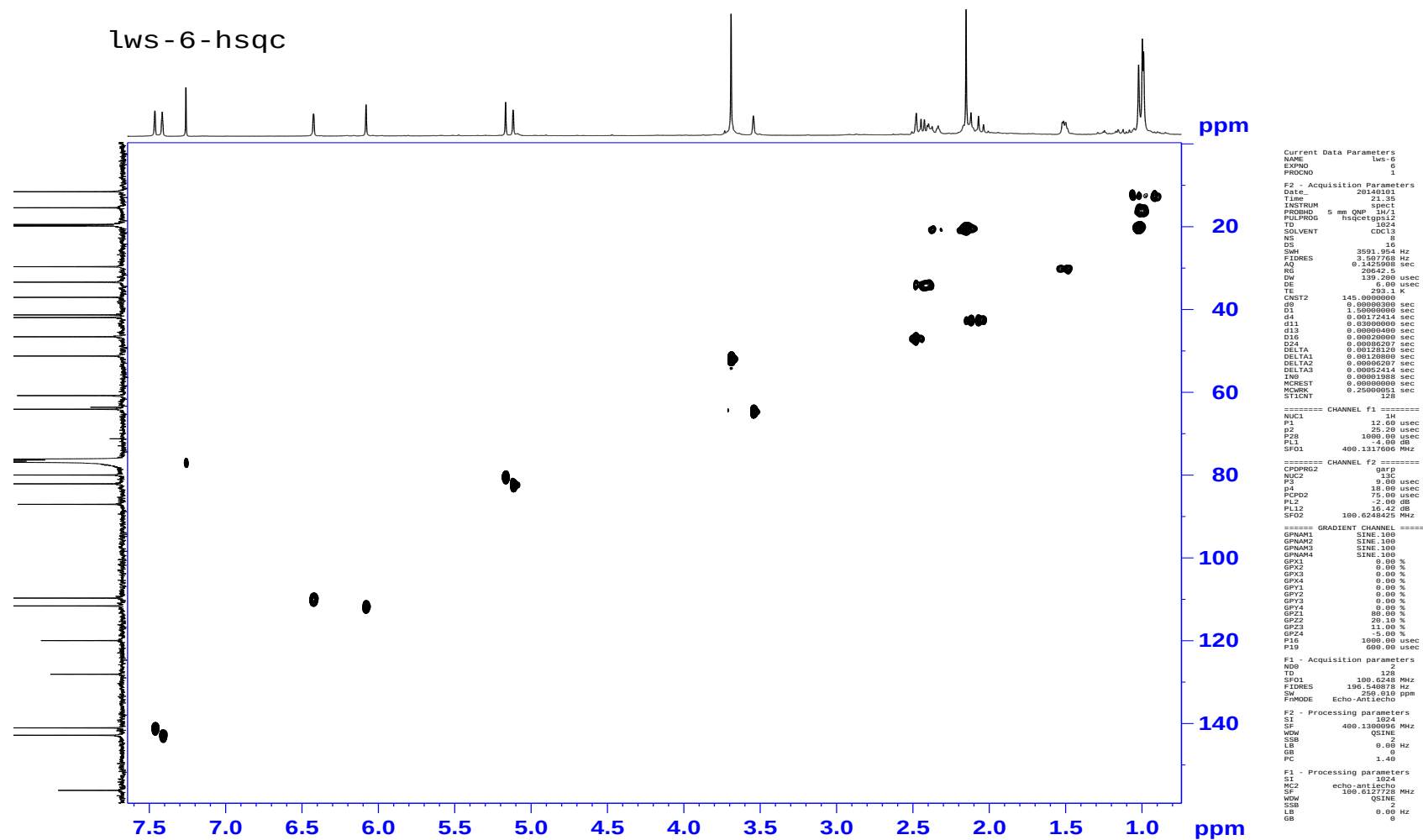


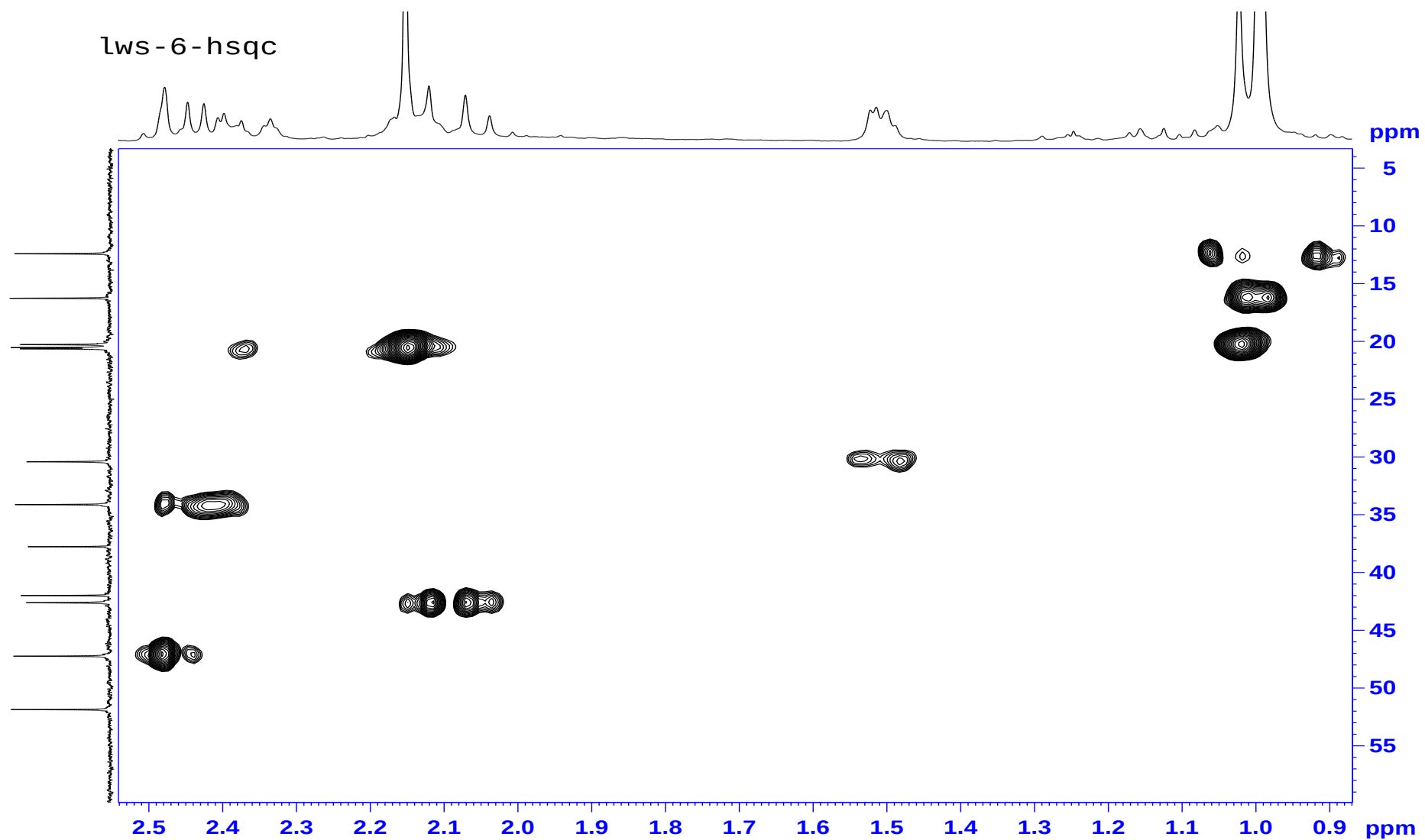


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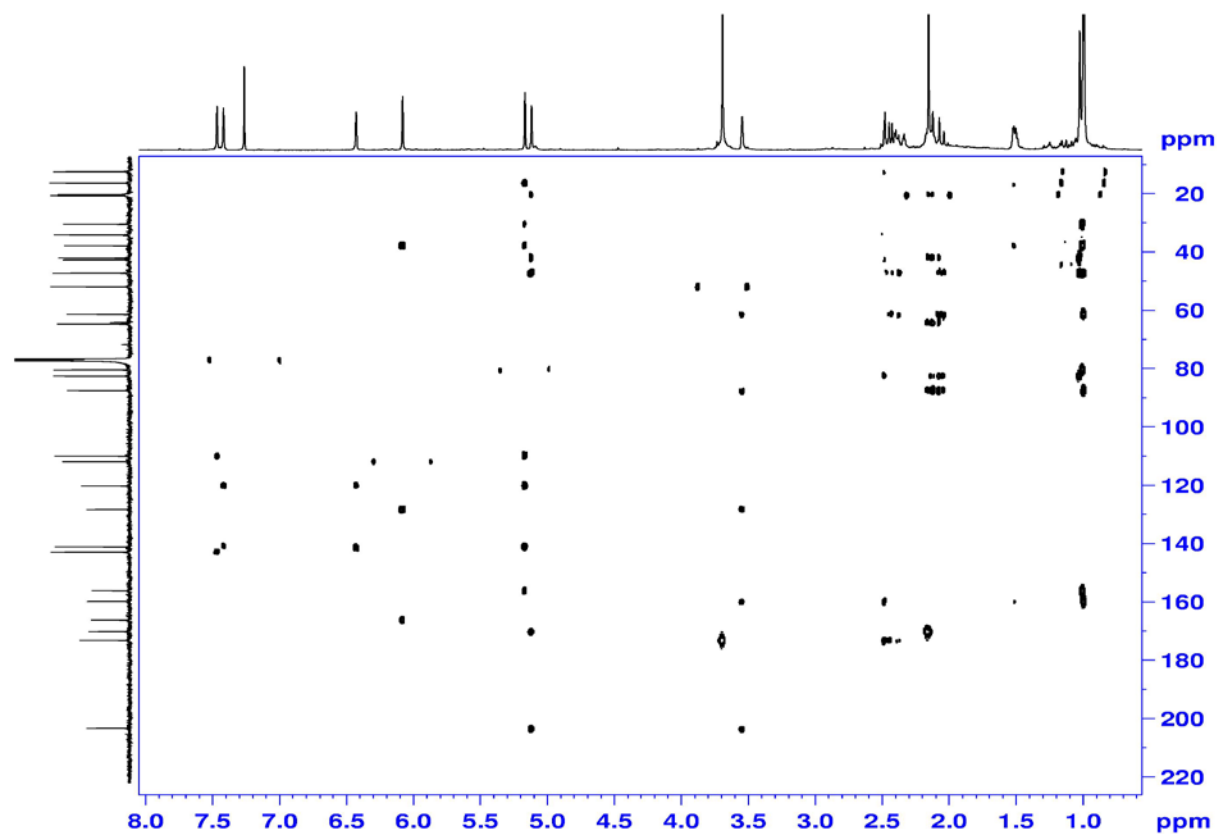
lws-6-hsqc





S20

HMBC (400 MHz) spectrum of Thaixylomolin M (7) in CDCl₃



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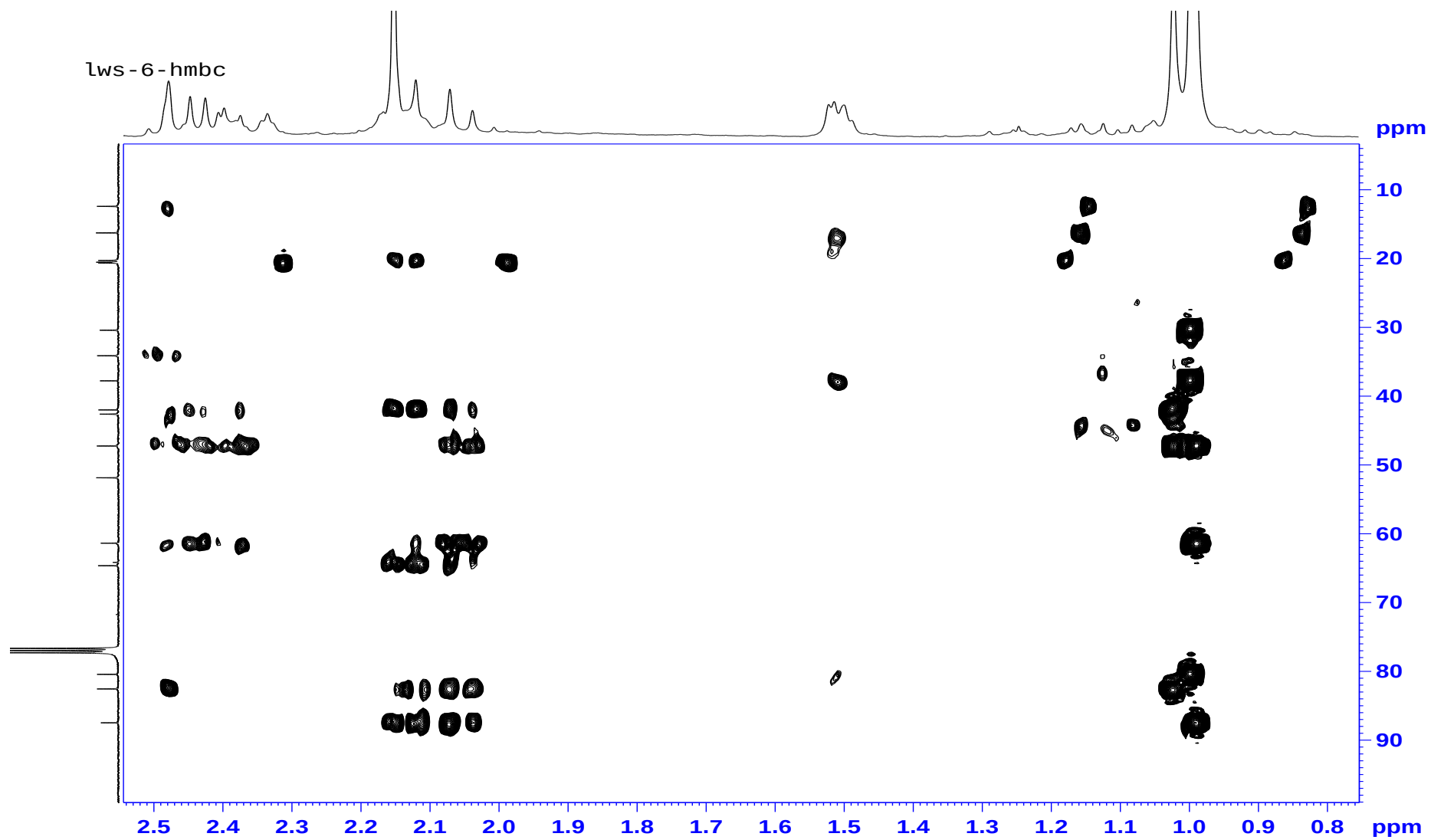
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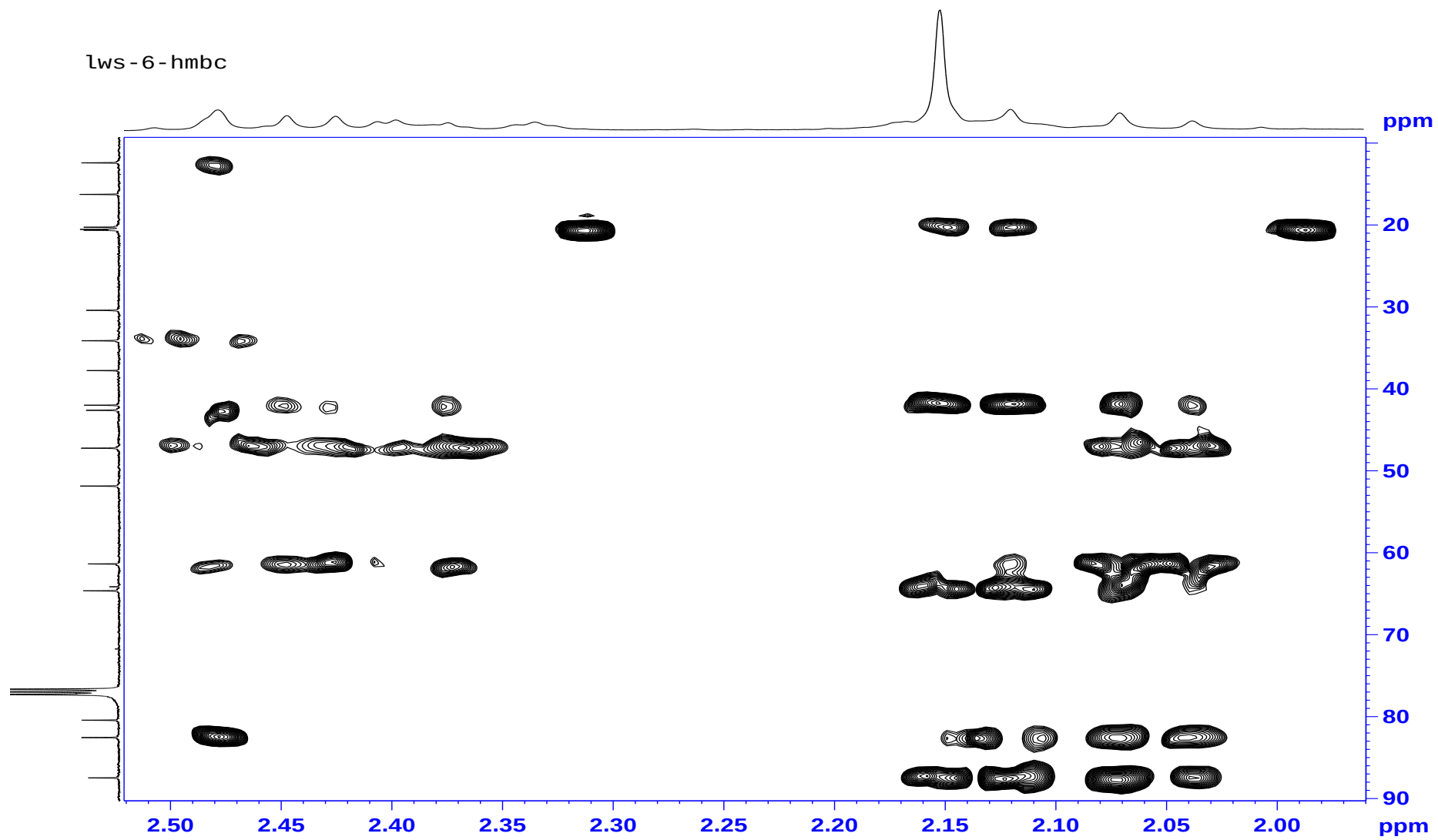
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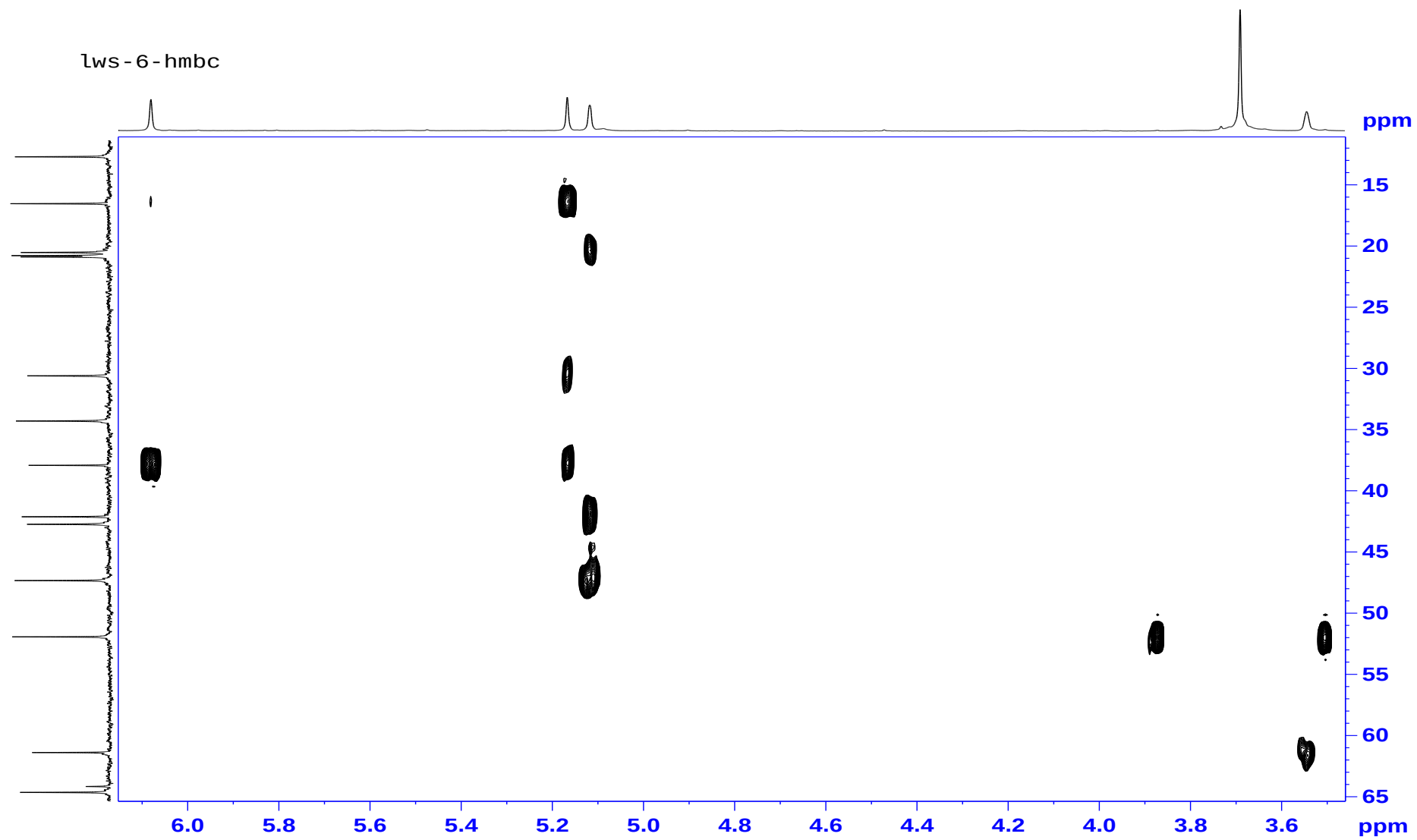
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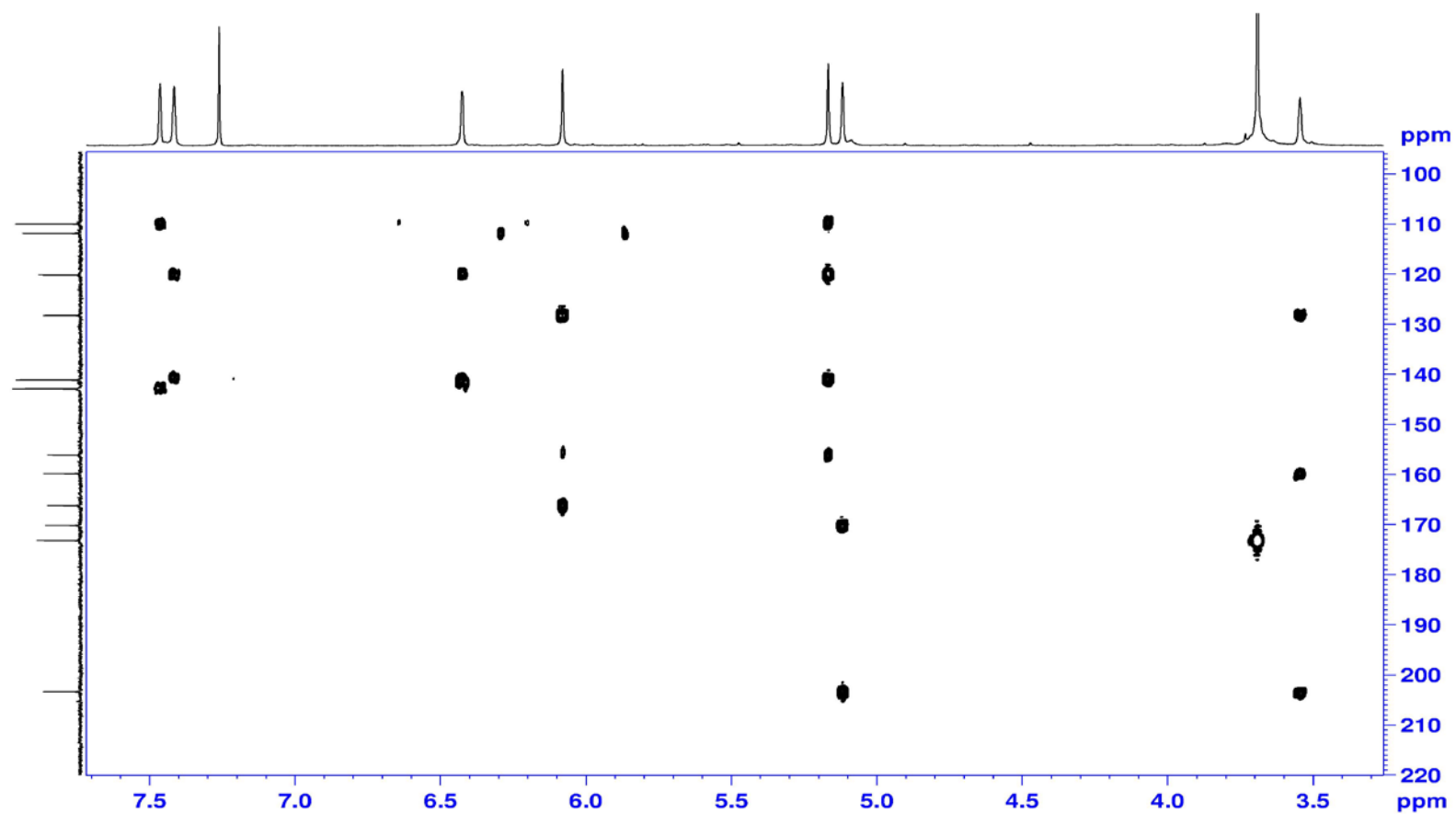
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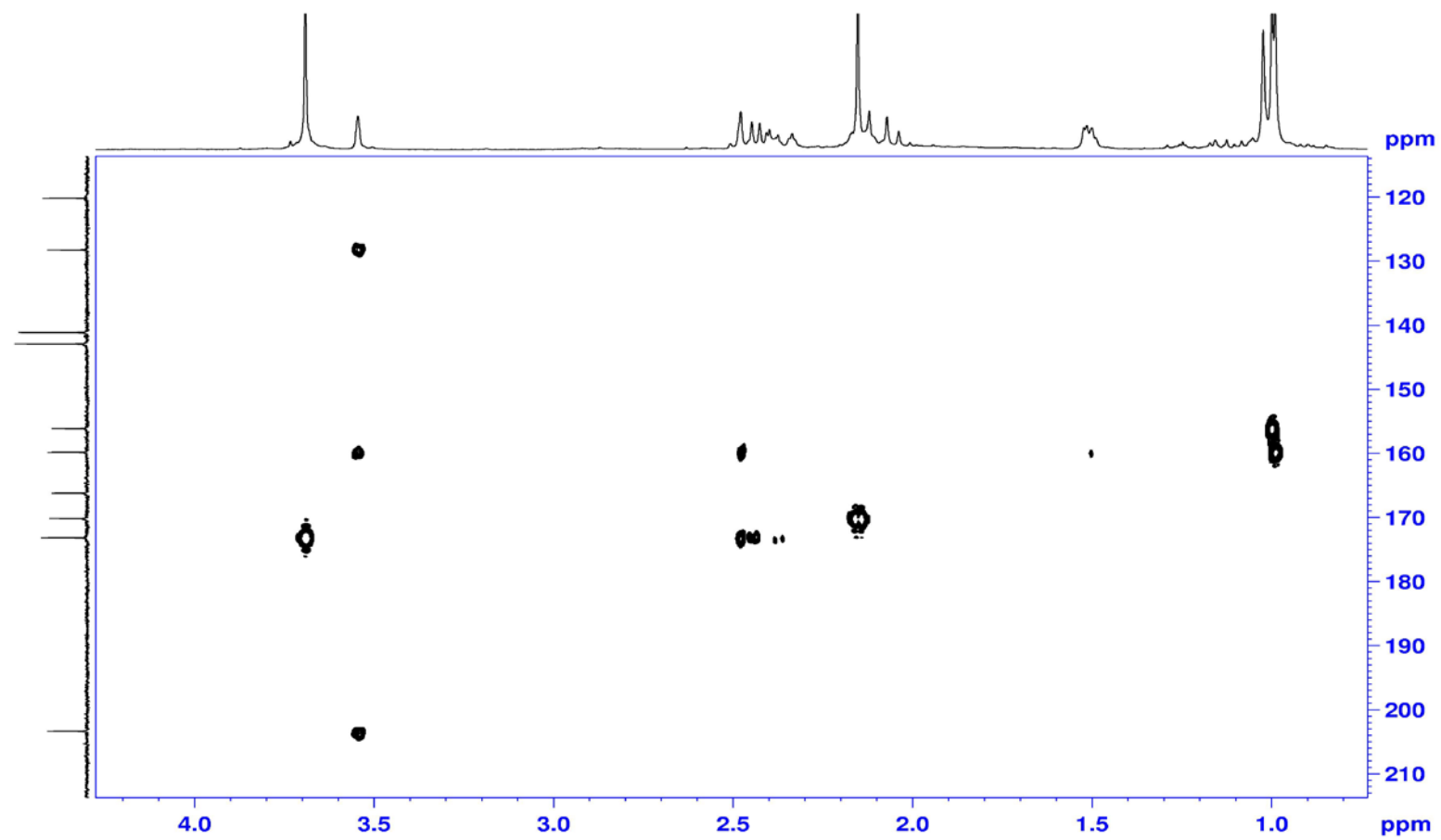
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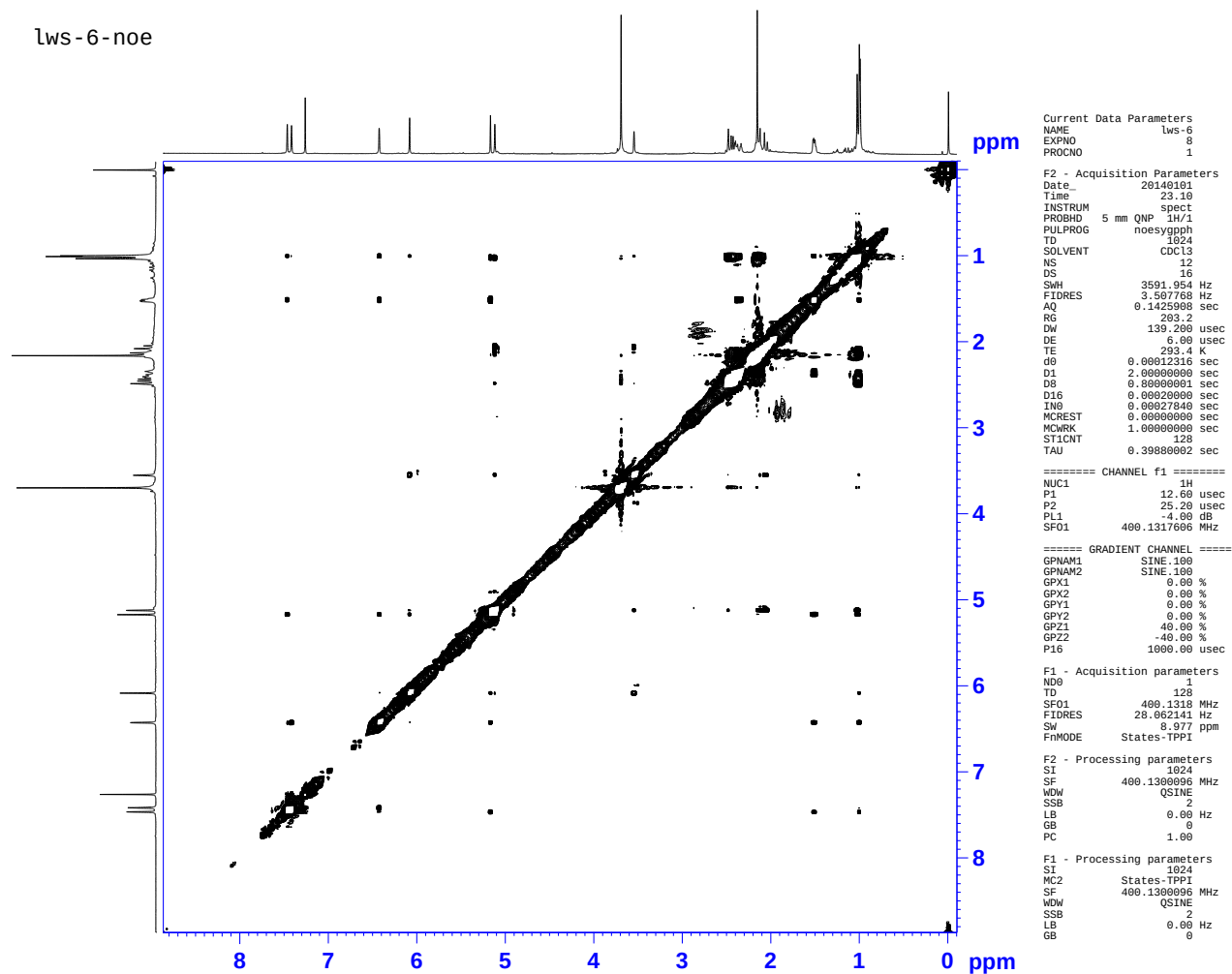
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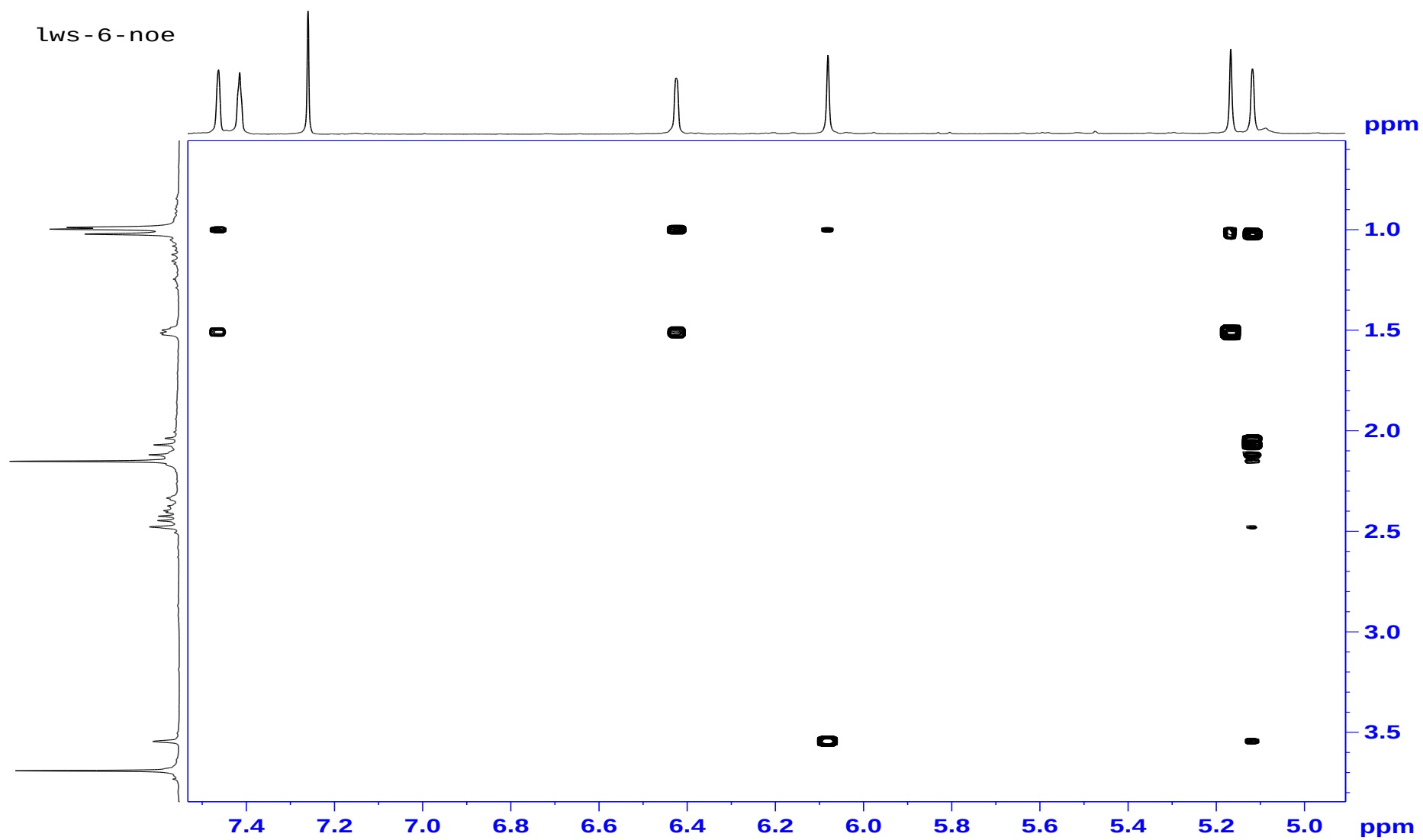


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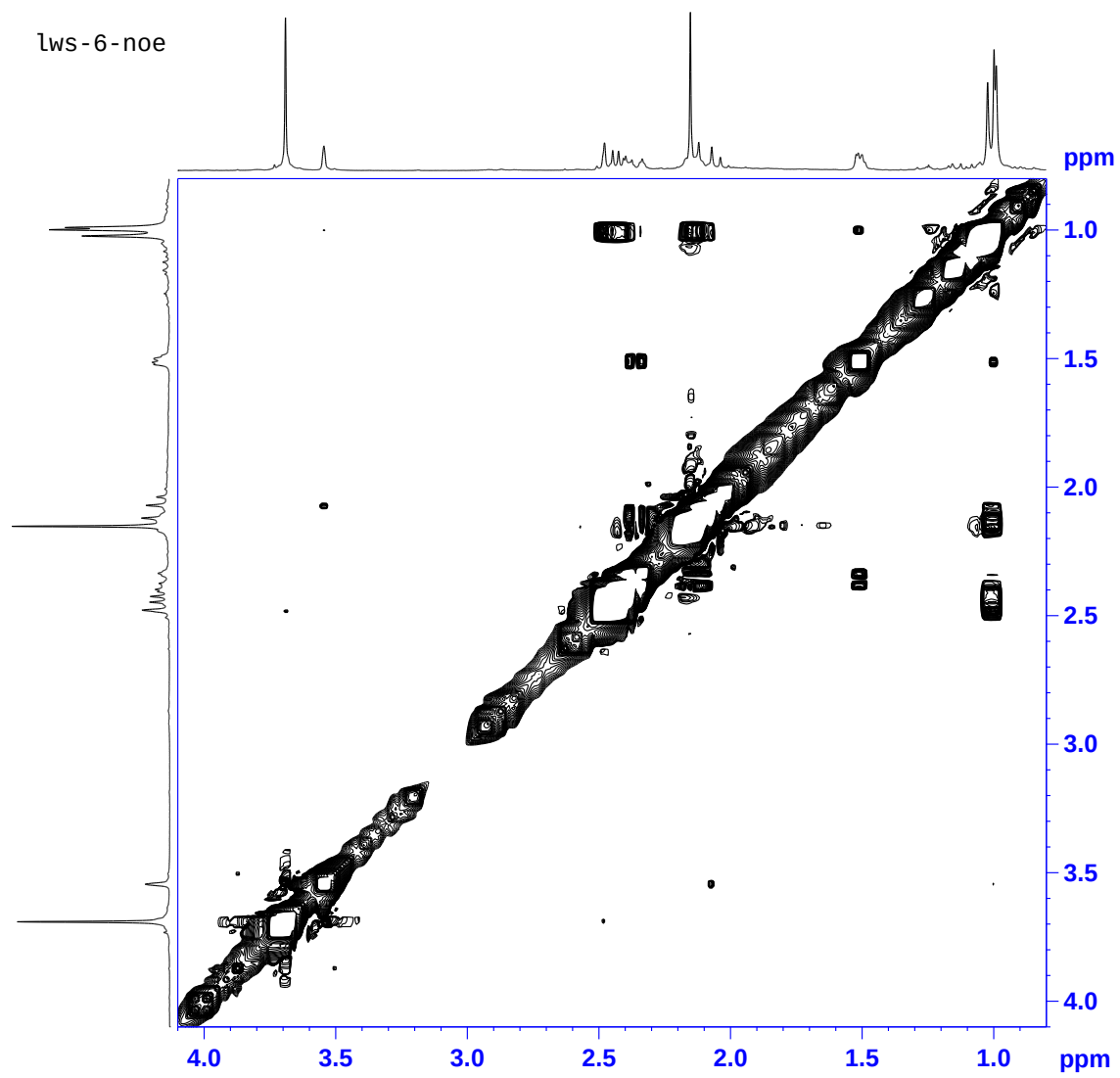
NOESY (400 MHz) spectrum of Thaixylomolin M (7) in CDCl₃

lws-6-noe

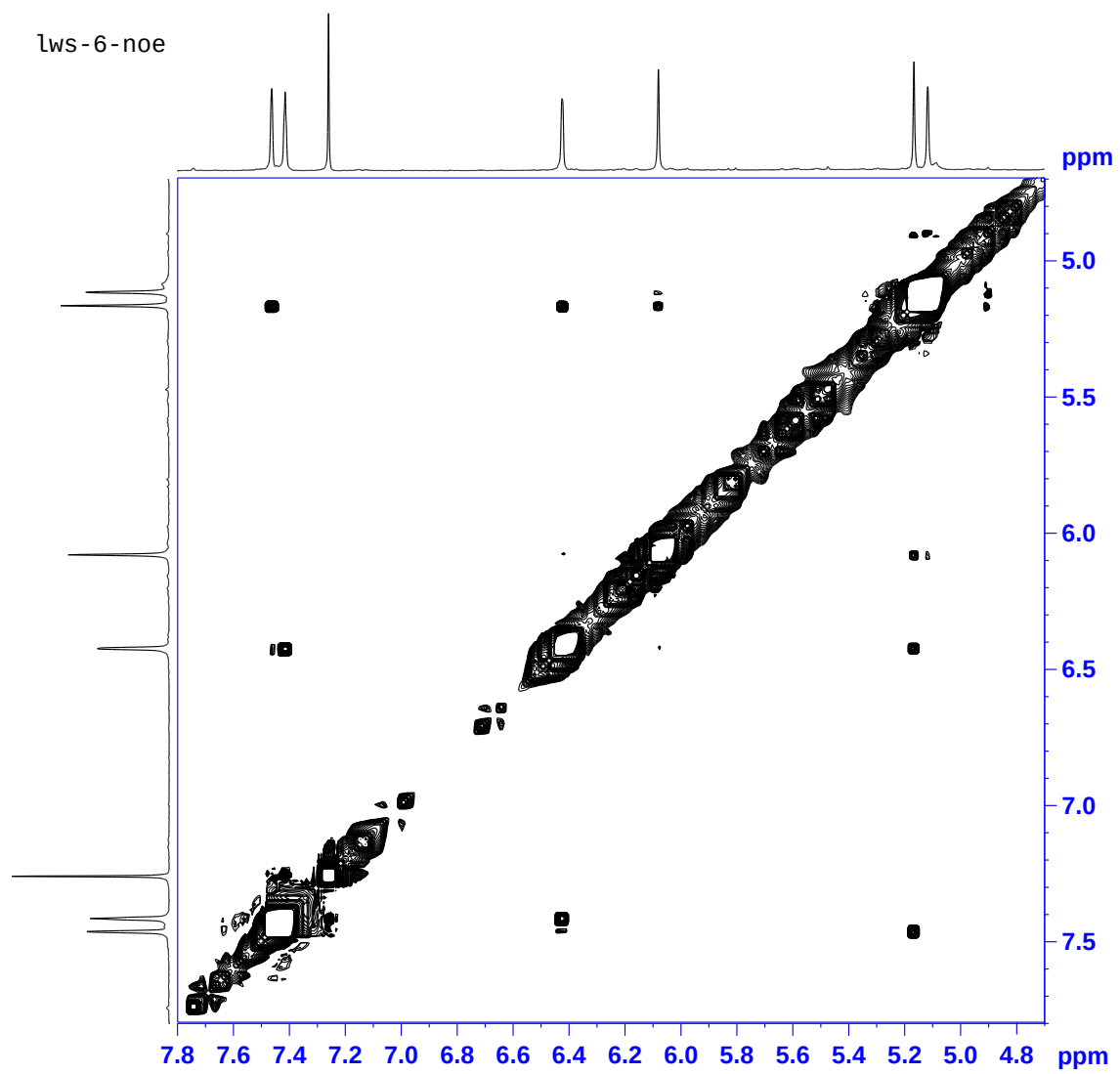




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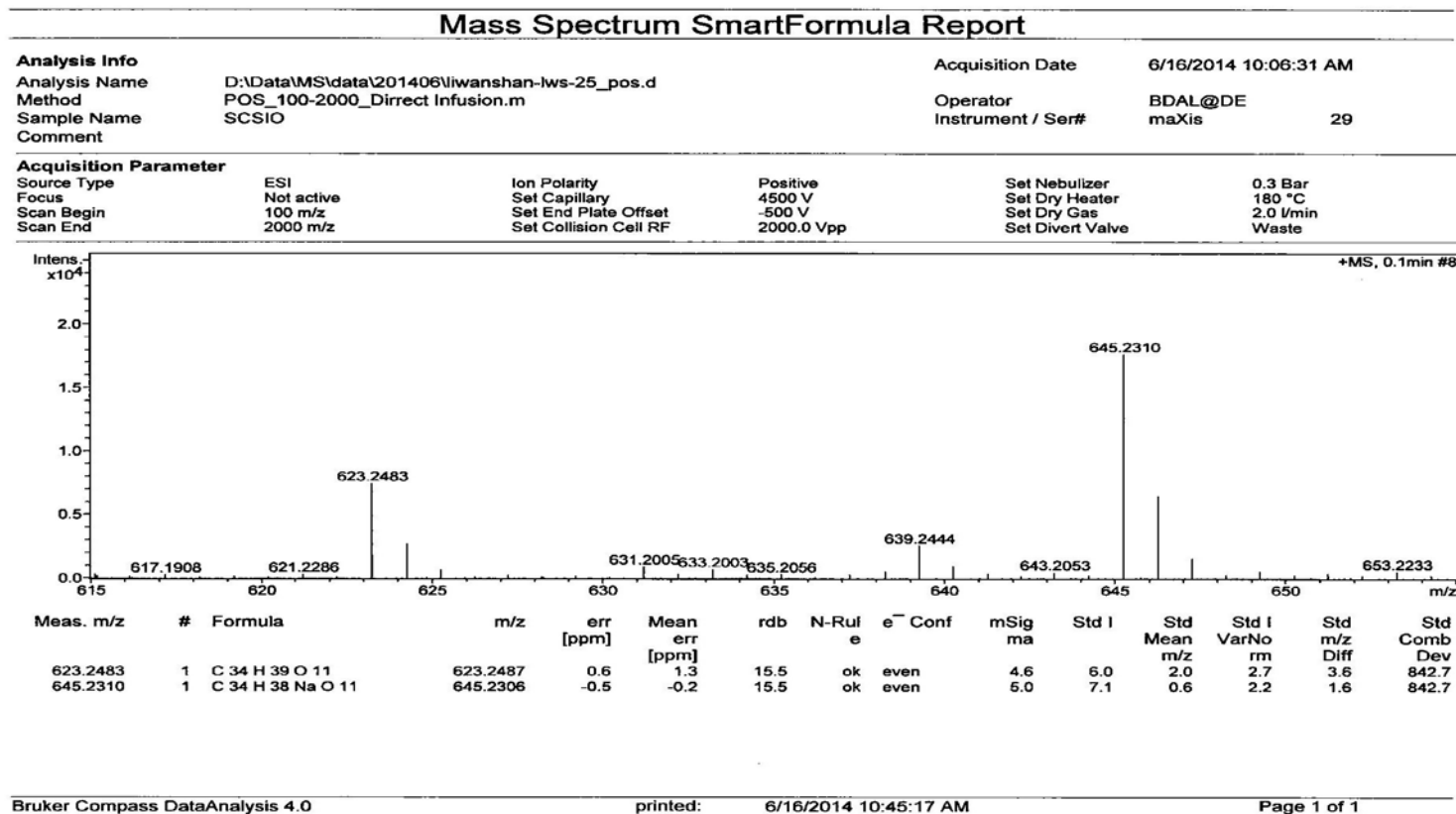


S29



S30

HR-ESIMS of Thaixylomolin N (8)



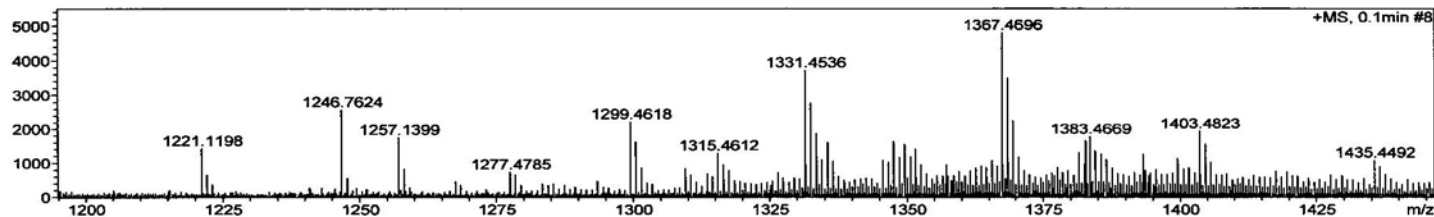
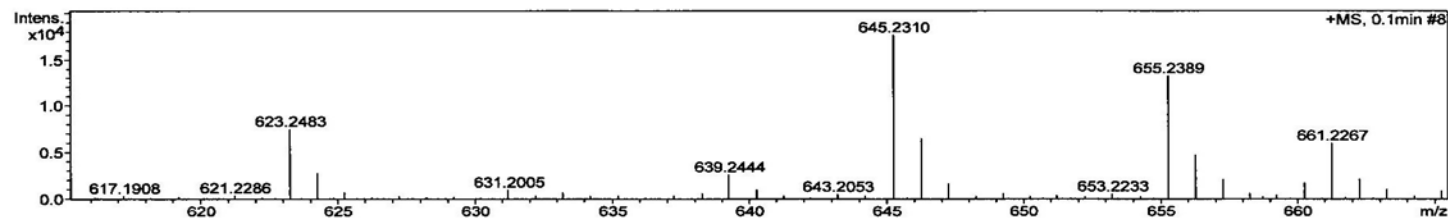
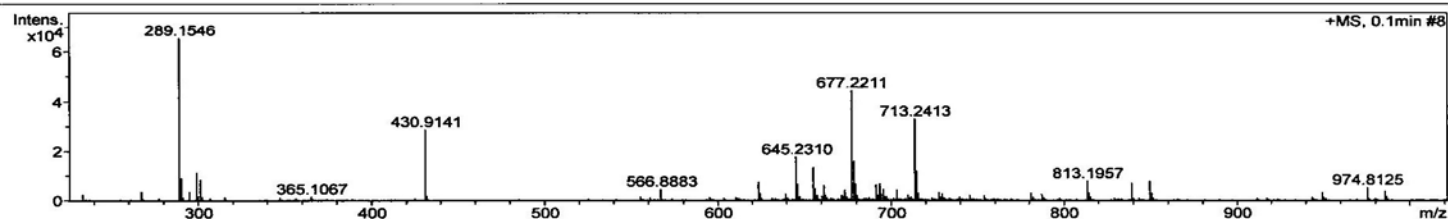
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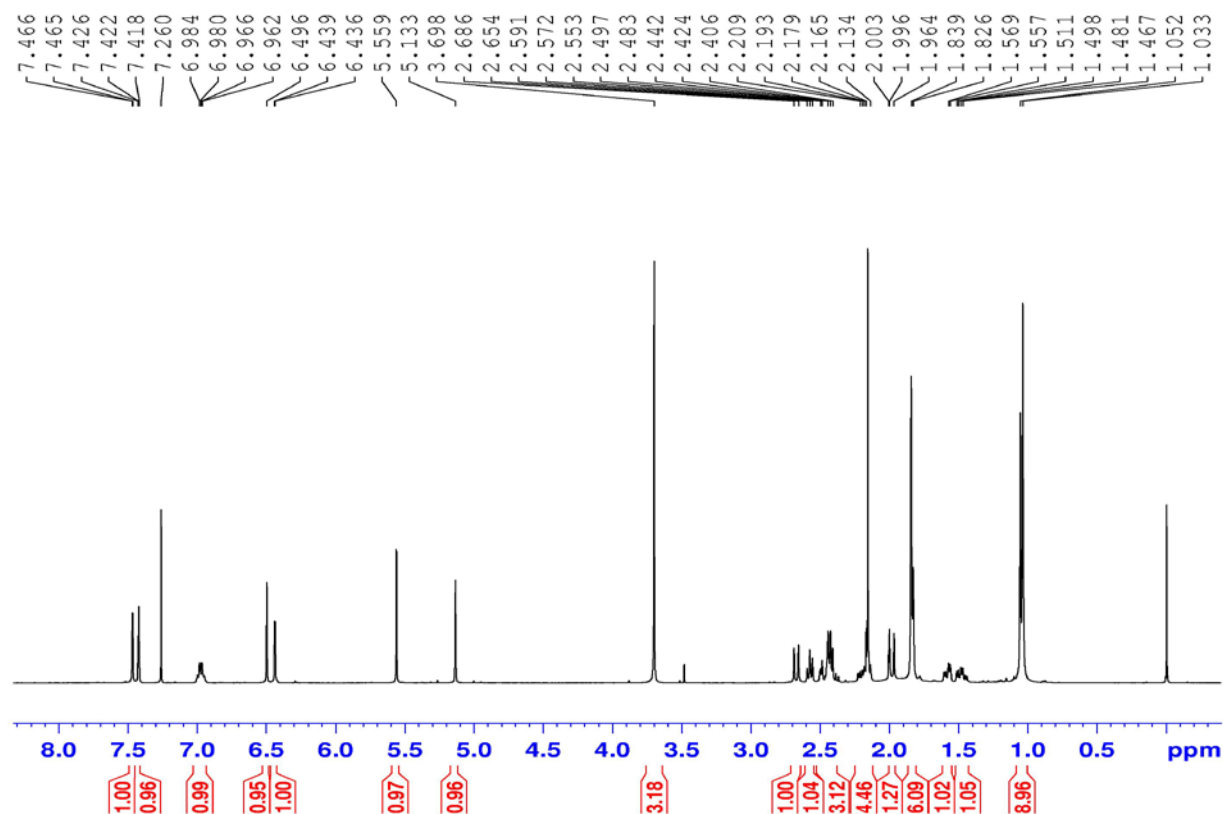
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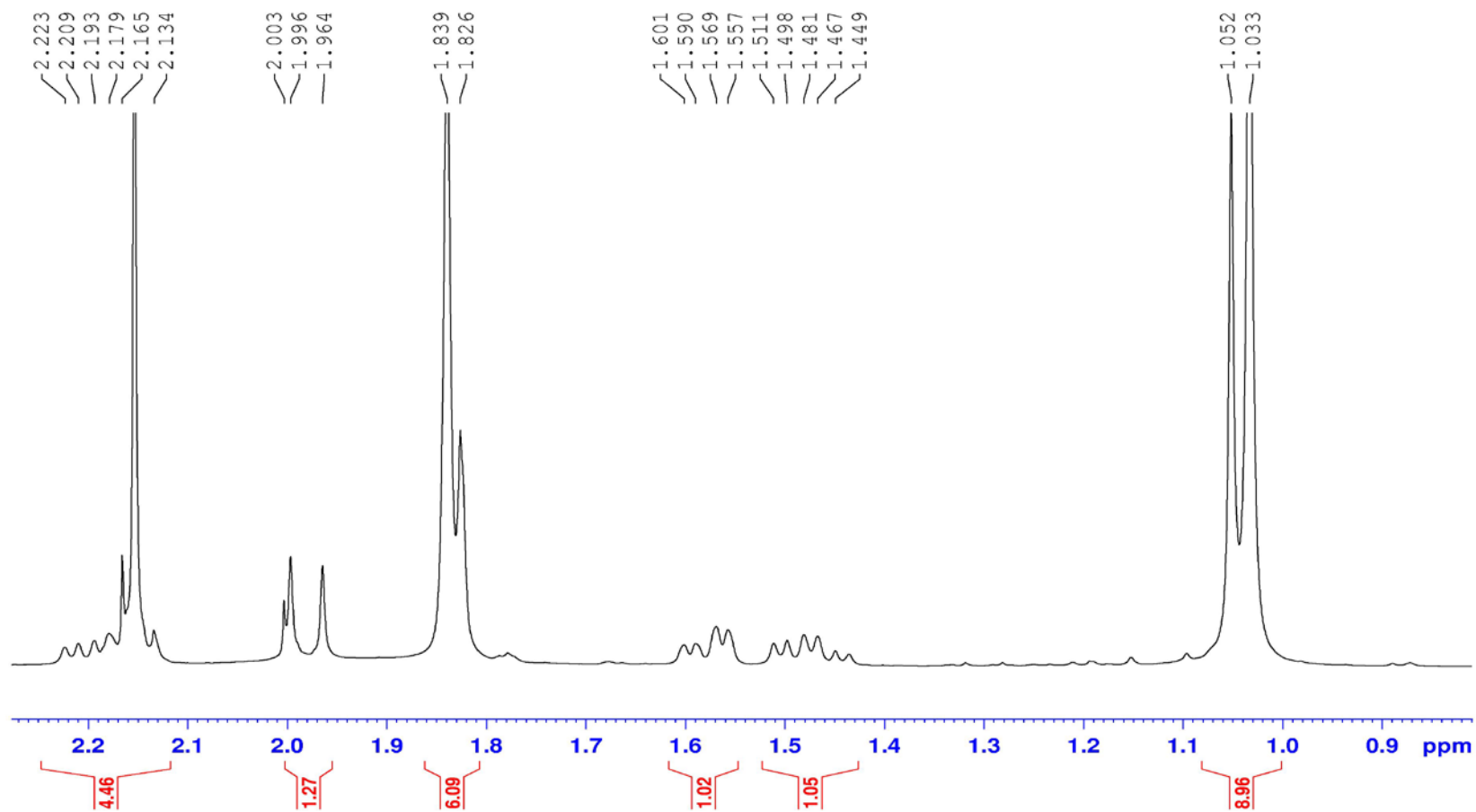
^1H NMR (400 MHz) spectrum of Thaixylomolin N (**8**) in CDCl_3

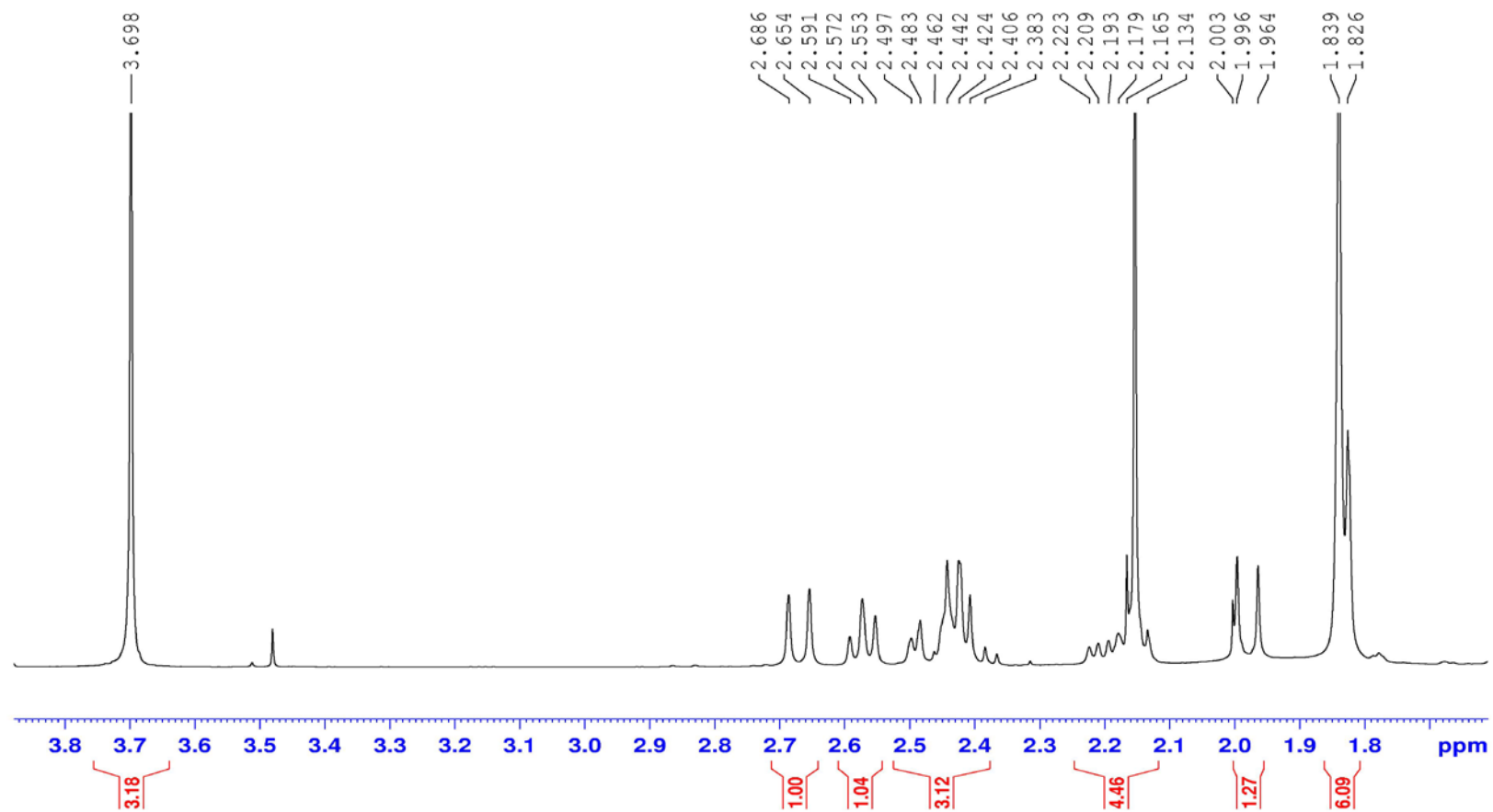


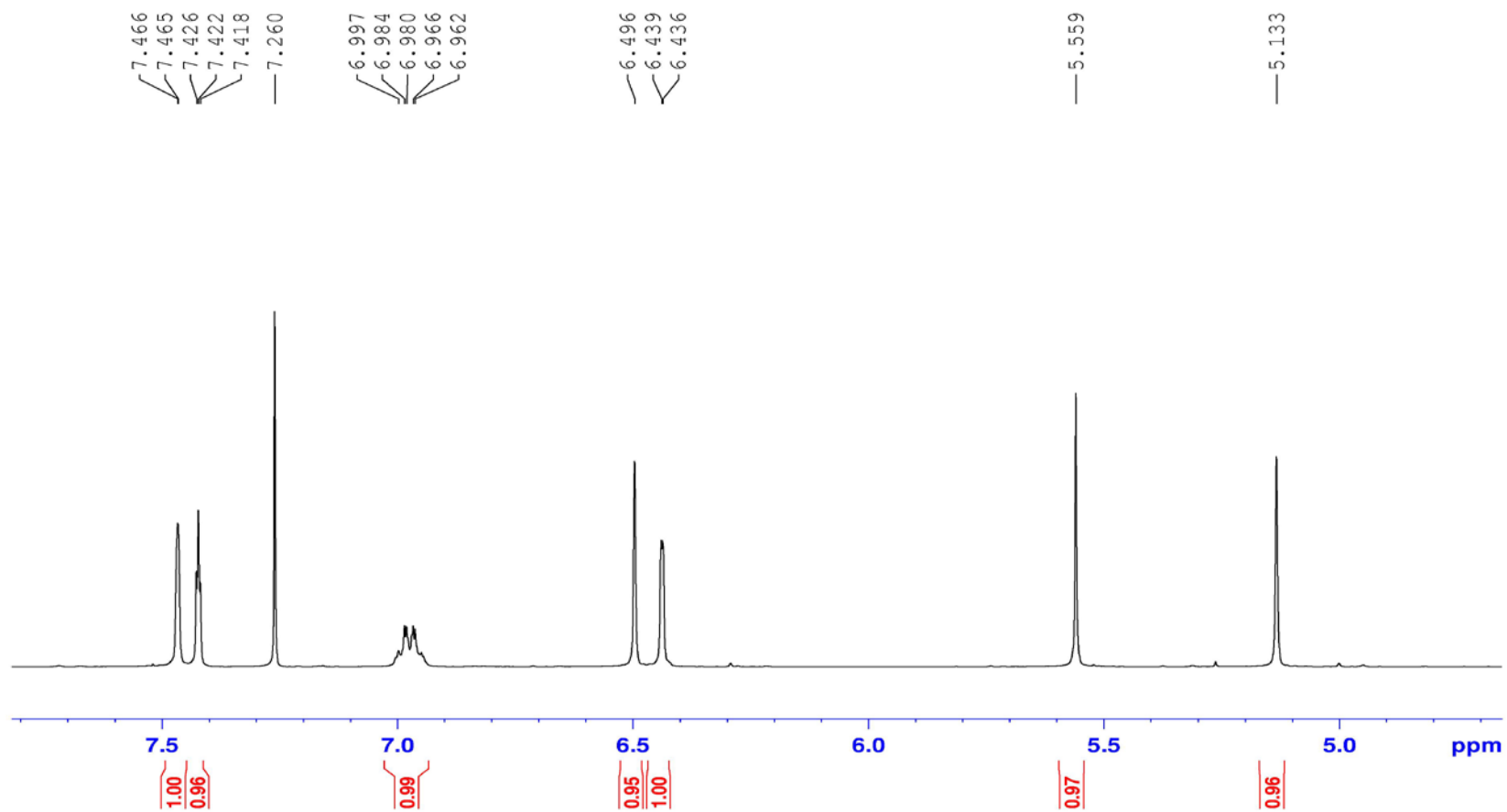
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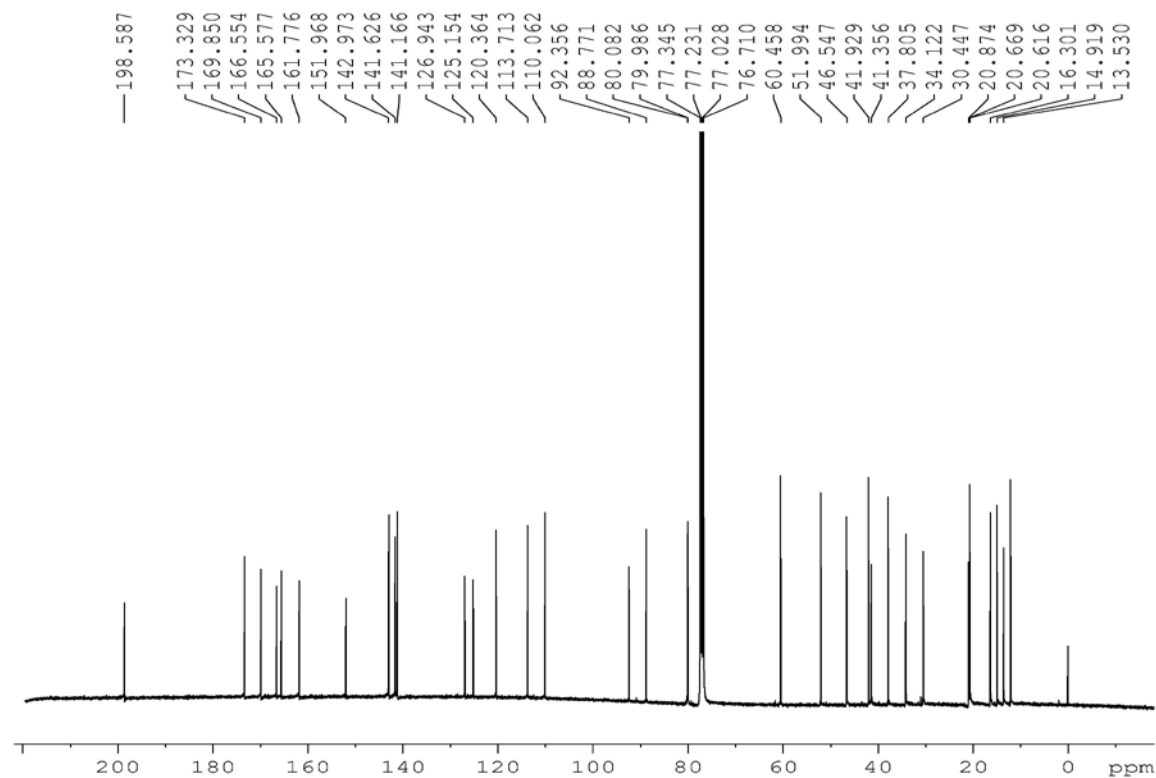
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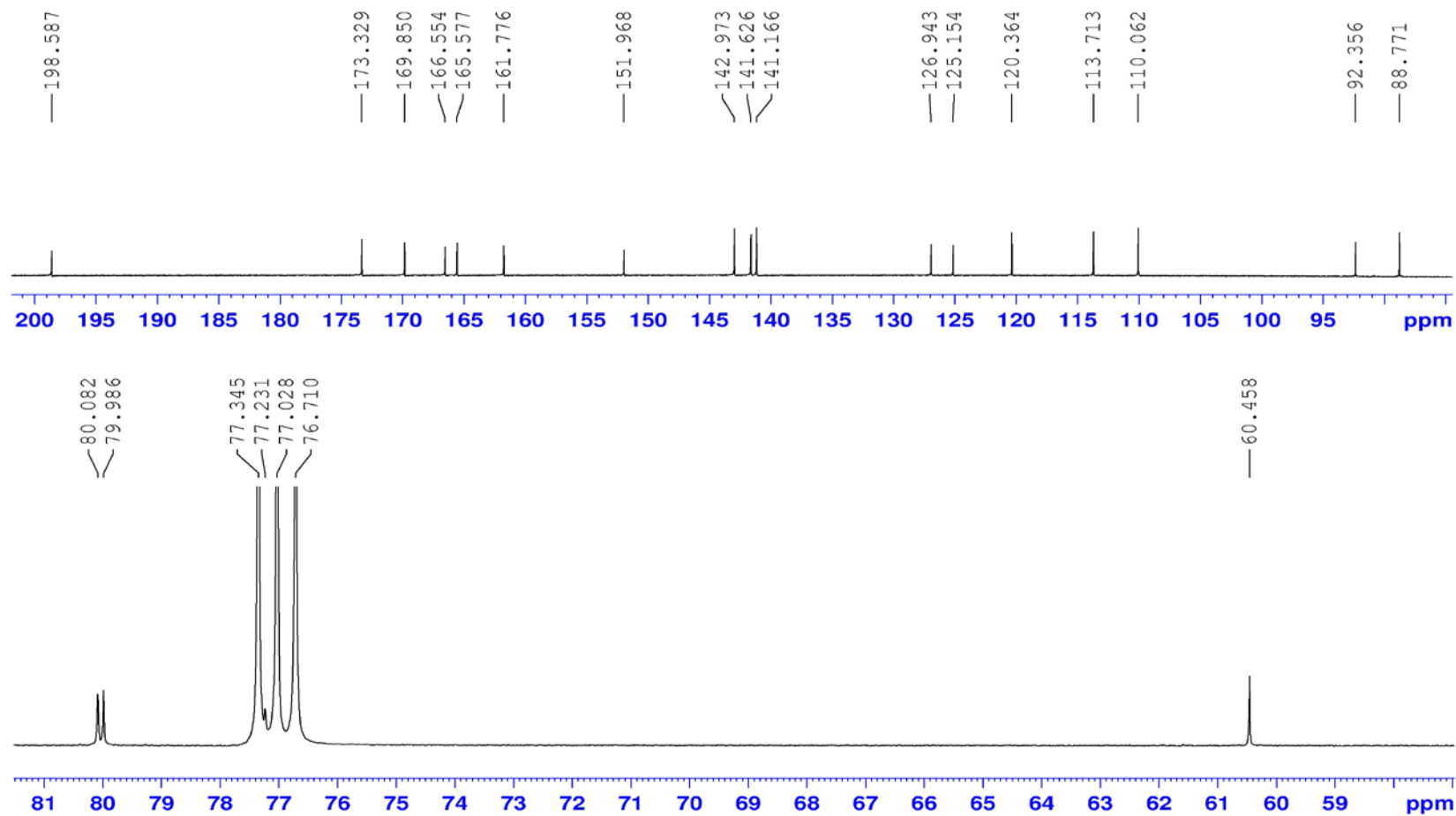
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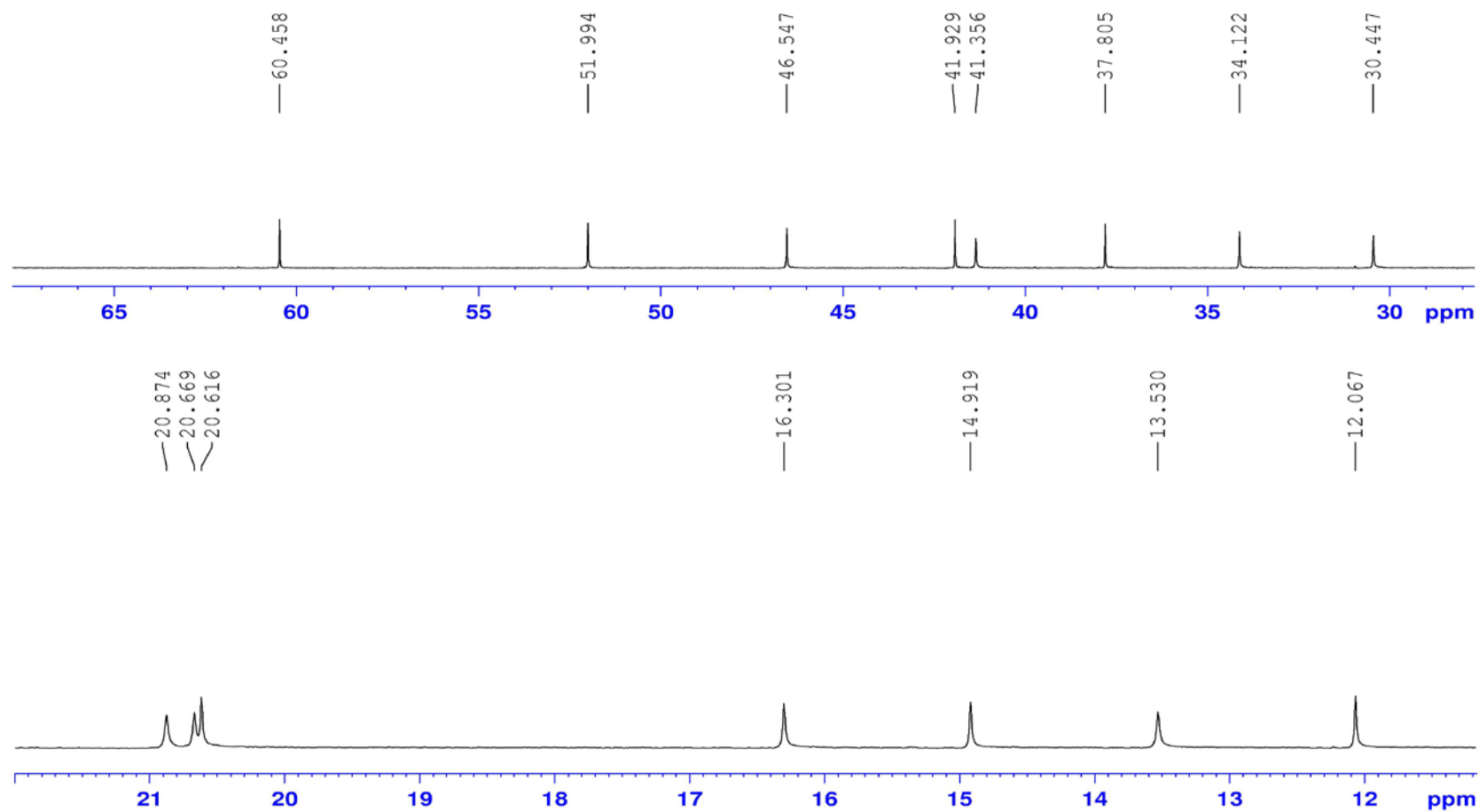


