Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Cyperane and Eudesmane-Type Sesquiterpenoids from the Chinese Liverwort and Their Anti-Diabetic Nephropathy Potential

Jiaozhen Zhang[a] , Yongjie Wang[b], Rongxiu Zhu[c], Yi Li[a], Yuelan Li[a], Yanan Qiao[a], Jinchuan Zhou[d], and Hongxiang Lou[a,]*

[a] Department of Natural Products Chemistry, Key Lab of Chemical Biology of the Ministry of Education, Shandong University, Jinan 250012, People's Republic of China

[b] Department of Pharmacy, The Second Hospital of Shandong University, Jinan, Shandong 250033

[c] School of Chemistry and Chemical Engineering, Shandong University, Jinan 250010, People's Republic of China

[d] School of pharmacy, Linyi University, Linyi 276000, People's Republic of China

* To whom correspondences should be addressed.

Tel: +86-531-8838-2012. Fax: +86-531-8838-2019. E-mail: louhongxiang@sdu.edu.cn.

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Theory and Calculation Details.

The calculations were performed by the Gaussian 03 program package.[1] The semi-empirical AM1 method[2] and a DFT approach[3] B3LYP/6-31G* were employed to scan the potential energy surface (PES). The geometries of all ground-state conformations obtained were further optimized at the B3LYP/6-31G* level at 298.15 K, followed by calculations of their harmonic frequency analysis to confirm these minima and thence calculations of room-temperature free energies.

Time-dependent density functional theory (TDDFT)[4] at the same level was used to calculate the electronic excitation energies and rotational strengths in gas phase for the first 30 states. The rotatory strengths were summed and energetically weighted following the Boltzmann statistics and the final ECD spectra were then simulated by overlapping Gaussian functions according to the following equation.[5]

$$\Delta\varepsilon(E) = \frac{1}{2.296 \times 10^{-39}} \frac{1}{\sigma\sqrt{\pi}} \times \sum_i \Delta E_i R_i e^{-[(E-\Delta E_i)/\sigma]^2}$$

Where σ is the width of the band at $1/e$ height, while ΔE_i and R_i are the excitation energies and rotatory strengths for transition, respectively. σ = 0.1 eV and R_{vel} were used.

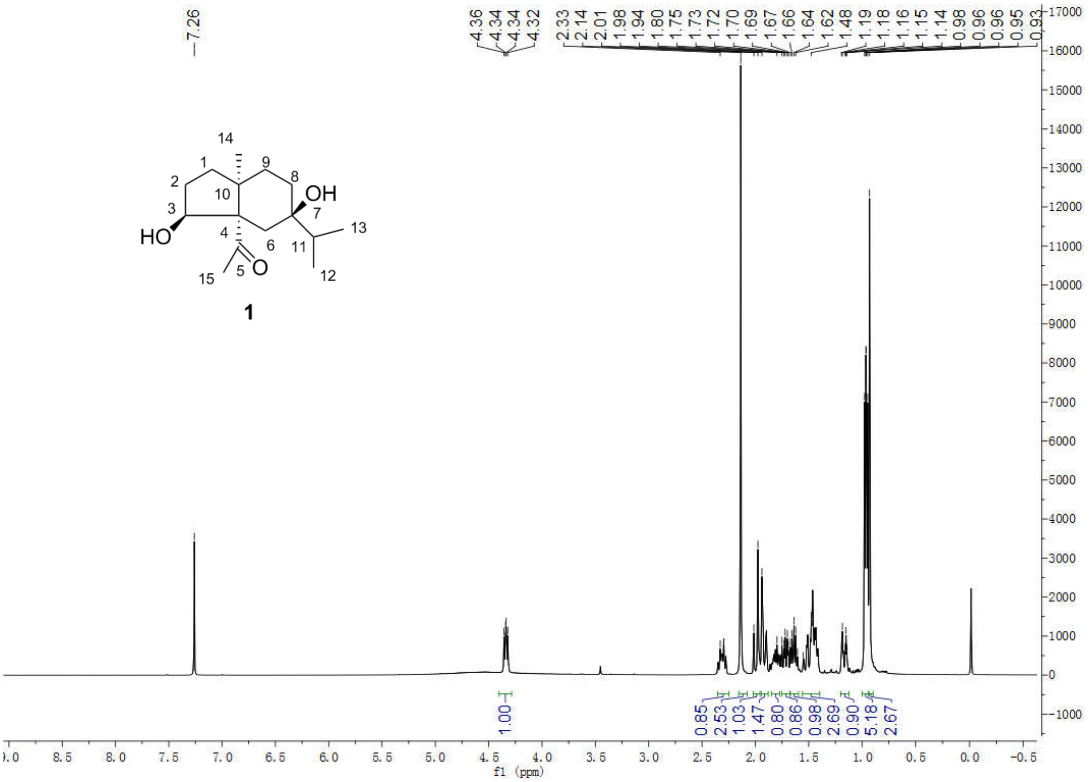


Figure S1. ^{1}H NMR spectrum (400 MHz) of **1** in $CDCl_3$.

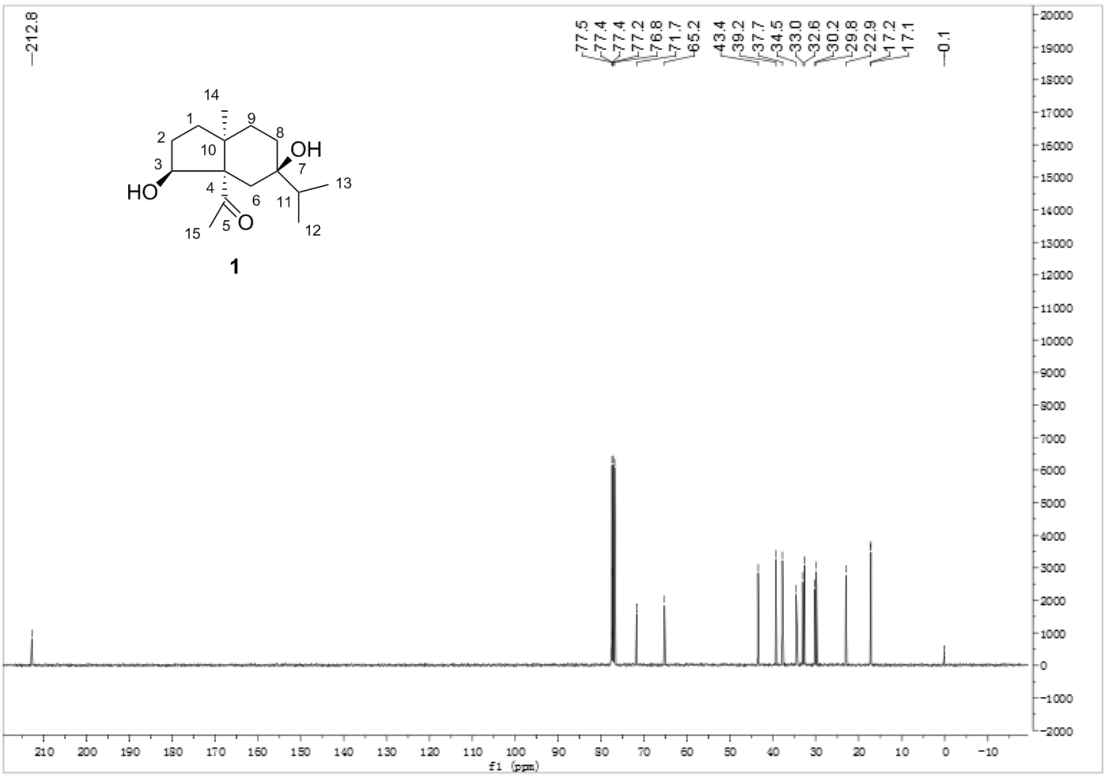


Figure S2. ^{13}C NMR spectrum (100 MHz) of **1** in $CDCl_3$.

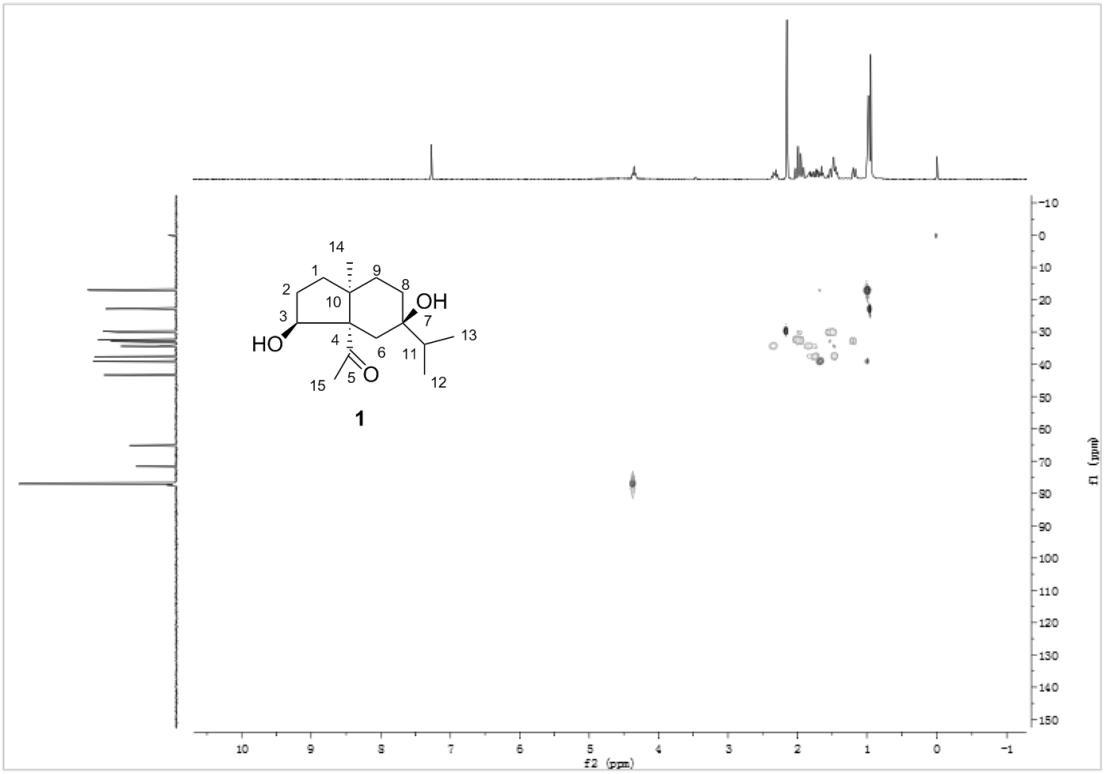


Figure S3. HSQC spectrum (400 MHz) of **1** in $CDCl_3$

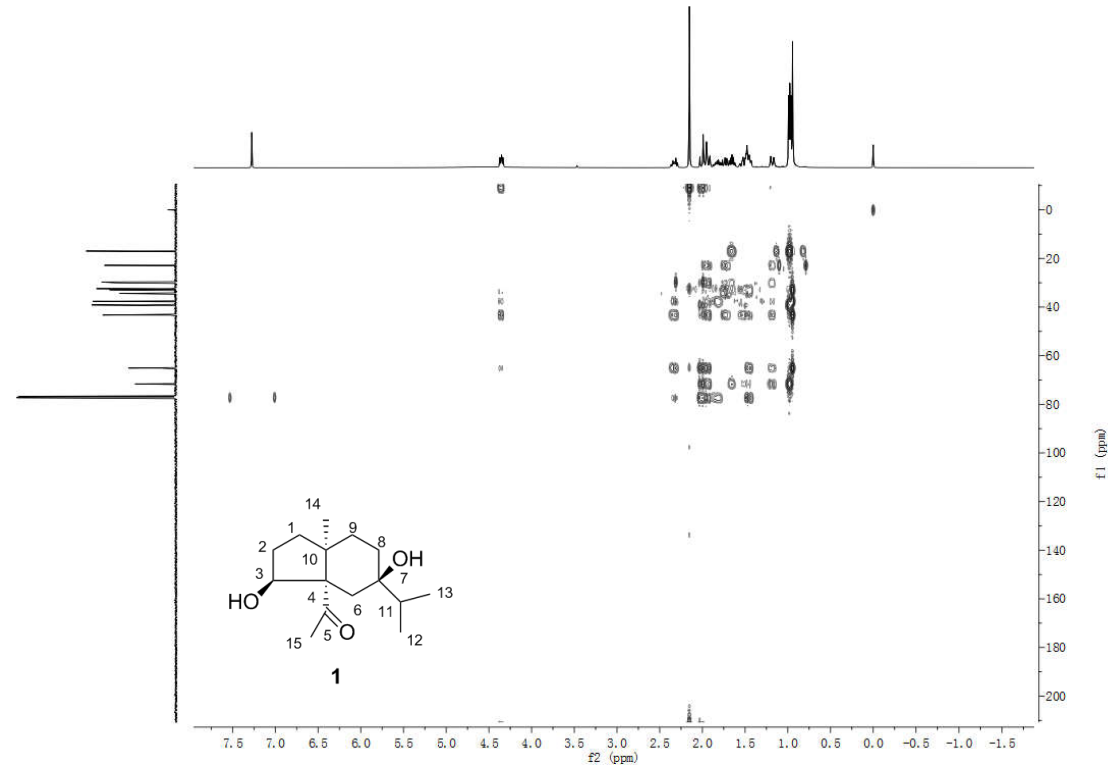


Figure S4. HMBC spectrum (400 MHz) of **1** in $CDCl_3$.

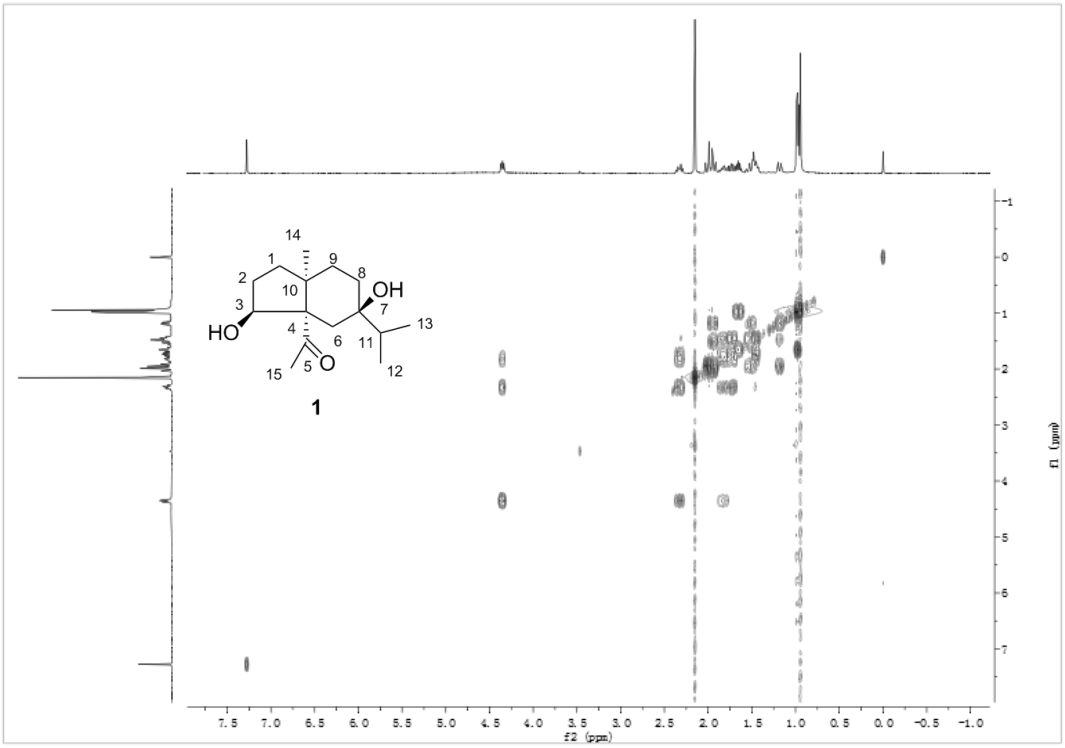


Figure S5. ^{1}H-^{1}H COSY spectrum (400 MHz) of **1** in $CDCl_3$.

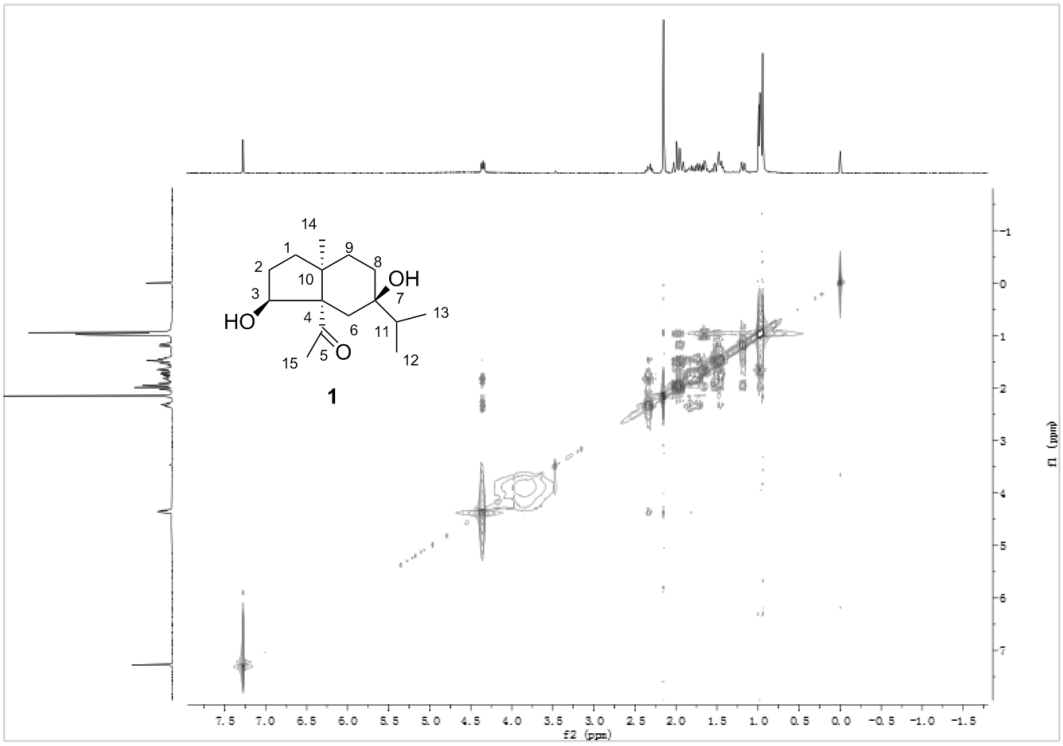


Figure S6. NOESY spectrum (400 MHz) of **1** in $CDCl_3$.

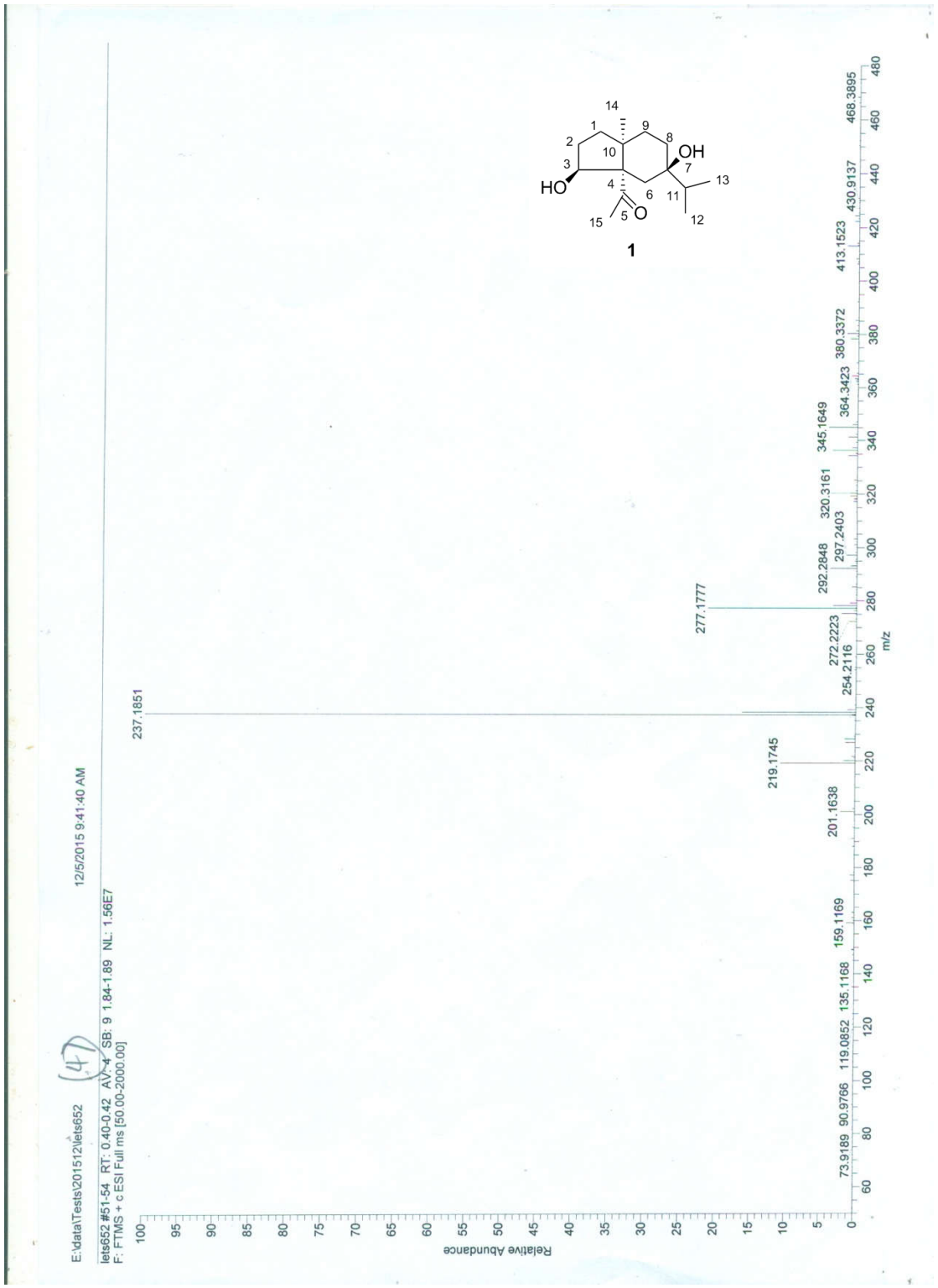


Figure S7. HRESIMS spectrum of **1**.

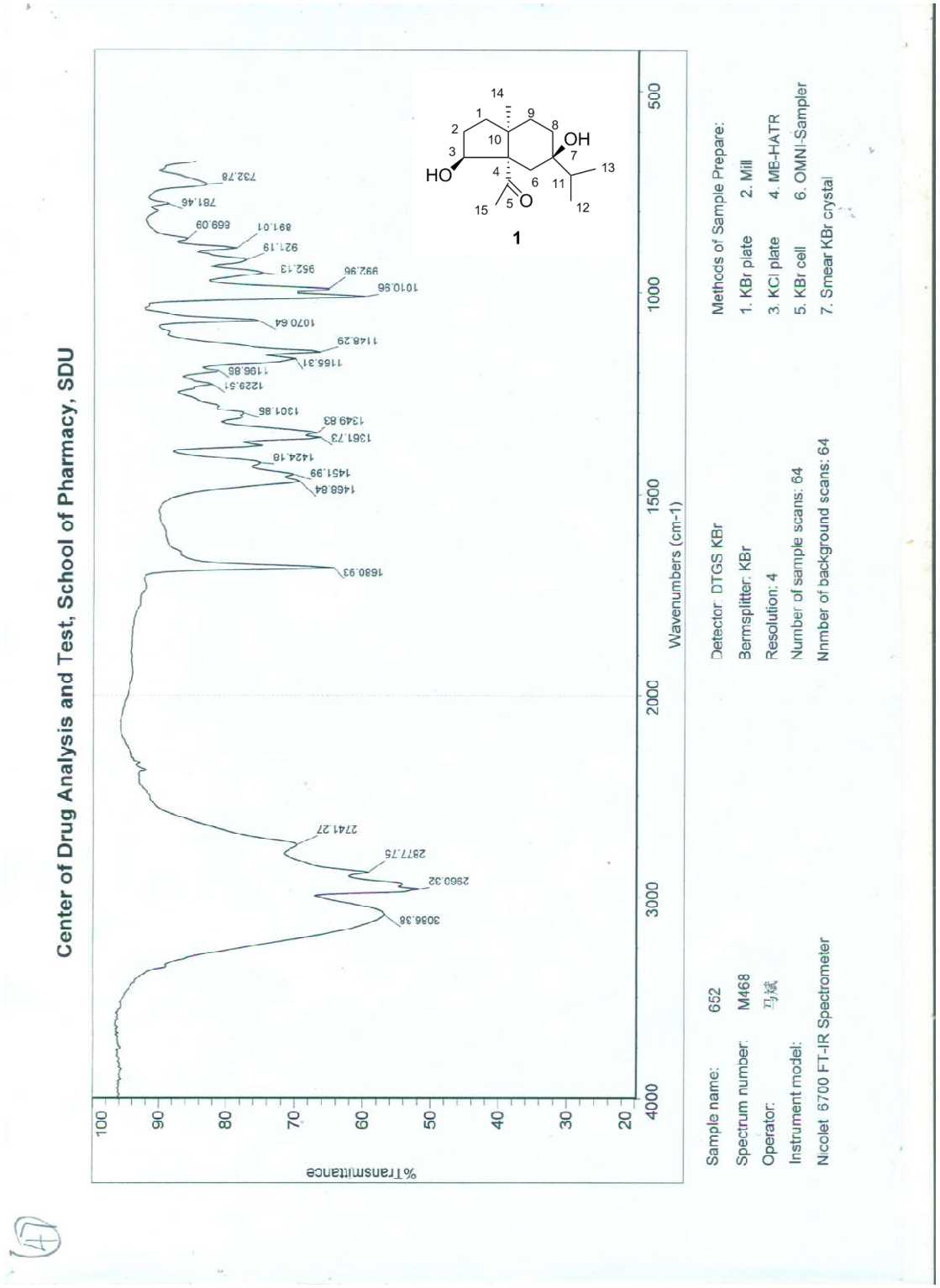


Figure S8. IR (KBr disc) spectrum of **1**.

