

Supplementary data

The influence of glycosylation of natural and synthetic prenylated flavonoids on binding to human serum albumin and inhibition of cyclooxygenases COX-1 and COX-2

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Figure S1. ^1H NMR spectrum of α,β -dihydroxanthohumol (**2**) (600 MHz, CD_3OD , Temp. 25 °C)

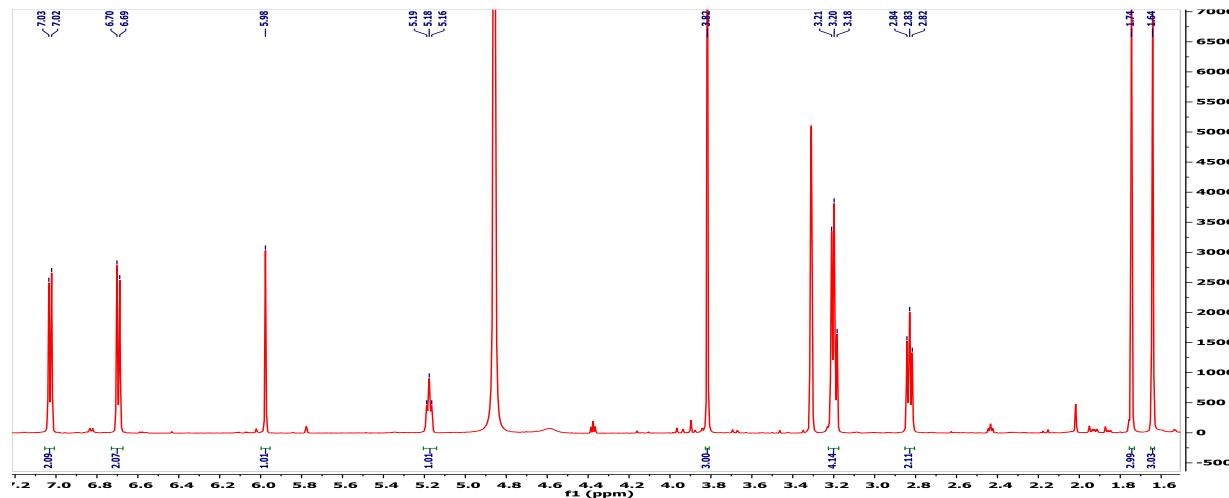


Figure S2. ^{13}C NMR and DEPT 135° spectra of α,β -dihydroxanthohumol (**2**) (151 MHz, CD_3OD , Temp. 25 °C)

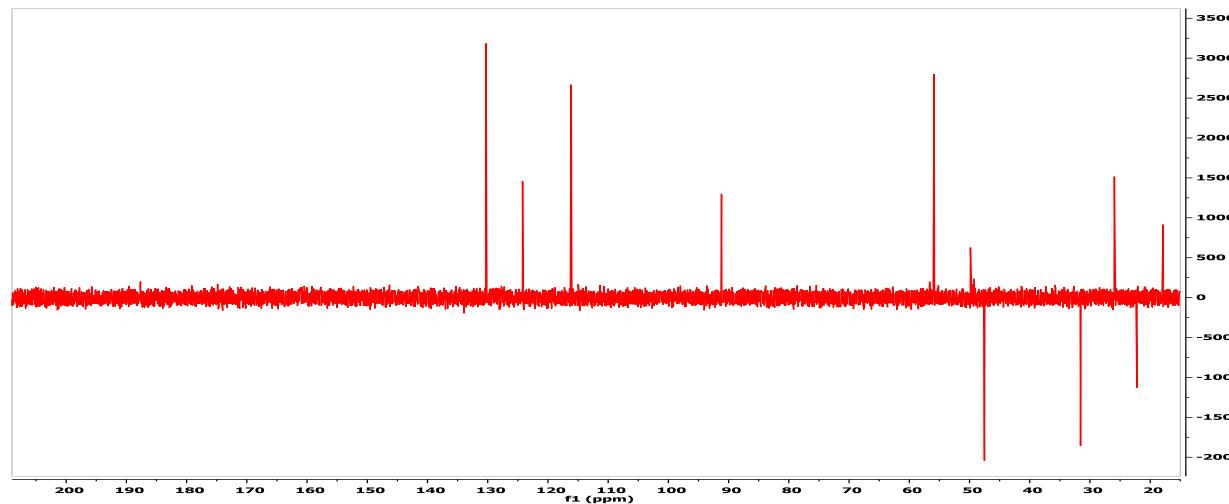
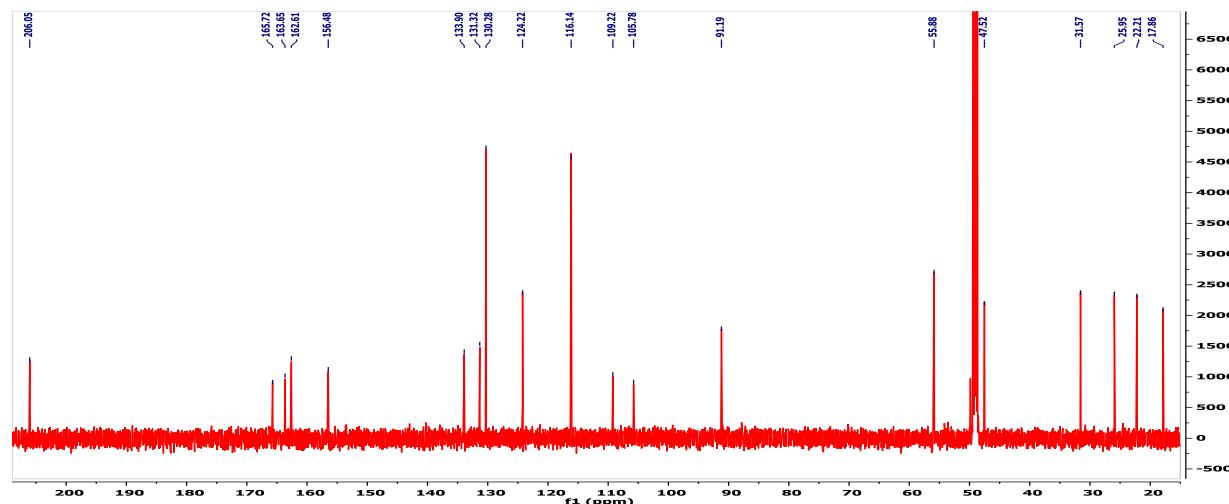


Figure S3: UV spectra of: A xanthohumol (**1**), B (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone (**3**) (MeOH, Temp. 20 °C)

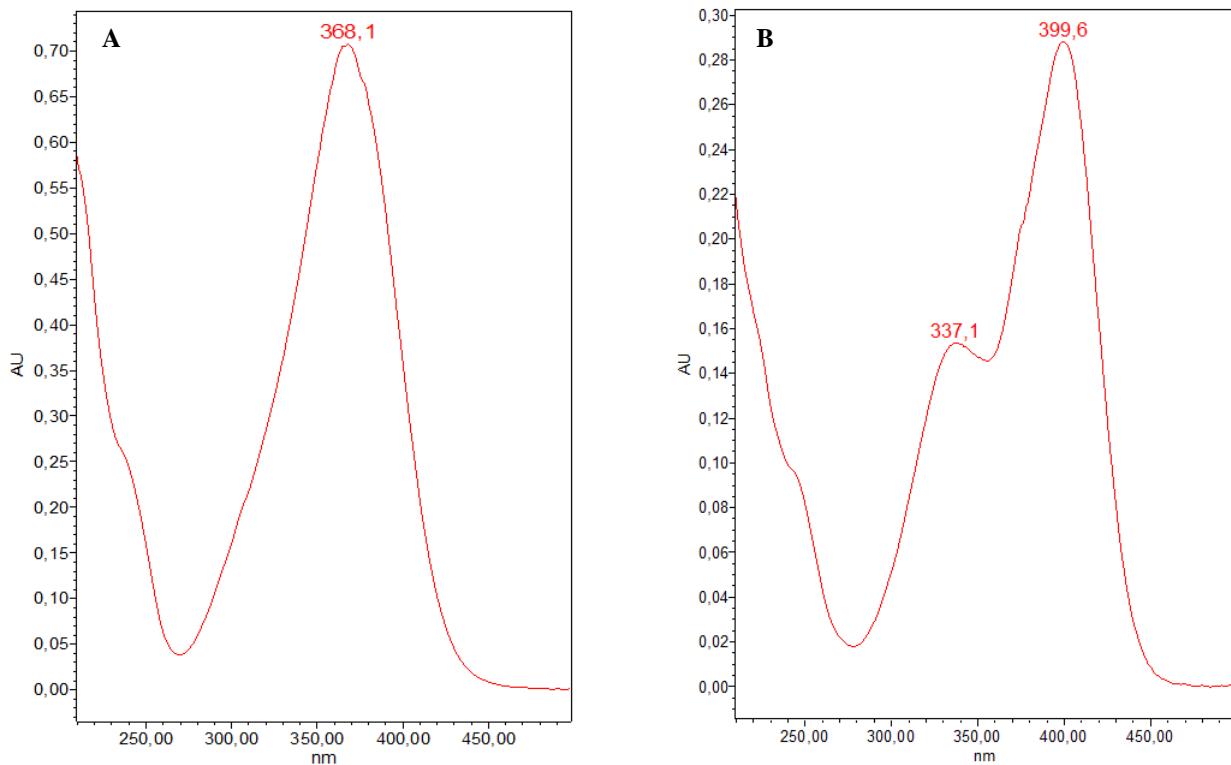


Figure S4. HRMS spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone (**3**)

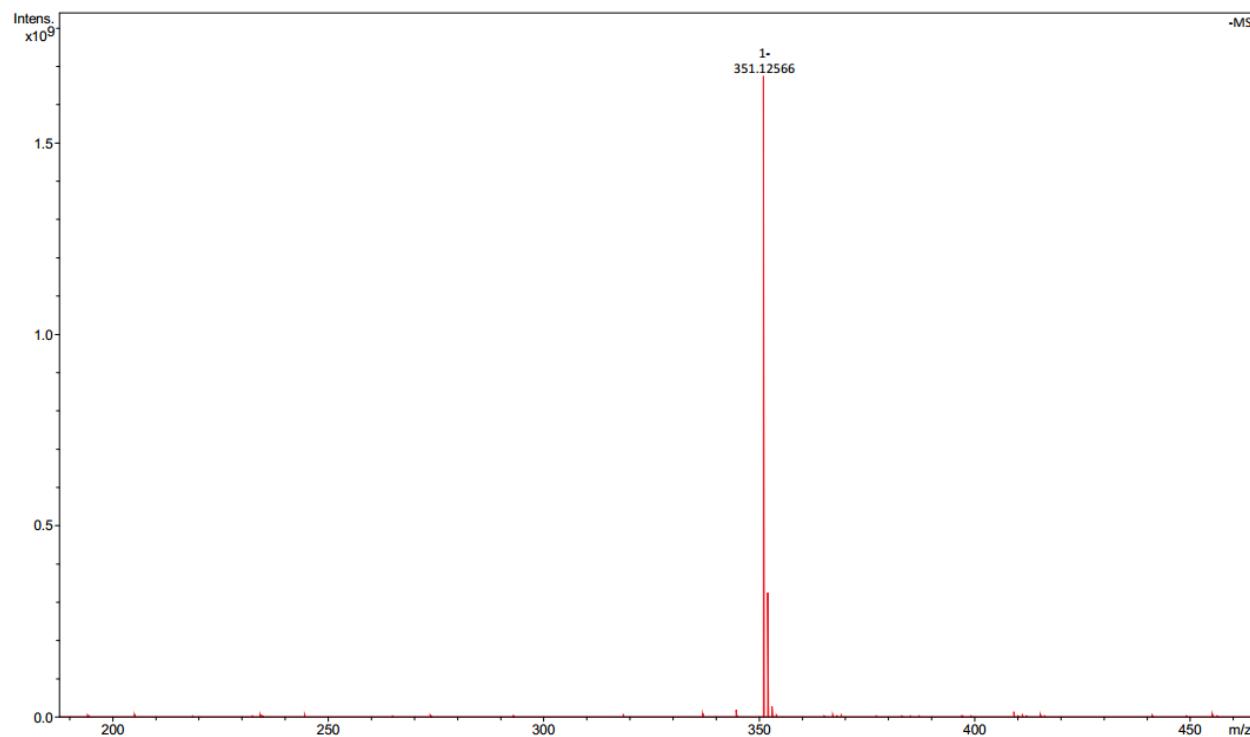


Figure S5. ^1H NMR spectra of: A xanthohumol (**1**) (600 MHz, $\text{DMSO}-d_6$), B (Z)-6,4'-dihydroxy-4-methoxy-7-prenyllaurone (**3**) (300 MHz, $\text{DMSO}-d_6$, Temp. 25 °C)

