New Cytotoxic Cerebrosides from the Red Sea Cucumber *Holothuria spinifera* Supported by *In-Silico* Studies

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Table of Contents

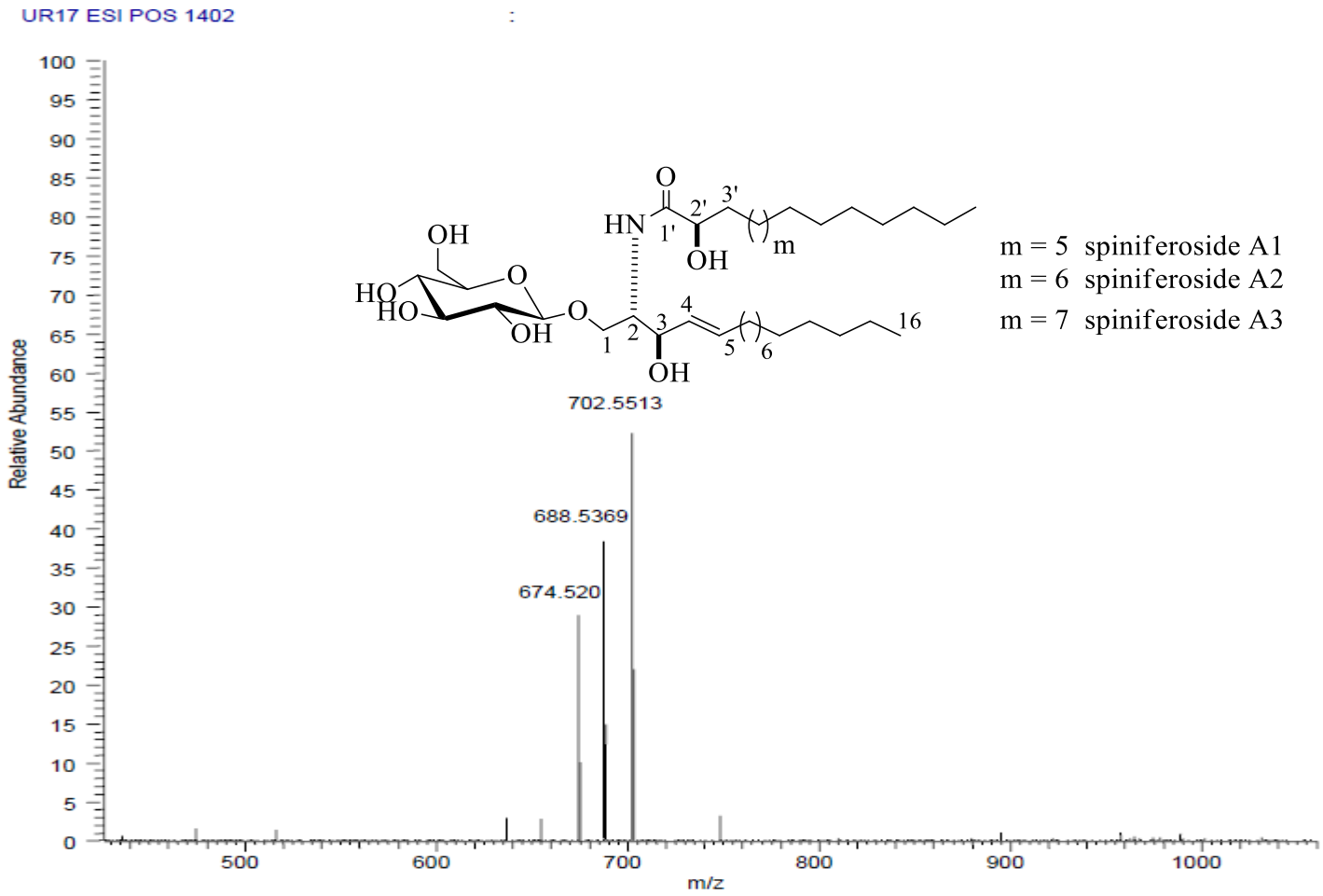


Figure S1. LC-HRESIMS of compound **1** $(M+H)^+$.

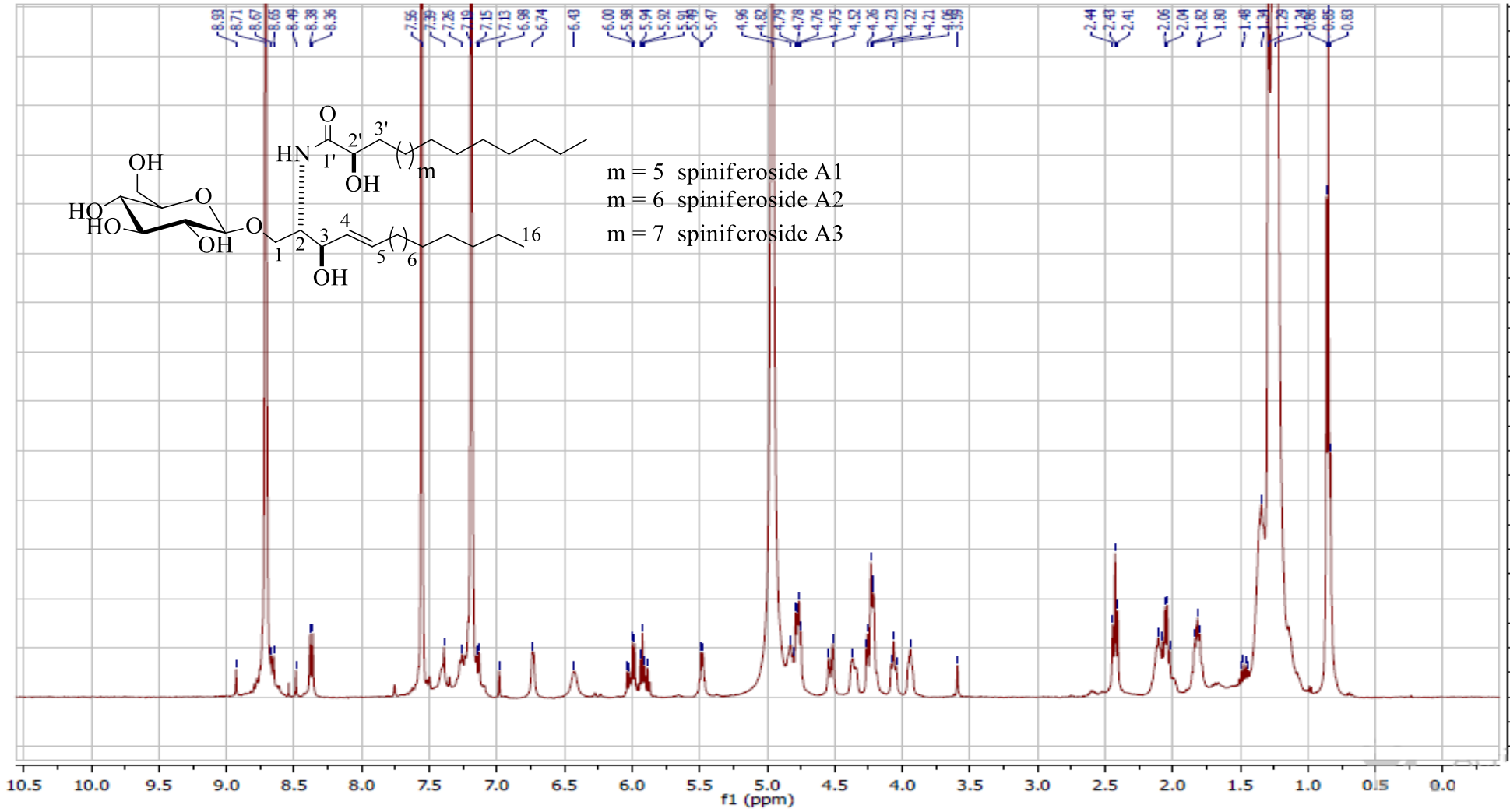


Figure S2. ^{1}H NMR spectrum of compound **1** (in C_5D_5N, 400 MHz).

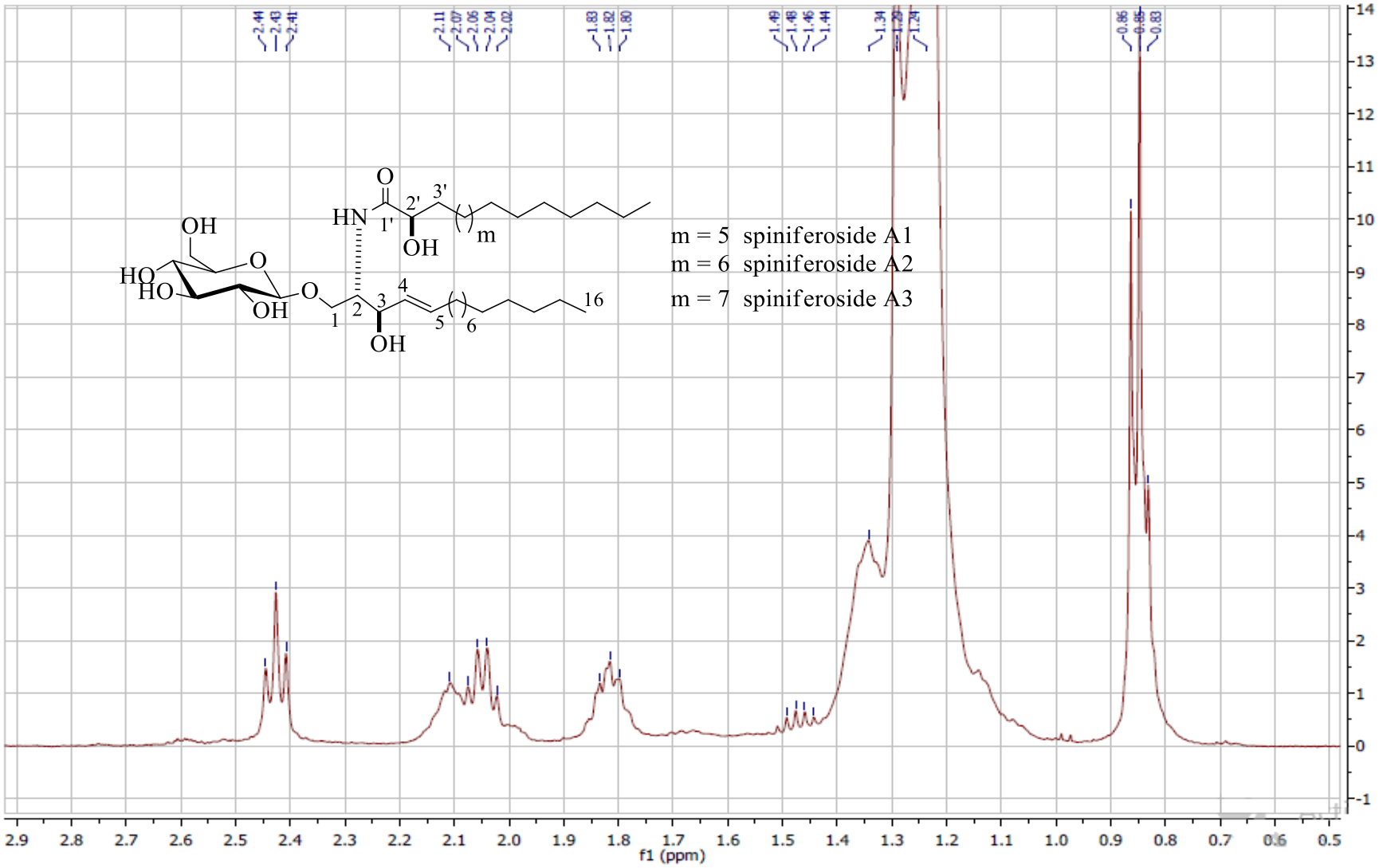


Figure S3. Partial expansion of the ^{1}H NMR spectrum of compound **1** (in C_5D_5N, 400 MHz).

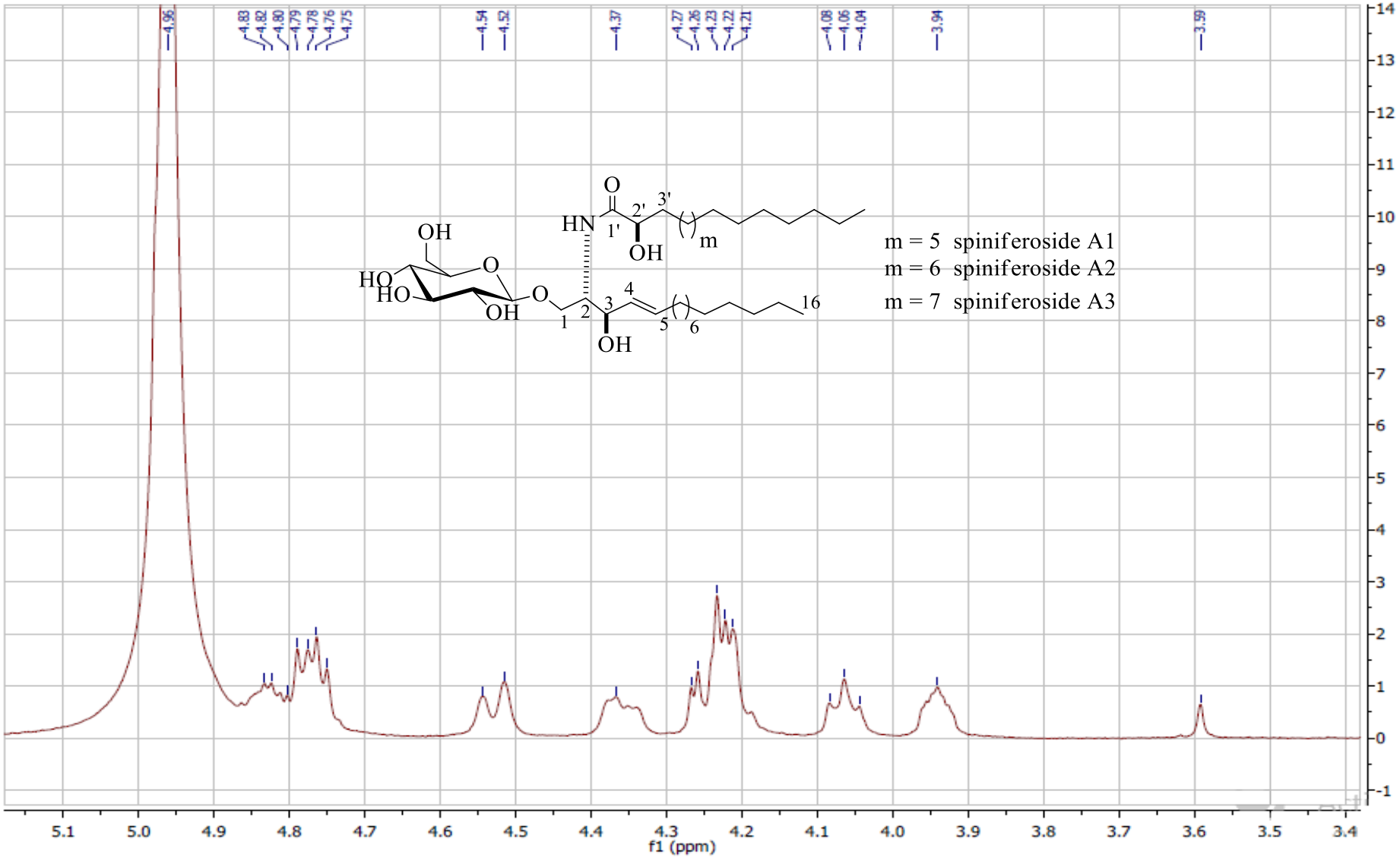


Figure S4. Partial expansion of the ^{1}H NMR spectrum of compound **1** (in C_5D_5N, 400 MHz).

