

Supplementary Materials: *ent*-Pimarane and *ent*-Kaurane Diterpenes from *Aldama discolor* (Asteraceae) and Their Antiprotozoal Activity

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1. Supporting Information

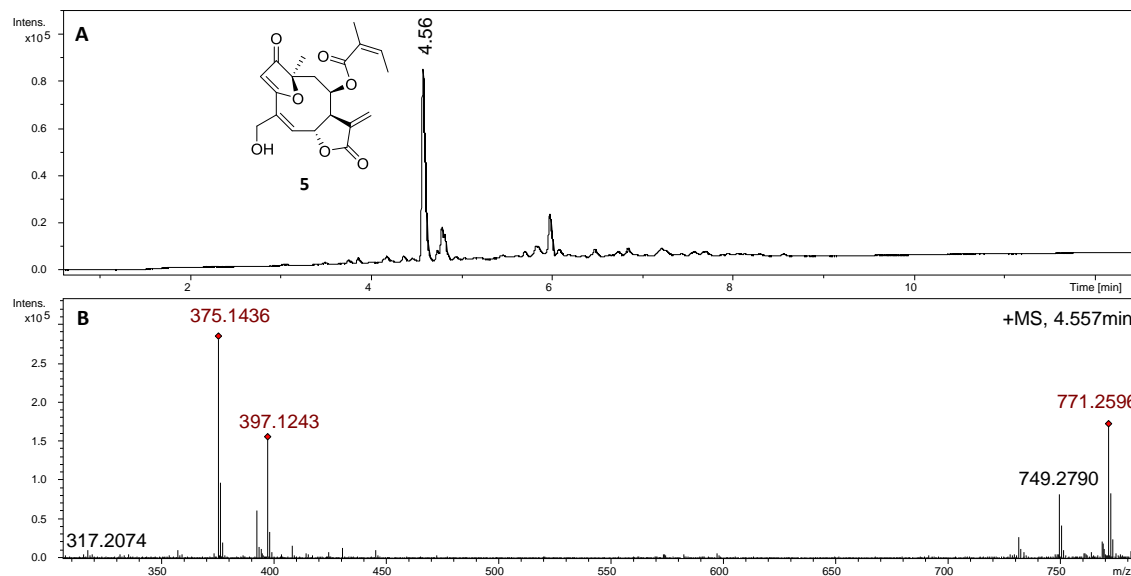


Figure S1. (A) LC-MS-chromatogram of the last fraction (elution with EtOAc) of the CC on silica gel of the dichloromethane extract of *A. discolor* leaves; (B) +ESI-MS of its major compound, budlein A. $[M + H]^+$: 375.1436 ($C_{20}H_{23}O_7$).

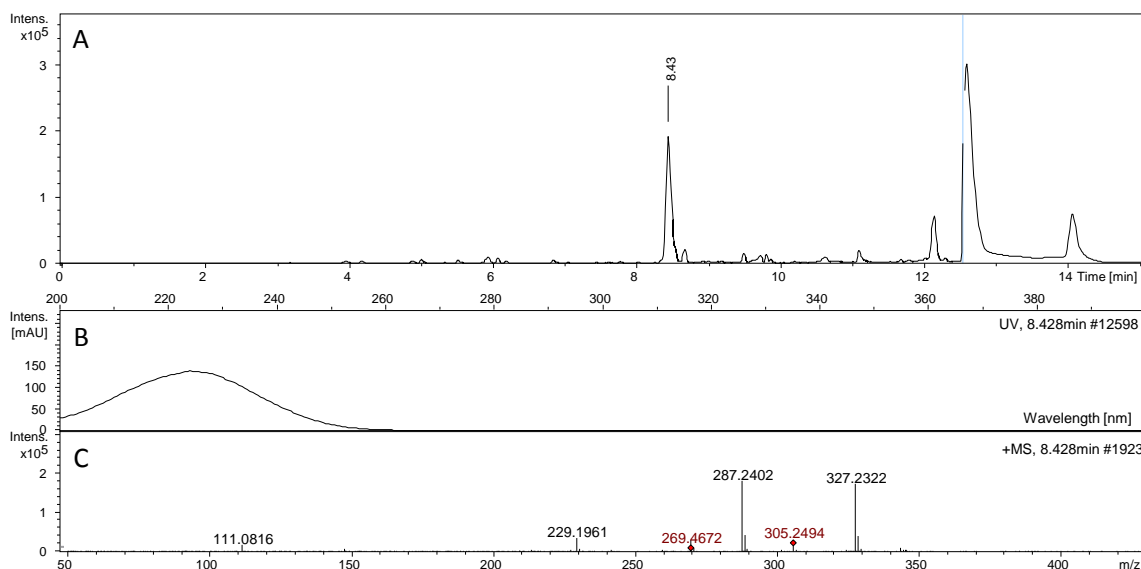


Figure S2. +ESI-QqTOF-MS chromatogram (A); UV spectrum (B); +ESI-MS (C) of compound 1, $[M + H]^+$: 305.2494 ($C_{20}H_{33}O_2$) and $[M + Na]^+$: 327.2322 ($C_{20}H_{32}O_2Na$). Internal calibrant sodium formate: 12.6 min.

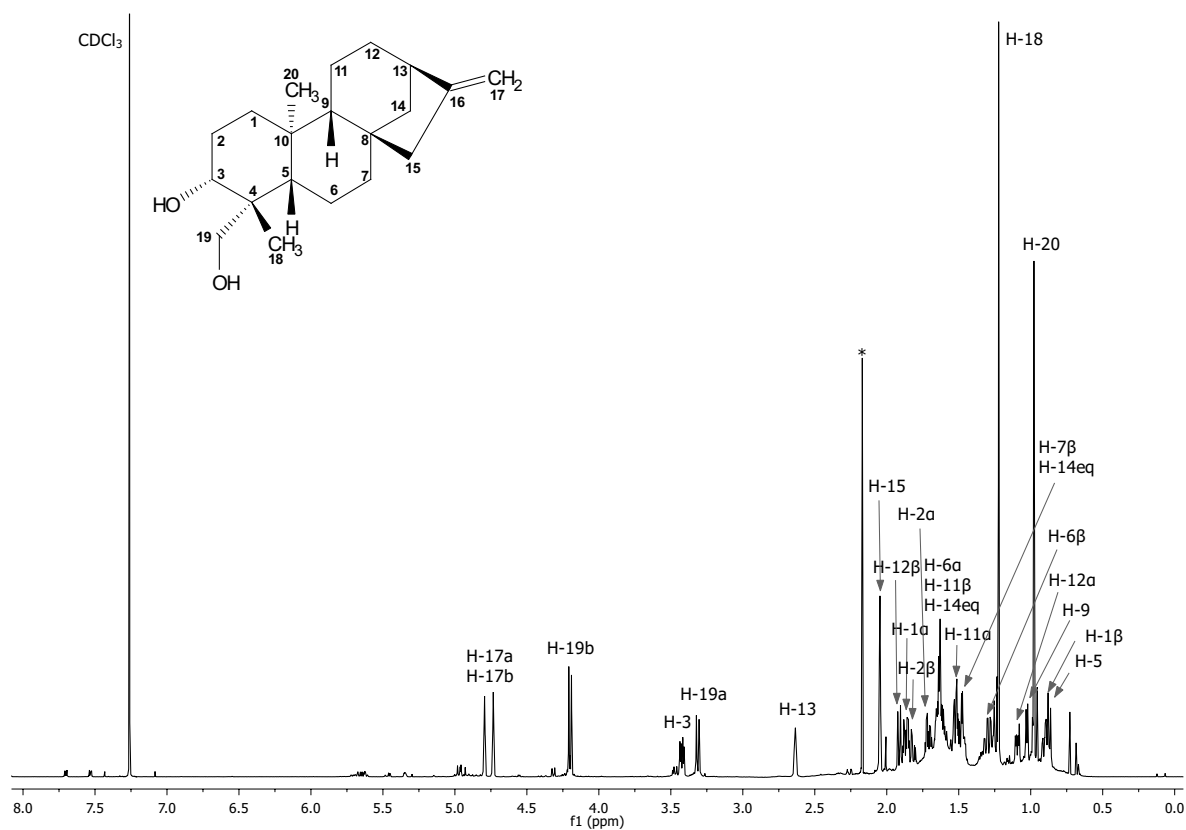


Figure S3. ^1H NMR spectrum of compound 1 (CDCl_3 , 600 MHz). *- CH_3 protons from acetone.

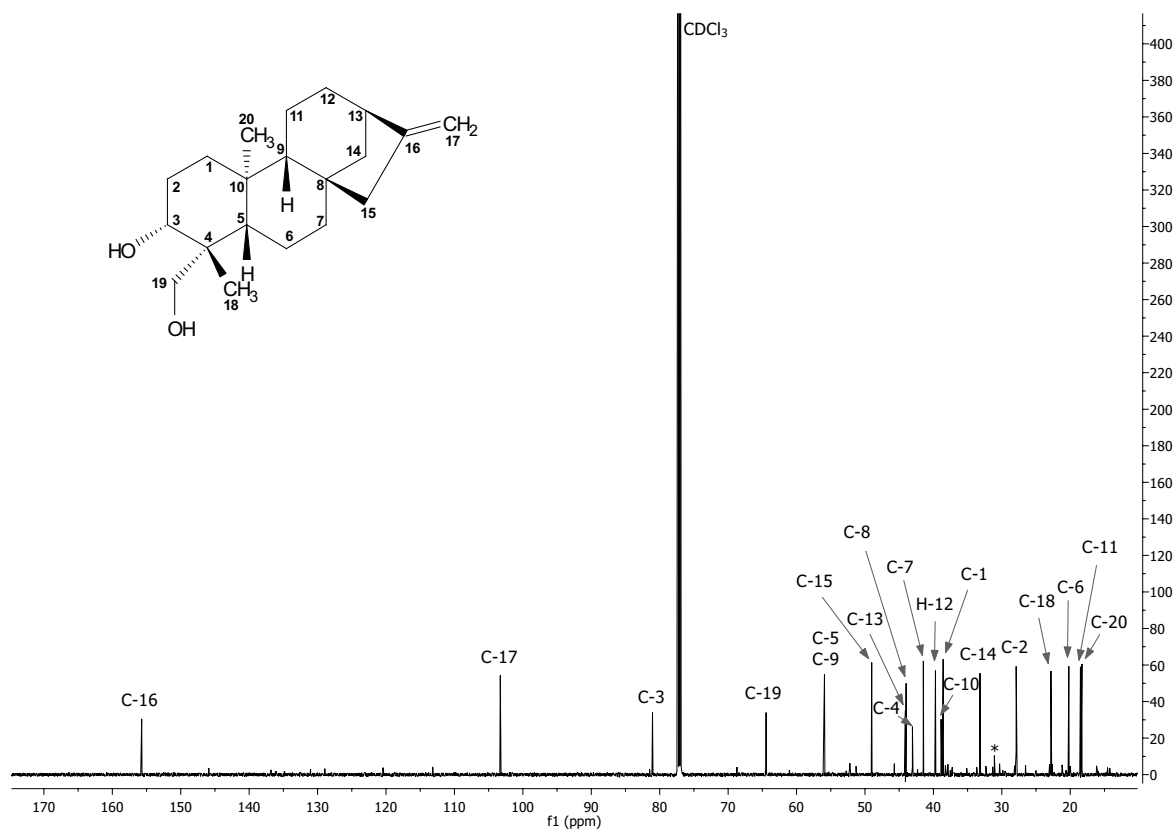


Figure S4. ^{13}C NMR spectrum of compound 1 (CDCl_3 , 150 MHz). *- CH_3 from acetone.