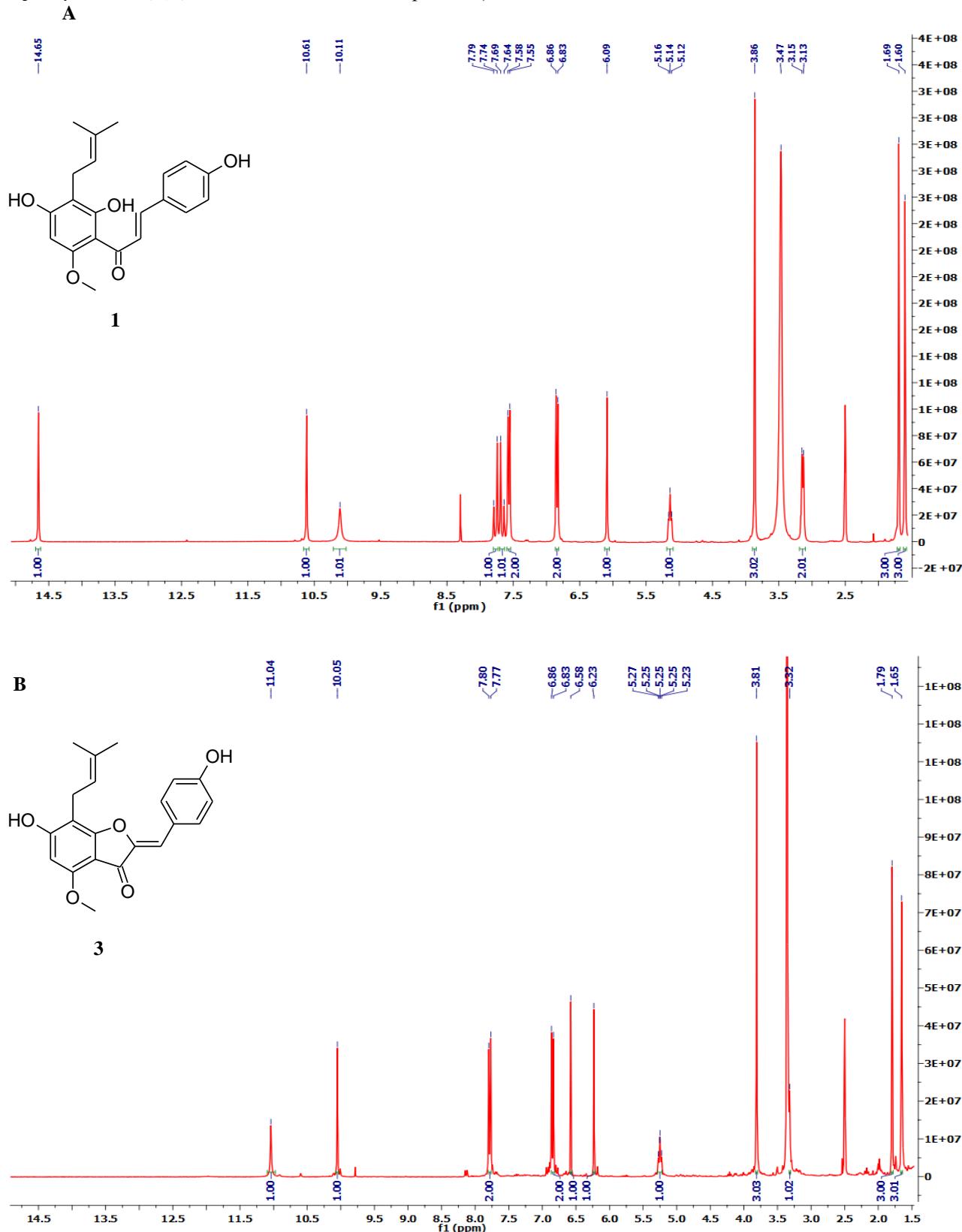
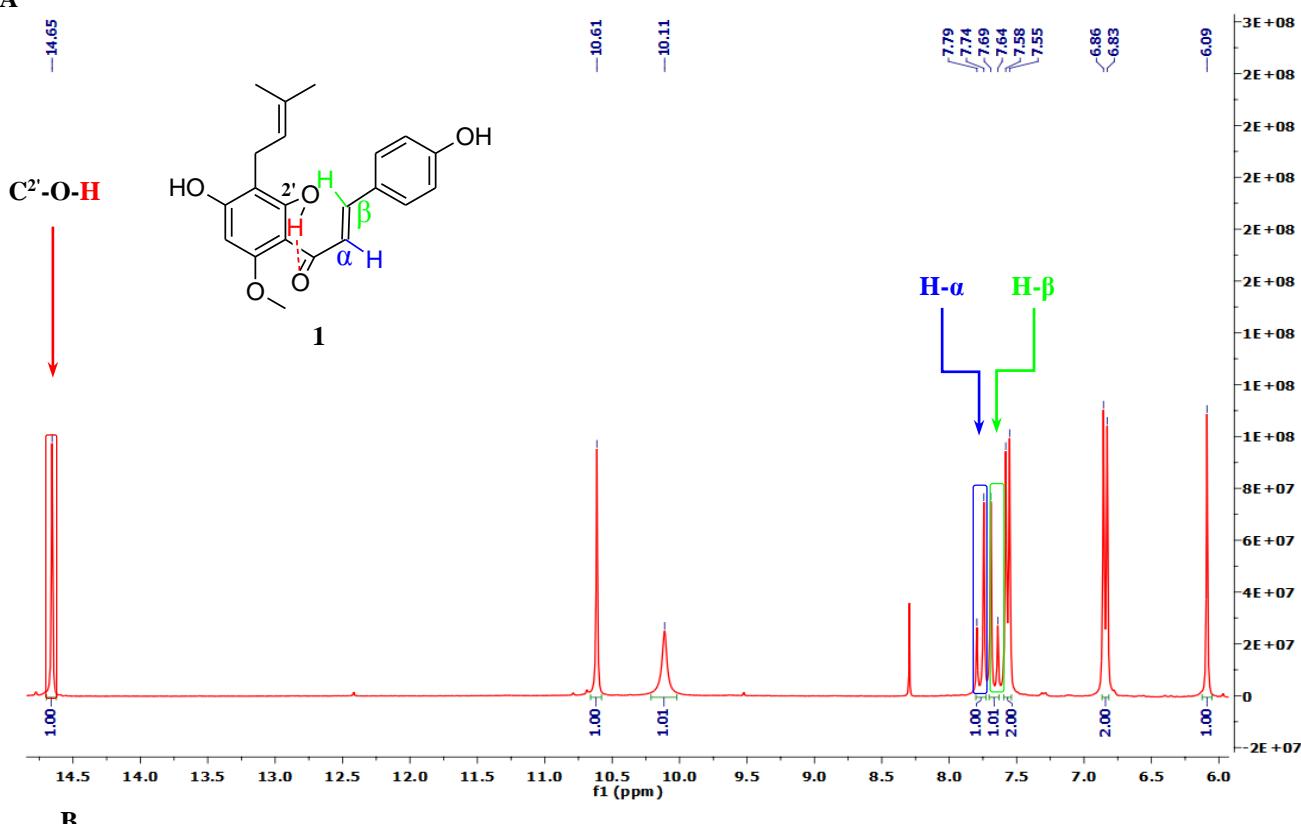


Figure S6. Fragments of ^1H NMR spectra of: A xanthohumol (**1**) (600 MHz, $\text{DMSO}-d_6$), B aurone (**3**) (300 MHz, $\text{DMSO}-d_6$, Temp. 25 °C)

A



B

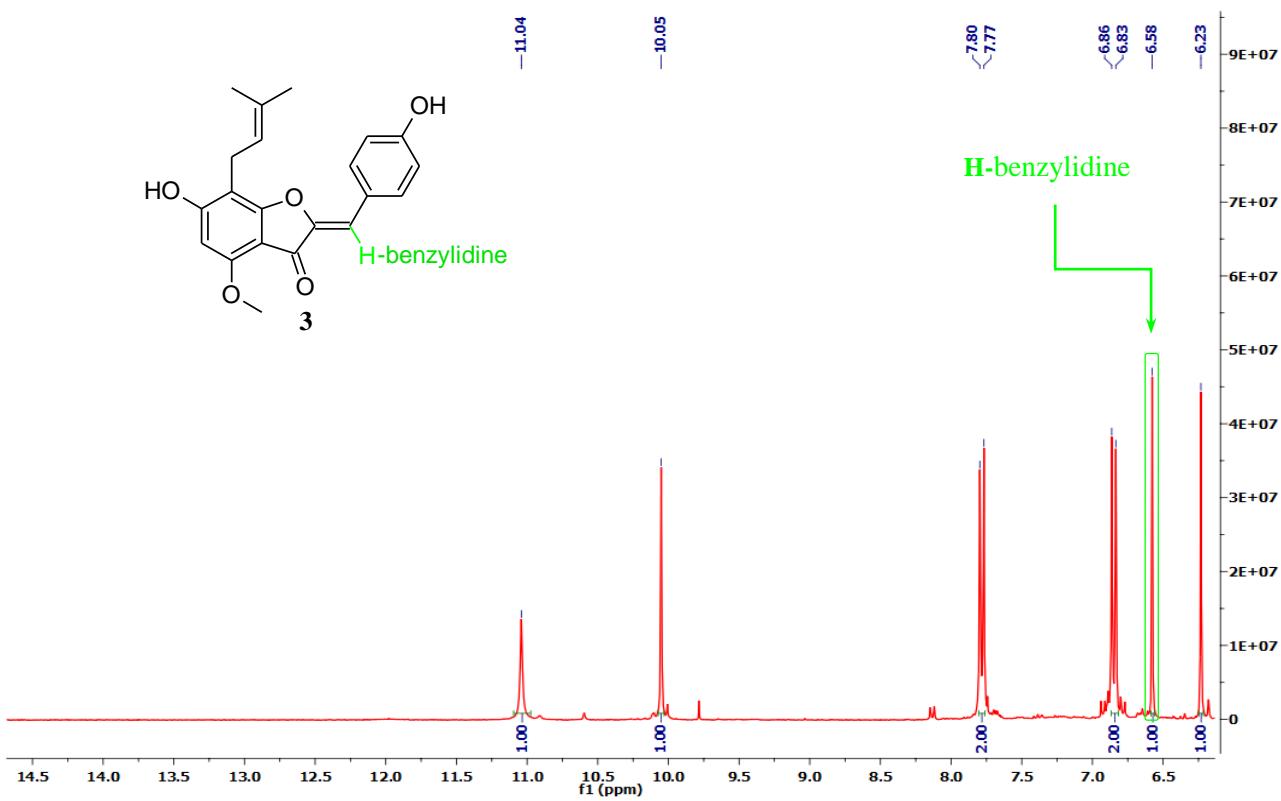


Figure S7. ^{13}C NMR spectra of: **A** xanthohumol (**1**) (151 MHz, DMSO-d_6), **B** auron (**3**) (75 MHz, DMSO-d_6 , Temp. 25 °C)