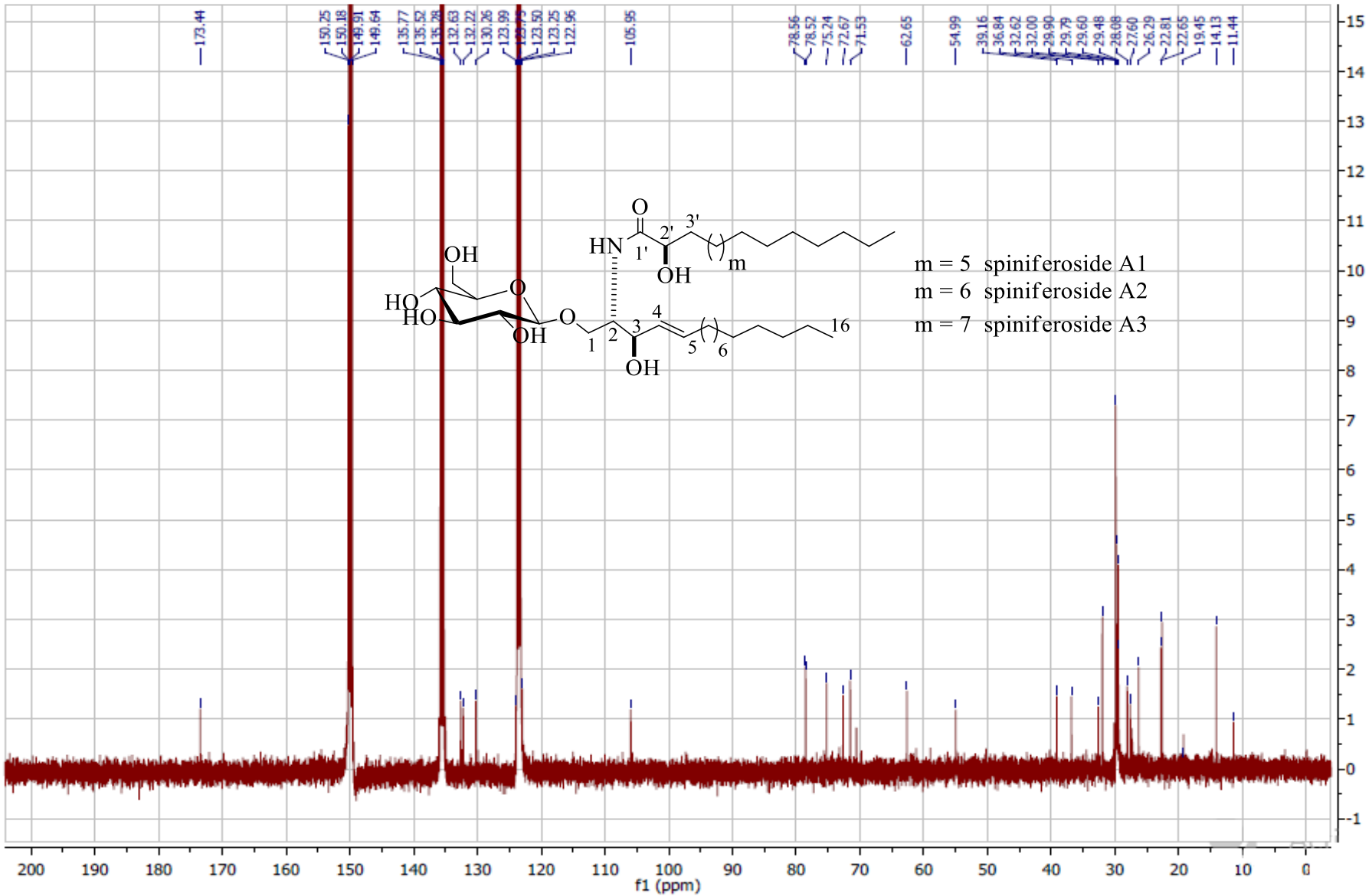


Figure S5. ^{13}C NMR spectrum of compound **1** (in C_5D_5N, 100 MHz).

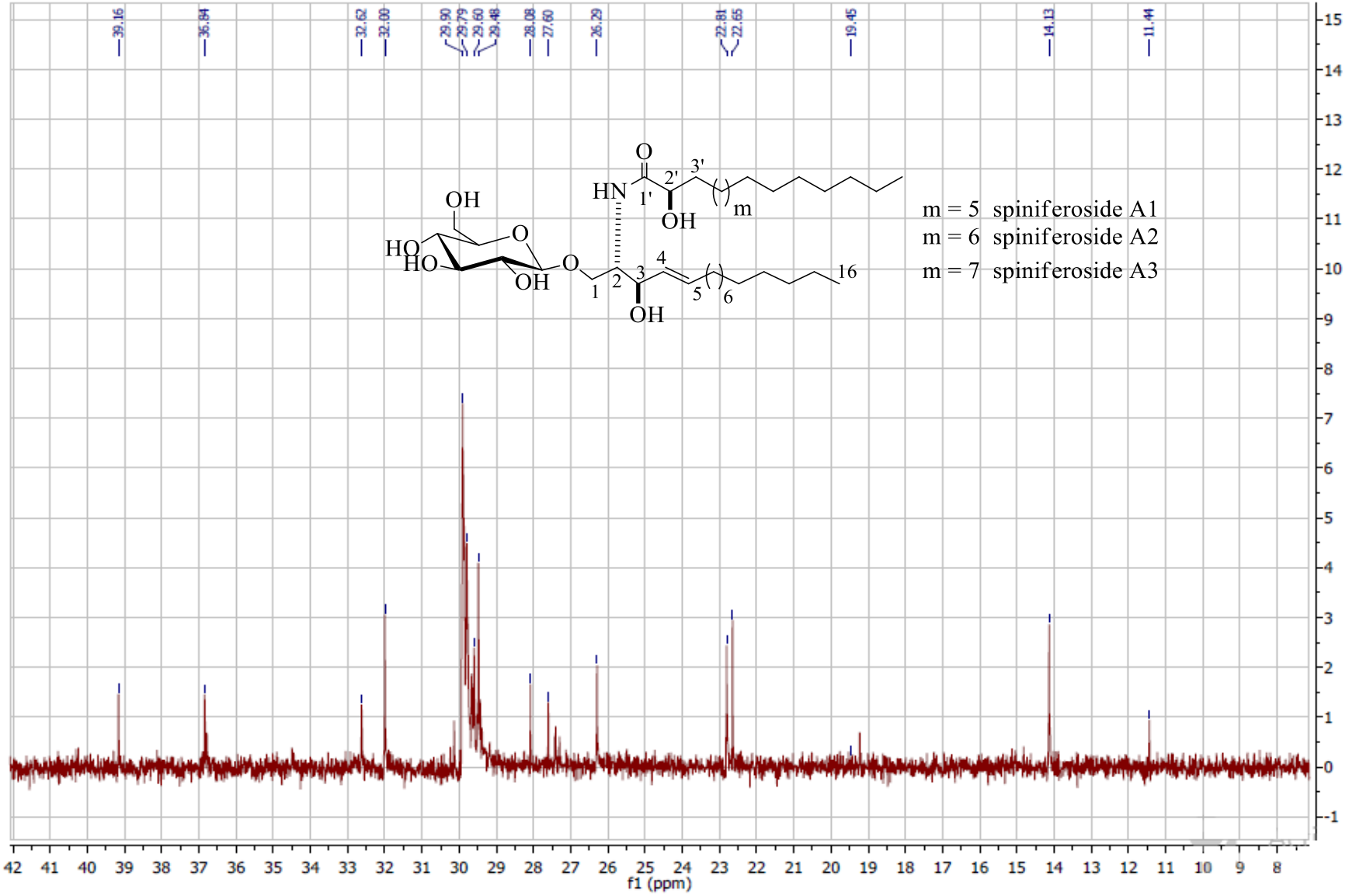


Figure S6. Partial expansion of the ^{13}C NMR spectrum of compound **1** (in C_5D_5N, 100 MHz).

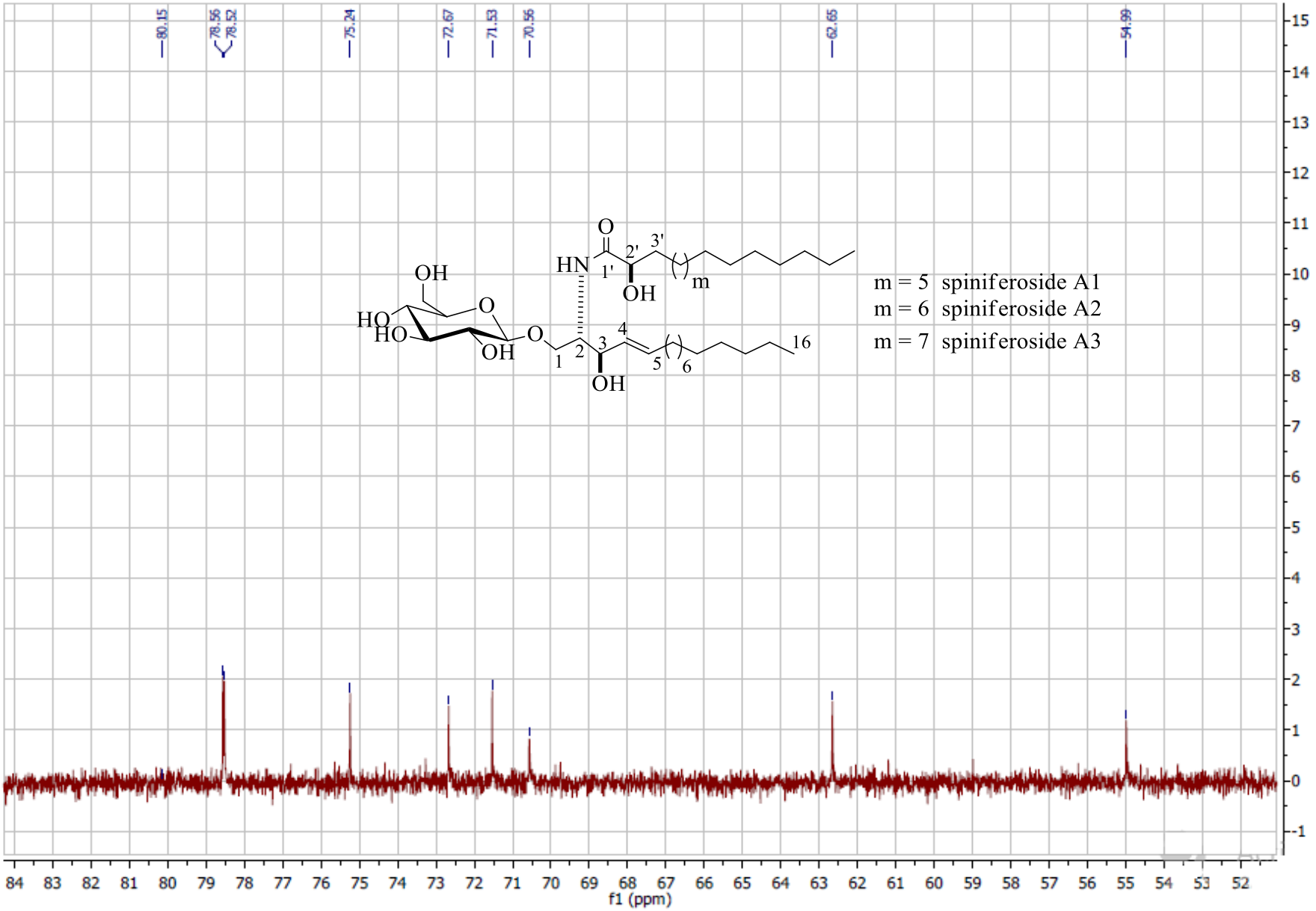


Figure S7. Partial expansion of the ^{13}C NMR spectrum of compound **1** (in C_5D_5N, 100 MHz).

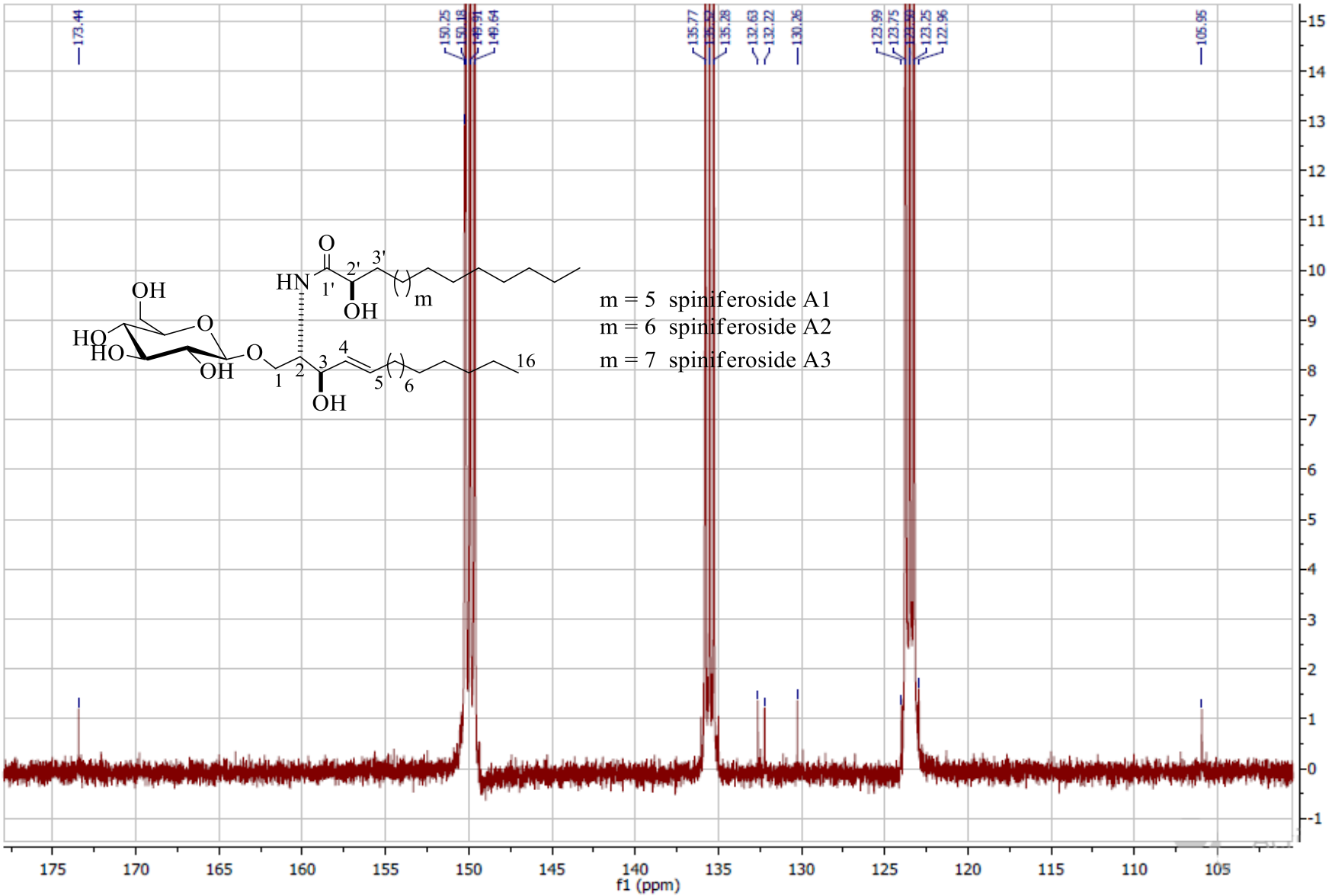


Figure S8. Partial expansion of the ^{13}C NMR spectrum of compound **1** (in C_5D_5N, 100 MHz).

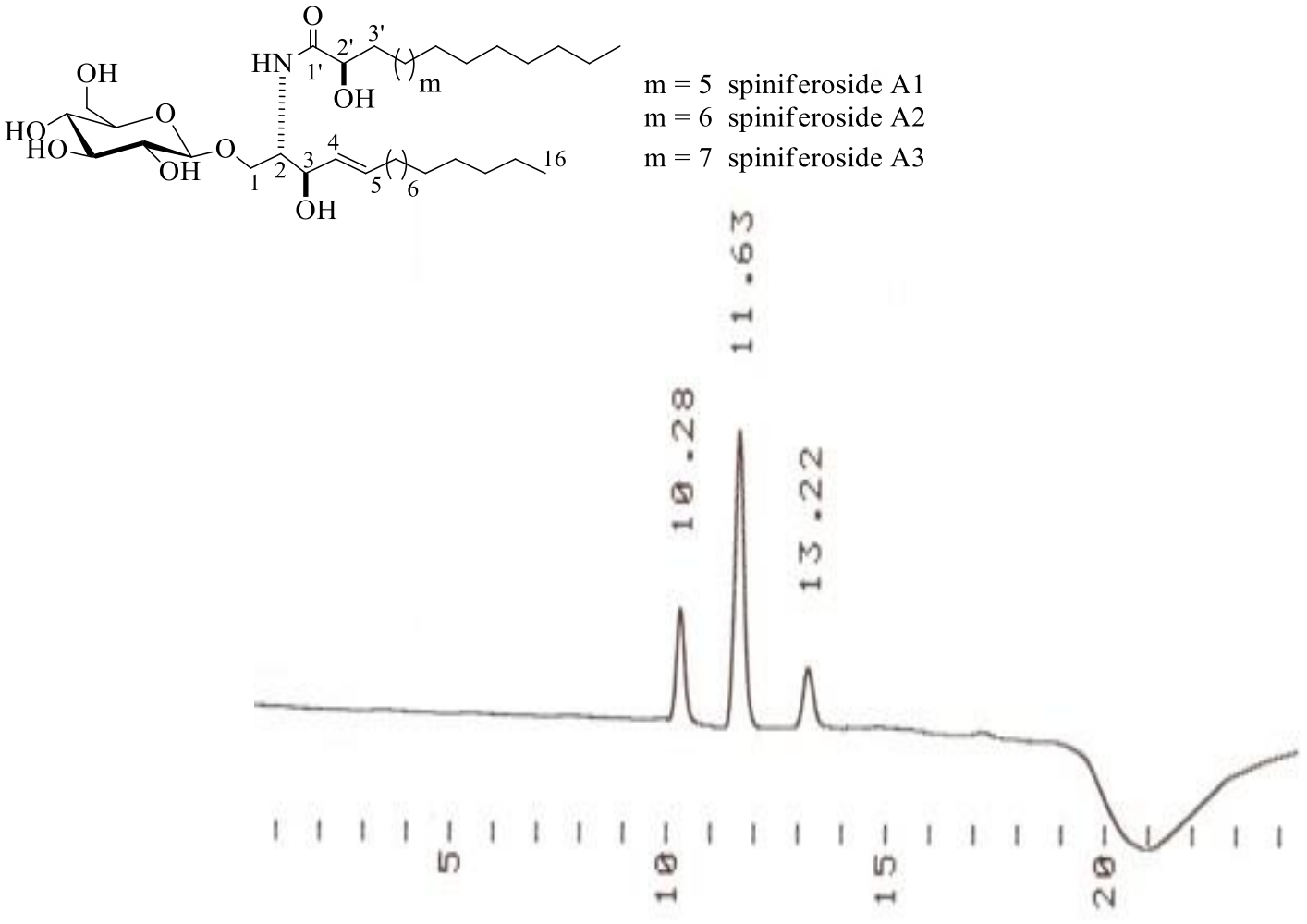
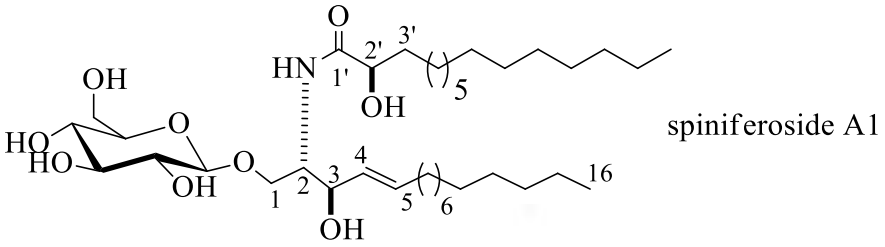


Figure S9. Chromatogram of semi-preparative HPLC purification of compound **1**.



