

Supplementary materials

Lutein isomers: preparation, separation, structure elucidation and occurrence in twenty medicinal plants

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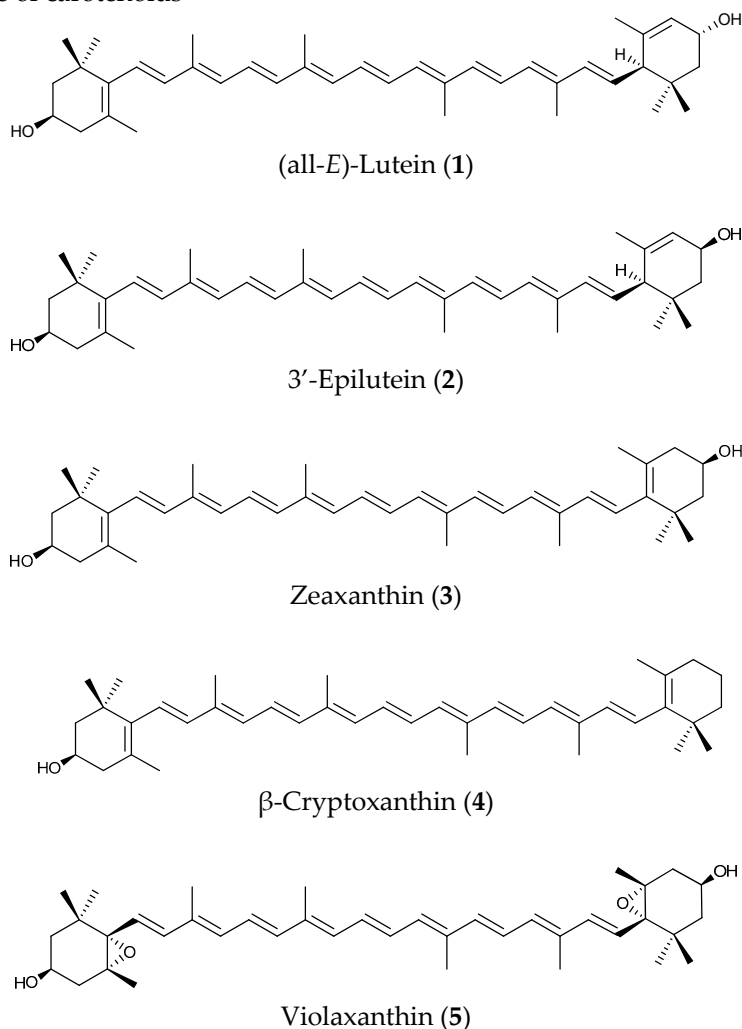
¹ Department of Biochemistry and Medical Chemistry, Medical School, University of Pécs, Szigeti út 12., H-7624 Pécs, Hungary

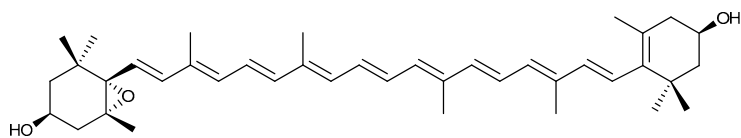
² Department of Pharmacognosy, Faculty of Pharmacy, University of Pécs, Rókus u. 2., H-7624 Pécs, Hungary

³ Institute of Bioanalytics, Medical School, University of Pécs, Szigeti út 12., H-7624 Pécs, Hungary

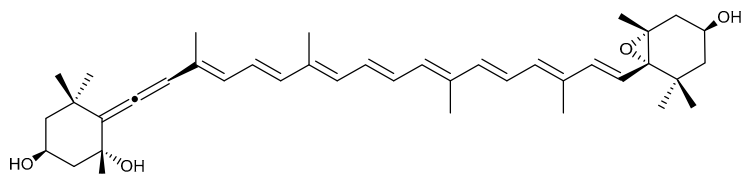
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Figure S1. Structure of carotenoids

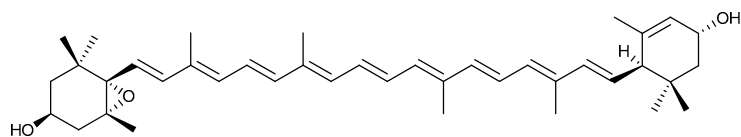




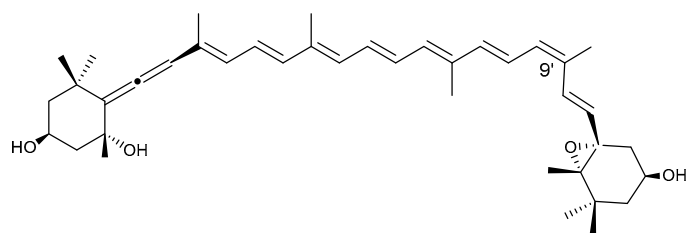
Antheraxanthin (6)



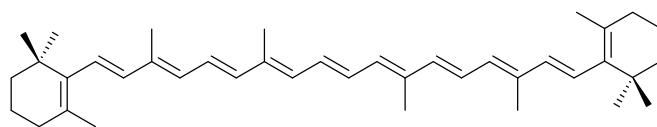
(all-*E*)-Neoxanthin (7)



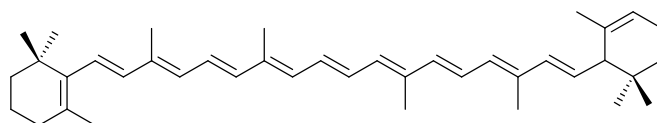
Lutein 5,6-epoxide (8)



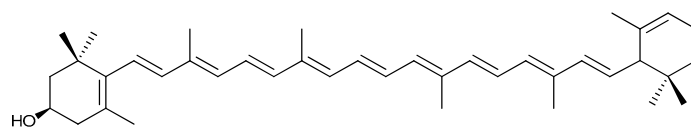
(9'*Z*)-Neoxanthin (9)



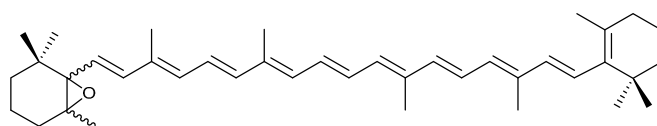
β-Carotene (10)



α-Carotene (11)



α-Cryptoxanthin (12)



β-Carotene 5,6-epoxide (13)

Figure S2. NMR spectra of lutein isomers, in CDCl₃, (500/125 MHz for ¹H/¹³C)

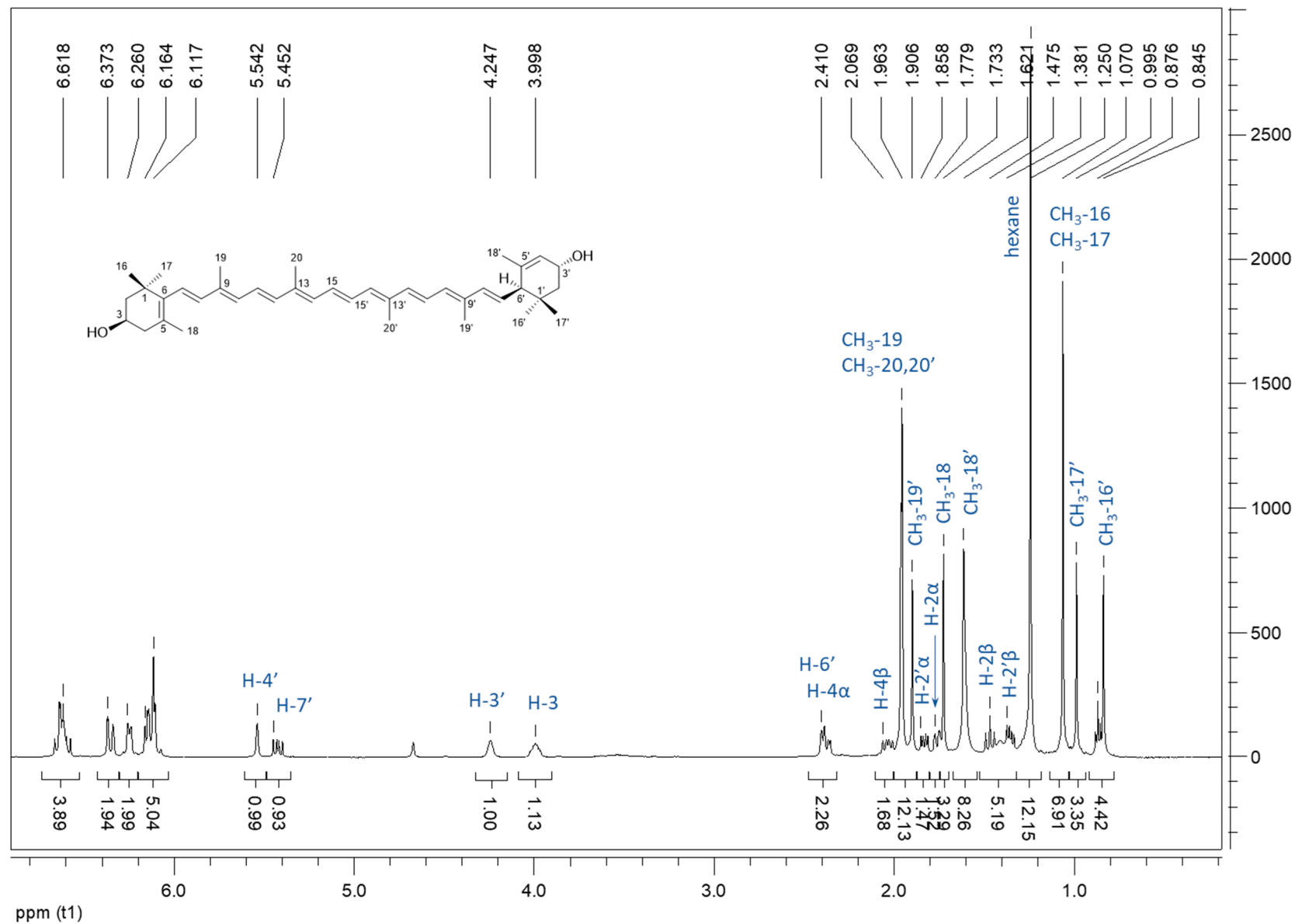


Figure S2.1. ¹H-NMR spectrum of (all-E)-lutein in CDCl₃, (500/125 MHz for ¹H/¹³C)

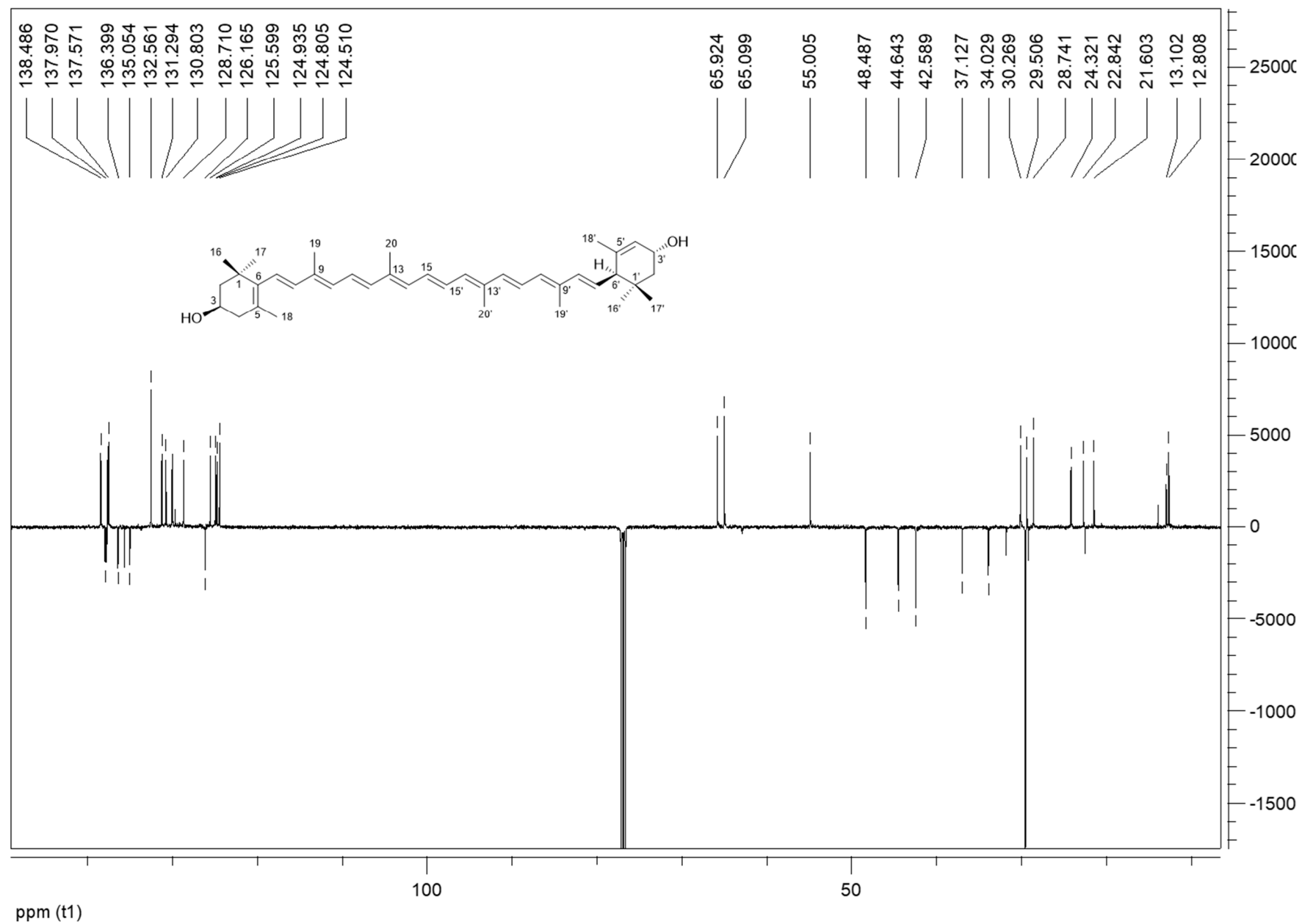


Figure S2.3. ¹³C-NMR spectrum of (all-*E*)-lutein in CDCl₃, (500/125 MHz for ¹H/¹³C)

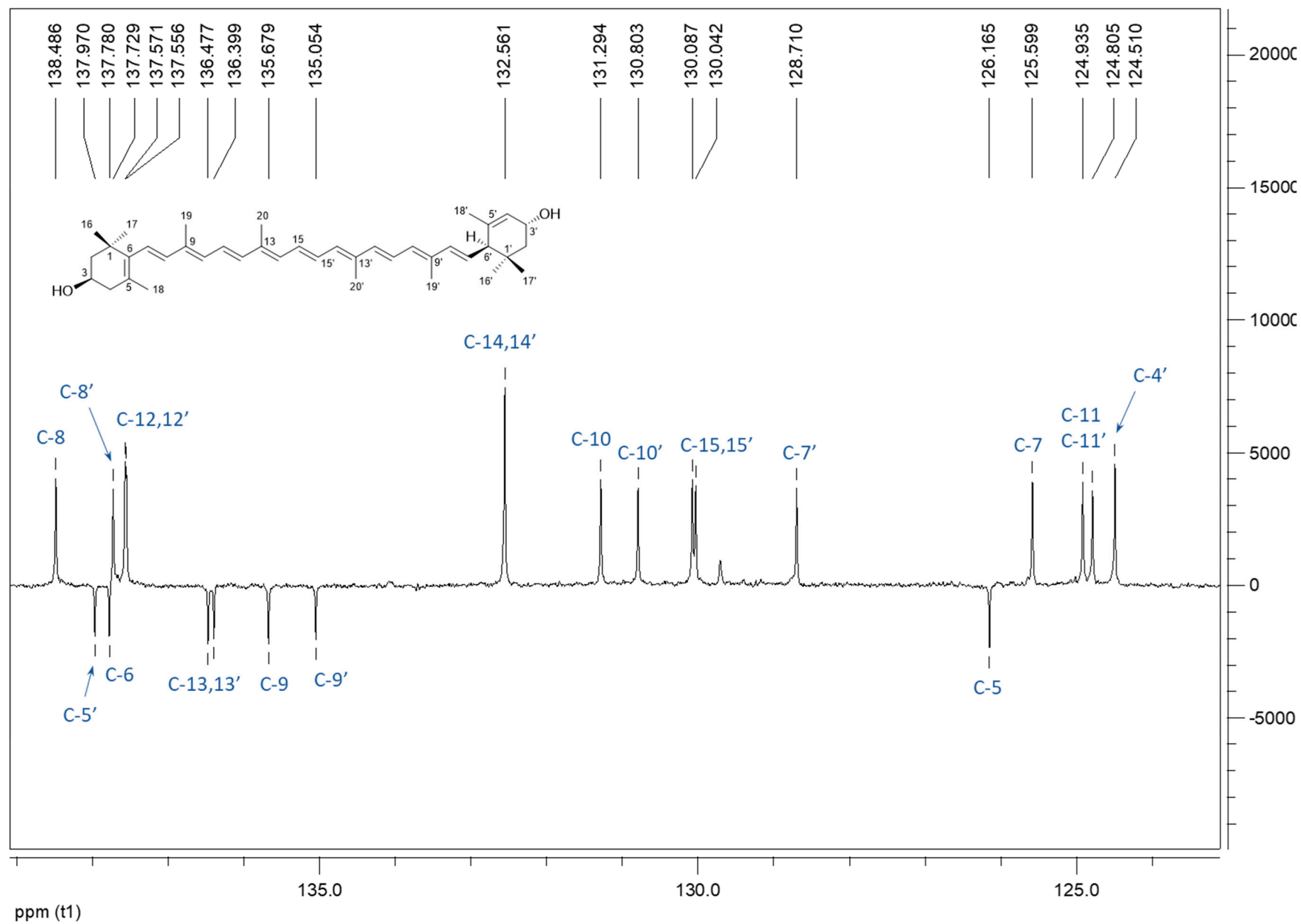


Figure S2.4. ^{13}C -NMR spectrum of (all-*E*)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

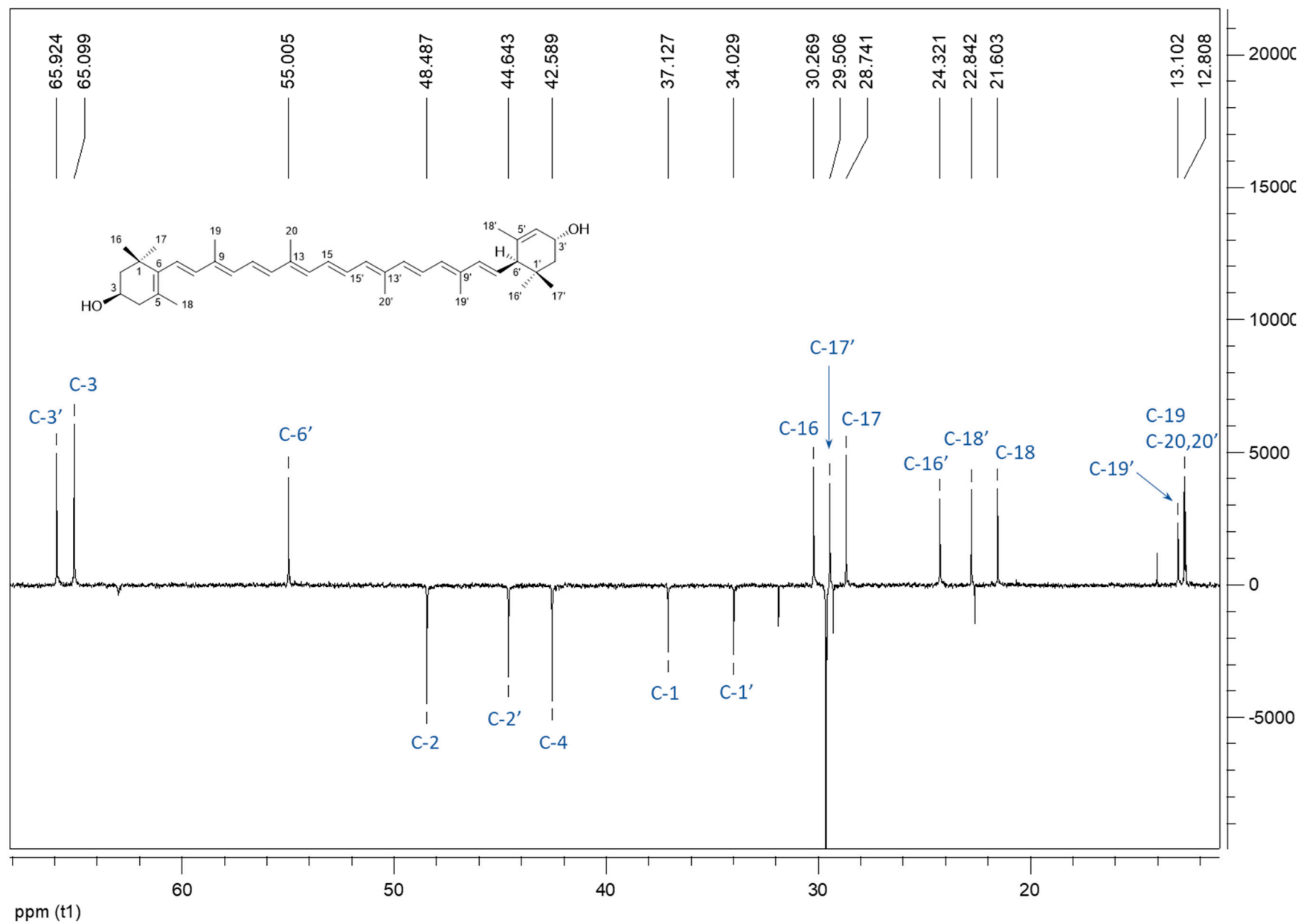


Figure S2.5. ^{13}C -NMR spectrum of (all-*E*)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

