

Supporting Information for

Secoemestrin D, A Cytotoxic Epitetrahydrodioxopiperazine and Emericellenes A–E, Five Sesterterpenoids from *Emericella* sp. AST0036, a Fungal Endophyte of *Astragalus lentiginosus*¹

Ya-ming Xu,[†] Patricia Espinosa-Artiles,[†] Mangping X. Liu,[†] A. Elizabeth Arnold,[‡] and A. A. Leslie Gunatilaka^{†,*}

[†]Southwest Center for Natural Products Research and Commercialization, School of Natural Resources and the Environment, College of Agriculture and Life Sciences, University of Arizona, 250 E. Valencia Road, Tucson, Arizona 85706, United States

[‡]School of Plant Sciences, College of Agriculture and Life Sciences, University of Arizona, Tucson, Arizona 85721, United States

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Figure S1. ^1H NMR Spectrum (400 MHz) of Secoemestrin D (**1**) in CDCl_3

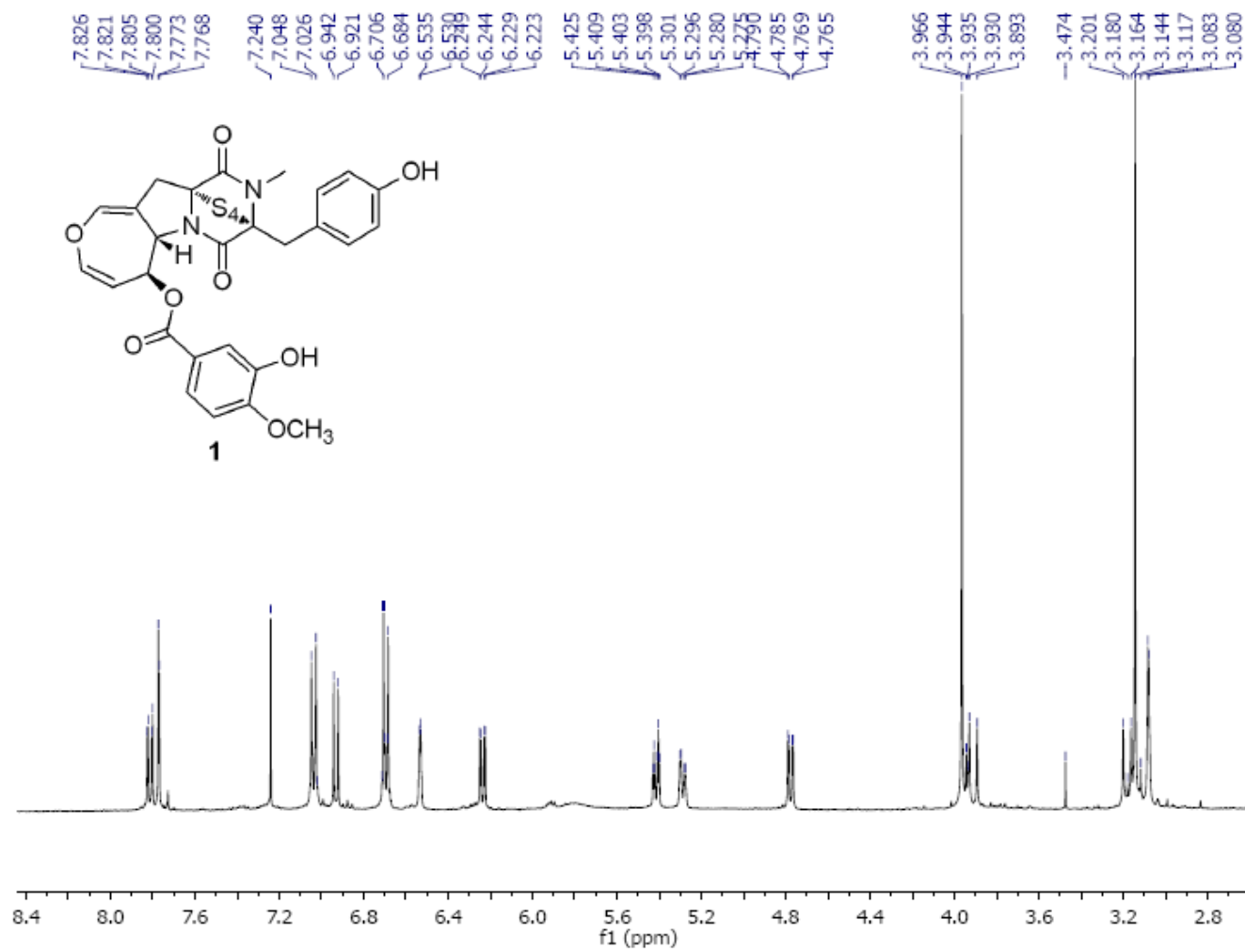
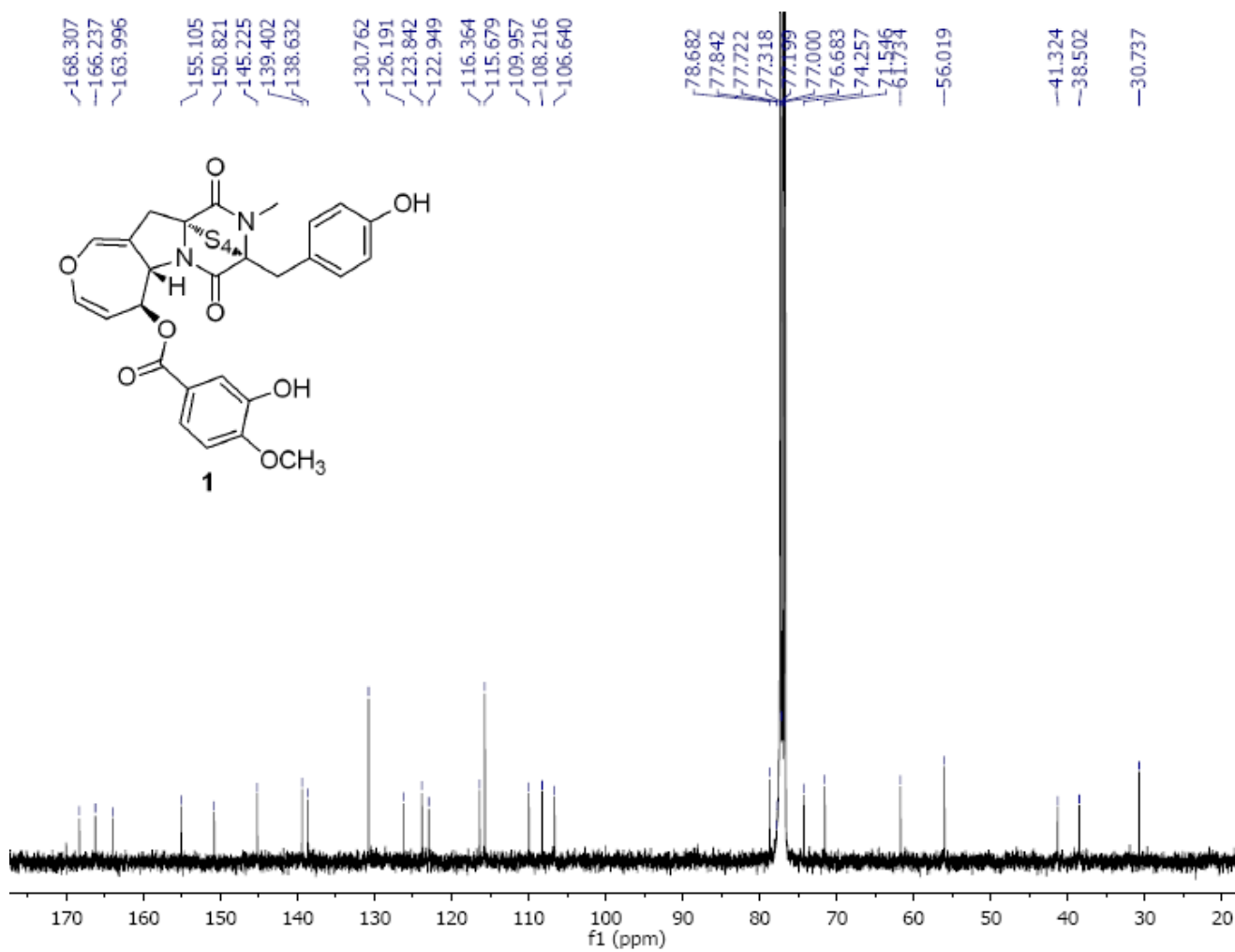


Figure S2. ^{13}C NMR Spectrum (100 MHz) of Secoemestrin D (**1**) in CDCl_3



168.307
166.237
163.996
155.105
150.821
145.225
139.402
138.632
130.762
126.191
123.842
122.949
116.364
115.679
109.957
108.216
106.640

78.682
77.842
77.722
77.318
77.199
77.000
76.683
74.257
61.546
61.534
56.019
41.324
38.502
30.737