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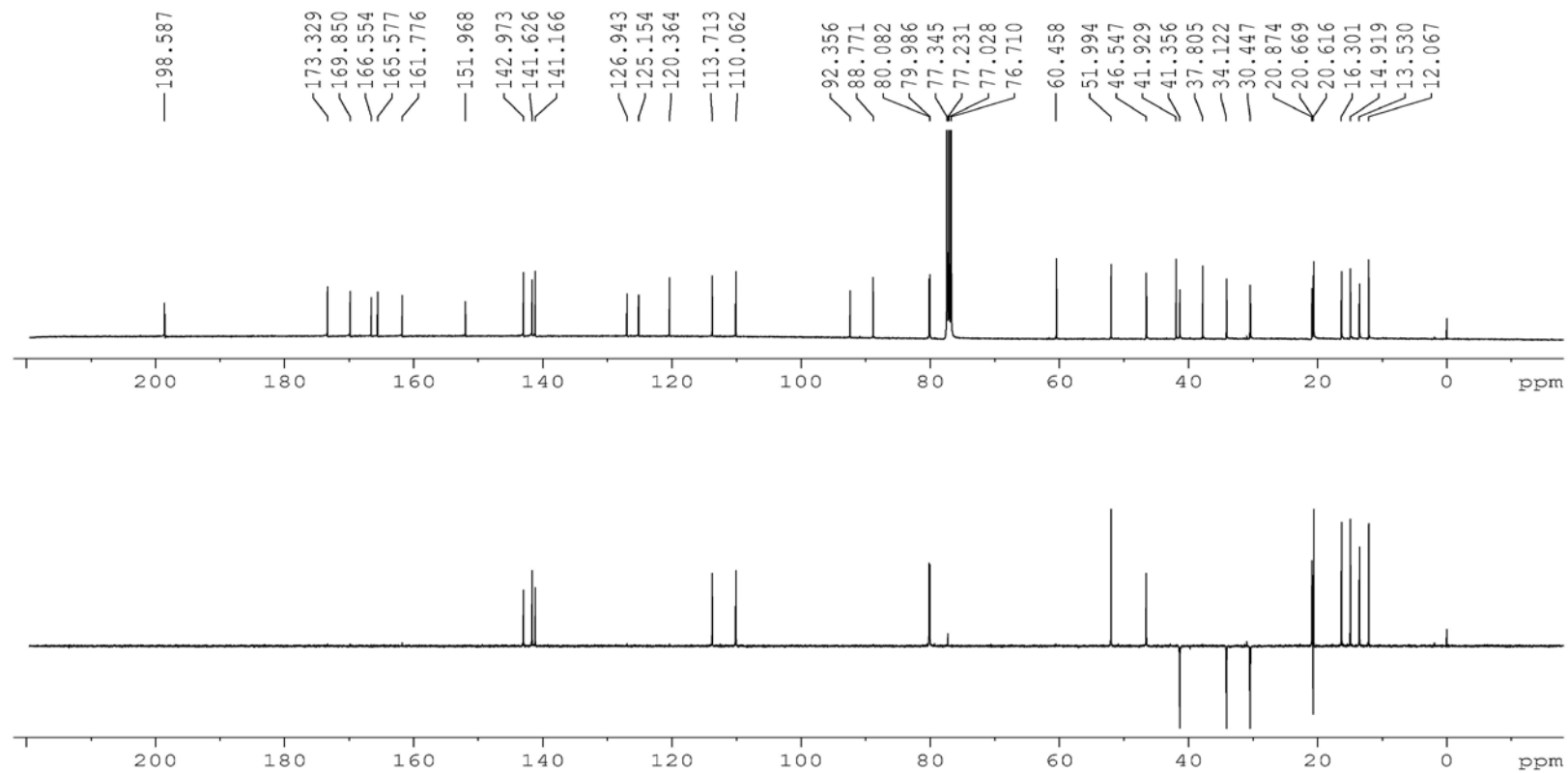
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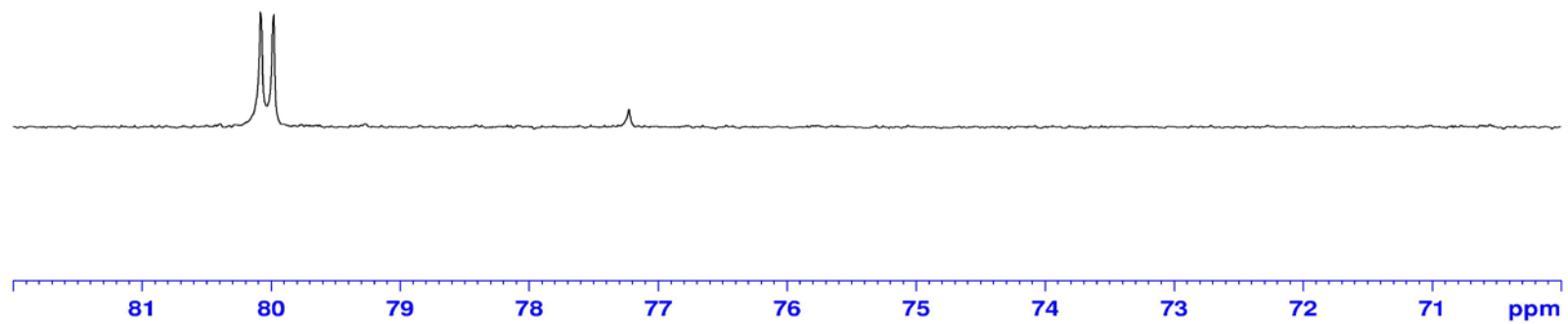
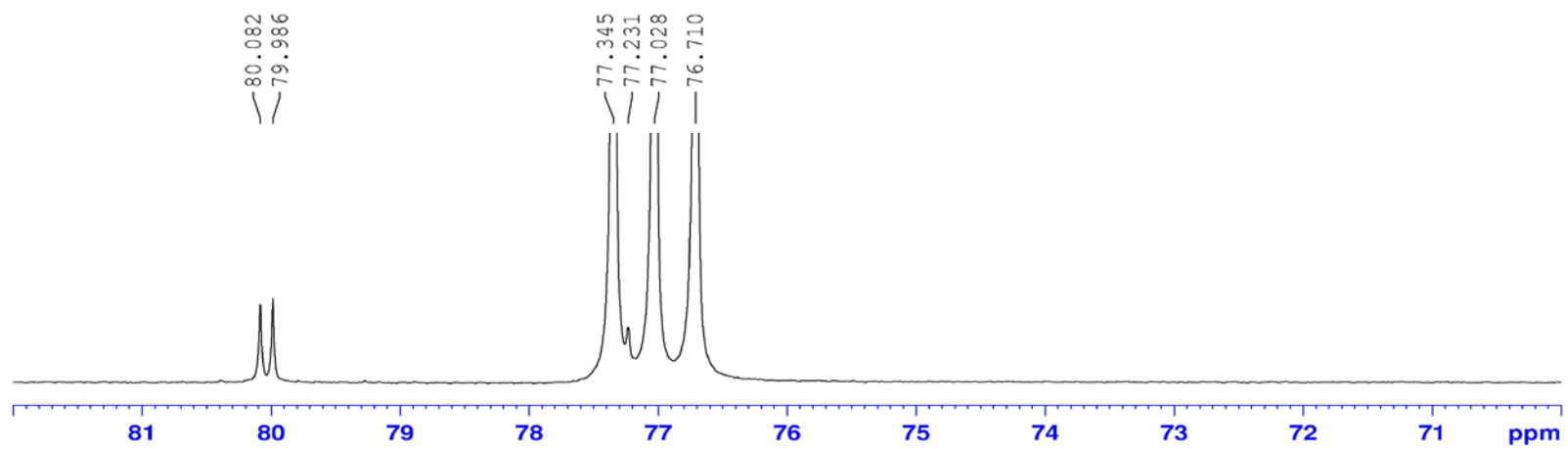
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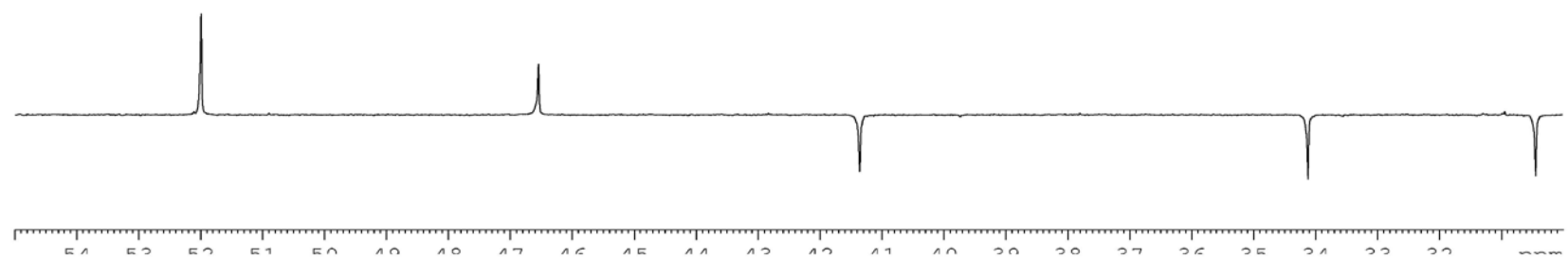
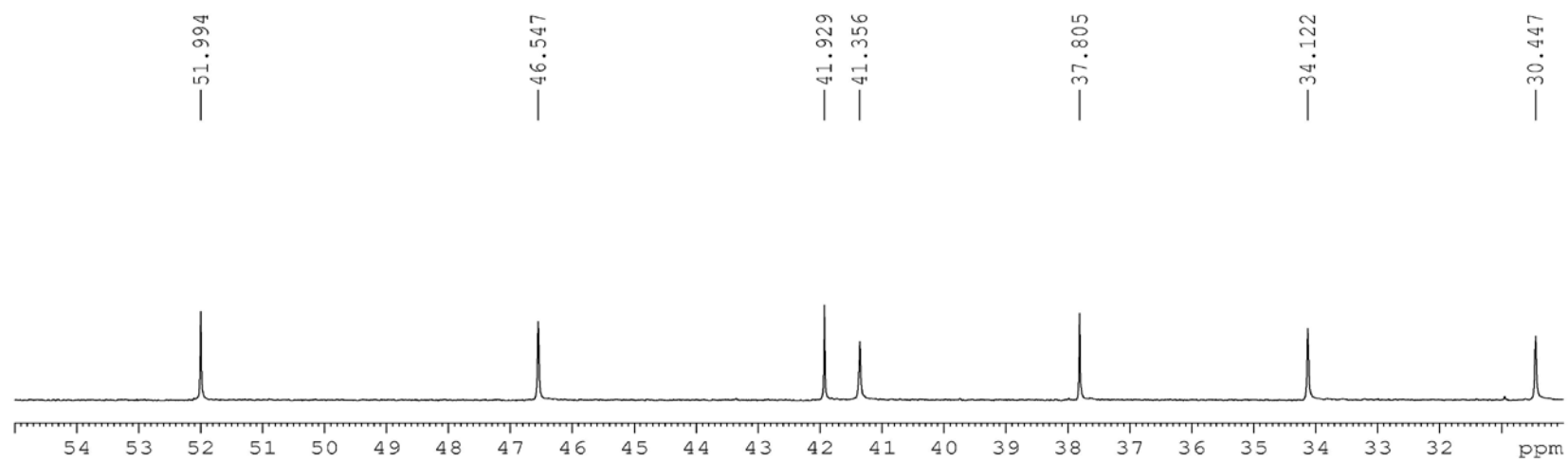


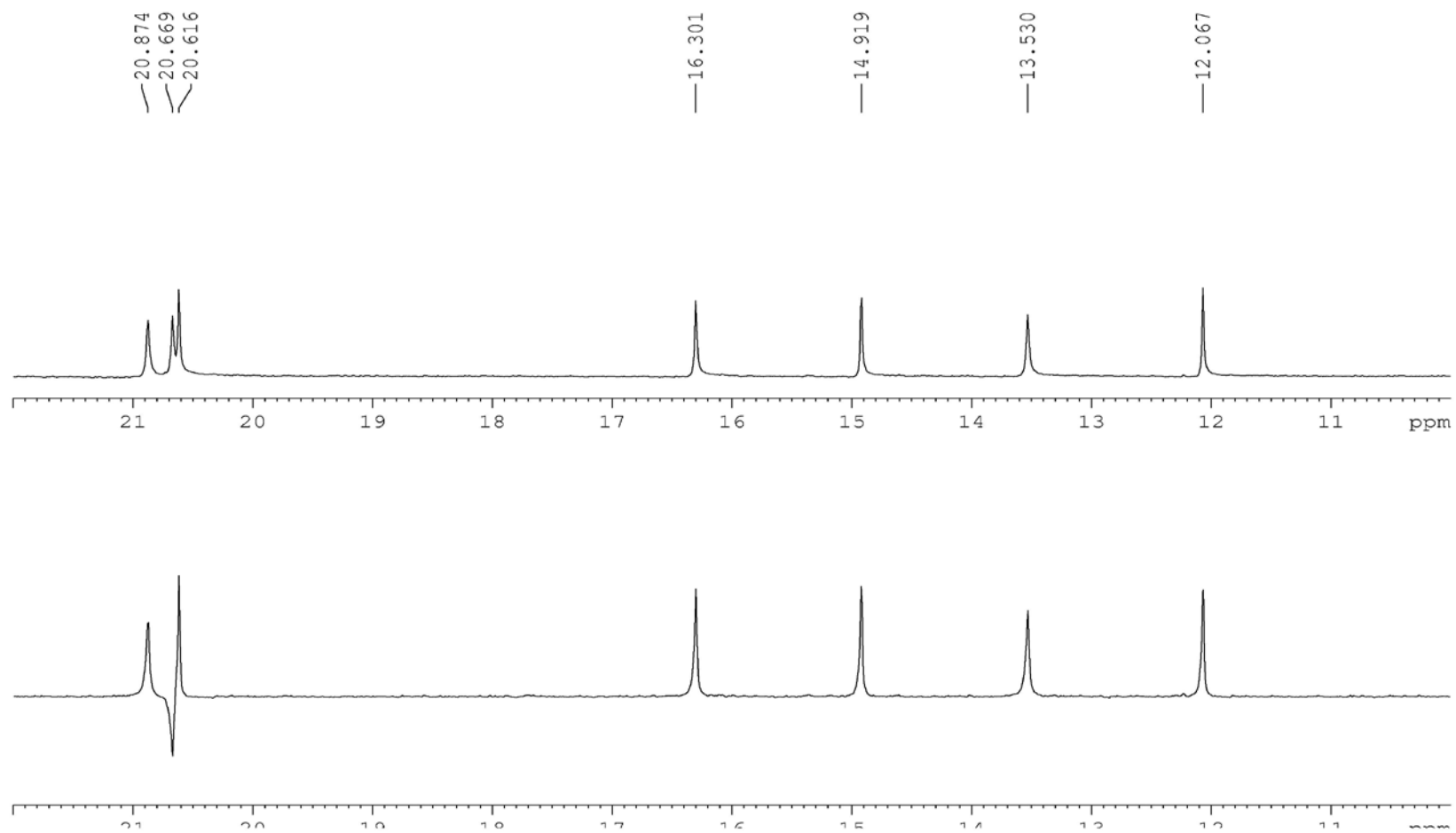


DEPT135° (100 MHz) spectrum of Thaixylomolin N (**8**) in CDCl₃

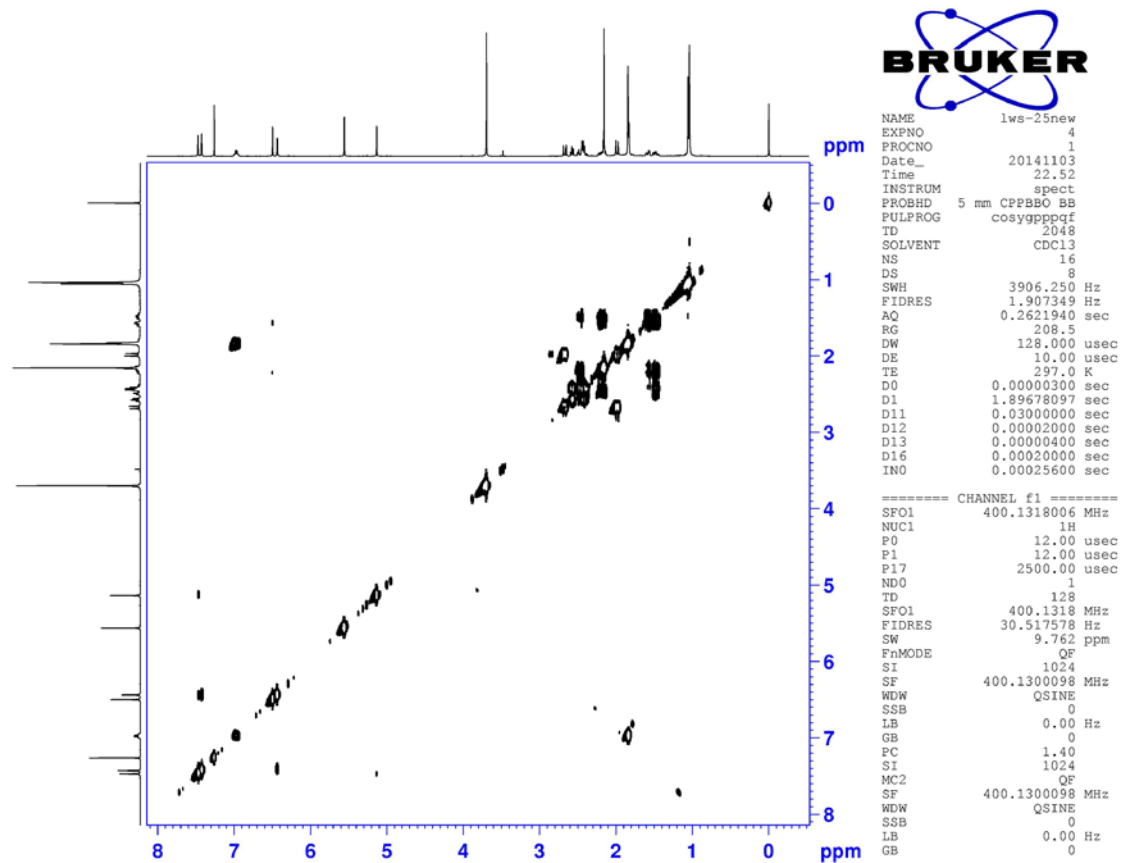


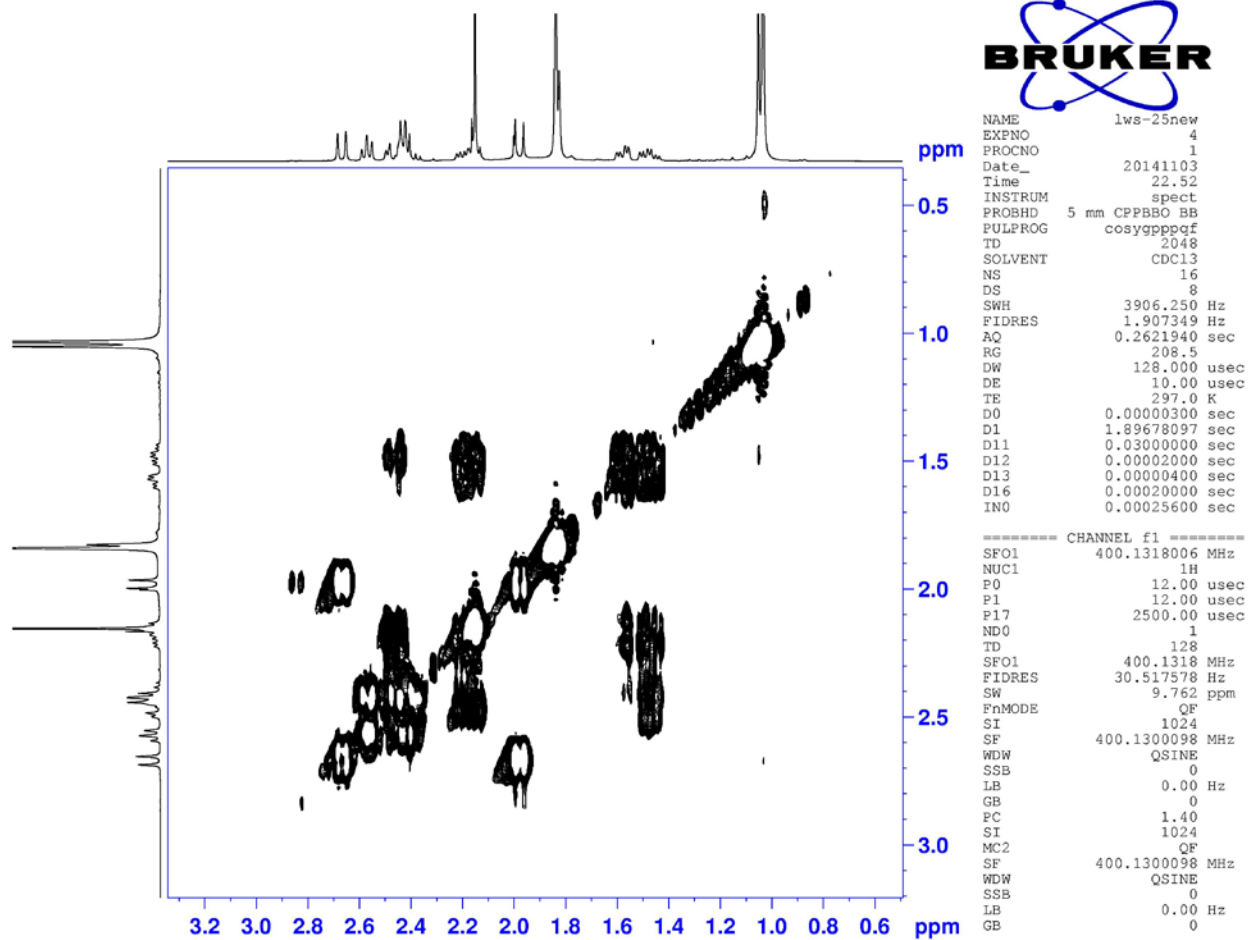




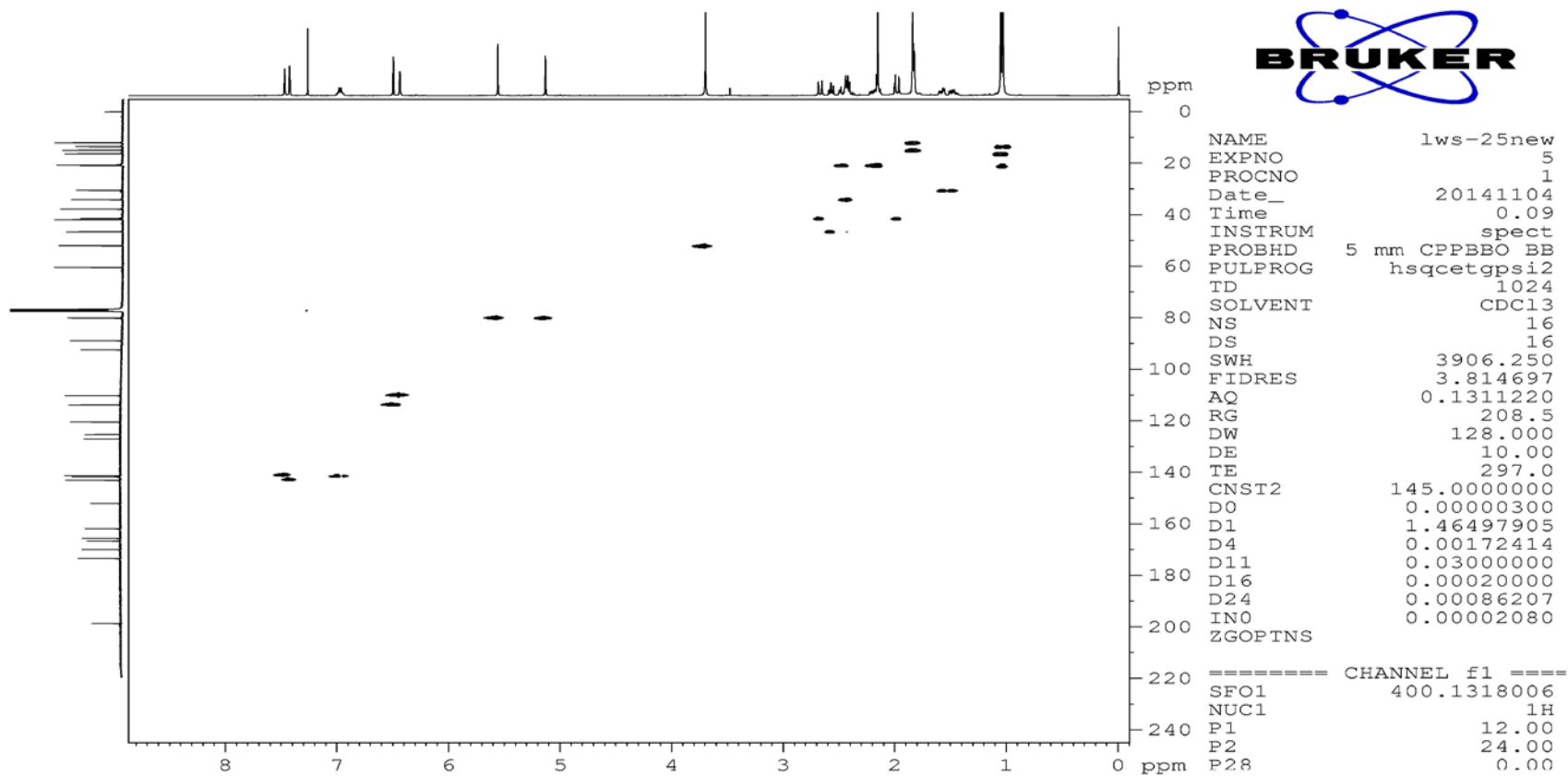


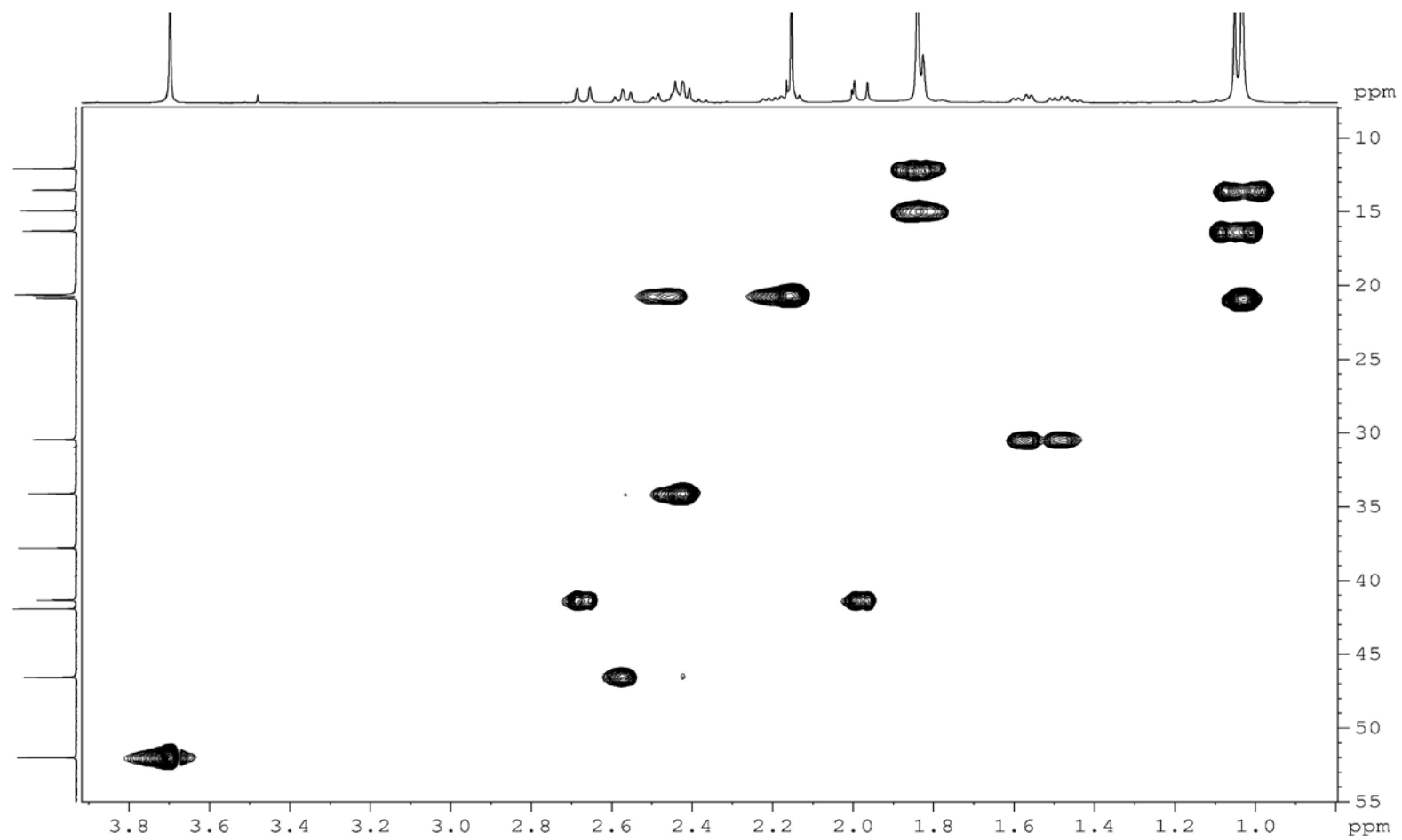
^1H - ^1H COSY (400 MHz) spectrum of Thaixylomolin N (**8**) in CDCl_3



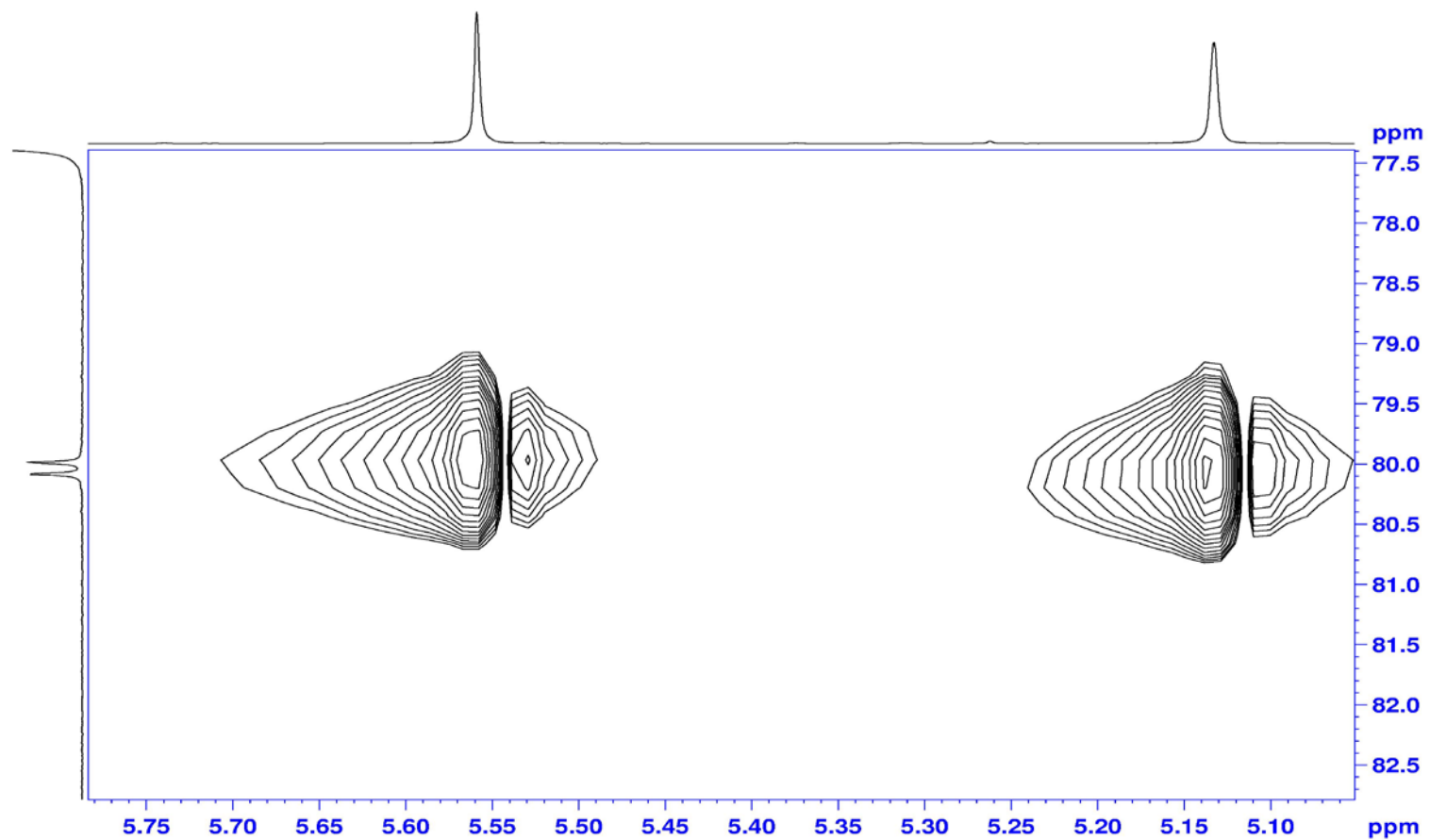


HSQC (400 MHz) spectrum of Thaixylomolin N (**8**) in CDCl₃

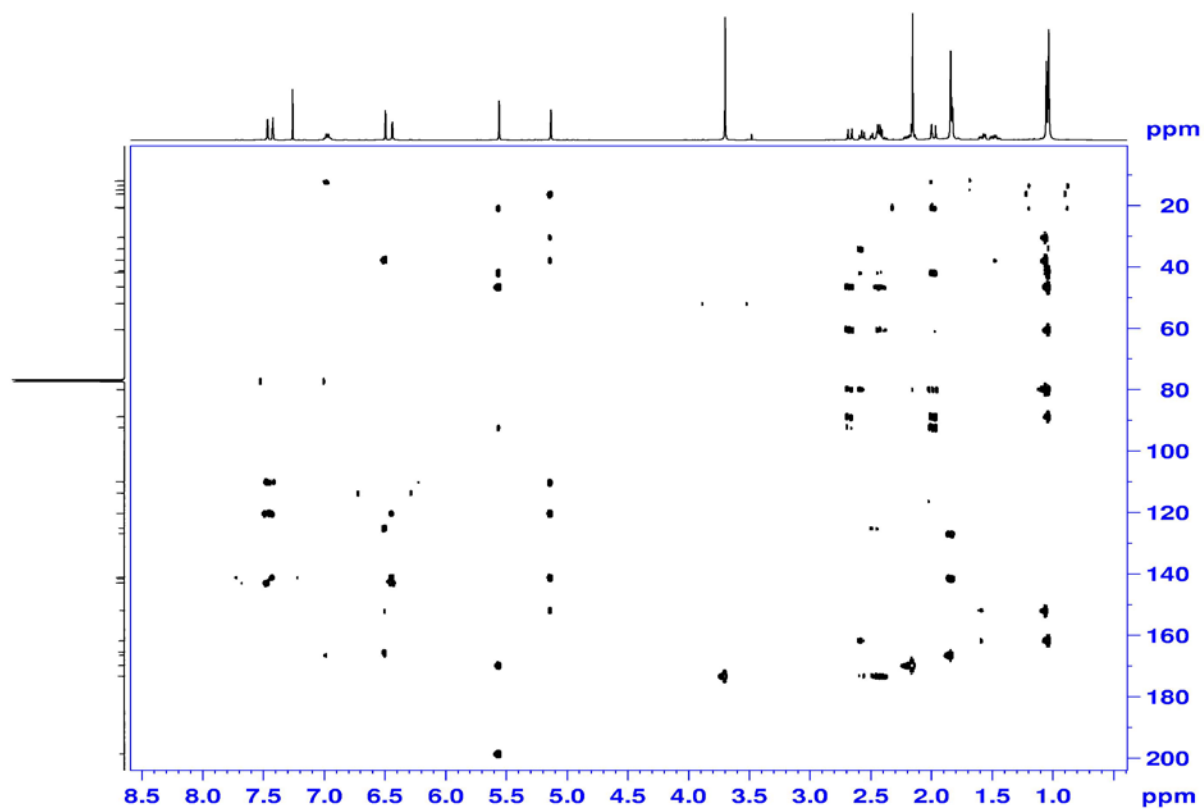




S47



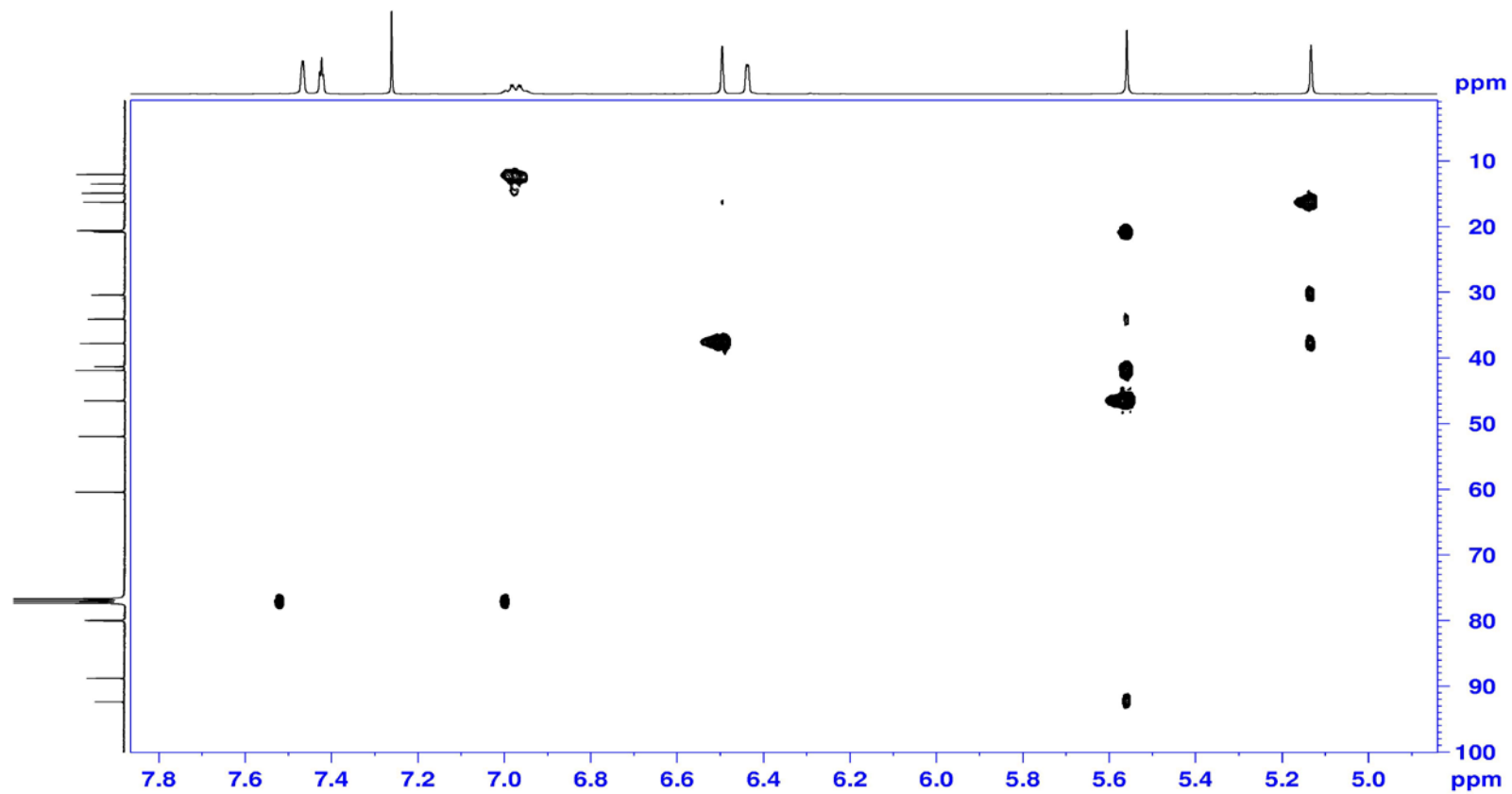
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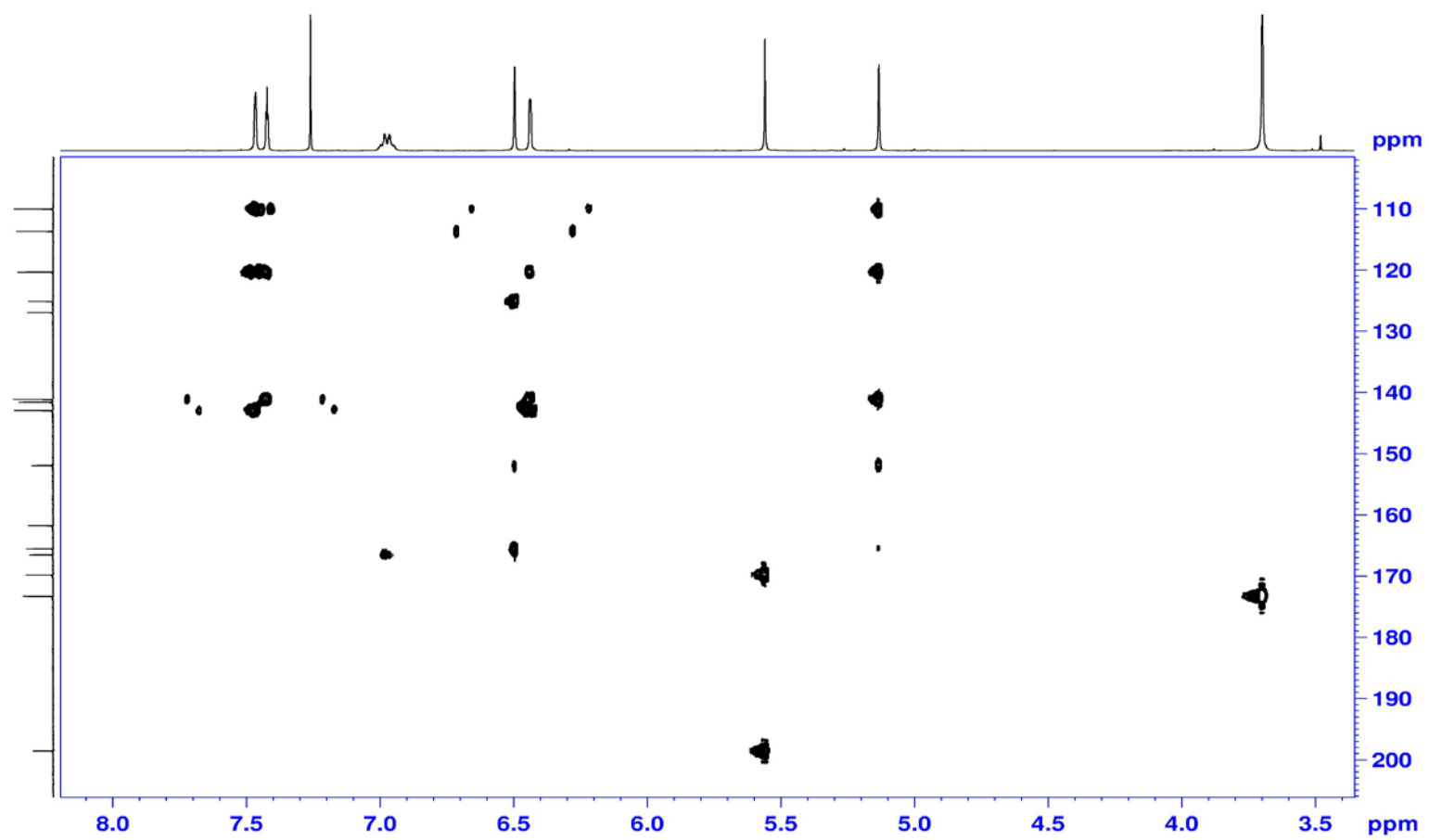
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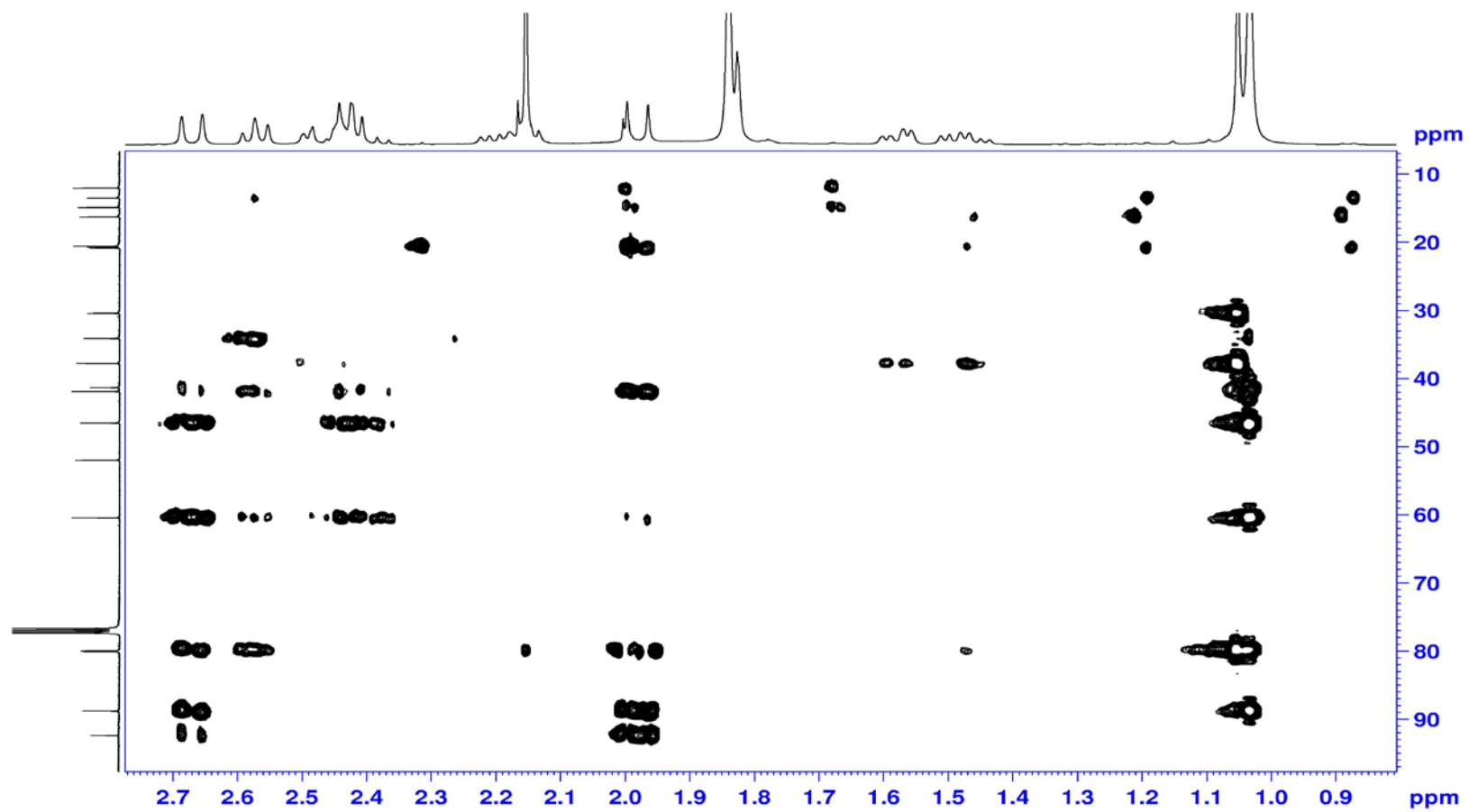
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D6         0.05000000 sec
D16        0.00020000 sec
IN0        0.00002080 sec

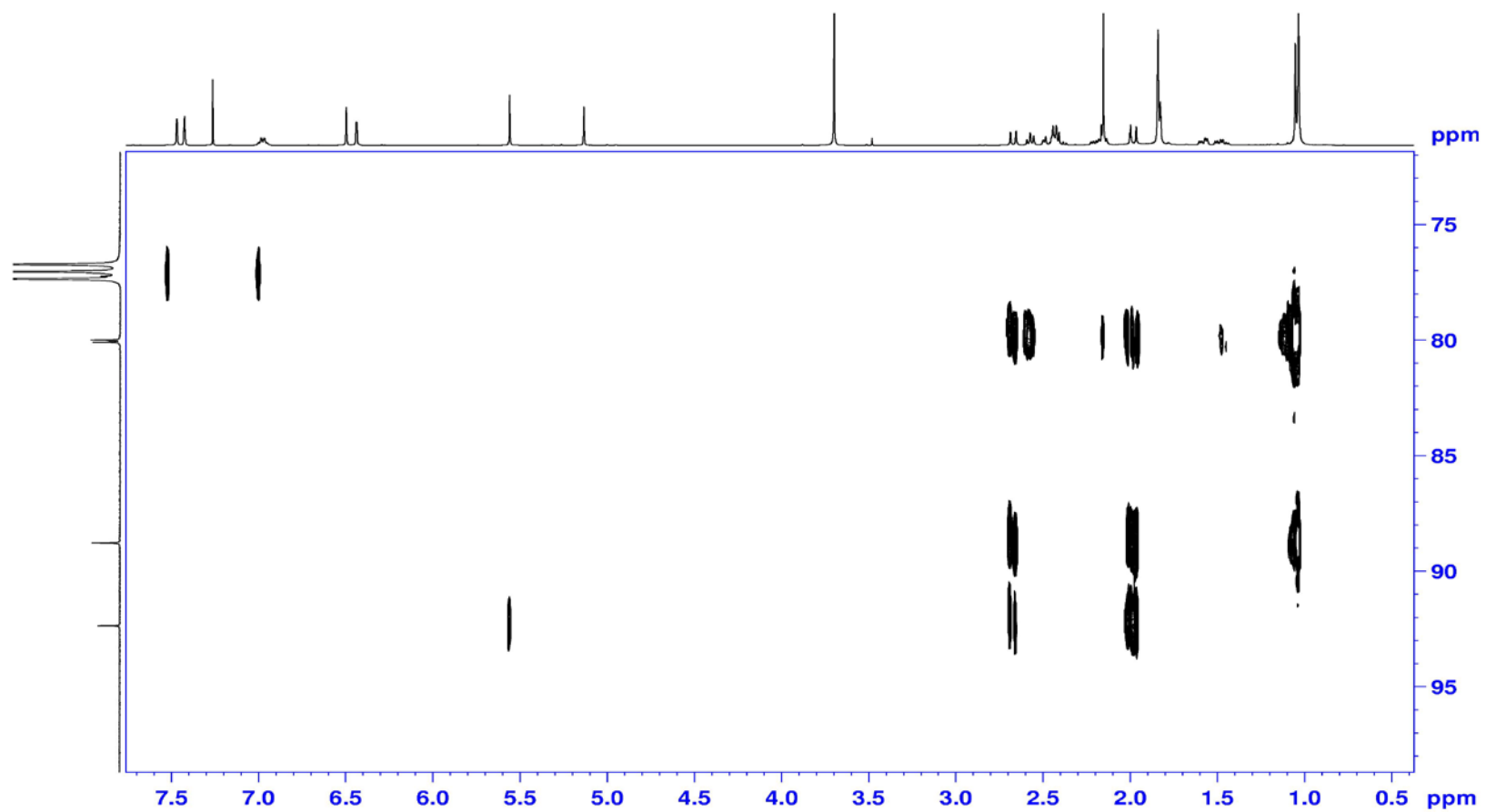
===== CHANNEL f1 =====
SFO1      400.1323208 MHz
NUC1       1H
P1         12.00 usec
P2         24.00 usec
ND0        2
TD         128
SFO1      100.6228 MHz
FIDRES     187.800476 Hz
SW         238.897 ppm
FnMODE     QF
SI         2048
SF         400.1300080 MHz
WDW        SINE
SSB         0
LB         0.00 Hz
GB         0
PC         1.40
SI         1024
MC2        QF
SF         100.6127693 MHz
WDW        SINE
SSB         0
LB         0.00 Hz
  
```

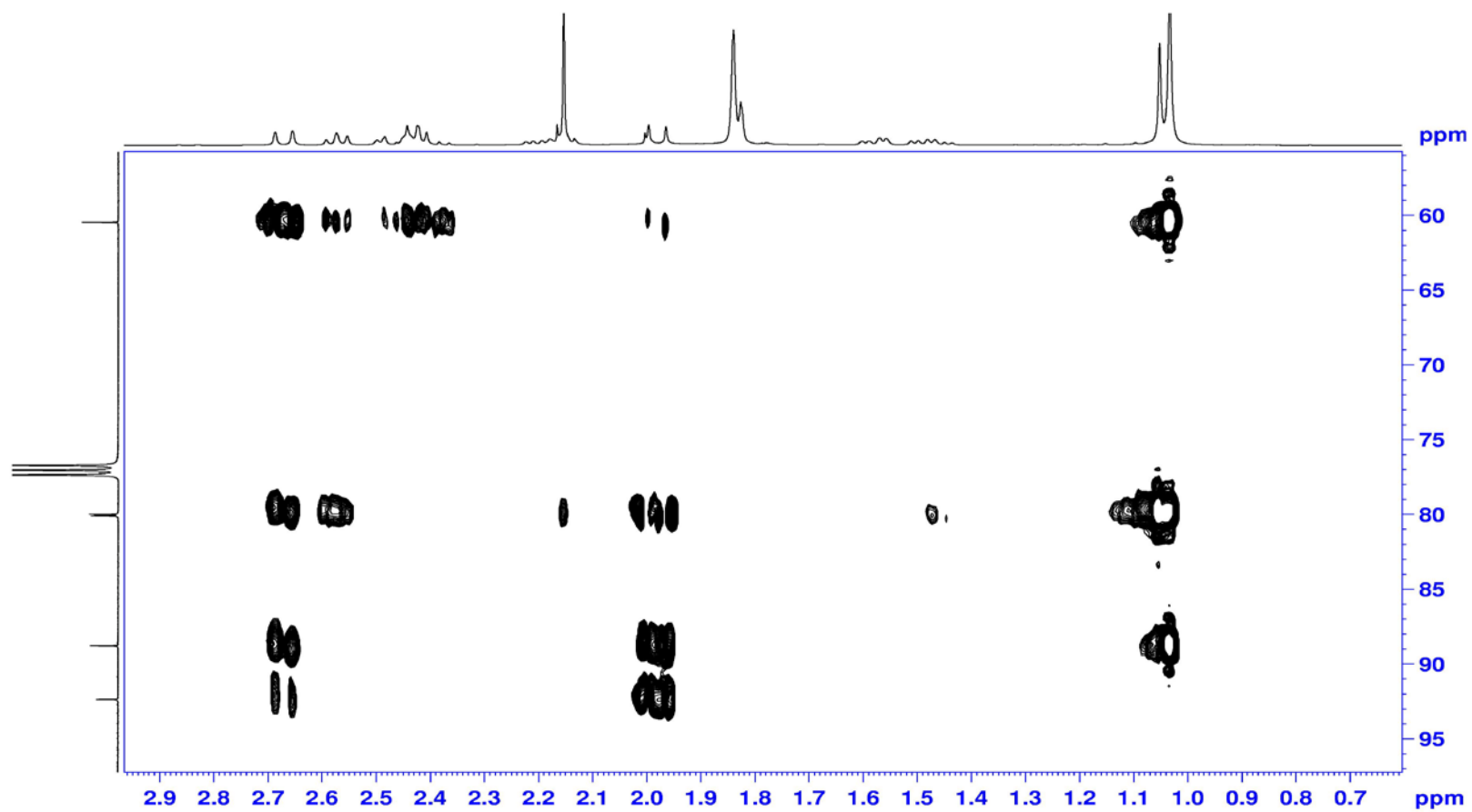


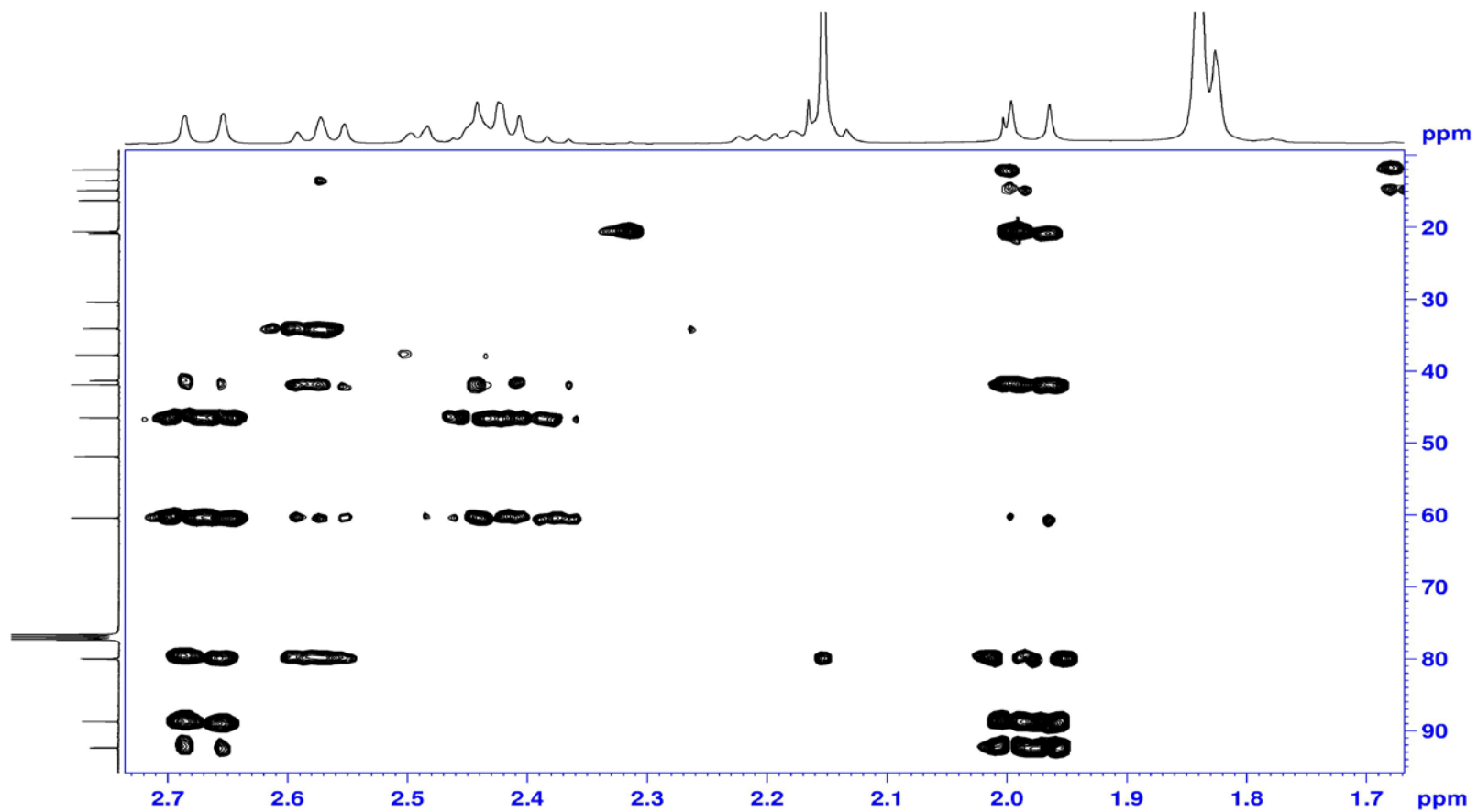
S50

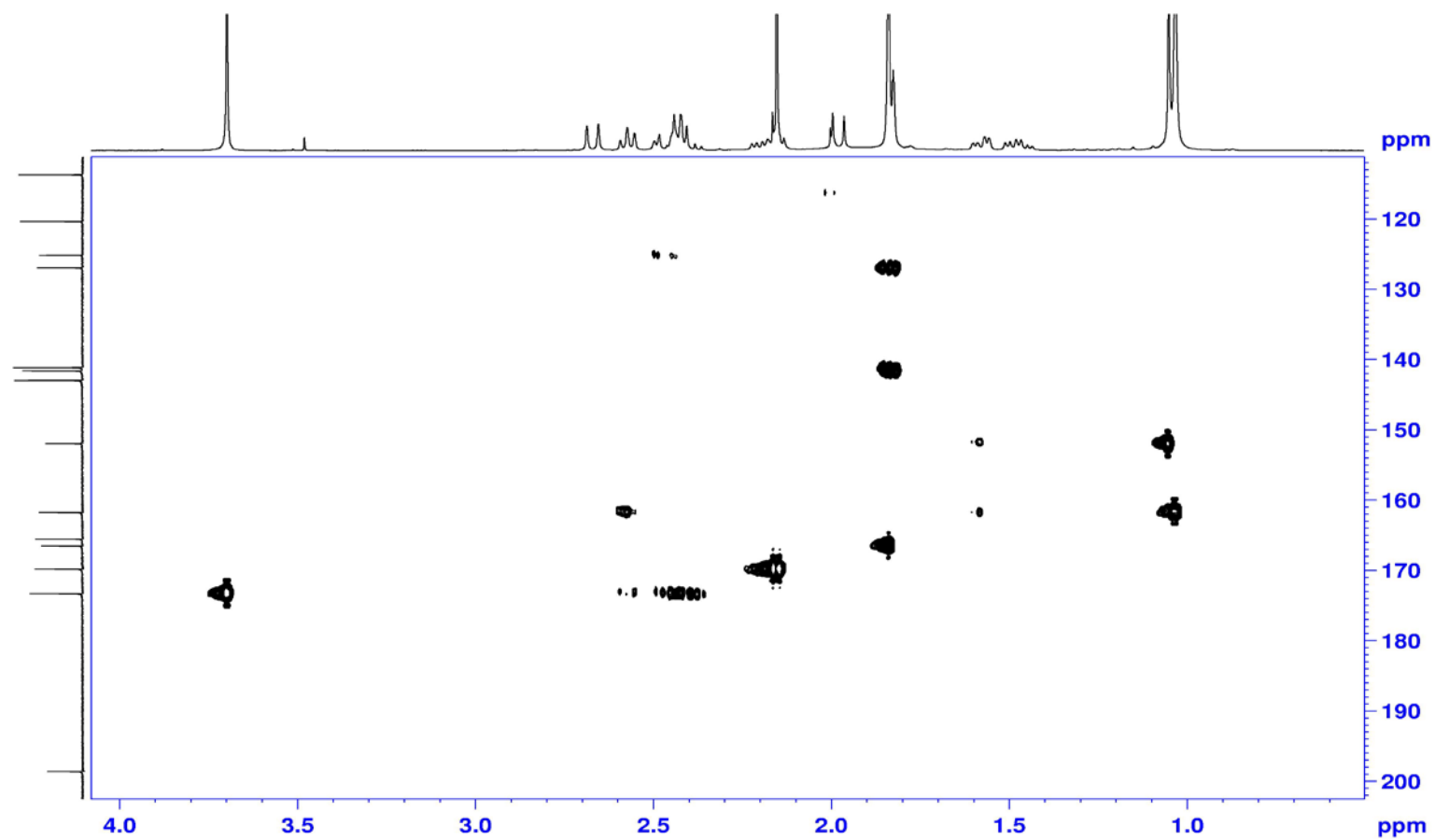






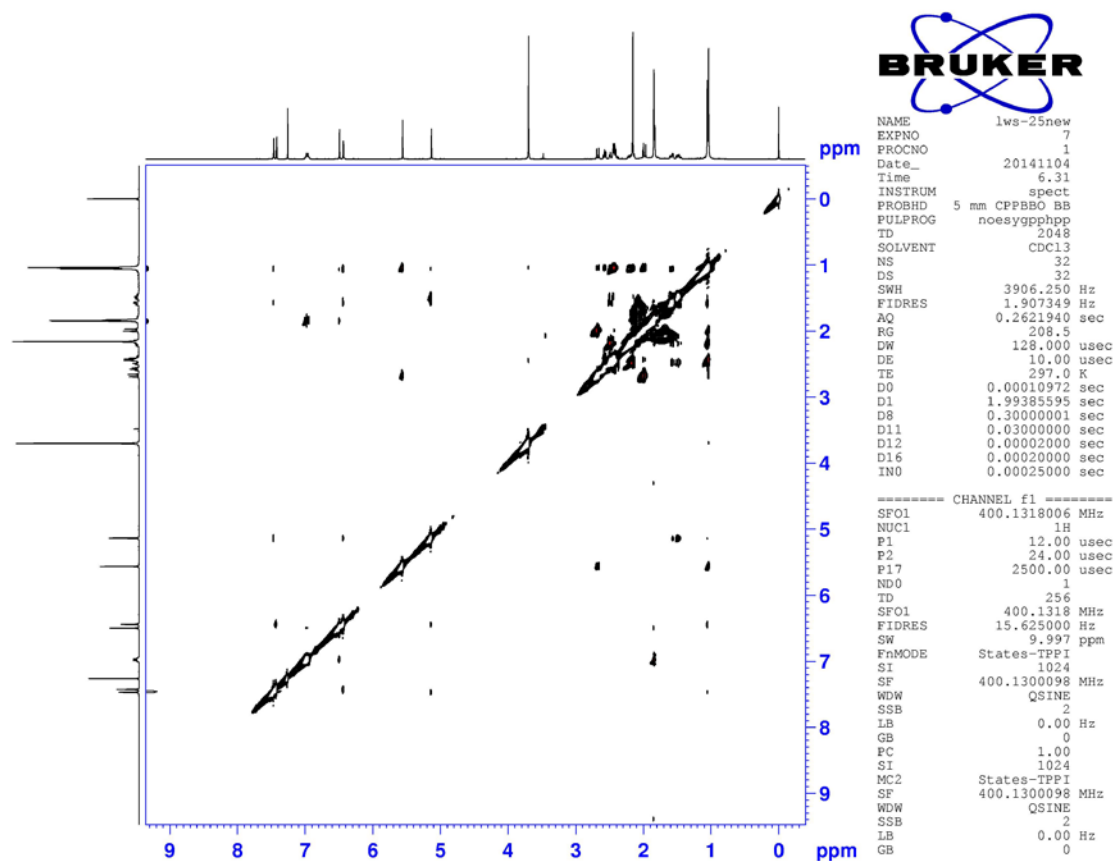


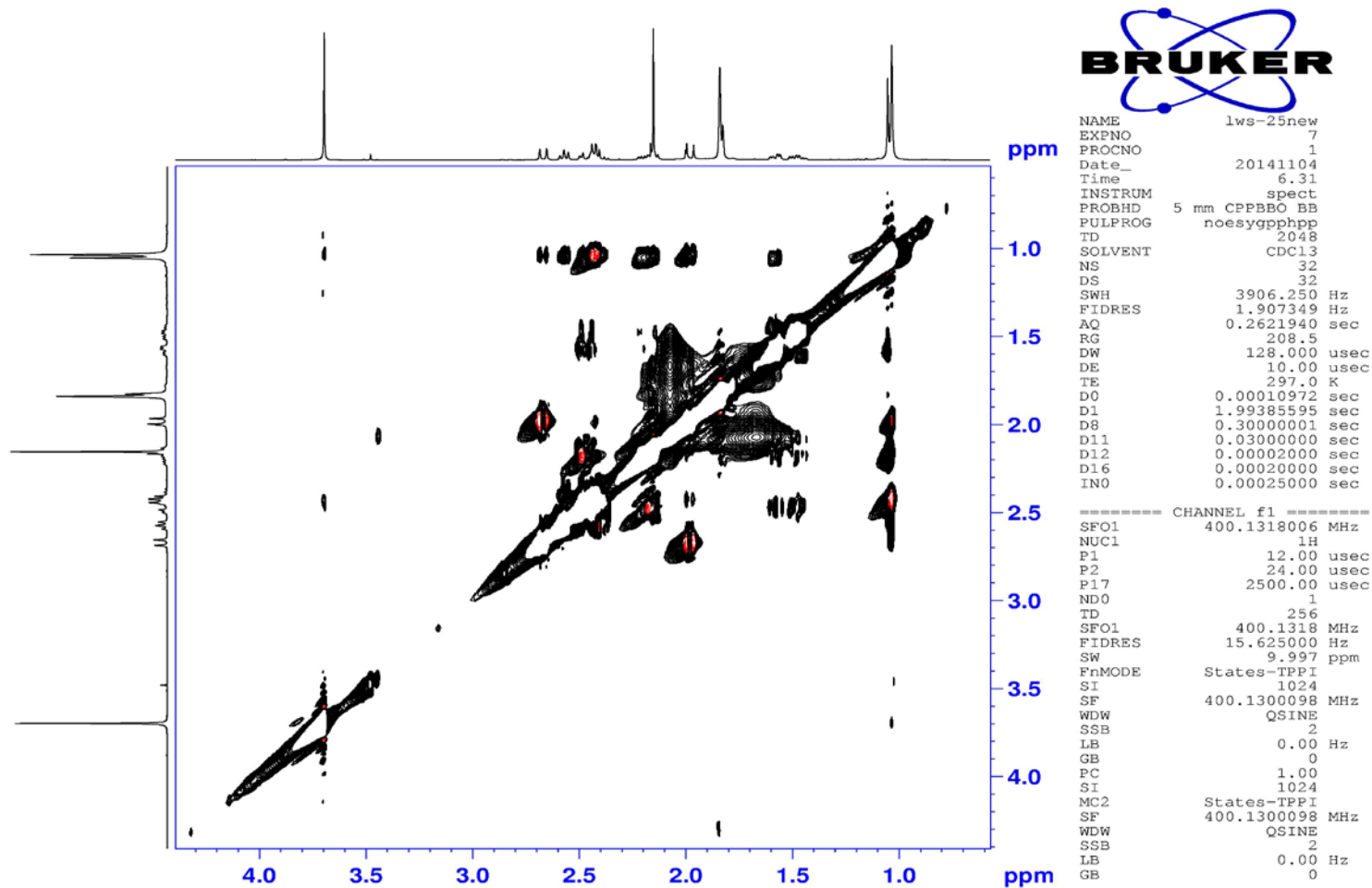


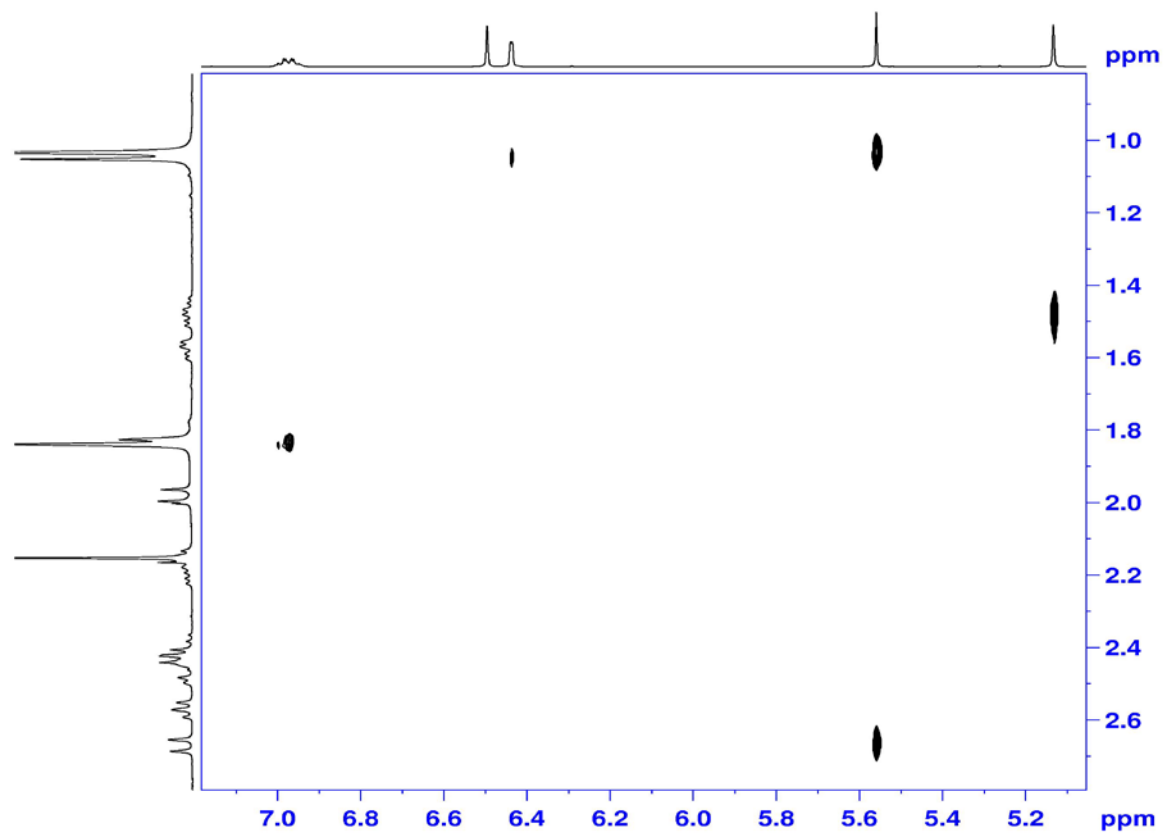


S56

NOESY (400 MHz) spectrum of Thaixylomolin N (**8**) in CDCl₃