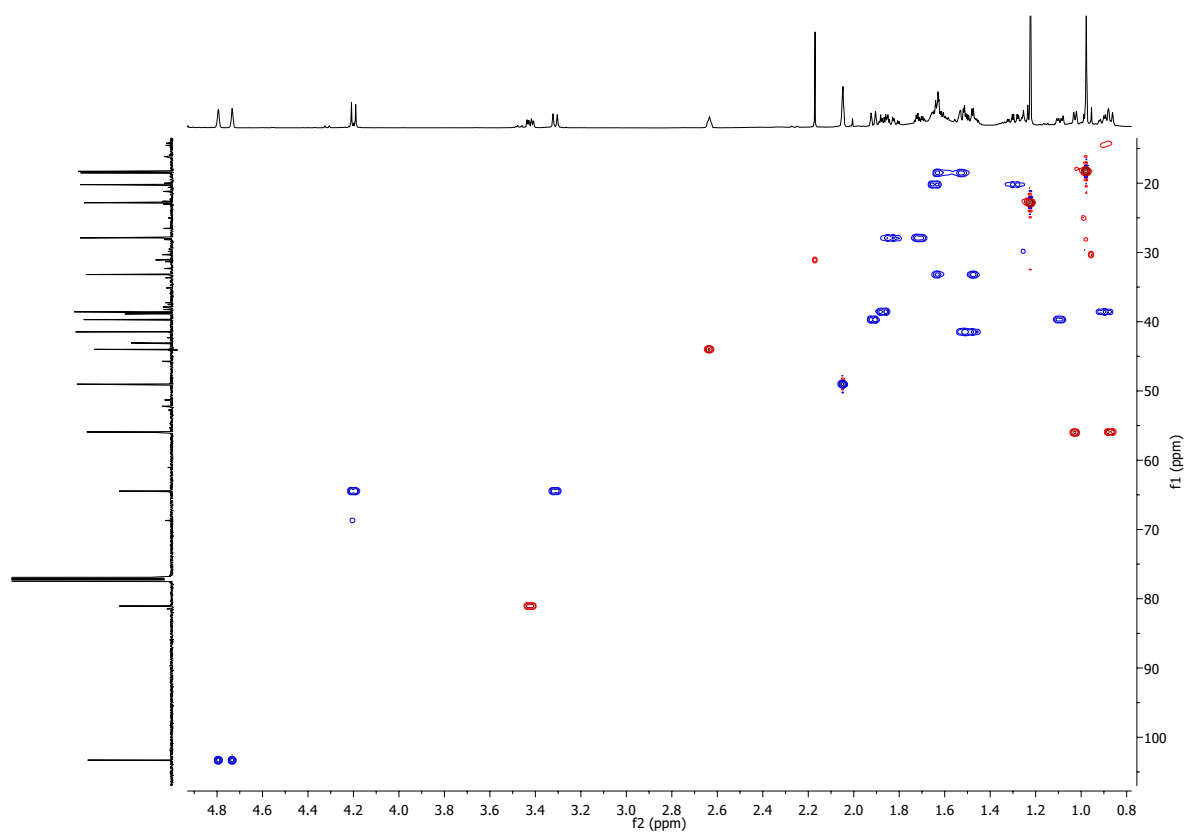


Figure S5. $^1\text{H}/^{13}\text{C}$ -HSQC spectrum of compound **1** (600/150 MHz, CDCl_3).

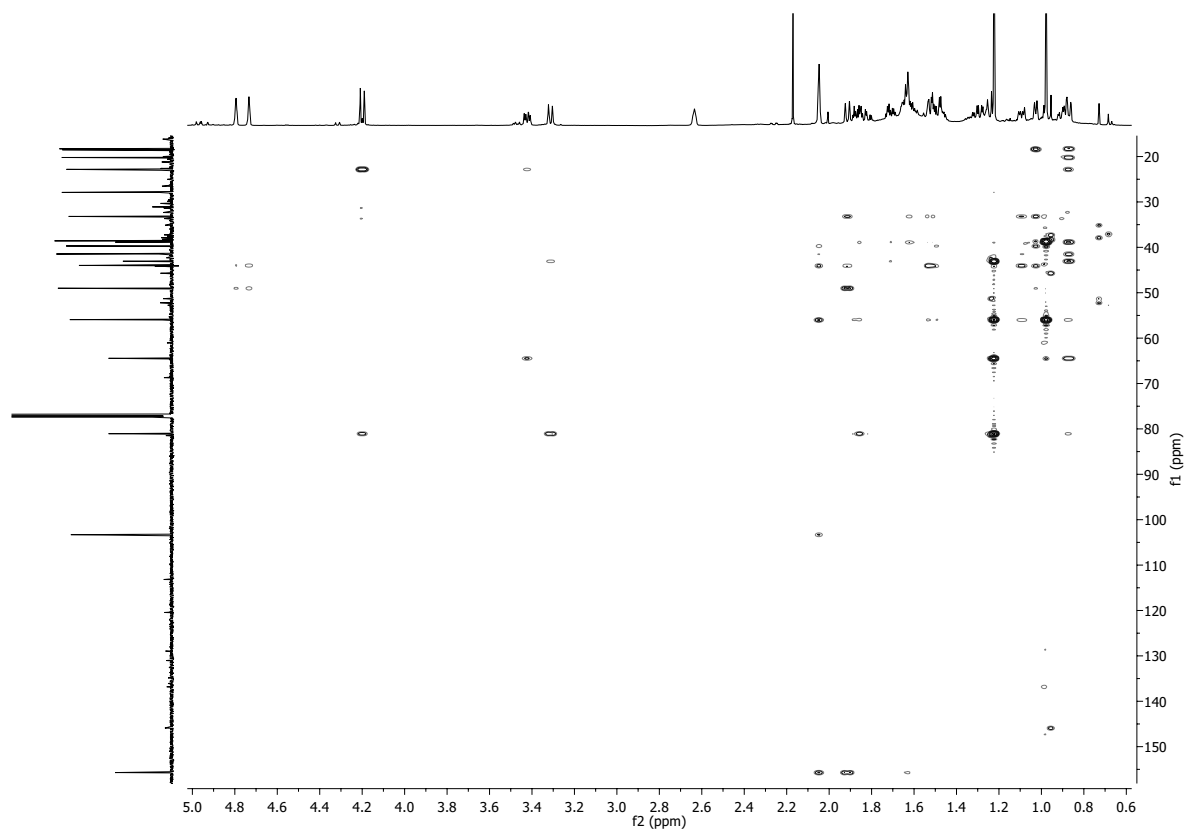


Figure S6. $^1\text{H}/^{13}\text{C}$ -HMBC spectrum of compound **1** (600/150 MHz, CDCl_3).

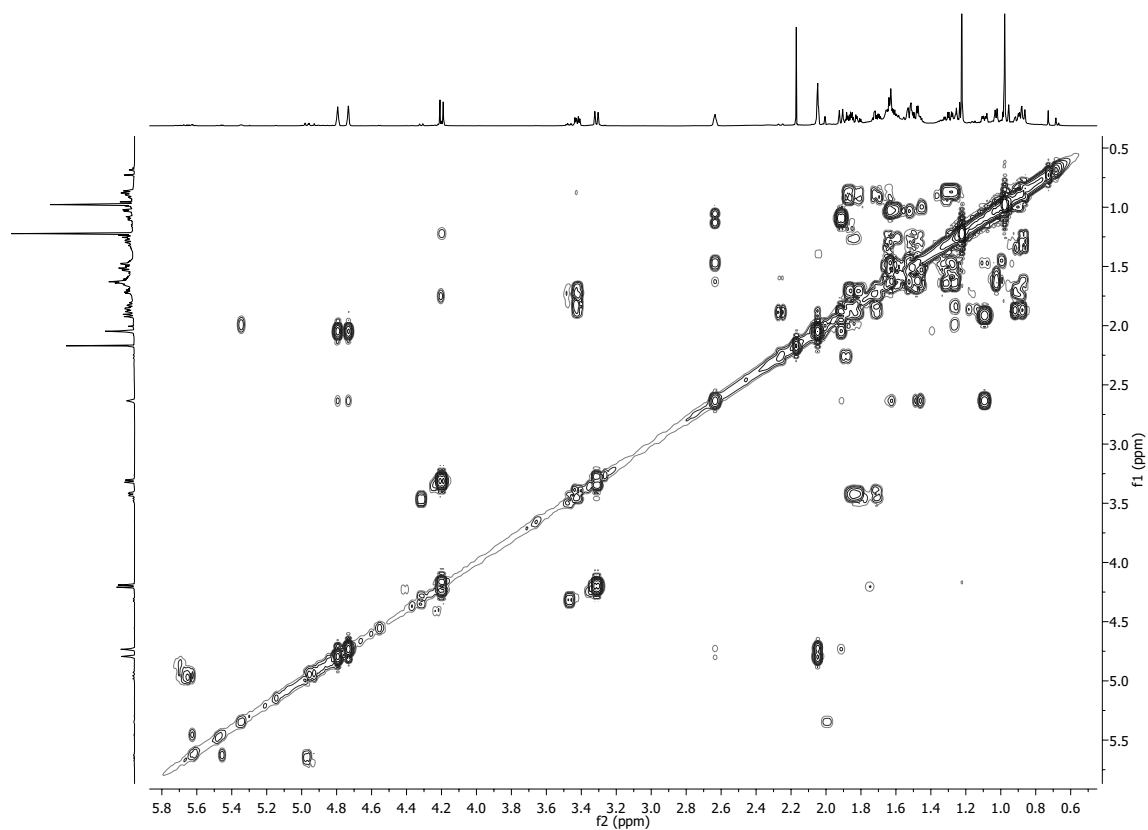


Figure S7. $^1\text{H}/^1\text{H}$ -COSY spectrum of compound 1 (600 MHz, CDCl_3).

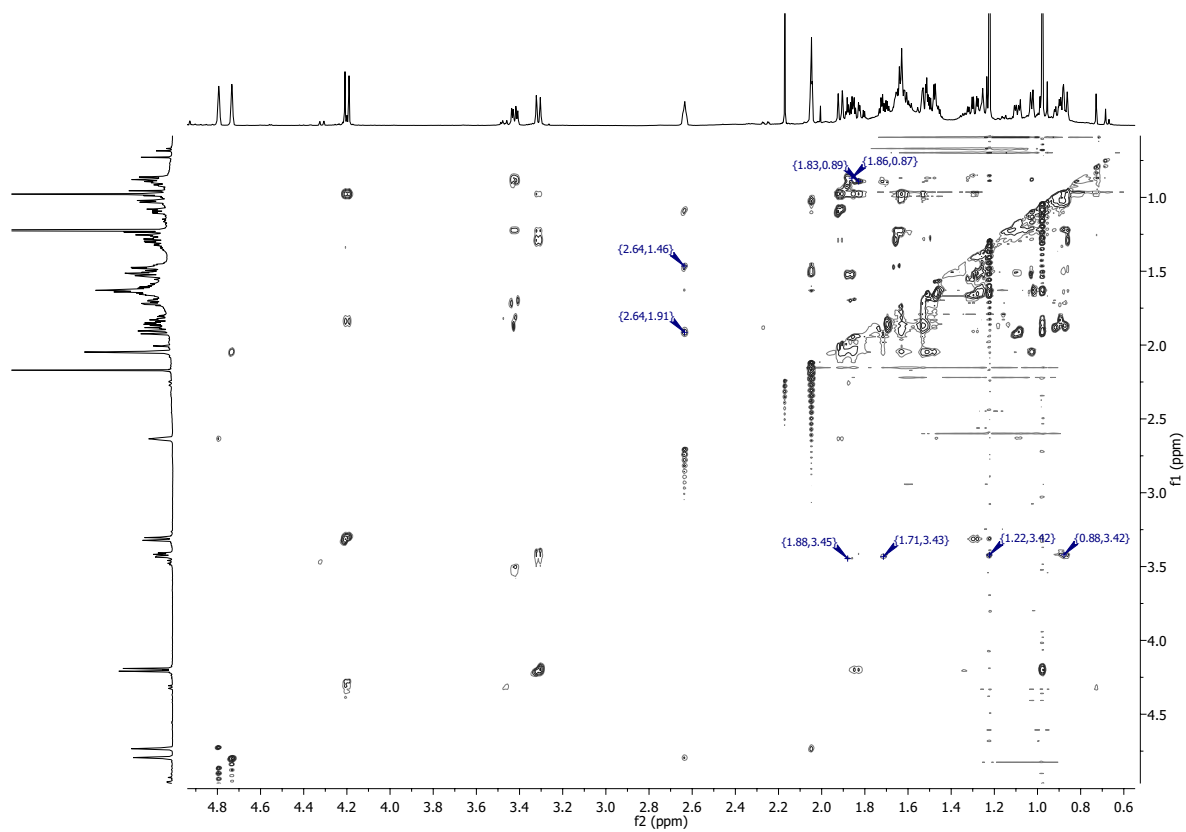


Figure S8. $^1\text{H}/^1\text{H}$ -NOESY spectrum of compound 1 (600 MHz, CDCl_3).