Figure S3. HSQC Spectrum (400 MHz) of Secoemestrin D (1) A in CDCl₃

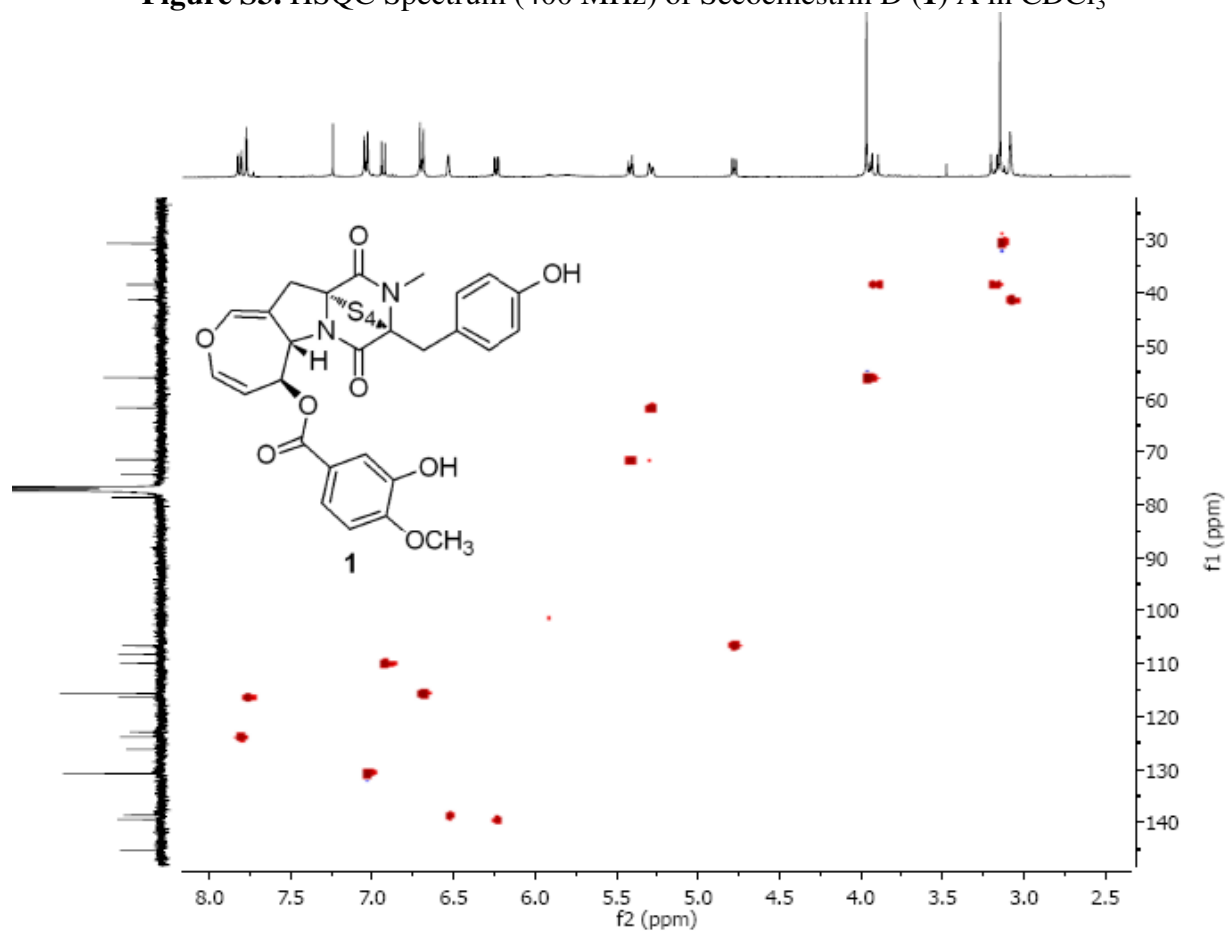


Figure S4. HMBC Spectrum (400 MHz) of Secoemestrin D (1) A in CDCl₃

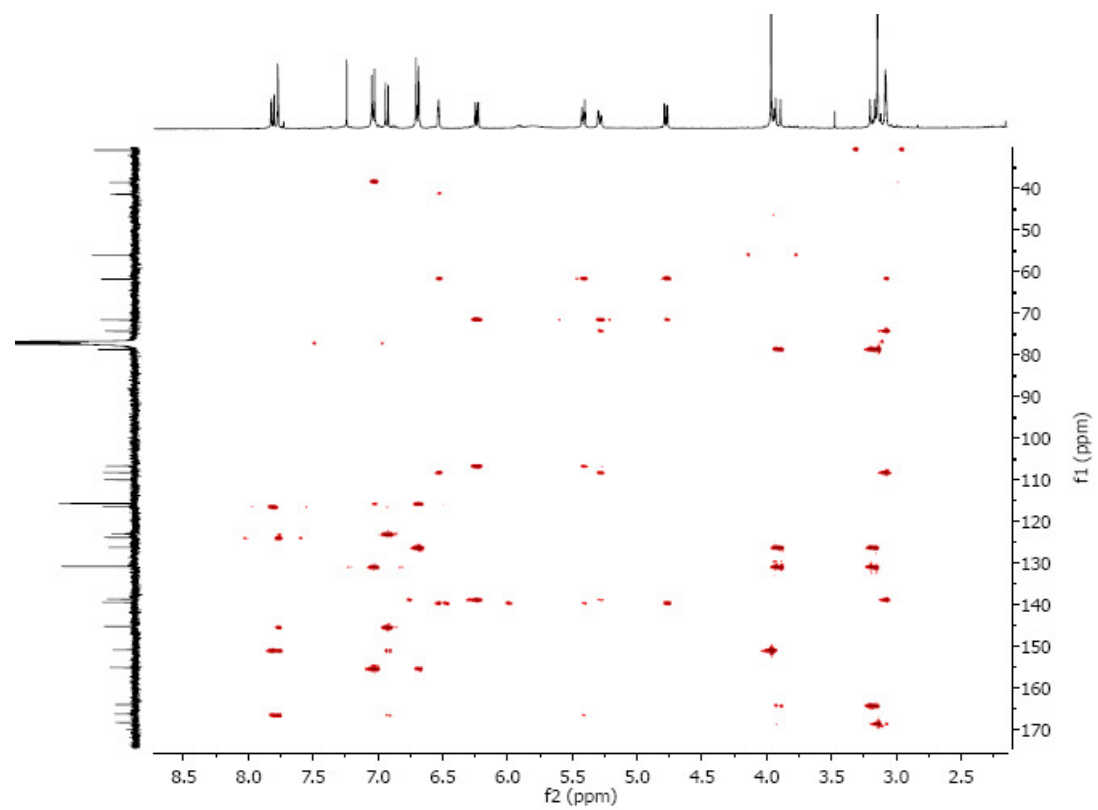


Figure S5. ^1H NMR Spectrum (400 MHz) of Emericellene A (**2**) in CDCl_3

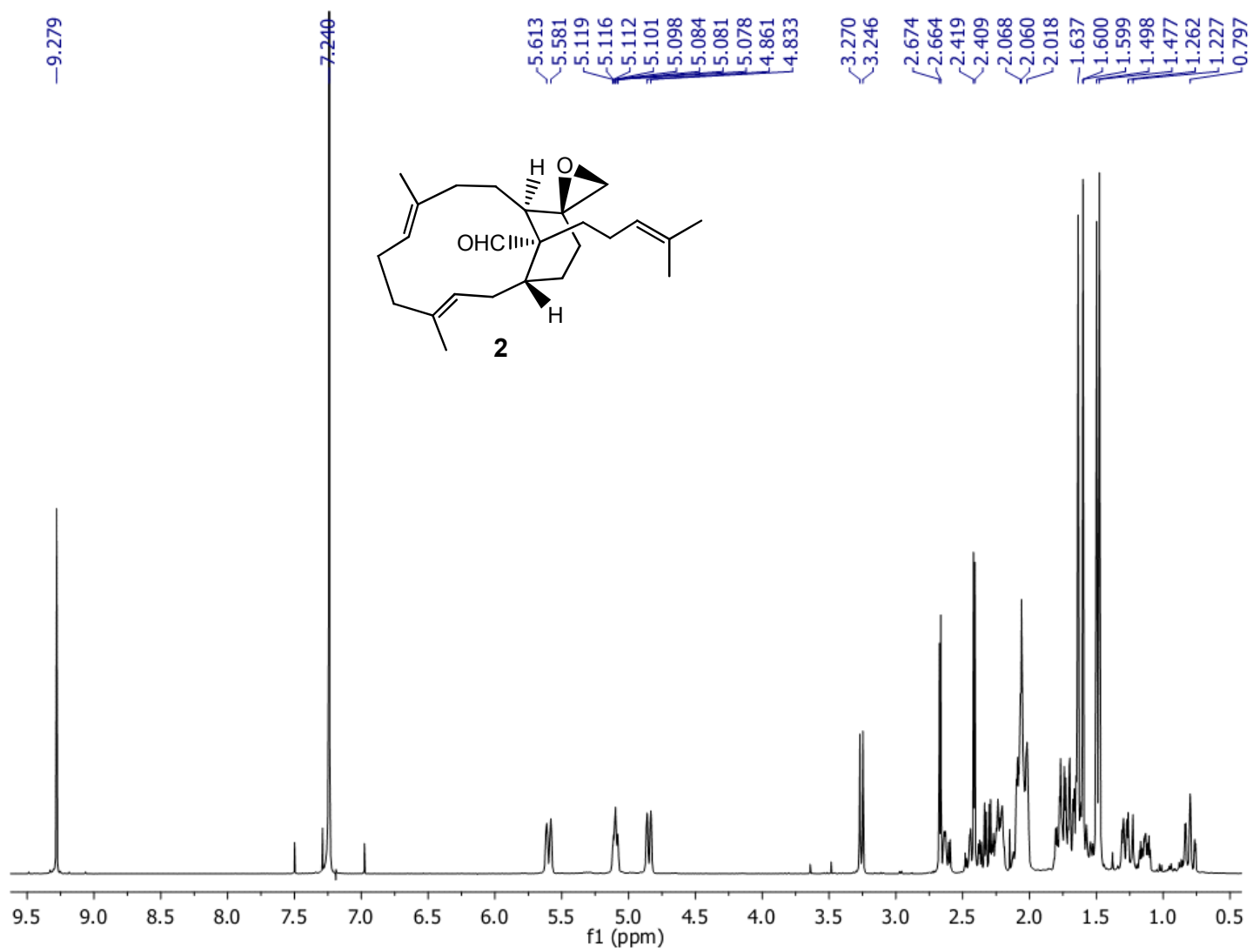


Figure S6. ^{13}C NMR Spectrum (100 MHz) of Emericellene A (**2**) in CDCl_3