```

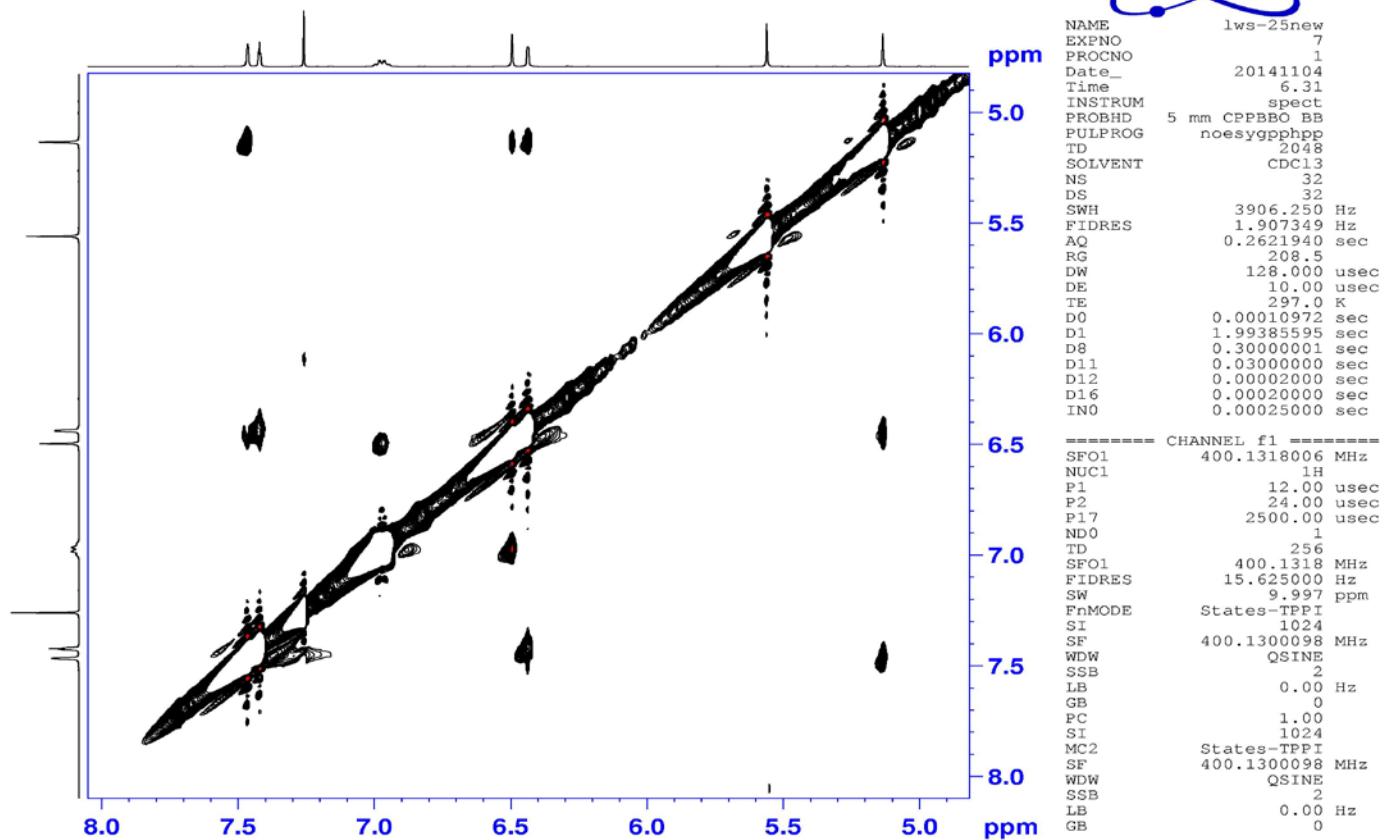
NAME          lws-25new
EXPNO          7
PROCNO         1
Date_         20141104
Time          6.31
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       noesygpphph
TD            2048
SOLVENT       CDC13
NS            32
DS            32
SWH           3906.250 Hz
FIDRES        1.907349 Hz
AQ            0.2621940 sec
RG            208.5
DW            128.000 usec
DE            10.00 usec
TE            297.0 K
D0            0.00010972 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

```

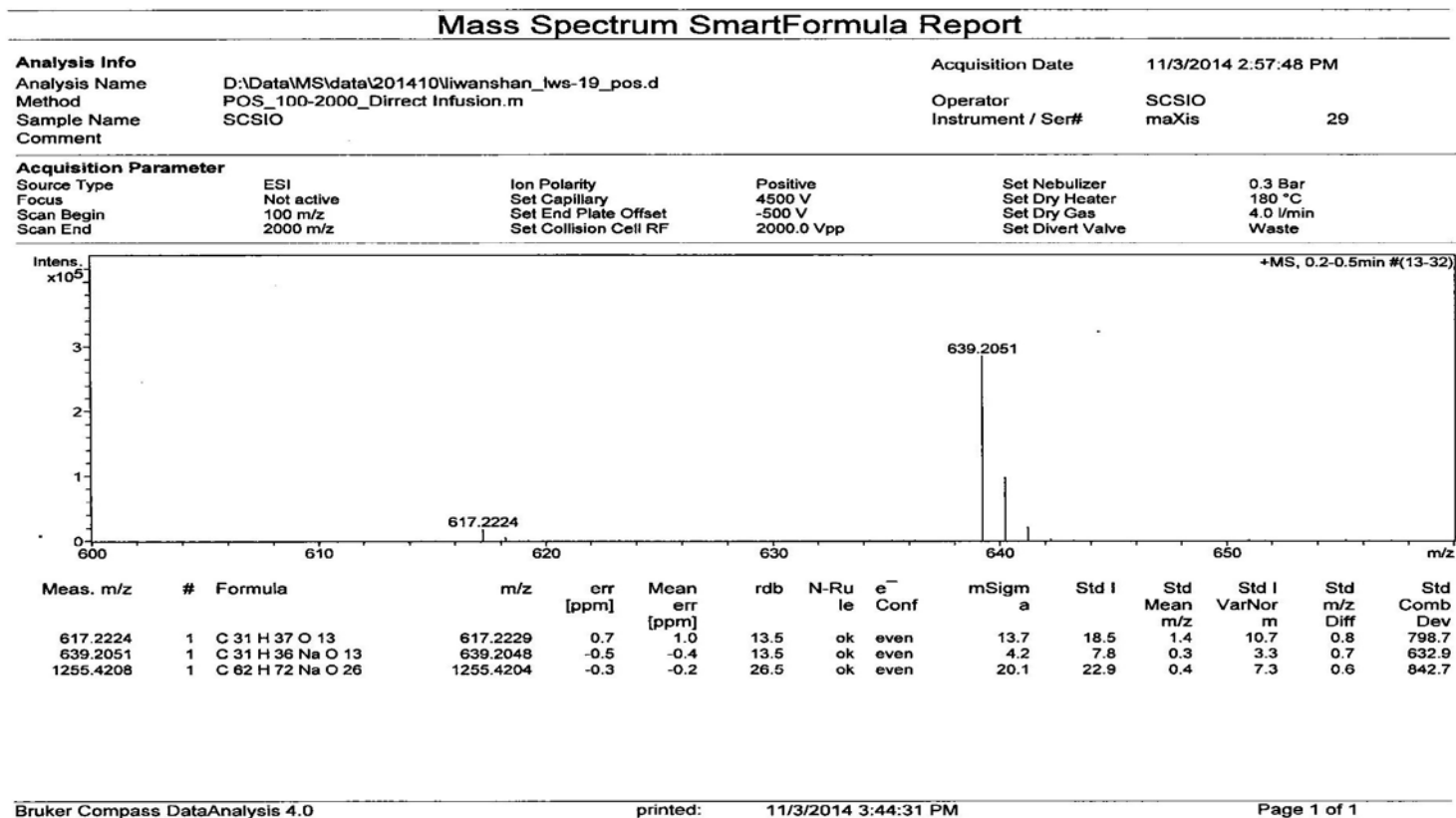
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===== CHANNEL f1 =====
SFO1          400.1318006 MHz
NUC1           1H
P1             12.00 usec
P2             24.00 usec
P17            2500.00 usec
ND0            1
TD             256
SFO1          400.1318 MHz
FIDRES        15.625000 Hz
SW             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
GB             0

```



HR-ESIMS of Compound 9



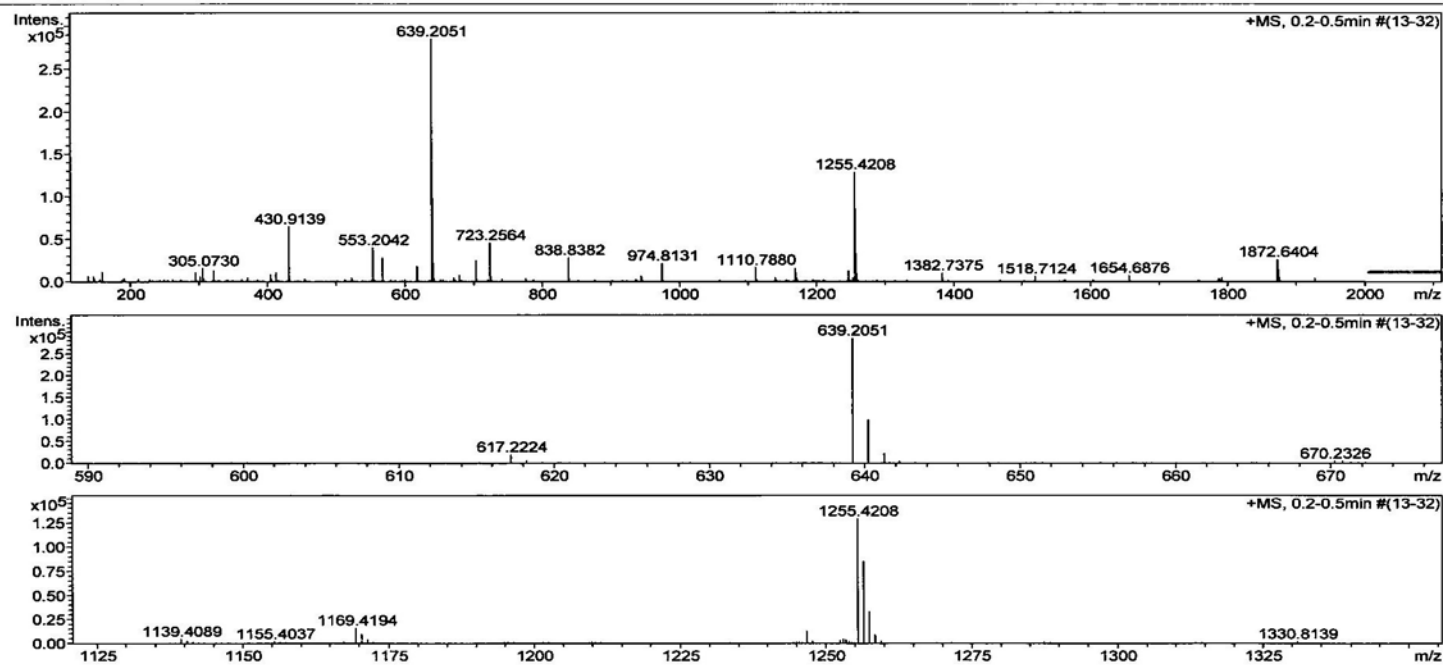
Generic Display Report

Analysis Info

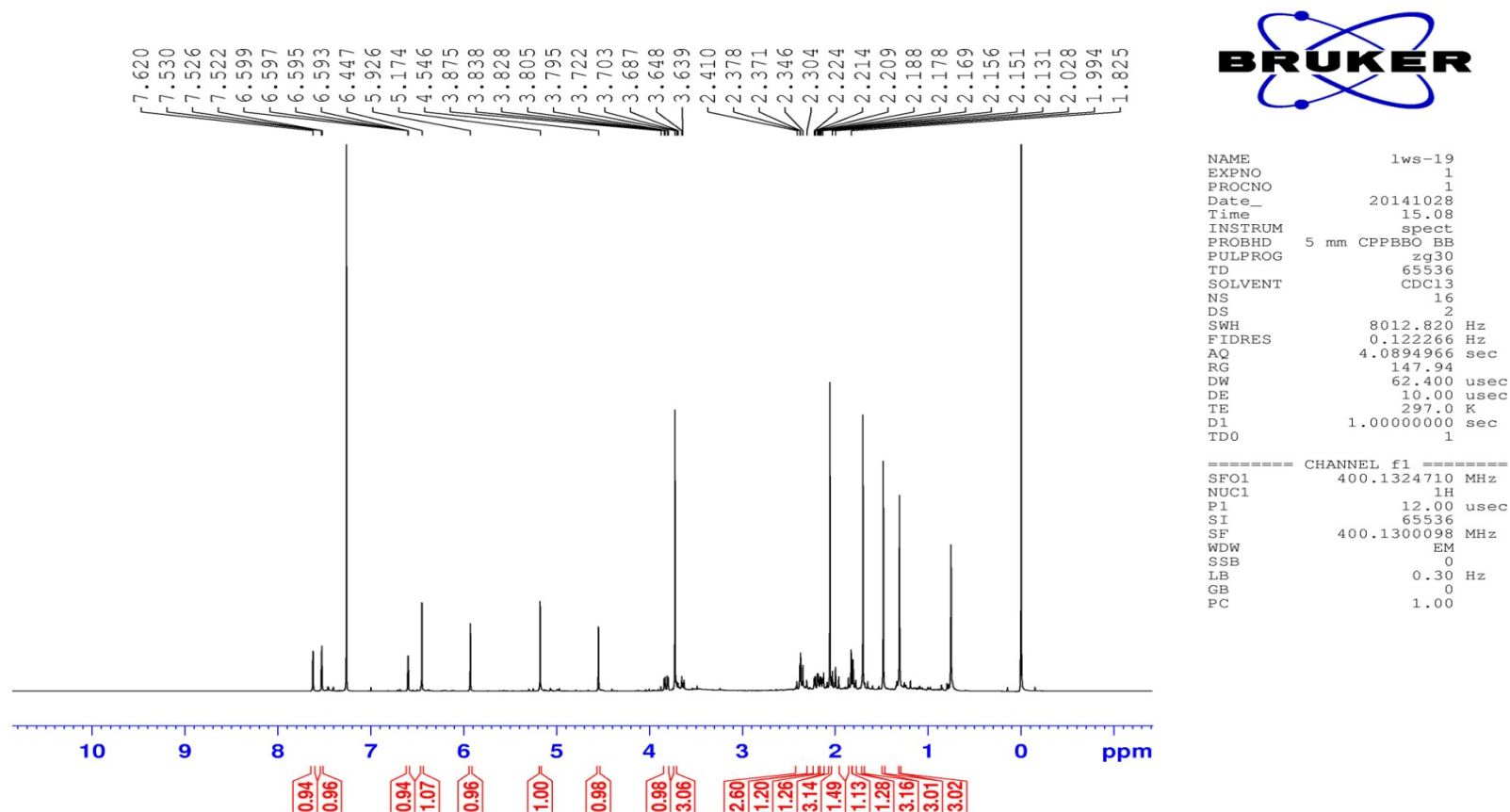
Analysis Name D:\Data\MS\data\201410\liwanshan_lws-19_pos.d
Method POS_100-2000_Direct Infusion.m
Sample Name SCSIO
Comment

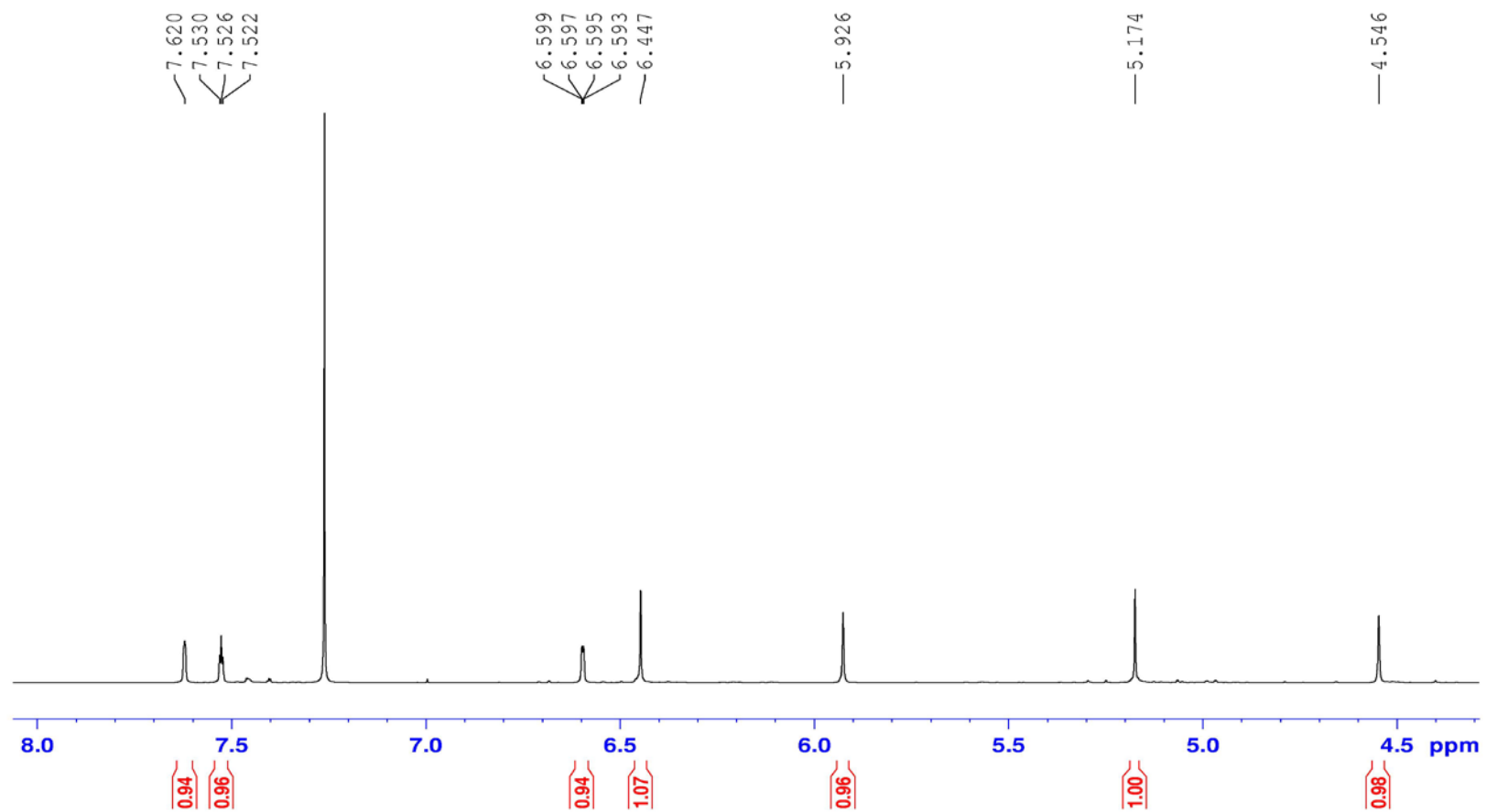
Acquisition Date 11/3/2014 2:57:48 PM

Operator SCSIO
Instrument maXis

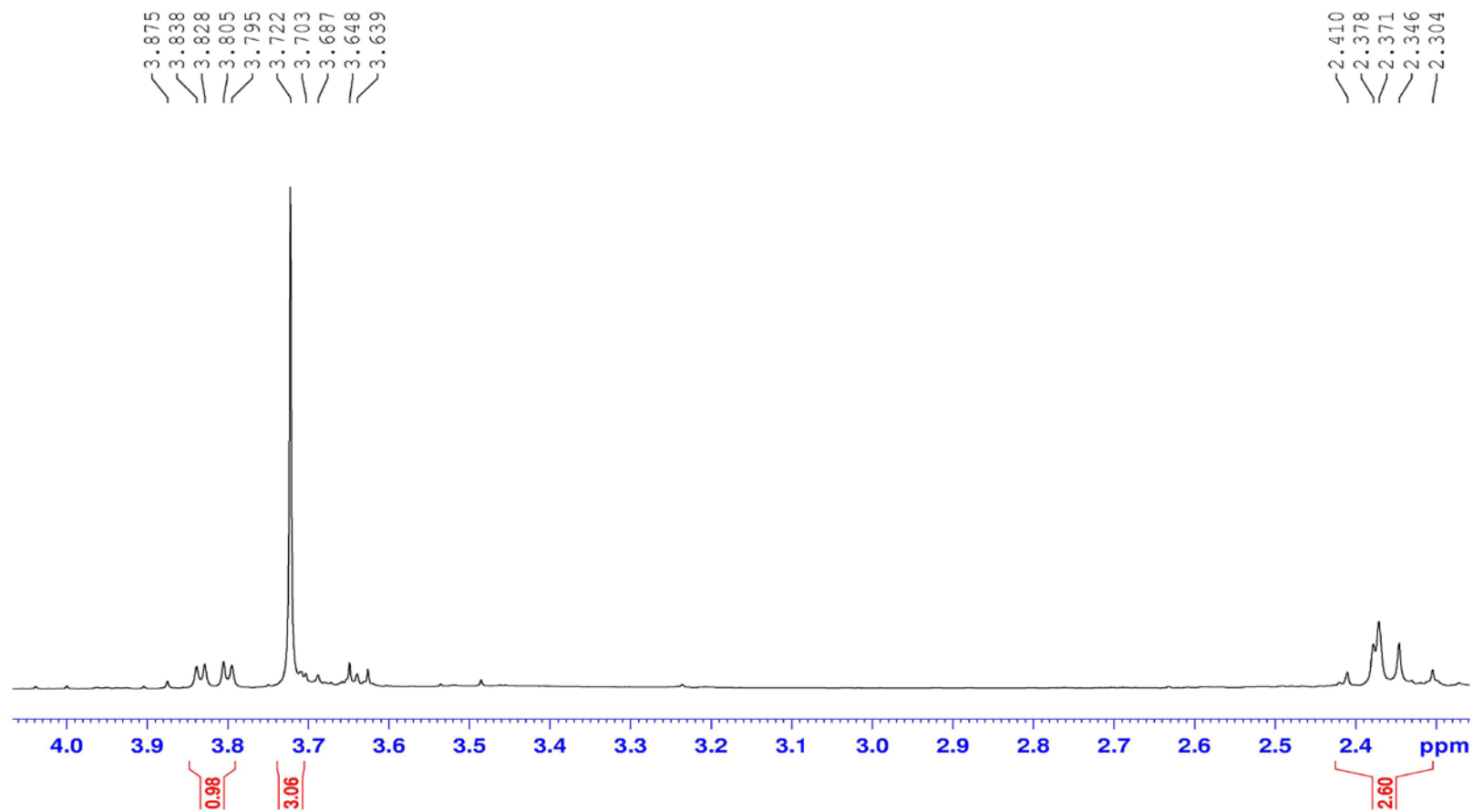


^1H NMR (400 MHz) spectrum of Compound **9** in CDCl_3

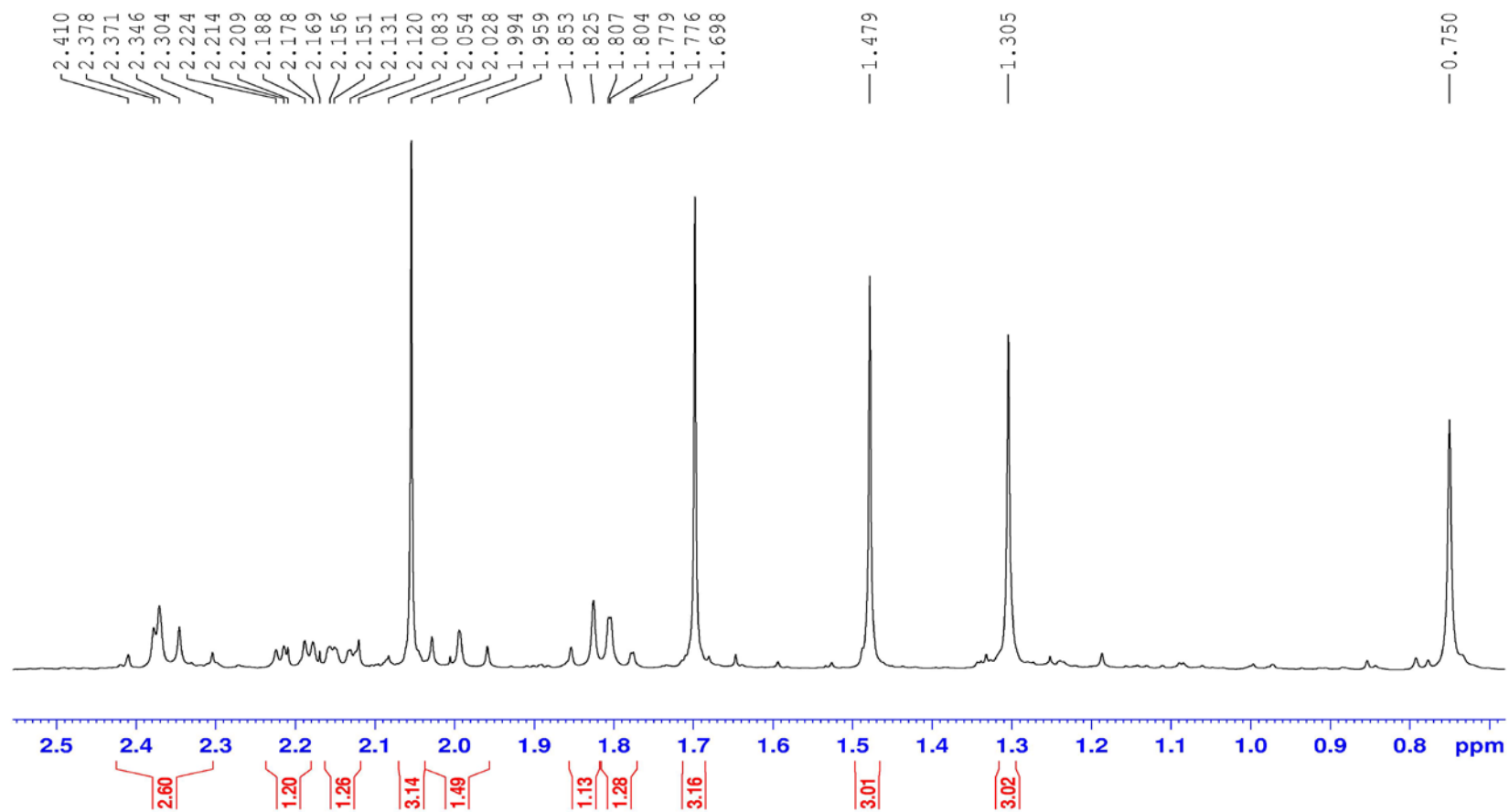




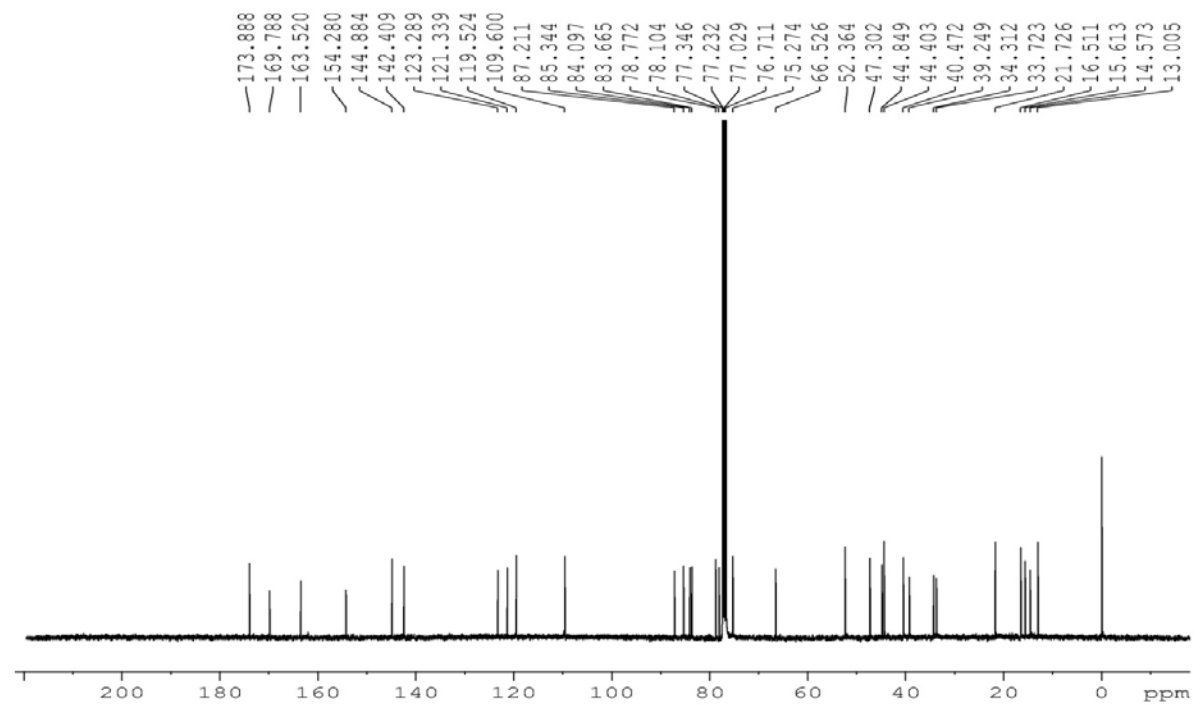
S64



S65



^{13}C NMR (100 MHz) spectrum of Compound **9** in CDCl_3

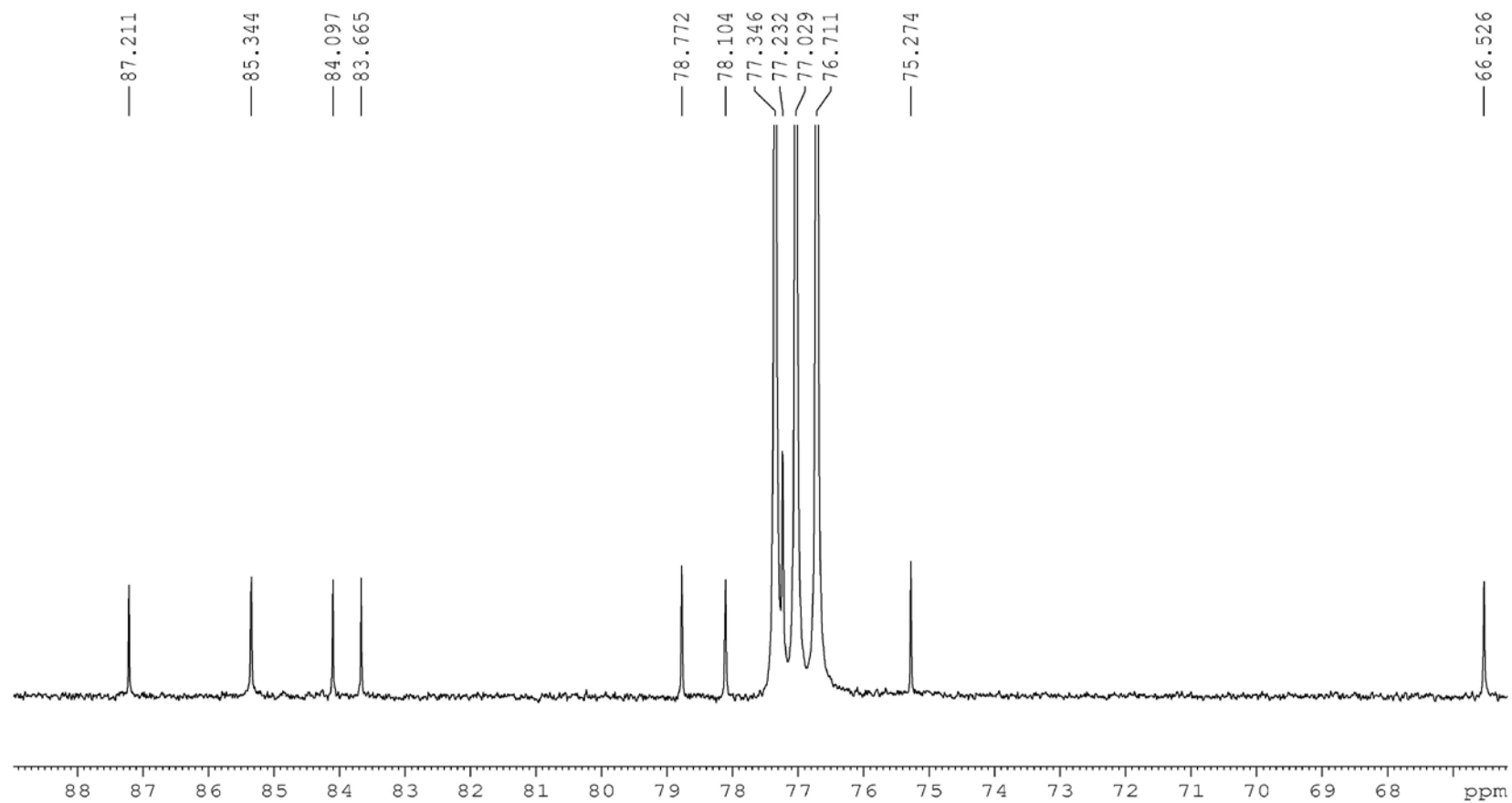


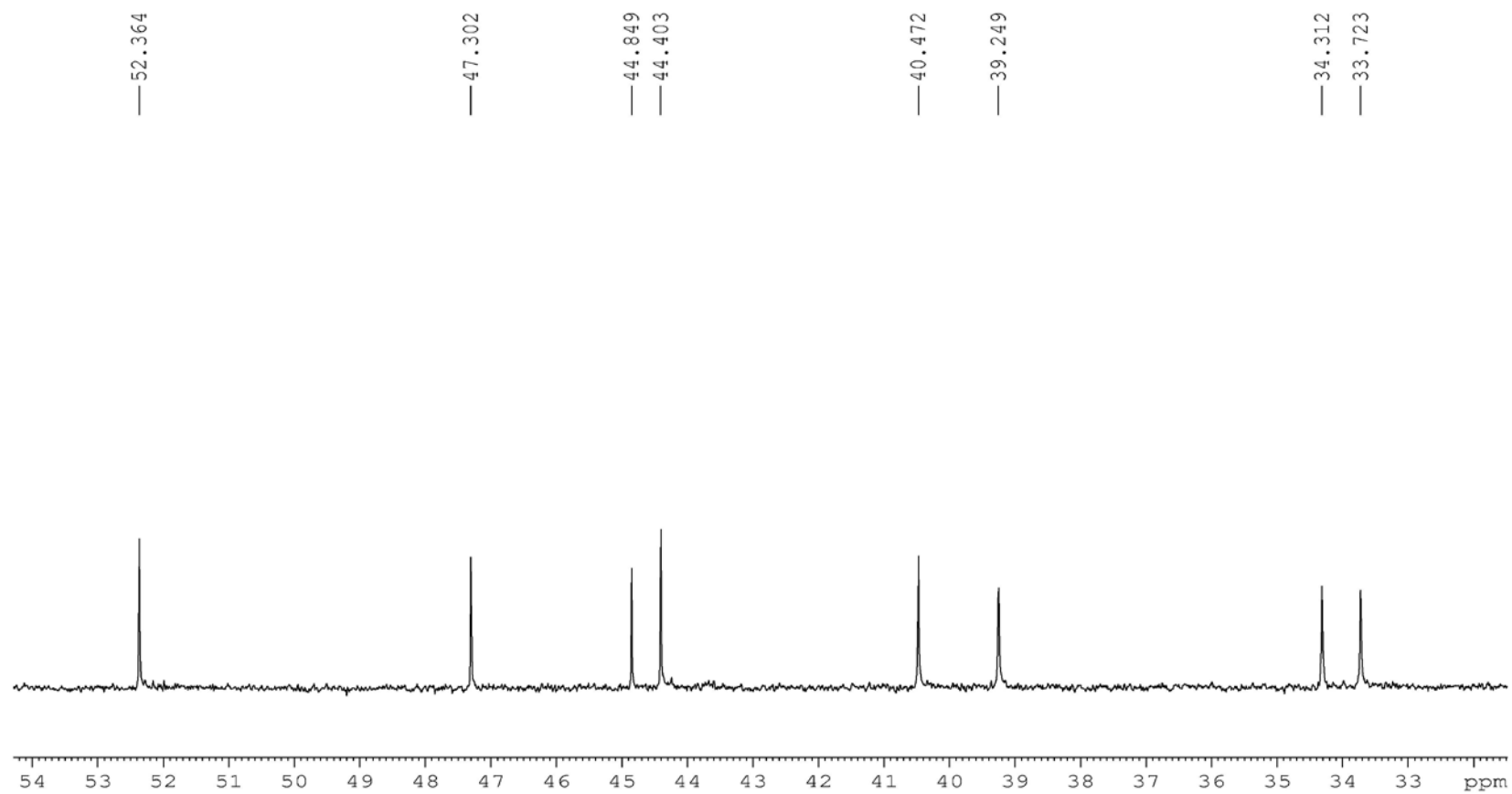
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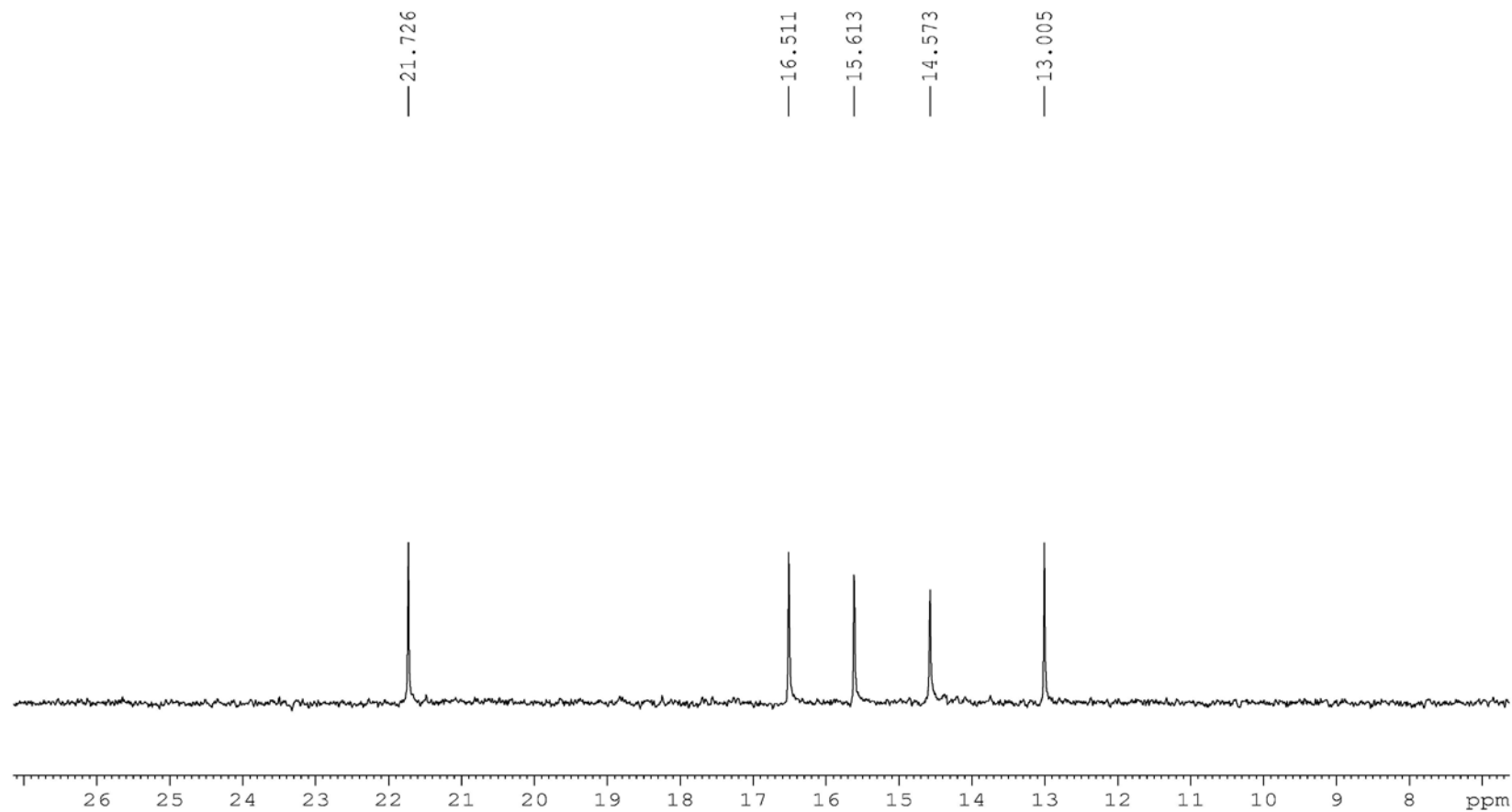
NAME                lws-19
EXPNO                2
PROCNO               1
Date_                20141028
Time_                15.27
INSTRUM              spect
PROBHD               5 mm CFPBBO BB
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                   1024
DS                    4
SWH                  24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631988 sec
RG                   147.94
DW                   20.800 use
DE                   18.00 use
TE                   297.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                  1
  
```

```

----- CHANNEL f1 -----
SFO1                100.6228293 MHz
NUC1                 13C
P1                   10.00 use
SI                   32768
SF                   100.6127686 MHz
WDW                  EM
SSB                   0
LB                   1.00 Hz
GB                   0
PC                   1.40
  
```

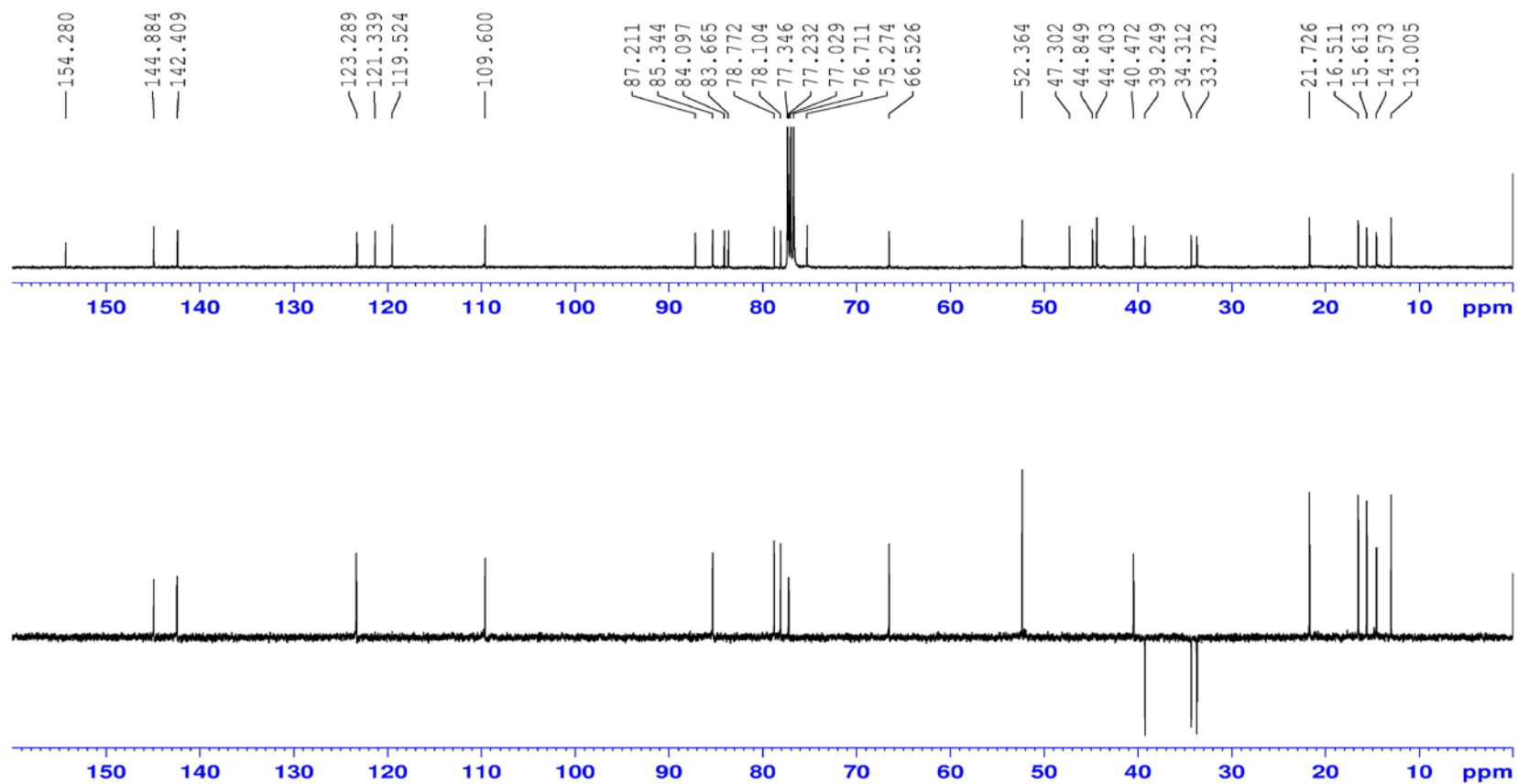




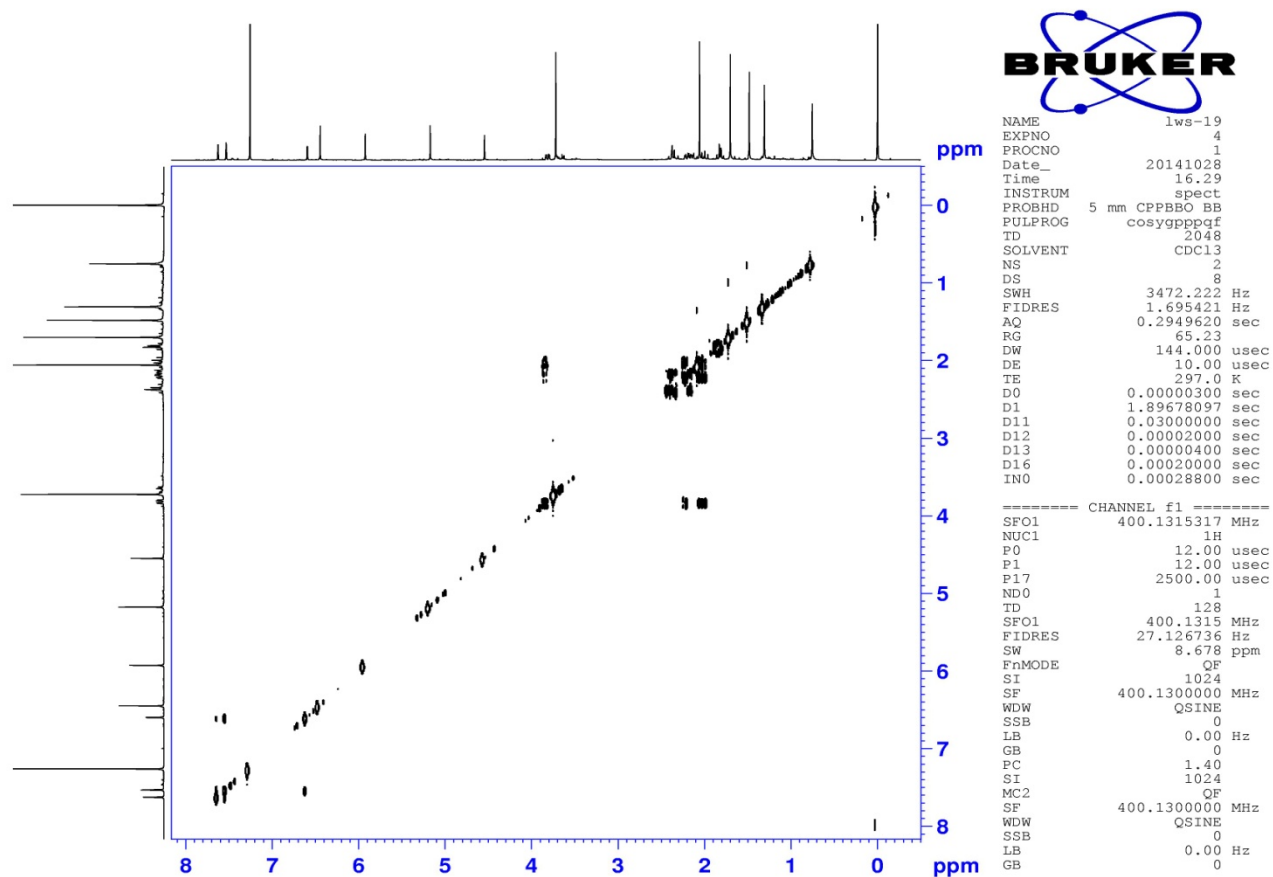


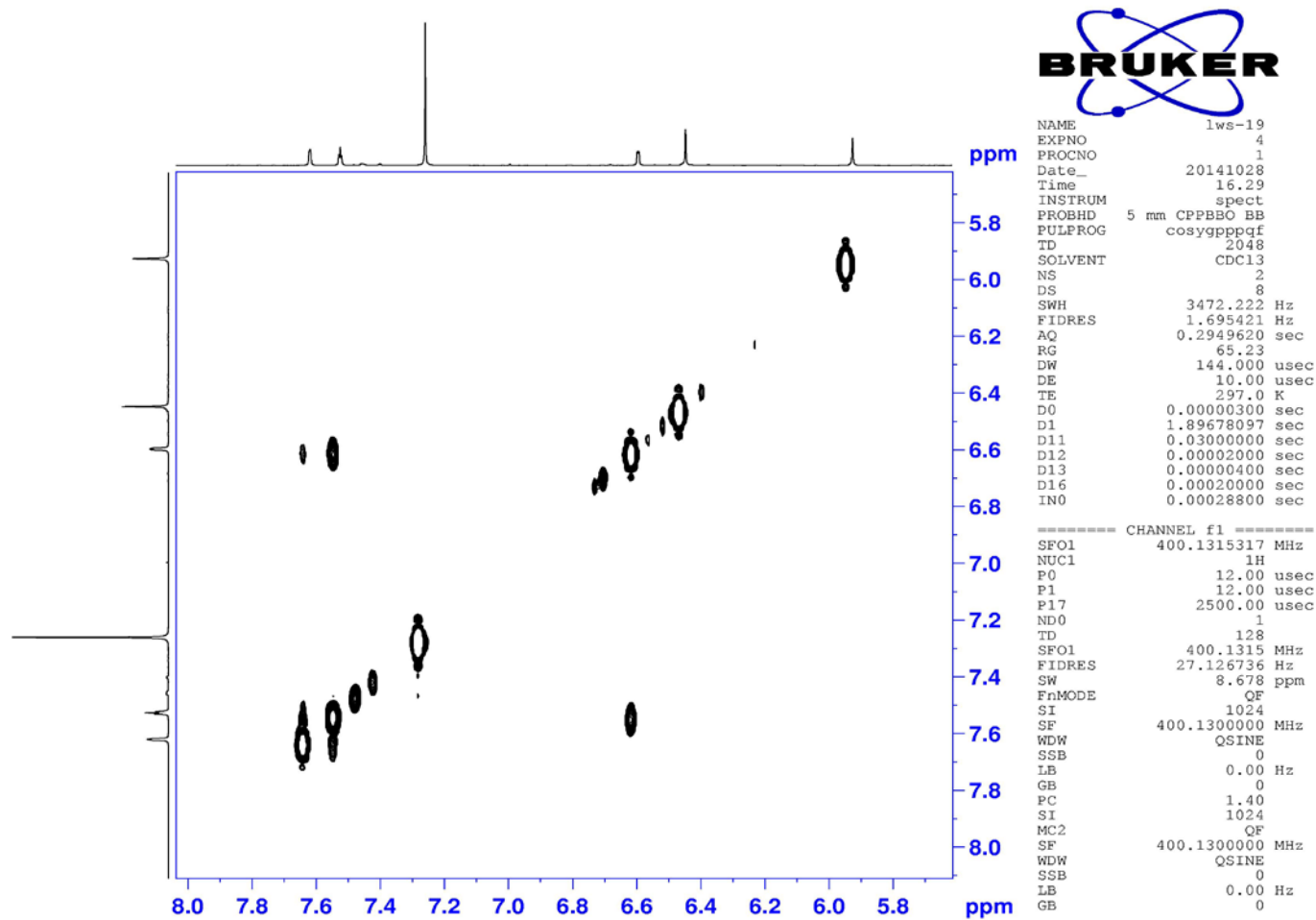
S70

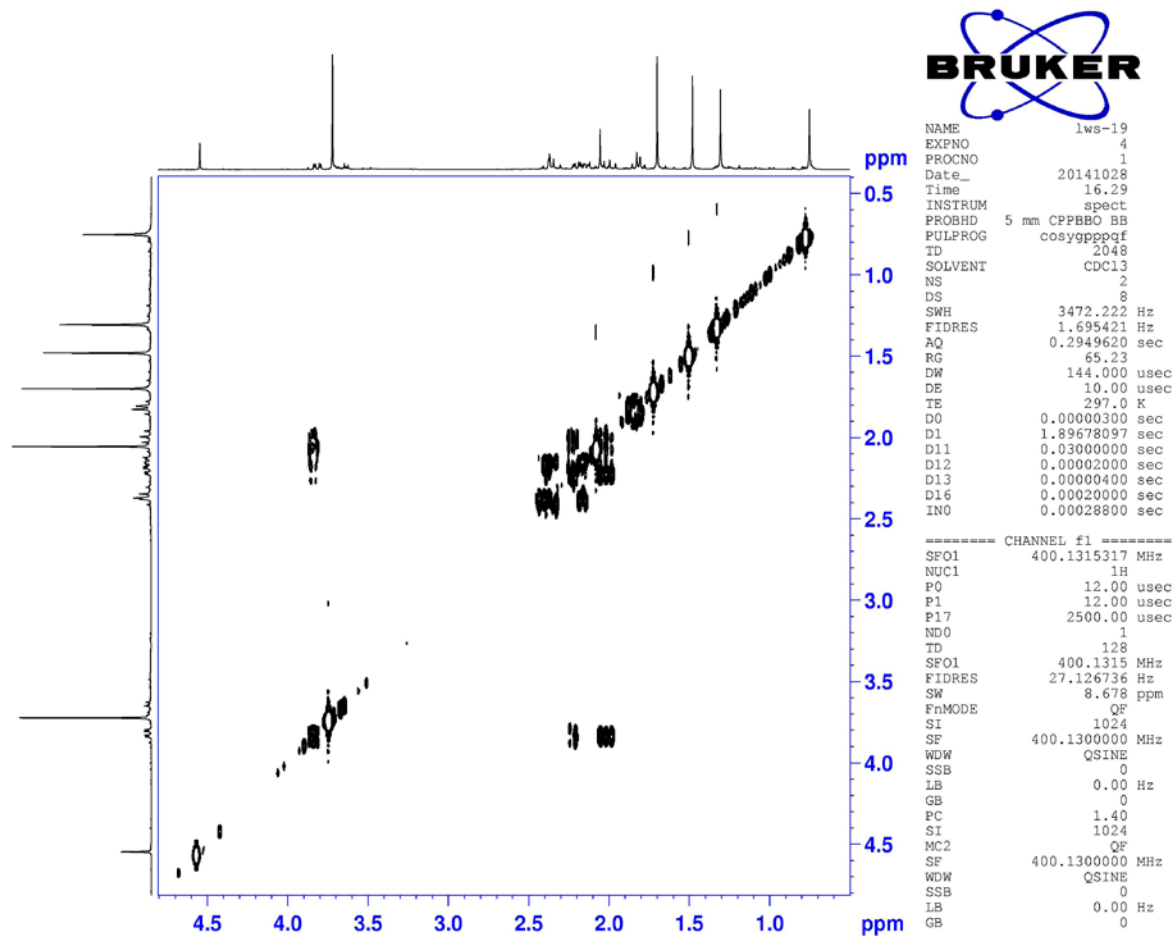
DEPT135° (100 MHz) spectrum of Compound **9** in CDCl₃



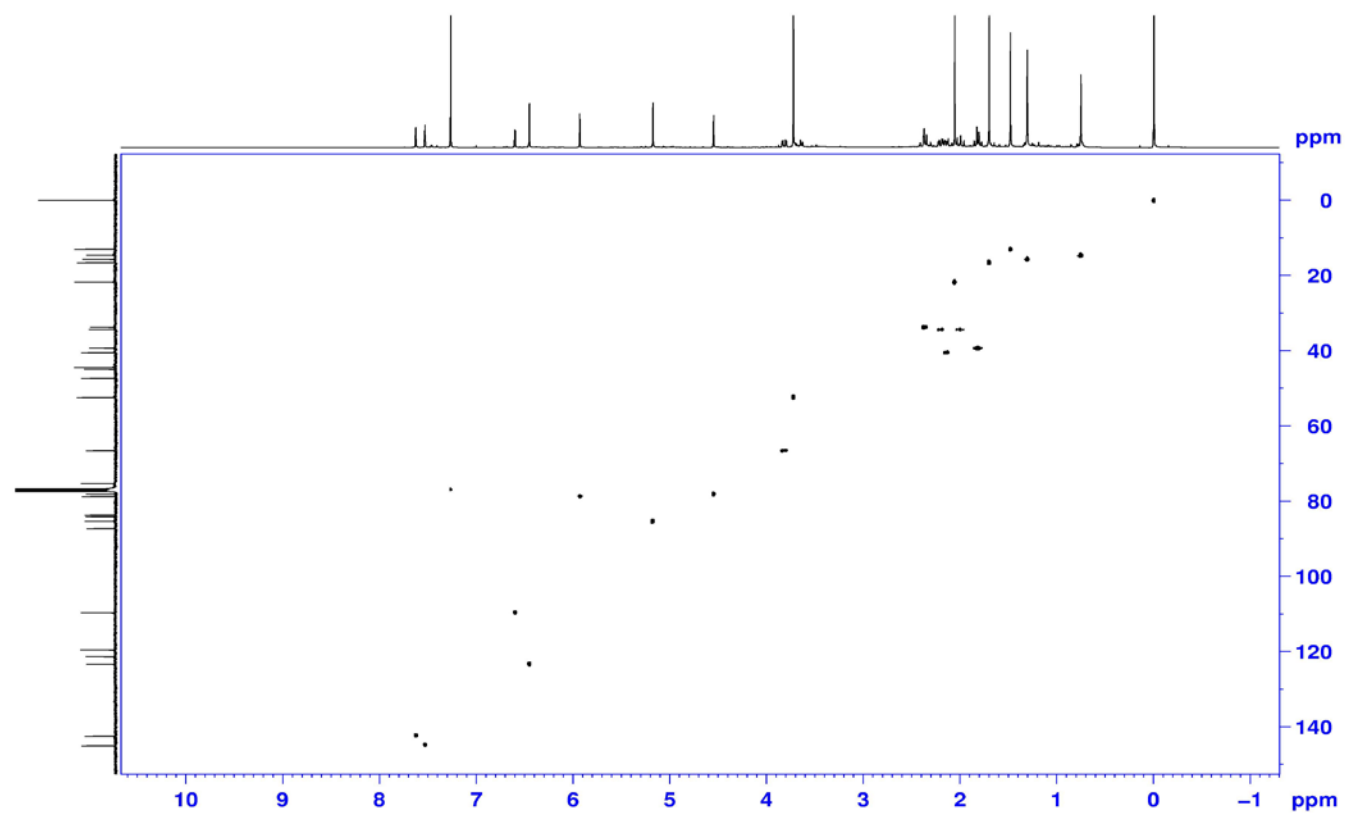
^1H - ^1H COSY (400 MHz) spectrum of Compound **9** in CDCl_3

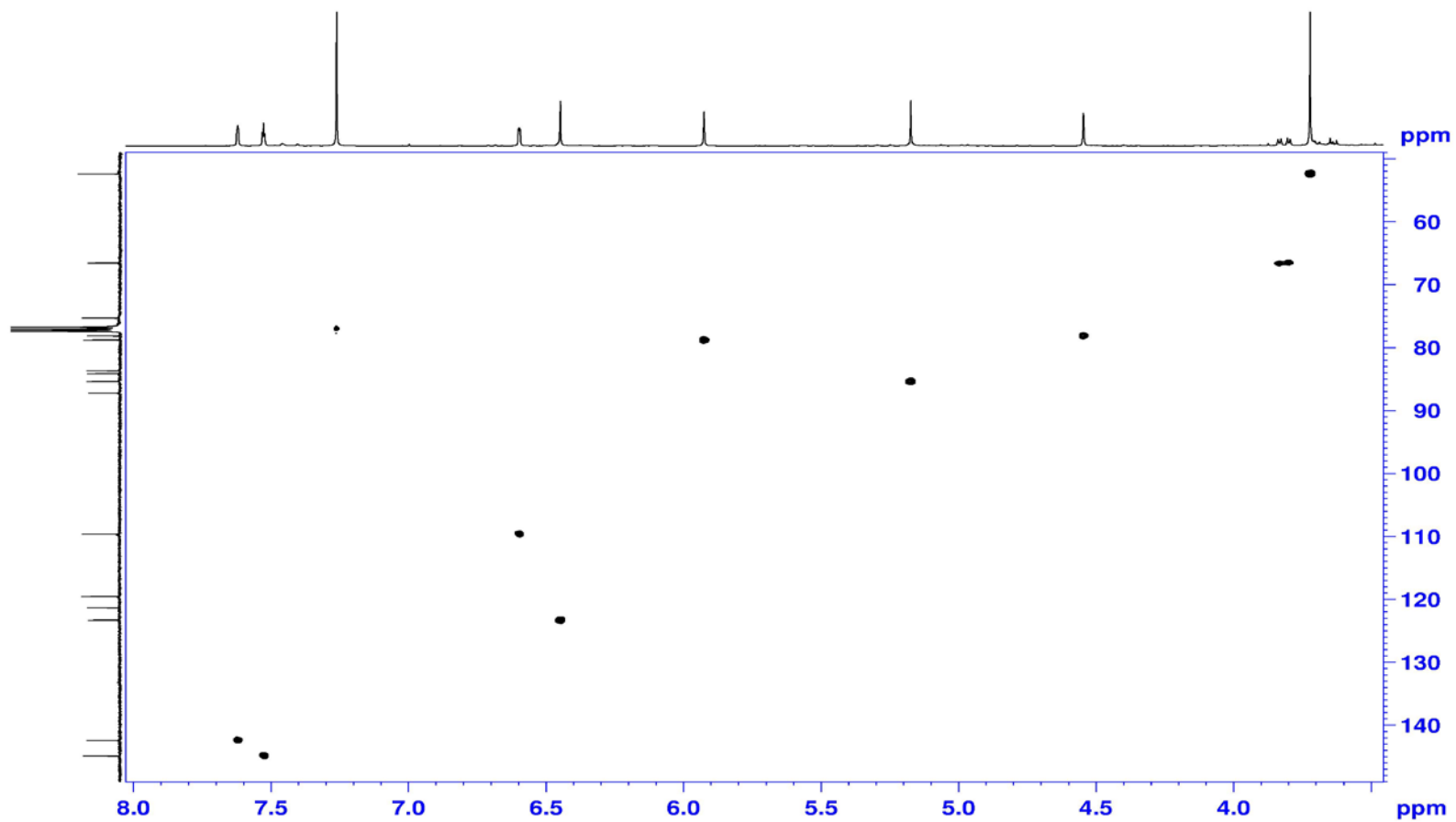




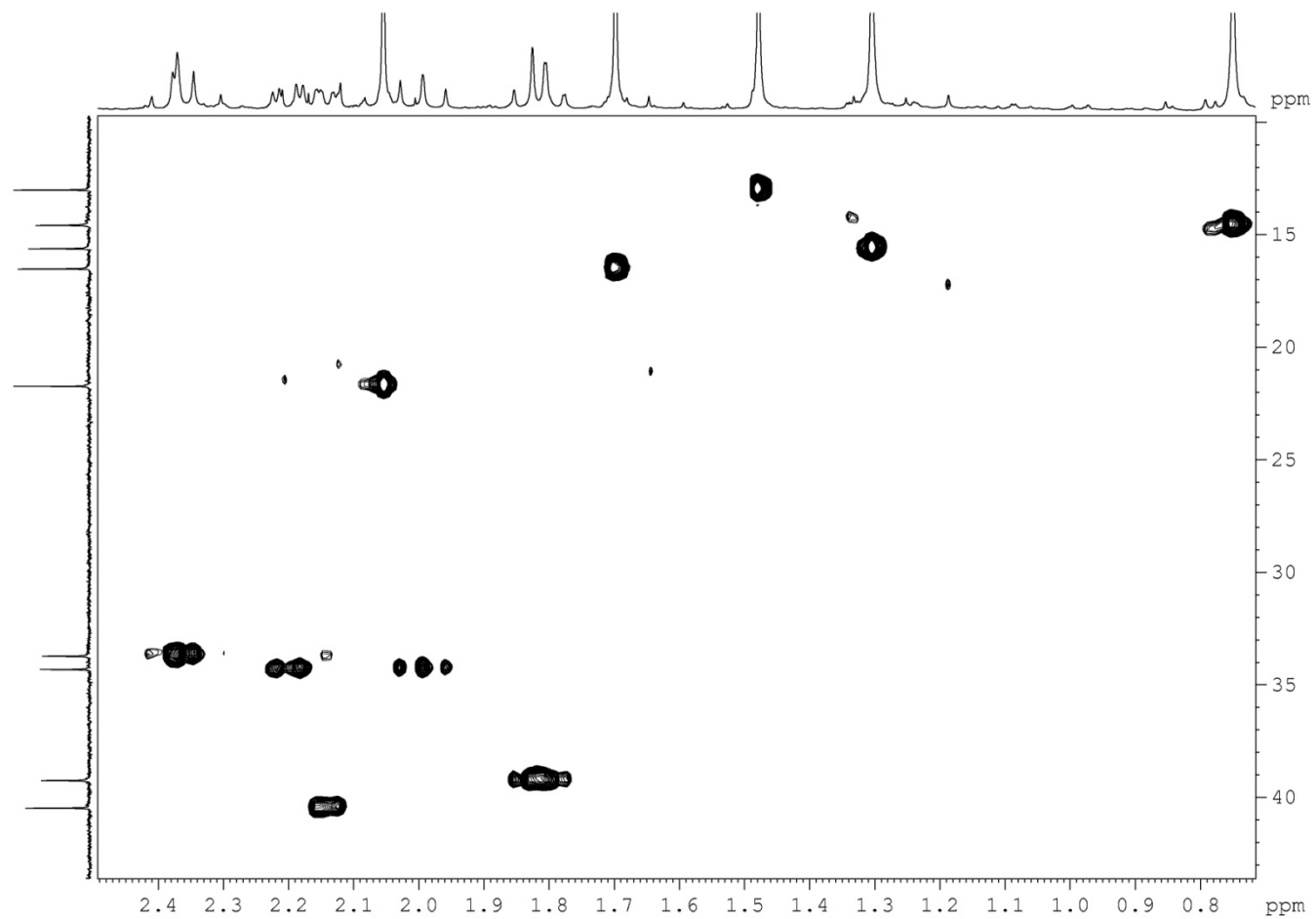


HSQC (400 MHz) spectrum of Compound **9** in CDCl₃

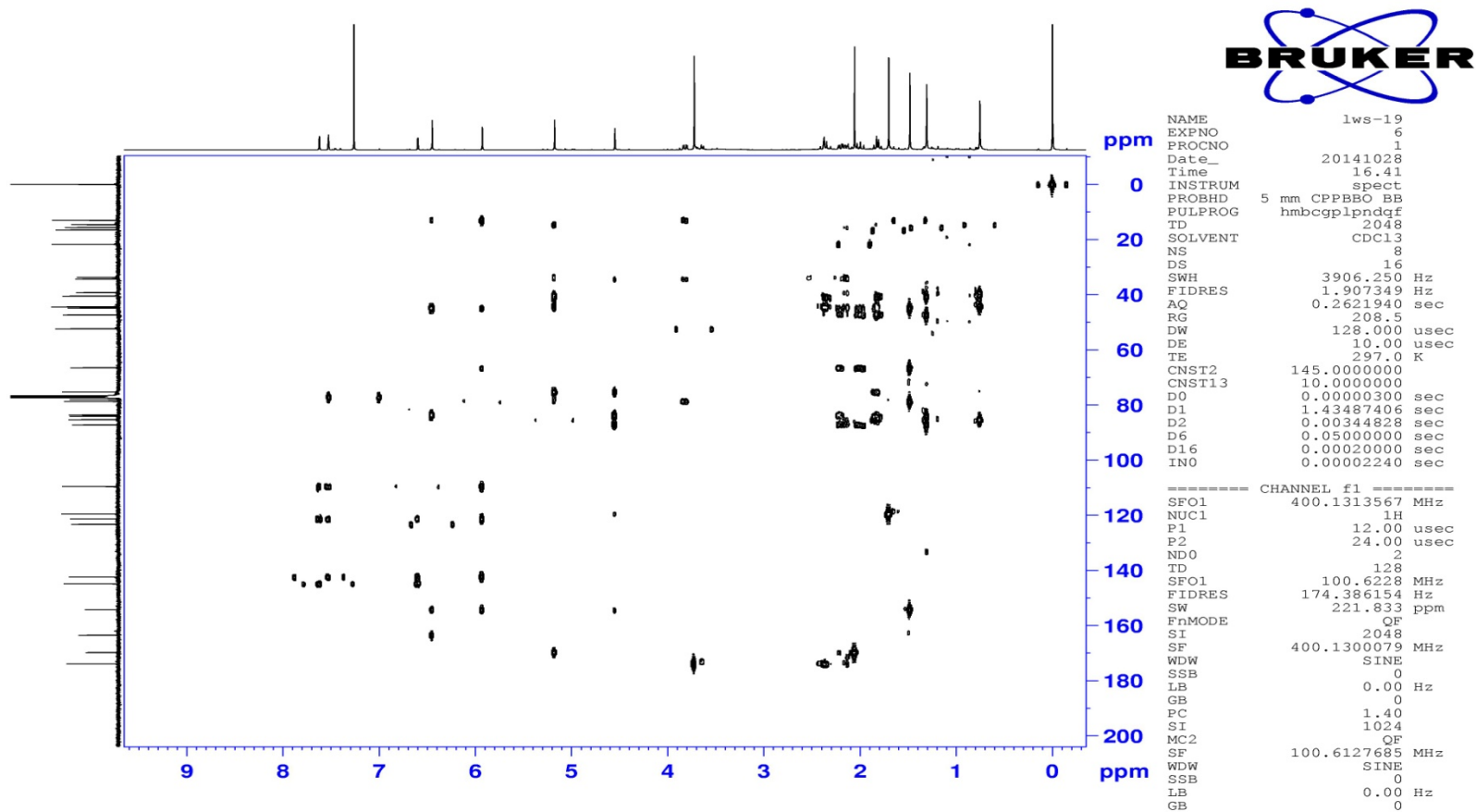


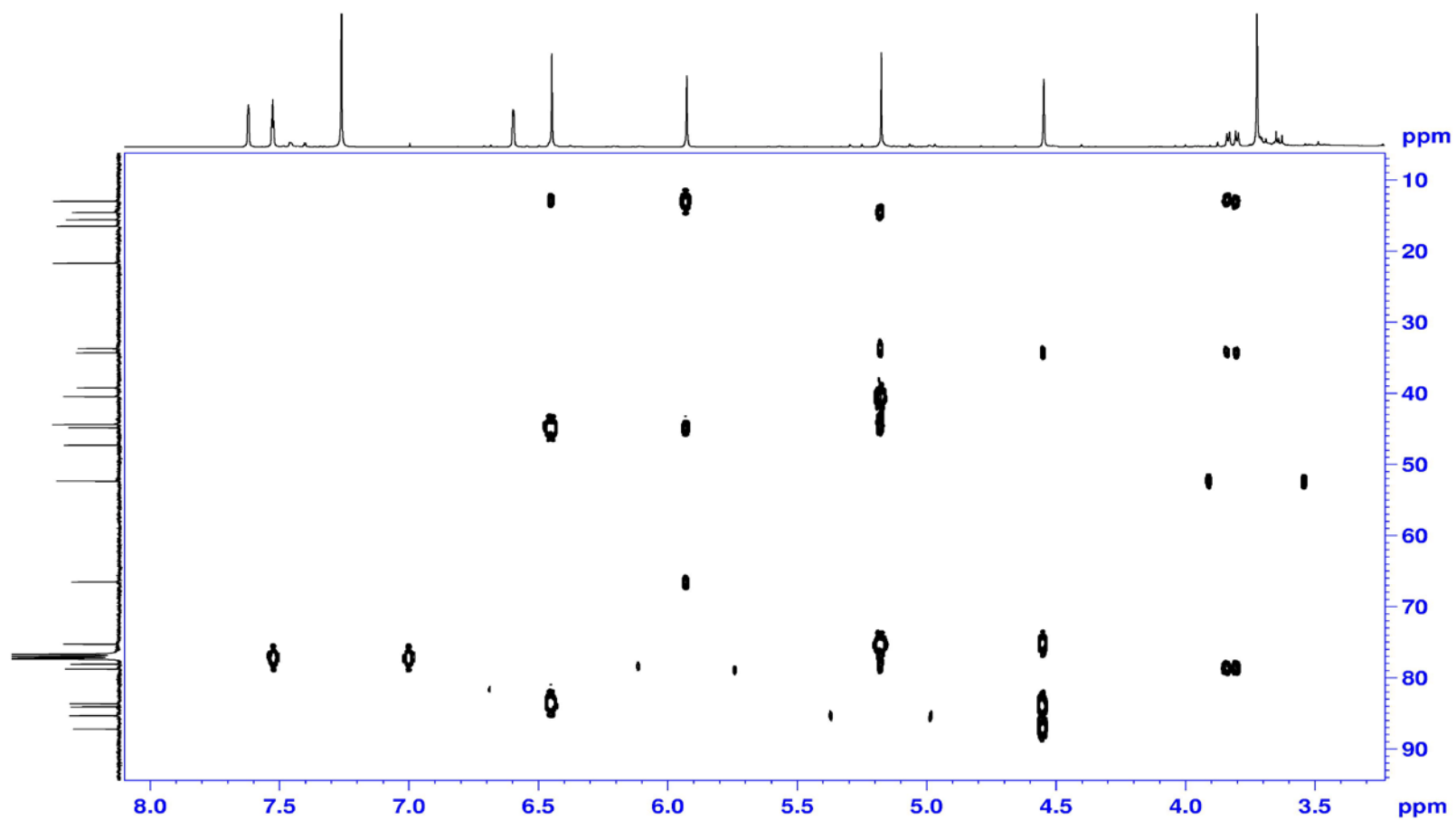


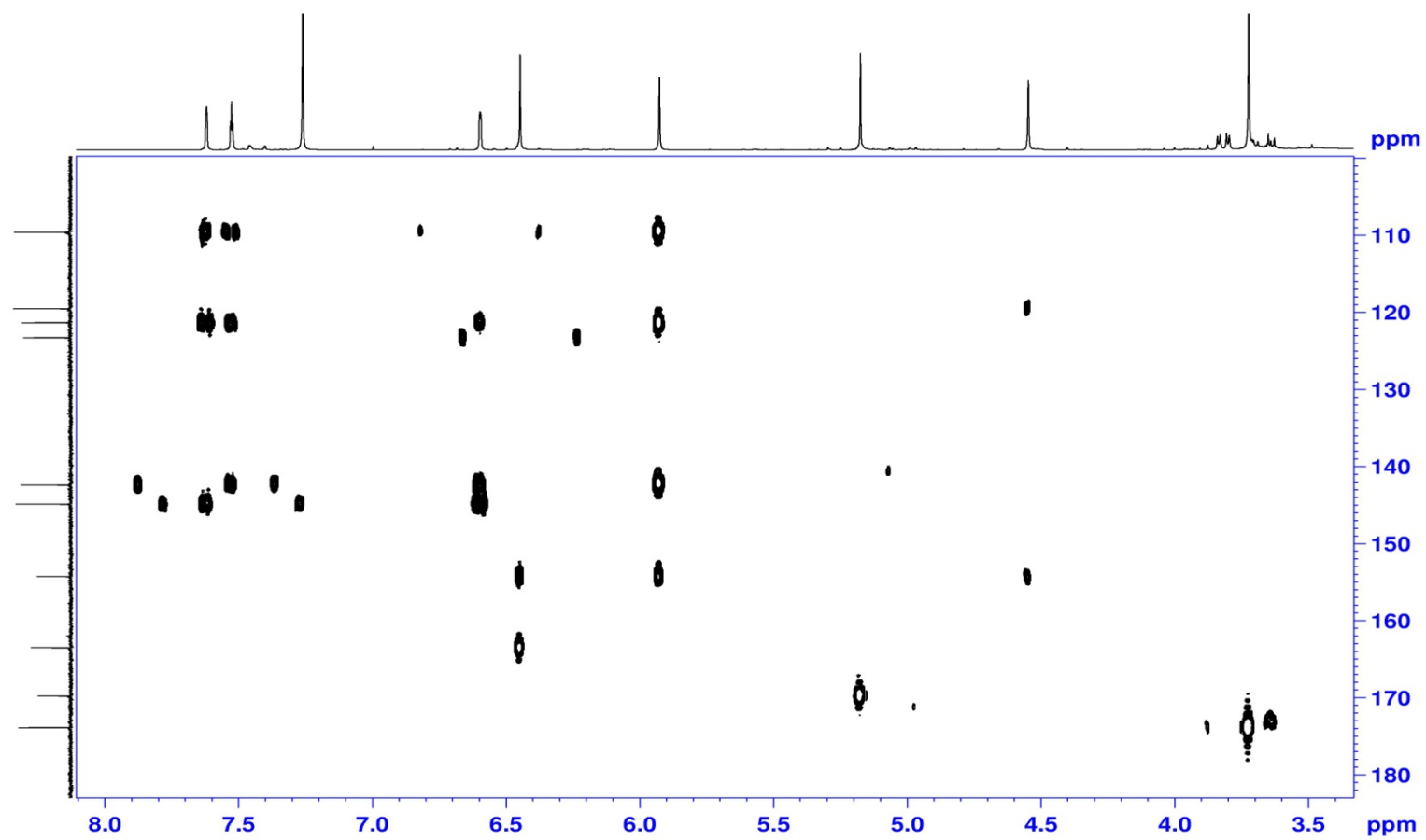
S76



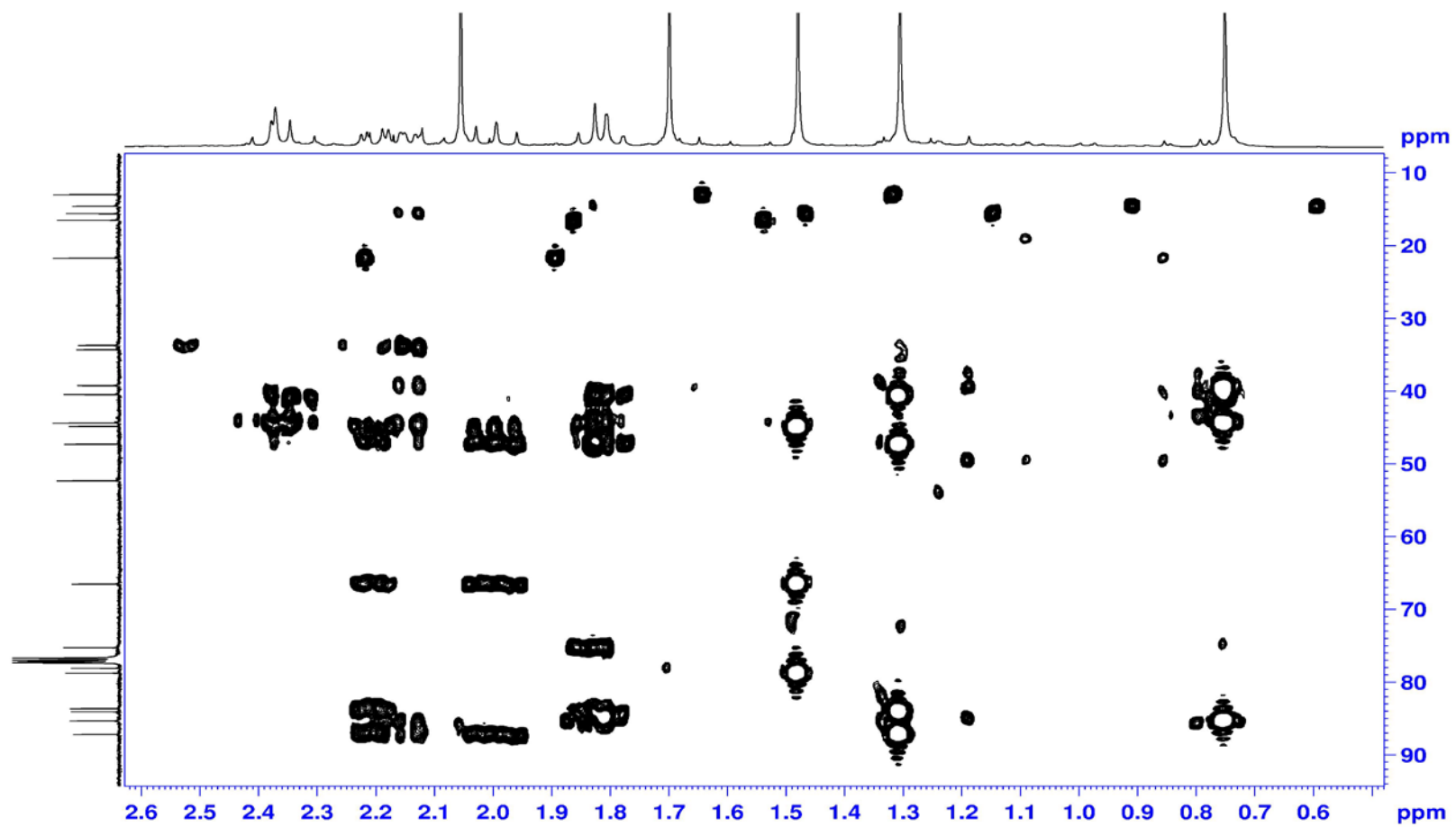
HMBC (400 MHz) spectrum of Compound **9** in CDCl₃

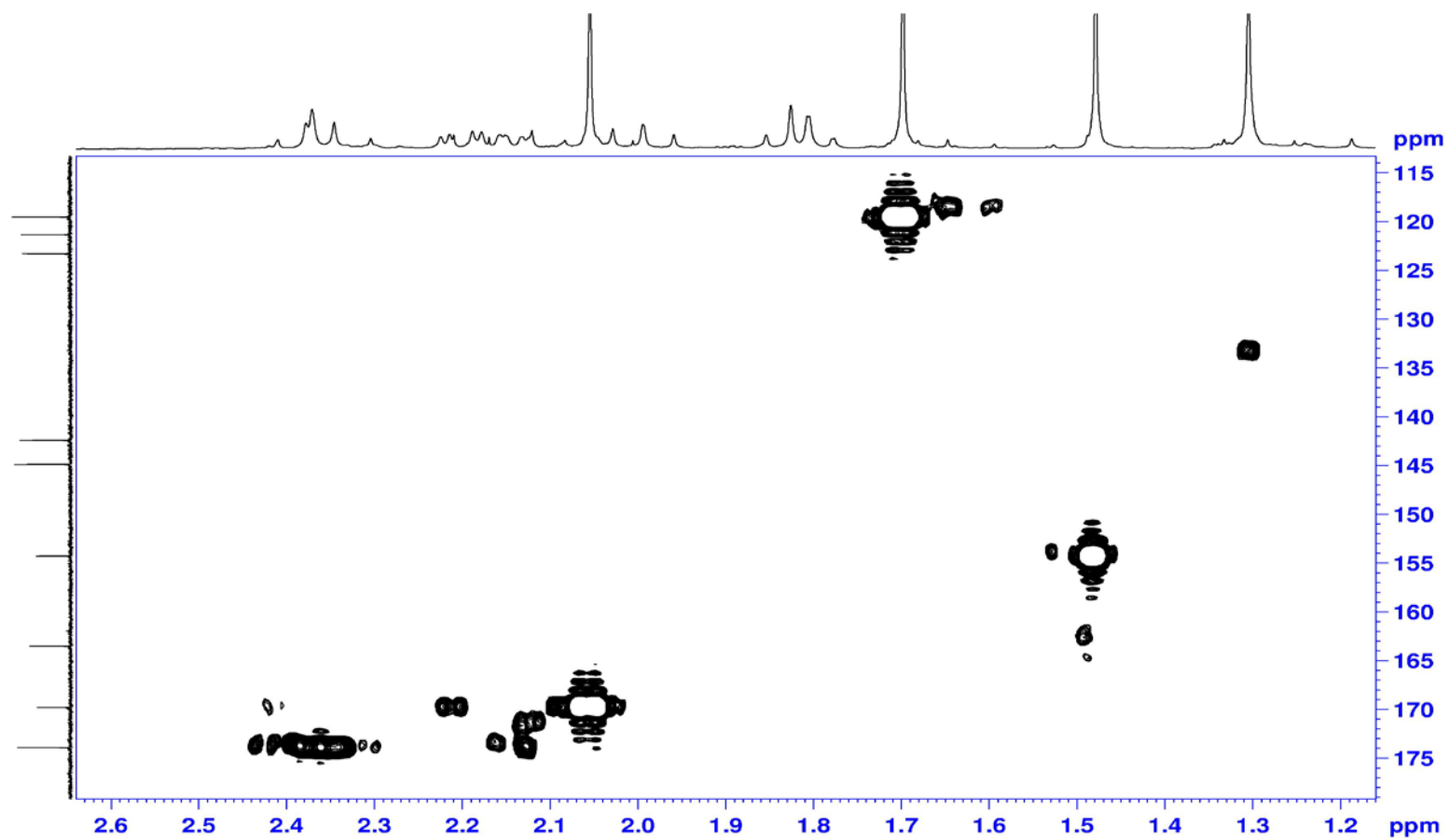




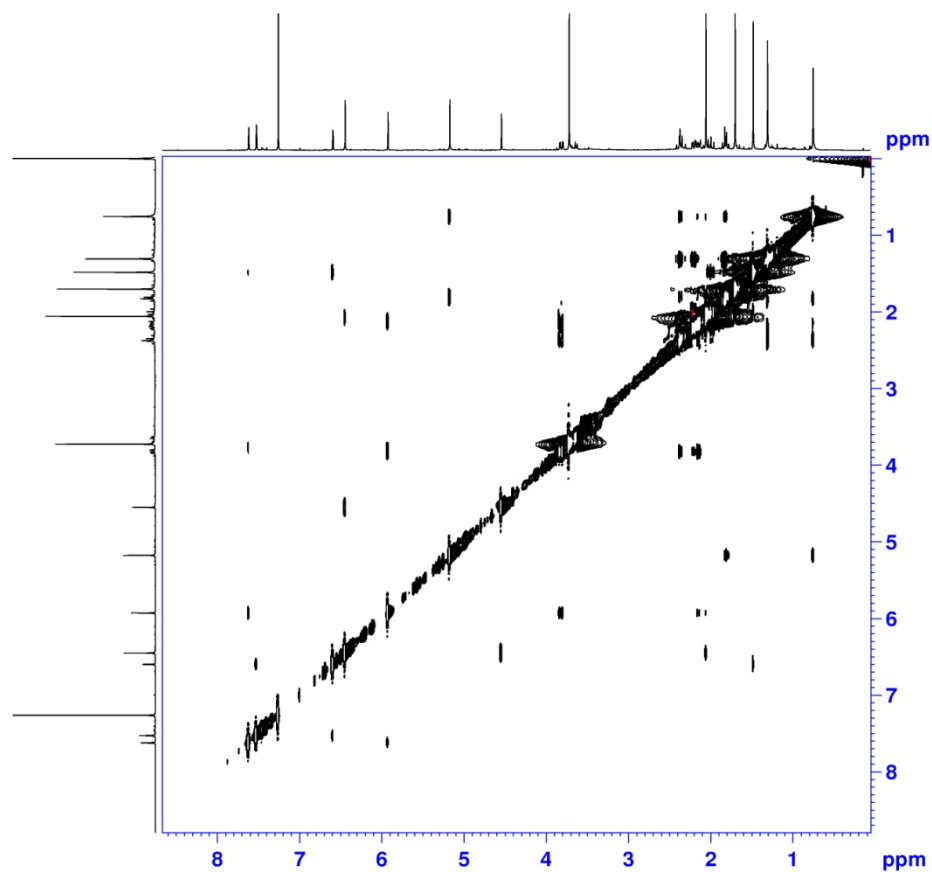


S80





NOESY (400 MHz) spectrum of Compound **9** in CDCl₃

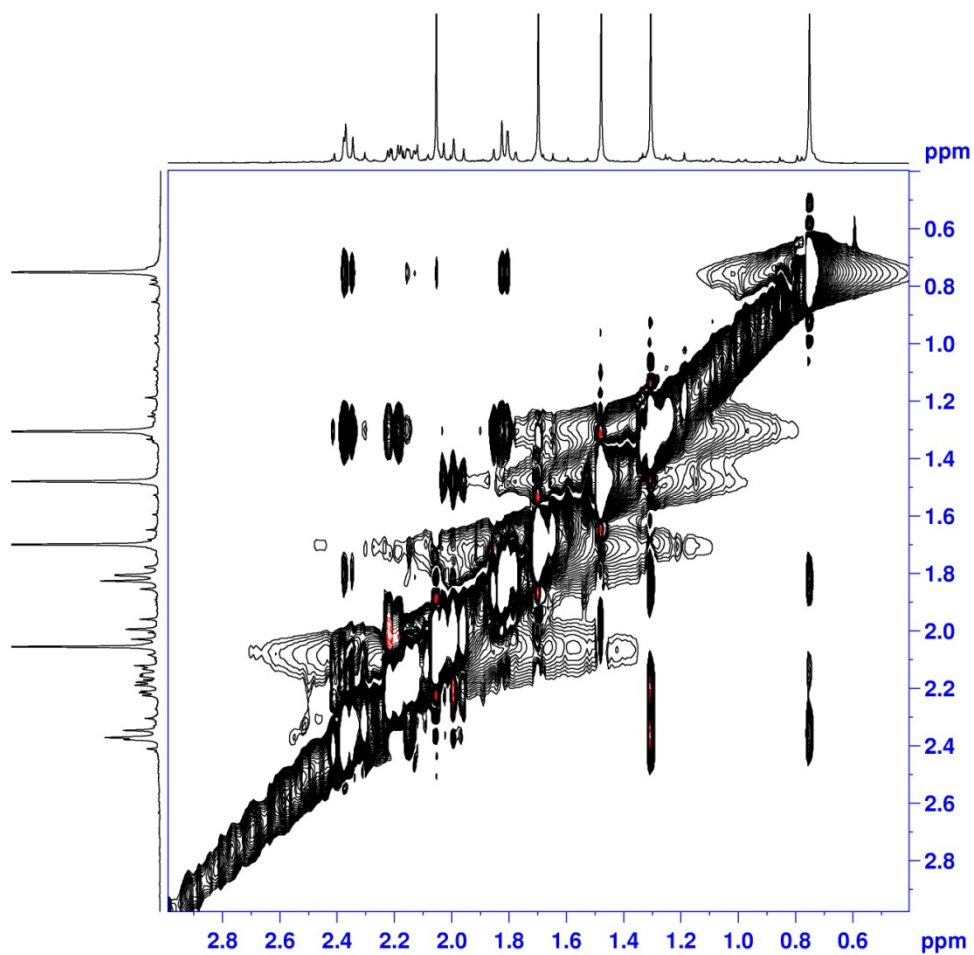


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NAME          lws-19
EXPNO         7
PROCNO        1
Date_         20141028
Time          17.54
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       noesygpphph
TD            2048
SOLVENT       CDCl3
NS            8
DS            32
SWH           3906.250 Hz
FIDRES        1.907349 Hz
AQ            0.2621940 sec
RG            65.23
DW            128.000 usec
DE            10.00 usec
TE            297.0 K
D0            0.00011272 sec
D1            1.99385595 sec
D8            0.30000001 sec
D11           0.03000000 sec
D12           0.00020000 sec
D16           0.00020000 sec
IN0           0.00025600 sec
  