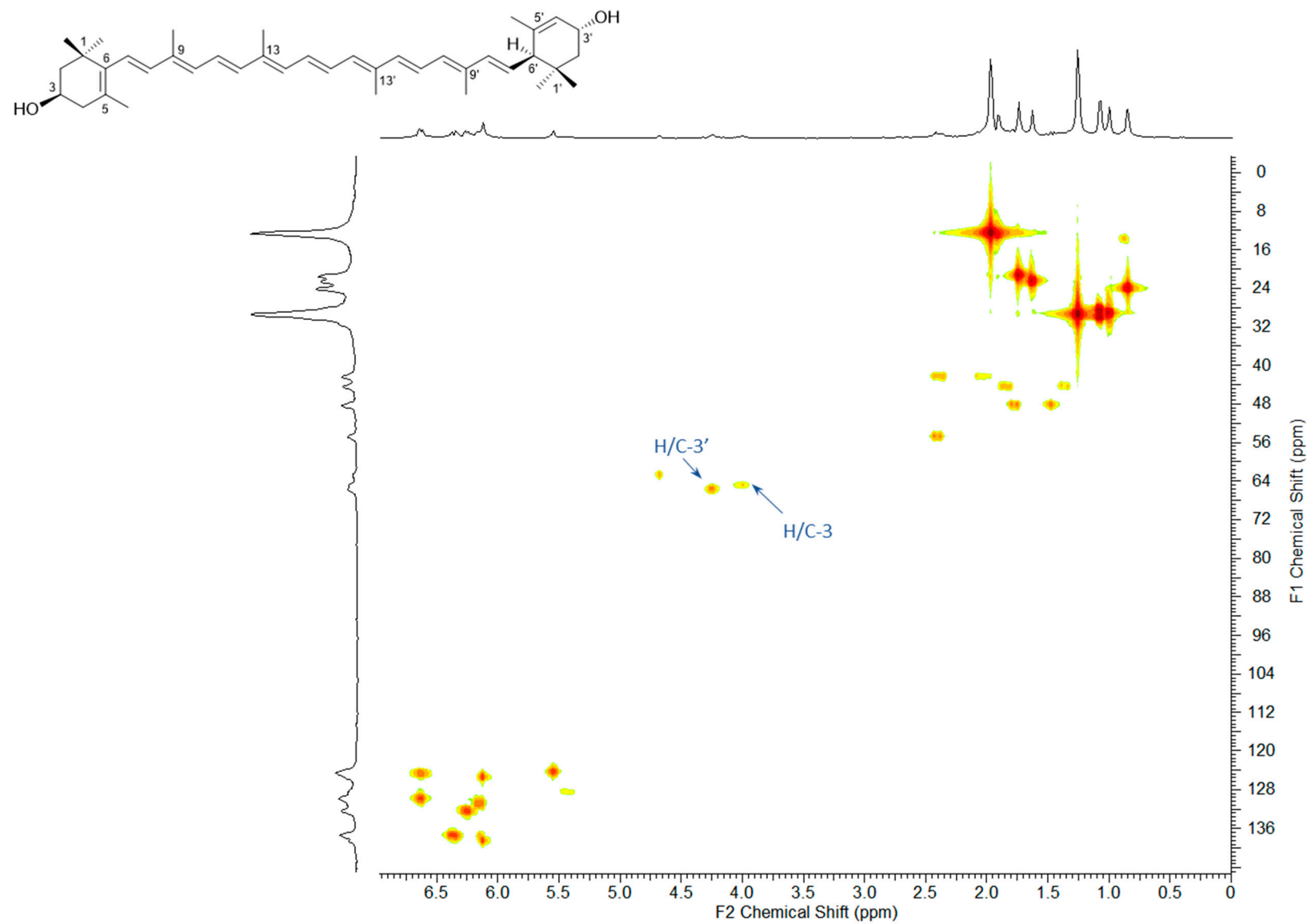


Figure S2.6. ^{13}C - ^1H -HSQC spectrum of (all-*E*)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

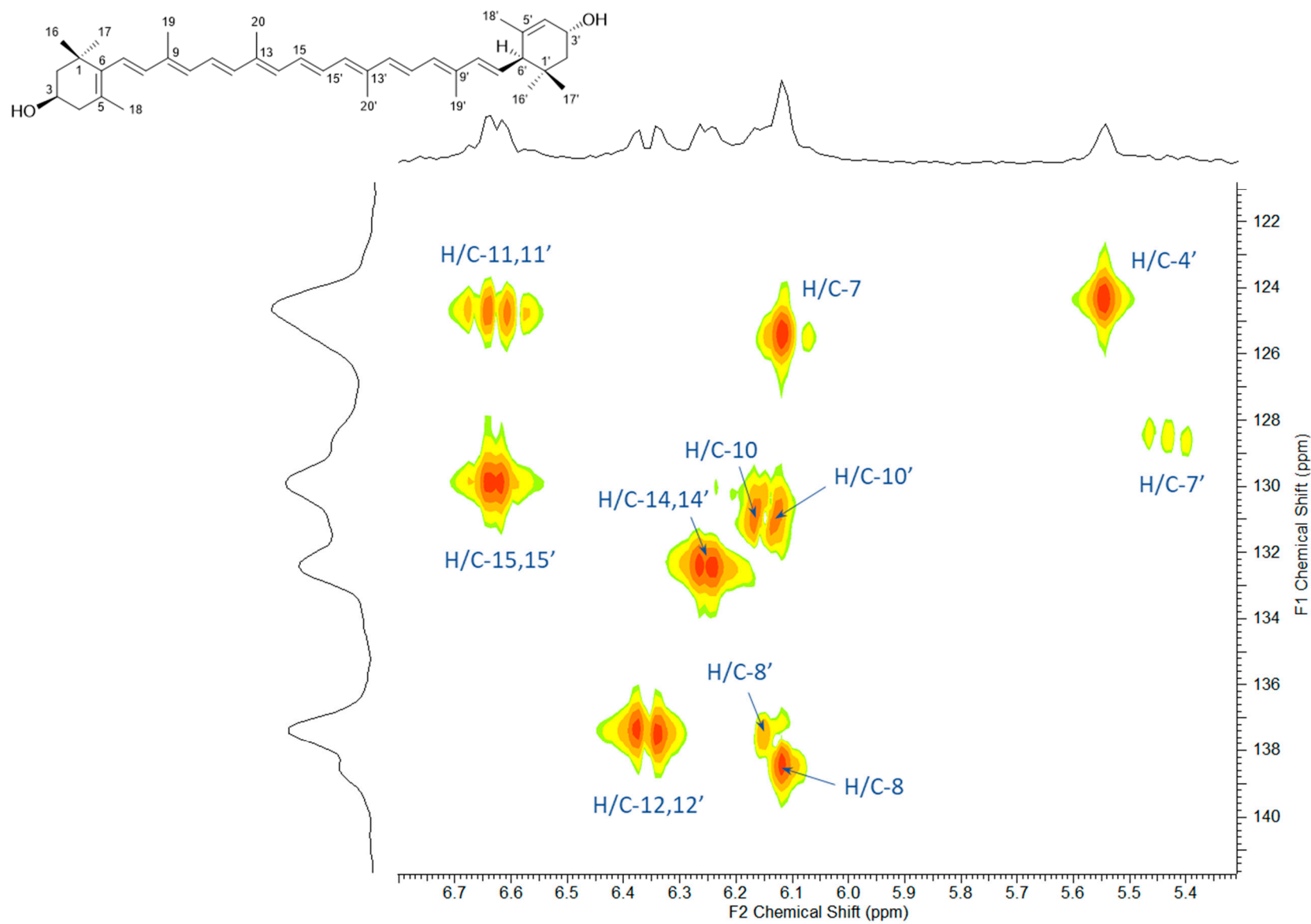


Figure S2.7. ^{13}C - ^1H -HSQC spectrum of (all-*E*)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

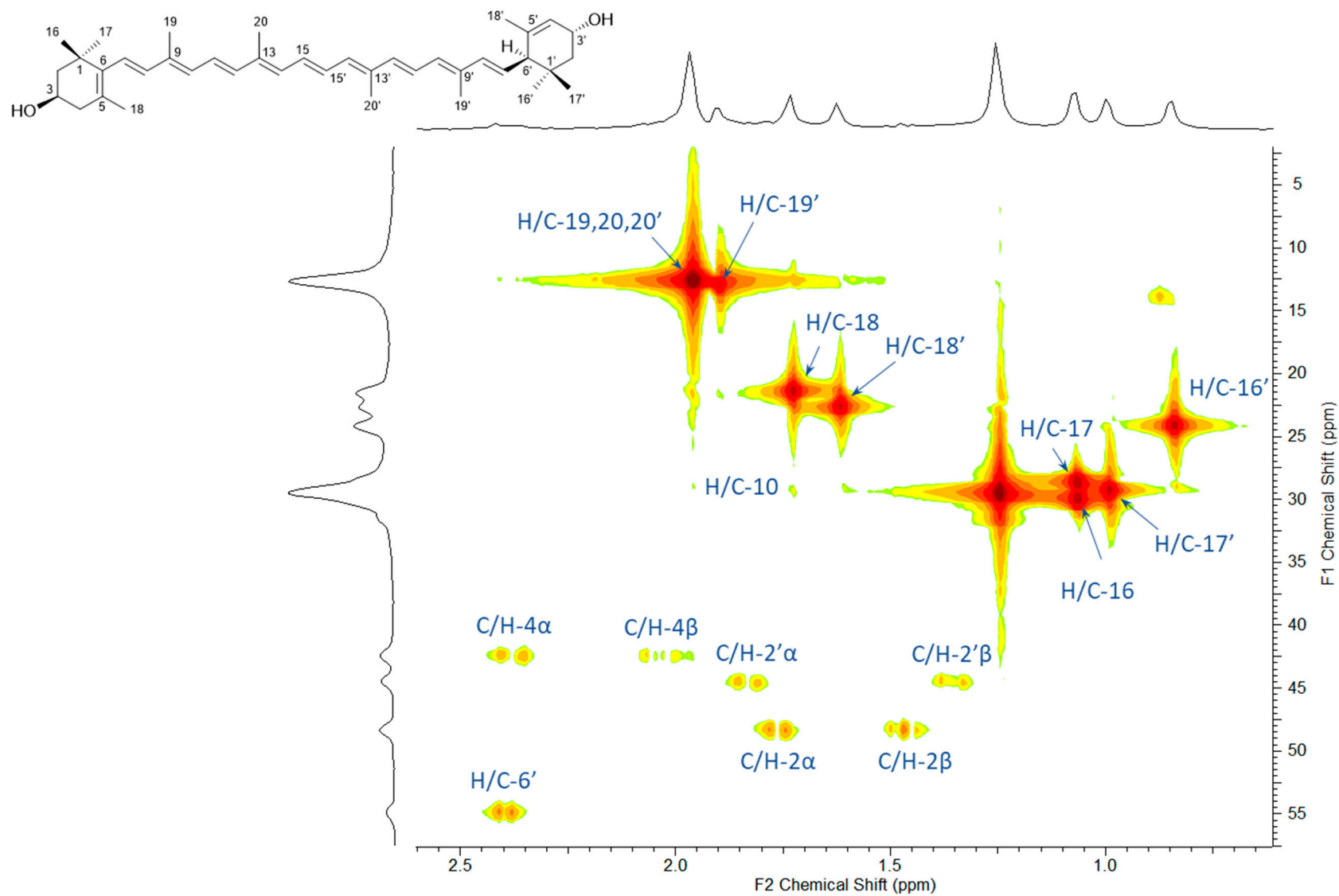


Figure S2.8. ^{13}C - ^1H -HSQC spectrum of (all-*E*)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

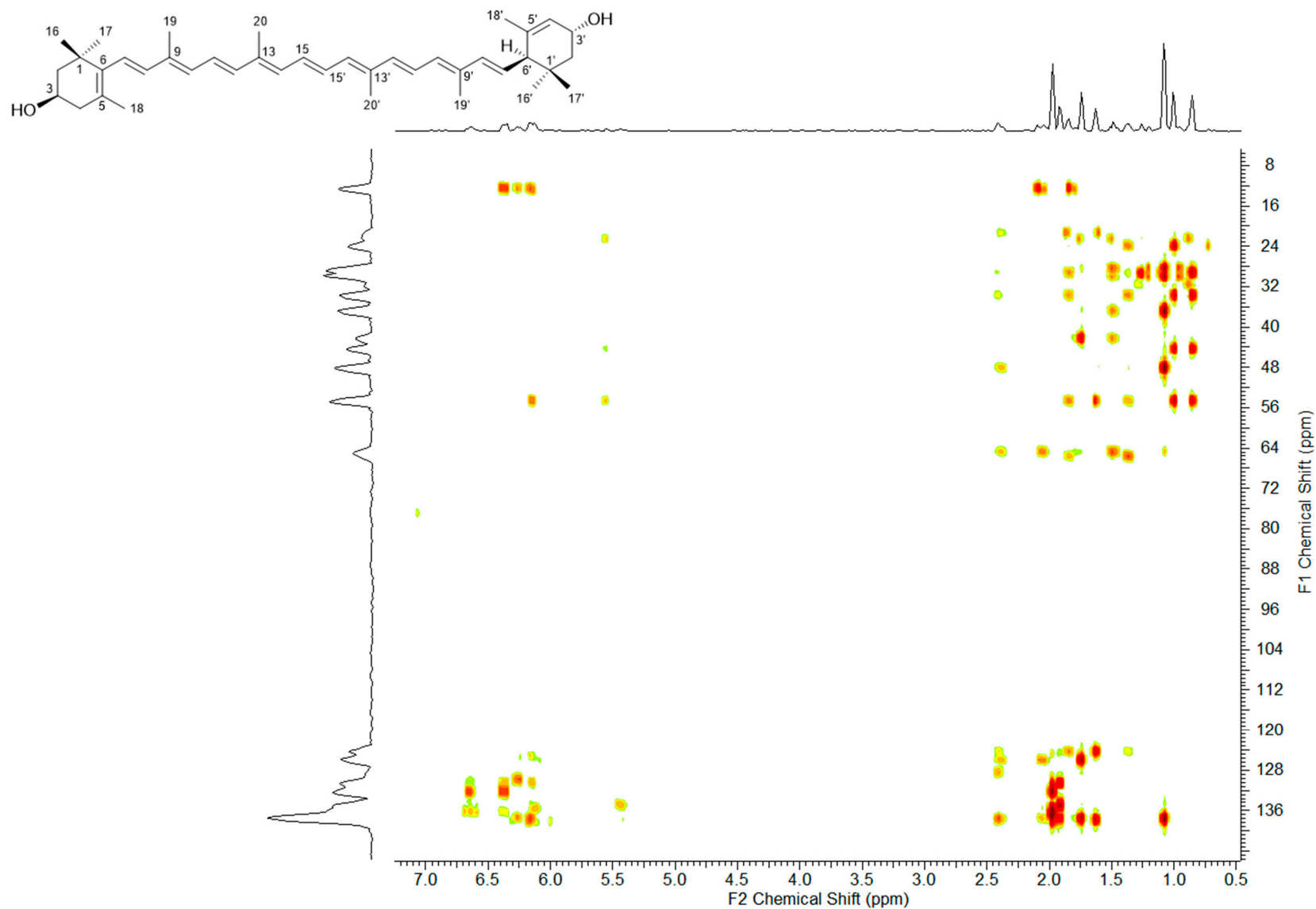


Figure S2.9. ^{13}C - ^1H -HMBC spectrum of (all-*E*)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

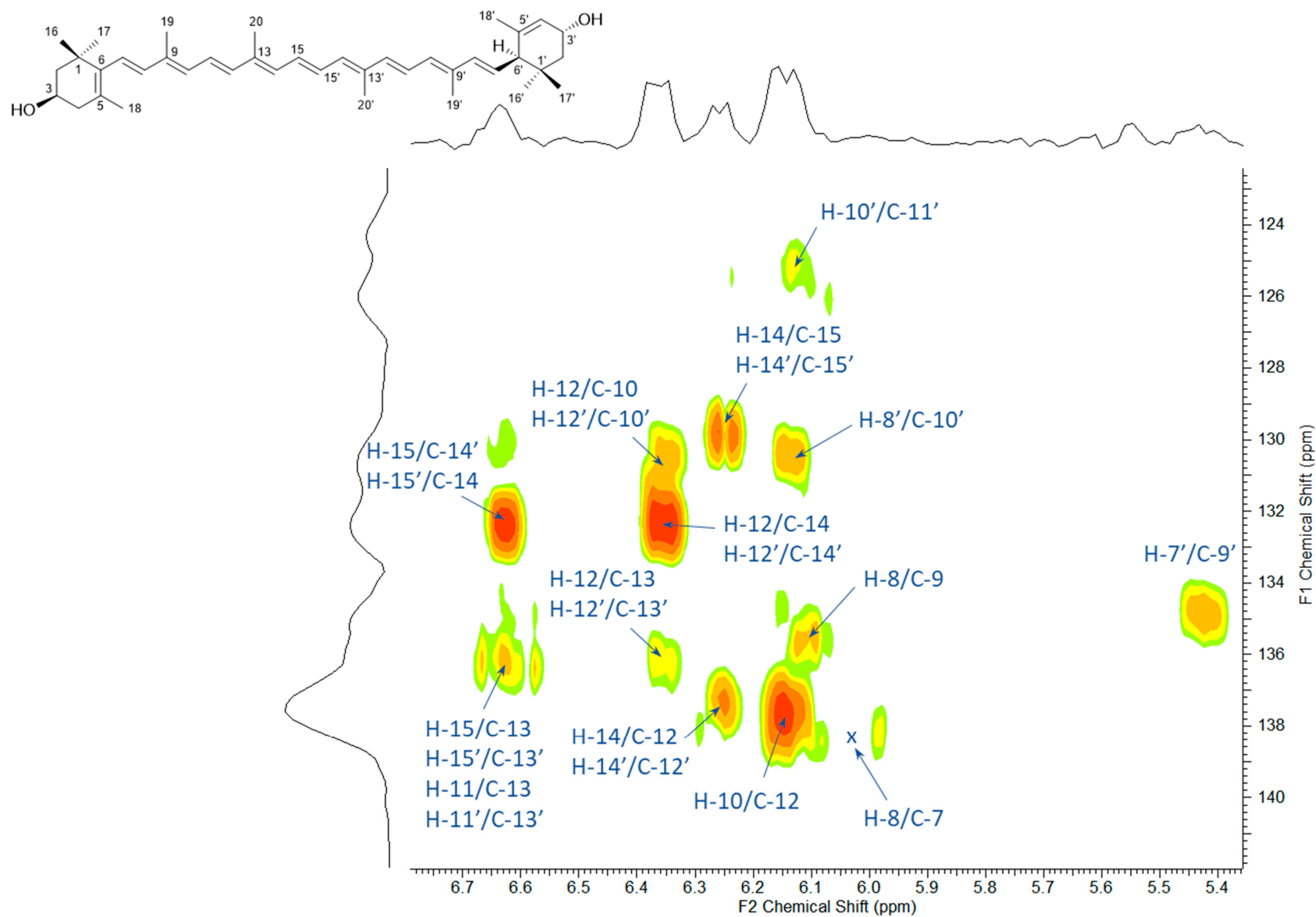


Figure S2.10. ^{13}C - ^1H -HMBC spectrum of (all-*E*)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

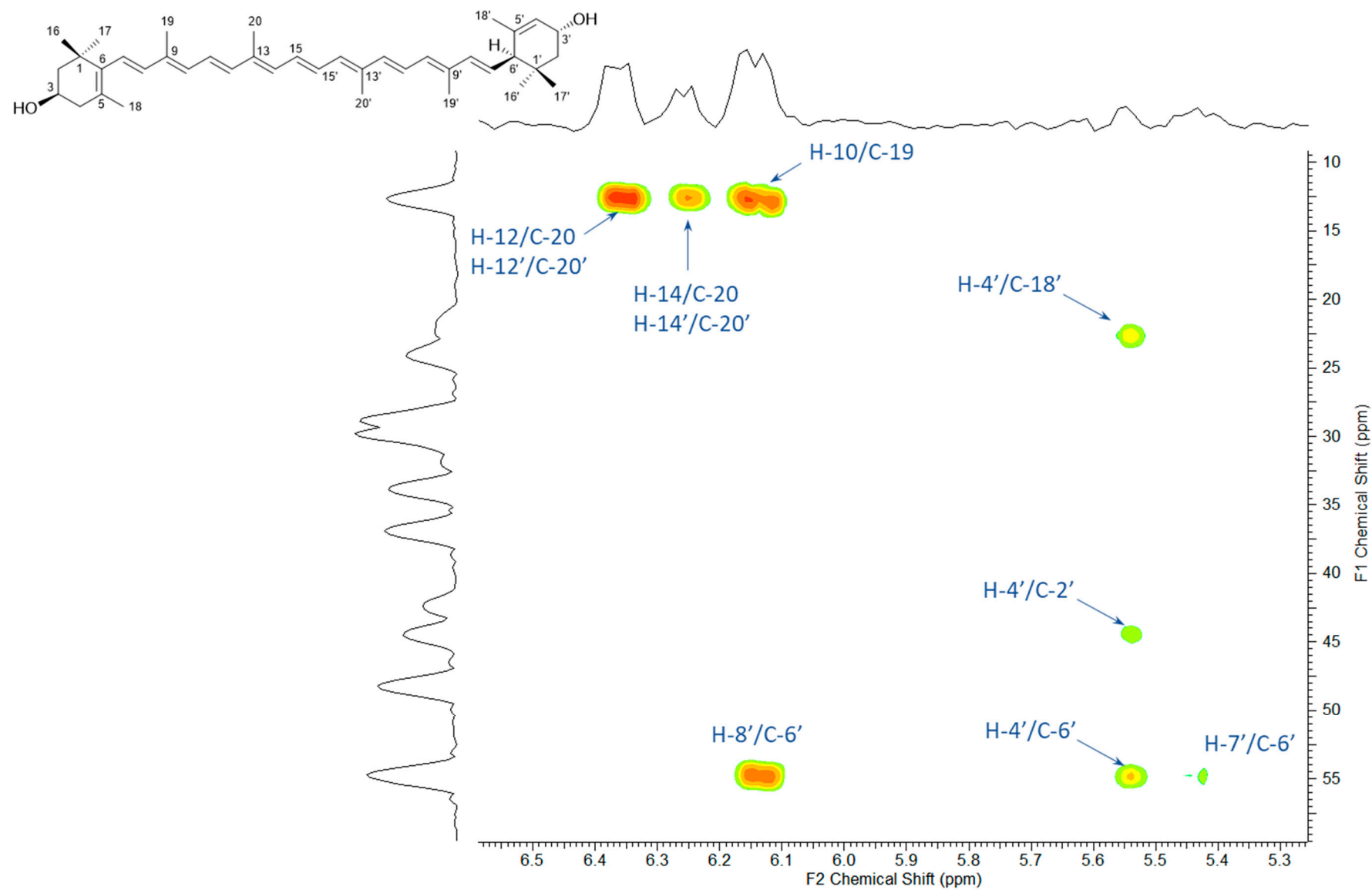


Figure S2.11. ^{13}C - ^1H -HMBC spectrum of (all-*E*)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

