

Electronic Supplementary Information for:

Total synthesis of ceramides and β -O-glucosylceramides via intramolecular fatty acyl group migration

Jaggaiah N. Gorantla,^{a,b,*} Maniganda Santhi,^{a,b} Yanling Hua,^{a,c} James R. Ketudat Cairns^{a,b,*}

^aCenter for Biomolecular Structure, Function and Application, ^bSchool of Chemistry, Institute of Science, and ^cCenter for Scientific and Technological Equipment, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand.

*Corresponding authors. E-mail address: cairns@sut.ac.th and gjhnaidu@gmail.com

New Journal of Chemistry

Electronic Supplementary Information

Table of Contents

Figure S1. ¹ H-NMR (500 MHz, CDCl ₃) spectrum of compound 3a .	ESI-3
Figure S2. ¹³ C-NMR (125 MHz, CDCl ₃) spectrum of compound 3a .	ESI-4
Figure S3. ¹ H-NMR (500 MHz, CDCl ₃) spectrum of compound 3b .	ESI-5
Figure S4. ¹³ C-NMR (125 MHz, CDCl ₃) spectrum of compound 3b .	ESI-6
Figure S5. ¹ H-NMR (500 MHz, CDCl ₃) spectrum of compound 4a .	ESI-7
Figure S6. ¹³ C-NMR (125 MHz, CDCl ₃) spectrum of compound 4a .	ESI-8
Figure S7. ¹ H-NMR (500 MHz, CDCl ₃) spectrum of compound 4b .	ESI-9
Figure S8. ¹³ C-NMR (125 MHz, CDCl ₃) spectrum of compound 4b .	ESI-10
Figure S9. ¹ H-NMR (500 MHz, CDCl ₃) spectrum of compound 5a .	ESI-11
Figure S10. ¹³ C-NMR (125 MHz, CDCl ₃) spectrum of compound 5a .	ESI-12
Figure S11. ¹ H-NMR (500 MHz, CDCl ₃) spectrum of compound 5b .	ESI-13
Figure S12. ¹³ C-NMR (125 MHz, CDCl ₃) spectrum of compound 5b .	ESI-14
Figure S13. ¹ H-NMR (400 MHz, CDCl ₃) spectrum of compound 8a .	ESI-15
Figure S14. ¹³ C-NMR (100 MHz, CDCl ₃) spectrum of compound 8a .	ESI-16

Figure S15. HMBC (400 MHz, CDCl ₃) spectrum of compound 8a .	ESI-17
Figure S16. ¹ H-NMR (500 MHz, CDCl ₃) spectrum of compound 8b .	ESI-18
Figure S17. ¹³ C-NMR (125 MHz, CDCl ₃) spectrum of compound 8b .	ESI-19
Figure S18. ¹ H-NMR (500 MHz, CDCl ₃) spectrum of compound 9a .	ESI-20
Figure S19. ¹³ C-NMR (125 MHz, CDCl ₃) spectrum of compound 9a .	ESI-21
Figure S20. HMBC (500 MHz, CDCl ₃) spectrum of compound 9a .	ESI-22
Figure S21. ¹ H-NMR (500 MHz, CDCl ₃) spectrum of compound 9b .	ESI-23
Figure S22. ¹³ C-NMR (125 MHz, CDCl ₃) spectrum of compound 9b .	ESI-24
Figure S23. ¹ H-NMR (500 MHz, CD ₃ OD: CDCl ₃) spectrum of compound 10 .	ESI-25
Figure S24. ¹³ C-NMR (125 MHz, CD ₃ OD: CDCl ₃) spectrum of compound 10 .	ESI-26
Figure S25. ¹ H-NMR (500 MHz, CD ₃ OD: CDCl ₃) spectrum of compound 11 .	ESI-27
Figure S26. ¹³ C-NMR (125 MHz, CD ₃ OD: CDCl ₃) spectrum of compound 11 .	ESI-28

Solvent: CDCl₃, Frequency: 500MHz

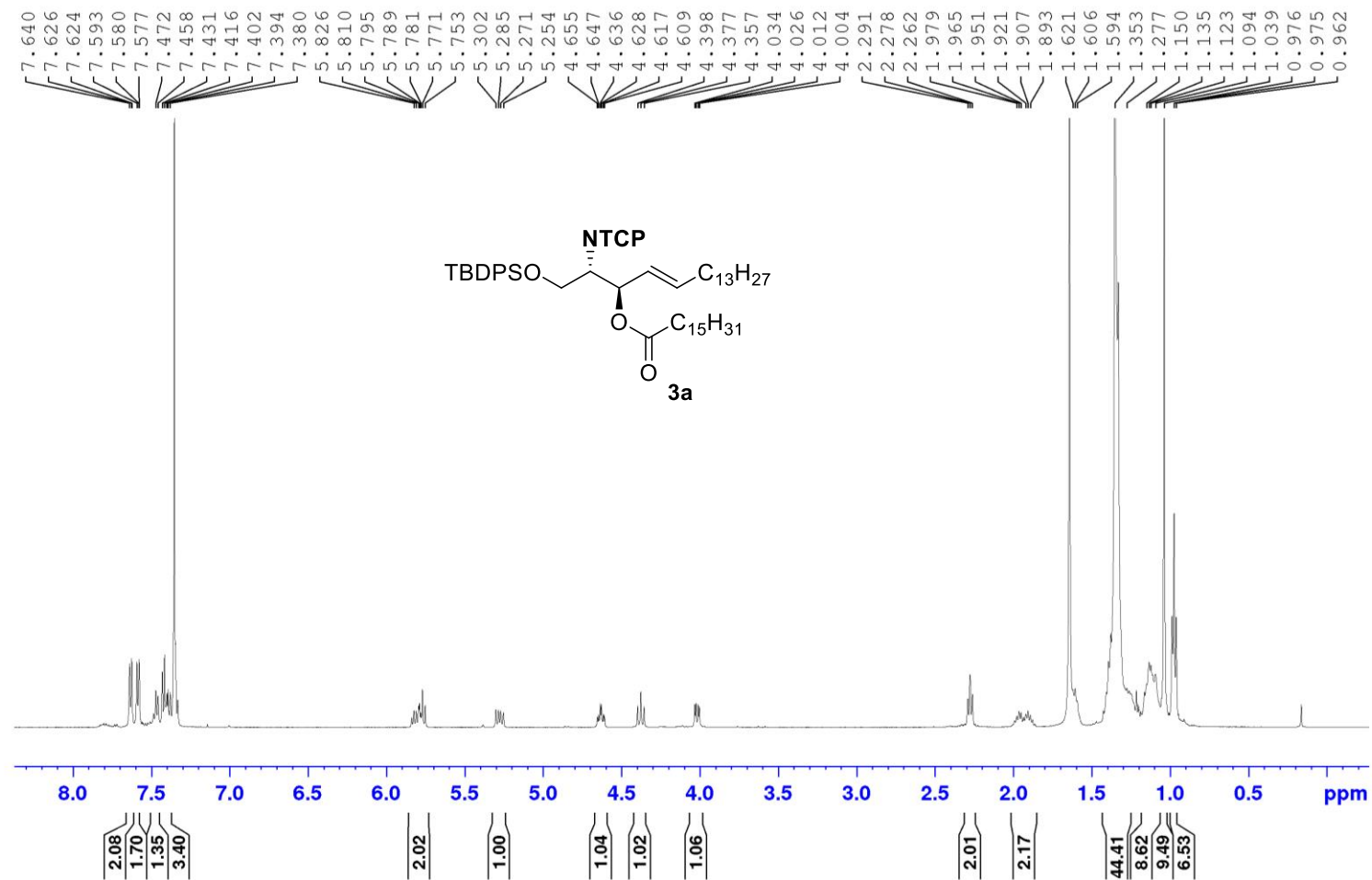


Figure S1. ¹H-NMR (500 MHz, CDCl₃) spectrum of compound **3a**.

Solvent: CDCl₃, Frequency: 125MHz

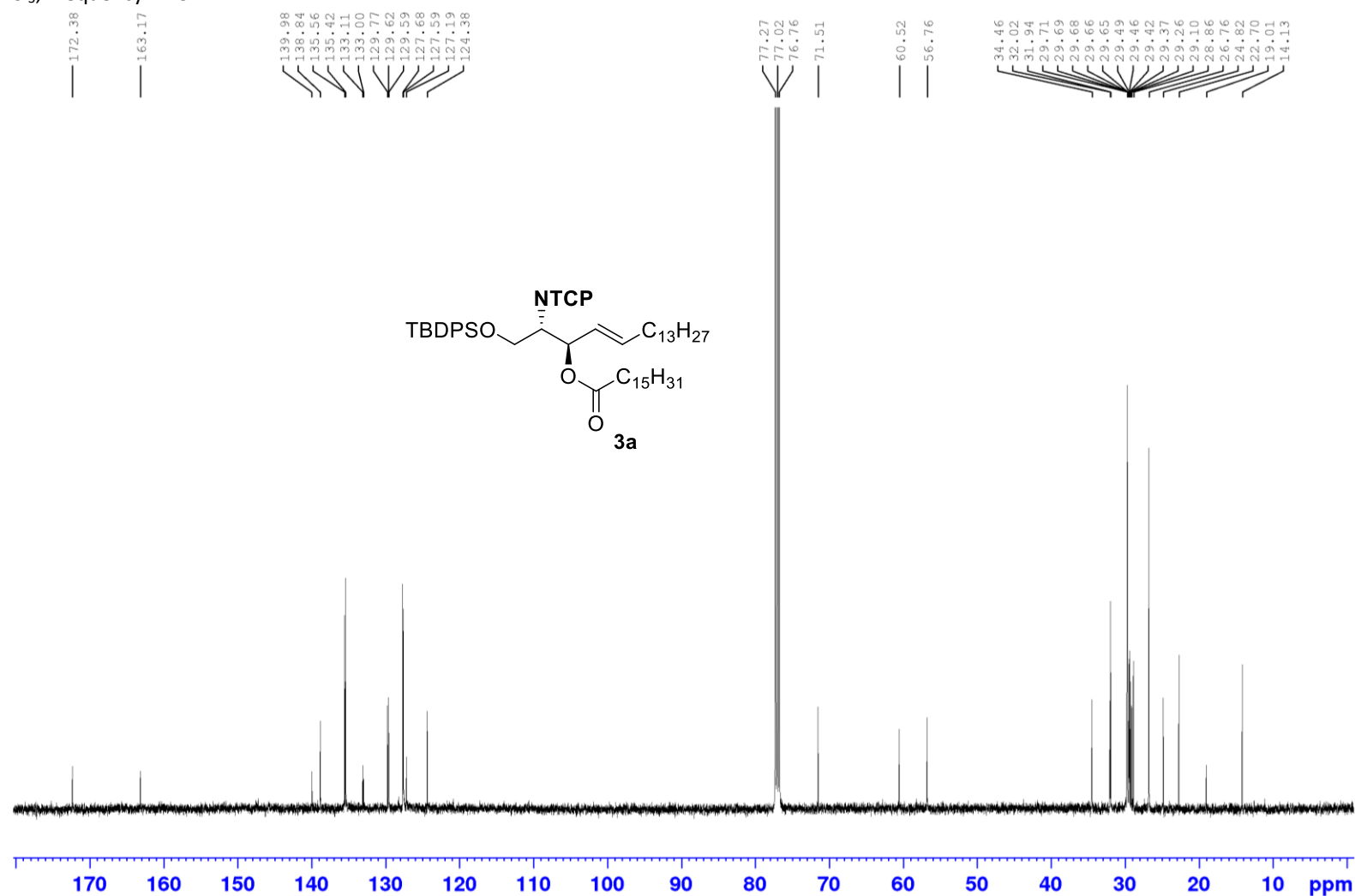


Figure S2. ¹³C-NMR (125 MHz, CDCl₃) spectrum of compound 3a.

