Fungal Biotransformation of Chloroflavanones and Antimicrobial Activity of Parent Compounds and Derived Products

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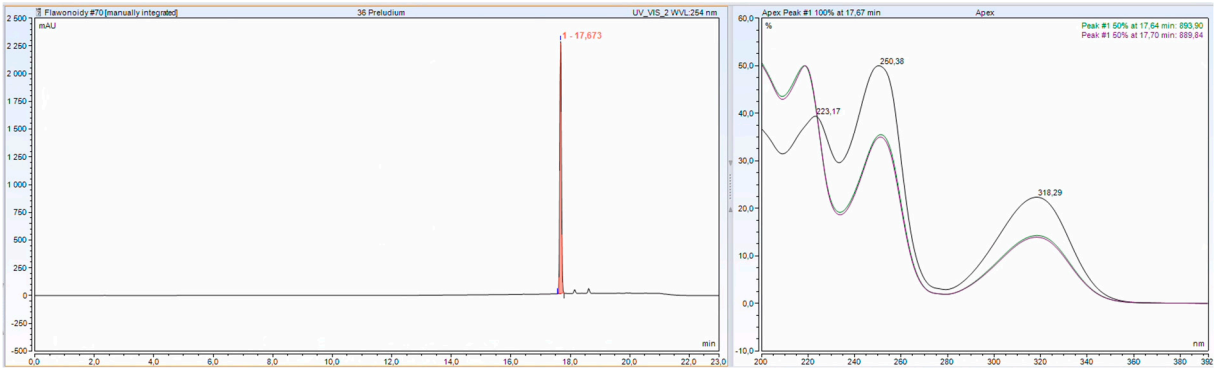


Figure S1. HPLC analysis of 2′-chloroflavanone (**1**).

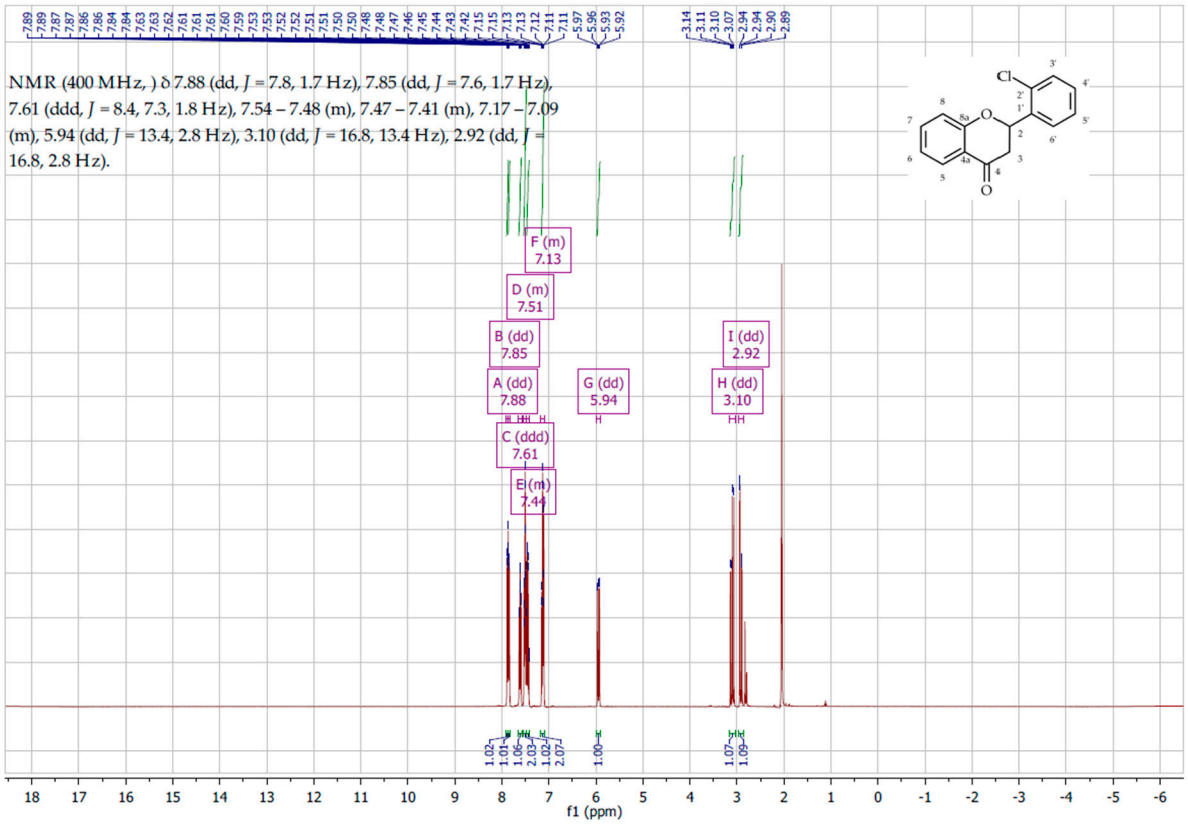


Figure S2. ^{1}H NMR spectrum (δ, acetone-d6, 600 MHz) of 2′-chloroflavanone (**1**).

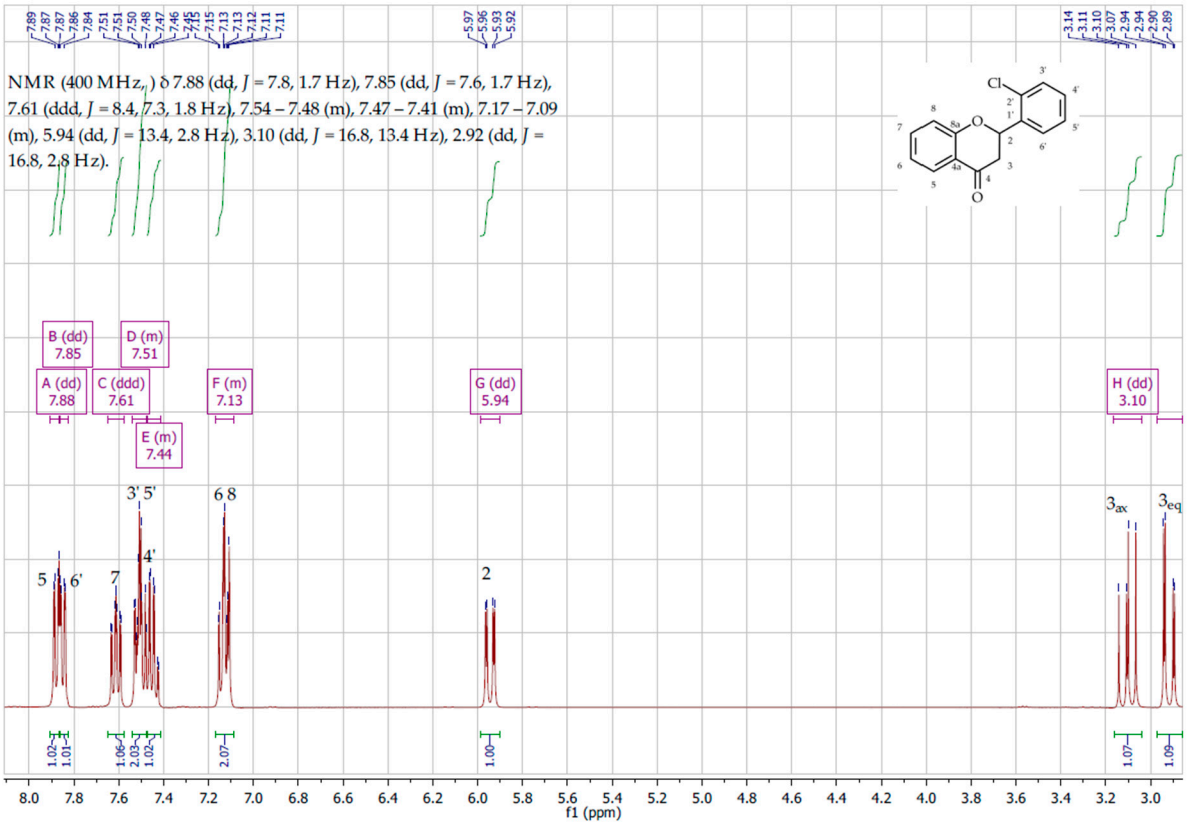


Figure S3. ^{1}H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 2′-chloroflavanone (**1**).

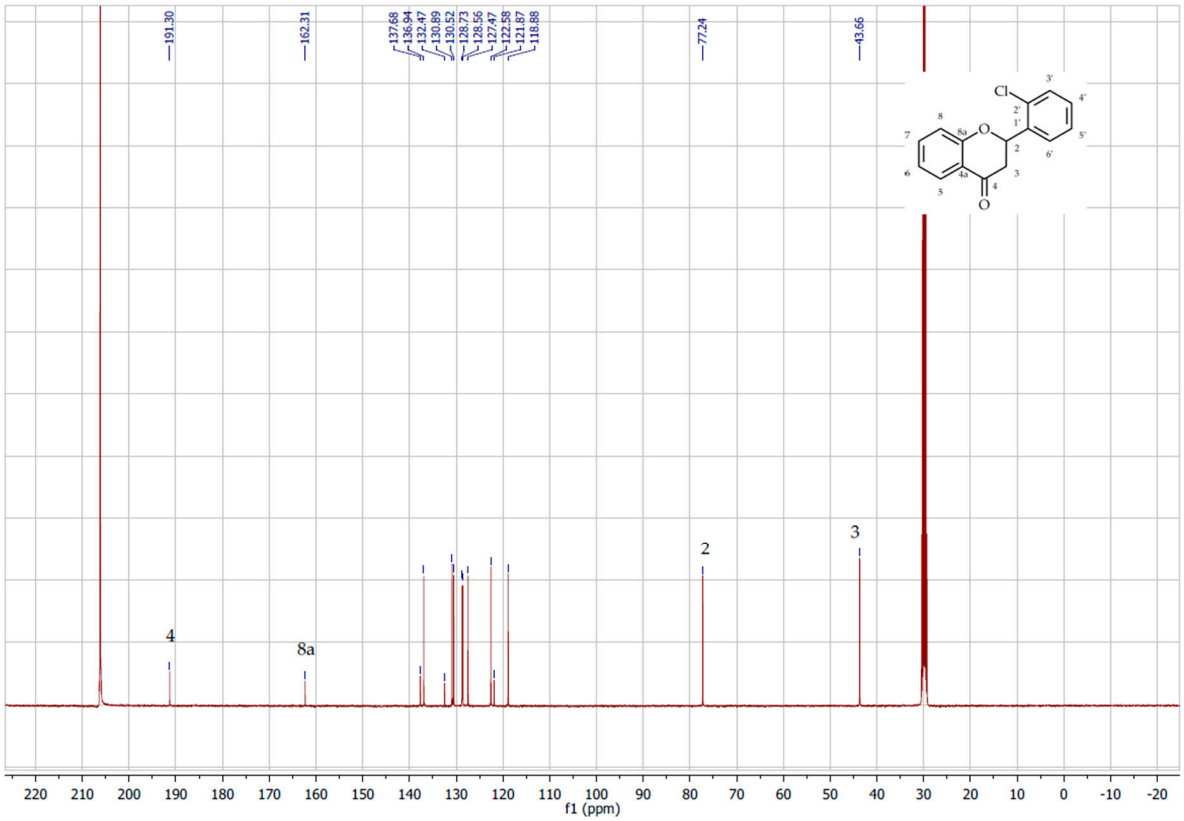


Figure S4. ^{13}C NMR spectrum (δ, acetone-d6, 151 MHz) of 2′-chloroflavanone (**1**).

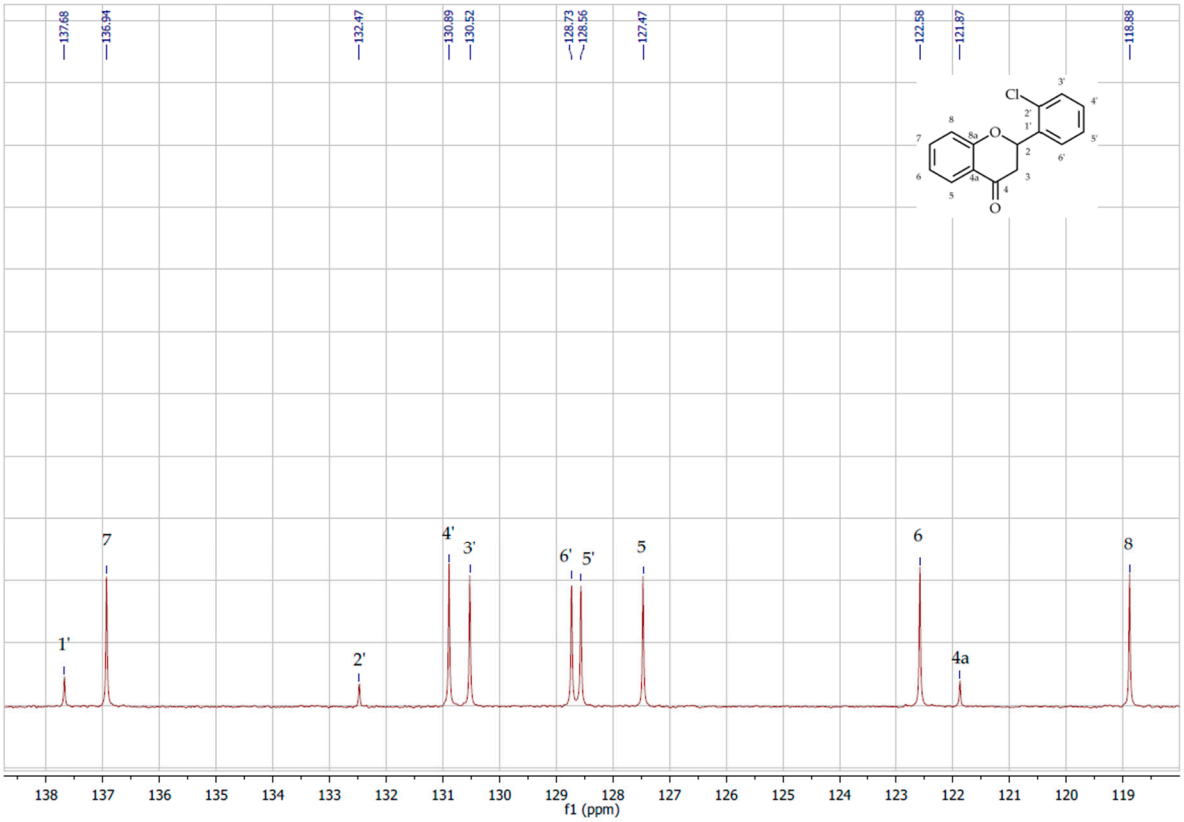


Figure S5. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 2′-chloroflavanone (**1**).

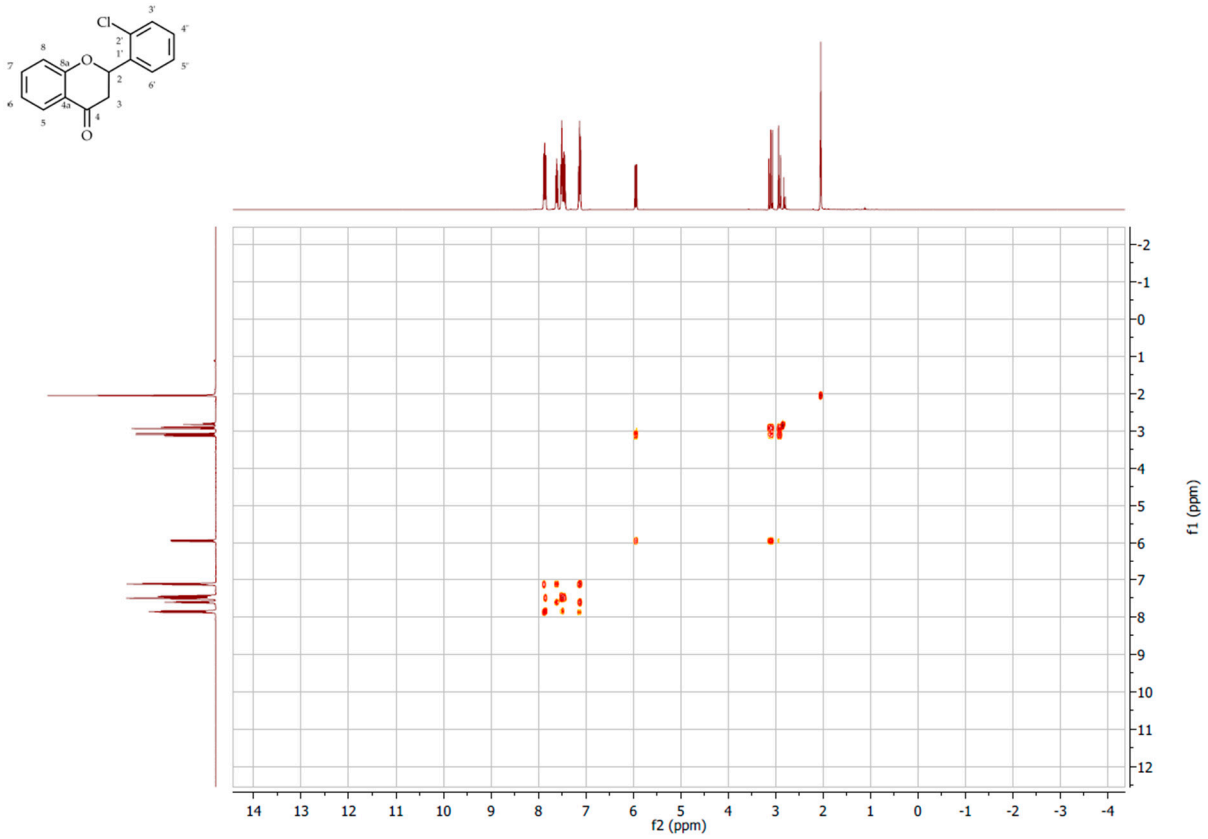


Figure S6. COSY contour map – ^{1}H x ^{1}H of 2′-chloroflavanone (**1**).

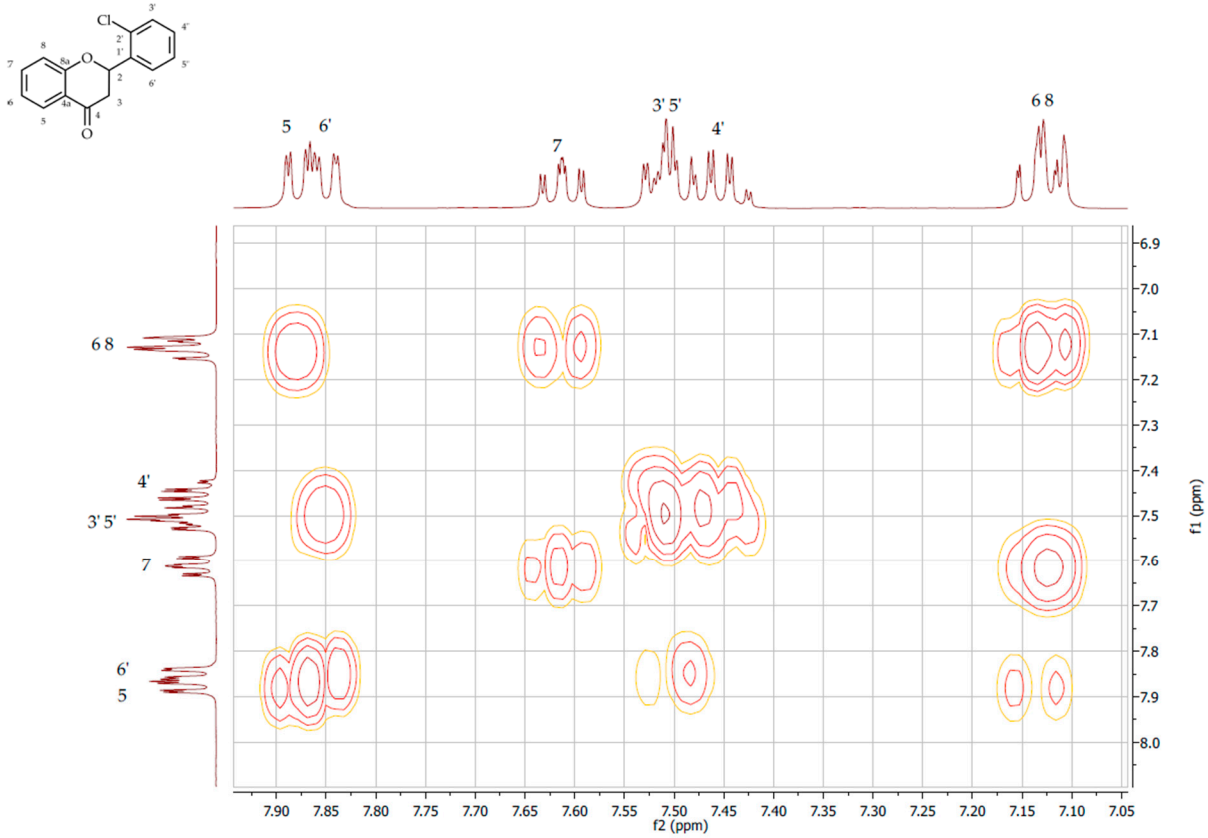


Figure S7. COSY contour map – ^{1}H x ^{1}H expansion of 2′-chloroflavanone (**1**).

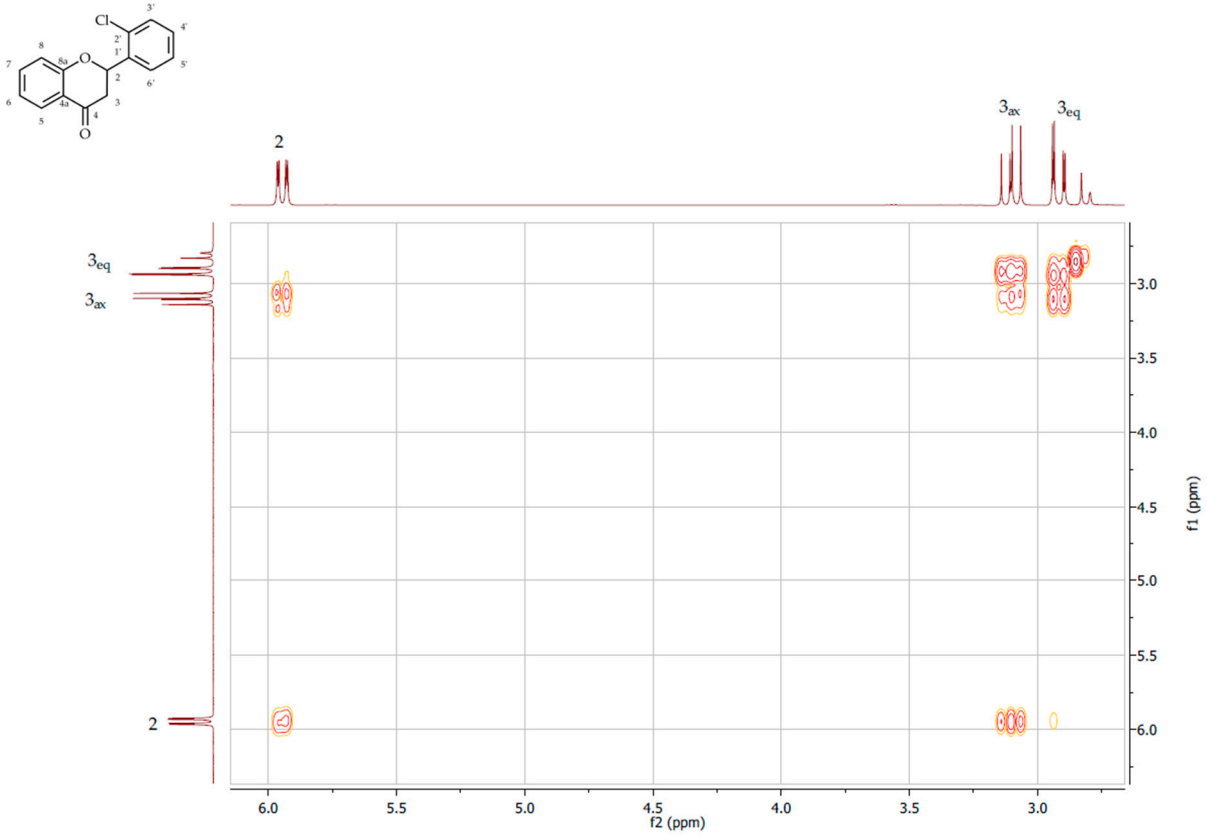


Figure S8. COSY contour map – ^{1}H x ^{1}H expansion of 2′-chloroflavanone (**1**).

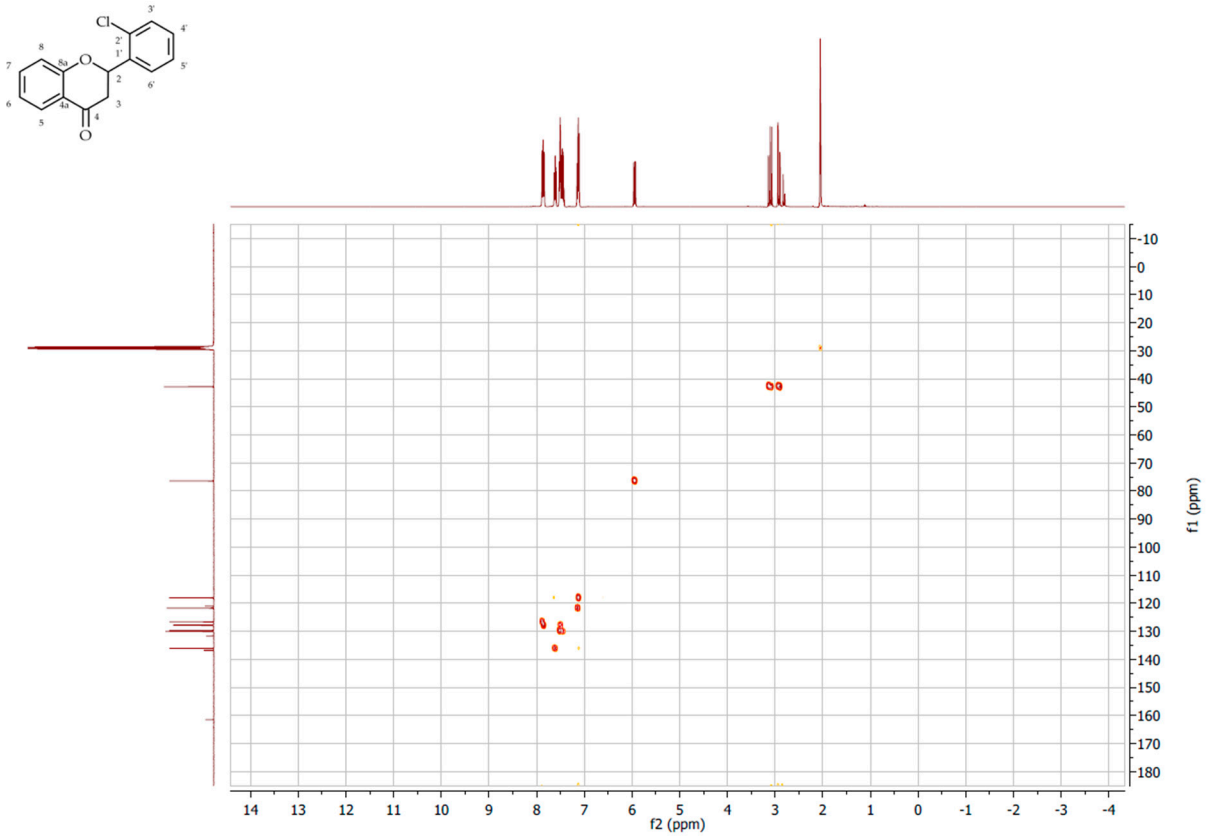


Figure S9. HMQC contour map – ^{1}H x ^{13}C of 2′-chloroflavanone (**1**).

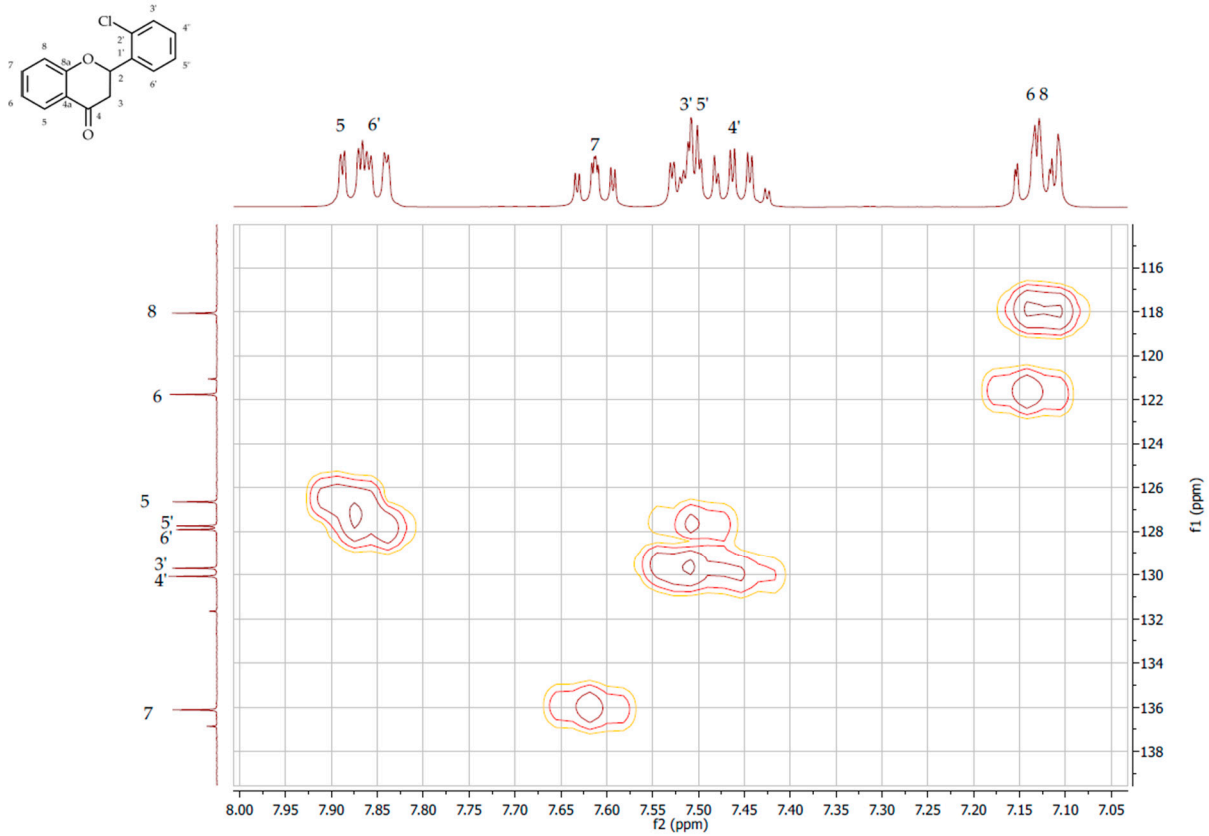


Figure S10. HMQC contour map – ^{1}H x ^{13}C expansion of 2′-chloroflavanone (**1**).

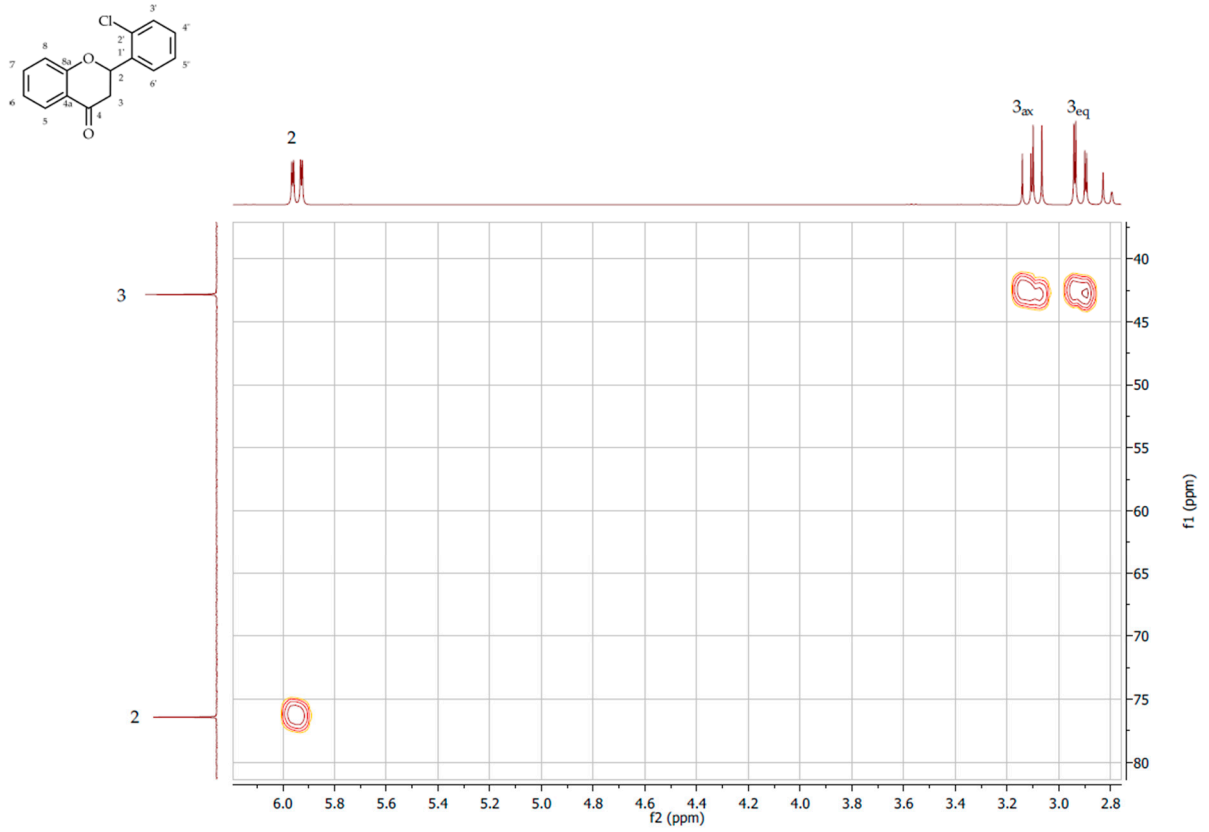


Figure S11. HMQC contour map – ^{1}H x ^{13}C expansion of 2′-chloroflavanone (**1**).

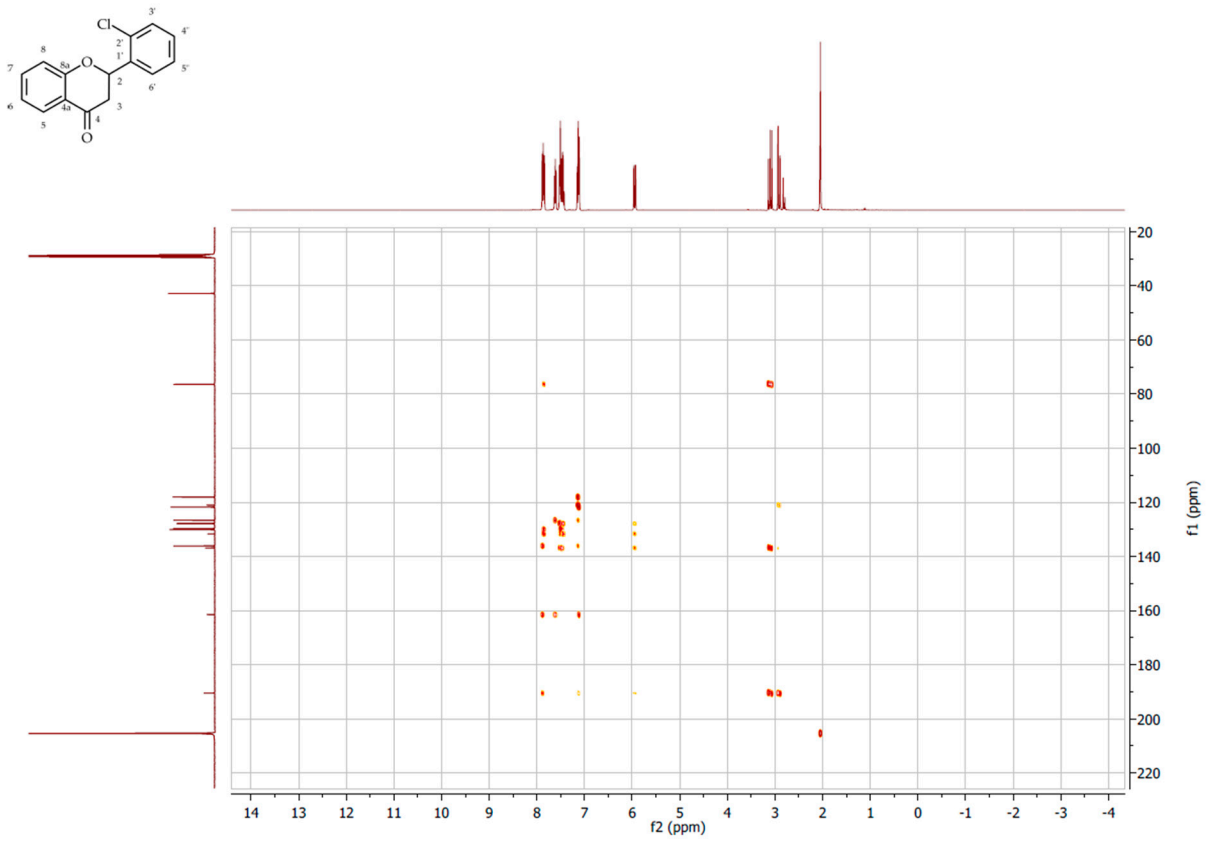


Figure S12. HMBC contour map – ^{1}H x ^{13}C of 2′-chloroflavanone (**1**).

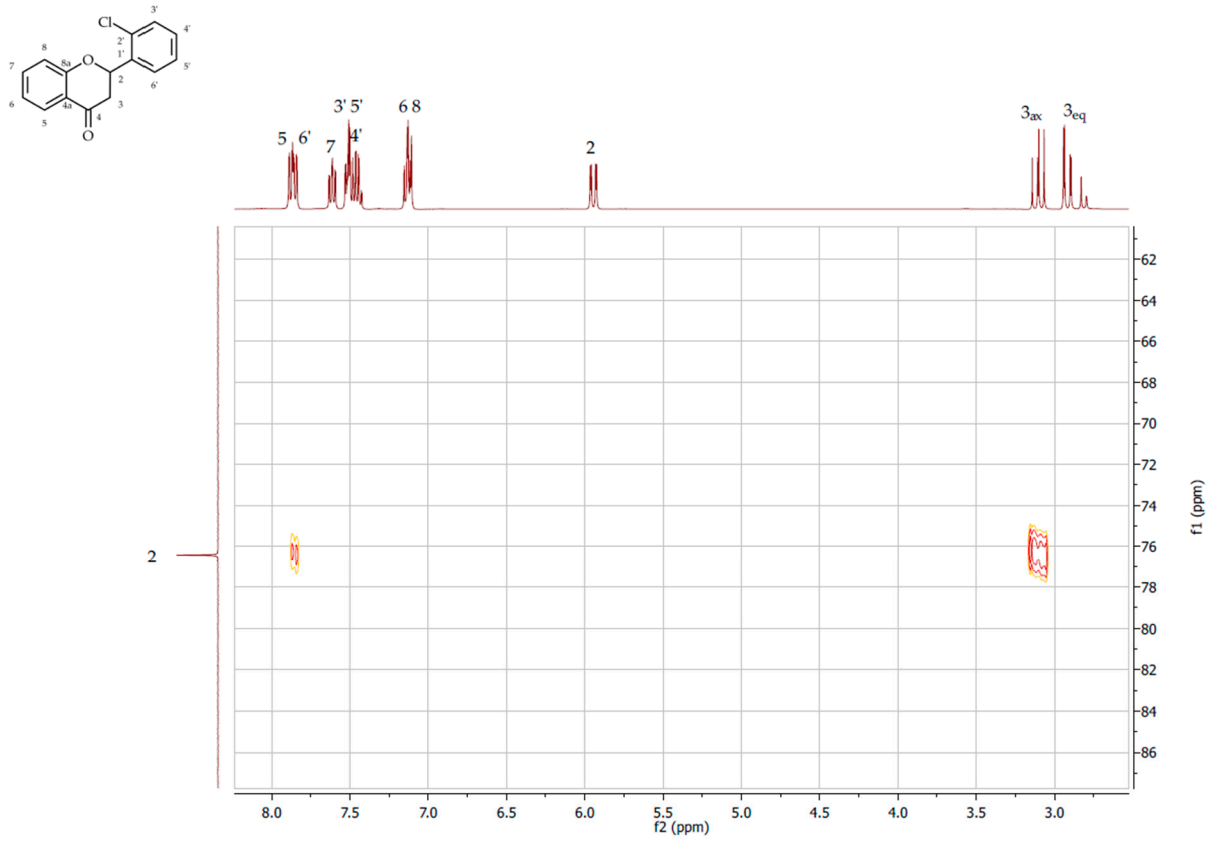


Figure S13. HMBC contour map – ^{1}H x ^{13}C expansion of 2′-chloroflavanone (**1**).

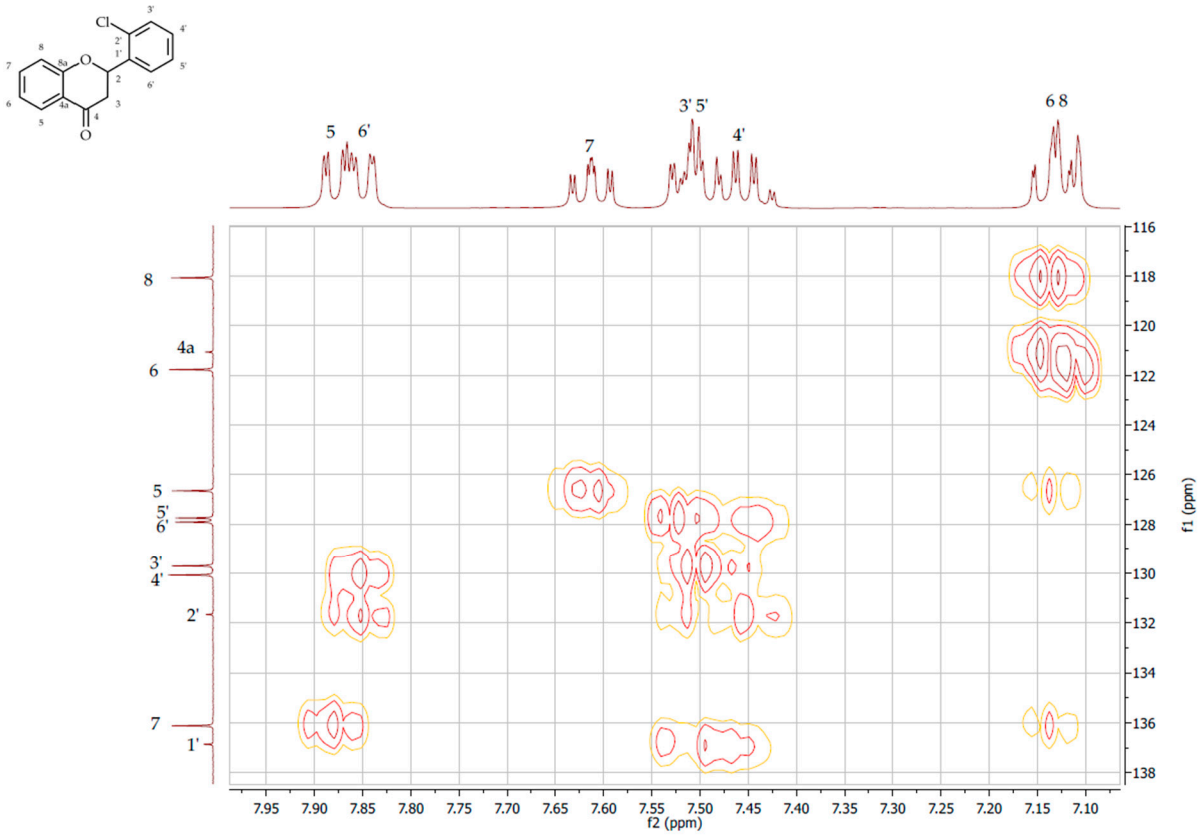


Figure S14. HMBC contour map – ^{1}H x ^{13}C expansion of 2′-chloroflavanone (**1**).

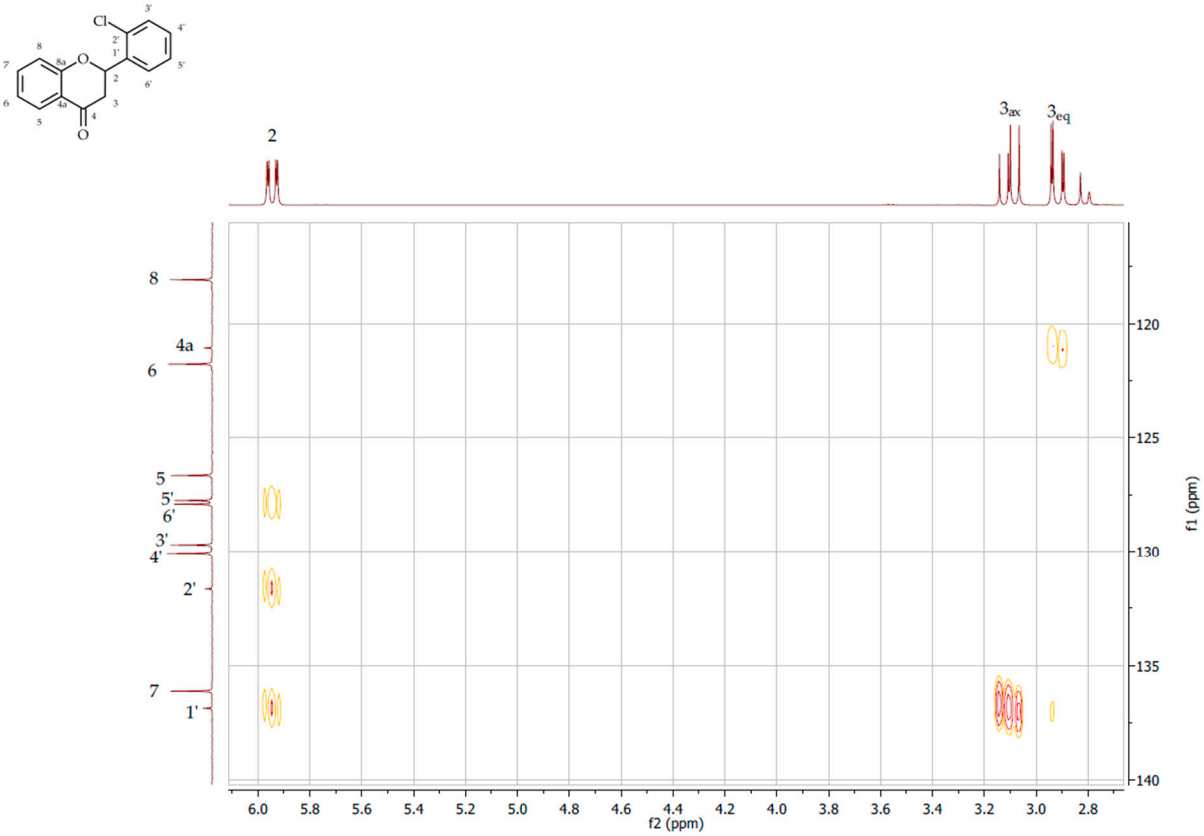


Figure S15. HMBC contour map – ^{1}H x ^{13}C expansion of 2′-chloroflavanone (**1**).

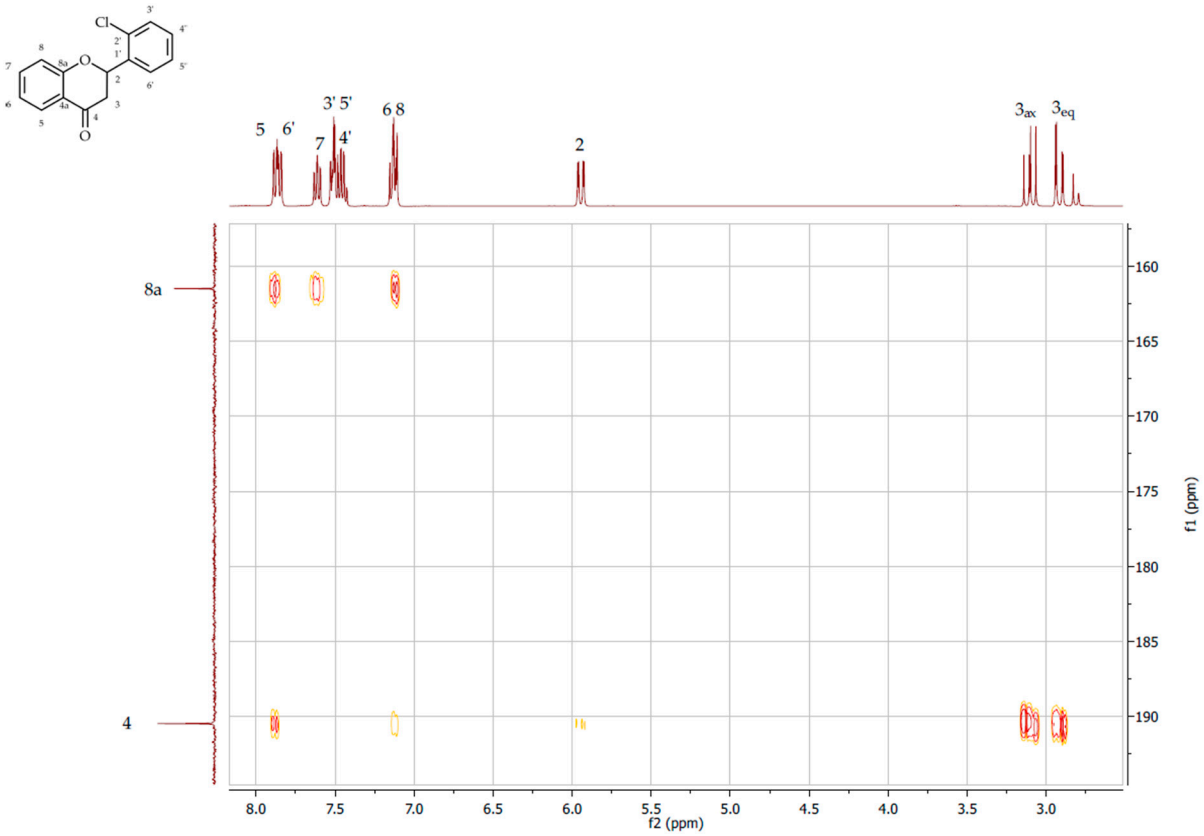
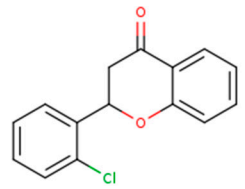
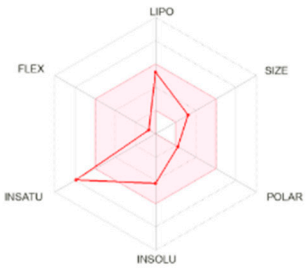


Figure S16. HMBC contour map – ^{1}H x ^{13}C expansion of 2′-chloroflavanone (**1**).

Molecule 1





SMILES Clc1ccccc1C1CC(=O)c2c(O1)cccc2

Physicochemical Properties	
Formula	C15H11ClO2
Molecular weight	258.70 g/mol
Num. heavy atoms	18
Num. arom. heavy atoms	12
Fraction Csp3	0.13
Num. rotatable bonds	1
Num. H-bond acceptors	2
Num. H-bond donors	0
Molar Refractivity	70.51
TPSA	26.30 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.63
Log $P_{o/w}$ (XLOGP3)	3.77
Log $P_{o/w}$ (WLOGP)	3.72
Log $P_{o/w}$ (MLOGP)	2.98
Log $P_{o/w}$ (SILICOS-IT)	4.18
Consensus Log $P_{o/w}$	3.46

Water Solubility	
Log *S* (ESOL)	-4.25
Solubility	1.47e-02 mg/ml ; 5.67e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-4.02
Solubility	2.50e-02 mg/ml ; 9.65e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-5.76
Solubility	4.48e-04 mg/ml ; 1.73e-06 mol/l
Class	Moderately soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.20 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.90

Figure S17. 2′-Chloroflavanone (**1**) physicochemical and ADME parameters prediction using the SwissADME modelling.