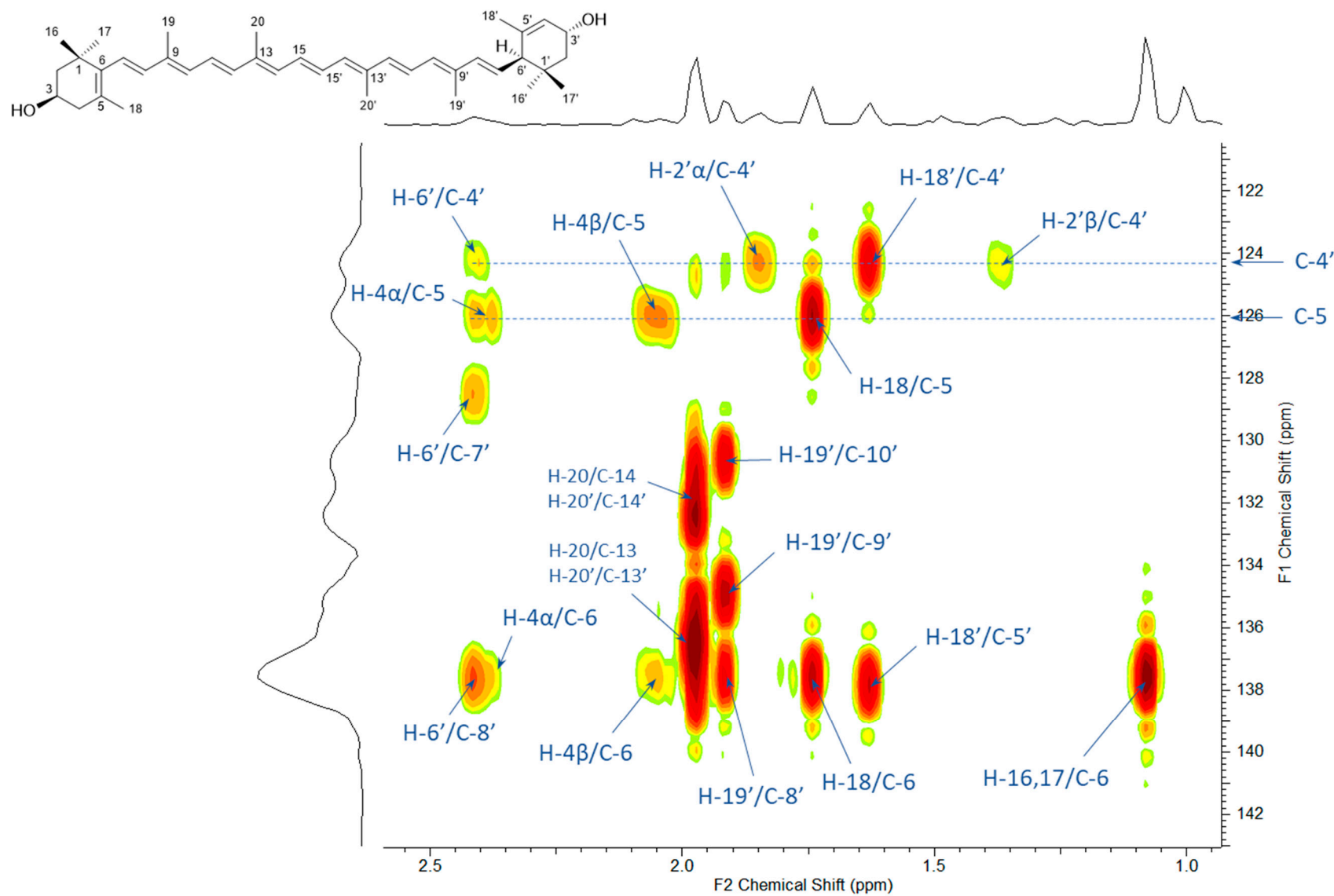


Figure S2.12. ^{13}C - ^1H -HMBC spectrum of (all-*E*)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

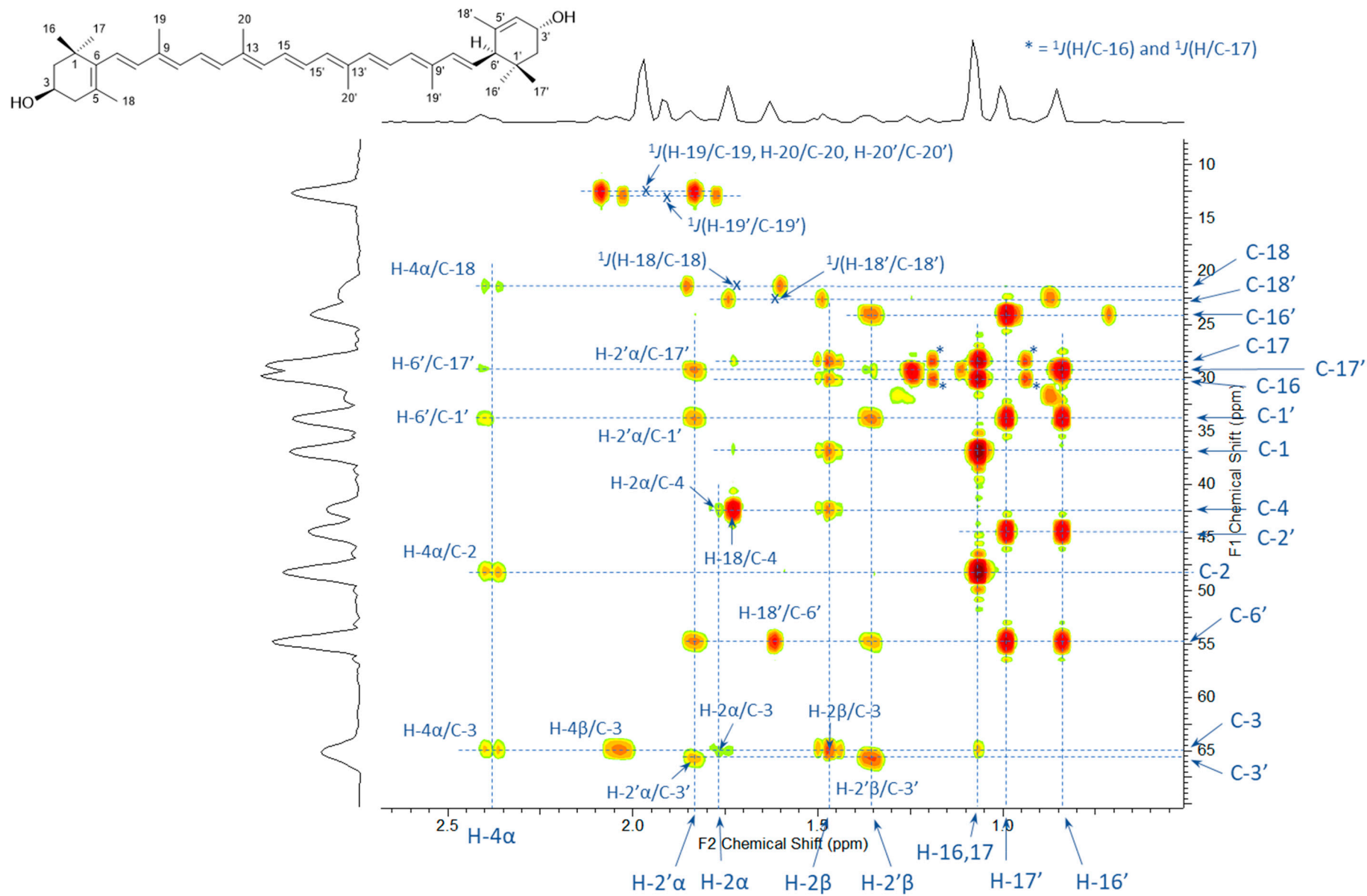


Figure S2.13. ^{13}C - ^1H -HMBC spectrum of (all-*E*)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

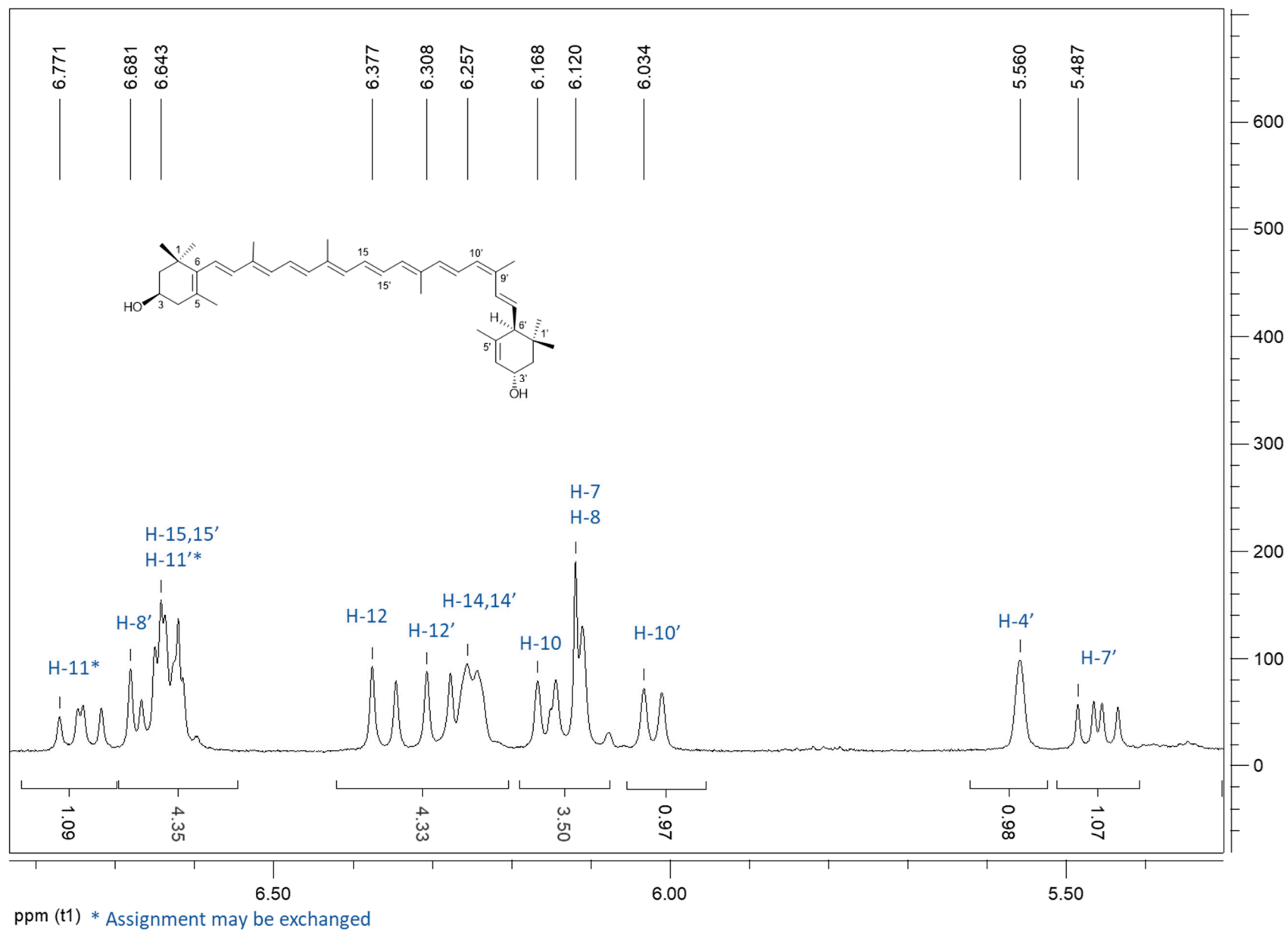


Figure S2.15. ^1H -NMR spectrum of (9'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

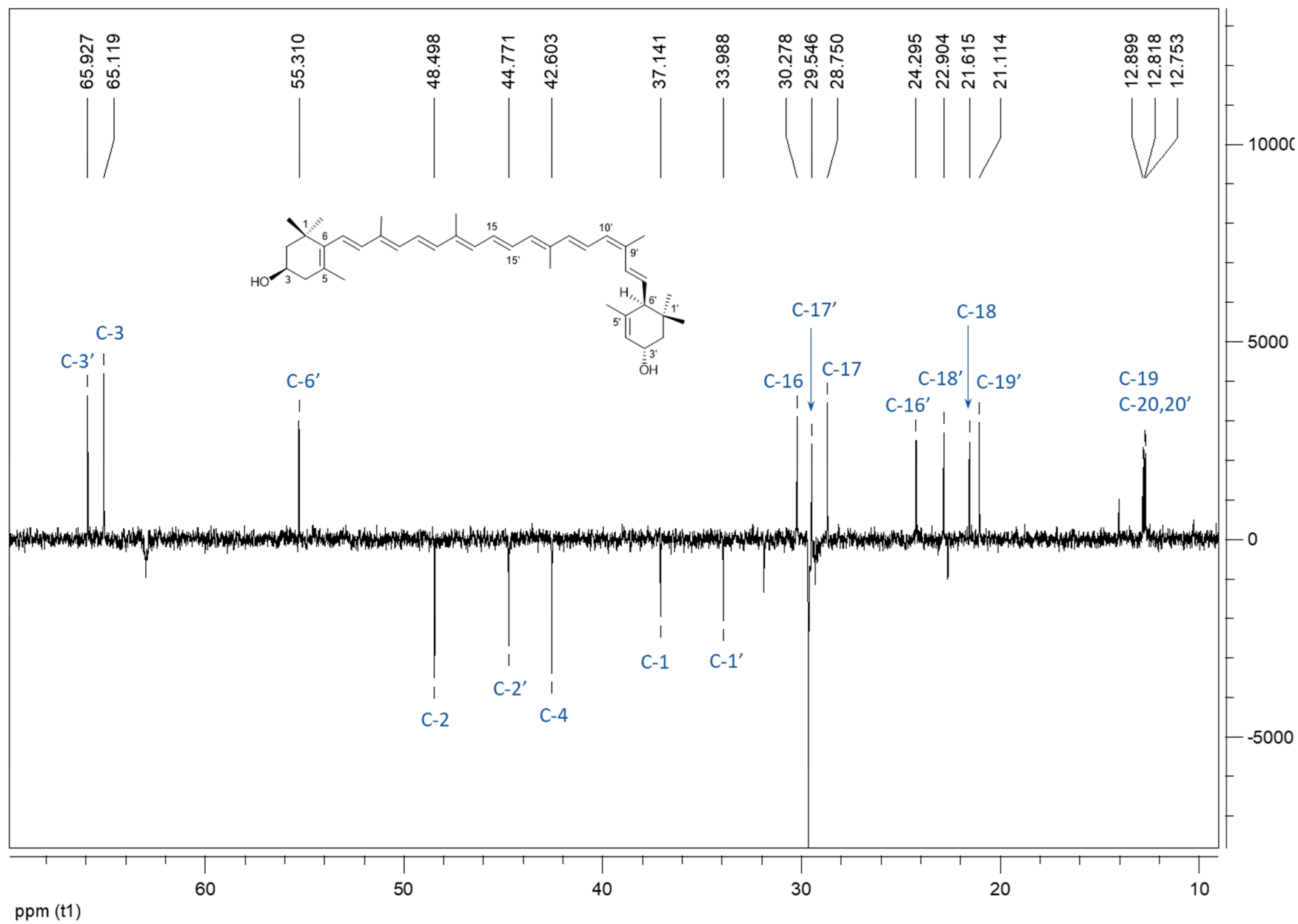


Figure S2.18. ^{13}C -NMR spectrum of (9'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

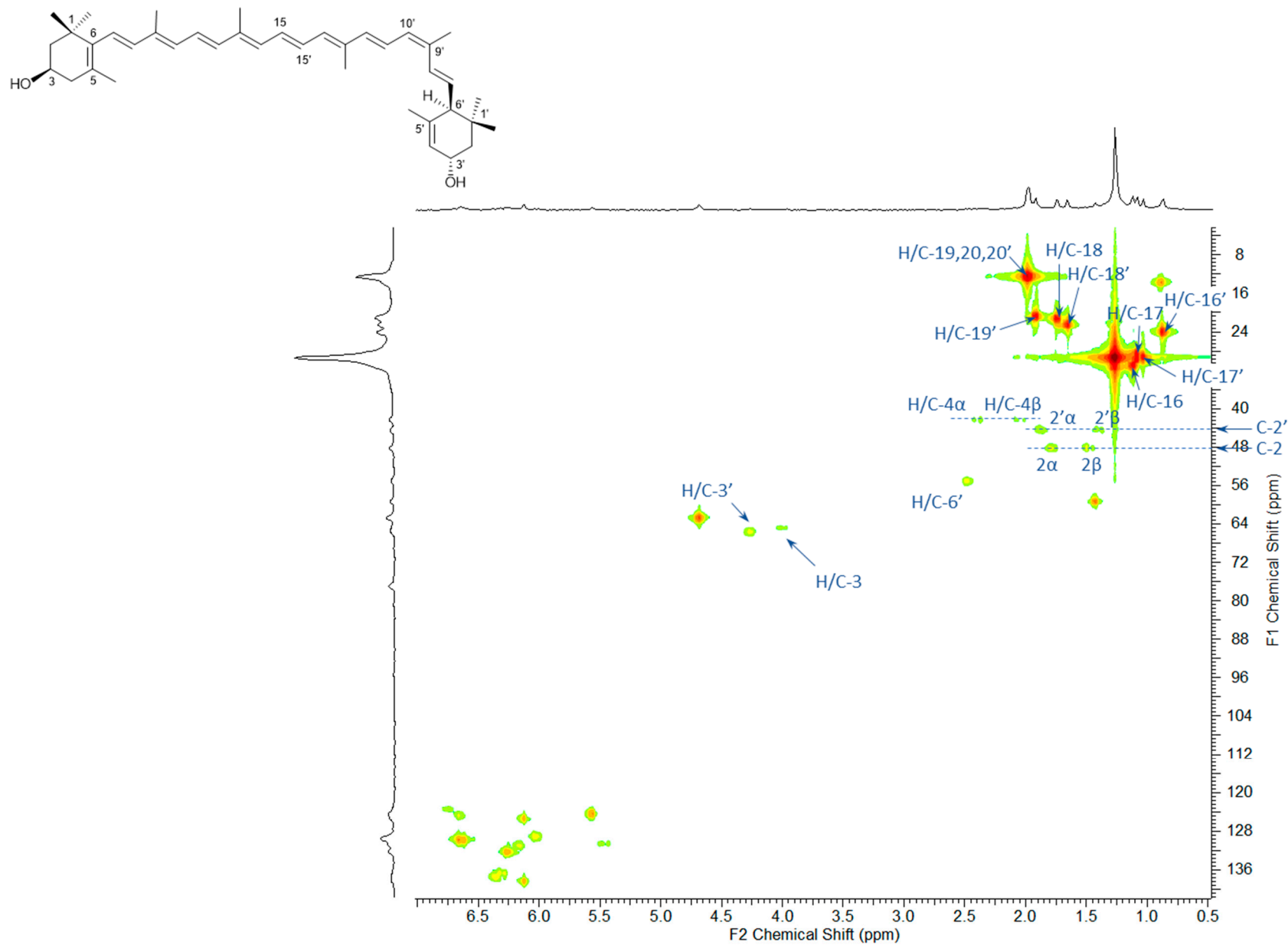


Figure S2.19. ^{13}C - ^1H -HSQC spectrum of (9'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