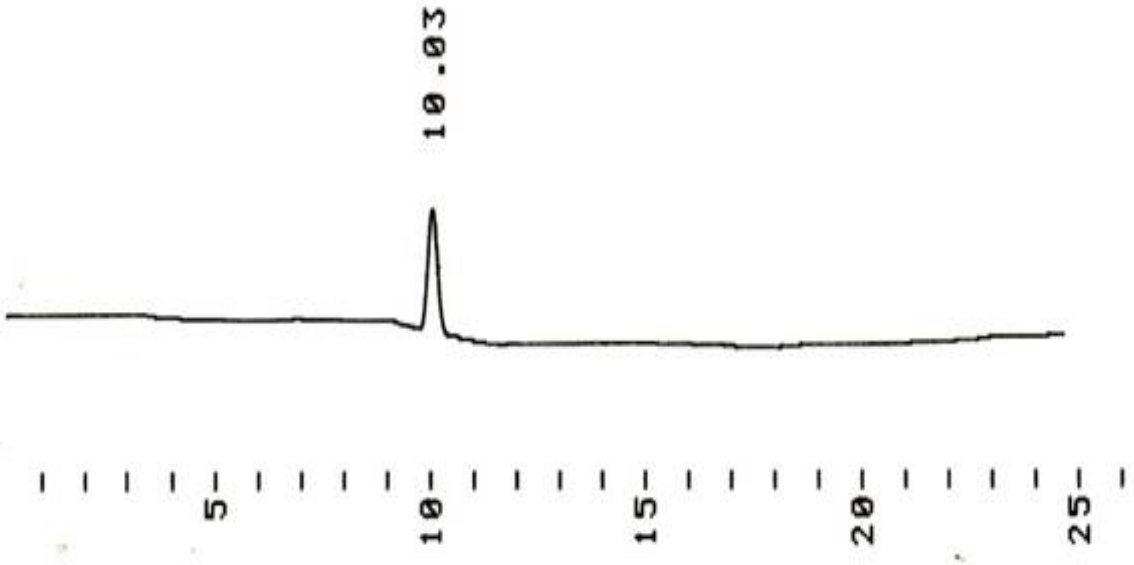


Figure S10. Chromatogram of semi-preparative HPLC purification of spiniferoside A1 (**1a**).

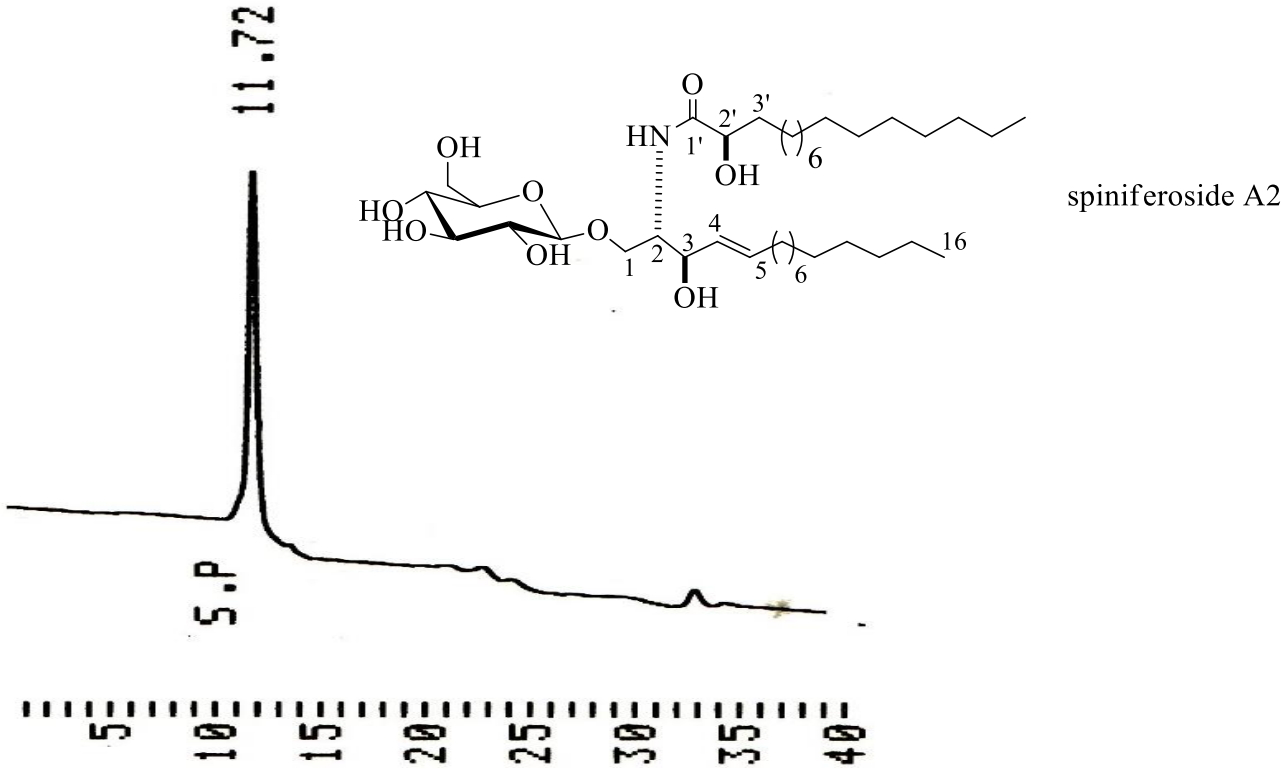


Figure S11. Chromatogram of semi-preparative HPLC purification of spiniferoside A2 (**1b**).

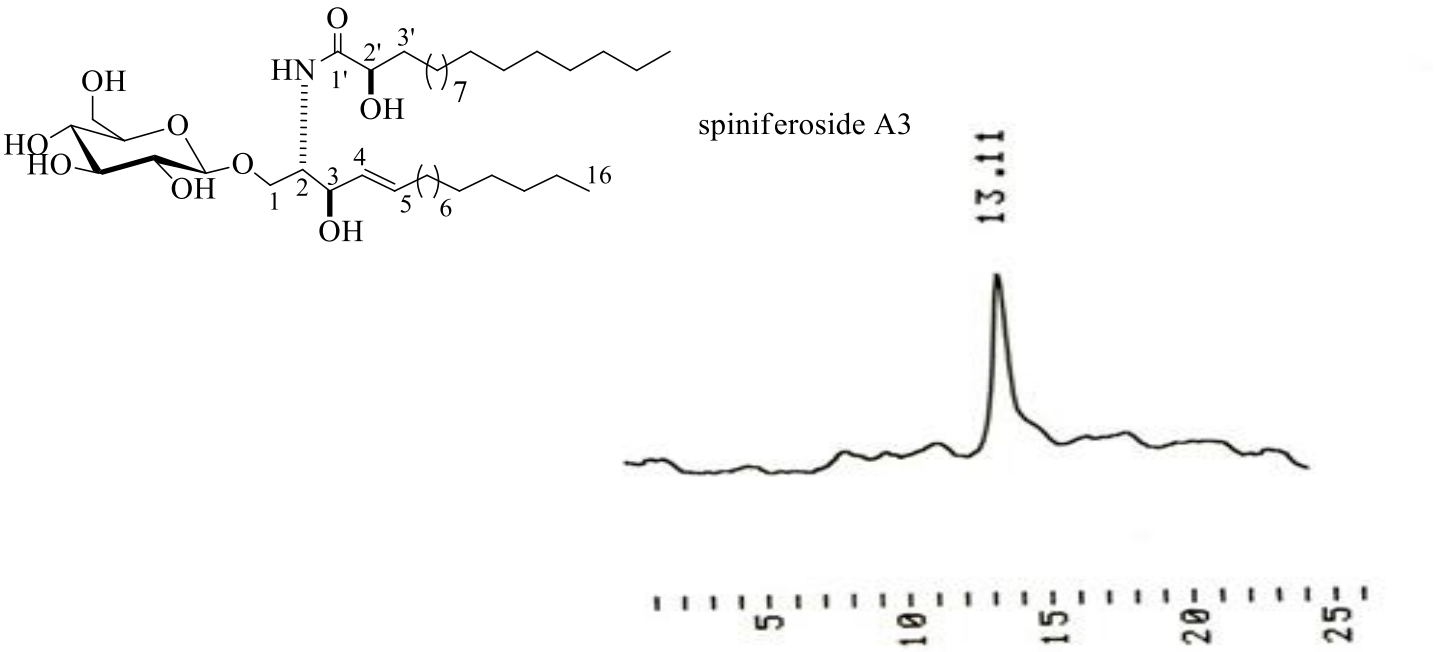


Figure S12. Chromatogram of semi-preparative HPLC purification of spiniferoside A3 (**1c**).

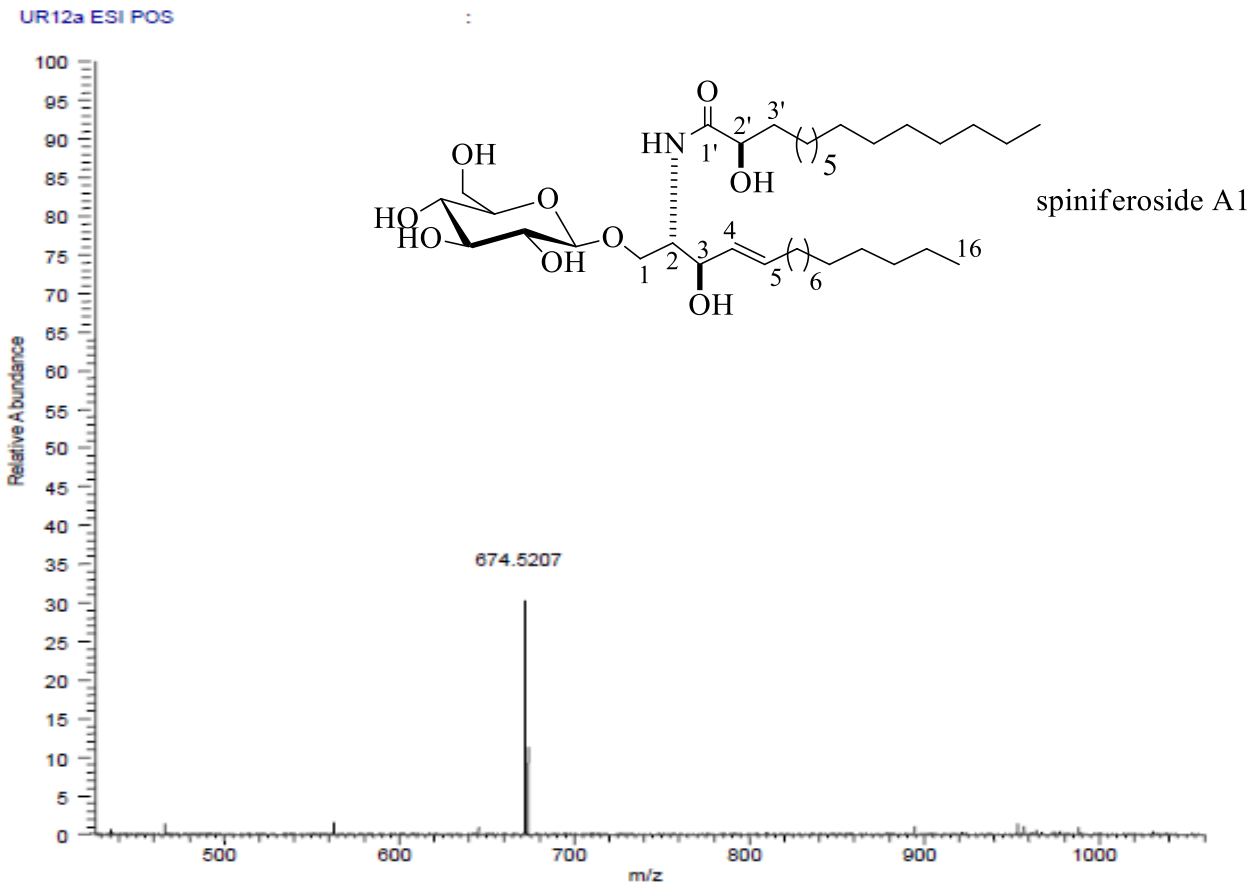


Figure S13. LC-HRESIMS for spiniferoside A1 (**1a**).

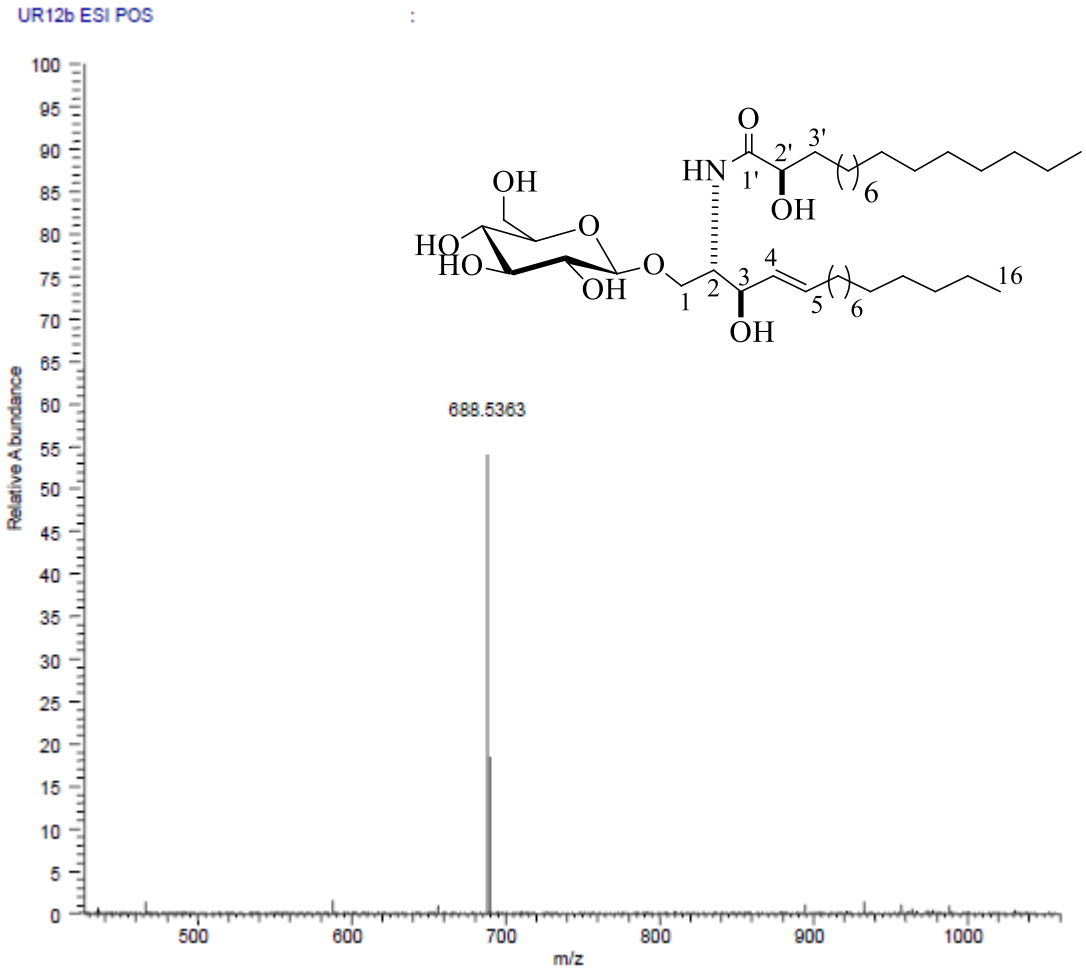


Figure S14. LC-HRESIMS for spiniferoside A2 (**1b**).

