

# Silibinin Derivatives as Anti-Prostate Cancer Agents: Synthesis and Cell-Based Evaluations

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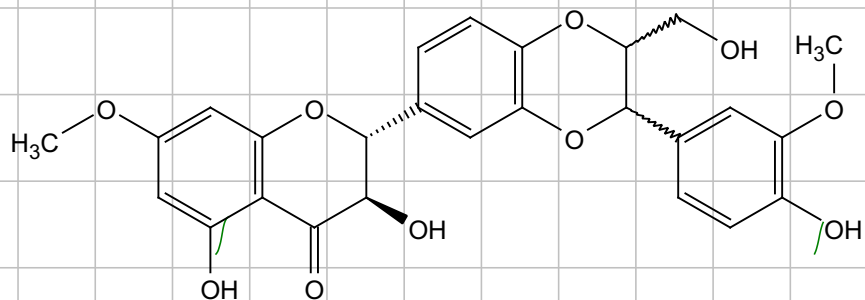
<sup>b</sup>RCMI Cancer Research Center and <sup>c</sup>Department of Chemistry, Xavier University of Louisiana, 1 Drexel Drive, New Orleans, LA 70125, USA

\* Corresponding author. Tel.: +1 559 2782394.

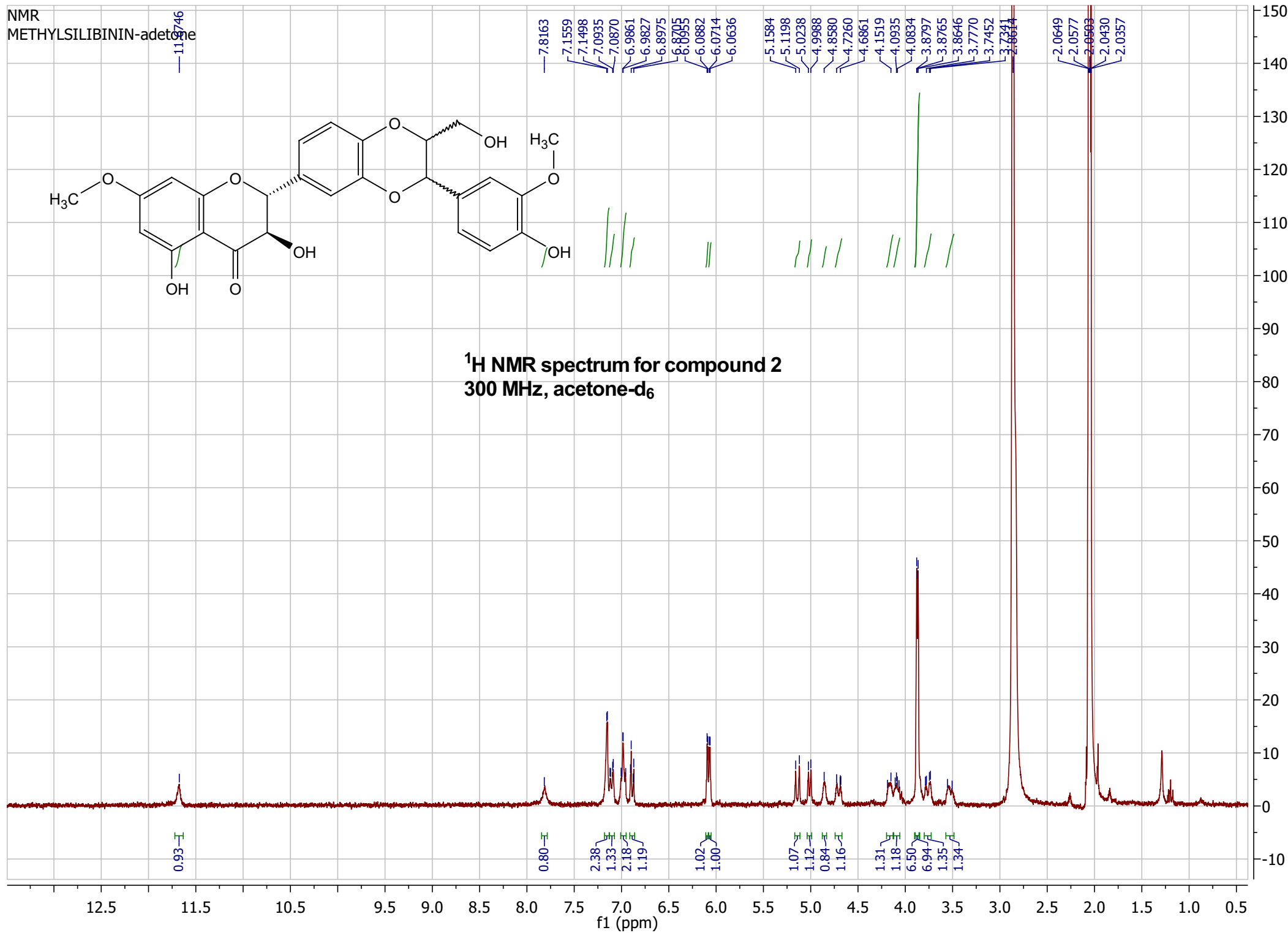
E-mail address: qchen@csufresno.edu

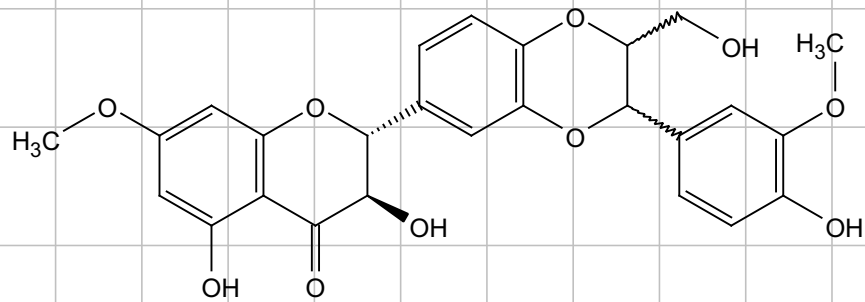
**Supporting Information:** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of final compounds

NMR  
METHYLSILIBININ-acetone



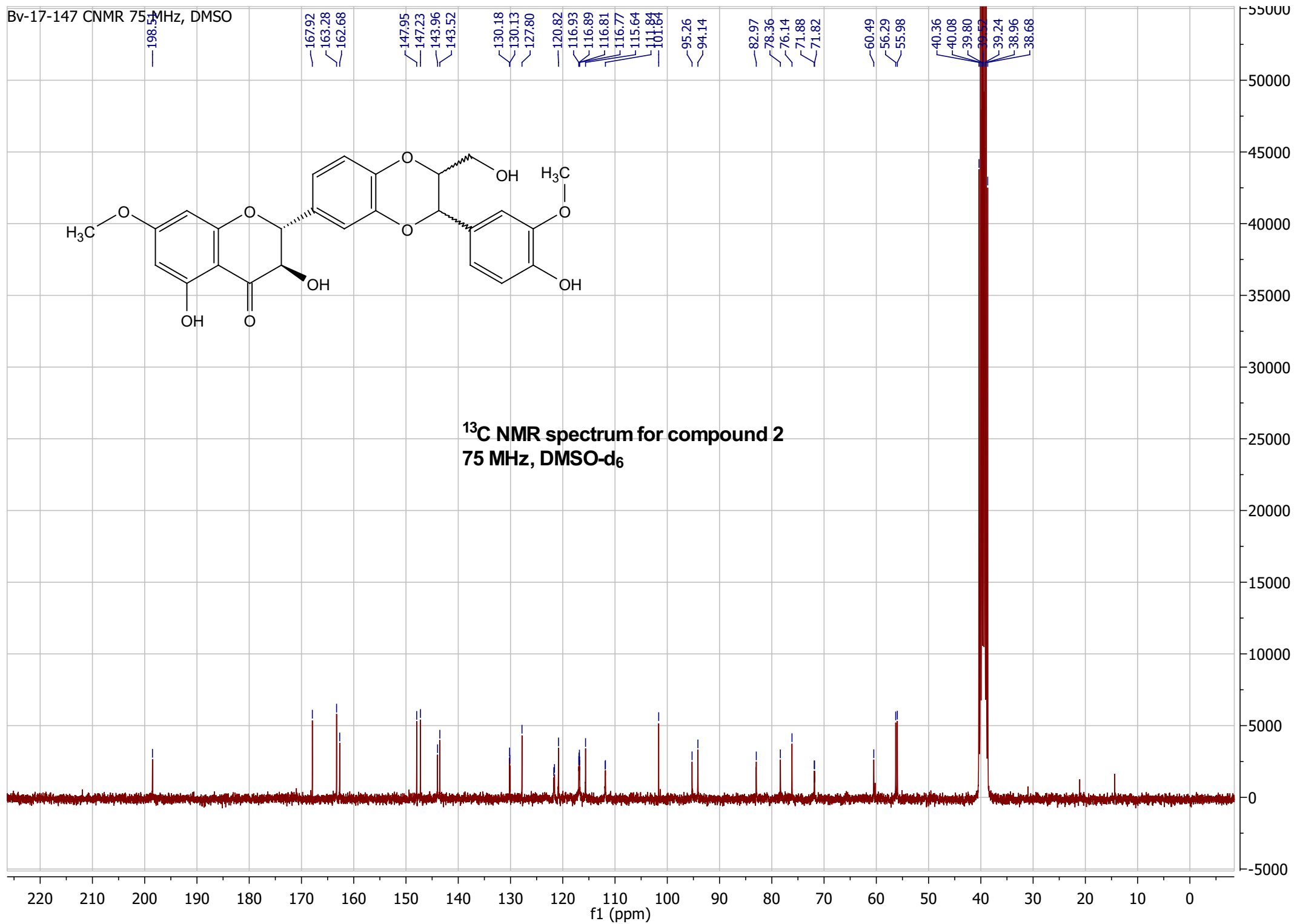
<sup>1</sup>H NMR spectrum for compound 2  
300 MHz, acetone-d<sub>6</sub>

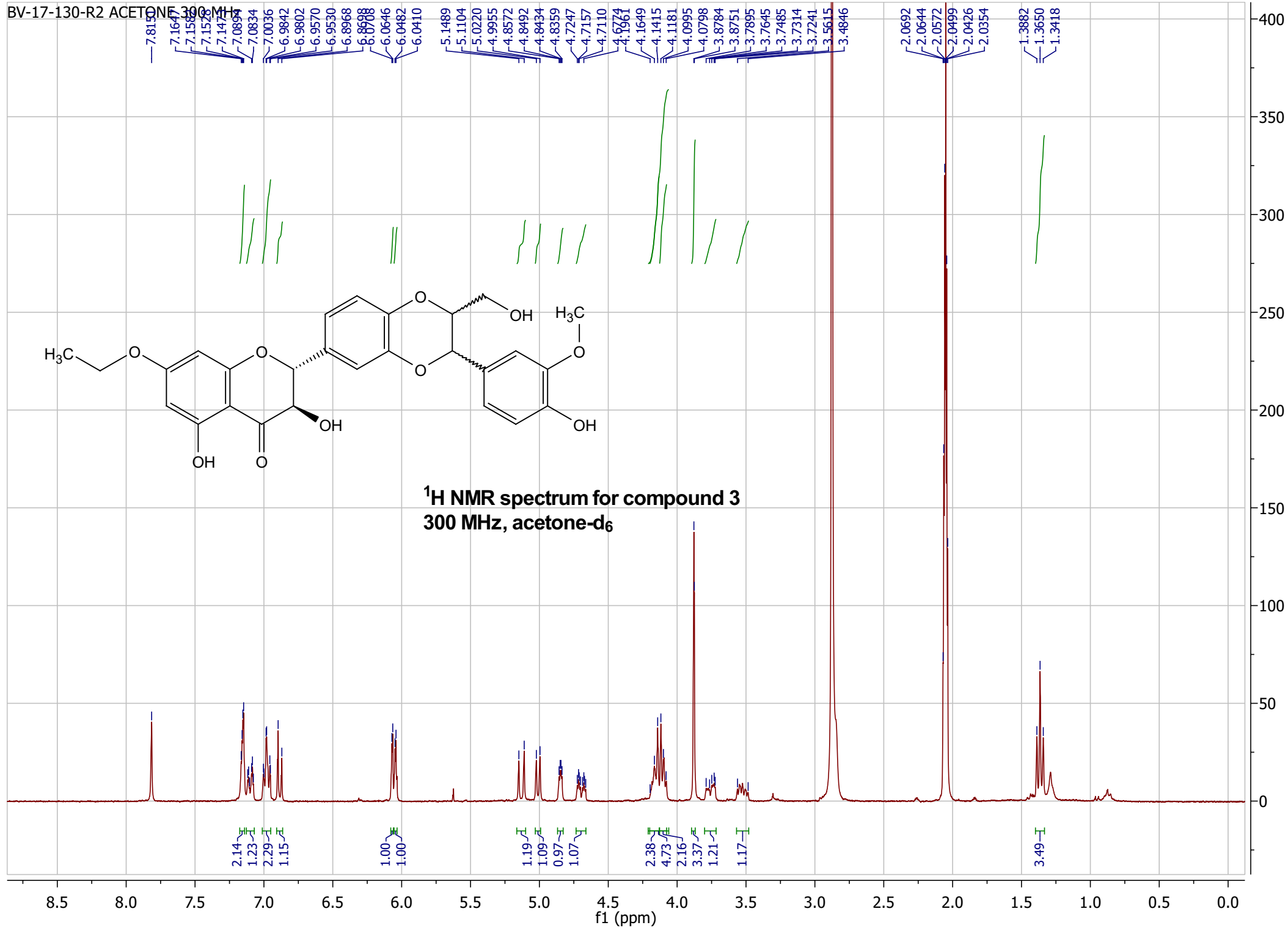




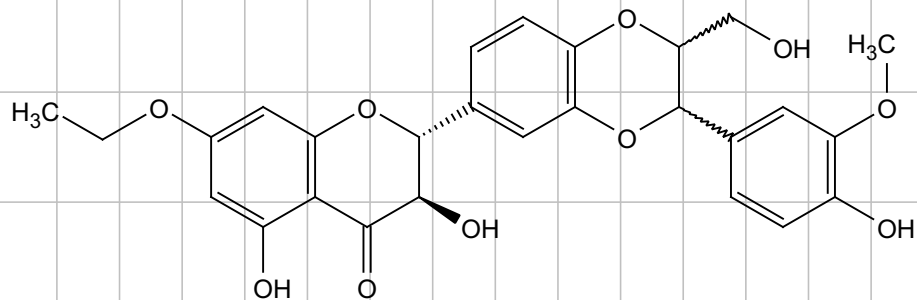
- 198.5
- 167.92
- 163.28
- 162.68
- 147.95
- 147.23
- 143.96
- 143.52
- 130.18
- 130.13
- 127.80
- 120.82
- 116.93
- 116.89
- 116.81
- 116.77
- 115.64
- 101.84
- 95.26
- 94.14
- 82.97
- 78.36
- 76.14
- 71.88
- 71.82
- 60.49
- 56.29
- 55.98
- 40.36
- 40.08
- 39.80
- 39.52
- 39.24
- 38.96
- 38.68

<sup>13</sup>C NMR spectrum for compound 2  
75 MHz, DMSO-d<sub>6</sub>

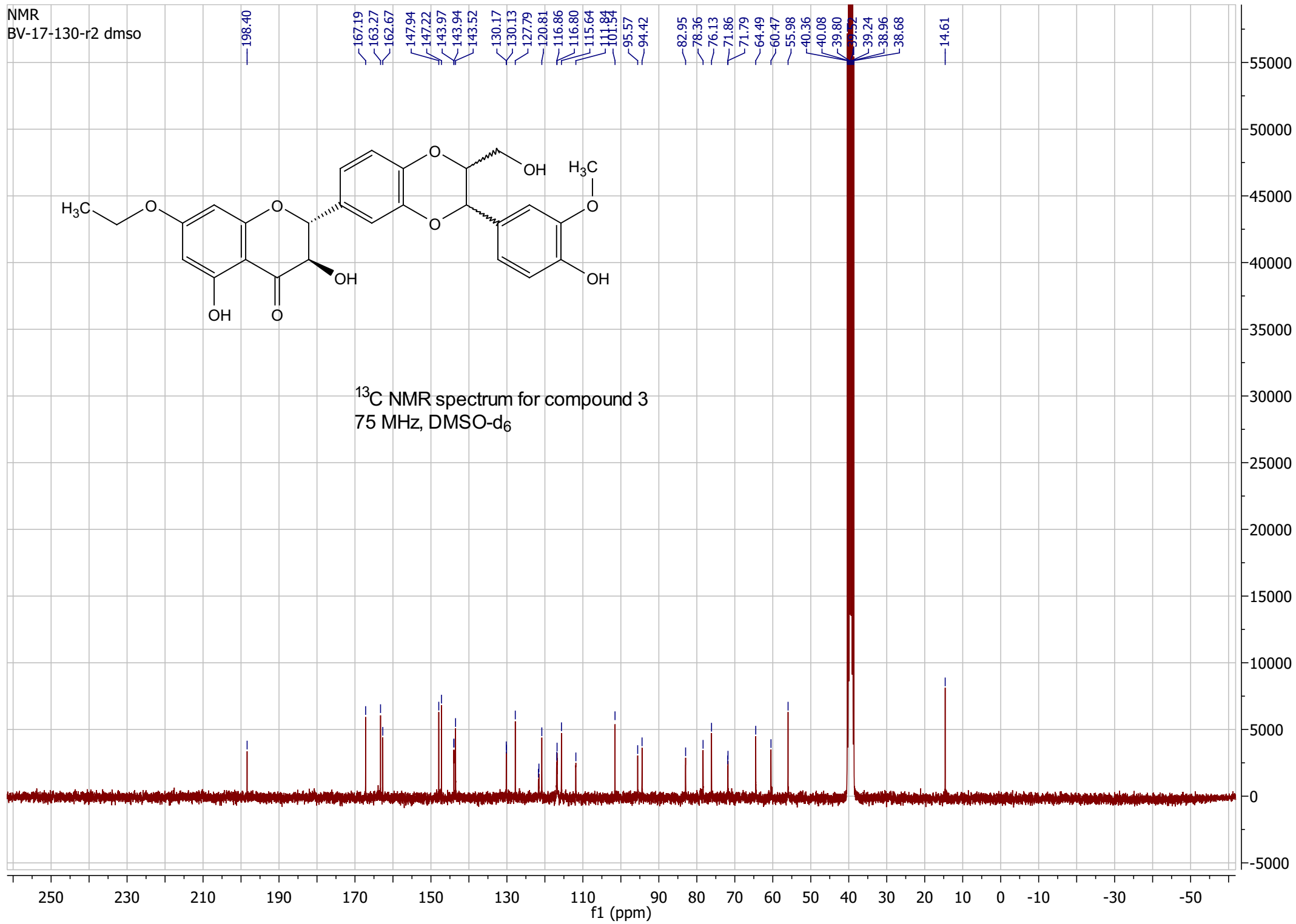


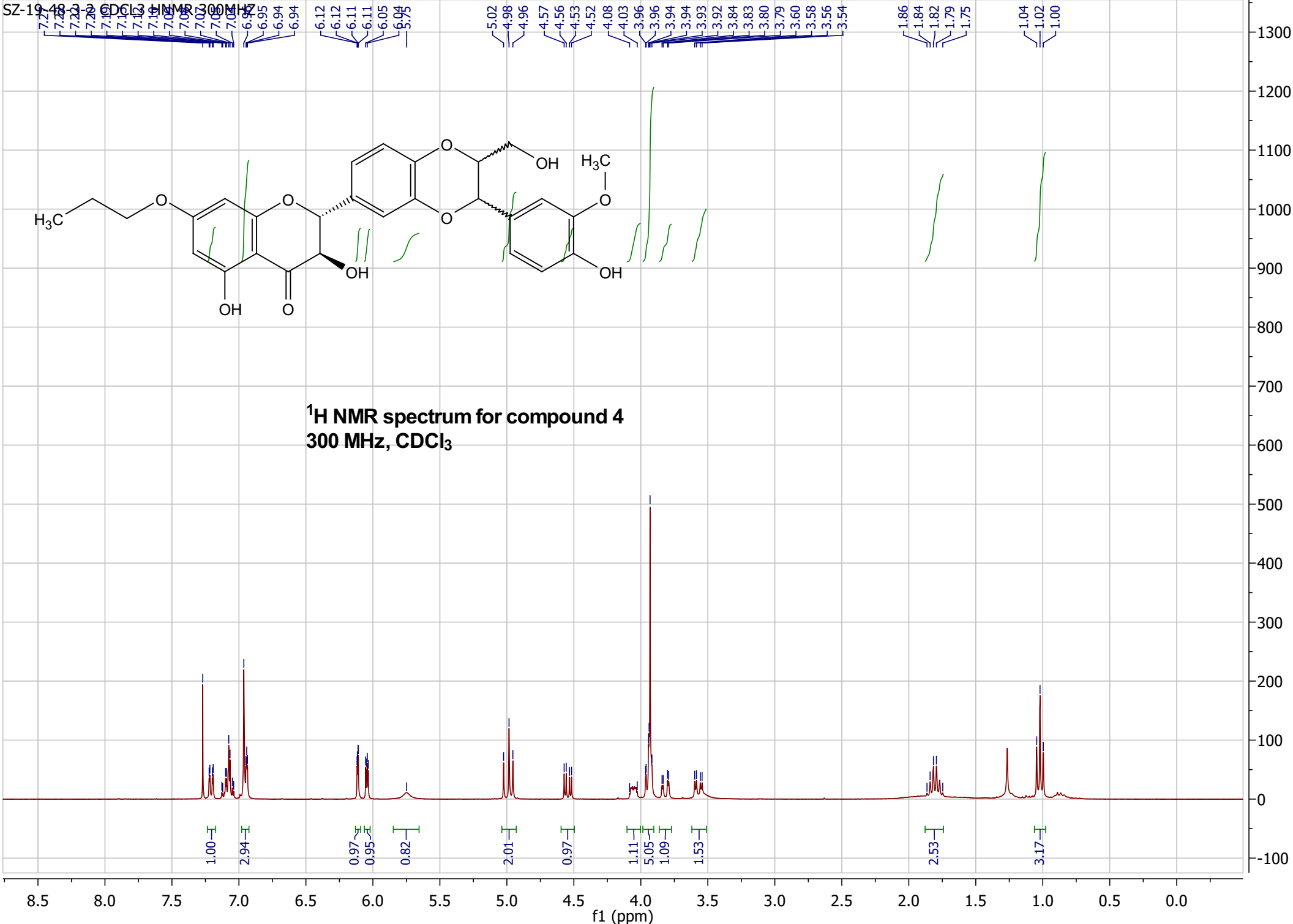


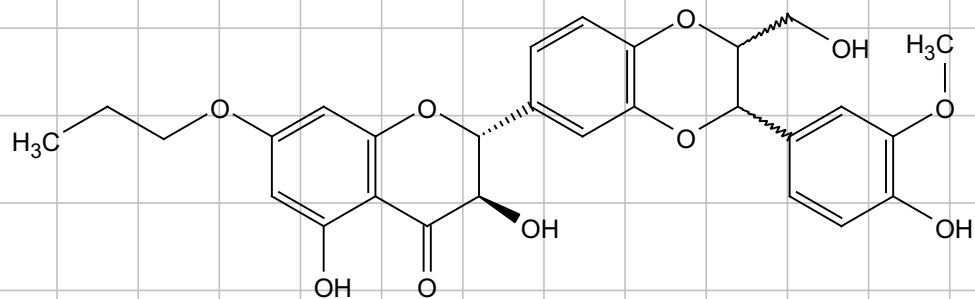
NMR  
BV-17-130-r2 dmso



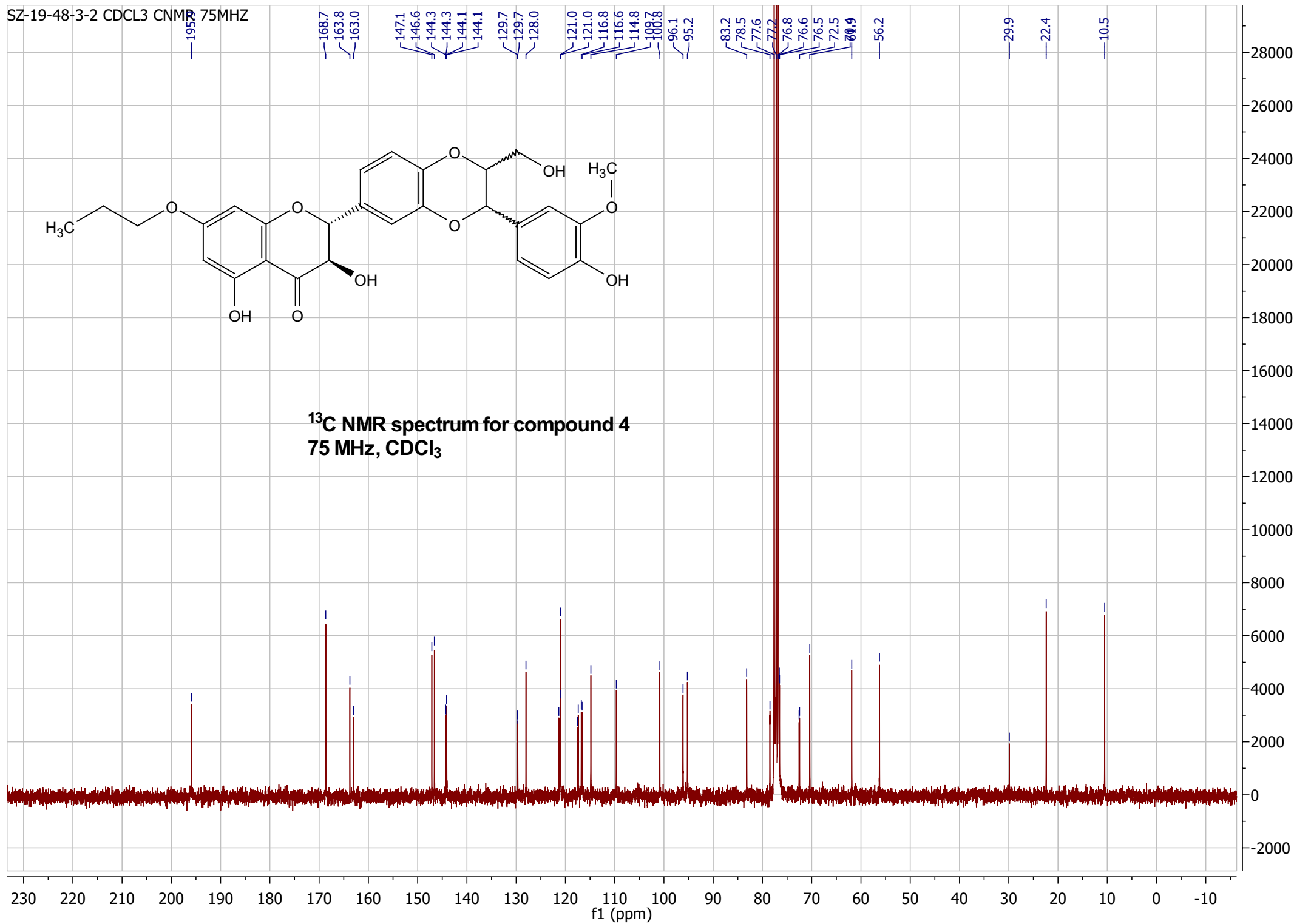
<sup>13</sup>C NMR spectrum for compound 3  
75 MHz, DMSO-d<sub>6</sub>