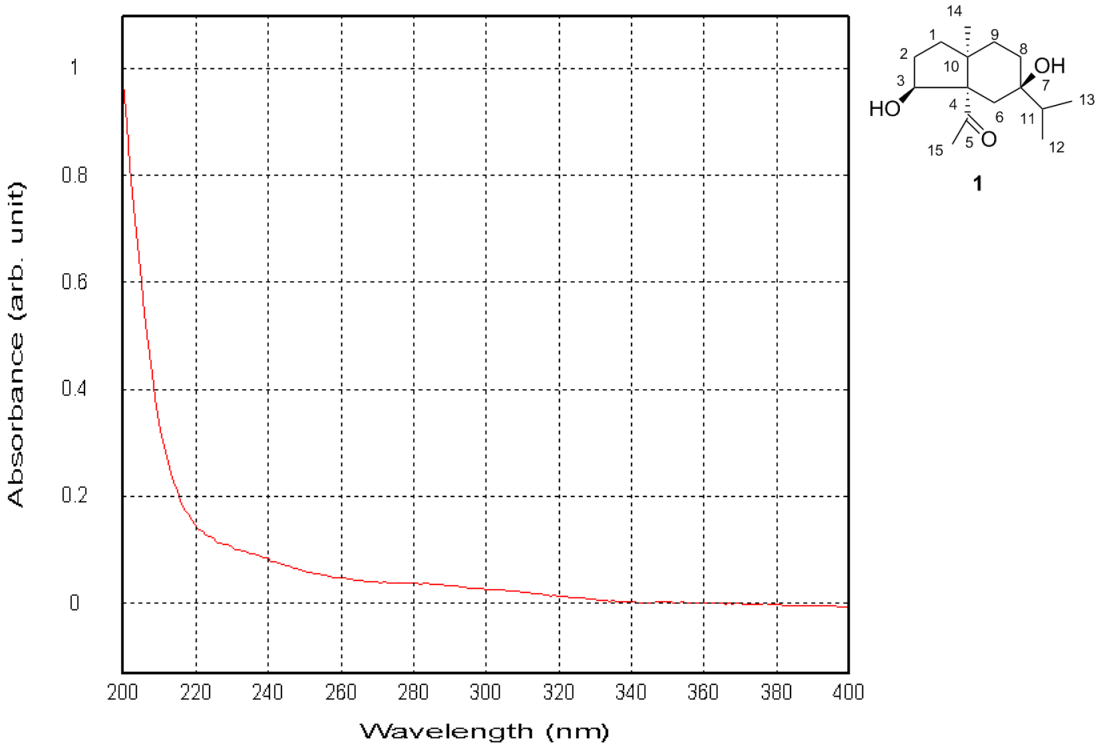


Figure S9. UV spectrum of **1**.

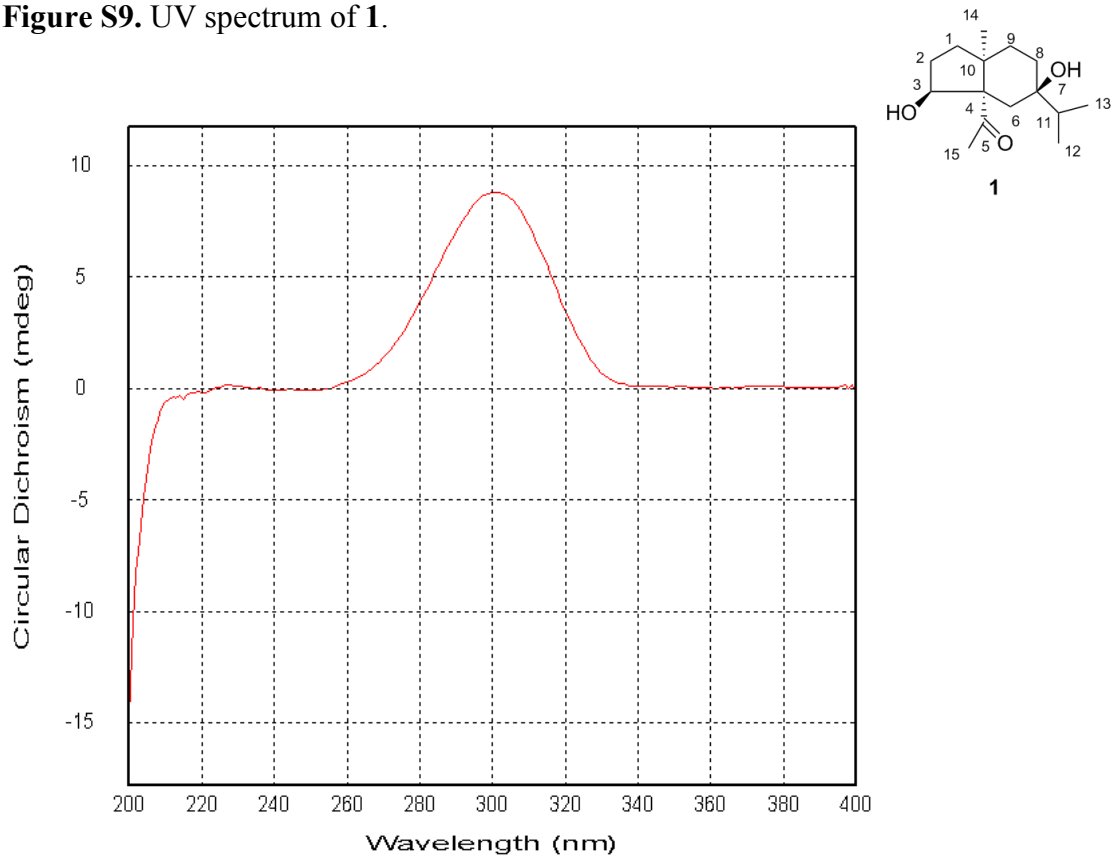


Figure S10. ECD spectrum of **1**.

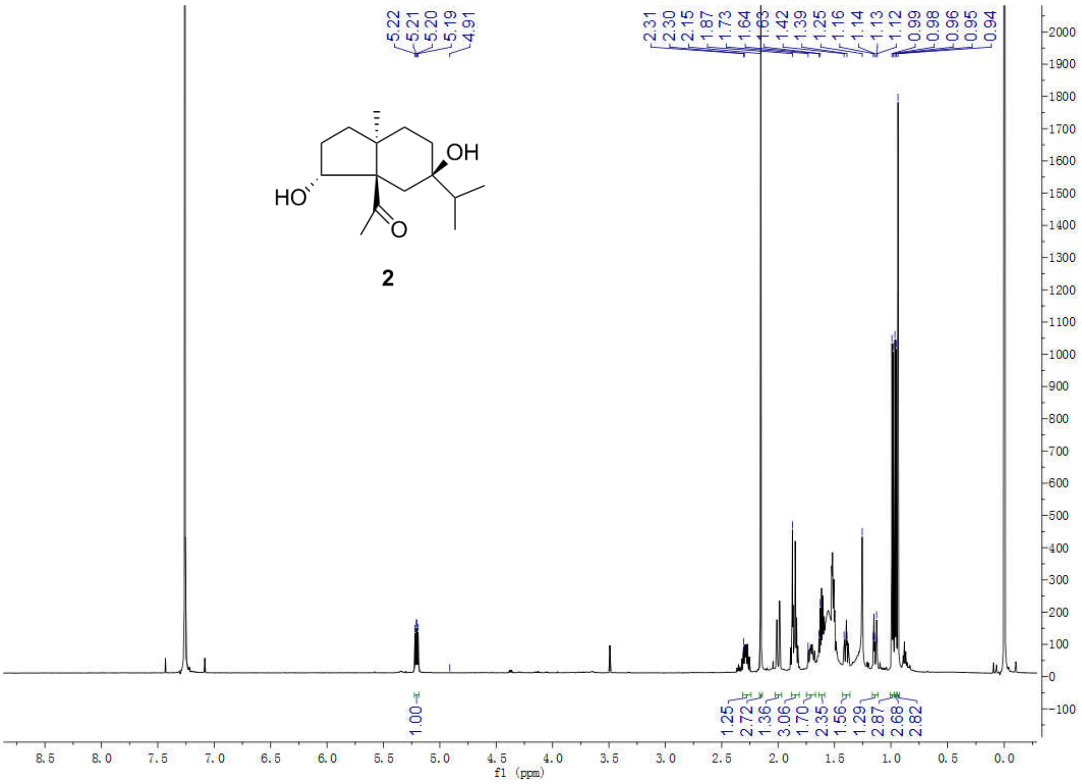


Figure S11. ^{1}H NMR spectrum (400 MHz) of **2** in $CDCl_3$.

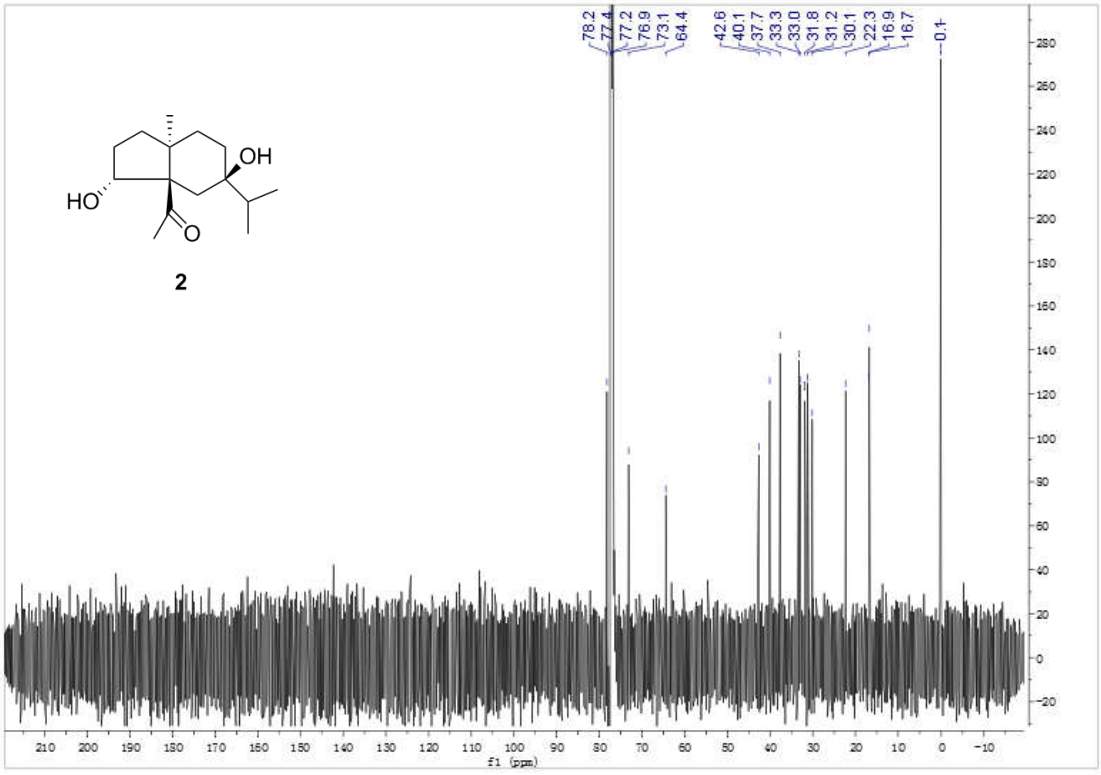


Figure S12. ^{13}C NMR spectrum (100 MHz) of **2** in $CDCl_3$.

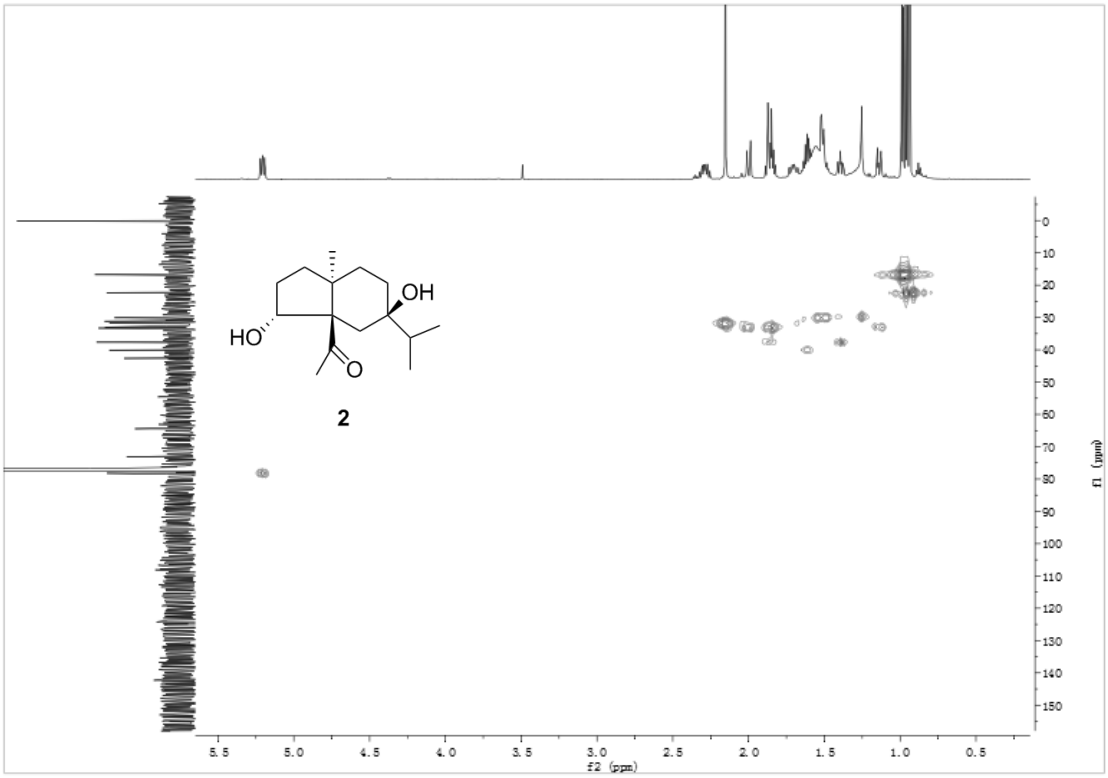


Figure S13. HSQC spectrum (400 MHz) of **2** in $CDCl_3$.

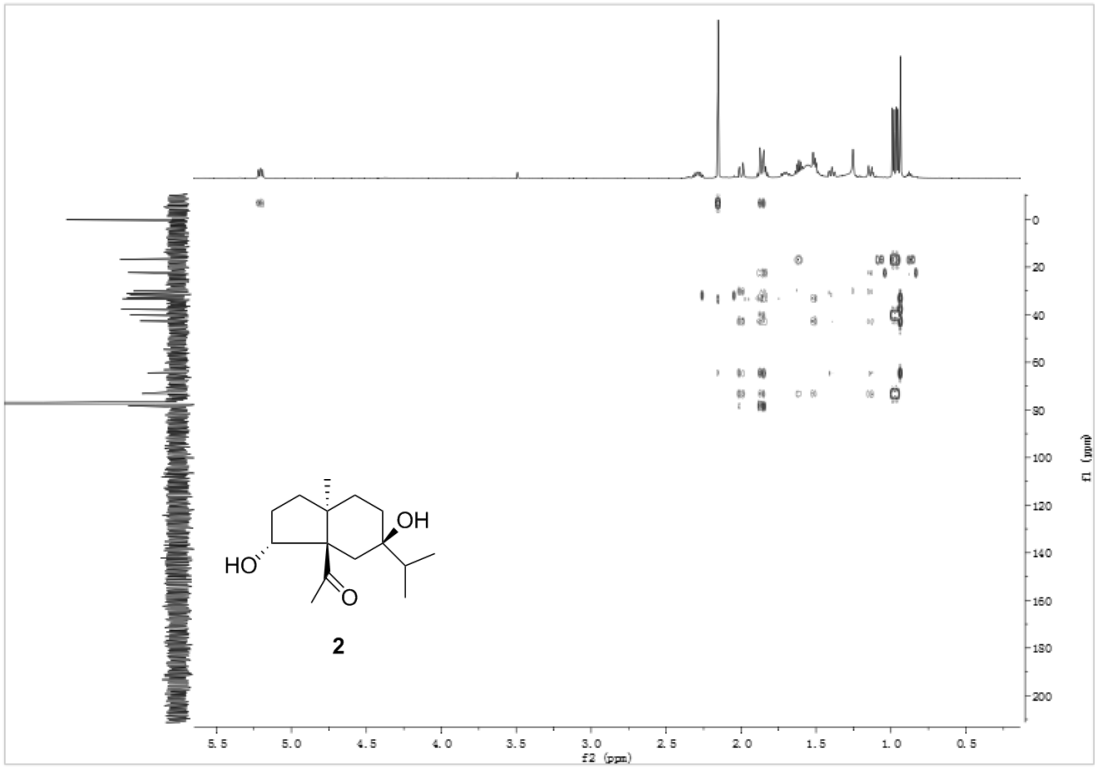


Figure S14. HMBC spectrum (400 MHz) of **2** in $CDCl_3$.

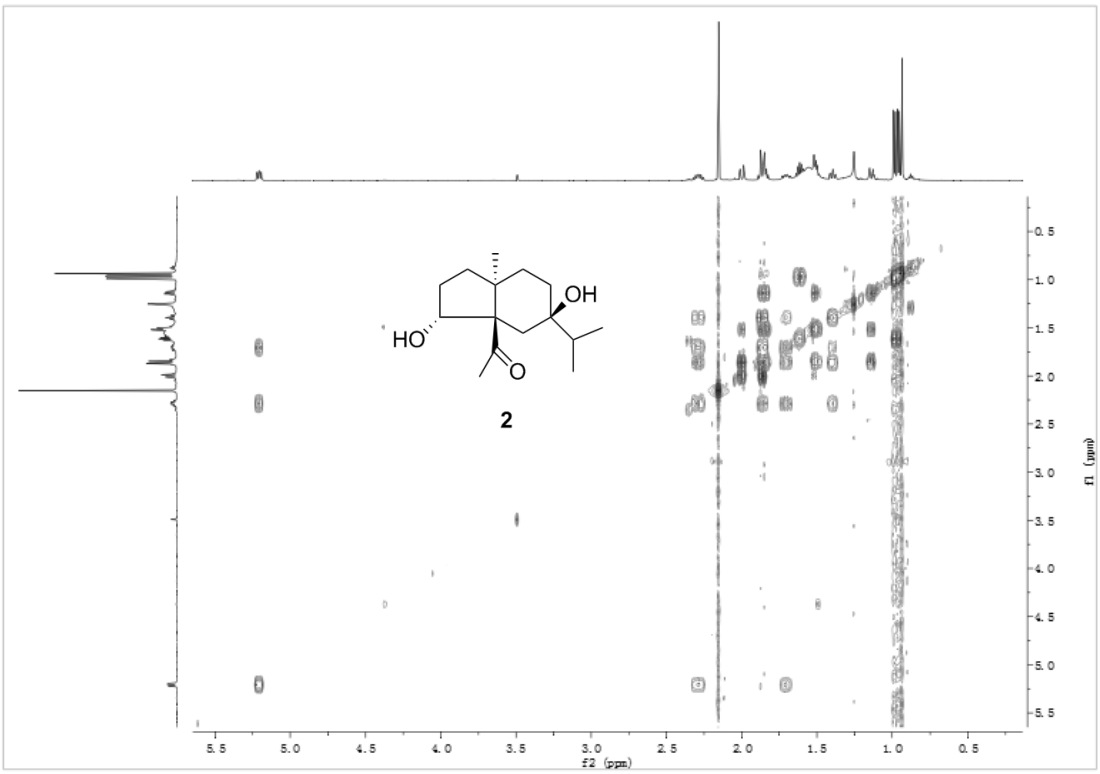


Figure S15. ^{1}H-^{1}H COSY spectrum (400 MHz) of **2** in $CDCl_3$.

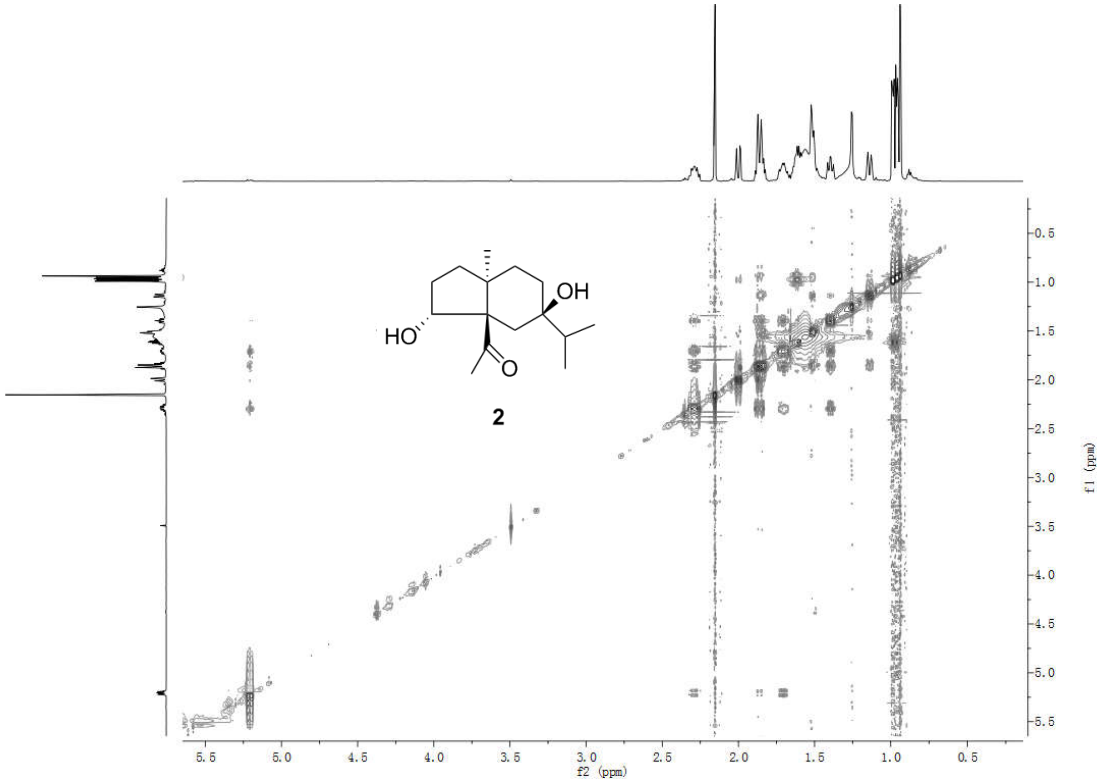


Figure S16. NOESY spectrum (400 MHz) of **2** in $CDCl_3$.

