

Supporting Information

Penicurvularins A and B, macrolides from an ascomycete fungus *Alternaria* sp.

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CDCl₃)

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Figure S1. ^1H NMR Spectrum of Penicurvularin A (**1**; 600 MHz, Acetone- d_6)

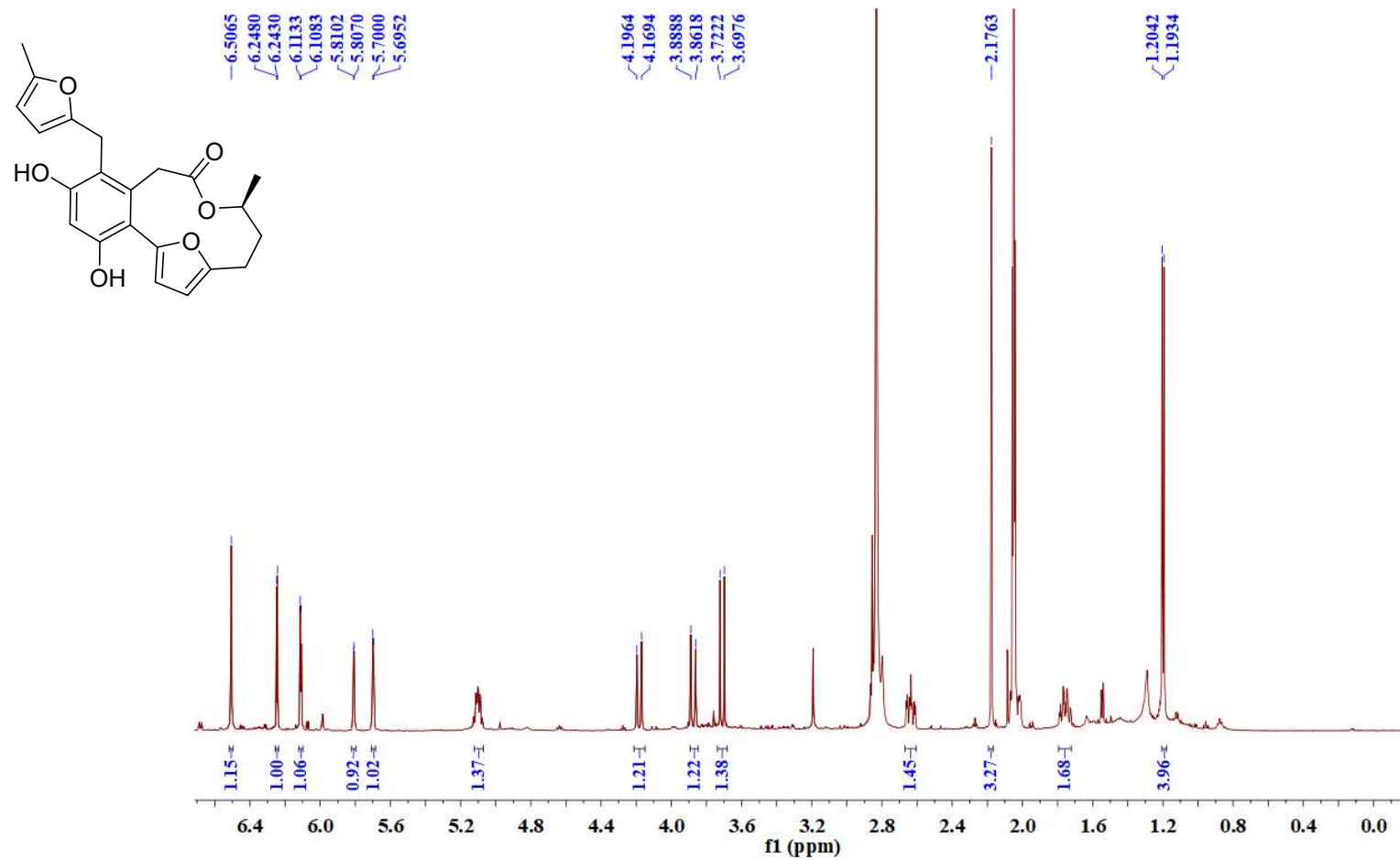


Figure S2. ^{13}C NMR Spectrum of Penicurvularin A (**1**; 150 MHz, Acetone- d_6)

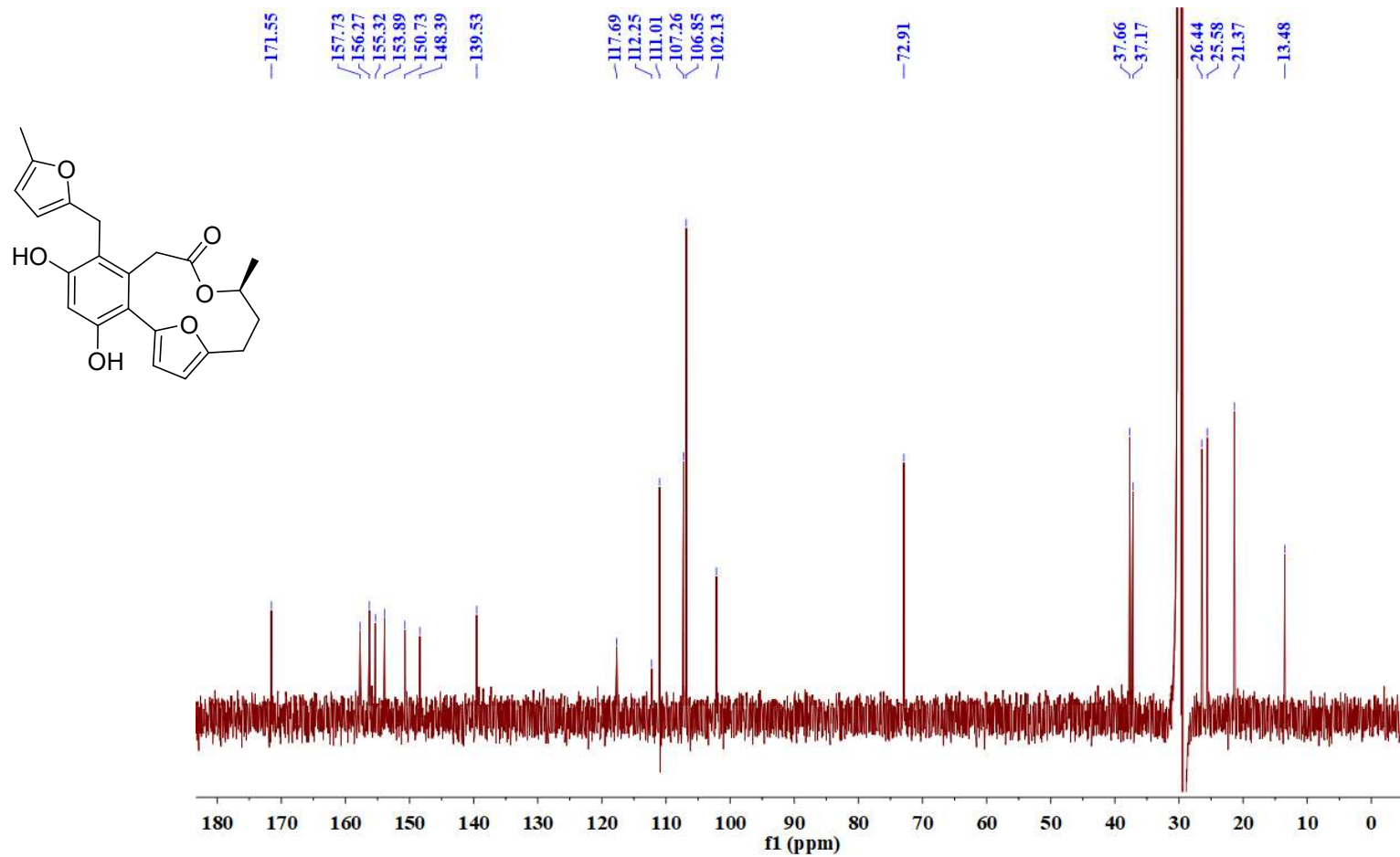


Figure S3. HSQC Spectrum of Penicurvularin A (**1**; 600 MHz, Acetone-*d*₆)

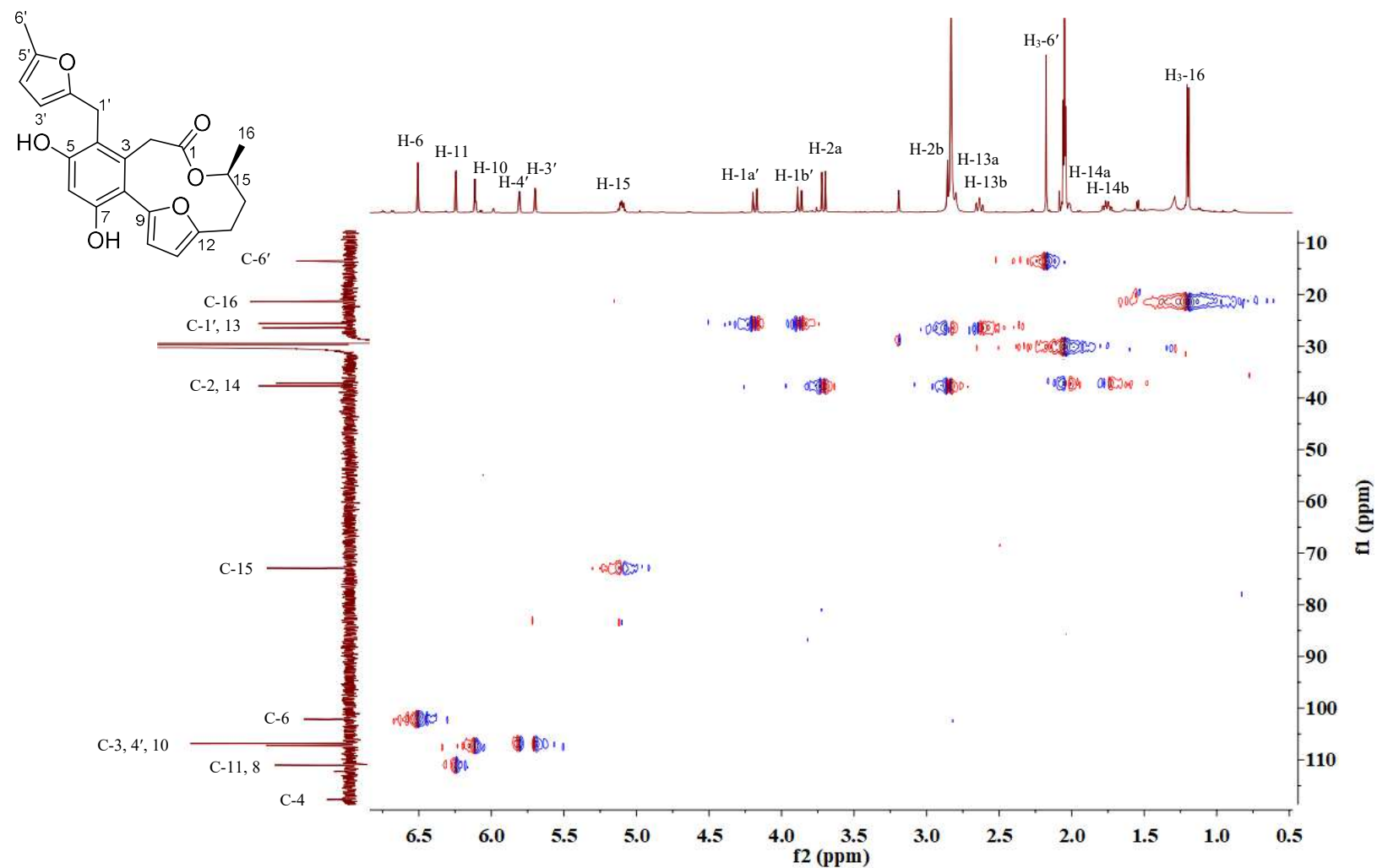


Figure S4. ^1H – ^1H COSY Spectrum of Penicurvularin A (**1**; 600 MHz, Acetone- d_6)