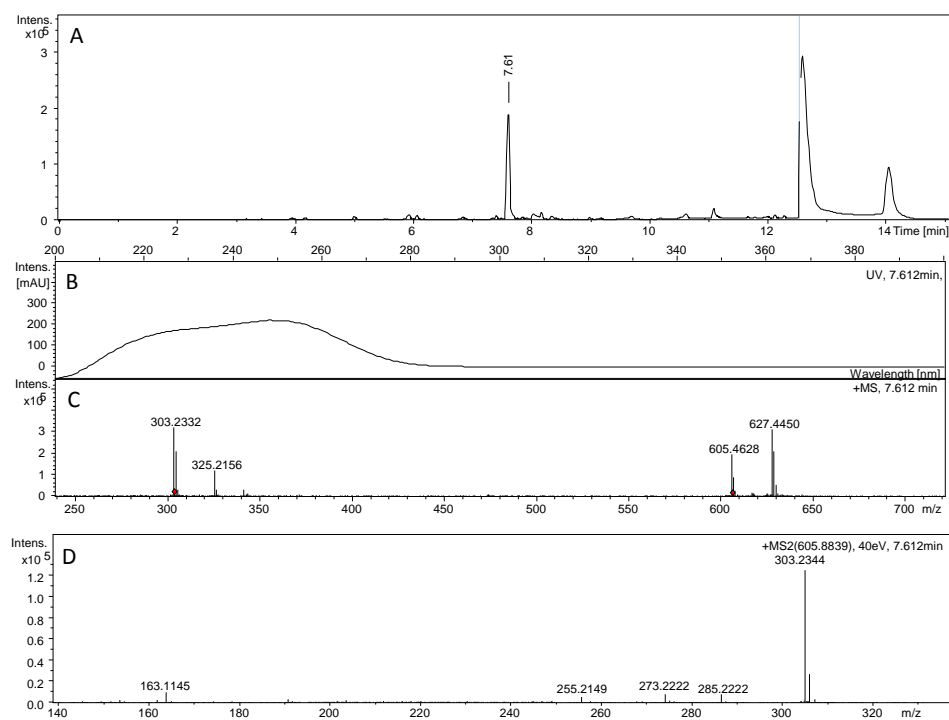


Figure S9. +ESI-QqTOF-MS chromatogram (A); UV spectrum (B); +ESI-MS (C) and +ESI-MS2 (D) spectra of compound 2, $[M + H]^+$: 303.2346 ($C_{20}H_{31}O_2$). Internal calibrant sodium formate: 12.6 min.

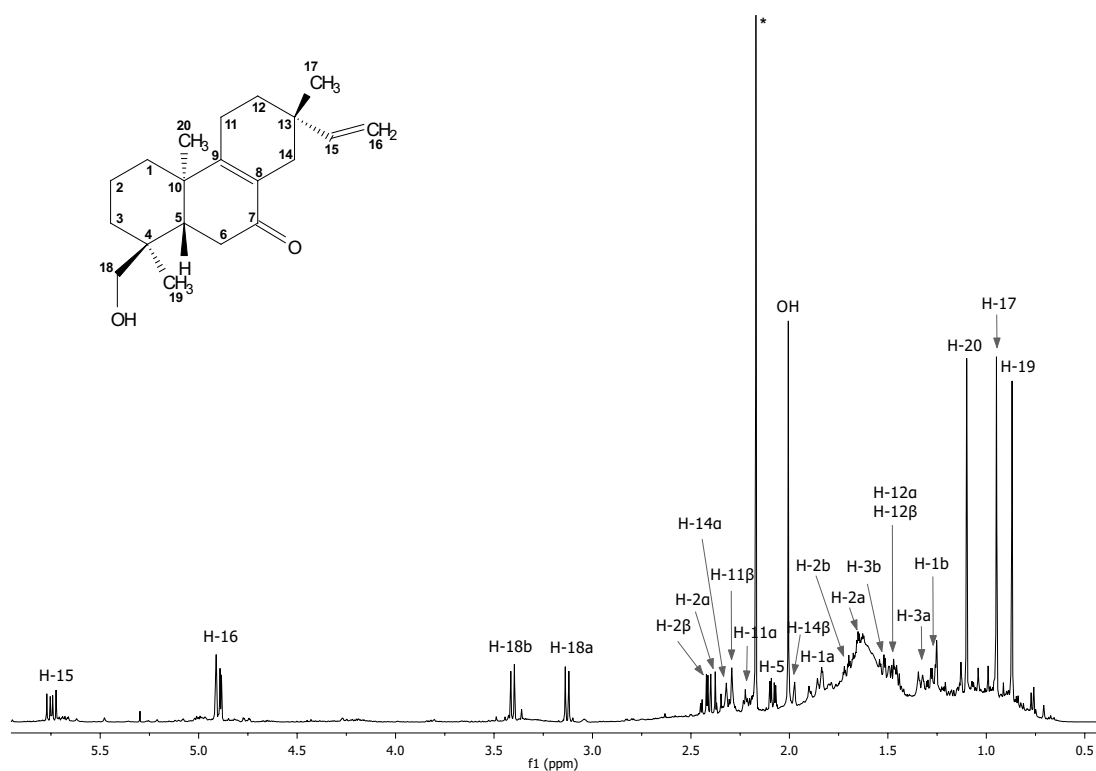


Figure S10. 1H NMR spectrum of compound 2 ($CDCl_3$, 600 MHz). *- CH_3 protons from acetone.

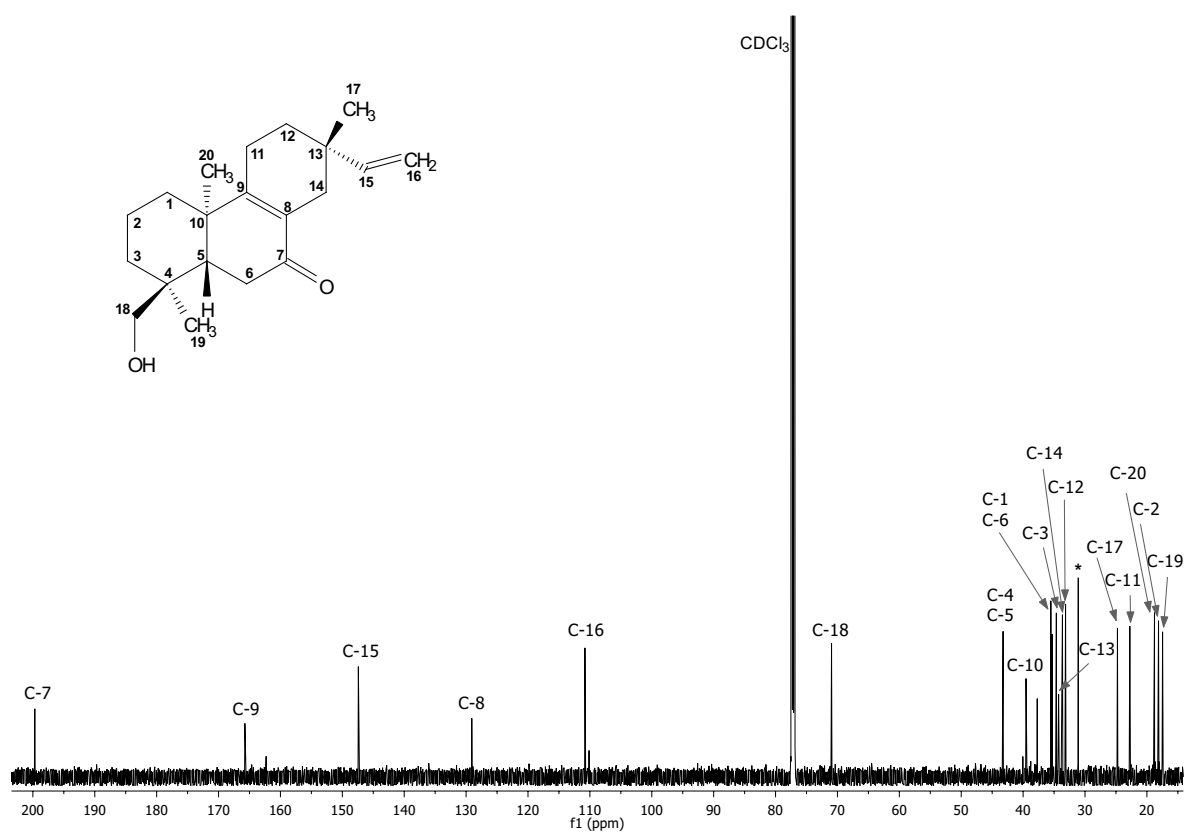


Figure S11. ^{13}C NMR spectrum of compound 2 (CDCl₃, 150 MHz). *-CH₃ from acetone.