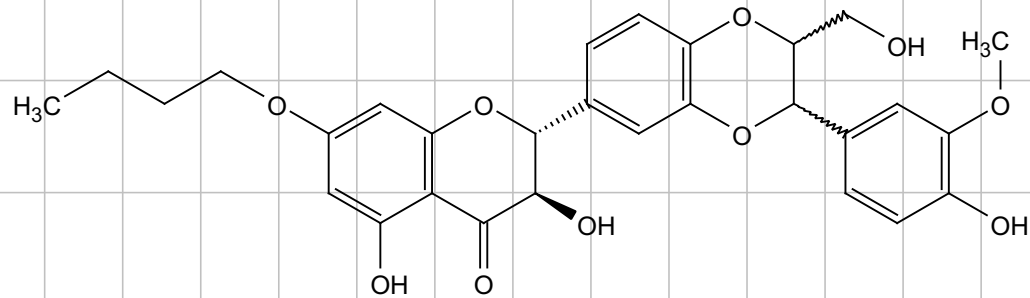




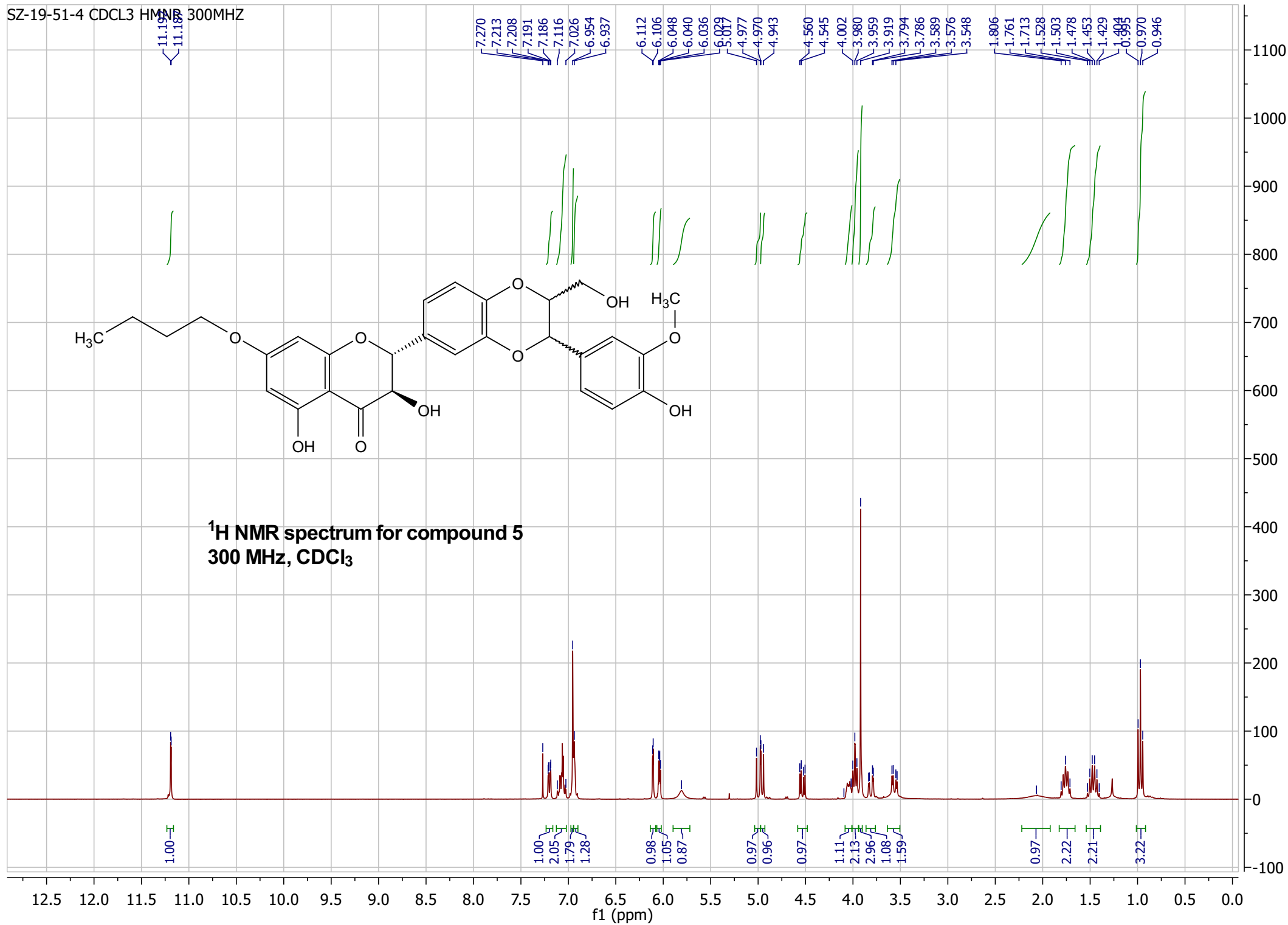


**<sup>13</sup>C NMR spectrum for compound 4**  
**75 MHz, CDCl<sub>3</sub>**



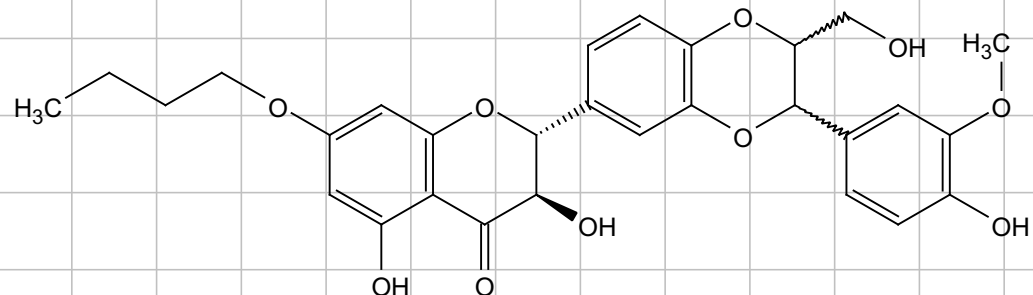


**<sup>1</sup>H NMR spectrum for compound 5  
300 MHz, CDCl<sub>3</sub>**

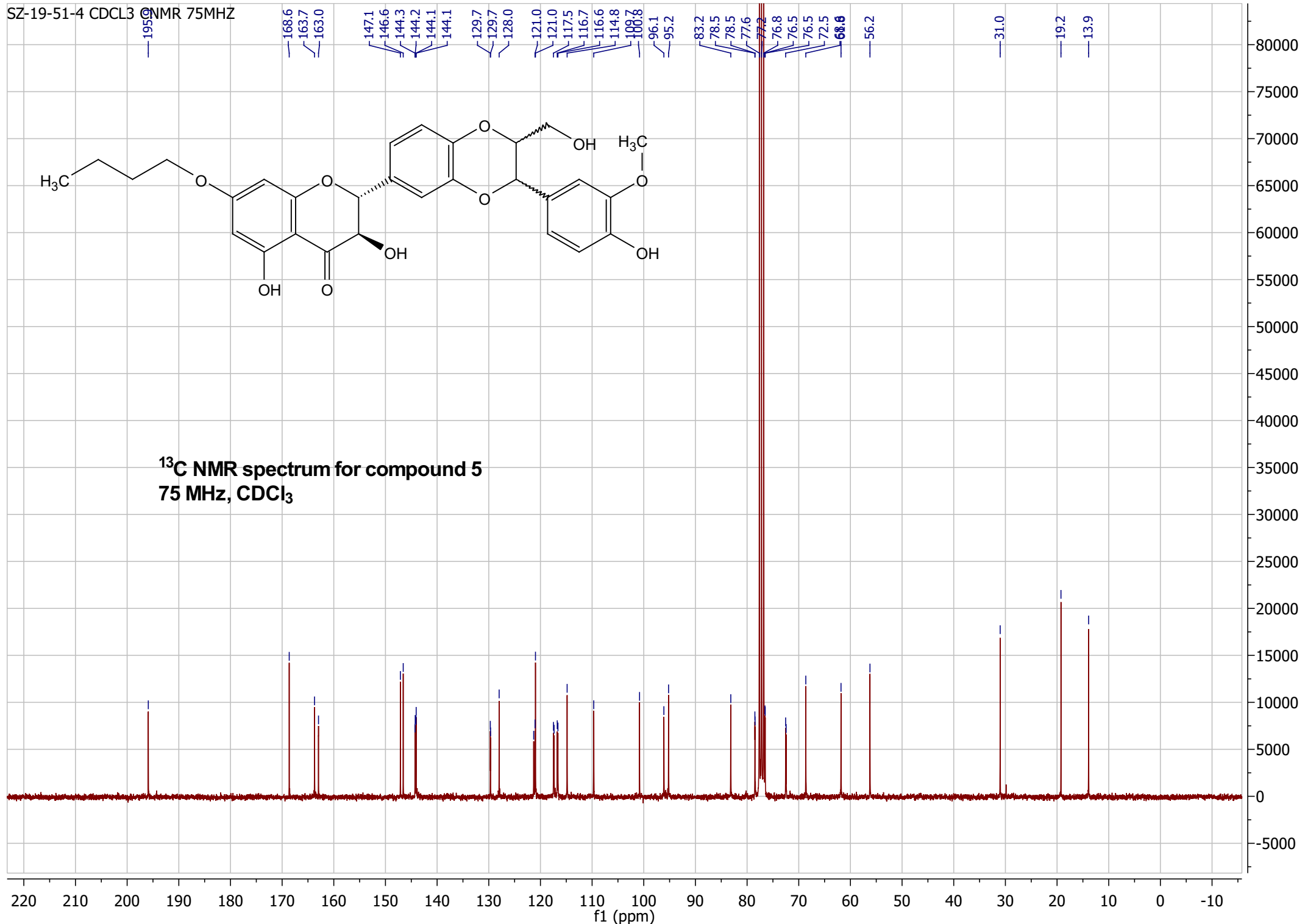




SZ-19-51-4 CDCl<sub>3</sub> NMR 75MHZ

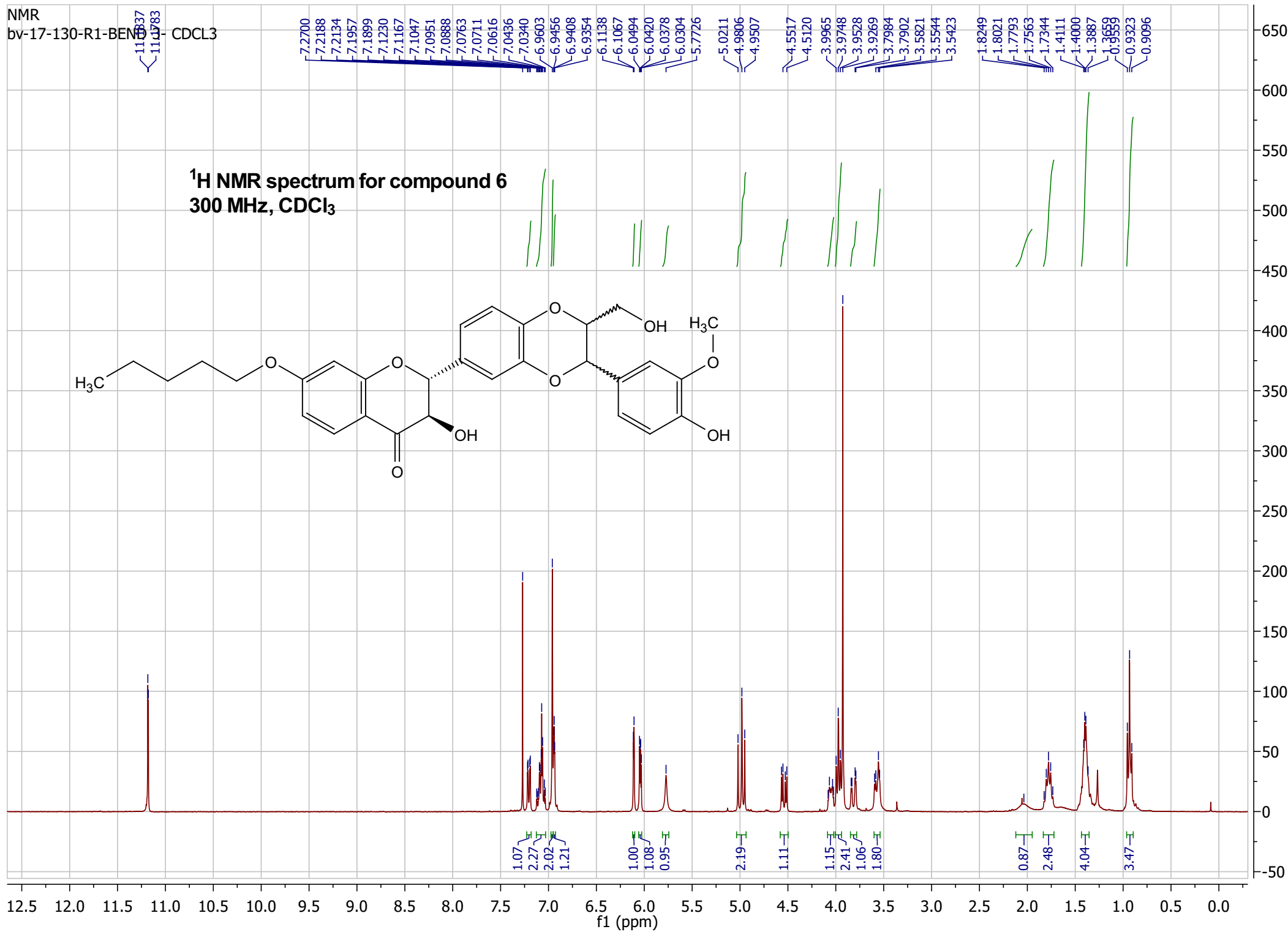
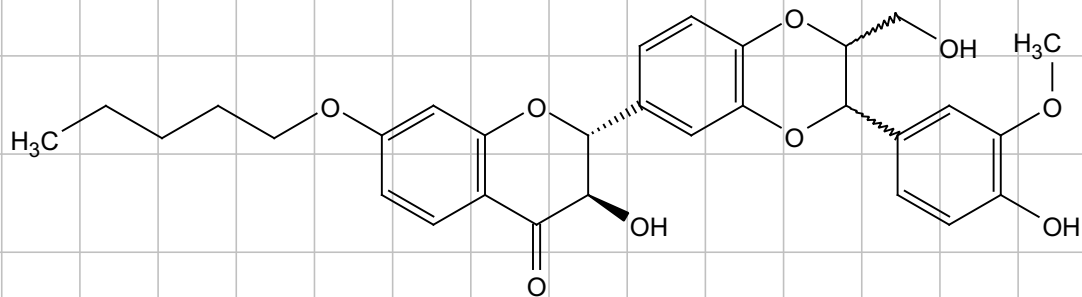


<sup>13</sup>C NMR spectrum for compound 5  
75 MHz, CDCl<sub>3</sub>

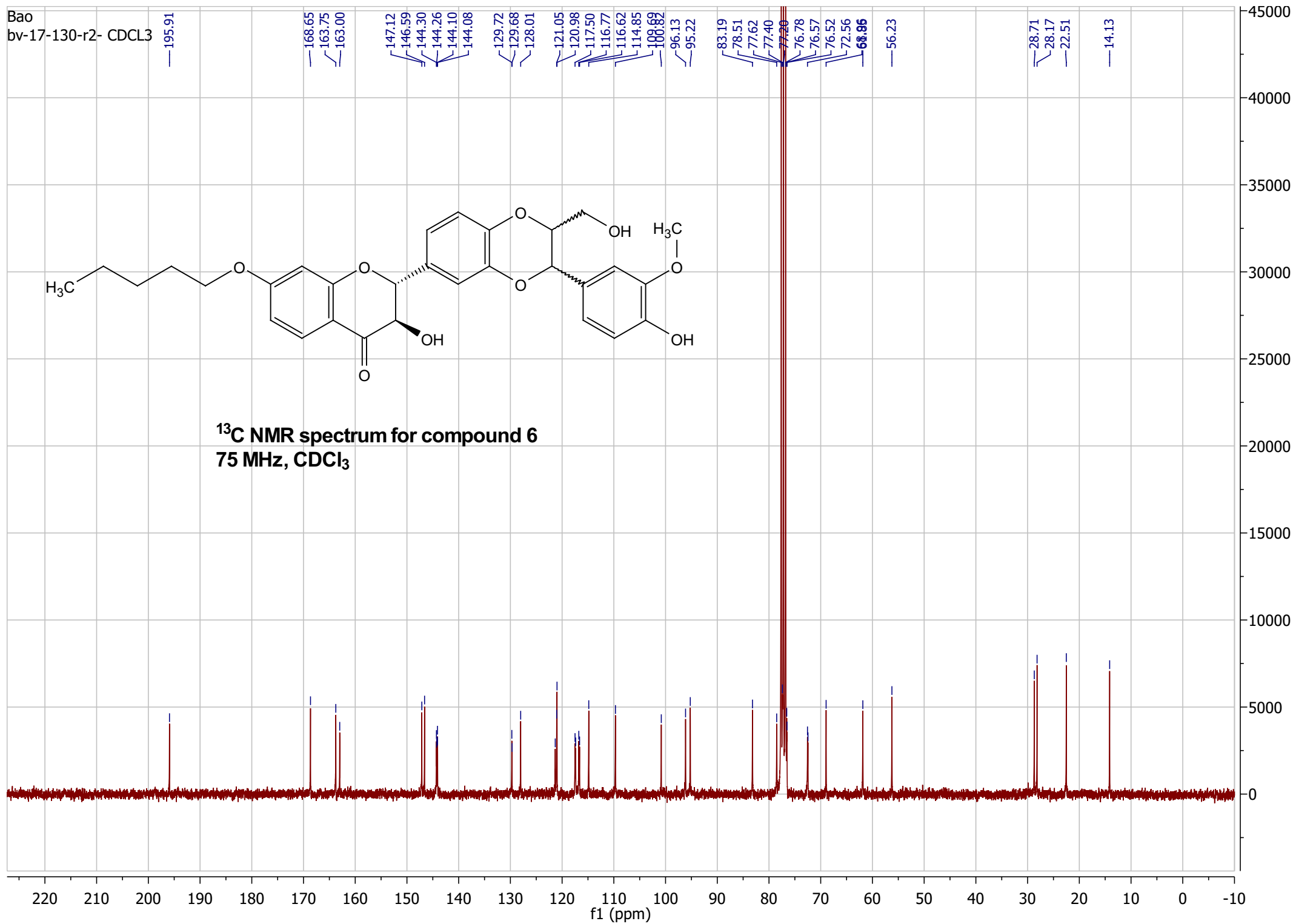


NMR  
bv-17-130-R1-BEN  
CDCl<sub>3</sub>

**<sup>1</sup>H NMR spectrum for compound 6**  
300 MHz, CDCl<sub>3</sub>

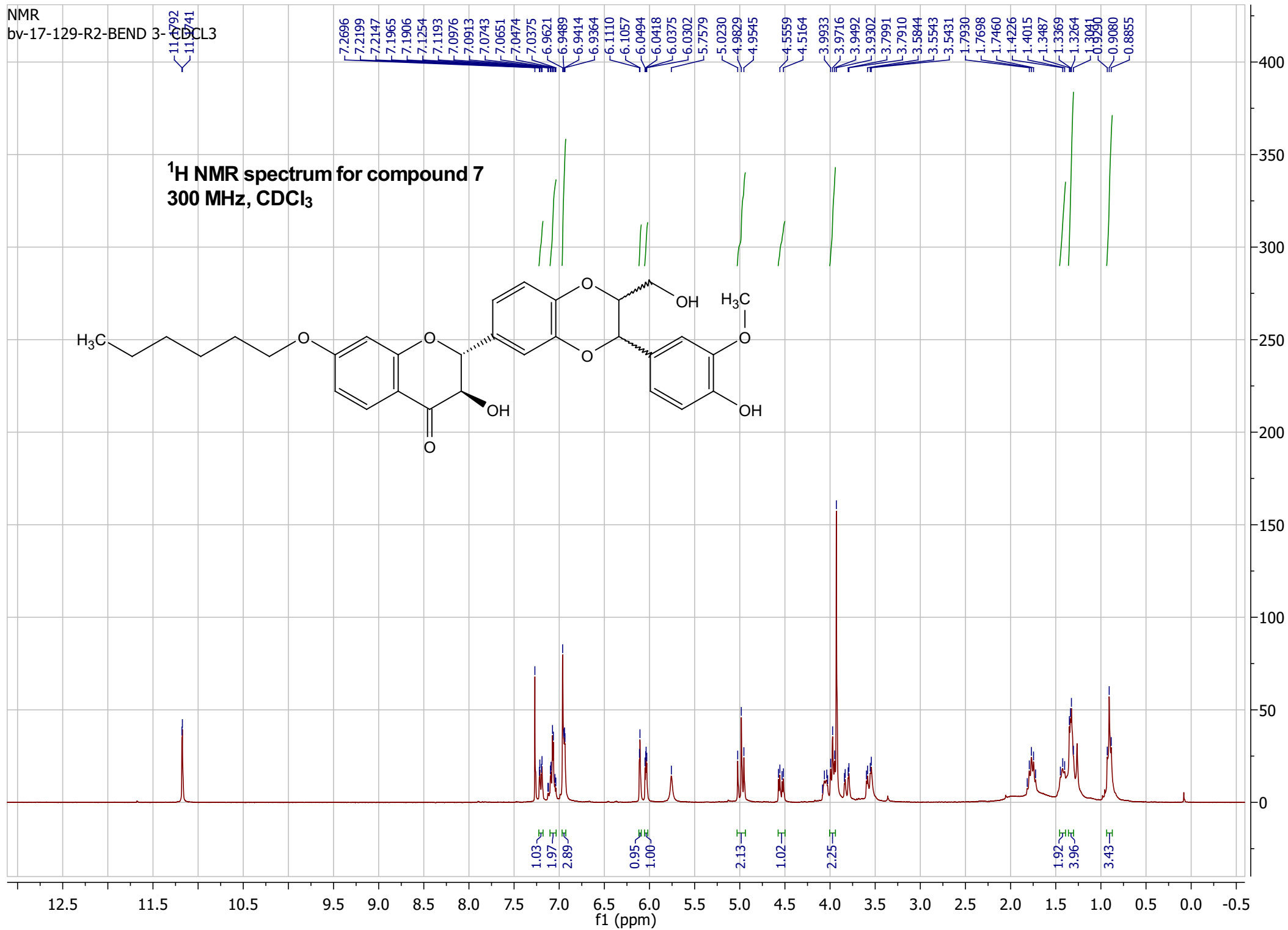
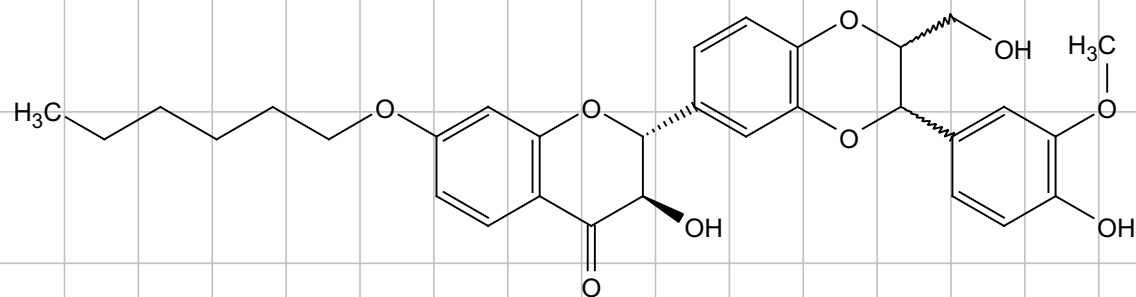