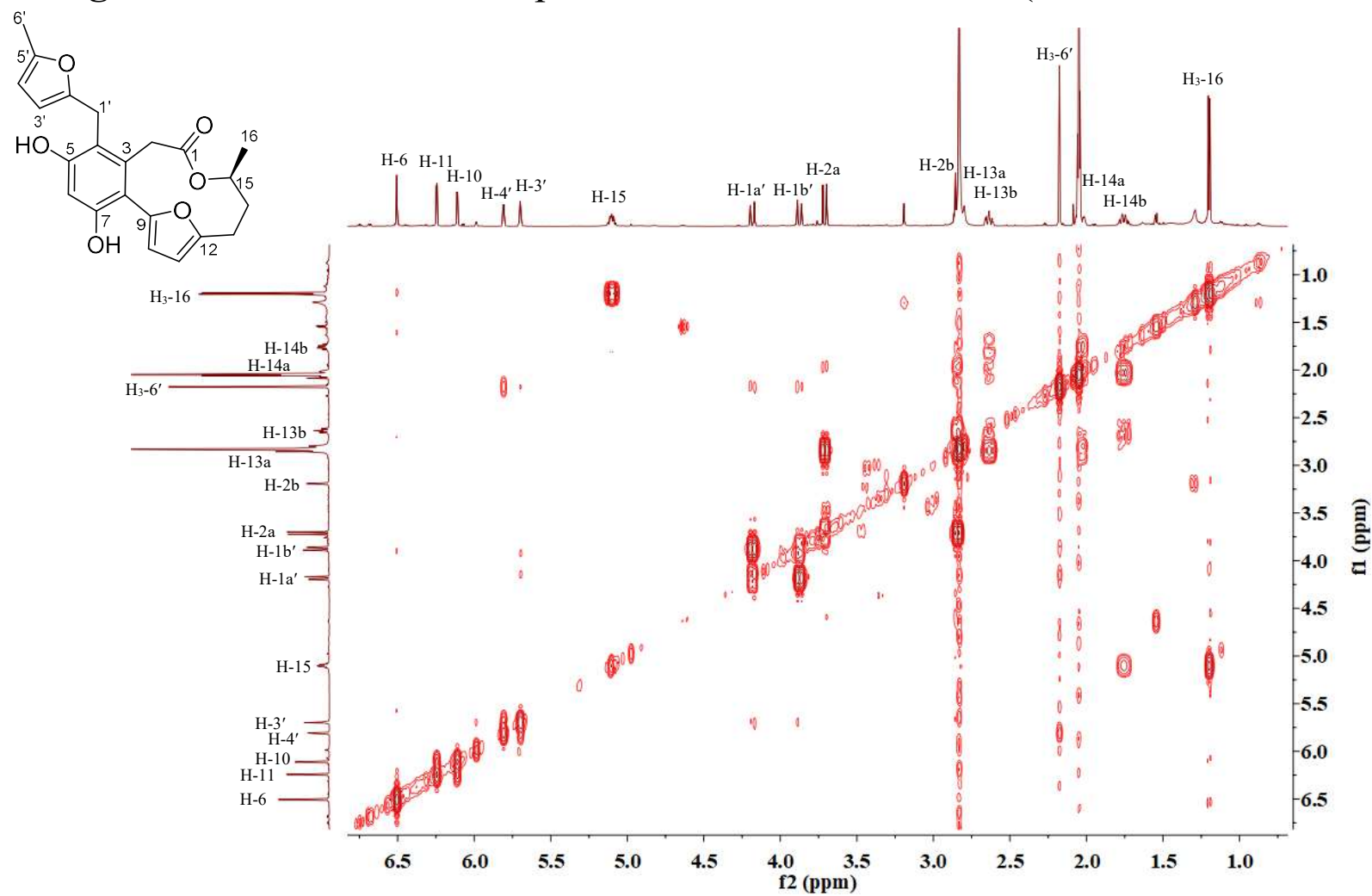


Figure S5. HMBC Spectrum of Penicurvarin A (1; 600 MHz, Acetone- d_6)

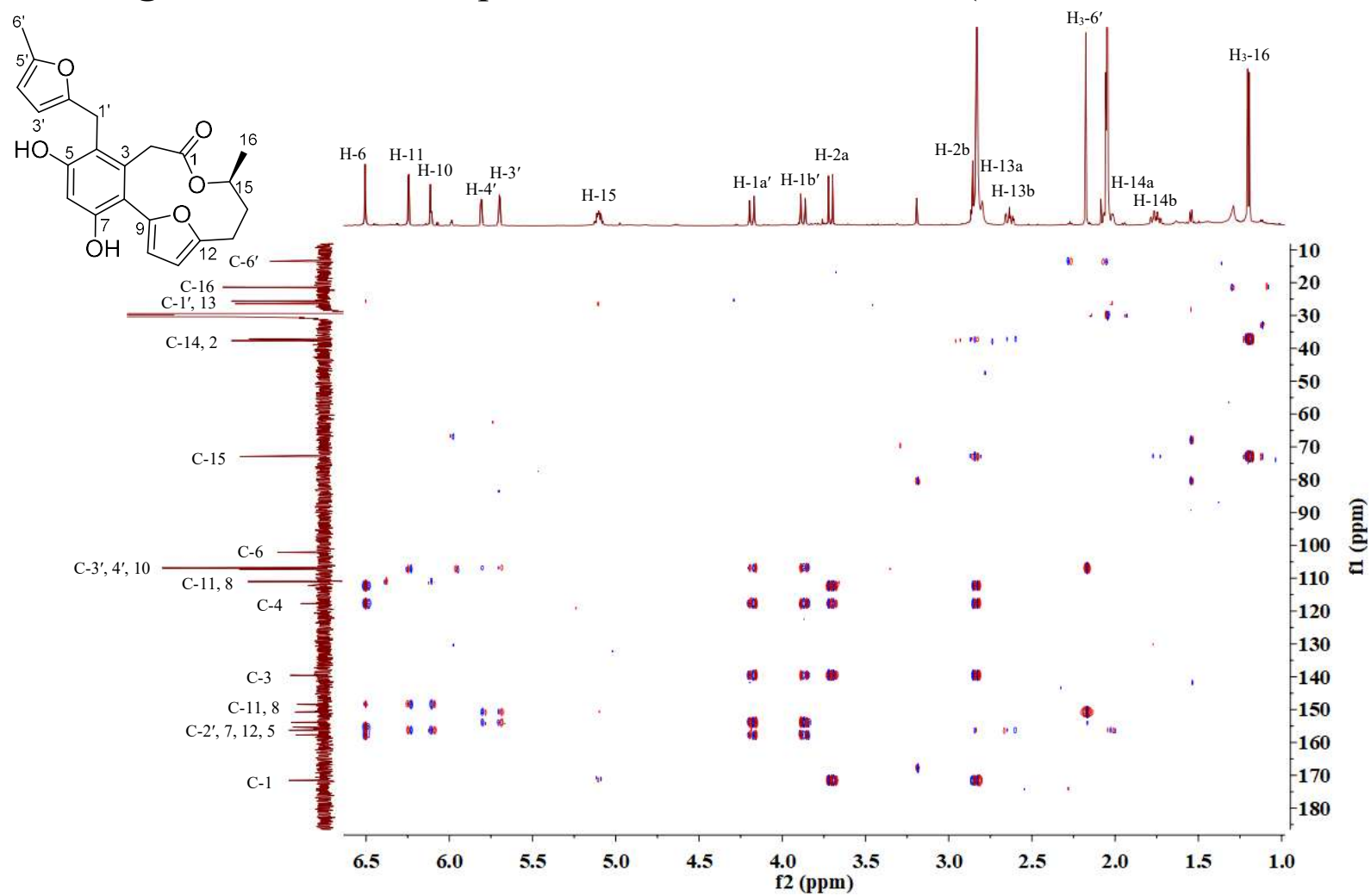


Figure S6. NOESY Spectrum of Penicurvarin A (**1**; 600 MHz, Acetone-*d*₆)

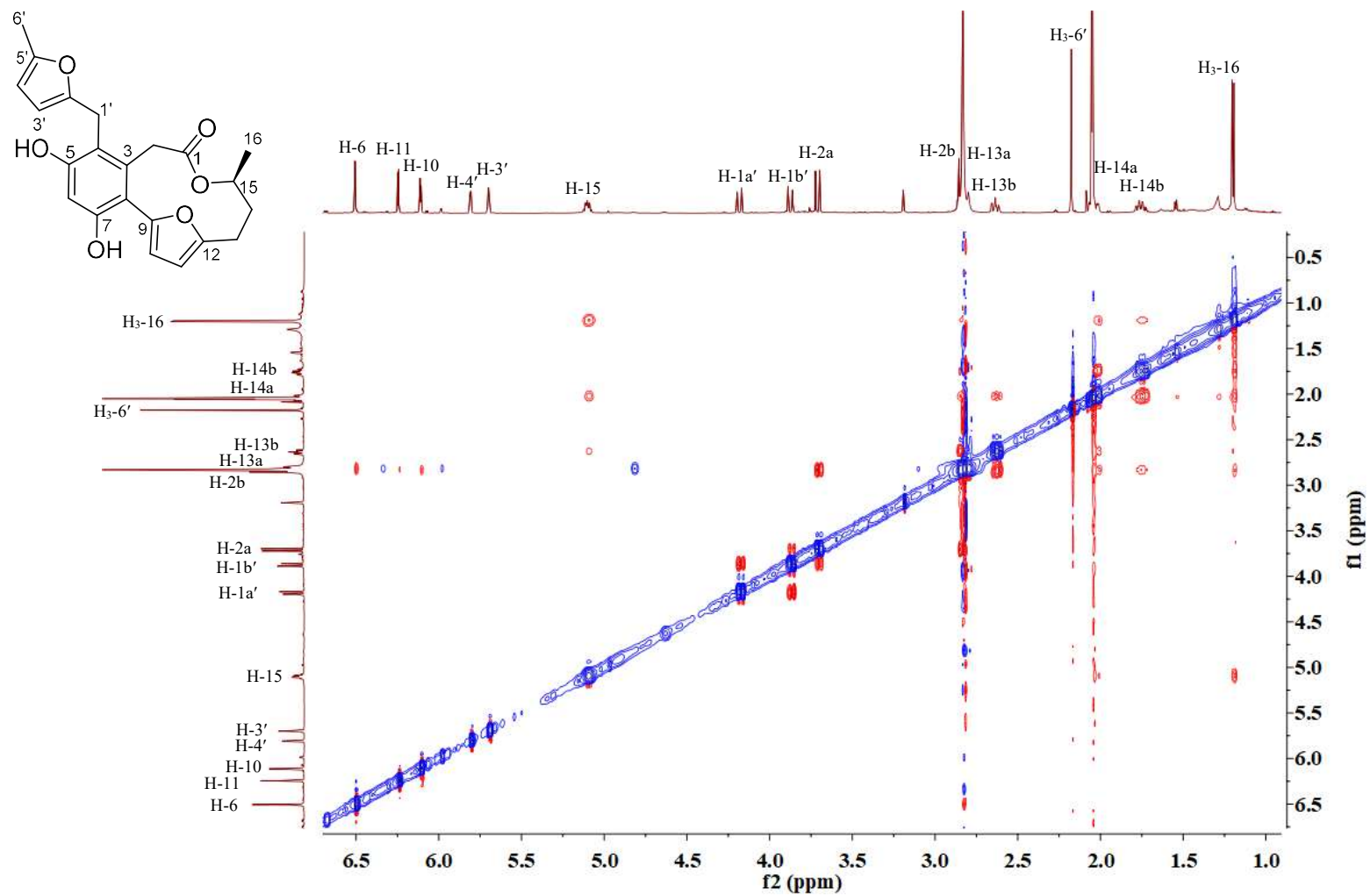


Figure S7. HRESIMS Spectrum of Penicurvularin A (1)