[illegible]

ESI-5

Solvent: CDCl₃, Frequency: 125MHz

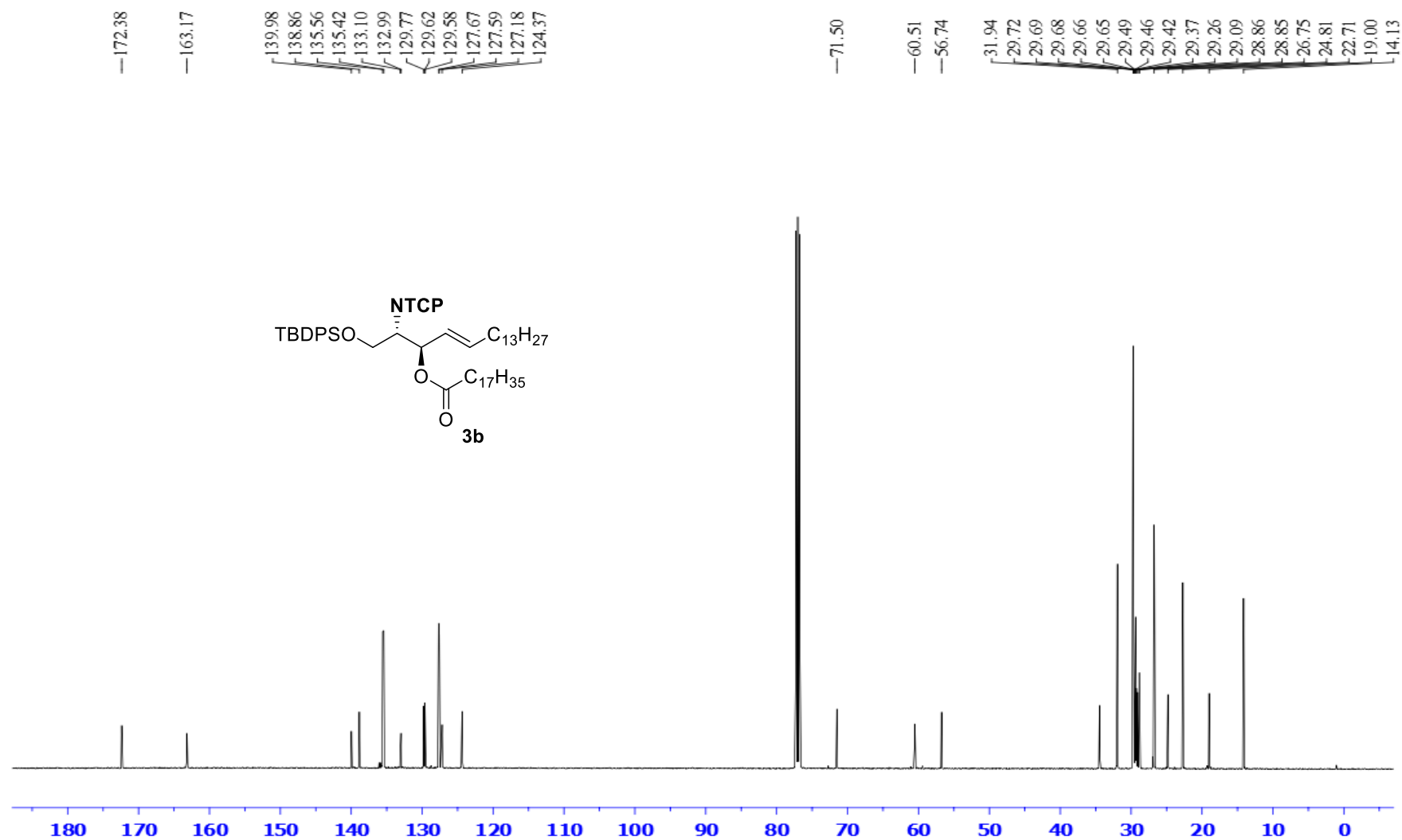


Figure S4. ¹³C-NMR (125 MHz, CDCl₃) spectrum of compound **3b**.

Solvent: CDCl₃, Frequency: 500MHz

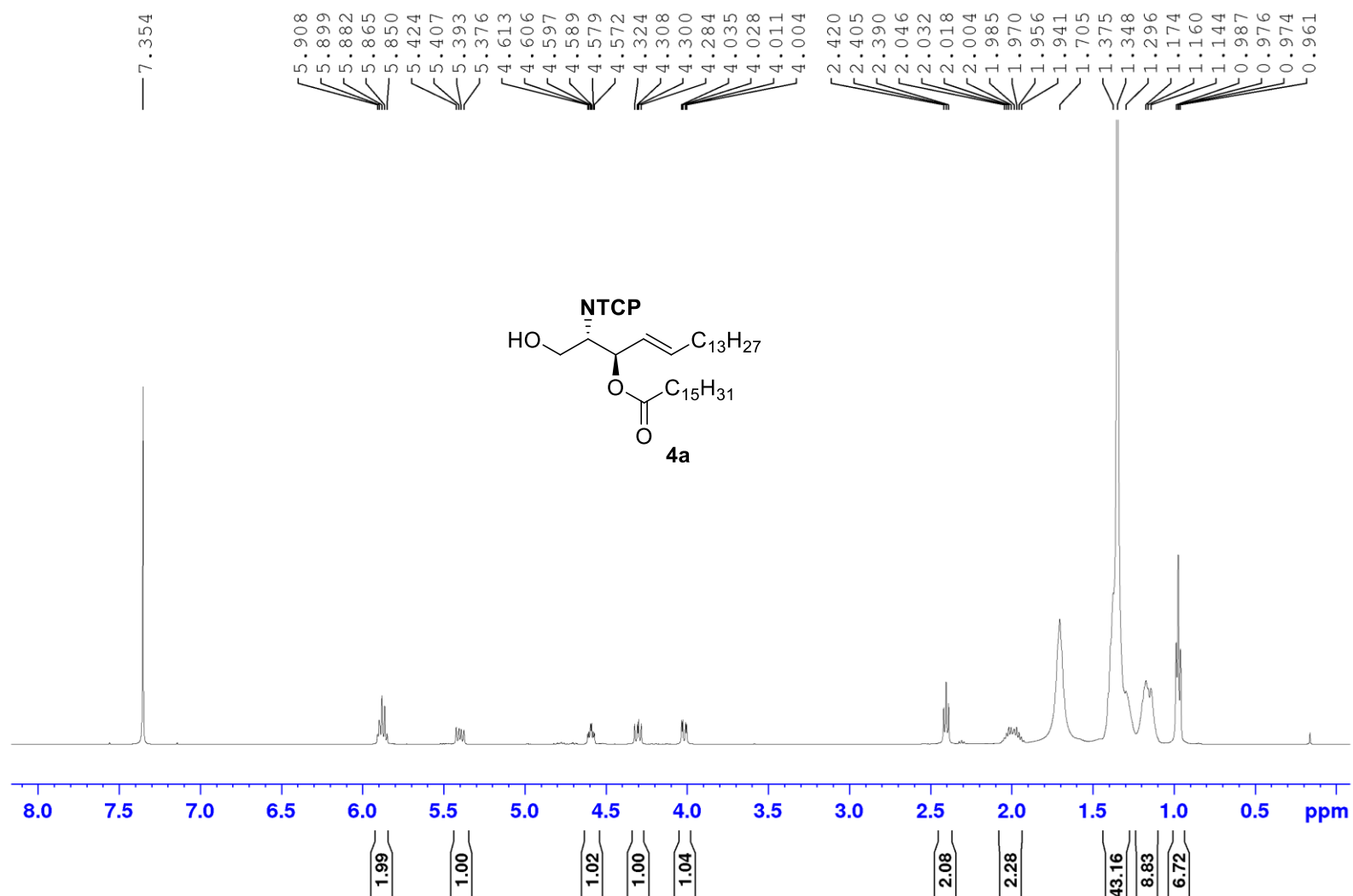


Figure S5. ¹H-NMR (500 MHz, CDCl₃) spectrum of compound **4a**.

Solvent: CDCl₃, Frequency: 125MHz

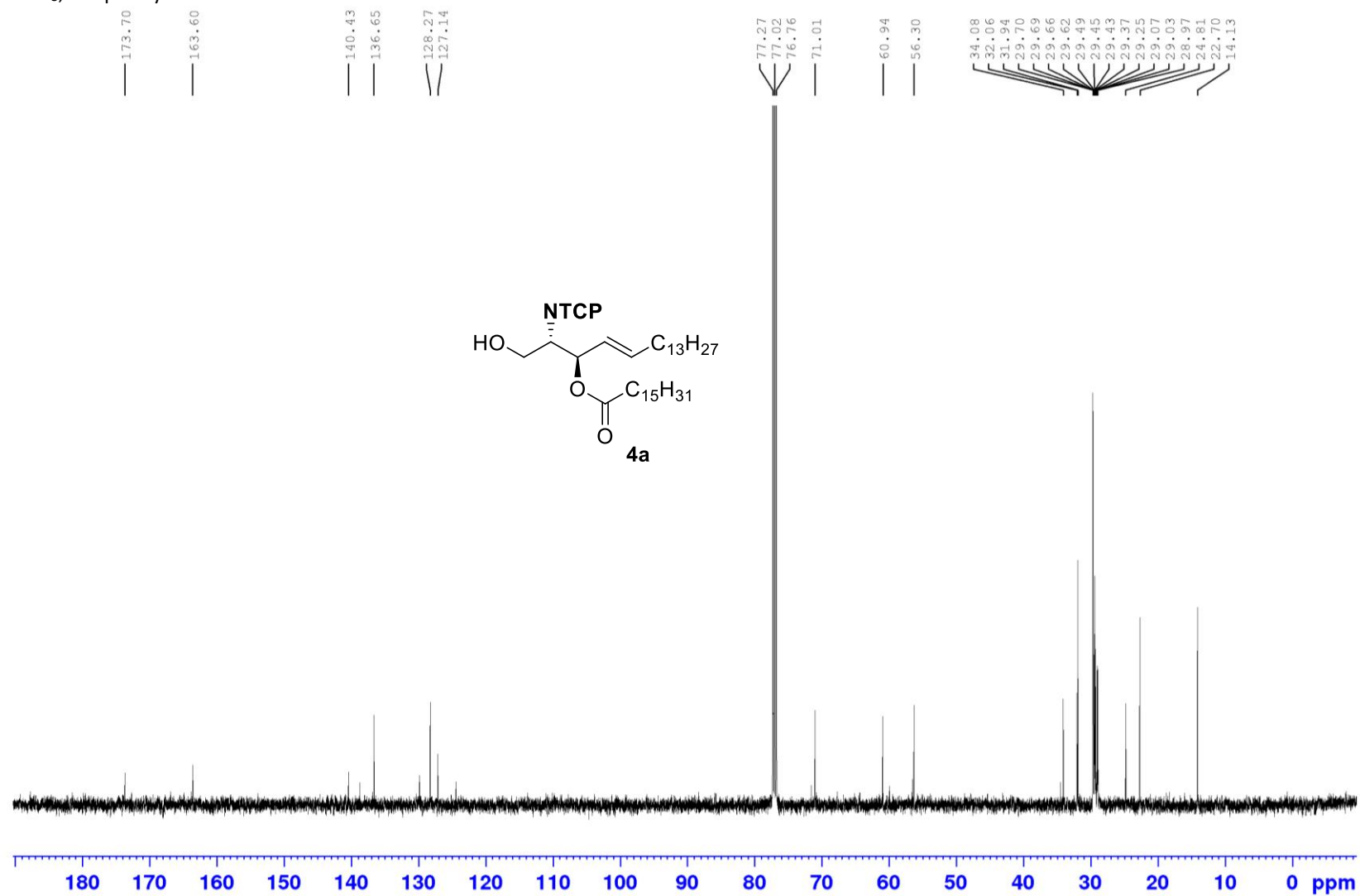


Figure S6. ¹³C-NMR (125 MHz, CDCl₃) spectrum of compound **4a**.

Solvent: CDCl₃, Frequency: 500MHz

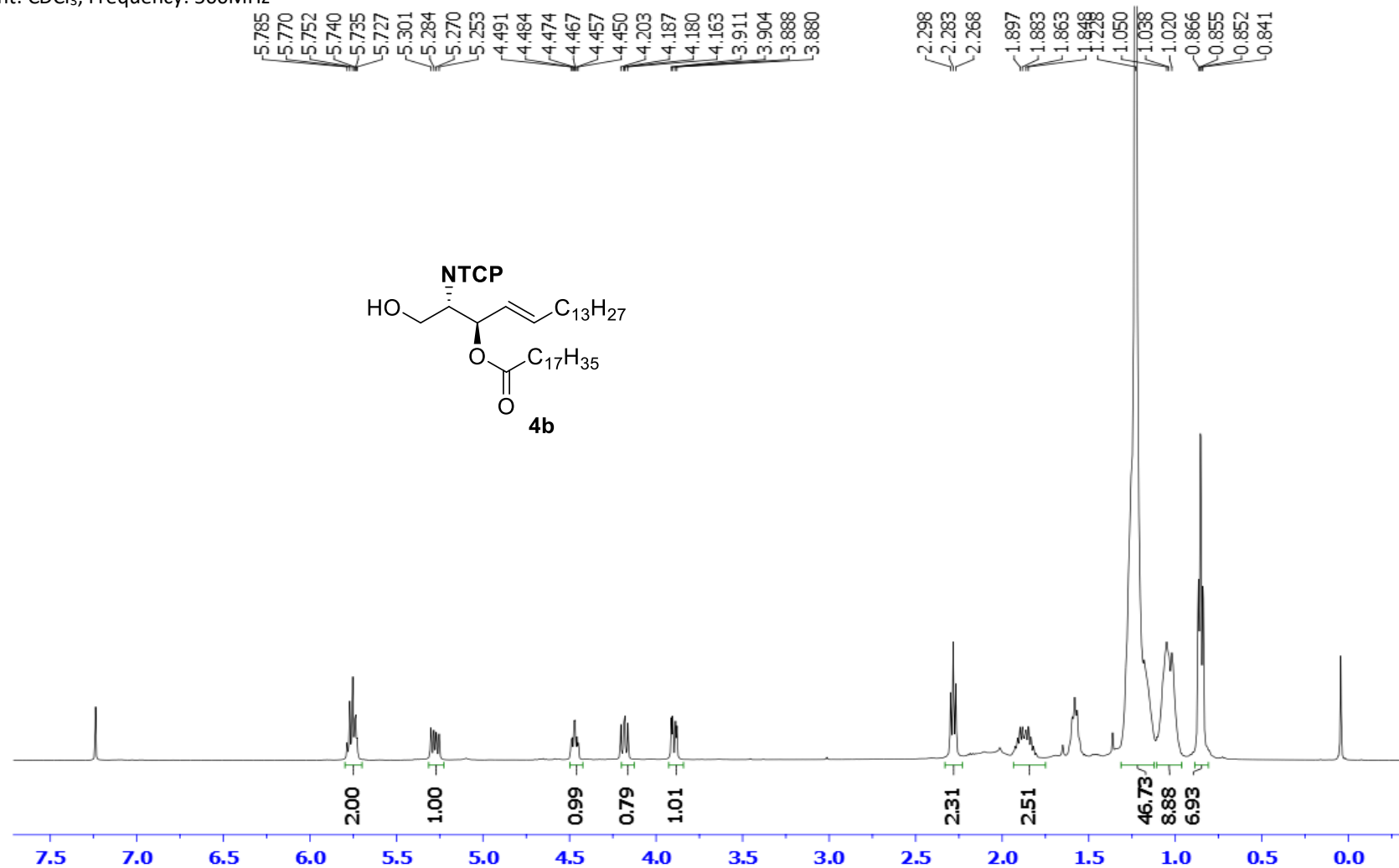


Figure S7. ¹H-NMR (500 MHz, CDCl₃) spectrum of compound **4b**.

