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

Tomasz Tronina*[1], Paulina Strugała[2], Jarosław Popłoński[1], Aleksandra Włoch[2], Sandra Sordon[1], Agnieszka Bartmańska[1] and Ewa Huszcza[1]

[1]Department of Chemistry, Wrocław University of Environmental and Life Sciences, Norwida 25, 50-375 Wrocław, Poland.[2]Department of Physics and Biophysics, Wrocław University of Environmental and Life Sciences, Norwida 25, 50-375 Wrocław, Poland. *Corresponding Author: E-mail address: tomasz.tronina@upwr.edu.pl, Phone: +48 713205197; fax: +48 3207744

Table of Contents:

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

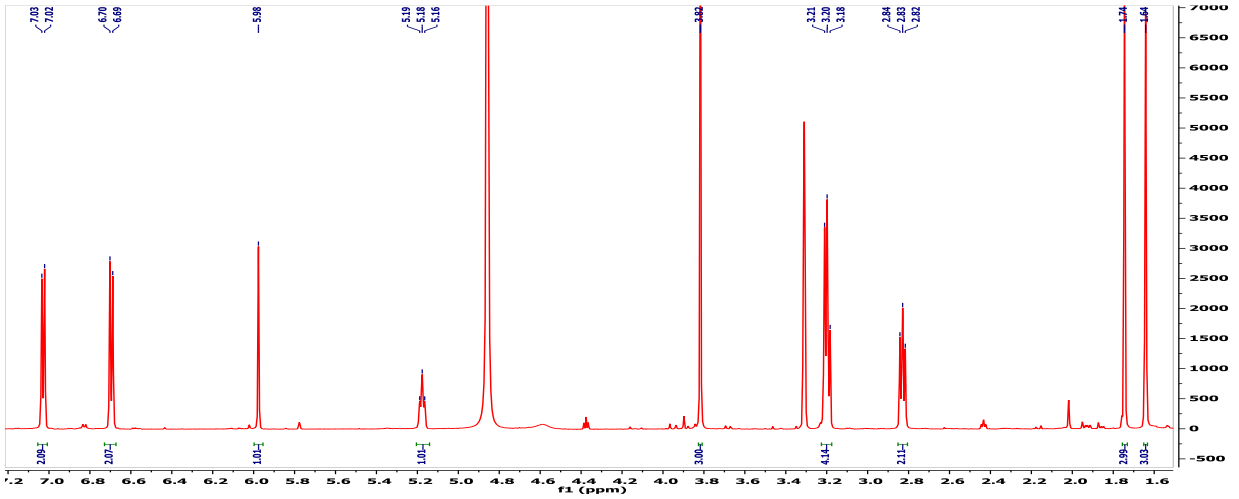


Figure S2. *^{13}C NMR and DEPT 135° spectra of α,β-dihydroxanthohumol (**2**) (151 MHz, CD_3OD, Temp. 25 ºC)*

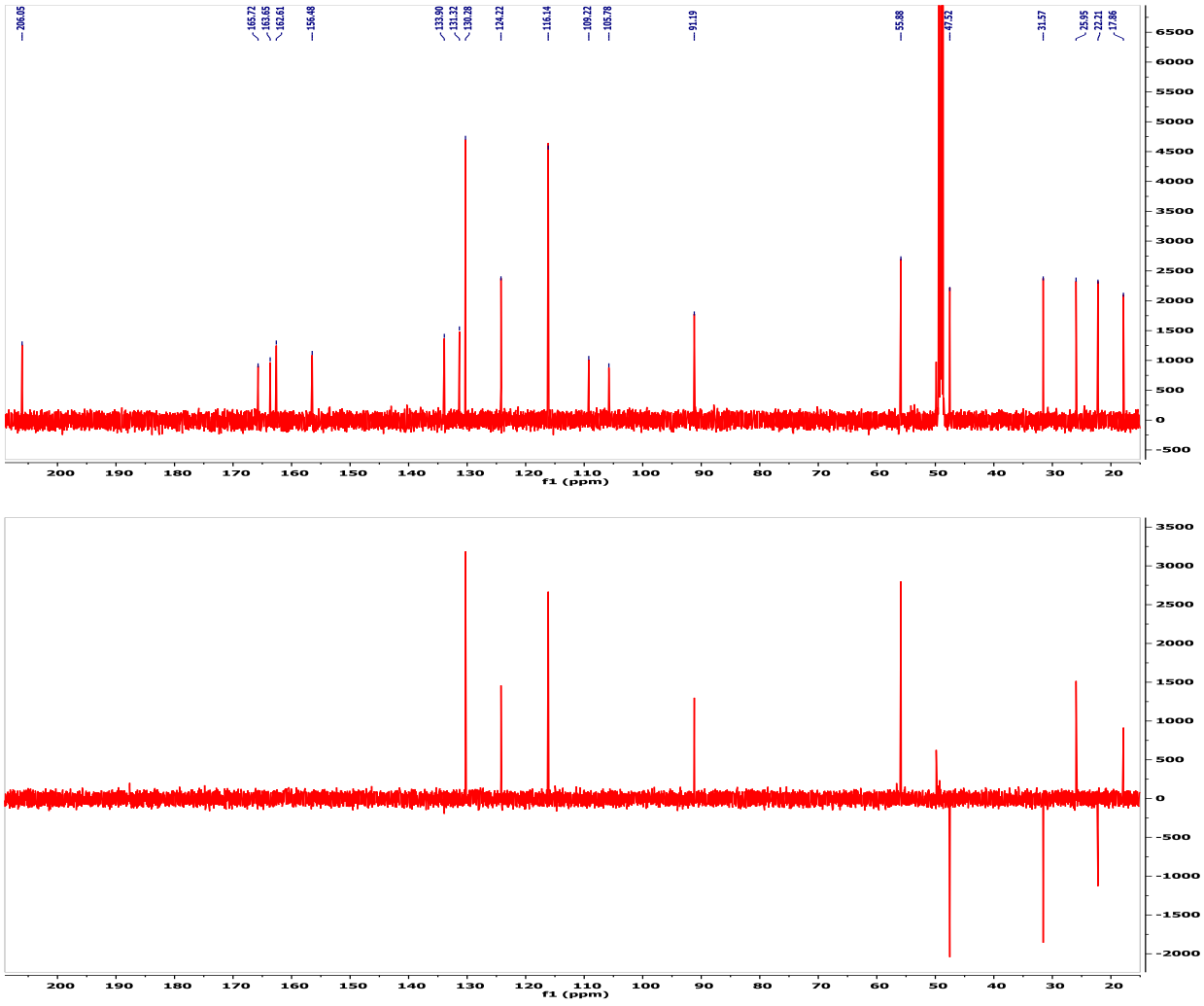


Figure S3*: UV spectra of:* ***A*** *xanthohumol* ***(1)****,* ***B*** *(Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone* ***(3)*** *(MeOH, Temp. 20 °C)*

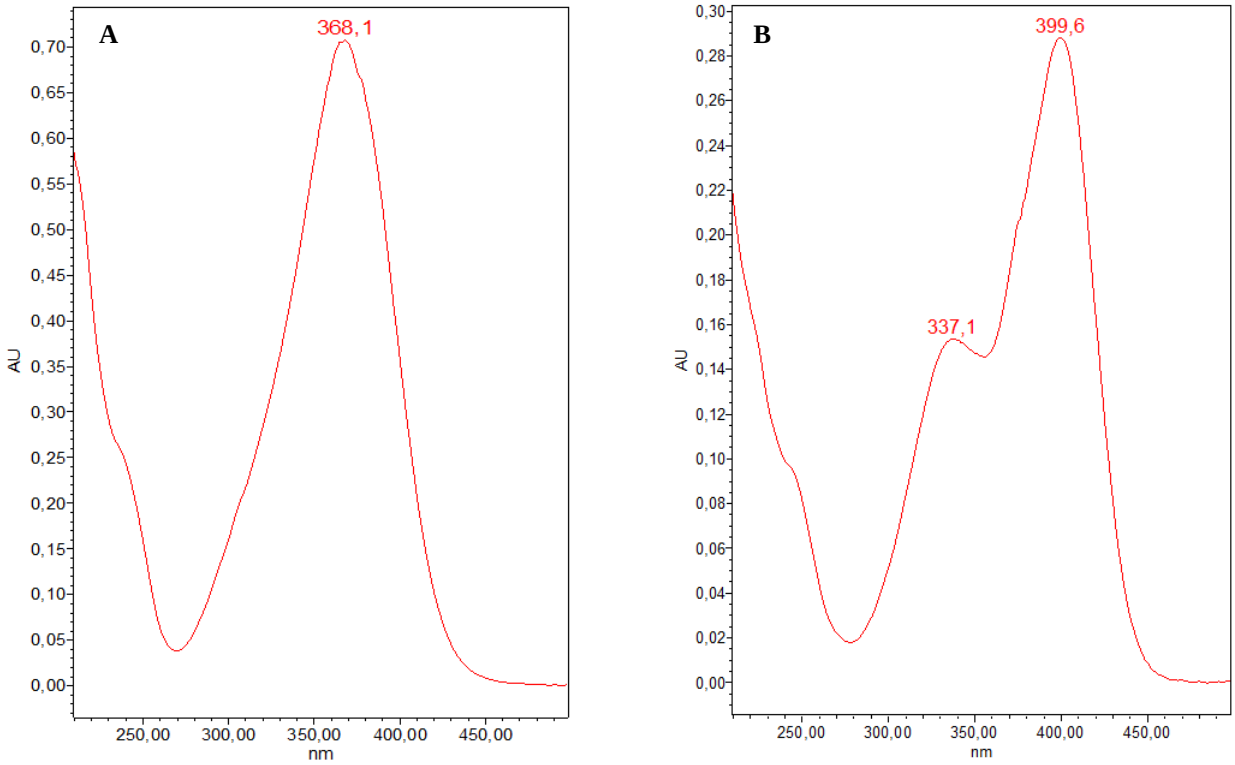


Figure S4. *HRMS spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone* ***(3)***

