

Electronic Supplementary Information

Neogenkwanines A–H: Daphnane-Type Diterpenes Containing 4,7 or 4,6- Ether Group from the Flower Bud of *Daphne genkwa*

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1:HRESIMS spectrum of compound 1

 Compound Mass Spectrum List Report

Analysis Info

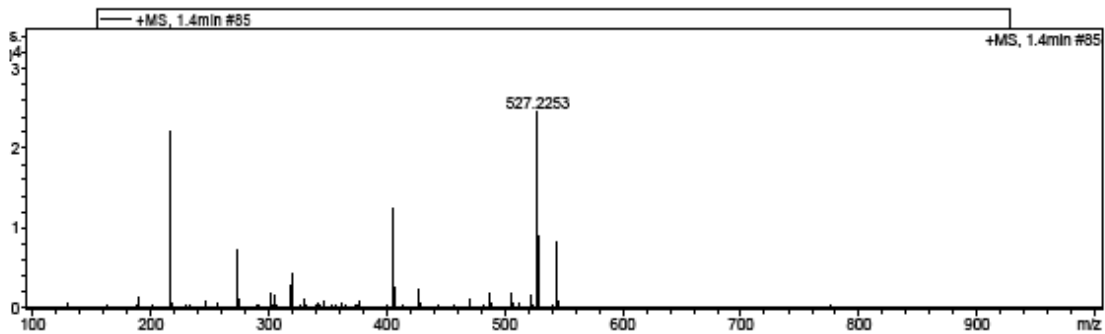
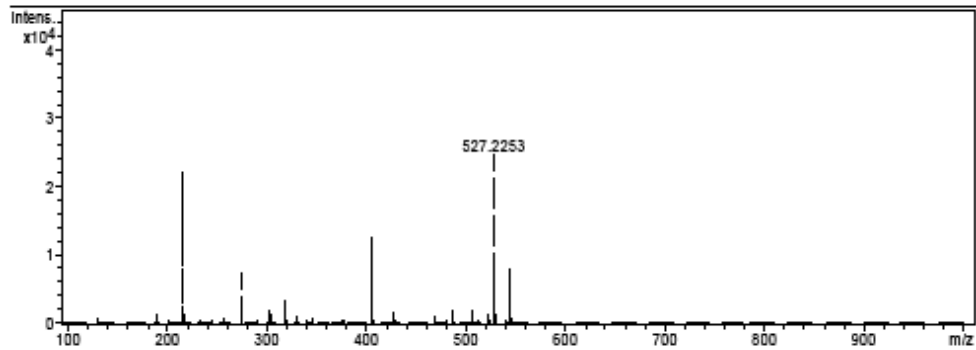
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 Comment

Acquisition Date 2009-7-7 17:58:38

Operator Bruker Customer
 Instrument / Ser# micrOTOF-Q 125

Acquisition Parameter

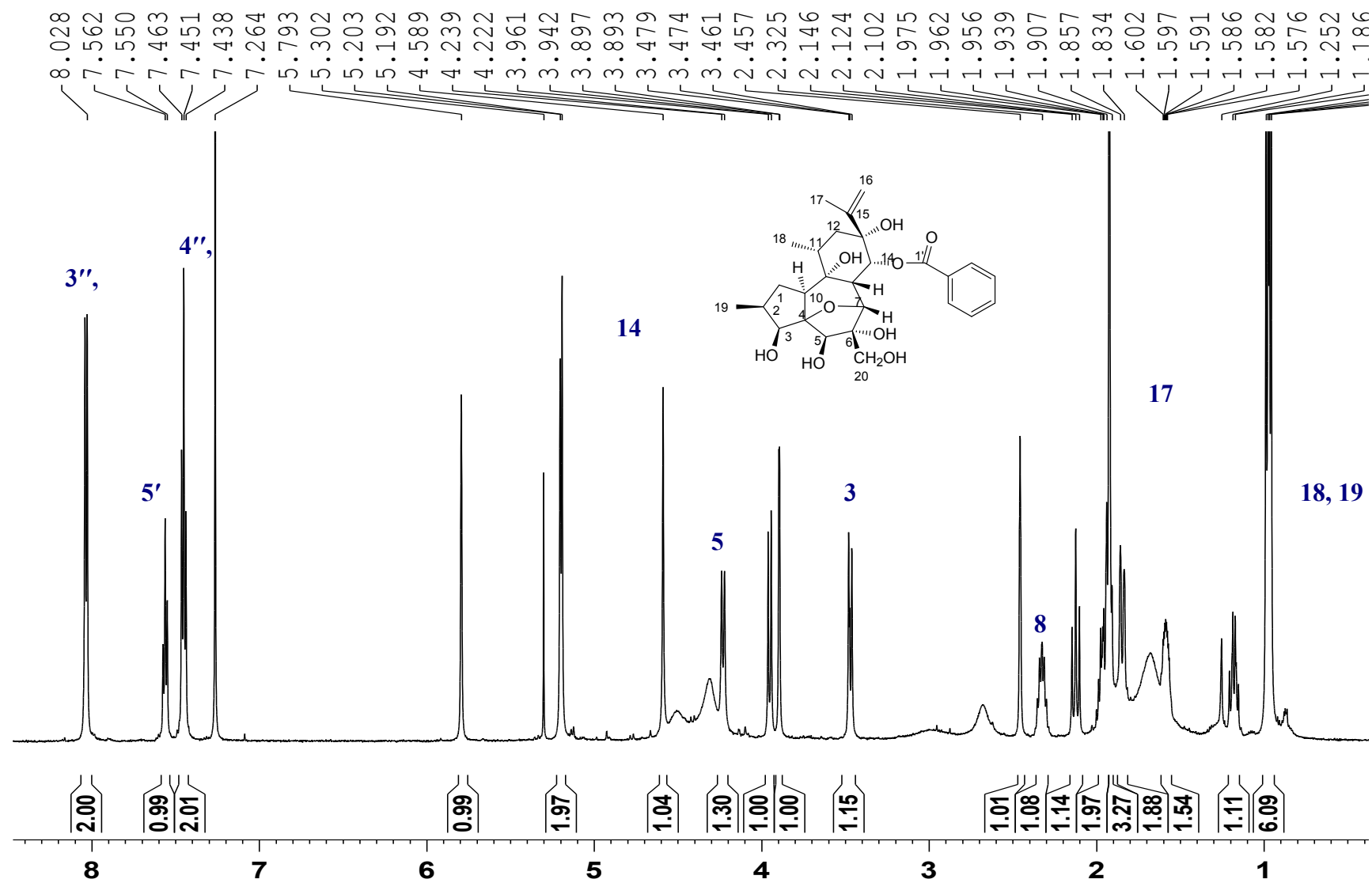
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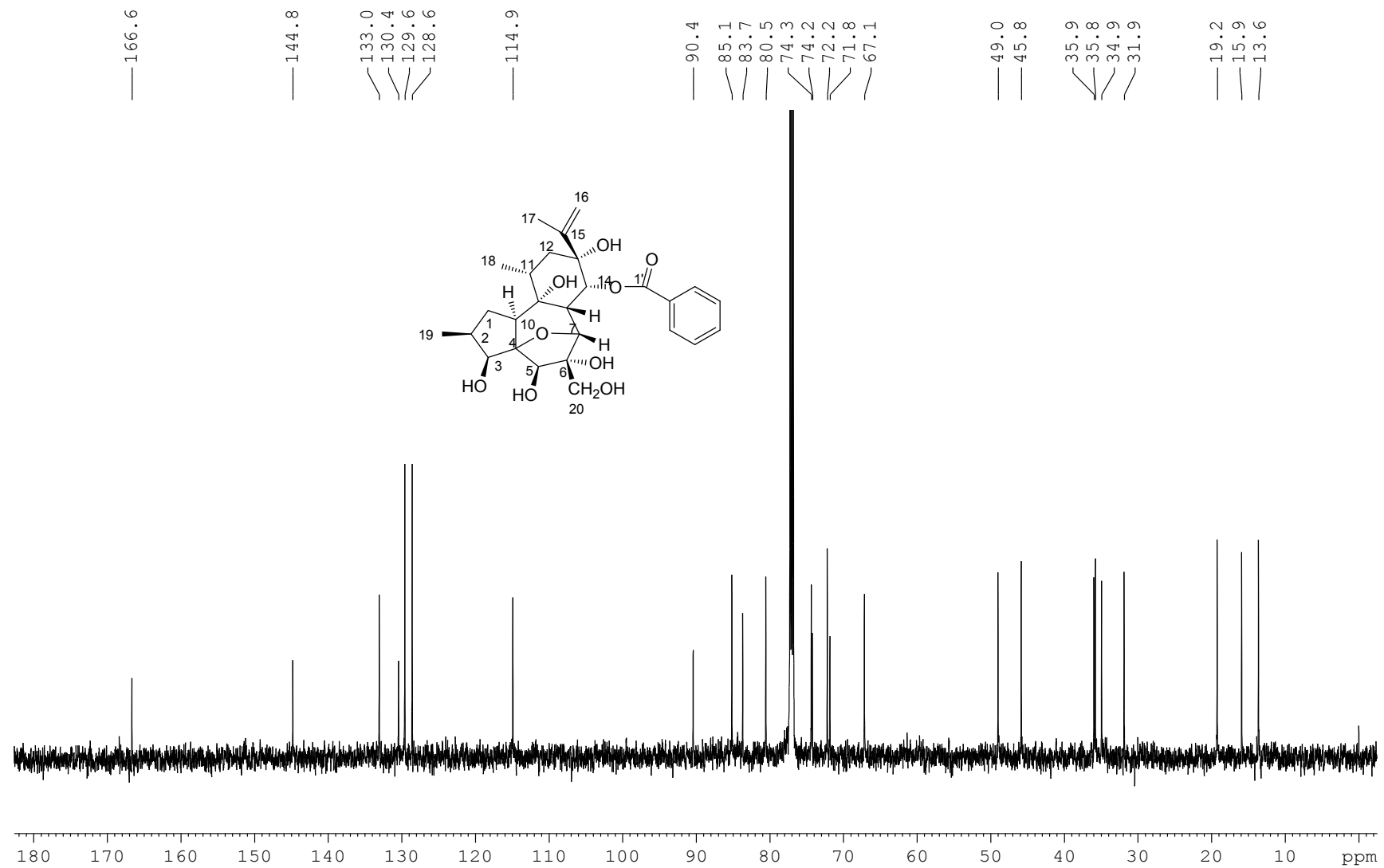
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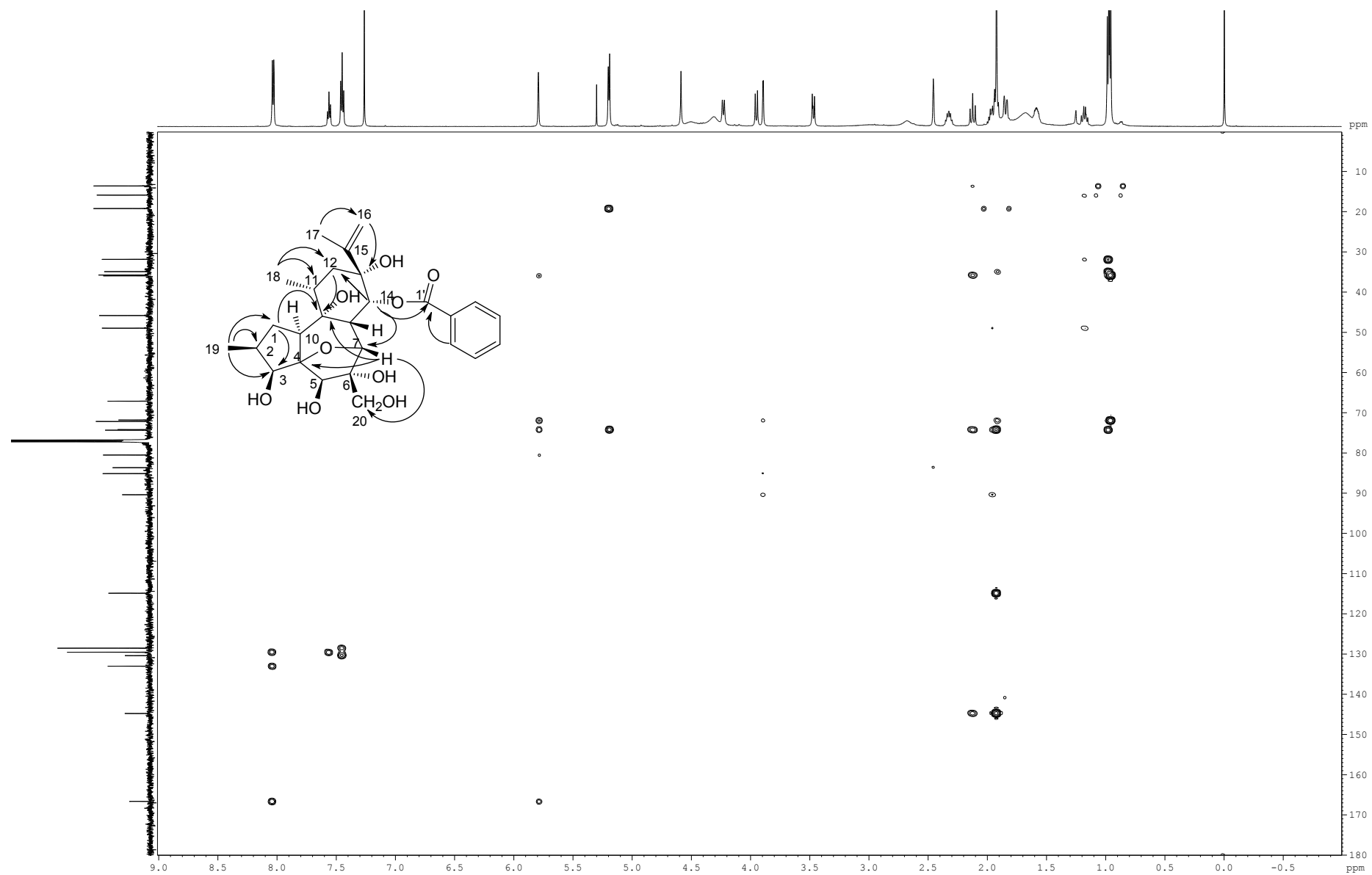
2: ^1H NMR spectrum for compound **1** recorded in CDCl_3 at 600 MHz.



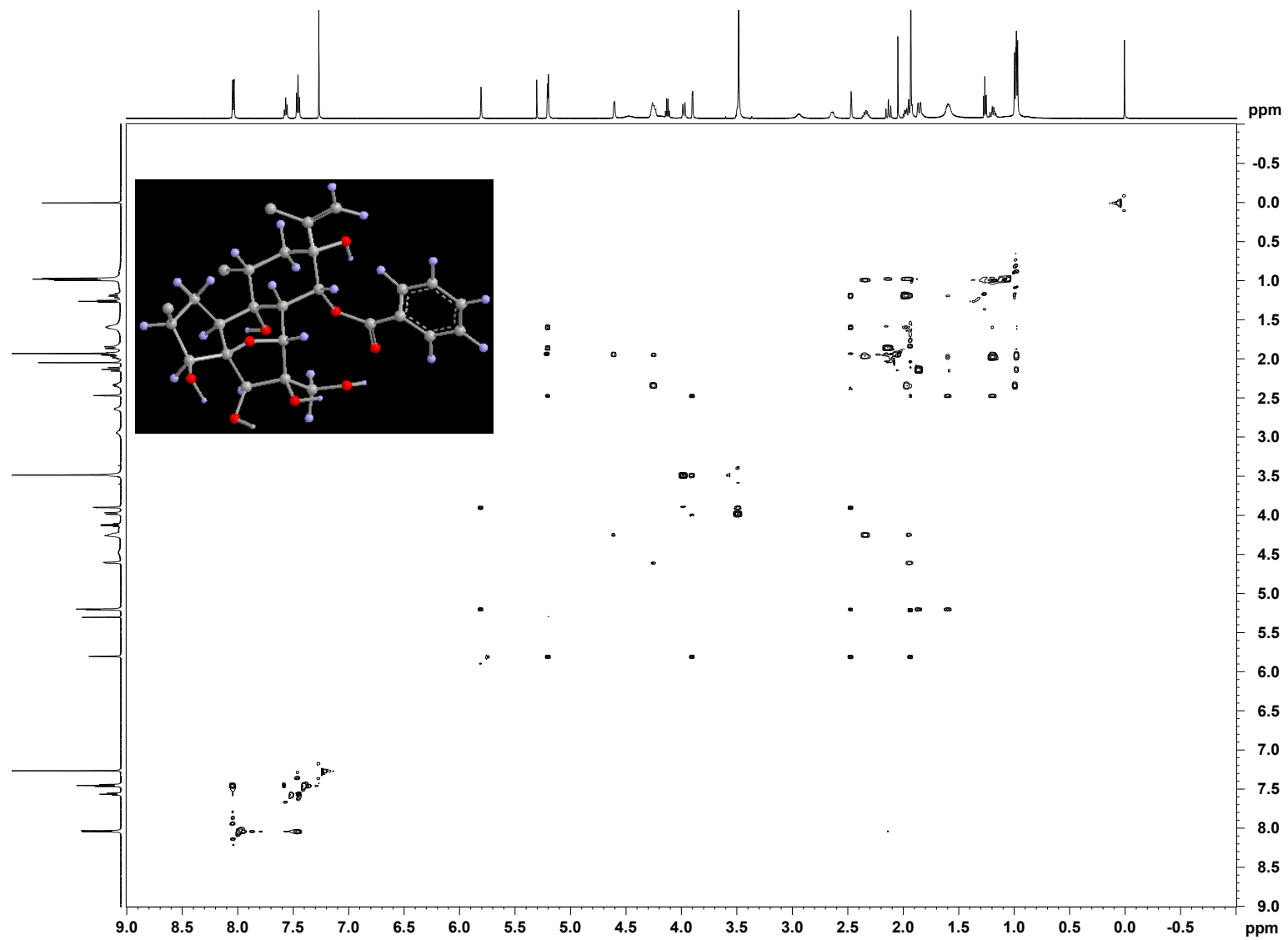
3: ^{13}C NMR spectrum for compound **1** recorded in CDCl_3 at 125 MHz.



4:HMBC spectrum for compound **1** recorded in CDCl₃ at 600 MHz.

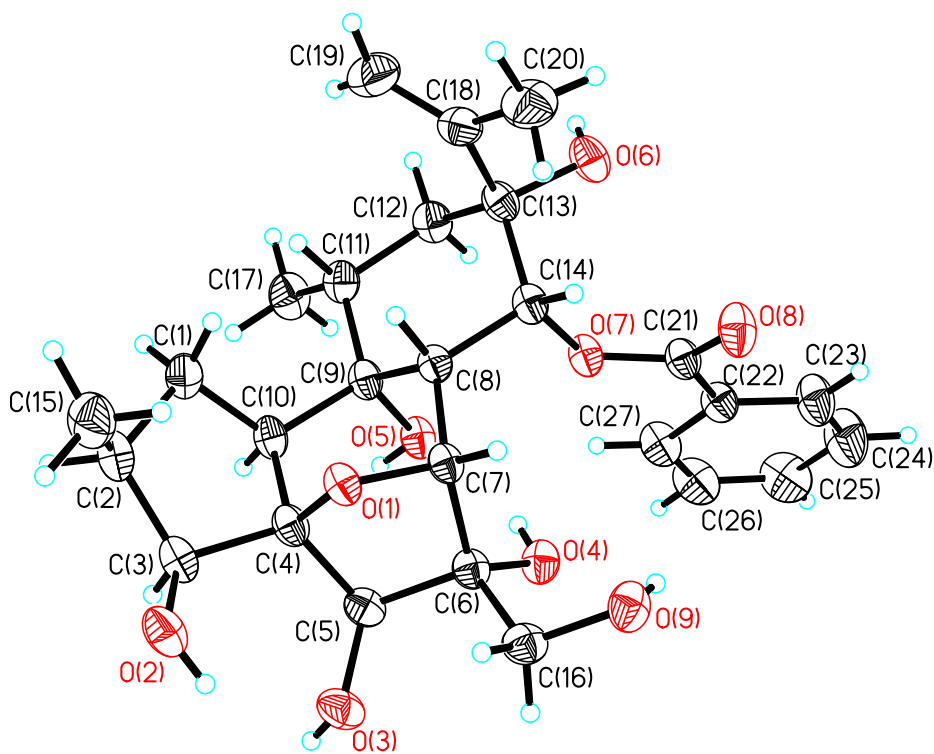


5:NOESY spectrum for compound **1** recorded in CDCl₃ at 600 MHz.



6. Single crystal X-ray diffraction analysis of genkdaphnin A (1)

Crystallization of genkdaphnin A (1) from n-hexane/ethyl acetate gave flaky cocrystal (1: 1) of 1 and ethyl acetate. All measurements were made on a Bruker SMART APEX-II with RAPID diffractometer using filtered $\text{CuK}\alpha$ radiation ($\lambda = 1.54187 \text{ \AA}$). Crystal data: Formula $\text{C}_{27}\text{H}_{36}\text{O}_9$, Formula weight 504.24, Orthorhombic system, Space group: P 21 21 21, $a = 11.7035(7) \text{ \AA}$, $b = 12.7664(9) \text{ \AA}$, $c = 21.1157(14) \text{ \AA}$, $\alpha = \beta = \gamma = 90.00^\circ$, $V = 3154.9(4) \text{ \AA}^3$, $Z = 4$, $T = 296(2) \text{ K}$, $d = 1.248 \text{ g cm}^{-3}$, specimen: $0.05 \times 0.20 \times 0.010 \text{ mm}^3$. The total number of independent reflections measured was 9697, 4408 reflections unique, of which 4183 were observed ($|F|^2 \geq 2\sigma|F|^2$). All calculations were performed using Crystal Structure except for refinement, which was performed using direct method SHELXL-97, expanded by using difference Fourier techniques, and refined by the full-matrix least-squares calculations. The non-hydrogen atoms were refined anisotropically, and hydrogen atoms were included at their calculated positions. The final indices were $R_1 = 0.0429$, $wR_2 = 0.1181$ ($w = 1/\sigma|F|^2$), $S = 1.030$. Crystallographic data for genkdaphnin A (1) have been deposited at the Shanghai Institute of Pharmaceutical Industry.



ORTEP drawing of genkdaphnin A (1).