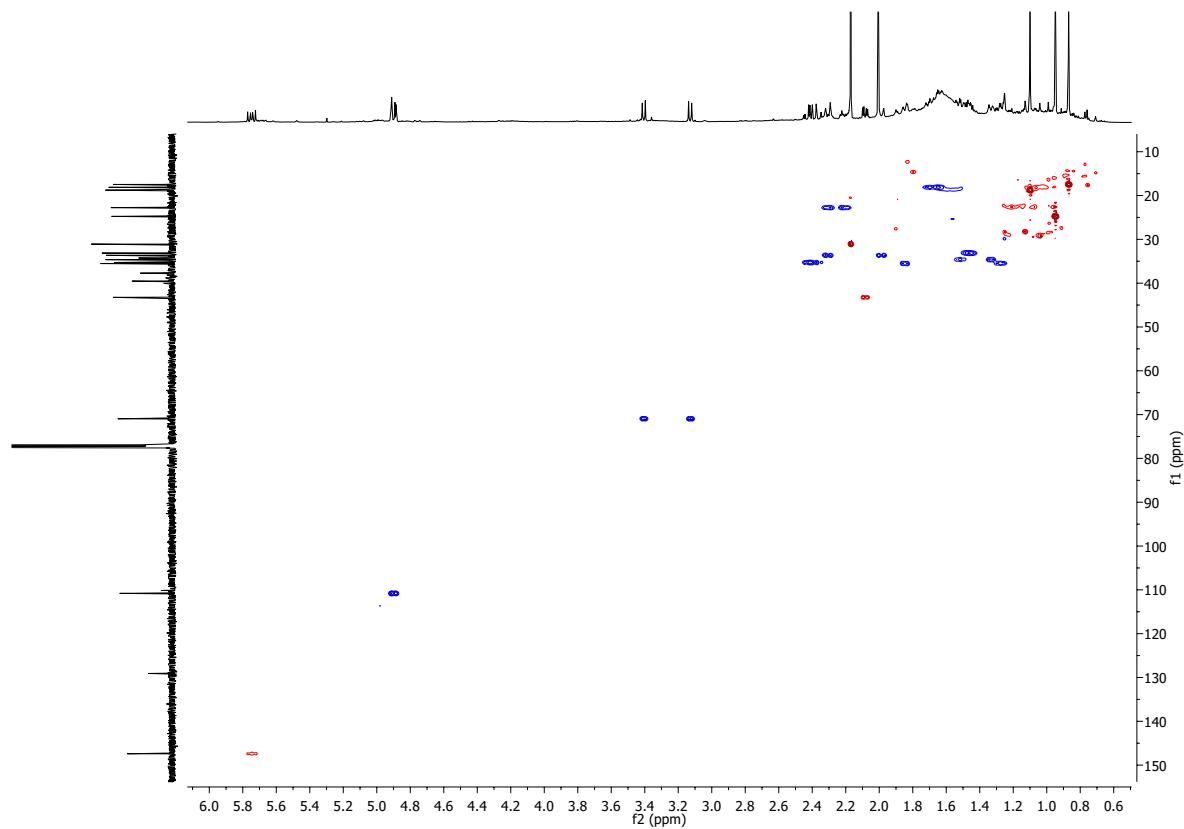


Figure S12. $^1\text{H}/^{13}\text{C}$ -HSQC spectrum of compound 2 (600/150 MHz, CDCl₃).

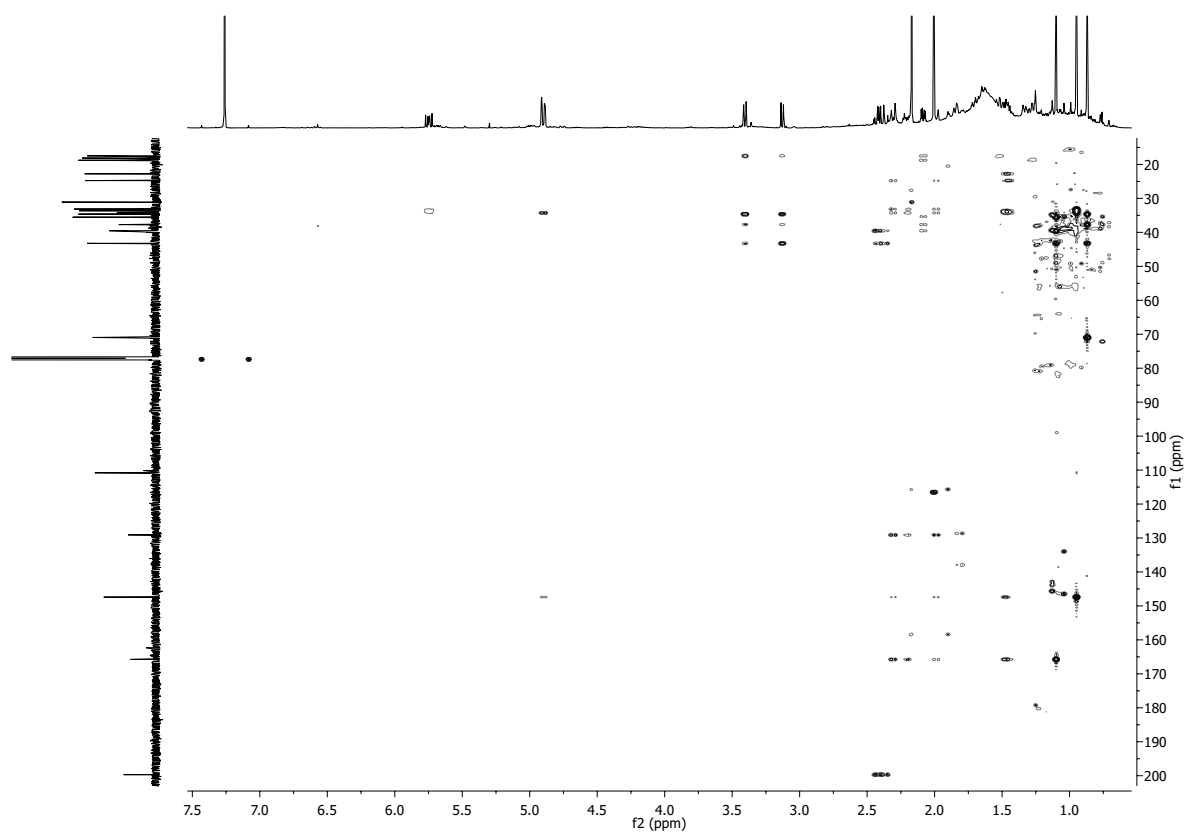


Figure S13. $^1\text{H}/^{13}\text{C}$ -HMBC spectrum of compound **2** (600/150 MHz, CDCl_3).

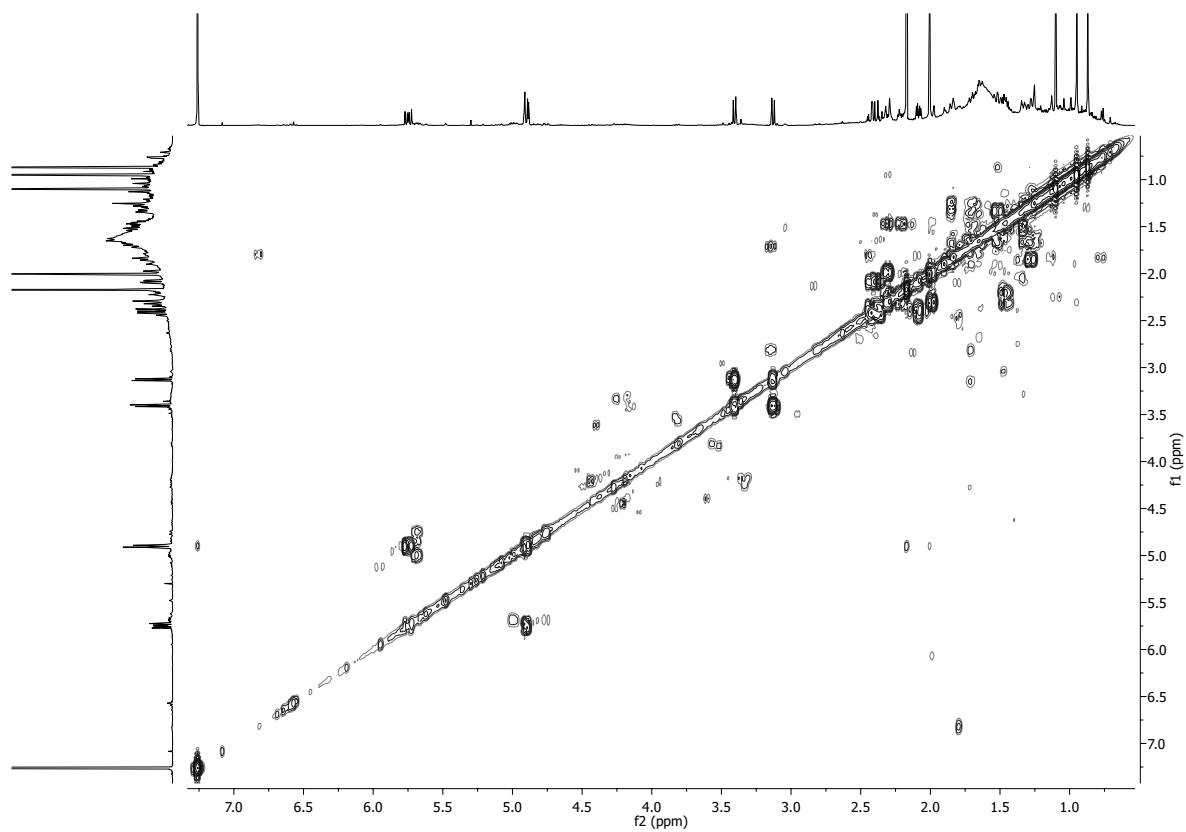


Figure S14. $^1\text{H}/^1\text{H}$ -COSY spectrum of compound **2** (600 MHz, CDCl_3).

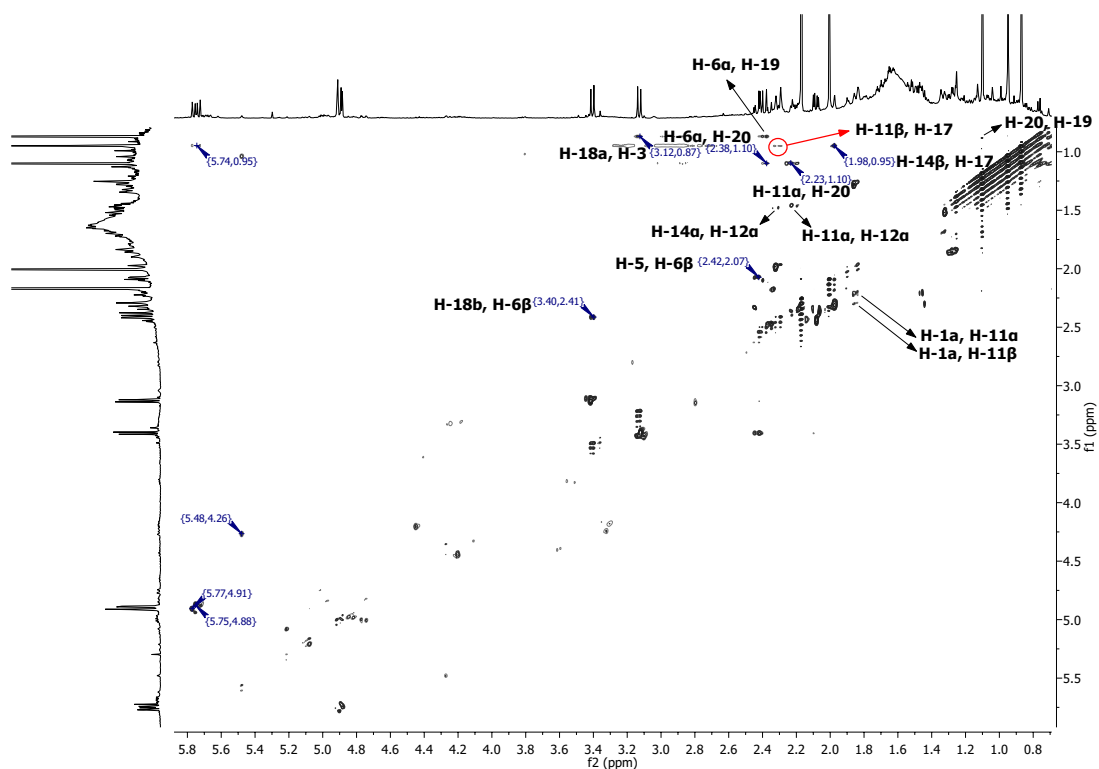


Figure S15. $^1\text{H}/^1\text{H}$ -NOESY spectrum of compound **2** (600 MHz, CDCl_3). Cross-correlated peak (red circle) enabled the determination of the stereochemistry at C-13.