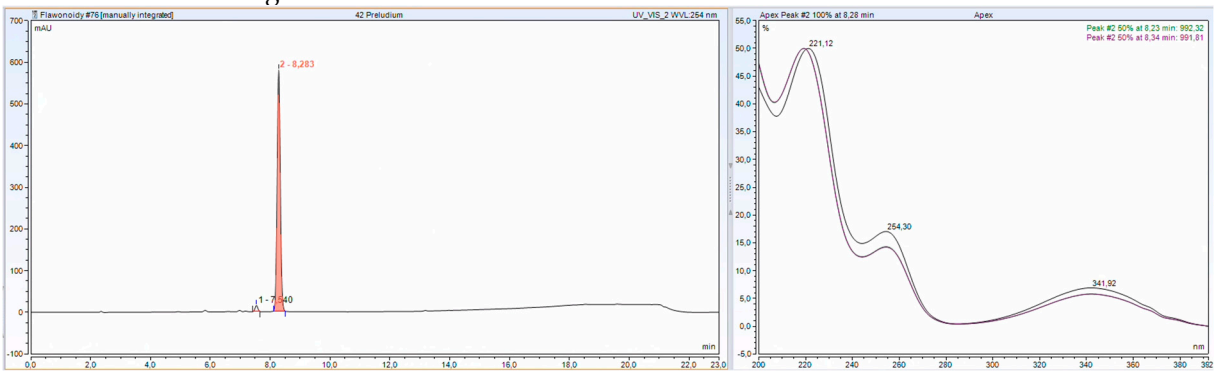


Figure S18. HPLC analysis of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

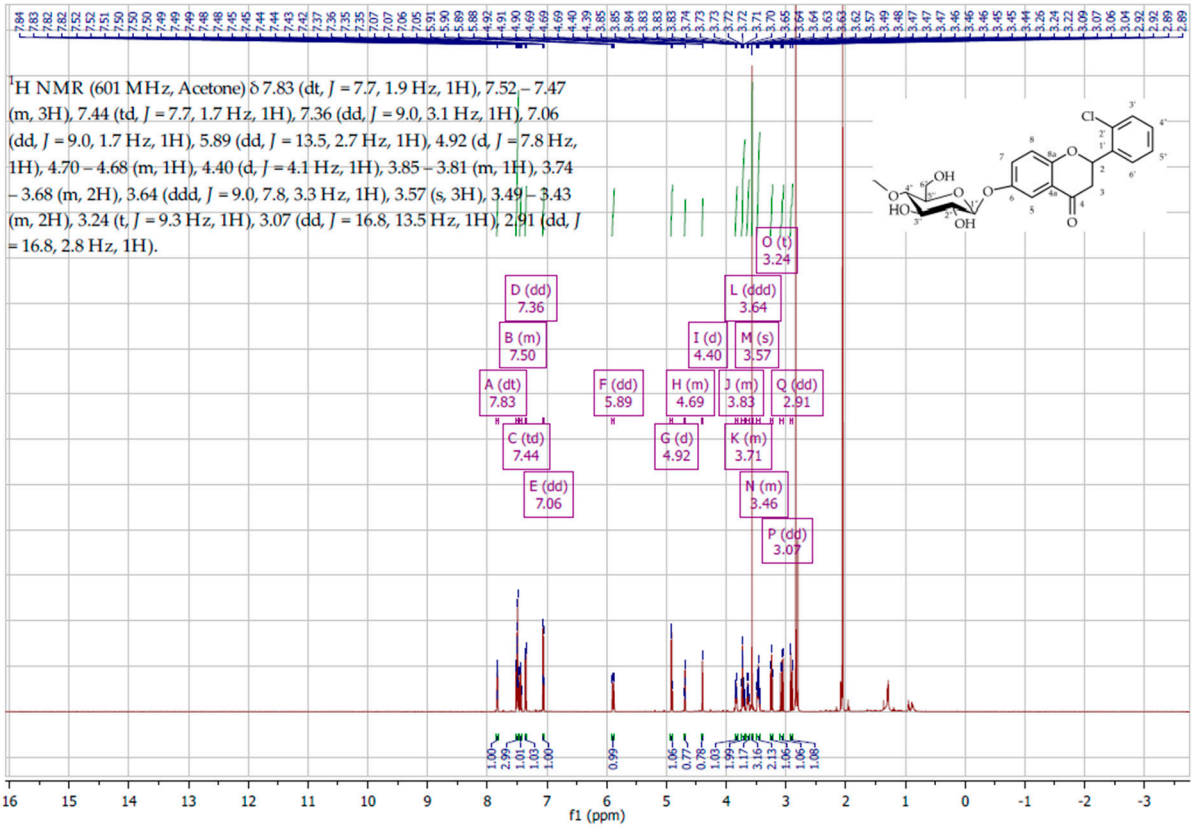


Figure S19. ¹H NMR spectrum (δ, acetone-d6, 600 MHz) of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

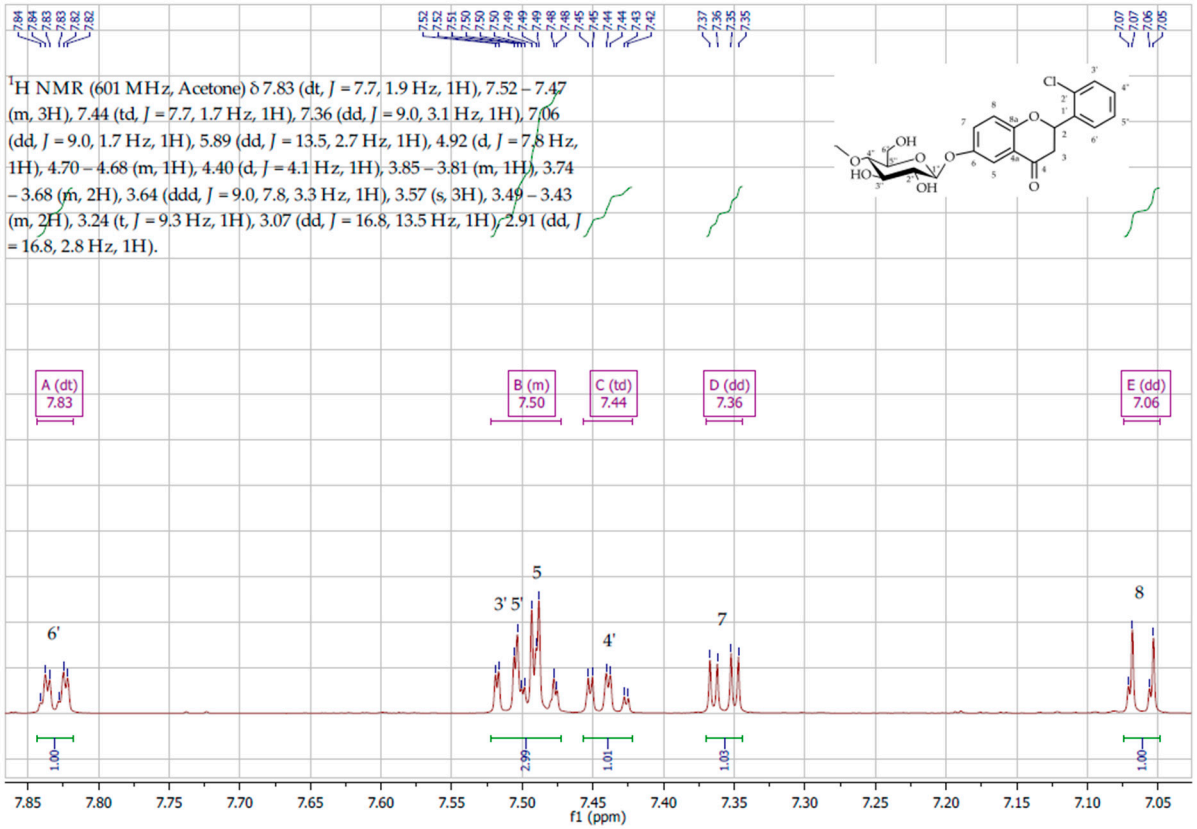


Figure S20. ¹H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

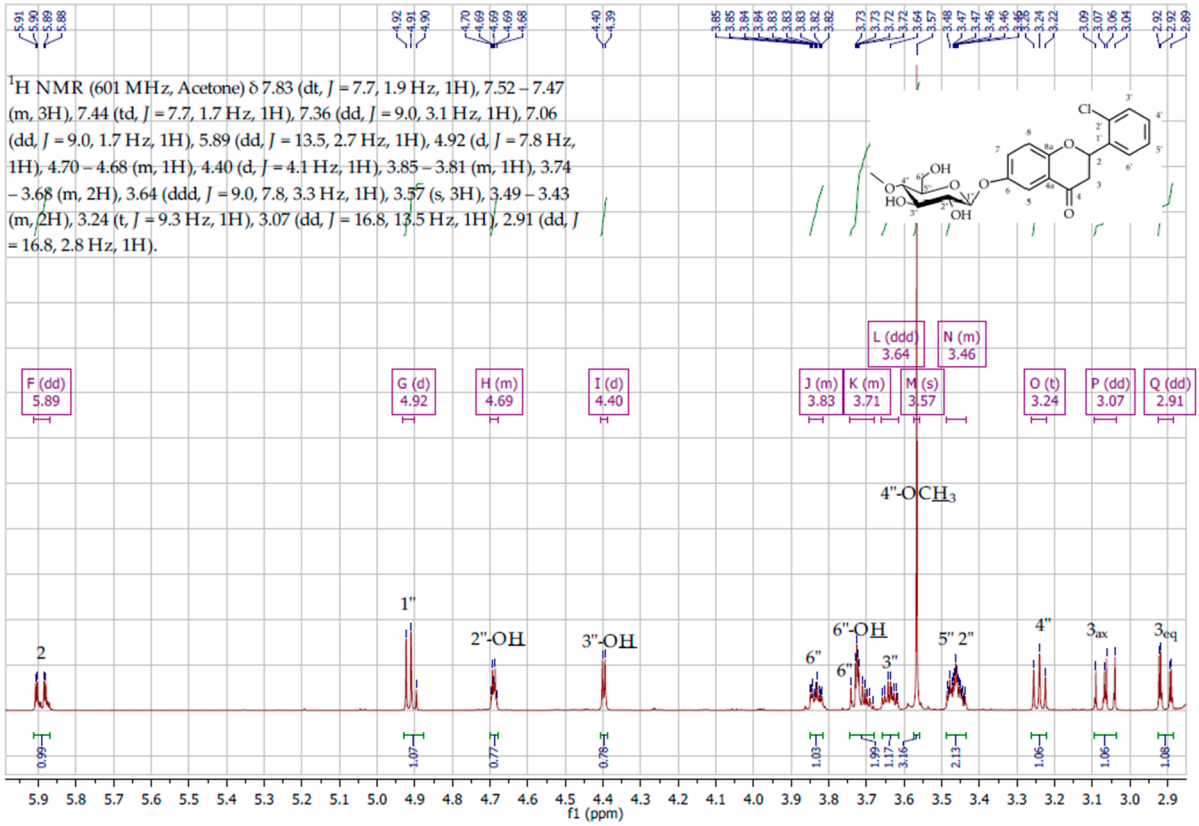


Figure S21. ¹H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

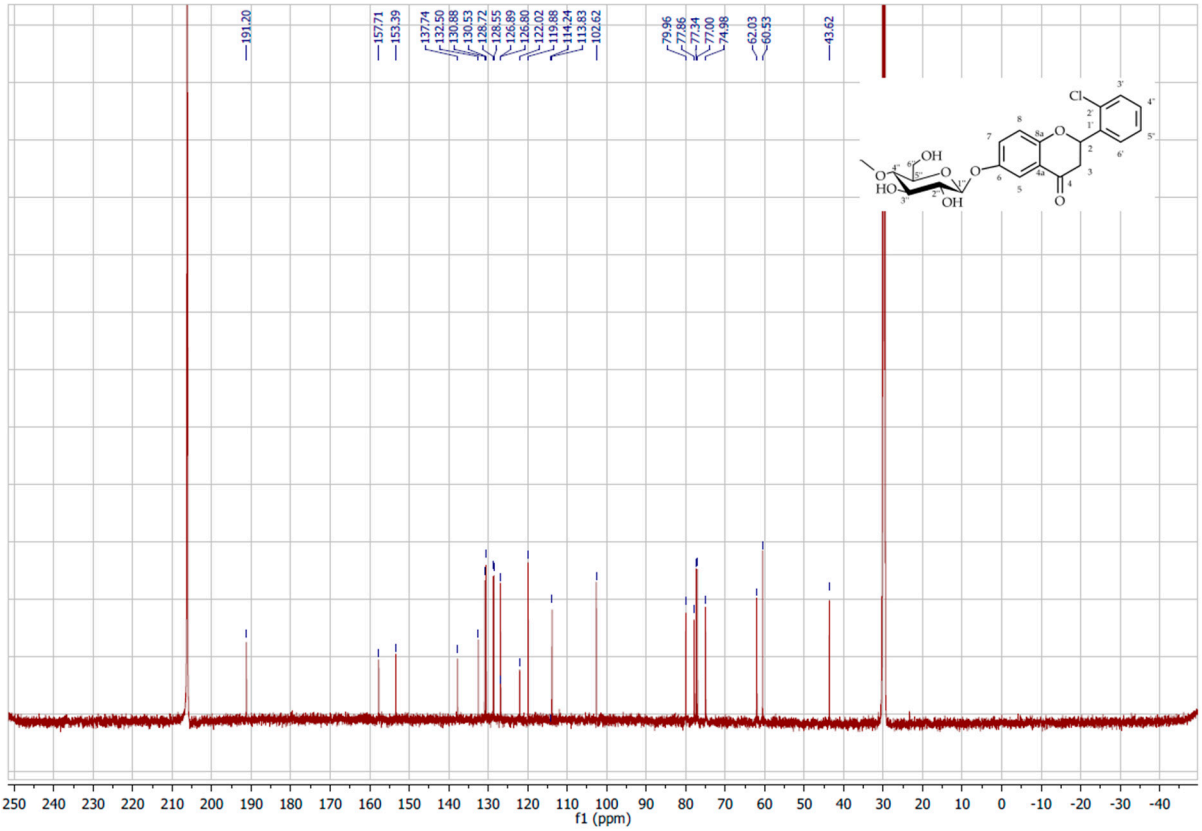


Figure S22. ^{13}C NMR spectrum (δ, acetone-d6, 151 MHz) of 2′-chloroflavanone 6-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

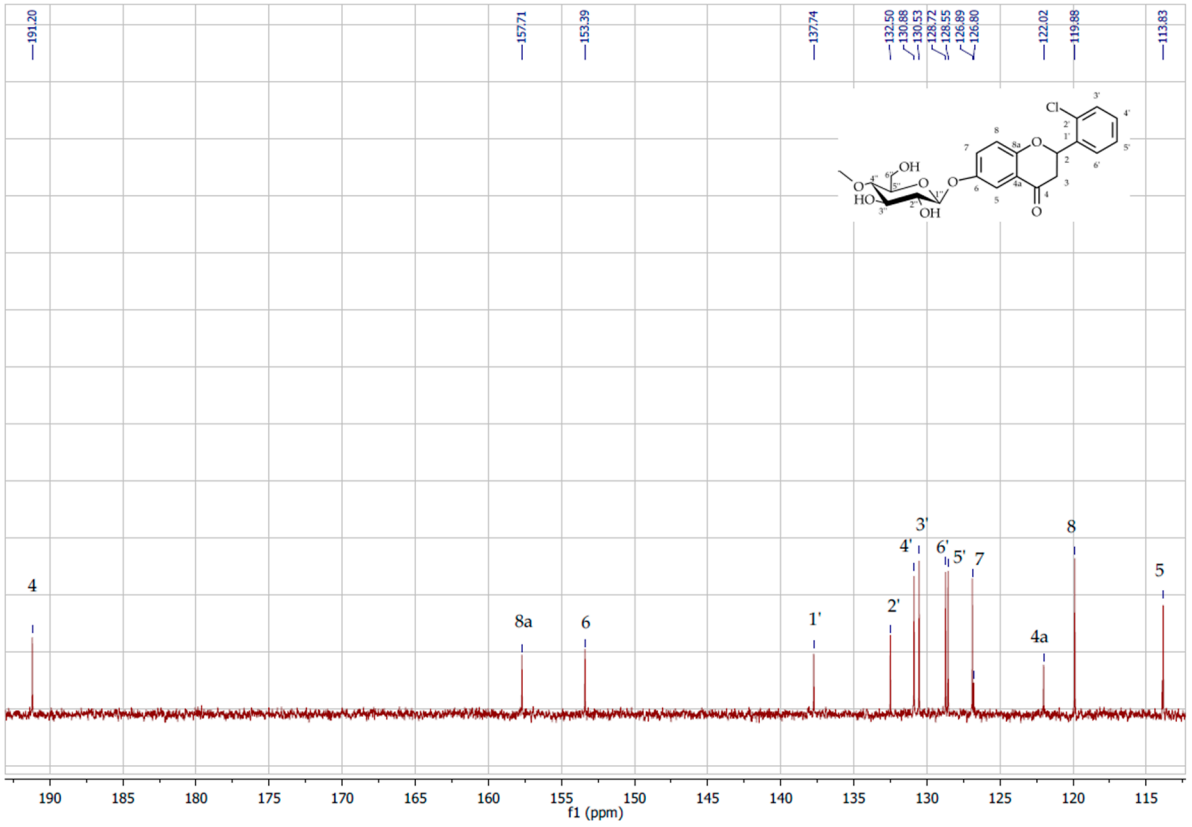


Figure S23. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 2′-chloroflavanone 6-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

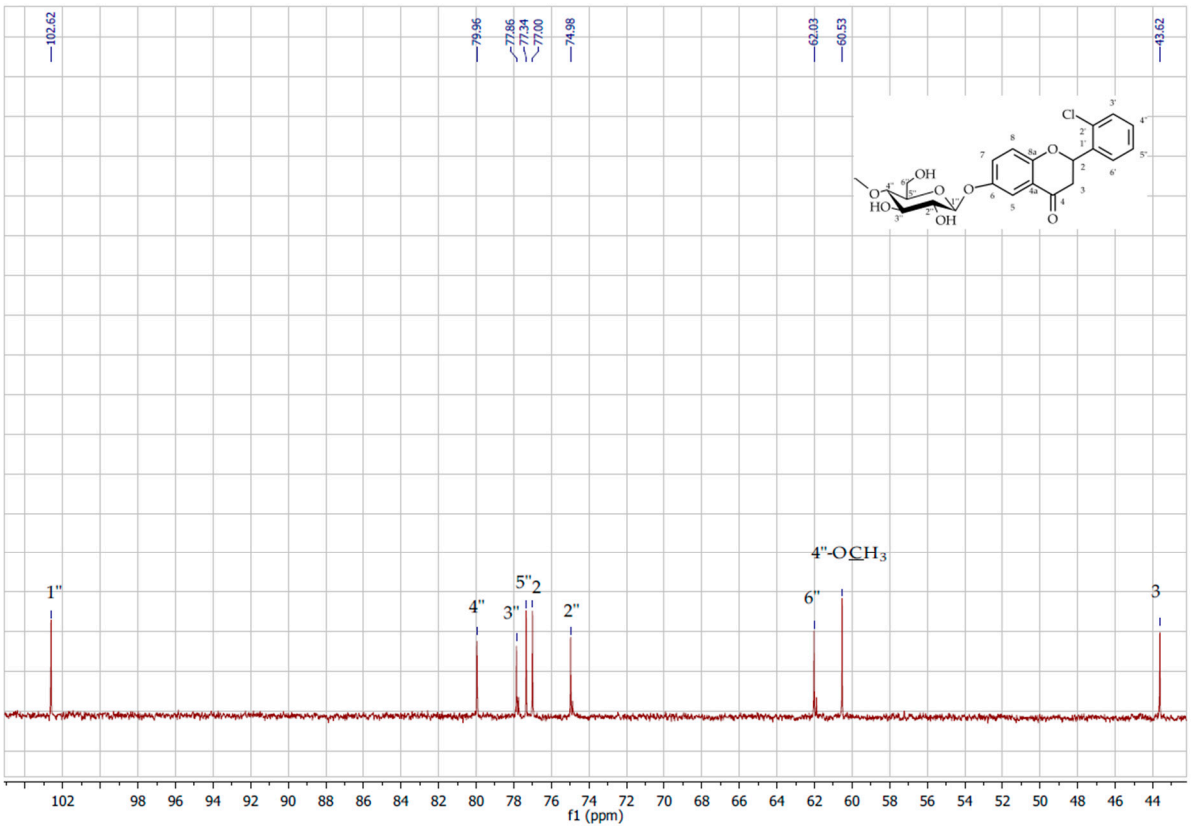


Figure S24. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 2′-chloroflavanone 6-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

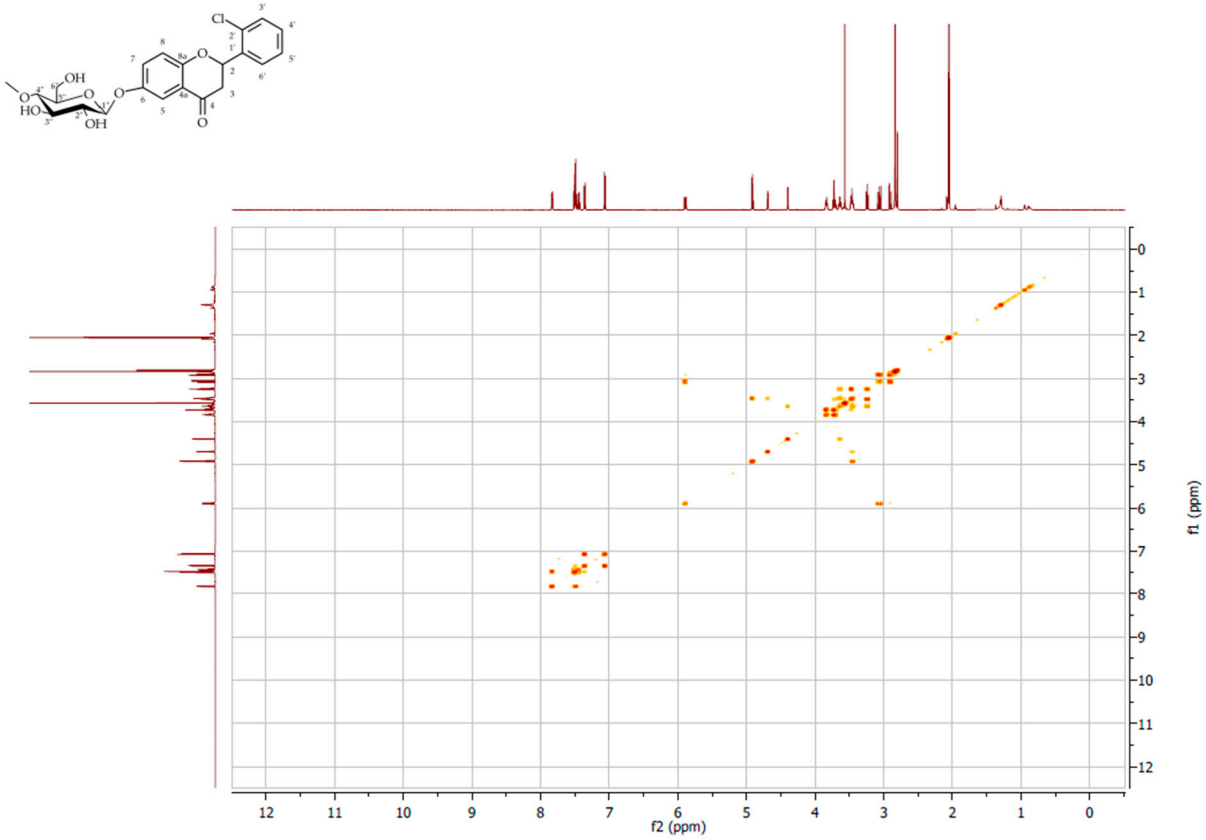


Figure S25. COSY contour map – ^{1}H x ^{1}H of 2′-chloroflavanone 6-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

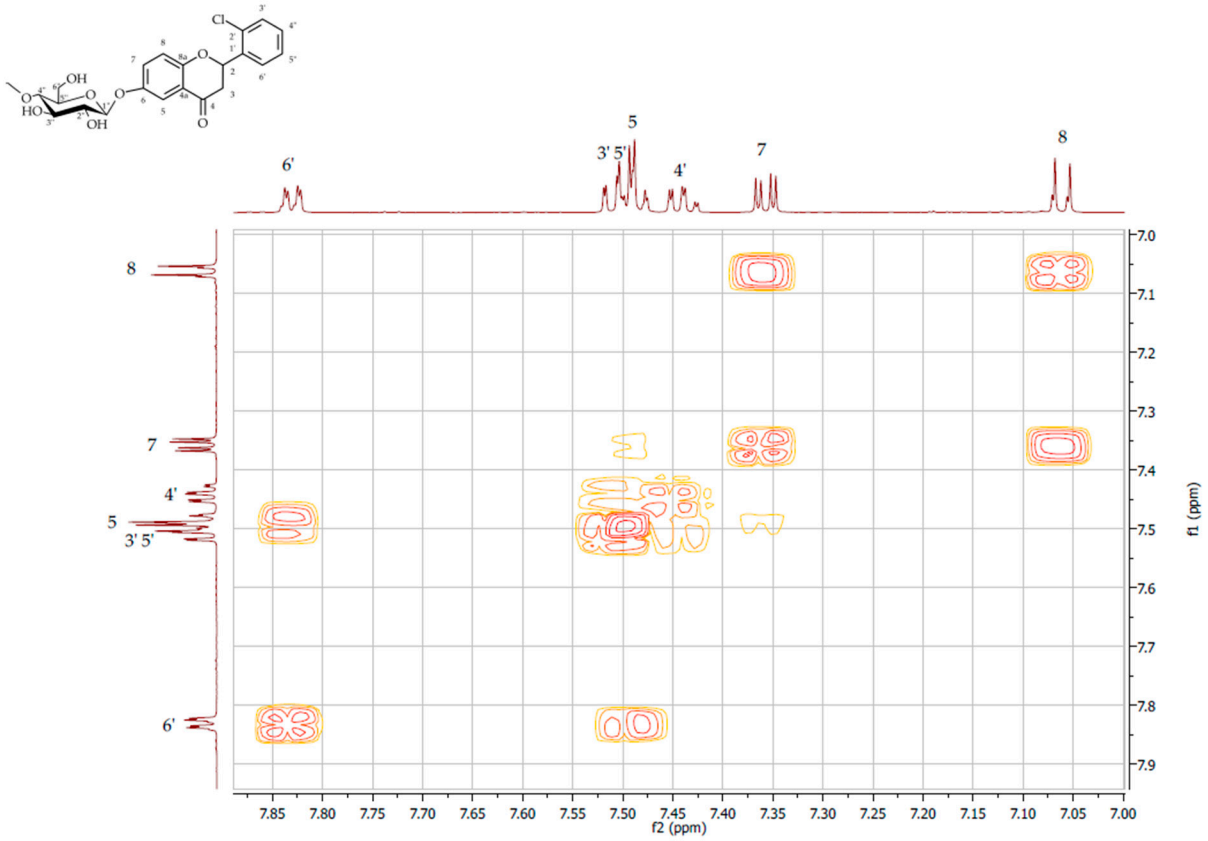


Figure S26. COSY contour map – ^{1}H x ^{1}H expansion of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

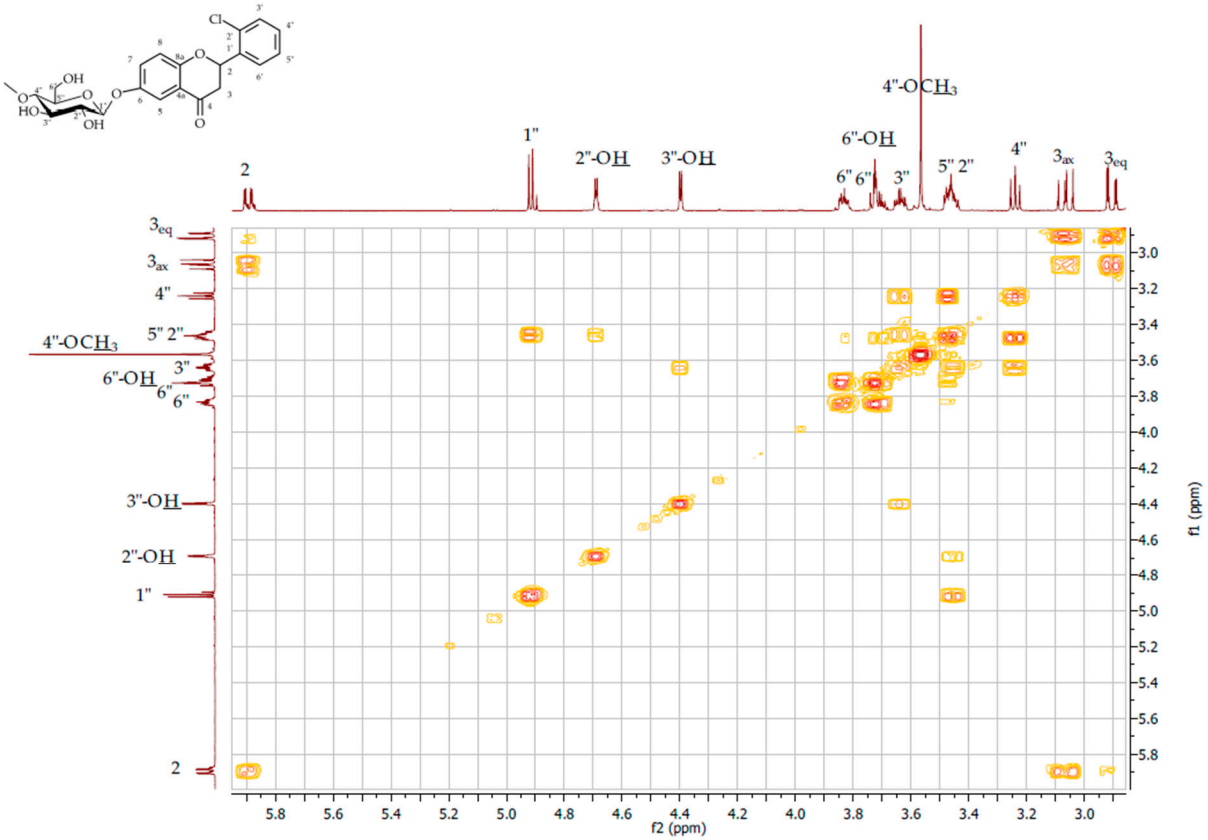


Figure S27. COSY contour map – ^{1}H x ^{1}H expansion of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

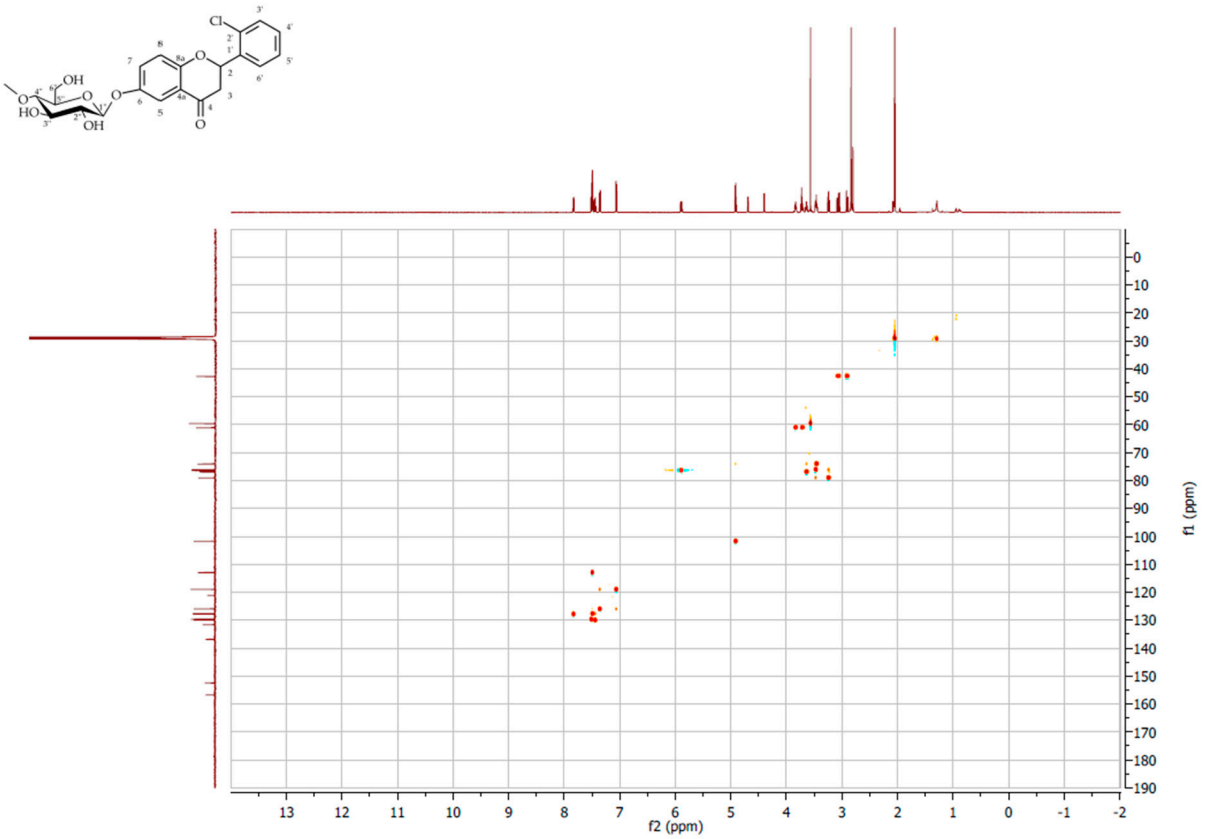


Figure S28. HMQC contour map – ^{1}H x ^{13}C of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

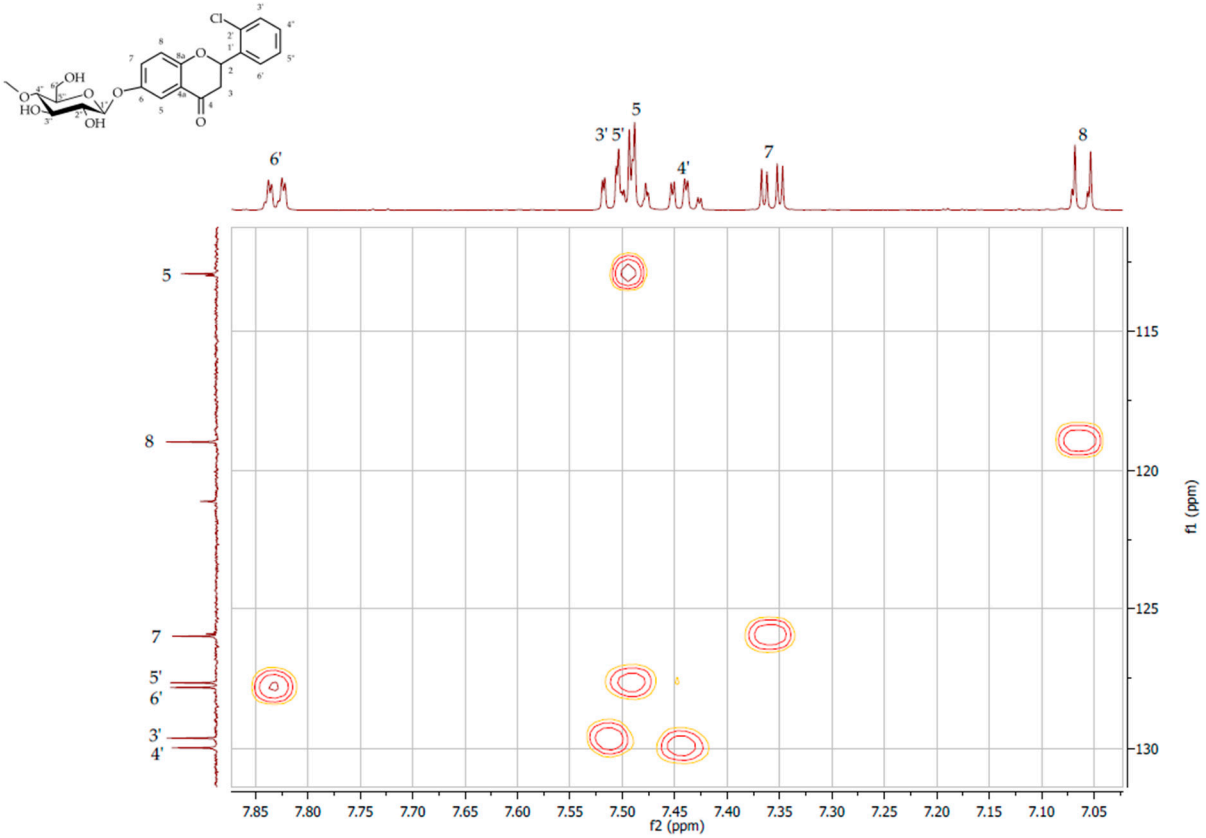


Figure S29. HMQC contour map – ^{1}H x ^{13}C expansion of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

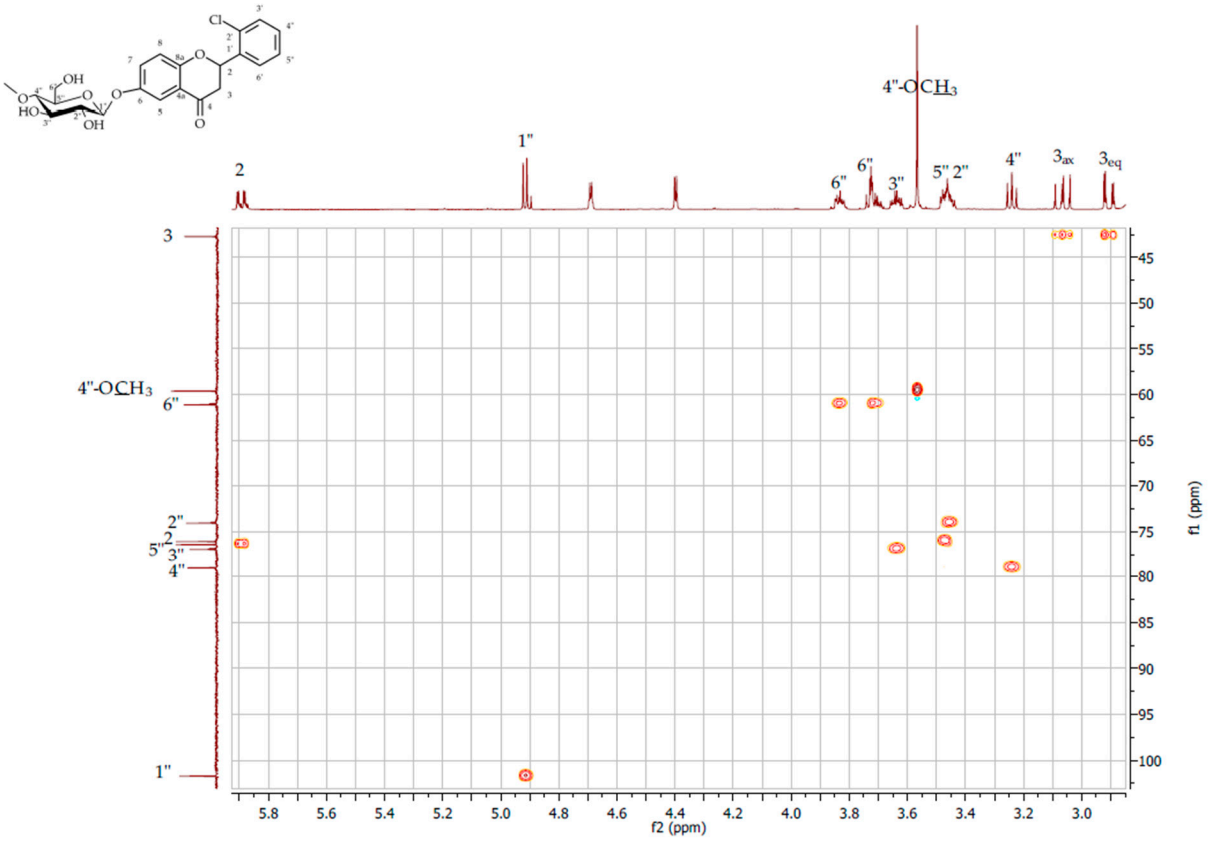


Figure S30. HMQC contour map – ^{1}H x ^{13}C expansion of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

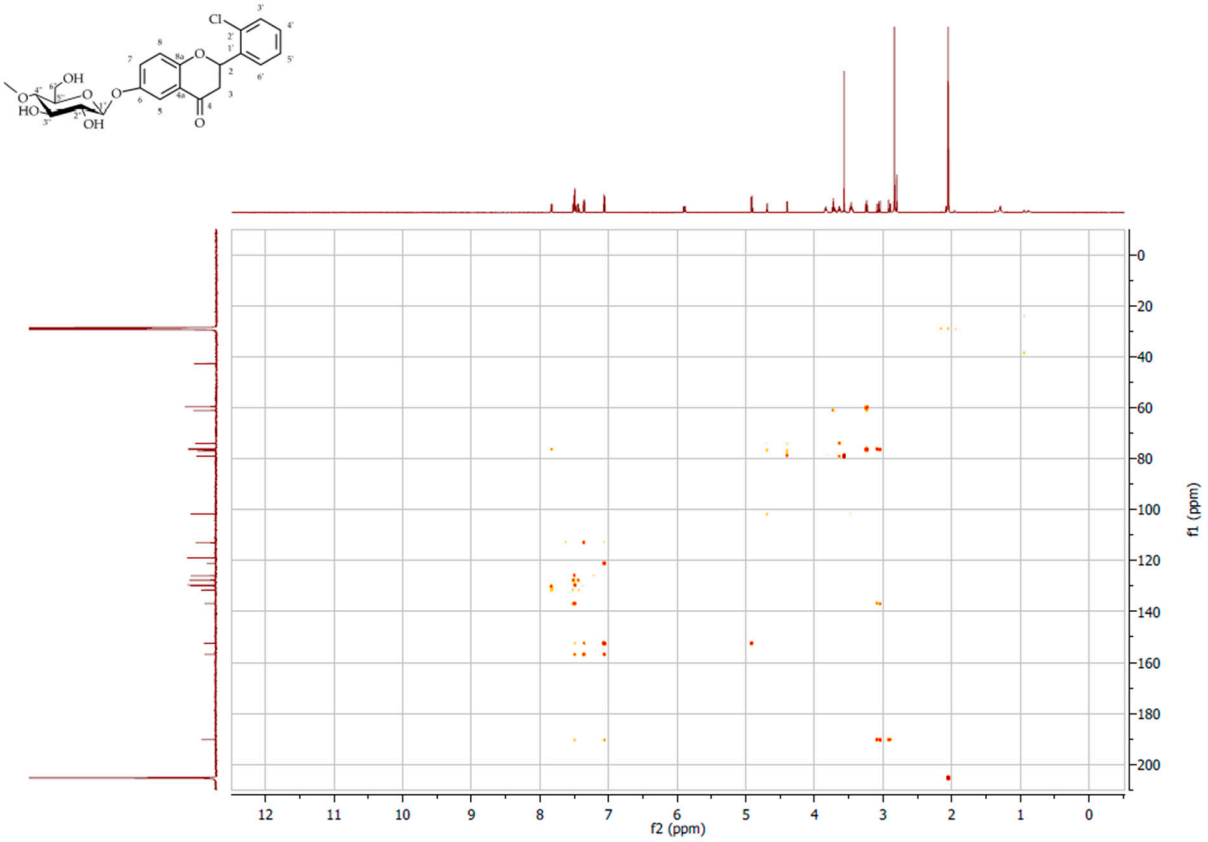


Figure S31. HMBC contour map – ^{1}H x ^{13}C of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

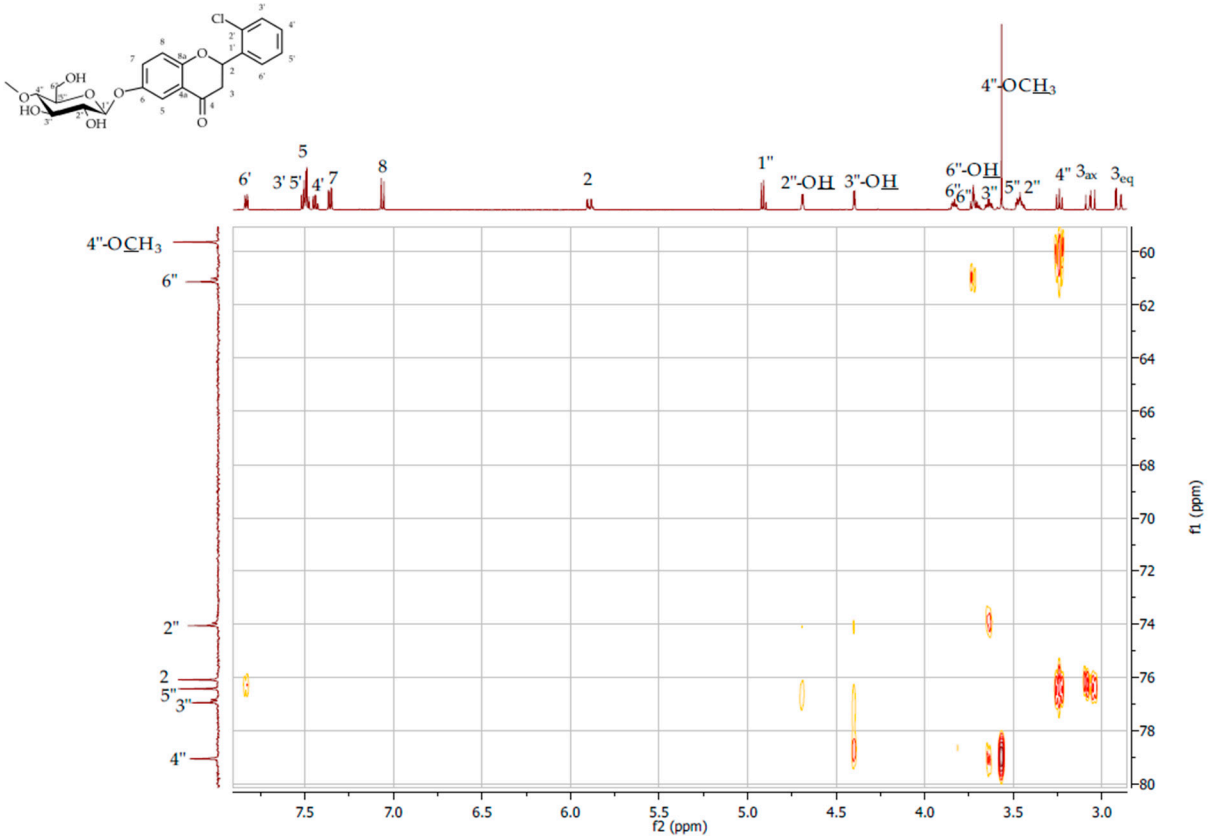


Figure S32. HMBC contour map – ^{1}H x ^{13}C expansion of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

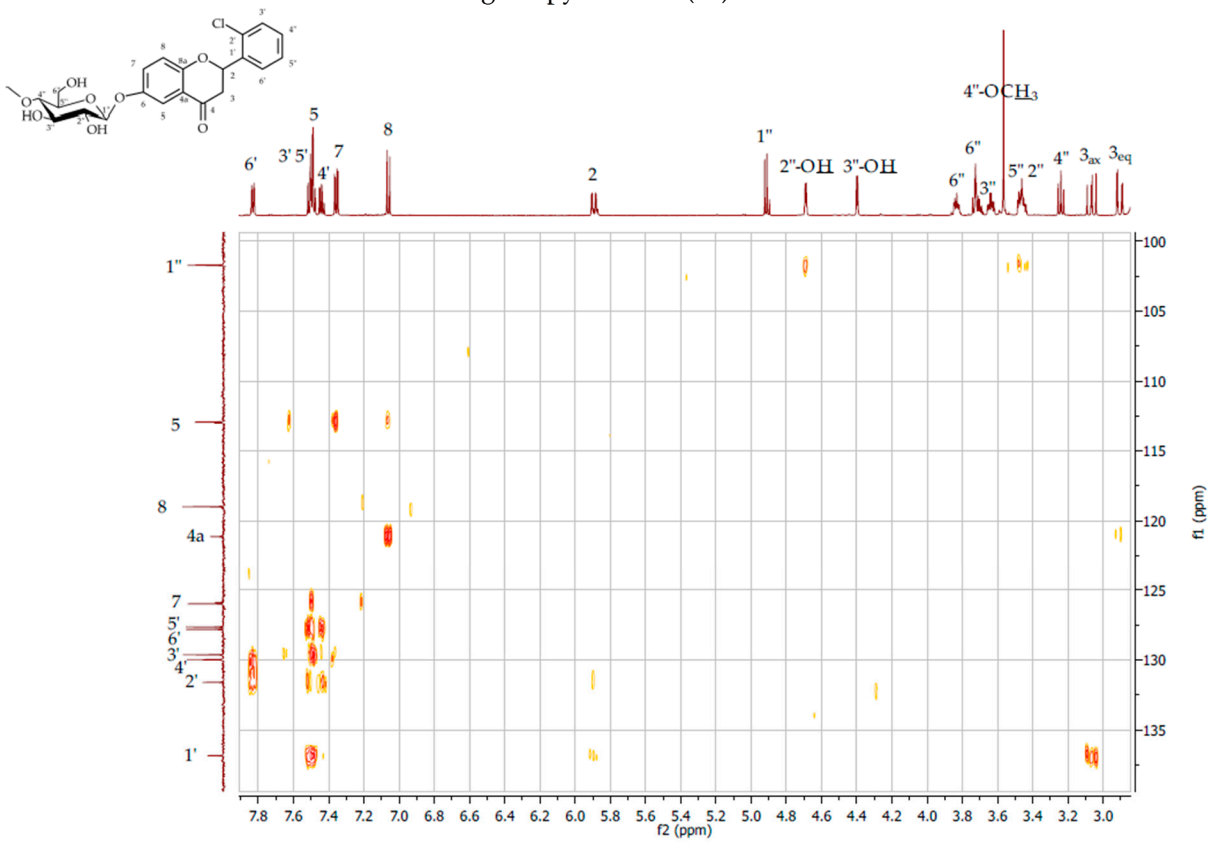


Figure S33. HMBC contour map – ^{1}H x ^{13}C expansion of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

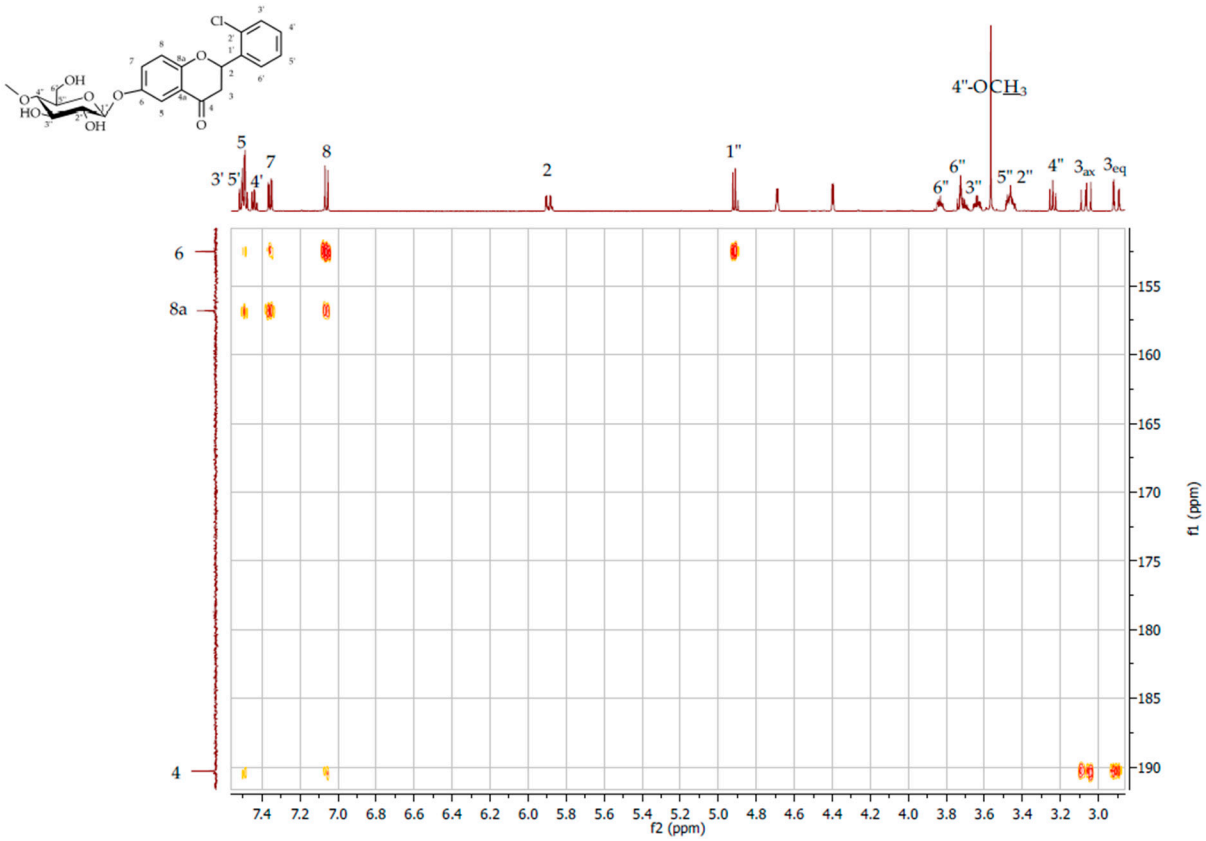


Figure S34. HMBC contour map – ^{1}H x ^{13}C expansion of 2′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**).