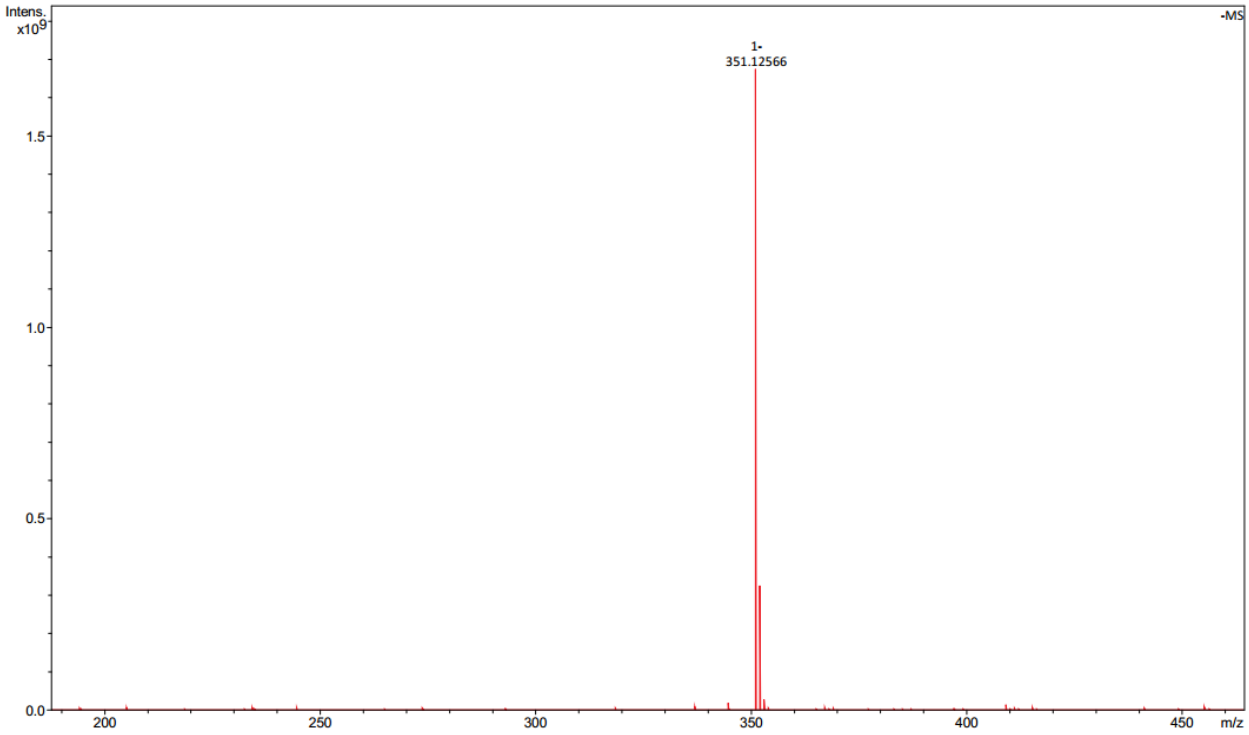
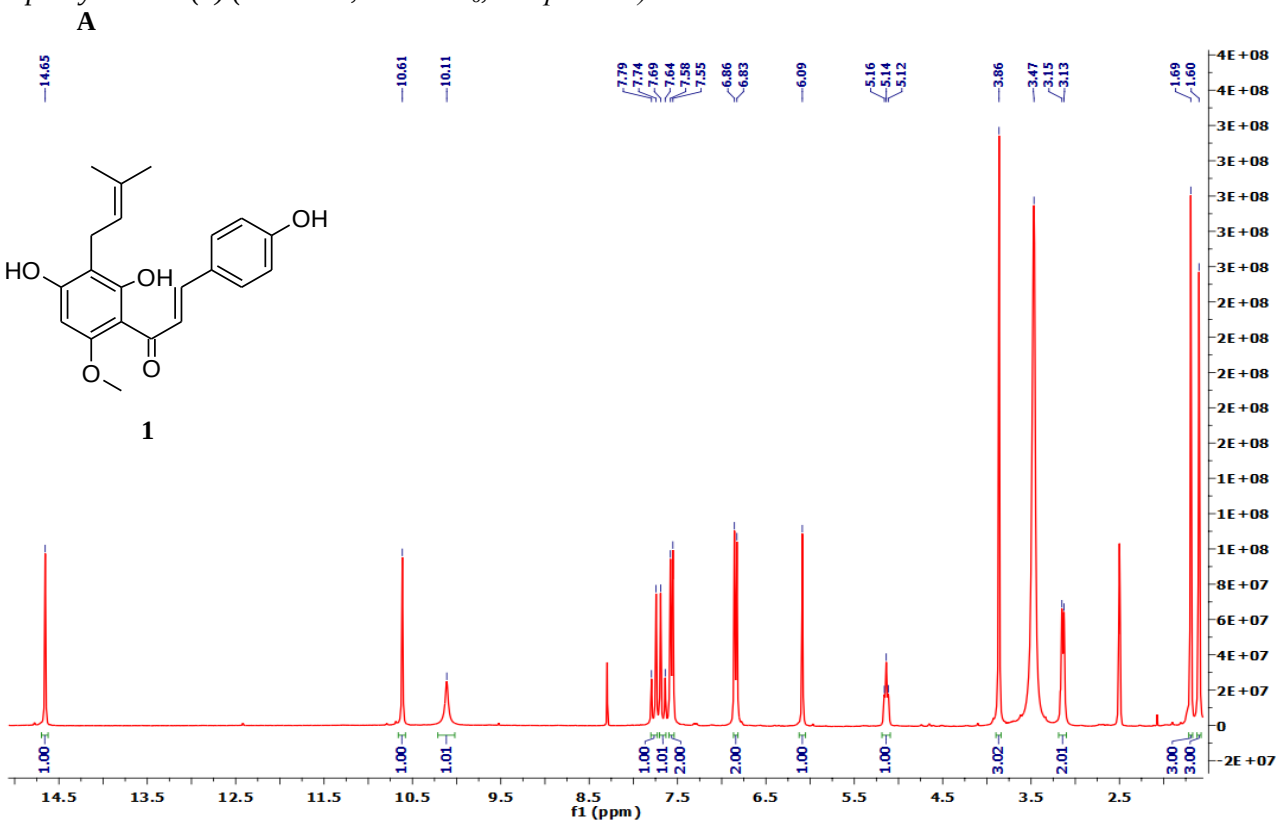


Figure S5. *[1]H NMR spectra of:* ***A*** *xanthohumol* ***(1)*** *(600 MHz, DMSO-d_6),* ***B*** *(Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone* ***(3)*** *(300 MHz, DMSO-d_6, Temp. 25 ºC)*



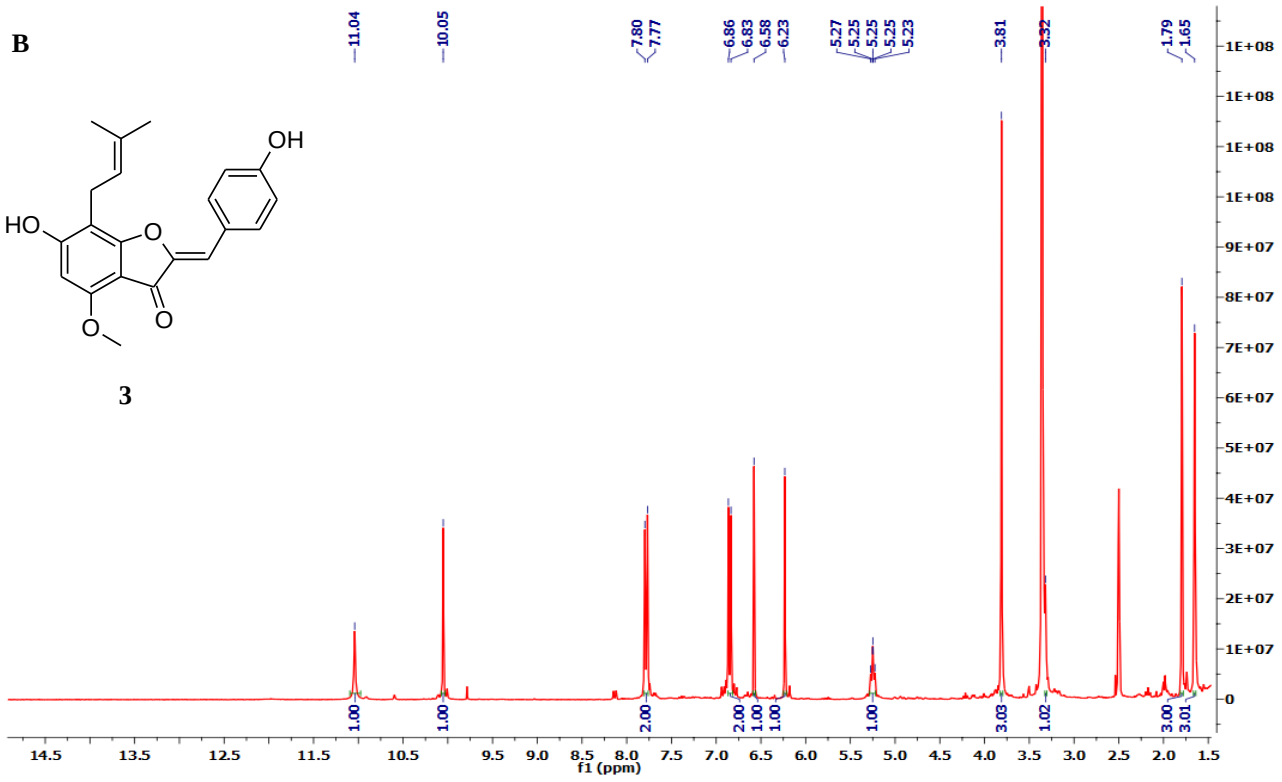
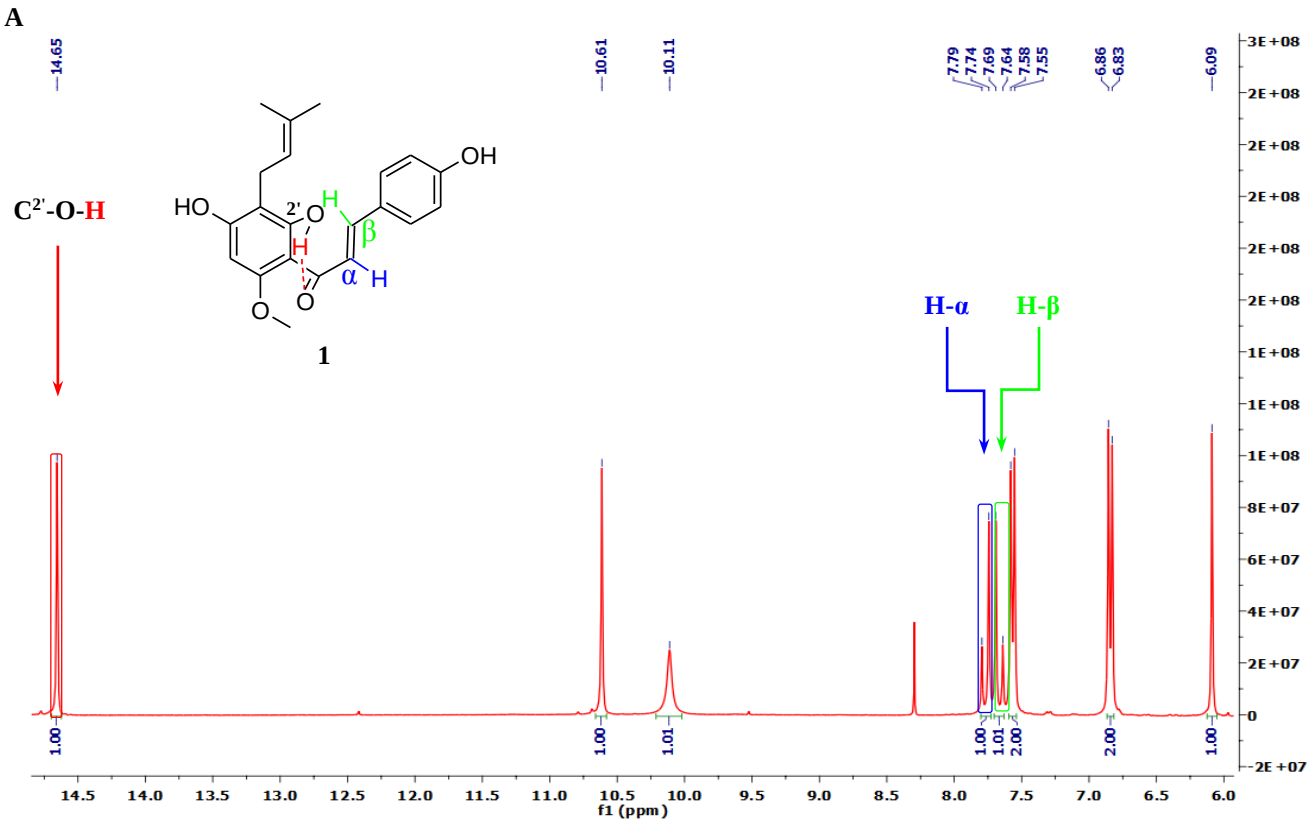


Figure S6. *Fragments of ^{1}H NMR spectra of:* ***A*** *xanthohumol (**1**) (600 MHz, DMSO-d_6),* ***B*** *aurone (**3**) (300 MHz, DMSO-d_6, Temp. 25 ºC)*