Solvent: CDCl₃, Frequency: 125MHz

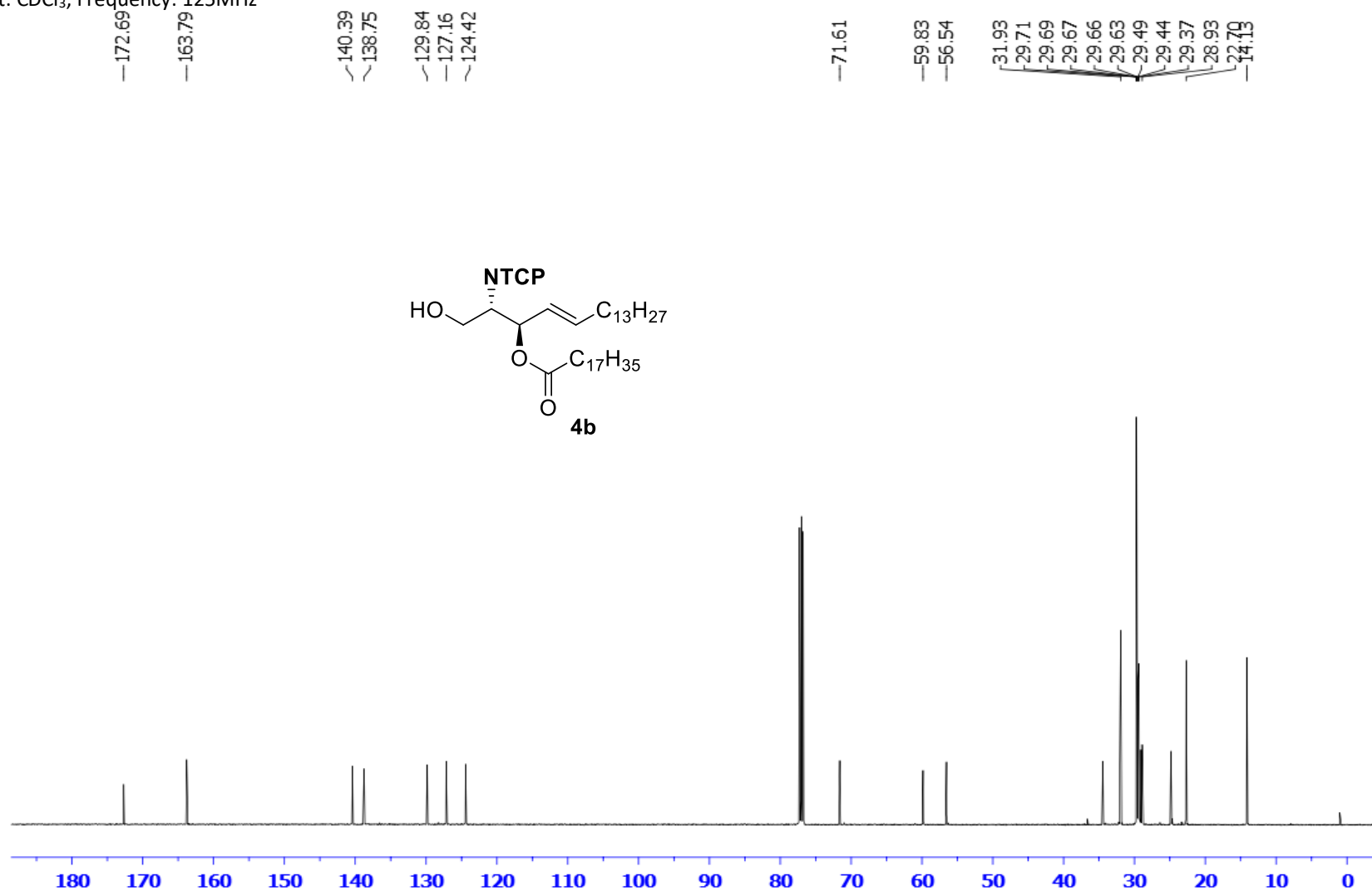


Figure S8. ¹³C-NMR (125 MHz, CDCl₃) spectrum of compound **4b**.

Solvent: CDCl₃, Frequency: 500MHz

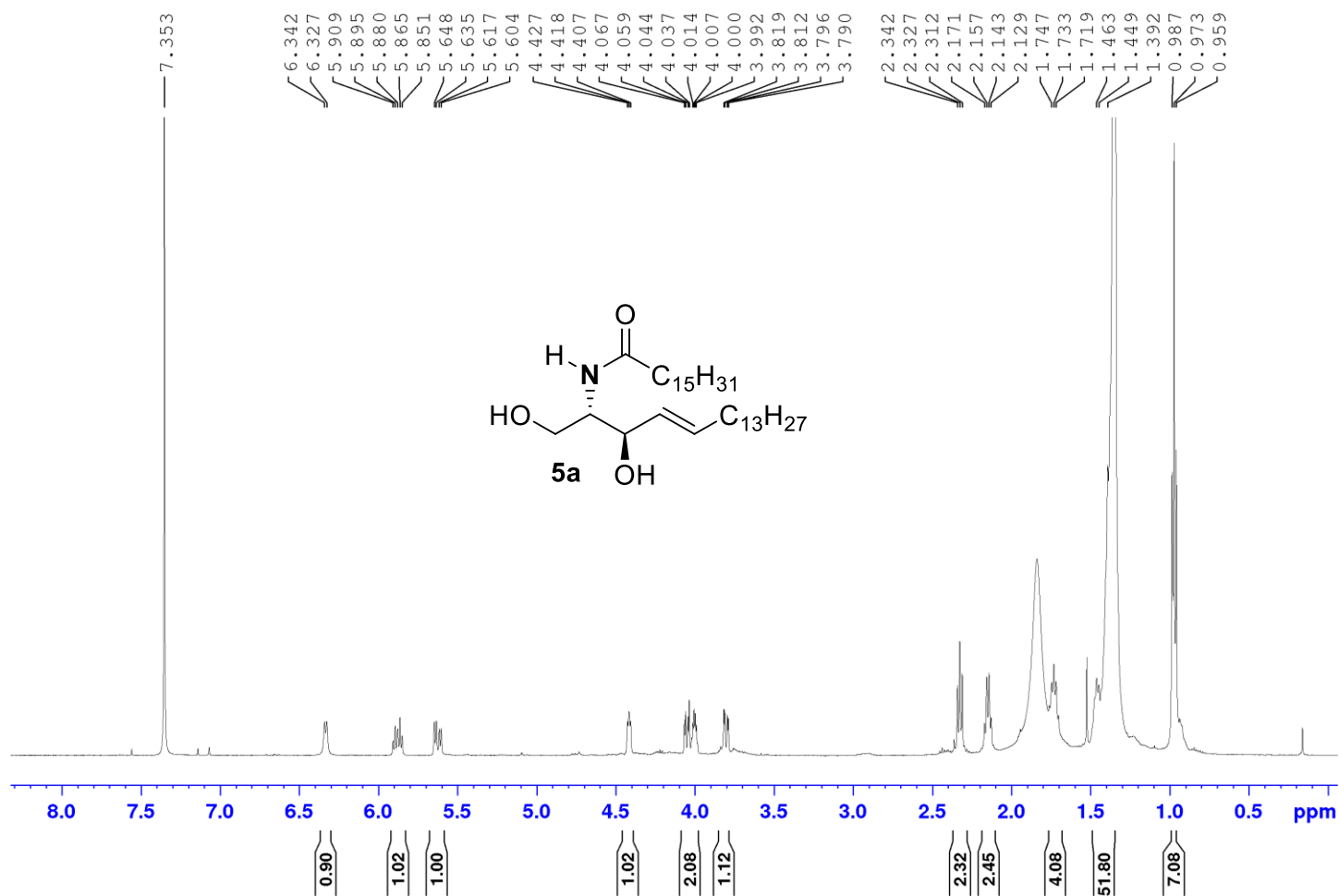


Figure S9. ¹H-NMR (500 MHz, CDCl₃) spectrum of compound **5a**.

Solvent: CDCl₃, Frequency: 125MHz

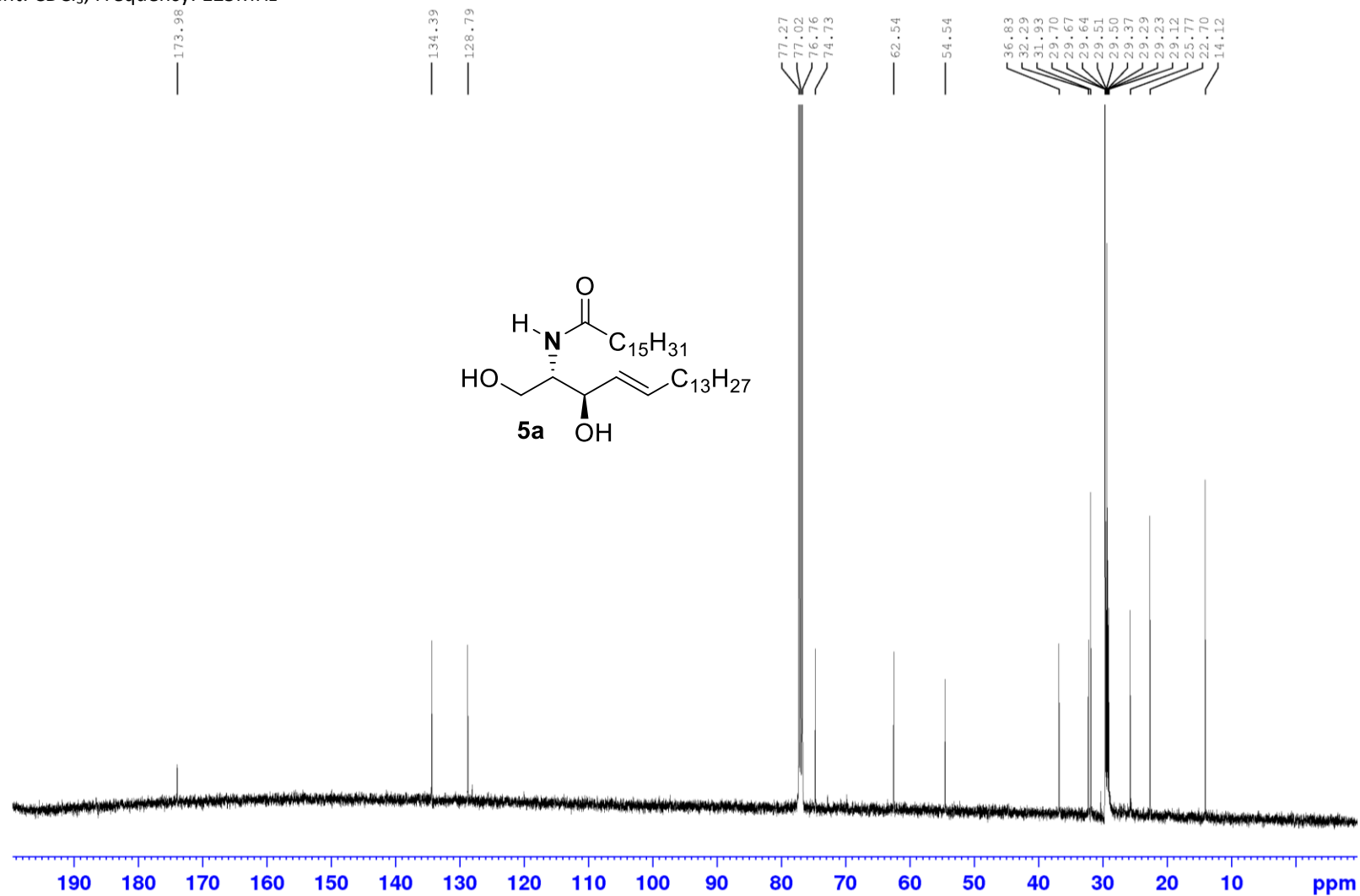


Figure S10. ¹³C-NMR (125 MHz, CDCl₃) spectrum of compound **5a**.