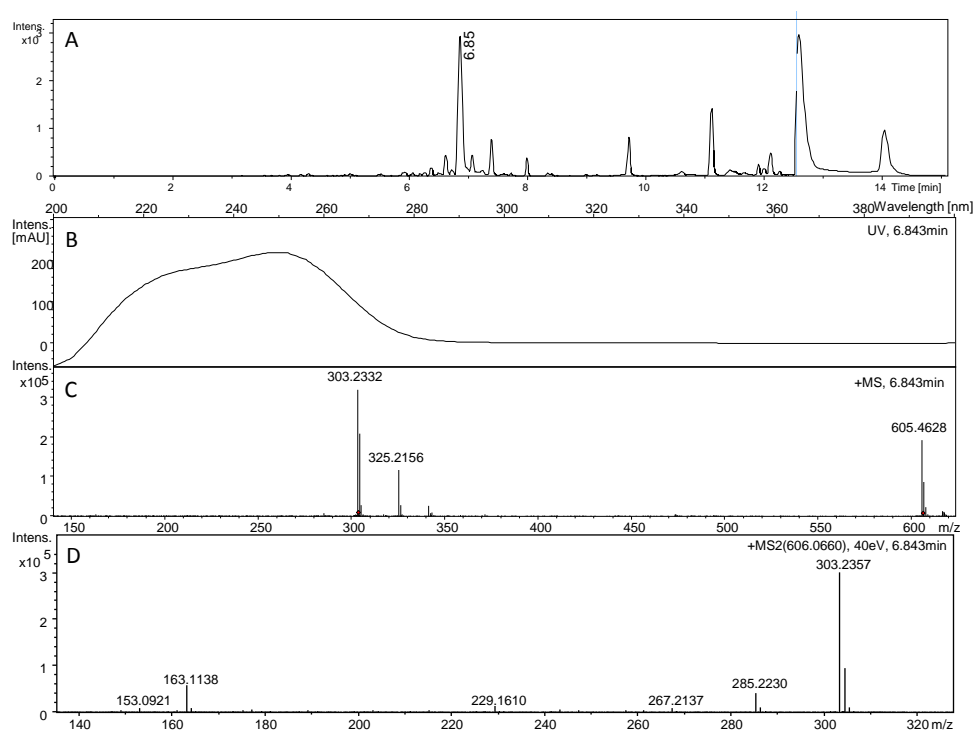
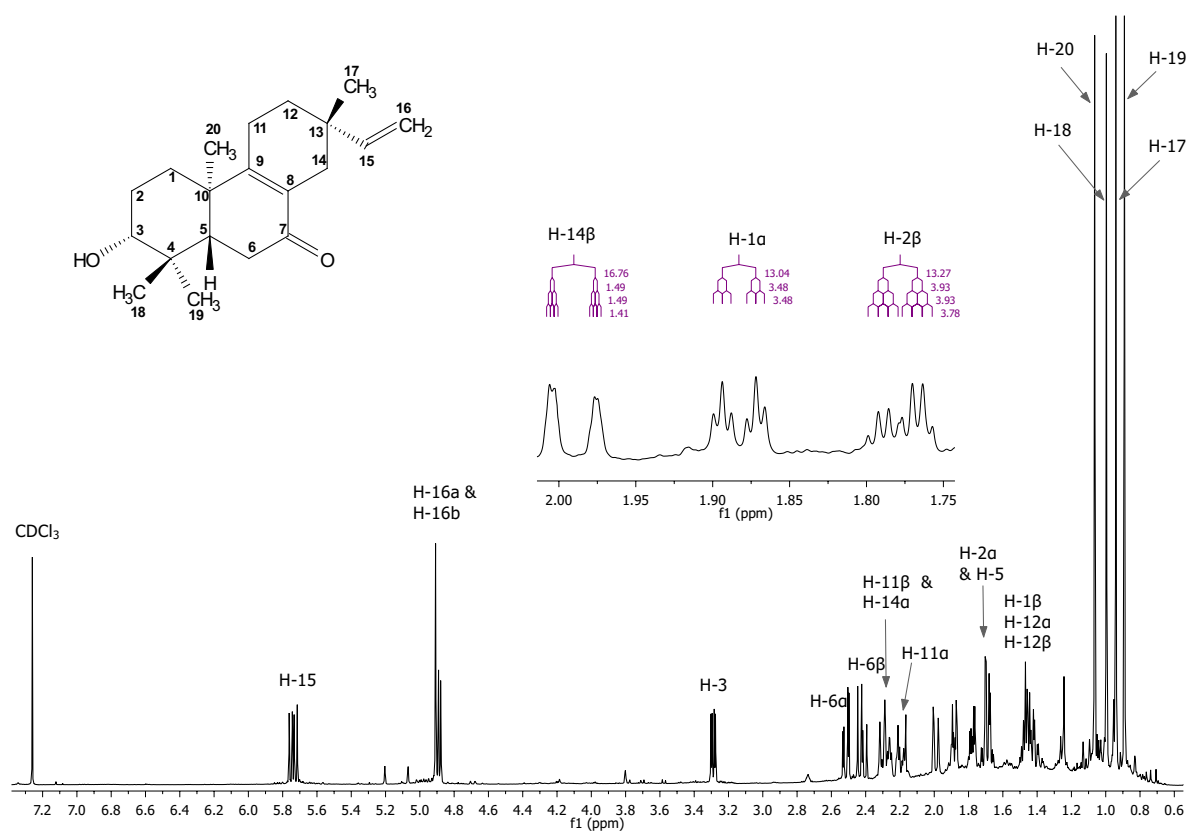
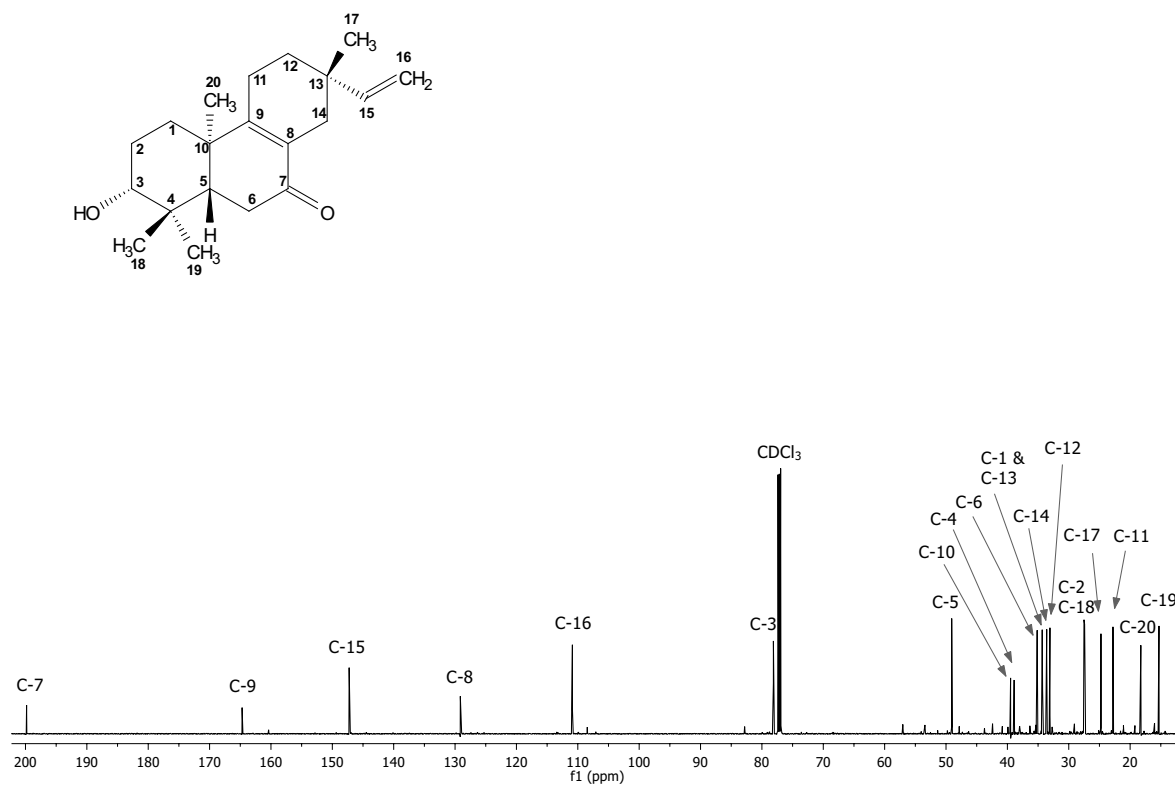


Figure S16. +ESI-QqTOF-MS chromatogram (A); UV spectrum (B); +ESI-MS (C) and +ESI-MS2 (D) spectra of compound **3**, $[\text{M} + \text{H}]^+$: 303.2332 ($\text{C}_{20}\text{H}_{31}\text{O}_2$). Internal calibrant sodium formate: 12.6 min.

Figure S17. ^1H NMR spectrum of compound 3 (CDCl₃, 600 MHz).Figure S18. ^{13}C NMR spectrum of compound 3 (CDCl₃, 150 MHz).

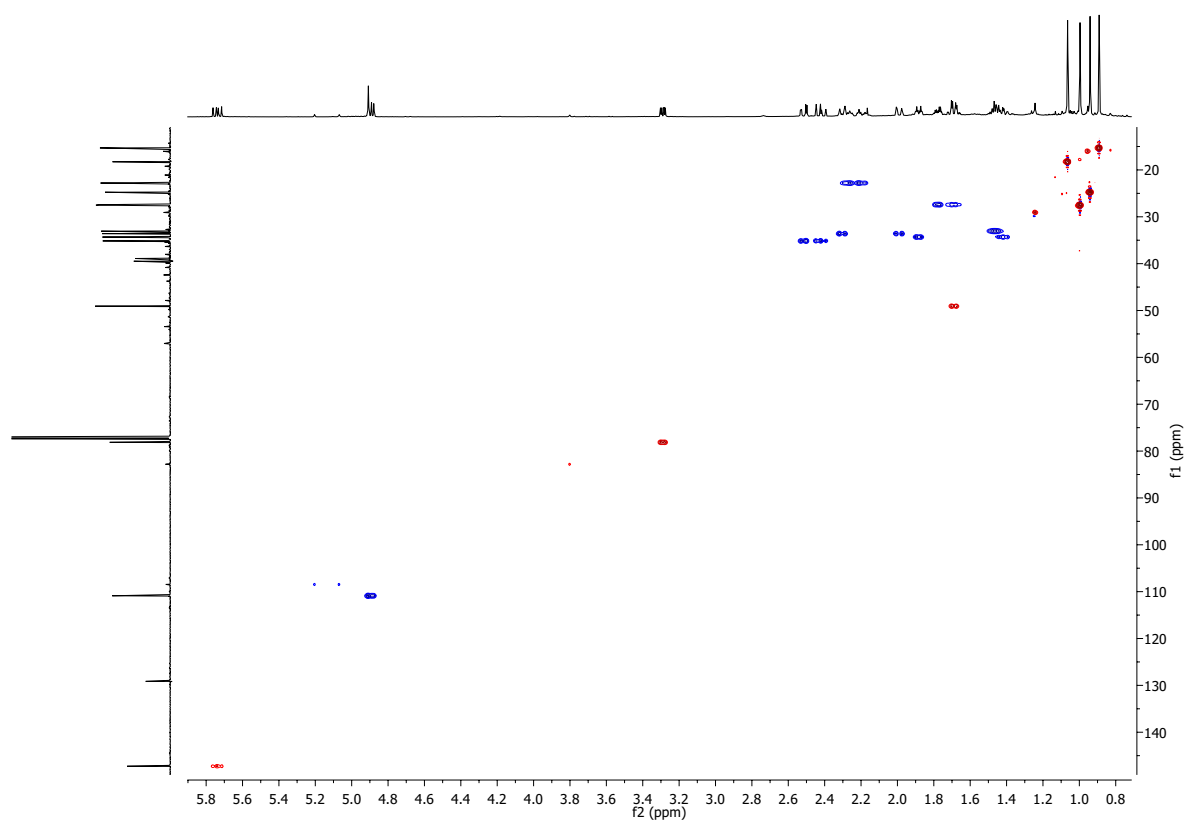


Figure S19. $^1\text{H}/^{13}\text{C}$ -HSQC spectrum of compound 3 (600/150 MHz, CDCl_3).