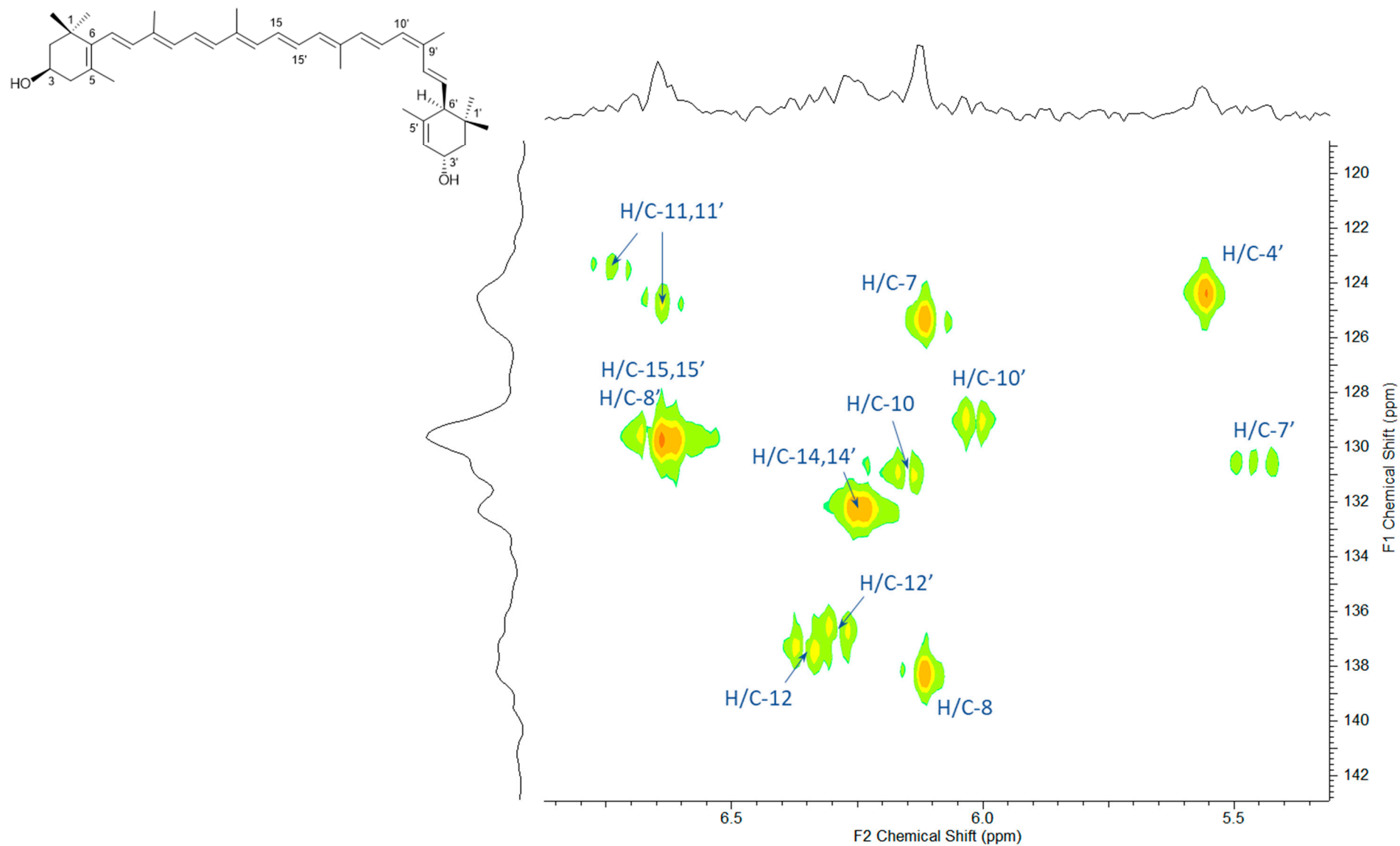


Figure S2.20. ^{13}C - ^1H -HSQC spectrum of (9'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

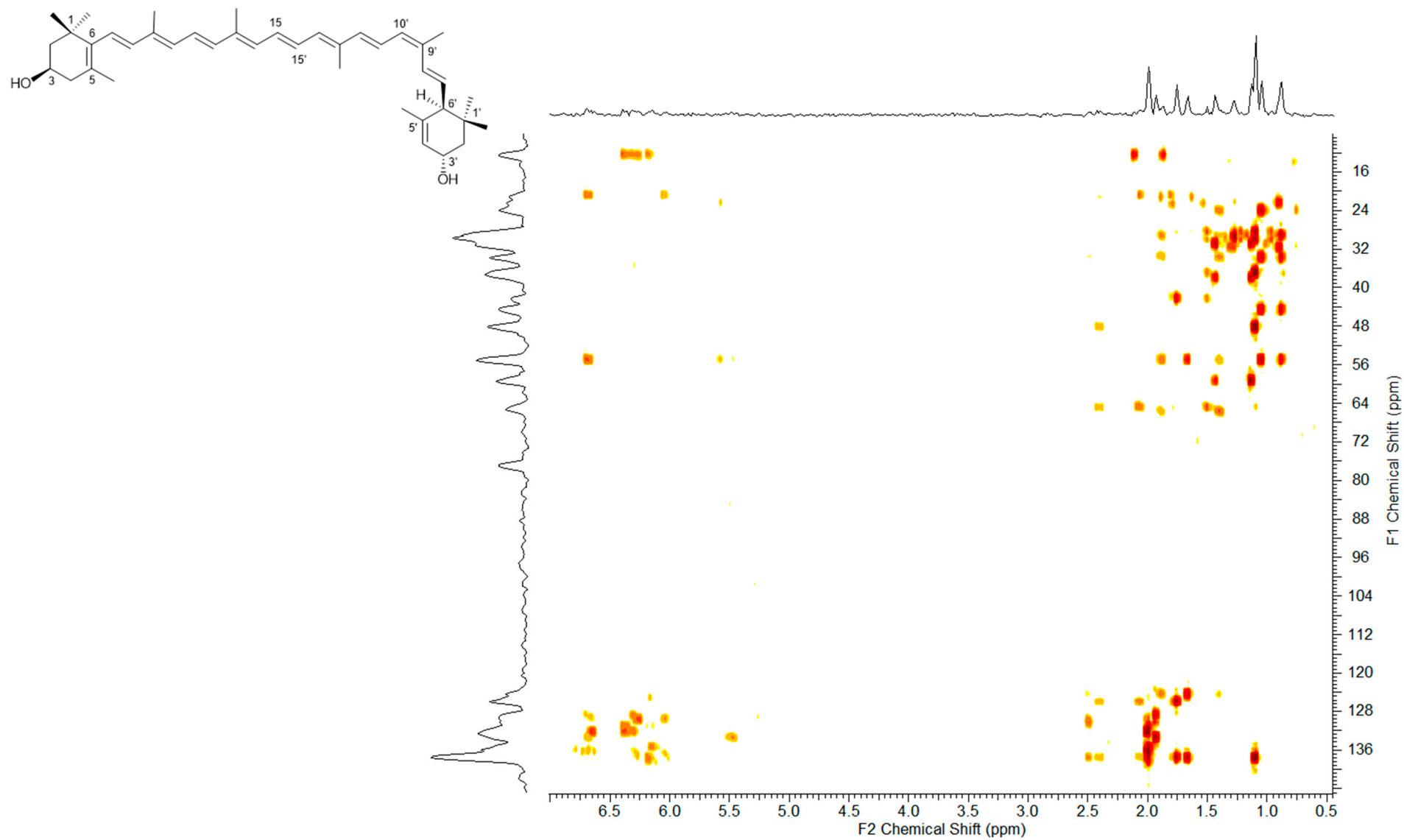


Figure S2.21. ^{13}C - ^1H -HMBC spectrum of (9'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

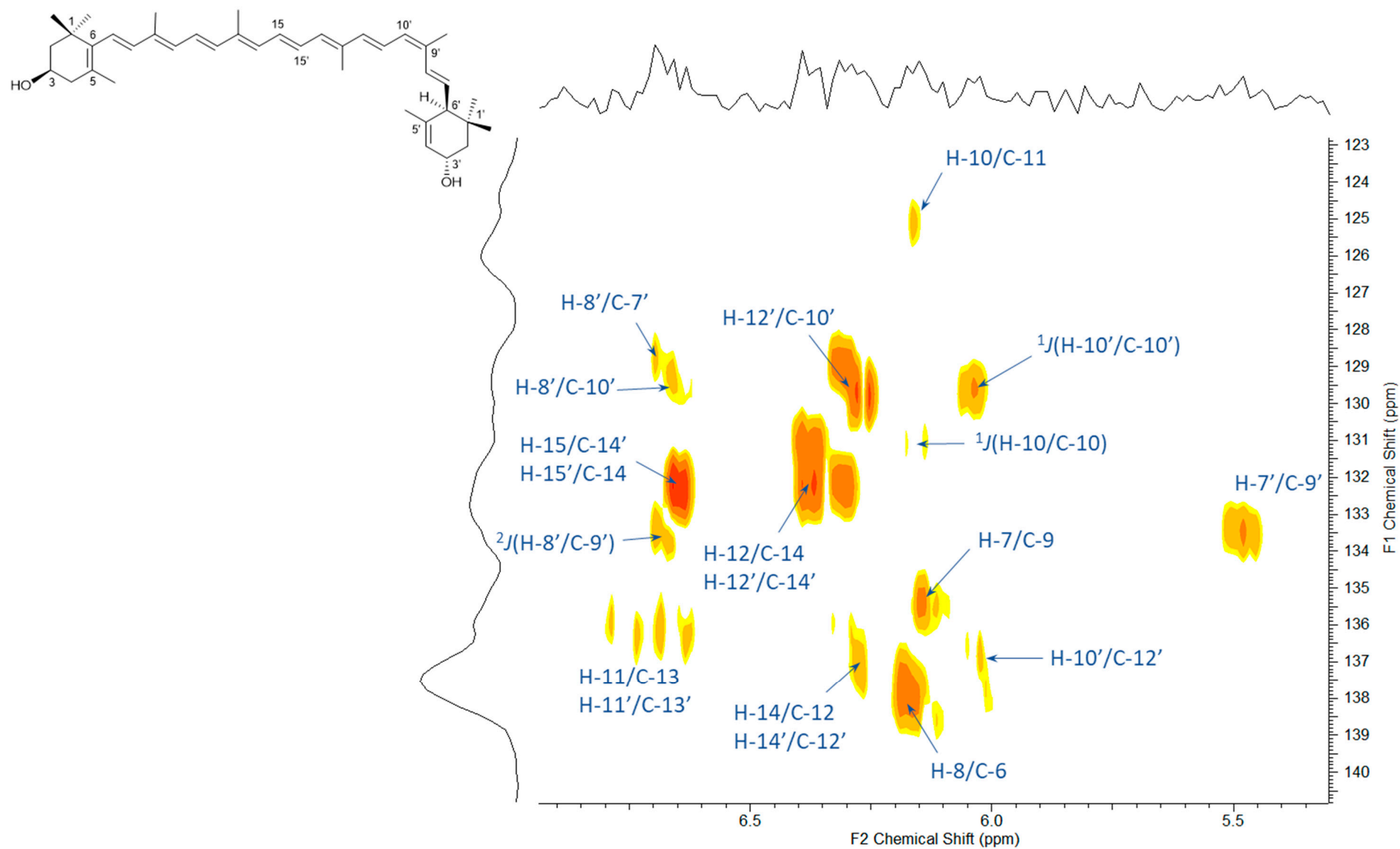


Figure S2.22. ¹³C-¹H-HMBC spectrum of (9'*Z*)-lutein in CDCl₃, (500/125 MHz for ¹H/¹³C)

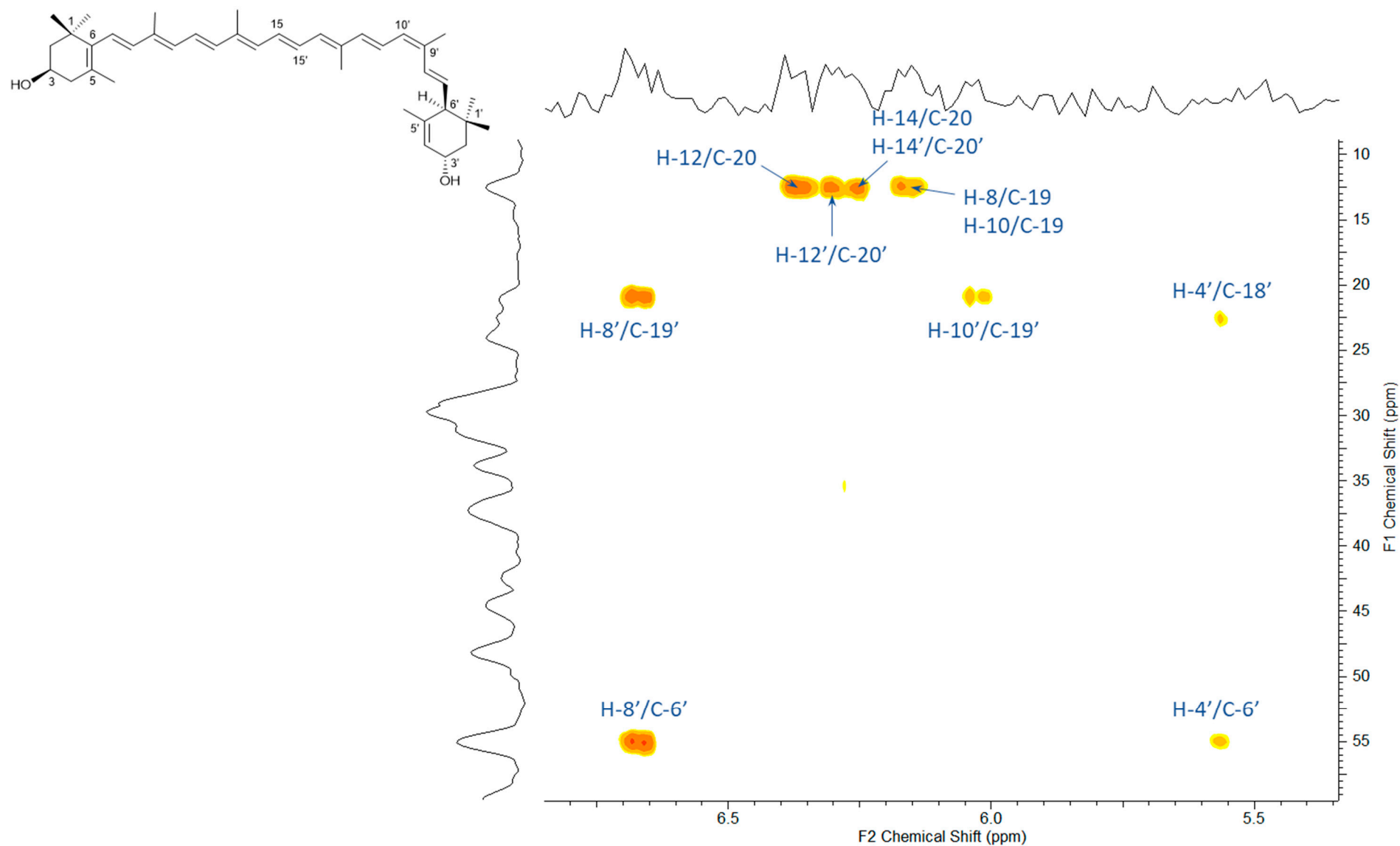


Figure S2.23. ^{13}C - ^1H -HMBC spectrum of (9'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

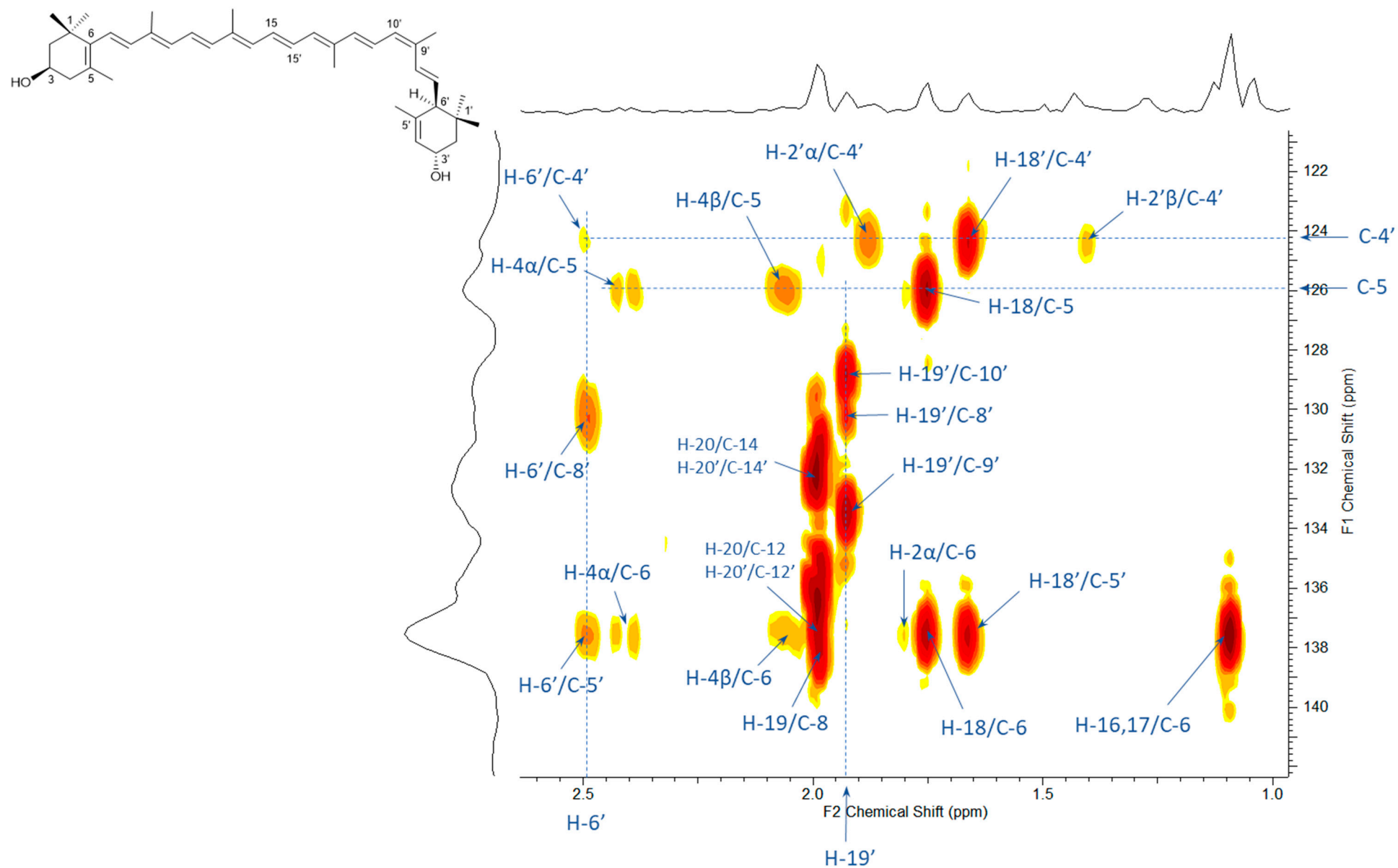


Figure S2.24. ^{13}C - ^1H -HMBC spectrum of (9'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

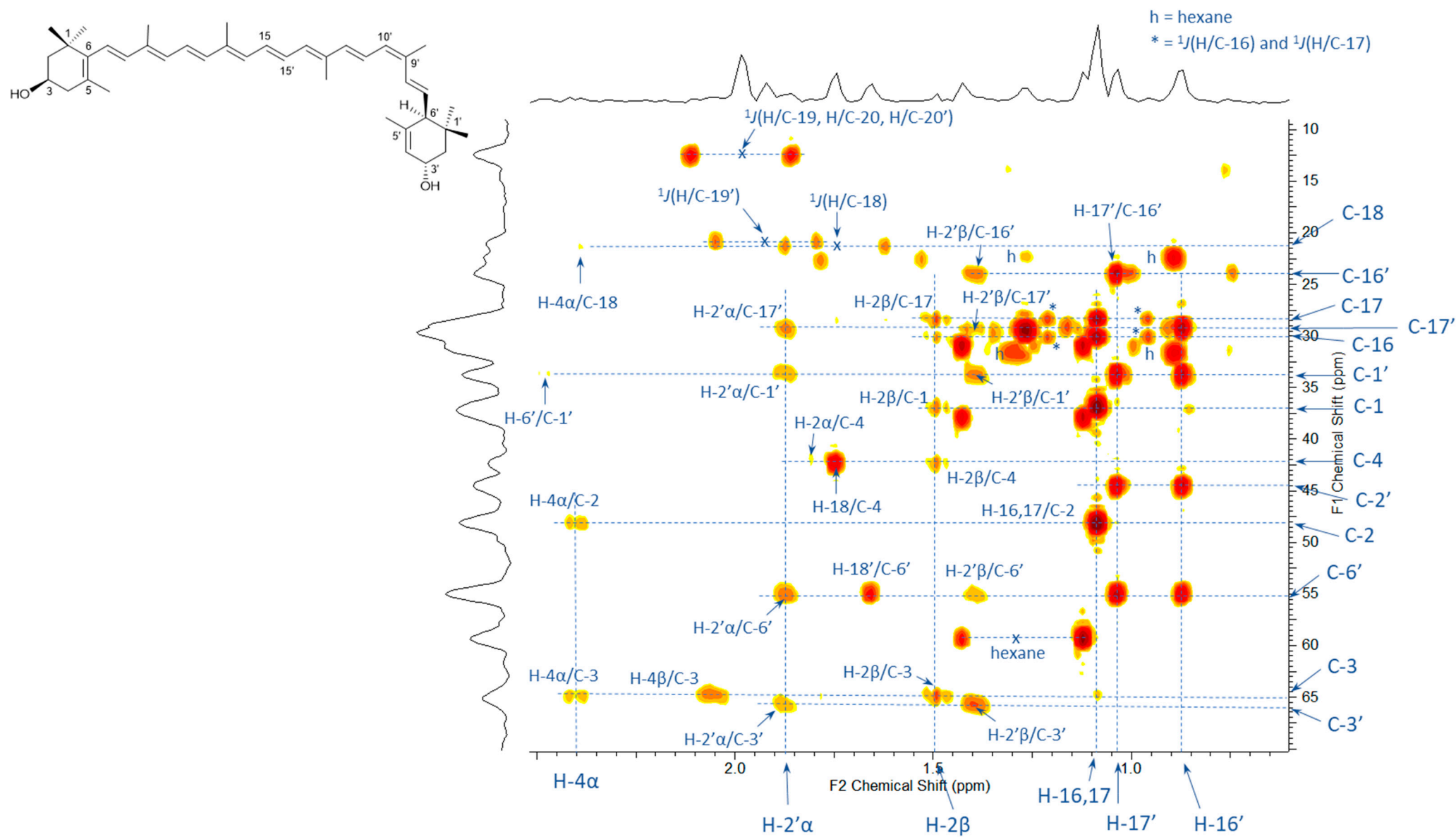


Figure S2.25. ^{13}C - ^1H -HMBC spectrum of (9'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