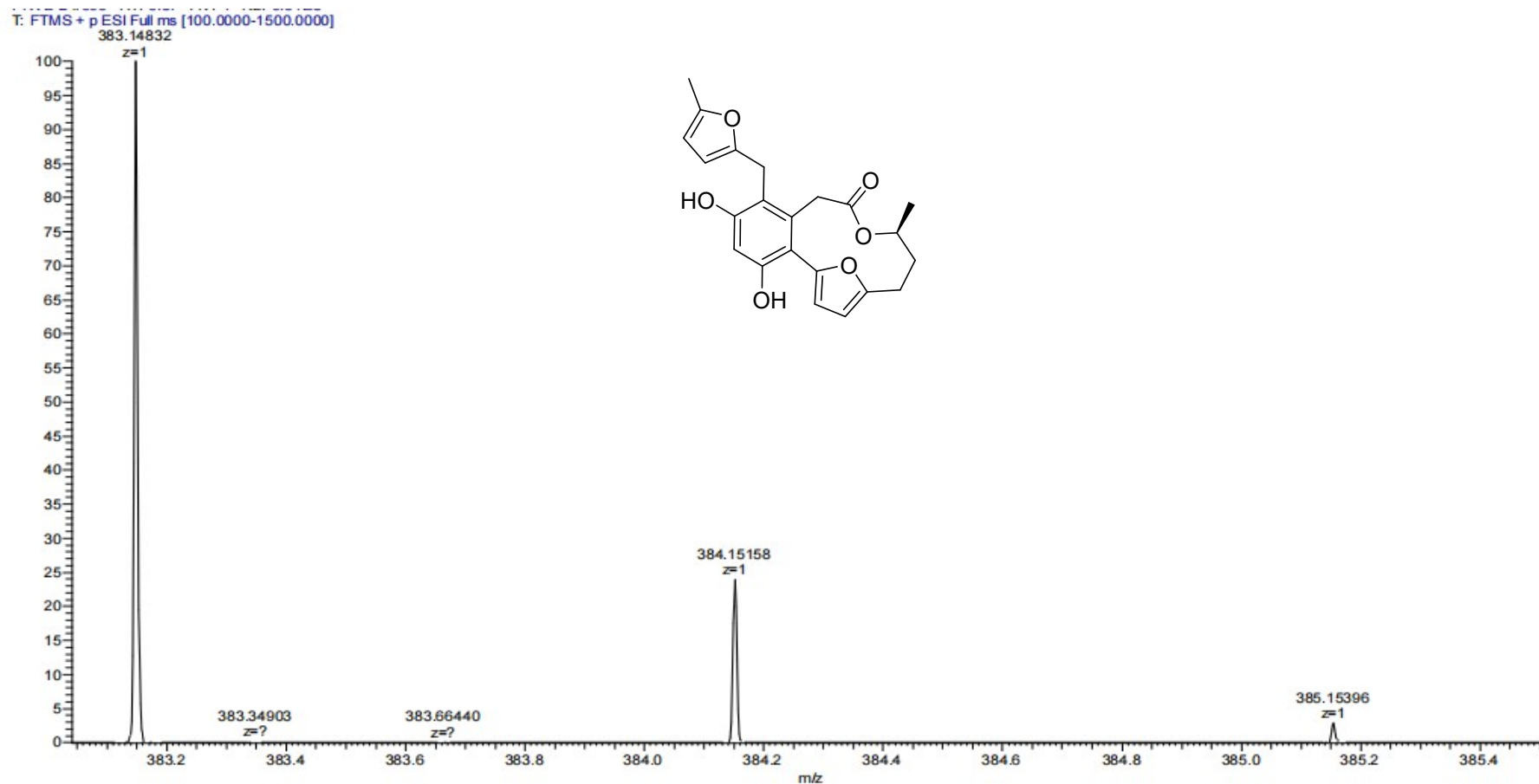


Figure S8. IR Spectrum of Penicurvularin A (1)

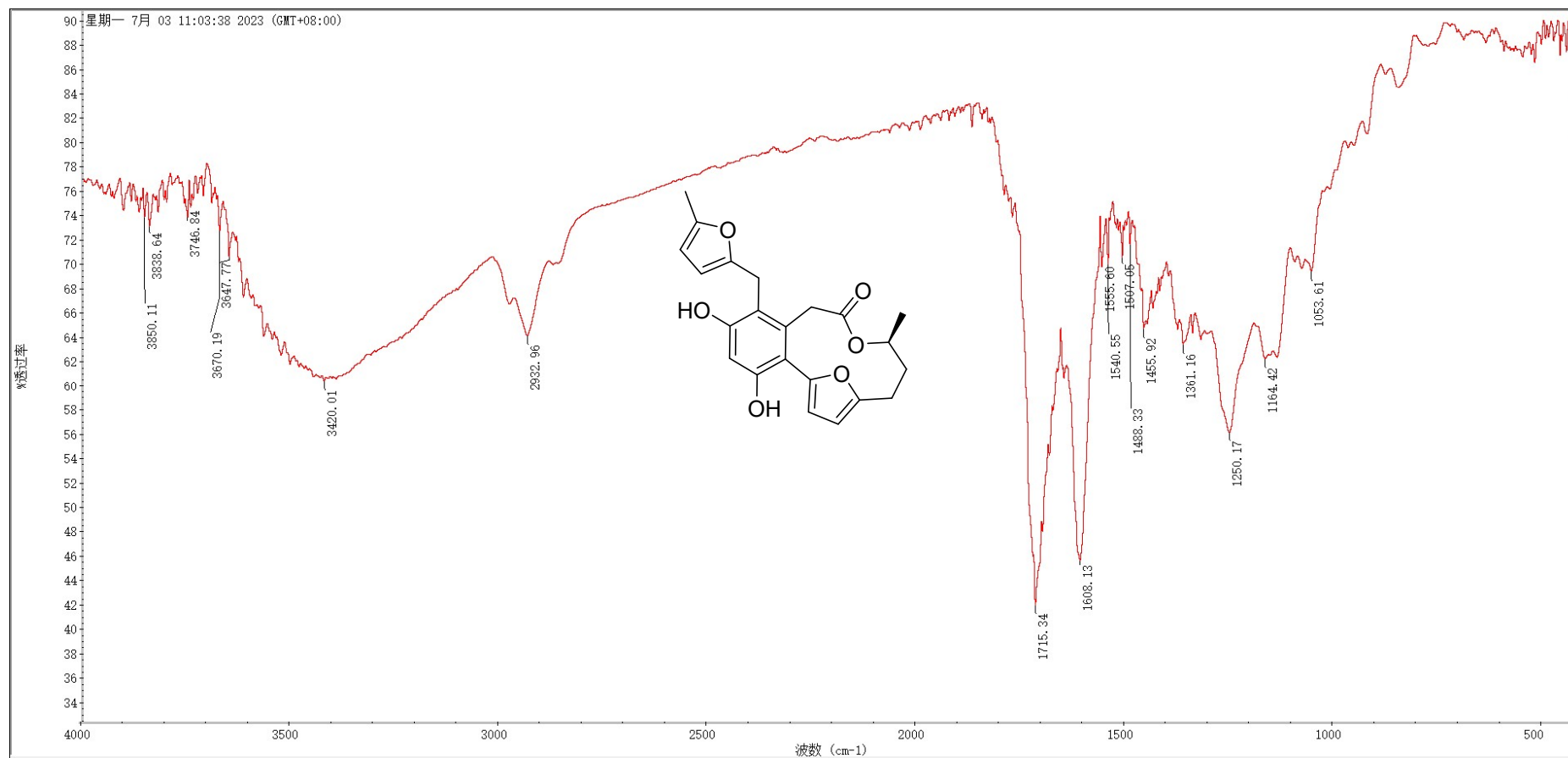


Figure S9. UV Spectrum of Penicurvularin A (**1**) in MeOH

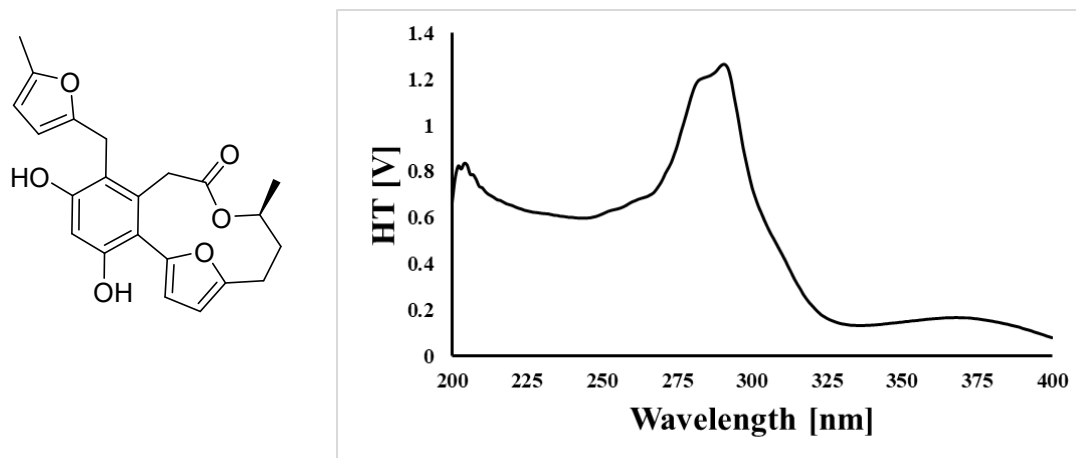


Figure S10. ECD Spectrum of Penicurvularin A (**1**) in MeOH

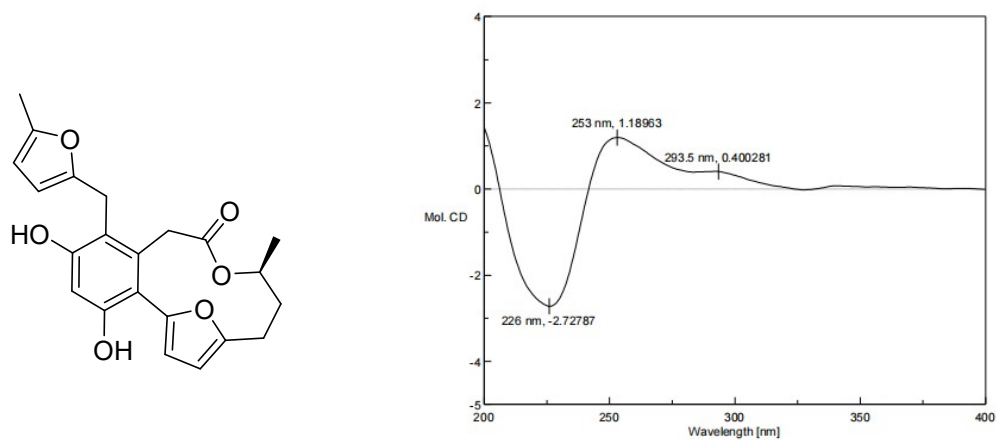


Figure S11. The Optimized Conformers for **1a**

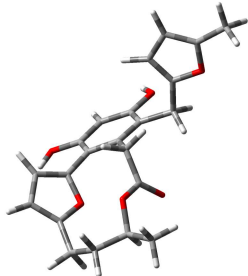
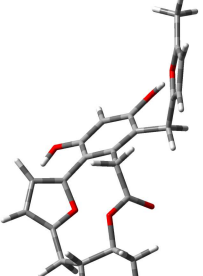
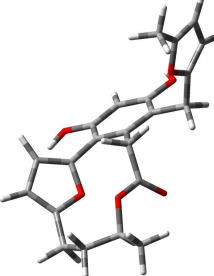
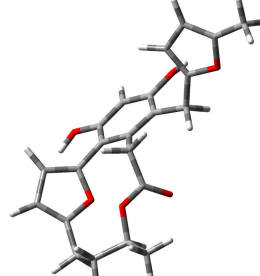
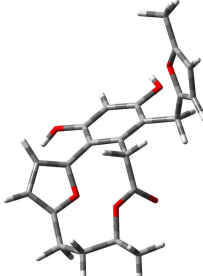
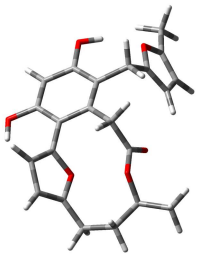
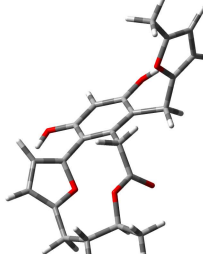
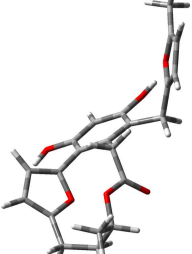
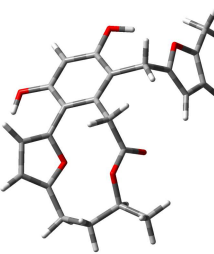
				