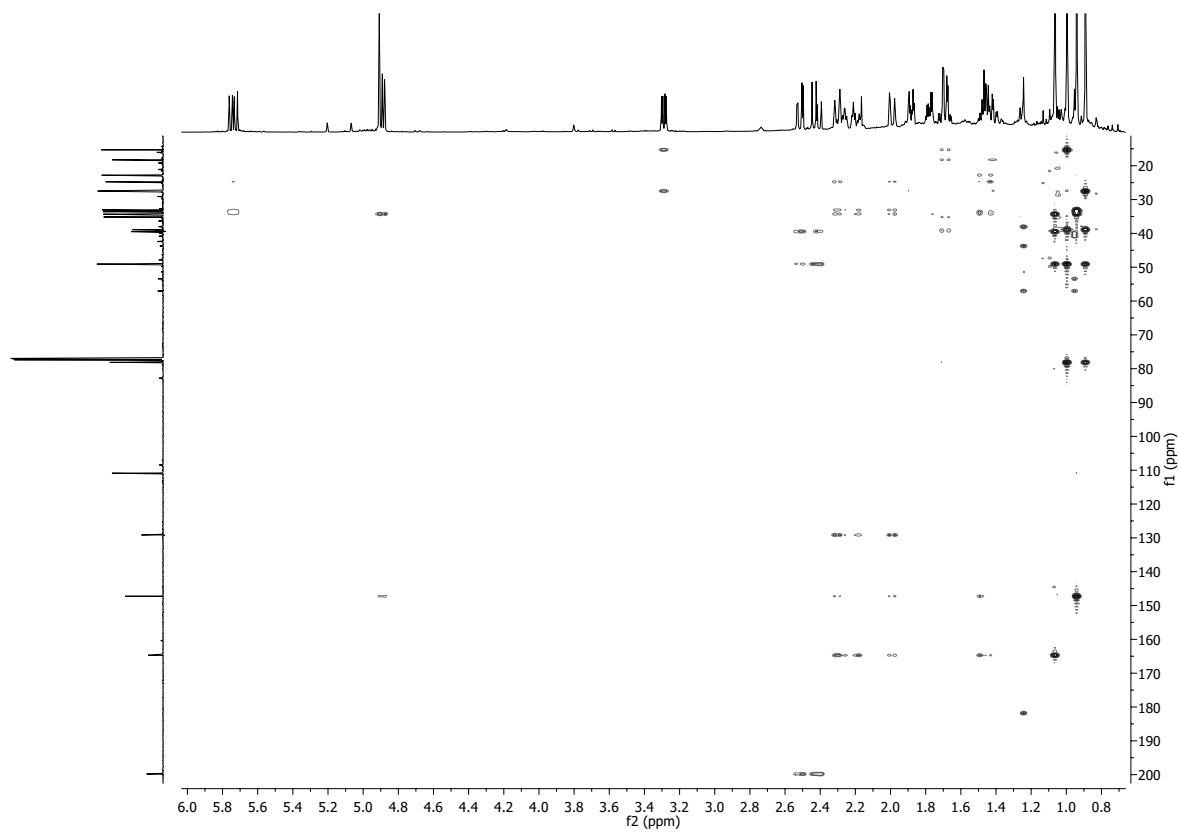


Figure S20. $^1\text{H}/^{13}\text{C}$ -HMBC spectrum of compound 3 (600/150 MHz, CDCl_3).

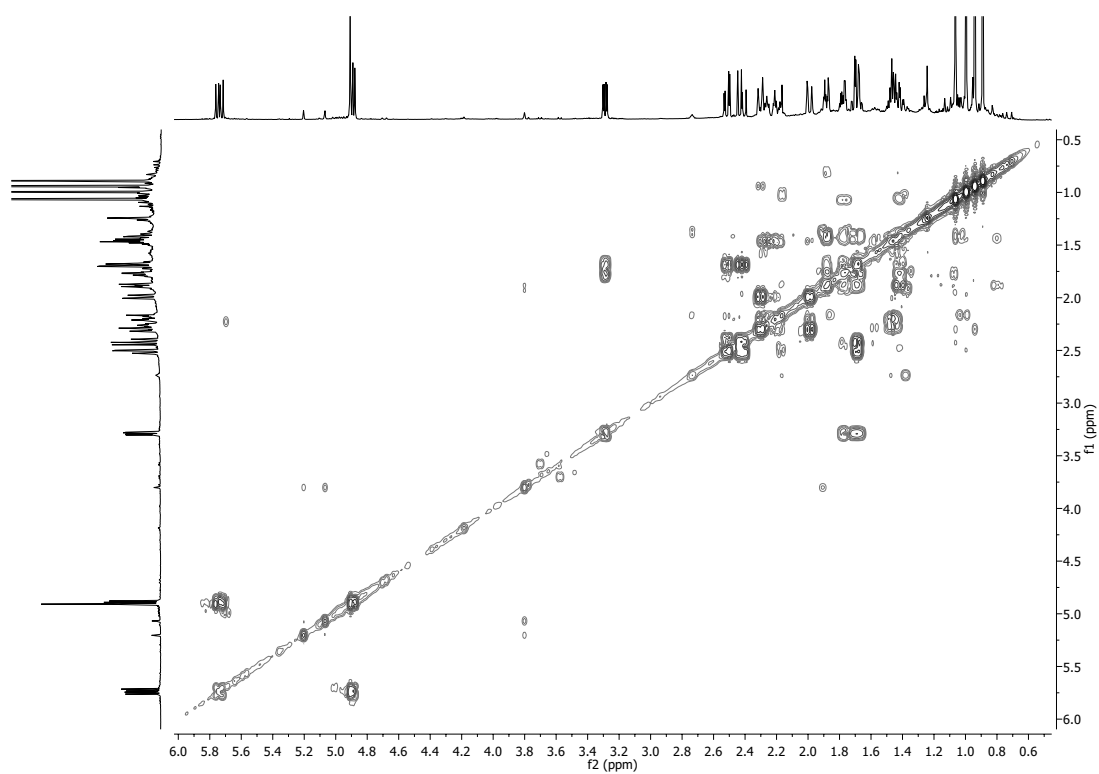


Figure S21. $^1\text{H}/^1\text{H}$ -COSY spectrum of compound **3** (600 MHz, CDCl_3).

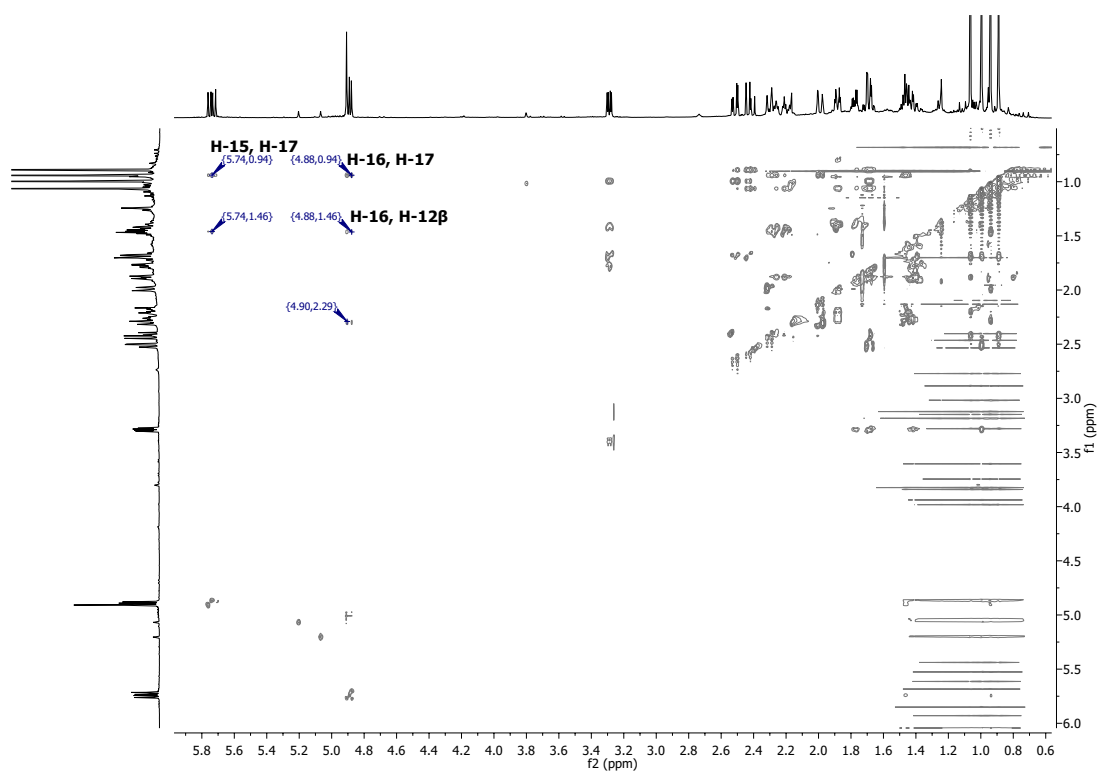


Figure S22. Partial $^1\text{H}/^1\text{H}$ -NOESY spectrum of compound **3** (600 MHz, CDCl_3) highlighting correlations in the downfield region.

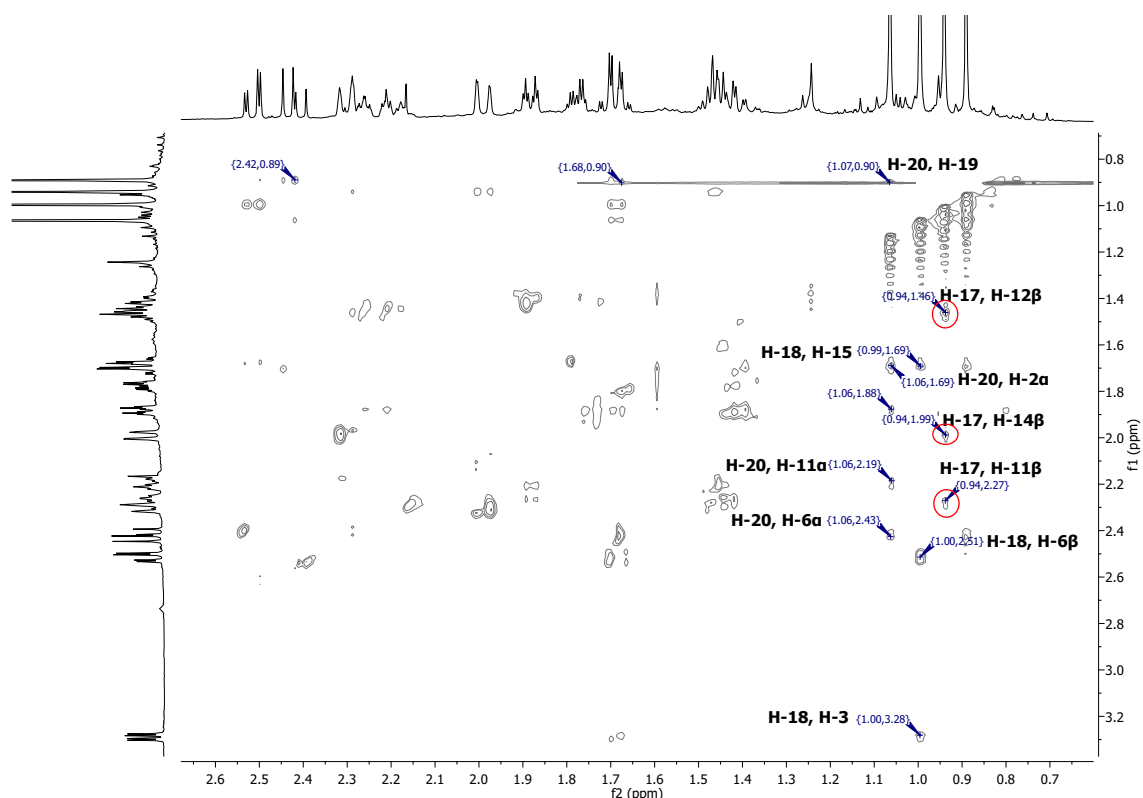


Figure S23. Partial $^1\text{H}/^1\text{H}$ -NOESY spectrum of compound **3** (600 MHz, CDCl_3) showing correlations in the upfield region. Stereochemistry at C-13 in compound **4** is justified by the NOE effects circled in red.