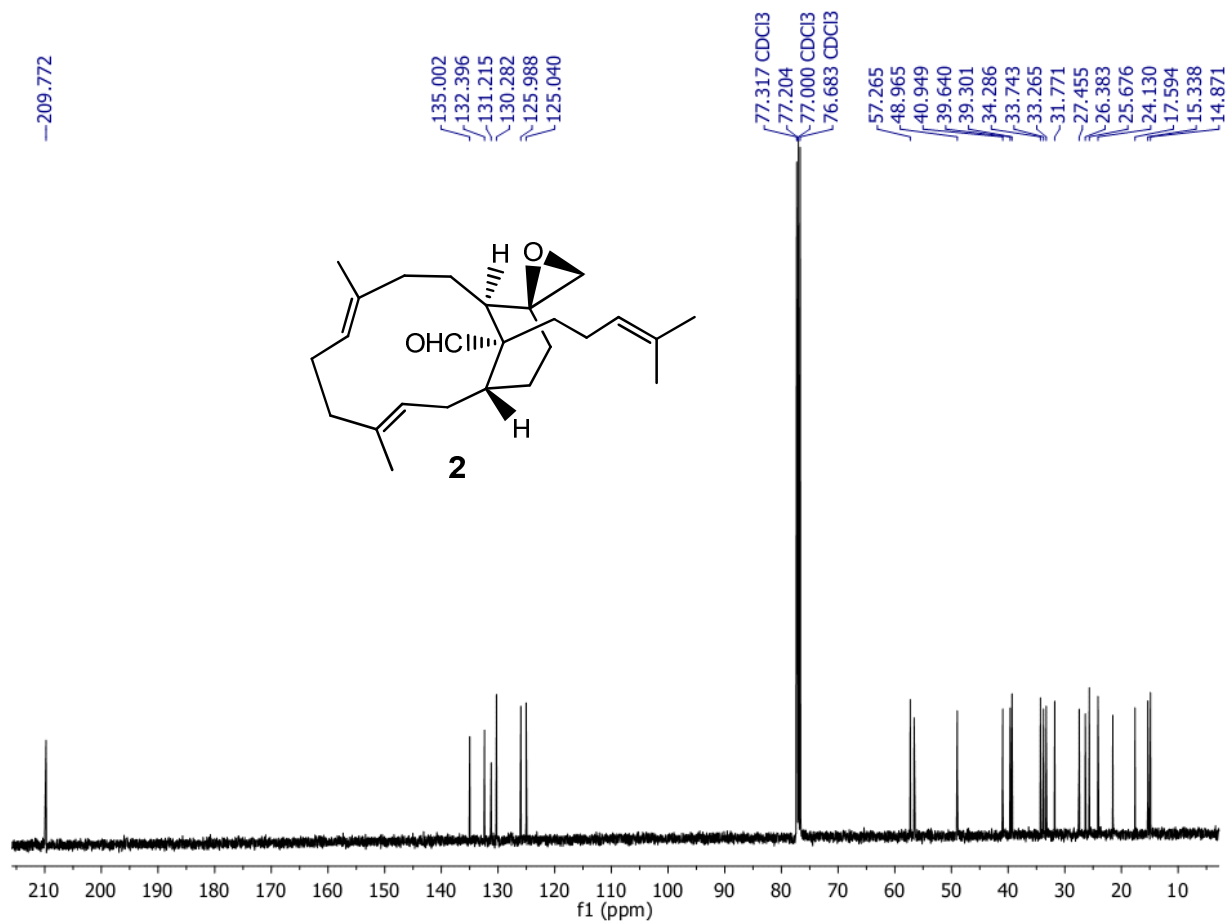


Figure S7. HSQC Spectrum (400 MHz) of Emericellene A (**2**) in CDCl₃

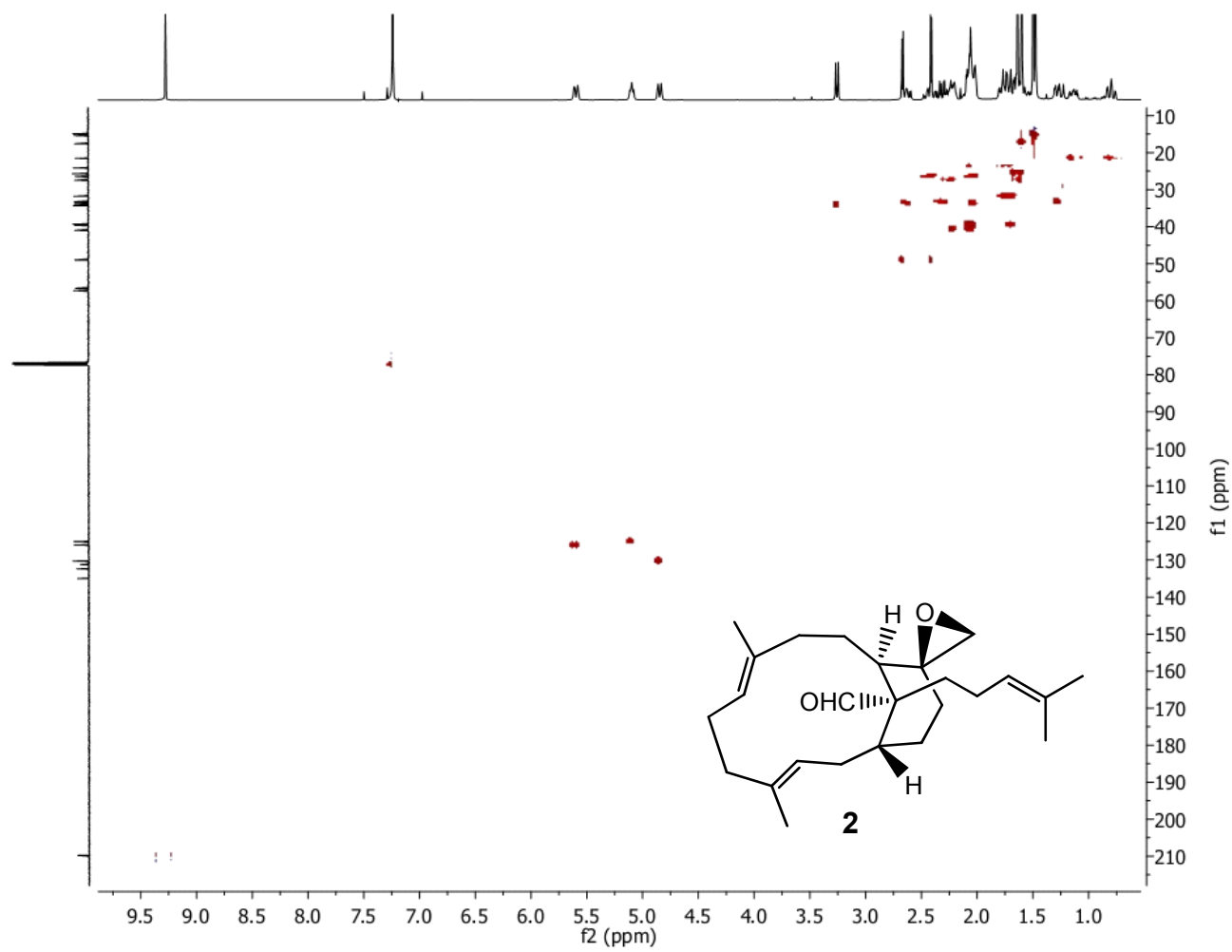


Figure S8. HMBC Spectrum (400 MHz) of Emericellene A (**2**) in CDCl₃

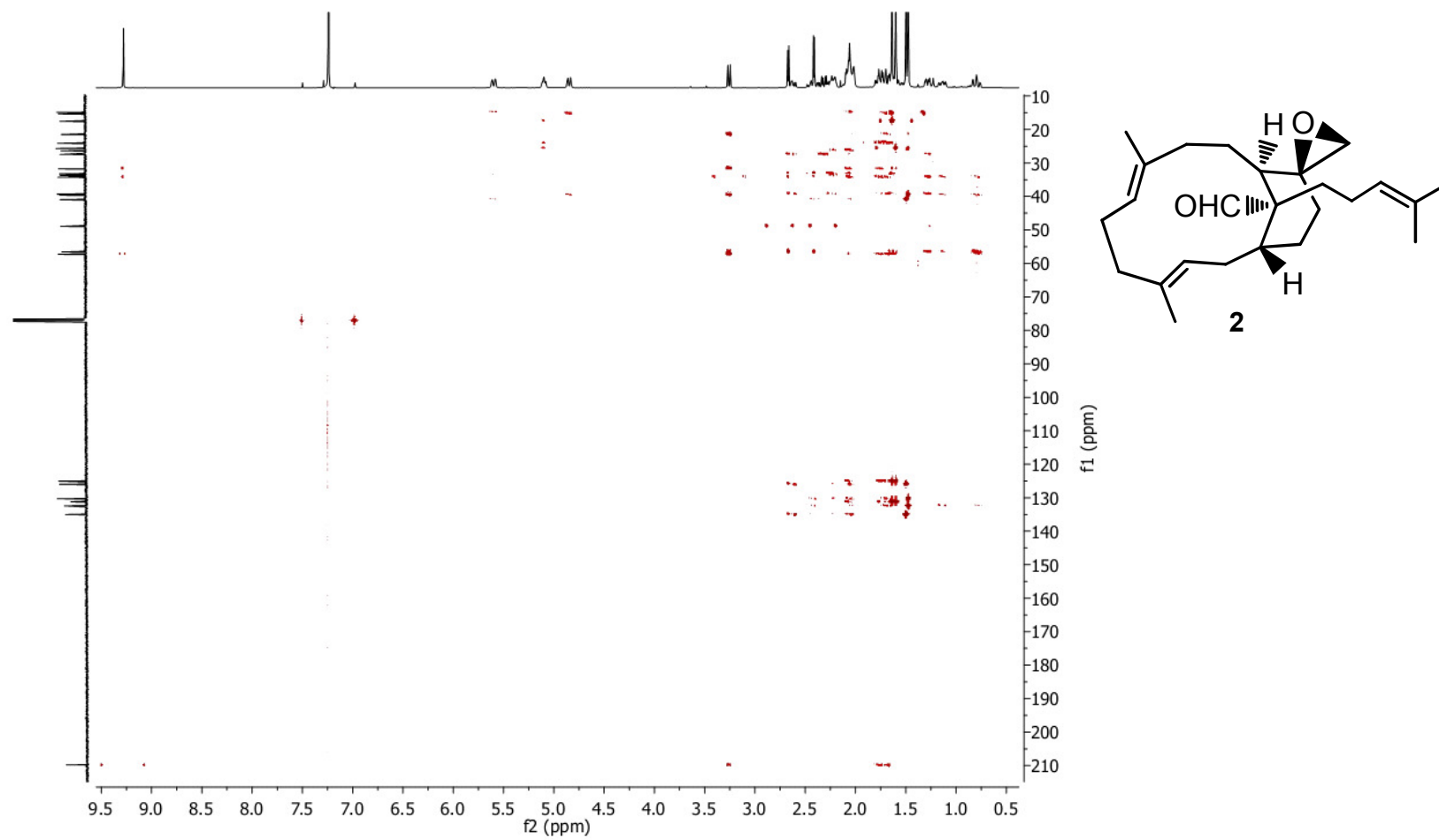


Figure S10. ^{13}C NMR Spectrum (100 MHz) of Emericellene B (**3**) in CDCl_3

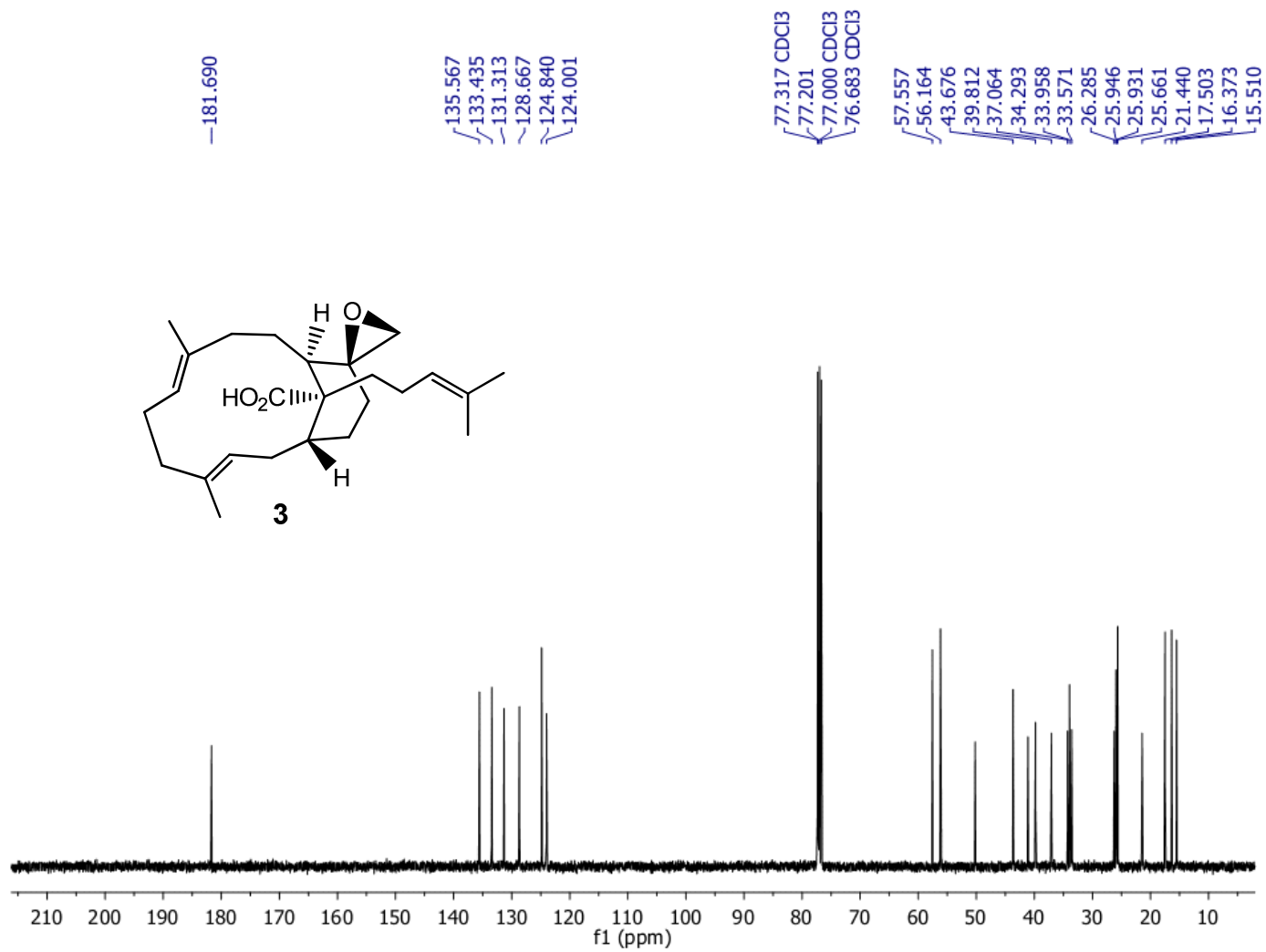


Figure S11. HSQC Spectrum (400 MHz) of Emericellene B (**3**) in CDCl₃