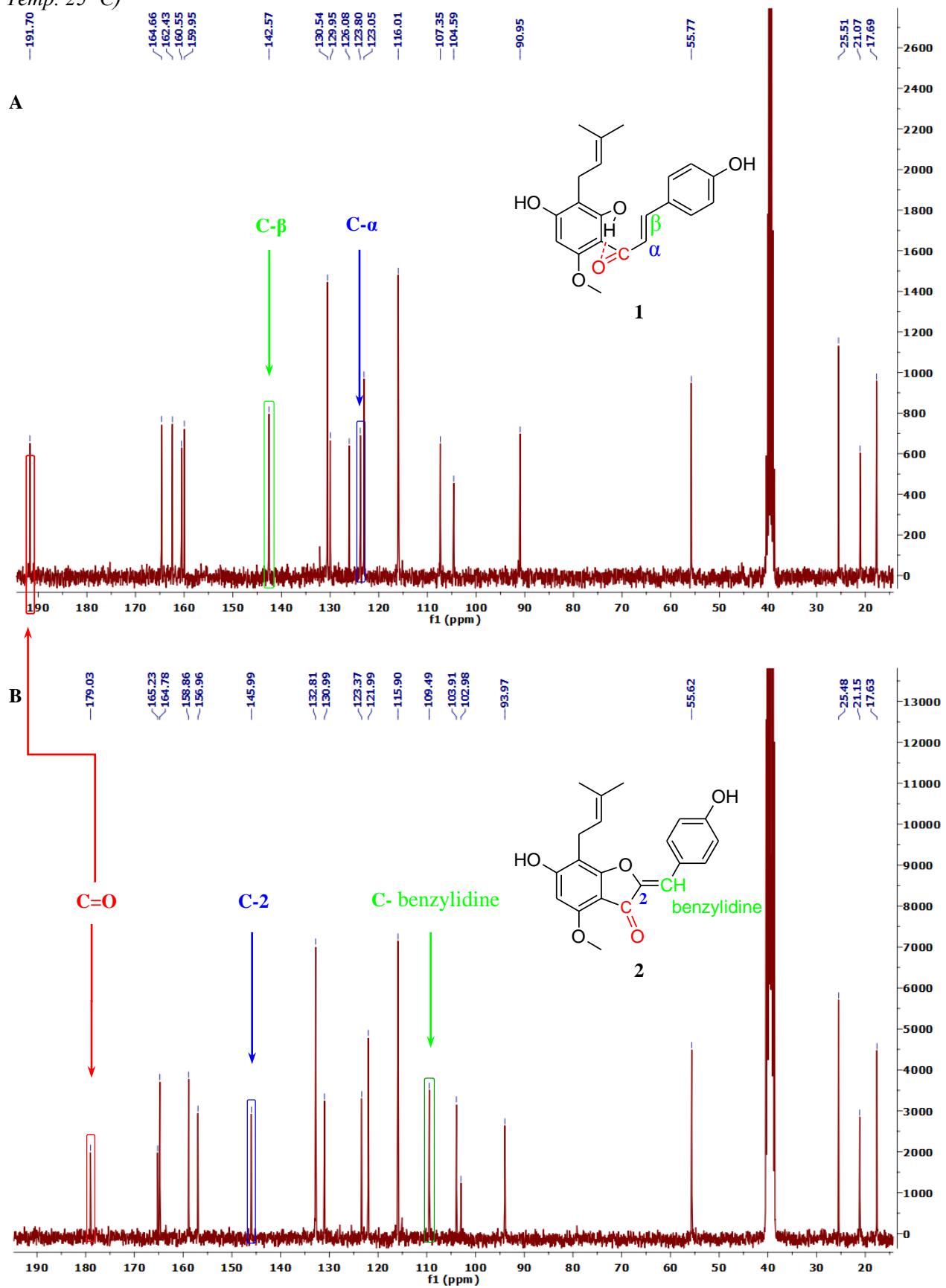


Figure S8. ^1H - ^1H NMR (COSY) spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone (**3**) (300 MHz/300 MHz, DMSO- d_6 , Temp. 25°)

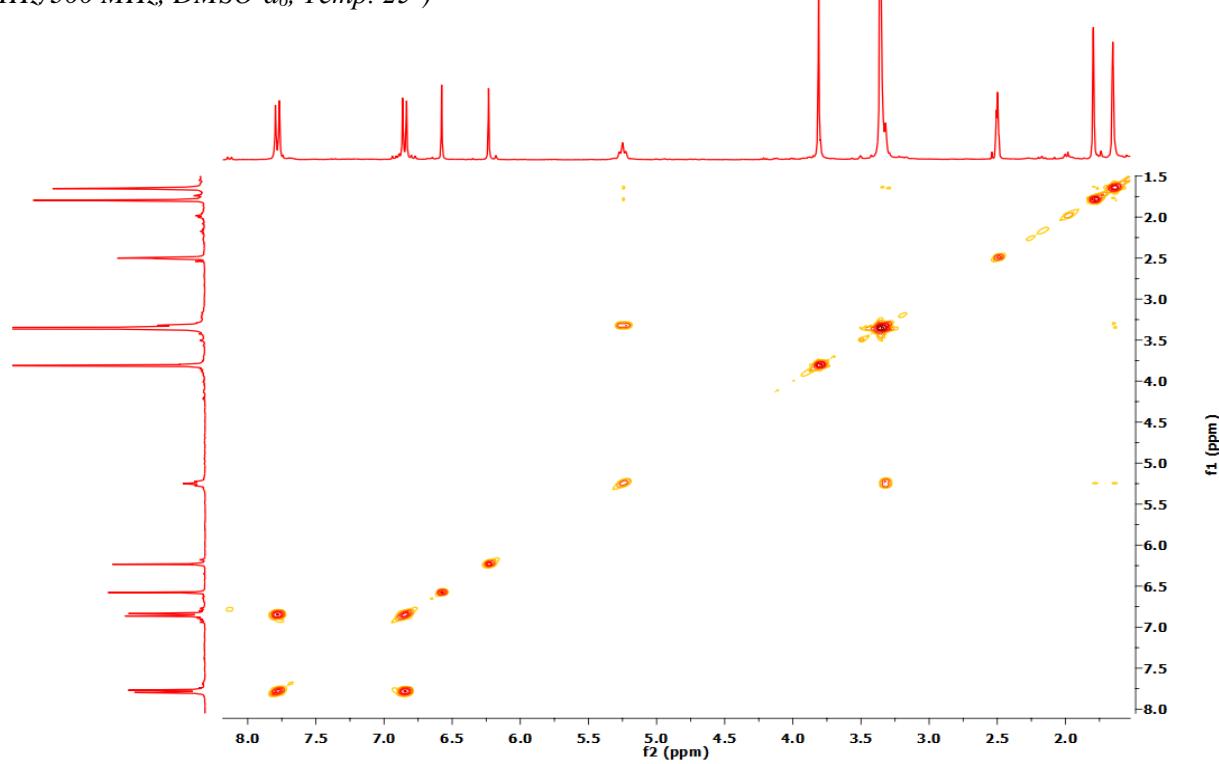


Figure S9. ^1H - ^{13}C NMR (HSQC) spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone (**3**) (300 MHz/75 MHz, DMSO- d_6 , Temp. 25°)

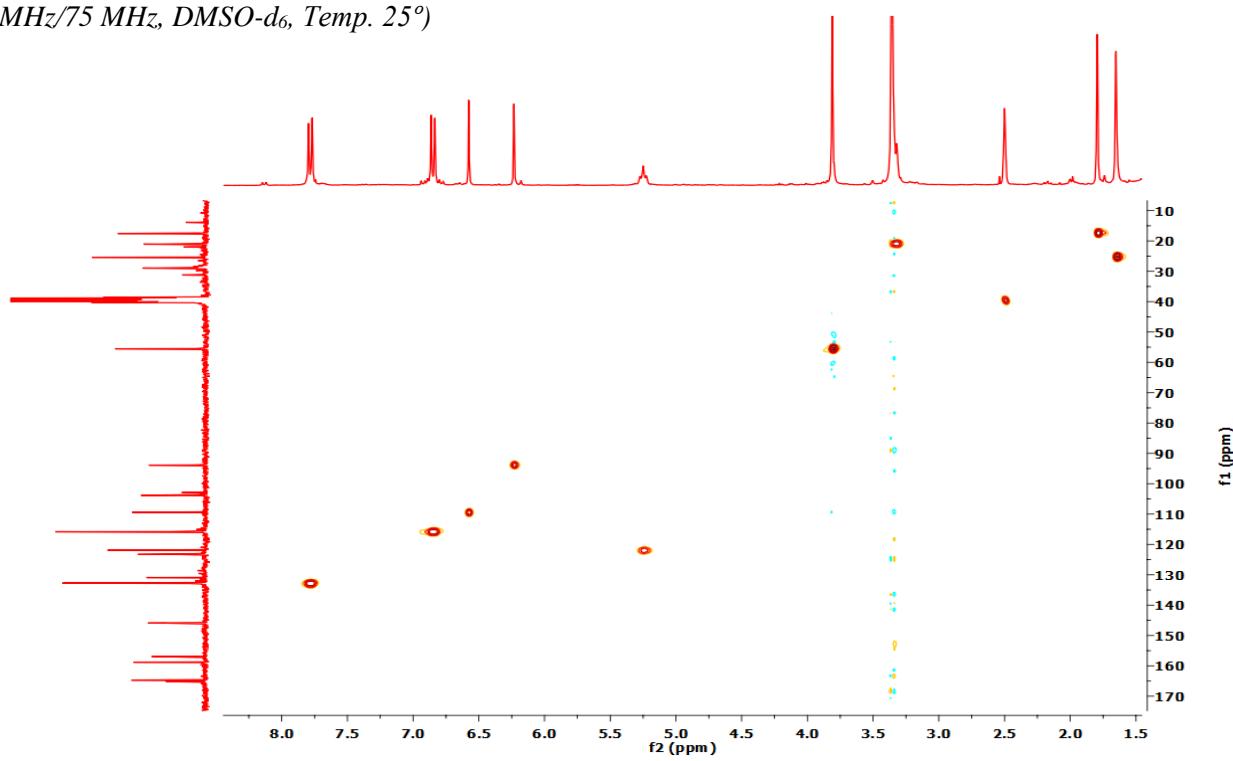


Figure S10. UV spectrum of α,β -dihydroxanthohumol 4' -O- β -D-glucopyranoside (**6**) (MeOH, Temp. 20 °C)

