molecules

MDPI

Supplementary material for the article:

Study on the synthesis, antioxidant properties, and self-assembly of carotenoid-flavonoid conjugates

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[3] University of Pécs, Faculty of Pharmacy, Department of Pharmacognosy, Rókus u. 2, H-7624 Pécs, Hungary
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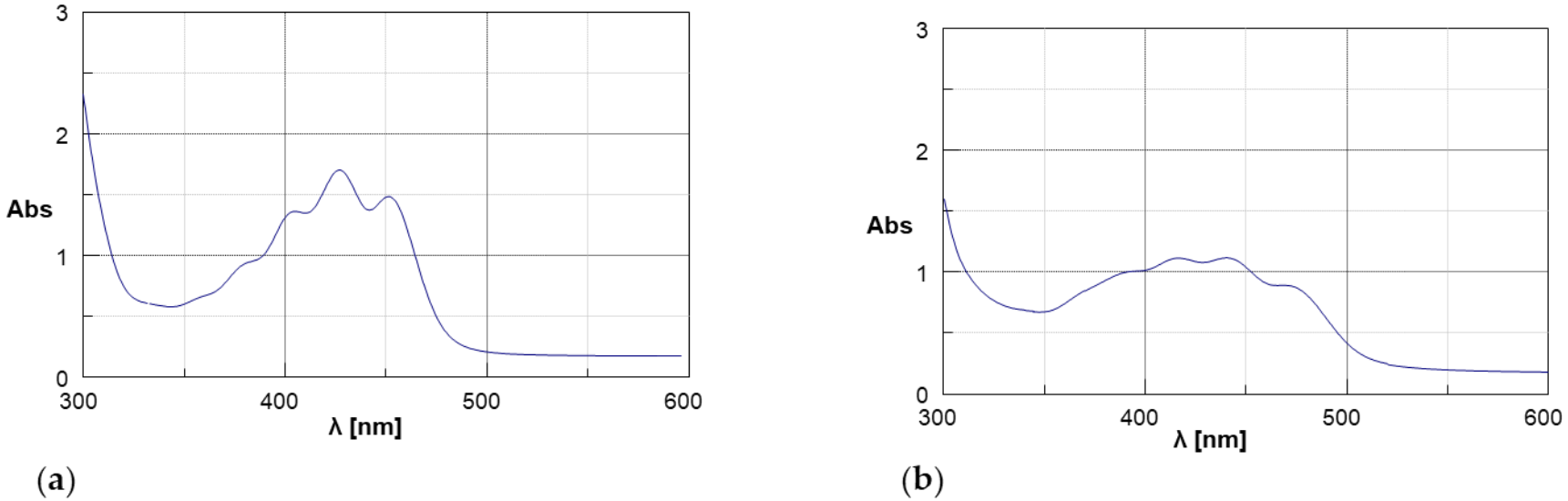


Figure S1. UV-vis spectra of daidzein-8′-apo-β-carotenol conjugate **(16)** in (**a**) acetone/ethanol 1:2; (**b**) acetone/ethanol/water 1:1:2.

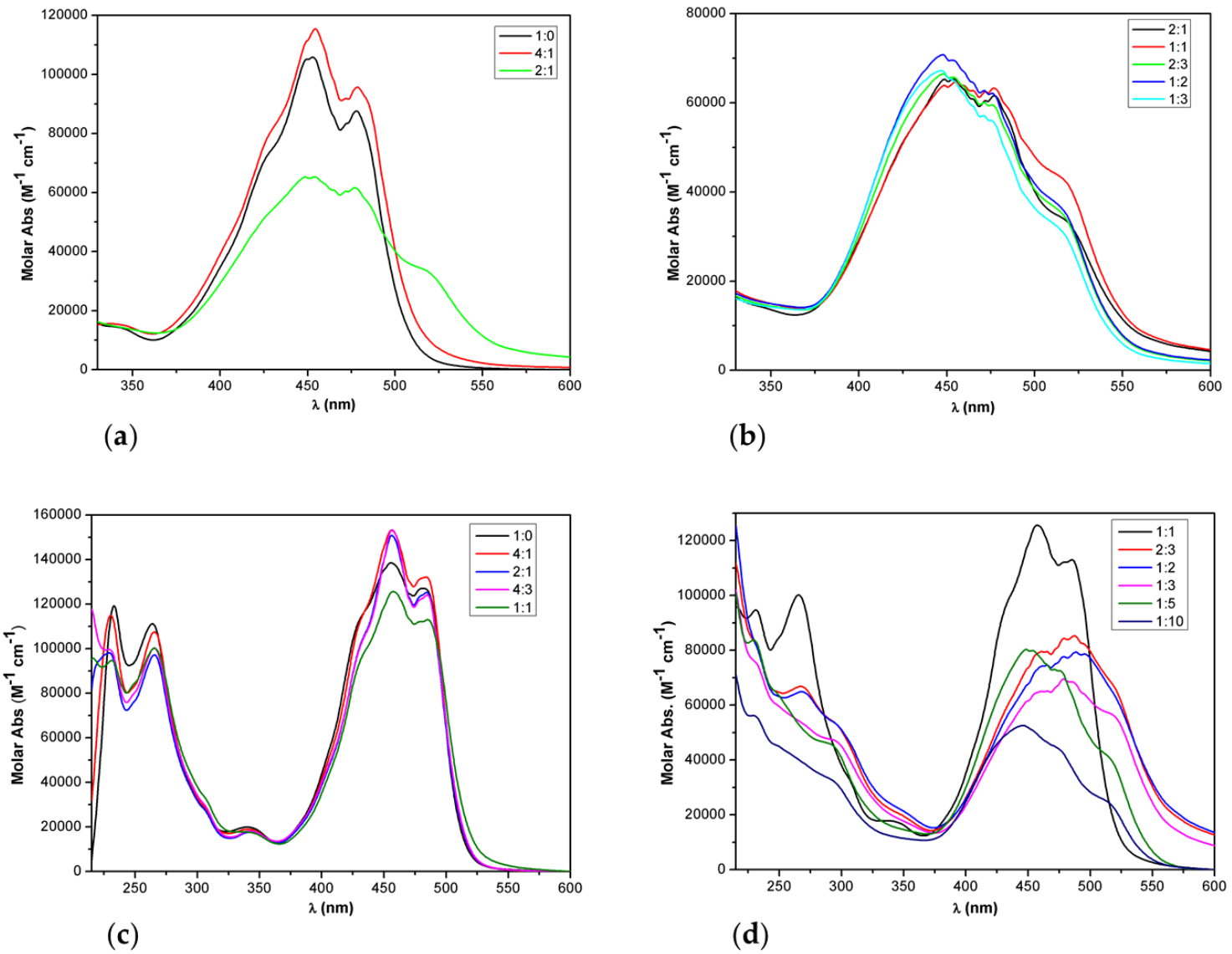


Figure S2. UV-vis spectra of ditriazole daidzein-zeaxanthin conjugate **(17)** in (**a**) acetone/water 1:0-2:1; (**b**) acetone/water 2:1-1:3 (**c**) THF/water 1:0-1:1. (**d**) THF/water 1:1-1:10.

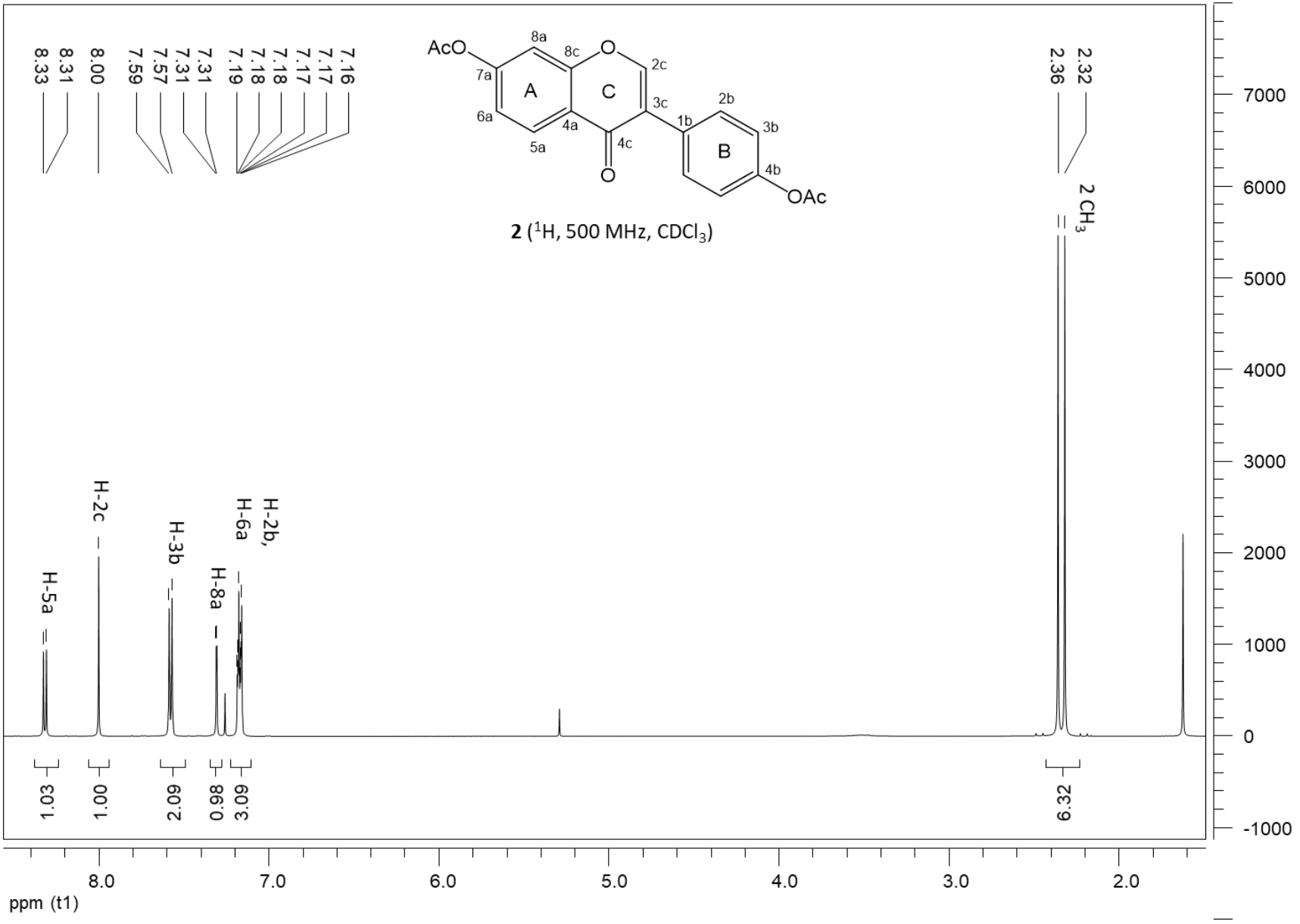


Figure S3. ^{1}H NMR spectrum of diacetyl daidzein (**2**)

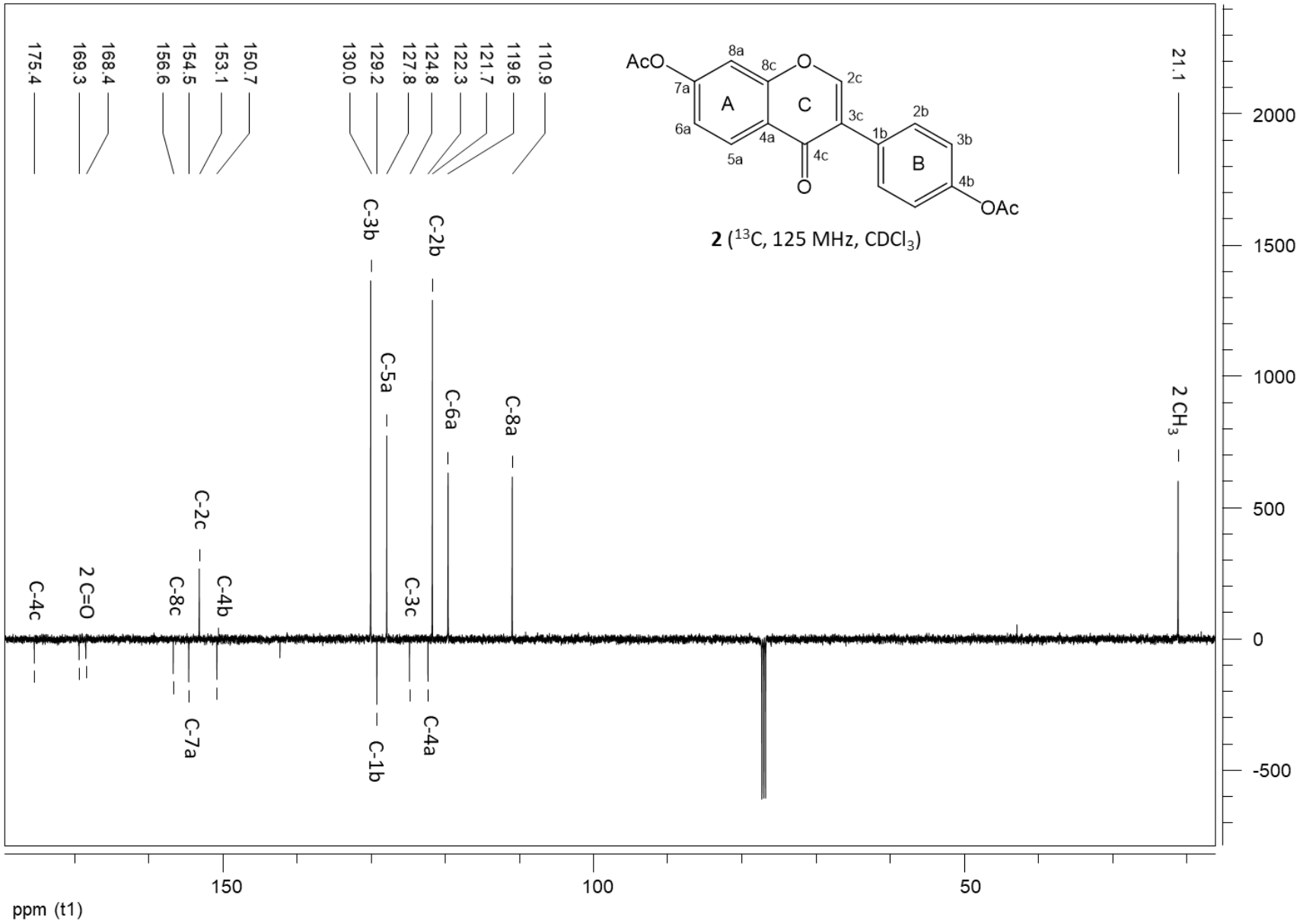


Figure S4. ^{13}C-apt NMR spectrum of diacetyl daidzein (**2**)

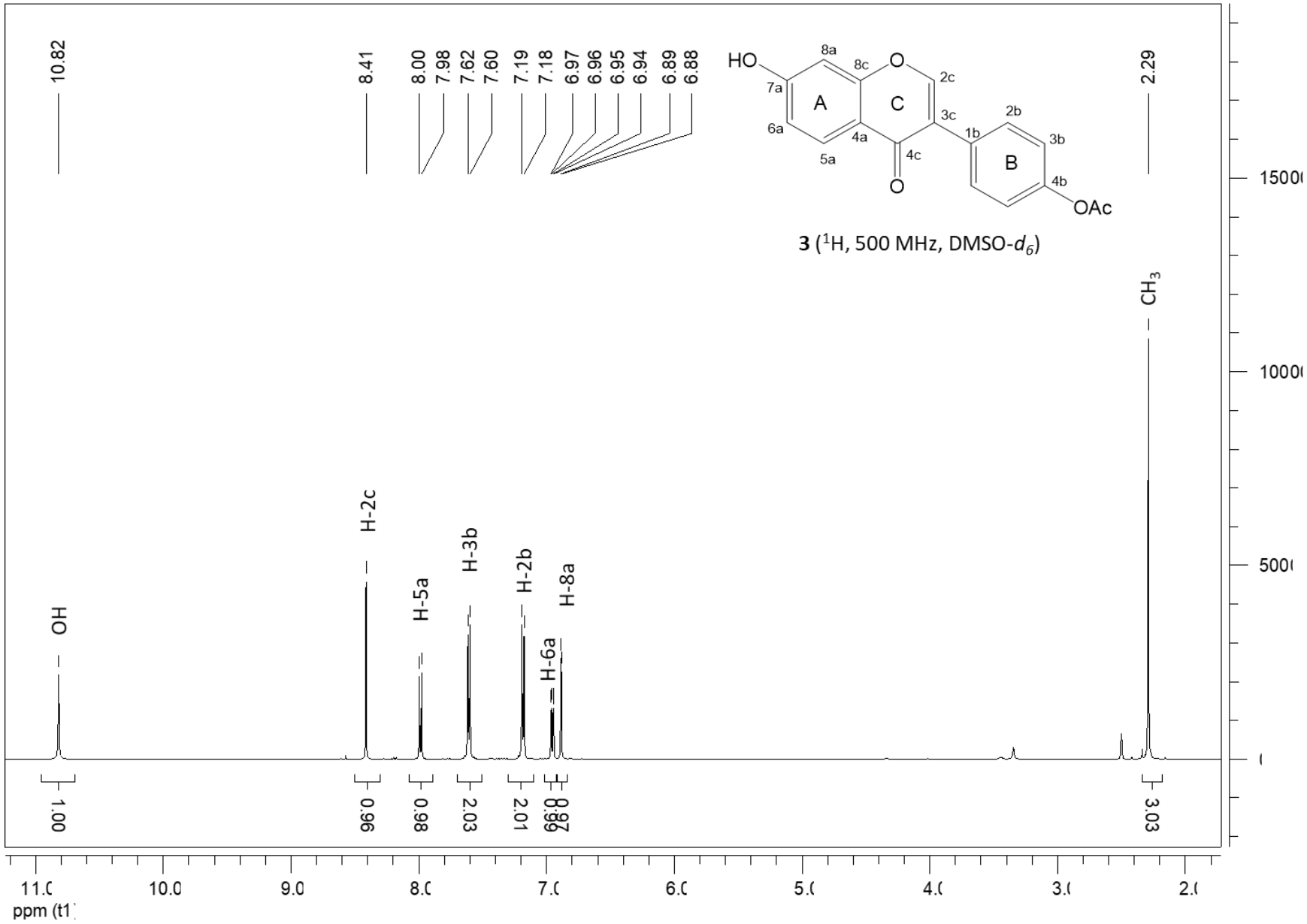


Figure S5. [1]H NMR spectrum of 4-acetyldaidzein (**3**)

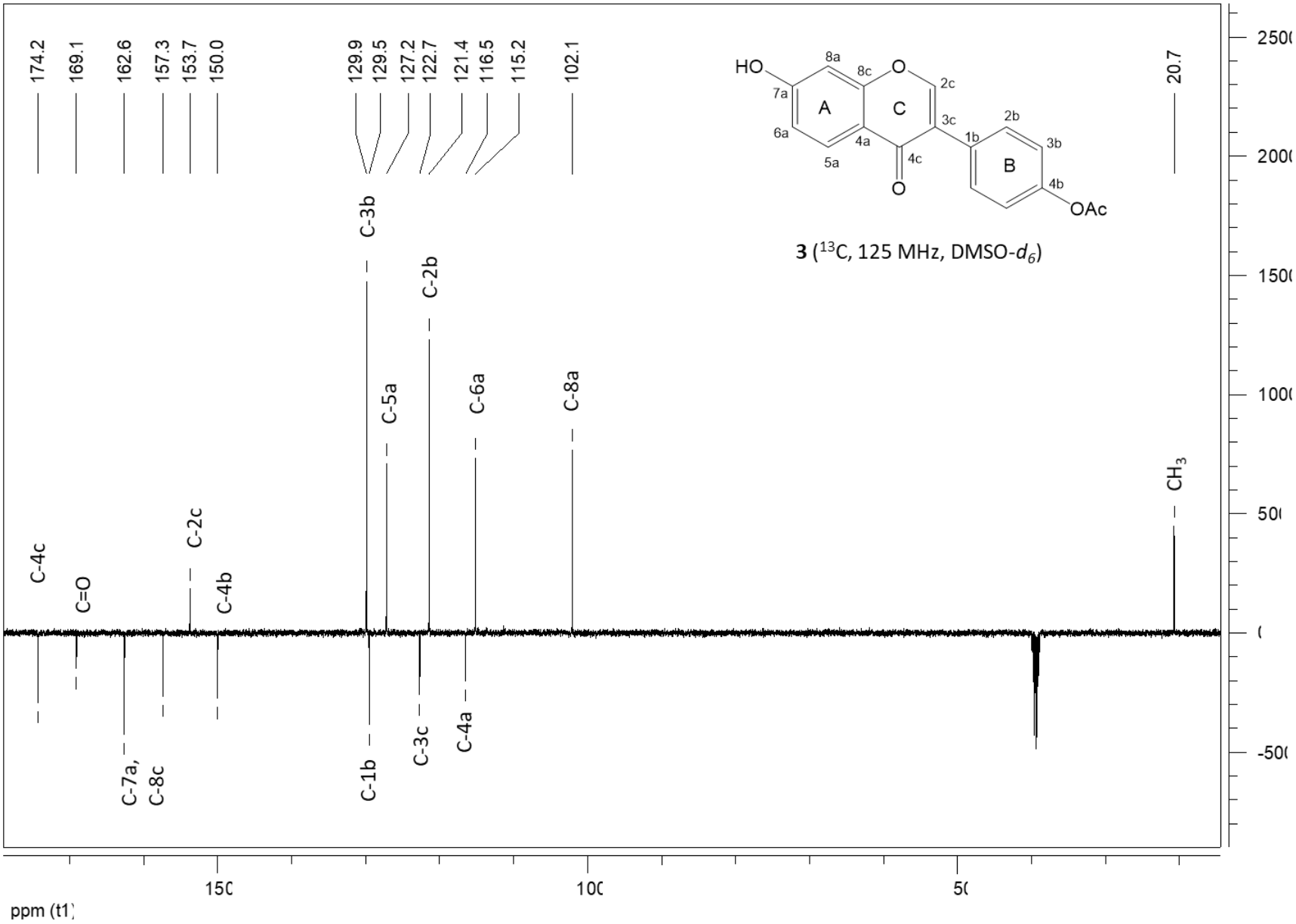


Figure S6. ^{13}C-apt NMR spectrum of 4-acetyldaidzein (**3**)

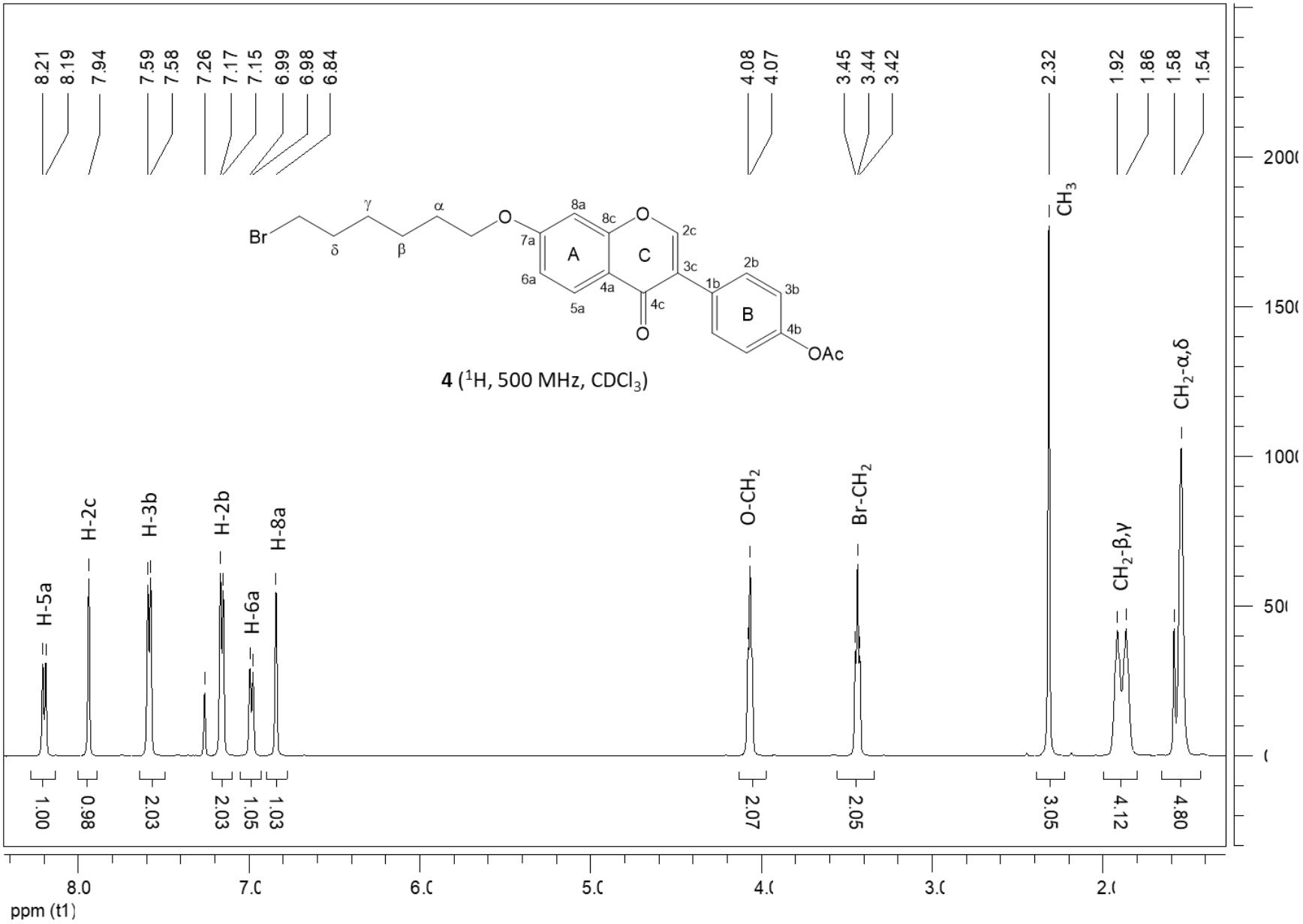


Figure S7. [1]H NMR spectrum of 7-bromohexyl-4-acetyldaidzein (**4**)