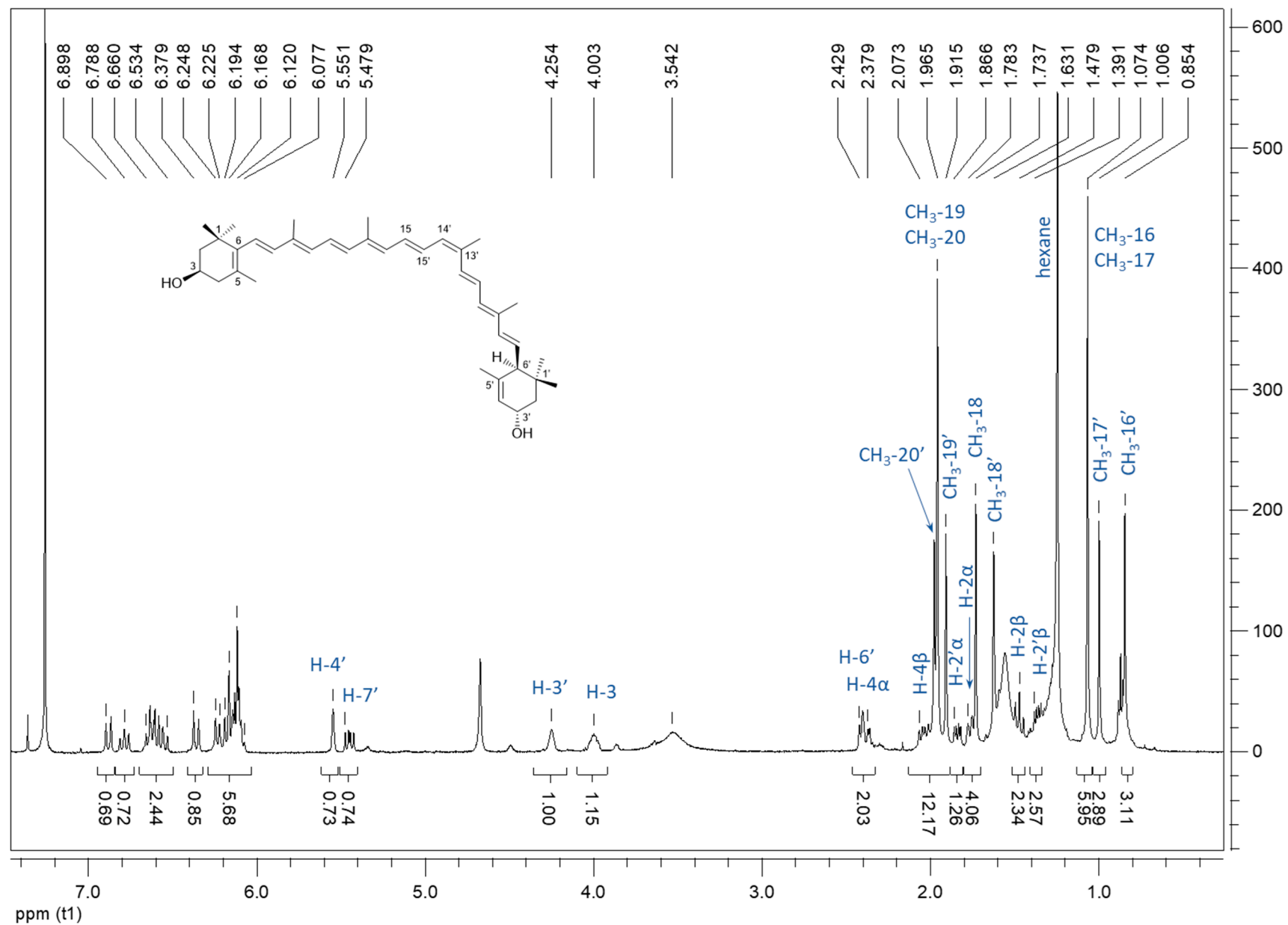


Figure S2.26. ^1H -NMR spectrum of (13'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

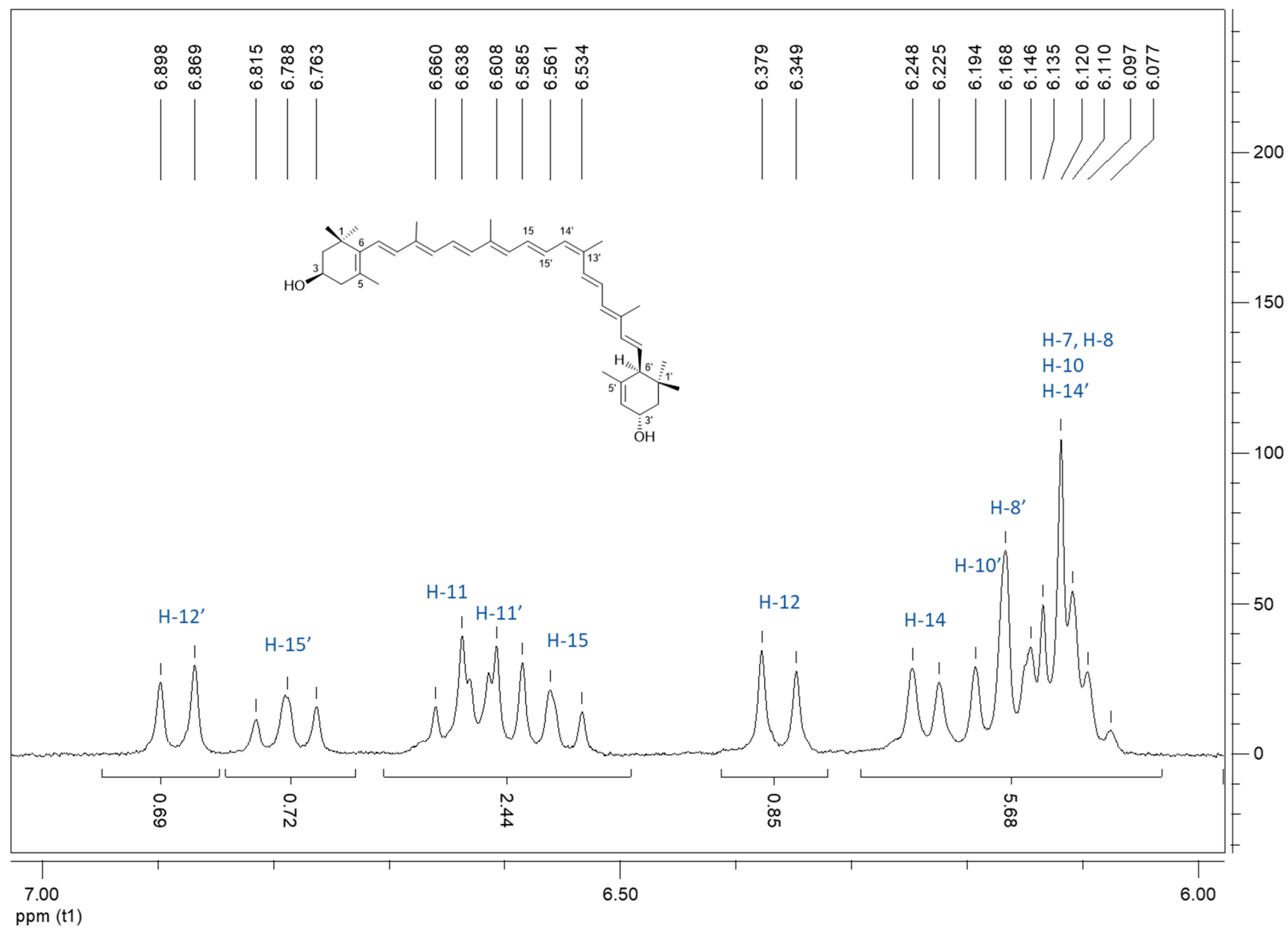


Figure S2.27. ^1H -NMR spectrum of (13'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

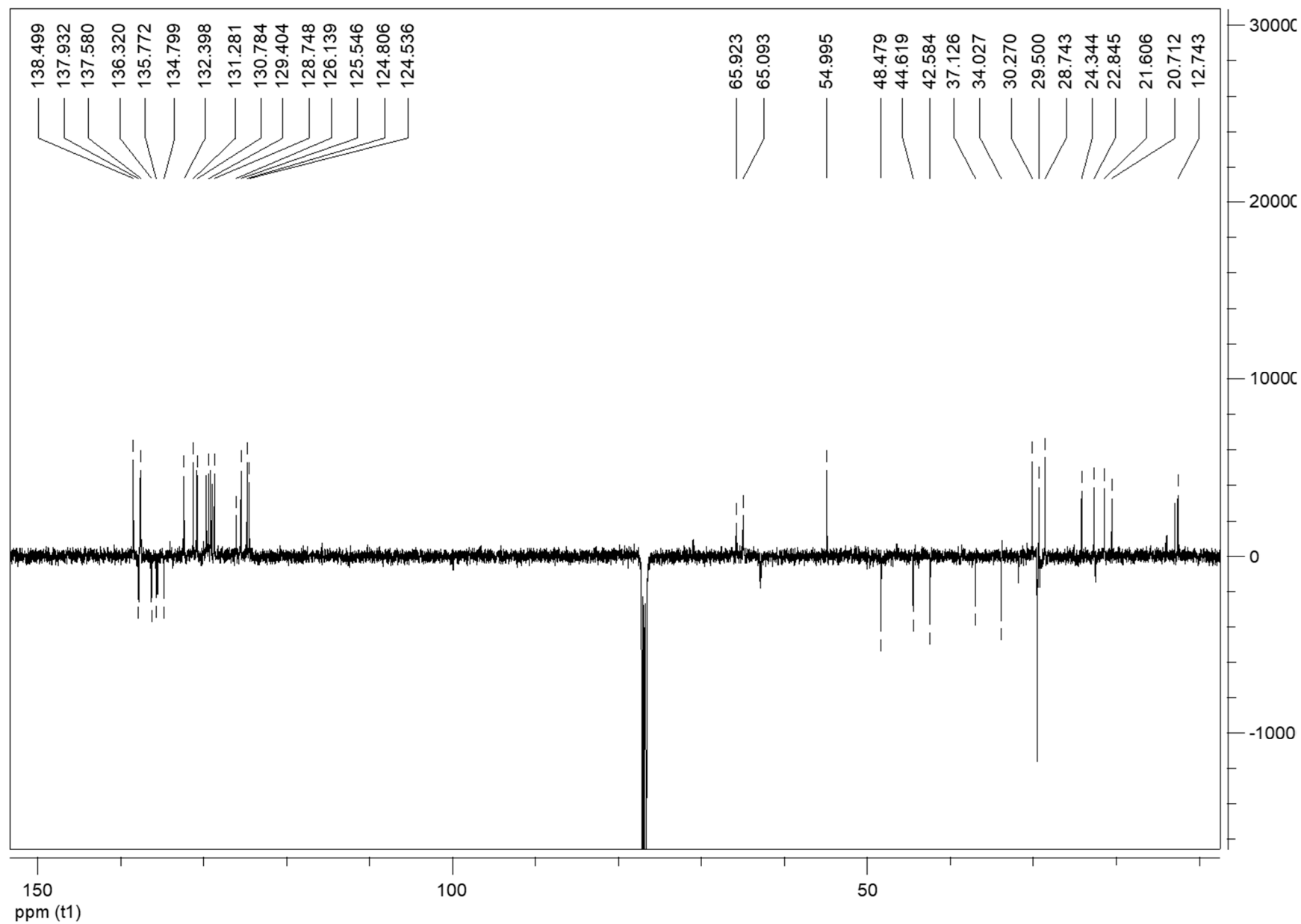


Figure S2.28. ¹³C-NMR spectrum of (13'Z)-lutein in CDCl₃, (500/125 MHz for ¹H/¹³C)

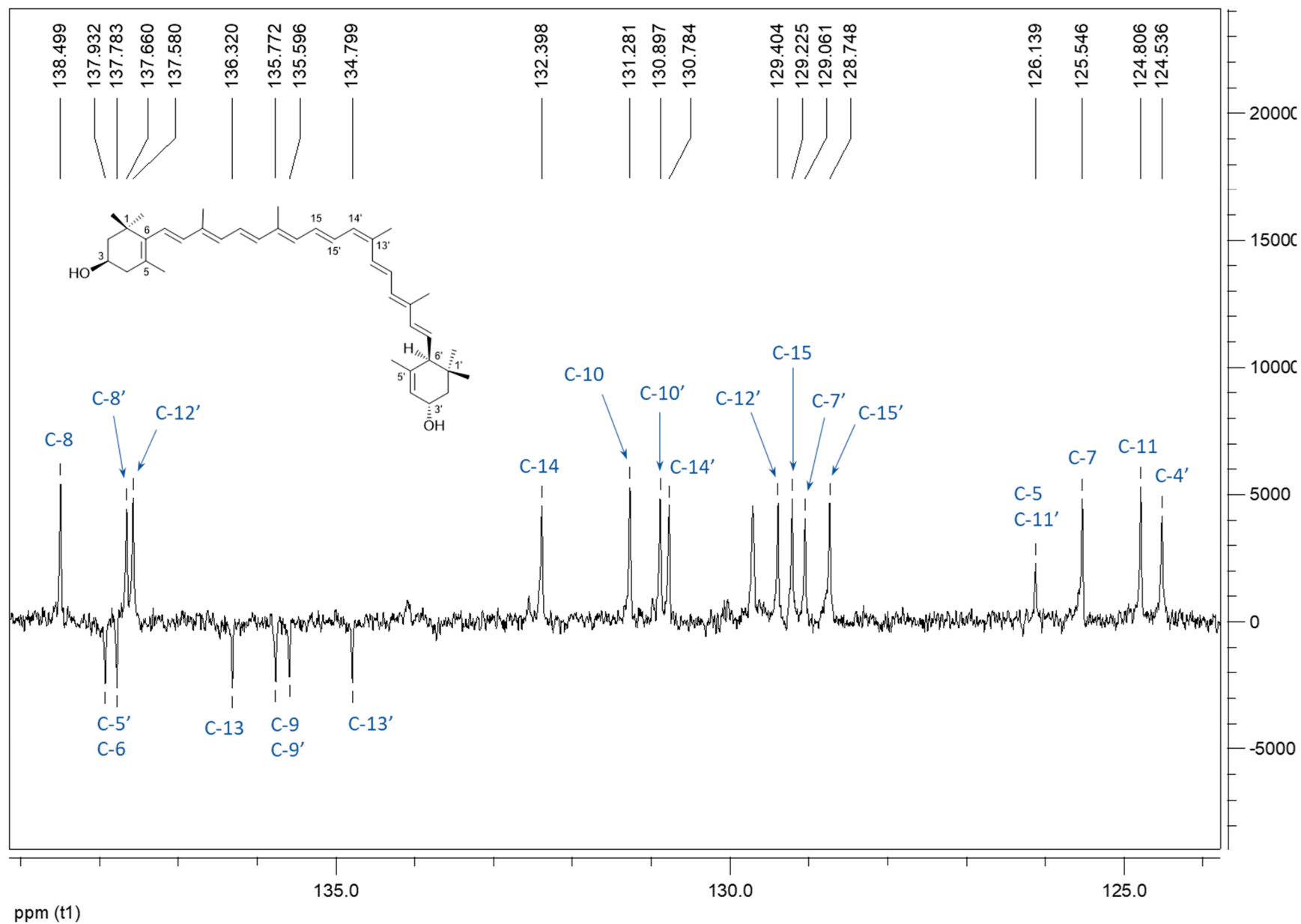


Figure S2.29. ^{13}C -NMR spectrum of (13'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

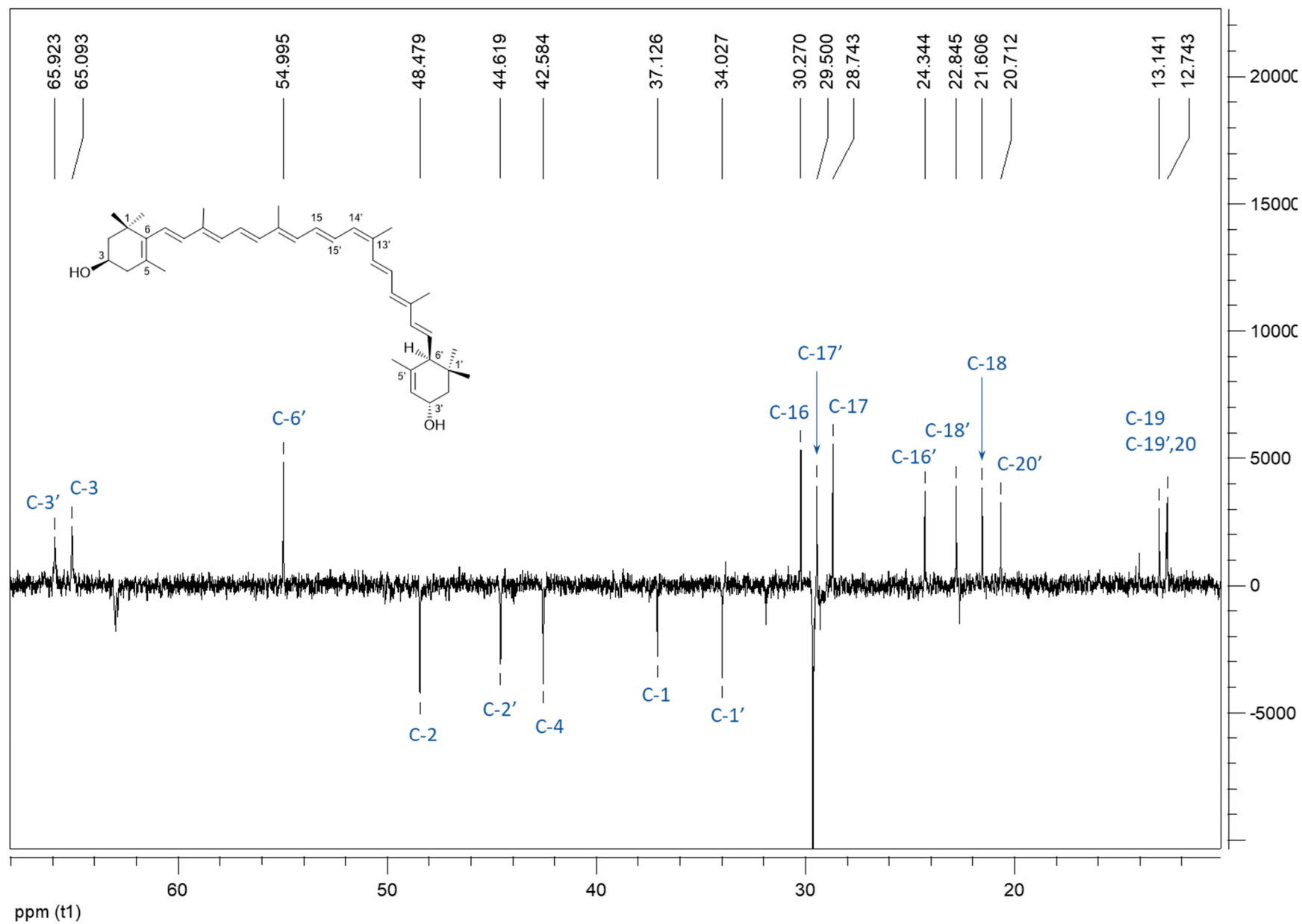


Figure S2.30. ^{13}C -NMR spectrum of (13'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

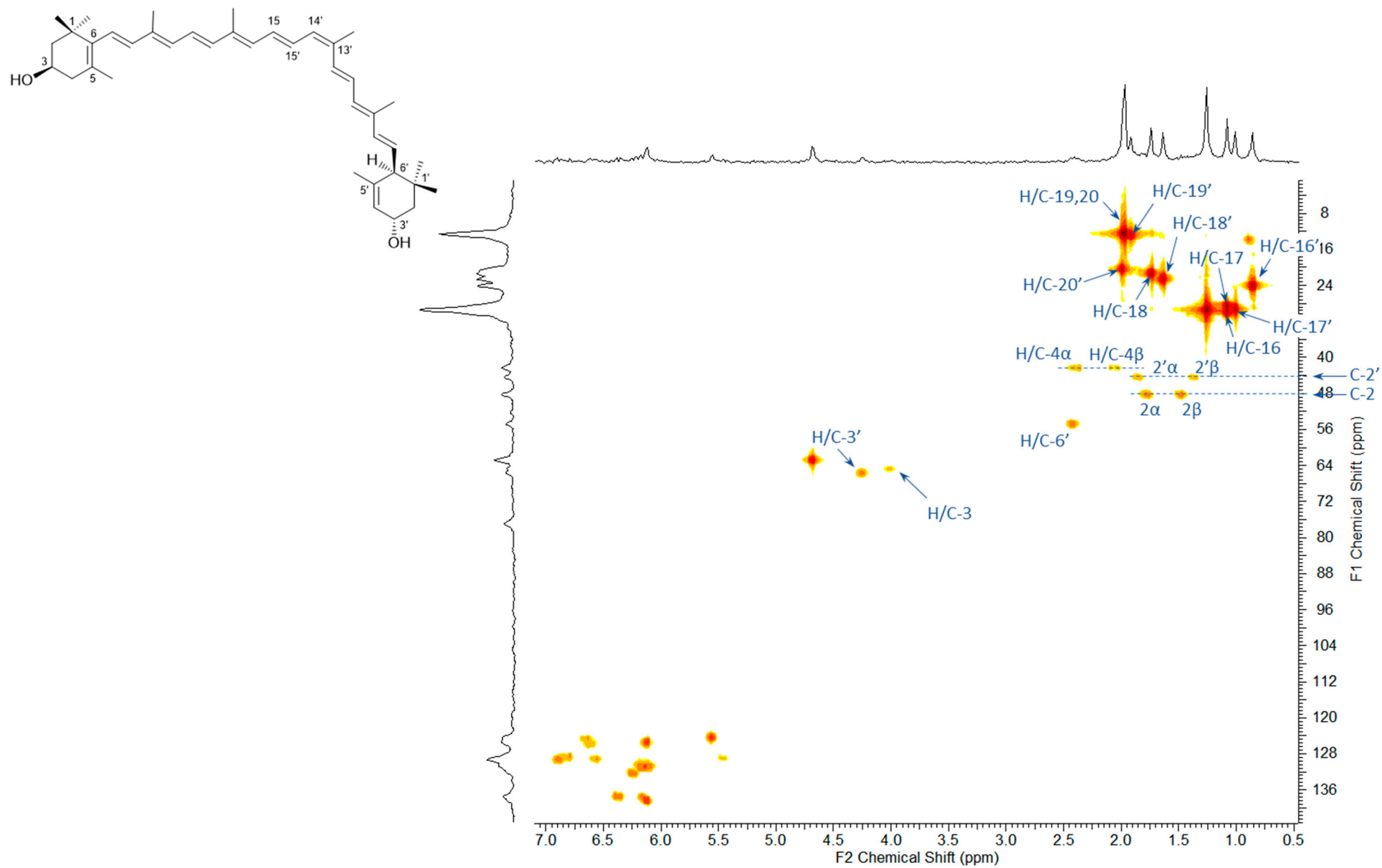


Figure S2.31. ^{13}C - ^1H -HSQC spectrum of (13'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

