

Supplementary materials

Fungal biotransformation of 2'-methylflavanone and 2'-methylflavone as a method to obtain glycosylated derivatives

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Figure S154. ^1H NMR spectrum expansion (δ , acetone- d_6 , 600 MHz) of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S155. ^1H NMR spectrum expansion (δ , acetone- d_6 , 600 MHz) of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S156. ^{13}C NMR spectrum (δ , acetone- d_6 , 151 MHz) of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S157. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S158. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S159. COSY contour map – $^1\text{H} \times ^1\text{H}$ of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S160. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S161. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S162. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S163. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S164. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S165. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S166. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Figure S167. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

Molecular formula: C₁₆H₁₄O₂

Formula weight: 238.10

Ionization mode: positive

Precursor: [M + H]⁺ 239.30

239.3000>121.1000 CE (Collision Energy): -22.0

239.3000>224.1000 CE: -17.0

239.3000>198.1500 CE: -8.0

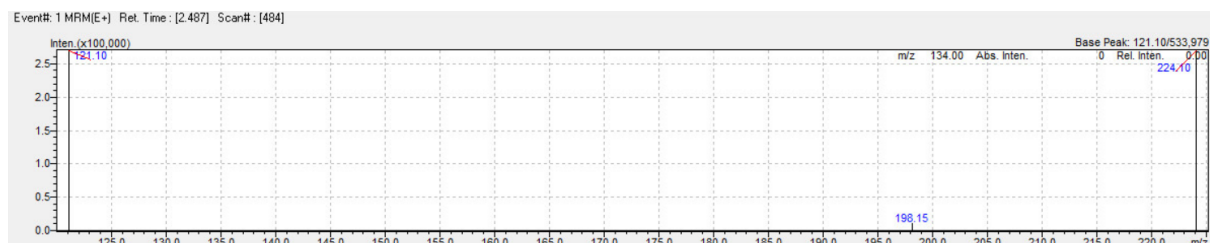
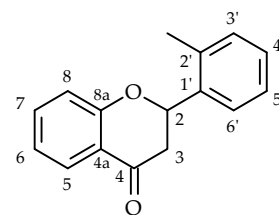


Figure S1. MS analysis of 2'-methyflavanone (4)

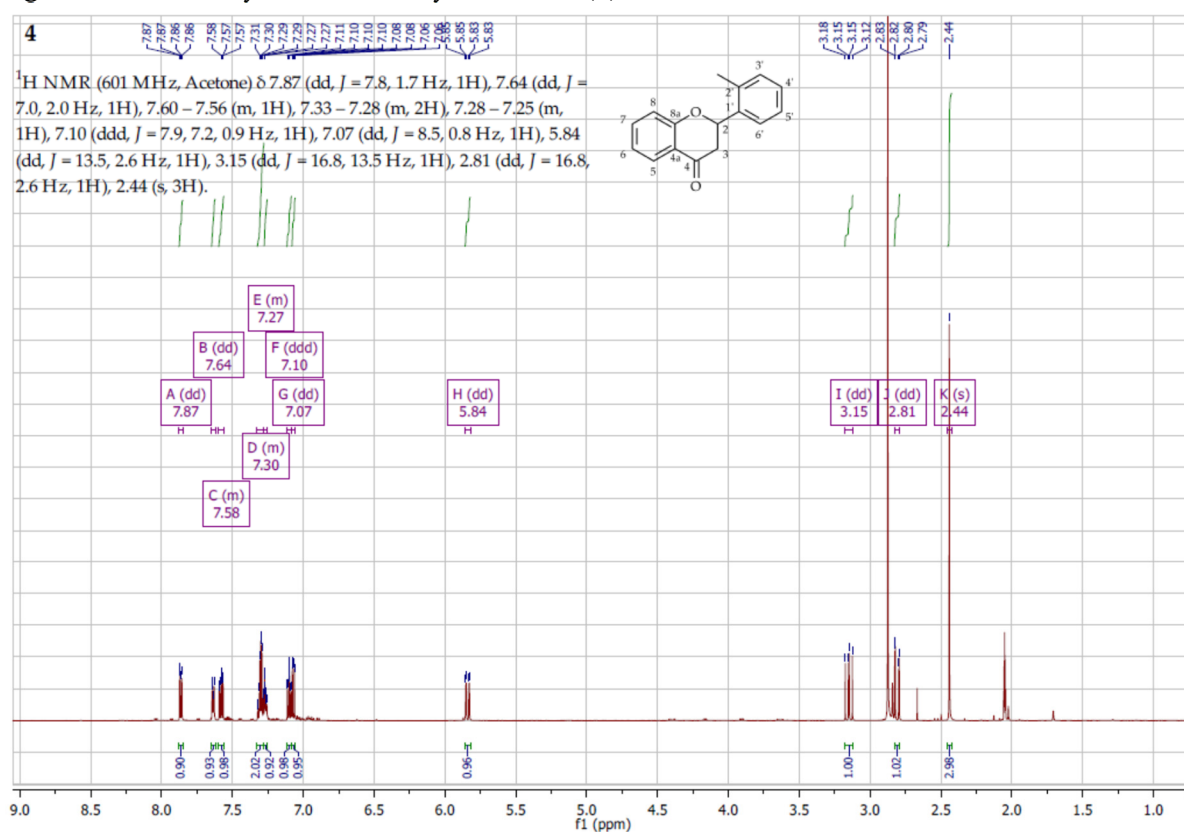


Figure S2. ¹H NMR spectrum (δ, acetone-d₆, 600 MHz) of 2'-methyflavanone (4)

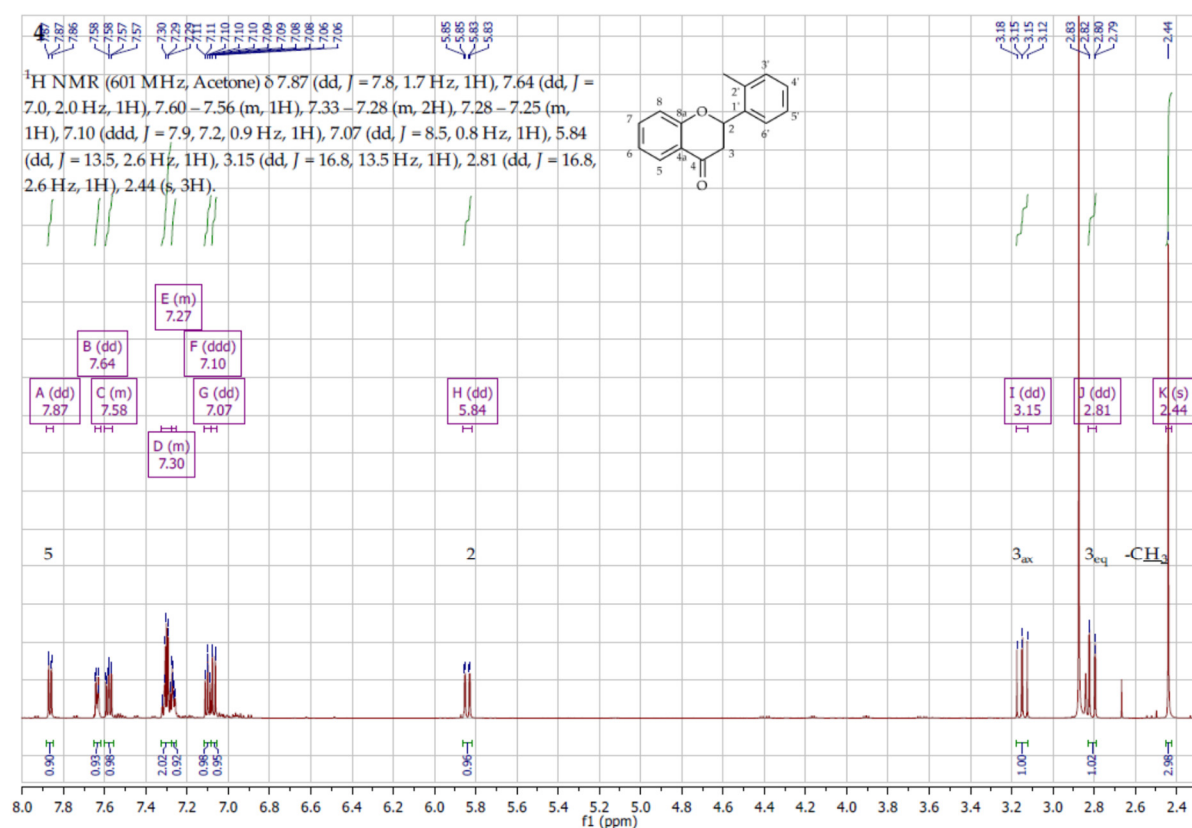


Figure S3 ^1H NMR spectrum expansion (δ , acetone- d_6 , 600 MHz) of 2'-methyflavanone (**4**)

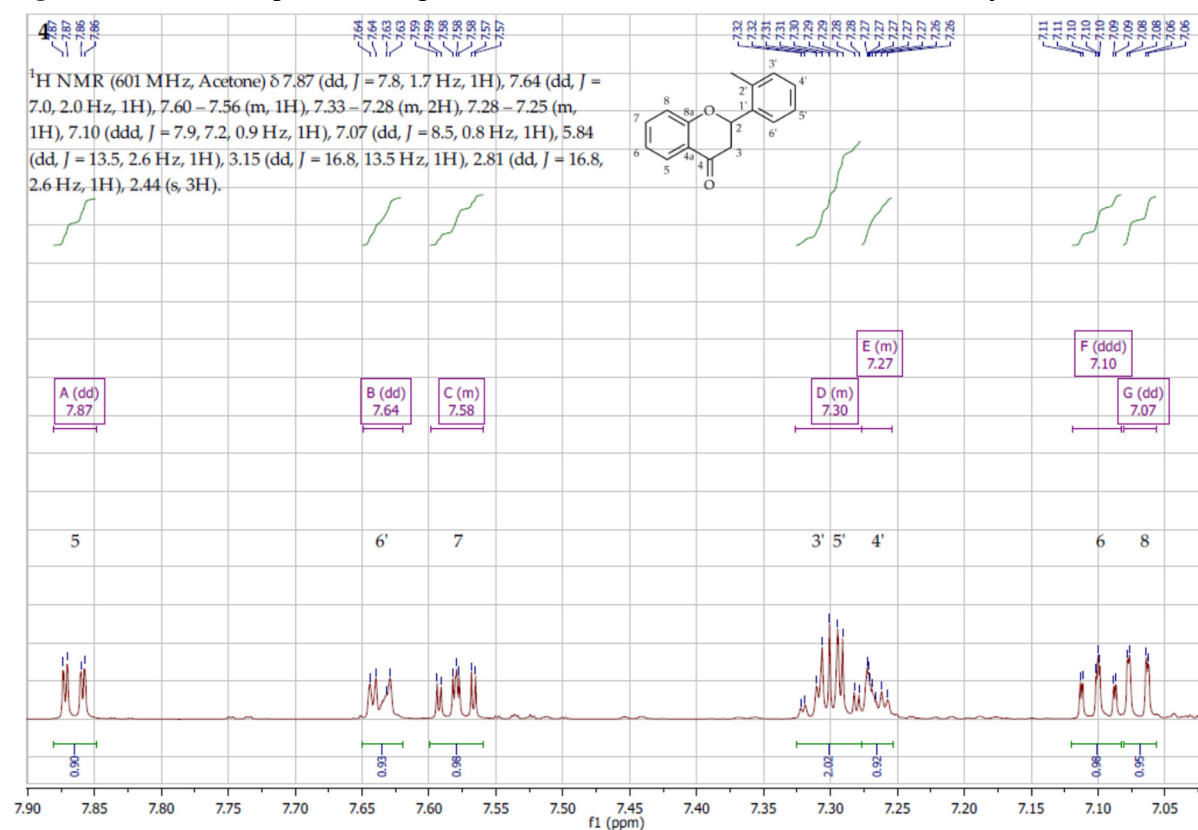


Figure S4. ^1H NMR spectrum expansion (δ , acetone- d_6 , 600 MHz) of 2'-methyflavanone (**4**)

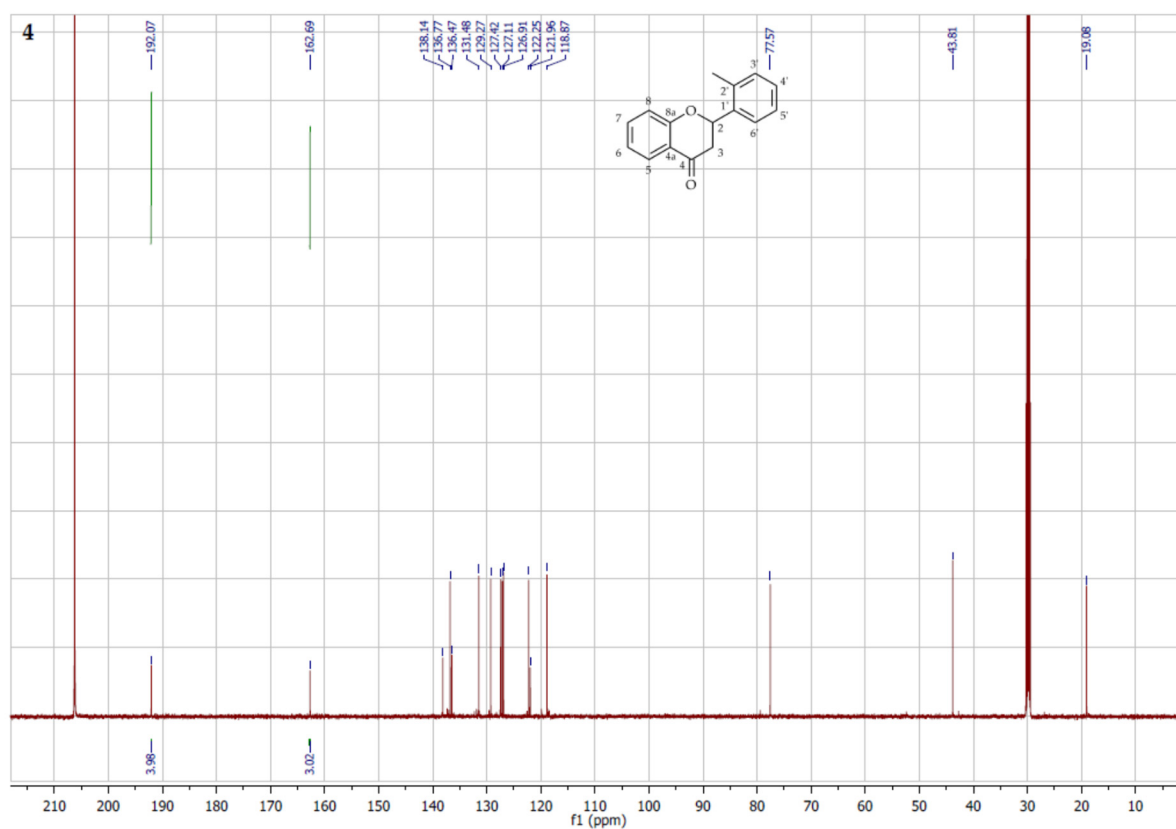


Figure S5. ^{13}C NMR spectrum (δ , acetone- d_6 , 151 MHz) of 2'-methyflavanone (**4**)

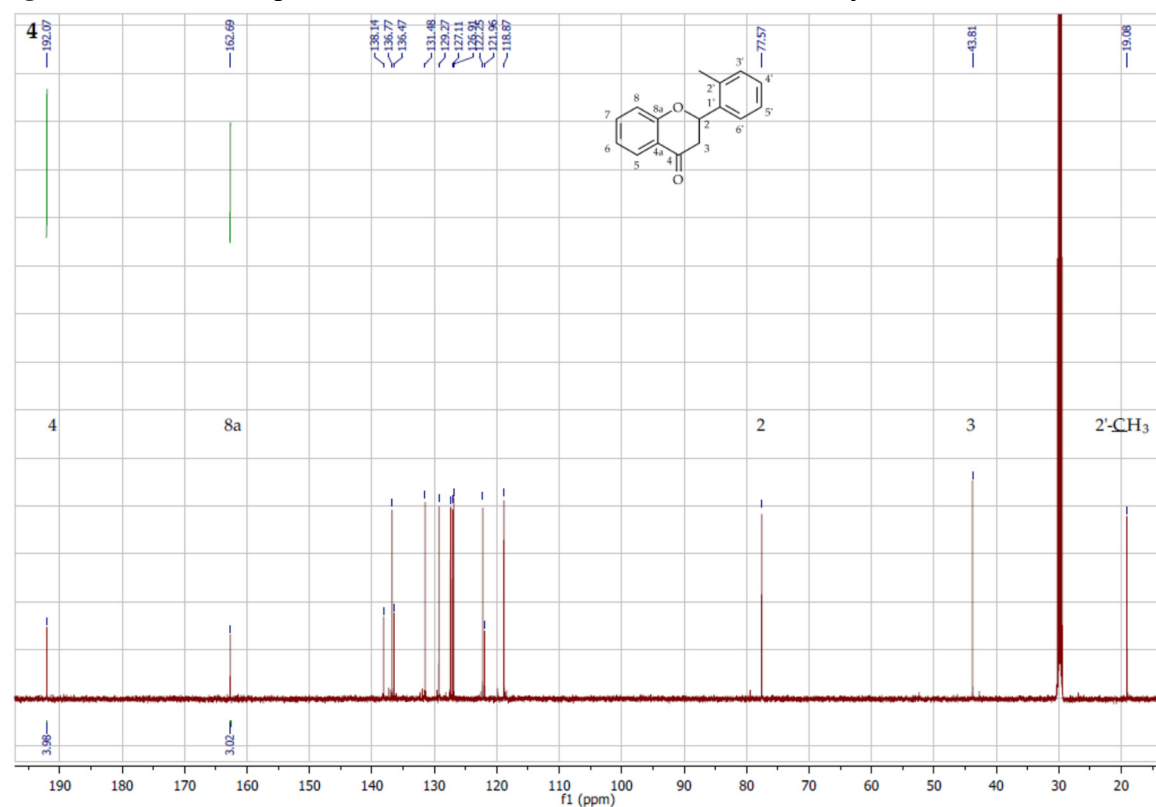


Figure S6. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methyflavanone (**4**)

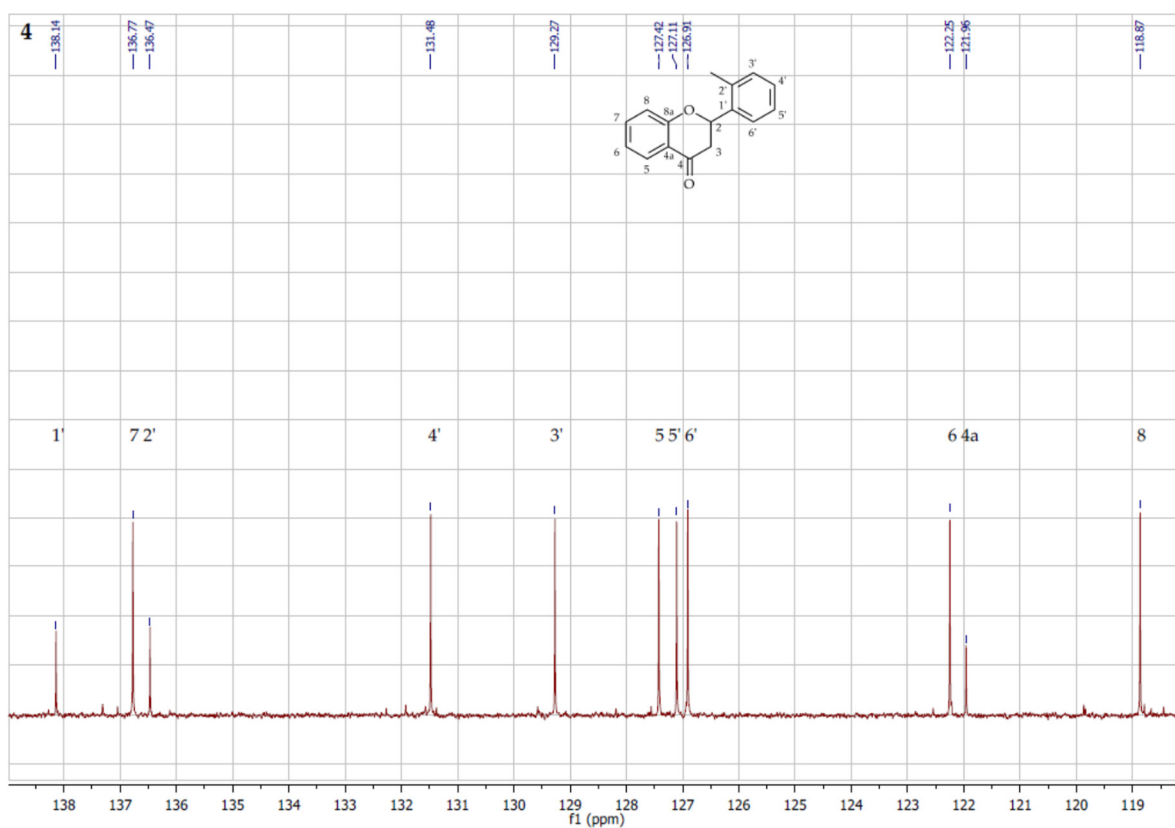


Figure S7. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methyflavanone (**4**)

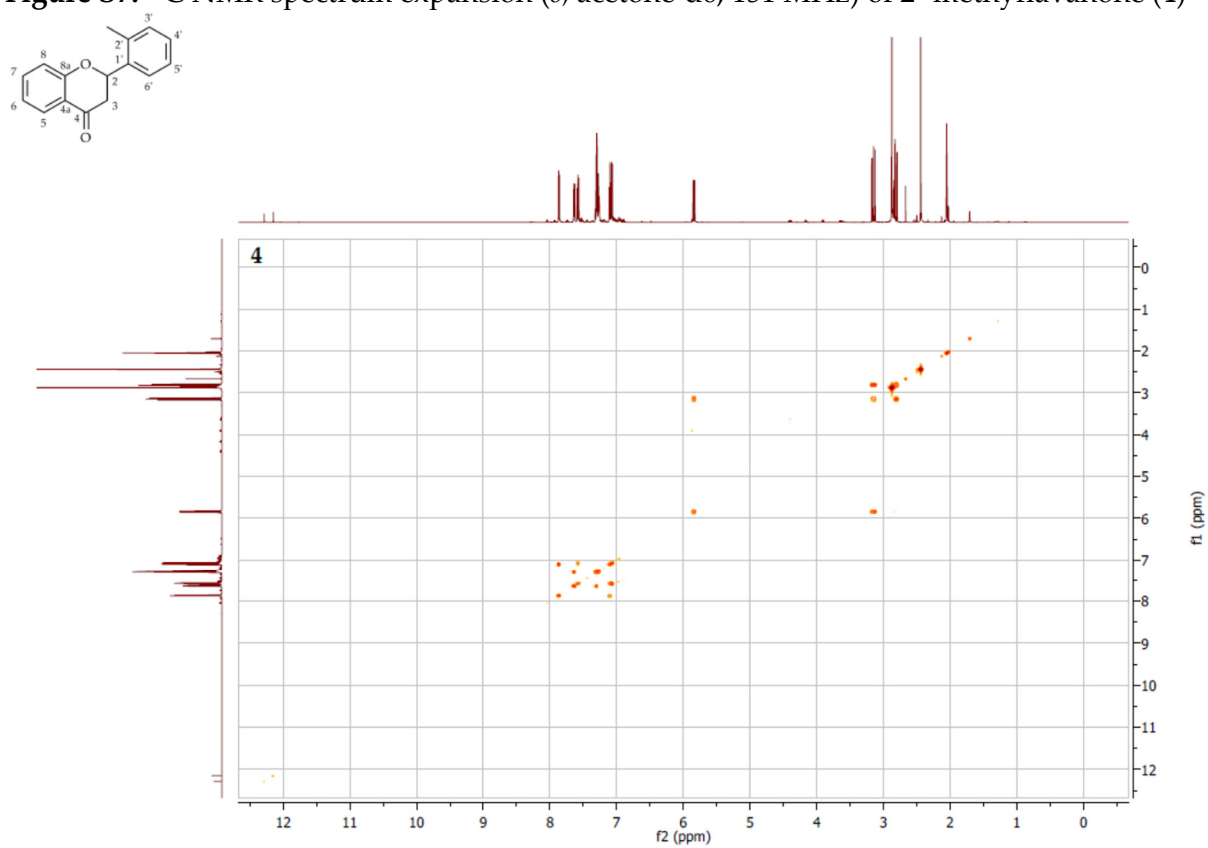


Figure S8. COSY contour map – $^1\text{H} \times ^1\text{H}$ of 2'-methyflavanone (**4**)

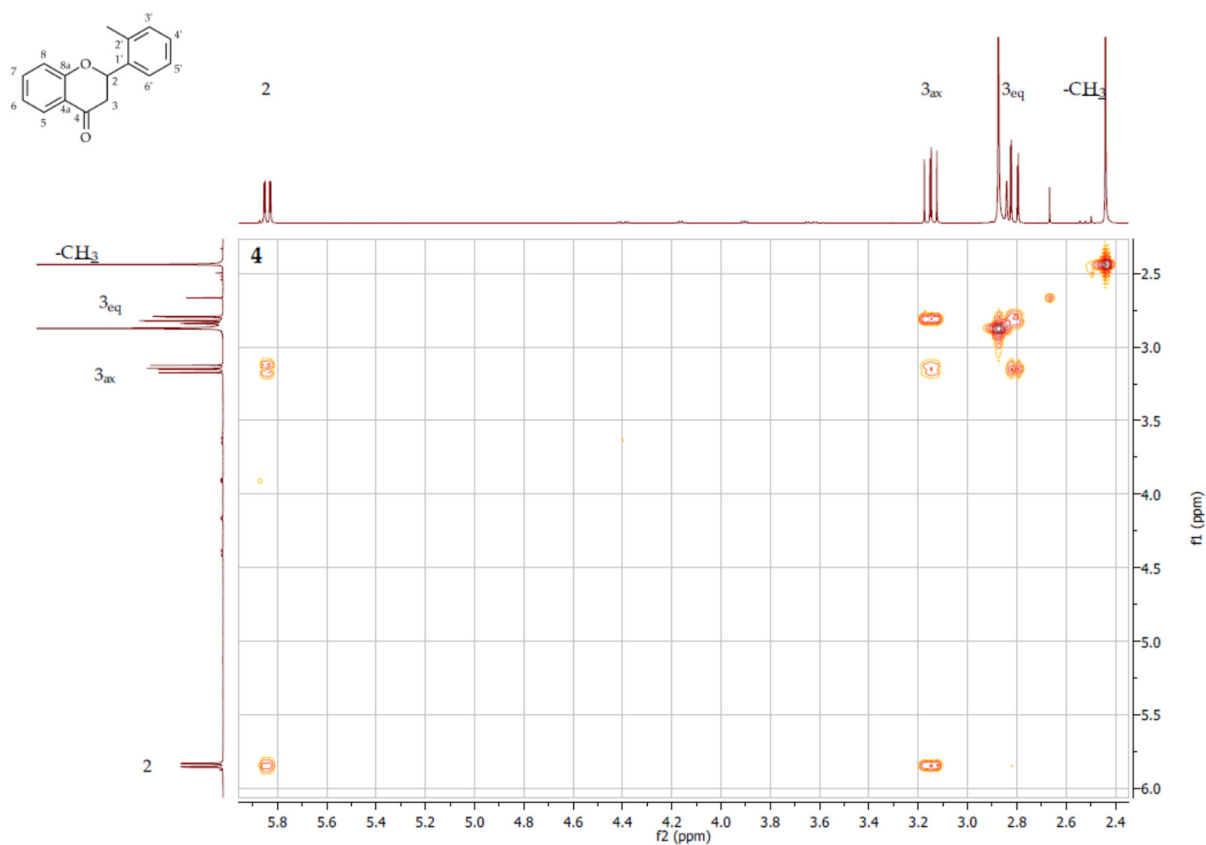


Figure S9. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methyflavanone (4)

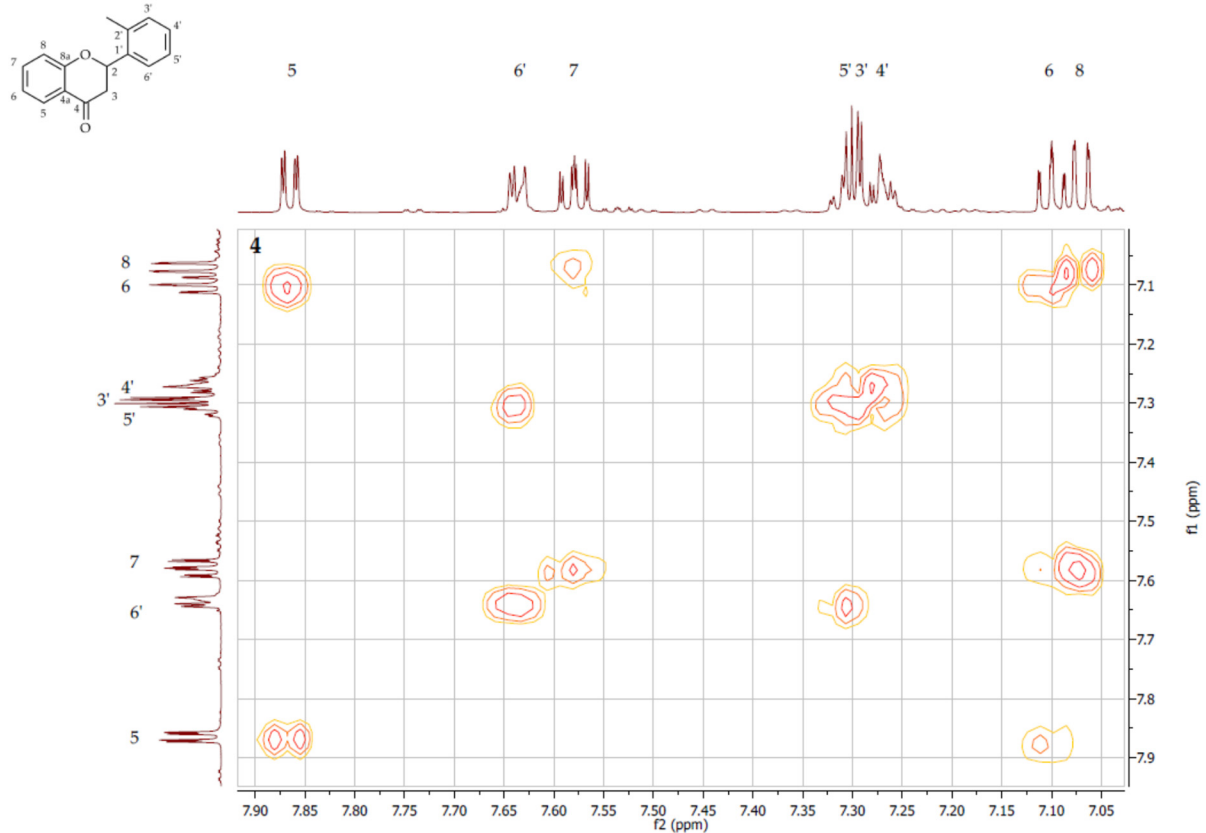


Figure S10. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methyflavanone (4)

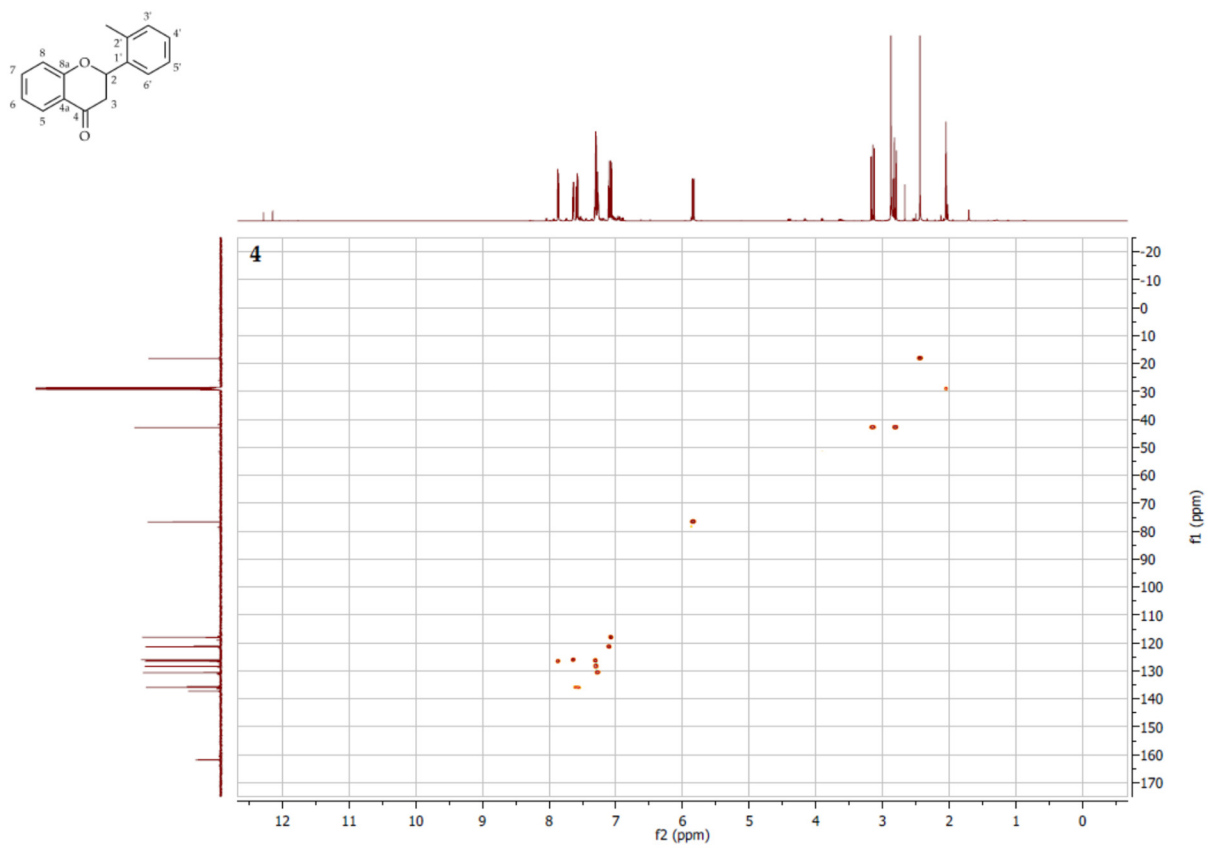


Figure S11. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methyflavanone (4)

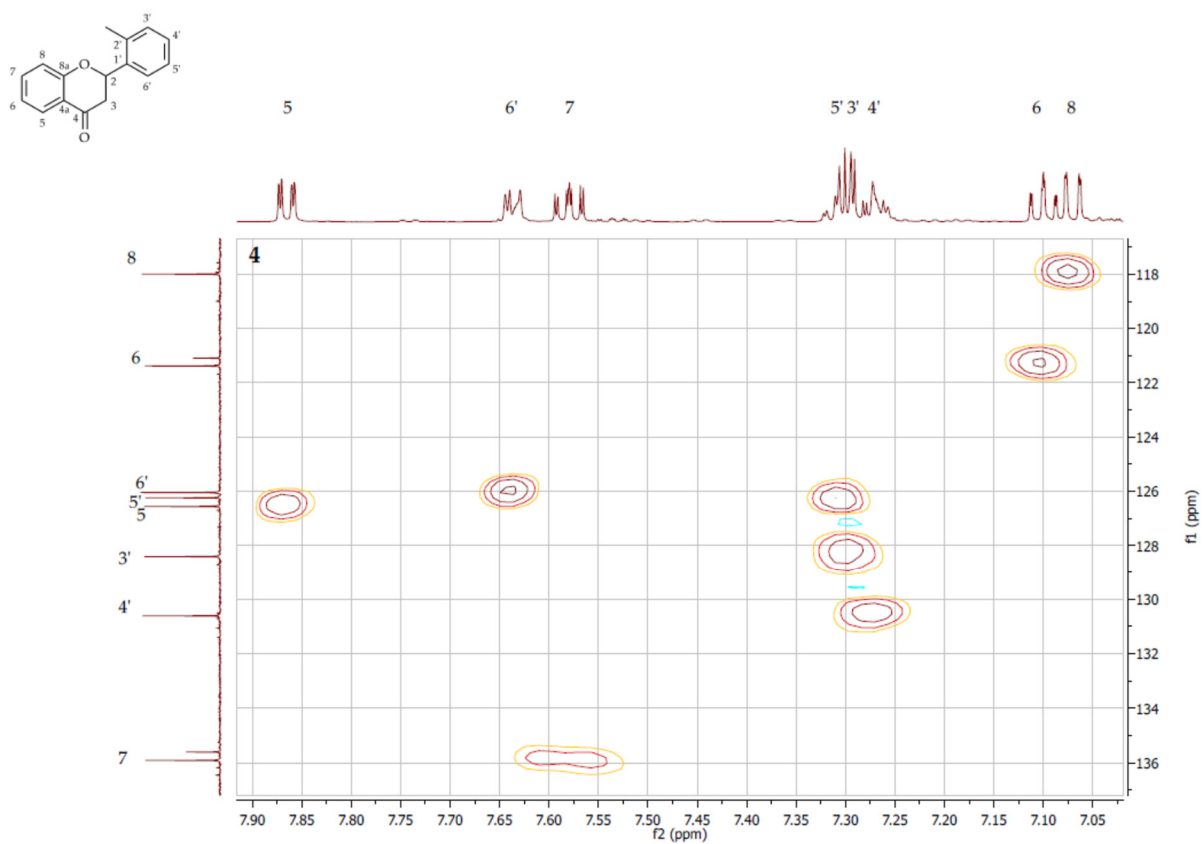


Figure S12. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methyflavanone (4)

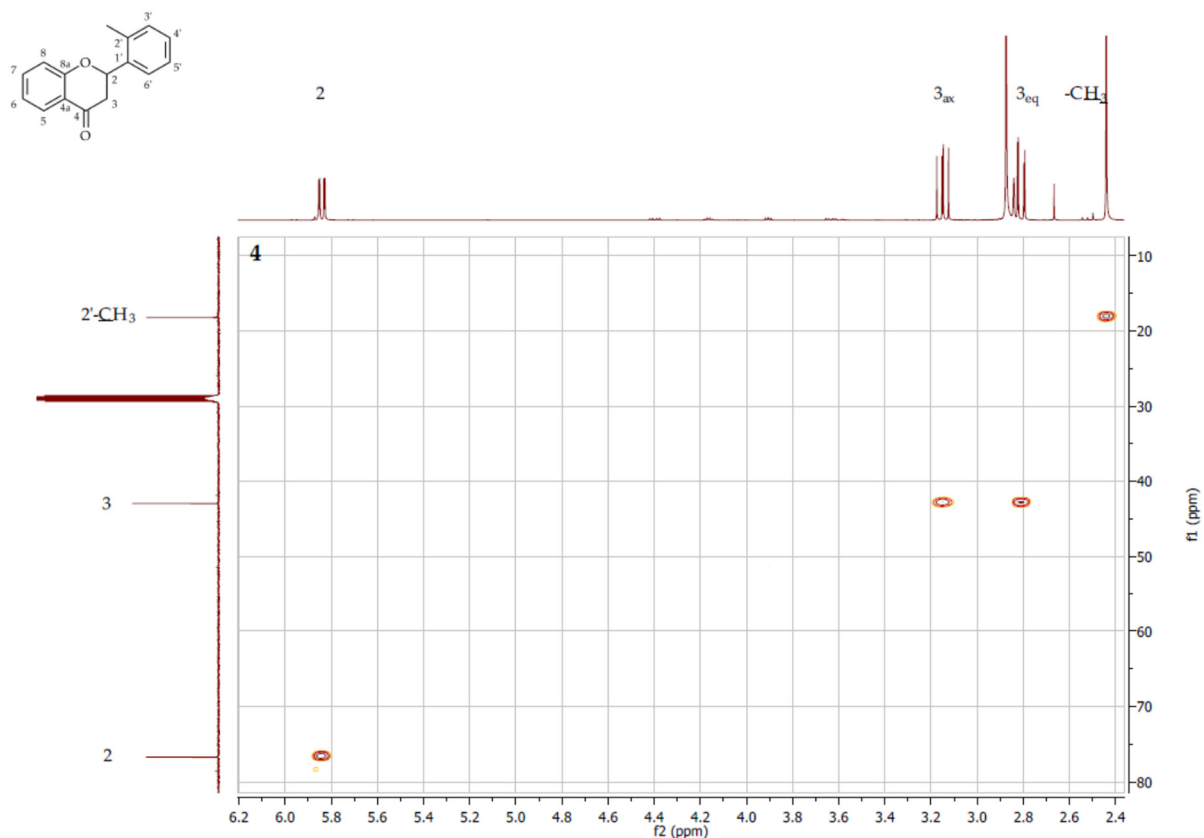


Figure S13. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methyflavanone (4)

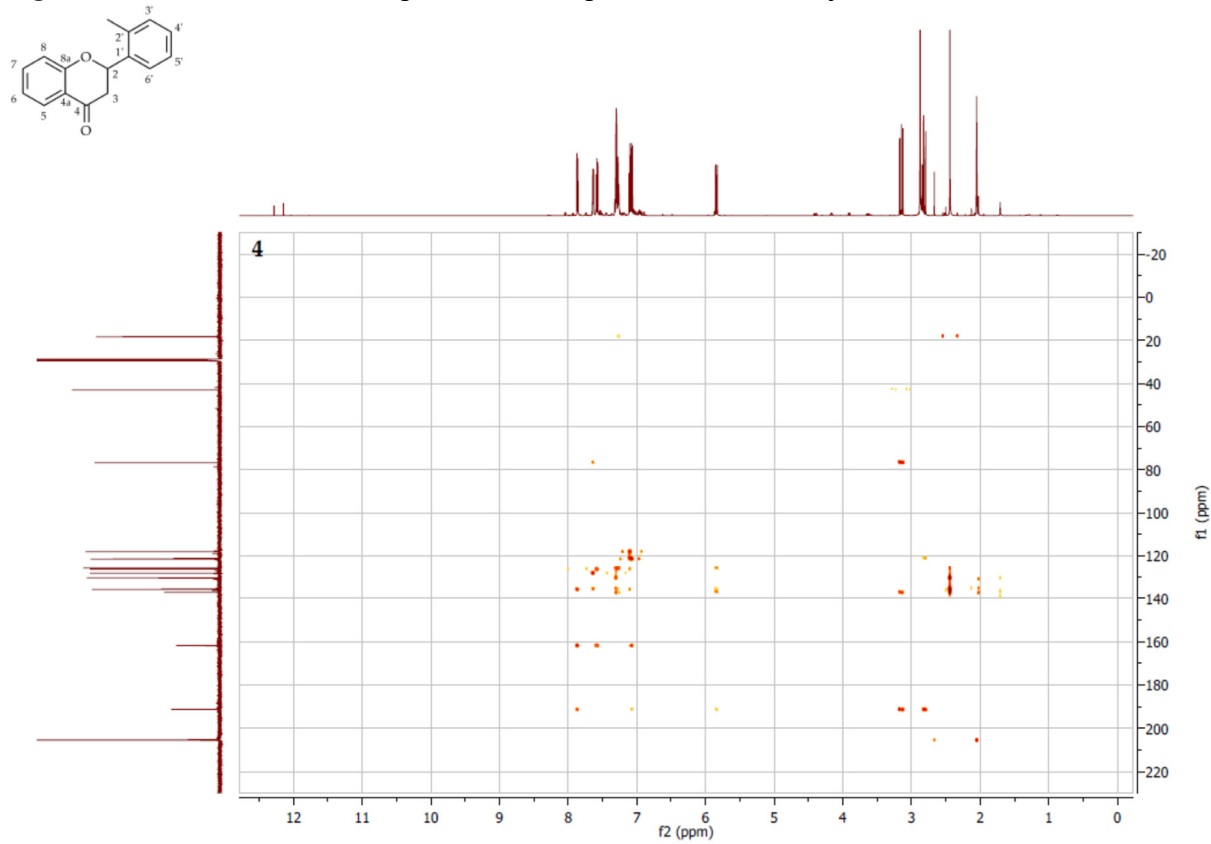


Figure S14. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methyflavanone (4)

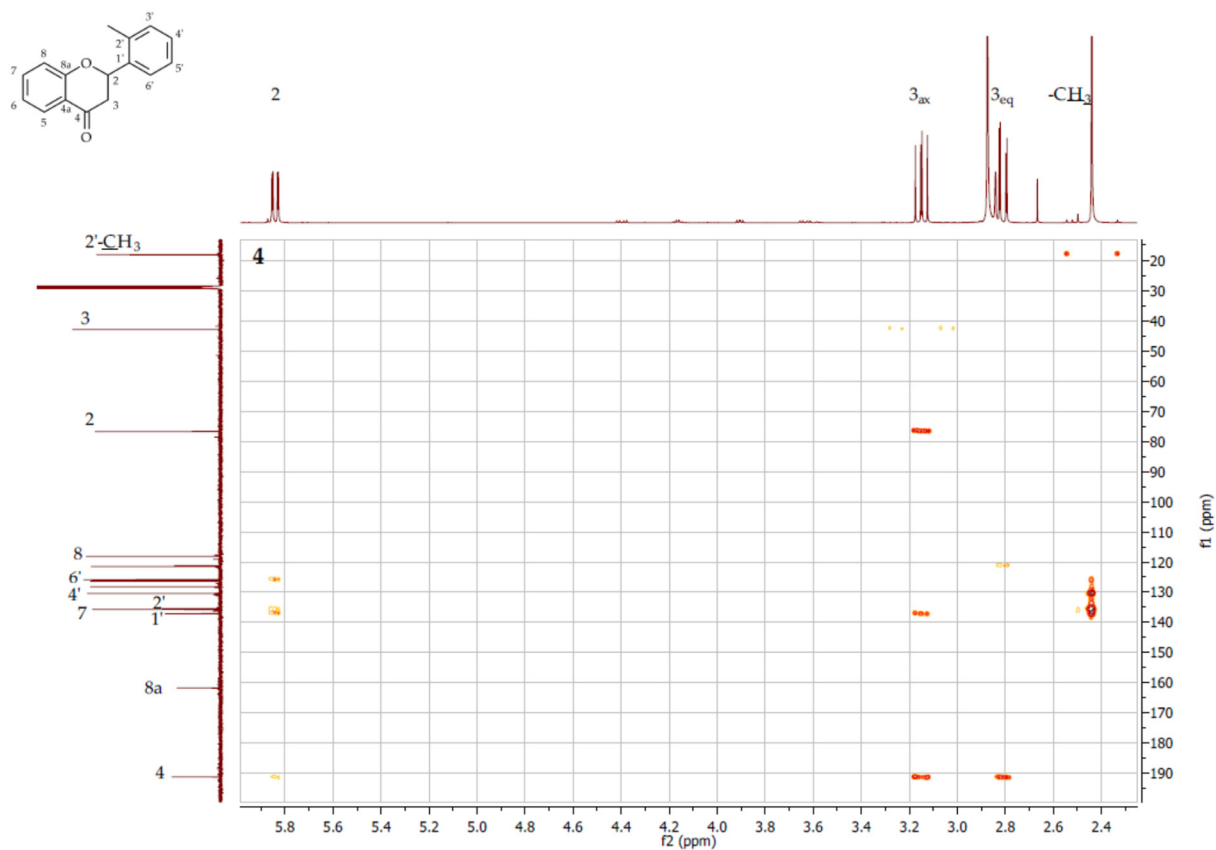


Figure S15. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methyflavanone (4)

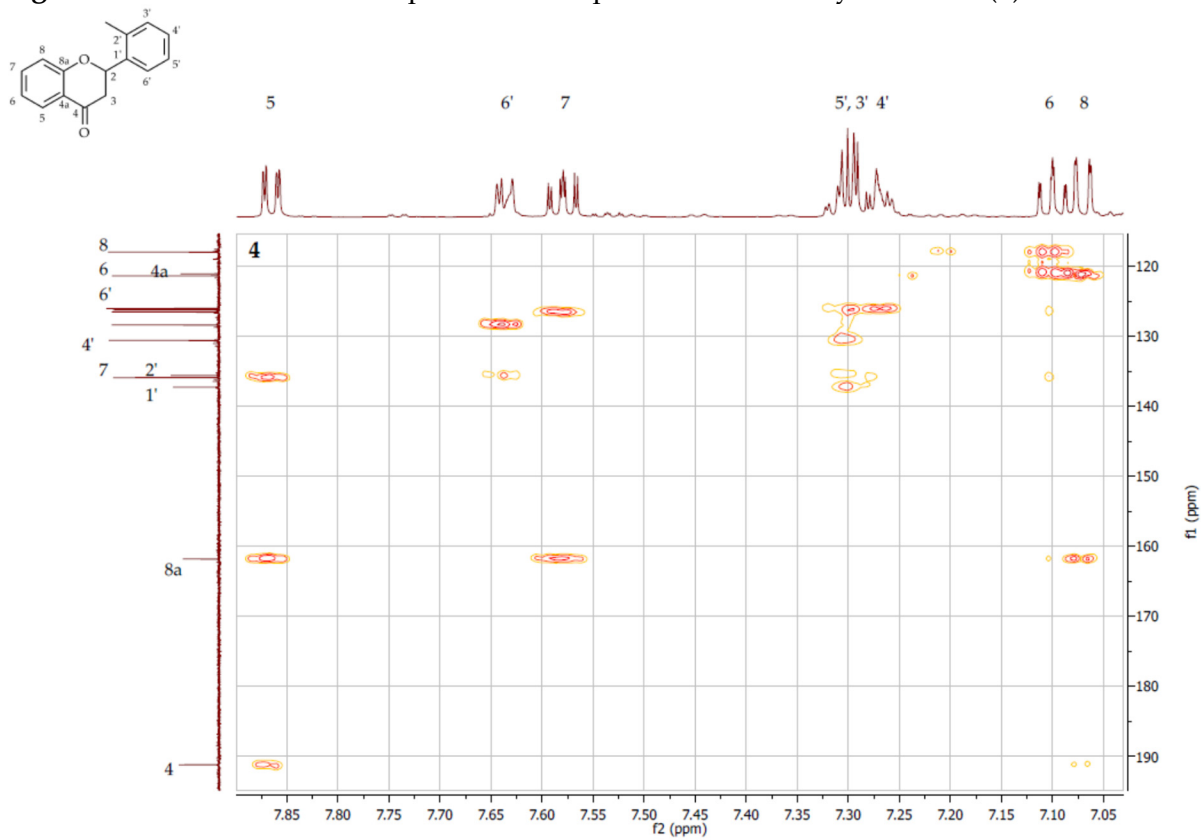


Figure S16. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methyflavanone (4)

Molecular formula: C₂₃H₂₆O₈

Formula weight: 430.16

Ionization mode: positive

Precursor: [M + H]⁺ 430.70

430.7000>311.2500 CE: -24.0

430.7000>226.8500 CE: -17.0

430.7000>362.9000 CE: -10.0

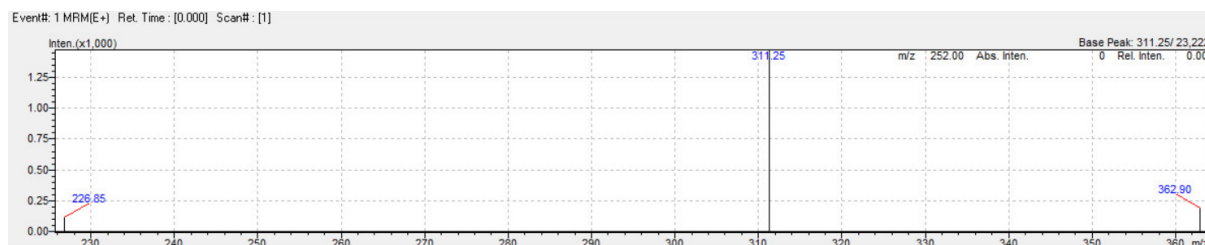
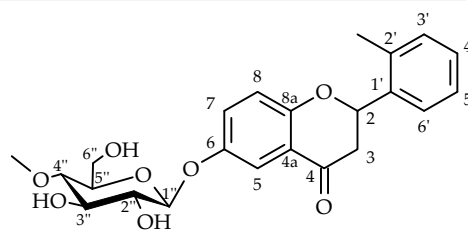


Figure S17. MS analysis of 2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4a**)

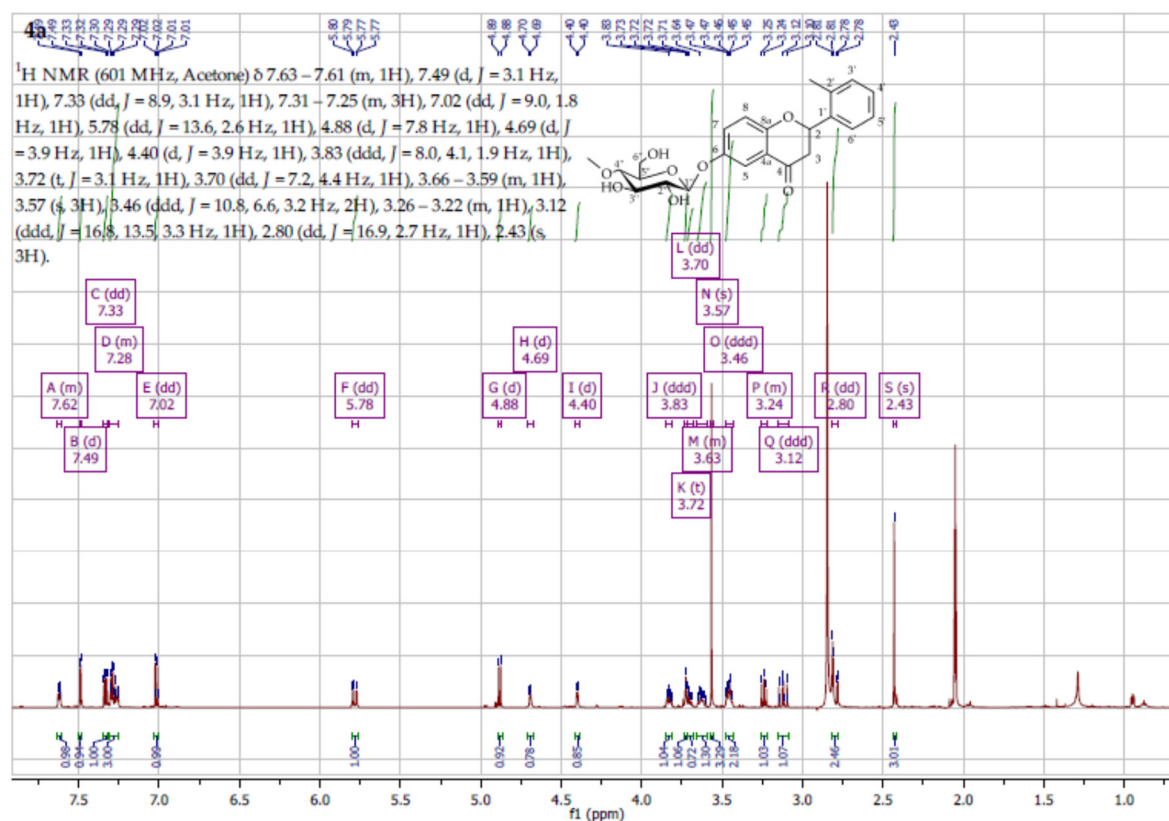


Figure S18. ¹H NMR spectrum (δ , acetone-d₆, 600 MHz) of 2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4a**)

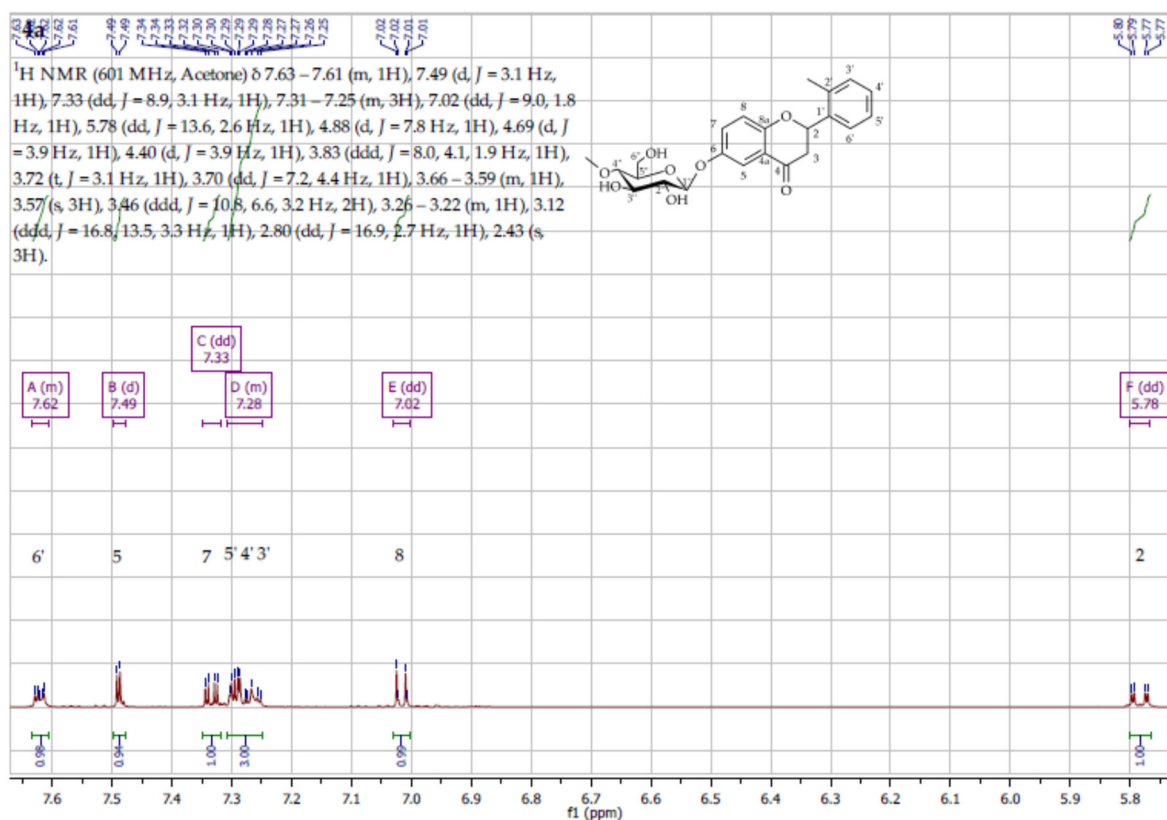


Figure S19. ¹H NMR spectrum expansion (δ , acetone-d₆, 600 MHz) of 2'-methylflavanone 6-*O*- β -D-(4''-*O*-methyl)-glucopyranoside (**4a**)

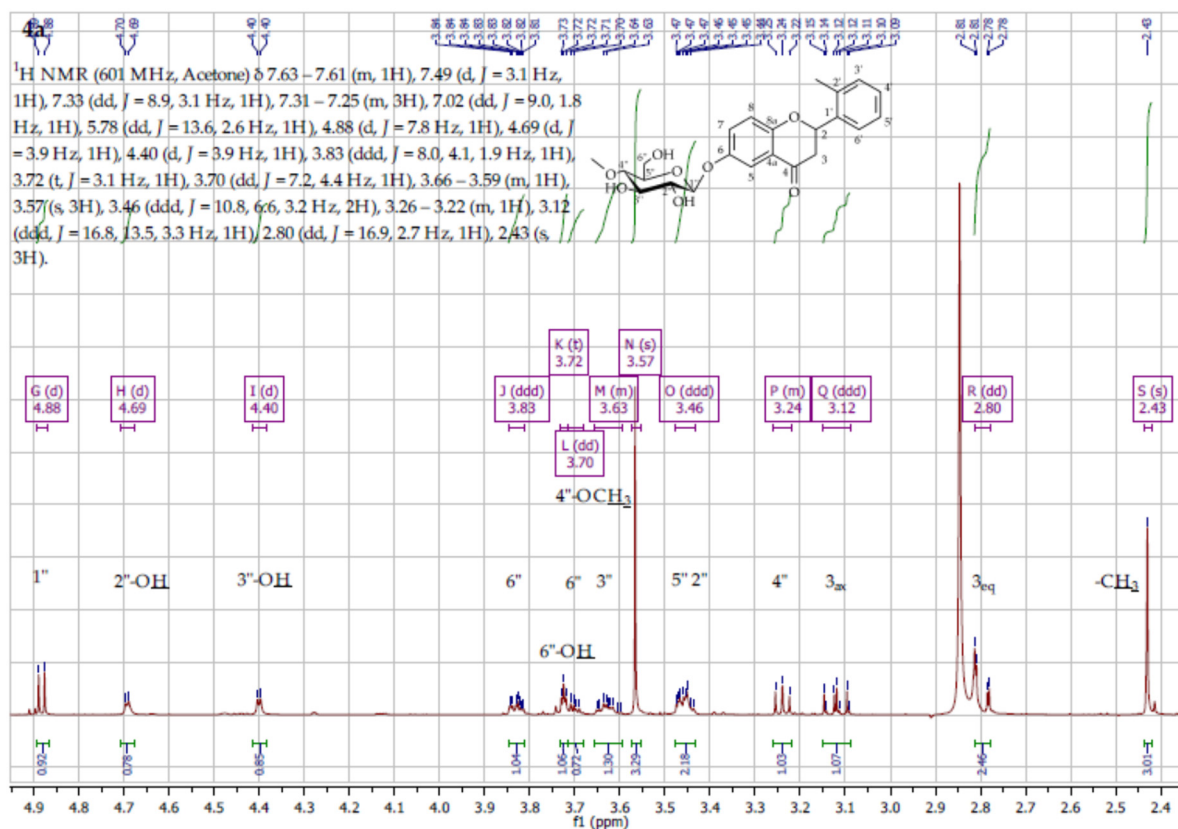


Figure S20. ¹H NMR spectrum expansion (δ , acetone-d₆, 600 MHz) of 2'-methylflavanone 6-*O*- β -D-(4''-*O*-methyl)-glucopyranoside (**4a**)

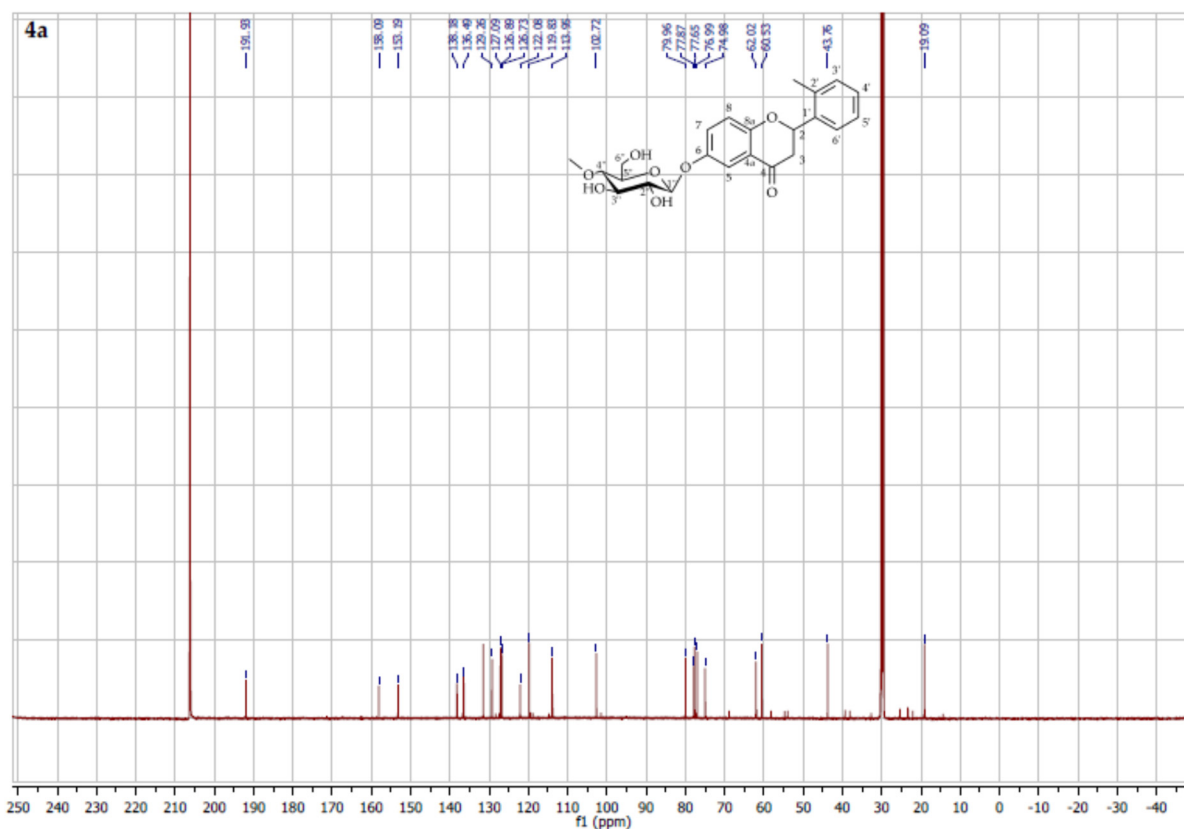


Figure S21. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (4a)