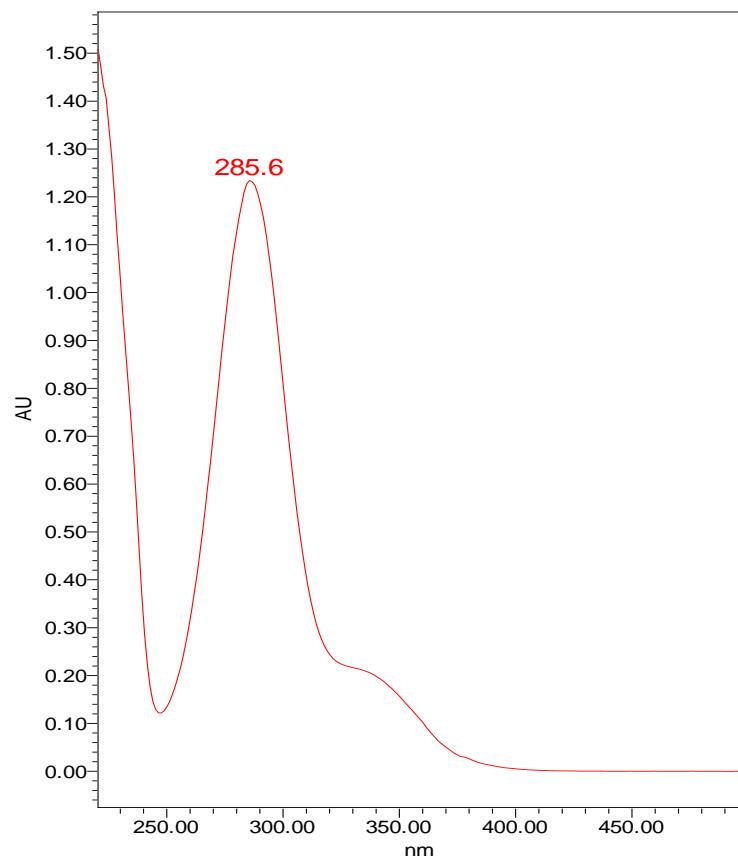


Figure S11. HRMS spectrum of α,β -dihydroxanthohumol 4' -O- β -D-glucopyranoside (**6**)

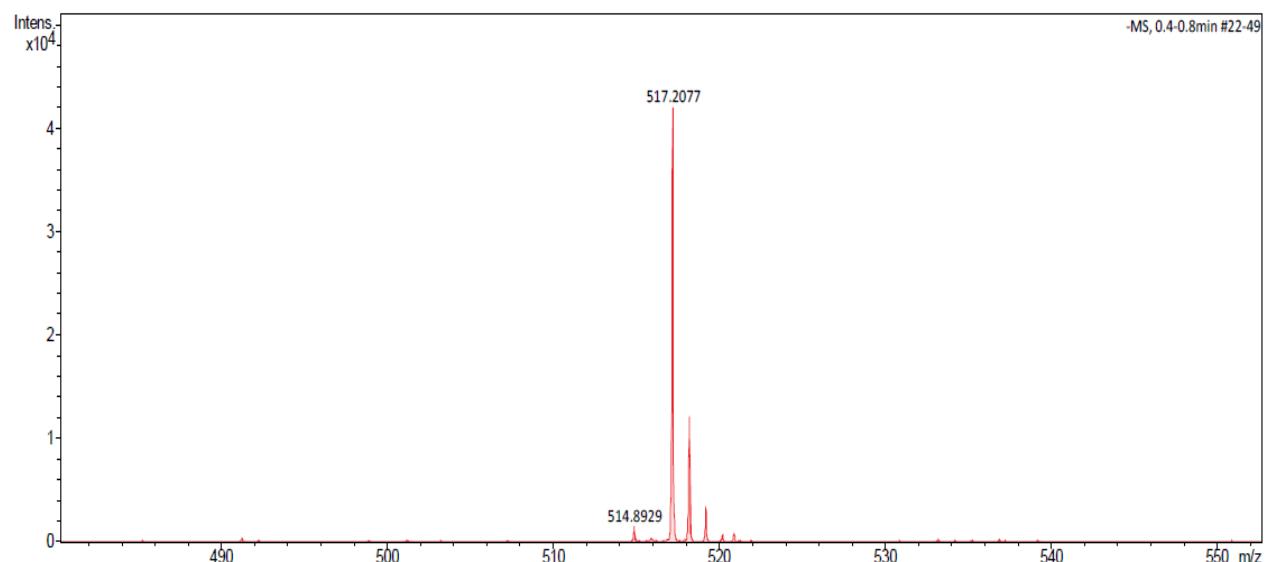


Figure S12. ^1H NMR (600 MHz) and ^{13}C NMR (151 MHz) spectra of α,β -dihydroxanthohumol 7-O- β -D-glucopyranoside (**6**) (Acetone- d_6 , Temp. 25 °C)

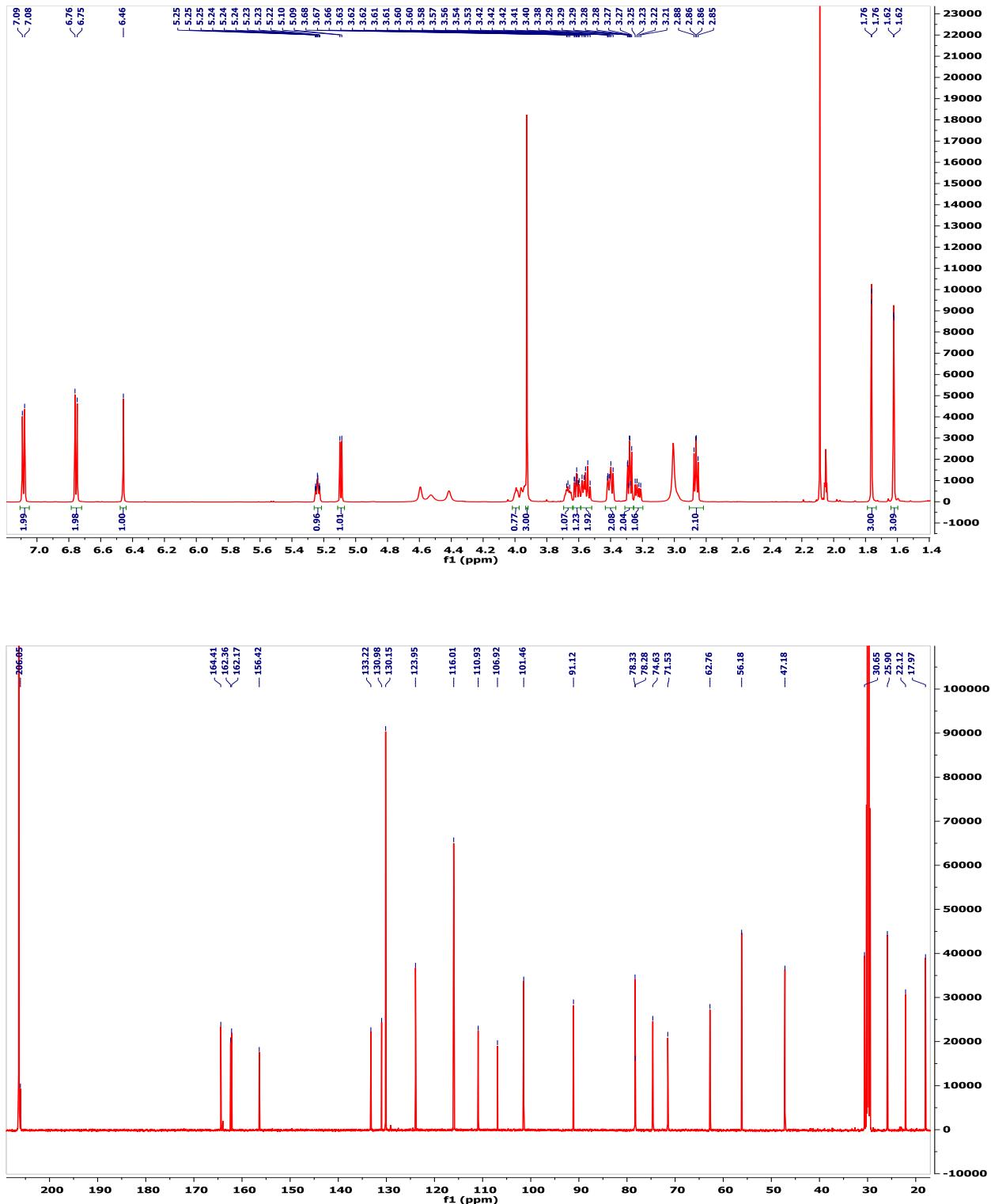


Figure S13. ^1H NMR - ^1H NMR (COSY) spectrum of α,β -dihydroxanthohumol 7-O- β -D-glucopyranoside (**6**) (600 MHz/600 MHz, Acetone- d_6 , Temp. 25°)

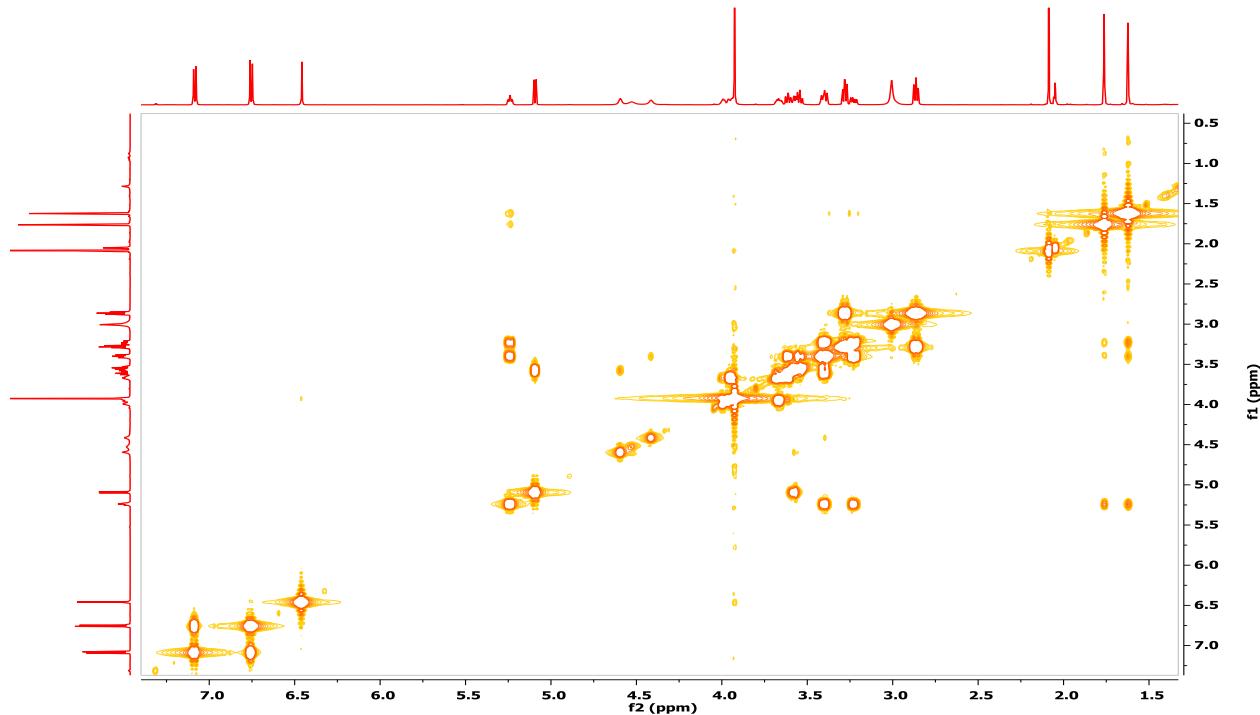


Figure S14. ^1H NMR - ^{13}C NMR (HSQC) spectrum of α,β -dihydroxanthohumol 7-O- β -D-glucopyranoside (**6**) (600 MHz/151 MHz, Acetone- d_6 , Temp. 25°)