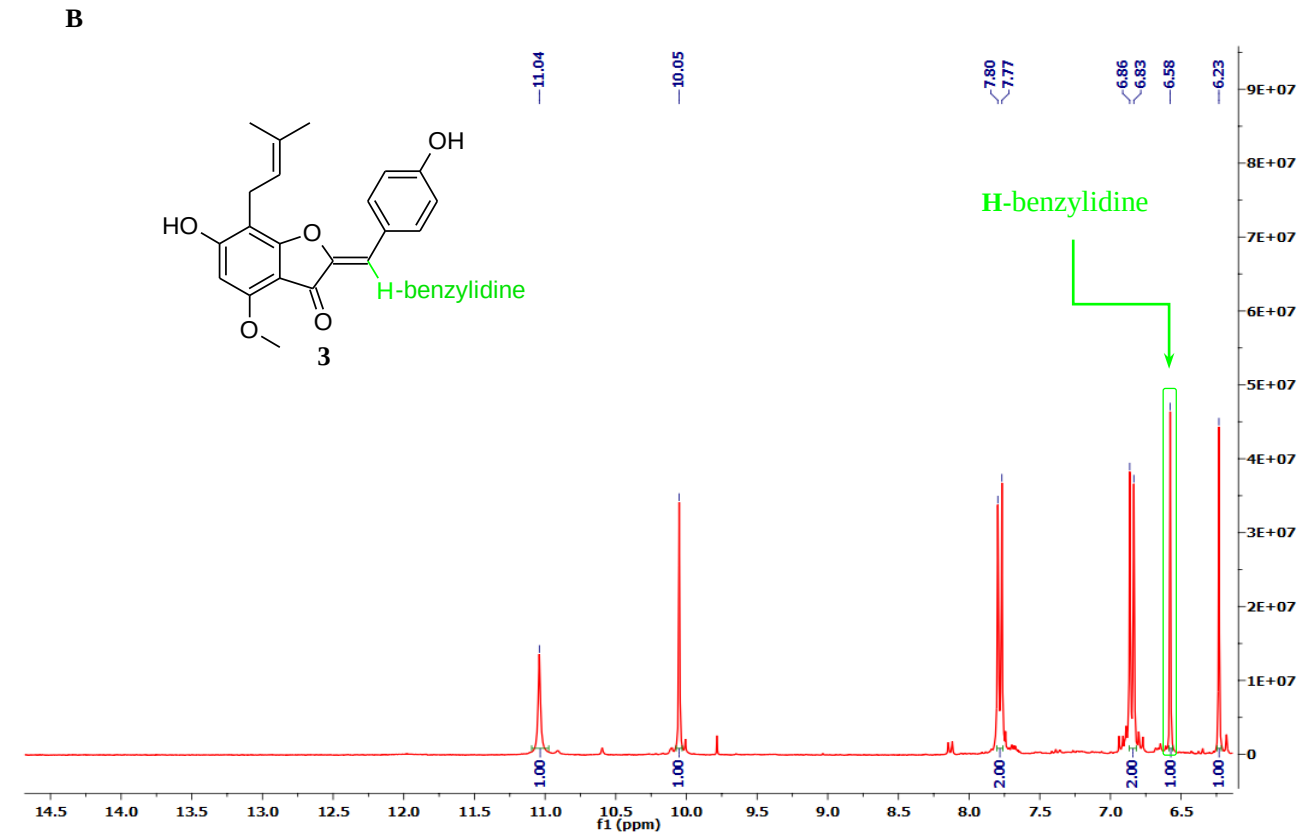


Figure S7. *^{13}C NMR spectra of:* ***A*** *xanthohumol* ***(1)*** *(151 MHz, DMSO-d_6),* ***B*** *auron* ***(3)*** *(75 MHz, DMSO-d_6, Temp. 25 ºC)*

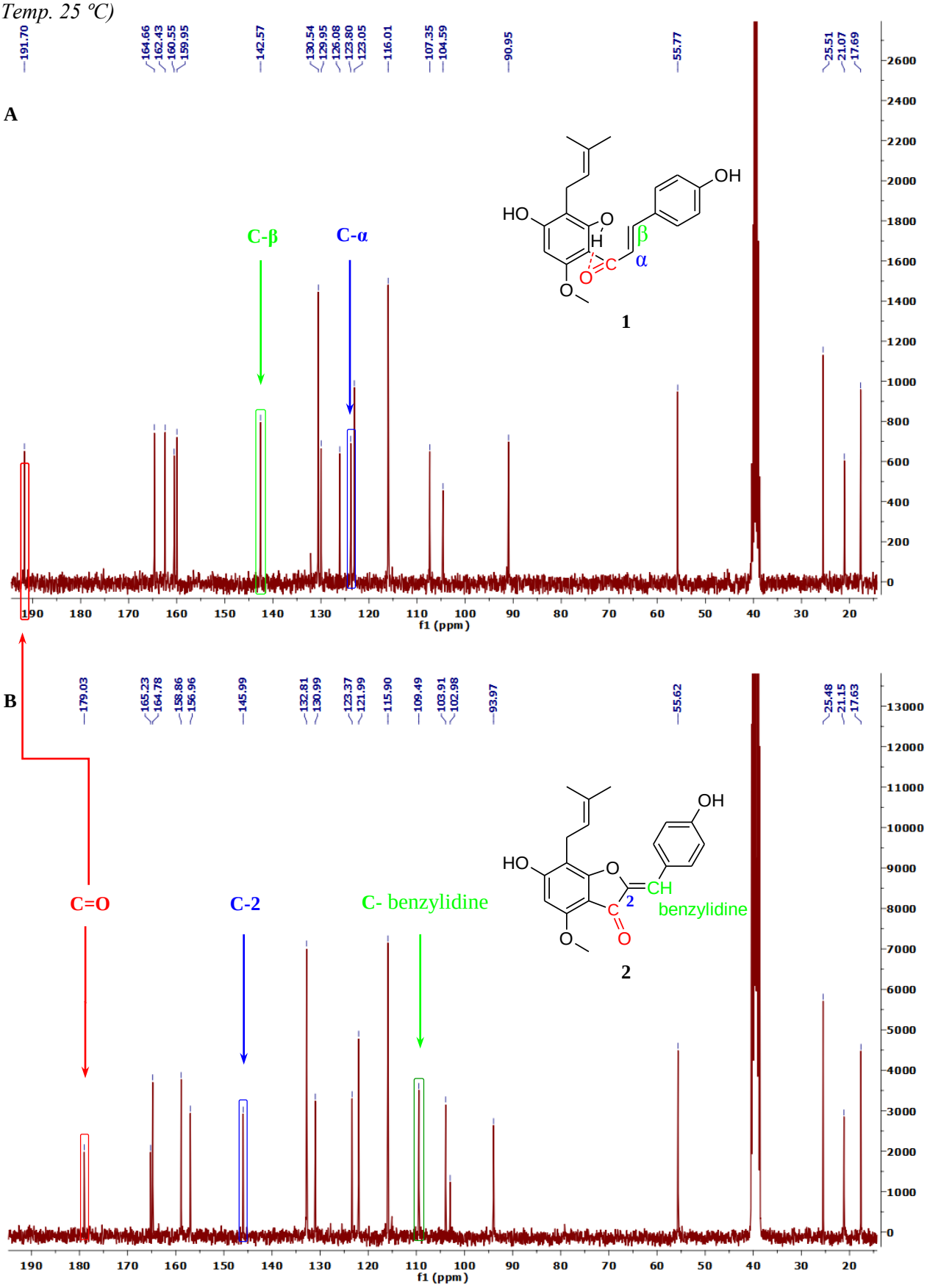


Figure S8. *^{1}H-^{1}H NMR (COSY) spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone (**3**)(300 MHz/300 MHz, DMSO-d_6, Temp. 25°)*

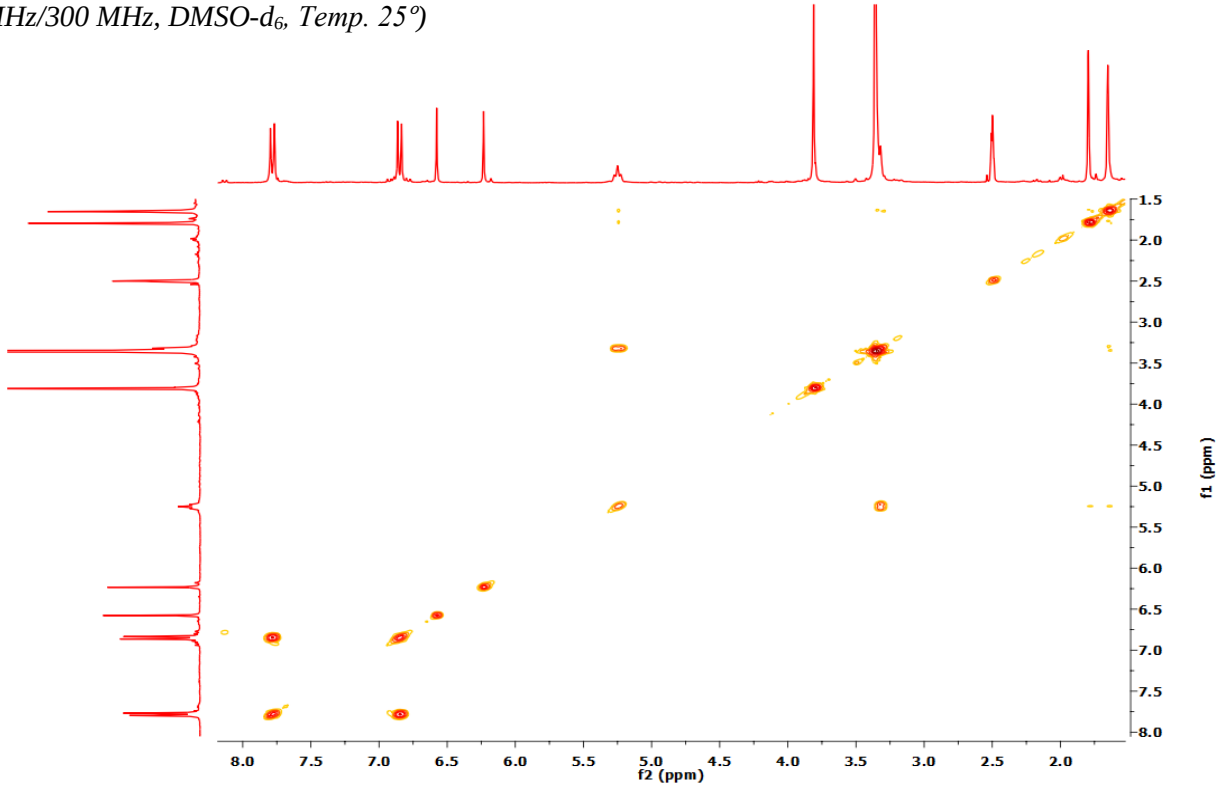


Figure S9. *^{1}H– ^{13}C NMR (HSQC) spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone (**3**))(300 MHz/75 MHz, DMSO-d_6, Temp. 25°)*

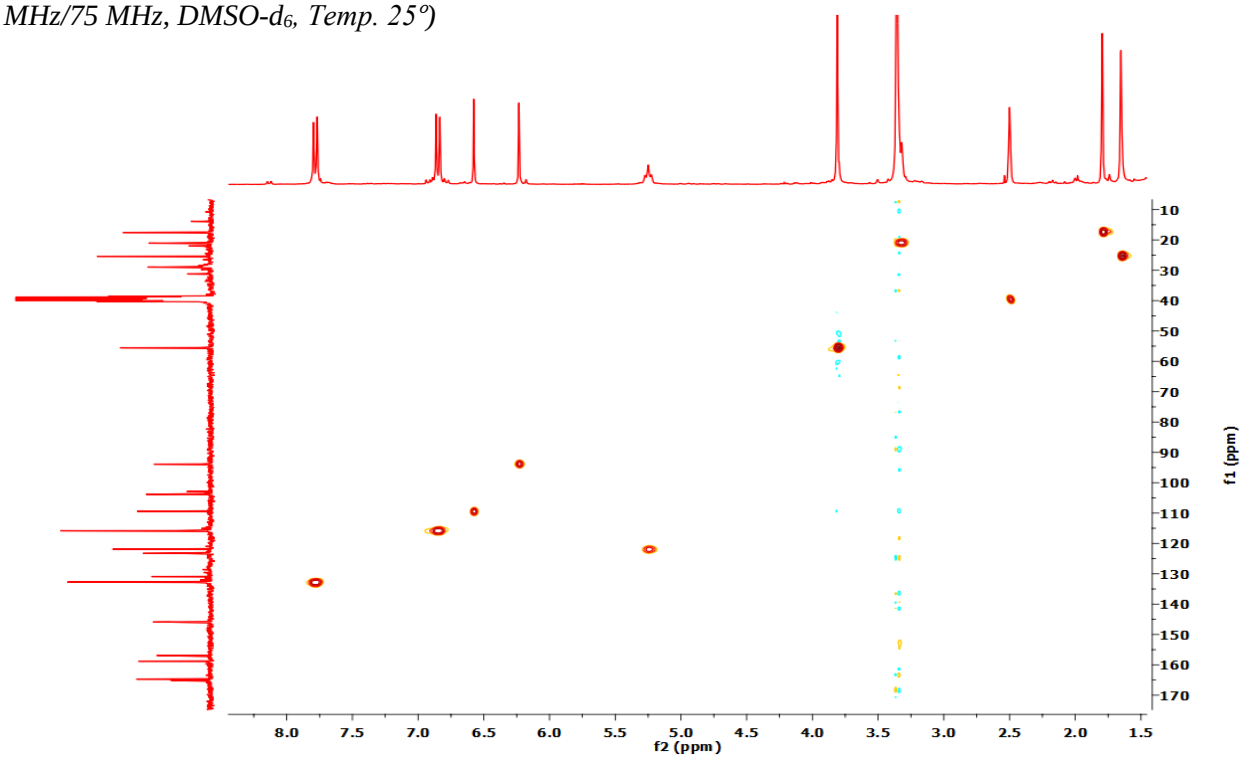


Figure S10. *UV spectrum of α,β-dihydroxanthohumol 4' -O-β-D-glucopyranoside (**6**) (MeOH, Temp. 20 °C)*