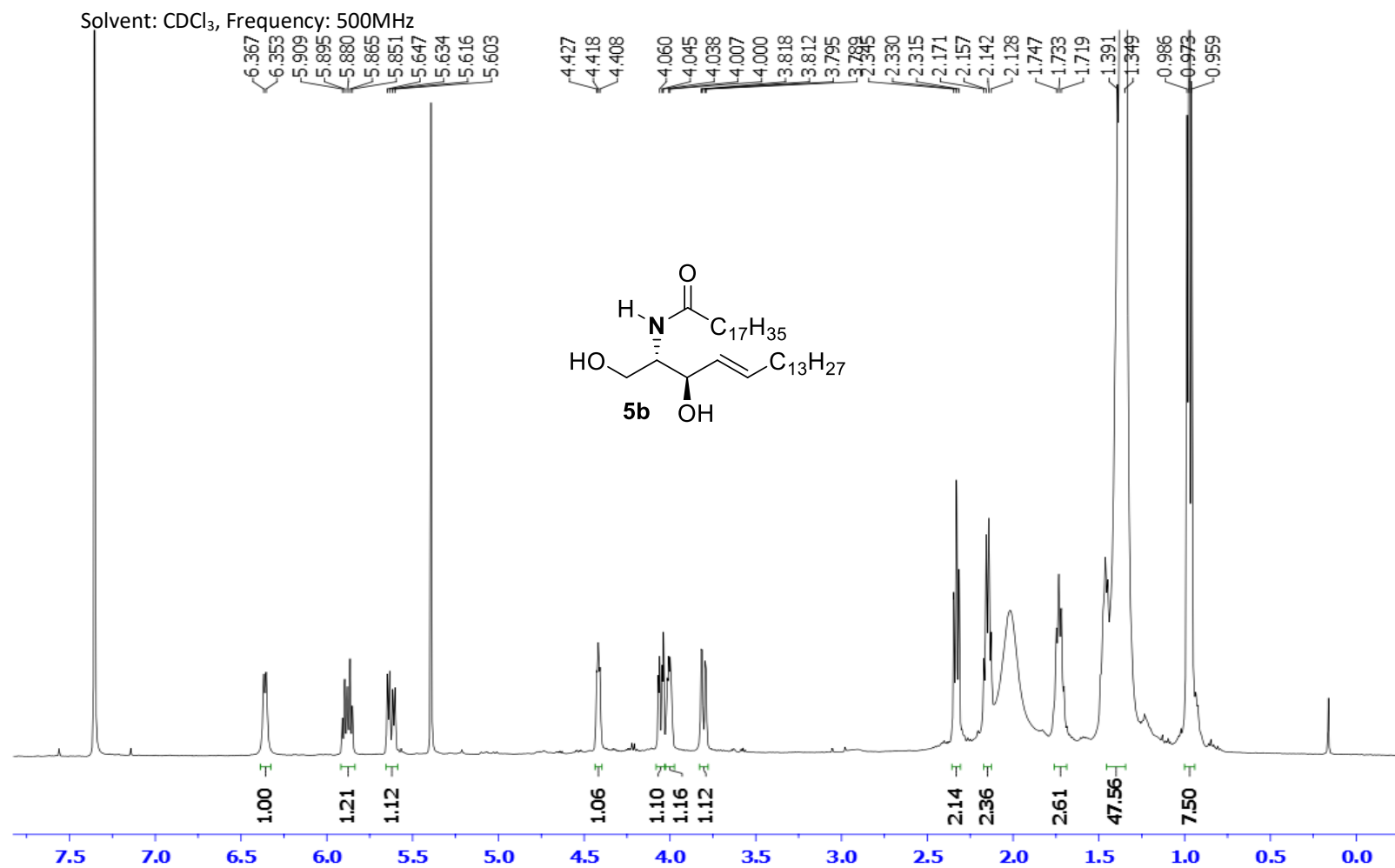


Figure S11. ¹H-NMR (500 MHz, CDCl₃) spectrum of compound **5b**.

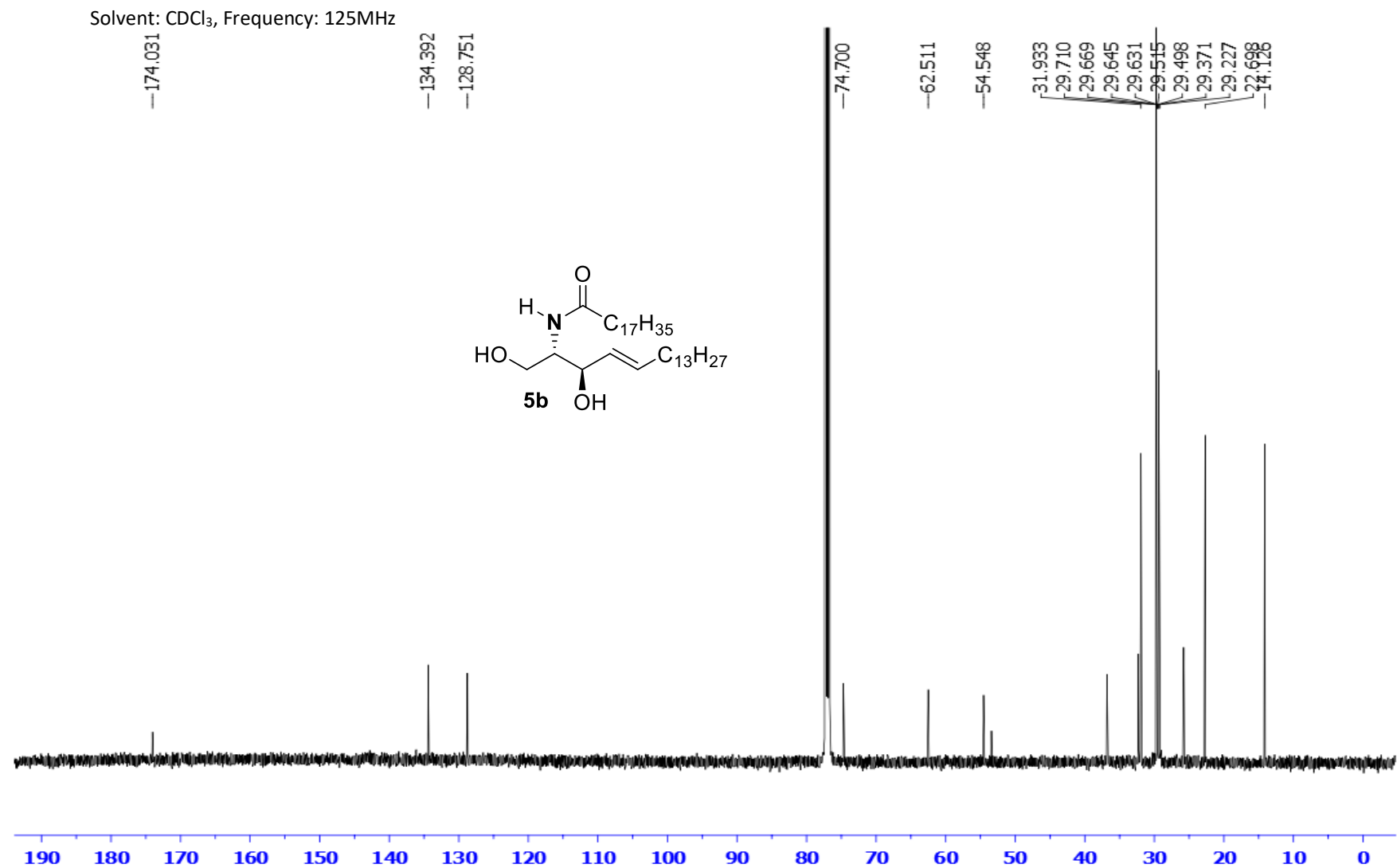


Figure S12. ¹³C-NMR (125 MHz, CDCl₃) spectrum of compound **5b**.

Solvent: CDCl₃, Frequency: 400MHz

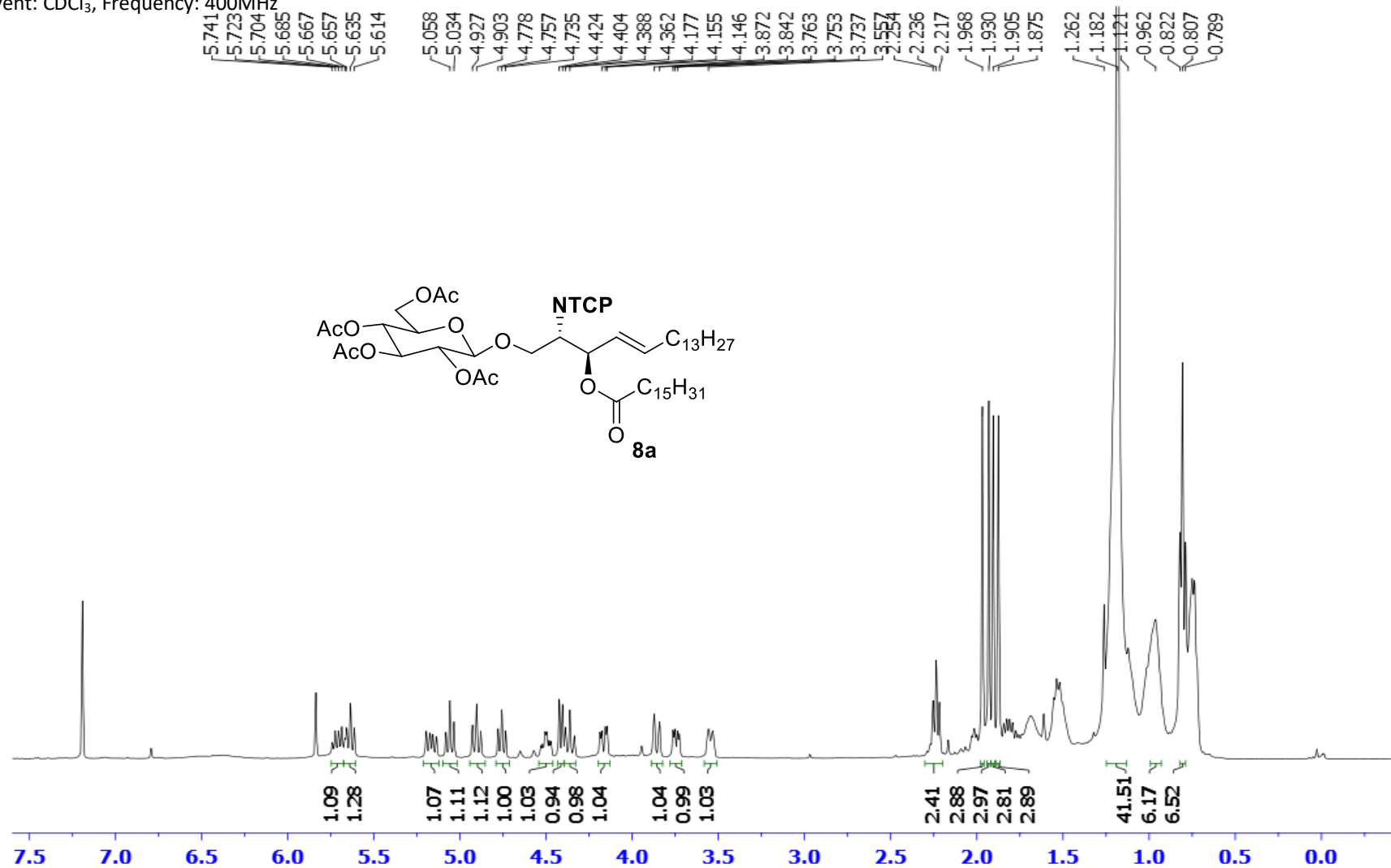


Figure S13. ¹H-NMR (400 MHz, CDCl₃) spectrum of compound **8a**.