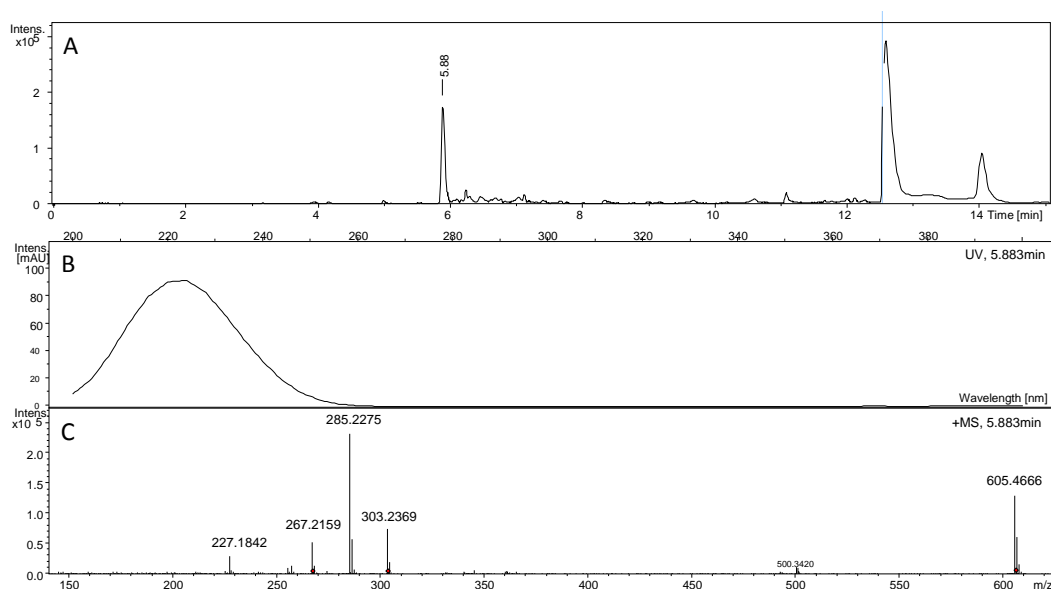


Figure S24. +ESI-QqTOF-MS chromatogram (A); UV spectrum (B); +ESI-MS (C) and +ESI-MS2 (D) spectra of compound **4**, $[\text{M} + \text{H}]^+$: 303.2369 ($\text{C}_{20}\text{H}_{31}\text{O}_2$). Internal calibrant sodium formate: 12.6 min.

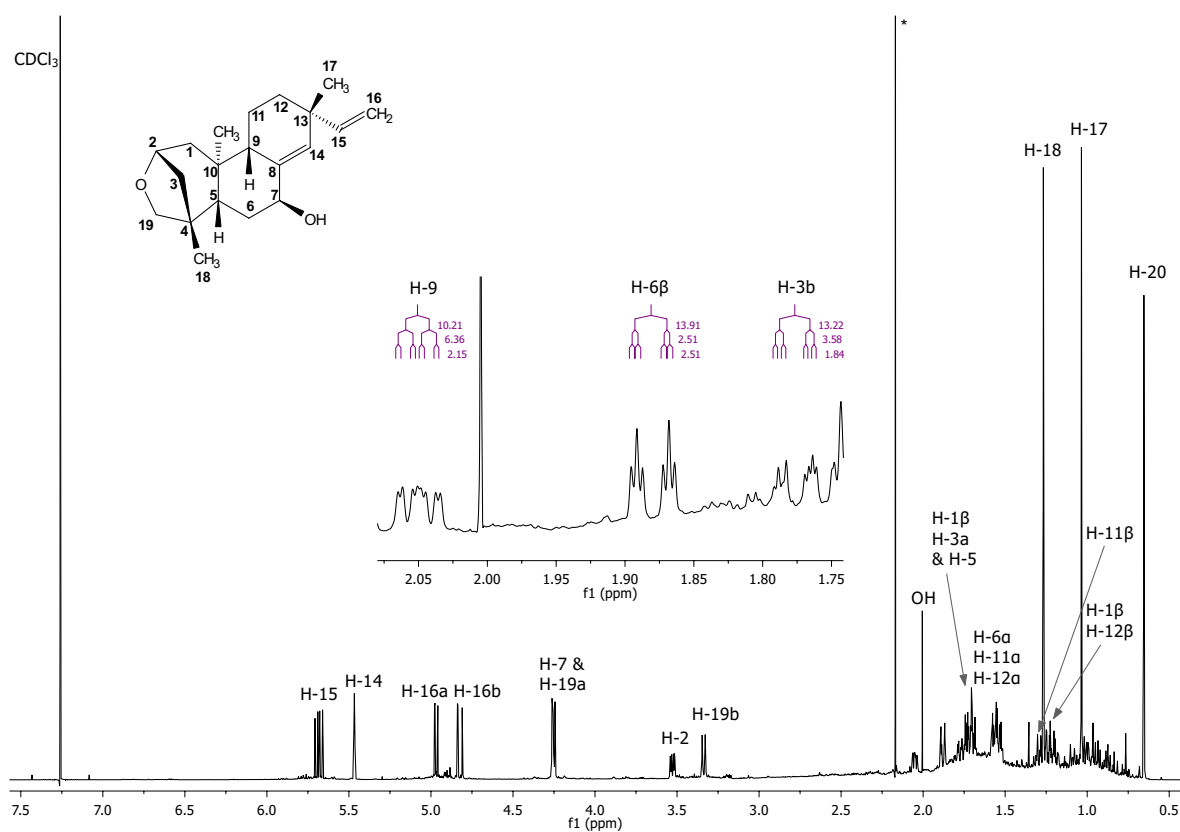


Figure S25. ^1H NMR spectrum of compound **4** (CDCl_3 , 600 MHz). *- CH_3 protons from acetone.

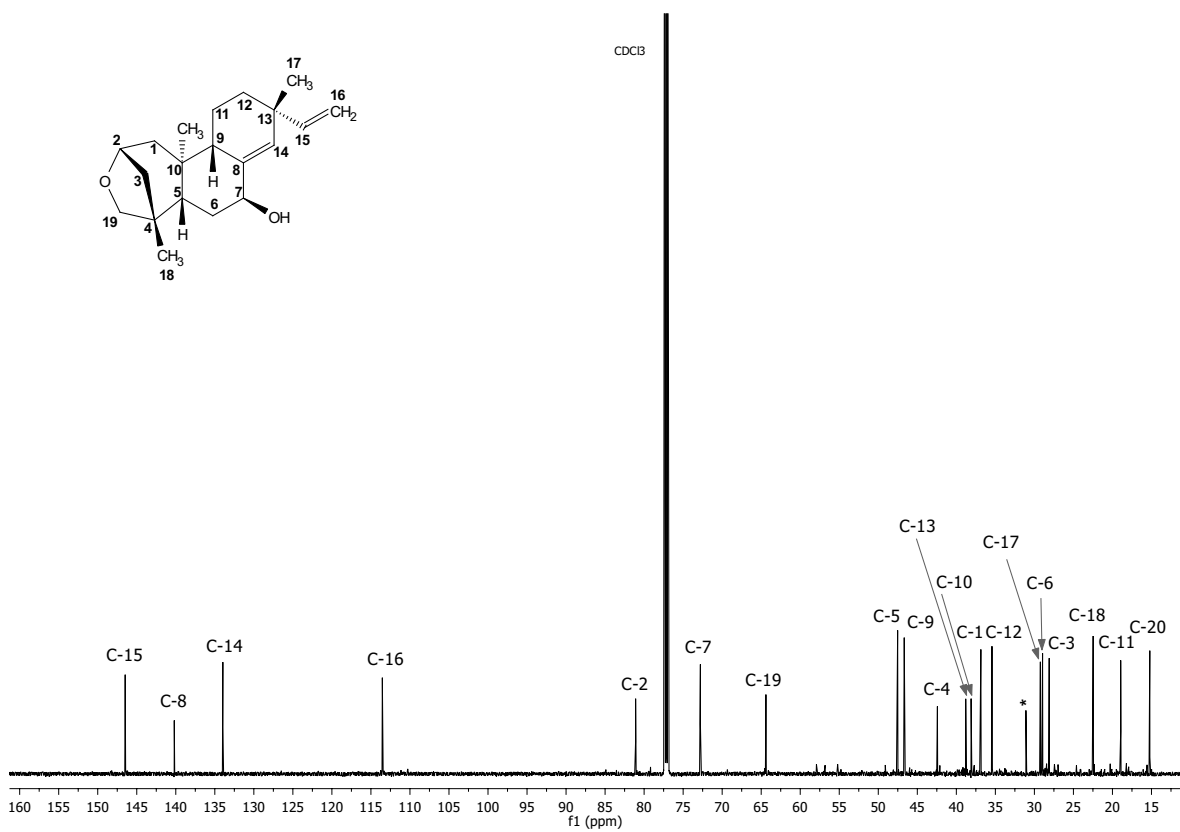


Figure S26. ^{13}C NMR spectrum of compound **4** (CDCl_3 , 150 MHz). *- CH_3 from acetone.

