

Supporting Information

Anti-proliferative effects of diterpenoids from *Sagittaria trifolia L.* tubers on colon cancer cells by targeting NF- κ B pathway

Israa Assani^a, Ying Du^a, Chun-Gu Wang^a, Lei Chen^a, Pei-Lei Hou^a, Shi-Feng Zhao^a, Yan Feng^a, Ling-Fei Liu^a, Bo Sun^a, Yan Li^a, Zhi-Xin Liao^{a*} and Ri-Zhen Huang^{b*}

^aDepartment of Pharmaceutical Engineering, School of Chemistry and Chemical Engineering, Jiangsu Province Hi-Tech Key Laboratory for Biomedical Research, Southeast University, Nanjing 211189, China

^bCollege of Biotechnology, Guilin Medical University, Guilin 541100.

*Corresponding authors at ^aDepartment of Pharmaceutical Engineering, School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, China. ^bCollege of Biotechnology, Guilin Medical University, Guilin 541100.

E-mail addresses: zxliao@seu.edu.cn (Z. -X. Liao) and rzhuang1783@163.com (R.-Z. Huang).

List of supporting information

EXPERIMENTAL SECTION

Figure S1.1 ^1H NMR spectrum (400 MHz) of **1** in CDCl_3

Figure S1.2 ^{13}C NMR spectrum (100 MHz) of **1** in CDCl_3

Figure S1.3 HMBC spectrum of **1** in CDCl_3

Figure S1.4 HMQC spectrum of **1** in CDCl_3

Figure S1.5 ROESY spectrum of **1** in CDCl_3

Figure S1.6 ^1H - ^1H COSY spectrum of **1** in CDCl_3

Figure S1.7 HRESIMS spectrum of **1**

Figure S2.1 ^1H NMR spectrum (400 MHz) of **2** in CDCl_3

Figure S2.2 ^{13}C NMR spectrum (100 MHz) of **2** in CDCl_3

Figure S3.1 ^1H NMR spectrum (400 MHz) of **3** in CDCl_3

Figure S3.2 ^{13}C NMR spectrum (100 MHz) of **3** in CDCl_3

Figure S4.1 ^1H NMR spectrum (400 MHz) of **4** in CDCl_3

Figure S4.2 ^{13}C NMR spectrum (100 MHz) of **4** in CDCl_3

Figure S5.1 ^1H NMR spectrum (400 MHz) of **5** in CDCl_3

Figure S5.2 ^{13}C NMR spectrum (100 MHz) of **5** in CDCl_3

Figure S6.1 ^1H NMR spectrum (400 MHz) of **6** in CDCl_3

Figure S6.2 ^{13}C NMR spectrum (100 MHz) of **6** in CDCl_3

Figure S7.1 ^1H NMR spectrum (400 MHz) of **7** in CDCl_3

Figure S7.2 ^{13}C NMR spectrum (100 MHz) of **7** in CDCl_3

Figure S8.1 ^1H NMR spectrum (400 MHz) of **8** in CDCl_3

Figure S8.2 ^{13}C NMR spectrum (100 MHz) of **8** in CDCl_3

Figure S9.1 ^1H NMR spectrum (400 MHz) of **9** in CDCl_3

Figure S9.2 ^{13}C NMR spectrum (100 MHz) of **9** in CDCl_3

Figure S10.1 ^1H NMR spectrum (400 MHz) of **10** in CDCl_3

Figure S10.2 ^{13}C NMR spectrum (100 MHz) of **10** in CDCl_3

Figure S10.3 The purity of **10** investigated by HPLC

Figure S11.1 ^1H NMR spectrum (400 MHz) of **11** in CDCl_3

Figure S11.2 ^{13}C NMR spectrum (100 MHz) of **11** in CDCl_3

Figure S11.3 The purity of **11** investigated by HPLC

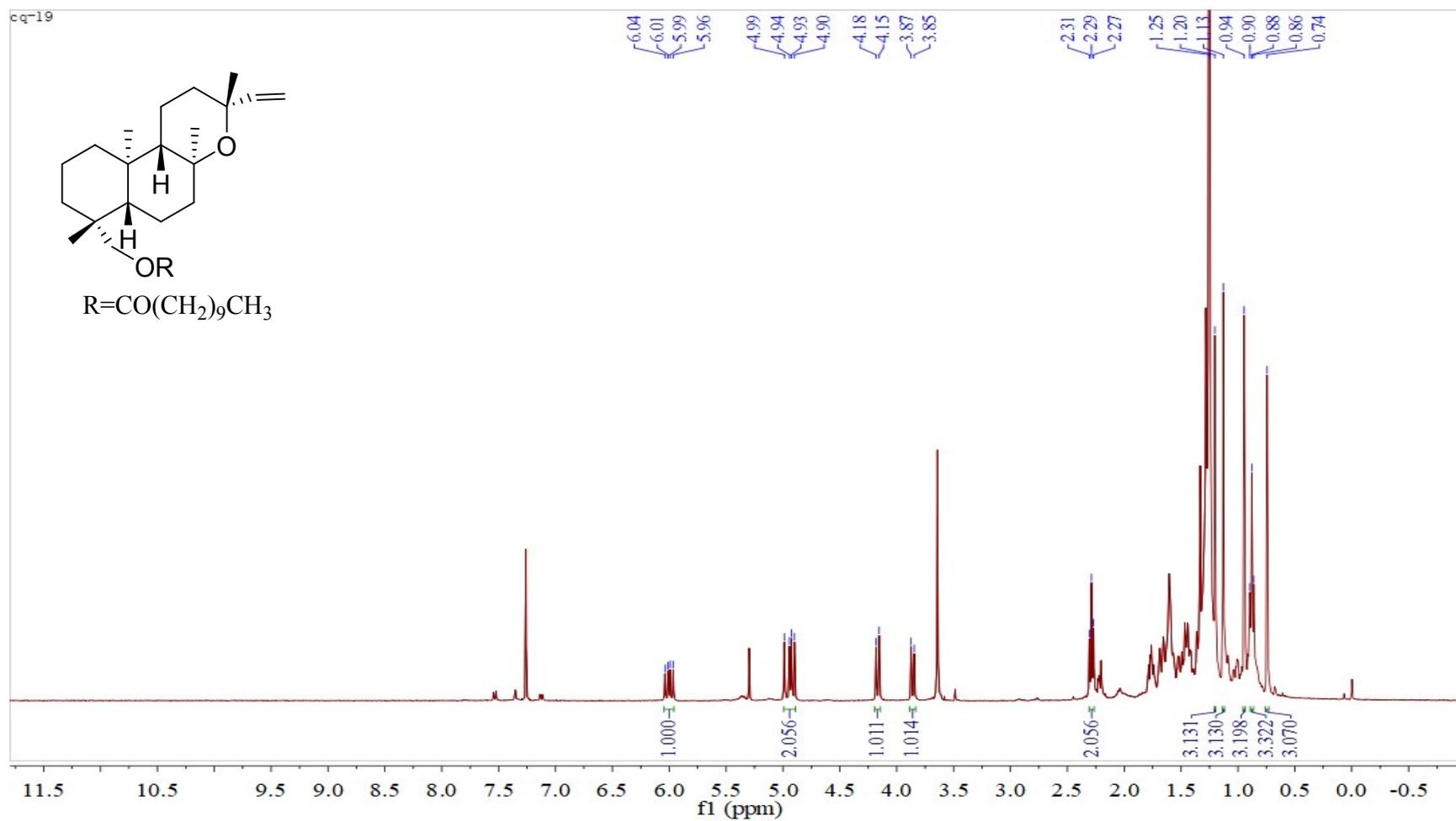


Figure S1.1 ¹H NMR spectrum (400 MHz) of **1** in CDCl₃

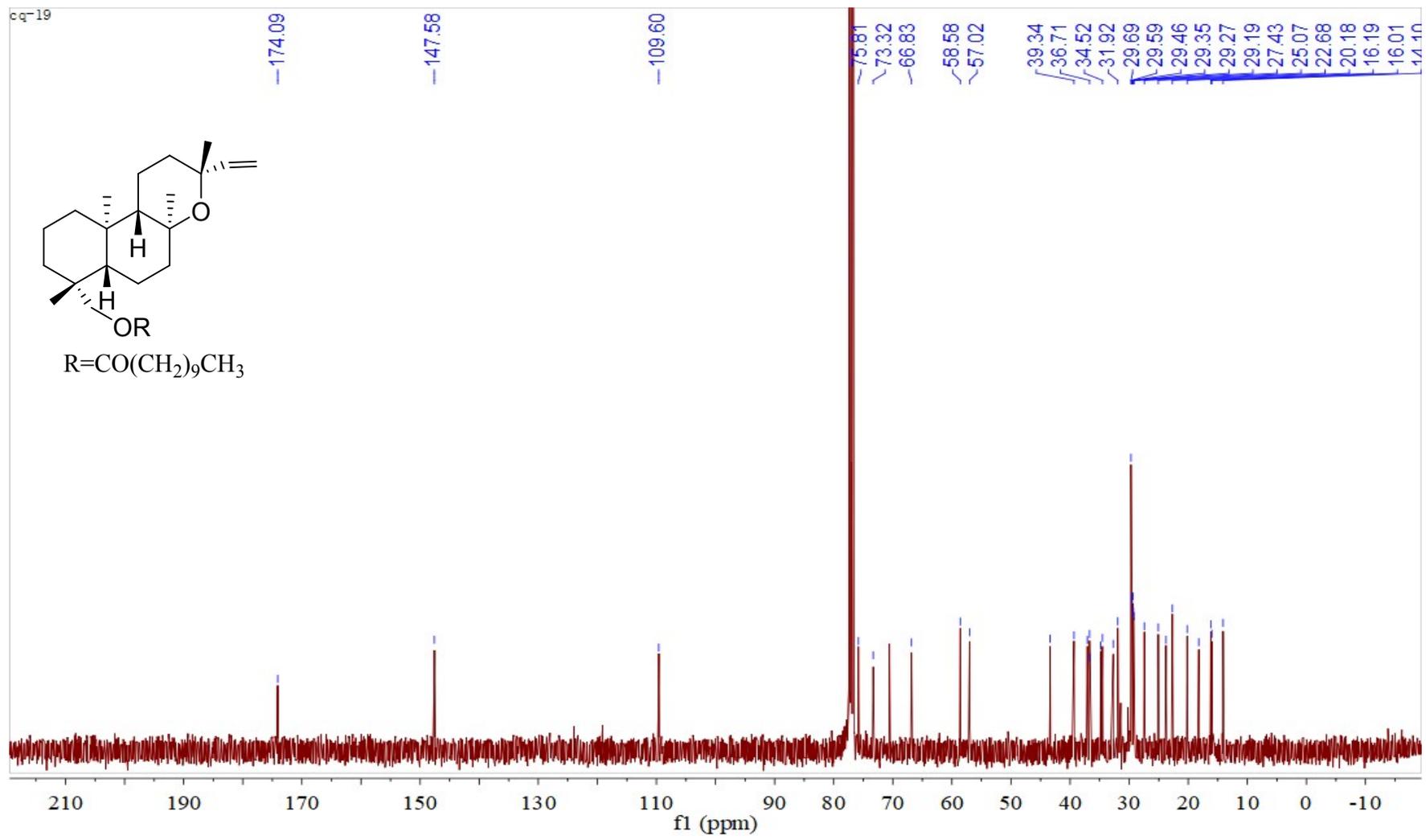


Figure S1.2 ¹³C NMR spectrum (100 MHz) of **1** in CDCl₃

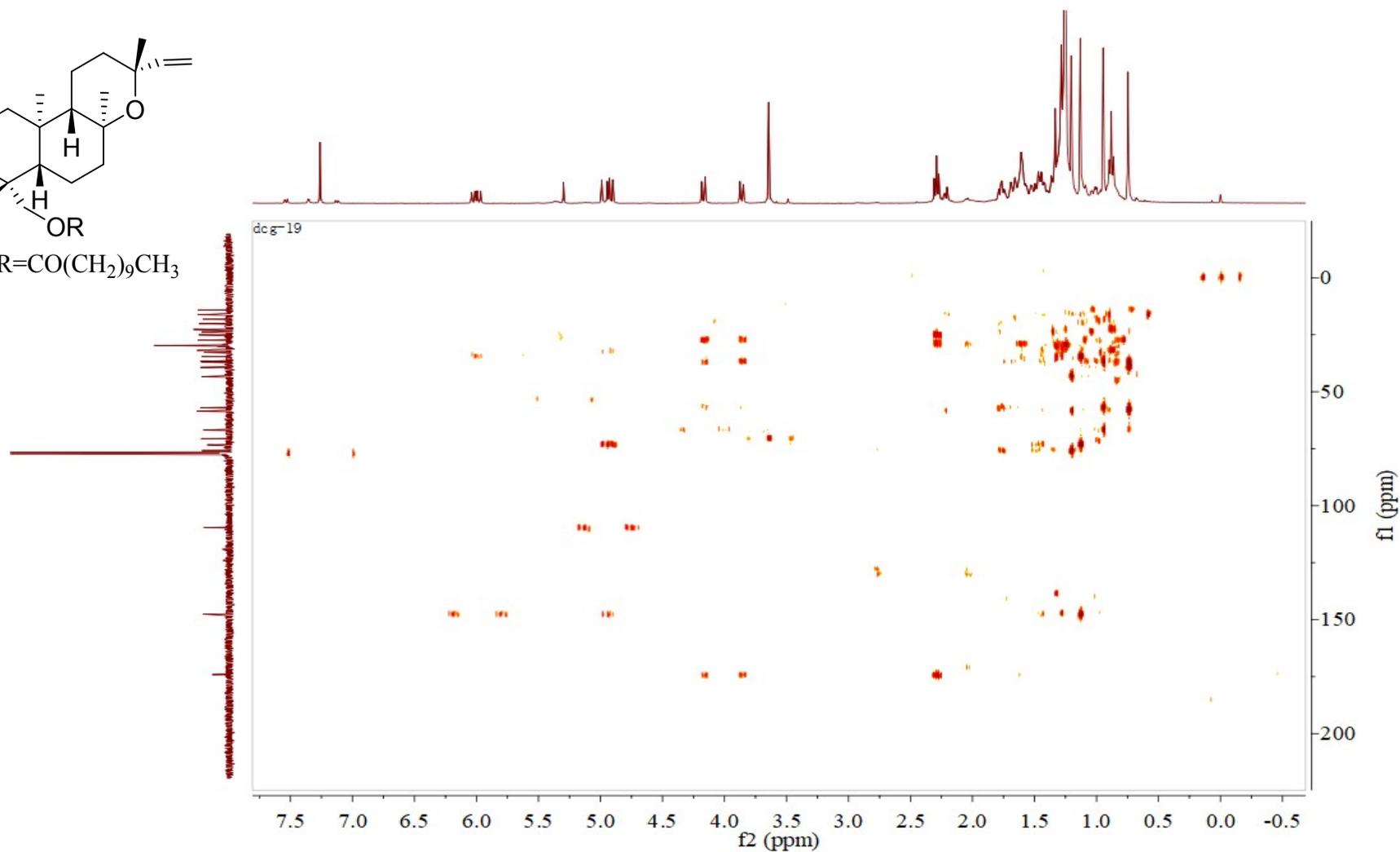
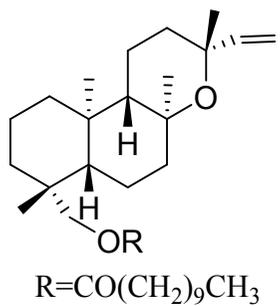