```

```

===== CHANNEL f1 =====
SFO1         400.1313567 MHz
NUC1          1H
P1            12.00 usec
P2            24.00 usec
P17           2500.00 usec
ND0           1
TD            256
SFO1         400.1314 MHz
FIDRES        15.258789 Hz
SW            9.762 ppm
FnmODE       States-TPPI
SI            1024
SF           400.1300079 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.00
SI            1024
MC2          States-TPPI
SF           400.1300079 MHz
WDW           QSINE
SSB           2
  
```

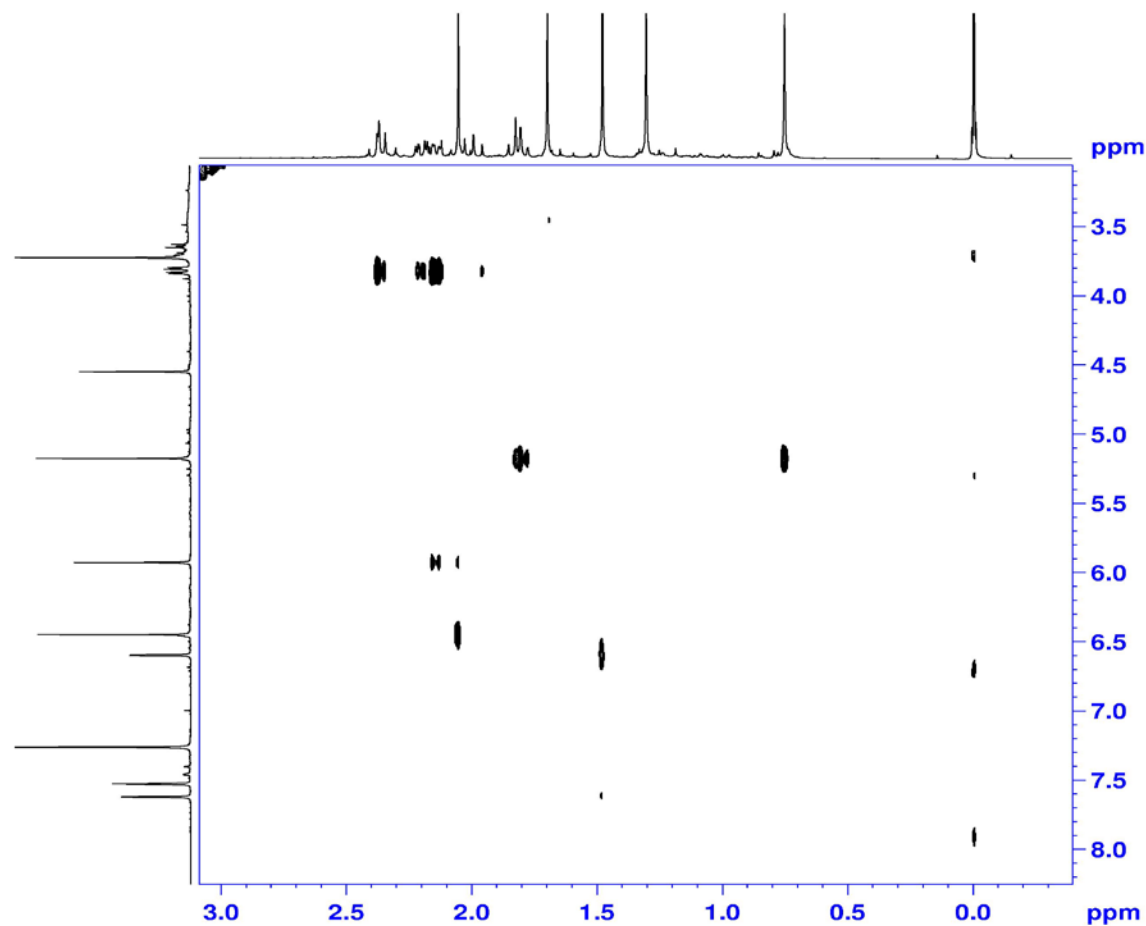


```

NAME          lws-19
EXPNO         7
PROCNO        1
Date_         20141028
Time          17.54
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       noesygpphpg
TD            2048
SOLVENT       CDCl3
NS            8
DS            32
SWH           3906.250 Hz
FIDRES        1.907349 Hz
AQ            0.2621940 sec
RG            65.23
DW            128.000 usec
DE            10.00 usec
TE            297.0 K
D0            0.00011272 sec
D1            1.99385595 sec
D8            0.30000001 sec
D11           0.03000000 sec
D12           0.00002000 sec
D16           0.00020000 sec
IN0           0.00025600 sec

===== CHANNEL f1 =====
SFO1          400.1313567 MHz
NUC1           1H
P1            12.00 usec
P2            24.00 usec
P17           2500.00 usec
ND0            1
TD            256
SFO1          400.1314 MHz
FIDRES        15.258789 Hz
SW            9.762 ppm
FnMODE        States-TPPI
SI            1024
SF            400.1300079 MHz
WDW           QSINE
SSB            2
LB            0.00 Hz
GB            0
PC            1.00
SI            1024
MC2           States-TPPI
SF            400.1300079 MHz
WDW           QSINE
SSB            2

```

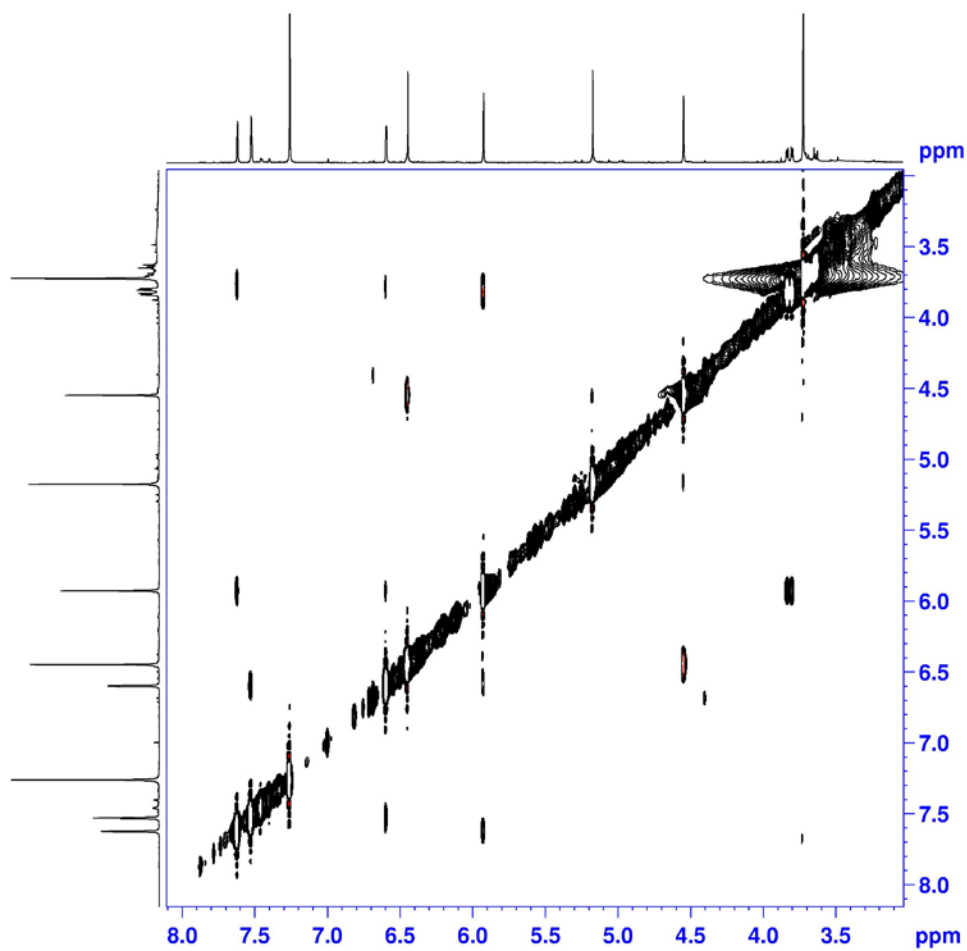



```

NAME          lws-19
EXPNO          7
PROCNO         1
Date_         20141028
Time          17.54
INSTRUM        spect
PROBHD         5 mm CPPBBO BB
PULPROG        noesygpphph
TD             2048
SOLVENT        CDCl3
NS              8
DS             32
SWH            3906.250 Hz
FIDRES         1.907349 Hz
AQ             0.2621940 sec
RG             65.23
DW            128.000 usec
DE             10.00 usec
TE             297.0 K
D0             0.00011272 sec
D1             1.99385595 sec
D8             0.30000001 sec
D11            0.030000000 sec
D12            0.000020000 sec
D16            0.00020000 sec
IN0            0.00025600 sec

===== CHANNEL f1 =====
SFO1          400.1313567 MHz
NUC1           1H
P1             12.00 usec
P2             24.00 usec
P17            2500.00 usec
ND0            1
TD             256
SFO1          400.1314 MHz
FIDRES         15.258789 Hz
SW             9.762 ppm
FnMODE         States-TPPI
SI             1024
SF            400.1300079 MHz
WDW            QSINE
SSB            2
LB             0.00 Hz
GB             0
PC             1.00
SI             1024
MC2            States-TPPI
SF            400.1300079 MHz
WDW            QSINE
SSB            2

```



```

NAME          lws-19
EXPNO         7
PROCNO        1
Date_         20141028
Time          17.54
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       noesygpphph
TD            2048
SOLVENT       CDC13
NS            8
DS            32
SWH           3906.250 Hz
FIDRES        1.907349 Hz
AQ            0.2621940 sec
RG            65.23
DW            128.000 usec
DE            10.00 usec
TE            297.0 K
D0            0.00011272 sec
D1            1.99385595 sec
D8            0.30000001 sec
D11           0.03000000 sec
D12           0.00002000 sec
D16           0.00020000 sec
IN0           0.00025600 sec

```

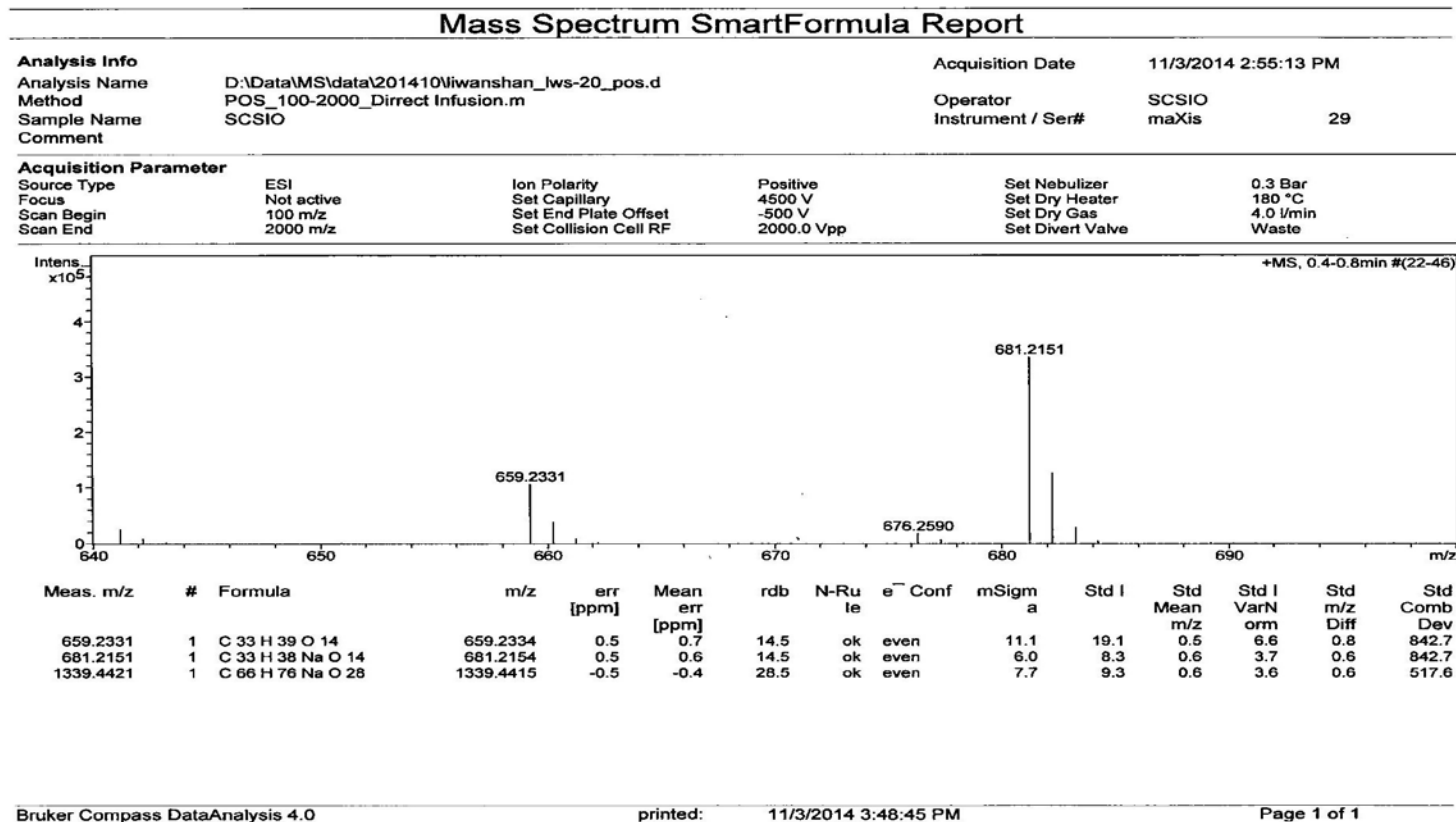
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===== CHANNEL f1 =====
SFO1         400.1313567 MHz
NUC1          1H
P1            12.00 usec
P2            24.00 usec
P17           2500.00 usec
ND0           1
TD            256
SFO1         400.1314 MHz
FIDRES        15.258789 Hz
SW            9.762 ppm
FnMODE        States-TPPI
SI            1024
SF            400.1300079 MHz
WDW           QSINE
SSB            2
LB            0.00 Hz
GB            0
PC            1.00
SI            1024
MC2           States-TPPI
SF            400.1300079 MHz
WDW           QSINE
SSB            2

```

HR-ESIMS of Compound 10

2.583



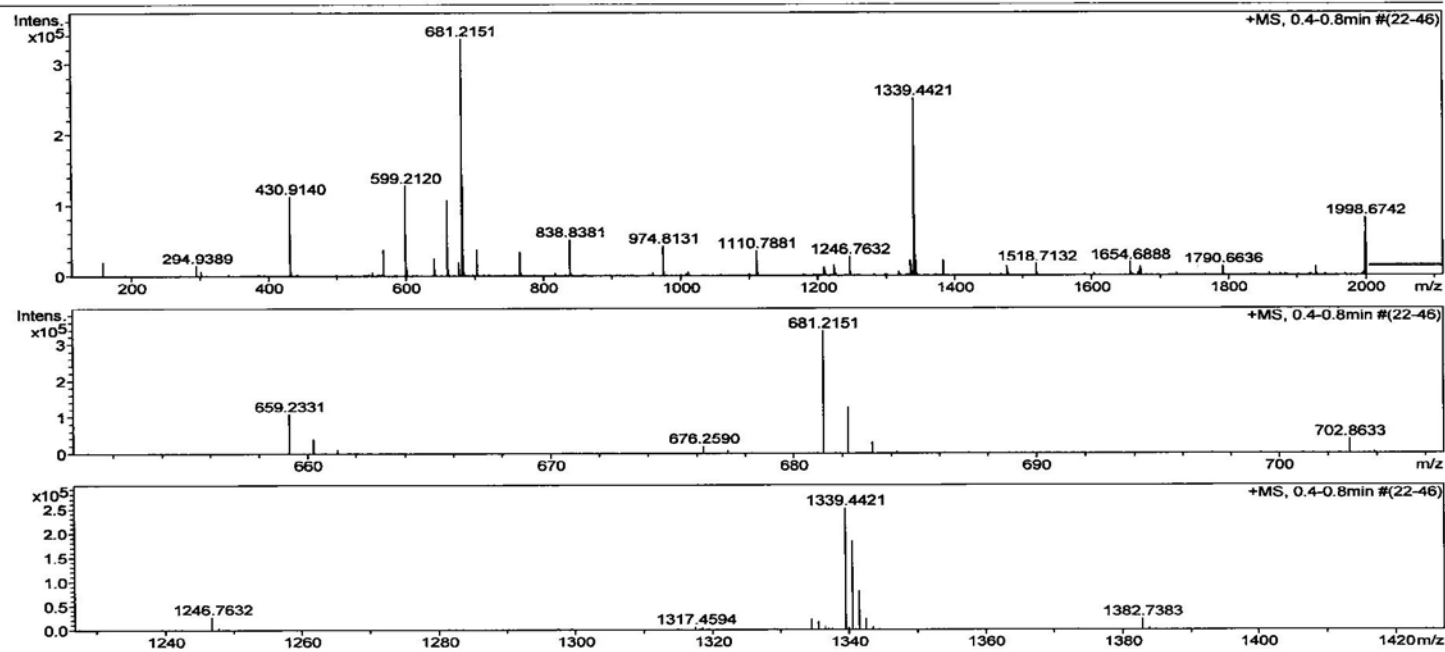
Generic Display Report

Analysis Info

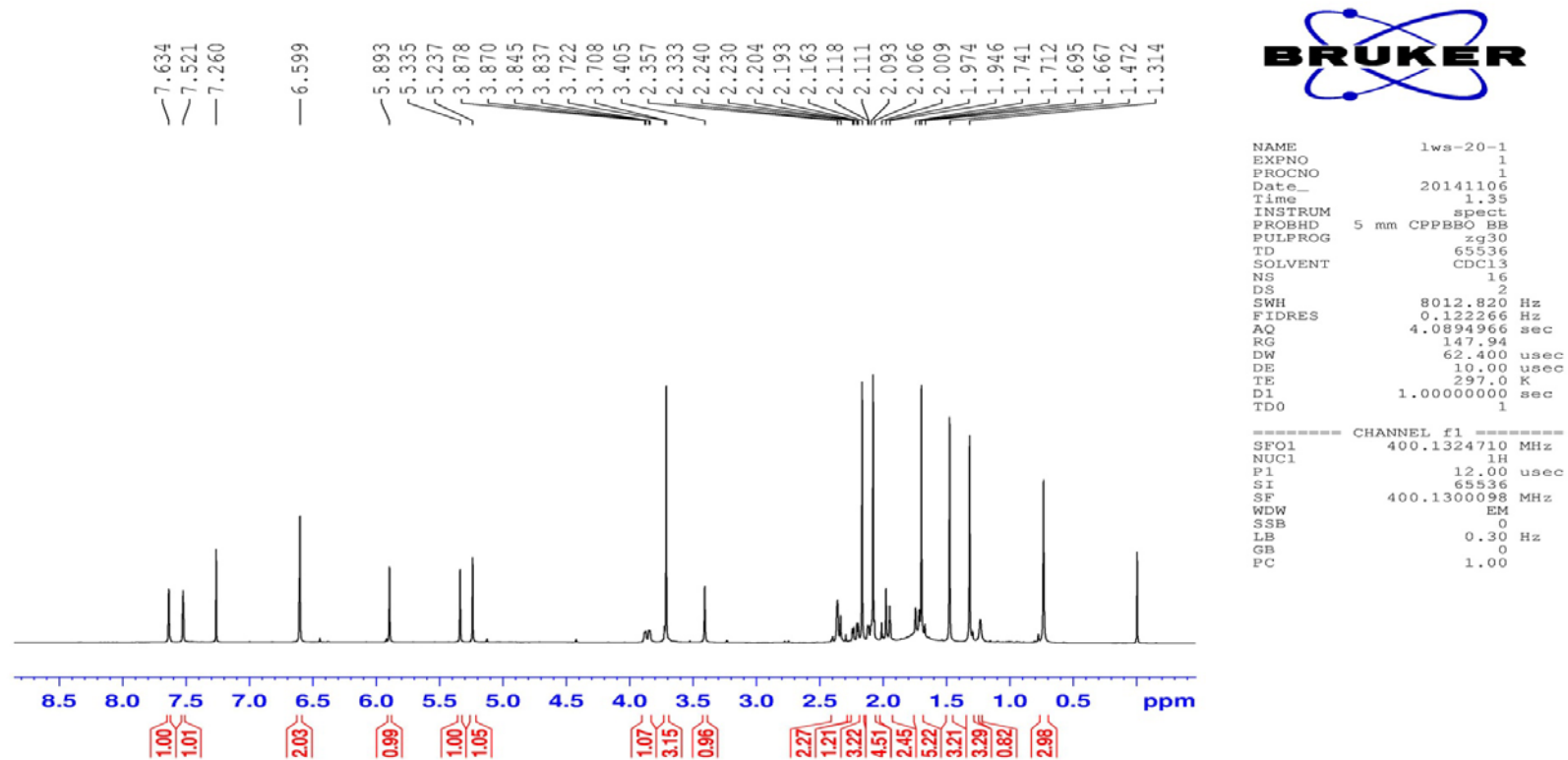
Analysis Name D:\Data\MS\data\201410\liwanshan_lws-20_pos.d
Method POS_100-2000_Direct Infusion.m
Sample Name SCSIO
Comment

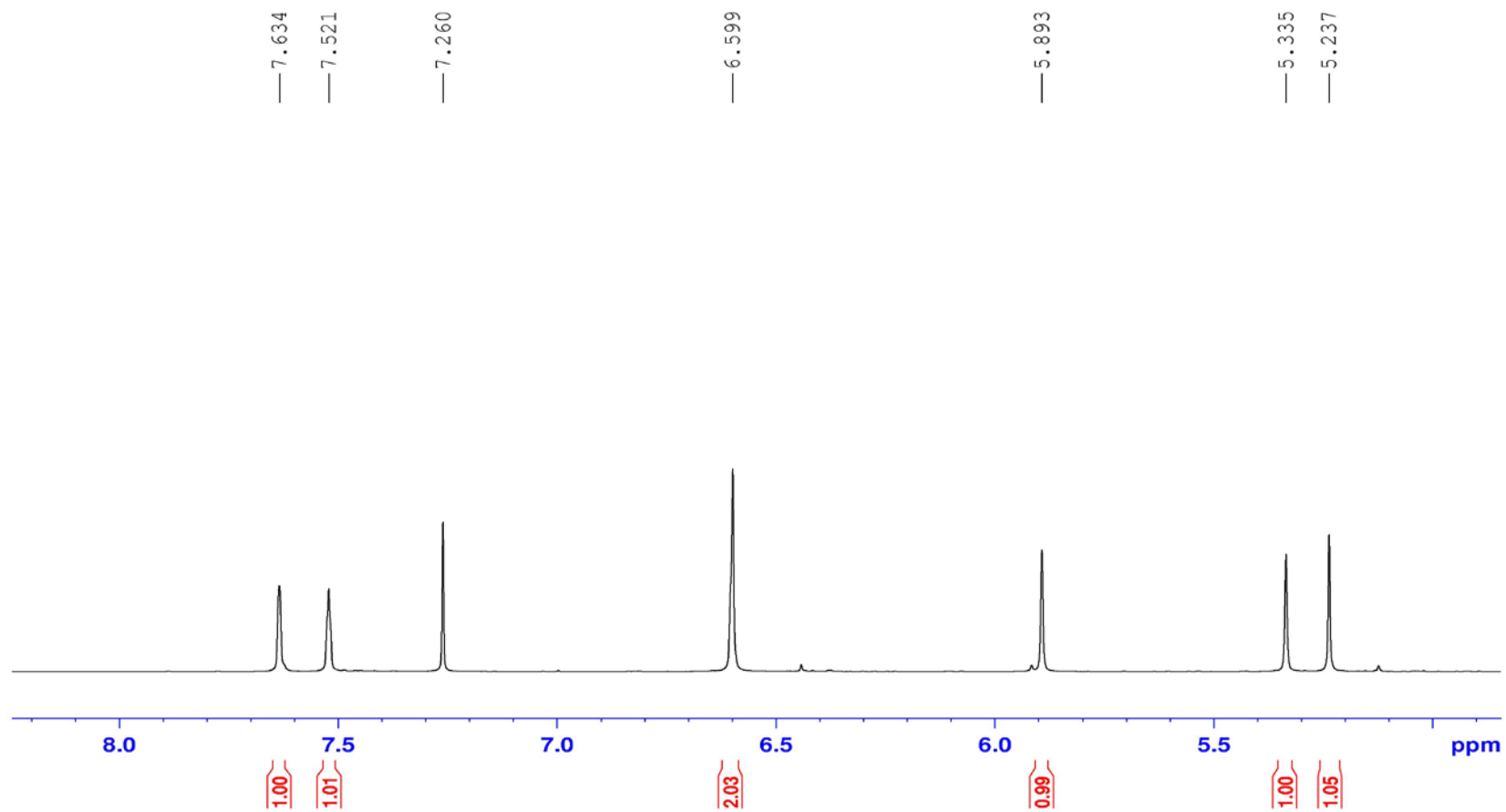
Acquisition Date 11/3/2014 2:55:13 PM

Operator SCSIO
Instrument maXis

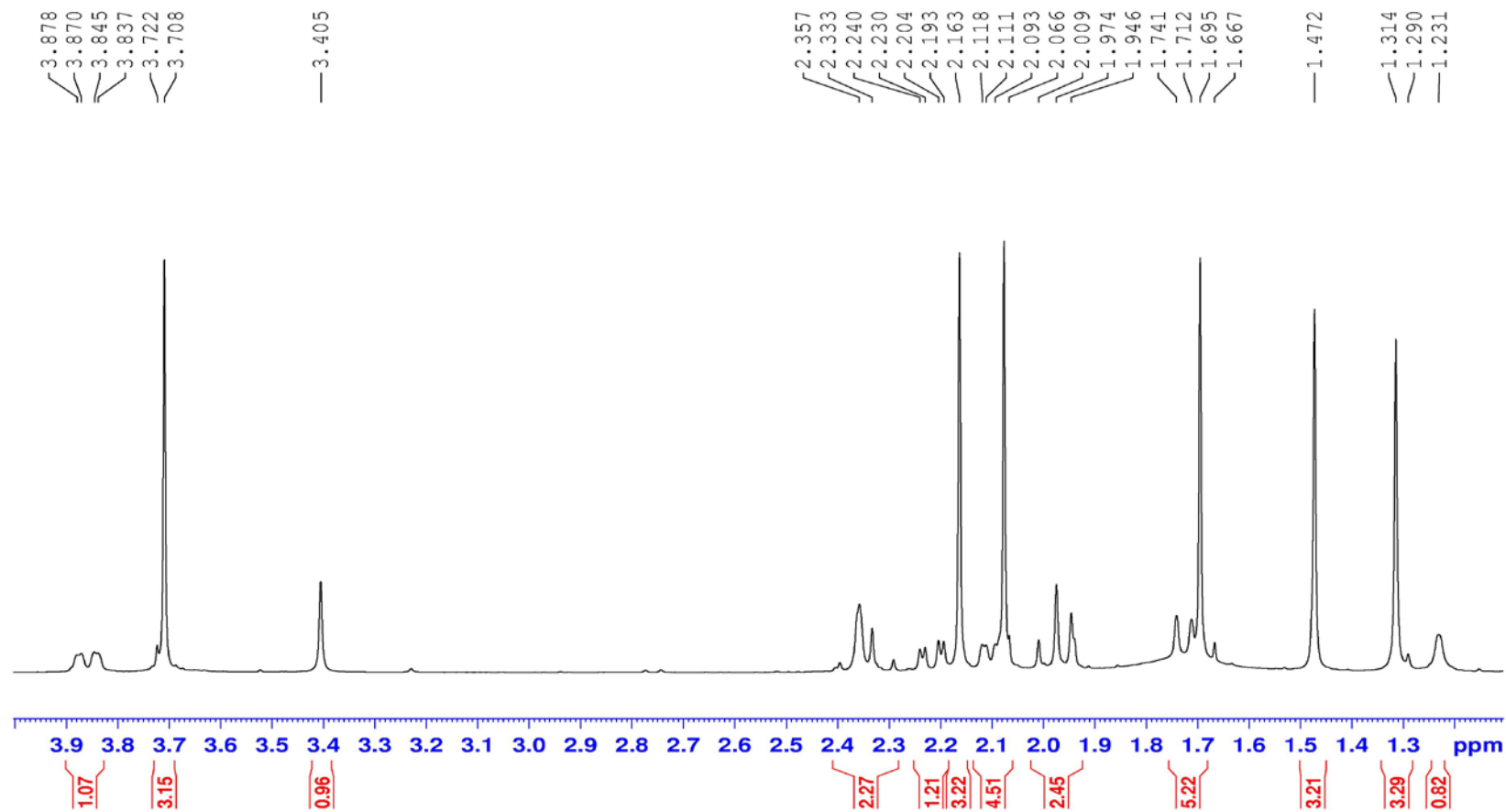


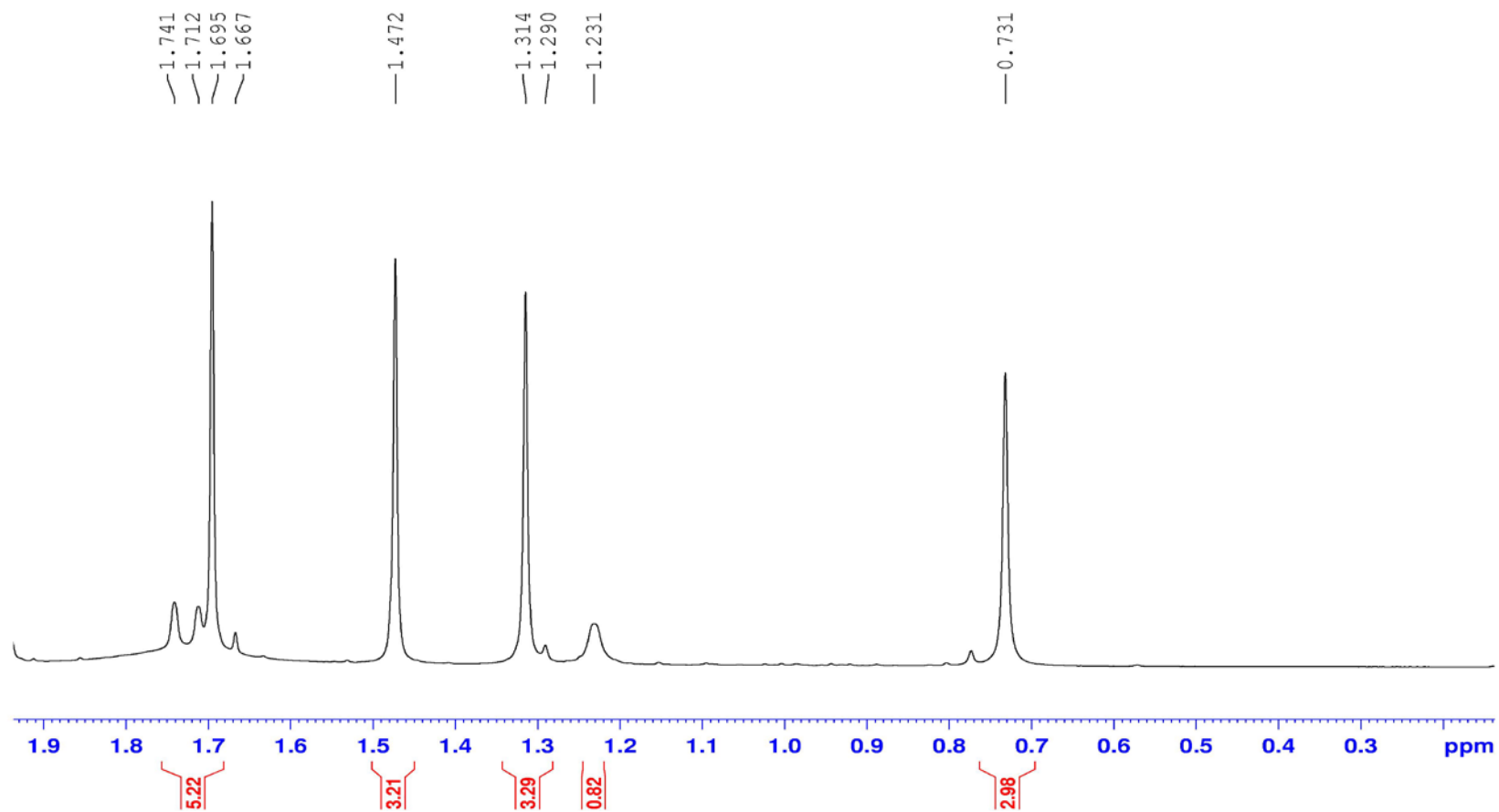
^1H NMR (400 MHz) spectrum of Compound **10** in CDCl_3



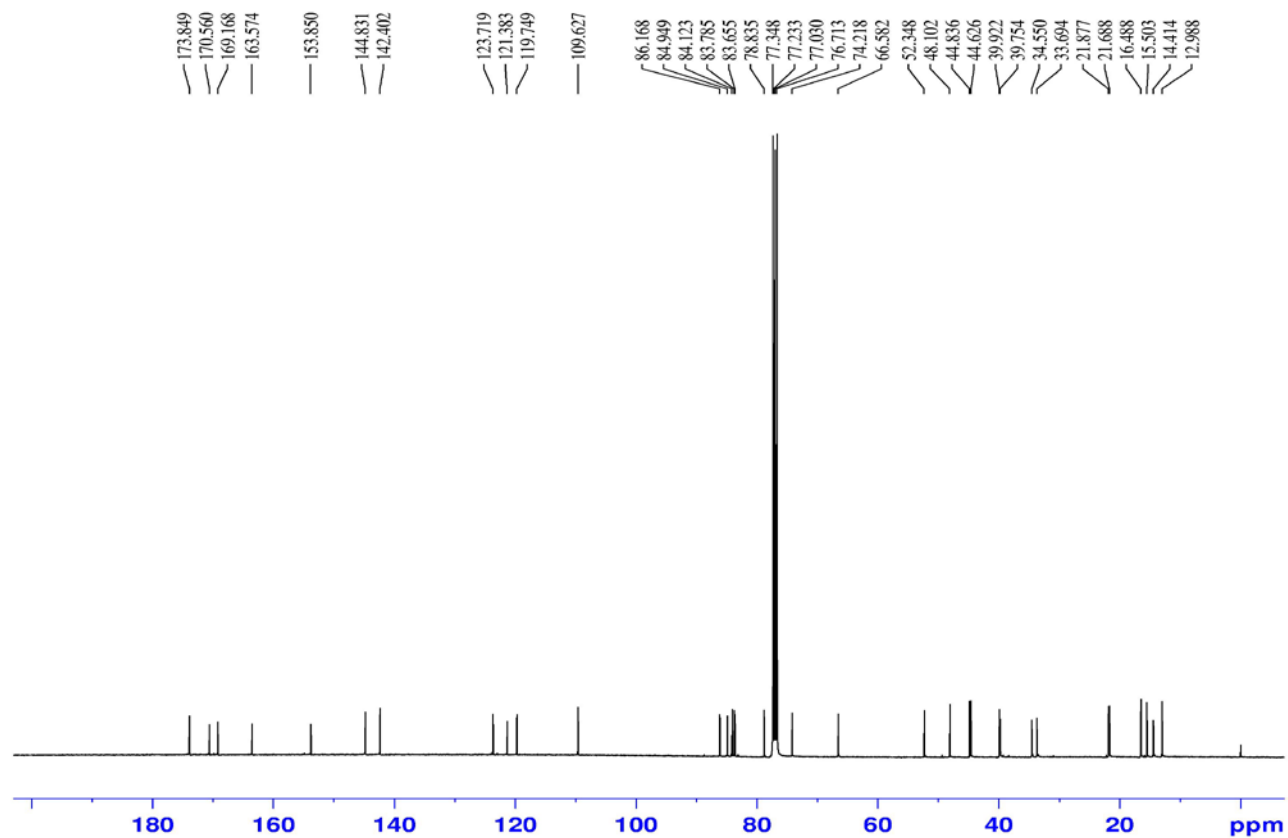


S90





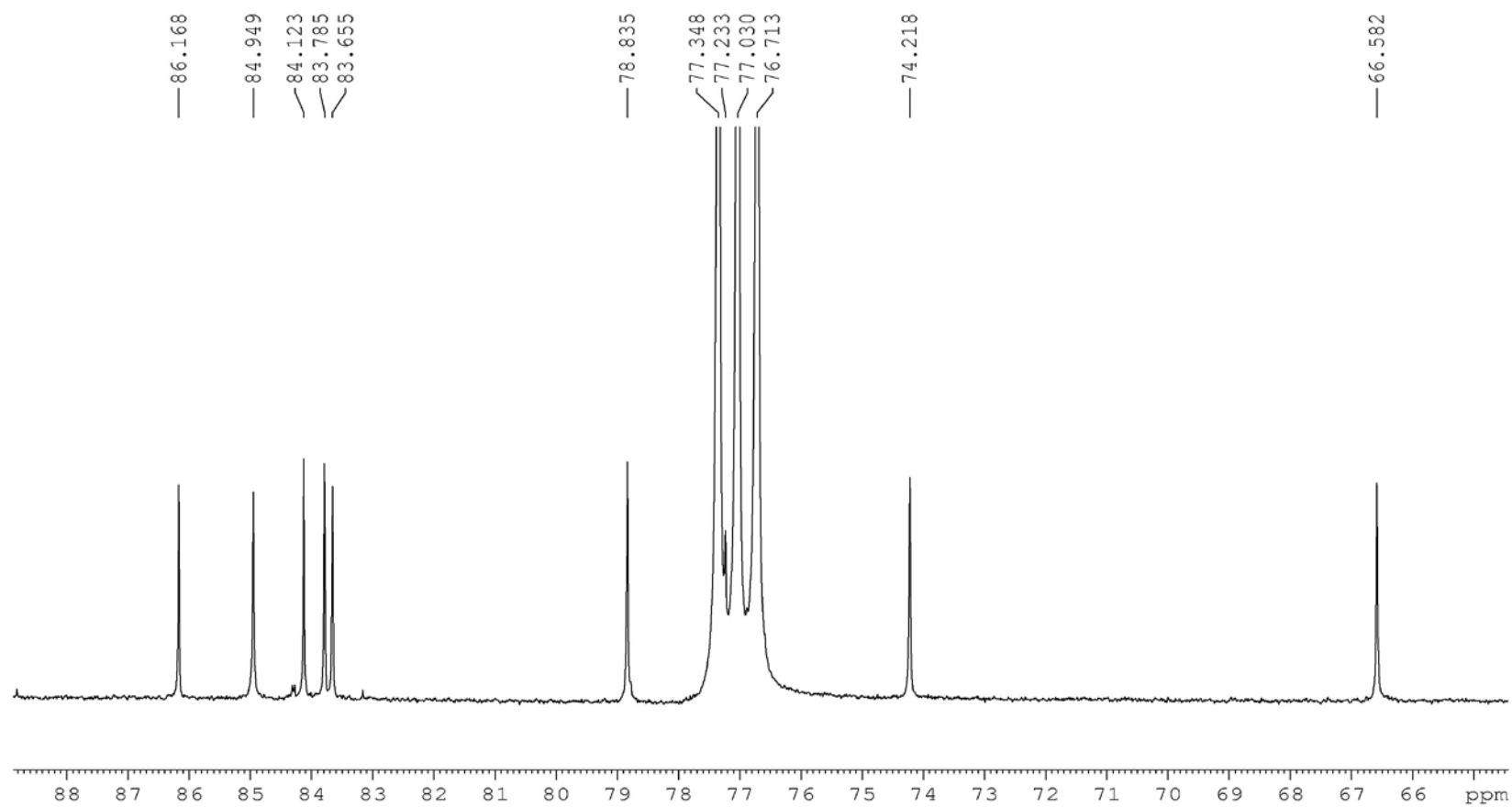
^{13}C NMR (100 MHz) spectrum of Compound **10** in CDCl_3

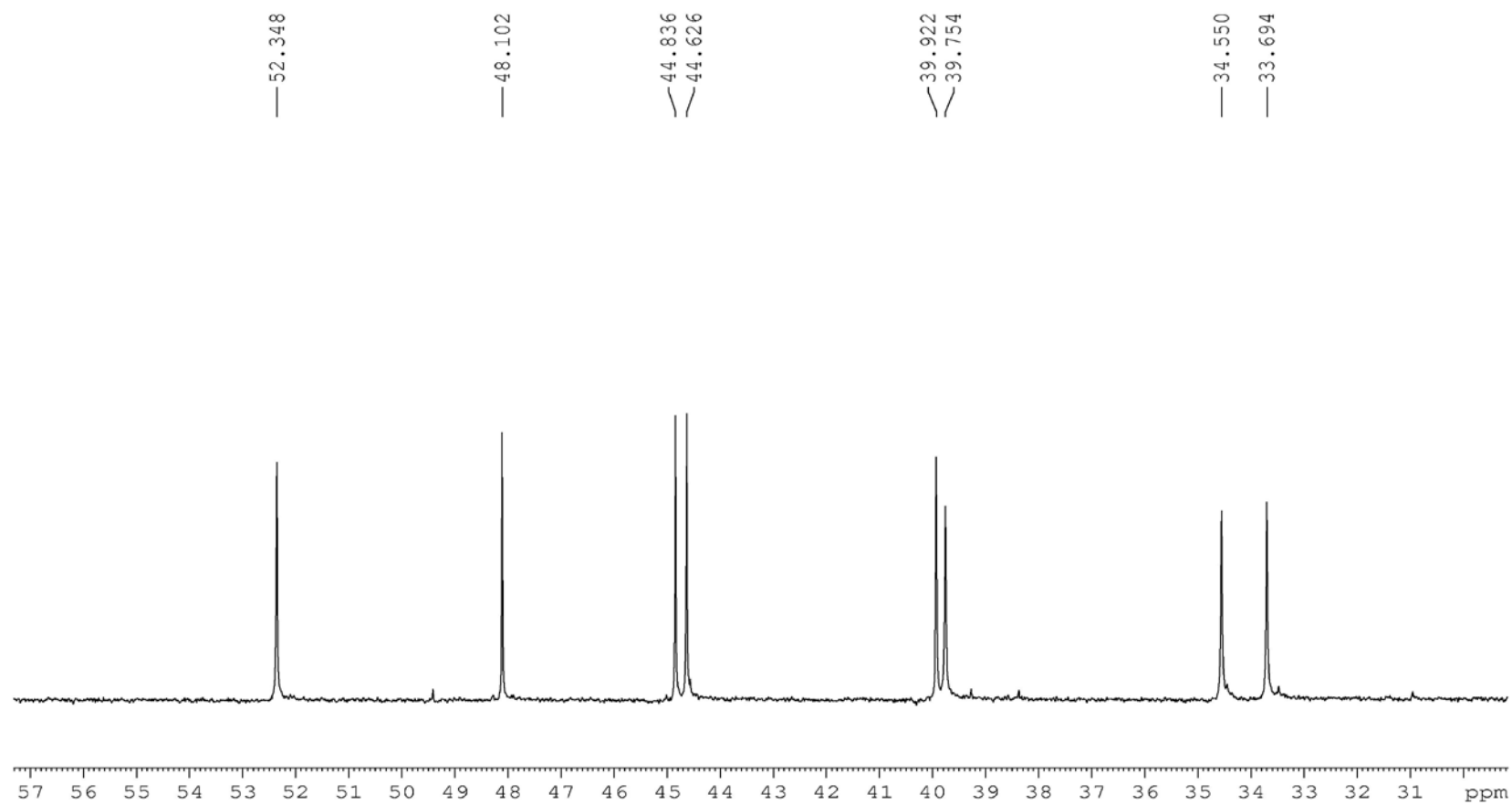


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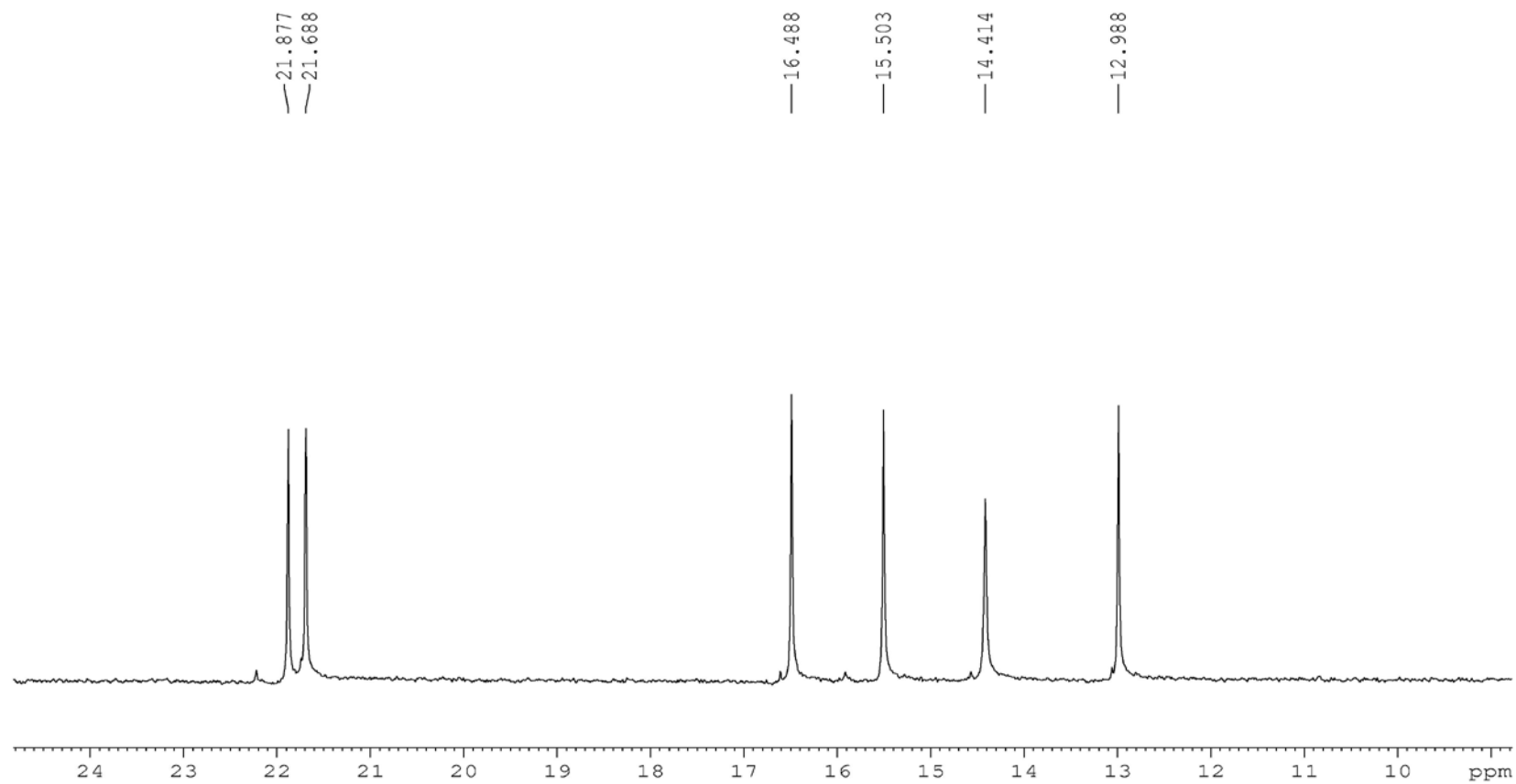
NAME          lws-20-1
EXPNO          2
PROCNO         1
Date_         20141106
Time           9.14
INSTRUM        spect
PROBHD         5 mm CPMBO BB
PULPROG        zgpg30
TD             65536
SOLVENT        CDCl3
NS             8000
DS             4
SWH            24038.461 Hz
FIDRES         0.366798 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          100.6228293 MHz
NUC1           13C
P1            10.00 usec
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB            0
LB             1.00 Hz
GB             0
PC             1.40
  