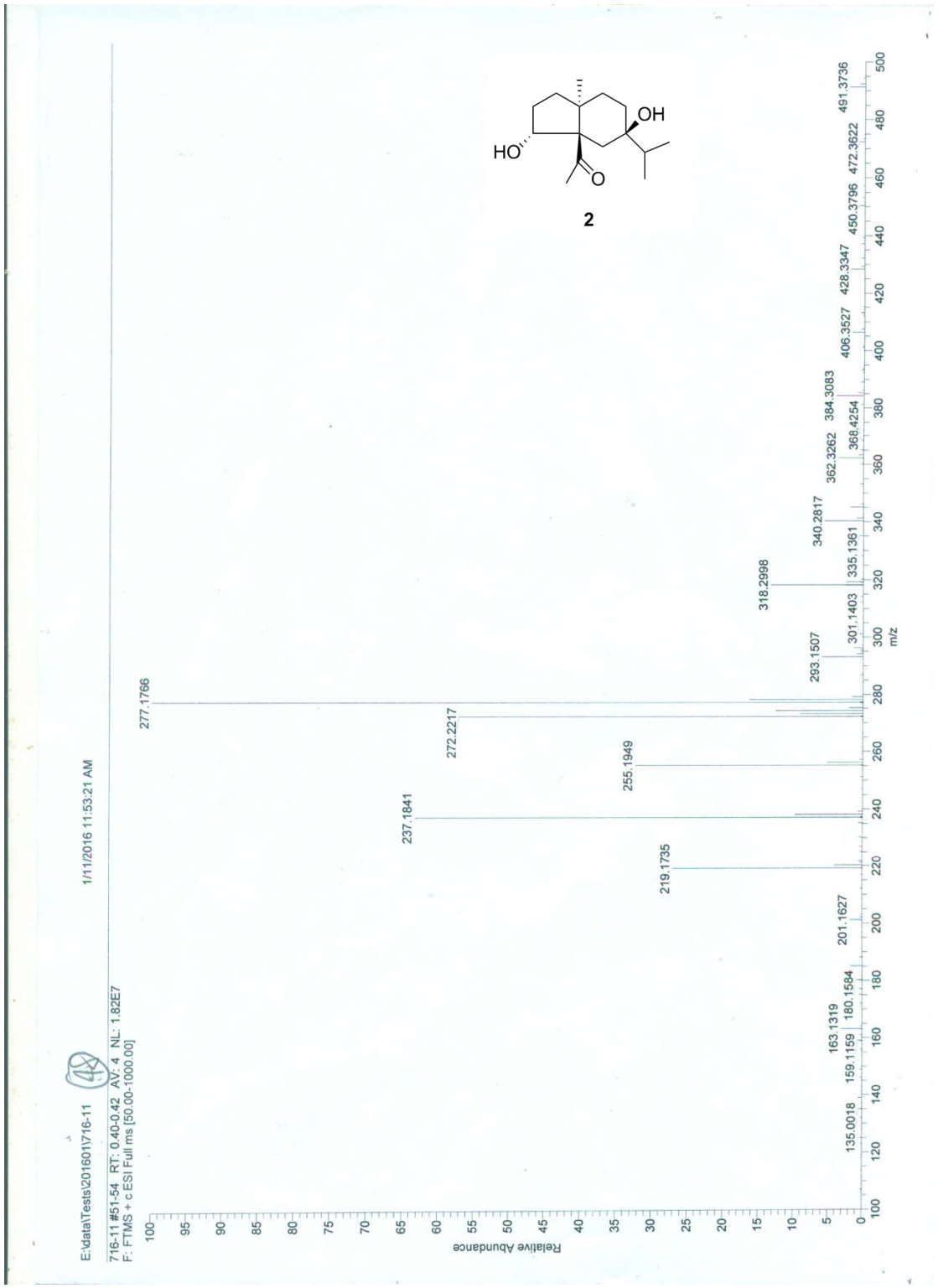


Figure S17. HRESIMS spectrum of **2**.

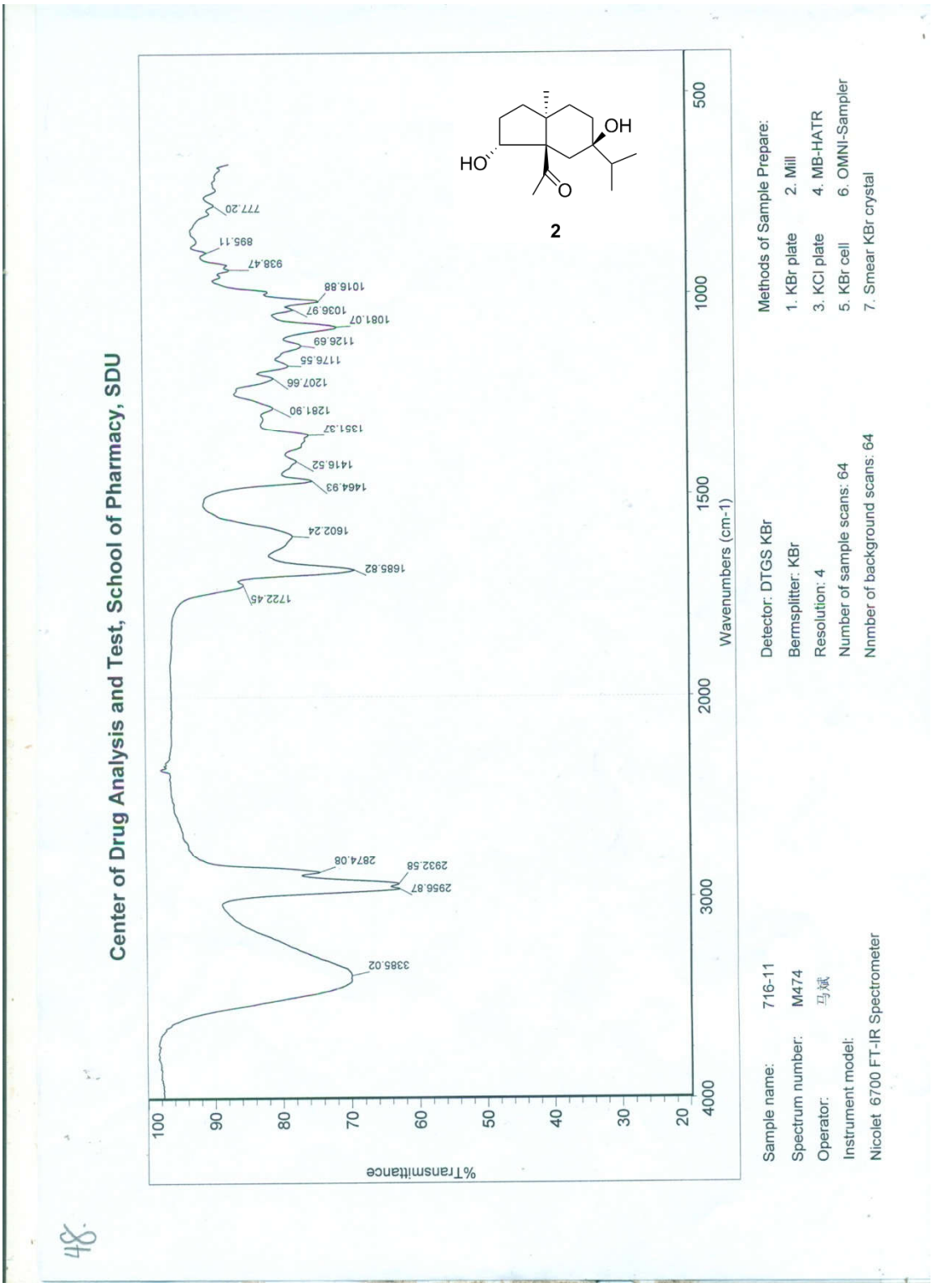


Figure S18. IR (KBr disc) spectrum of **2**.

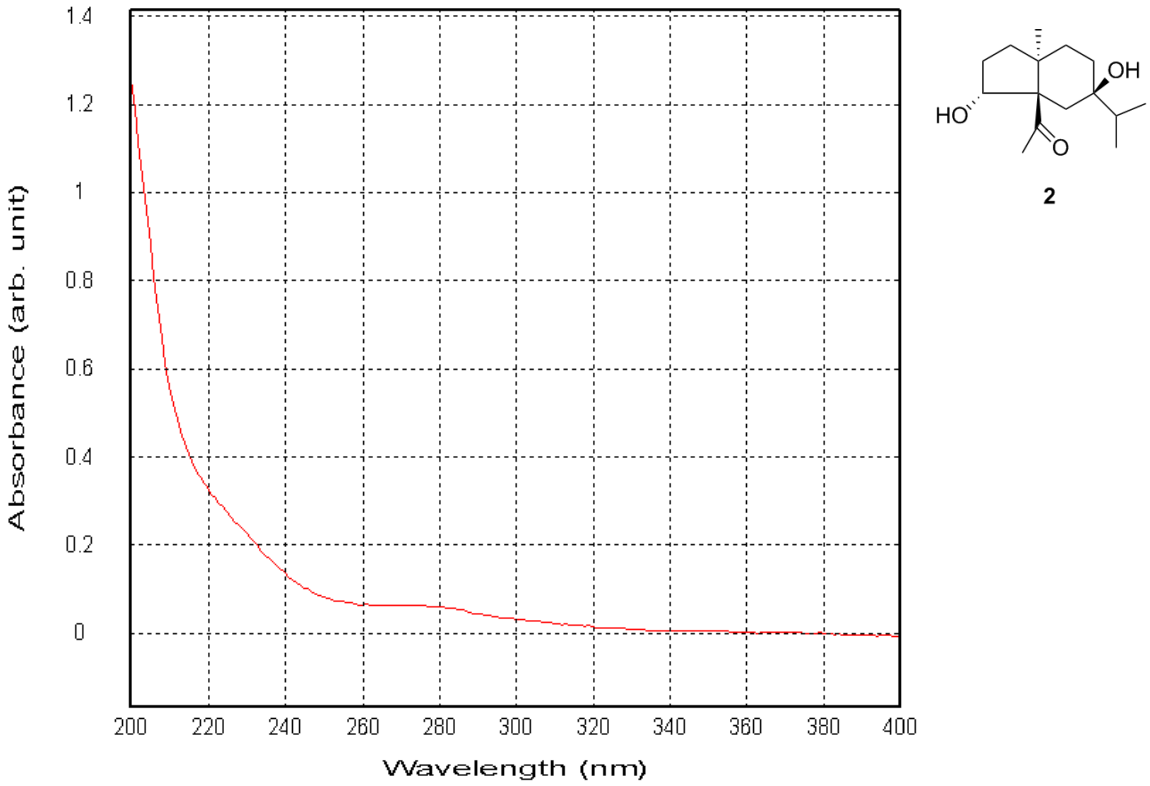


Figure S19. UV spectrum of **2**.

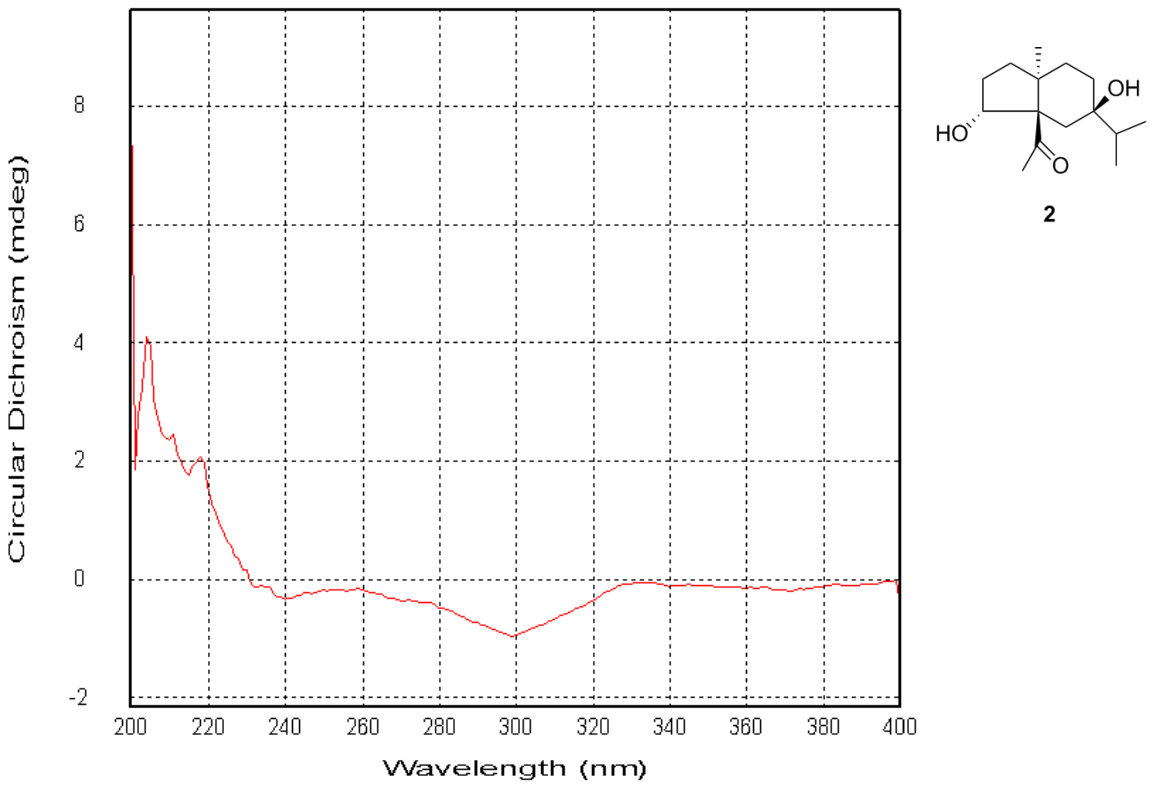
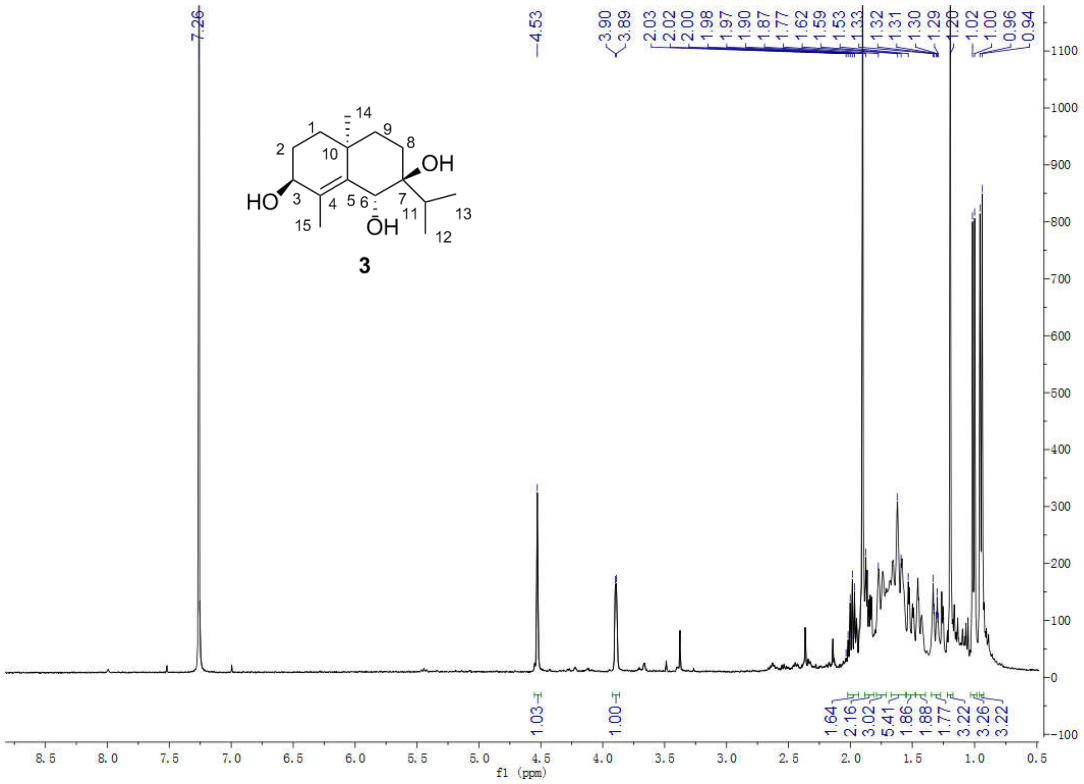
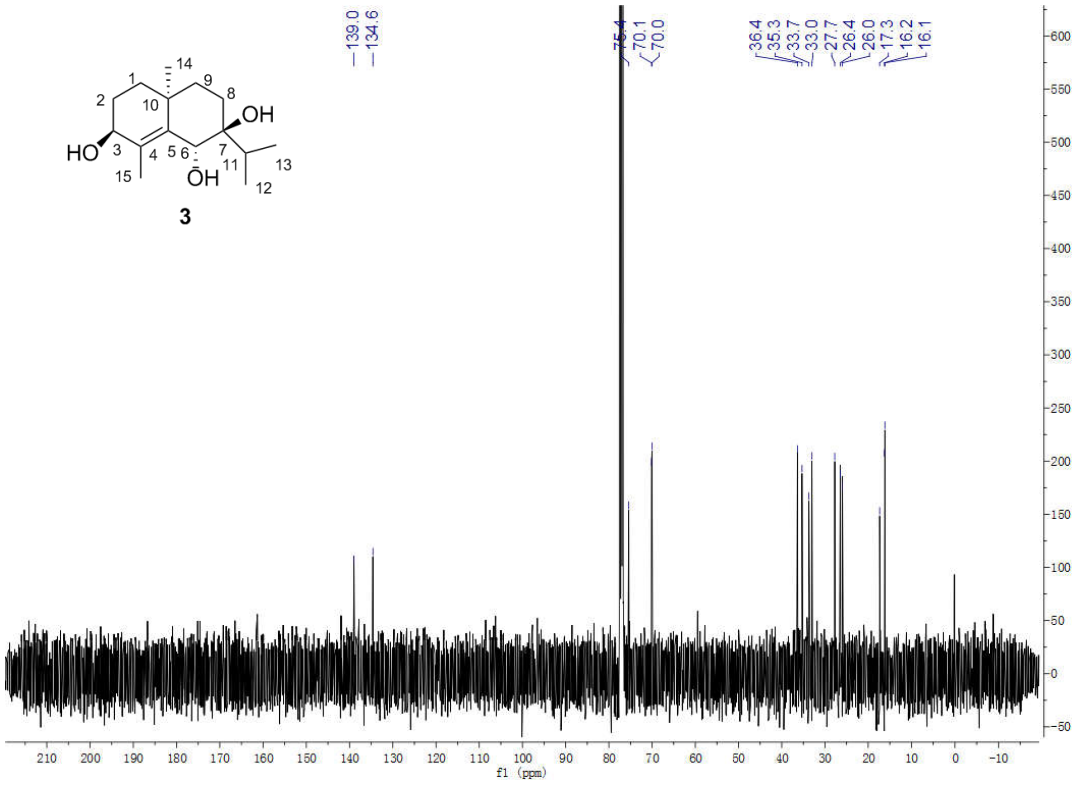


Figure S20. ECD spectrum of **2**.



3

Figure S21 ^{1}H NMR spectrum (400 MHz) of **3** in $CDCl_3$.



3

Figure S22. ^{13}C NMR spectrum (100 MHz) of **3** in $CDCl_3$.

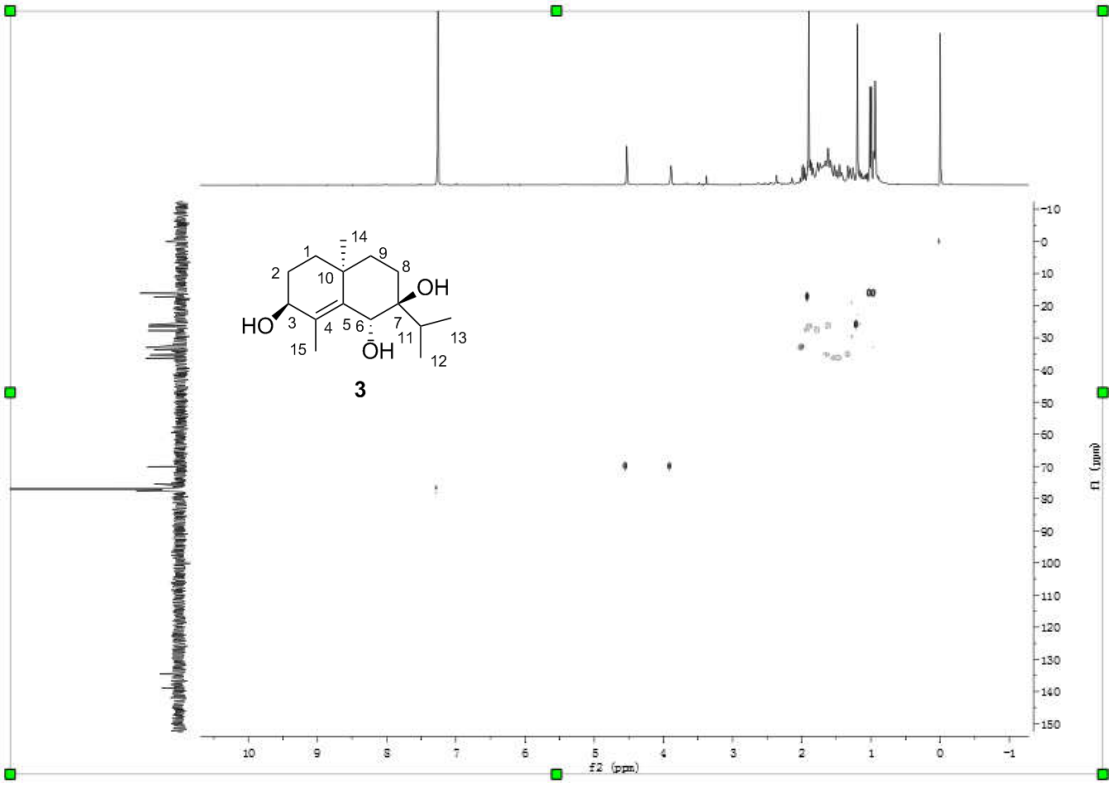


Figure S23. HSQC spectrum (400 MHz) of **3** in $CDCl_3$.

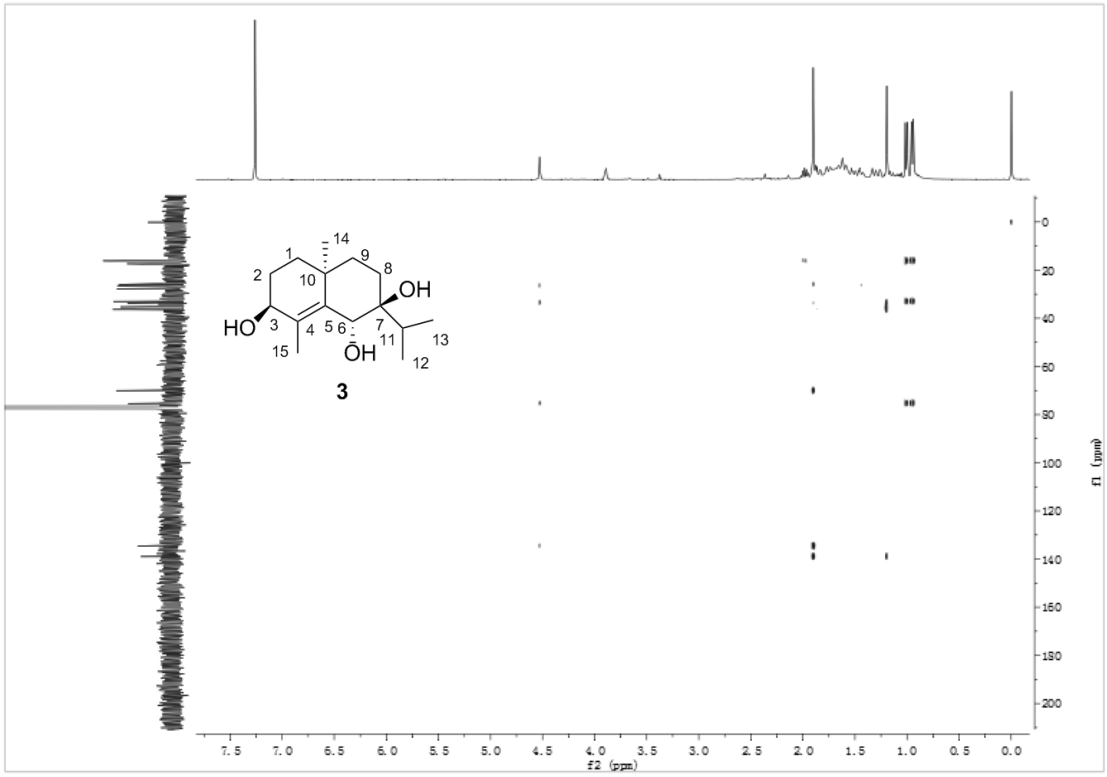


Figure S24. HMBC spectrum (400 MHz) of **3** in $CDCl_3$.