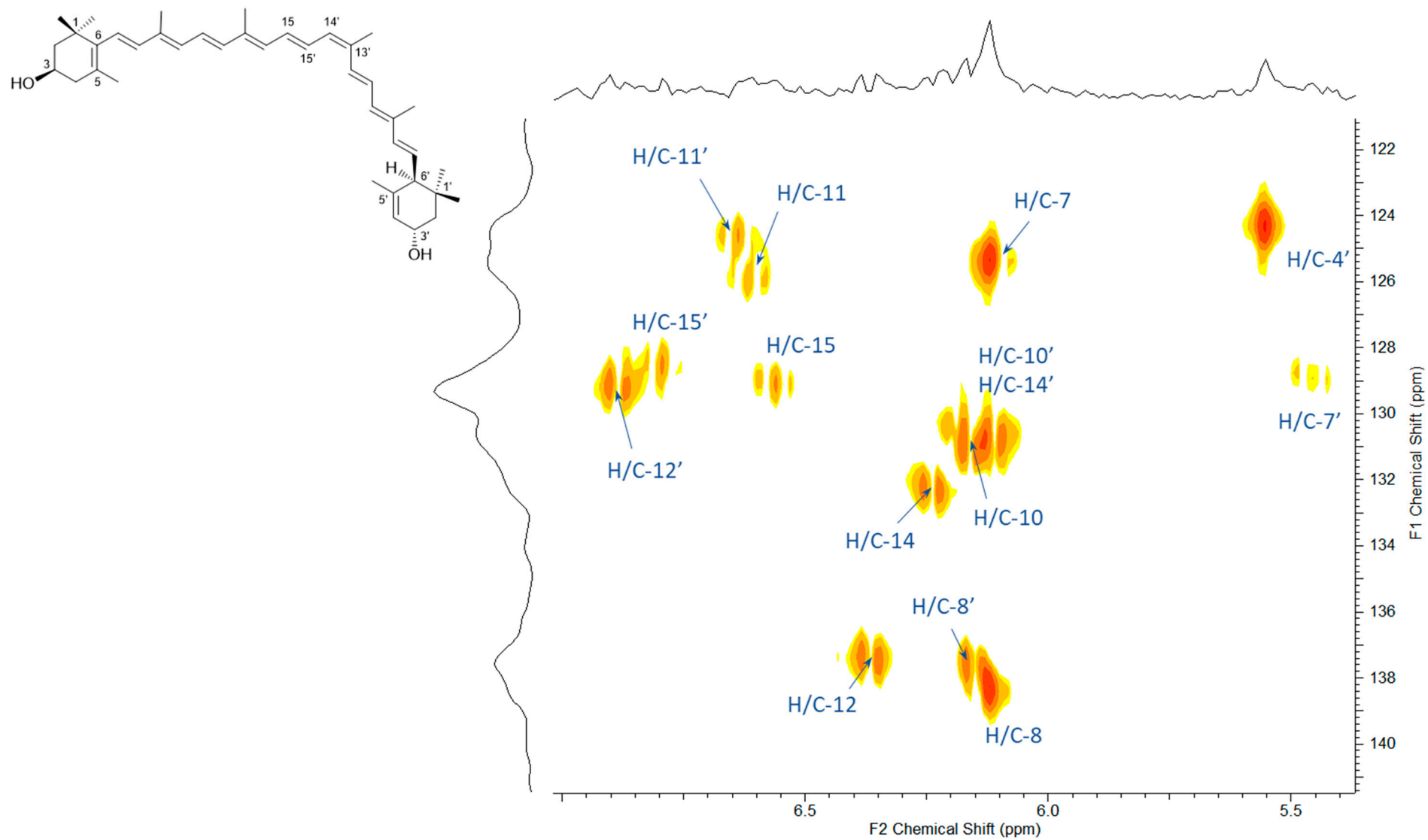


Figure S2.32. ^{13}C - ^1H -HSQC spectrum of (13'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

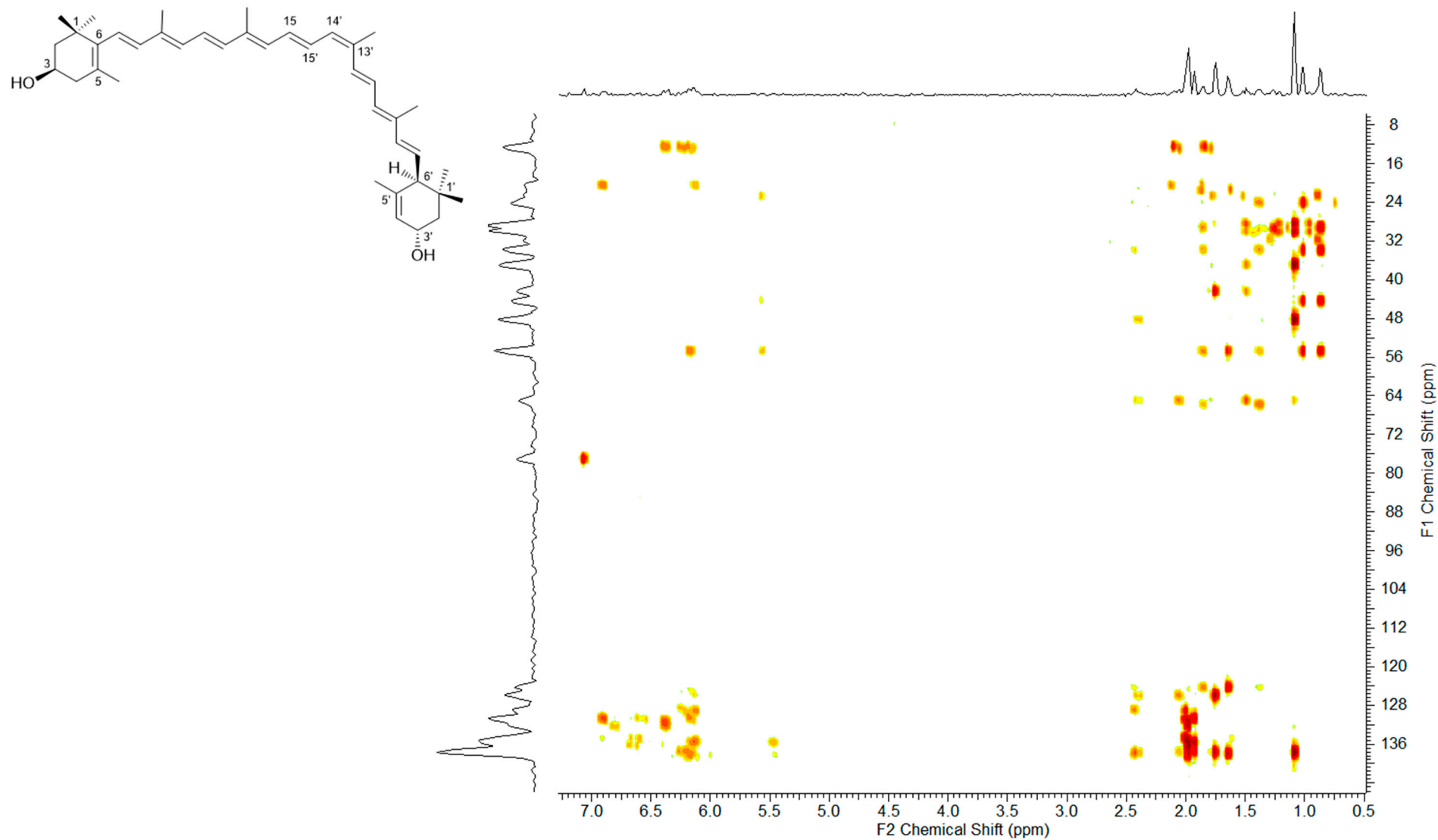


Figure S2.33. ^{13}C - ^1H -HMBC spectrum of (13'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

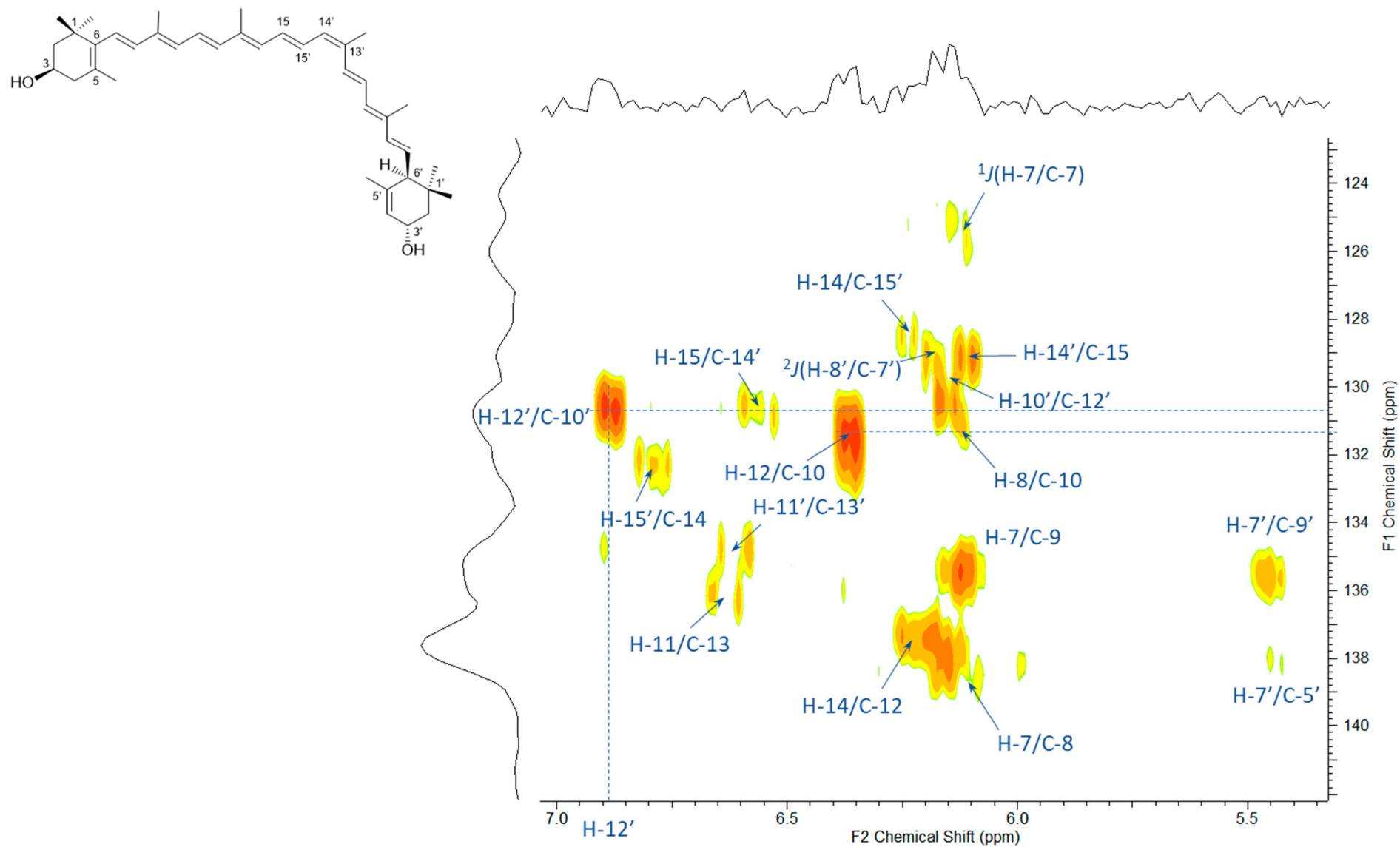


Figure S2.34. ^{13}C - ^1H -HMBC spectrum of (13'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

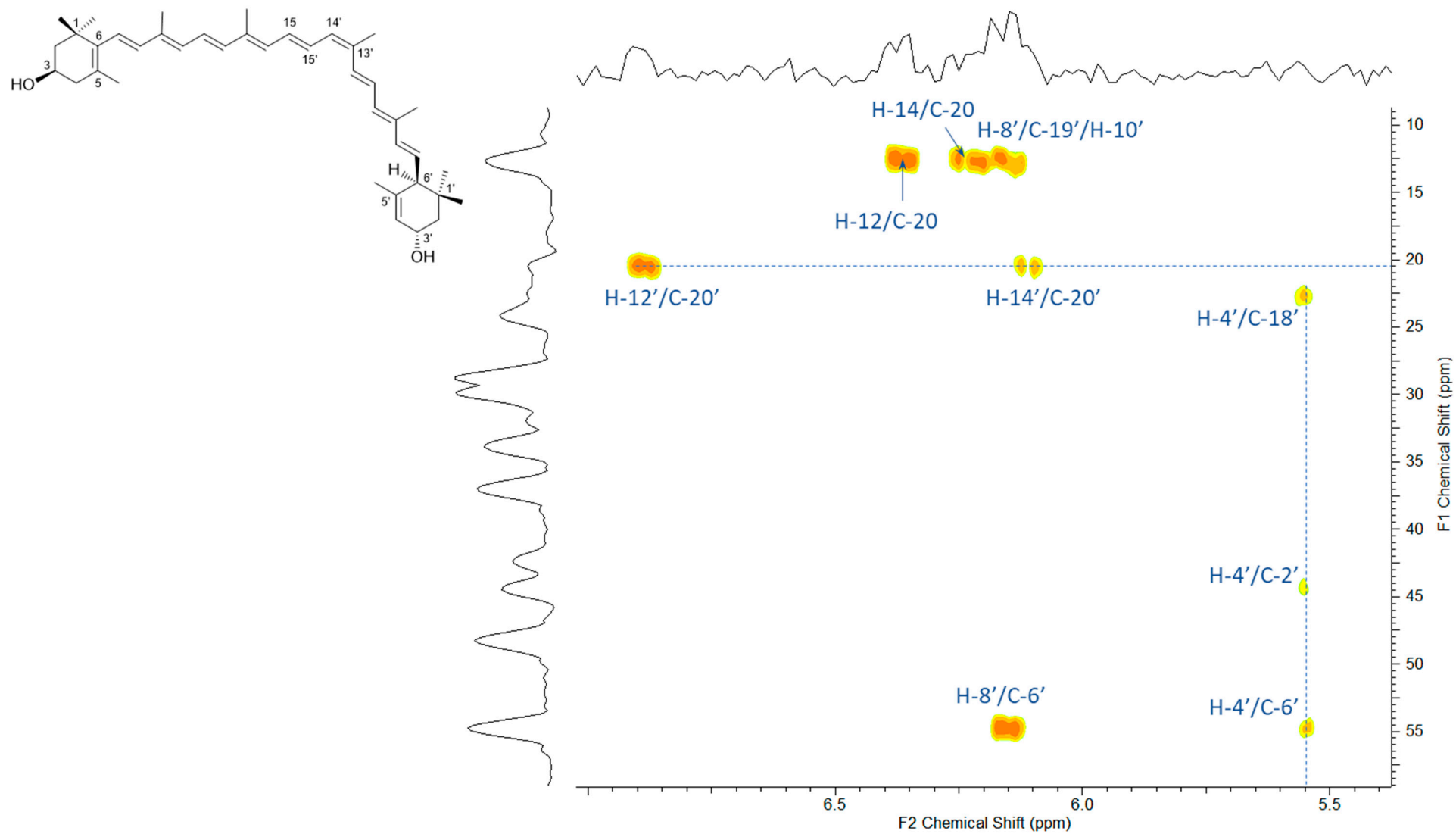


Figure S2.35. ^{13}C - ^1H -HMBC spectrum of (13'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

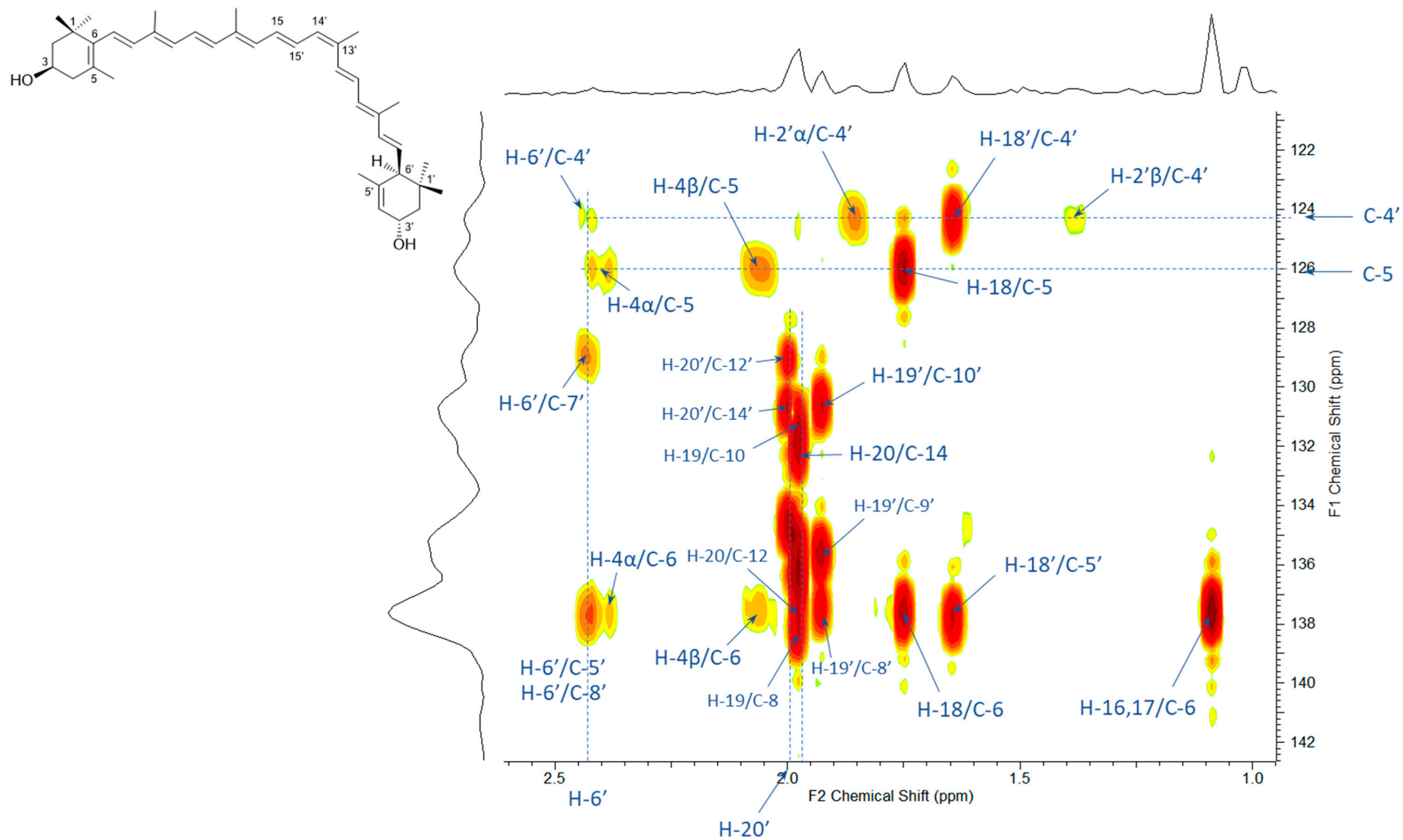


Figure S2.36. ¹³C-¹H-HMBC spectrum of (13'Z)-lutein in CDCl₃, (500/125 MHz for ¹H/¹³C)