7:HRESIMS spectrum for compound 2

 Compound Mass Spectrum List Report

Analysis Info

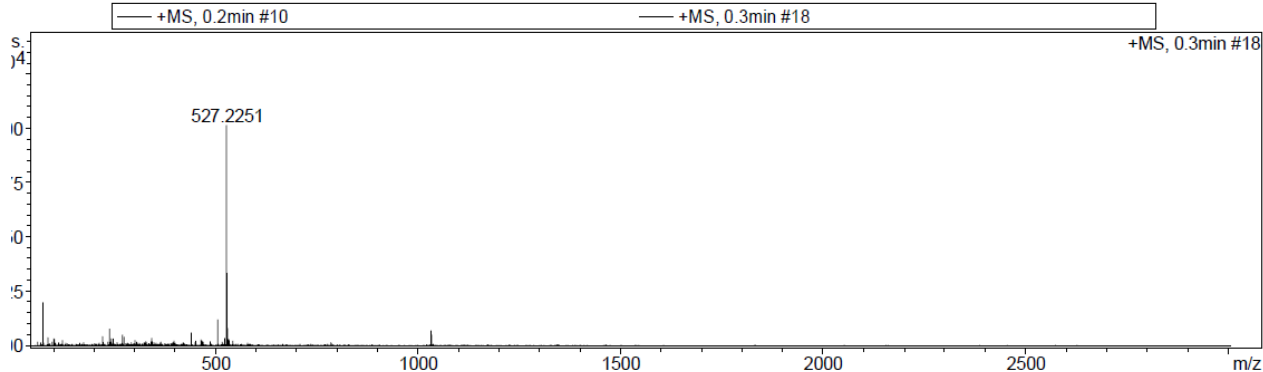
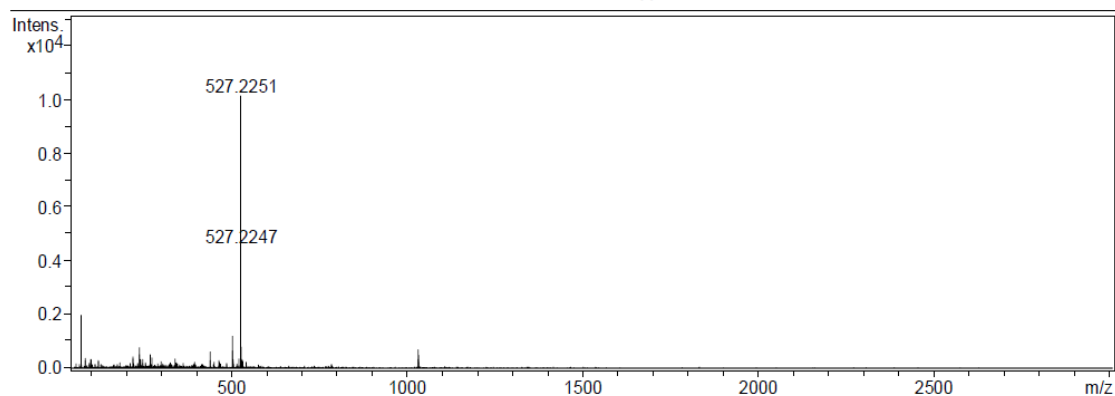
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 Sample Name sg
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Operator Bruker Customer
 Instrument / Ser# micrOTOF-Q 125

Acquisition Parameter

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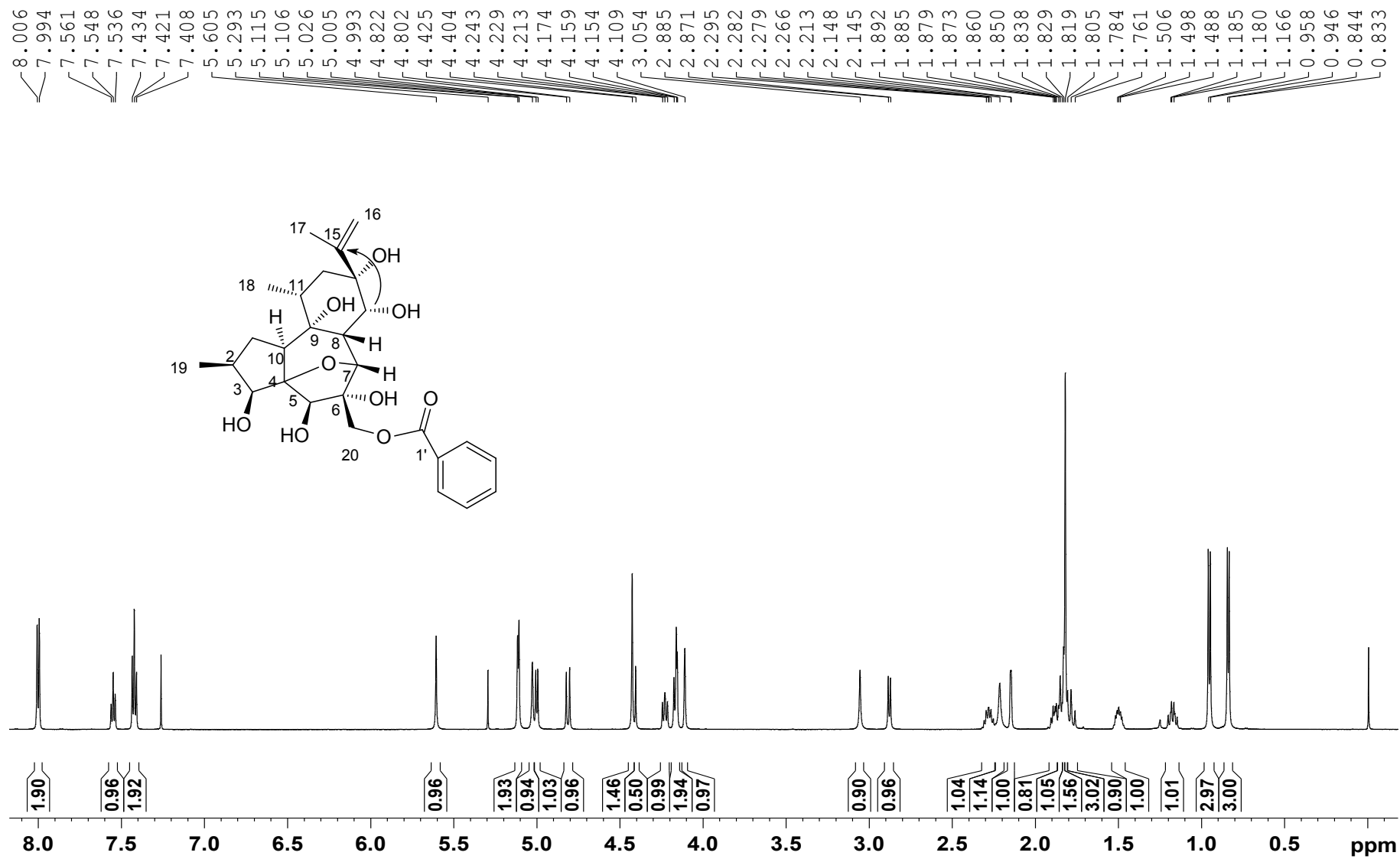


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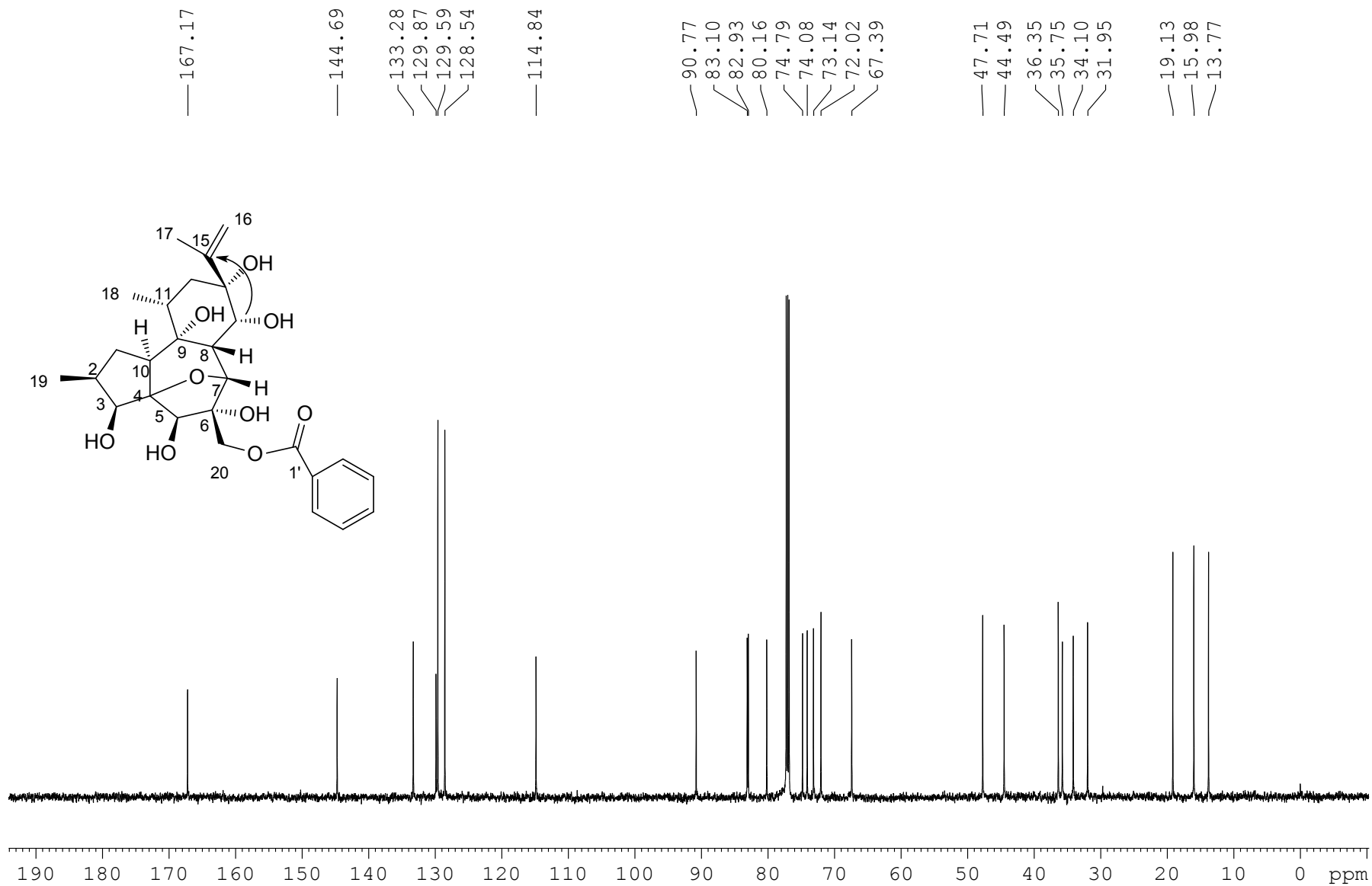
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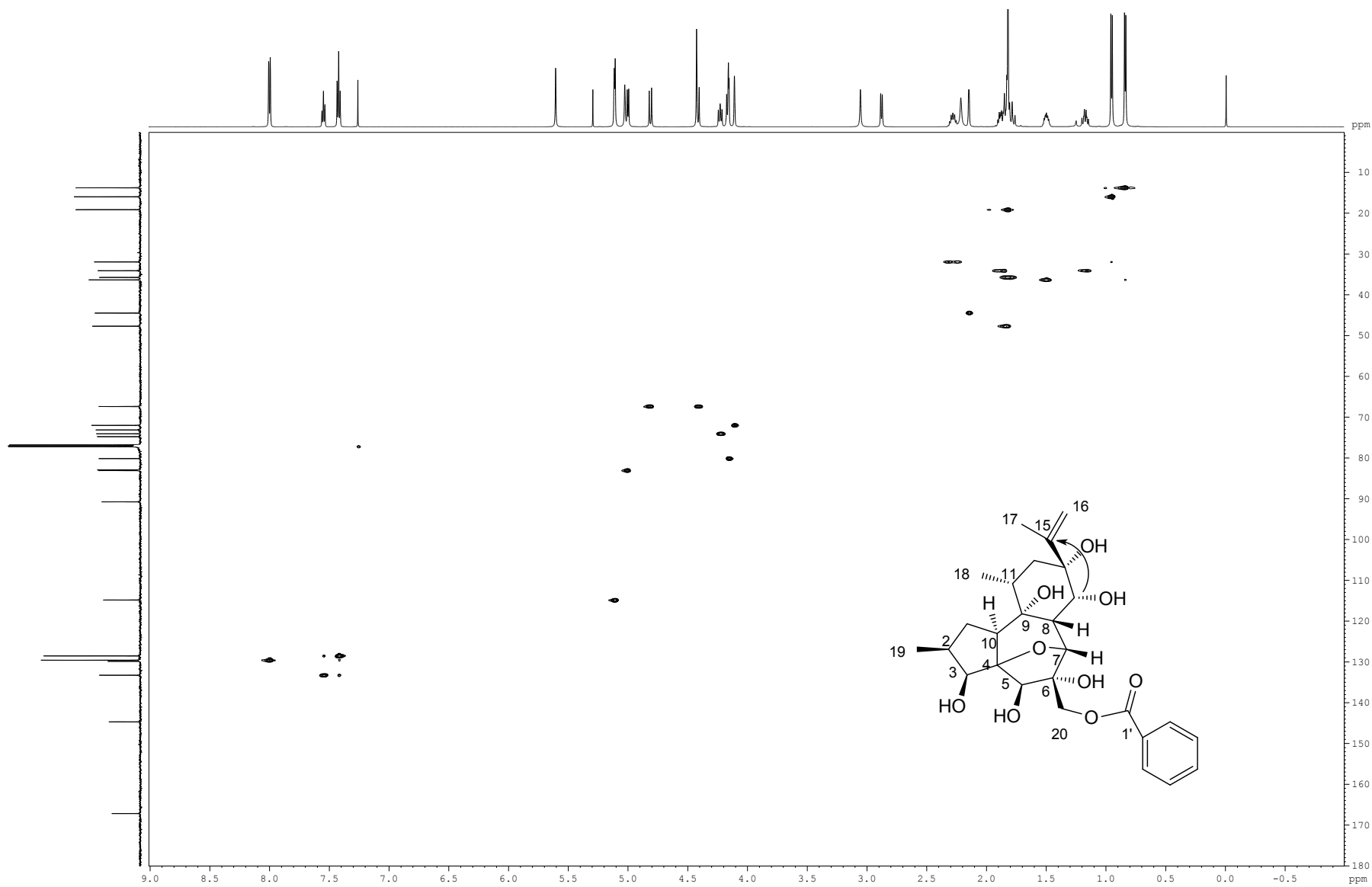
8: ^1H NMR spectrum for compound **2** recorded in CDCl_3 at 600 MHz.

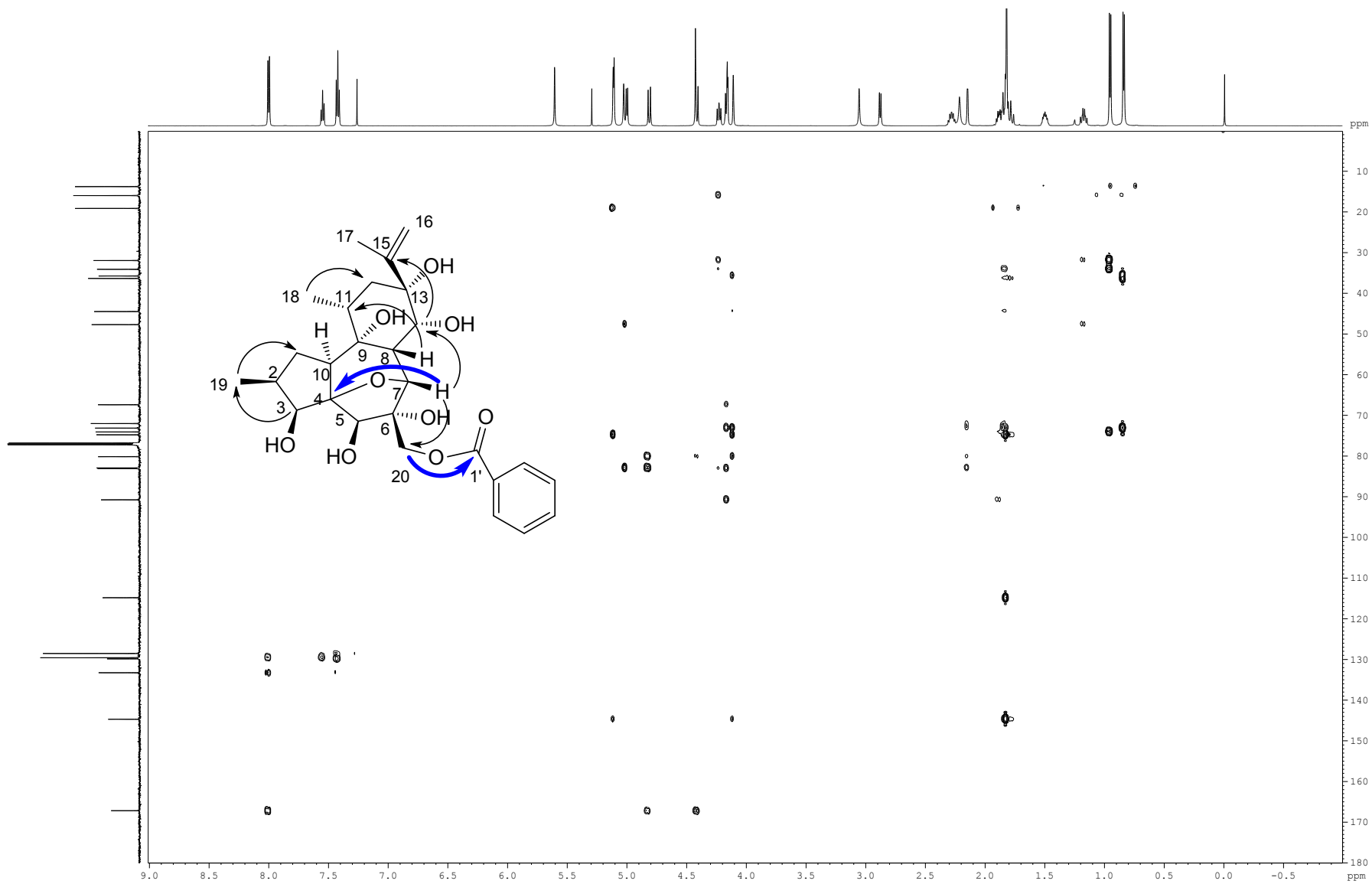


9: ^{13}C NMR spectrum for compound **2** recorded in CDCl_3 at 125 MHz.

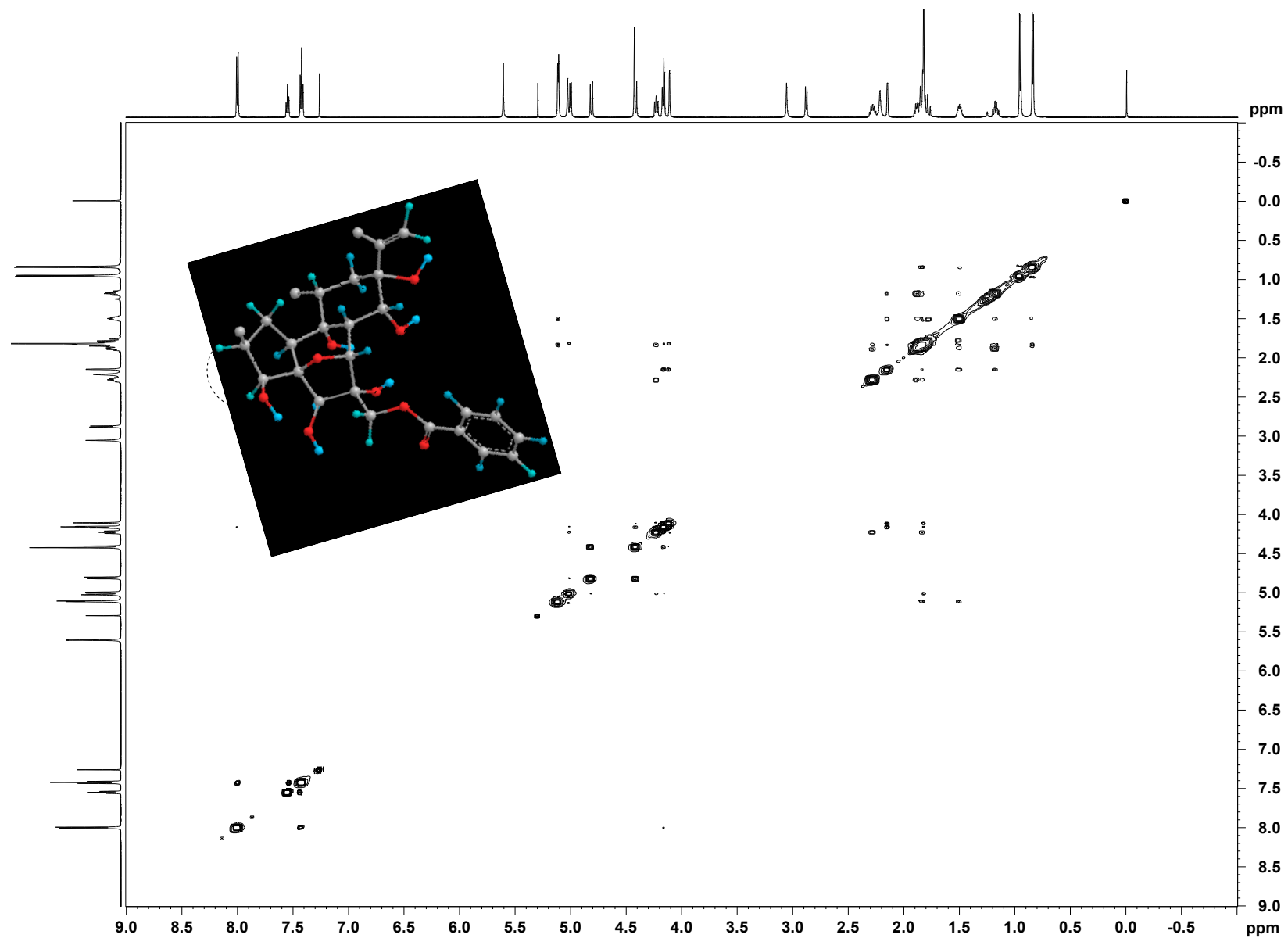


10:HSQC spectrum for compound **2** recorded in CDCl₃ at 600 MHz.