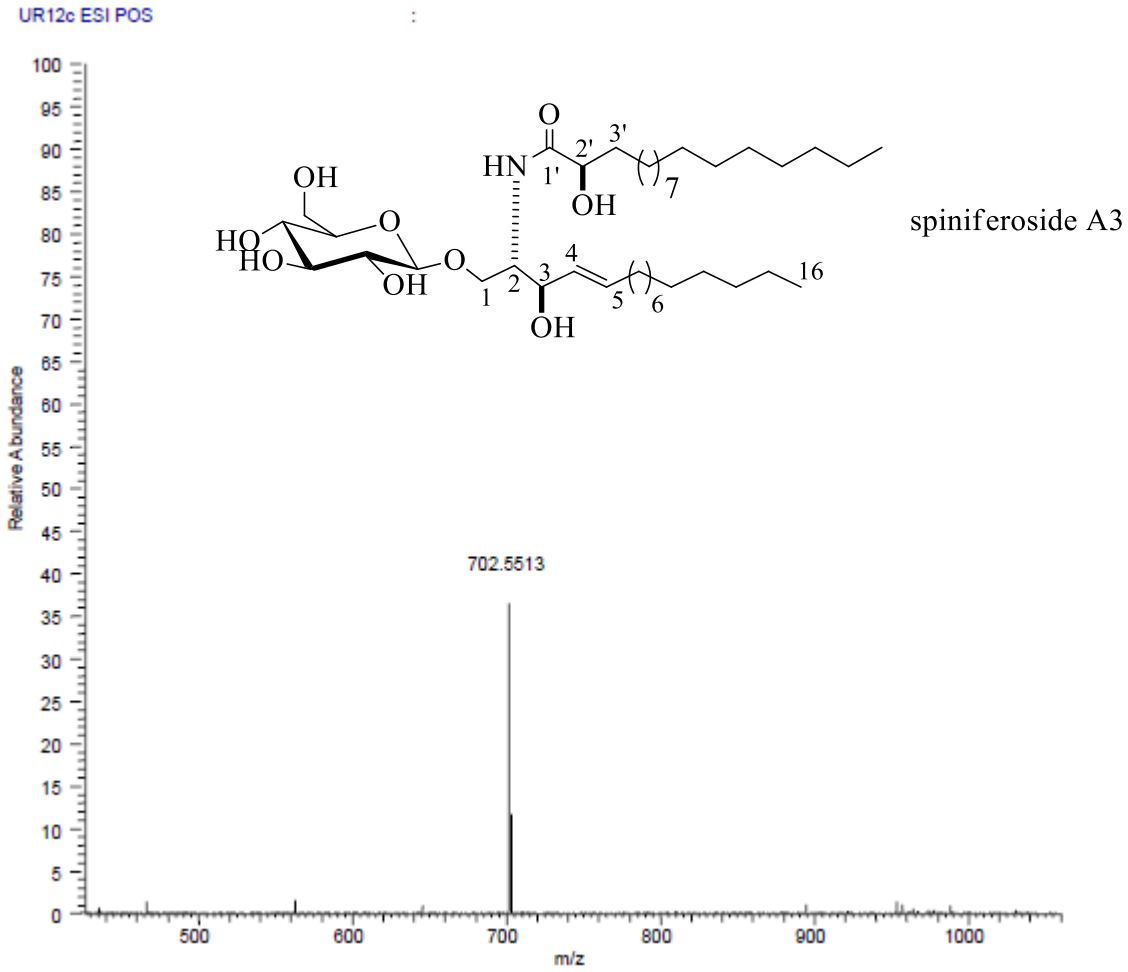


Figure S15: LC-HRESIMS for spiniferoside A3 (**1c**).

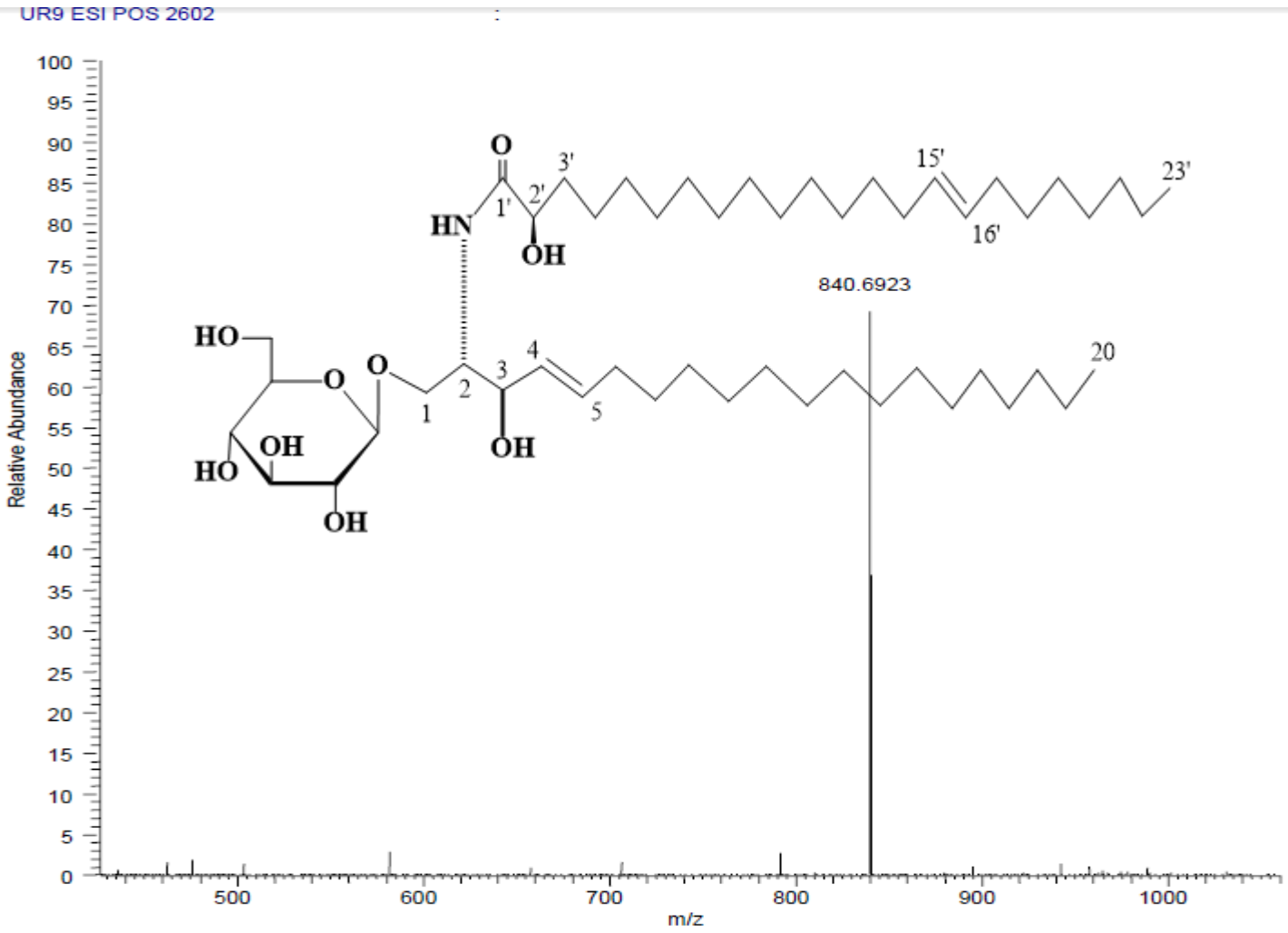


Figure S16. LC-HRESIMS of compound **2** $(M+H)^+$

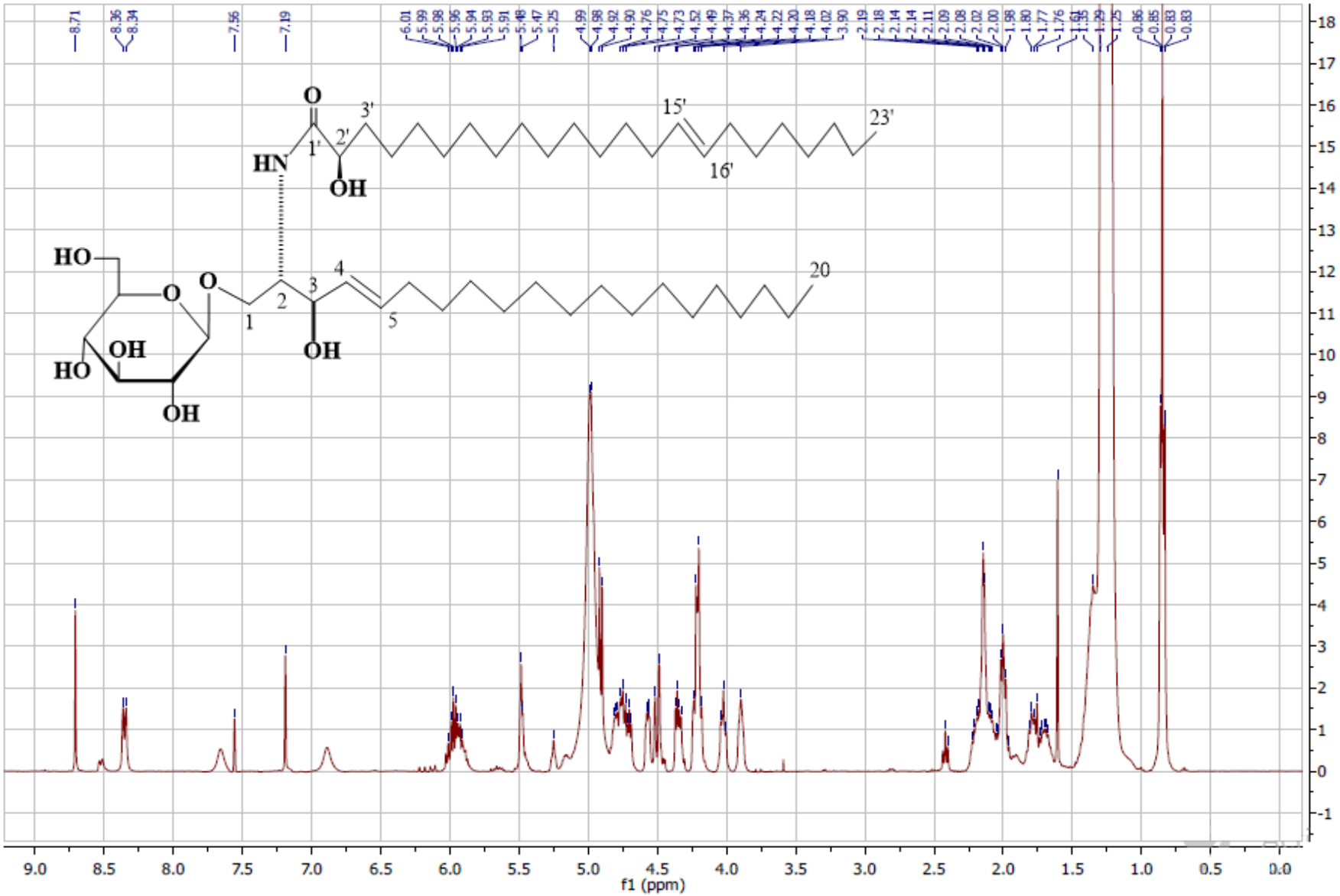


Figure S17. ^{1}H NMR spectrum of compound **2** (in C_5D_5N, 400 MHz).

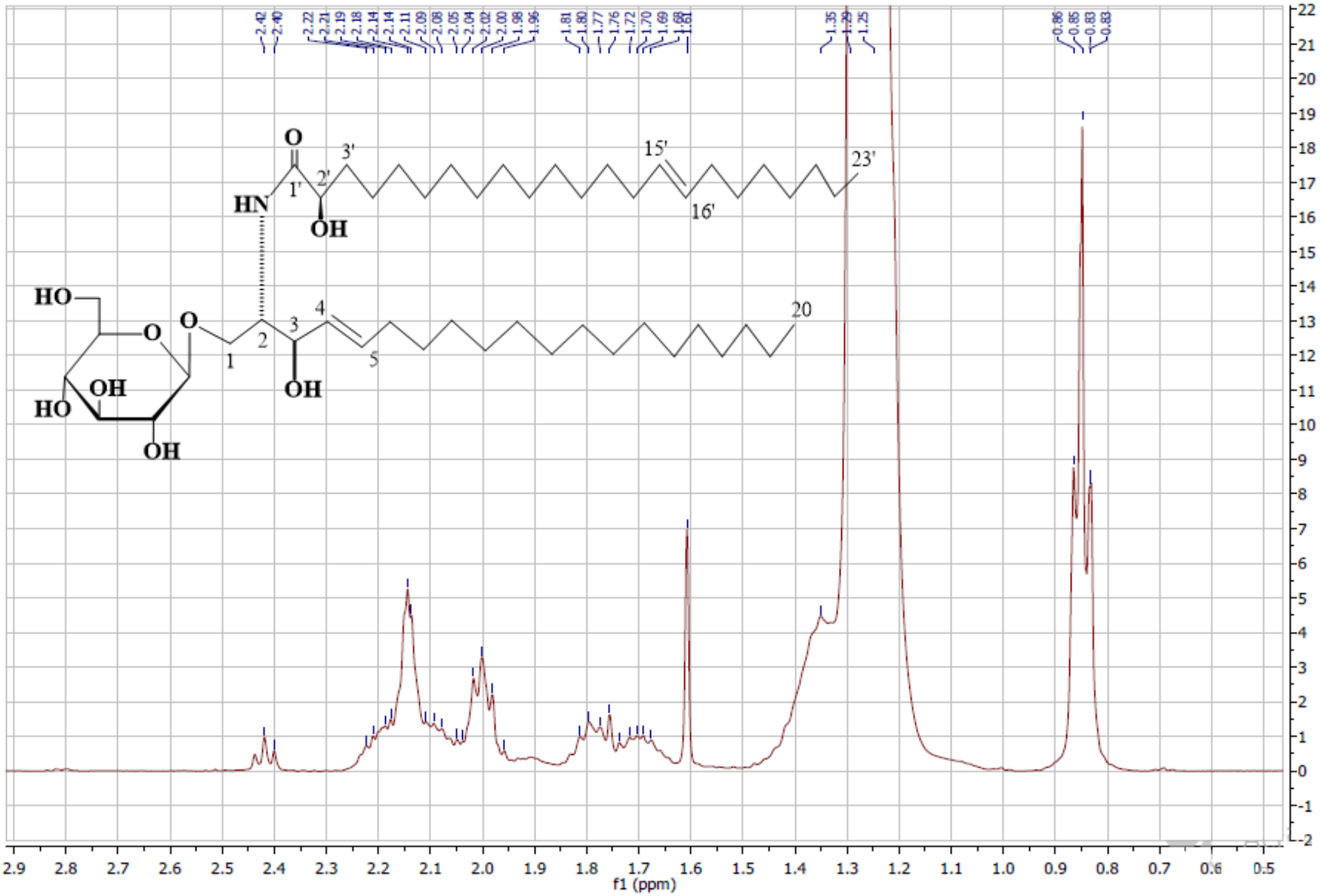


Figure S18. Partial expansions of the ^{1}H NMR spectrum of compound **2** (in C_5D_5N, 400 MHz).

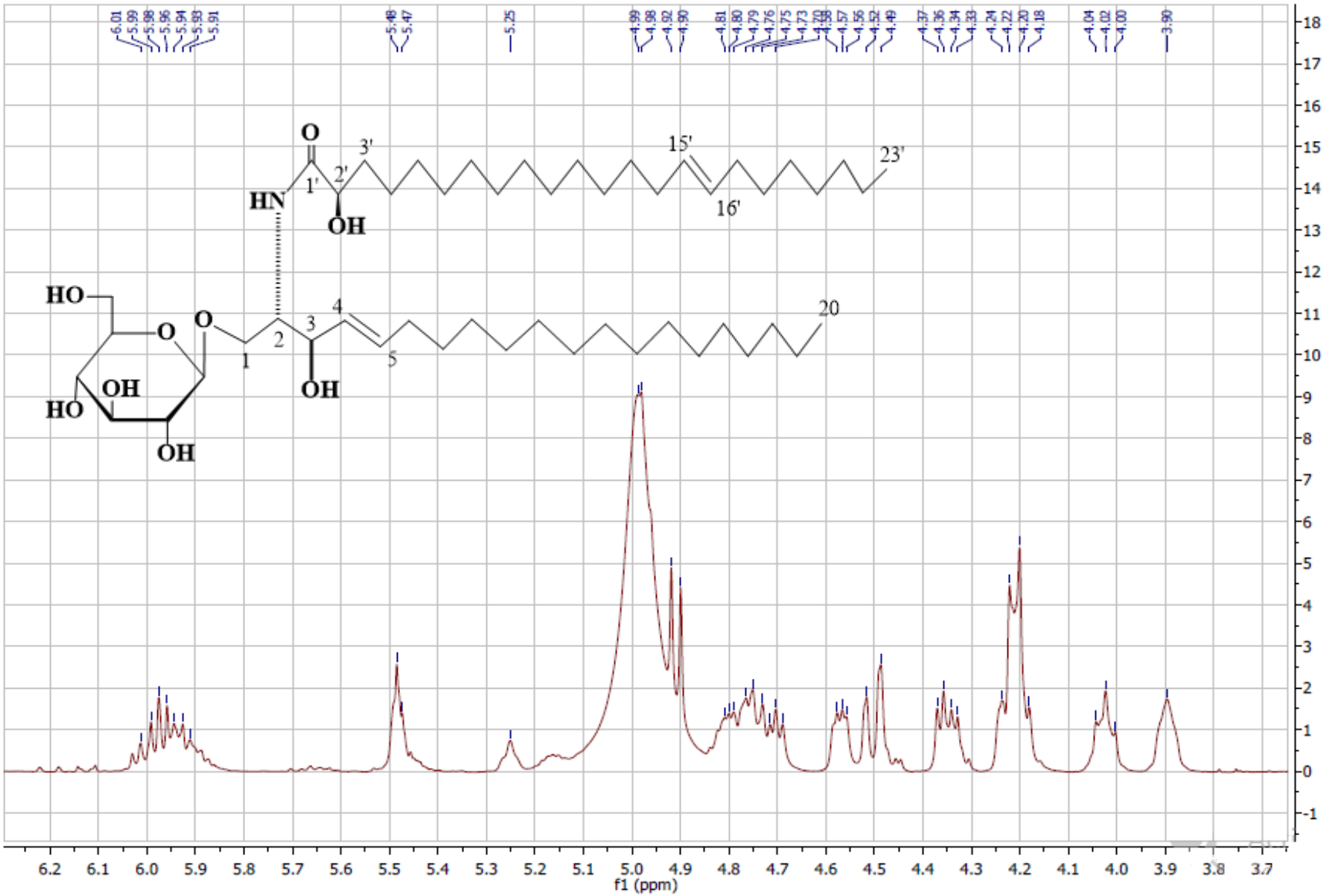


Figure S19. Partial expansions of the ^{1}H NMR spectrum of compound **2** (in C_5D_5N, 400 MHz).