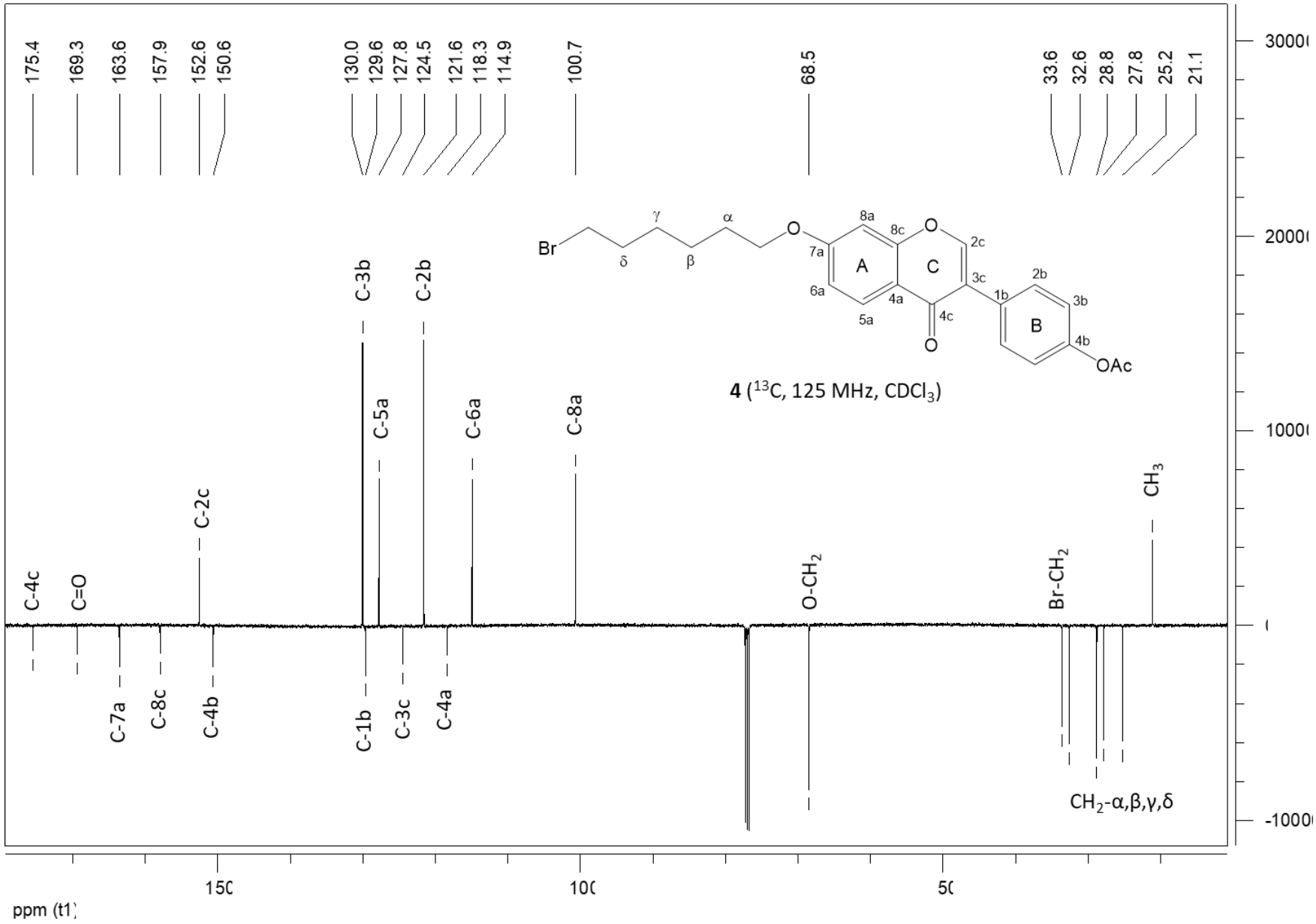


Figure S8. ^{13}C-apt NMR spectrum of 7-bromohexyl-4-acetyldaidzein (**4**)

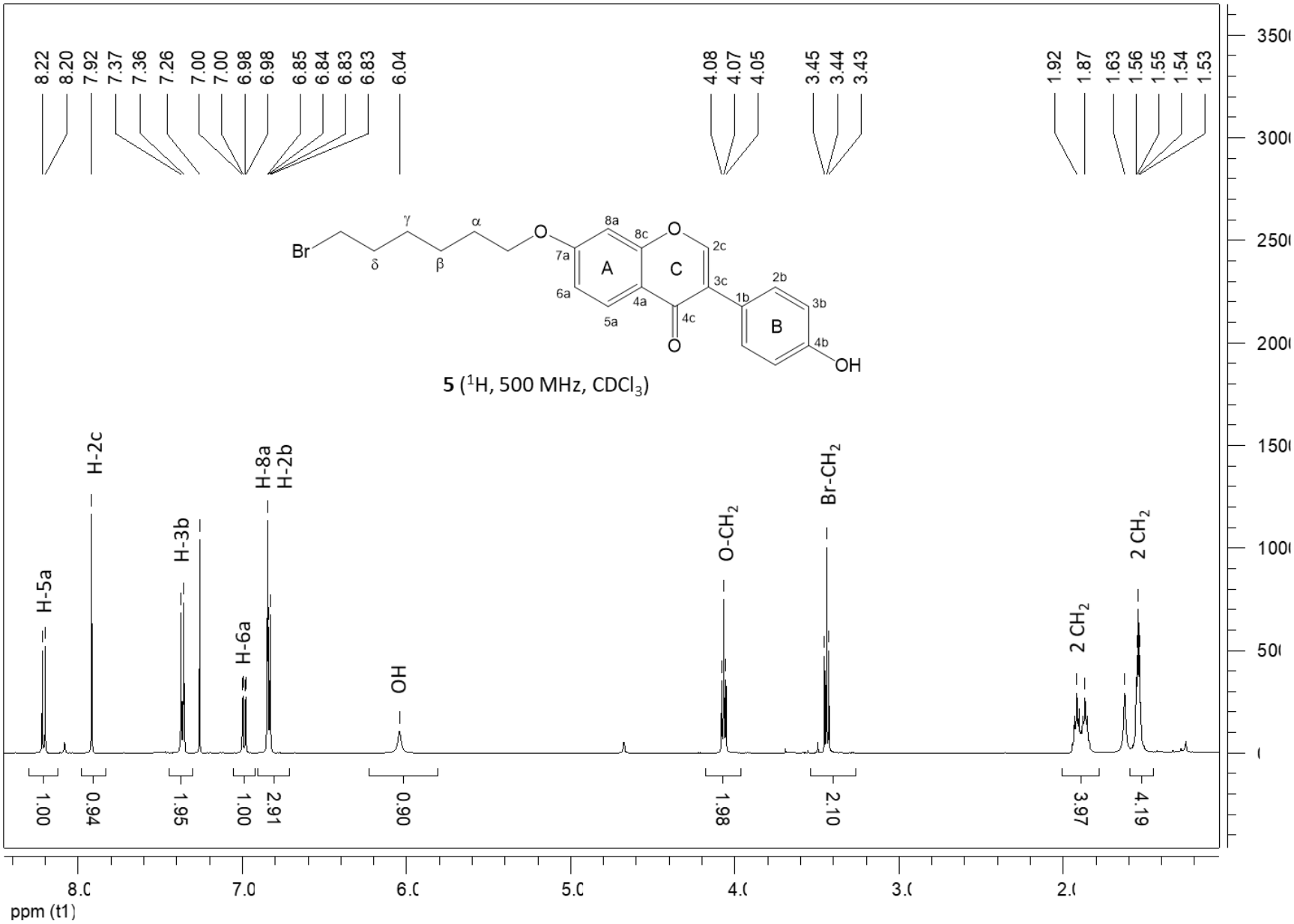


Figure S9. ^{1}H NMR spectrum of 7-bromohexyl-daidzein (**5**)

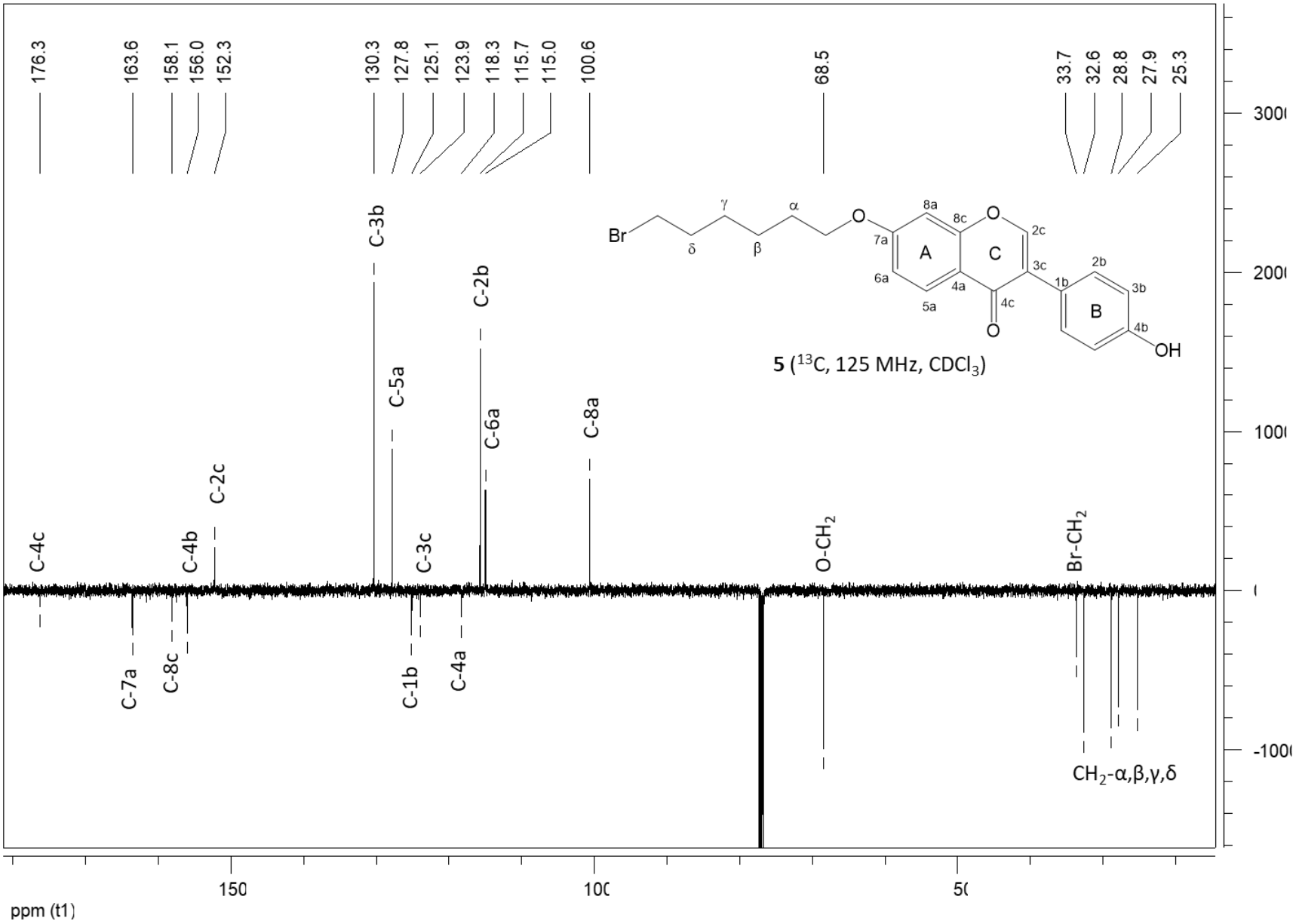


Figure S10. ^{13}C-apt NMR spectrum of 7-bromohexyl-daidzein (**5**)

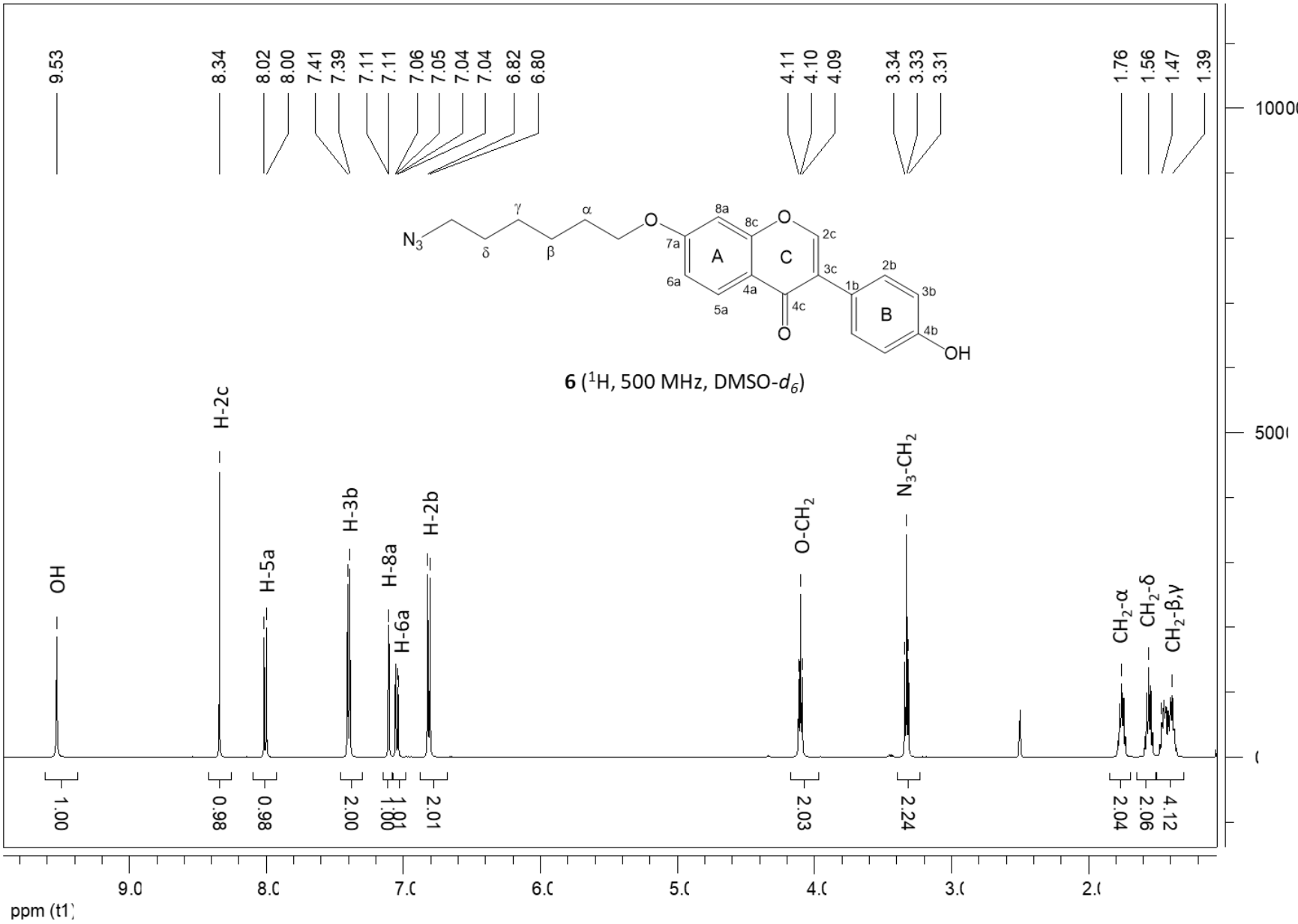


Figure S11. [1]H NMR spectrum of 7-azidohexyl-daidzein (**6**)

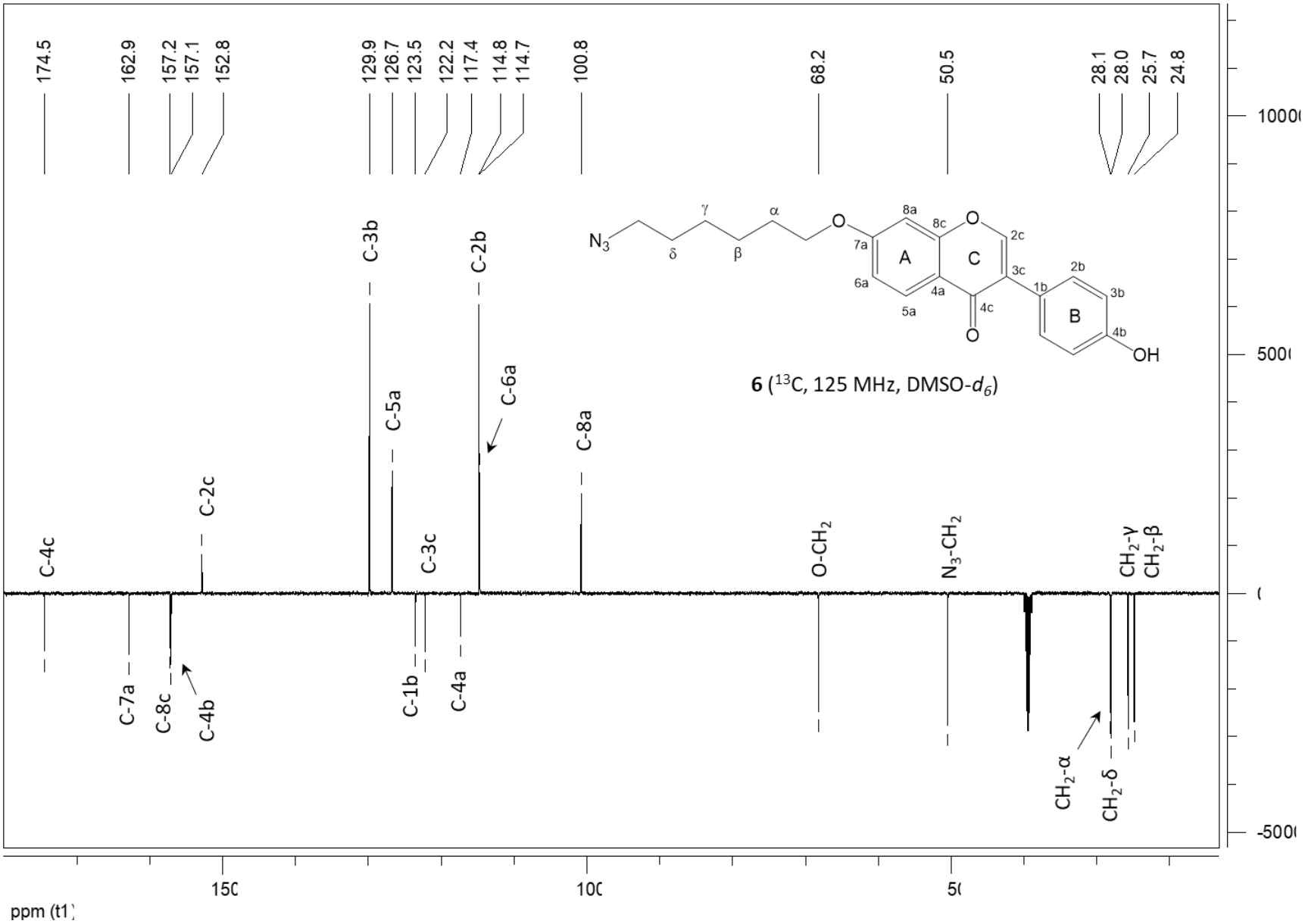


Figure S12. ^{13}C-apt NMR spectrum of 7-azidohexyl-daidzein (**6**)

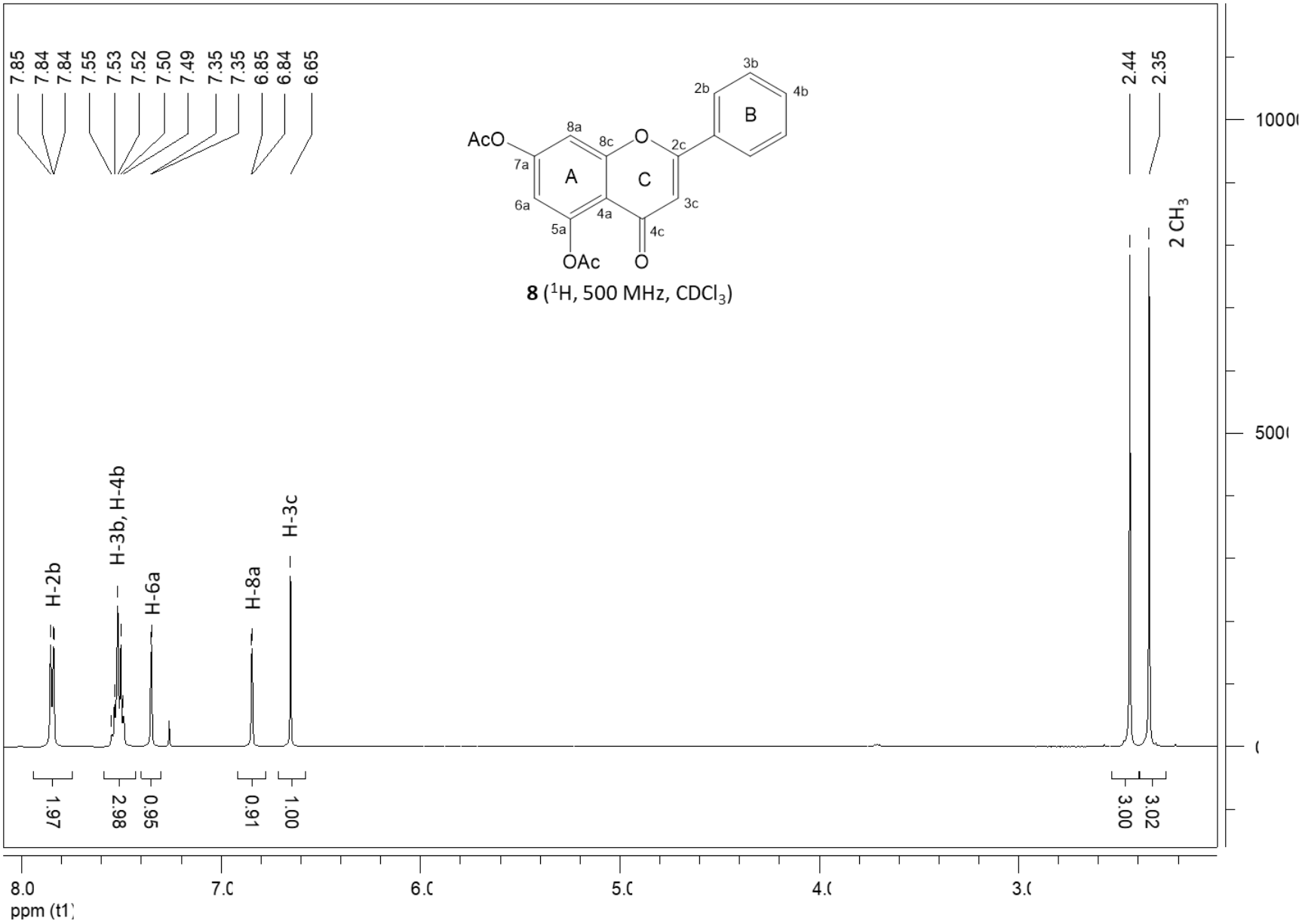


Figure S13. [1]H NMR spectrum of diacetyl chrysin (**8**)

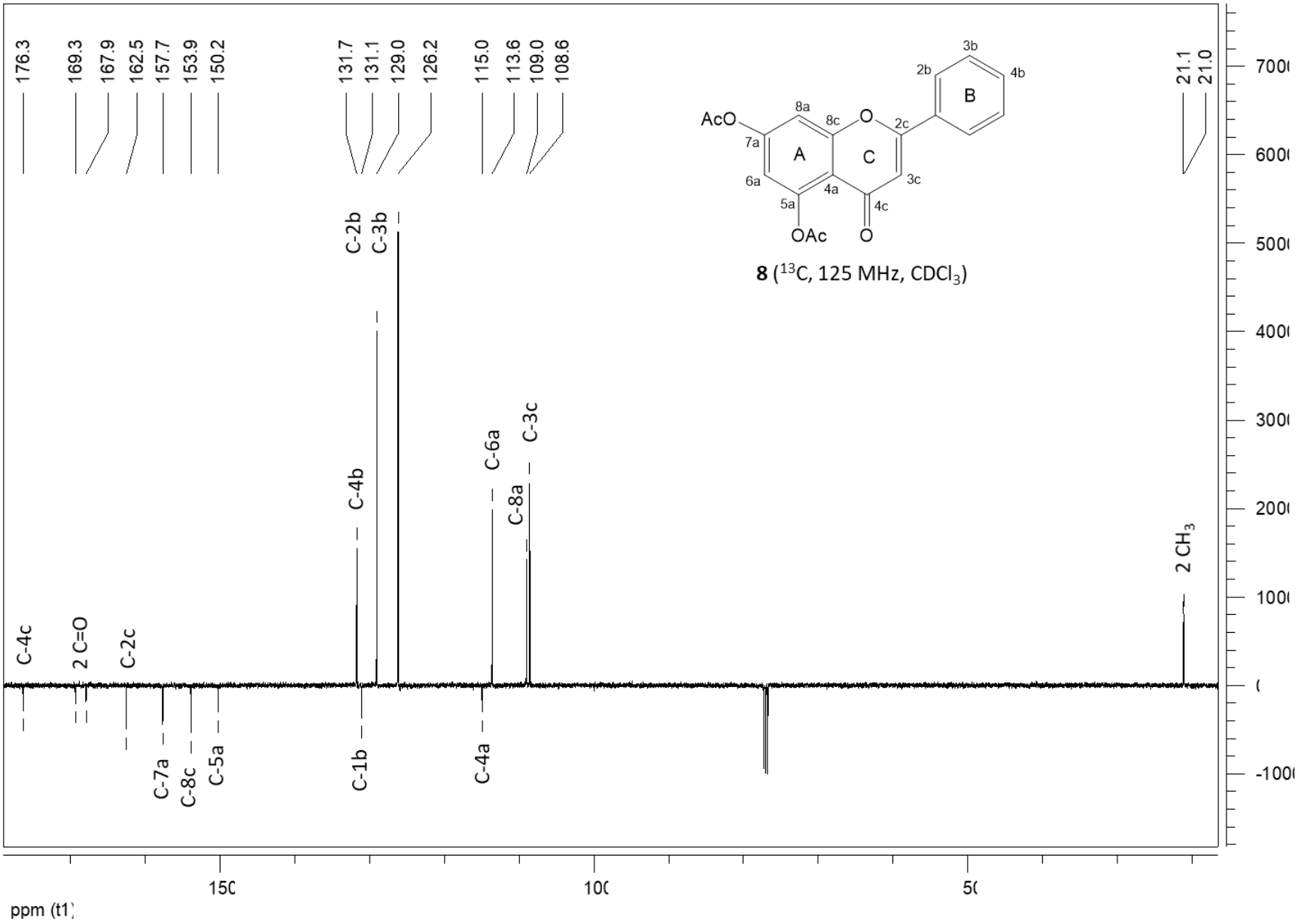


Figure S14. ^{13}C-apt NMR spectrum of diacetyl chrysin (**8**)

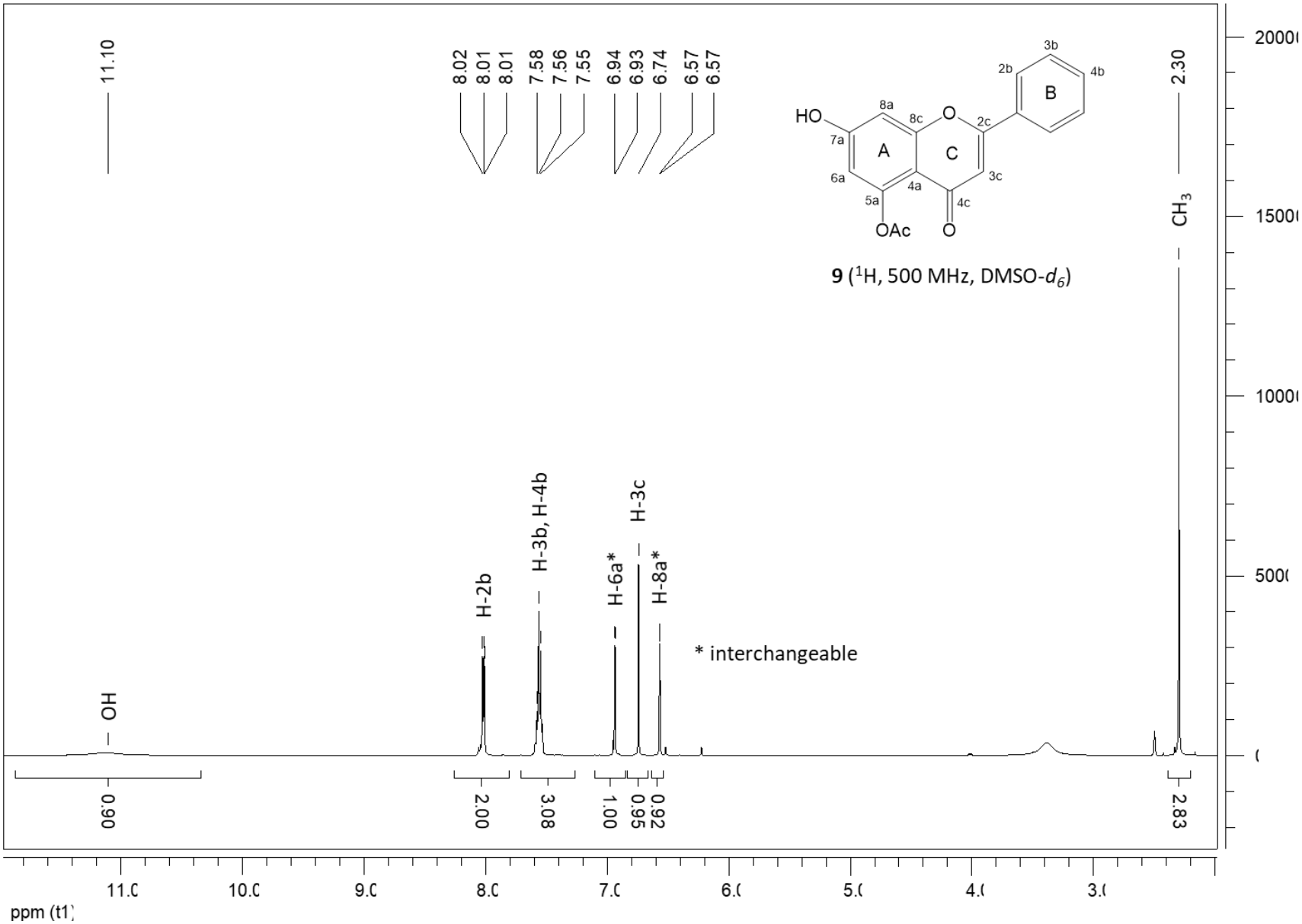


Figure S15. [1]H NMR spectrum of 5-acetylchrysin (**9**)