Figure S1.3 HMBC spectrum of **1** in CDCl_3

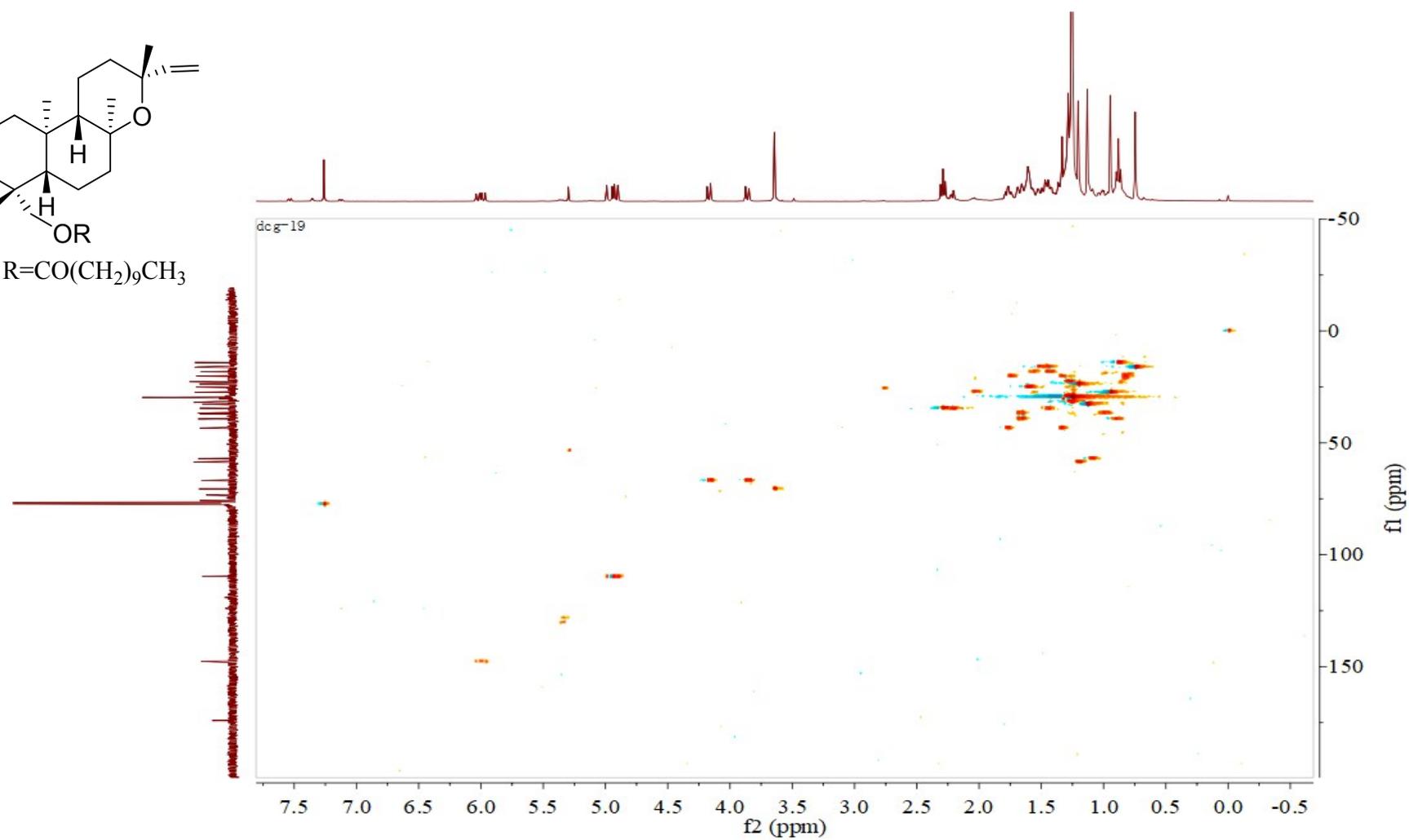
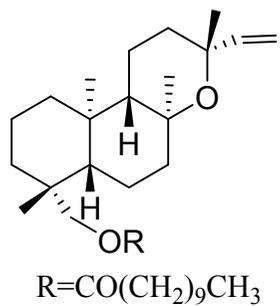


Figure S1.4 HMQC spectrum of **1** in CDCl_3

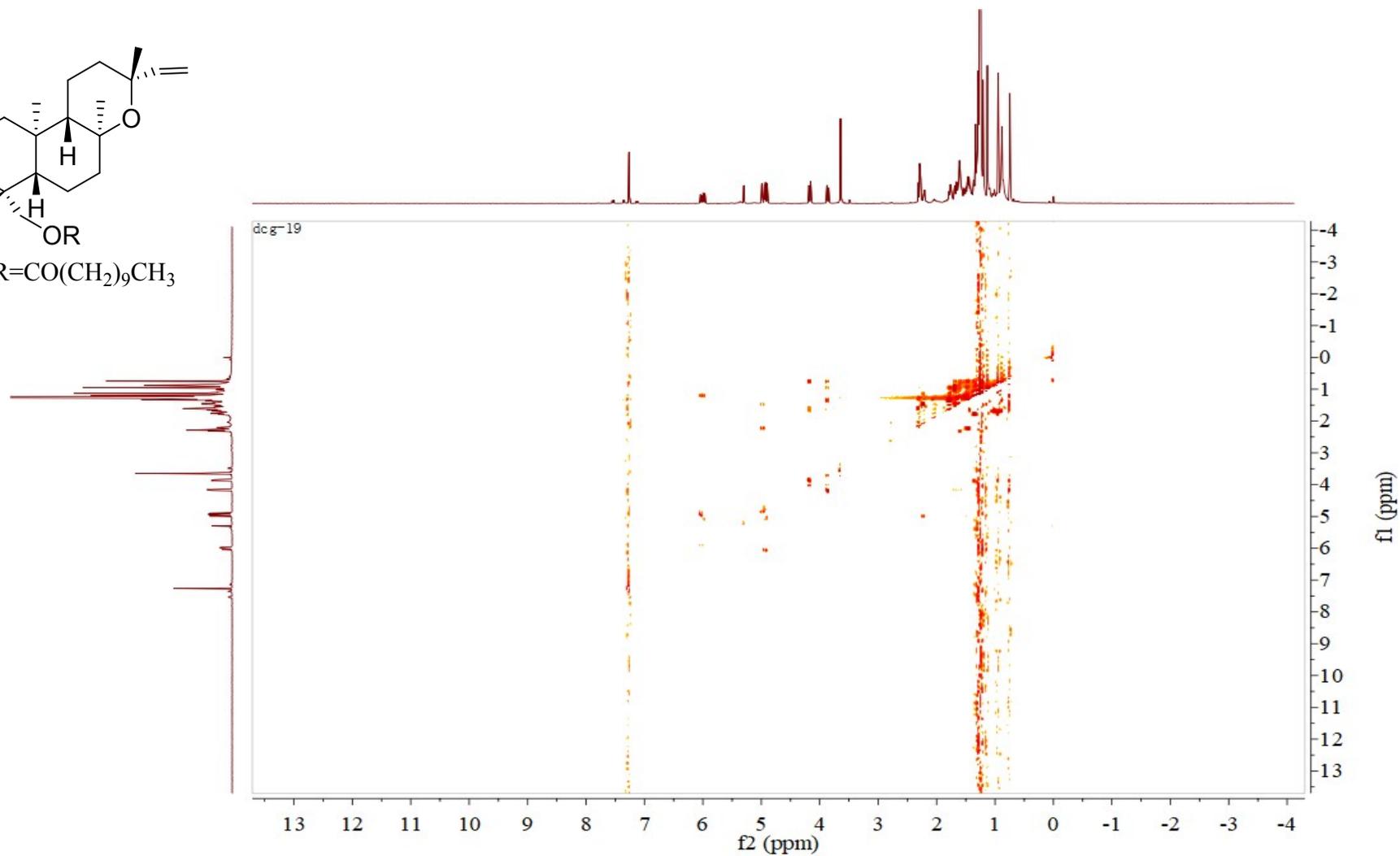
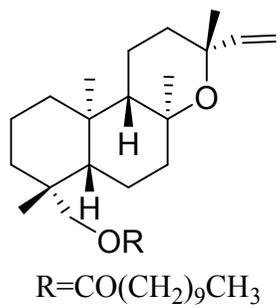


Figure S1.5 ROESY spectrum of **1** in CDCl₃

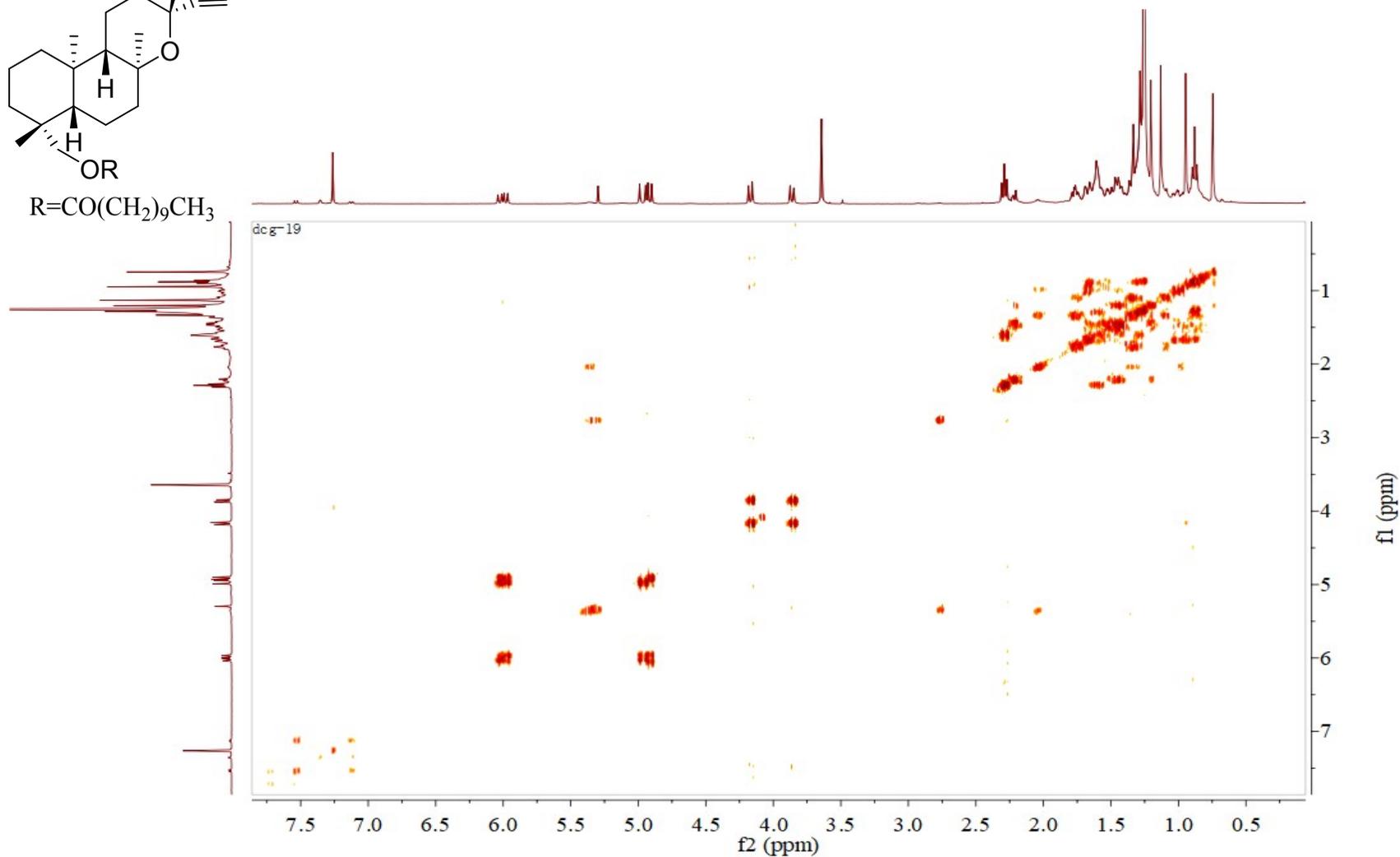
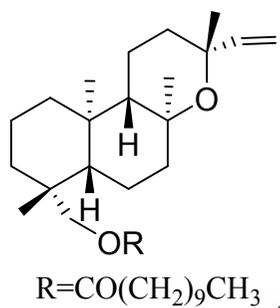


Figure S1.6 ^1H - ^1H COSY spectrum of **1** in CDCl_3

cg-19 #21 RT: 0.07 AV: 1 NL: 1.95E6
T: FTMS - p ESI Full ms [200.00-1000.00]