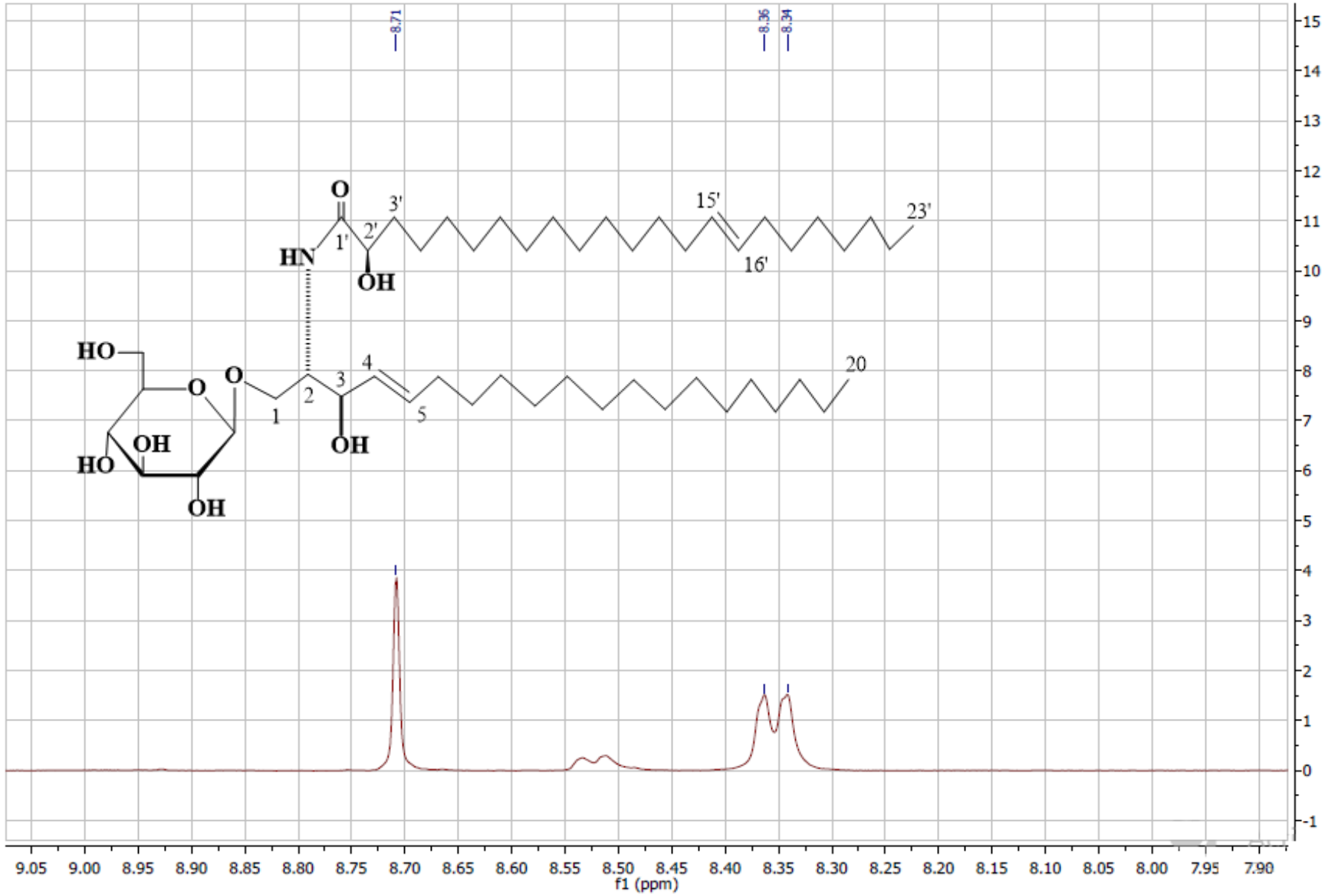


Figure S20. Partial expansions of the ^{1}H NMR spectrum of compound **2** (in C_5D_5N, 400 MHz).

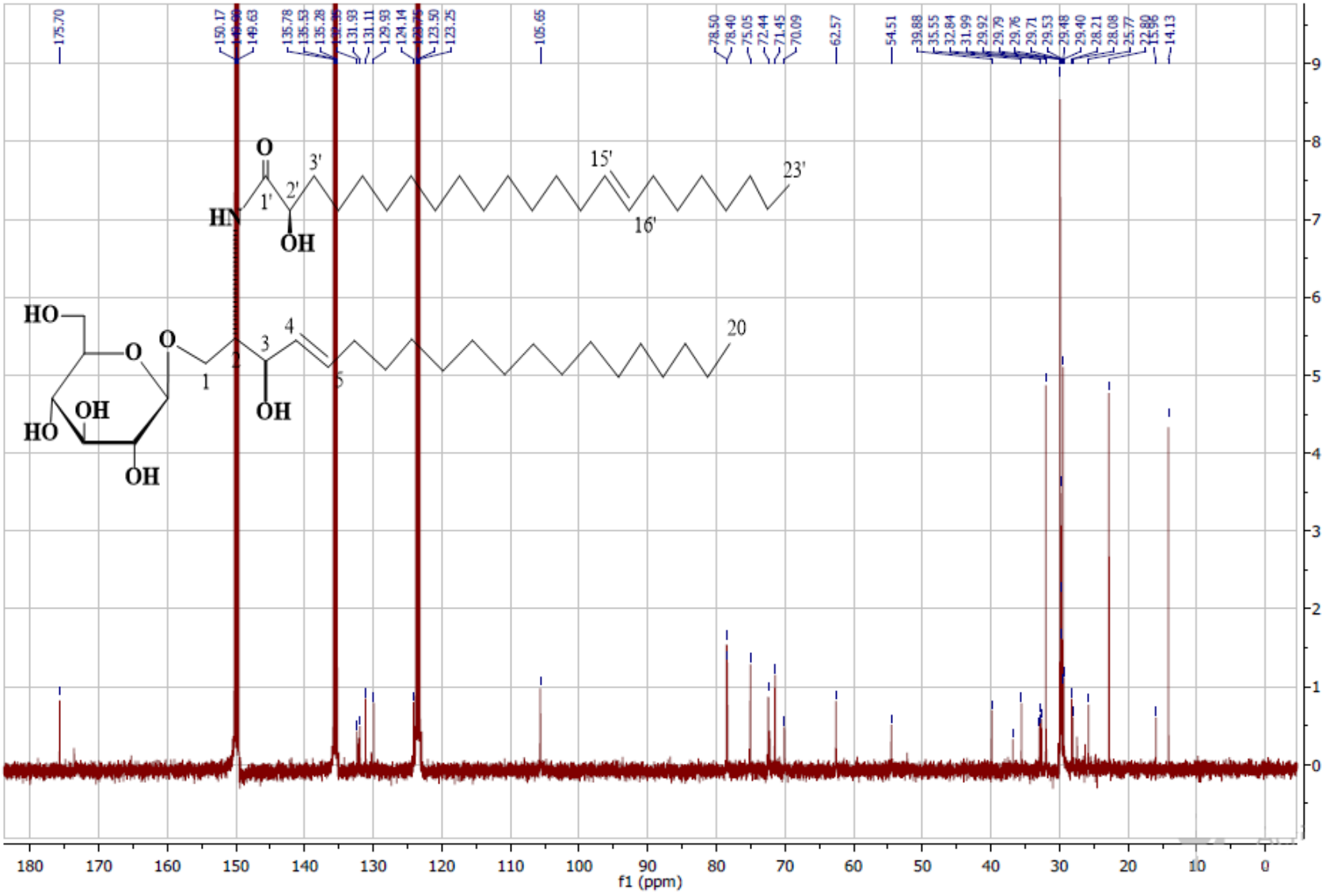


Figure S21. ^{13}C NMR spectrum of compound **2** (in C_5D_5N, 100 MHz).

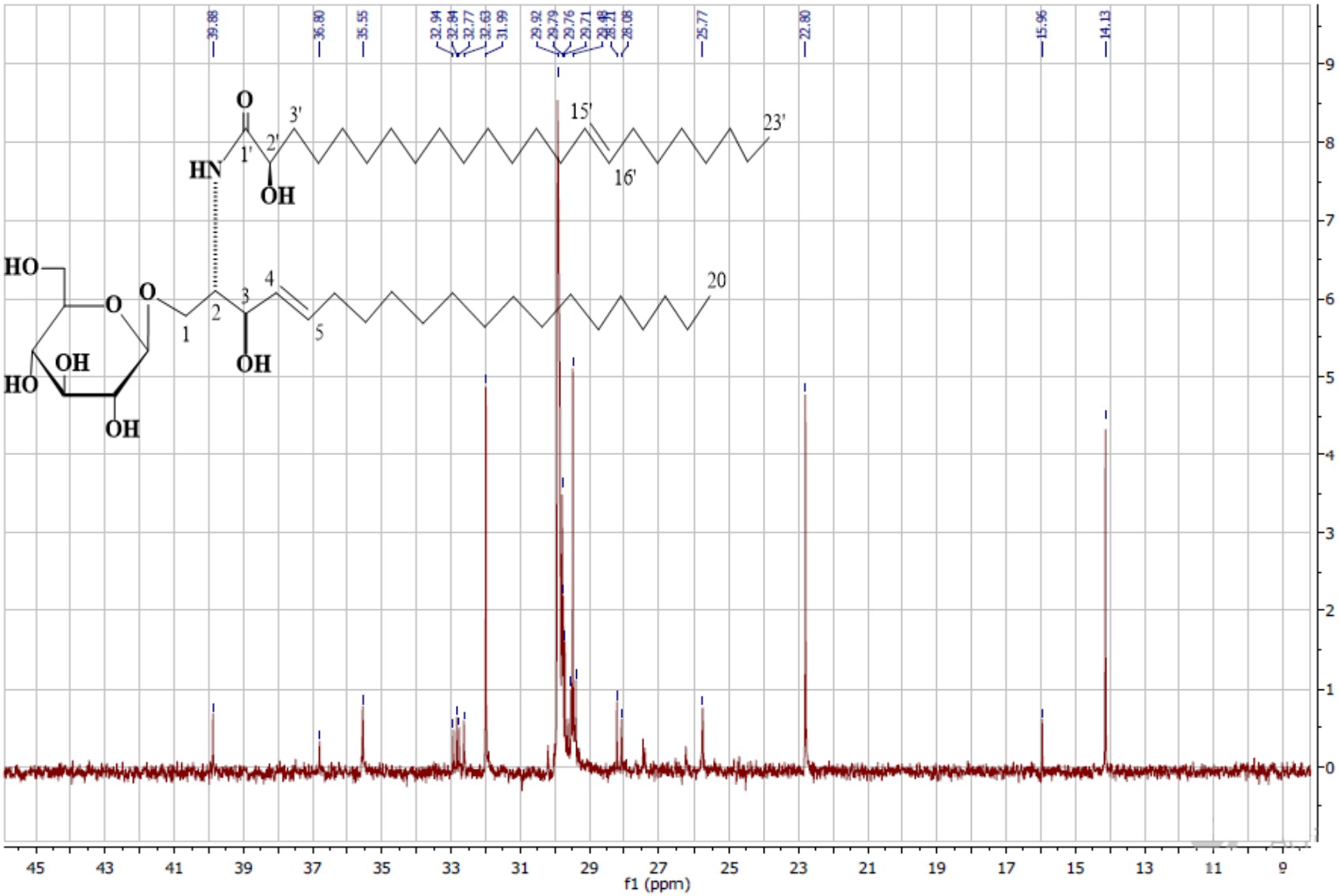


Figure S22. Partial expansion of the ^{13}C NMR spectrum of compound **2** (in C_5D_5N, 100 MHz).

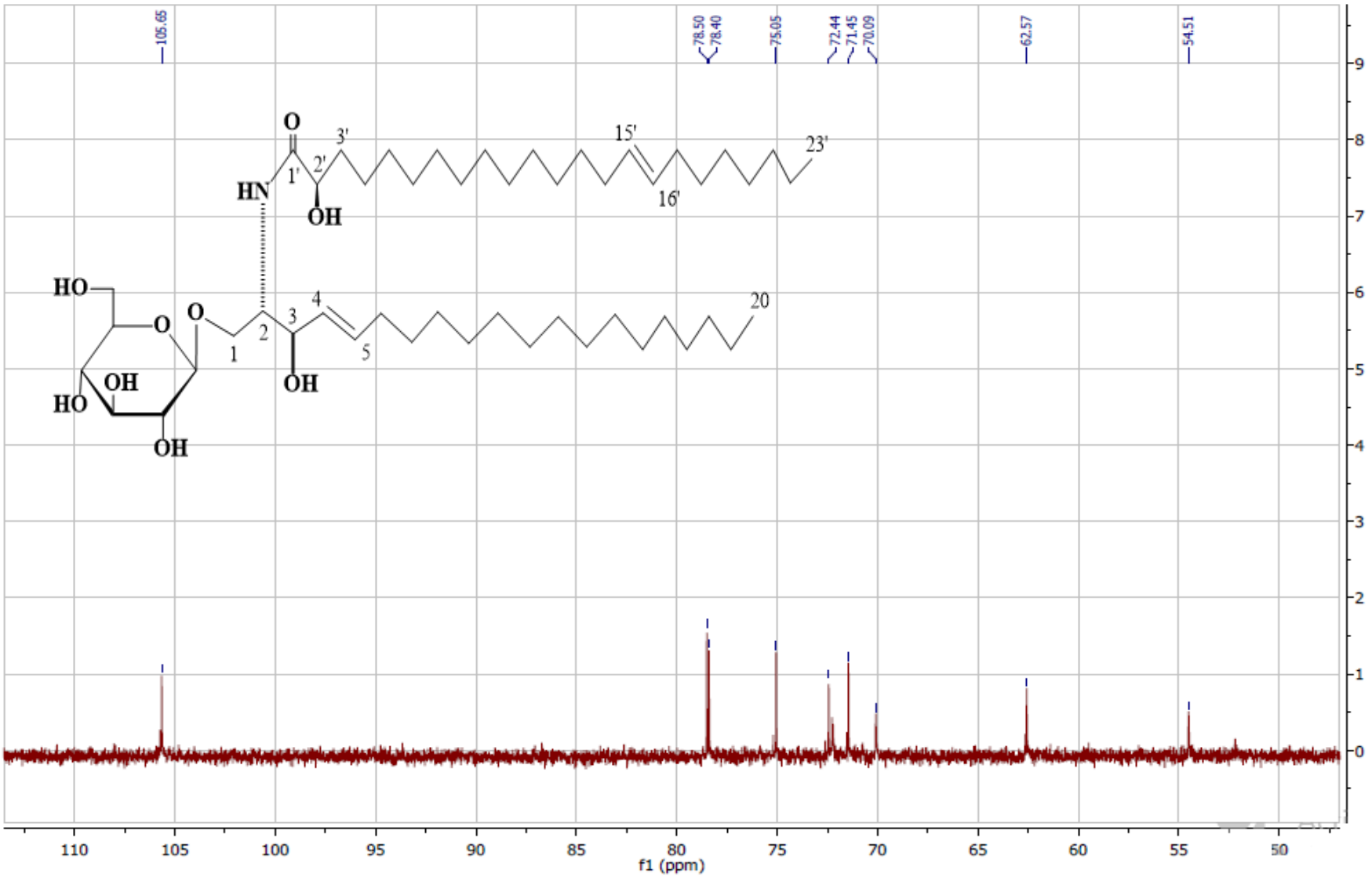


Figure S23. Partial expansion of the ^{13}C NMR spectrum of compound **2** (in C_5D_5N, 100 MHz).