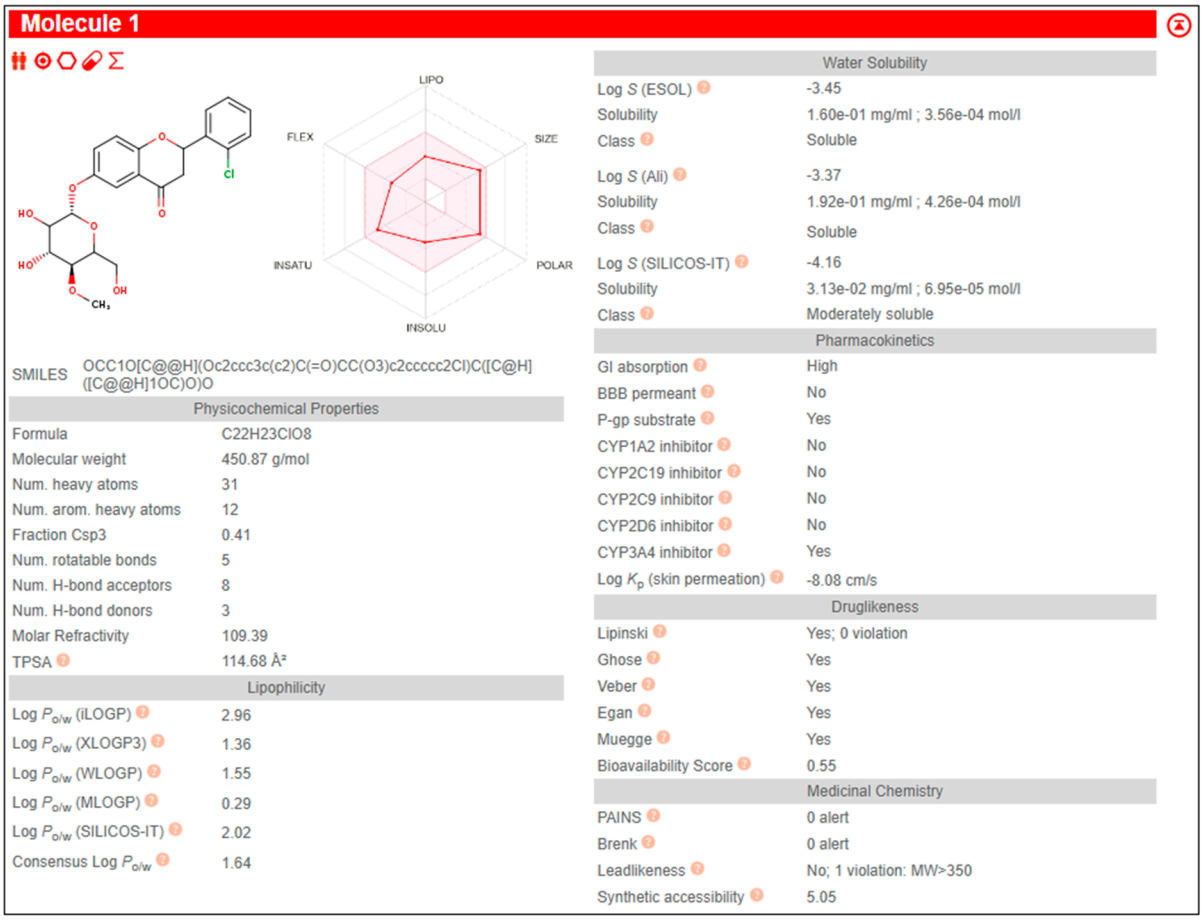


Figure S35. 2′-Chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**1a**) physicochemical and ADME parameters prediction using the SwissADME modelling.

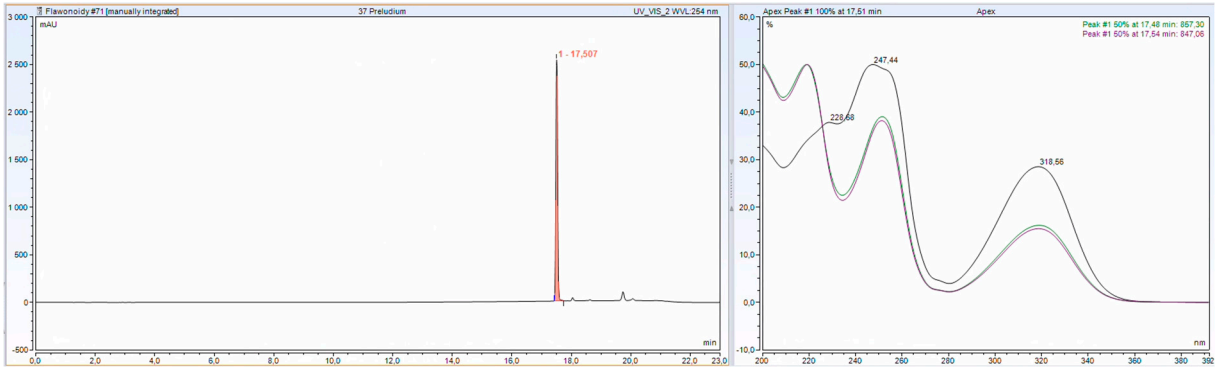


Figure S36. HPLC analysis of 3′-chloroflavanone (**2**).

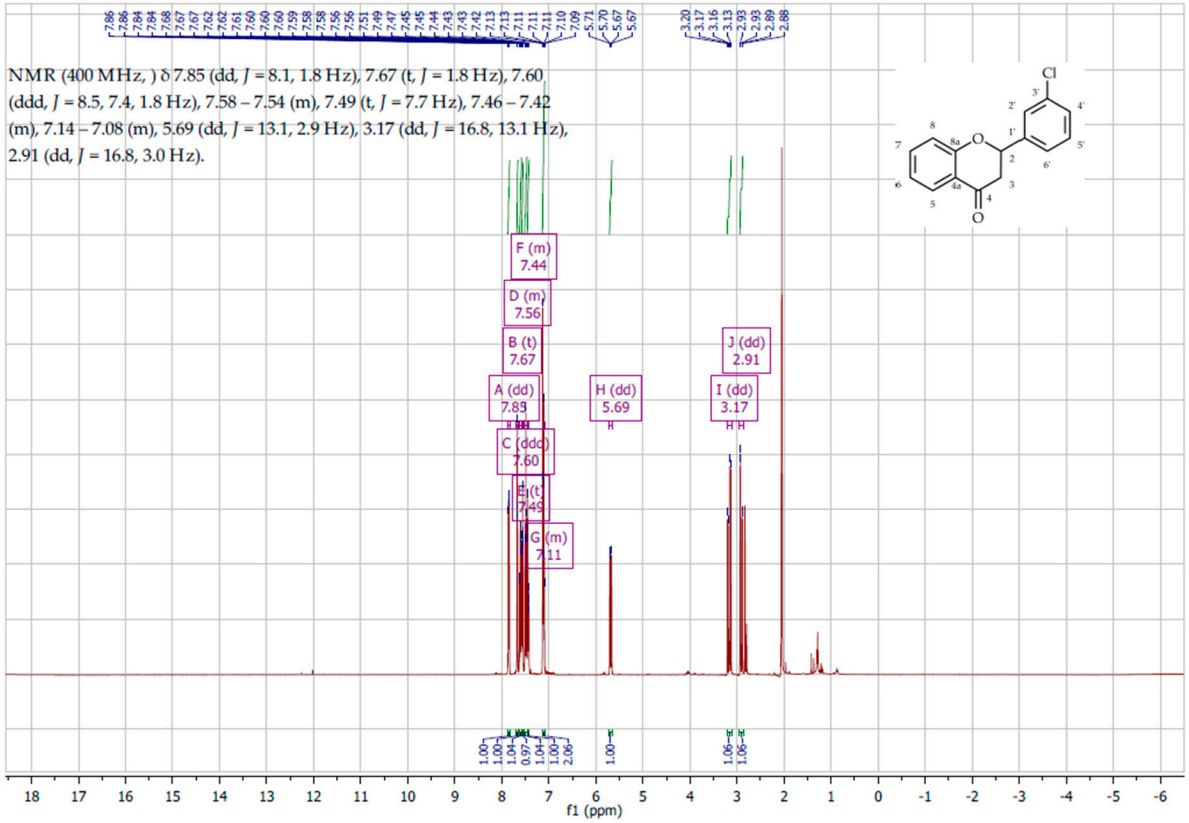


Figure S37. ^{1}H NMR spectrum (δ, acetone-d6, 600 MHz) of 3′-chloroflavanone (**2**).

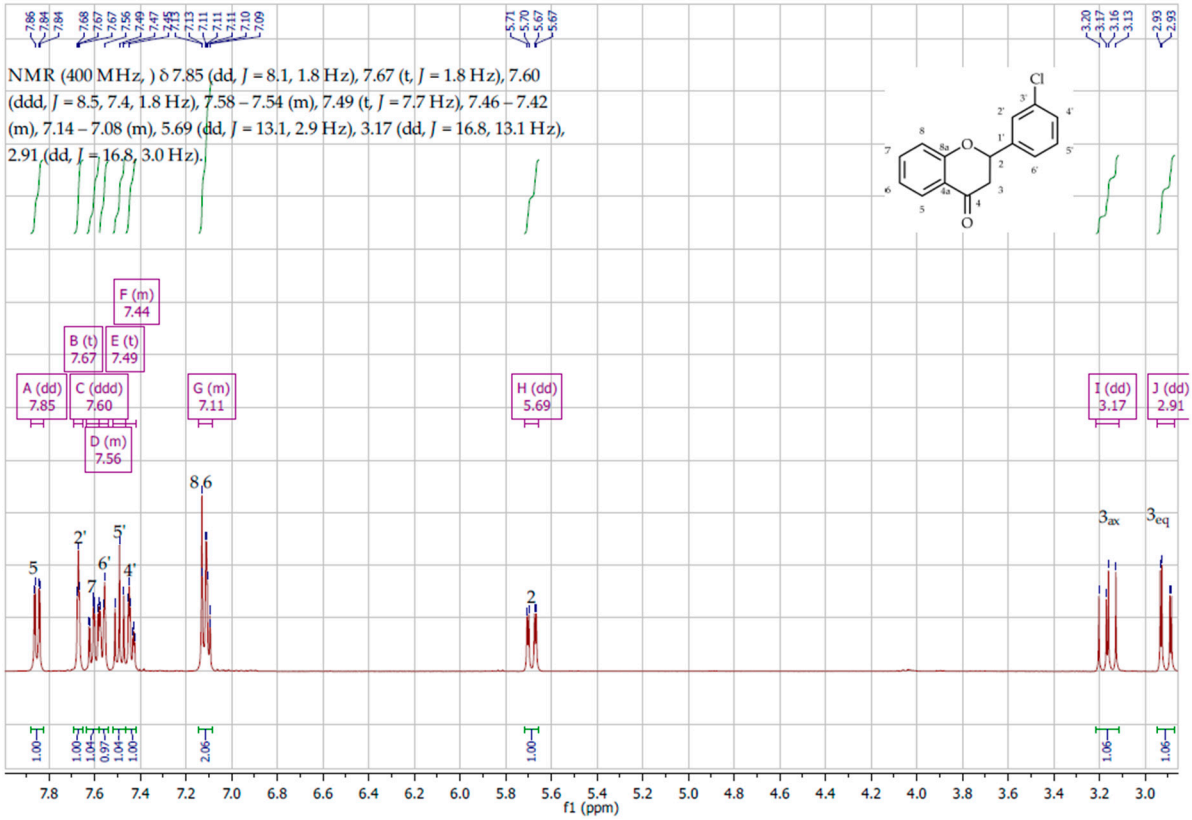


Figure S38. ^{1}H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 3′-chloroflavanone (**2**).

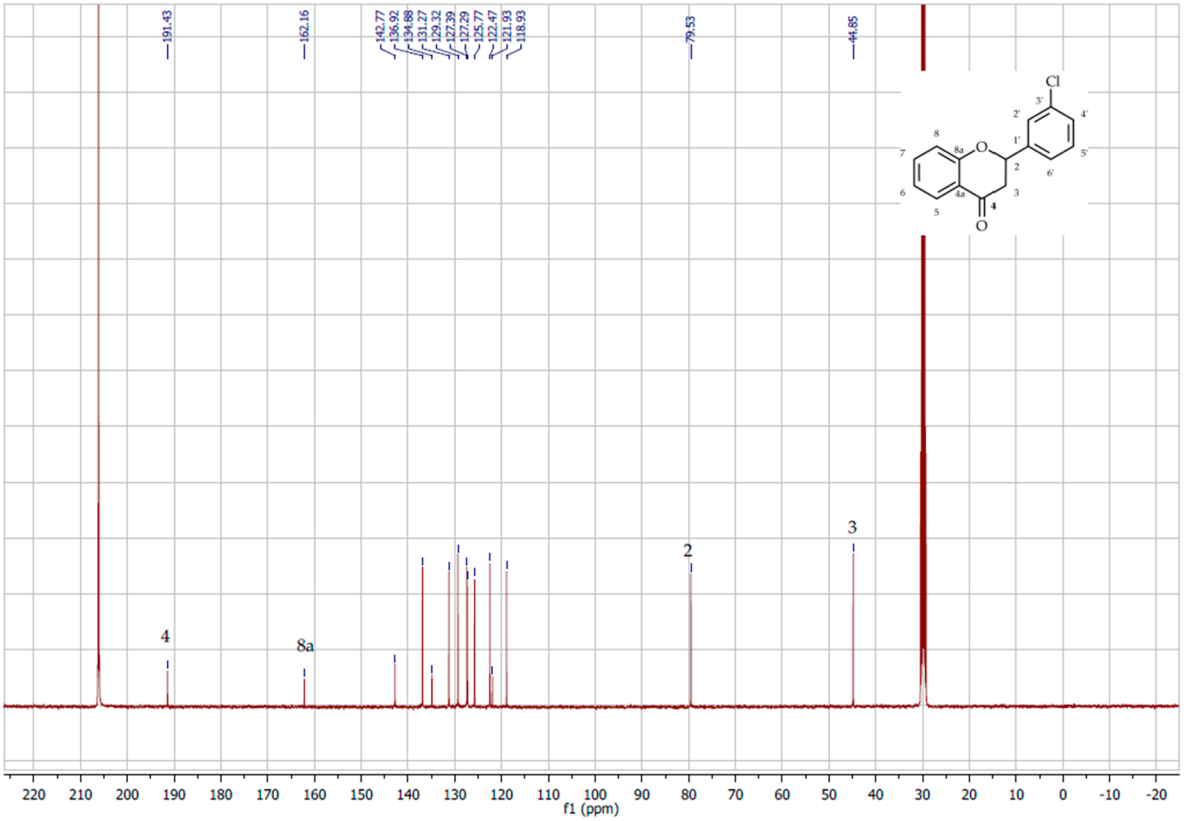


Figure S39. ^{13}C NMR spectrum (δ, acetone-d6, 151 MHz) of 3′-chloroflavanone (**2**).

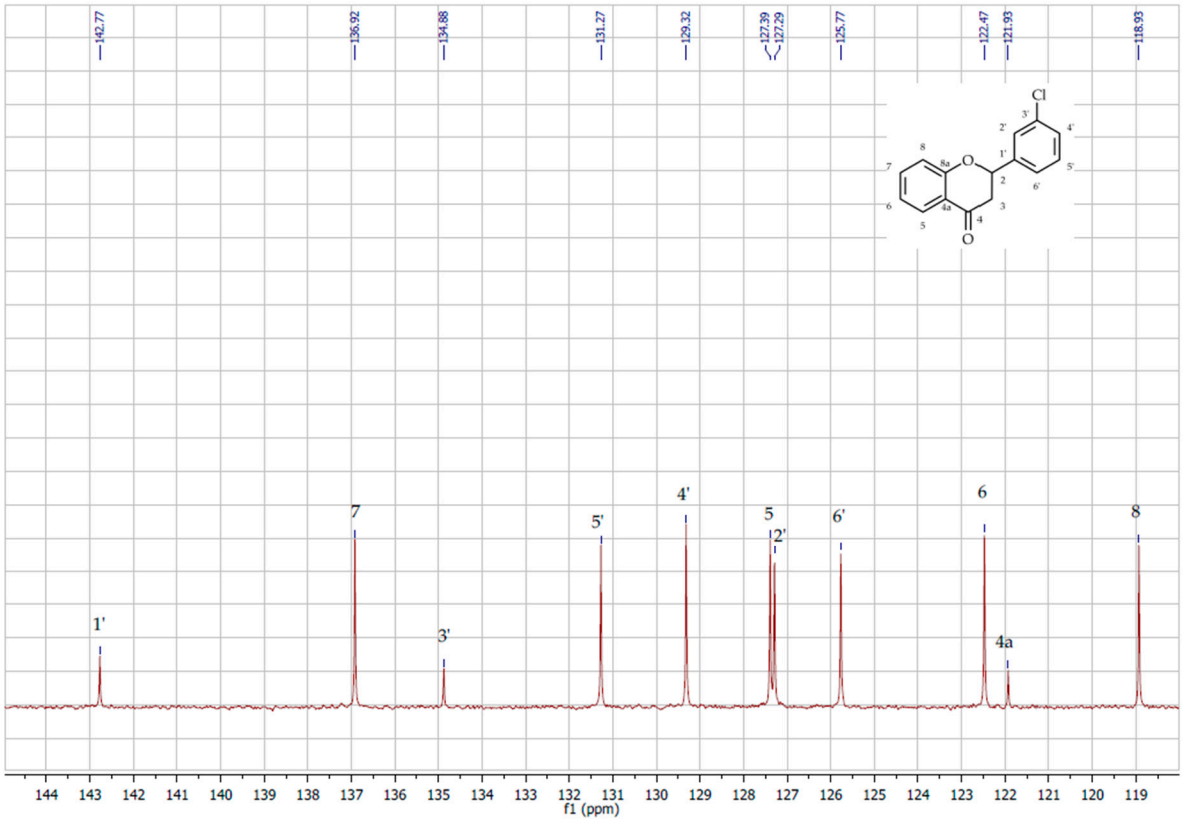


Figure S40. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 3′-chloroflavanone (**2**).

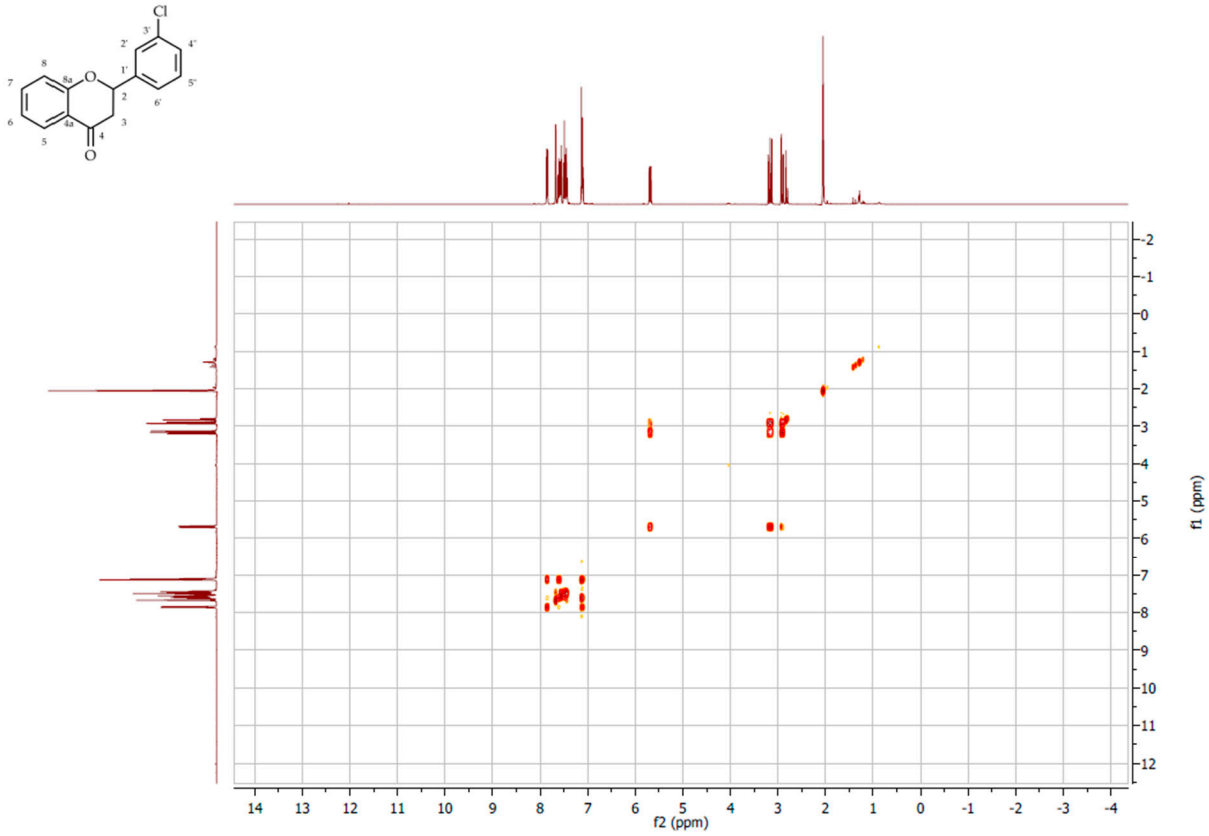


Figure S41. COSY contour map – ^{1}H x ^{1}H of 3′-chloroflavanone (**2**).

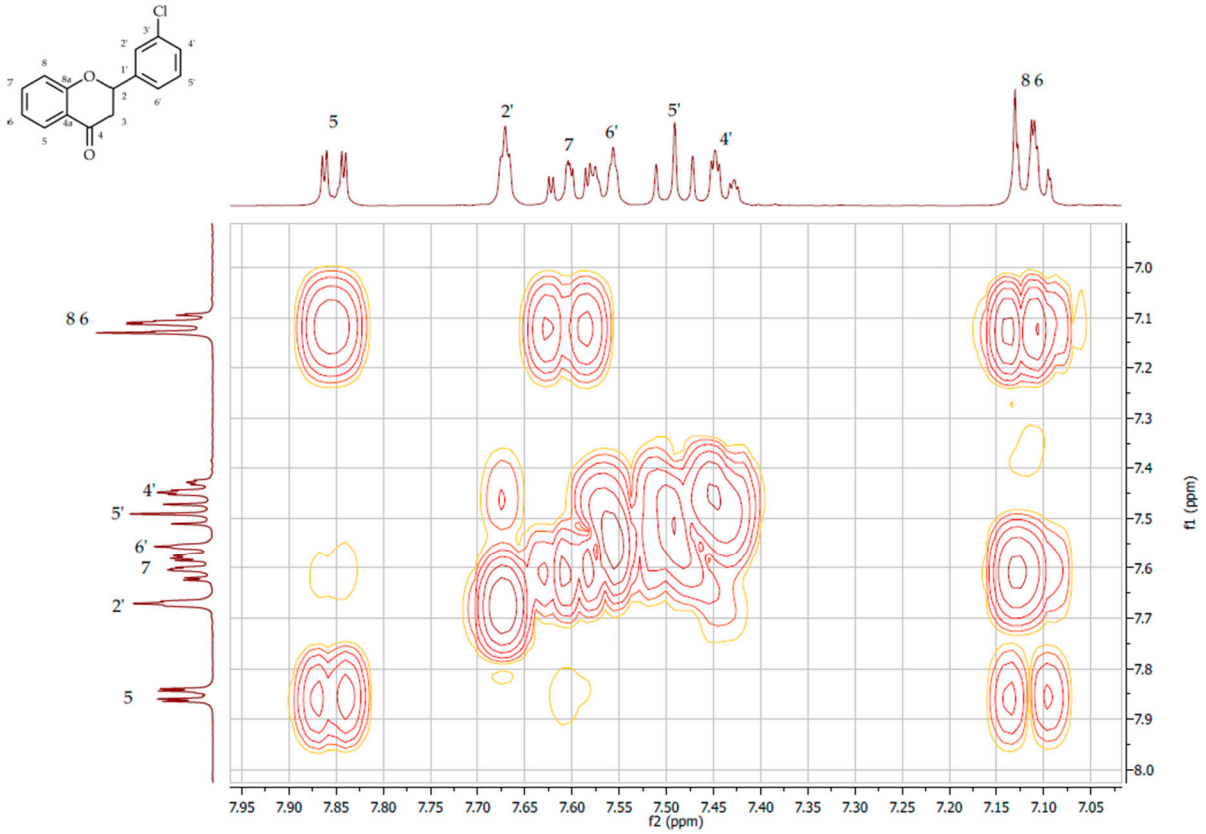


Figure S42. COSY contour map – ^{1}H x ^{1}H expansion of 3′-chloroflavanone (**2**).

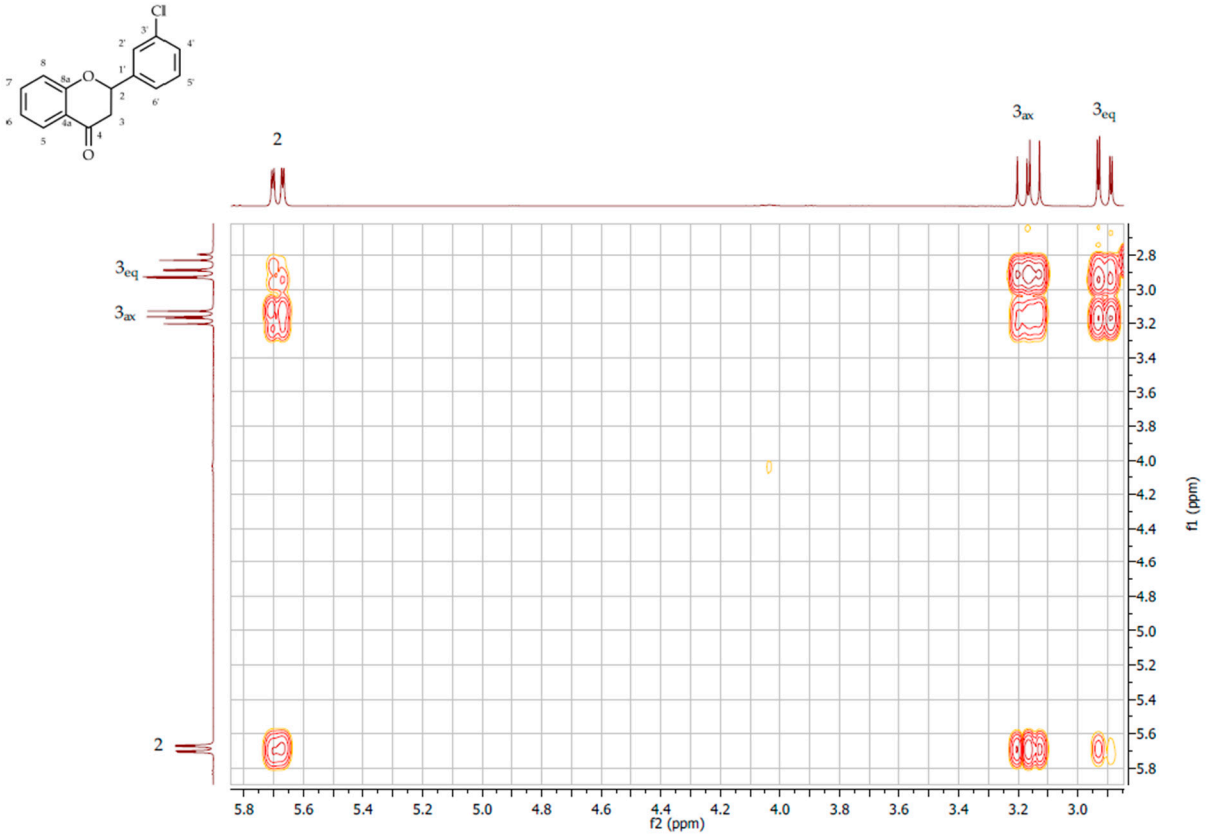


Figure S43. COSY contour map – ^{1}H x ^{1}H expansion of 3′-chloroflavanone (**2**).

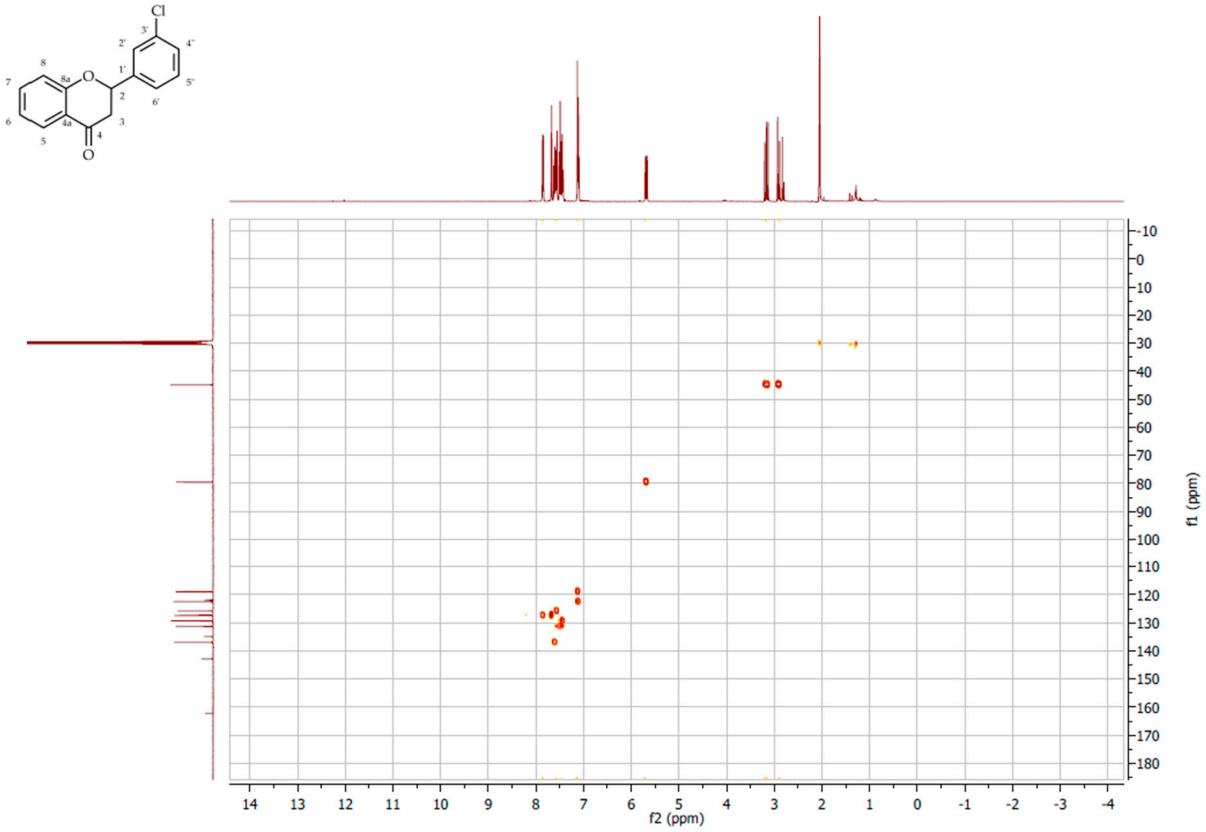


Figure S44. HMQC contour map – ^{1}H x ^{13}C of 3′-chloroflavanone (**2**).

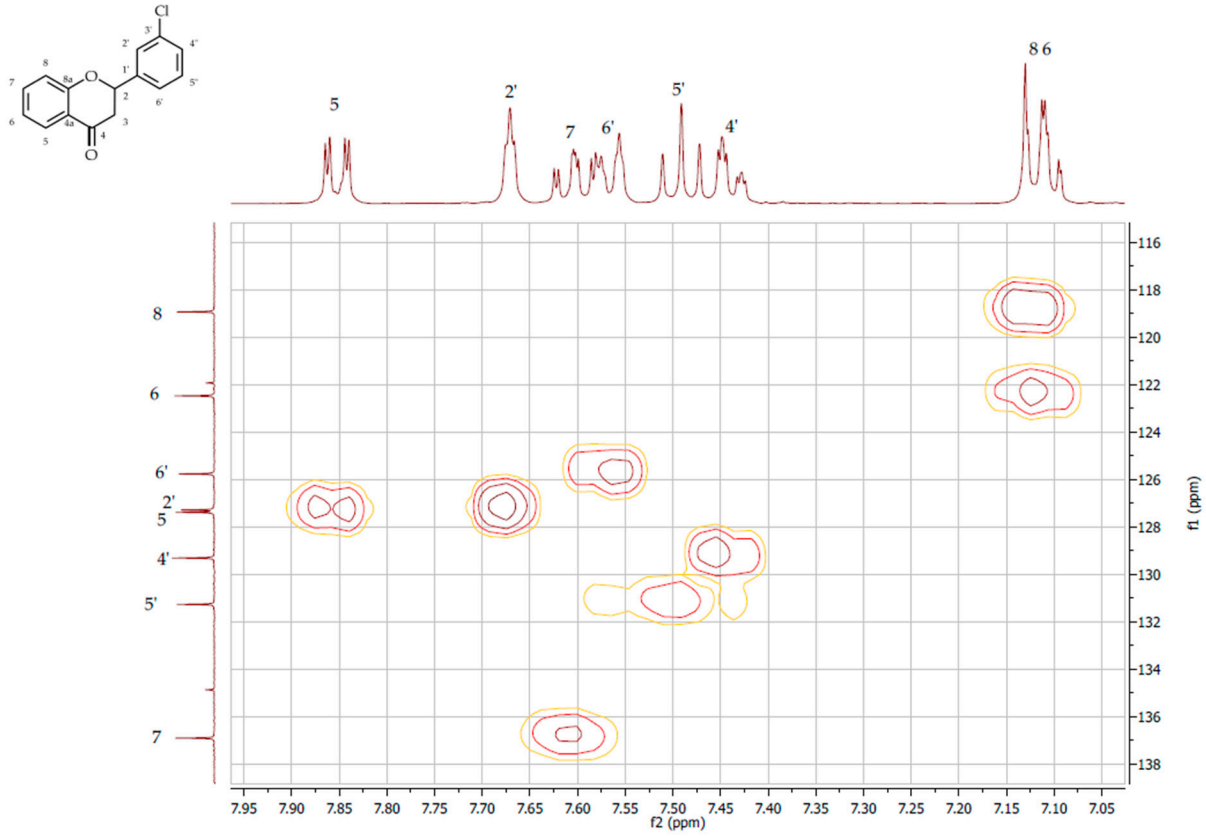


Figure S45. HMQC contour map – ^{1}H x ^{13}C expansion of 3′-chloroflavanone (**2**).

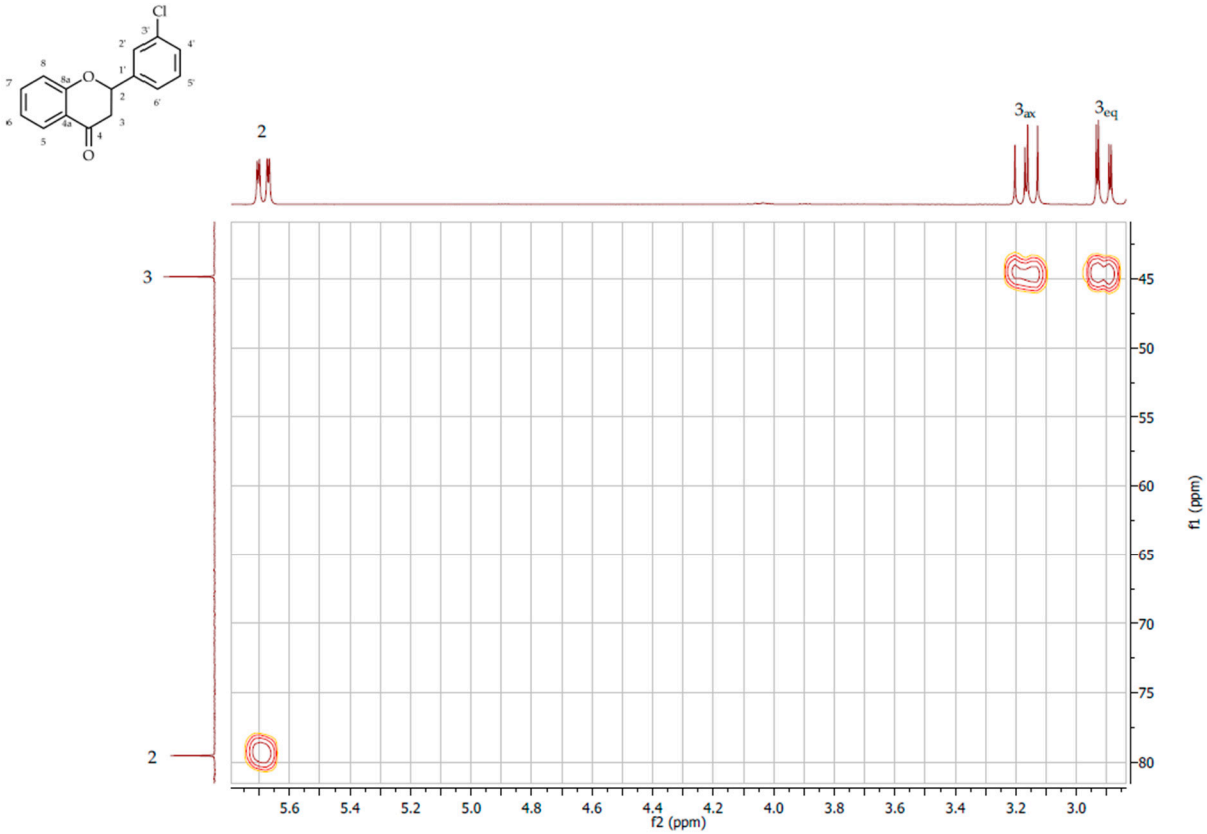


Figure S46. HMQC contour map – ^{1}H x ^{13}C expansion of 3′-chloroflavanone (**2**).

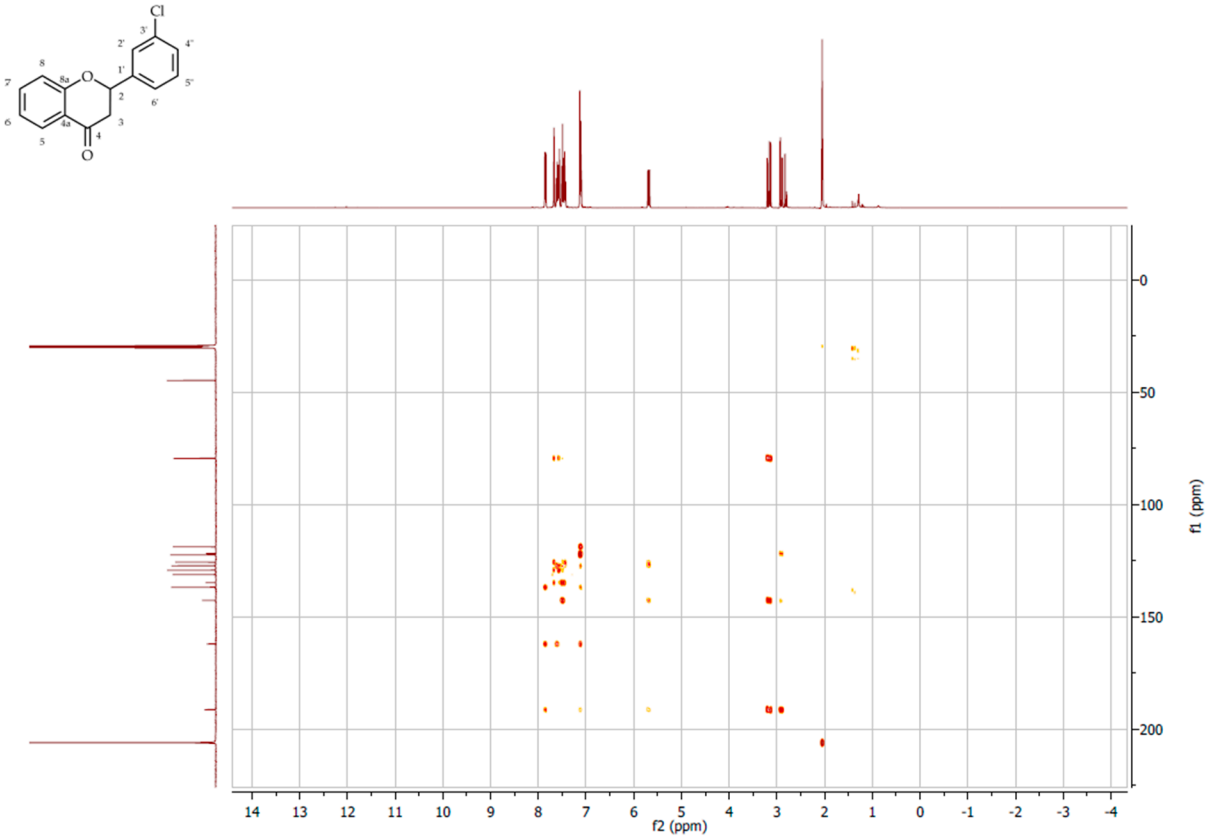


Figure S47. HMBC contour map – ^{1}H x ^{13}C of 3′-chloroflavanone (**2**).

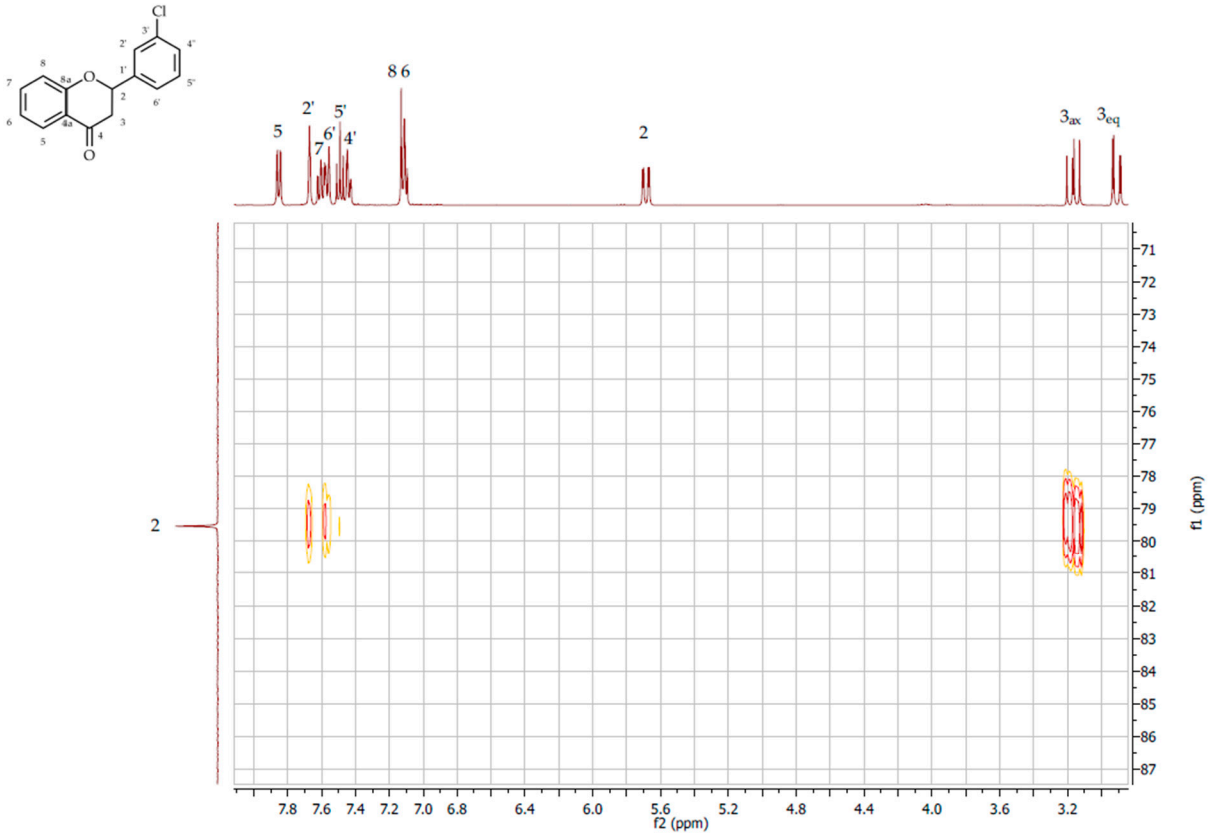


Figure S48. HMBC contour map – ^{1}H x ^{13}C expansion of 3′-chloroflavanone (**2**).

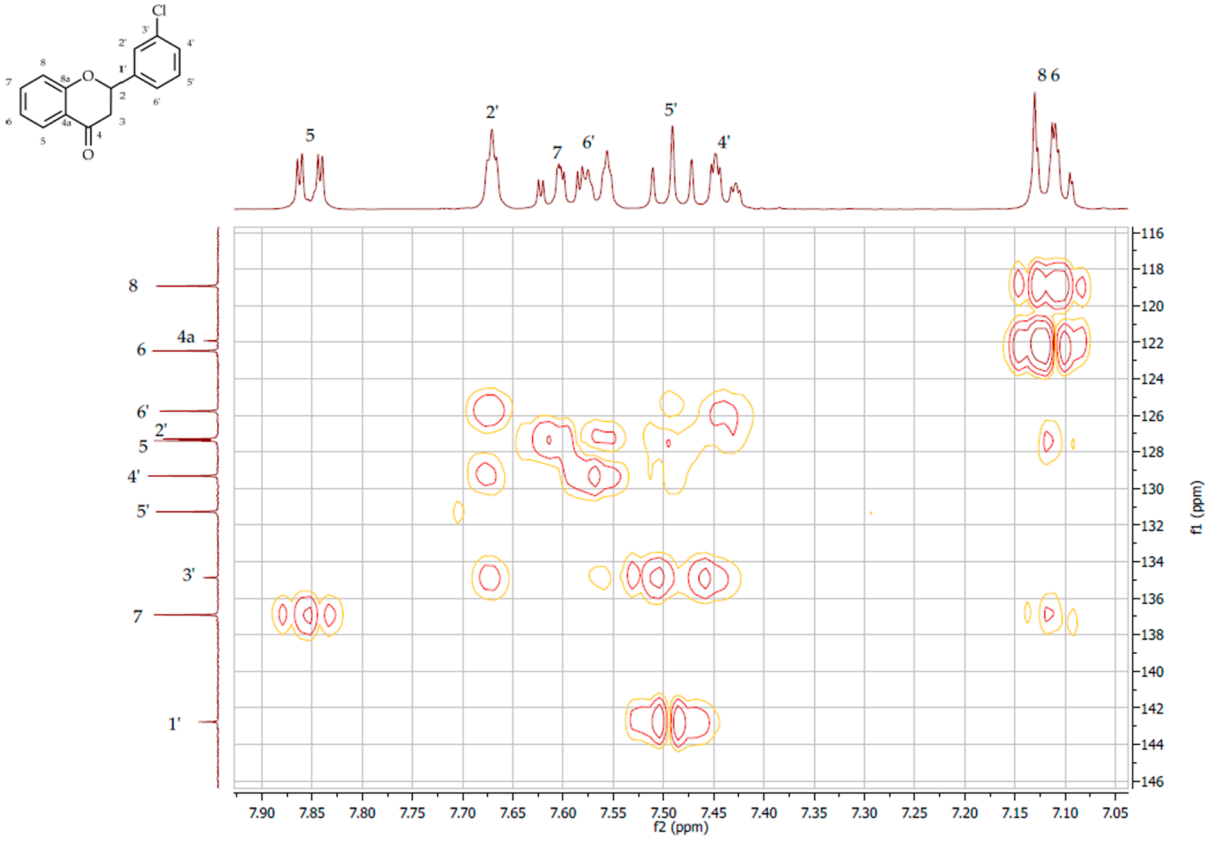


Figure S49. HMBC contour map – ^{1}H x ^{13}C expansion of 3′-chloroflavanone (**2**).

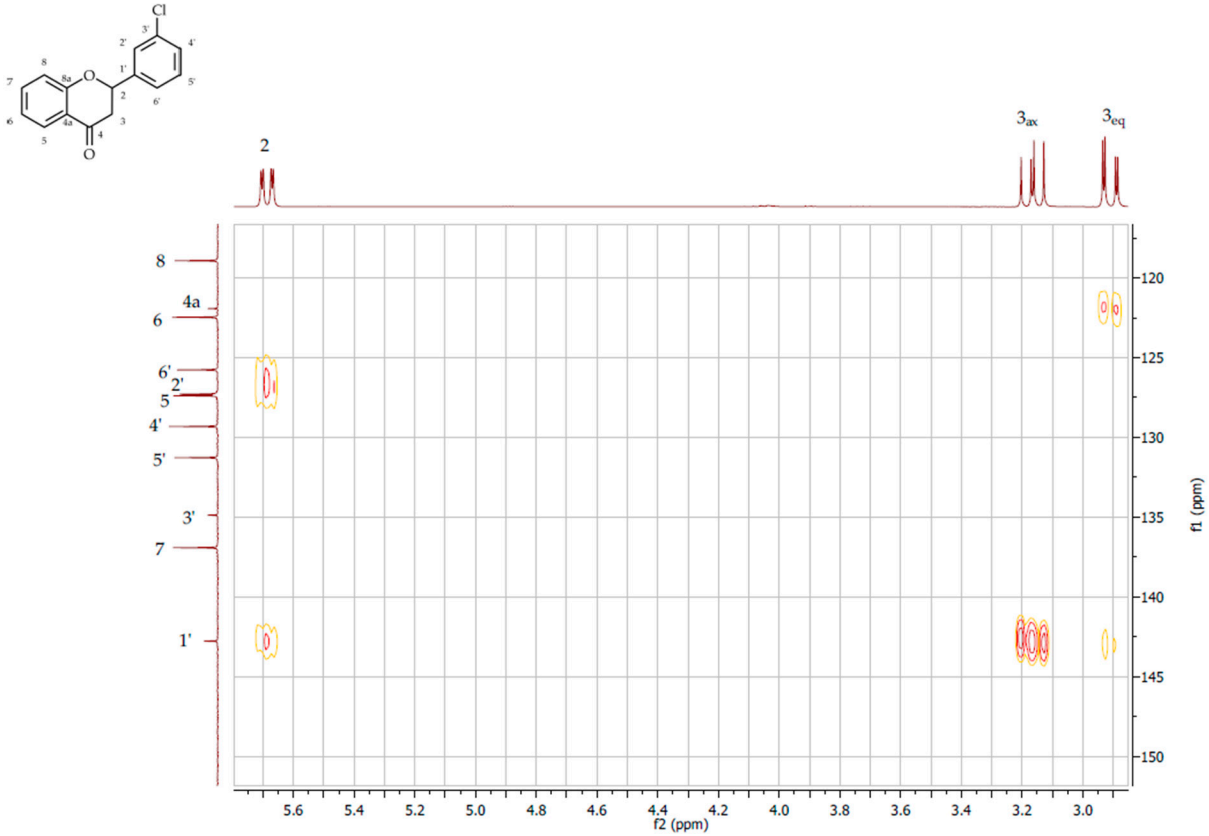


Figure S50. HMBC contour map – ^{1}H x ^{13}C expansion of 3′-chloroflavanone (**2**).