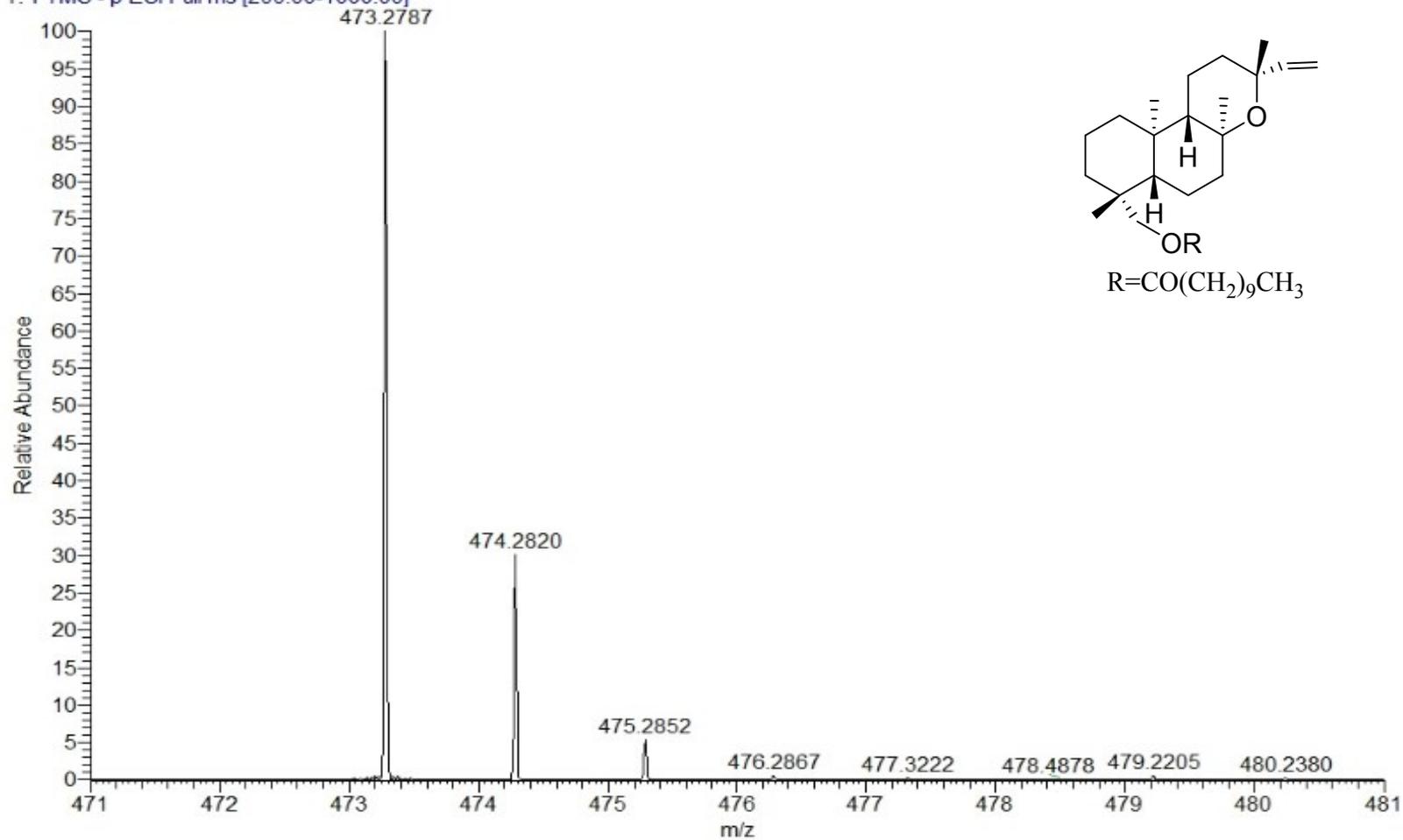


Figure S1.7 HRESIMS spectrum of **1**

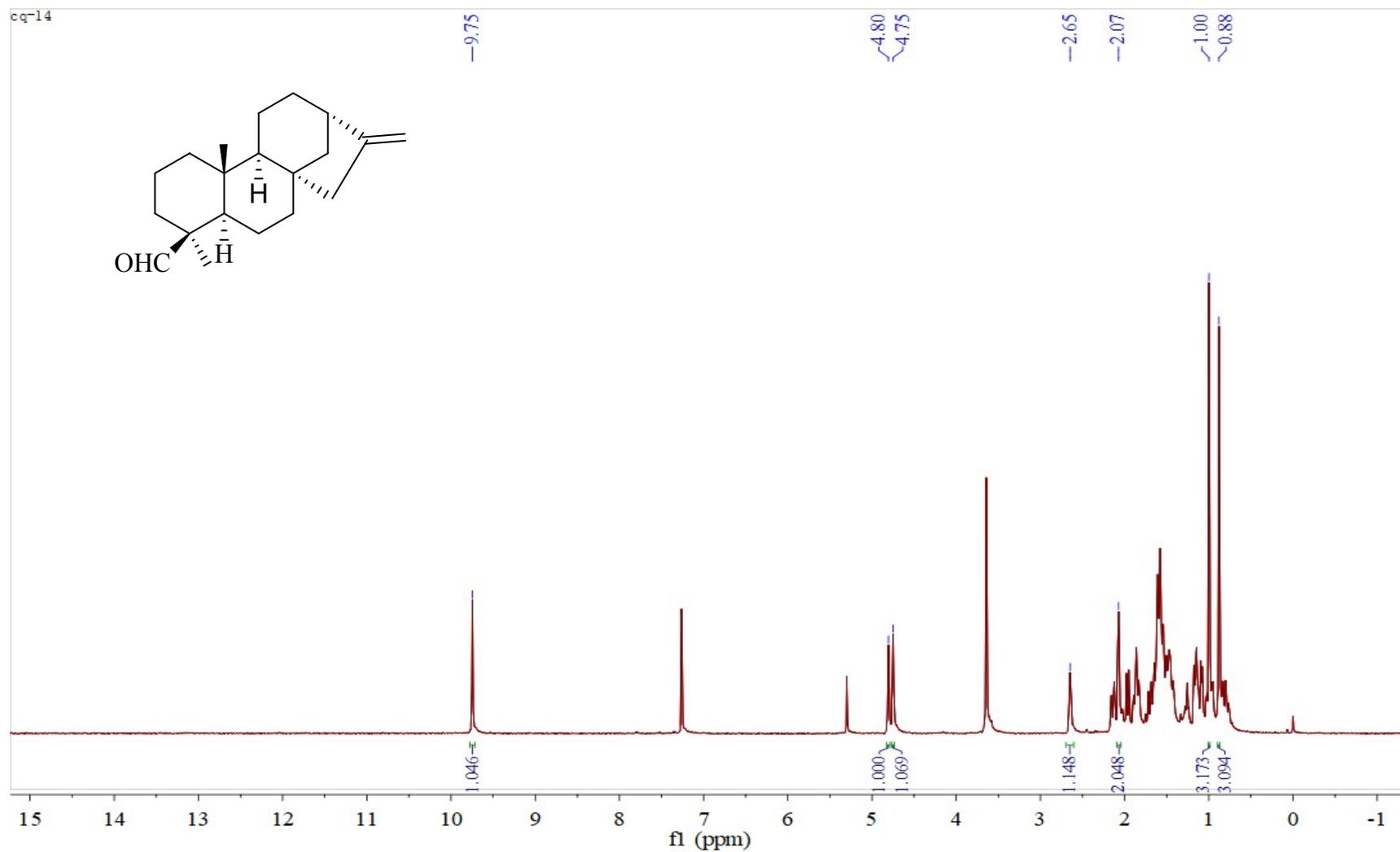


Figure S2.1 ^1H NMR spectrum (400 MHz) of **2** in CDCl_3

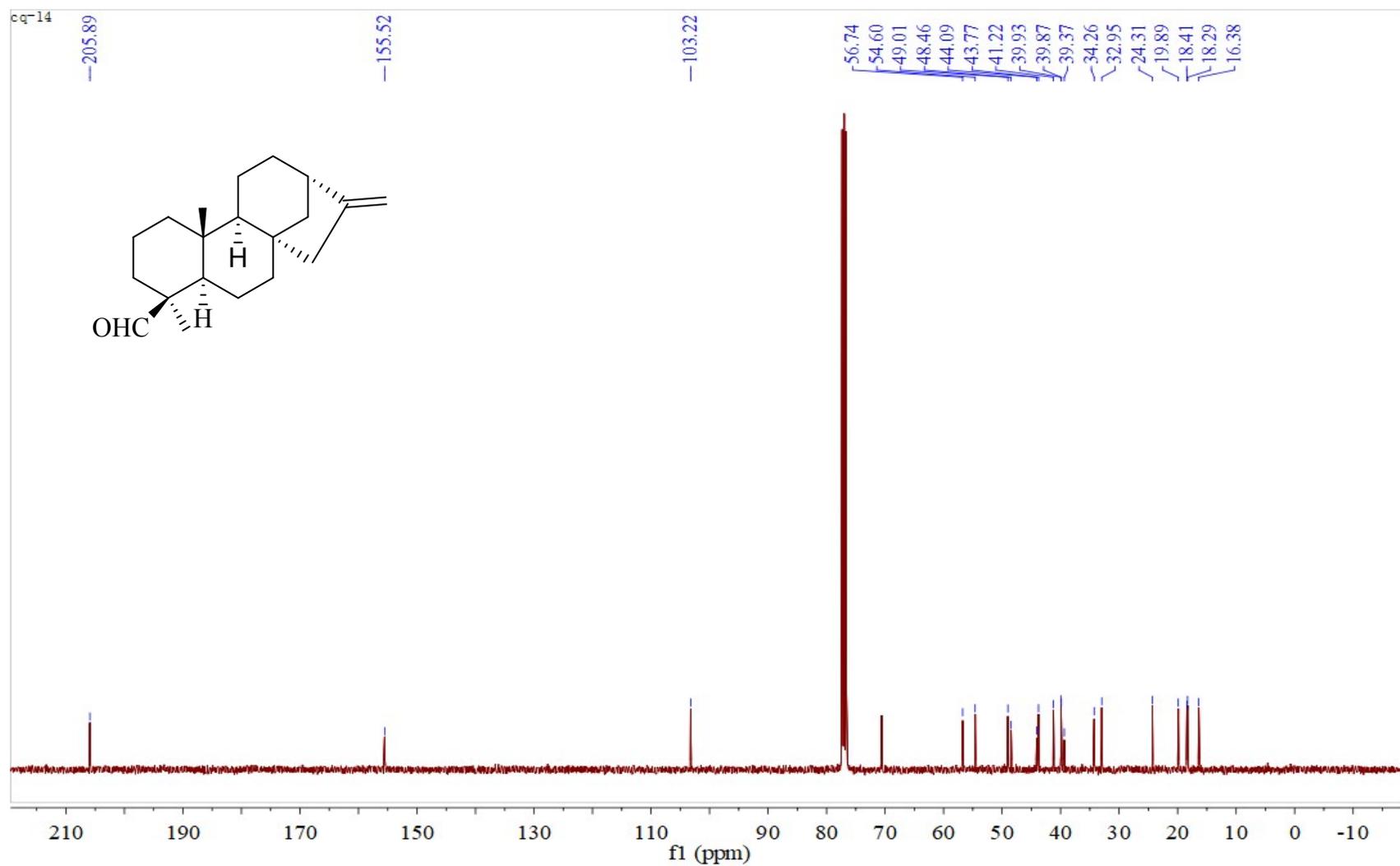


Figure S2.2 ¹³C NMR spectrum (100 MHz) of 2 in CDCl₃

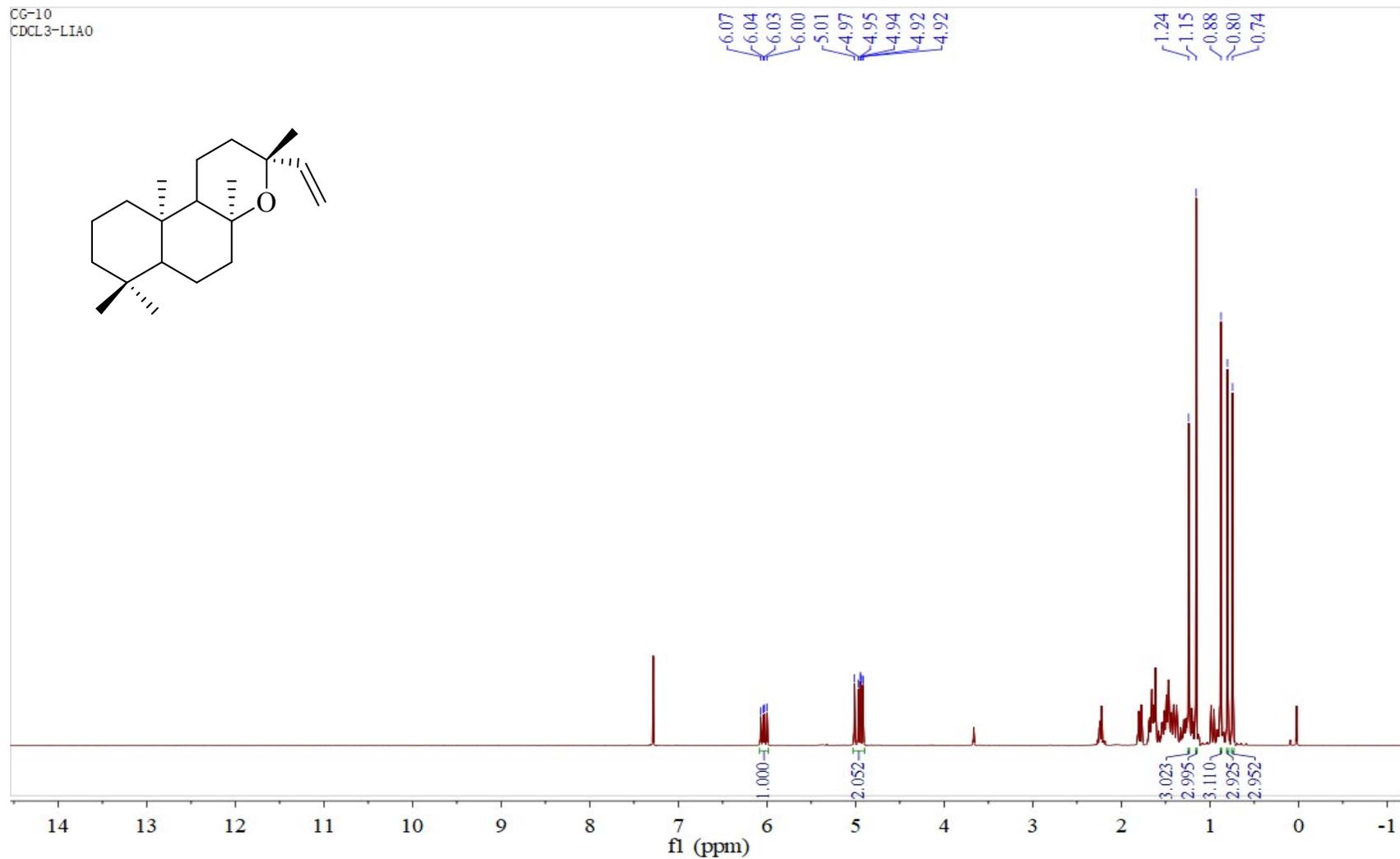


Figure S3.1 ¹H NMR spectrum (400 MHz) of **3** in CDCl₃