Bao  
bv-17-130-r2- CDCL3

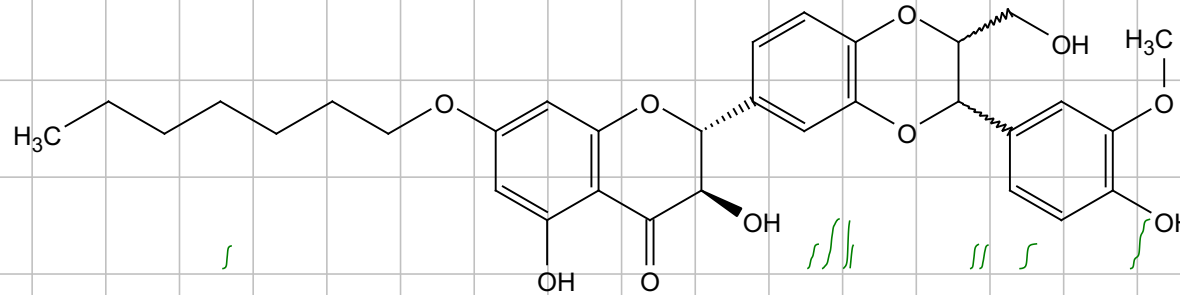


NMR  
bv-17-129-R2-BEND 3-  
CDCl<sub>3</sub>

**<sup>1</sup>H NMR spectrum for compound 7**  
300 MHz, CDCl<sub>3</sub>

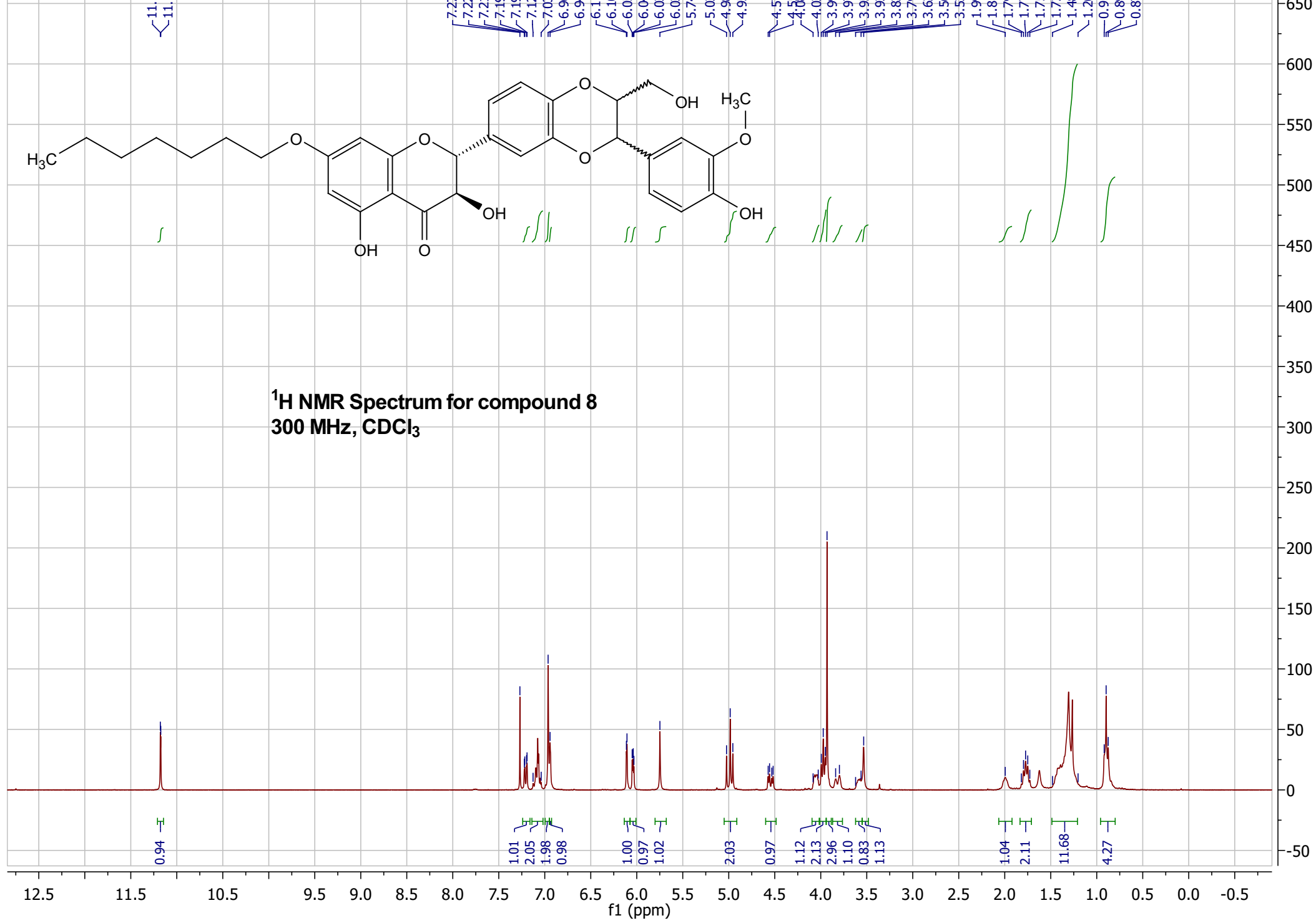


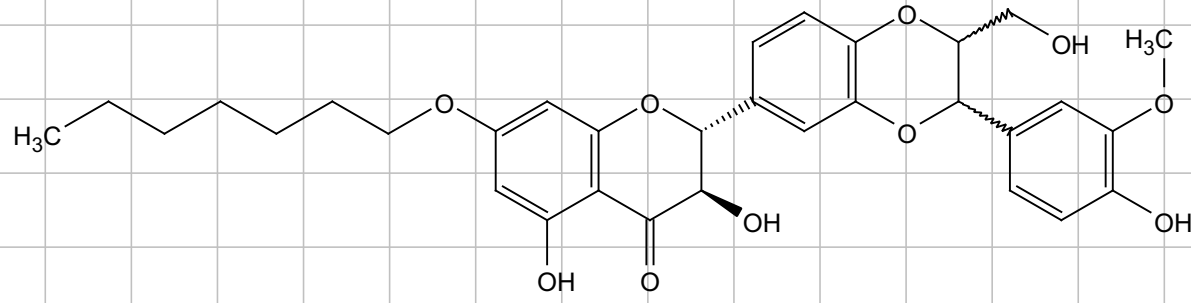




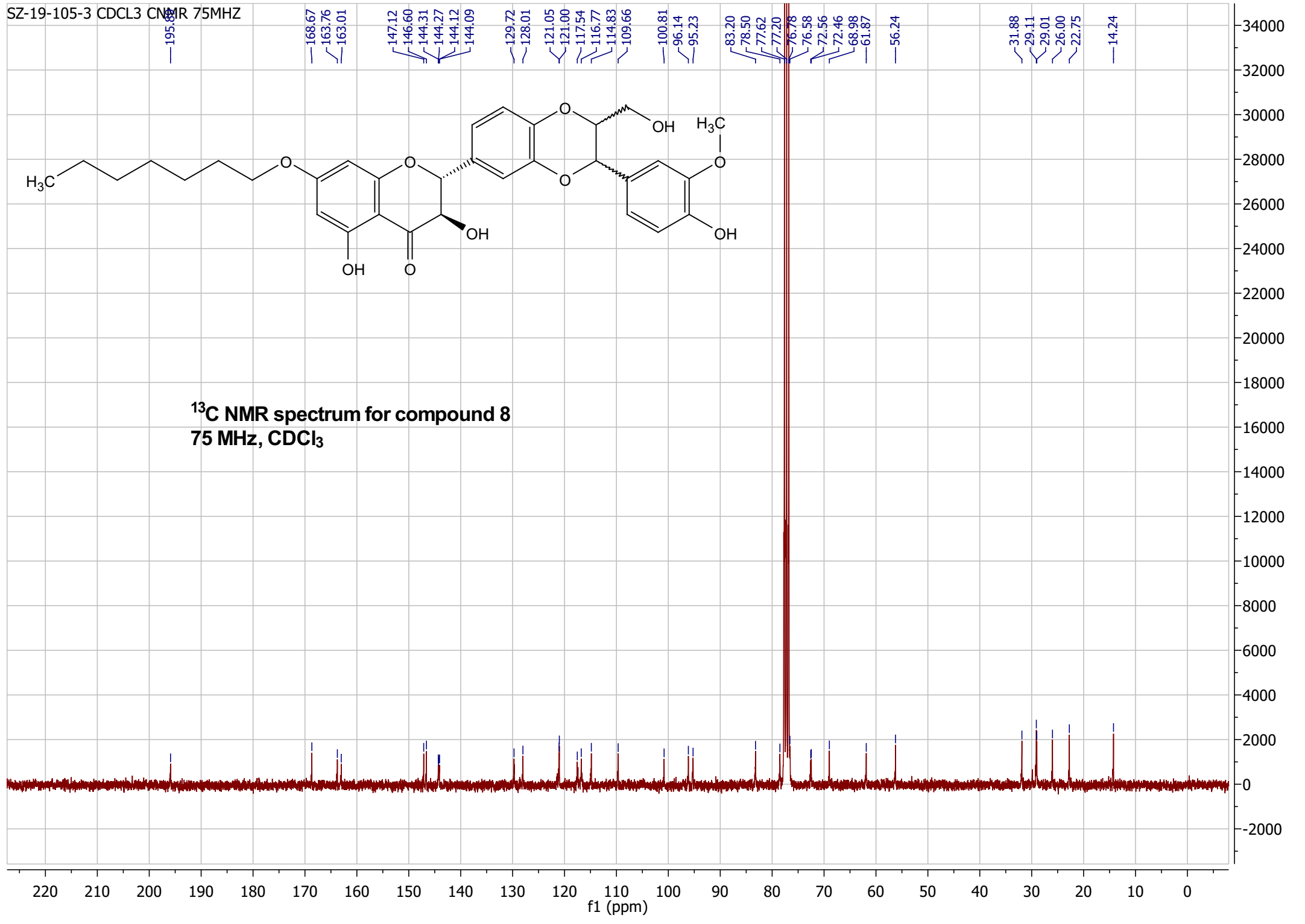
11.177  
11.172  
7.270  
7.222  
7.217  
7.198  
7.193  
7.127  
7.039  
6.964  
6.942  
6.112  
6.106  
6.050  
6.043  
6.038  
6.031  
5.748  
5.024  
4.984  
4.956  
4.571  
4.556  
4.553  
4.028  
3.994  
3.973  
3.950  
3.932  
3.838  
3.797  
3.621  
3.562  
3.533  
1.995  
1.819  
1.796  
1.773  
1.750  
1.728  
1.480  
1.203  
0.919  
0.898  
0.876

**<sup>1</sup>H NMR Spectrum for compound 8**  
300 MHz, CDCl<sub>3</sub>

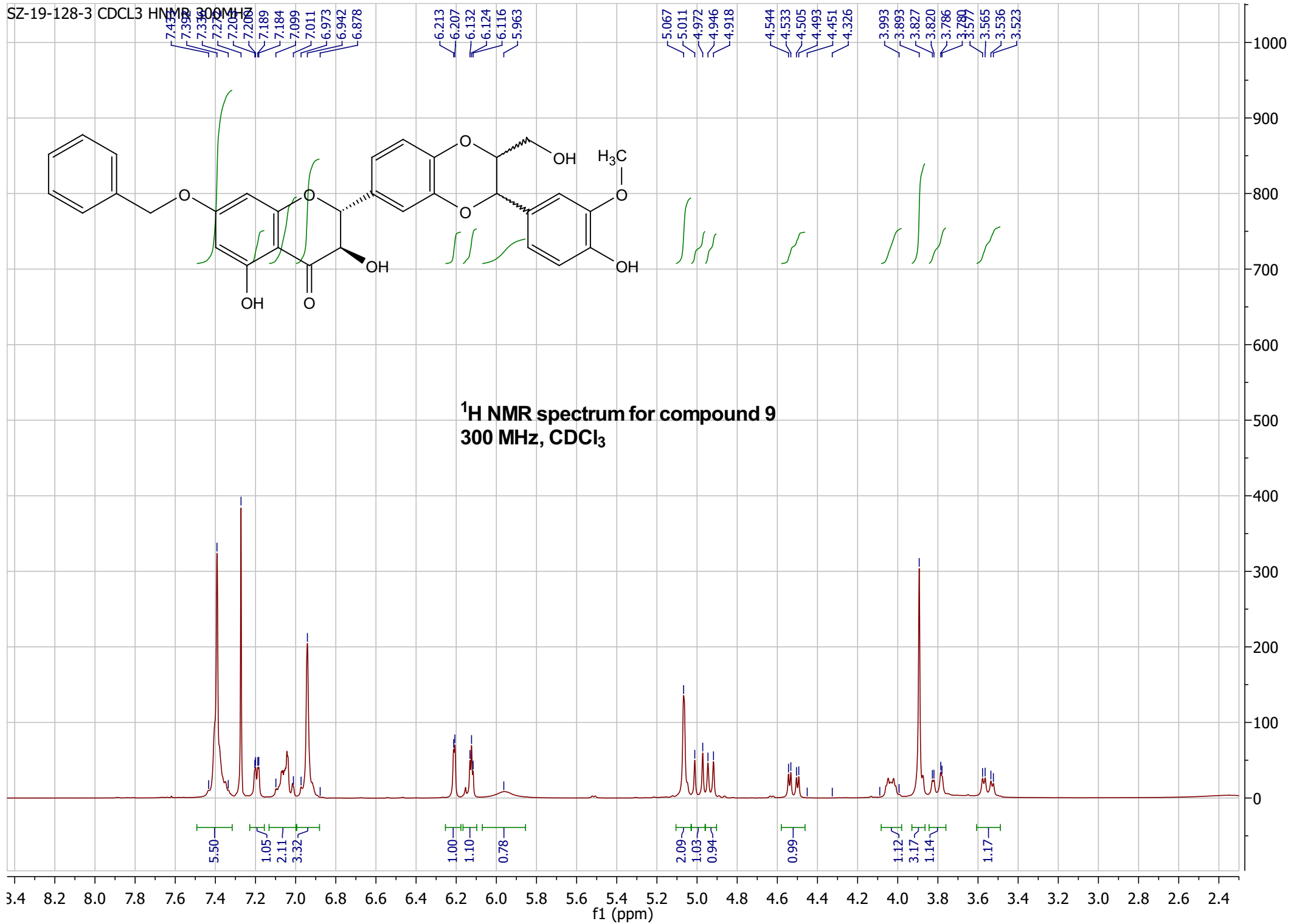




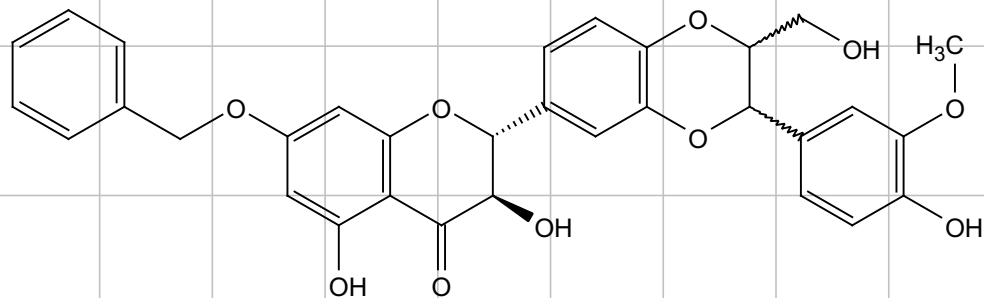
<sup>13</sup>C NMR spectrum for compound 8  
75 MHz, CDCl<sub>3</sub>



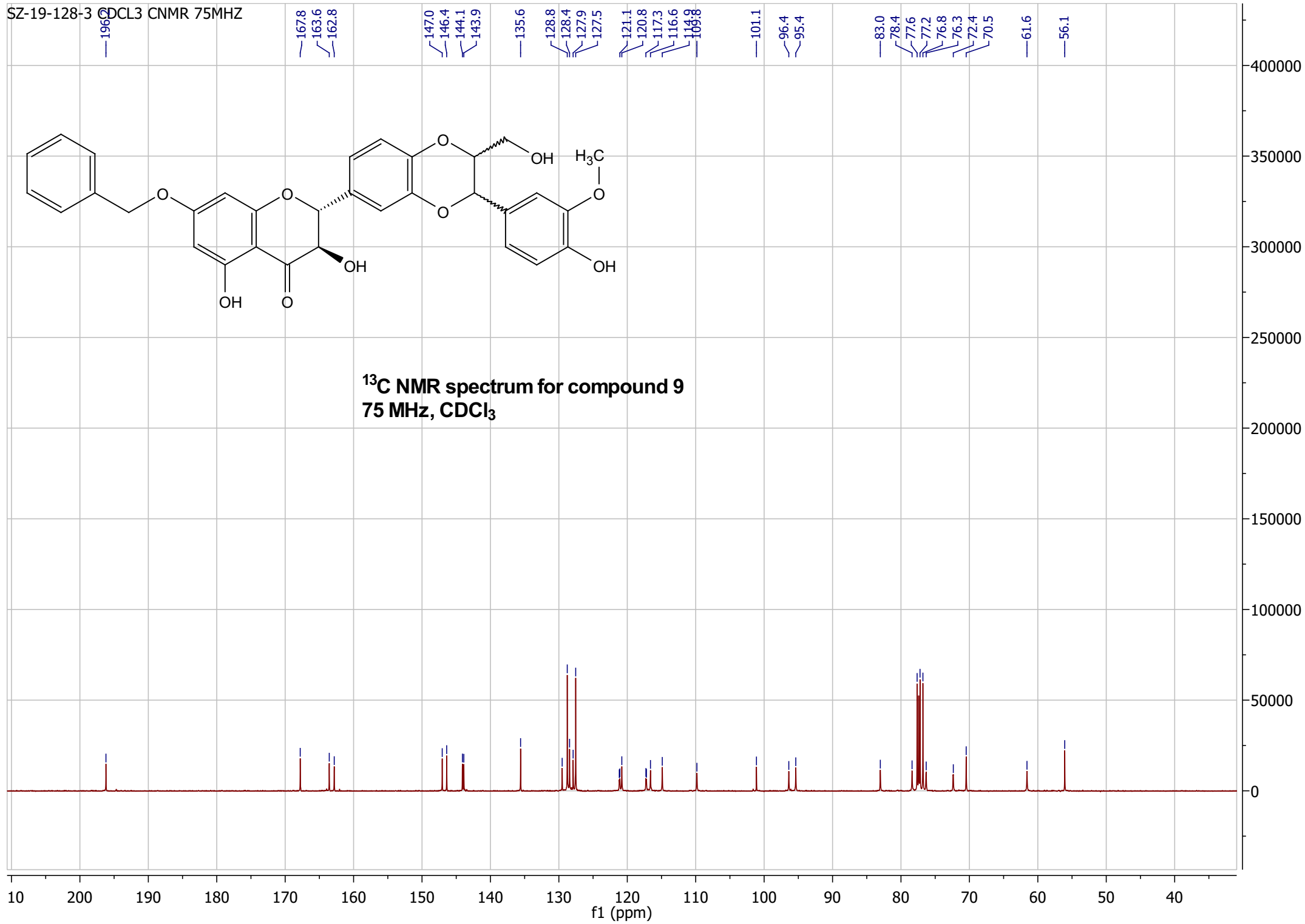
SZ-19-128-3 CDCl<sub>3</sub> HNMR 300MHz





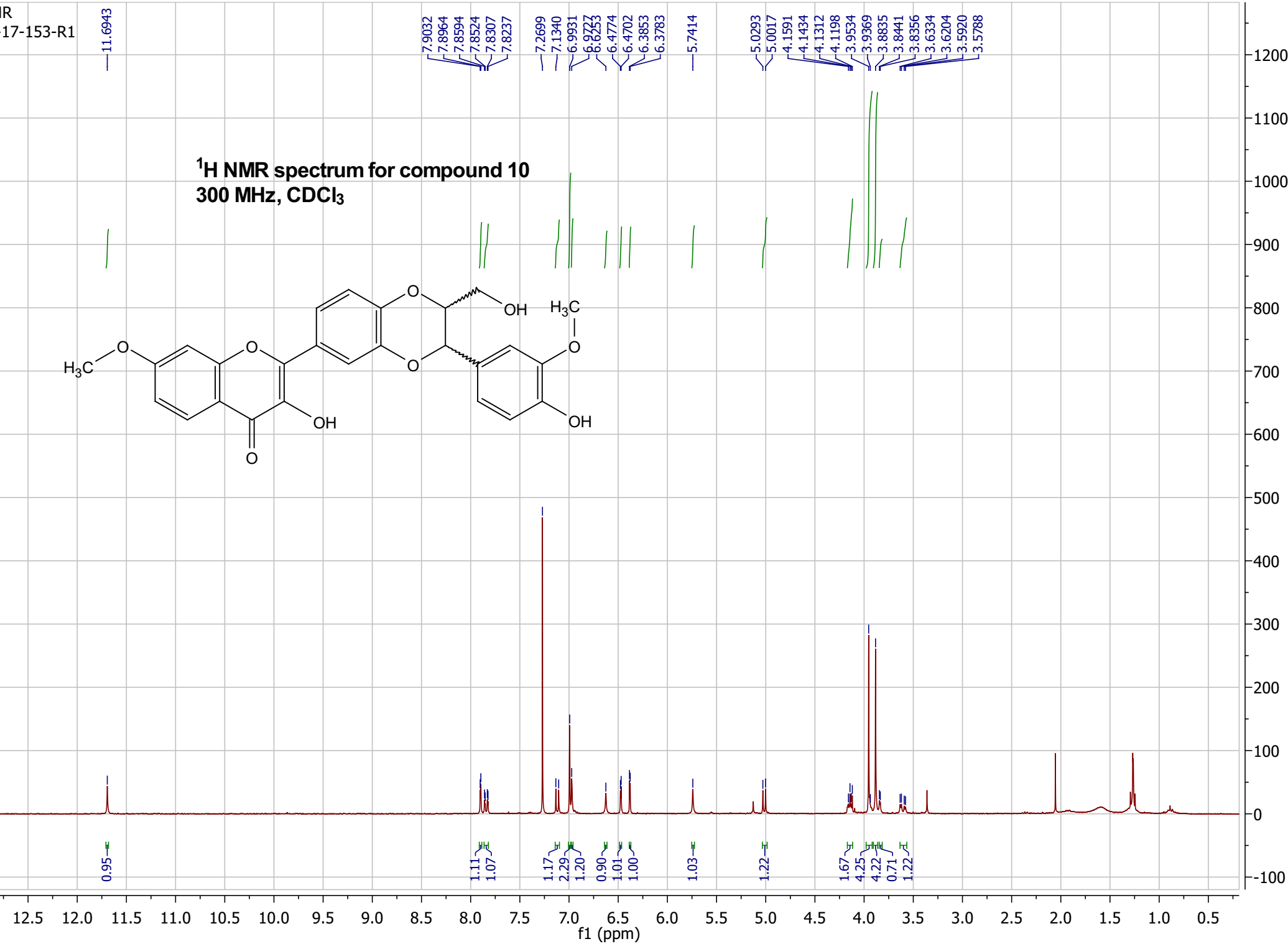
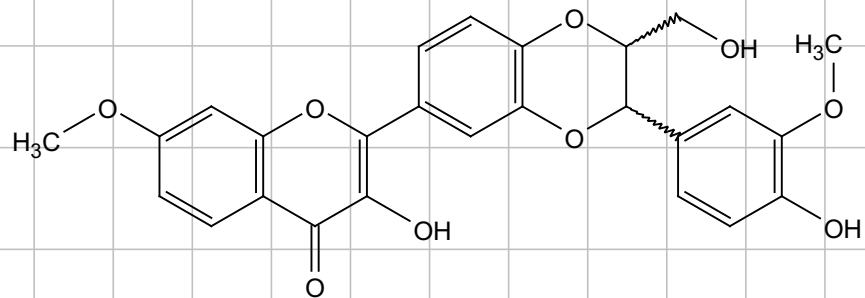


**<sup>13</sup>C NMR spectrum for compound 9**  
75 MHz, CDCl<sub>3</sub>

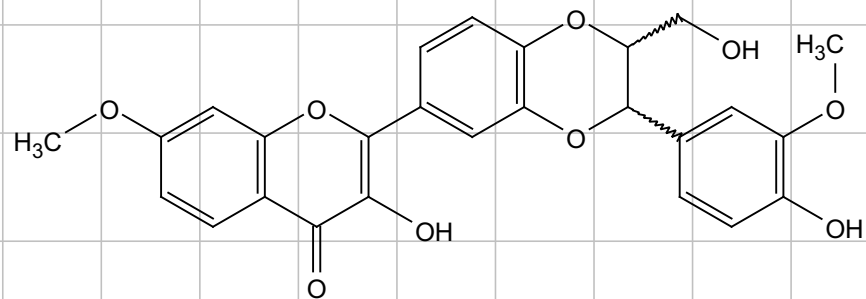


NMR  
bv-17-153-R1

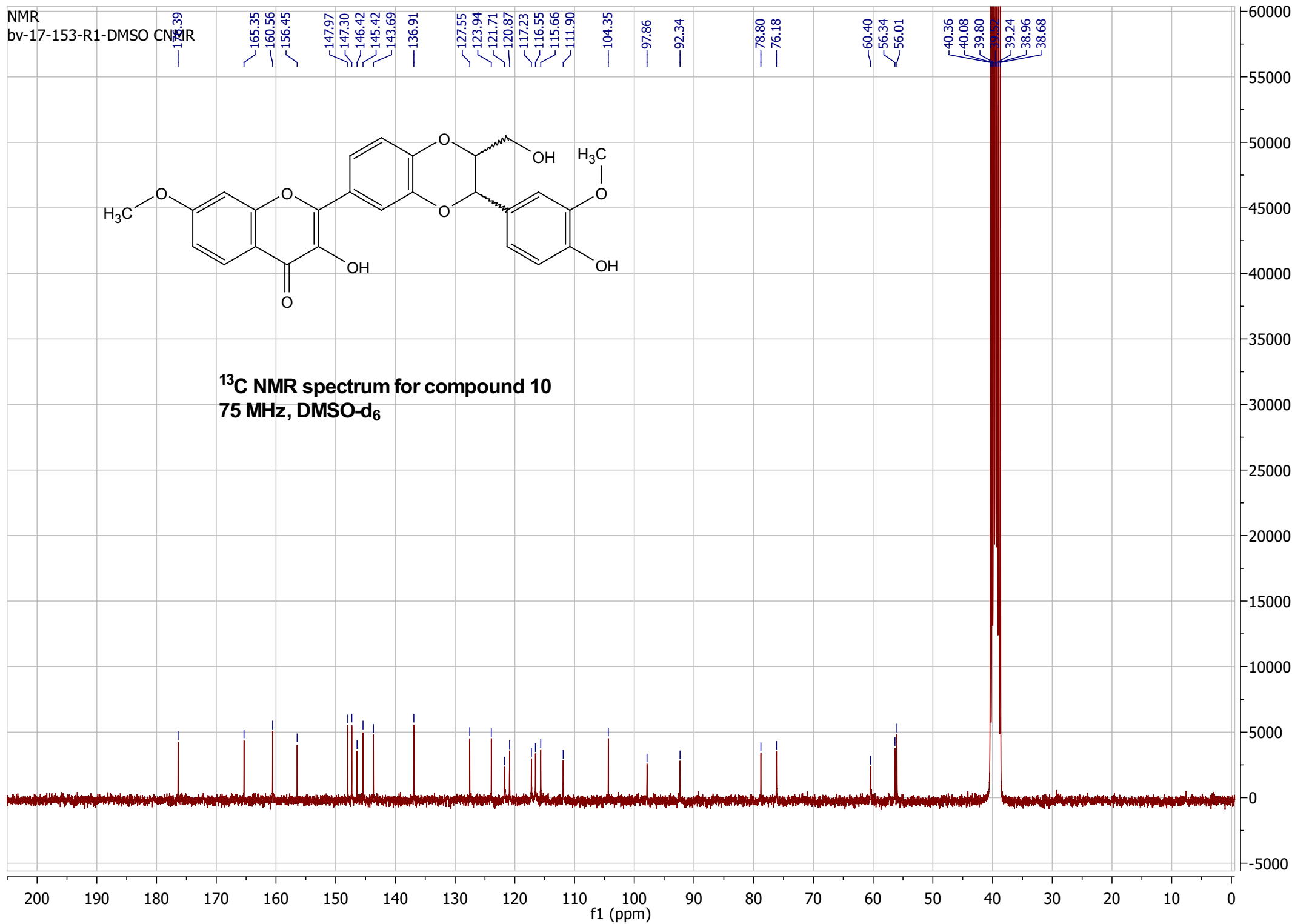
**<sup>1</sup>H NMR spectrum for compound 10**  
300 MHz, CDCl<sub>3</sub>