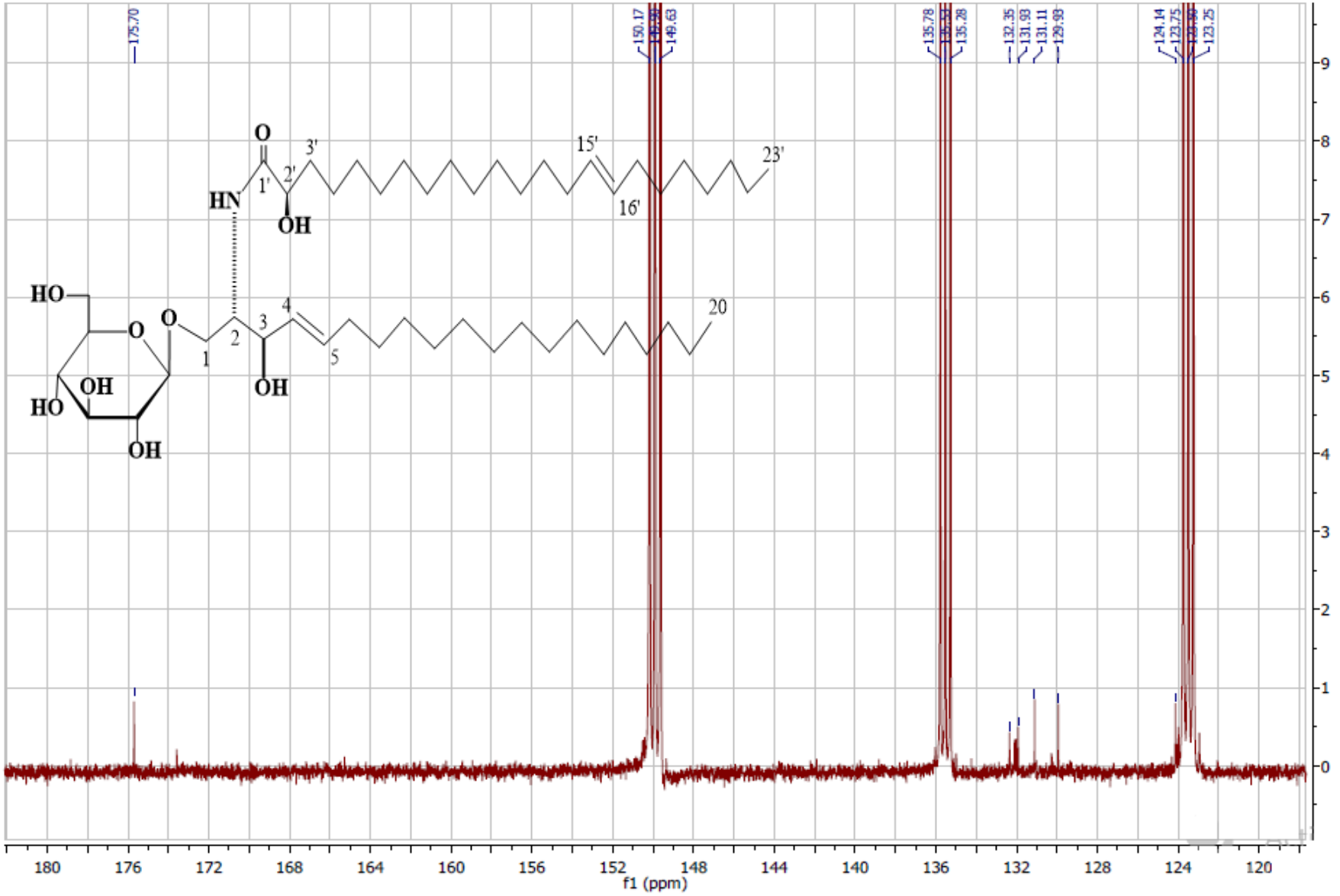


Figure S24. Partial expansion of the ^{13}C NMR spectrum of compound **2** (in C_5D_5N, 100 MHz).

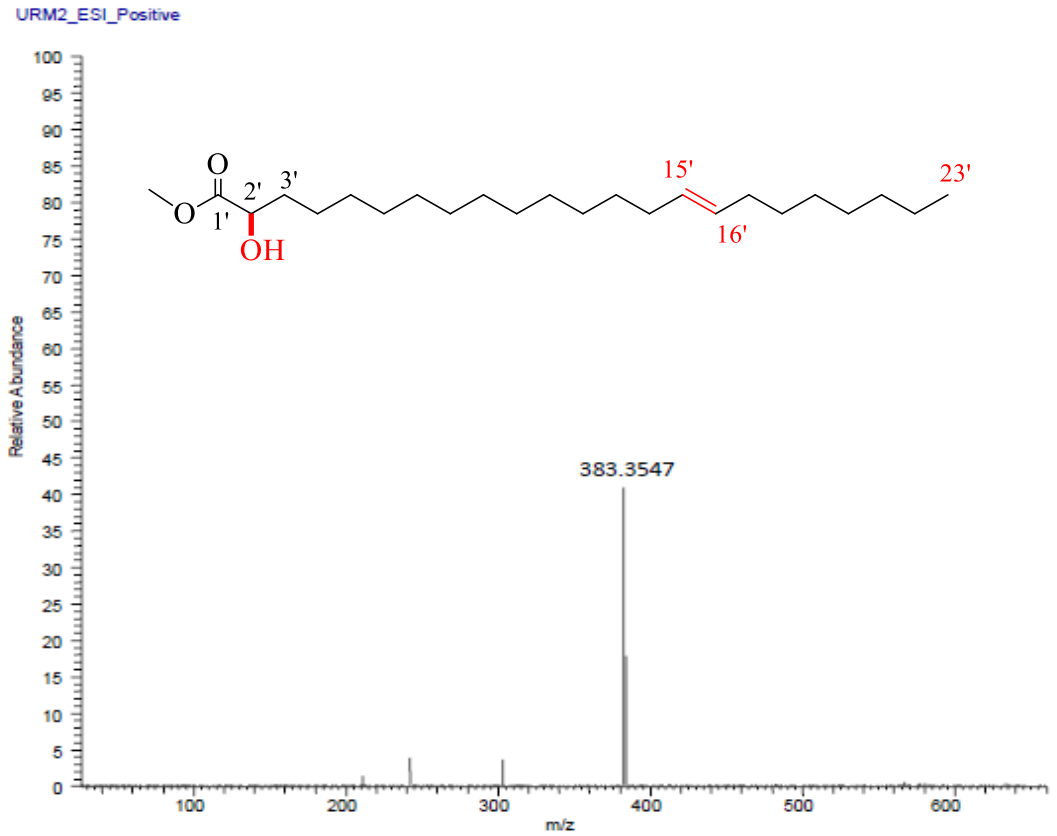


Figure S25. LC-HRESIMS for α-hydroxy fatty acid methyl ester after hydrolysis of compound **2**

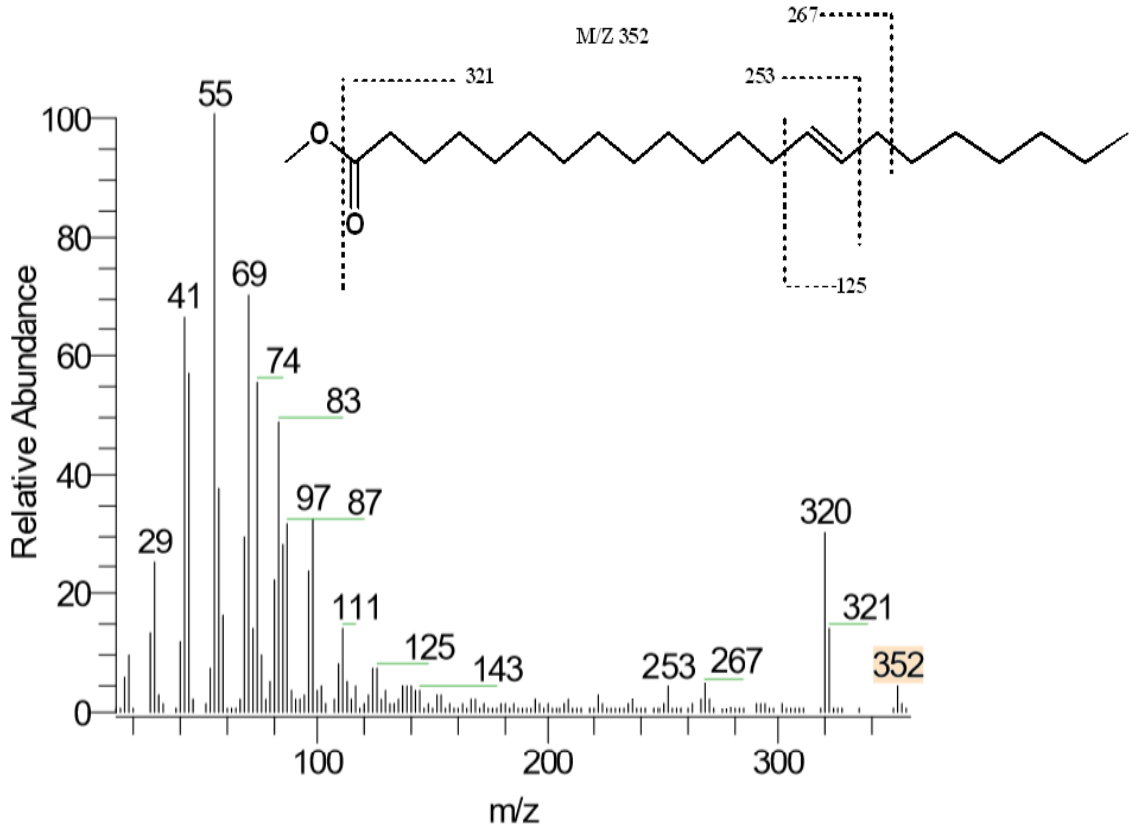


Figure S26. GC-MS analysis of fatty acids methyl esters carried out after oxidation of α-hydroxy fatty acid methyl ester (Compound 2)

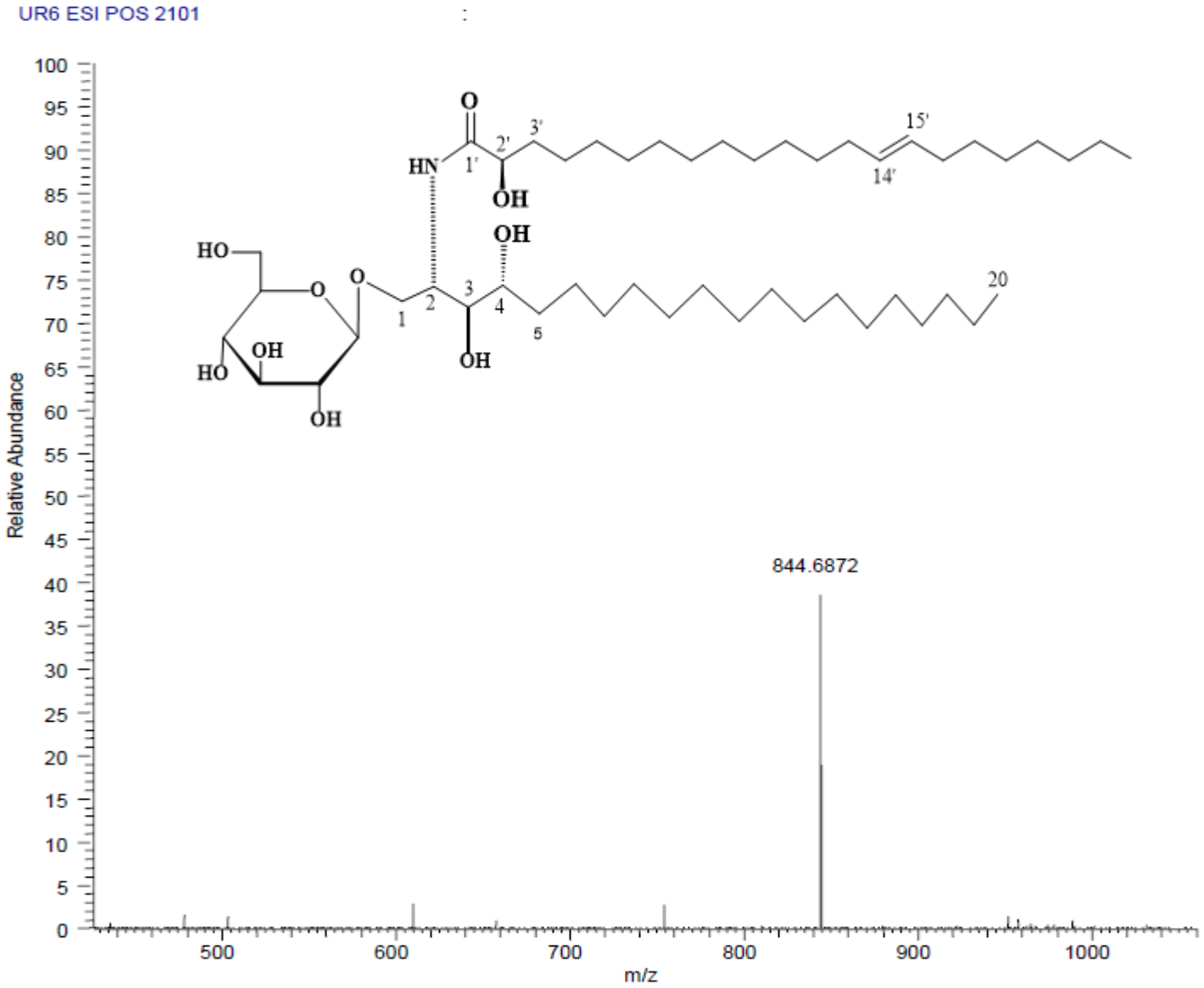


Figure S27. LC-HRESIMS of Compound **3** $(M+H)^+$.

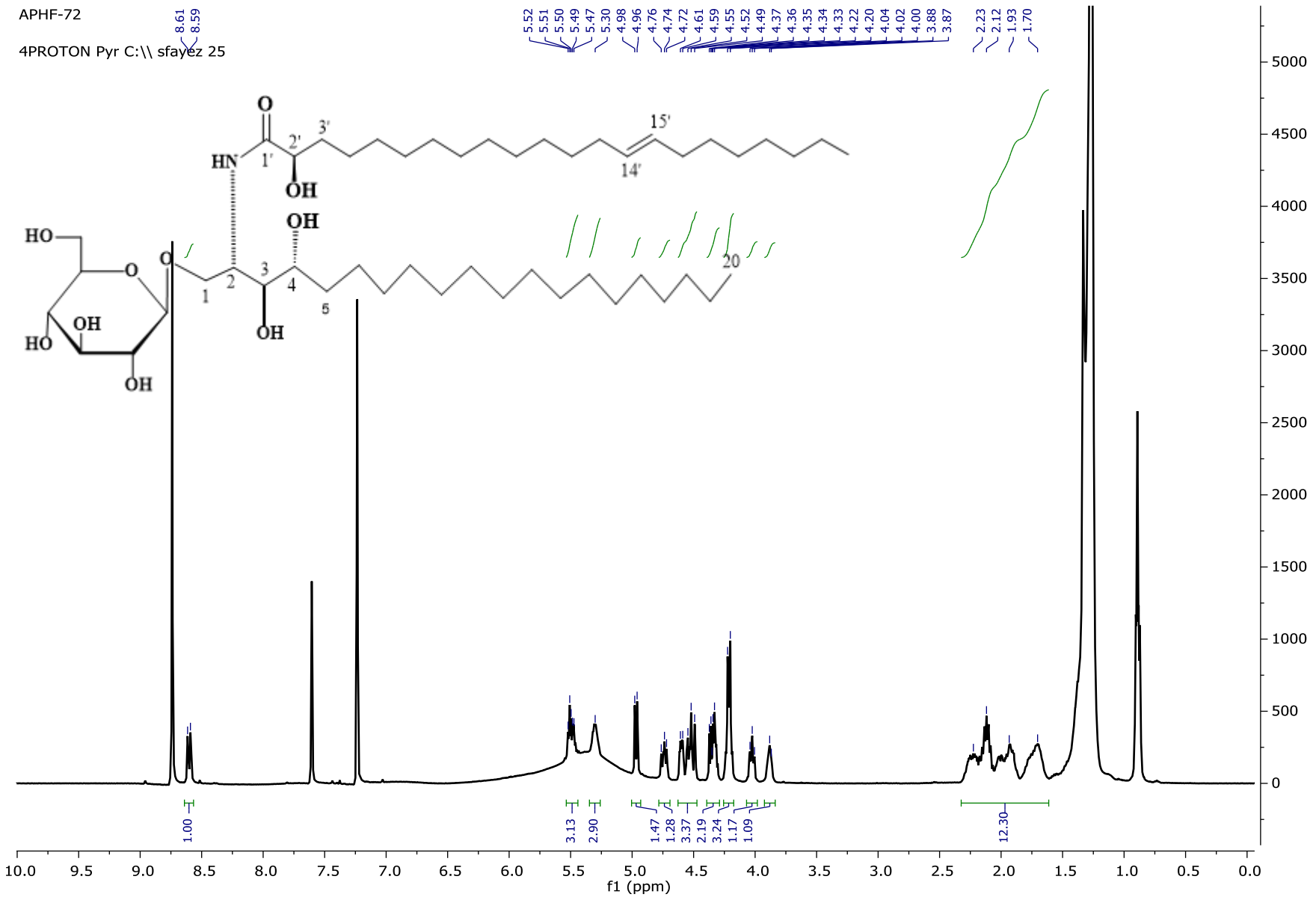


Figure S28. ^{1}H NMR spectrum of compound **3** (in C_5D_5N, 400 MHz).