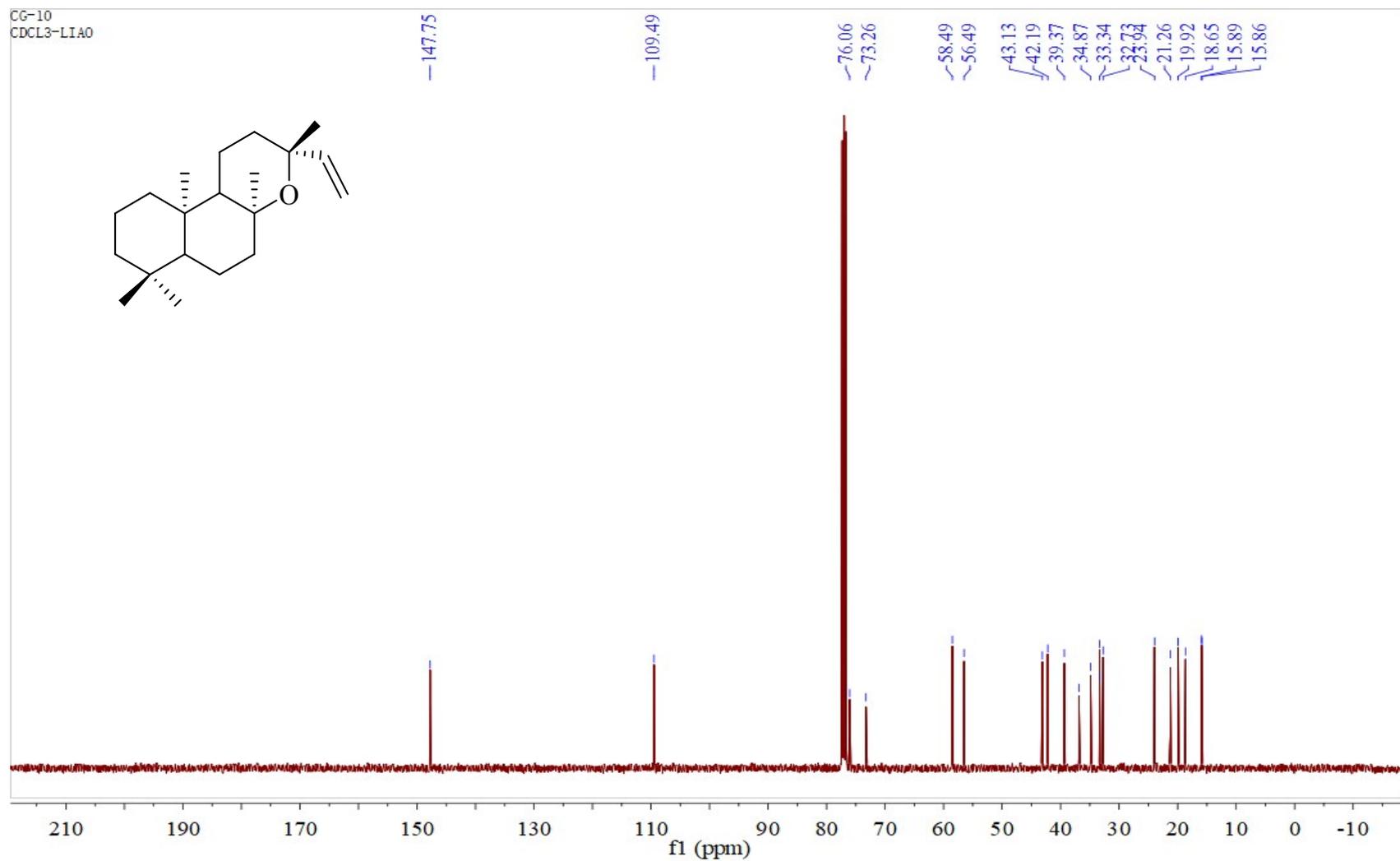


Figure S3.2 ^{13}C NMR spectrum (100 MHz) of **3** in CDCl_3

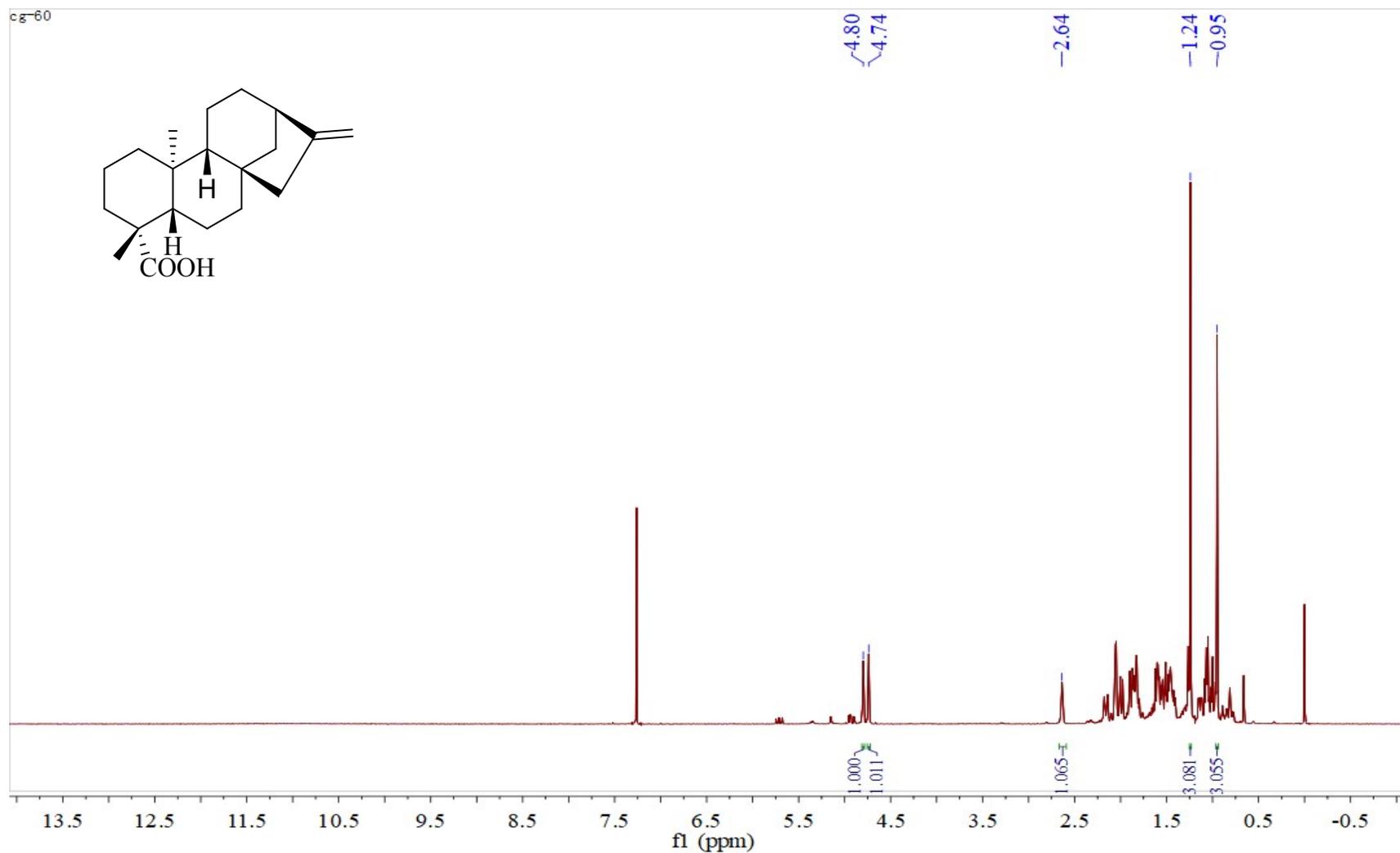


Figure S4.1 ^1H NMR spectrum (400 MHz) of **4** in CDCl_3

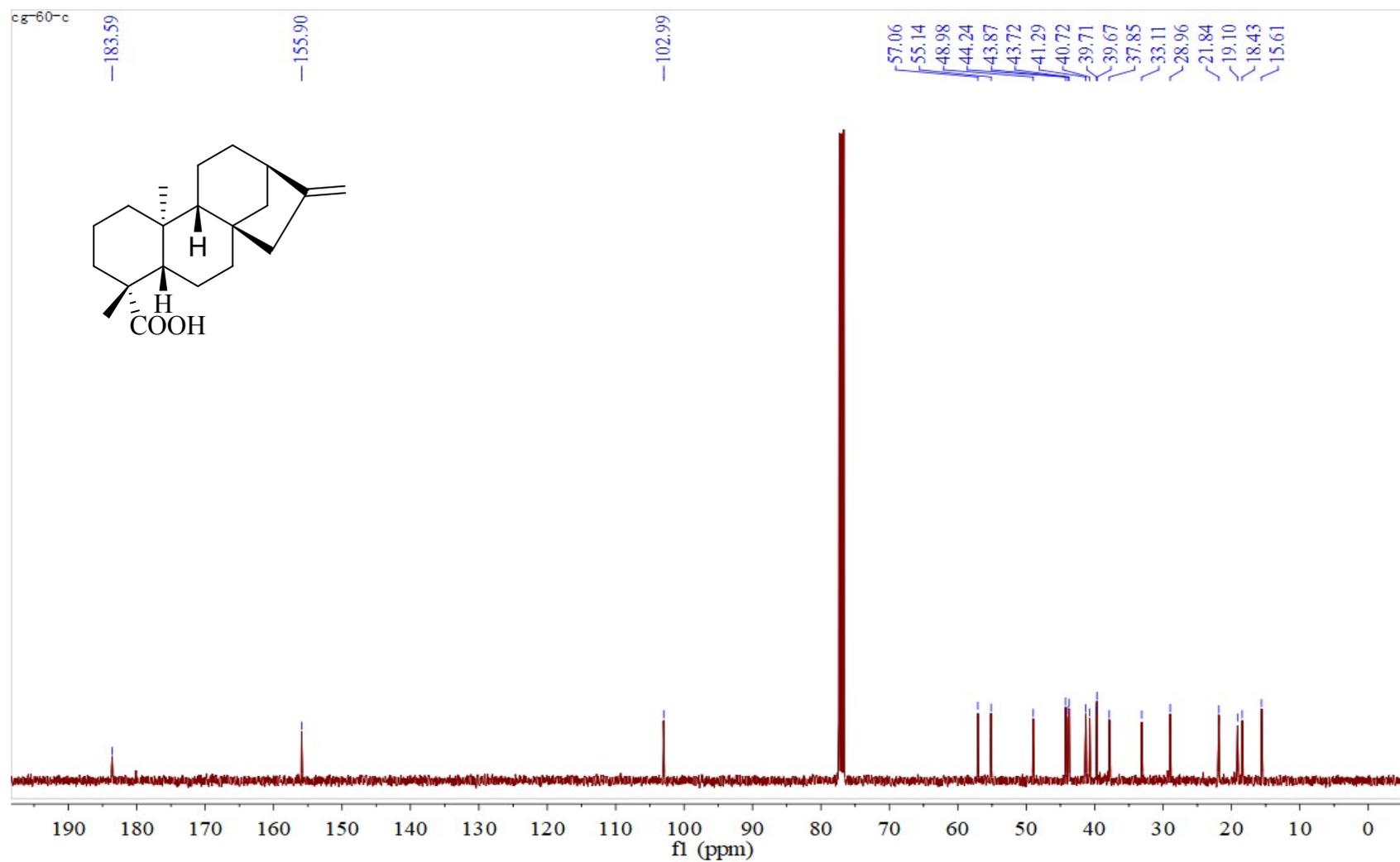


Figure S4.2 ¹³C NMR spectrum (100 MHz) of 4 in CDCl₃

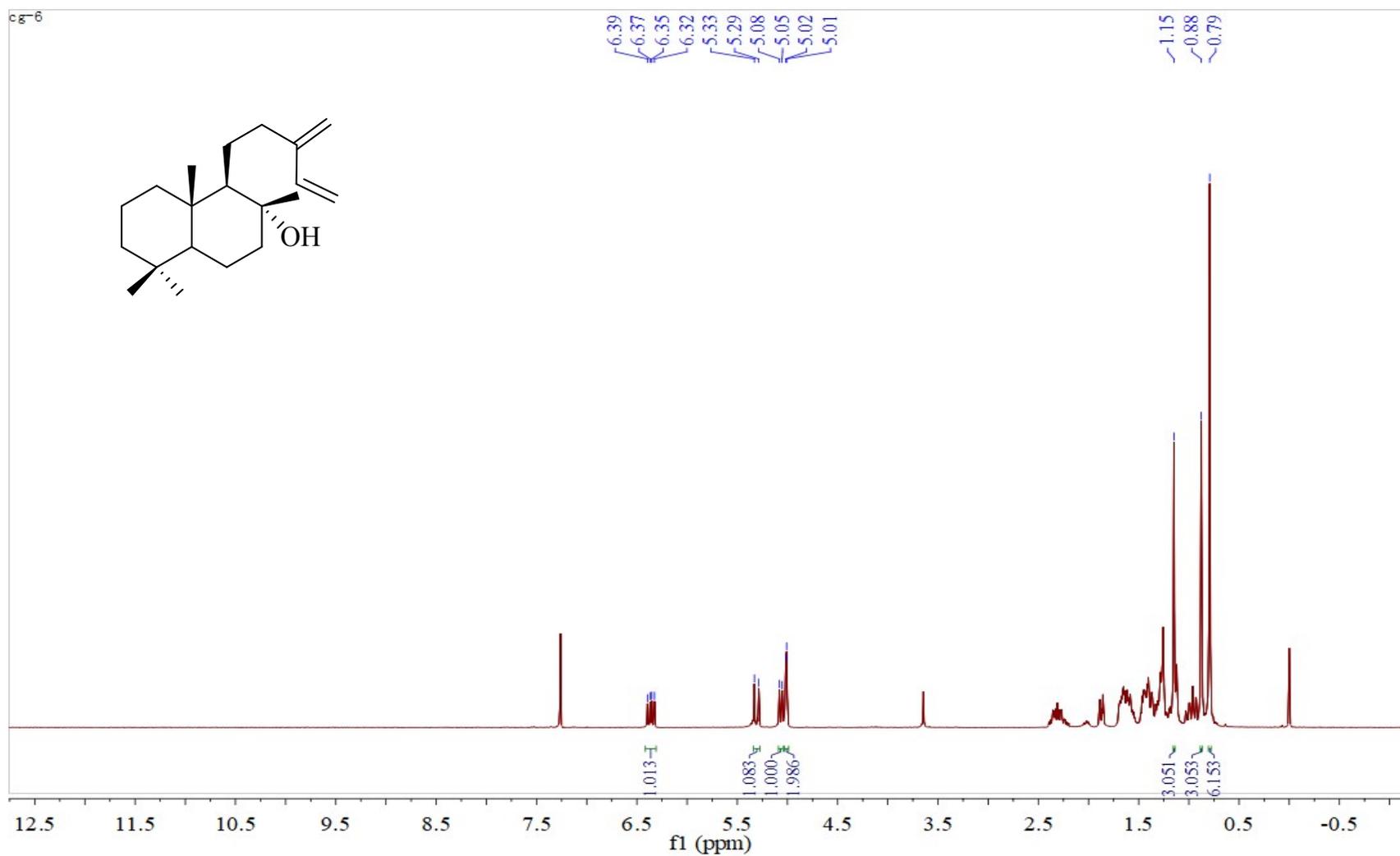


Figure S5.1 ^1H NMR spectrum (400 MHz) of **5** in CDCl_3