1aC1 (2.49%)	1aC2 (50.80%)	1aC3 (4.71%)	1aC4 (4.55%)	1aC6 (1.14%)
				
1aC7 (13.67%)	1aC9 (6.35%)	1aC13 (3.12%)	1aC14 (13.17%)	

Figure S12. ^1H NMR Spectrum of Penicurvularin B (2; 600 MHz, CDCl_3)

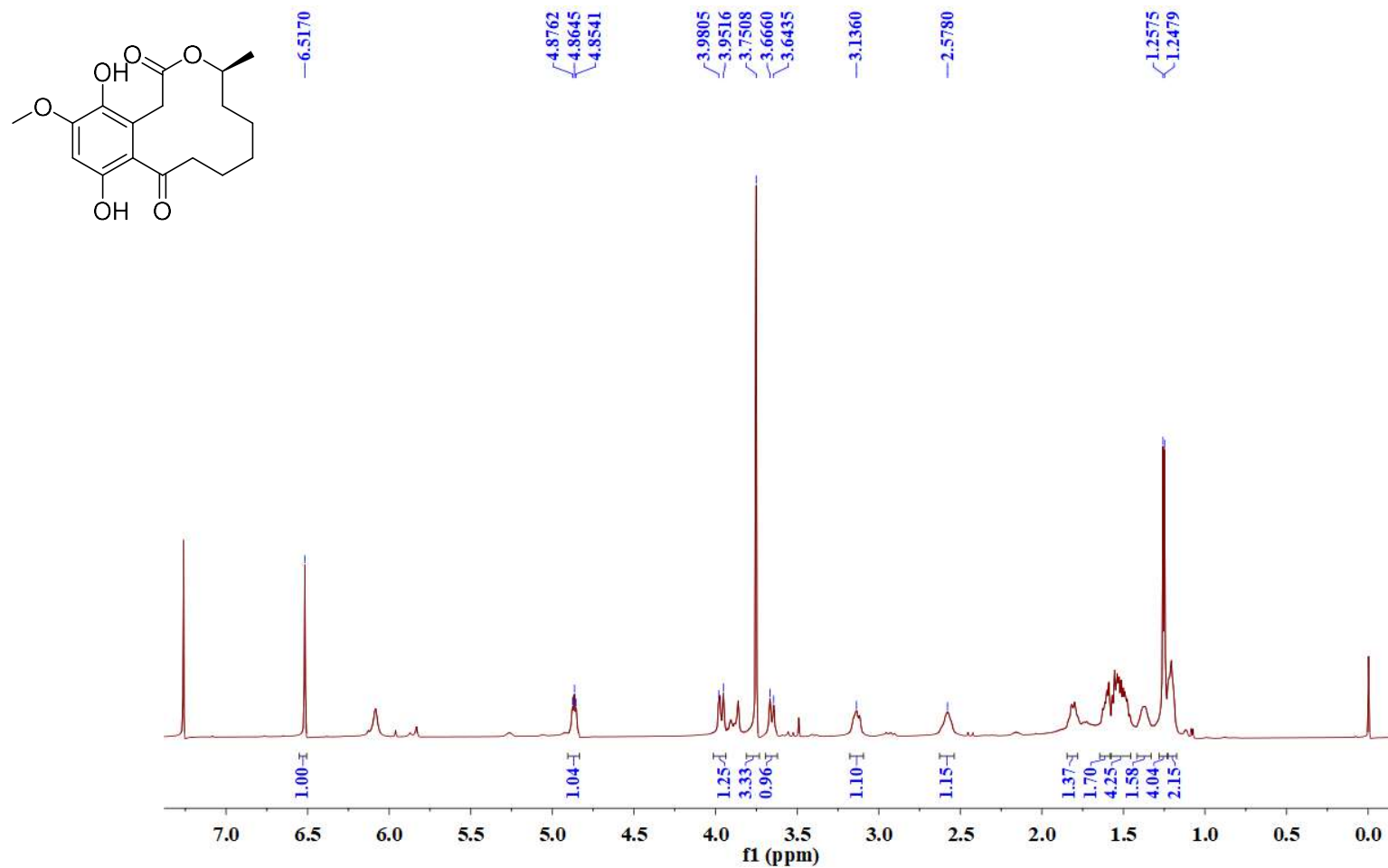


Figure S13. ^{13}C NMR Spectrum of Penicurvularin B (**2**; 150 MHz, CDCl_3)

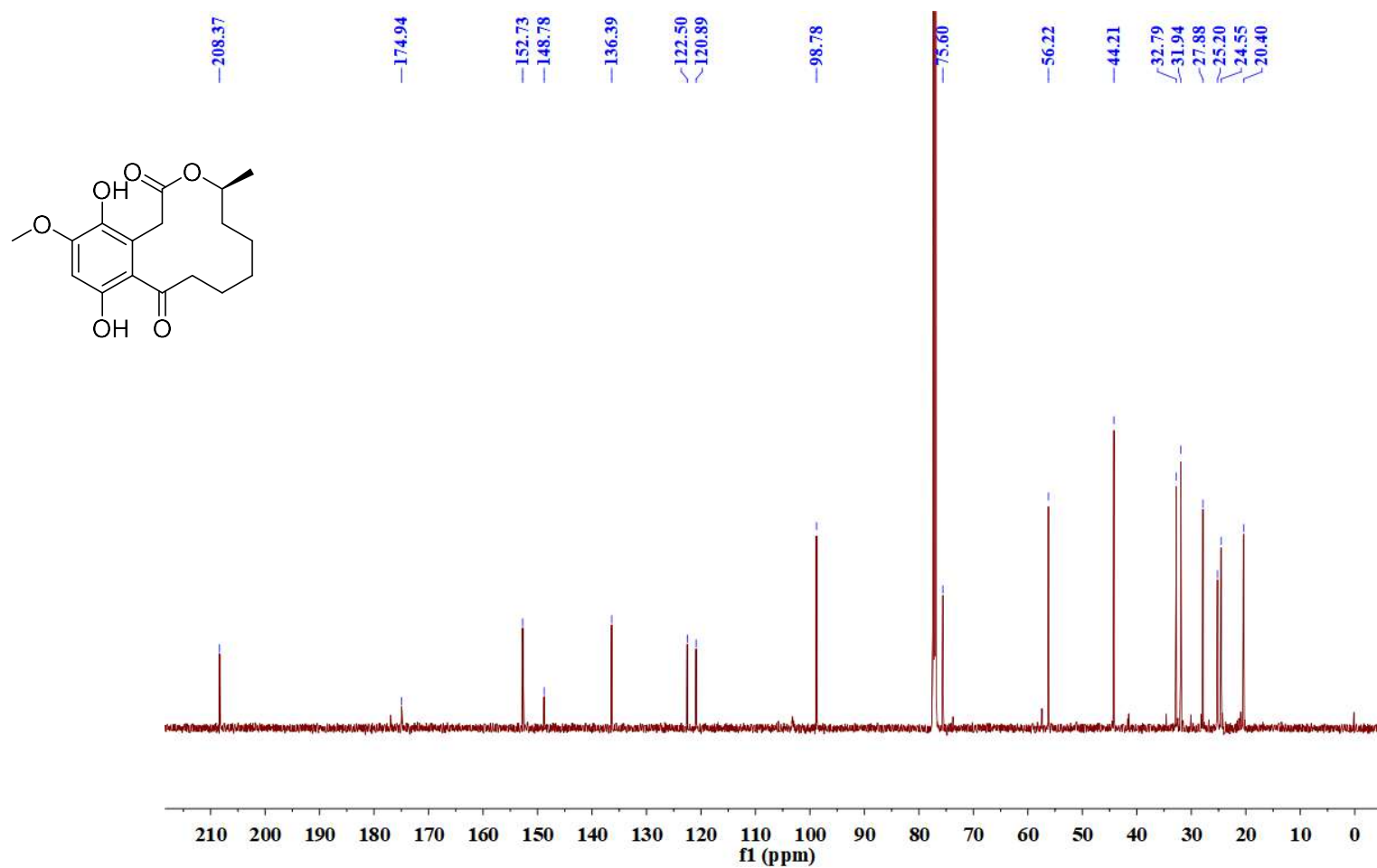


Figure S14. HSQC Spectrum of Penicurvularin B (**2**; 600 MHz, CDCl₃)

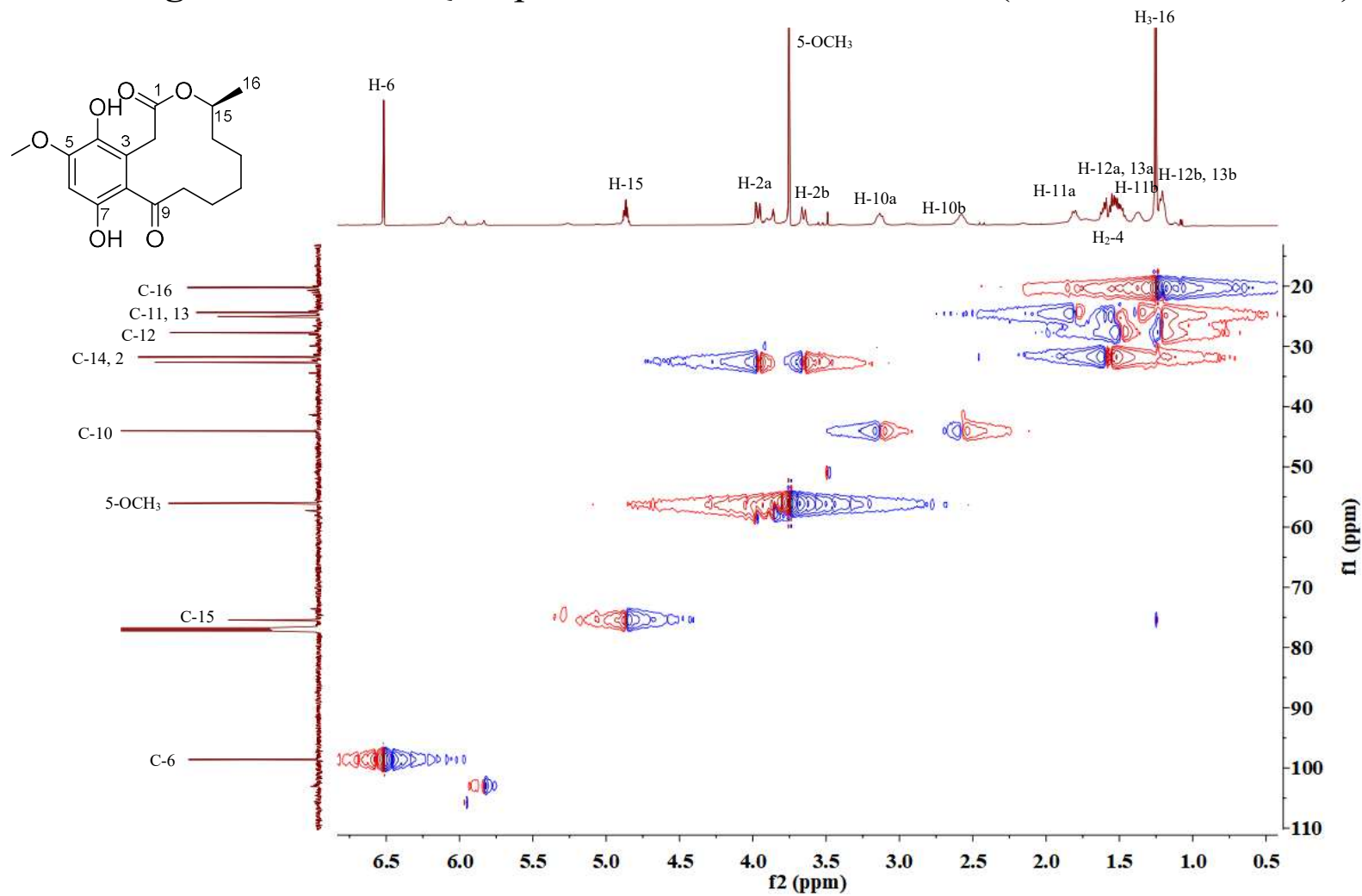


Figure S15. ^1H - ^1H COSY Spectrum of Penicurvularin B (**2**; 600 MHz, CDCl_3)