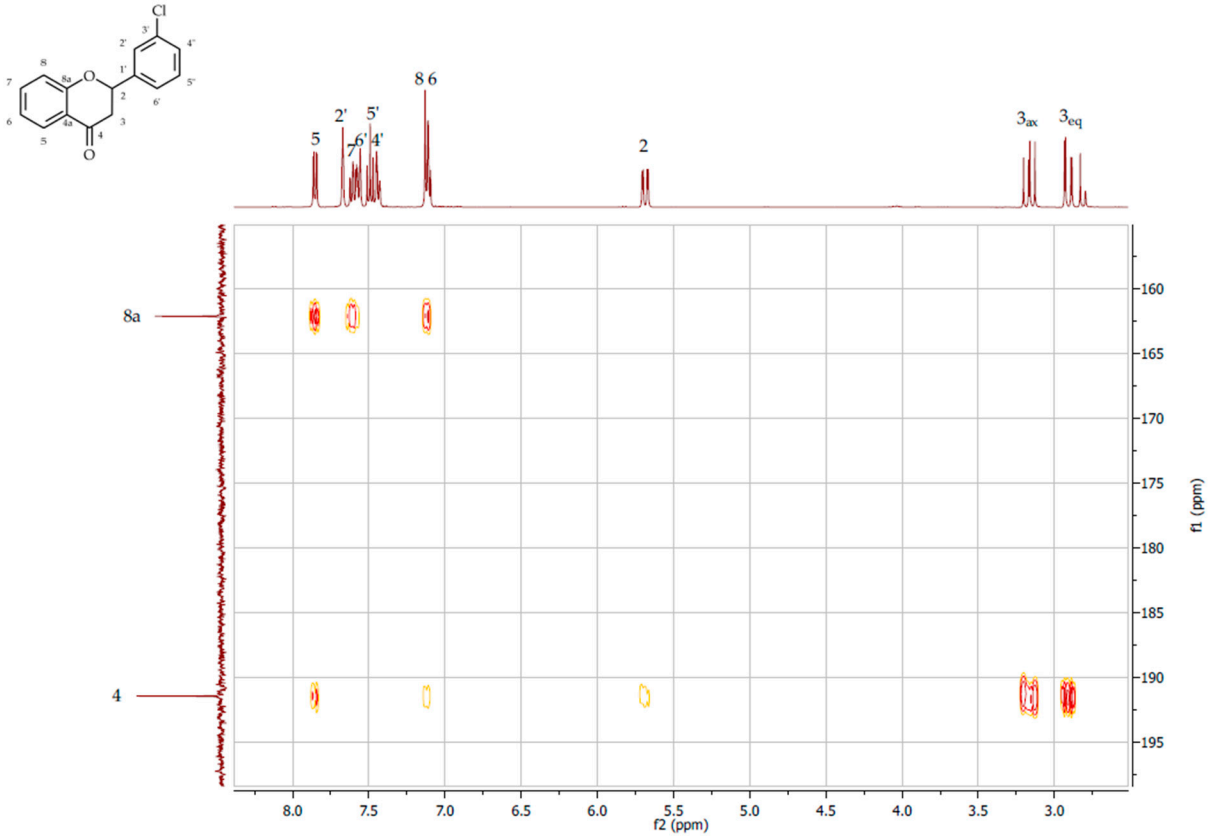


Figure S51. HMBC contour map – ^{1}H x ^{13}C expansion of 3′-chloroflavanone (**2**).

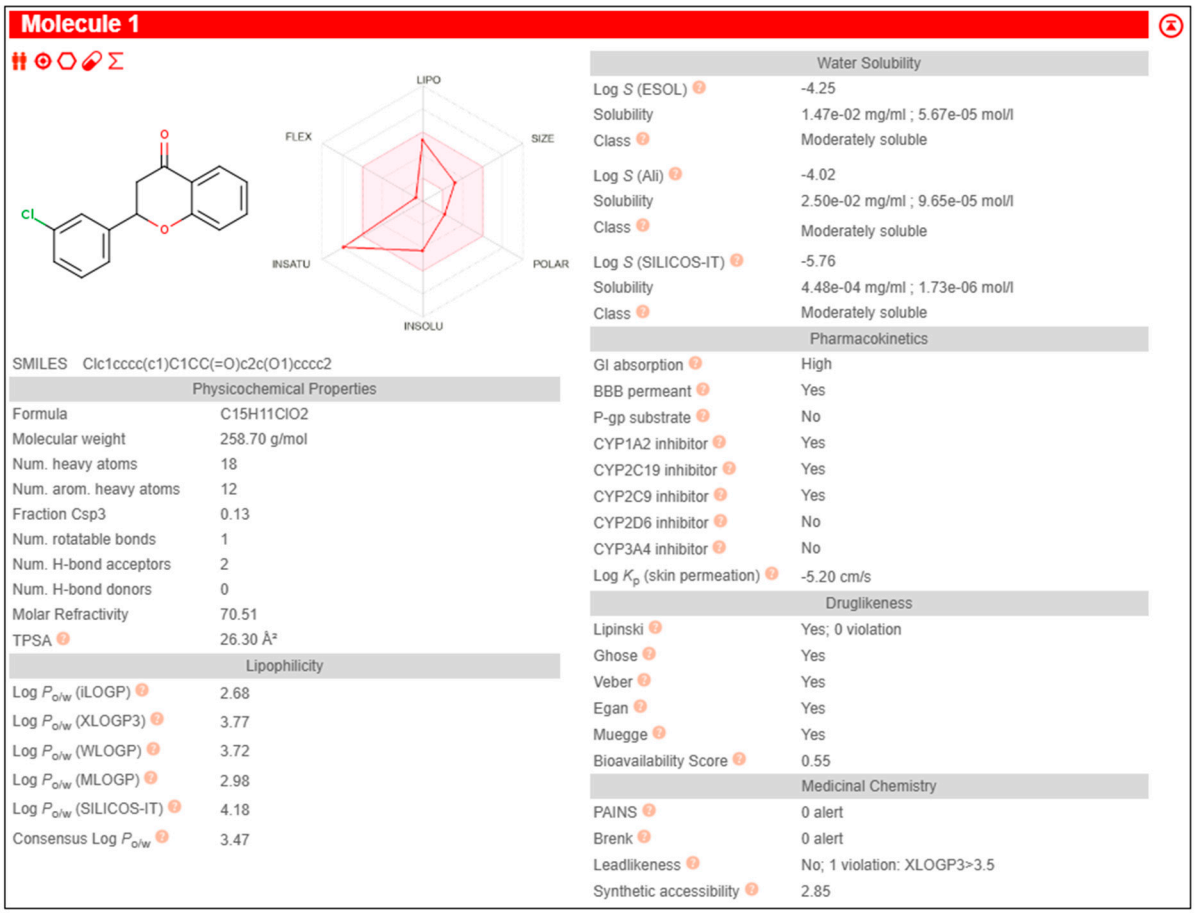


Figure S52. 3′-Chloroflavanone (**2**) physicochemical and ADME parameters prediction using the SwissADME modelling.

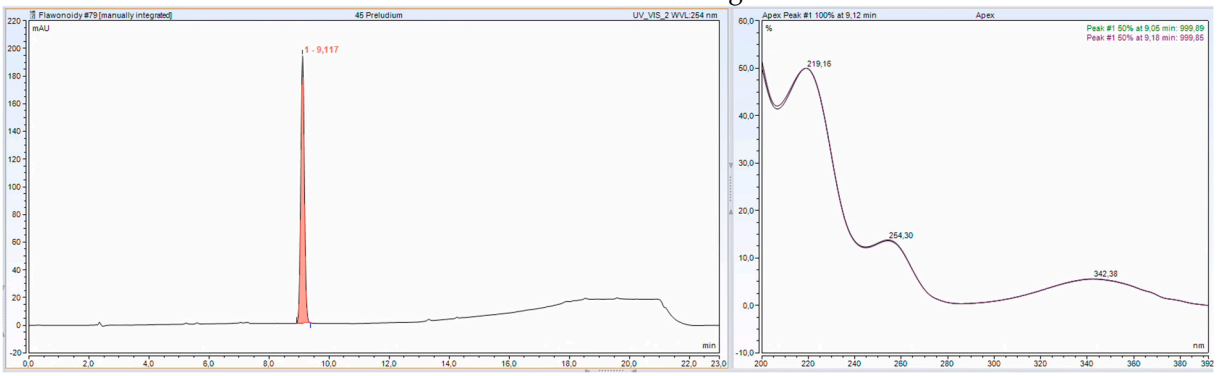


Figure S53. HPLC analysis of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

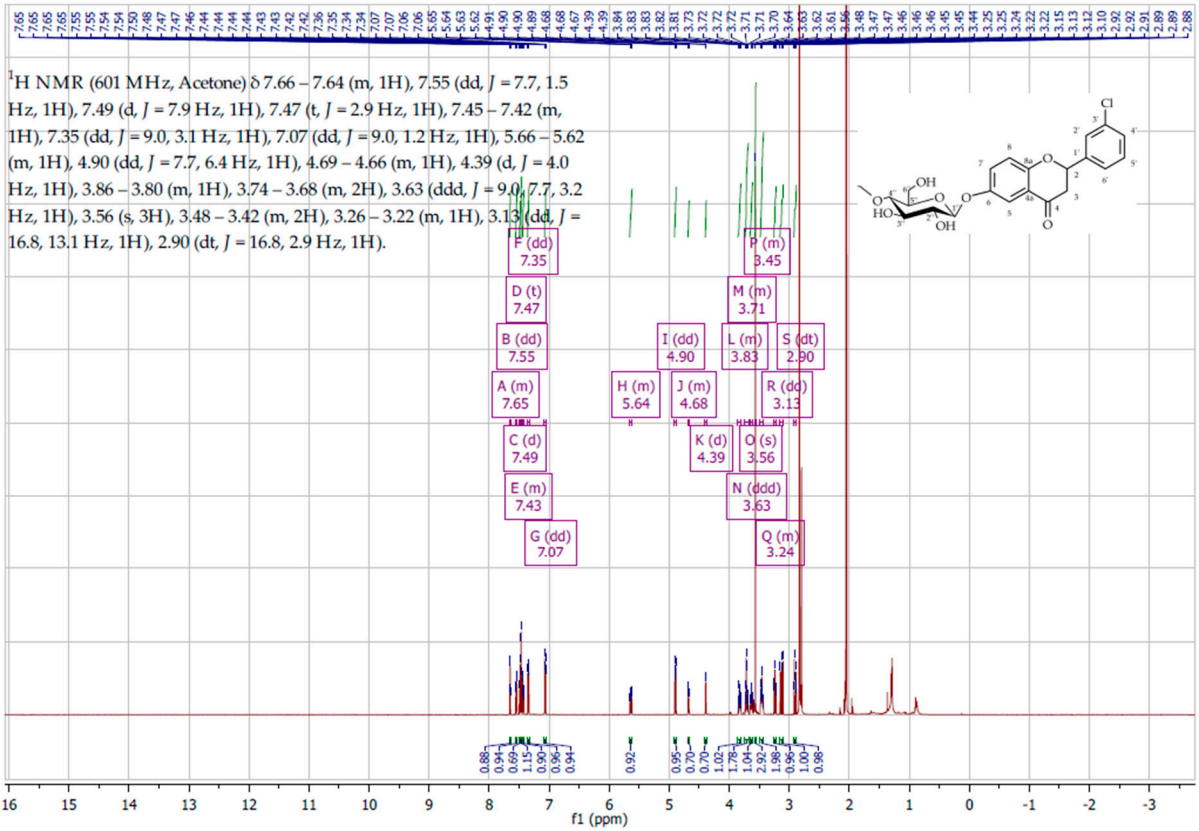


Figure S54. ^{1}H NMR spectrum (*δ*, acetone-d6, 600 MHz) of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

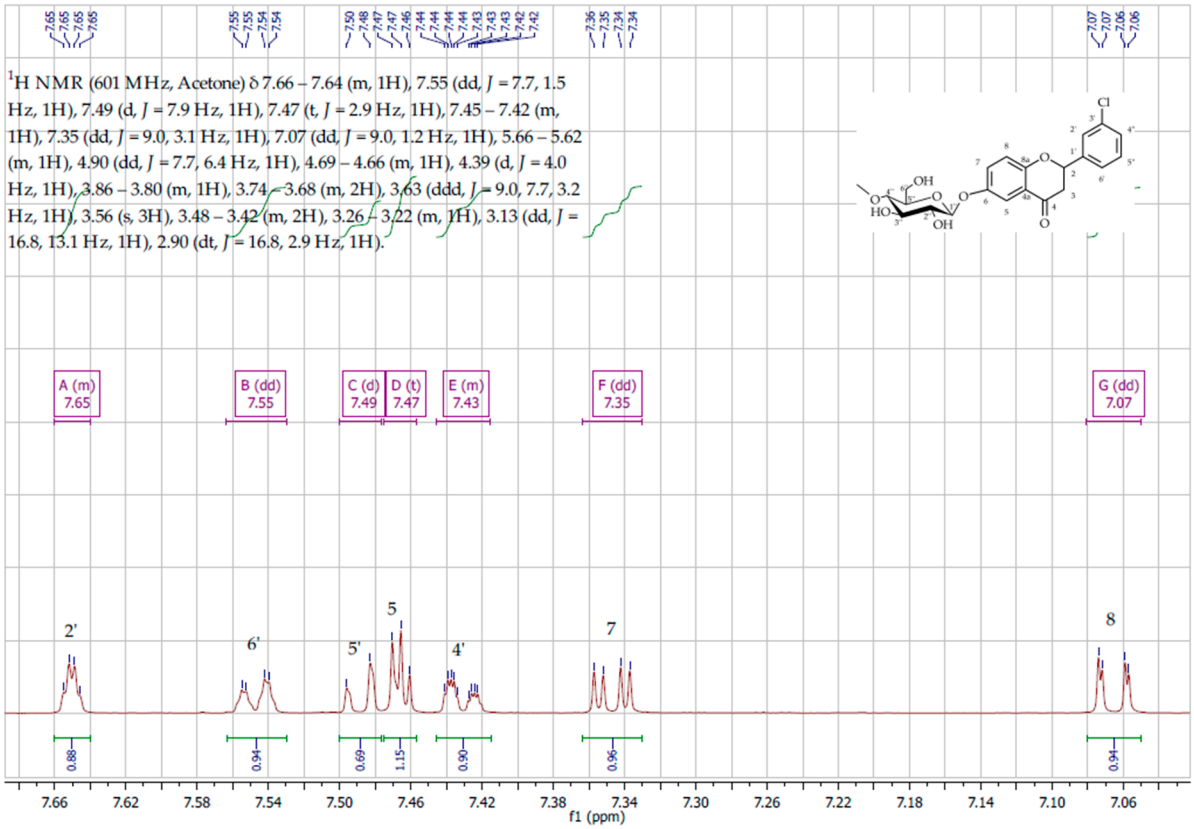


Figure S55. ^{1}H NMR spectrum expansion (*δ*, acetone-d6, 600 MHz) of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

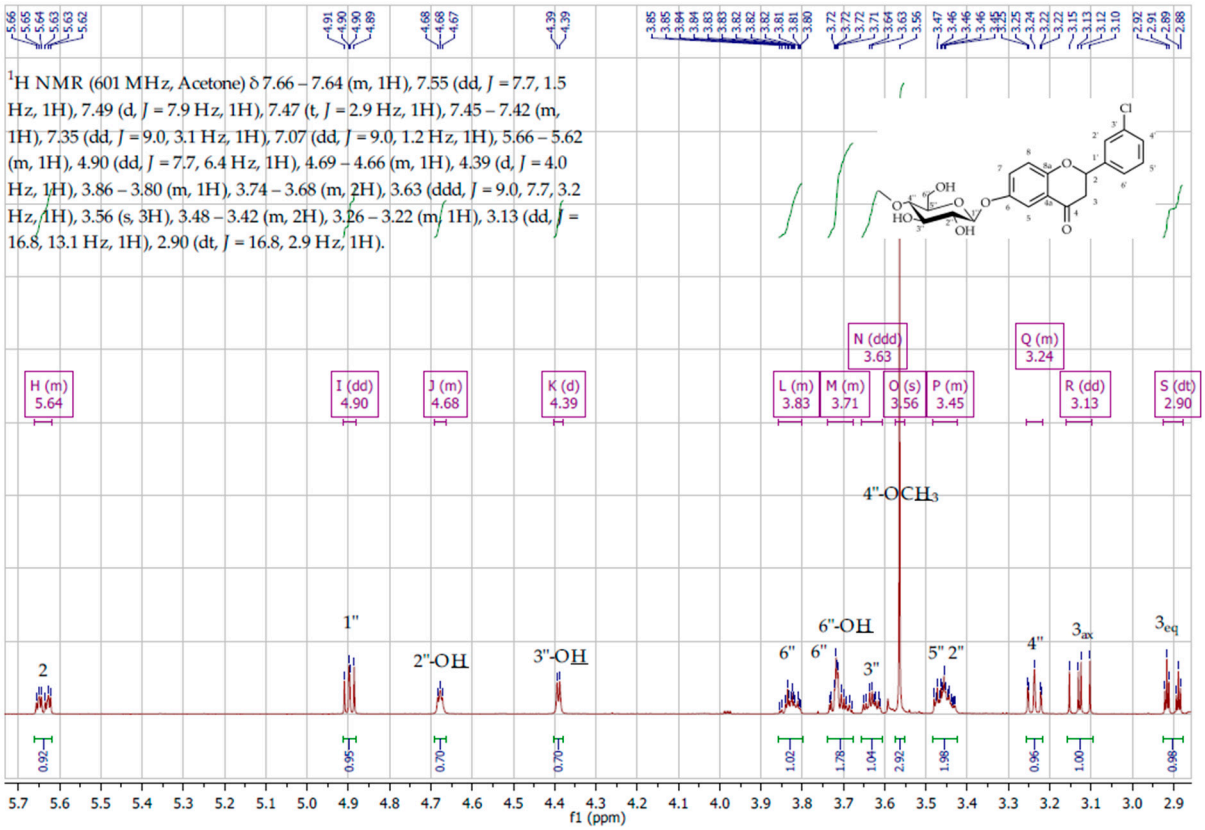


Figure S56. ^{1}H NMR spectrum expansion (*δ*, acetone-d6, 600 MHz) of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

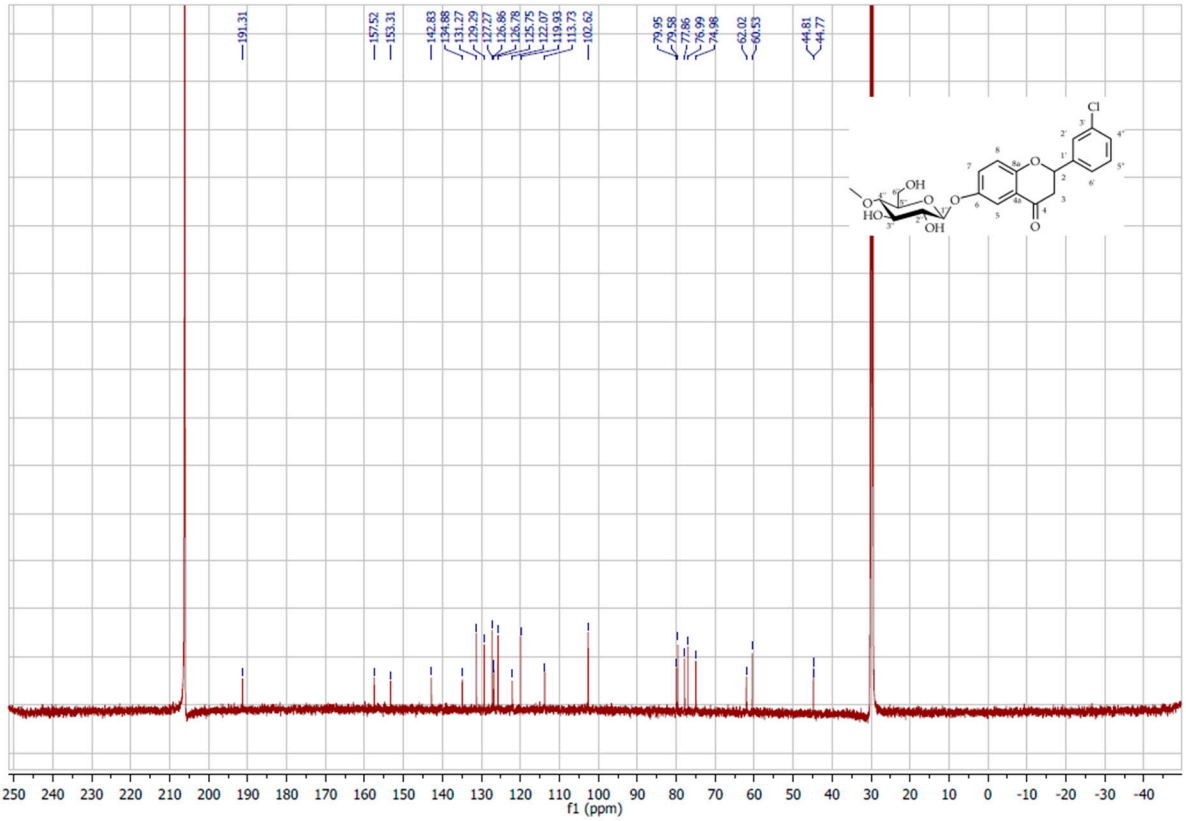


Figure S57. ^{13}C NMR spectrum (*δ*, acetone-d6, 151 MHz) of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

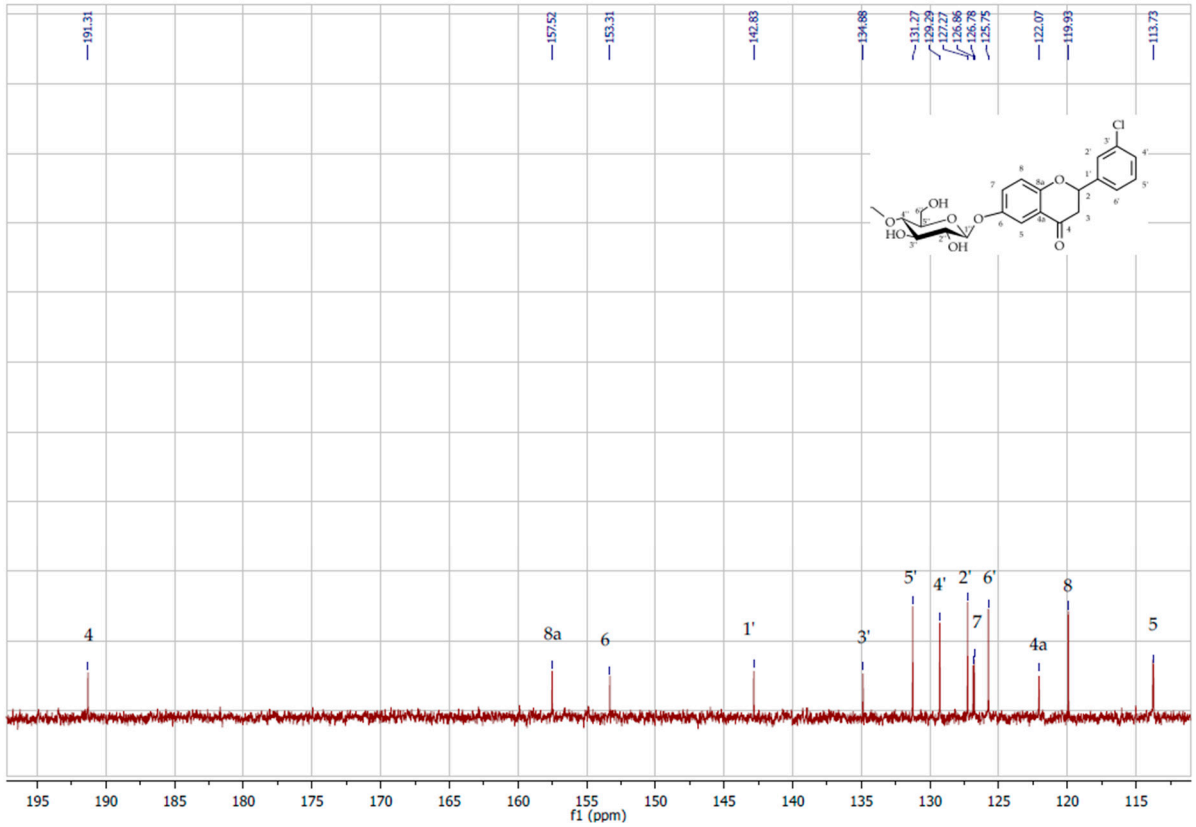


Figure S58. ^{13}C NMR spectrum expansion (*δ*, acetone-d6, 151 MHz) of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

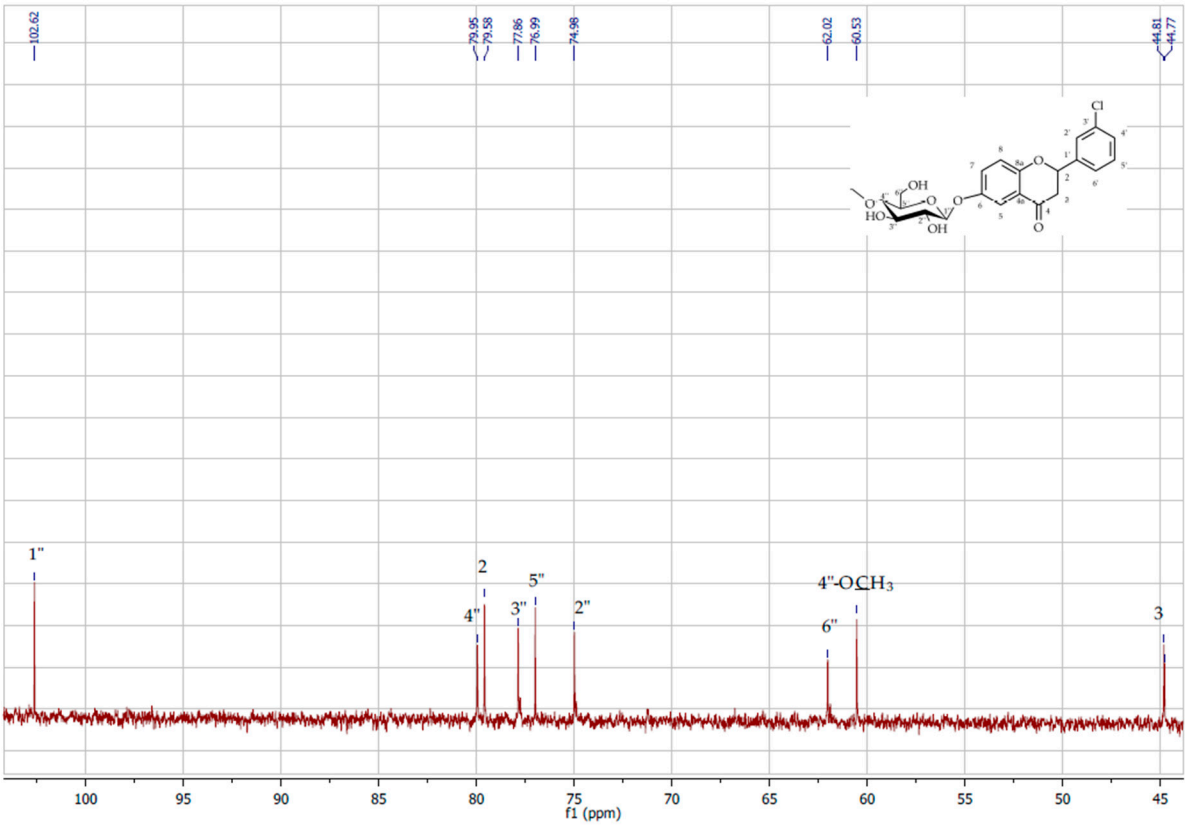


Figure S59. ^{13}C NMR spectrum expansion (*δ*, acetone-d6, 151 MHz) of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

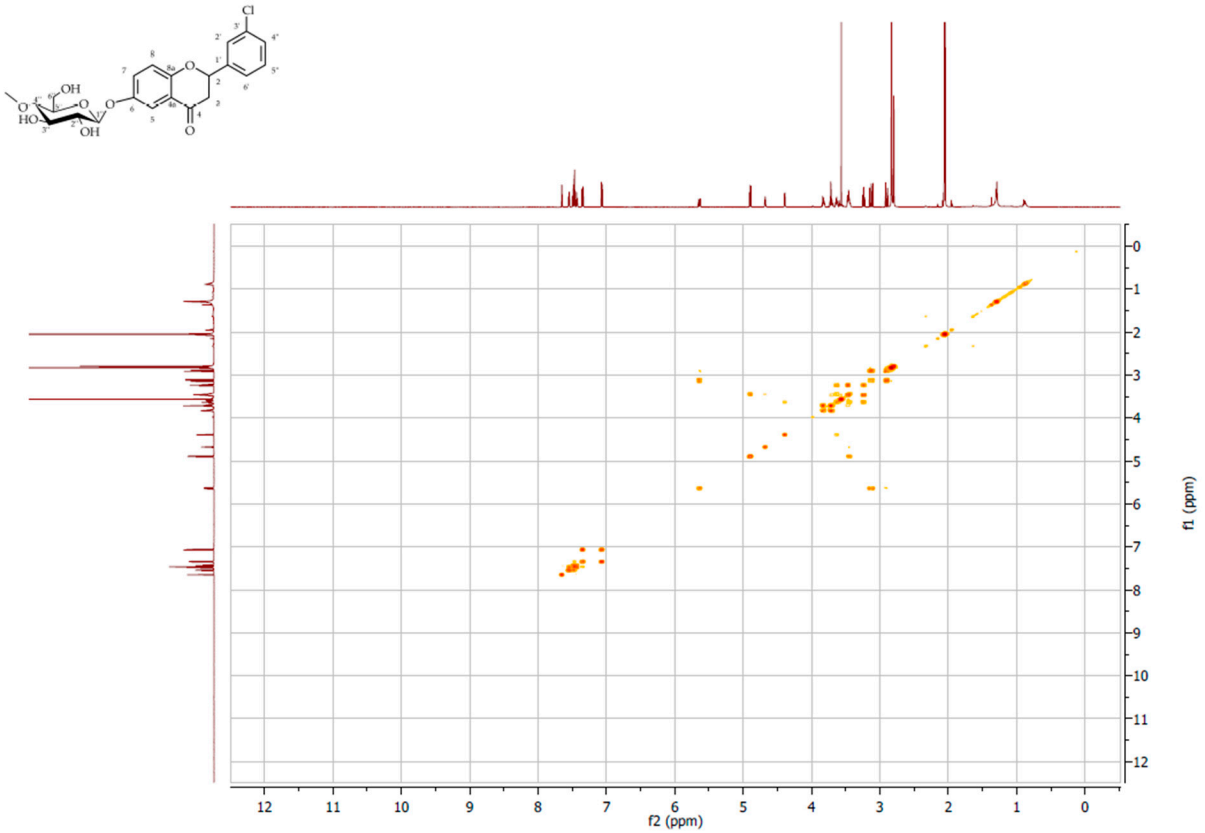


Figure S60. COSY contour map – ^{1}H x ^{1}H of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

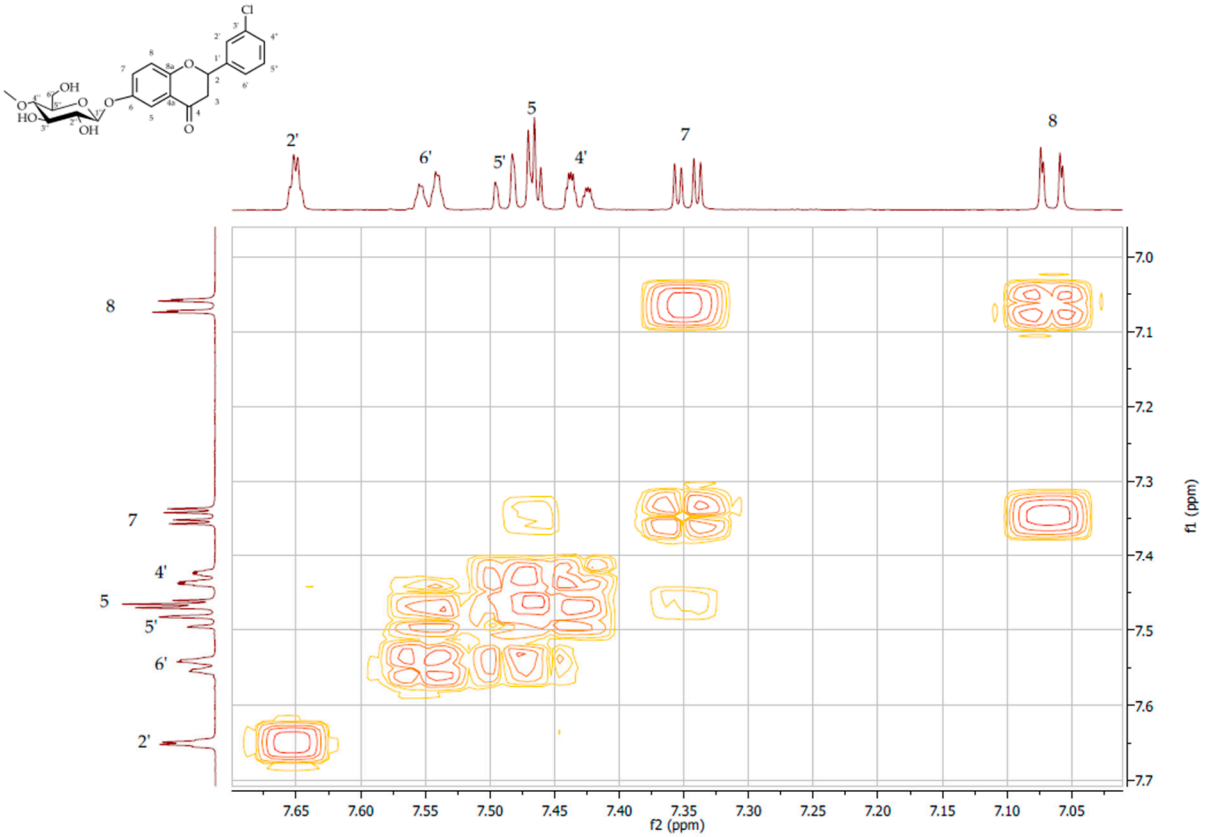


Figure S61. COSY contour map – ^{1}H x ^{1}H expansion of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

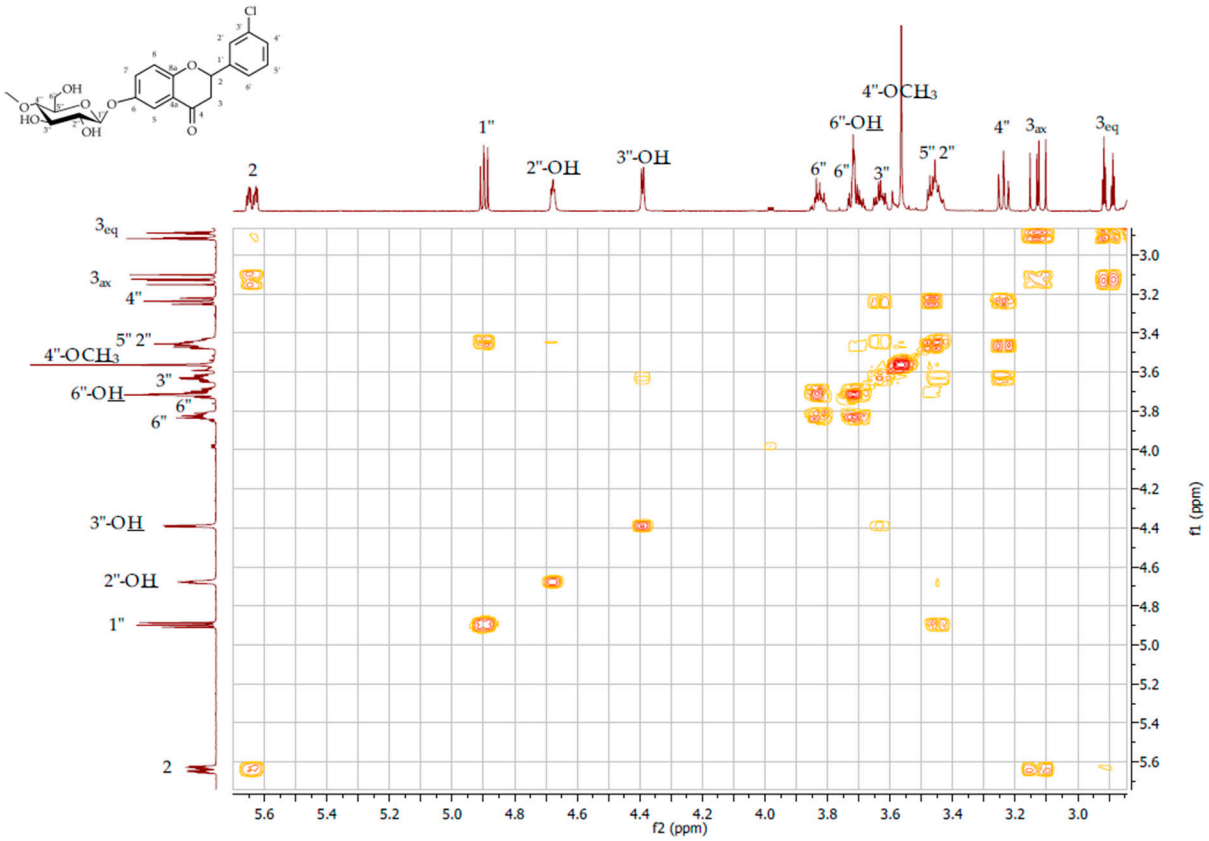


Figure S62. COSY contour map – ^{1}H x ^{1}H expansion of 3′-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

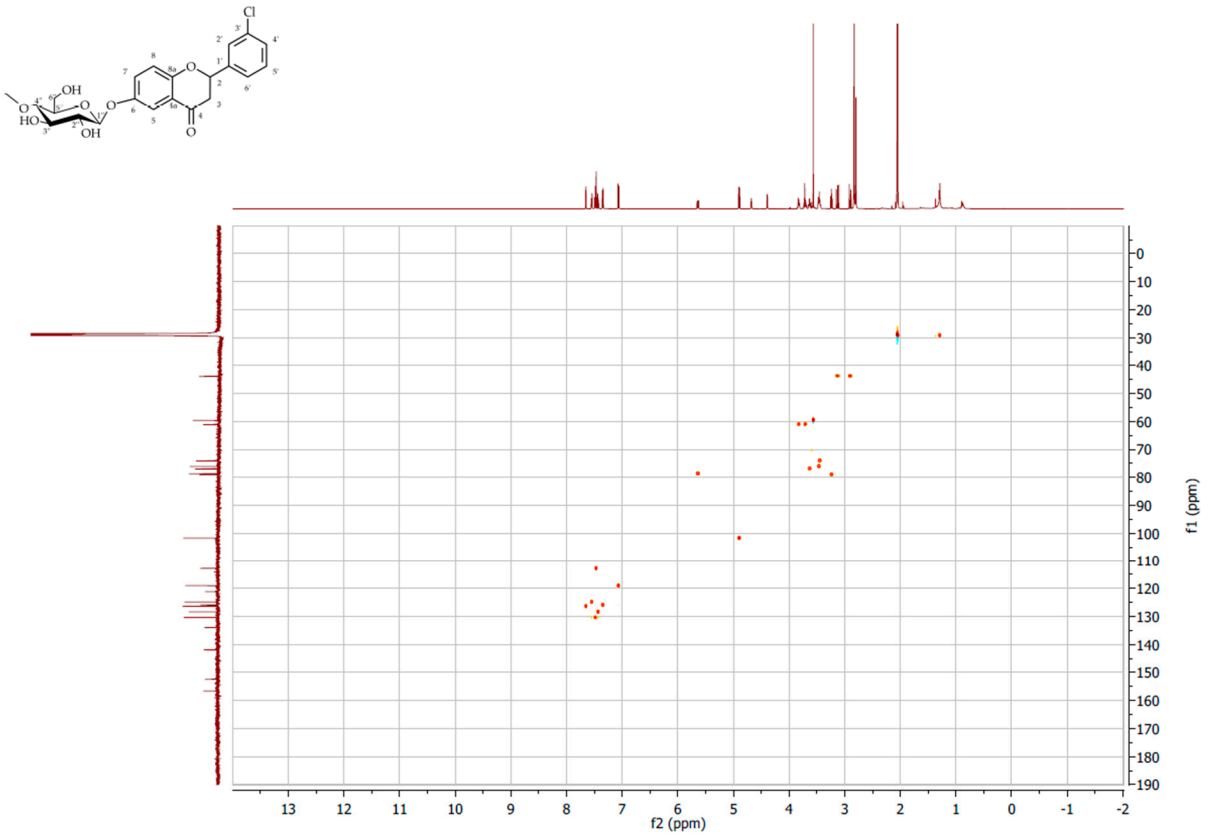


Figure S63. HMQC contour map – ^{1}H x ^{13}C of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

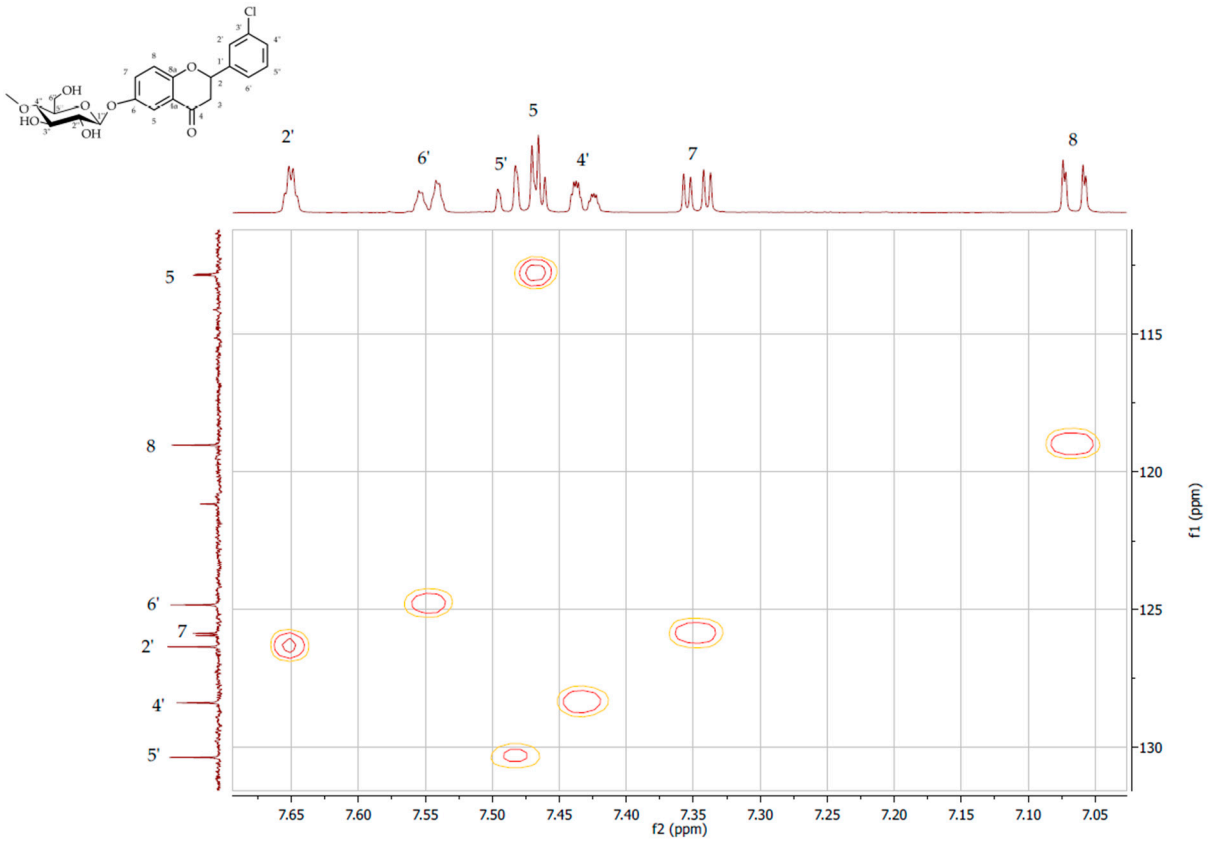


Figure S64. HMQC contour map – ^{1}H x ^{13}C expansion of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

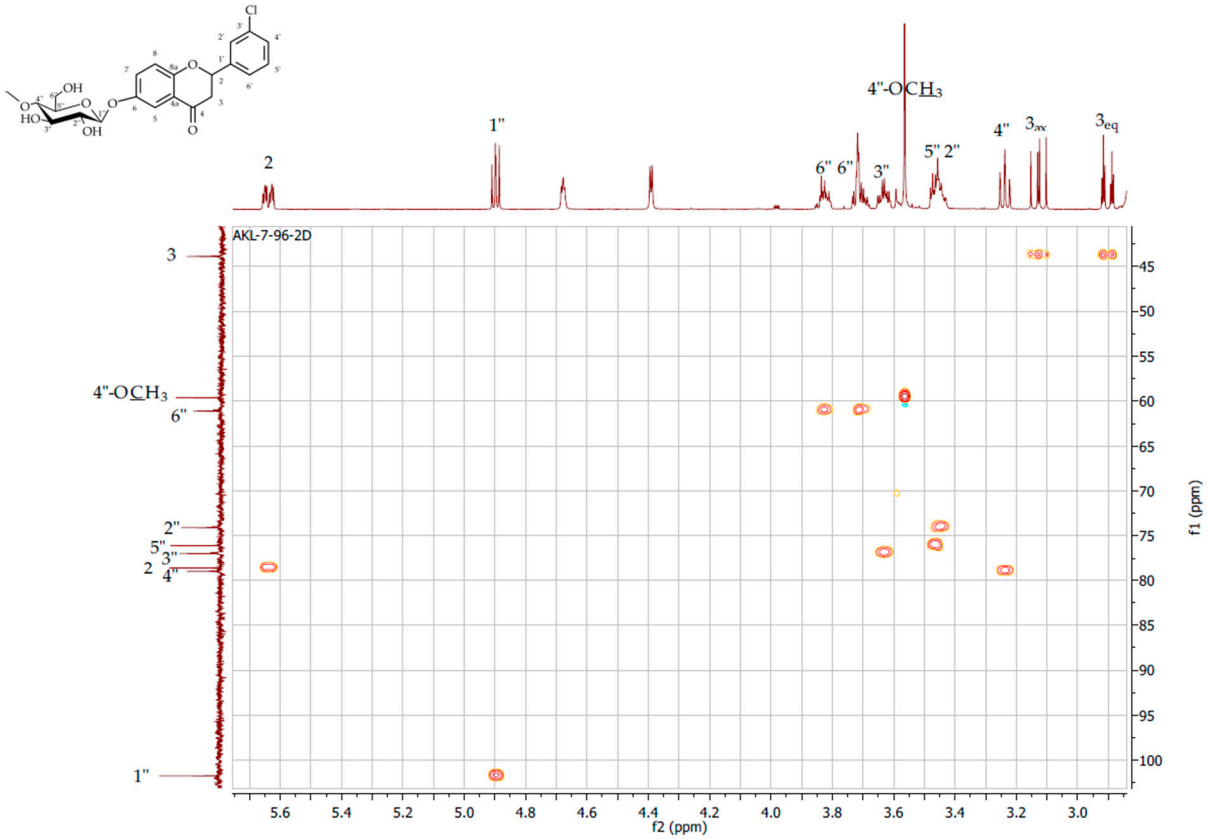


Figure S65. HMQC contour map – ^{1}H x ^{13}C expansion of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

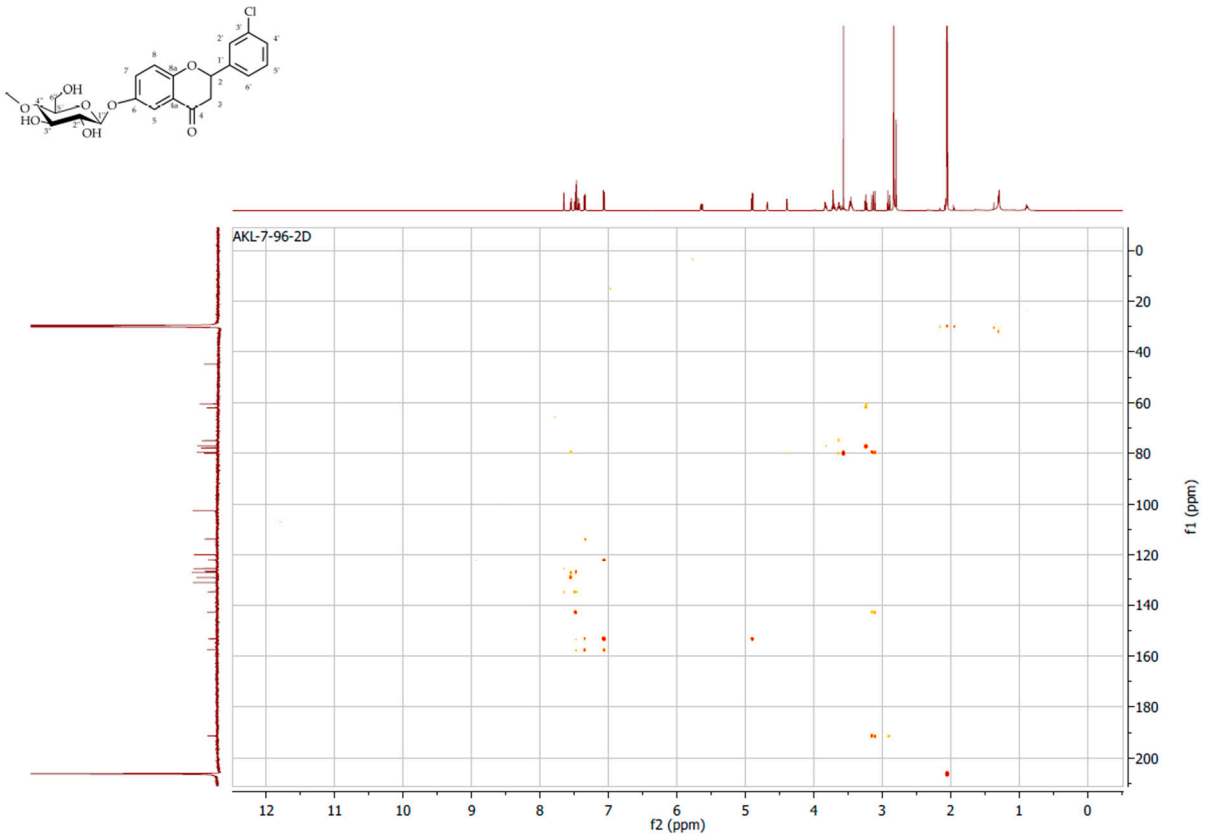


Figure S66. HMBC contour map – ^{1}H x ^{13}C of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