Solvent: CDCl₃, Frequency: 100MHz

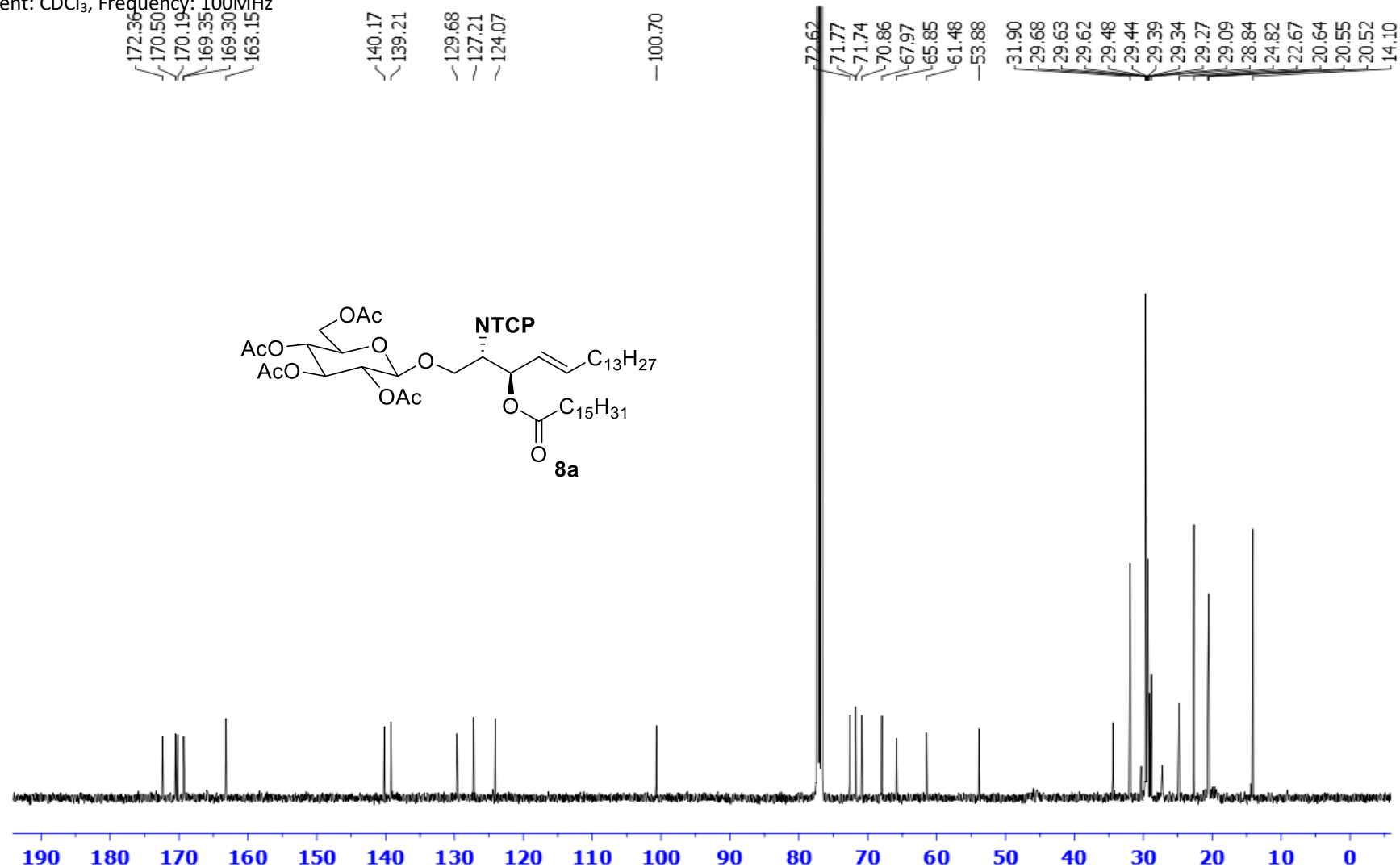


Figure S14. ¹³C-NMR (100 MHz, CDCl₃) spectrum of compound **8a**.

Solvent: CDCl₃, Frequency: 400MHz

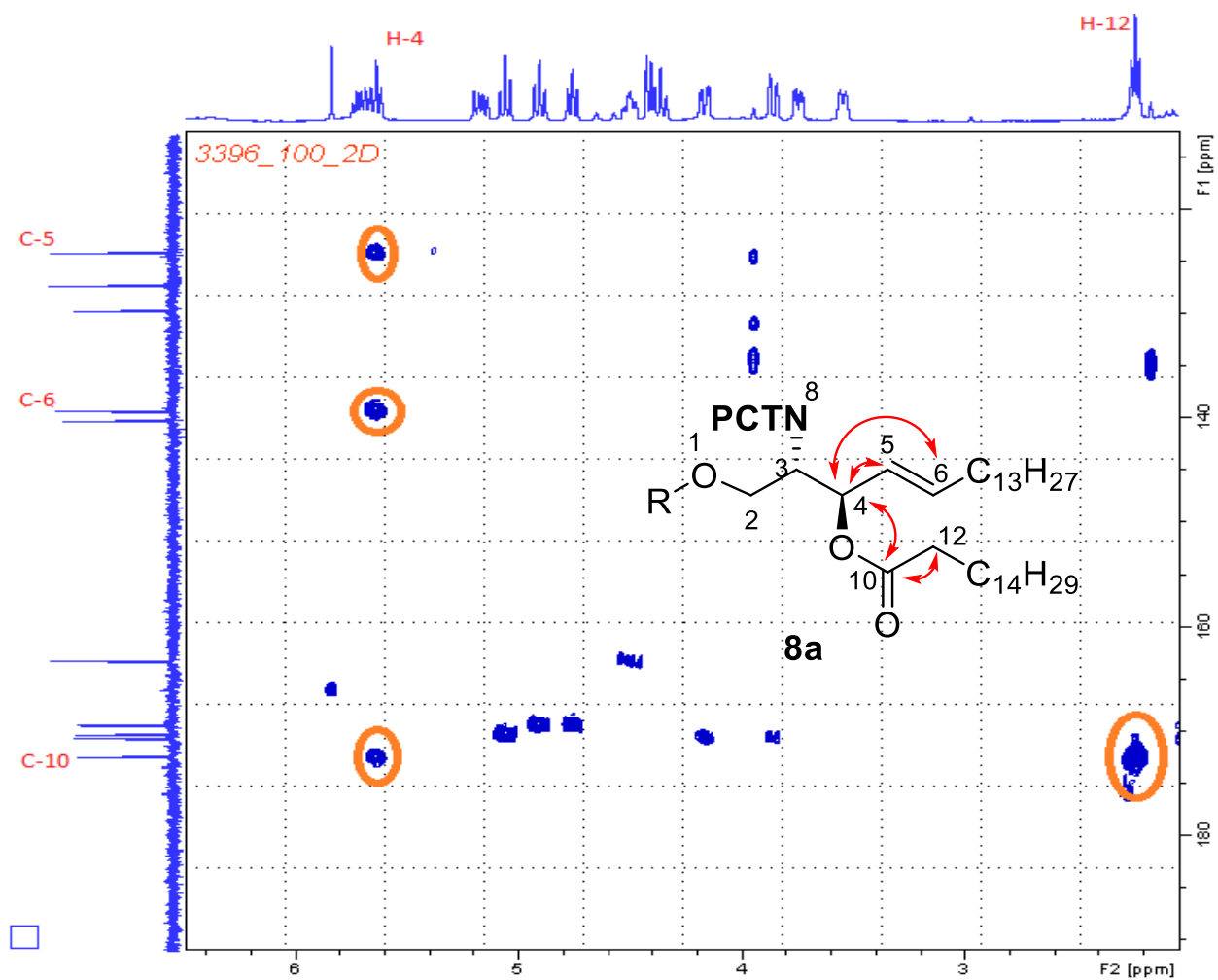


Figure S15. HMBC (400 MHz, CDCl₃) spectrum of compound **8a**.

Solvent: CDCl₃, Frequency: 500MHz

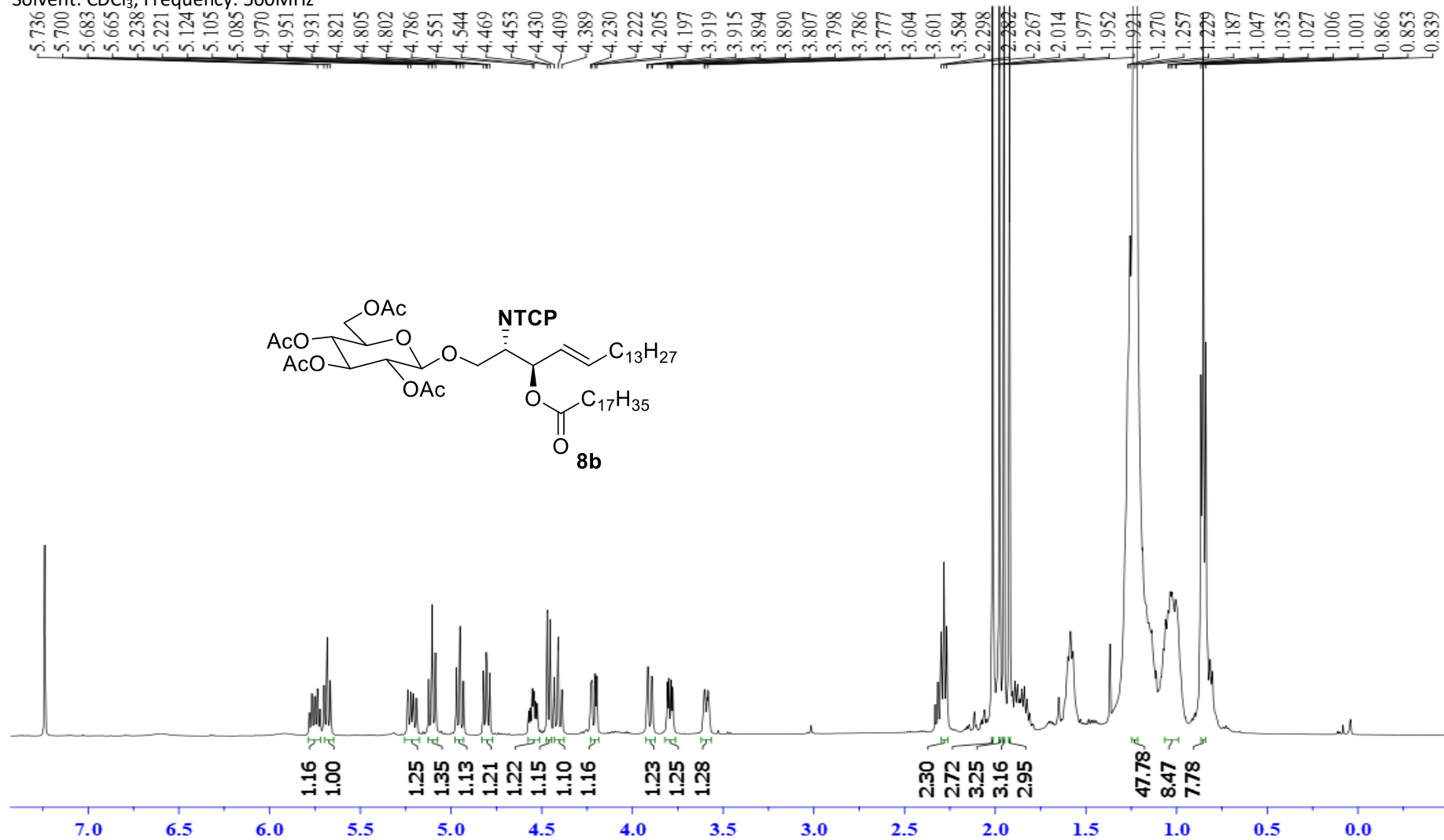


Figure S16. ¹H-NMR (500 MHz, CDCl₃) spectrum of compound **8b**.