11:HMBC spectrum for compound **2** recorded in CDCl₃ at 600 MHz.

12:NOESY spectrum for compound **2** recorded in CDCl₃ at 600 MHz.



13. HRESIMS spectrum for compound 3 .

 Compound Mass Spectrum List Report

Analysis Info

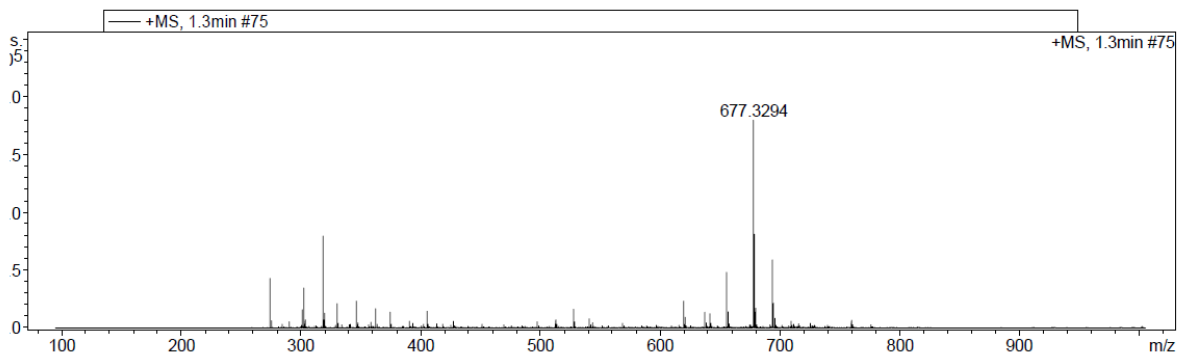
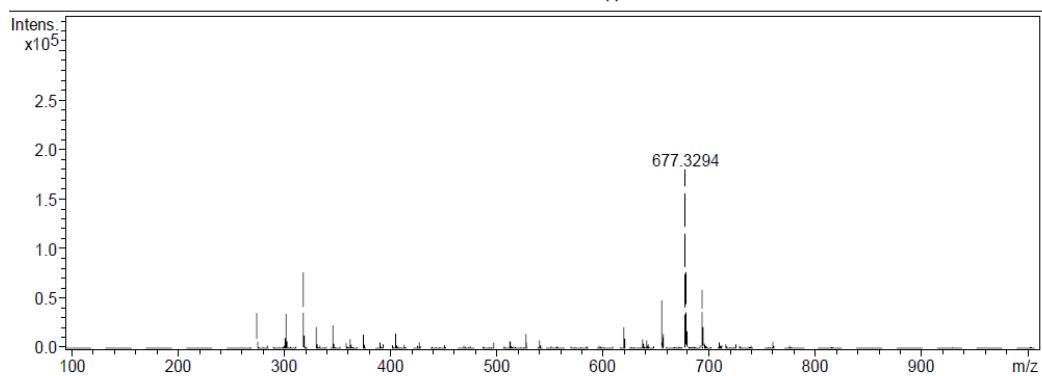
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Operator Bruker Customer
 Instrument / Ser# microTOF-Q 125

Acquisition Parameter

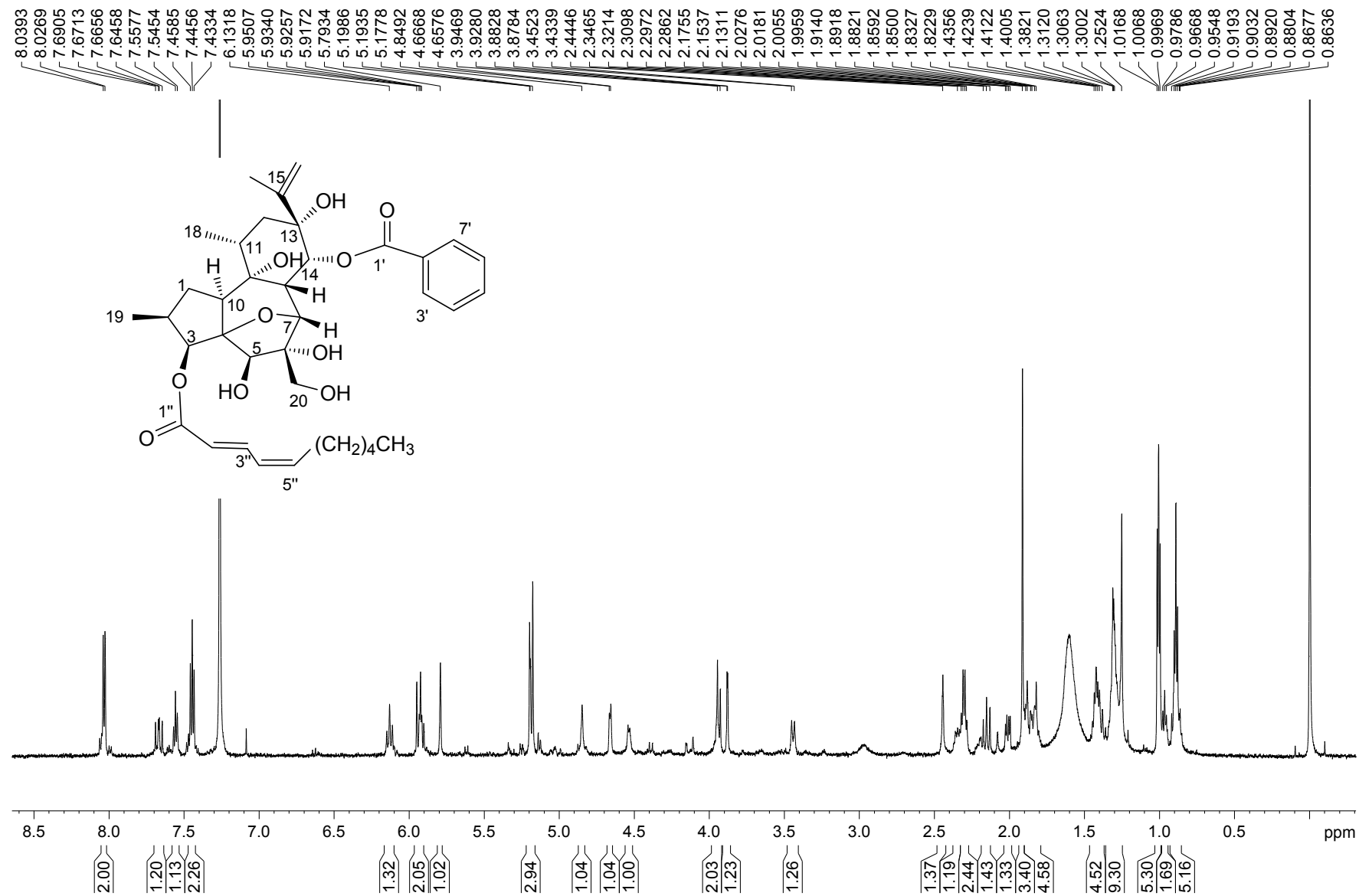
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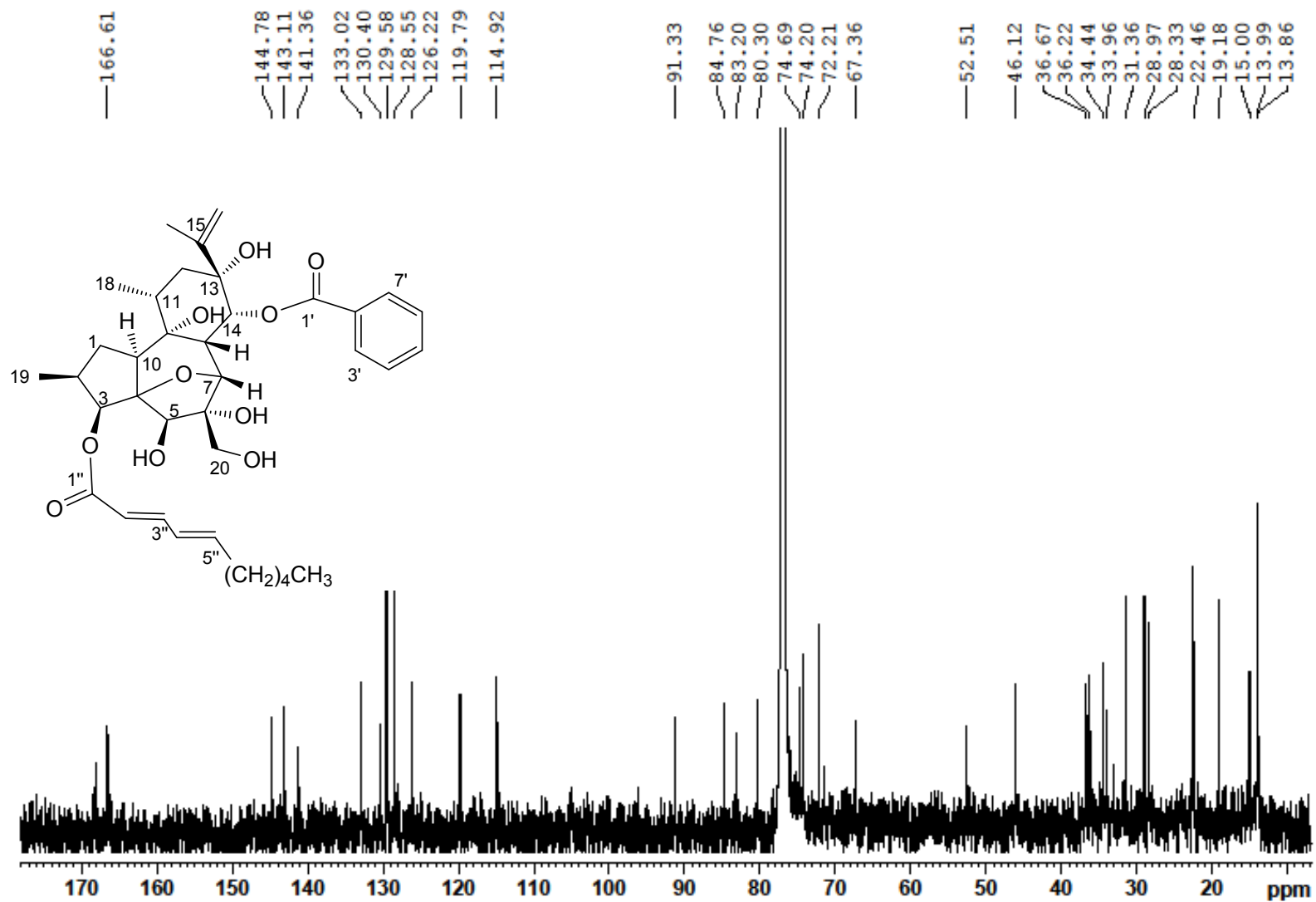
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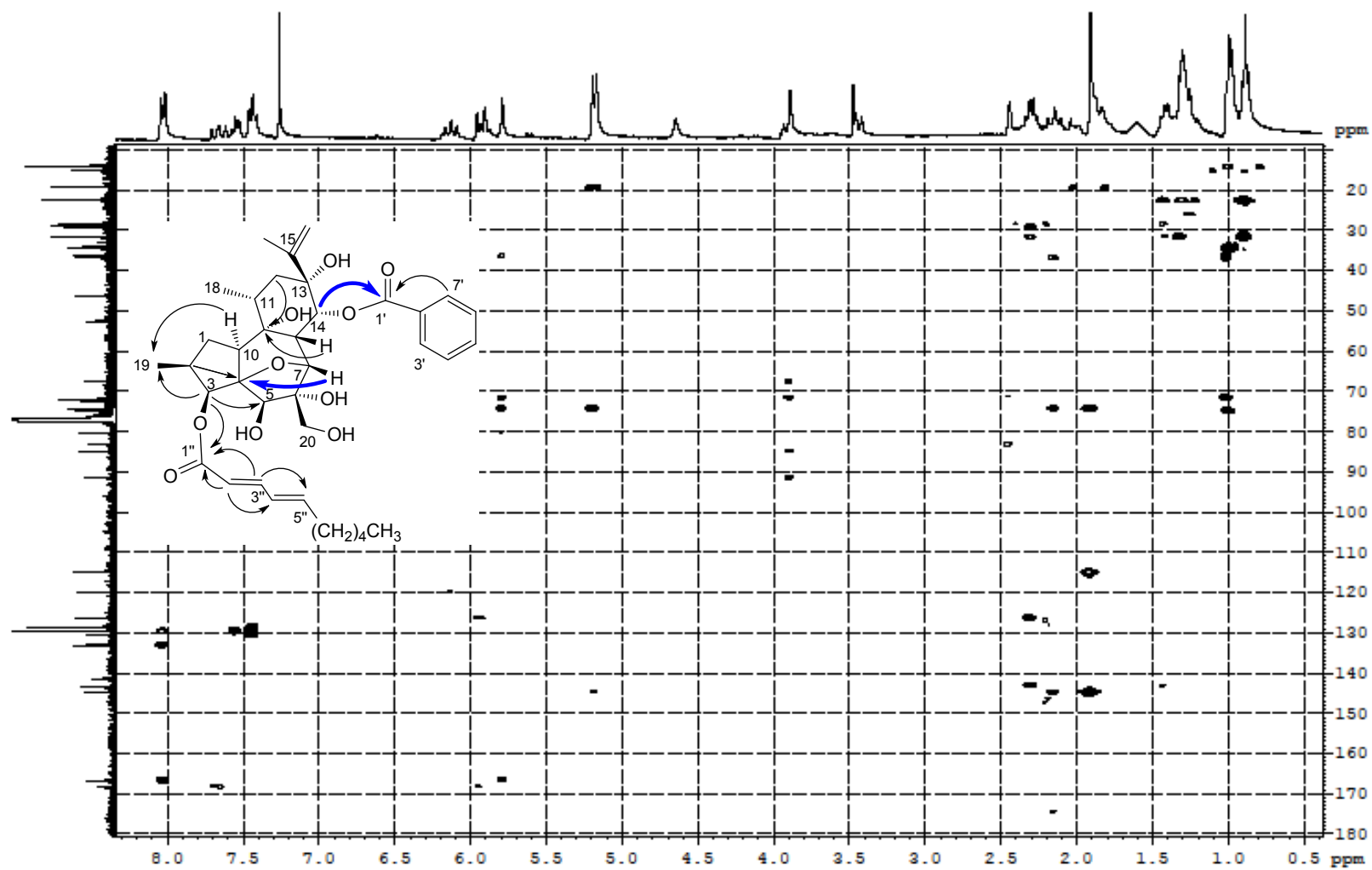
14: ^1H NMR spectrum for compound **3** recorded in CDCl_3 at 125 MHz.



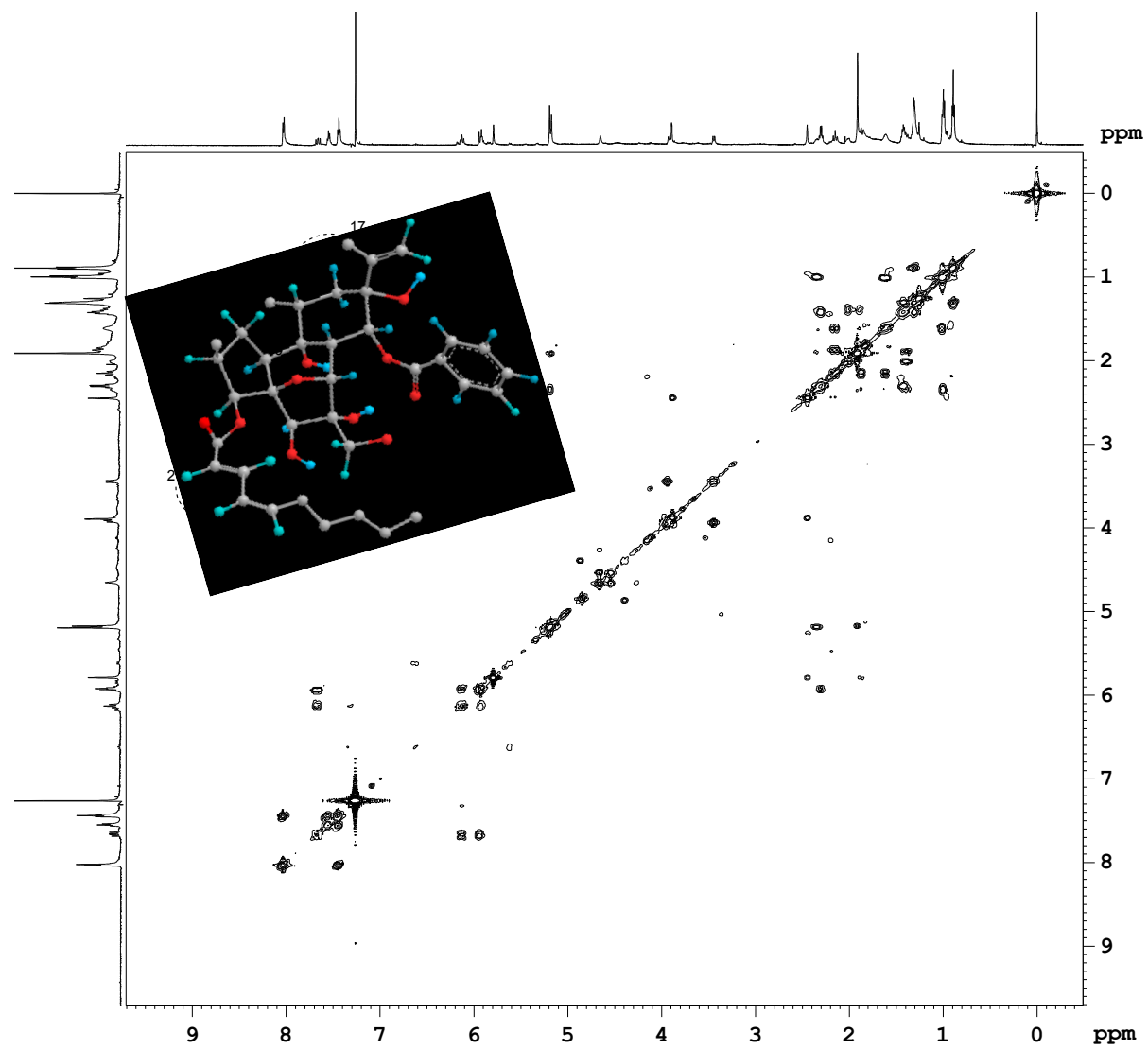
15: ^{13}C NMR spectrum for compound 3 recorded in CDCl_3 at 600 MHz.



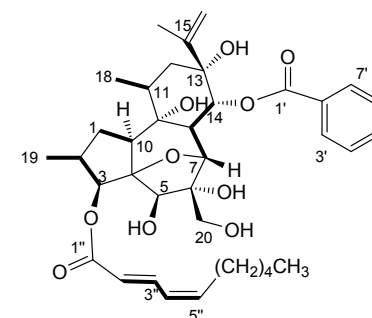
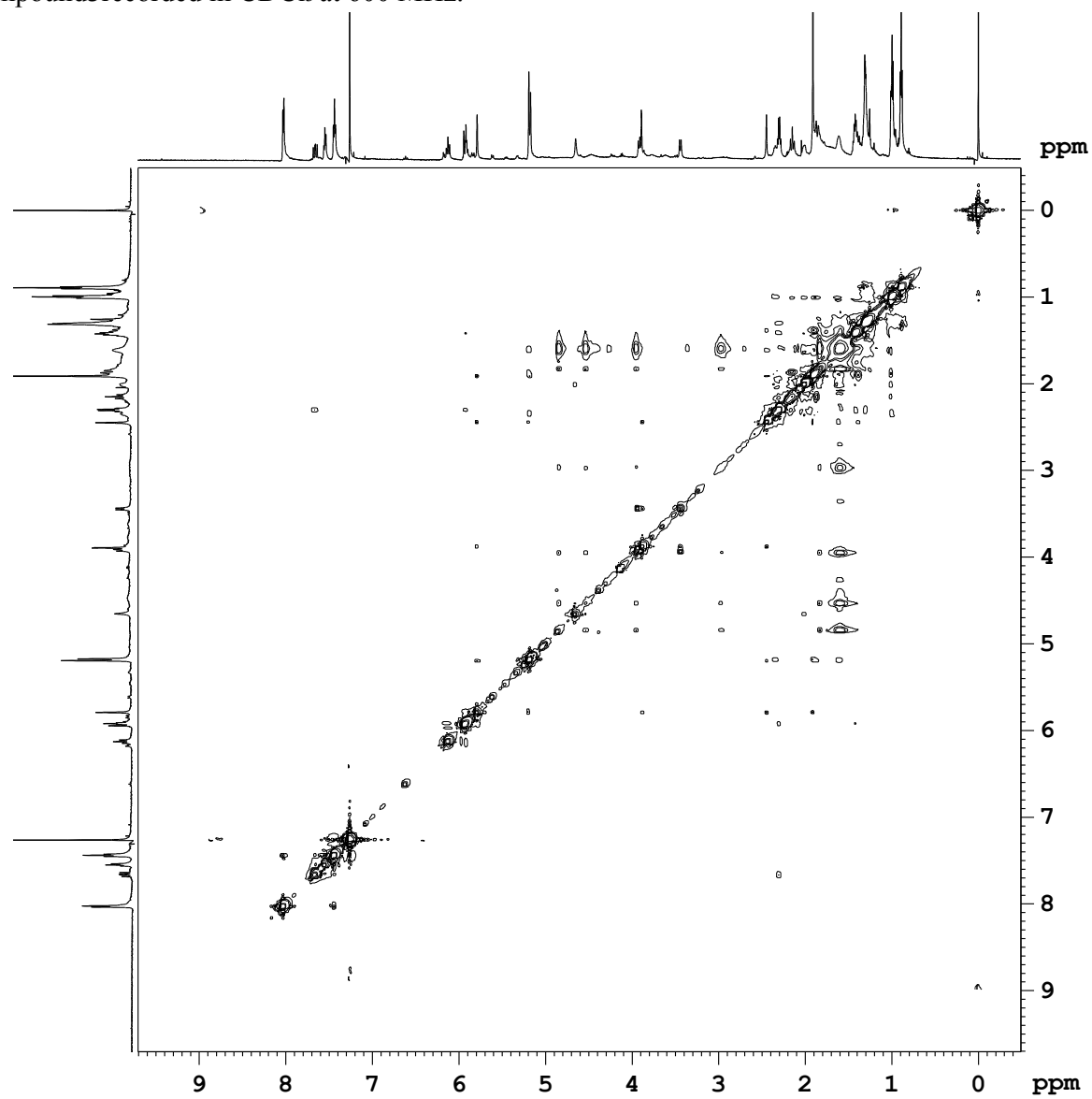
16:HMBC spectrum for compound 3 recorded in CDCl₃ at 600 MHz.