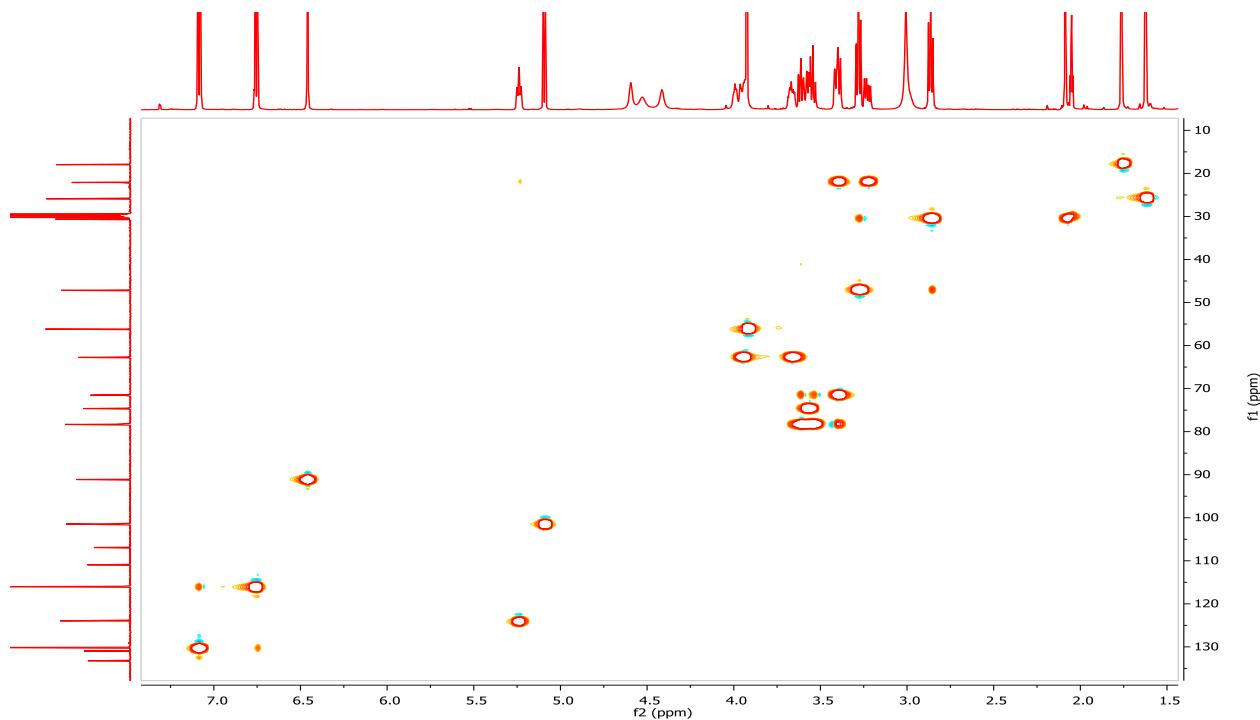


Figure S15. UV spectrum of α,β -dihydroxanthohumol 7-O- β -D-(4''-O-methyl)glucopyranoside (**7**) (MeOH, Temp. 20 °C)

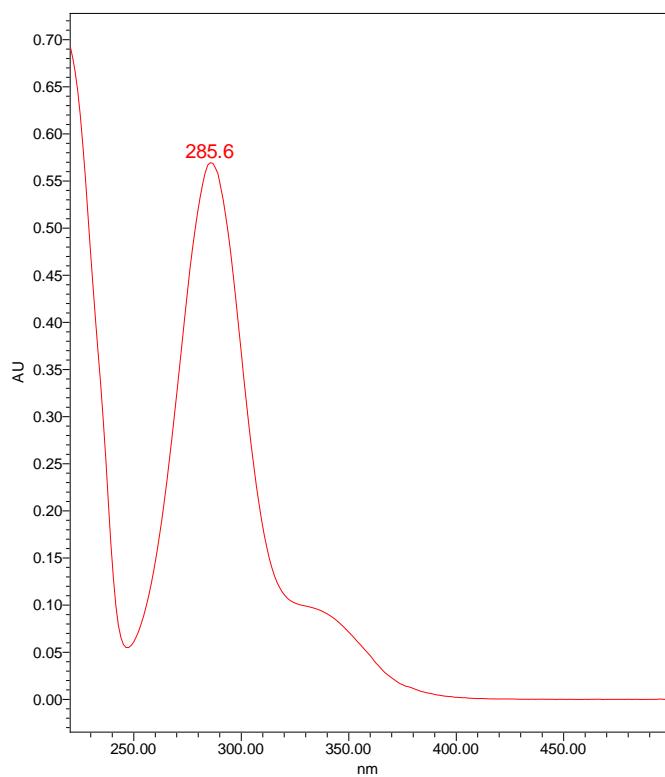


Figure S16. HRMS spectrum of α,β -dihydroxanthohumol 7-O- β -D-(4''-O-methyl)glucopyranoside (**7**)

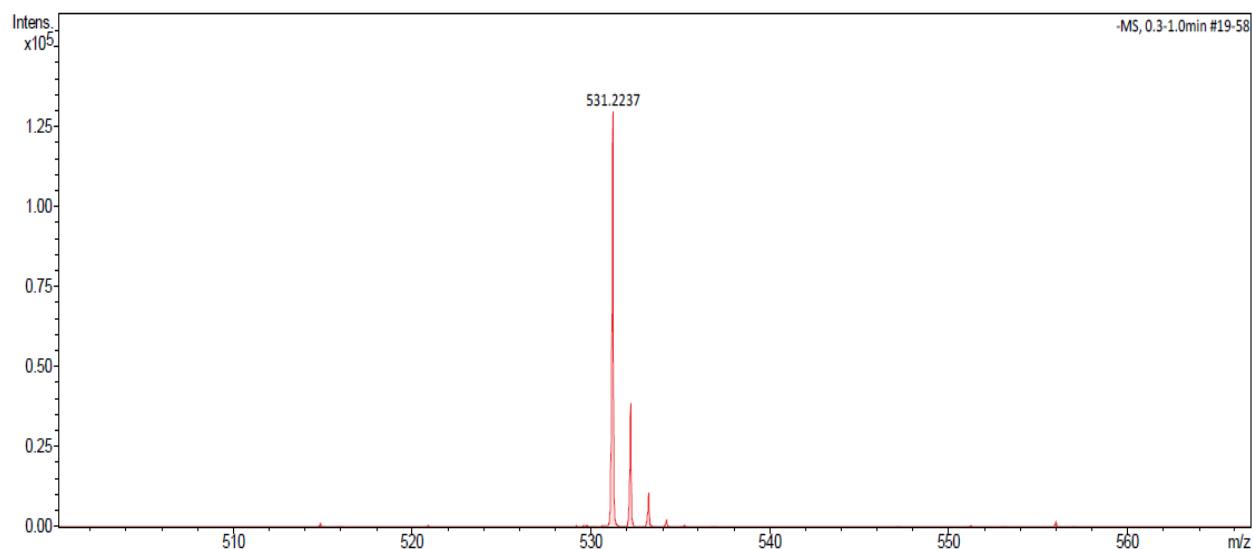


Figure S17. ^1H NMR (600 MHz) and ^{13}C NMR (151 MHz) spectra of α,β -dihydroxanthohumol 7-O- β -D-(4''-O-methyl)glucopyranoside (**7**) (Acetone- d_6 , Temp. 25 °C).

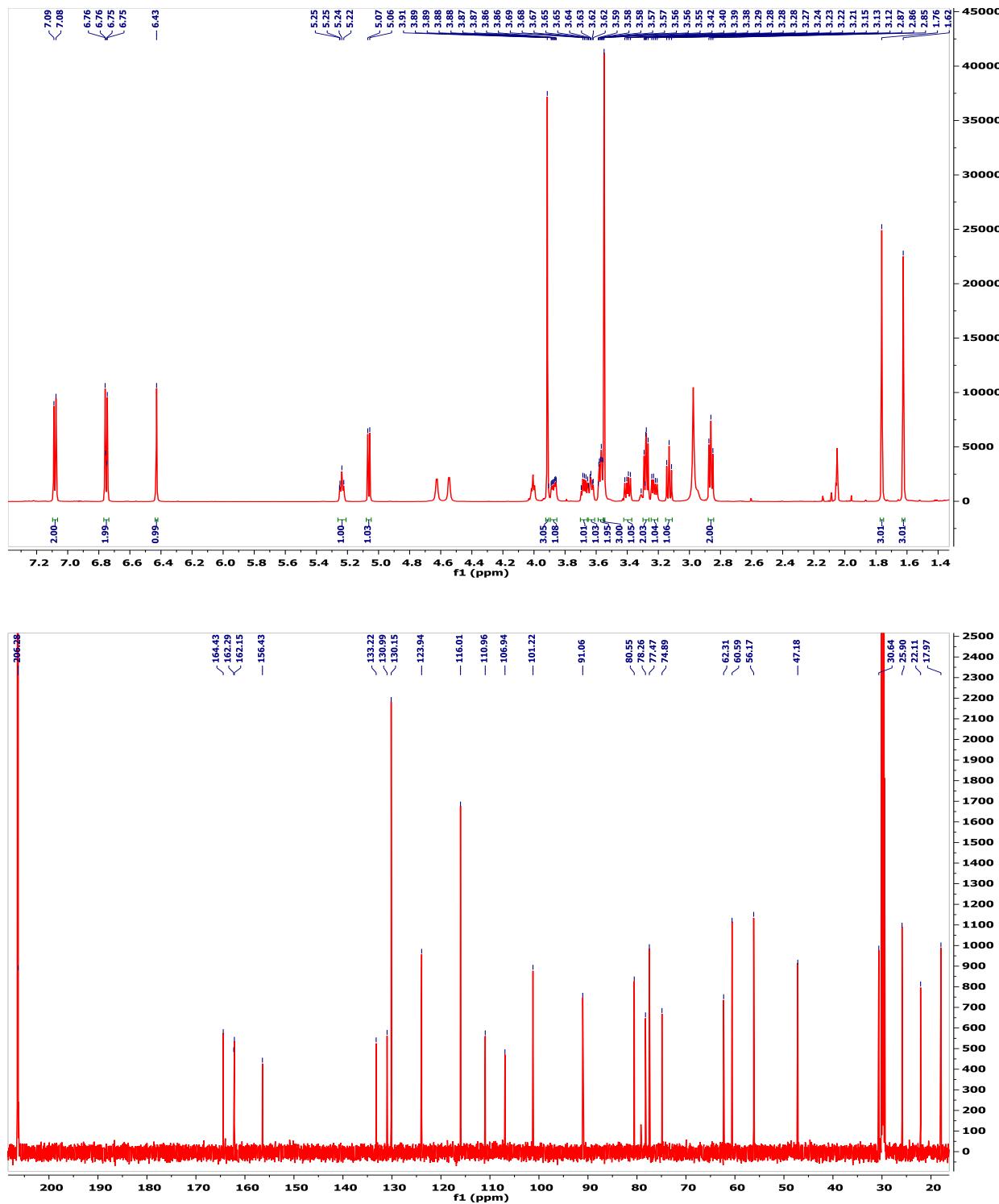


Figure S18. ^1H NMR - ^1H NMR (COSY) spectrum of α,β -dihydroxanthohumol 7-O- β -D-(4''-O-methyl)glucopyranoside (**7**) (600 MHz/600 MHz, Acetone- d_6 , Temp. 25°)