```

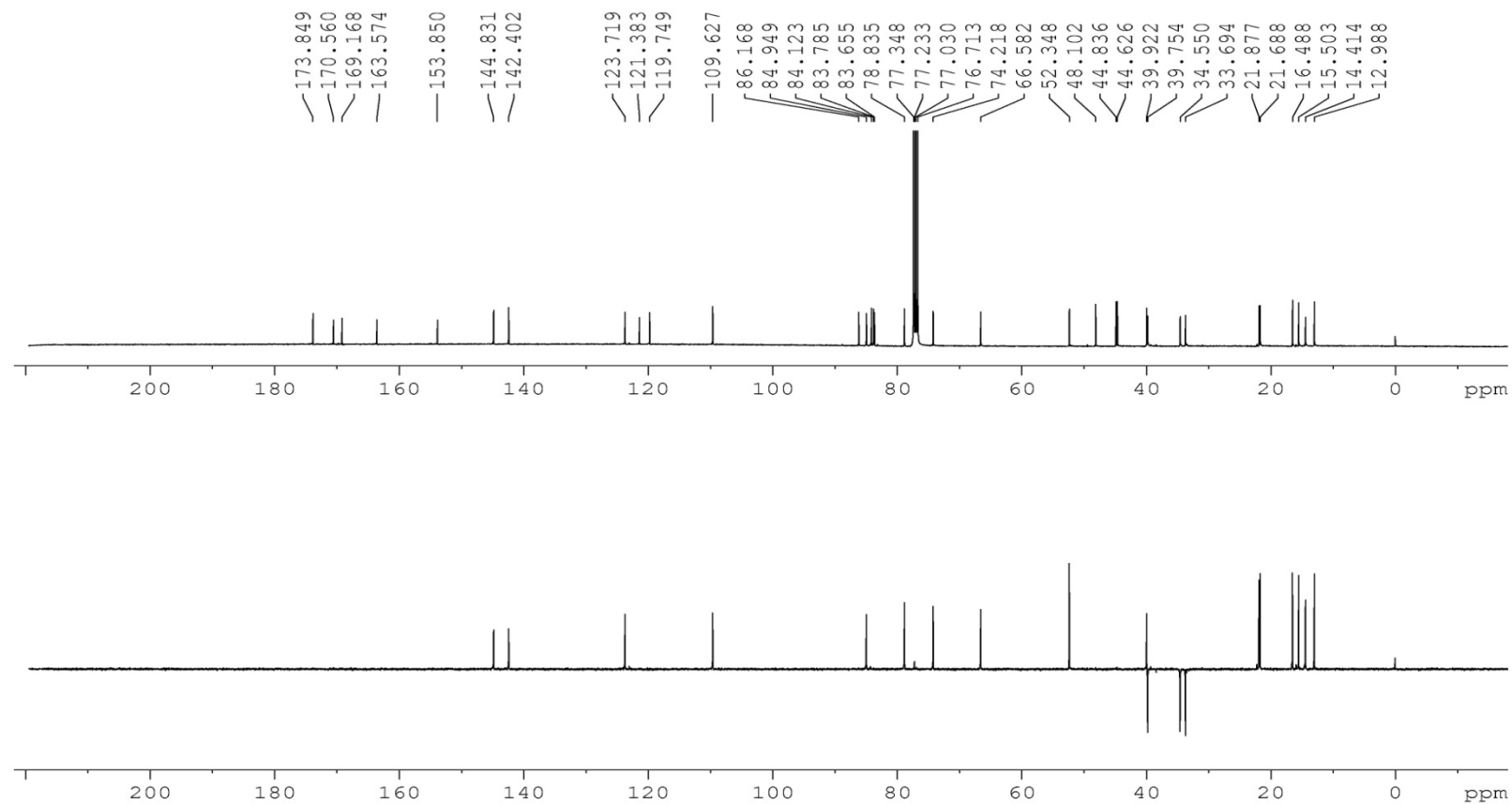


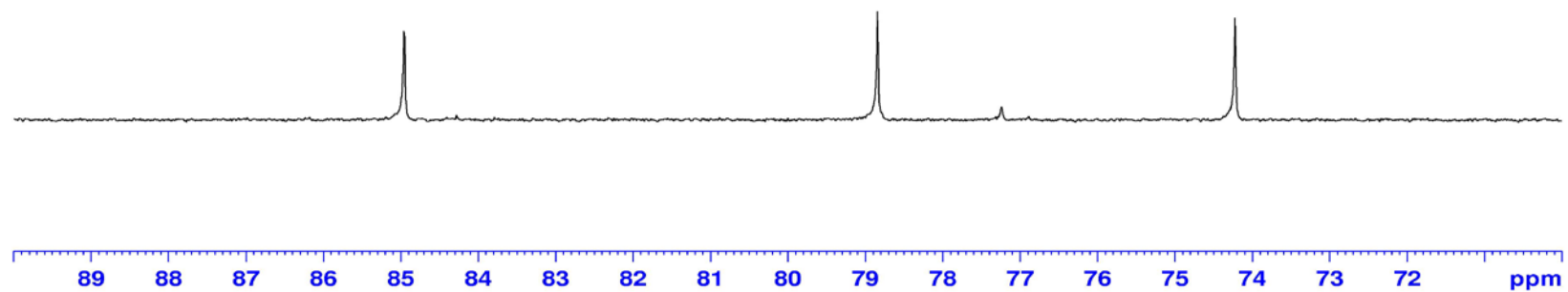
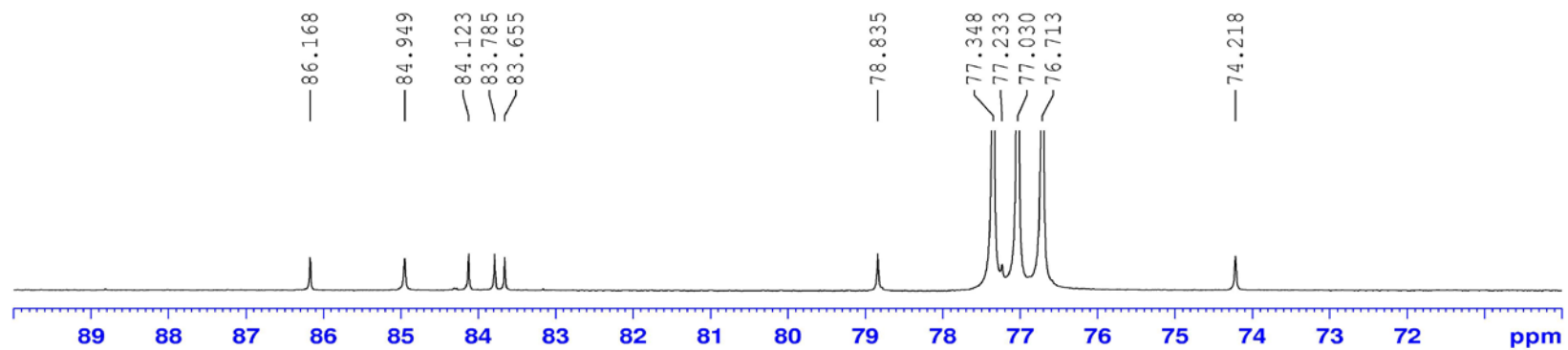


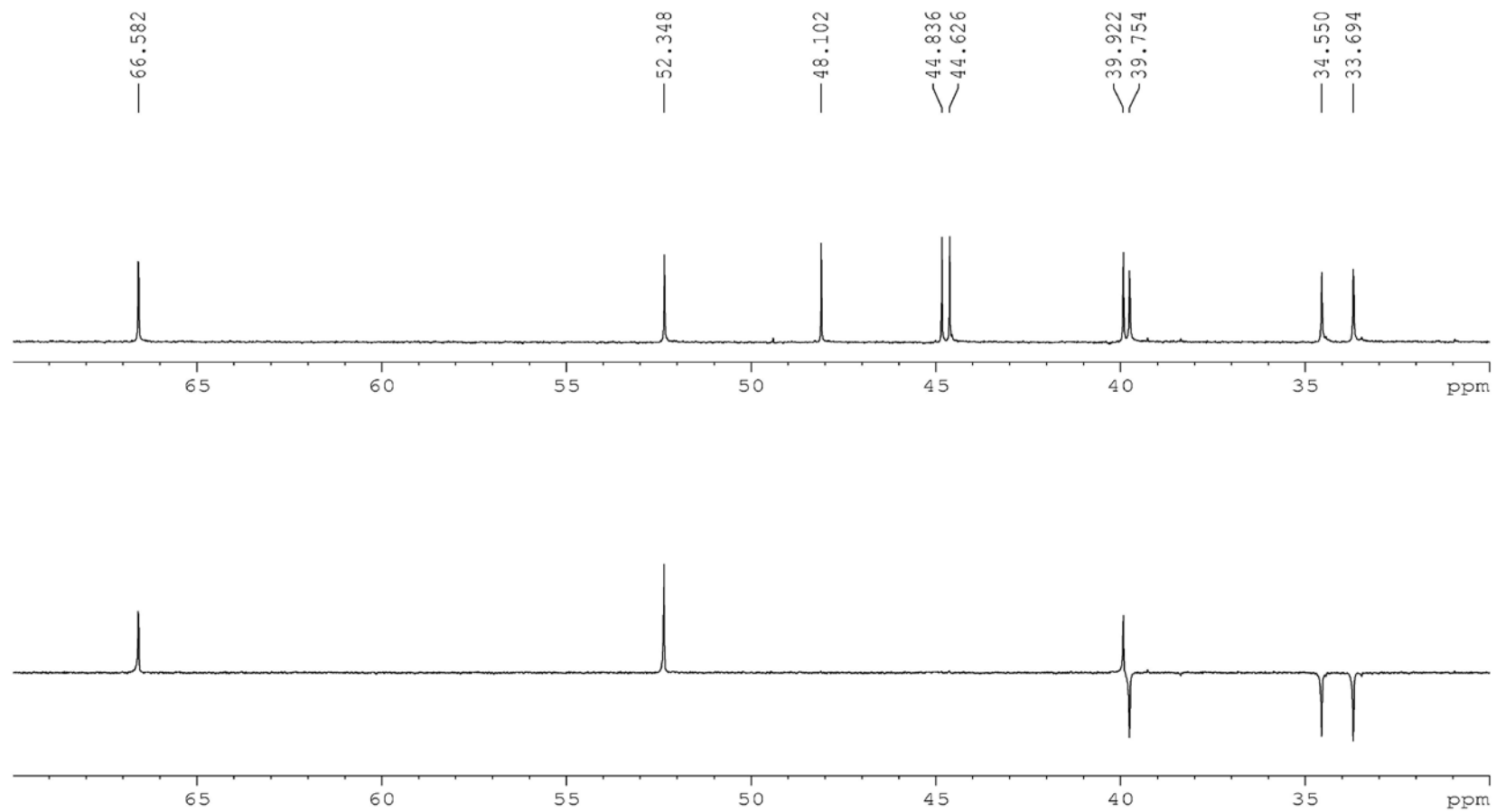
S95

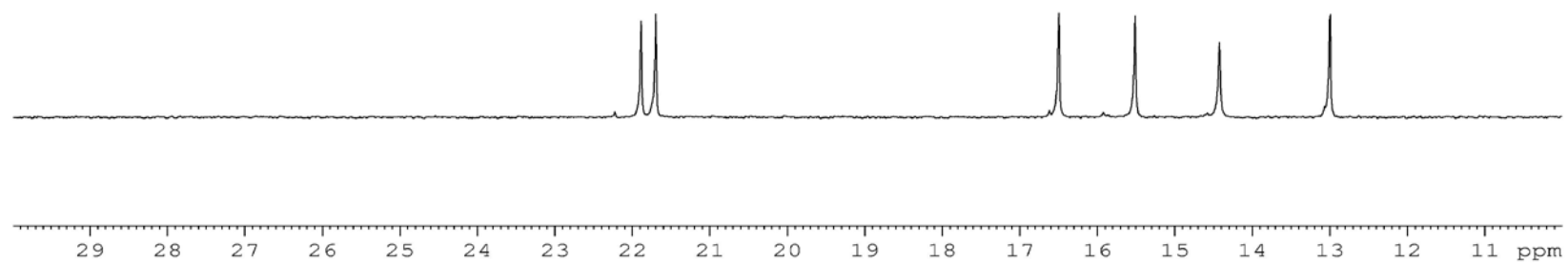
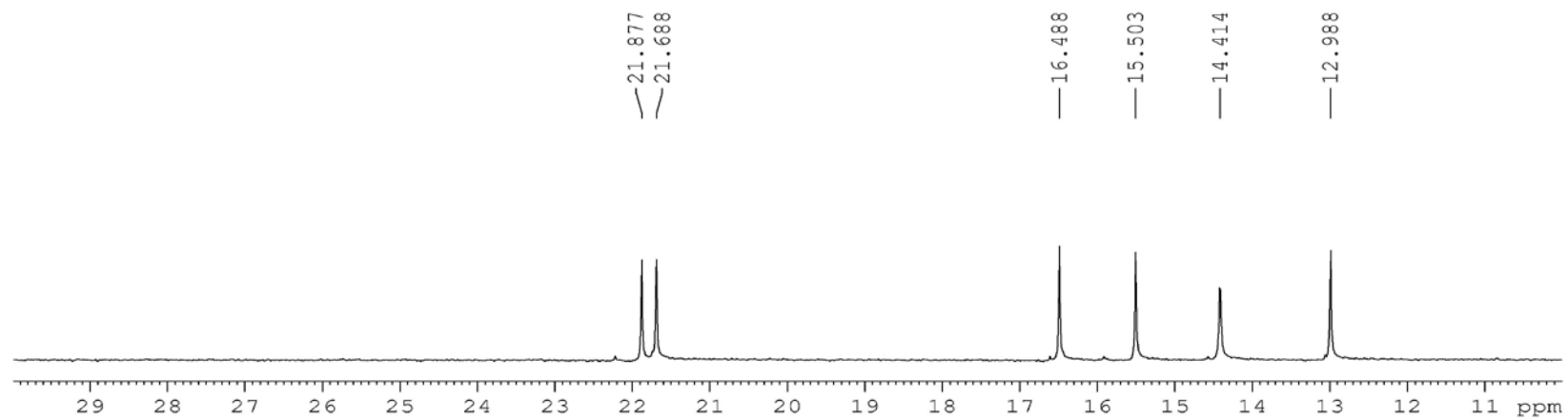


DEPT135° (100 MHz) spectrum of Compound **10** in CDCl₃



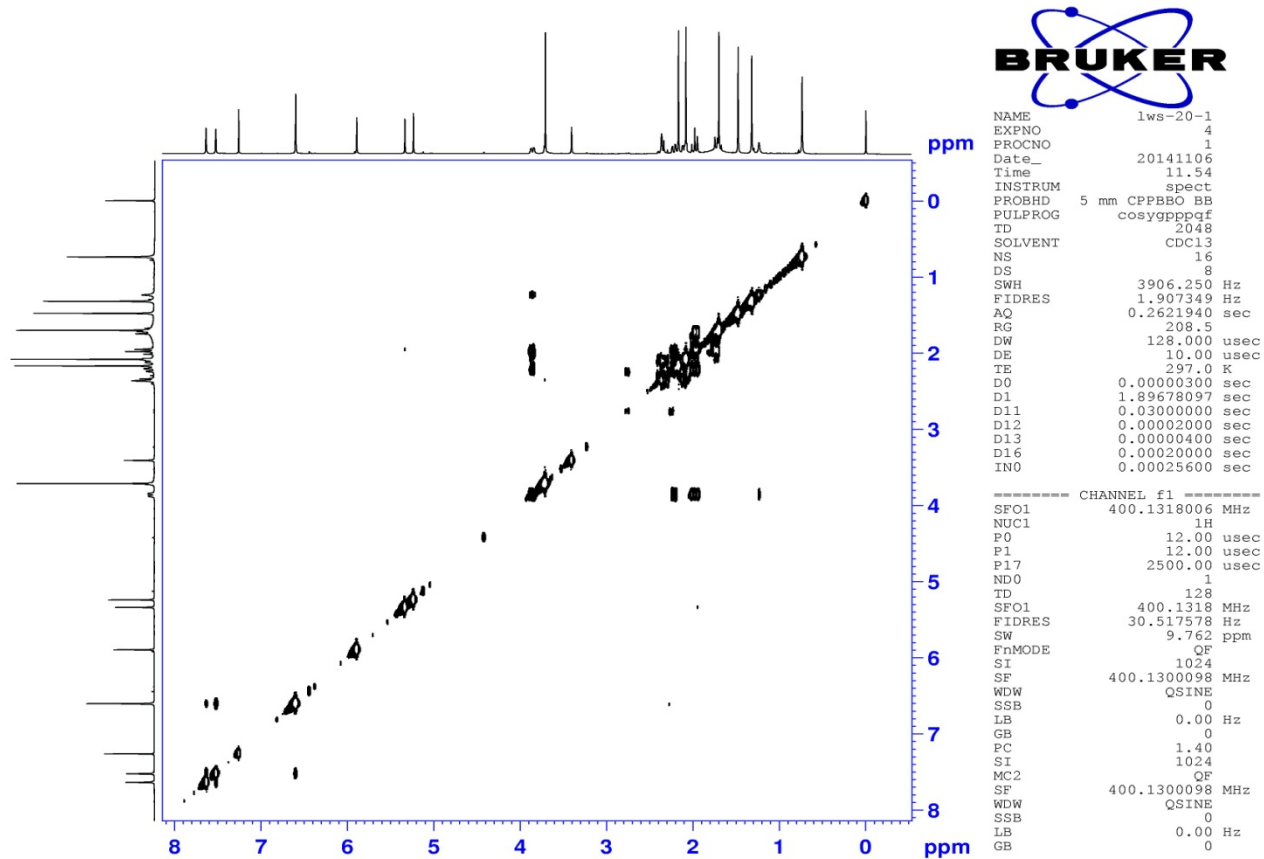


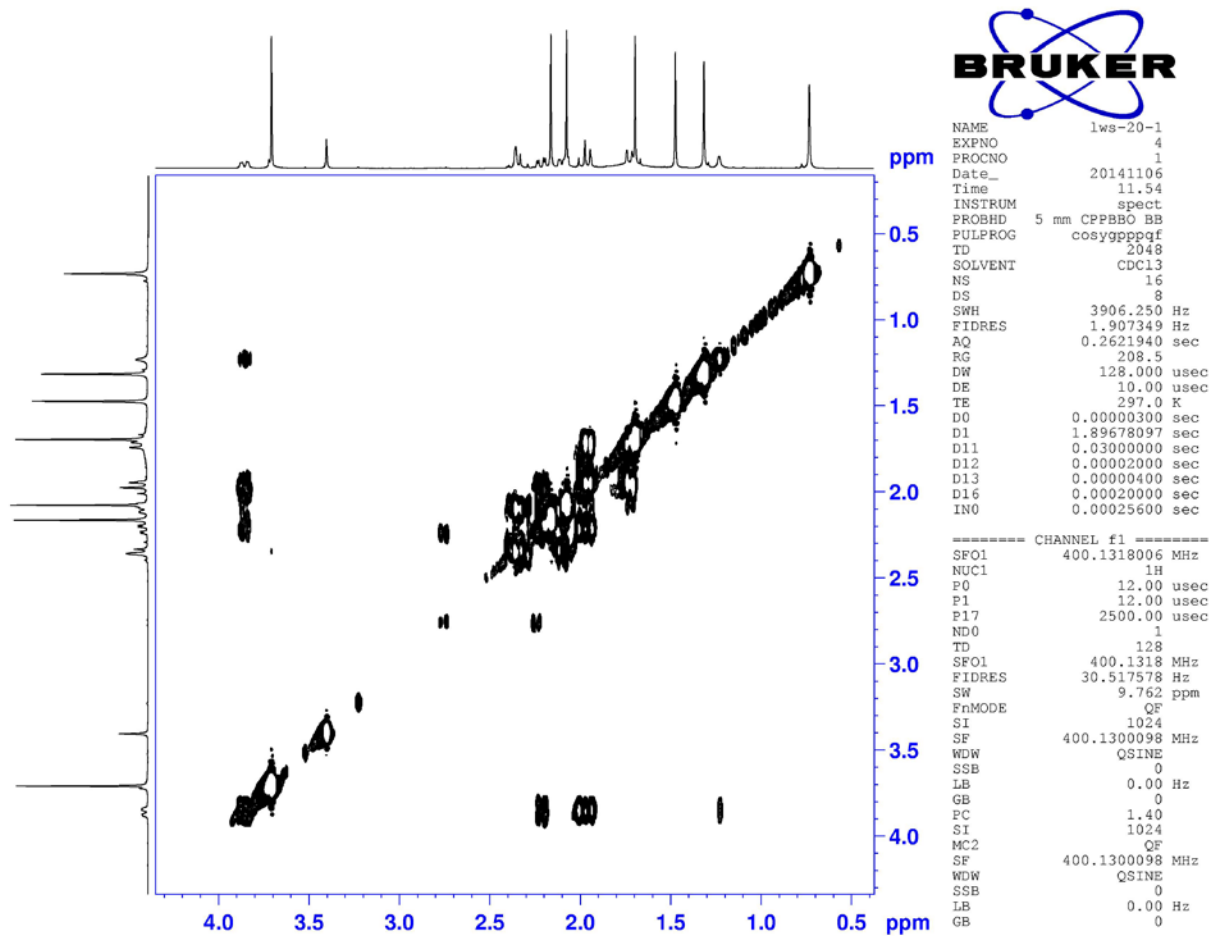




S100

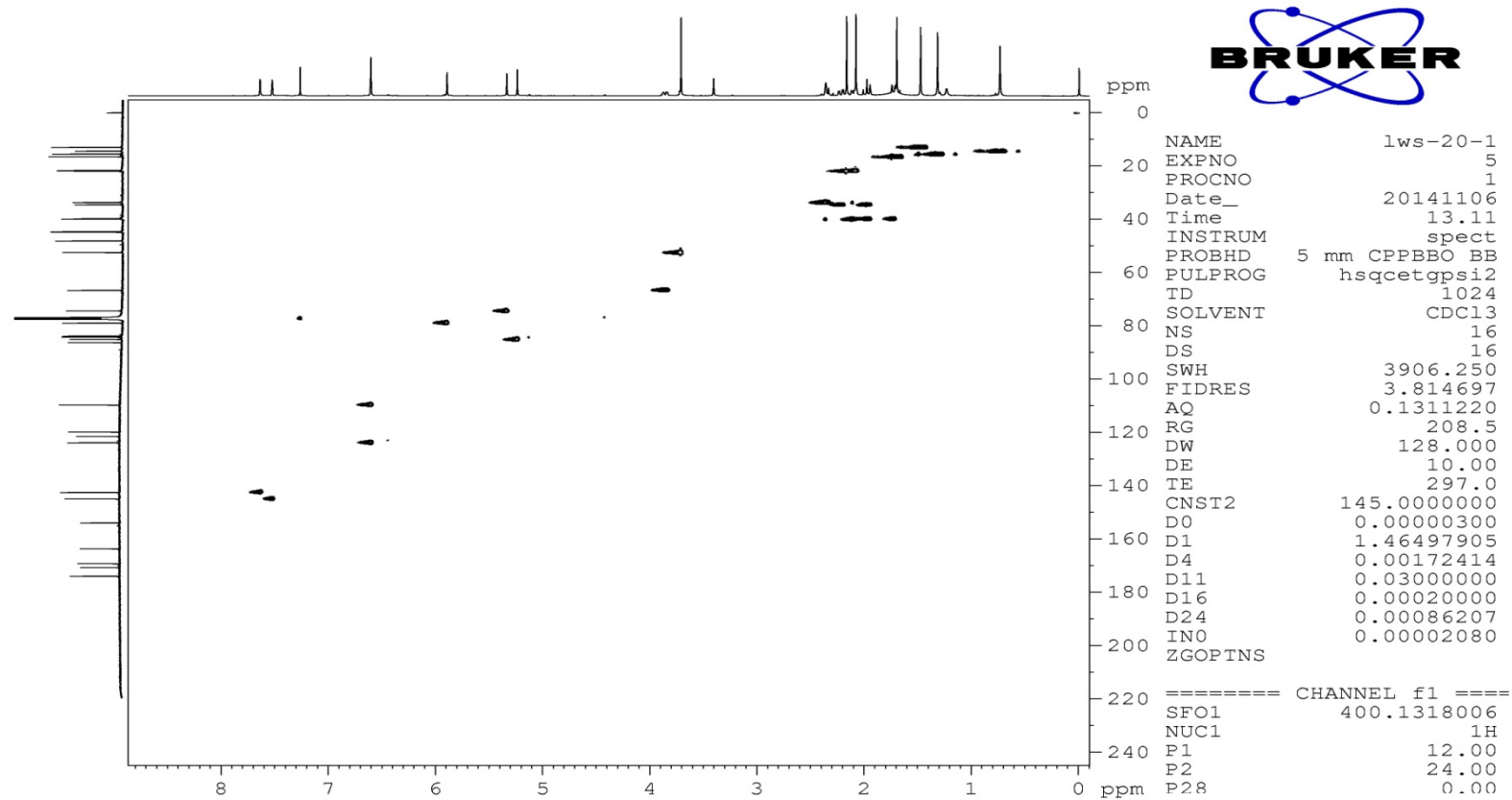
^1H - ^1H COSY (400 MHz) spectrum of Compound **10** in CDCl_3

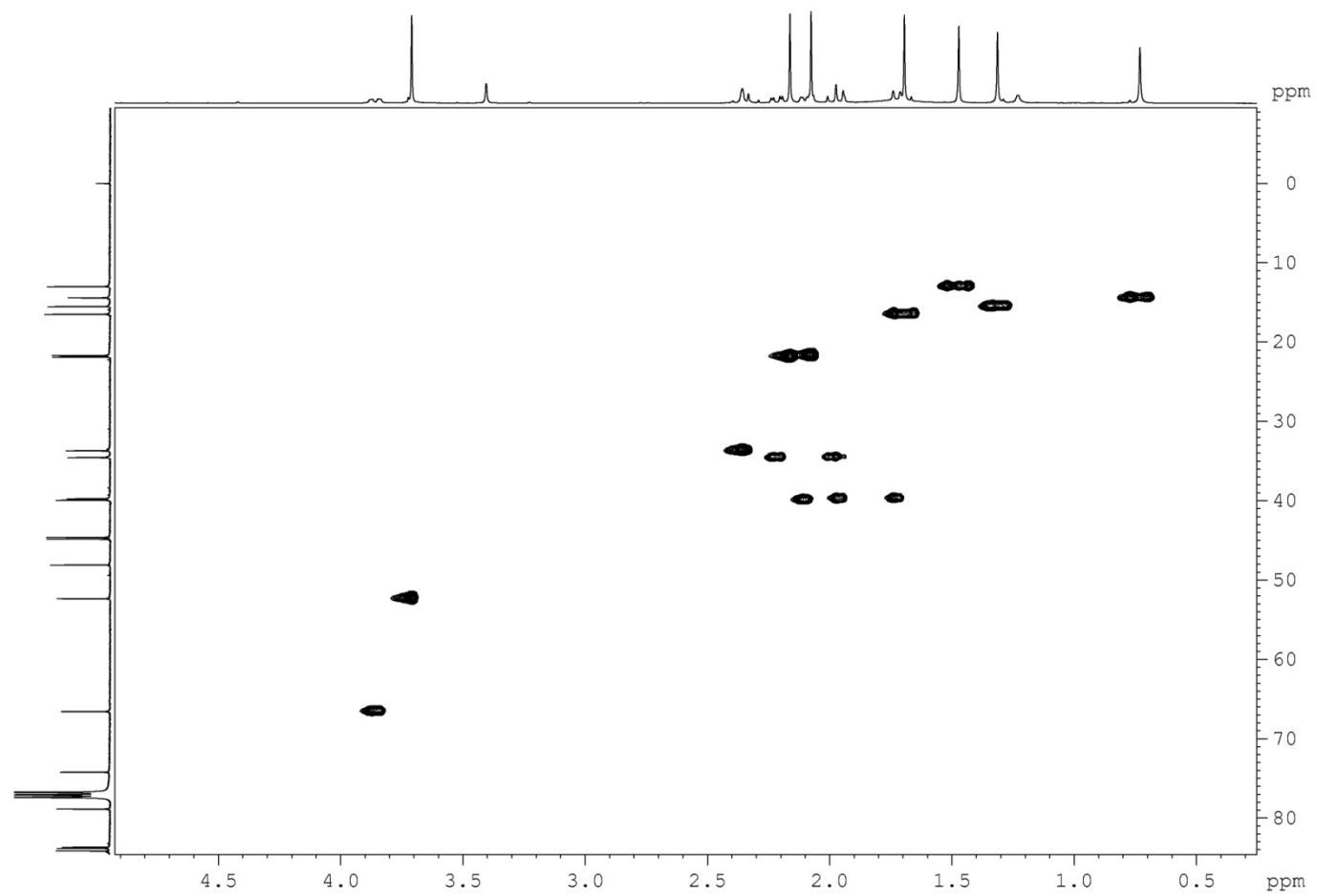




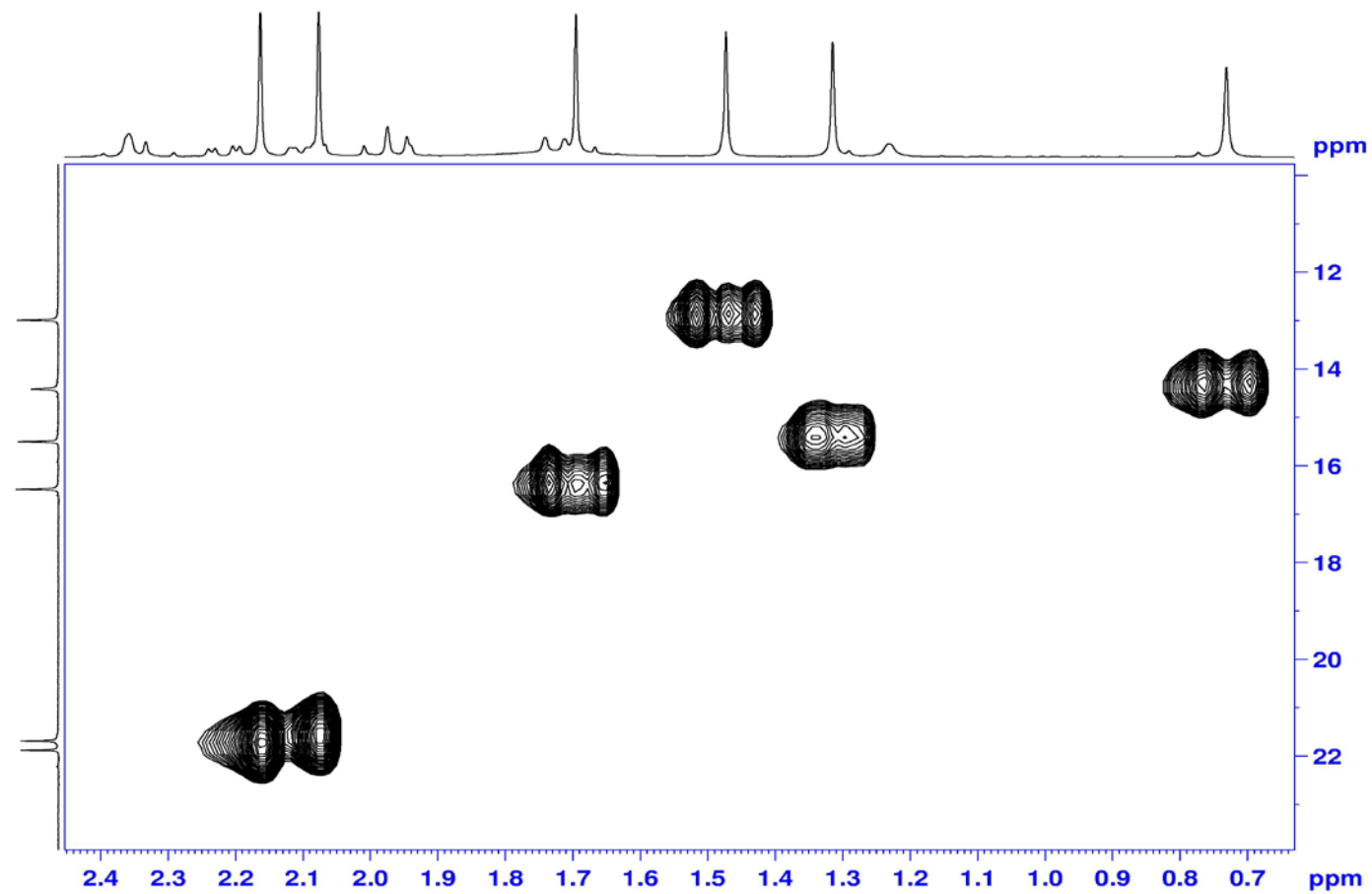
S102

HSQC (400 MHz) spectrum of Compound **10** in CDCl₃



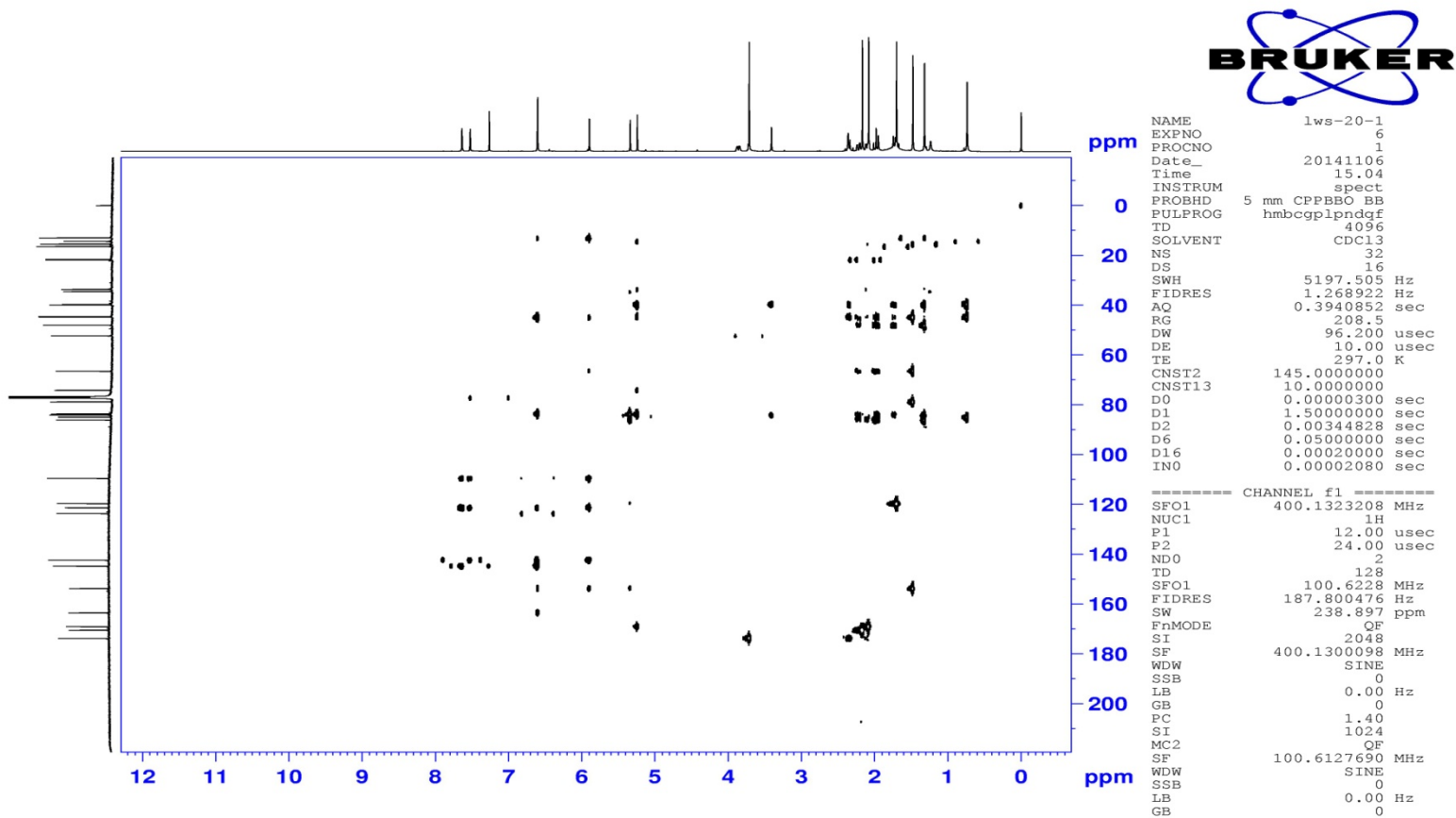


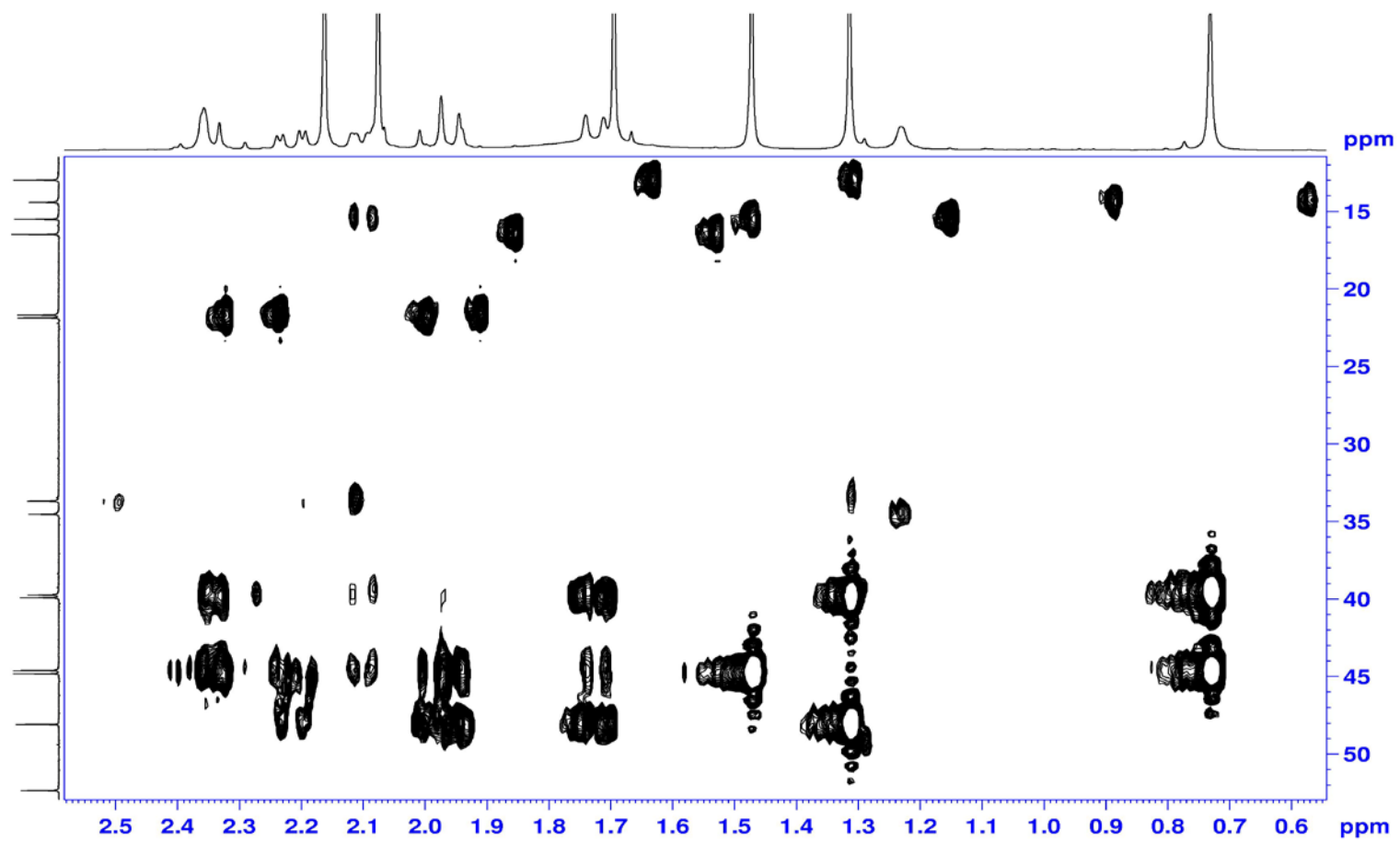
S104



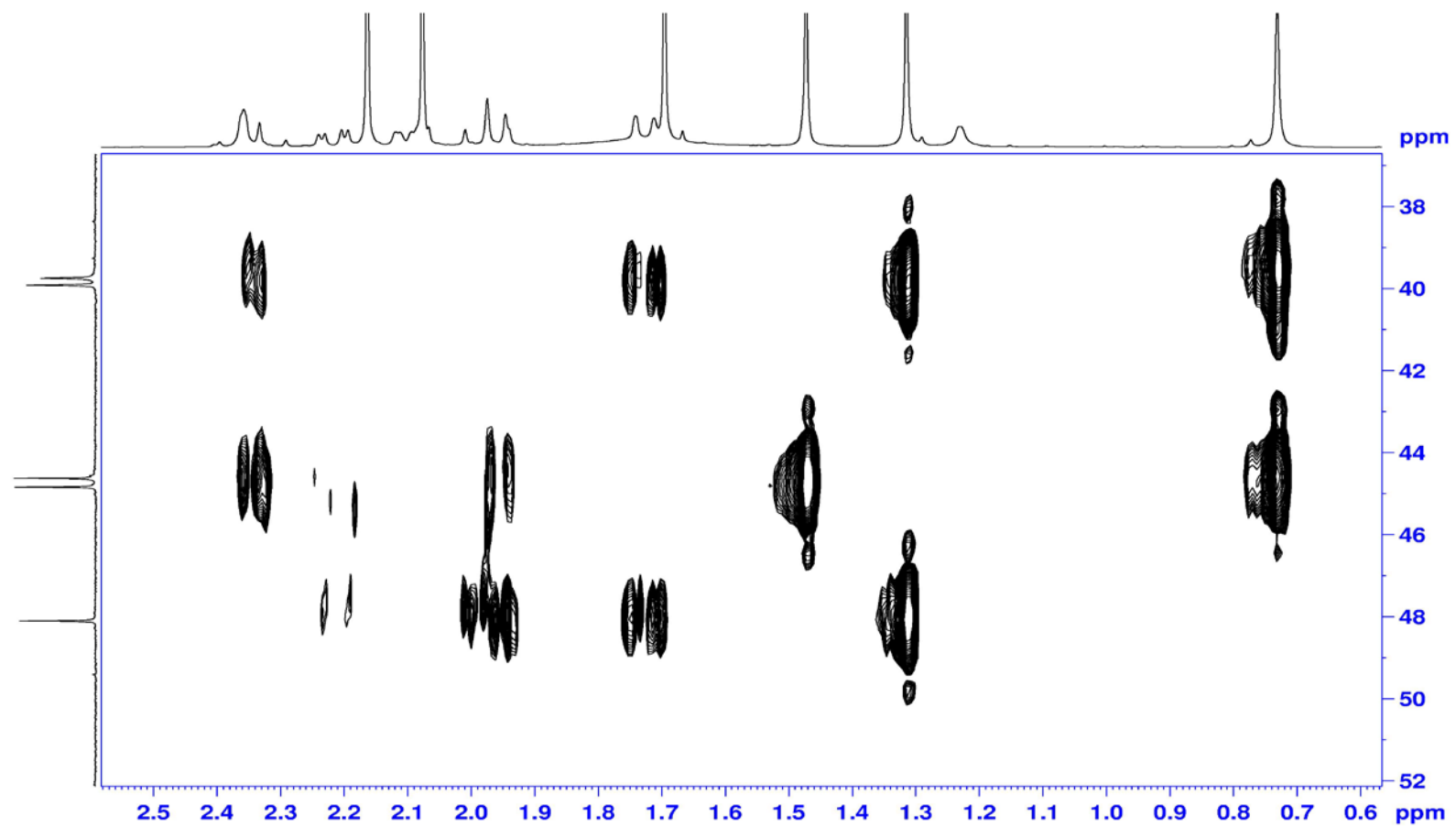
S105

HMBC (400 MHz) spectrum of Compound **10** in CDCl₃

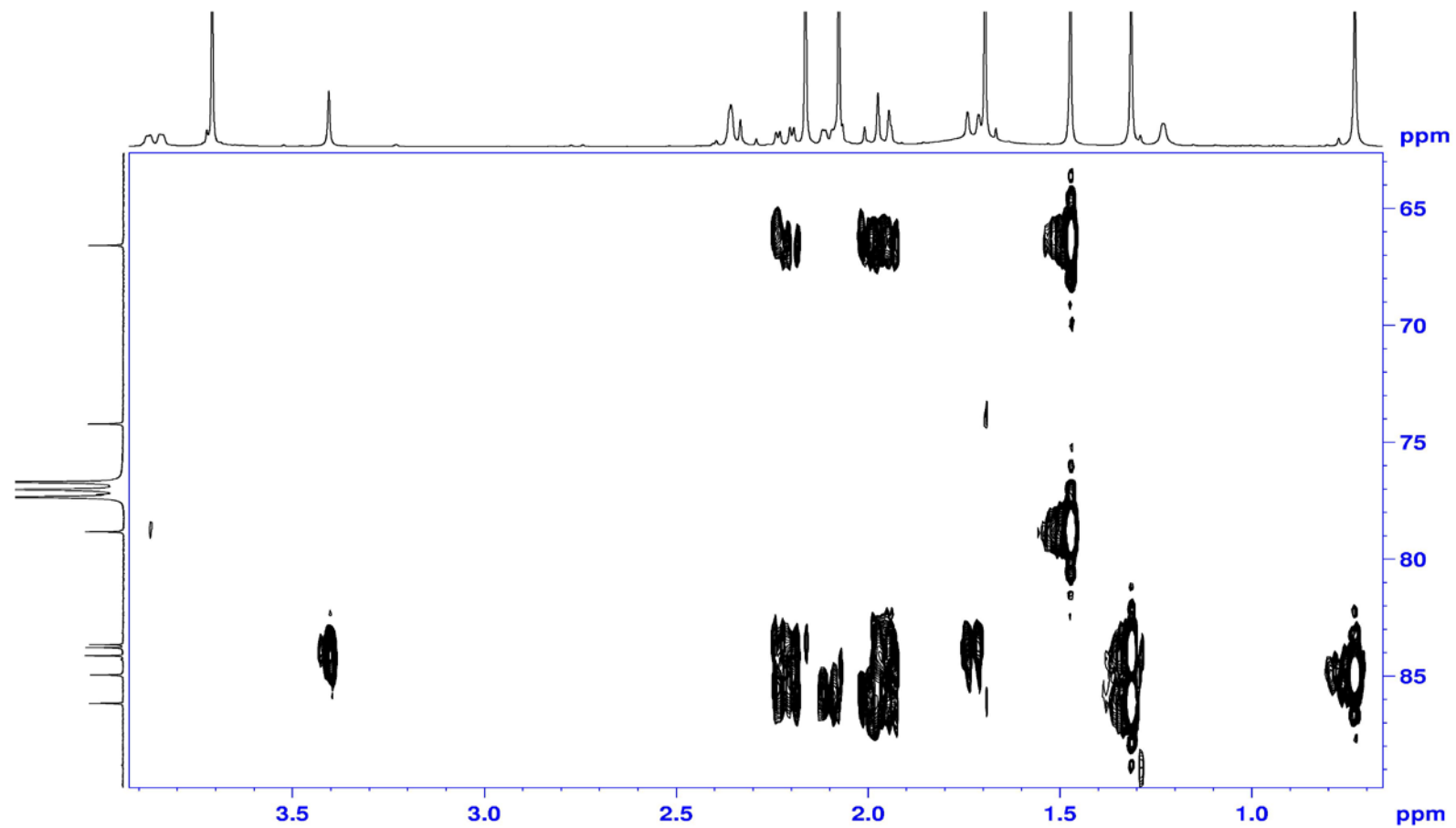




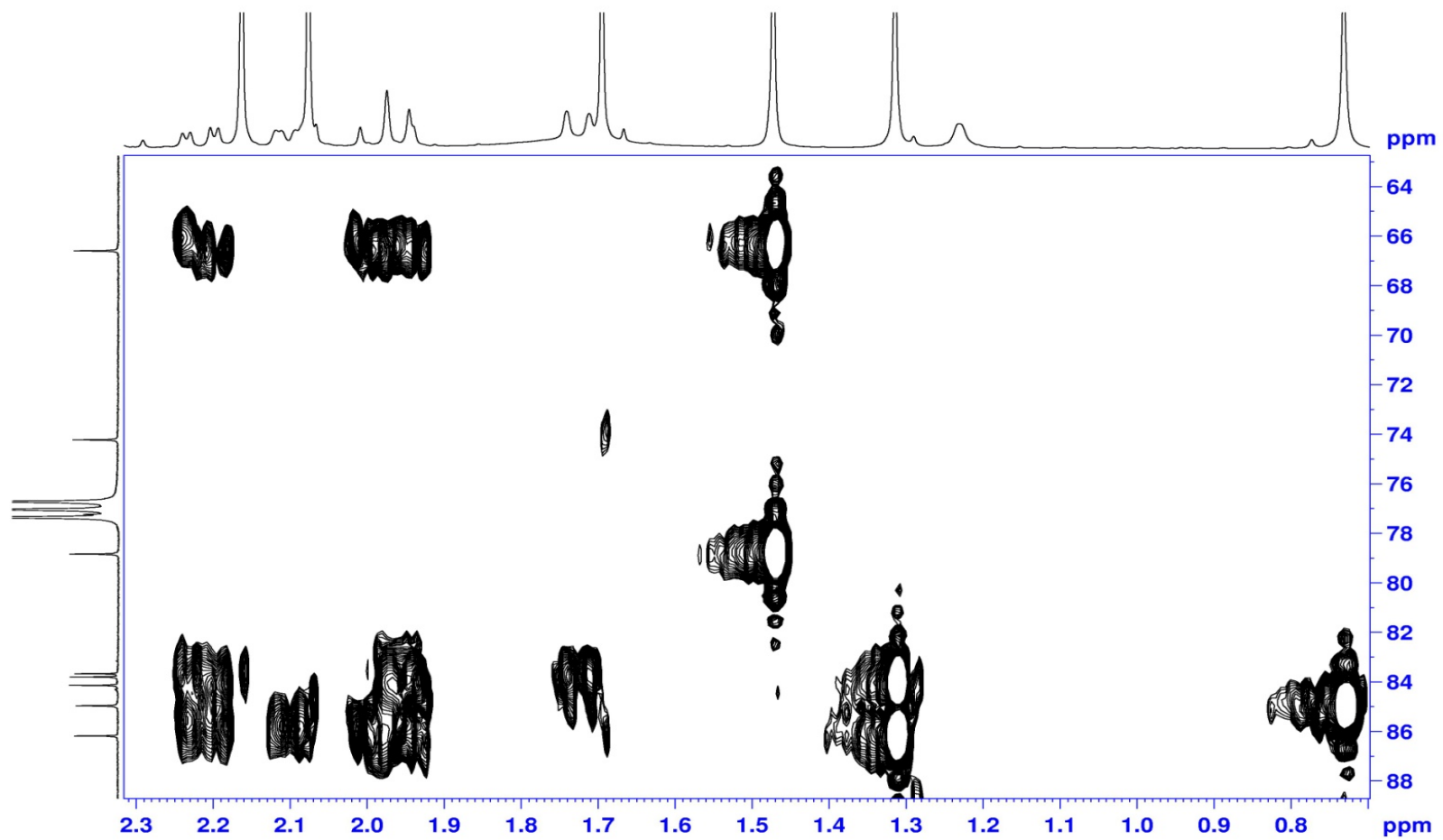
S107



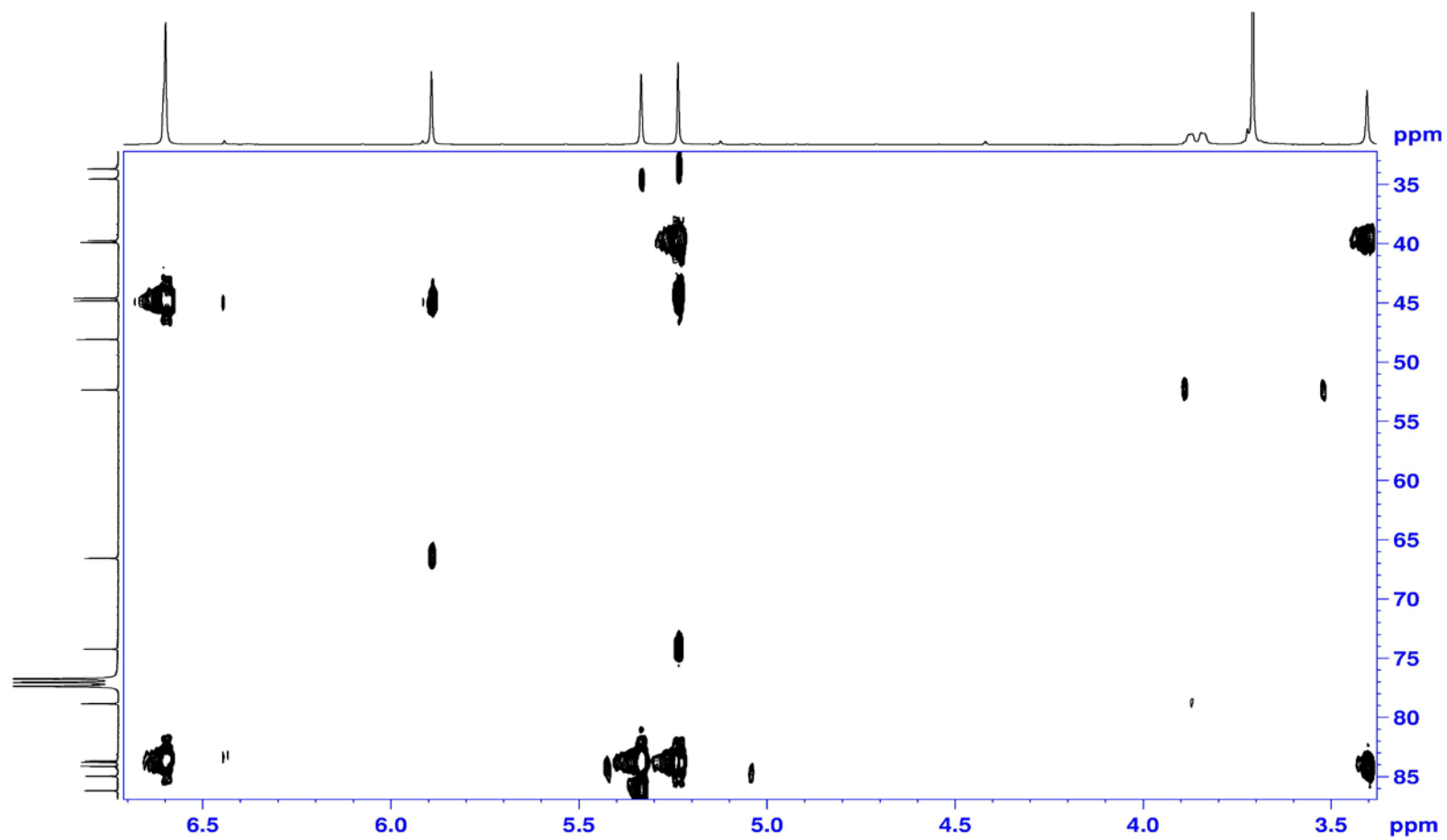
S108



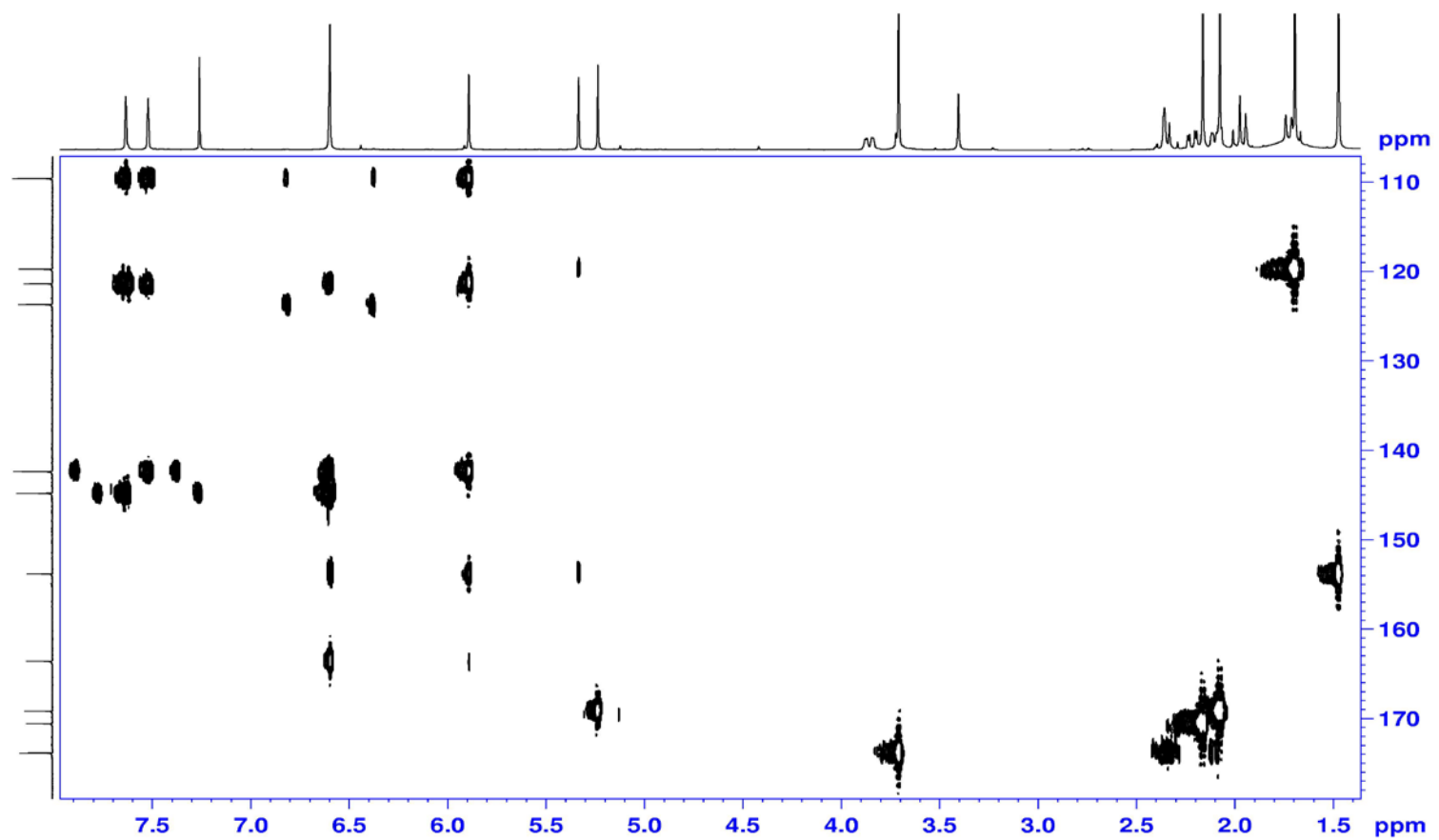
S109



S110

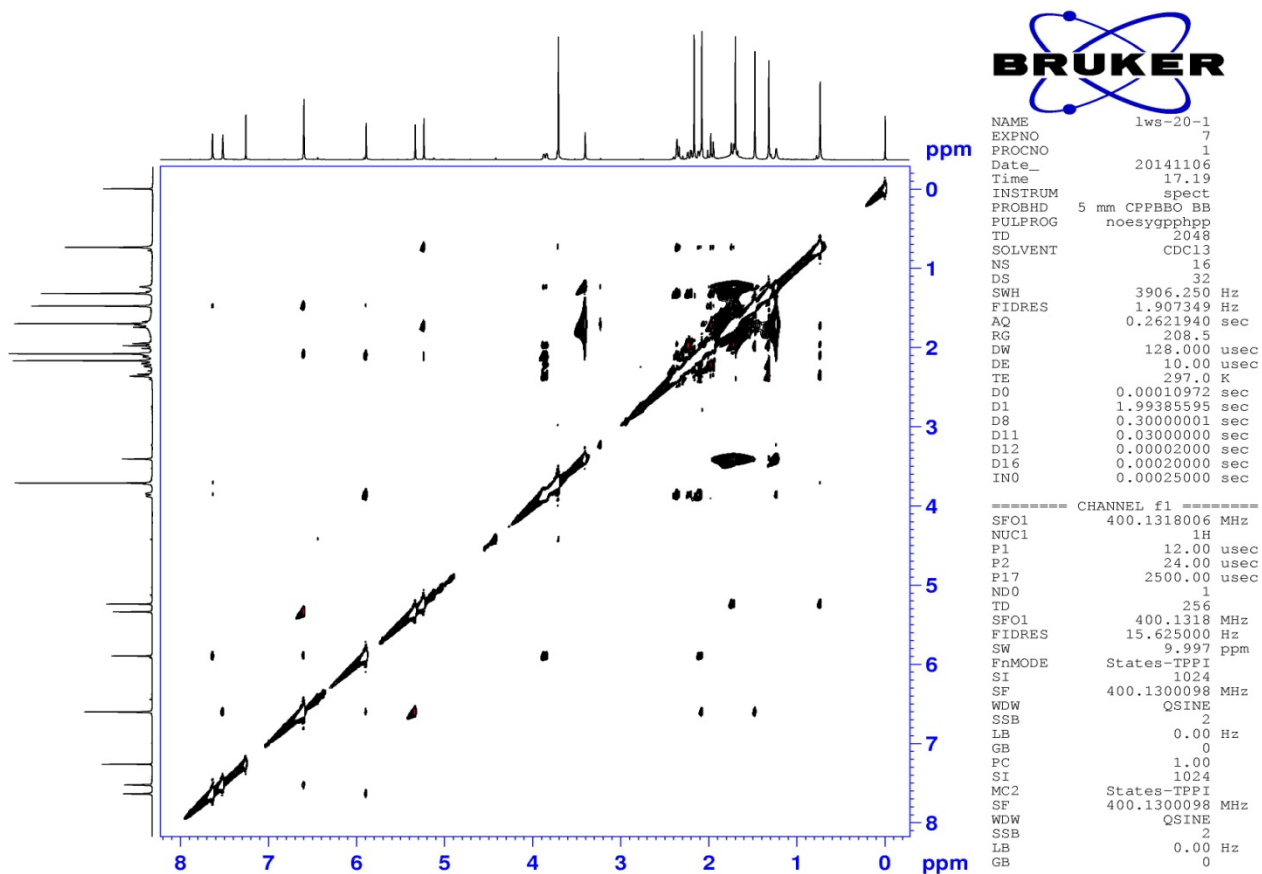


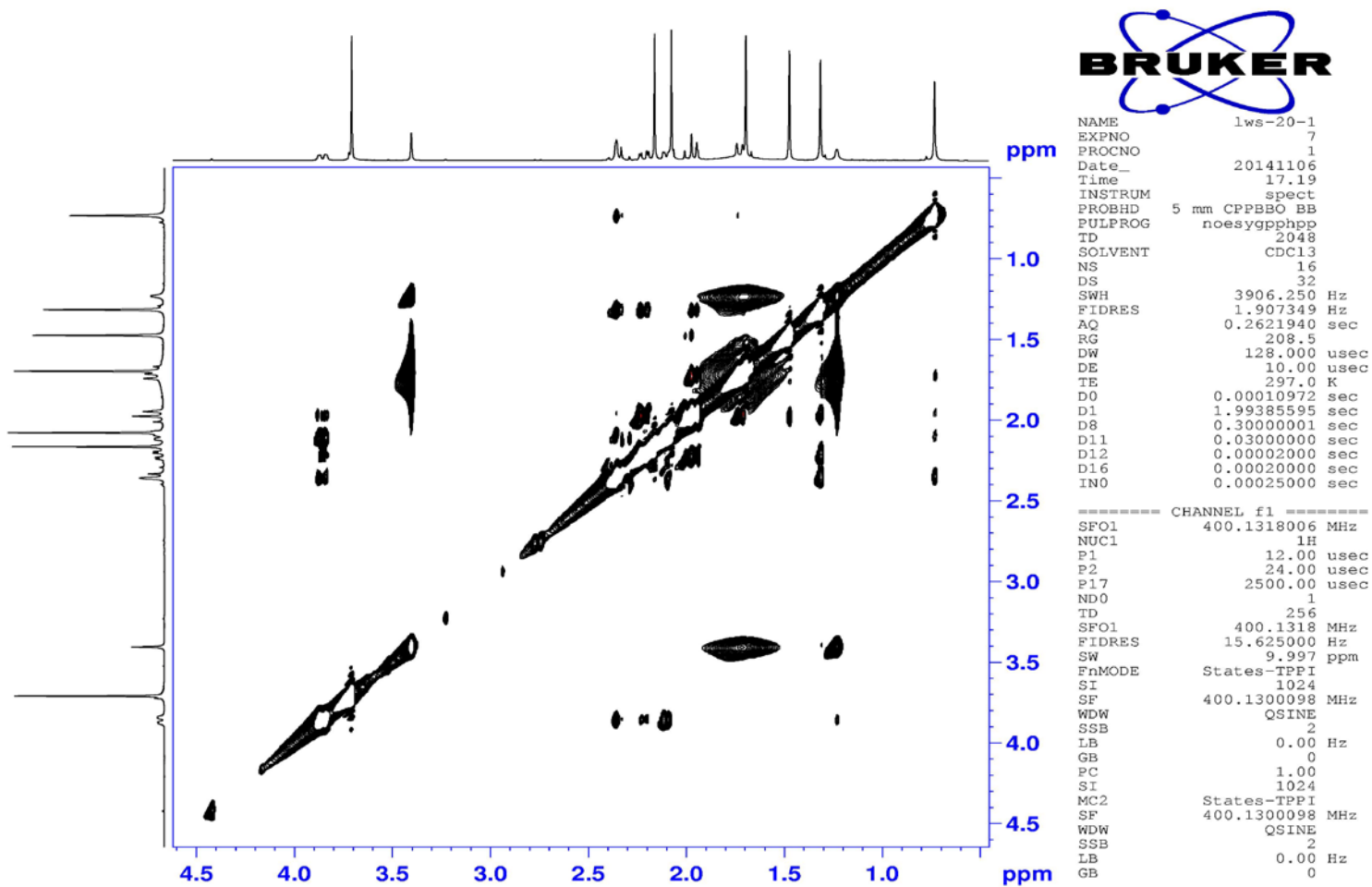
S111

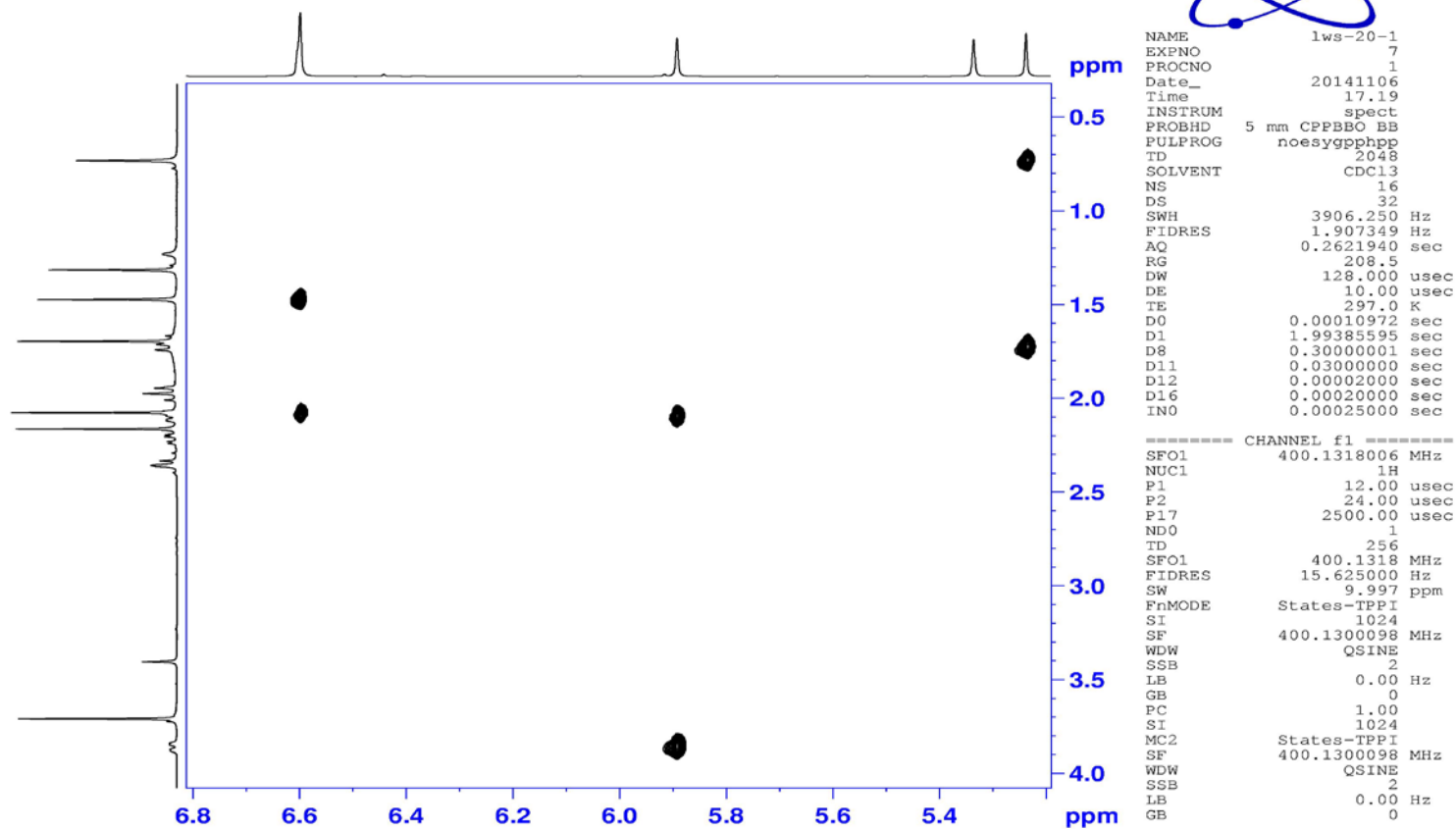


S112

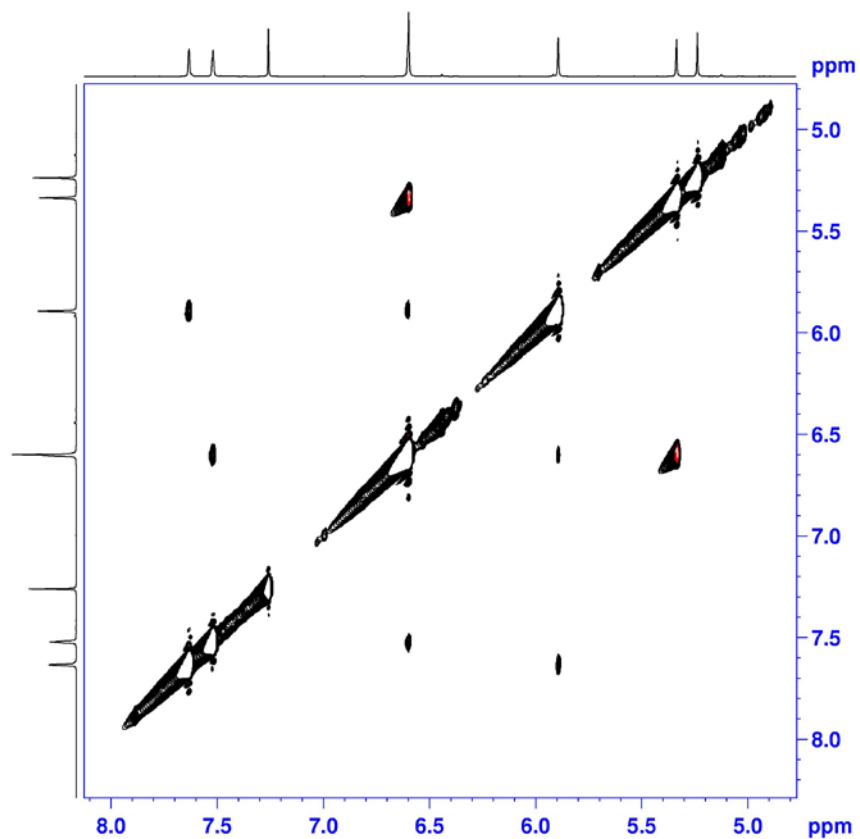
NOESY (400 MHz) spectrum of Compound **10** in CDCl₃