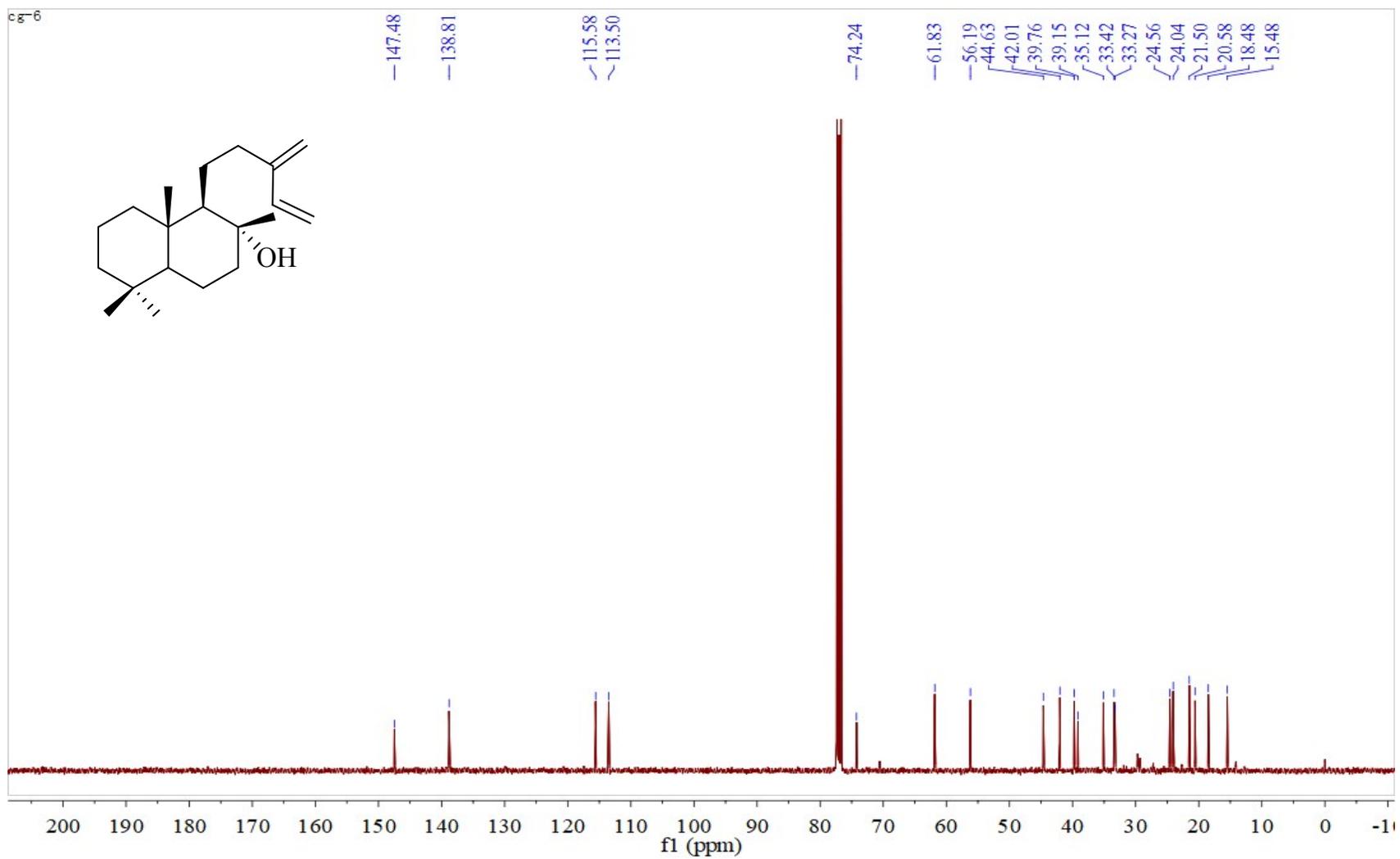


Figure S5.2 ^{13}C NMR spectrum (100 MHz) of **5** in CDCl_3

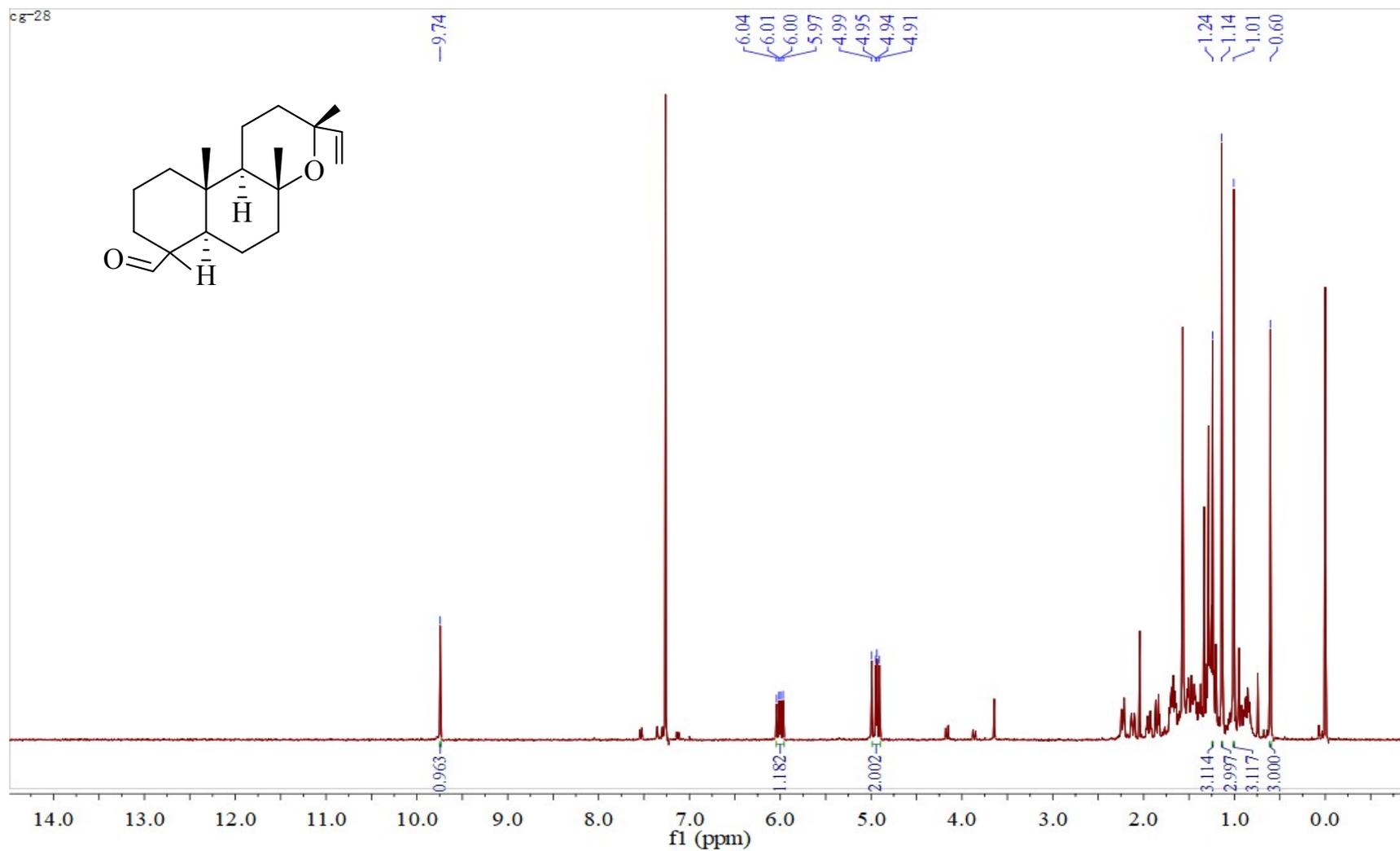


Figure S6.1 ^1H NMR spectrum (400 MHz) of **6** in CDCl_3

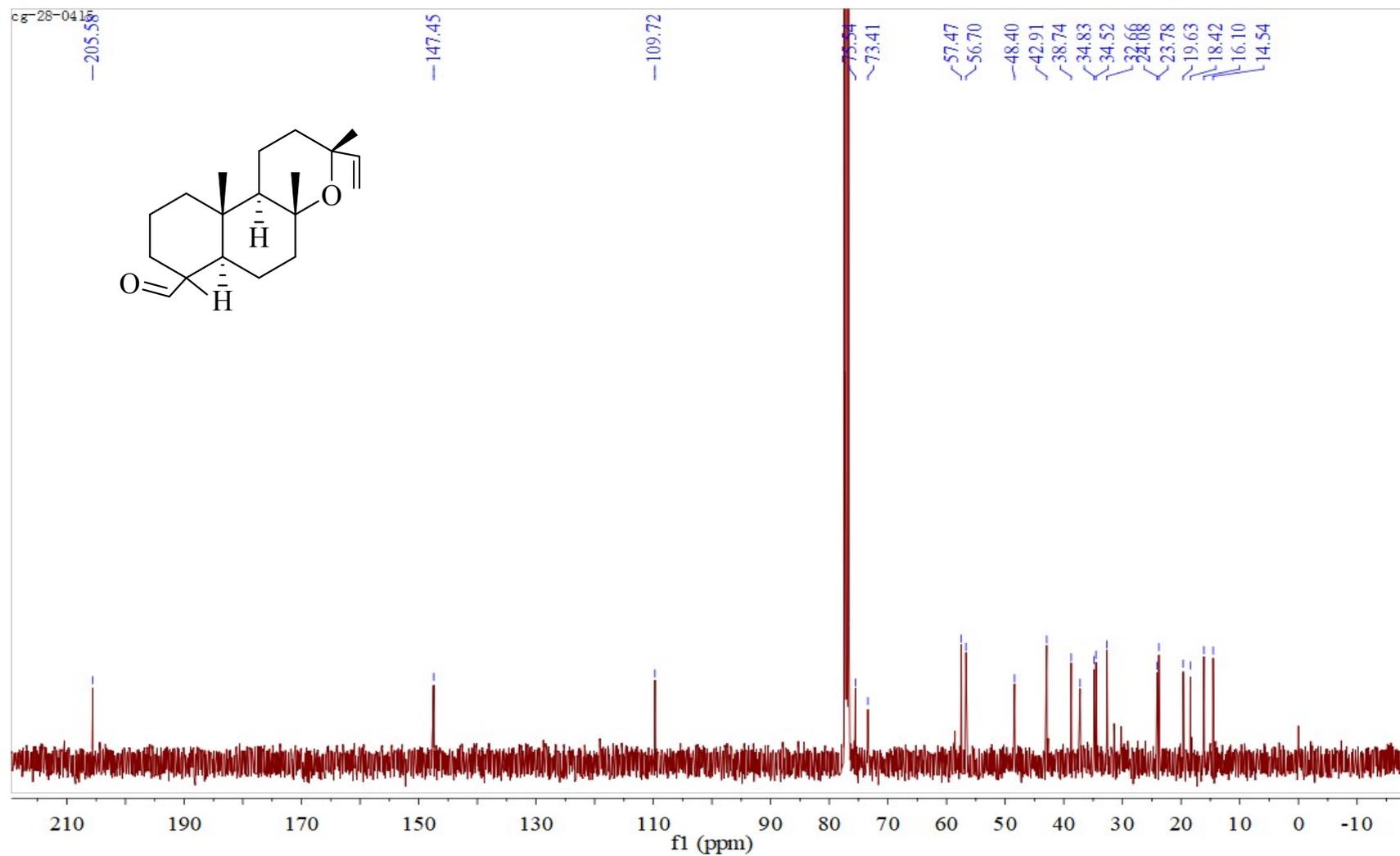


Figure S6.2 ^{13}C NMR spectrum (100 MHz) of **6** in CDCl_3

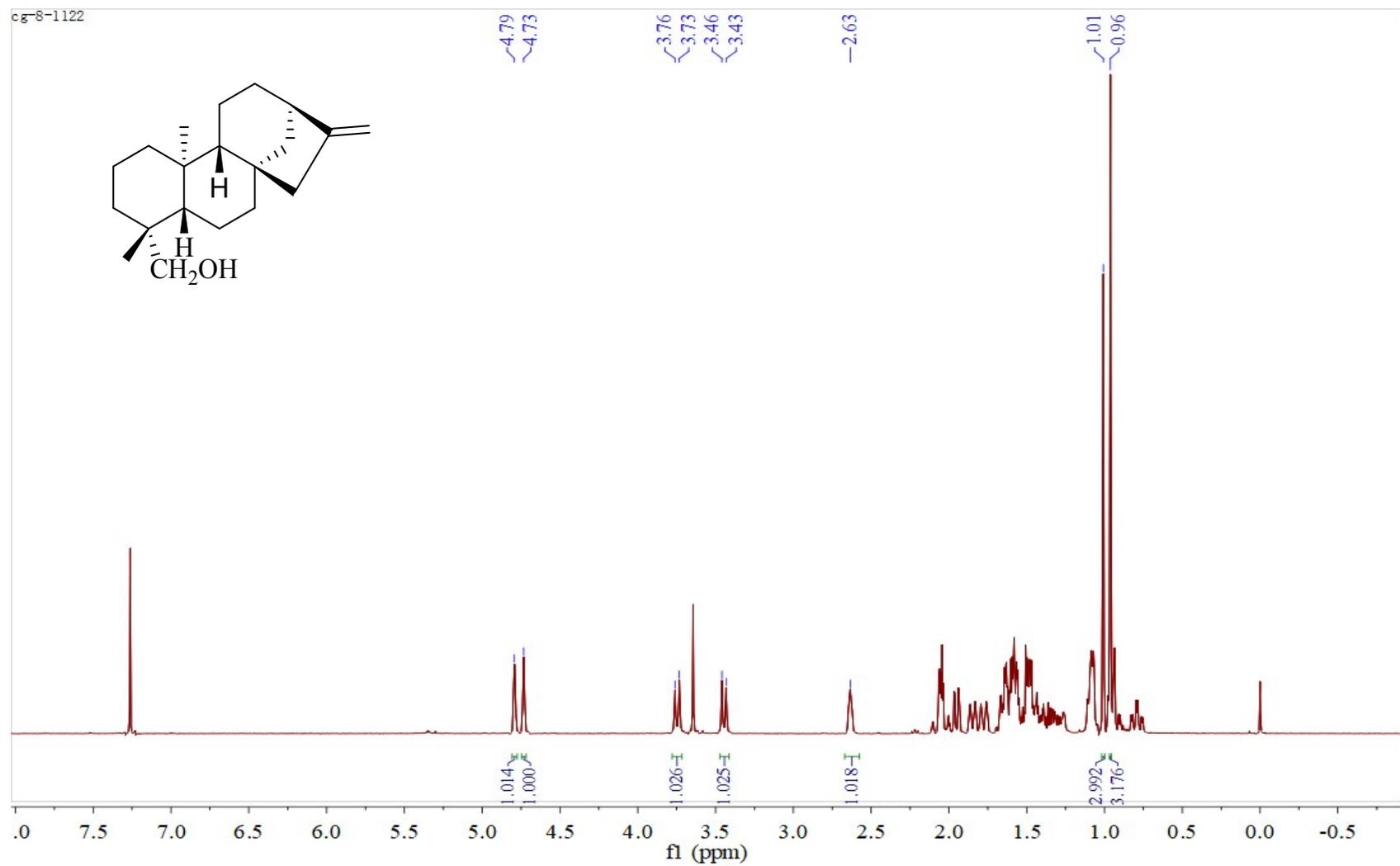