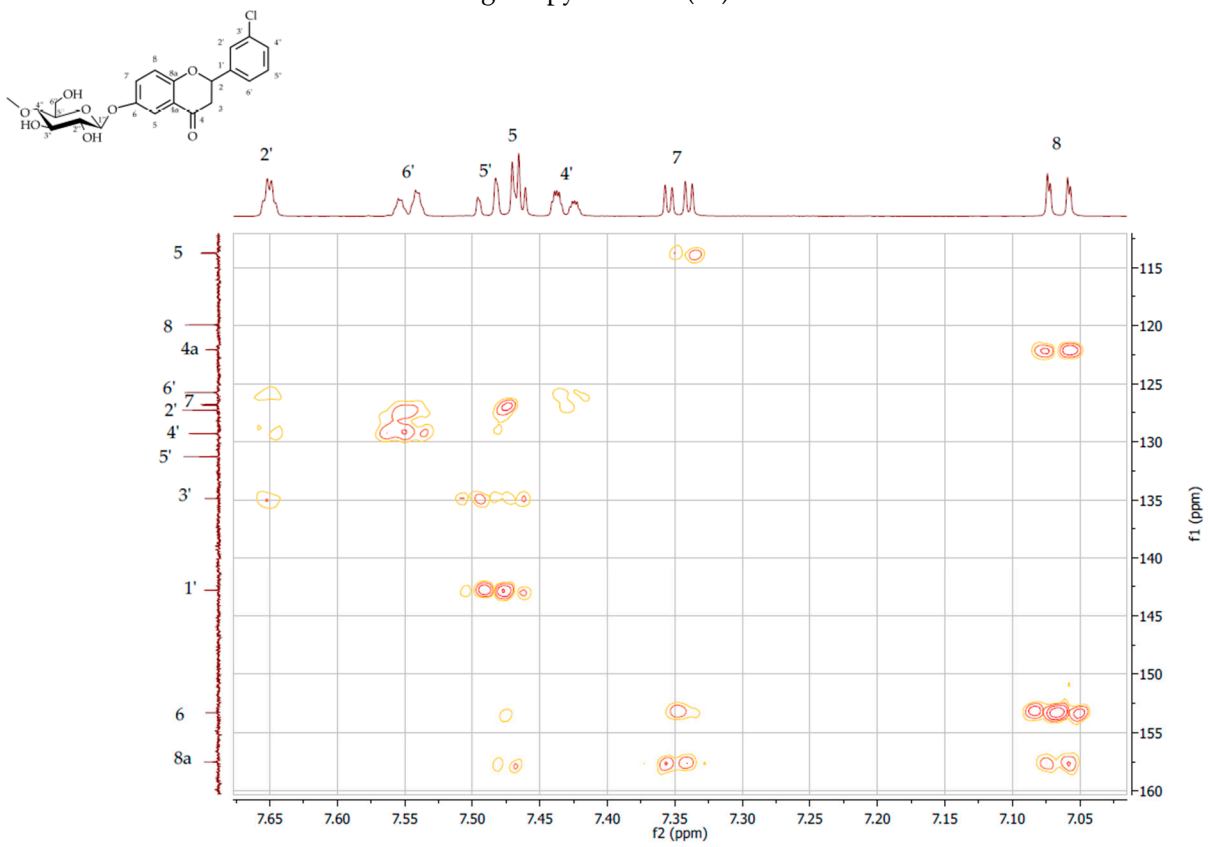


Figure S67. HMBC contour map – ^{1}H x ^{13}C expansion of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

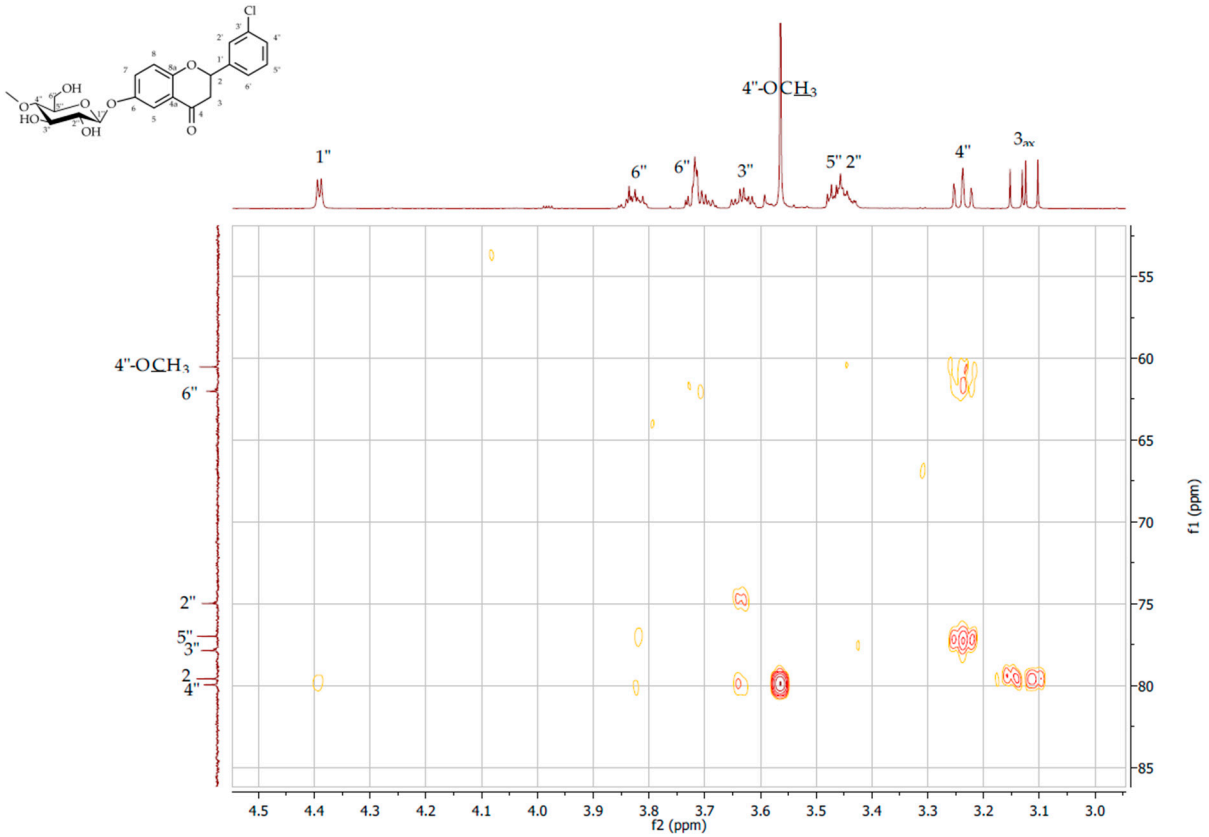


Figure S68. HMBC contour map – ^{1}H x ^{13}C expansion of 3′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

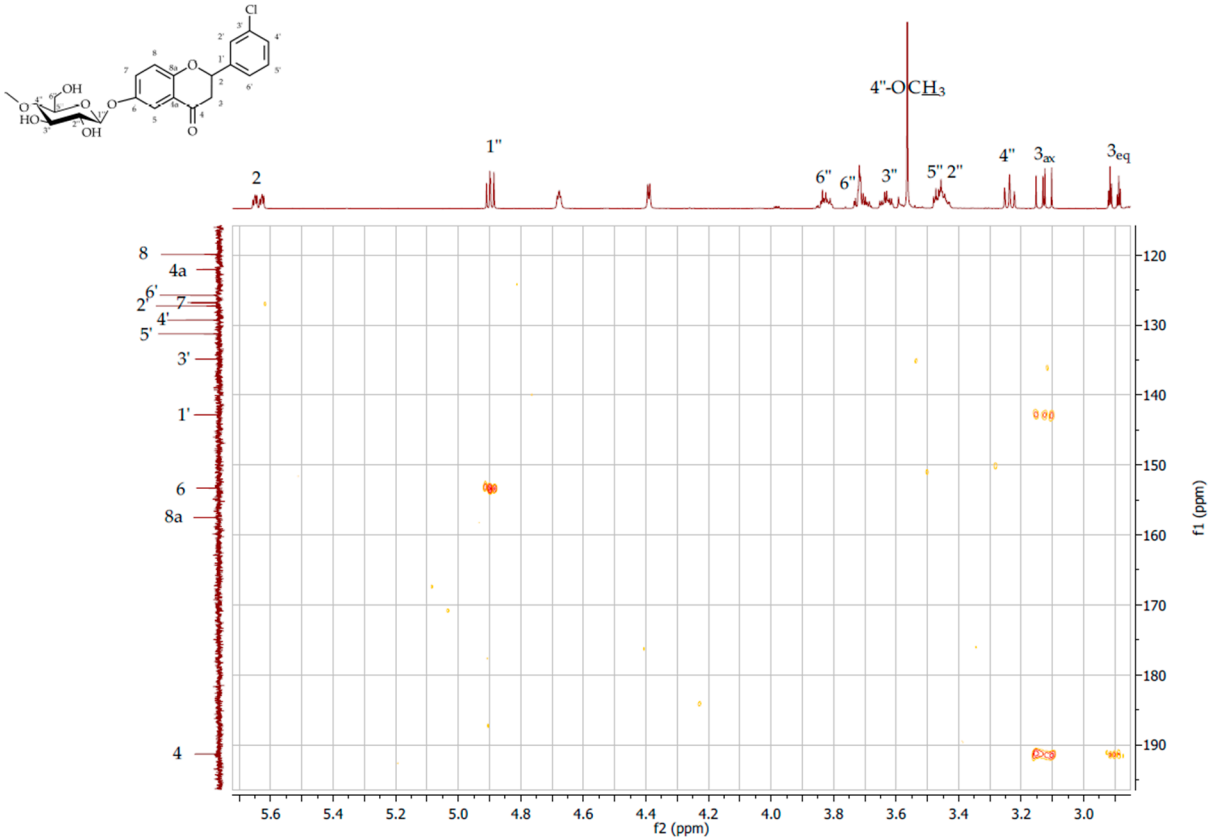


Figure S69. HMBC contour map – ^{1}H x ^{13}C expansion of 3′-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**).

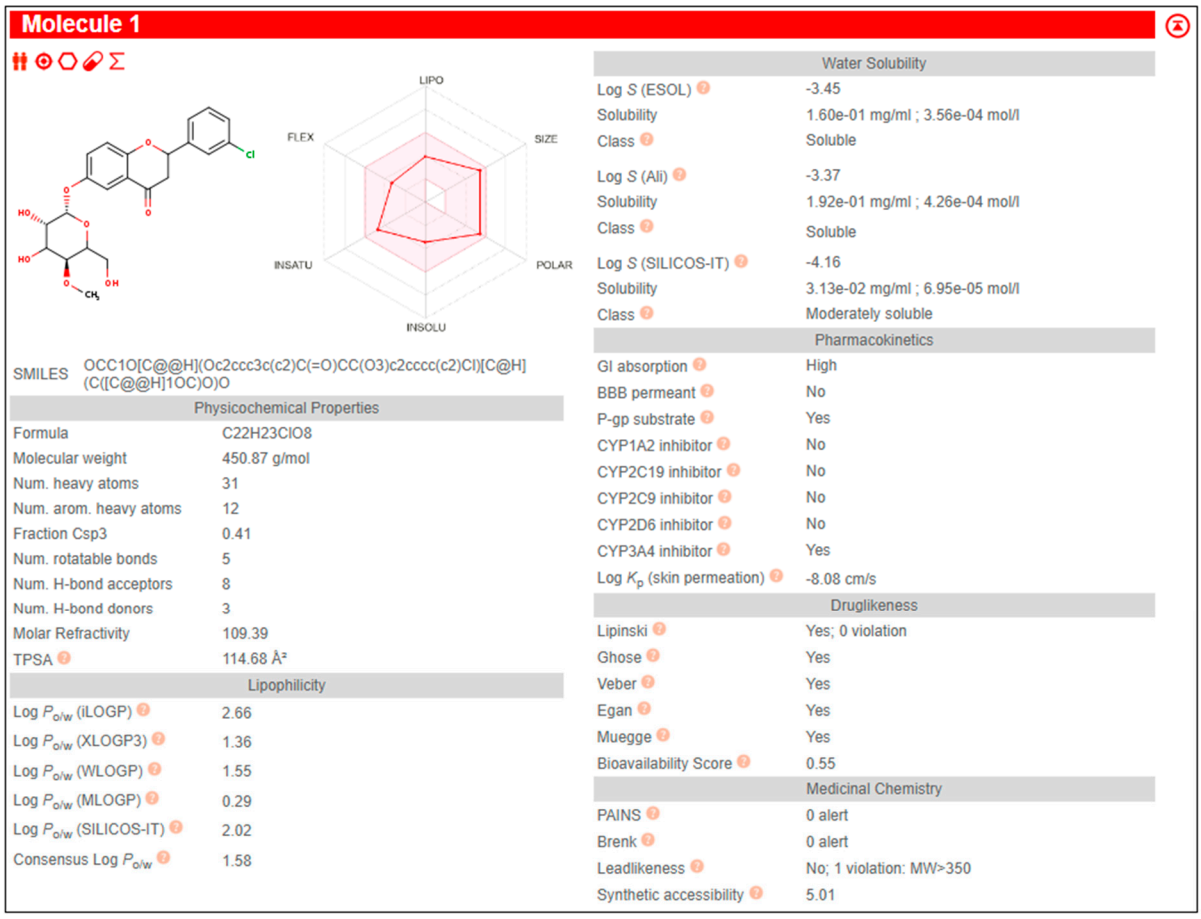


Figure S70. 3′-Chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**2a**) physicochemical and ADME parameters prediction using the SwissADME modelling.

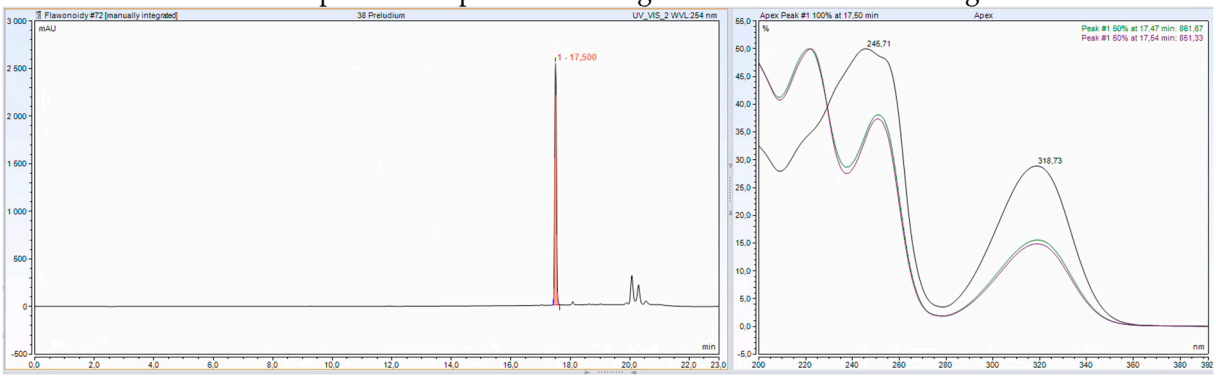


Figure S71. HPLC analysis of 4′-chloroflavanone (**3**).

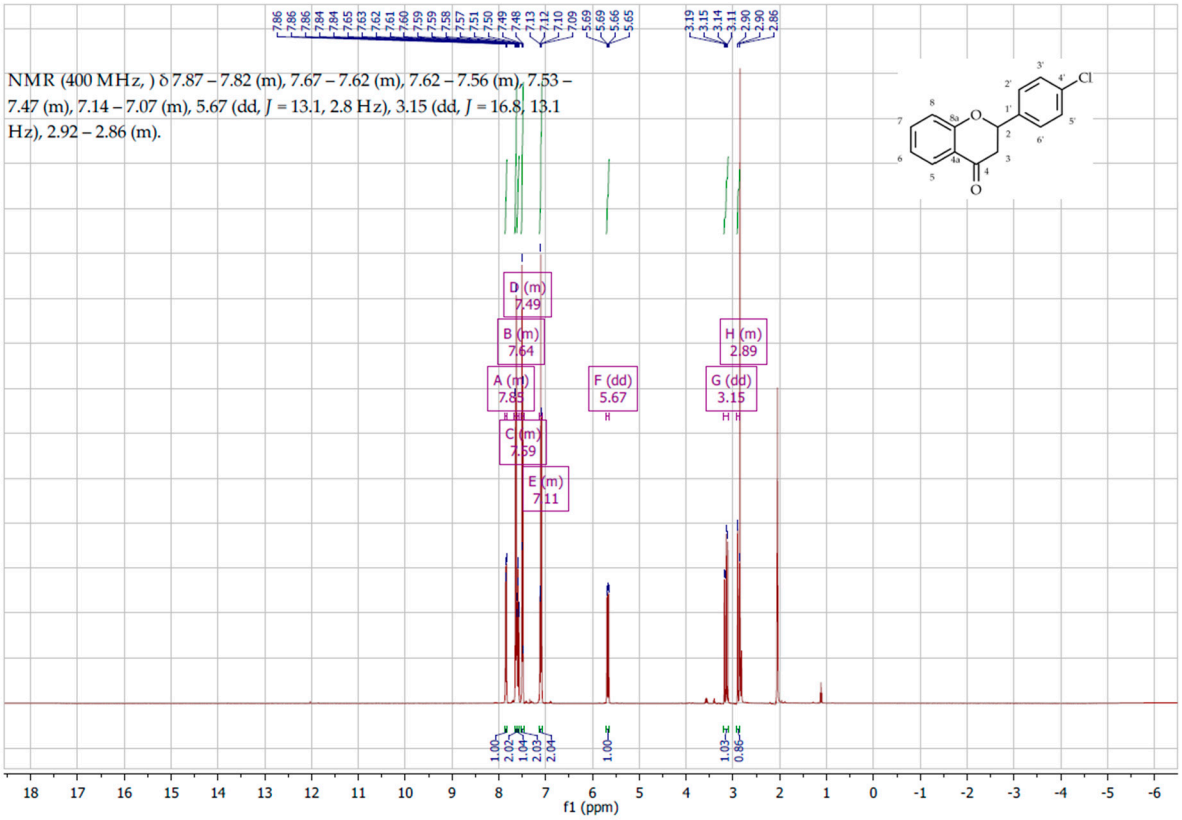


Figure S72. ^{1}H NMR spectrum (δ, acetone-d6, 600 MHz) of 4′-chloroflavanone (**3**).

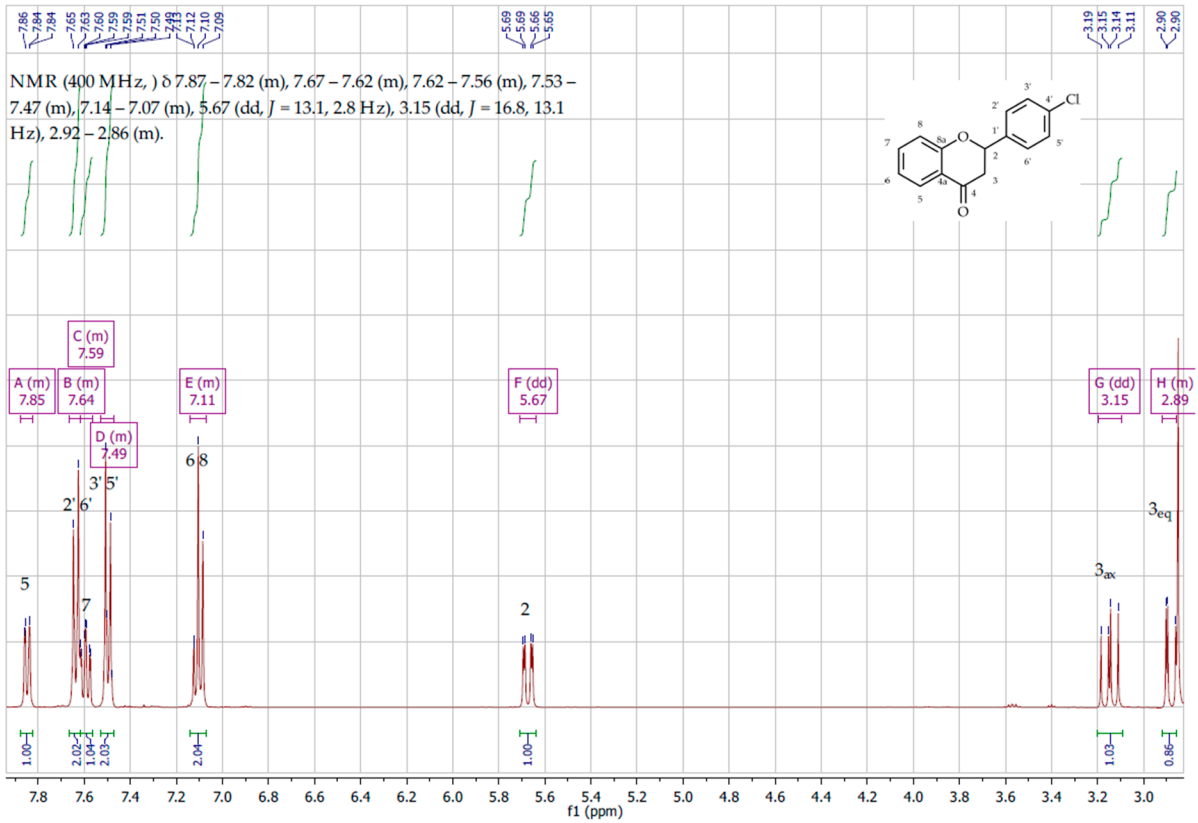


Figure S73. ^{1}H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 4′-chloroflavanone (**3**).

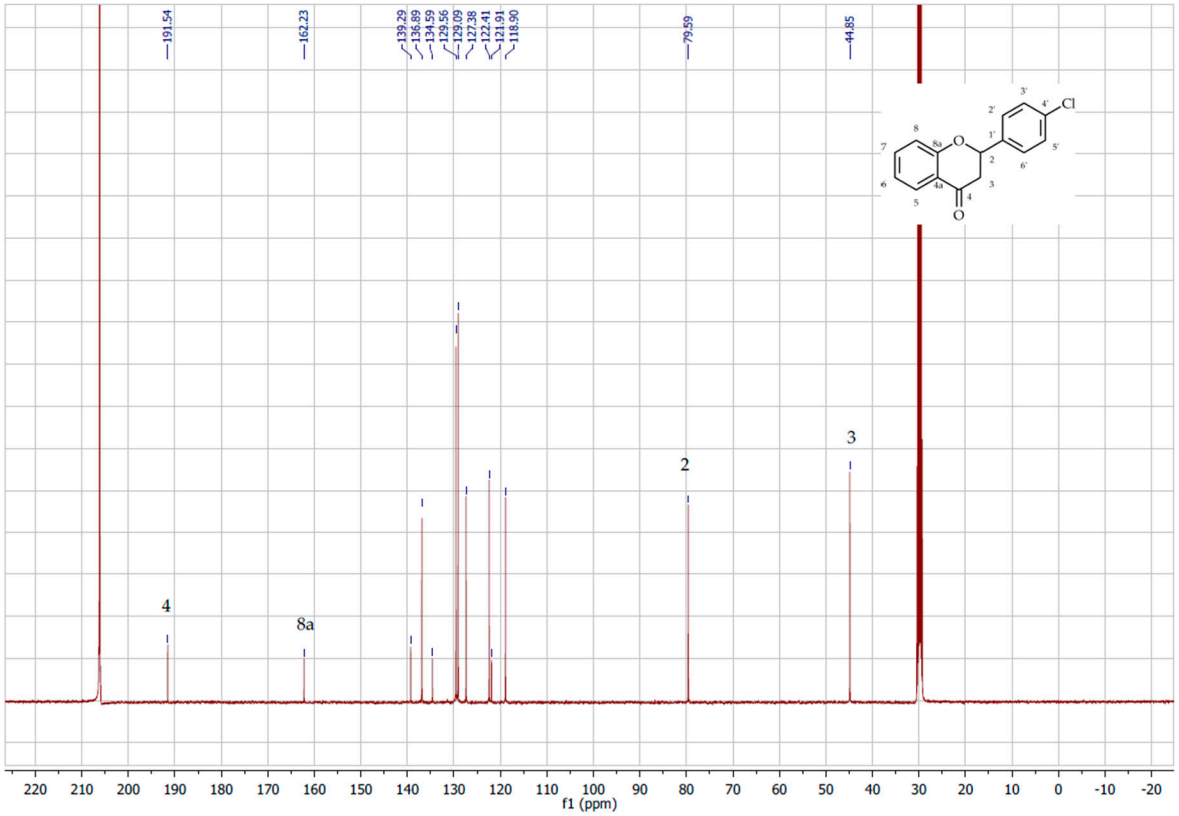


Figure S74. ^{13}C NMR spectrum (δ, acetone-d6, 151 MHz) of 4′-chloroflavanone (**3**).

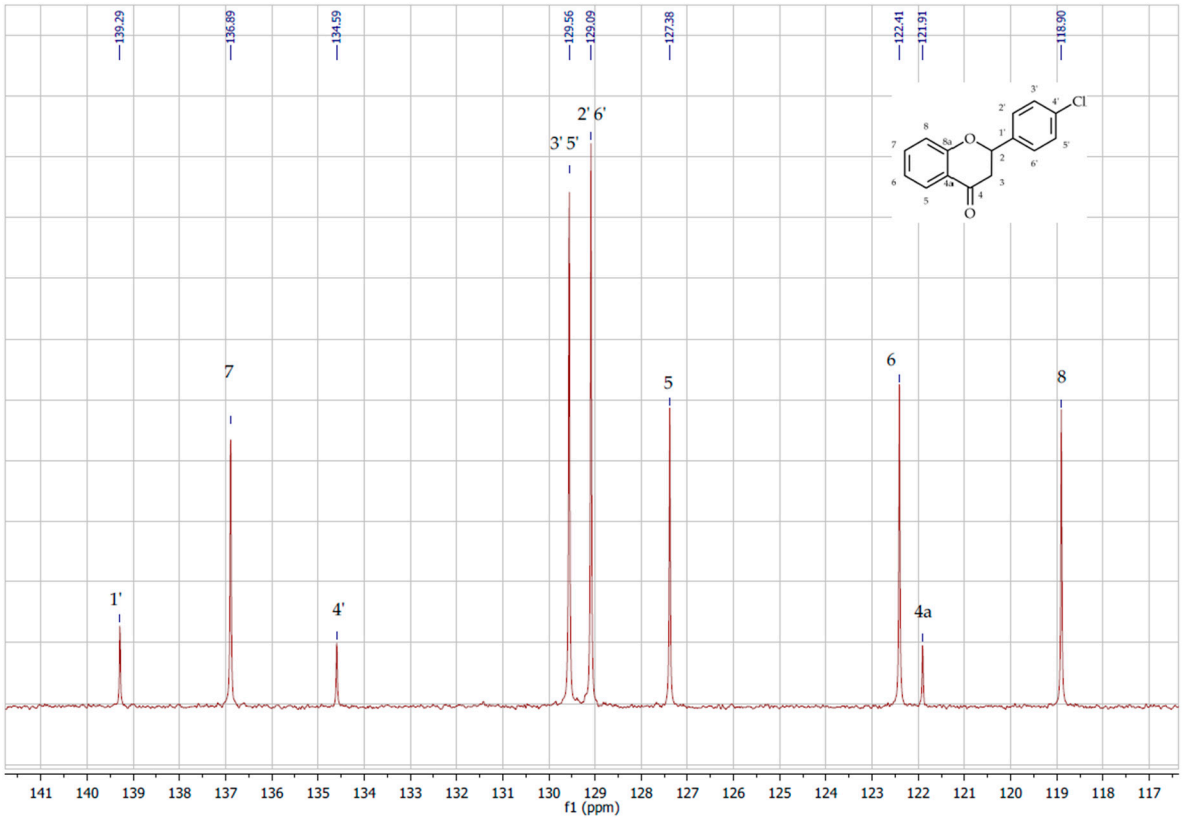


Figure S75. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 4′-chloroflavanone (**3**).

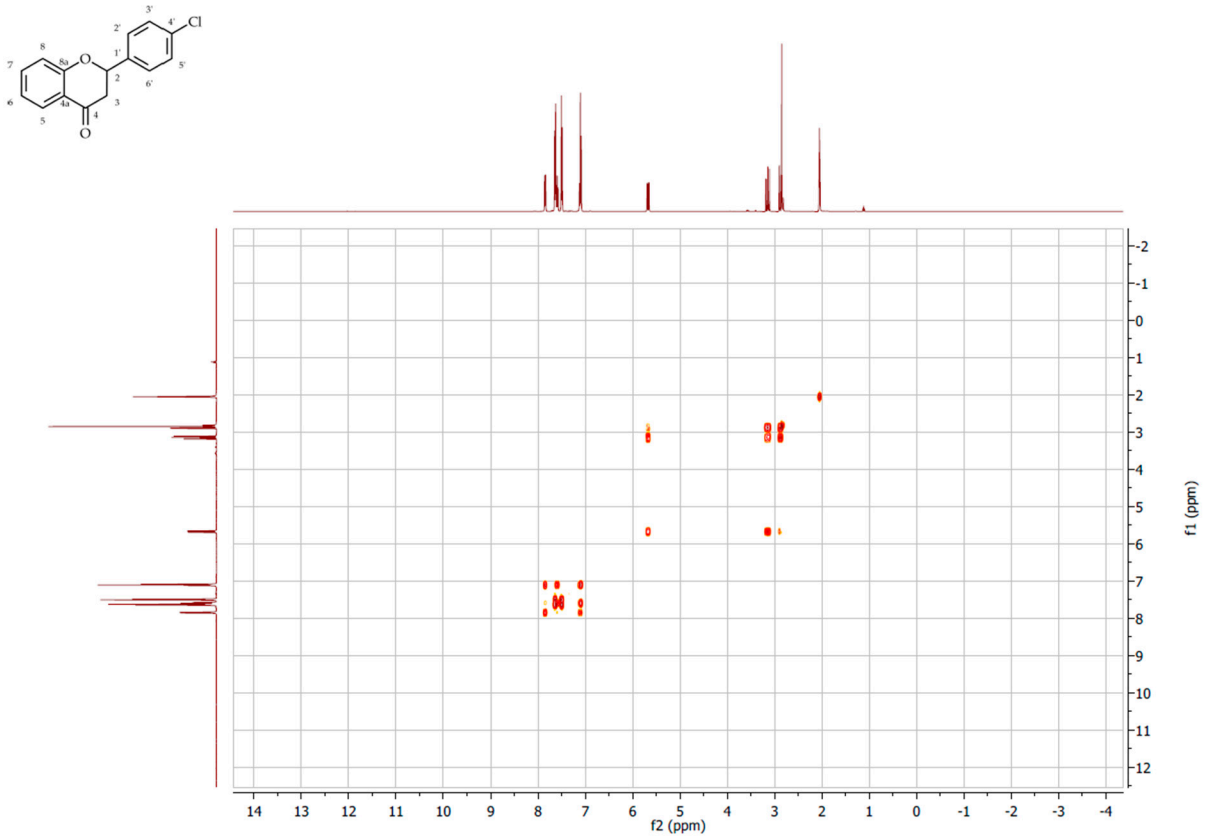


Figure S76. COSY contour map – ^{1}H x ^{1}H of 4′-chloroflavanone (**3**).

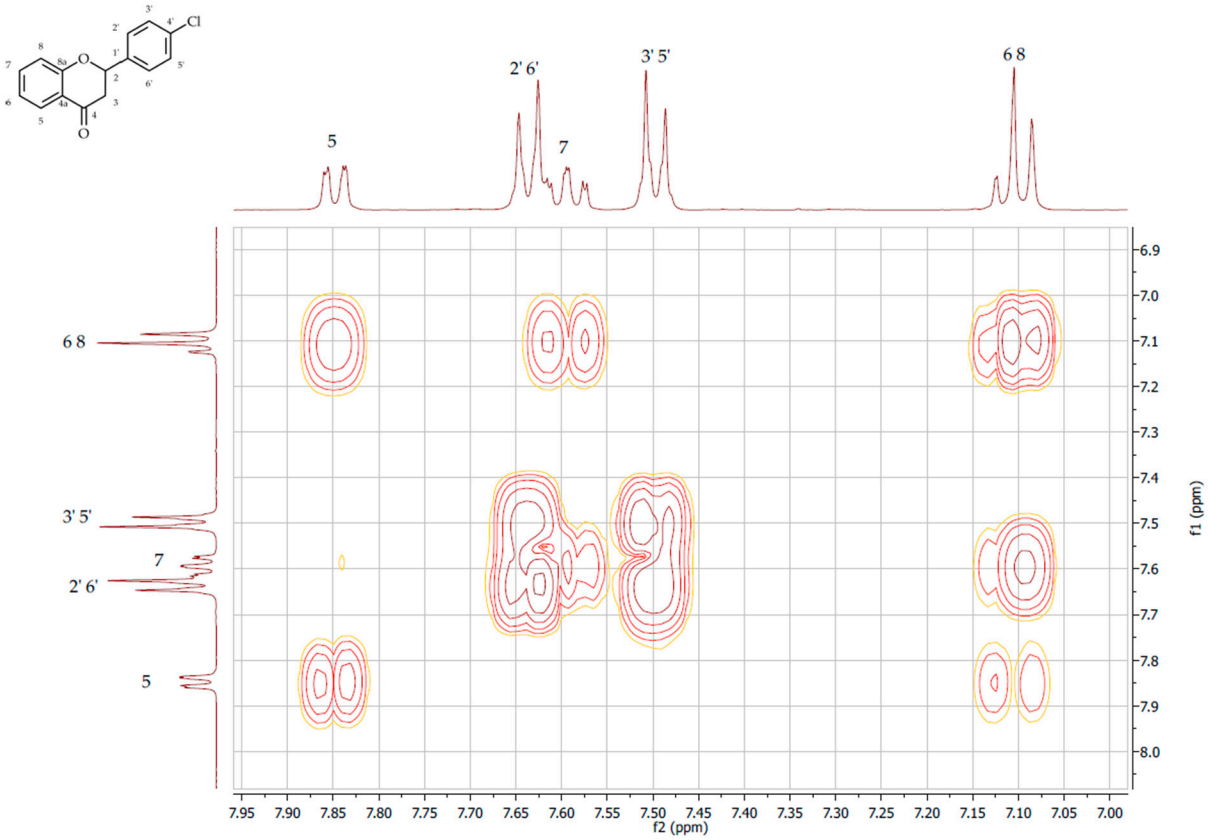


Figure S77. COSY contour map – ^{1}H x ^{1}H expansion of 4′-chloroflavanone (**3**).

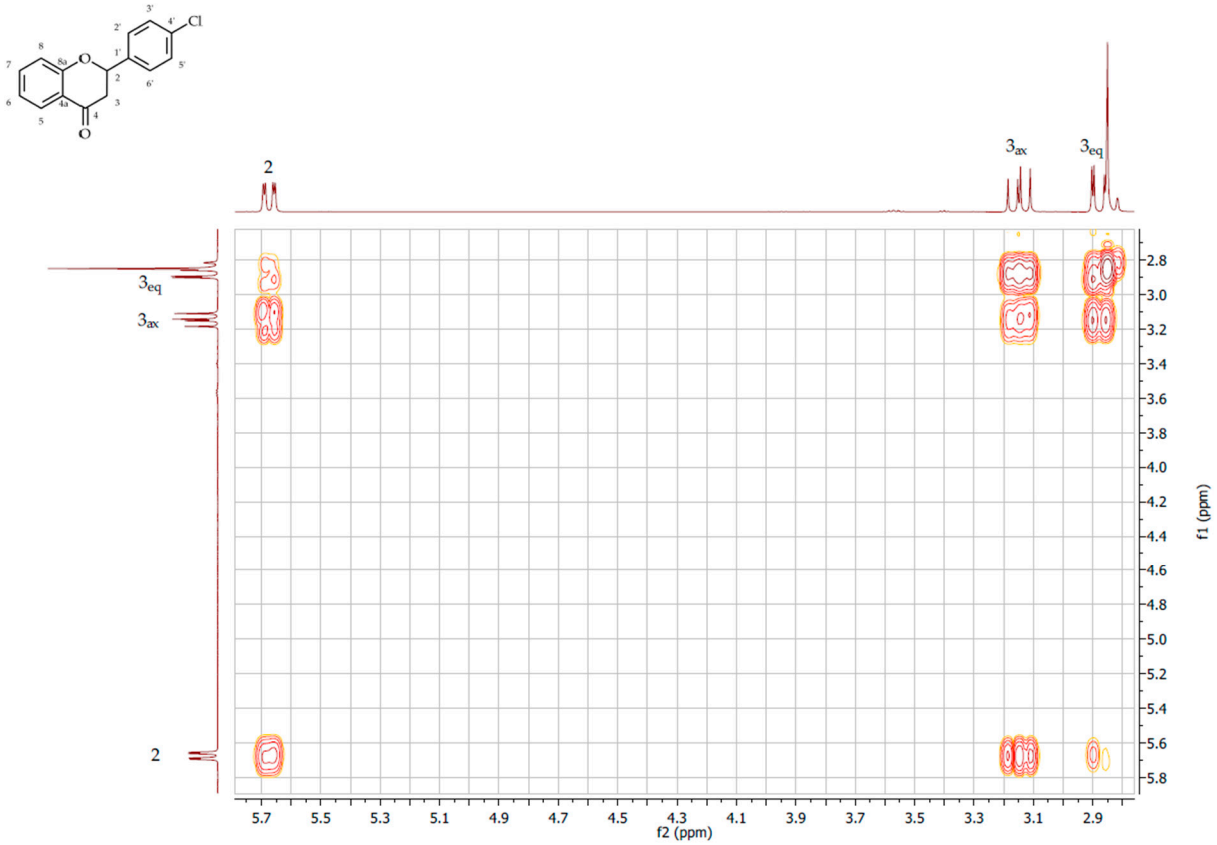


Figure S78. COSY contour map – ^{1}H x ^{1}H expansion of 4′-chloroflavanone (**3**).

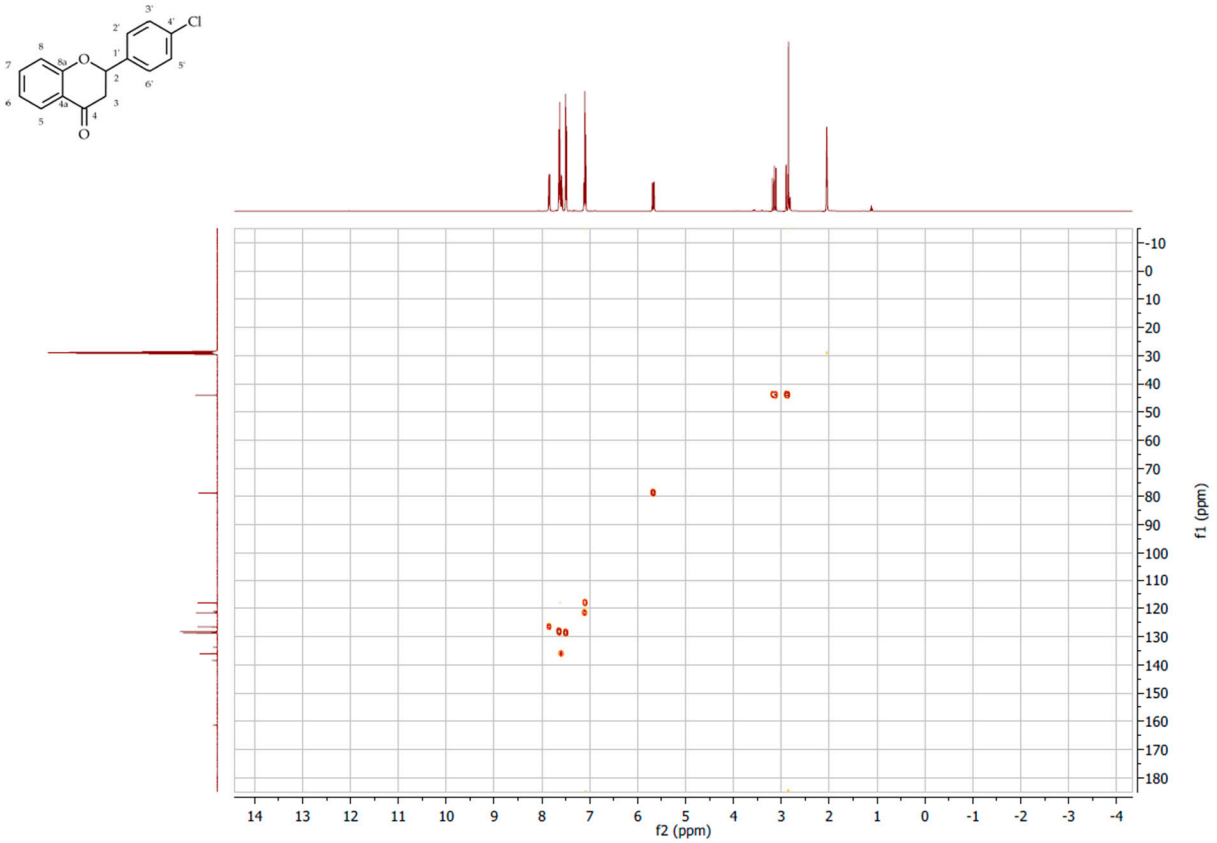


Figure S79. HMQC contour map – ^{1}H x ^{13}C of 4′-chloroflavanone (**3**).

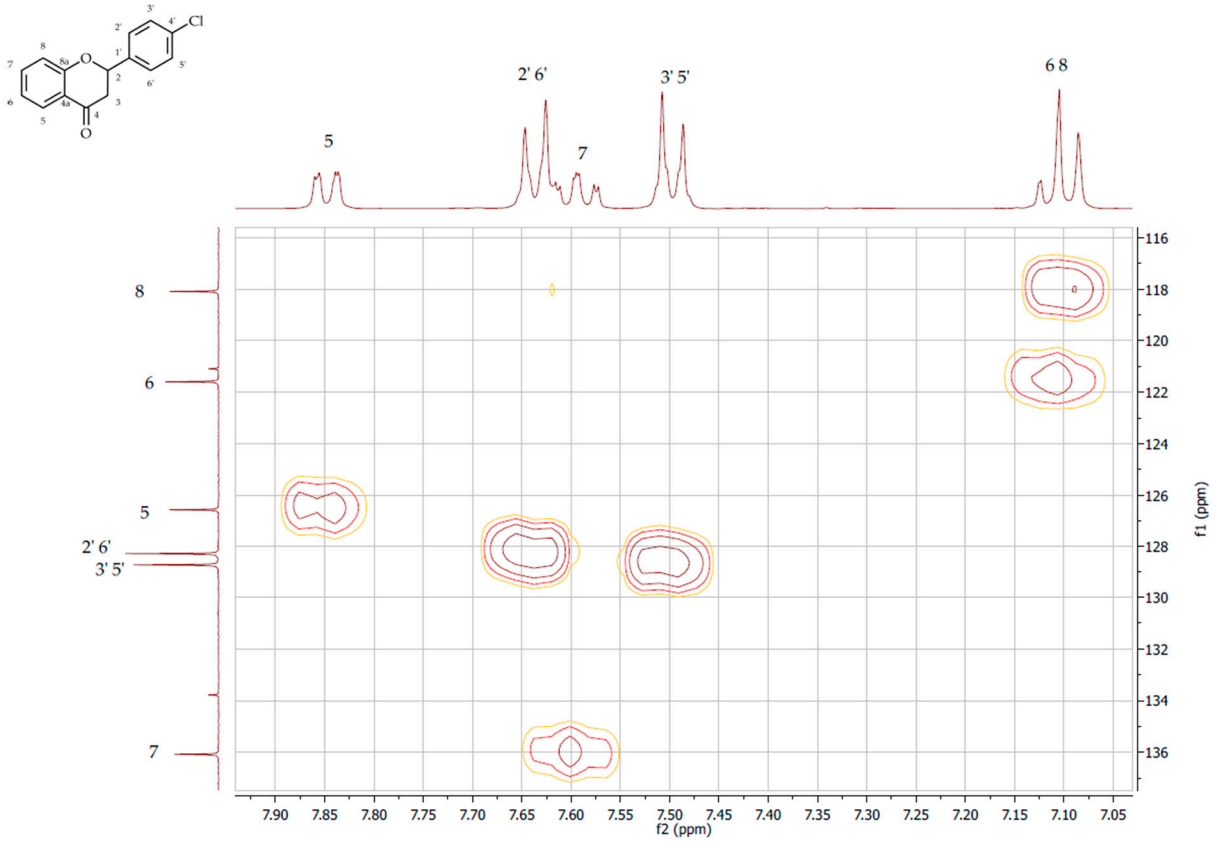


Figure S80. HMQC contour map – ^{1}H x ^{13}C expansion of 4′-chloroflavanone (**3**).

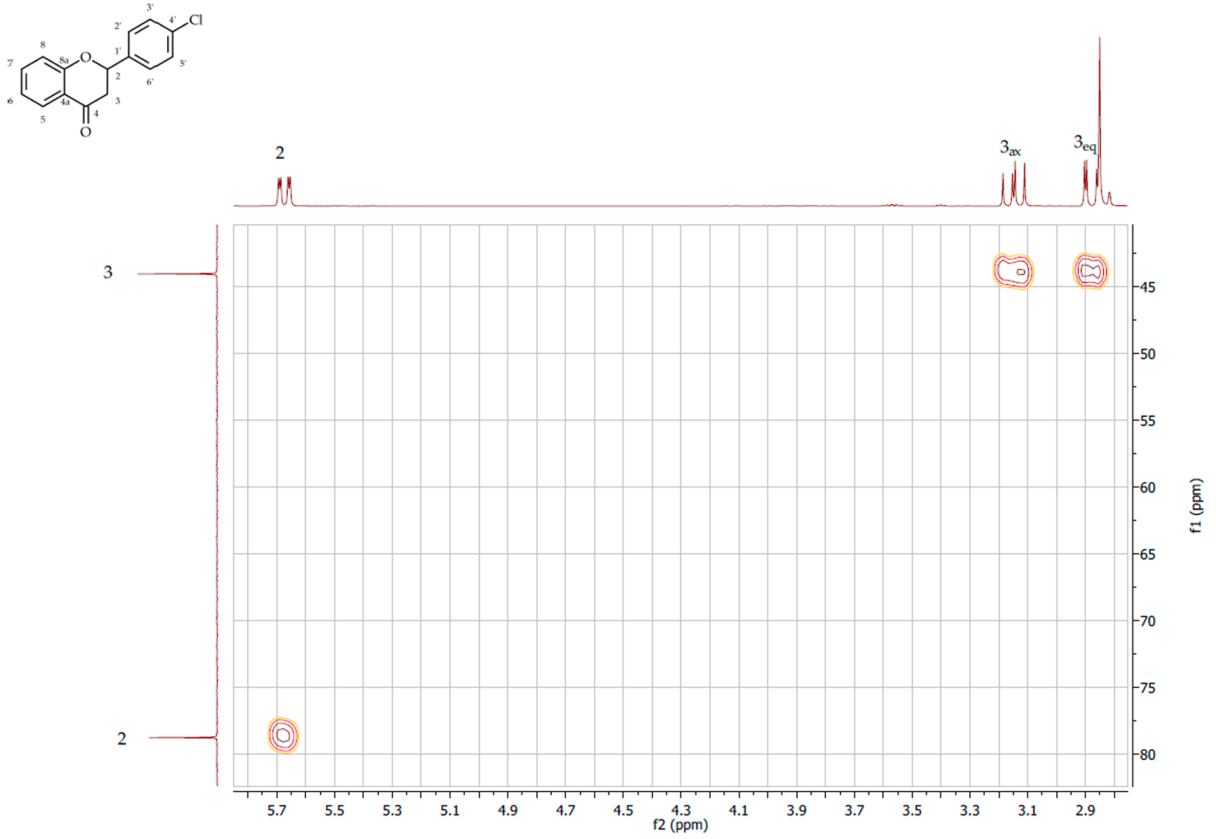


Figure S81. HMQC contour map – ^{1}H x ^{13}C expansion of 4′-chloroflavanone (**3**).

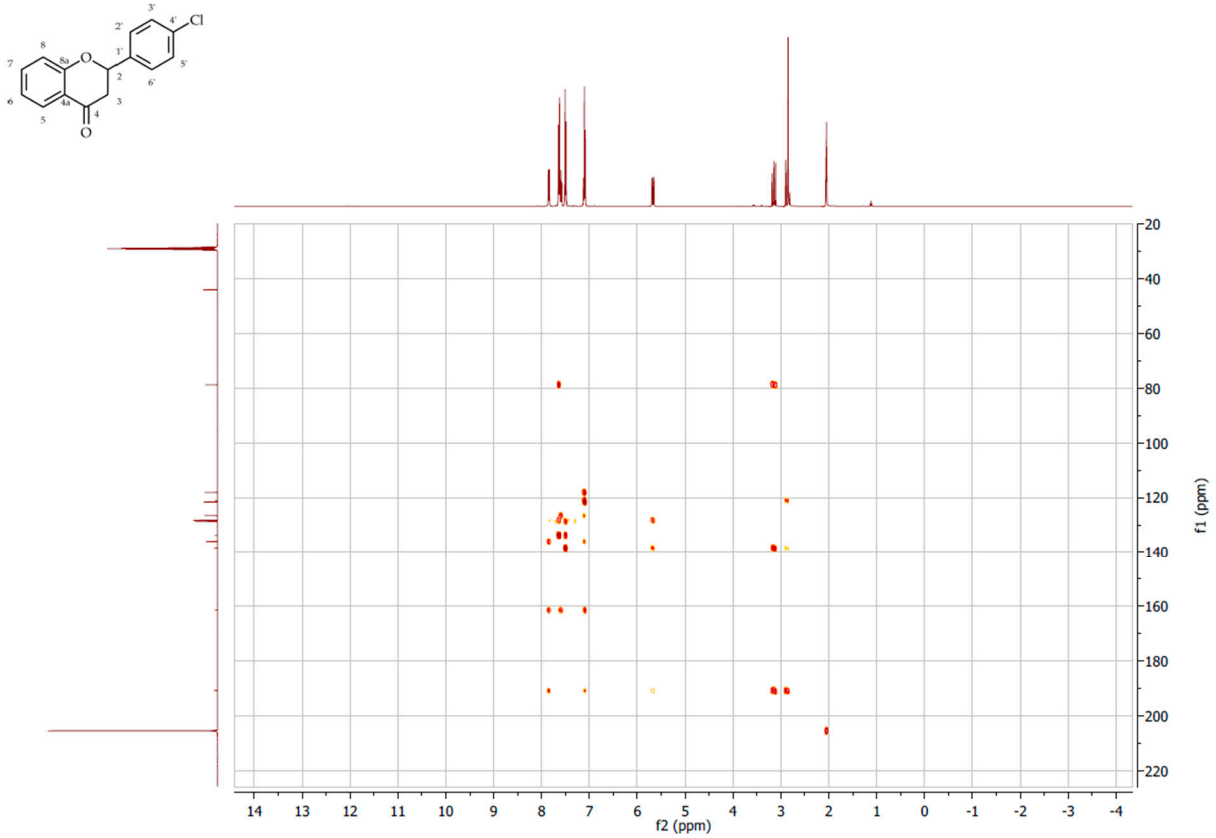


Figure S82. HMBC contour map – ^{1}H x ^{13}C of 4′-chloroflavanone (**3**).

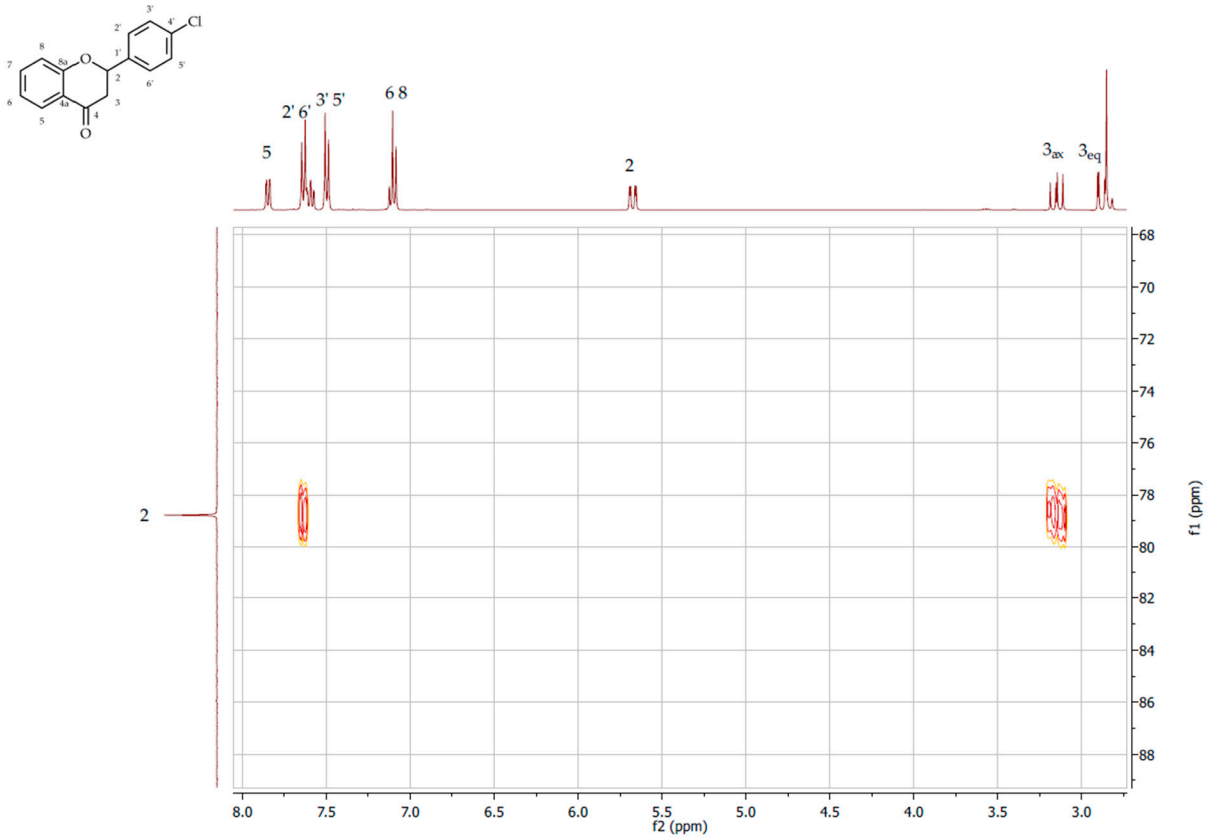


Figure S83. HMBC contour map – ^{1}H x ^{13}C expansion of 4′-chloroflavanone (**3**).