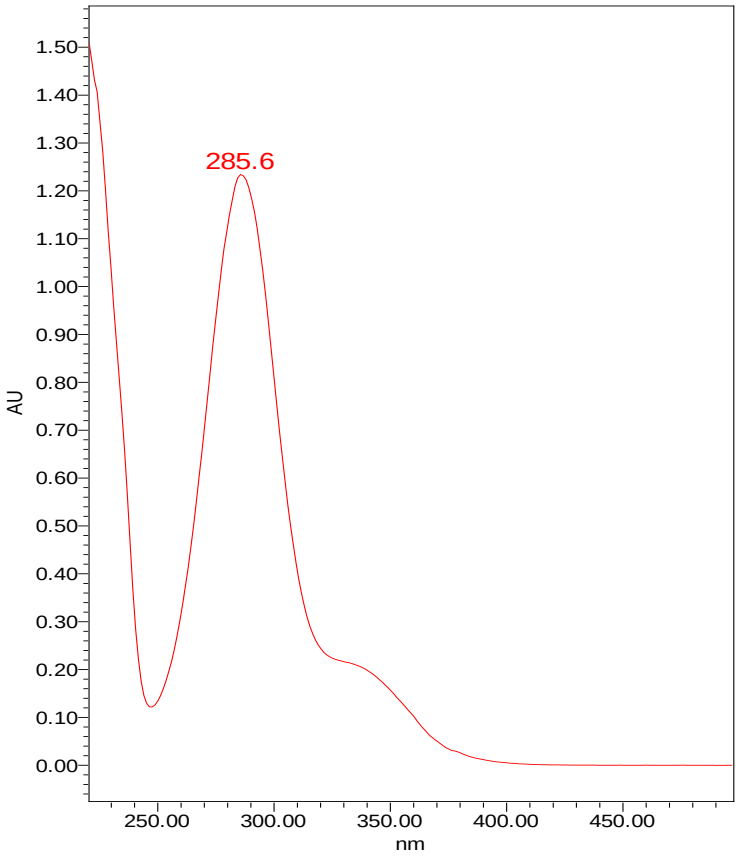


Figure S11. *HRMS spectrum of α,β-dihydroxanthohumol 4' -O-β-D-glucopyranoside (**6**)*

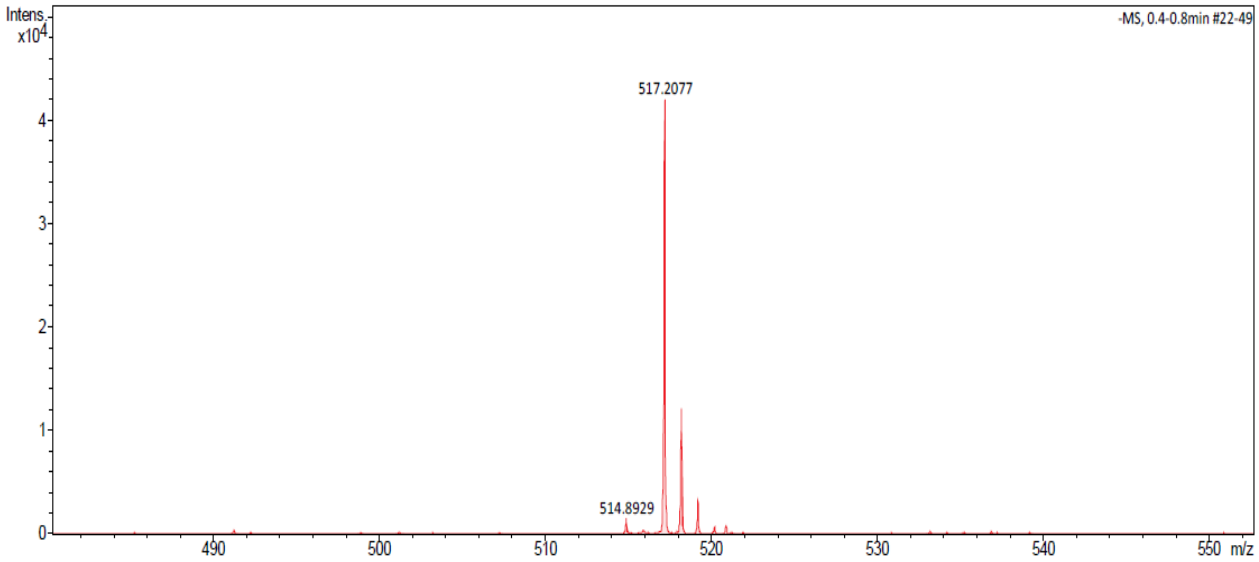


Figure S12. *^{1}H NMR (600 MHz) and ^{13}C NMR (151 MHz) spectra of α,β-dihydroxanthohumol 7-O-β-D-glucopyranoside* ***(6)*** *(Acetone-d_6,Temp. 25 ºC)*

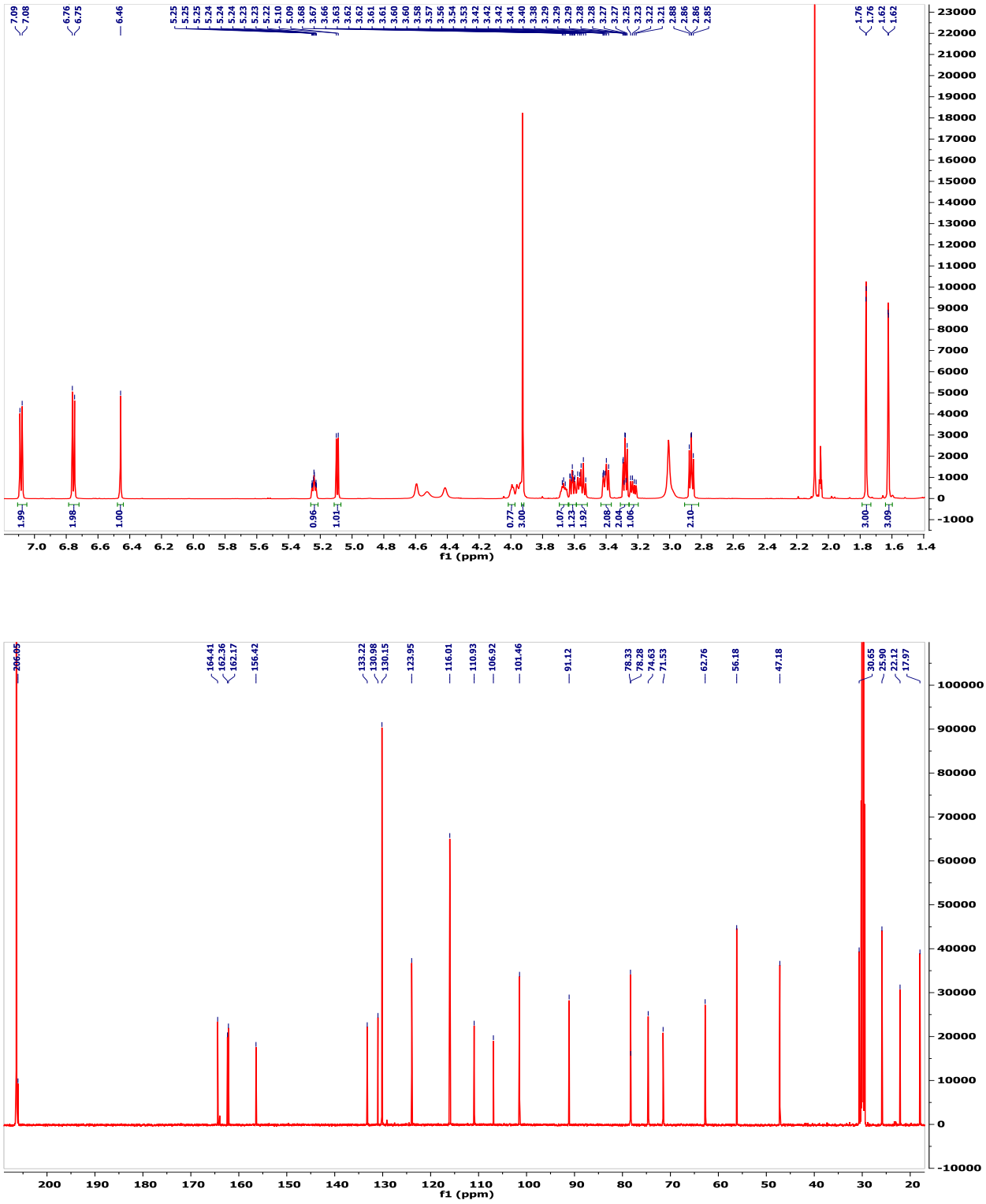


Figure S13. *^{1}H NMR - ^{1}H NMR (COSY) spectrum of α,β-dihydroxanthohumol 7-O-β-D-glucopyranoside* ***(6)*** *)(600 MHz/600 MHz, Acetone-d_6, Temp. 25°)*

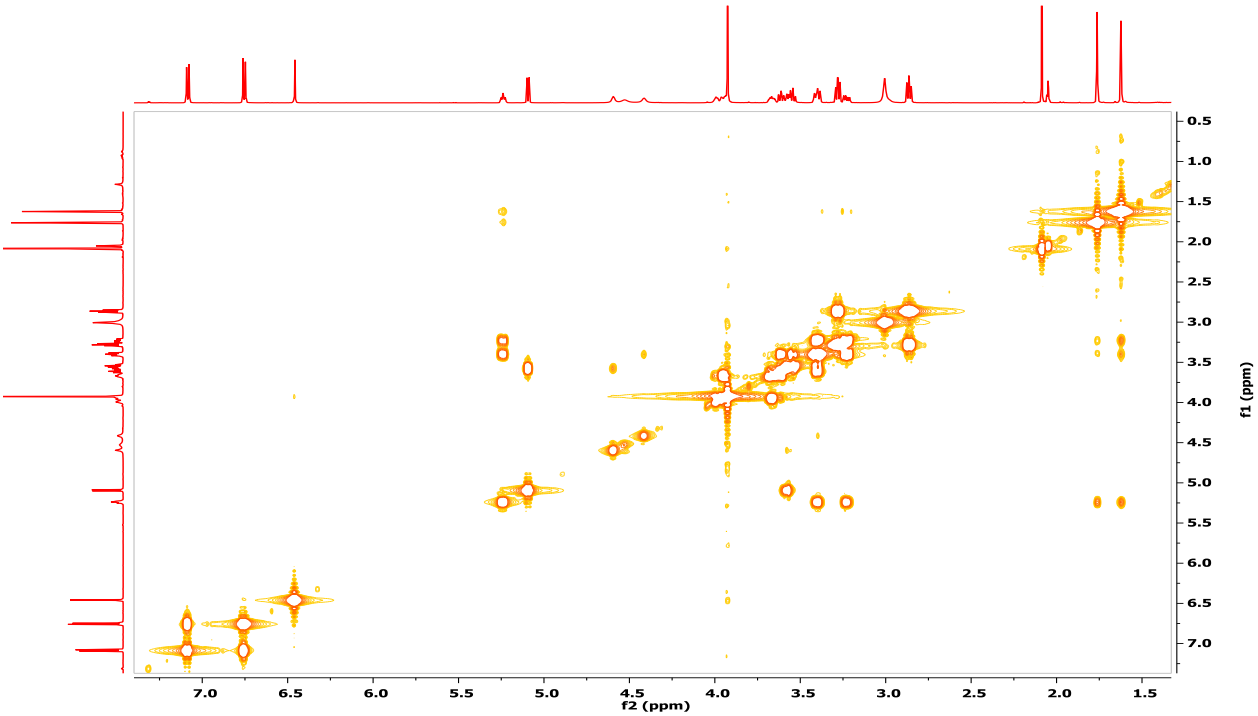


Figure S14. *^{1}H NMR - ^{13}C NMR (HSQC) spectrum of α,β-dihydroxanthohumol 7-O-β-D-glucopyranoside* ***(6)*** *)(600 MHz/151 MHz, Acetone-d_6, Temp. 25°)*