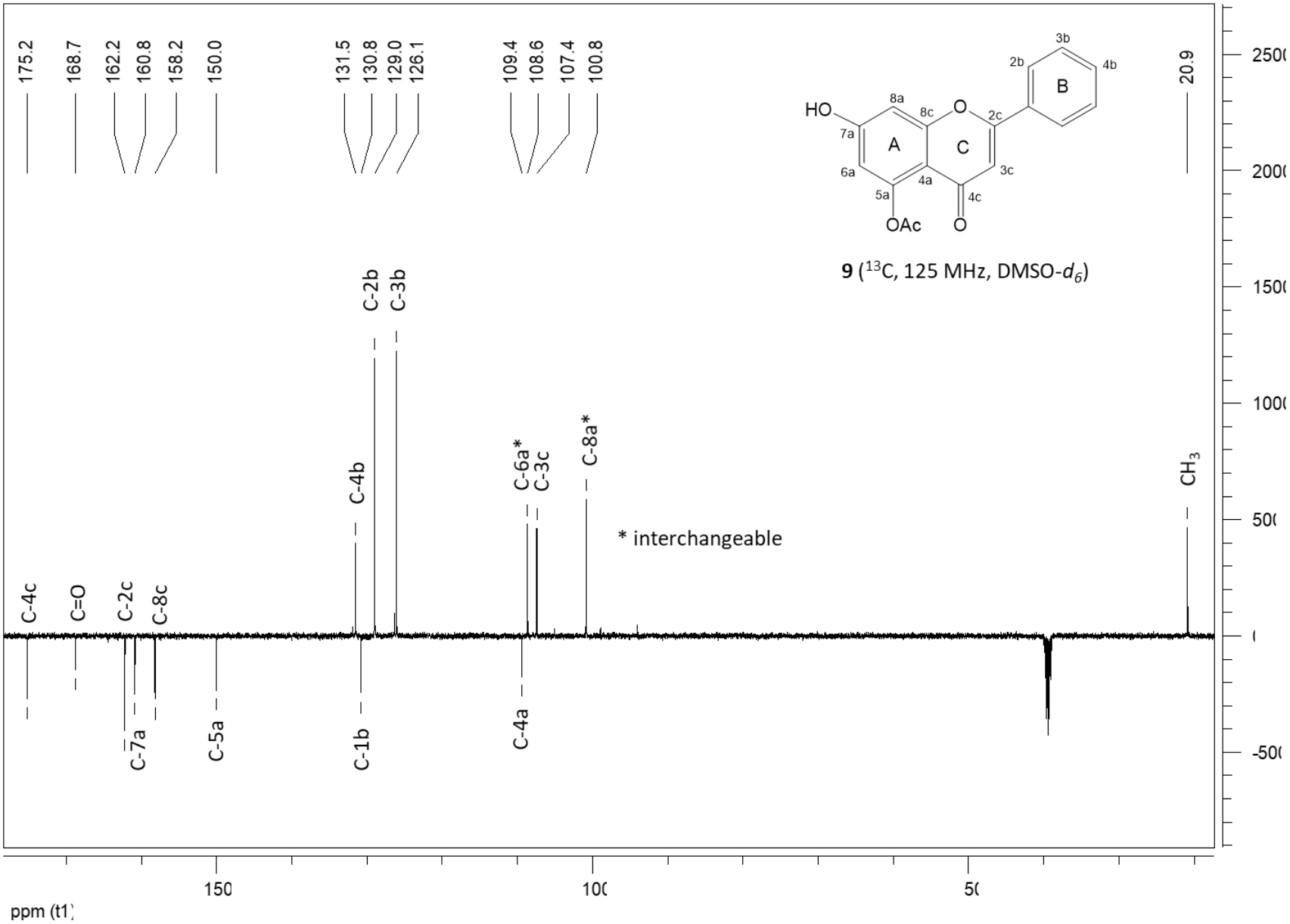


Figure S16. [13]C-apt NMR spectrum of 5-acetylchrysin (**9**)

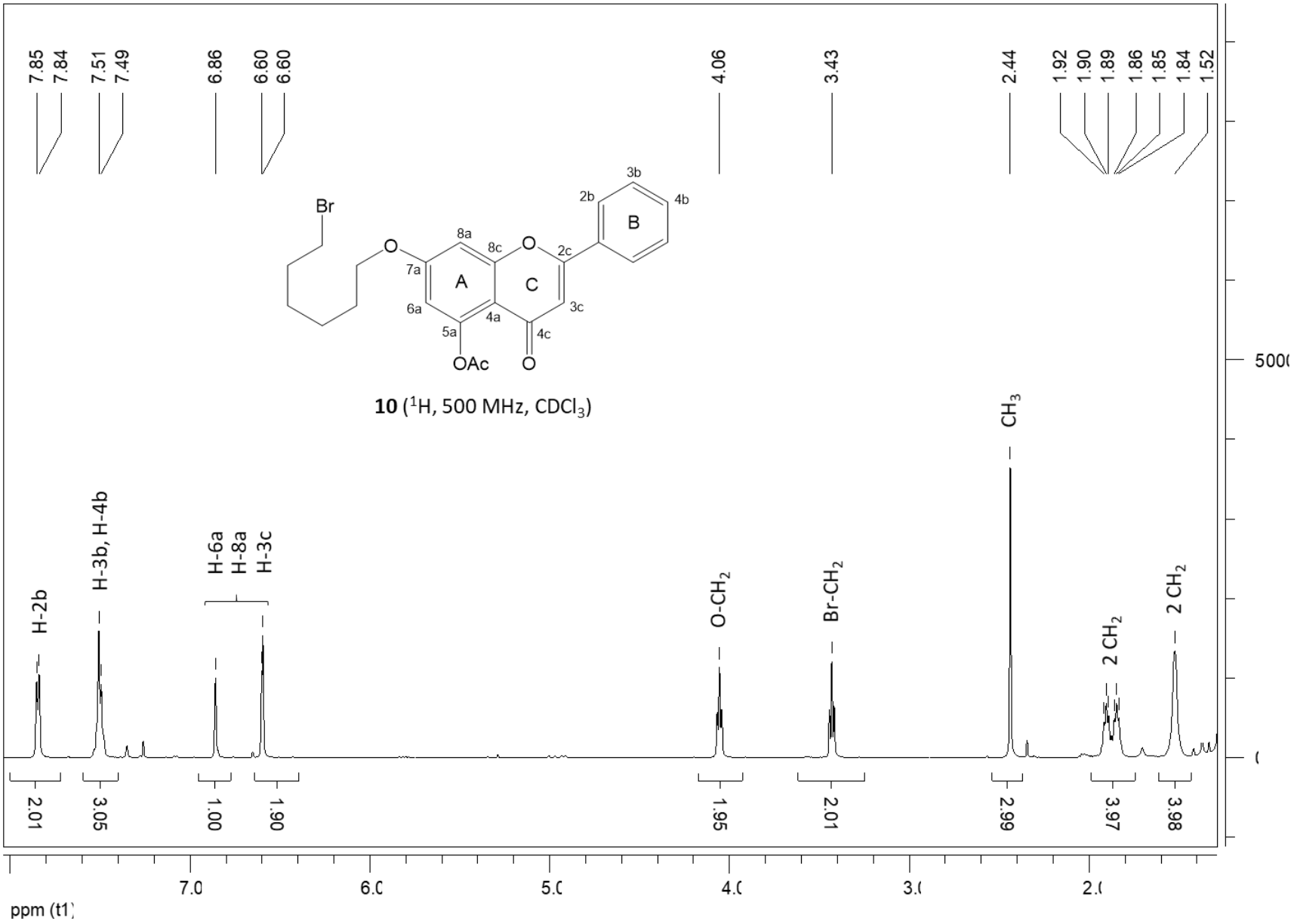


Figure S17. [1]H NMR spectrum of 7-bromohexyl-5-acetylchrysin (**10**)

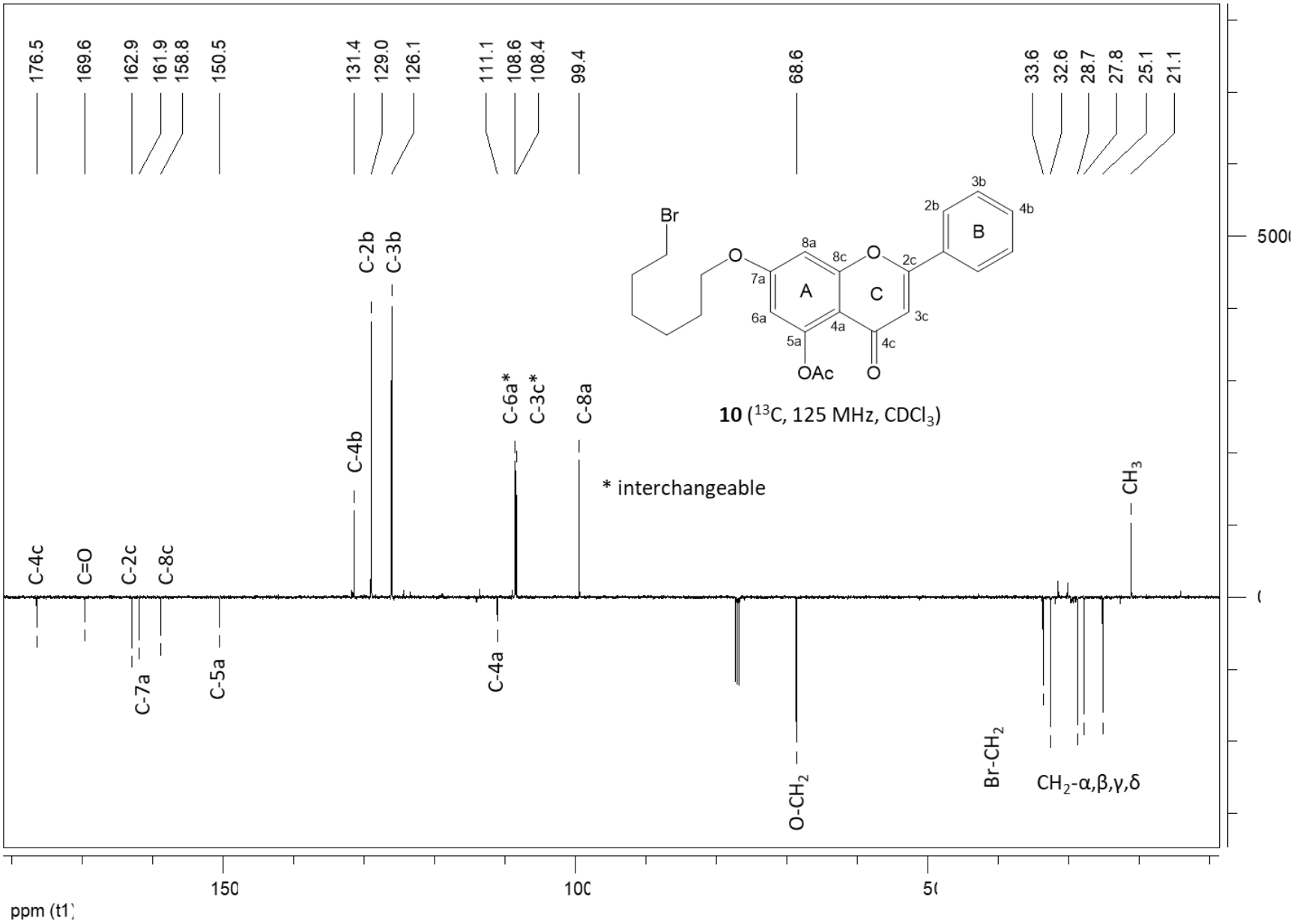


Figure S18. ^{13}C-apt NMR spectrum of 7-bromohexyl-5-acetylchrysin (**10**)

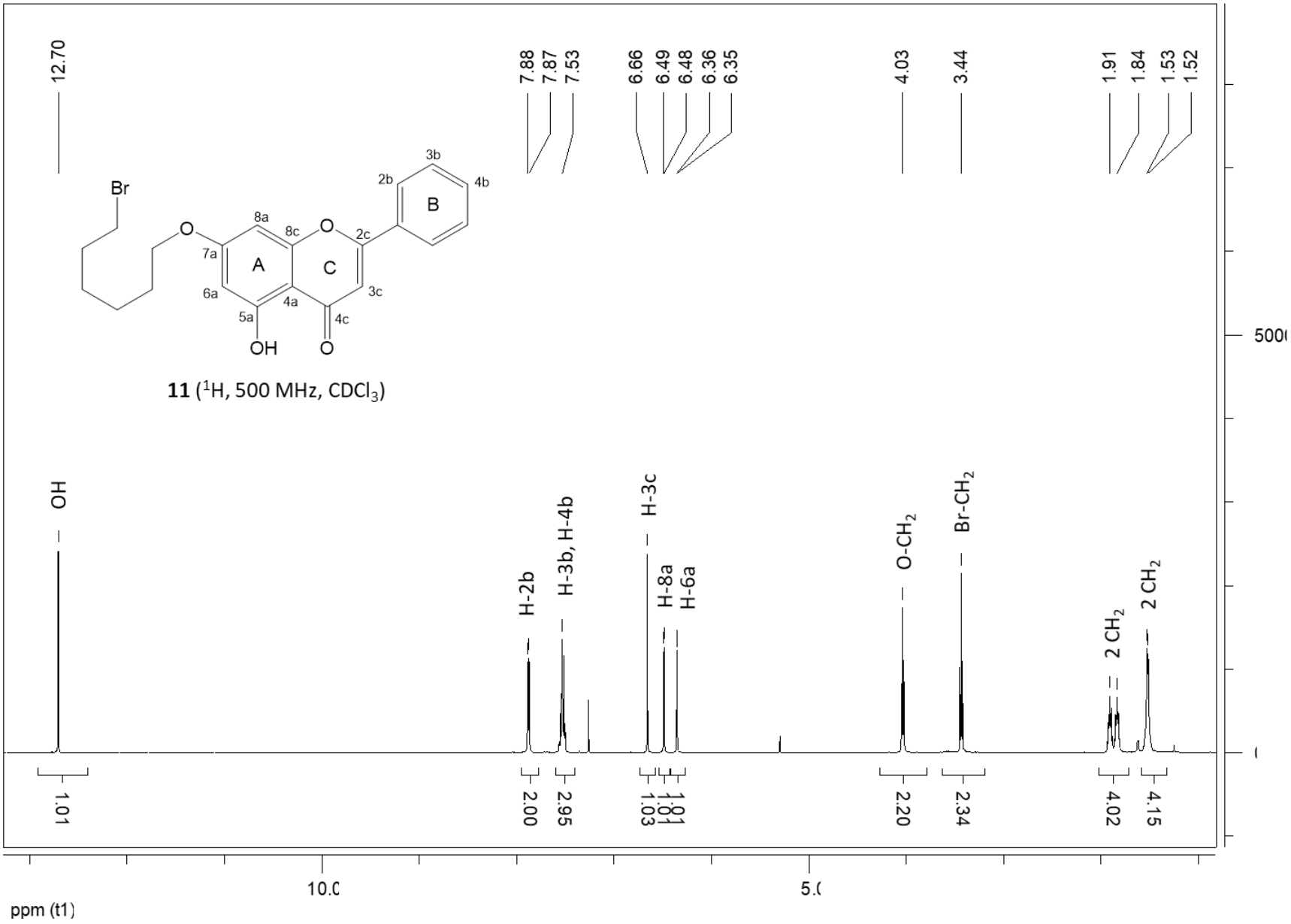


Figure S19. [1]H NMR spectrum of 7-bromohexyl-chrysin (**11**)

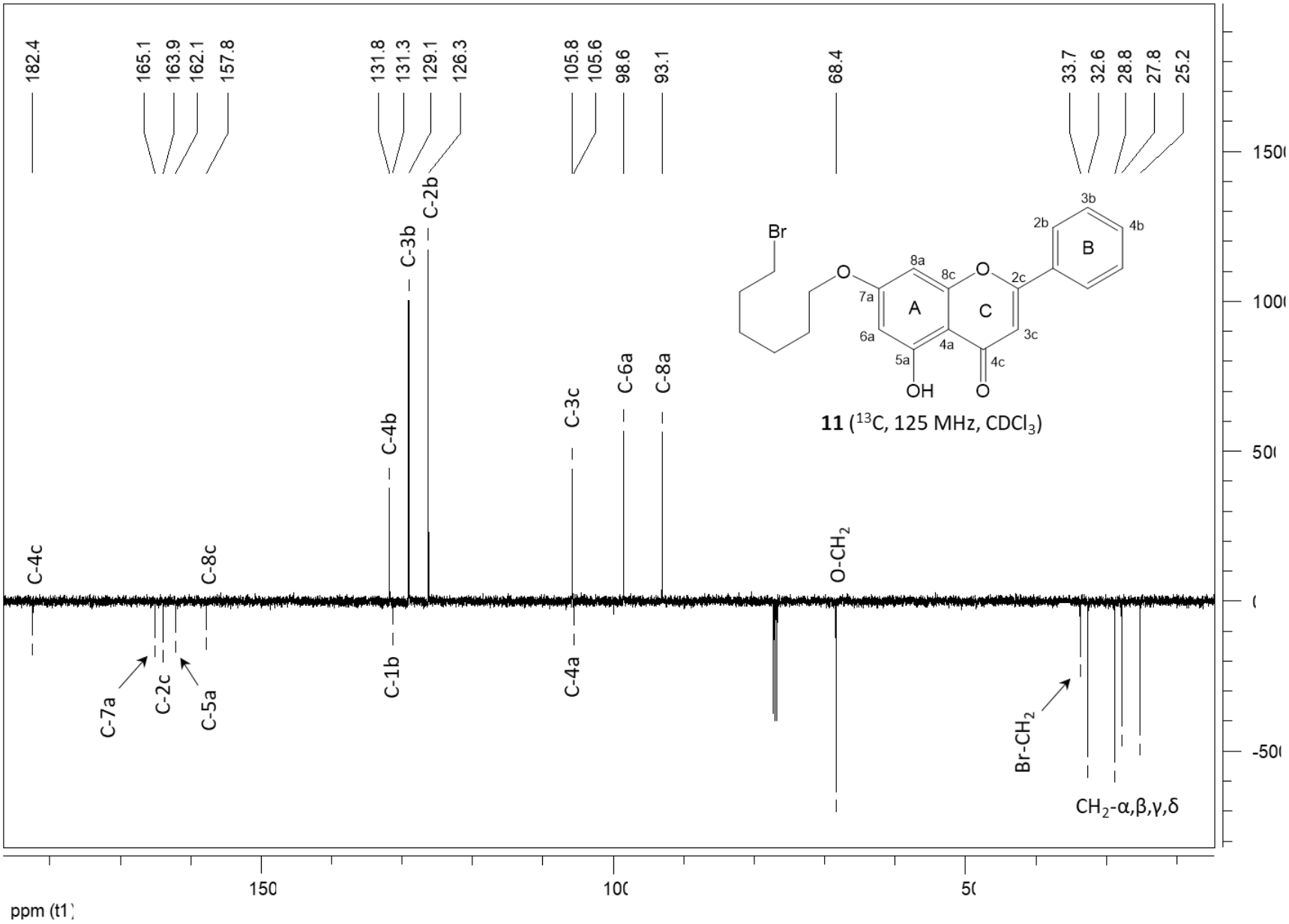


Figure S20. ^{13}C-apt NMR spectrum of 7-bromohexyl-chrysin (**11**)

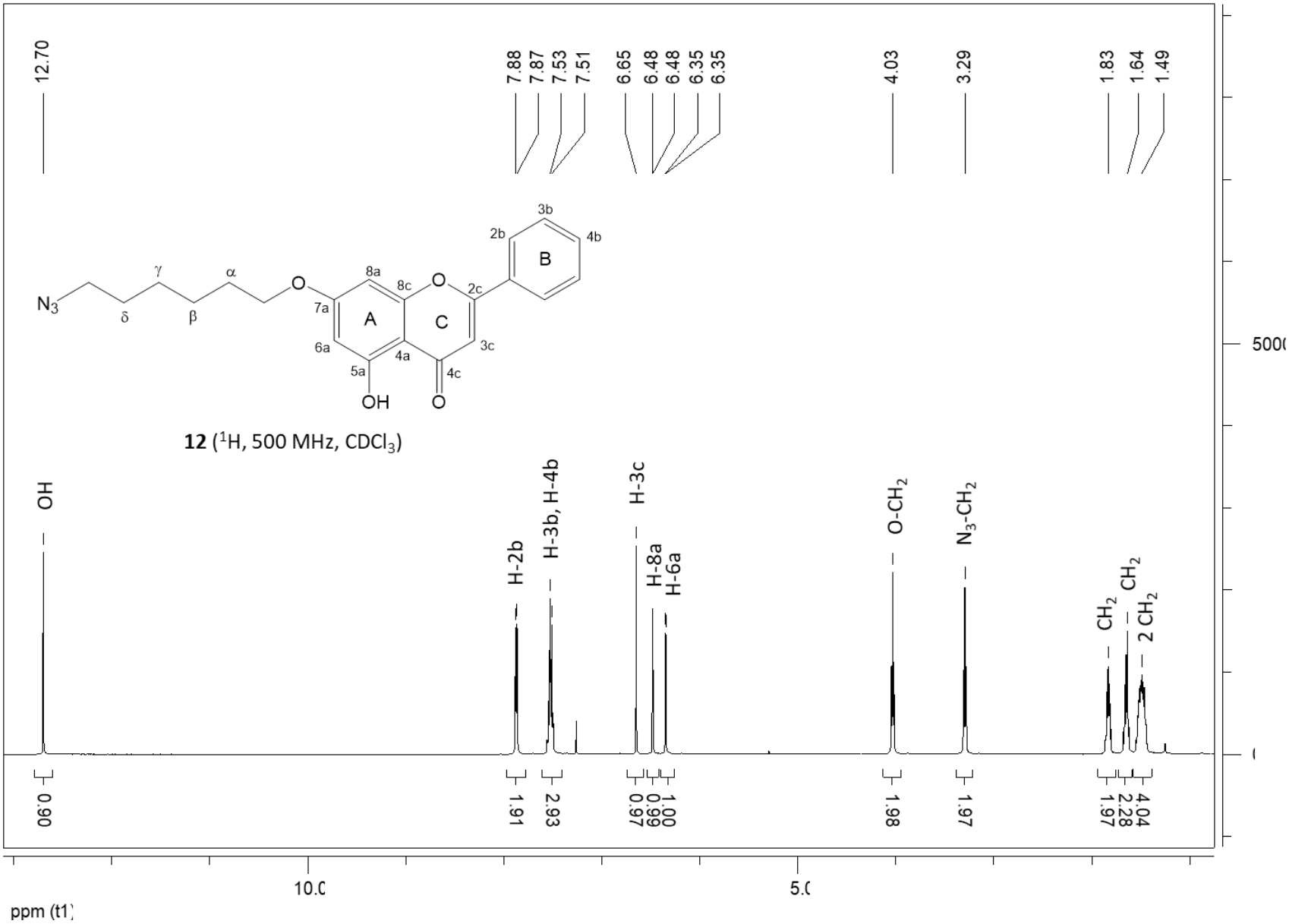


Figure S21. [1]H NMR spectrum of 7-azidohexyl-chrysin (**12**)

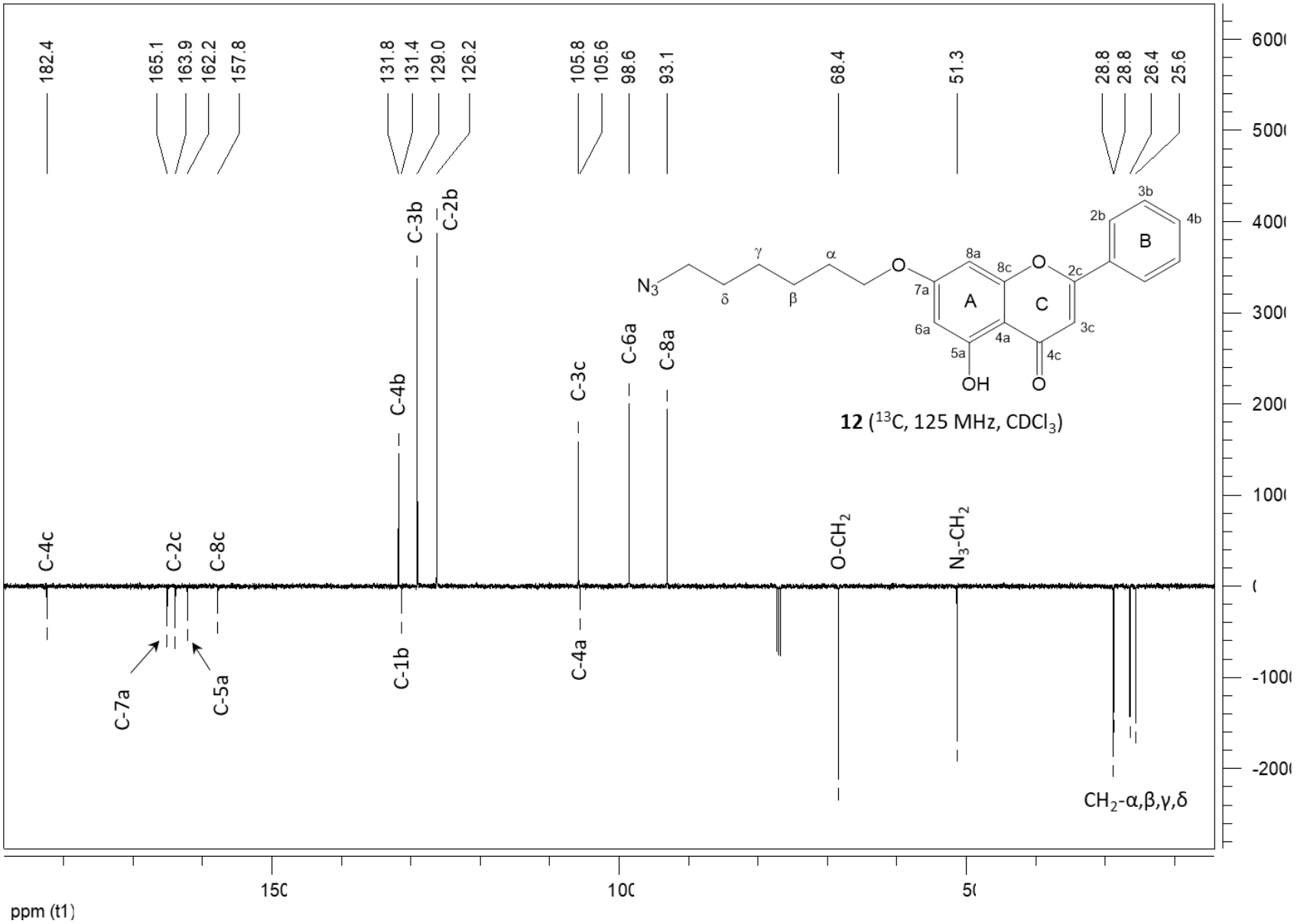


Figure S22. ^{13}C-apt NMR spectrum of 7-azidohexyl-chrysin (**12**)