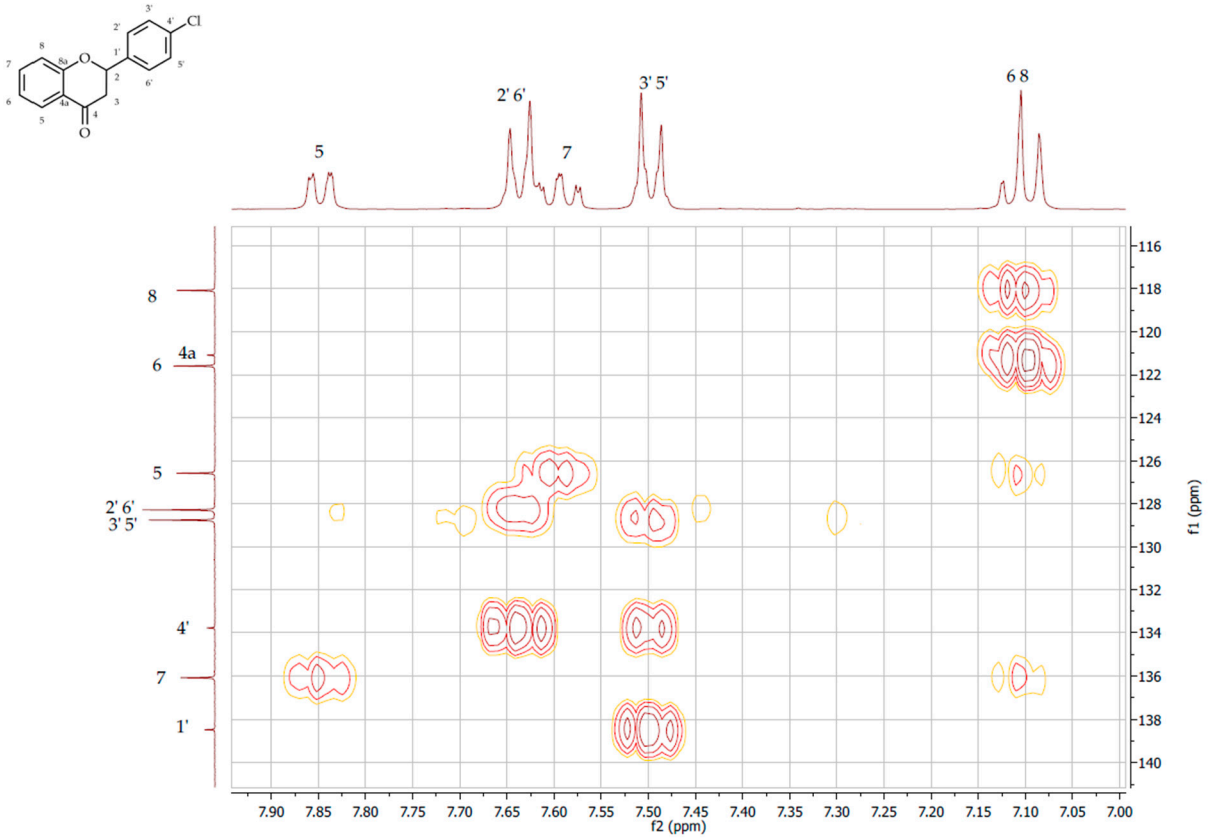


Figure S84. HMBC contour map – ^{1}H x ^{13}C expansion of 4′-chloroflavanone (**3**).

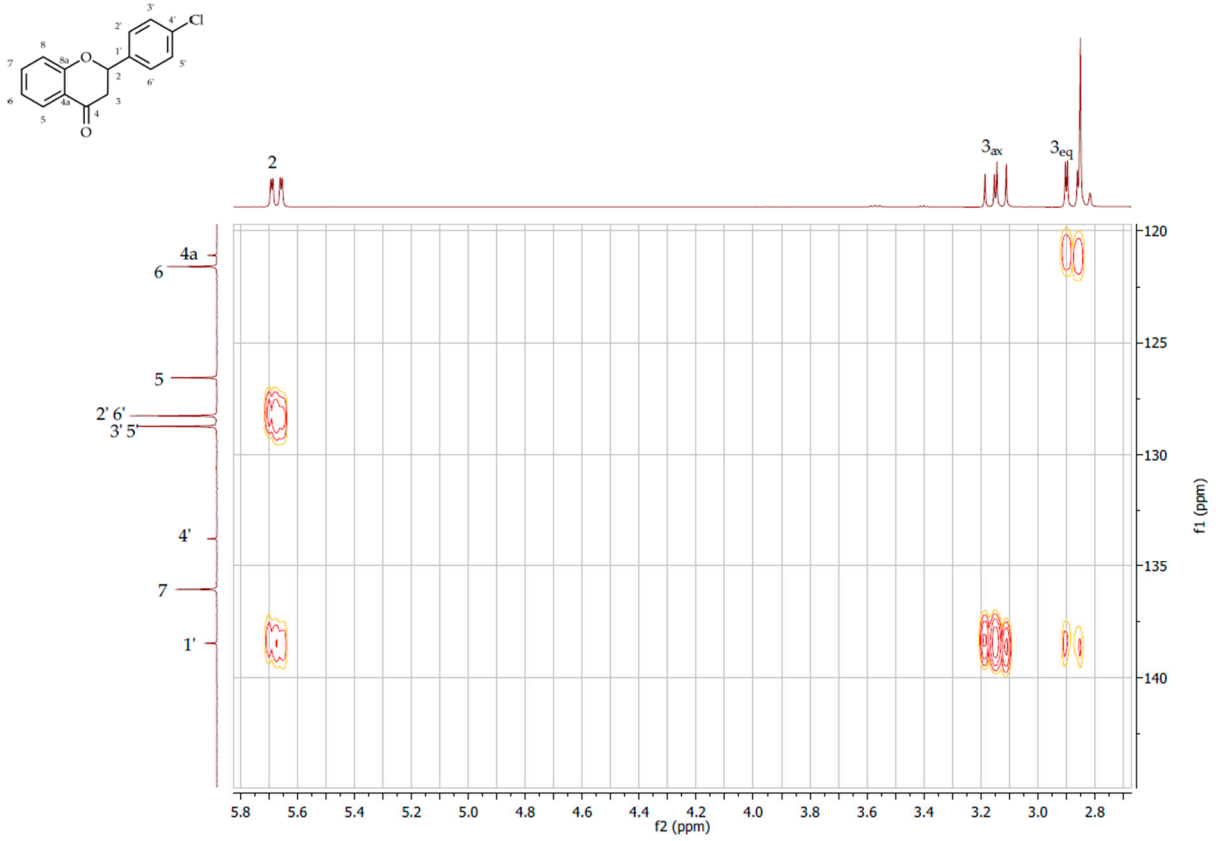


Figure S85. HMBC contour map – ^{1}H x ^{13}C expansion of 4′-chloroflavanone (**3**).

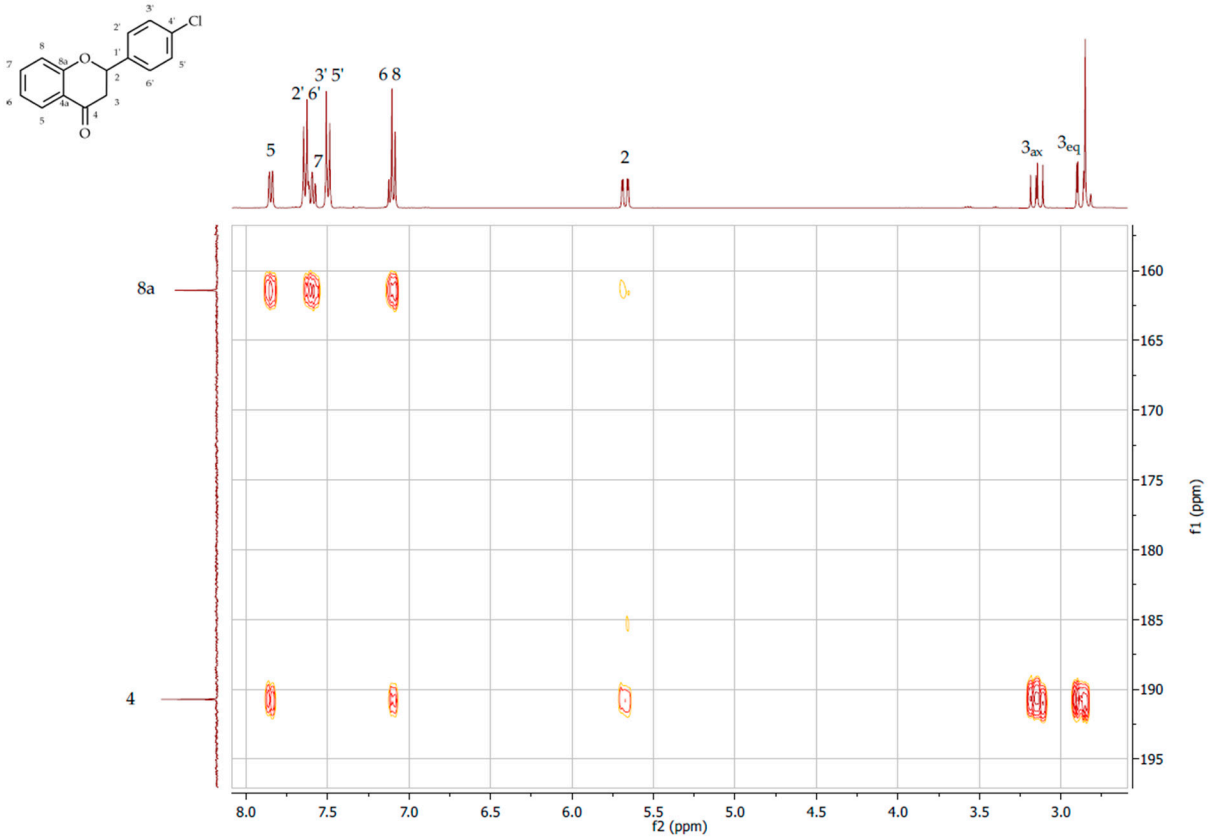
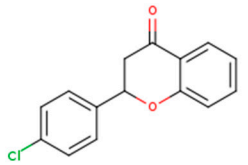
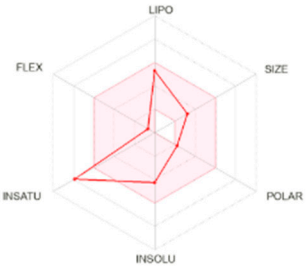


Figure S86. HMBC contour map – ^{1}H x ^{13}C expansion of 4′-chloroflavanone (**3**).

Molecule 1





SMILES Clc1ccc(cc1)C1CC(=O)c2c(O1)cccc2

Physicochemical Properties	
Formula	C15H11ClO2
Molecular weight	258.70 g/mol
Num. heavy atoms	18
Num. arom. heavy atoms	12
Fraction Csp3	0.13
Num. rotatable bonds	1
Num. H-bond acceptors	2
Num. H-bond donors	0
Molar Refractivity	70.51
TPSA	26.30 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.68
Log $P_{o/w}$ (XLOGP3)	3.77
Log $P_{o/w}$ (WLOGP)	3.72
Log $P_{o/w}$ (MLOGP)	2.98
Log $P_{o/w}$ (SILICOS-IT)	4.18
Consensus Log $P_{o/w}$	3.47

Water Solubility	
Log *S* (ESOL)	-4.25
Solubility	1.47e-02 mg/ml ; 5.67e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-4.02
Solubility	2.50e-02 mg/ml ; 9.65e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-5.76
Solubility	4.48e-04 mg/ml ; 1.73e-06 mol/l
Class	Moderately soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.20 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.80

Figure S87. 4′-Chloroflavanone (**3**) physicochemical and ADME parameters prediction using the SwissADME modelling.

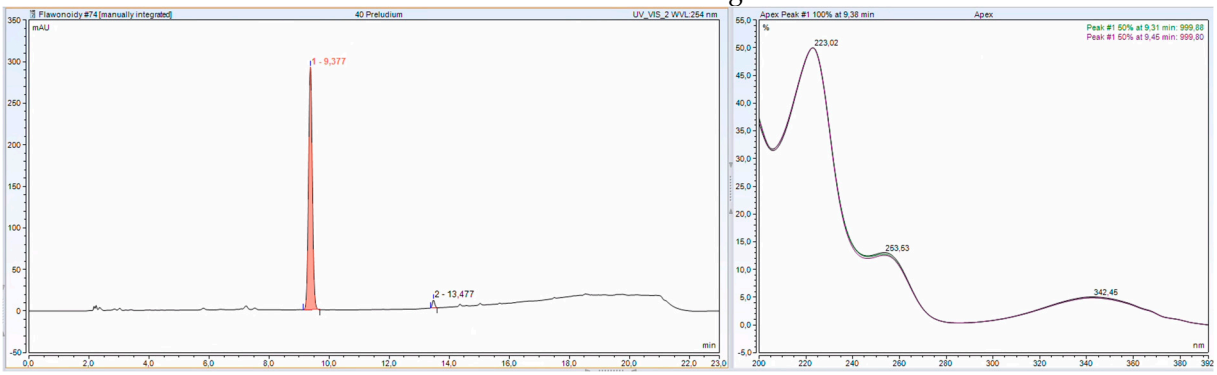


Figure S88. HPLC analysis of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

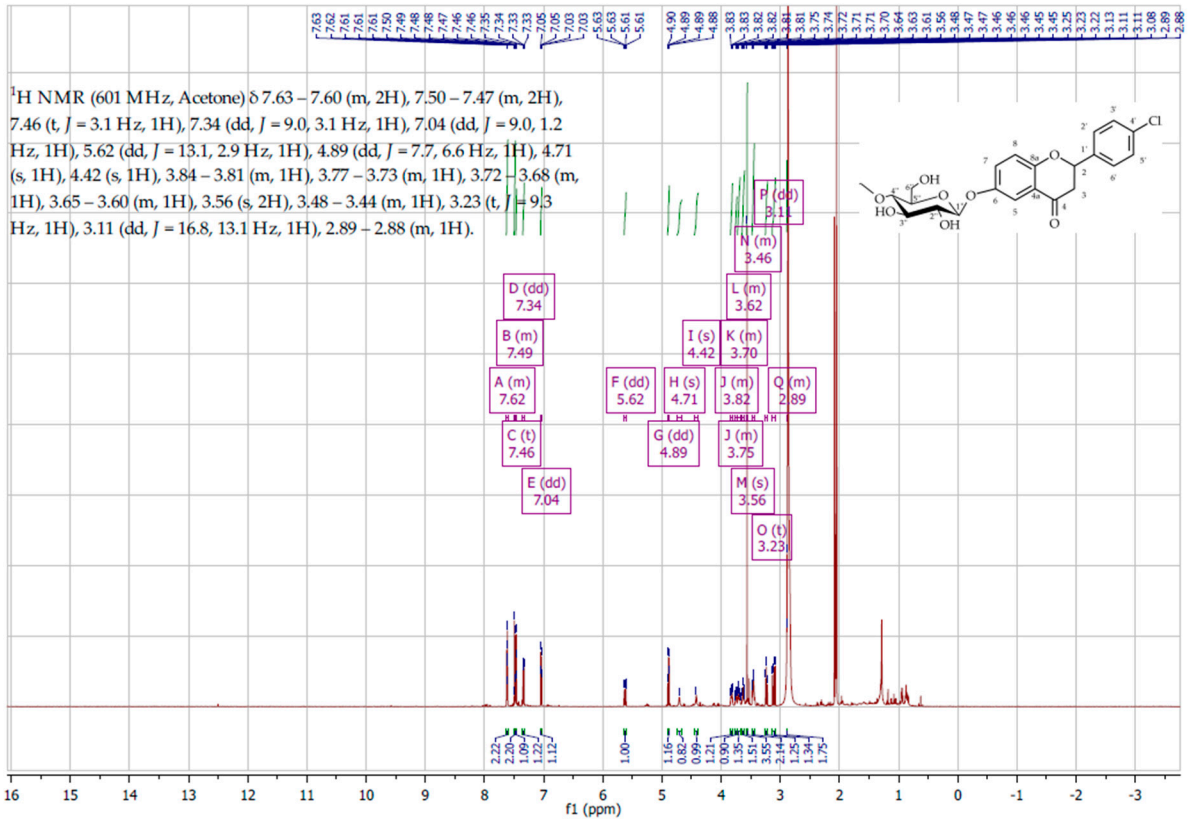


Figure S89. ^{1}H NMR spectrum (*δ*, acetone-d6, 600 MHz) of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

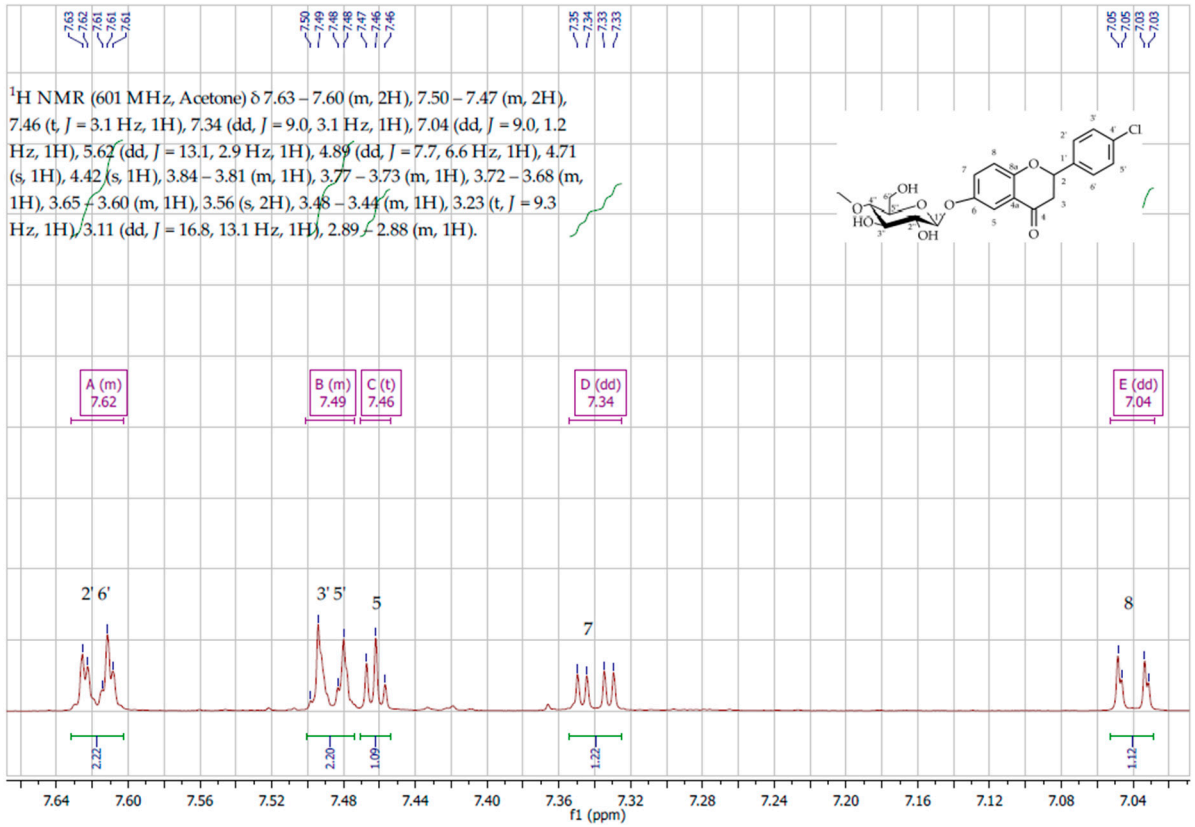


Figure S90. ^{1}H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

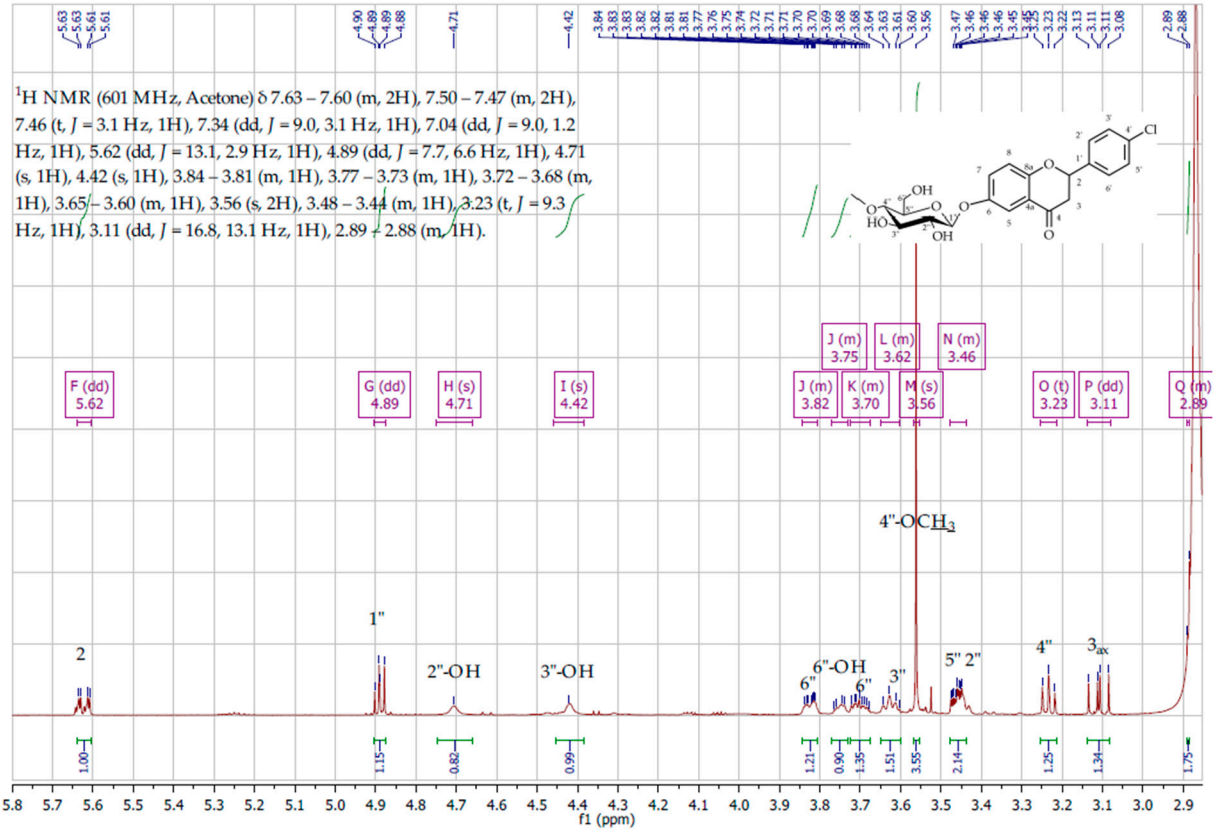


Figure S91. ^{1}H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

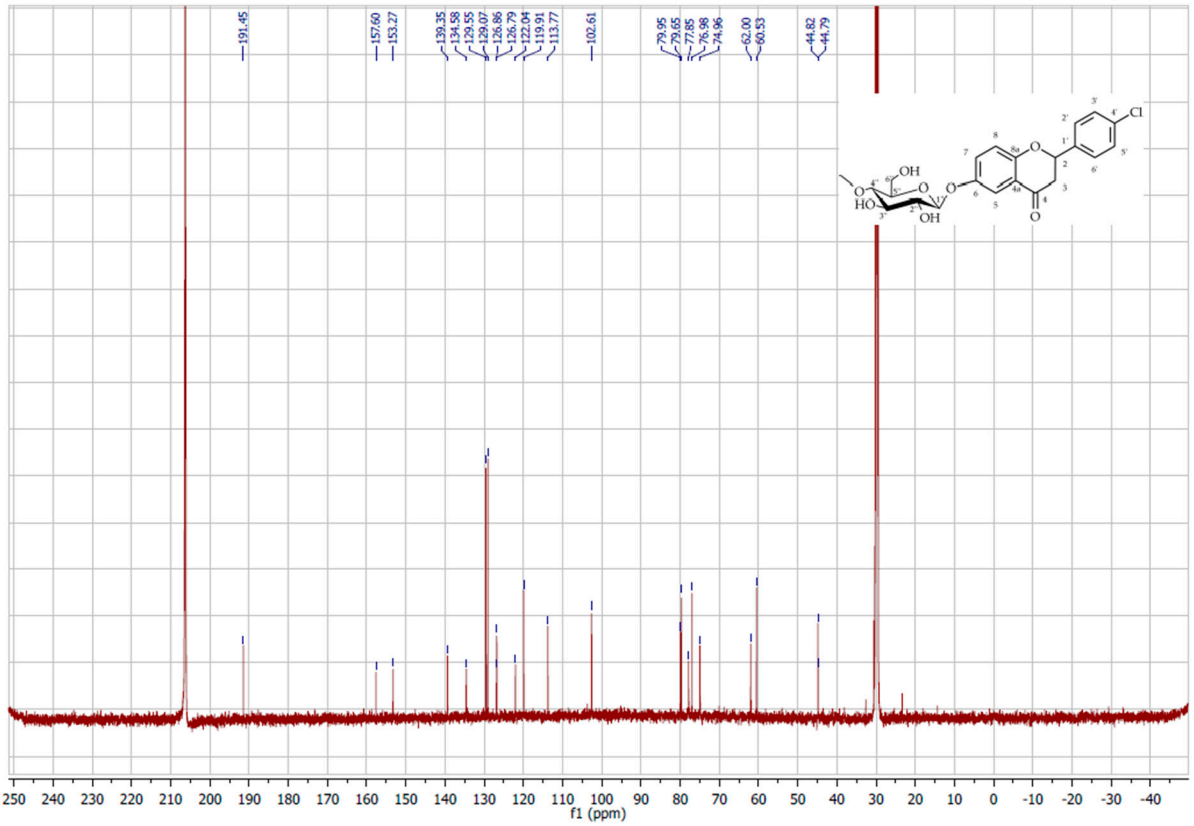


Figure S92. ^{13}C NMR spectrum (δ, acetone-d6, 151 MHz) of 4′-chloroflavanone 6-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

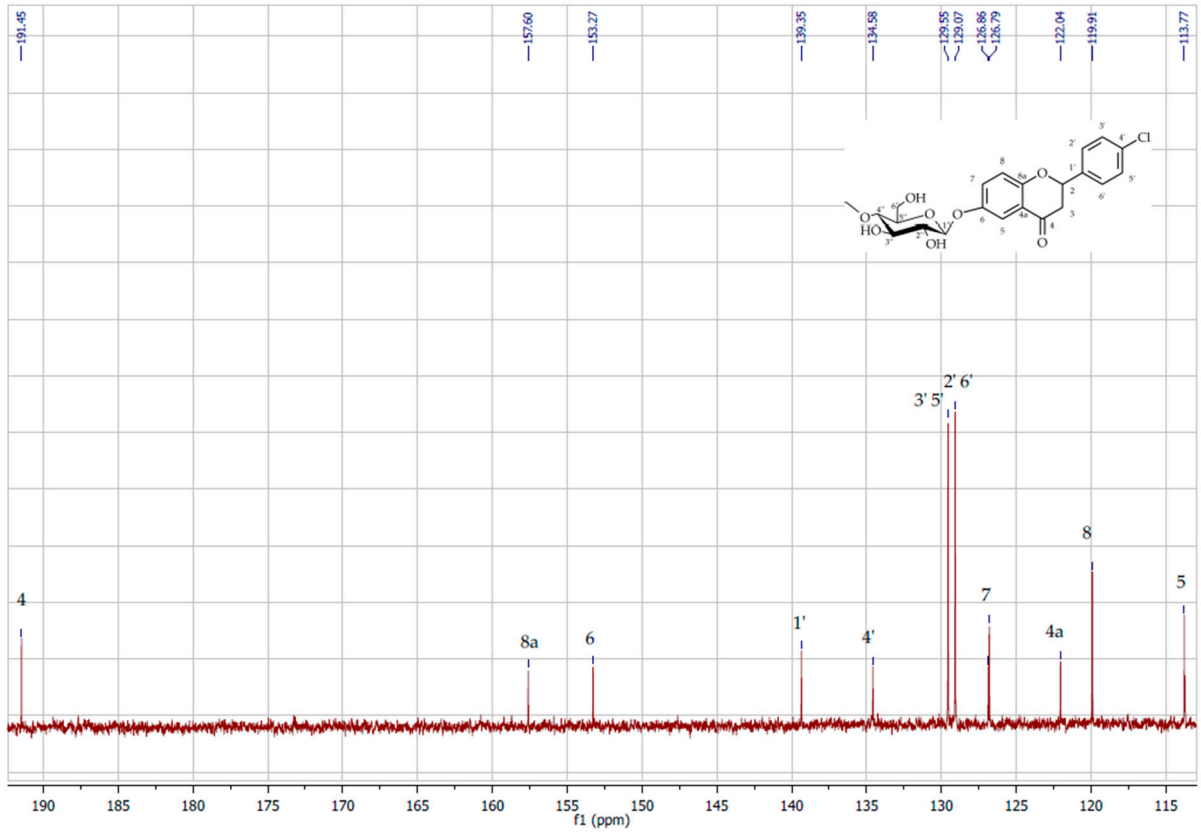


Figure S93. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 4′-chloroflavanone 6-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

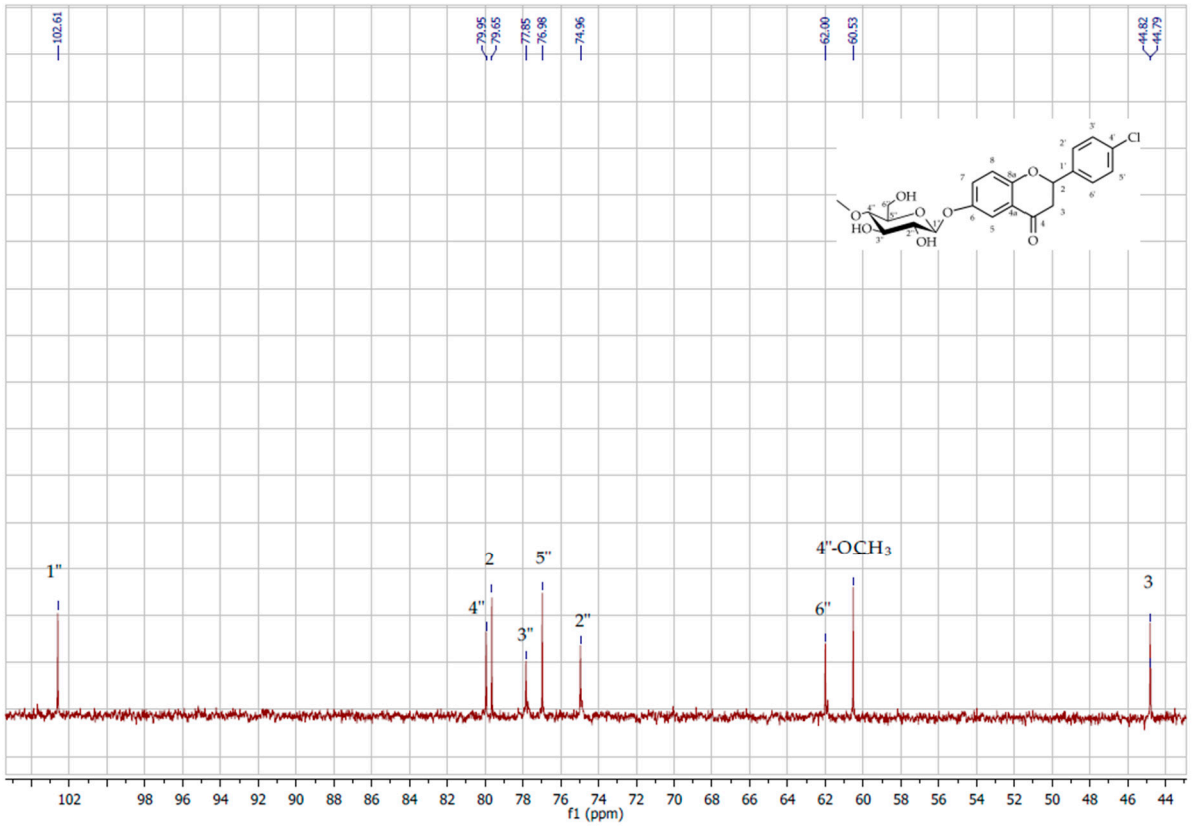


Figure S94. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 4′-chloroflavanone 6-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

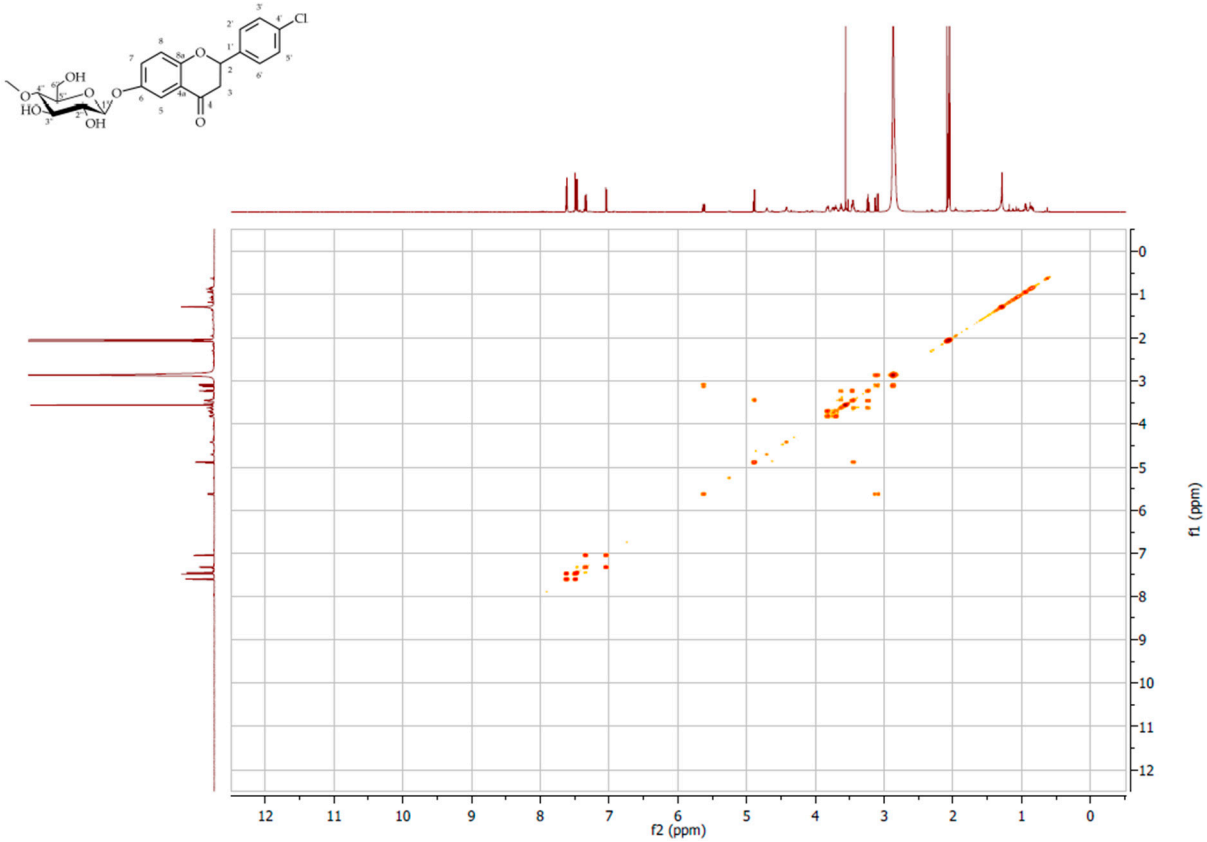


Figure S95. COSY contour map – ^{1}H x ^{1}H of 4′-chloroflavanone 6-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

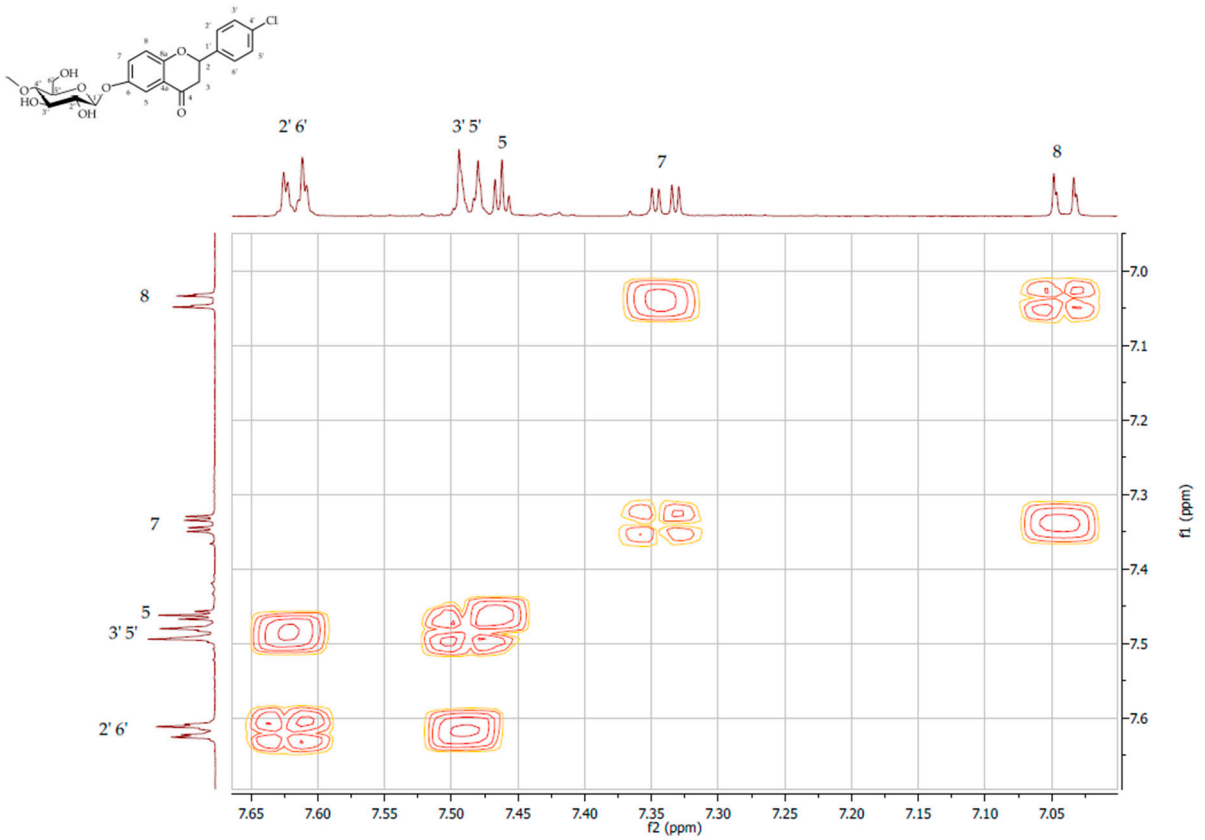


Figure S96. COSY contour map – ^{1}H x ^{1}H expansion of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

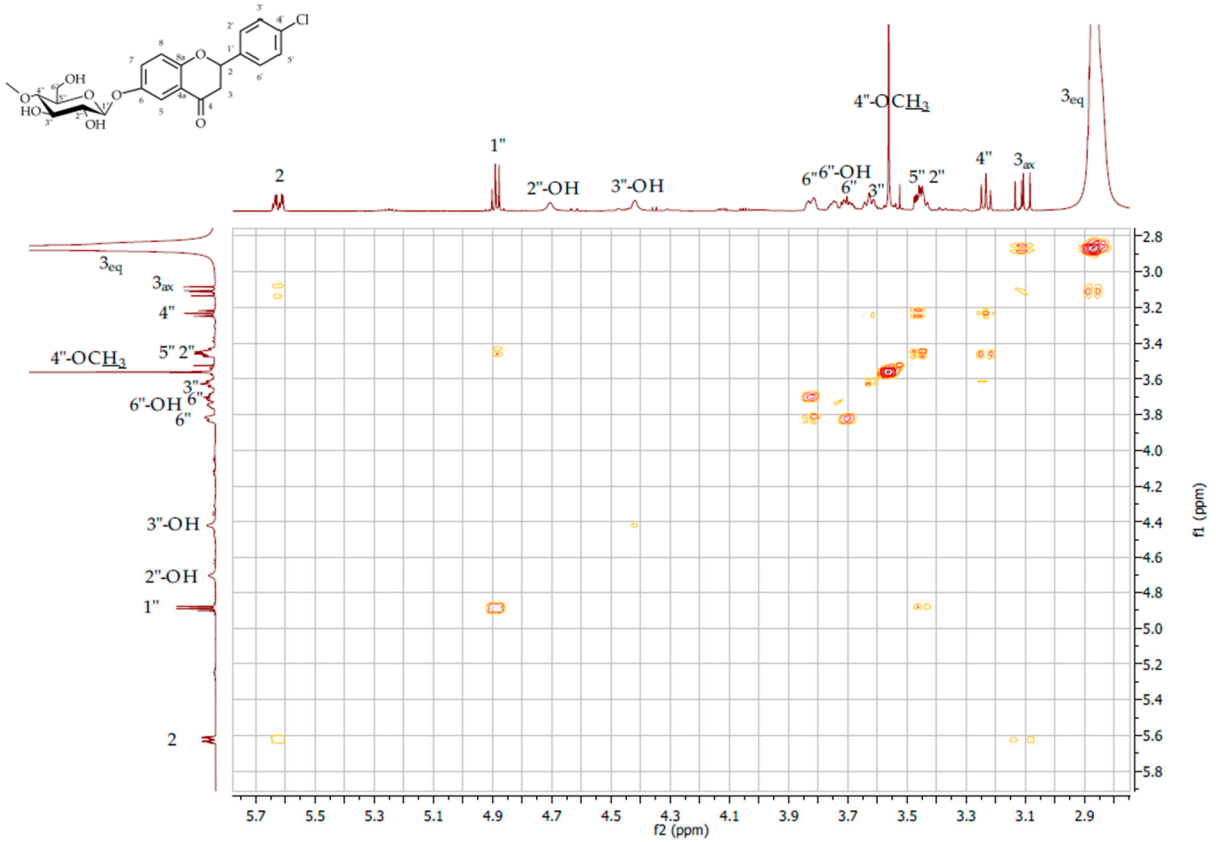


Figure S97. COSY contour map – ^{1}H x ^{1}H expansion of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

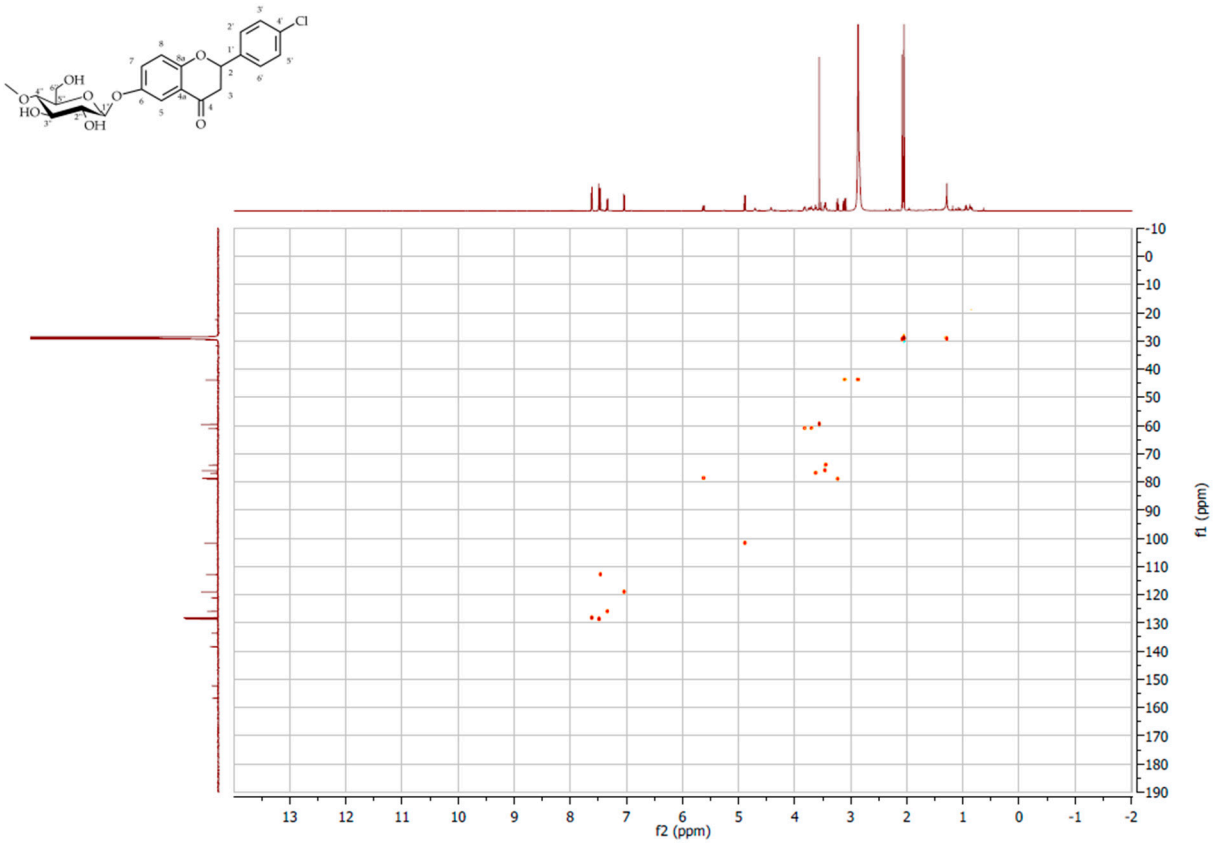


Figure S98. HMQC contour map – ^{1}H x ^{13}C of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

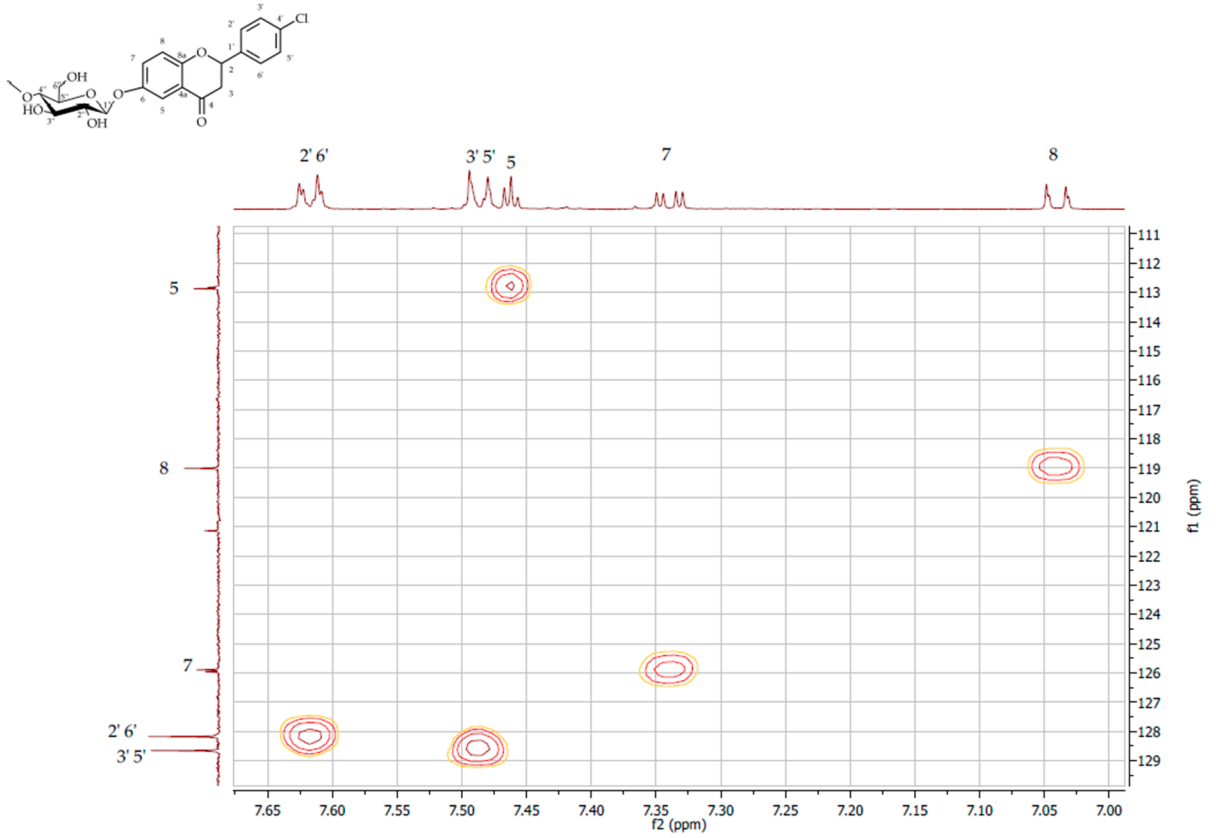


Figure S99. HMQC contour map – ^{1}H x ^{13}C expansion of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