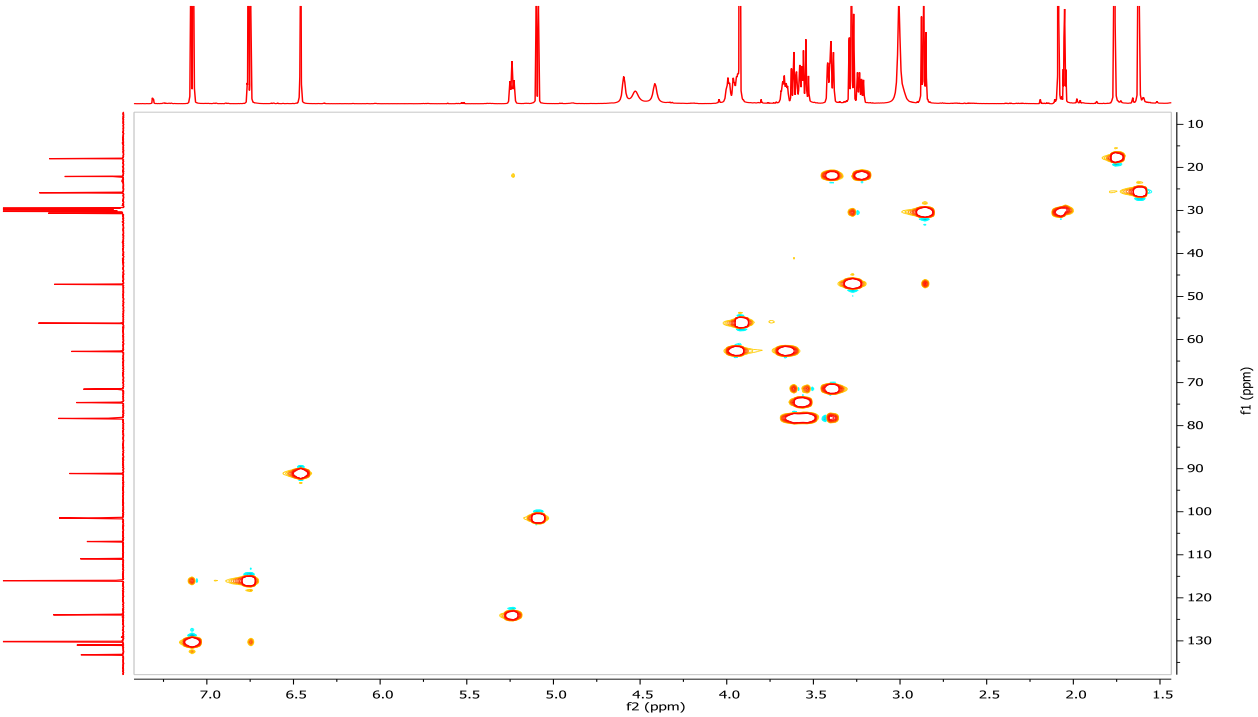


Figure S15. *UV spectrum of α,β-dihydroxanthohumol 7-O-β-D-(4'''-O-methyl)glucopyranoside* ***(7)*** *(MeOH, Temp. 20 °C)*

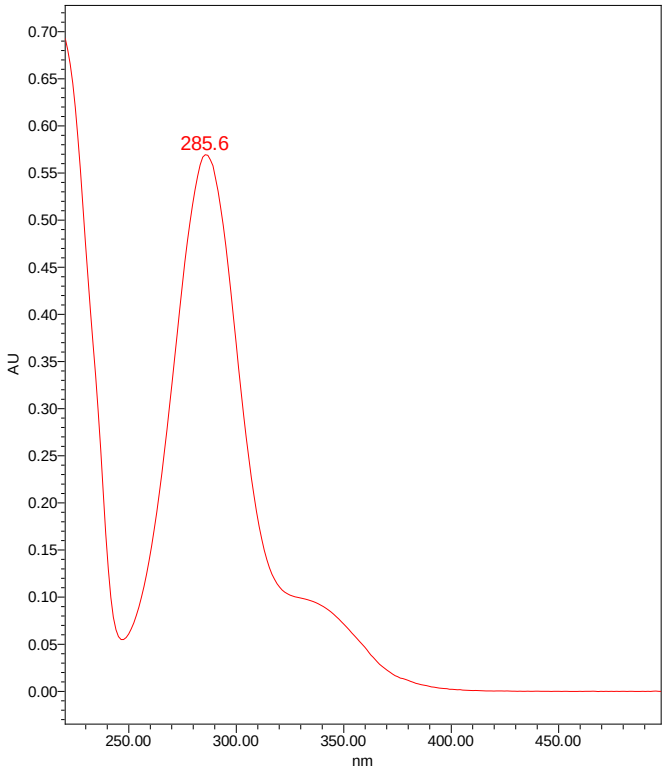


Figure S16. *HRMS spectrum of α,β-dihydroxanthohumol 7-O-β-D-(4'''-O-methyl)glucopyranoside* ***(7)***

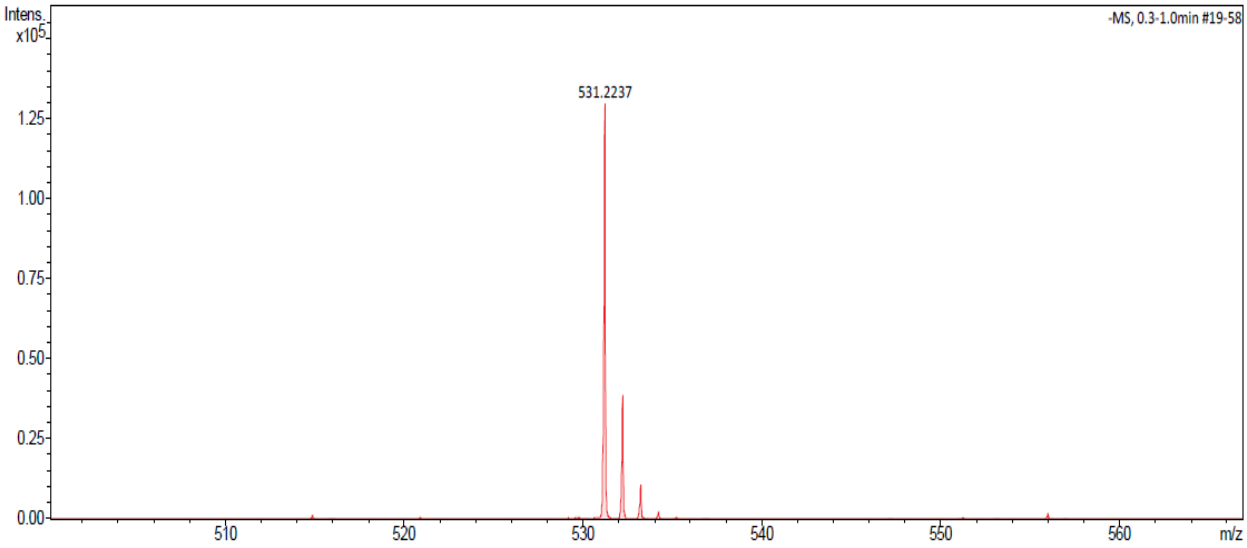
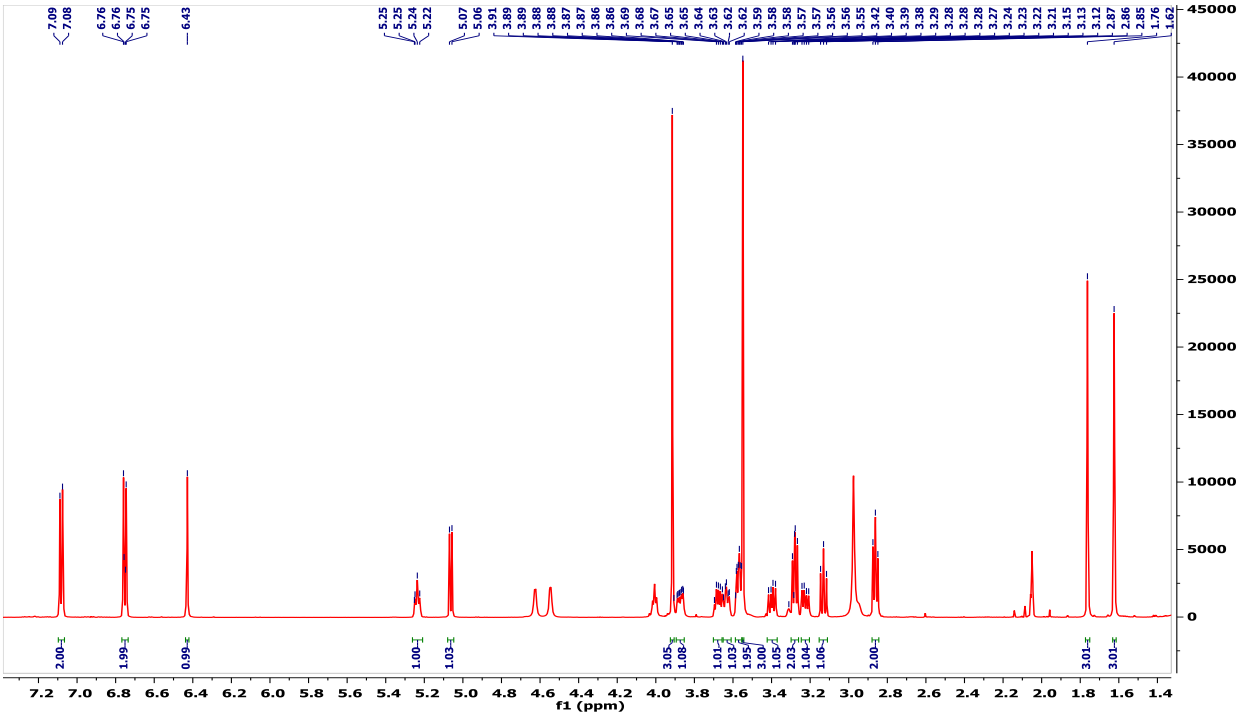


Figure S17. *^{1}H NMR (600 MHz) and ^{13}C NMR (151 MHz) spectra of α,β-dihydroxanthohumol 7-O-β-D-(4'''-O-methyl)glucopyranoside* ***(7)*** *(Acetone-d_6, Temp. 25 ºC).*



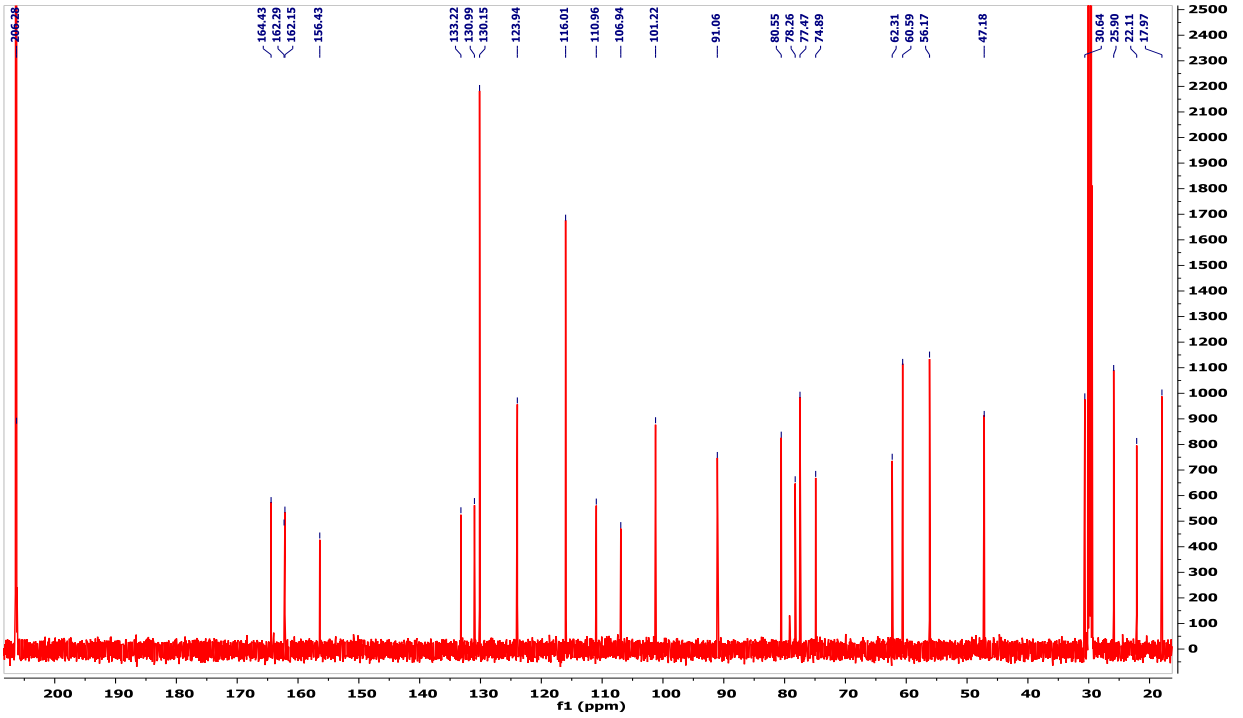


Figure S18. *^{1}H NMR - ^{1}H NMR (COSY) spectrum of α,β-dihydroxanthohumol 7-O-β-D-(4'''-O-methyl)glucopyranoside* ***(7)*** *(600 MHz/600 MHz, Acetone-d_6, Temp. 25°)*