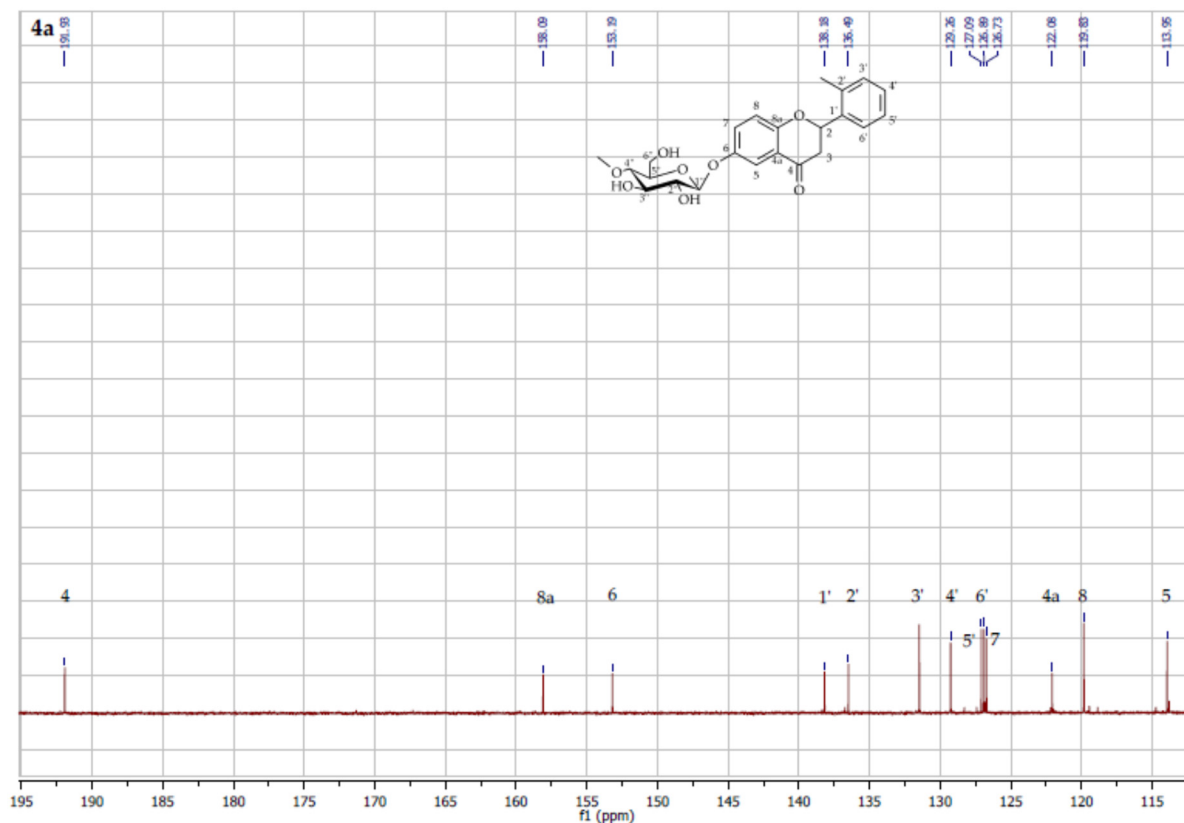


Figure S22. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (4a)

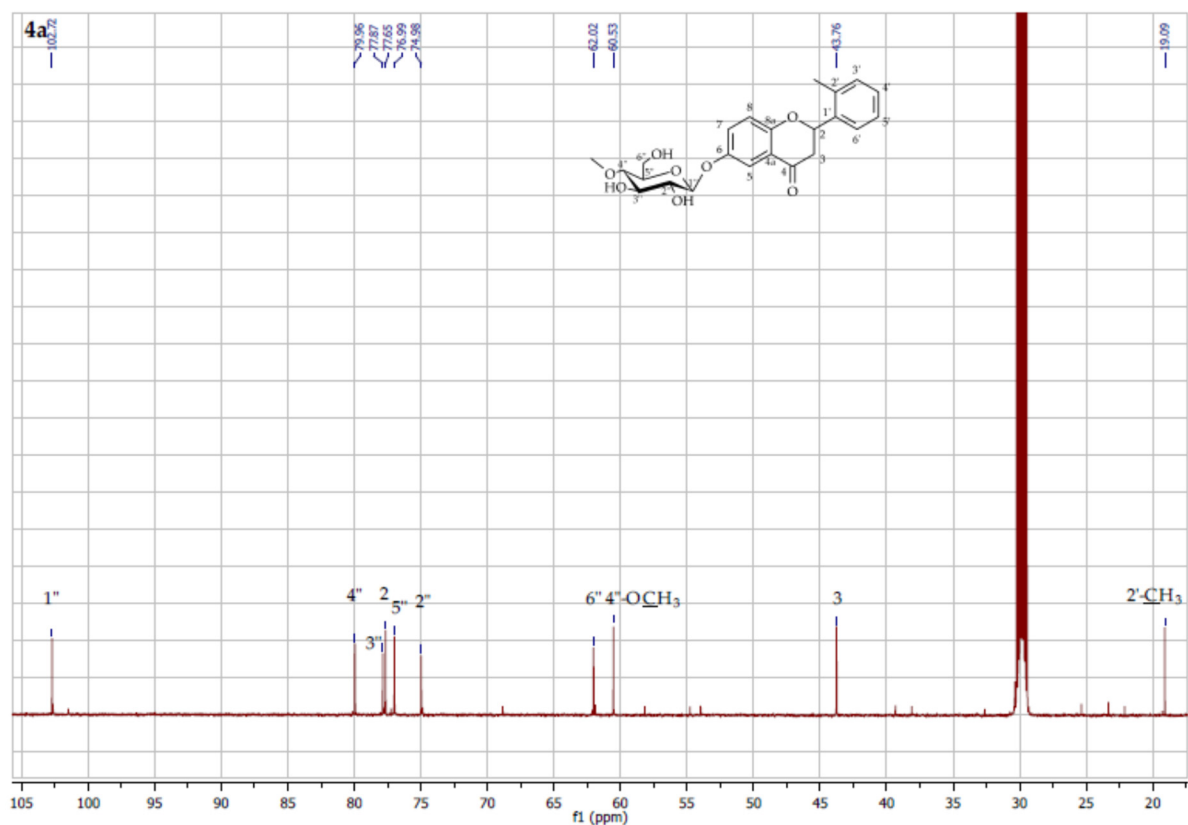


Figure S23. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4a**)

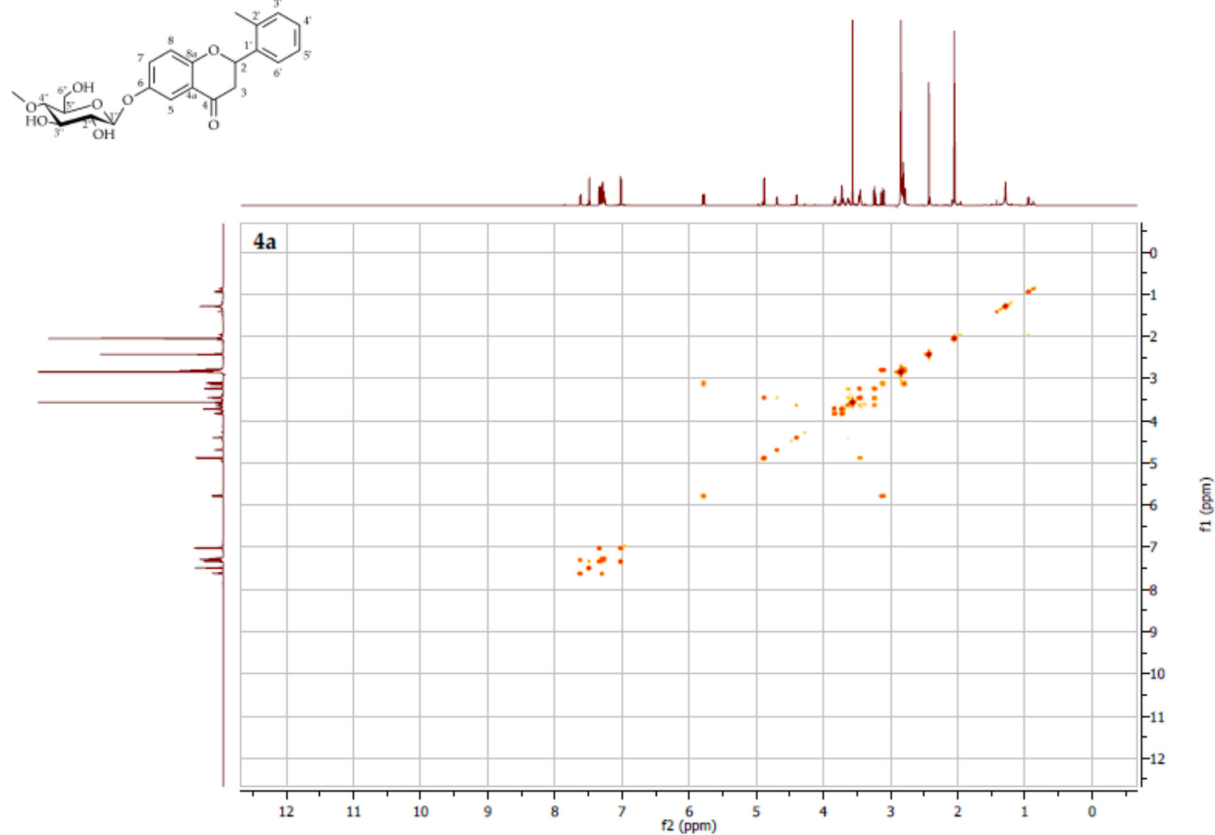


Figure S24. COSY contour map – $^1\text{H} \times ^1\text{H}$ of 2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4a**)

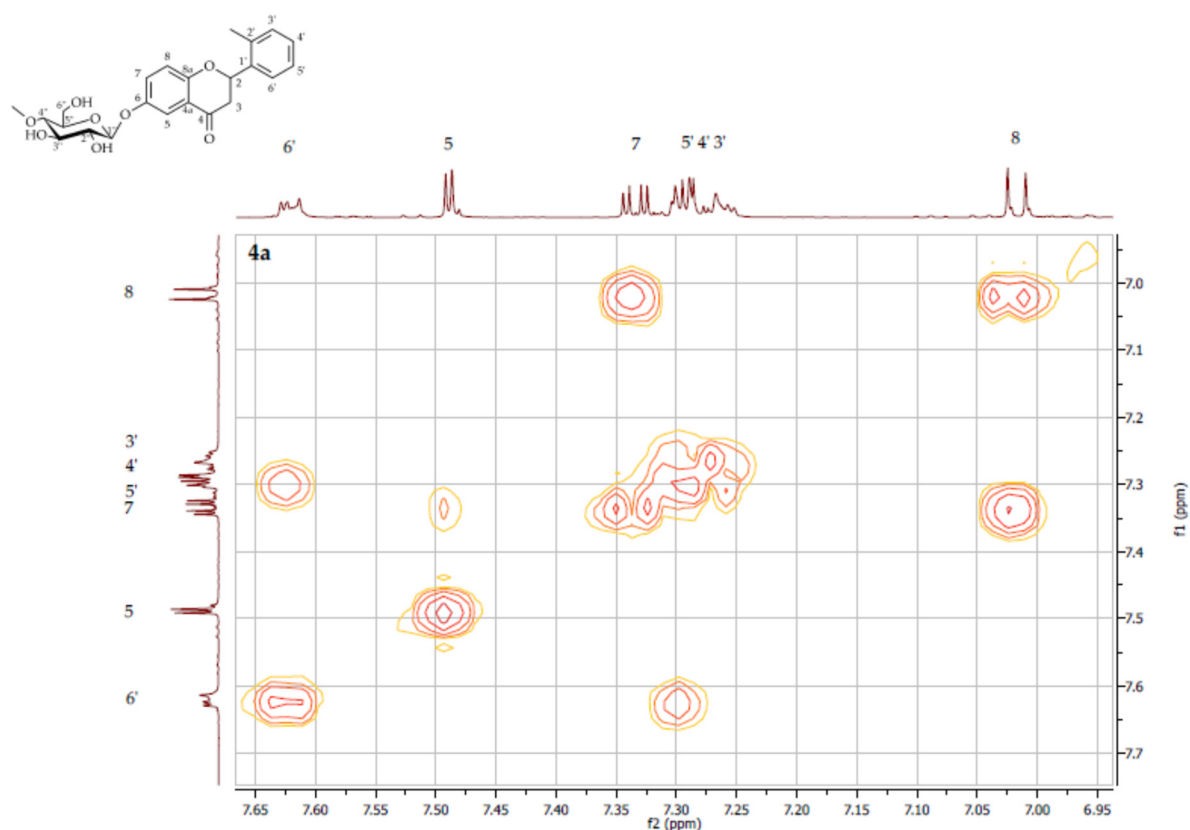


Figure S25. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4a**)

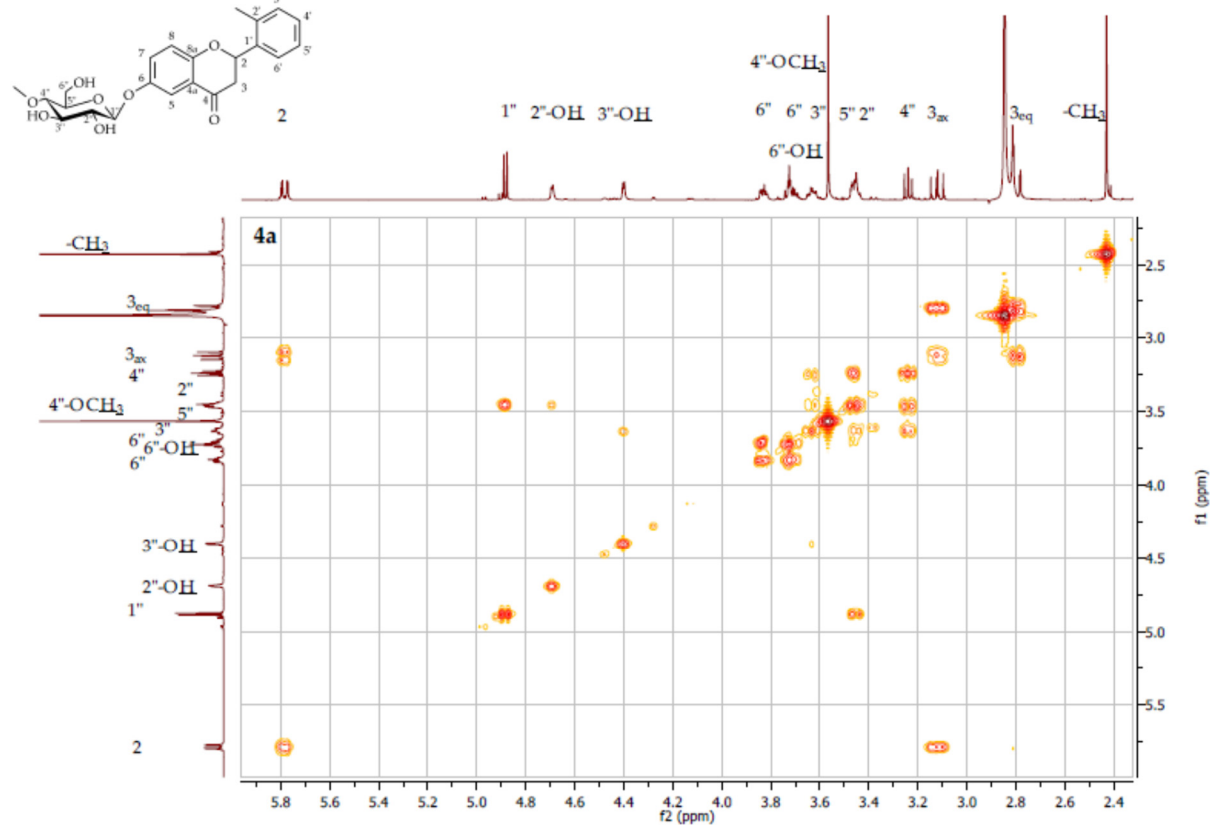


Figure S26. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4a**)

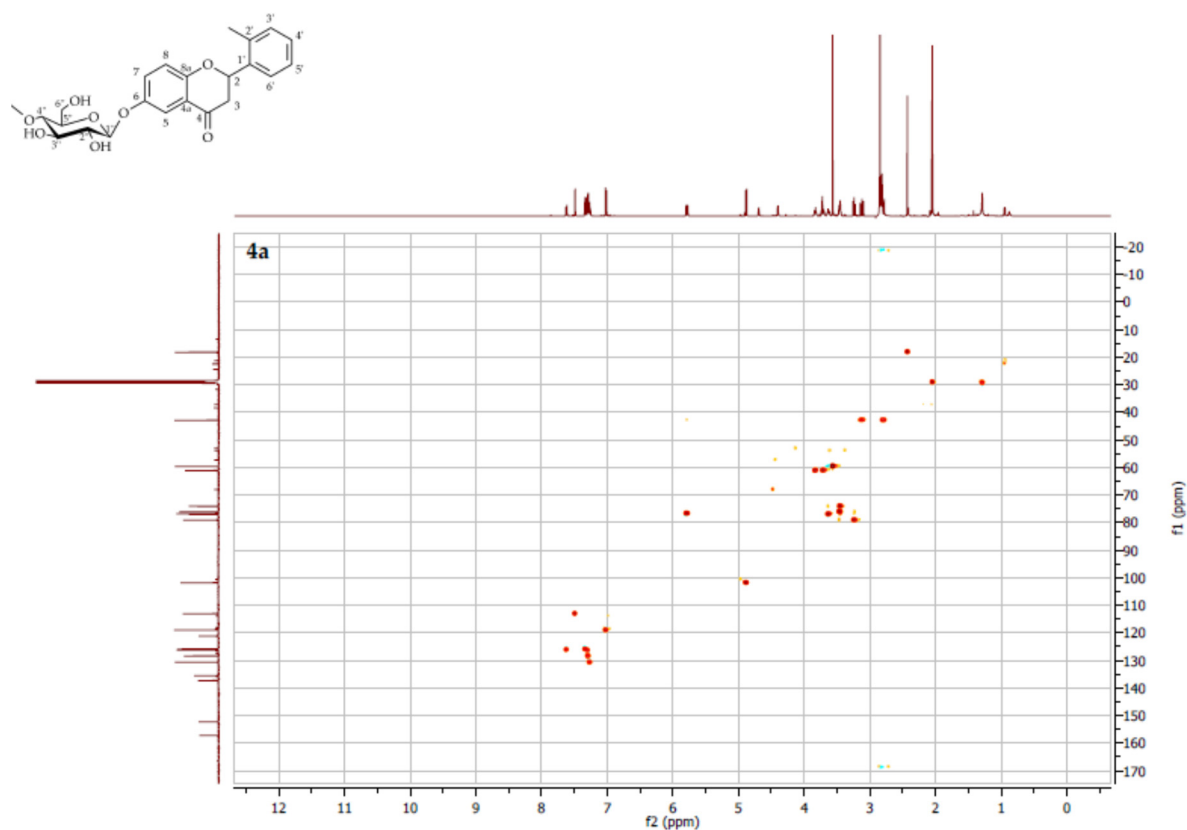


Figure S27. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavanone 6-*O*- β -D-(4''-*O*-methyl)-glucopyranoside (**4a**)

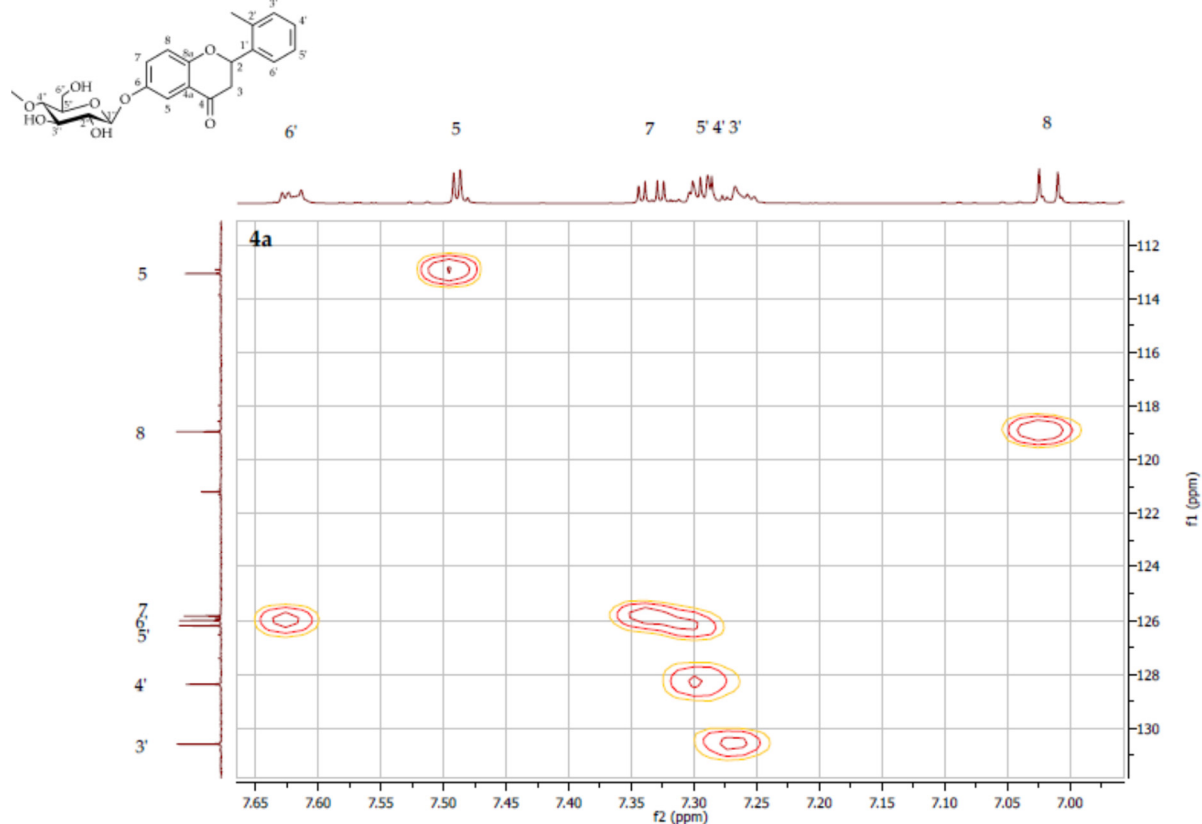


Figure S28. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavanone 6-*O*- β -D-(4''-*O*-methyl)-glucopyranoside (**4a**)

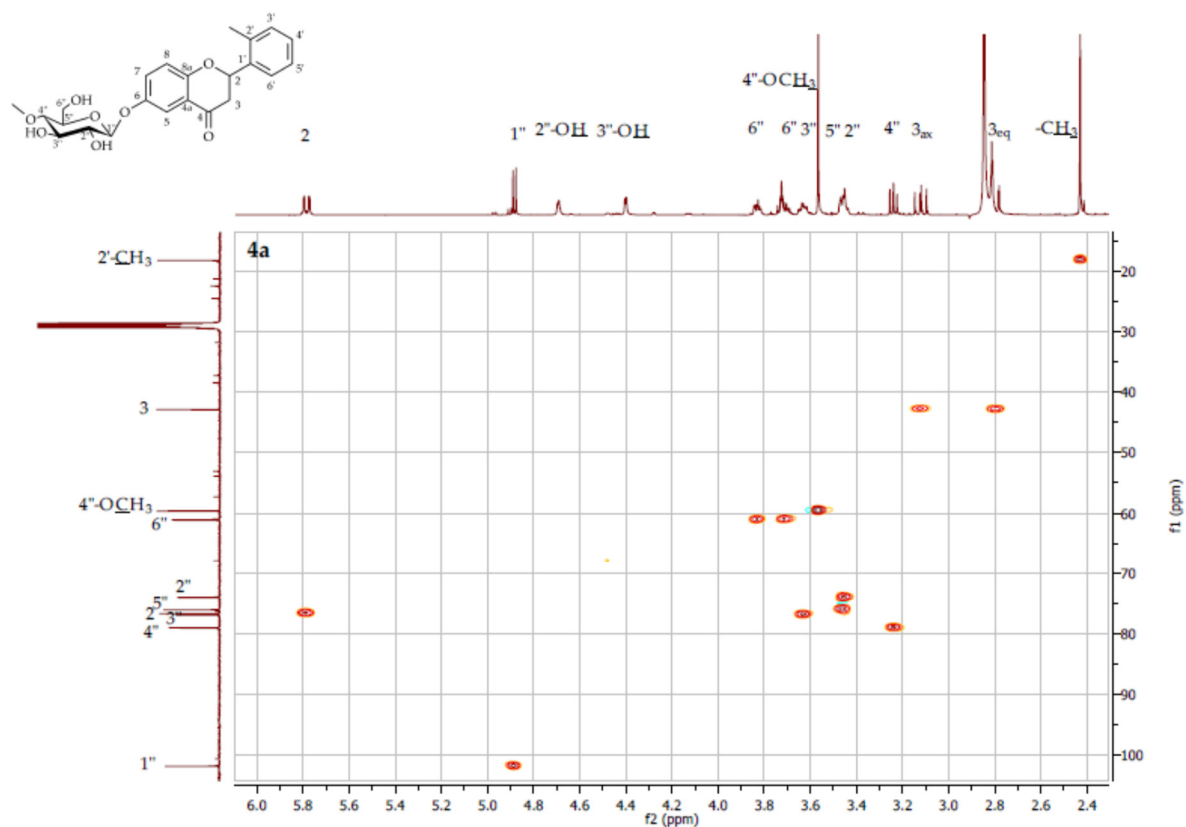


Figure S29. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4a**)

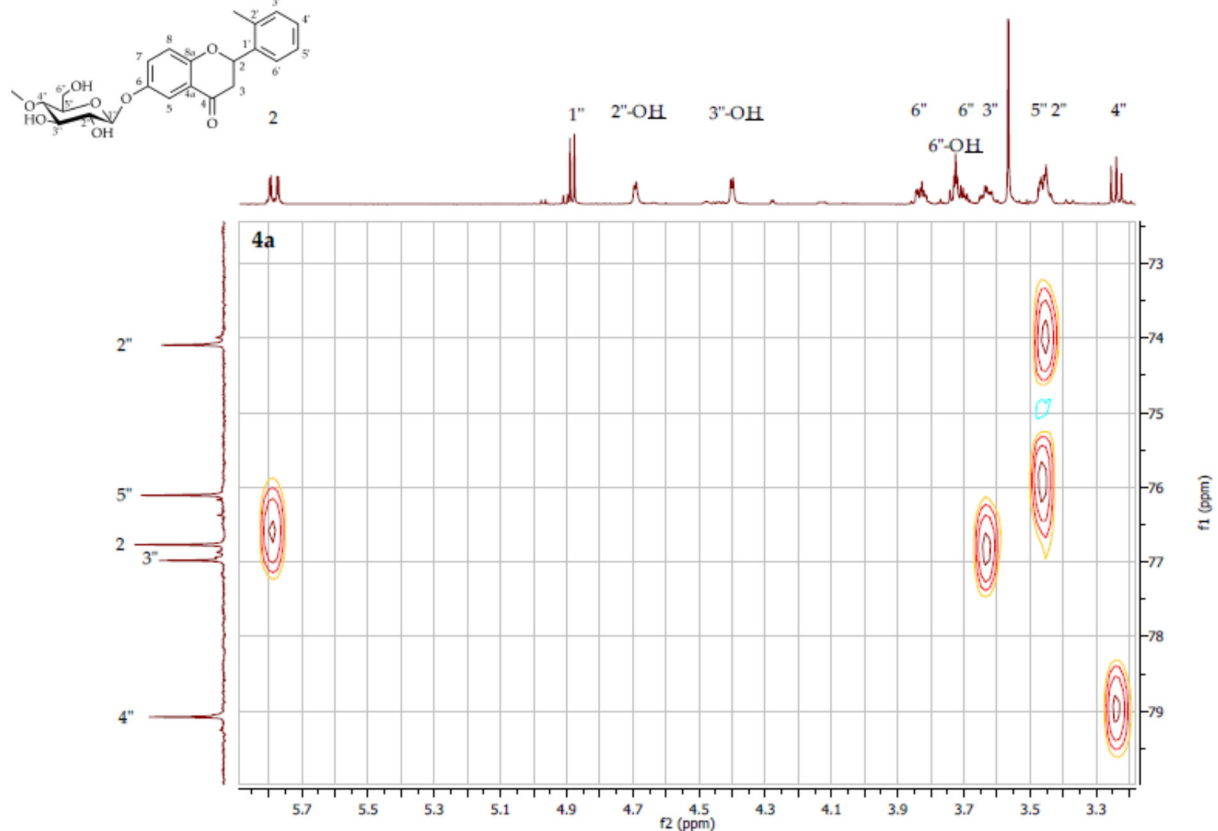


Figure S30. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4a**)

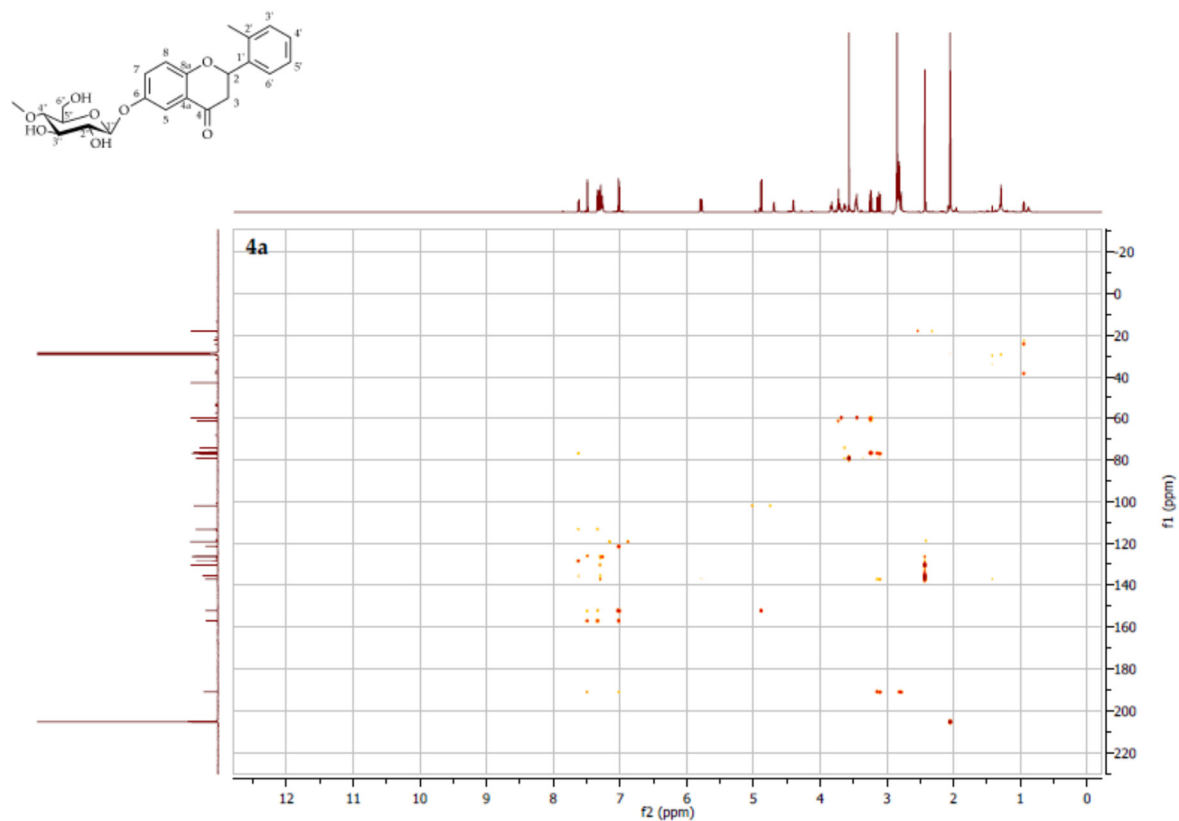


Figure S31. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavanone 6-*O*- β -D-(4''-*O*-methyl)-glucopyranoside (**4a**)

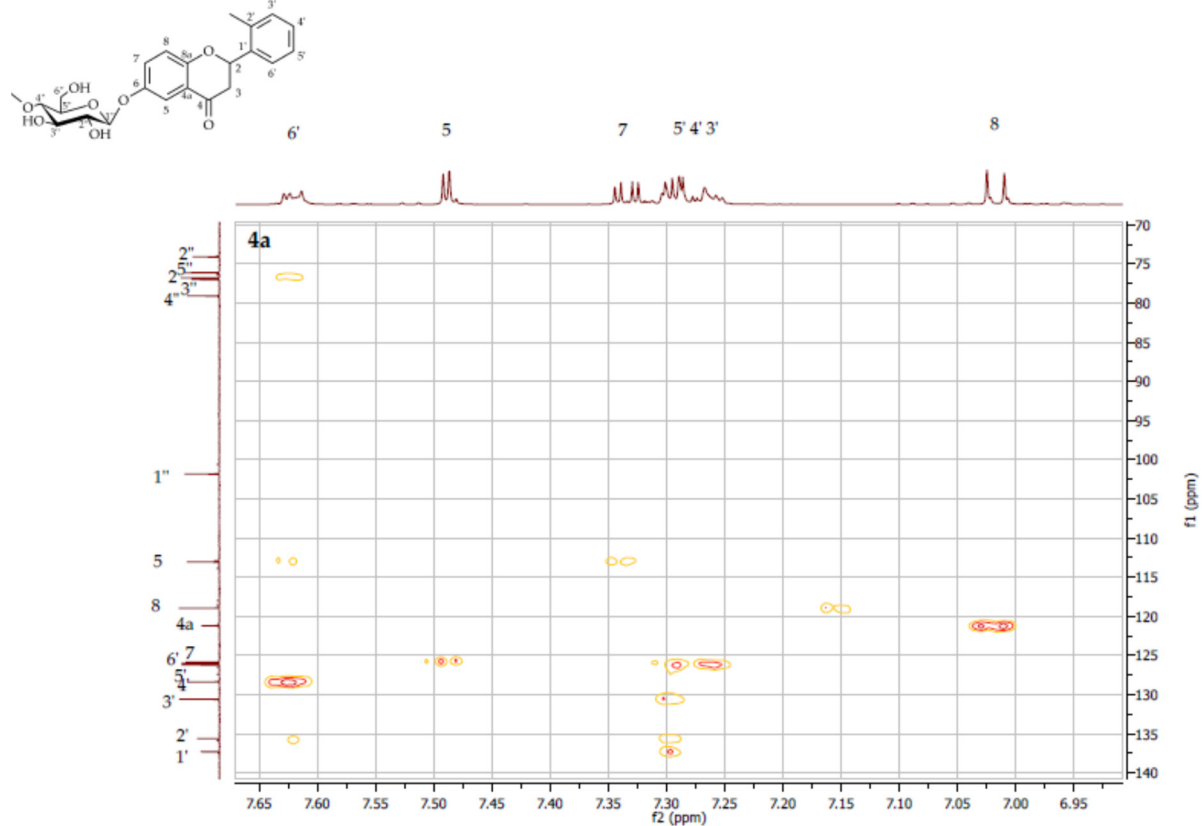


Figure S32. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavanone 6-*O*- β -D-(4''-*O*-methyl)-glucopyranoside (**4a**)

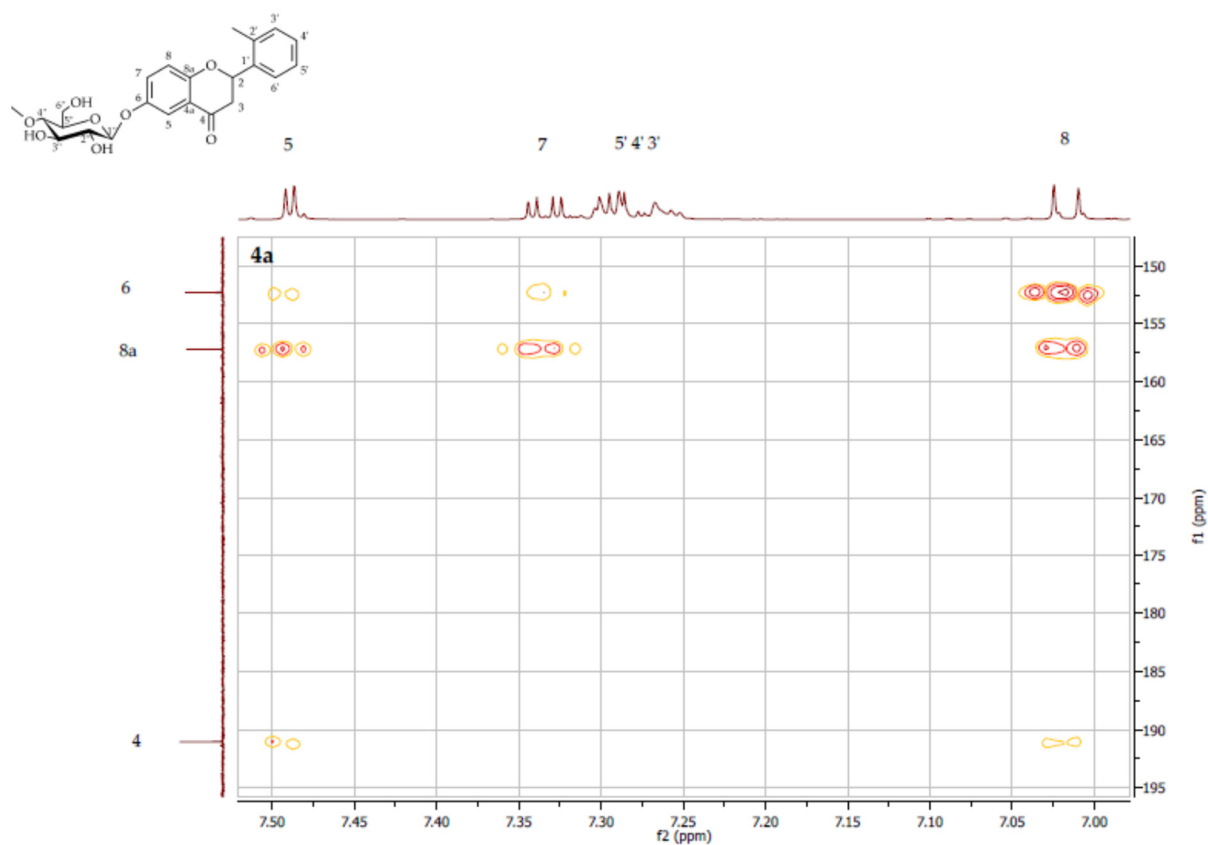


Figure S33. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4a**)

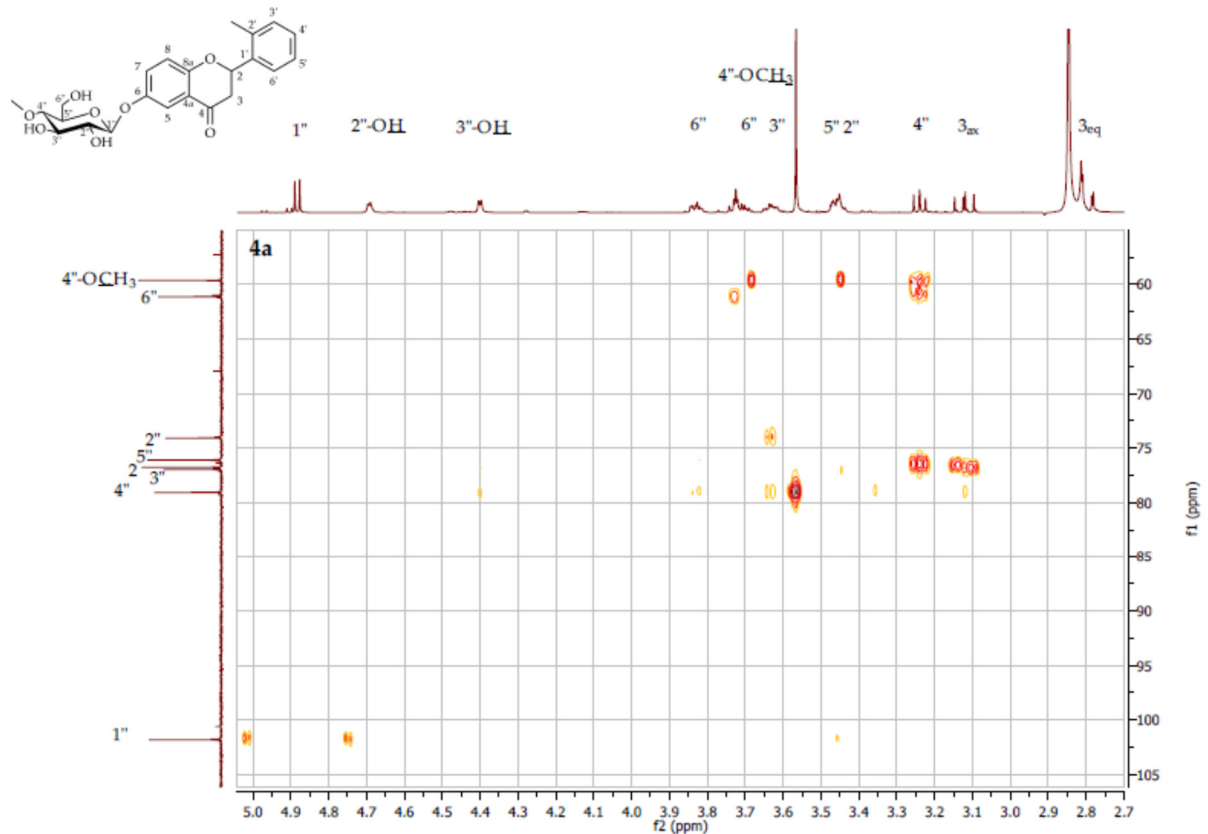


Figure S34. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4a**)

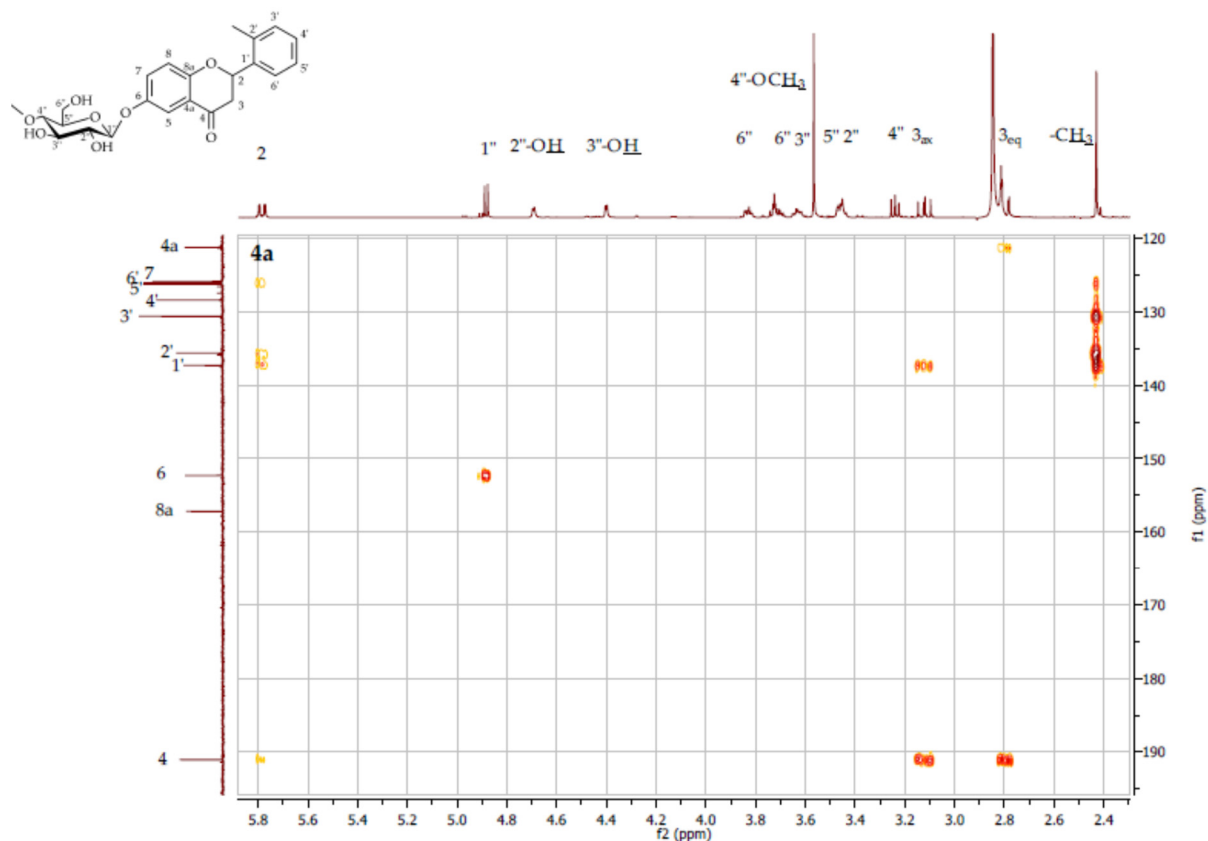


Figure S35. HMBC contour map – ¹H × ¹³C expansion of 2'-methylflavanone 6-O-β-D-(4''-O-methyl)-glucopyranoside (4a)

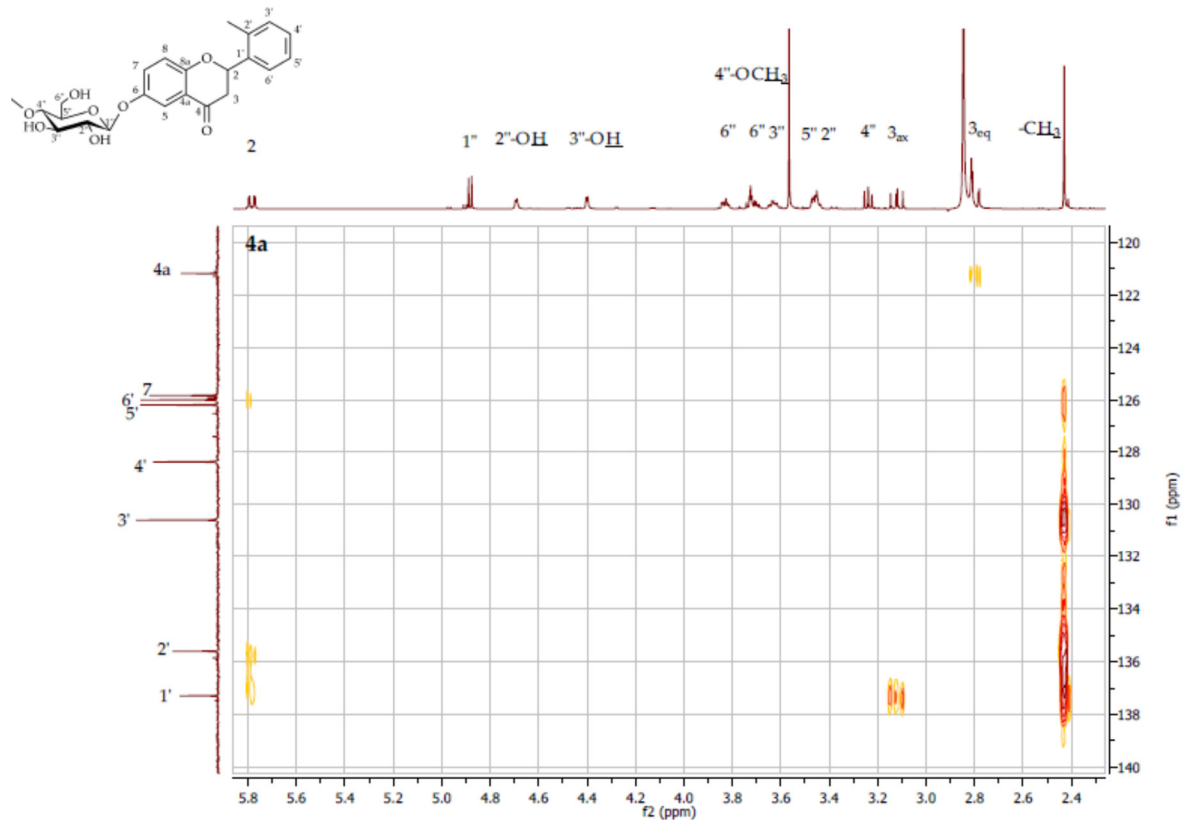


Figure S36. HMBC contour map – ¹H × ¹³C expansion of 2'-methylflavanone 6-O-β-D-(4''-O-methyl)-glucopyranoside (4a)

Molecular formula: C₂₃H₂₆O₉

Formula weight: 446.16

Ionization mode: negative

Precursor: [M - H]⁻ 445.30

445.3000 > 269.0500 CE: 18.0

445.3000 > 251.1000 CE: 29.0

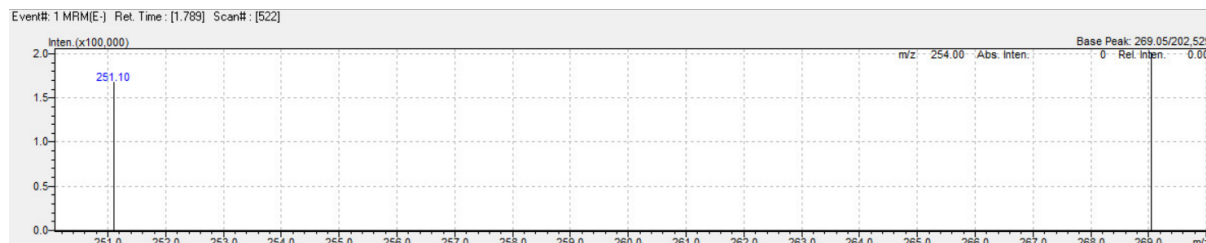
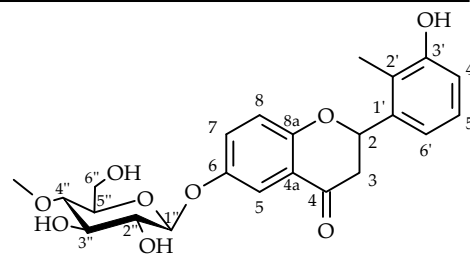


Figure S37. MS analysis of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

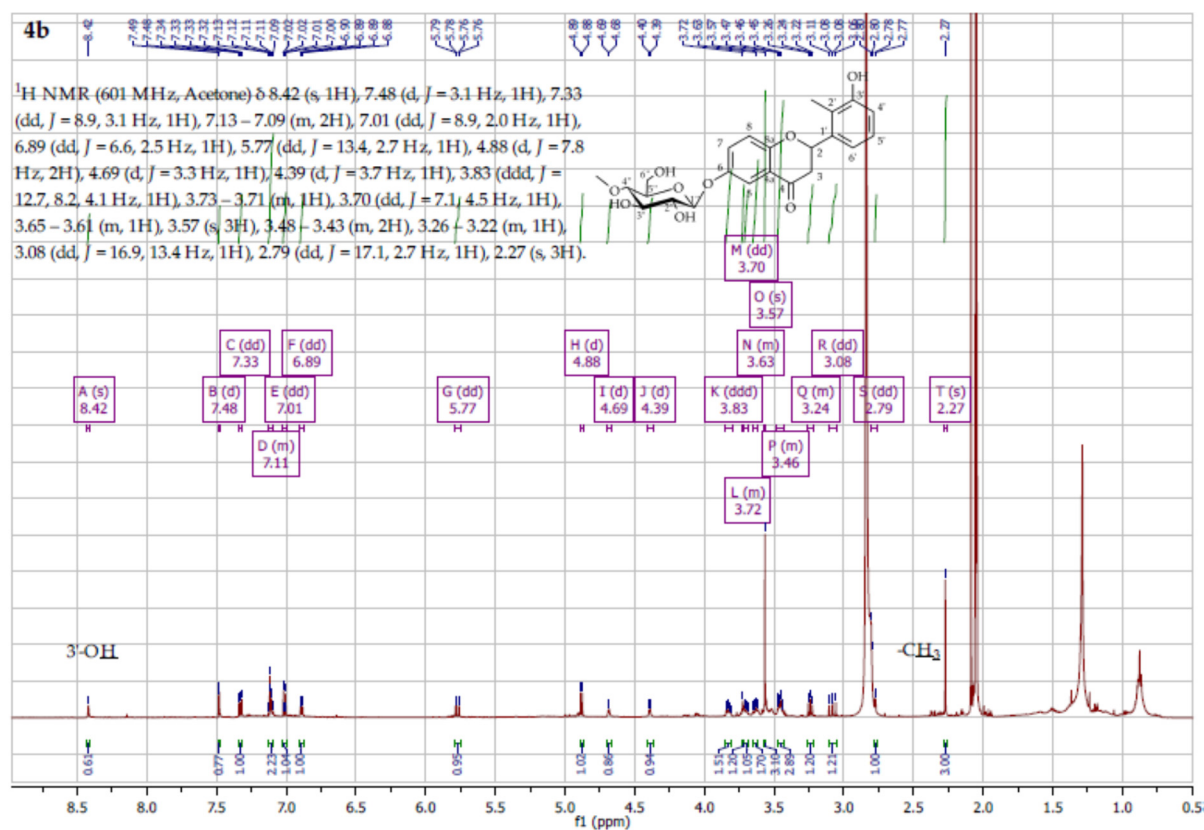


Figure S38. ¹H NMR spectrum (δ , acetone-*d*₆, 600 MHz) of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

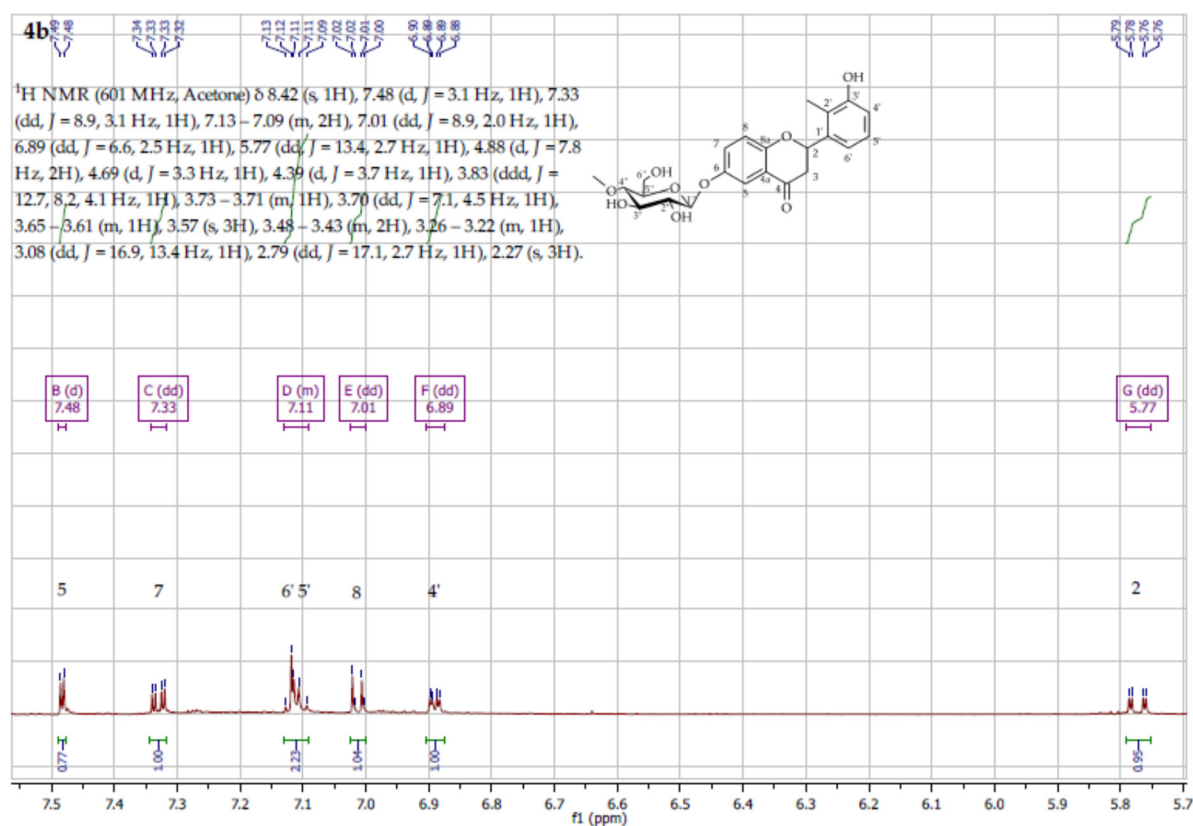


Figure S39. ¹H NMR spectrum expansion (δ, acetone-d₆, 600 MHz) of 3'-hydroxy-2'-methylflavanone 6-*O*-β-D-(4''-*O*-methyl)-glucopyranoside (**4b**)

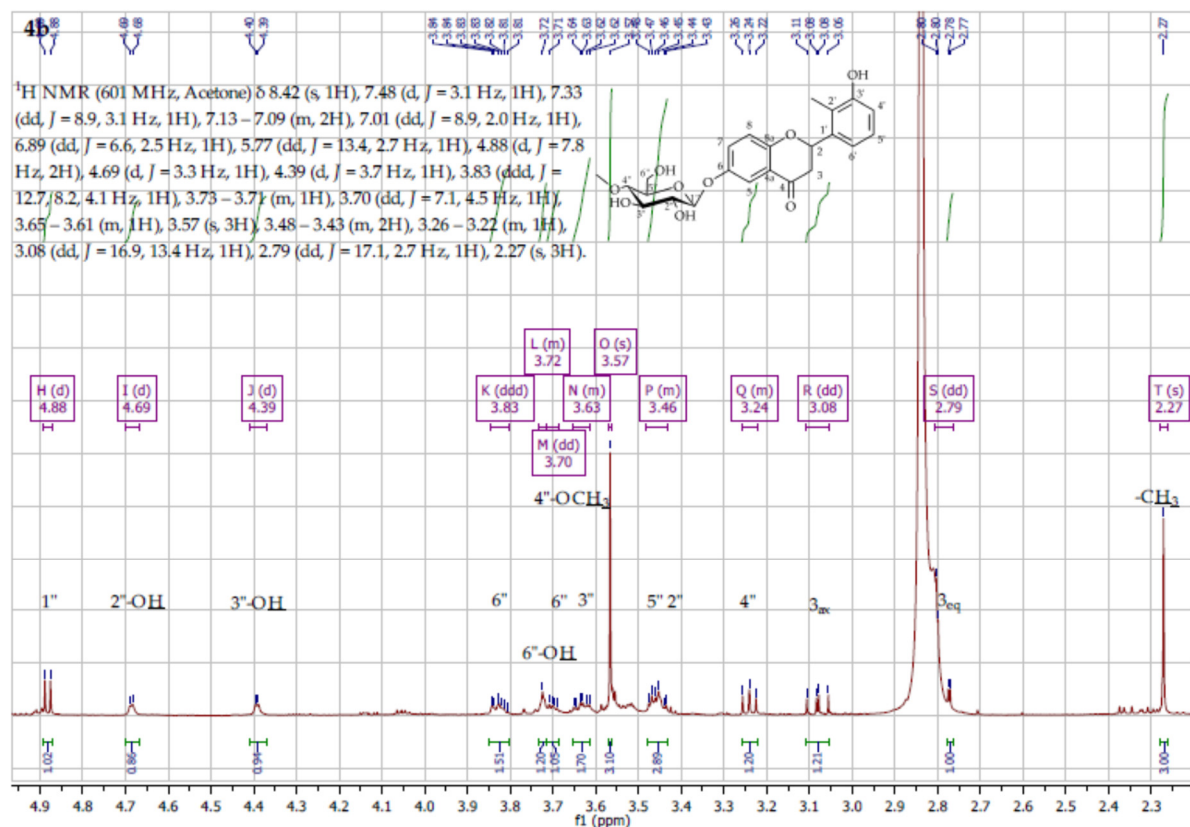


Figure S40. ¹H NMR spectrum expansion (δ, acetone-d₆, 600 MHz) of 3'-hydroxy-2'-methylflavanone 6-*O*-β-D-(4''-*O*-methyl)-glucopyranoside (**4b**)

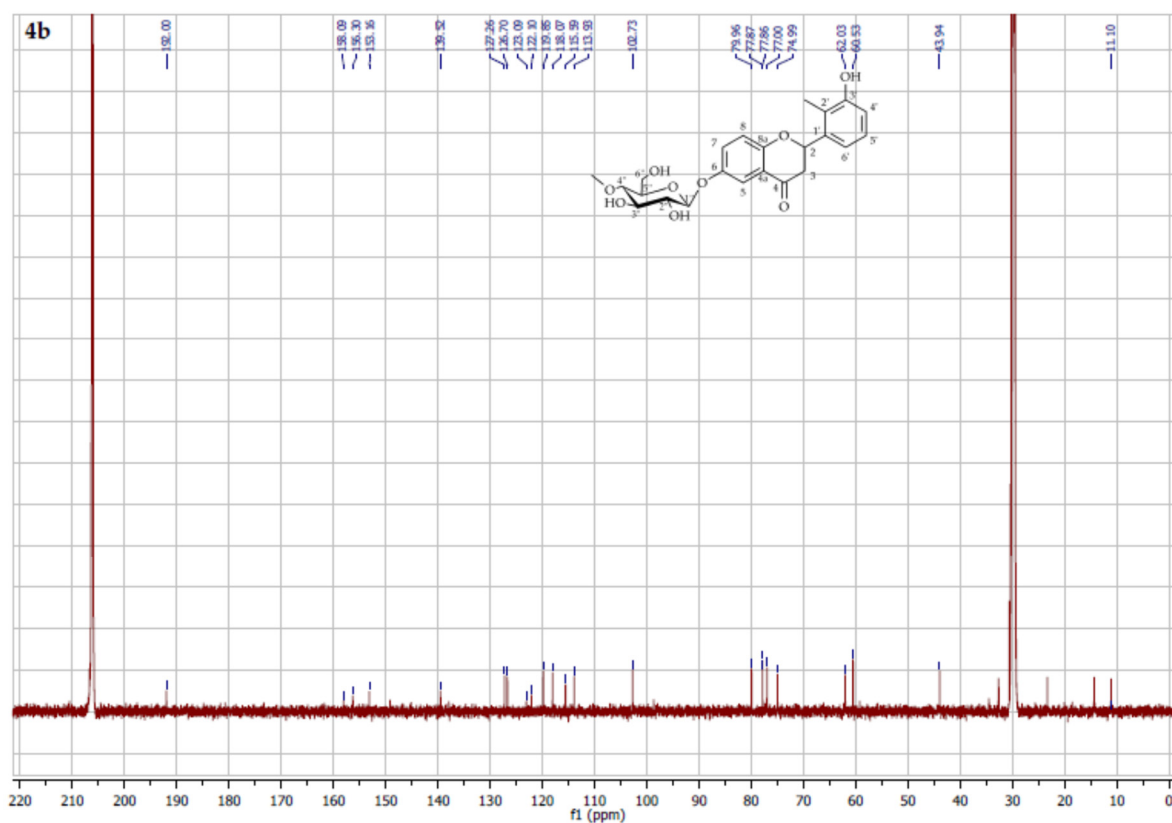


Figure S41. ^{13}C NMR spectrum (δ , acetone- d_6 , 151 MHz) of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