17:NOESY spectrum for compound **3** recorded in CDCl₃ at 600 MHz.



18:H-HCOSY spectrum for compound **3** recorded in CDCl₃ at 600 MHz.



19. HRESIMS spectrum for compound 4 .

 Compound Mass Spectrum List Report

Analysis Info

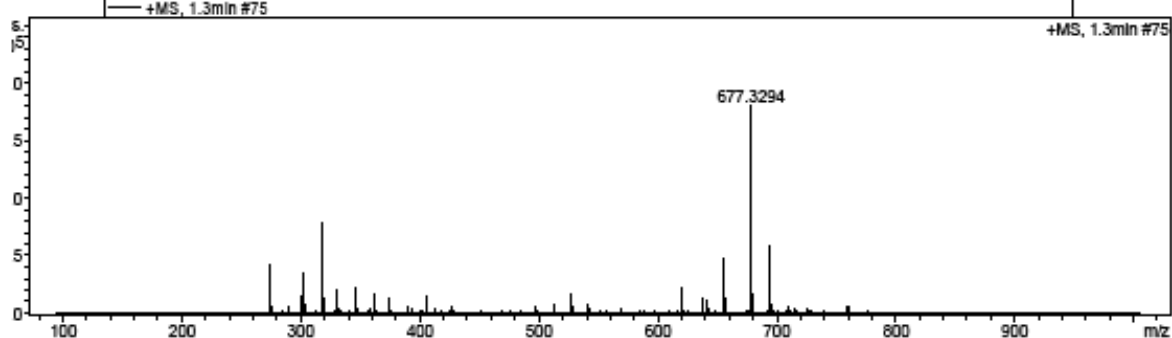
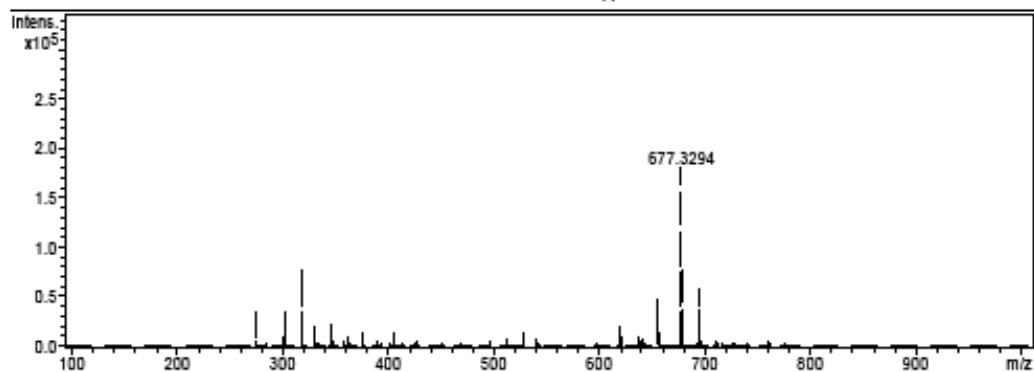
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 Method tune_low.m
 Sample Name 3(c)-1.5h-MS
 Comment

Acquisition Date 2009-7-7 18:08:40

Operator Bruker Customer
 Instrument / Ser# micrOTOF-Q 125

Acquisition Parameter

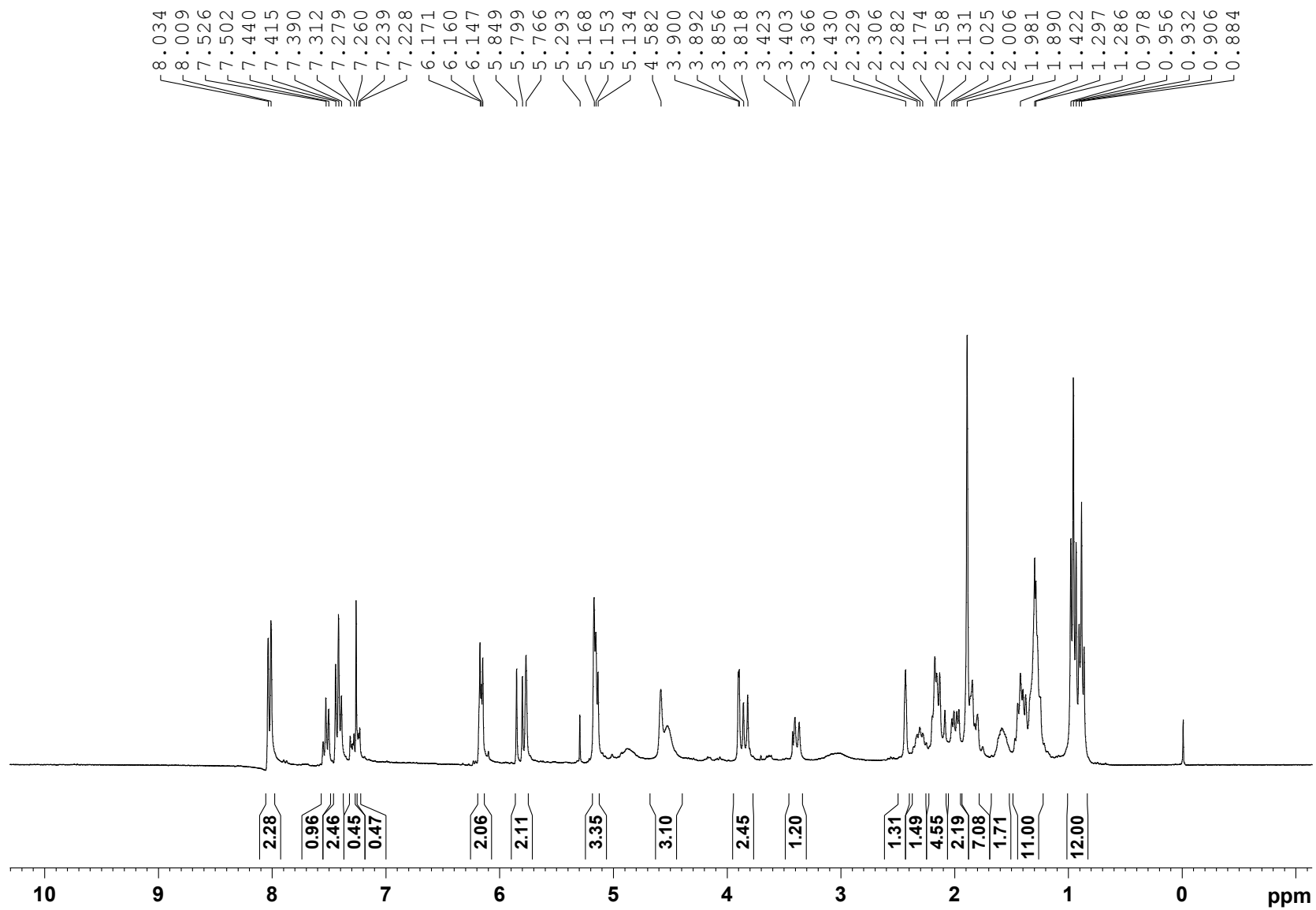
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Scan End	1000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Source

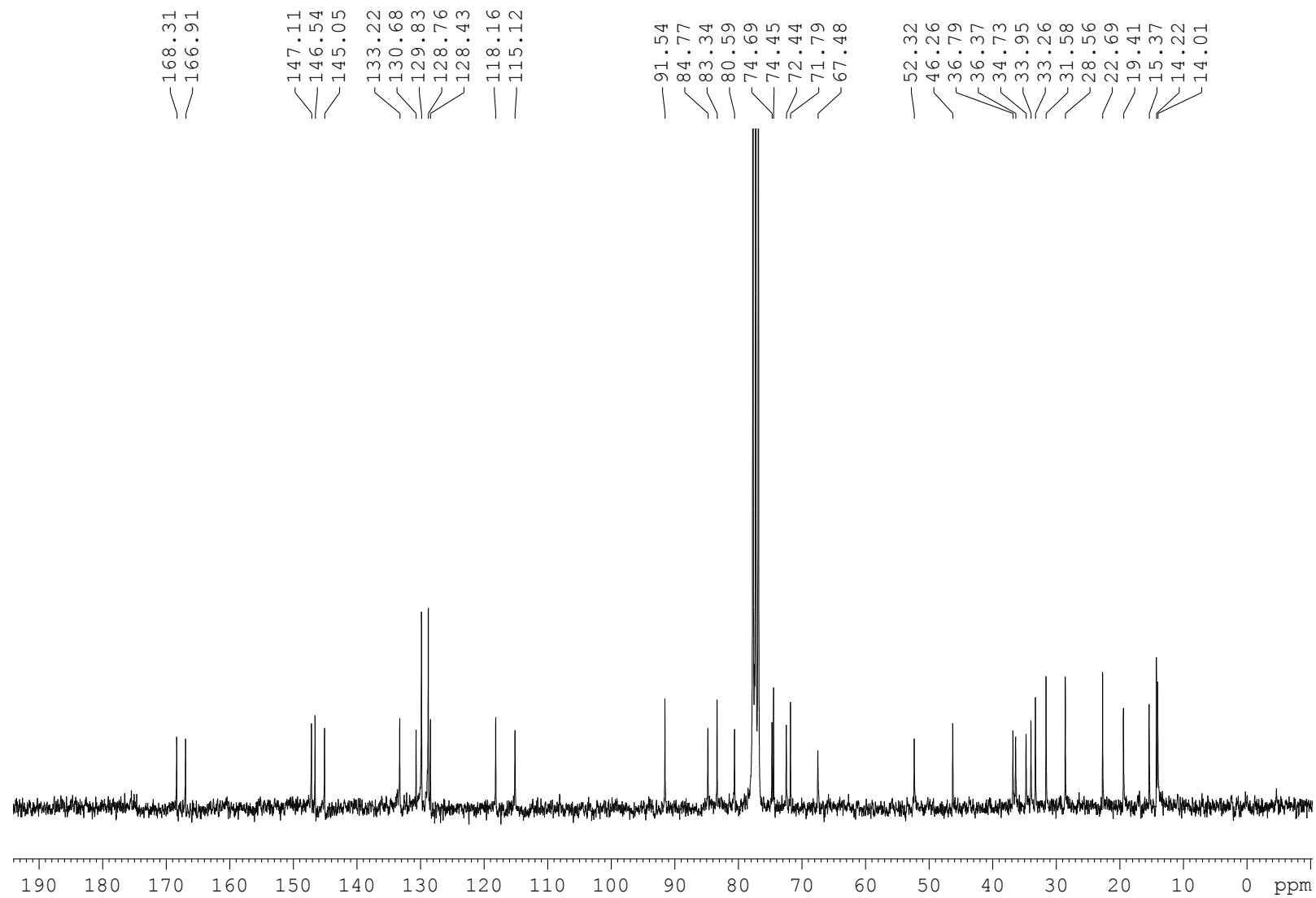


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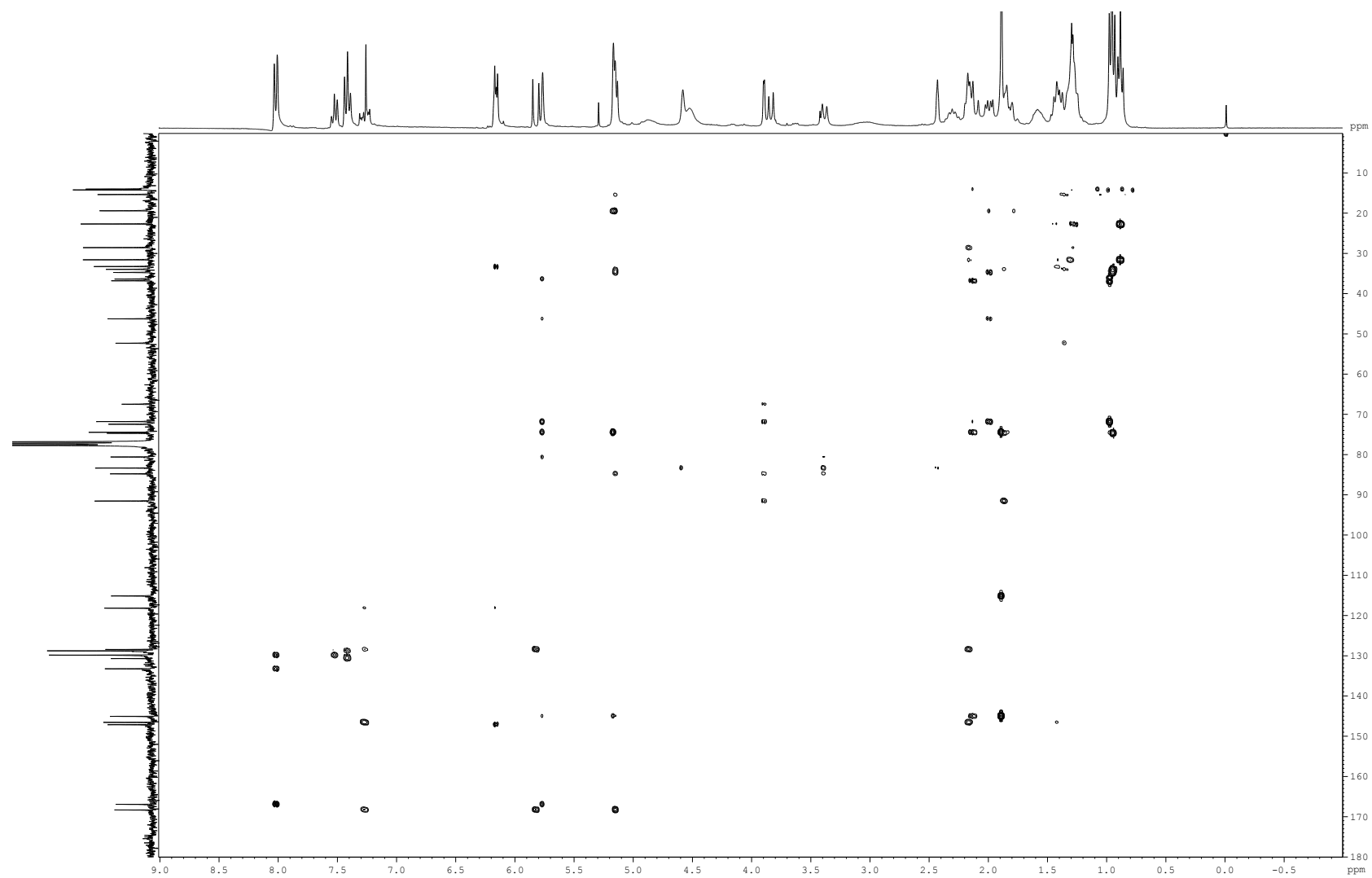
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20. ^1H NMR spectrum for compound **4** recorded in CDCl_3 at 600 MHz.



21. ^{13}C NMR spectrum for compound **4** recorded in CDCl_3 at 125 MHz.

22. HMBC spectrum for compound 4 recorded in CDCl₃ at 600 MHz.



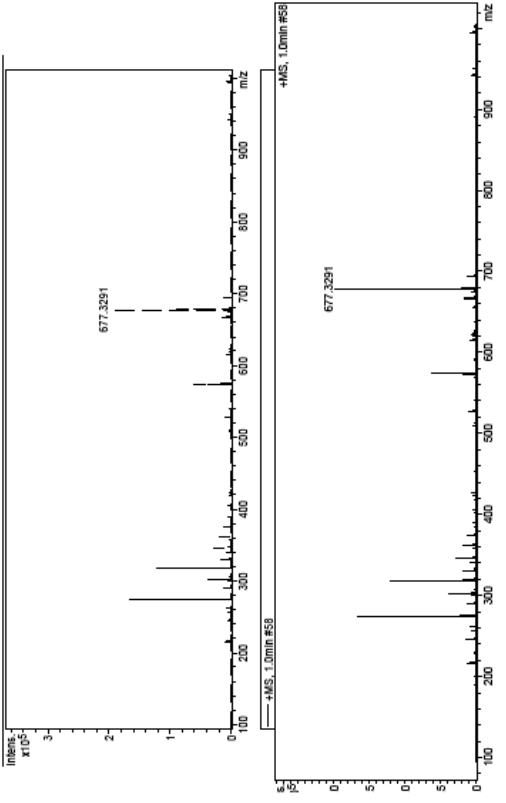
23. HRESIMS spectrum for compound 5.

S 23

Compound Mass Spectrum List Report

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 Operator Bruker Customer
 Sample Name 3(c)-1.5h-MS
 Instrument / Ser# micrOTOF-Q 125
 Comment

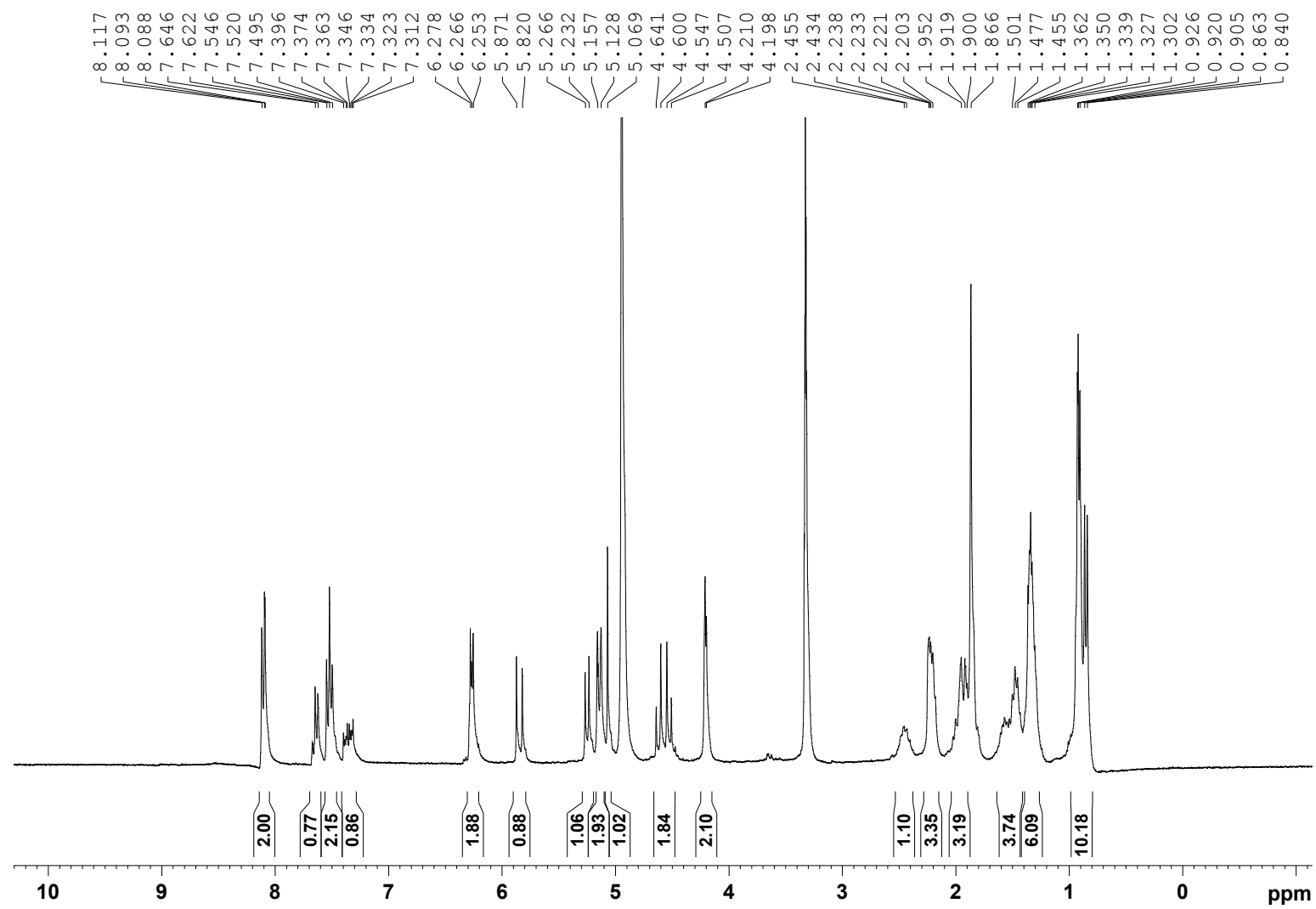
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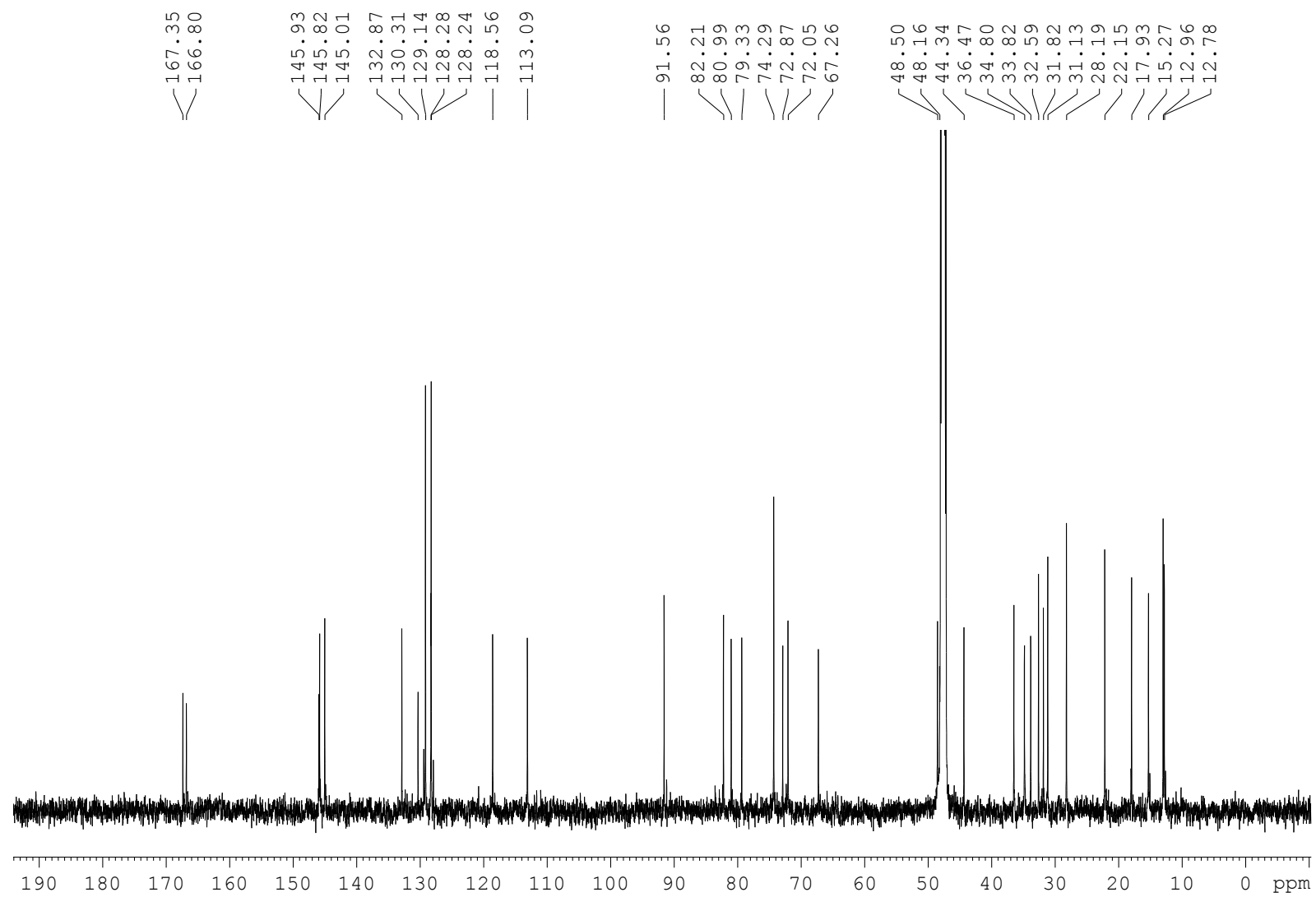