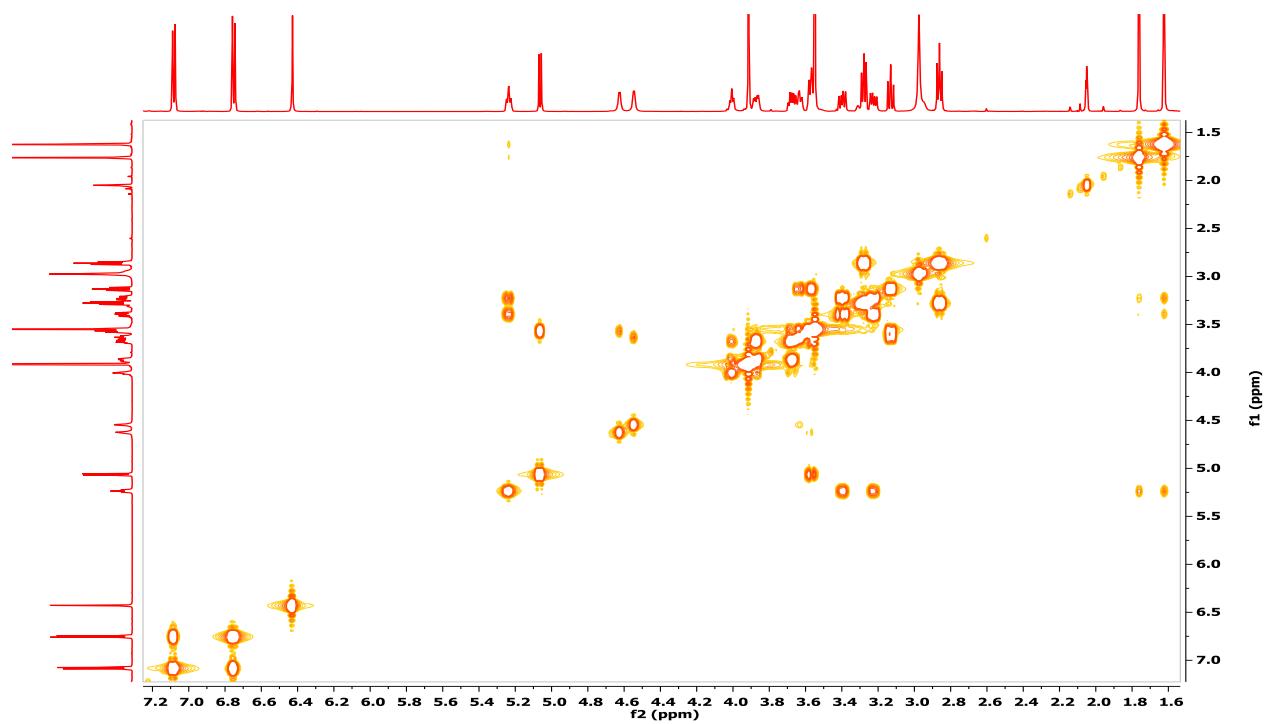


Figure S19. ^1H NMR - ^{13}C NMR (HSQC) spectrum of α,β -dihydroxanthohumol 7-O- β -D-(4''-O-methyl)glucopyranoside (**7**) (600 MHz/151 MHz, Acetone- d_6 , Temp. 25°)

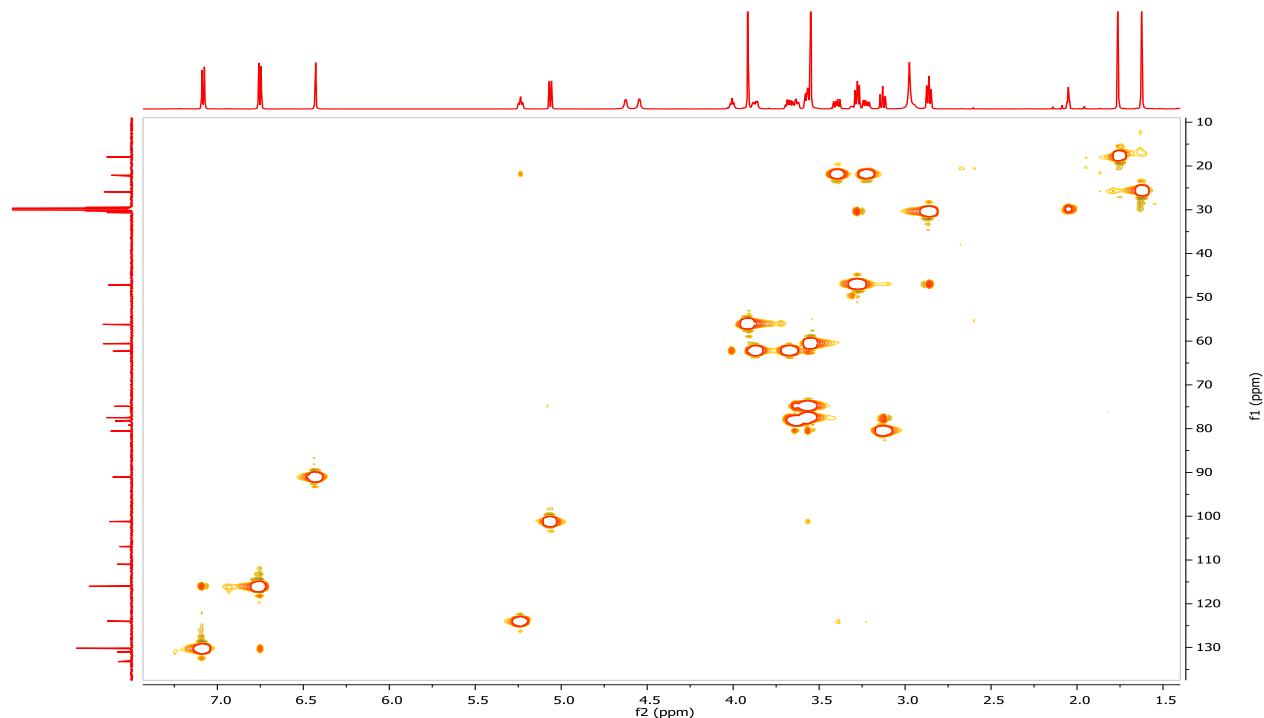


Figure S20. UV spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O- β -D-glucopyranoside (**8**) (MeOH, Temp. 20 °C)

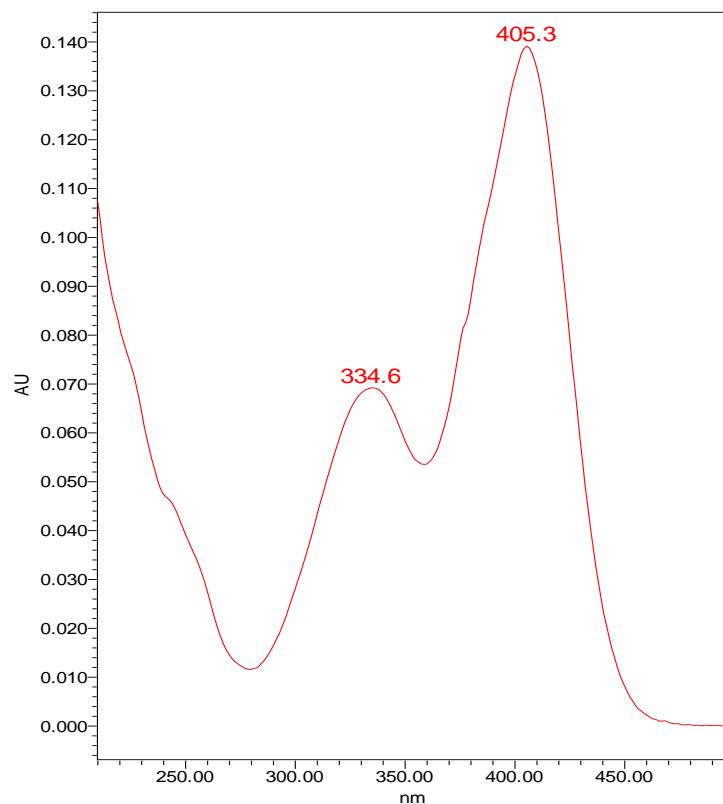


Figure S21. HRMS spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O- β -D-glucopyranoside (**8**)

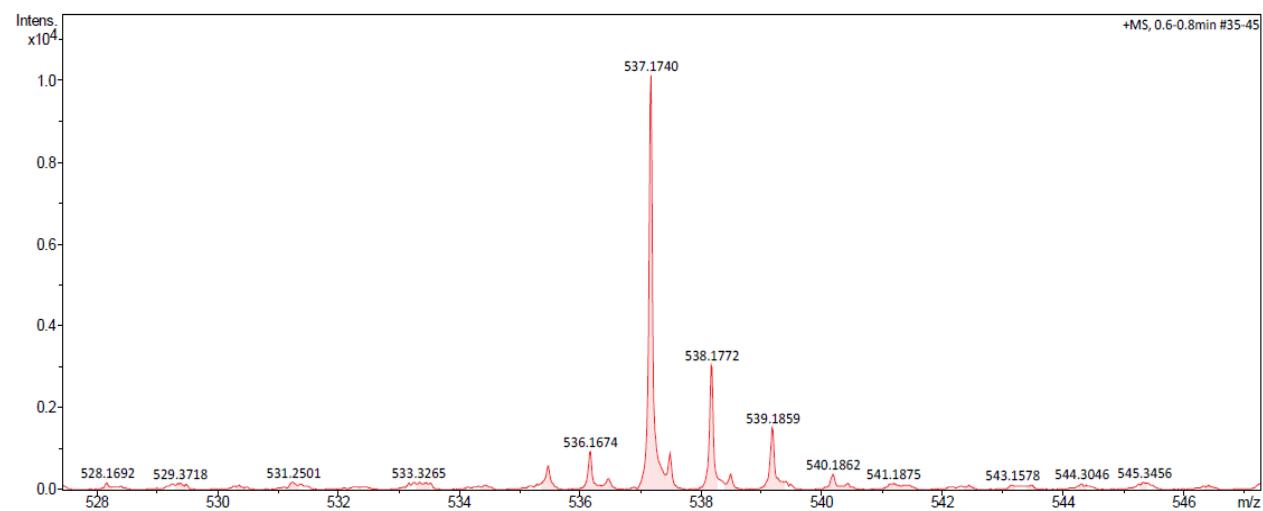


Figure S22. ^1H NMR (600 MHz) and ^{13}C NMR (151 MHz) spectra of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O- β -D-glucopyranoside (8) CD₃OD, Temp. 25 °C)