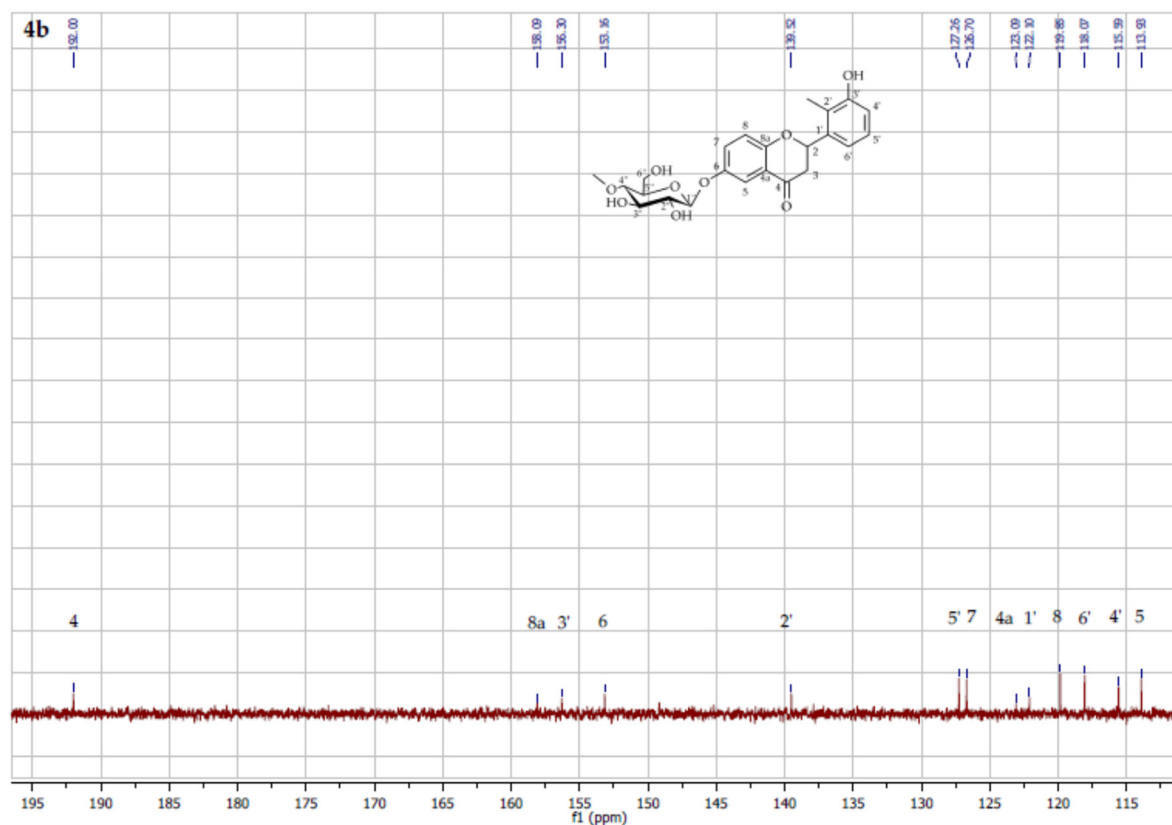


Figure S42. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

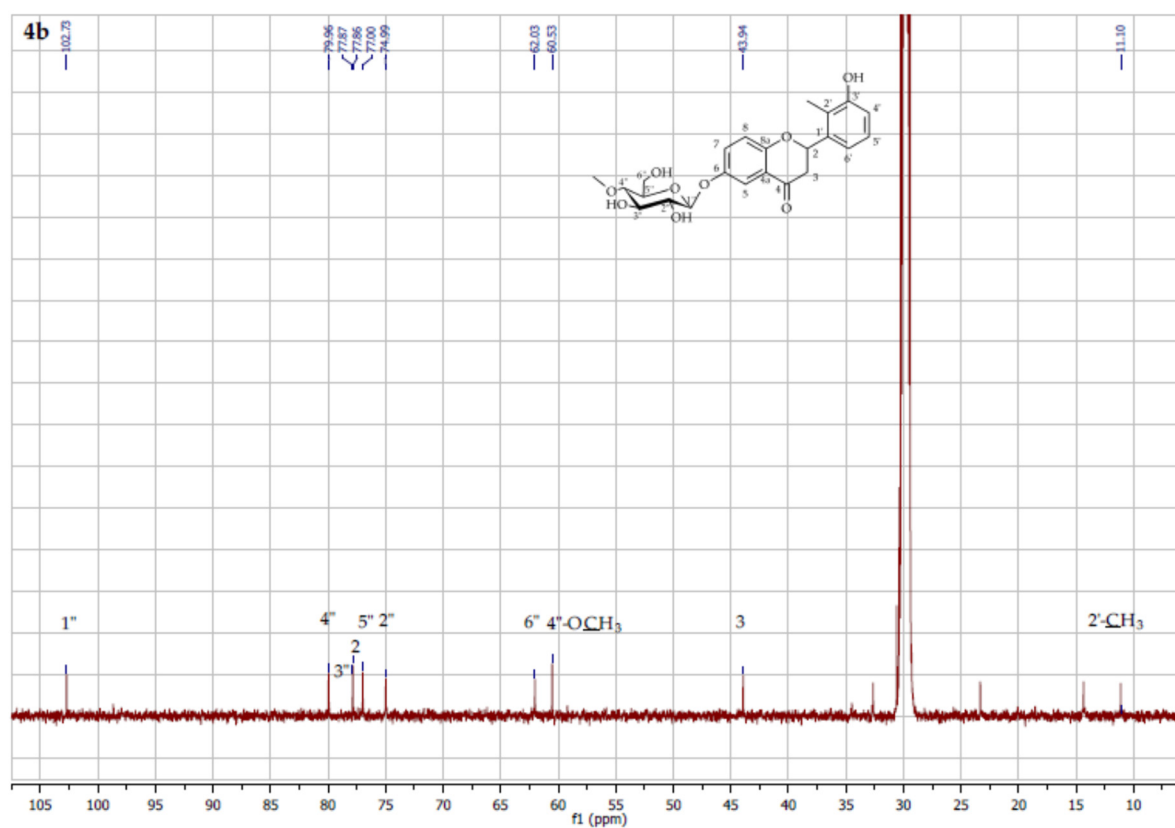


Figure S43. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

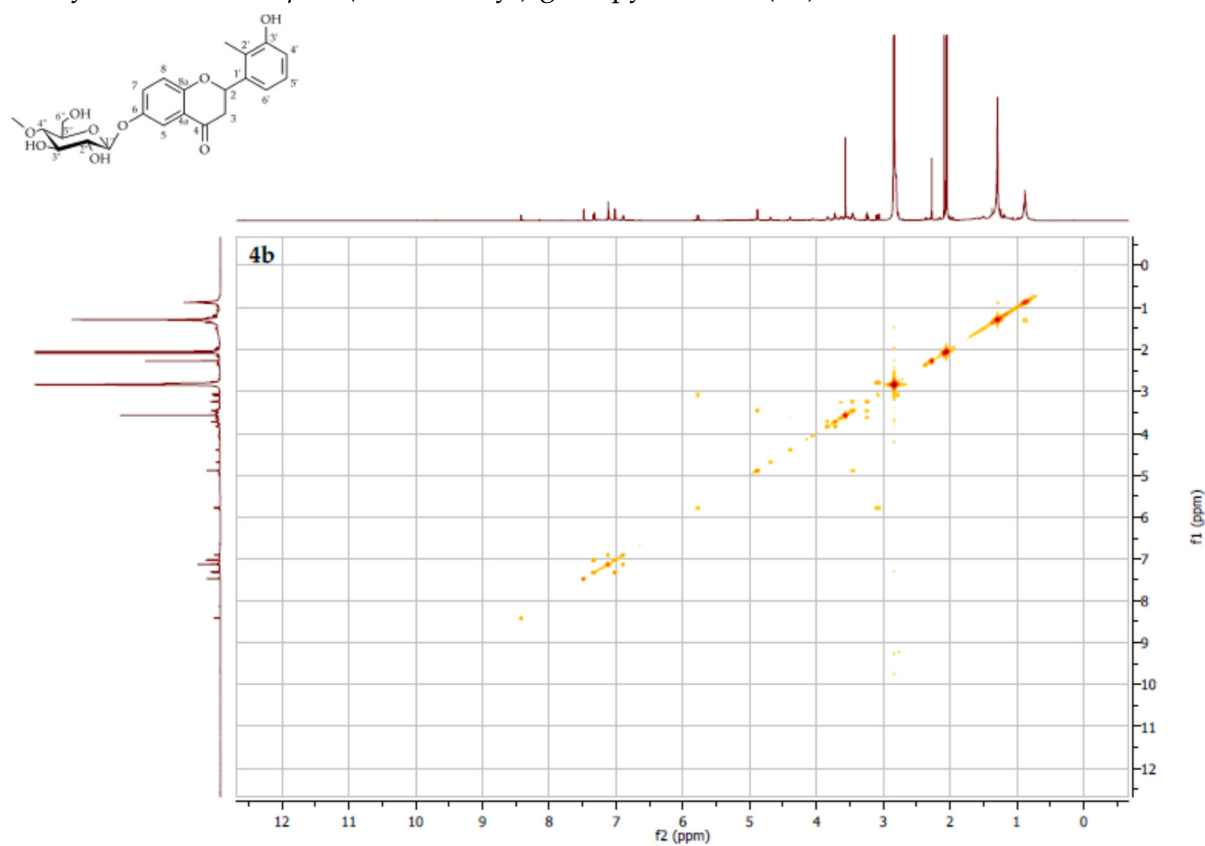


Figure S44. COSY contour map – $^1\text{H} \times ^1\text{H}$ of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

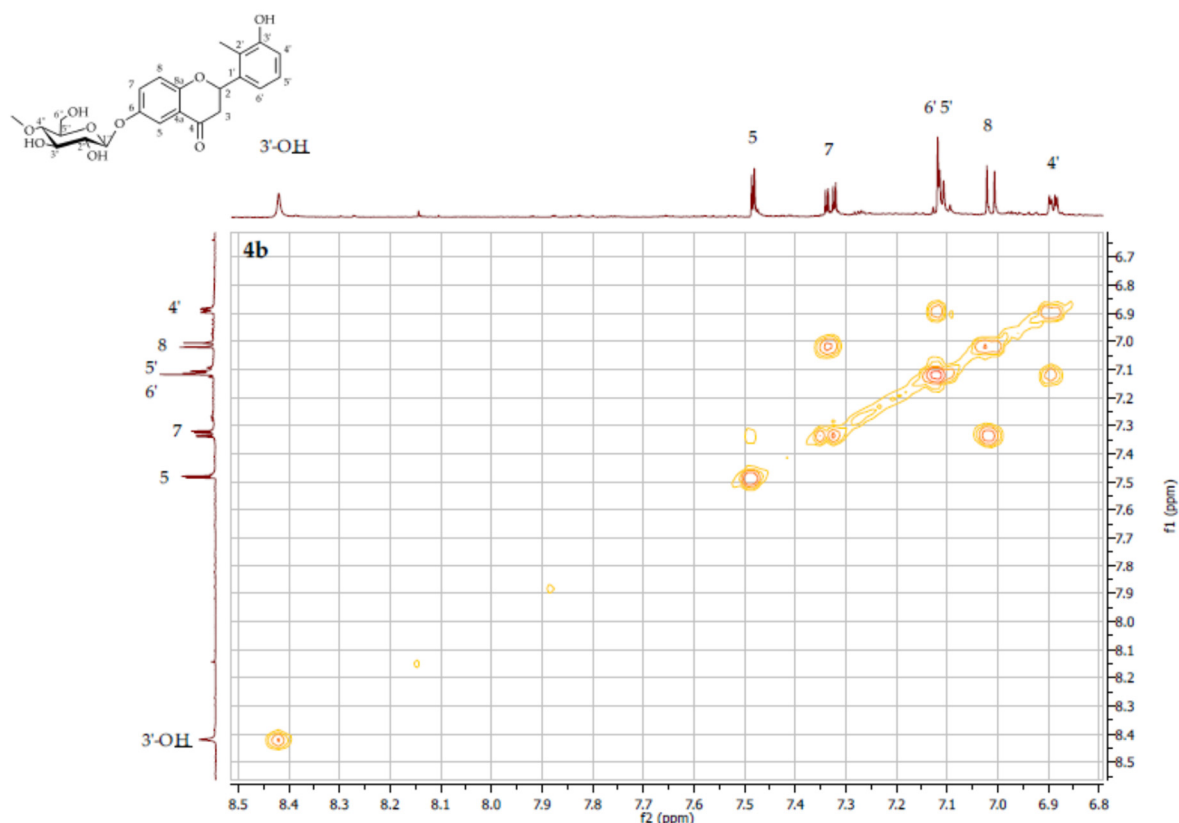


Figure S45. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

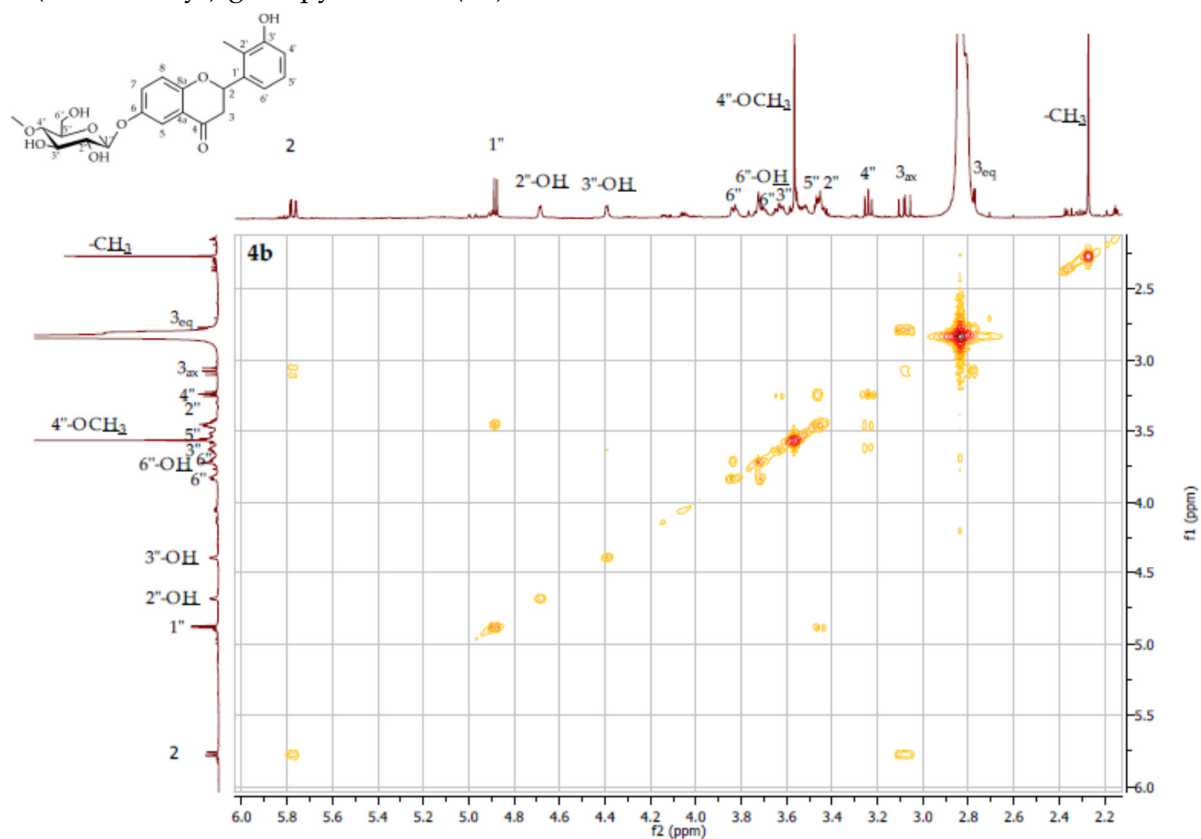


Figure S46. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

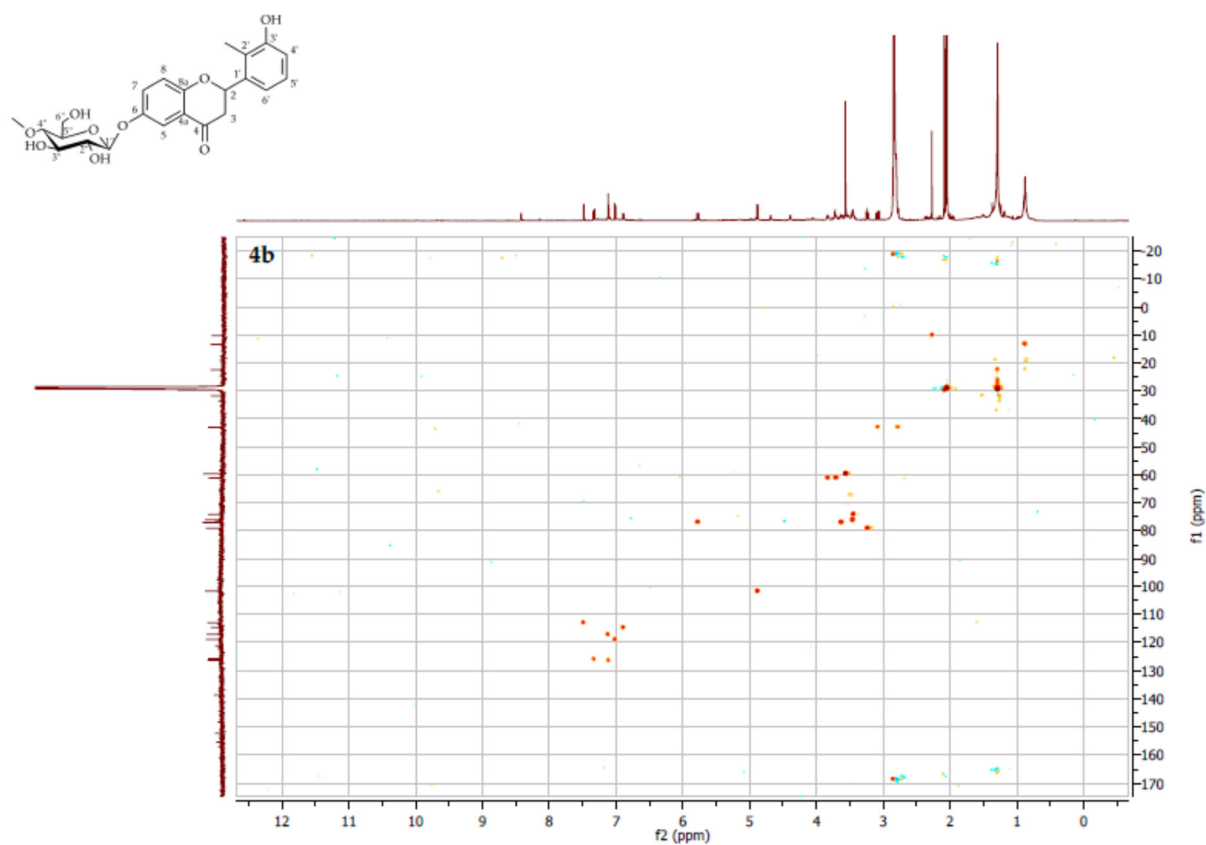


Figure S47. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

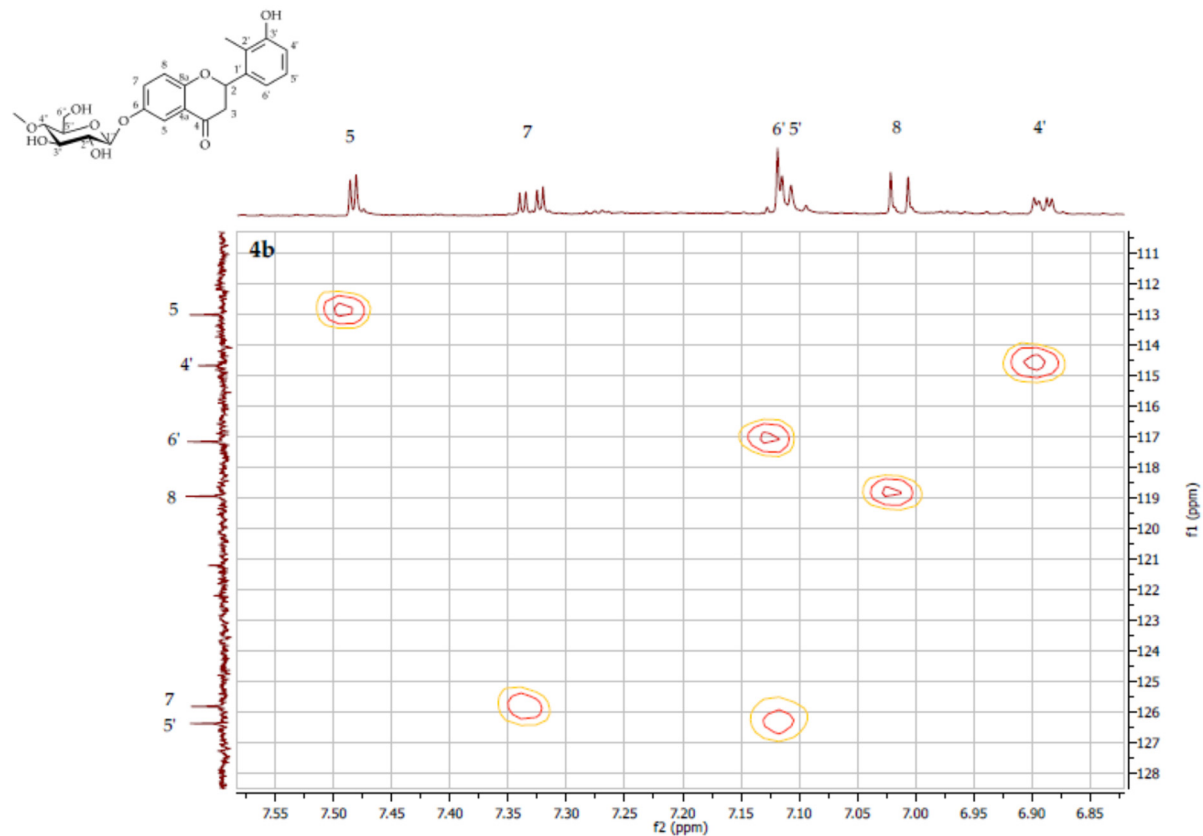


Figure S48. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

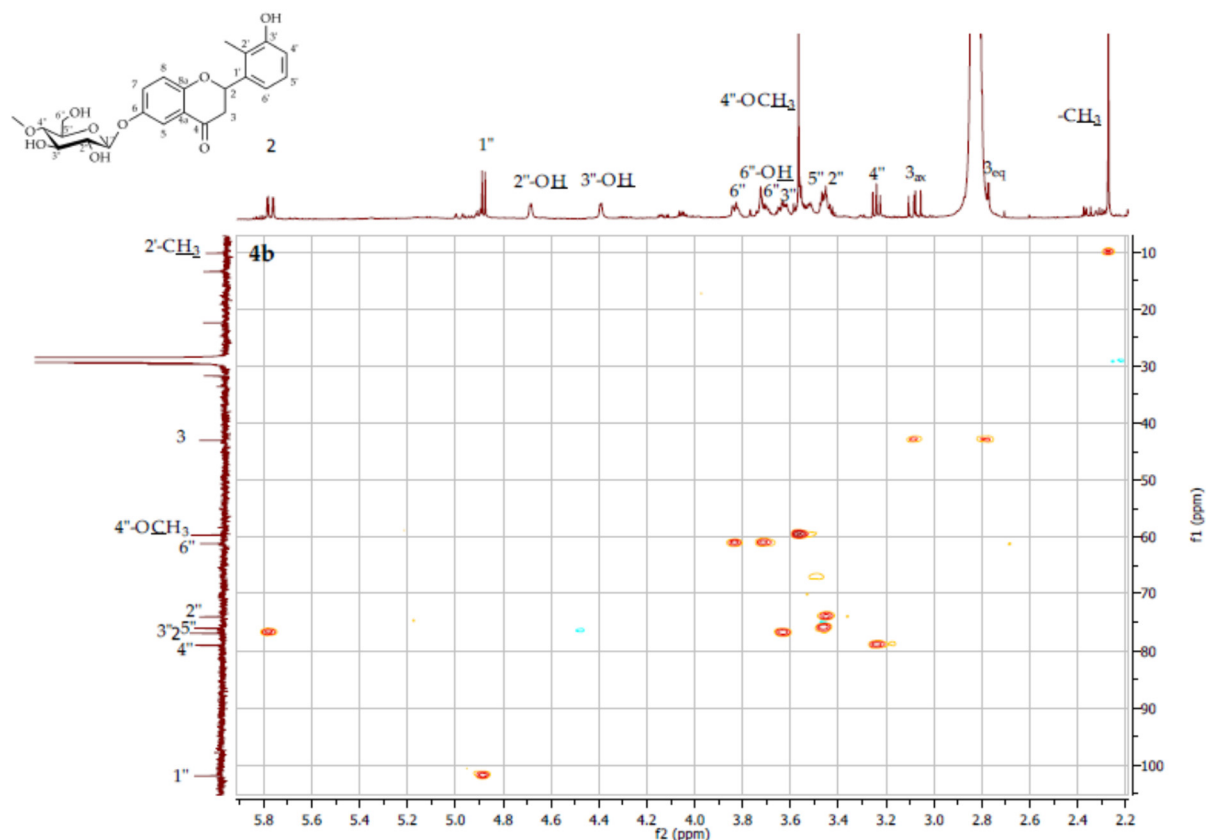


Figure S49. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

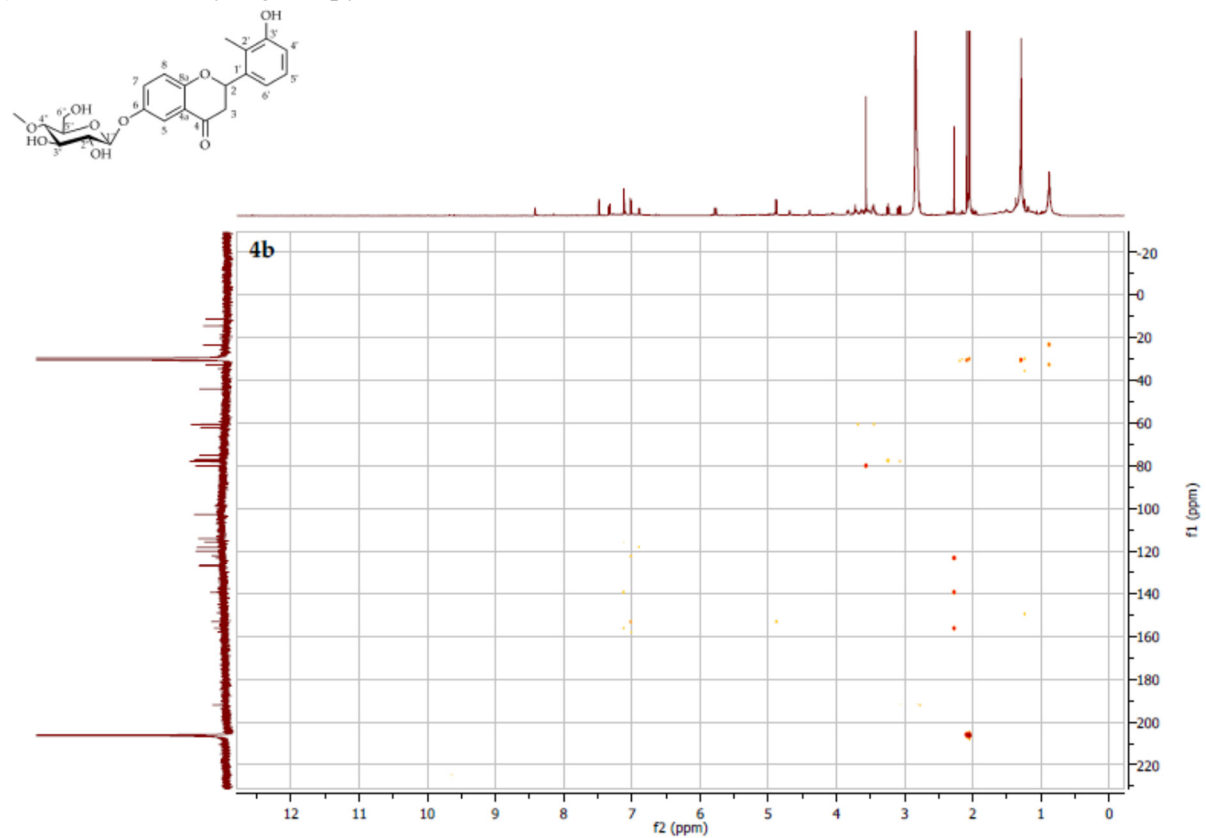


Figure S50. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

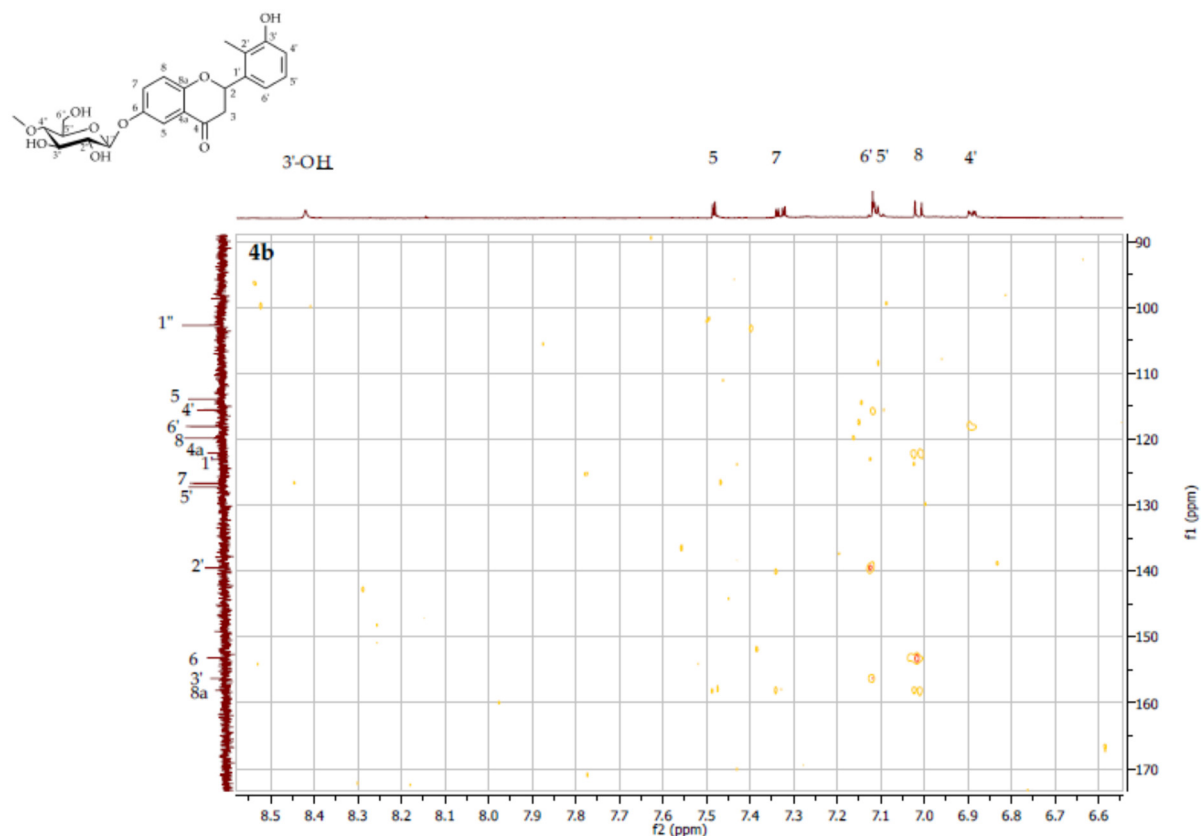


Figure S51. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

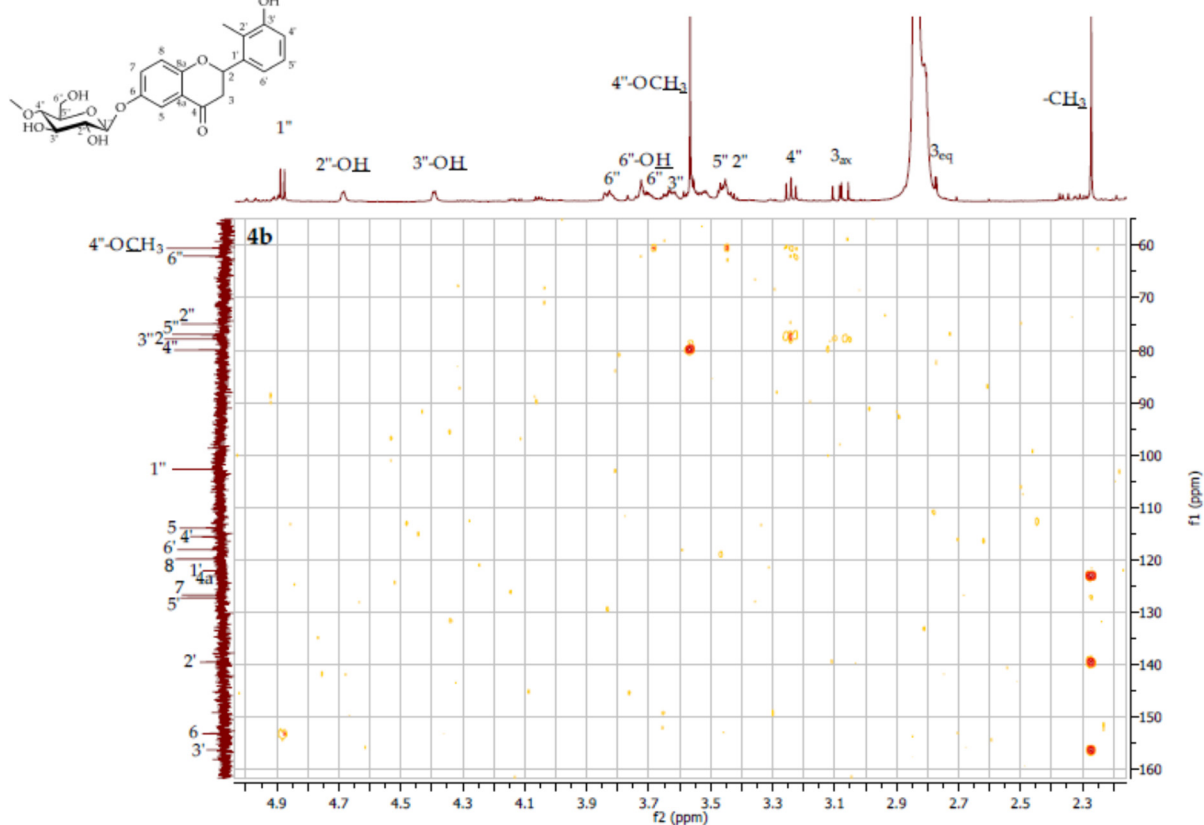


Figure S52. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 3'-hydroxy-2'-methylflavanone 6-O- β -D-(4''-O-methyl)-glucopyranoside (**4b**)

Molecular formula: C₂₃H₂₈O₇

Formula weight: 416.18

Ionization mode: negative

Precursor: adduct [M + 46 - H]⁻ ([M + HCOOH - H]⁻) 461.20

461.2000>45.0500 CE: 12.0

461.2000>309.1500 CE: 23.0

461.2000>325.1500 CE: 22.0

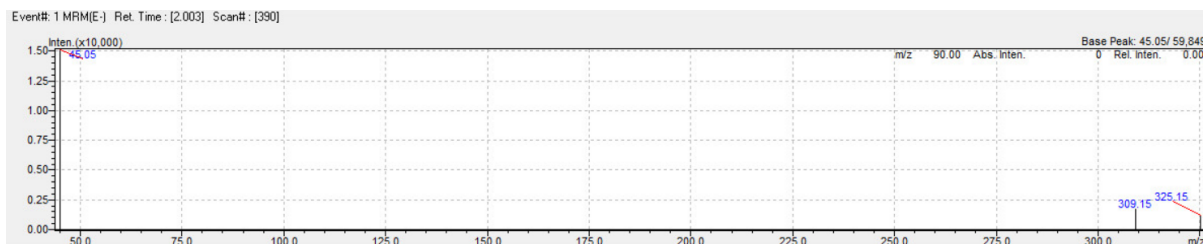
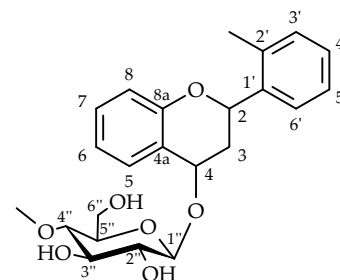


Figure S53. MS analysis of 2-(2'-methylphenyl)-chromane 4-O- β -D-(4''-O-methyl)-glucopyranoside (**4c**)

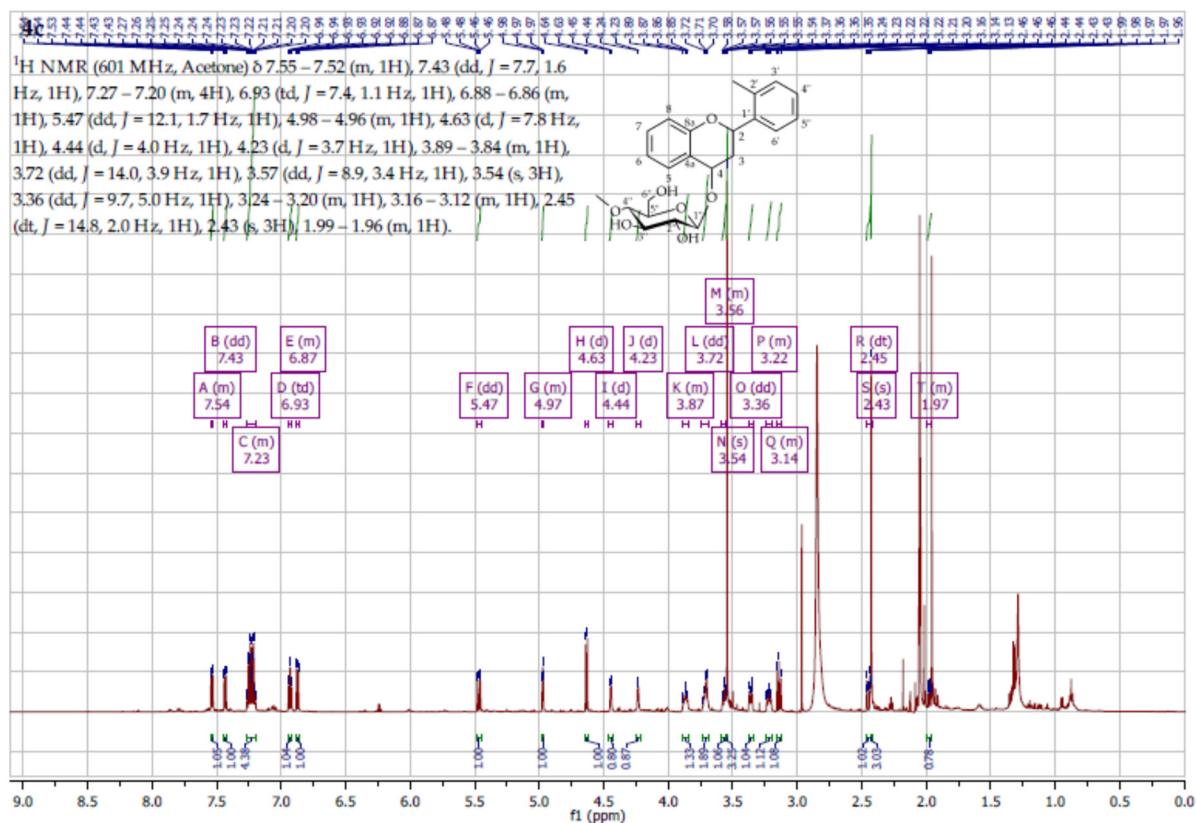


Figure S54. ¹H NMR spectrum (δ , acetone-d₆, 600 MHz) of 2-(2'-methylphenyl)-chromane 4-O- β -D-(4''-O-methyl)-glucopyranoside (**4c**)

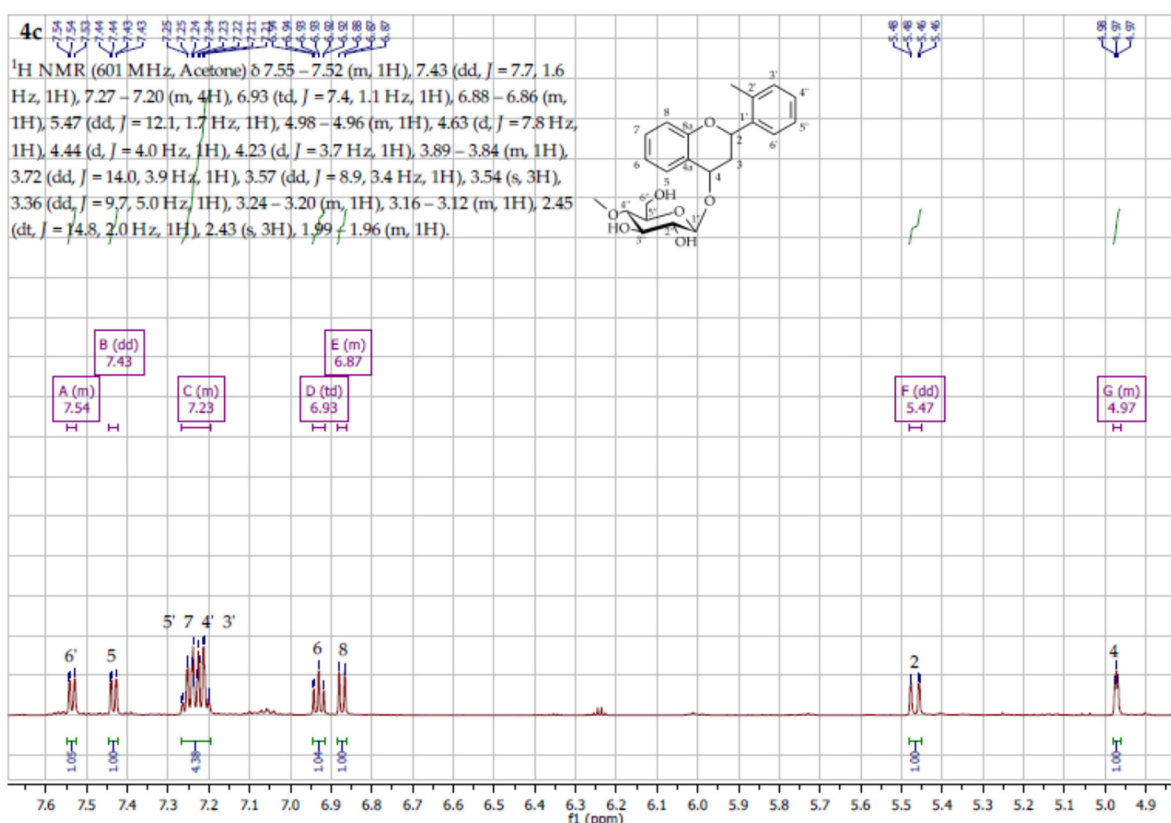


Figure S55. ¹H NMR spectrum expansion (δ, acetone-d₆, 600 MHz) of 2-(2'-methylphenyl)-chromane 4-*O*-β-D-(4''-*O*-methyl)-glucopyranoside (**4c**)

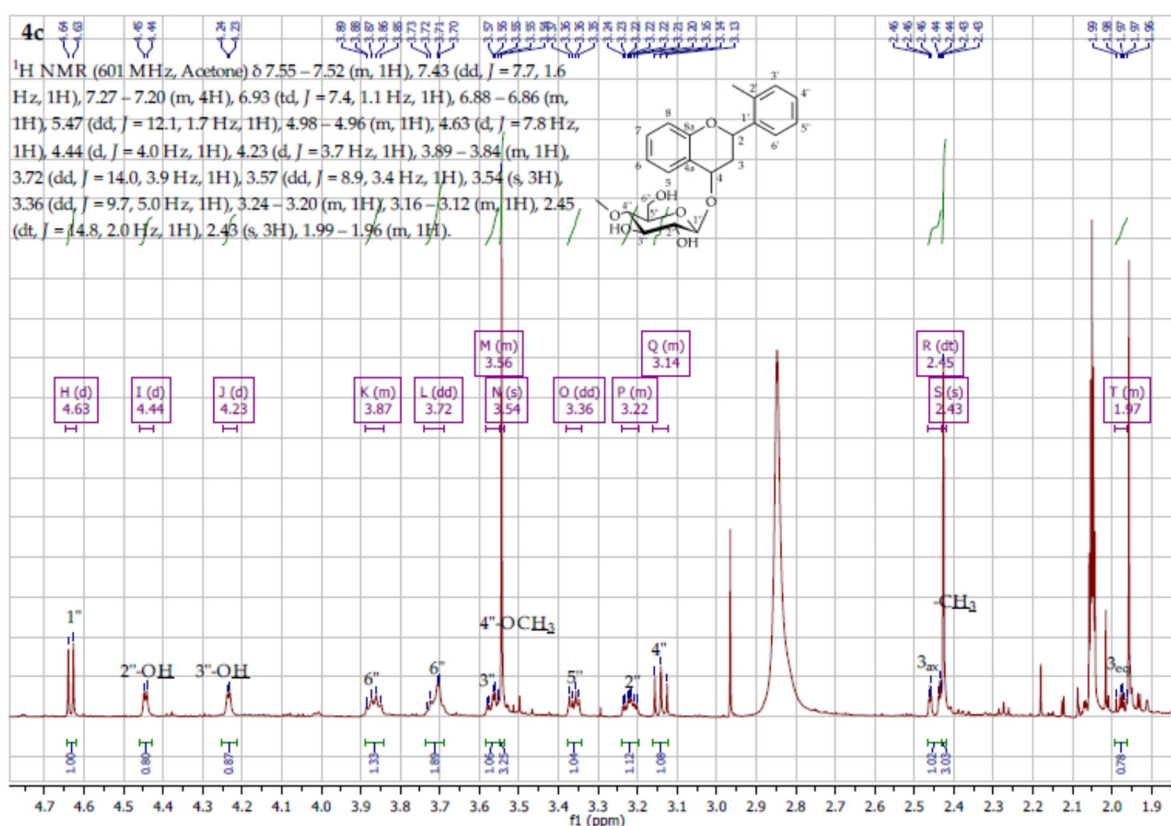


Figure S56. ¹H NMR spectrum expansion (δ, acetone-d₆, 600 MHz) of 2-(2'-methylphenyl)-chromane 4-*O*-β-D-(4''-*O*-methyl)-glucopyranoside (**4c**)

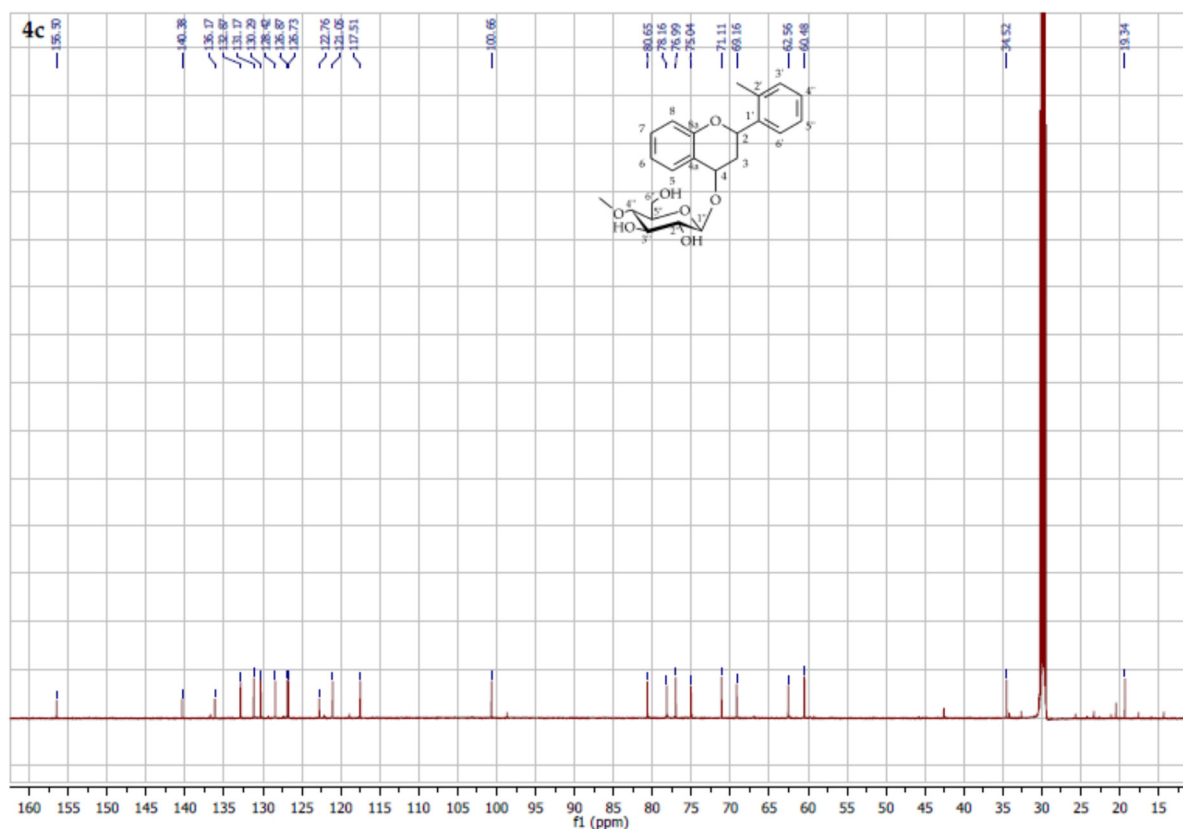


Figure S57. ^{13}C NMR spectrum (δ , acetone- d_6 , 151 MHz) of 2-(2'-methylphenyl)-chromane 4- O - β -D-(4''- O -methyl)-glucopyranoside (**4c**)

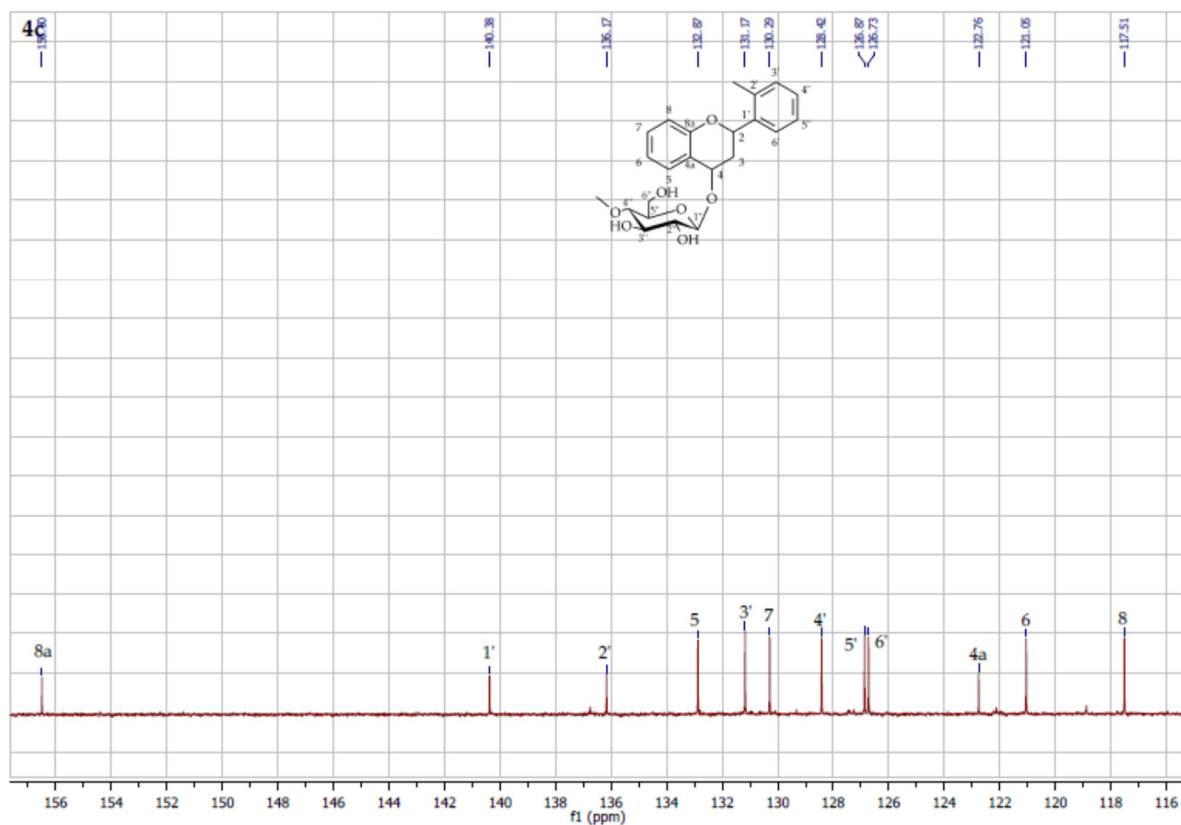


Figure S58. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2-(2'-methylphenyl)-chromane 4- O - β -D-(4''- O -methyl)-glucopyranoside (**4c**)

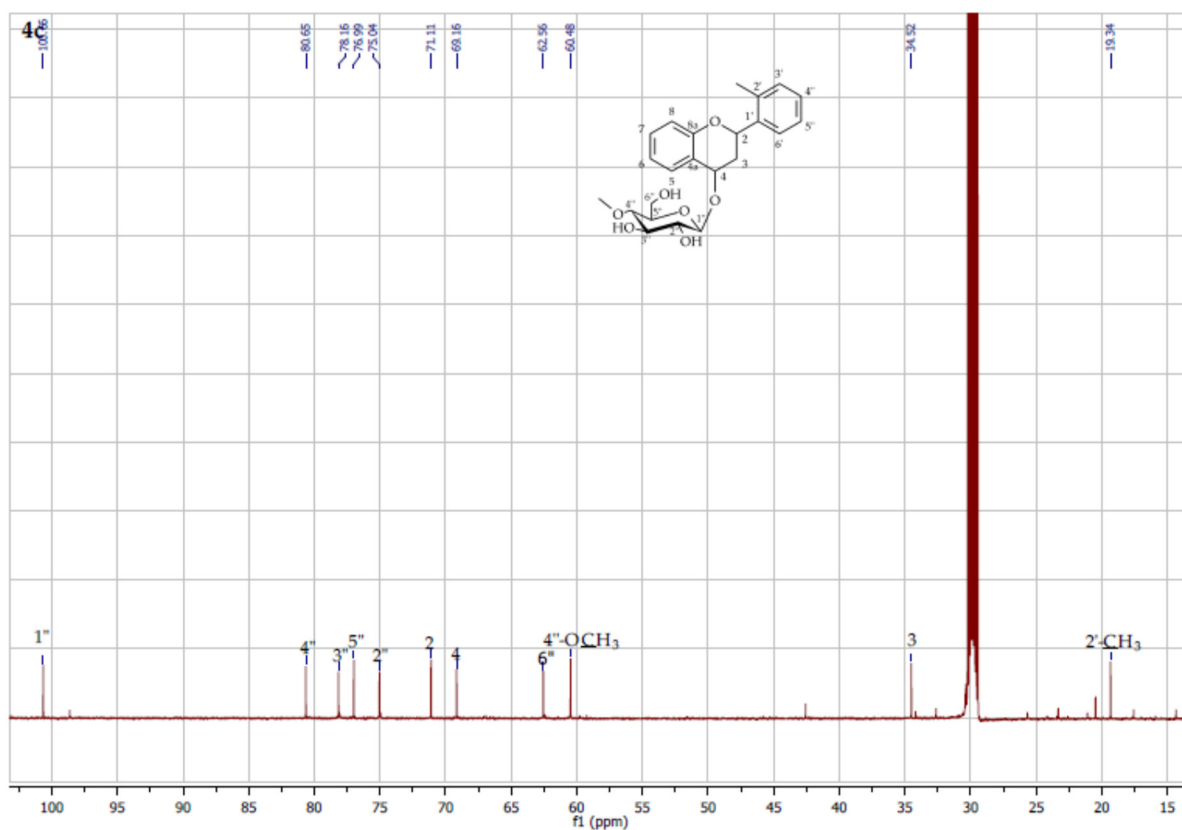


Figure S59. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2-(2'-methylphenyl)-chromane 4- O - β -D-(4''- O -methyl)-glucopyranoside (**4c**)

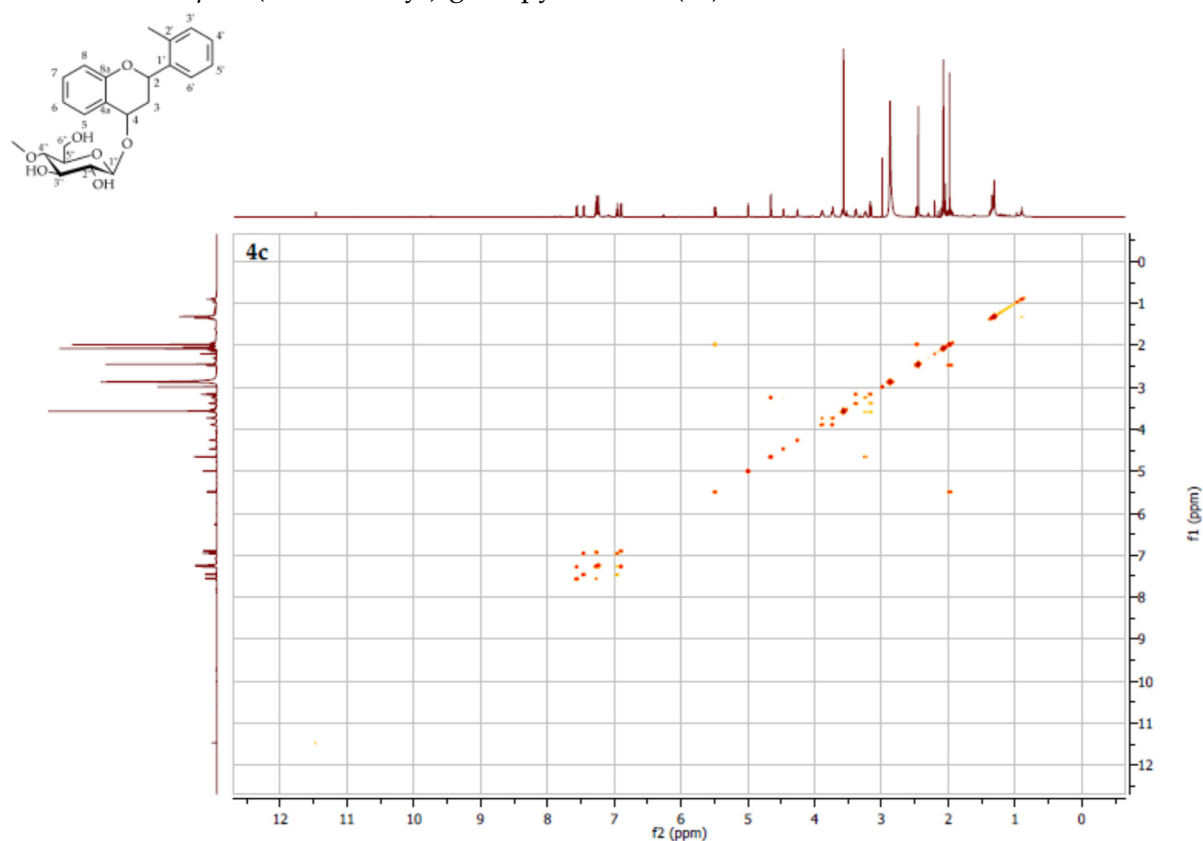


Figure S60. COSY contour map – $^1\text{H} \times ^1\text{H}$ of 2-(2'-methylphenyl)-chromane 4- O - β -D-(4''- O -methyl)-glucopyranoside (**4c**)

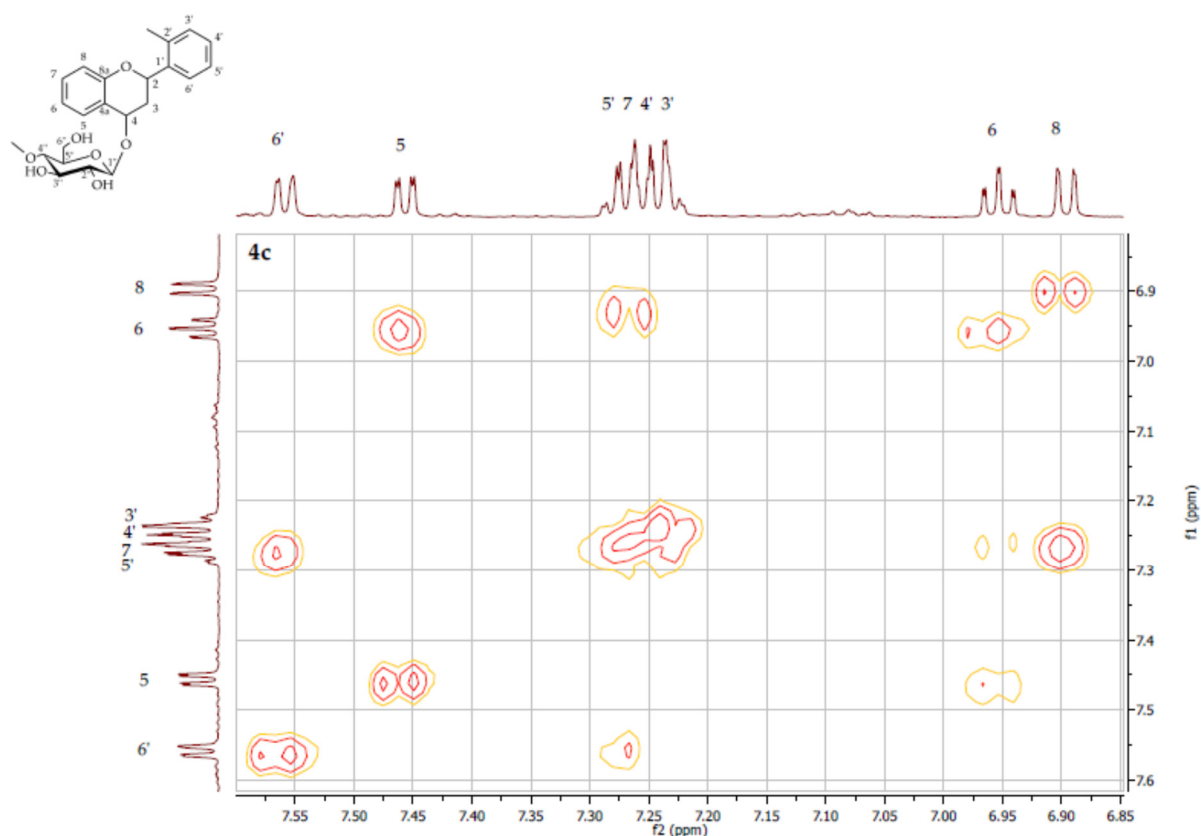


Figure S61. COSY contour map – ¹H x ¹H expansion of of 2-(2'-methylphenyl)-chromane 4-O-β-D-(4''-O-methyl)-glucopyranoside (**4c**)