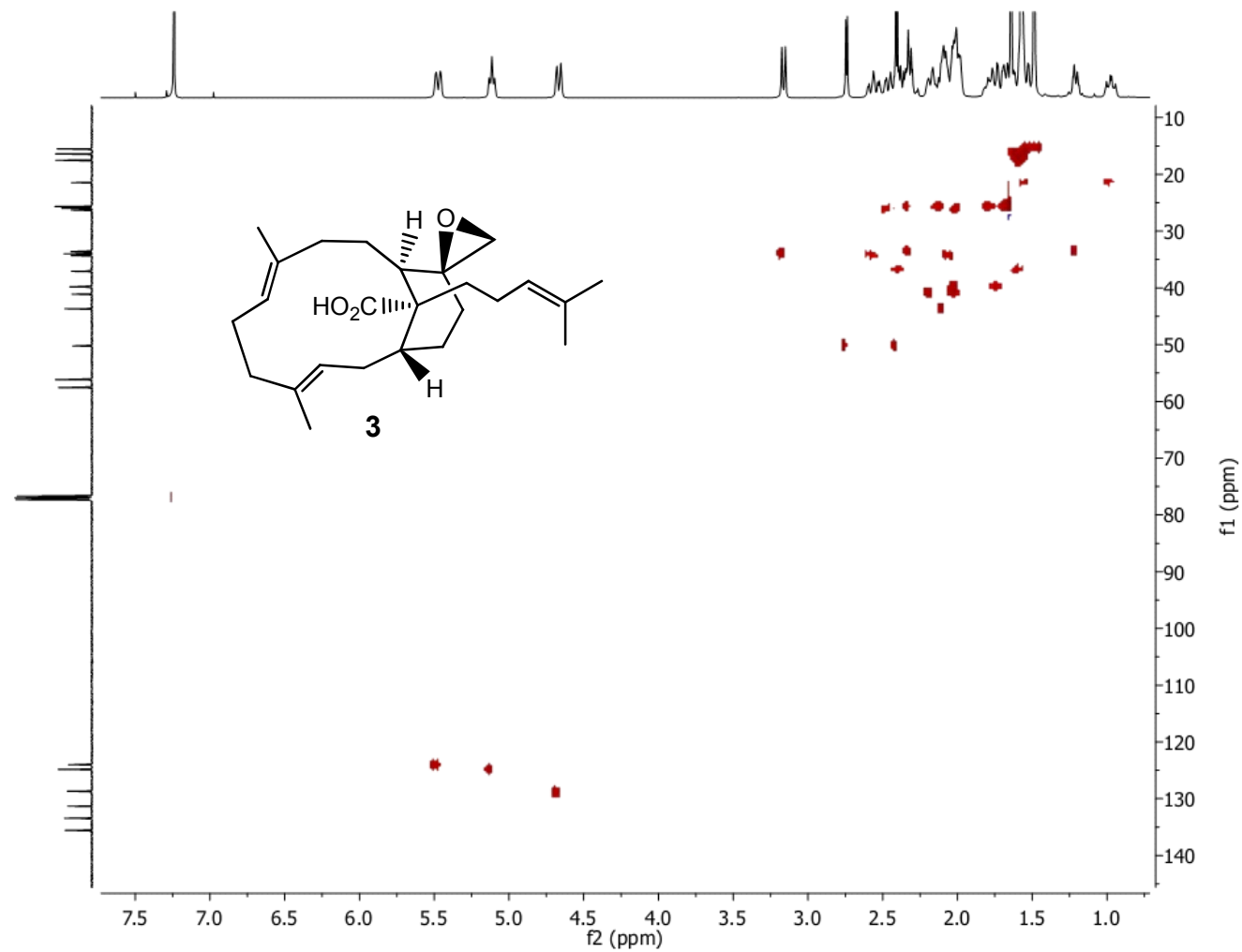


Figure S12. HMBC Spectrum (400 MHz) of Emericellene B (**3**) in CDCl₃

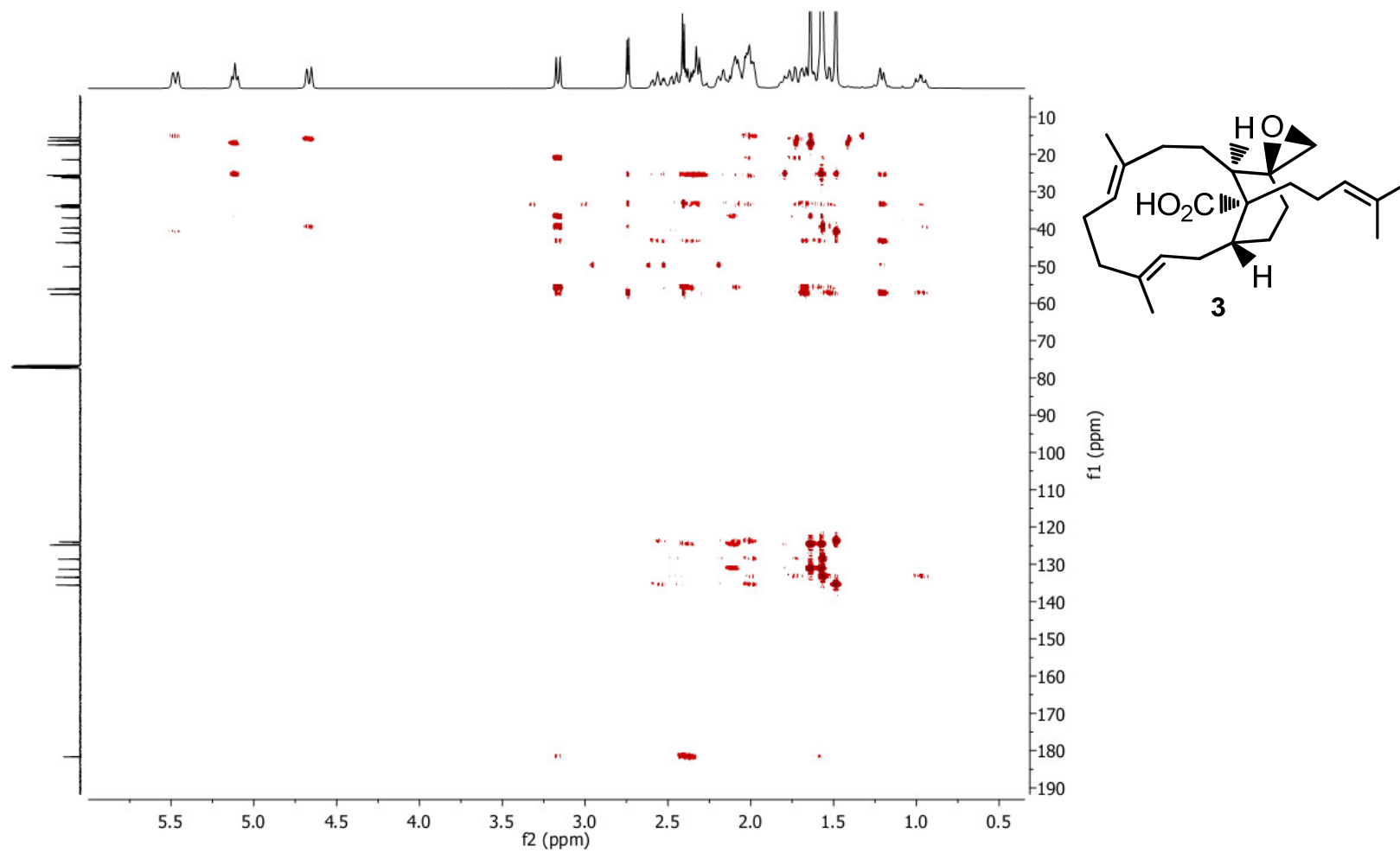


Figure S13. ^1H NMR Spectrum (400 MHz) of Emericellene C (**4**) in CDCl_3

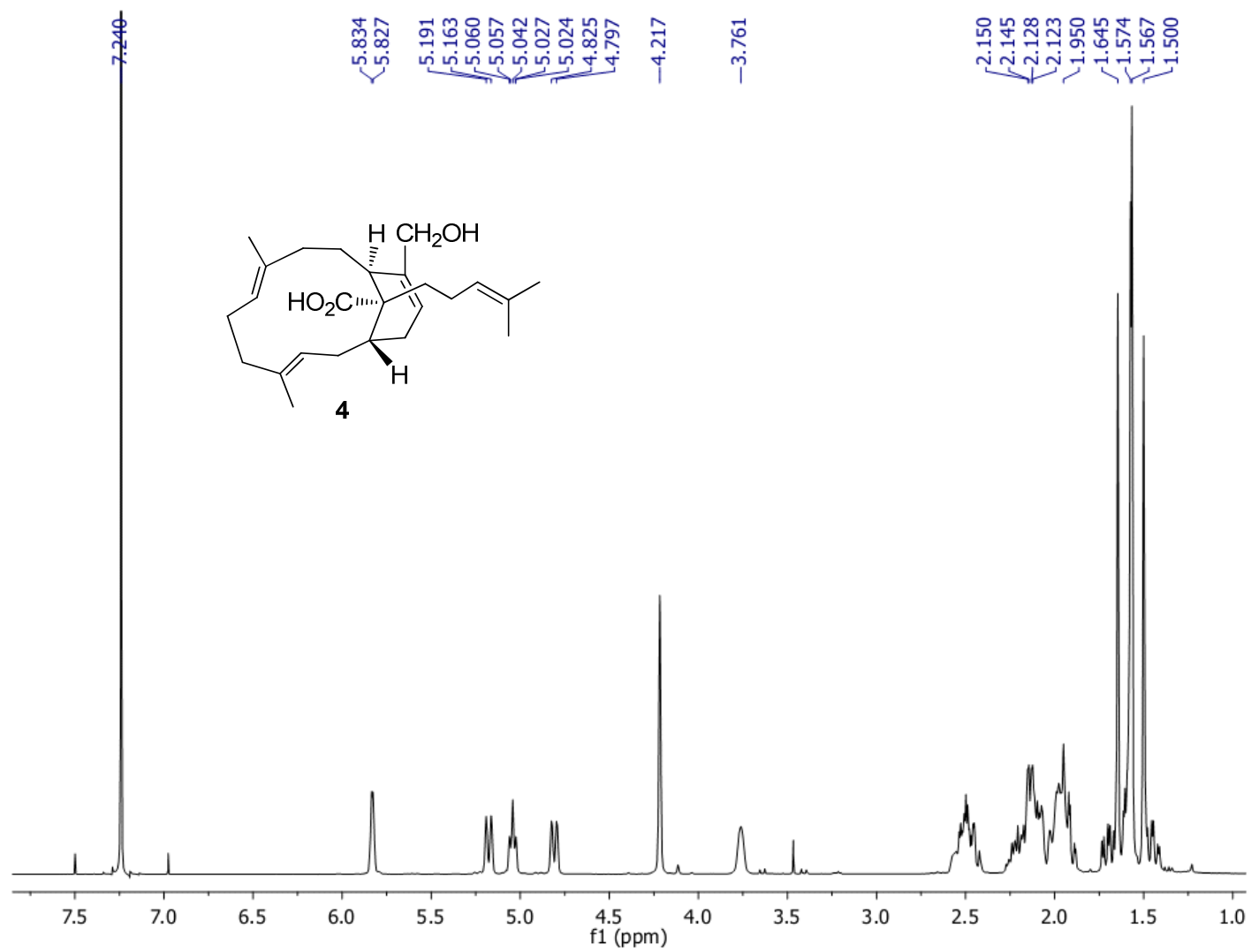


Figure S14. ^{13}C NMR Spectrum (100 MHz) of Emericellene C (**4**) in CDCl_3

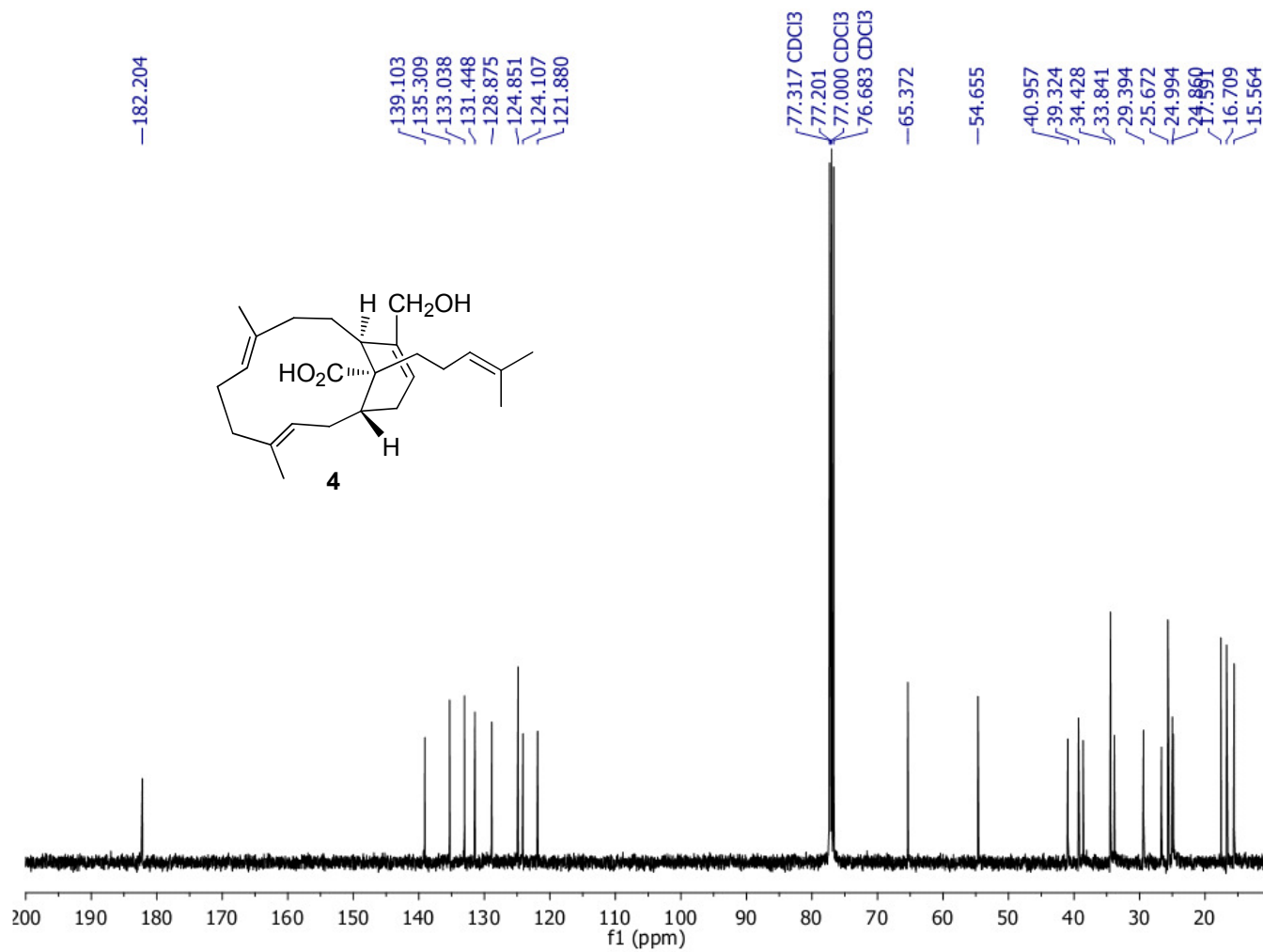