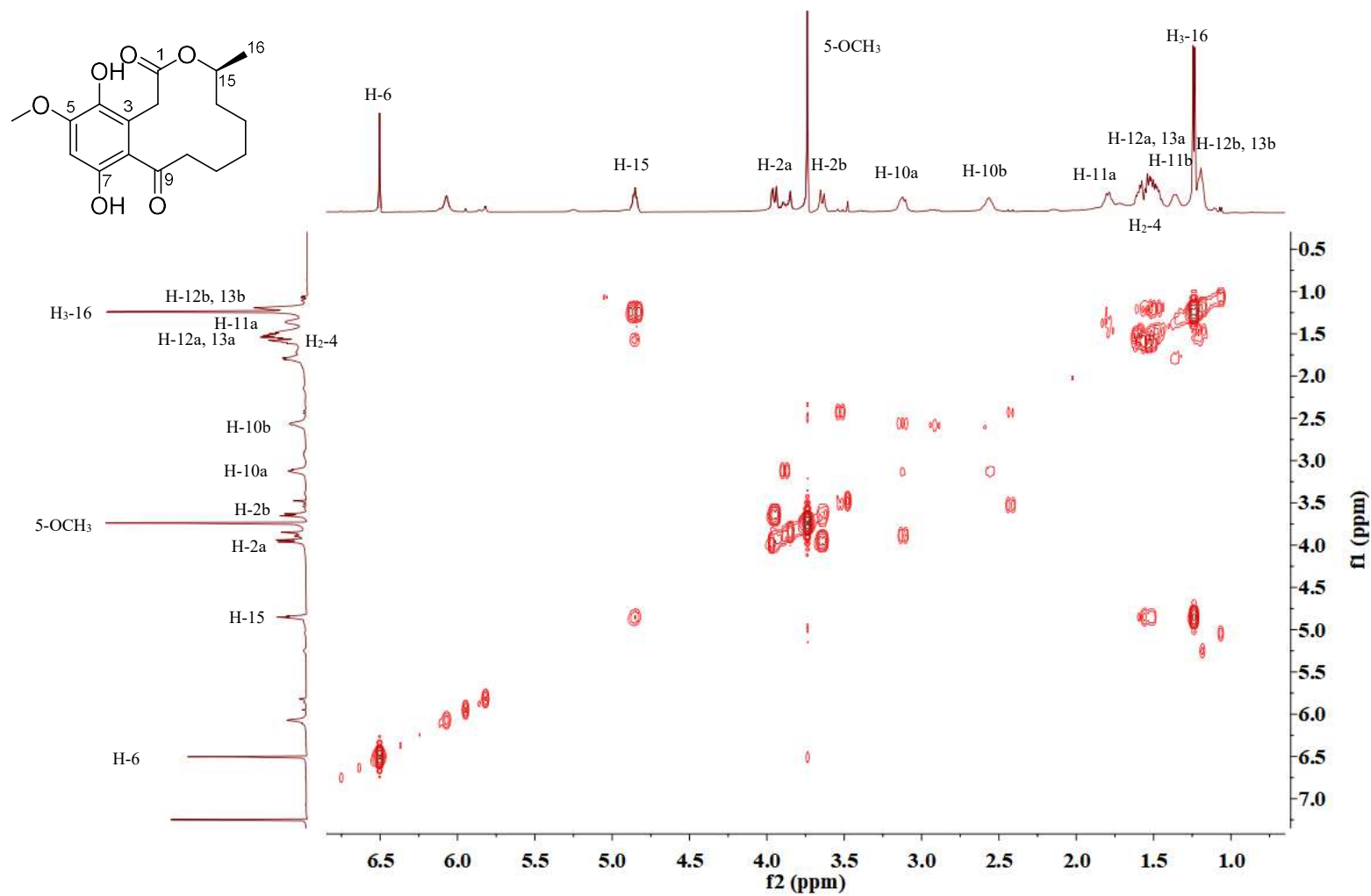


Figure S16. HMBC Spectrum of Penicurvularin B (**2**; 600 MHz, CDCl₃)

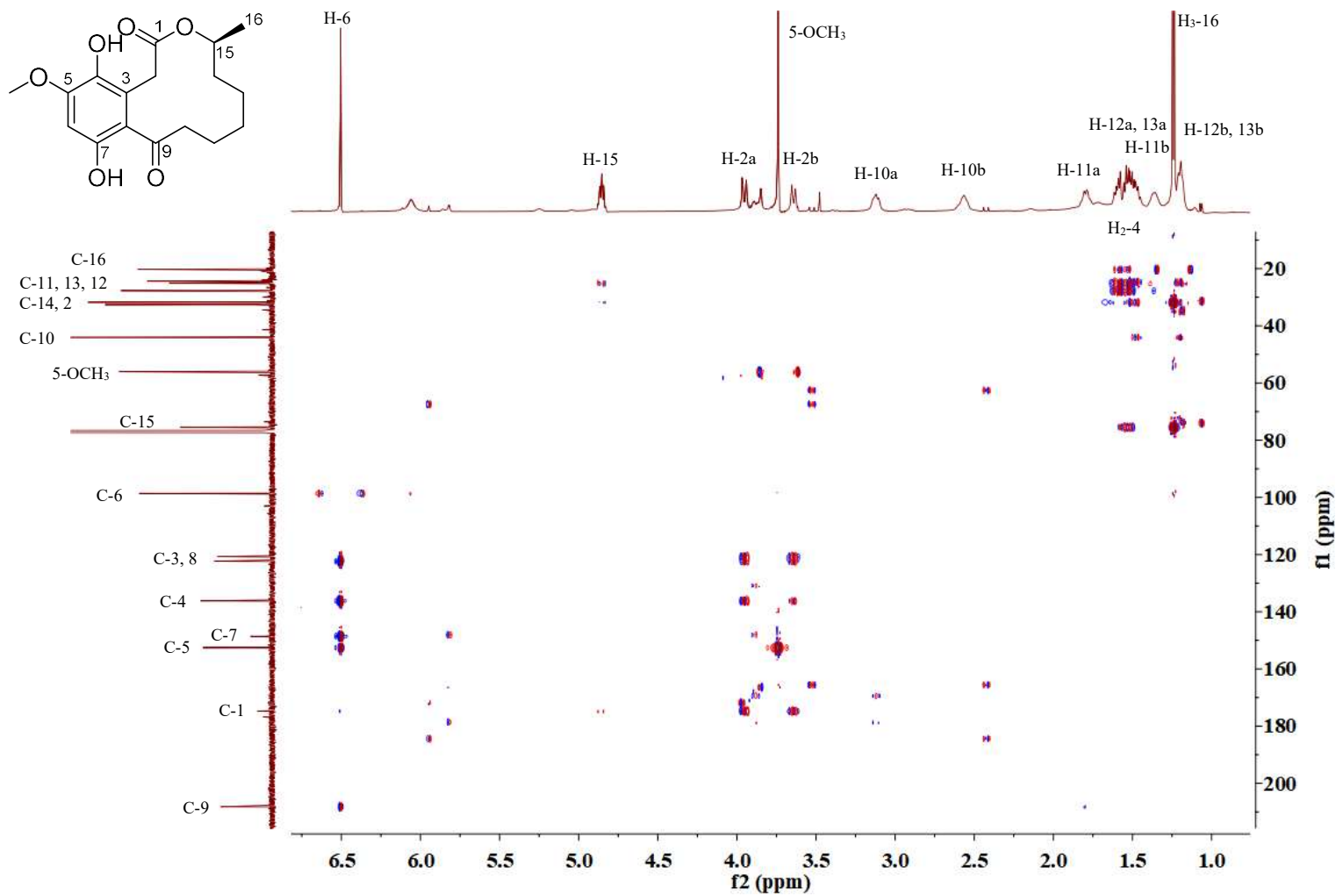


Figure S17. NOESY Spectrum of Penicurularin B (**2**; 600 MHz, CDCl₃)

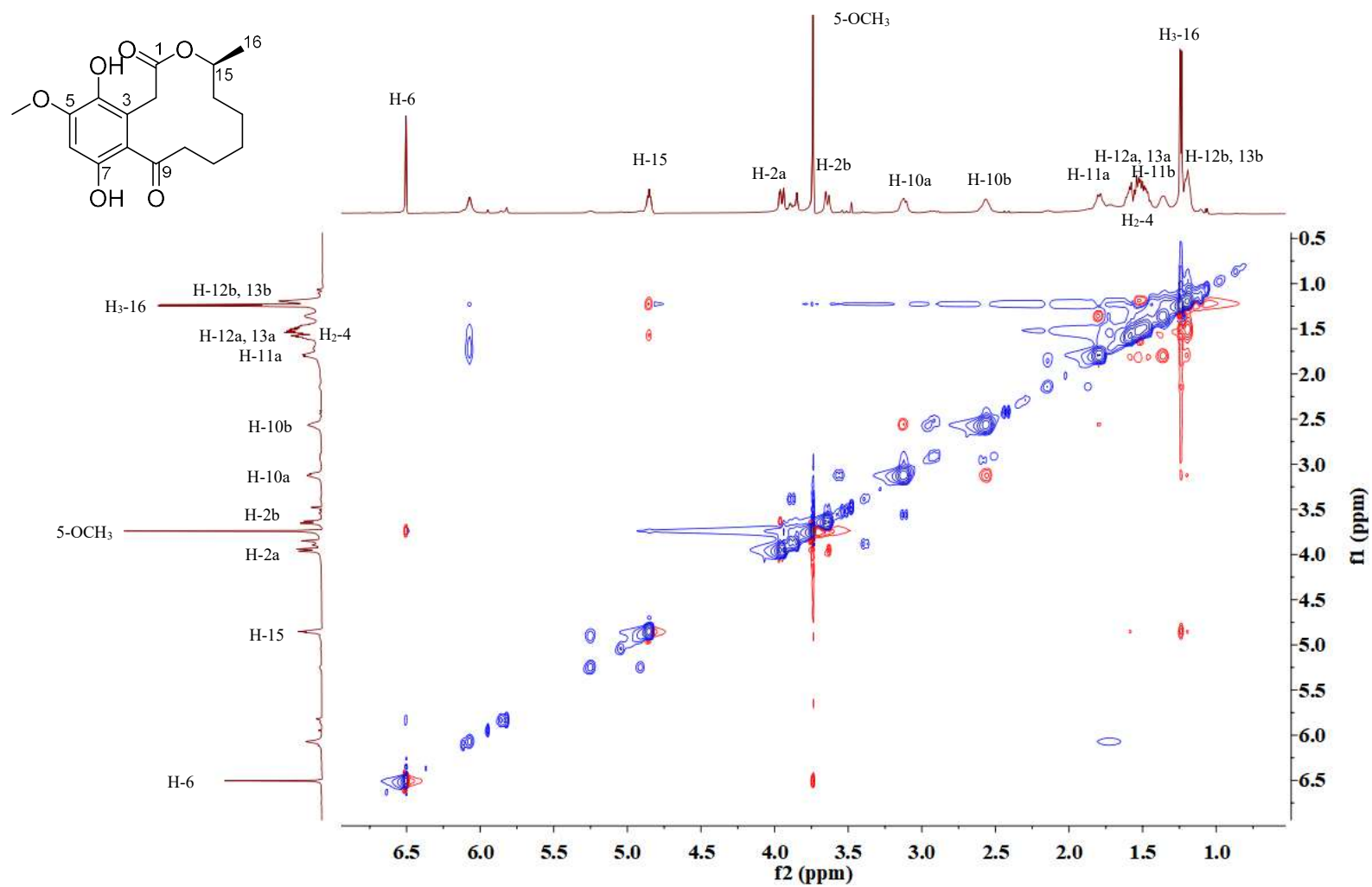


Figure S18. HRESIMS Spectrum of Penicurvularin B (2)