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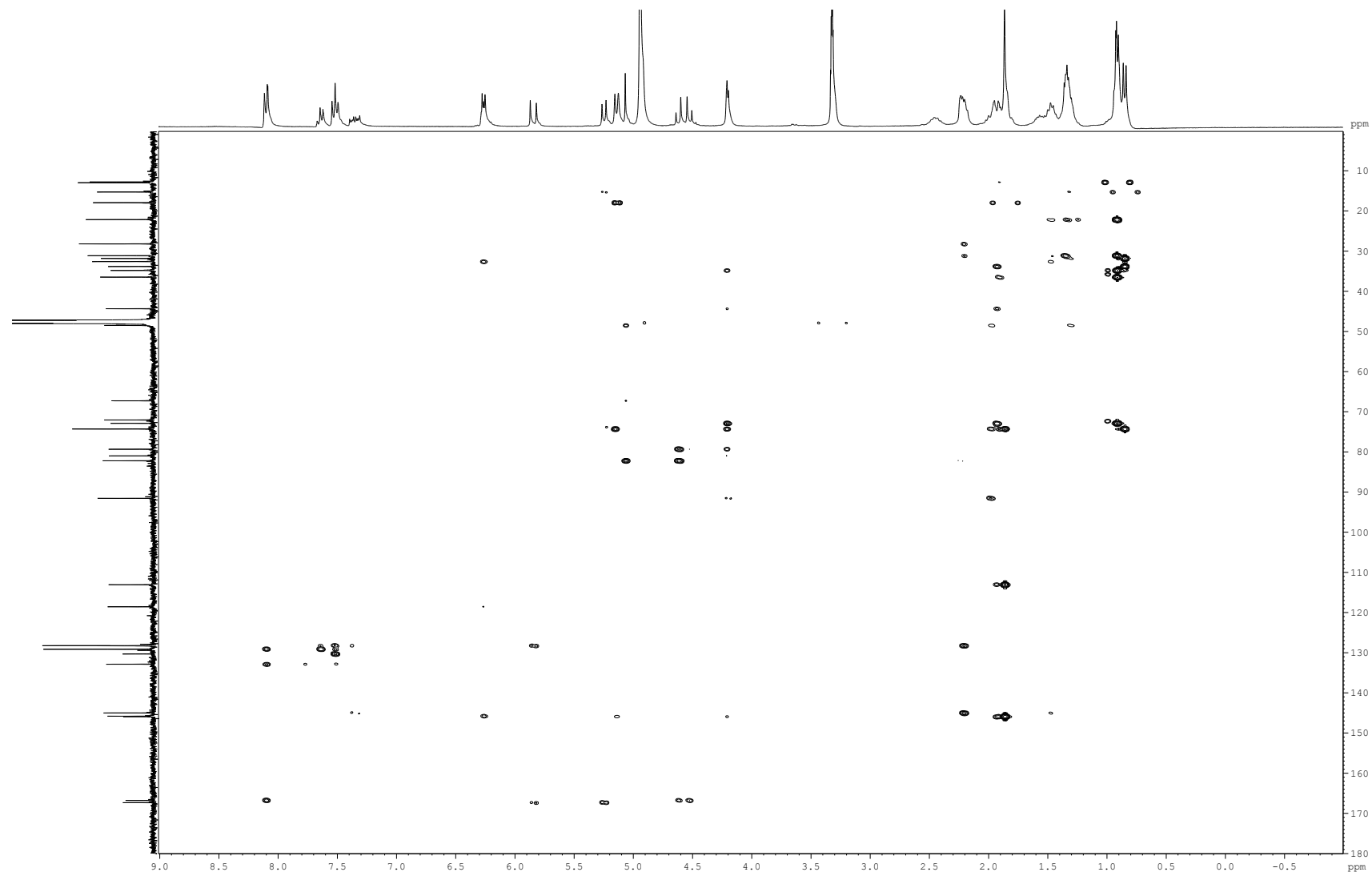
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24. ^1H NMR spectrum for compound **5** recorded in CDCl_3 at 600 MHz.



25. ^{13}C NMR spectrum for compound **5** recorded in CDCl_3 at 125 MHz.

26. HMBC spectrum for compound 5 recorded in CDCl₃ at 600 MHz.



27. HRESIMS spectrum for compound6.

Compound Mass Spectrum List Report

Analysis Info

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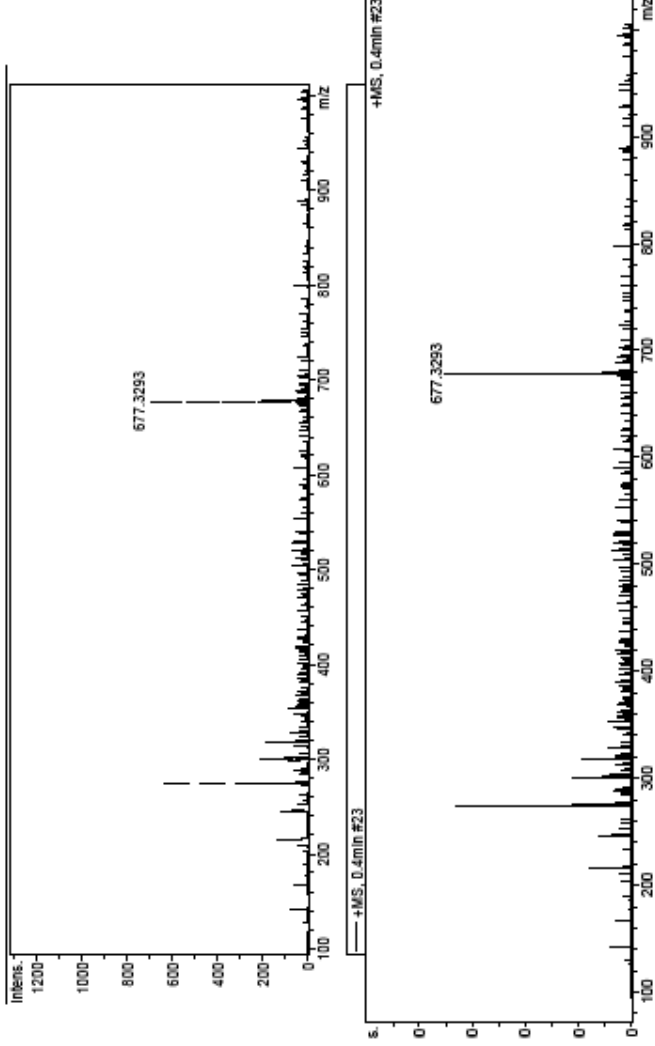
Operator Bruker Customer
 Instrument / Ser# micrOTOF-Q 125

Acquisition Parameter

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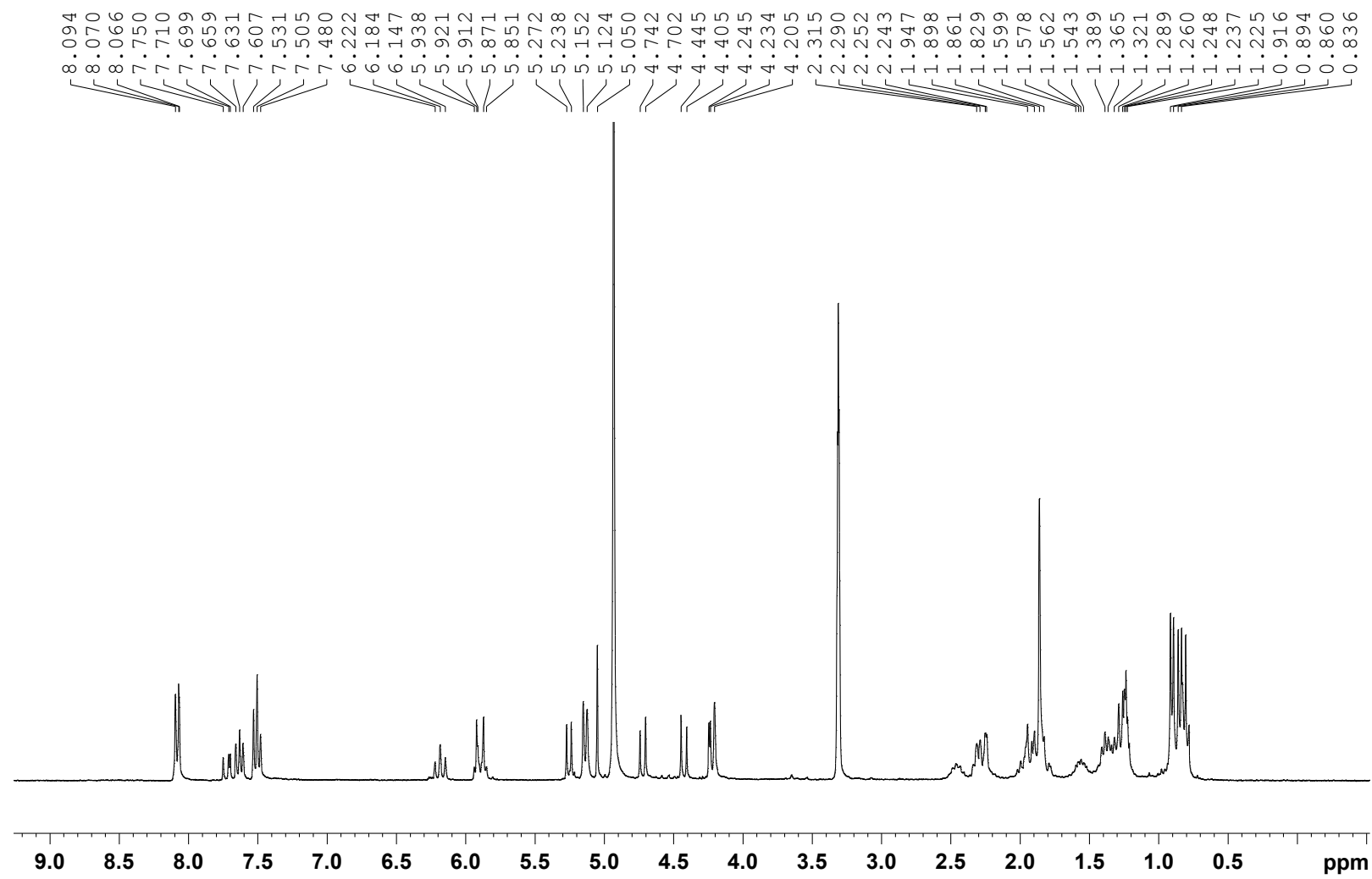
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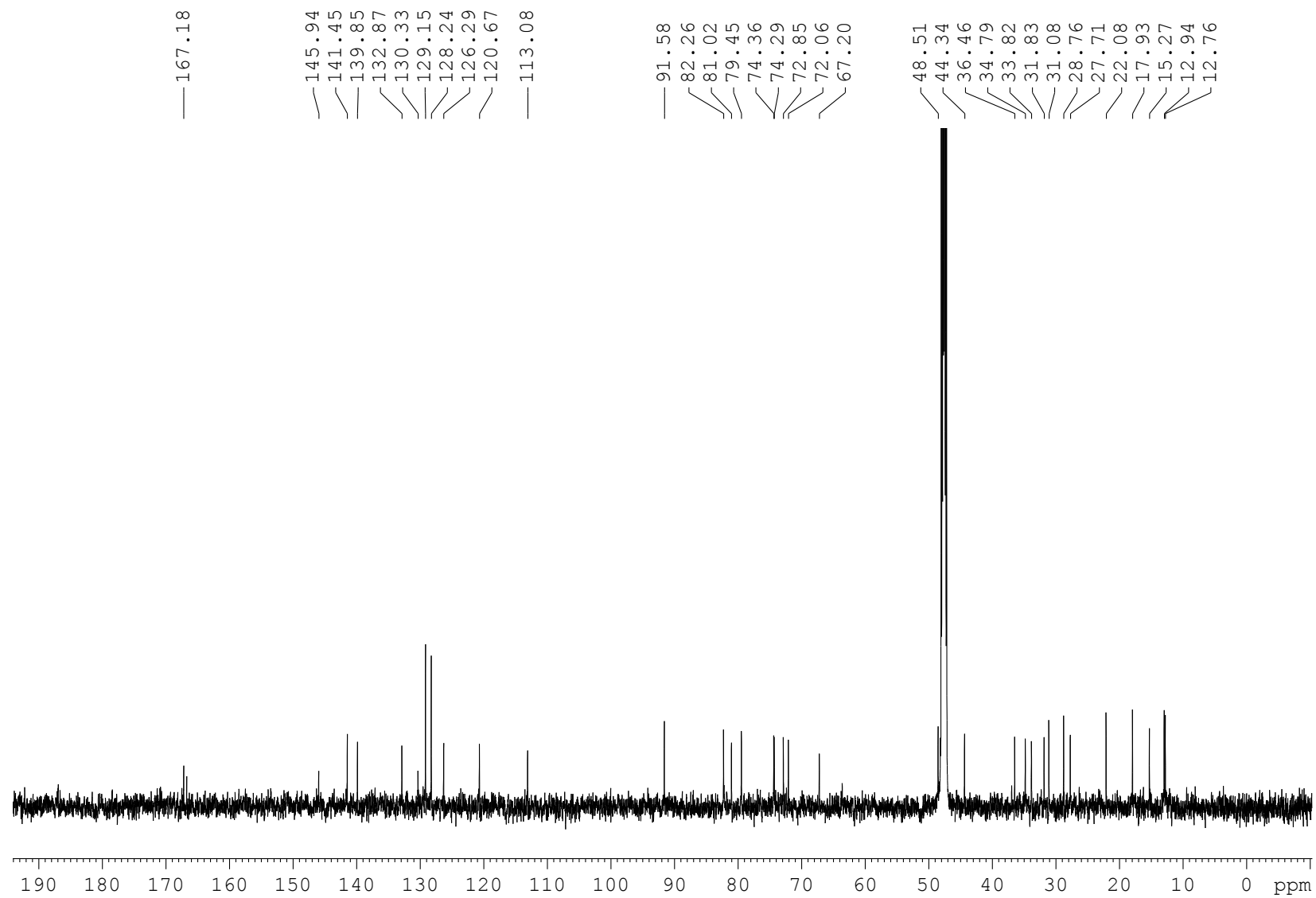
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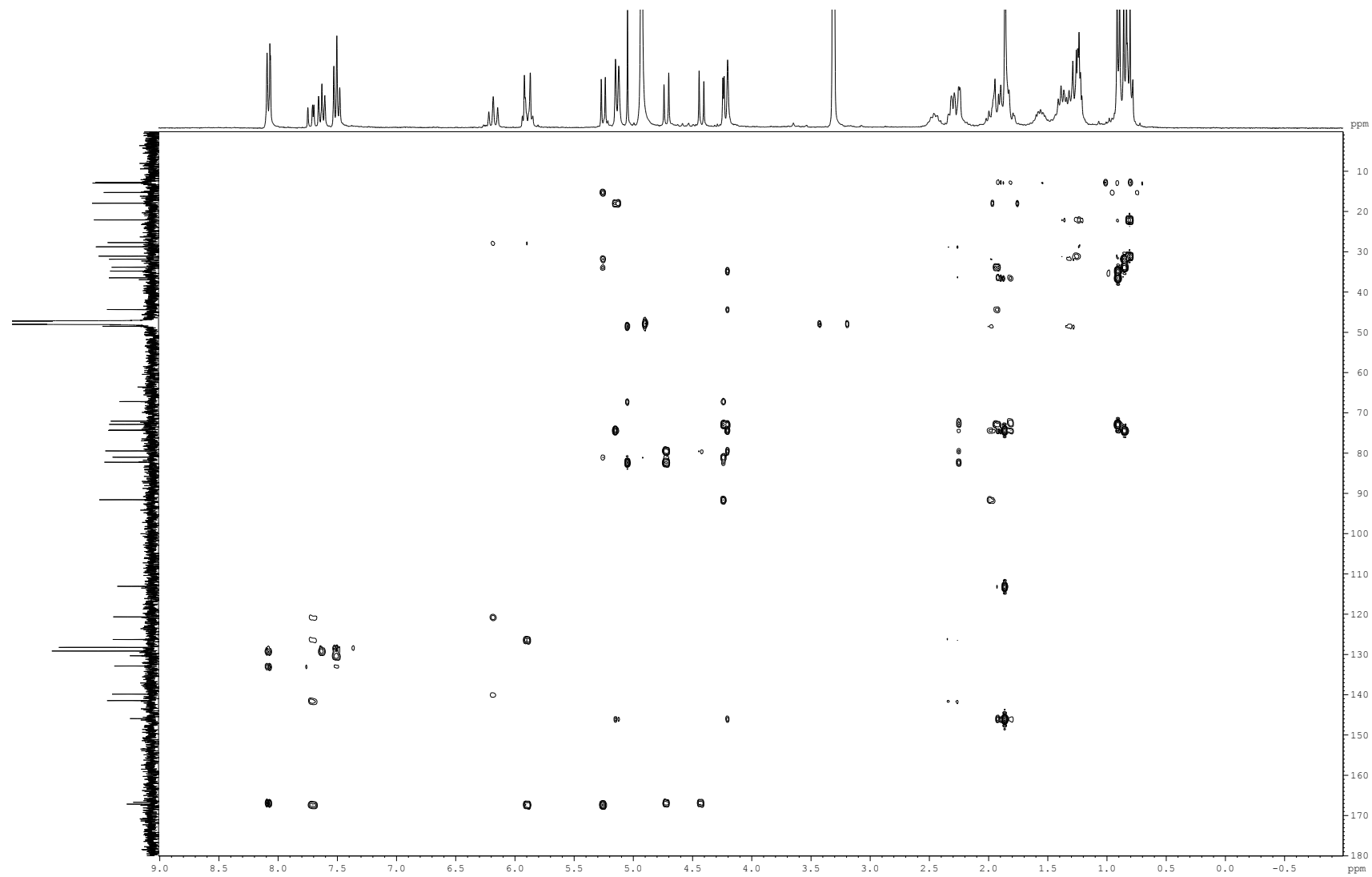
28. ^1H NMR spectrum for compound **6** recorded in CDCl_3 at 600 MHz.



29. ^{13}C NMR spectrum for compound **6** recorded in CDCl_3 at 125 MHz.