Figure S7.1 ^1H NMR spectrum (400 MHz) of 7 in CDCl_3

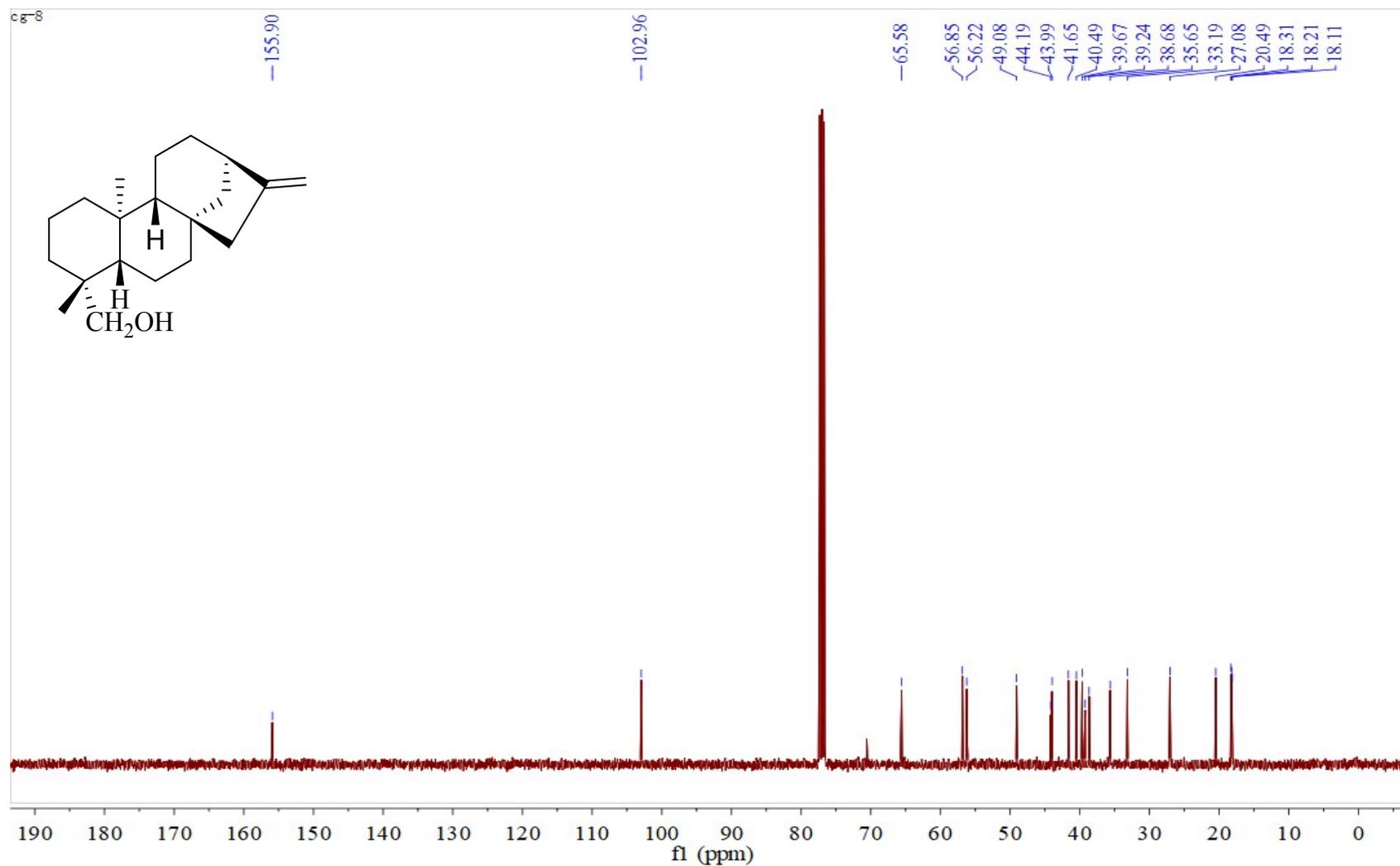


Figure S7.2 ¹³C NMR spectrum (100 MHz) of 7 in CDCl₃

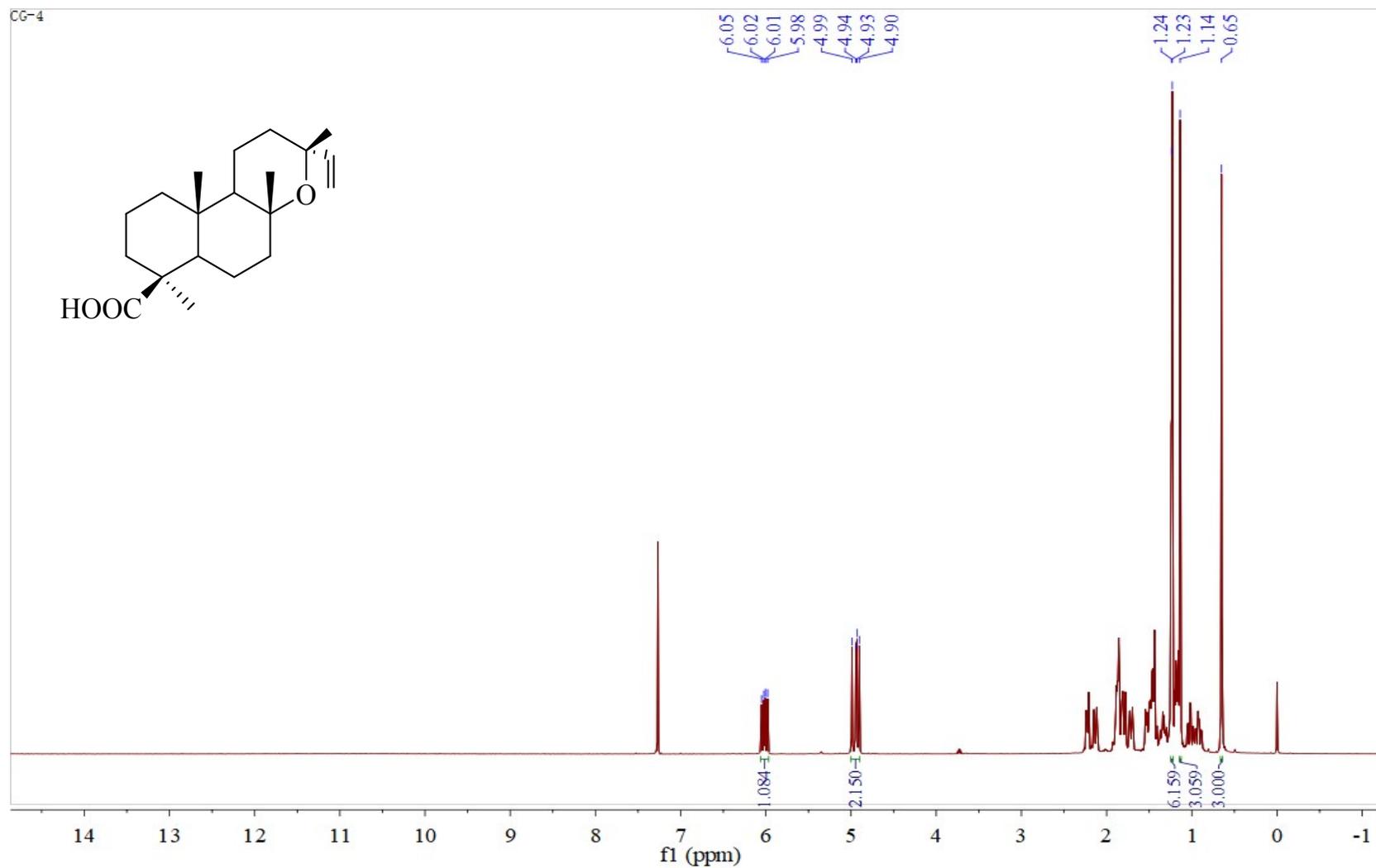


Figure S8.1 ^1H NMR spectrum (400 MHz) of **8** in CDCl_3

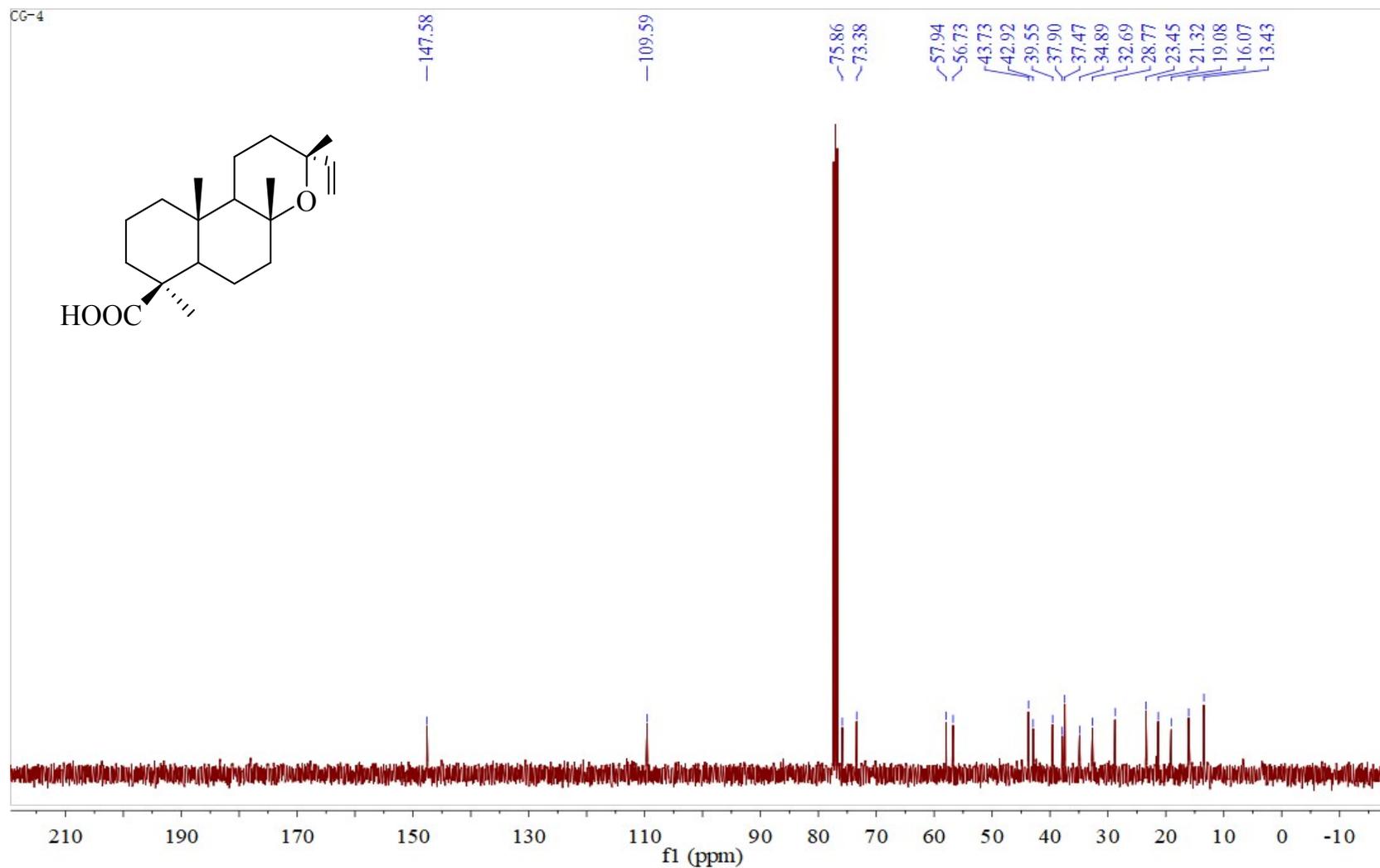


Figure S8.2 ^{13}C NMR spectrum (100 MHz) of **8** in CDCl_3

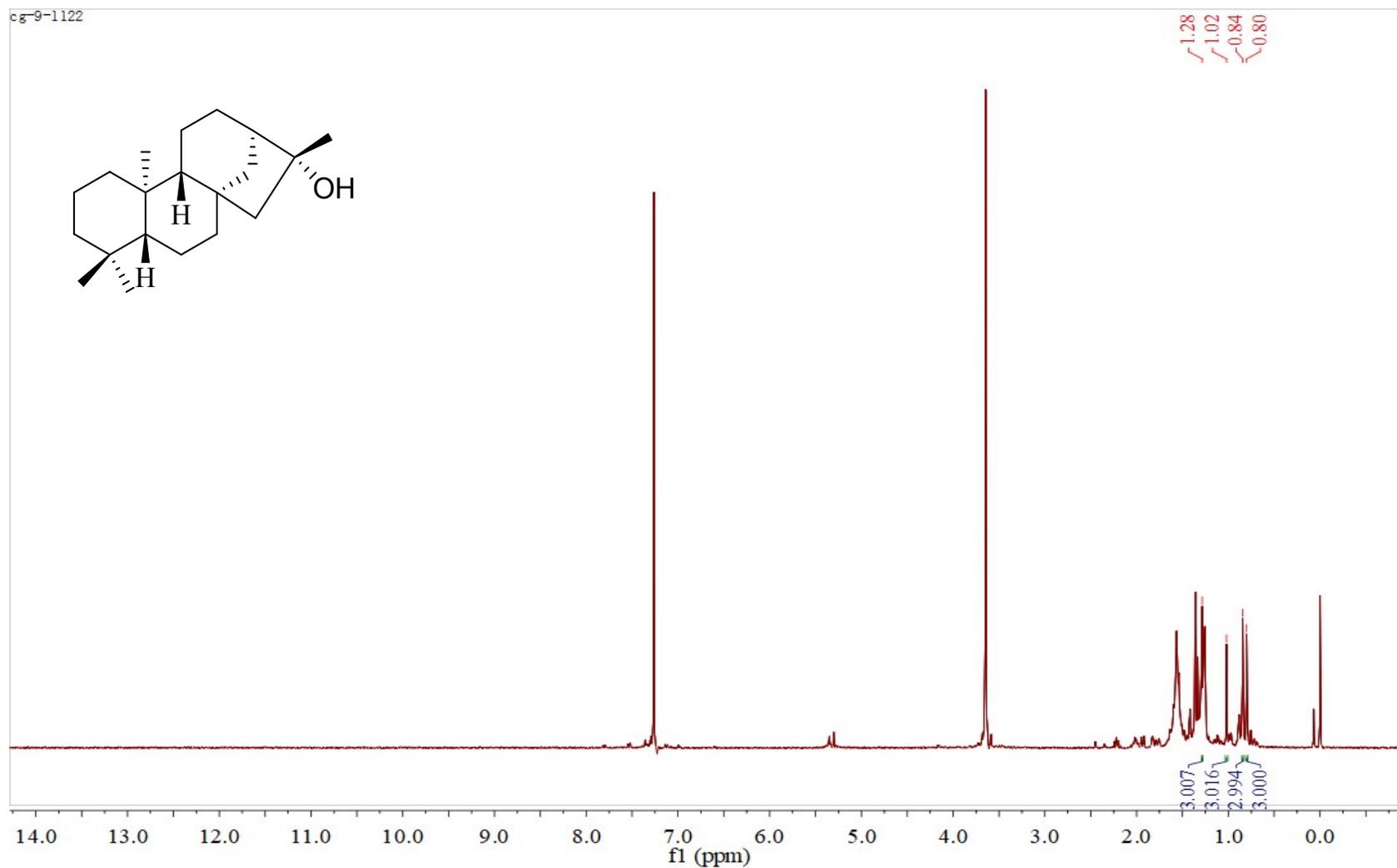