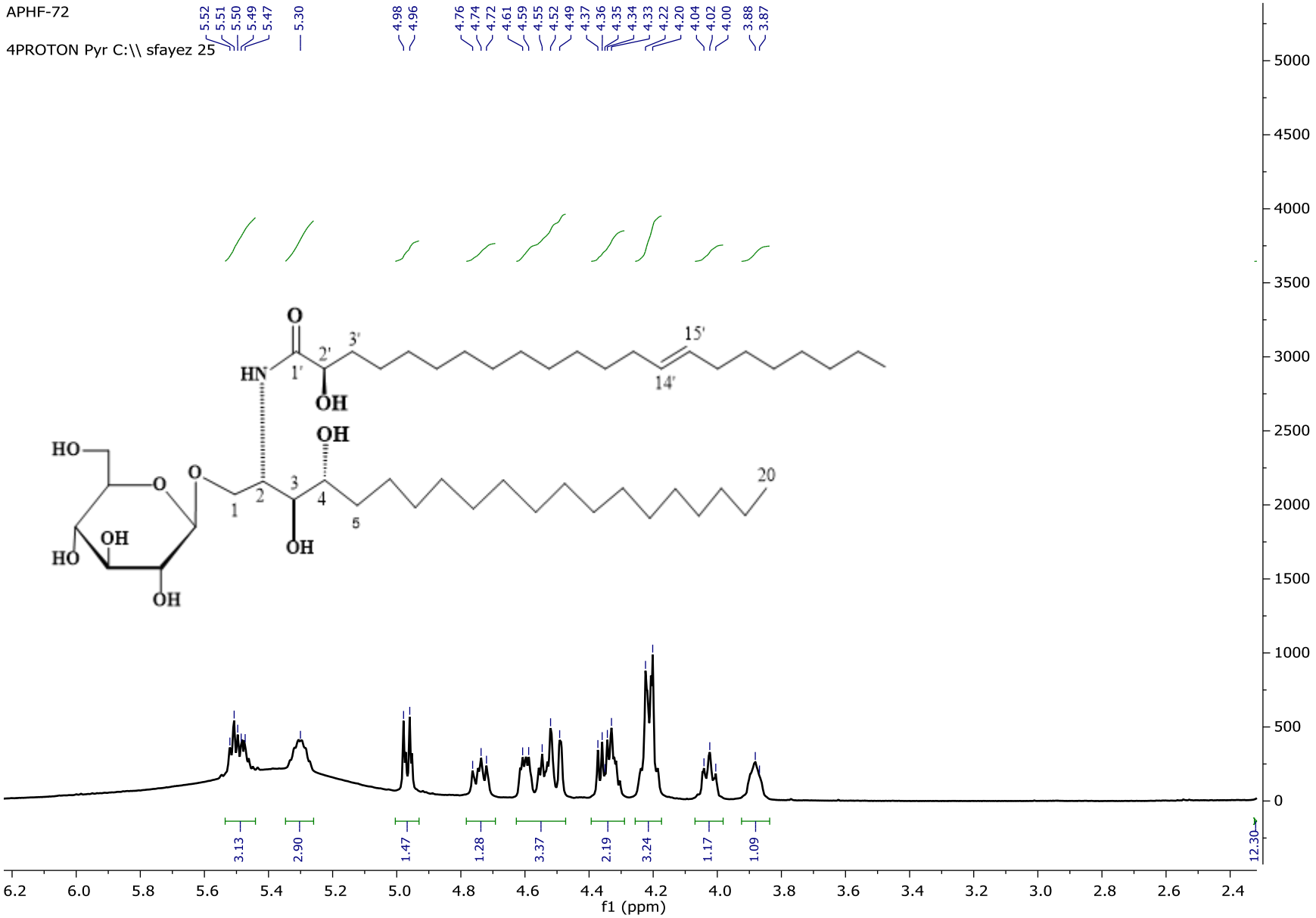


Figure S29. Partial expansion of the ^{1}H NMR spectrum of compound **3** (in C_5D_5N, 400 MHz).

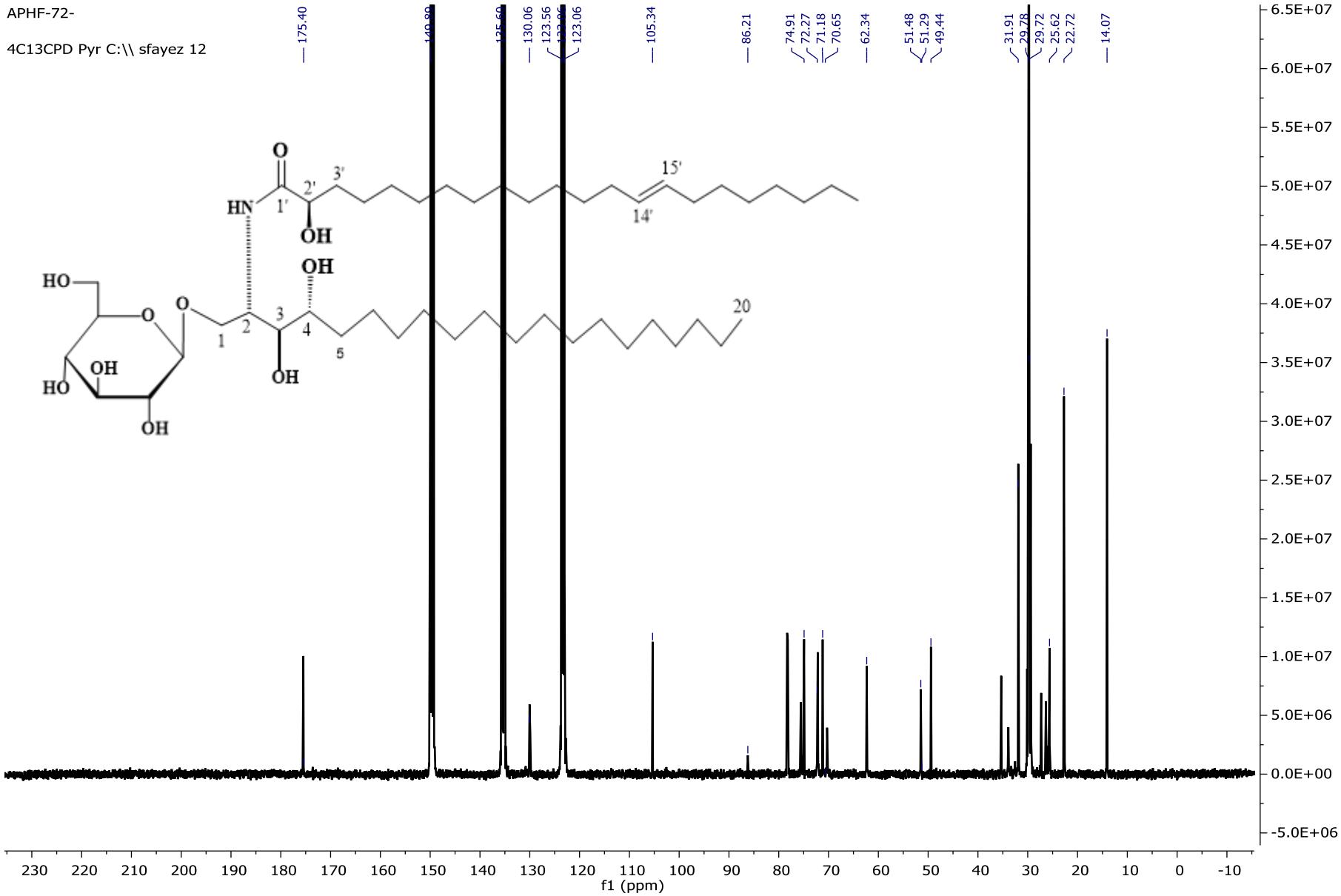


Figure S30. ^{13}C NMR spectrum of compound **3** (in C_5D_5N, 100 MHz).

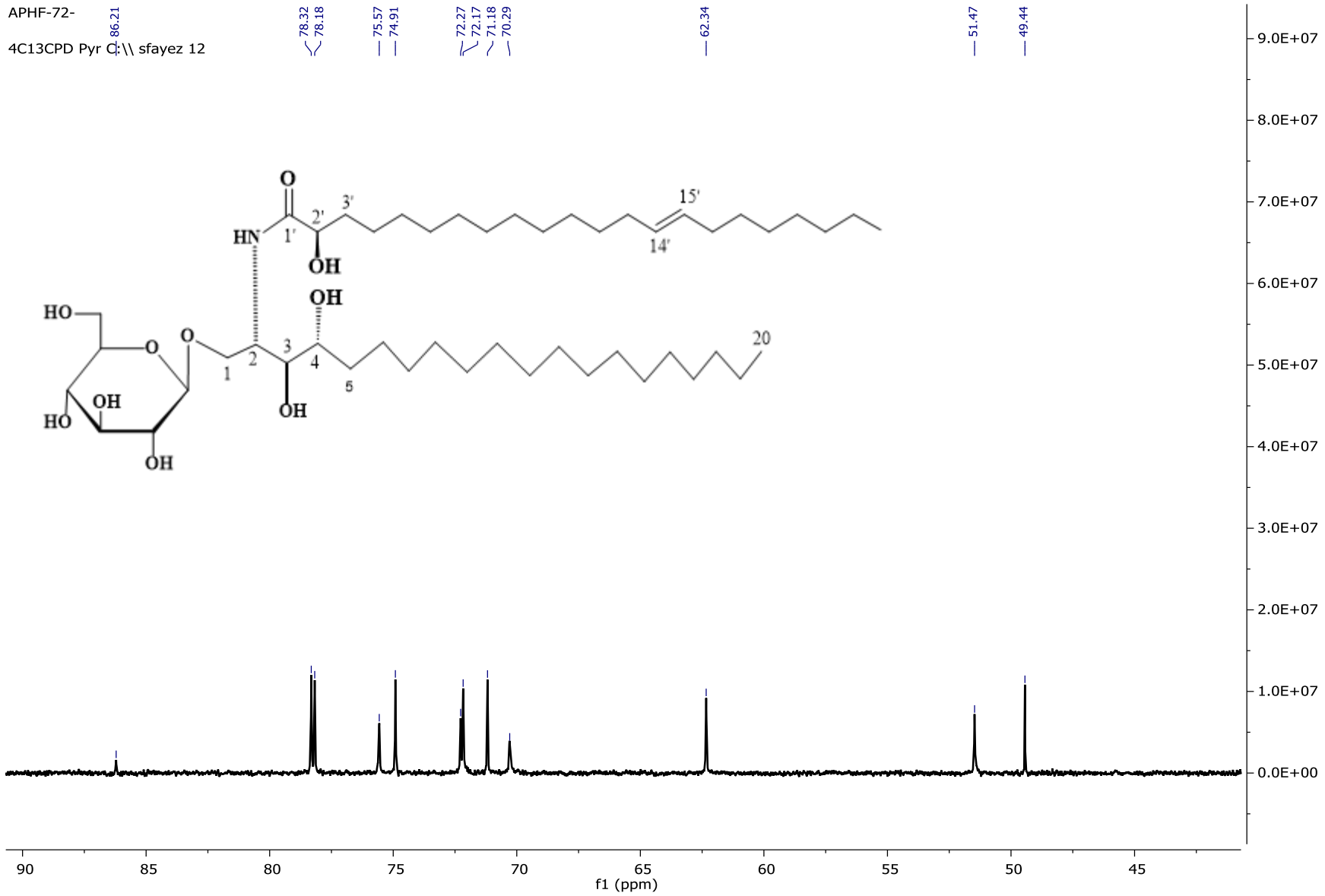


Figure S31. Partial expansion of the ^{13}C NMR spectrum of compound **3** (in C_5D_5N, 100 MHz).

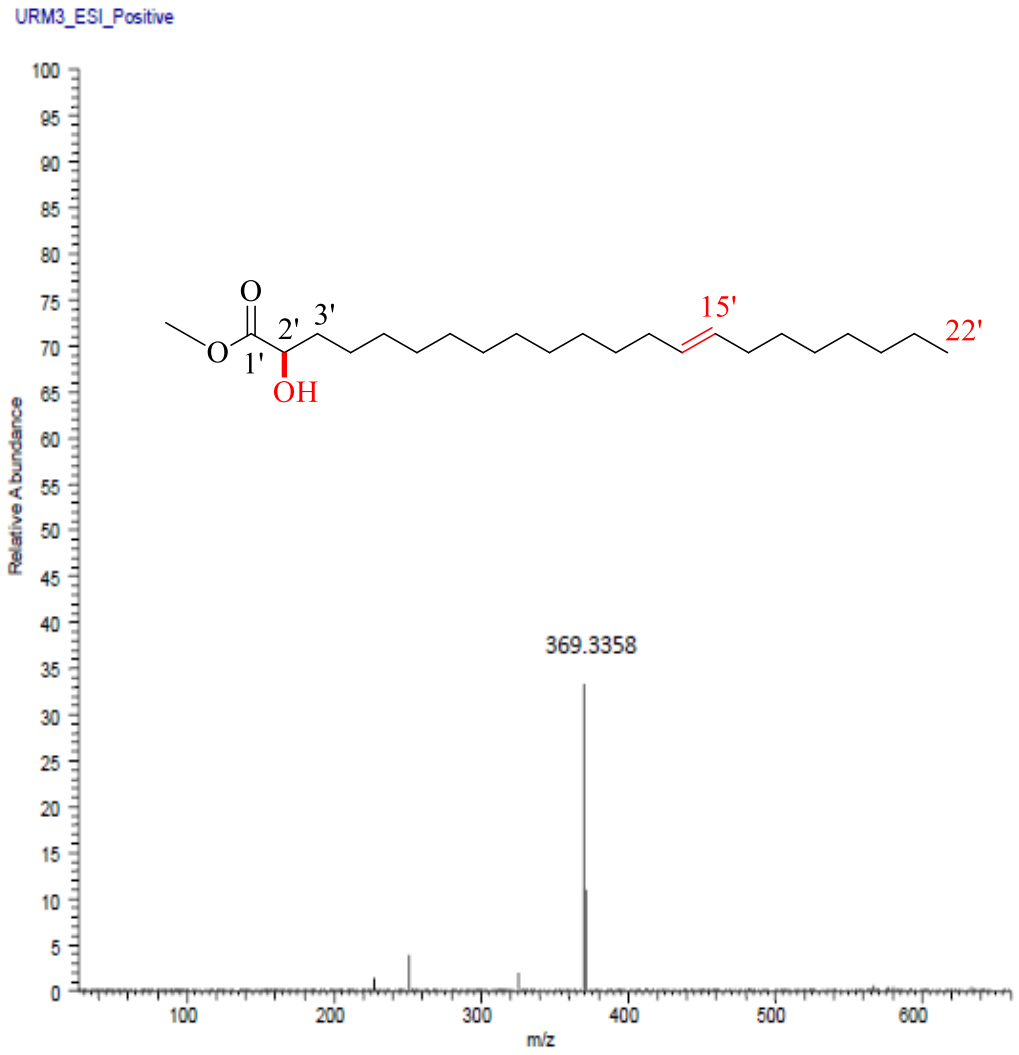


Figure S32. LC-HRESIMS for α-hydroxy fatty acid methyl ester after hydrolysis of compound **3**

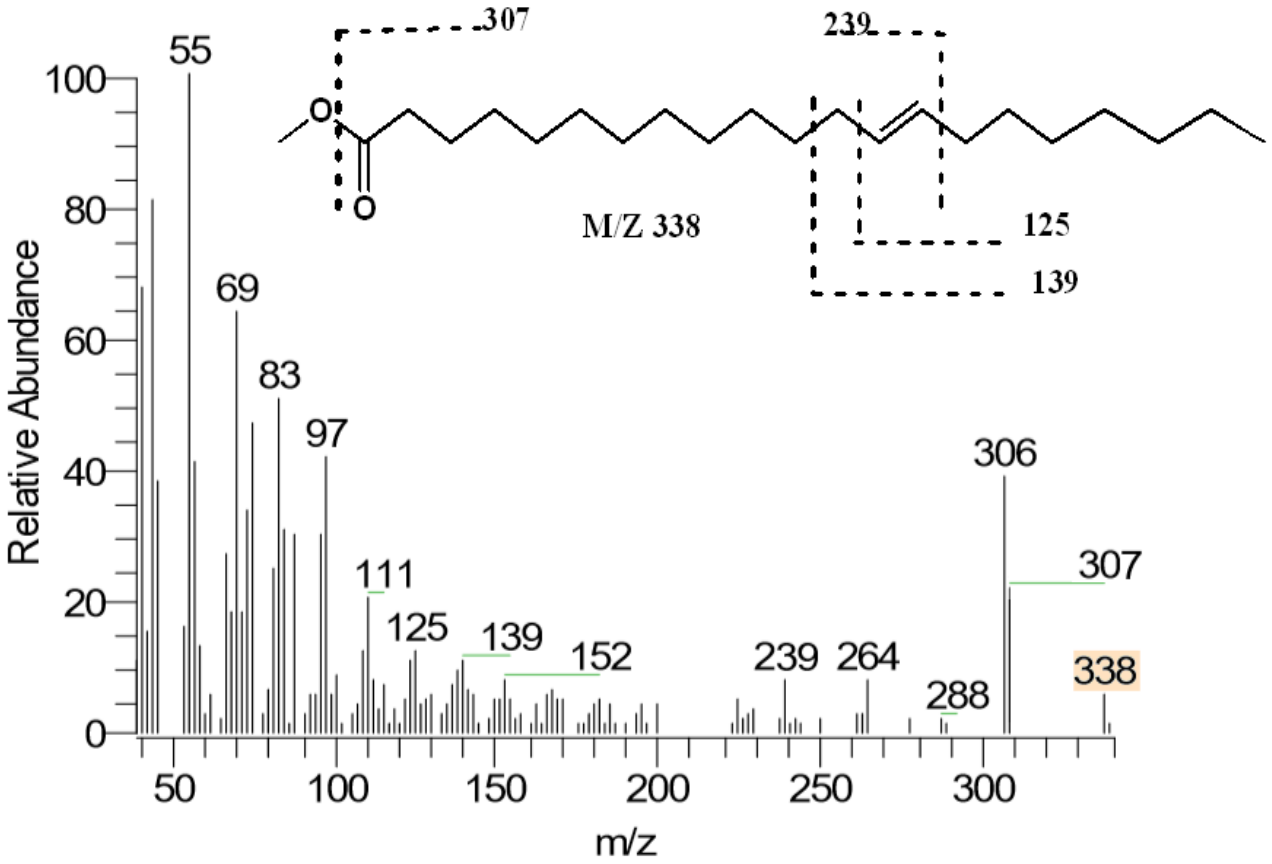


Figure S33. GC-MS analysis of fatty acids methyl esters carried out after oxidation of α-hydroxy fatty acid methyl ester (Compound 3)