Solvent: CDCl₃, Frequency: 125MHz

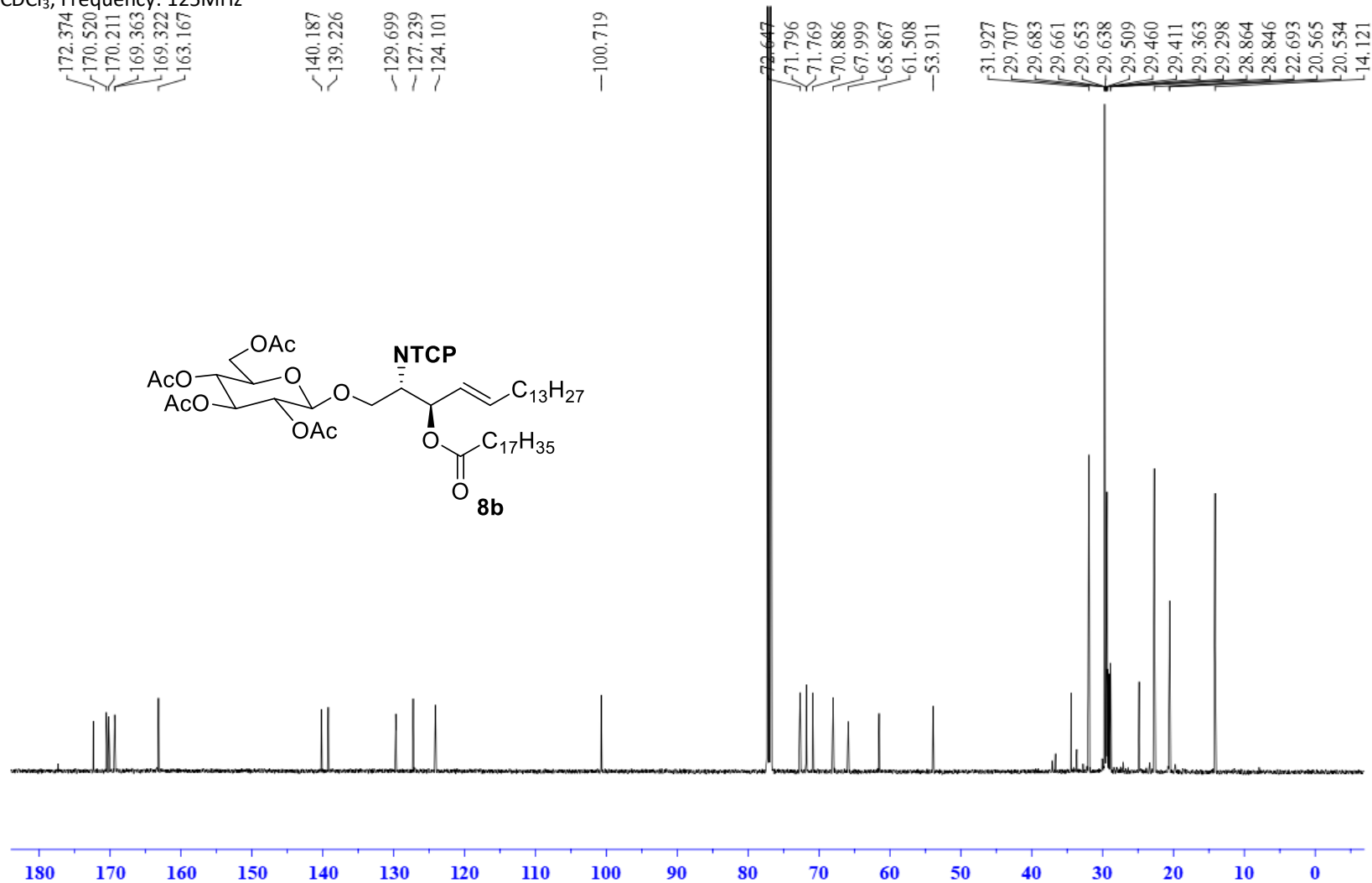


Figure S17. ¹³C-NMR (125 MHz, CDCl₃) spectrum of compound **8b**.

Solvent: CDCl₃, Frequency: 500MHz

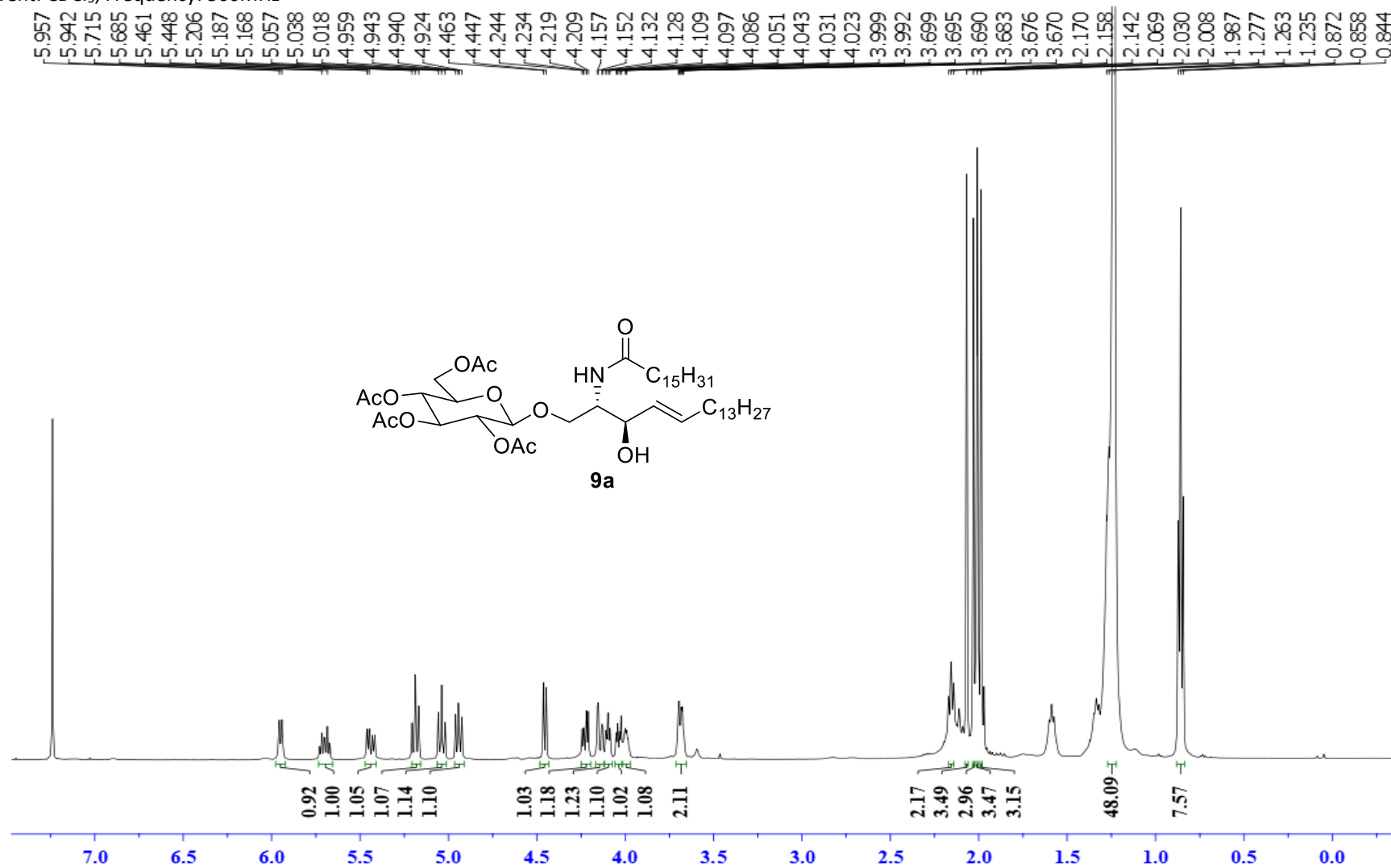


Figure S18. ¹H-NMR (500 MHz, CDCl₃) spectrum of compound **9a**.

Solvent: CDCl₃, Frequency: 125MHz

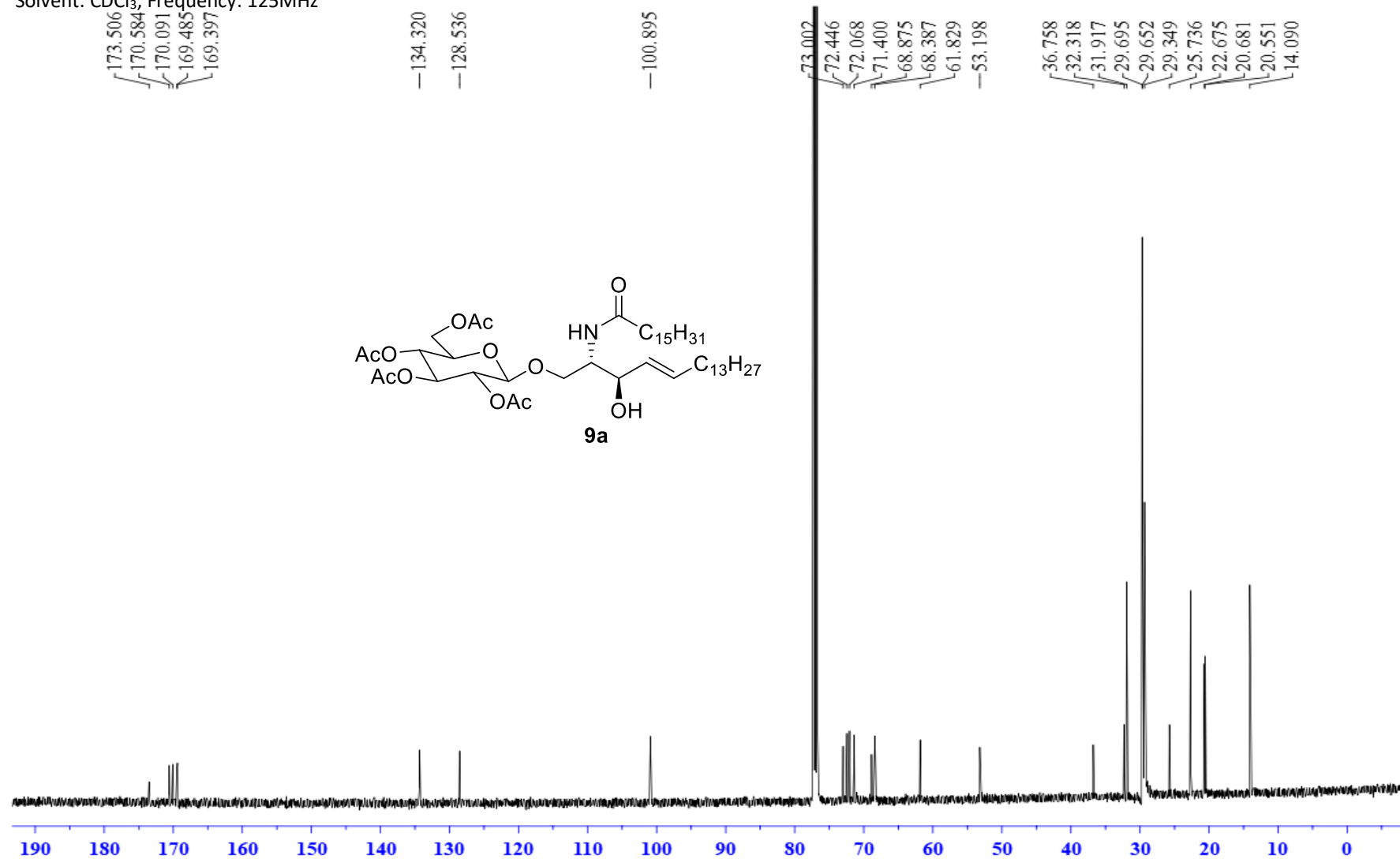


Figure S19. ¹³C-NMR (125 MHz, CDCl₃) spectrum of compound 9a.

Solvent: CDCl₃, Frequency: 500MHz

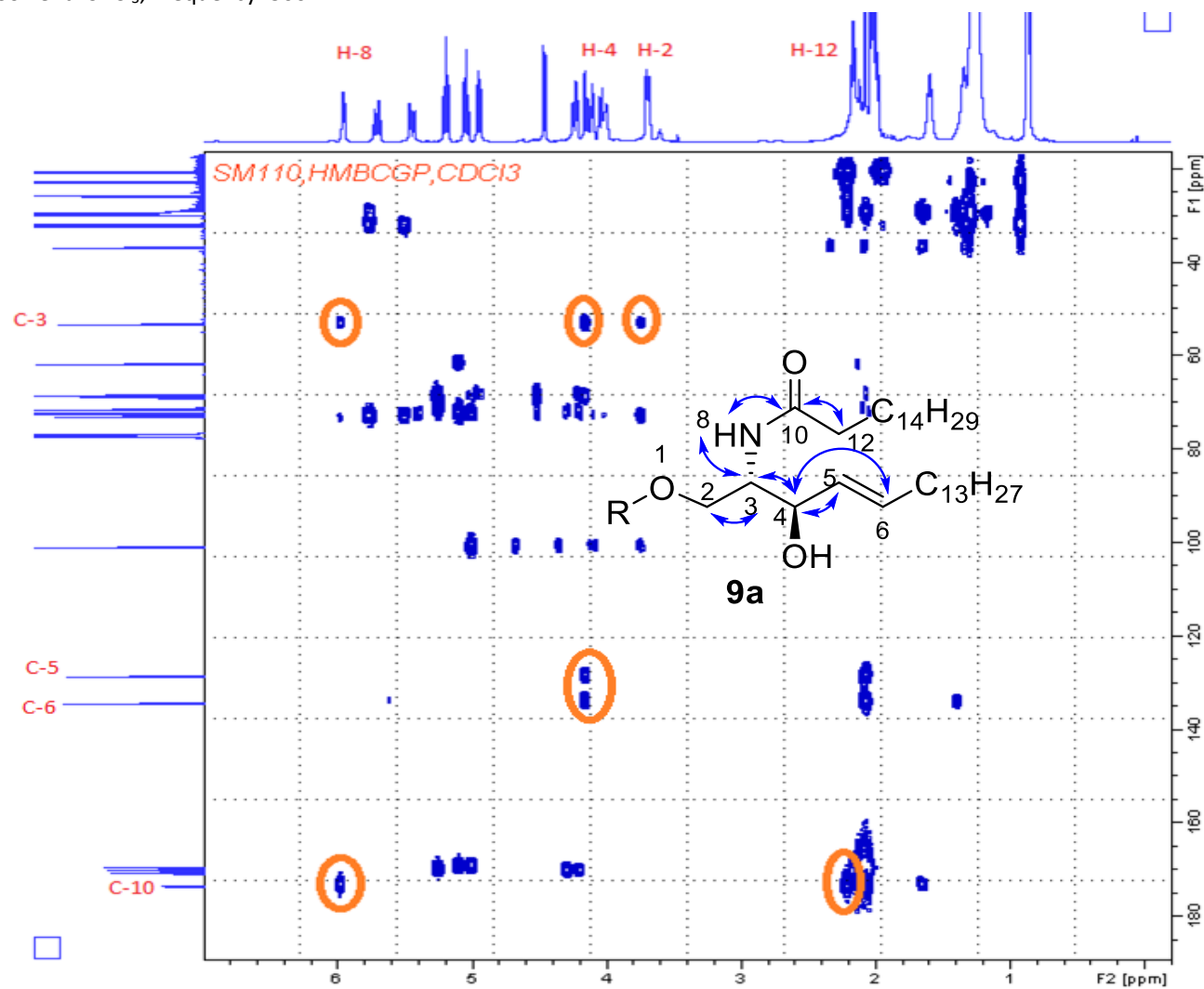


Figure S20. HMBC (500 MHz, CDCl₃) spectrum of compound **9a**.