30. HMBC spectrum for compound 6 recorded in CDCl₃ at 600 MHz.



31. HRESIMS spectrum for compound7.

S 31

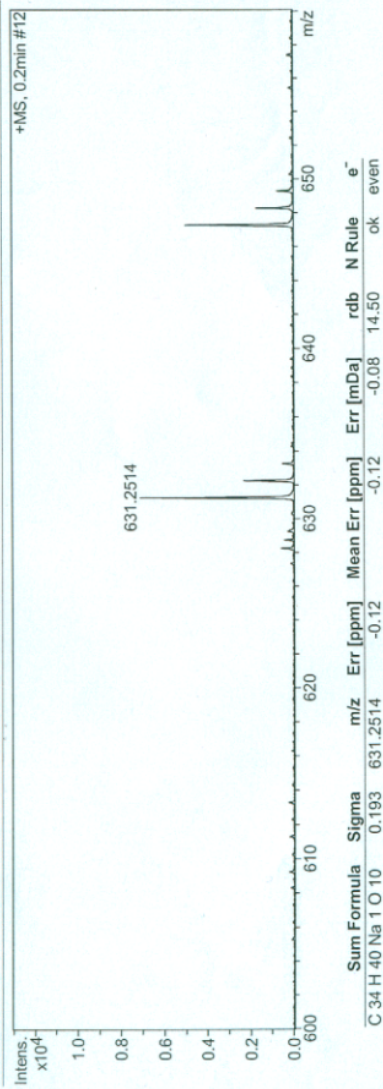
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 Comment
 Operator Bruker Customer
 Instrument / Ser# micrOTOF-Q 125

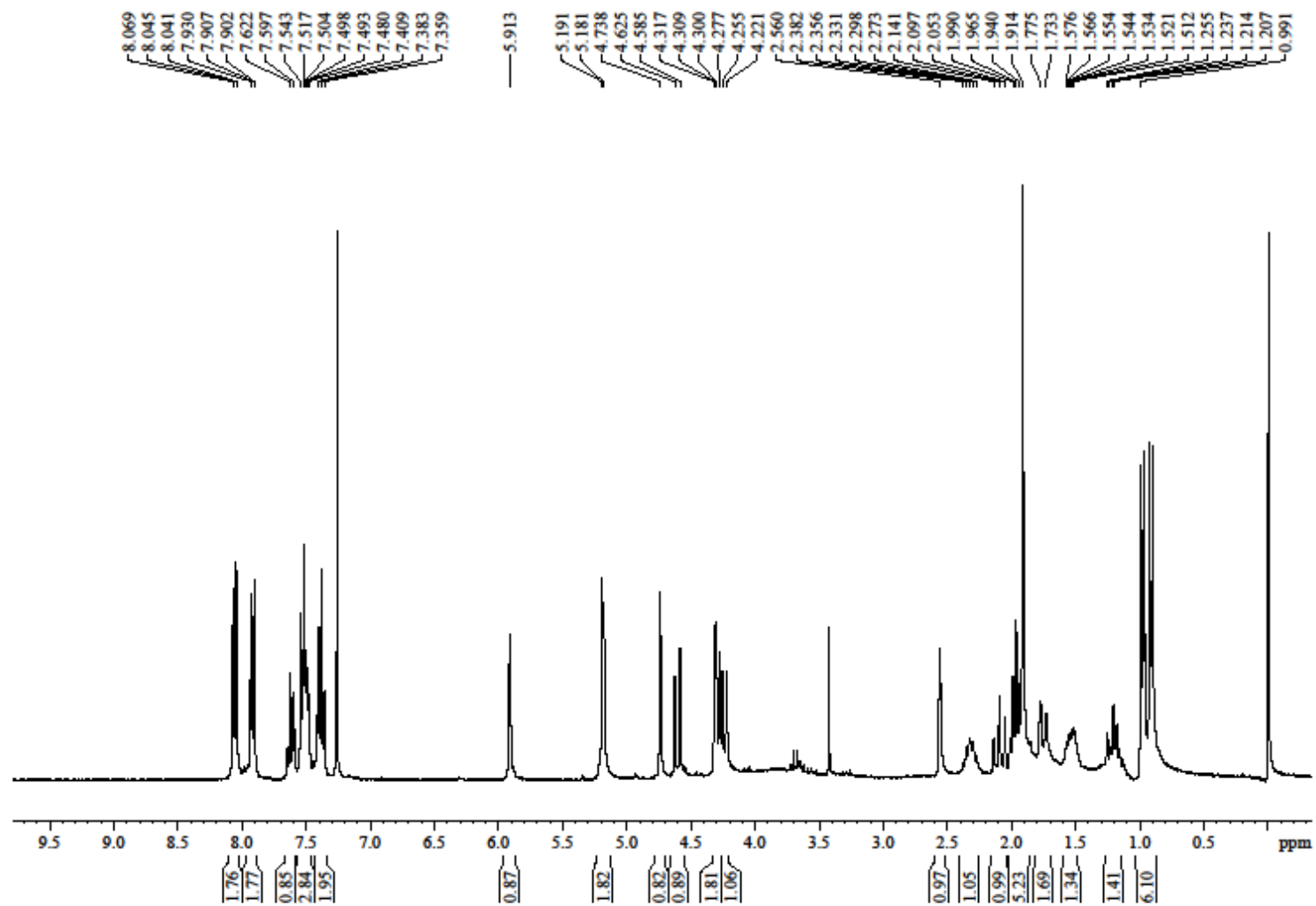
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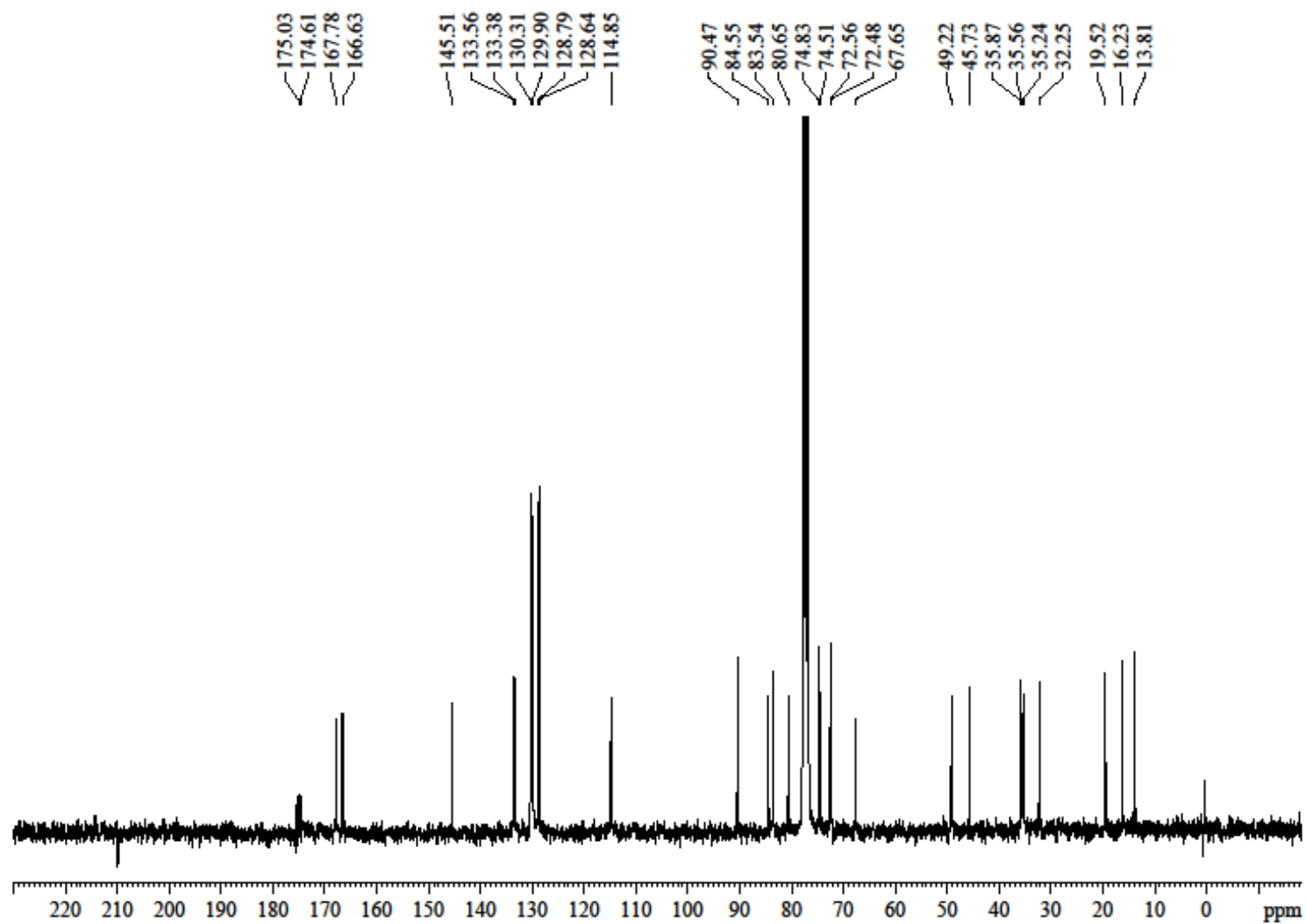
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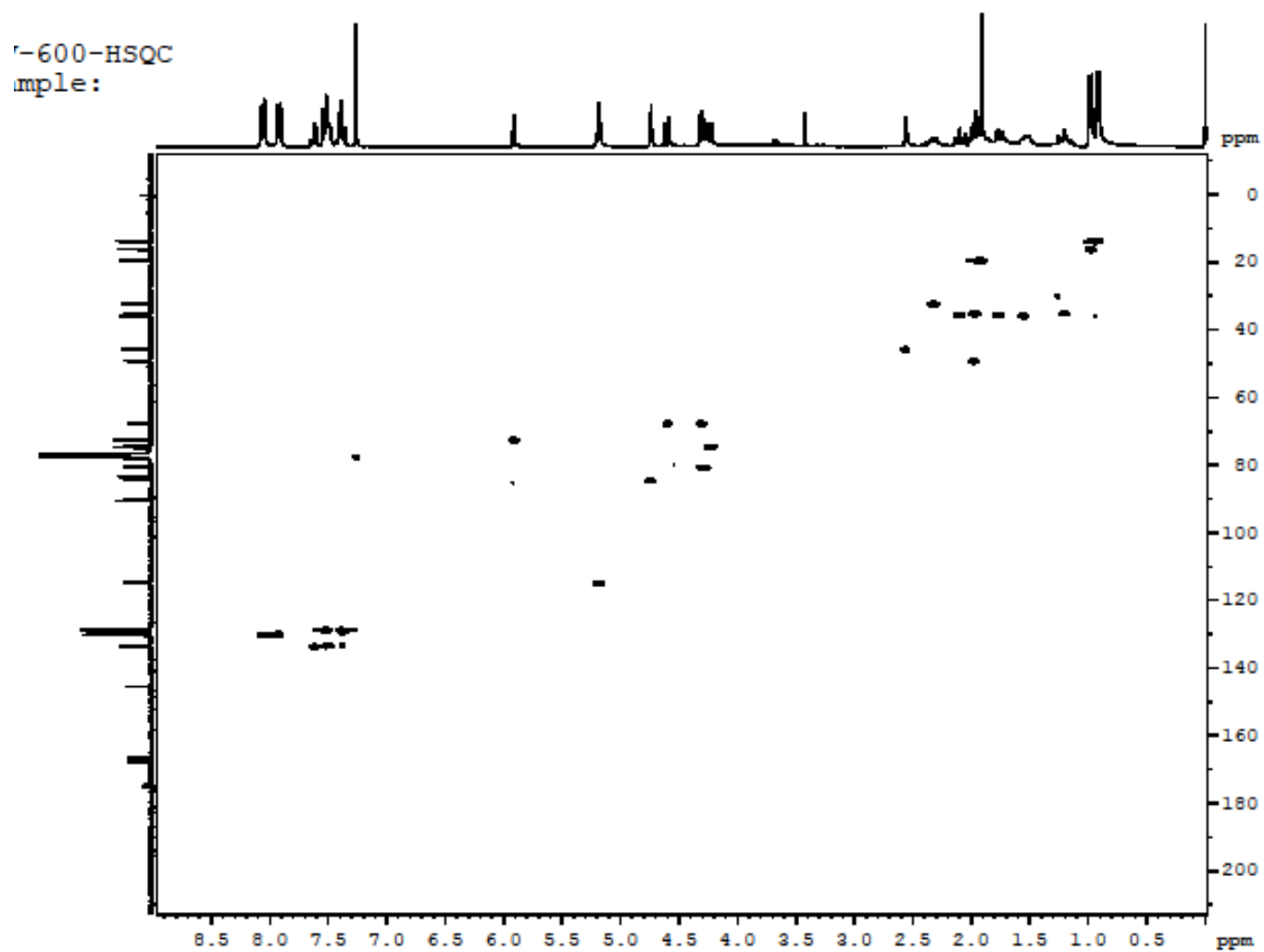
32. ^1H NMR spectrum for compound **8** recorded in CDCl_3 at 600 MHz.



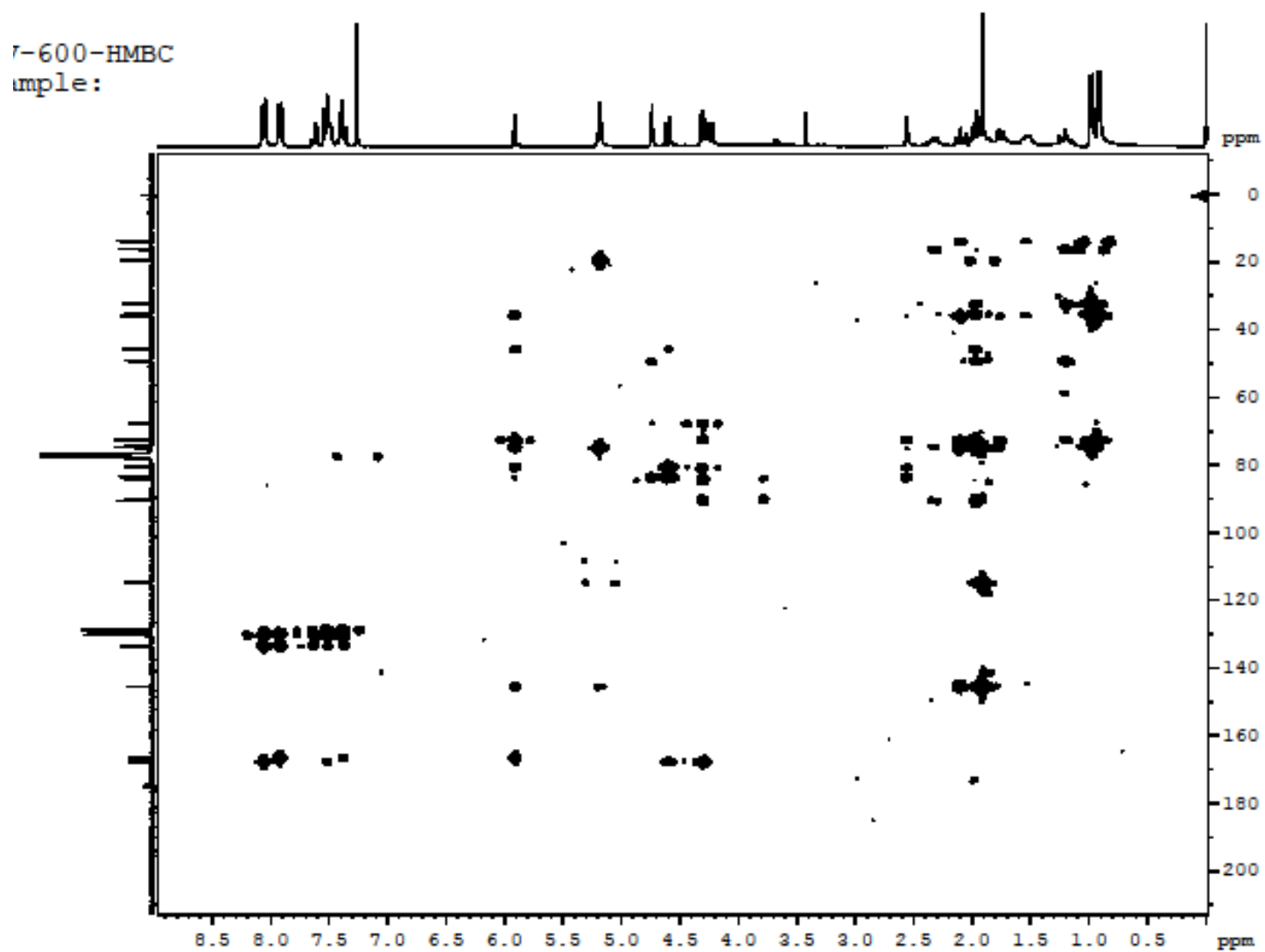
33. ^{13}C NMR spectrum for compound **8** recorded in CDCl_3 at 125 MHz.



34. HSQC spectrum for compound **8** recorded in CDCl₃ at 600 MHz.

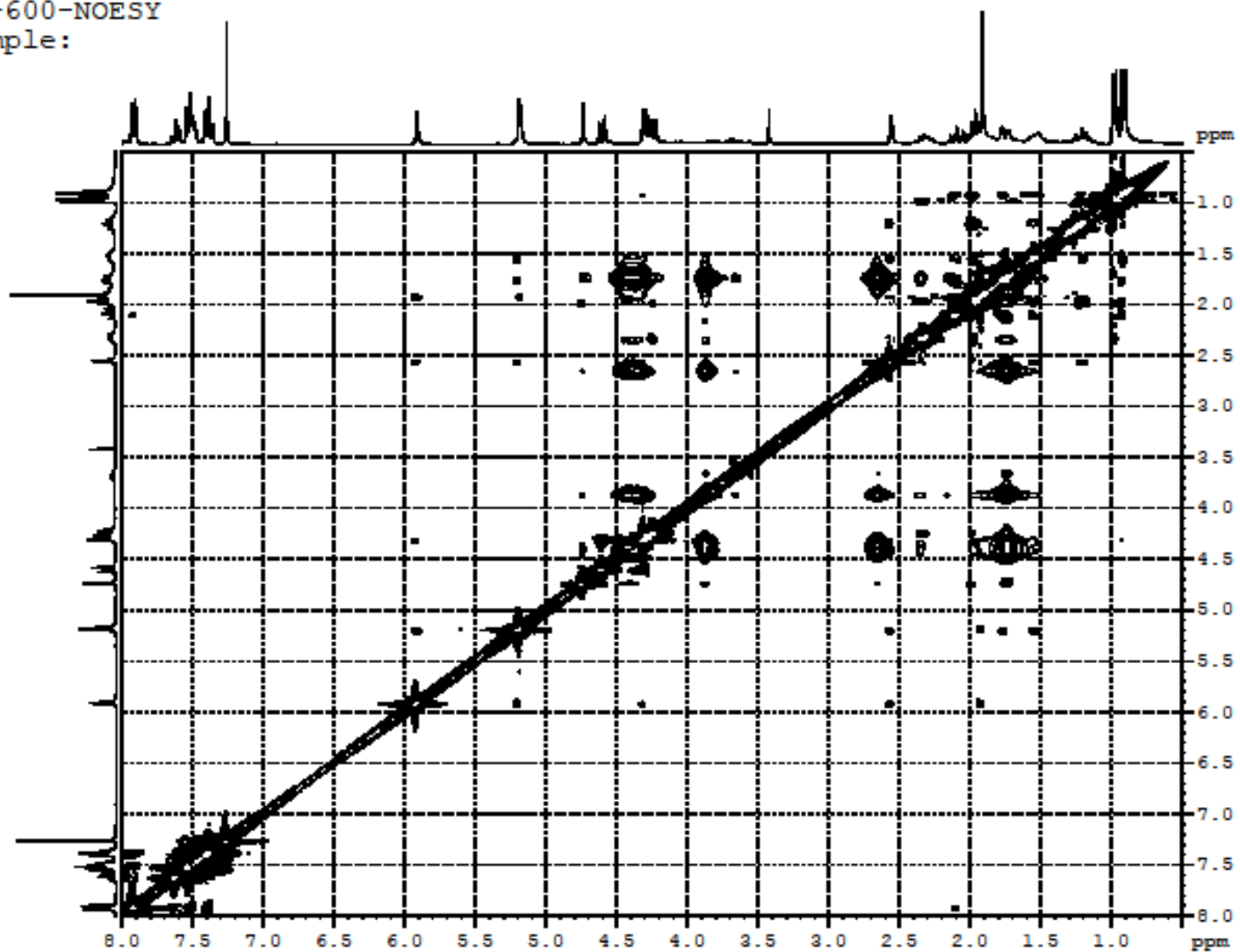


35.HMBC spectrum for compound **8** recorded in CDCl₃ at 600 MHz.



36.NOESY spectrum for compound **8** recorded in CDCl₃ at 600 MHz.

AV-600-NOESY
Sample:



37. HRESIMS spectrum for compound 8.

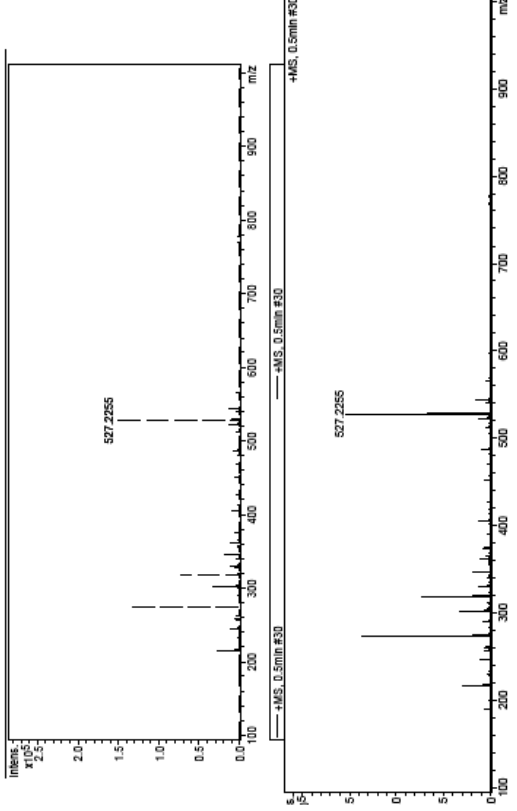
Compound Mass Spectrum List Report

Analysis Info
 Analysis Name D:\data\songs\haoliang\plotfiles\YH-22-B.d
 Method tune_low.m
 Sample Name 3(c)-1.5h-MS
 Comment

Acquisition Date 2008-7-7 18:01:16
 Operator Bruker Customer
 Instrument / Ser# mriOTOF-Q 125

Acquisition Parameter

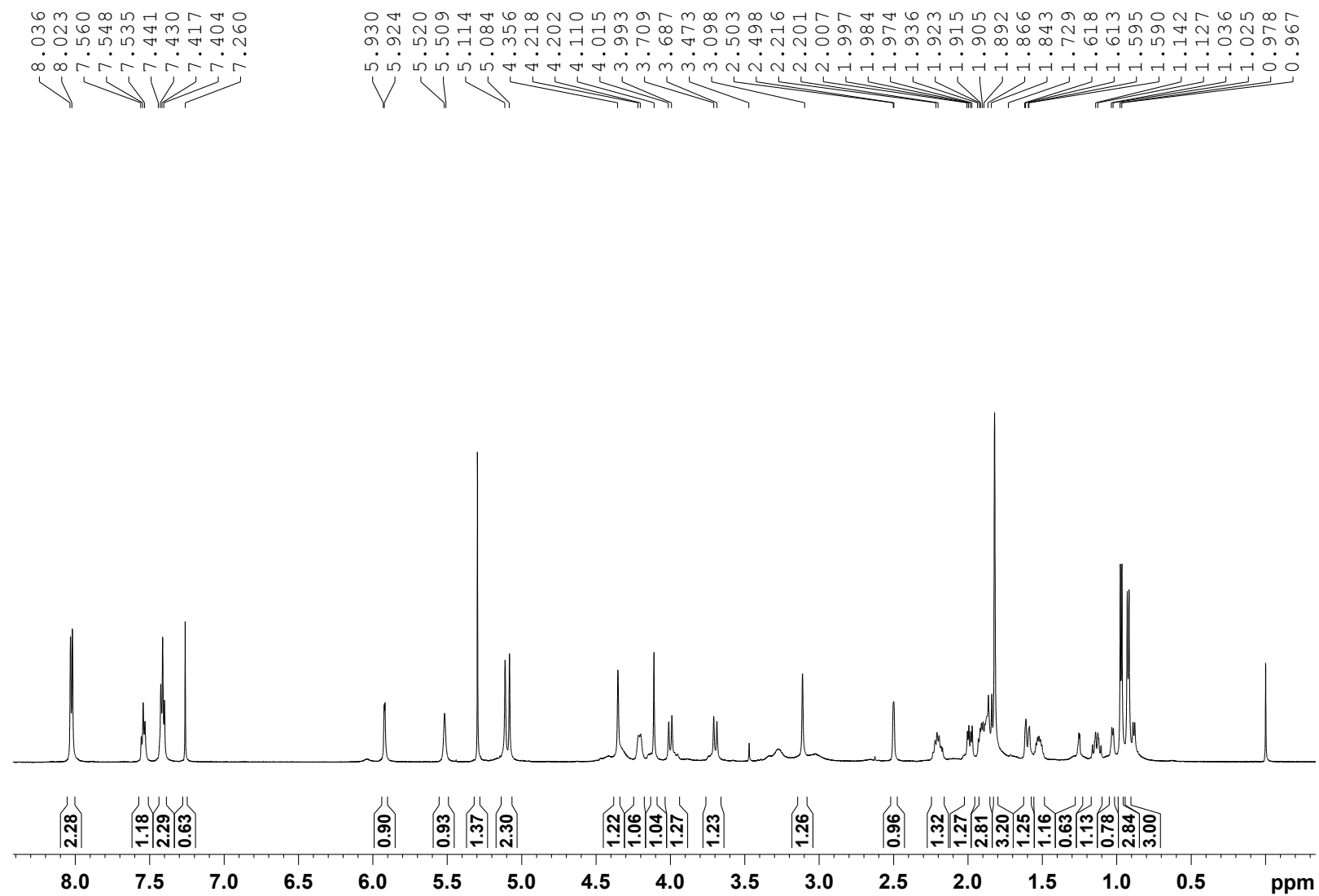
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Header	190 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell P1	200.0 Vpp	Set Divert Valve	Source