Figure S15. HSQC Spectrum (400 MHz) of Emericellene C (**4**) in CDCl₃

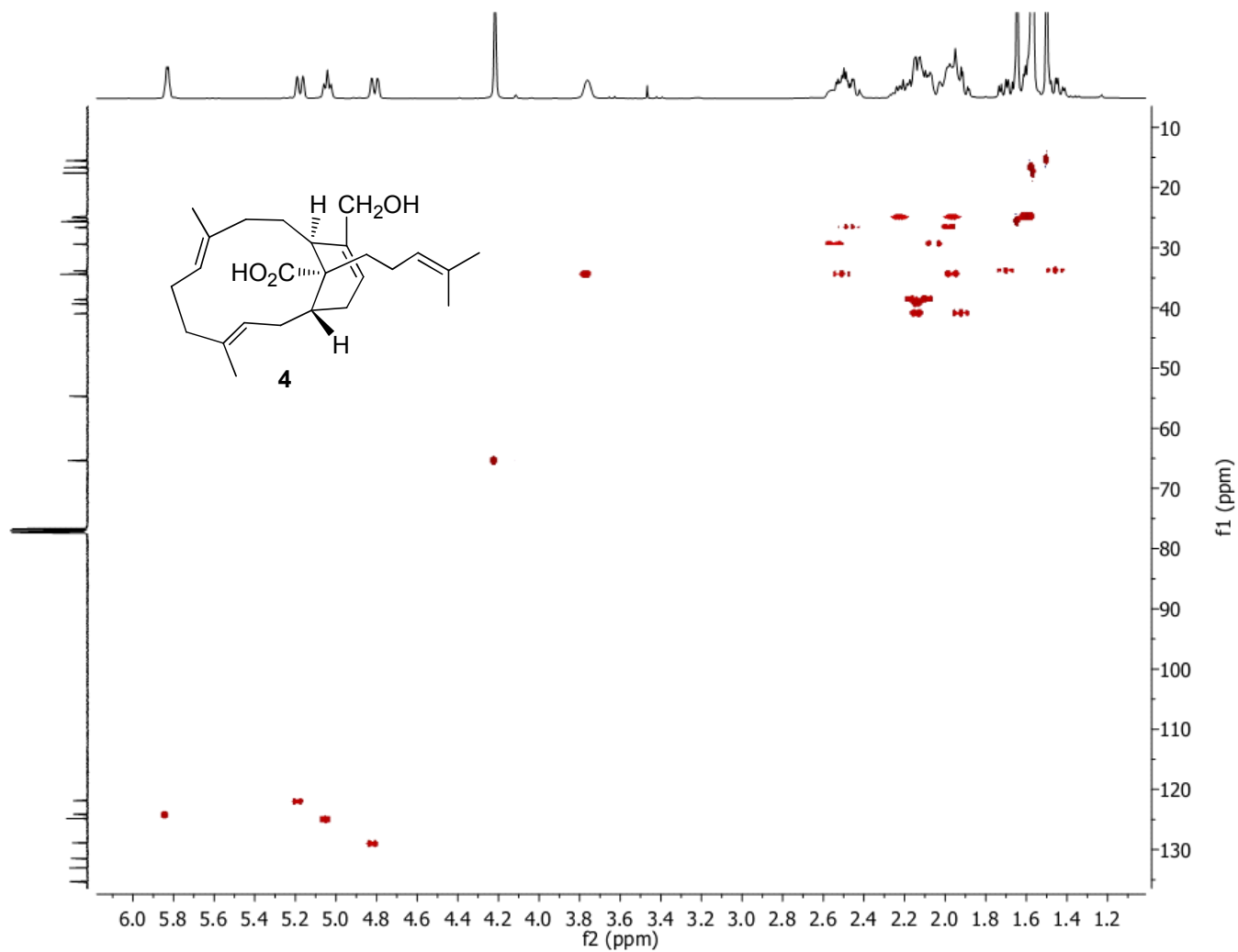


Figure S16. HMBC Spectrum (400 MHz) of Emericellene C (**4**) in CDCl₃

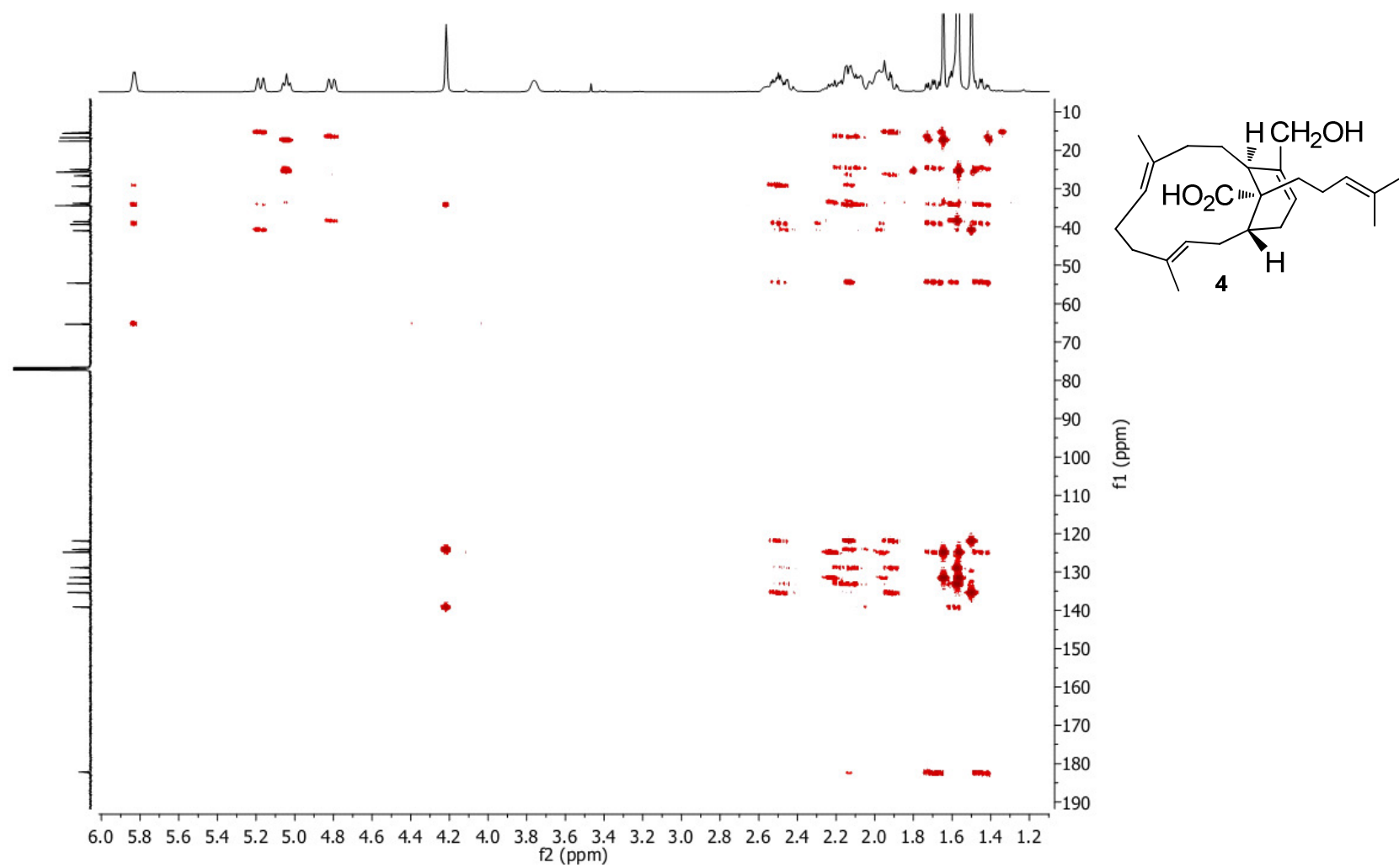


Figure S17. ^1H NMR Spectrum (400 MHz) of Emericellene D (**5**) in CDCl_3

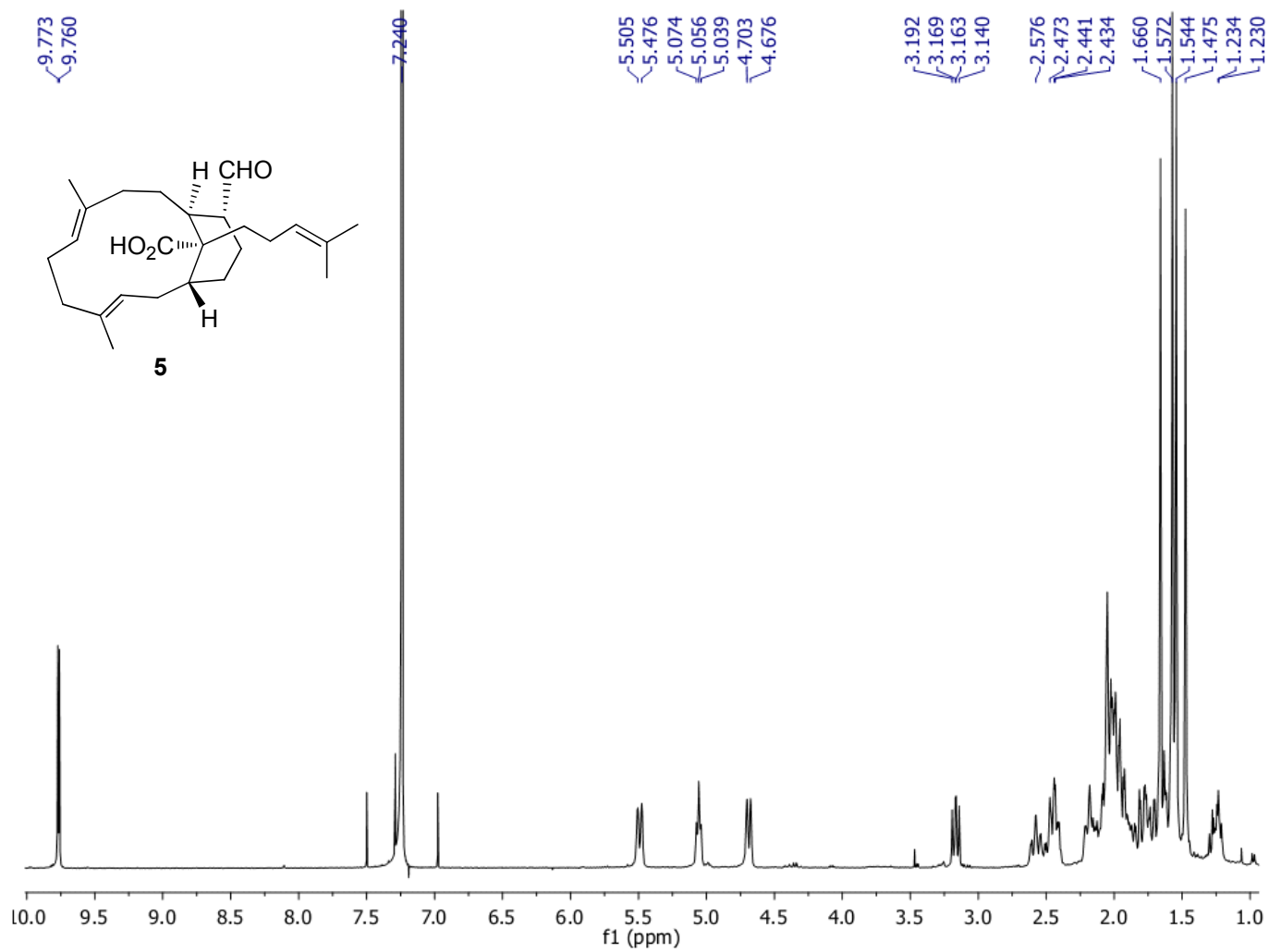


Figure S18. ^{13}C NMR Spectrum (100 MHz) of Emericellene D (**5**) in CDCl_3