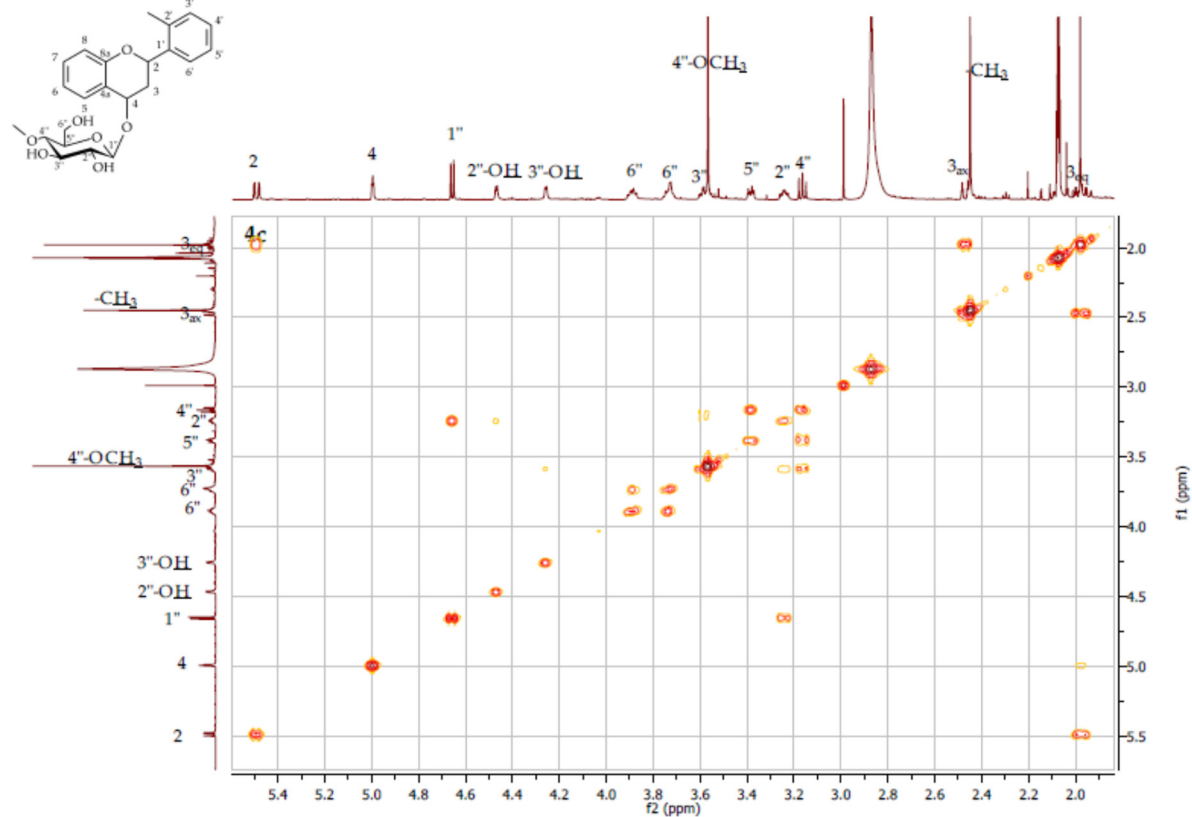


Figure S62. COSY contour map – ¹H x ¹H expansion of of 2-(2'-methylphenyl)-chromane 4-O-β-D-(4''-O-methyl)-glucopyranoside (**4c**)

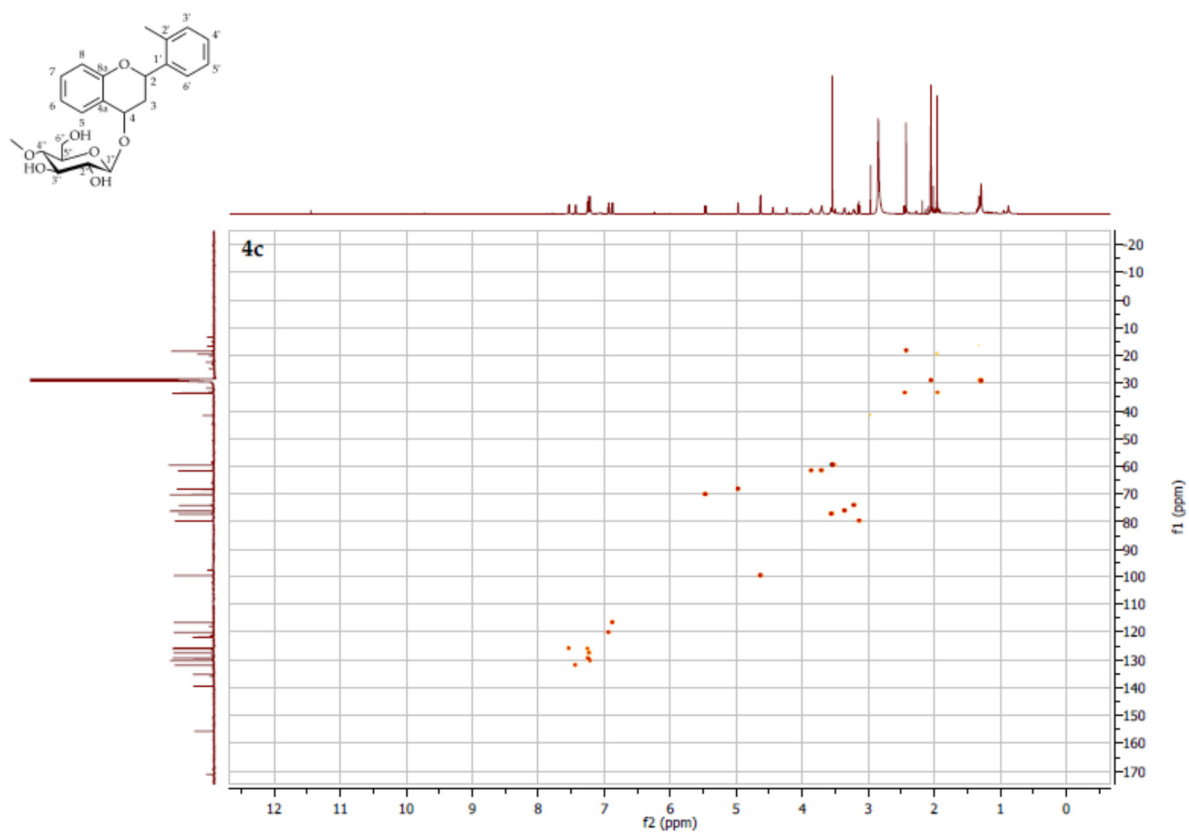


Figure S63. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2-(2'-methylphenyl)-chromane 4-O- β -D-(4''-O-methyl)-glucopyranoside (**4c**)

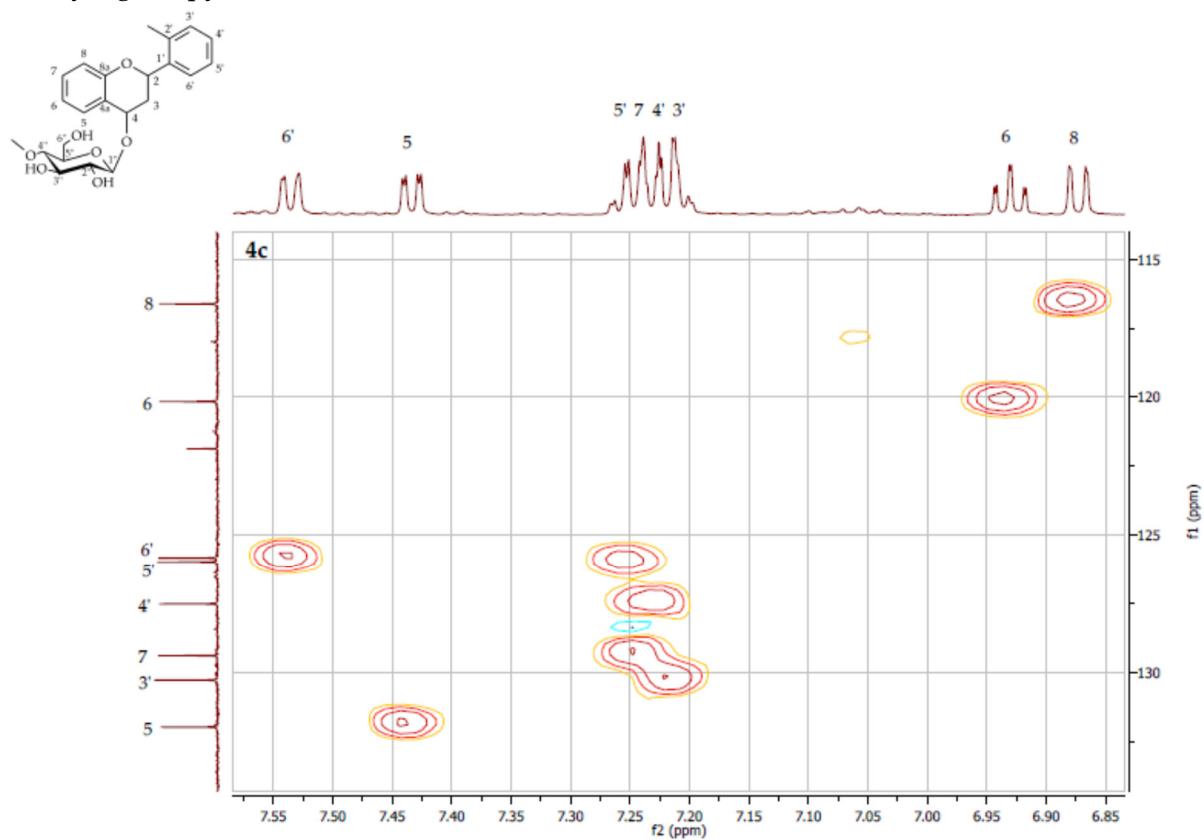


Figure S64. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2-(2'-methylphenyl)-chromane 4-O- β -D-(4''-O-methyl)-glucopyranoside (**4c**)

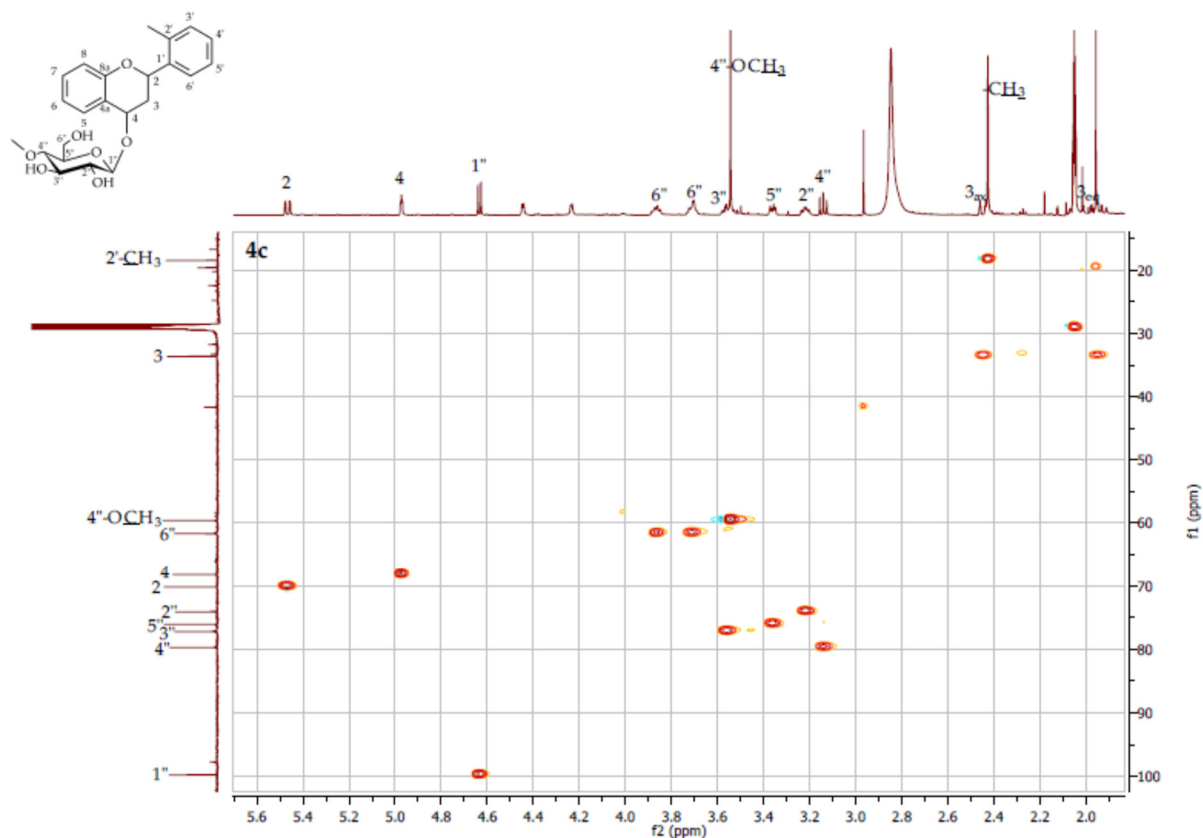


Figure S65. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2-(2'-methylphenyl)-chromane 4-O- β -D-(4''-O-methyl)-glucopyranoside (**4c**)

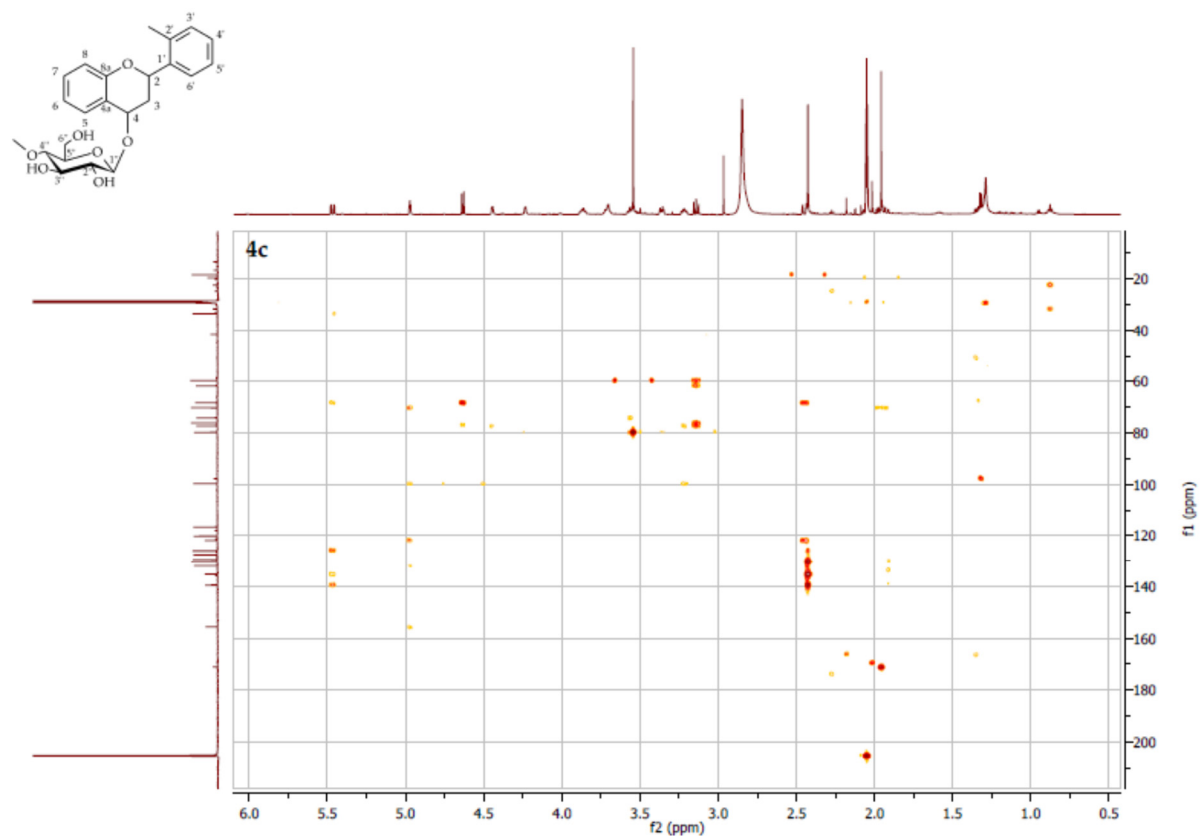


Figure S66. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2-(2'-methylphenyl)-chromane 4-O- β -D-(4''-O-methyl)-glucopyranoside (**4c**)

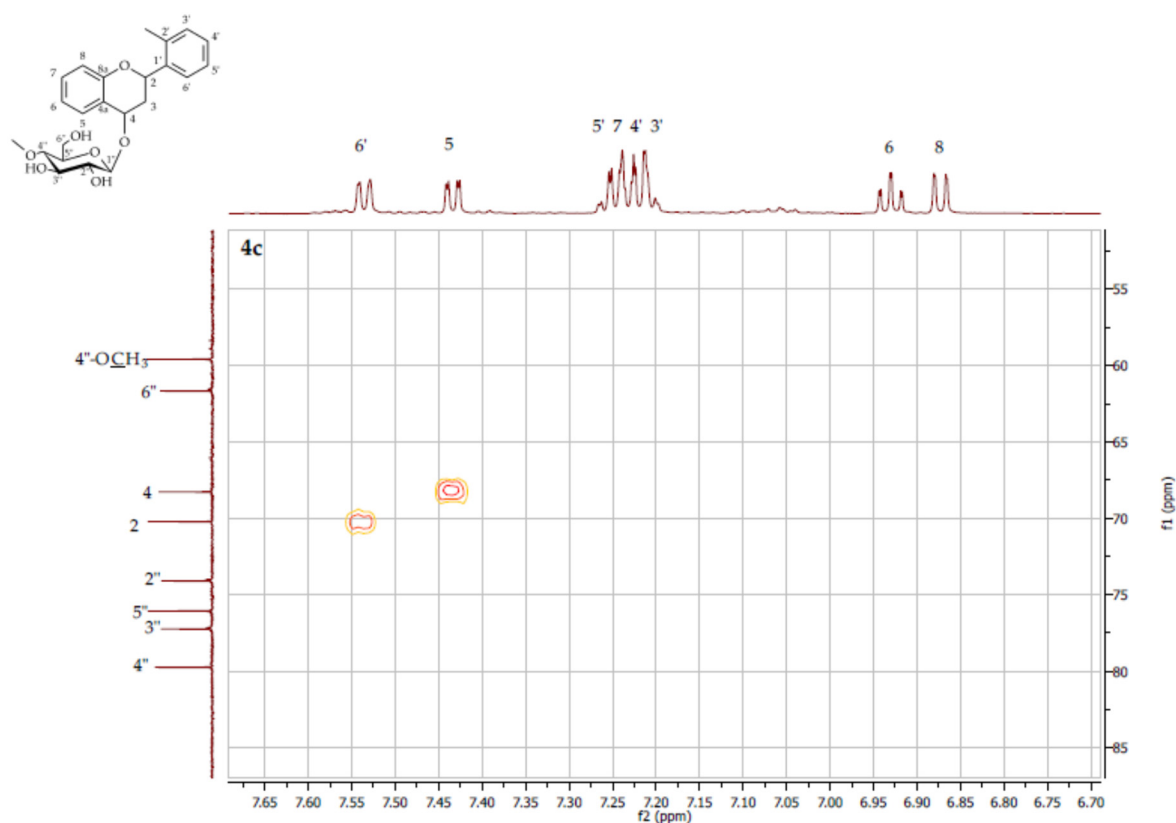


Figure S67. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2-(2'-methylphenyl)-chromane 4-O- β -D-(4''-O-methyl)-glucopyranoside (**4c**)

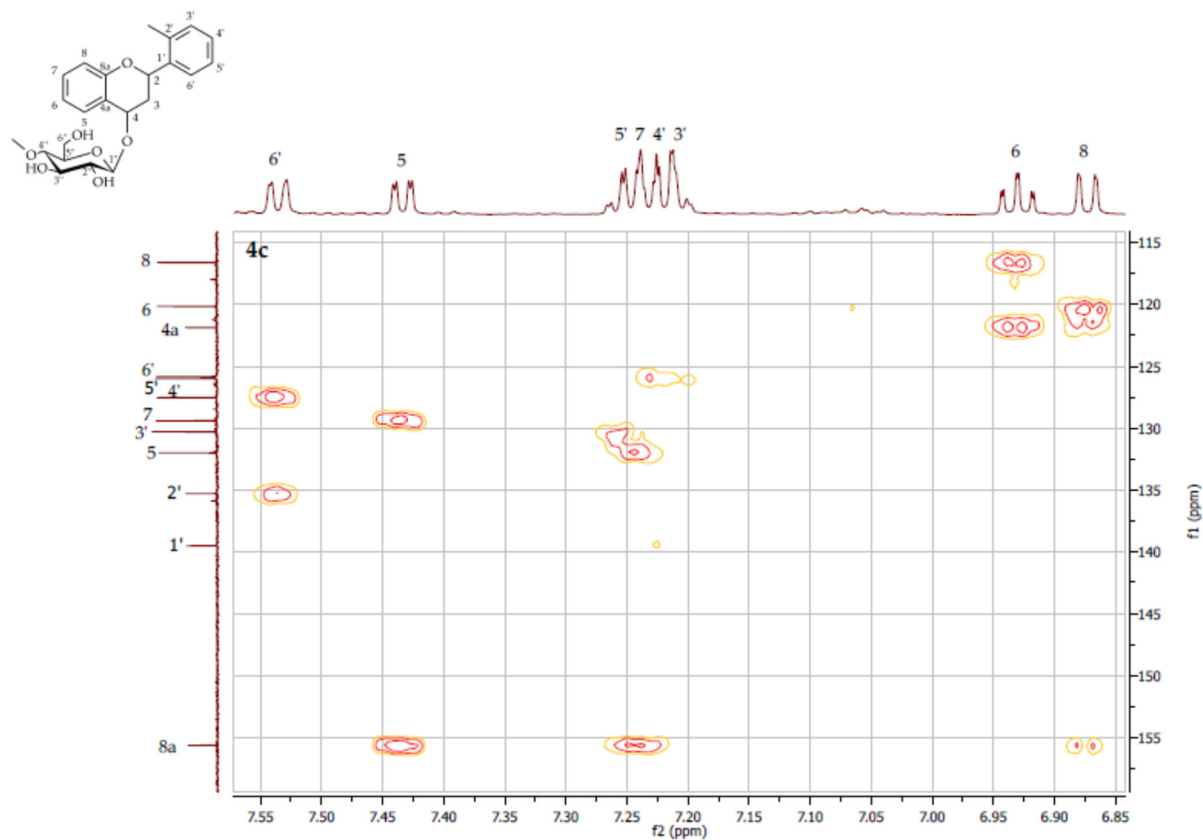


Figure S68. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2-(2'-methylphenyl)-chromane 4-O- β -D-(4''-O-methyl)-glucopyranoside (**4c**)

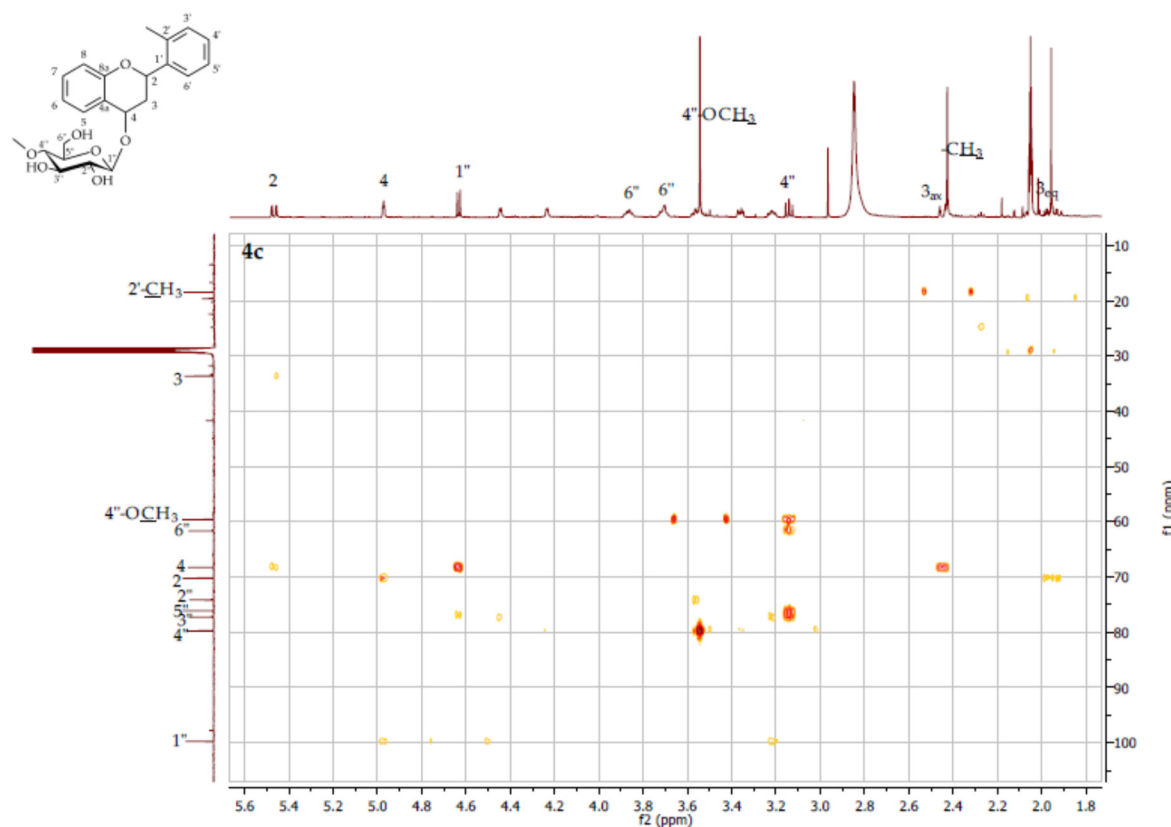


Figure S69. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2-(2'-methylphenyl)-chromane 4-O- β -D-(4''-O-methyl)-glucopyranoside (**4c**)

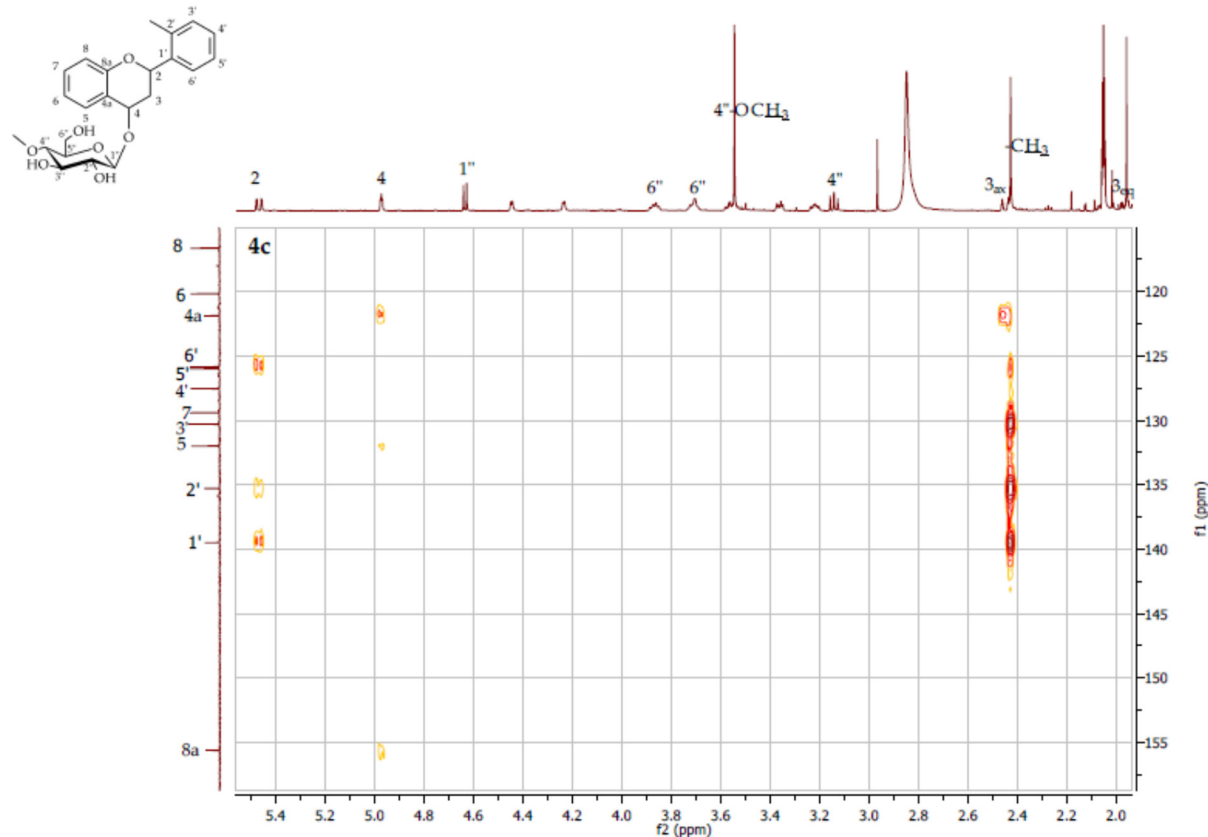


Figure S70. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2-(2'-methylphenyl)-chromane 4-O- β -D-(4''-O-methyl)-glucopyranoside (**4c**)

Molecular formula: C₂₃H₂₆O₈

Formula weight: 430.16

Ionization mode: positive

Precursor: [M + H]⁺ 431.20

431.2000>390.0500 CE: -8.0

431.2000>312.3000 CE: -23.0

431.2000>255.1000 CE: -15.0

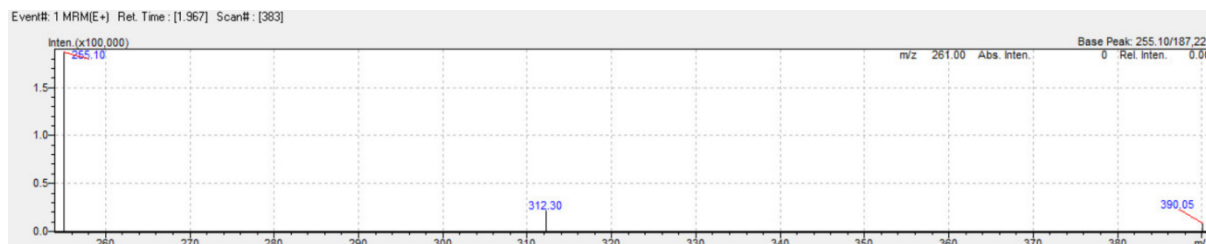
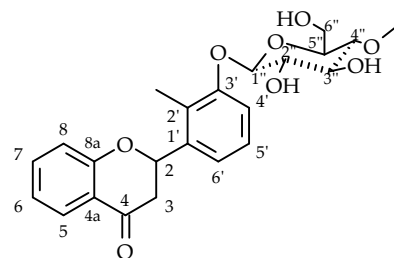


Figure S71. MS analysis of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**4d**)

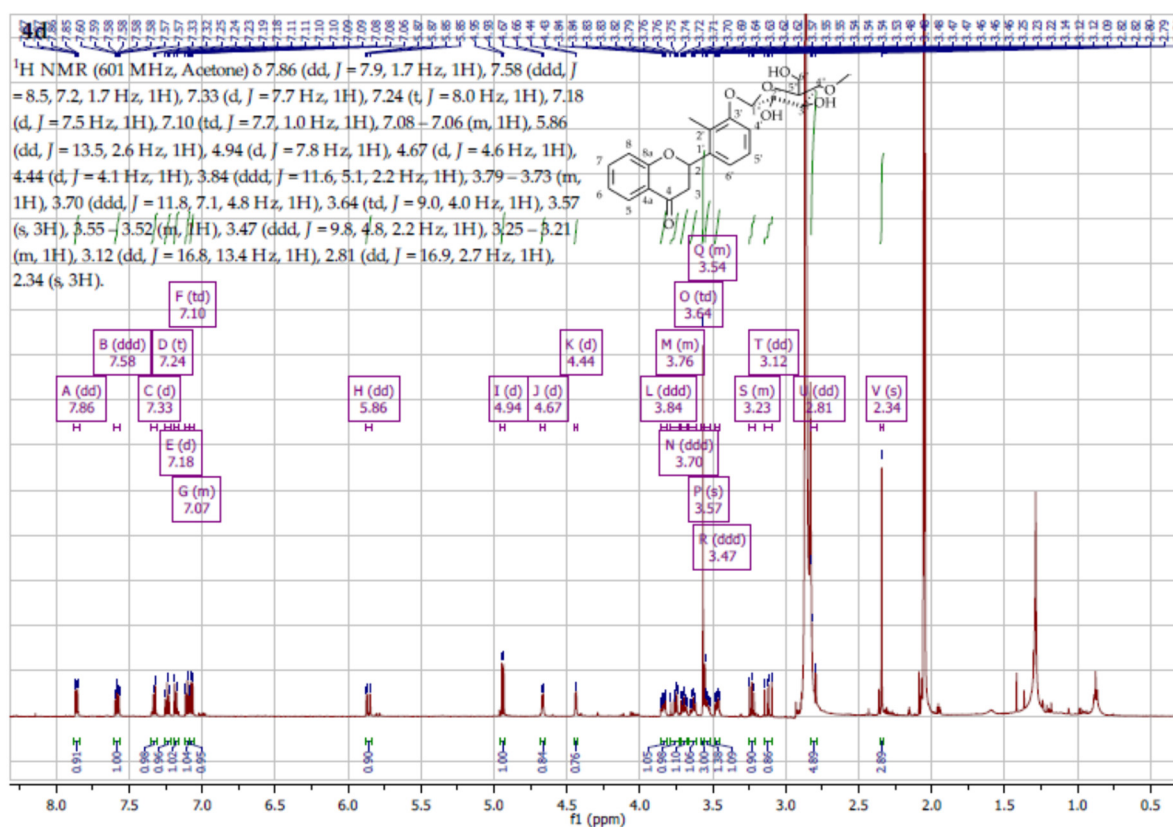


Figure S72. ¹H NMR spectrum (δ , acetone-d₆, 600 MHz) of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**4d**)

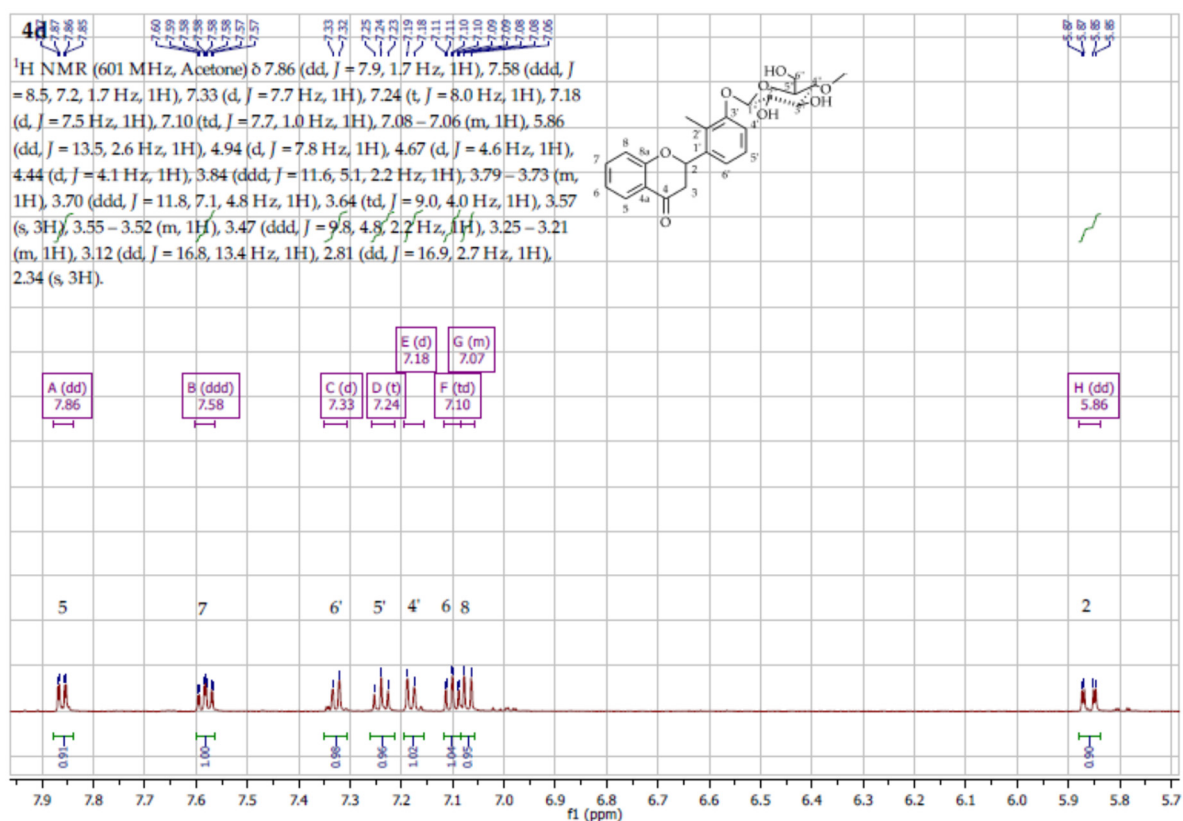


Figure S73. ¹H NMR spectrum expansion (δ, acetone-d₆, 600 MHz) of 2'-methylflavanone 3'-O-β-D-(4''-O-methyl)-glucopyranoside (**4d**)

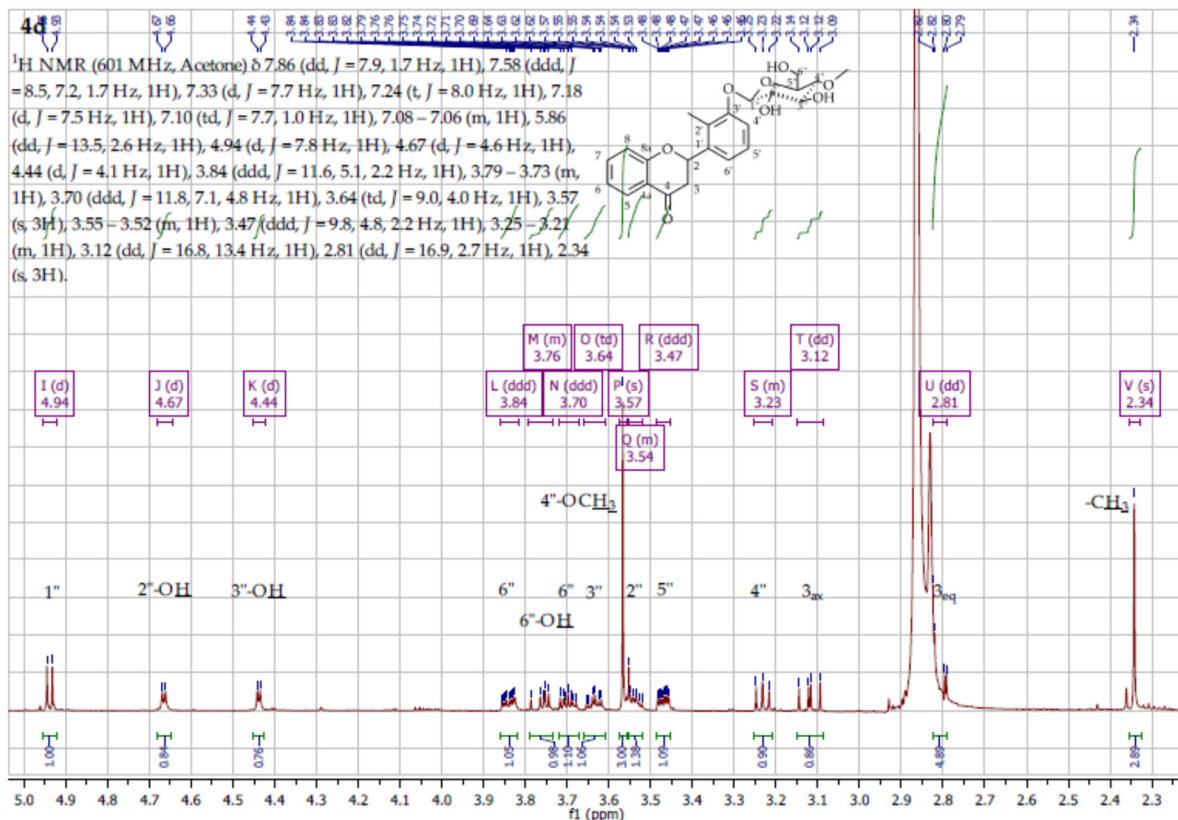


Figure S74. ¹H NMR spectrum expansion (δ, acetone-d₆, 600 MHz) of 2'-methylflavanone 3'-O-β-D-(4''-O-methyl)-glucopyranoside (**4d**)

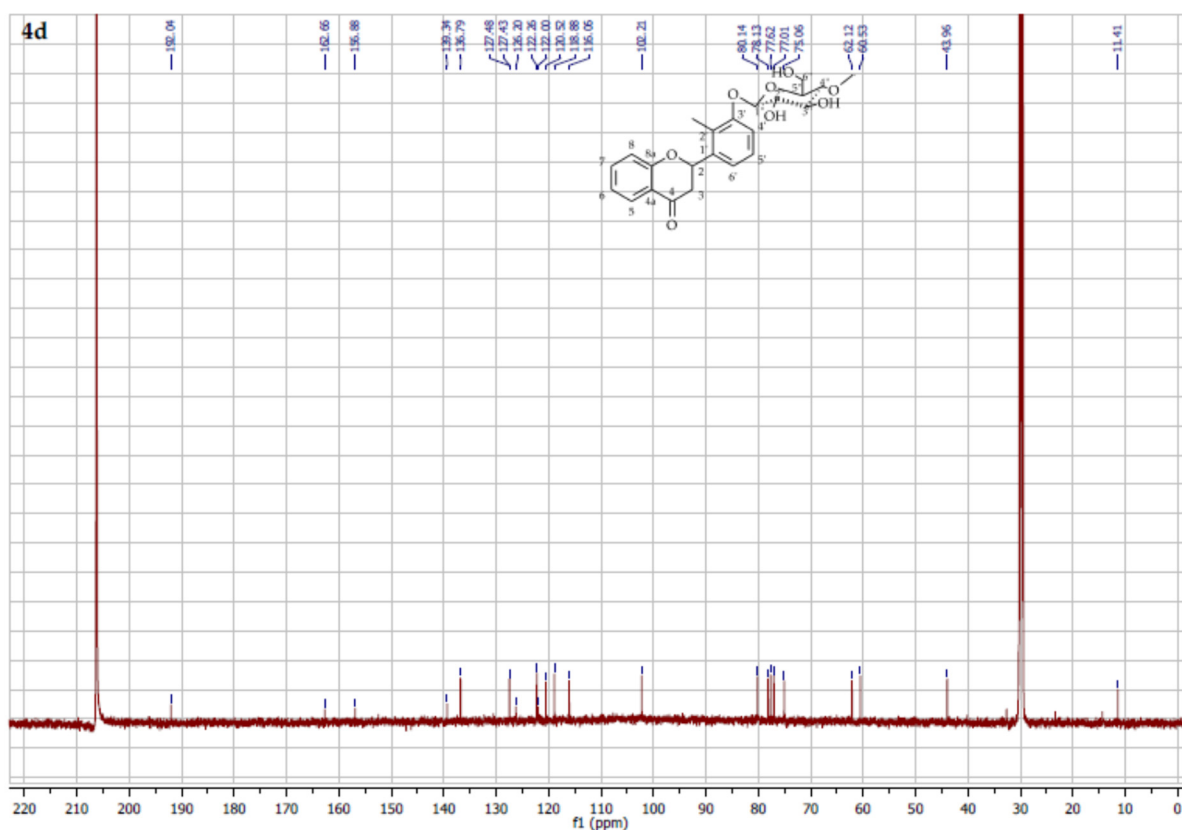


Figure S75. ^{13}C NMR spectrum (δ , acetone- d_6 , 151 MHz) of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**4d**)

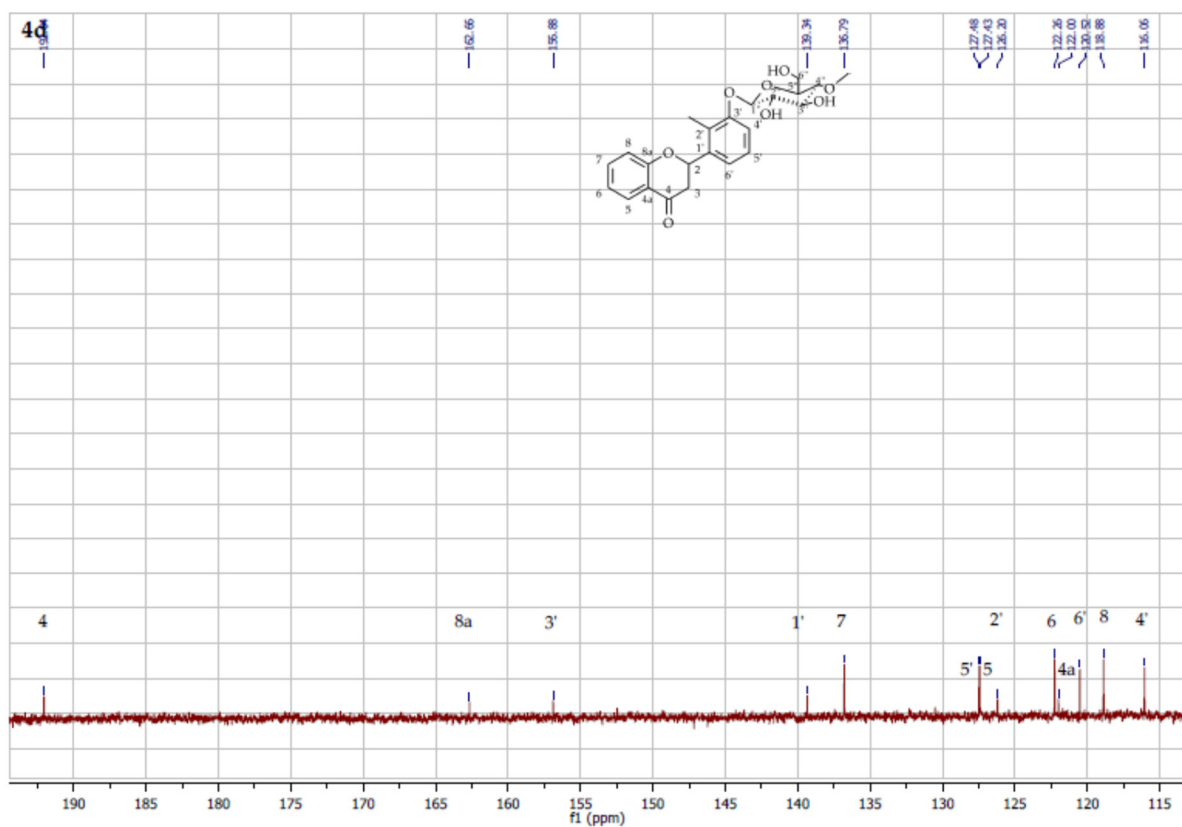


Figure S76. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**4d**)

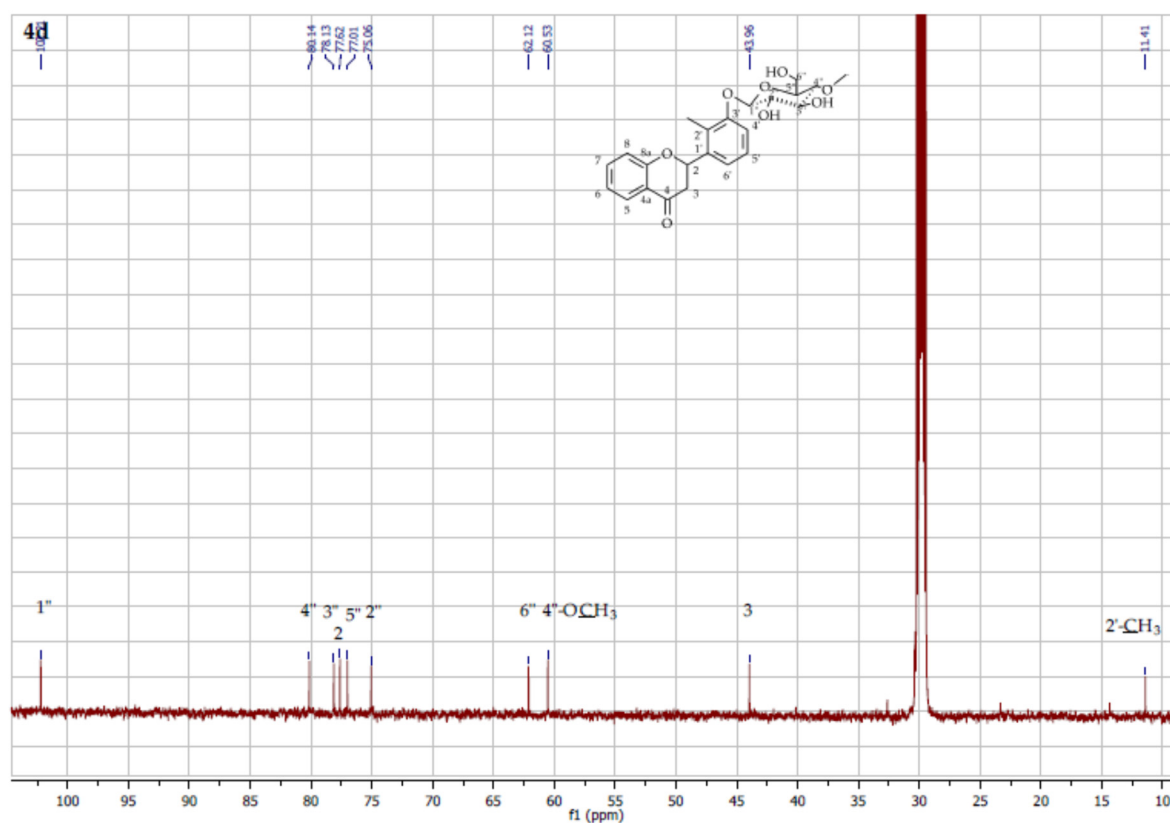


Figure S77. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavanone 3'- O - β -D-(4''- O -methyl)-glucopyranoside (**4d**)

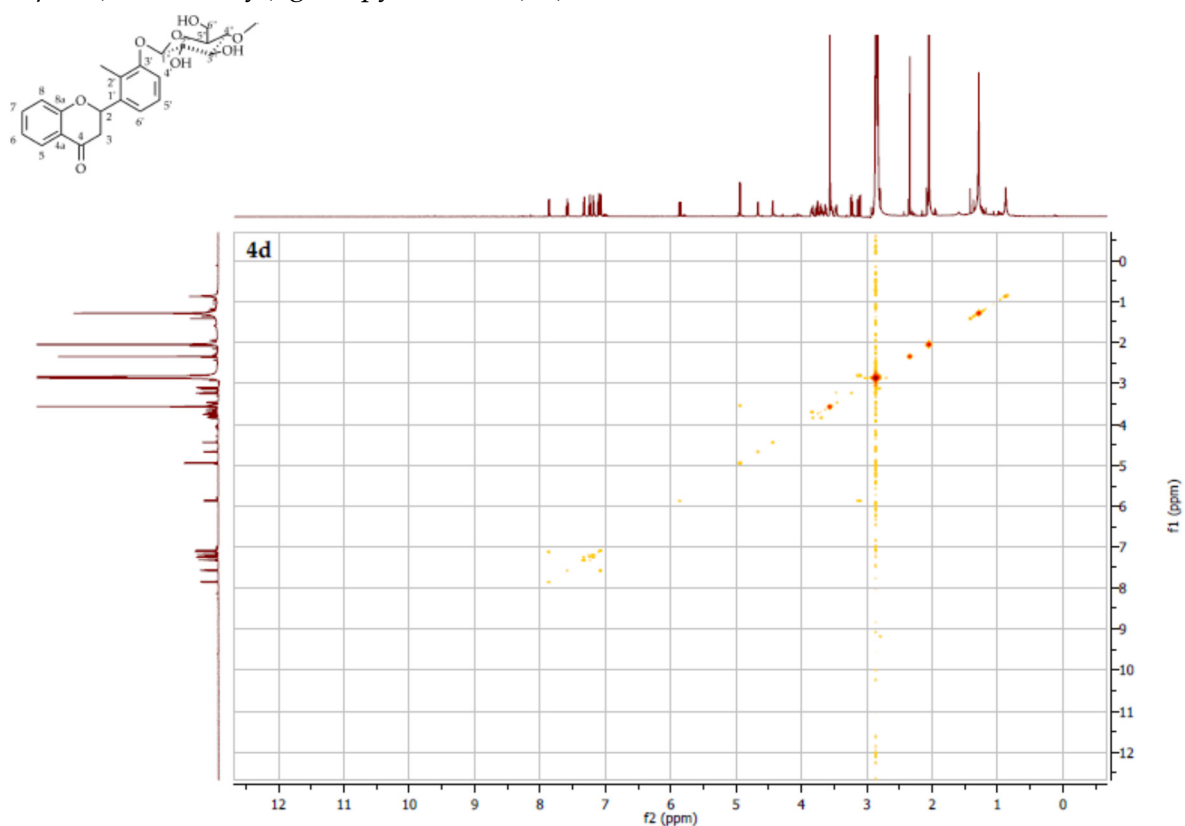


Figure S78. COSY contour map – $^1\text{H} \times ^1\text{H}$ of 2'-methylflavanone 3'- O - β -D-(4''- O -methyl)-glucopyranoside (**4d**)

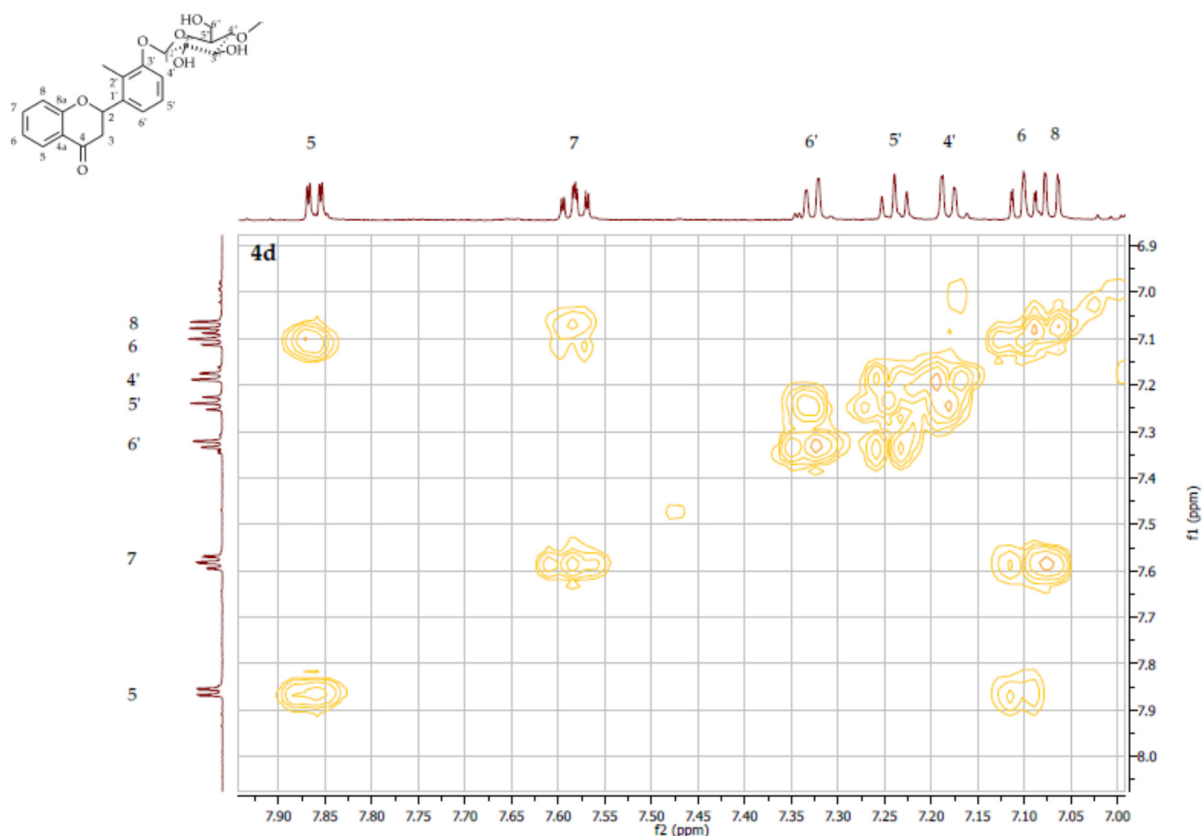


Figure S79. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**4d**)

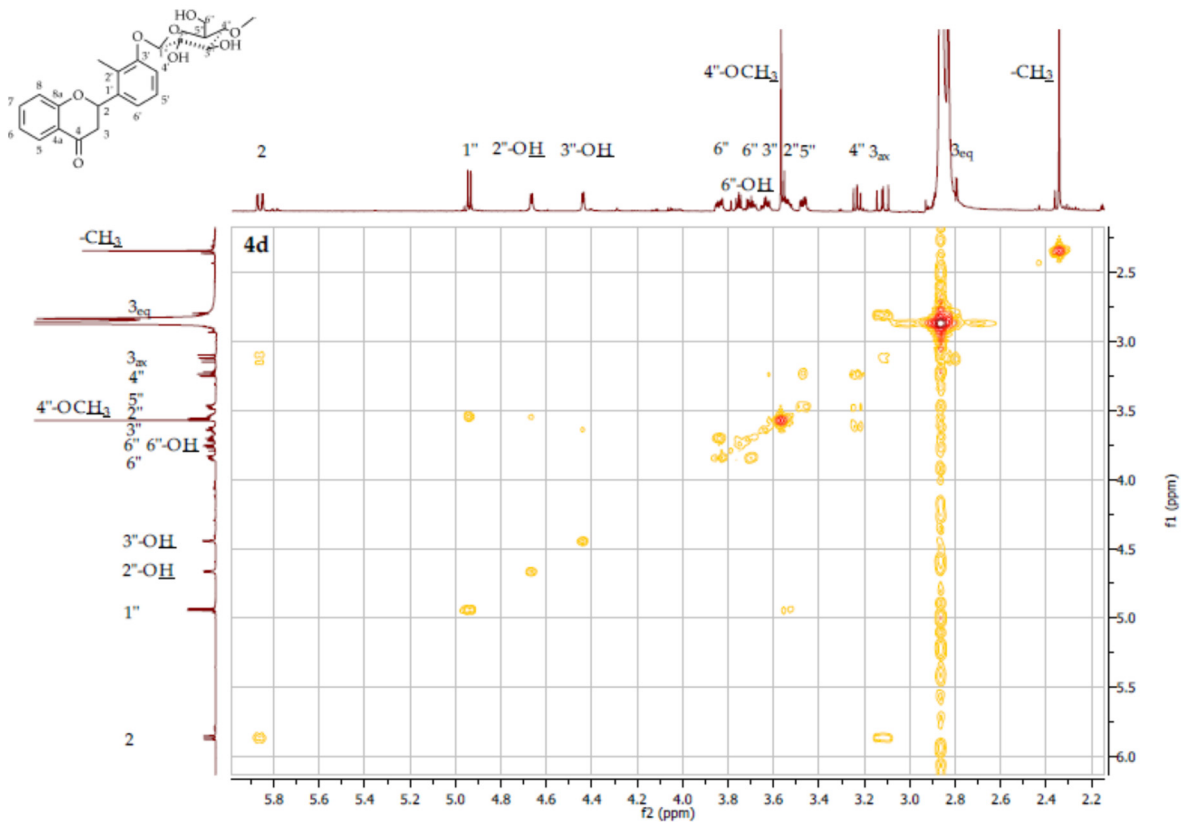


Figure S80. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**4d**)

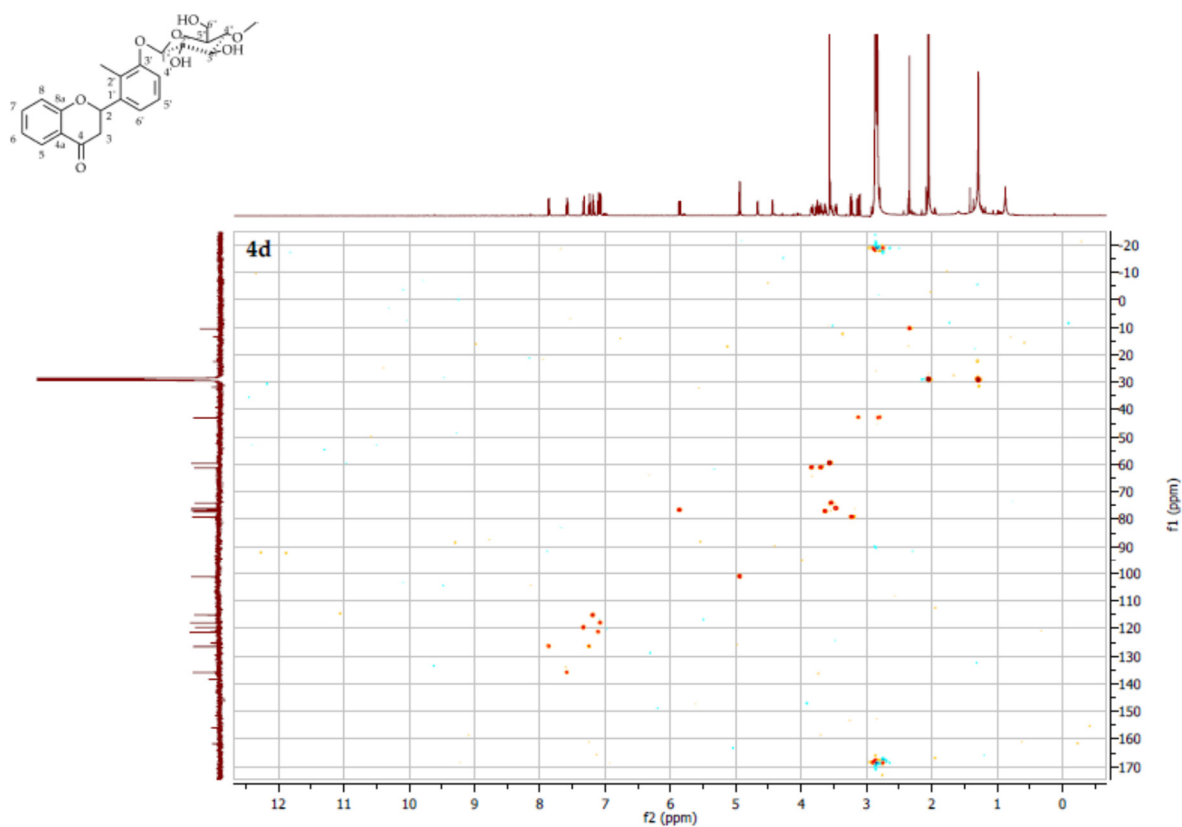


Figure S81. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**4d**)

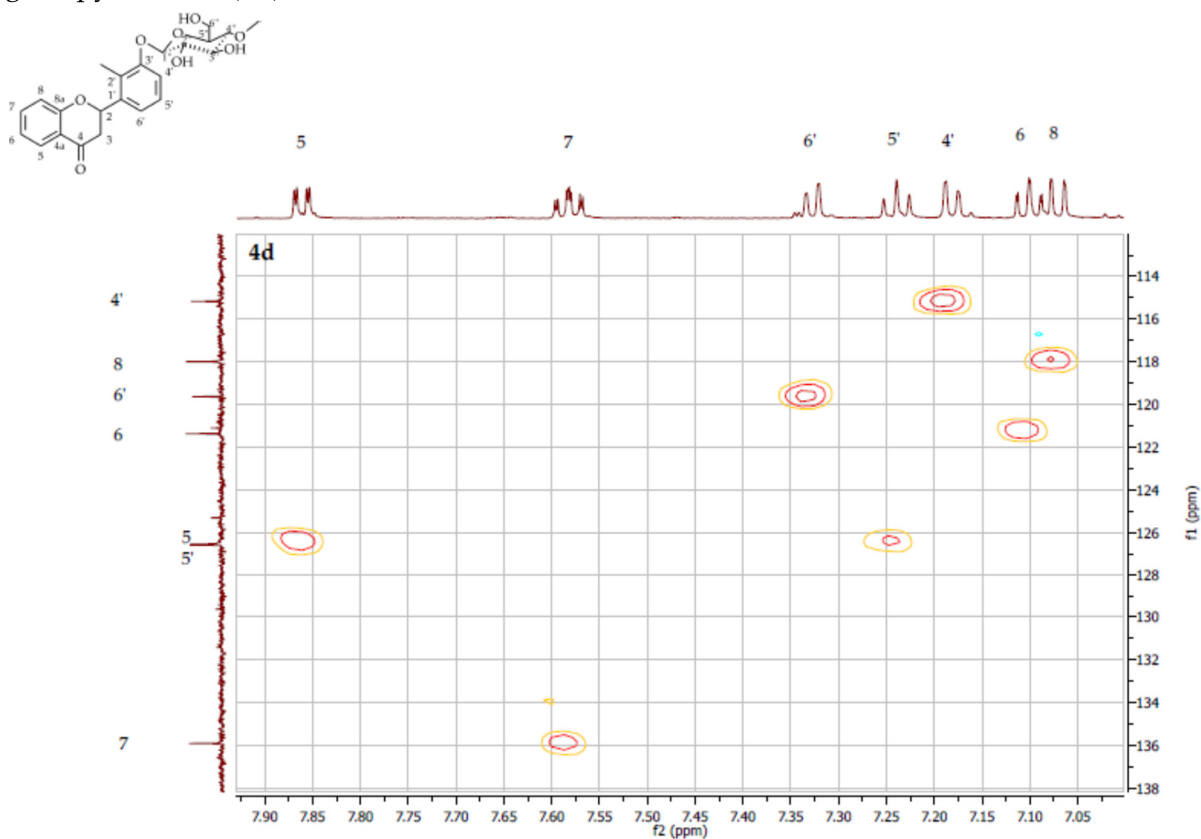


Figure S82. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**4d**)