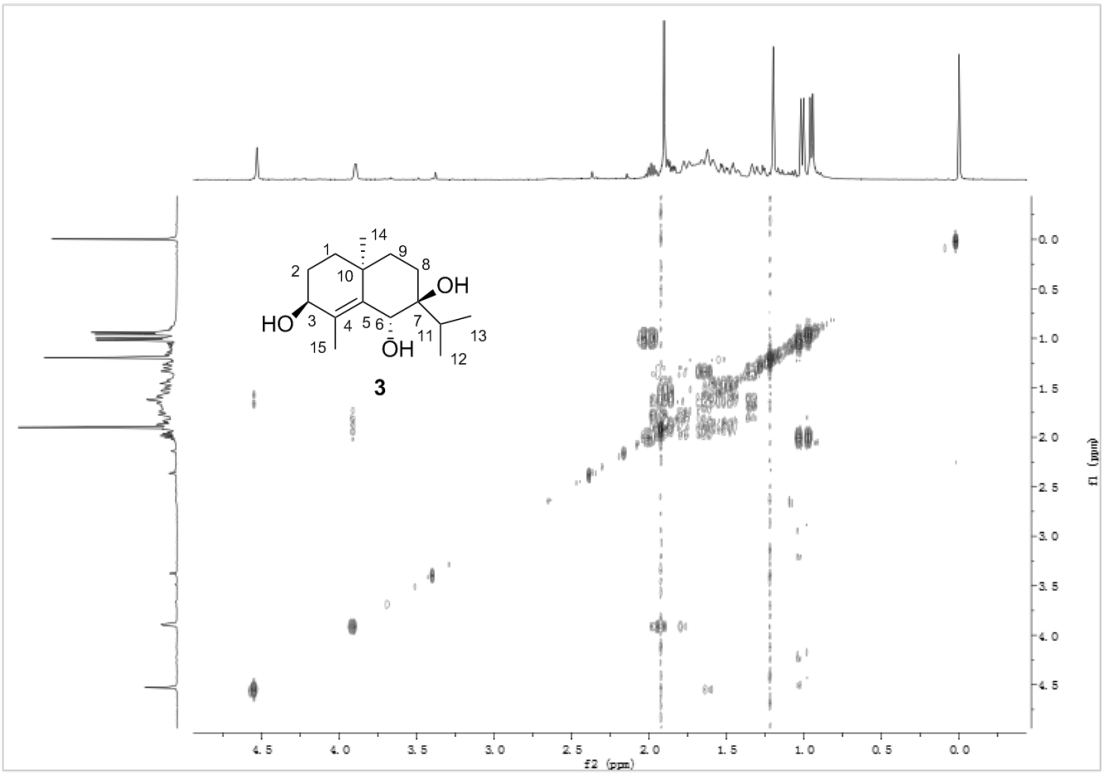


Figure S25. ^{1}H-^{1}H COSY spectrum (400 MHz) of **3** in $CDCl_3$.

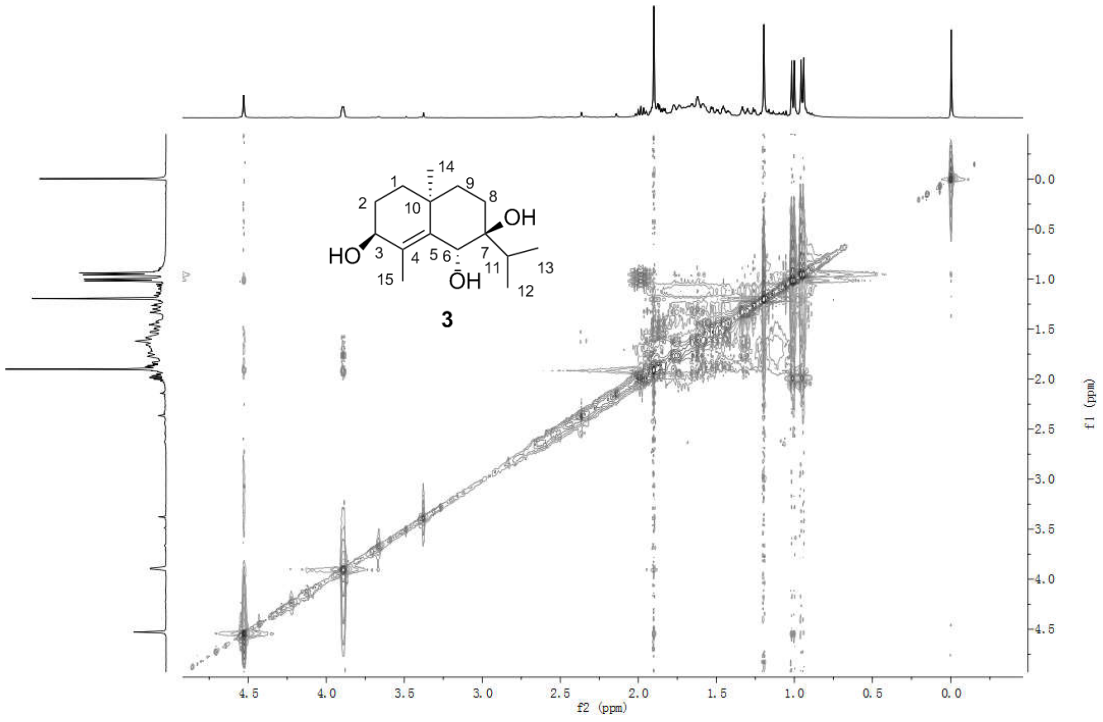


Figure S26. NOESY spectrum (400 MHz) of **3** in $CDCl_3$.

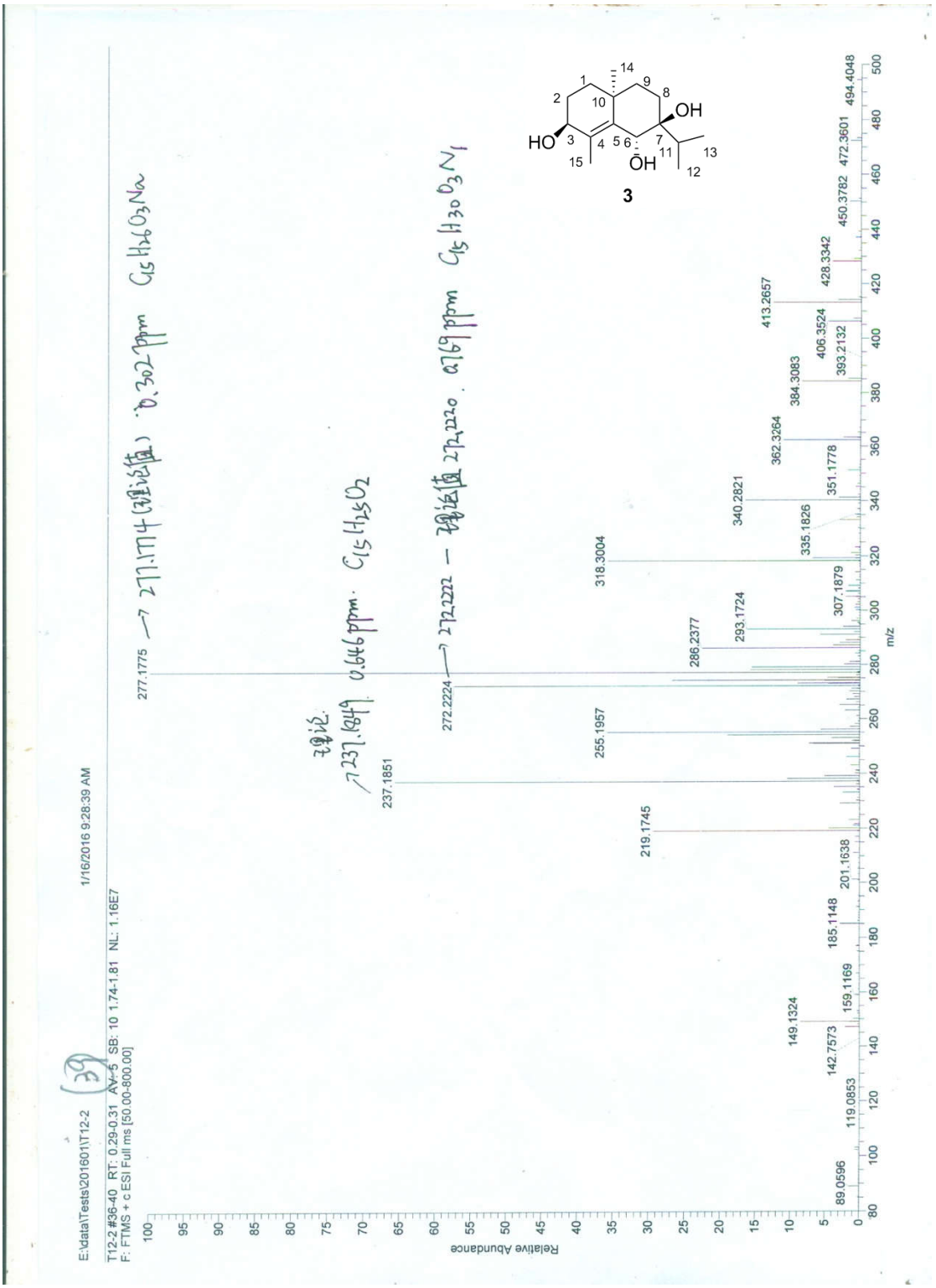


Figure S27. HRESIMS spectrum of **3**.

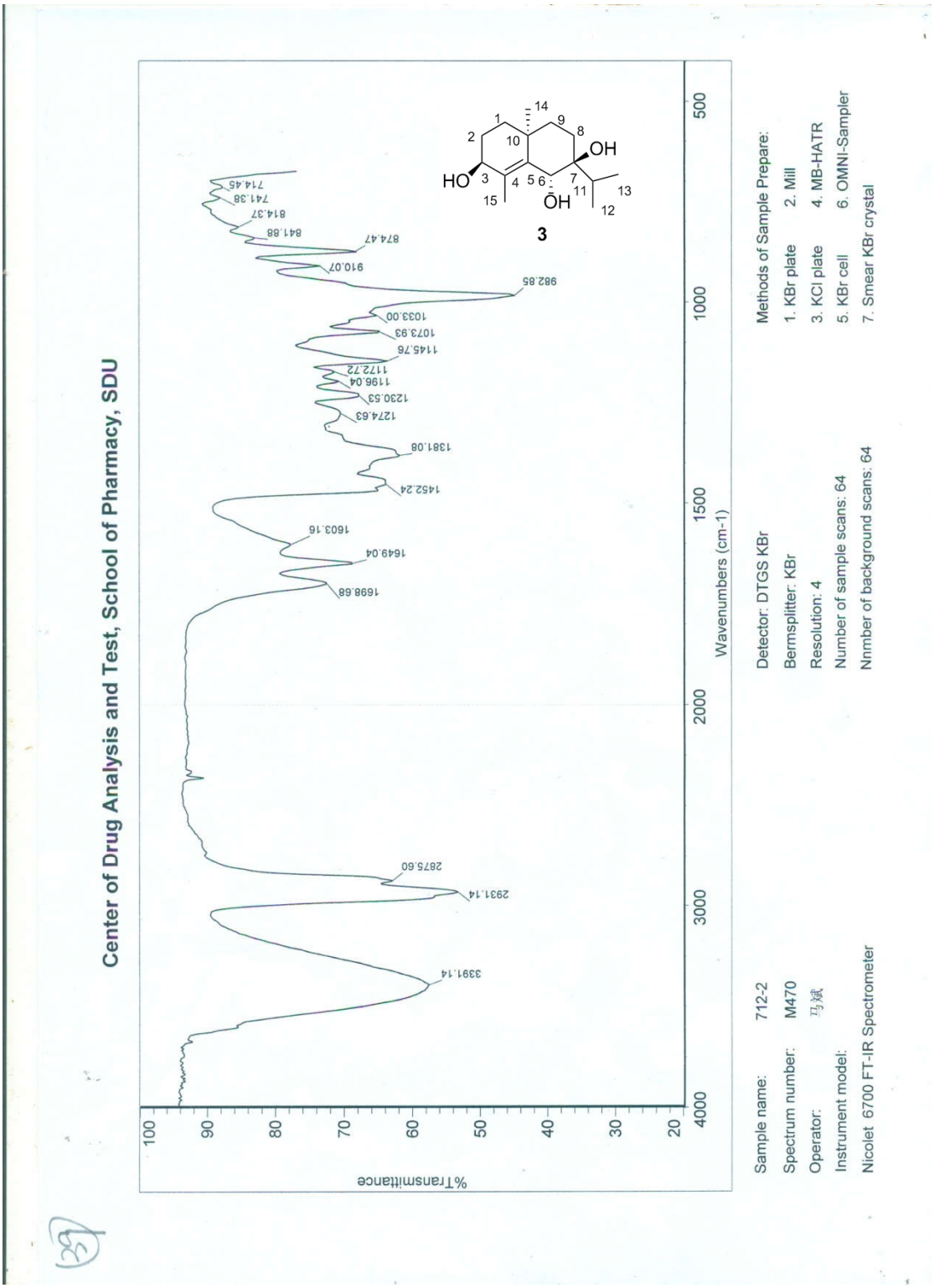


Figure S28. IR (KBr disc) spectrum of **3**.

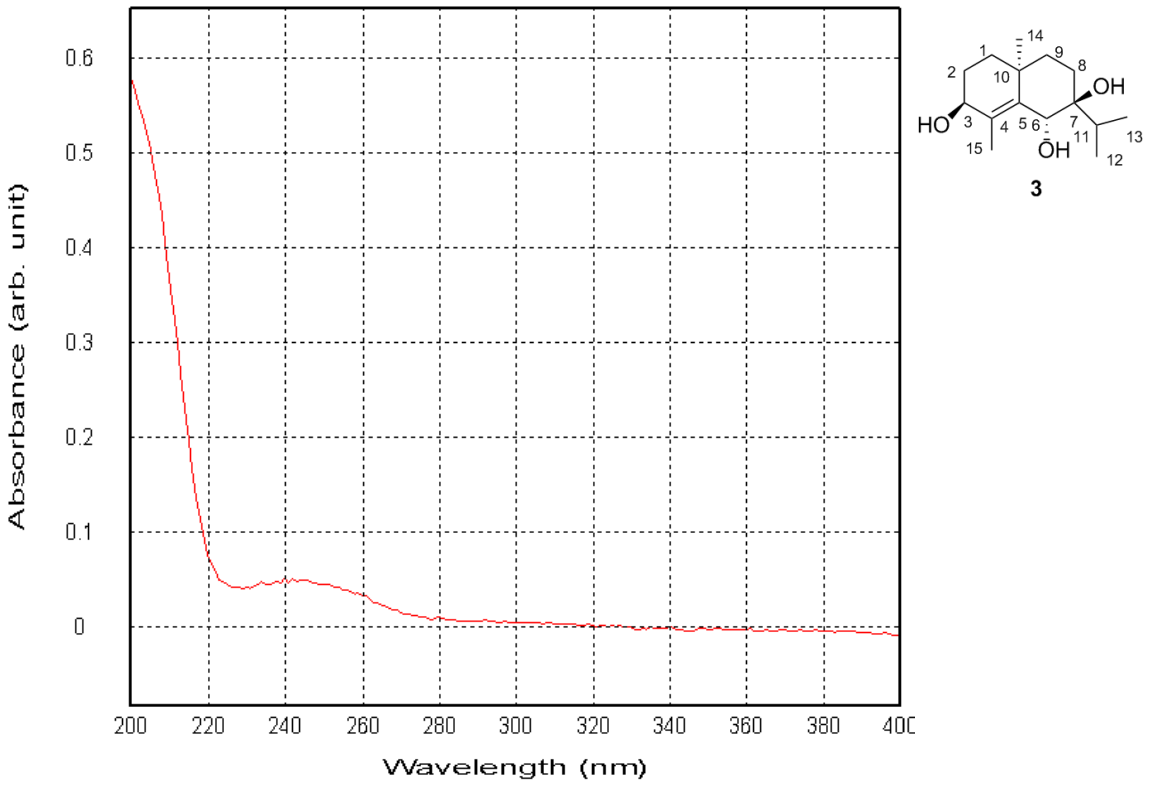


Figure S29. UV spectrum of **3**.

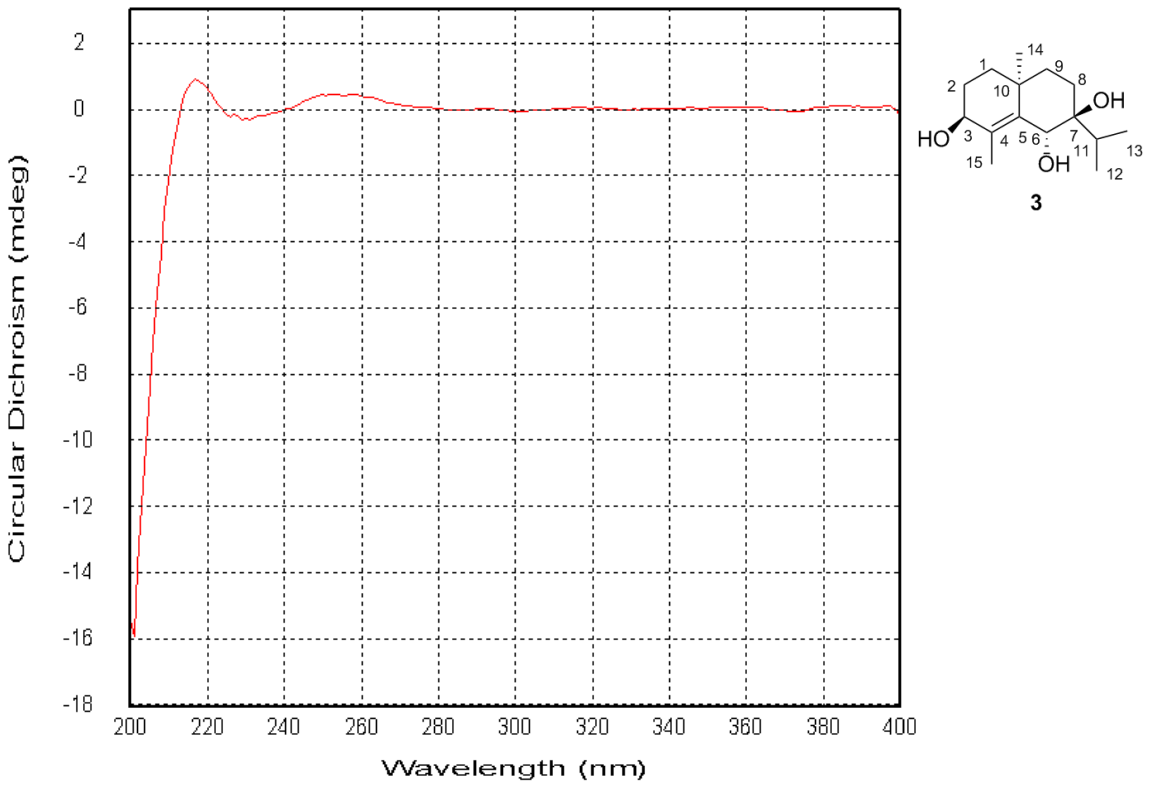


Figure S30. ECD spectrum of **3**.

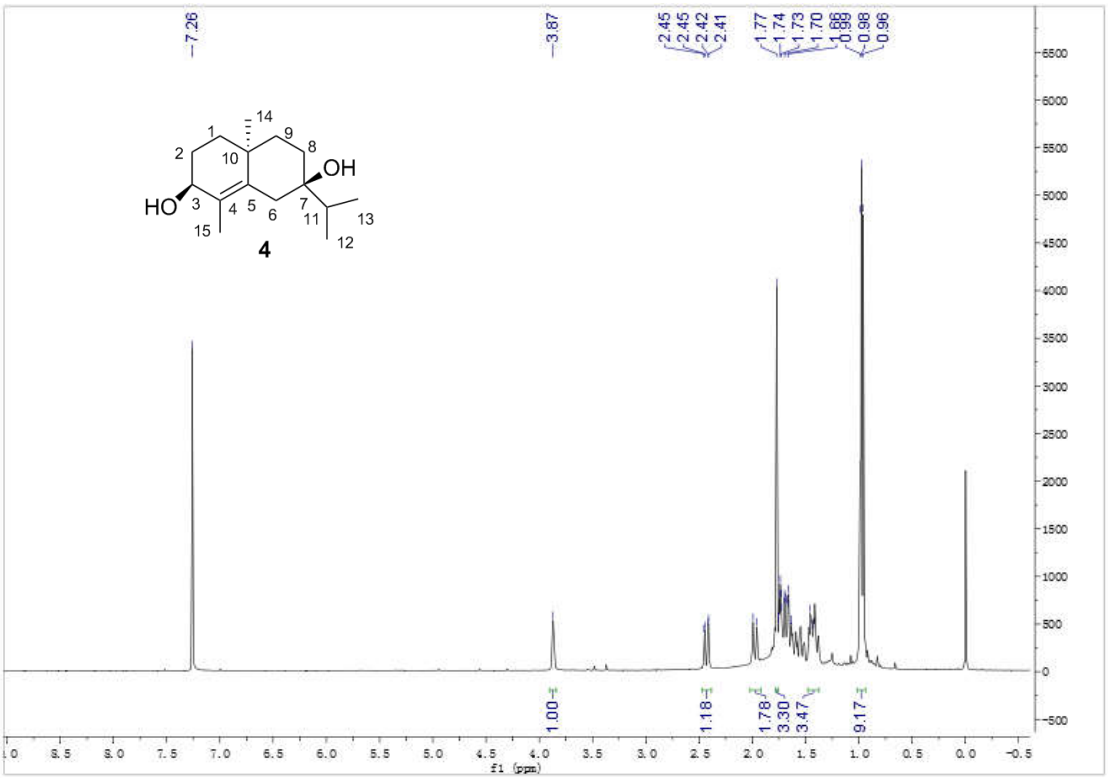


Figure S31. ^{1}H NMR spectrum (400 MHz) of **4** in $CDCl_3$.

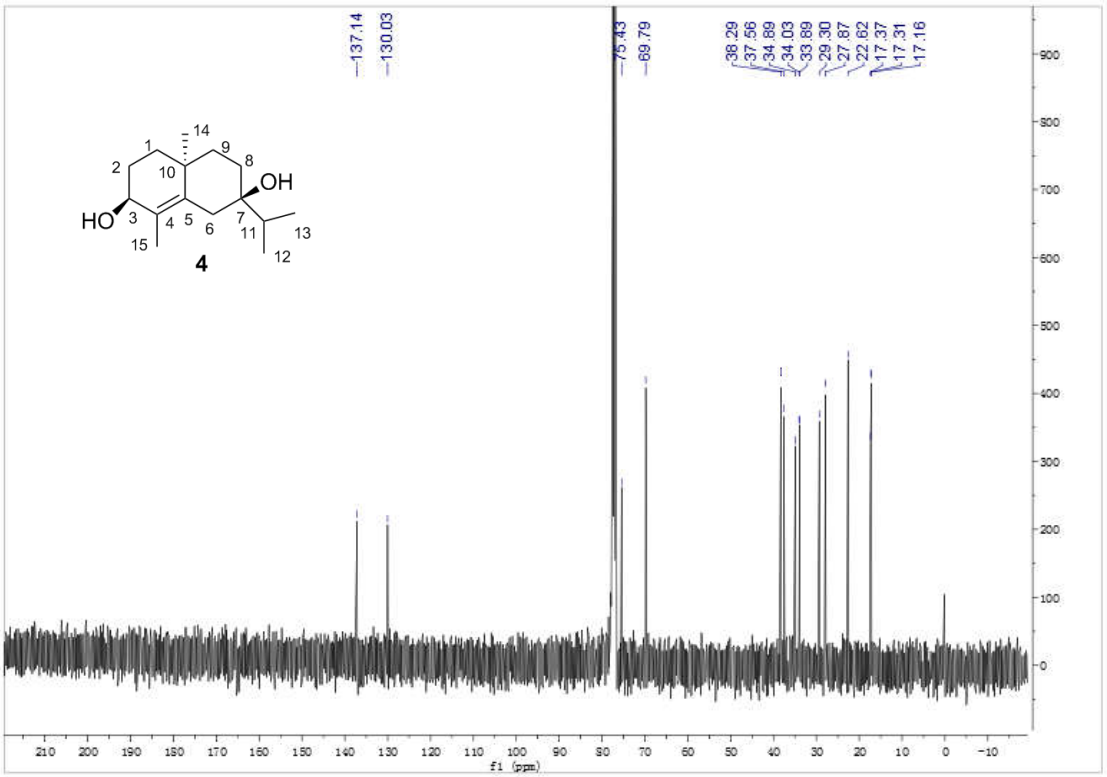


Figure S32. ^{13}C NMR spectrum (100 MHz) of **4** in $CDCl_3$.