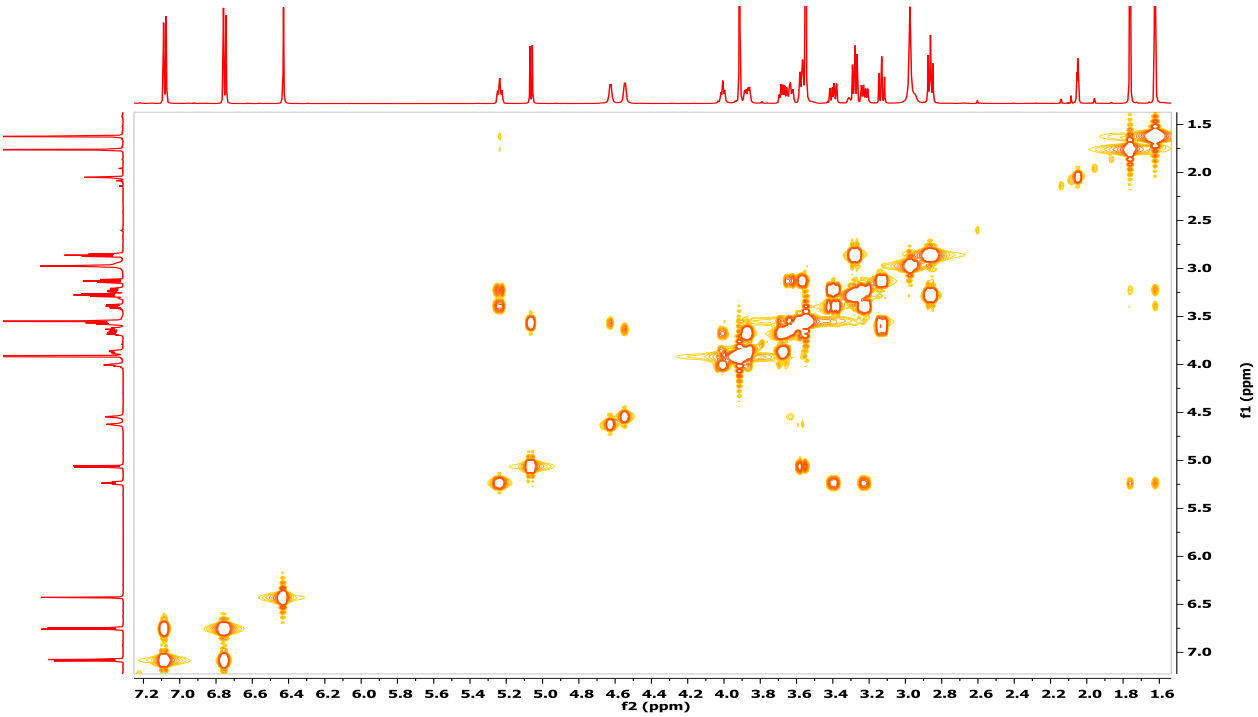


Figure S19. *^{1}H NMR - ^{13}C NMR (HSQC) spectrum of α,β-dihydroxanthohumol 7-O-β-D-(4'''-O-methyl)glucopyranoside* ***(7)*** *(600 MHz/151 MHz, Acetone-d_6, Temp. 25°)*

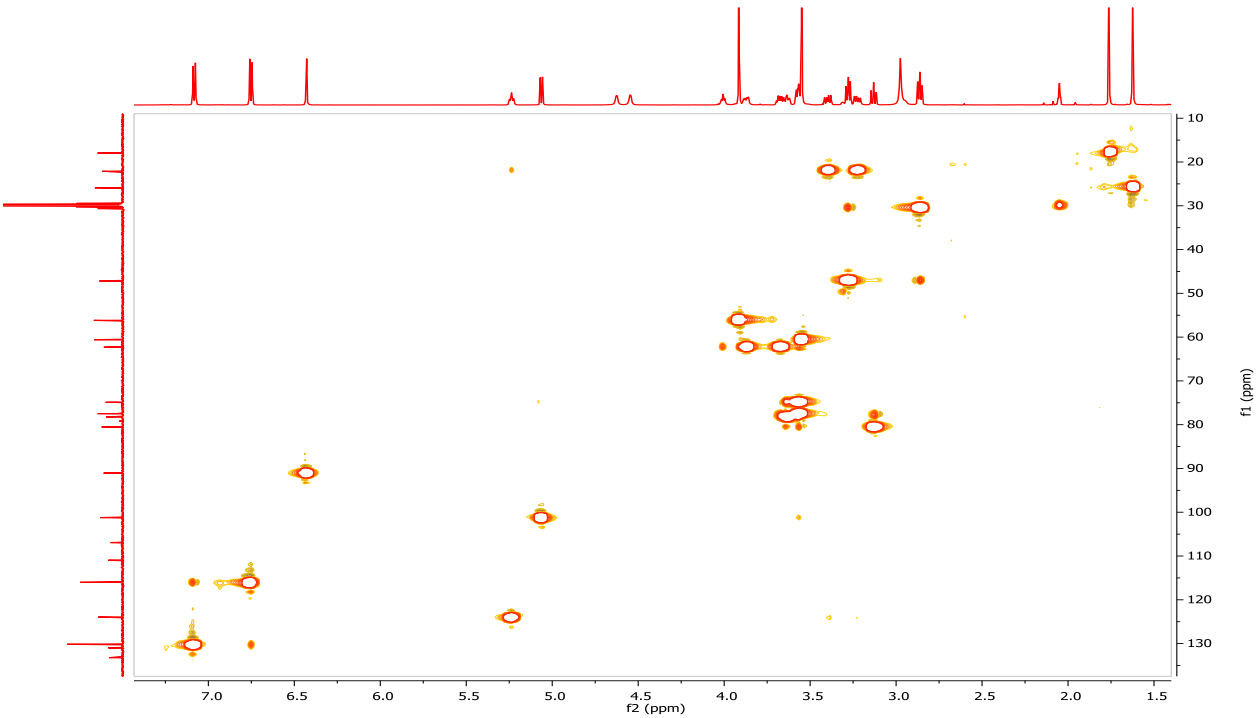


Figure S20. *UV spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O-β-D-glucopyranoside* ***(8)*** *(MeOH, Temp. 20 °C)*

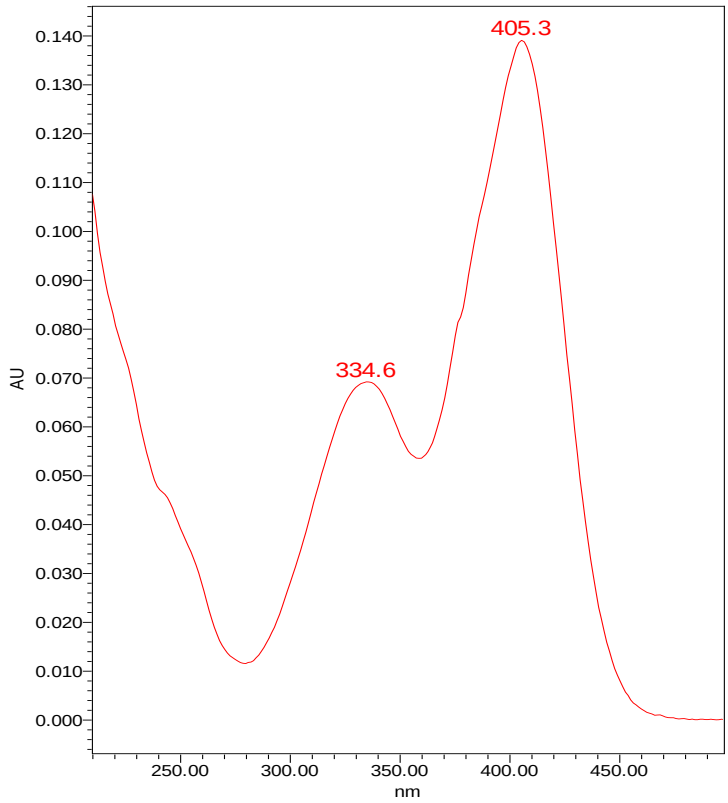


Figure S21. *HRMS spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O-β-D-glucopyranoside* ***(8)***

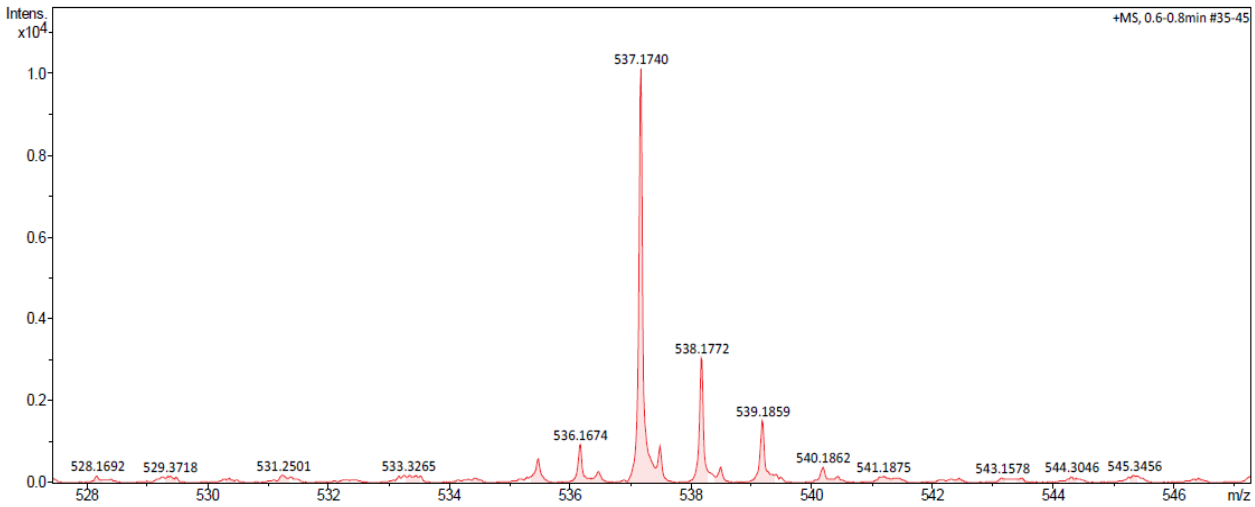
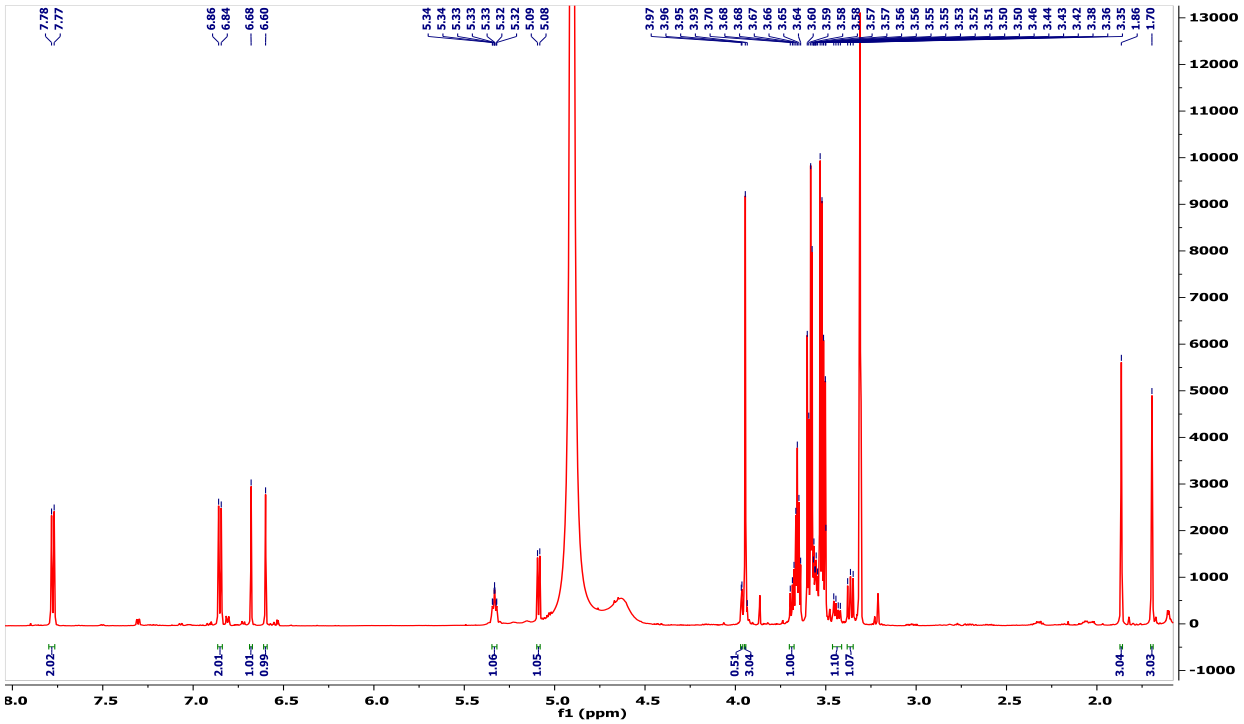


