

Article

Holospiniferoside: A New Antitumor Cerebroside from The Red Sea Cucumber *Holothuria spinifera*: In Vitro and In Silico Studies

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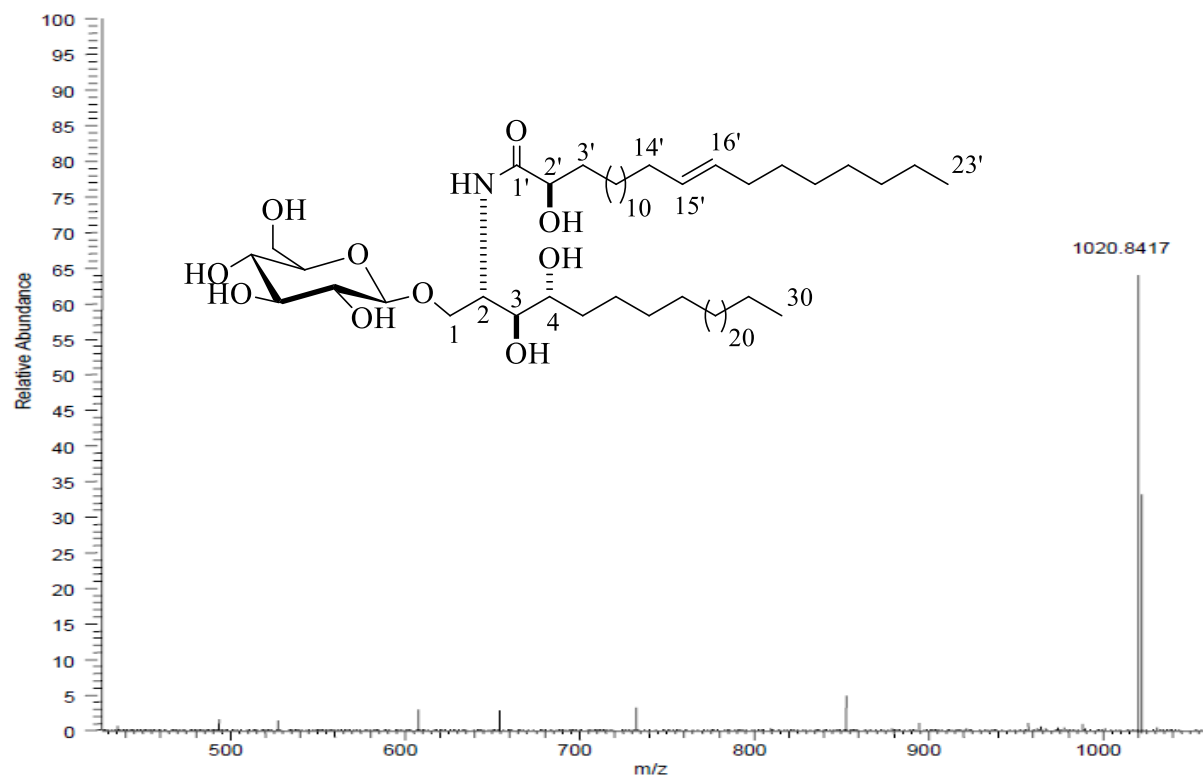


Figure S1: HRMS of Compound 1 $(M+Na)^+$.

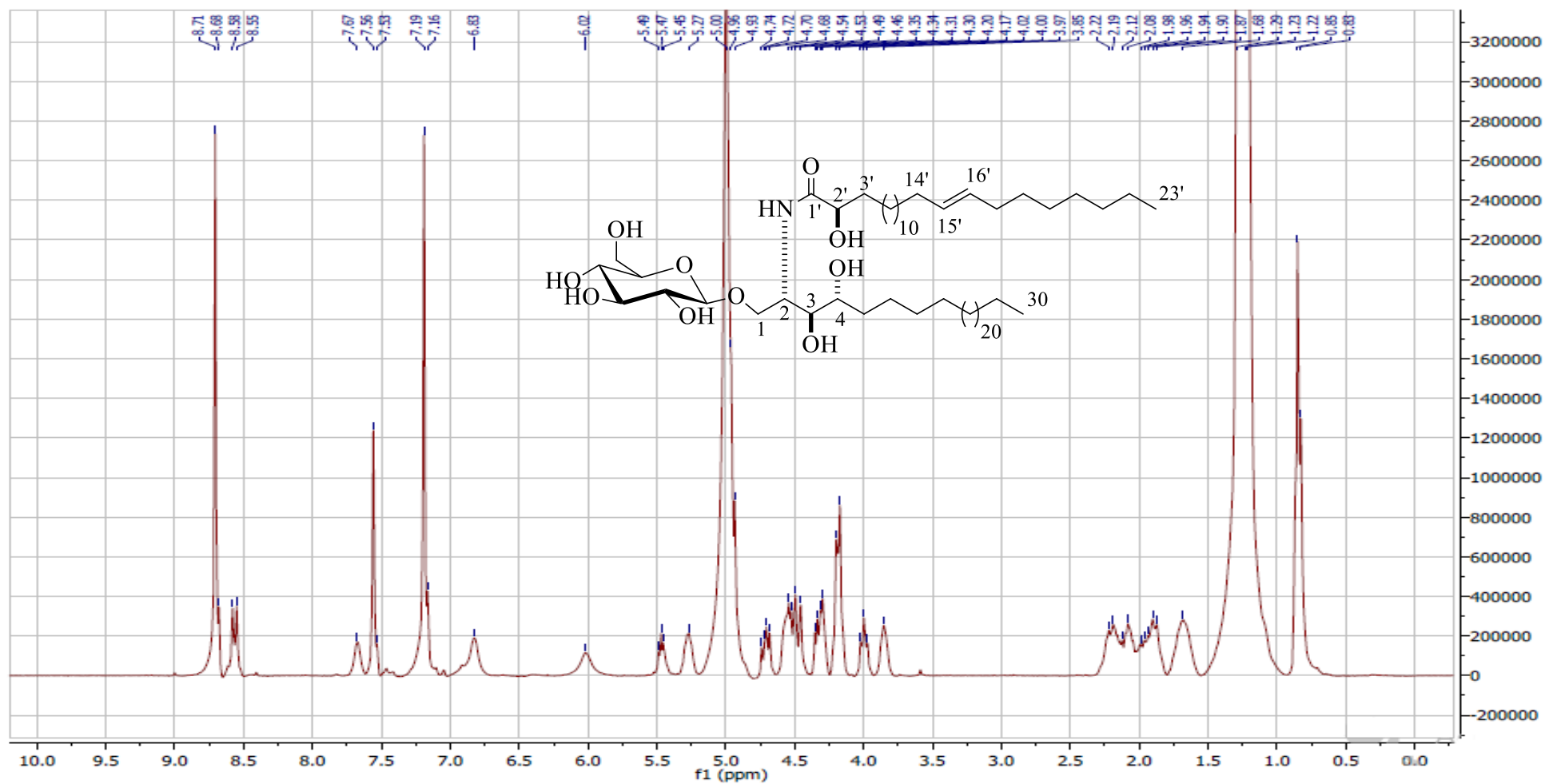


Figure S2: ¹H-NMR spectrum of compound 1 in (C₅D₅N, 400 MHz).

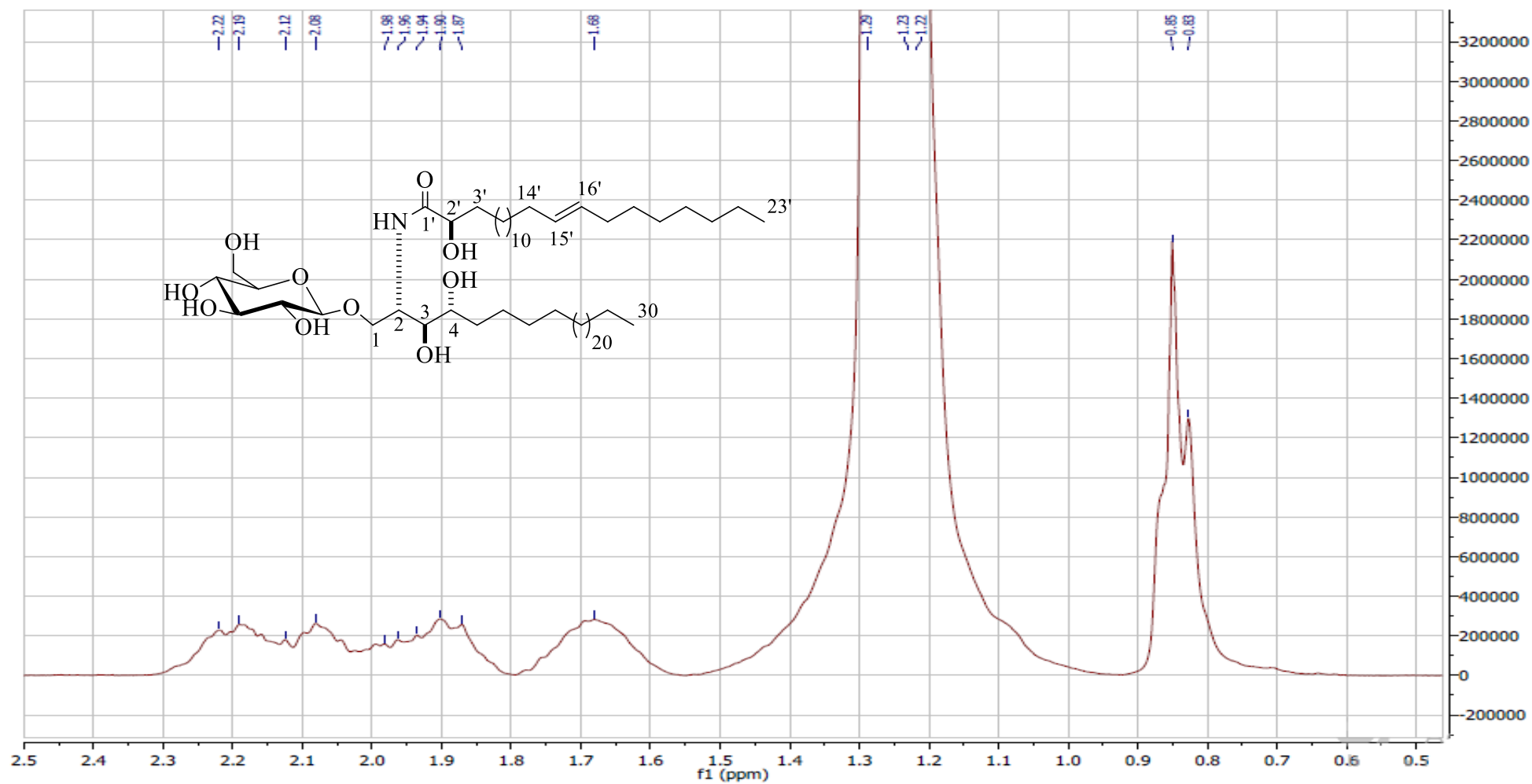


Figure S3: Partial expansion of the $^1\text{H-NMR}$ spectrum of compound 1 in $(\text{C}_5\text{D}_5\text{N}, 400 \text{ MHz})$.

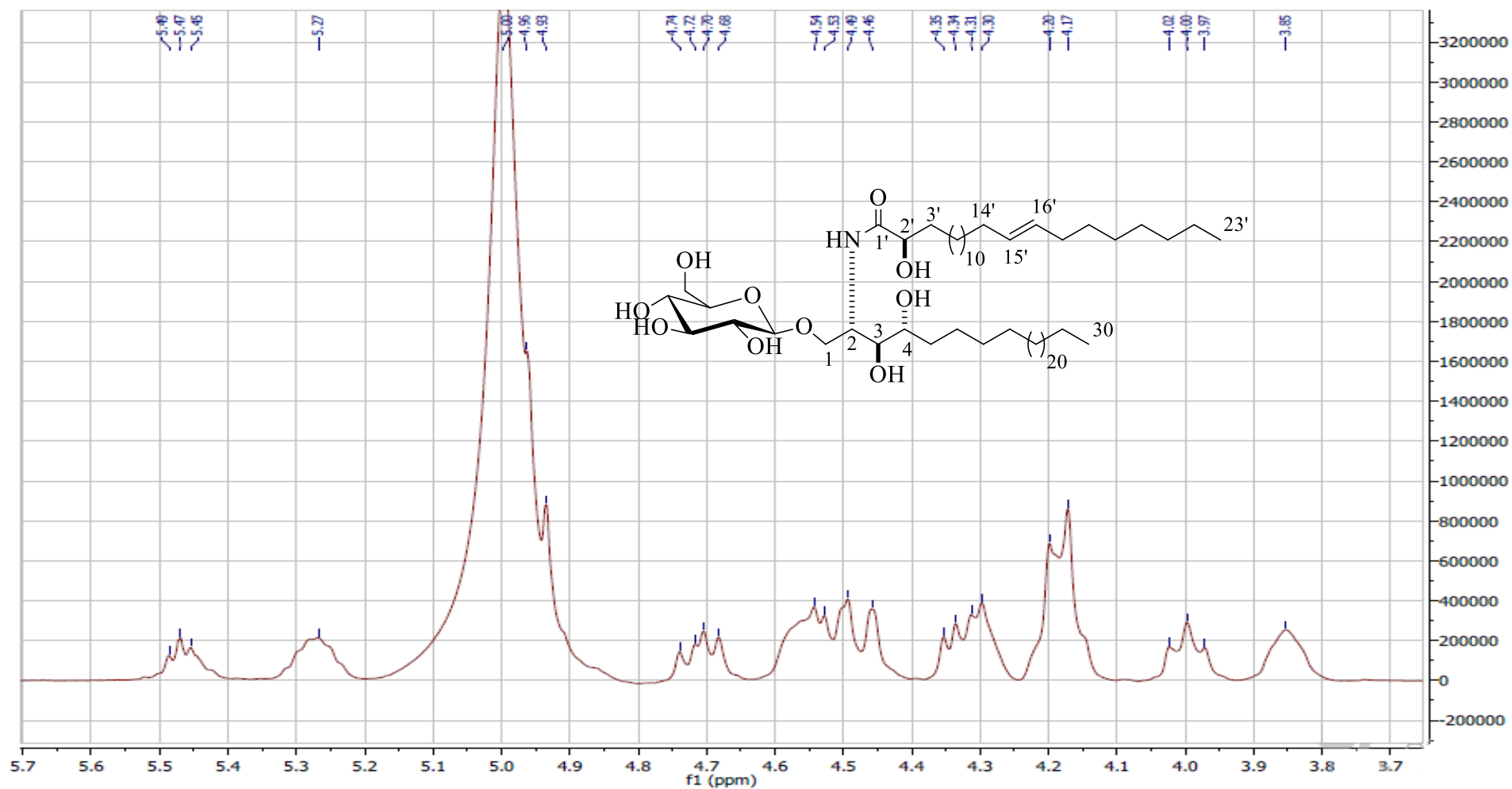


Figure S4: Partial expansion of the $^1\text{H-NMR}$ spectrum of compound 1 in ($\text{C}_5\text{D}_5\text{N}$, 400 MHz).