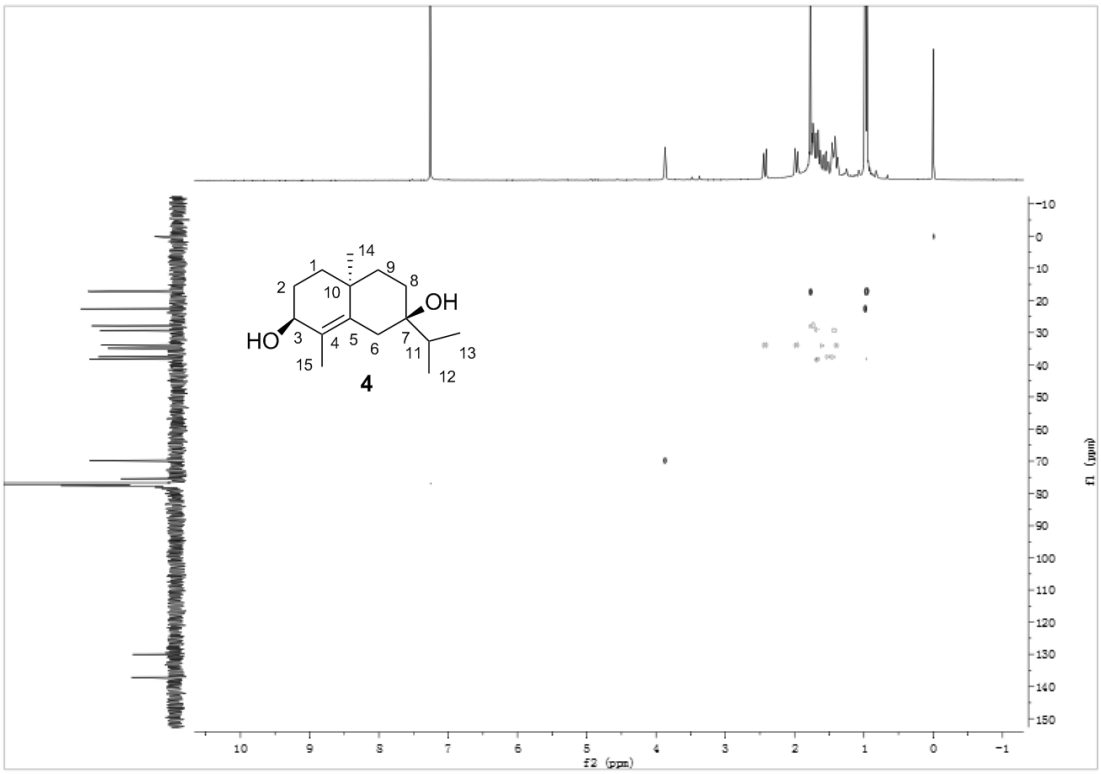


Figure S33. HSQC spectrum (400 MHz) of **4** in $CDCl_3$.

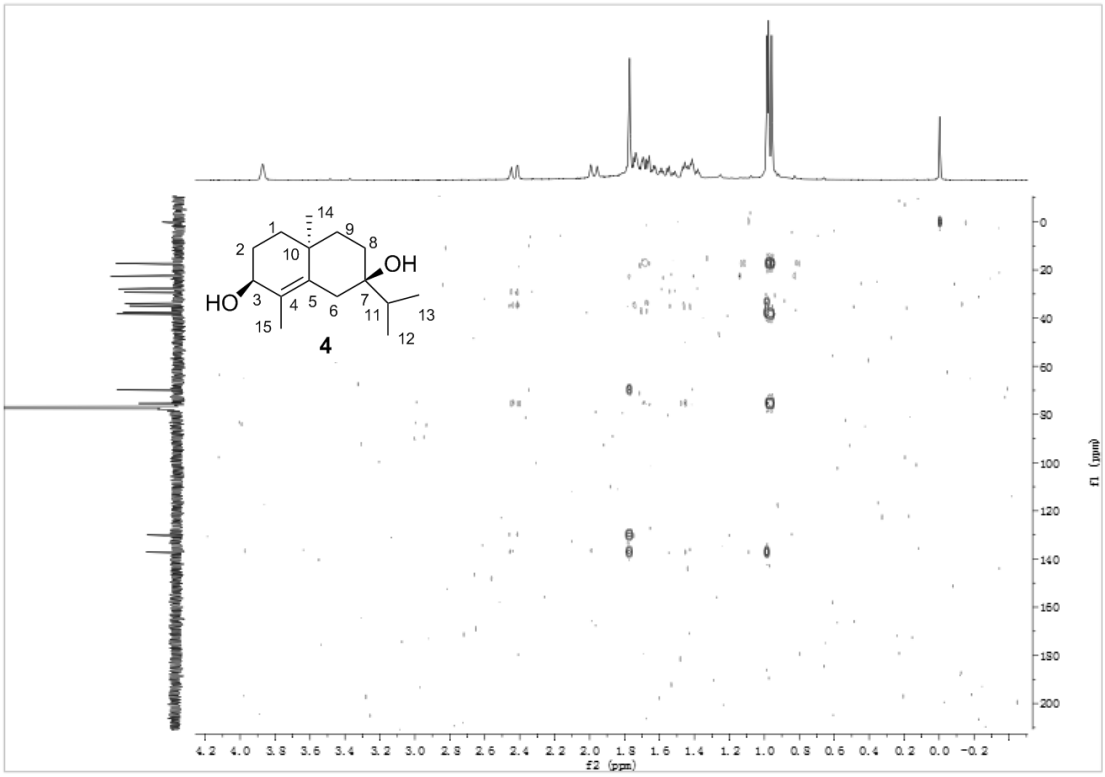


Figure S34. HMBC spectrum (400 MHz) of **4** in $CDCl_3$.

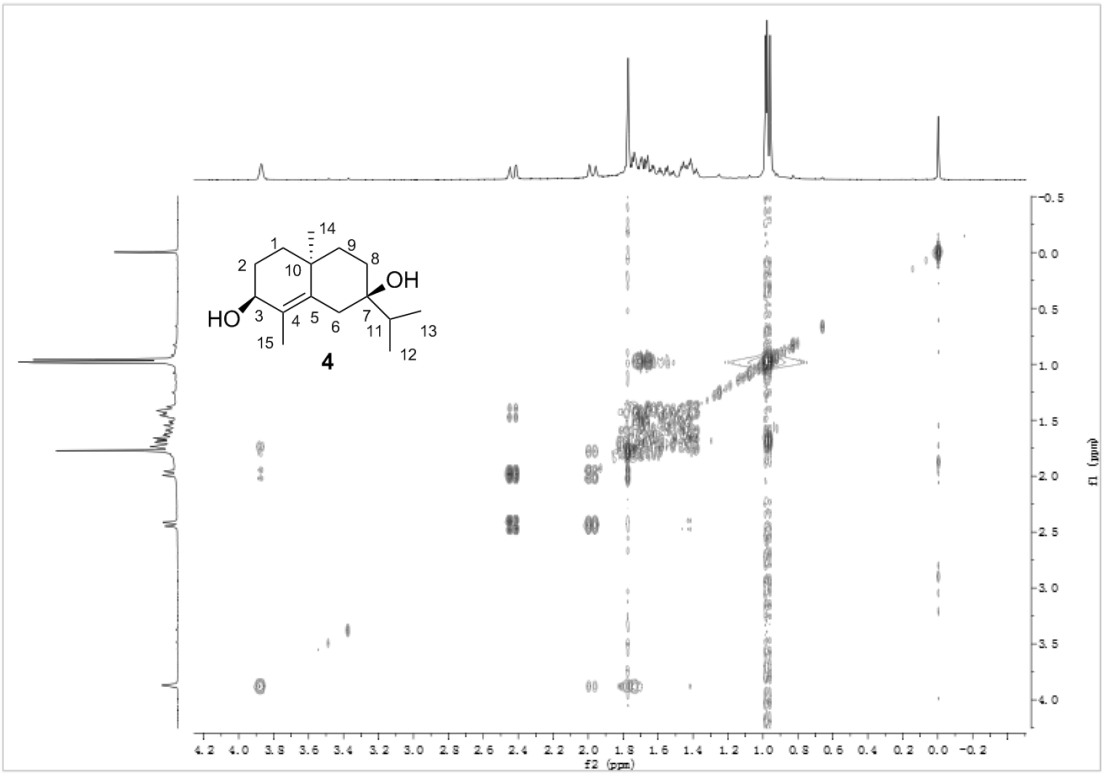


Figure S35. ^{1}H-^{1}H COSY spectrum (400 MHz) of **4** in $CDCl_3$.

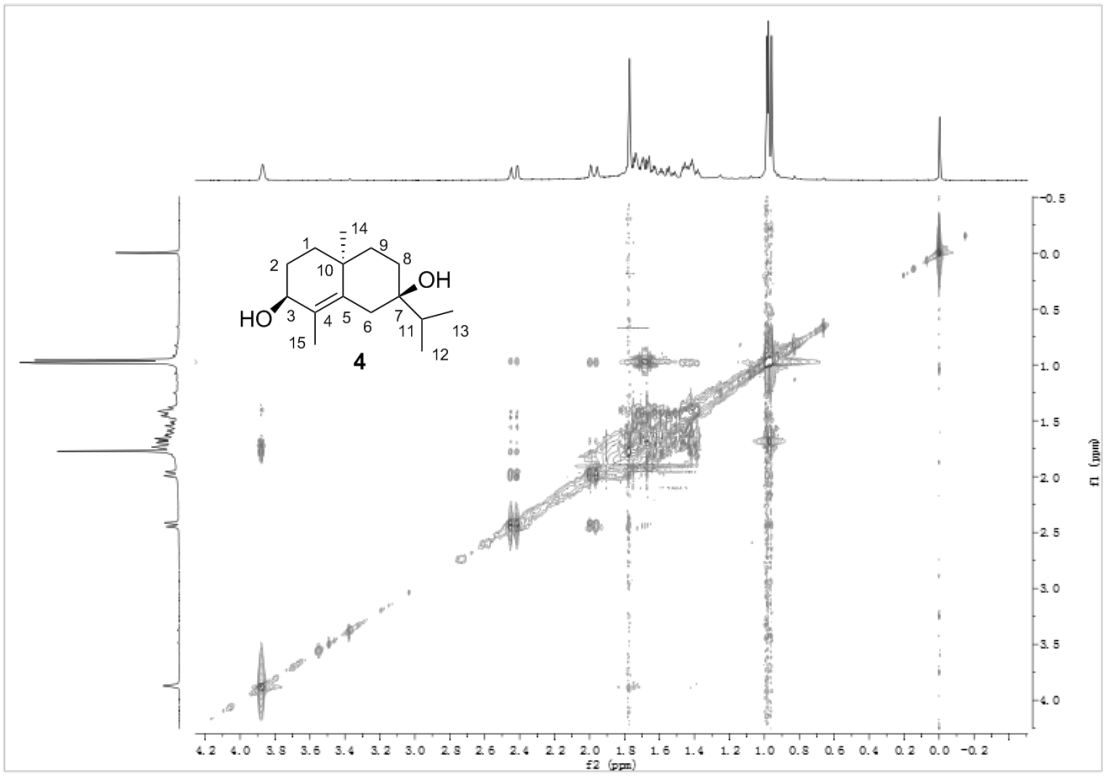


Figure S36. NOESY spectrum (400 MHz) of **4** in $CDCl_3$.

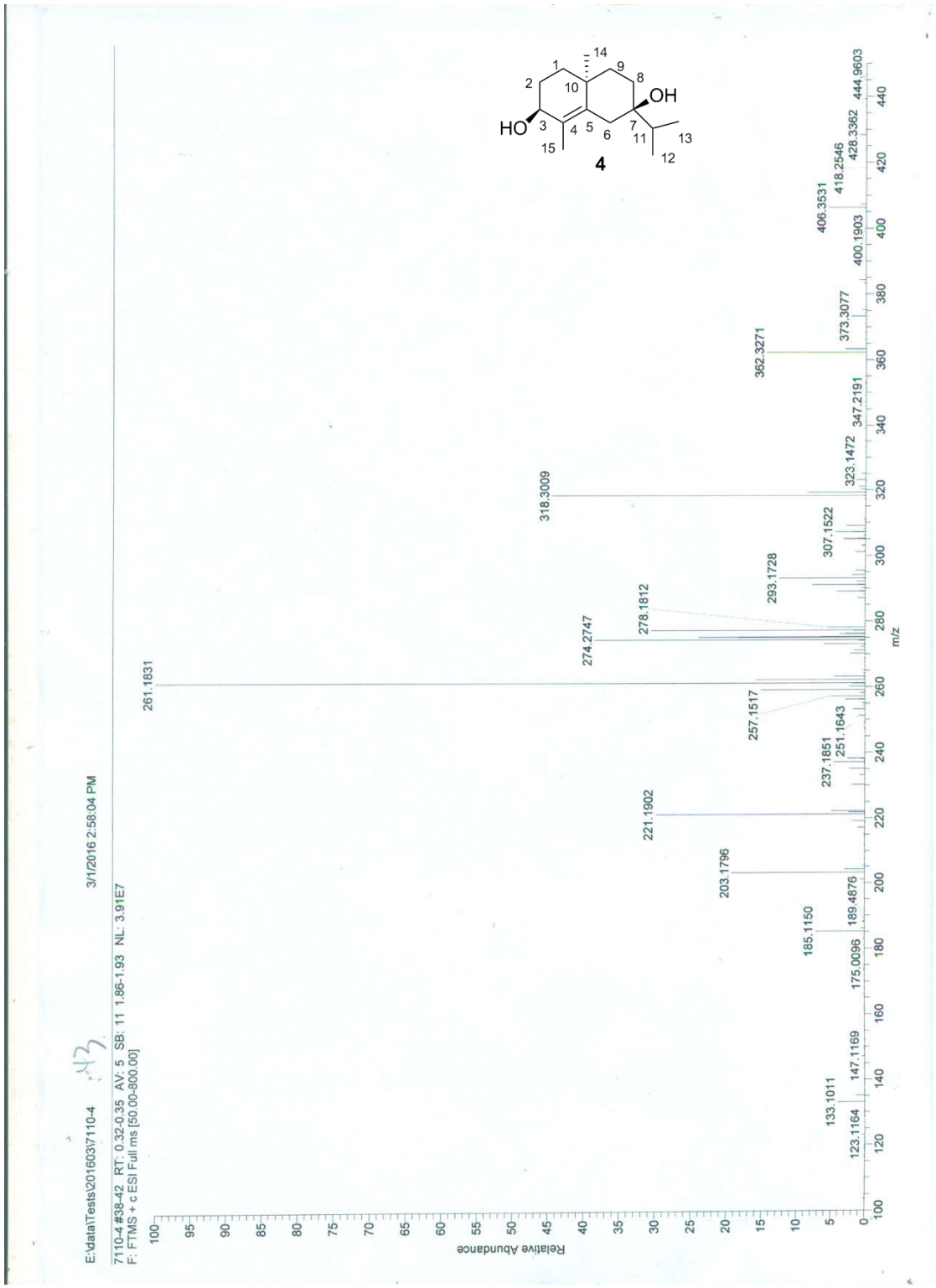


Figure S37. HRESIMS spectrum of **4**.

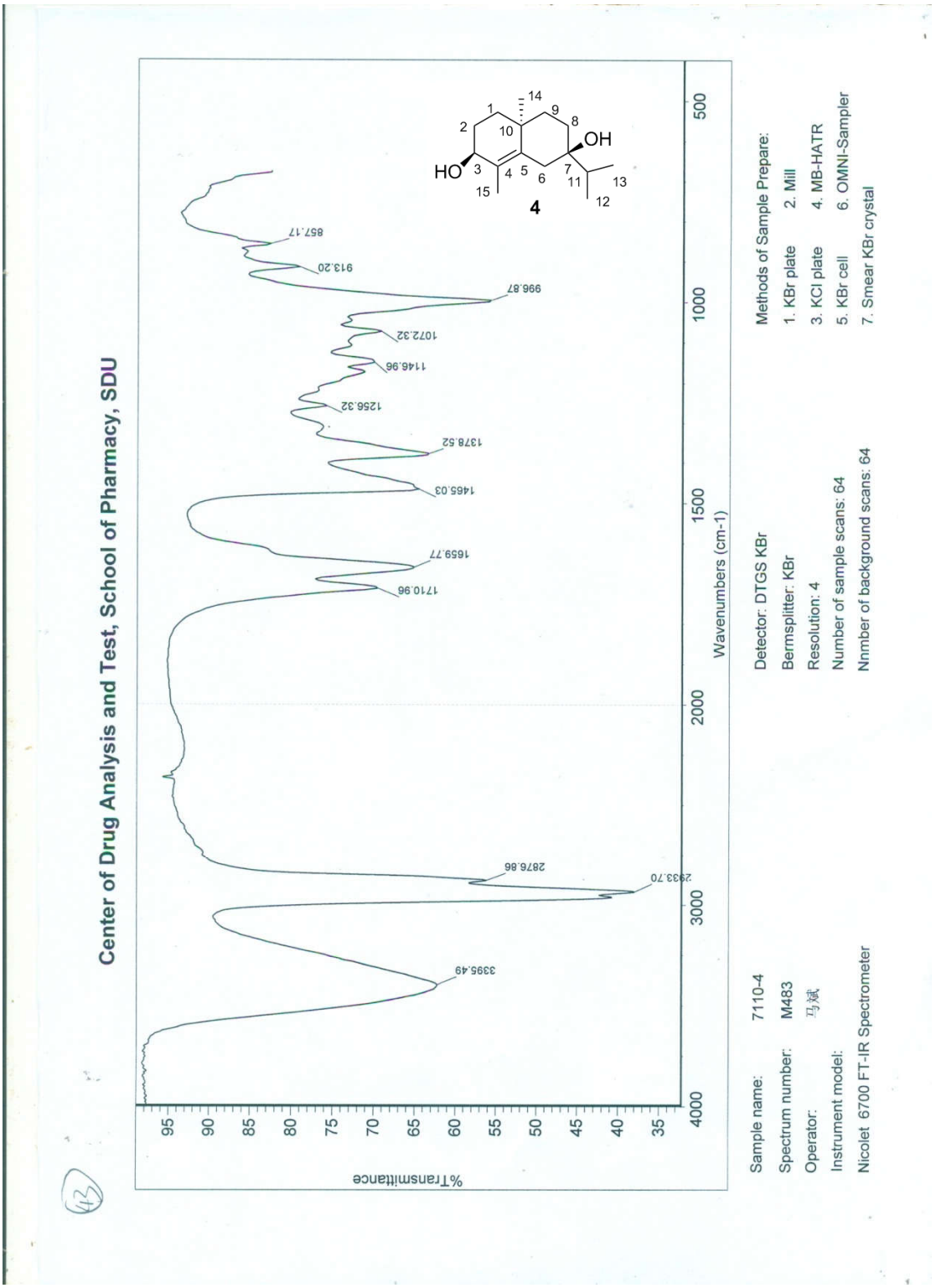


Figure S38. IR (KBr disc) spectrum of **4**.

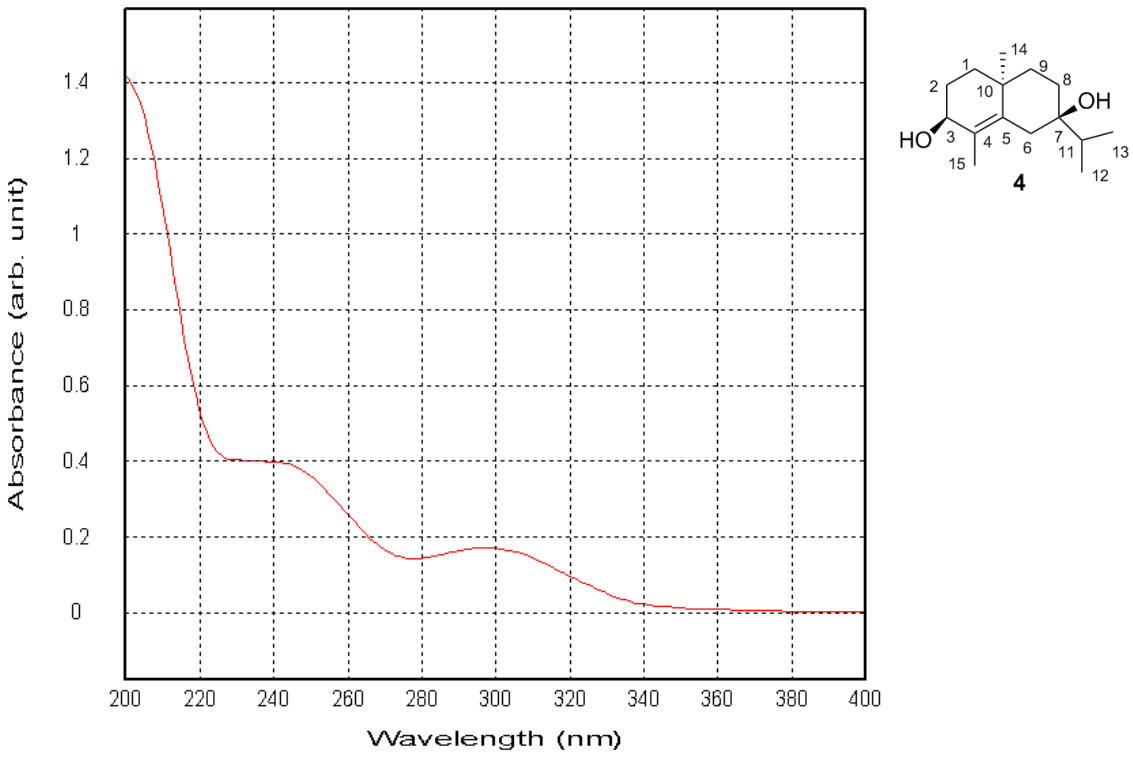


Figure S39. UV spectrum of **4**.

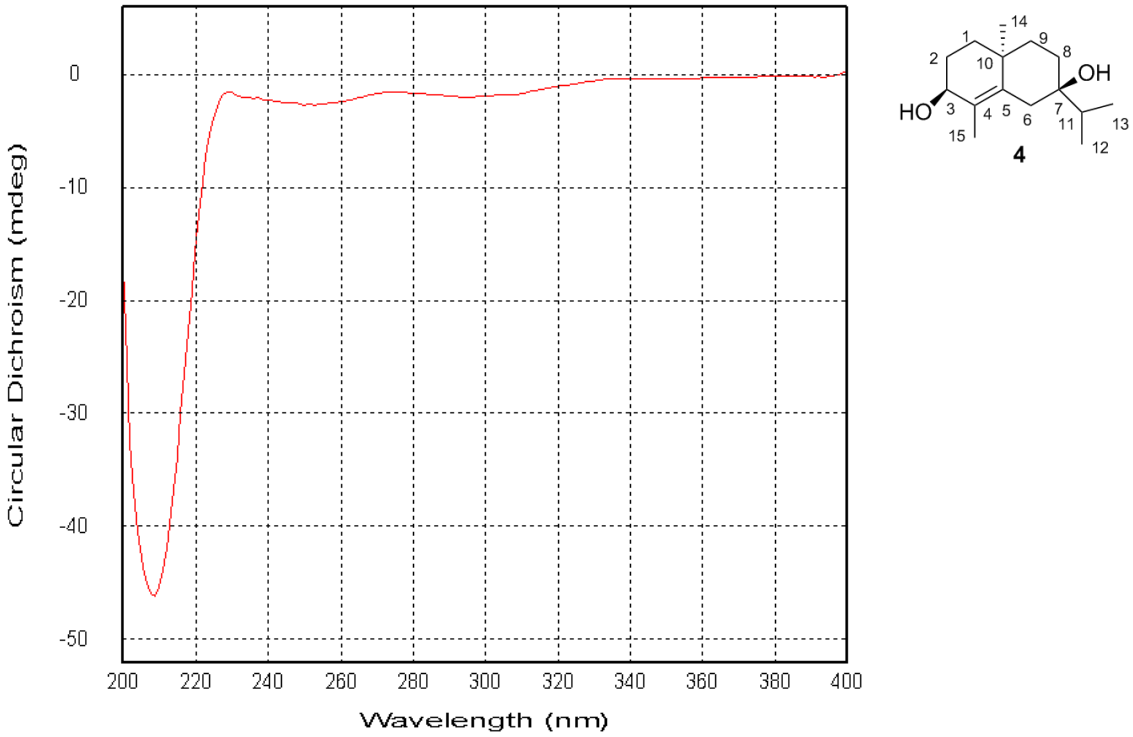


Figure S40. ECD spectrum of **4**.