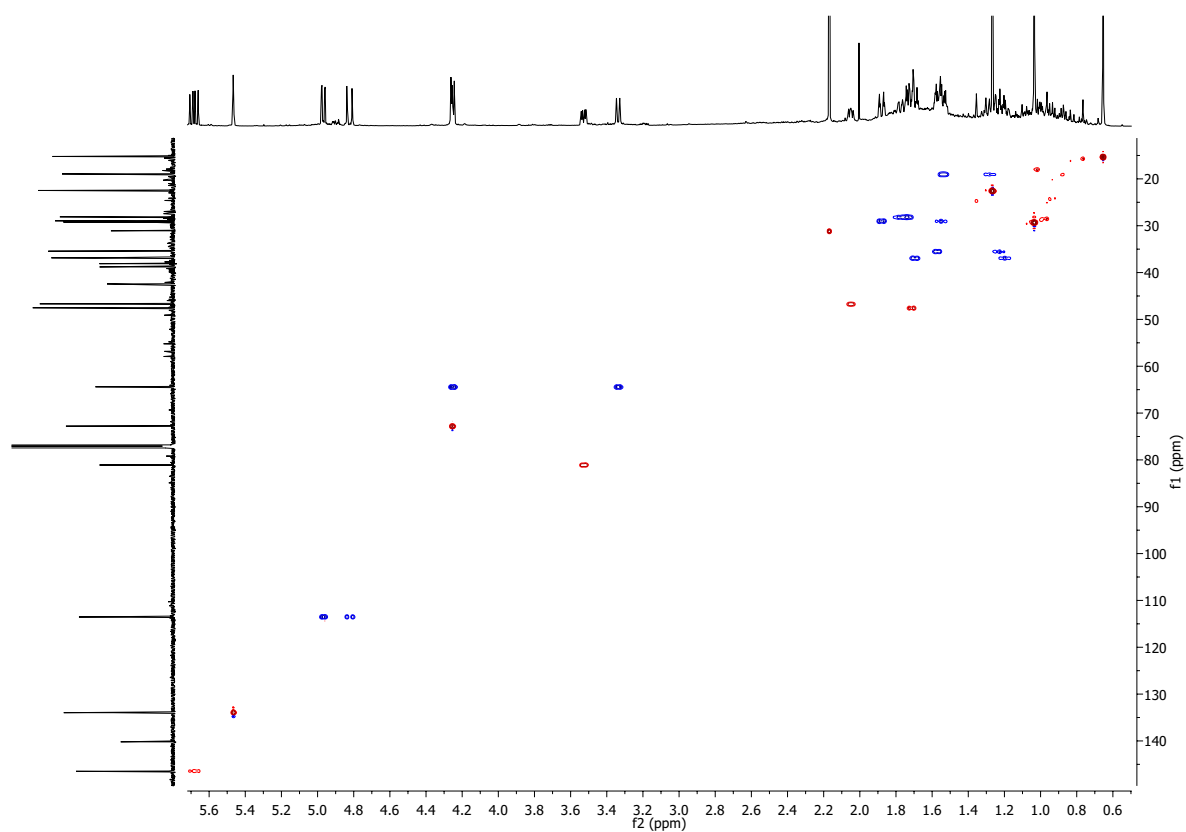


Figure S27. $^1\text{H}/^{13}\text{C}$ -HSQC spectrum of compound 4 (600/150 MHz, CDCl_3).

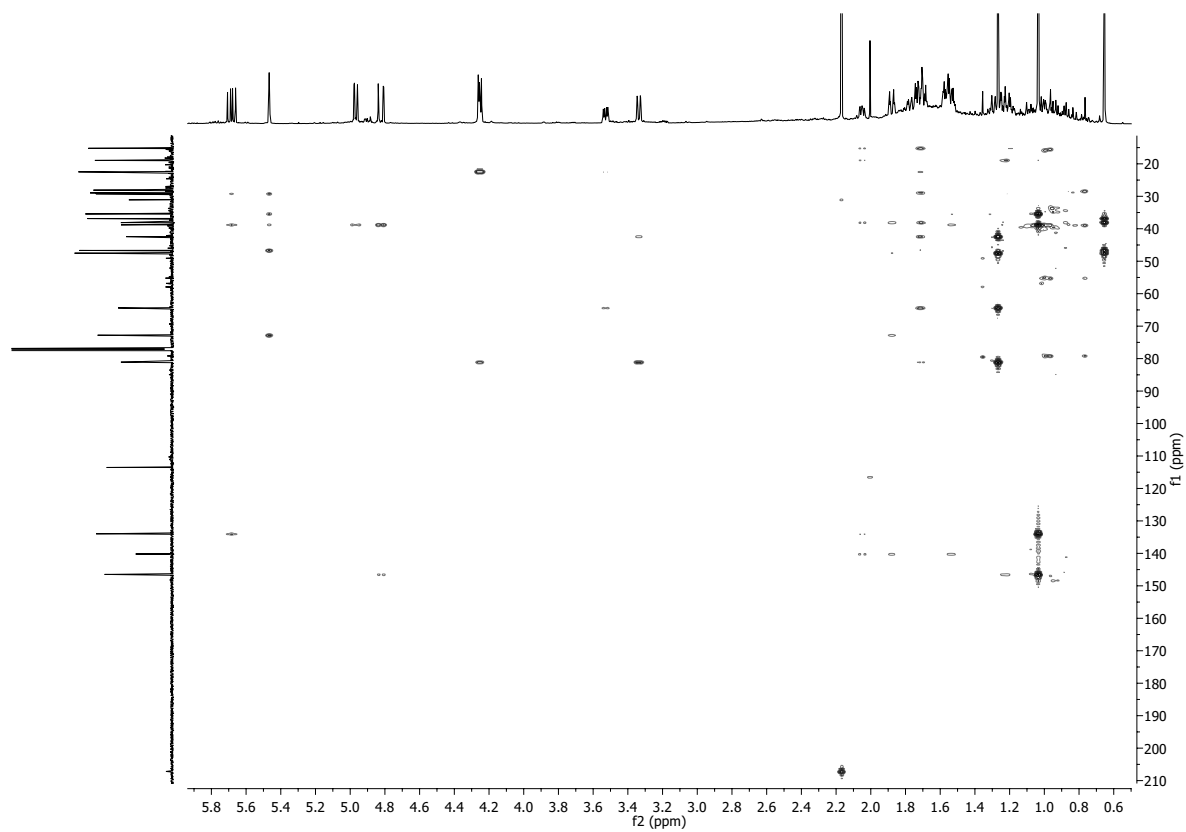
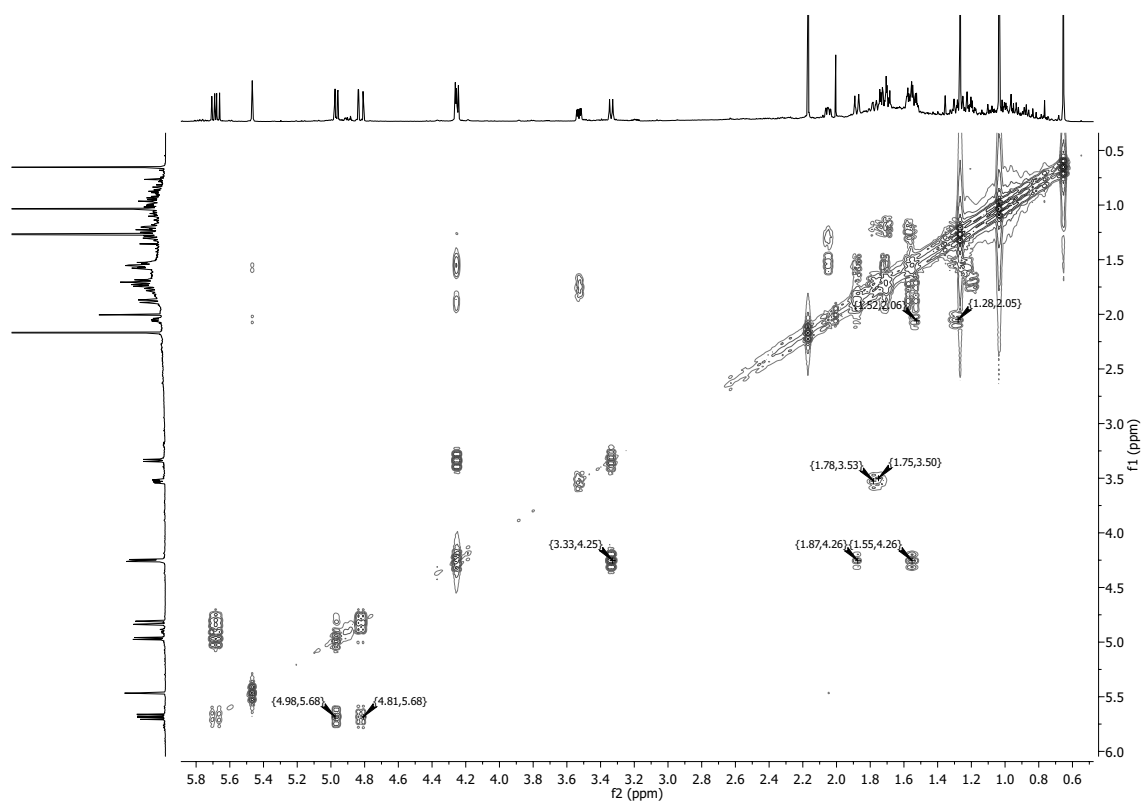
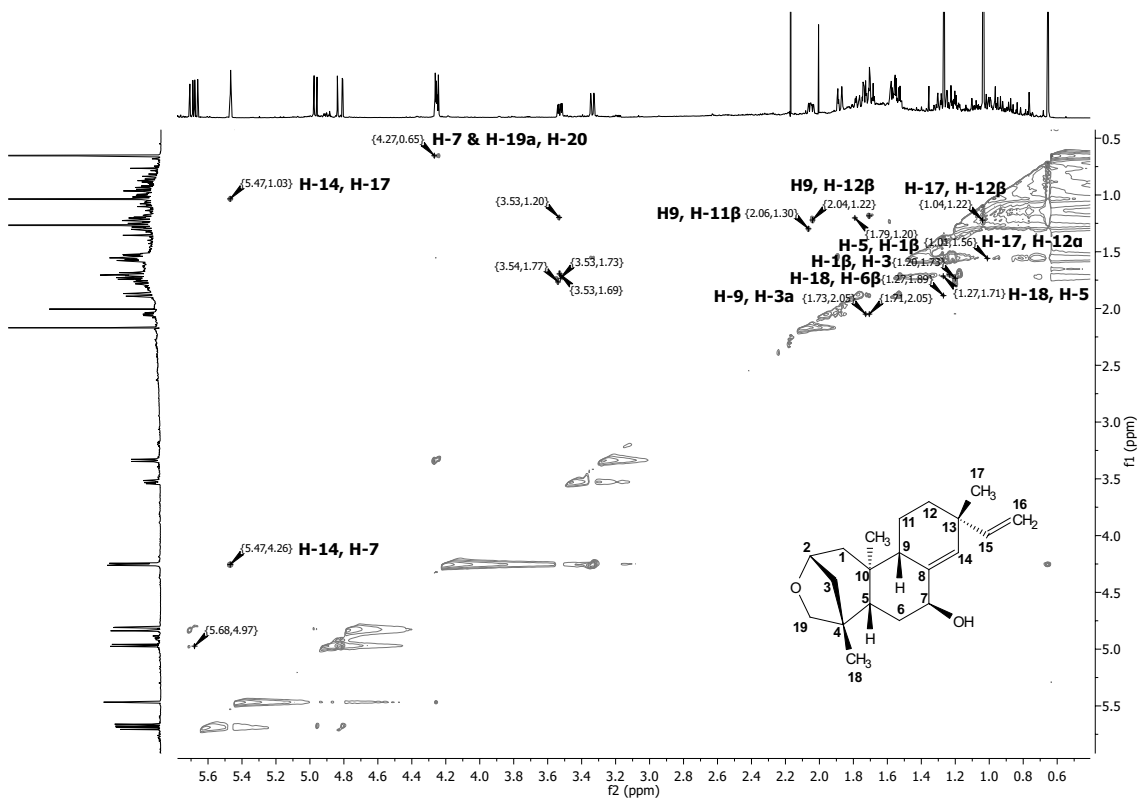


Figure S28. $^1\text{H}/^{13}\text{C}$ -HMBC spectrum of compound 4 (600/150 MHz, CDCl_3).

Figure S29. $^1\text{H}/^1\text{H}$ -COSY spectrum of compound **4** (600 MHz, CDCl_3).Figure S30. $^1\text{H}/^1\text{H}$ -NOESY spectrum of compound **4** (600 MHz, CDCl_3).