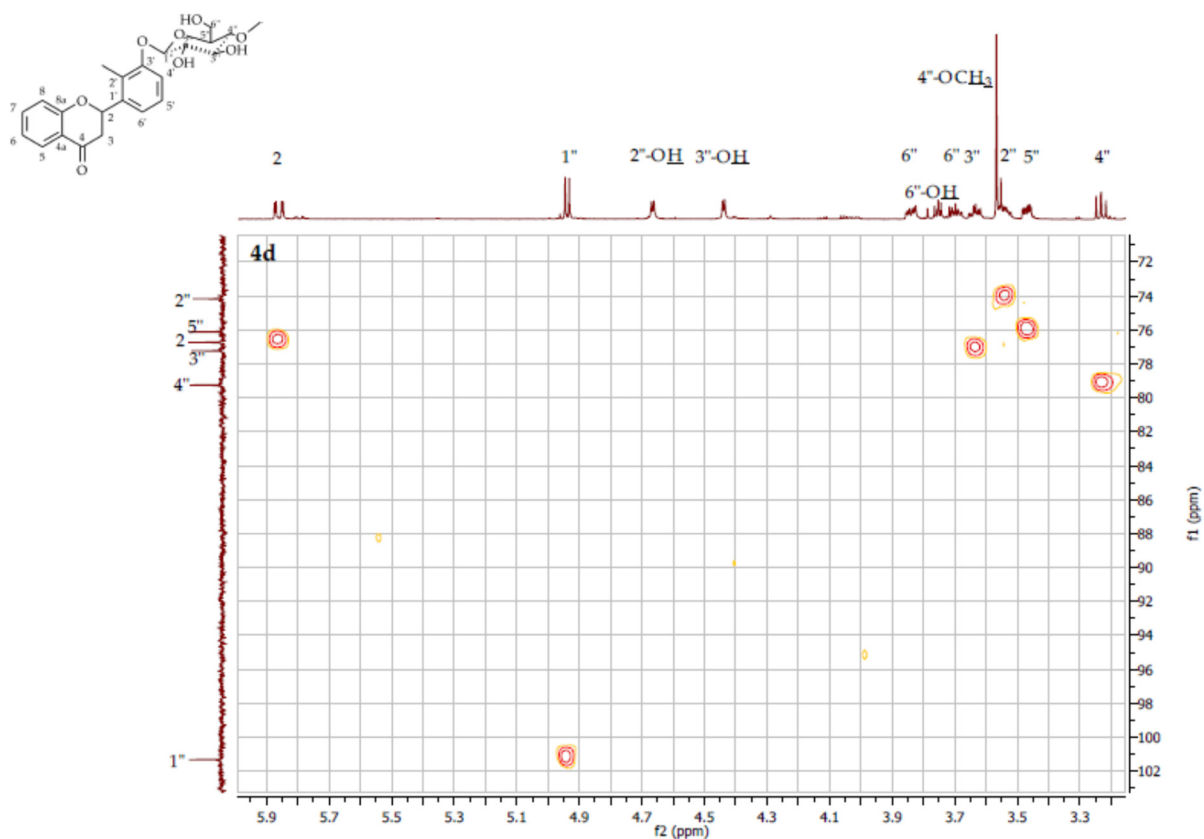


Figure S83. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (4d)

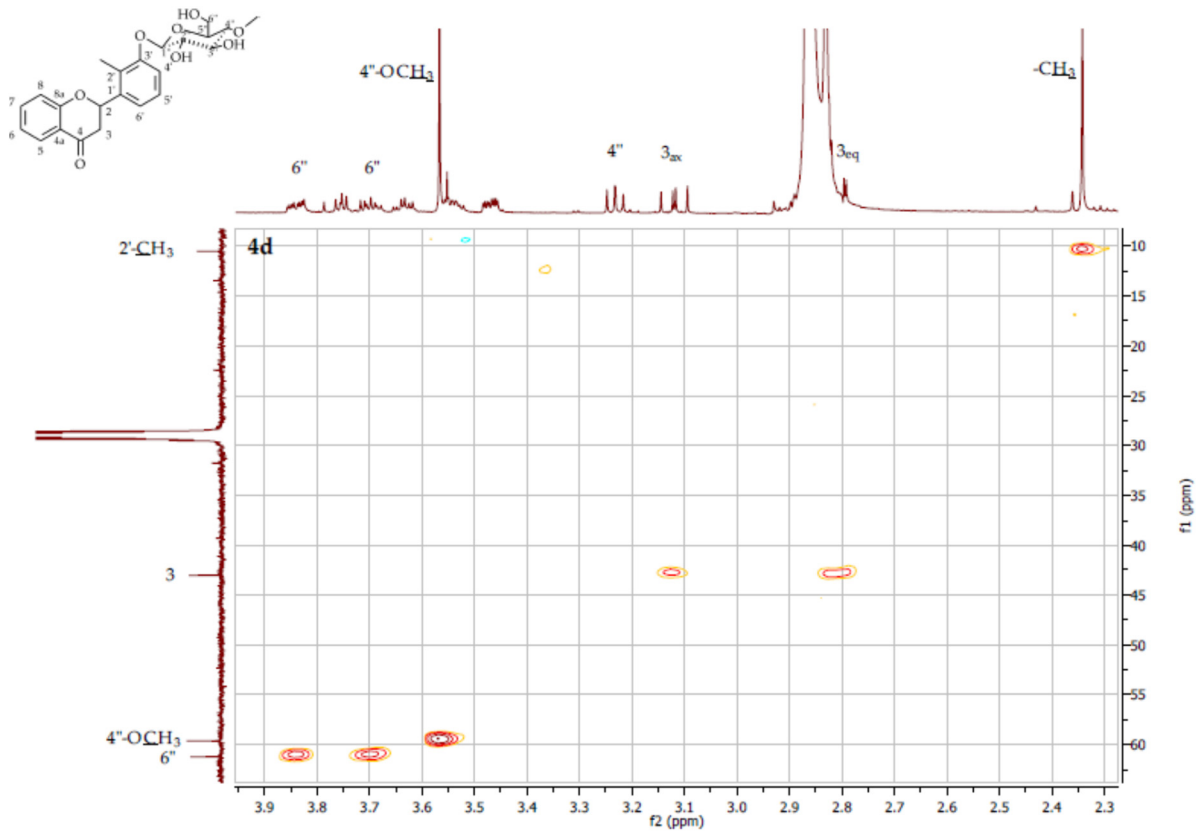


Figure S84. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (4d)

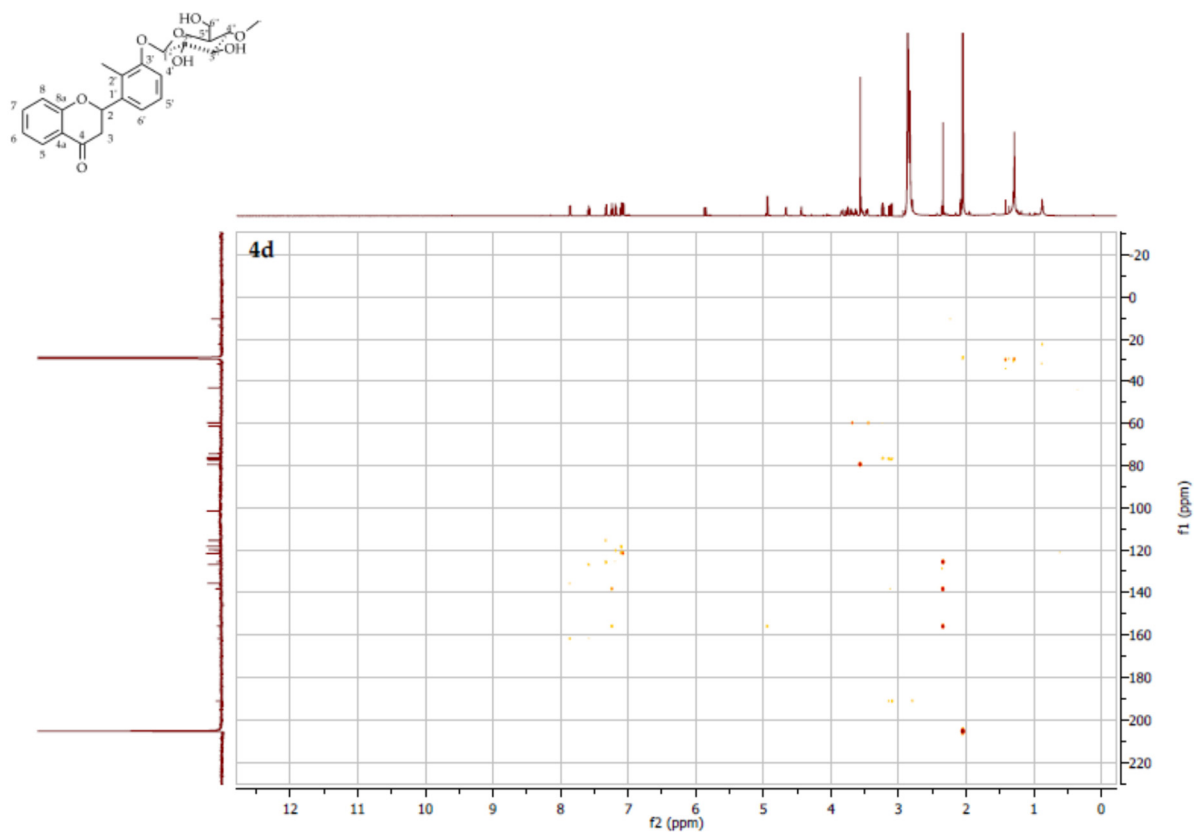


Figure S85. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**4d**)

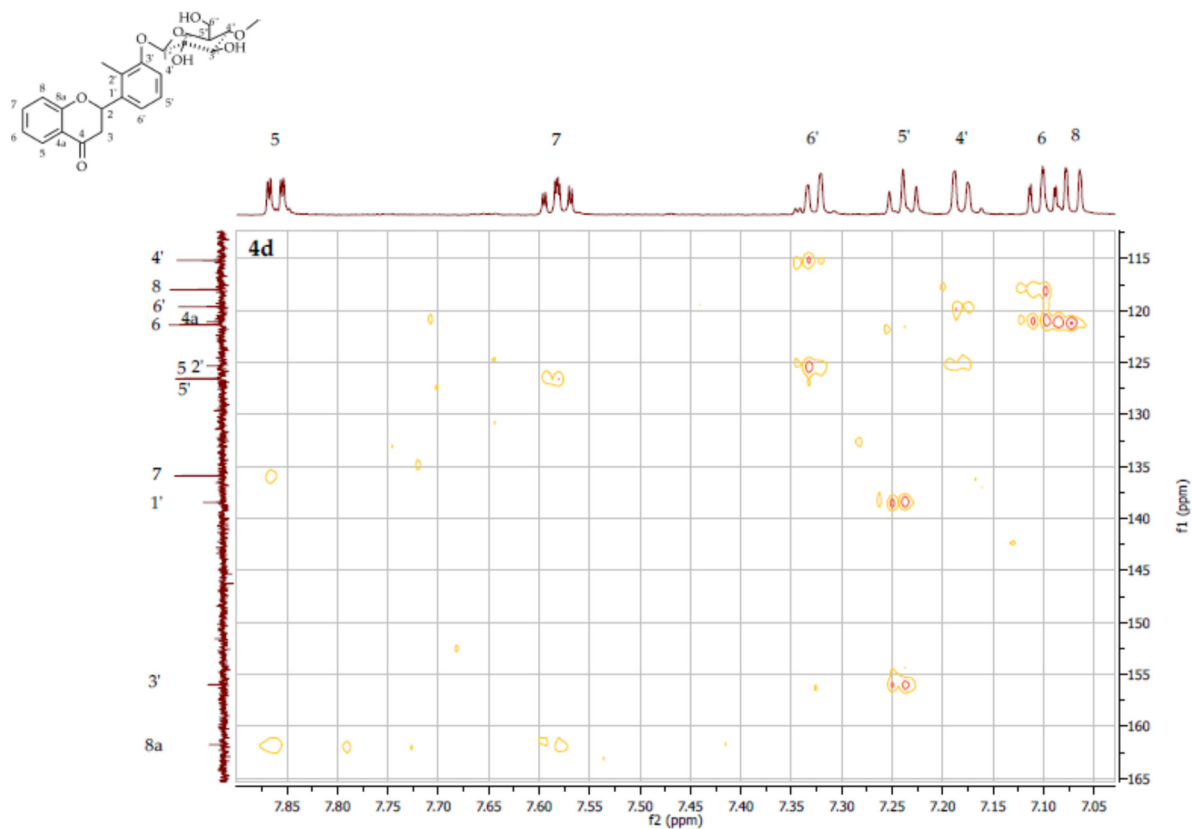


Figure S86. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**4d**)

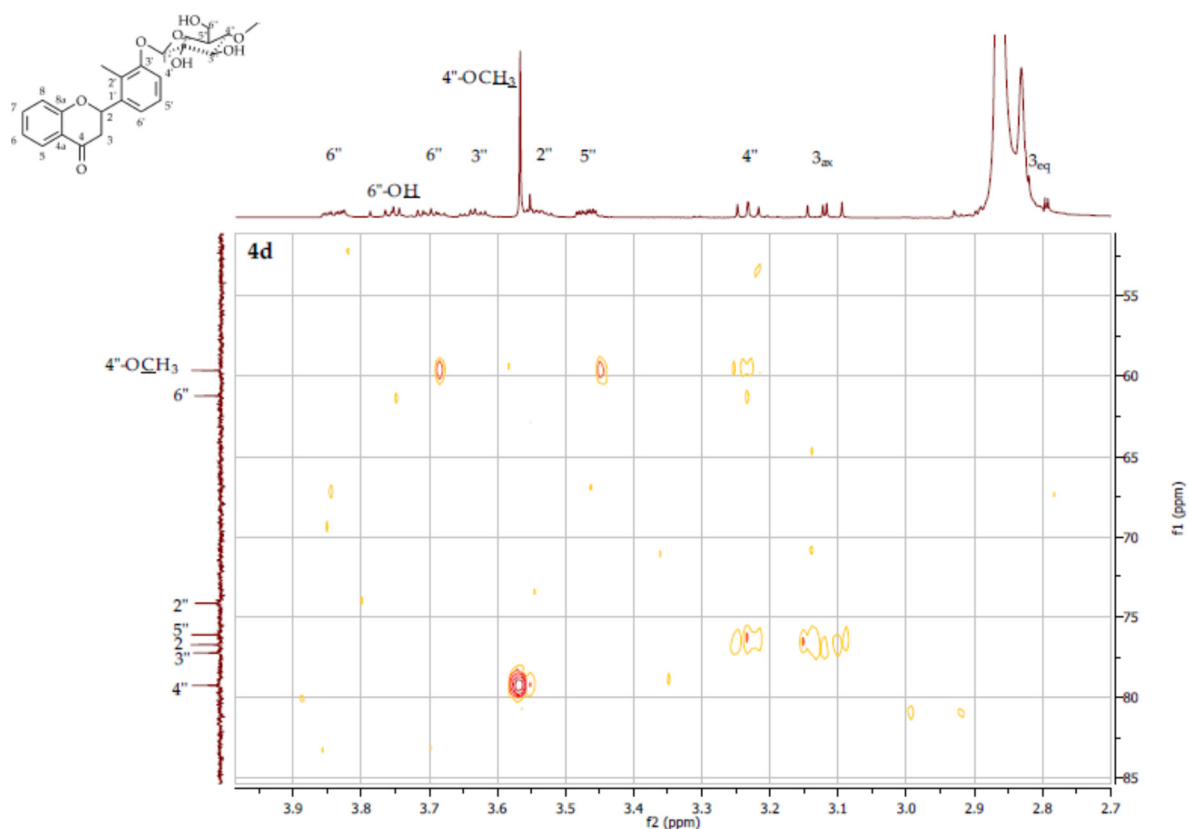


Figure S87. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (4d)

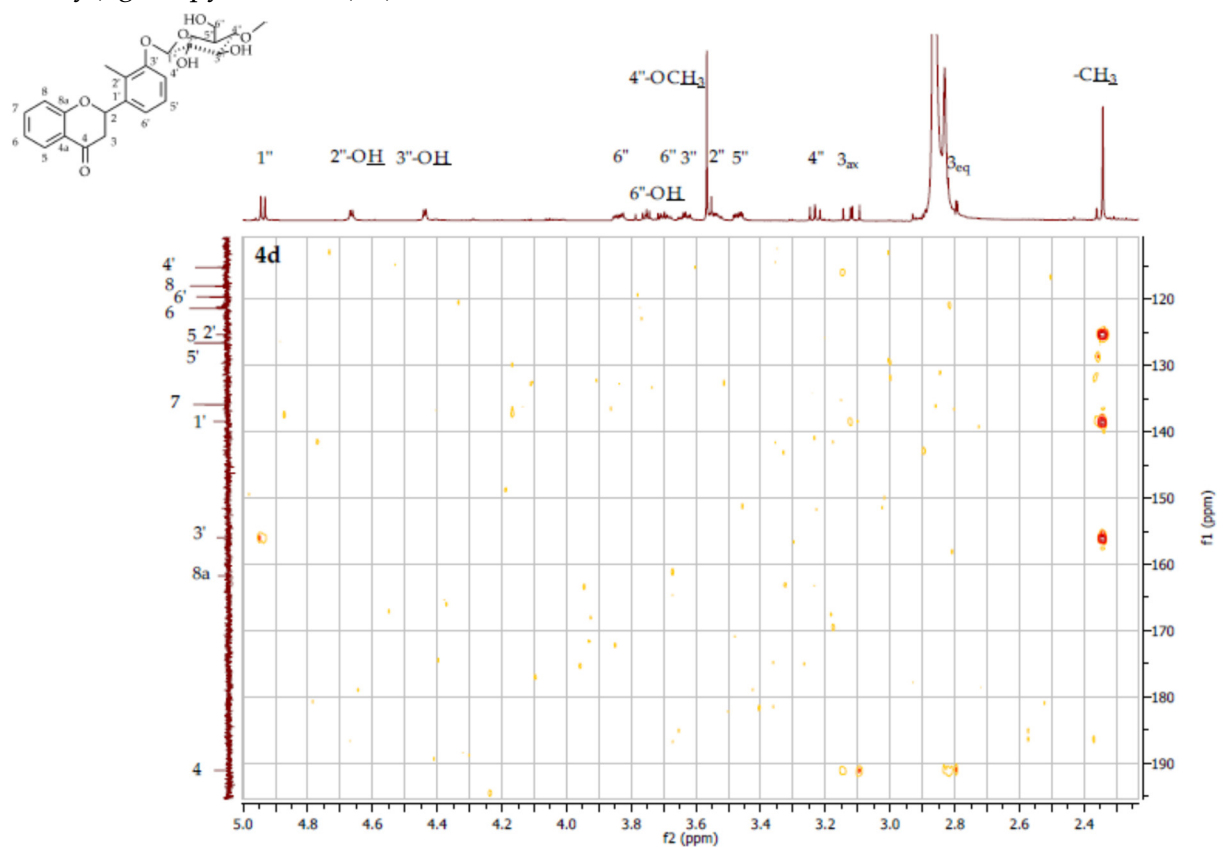


Figure S88. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavanone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (4d)

Molecular formula: C₁₅H₂₀O₈

Formula weight: 328.12

Ionization mode: negative

Precursor: [M - H]⁻ 327.40

327.4000>151.1000 CE: 15.0

327.4000>150.1000 CE: 27.0

327.4000>108.0500 CE: 33.0

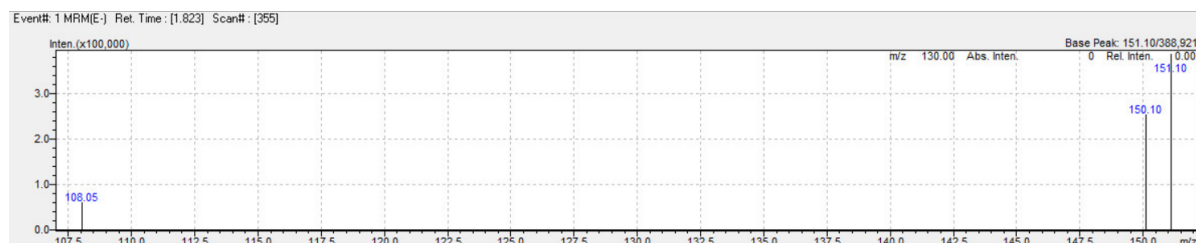
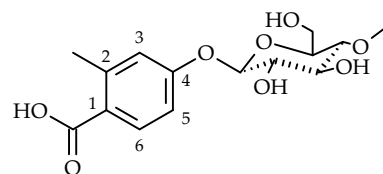


Figure S89. MS analysis of 2-methylbenzoic acid 4-*O*- β -D-(4'-*O*-methyl)-glucopyranoside (**4e**)

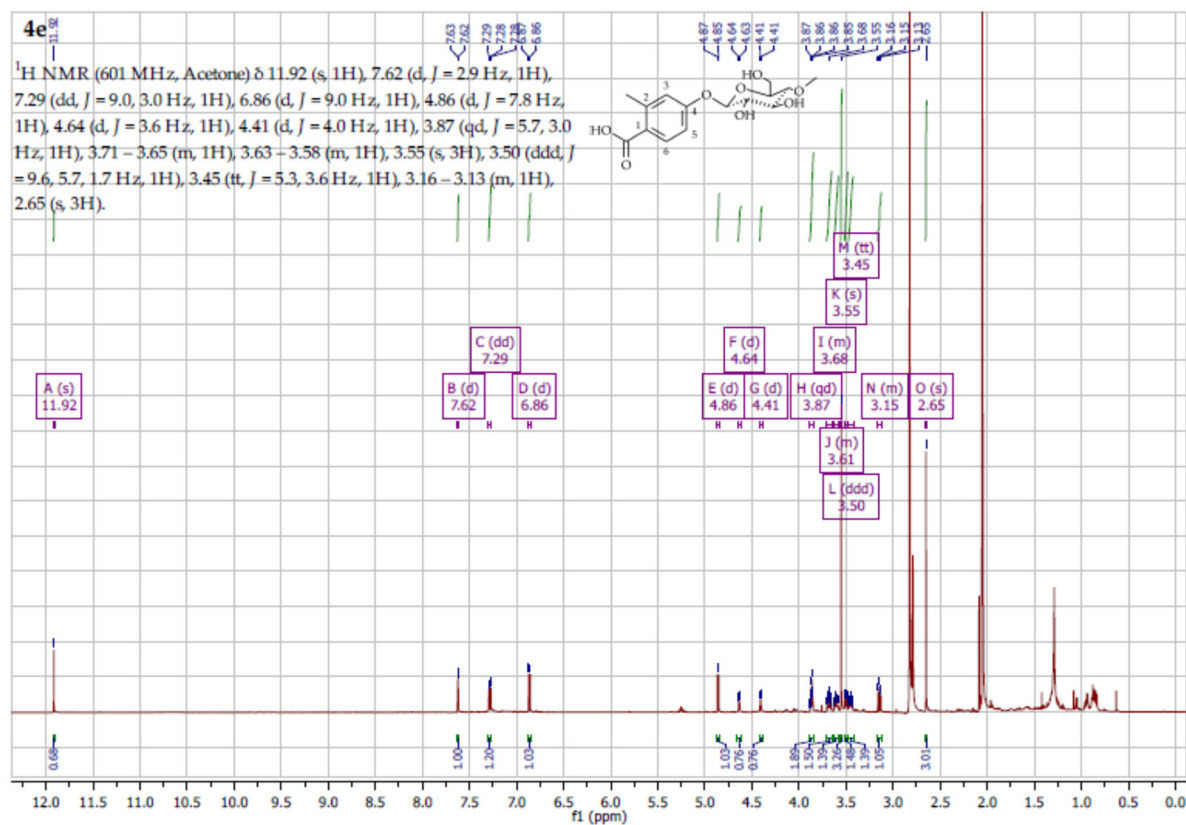


Figure S90. ¹H NMR spectrum (δ , acetone-*d*₆, 600 MHz) of 2-methylbenzoic acid 4-*O*- β -D-(4'-*O*-methyl)-glucopyranoside (**4e**)

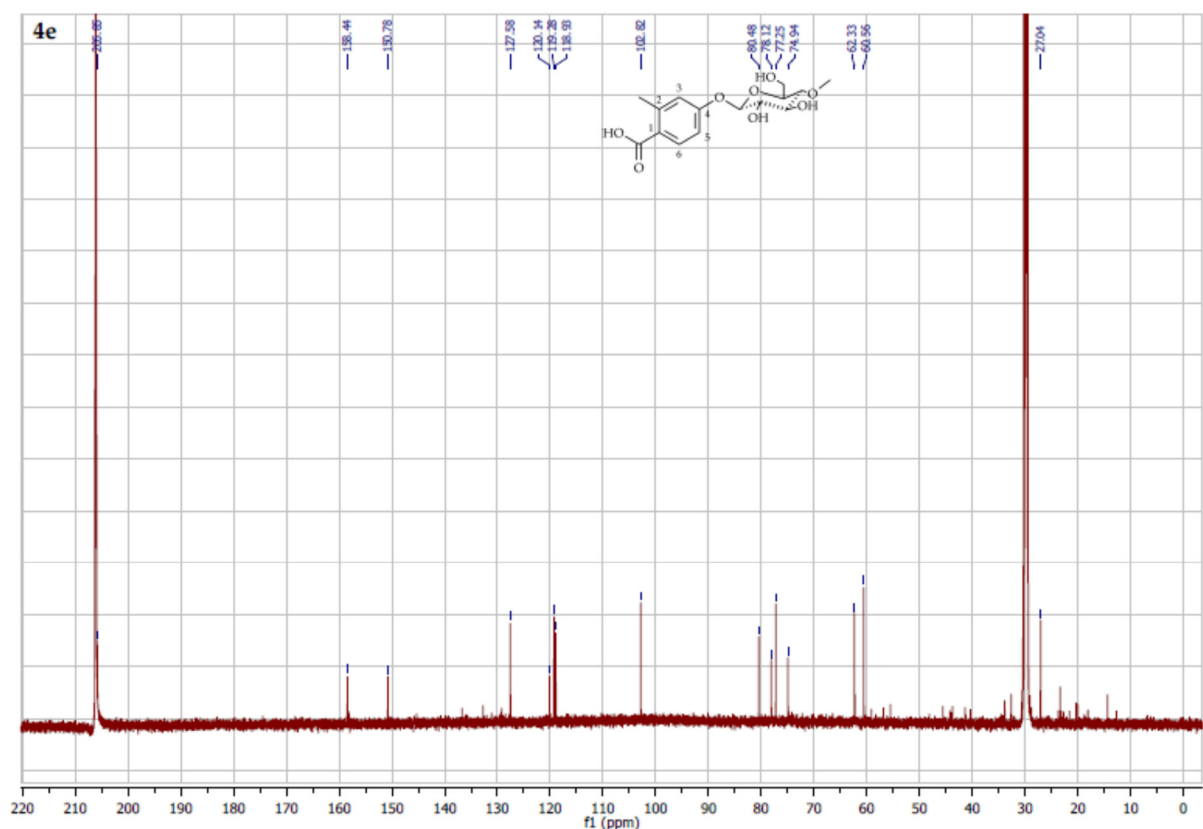


Figure S93. ^{13}C NMR spectrum (δ , acetone- d_6 , 151 MHz) of 2-methylbenzoic acid 4-O- β -D-(4'-O-methyl)-glucopyranoside (**4e**)

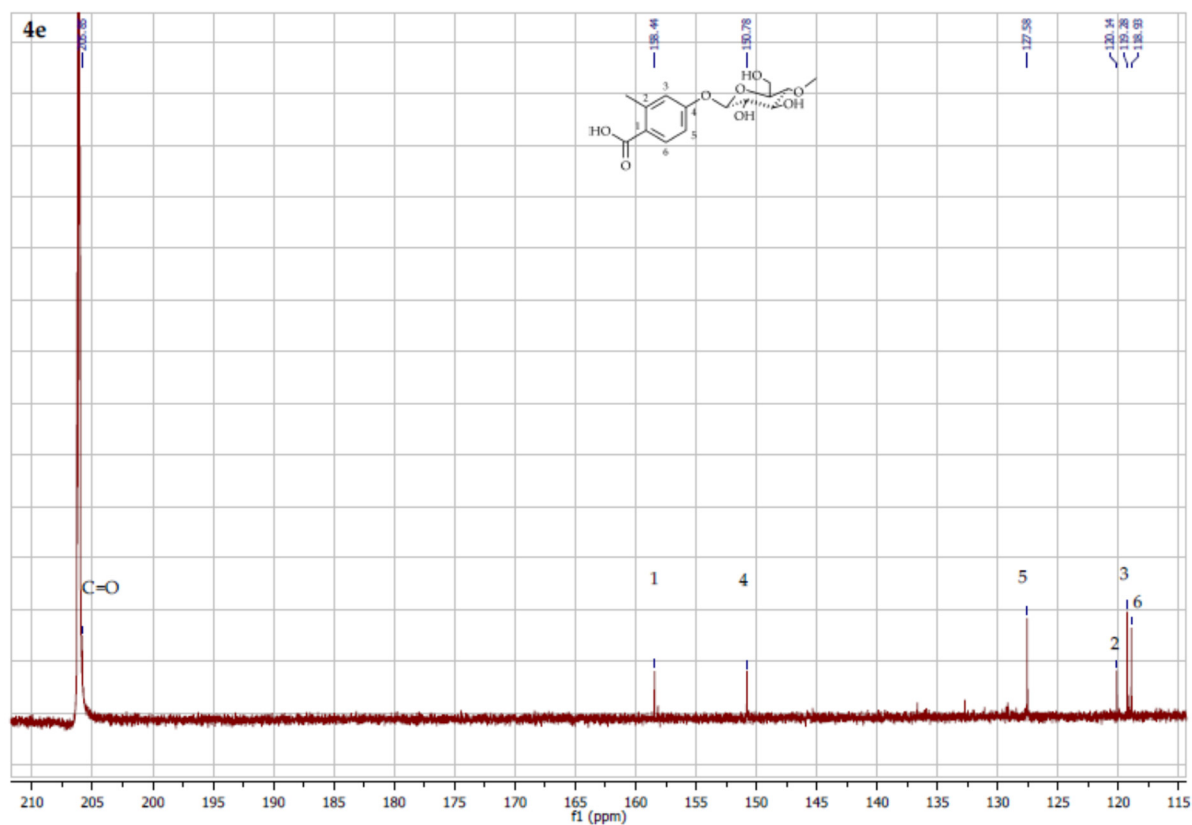


Figure S94. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2-methylbenzoic acid 4-O- β -D-(4'-O-methyl)-glucopyranoside (**4e**)

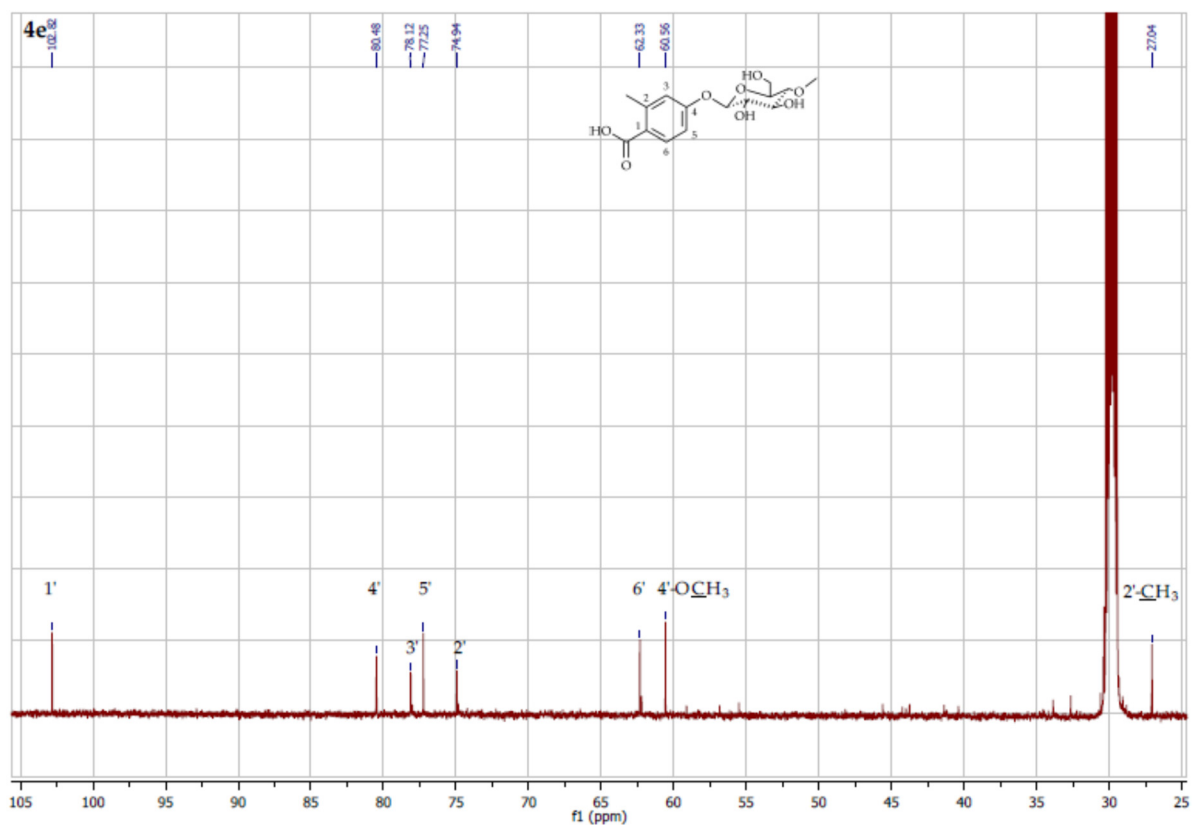


Figure S95. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2-methylbenzoic acid 4-O- β -D-(4'-O-methyl)-glucopyranoside (**4e**)

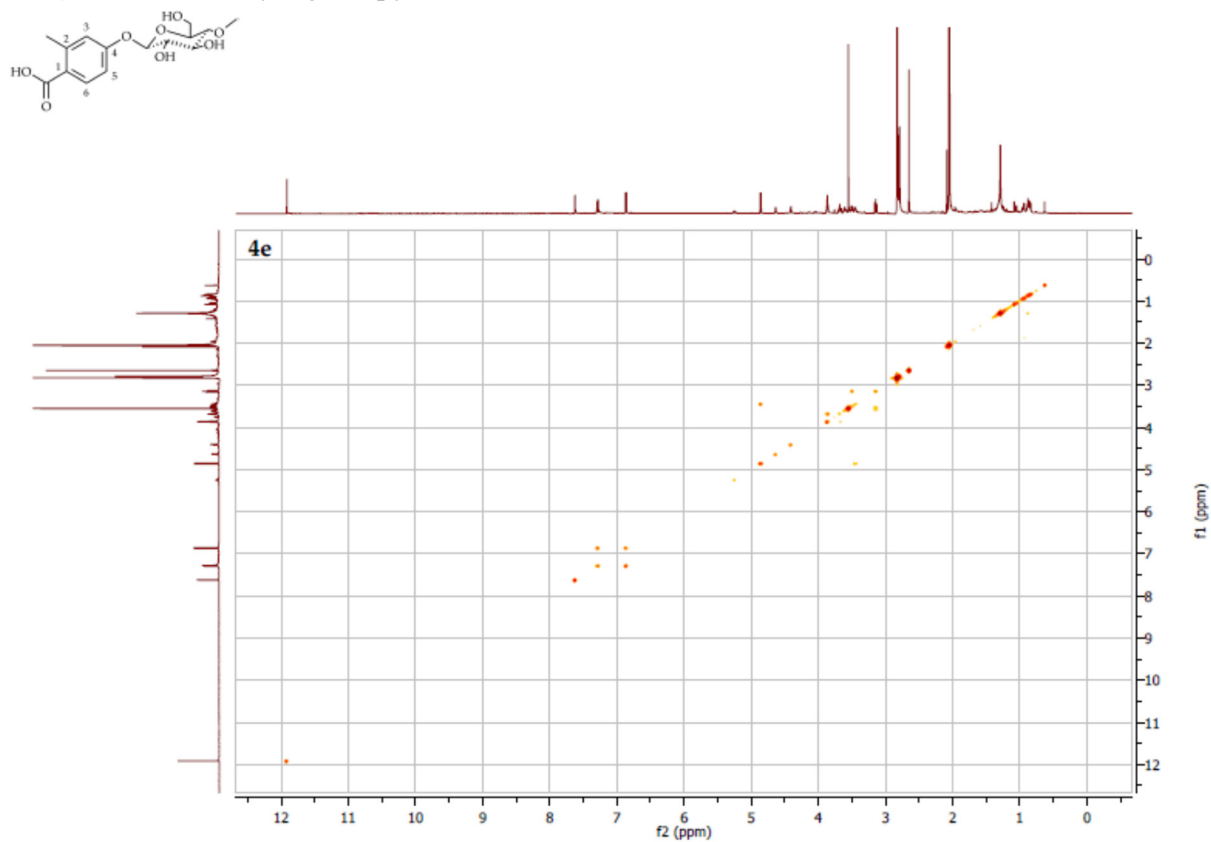


Figure S96. COSY contour map – $^1\text{H} \times ^1\text{H}$ of 2-methylbenzoic acid 4-O- β -D-(4'-O-methyl)-glucopyranoside (**4e**)

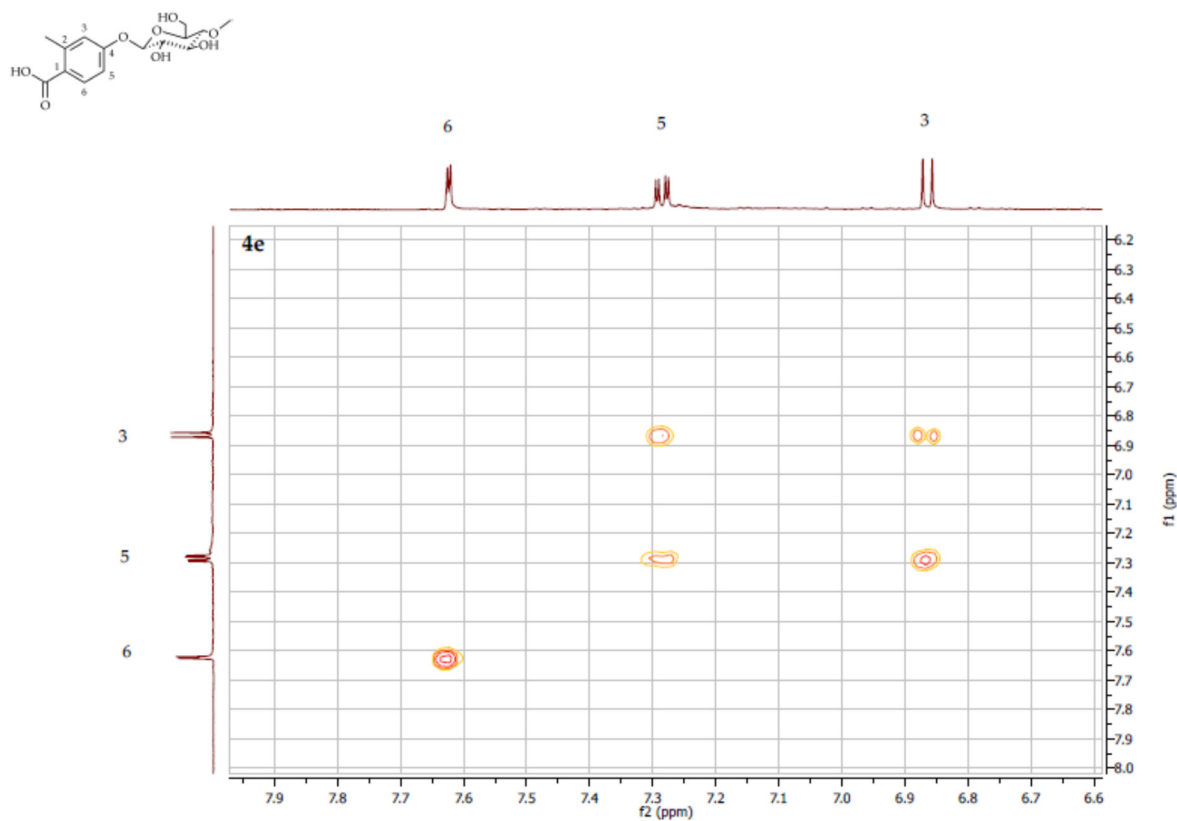


Figure S97. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2-methylbenzoic acid 4-O- β -D-(4'-O-methyl)-glucopyranoside (**4e**)

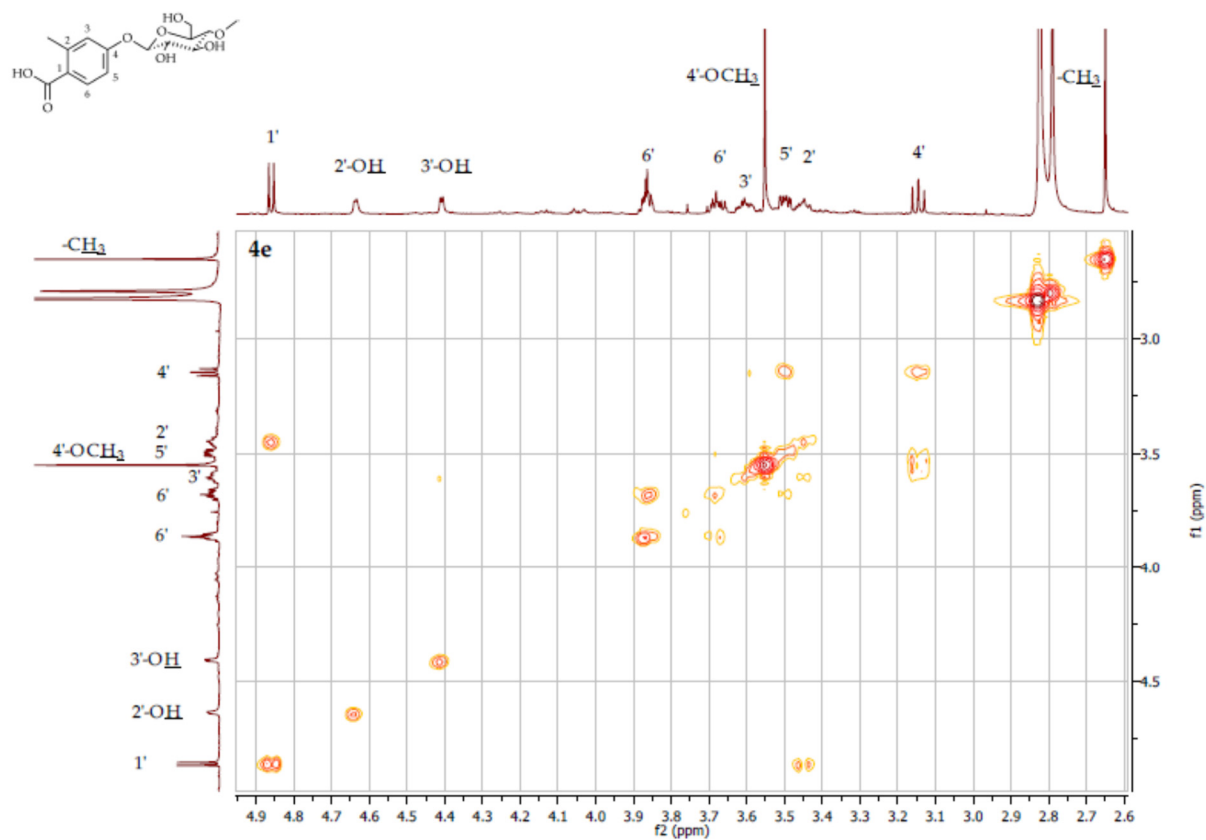


Figure S98. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2-methylbenzoic acid 4-O- β -D-(4'-O-methyl)-glucopyranoside (**4e**)

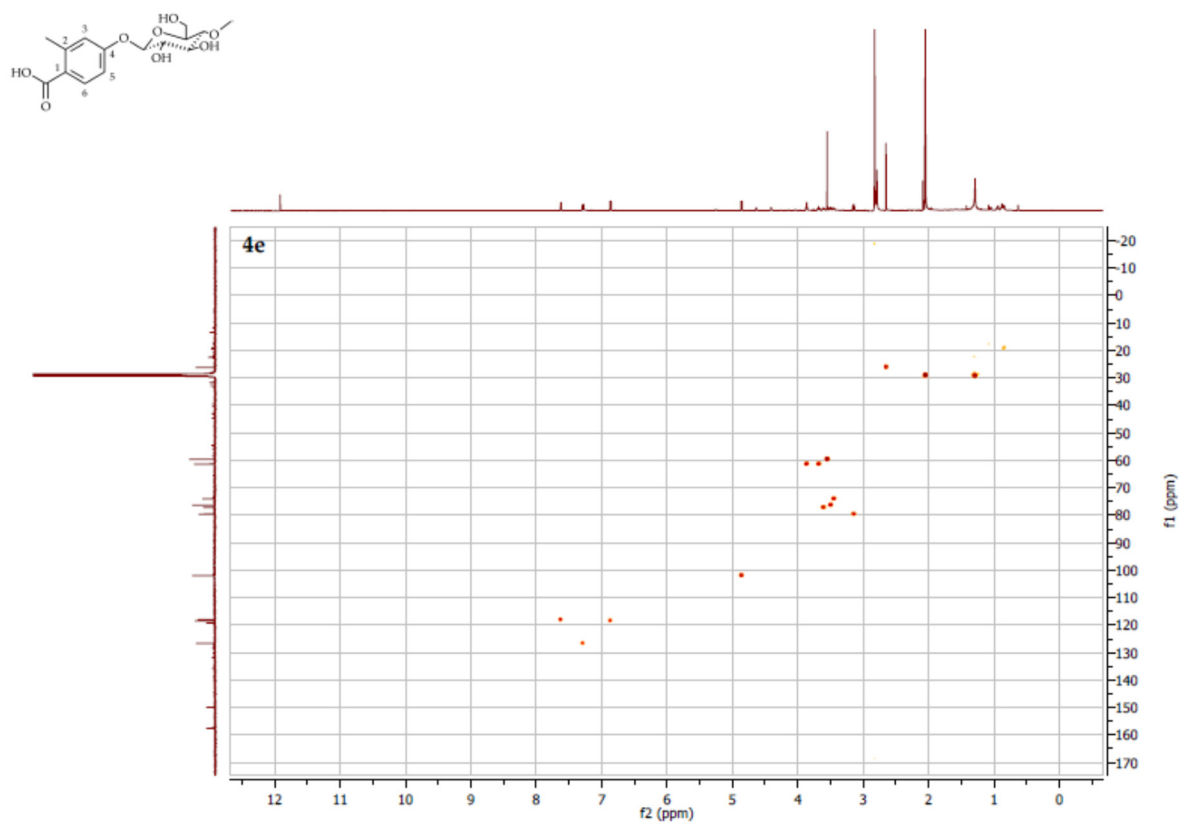


Figure S99. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ 2-methylbenzoic acid 4-O- β -D-(4'-O-methyl)-glucopyranoside (**4e**)

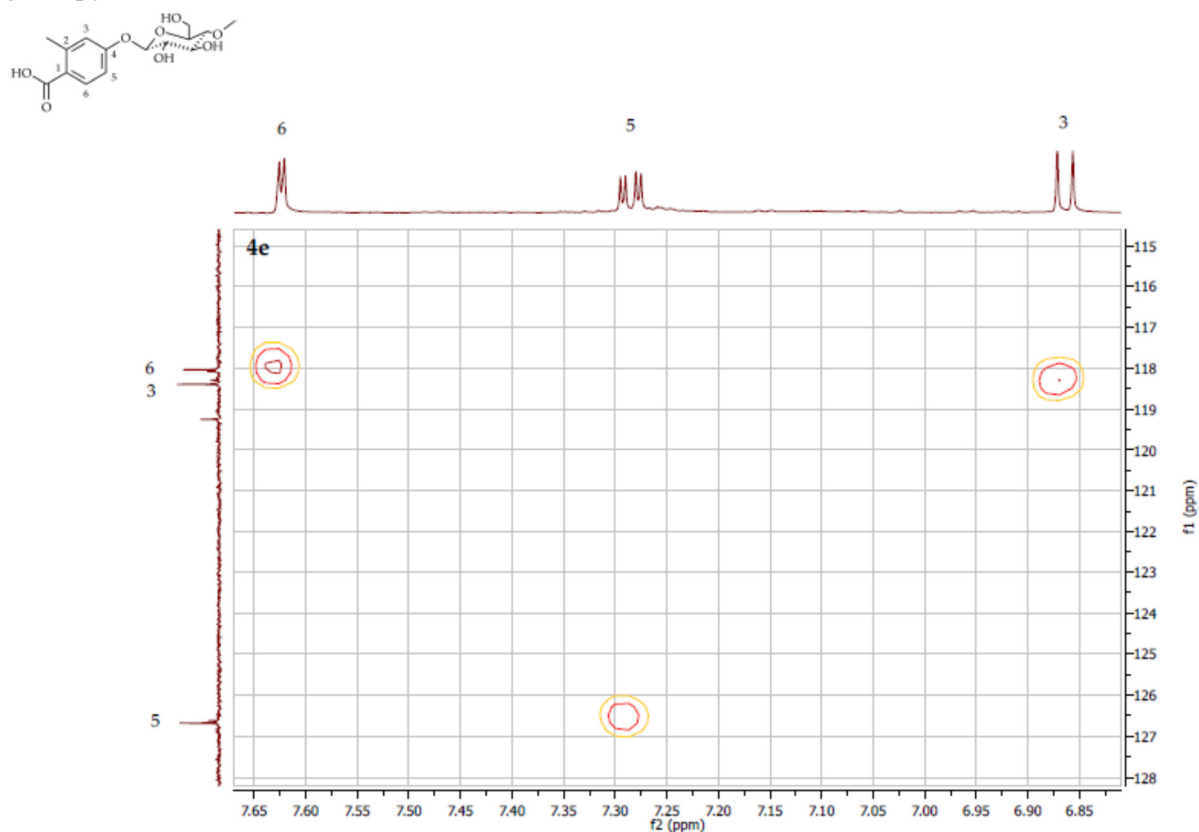


Figure S100. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2-methylbenzoic acid 4-O- β -D-(4'-O-methyl)-glucopyranoside (**4e**)

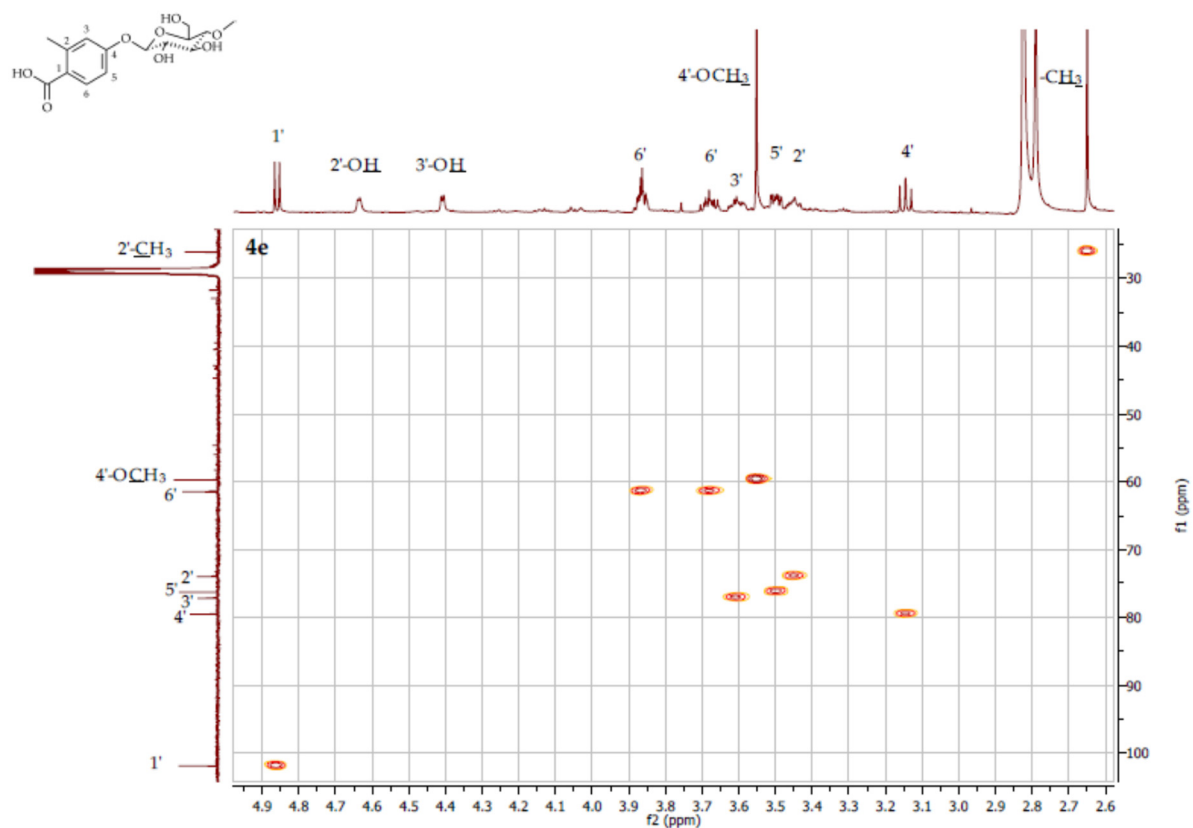


Figure S101. HSQC contour map – ¹H x ¹³C expansion of 2-methylbenzoic acid 4-O-β-D-(4'-O-methyl)-glucopyranoside (4e)

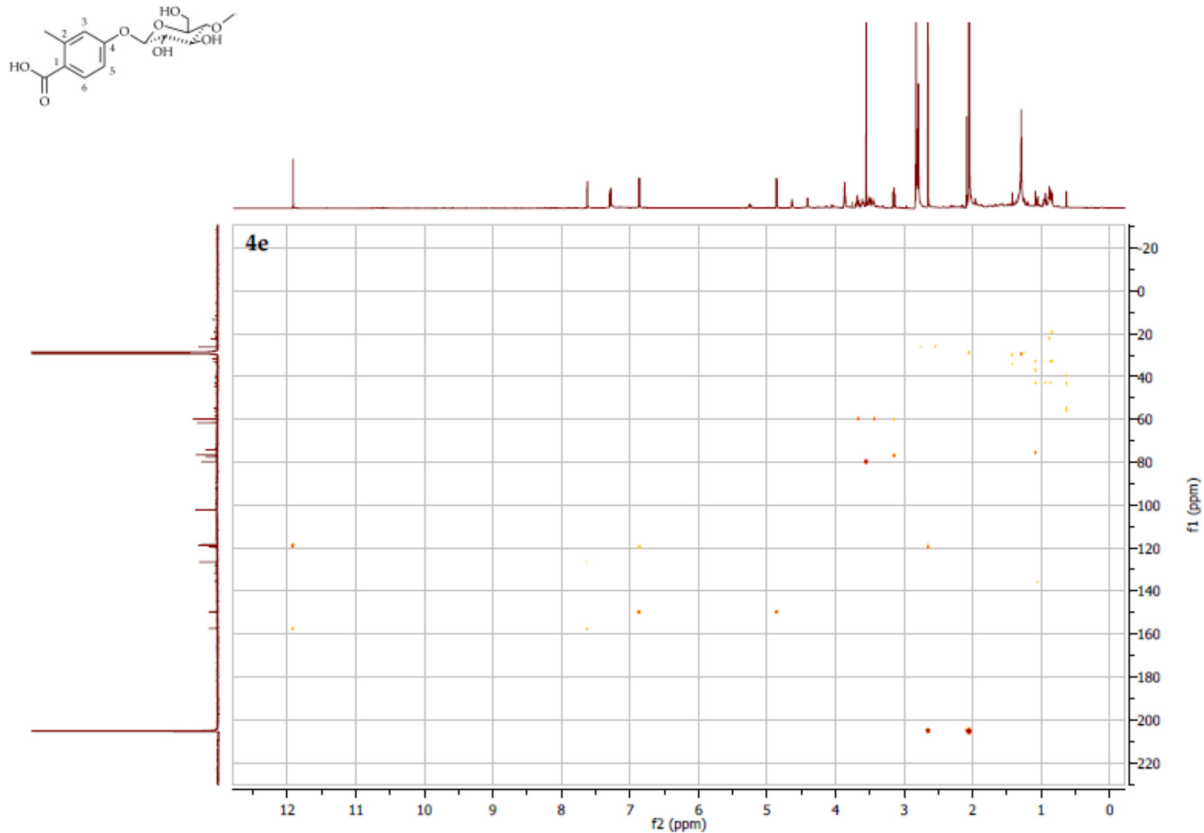


Figure S102. HMBC contour map – ¹H x ¹³C of 2-methylbenzoic acid 4-O-β-D-(4'-O-methyl)-glucopyranoside (4e)

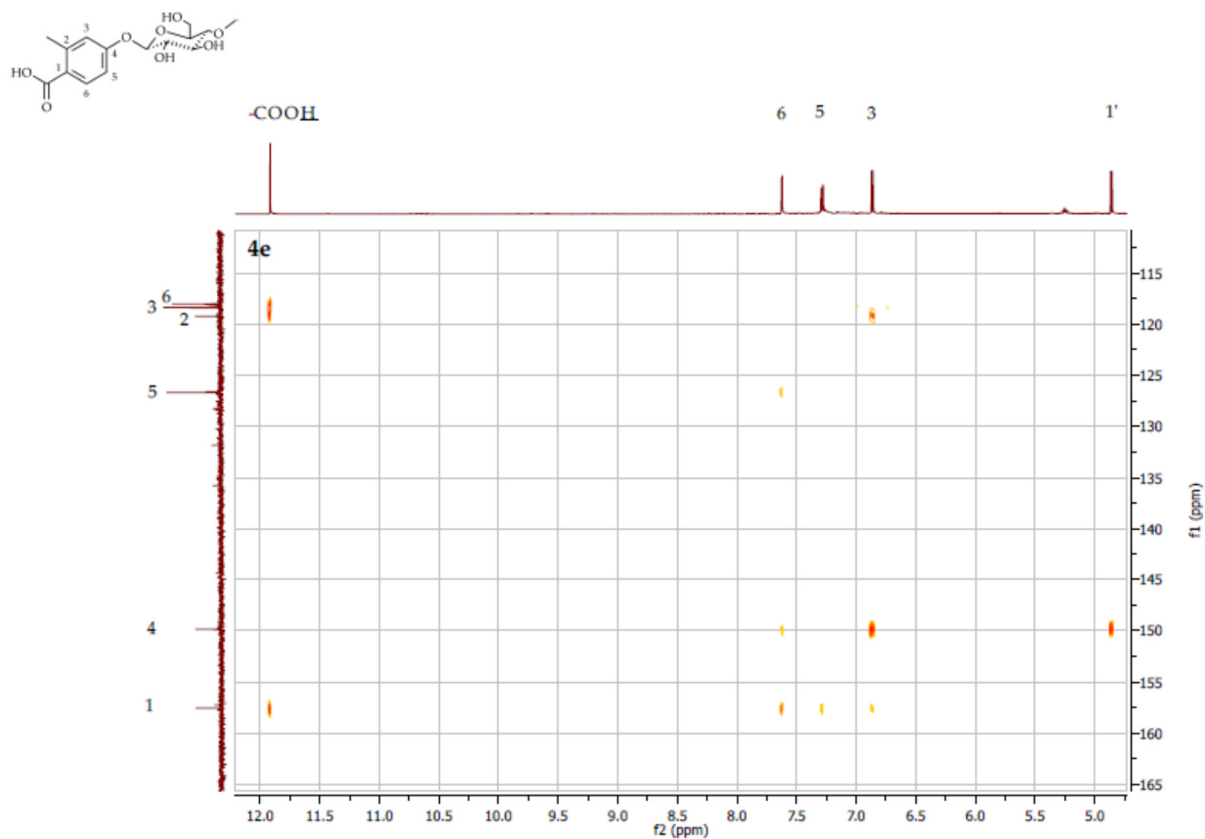


Figure S103. HMBC contour map – ^1H x ^{13}C expansion of 2-methylbenzoic acid 4-O- β -D-(4'-O-methyl)-glucopyranoside (**4e**)

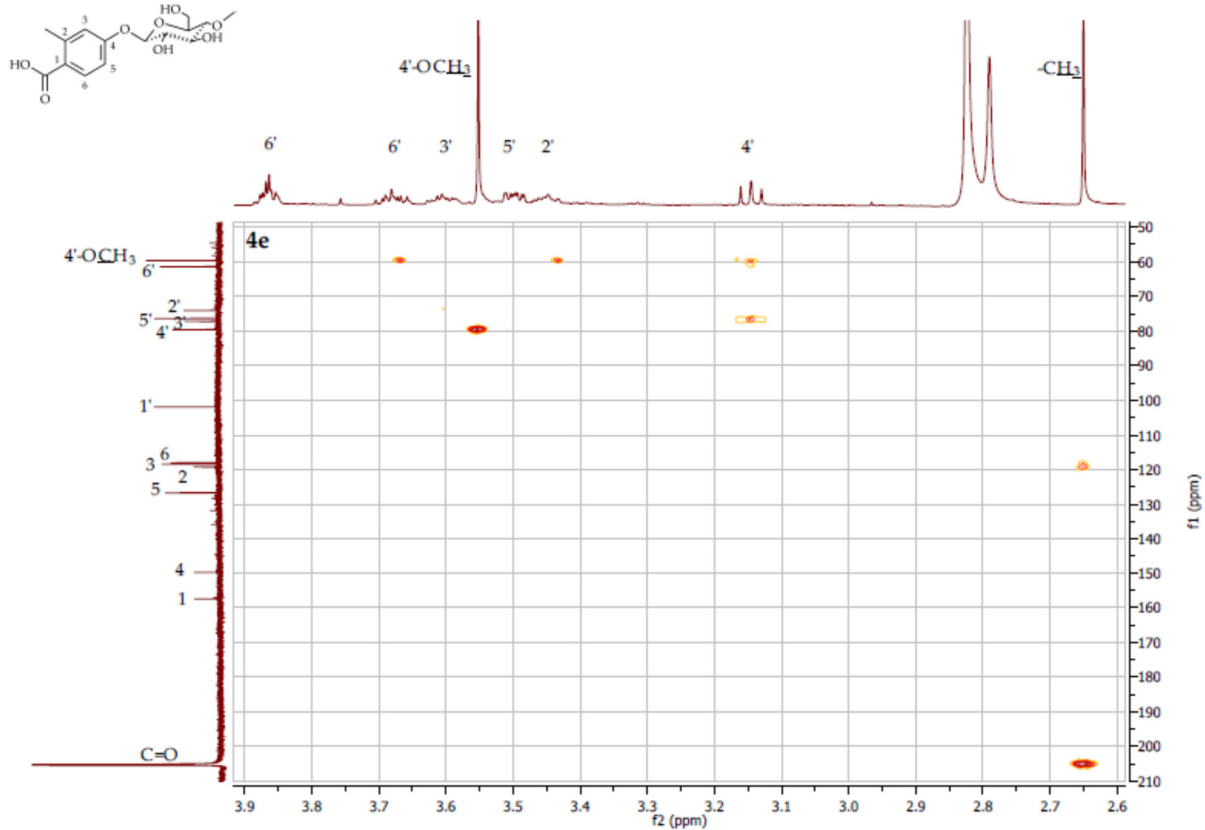


Figure S104. HMBC contour map – ^1H x ^{13}C expansion of 2-methylbenzoic acid 4-O- β -D-(4'-O-methyl)-glucopyranoside (**4e**)