Figure S22. *^{1}H NMR (600 MHz) and ^{13}C NMR (151 MHz) spectra of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O-β-D-glucopyranoside* ***(8)*** *CD_3OD, Temp. 25 ºC)*



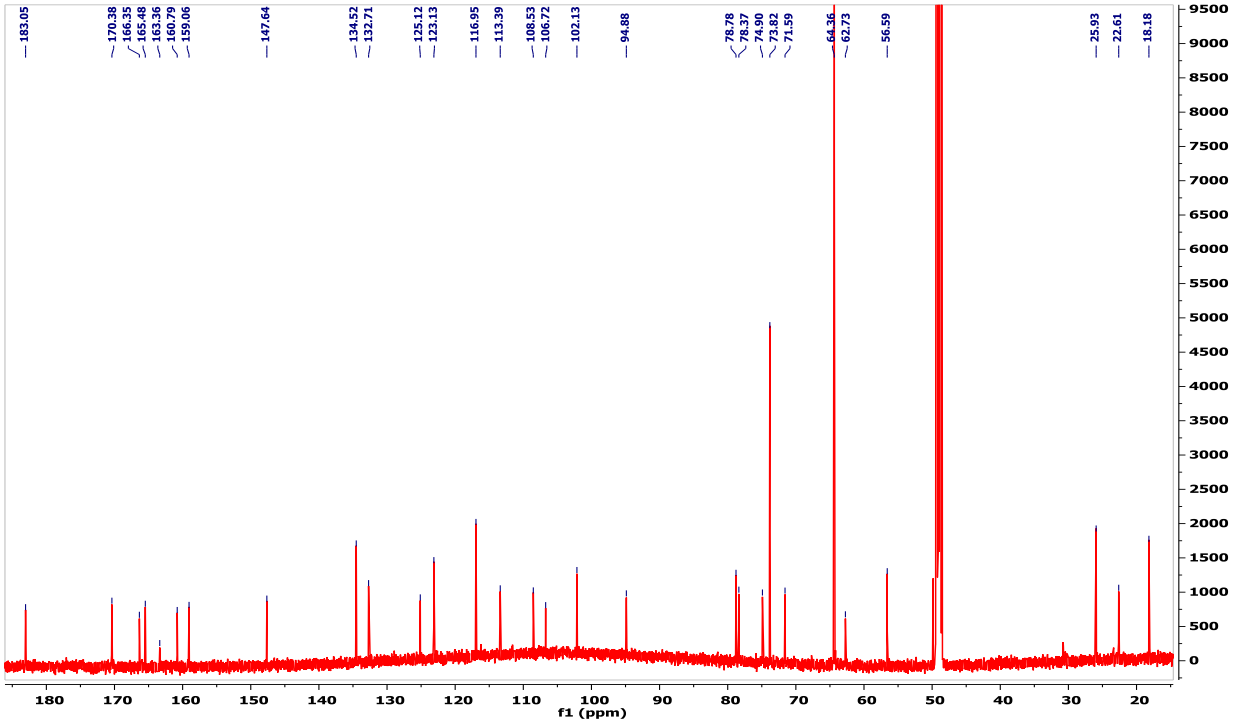


Figure S23. *^{1}H NMR - ^{1}H NMR (COSY) spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O-β-D-glucopyranoside* ***(8)*** *(600 MHz/600 MHz, CD_3OD, Temp. 25 ºC)*

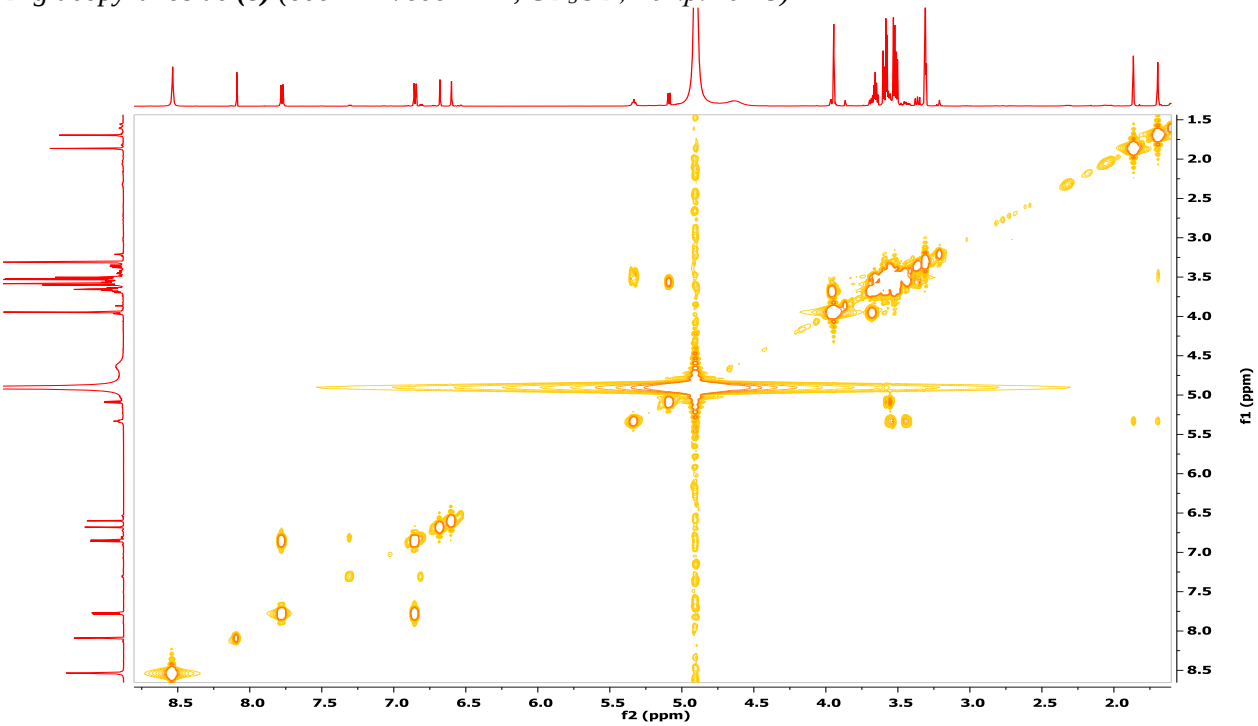


Figure S24. *^{1}H NMR - ^{13}C NMR (HSQC)spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O-β-D-glucopyranoside* ***(8)*** *(600 MHz/151 MHz, CD_3OD, Temp. 25 ºC)*

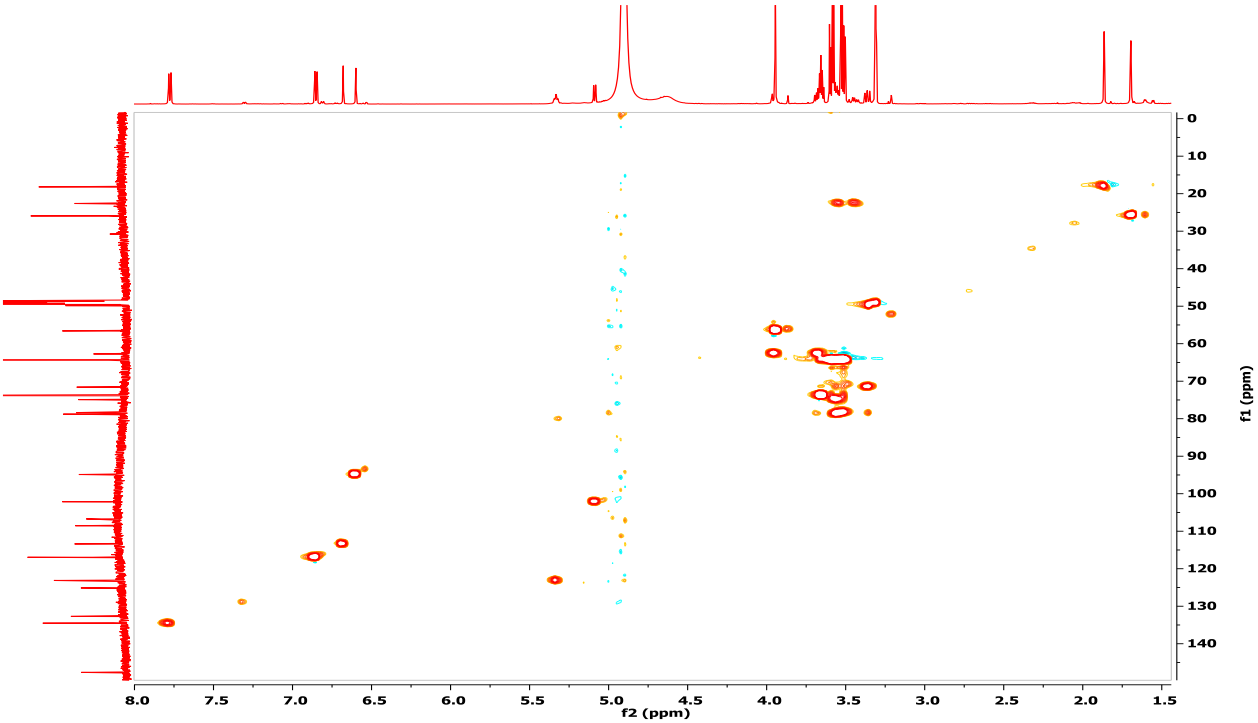


Figure S25. *UV spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O-β-D-(4'''-O-methyl)glucopyranoside (**9**)(MeOH, Temp. 20 °C)*

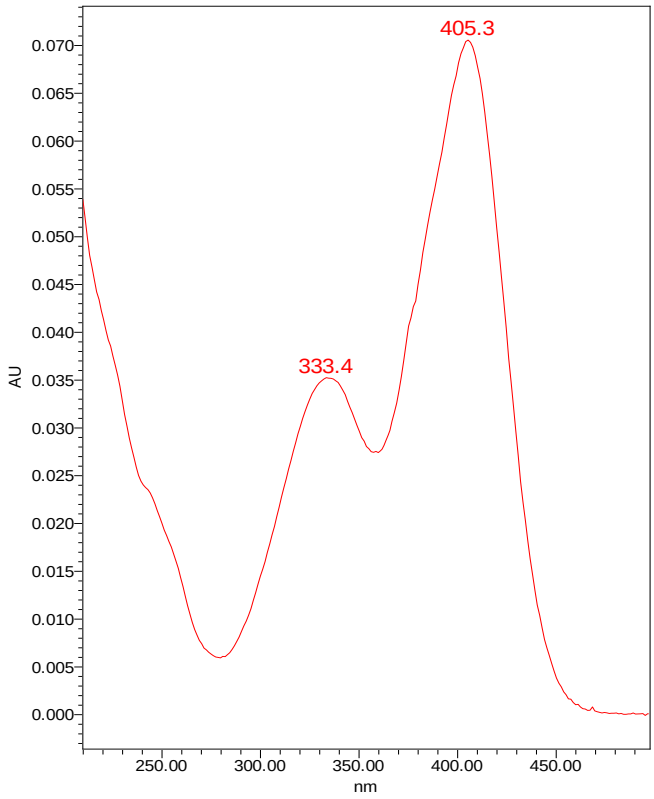


Figure S26. *HRMS spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O-β-D-(4'''-O-methyl)glucopyranoside (**9**)*