S115



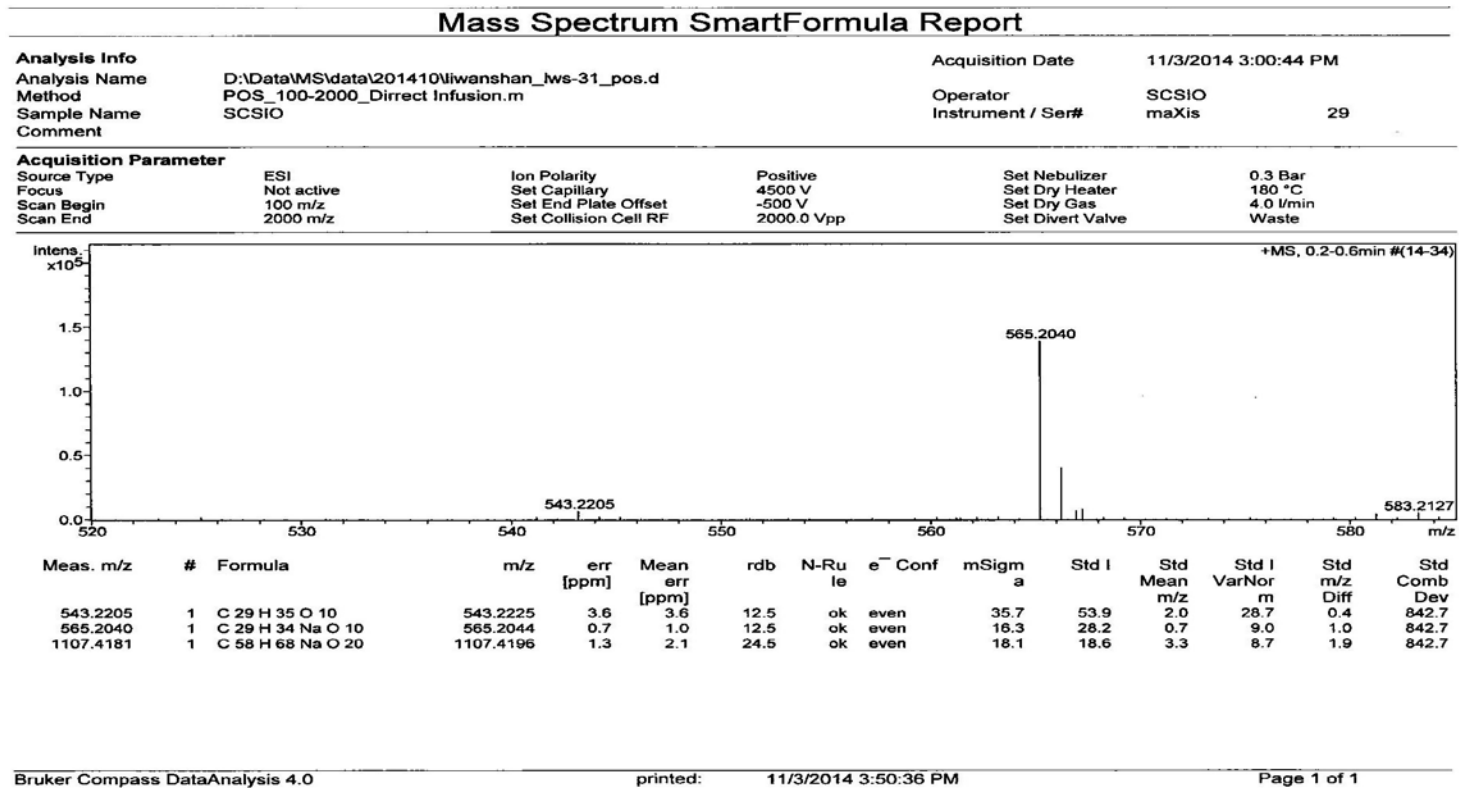
```

NAME          lws-20-1
EXPNO         7
PROCNO        1
Date_         20141106
Time          17.19
INSTRUM       spect
PROBHD        5 mm CFPBBO BB
PULPROG       noesygpphpp
TD            2048
SOLVENT       CDC13
NS            16
DS            32
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            0.00010972 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
GB            0

```


HR-ESIMS of Compound 11



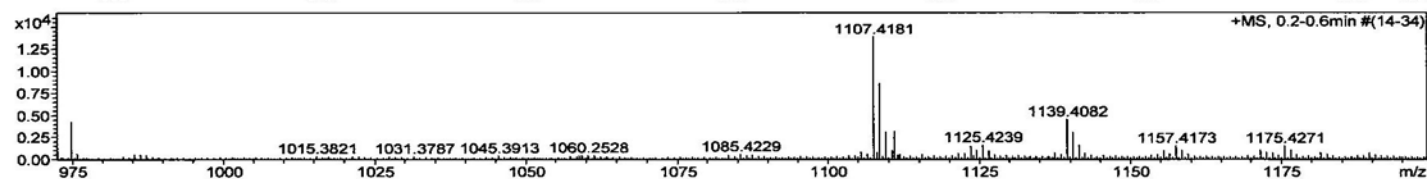
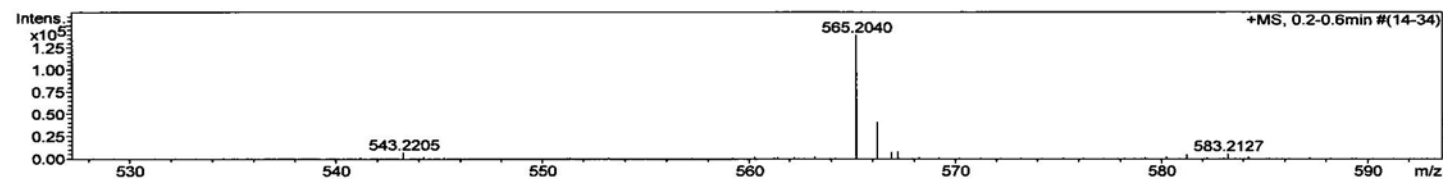
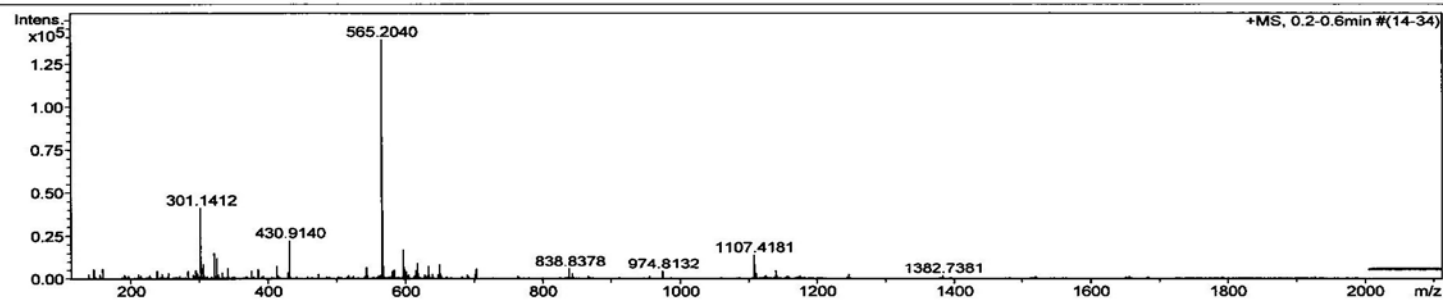
Generic Display Report

Analysis Info

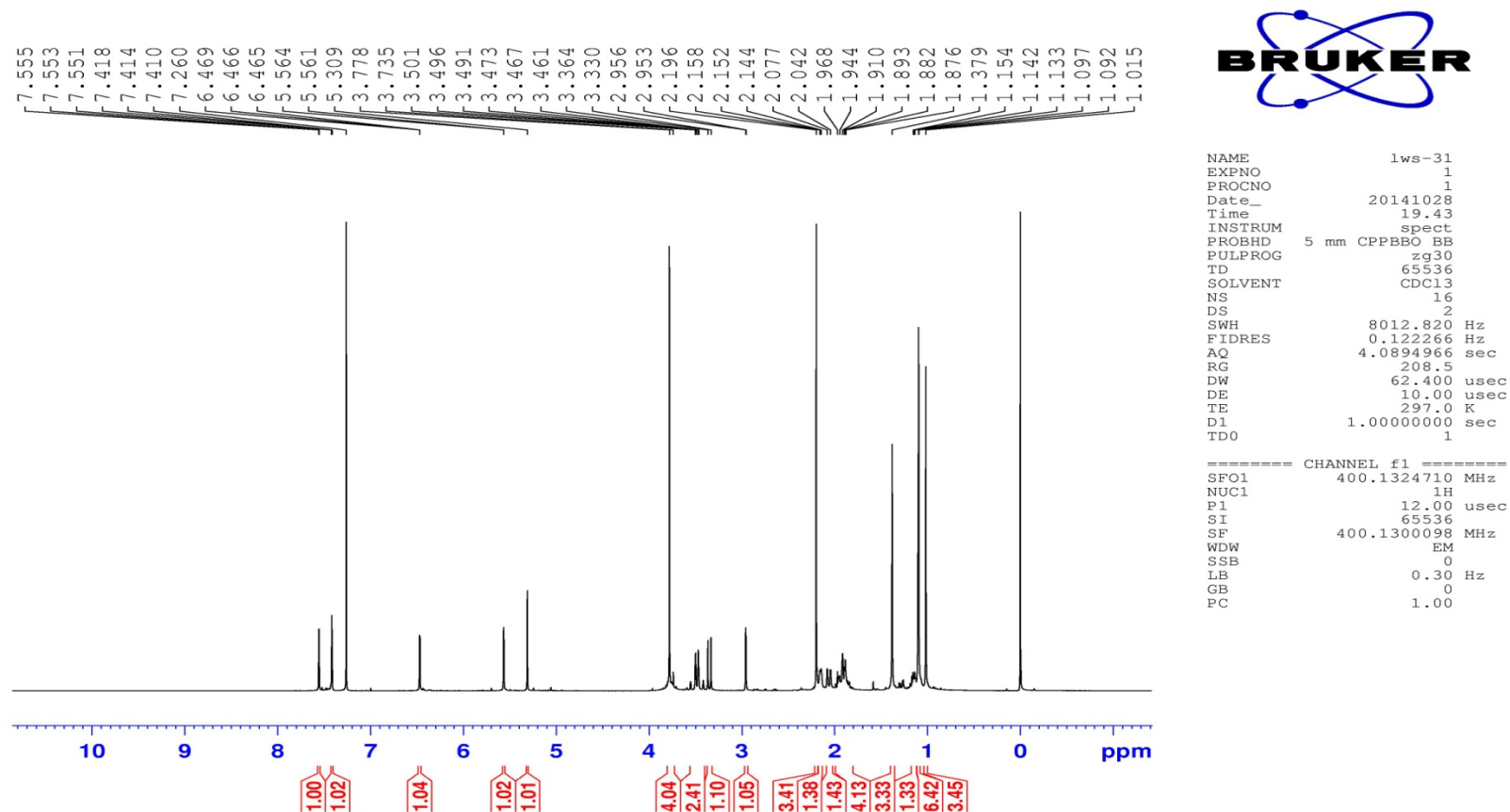
Analysis Name D:\Data\MS\data\201410\liwanshan_lws-31_pos.d
Method POS_100-2000_Direct Infusion.m
Sample Name SCSIO
Comment

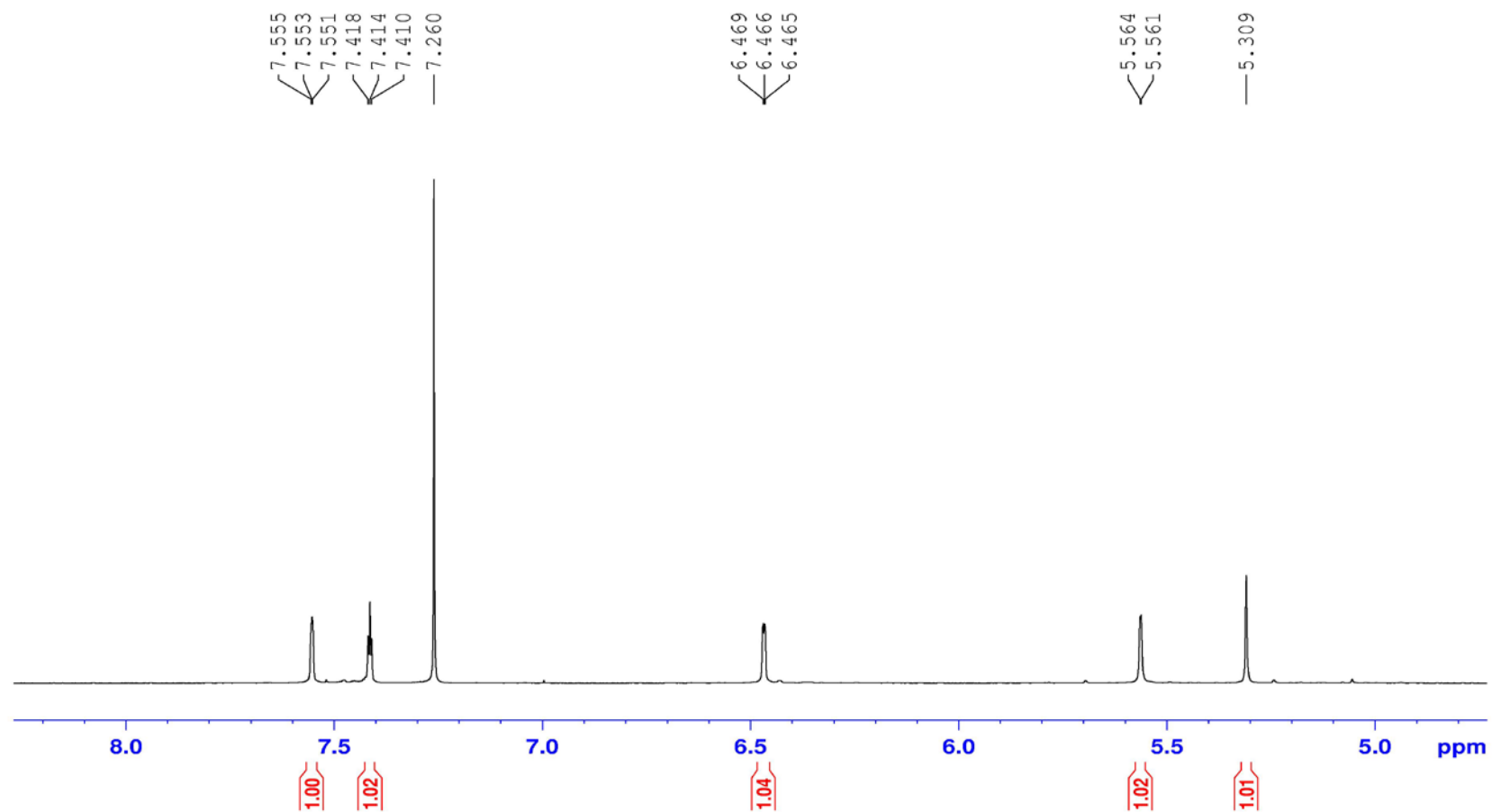
Acquisition Date 11/3/2014 3:00:44 PM

Operator SCSIO
Instrument maXis

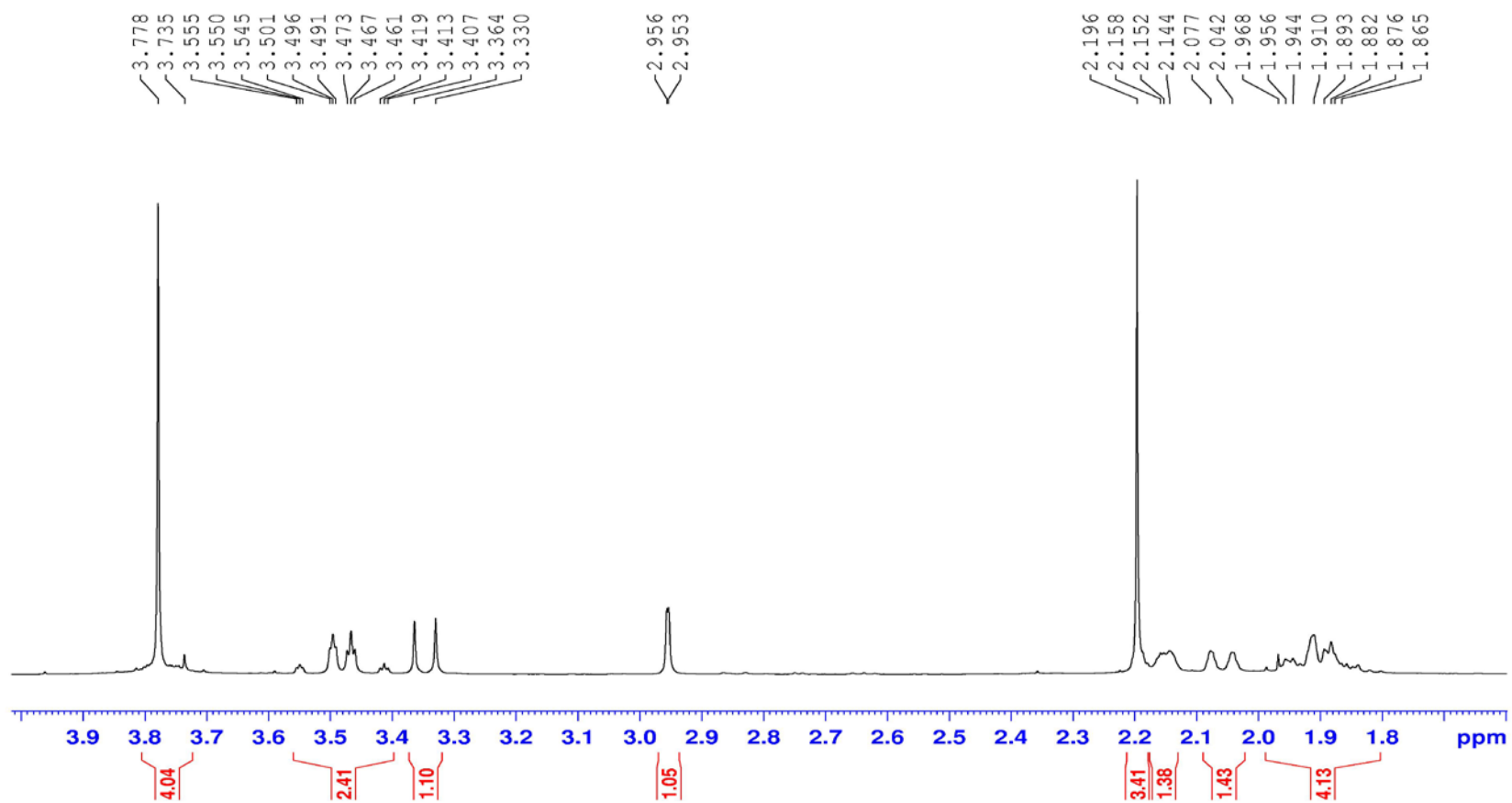


^1H NMR (400 MHz) spectrum of Compound **11** in CDCl_3

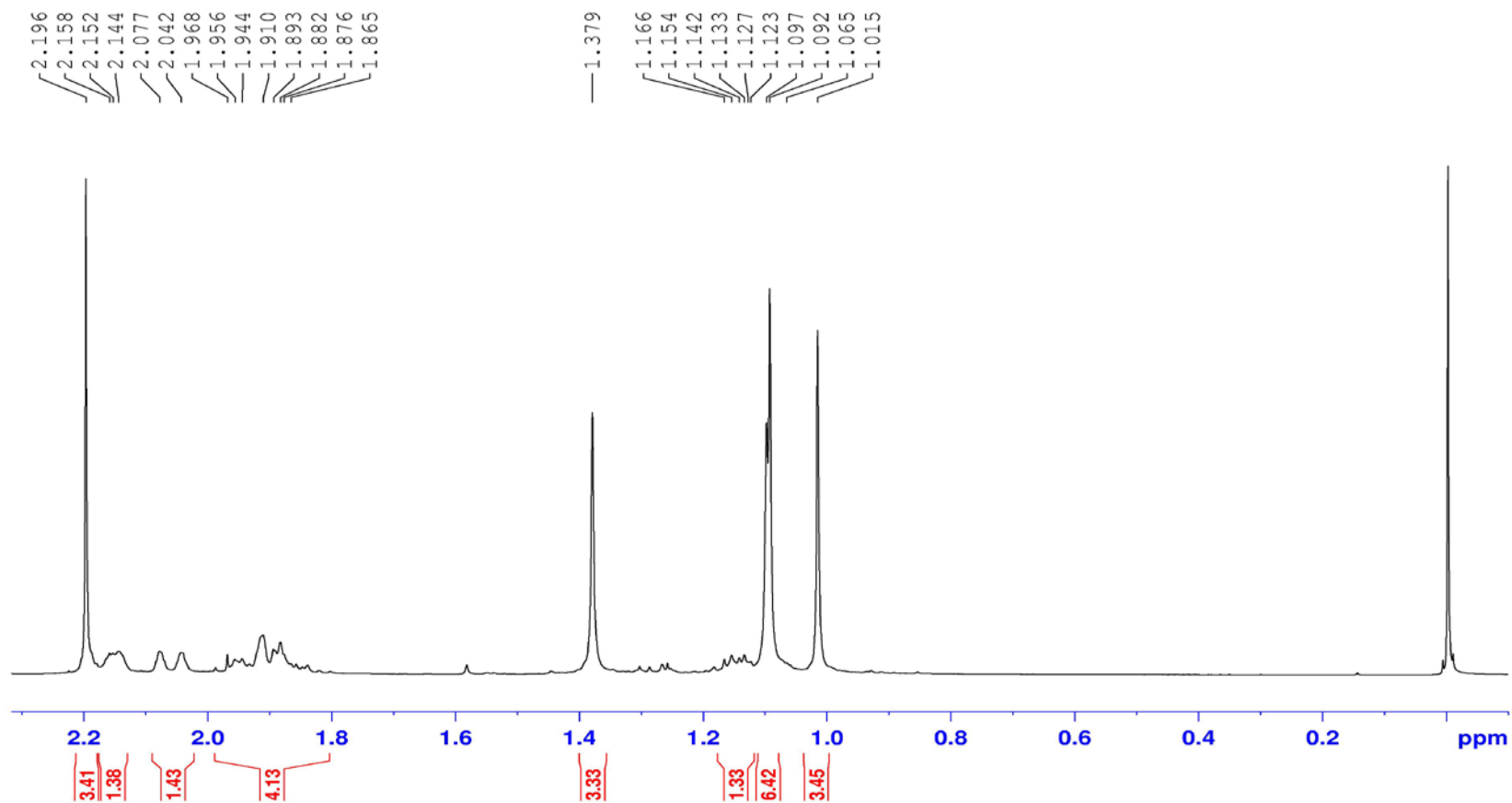




S120

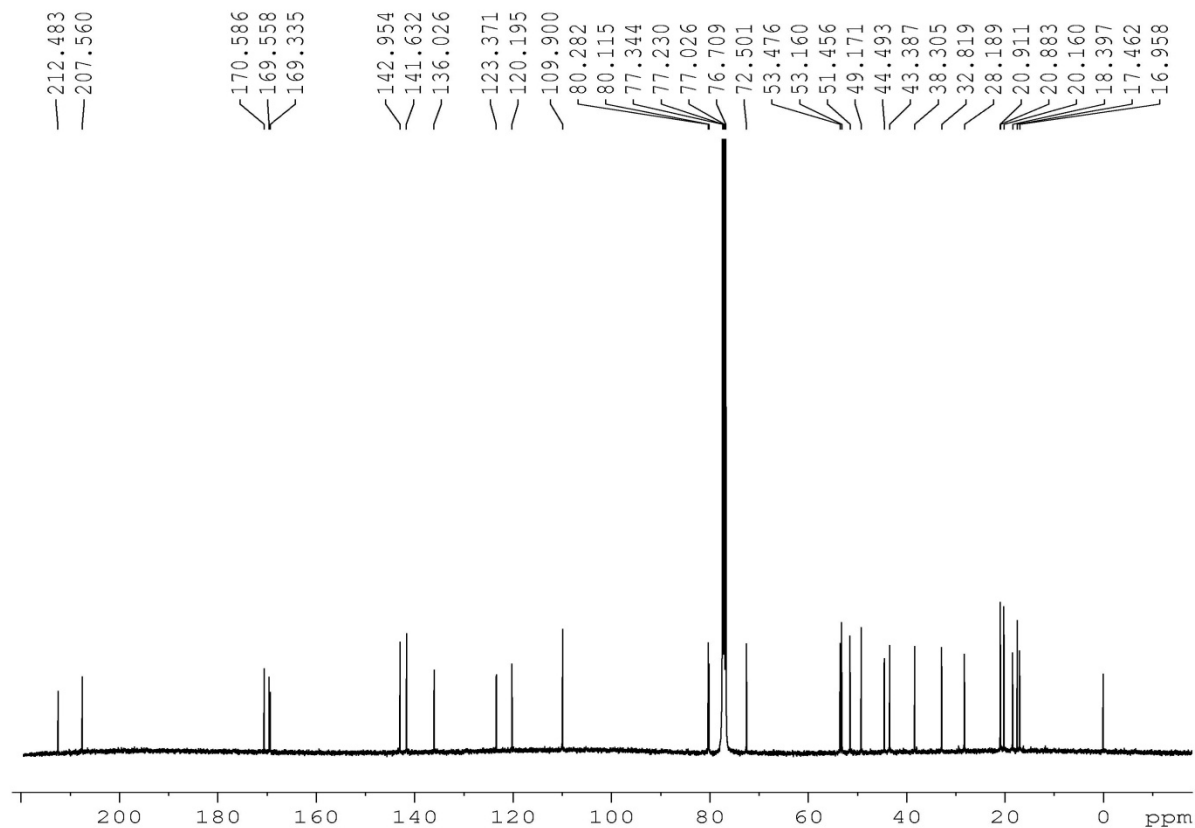


S121



S122

^{13}C NMR (100 MHz) spectrum of Compound **11** in CDCl_3

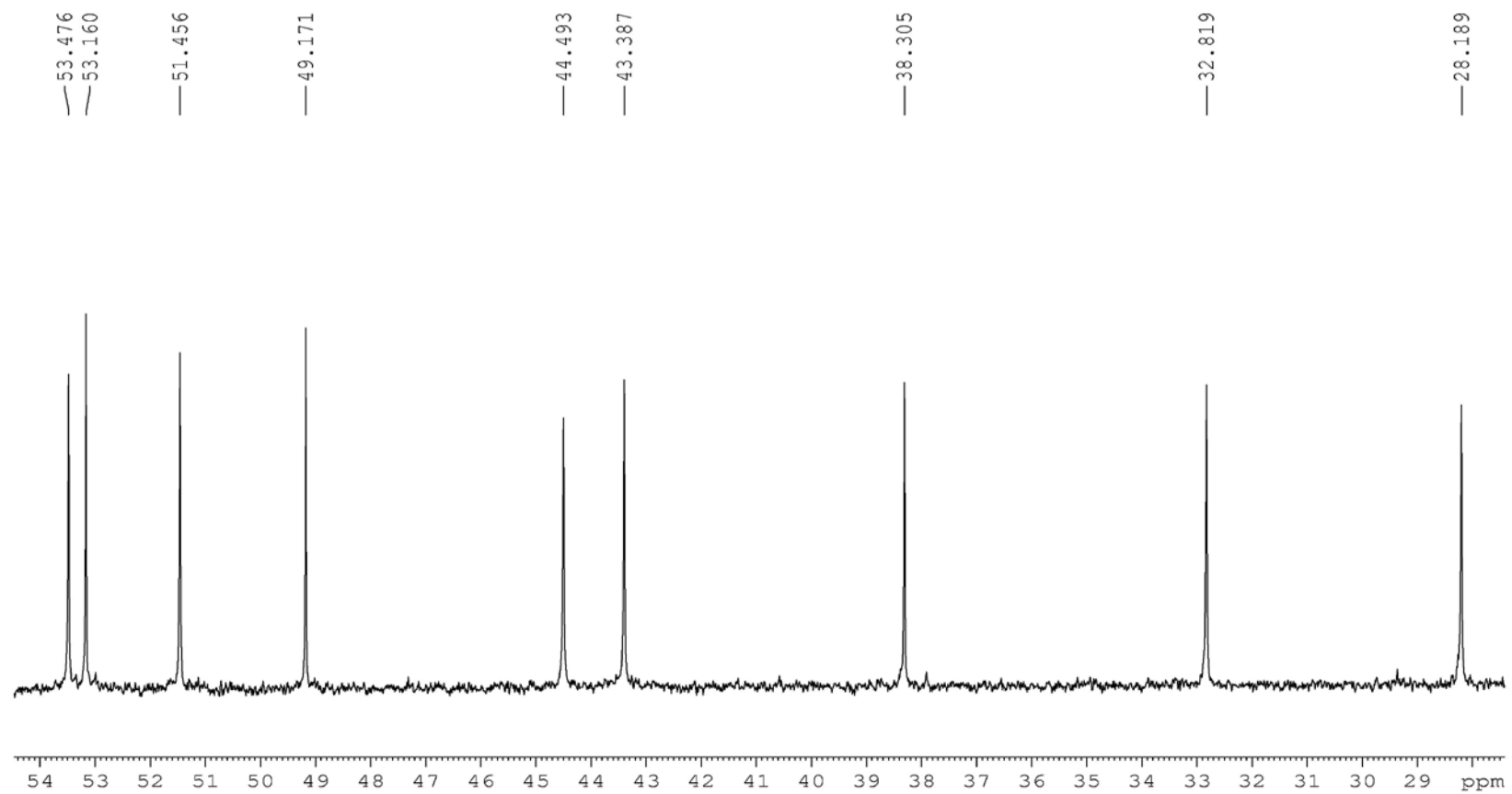


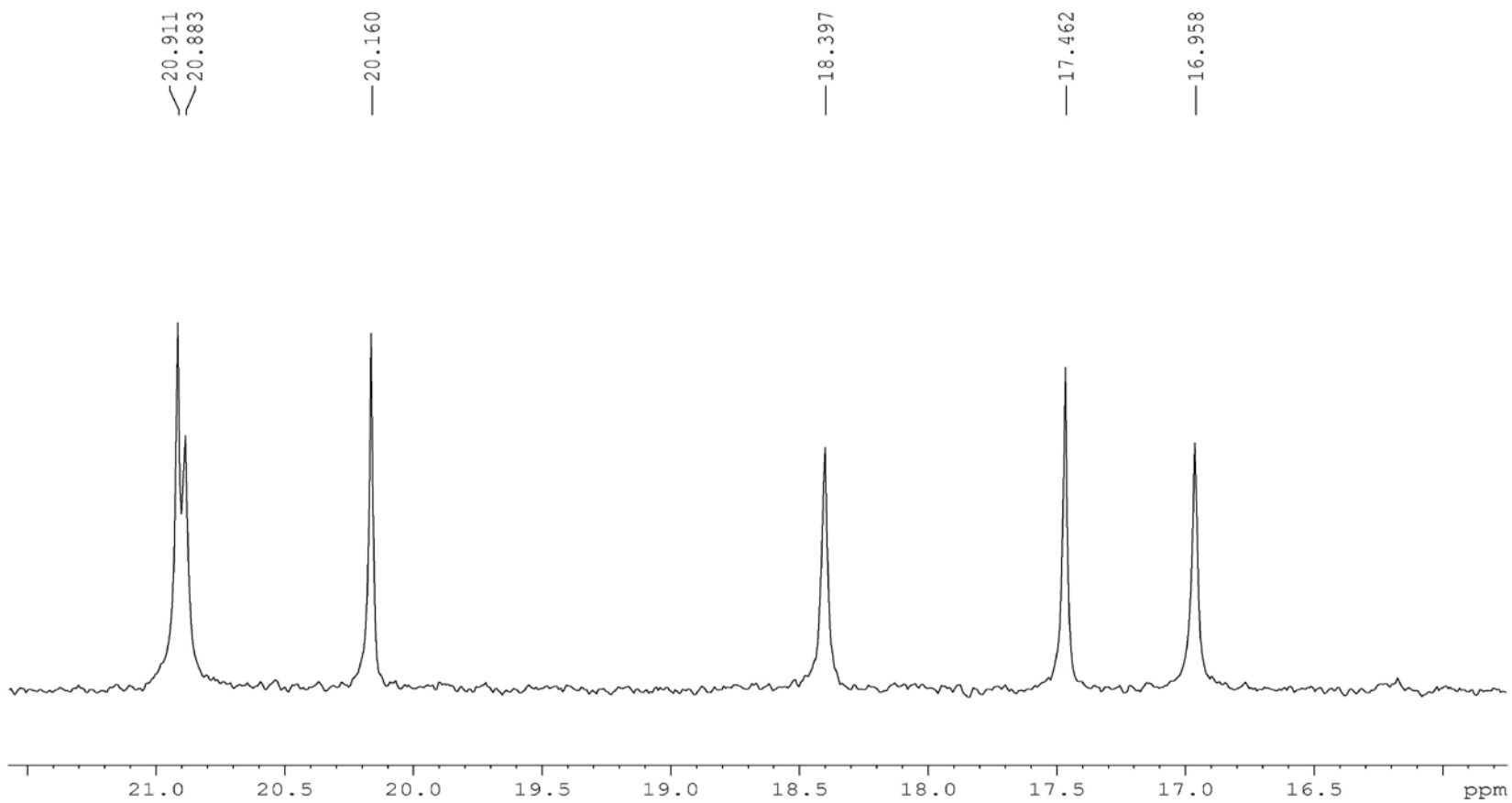
```

NAME                lws-31
EXPNO                2
PROCNO              1
Date_               20141029
Time                5.15
INSTRUM             spect
PROBHD              5 mm CPPBBO BB
PULPROG             zgpg30
TD                  65536
SOLVENT             CDC13
NS                  10000
DS                   4
SWH                 24038.461
FIDRES              0.366798
AQ                  1.3631988
RG                  147.94
DW                  20.800
DE                   18.00
TE                   297.0
D1                   2.00000000
D11                  0.03000000
TD0                  1
  
```

```

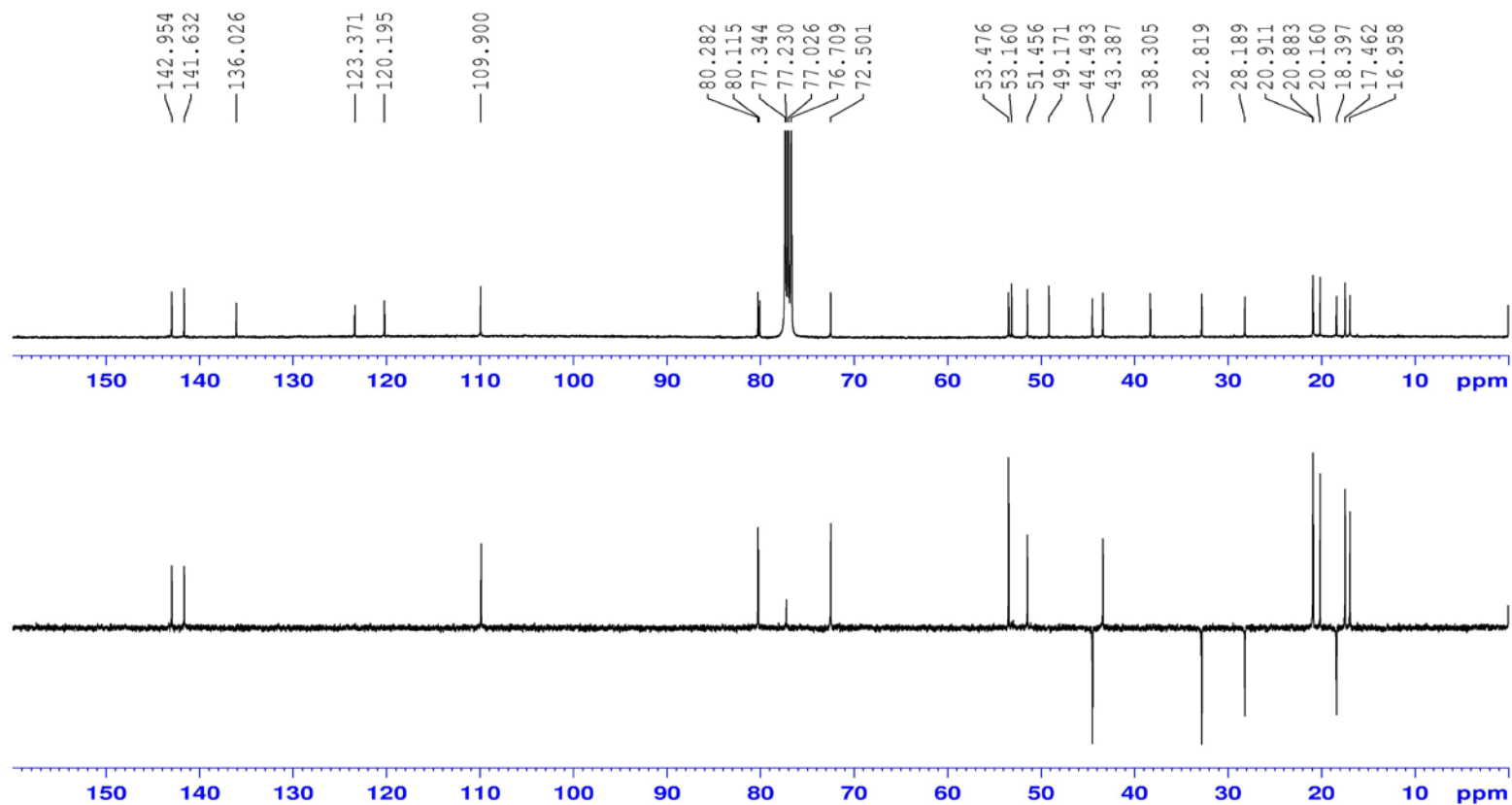
===== CHANNEL f1 =====
SFO1                100.6228293
NUC1                 13C
P1                   10.00
SI                   32768
SF                   100.6127681
WDW                  EM
SSB                   0
LB                   1.00
GB                   0
PC                   1 10
  
```

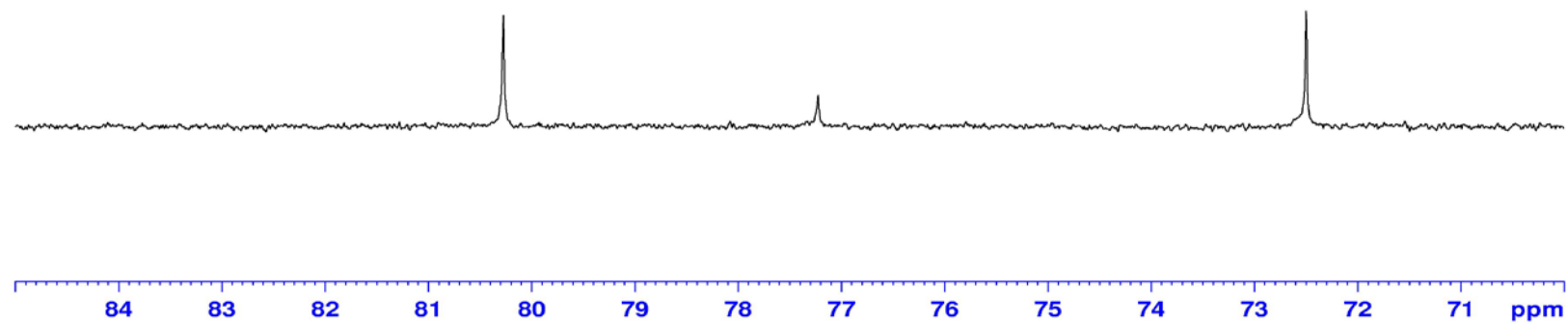
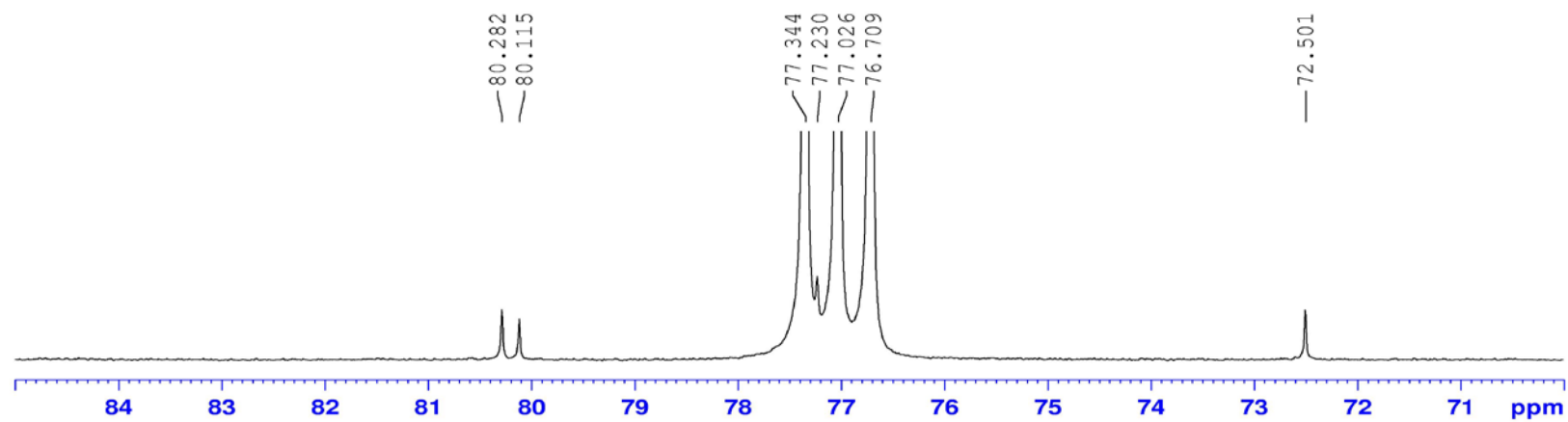




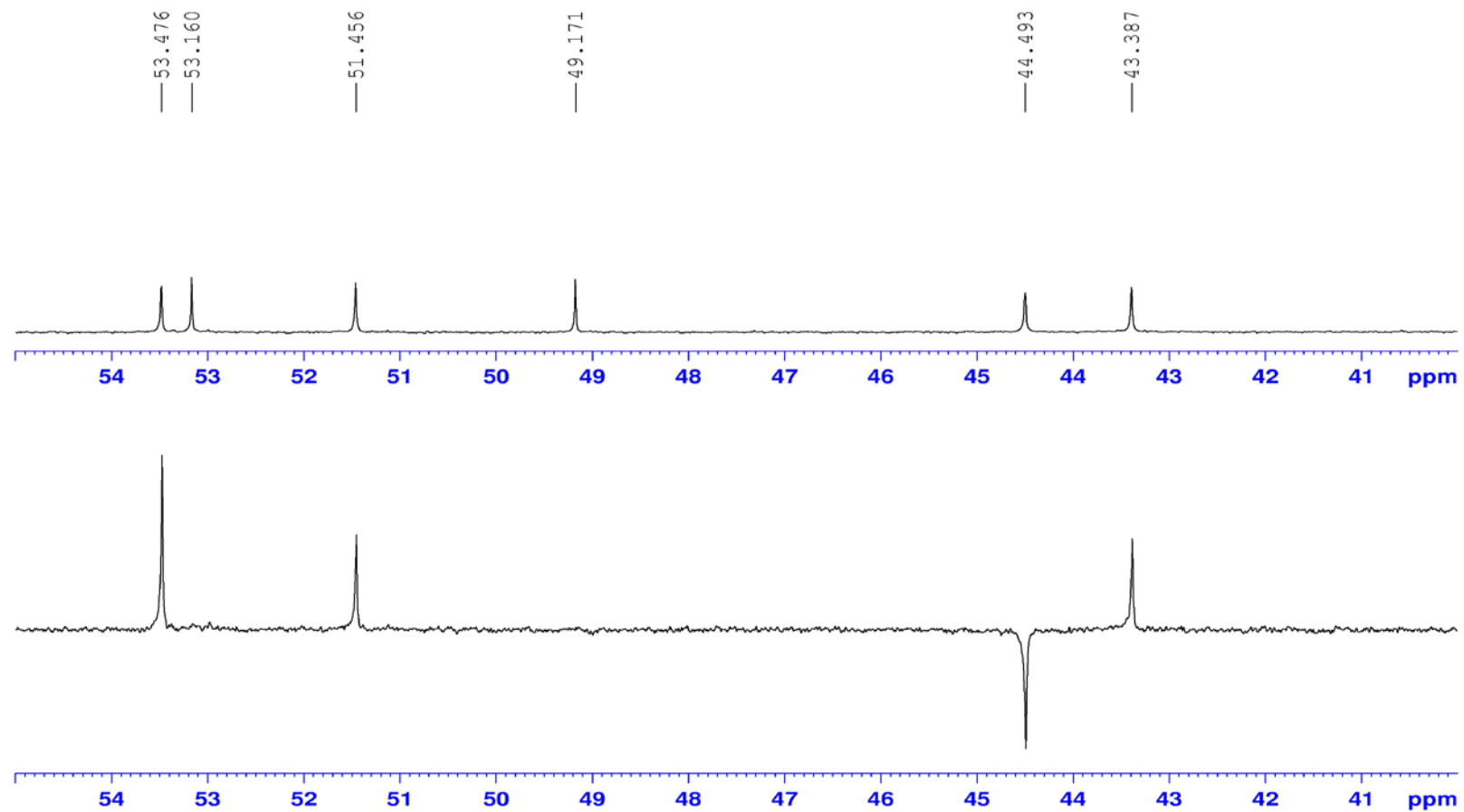
S125

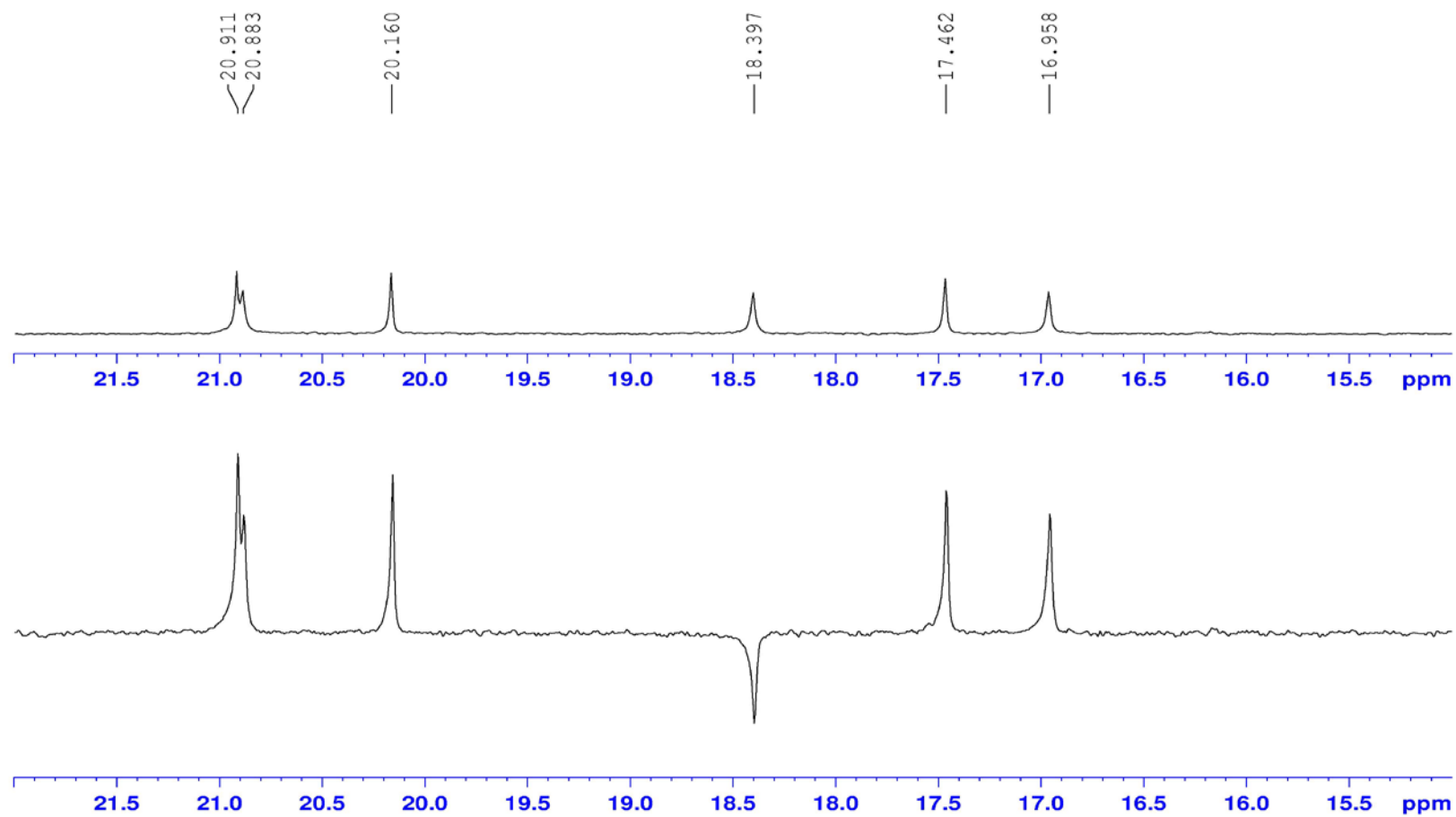
DEPT135° (100 MHz) spectrum of Compound **11** in CDCl₃



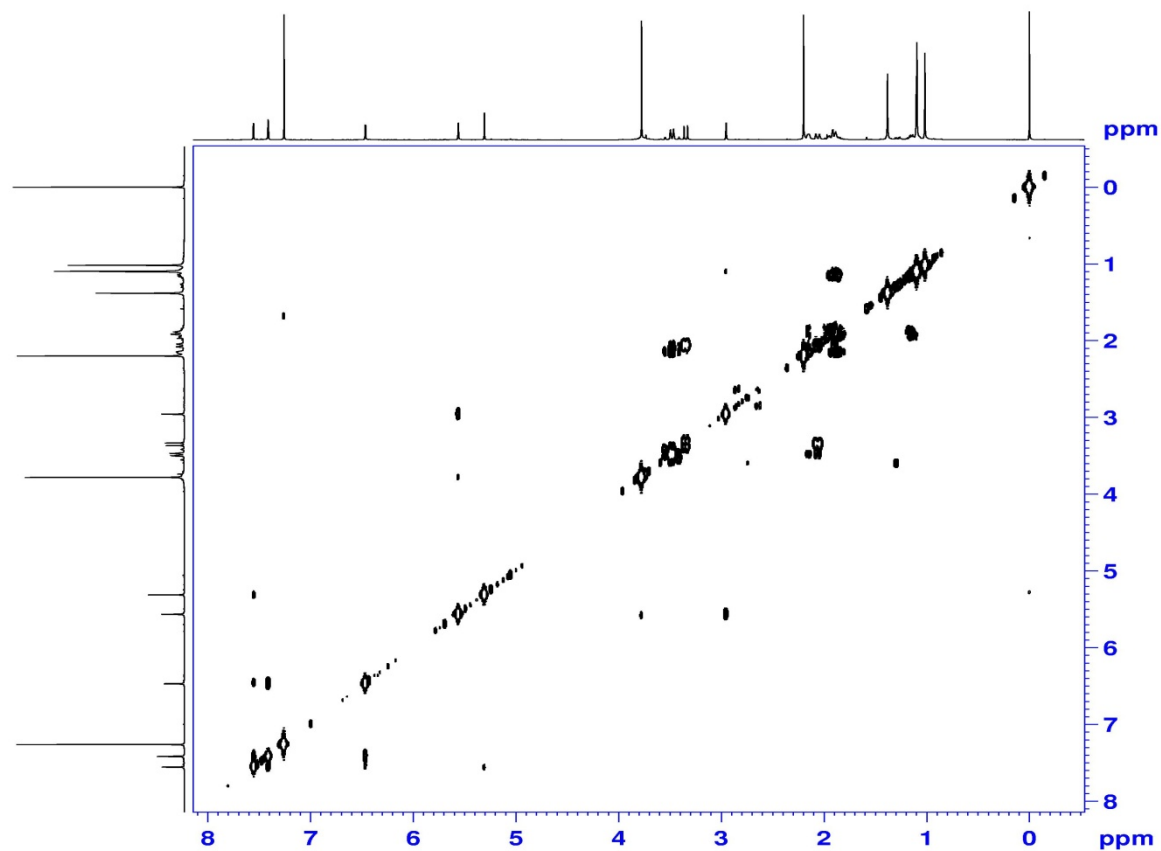


S127





^1H - ^1H COSY (400 MHz) spectrum of Compound **11** in CDCl_3

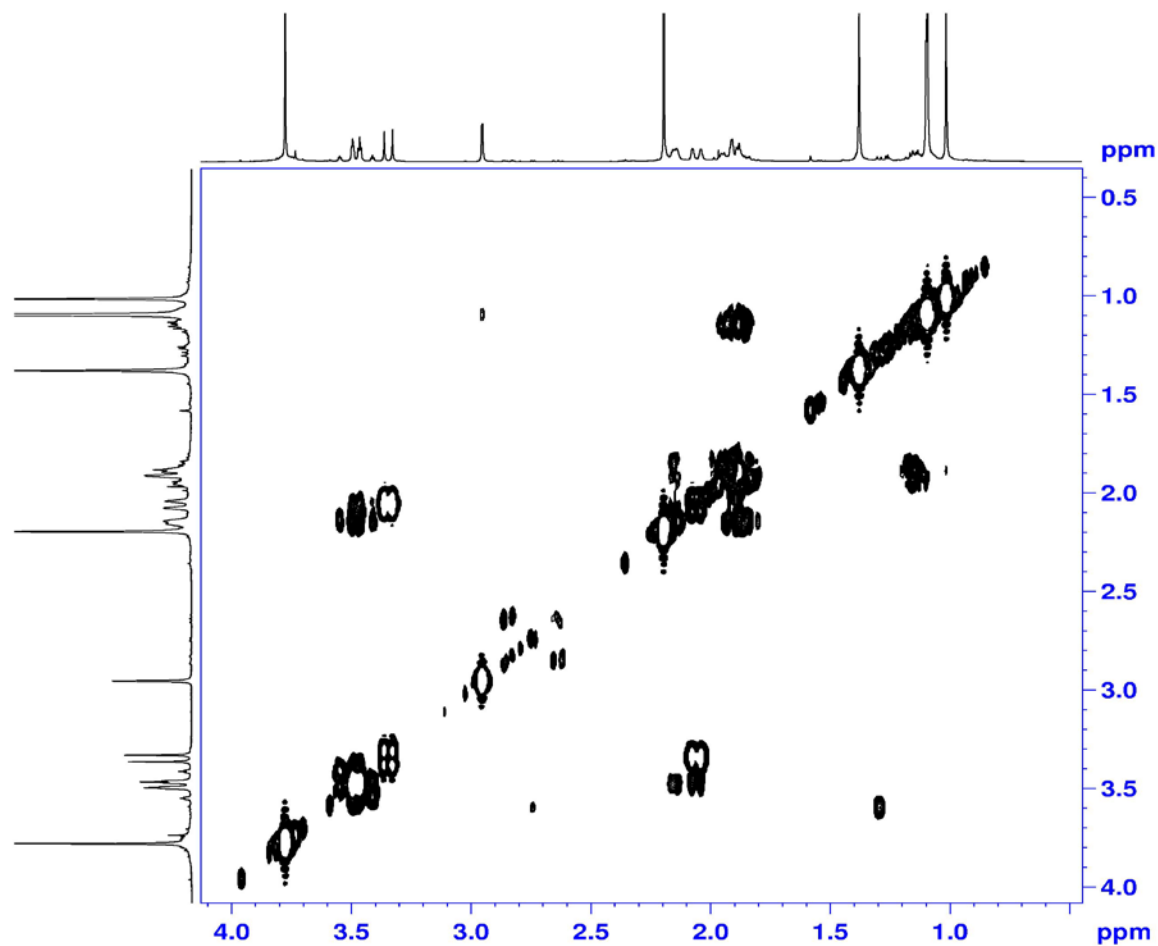


```

NAME                lws-31
EXPNO                4
PROCNO              1
Date_               20141102
Time                21.07
INSTRUM             spect
PROBHD              5 mm CFPBBO BB
PULPROG             cosygpppgf
TD                  2048
SOLVENT             CDCl3
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                    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
  
```



```

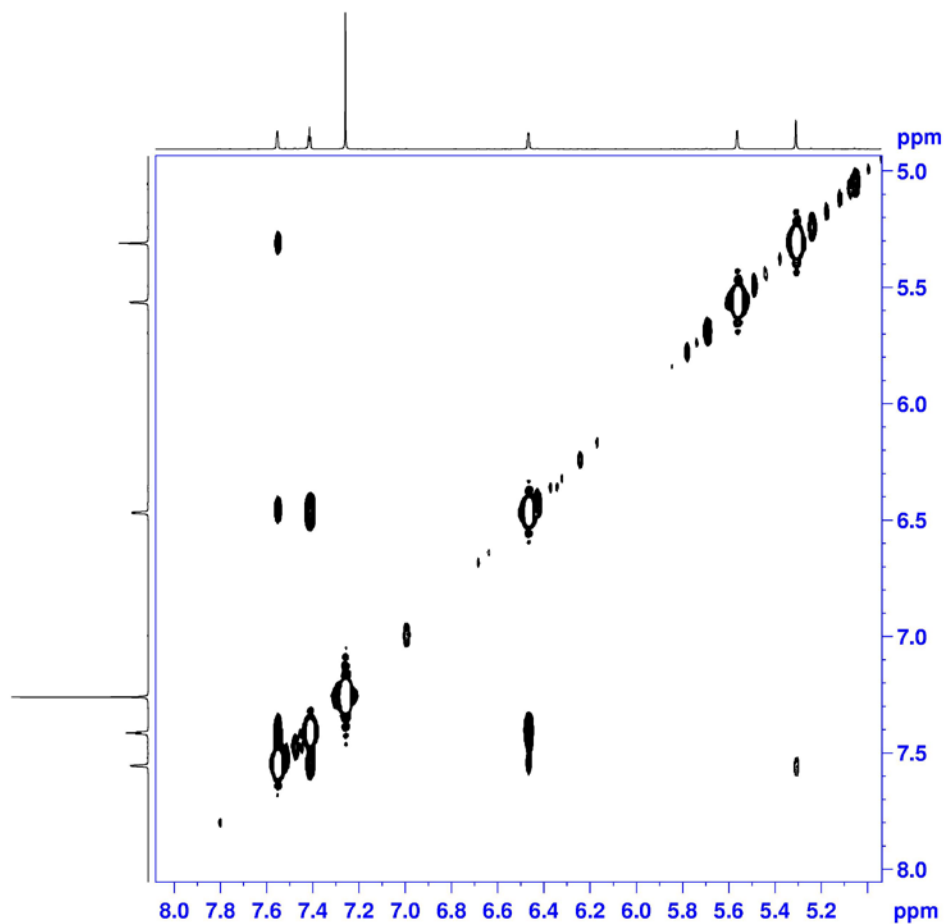
NAME                lws-31
EXPNO                4
PROCNO              1
Date_               20141102
Time                21.07
INSTRUM             spect
PROBHD              5 mm CPPBBO BB
PULPROG             cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                   16
DS                   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                   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
FhMODE              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

```



```

NAME          lws-31
EXPNO         4
PROCNO        1
Date_         20141102
Time          21.07
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       cosygpppqf
TD            2048
SOLVENT       CDCl3
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

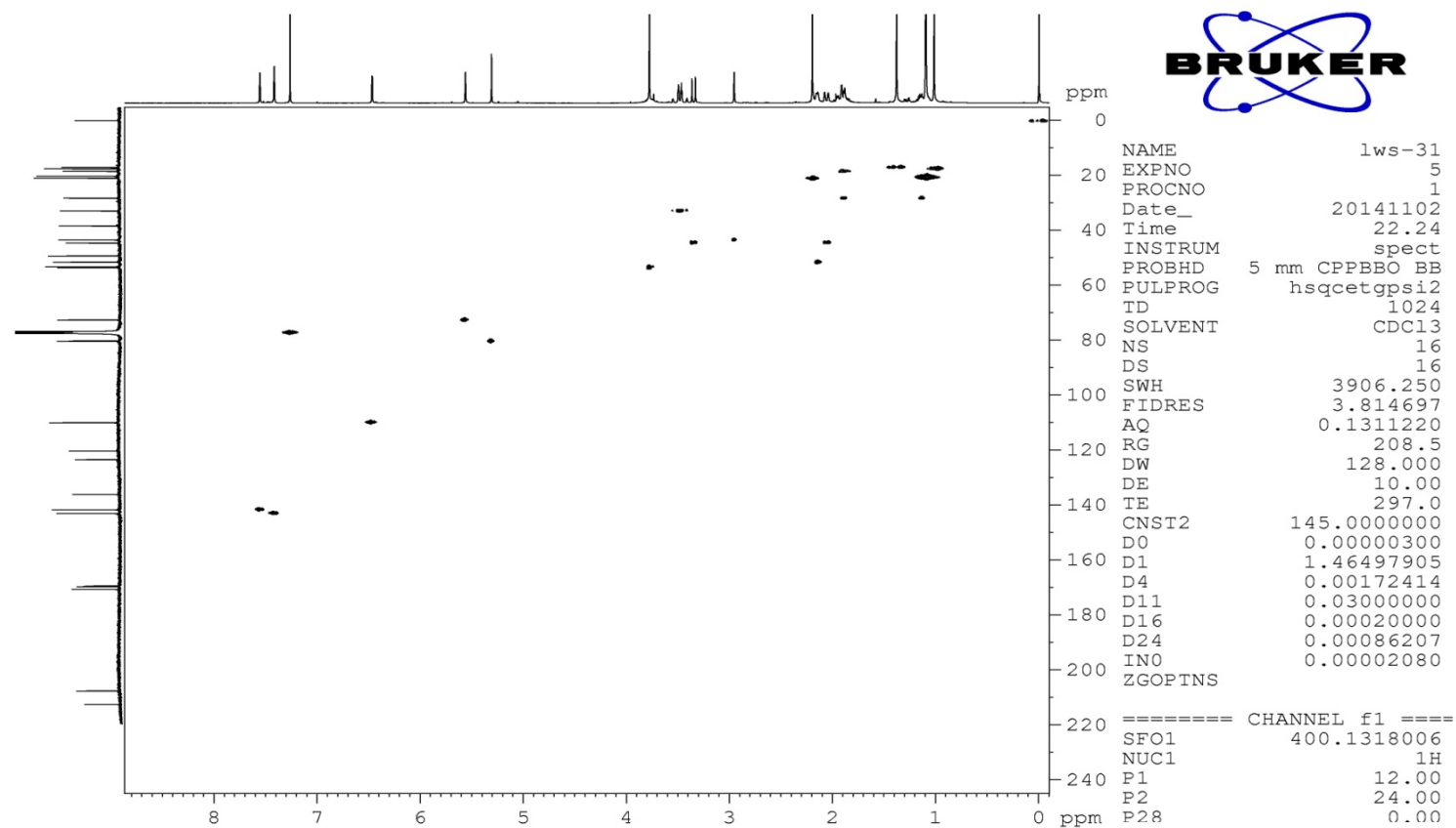
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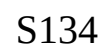
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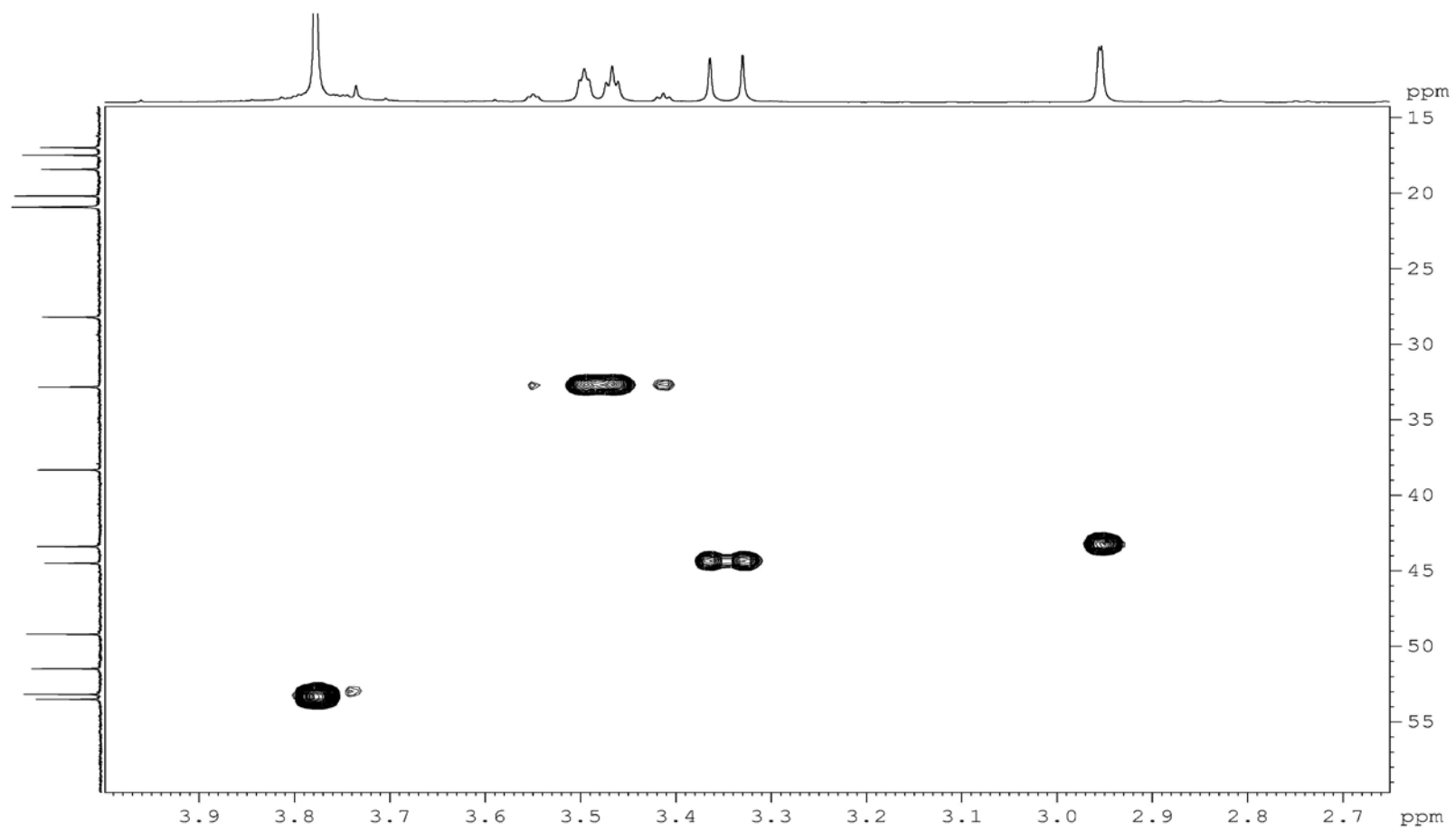
===== CHANNEL f1 =====
SFO1          400.1318006 MHz
NUC1           1H
P0            12.00 usec
P1            12.00 usec
P17           2500.00 usec
ND0            1
TD            128
SFO1          400.1318 MHz
FIDRES        30.517578 Hz
SW            9.762 ppm
FnMODE        QF
SI            1024
SF            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