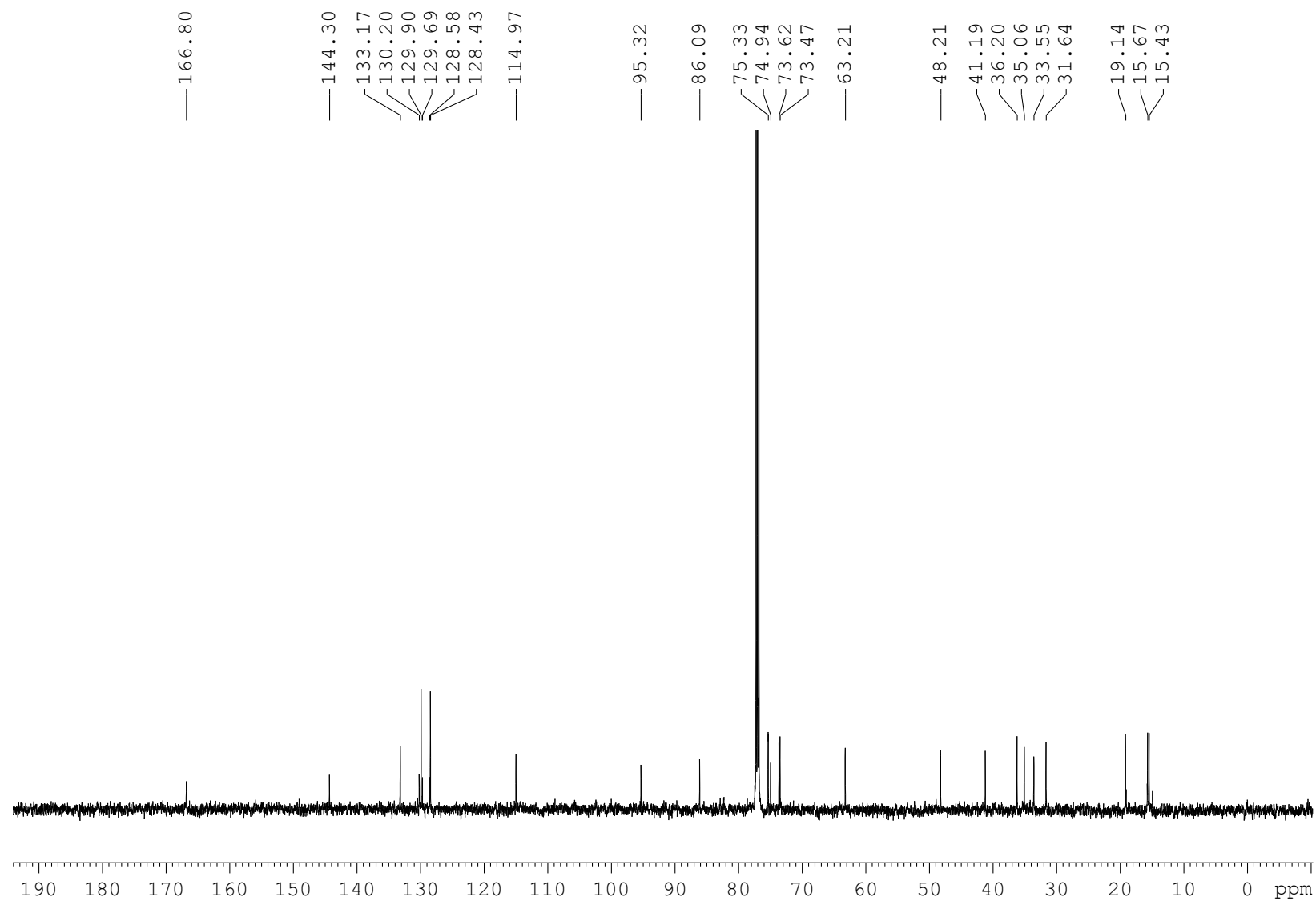
#	m/z	I
1	527.2255	153669
1	527.2255	153669

Sum Formula	Sigma	m/z	Err (ppm)	Mean Err (ppm)	Err (mDa)	rd	N Rule	e
C ₂₇ H ₃₆ Na ₂ O ₉	0.153	527.2252	-0.75	-0.75	-0.39	9.50	OK	even

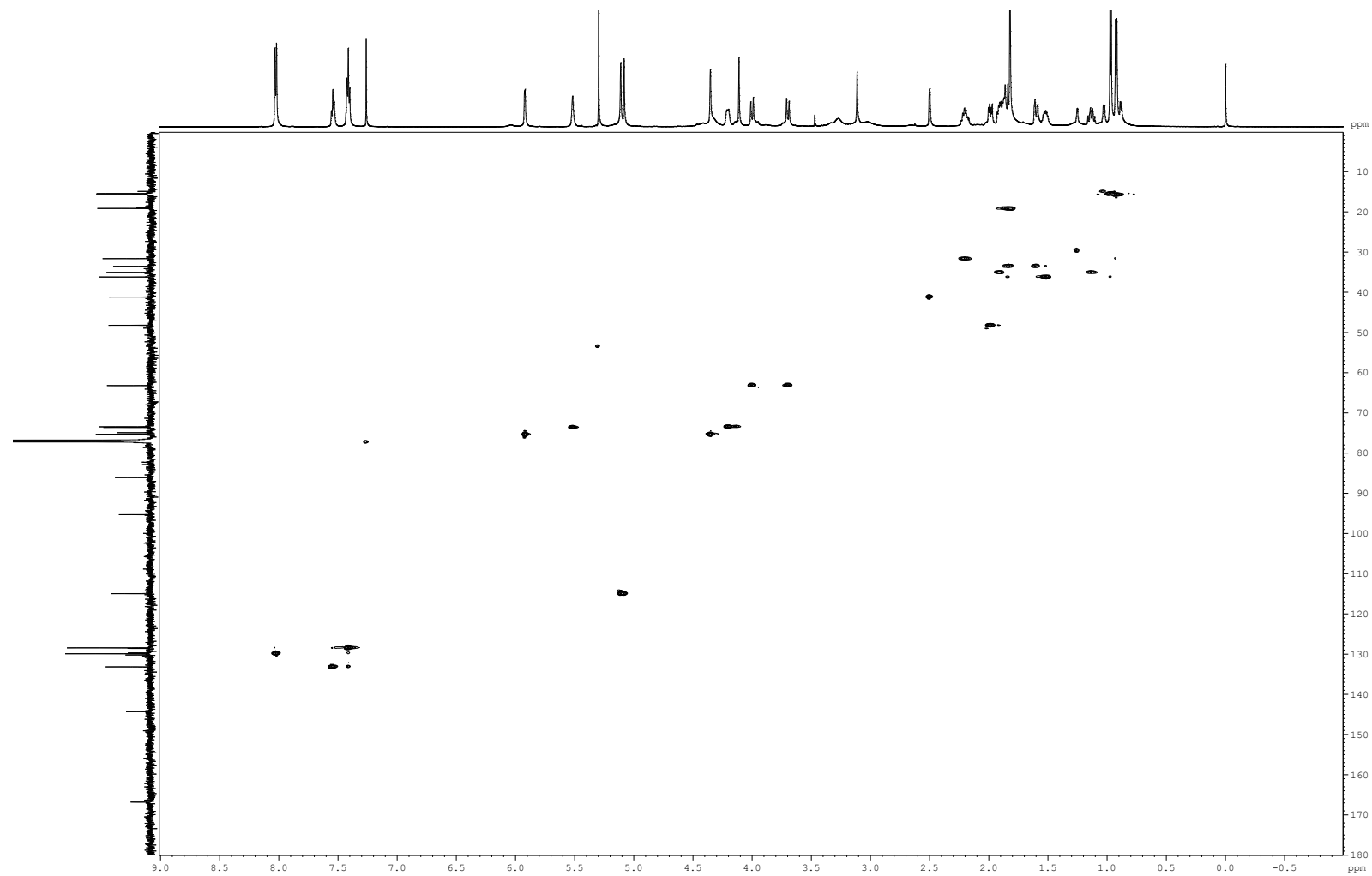
38. ^1H NMR spectrum for compound **8** recorded in CDCl_3 at 600 MHz.



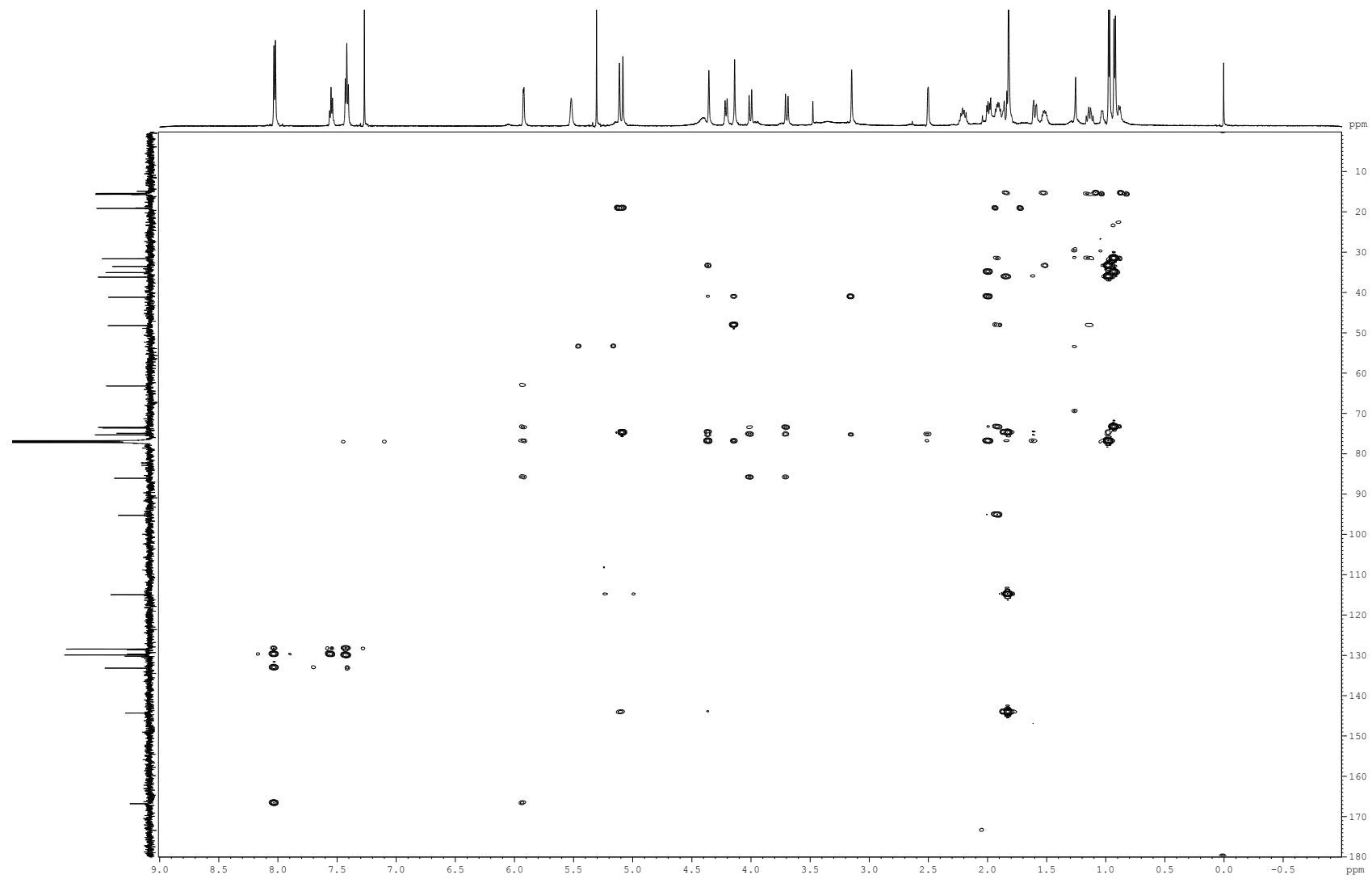
39. ^{13}C NMR spectrum for compound **8** recorded in CDCl_3 at 125 MHz.



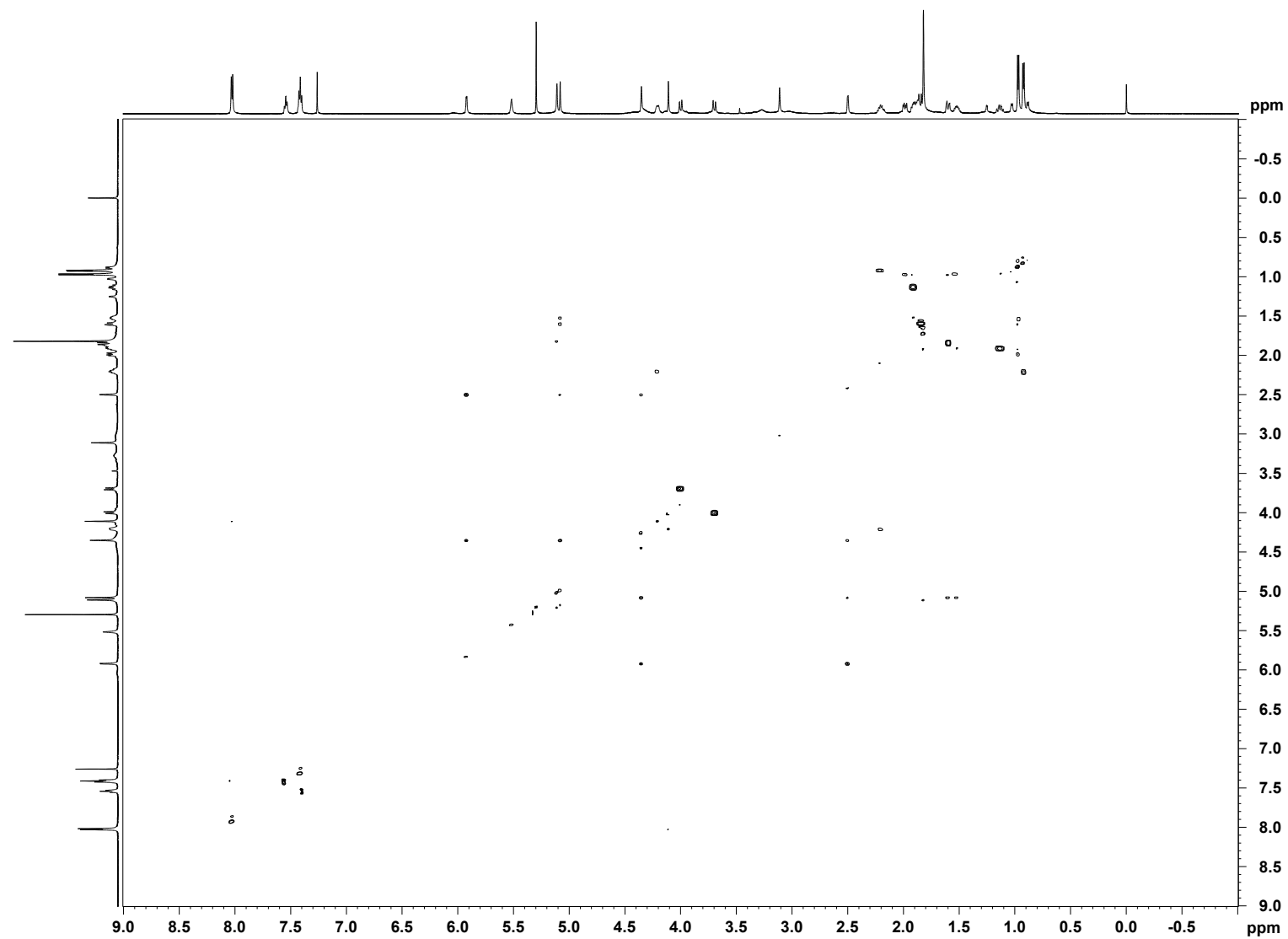
40. HSQC spectrum for compound **8** recorded in CDCl₃ at 600 MHz.



41.HMBC spectrum for compound **8** recorded in CDCl₃ at 600 MHz.



42.NOESY spectrum for compound **8** recorded in CDCl₃ at 600 MHz.



43. HRESIMS spectrum for compound 9.

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\20140320ceyang\YHS-1_1-b,1_01_2877.d
 Method 20131026ceyang.m
 Sample Name YHS-1
 Comment

Acquisition Date 3/20/2014 3:04:23 PM

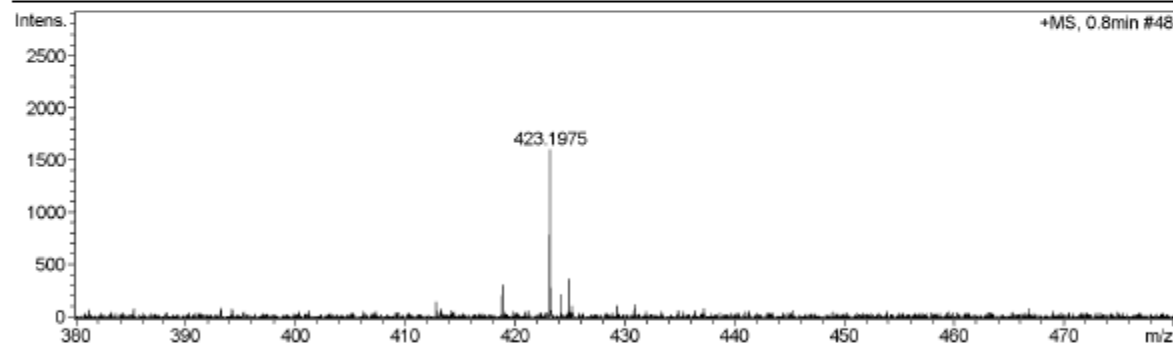
Operator Bruker Customer
 Instrument / Ser# micrOTOF-Q 125

Acquisition Parameter

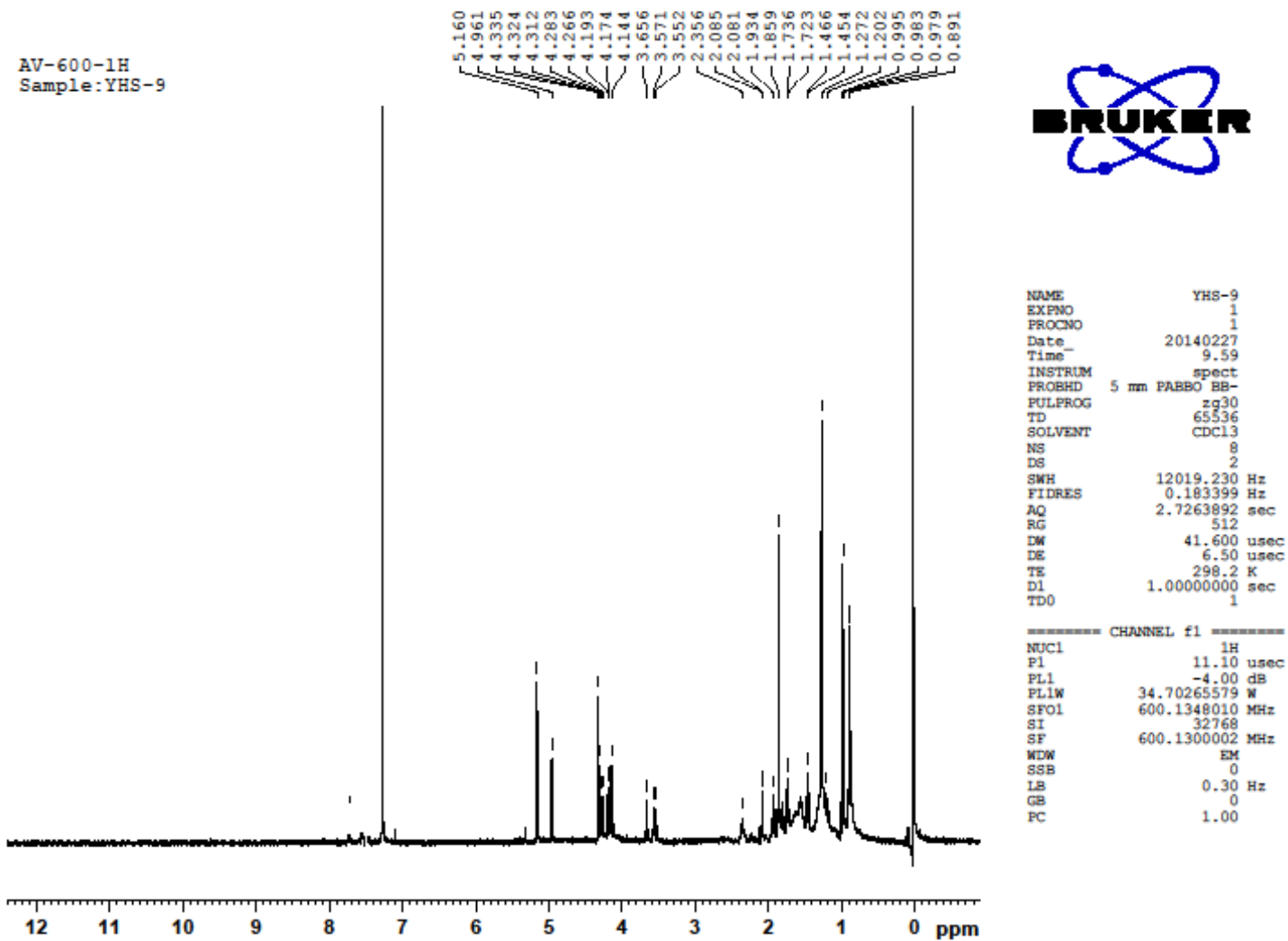
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C20H32O8Na				
Formula, max.					
Measured m/z	423.197	Tolerance	5 ppm	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nitrogen Rule	no	Electron Configuration	both		
Filter H/C Ratio	no	Minimum	0	Maximum	3
Estimate Carbon	yes				