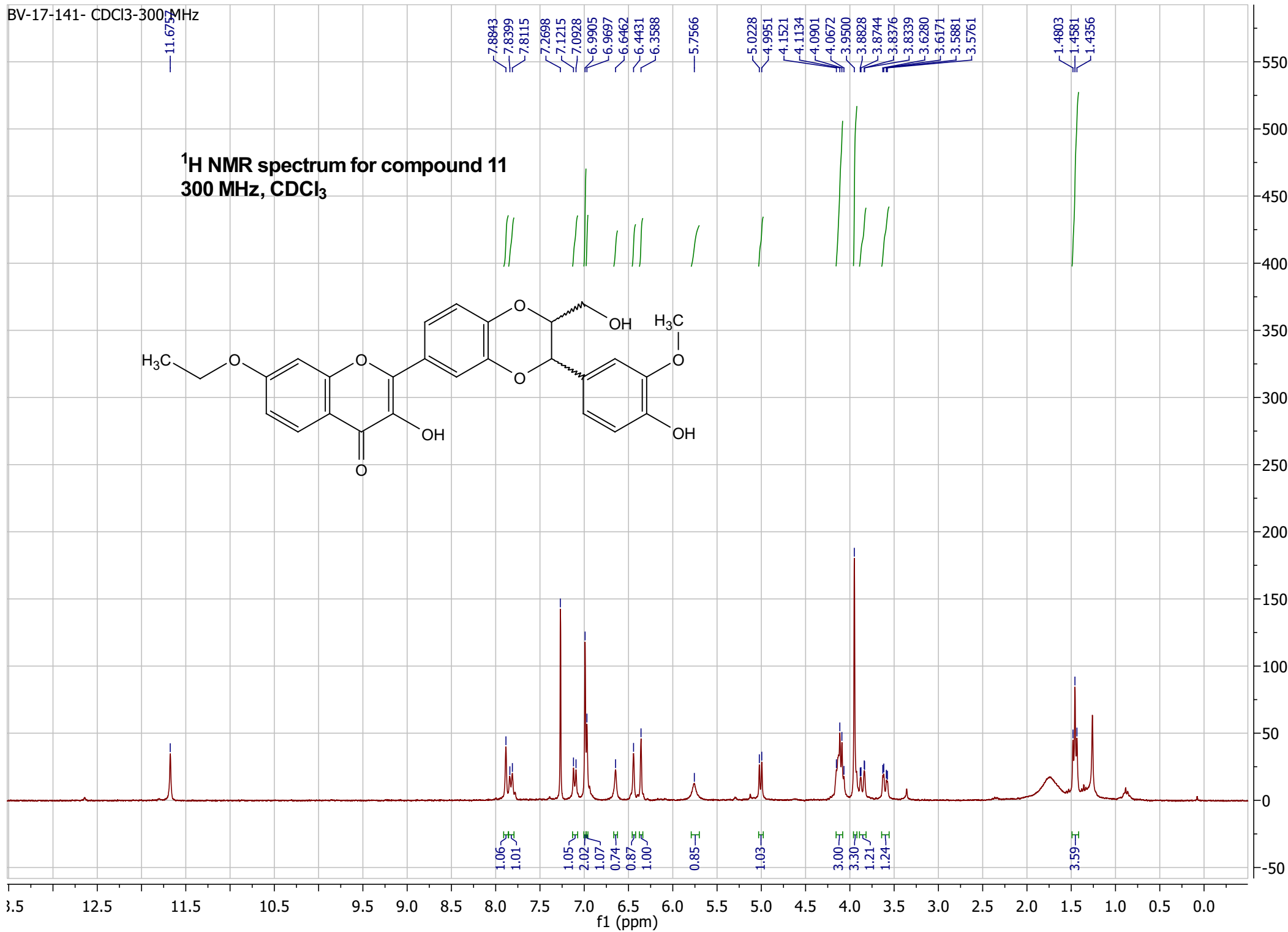
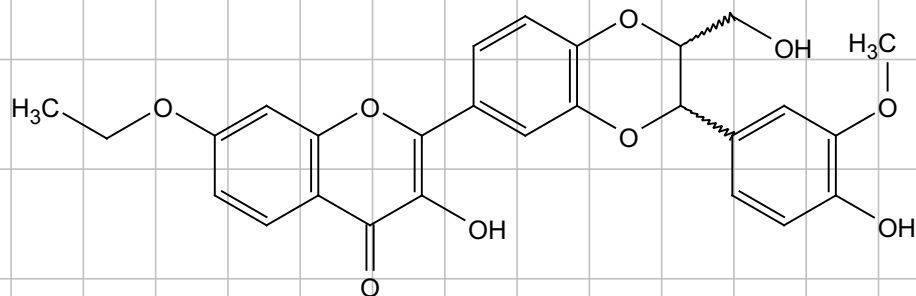
NMR  
bv-17-153-R1-DMSO CNMR



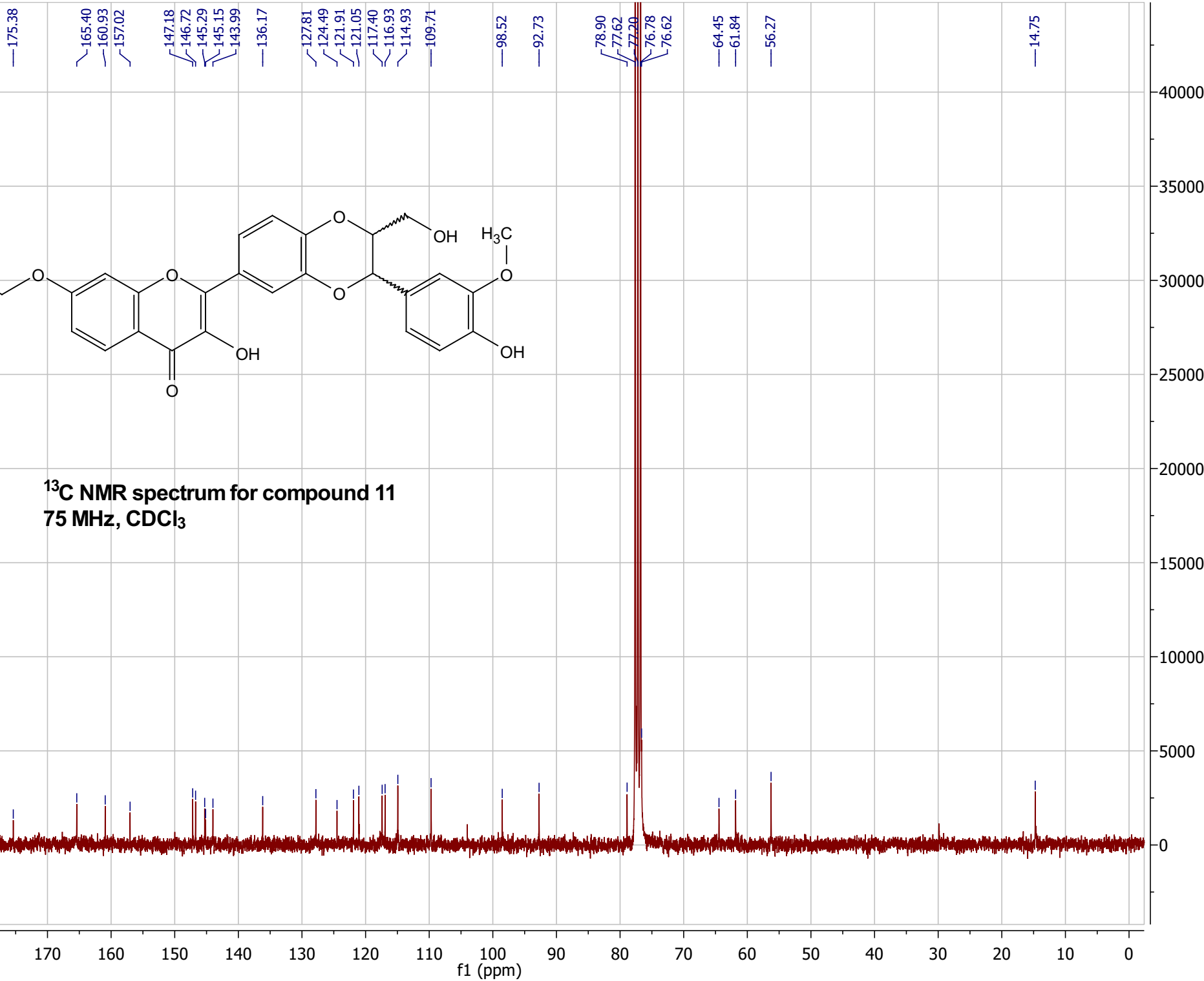
**<sup>13</sup>C NMR spectrum for compound 10**  
**75 MHz, DMSO-d<sub>6</sub>**

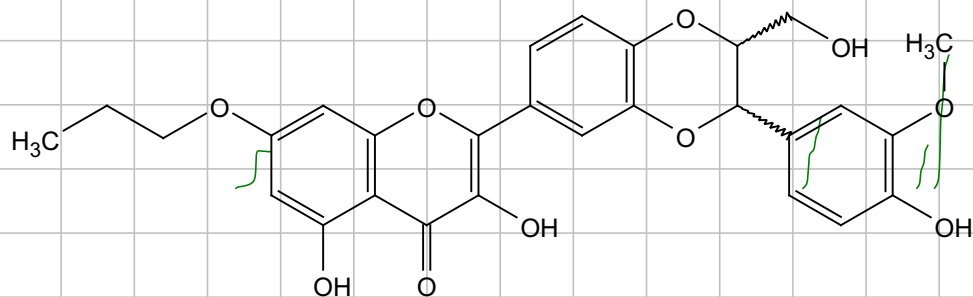


**<sup>1</sup>H NMR spectrum for compound 11**  
**300 MHz, CDCl<sub>3</sub>**

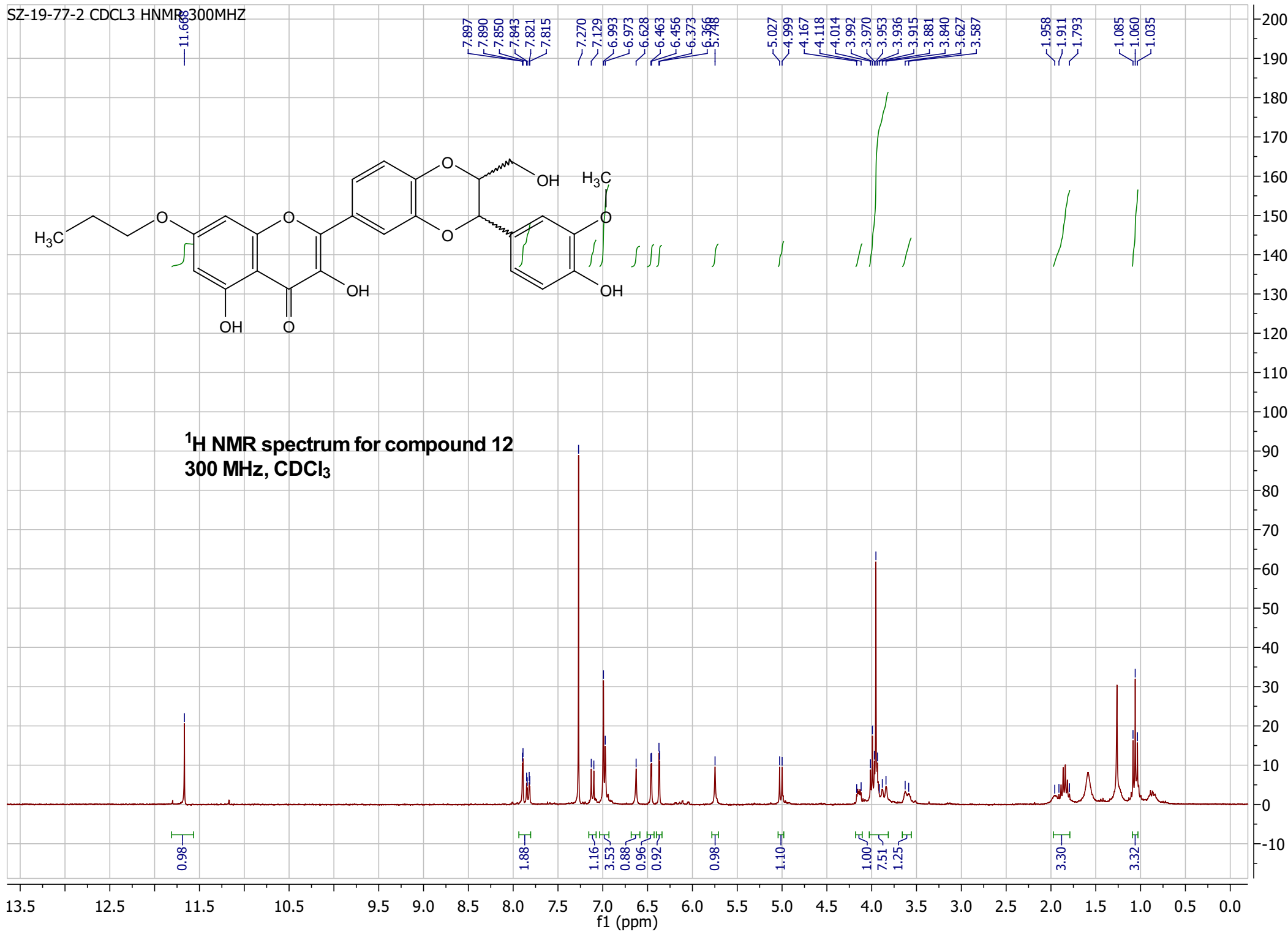


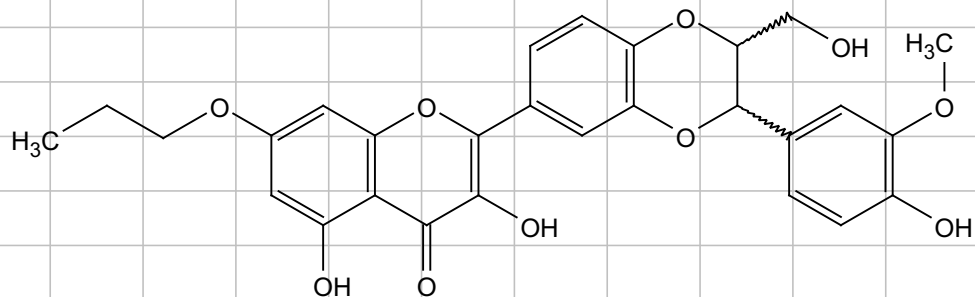
NMR  
BV-17-141-cnmr cdc3



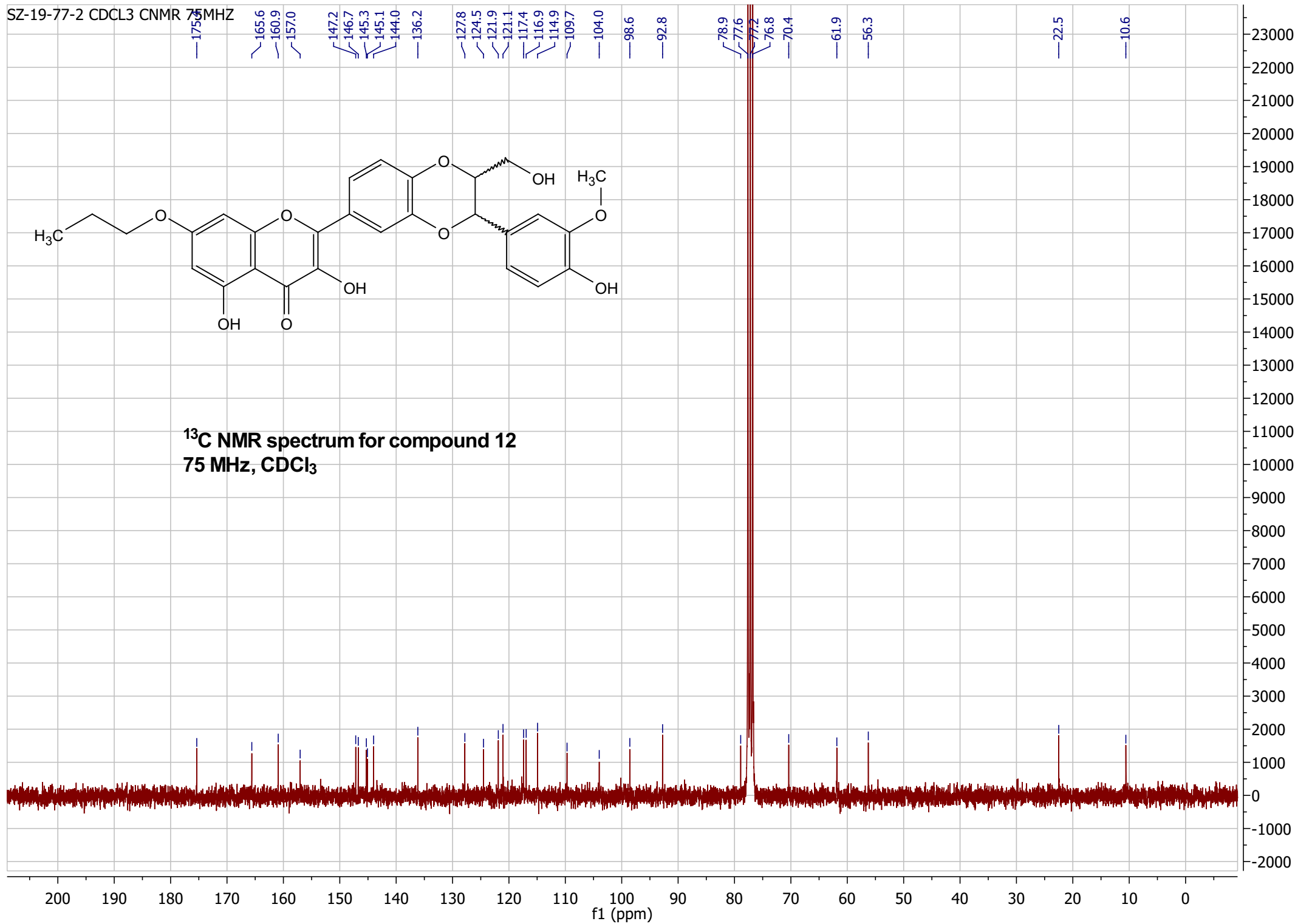


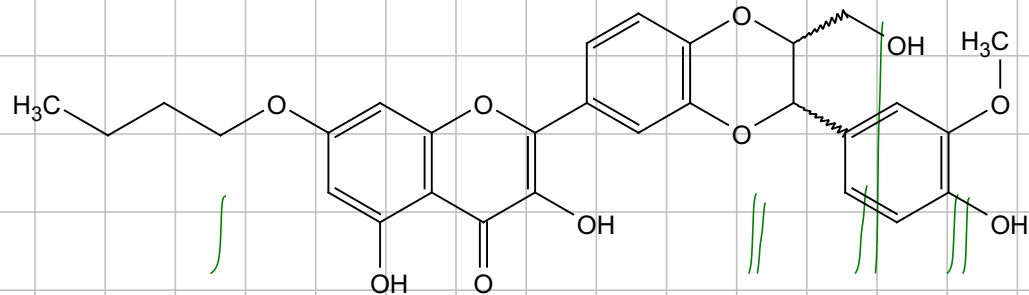
**<sup>1</sup>H NMR spectrum for compound 12**  
**300 MHz, CDCl<sub>3</sub>**



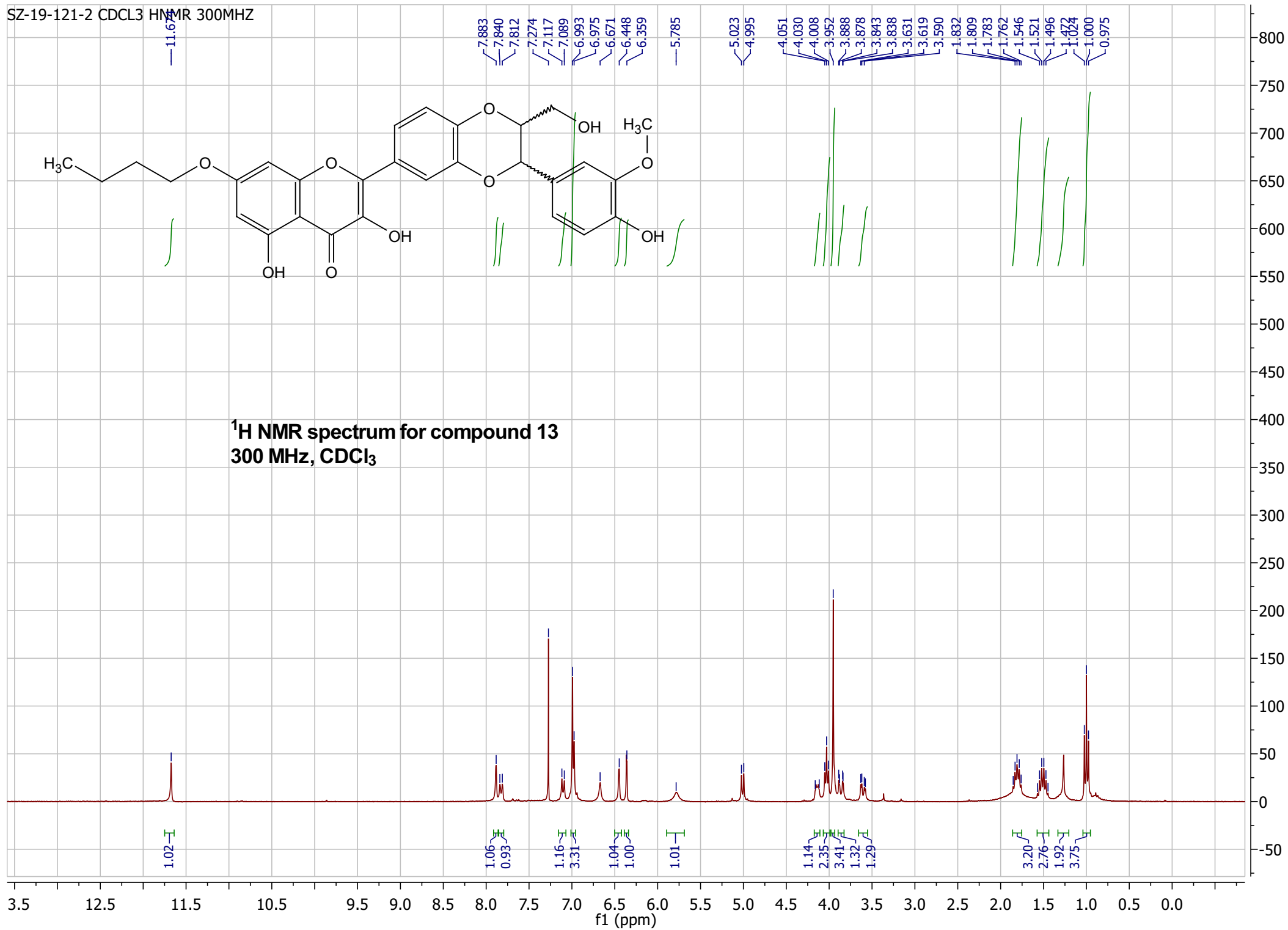


**<sup>13</sup>C NMR spectrum for compound 12**  
**75 MHz, CDCl<sub>3</sub>**

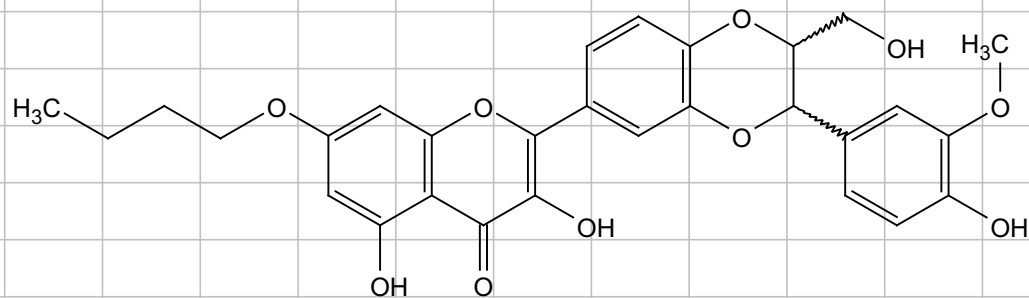




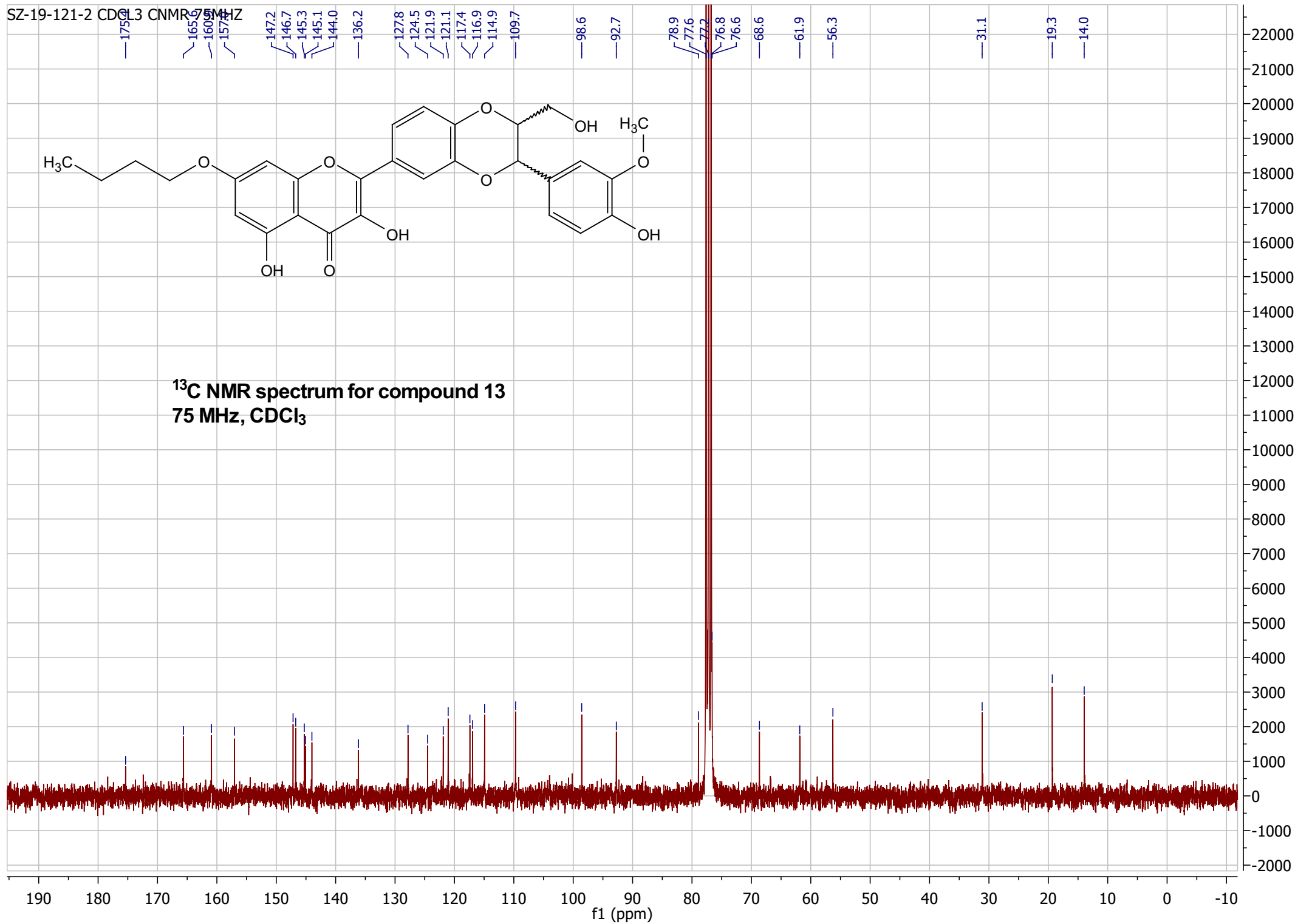
**<sup>1</sup>H NMR spectrum for compound 13  
300 MHz, CDCl<sub>3</sub>**