Figure S9.1 ^1H NMR spectrum (400 MHz) of **9** in CDCl_3

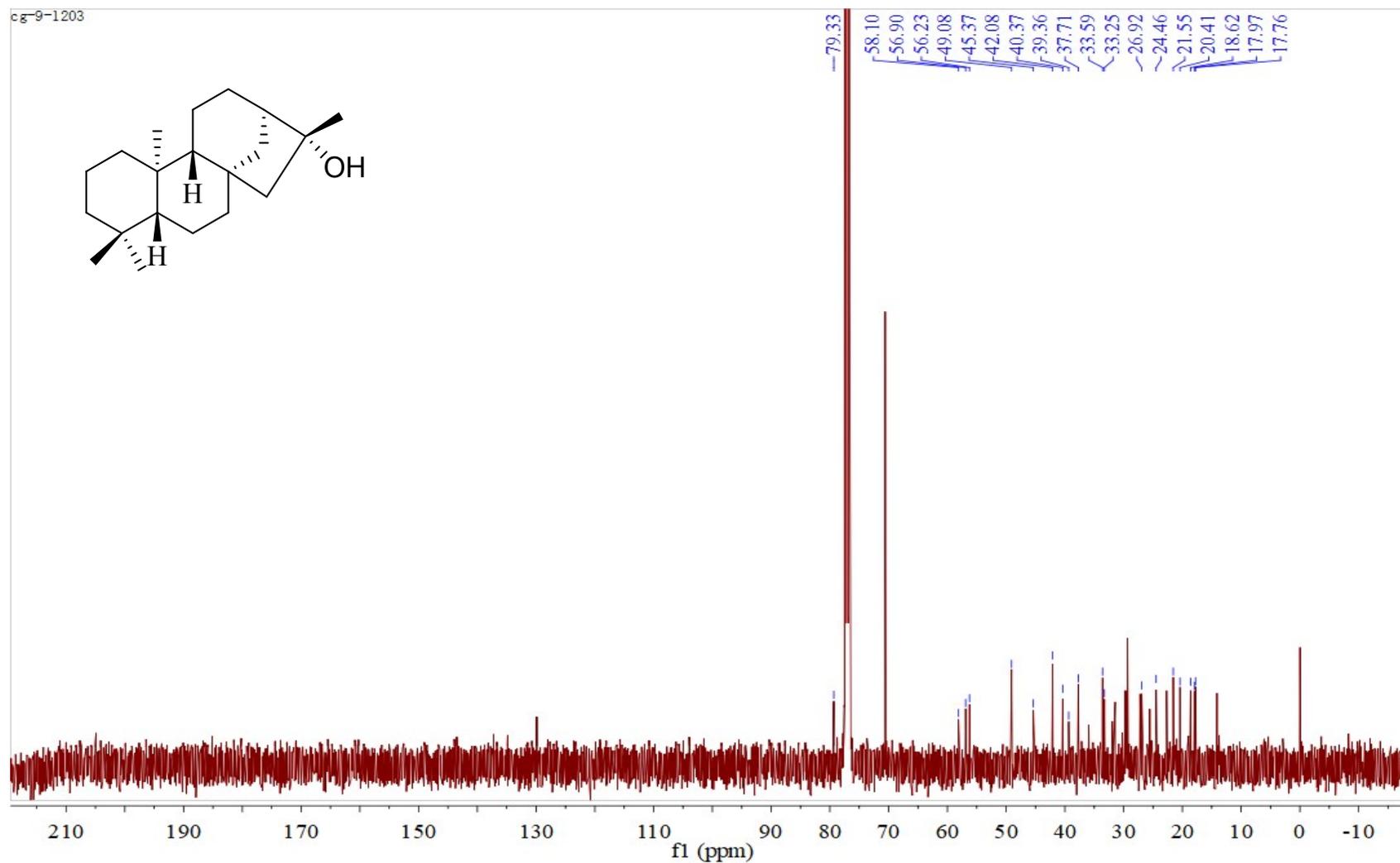


Figure S9.2 ¹³C NMR spectrum (100 MHz) of **9** in CDCl₃

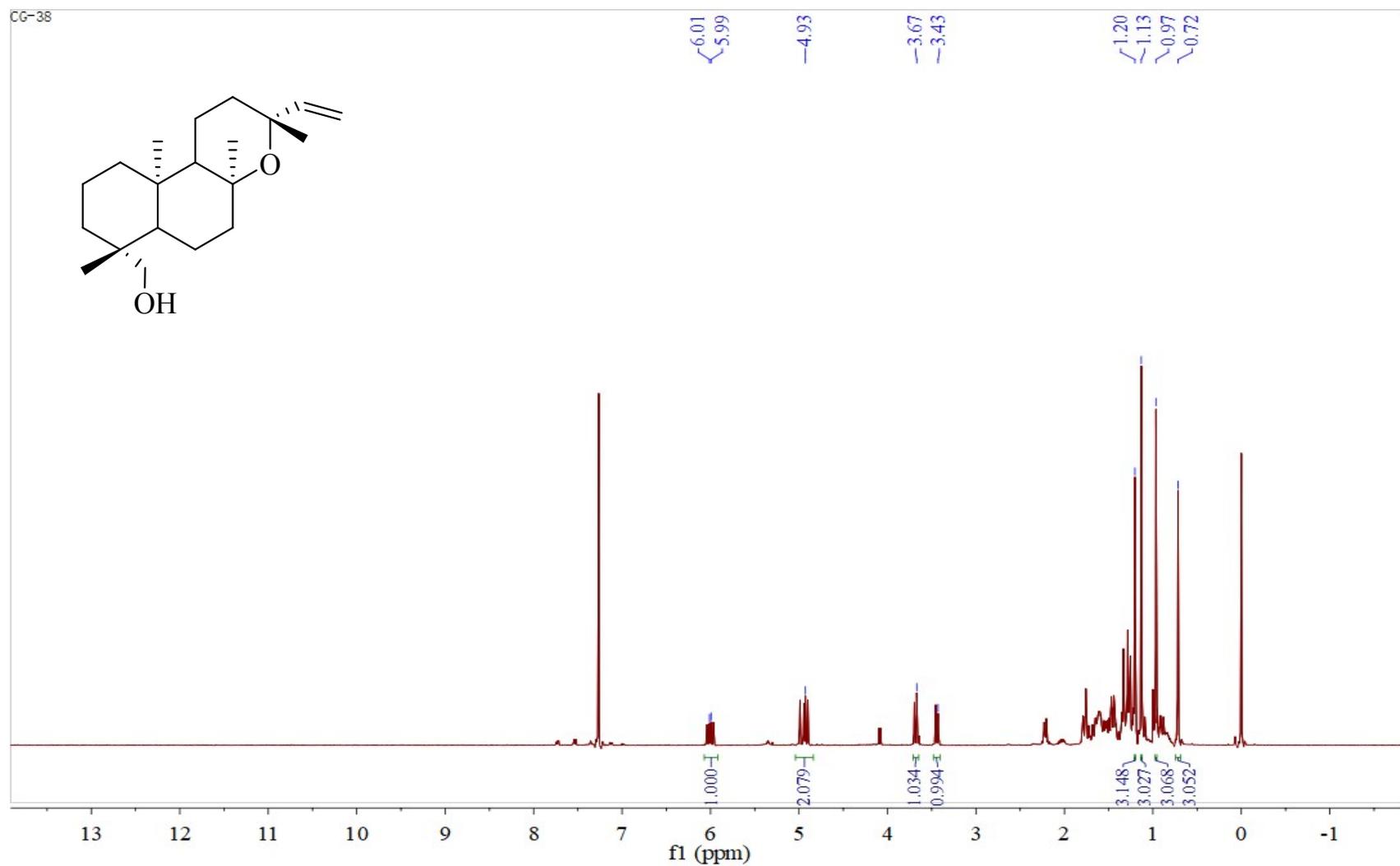


Figure S10.1 ^1H NMR spectrum (400 MHz) of **10** in CDCl_3

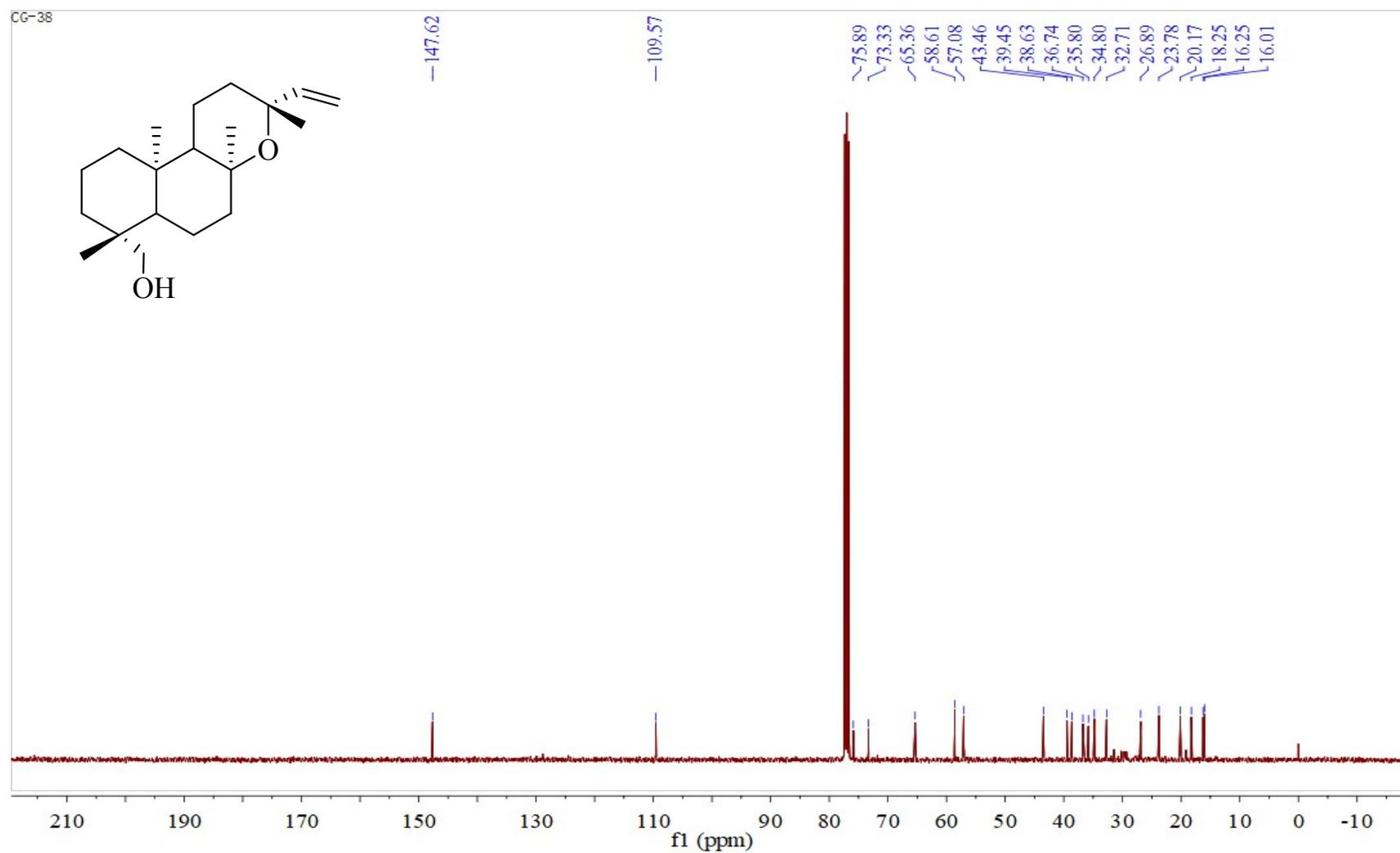


Figure S10.2 ^{13}C NMR spectrum (100 MHz) of **10** in CDCl_3

mAU