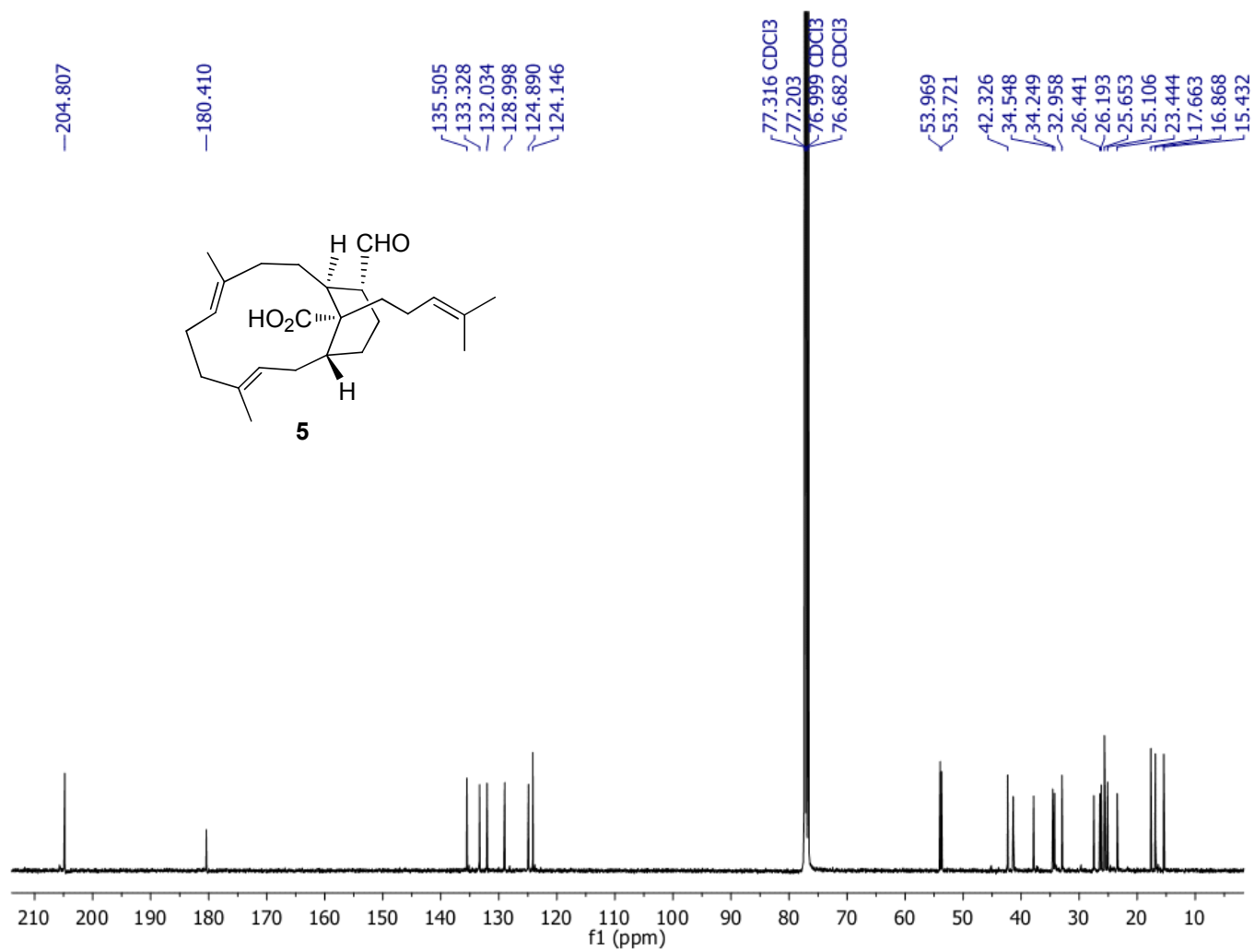


Figure S19. HSQC Spectrum (400 MHz) of Emericellene D (**5**) in CDCl₃

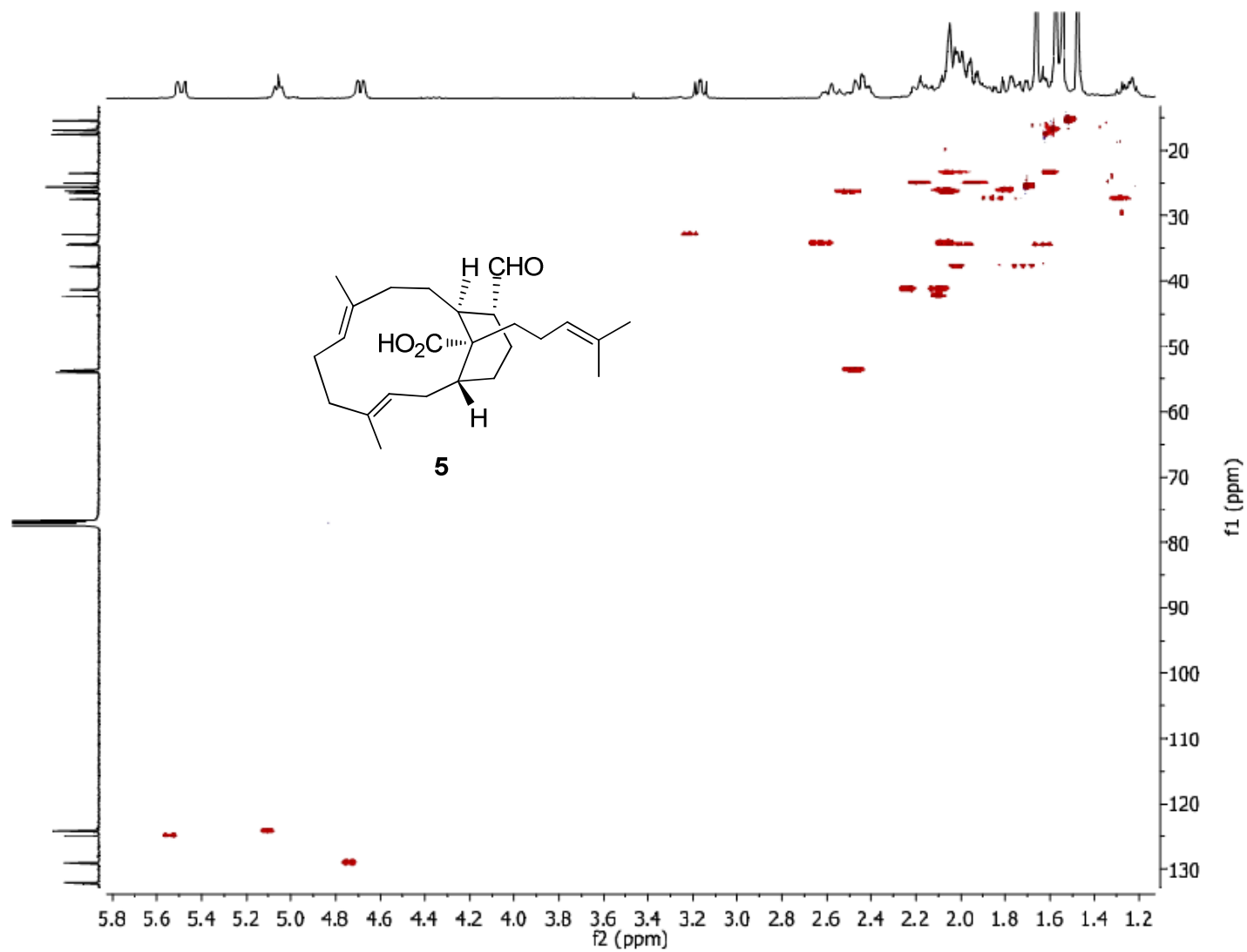


Figure S20. HMBC Spectrum (400 MHz) of Emericellene D (**5**) in CDCl₃

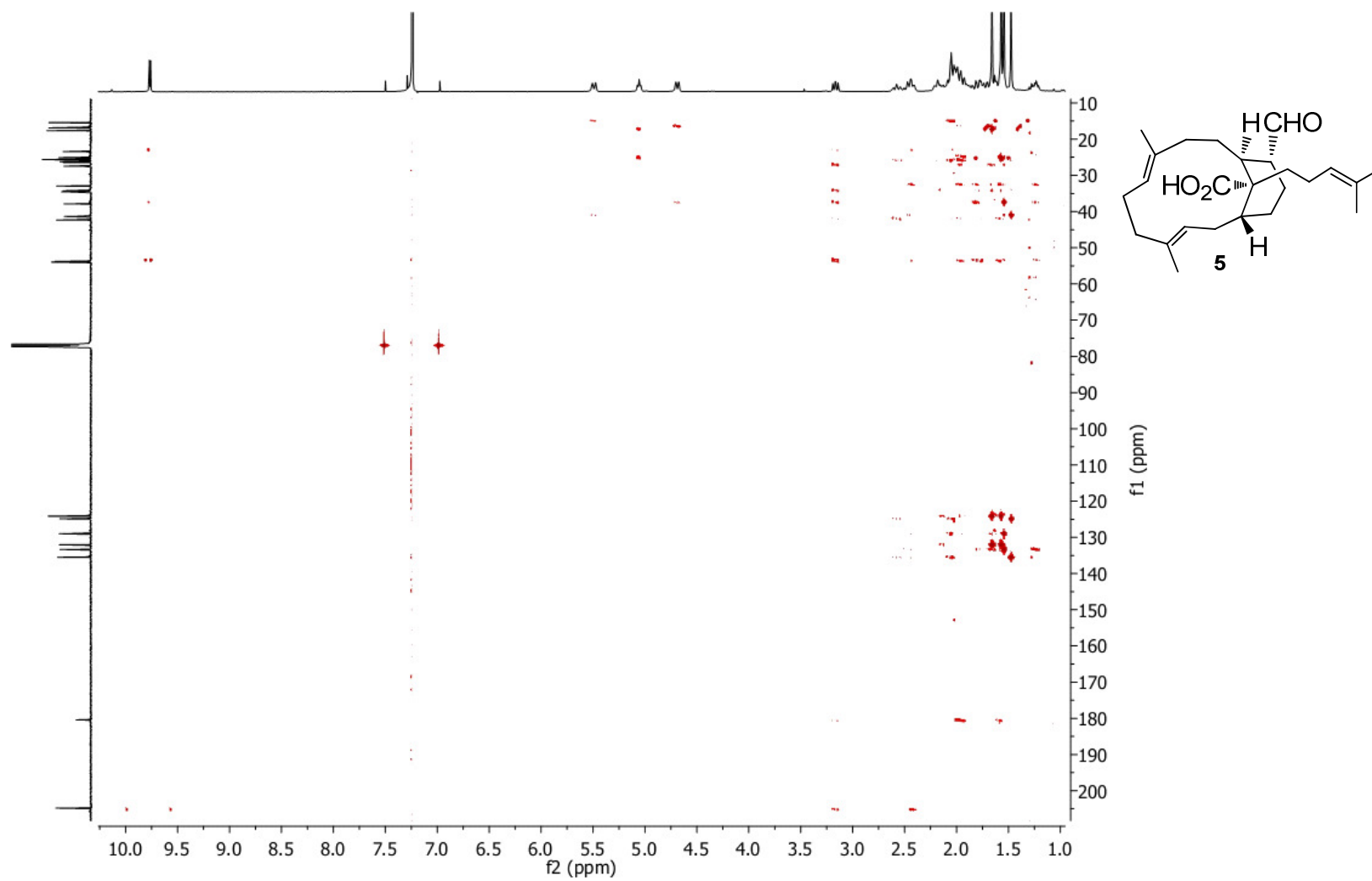


Figure S21. ^1H NMR Spectrum (400 MHz) of Emericellene E (**6**) in CDCl_3

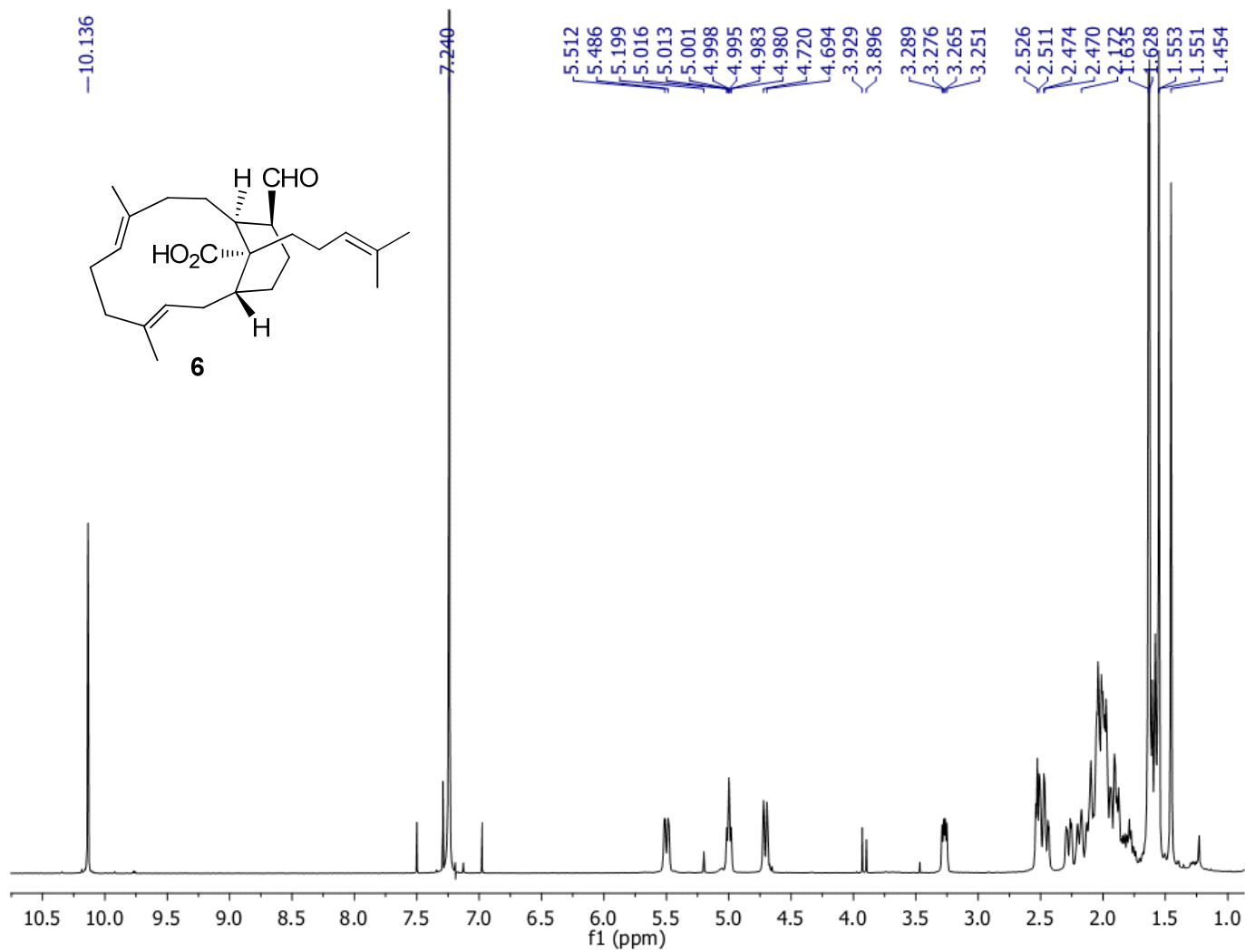