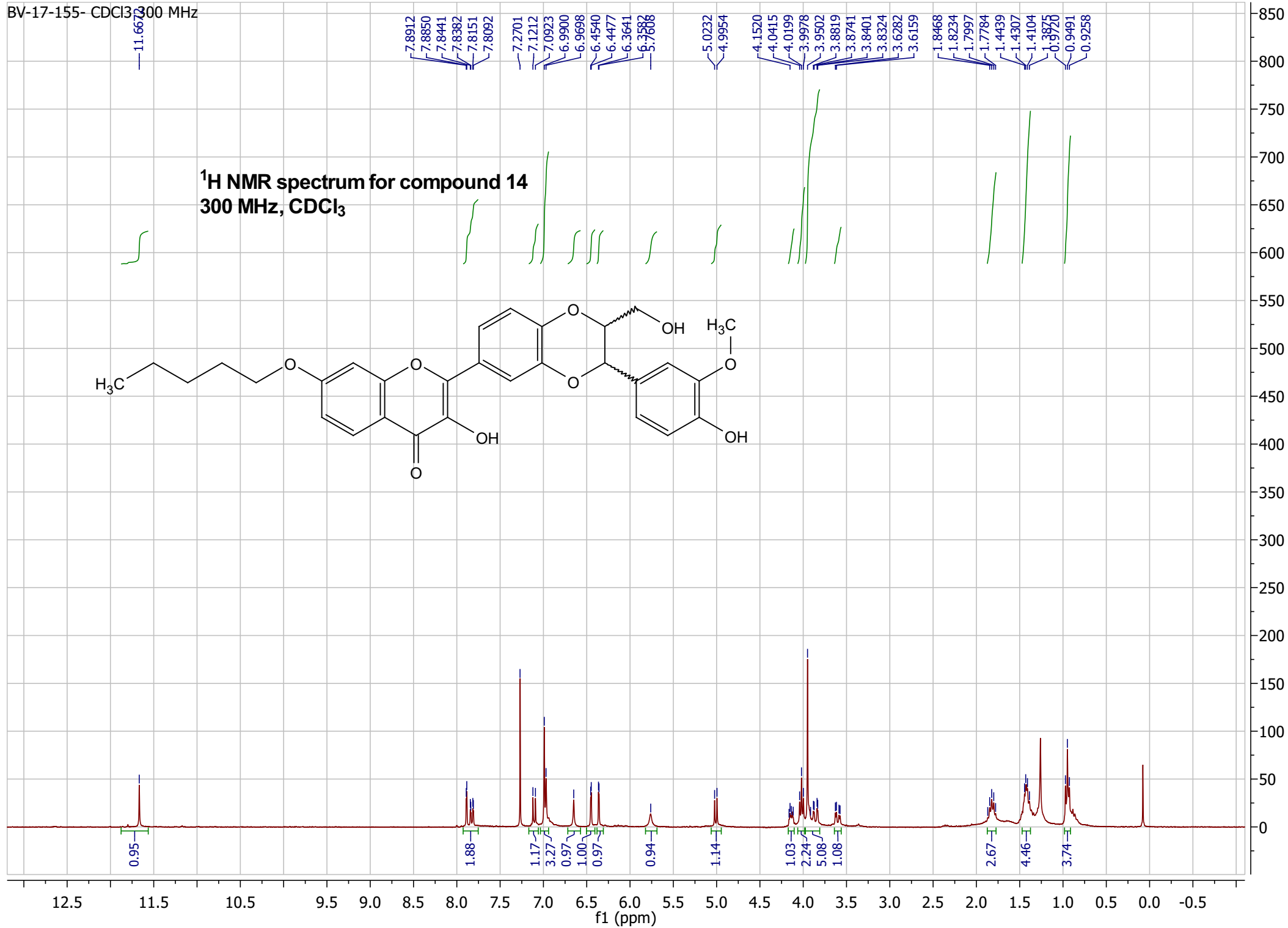
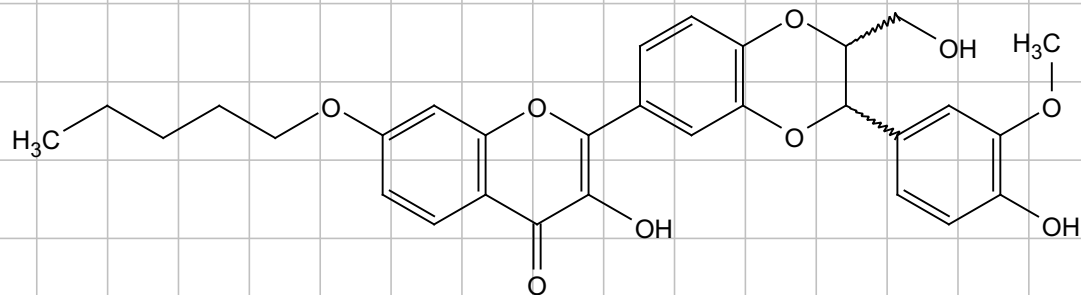


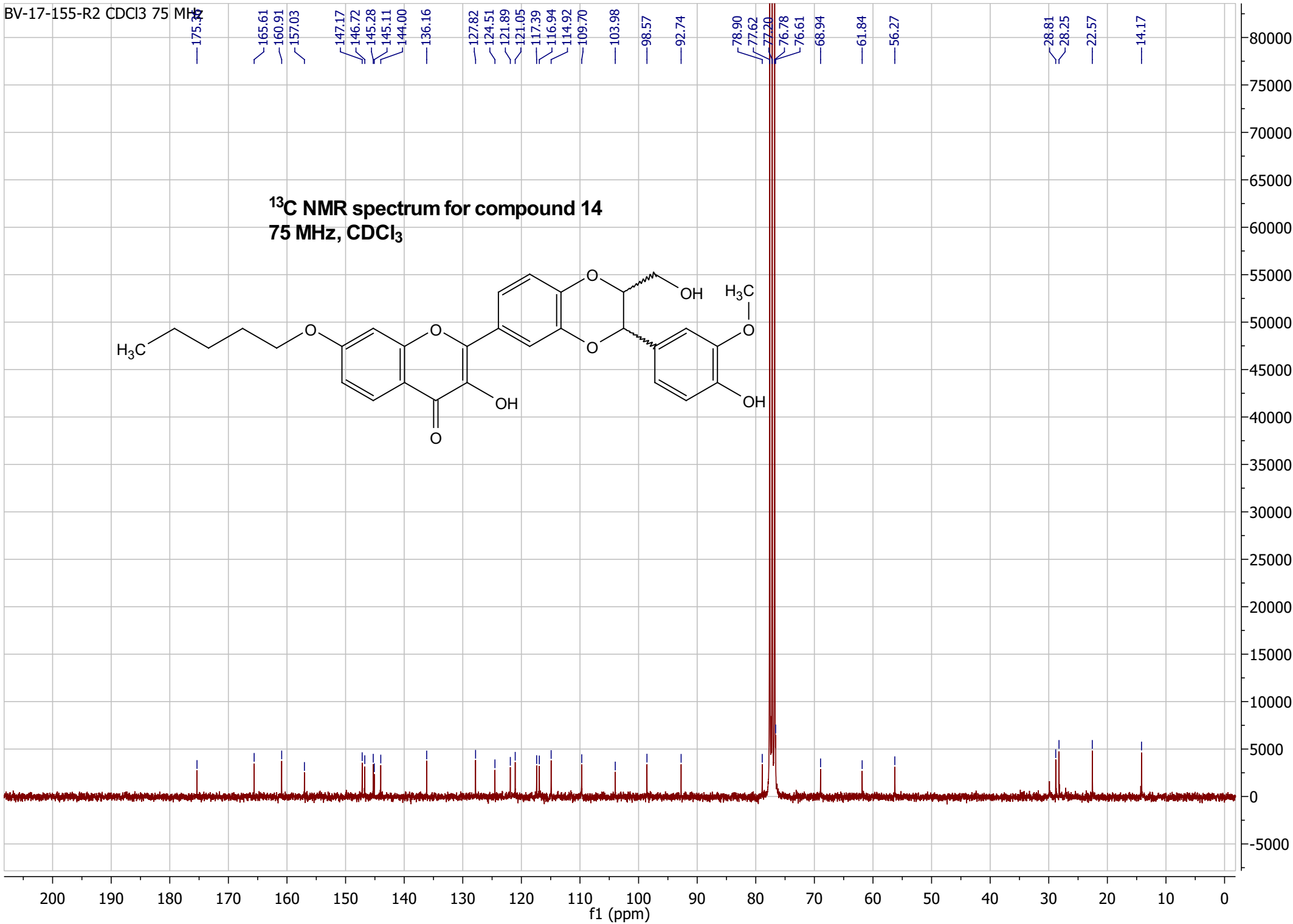


**<sup>13</sup>C NMR spectrum for compound 13**  
75 MHz, CDCl<sub>3</sub>

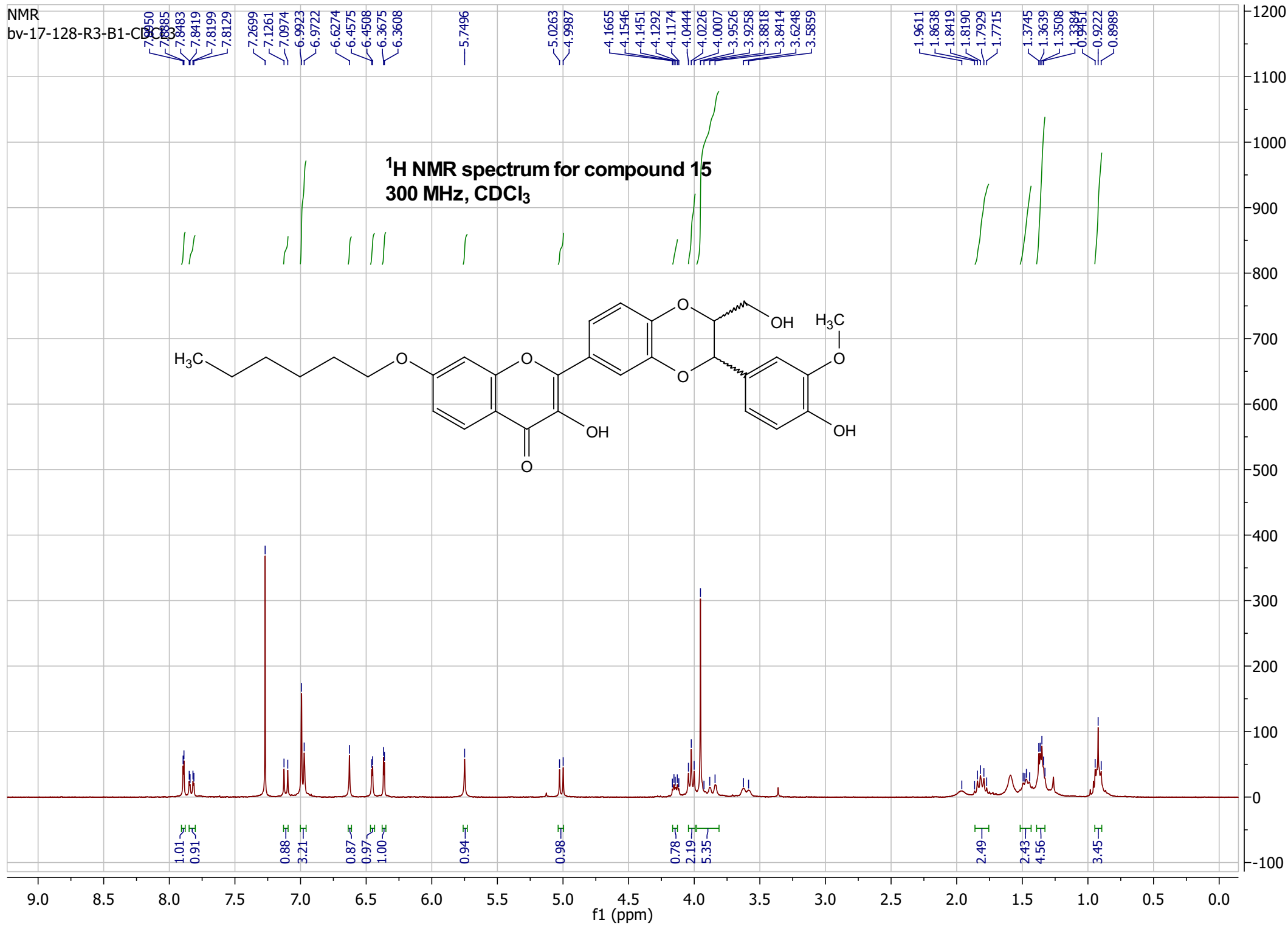


**<sup>1</sup>H NMR spectrum for compound 14**  
300 MHz, CDCl<sub>3</sub>

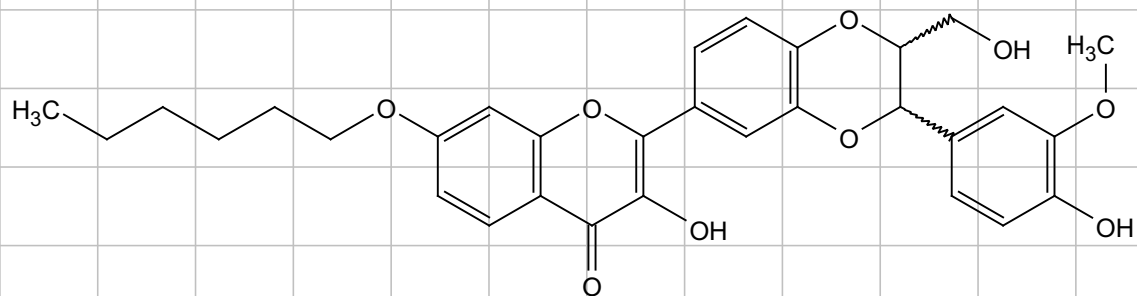




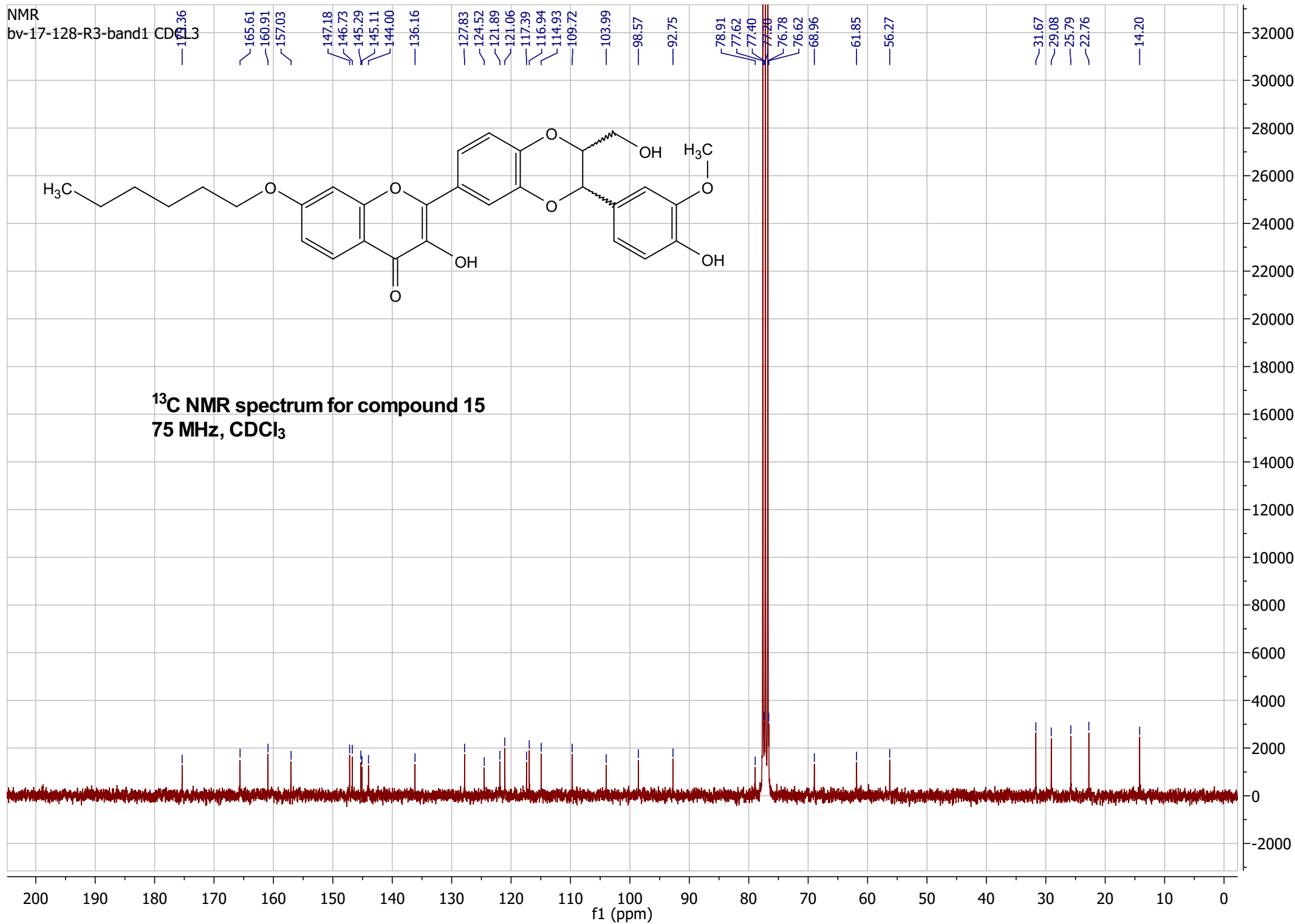
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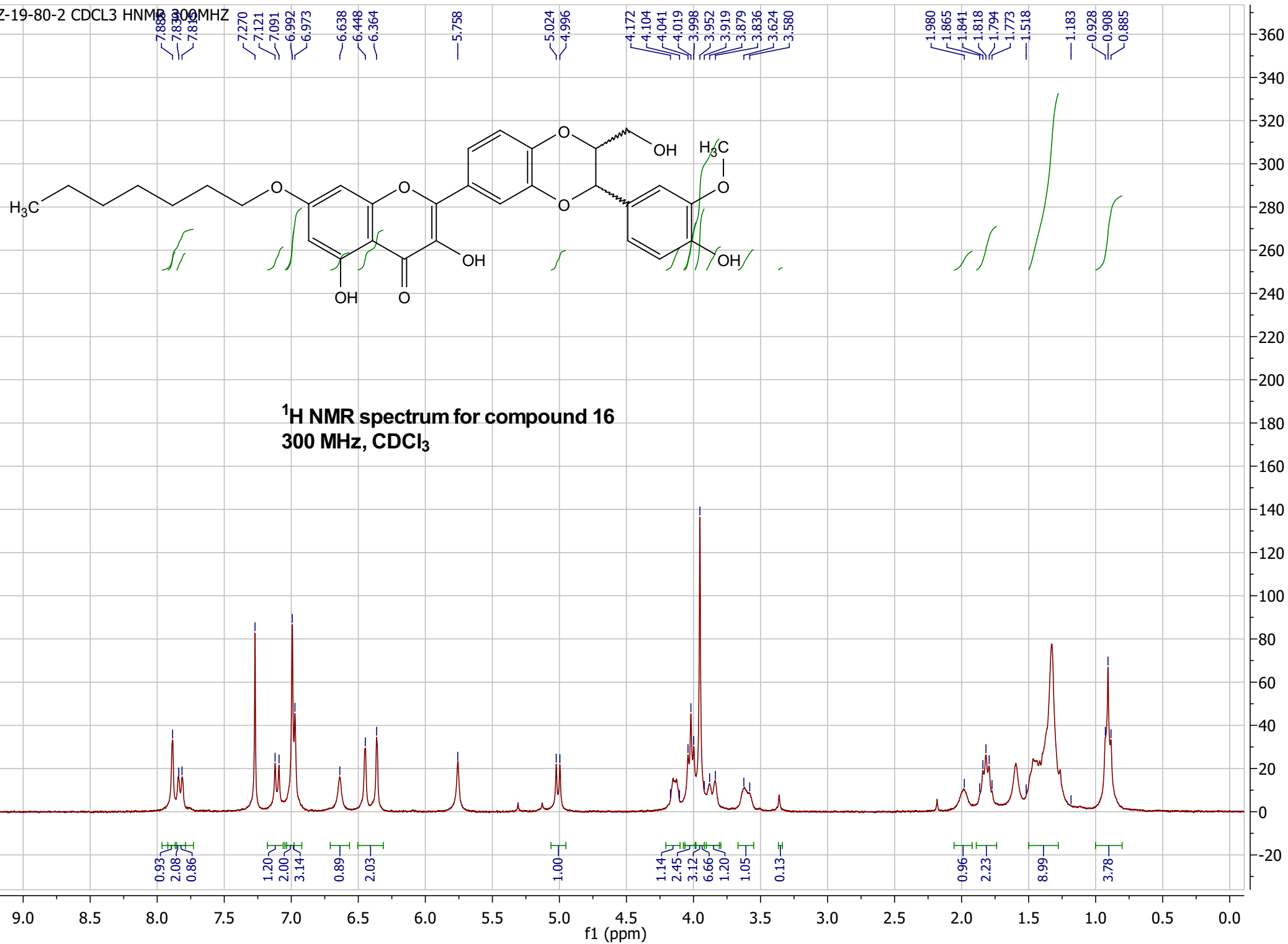
NMR  
bv-17-128-R3-band1 CDCl<sub>3</sub>