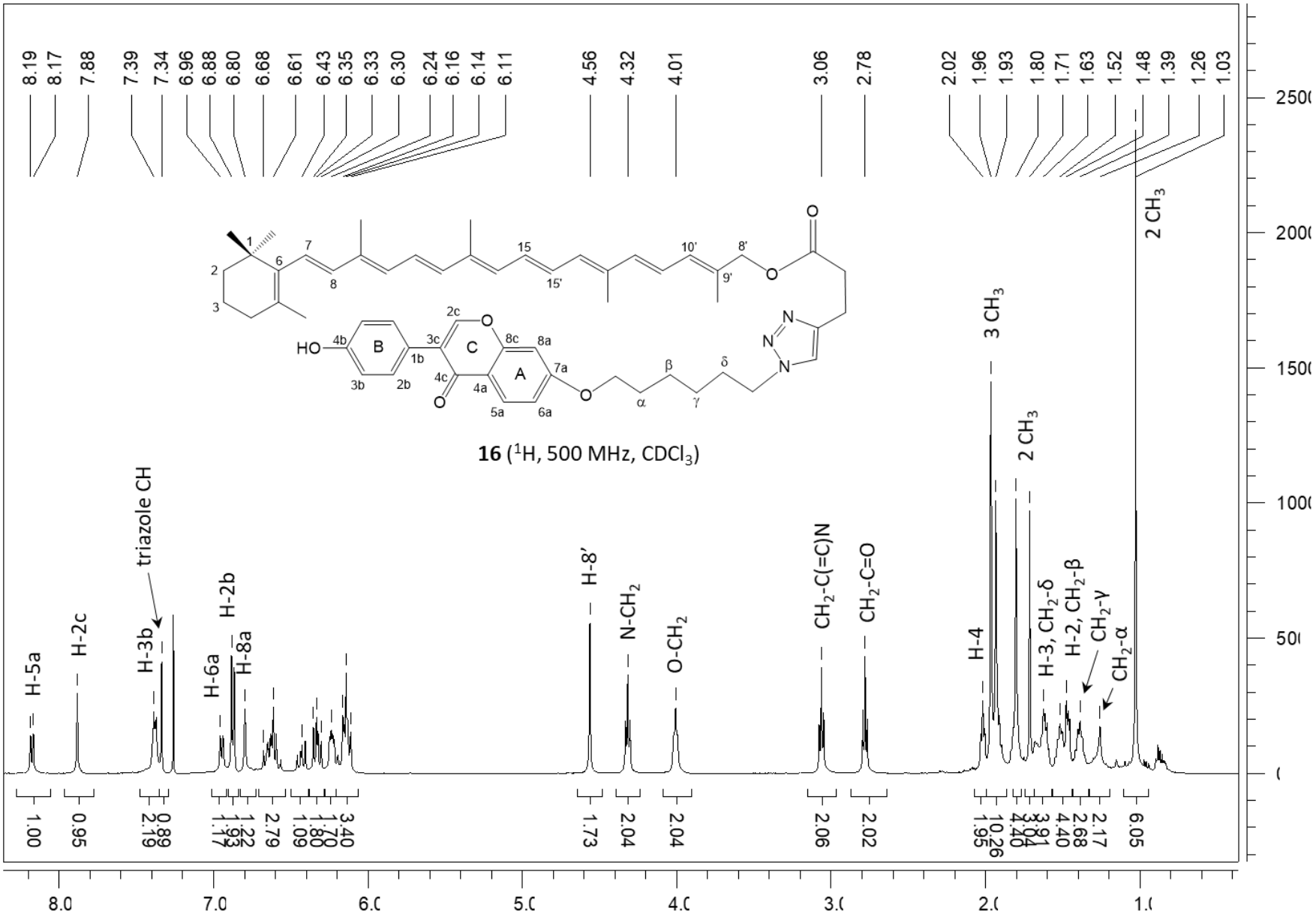


Figure S23.a. [1]H NMR spectrum of daidzein-8′-apo-β-carotenol conjugate (**16**)

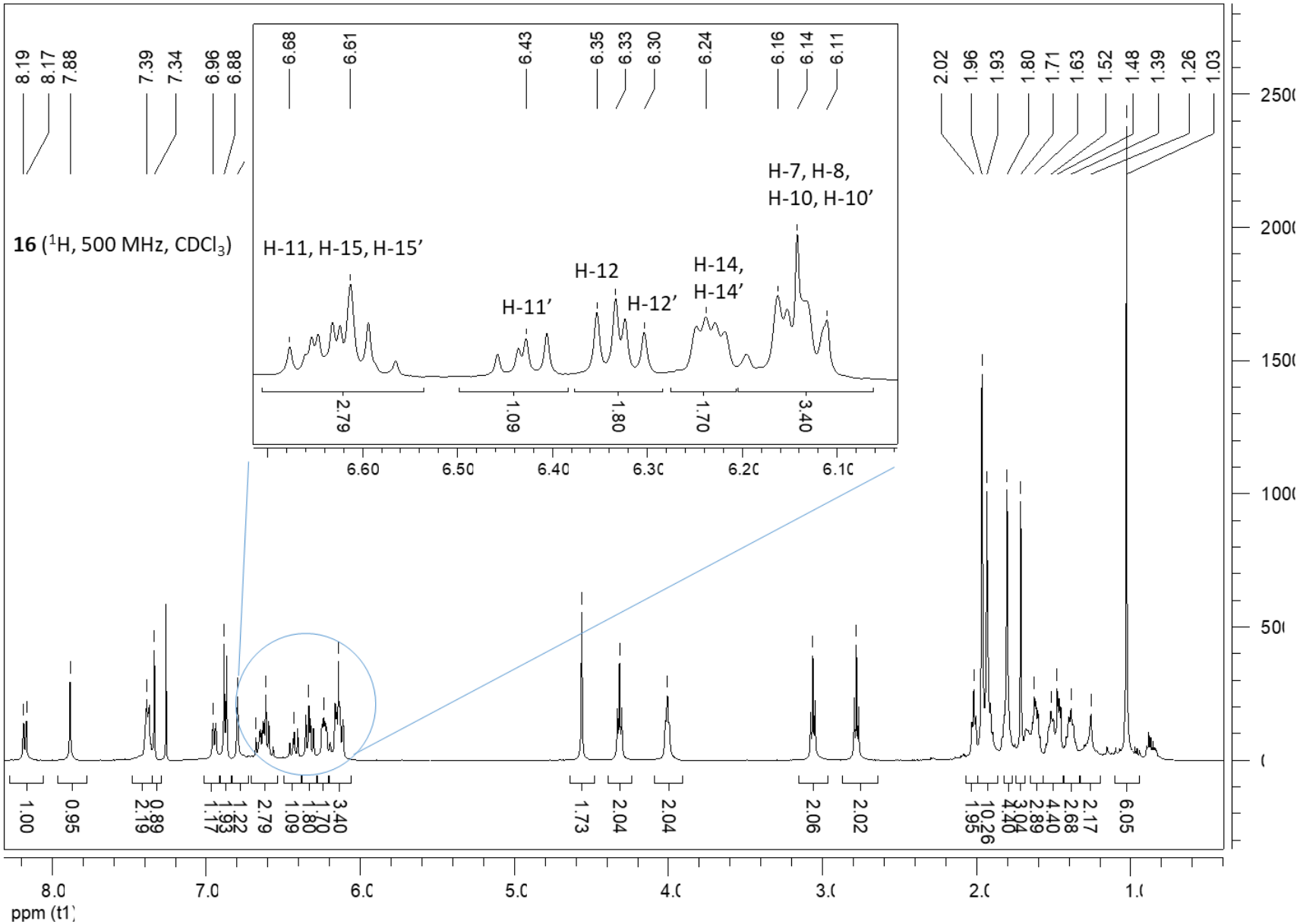


Figure S23.b. ^{1}H NMR spectrum of daidzein-8′-apo-β-carotenol conjugate (**16**)

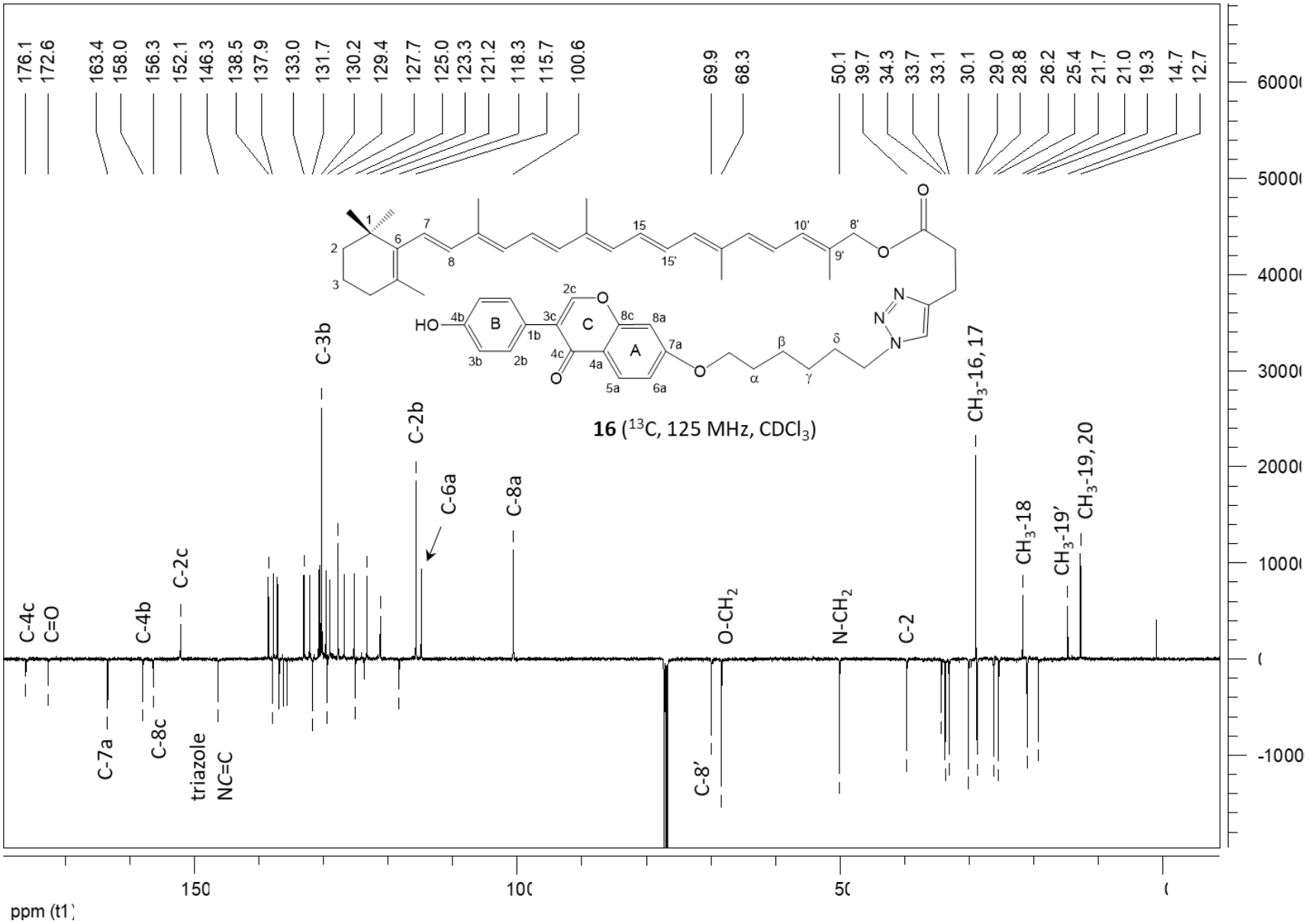


Figure S24.a. ^{13}C-apt NMR spectrum of daidzein-8′-apo-β-carotenol conjugate (**16**)

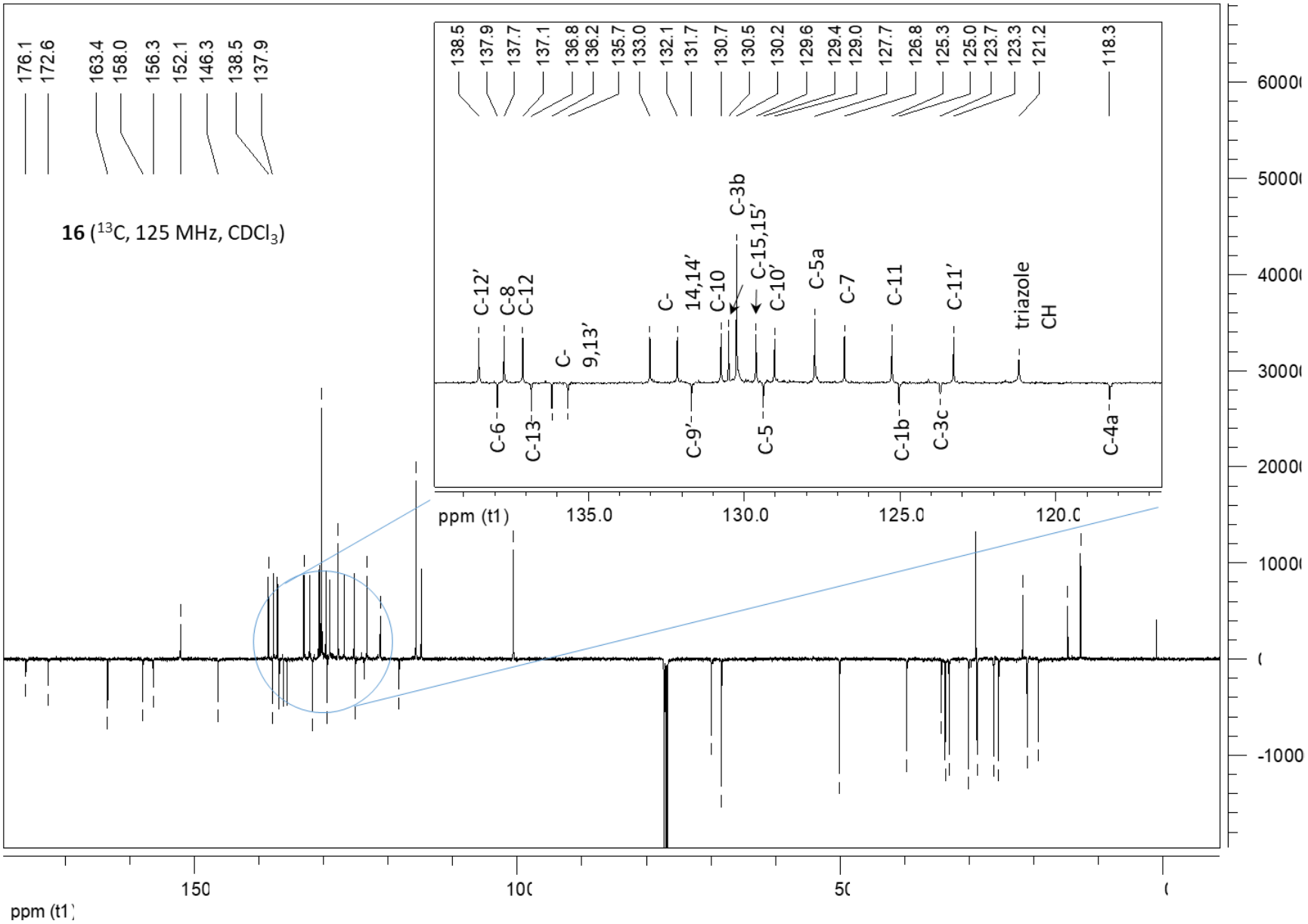


Figure S24.b. [13]C-apt NMR spectrum of daidzein-8′-apo-β-carotenol conjugate (**16**)

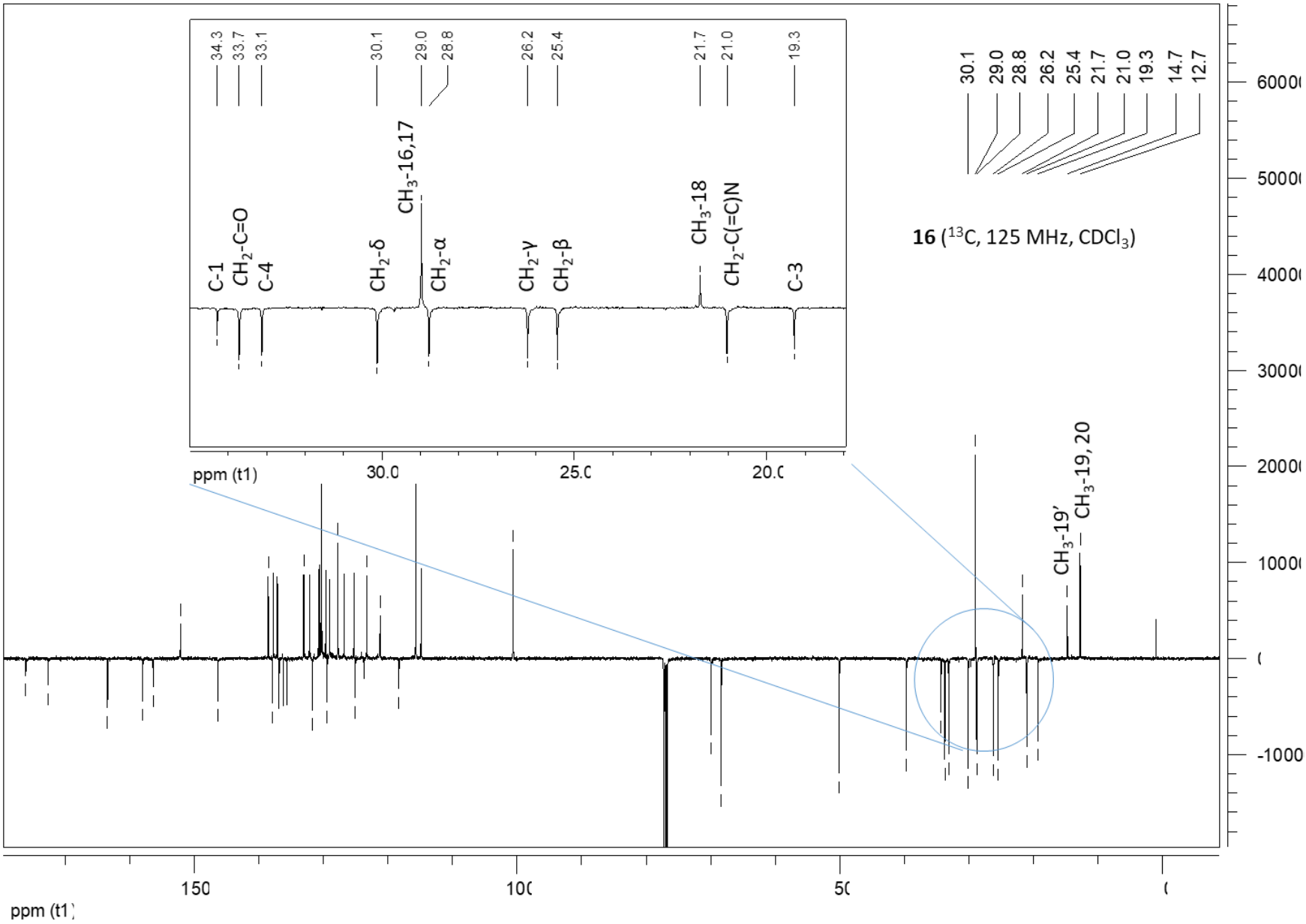


Figure S24.c. ^{13}C-apt NMR spectrum of daidzein-8′-apo-β-carotenol conjugate (**16**)

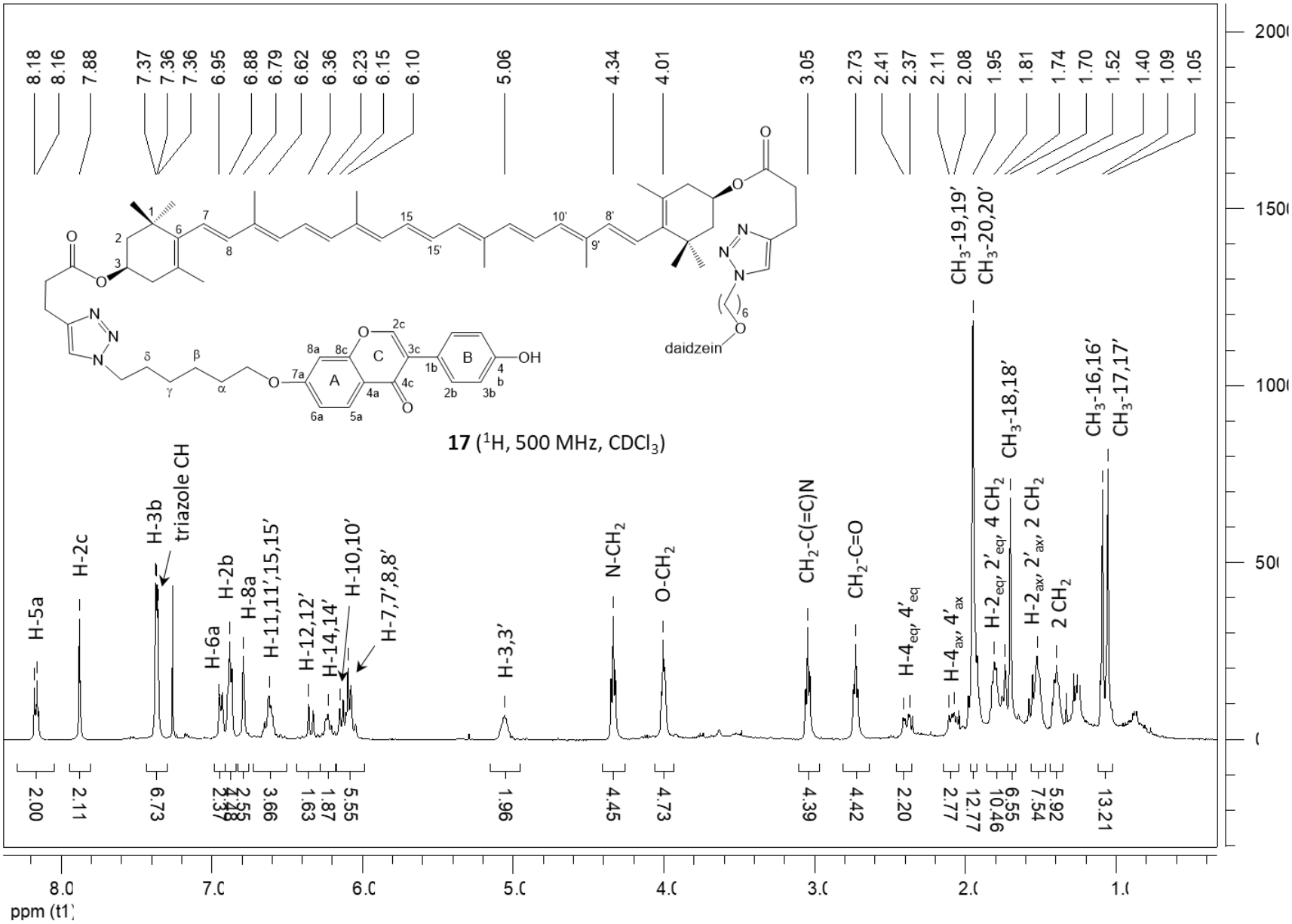


Figure S25. [1]H NMR spectrum of *bis*-daidzein-zeaxanthin conjugate (**17**)

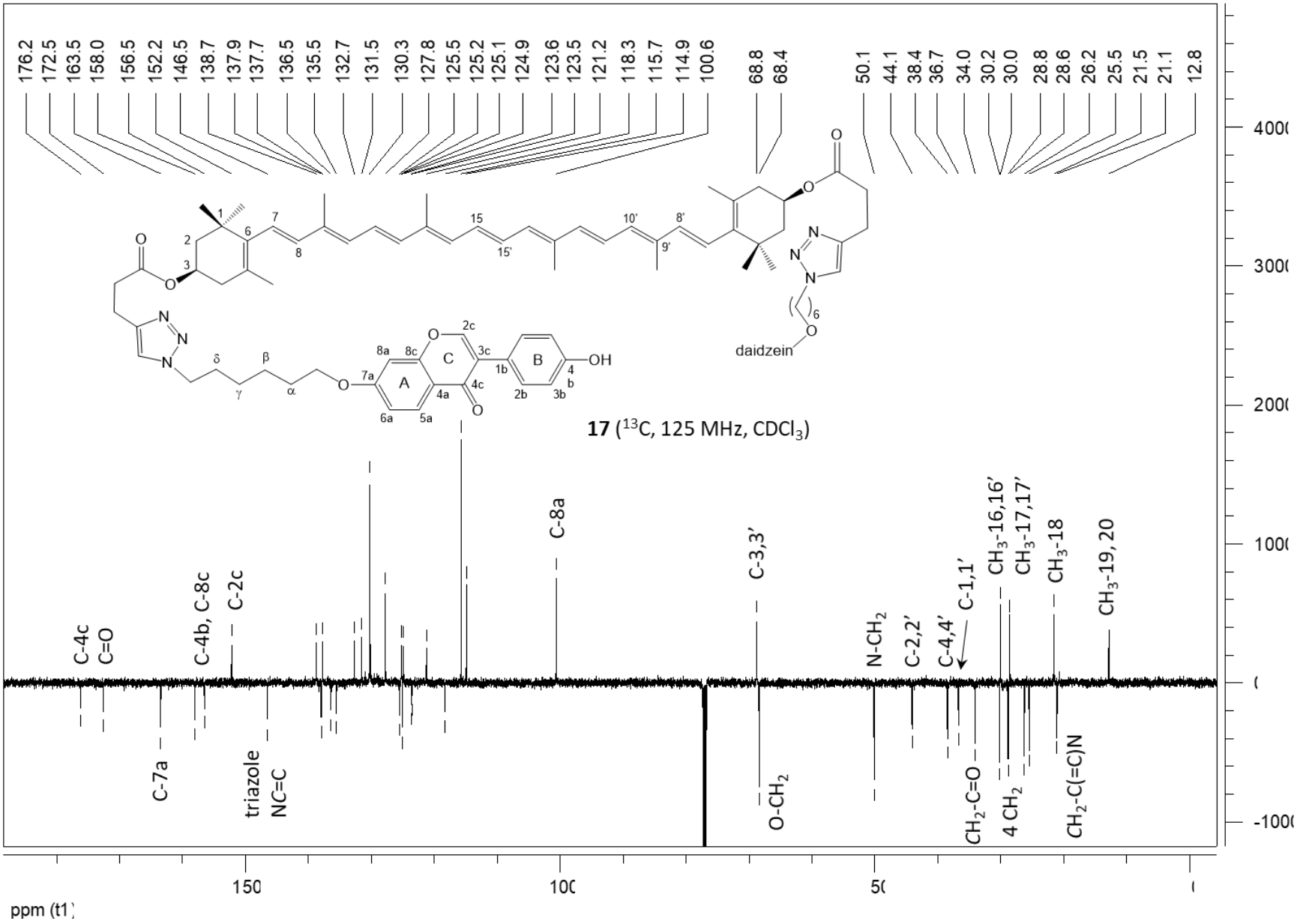


Figure S26.a. ^{13}C-apt NMR spectrum of *bis*-daidzein-zeaxanthin conjugate (**17**)