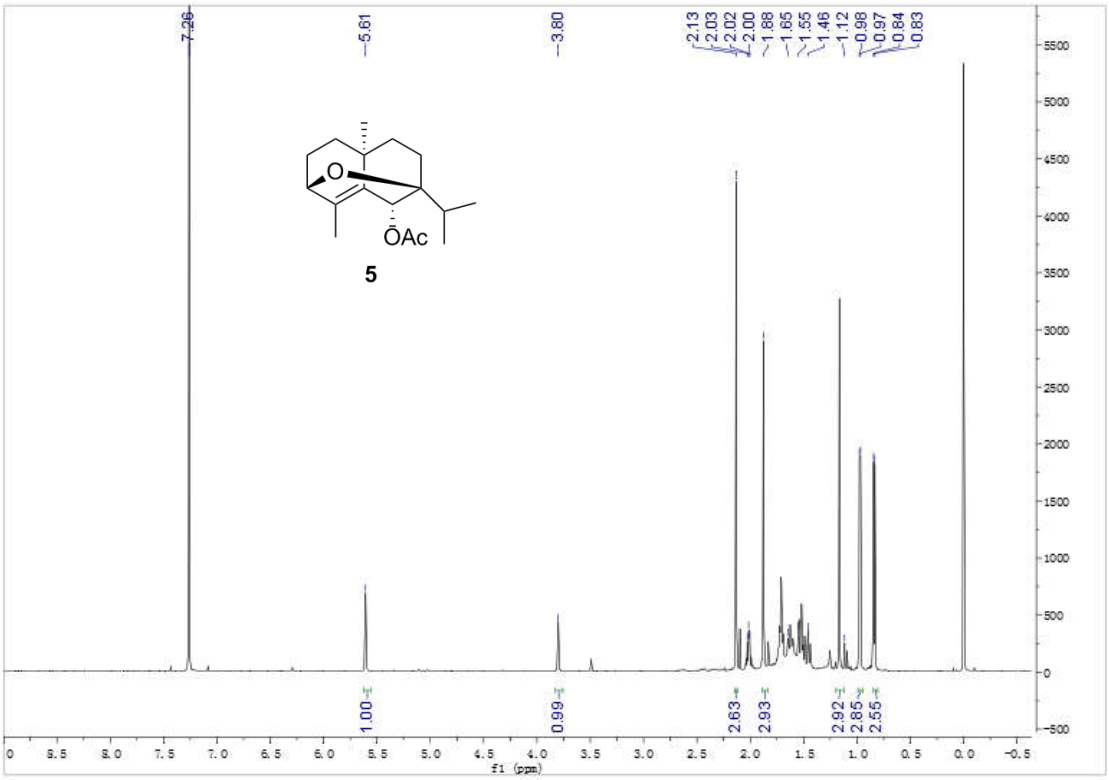


Figure S41. ^{1}H NMR spectrum (600 MHz) of **5** in $CDCl_3$.

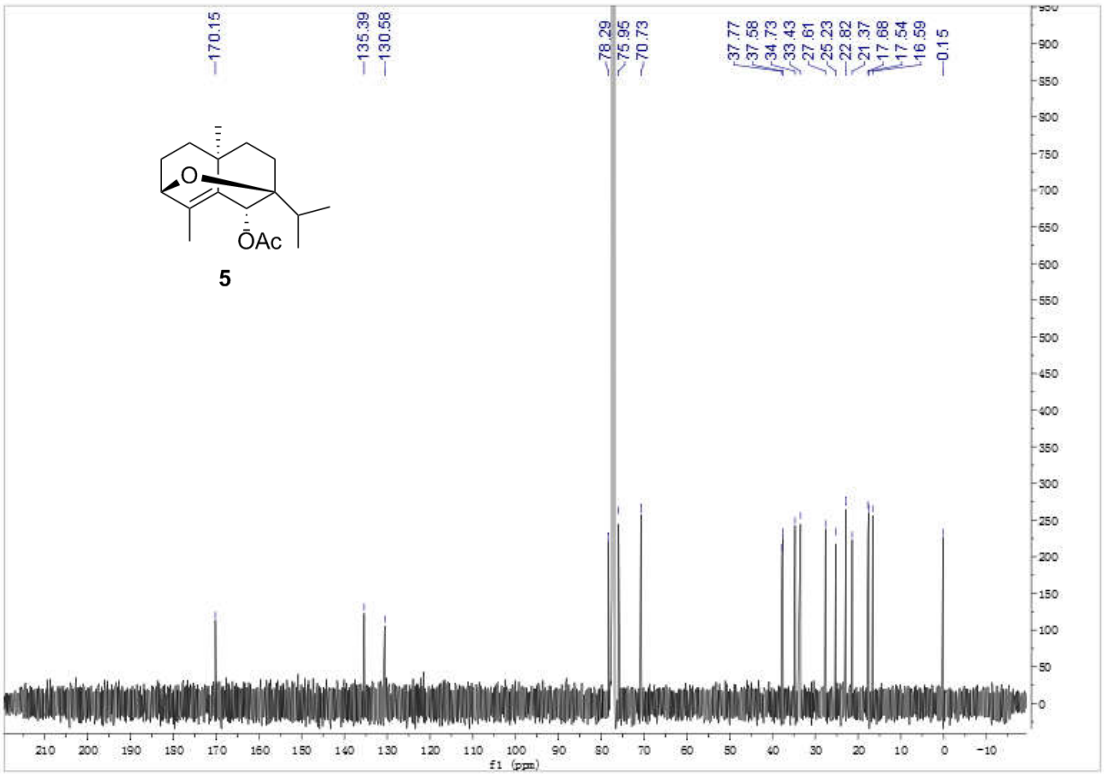


Figure S42. ^{13}C NMR spectrum (150 MHz) of **5** in $CDCl_3$.

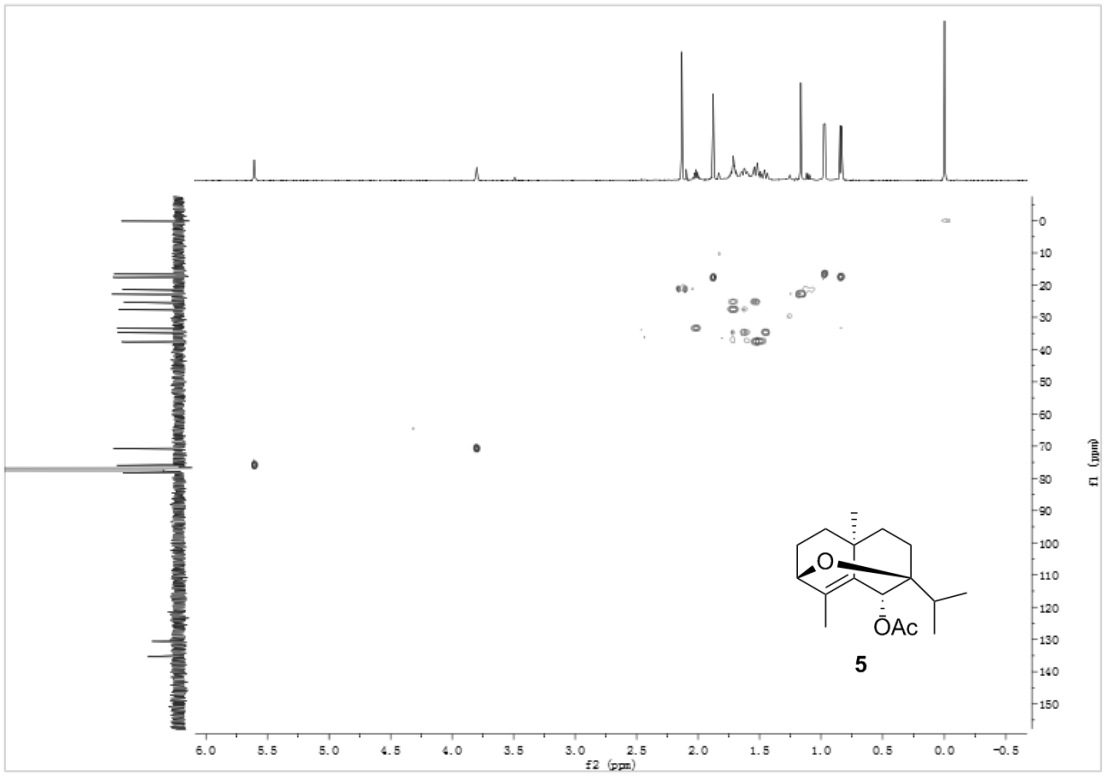


Figure S43. HSQC spectrum (600 MHz) of **5** in $CDCl_3$.

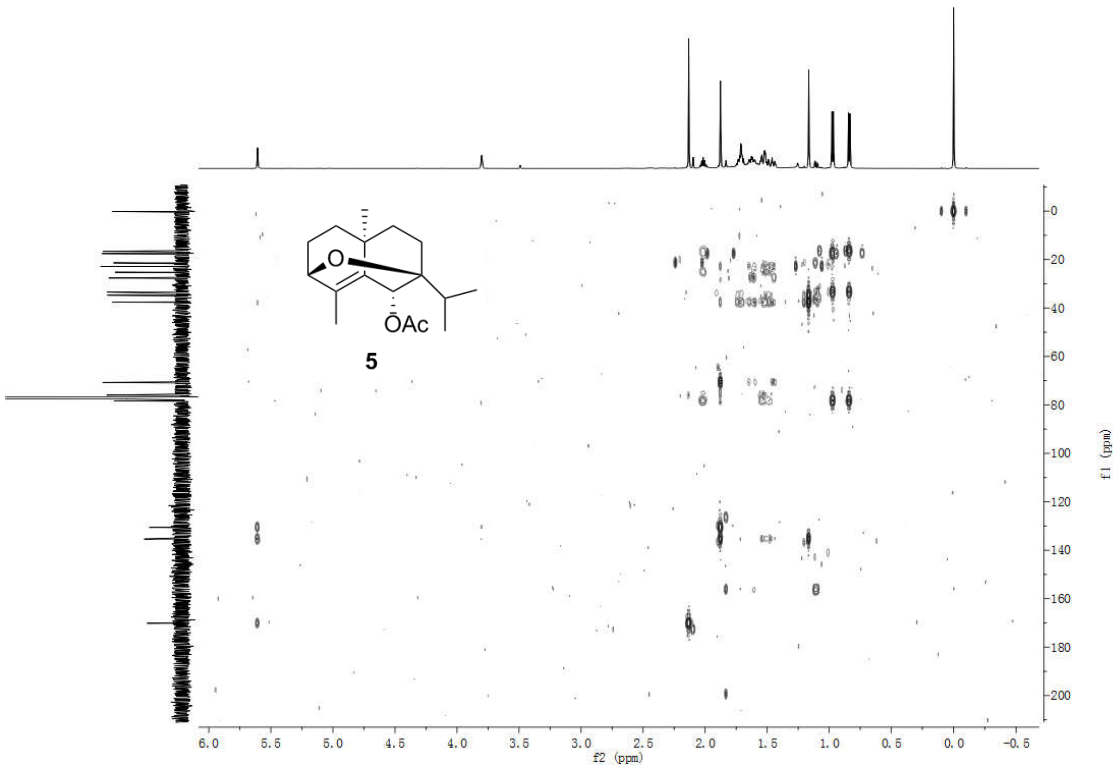


Figure S44. HMBC spectrum (600 MHz) of **5** in $CDCl_3$.

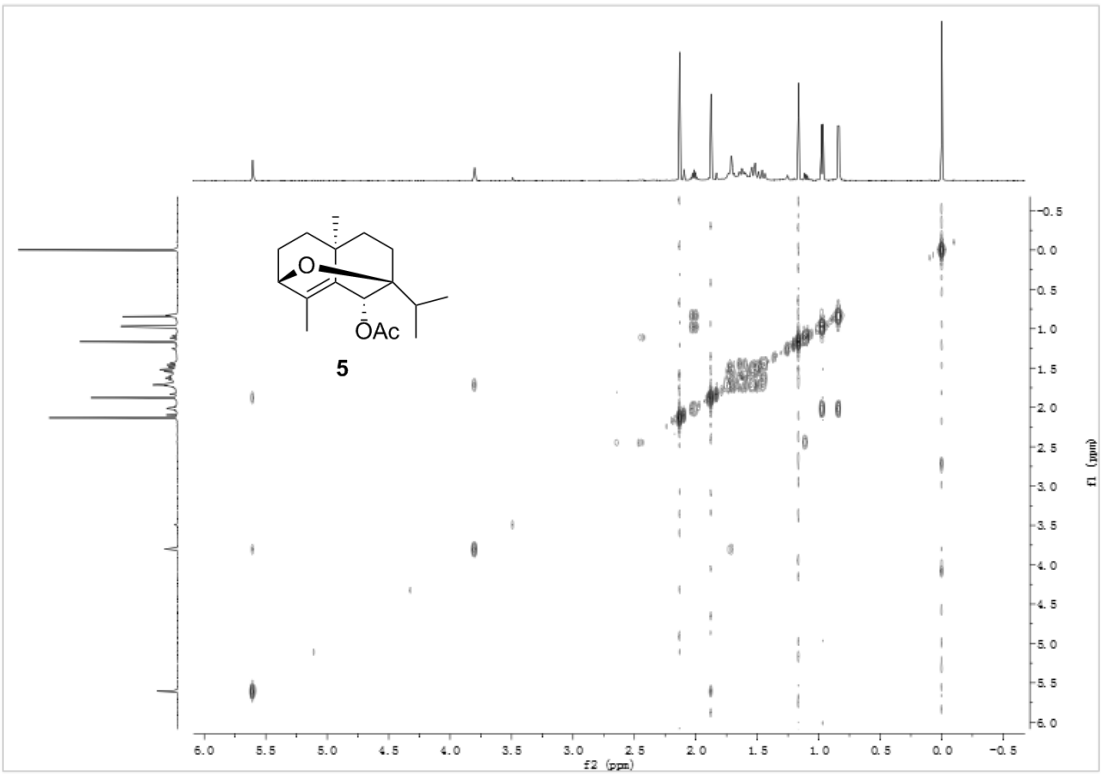


Figure S45. ^{1}H-^{1}H COSY spectrum (600 MHz) of **5** in $CDCl_3$.

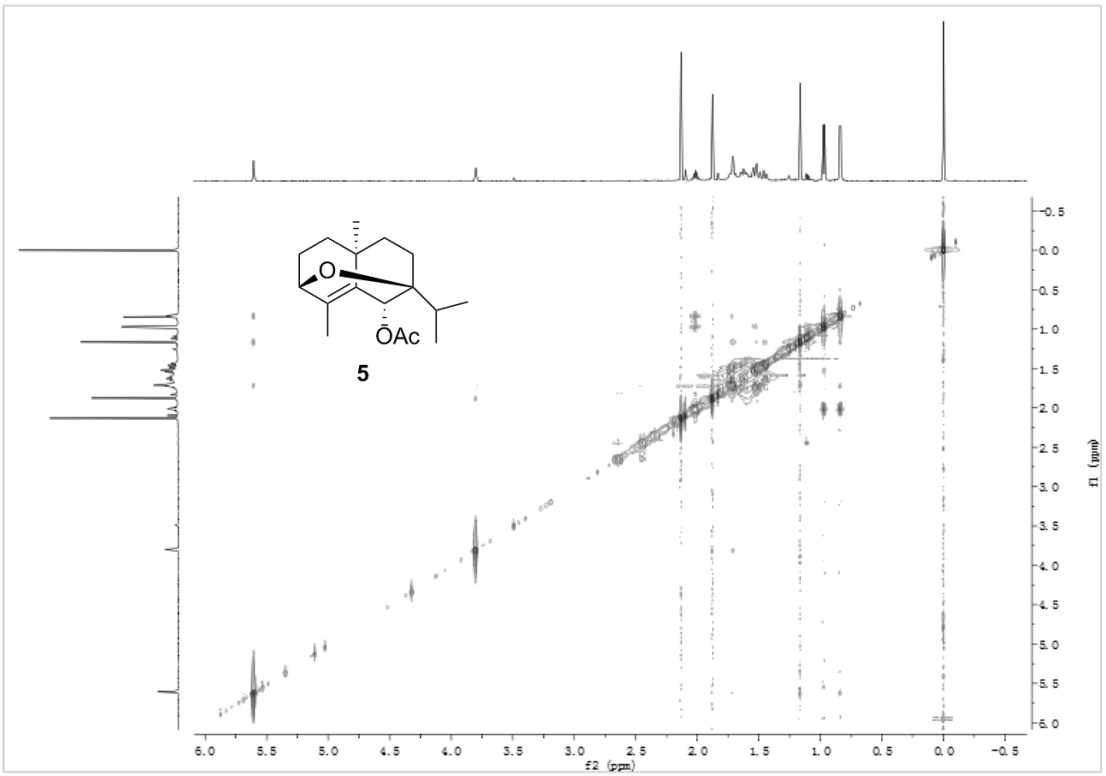


Figure S46. NOESY spectrum (600 MHz) of **5** in $CDCl_3$.

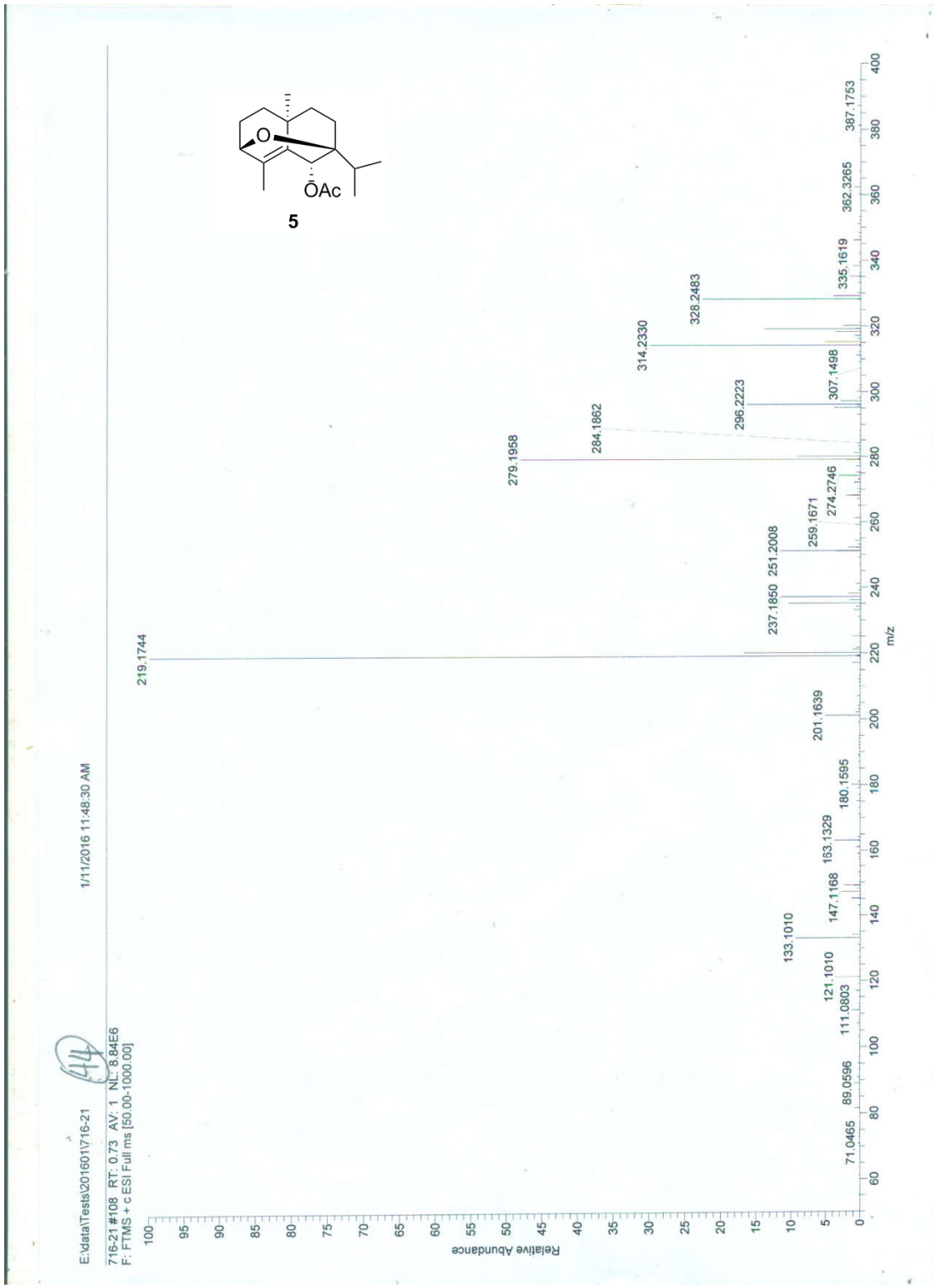


Figure S47. HRESIMS spectrum of **5**.

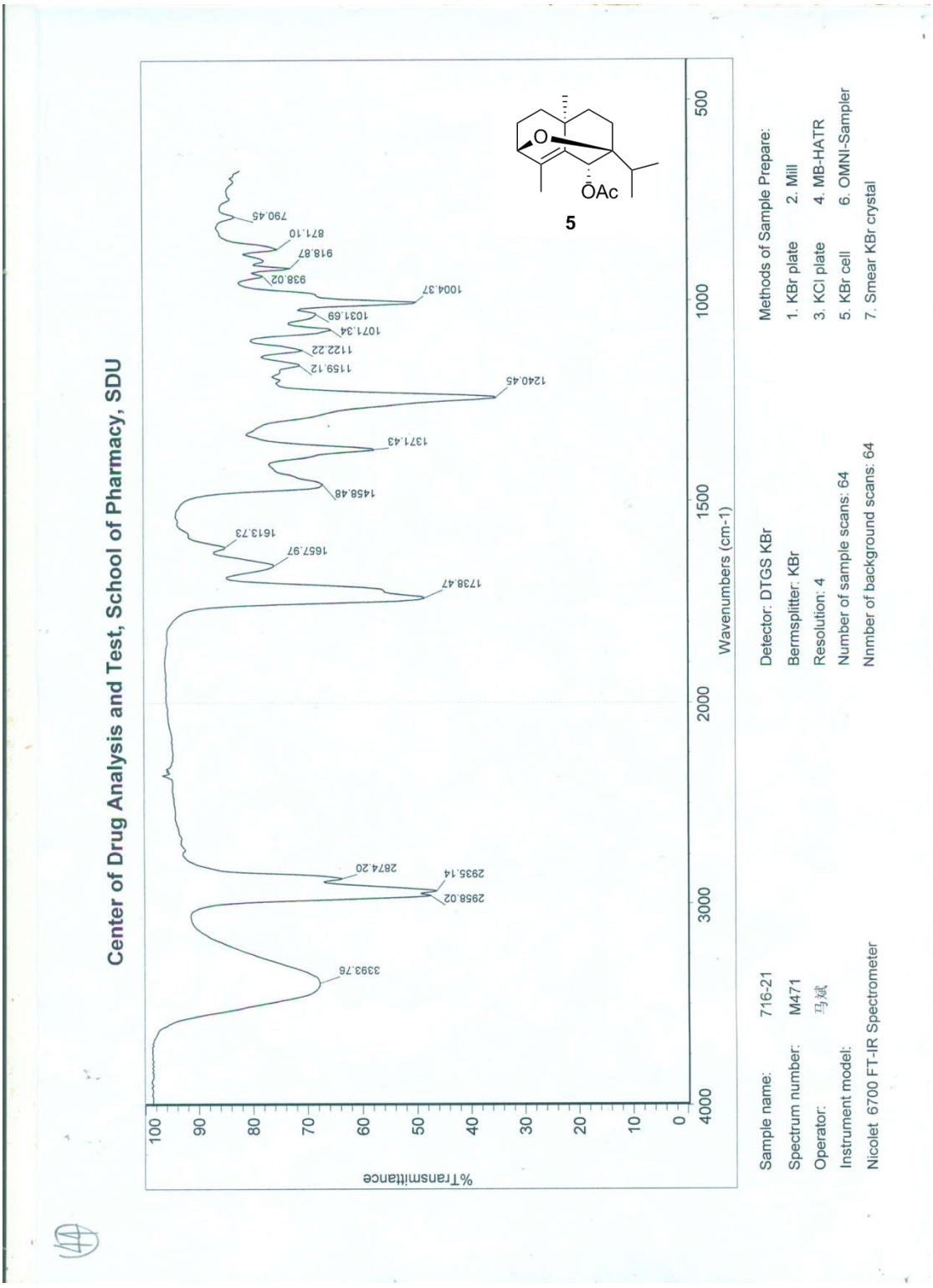


Figure S48. IR (KBr disc) spectrum of **5**.