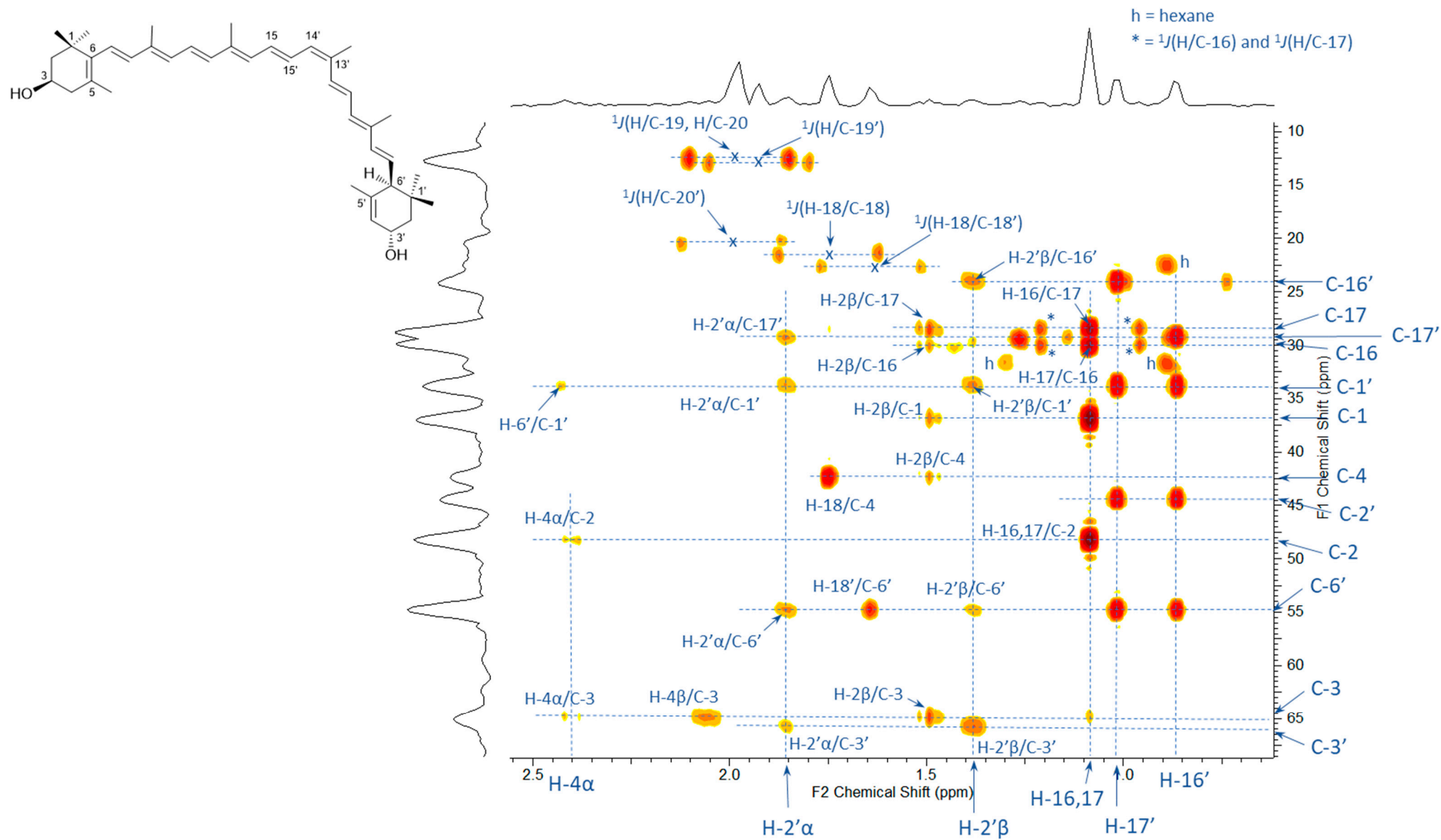


Figure S2.36. ^{13}C - ^1H -HMBC spectrum of (13'Z)-lutein in CDCl_3 , (500/125 MHz for $^1\text{H}/^{13}\text{C}$)

Figure S3. UV-vis spectra of lutein isomers, in the HPLC mobile phase

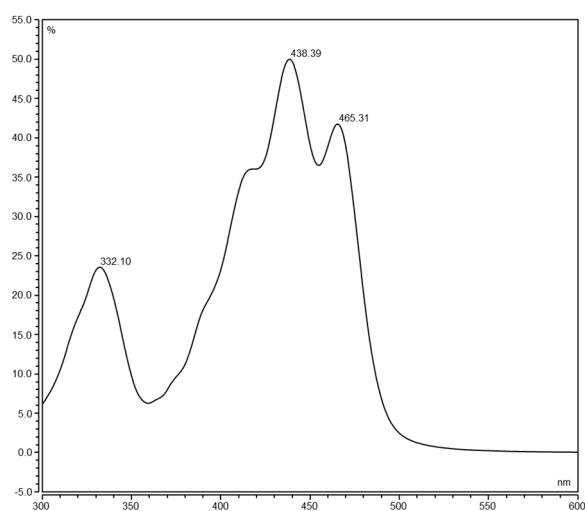


Figure S3.1. UV-vis spectrum of (13Z)-lutein in the HPLC mobile phase at 11.9 min. Q: 2.10, A_B/A_{II} : 47.2%

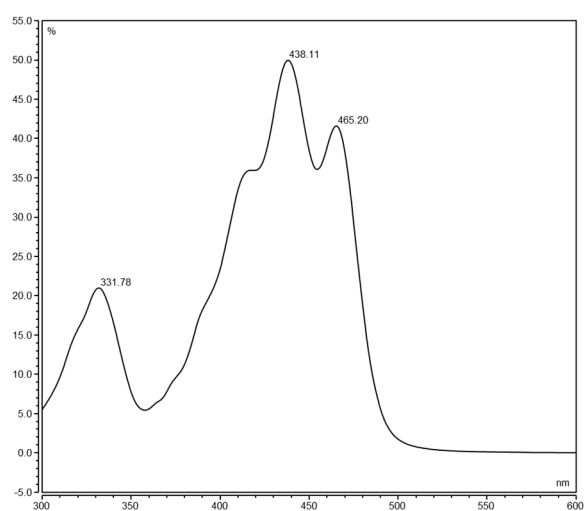


Figure S3.2. UV-vis spectrum of (13'Z)-lutein in the HPLC mobile phase at 12.4 min. Q: 2.37, A_B/A_{II} : 41.7%

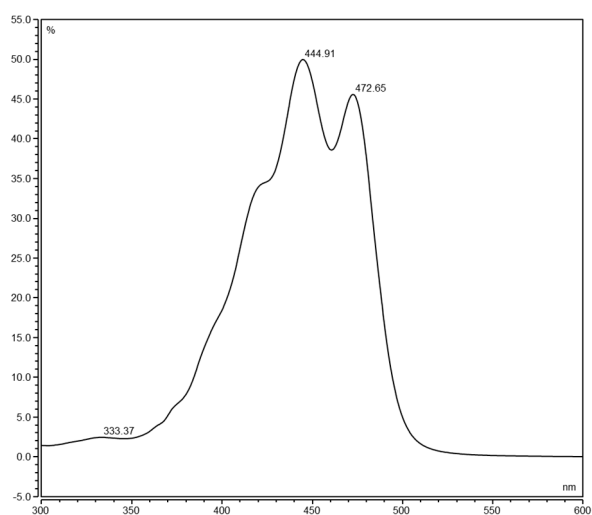


Figure S3.3. UV-vis spectrum of all-(*E*)-lutein in the HPLC mobile phase at 13.3 min.

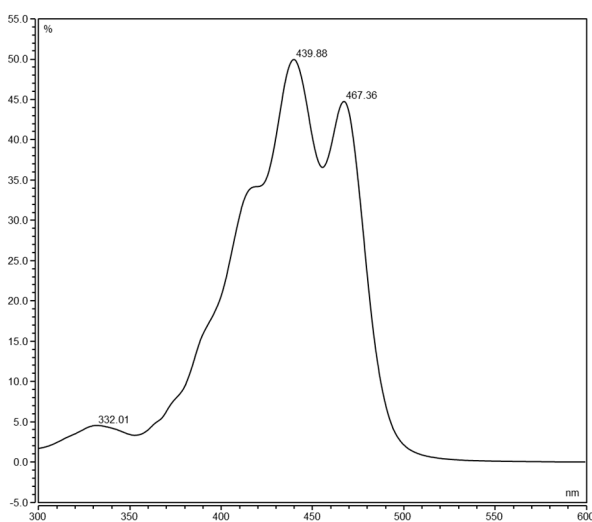


Figure S3.4. UV-vis spectrum of (9*Z*)-lutein in the HPLC mobile phase at 16.8 min. Q: 10.80, A_B/A_{II} : 9.7%

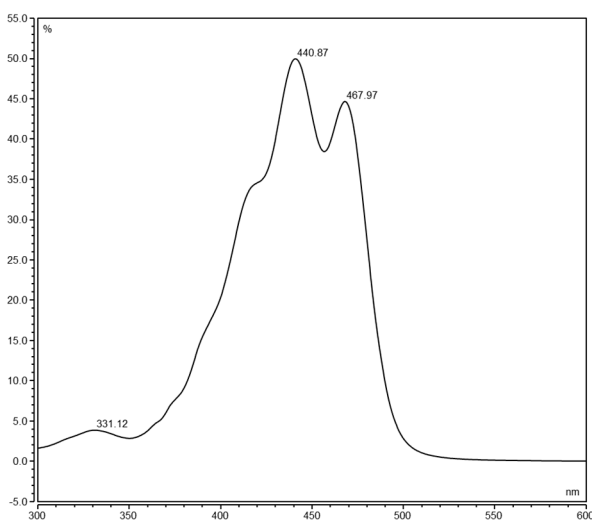


Figure S3.5. UV-vis spectrum of (9'*Z*)-lutein in the HPLC mobile phase at 19.6 min. Q: 13.56, A_B/A_{II} : 8.5%