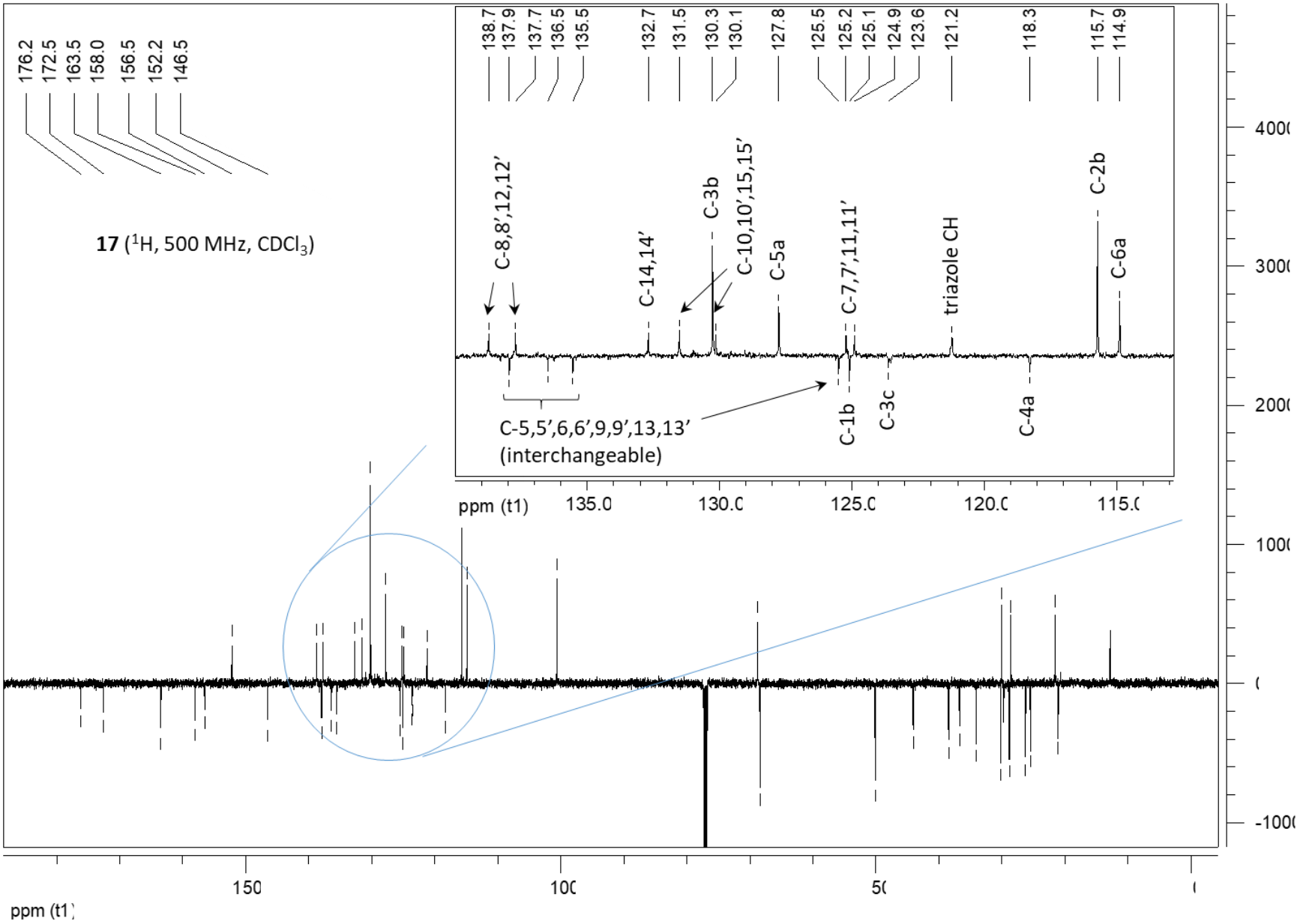


Figure S26.b. ^{13}C-apt NMR spectrum of *bis*-daidzein-zeaxanthin conjugate (**17**)

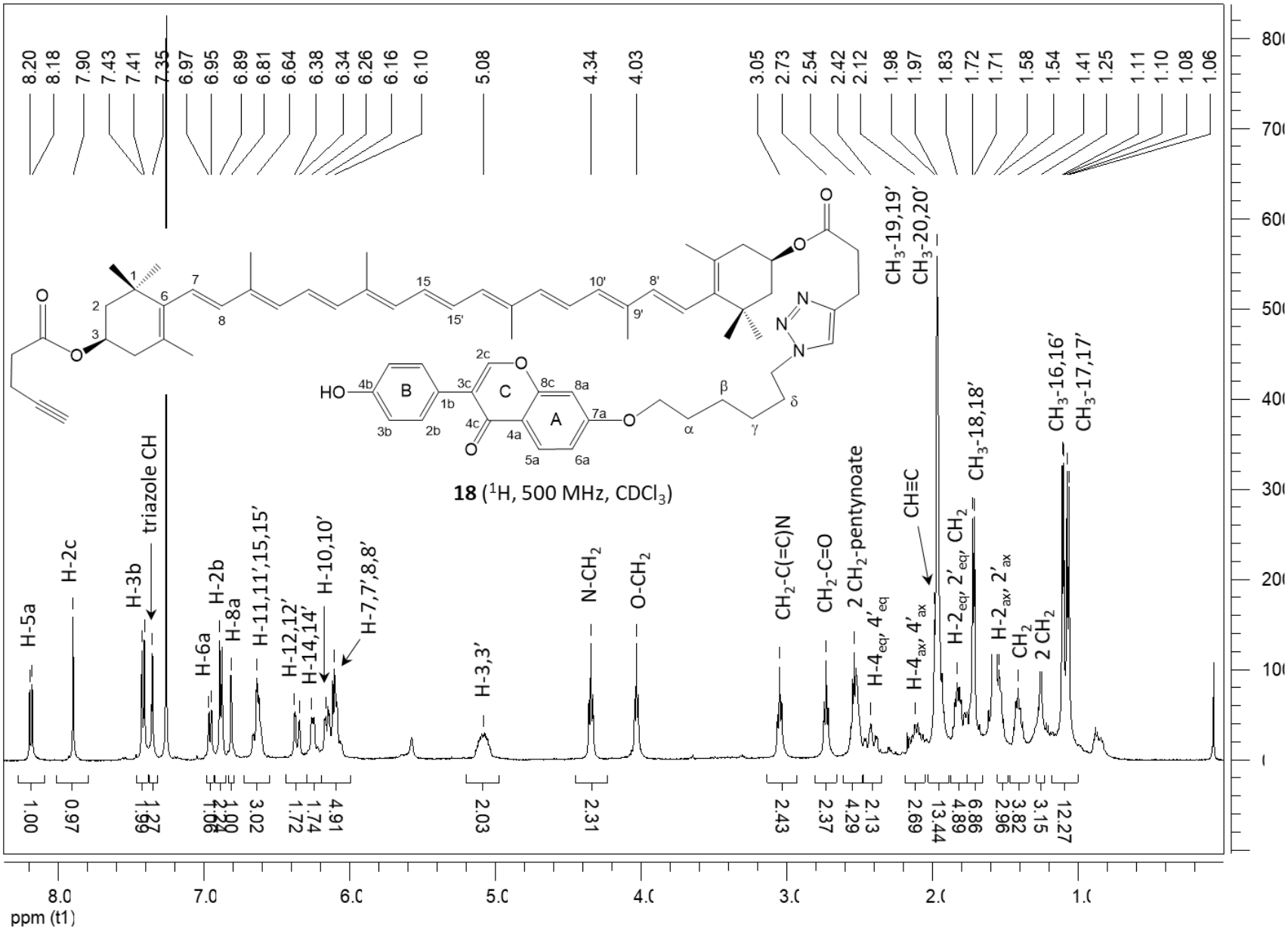


Figure S27. [1]H NMR spectrum of daidzein-zeaxanthin conjugate (**18**)

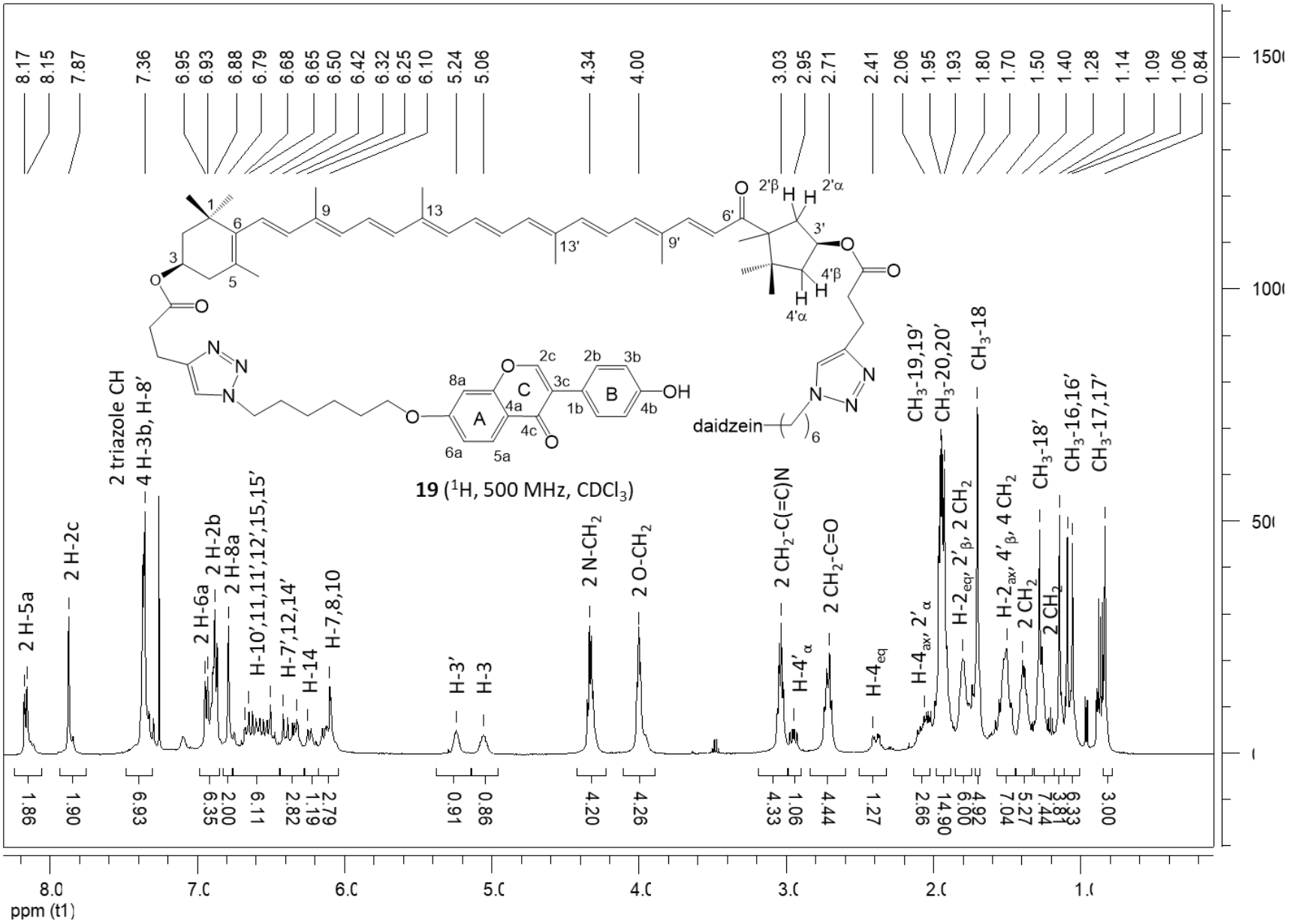


Figure S28. [1]H NMR spectrum of *bis*-daidzein-capsanthin conjugate (**19**)

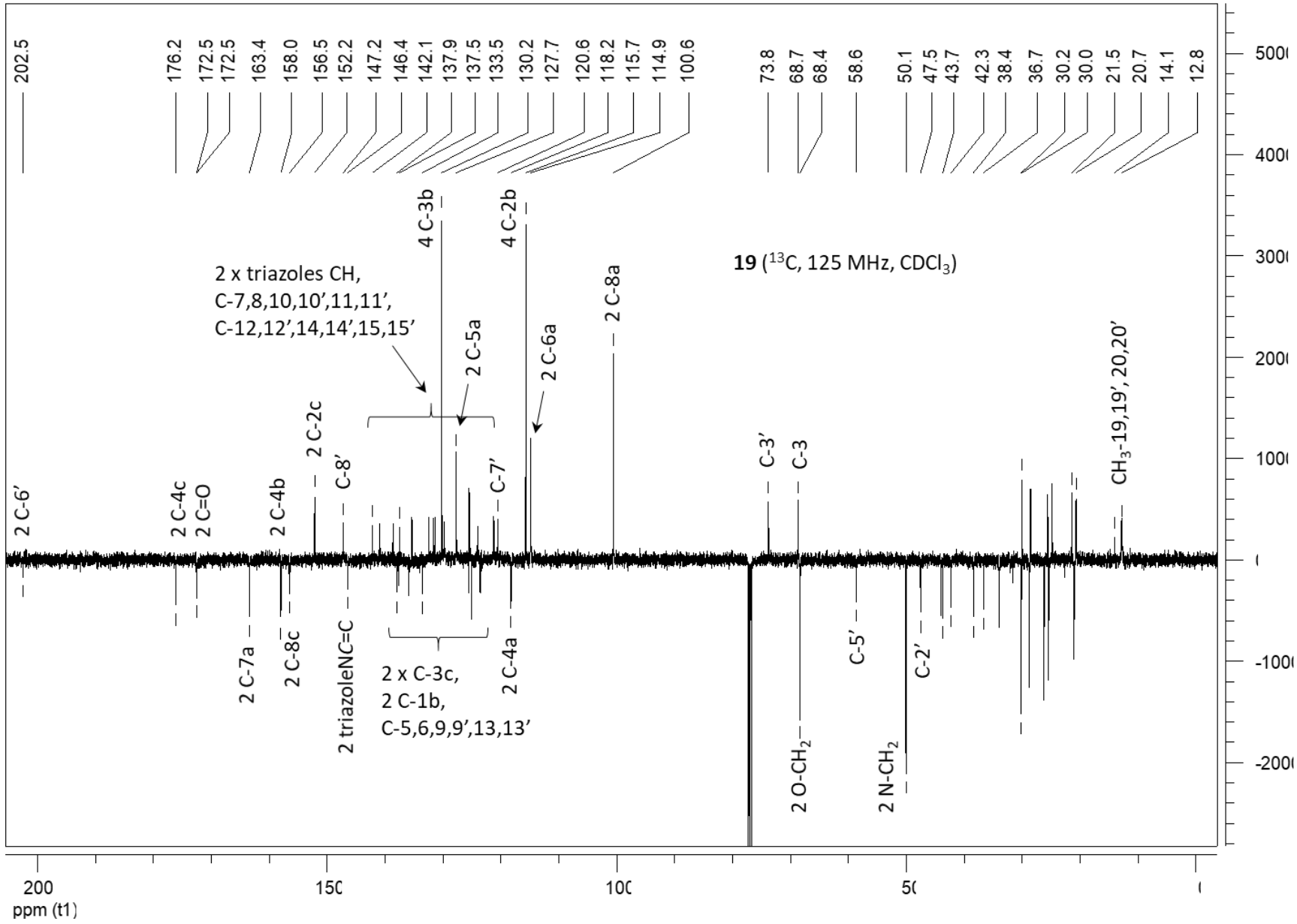
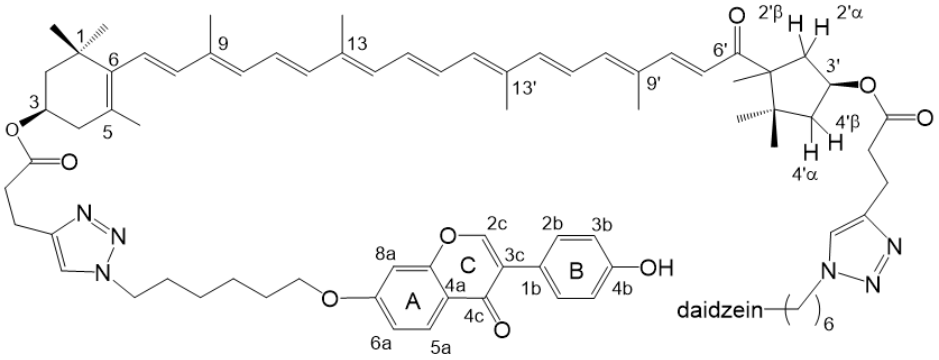


Figure S29.a. ^{13}C-apt NMR spectrum of *bis*-daidzein-capsanthin conjugate (**19**)



19 (^{13}C, 125 MHz, $CDCl_3$)

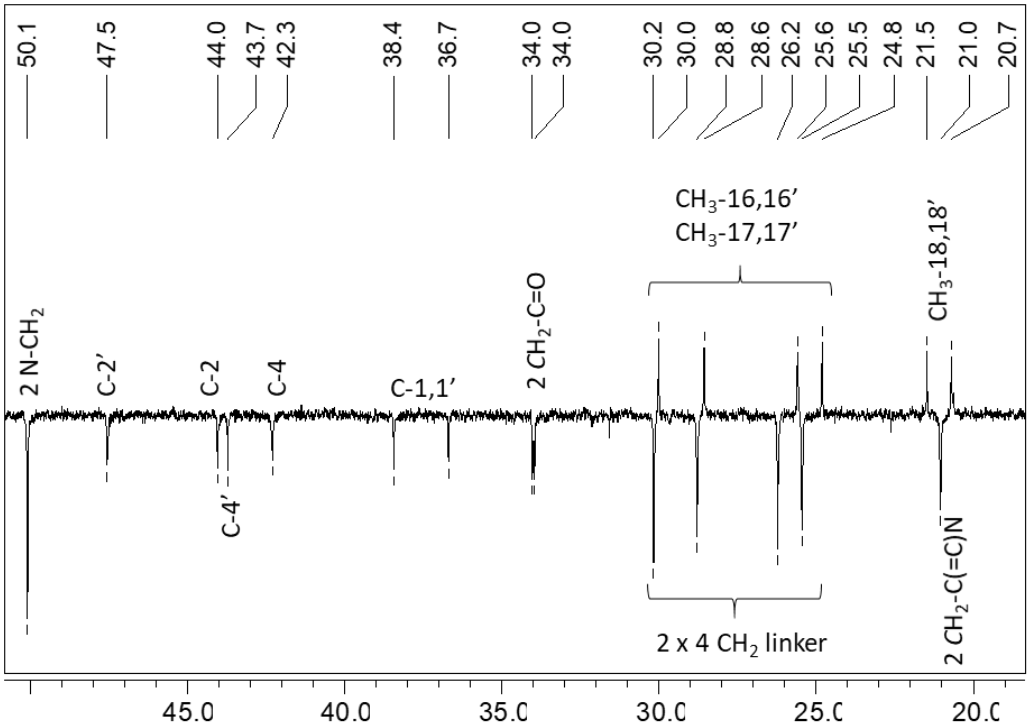


Figure S29.b. ^{13}C-apt NMR spectrum of *bis*-daidzein-capsanthin conjugate (**19**)

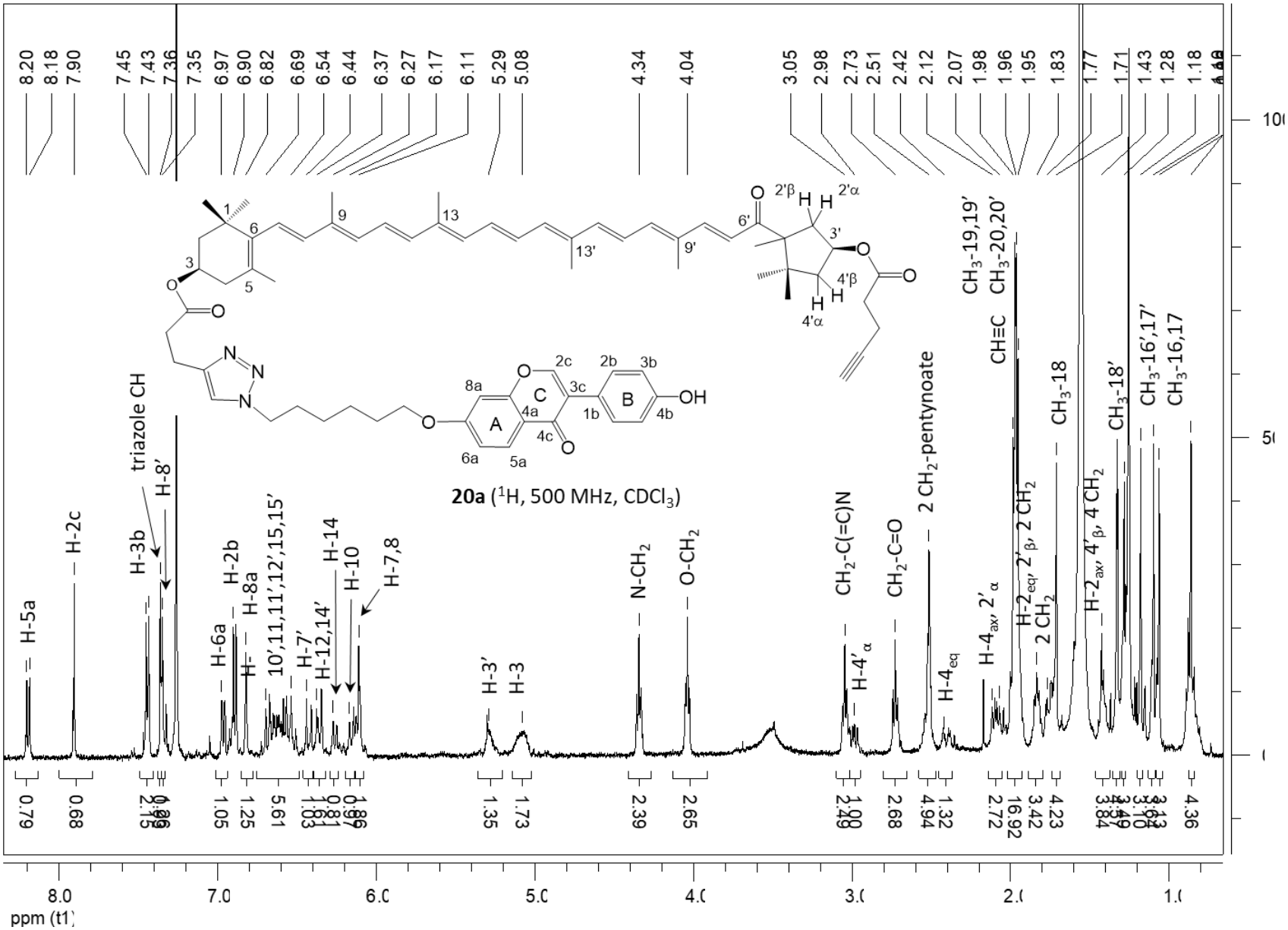


Figure S30. ^{1}H NMR spectrum of daidzein-capsanthin conjugate (**20a**)

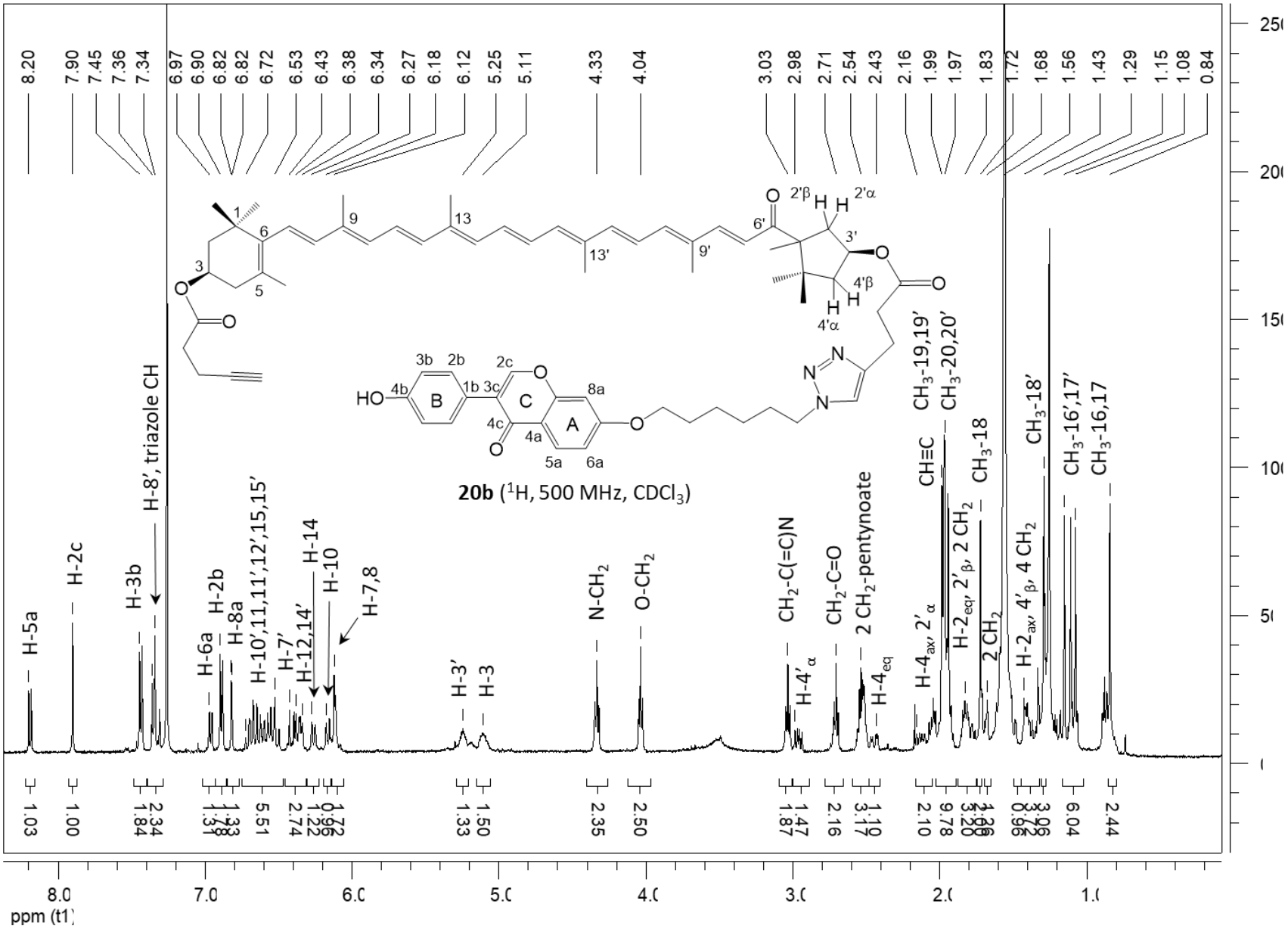


Figure S31. [1]H NMR spectrum of daidzein-capsanthin conjugate (**20b**)