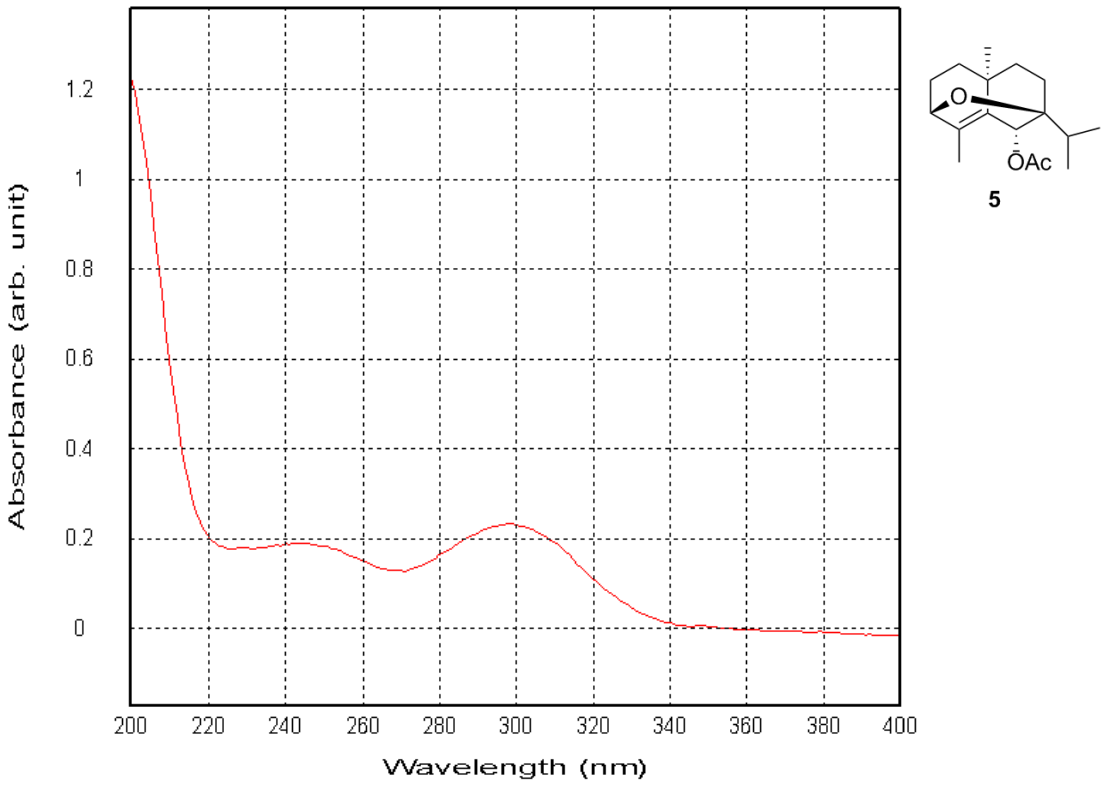


Figure S49. UV spectrum of **5**.

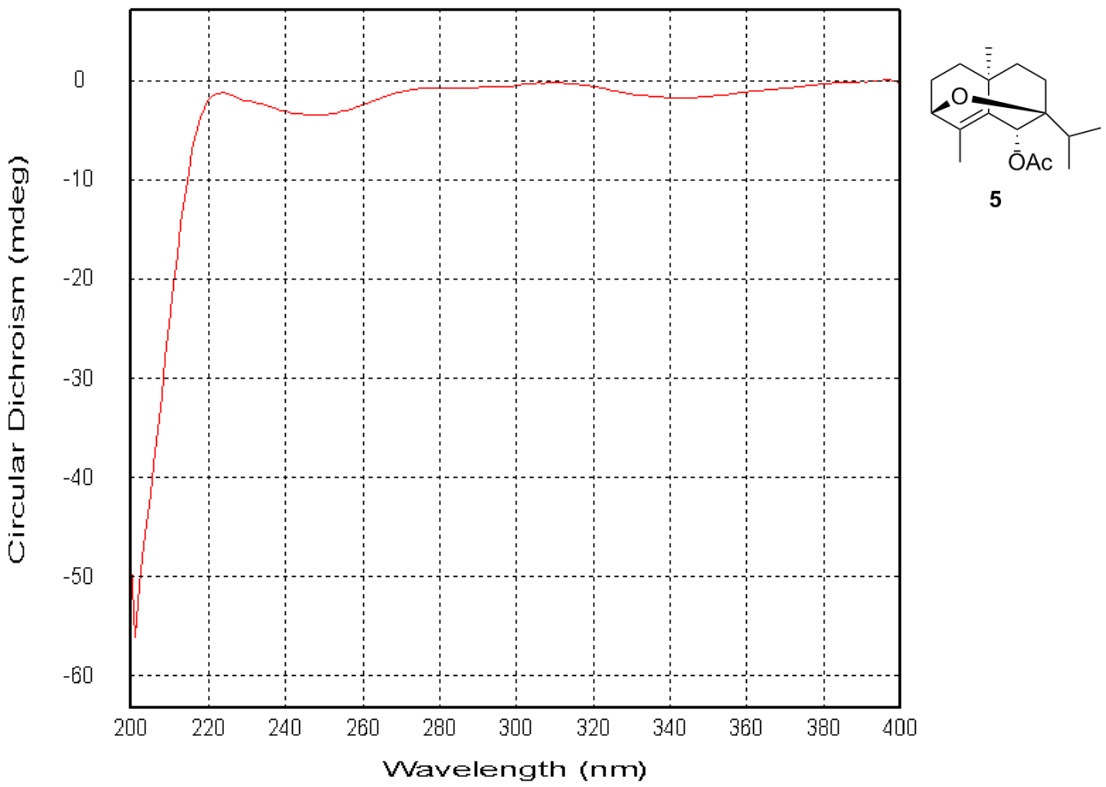


Figure S50. ECD spectrum of **5**.

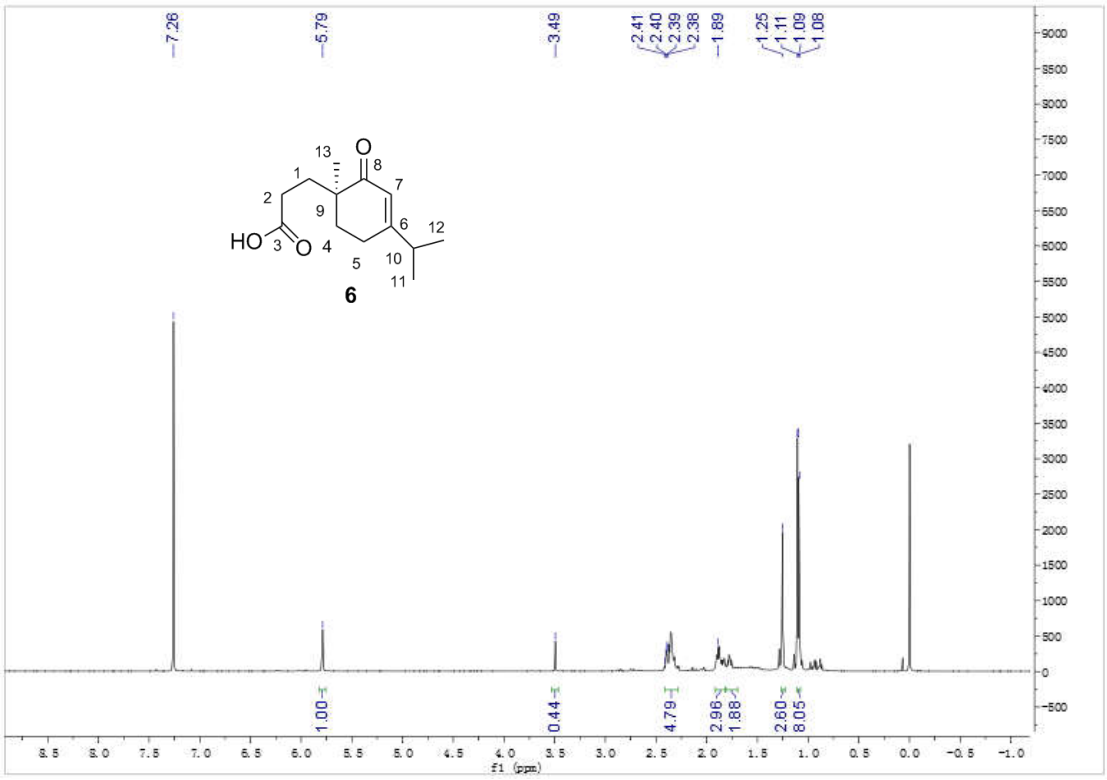


Figure S51. ^{1}H NMR spectrum (600 MHz) of **6** in $CDCl_3$.

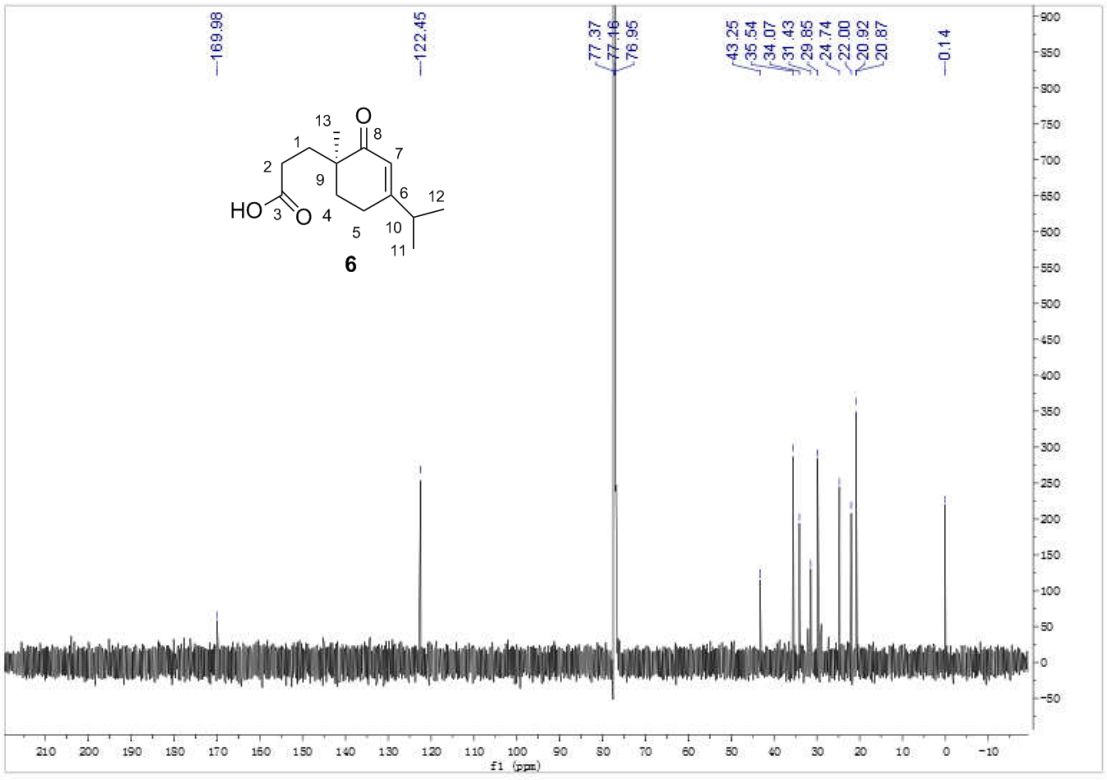


Figure S52. ^{13}C NMR spectrum (150 MHz) of **6** in $CDCl_3$.

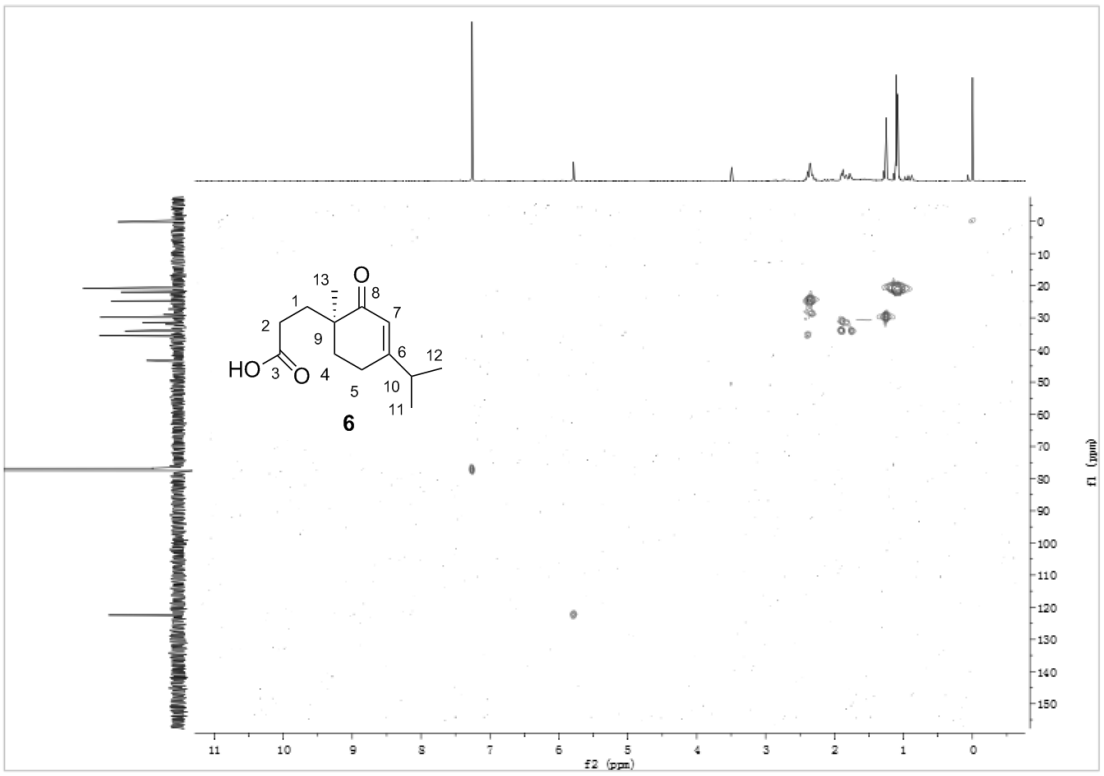


Figure S53. HSQC spectrum (600 MHz) of **6** in $CDCl_3$.

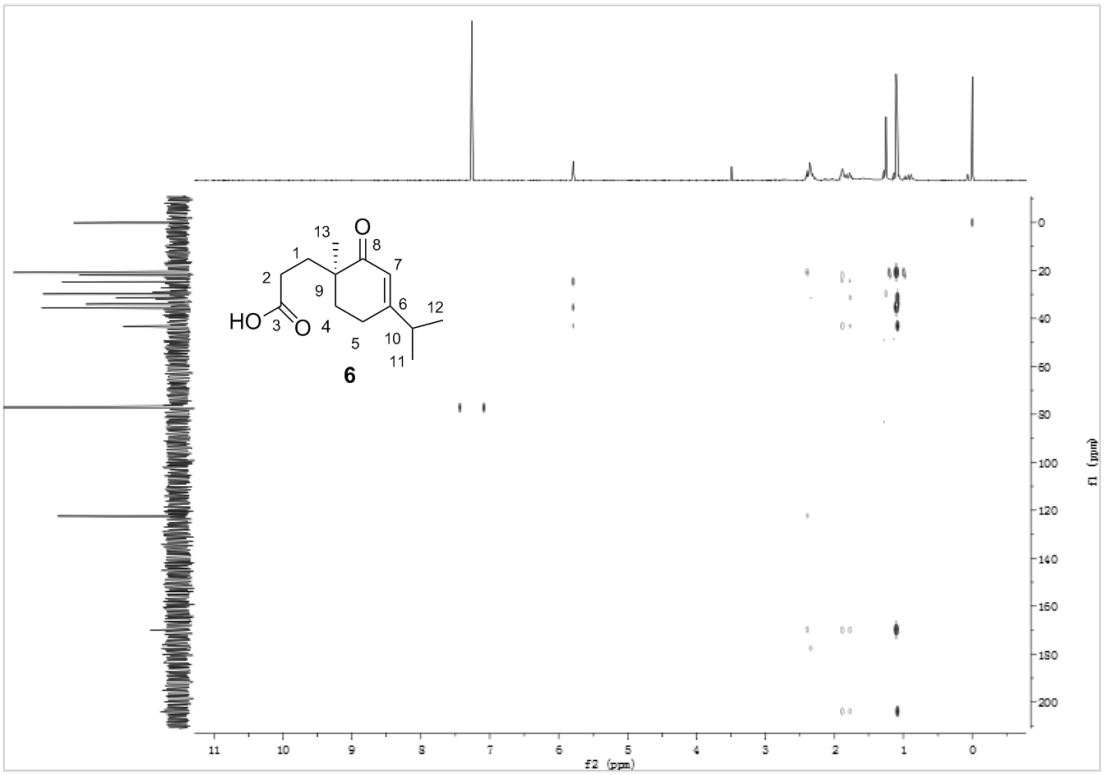


Figure S54. HMBC spectrum (600 MHz) of **6** in $CDCl_3$.

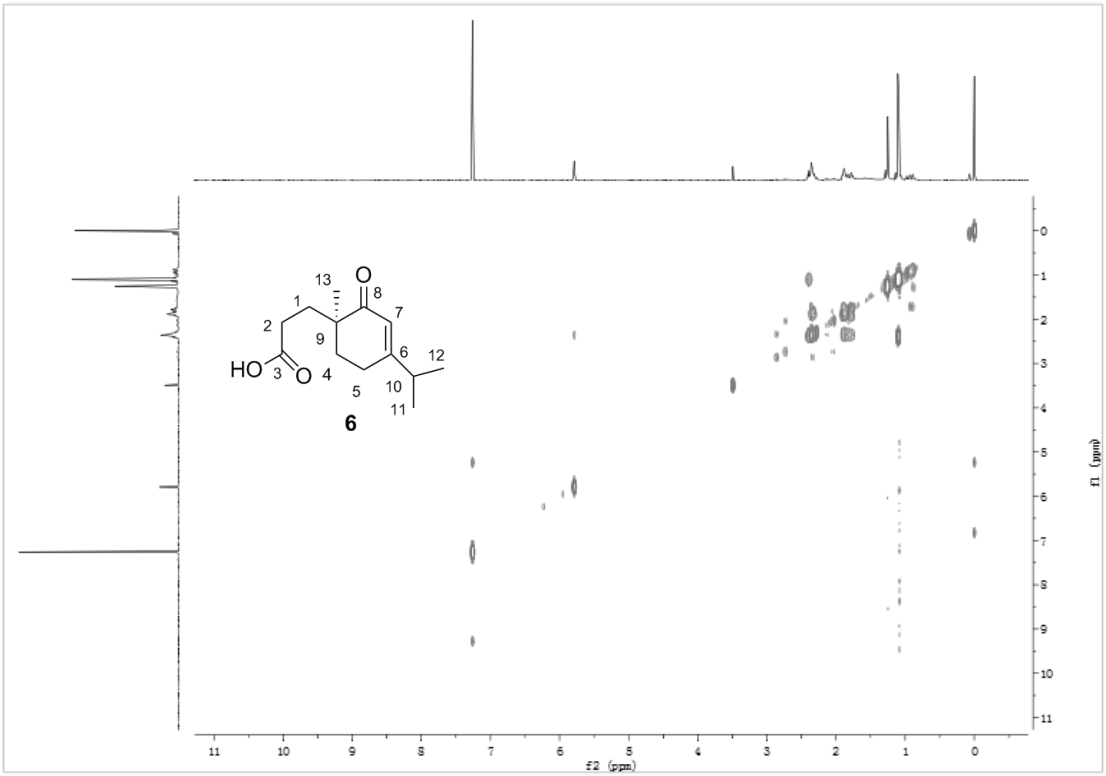


Figure S55. ^{1}H-^{1}H COSY spectrum (600 MHz) of **6** in $CDCl_3$.

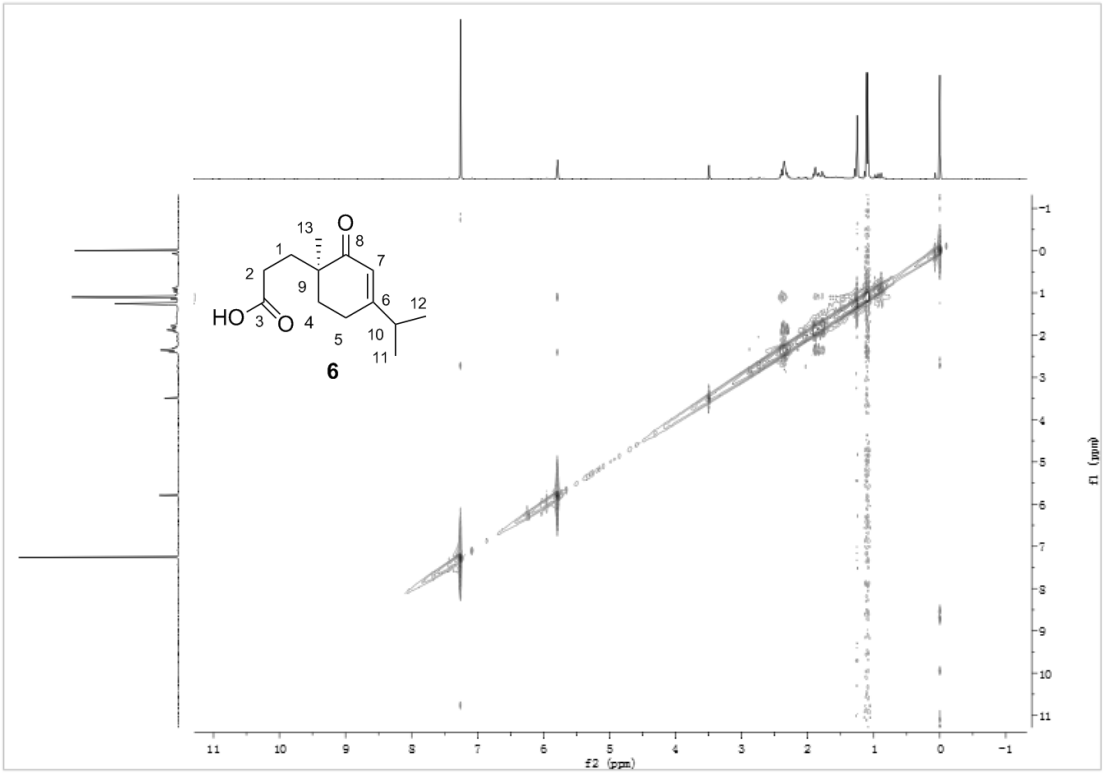


Figure S56. NOESY spectrum (600 MHz) of **6** in $CDCl_3$.