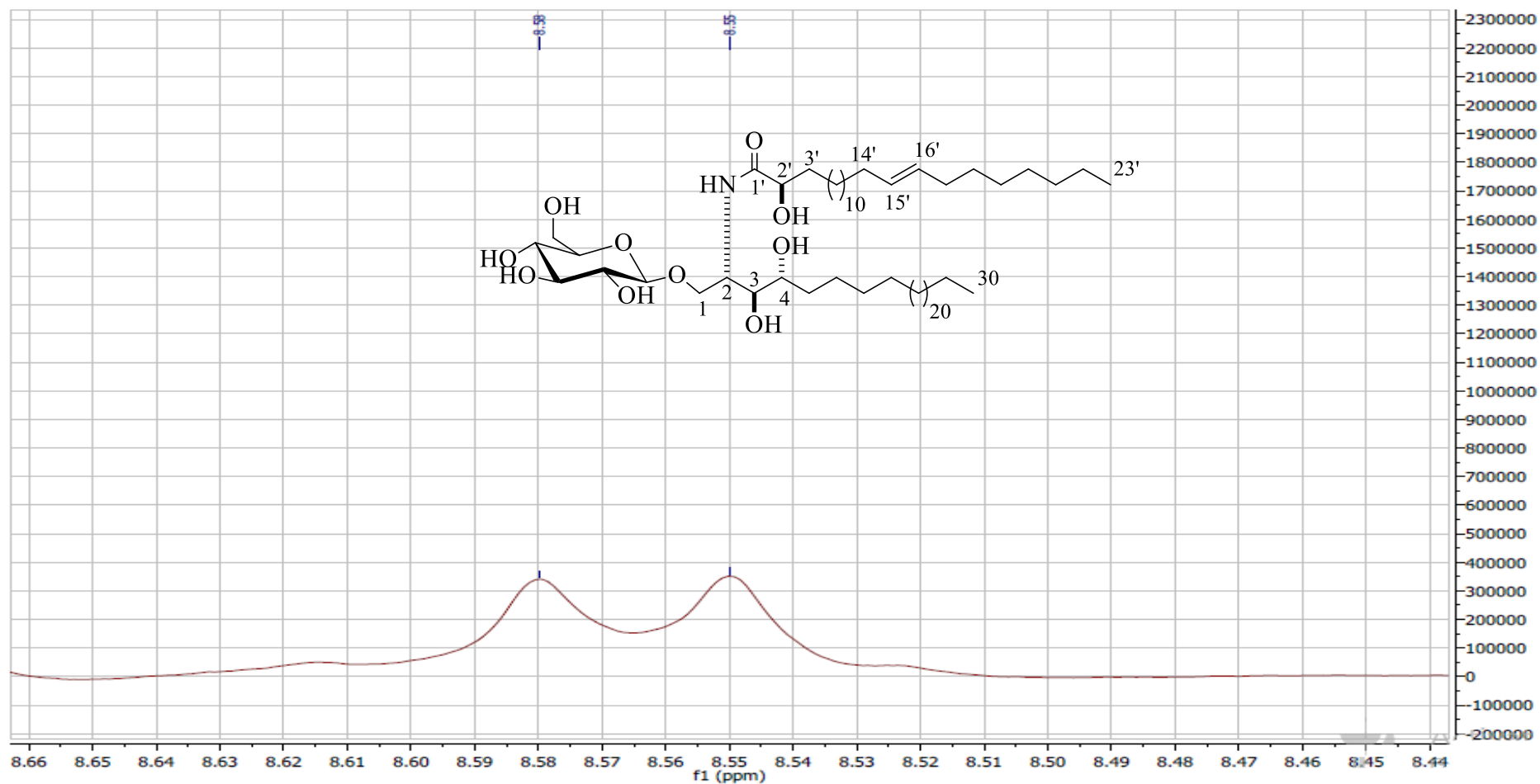


Figure S5: Partial expansion of the ¹H-NMR spectrum of compound 1 in (C₅D₅N, 400 MHz).

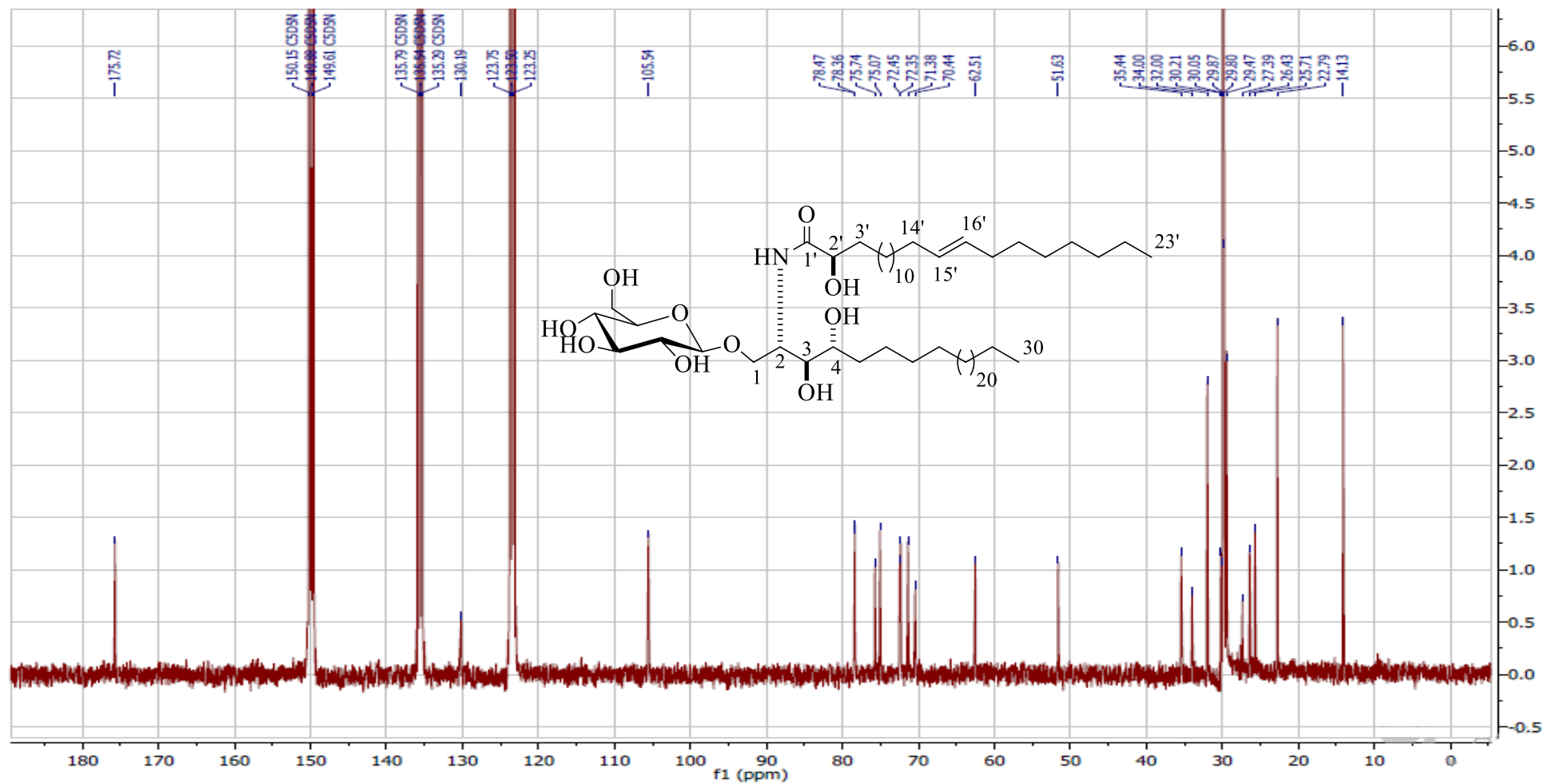


Figure S6: ^{13}C -NMR spectrum of compound 1 in ($\text{C}_5\text{D}_5\text{N}$, 100 MHz).

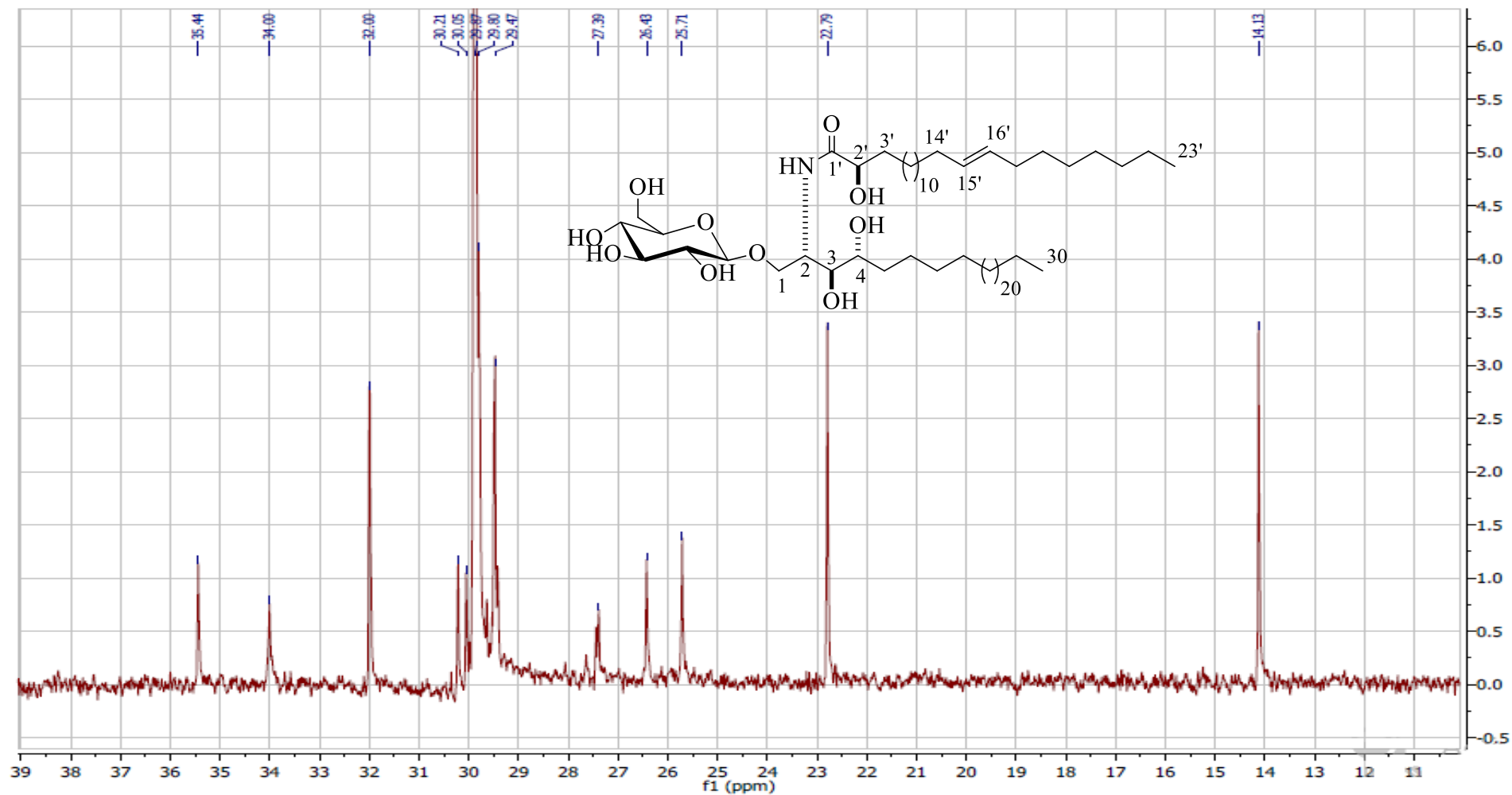


Figure S7: Partial expansion of the ^{13}C -NMR spectrum of compound 1 in ($\text{C}_5\text{D}_5\text{N}$, 100 MHz).