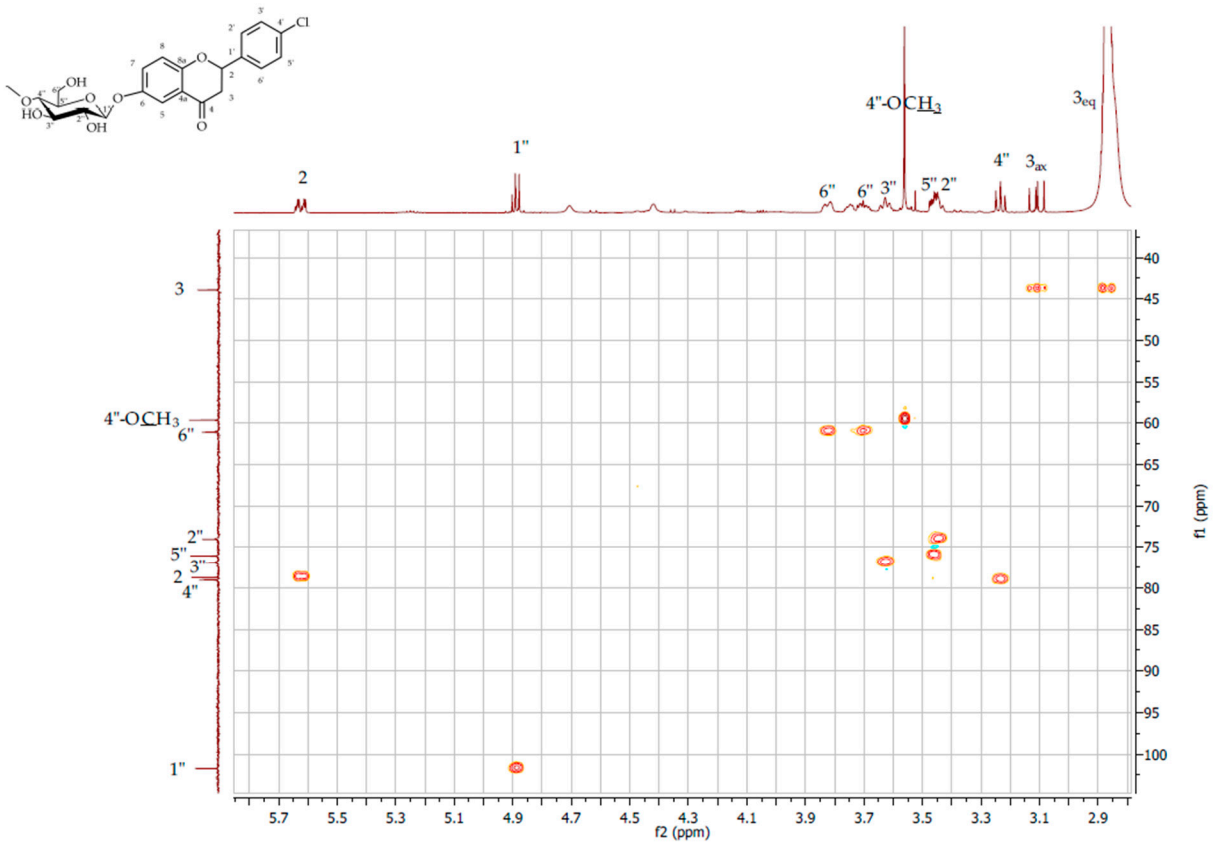


Figure S100. HMQC contour map – ^{1}H x ^{13}C expansion of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

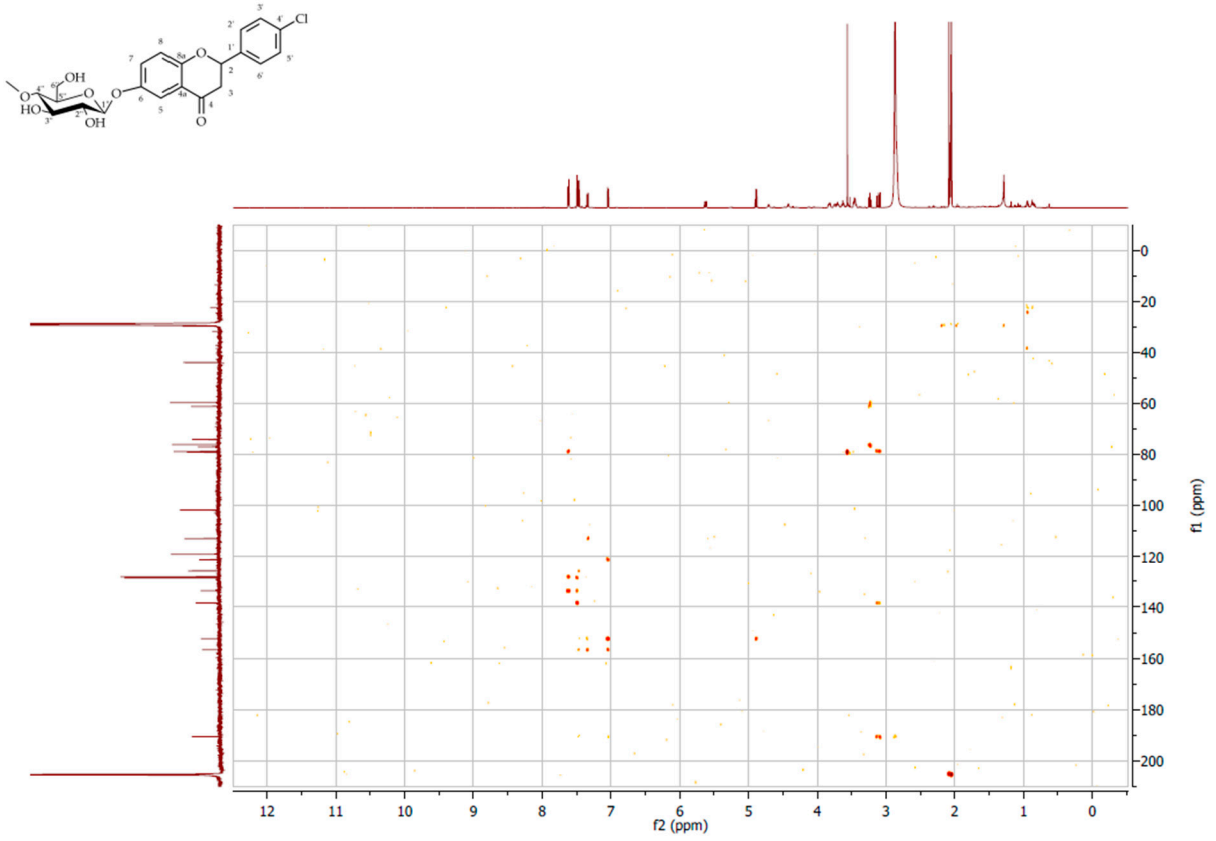


Figure S101. HMBC contour map – ^{1}H x ^{13}C of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

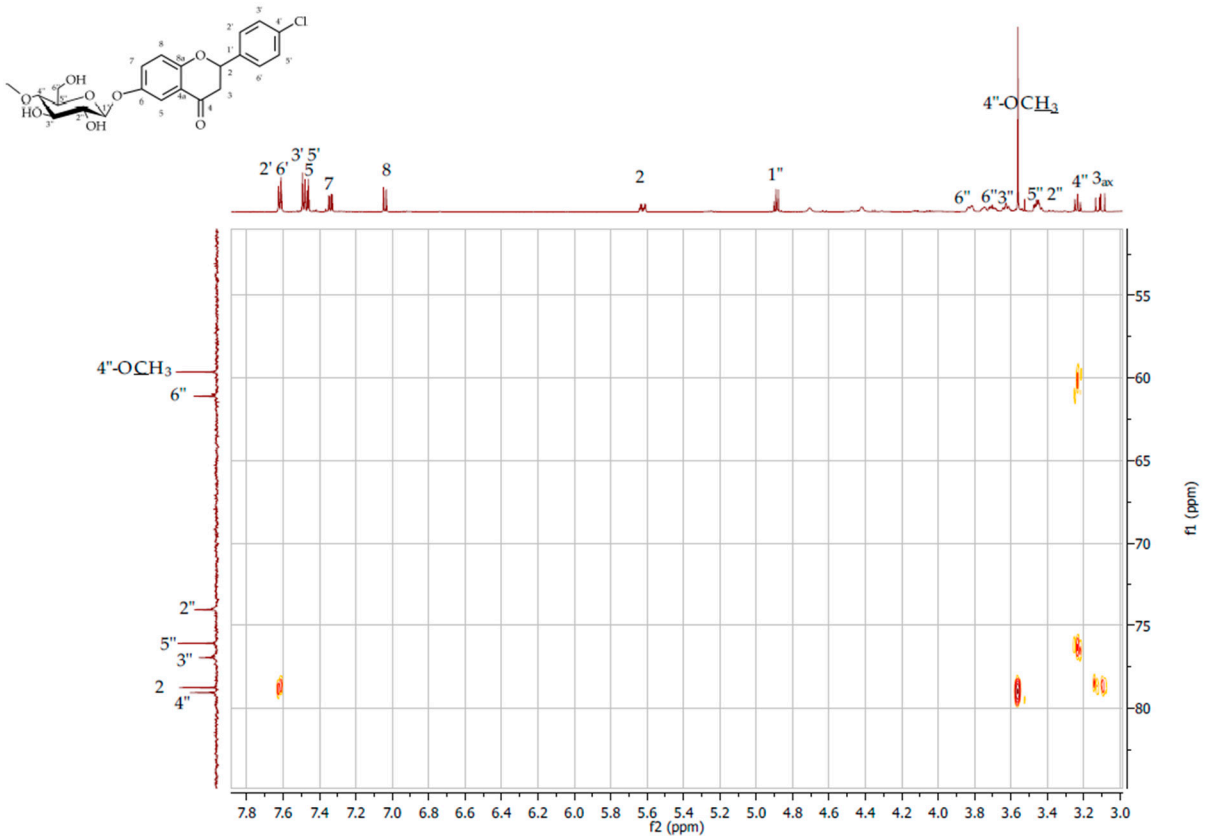


Figure S102. HMBC contour map – ^{1}H x ^{13}C expansion of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

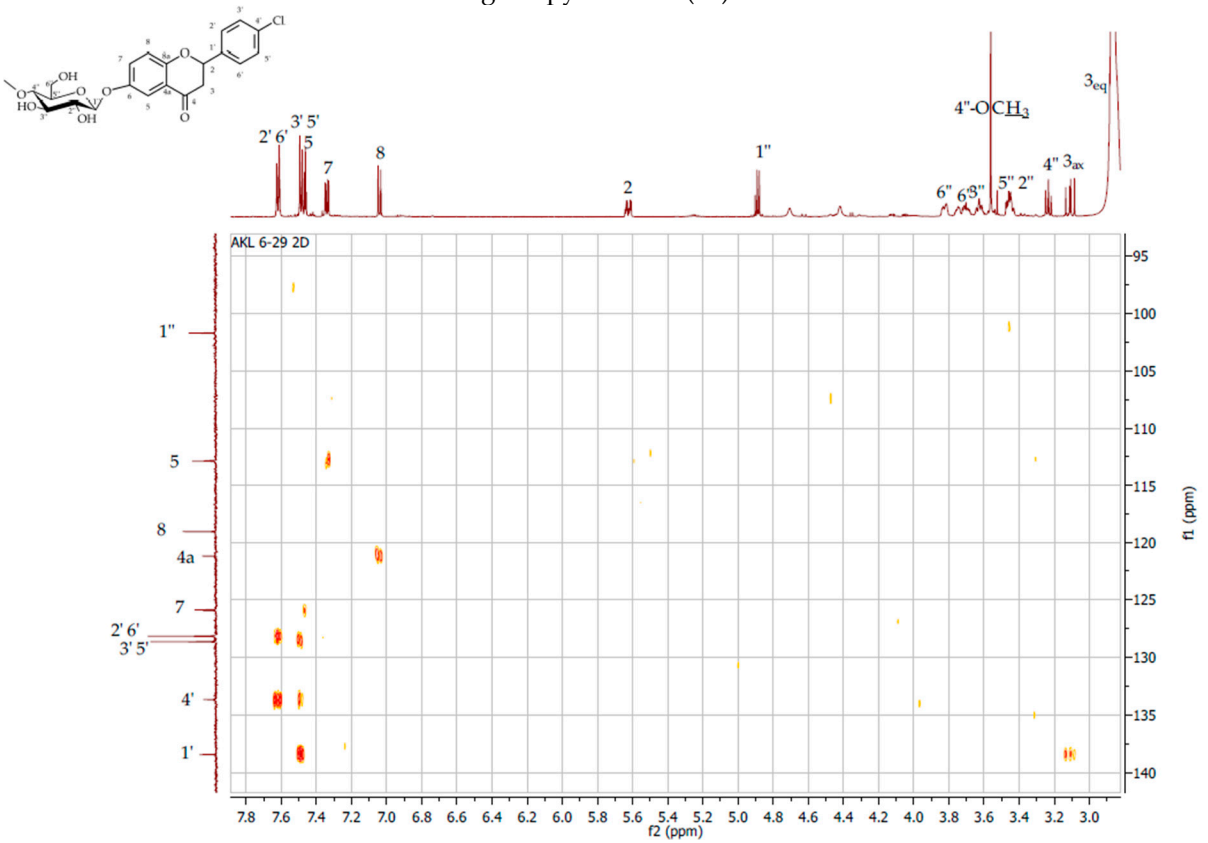


Figure S103. HMBC contour map – ^{1}H x ^{13}C expansion of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

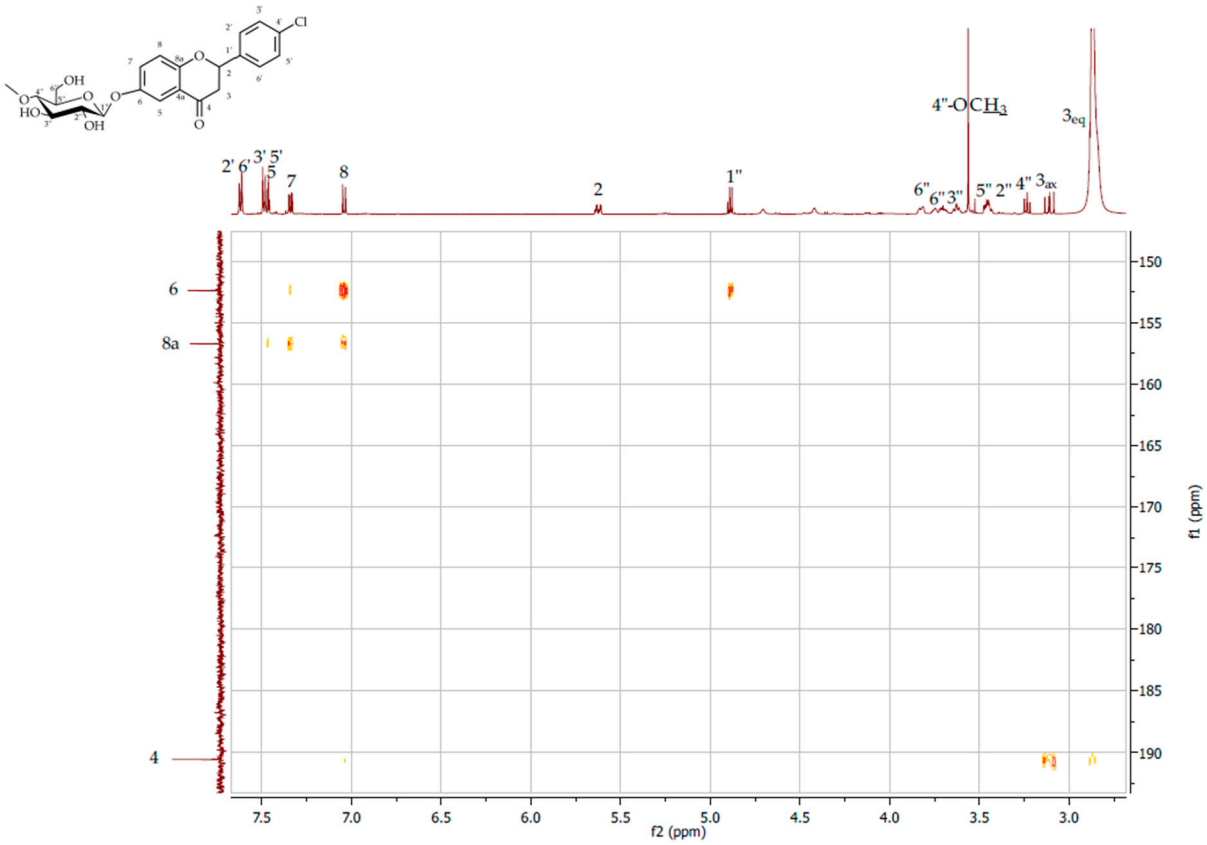


Figure S104. HMBC contour map – ^{1}H x ^{13}C expansion of 4′-chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**).

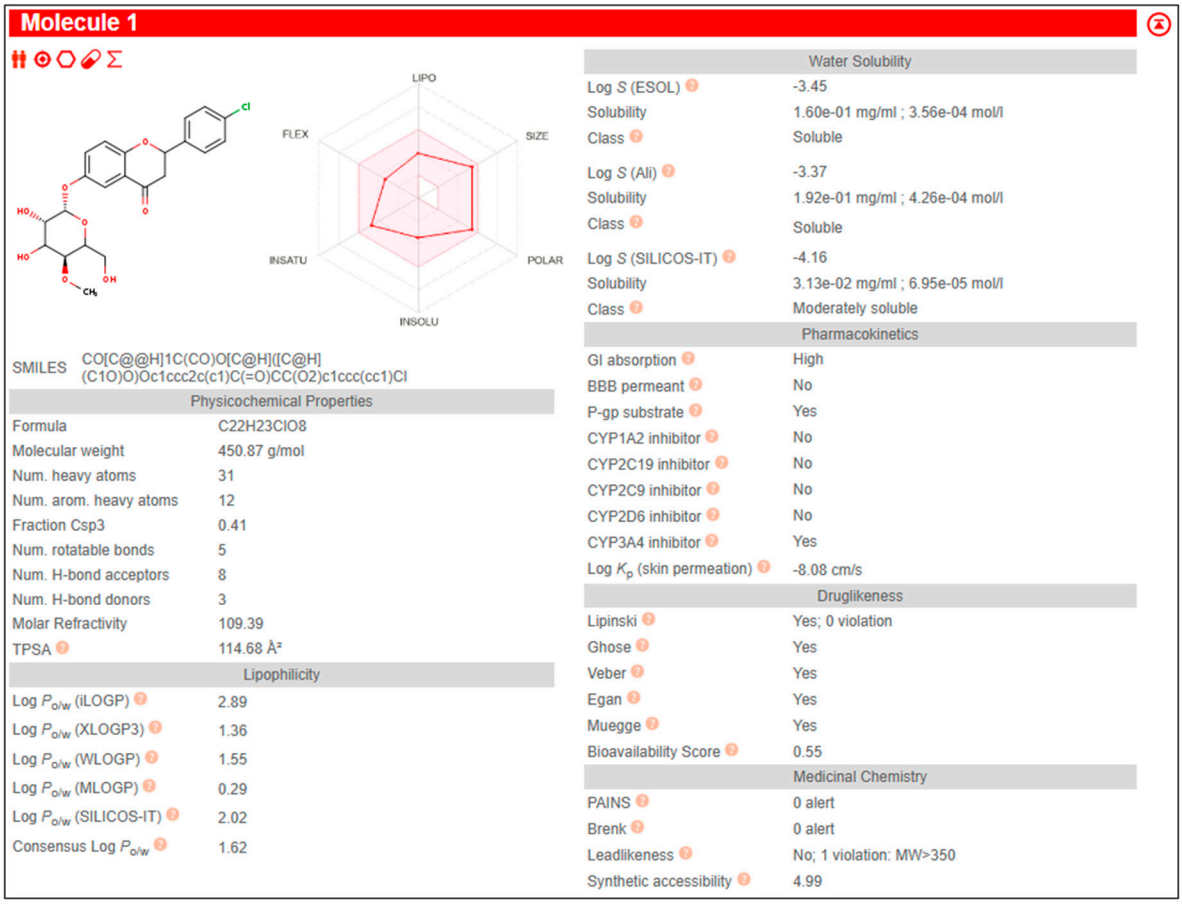


Figure S105. 4′-Chloroflavanone 6-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**) physicochemical and ADME parameters prediction using the SwissADME modelling.

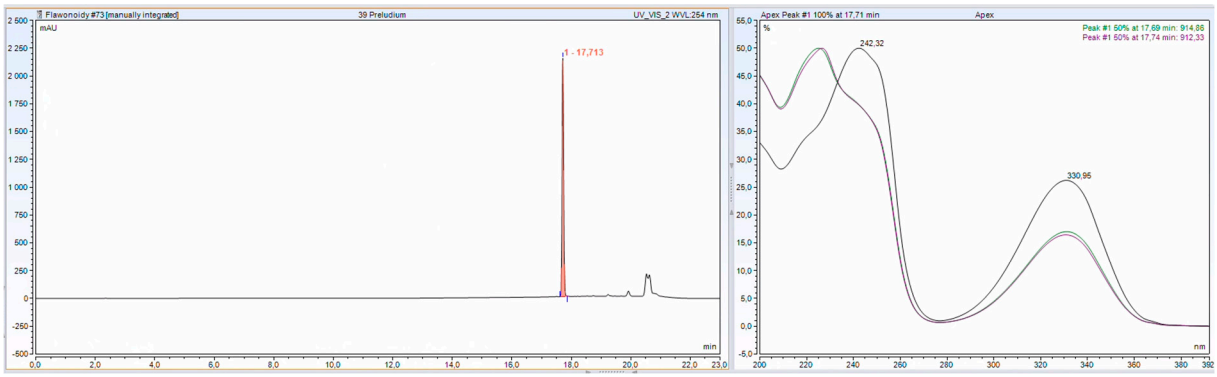


Figure S106. HPLC analysis of 6-chloroflavanone (**4**).

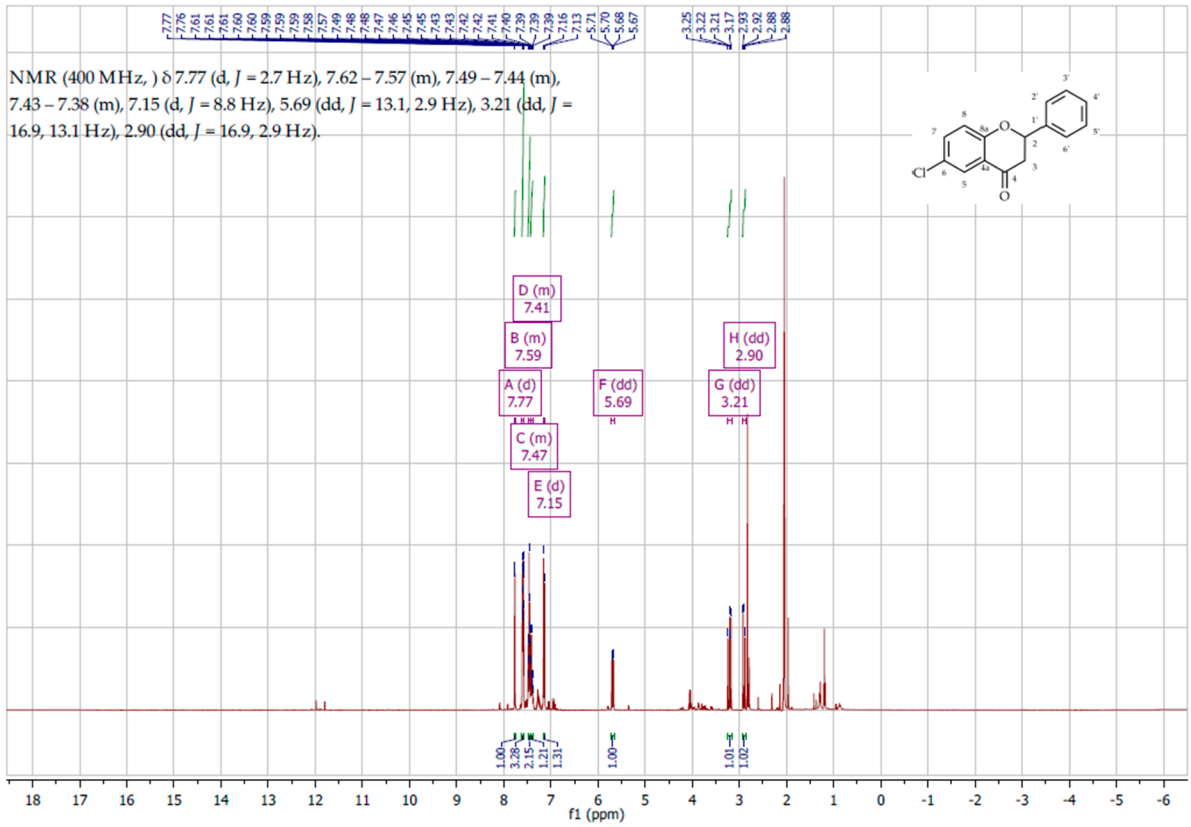


Figure S107. ^{1}H NMR spectrum (*δ*, acetone-d6, 600 MHz) of 6-chloroflavanone (**4**).

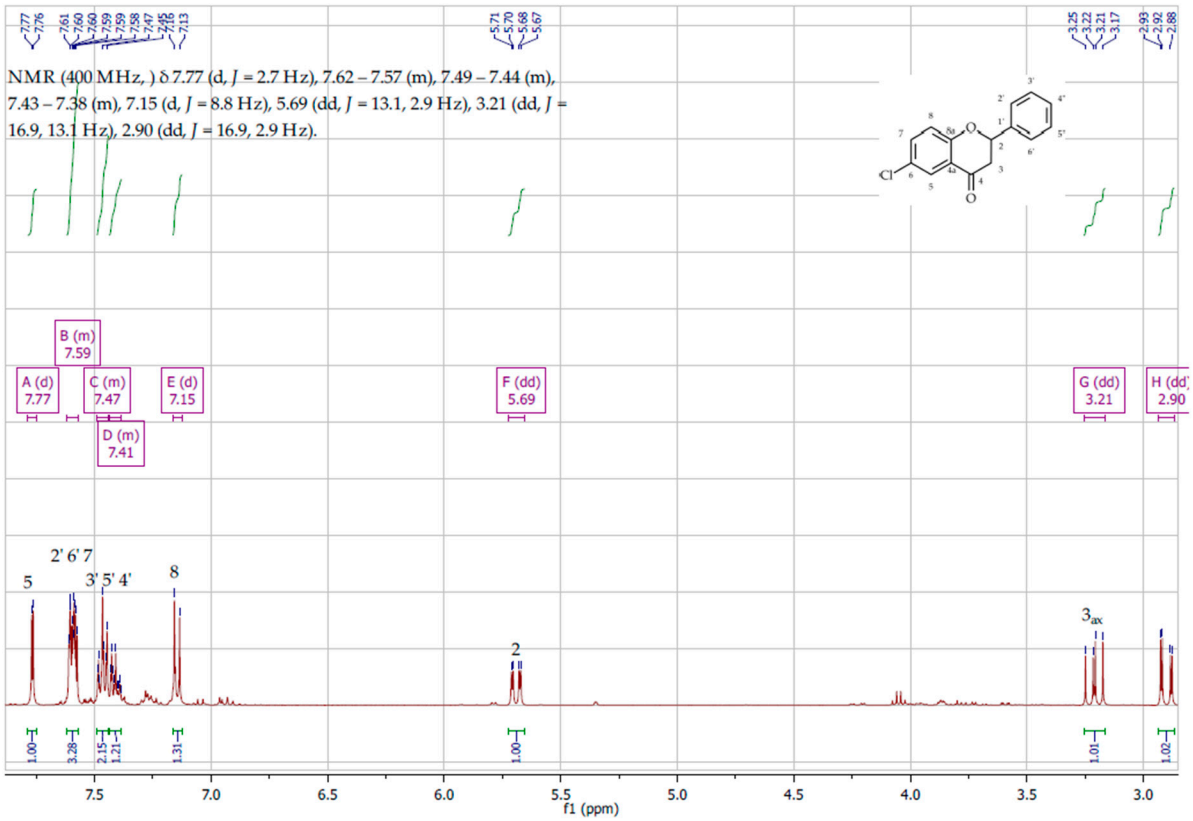


Figure S108. ^{1}H NMR spectrum (δ, acetone-d6, 600 MHz) of 6-chloroflavanone (**4**).

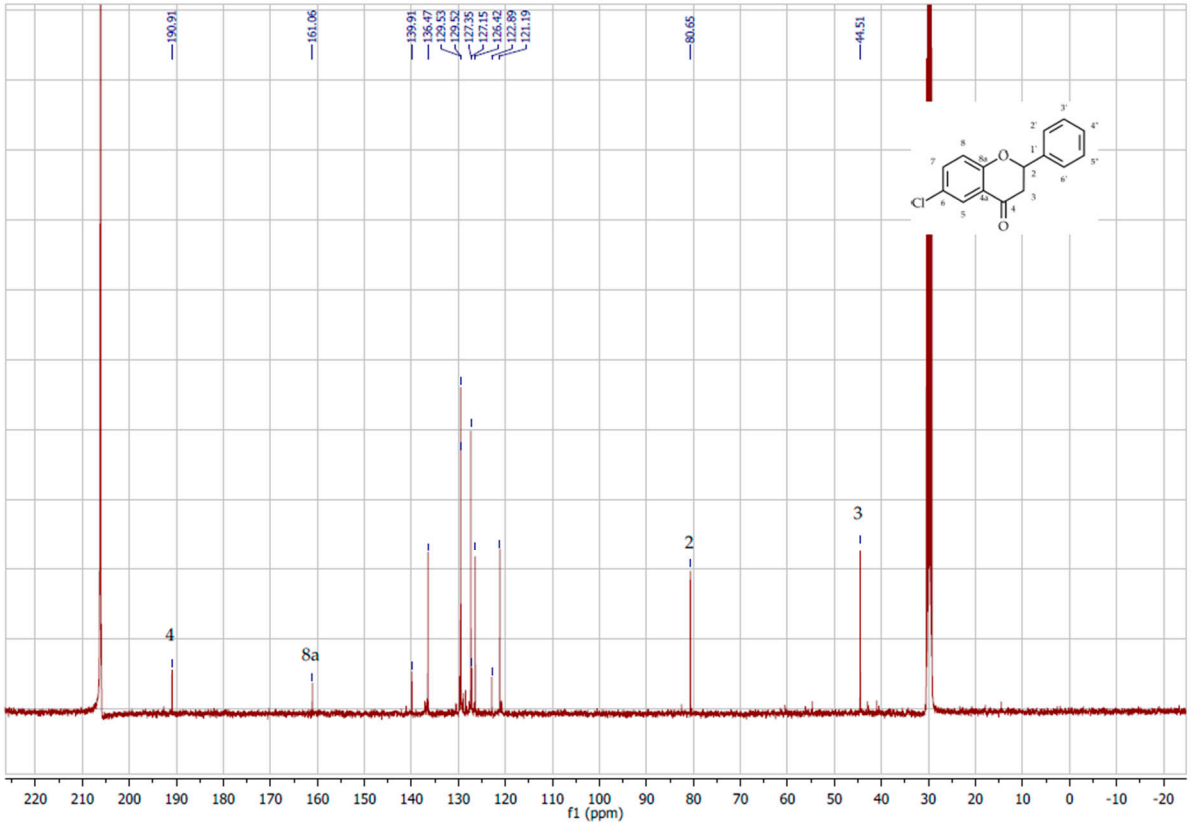


Figure S109. ^{13}C NMR spectrum (δ, acetone-d6, 151 MHz) of 6-chloroflavanone (**4**).

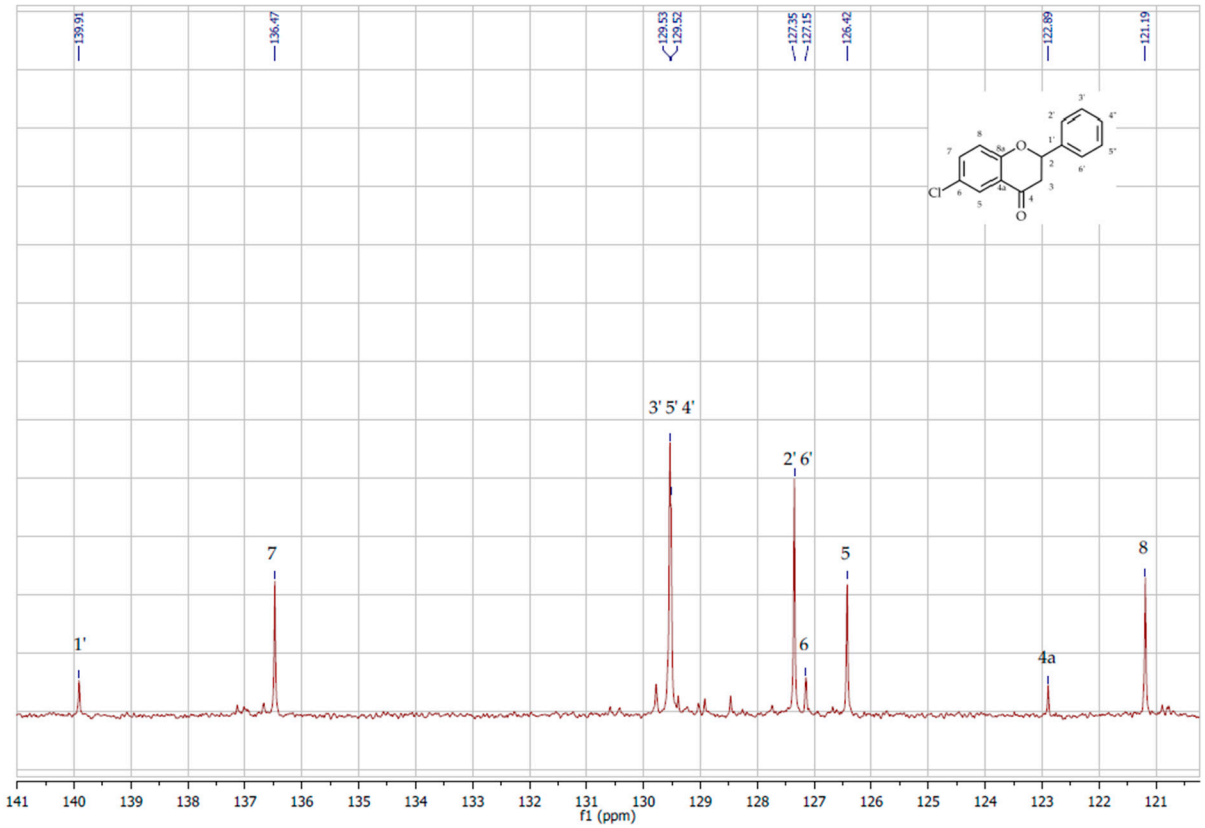


Figure S110. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 6-chloroflavanone (**4**).

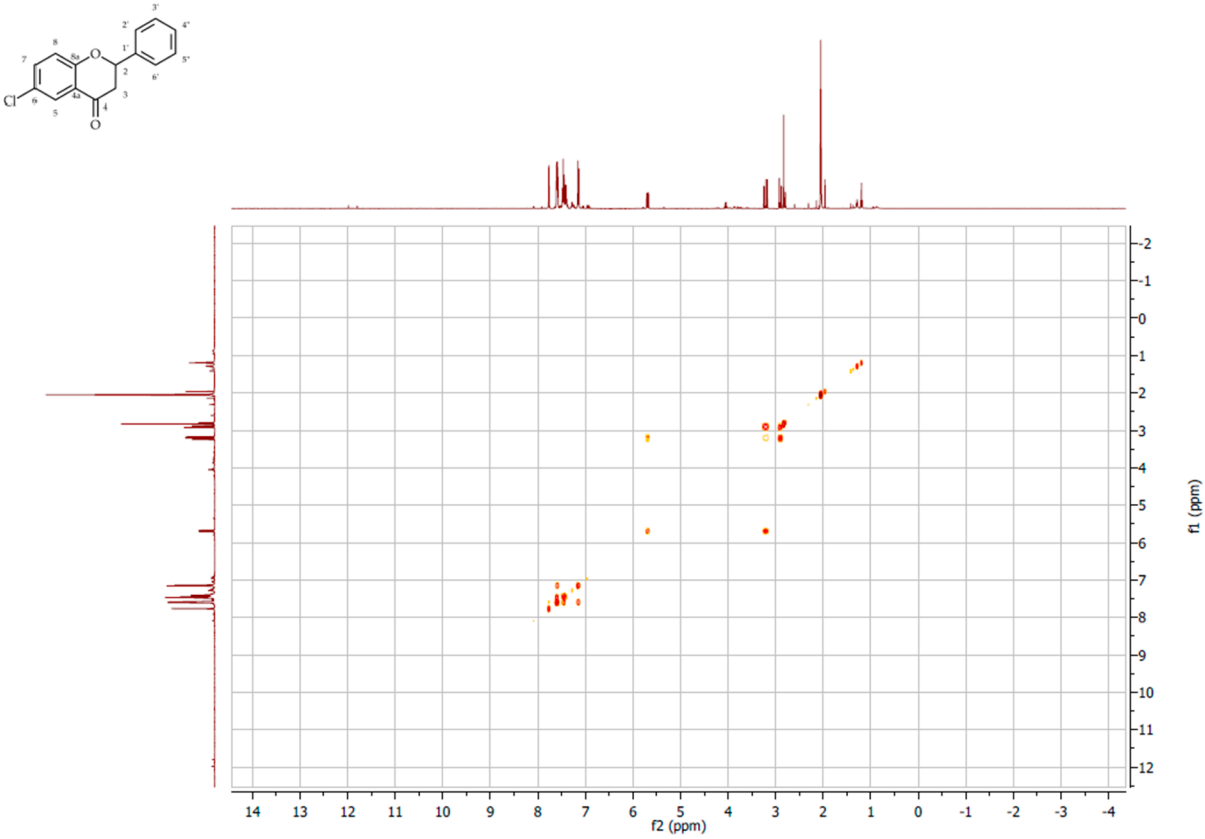


Figure S111. COSY contour map – ^{1}H x ^{1}H of 6-chloroflavanone (**4**).

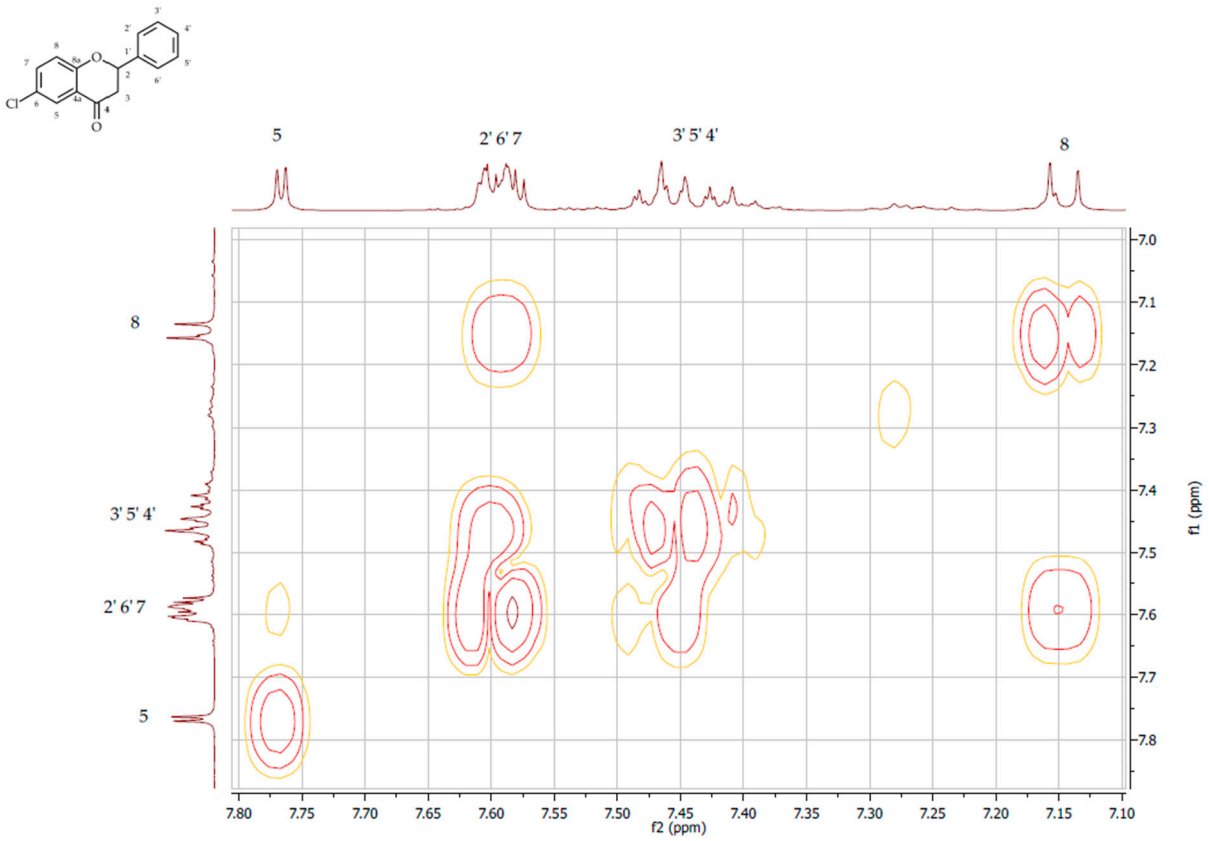


Figure S112. COSY contour map – ^{1}H x ^{1}H expansion of 6-chloroflavanone (**4**).

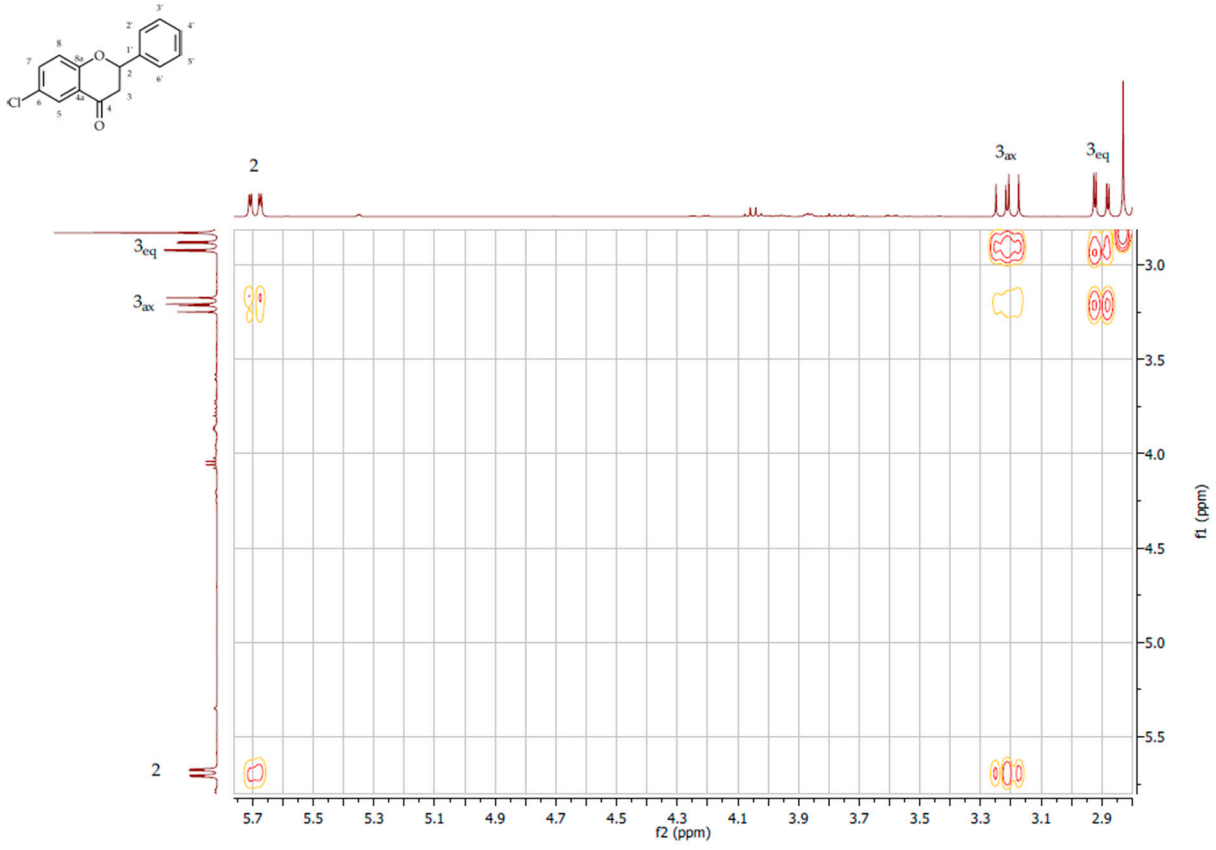


Figure S113. COSY contour map – ^{1}H x ^{1}H expansion of 6-chloroflavanone (**4**).

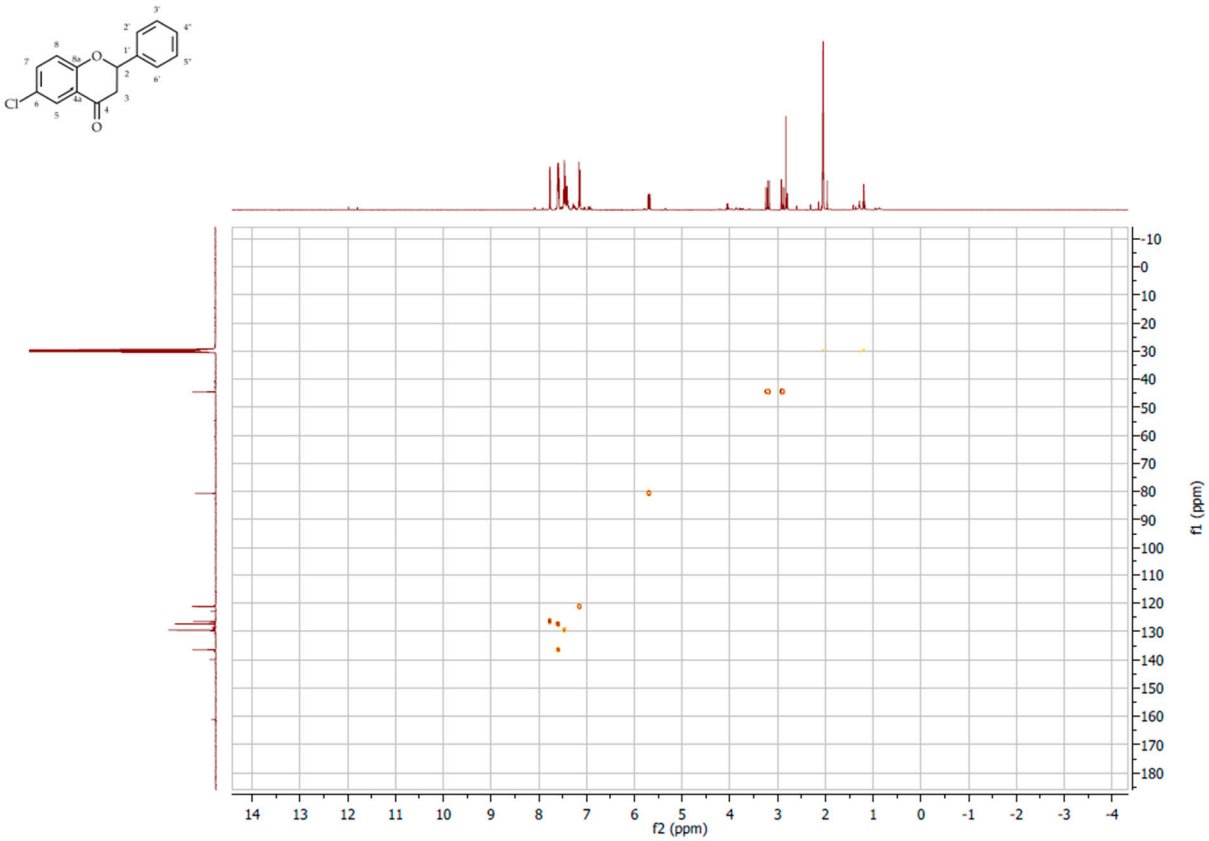


Figure S114. HMQC contour map – ^{1}H x ^{13}C of 6-chloroflavanone (**4**).

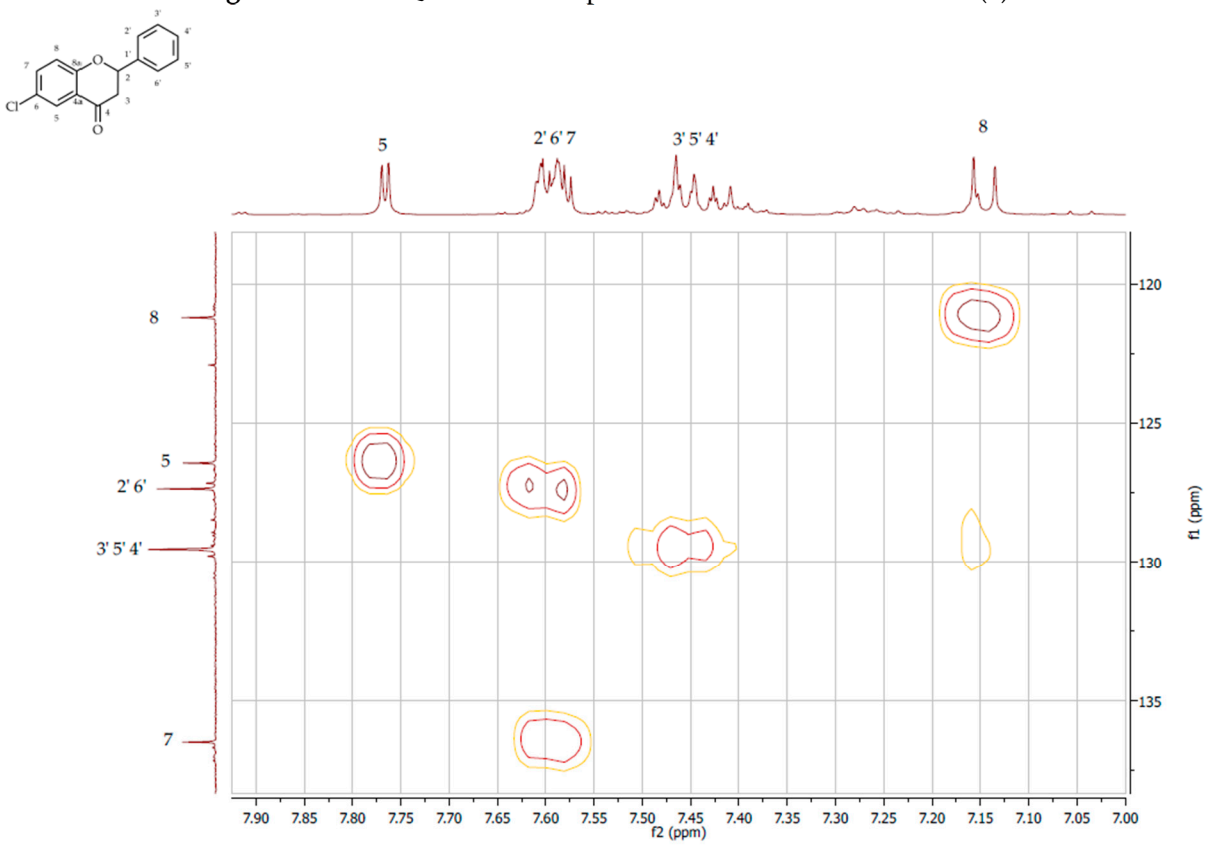


Figure S115. HMQC contour map – ^{1}H x ^{13}C expansion of 6-chloroflavanone (**4**).

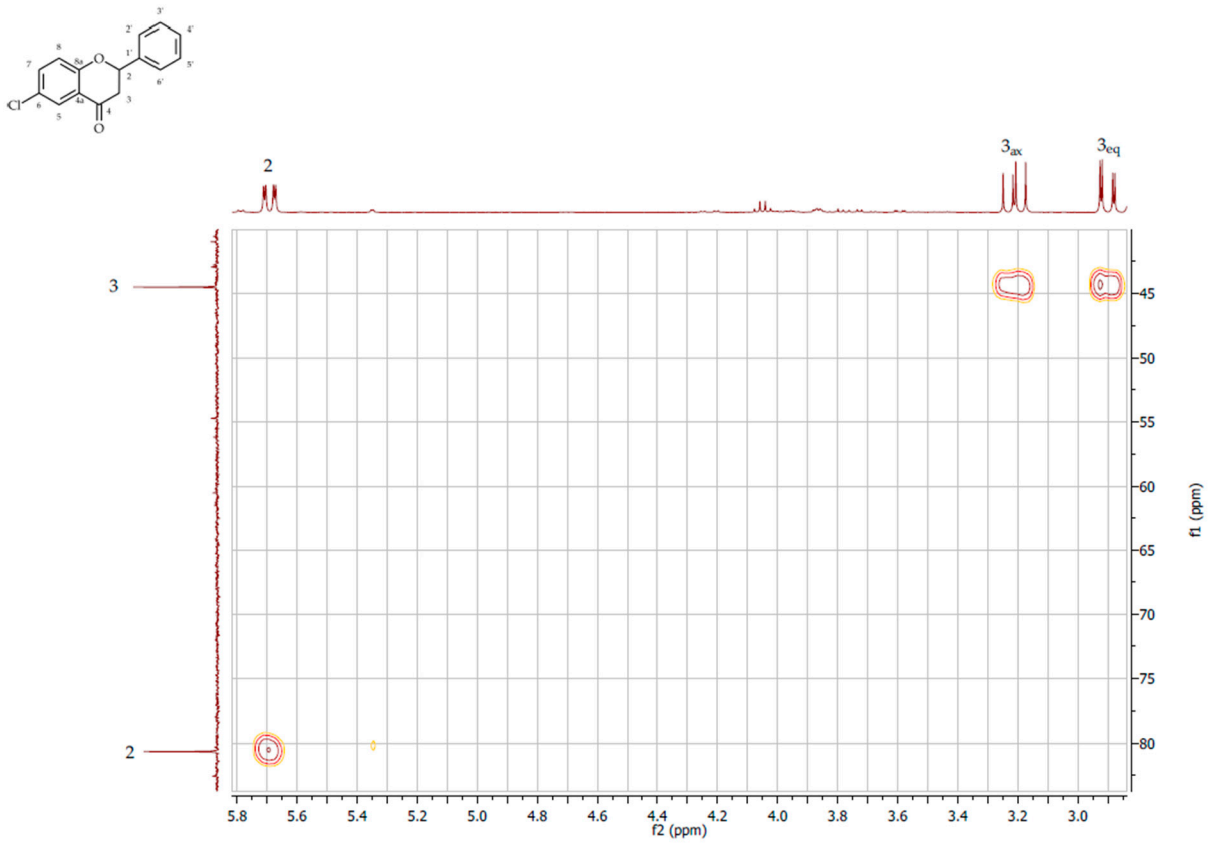


Figure S116. HMQC contour map – ^{1}H x ^{13}C expansion of 6-chloroflavanone (**4**).