Molecular formula: C₁₆H₁₂O₂

Formula weight: 236.08

Ionization mode: positive

Precursor: [M + H]⁺ 237.10

237.1000>65.0500 CE: -51.0

237.1000>121.0500 CE: -31.0

237.1000>115.1000 CE: -39.0

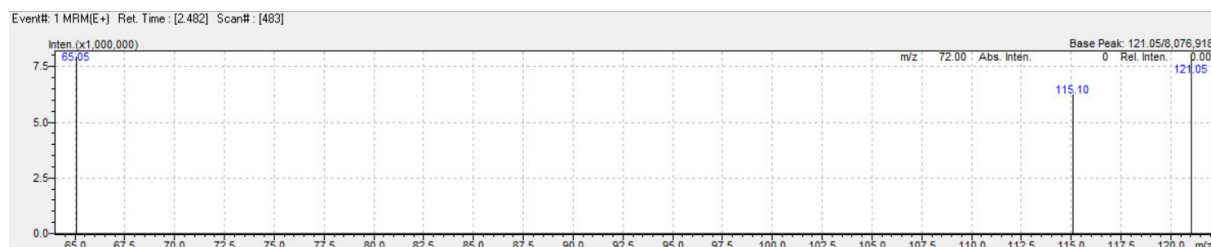
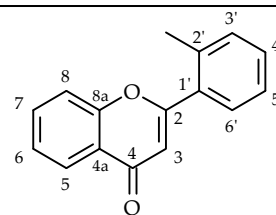


Figure S105. MS analysis of 2'-methylflavone (5)

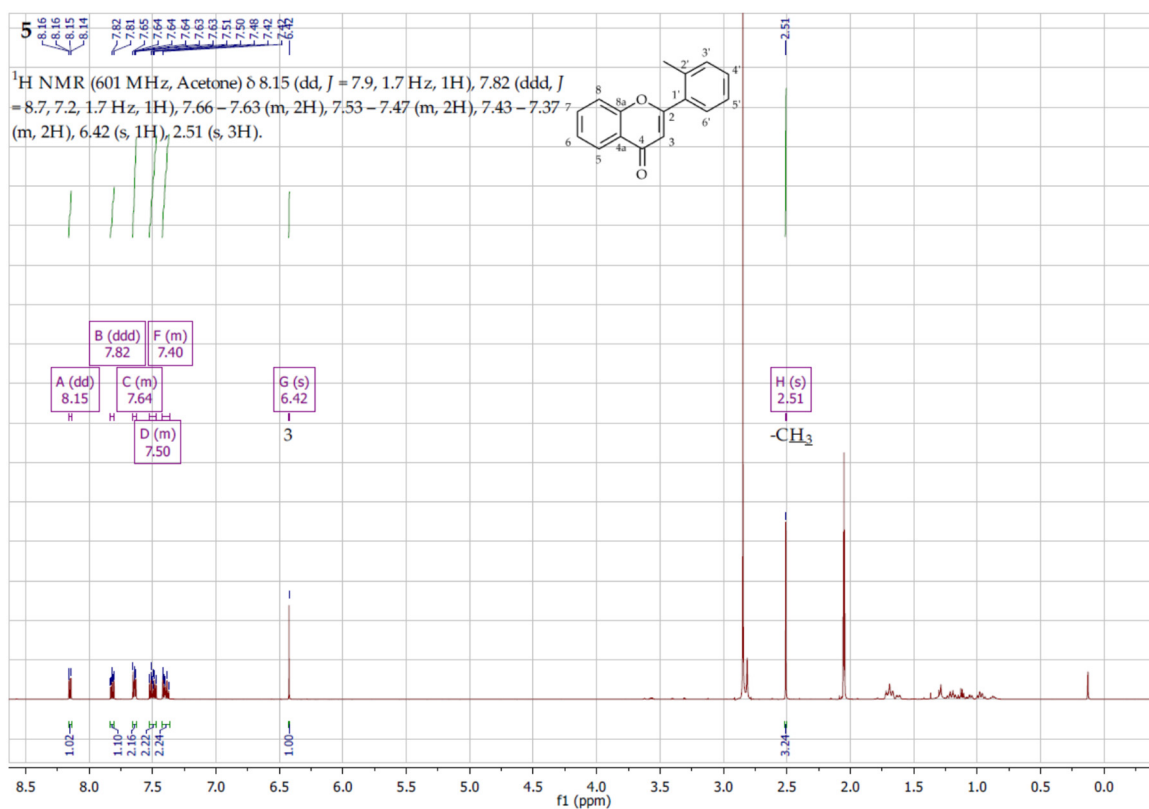


Figure S106. ¹H NMR spectrum (δ, acetone-d₆, 600 MHz) of 2'-methylflavone (5)

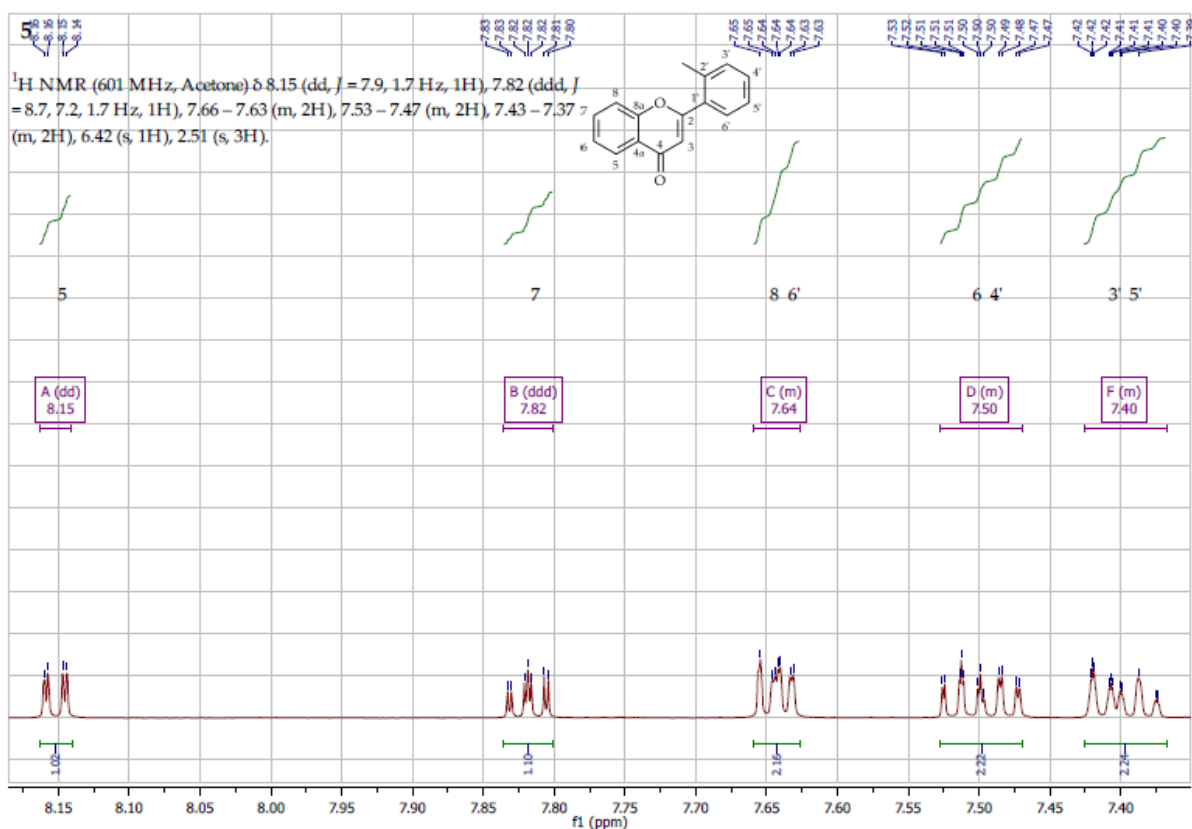


Figure S107. ¹H NMR spectrum expansion (δ, acetone-d₆, 600 MHz) 2'-methylflavone (**5**)

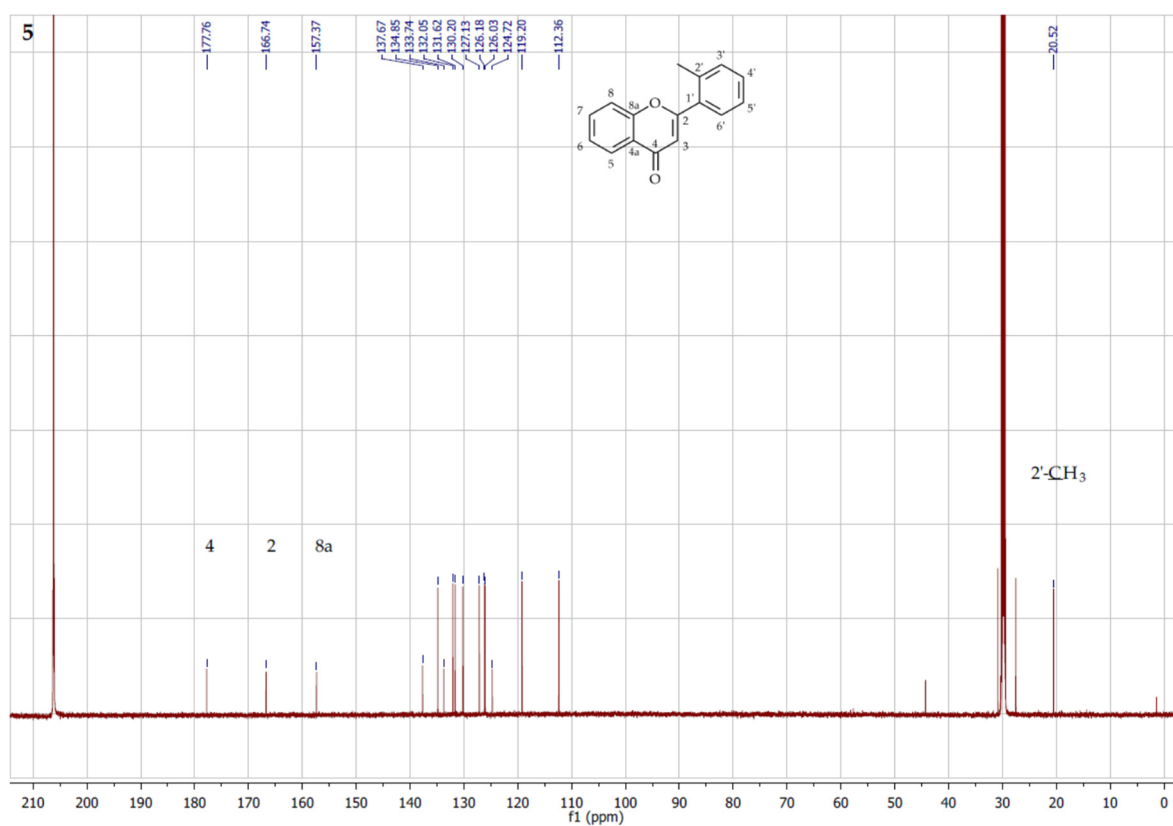


Figure S108. ¹³C NMR spectrum (δ, acetone-d₆, 151 MHz) of 2'-methylflavone (**5**)

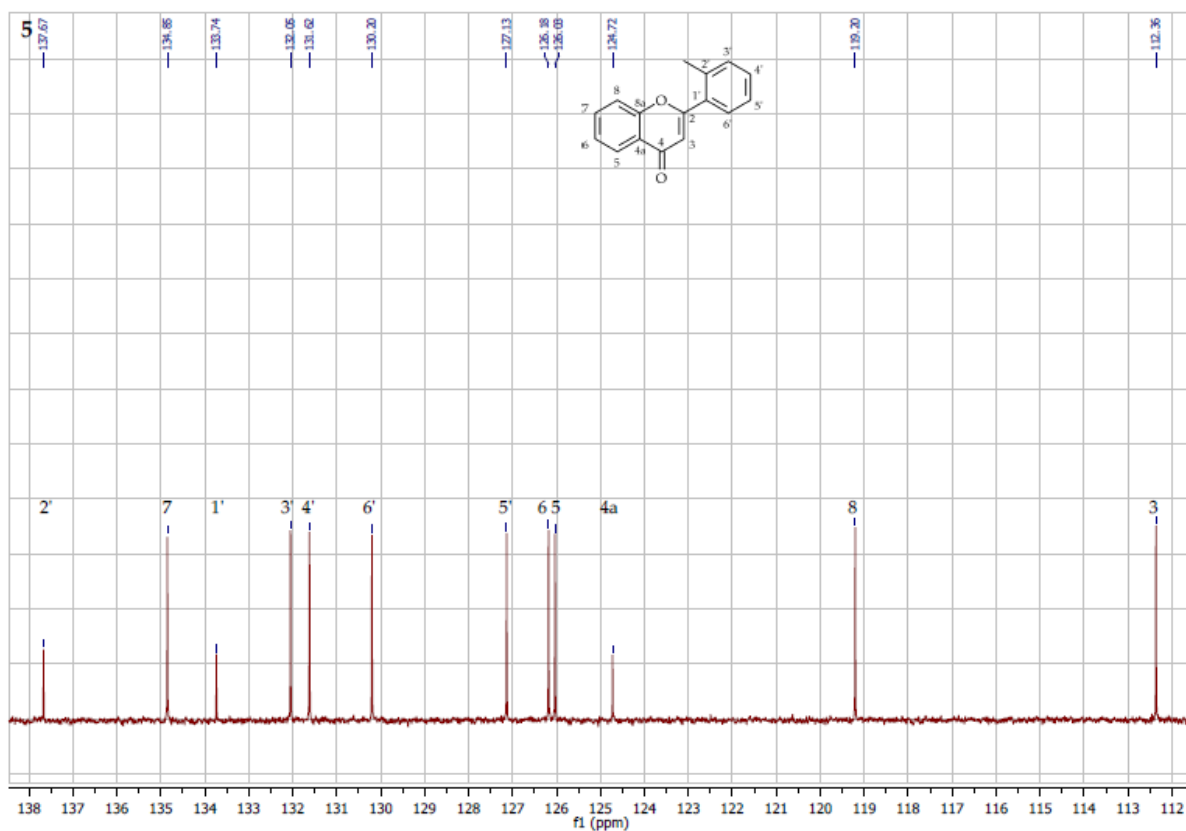


Figure S109. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavone (**5**)

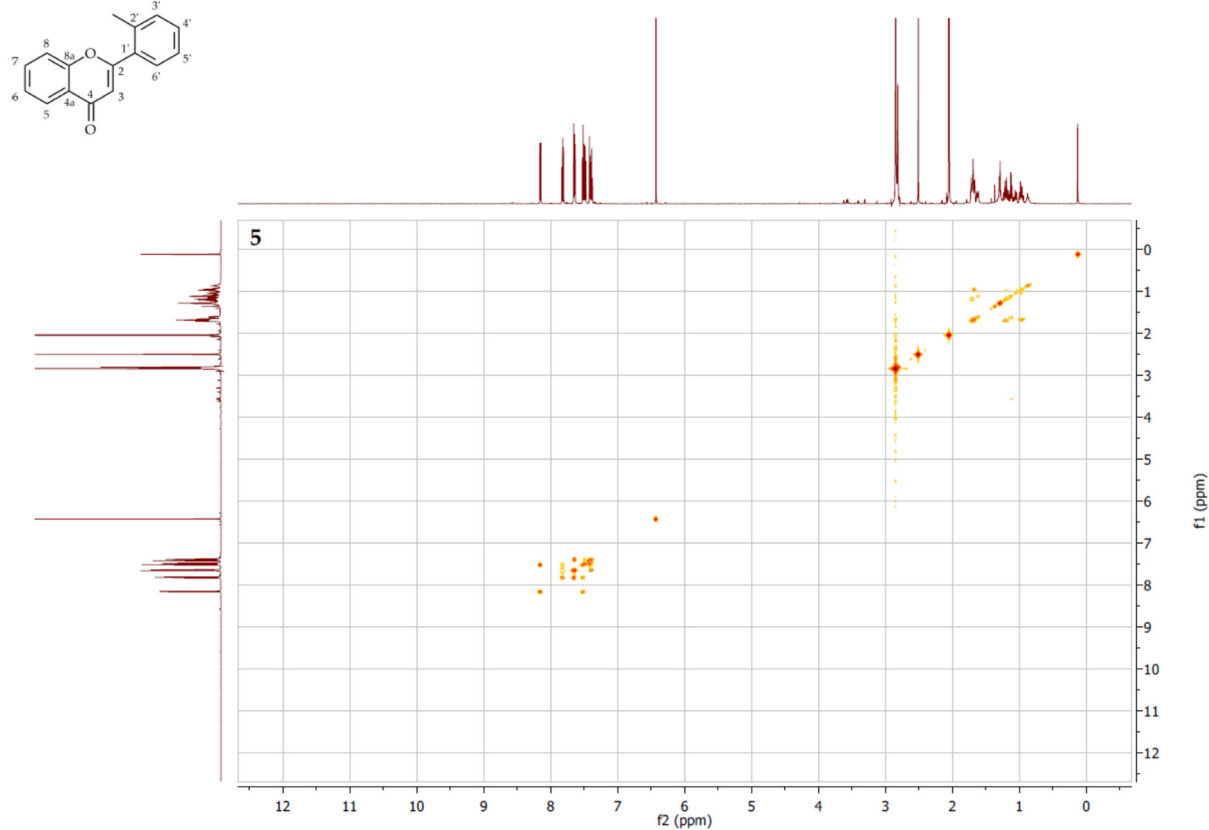


Figure S110. COSY contour map – $^1\text{H} \times ^1\text{H}$ of 2'-methylflavone (**5**)

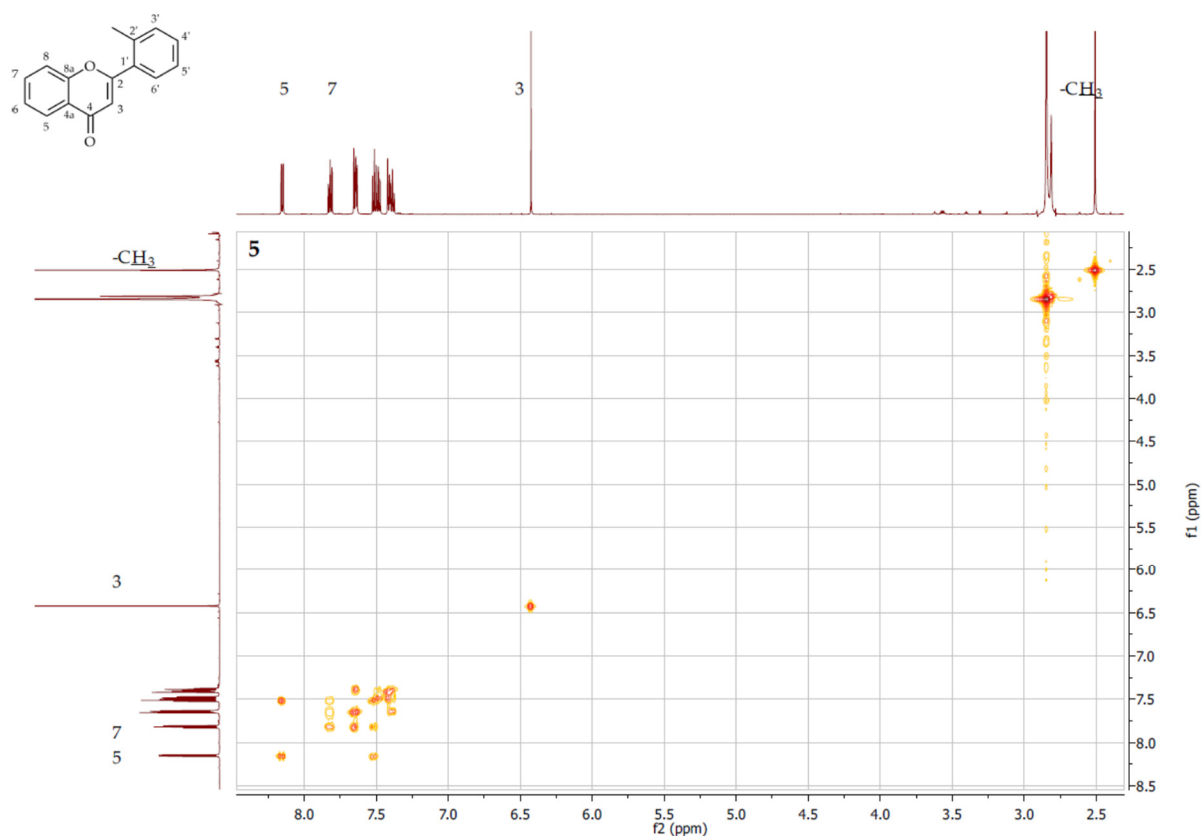


Figure S111. COSY contour map – ¹H x ¹H expansion of 2'-methylflavone (5)

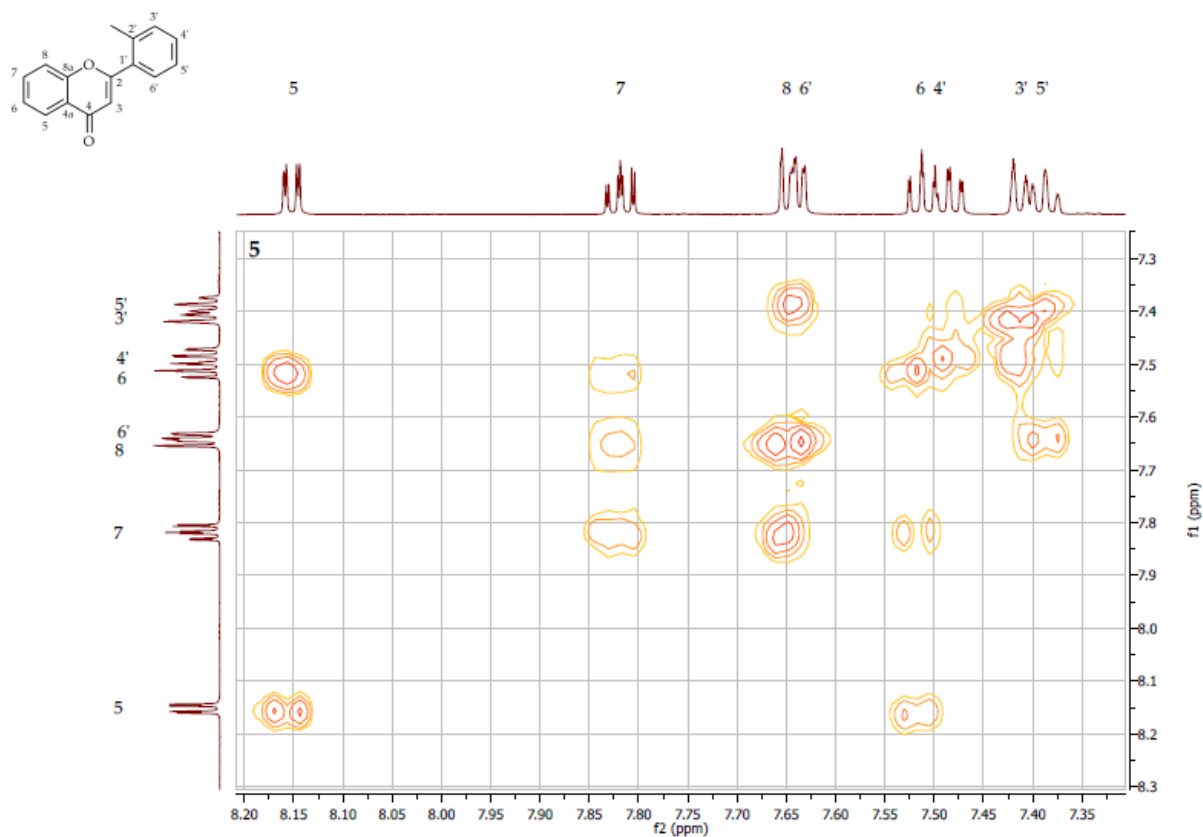


Figure S112. COSY contour map – ¹H x ¹H expansion of 2'-methylflavone (5)

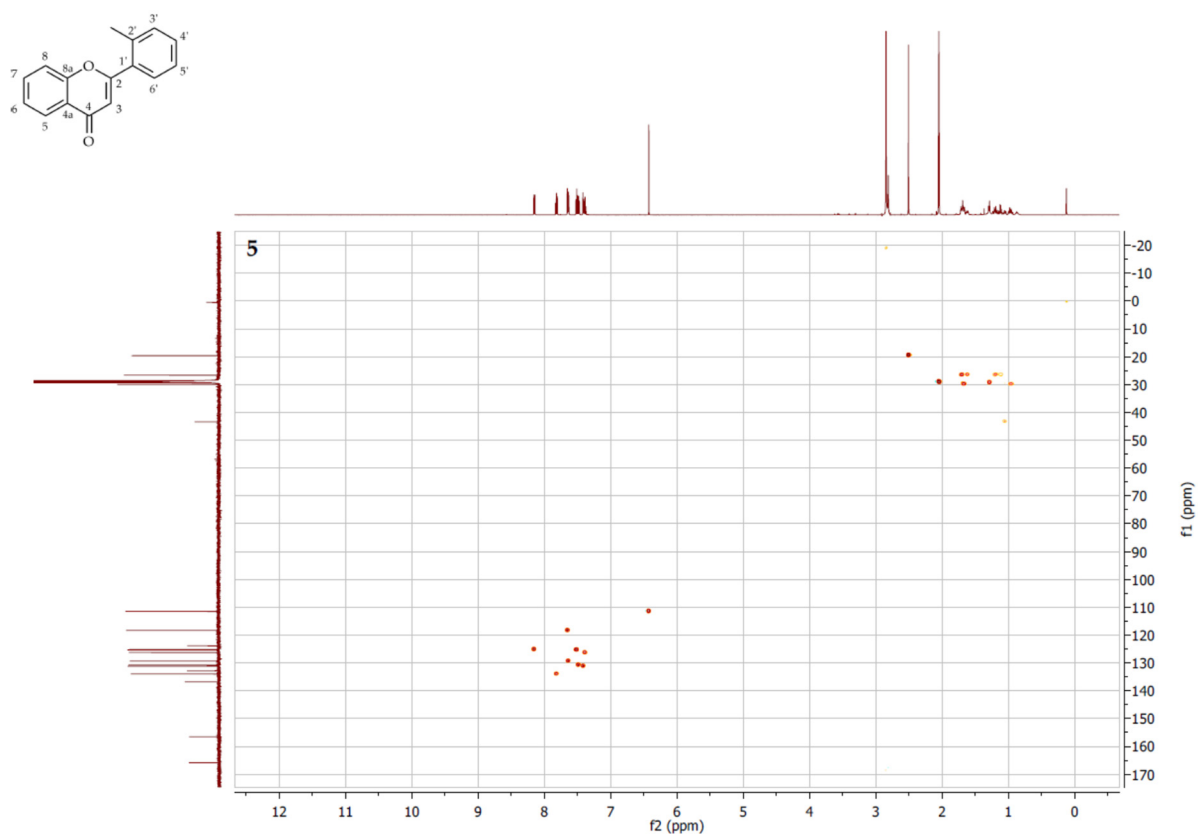


Figure S113. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavone (5)

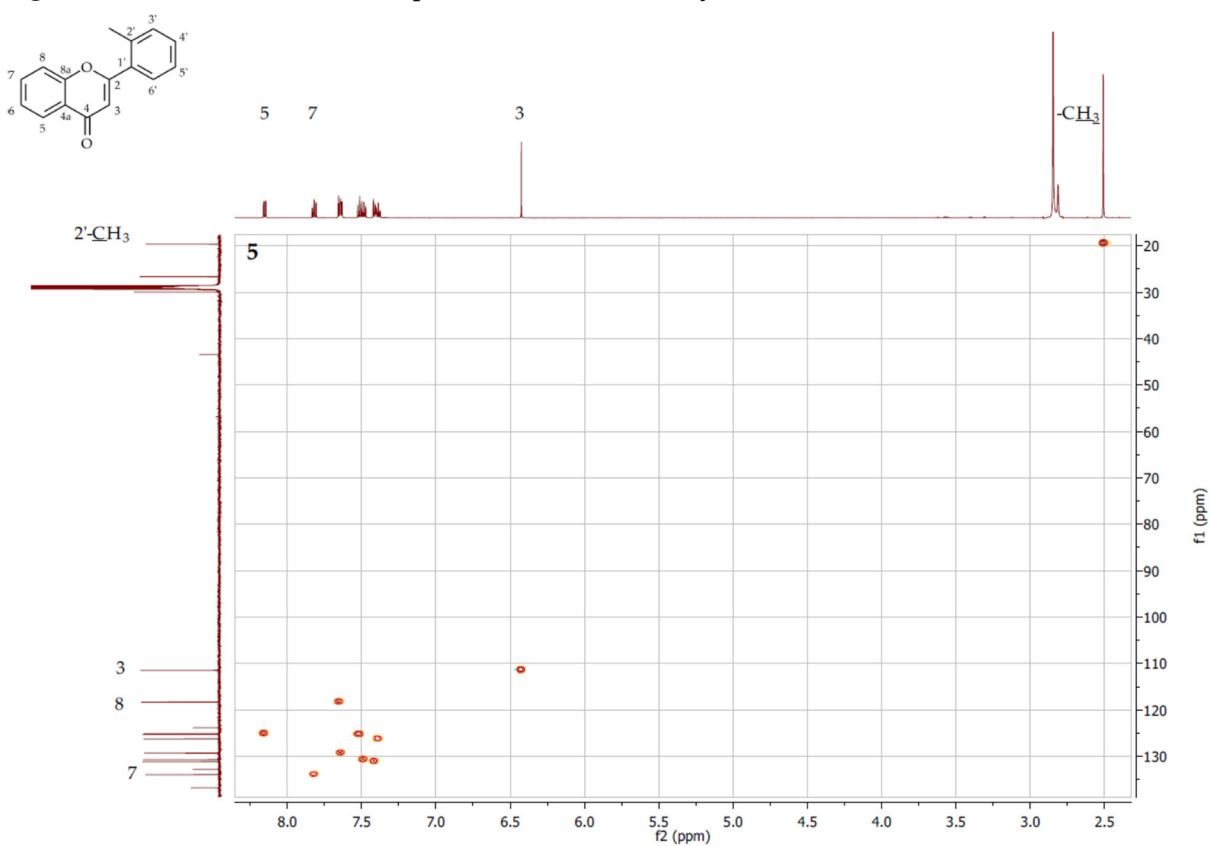


Figure S114. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone (5)

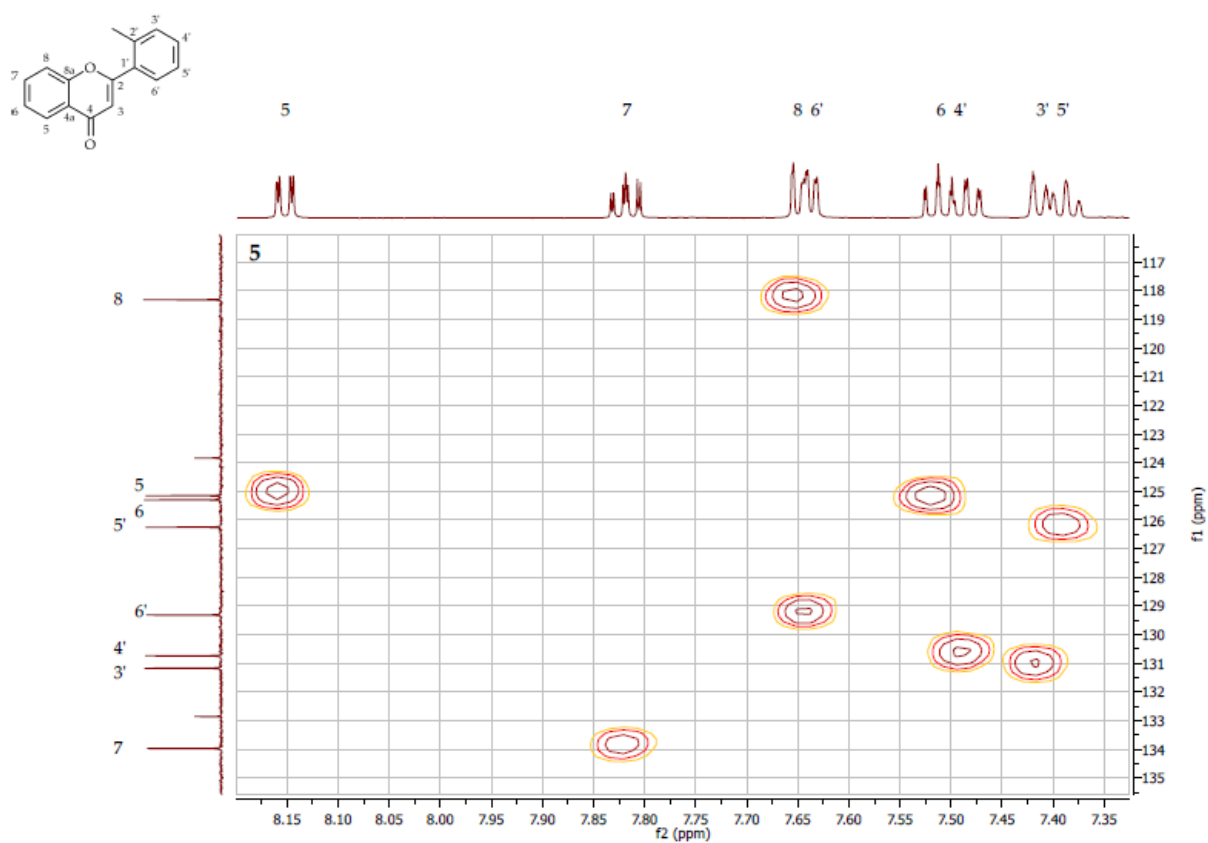


Figure S115. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone (5)

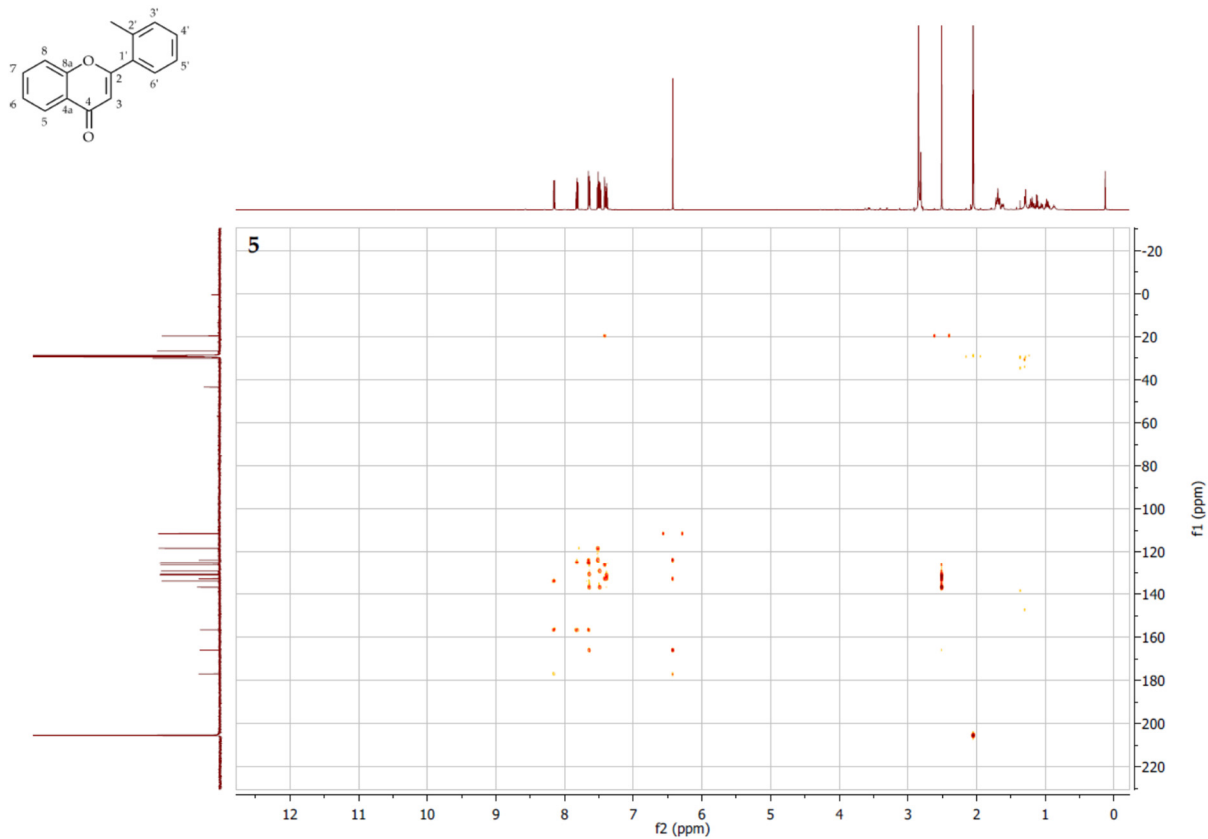


Figure S116. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavone (5)

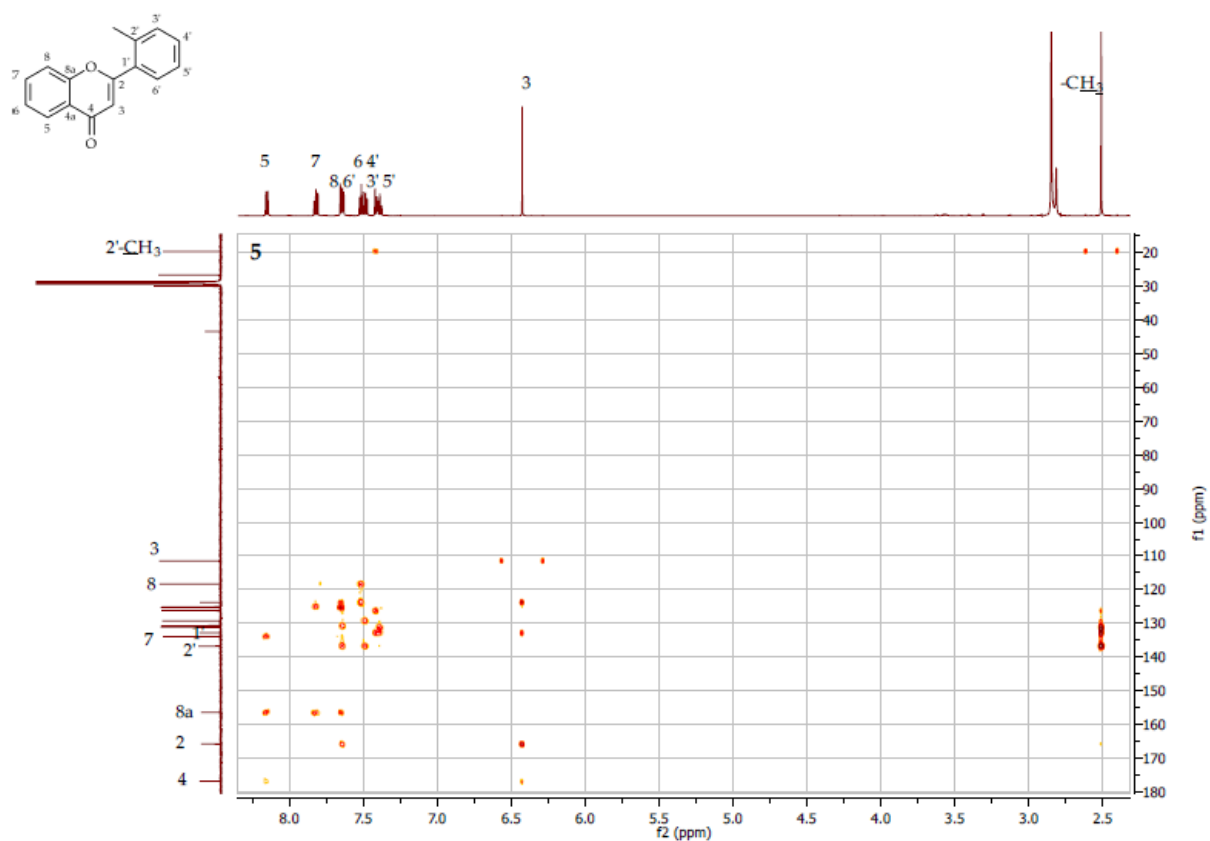


Figure S117. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone (5)

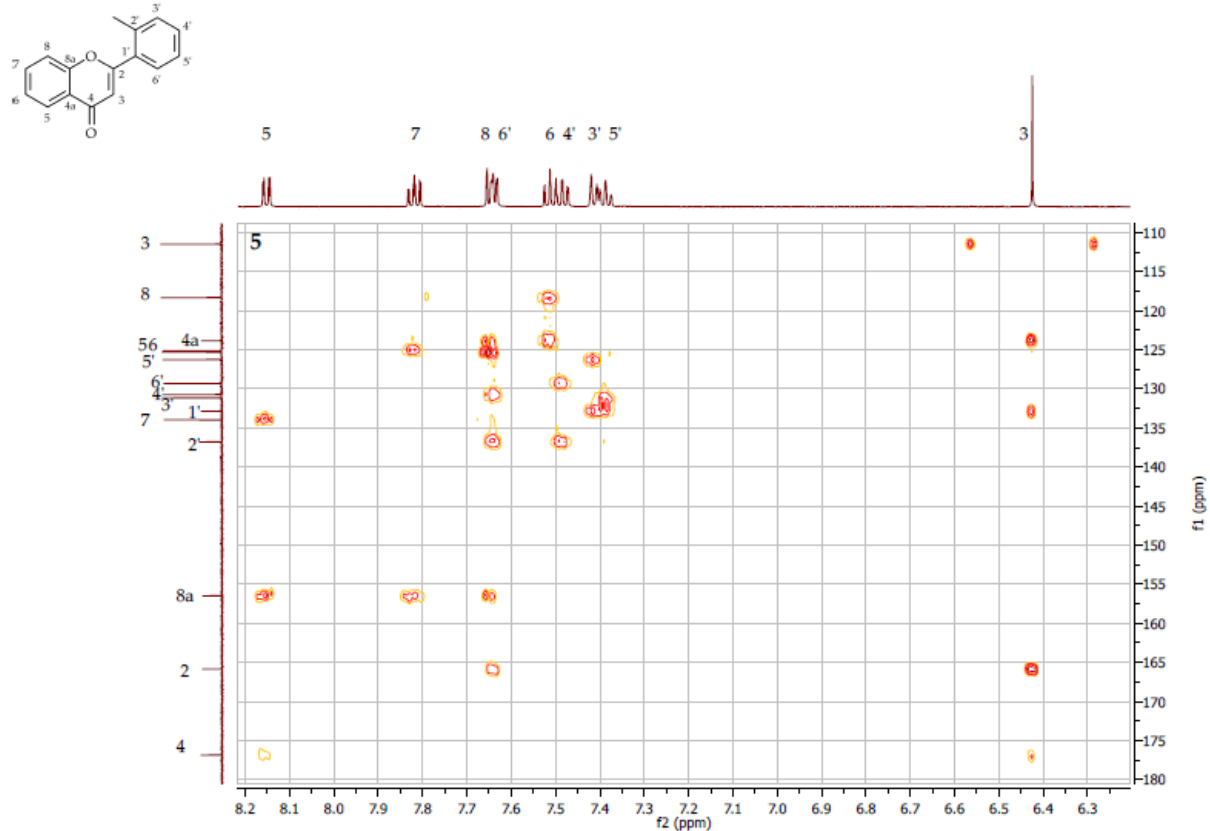


Figure S118. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone (5)

Molecular formula: C₂₃H₂₄O₈

Formula weight: 428.15

Ionization mode: positive

Precursor: [M + H]⁺ 429.10

429.1000>253.0500 CE: -31.0

429.1000>121.0500 CE: -55.0

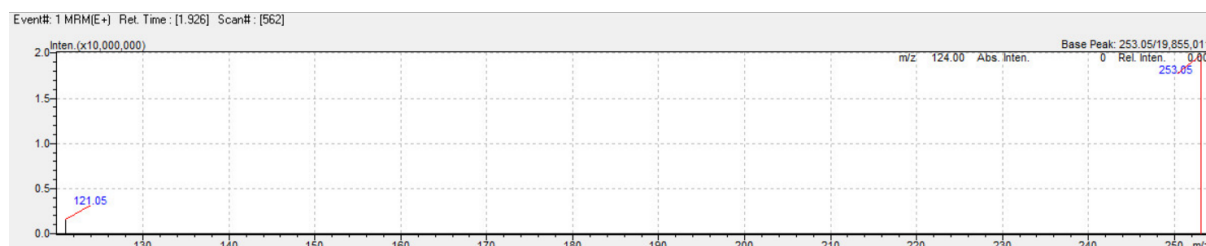
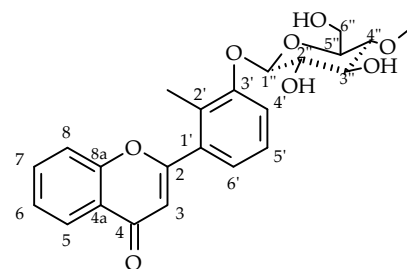


Figure S119. MS analysis of 2'-methylflavone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**5a**)

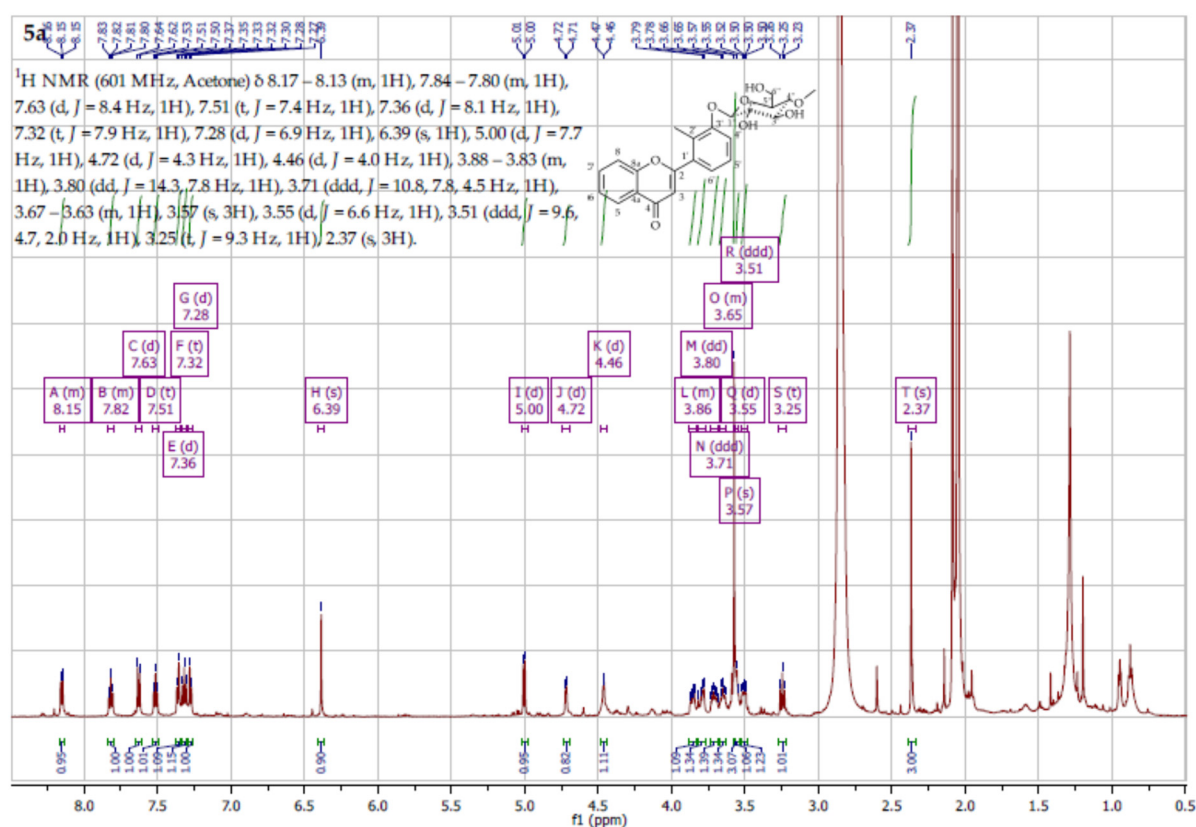


Figure S120. ¹H NMR spectrum (δ , acetone-d₆, 600 MHz) of 2'-methylflavone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**5a**)

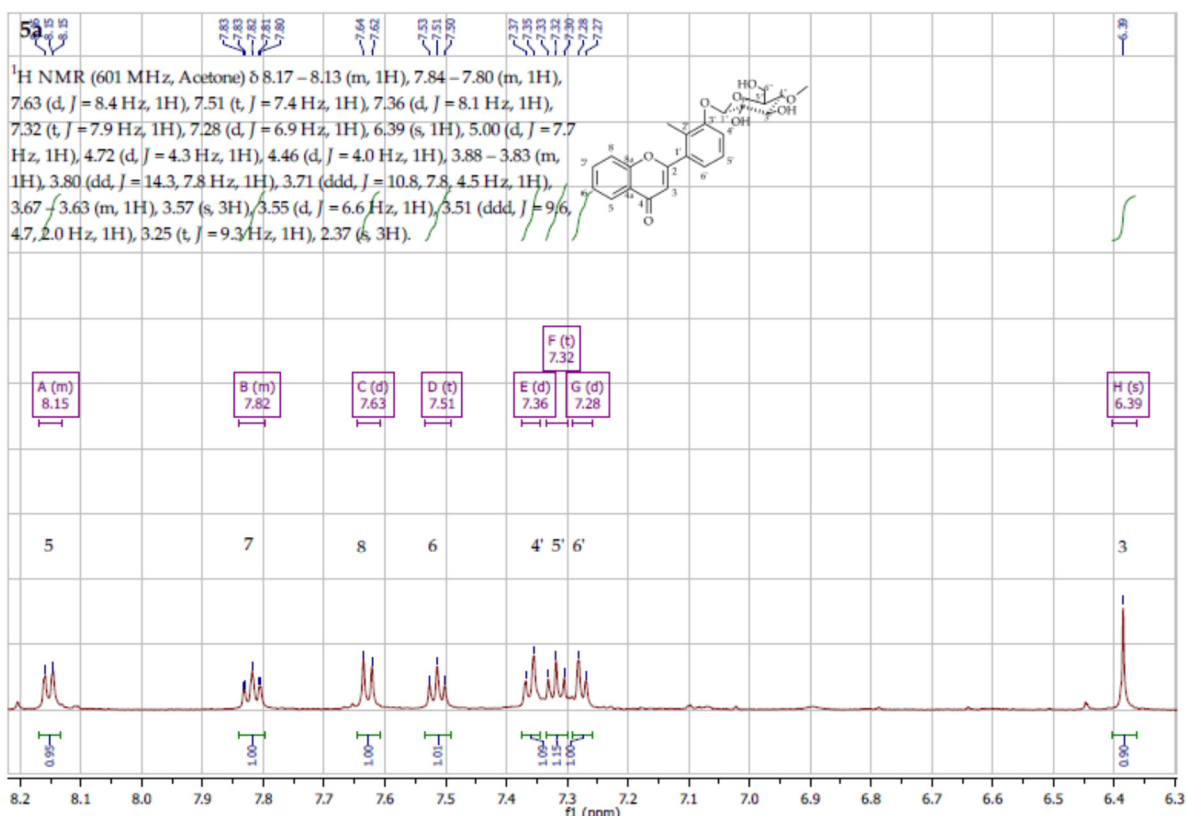


Figure S121. ¹H NMR spectrum expansion (δ, acetone-d₆, 600 MHz) of 2'-methylflavone 3'-O-β-D-(4''-O-methyl)-glucopyranoside (**5a**)

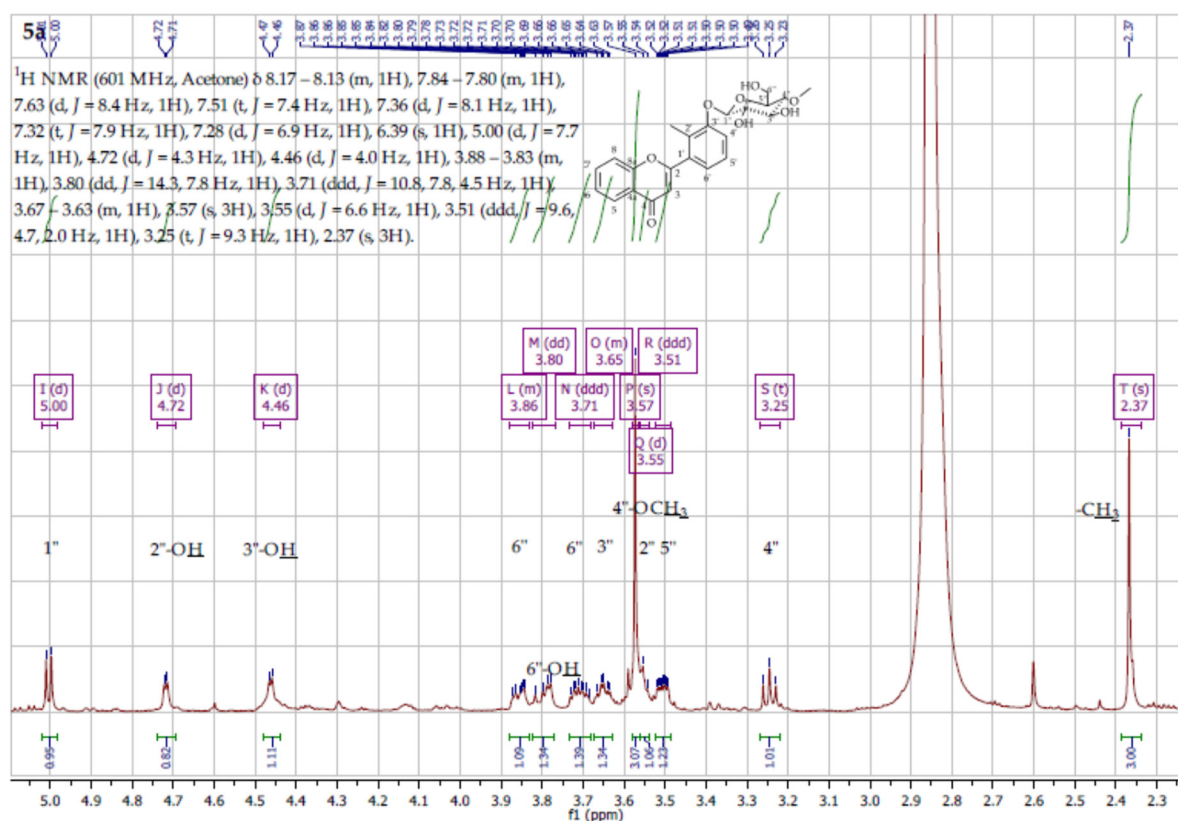


Figure S122. ¹H NMR spectrum expansion (δ, acetone-d₆, 600 MHz) of 2'-methylflavone 3'-O-β-D-(4''-O-methyl)-glucopyranoside (**5a**)

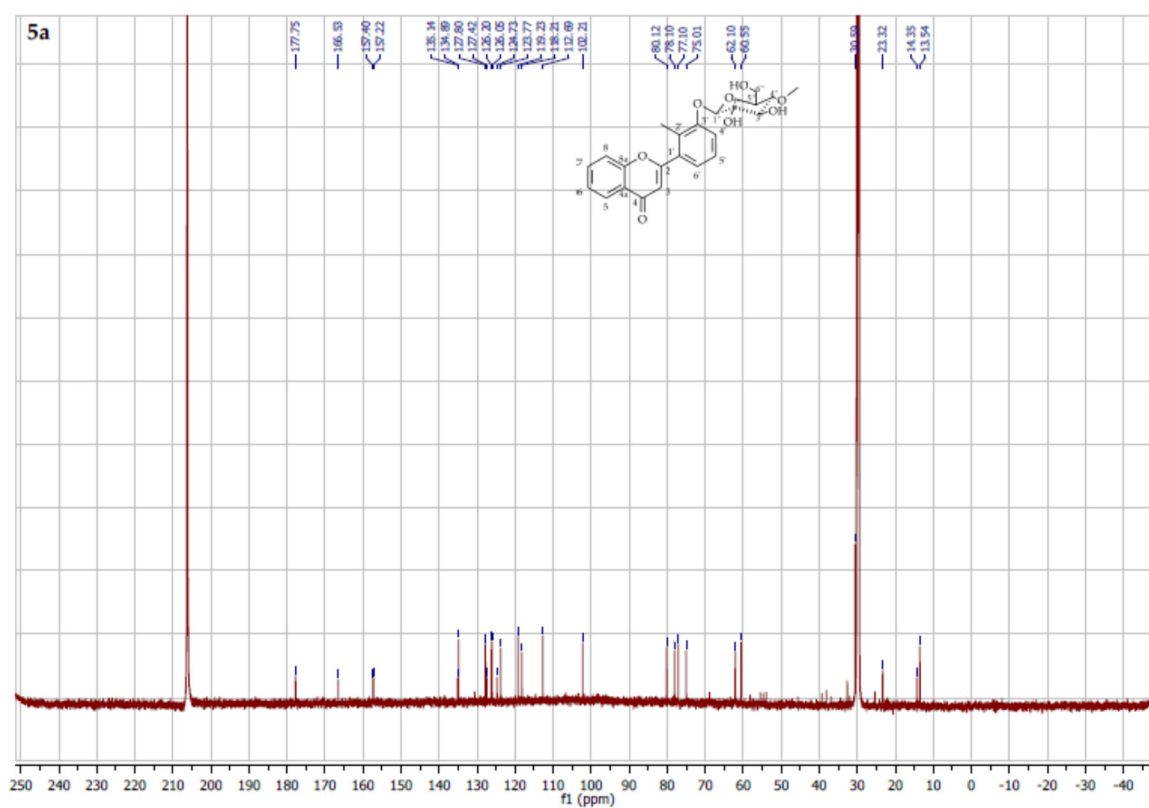


Figure S123. ^{13}C NMR spectrum (δ , acetone- d_6 , 151 MHz) of 2'-methylflavone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (5a)

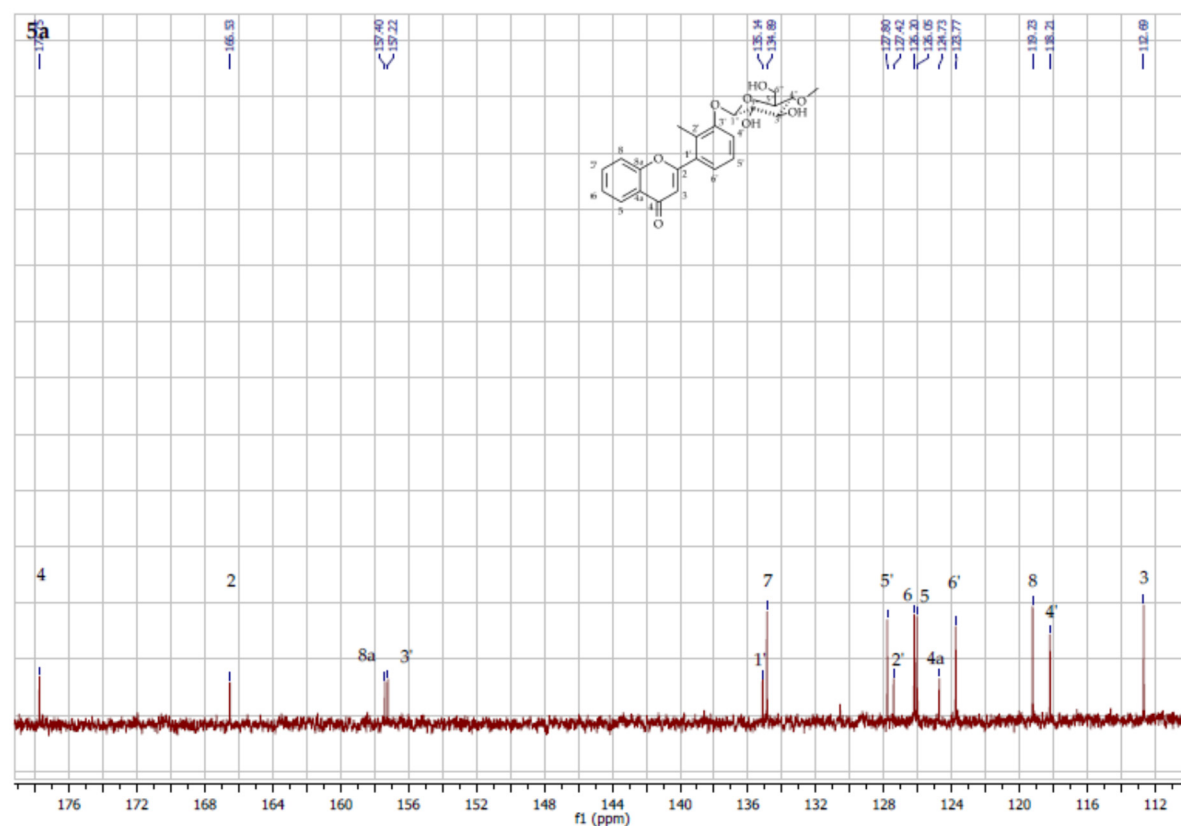


Figure S124. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (5a)

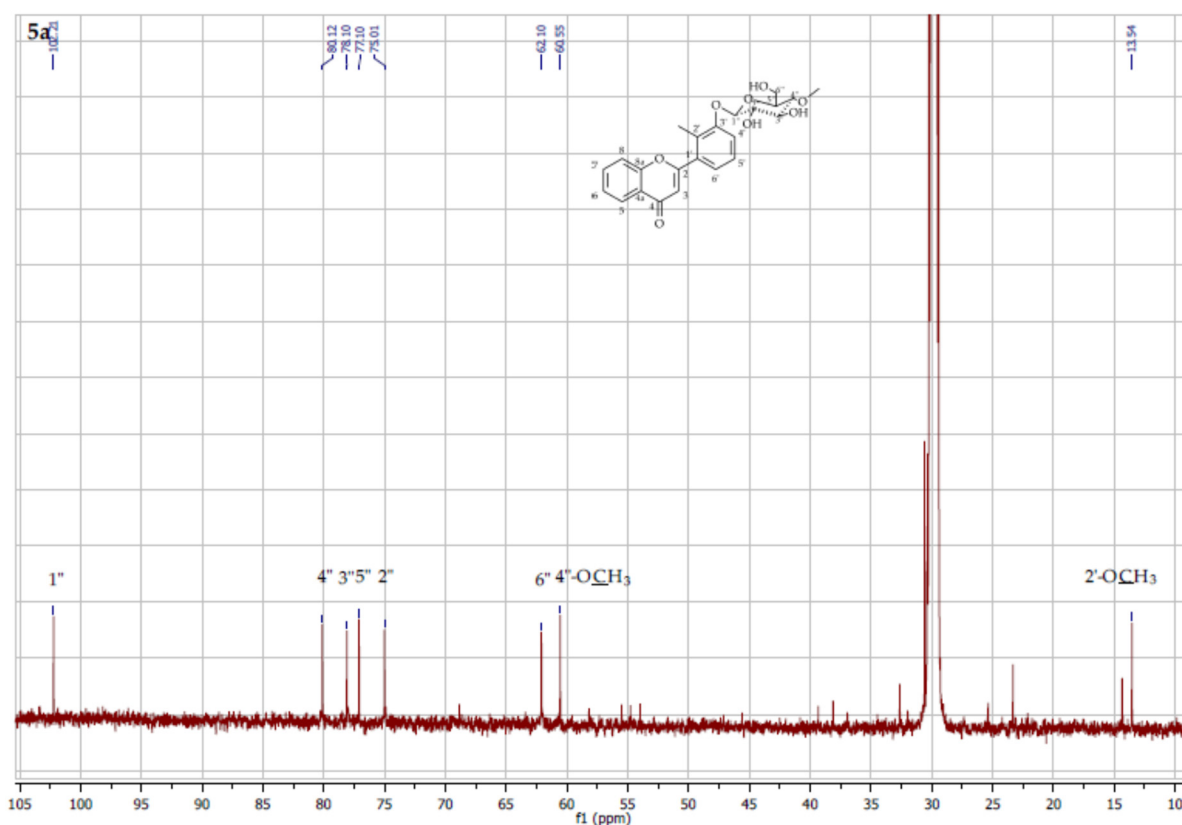


Figure S125. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavone 3'- O - β -D-(4''- O -methyl)-glucopyranoside (**5a**)