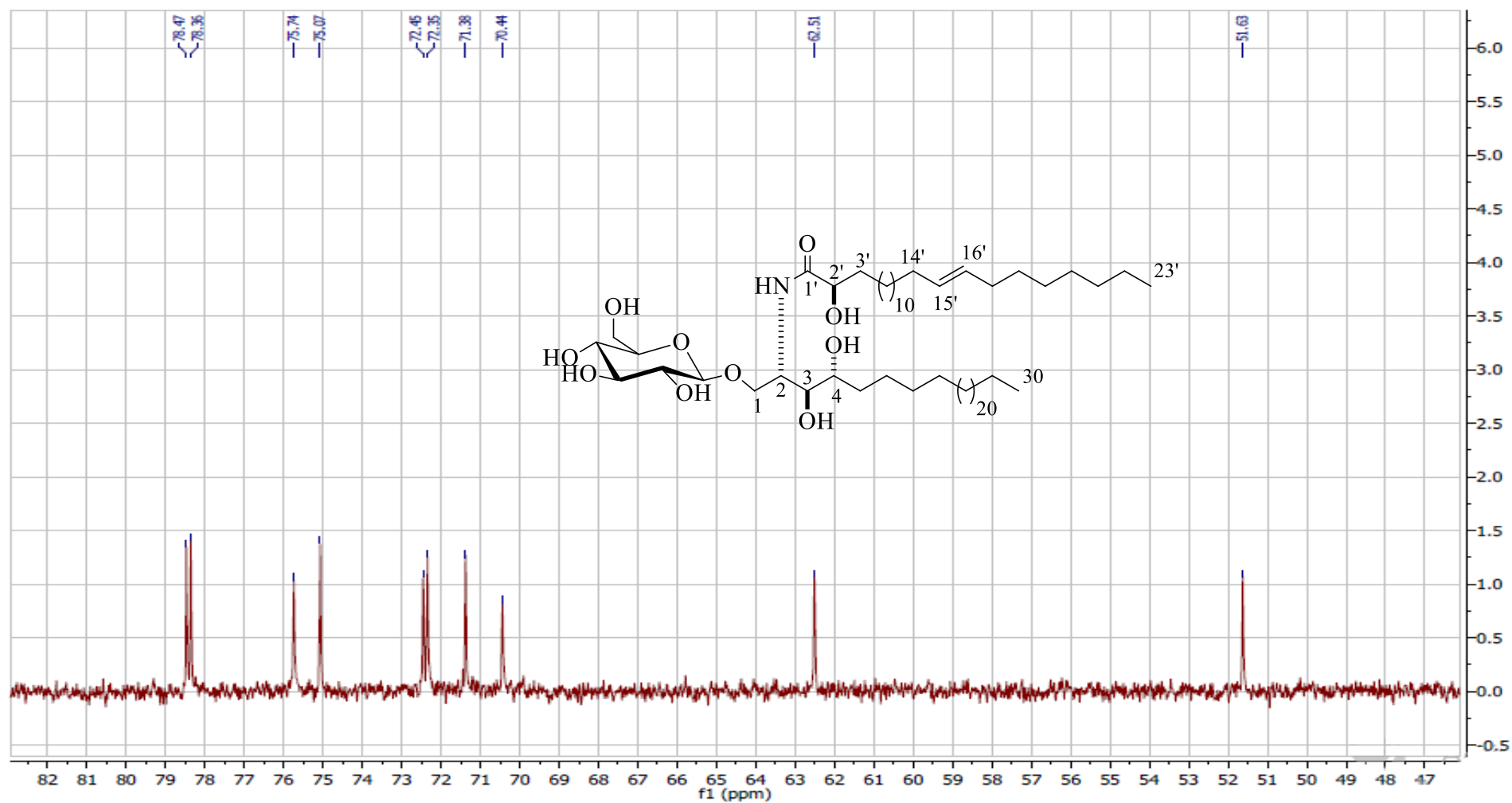


Figure S8: Partial expansion of the ^{13}C -NMR spectrum of compound 1 in ($\text{C}_5\text{D}_5\text{N}$, 100 MHz).

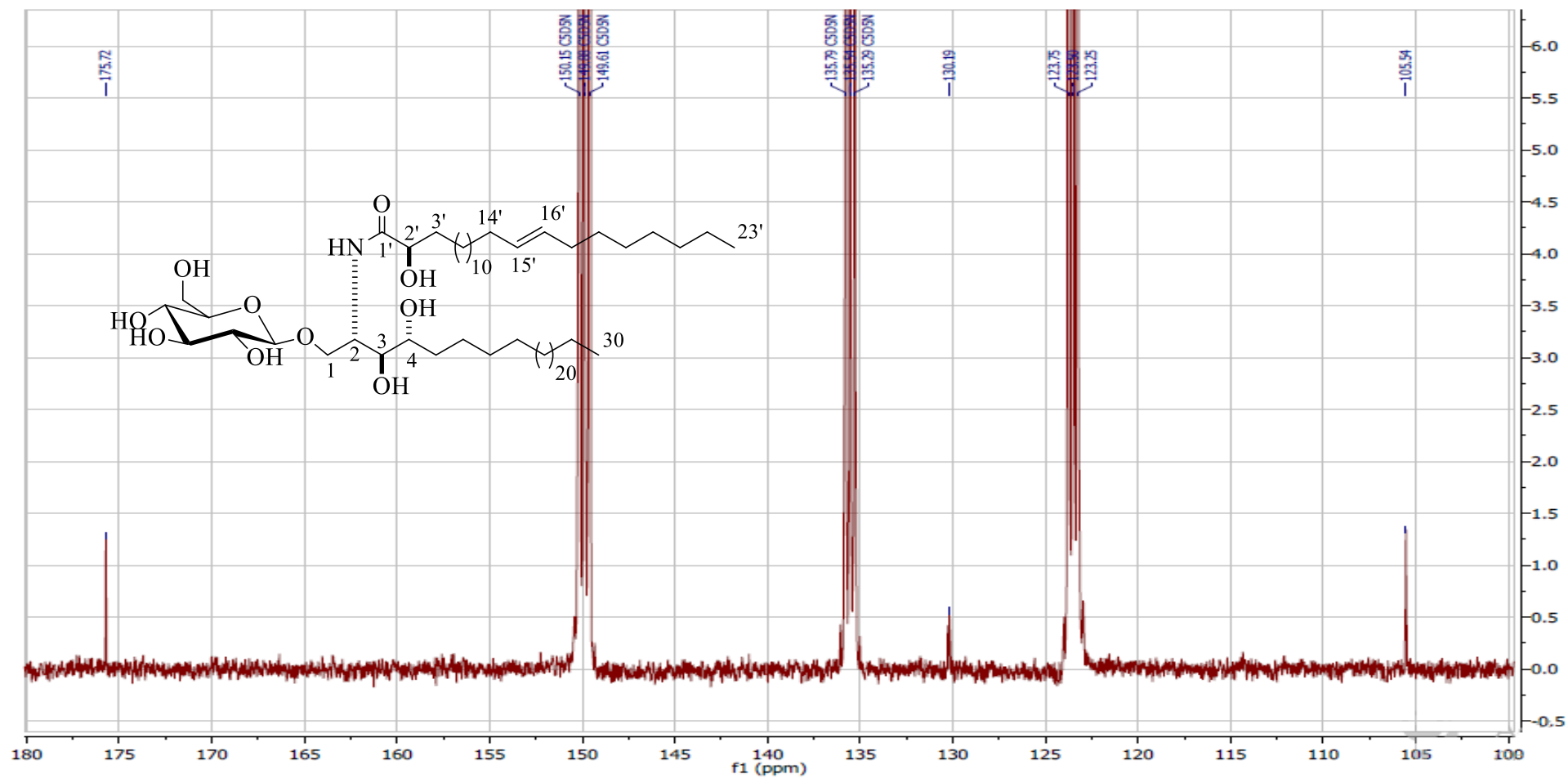


Figure S9: Partial expansion of the ^{13}C -NMR spectrum of compound 1 in ($\text{C}_5\text{D}_5\text{N}$, 100 MHz).

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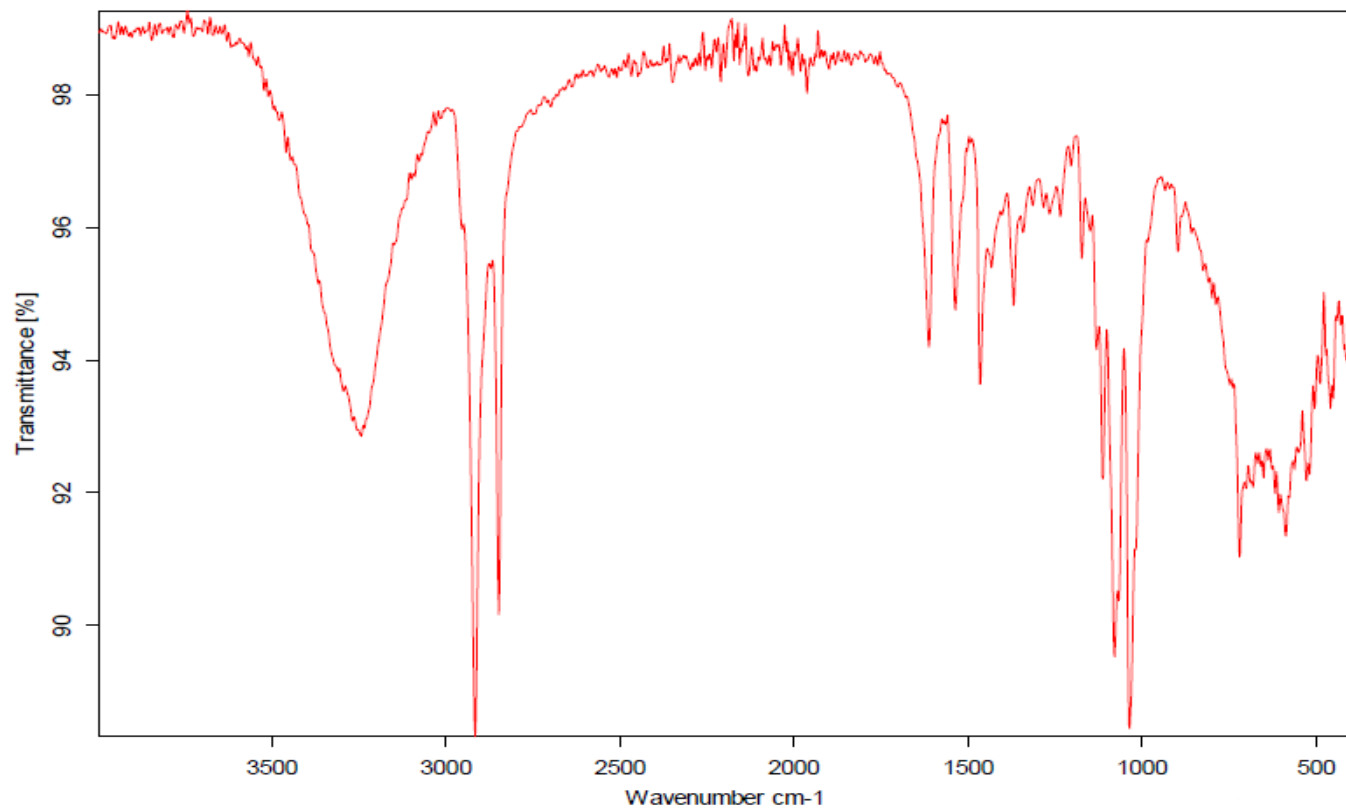


Figure S10: IR spectrum of compound 1.

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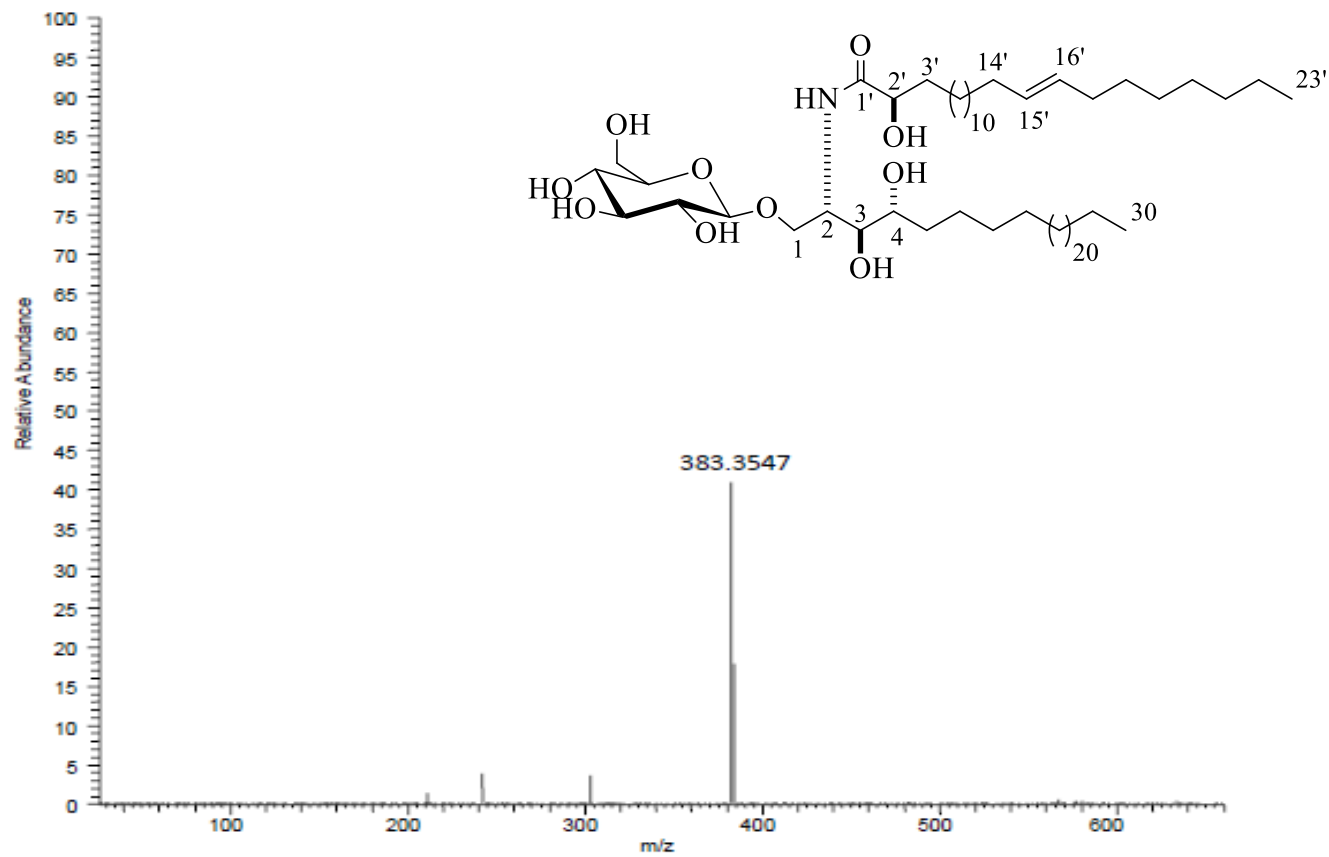


Figure S11: HRMS of α -hydroxy fatty acid methyl ester resulted from hydrolysis of compound 1