Solvent: CDCl₃, Frequency: 500MHz

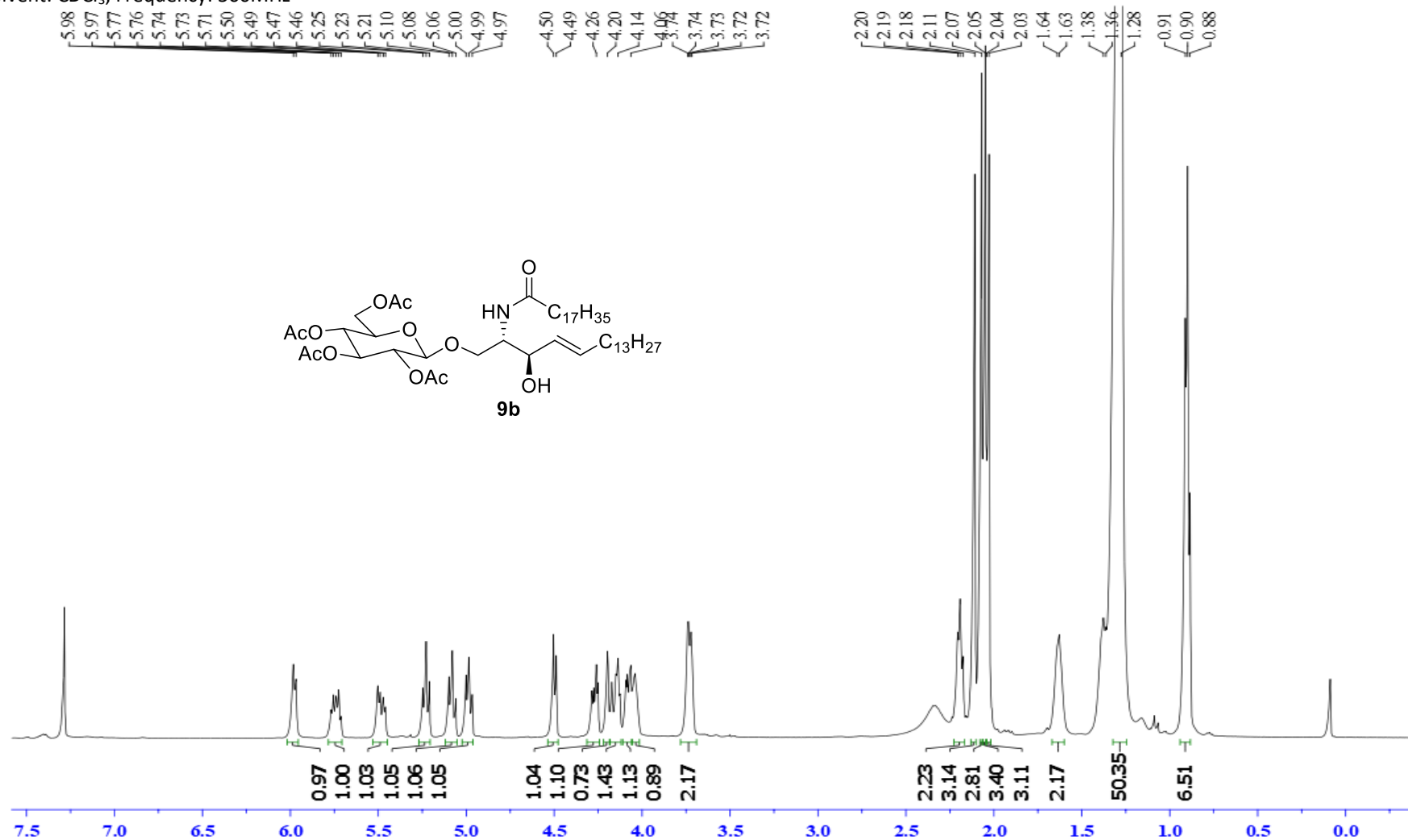


Figure S21. ¹H-NMR (500 MHz, CDCl₃) spectrum of compound **9b**.

Solvent: CDCl₃, Frequency: 125MHz

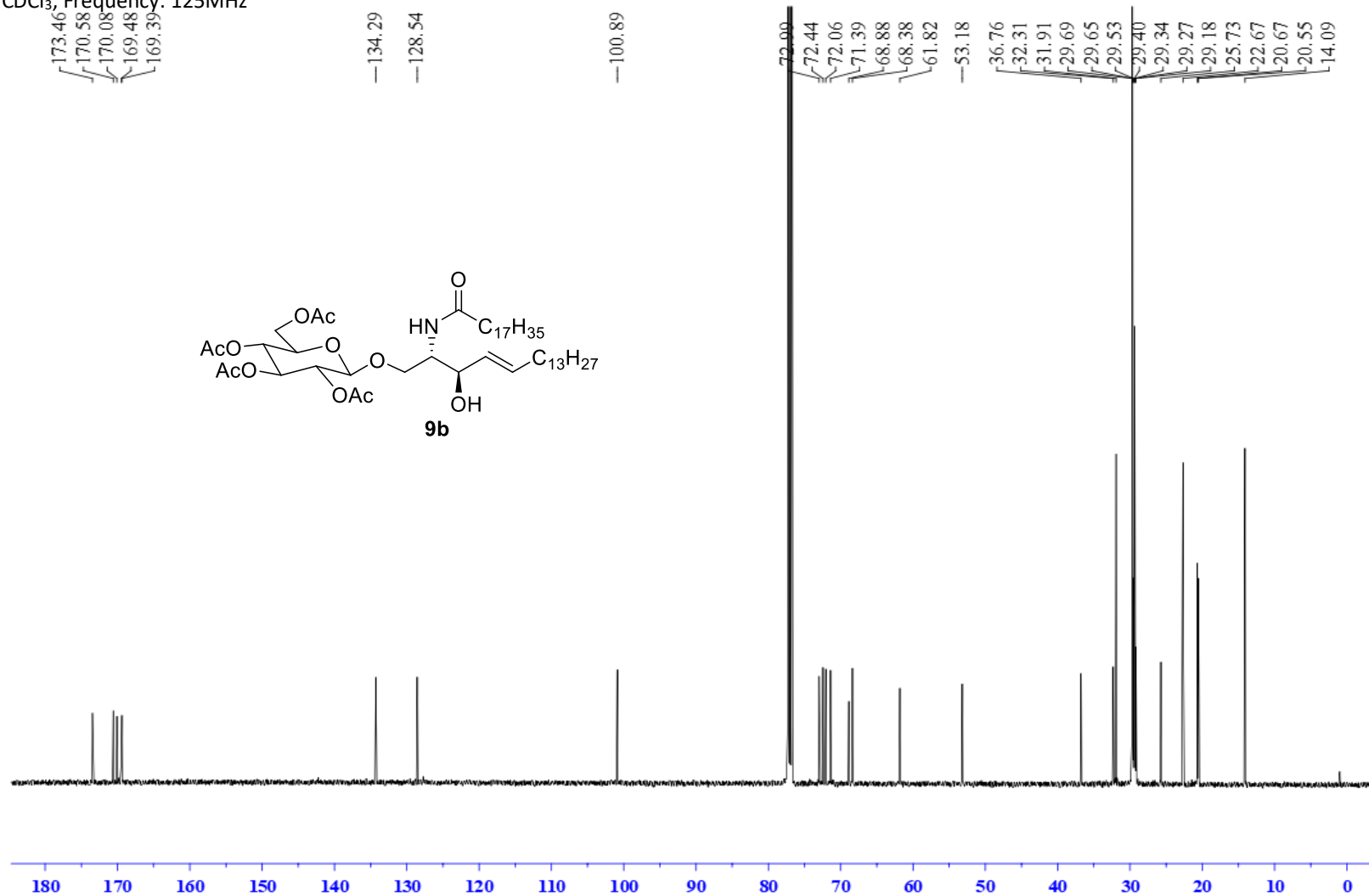


Figure S22. ¹³C-NMR (125 MHz, CDCl₃) spectrum of compound **9b**.

Solvent: CDCl₃:CD₃OD (6:1), Frequency: 500MHz

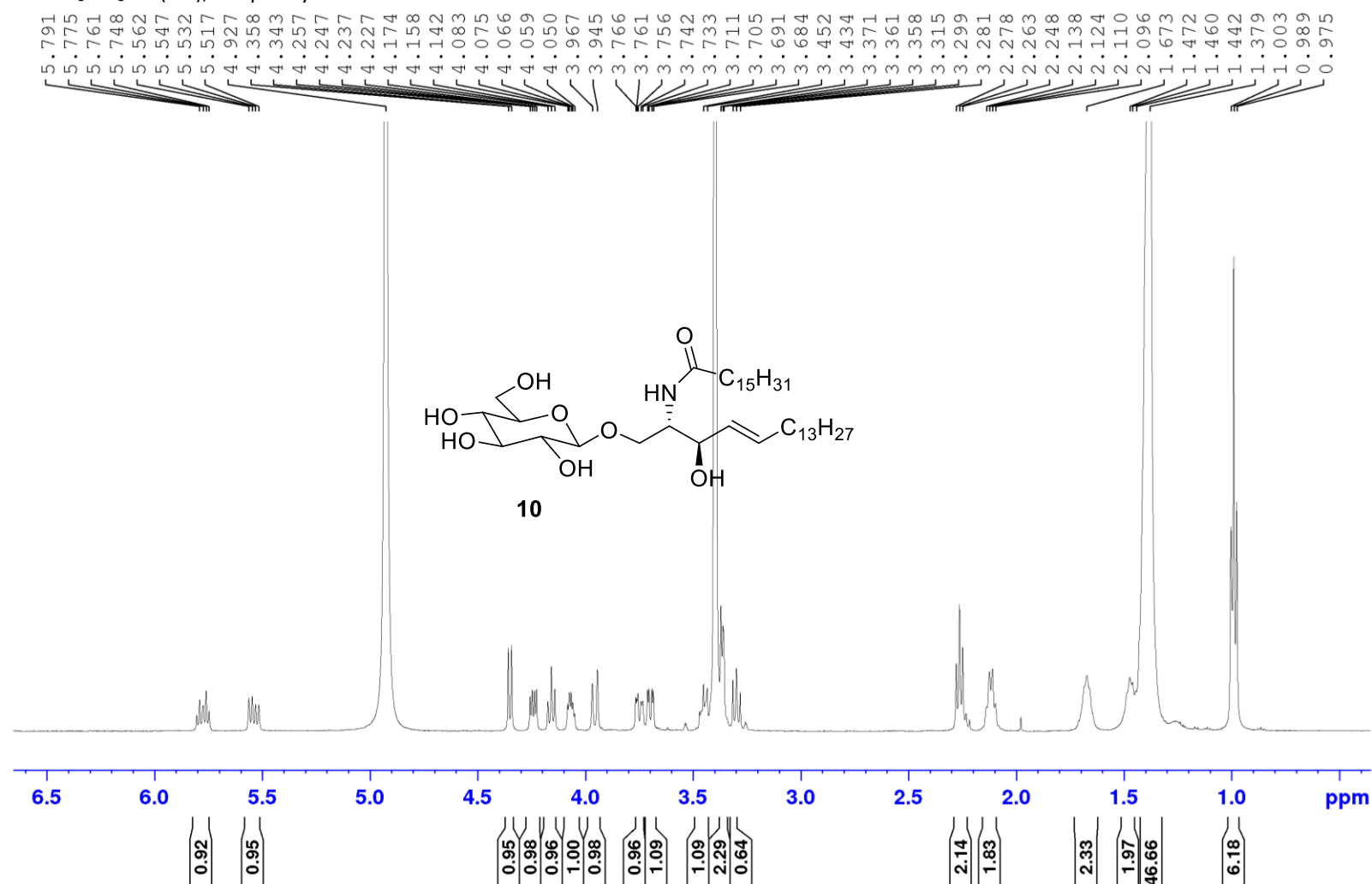


Figure S23. ¹H-NMR (500 MHz, CD₃OD: CDCl₃) spectrum of compound **10**.