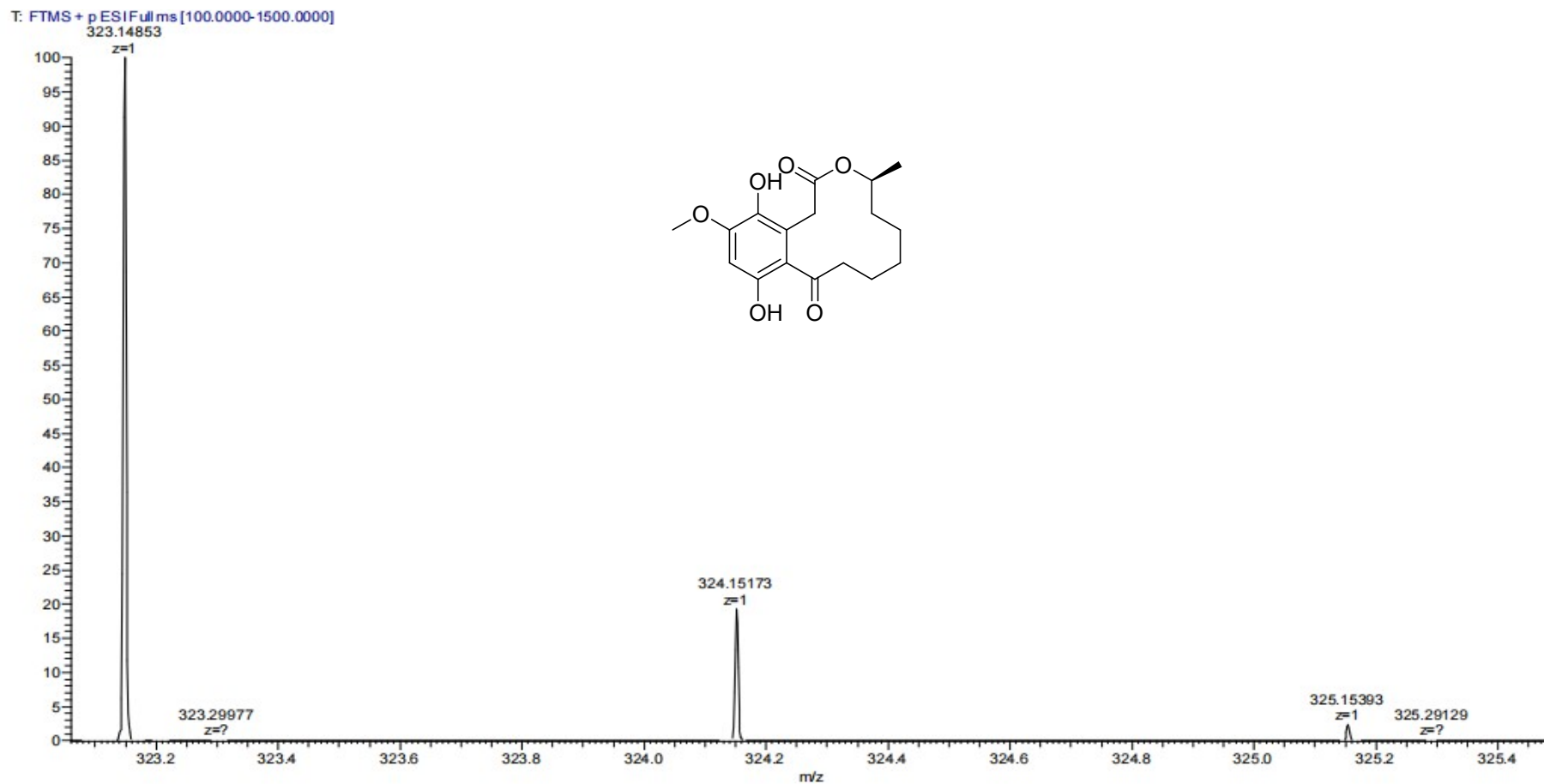


Figure S19. IR Spectrum of Penicurvularin B (2)

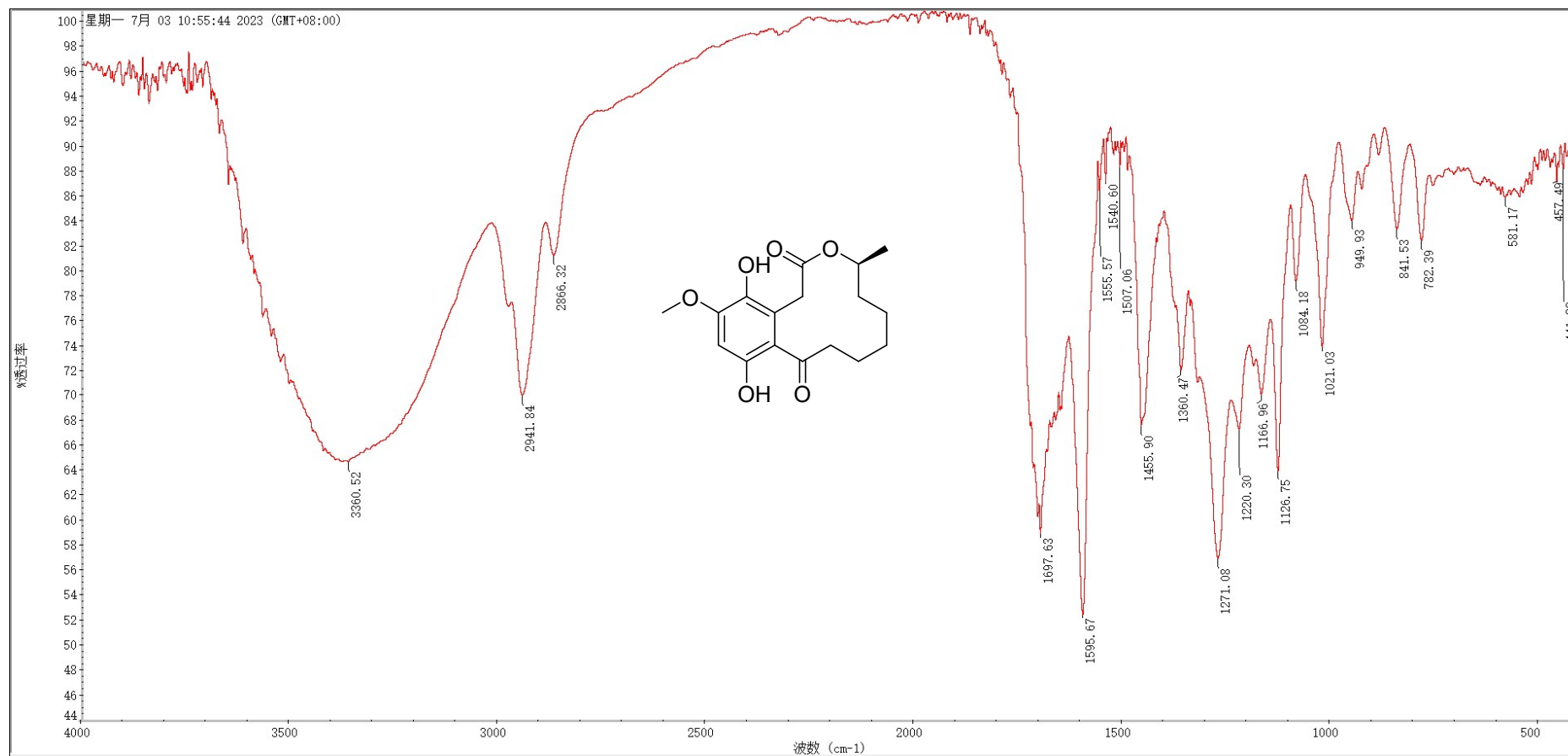


Figure S20. UV Spectrum of Penicurvularin B (2) in MeOH

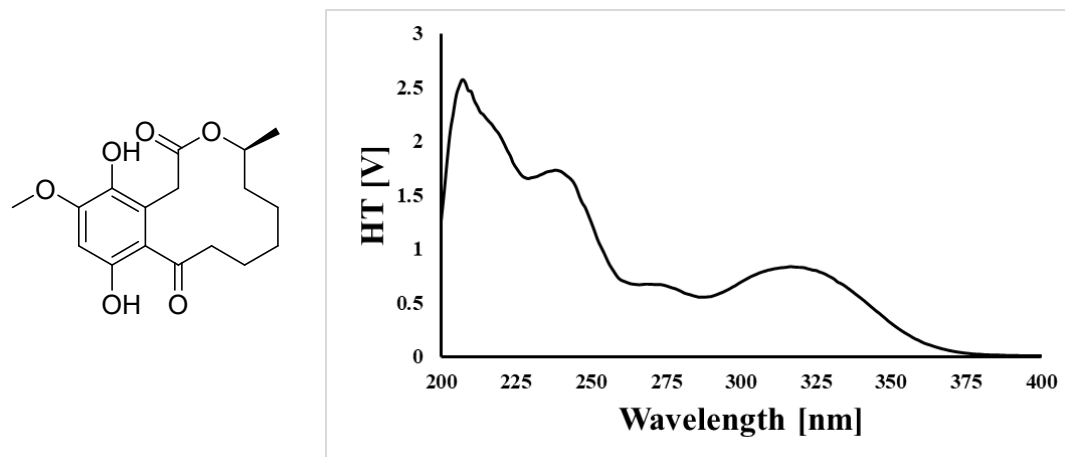


Figure S21. ECD Spectrum of Penicurvularin B (2) in MeOH

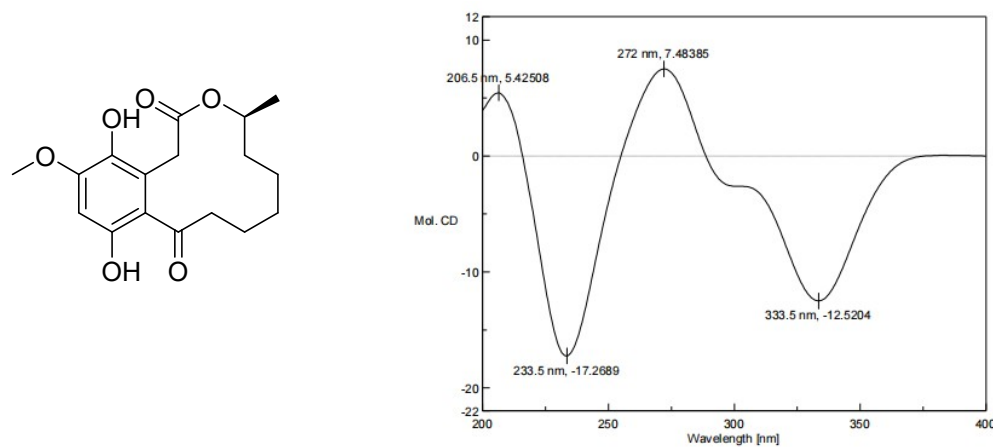


Figure S22. ^1H NMR Spectrum of 5-Methoxycurvularin (**3**; 600 MHz, Acetone- d_6)