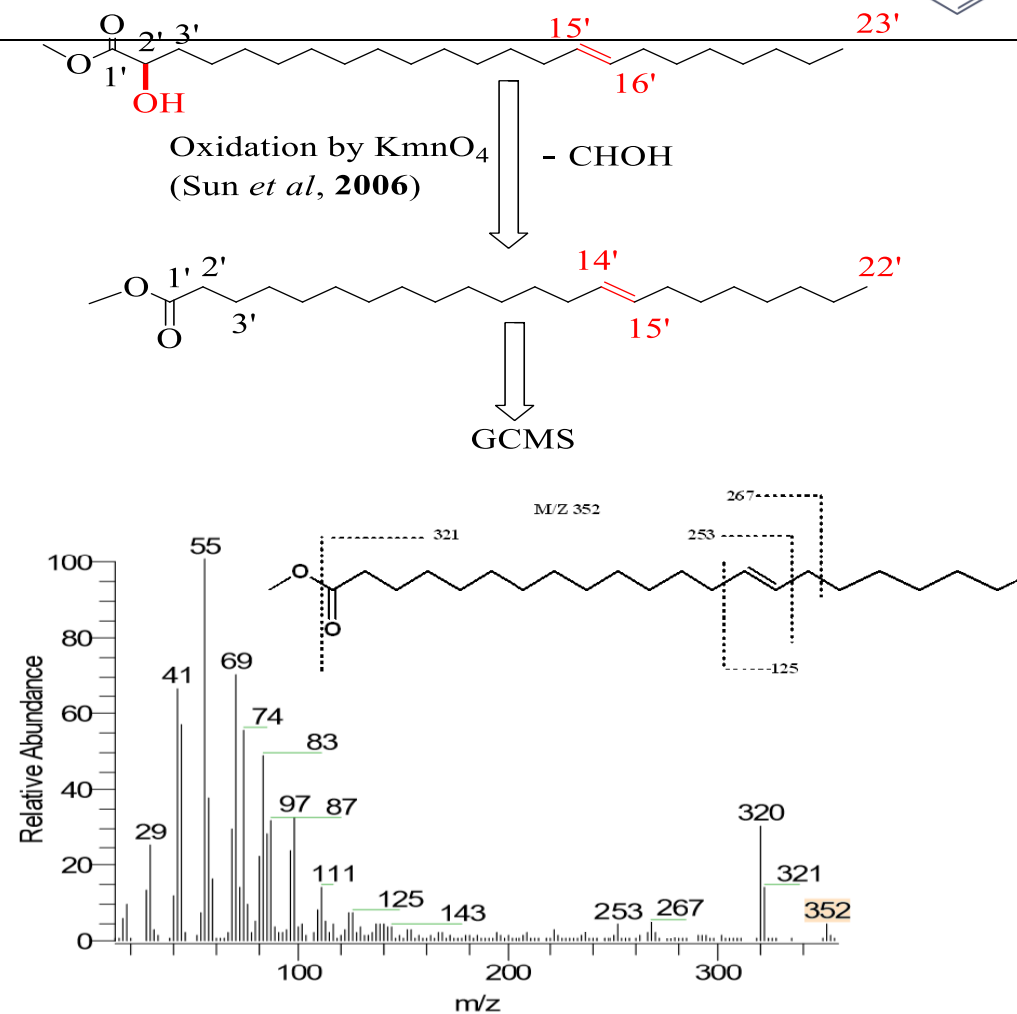
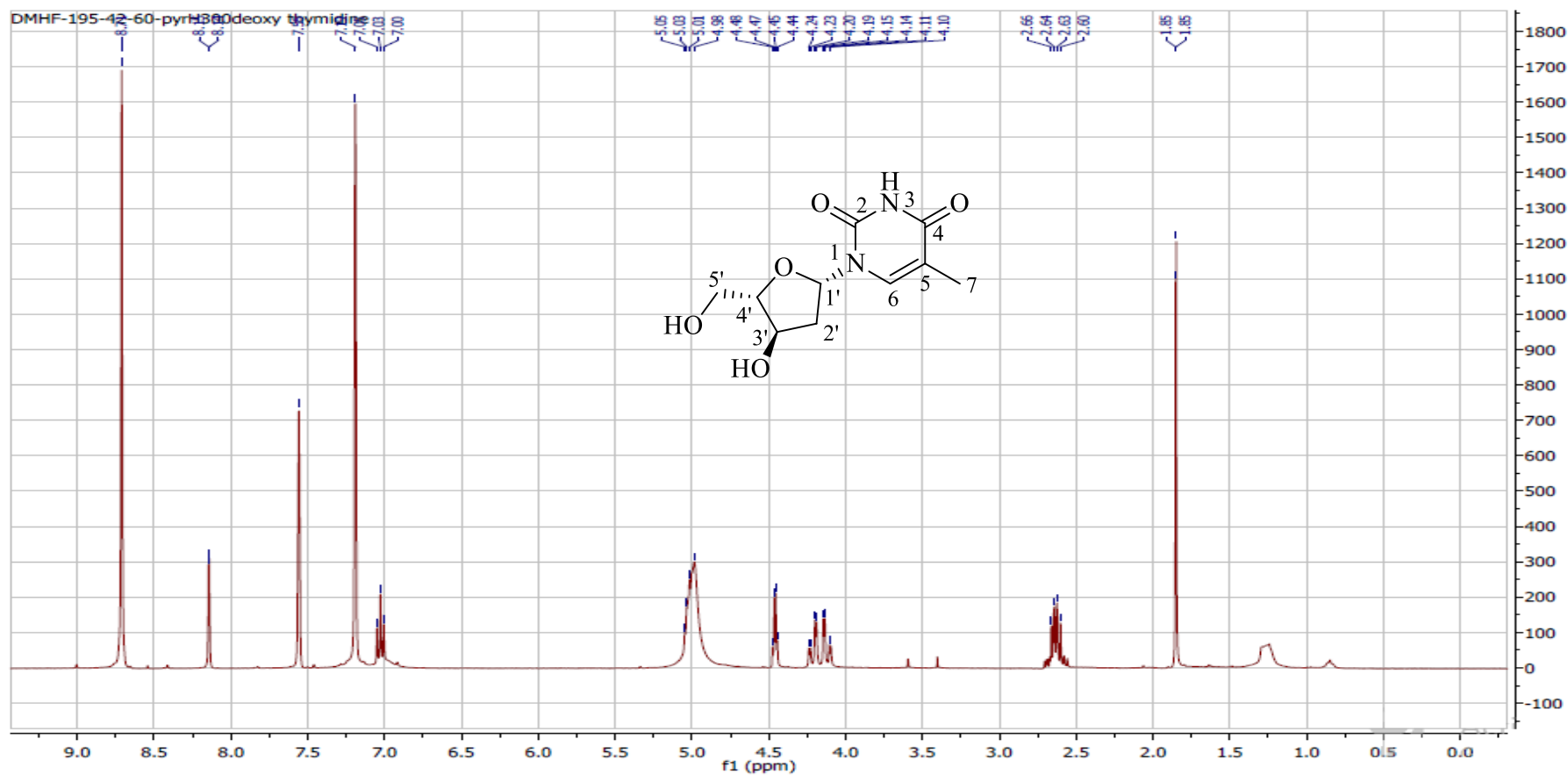


Figure S12: GC-MS analysis of fatty acids methyl ester carried out after oxidation of α -hydroxy fatty acid methyl ester (Compound 1)



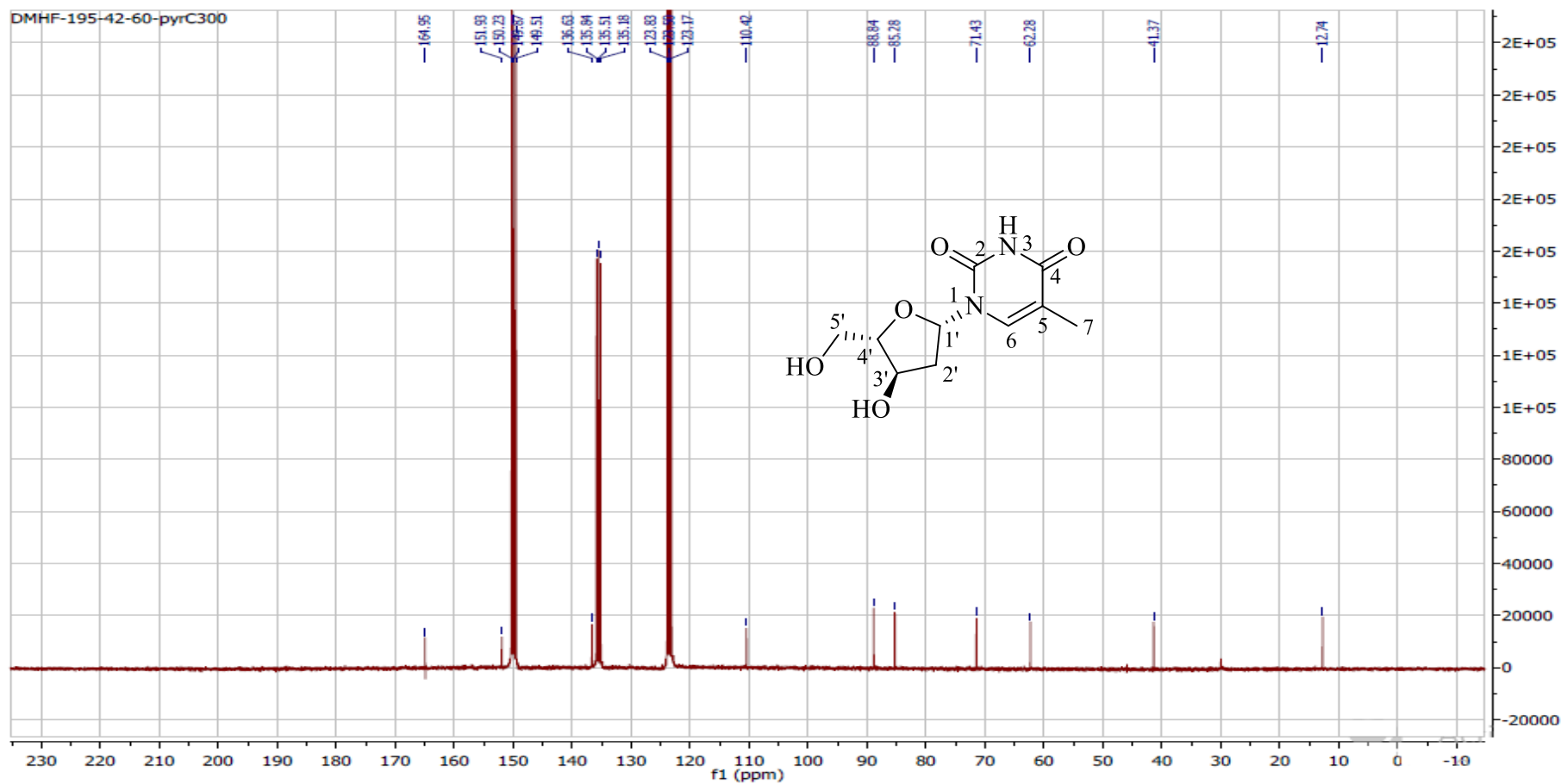


Figure S14: ^{13}C -NMR spectrum of compound 2 in ($\text{C}_5\text{D}_5\text{N}$, 100 MHz).

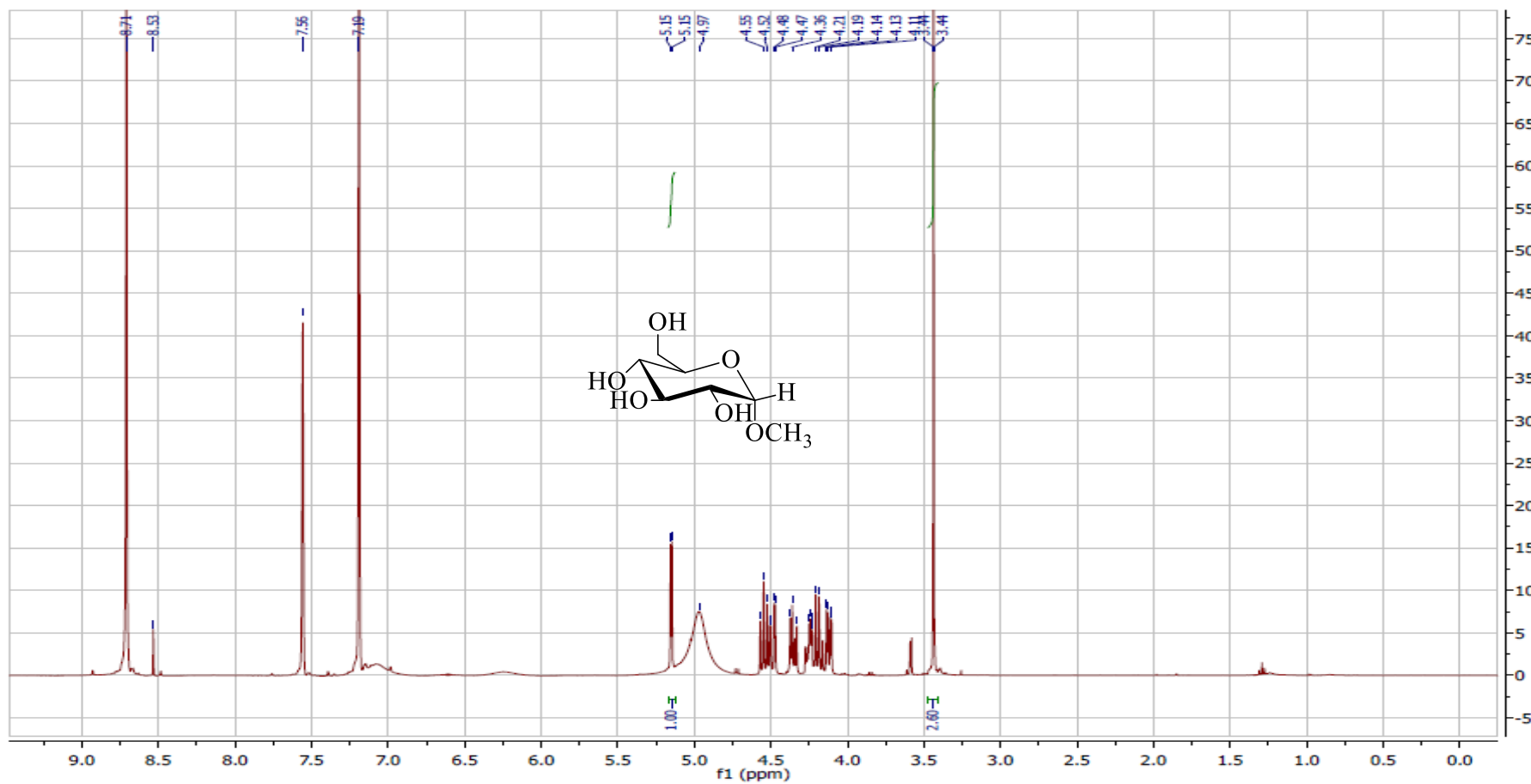


Figure S15: ¹H -NMR spectrum of Compound 3 in (C₅D₅N, 400 MHz).