```


HSQC (400 MHz) spectrum of Compound **11** in CDCl₃

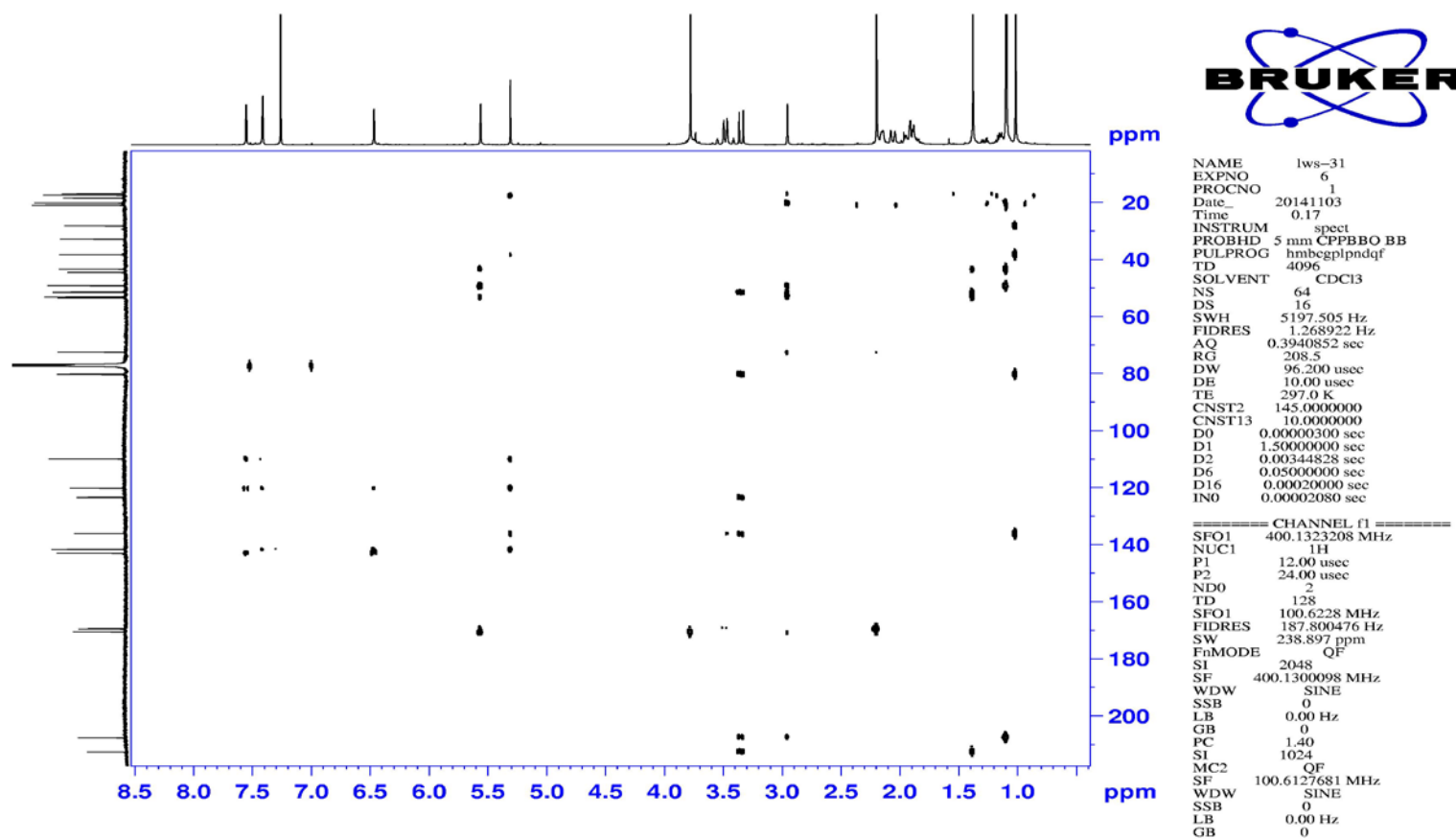


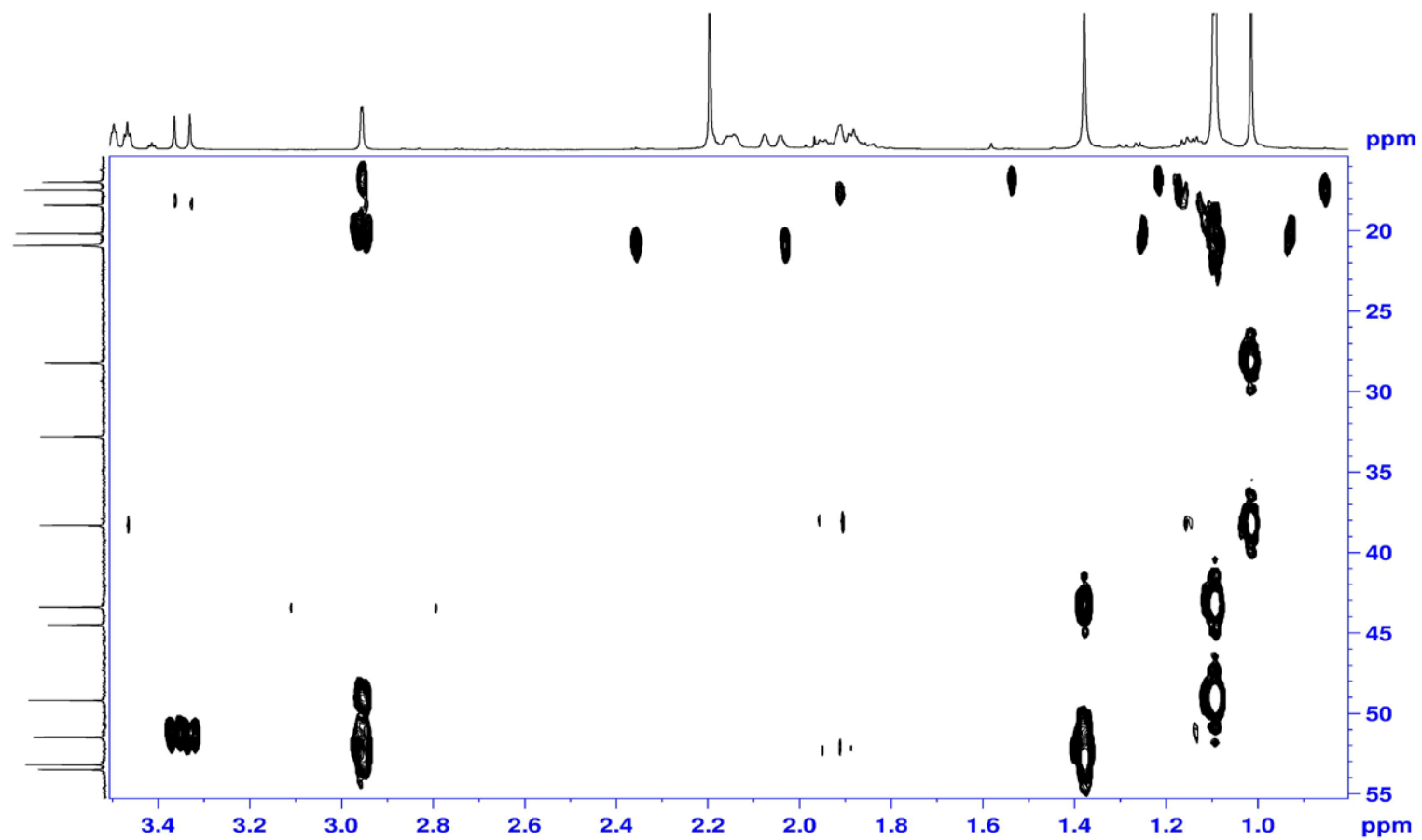




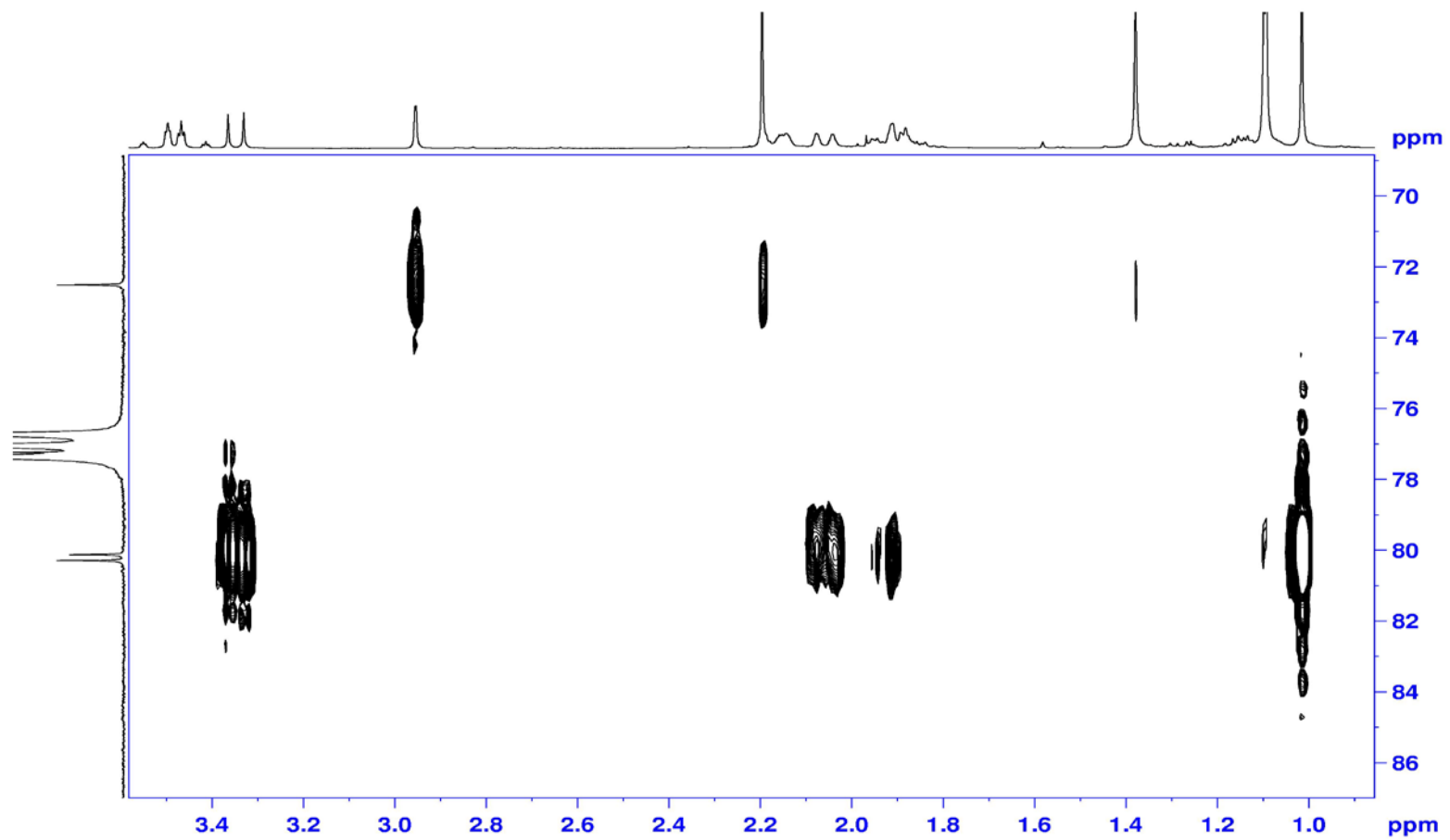
S135

HMBC (400 MHz) spectrum of Compound **11** in CDCl₃

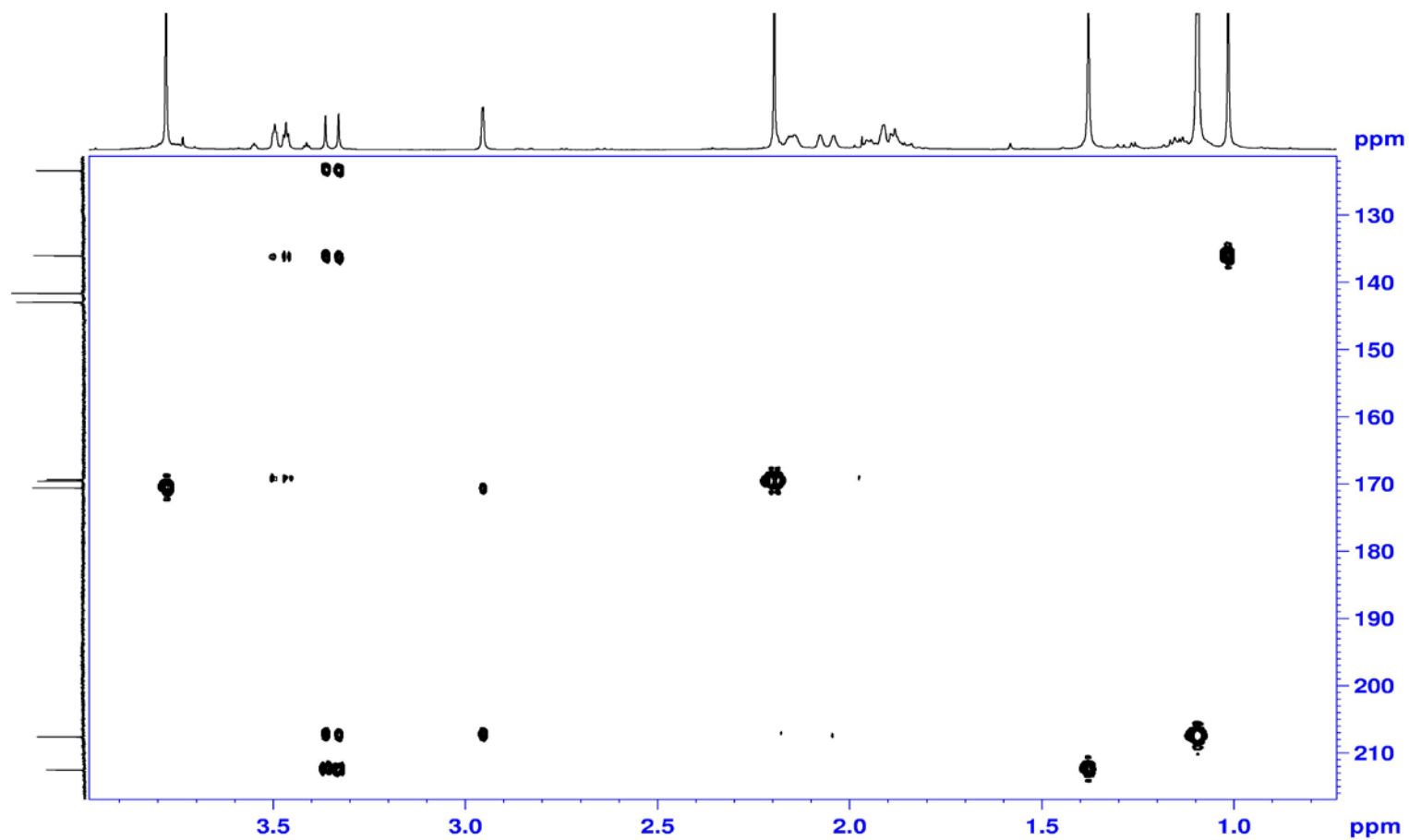




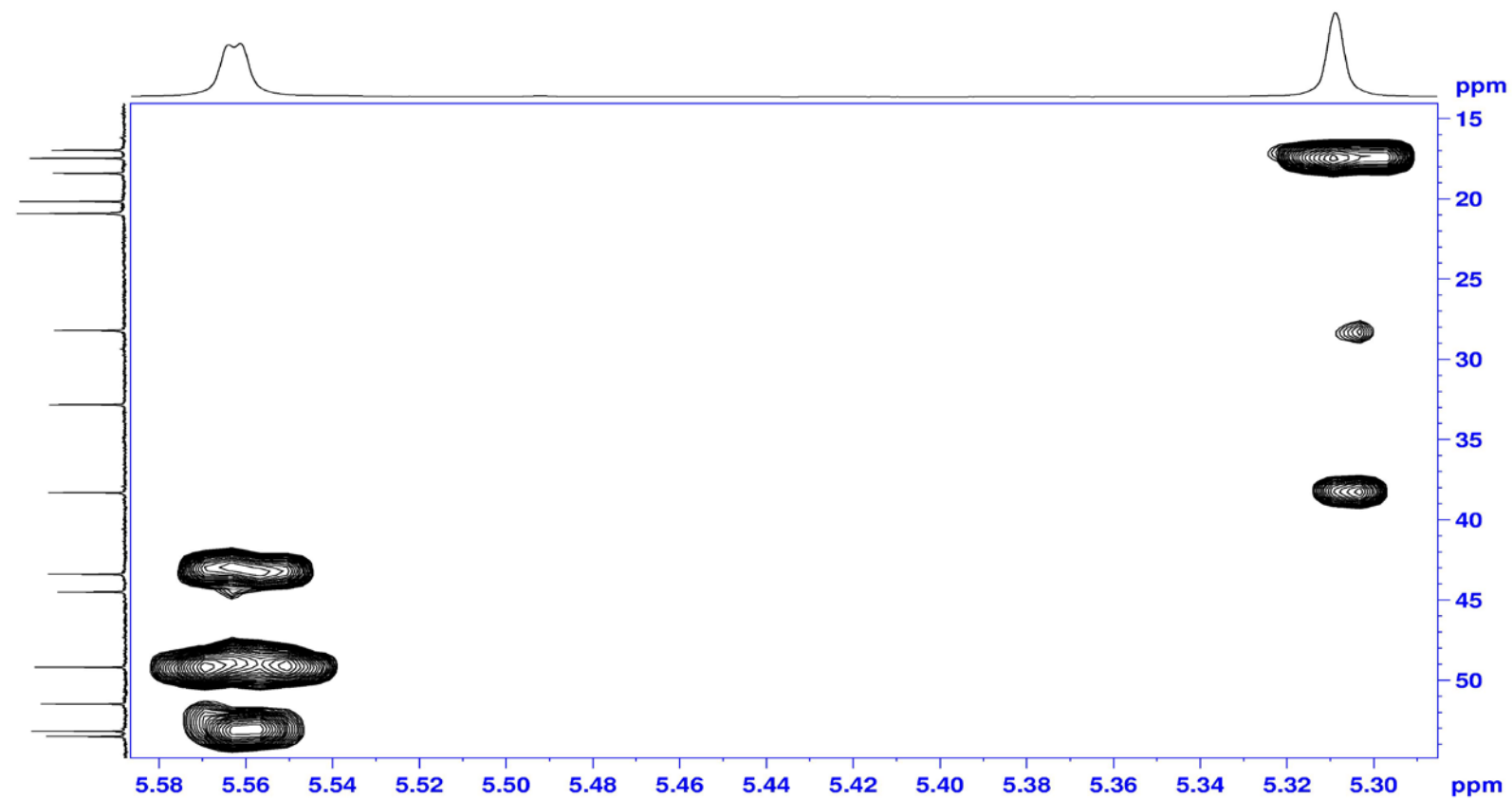
S137



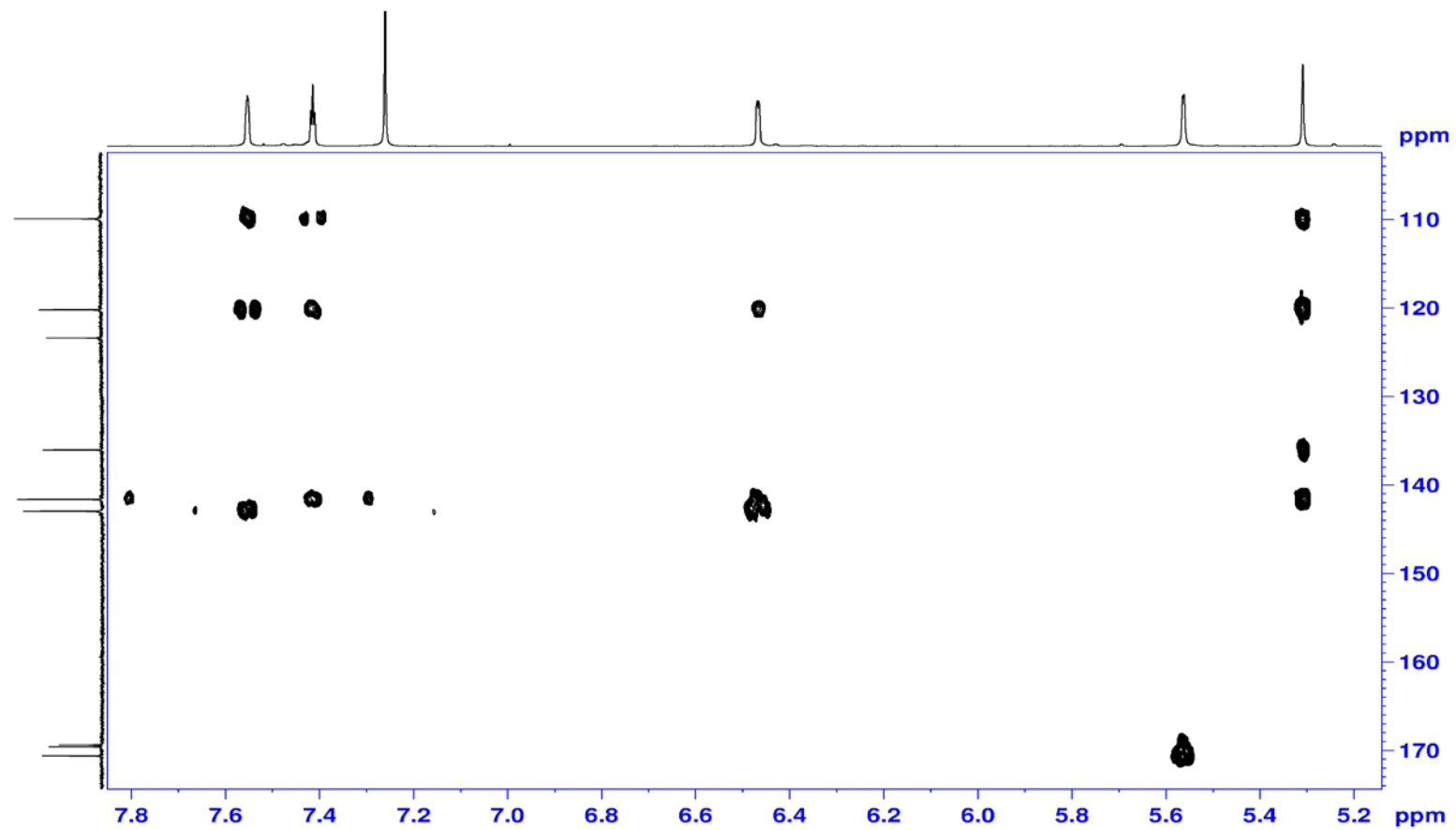
S138



S139

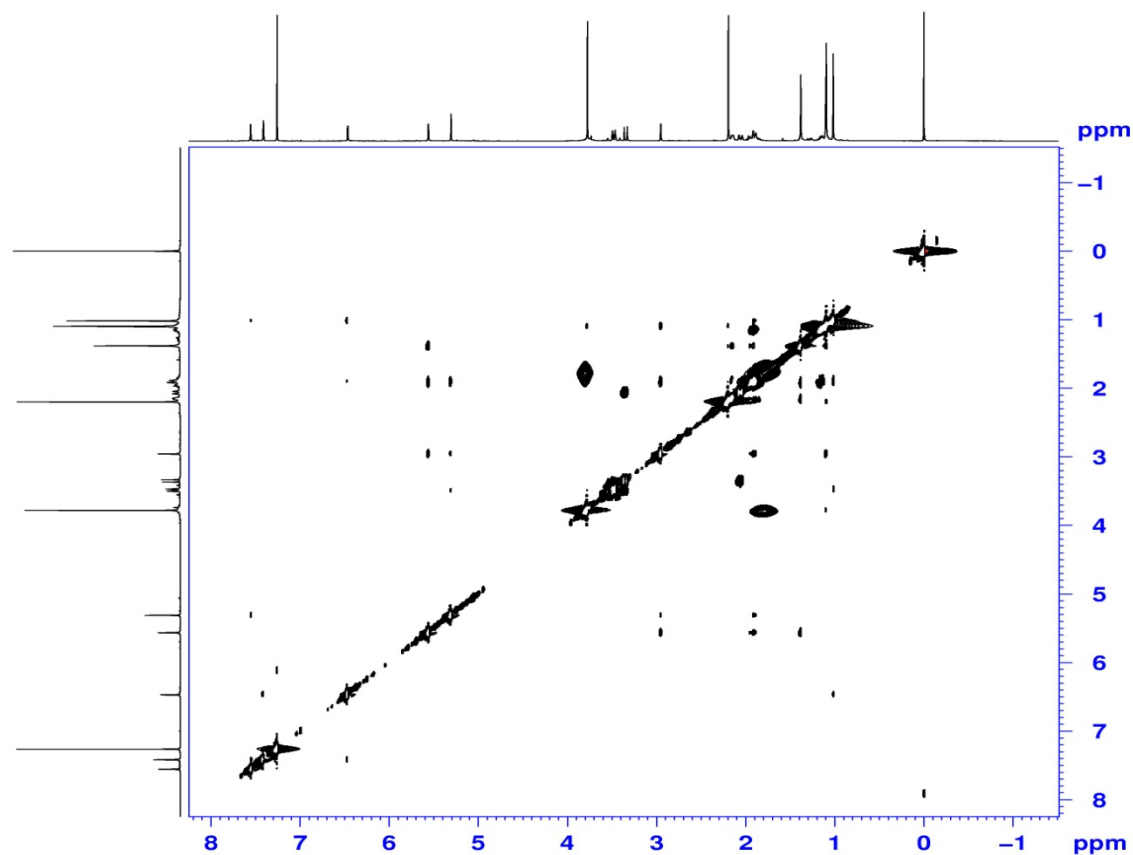


S140



S141

NOESY (400 MHz) spectrum of Compound **11** in CDCl₃

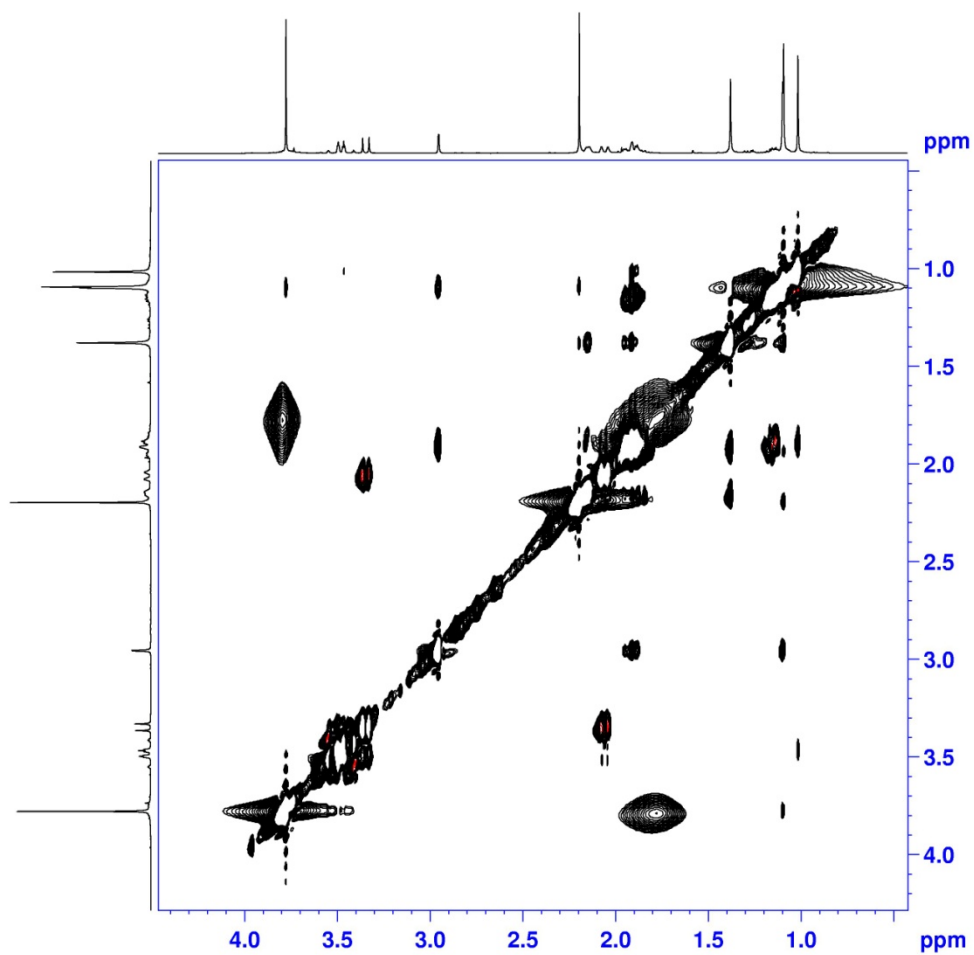


```

NAME                lws-31
EXPNO                7
PROCNO               1
Date_                20141103
Time                4.46
INSTRUM              spect
PROBHD               5 mm CFPBBO BB
PULPROG              noesygpphphpp
TD                   2048
SOLVENT              CDCl3
NS                   32
DS                   32
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                   0.00010972 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
  
```



```

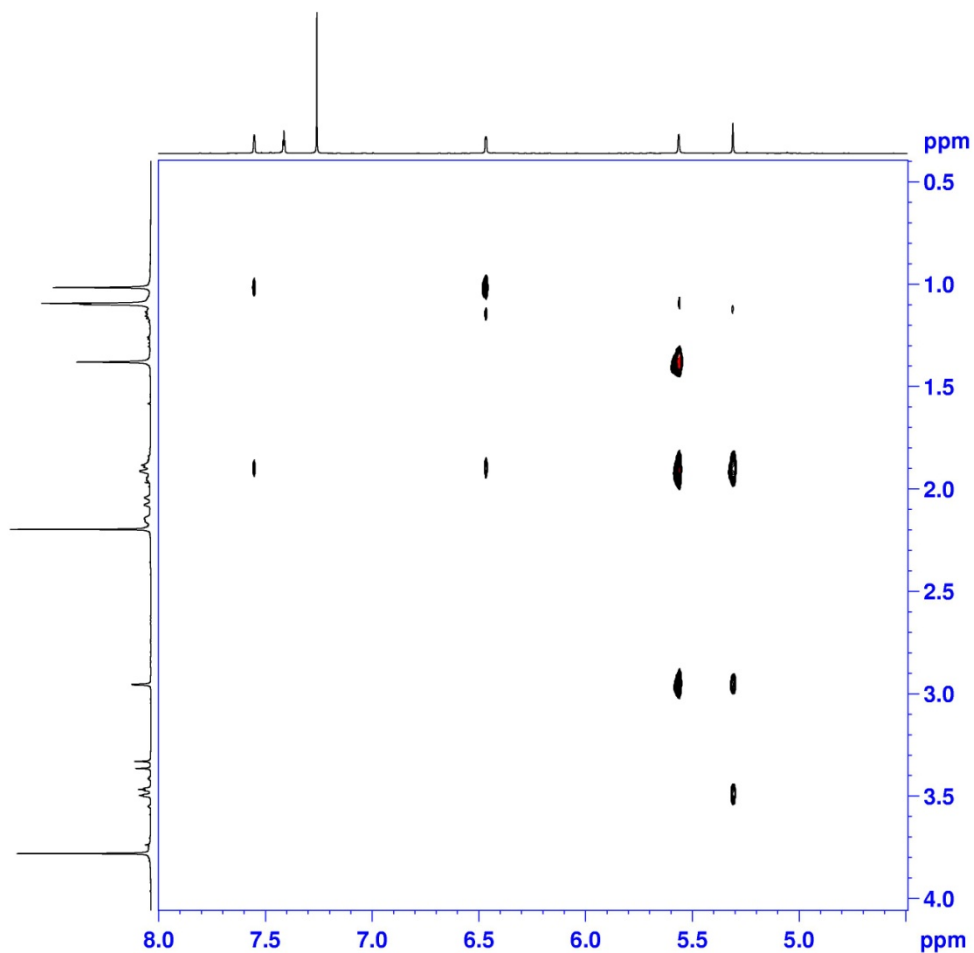
NAME          lws-31
EXPNO          7
PROCNO         1
Date_         20141103
Time           4.46
INSTRUM        spect
PROBHD         5 mm CPPBBO BB
PULPROG        noesygpph
TD             2048
SOLVENT        CDC13
NS             32
DS             32
SWH            3906.250 Hz
FIDRES         1.907349 Hz
AQ             0.2621940 sec
RG             208.5
DW             128.000 usec
DE             10.00 usec
TE             297.0 K
D0             0.00010972 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

```



```

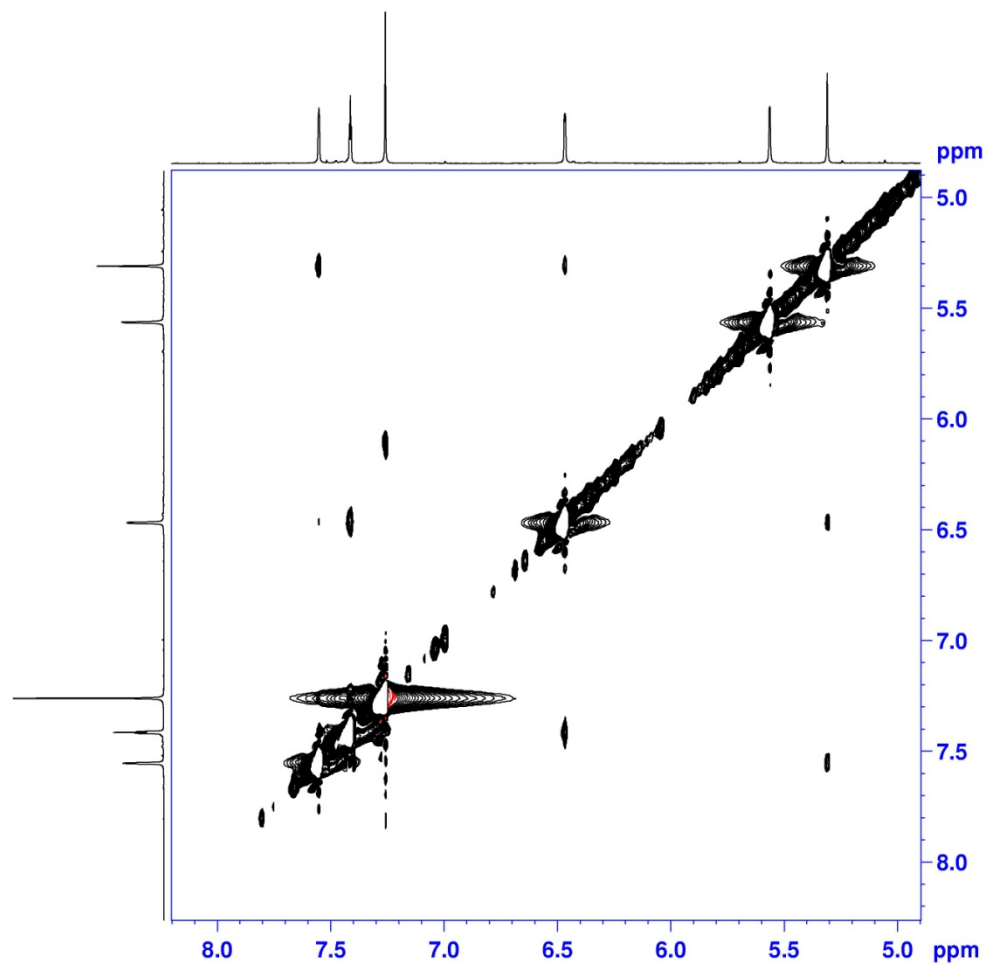
NAME          lws-31
EXPNO          7
PROCNO         1
Date_         20141103
Time           4.46
INSTRUM        spect
PROBHD         5 mm CPPBBO BB
PULPROG        noesygpphph
TD             2048
SOLVENT        CDCl3
NS              32
DS              32
SWH            3906.250 Hz
FIDRES         1.907349 Hz
AQ             0.2621940 sec
RG             208.5
DW             128.000 usec
DE             10.00 usec
TE             297.0 K
D0             0.00010972 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

```



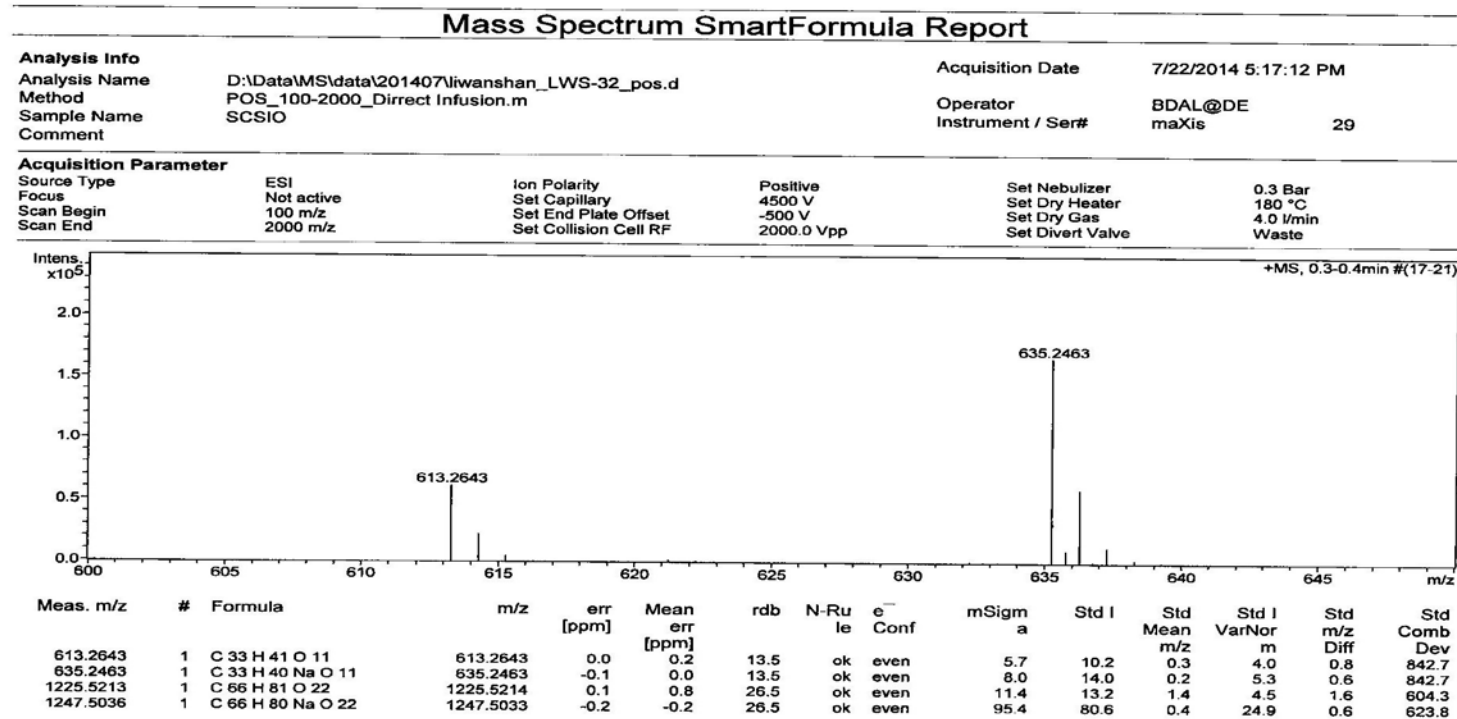
```

NAME          lws-31
EXPNO          7
PROCNO         1
Date_         20141103
Time          4.46
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       noesygpphph
TD            2048
SOLVENT       CDCl3
NS             32
DS             32
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            0.00010972 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
  
```

HR-ESIMS of Compound 12



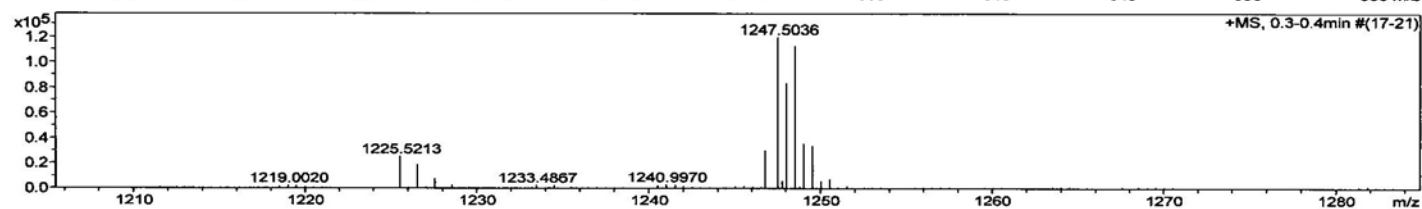
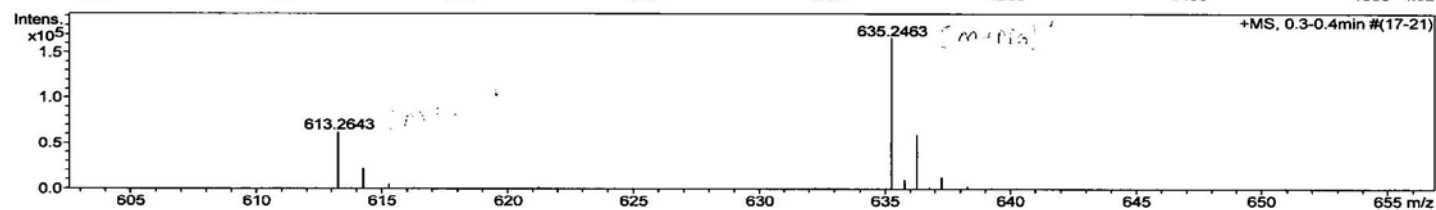
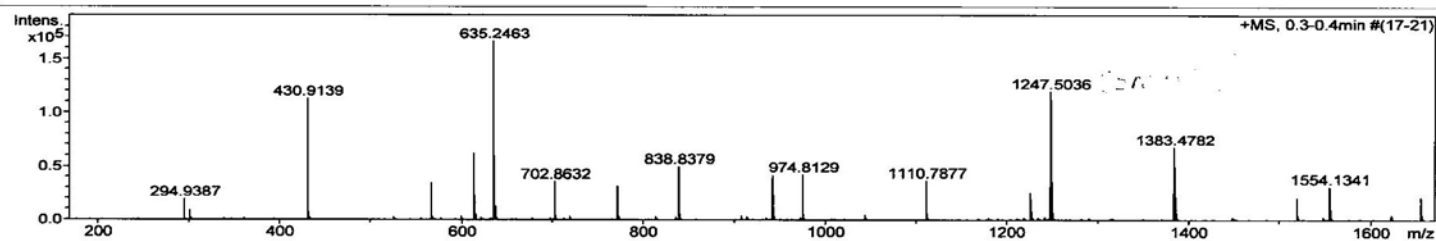
Generic Display Report

Analysis Info

Analysis Name D:\Data\MS\data\201407\liwanshan_LWS-32_pos.d
Method POS_100-2000_Direct Infusion.m
Sample Name SCSiO
Comment

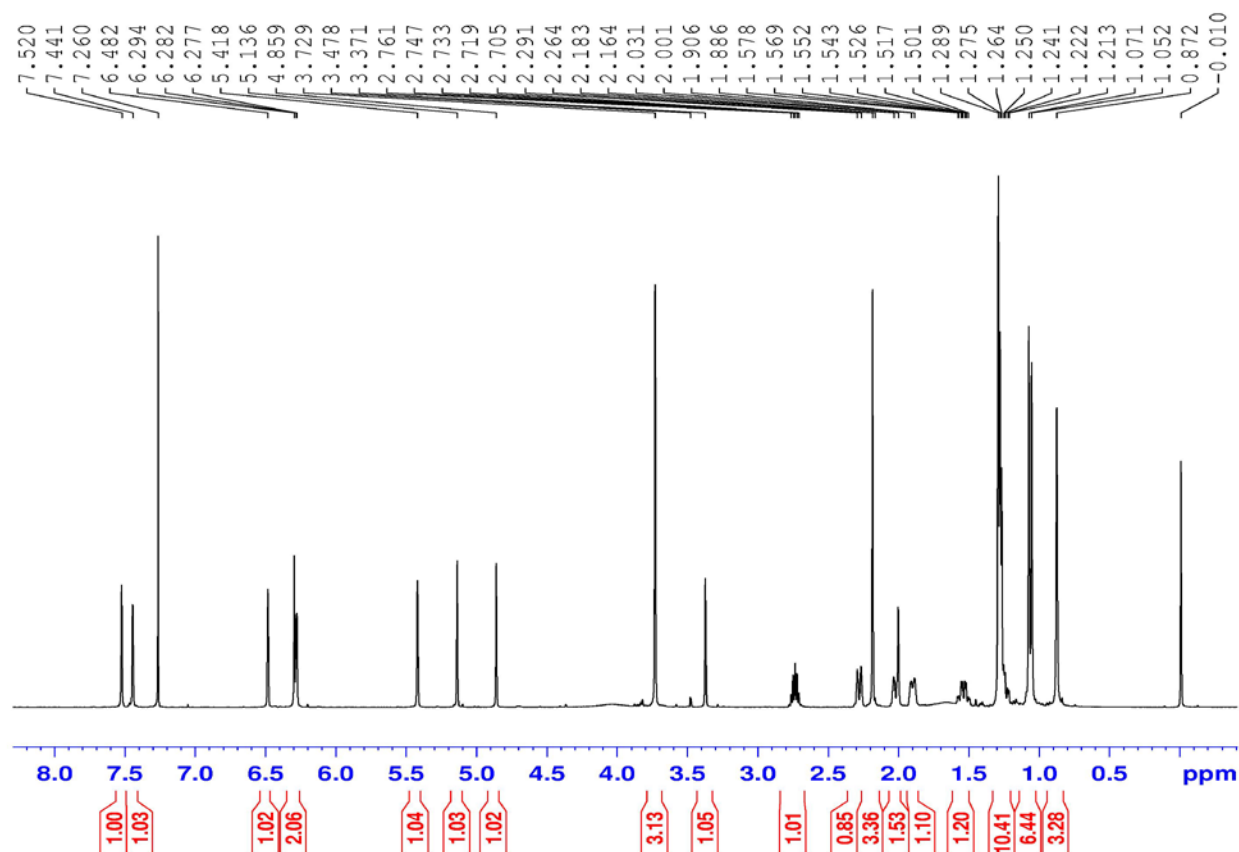
Acquisition Date 7/22/2014 5:17:12 PM

Operator BDAL@DE
Instrument maXis



^1H NMR (500 MHz) spectrum of Compound **12** in CDCl_3

^1H NMR Spectrum of lws-32

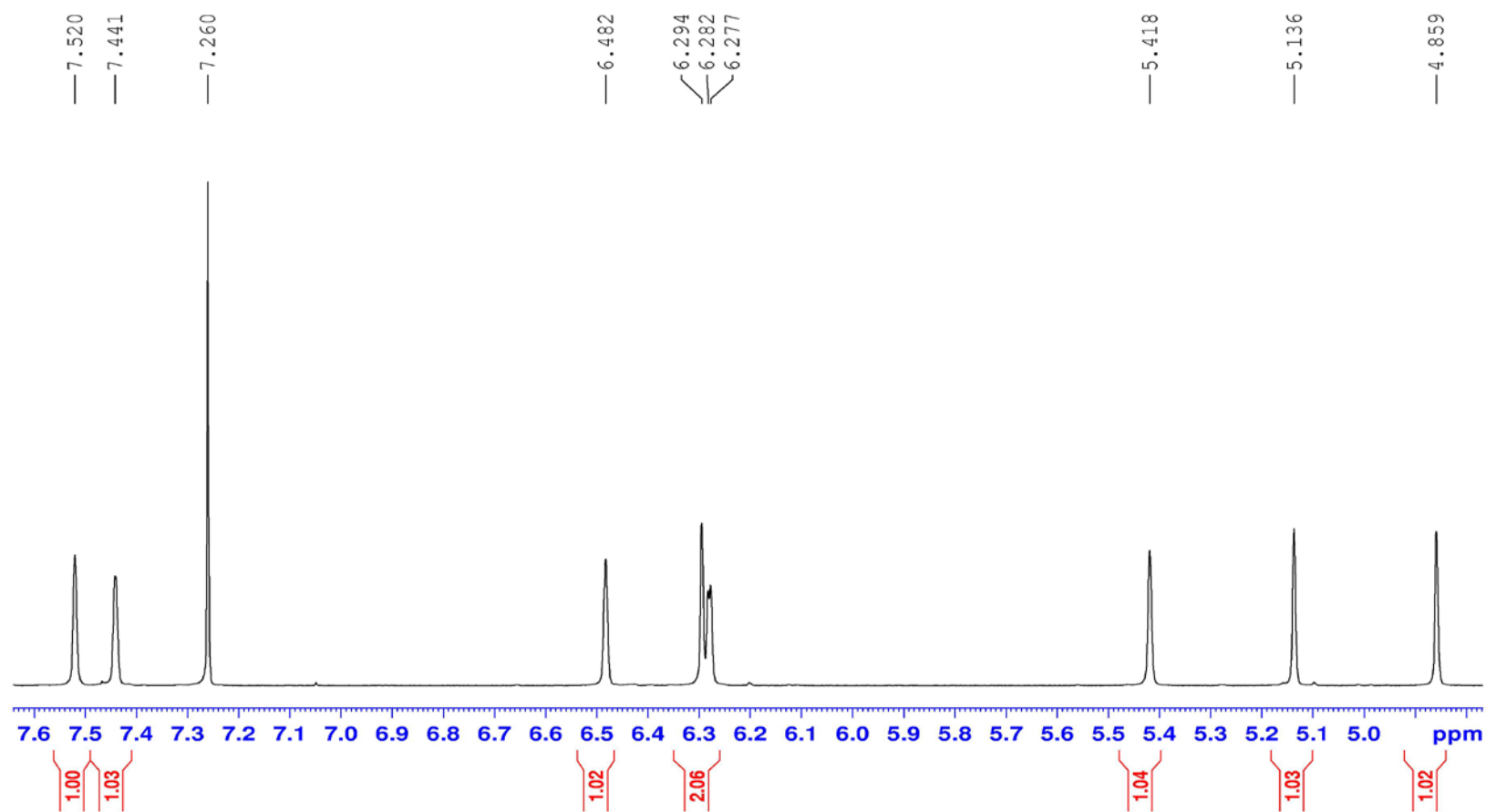


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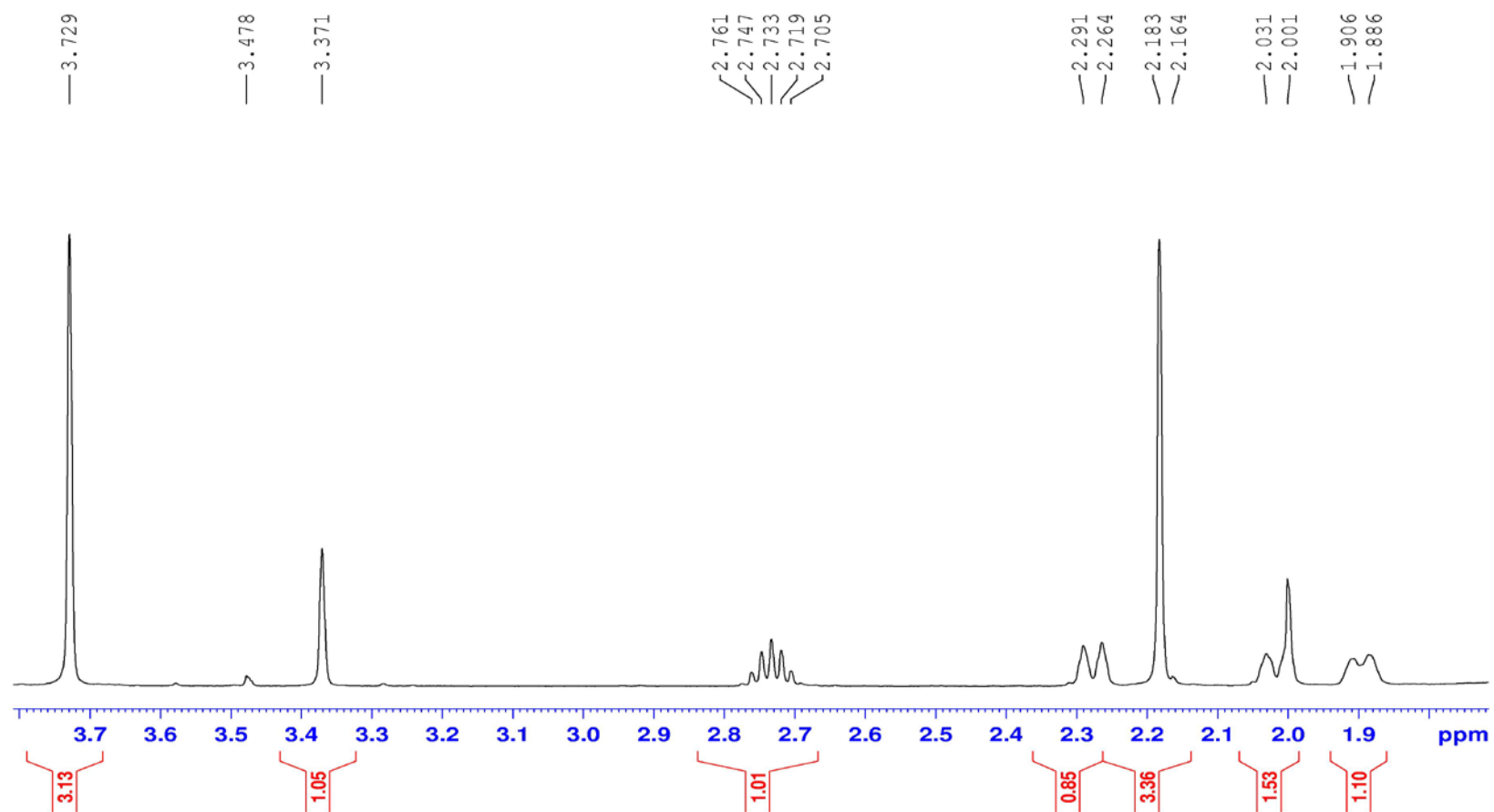
NAME      liwanshan-lws-32
EXPNO     1
PROCNO    1
Date_     20140716
Time      23.53
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        32768
SOLVENT   CDCl3
NS        8
DS        2
SWH       10330.578 Hz
FIDRES    0.315264 Hz
AQ        1.5860696 sec
RG        161.3
DW        48.400 usec
DE        6.50 usec
TE        296.3 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1        16.50 usec
PL1       -1.00 dB
PL1W      13.91402149 W
SFO1      500.1330885 MHz
SI        32768
SF        500.1300131 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

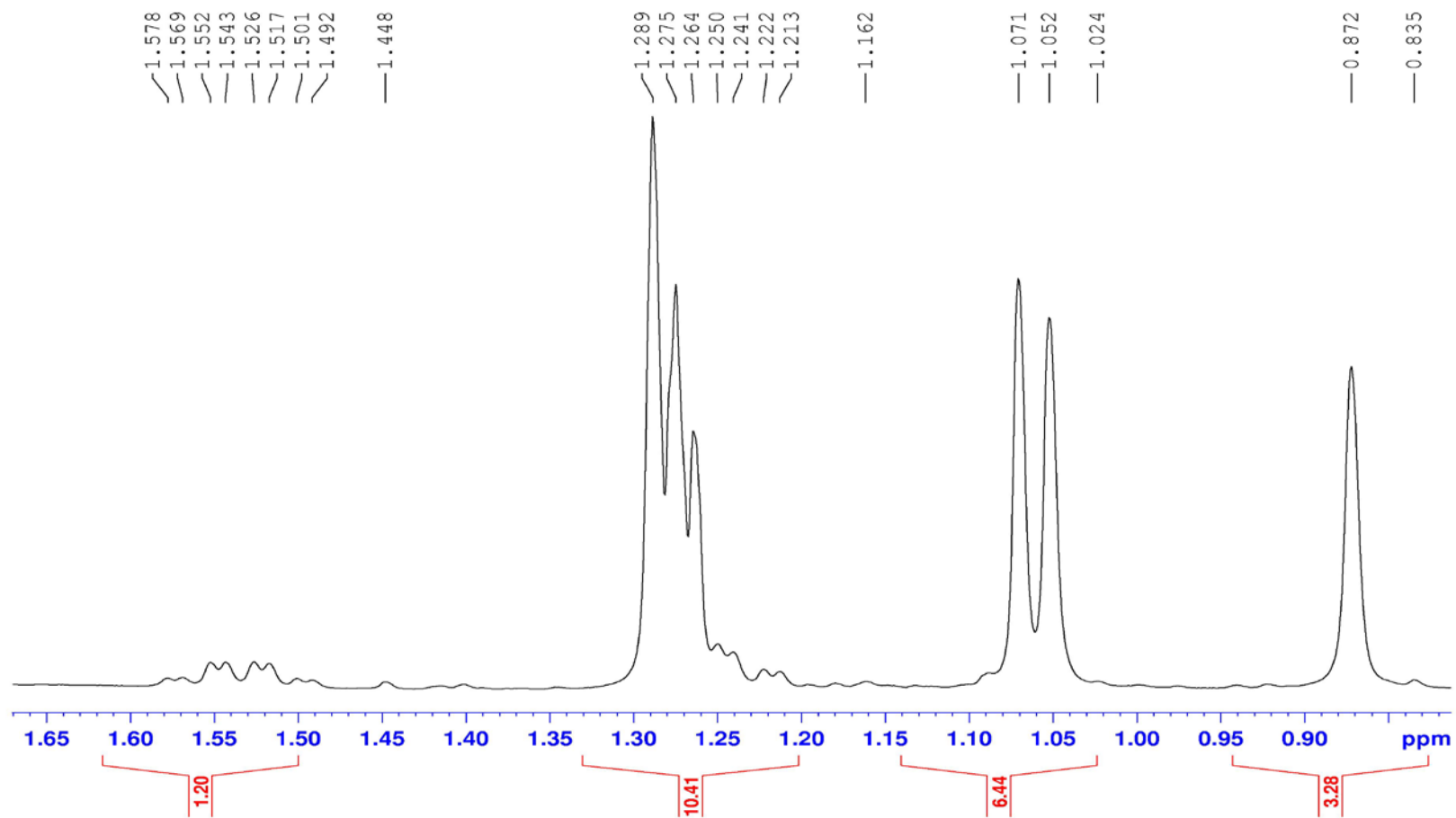

¹H NMR Spectrum of lws-32



¹H NMR Spectrum of lws-32

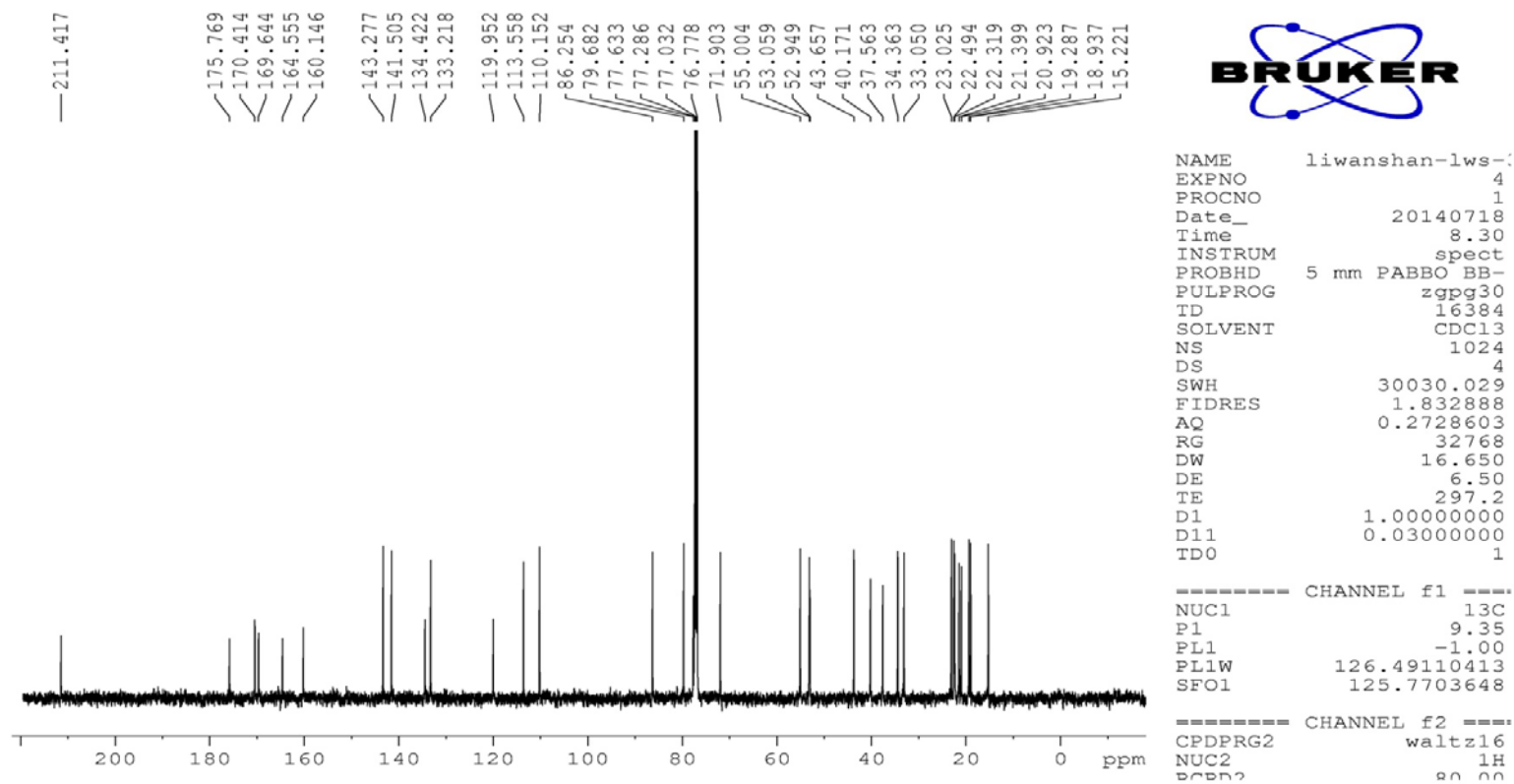


¹H NMR Spectrum of lws-32

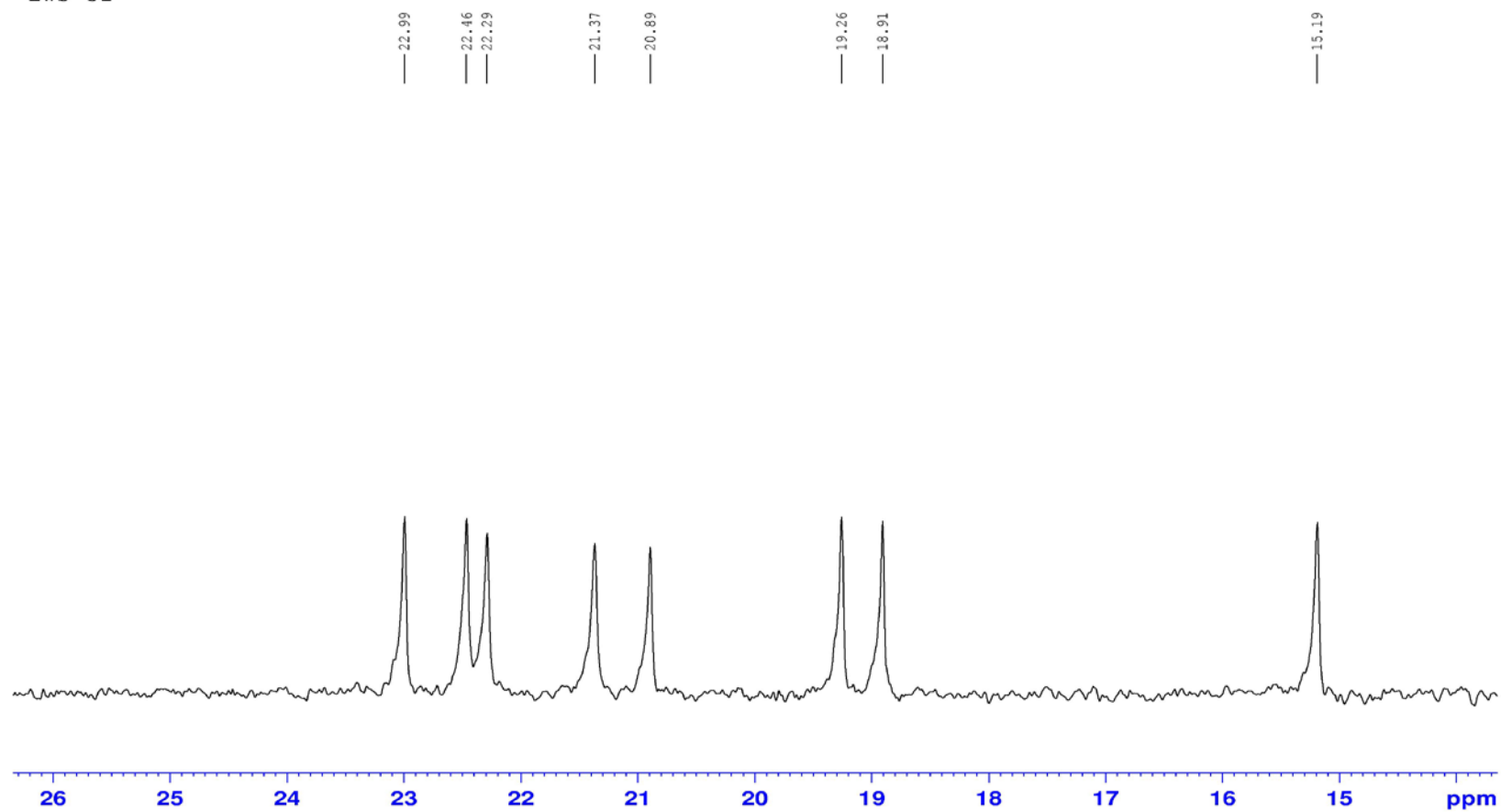


S151

^{13}C NMR (125 MHz) spectrum of Compound **12** in CDCl_3

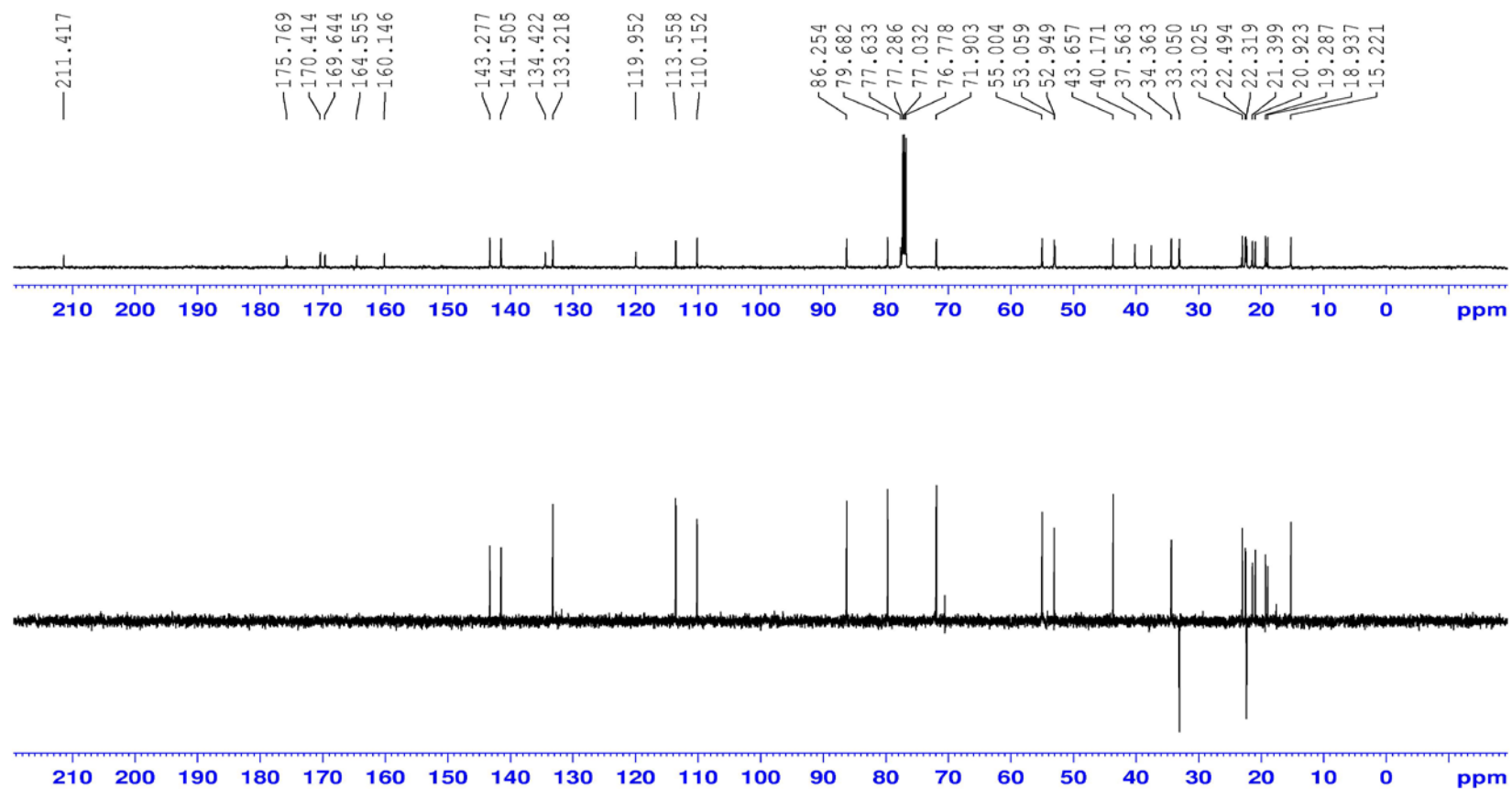


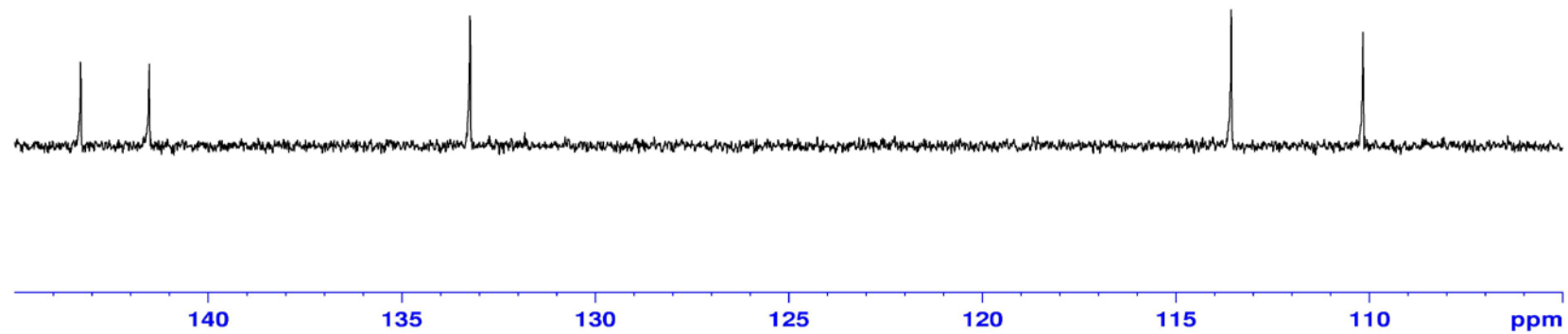
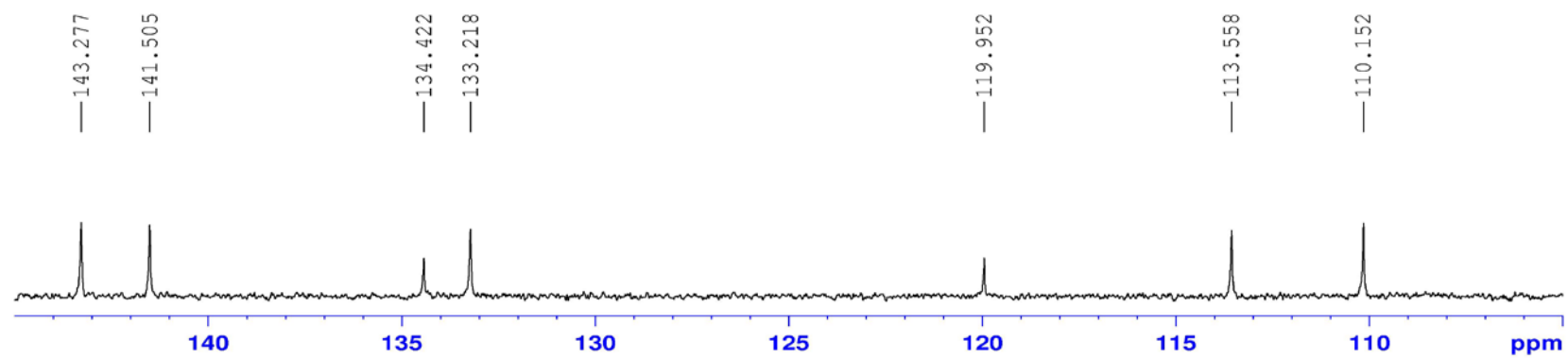
lws-32



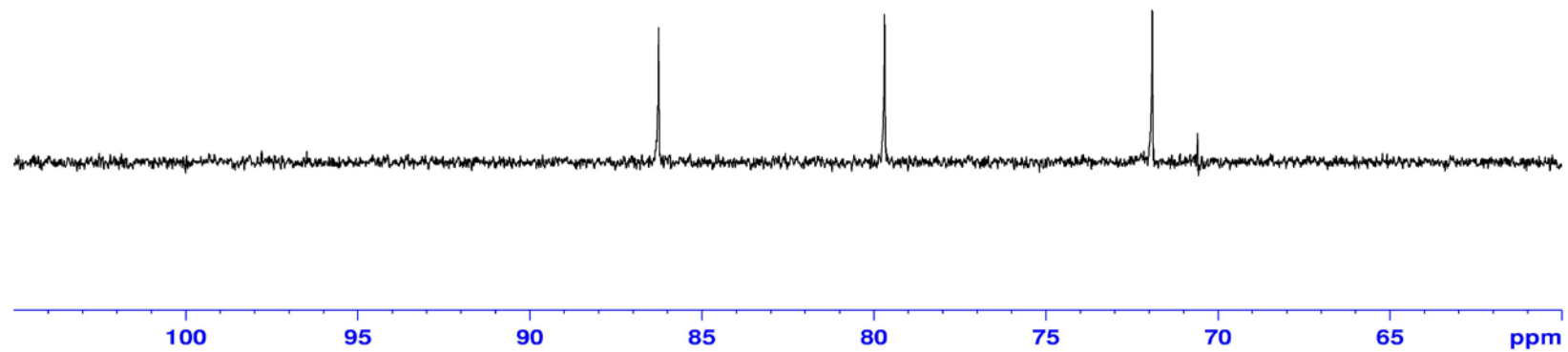
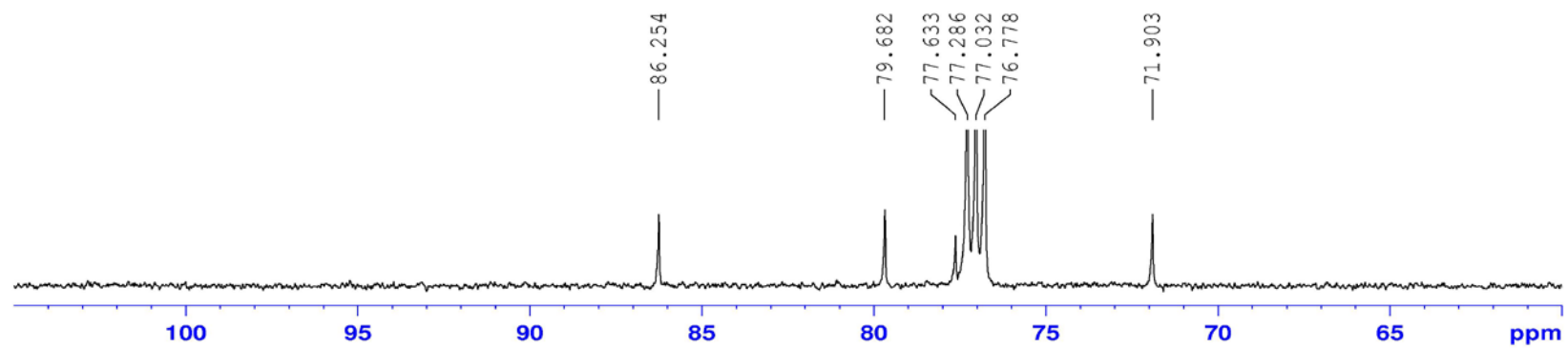
S153

DEPT135° (125 MHz) spectrum of Compound **12** in CDCl₃

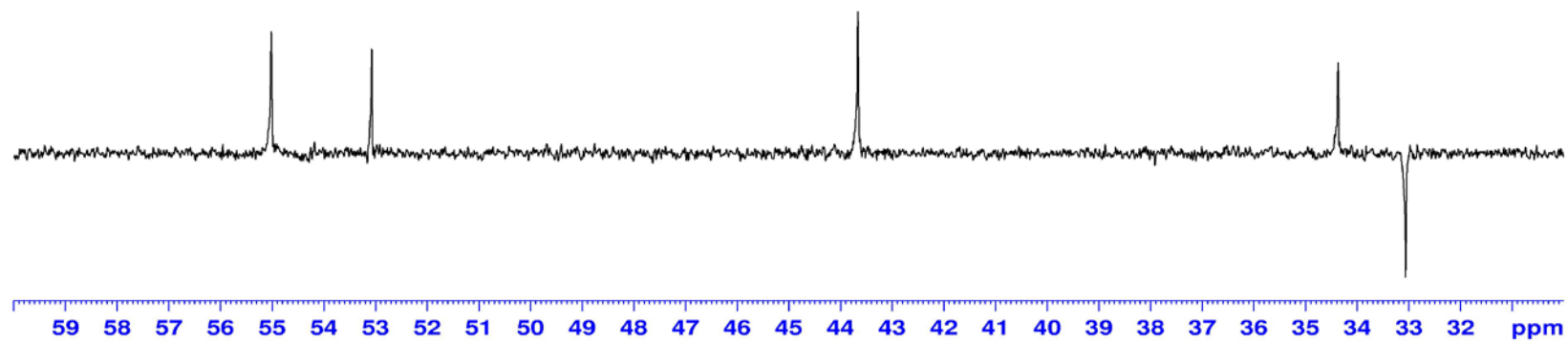
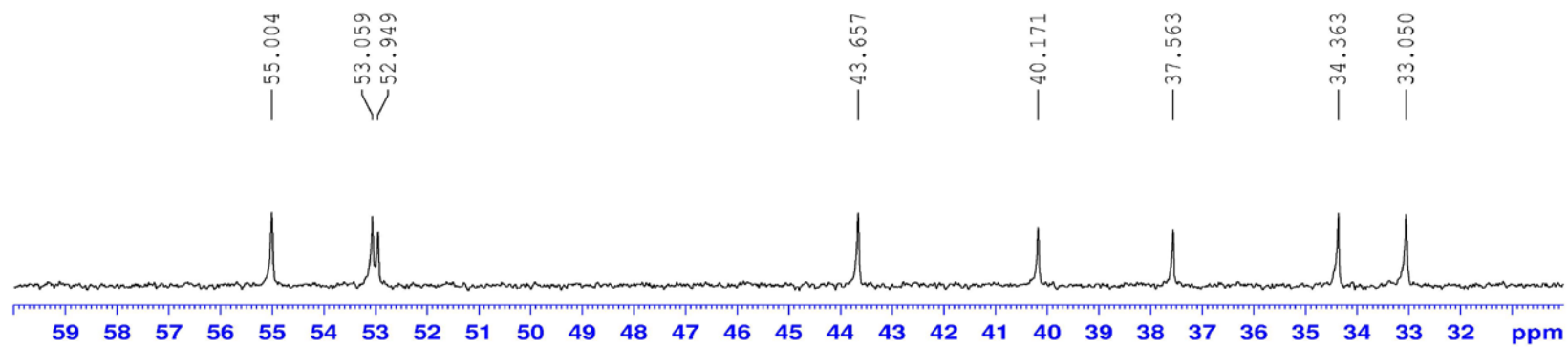