Figure S22. ^{13}C NMR Spectrum (100 MHz) of Emericellene E (**6**) in CDCl_3

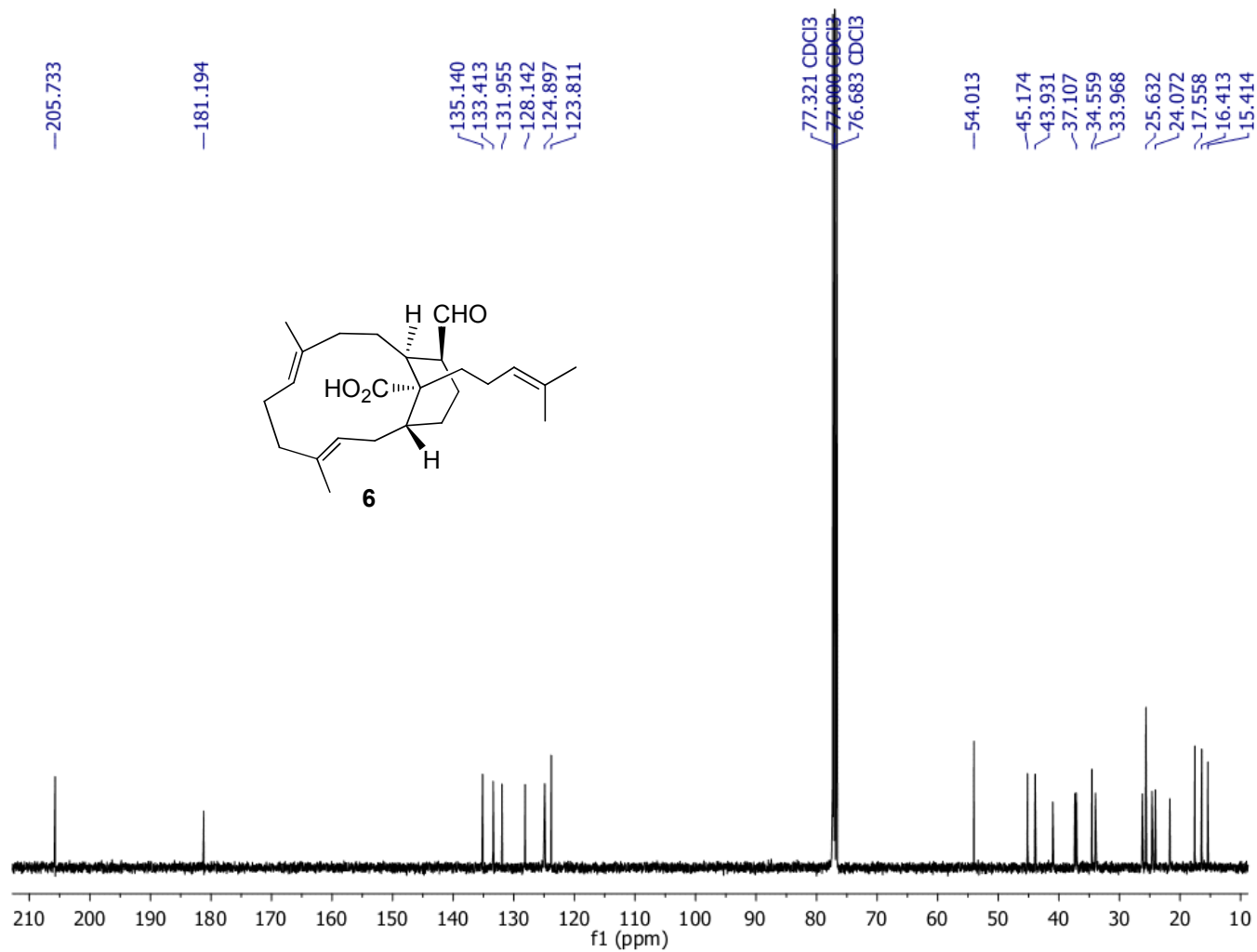


Figure S23. HSQC Spectrum (400 MHz) of Emericellene E (6) in CDCl₃

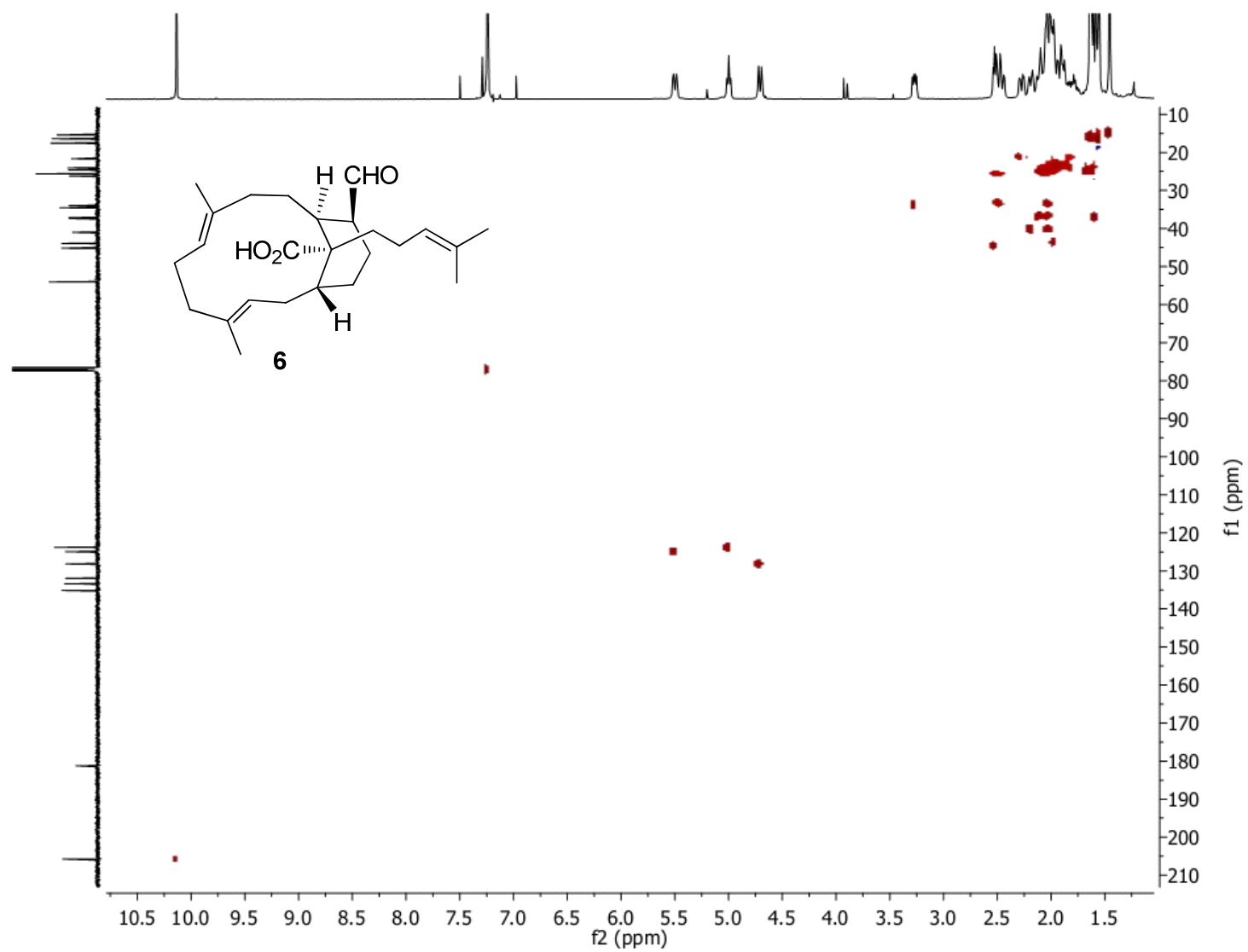


Figure S24. HMBC Spectrum (400 MHz) of Emericellene E (6) in CDCl₃

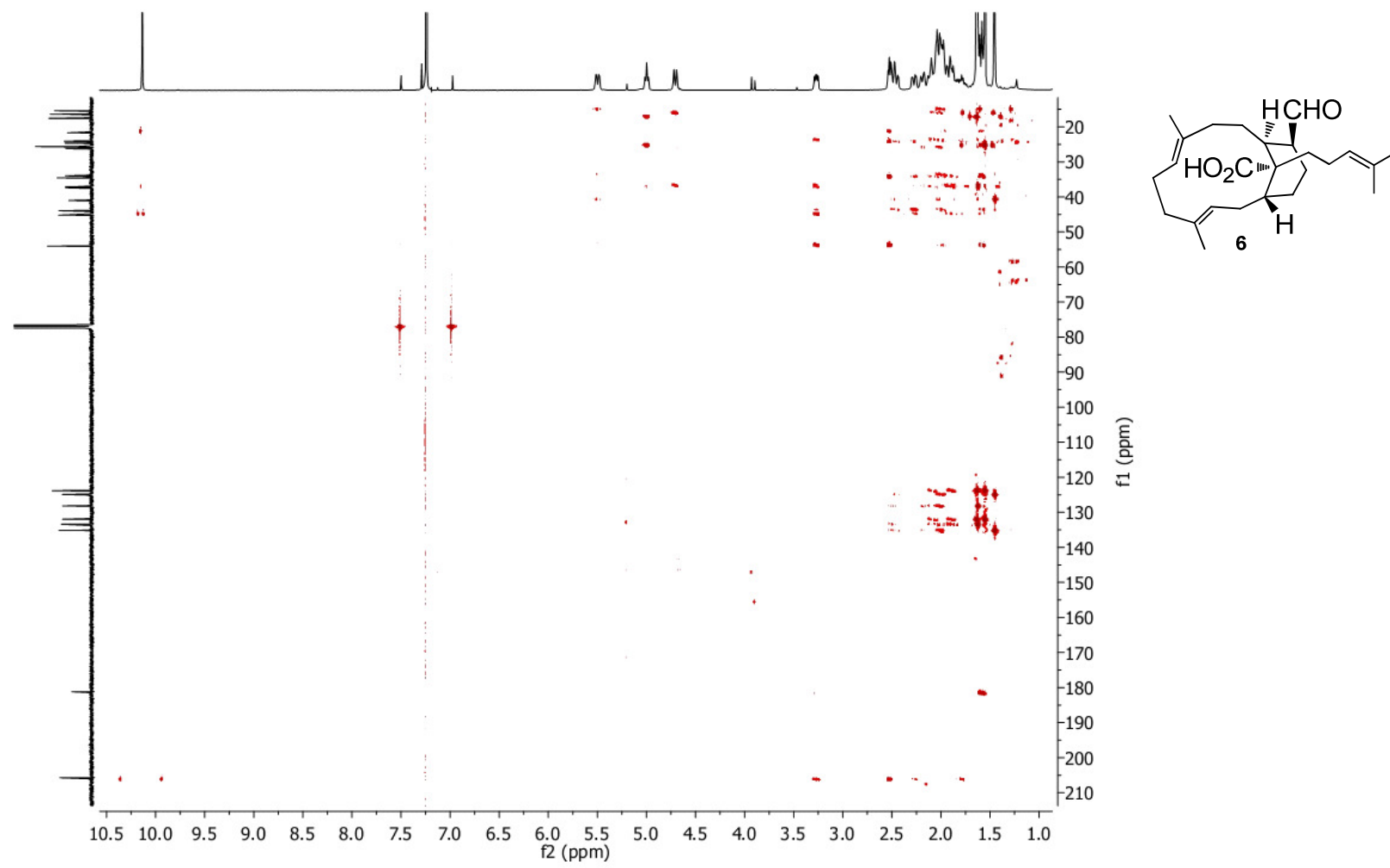


Figure S25. Significant HMBC Correlations of 3-6

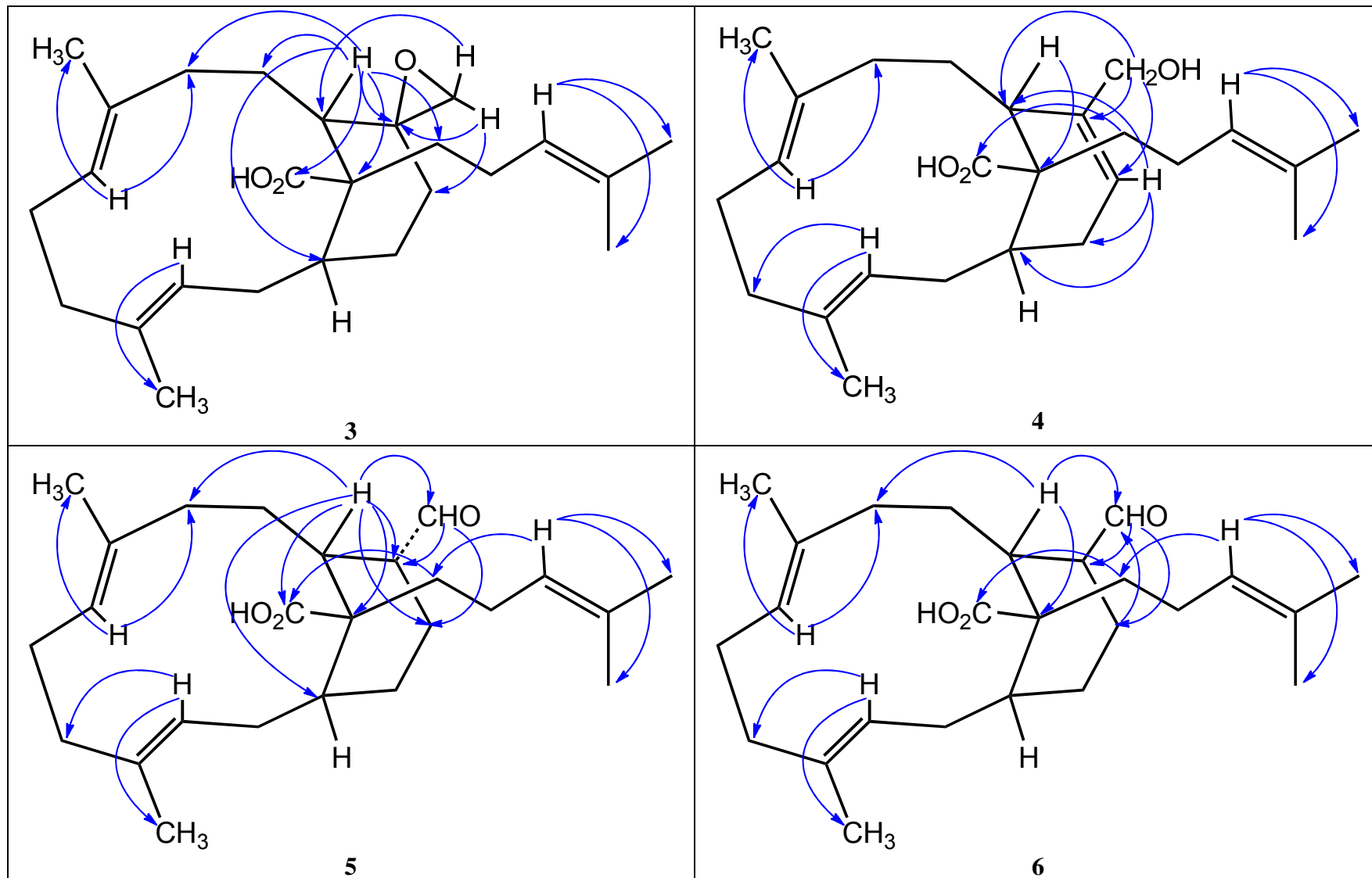