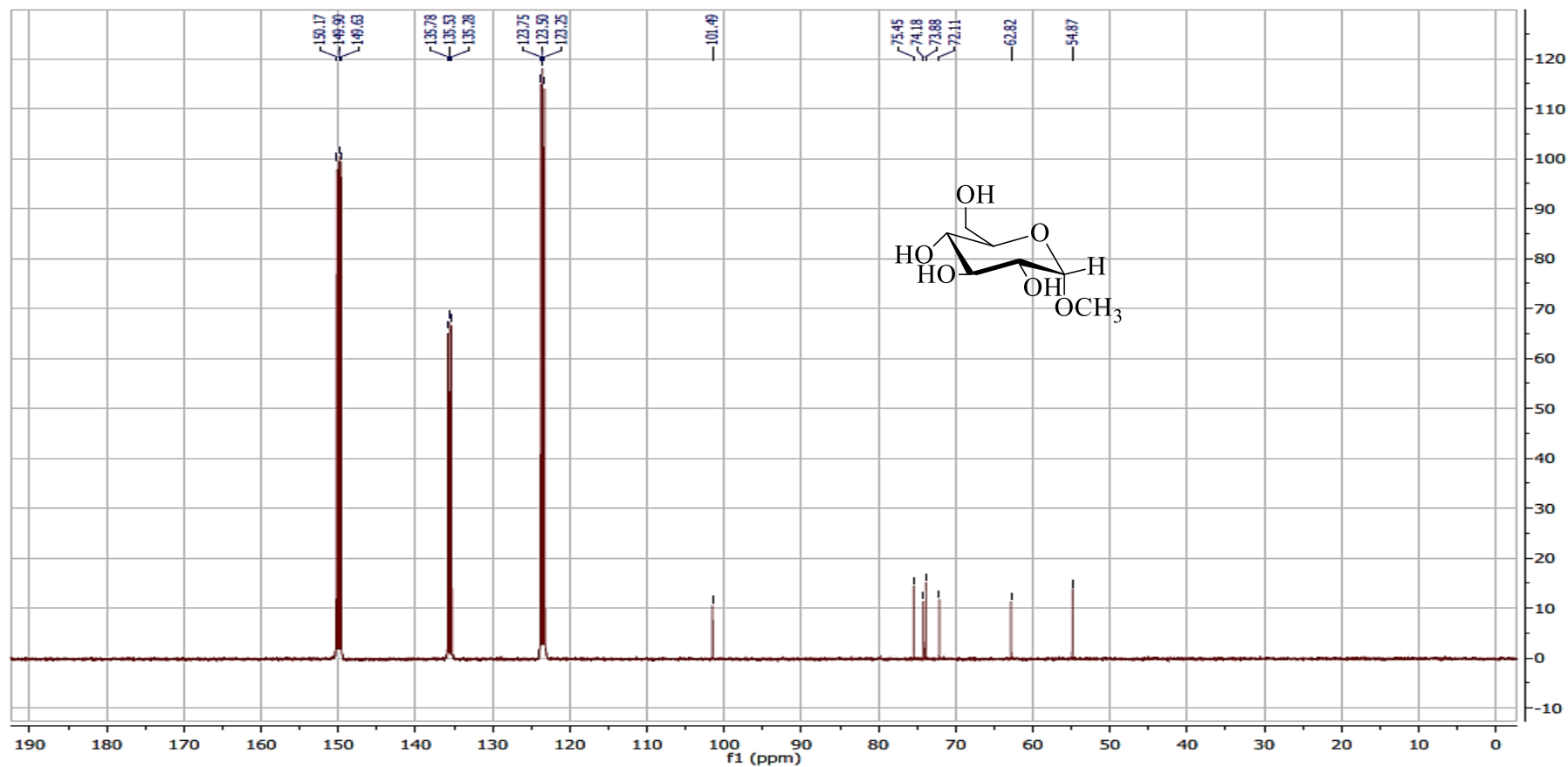


Figure S16: ^{13}C -NMR spectrum of Compound 3 ($\text{C}_5\text{D}_5\text{N}$, 100 MHz).

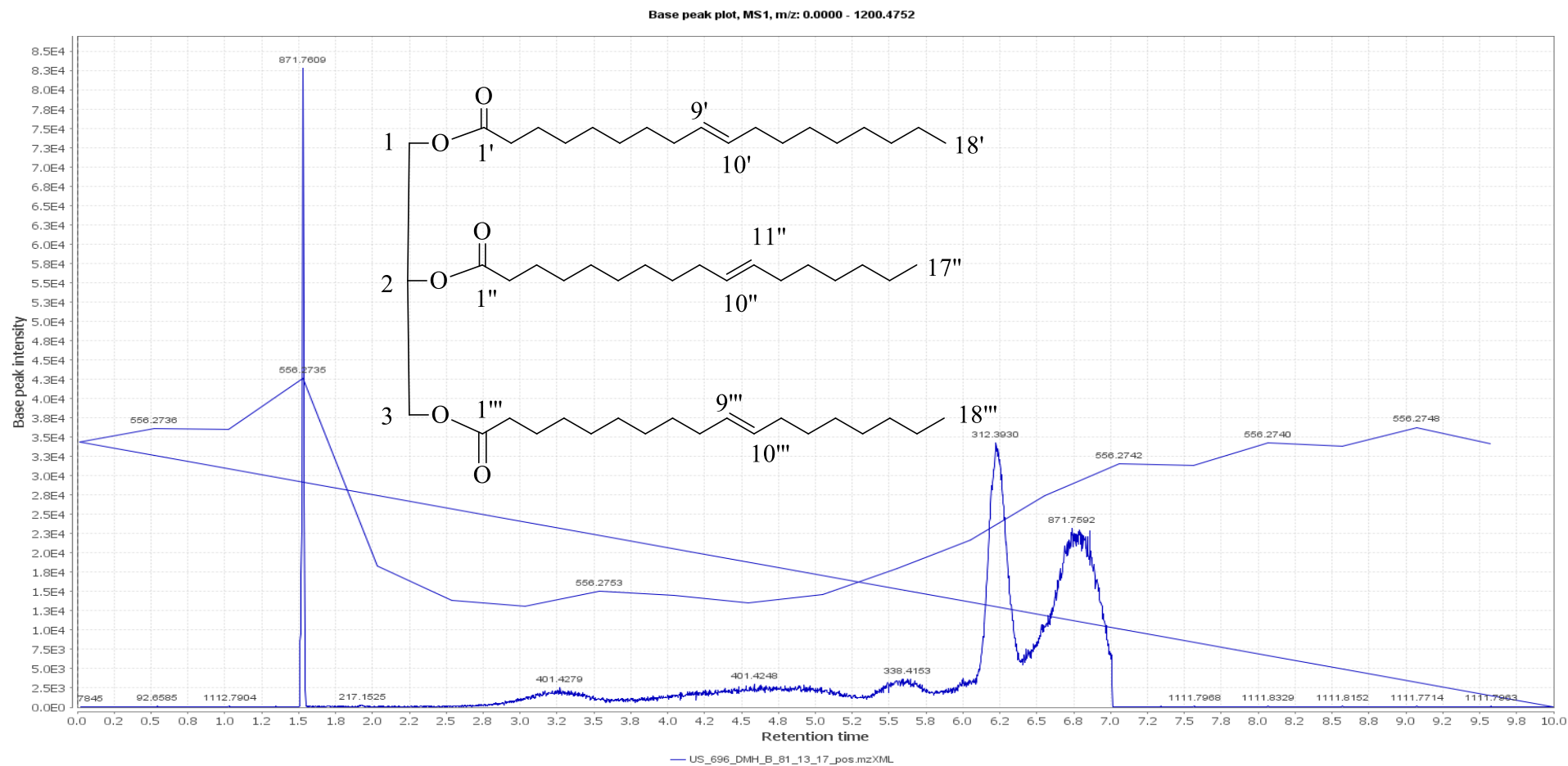
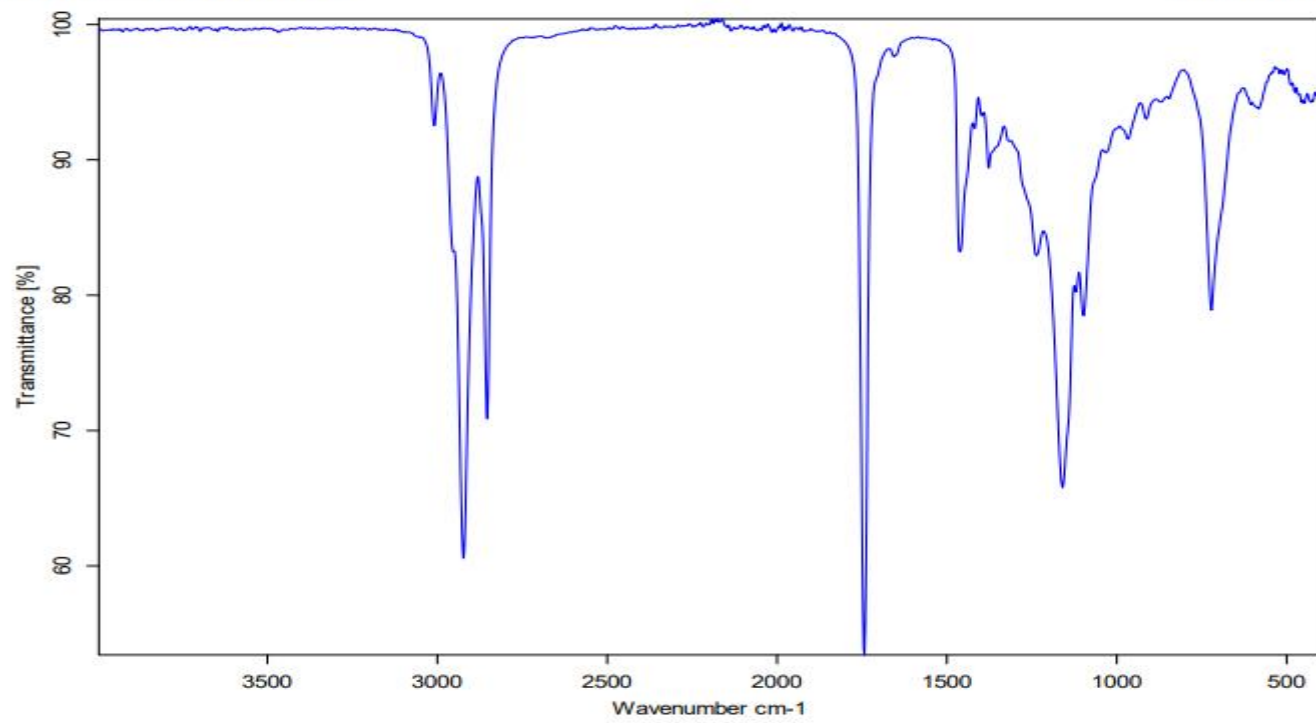


Figure S17: HRMS of Compound 4 (M+H)⁺

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Figure 16

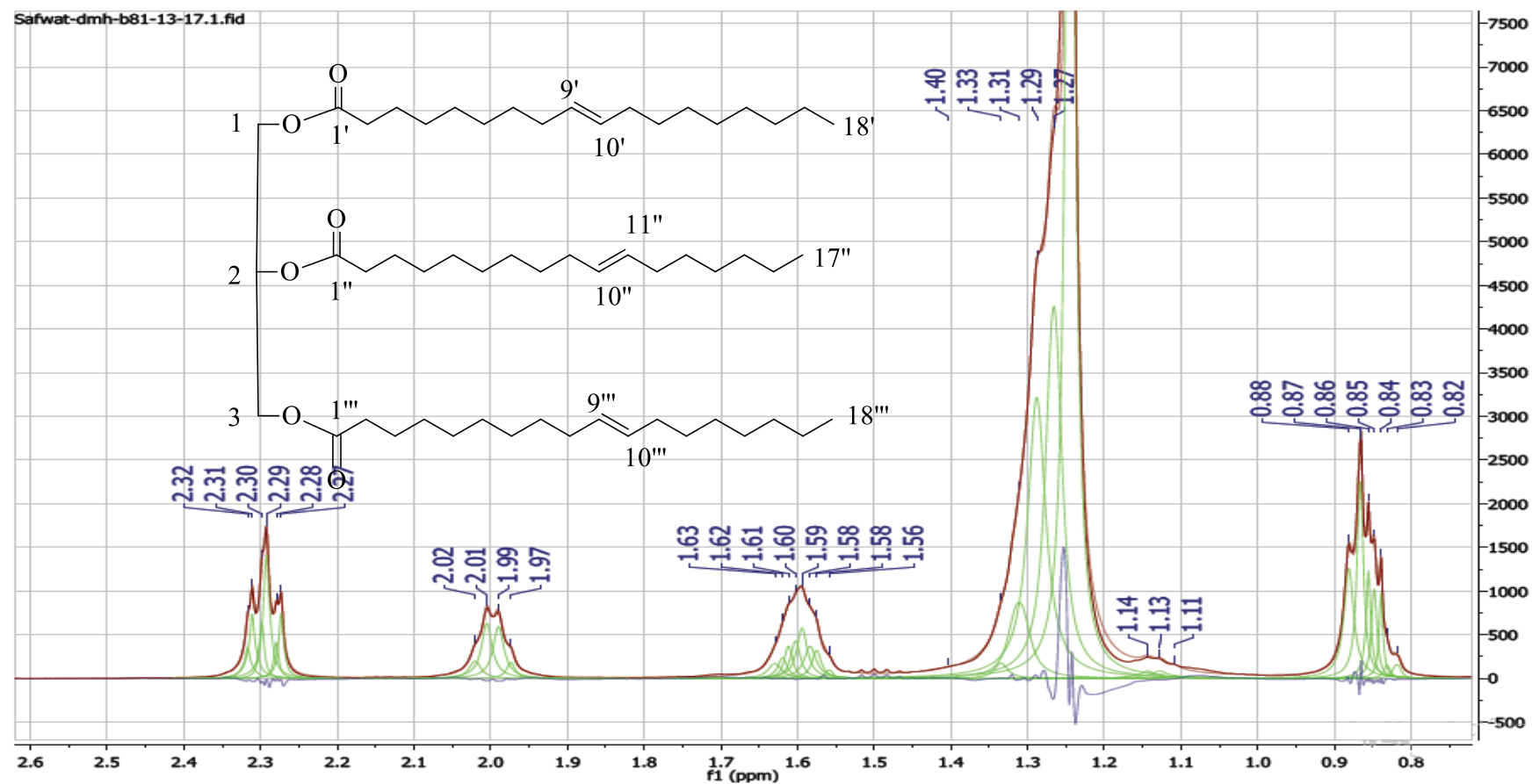


Figure S20: Partial expansions of the ¹H-NMR spectrum of compound 4 in (CDCl₃, 400 MHz)