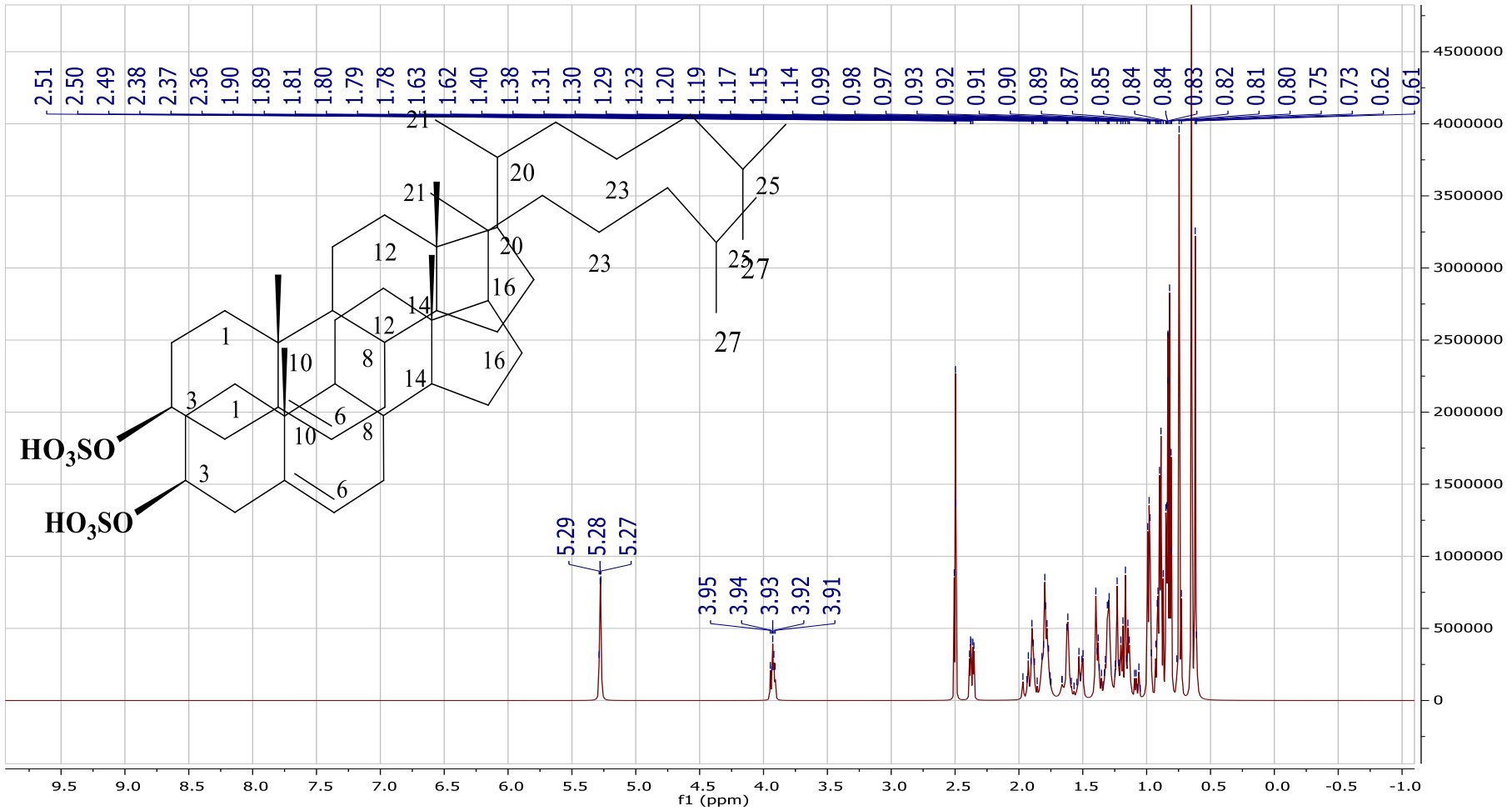


Figure S34. ^{1}H NMR spectrum of compound **4** (in DMSO, 400 MHz)

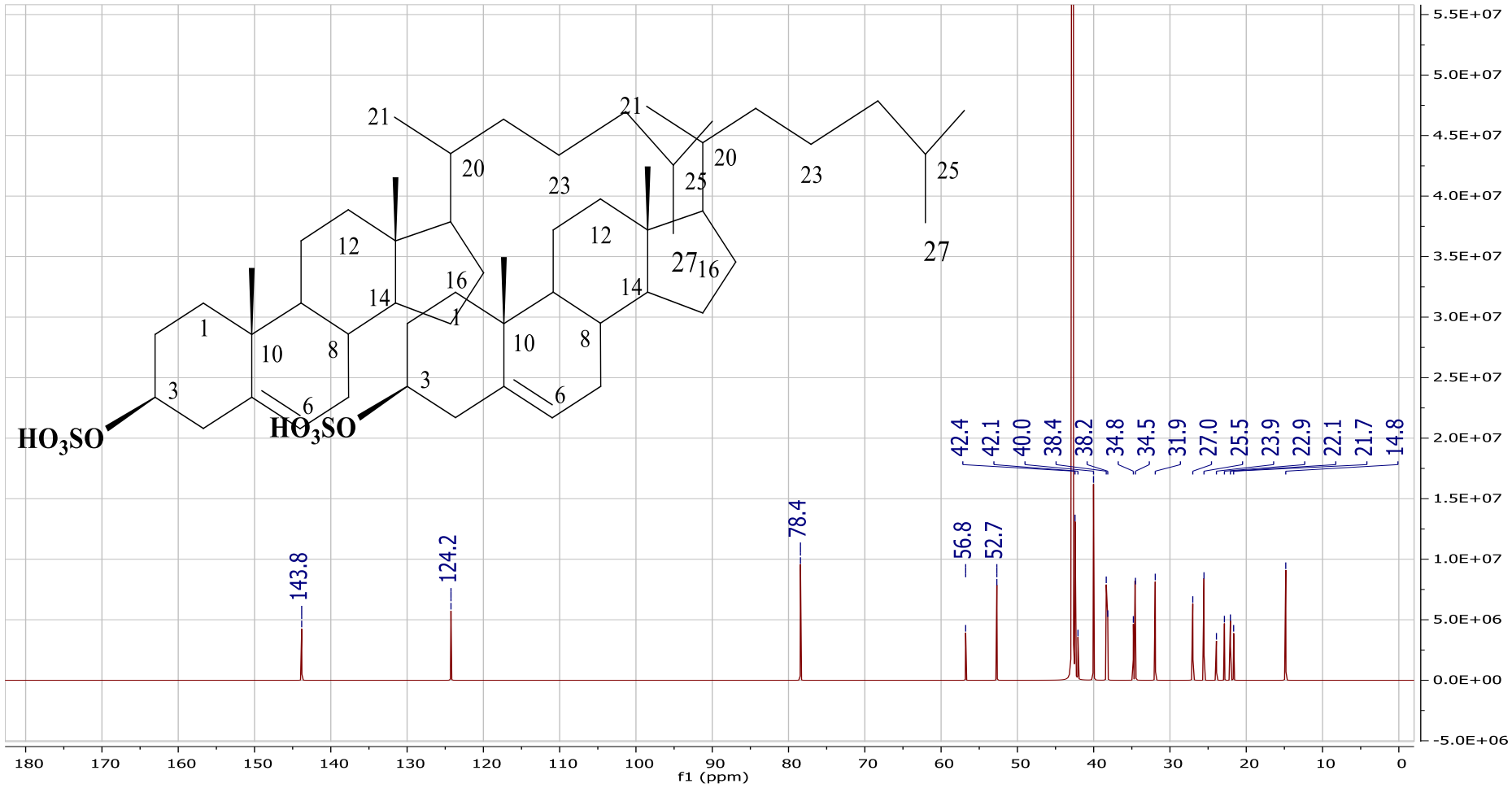


Figure S35. ^{13}C NMR spectrum of compound **4** (in DMSO, 400 MHz)

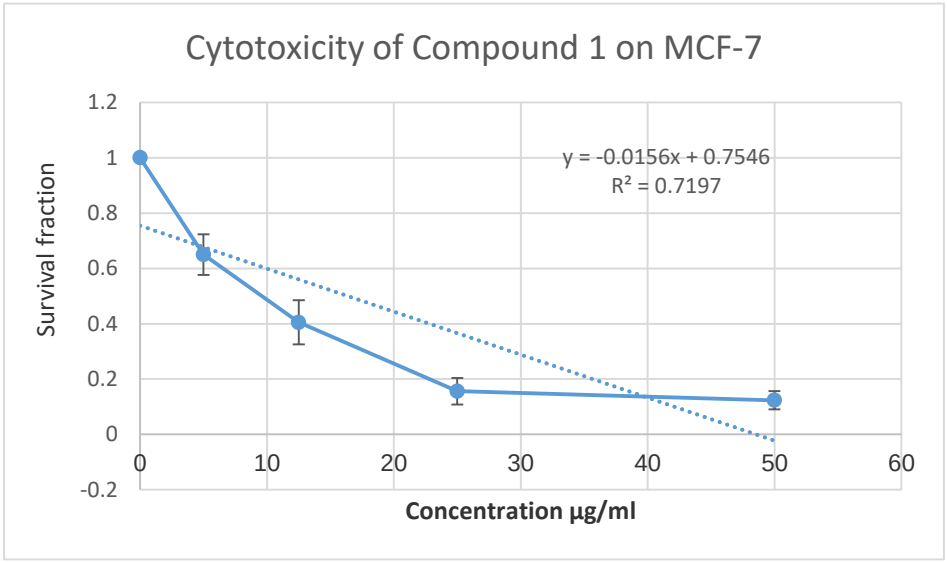


Figure S36. Cytotoxicity of compound **1** on MCF-7

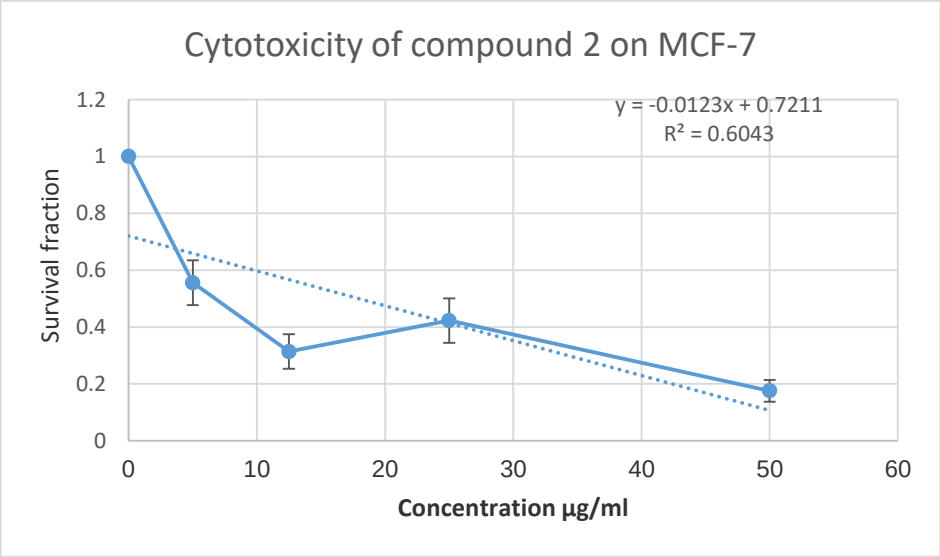


Figure S37. Cytotoxicity of compound **2** on MCF-7

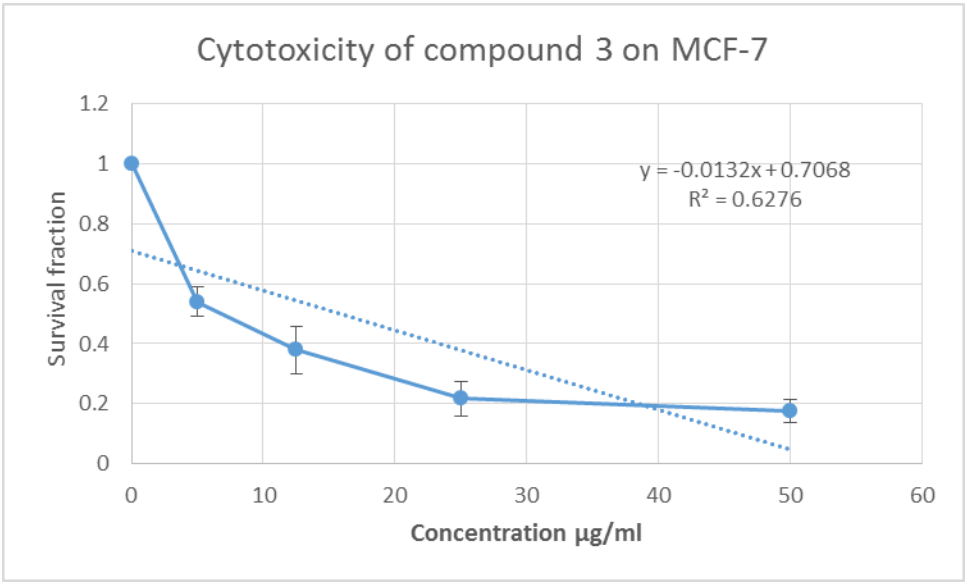


Figure S38. Cytotoxicity of compound **3** on MCF-7

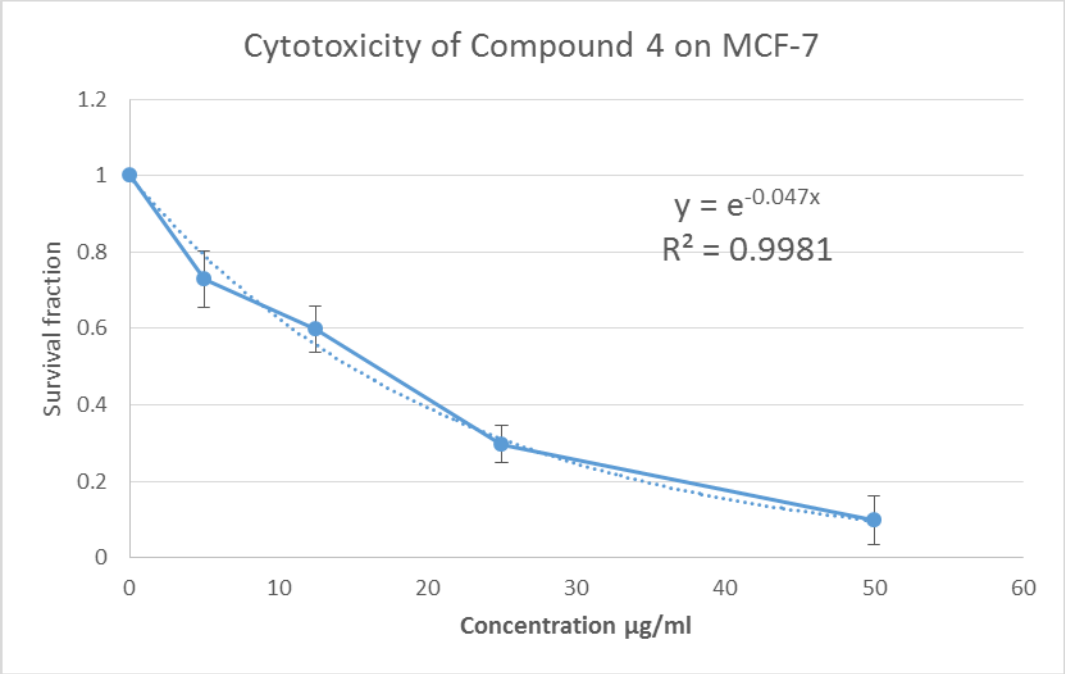


Figure S39. Cytotoxicity of compound **4** on MCF-7

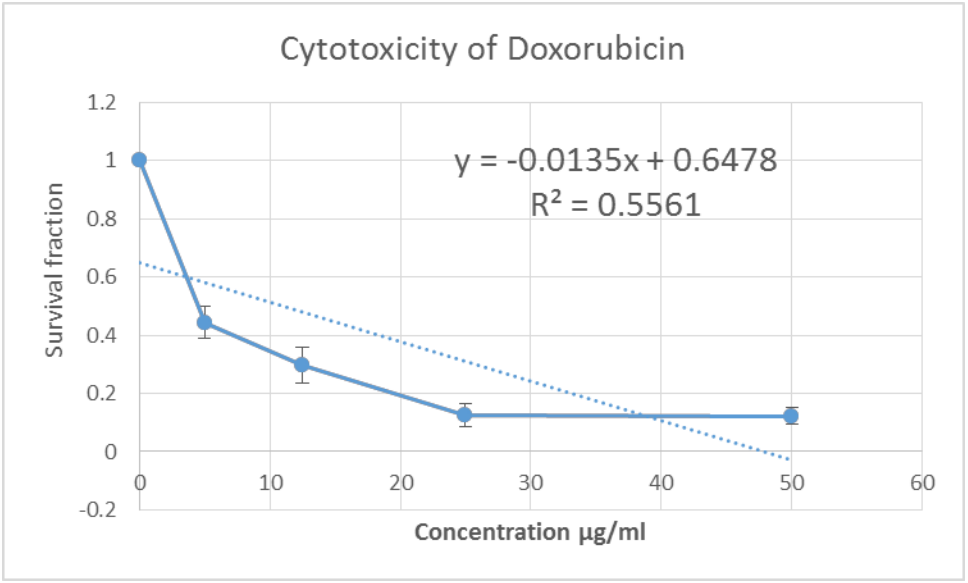


Figure S40. Cytotoxicity of Doxorubicin on MCF-7