Figure S4. UV-vis and EIC chromatograms of the investigated flowers

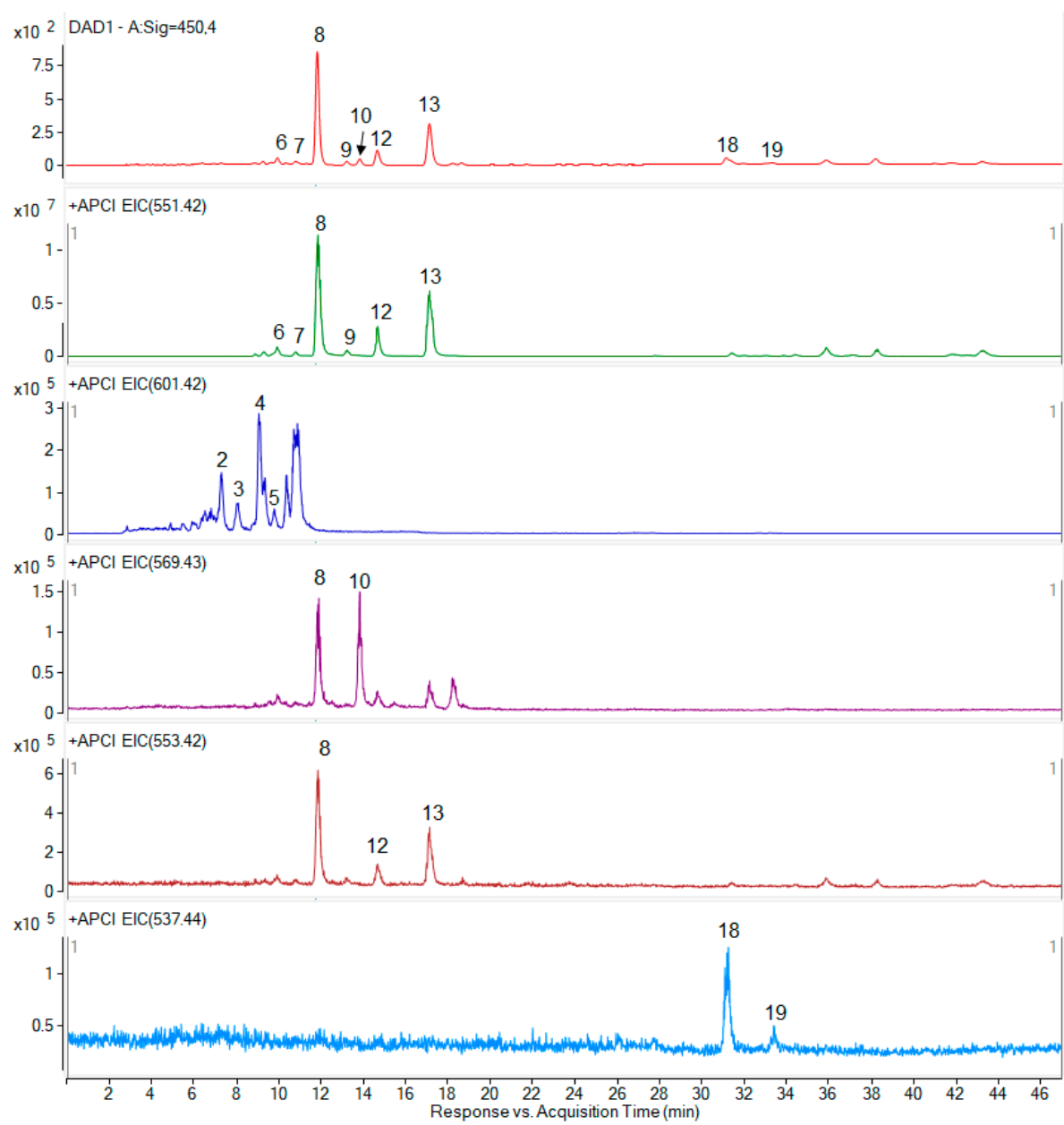


Figure S4.1. UV-vis and EIC chromatogram of *Anthemis tinctoria*

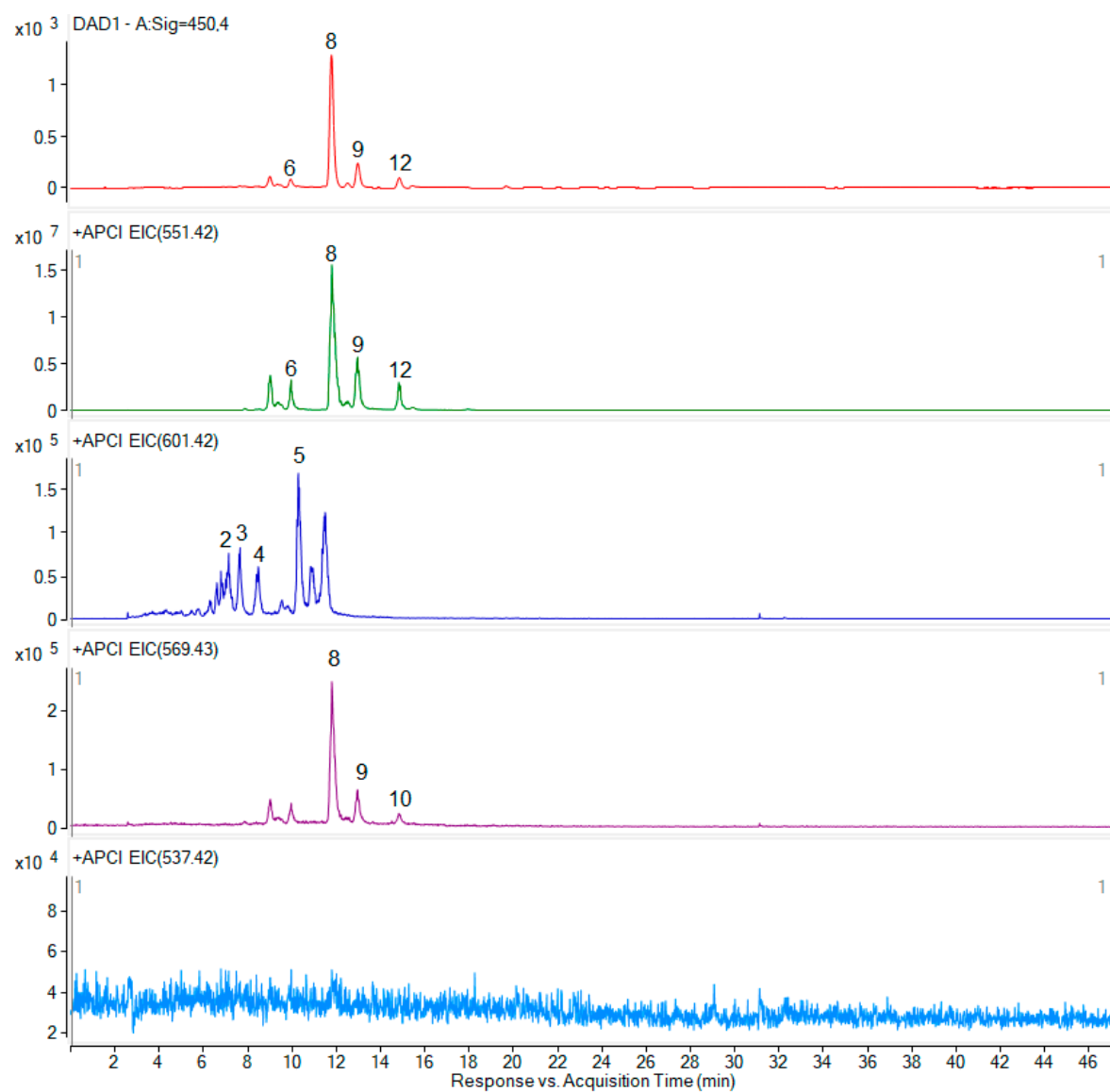


Figure S4.2. UV-vis and EIC chromatogram of *Cholicum autumnale*

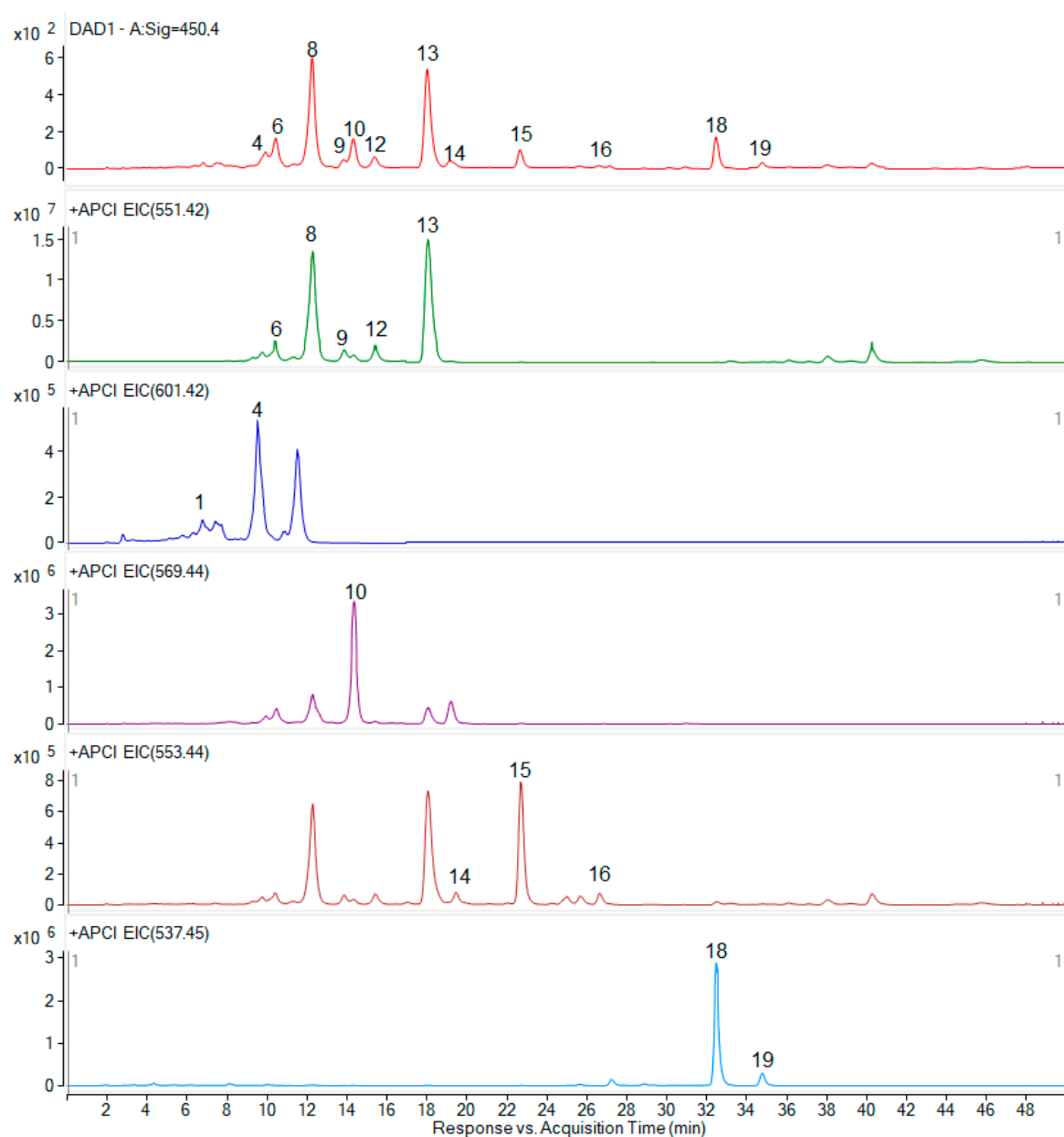


Figure S4.3. UV-vis and EIC chromatogram of *Helicrysum italicum*

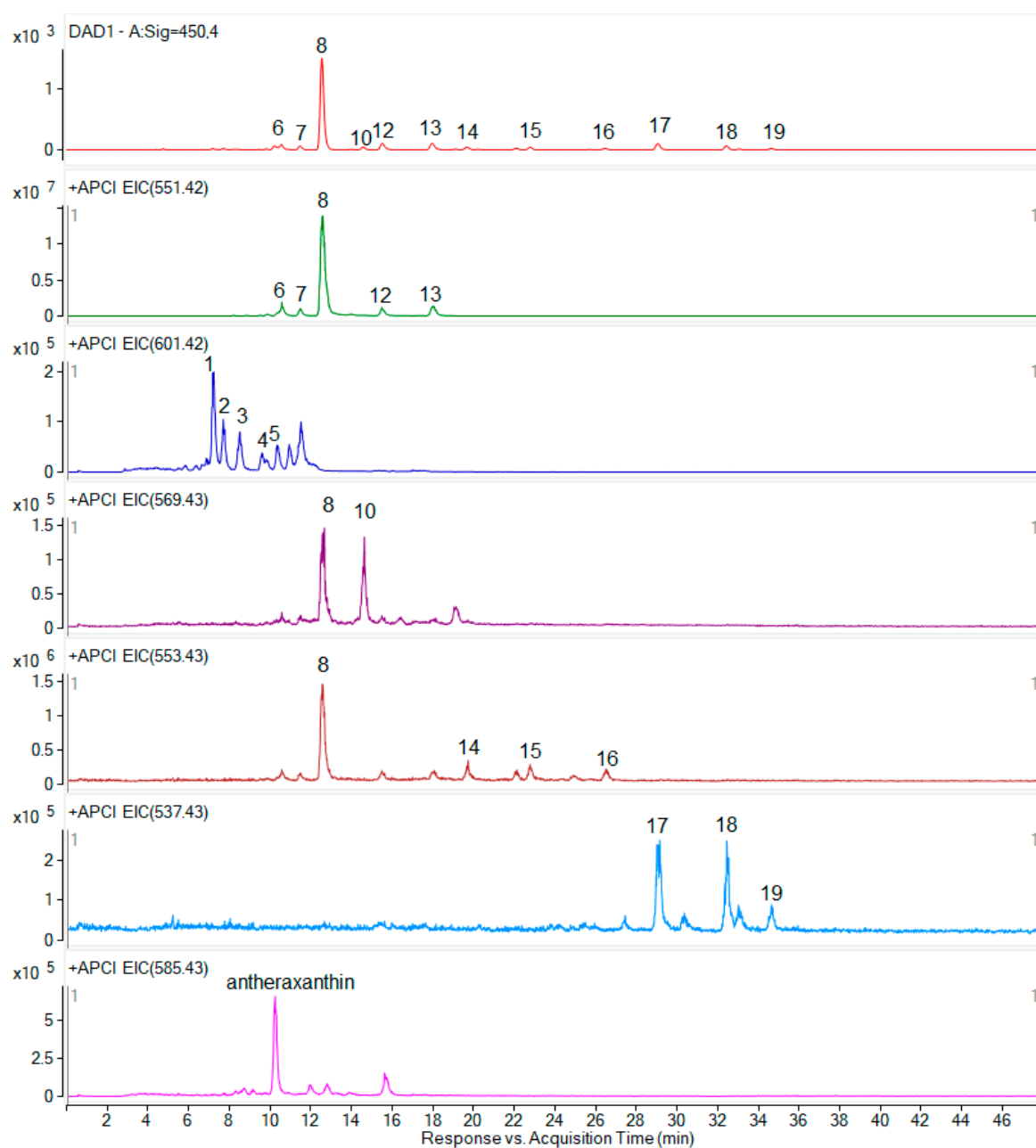


Figure S4.4. UV-vis and EIC chromatogram of *Helianthus angustifolius*

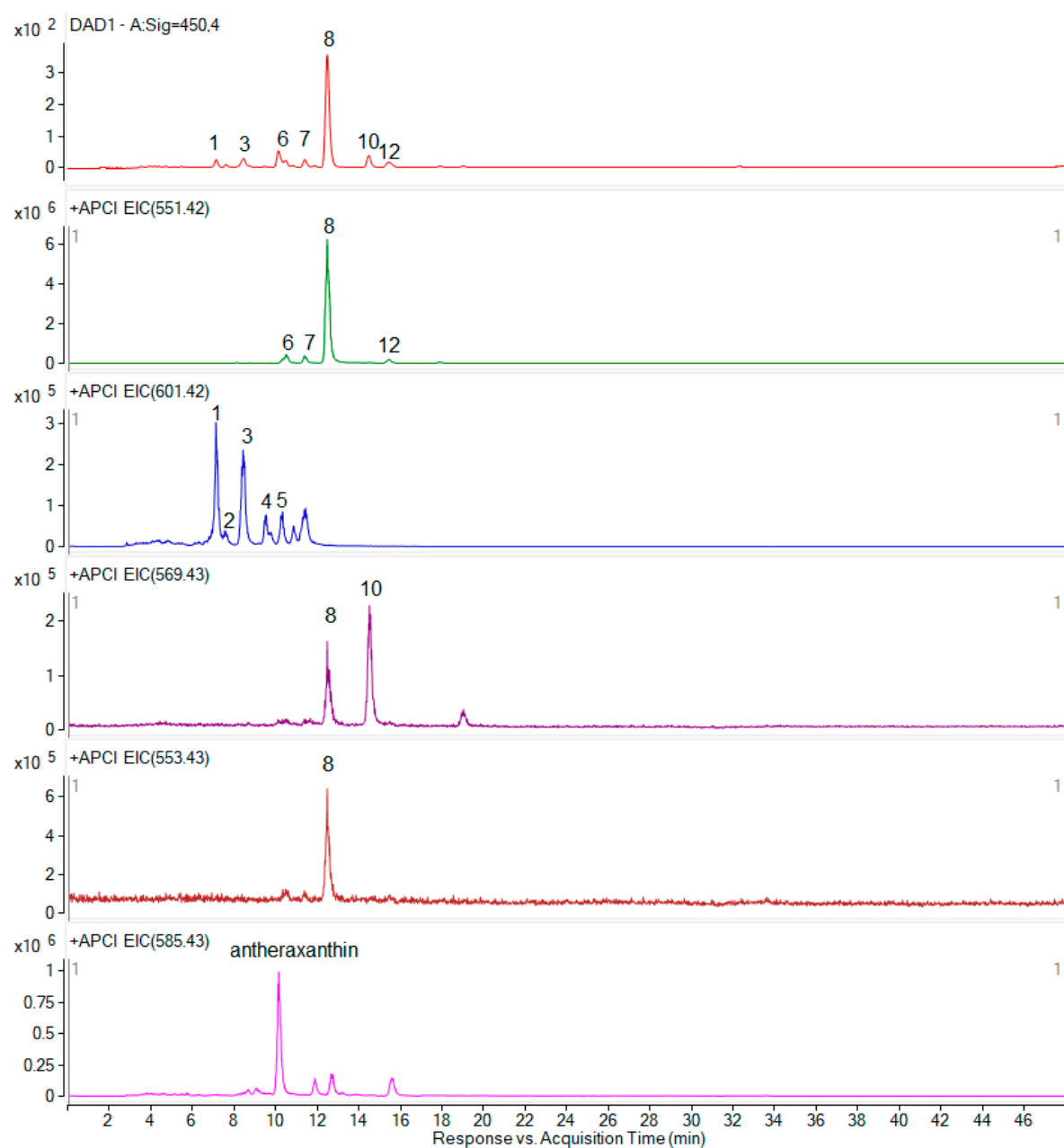


Figure S4.5. UV-vis and EIC chromatogram of *Helianthus tuberosus*

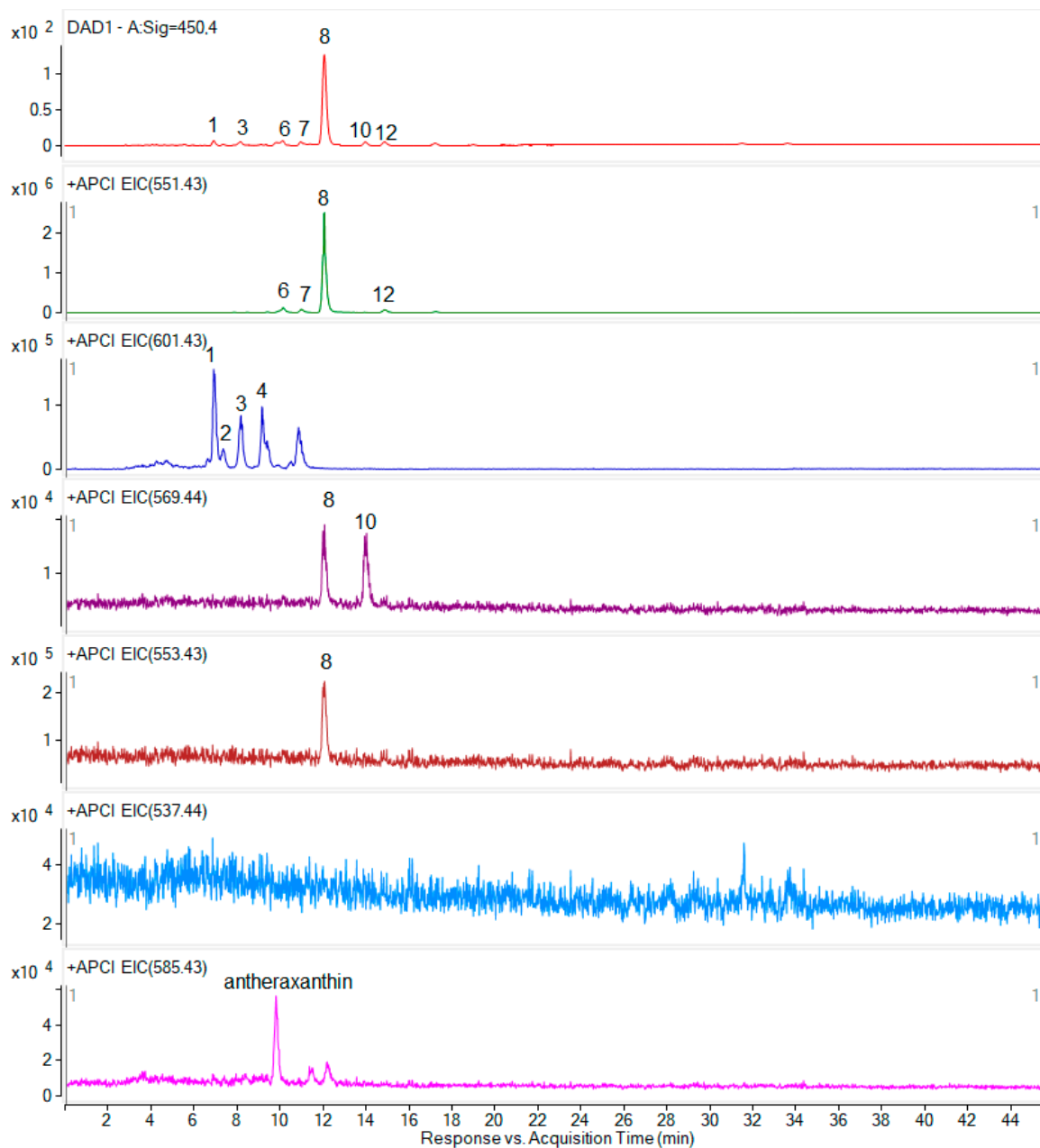


Figure S4.6. UV-vis and EIC chromatogram of *Sternbergia lutea*

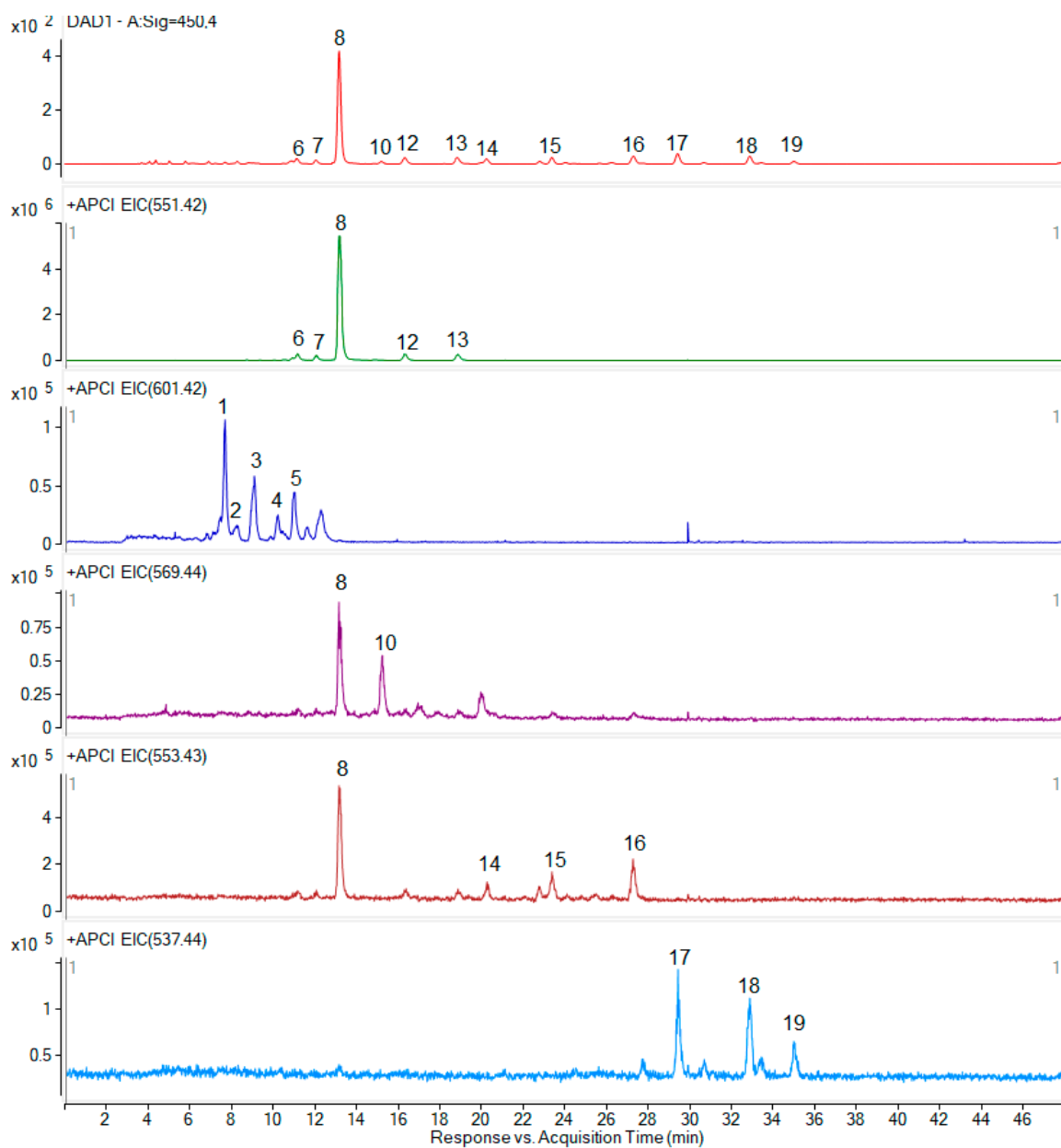


Figure S4.7. UV-vis and EIC chromatogram of *Coreopsis pubescens*

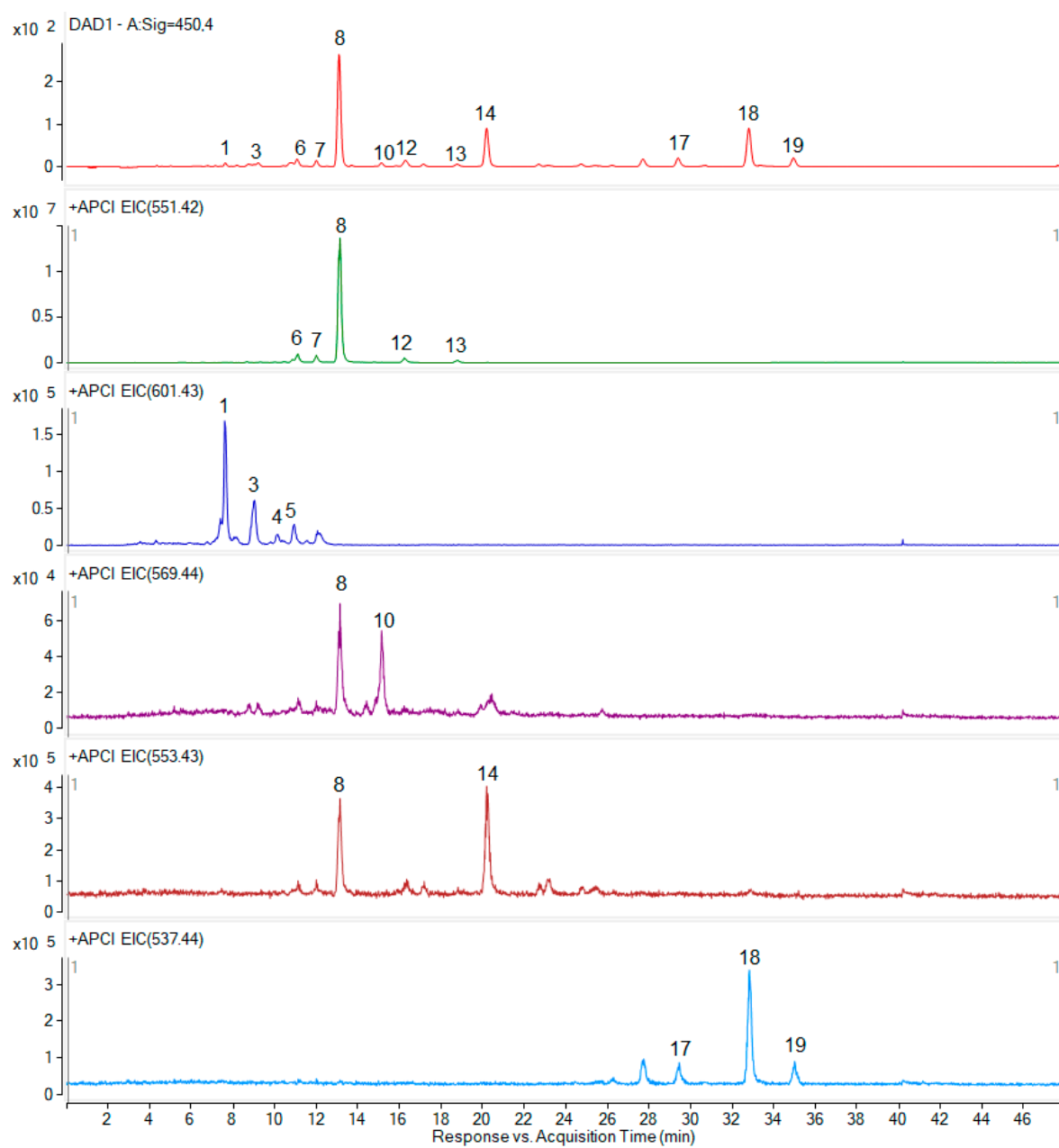


Figure S4.8. UV-vis and EIC chromatogram of *Cassia artemisioides*

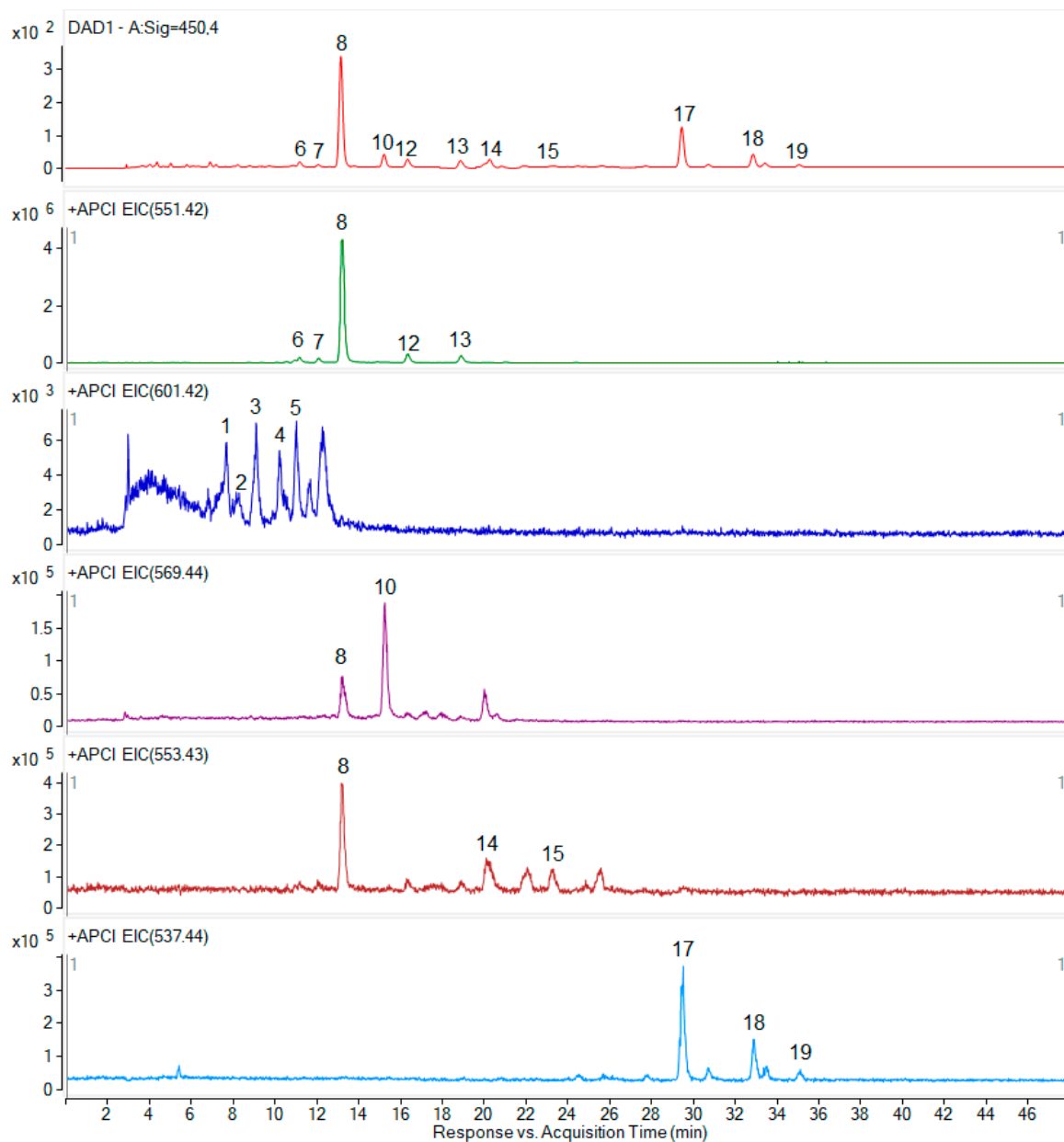


Figure S4.9. UV-vis and EIC chromatogram of *Echinacea paradoxa*