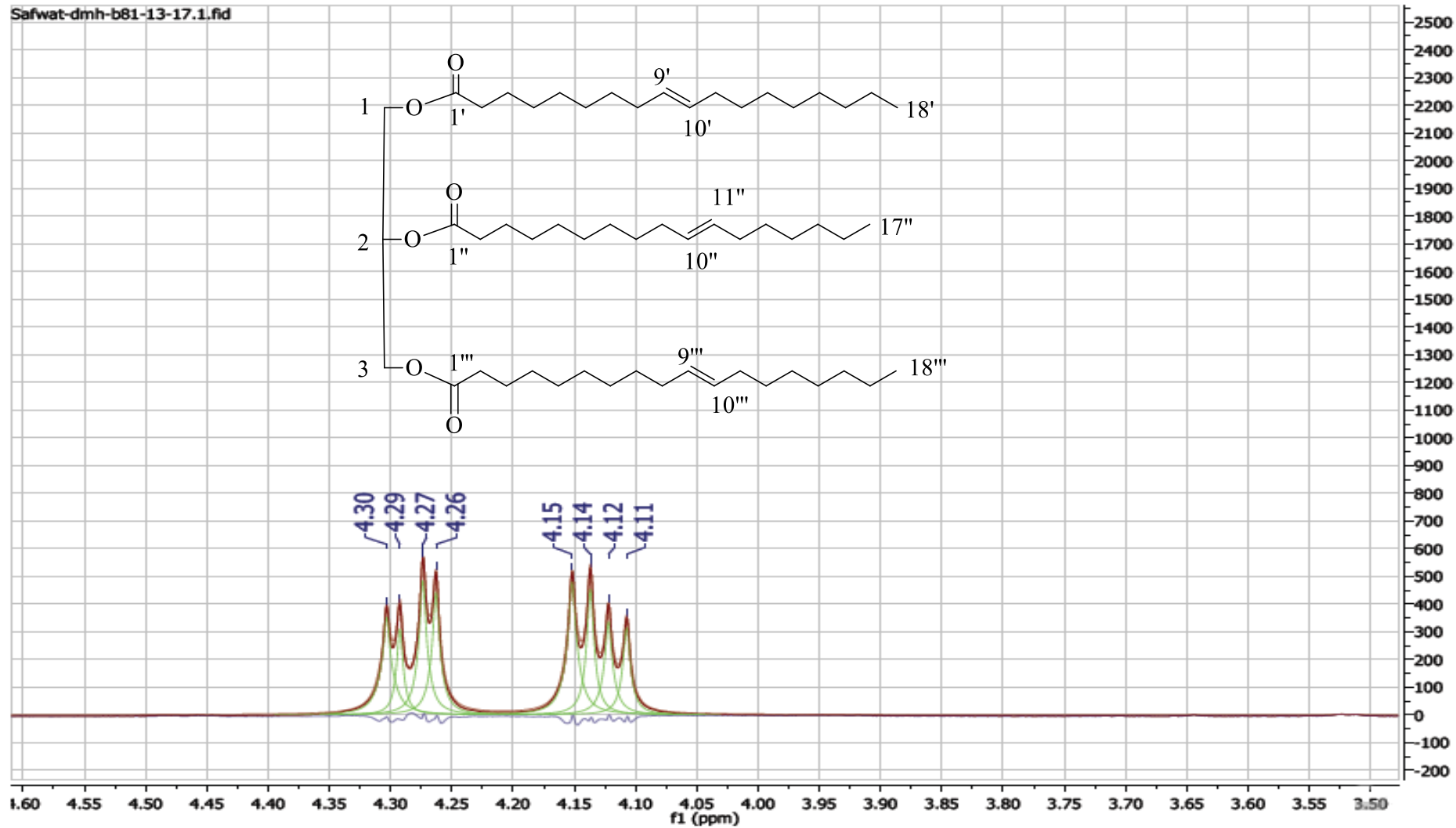


Figure S21: Partial expansions of the ¹H-NMR spectrum of compound 4 in (CDCl₃, 400 MHz)

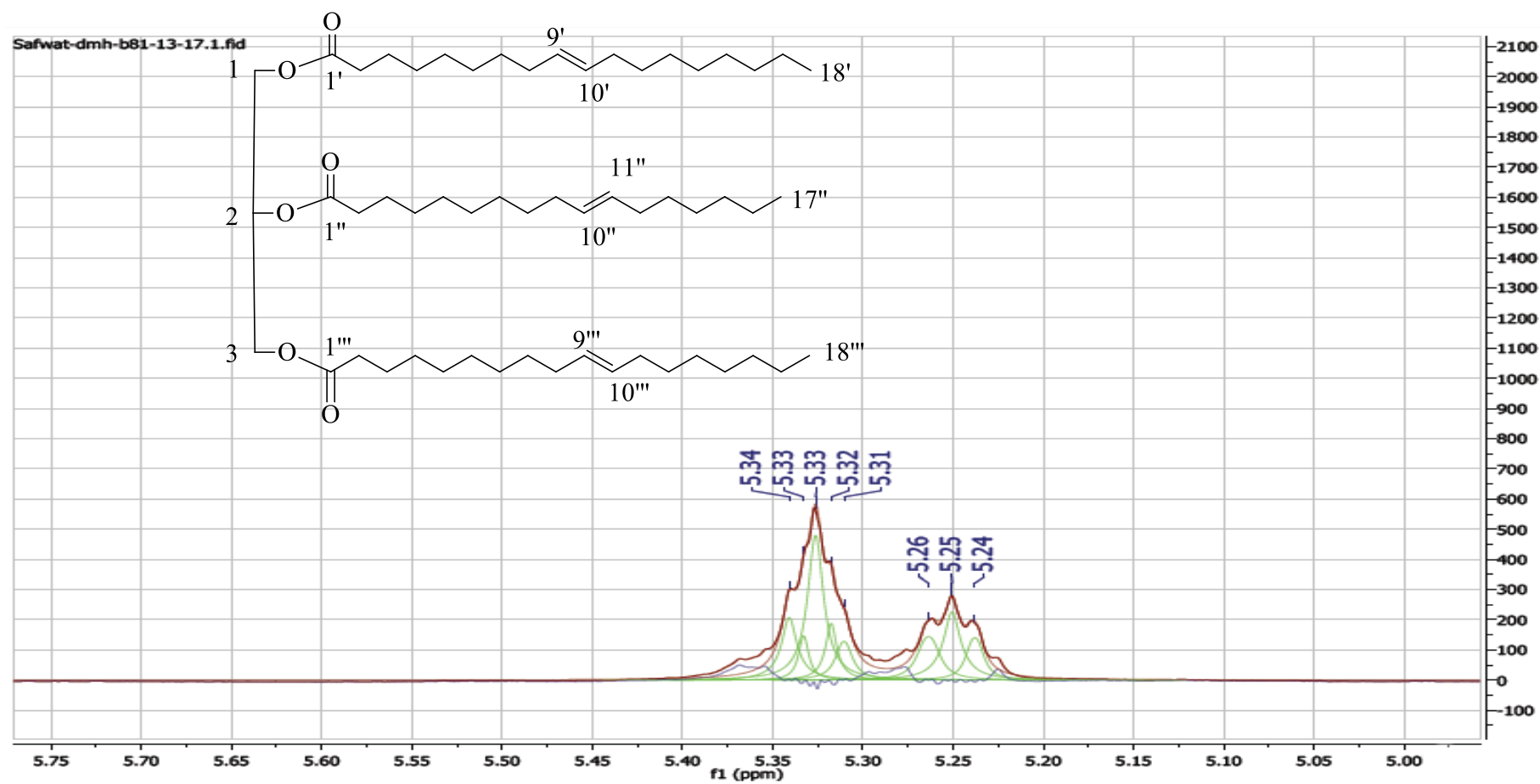


Figure S22: Partial expansions of the ¹H-NMR spectrum of compound 4 in (CDCl₃, 400 MHz)

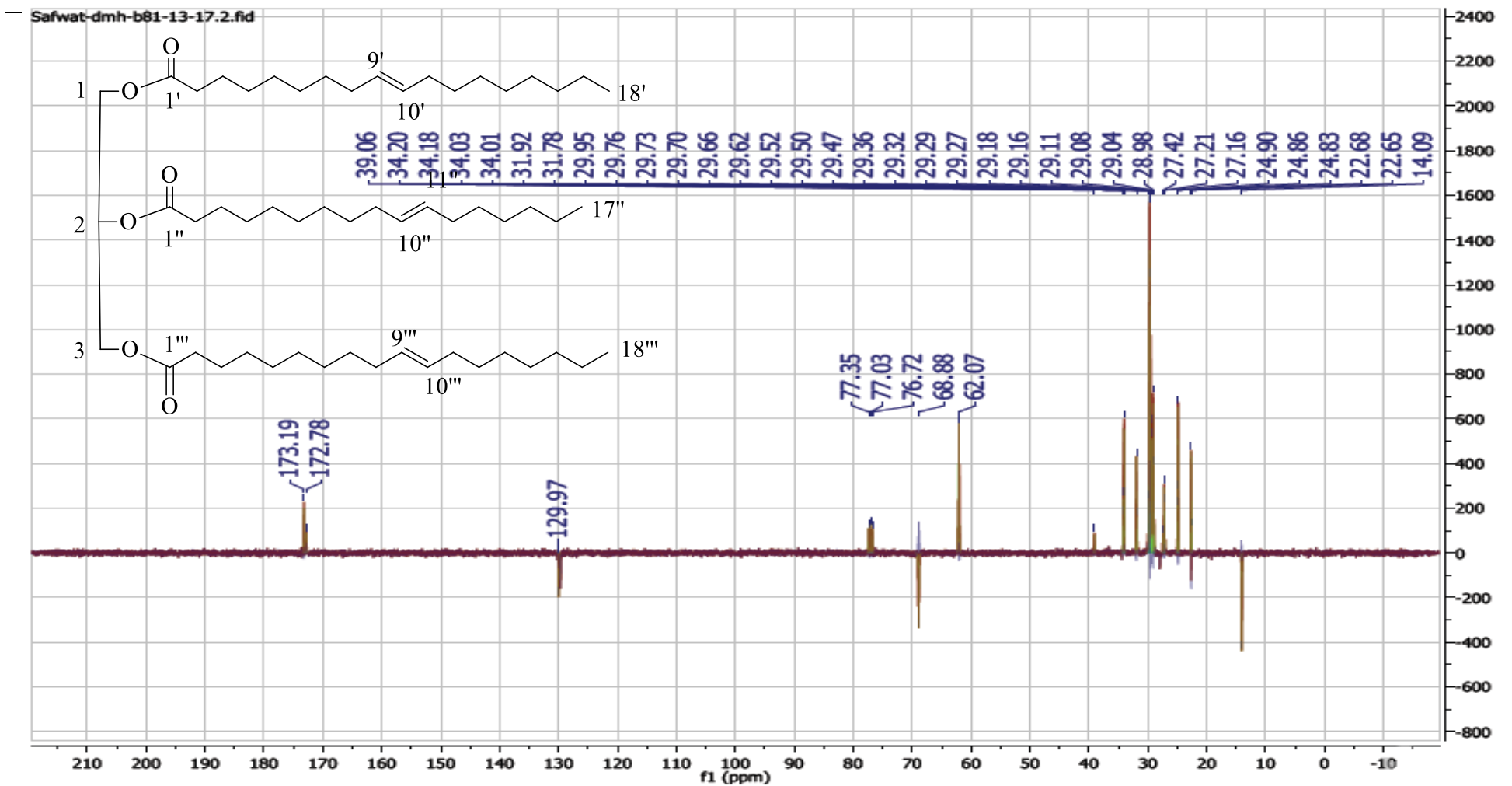


Figure S23: ^{13}C -NMR spectrum of compound 4 in (CDCl_3 , 400 MHz).