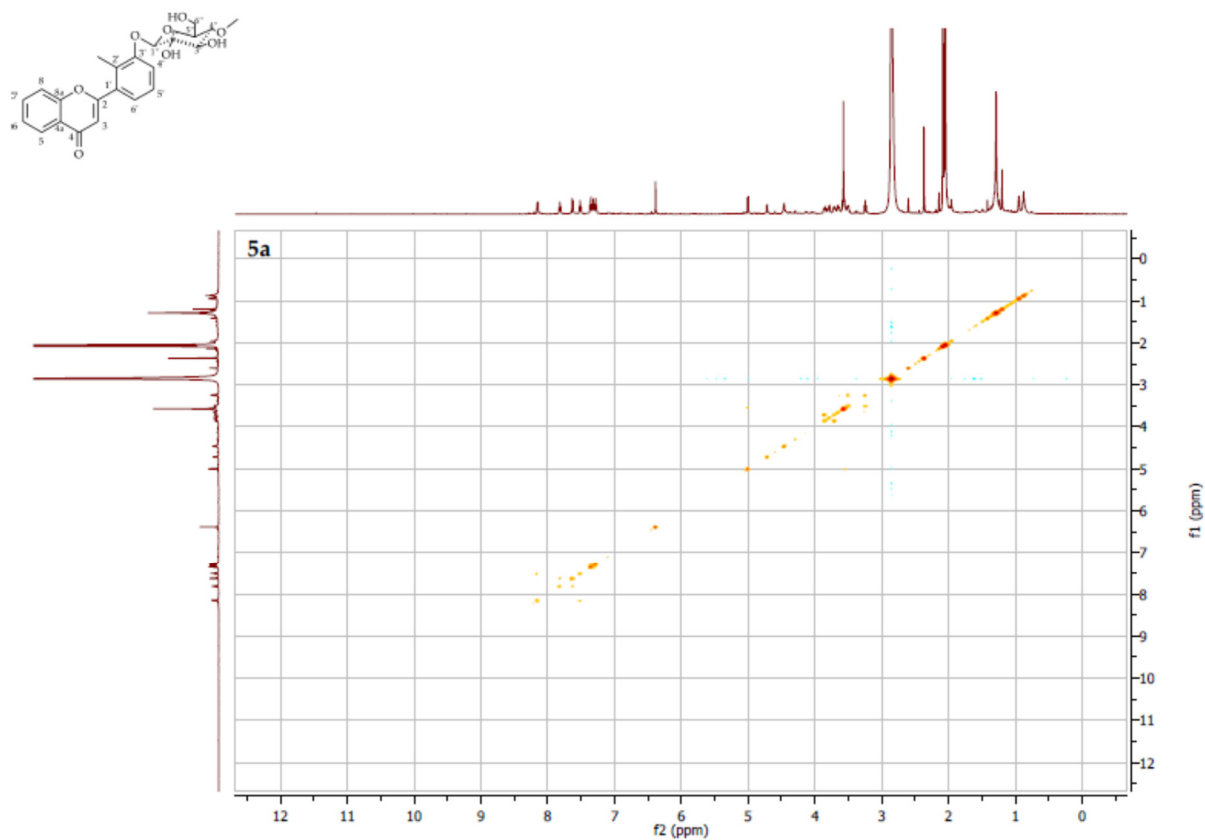


Figure S126. COSY contour map – $^1\text{H} \times ^1\text{H}$ of 2'-methylflavone 3'- O - β -D-(4''- O -methyl)-glucopyranoside (**5a**)

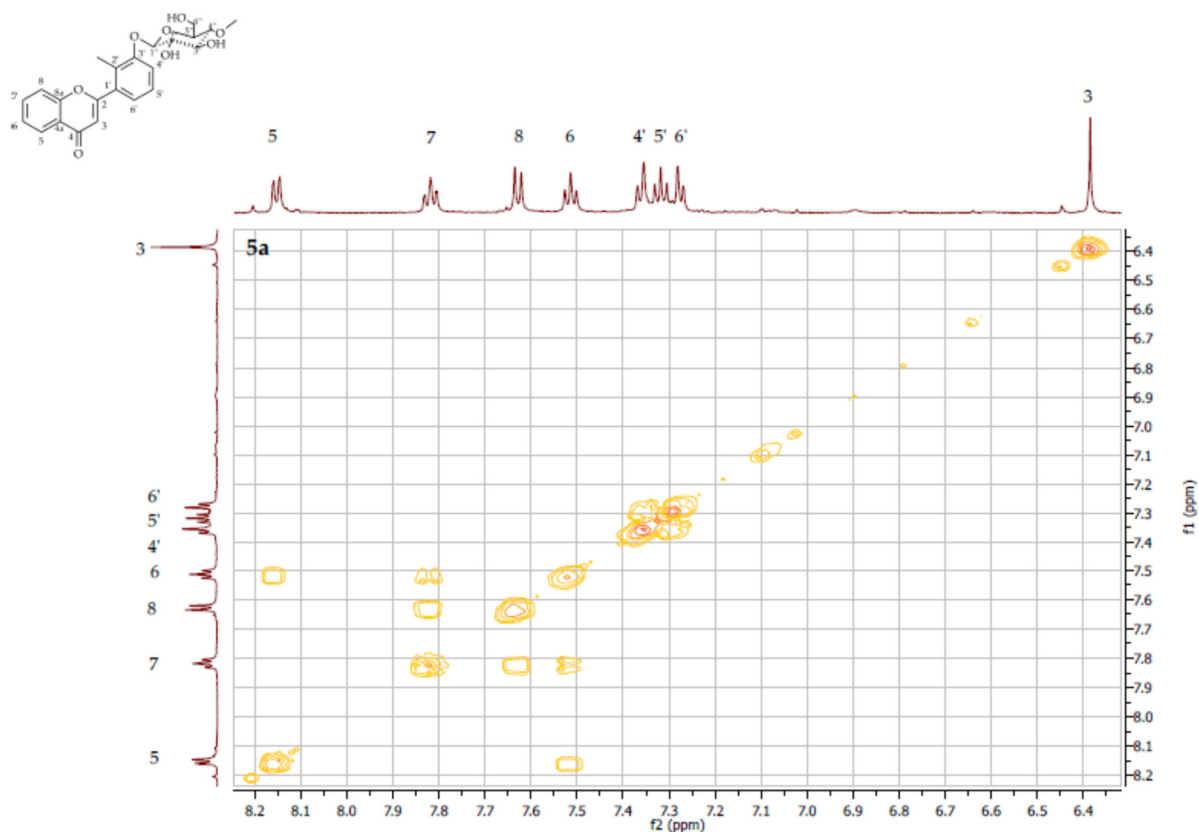


Figure S127. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methylflavone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**5a**)

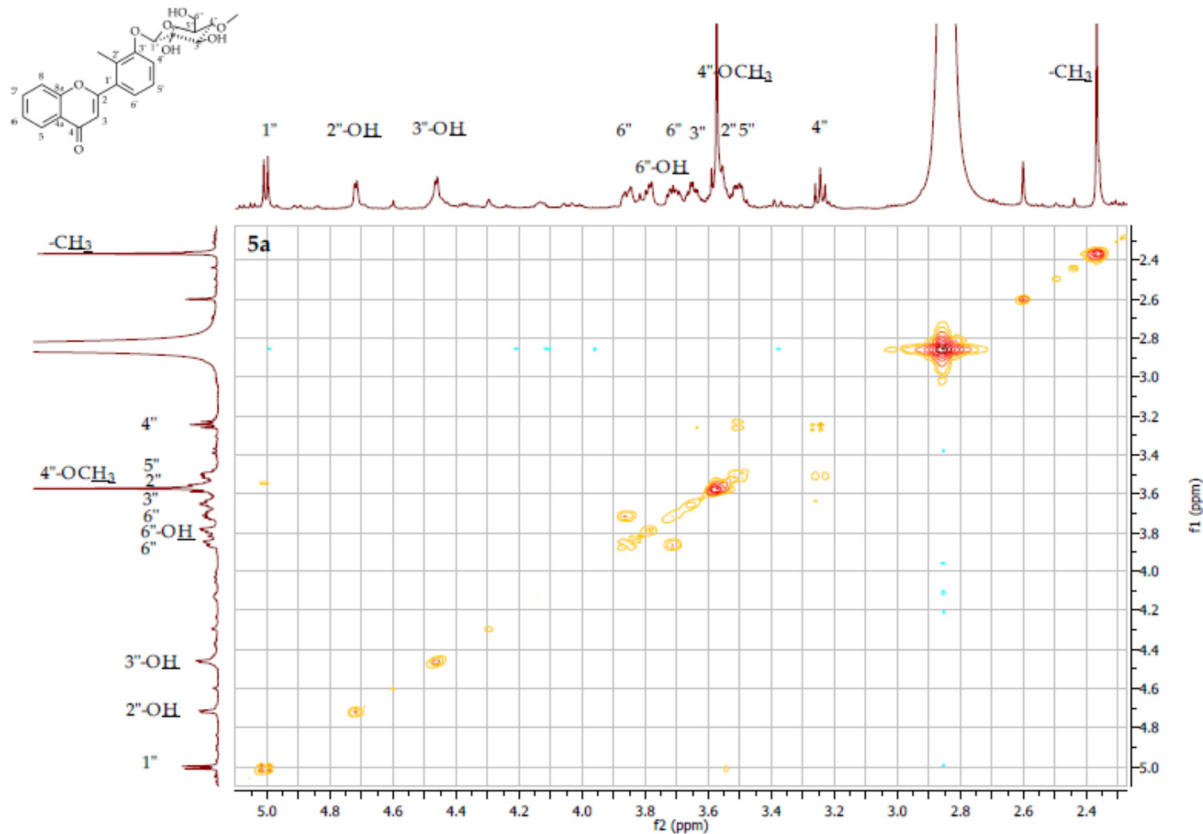


Figure S128. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methylflavone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**5a**)

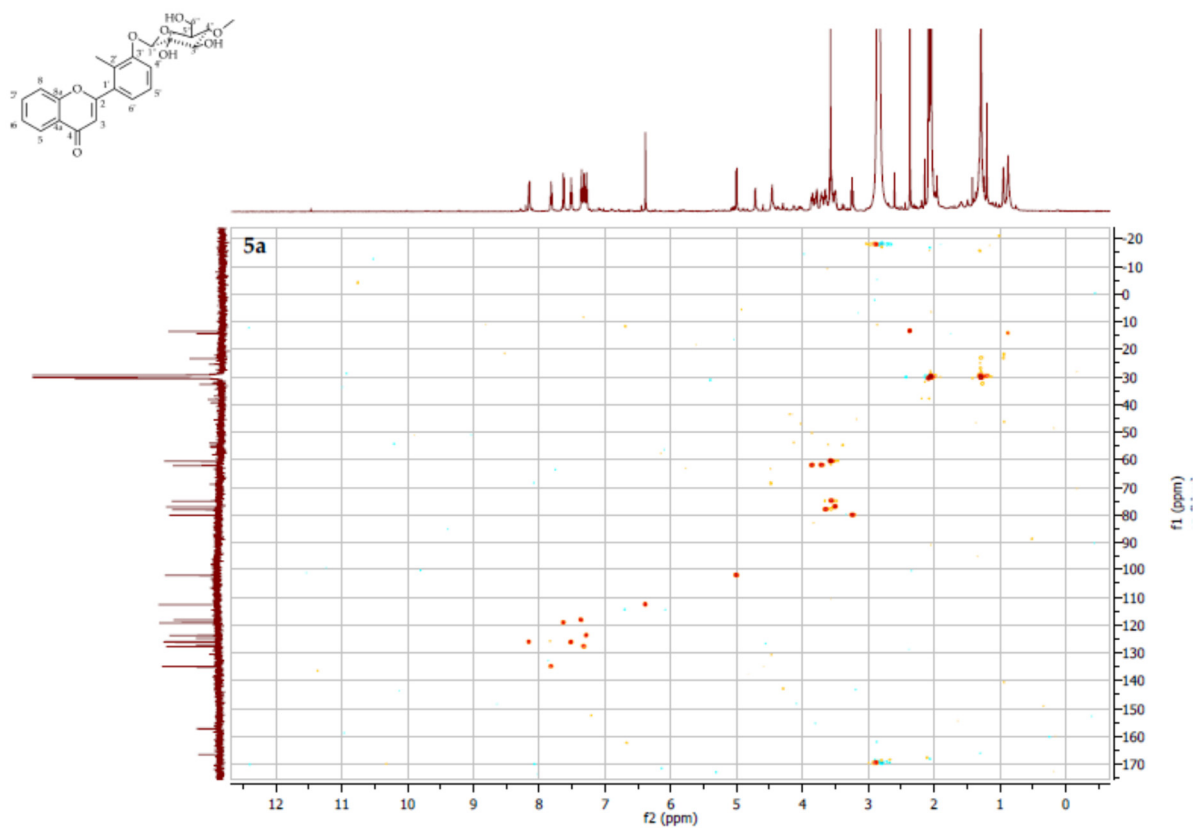


Figure S129. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**5a**)

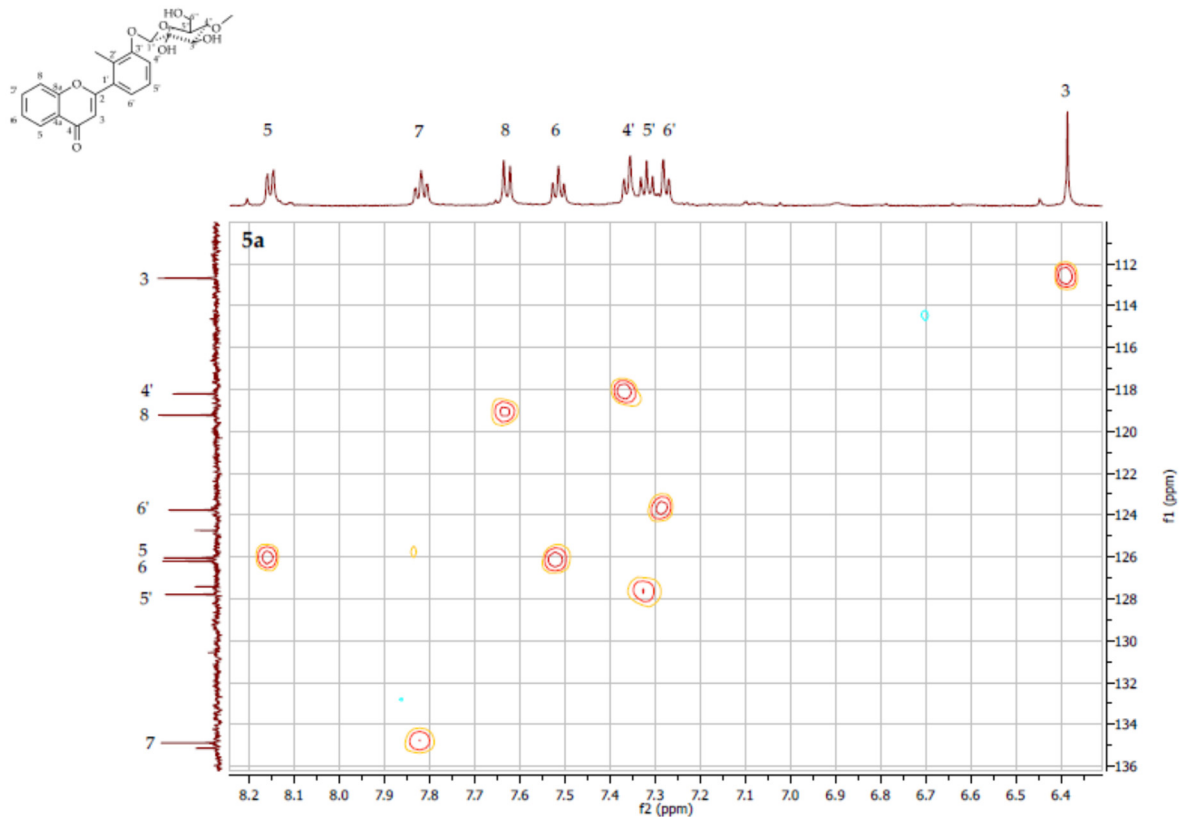


Figure S130. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**5a**)

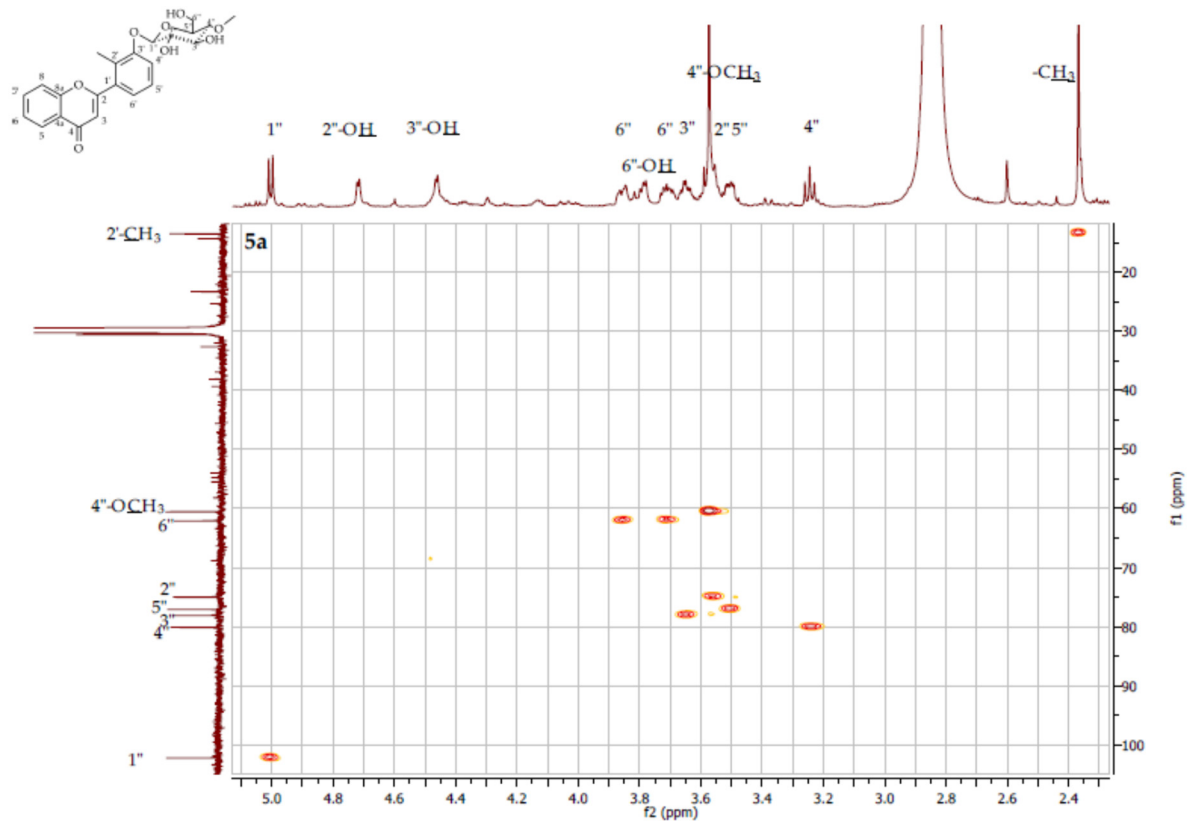


Figure S131. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**5a**)

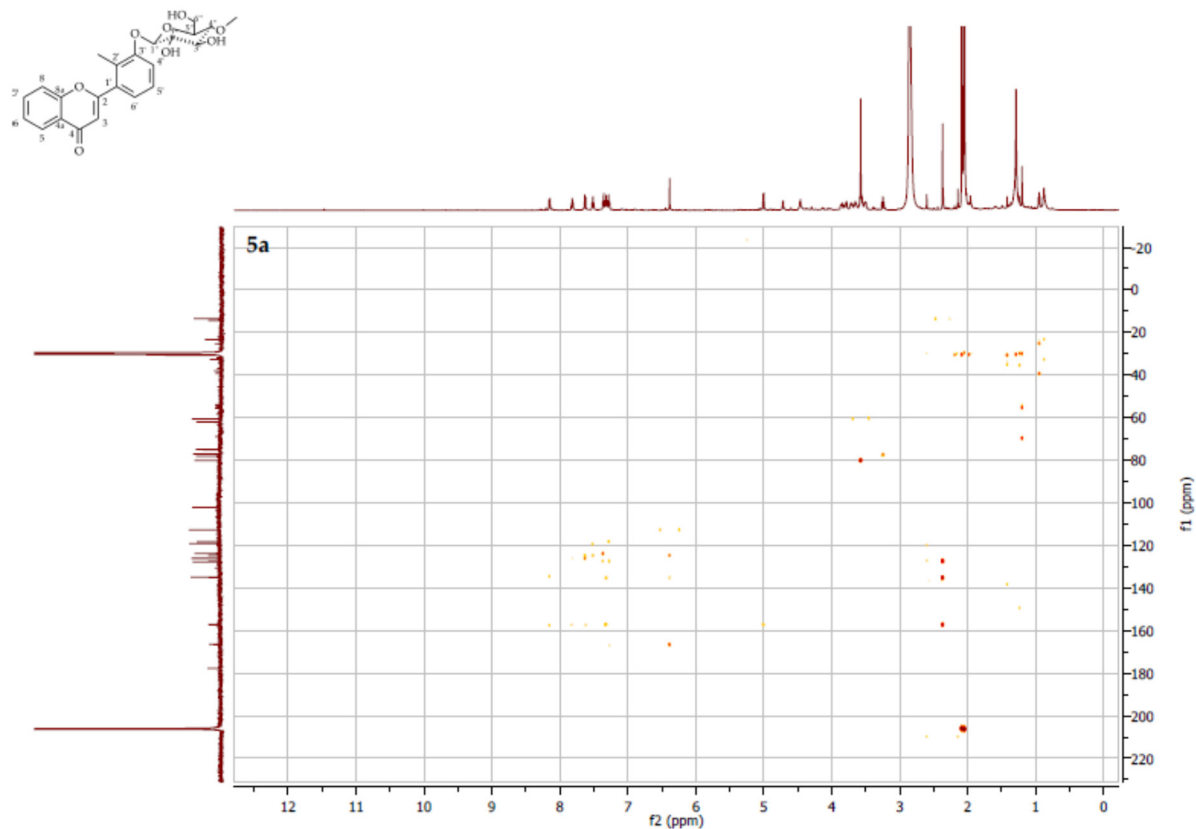


Figure S132. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 3'-O- β -D-(4''-O-methyl)-glucopyranoside (**5a**)

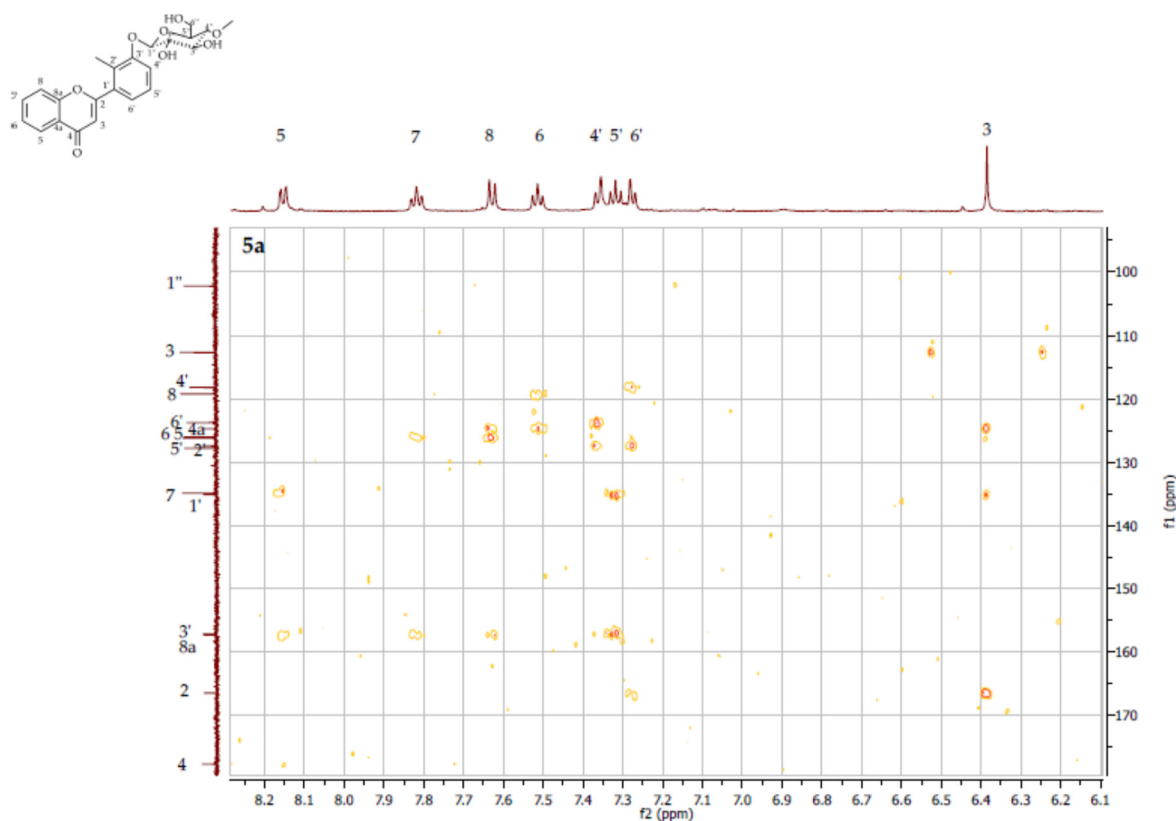


Figure S133. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 3'-O-β-D-(4''-O-methyl)-glucopyranoside (5a)

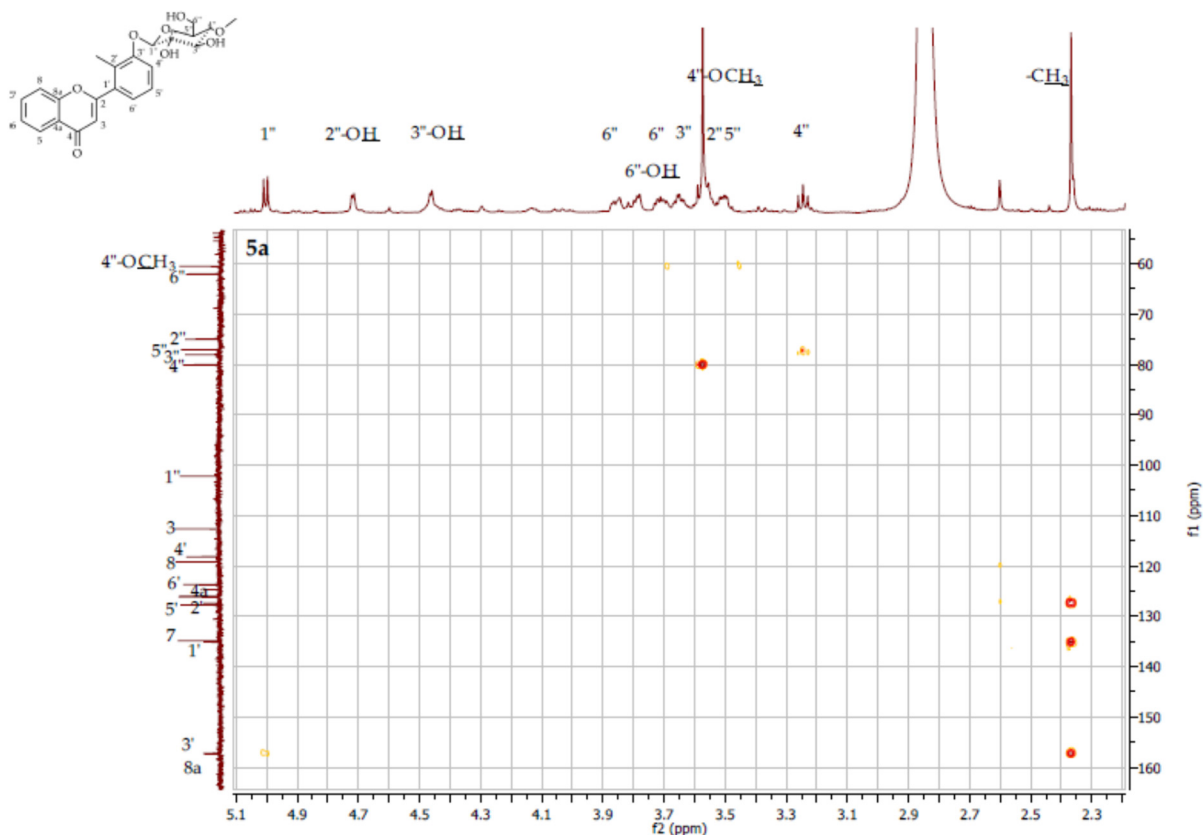


Figure S134. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 3'-O-β-D-(4''-O-methyl)-glucopyranoside (5a)

Molecular formula: C₂₃H₂₄O₈

Formula weight: 428.15

Ionization mode: positive

Precursor: [M + H]⁺ 429.10

429.1000>253.1000 CE: -22.0

429.1000>121.0000 CE: -55.0

429.1000>159.0000 CE: -53.0

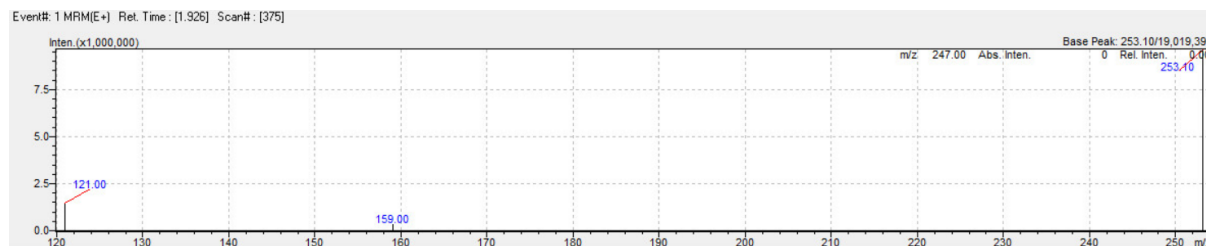
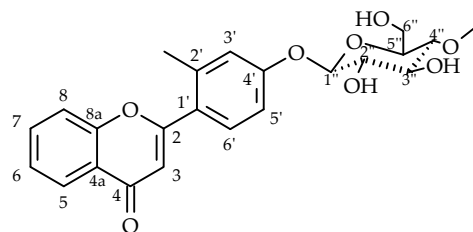


Figure S135. MS analysis of 2'-methylflavone 4'-O- β -D-(4''-O-methyl)-glucopyranoside (**5b**)

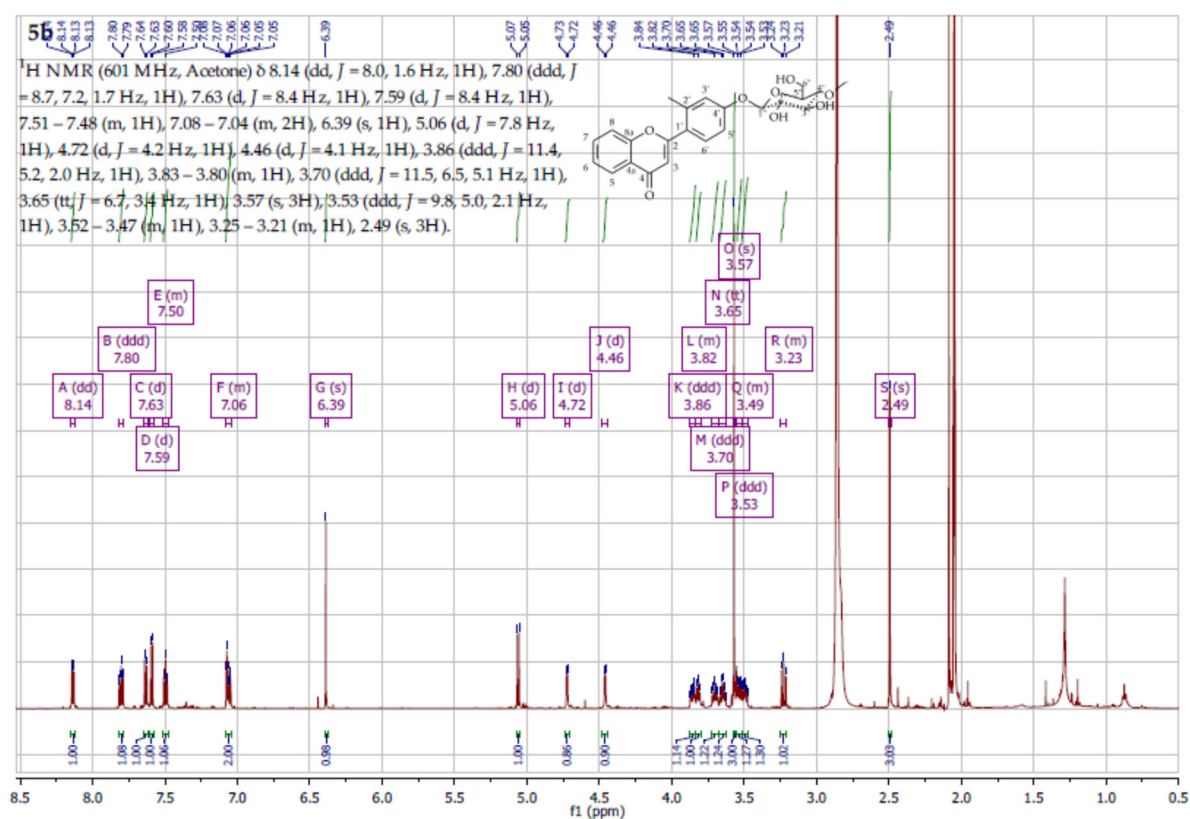


Figure S136. ¹H NMR spectrum (δ , acetone-d₆, 600 MHz) of 2'-methylflavone 4'-O- β -D-(4''-O-methyl)-glucopyranoside (**5b**)

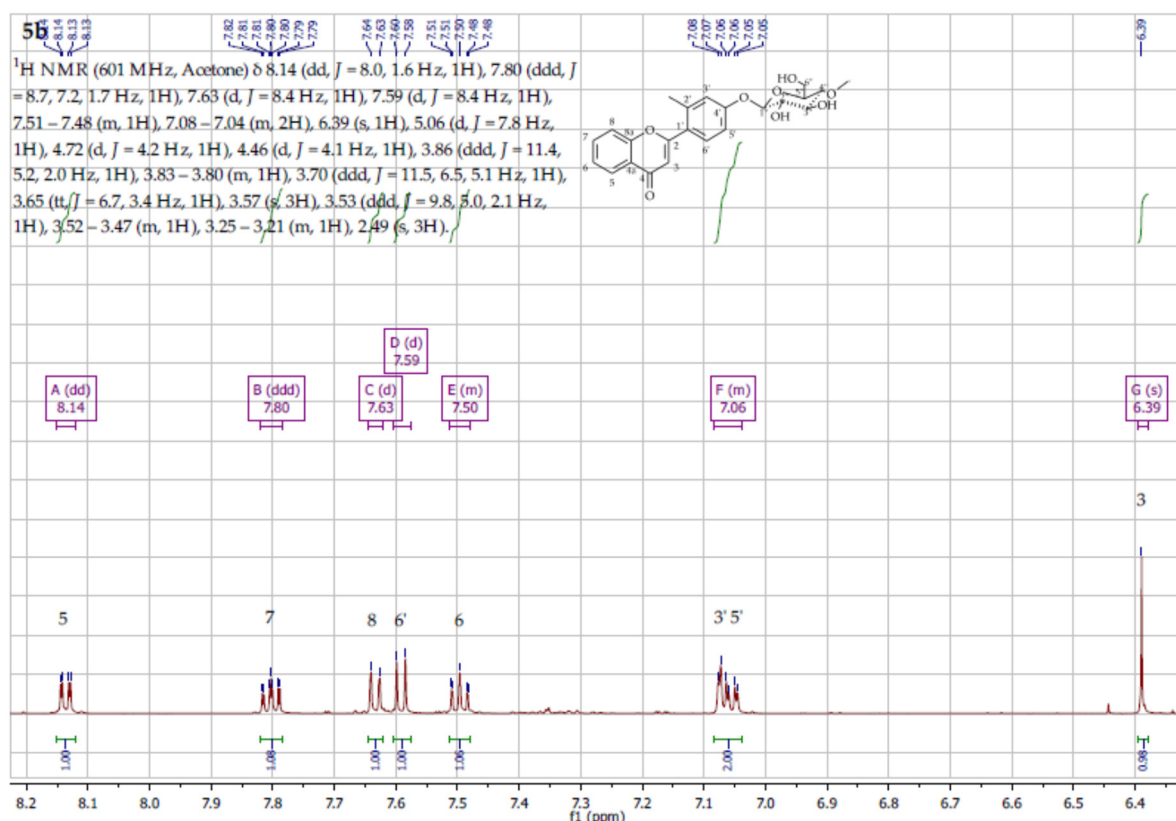


Figure S137. ¹H NMR spectrum expansion (δ, acetone-d₆, 600 MHz) of 2'-methylflavone 4'-O-β-D-(4''-O-methyl)-glucopyranoside (**5b**)

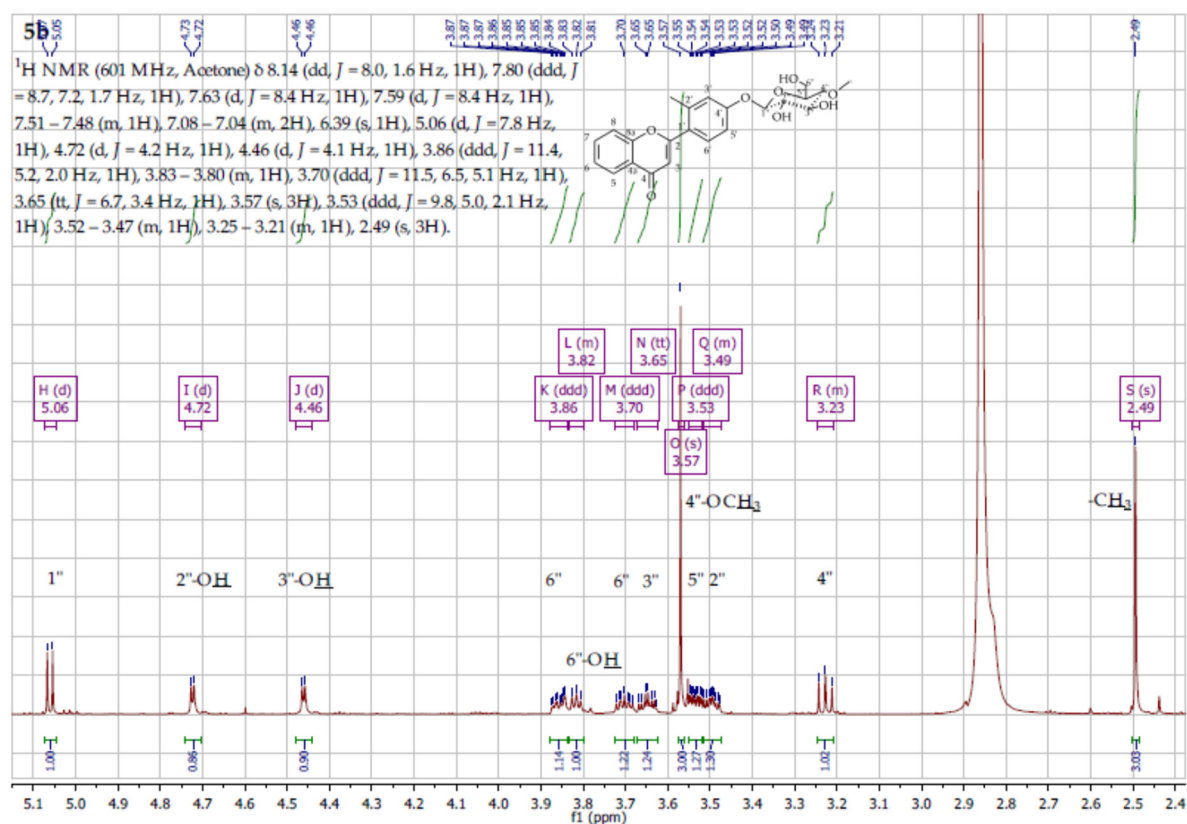


Figure S138. ^1H NMR spectrum expansion (δ , acetone- d_6 , 600 MHz) of 2'-methylflavone 4'- O - β -D-(4''- O -methyl)-glucopyranoside (**5b**)

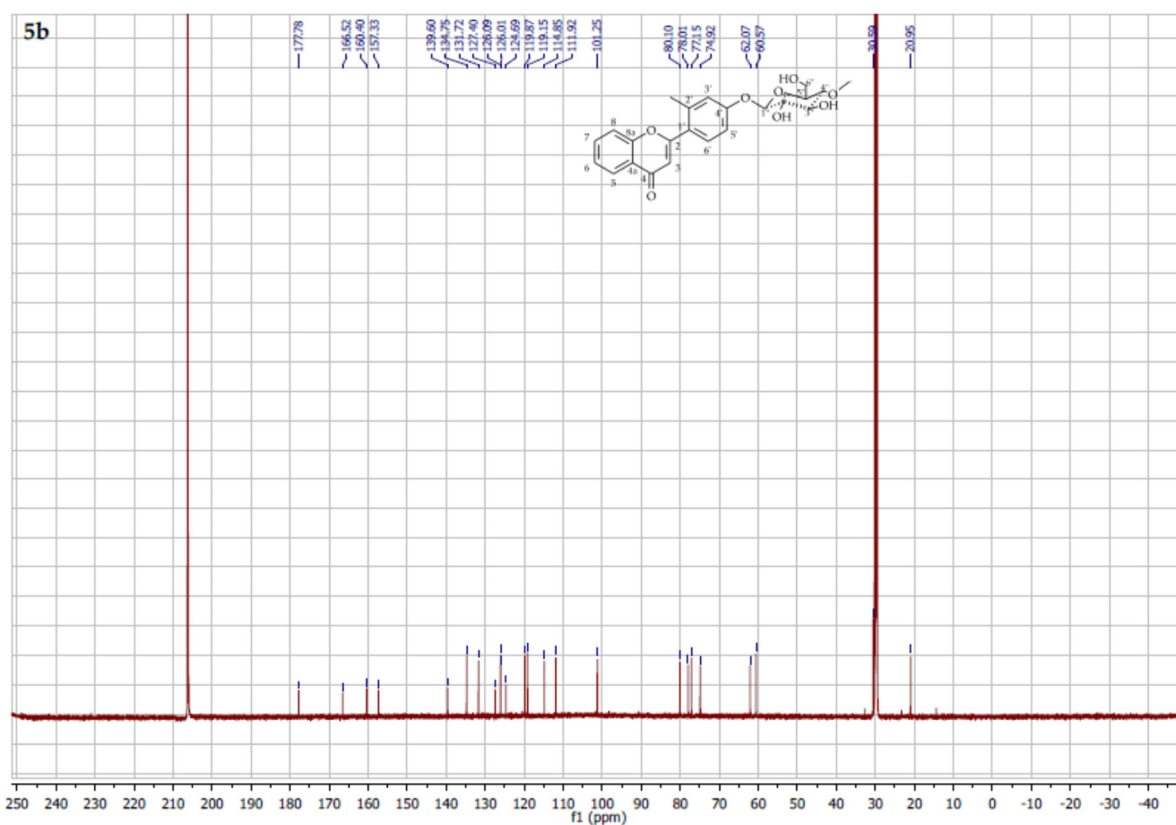


Figure S139. ^{13}C NMR spectrum of (δ , acetone- d_6 , 151 MHz) 2'-methylflavone 4'-O- β -D-(4''-O-methyl)-glucopyranoside (**5b**)

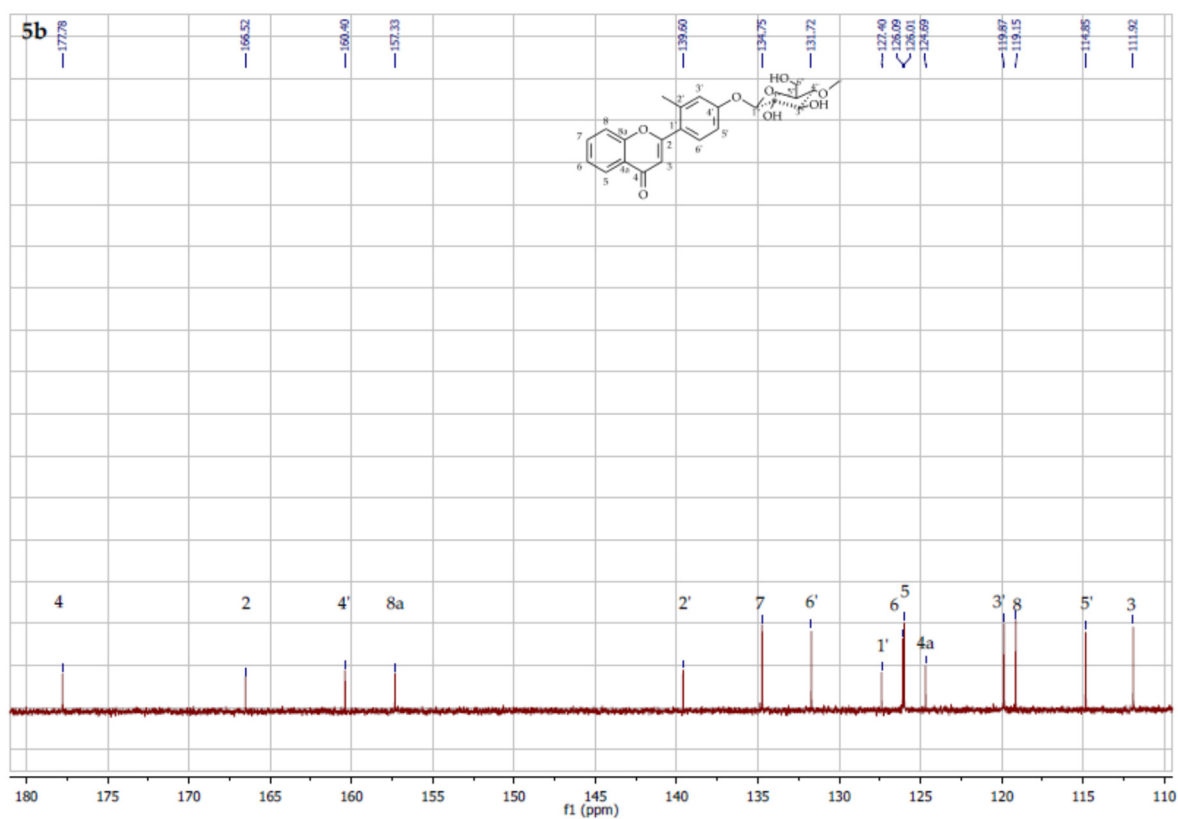


Figure S140. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavone 4'-O- β -D-(4''-O-methyl)-glucopyranoside (**5b**)

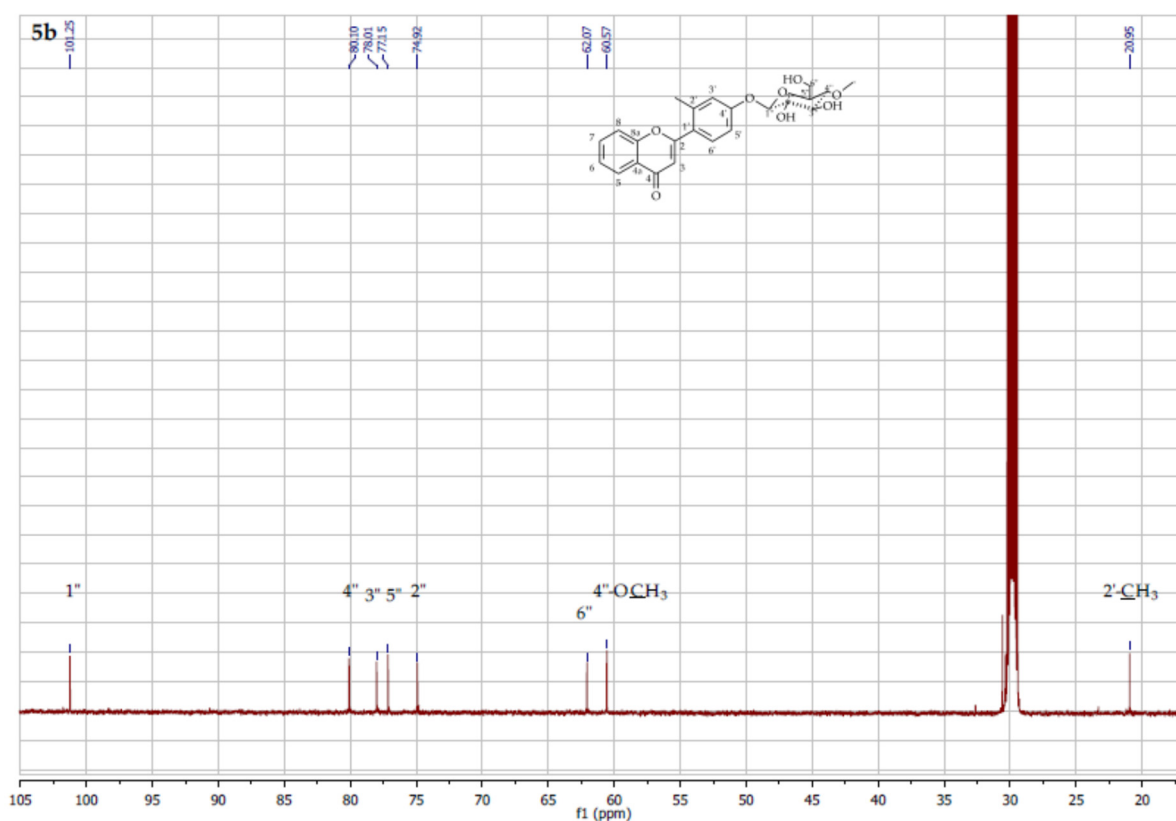


Figure S141. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavone 4'- O - β -D-(4''- O -methyl)-glucopyranoside (**5b**)

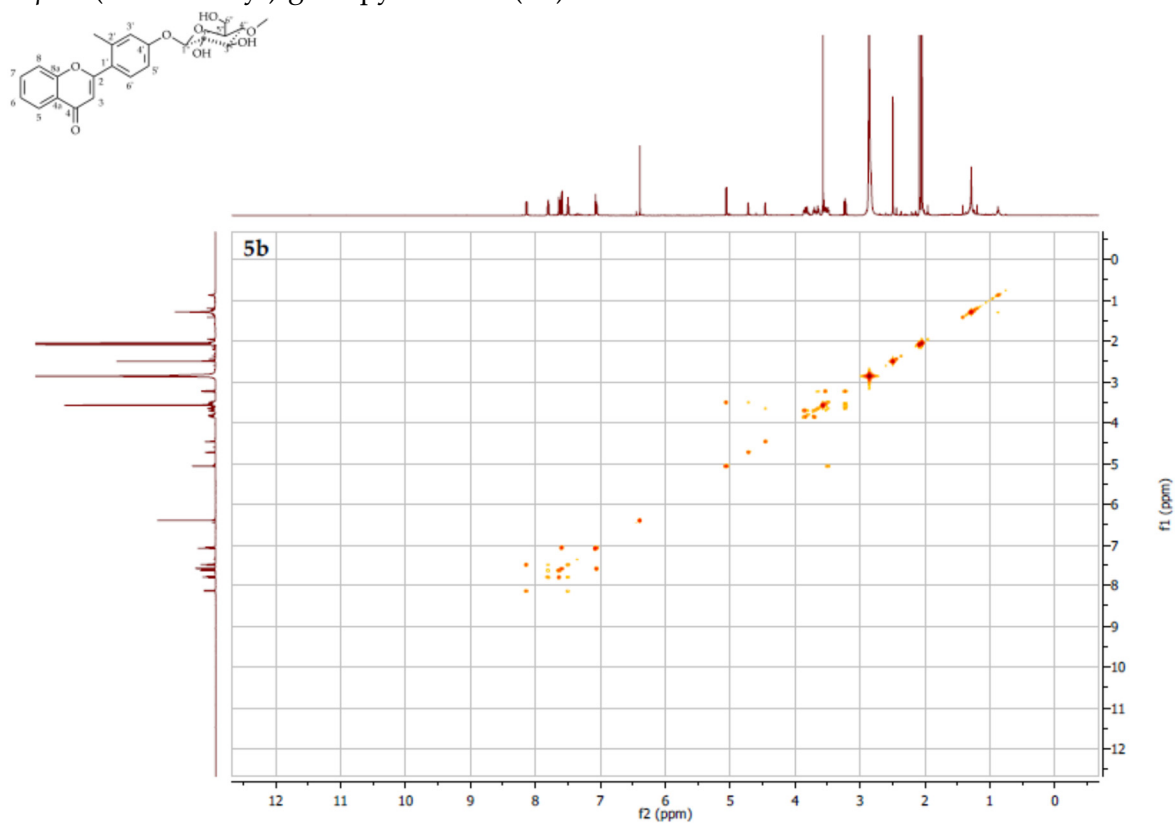


Figure S142. COSY contour map – $^1\text{H} \times ^1\text{H}$ 2'-methylflavone 4'- O - β -D-(4''- O -methyl)-glucopyranoside (**5b**)

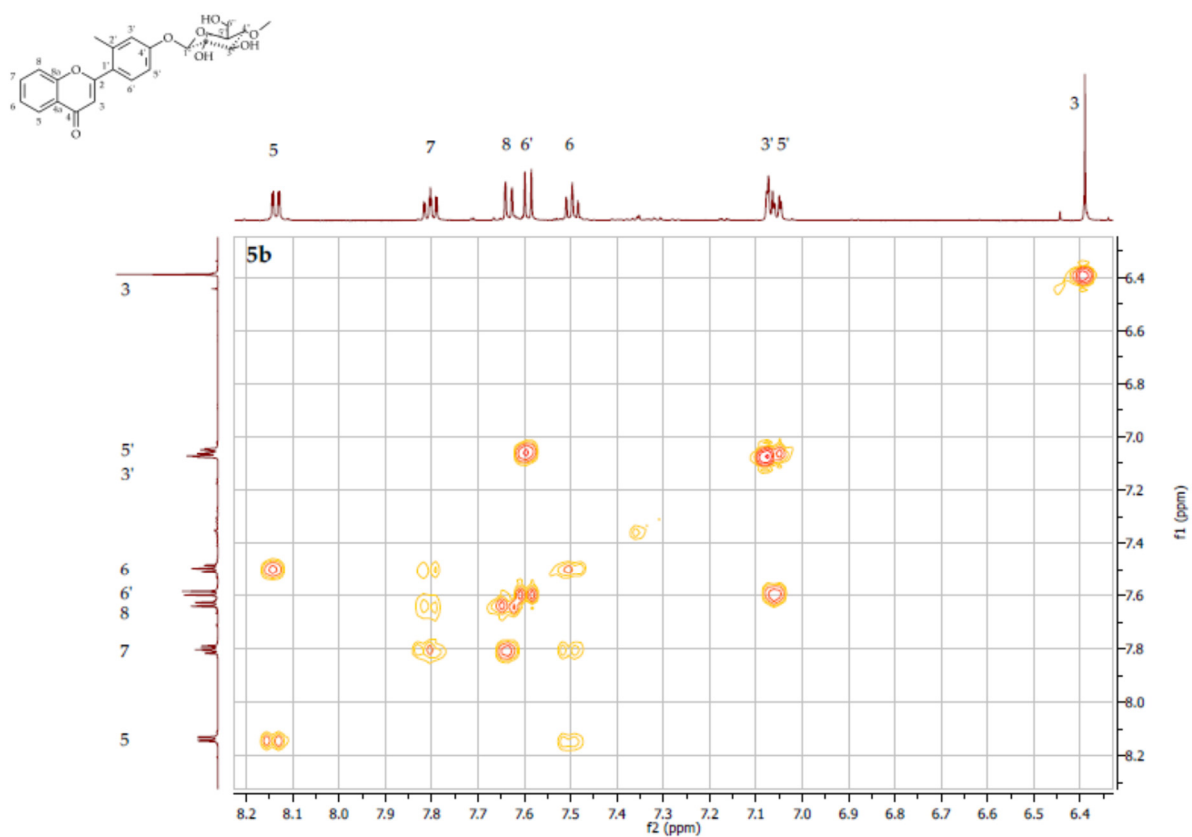


Figure S143. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methylflavone 4'-O- β -D-(4''-O-methyl)-glucopyranoside (**5b**)

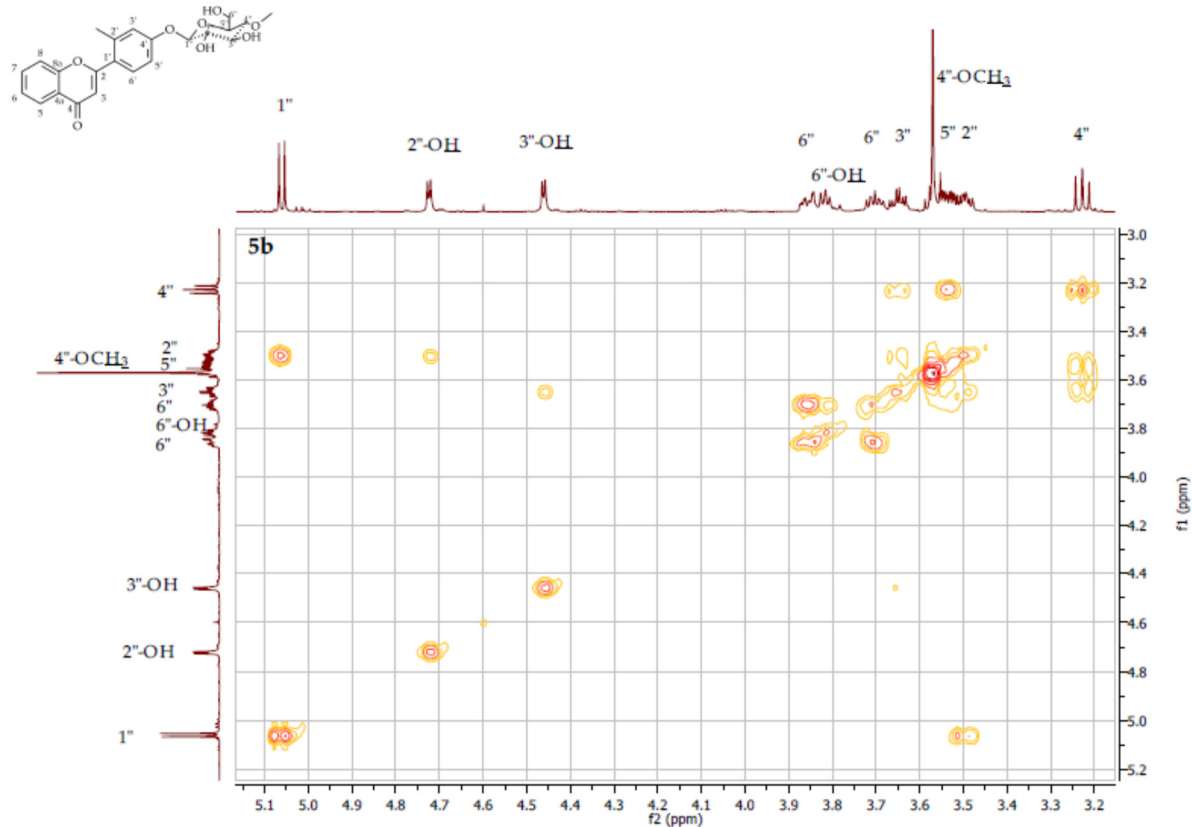


Figure S144. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methylflavone 4'-O- β -D-(4''-O-methyl)-glucopyranoside (**5b**)

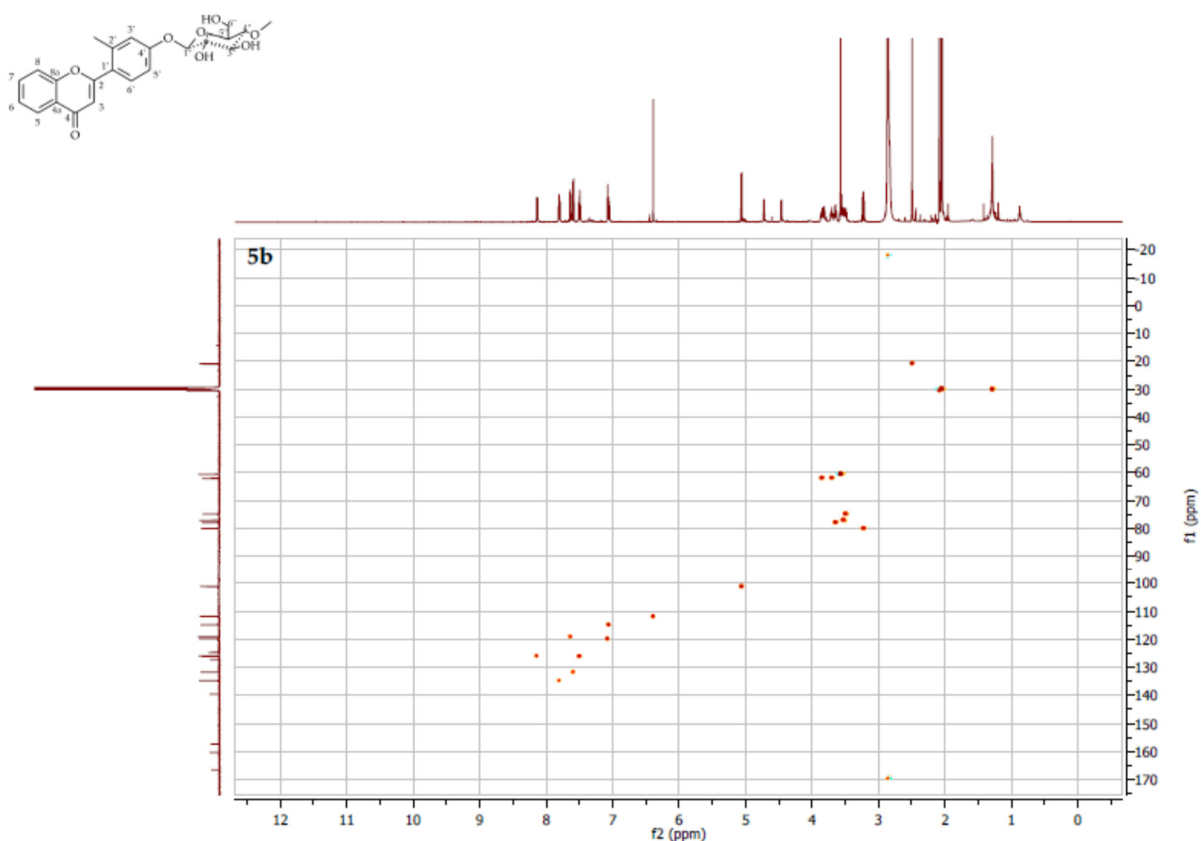


Figure S145. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavone 4'-O- β -D-(4''-O-methyl)-glucopyranoside (**5b**)