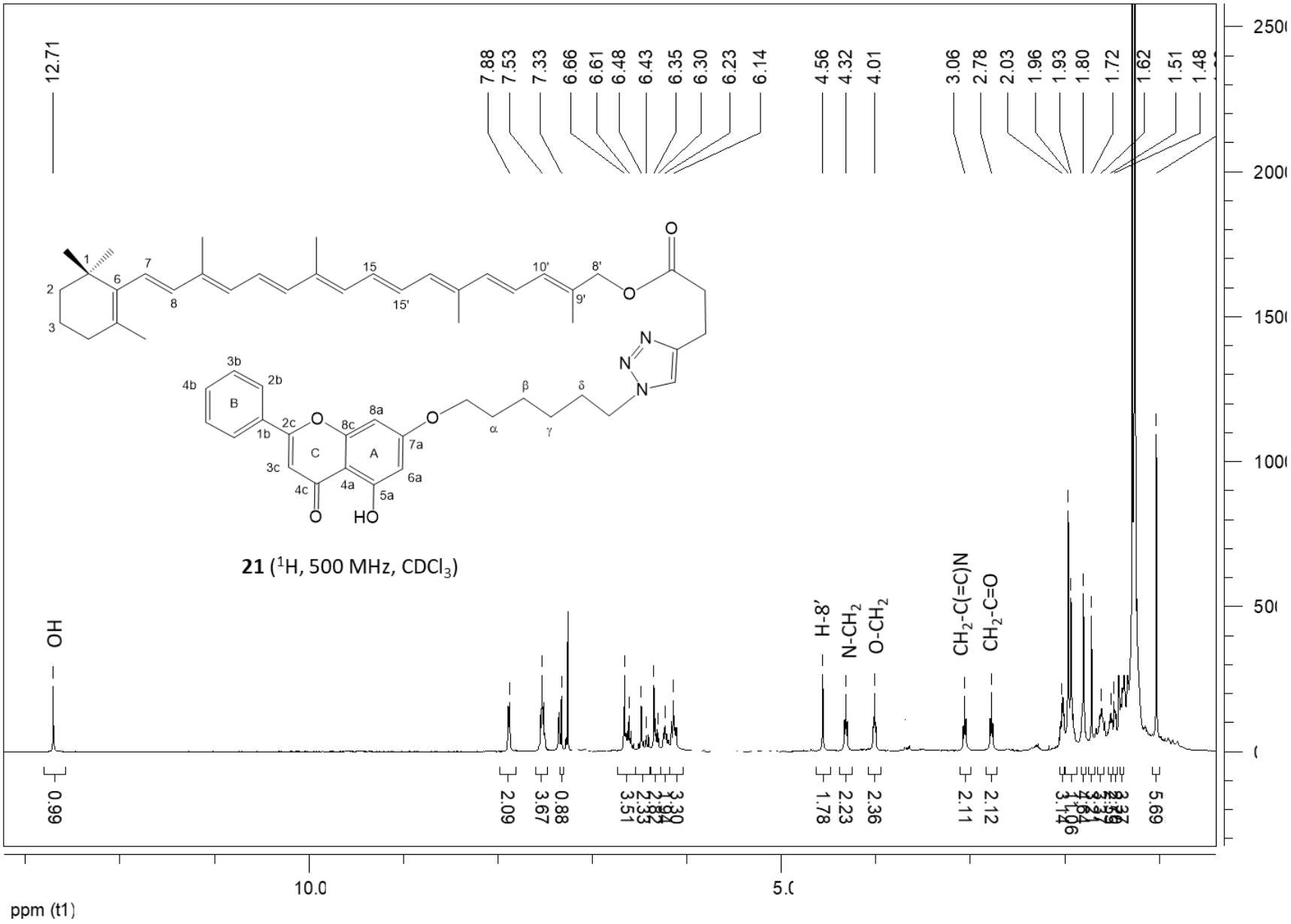


Figure S32.a. [1]H NMR spectrum of chrysin-8′-apo-β-carotenol conjugate (**21**)

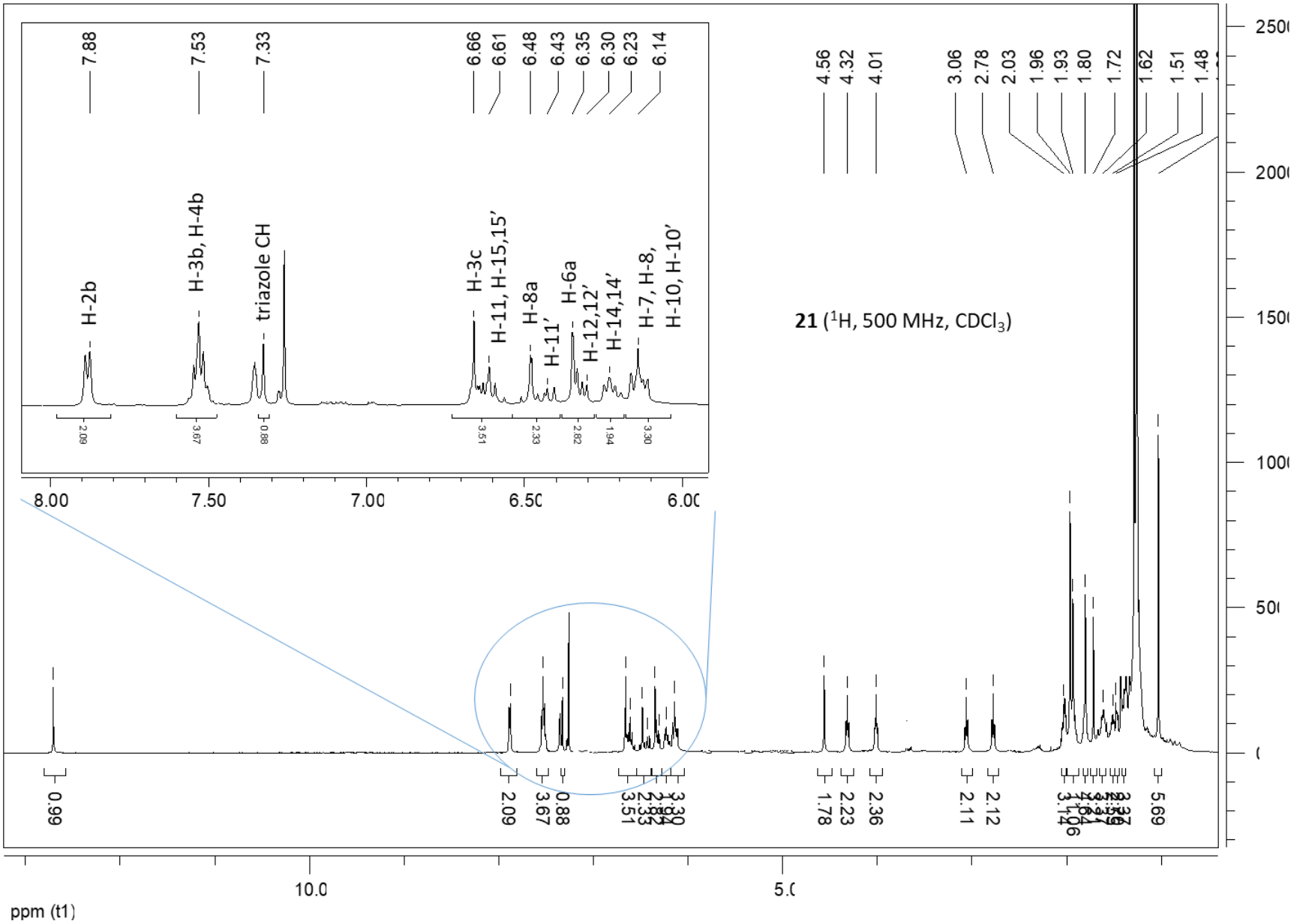


Figure S32.b. ^{1}H NMR spectrum of chrysin-8′-apo-β-carotenol conjugate (**21**)

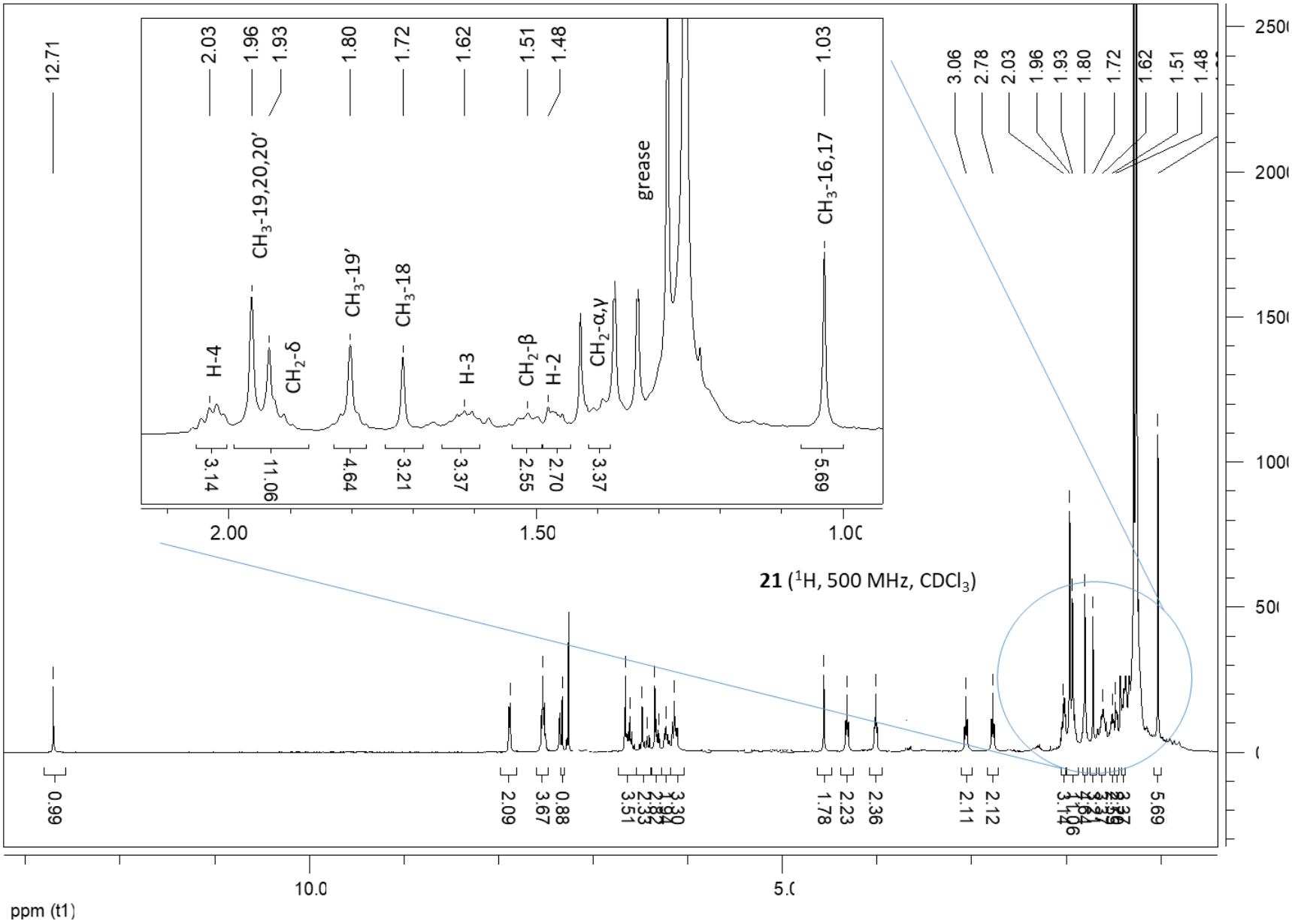


Figure S32.c. [1]H NMR spectrum of chrysin-8′-apo-β-carotenol conjugate (**21**)

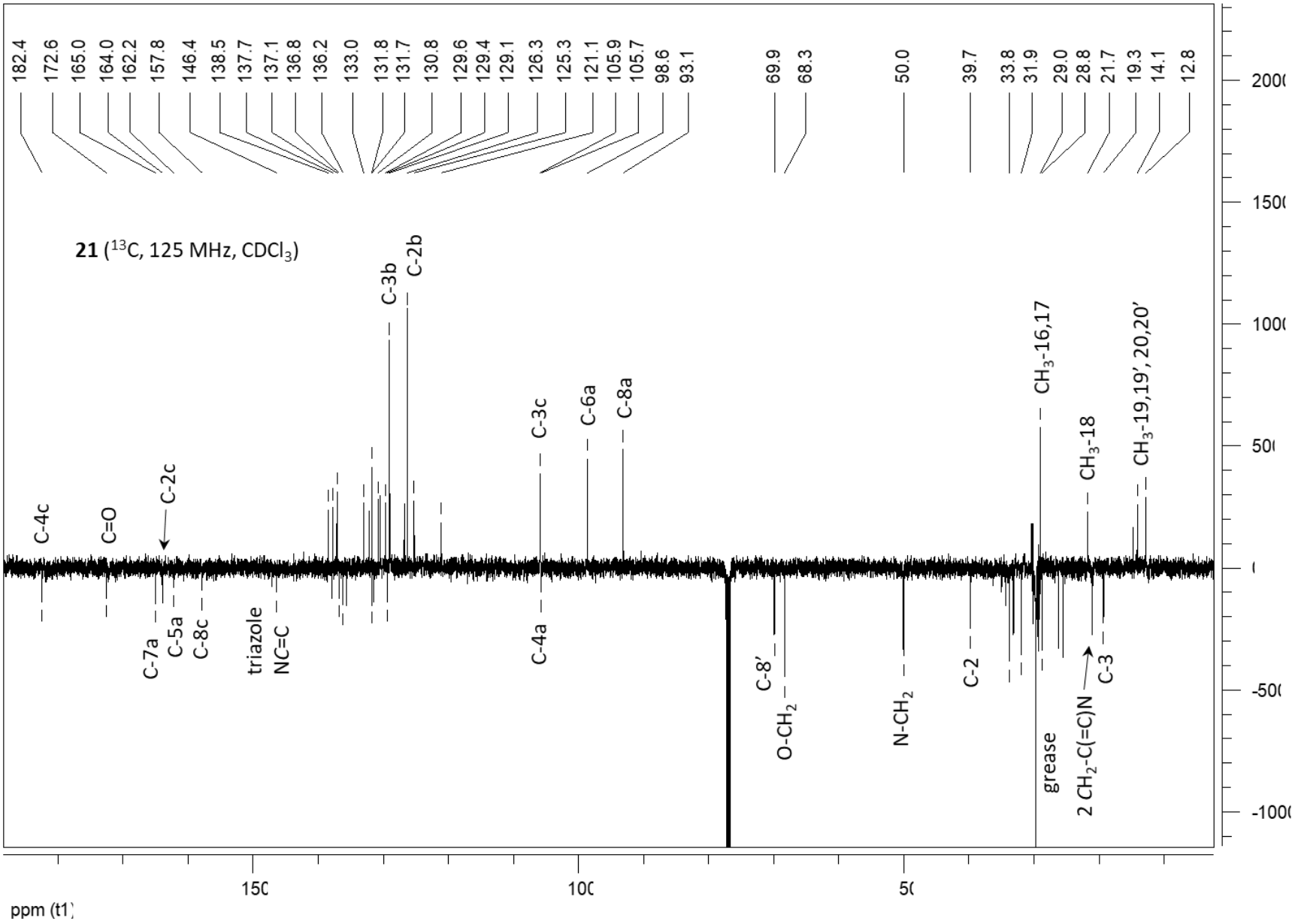
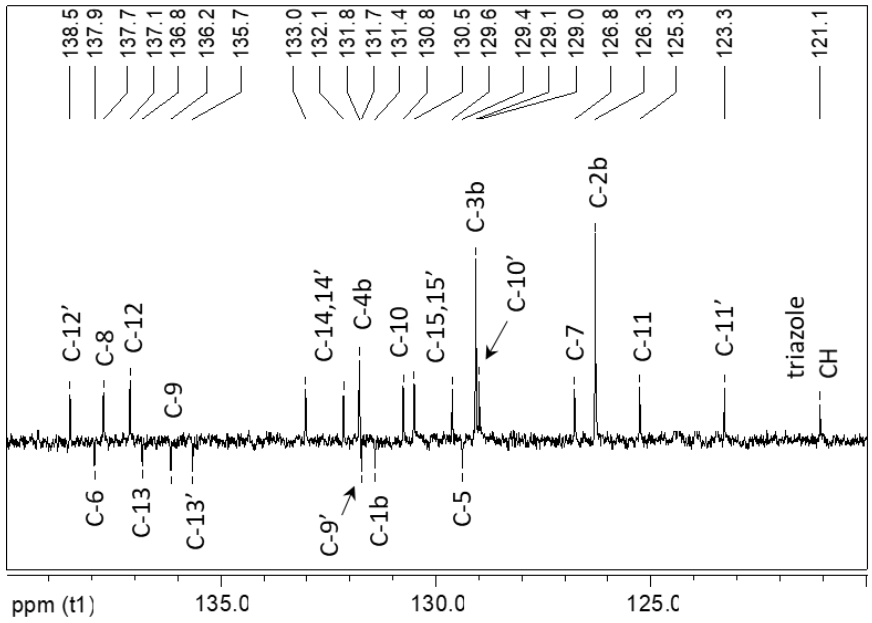
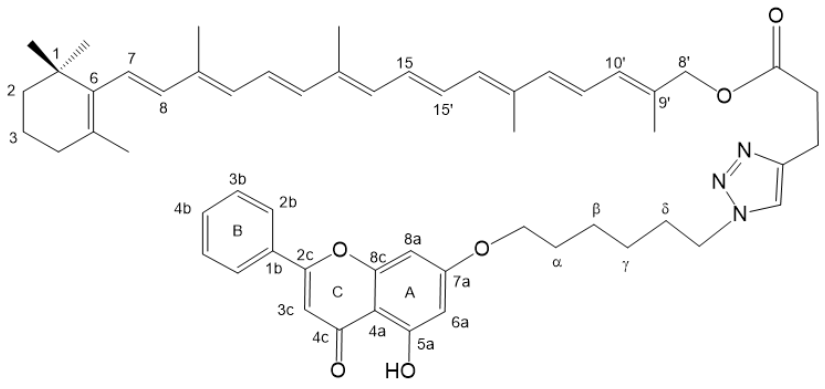


Figure S33.a. ^{13}C-apt NMR spectrum of chrysin-8′-apo-β-carotenol conjugate (**21**)





21 (^{13}C, 125 MHz, $CDCl_3$)

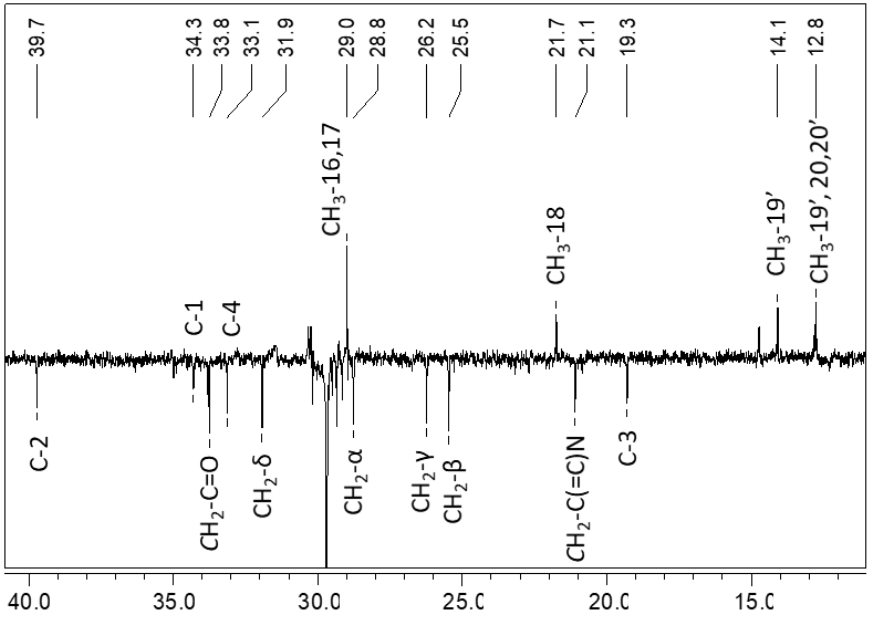


Figure S33.b. ^{13}C-apt NMR spectrum of chrysin-8′-apo-β-carotenol conjugate (**21**)

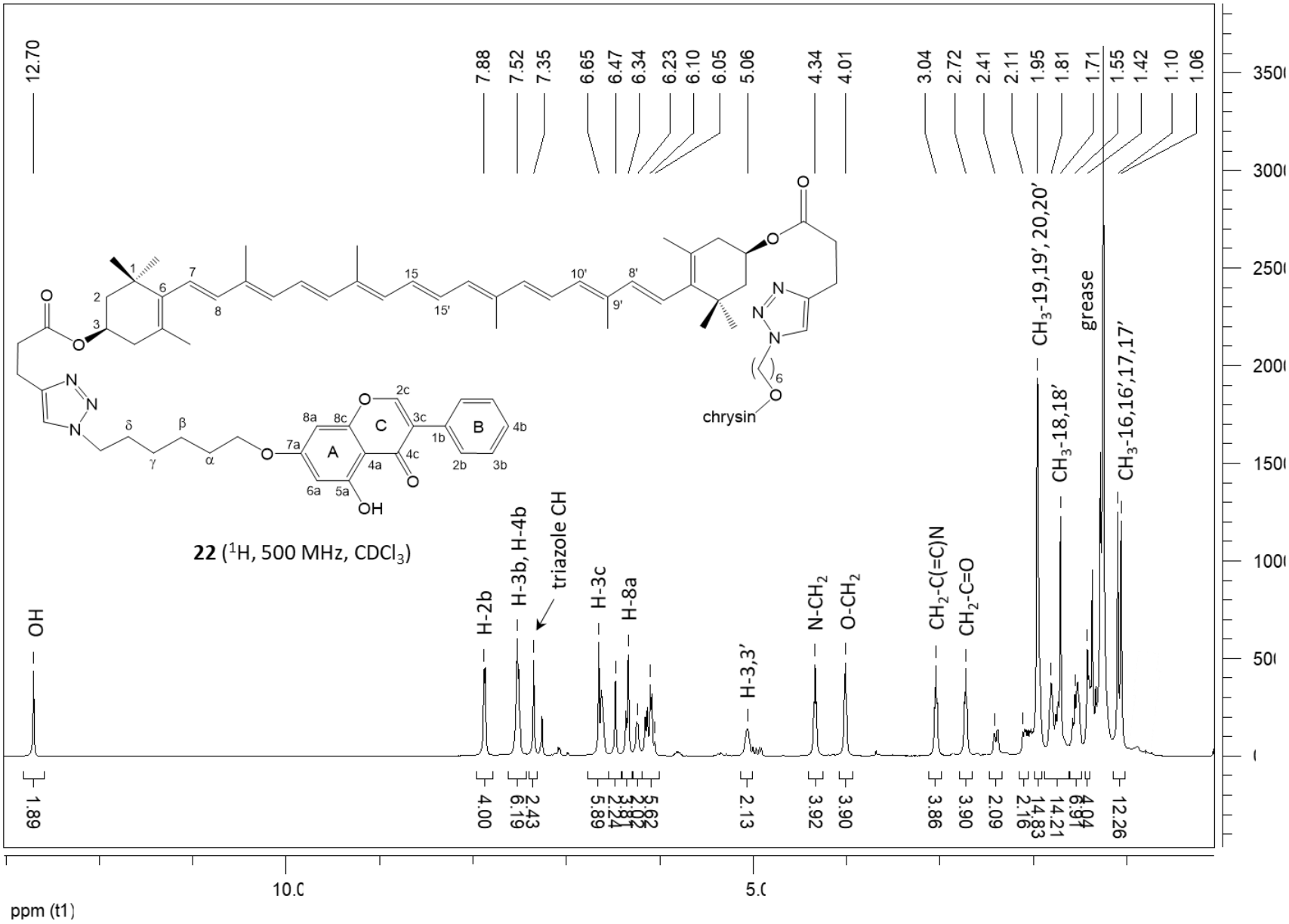


Figure S34.a. [1]H NMR spectrum of *bis*-chrysin-zeaxanthin conjugate (**22**)

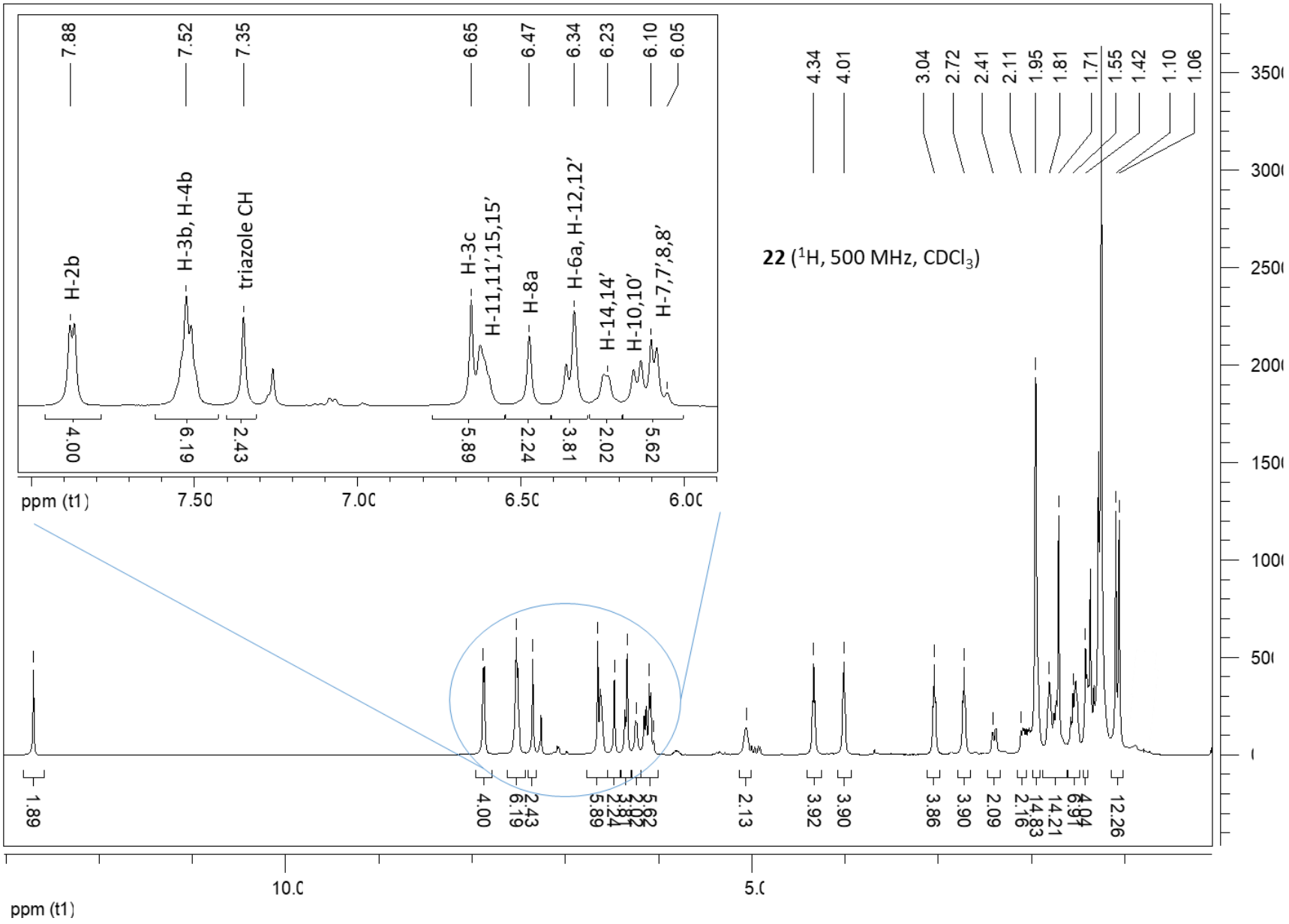


Figure S34.b. [1]H NMR spectrum of *bis*-chrysin-zeaxanthin conjugate (**22**)