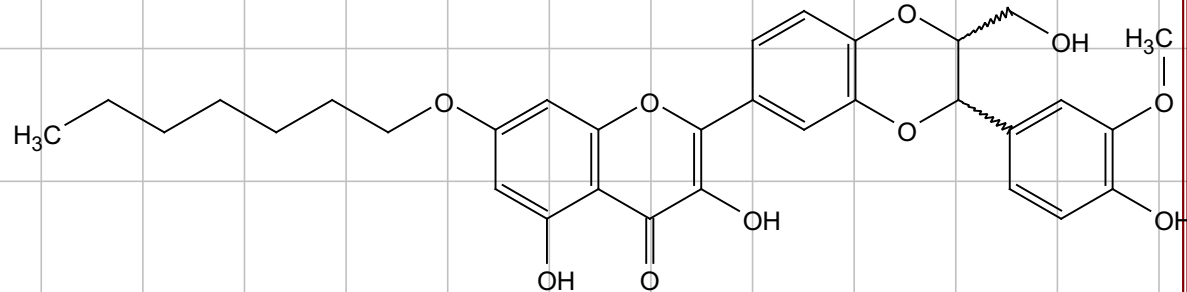


**<sup>13</sup>C NMR spectrum for compound 15**  
75 MHz, CDCl<sub>3</sub>

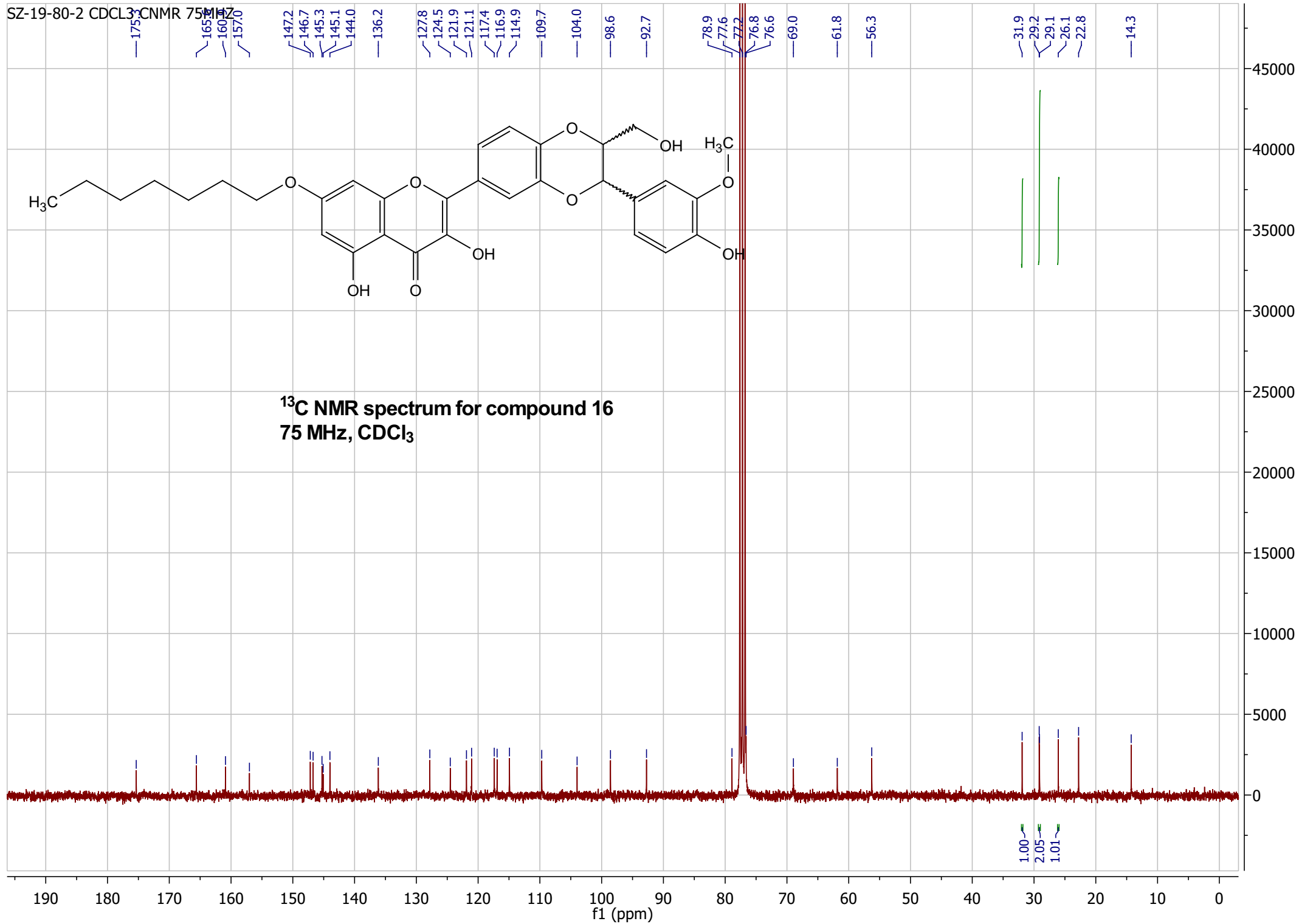


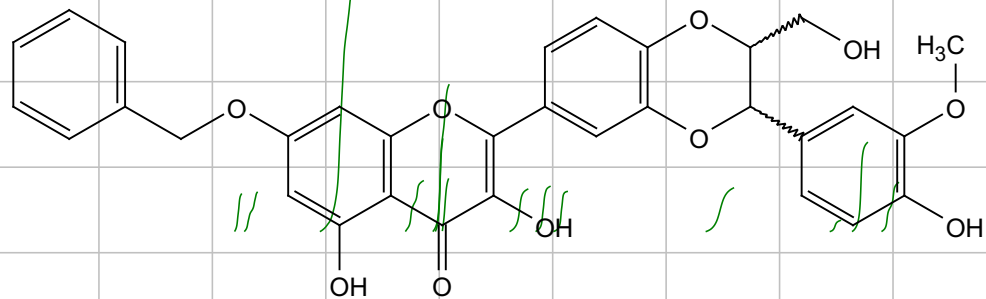
SZ-19-80-2 CDCL3 HNMR 300MHZ



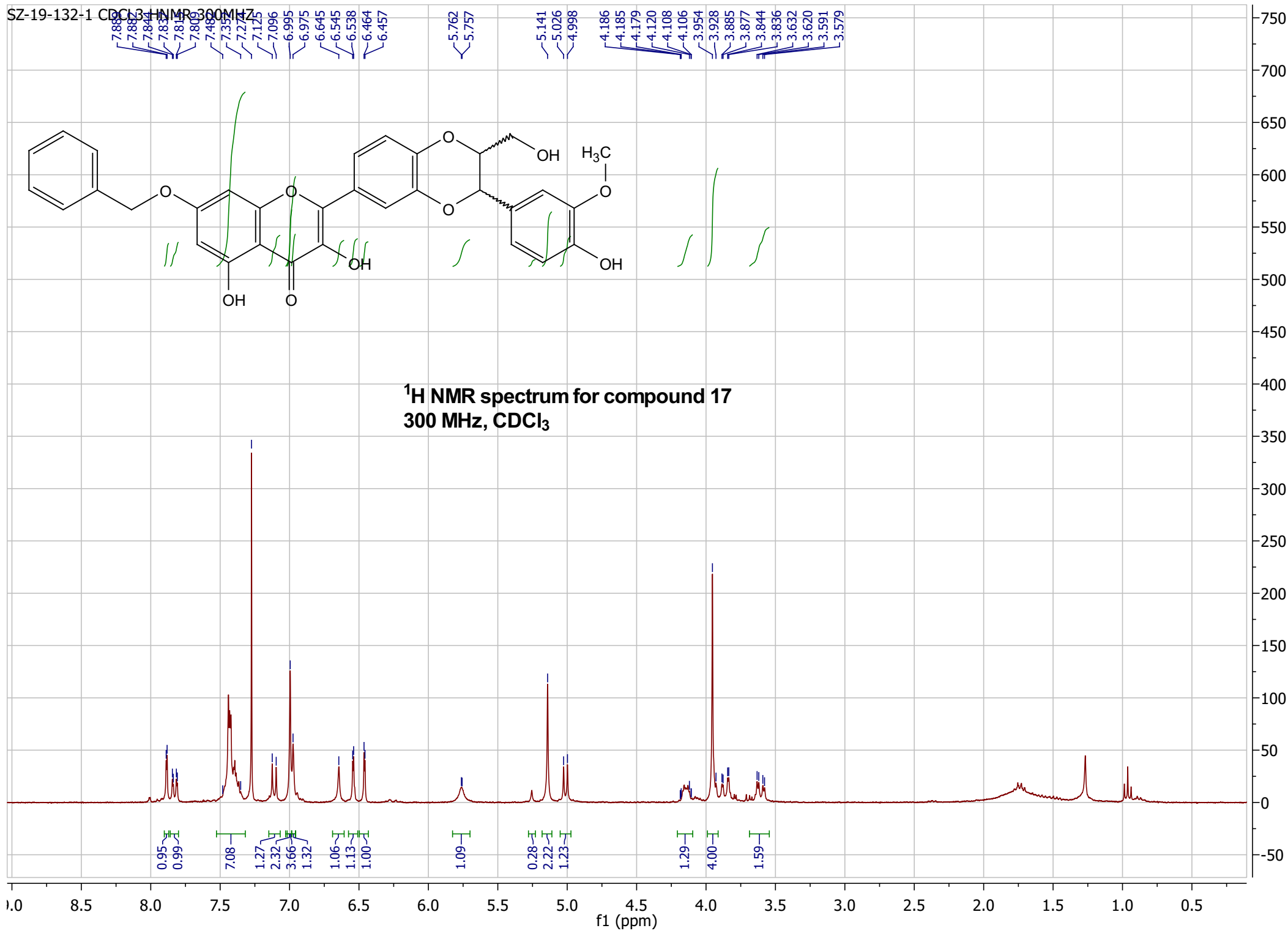


**<sup>13</sup>C NMR spectrum for compound 16**  
75 MHz, CDCl<sub>3</sub>



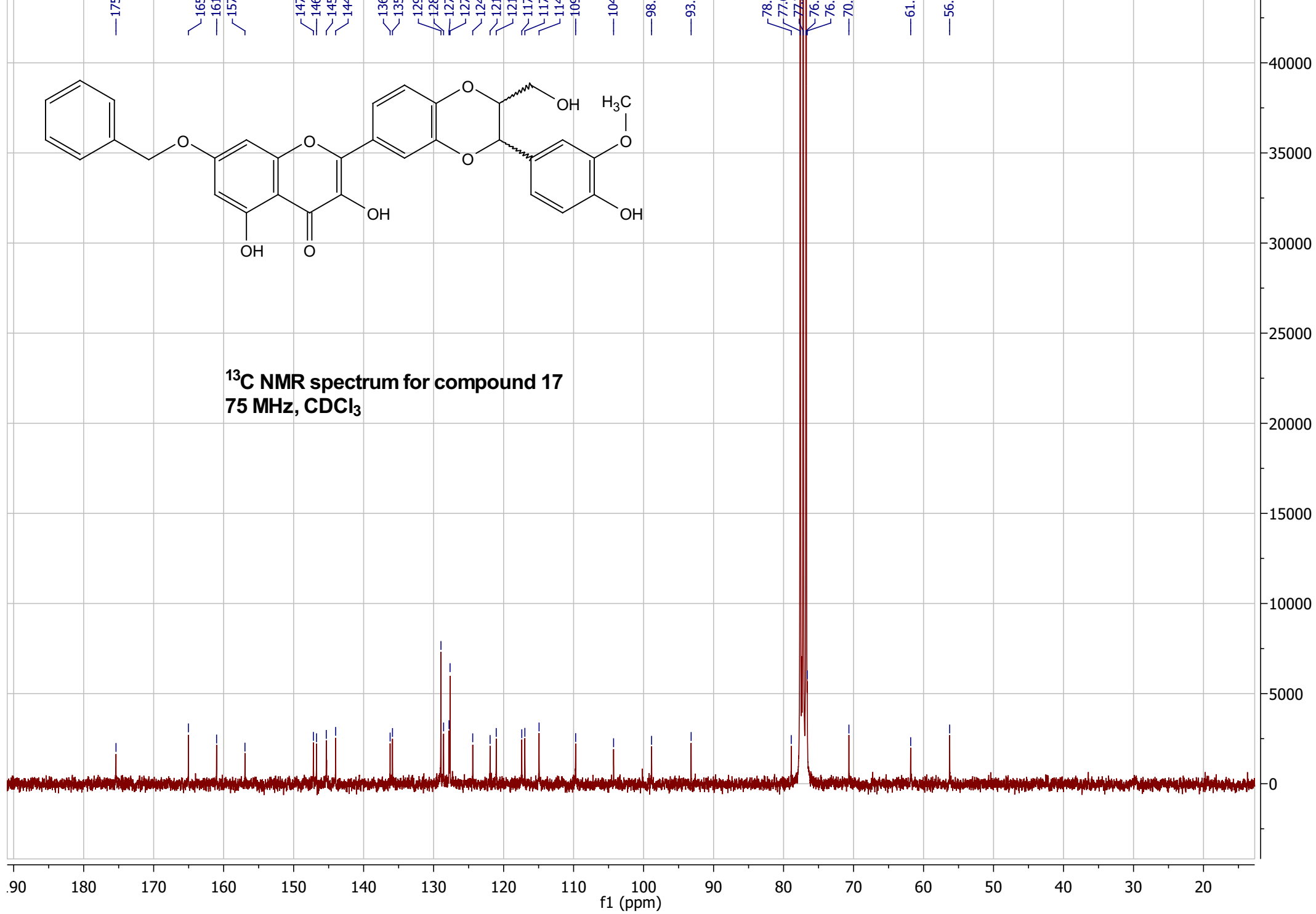


**<sup>1</sup>H NMR spectrum for compound 17**  
**300 MHz, CDCl<sub>3</sub>**

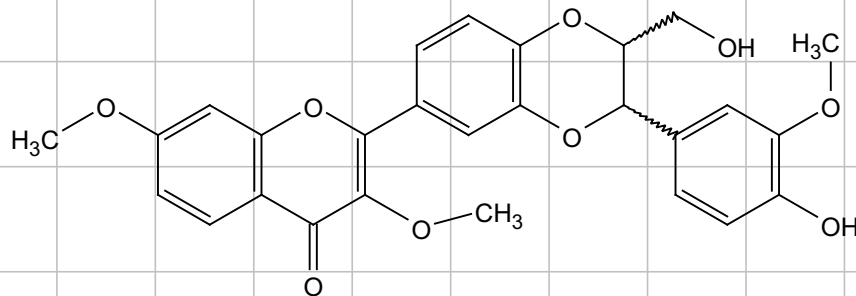




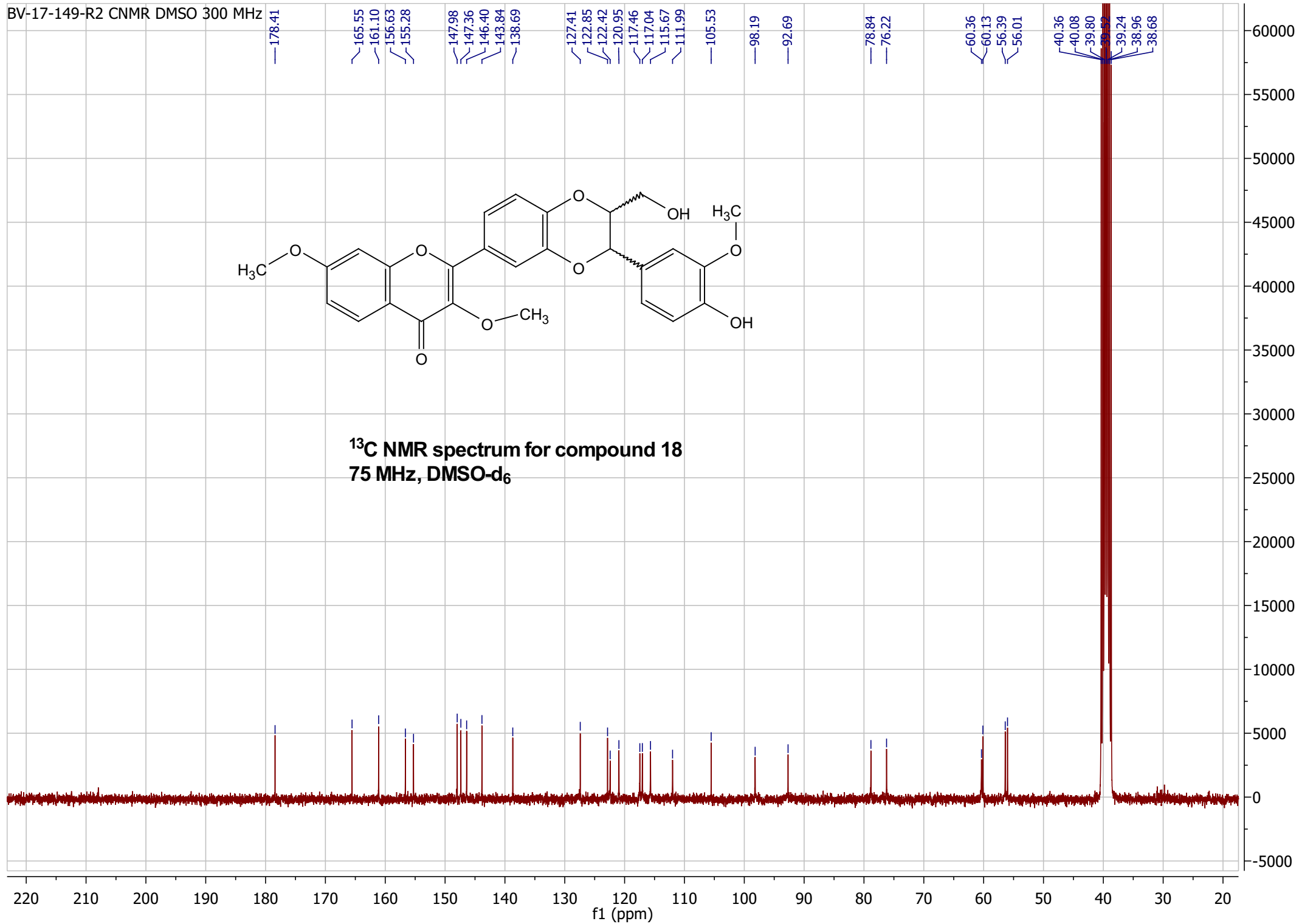
SZ-19-132-1 CDCl3 CNMR 75 MHz



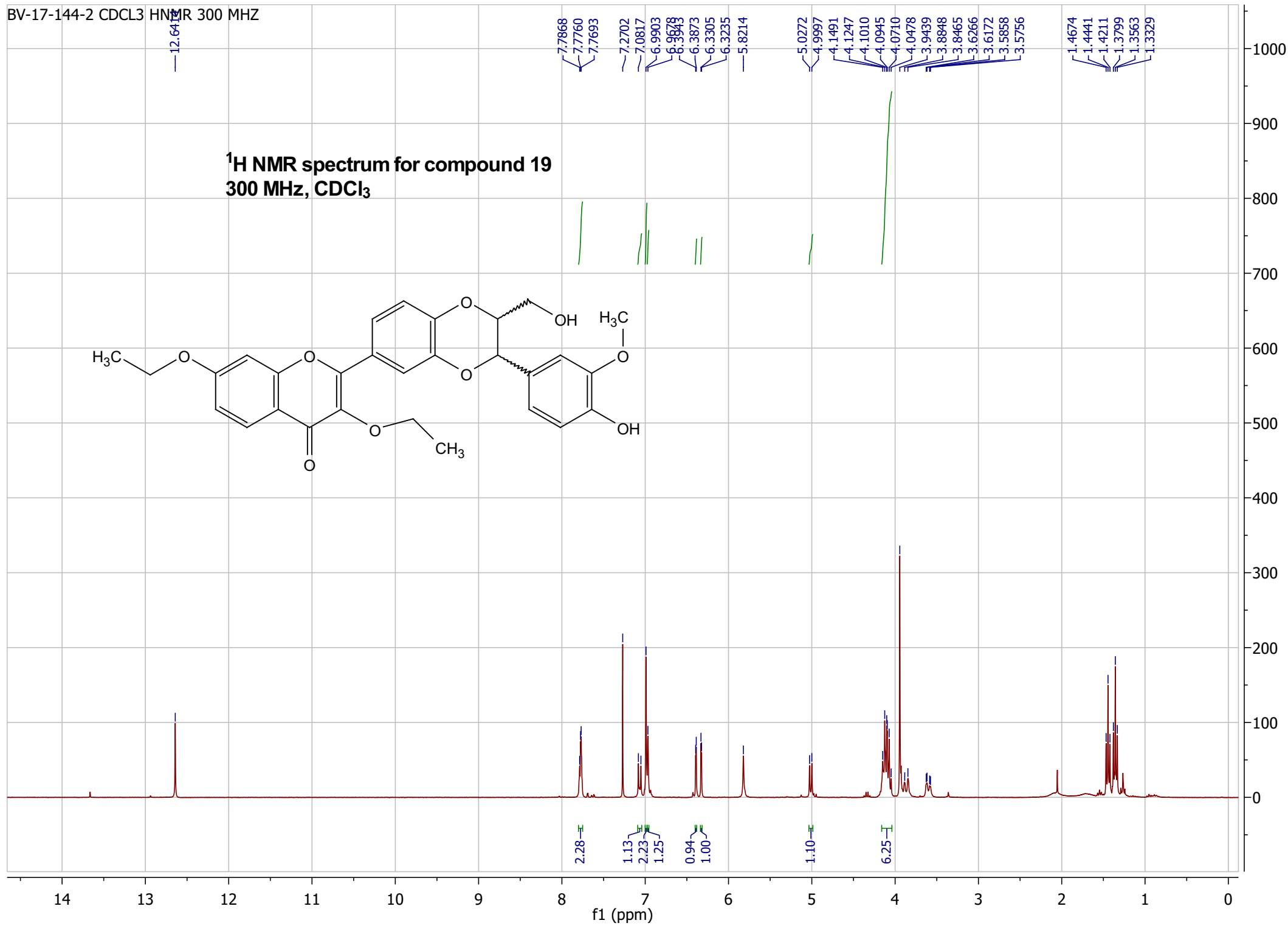
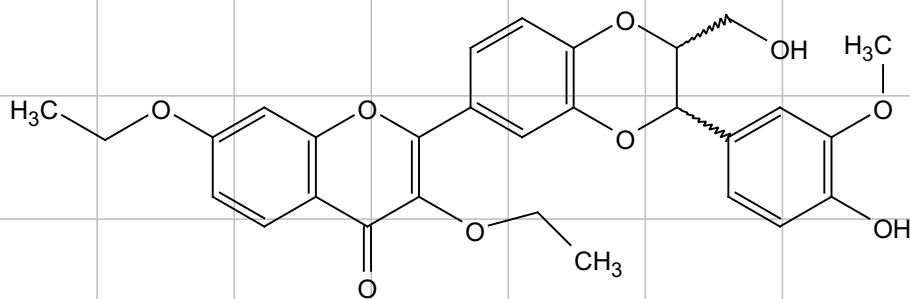




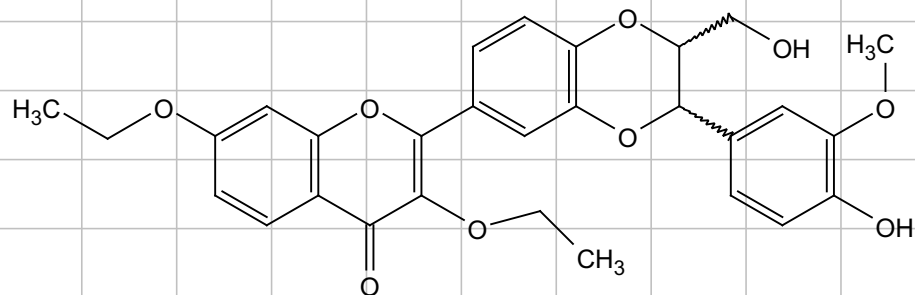
<sup>13</sup>C NMR spectrum for compound 18  
75 MHz, DMSO-d<sub>6</sub>



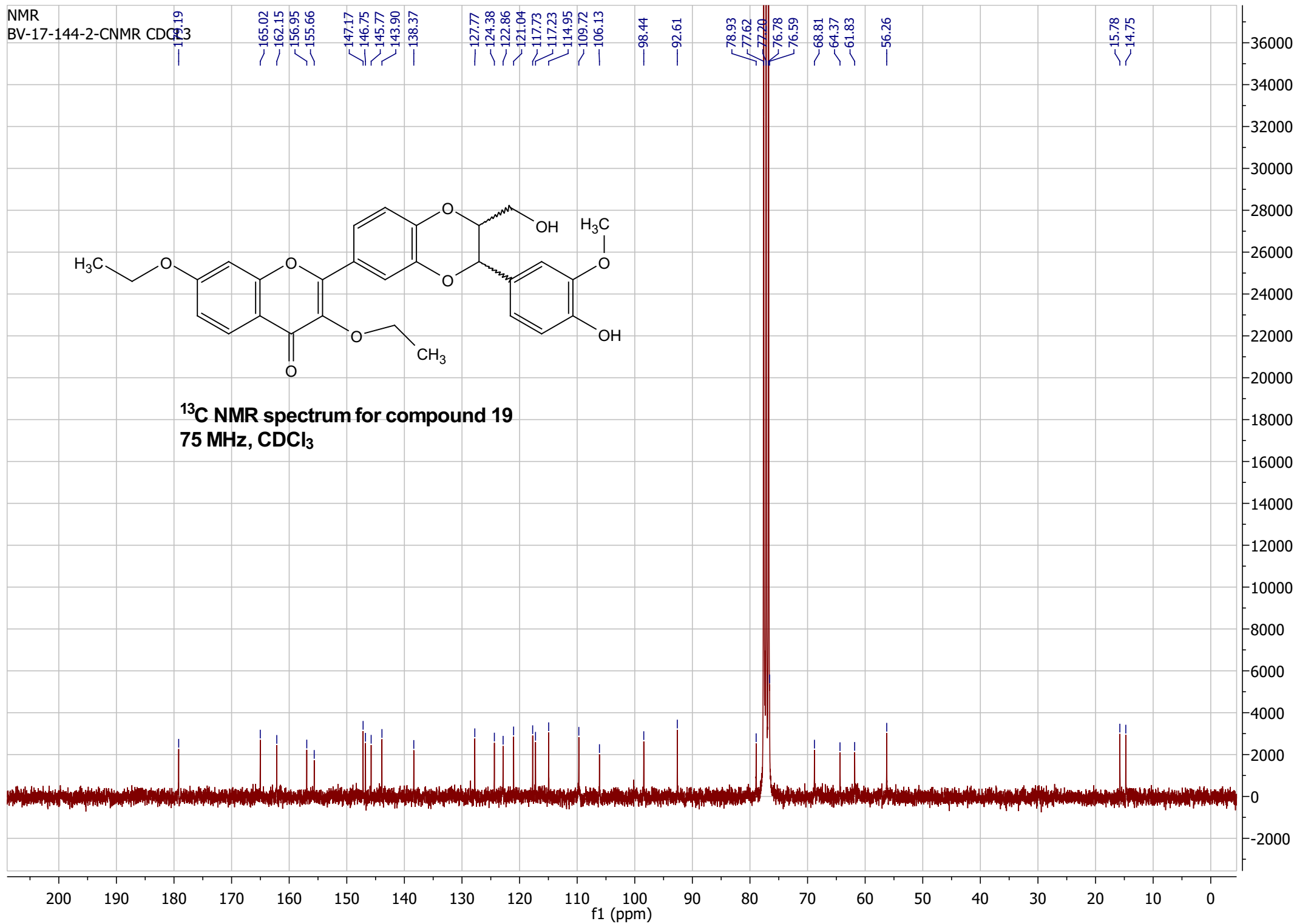
**<sup>1</sup>H NMR spectrum for compound 19**  
**300 MHz, CDCl<sub>3</sub>**



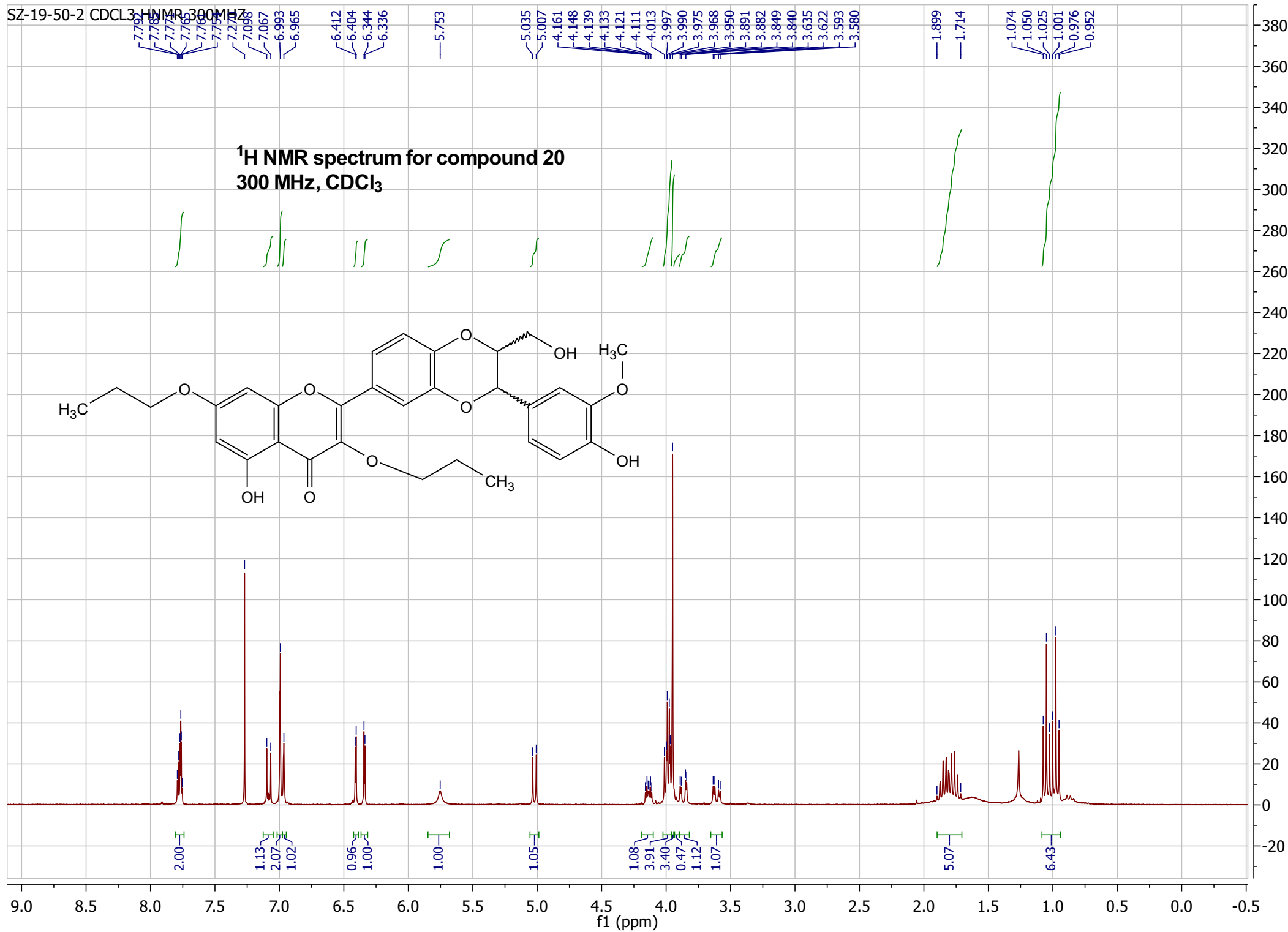
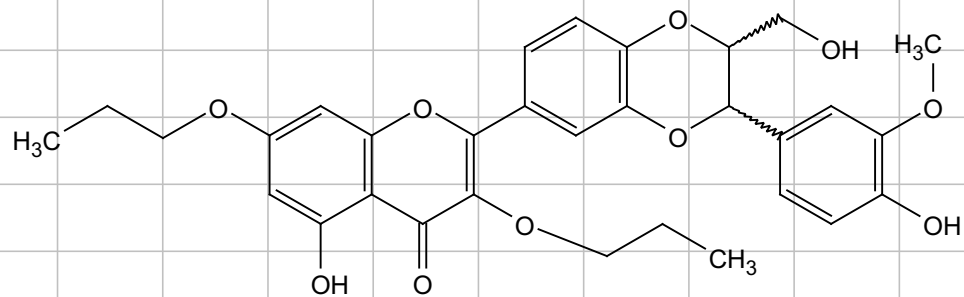
NMR  
BV-17-144-2-CNMR CDCl<sub>3</sub>