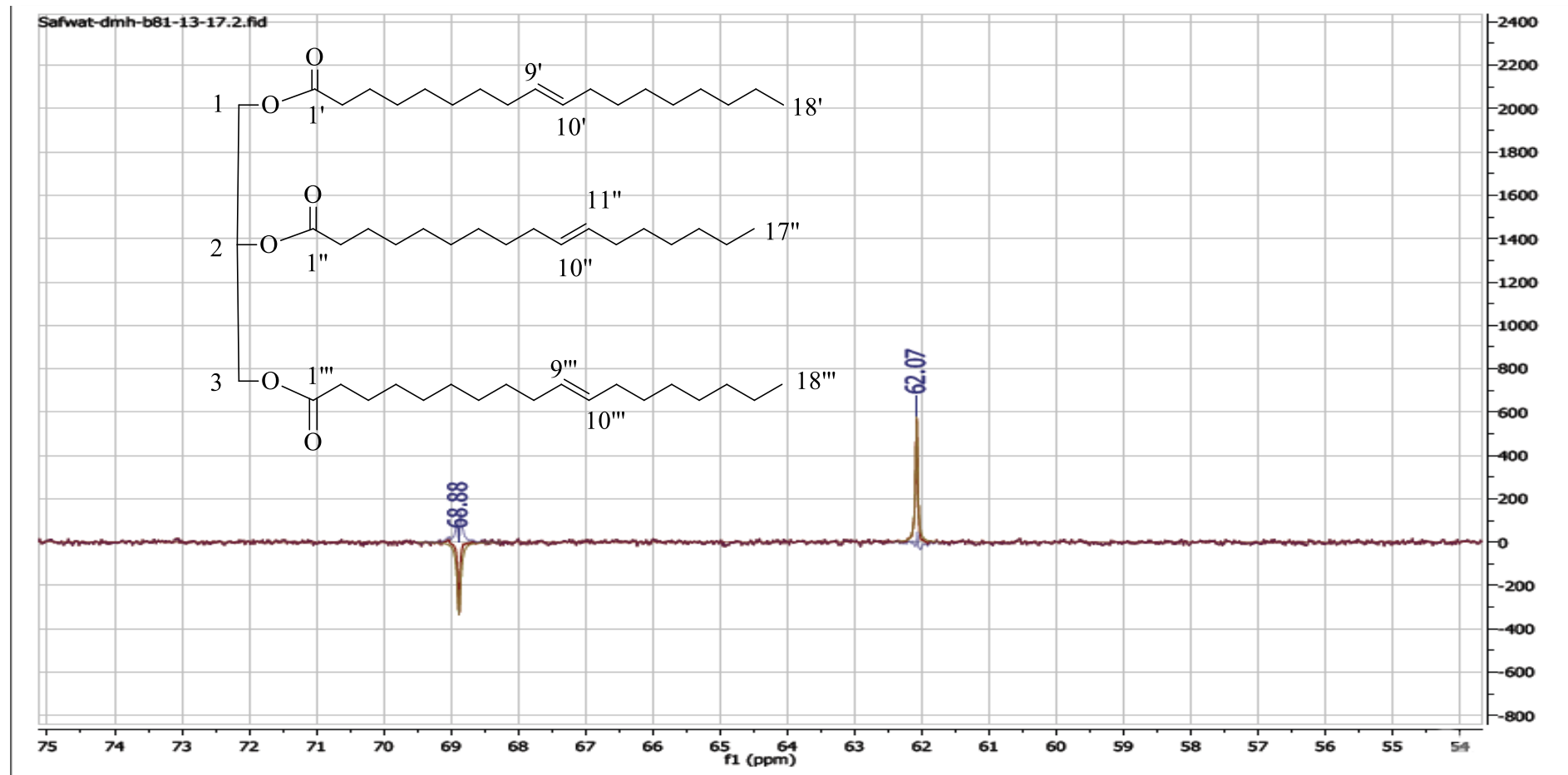


Figure S24: Partial expansion ^{13}C -NMR spectrum of compound 4 in (CDCl_3 , 400 MHz).

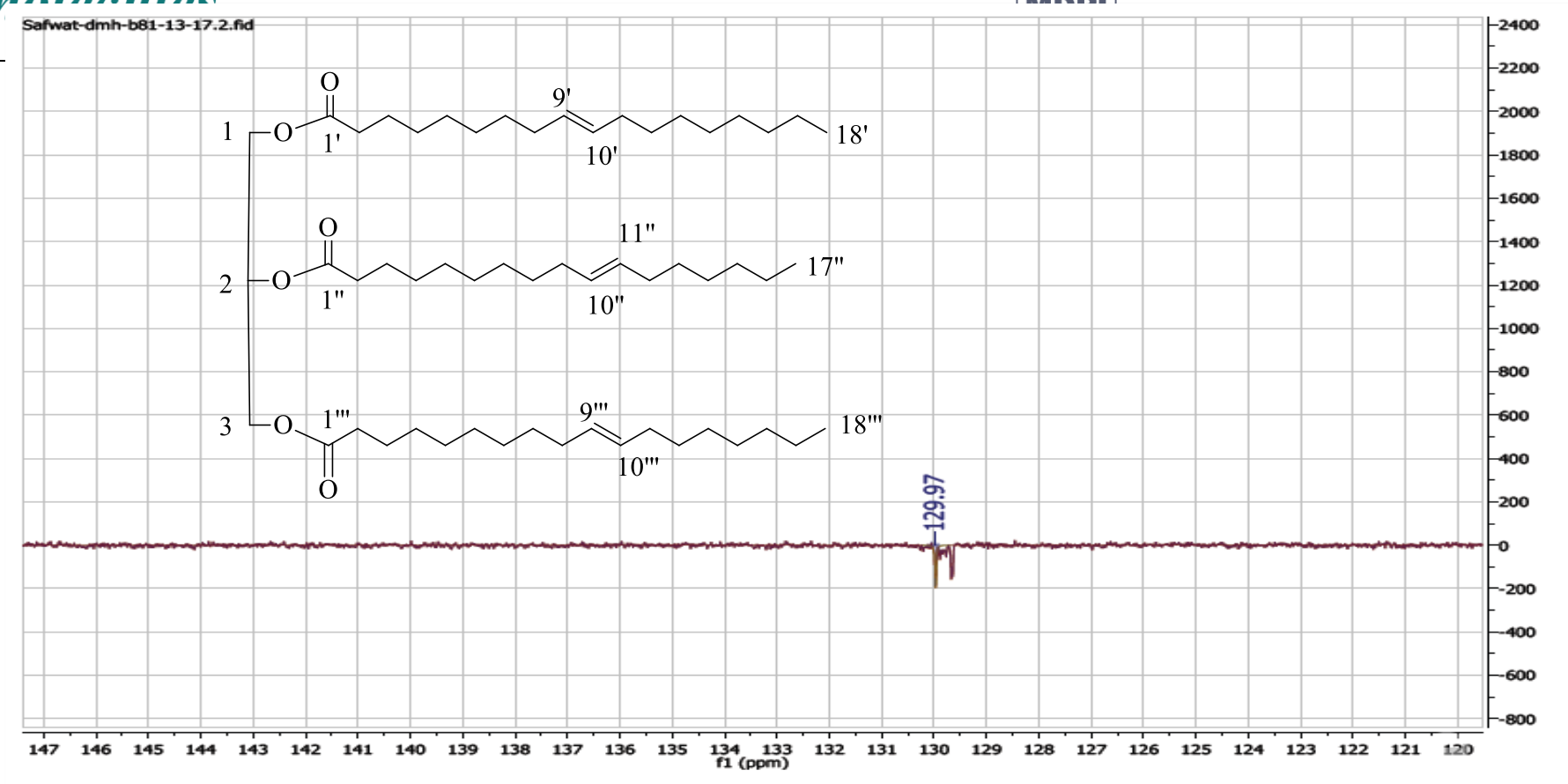


Figure S25: Partial expansion ¹³C-NMR spectrum of compound 4 in (CDCl₃, 400 MHz).

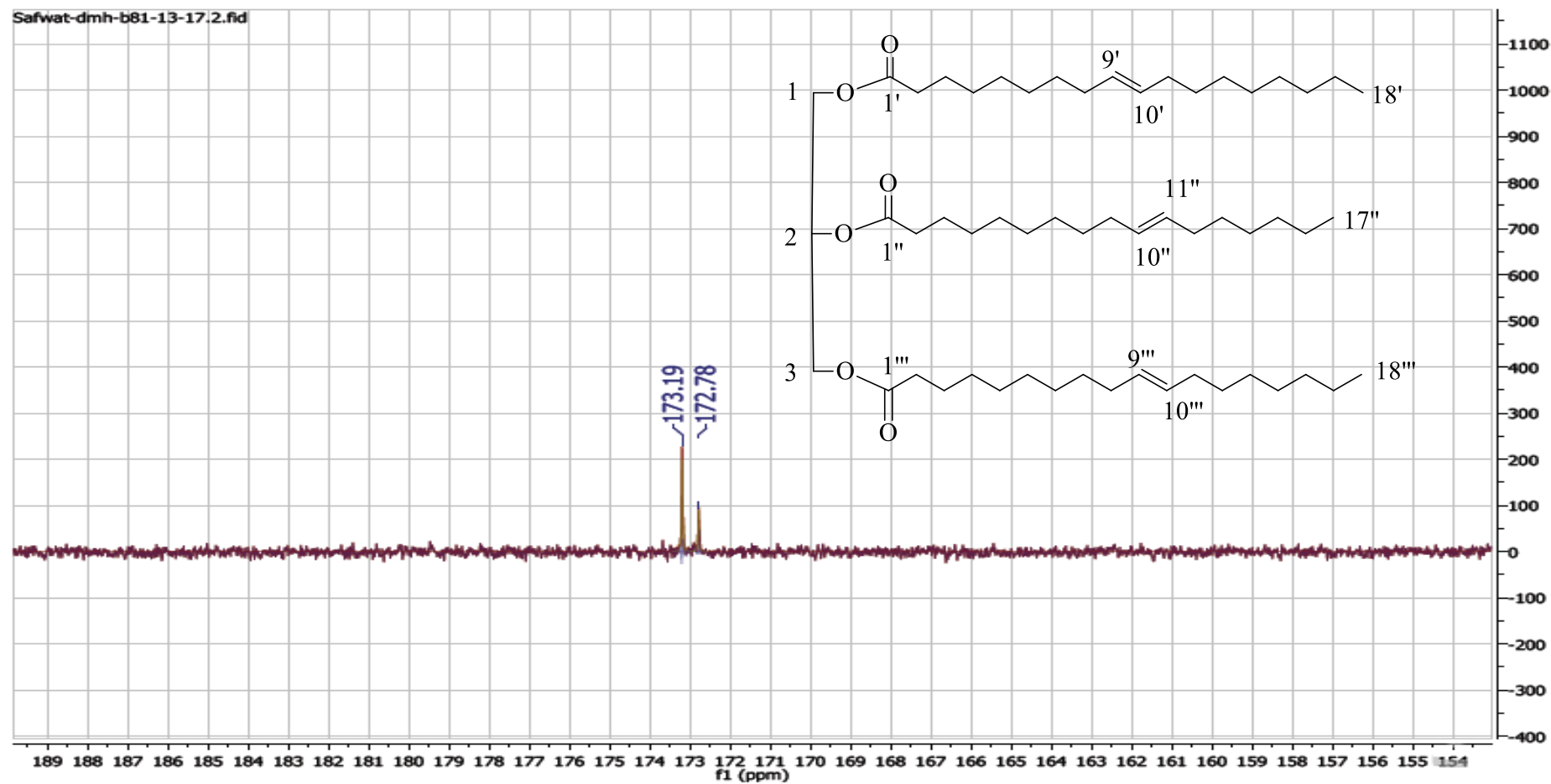


Figure S26: Partial expansion ^{13}C -NMR spectrum of compound 4 in (CDCl_3 , 400 MHz).

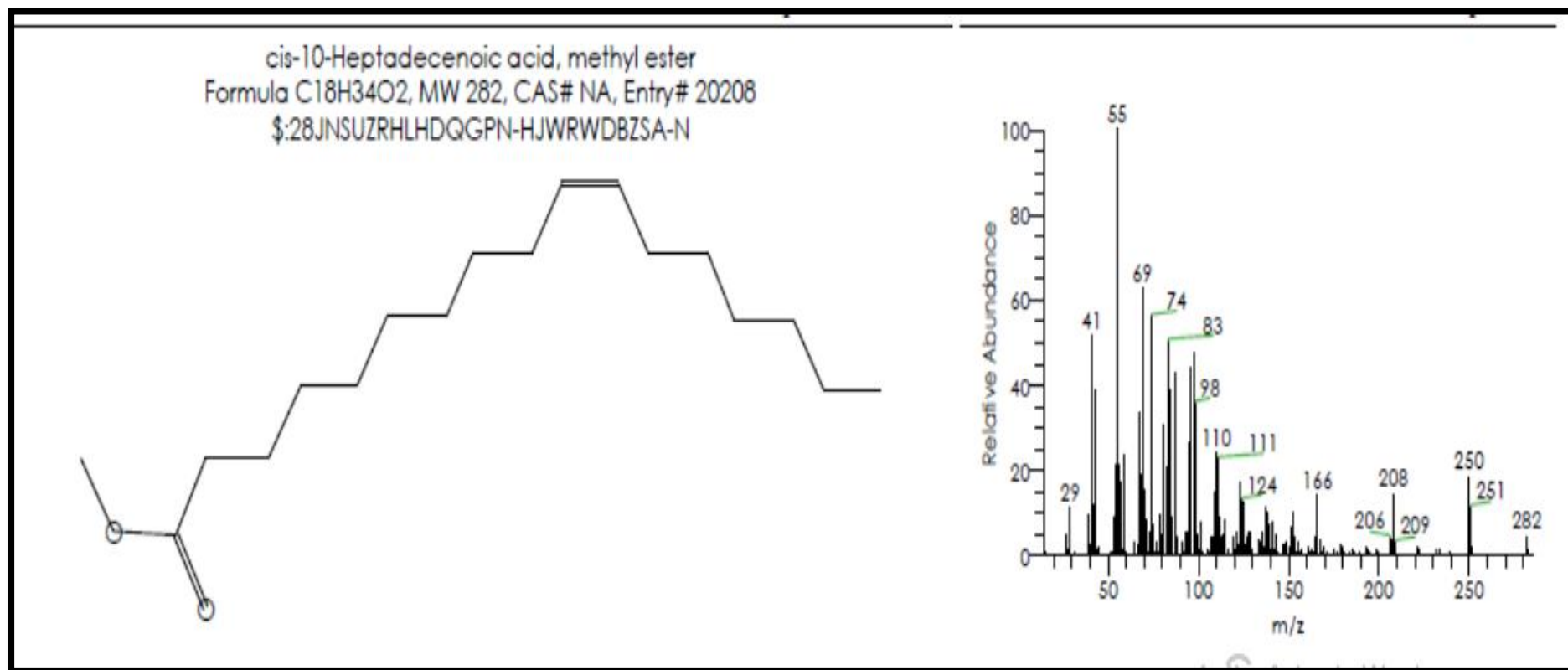


Figure S27: MS spectrum for 10-Heptadecenoic acid (z)- methyl ester.