Solvent: CDCl₃:CD₃OD (6:1), Frequency: 125MHz

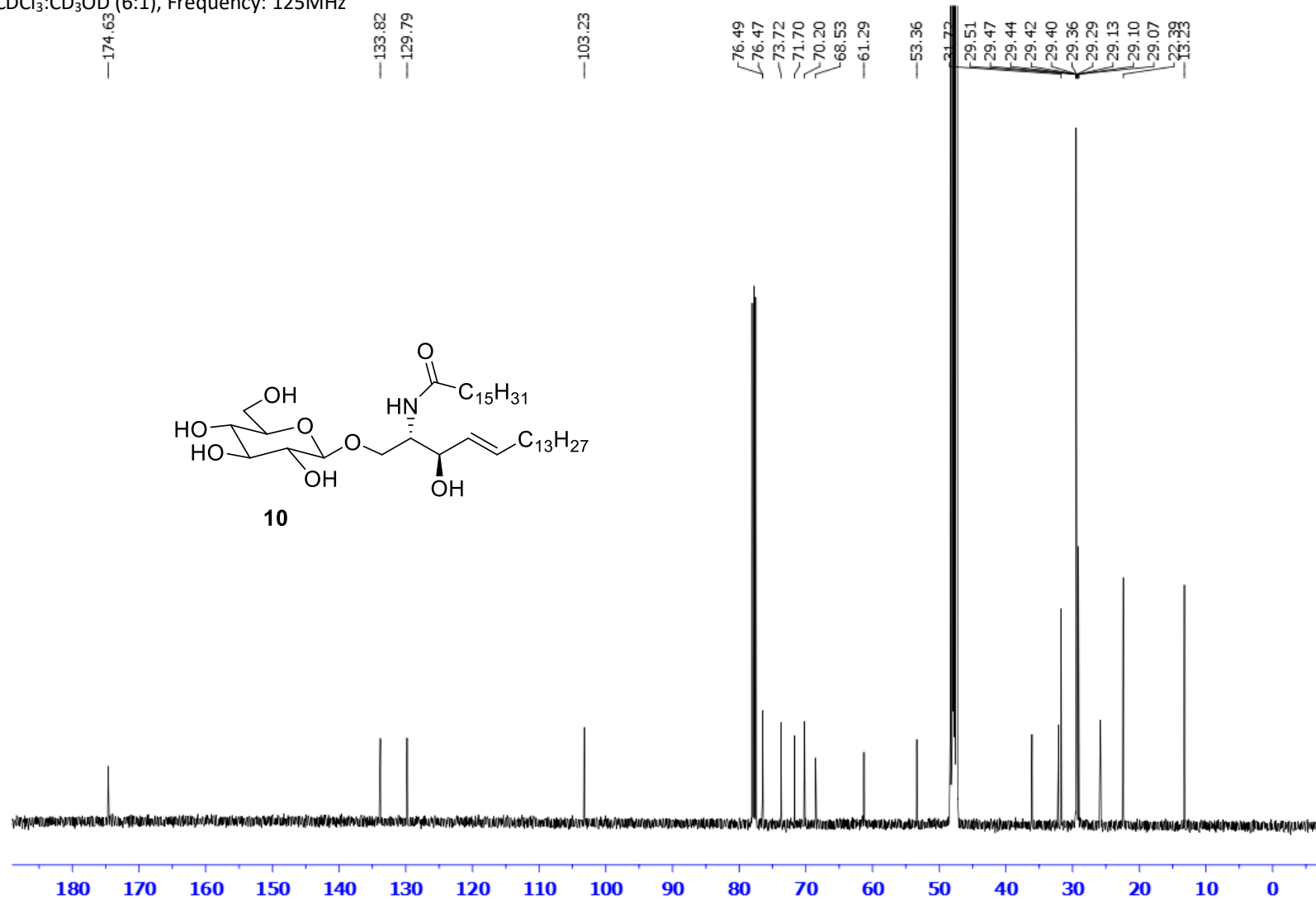


Figure S24. ¹³C-NMR (125 MHz, CD₃OD: CDCl₃) spectrum of compound 10.

Solvent: CDCl₃:CD₃OD (6:1), Frequency: 500MHz

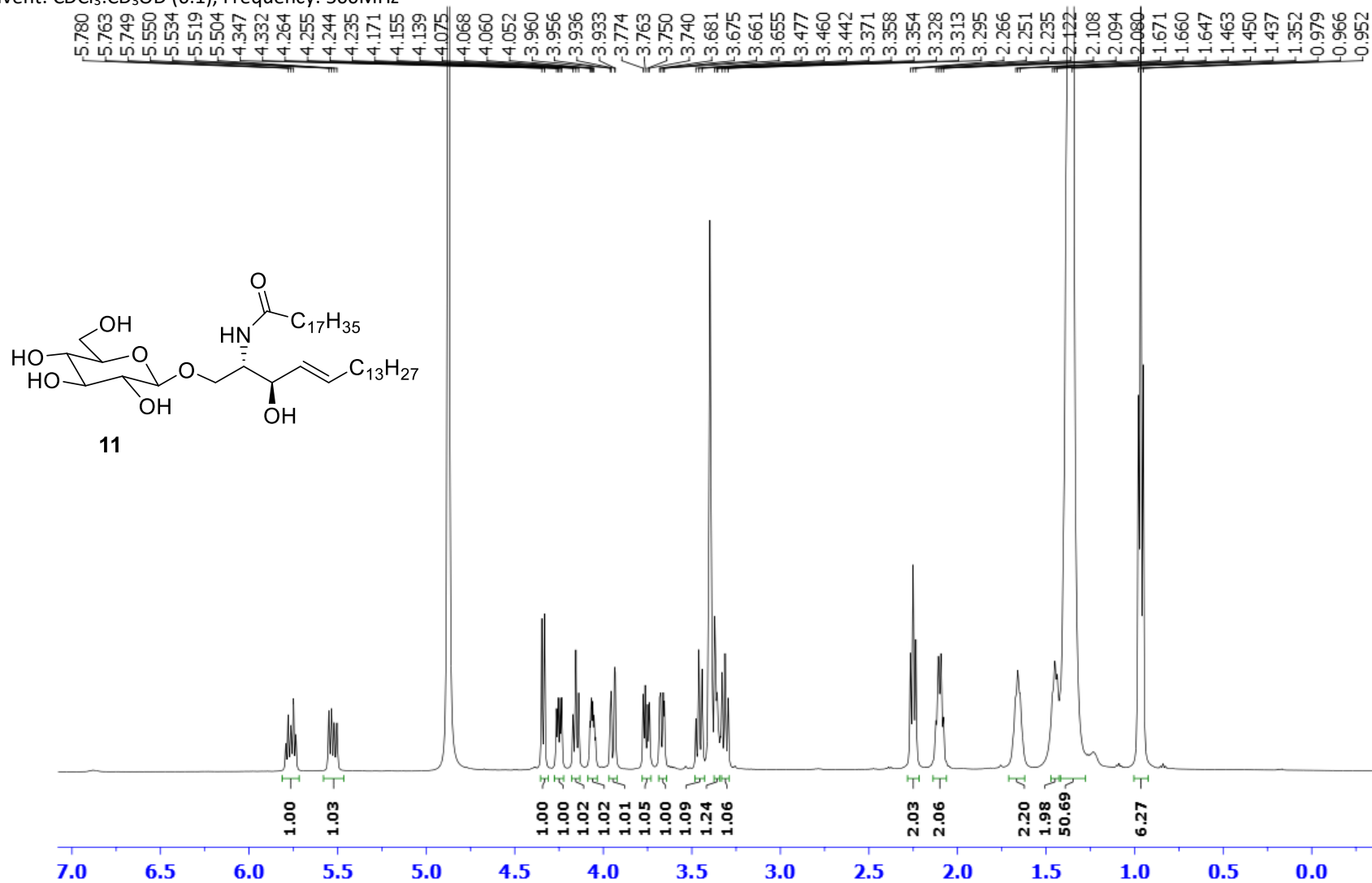


Figure S25. ¹H-NMR (500 MHz, CD₃OD: CDCl₃) spectrum of compound **11**.

Solvent: CDCl₃:CD₃OD (6:1), Frequency: 125MHz

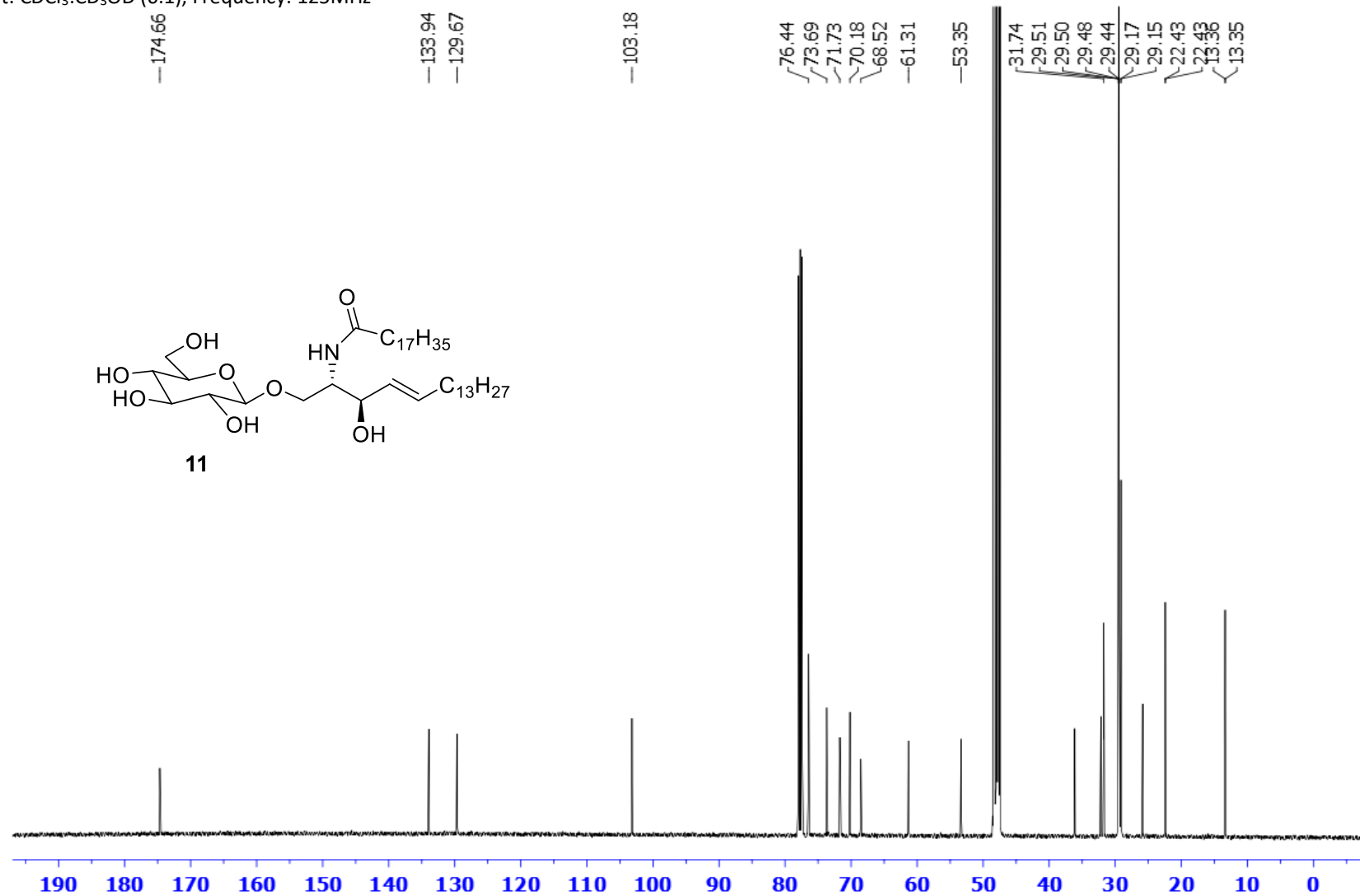


Figure S26. ¹³C-NMR (125 MHz, CD₃OD: CDCl₃) spectrum of compound 11.