Figure S26. Key NOE Correlations of 3-6

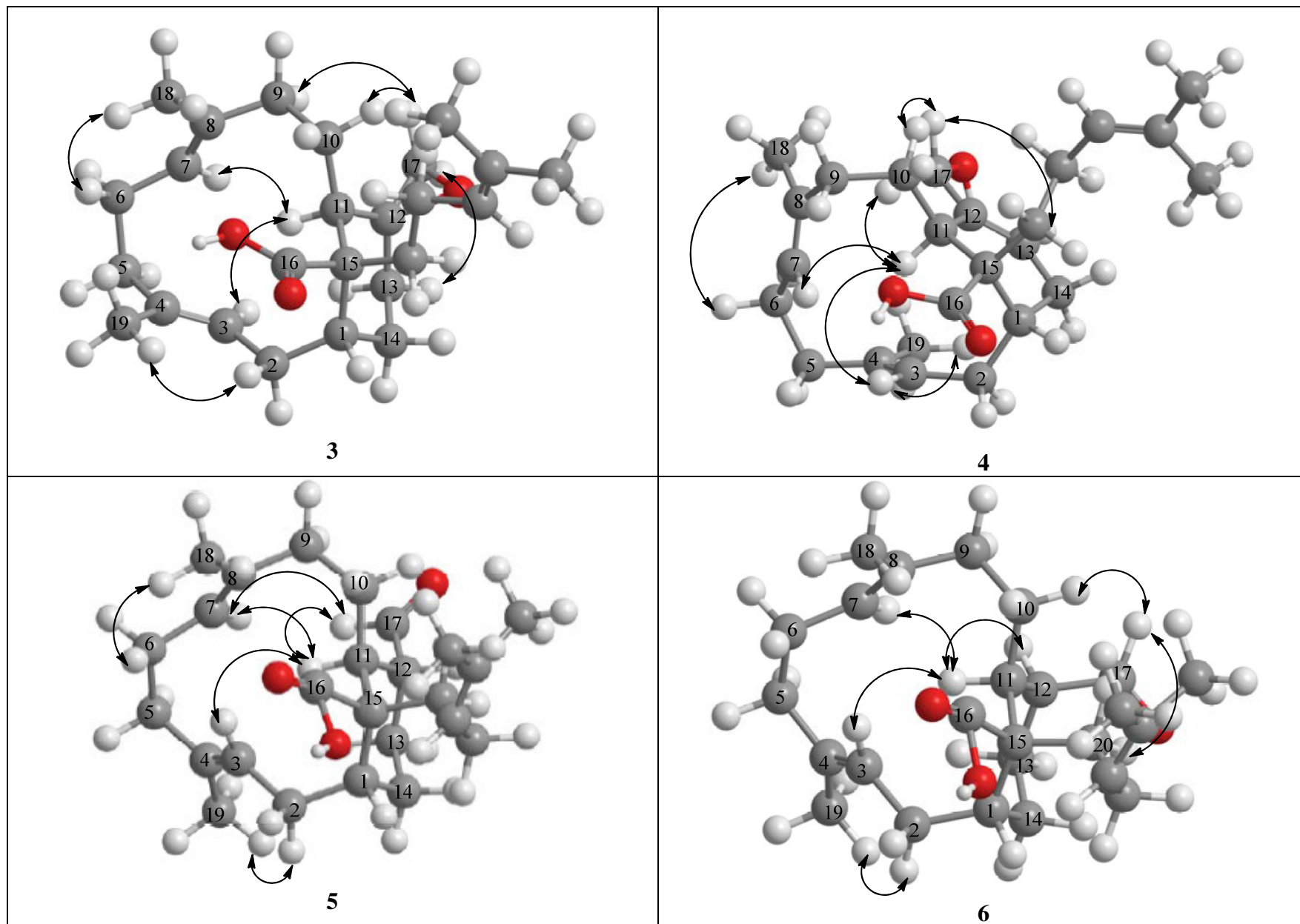


Figure S27. Probable Biosynthetic Conversion of Emericellene B (3) to Emericellenes C-E (4-6)

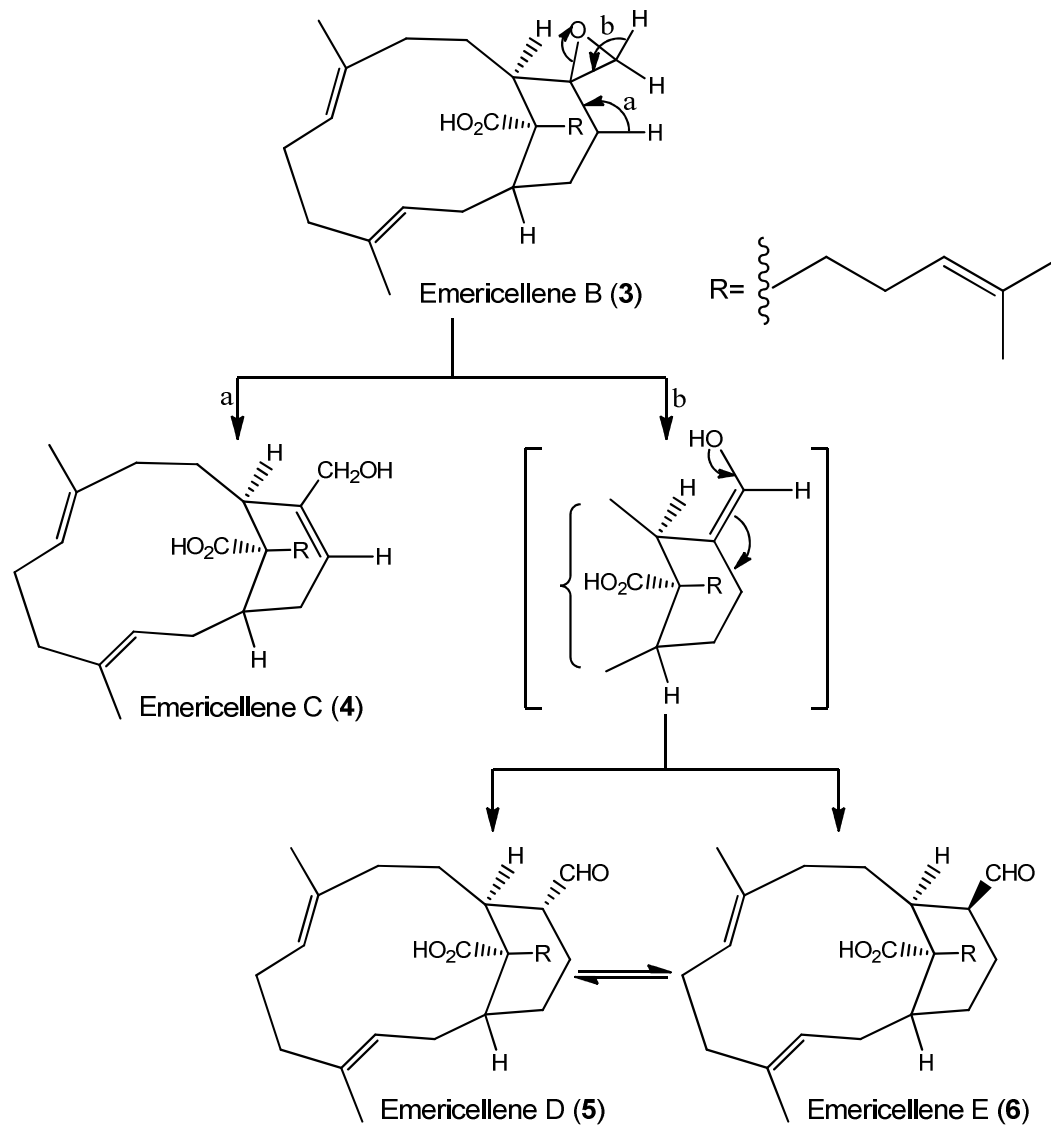


Figure S28. Results of Maximum Likelihood Analysis of ITSrDNA Data Revealing Strongly Supported Placement of AST0036 in *Emericella*. Values above Branches Indicate Relevant Maximum Likelihood Bootstrap Support >70%