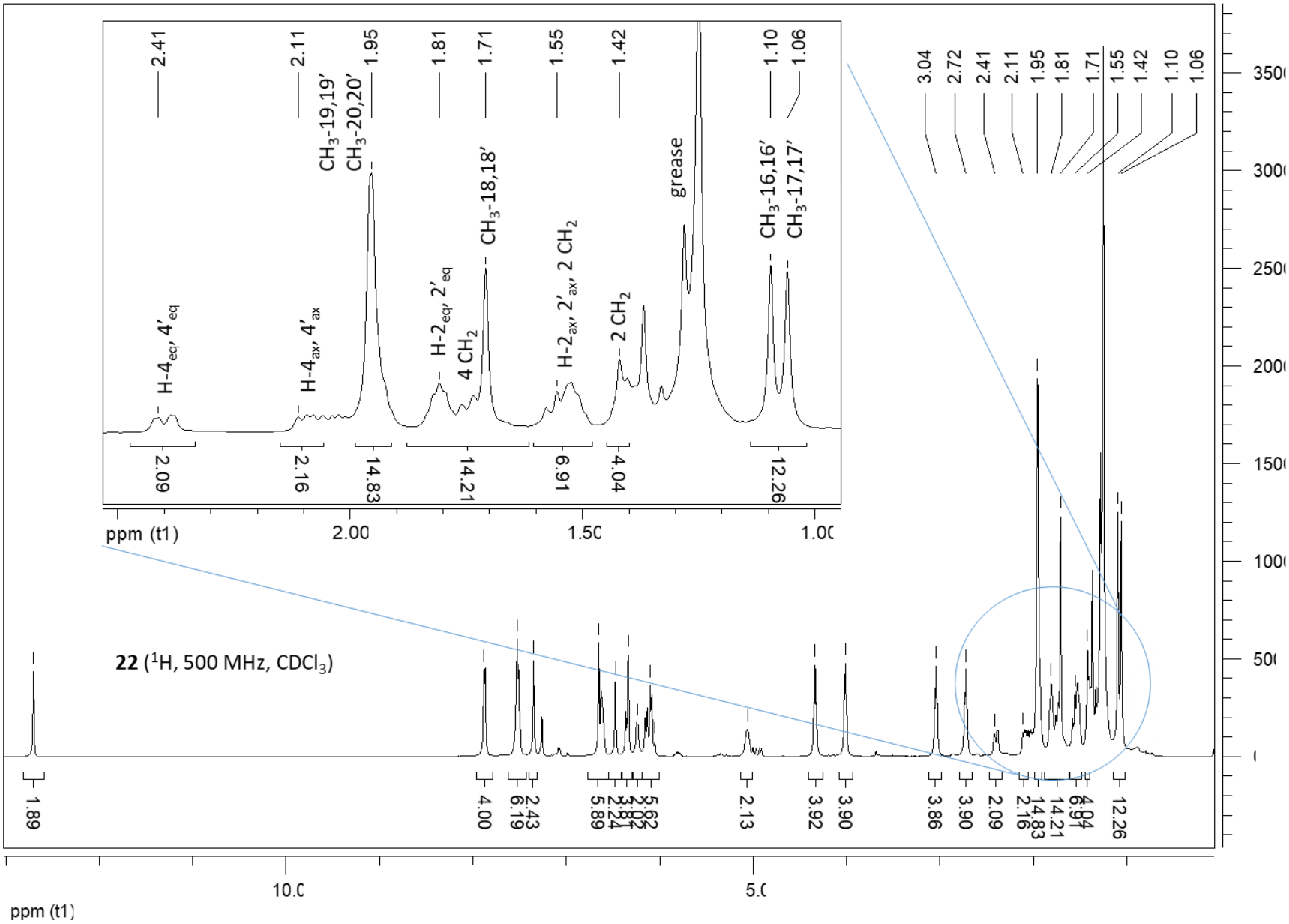


Figure S34.c. [1]H NMR spectrum of *bis*-chrysin-zeaxanthin conjugate (**22**)

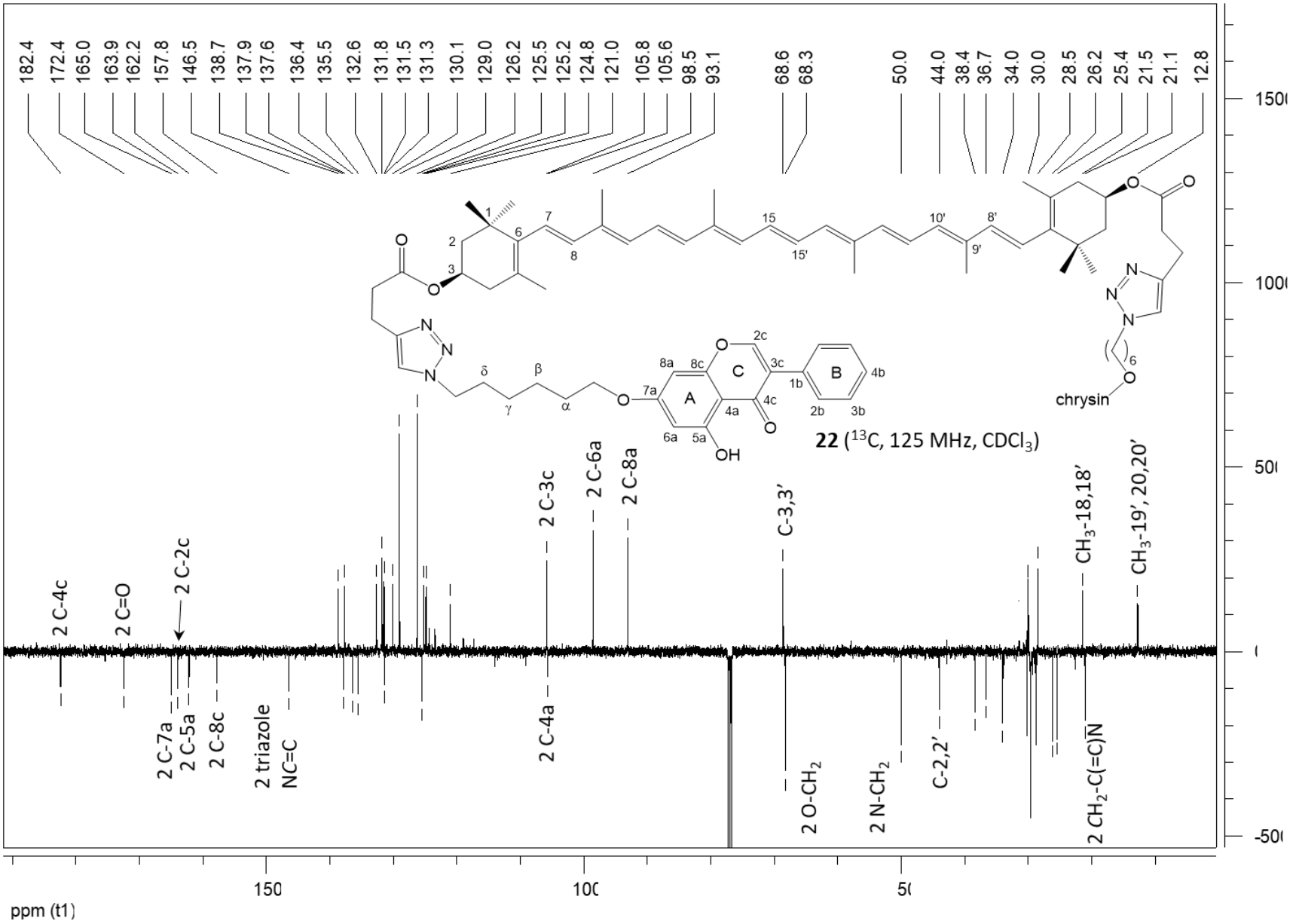
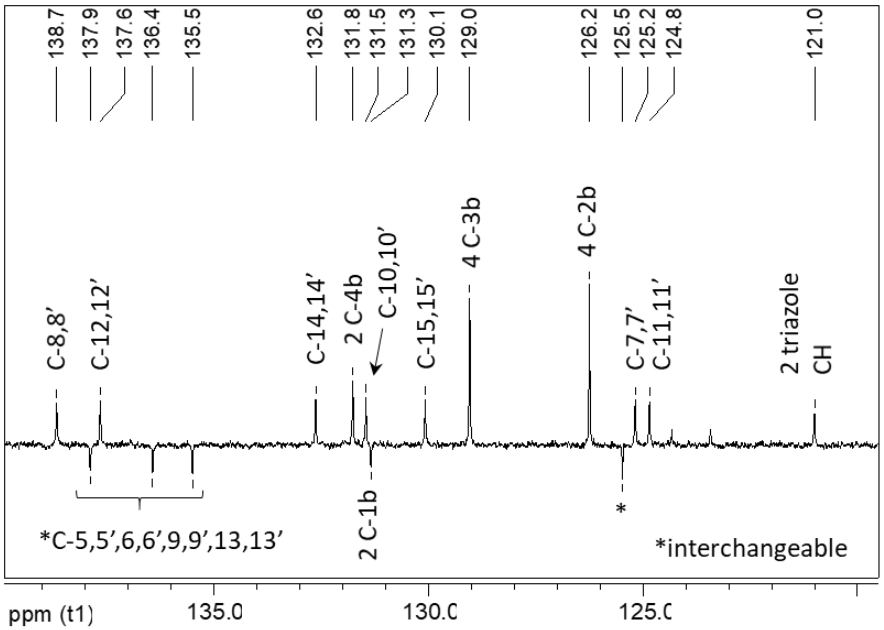
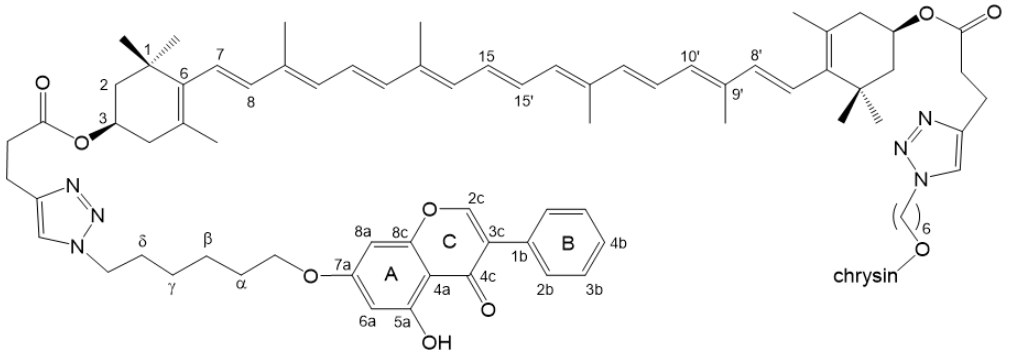


Figure S35.a. ^{13}C-apt NMR spectrum of *bis*-chrysin-zeaxanthin conjugate (**22**)





22 (^{13}C, 125 MHz, $CDCl_3$)

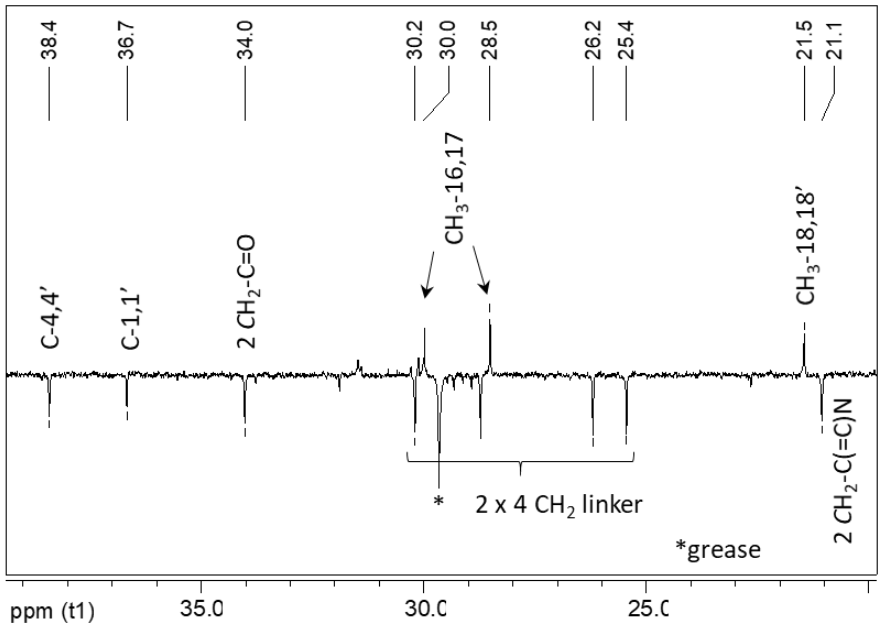


Figure S35.b. ^{13}C-apt NMR spectrum of *bis*-chrysin-zeaxanthin conjugate (**22**)

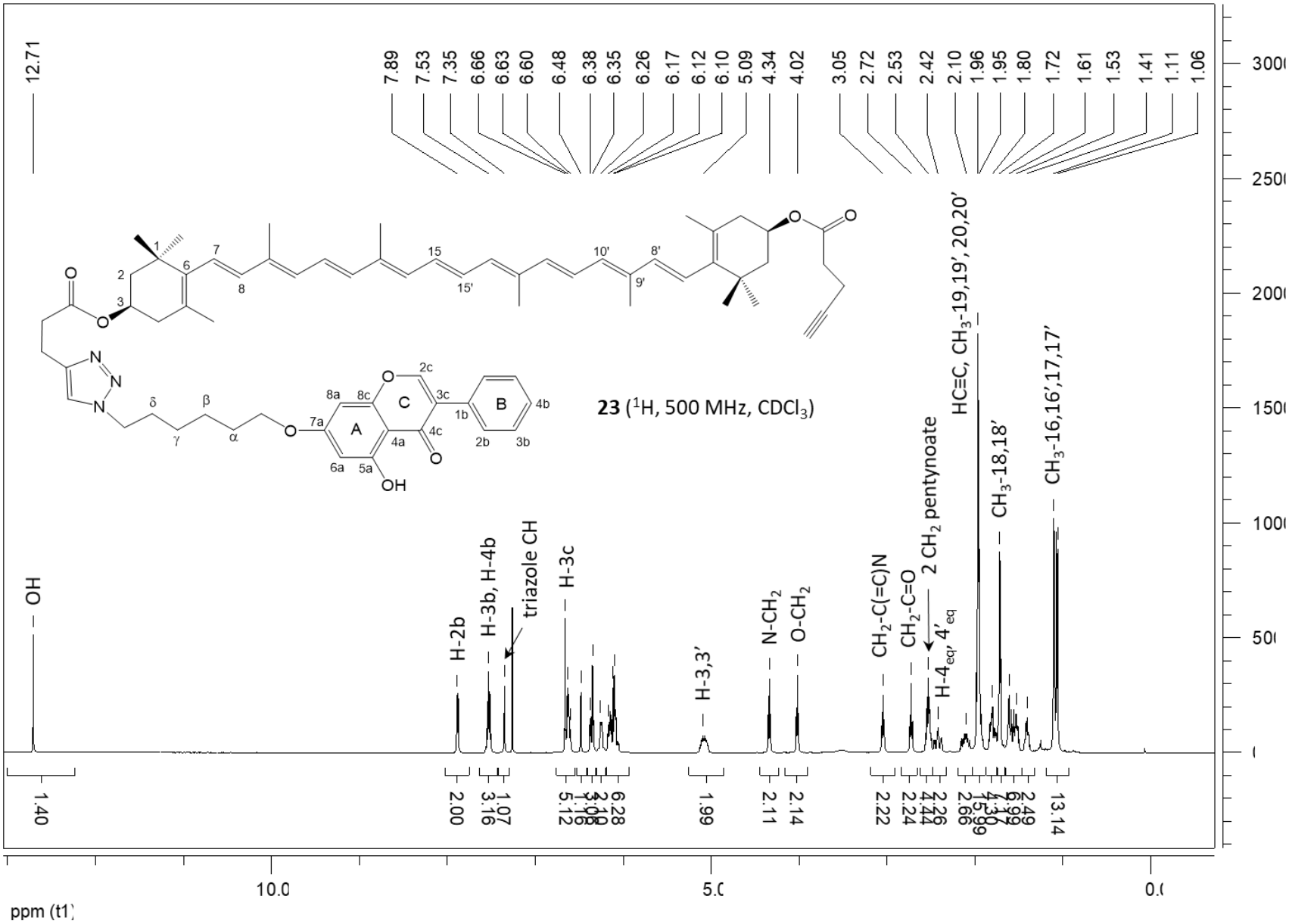


Figure S36.a. ^{1}H NMR spectrum of chrysin-zeaxanthin conjugate (**23**)

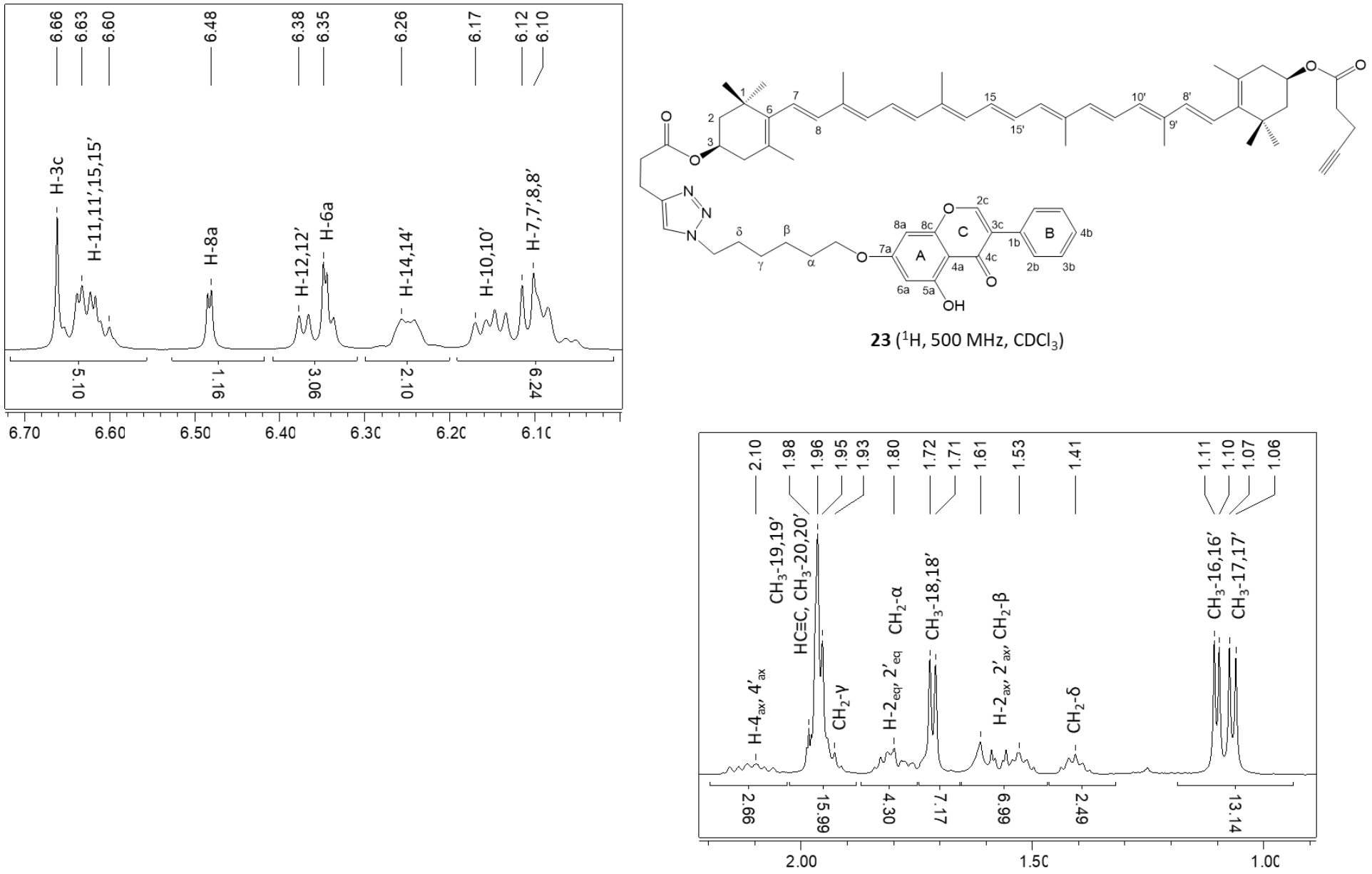


Figure S36.b. [1]H NMR spectrum of chrysin-zeaxanthin conjugate (**23**)

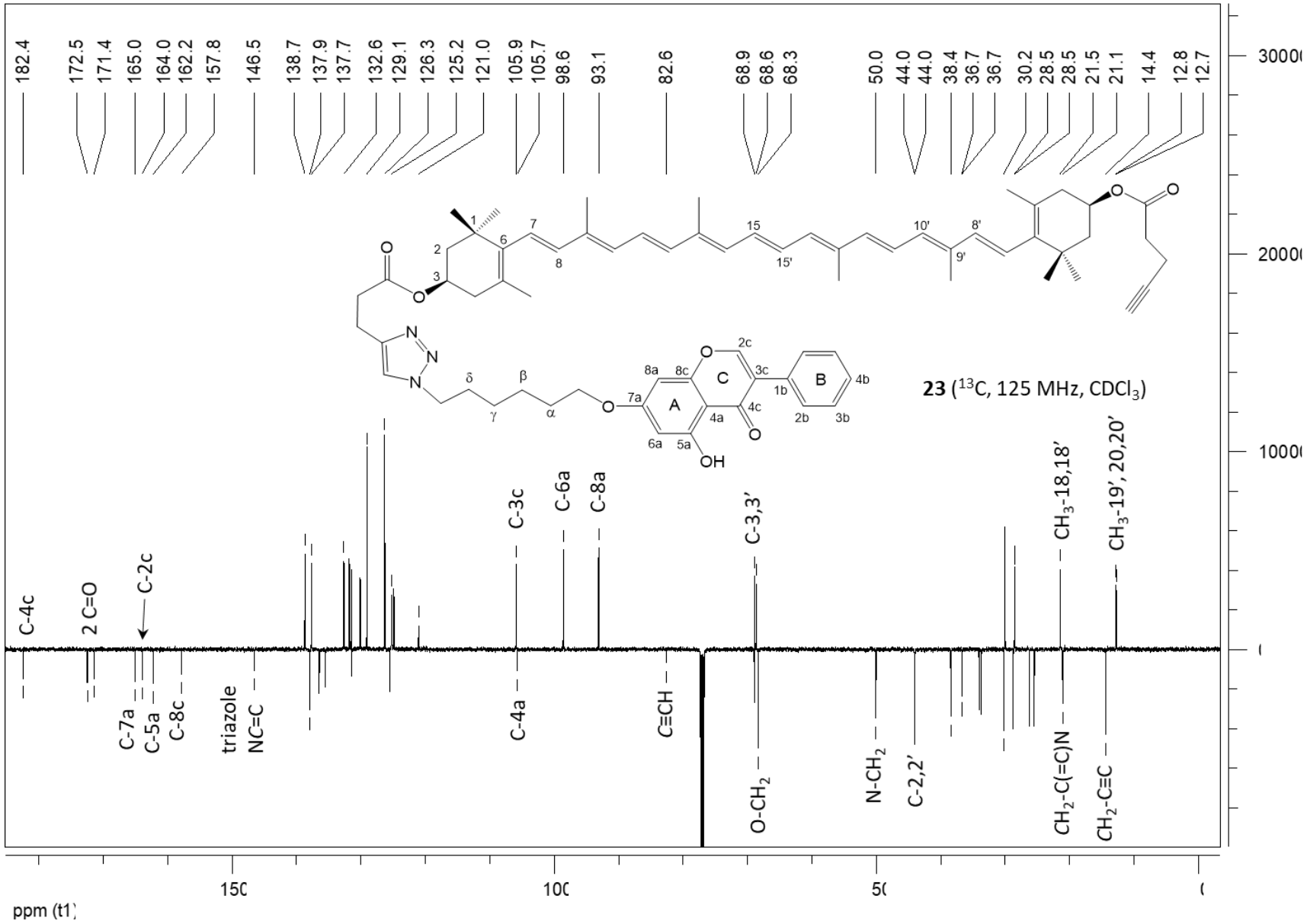


Figure S37.a. ^{13}C-apt NMR spectrum of chrysin-zeaxanthin conjugate (**23**)

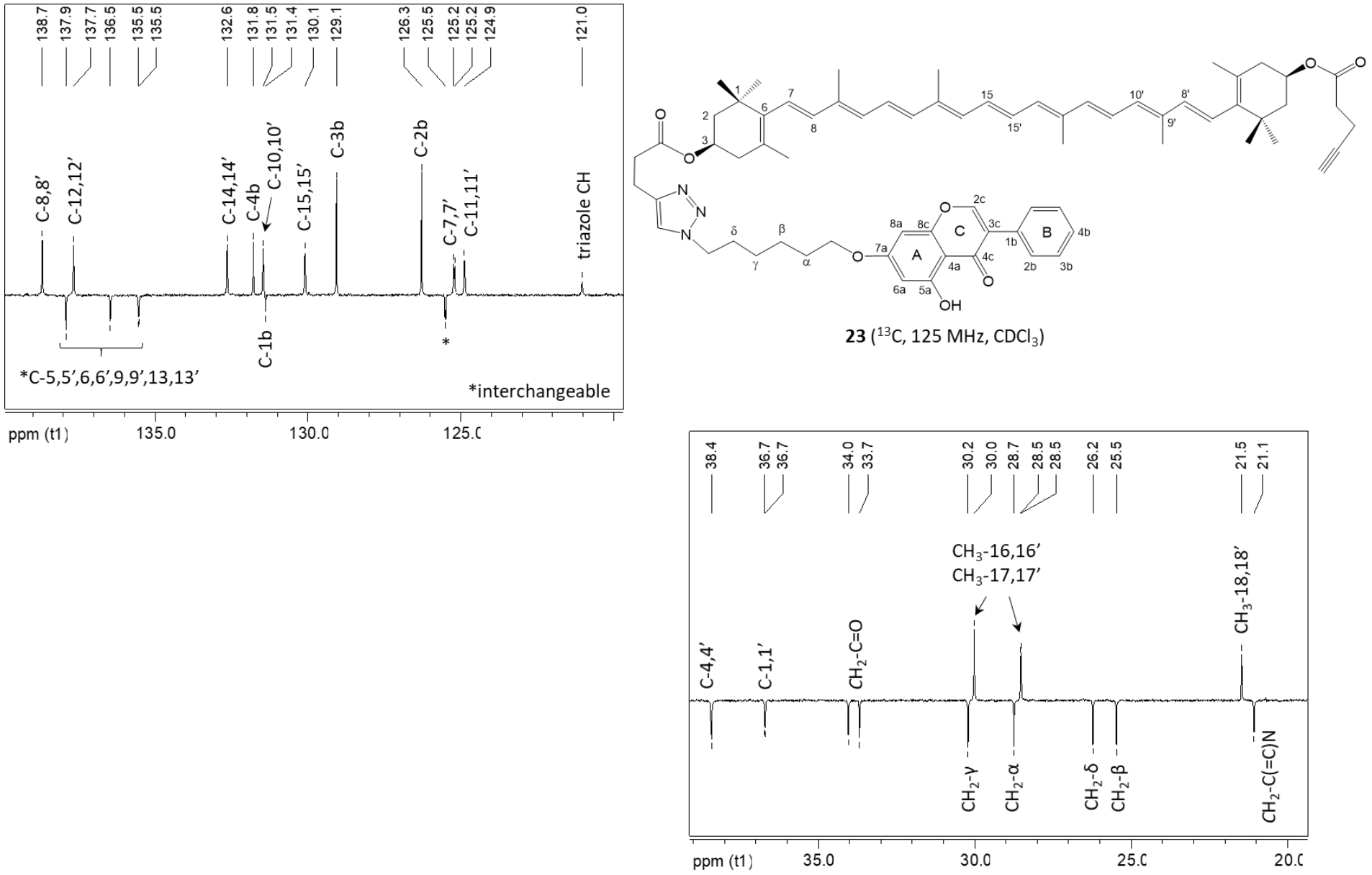


Figure S37.b. ^{13}C-apt NMR spectrum of chrysin-zeaxanthin conjugate (**23**)