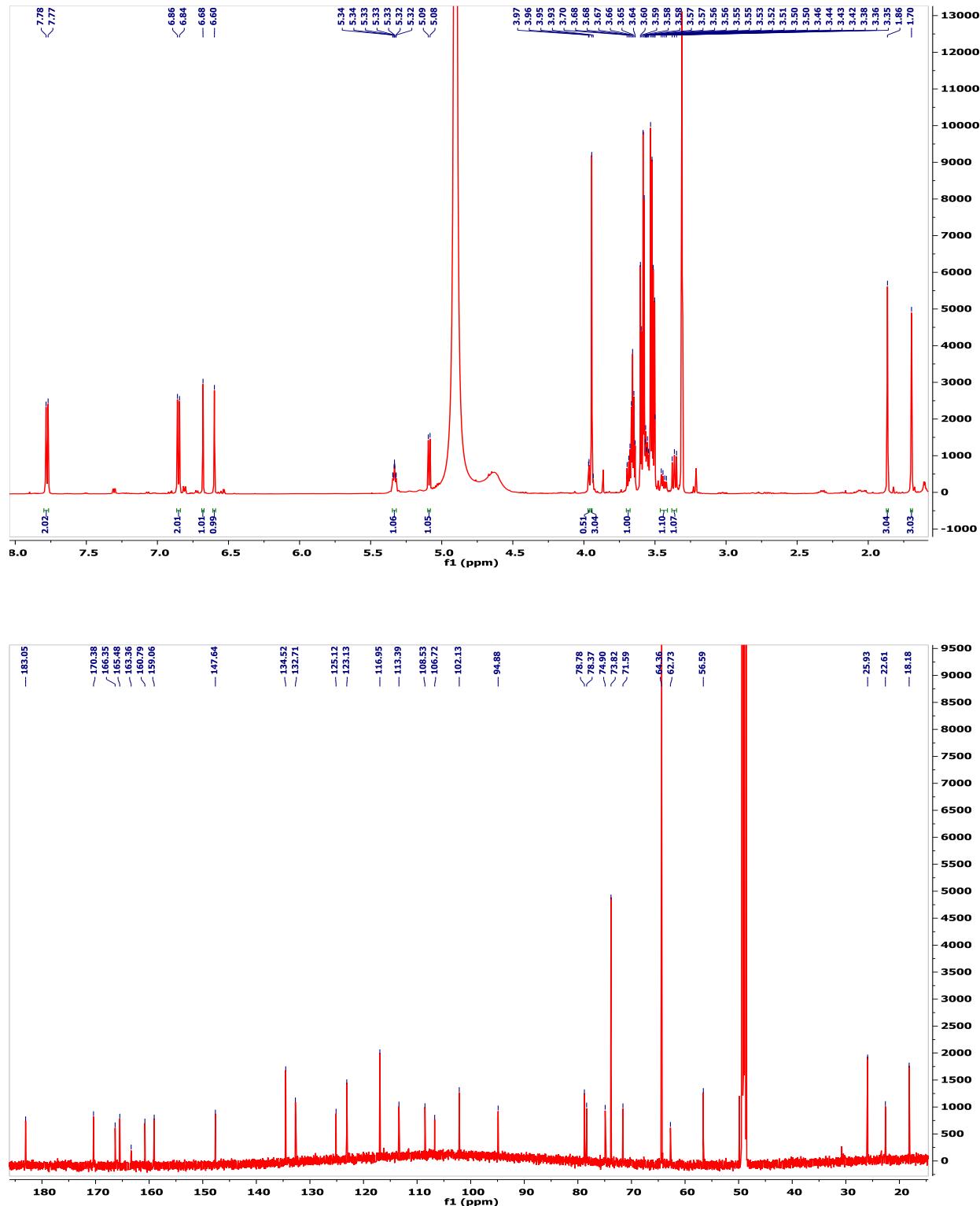


Figure S23. ^1H NMR - ^1H NMR (COSY) spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O- β -D-glucopyranoside (**8**) (600 MHz/600 MHz, CD_3OD , Temp. 25 °C)

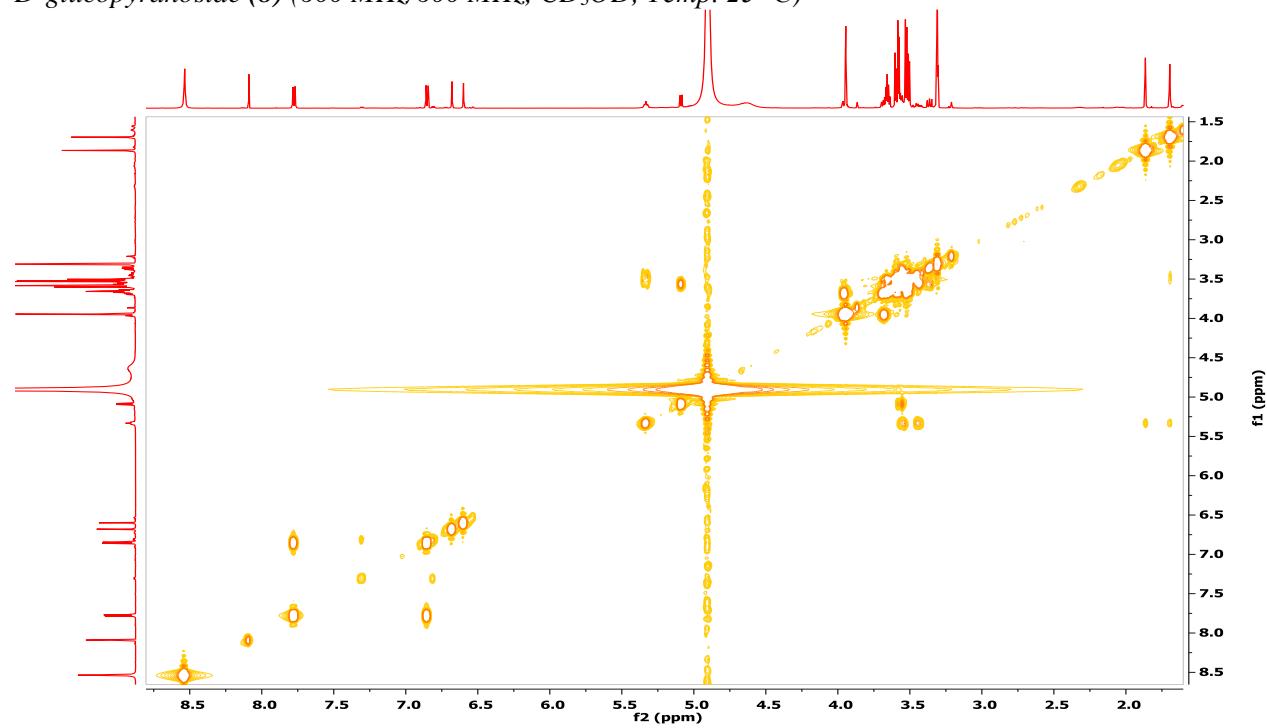


Figure S24. ^1H NMR - ^{13}C NMR (HSQC) spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O- β -D-glucopyranoside (**8**) (600 MHz/151 MHz, CD_3OD , Temp. 25 °C)

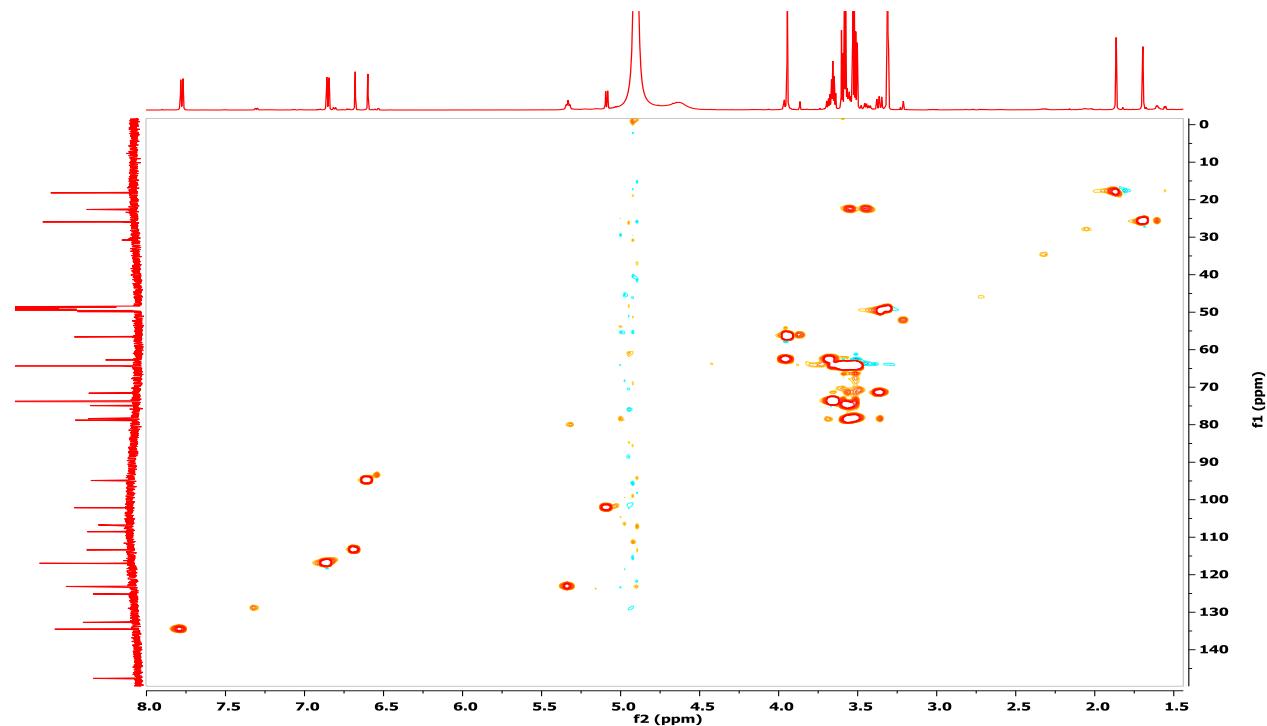


Figure S25. UV spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O- β -D-(4'''-O-methyl)glucopyranoside (**9**) (MeOH, Temp. 20 °C)