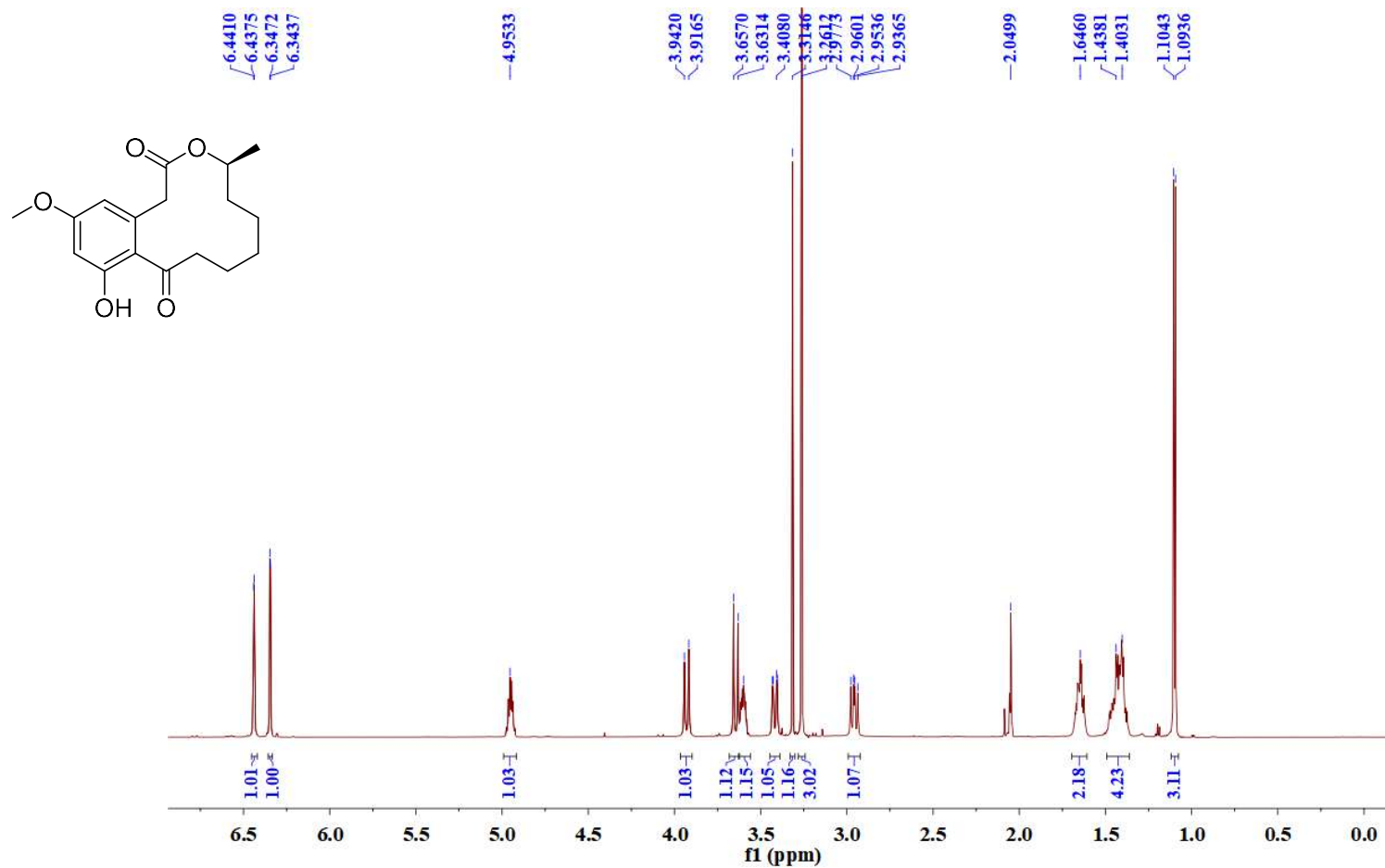


Figure S23. ^{13}C NMR Spectrum of 5-Methoxycurvularin (**3**; 150 MHz, Acetone- d_6)

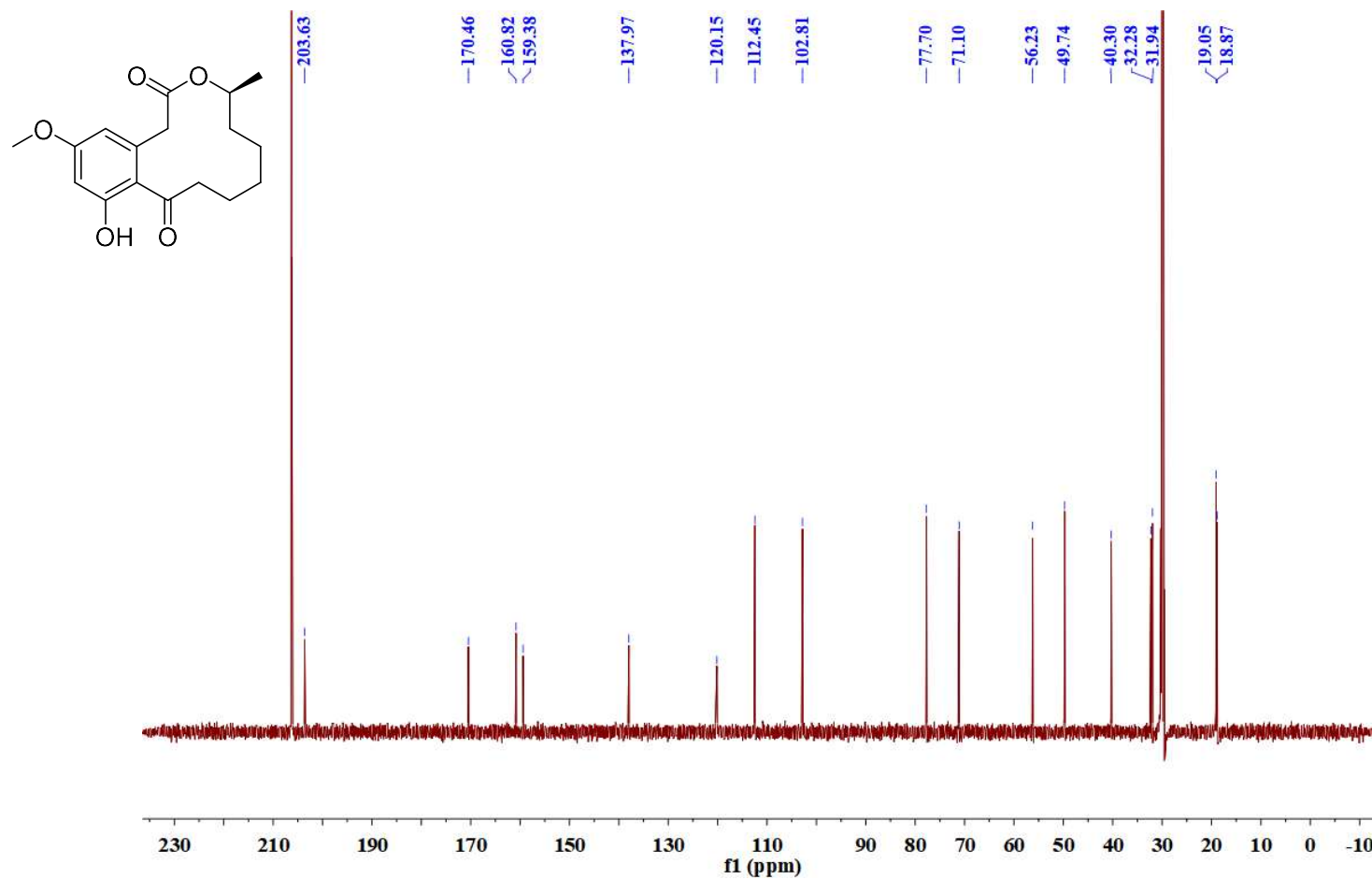


Figure S24. ^1H NMR Spectrum of Curvularin (**4**; 600 MHz, Acetone- d_6)

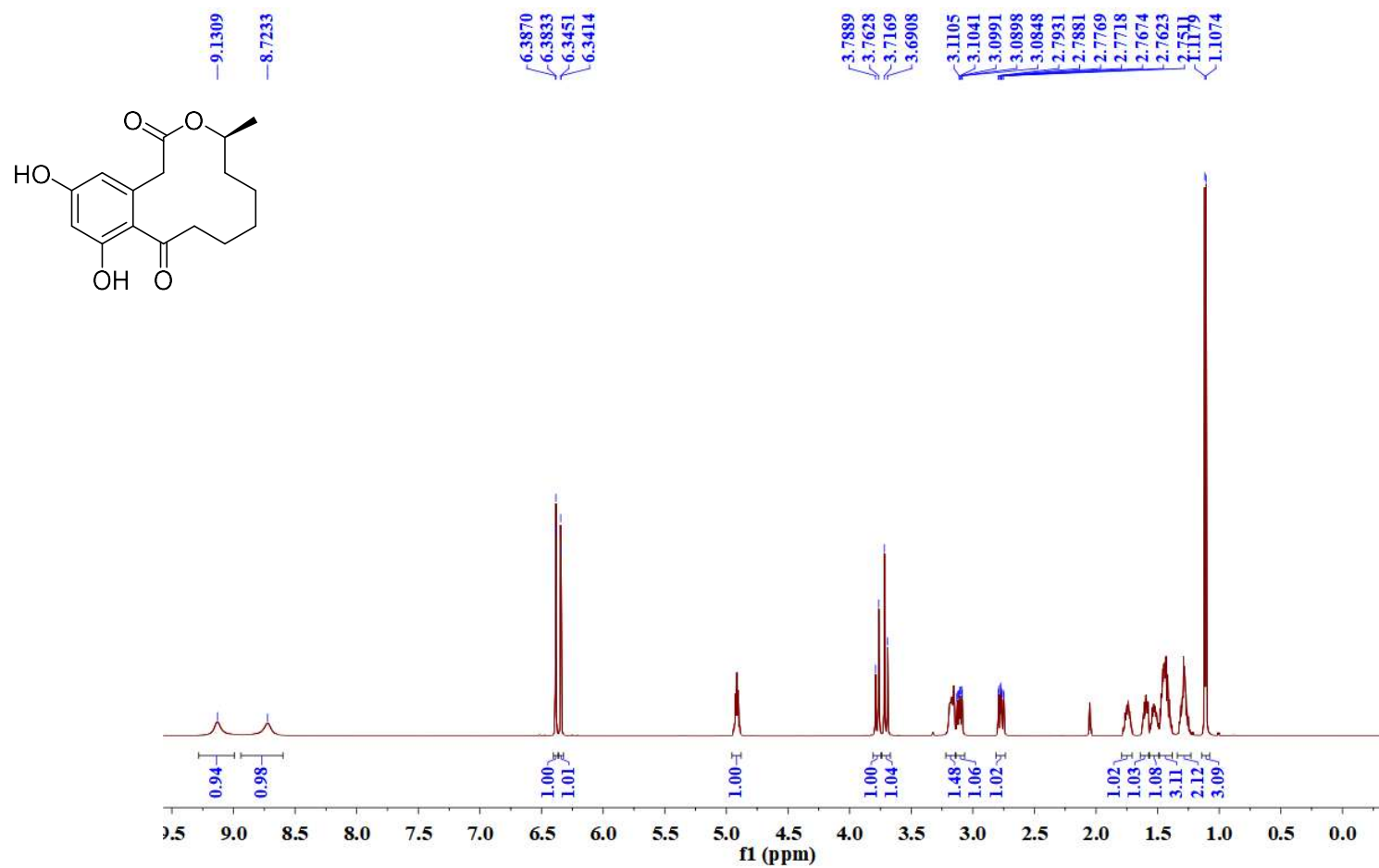


Figure S25. ^{13}C NMR Spectrum of Curvularin (**4**; 150 MHz, Acetone- d_6)