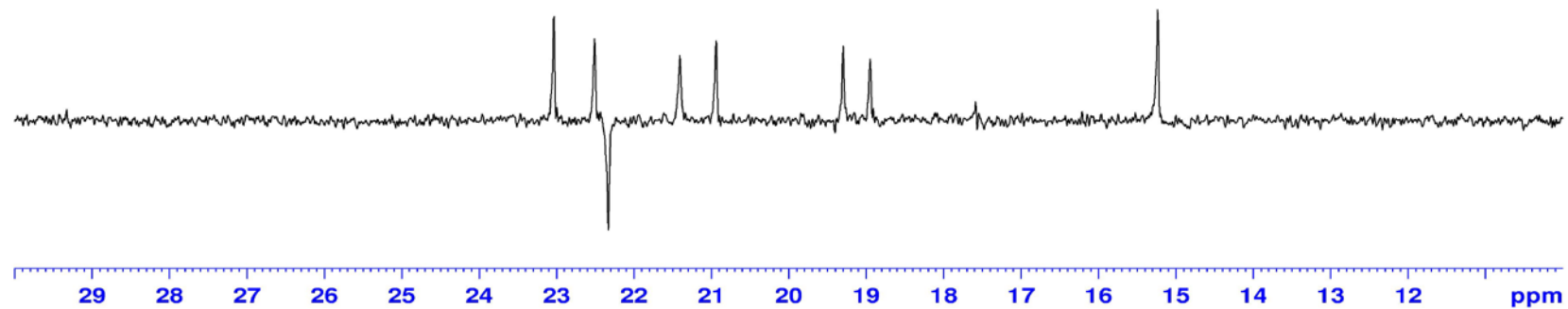
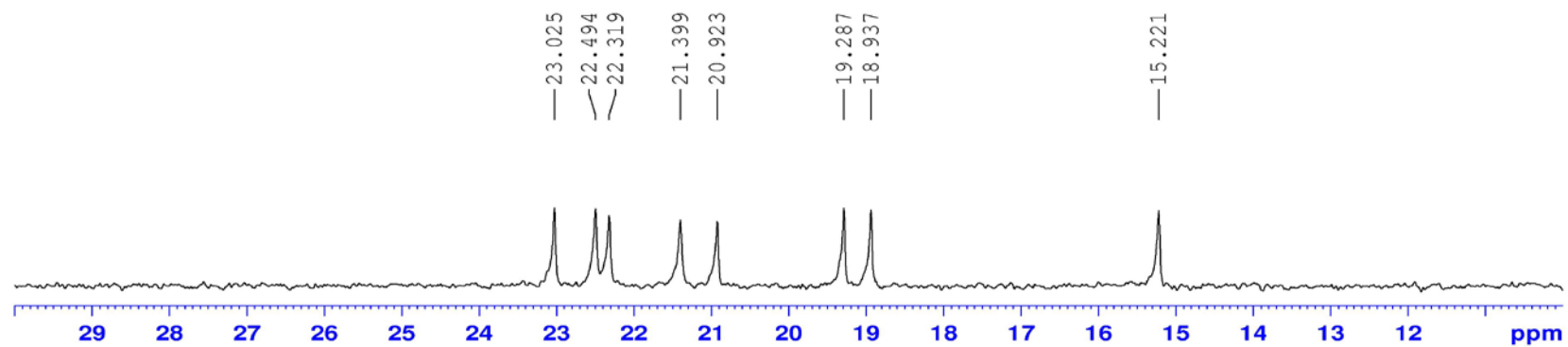


S155



S156

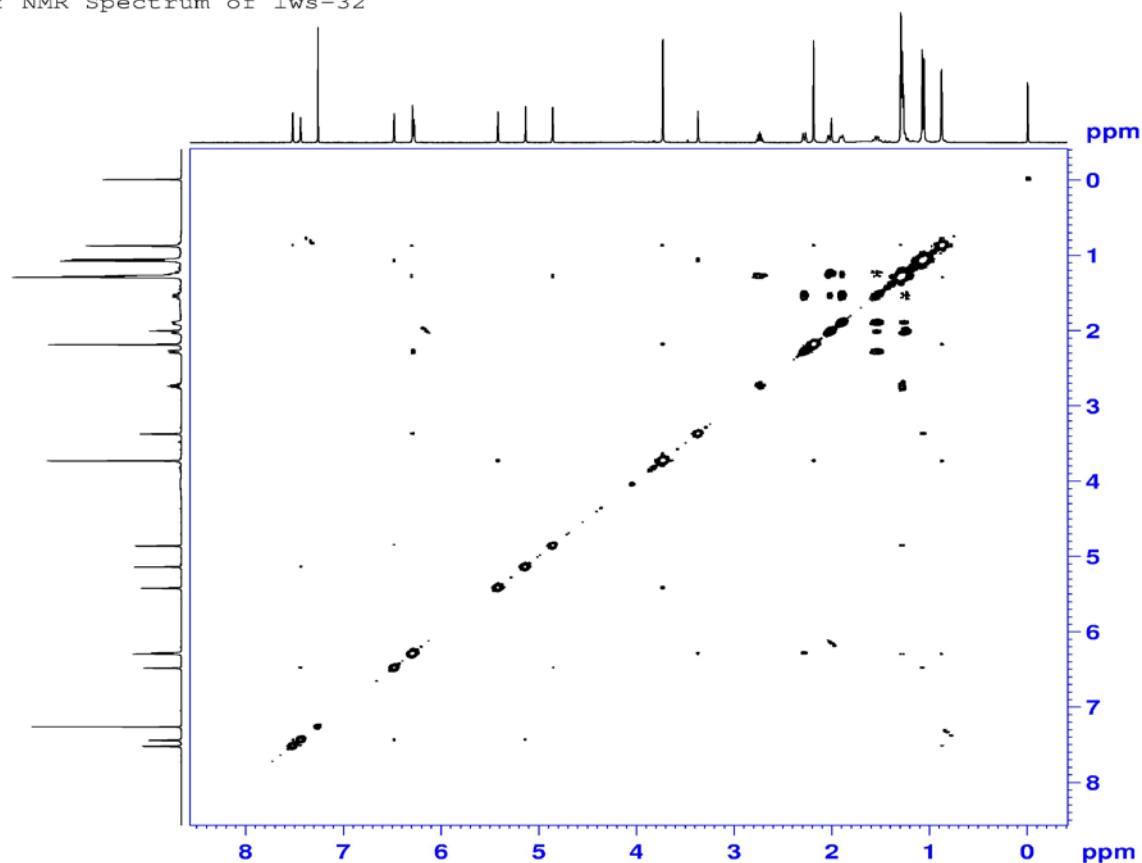




S158

^1H - ^1H COSY (500 MHz) spectrum of Compound **12** in CDCl_3

COSY NMR Spectrum of lws-32



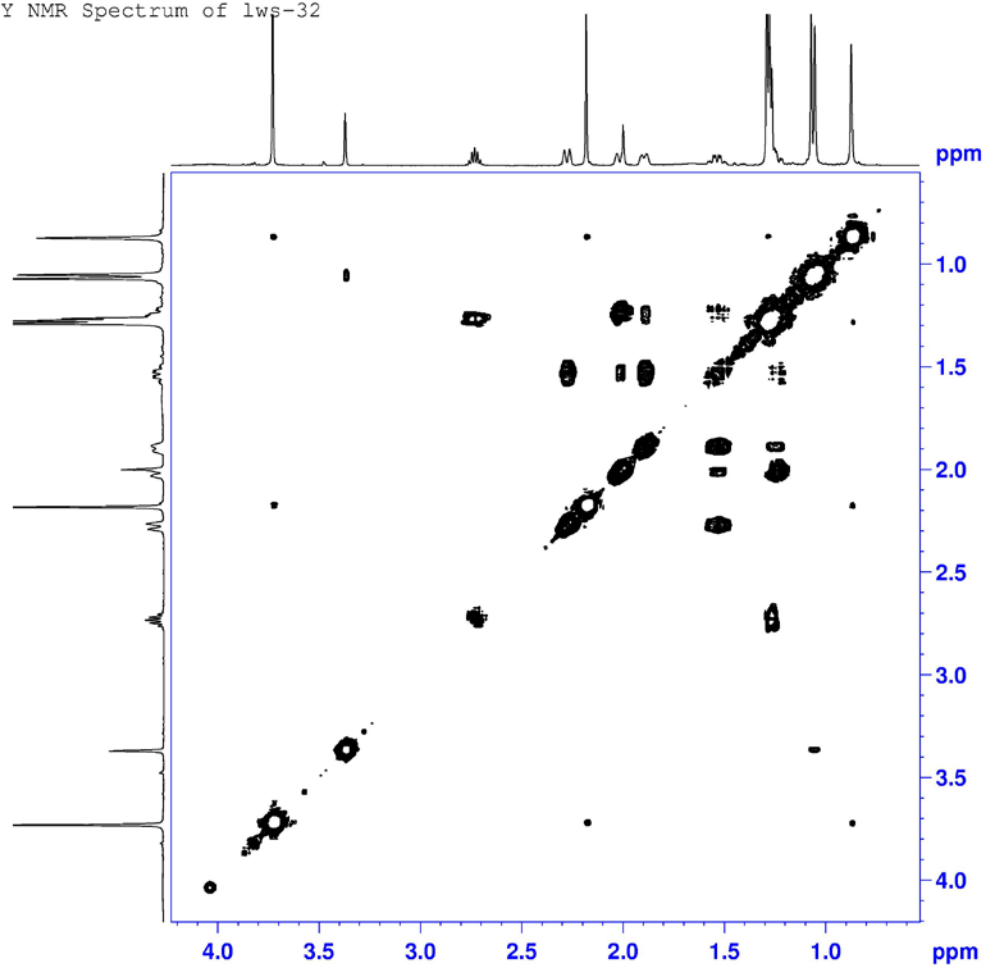
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NAME      liwanshan-lws-32
EXPNO     7
PROCNO    1
Date_     20140723
Time      1.49
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   cosygpgpf
TD        2048
SOLVENT   CDCl3
NS         8
DS         8
SWH       4496.403 Hz
FIDRES    2.195509 Hz
AQ        0.2278988 sec
RG         64
DW        111.200 usec
DE        6.50 usec
TE        299.0 K
D0        0.00000300 sec
D1        1.00000000 sec
D13       0.00000400 sec
D16       0.00020000 sec
IN0       0.00022240 sec

===== CHANNEL f1 =====
NUC1      1H
P0        16.50 usec
P1        16.50 usec
PL1       -1.00 dB
PL1W      13.91402149 W
SFO1      500.1320505 MHz

===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPZ1      10.00 %
P16       1000.00 usec
ND0       1
TD        128
SFO1      500.1321 MHz
FIDRES    35.128025 Hz
SW        8.990 ppm
FhMODE    QF
SI        1024
SF        500.1300131 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
PC        1.40
SI        1024
MC2       QF
SF        500.1300131 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
    
```

COSY NMR Spectrum of lws-32

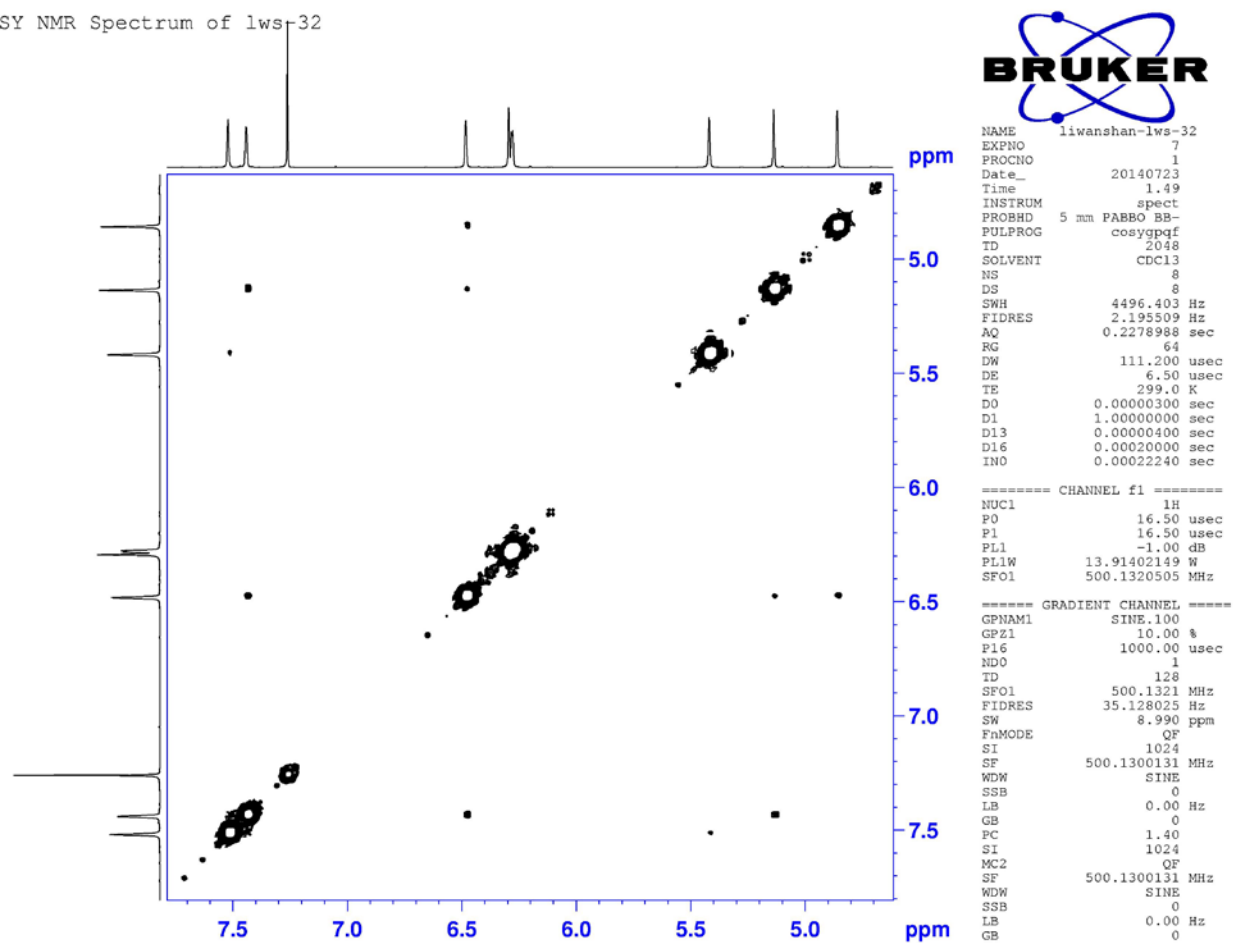


NAME liwanshan-lws-32
 EXPNO 7
 PROCNO 1
 Date_ 20140723
 Time 1.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG cosygpgf
 TD 2048
 SOLVENT CDCl3
 NS 8
 DS 8
 SWH 4496.403 Hz
 FIDRES 2.195509 Hz
 AQ 0.2278988 sec
 RG 64
 DW 111.200 usec
 DE 6.50 usec
 TE 299.0 K
 D0 0.00000300 sec
 D1 1.00000000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00022240 sec

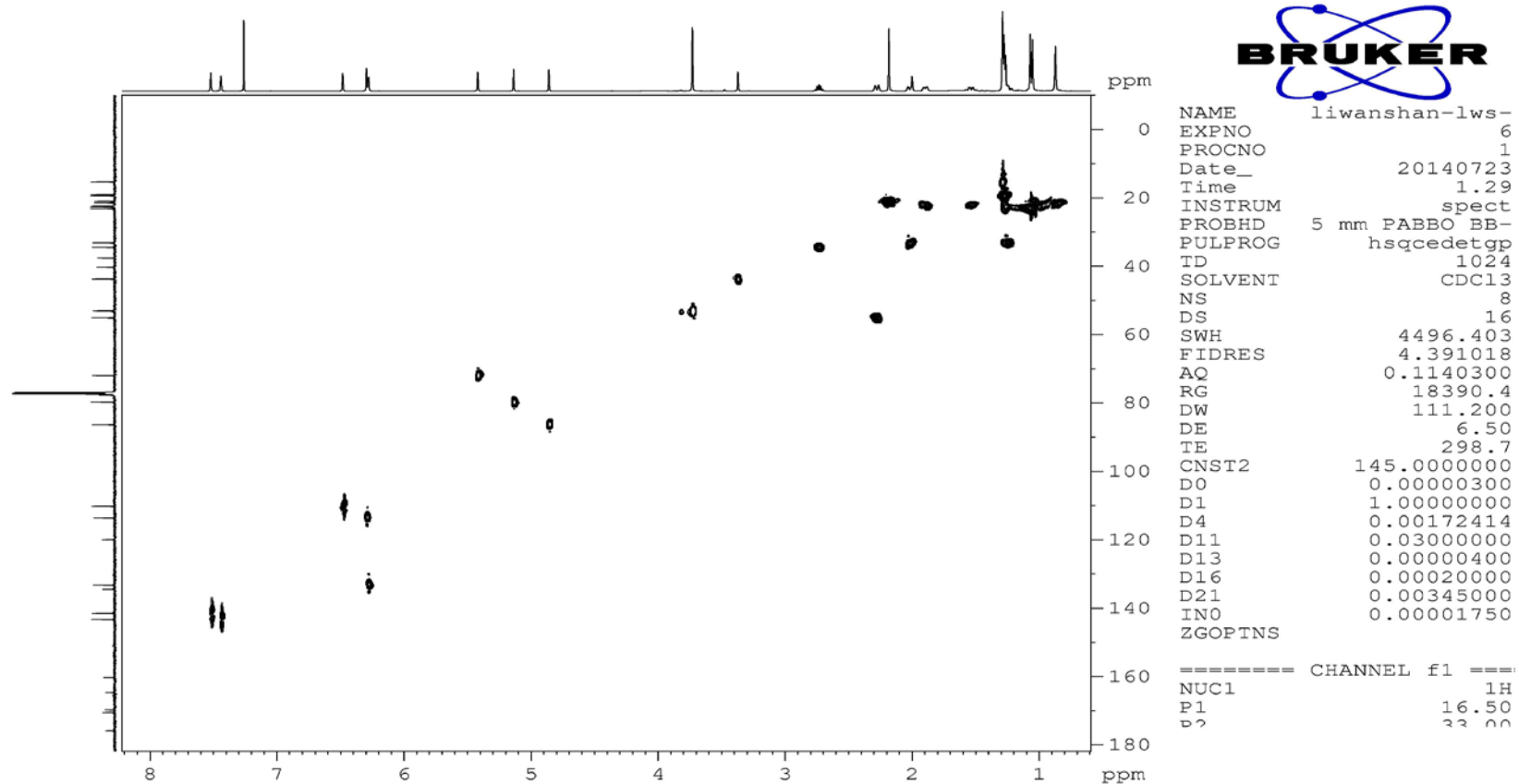
===== CHANNEL f1 =====
 NUC1 1H
 P0 16.50 usec
 P1 16.50 usec
 PL1 -1.00 dB
 PL1W 13.91402149 W
 SFO1 500.1320505 MHz

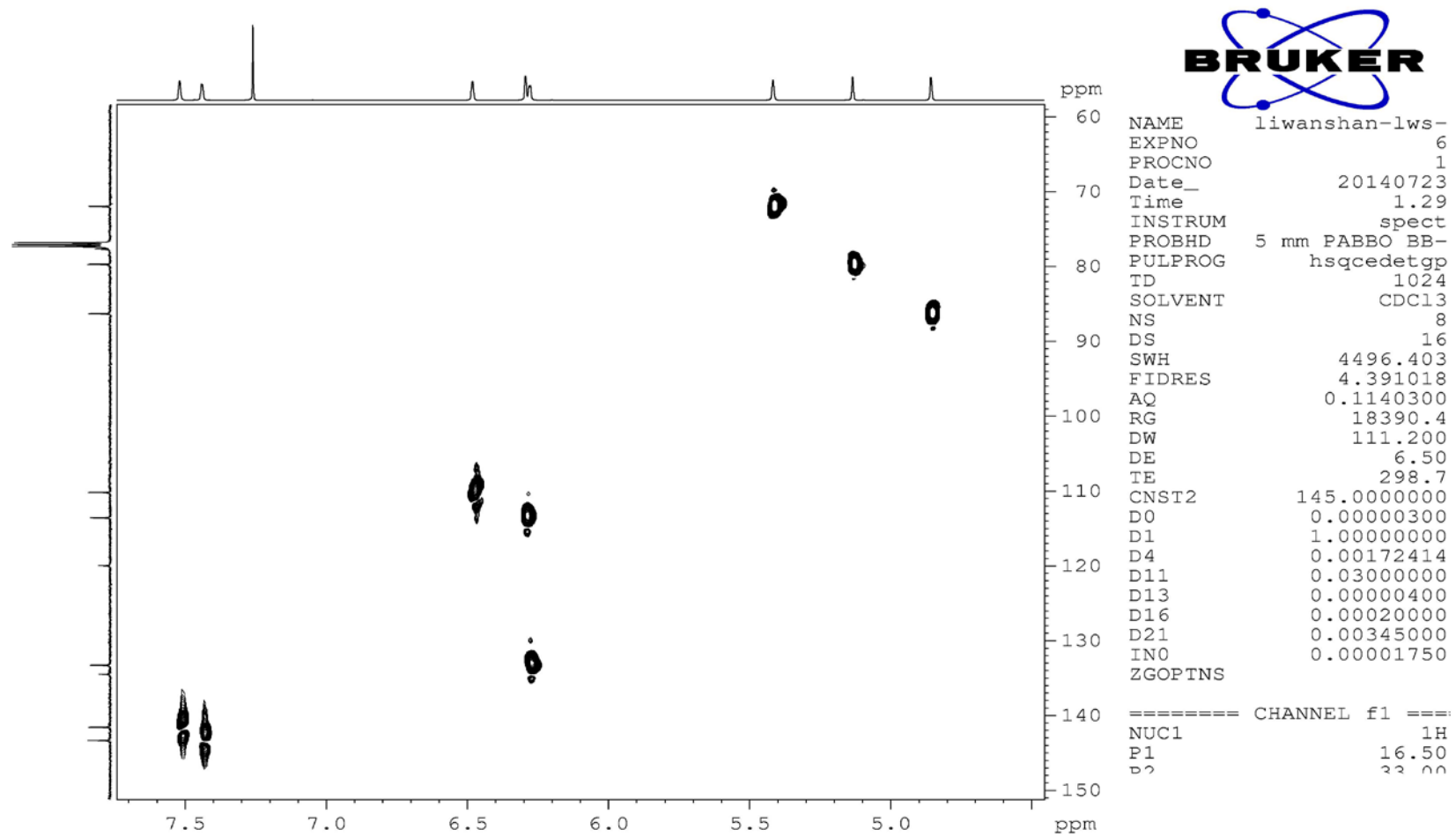
===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPZ1 10.00 %
 P16 1000.00 usec
 ND0 1
 TD 128
 SFO1 500.1321 MHz
 FIDRES 35.128025 Hz
 SW 8.990 ppm
 FnmODE QF
 SI 1024
 SF 500.1300131 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 QF
 SF 500.1300131 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

COSY NMR Spectrum of lws-32

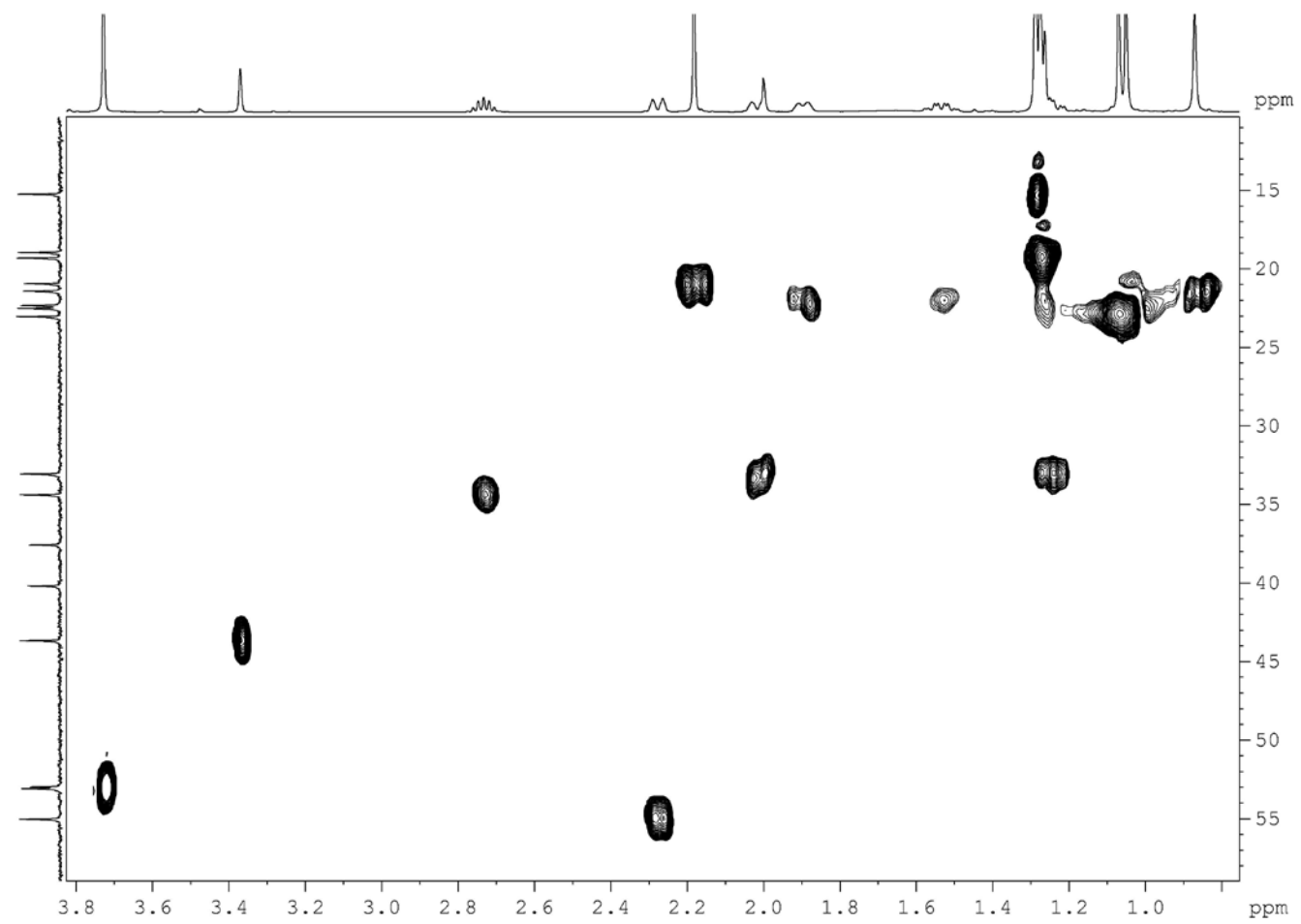


HSQC (500 MHz) spectrum of Compound **12** in CDCl₃





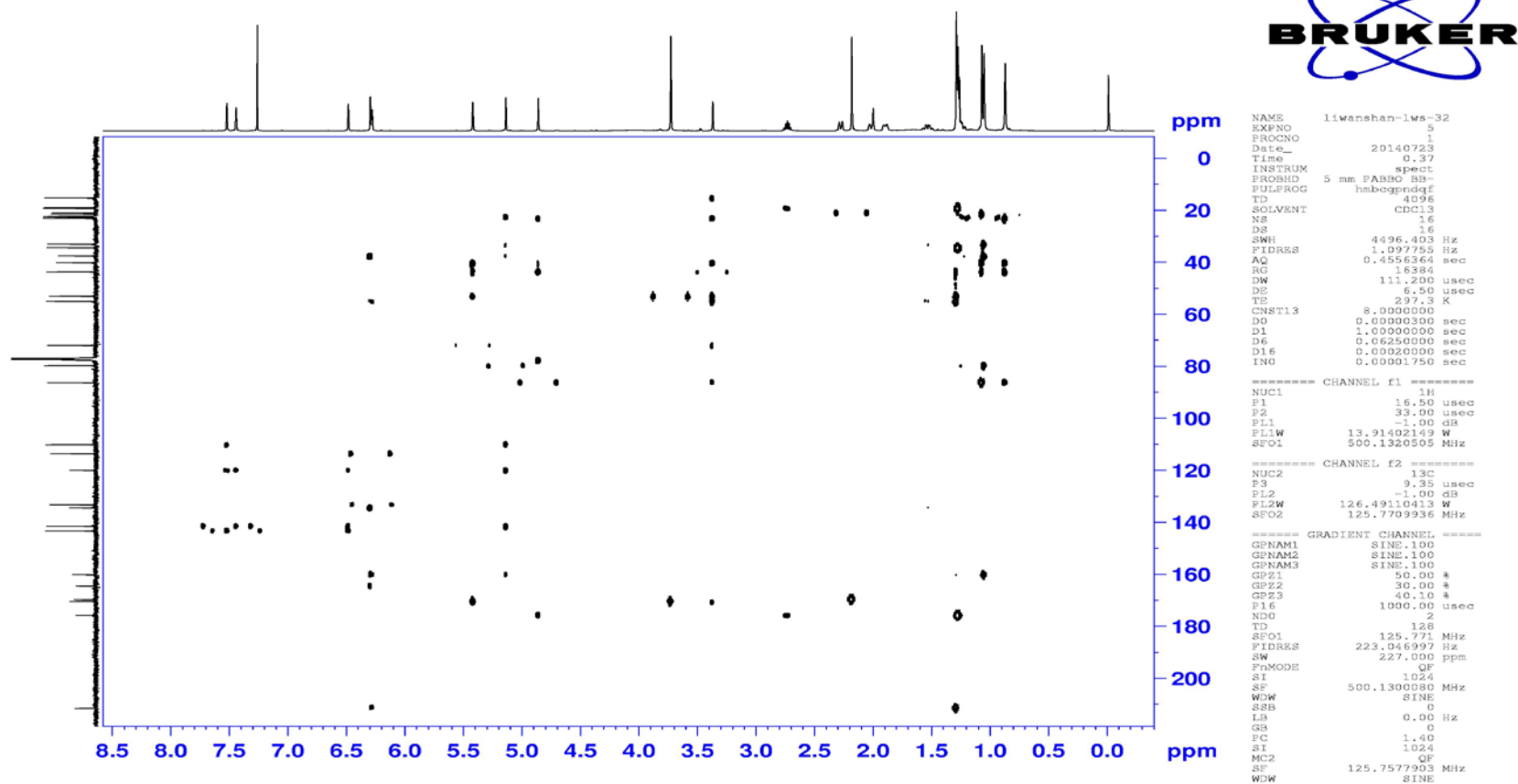
S163



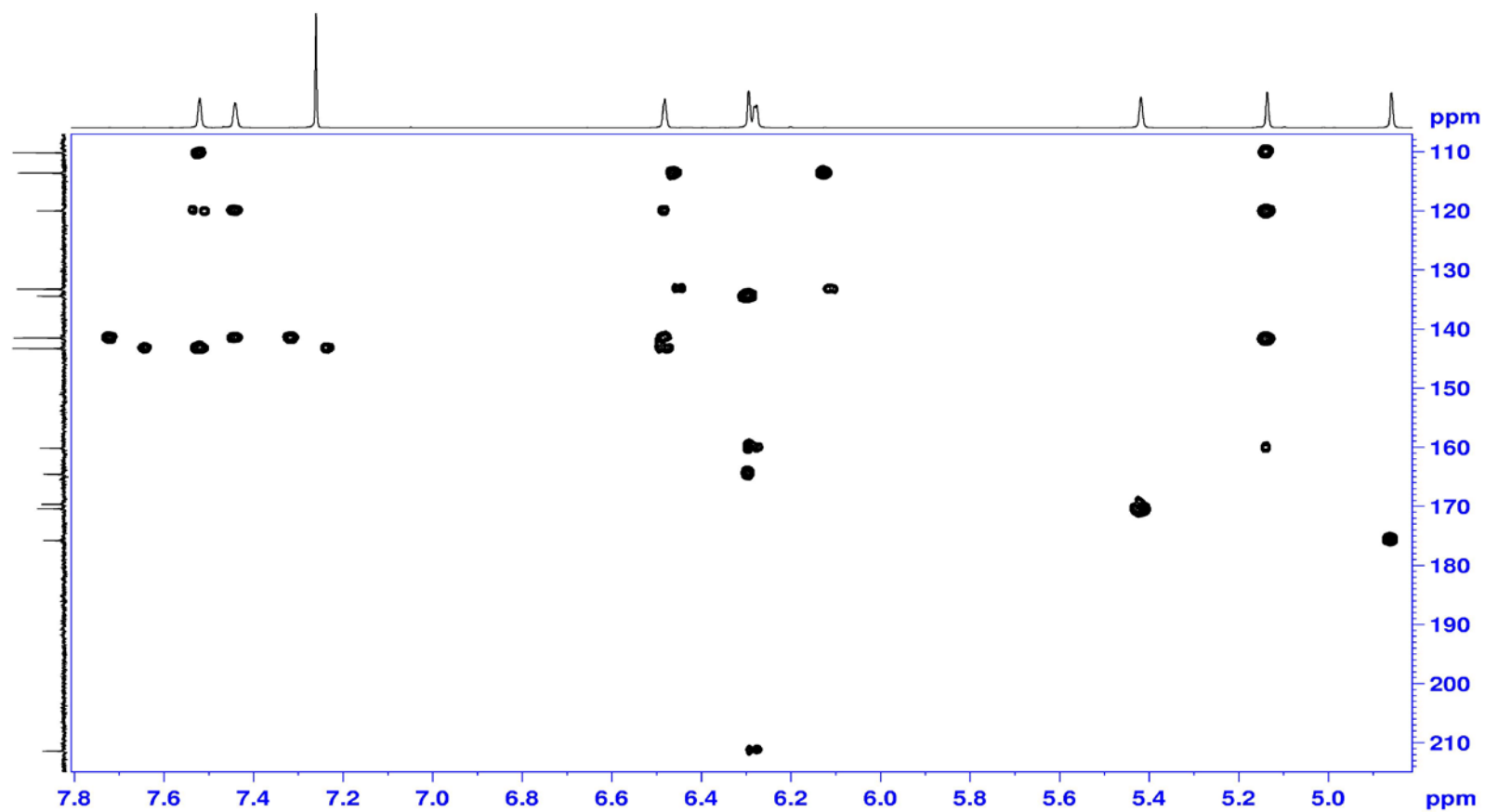
S164

HMBC (500 MHz) spectrum of Compound **12** in CDCl₃

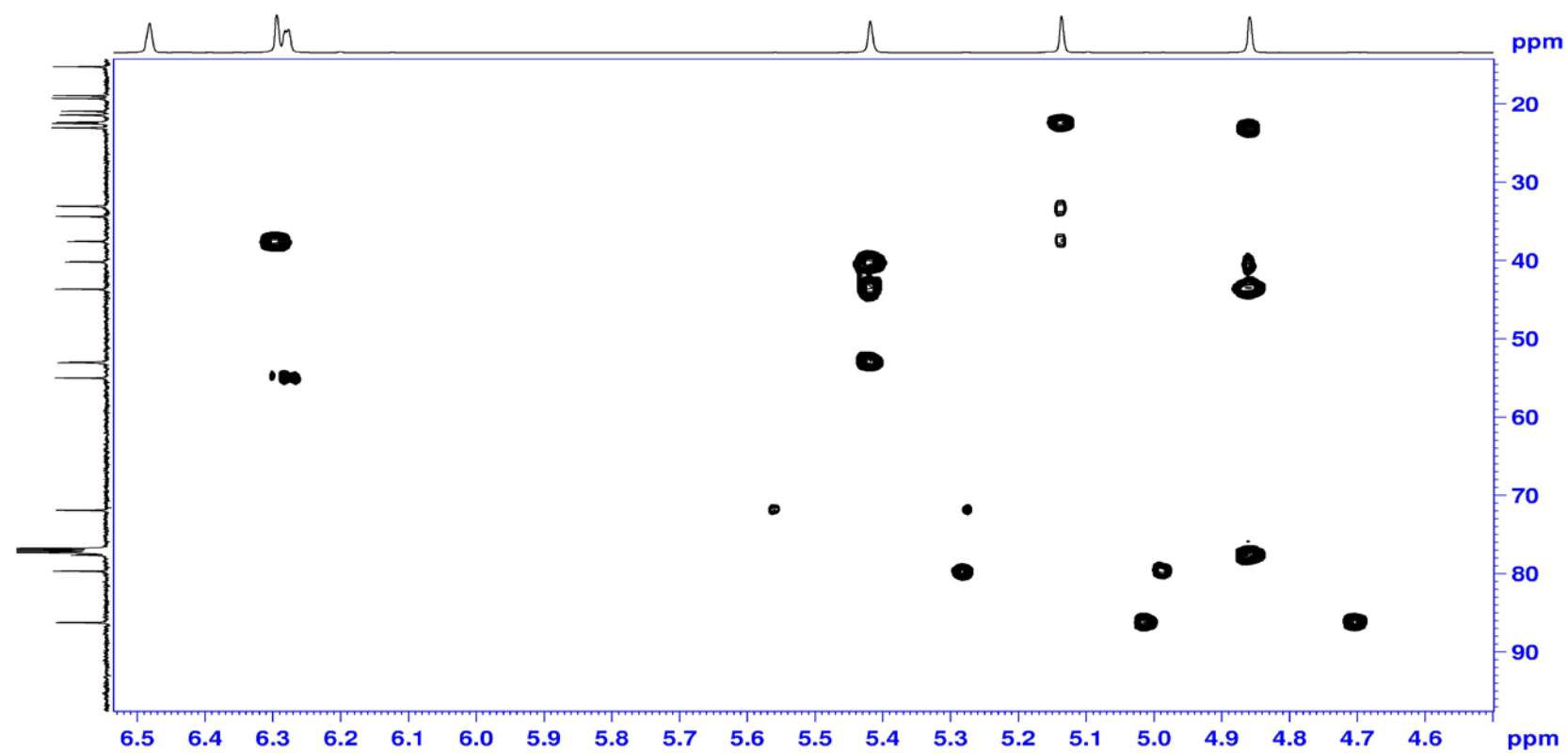
HMBC NMR Spectrum of lws-32



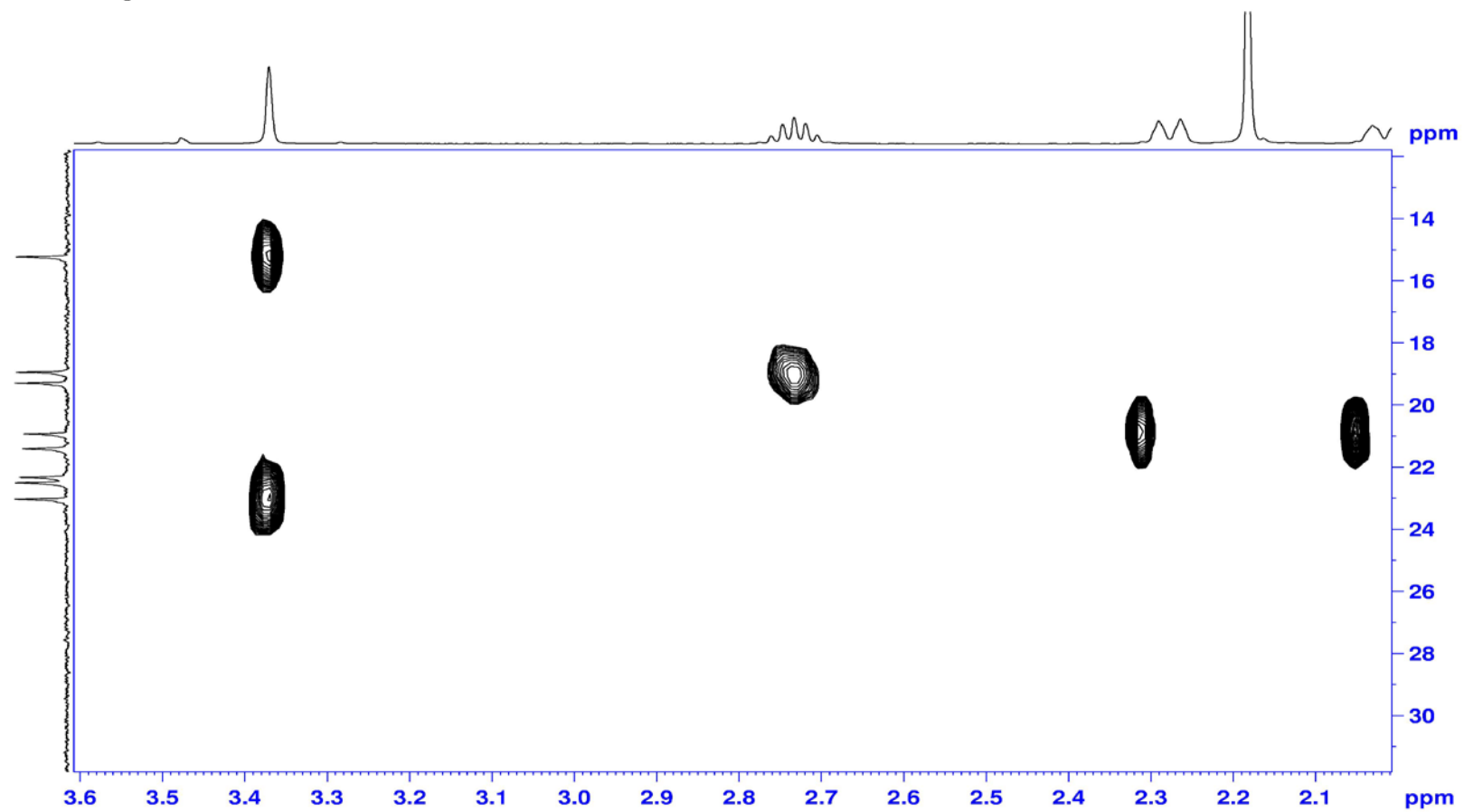
HMBC NMR Spectrum of lws-32



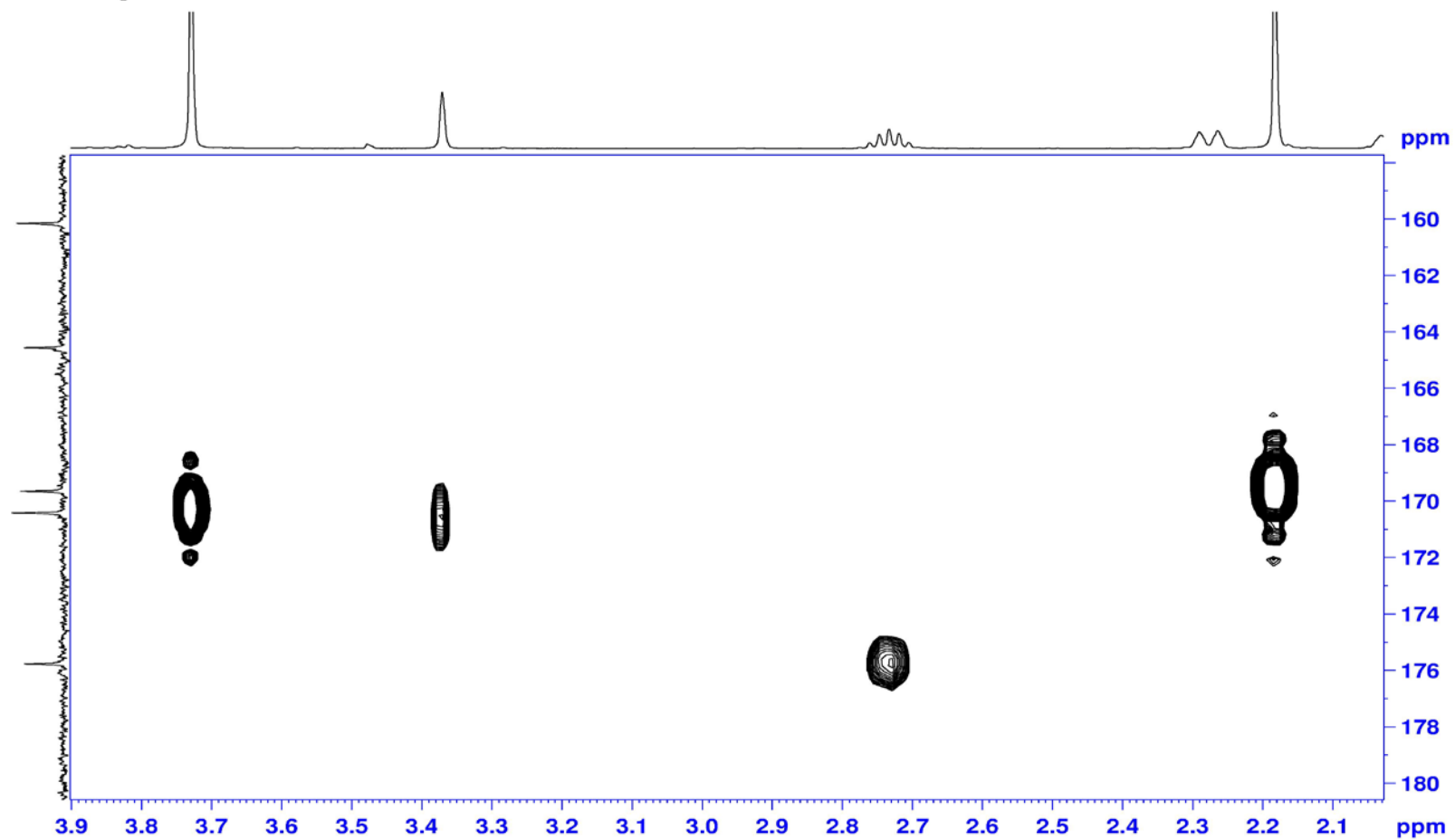
HMBC NMR Spectrum of lws-32



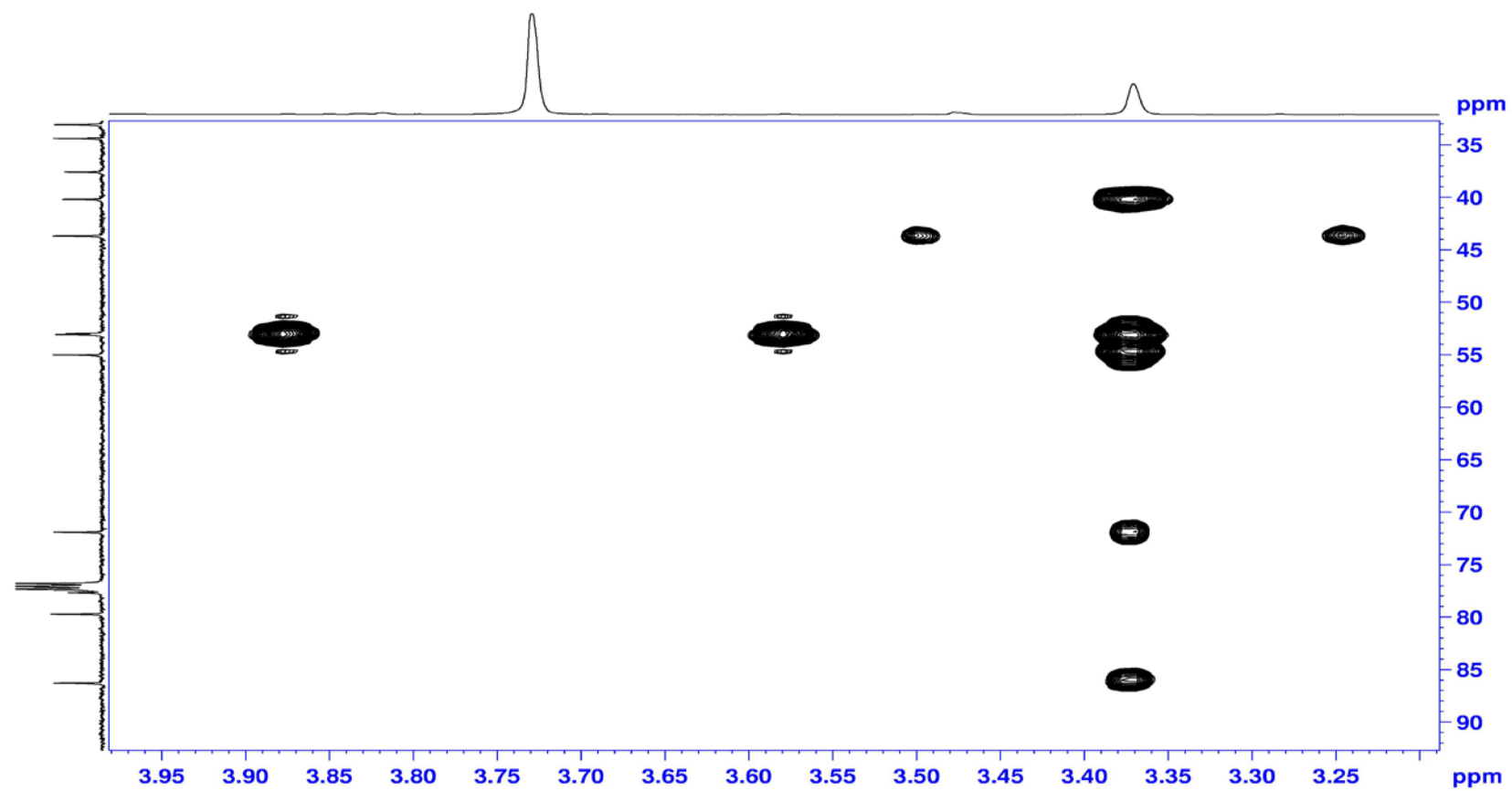
HMBC NMR Spectrum of lws-32



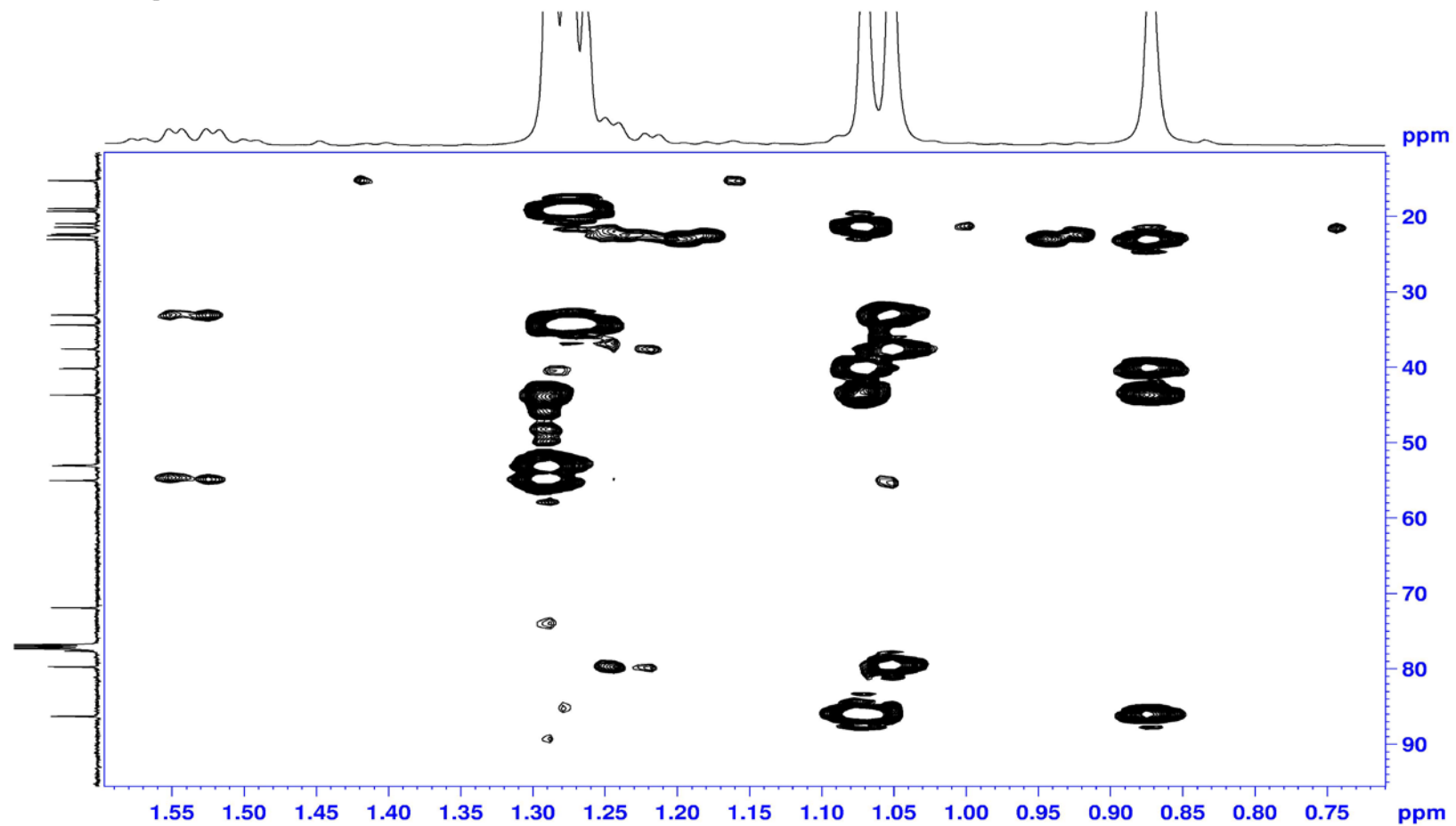
HMBC NMR Spectrum of lws-32



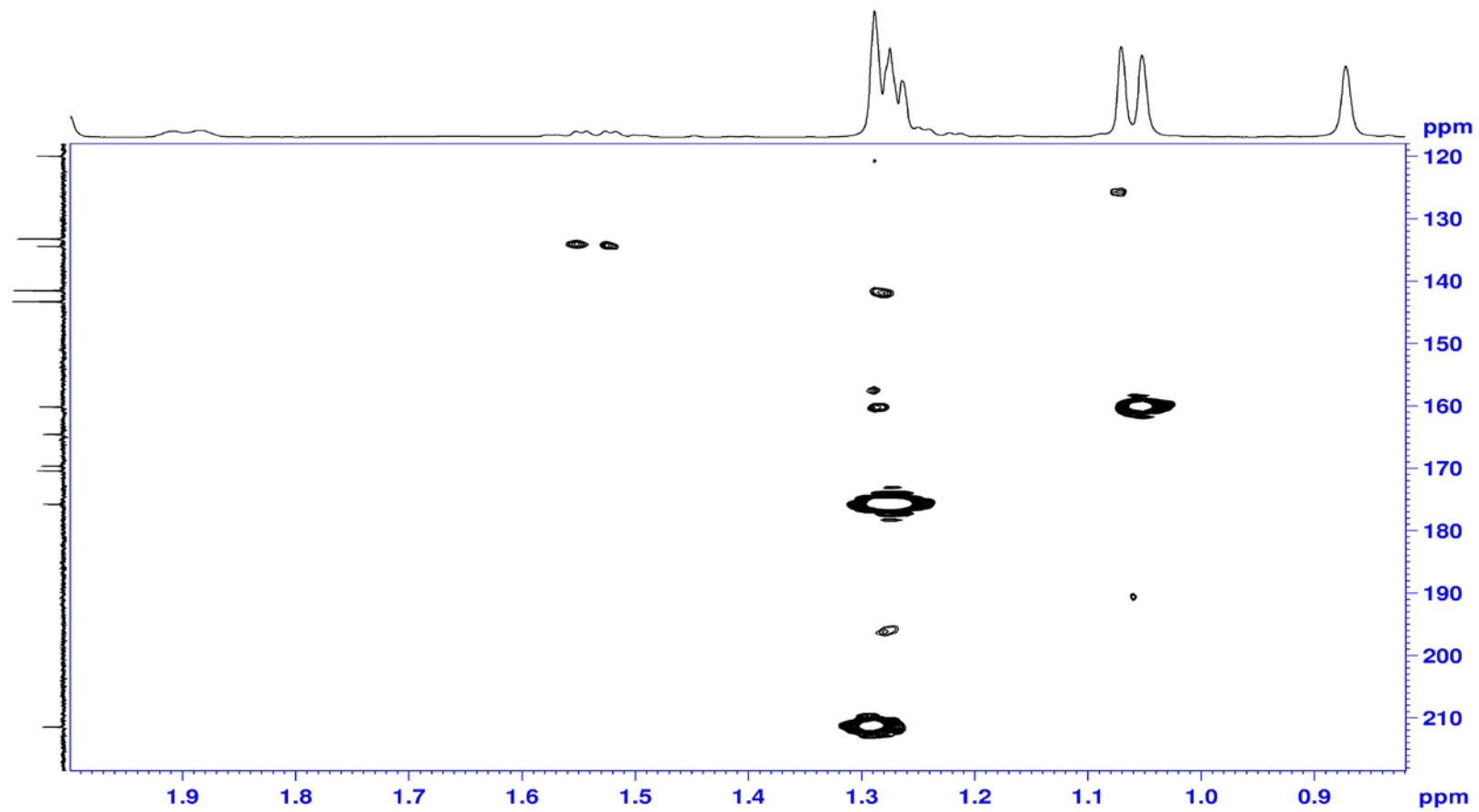
HMBC NMR Spectrum of lws-32



HMBC NMR Spectrum of lws-32

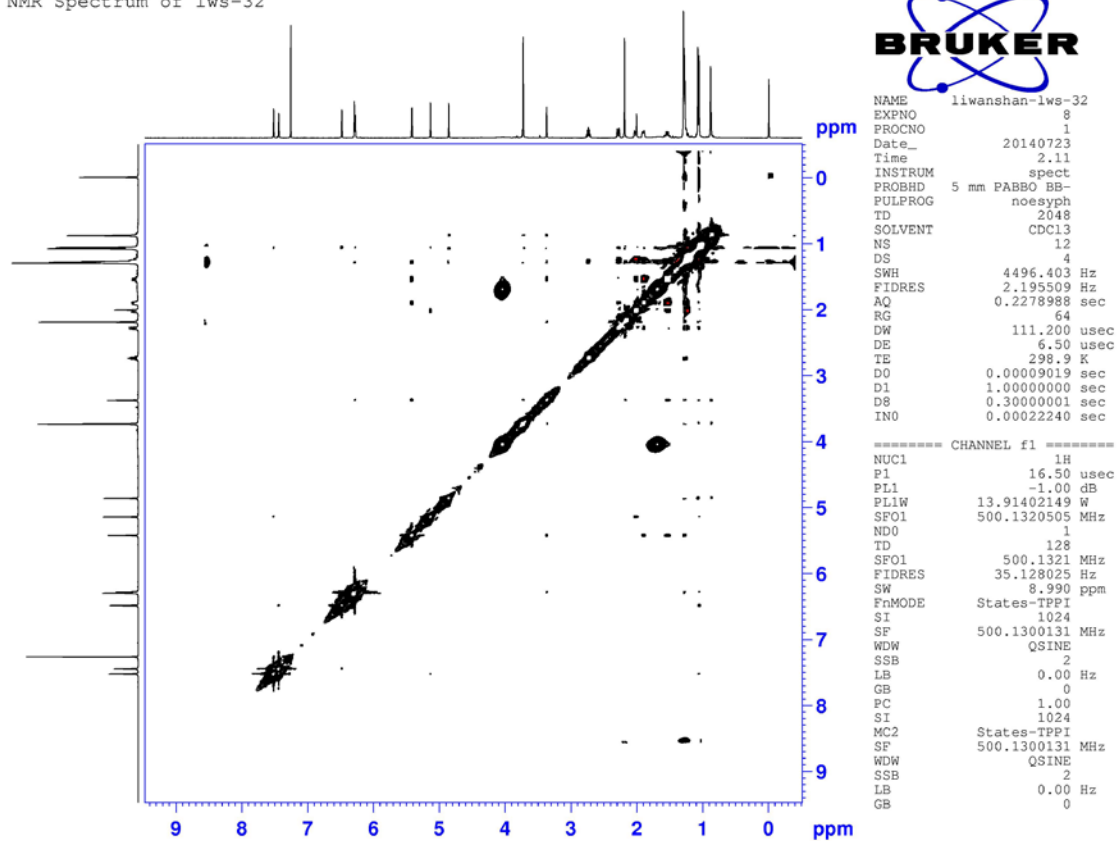


HMBC NMR Spectrum of lws-32

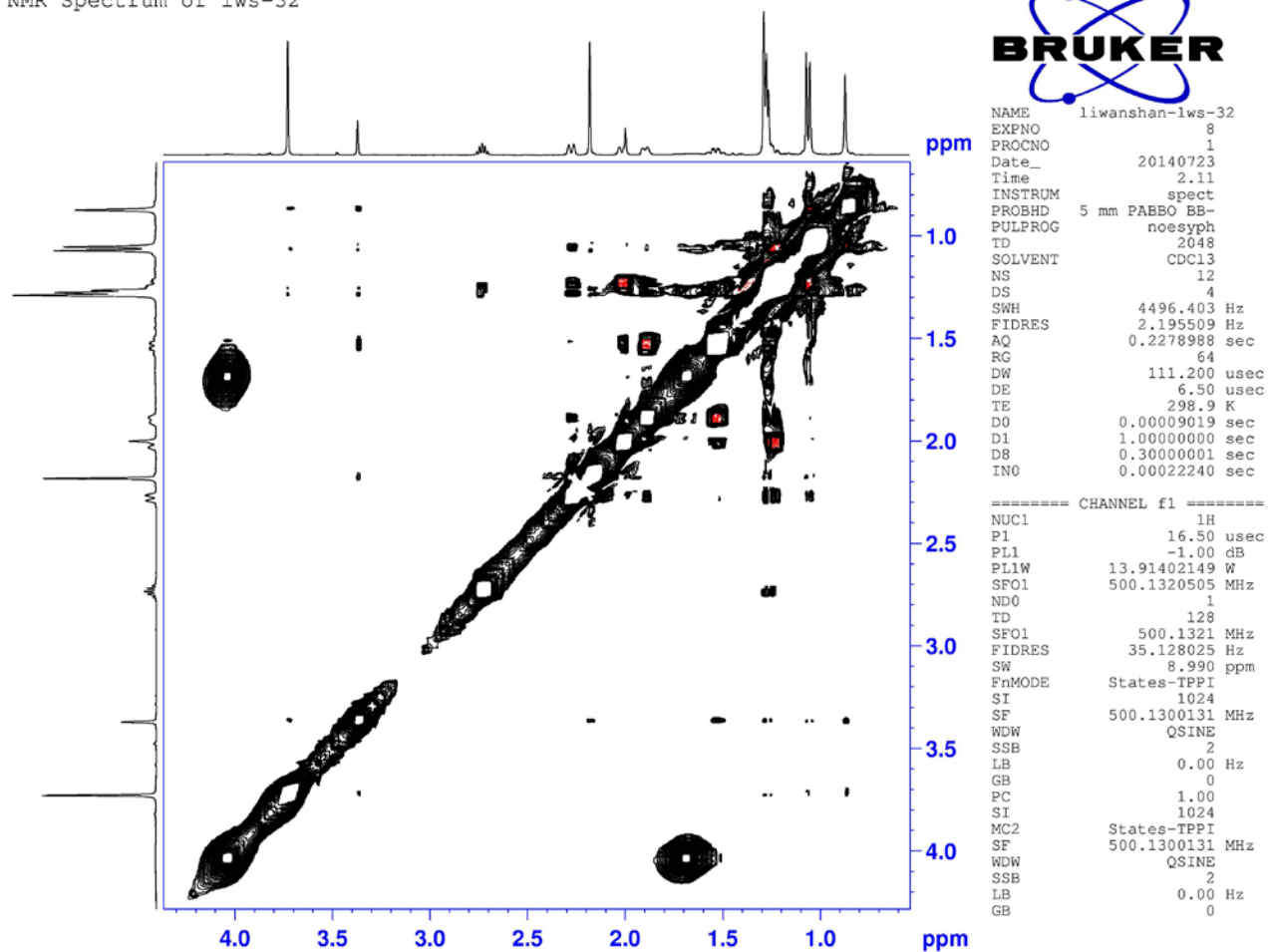


NOESY (500 MHz) spectrum of Compound **12** in CDCl₃

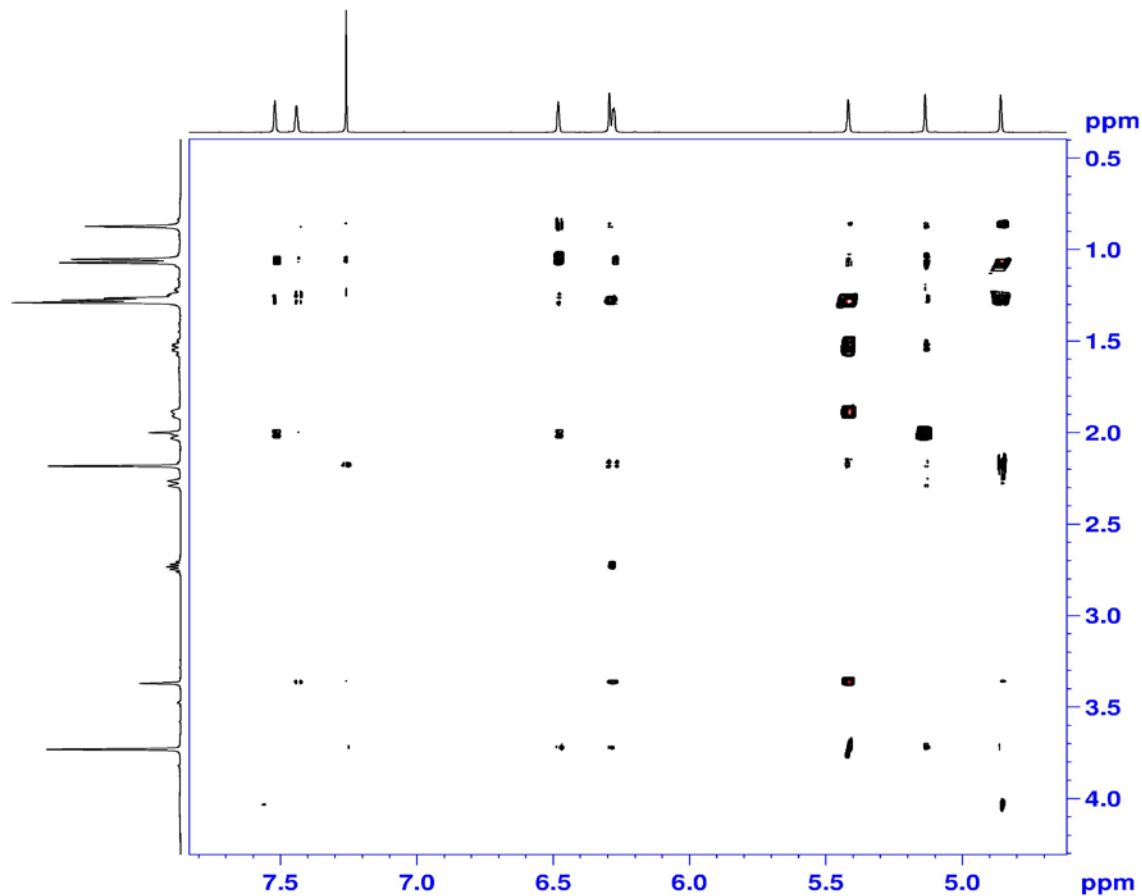
NOE NMR Spectrum of lws-32



NOE NMR Spectrum of lws-32



NOE NMR Spectrum of lws-32



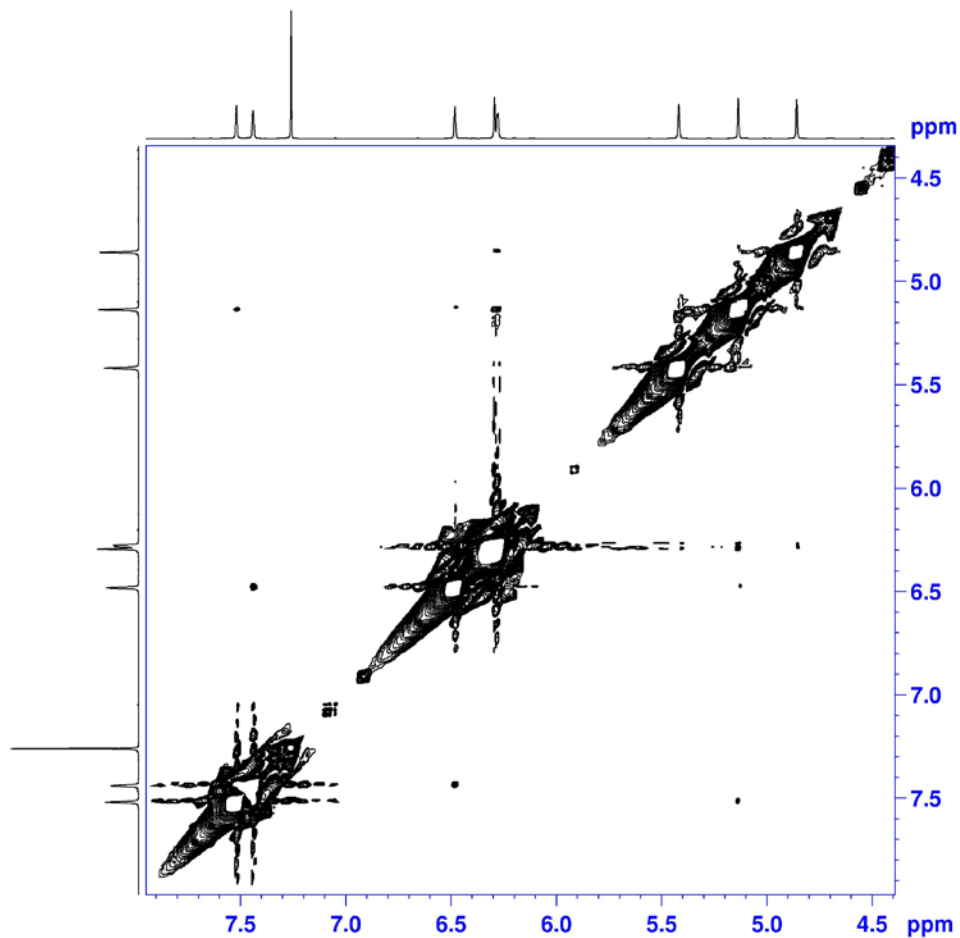
```

NAME      liwanshan-lws-32
EXPNO     8
PROCNO    1
Date_     20140723
Time      2.11
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   noesyph
TD        2048
SOLVENT   CDCl3
NS        12
DS        4
SWH       4496.403 Hz
FIDRES    2.195509 Hz
AQ        0.2278988 sec
RG        64
DW        111.200 usec
DE        6.50 usec
TE        298.9 K
D0        0.00009019 sec
D1        1.00000000 sec
D8        0.30000001 sec
IN0       0.00022240 sec
    
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        16.50 usec
PL1       -1.00 dB
PL1W      13.91402149 W
SF01      500.1320505 MHz
ND0       1
TD        128
SF01      500.1321 MHz
FIDRES    35.128025 Hz
SW        8.990 ppm
FnMODE    States-TPPI
SI        1024
SF        500.1300131 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
PC        1.00
SI        1024
MC2       States-TPPI
SF        500.1300131 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
    
```

NOE NMR Spectrum of lws-32



```

NAME      liwanshan-lws-32
EXPNO     8
PROCNO    1
Date_     20140723
Time      2.11
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   noesyph
TD        2048
SOLVENT   CDCl3
NS        12
DS        4
SWH       4496.403 Hz
FIDRES    2.195509 Hz
AQ        0.2278988 sec
RG        64
DW        111.200 usec
DE        6.50 usec
TE        298.9 K
D0        0.00009019 sec
D1        1.00000000 sec
D8        0.30000001 sec
IN0       0.00022240 sec
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        16.50 usec
PL1       -1.00 dB
PL1W      13.91402149 W
SF01      500.1320505 MHz
ND0       1
TD        128
SF01      500.1321 MHz
FIDRES    35.128025 Hz
SW        8.990 ppm
FnMODE    States-TPPI
SI        1024
SF        500.1300131 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
PC        1.00
SI        1024
MC2       States-TPPI
SF        500.1300131 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
  
```