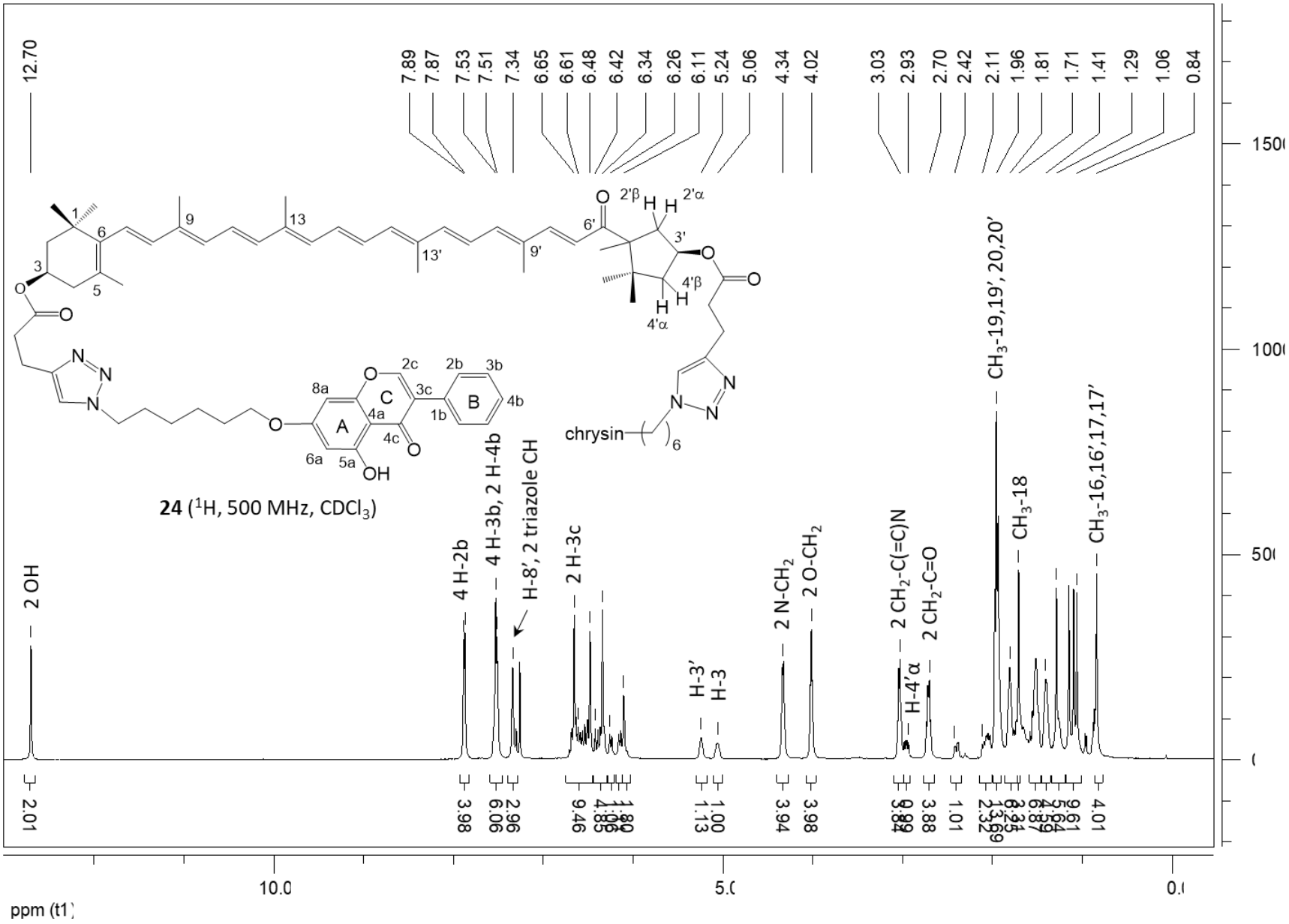


Figure S38.a. [1]H NMR spectrum of *bis*-chrysin-capsanthin conjugate (**24**)

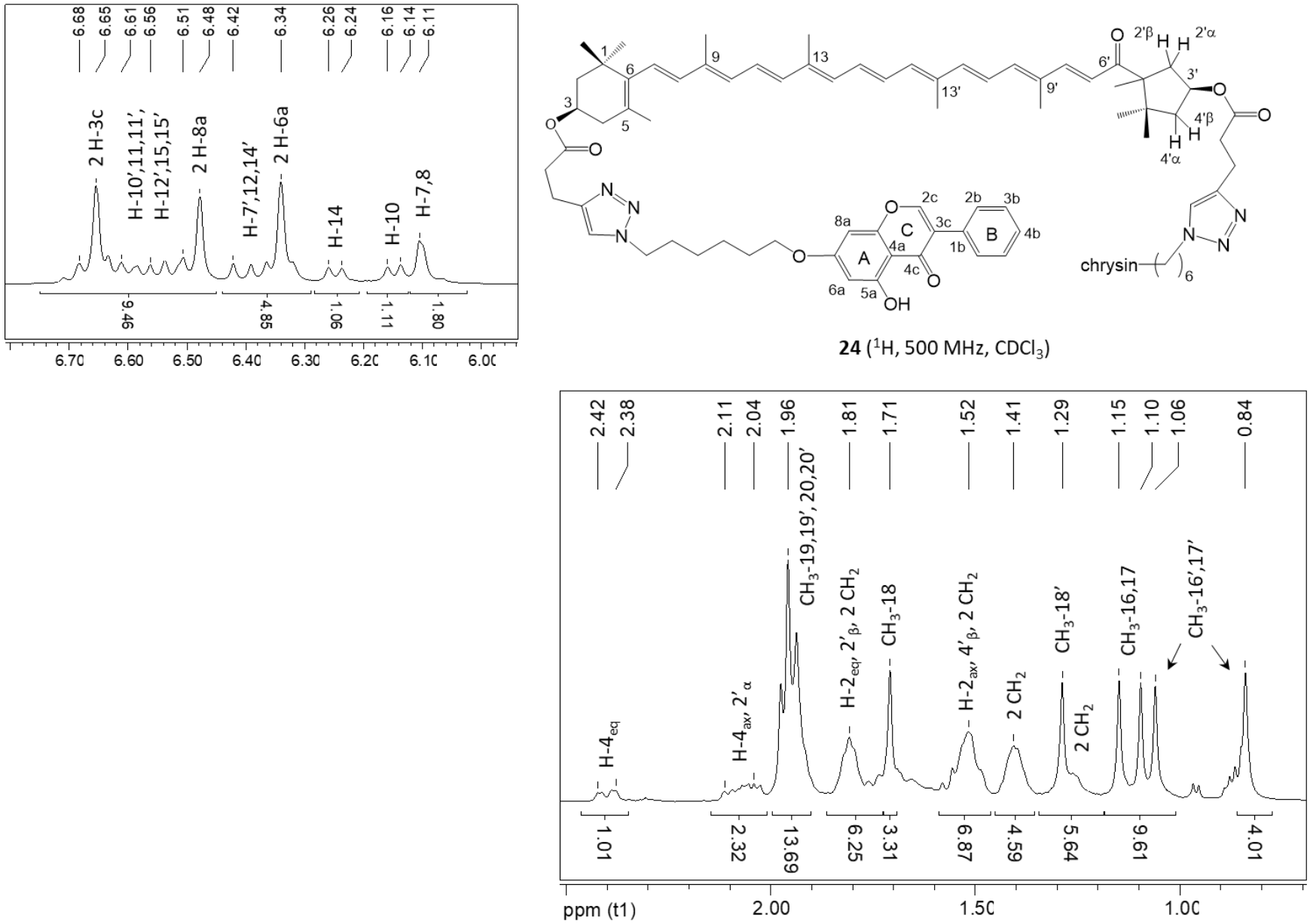


Figure S38.b. [1]H NMR spectrum of *bis*-chrysin-capsanthin conjugate (**24**)

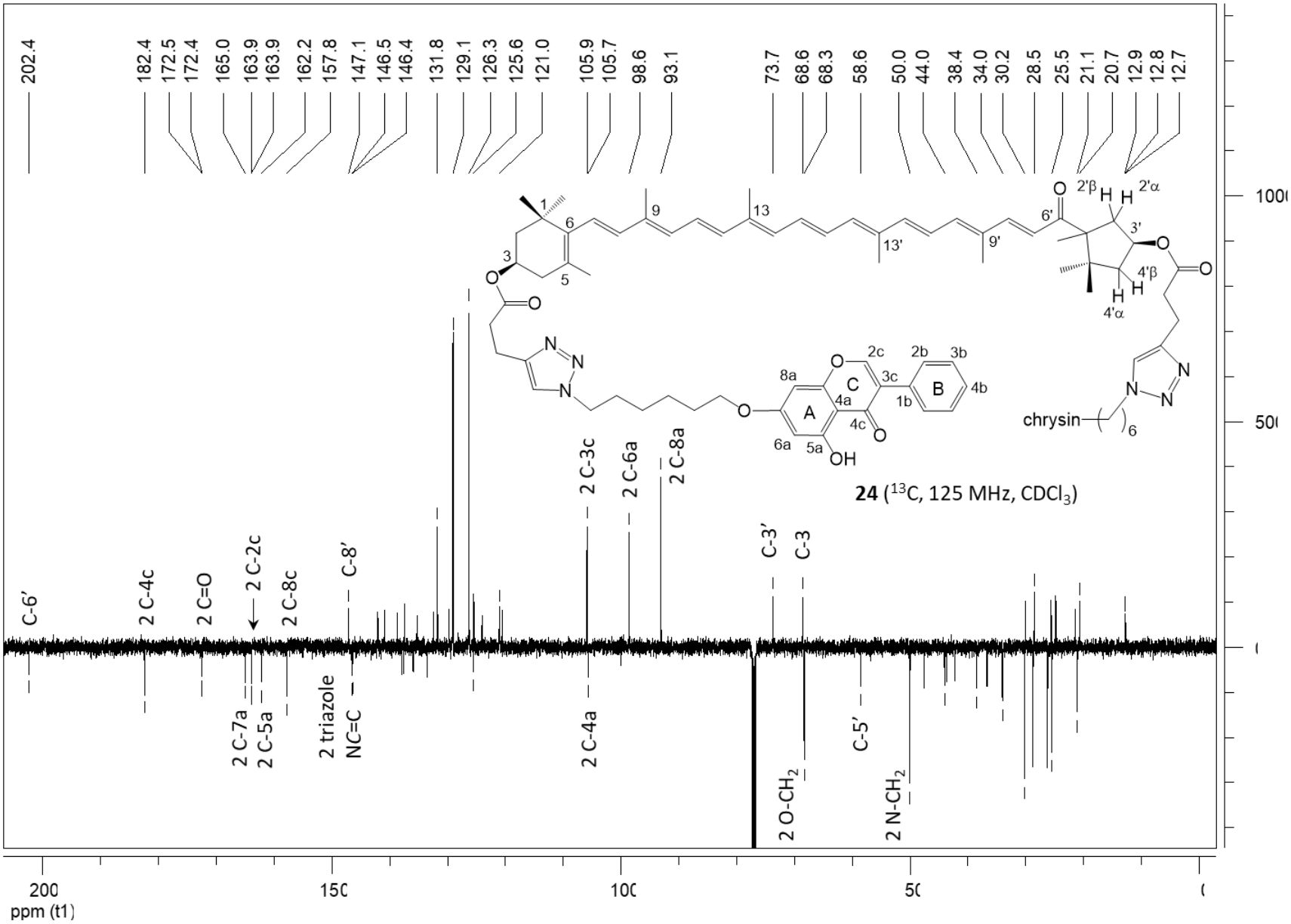


Figure S39.a. ^{13}C-apt NMR spectrum of *bis*-chrysin-capsanthin conjugate (**24**)

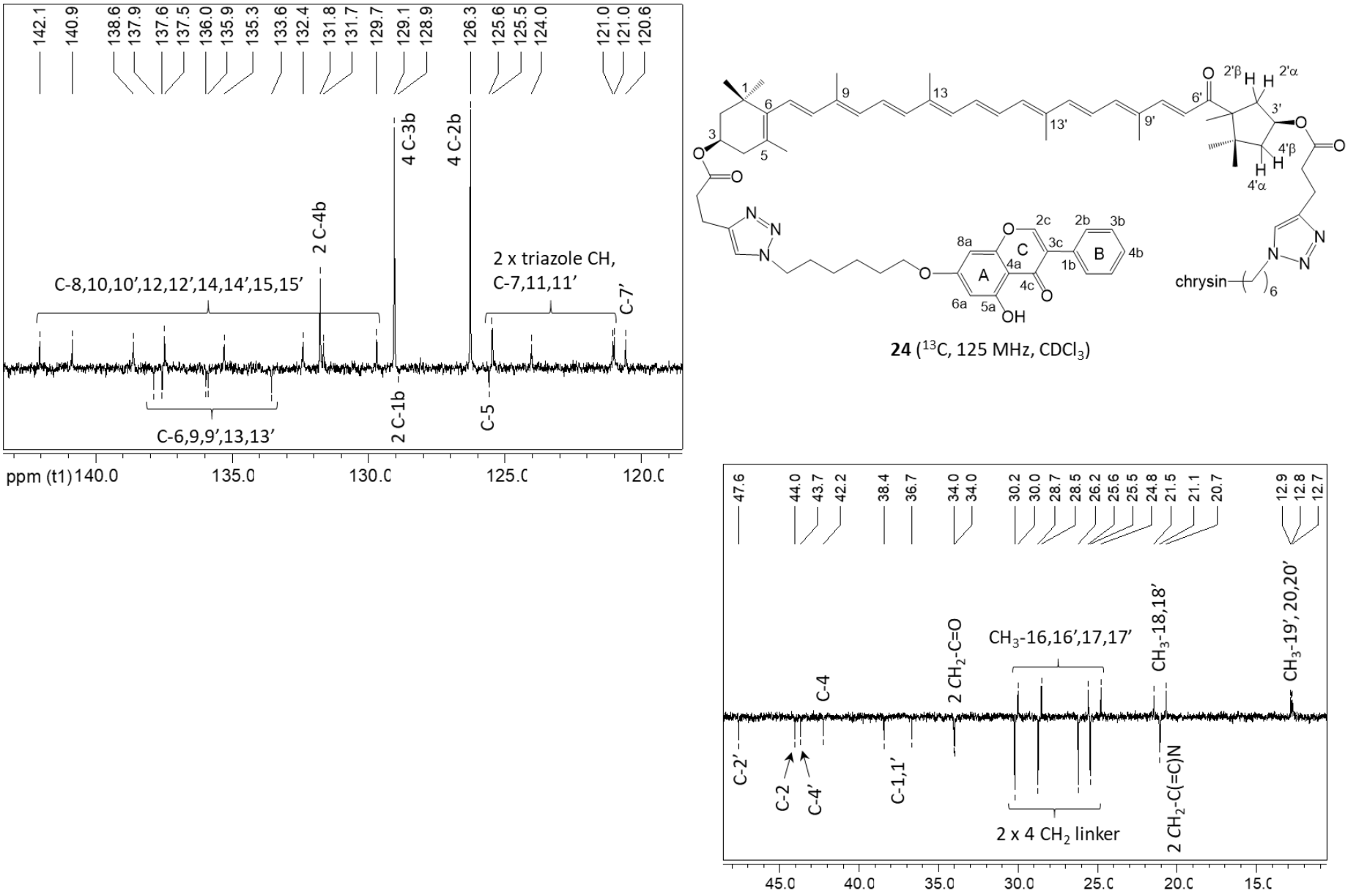


Figure S39.b. ^{13}C-apt NMR spectrum of *bis*-chrysin-capsanthin conjugate (**24**)

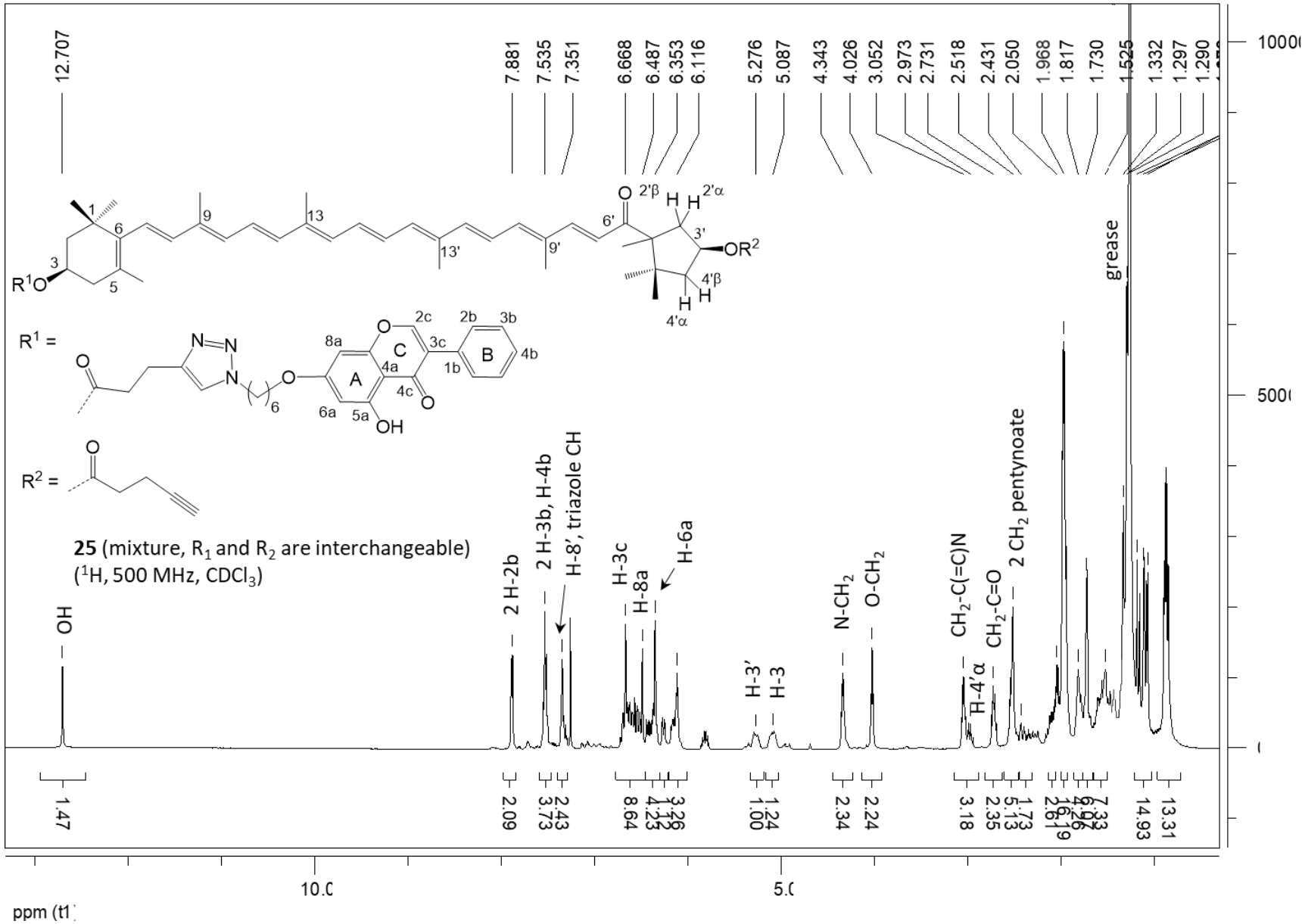
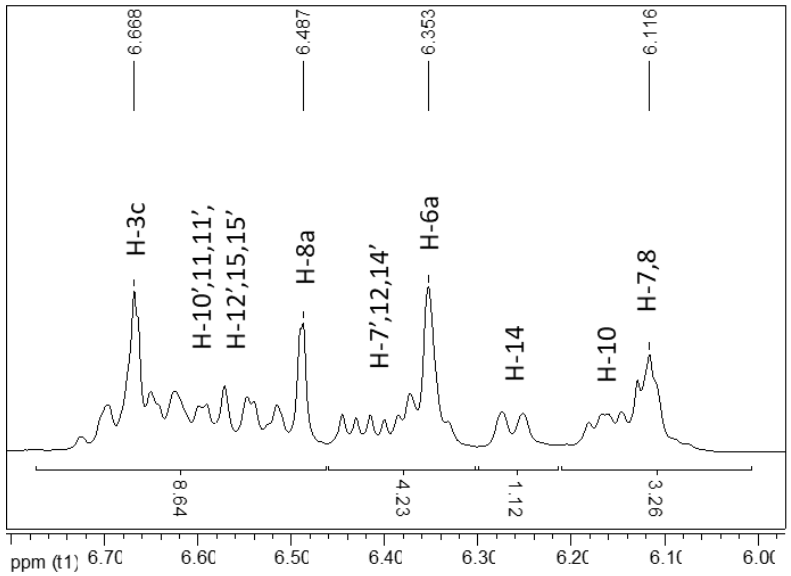
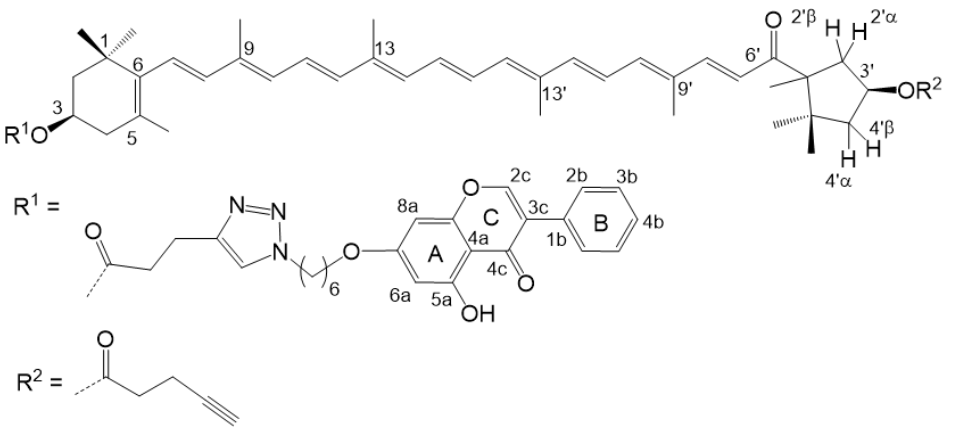


Figure S40.a. ^{1}H NMR spectrum of the mixture of regioisomers of chrysin-capsanthin conjugate (**25**)





25 (mixture, R_1 and R_2 are interchangeable)
(^{1}H, 500 MHz, $CDCl_3$)

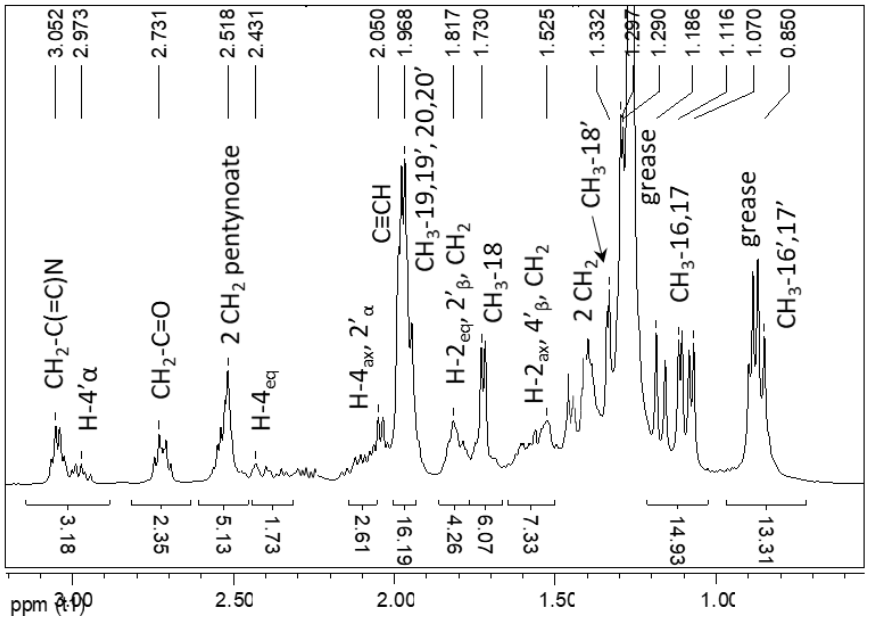


Figure S40.b. ^{1}H NMR spectrum of the mixture of regioisomers of chrysin-capsanthin conjugate (**25**)

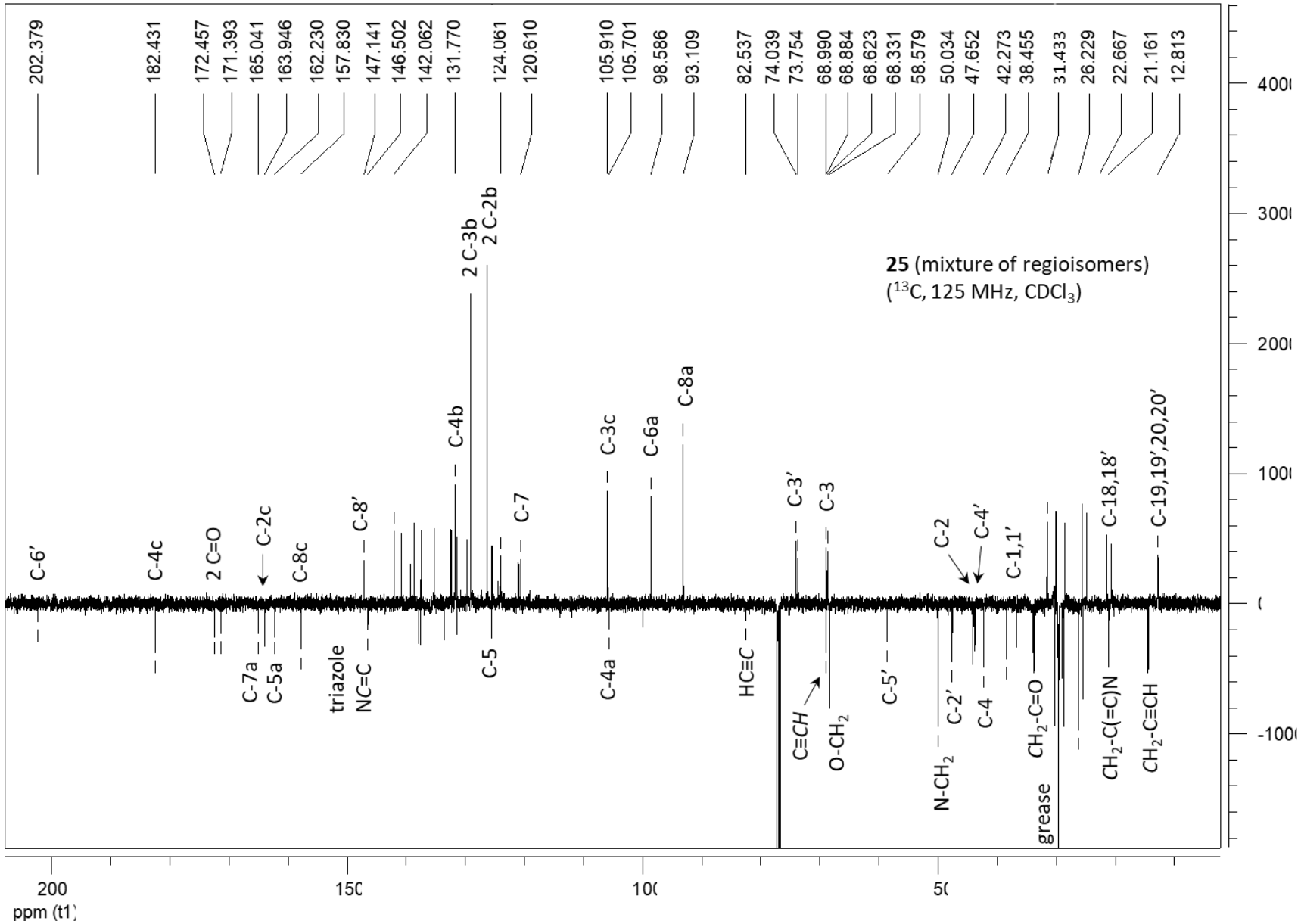


Figure S41. ^{13}C-apt NMR spectrum of the mixture of regioisomers of chrysin-capsanthin conjugate (**25**)