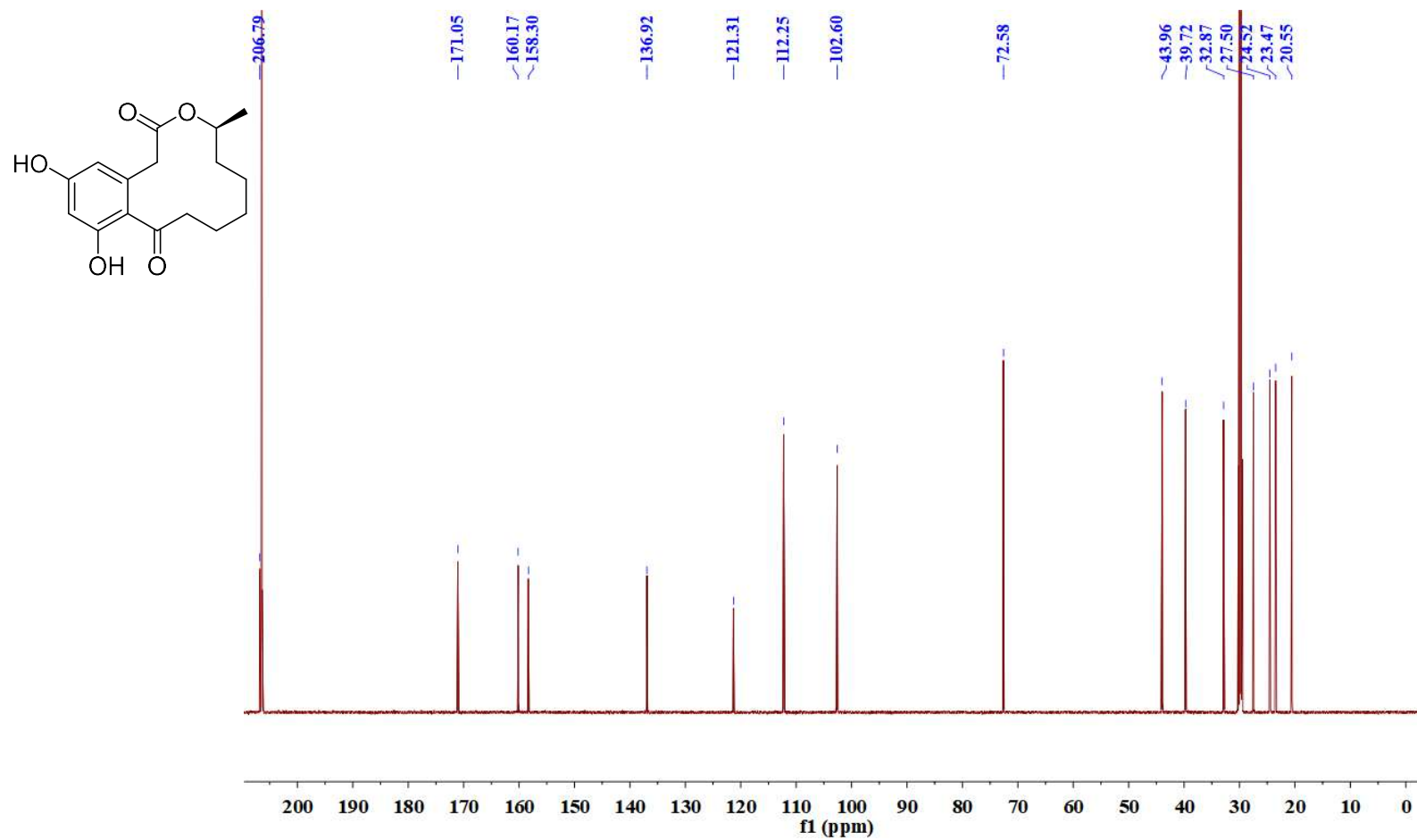


Figure S26. ^1H NMR Spectrum of Dehydrocurvularin (**5**; 600 MHz, Acetone- d_6)

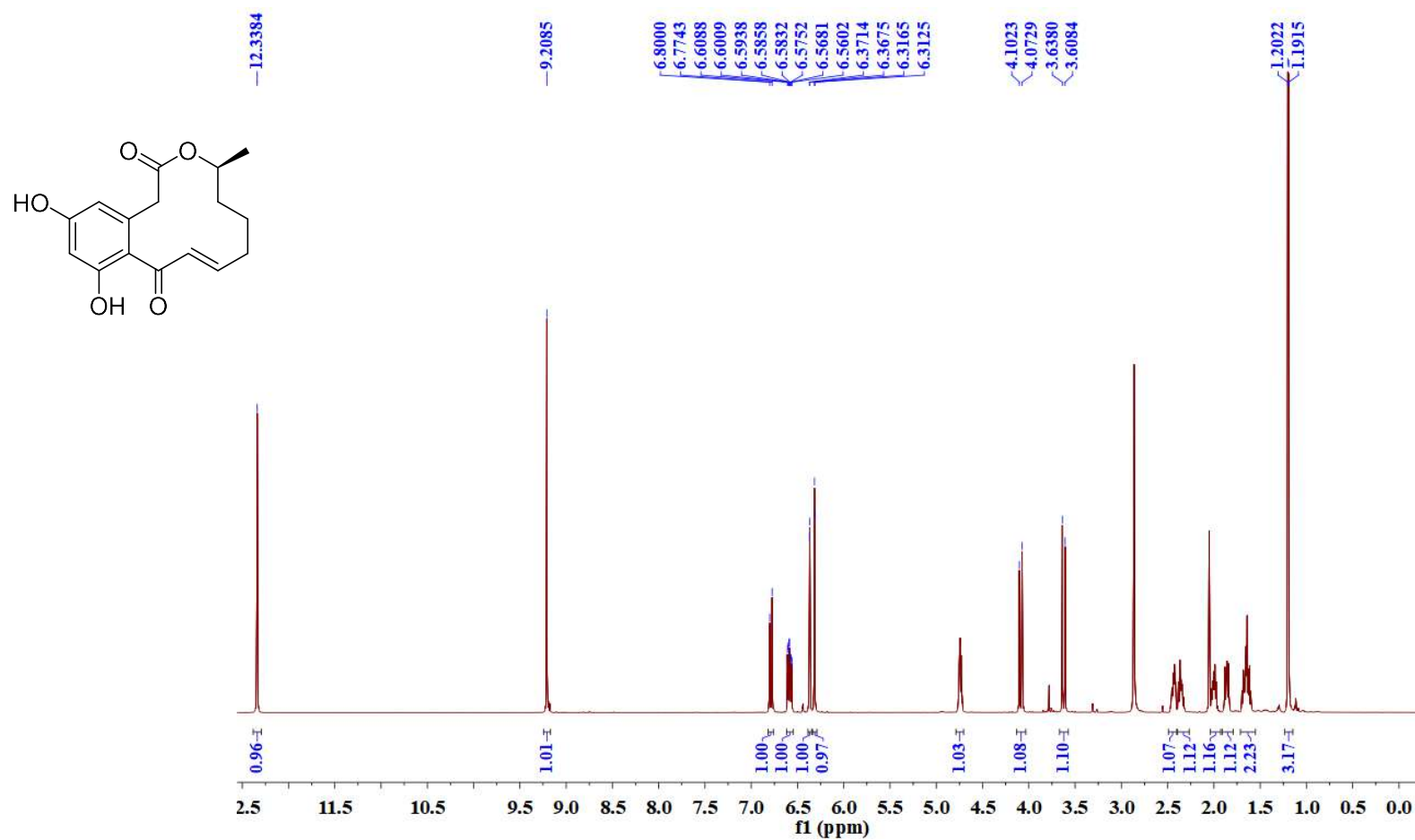


Figure S27. ^{13}C NMR Spectrum of Dehydrocurvularin (**5**; 150 MHz, Acetone- d_6)

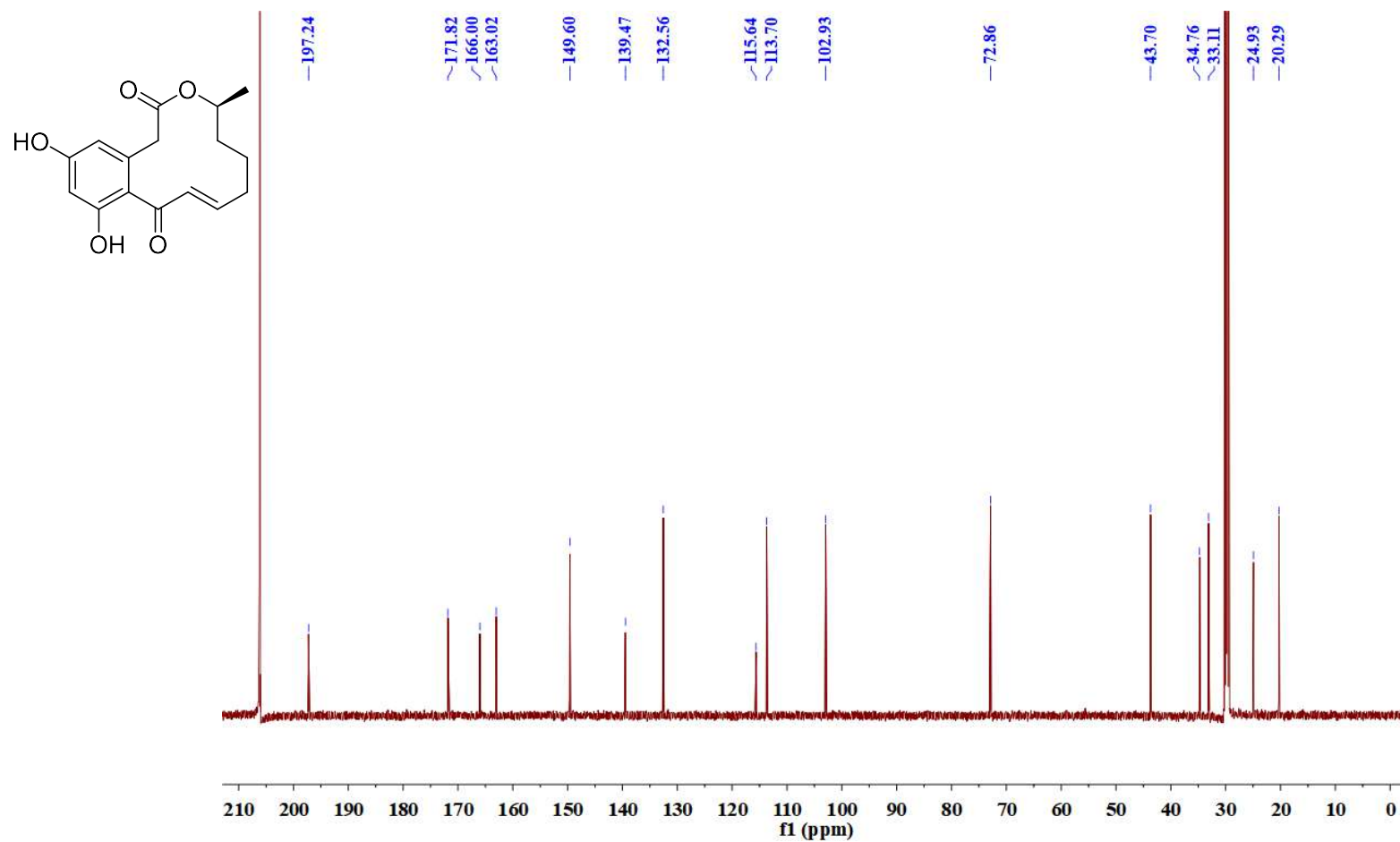


Table S1. Relative energies of dominant conformers and their Boltzmann population distributions of **1a**

conformers	population (%)	Energy (hartree)
1	2.49	-1303.260749
2	50.8	-1303.263594
3	4.71	-1303.26135
4	4.55	-1303.261317
6	1.14	-1303.260015
7	13.67	-1303.262355
9	6.35	-1303.261633
13	3.12	-1303.260963
14	13.17	-1303.262321