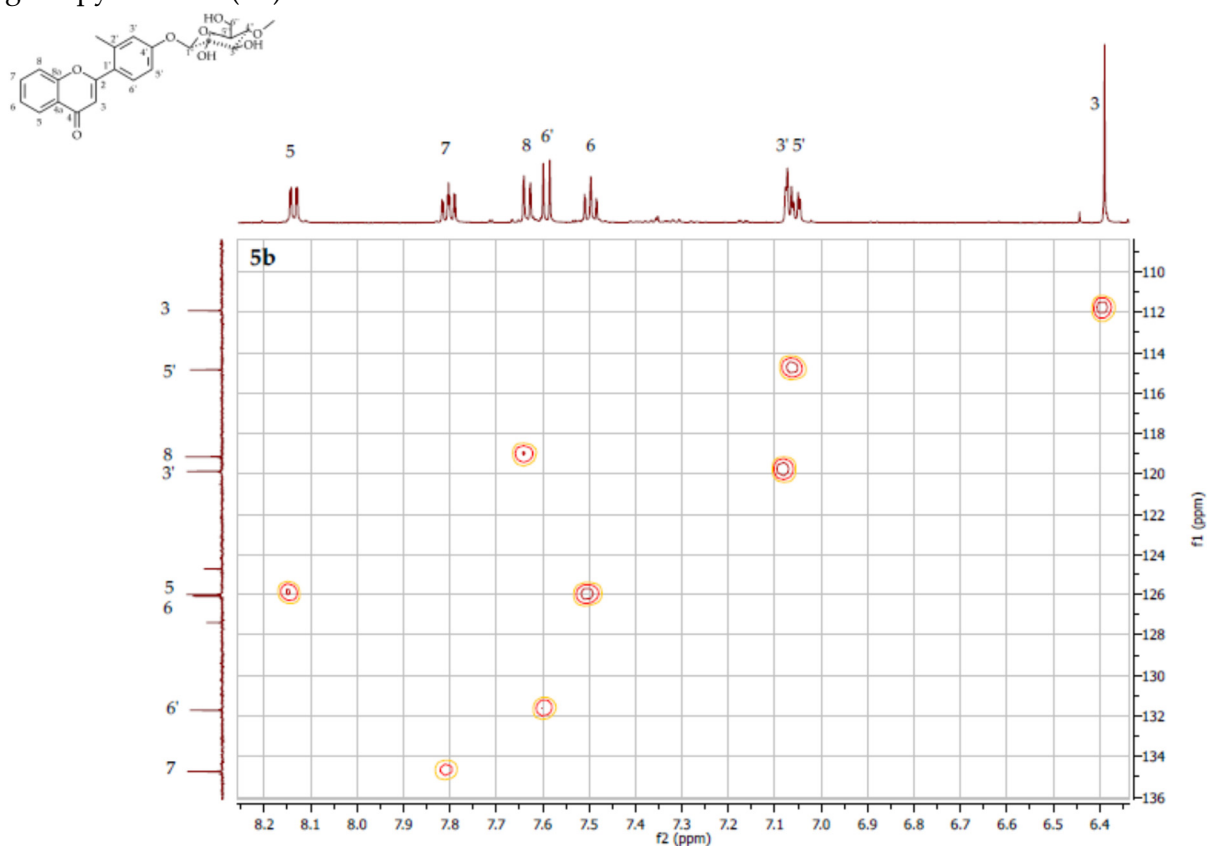


Figure S146. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 4'-O- β -D-(4''-O-methyl)-glucopyranoside (**5b**)

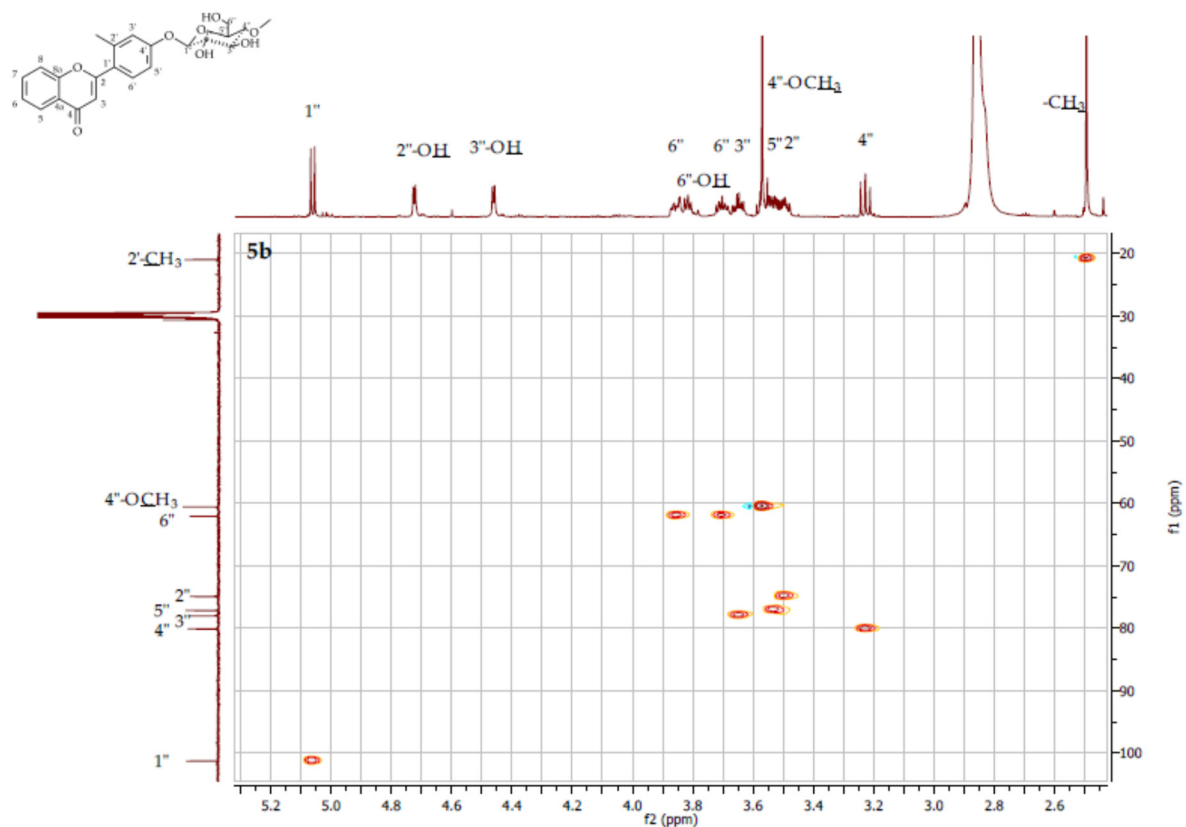


Figure S147. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 4'-O- β -D-(4''-O-methyl)-glucopyranoside (**5b**)

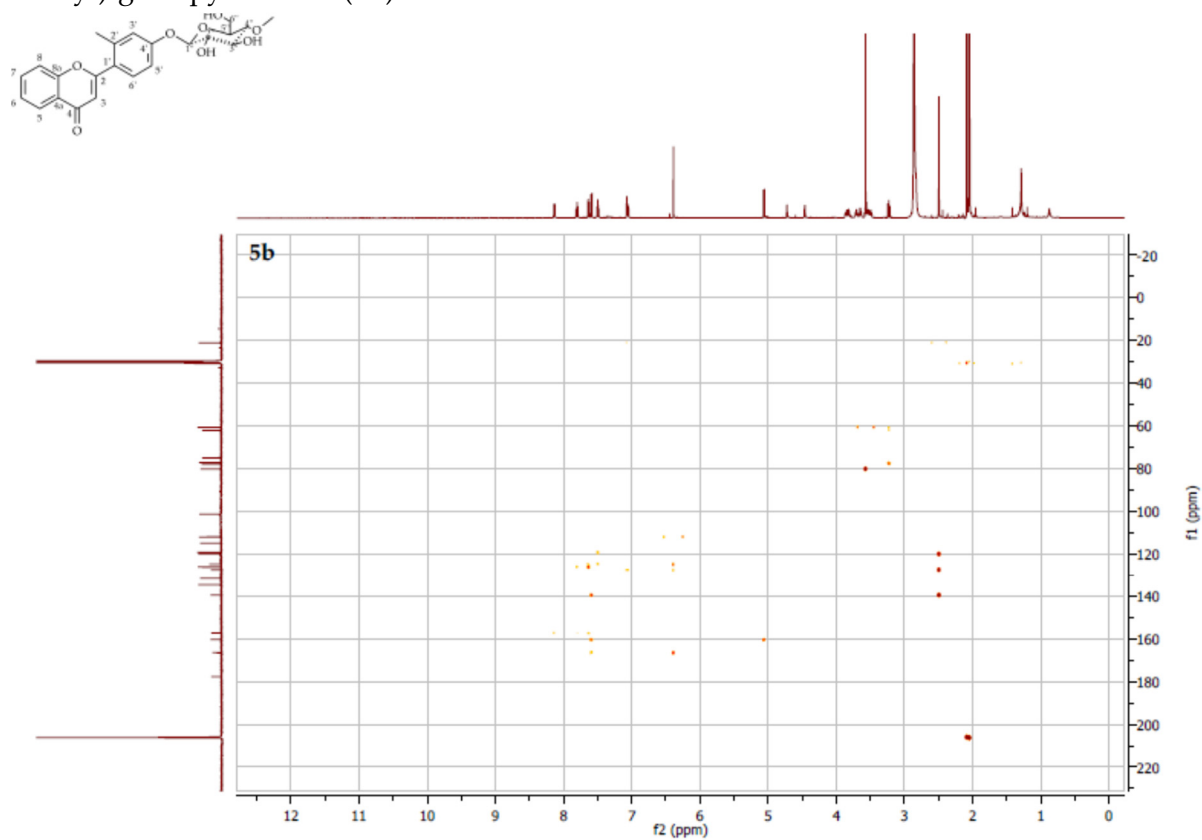


Figure S148. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavone 4'-O- β -D-(4''-O-methyl)-glucopyranoside (**5b**)

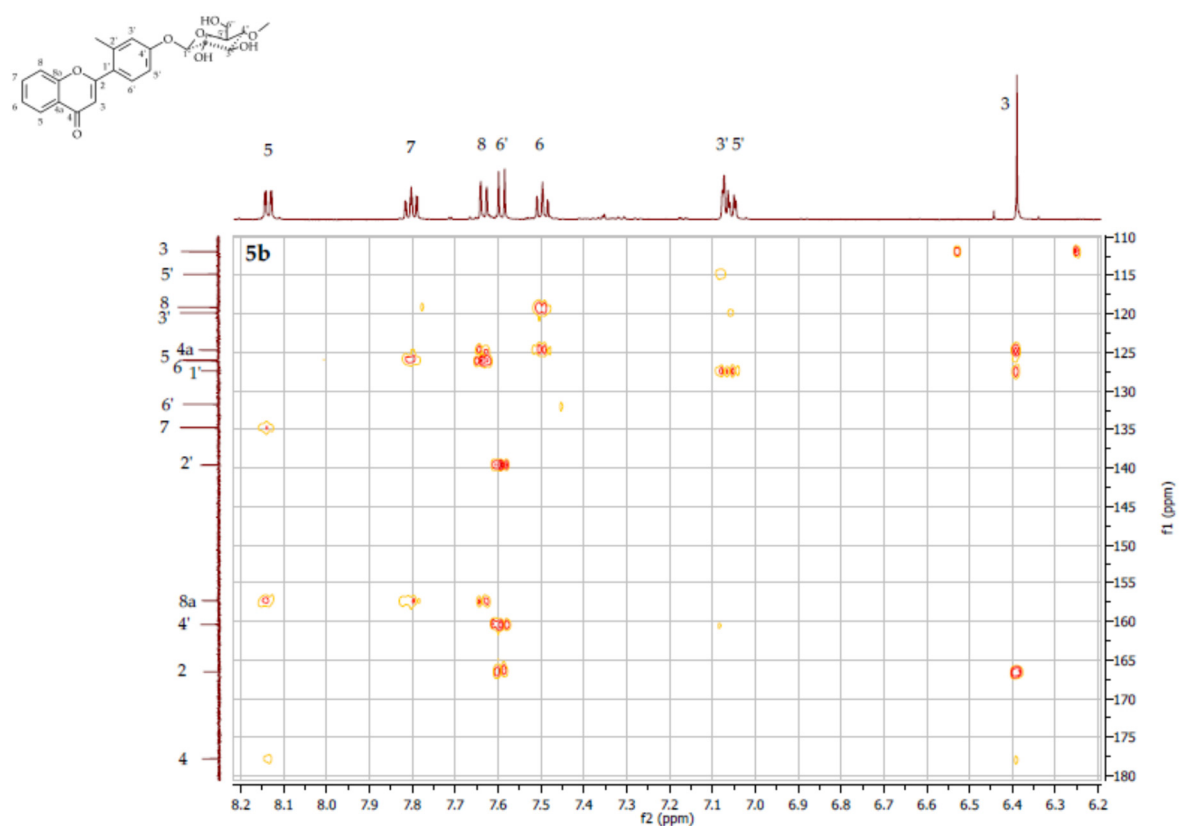


Figure S149. HMBC contour map – ¹H × ¹³C expansion of 2'-methylflavone 4'-O-β-D-(4''-O-methyl)-glucopyranoside (**5b**)

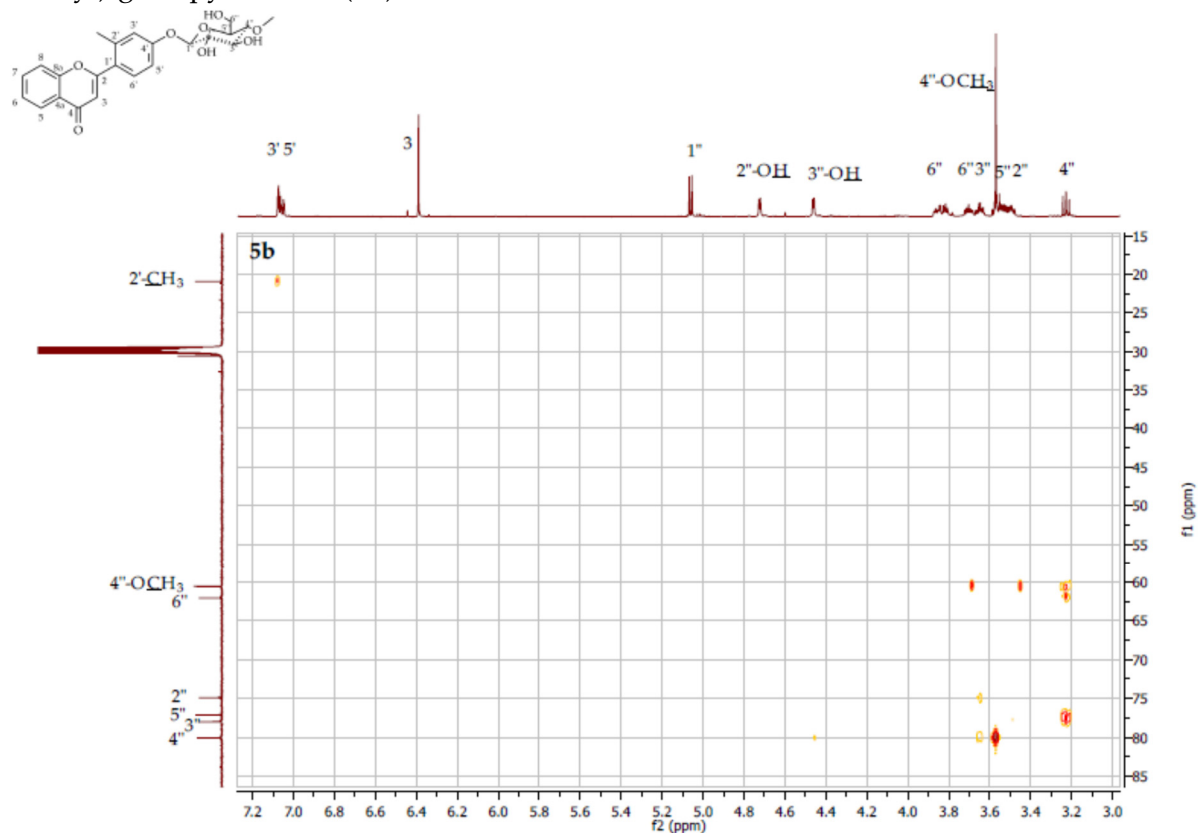


Figure S150. HMBC contour map – ¹H × ¹³C expansion of 2'-methylflavone 4'-O-β-D-(4''-O-methyl)-glucopyranoside (**5b**)

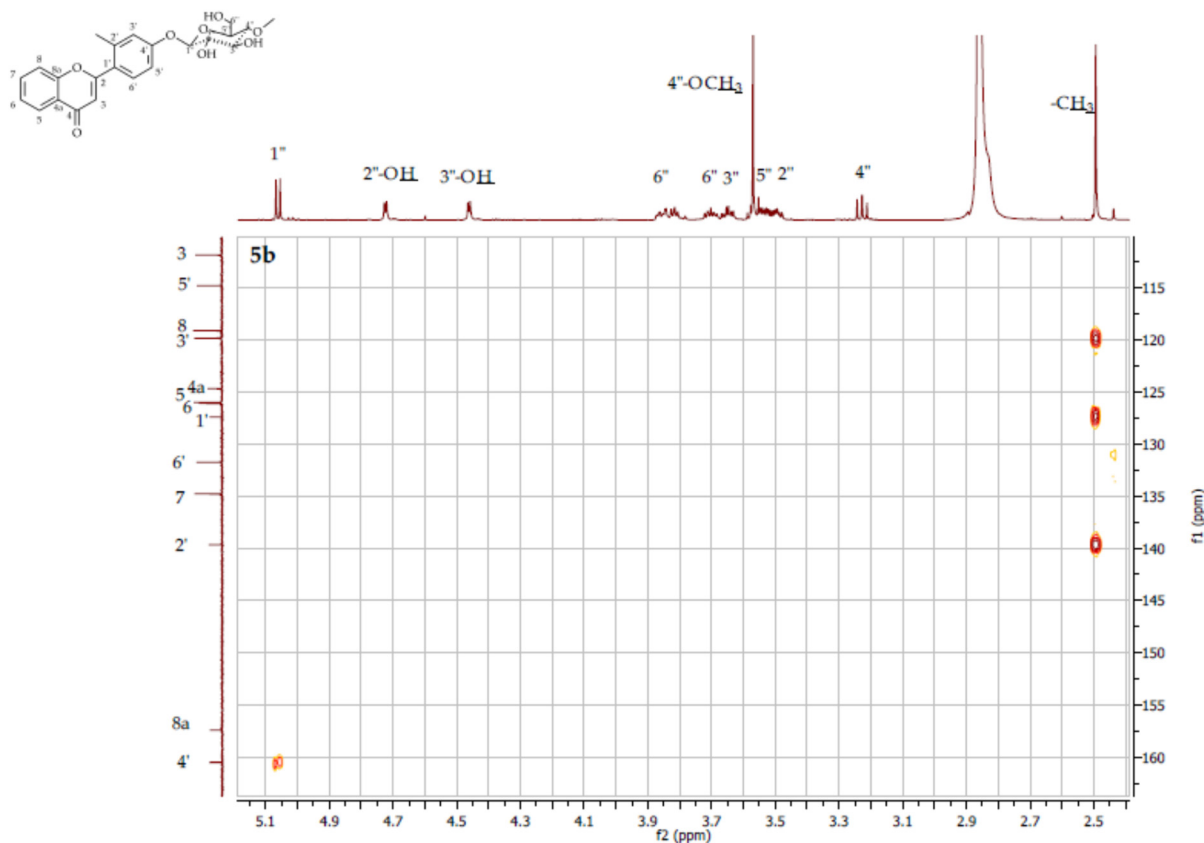


Figure S151. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 4'-O- β -D-(4''-O-methyl)-glucopyranoside (**5b**)

Molecular formula = $\text{C}_{23}\text{H}_{24}\text{O}_8$

Formula weight = 428.15

Ionization mode = positive

Precursor: $[\text{M} + \text{H}]^+ 429.20$

429.2000 > 253.0500 CE: -32.0

429.2000 > 294.9500 CE: -25.0

429.2000 > 121.0500 CE: -55.0

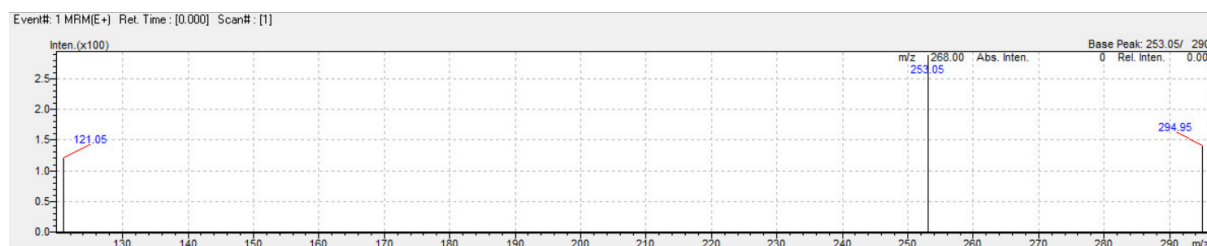
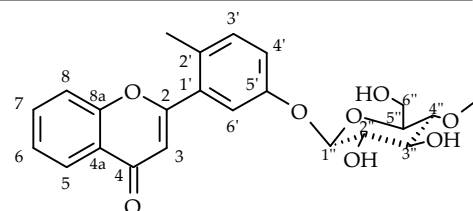


Figure S152. MS analysis of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

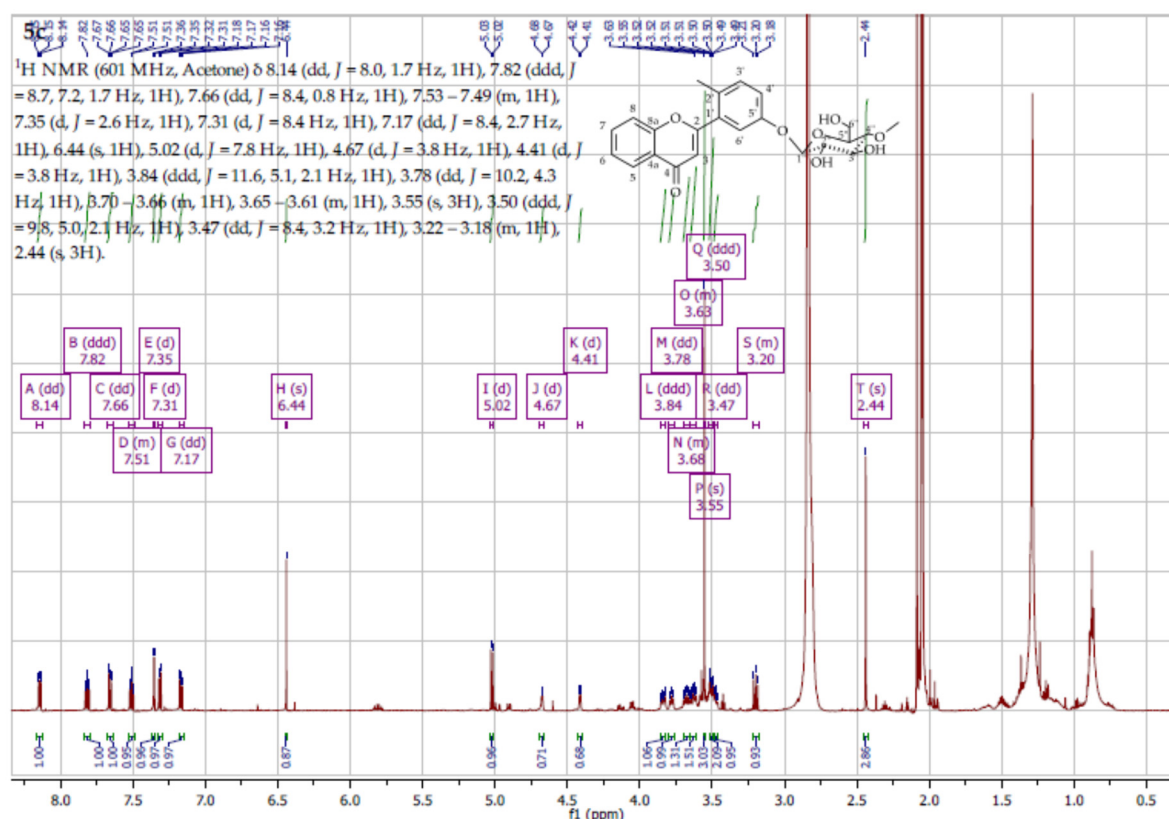


Figure S153. ¹H NMR spectrum (δ, acetone-d₆, 600 MHz) of 2'-methylflavone 5'-O-β-D-(4''-O-methyl)-glucopyranoside (5c)

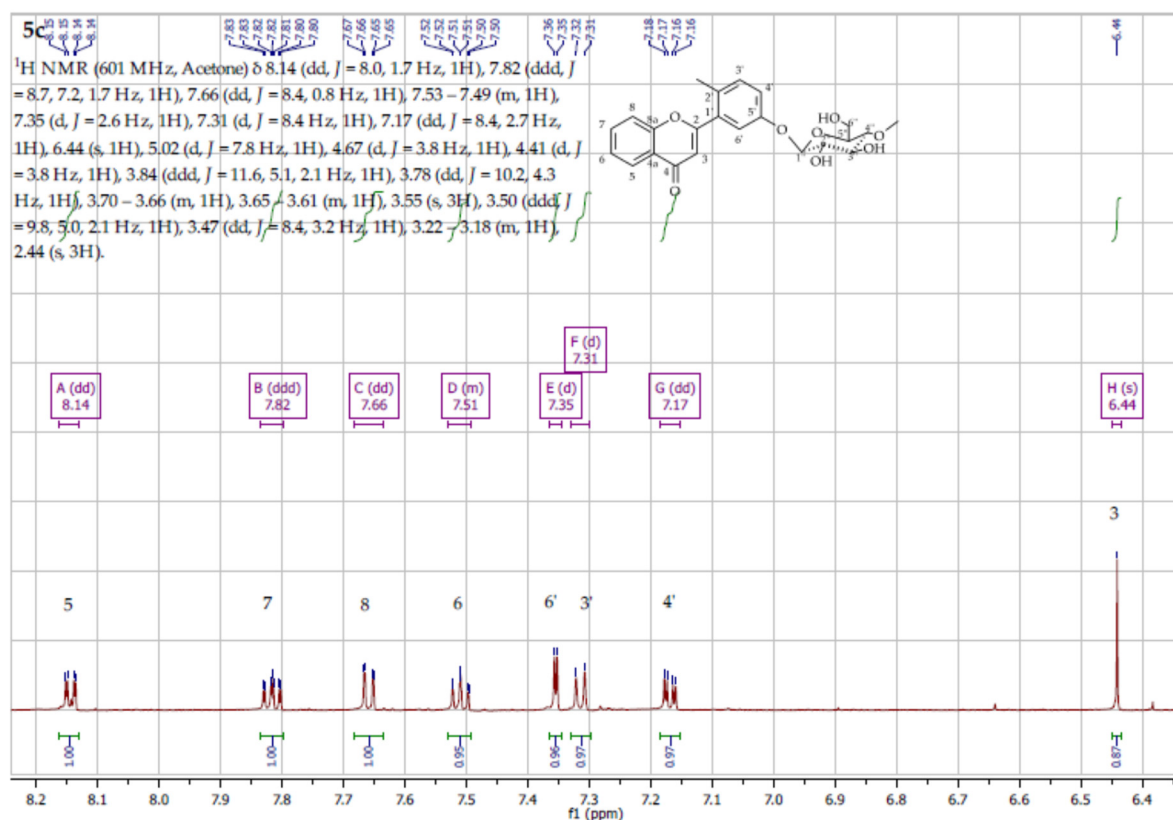
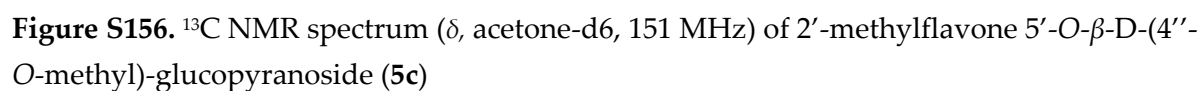
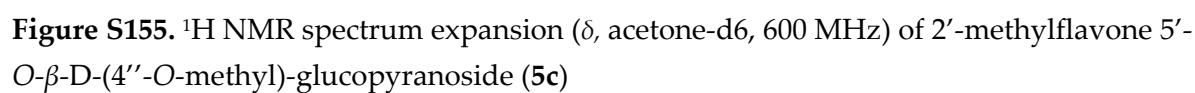


Figure S154. ¹H NMR spectrum expansion (δ, acetone-d₆, 600 MHz) of 2'-methylflavone 5'-O-β-D-(4''-O-methyl)-glucopyranoside (5c)



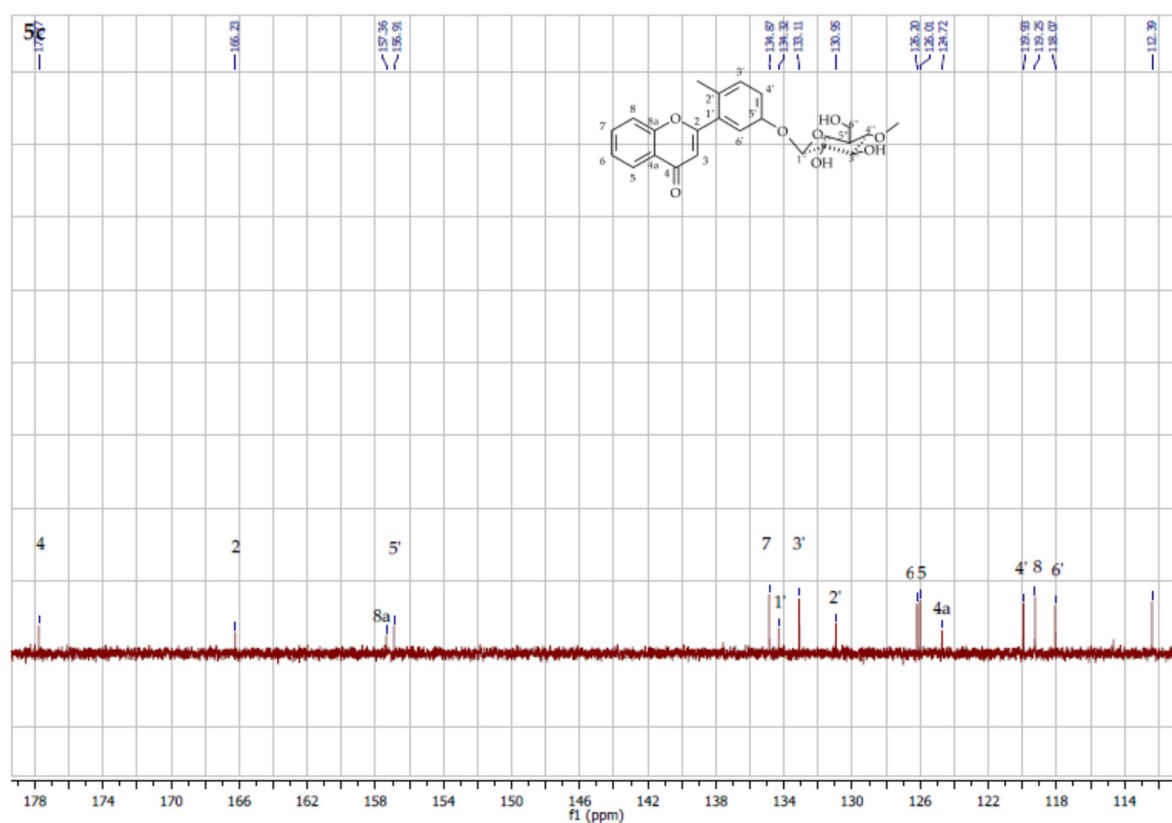


Figure S157. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavone 5'- O - β -D-(4''- O -methyl)-glucopyranoside (**5c**)

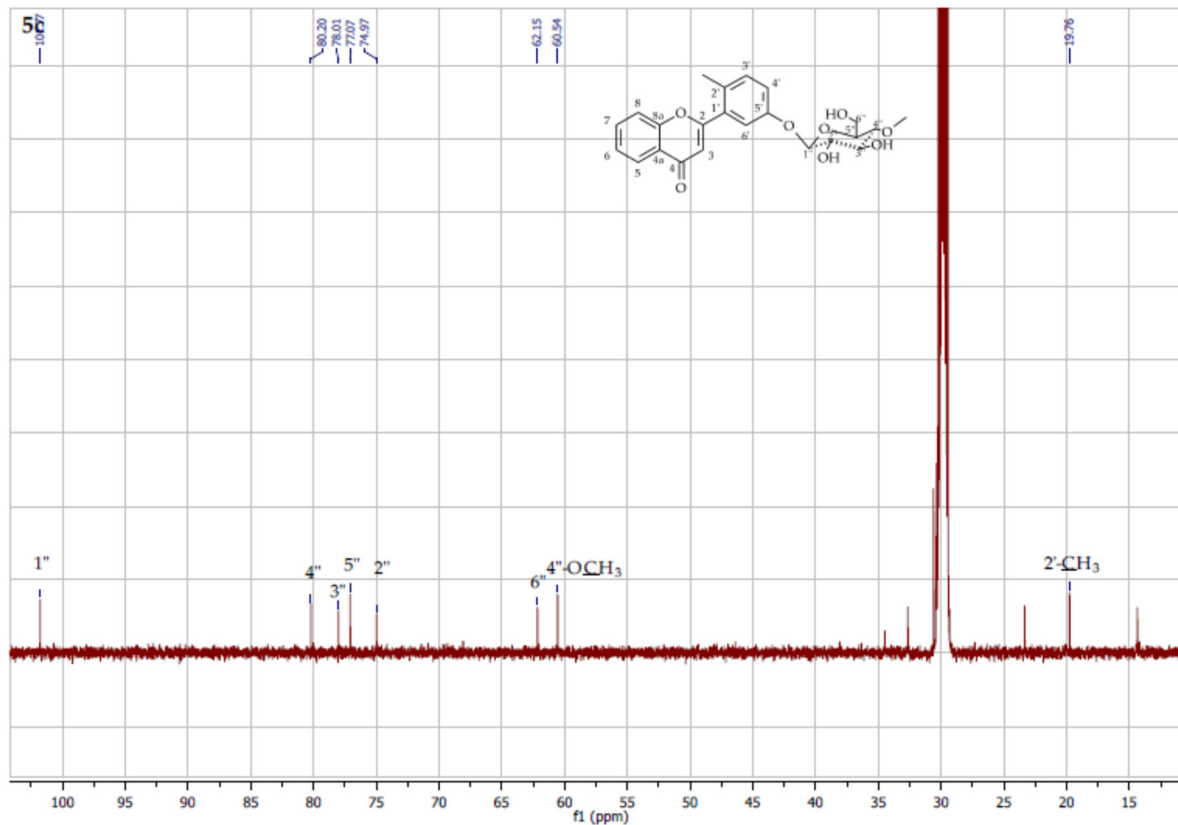


Figure S158. ^{13}C NMR spectrum expansion (δ , acetone- d_6 , 151 MHz) of 2'-methylflavone 5'- O - β -D-(4''- O -methyl)-glucopyranoside (**5c**)

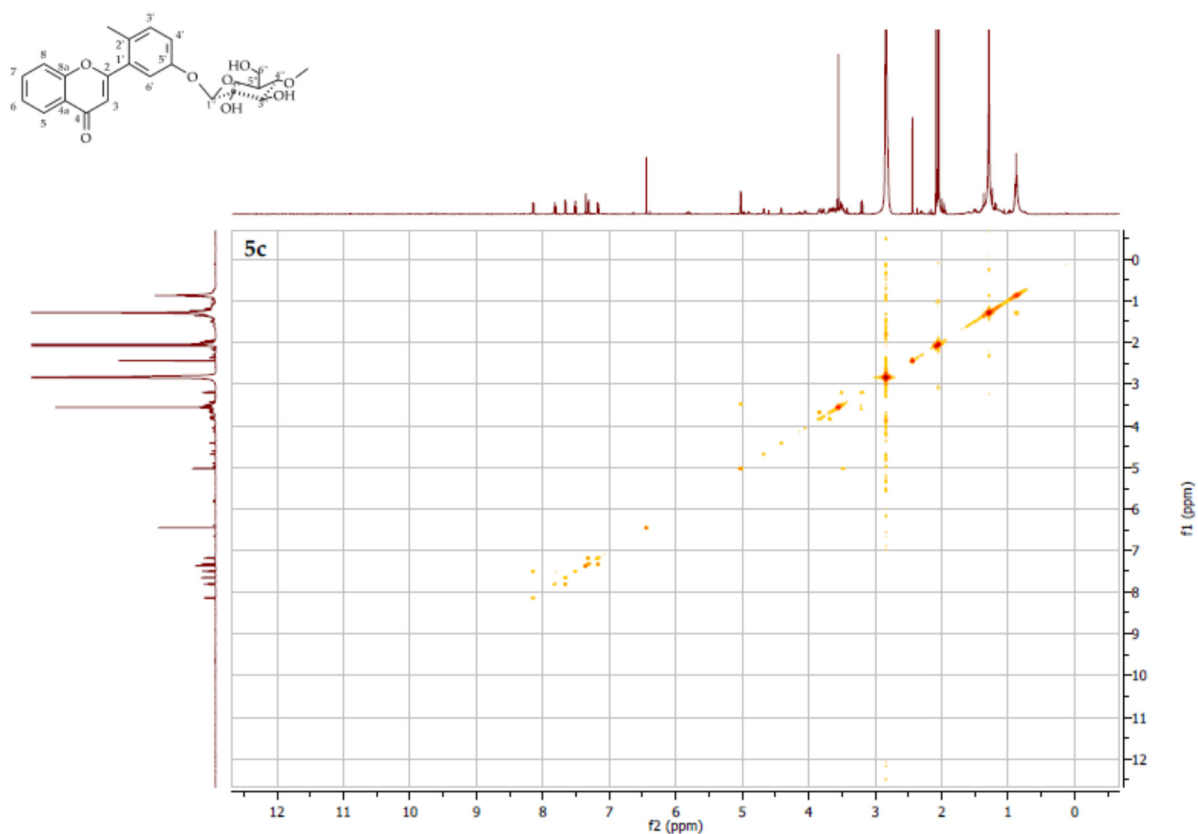


Figure S159. COSY contour map – $^1\text{H} \times ^1\text{H}$ of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

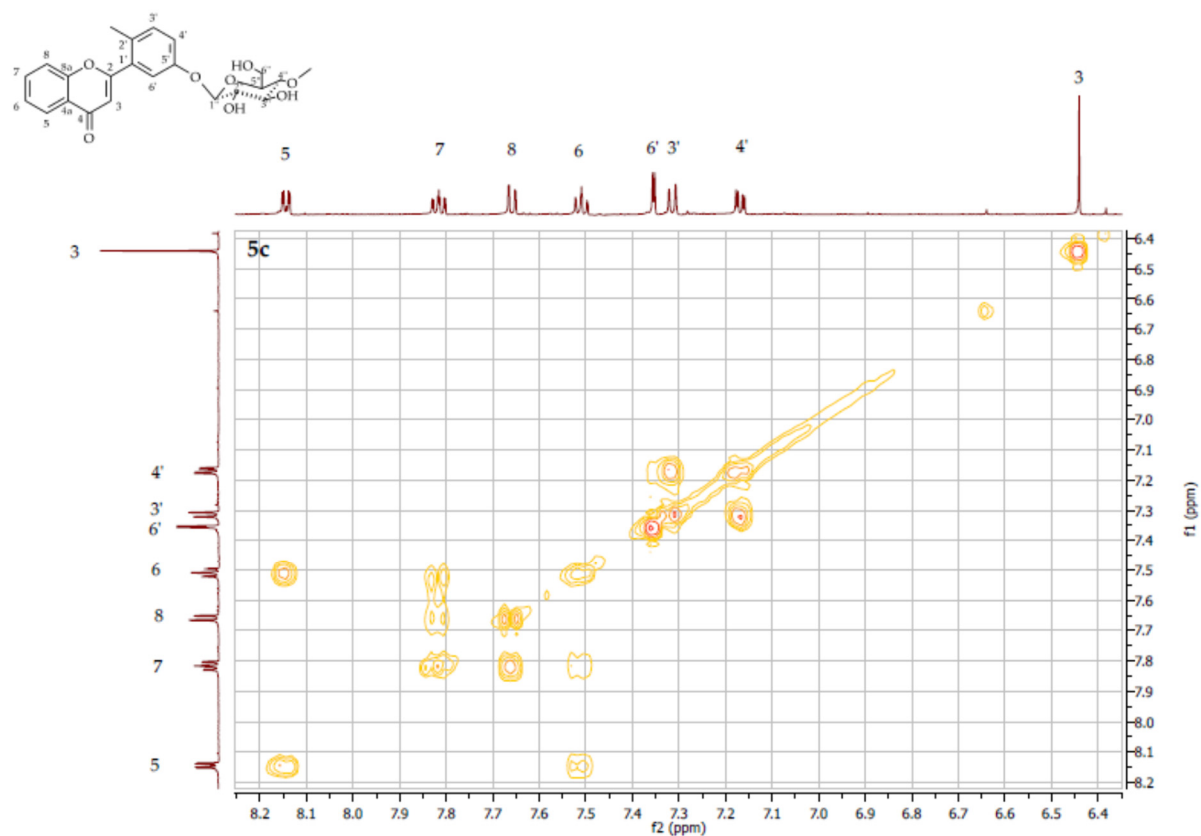


Figure S160. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

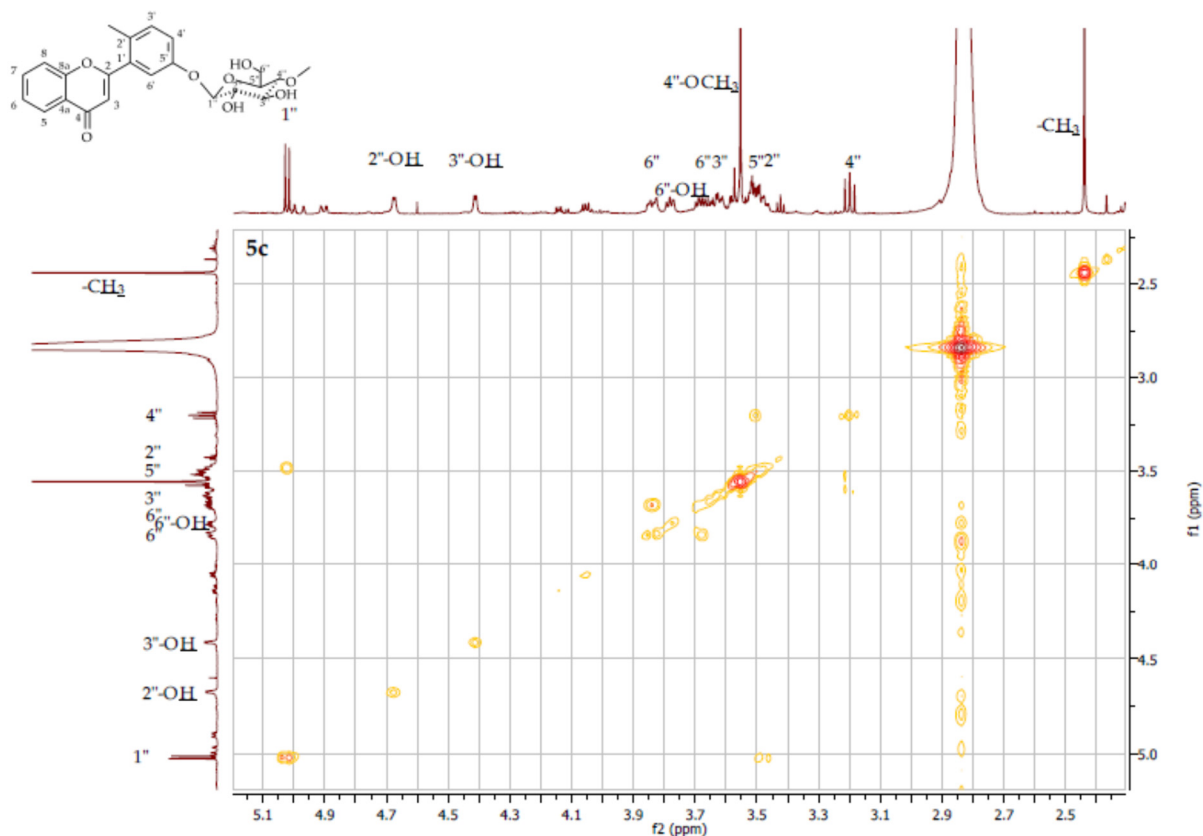


Figure S161. COSY contour map – $^1\text{H} \times ^1\text{H}$ expansion of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

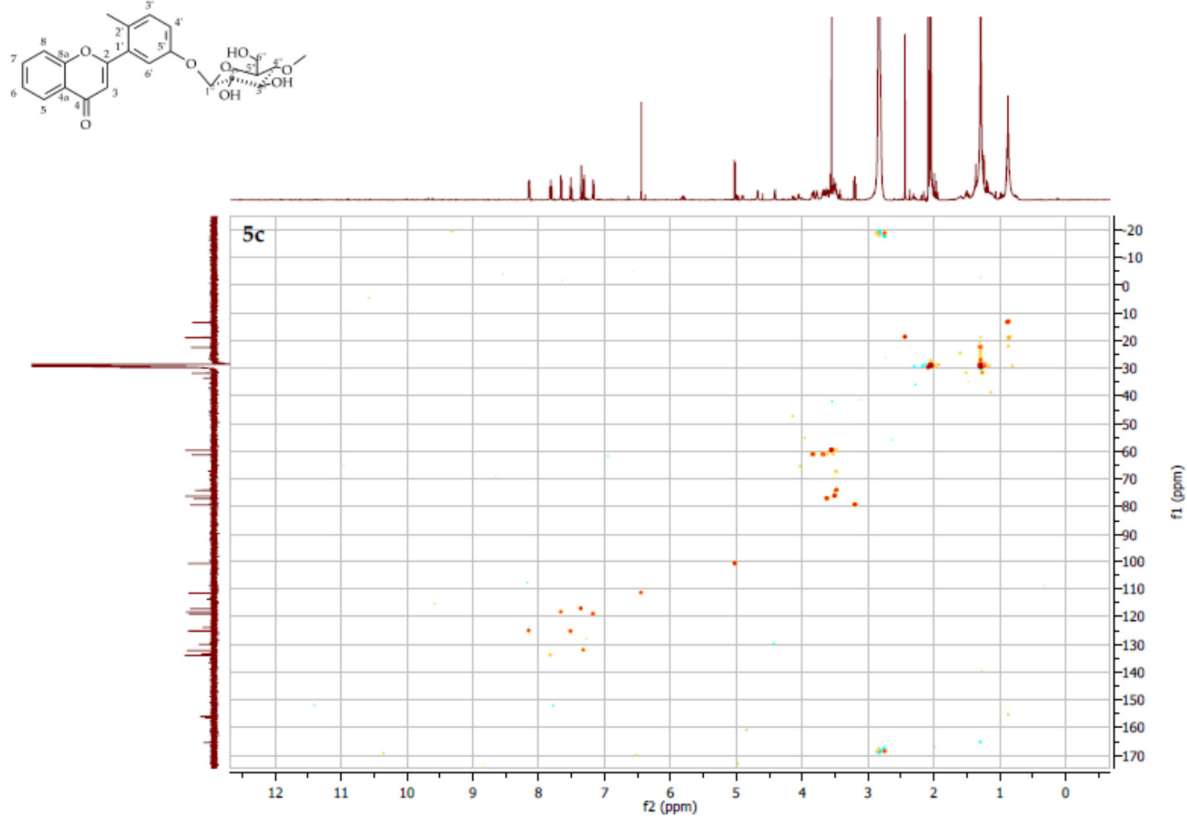


Figure S162. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

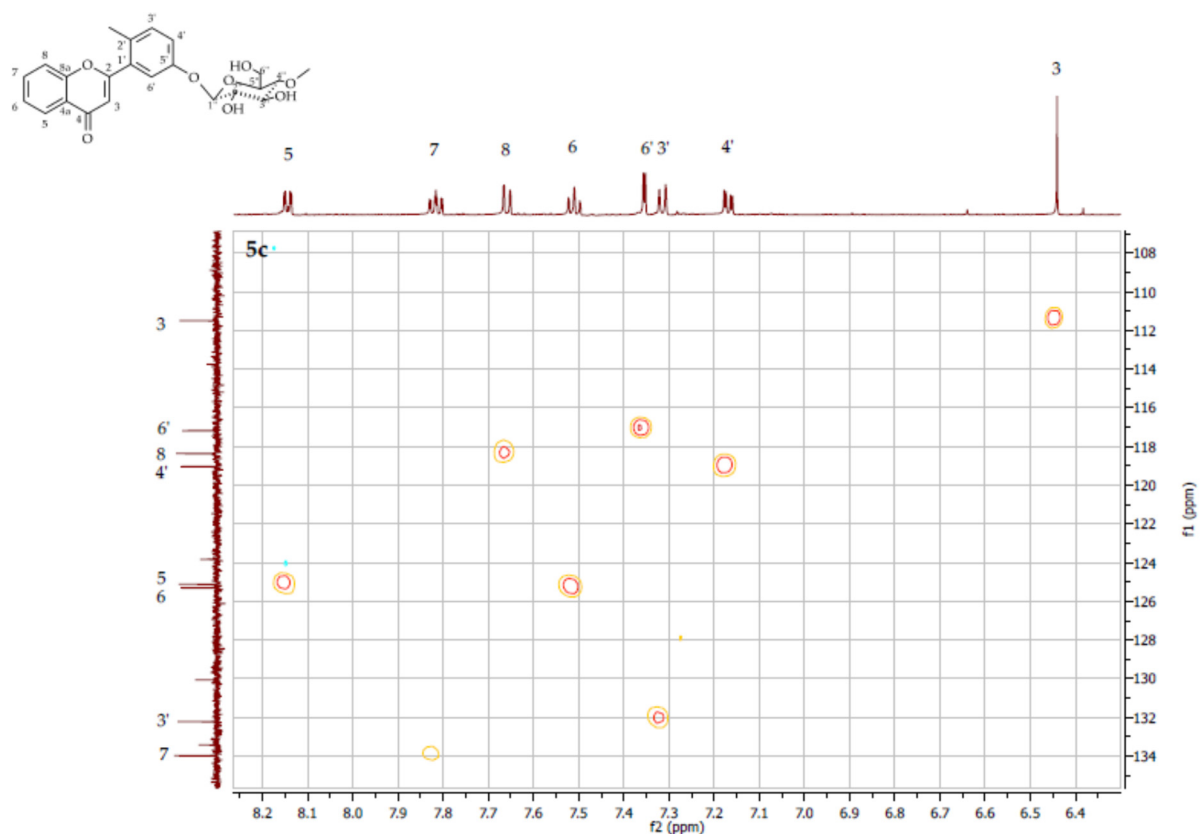


Figure S163. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

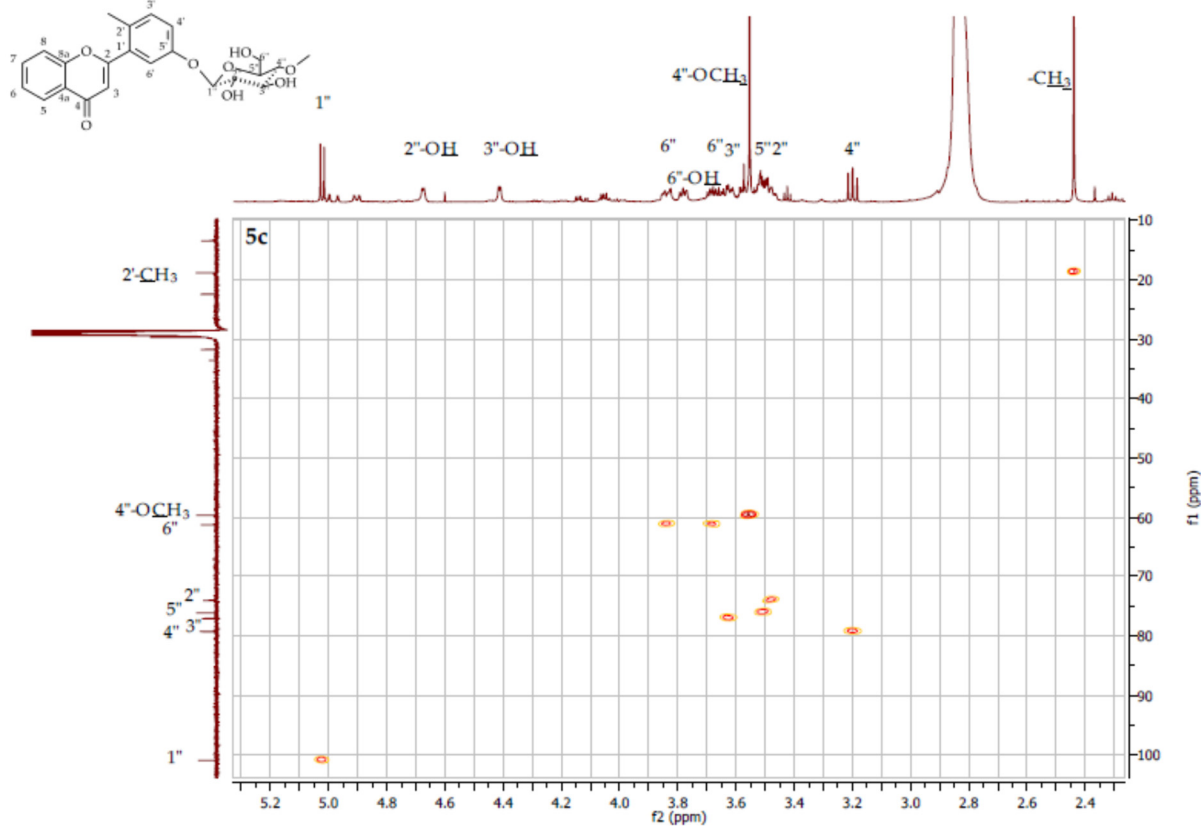


Figure S164. HSQC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

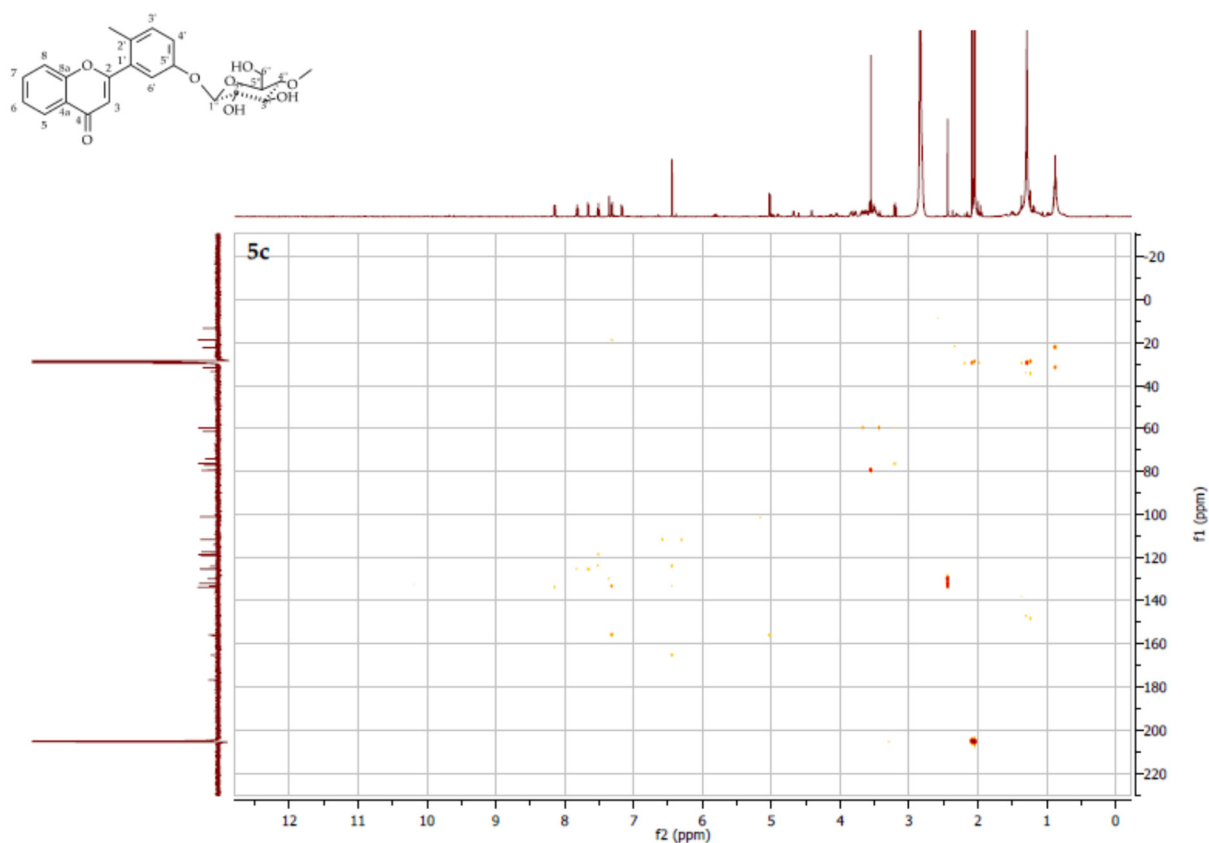


Figure S165. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

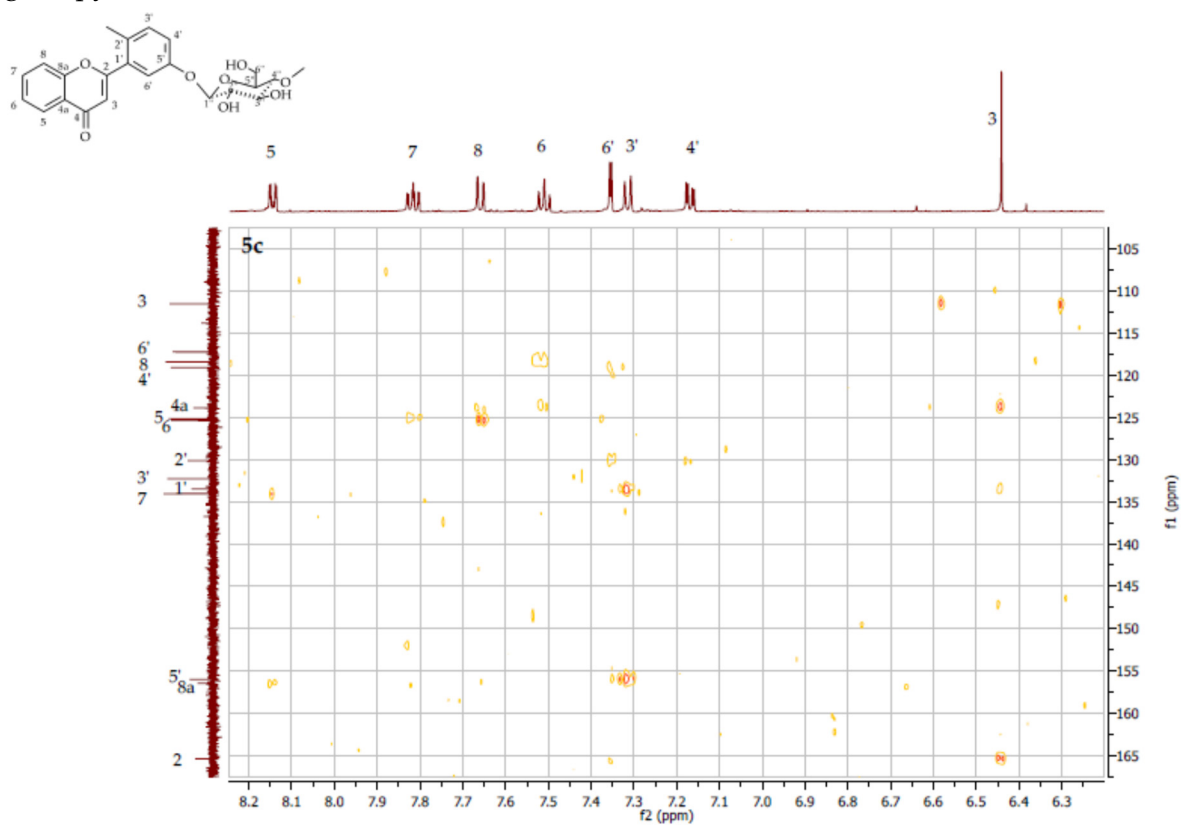


Figure S166. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 5'-O- β -D-(4''-O-methyl)-glucopyranoside (**5c**)

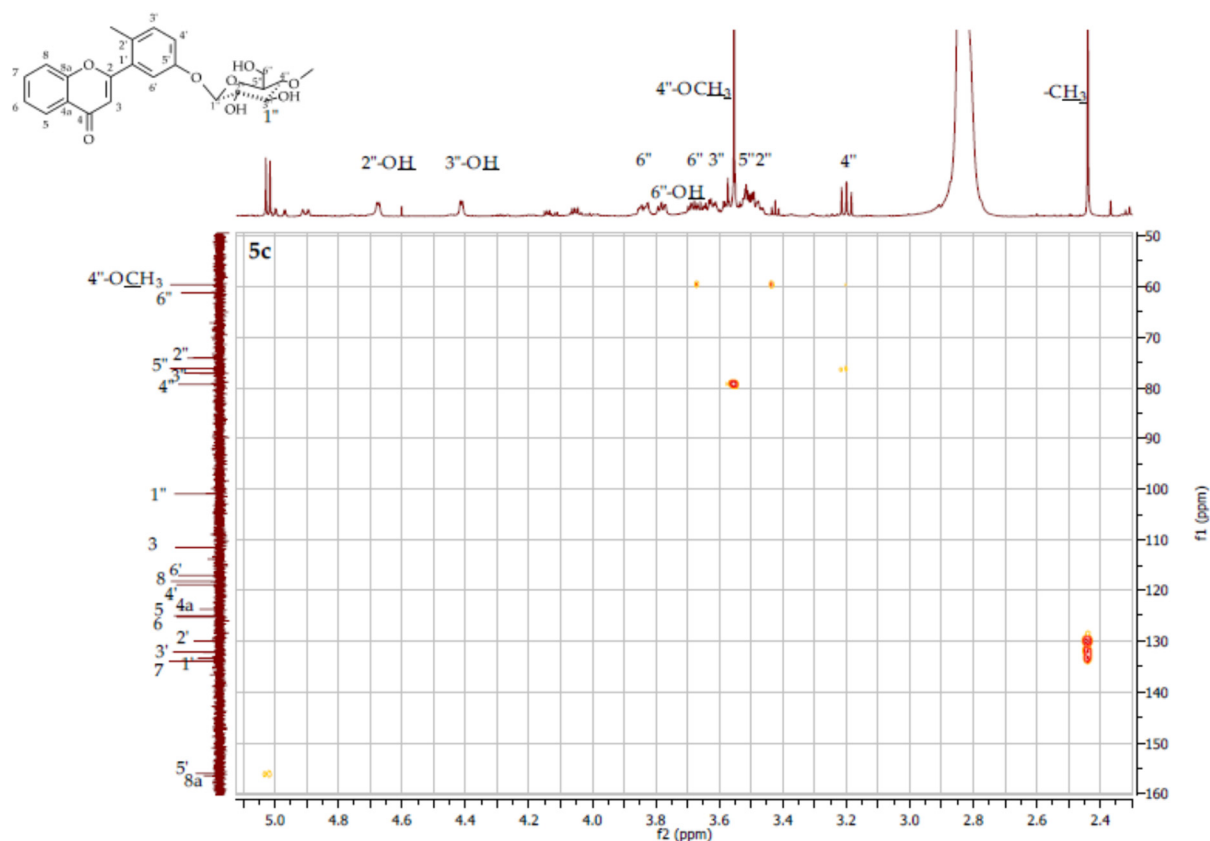


Figure S167. HMBC contour map – $^1\text{H} \times ^{13}\text{C}$ expansion of 2'-methylflavone 5'-O-β-D-(4''-O-methyl)-glucopyranoside (5c)