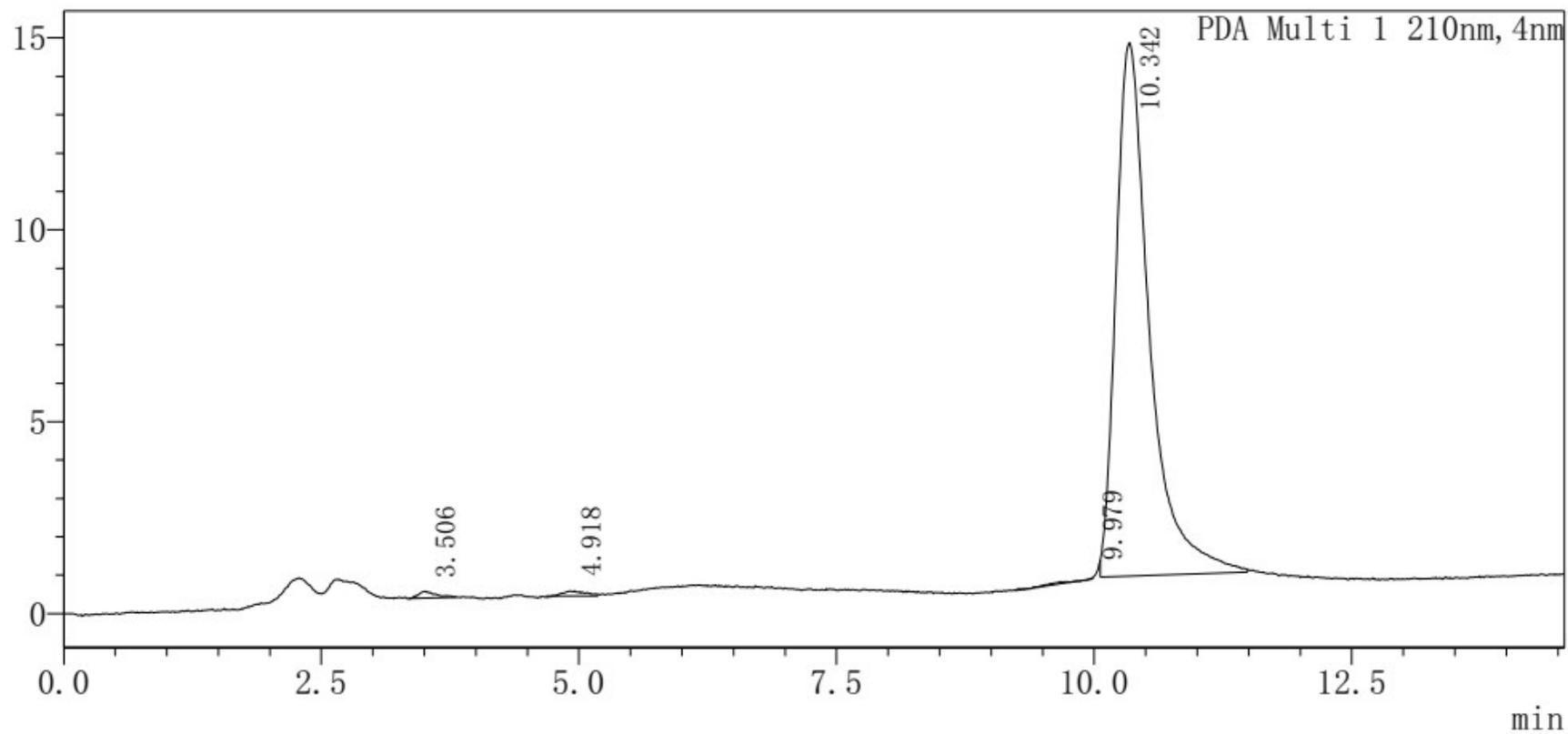


Figure S10.3 The purity of **10** investigated by HPLC

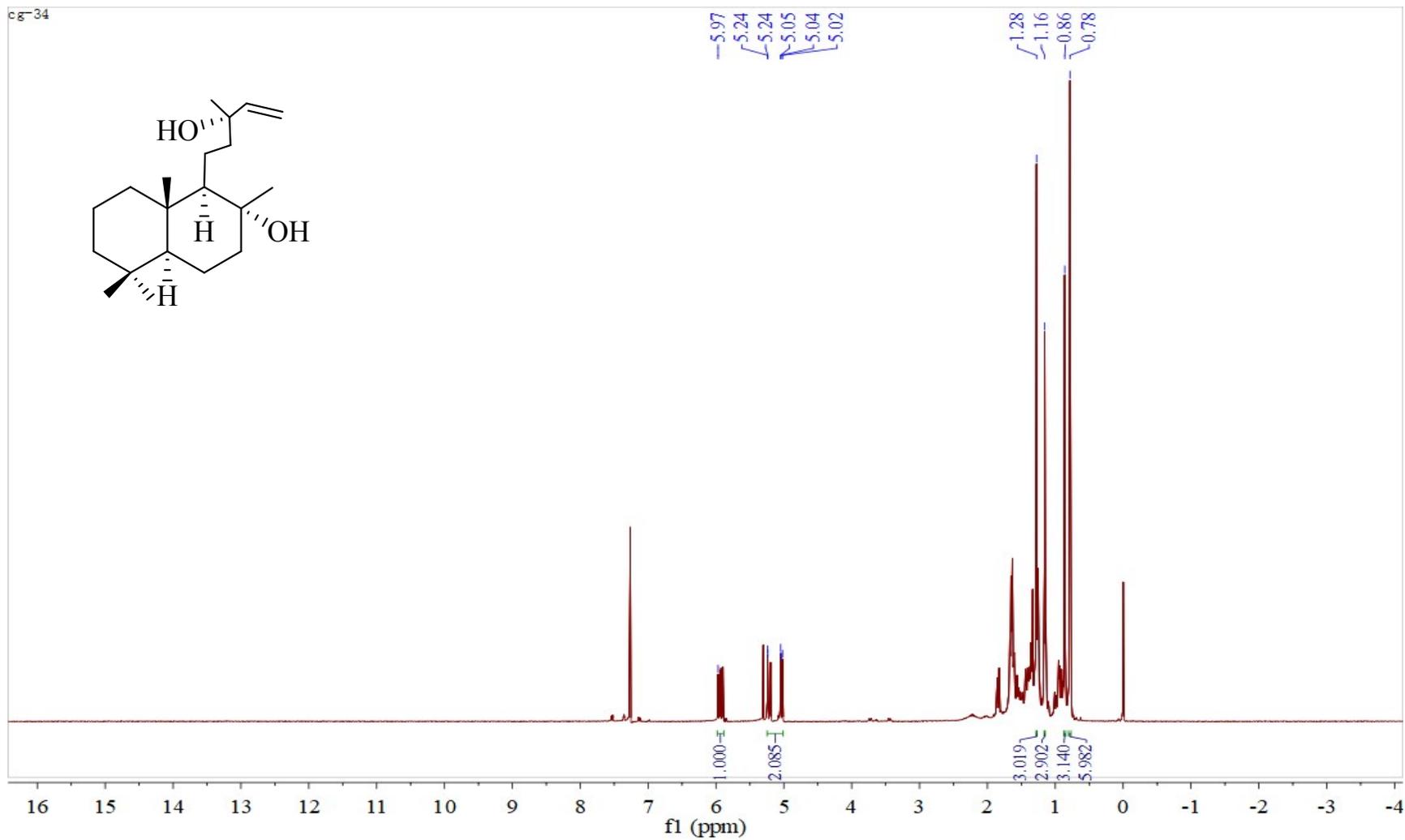


Figure S11.1 ^1H NMR spectrum (400 MHz) of **11** in CDCl_3

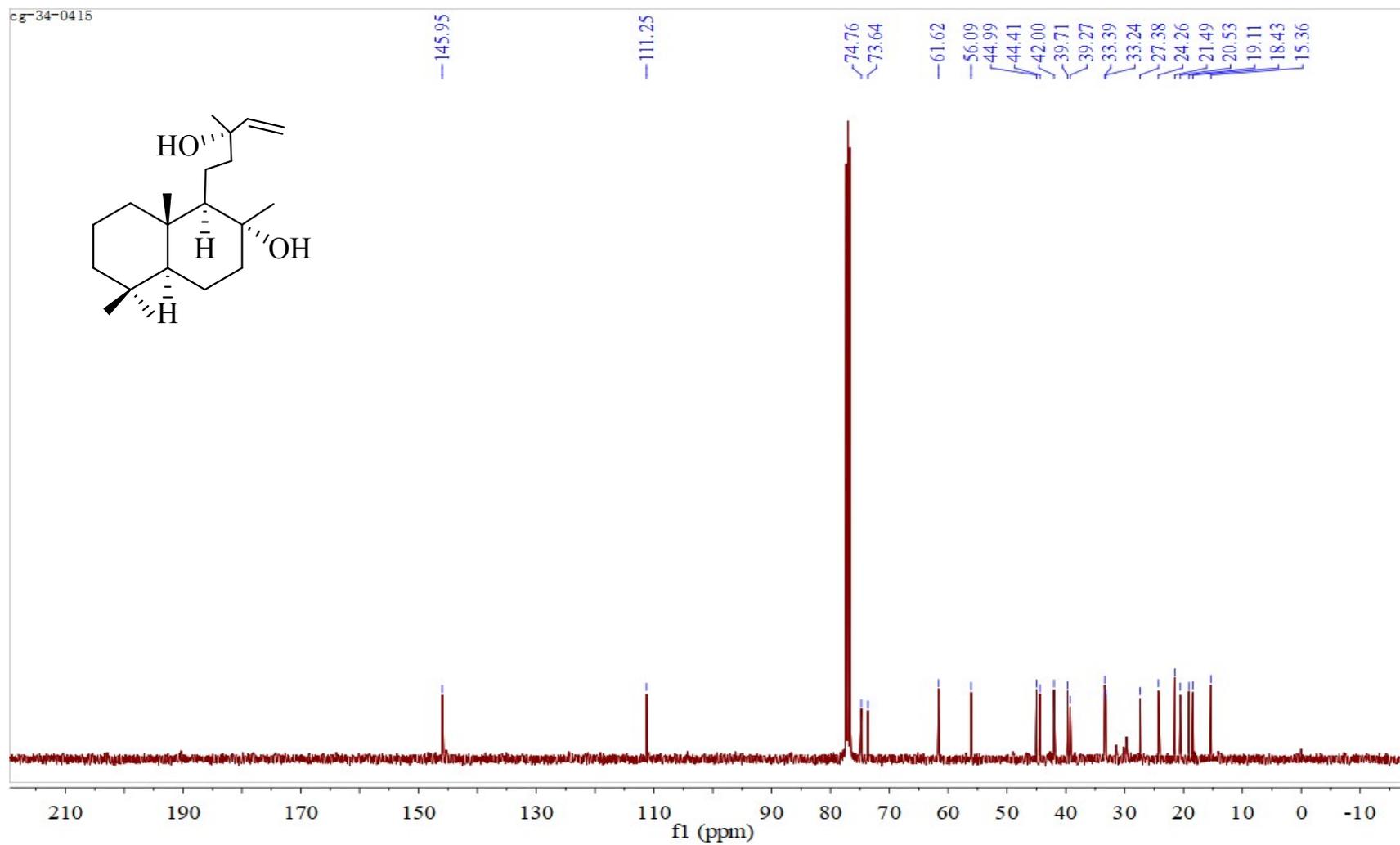


Figure S11.2 ¹³C NMR spectrum (100 MHz) of **11** in CDCl₃

mAU

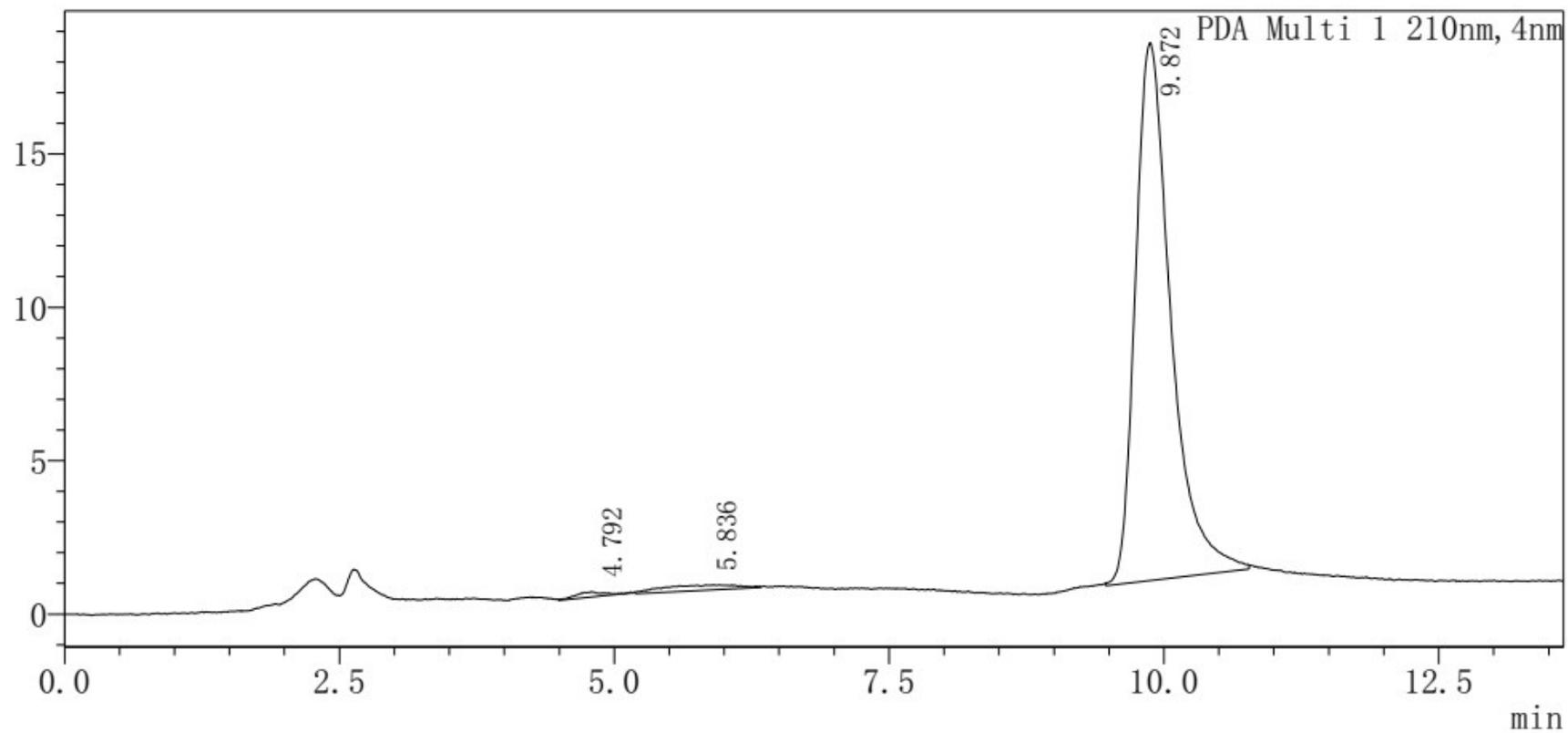


Figure S11.3 The purity of **11** investigated by HPLC