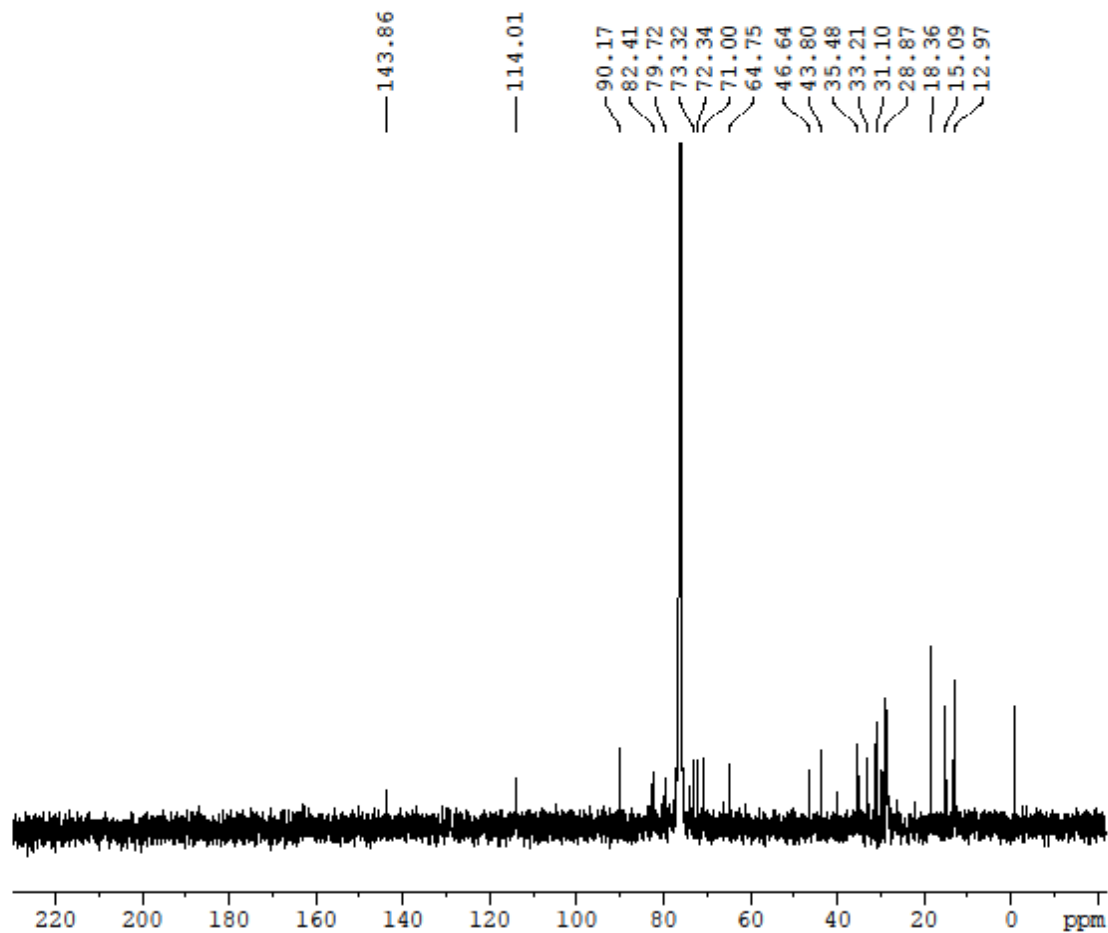


Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C ₂₀ H ₃₂ Na ₁ O ₈	0.052	423.1989	3.36	3.09	1.42	4.50	ok	even

44. ^1H NMR spectrum for compound **9** recorded in CDCl_3 at 600 MHz

45. ^{13}C NMR spectrum for compound **9** recorded in CDCl_3 at 125 MHz.

AV-600-13C
Sample:YHS-9



```

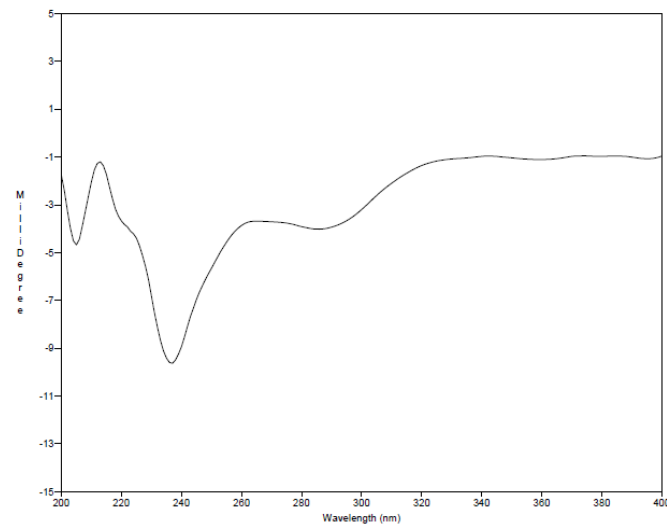
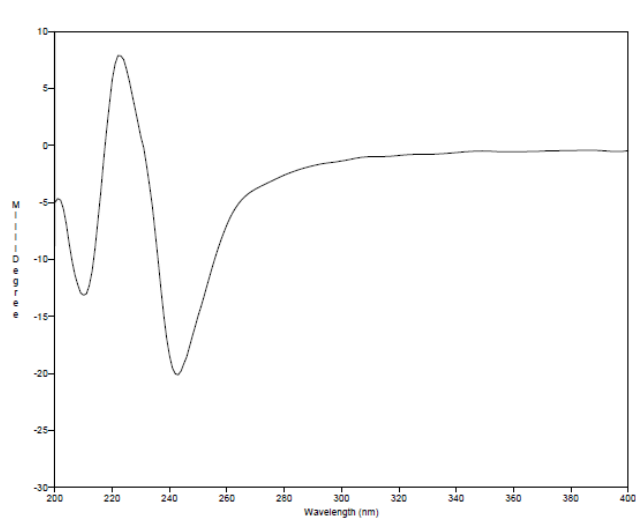
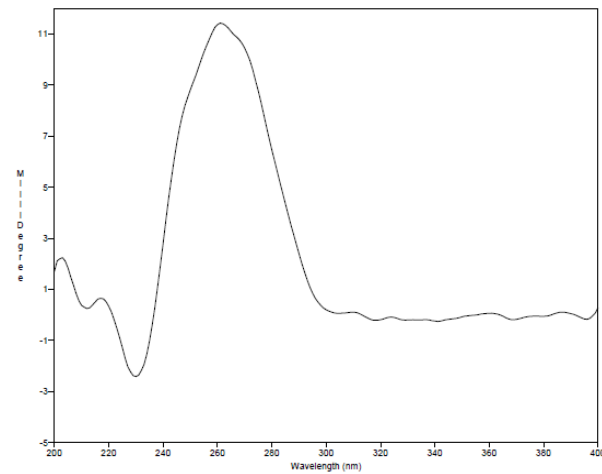
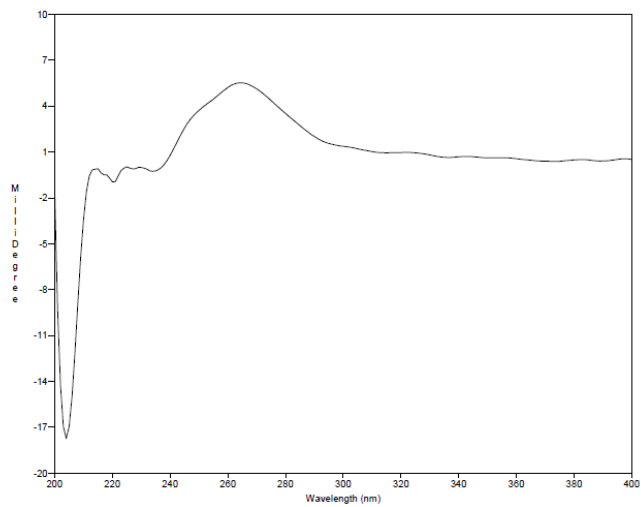
NAME          YHS-9(2)
EXPNO         2
PROCNO        1
Date_         20140624
Time          7.53
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            13757
DS            2
SWH           45454.547 Hz
FIDRES        0.693581 Hz
AQ            0.7209570 sec
RG            23100
DW            11.000 usec
DE            6.50 usec
TE            296.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
  
```

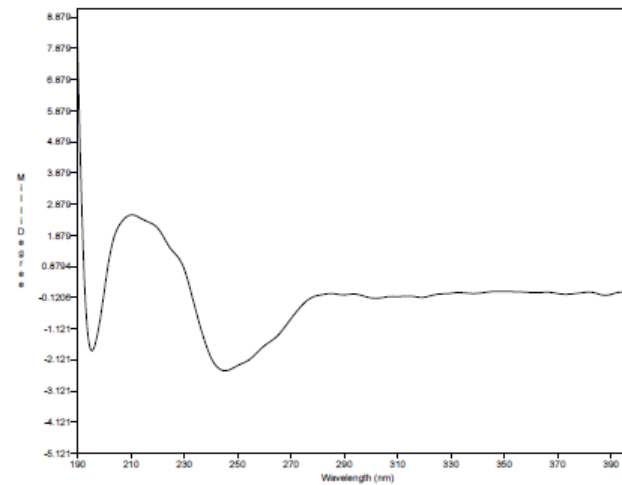
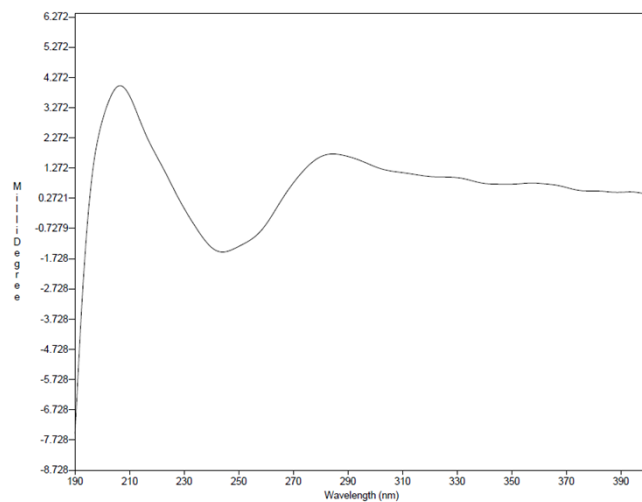
```

===== CHANNEL #1 =====
NUC1          13C
P1            6.00 usec
PL1           1.00 dB
PL1W          83.20243835 W
SFO1          150.9178993 MHz
  
```

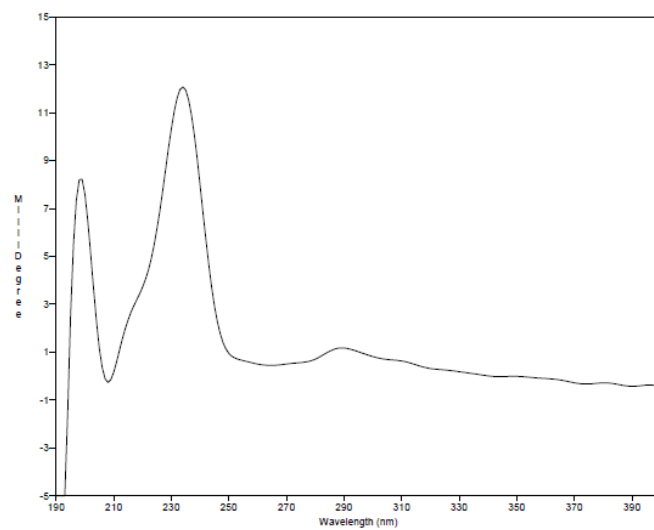
```

===== CHANNEL #2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -4.00 dB
PL12          13.16 dB
PL13          16.00 dB
PL2W          34.70265579 W
PL12W         0.66736388 W
PL13W         0.34702653 W
SFO2          600.1324005 MHz
SI            32768
SF            150.9029343 MHz
WDW           EM
SSB           0
LB            3.00 Hz
GB            0
PC            1.40
  
```

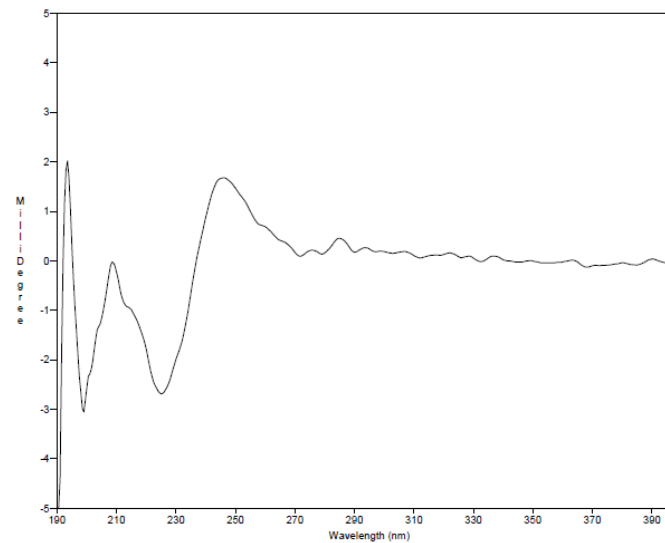

46. CD spectrum for compounds **1-8**.CD spectrum for compound **1** . CD spectrum for compound **2**CD spectrum for compound **3** . CD spectrum for compound **4** .



CD spectrum for compound 5 .CD spectrum for compound 6 .

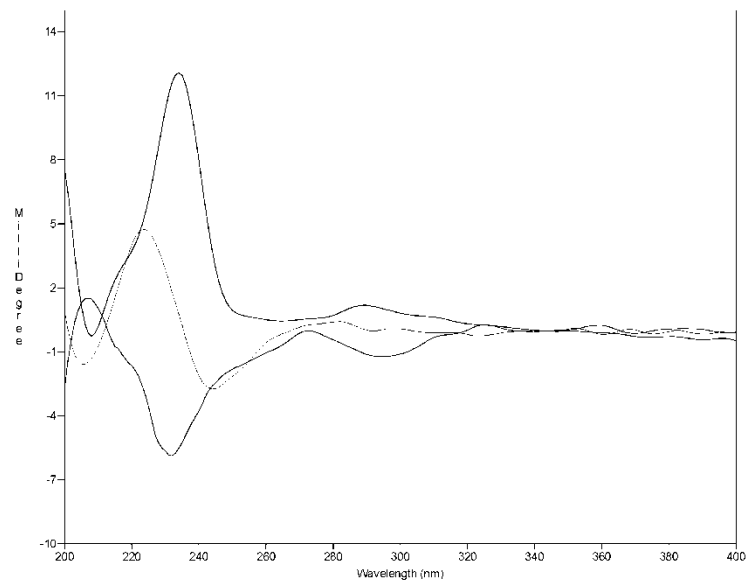


CD spectrum for compound 7 .



CD spectrum for compound 8

47. CD spectrum for the combination of several compounds
CD spectrum for compounds **1,2** and **8**



Bio-Kine Software V4.71 Date : 2014-4-1 Time : 9:31:10

PLOT 1 COMMENTS :

File name : d:\E307\yh-22-a.bka
Savitzky-Golay Smooth of sav-golay
Window Points=15
Polynomial Order=3
Derivative=0

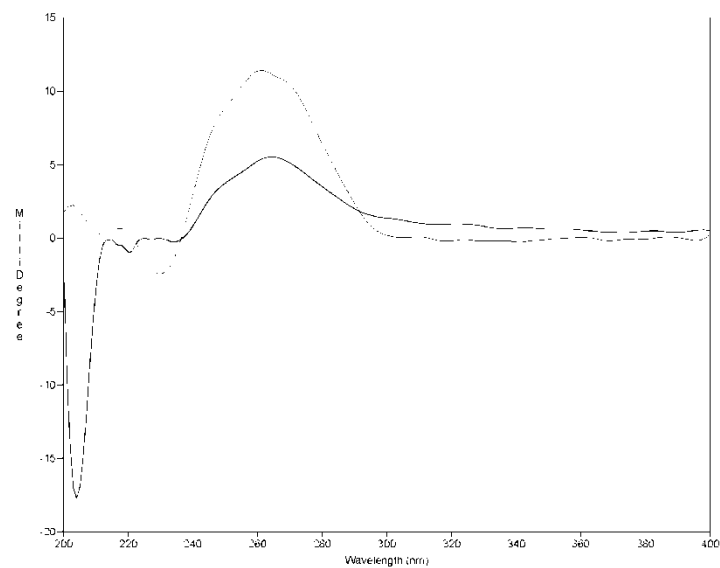
PLOT 2 COMMENTS :

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Savitzky-Golay Smooth of sav-golay
Window Points=15
Polynomial Order=3
Derivative=0

PLOT 3 COMMENTS :

File name : d:\E307\yh-3--bka
Savitzky-Golay Smooth of sav-golay
Window Points=15
Polynomial Order=3
Derivative=0

CD spectrum for compounds **3** and **4**



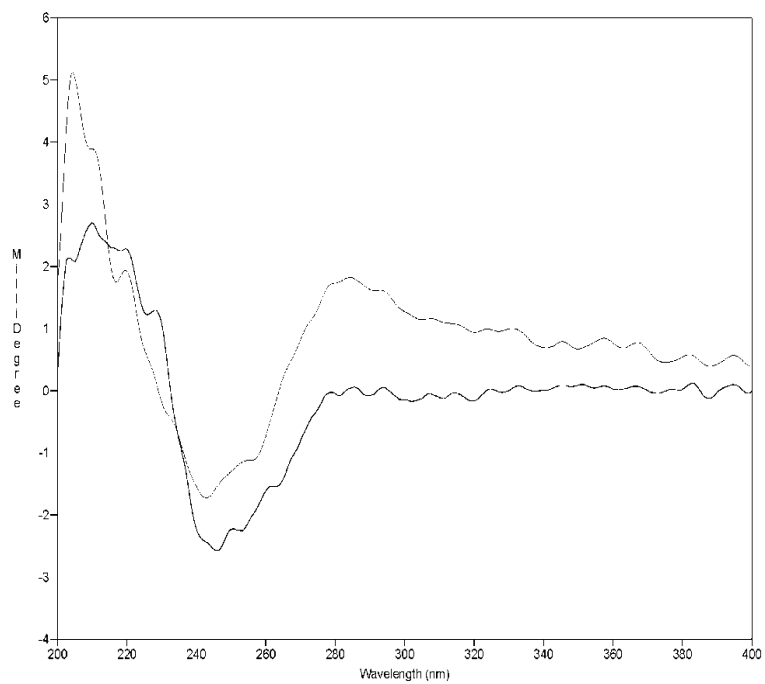
Bio-Kine Software V4.71 Date : 2014-4-1 Time : 11:01:40

PLOT 1 COMMENTS

File name : d:\E307\yh-38-2.bka
Savitzky-Golay Smooth of sav-golay
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Polynomial Order=3
Derivative=0

PLOT 2 COMMENTS

File name : d:\E307\yh-38-4-1.bka
Savitzky-Golay Smooth of sav-golay
Window Points=15
Polynomial Order=3
Derivative=0

CD spectrum for compounds **5** and **6**

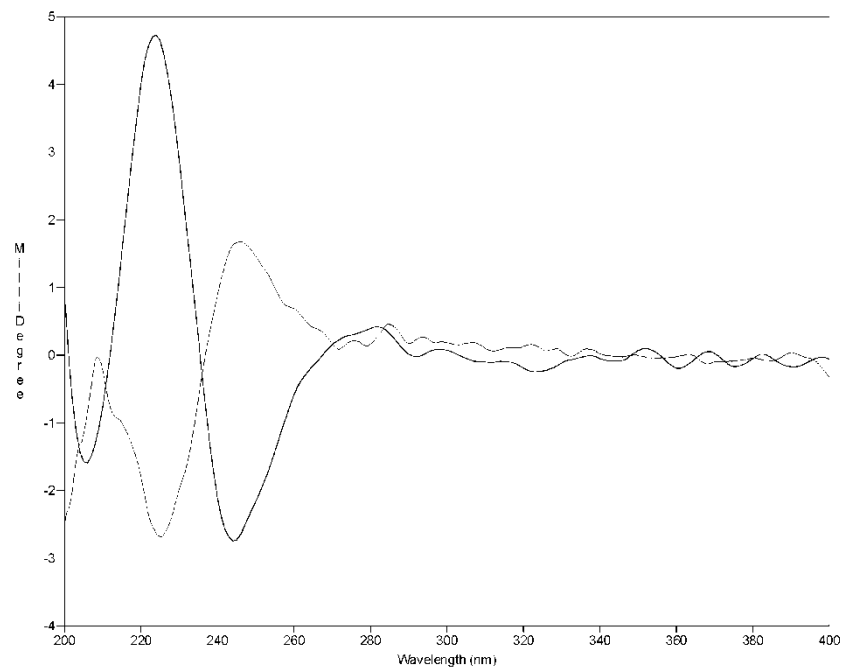
Bio-Kine Software V4.71 Date : 2014-4-1 Time : 11:02:34

PLOT 1 COMMENTS :

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Savitzky-Golay Smooth of sav-golay
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Polynomial Order=3
Derivative=0

PLOT 2 COMMENTS :

File name : d:\李玲芝\39-2-16.bka
Savitzky-Golay Smooth of sav-golay
Window Points=15

CD spectrum for compounds **8** and **8**

Bio-Kine Software V4.71 Date : 2014-4-1 Time : 9:37:59

PLOT 1 COMMENTS :

File name : d:\李玲芝\22-b.bka
Savitzky-Golay Smooth of sav-golay
Window Points=15
Polynomial Order=3
Derivative=0

PLOT 2 COMMENTS :

File name : d:\李玲芝\22-a.bka
Savitzky-Golay Smooth of sav-golay
Window Points=15
Polynomial Order=3
Derivative=0

48. Stereoviews of compounds 1-8