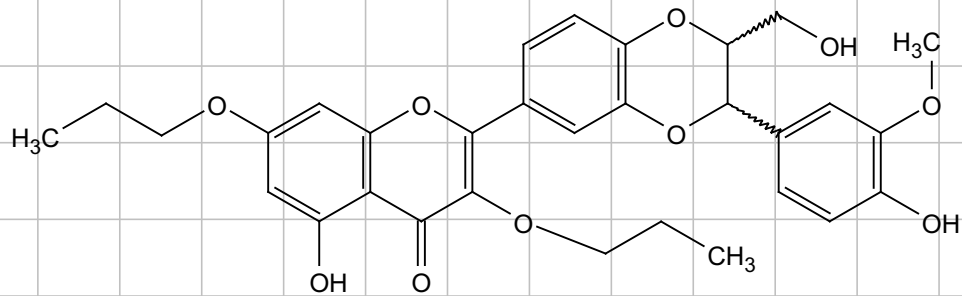


**<sup>13</sup>C NMR spectrum for compound 19**  
**75 MHz, CDCl<sub>3</sub>**

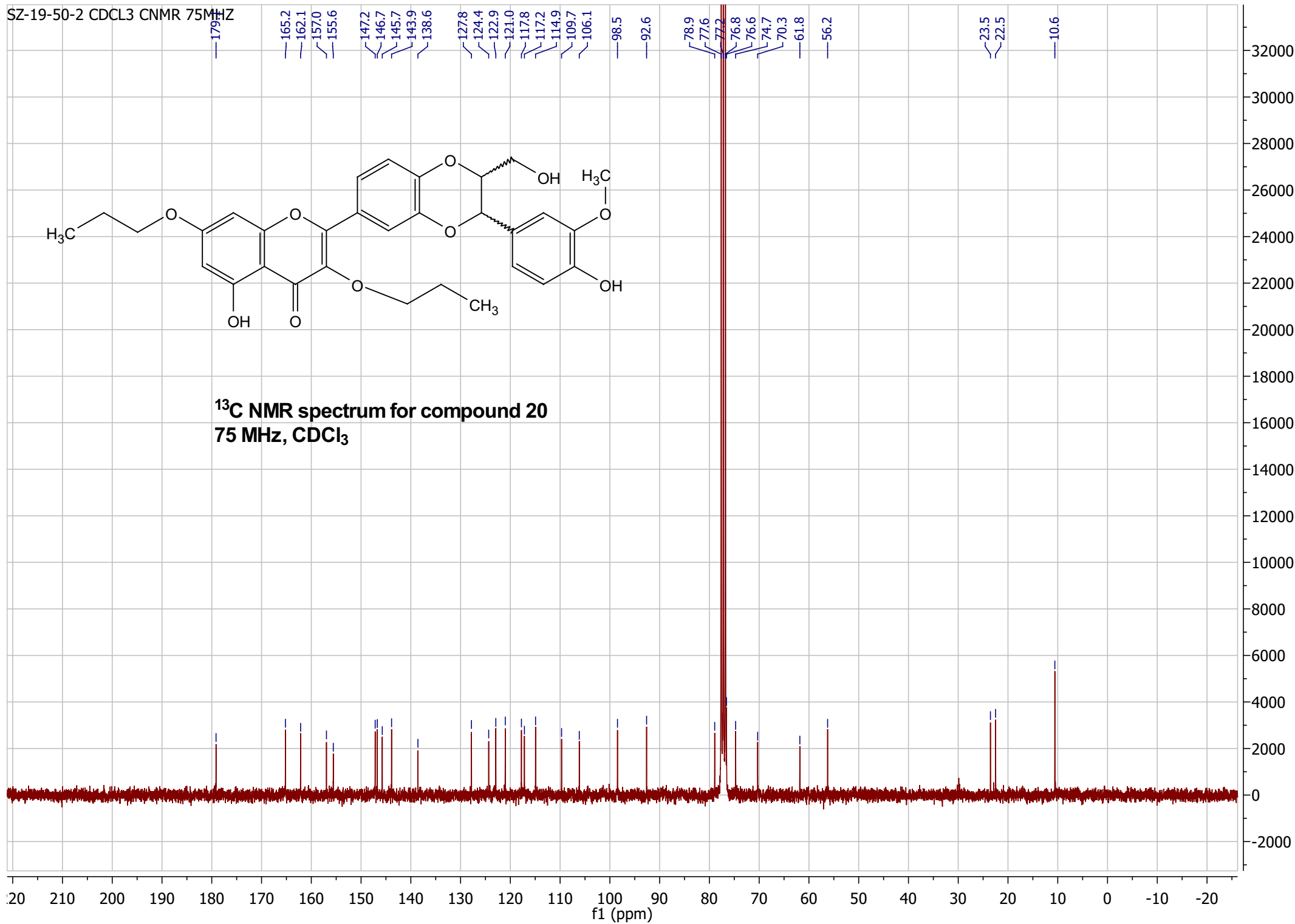


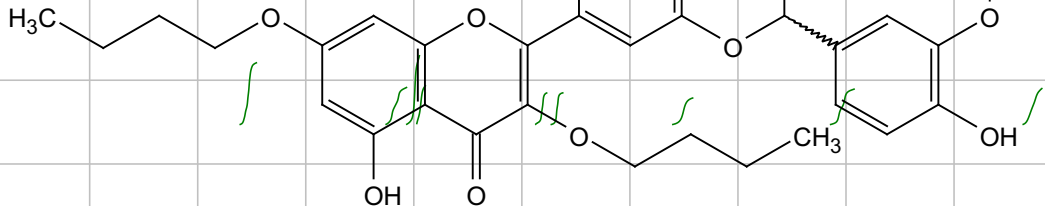
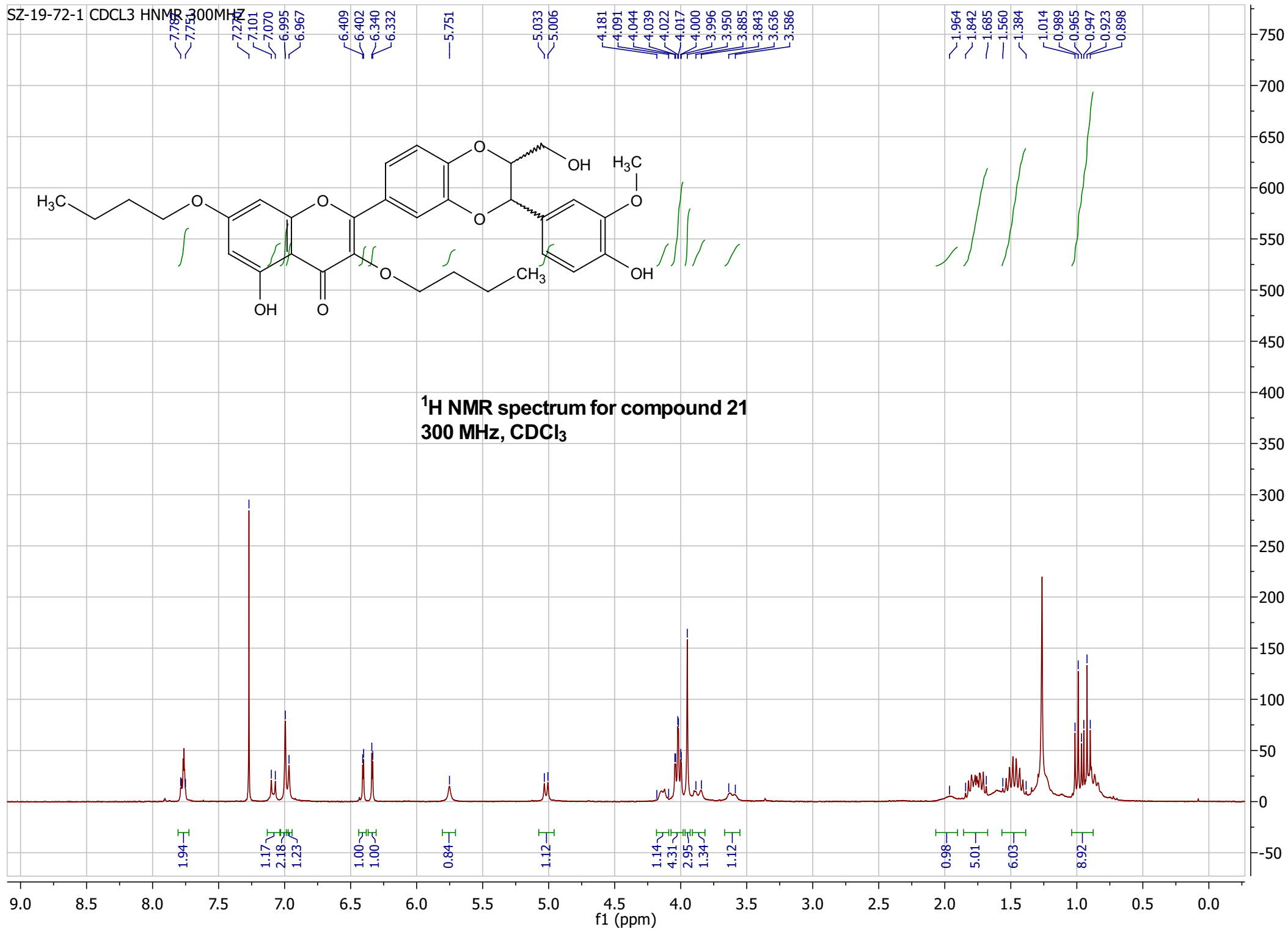
**<sup>1</sup>H NMR spectrum for compound 20**  
**300 MHz, CDCl<sub>3</sub>**



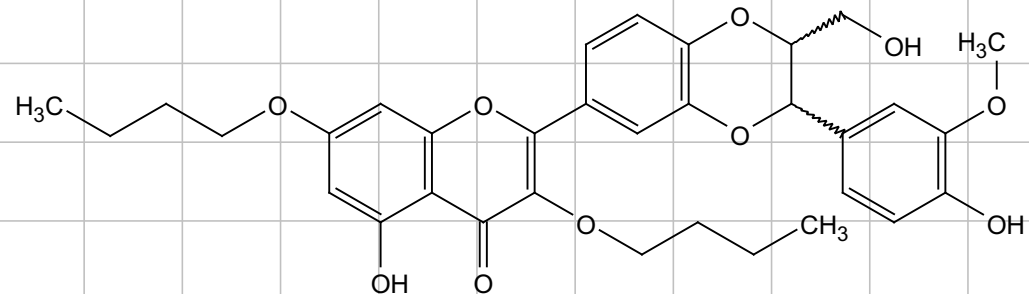


**<sup>13</sup>C NMR spectrum for compound 20**  
**75 MHz, CDCl<sub>3</sub>**

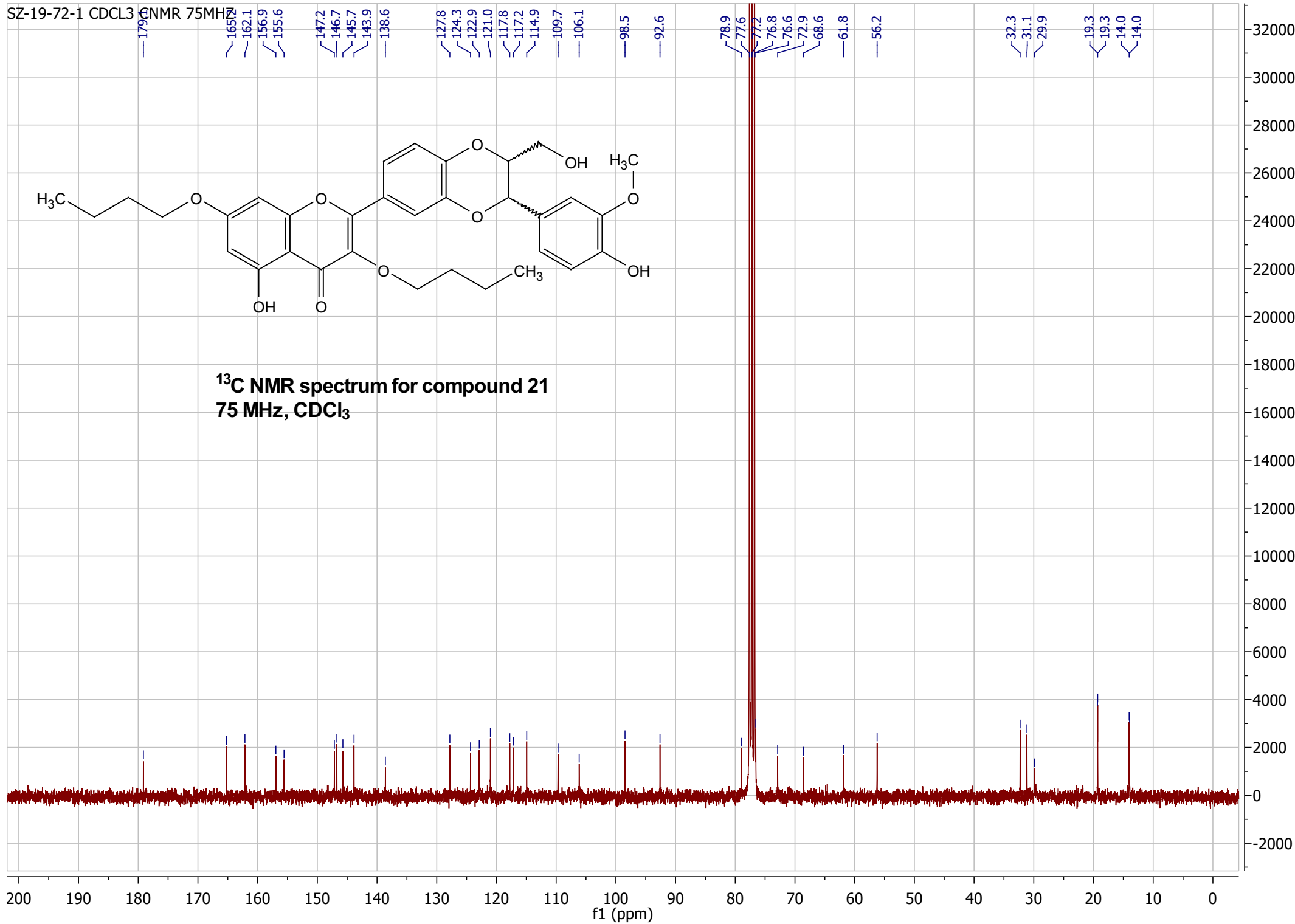




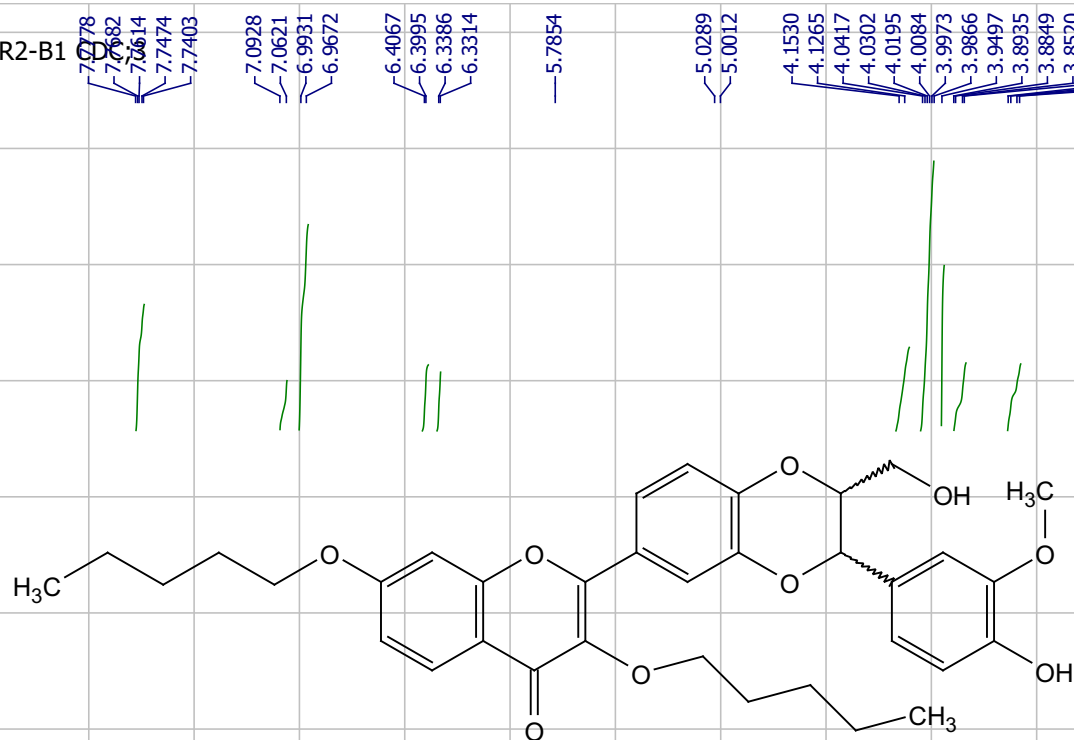




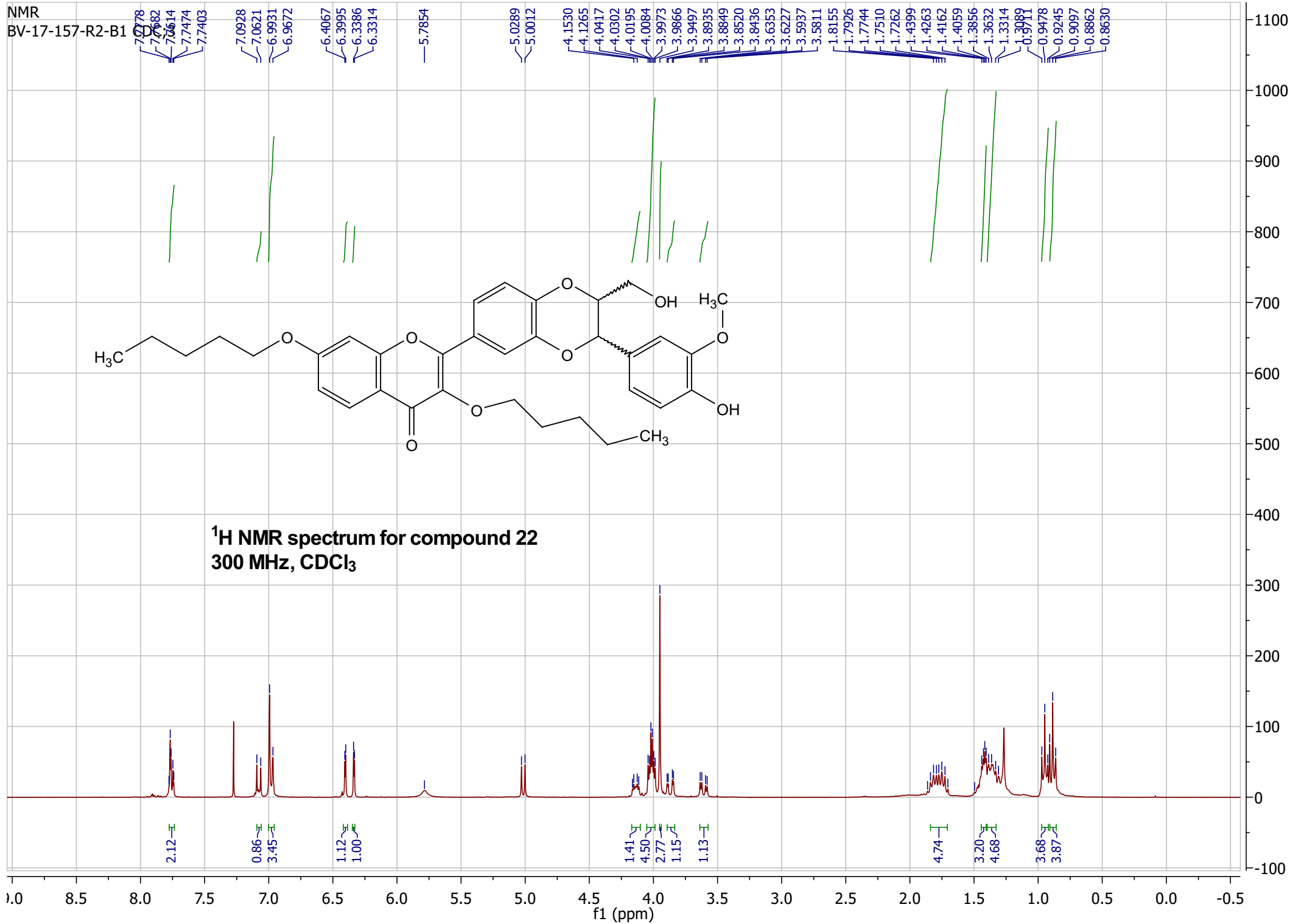
**<sup>13</sup>C NMR spectrum for compound 21**  
**75 MHz, CDCl<sub>3</sub>**



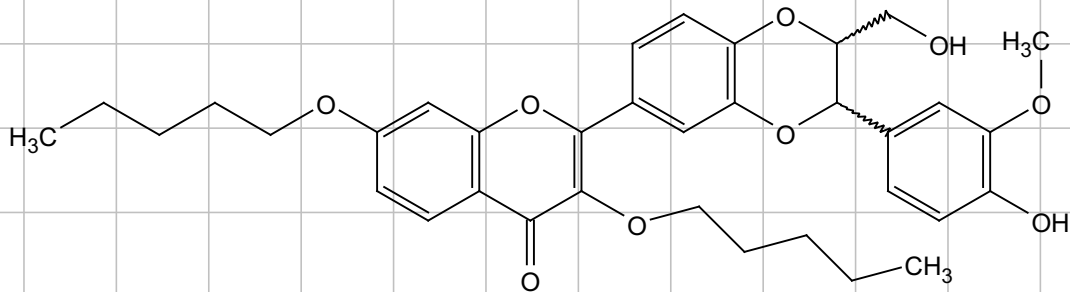
NMR  
BV-17-157-R2-B1



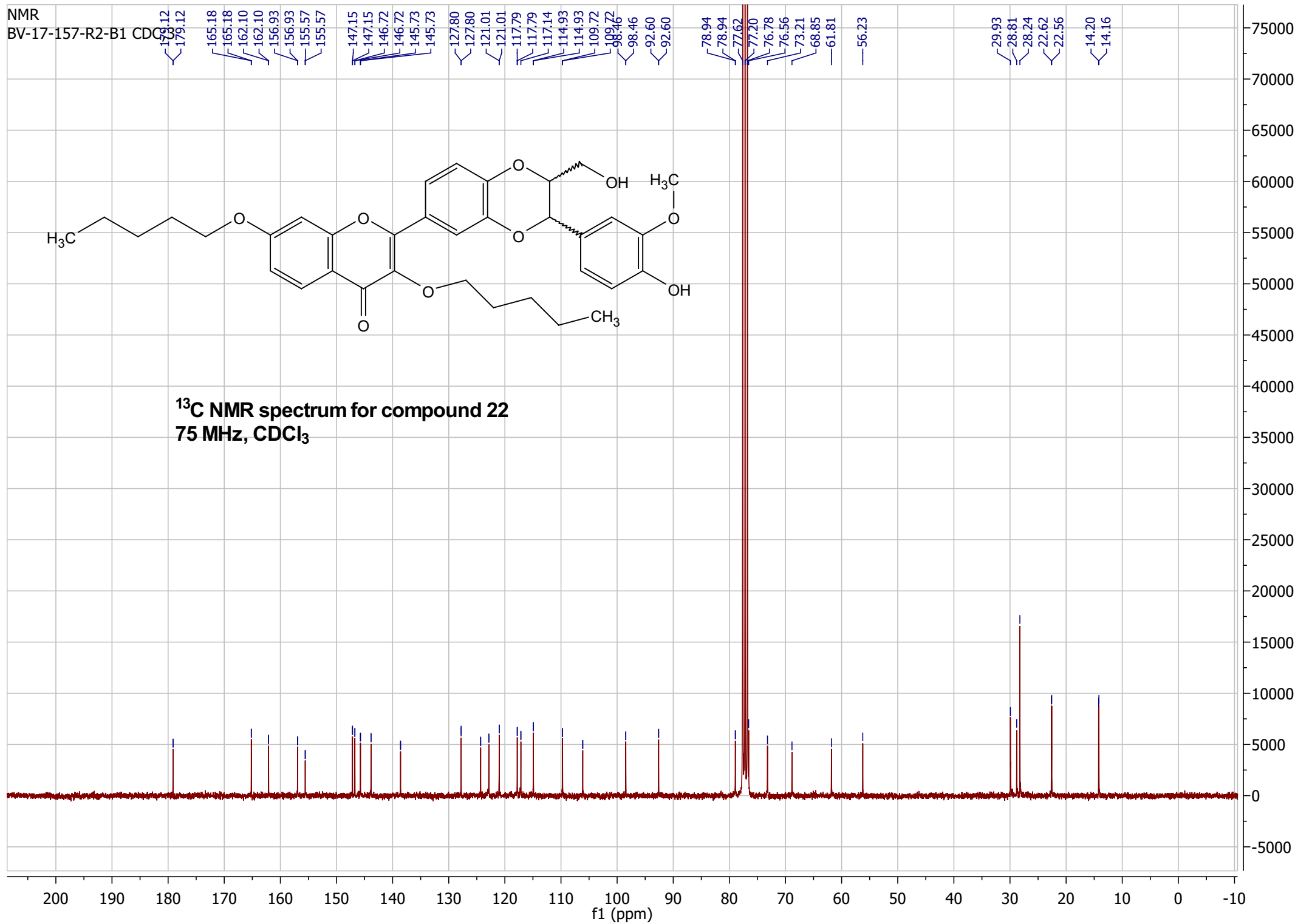
**<sup>1</sup>H NMR spectrum for compound 22**  
**300 MHz, CDCl<sub>3</sub>**