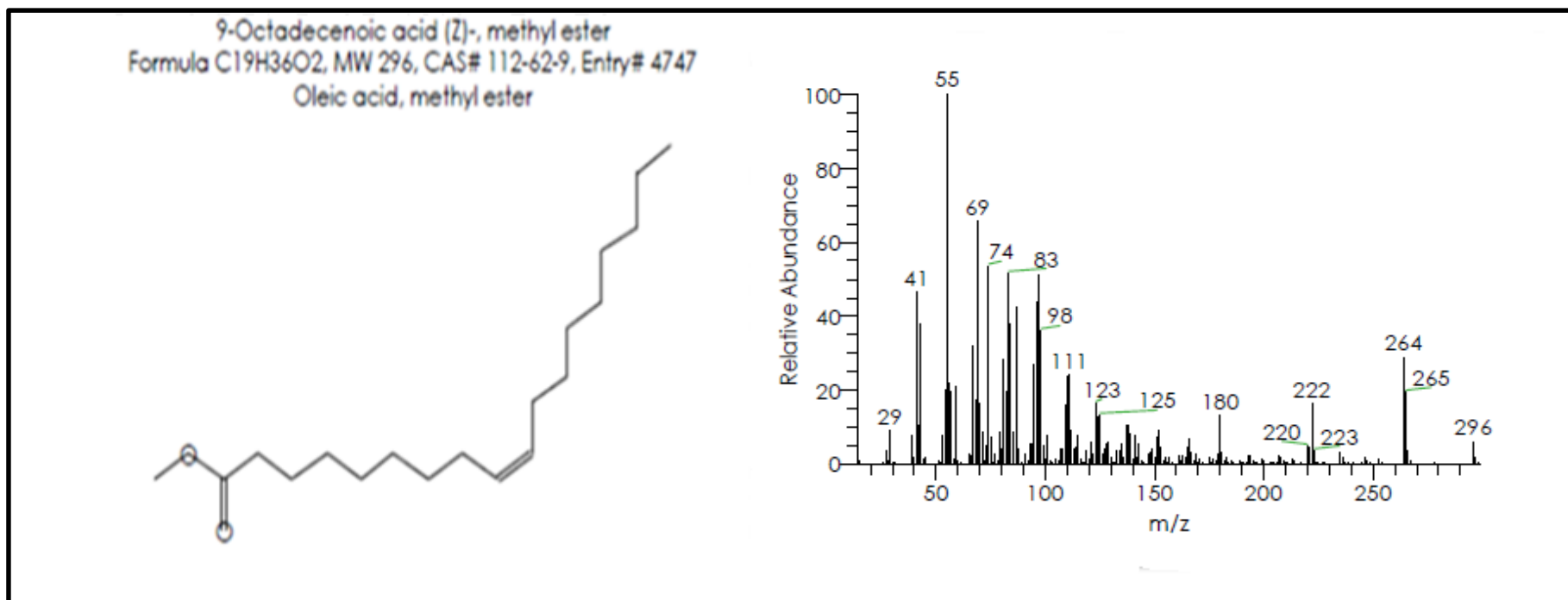


Figure S28: MS spectrum for 9-Octadecenoic acid (z)-methyl ester

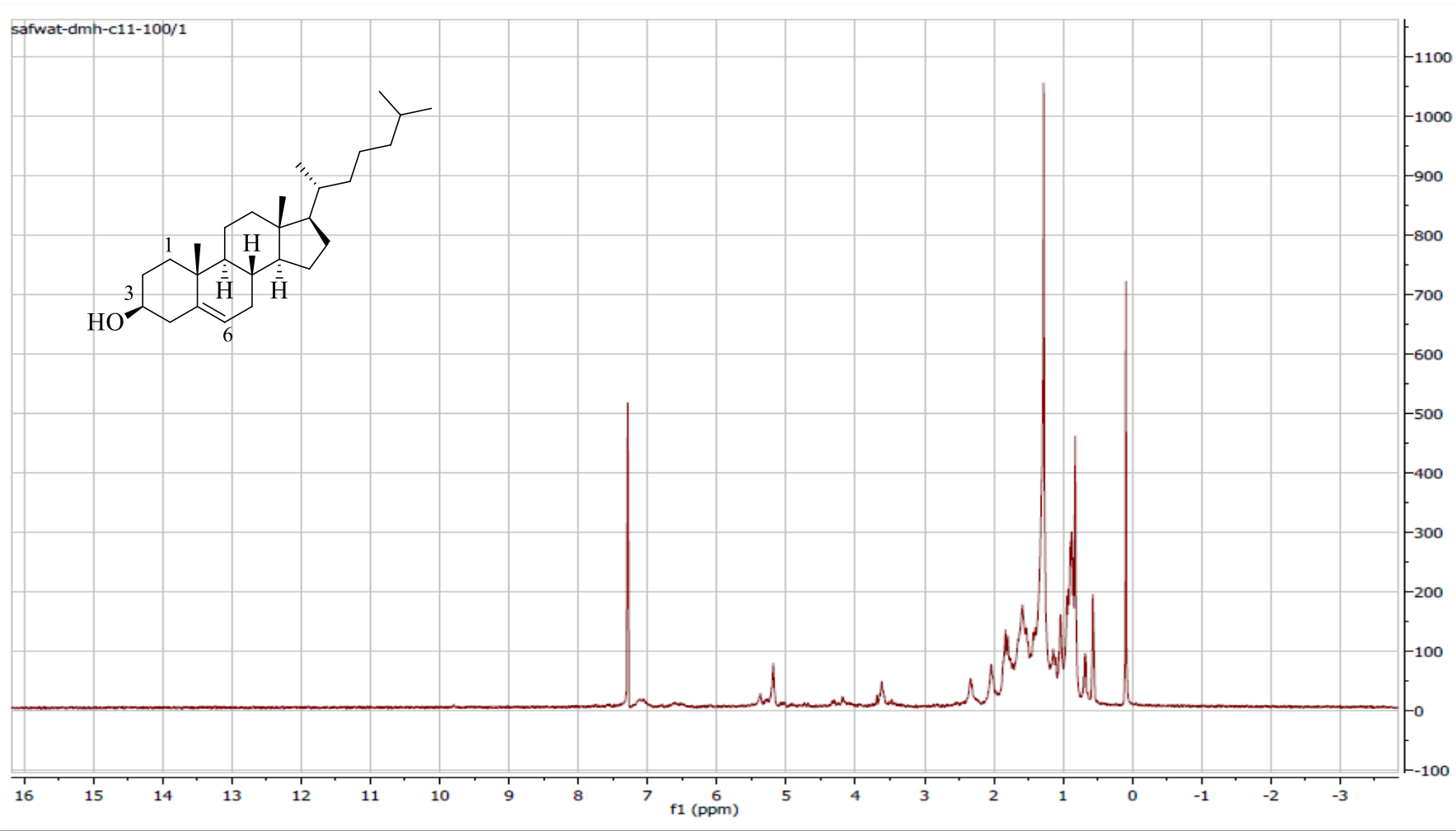


Figure S29: ¹H -NMR spectrum of Compound 5 in (CDCl₃, 400 MHz).

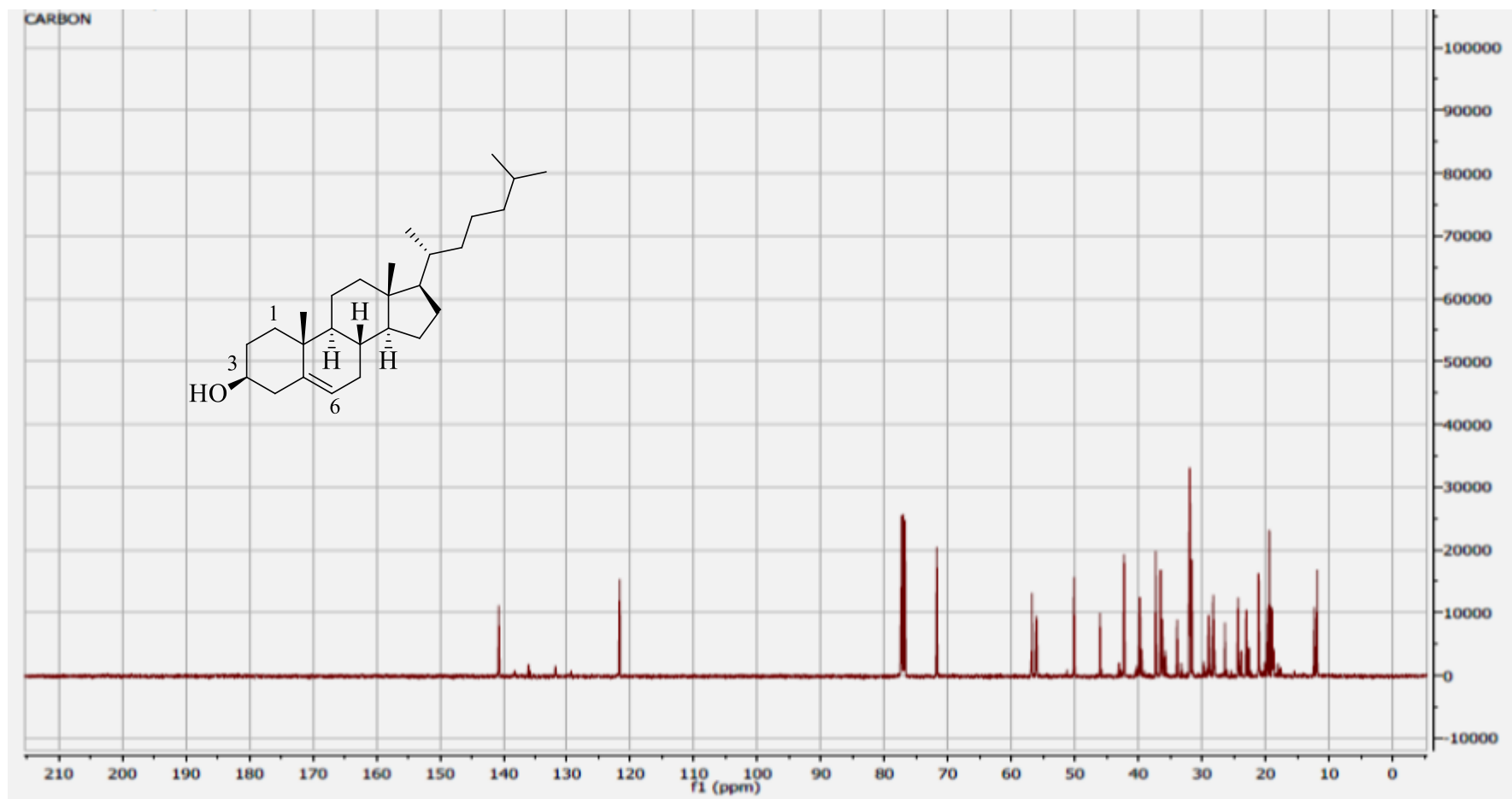


Figure S30: ^{13}C -NMR spectrum of Compound 5 (CDCl_3 , 100 MHz).

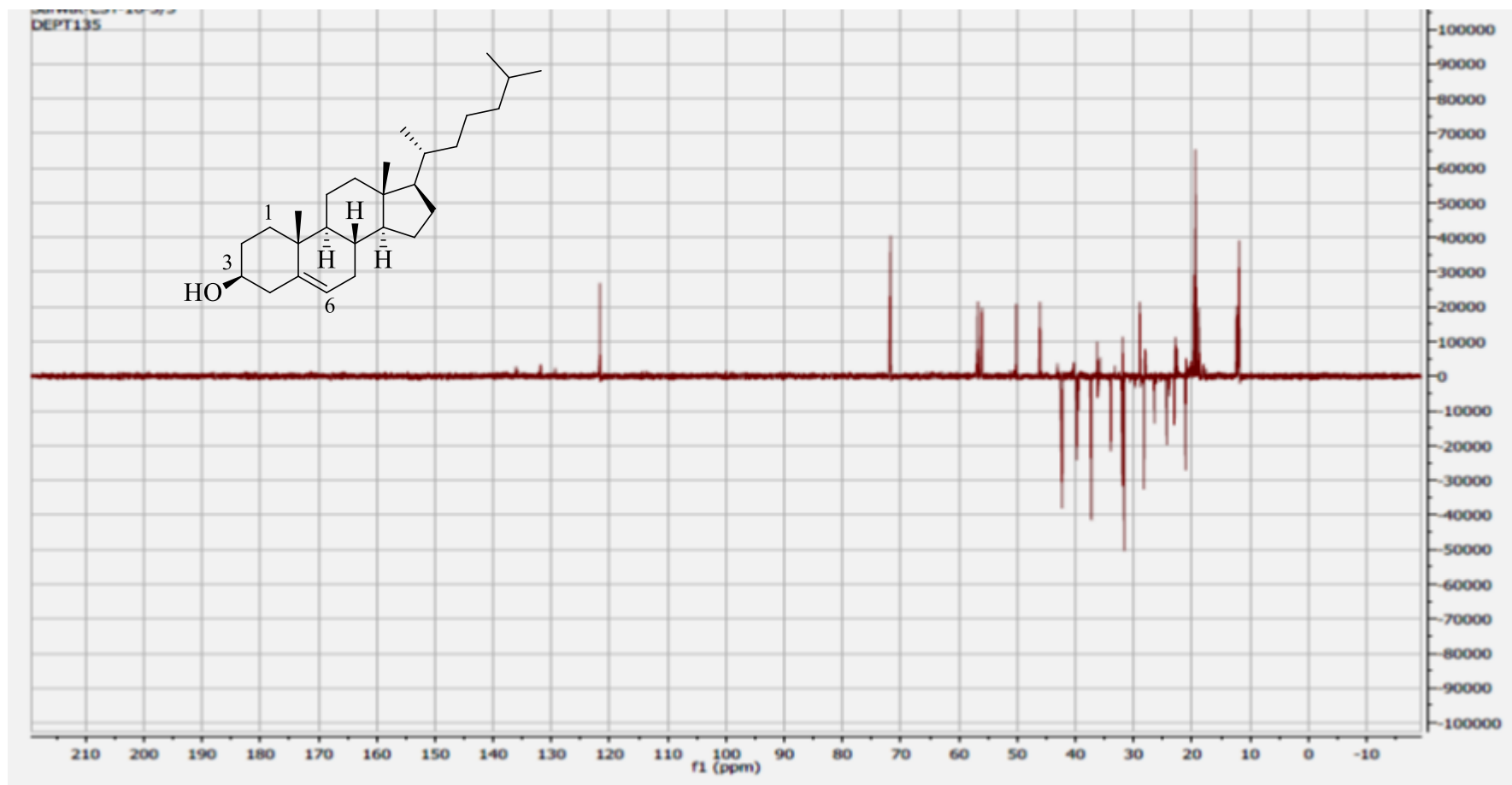


Figure S31: DEPT spectrum of Compound 5 in (CDCl₃, 100 MHz).