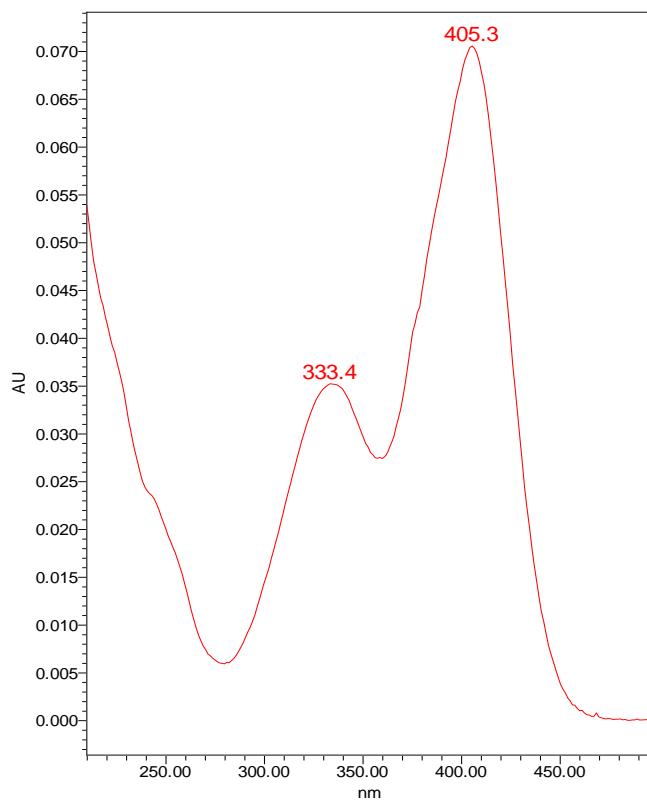


Figure S26. HRMS spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O- β -D-(4'''-O-methyl)glucopyranoside (**9**)

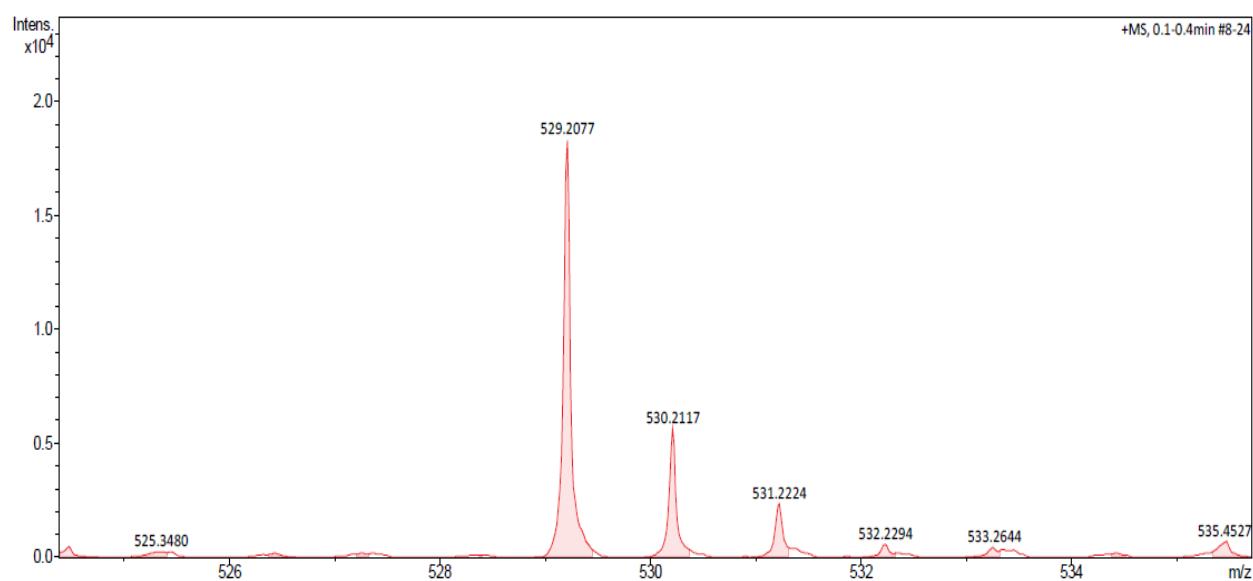


Figure S27. ^1H NMR (300 MHz) and ^{13}C NMR (75 MHz,) spectra of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O- β -D-(4'''-O-methyl)glucopyranoside (**9**) (DMSO- d_6 , Temp. 25 °C)

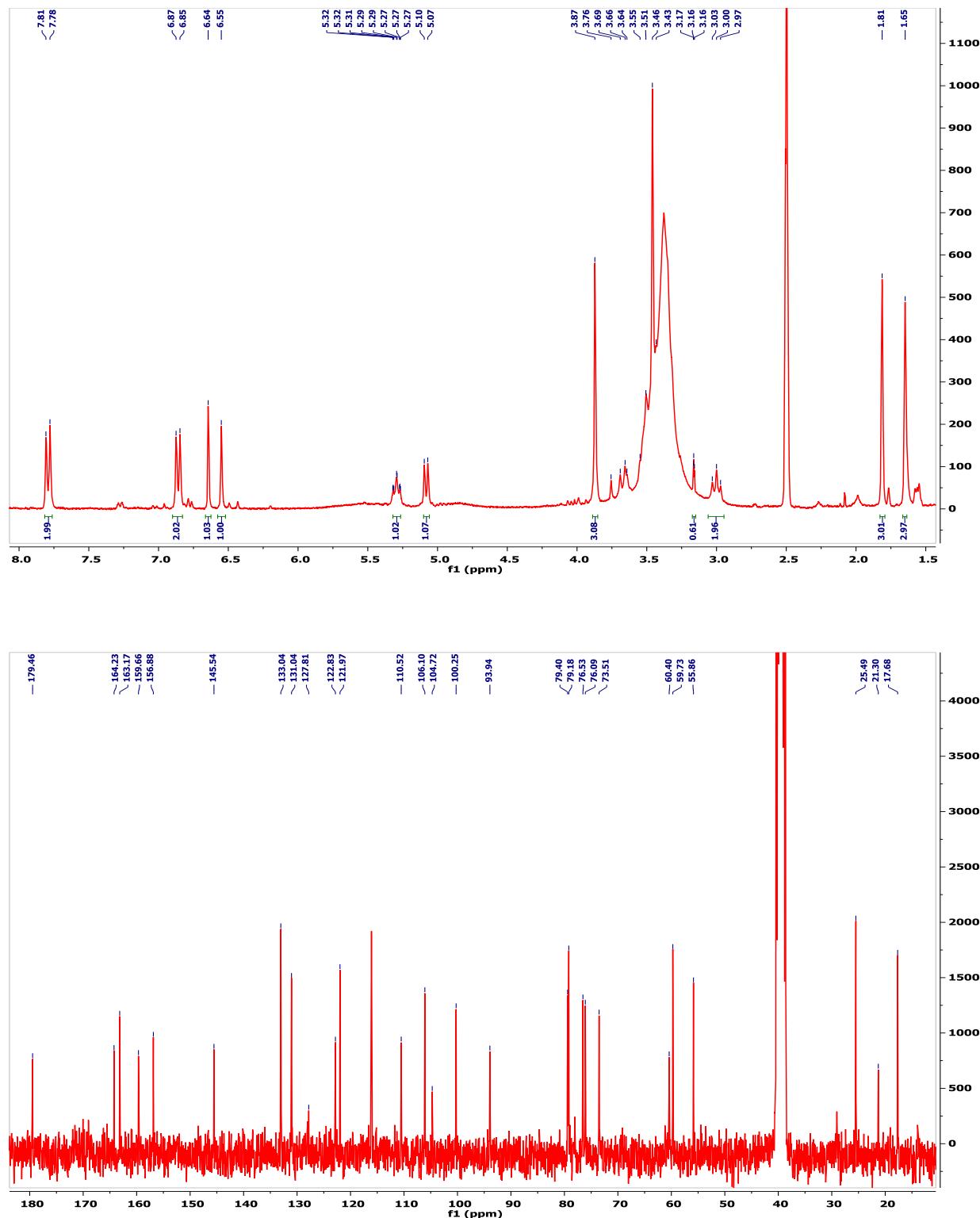


Figure S28. ^1H NMR - ^1H NMR (COSY) spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O- β -D-(4'''-O-methyl)glucopyranoside (**9**) (600 MHz/600 MHz, $\text{DMSO}-d_6$, Temp. 25 °C)

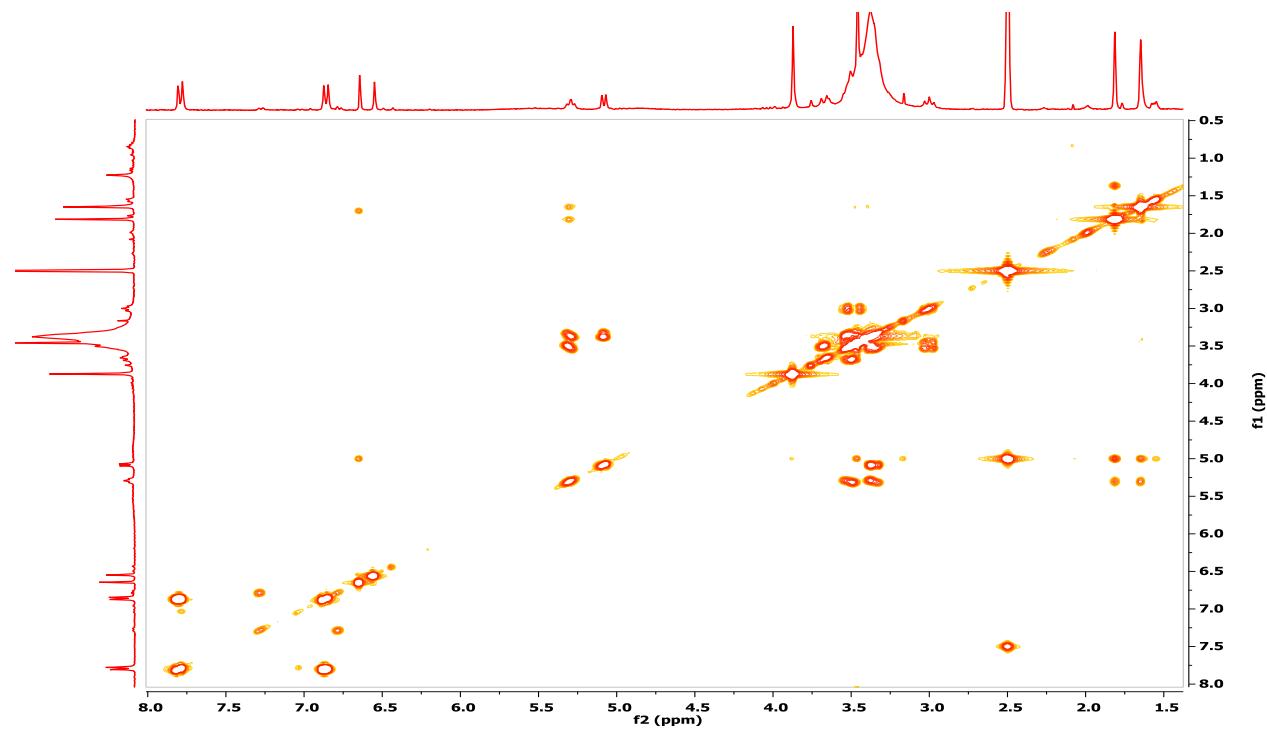


Figure S29. ^1H NMR - ^{13}C NMR (HSQC) spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O- β -D-(4'''-O-methyl)glucopyranoside (**9**) (600 MHz/151 MHz, $\text{DMSO}-d_6$, Temp. 25 °C)