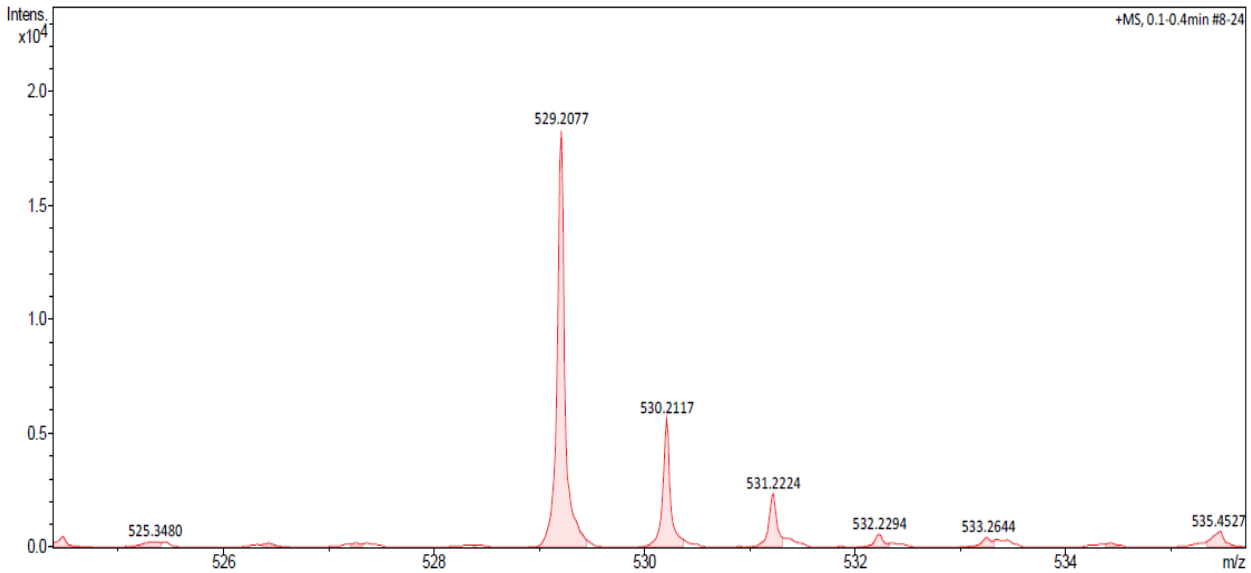
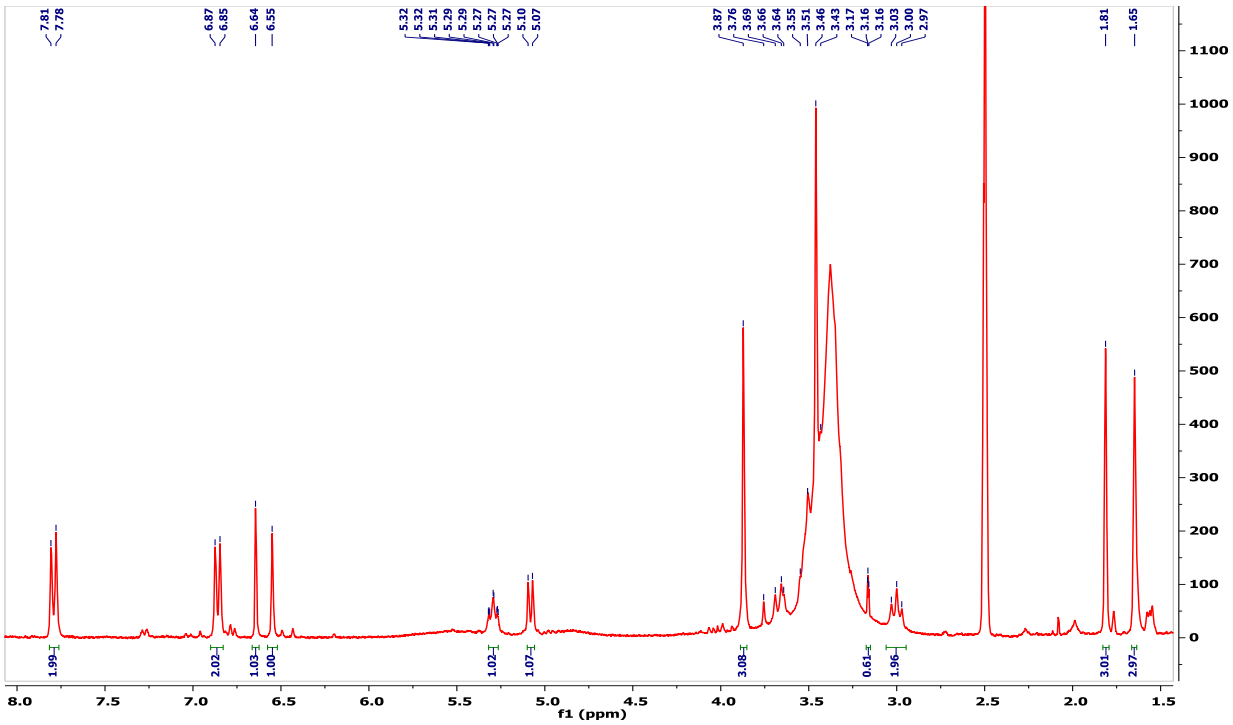


Figure S27. *^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz,) spectra of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O-β-D-(4'''-O-methyl)glucopyranoside (**9**) (DMSO-d_6, Temp. 25 ºC)*



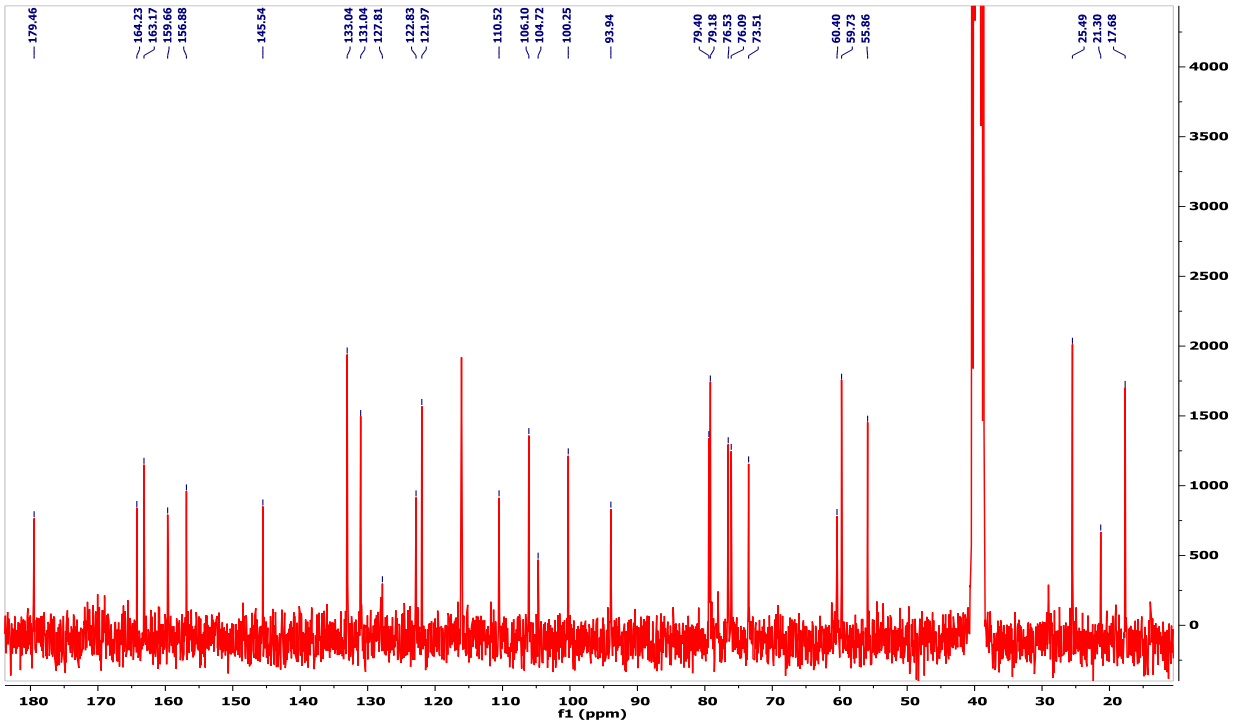


Figure S28. *^{1}H NMR - ^{1}H NMR (COSY) spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O-β-D-(4'''-O-methyl)glucopyranoside* ***(9)*** *) (600 MHz/600 MHz, DMSO-d_6, Temp. 25 ºC)*

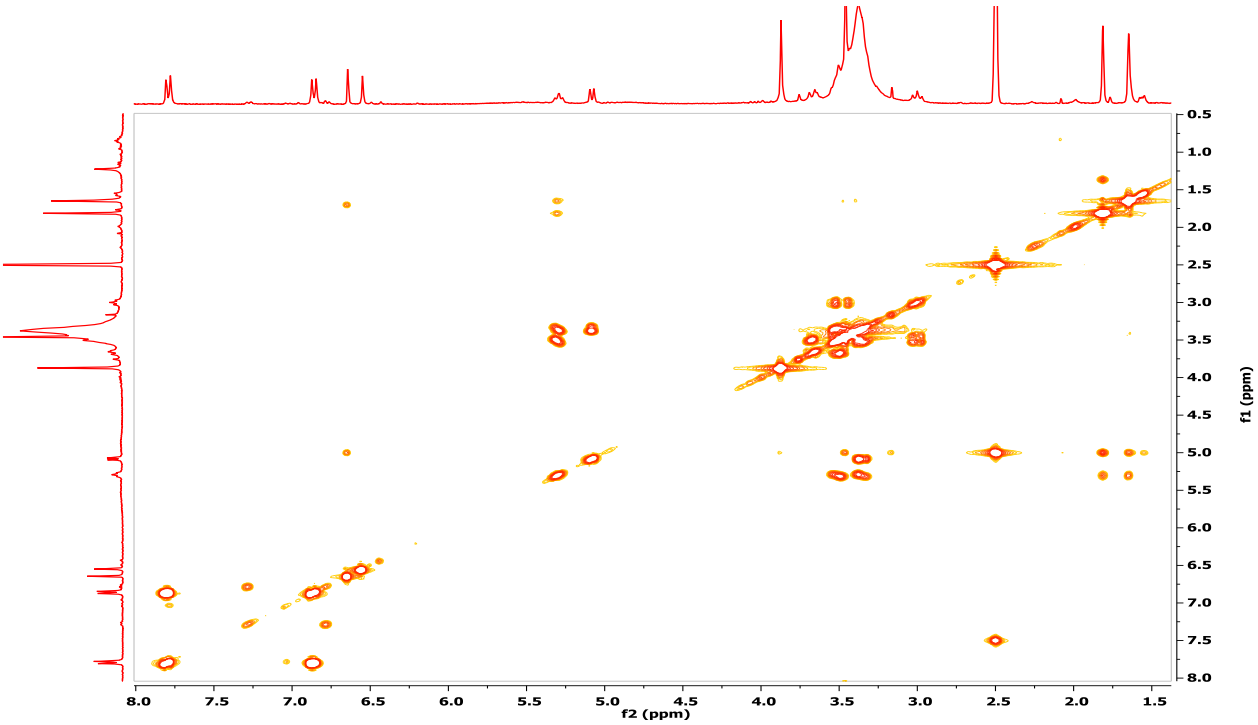


Figure S29. *^{1}H NMR - ^{13}C NMR (HSQC) spectrum of (Z)-6,4'-dihydroxy-4-methoxy-7-prenylaurone 6-O-β-D-(4'''-O-methyl)glucopyranoside* ***(9)*** *(600 MHz/151 MHz, DMSO-d_6, Temp. 25 ºC)*