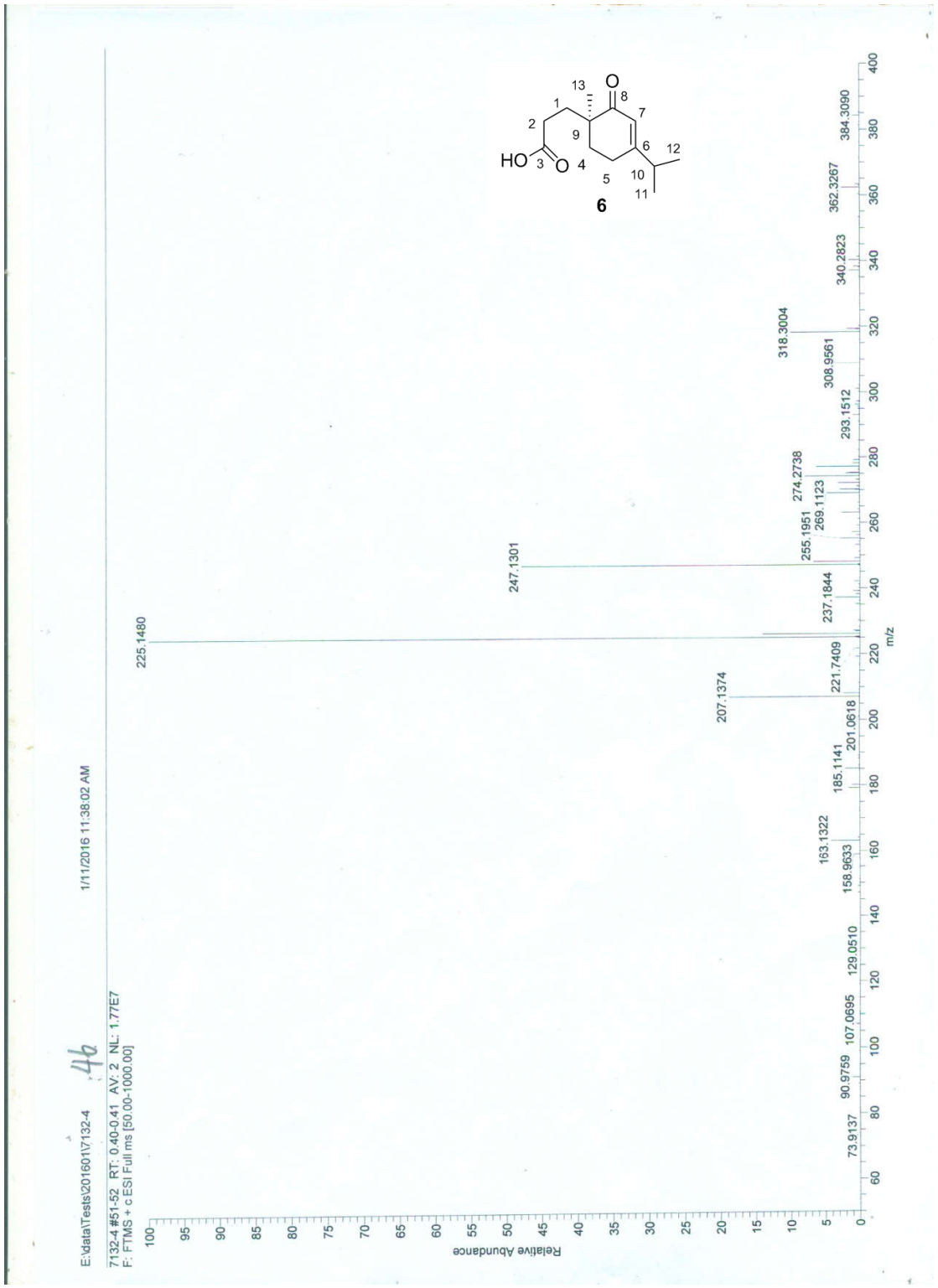


Figure S57. HRESIMS spectrum of **6**.

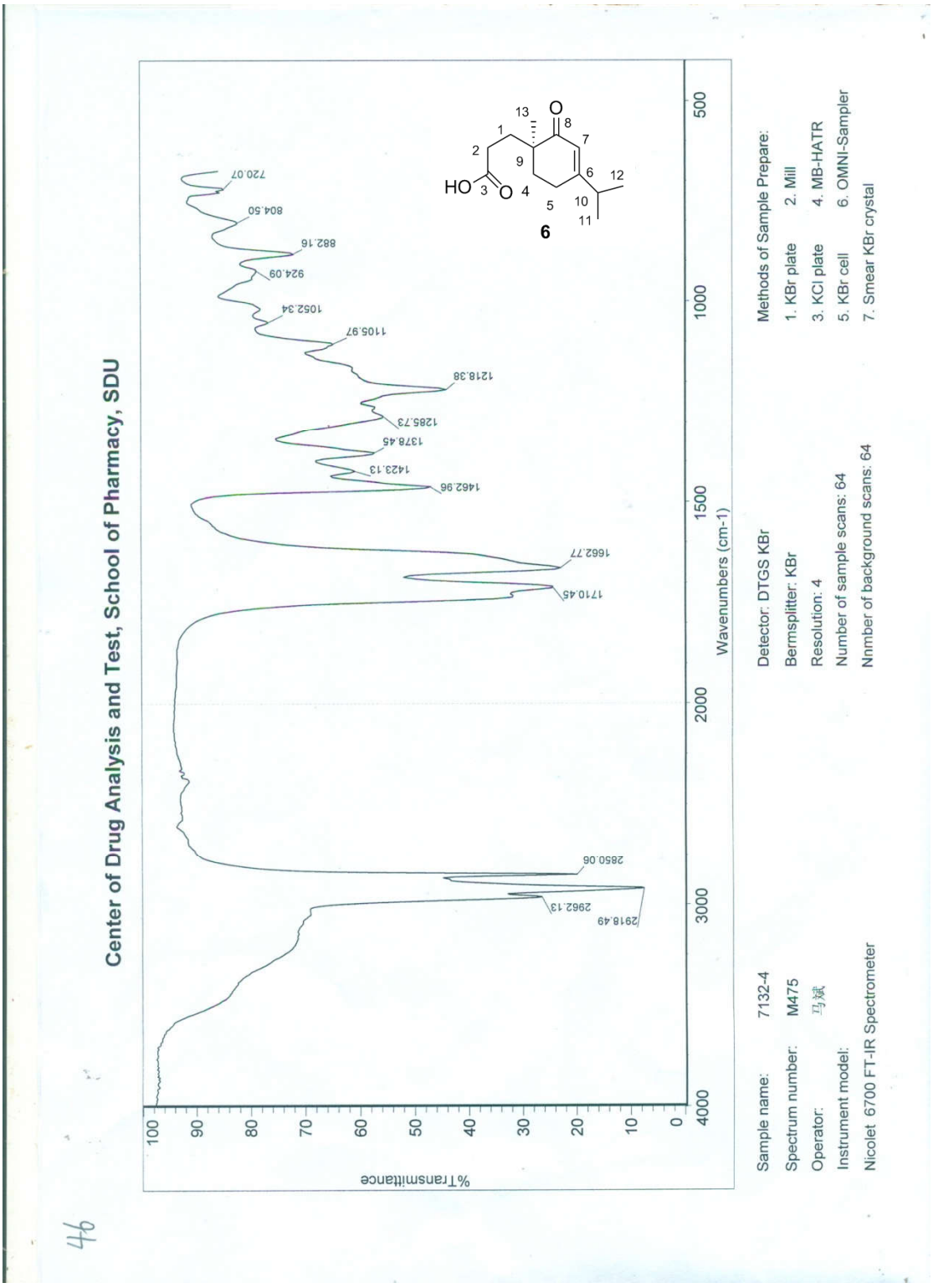


Figure S58. IR (KBr disc) spectrum of **6**.

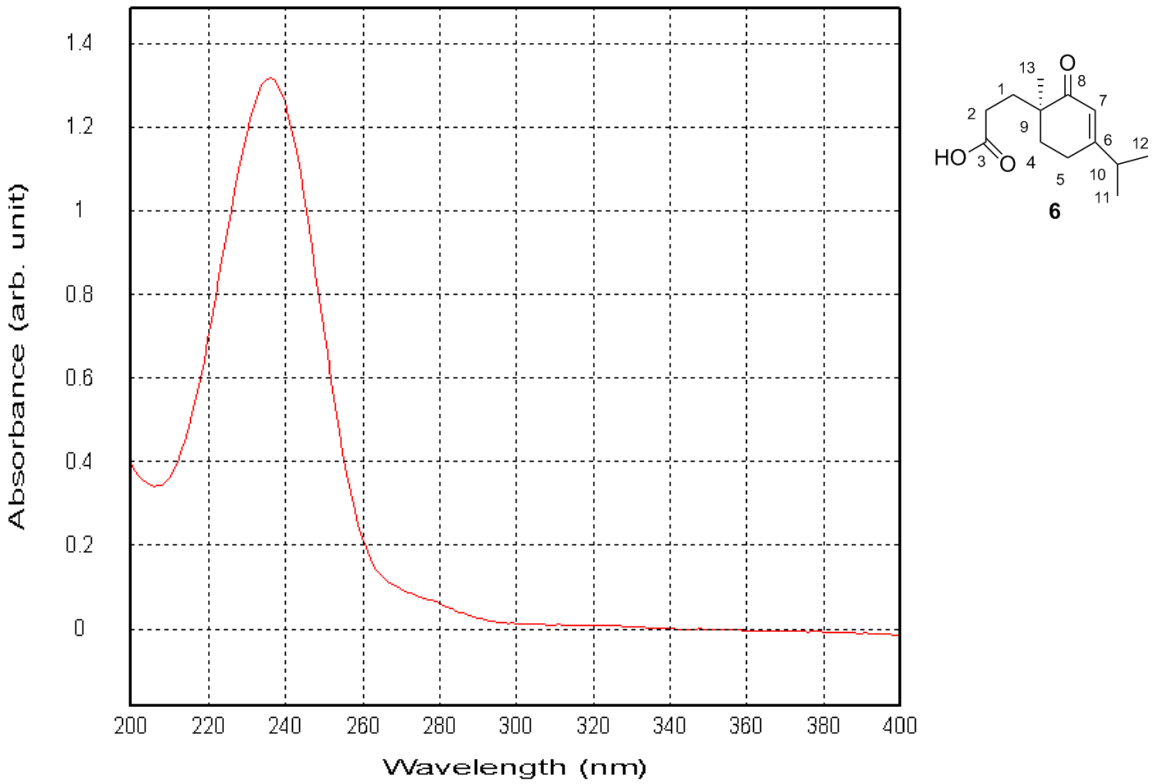


Figure S59. UV spectrum of **6**.

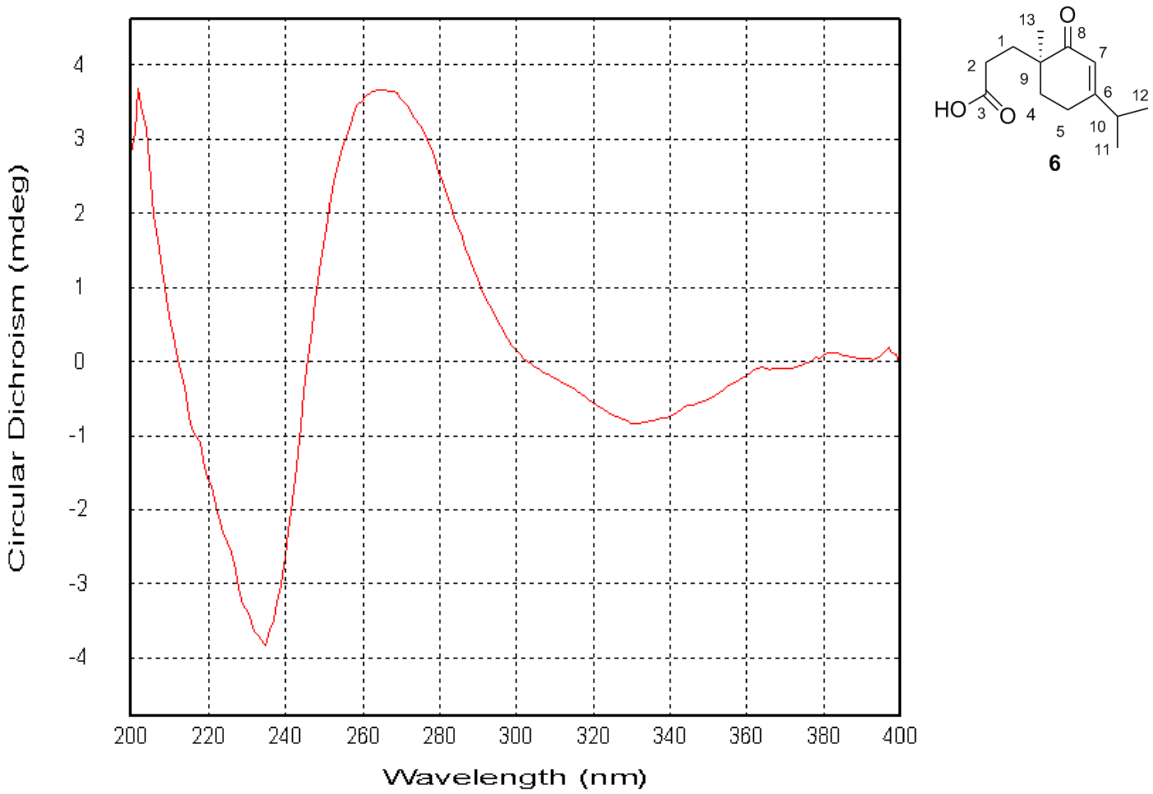


Figure S60. ECD spectrum of **6**.

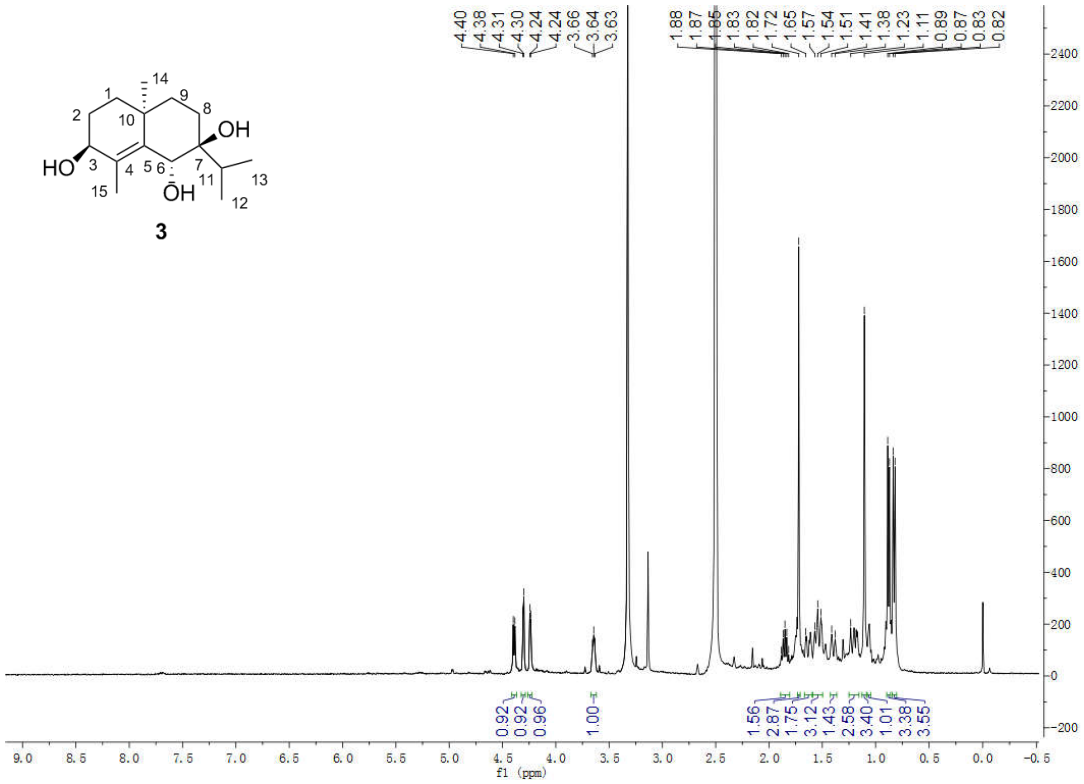


Figure S61. ^{1}H NMR spectrum (400 MHz) of **3** in DMSO-d_6.

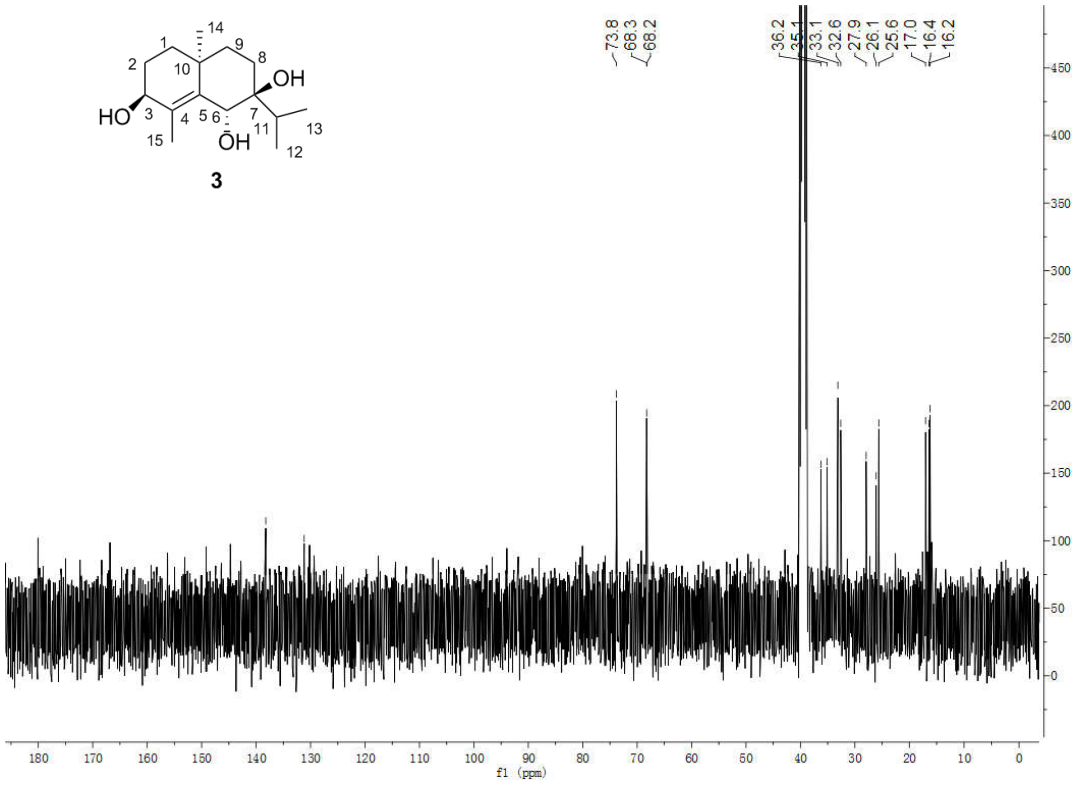


Figure S62. ^{13}C NMR spectrum (100 MHz) of **3** in DMSO-d_6.

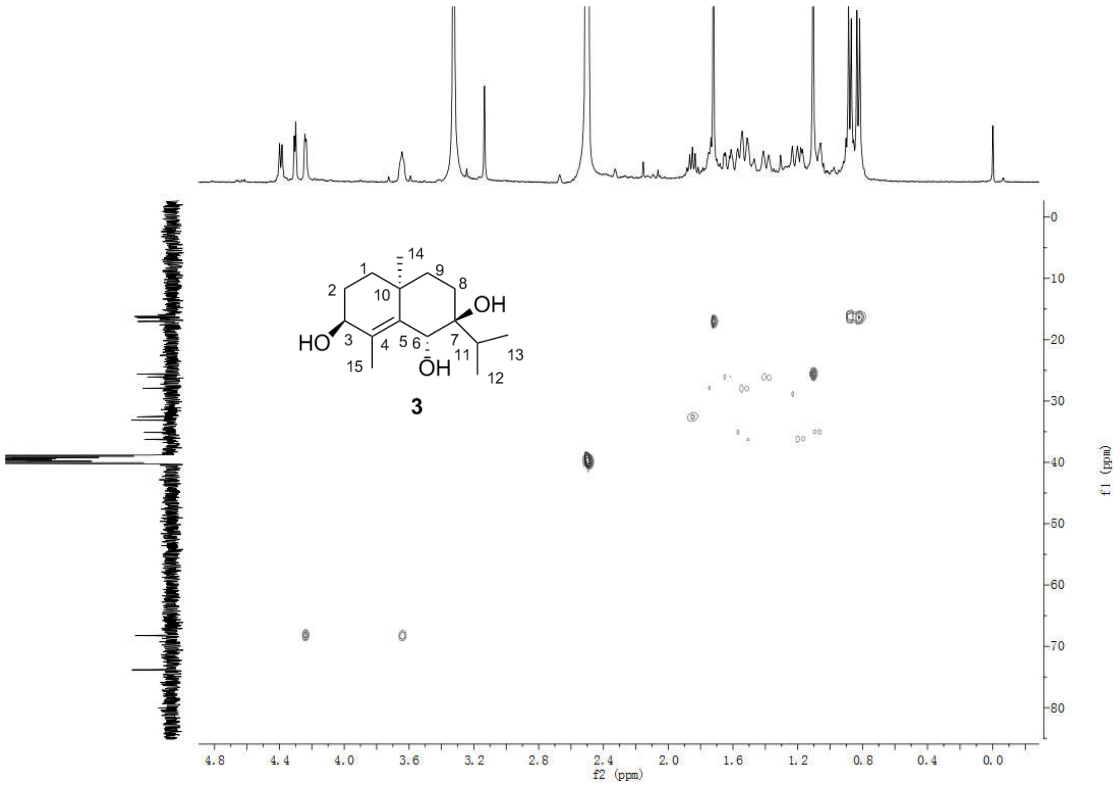


Figure S63. HSQC spectrum (400 MHz) of **3** in DMSO-d_6.

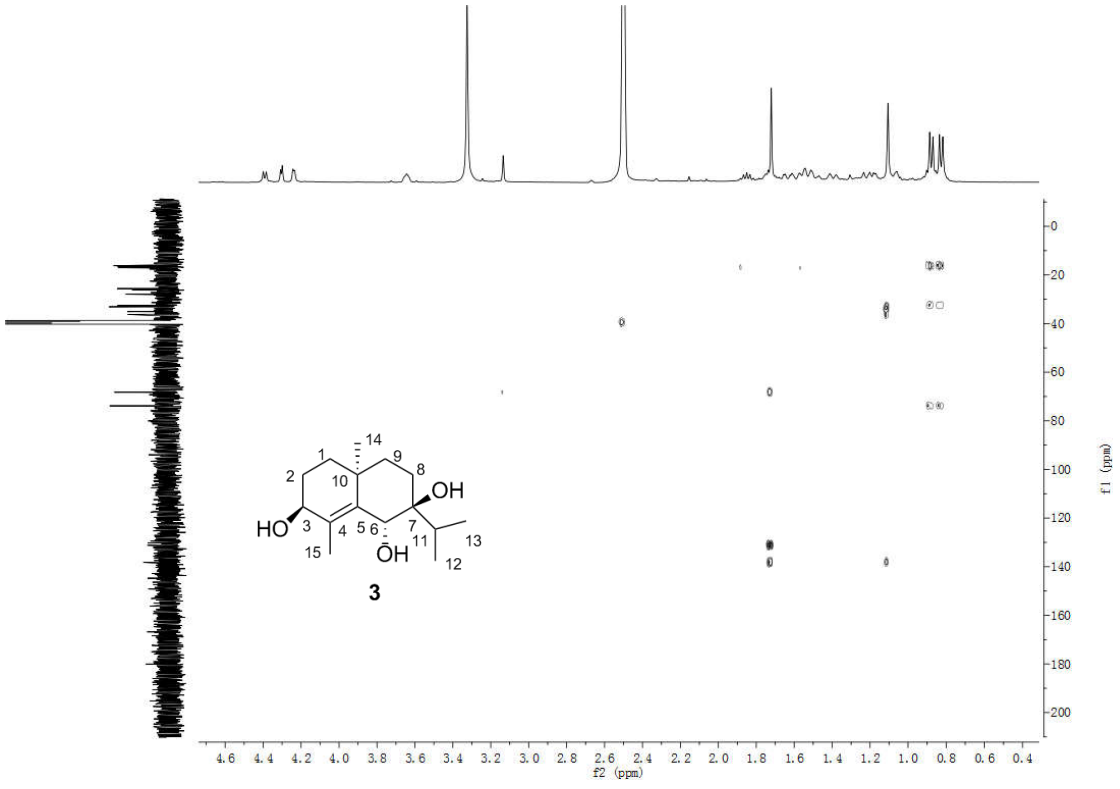


Figure S64. HMBC spectrum (400 MHz) of **3** in DMSO-d_6.

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