NMR  
BV-17-157-R2-B1 CDCl<sub>3</sub>

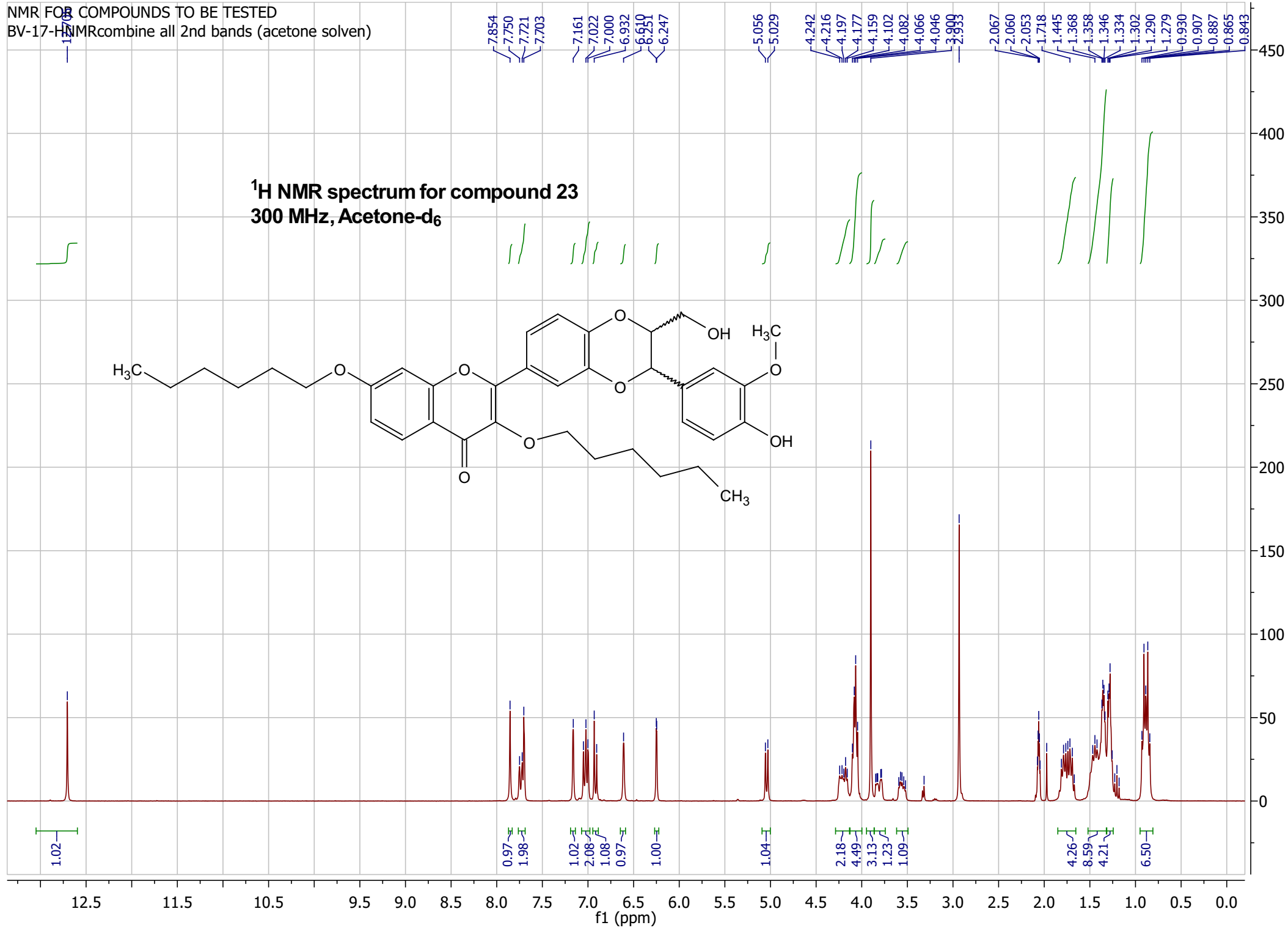
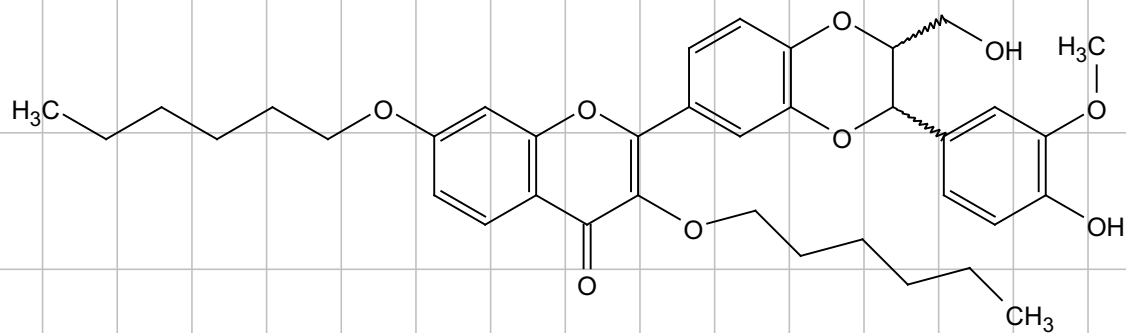


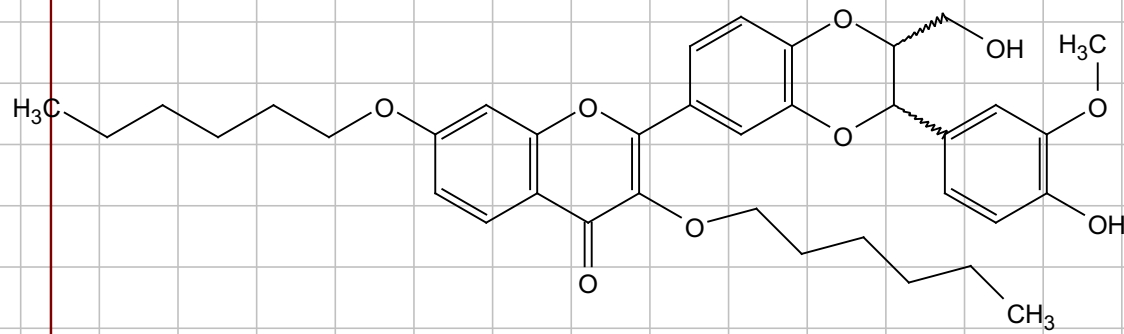
**<sup>13</sup>C NMR spectrum for compound 22**  
75 MHz, CDCl<sub>3</sub>



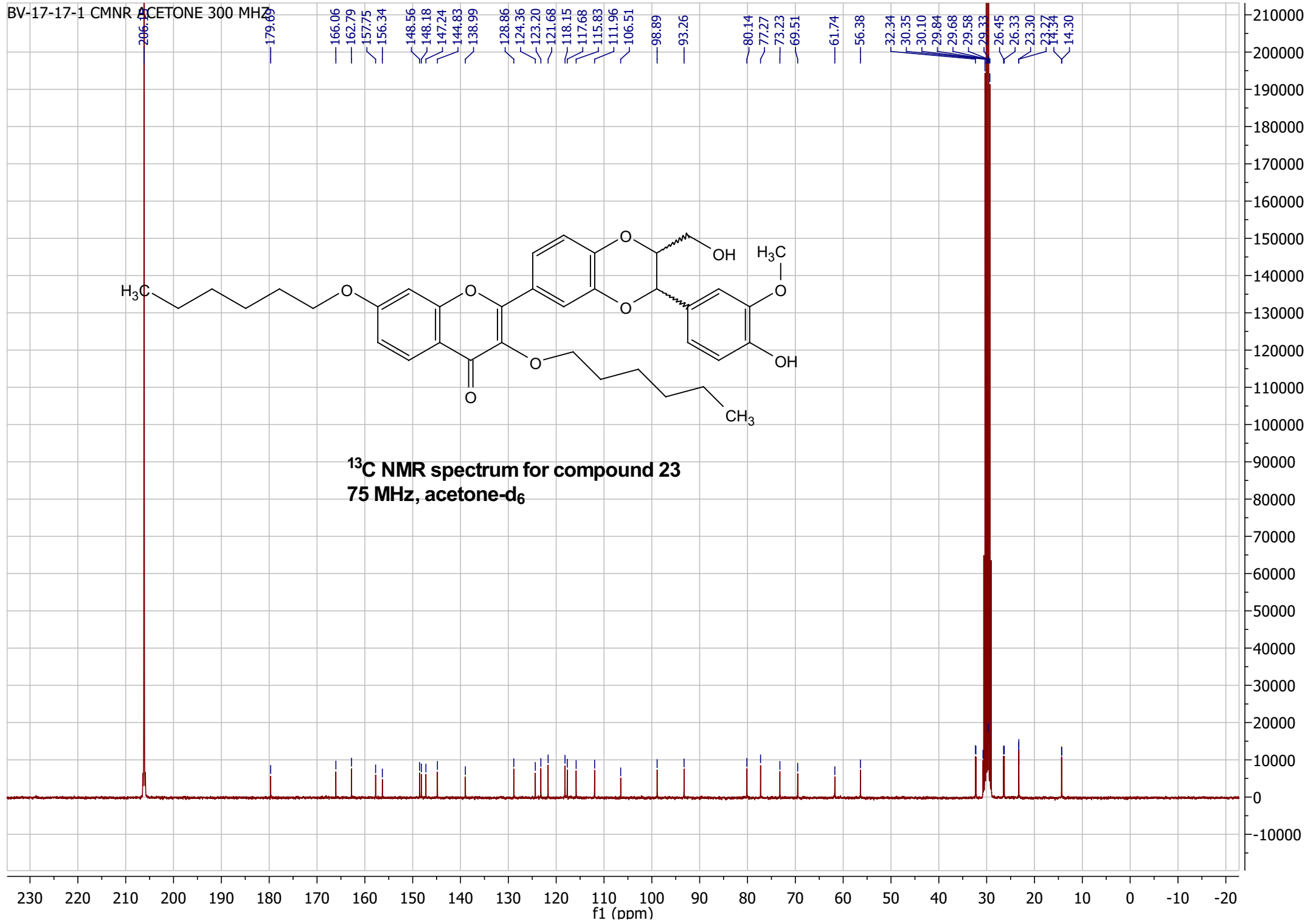
NMR FOR COMPOUNDS TO BE TESTED  
BV-17-H-NMRcombine all 2nd bands (acetone solven)

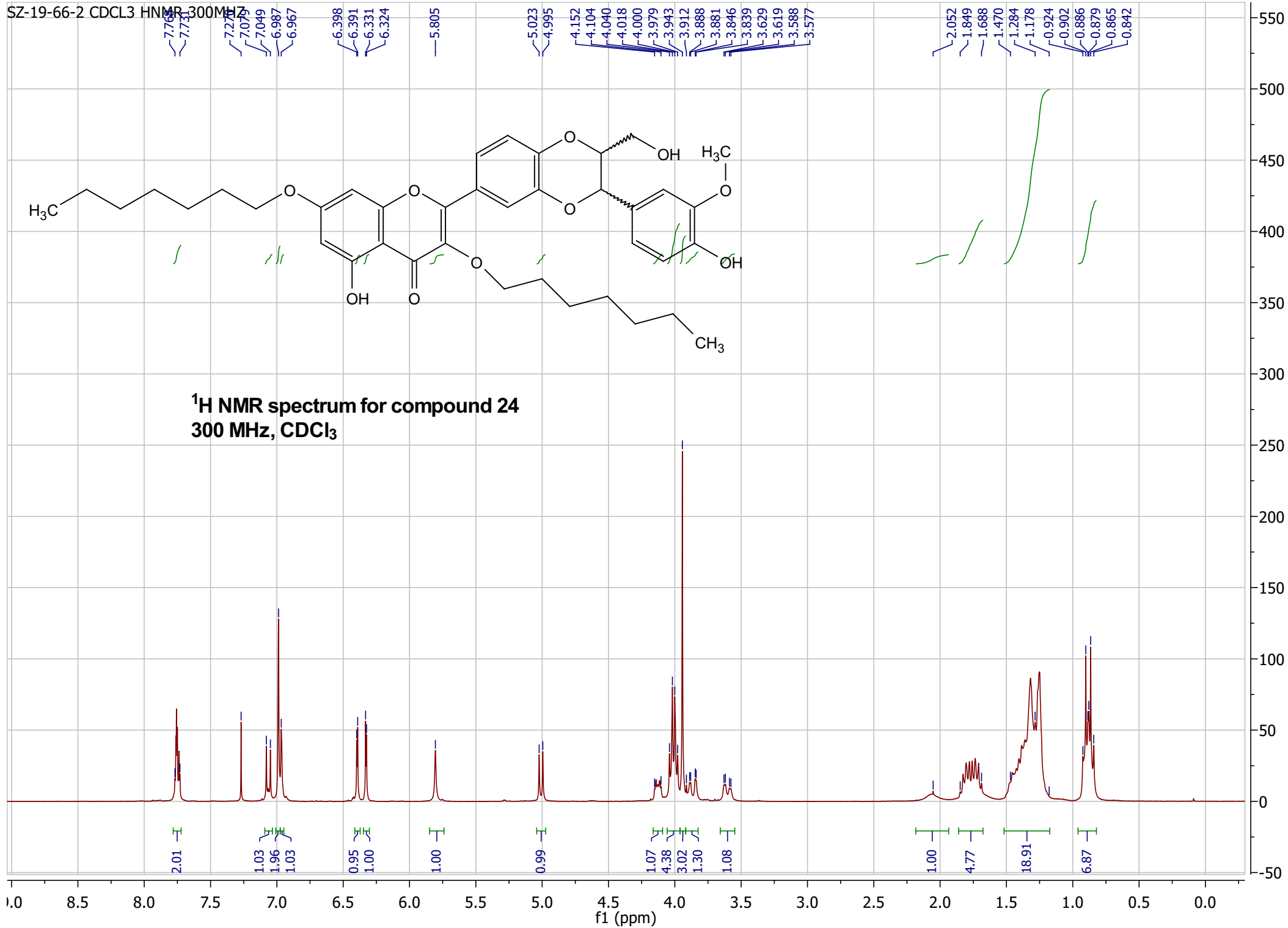
**<sup>1</sup>H NMR spectrum for compound 23**  
300 MHz, Acetone-d<sub>6</sub>

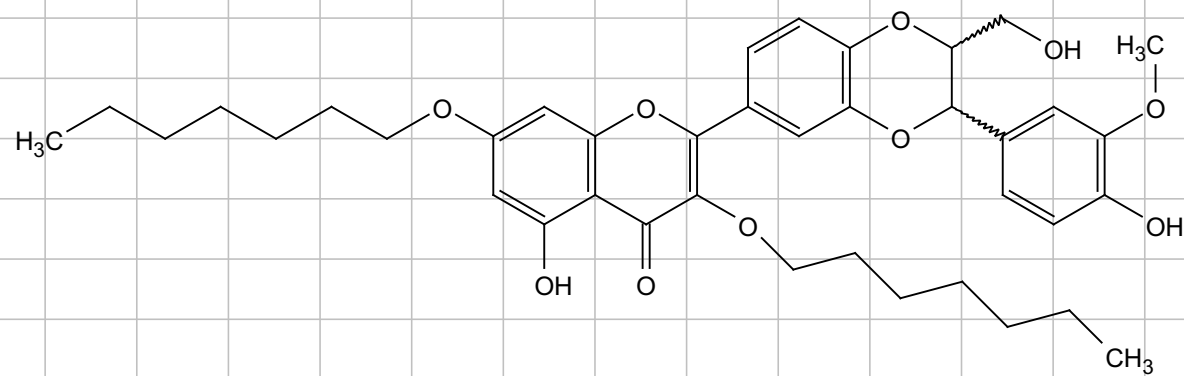




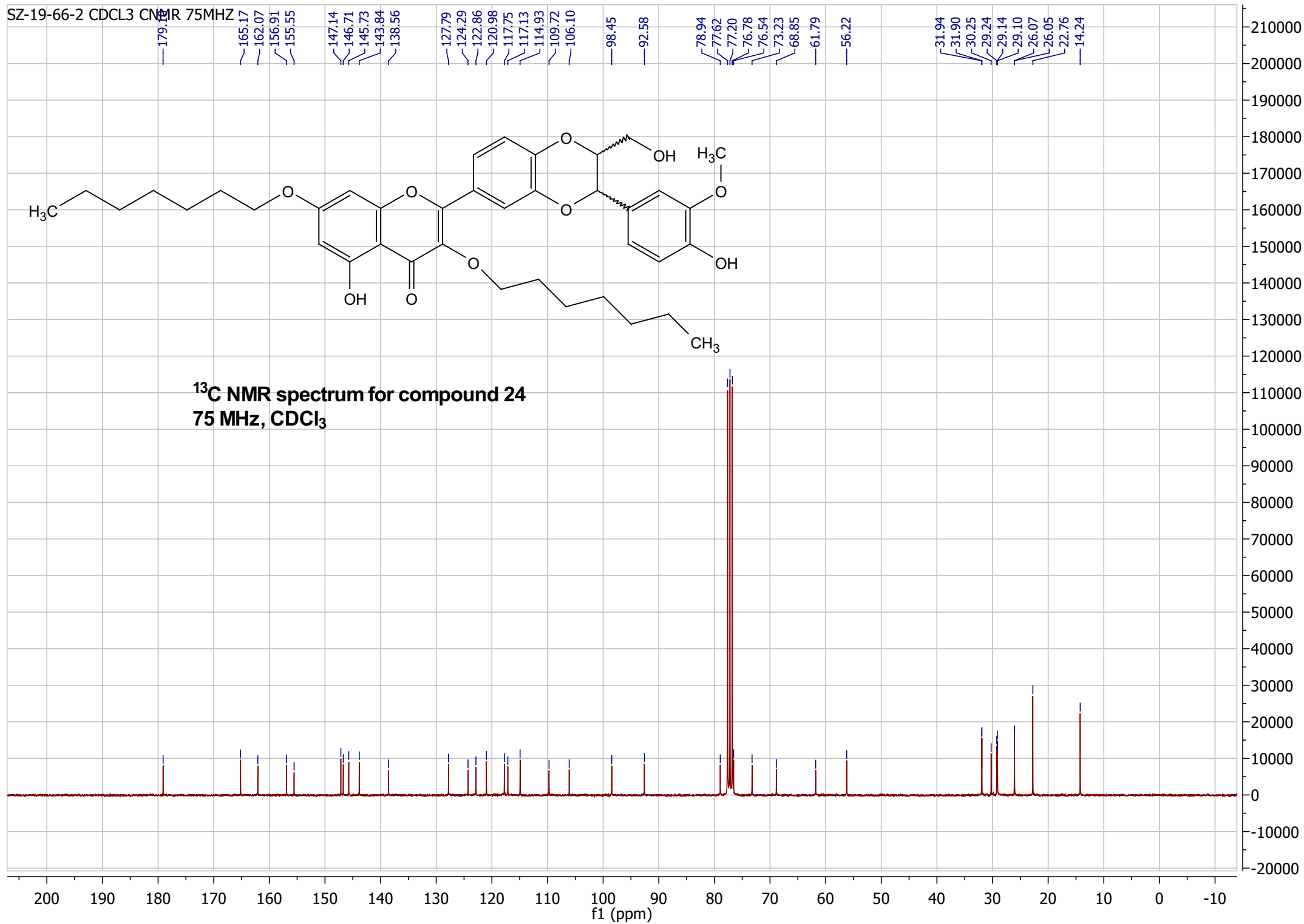
<sup>13</sup>C NMR spectrum for compound 23  
75 MHz, acetone-d<sub>6</sub>



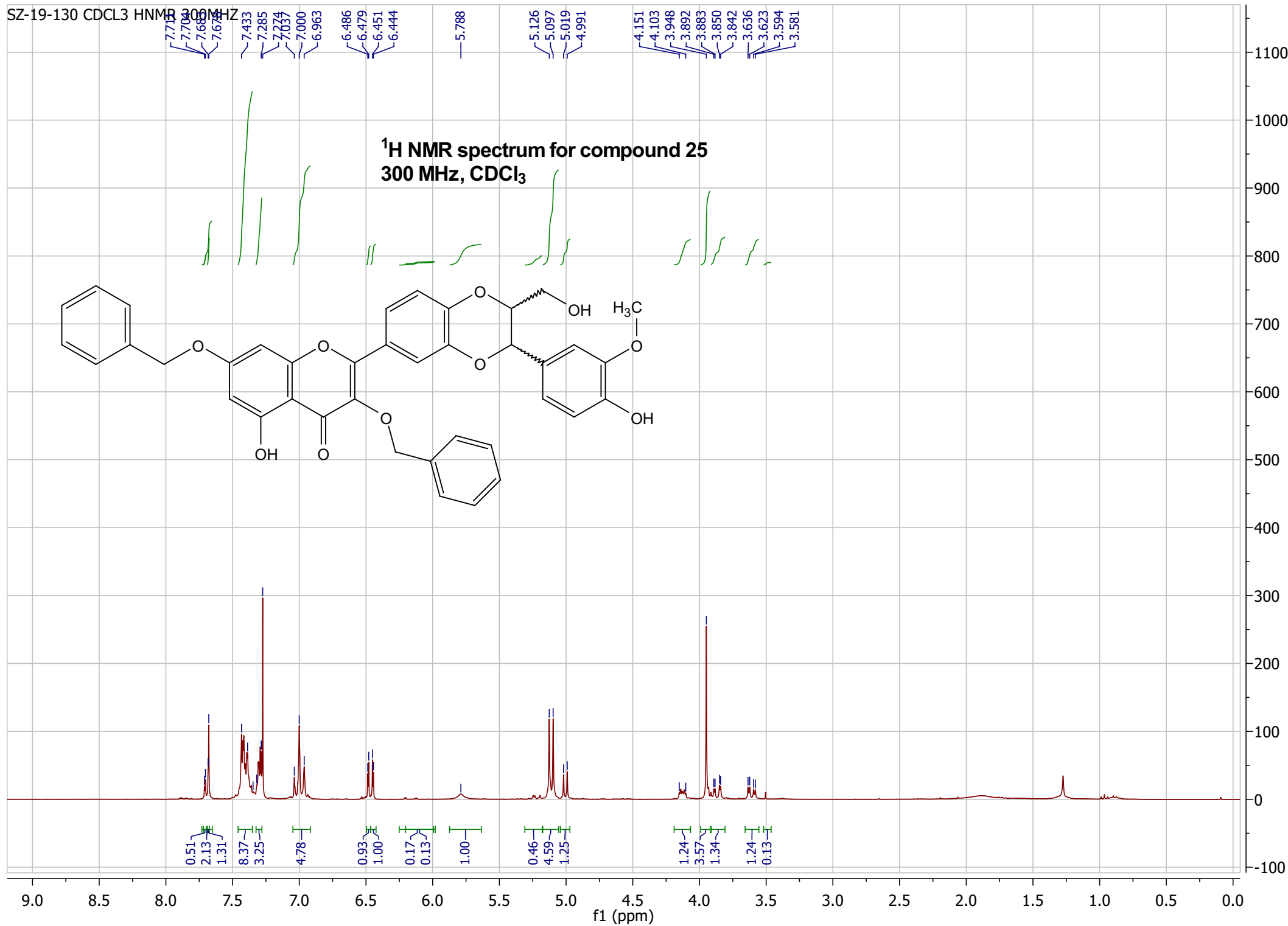
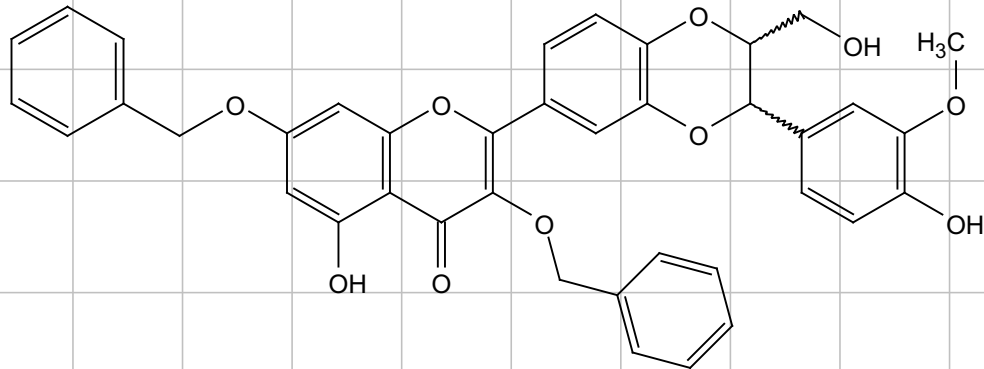




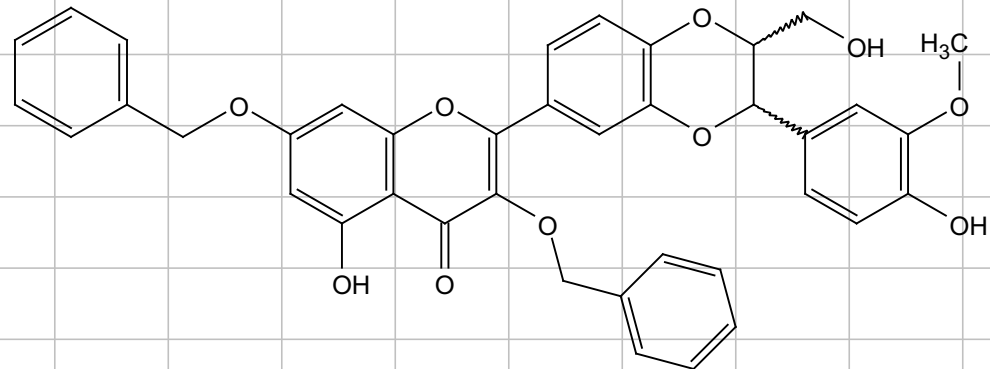
**<sup>13</sup>C NMR spectrum for compound 24**  
**75 MHz, CDCl<sub>3</sub>**



**<sup>1</sup>H NMR spectrum for compound 25**  
**300 MHz, CDCl<sub>3</sub>**







<sup>13</sup>C NMR spectrum for compound 25  
75 MHz, CDCl<sub>3</sub>