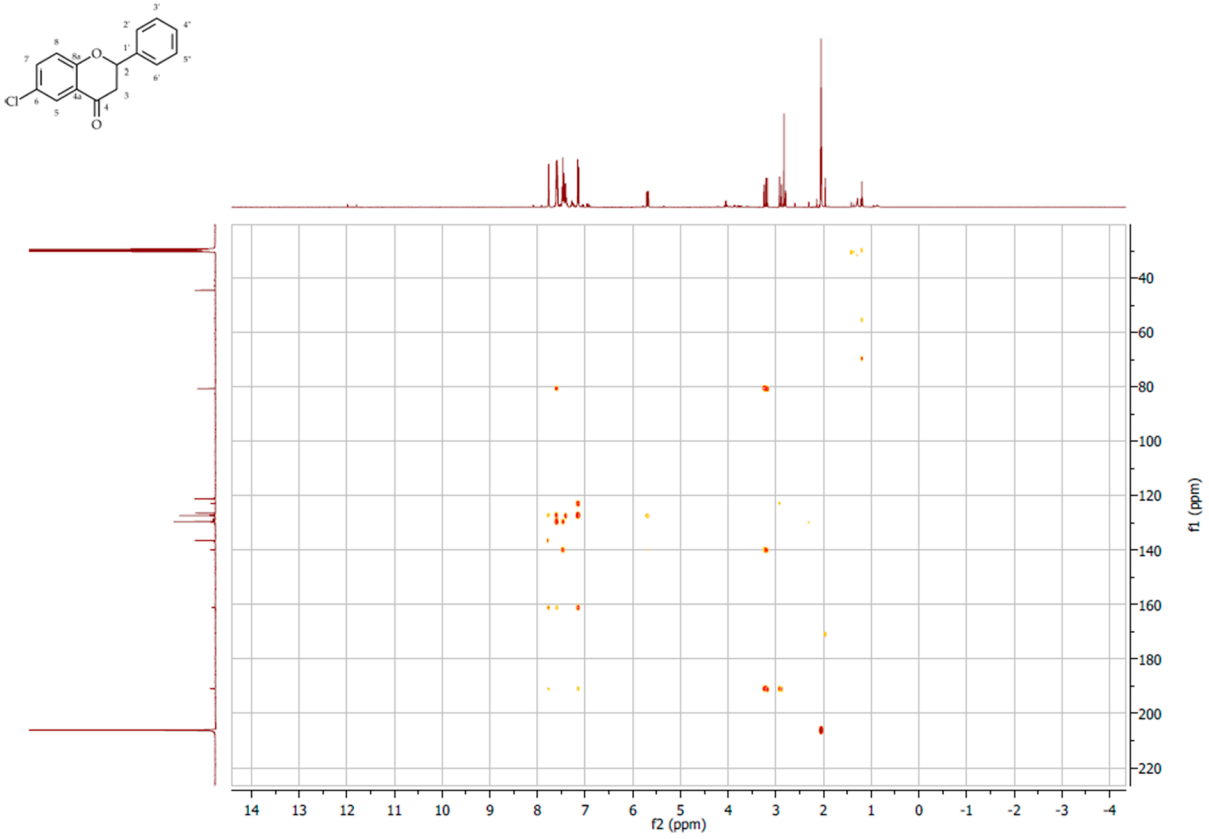


Figure S117. HMBC contour map – ^{1}H x ^{13}C of 6-chloroflavanone (**4**).

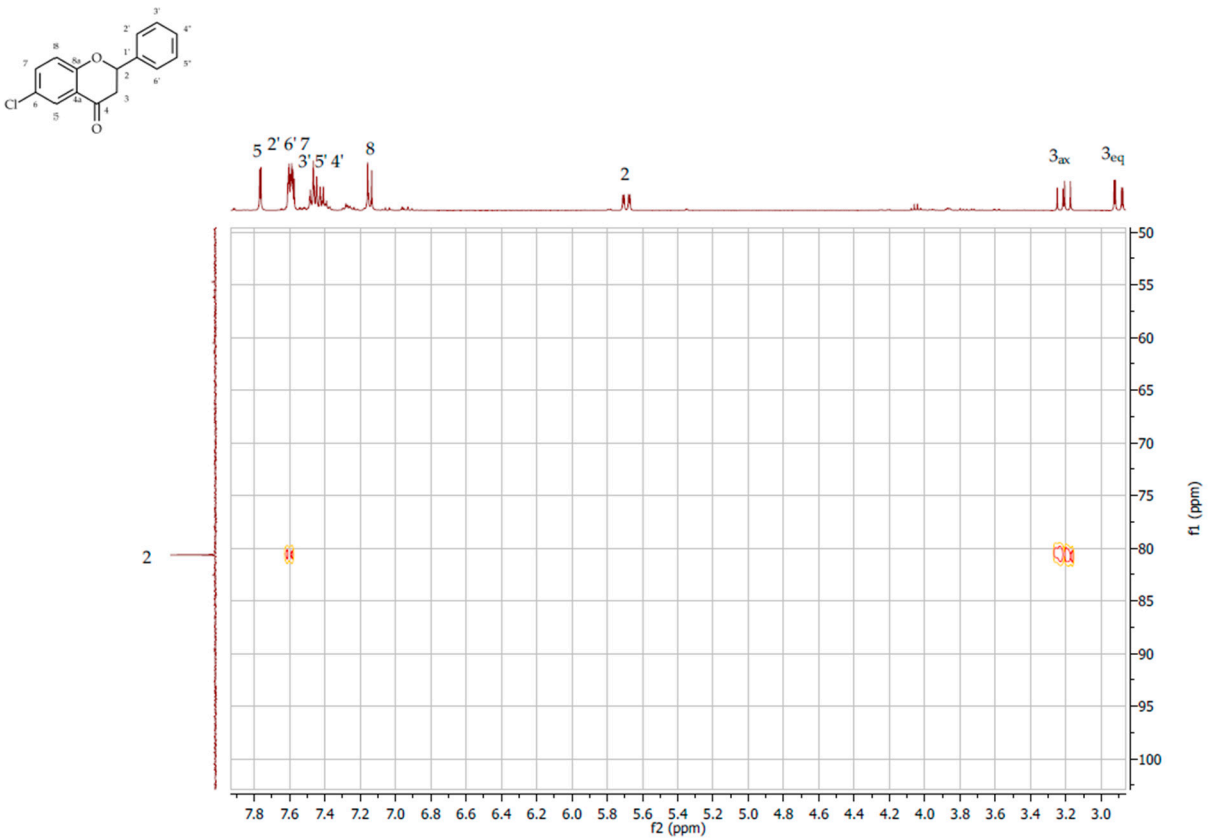


Figure S118. HMBC contour map – ^{1}H x ^{13}C expansion of 6-chloroflavanone (**4**).

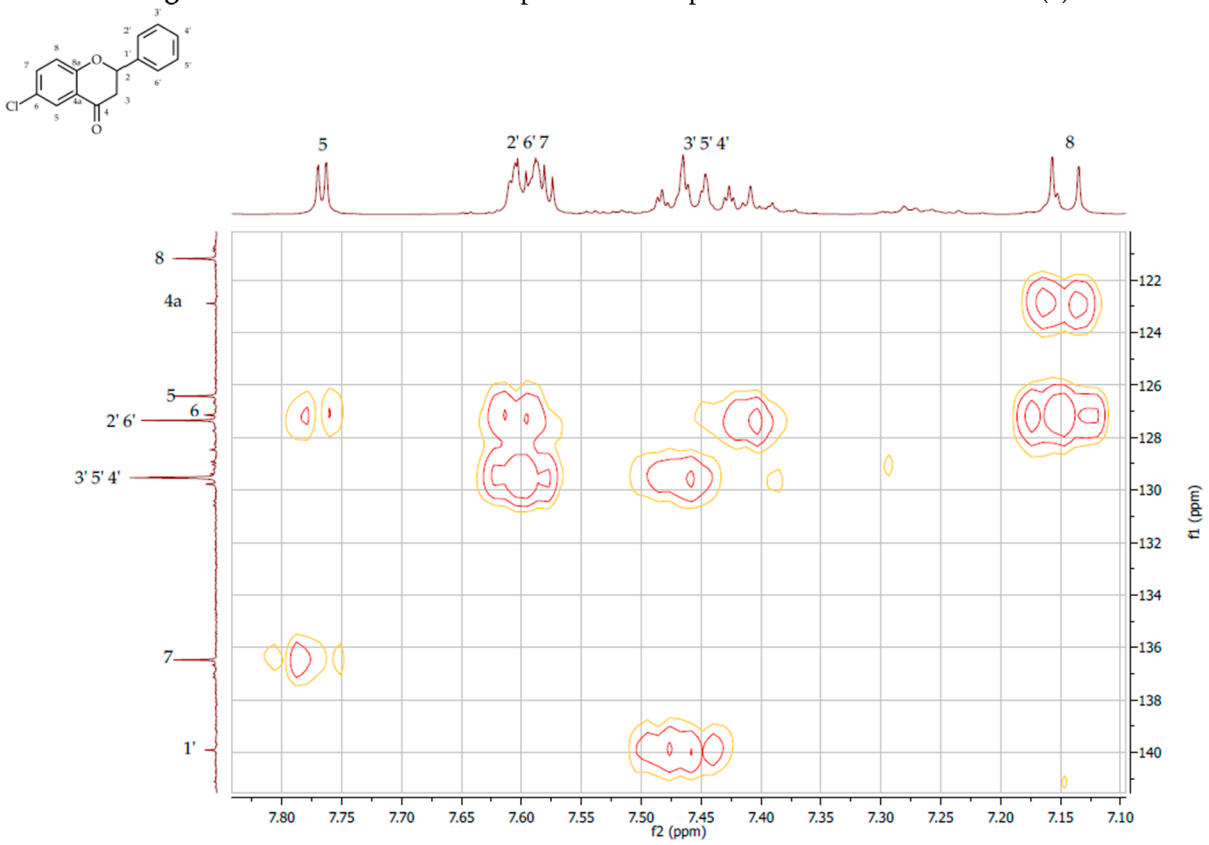


Figure S119. HMBC contour map – ^{1}H x ^{13}C expansion of 6-chloroflavanone (**4**).

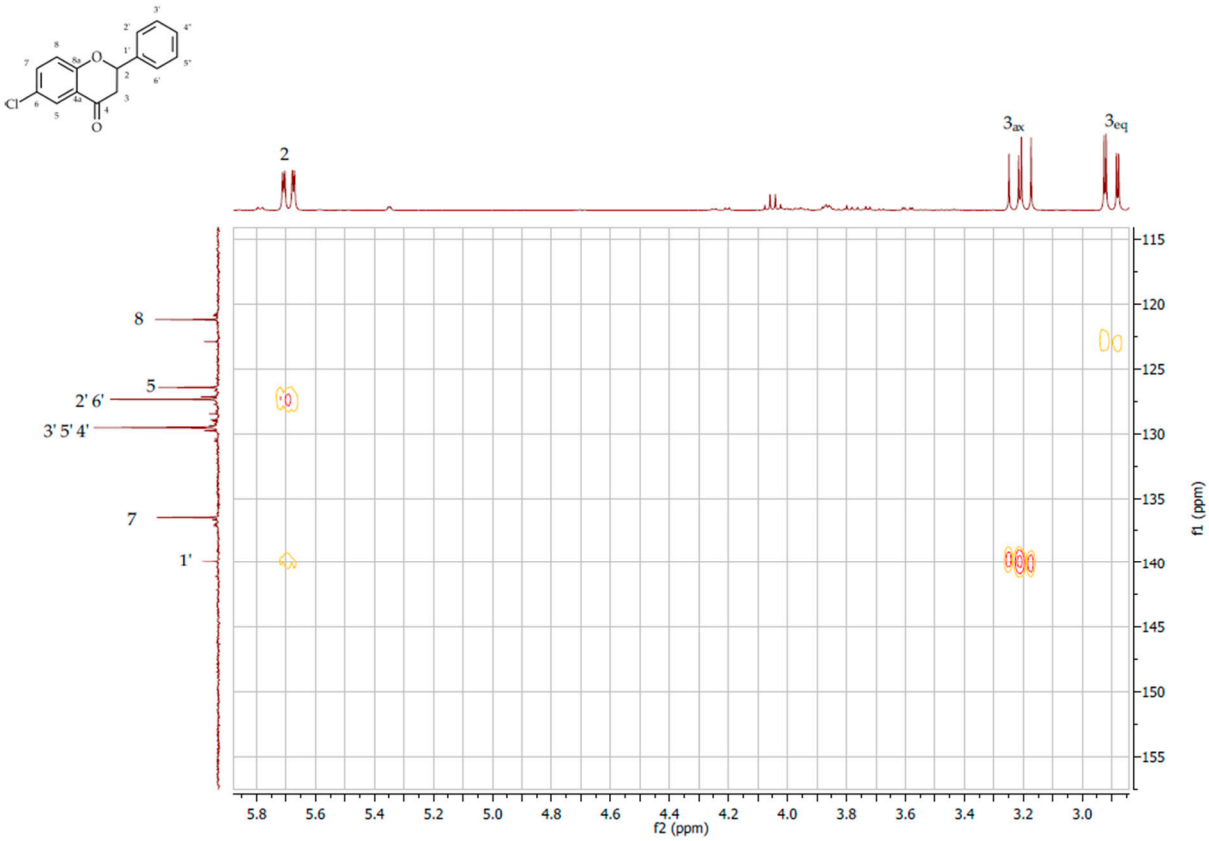


Figure S120. HMBC contour map – ^{1}H x ^{13}C expansion of 6-chloroflavanone (**4**).

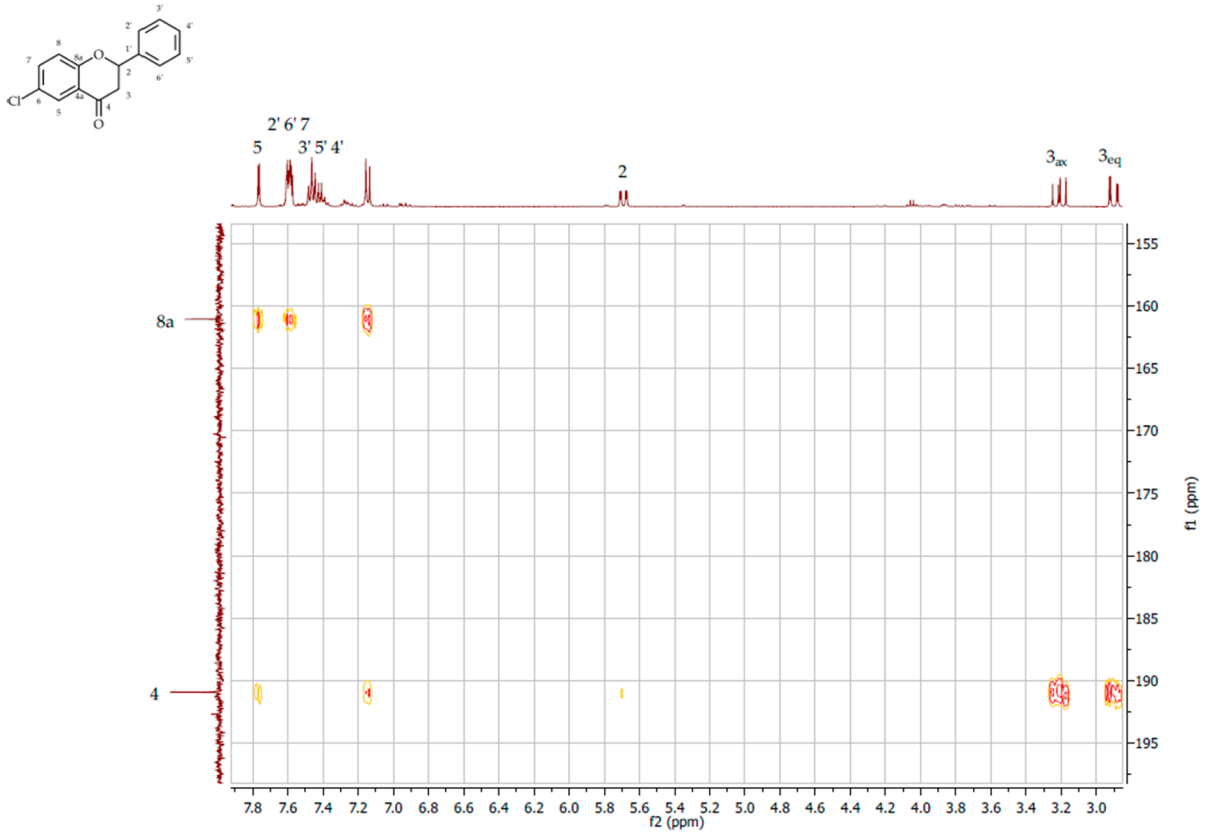


Figure S121. HMBC contour map – ^{1}H x ^{13}C expansion of 6-chloroflavanone (**4**).

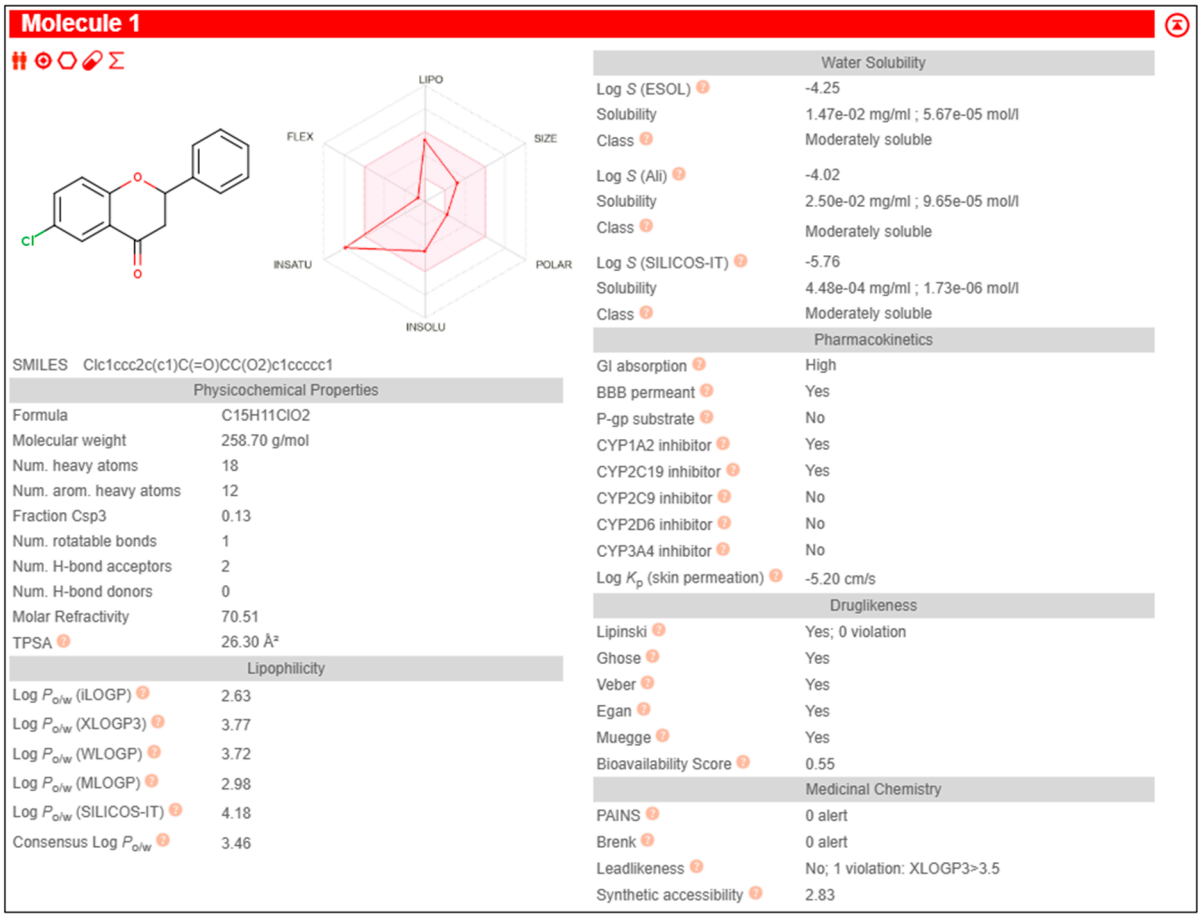


Figure S122. 6-Chloroflavanone (**4**) physicochemical and ADME parameters prediction using the SwissADME modelling.

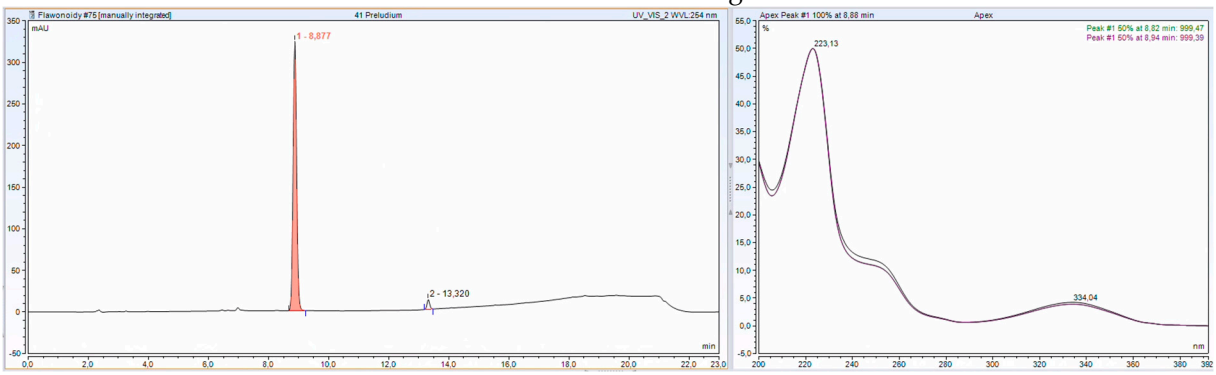


Figure S123. HPLC analysis of 6-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

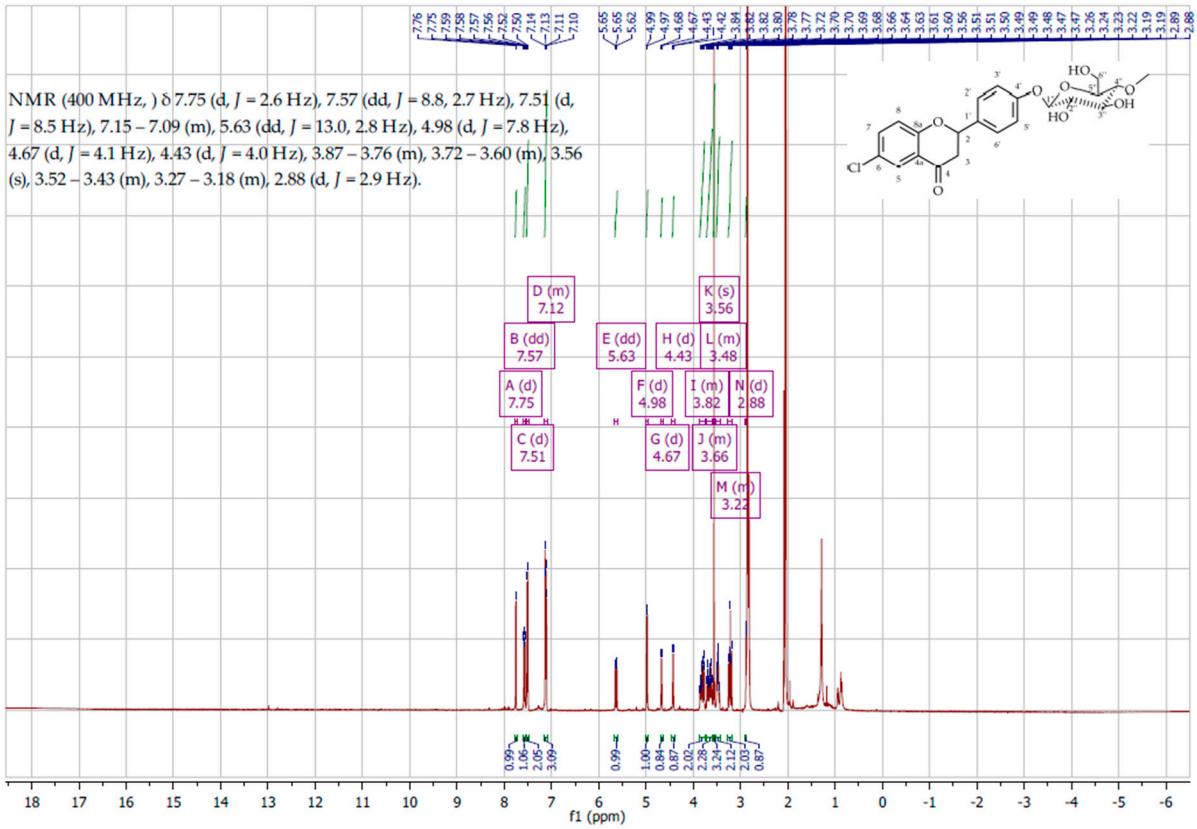


Figure S124. ^{1}H NMR spectrum (δ, acetone-d6, 600 MHz) of 6-chloroflavanone 4′-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

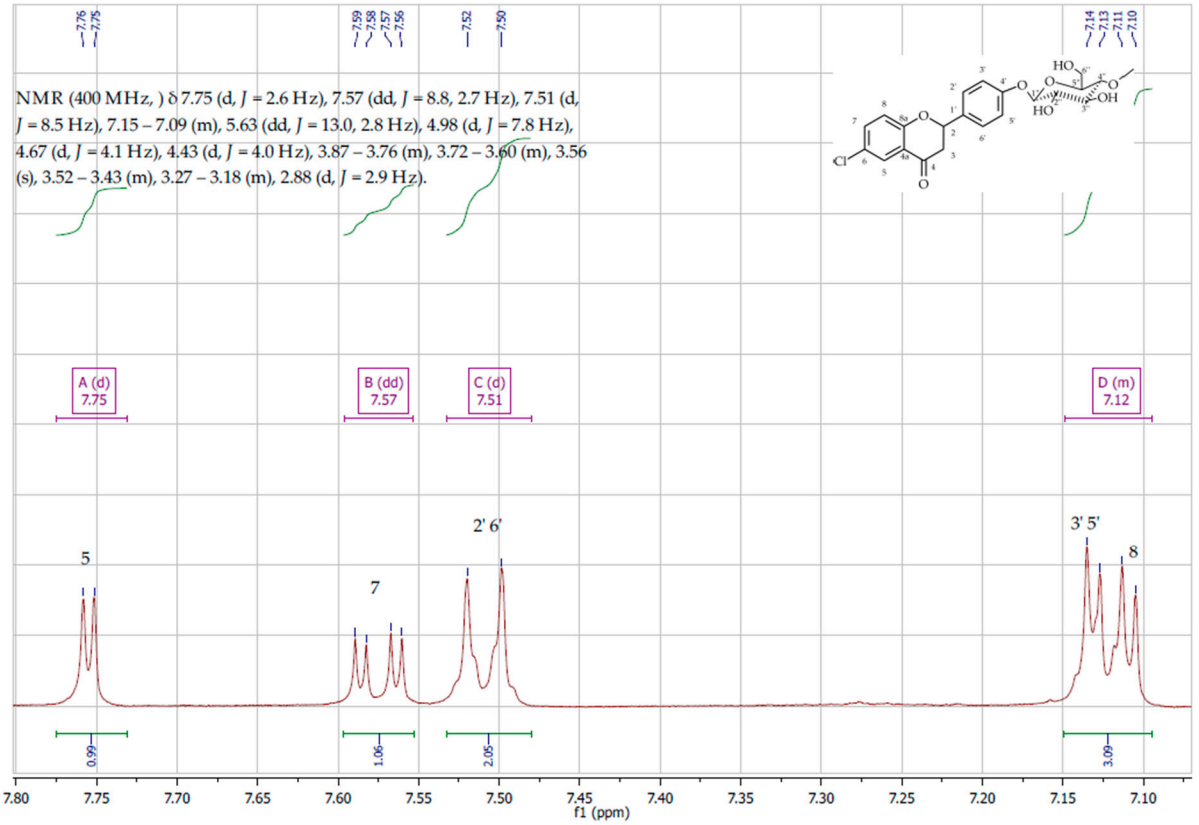


Figure S125. ^{1}H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 6-chloroflavanone 4′-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

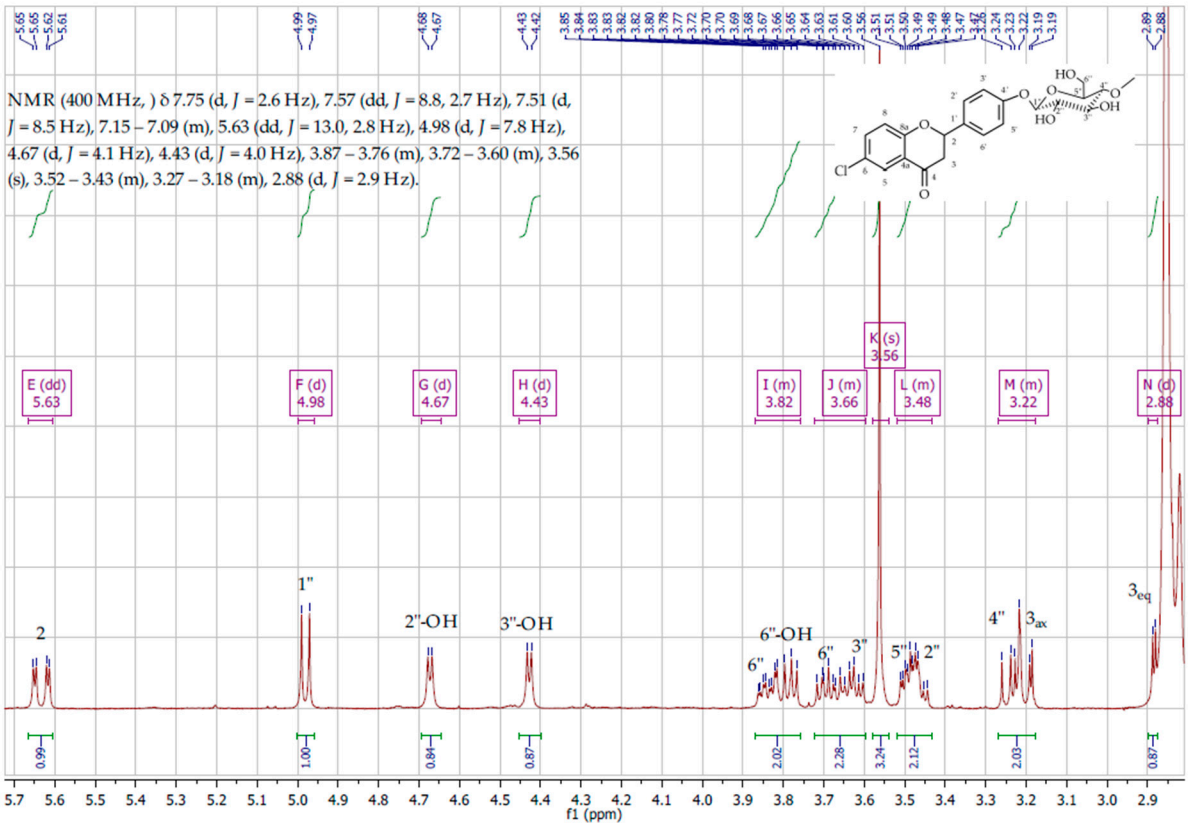


Figure S126. ^{1}H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 6-chloroflavanone 4′-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

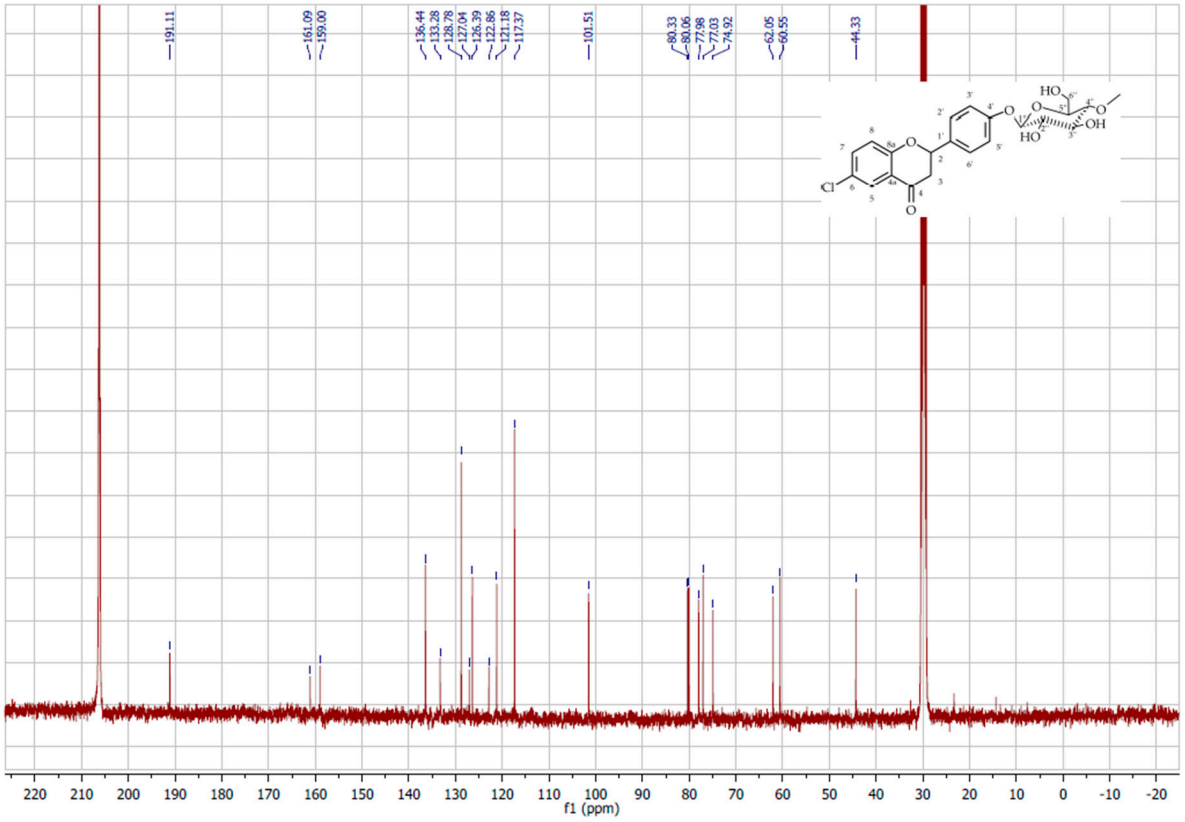


Figure S127. ^{13}C NMR spectrum (δ, acetone-d6, 151 MHz) of 6-chloroflavanone 4′-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

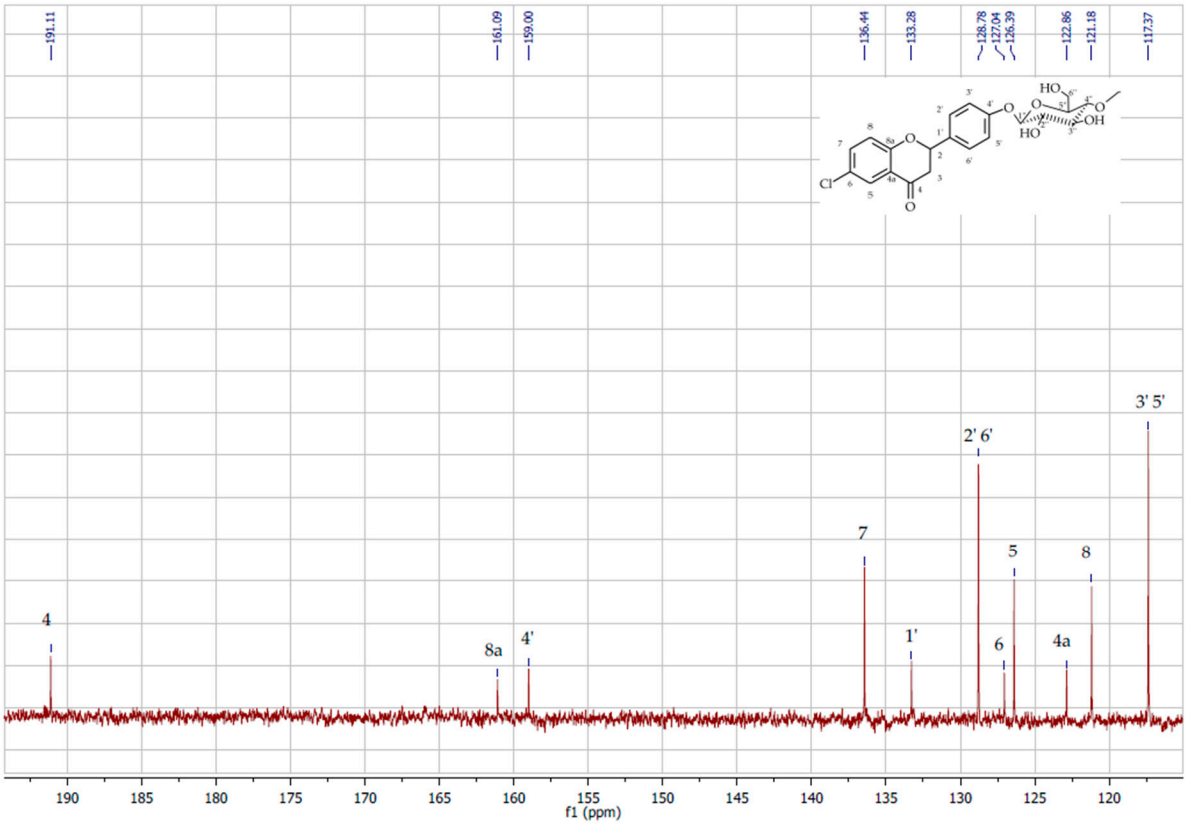


Figure S128. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 6-chloroflavanone 4′-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

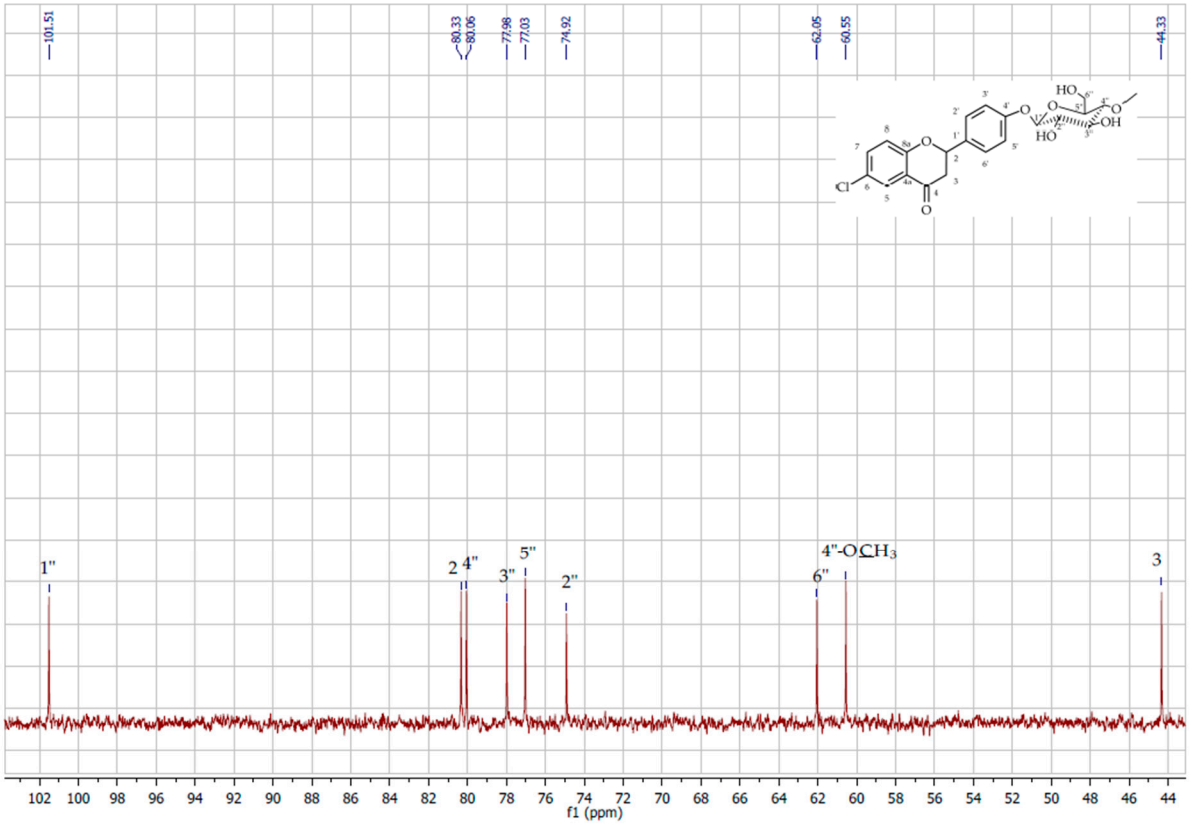


Figure S129. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 6-chloroflavanone 4′-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

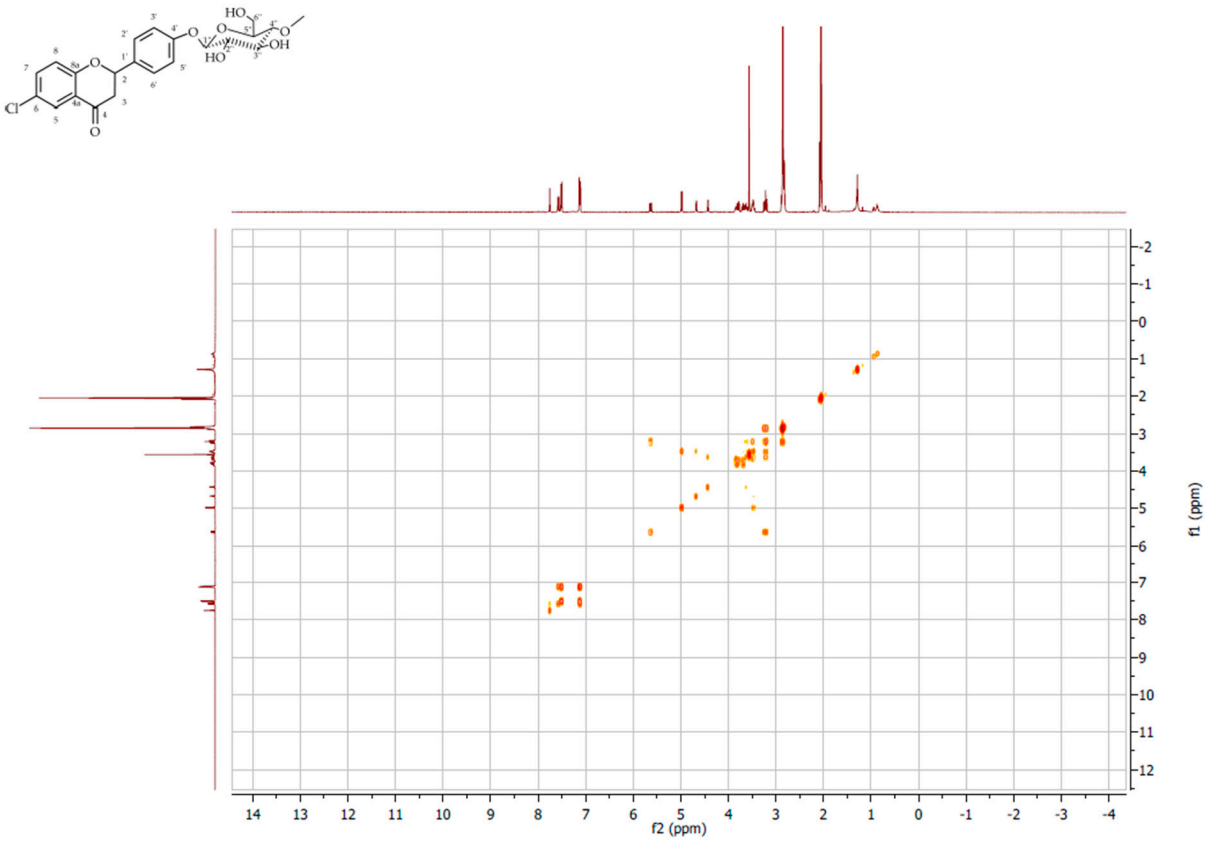


Figure S130. COSY contour map – ^{1}H x ^{1}H of 6-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

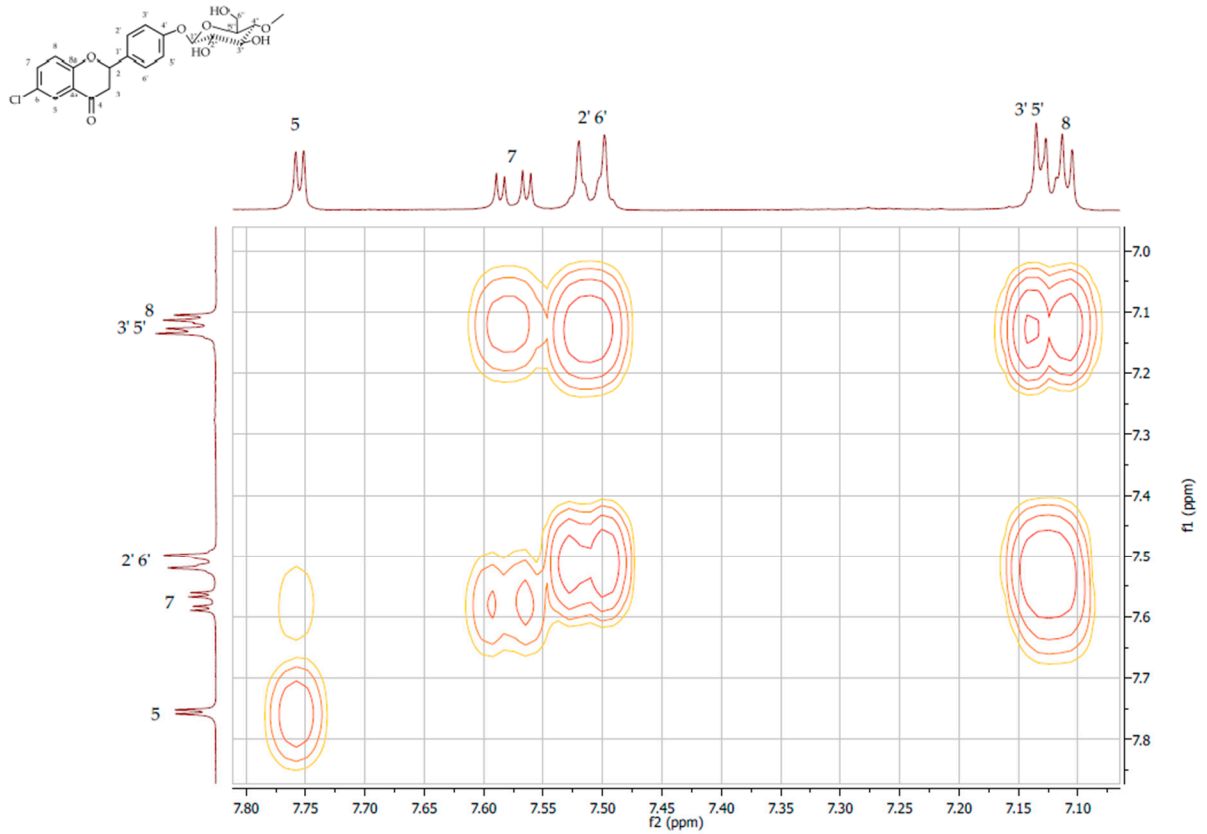


Figure S131. COSY contour map – ^{1}H x ^{1}H expansion of 6-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

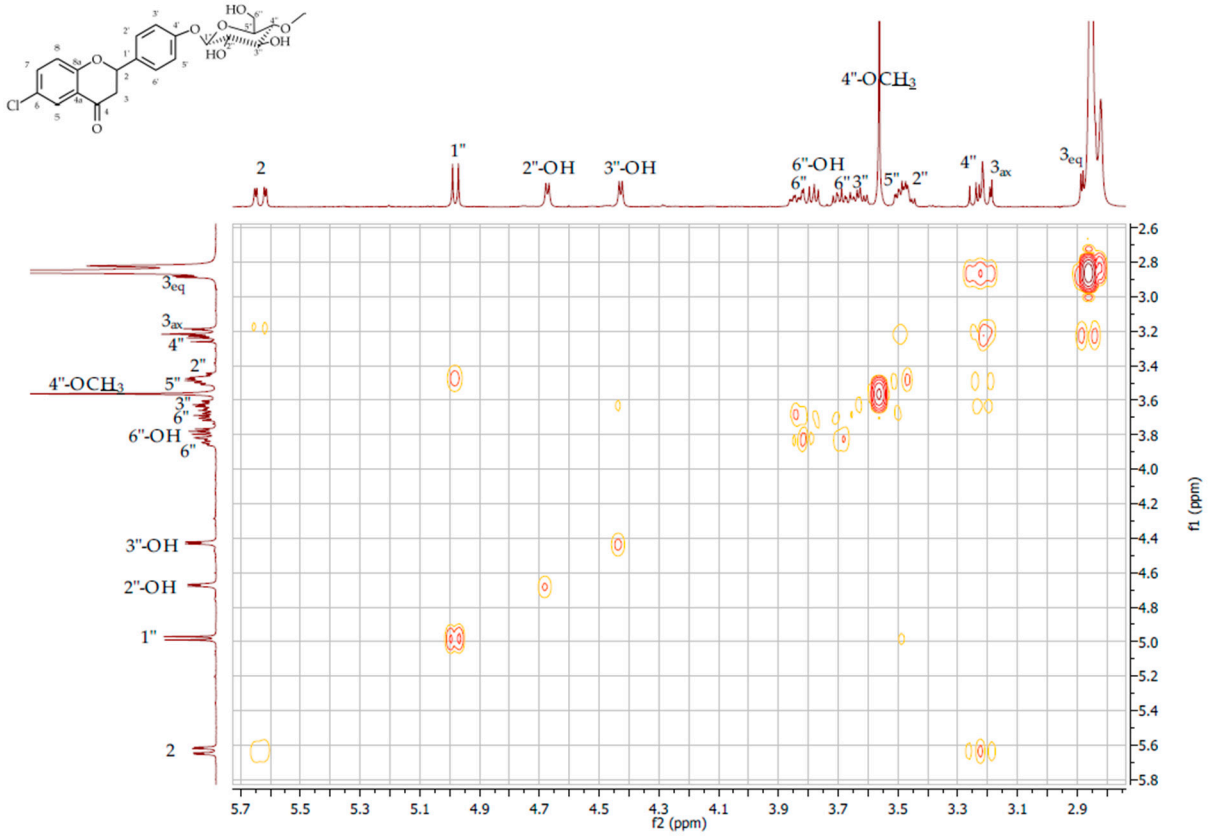


Figure S132. COSY contour map – ^{1}H x ^{1}H expansion of 6-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

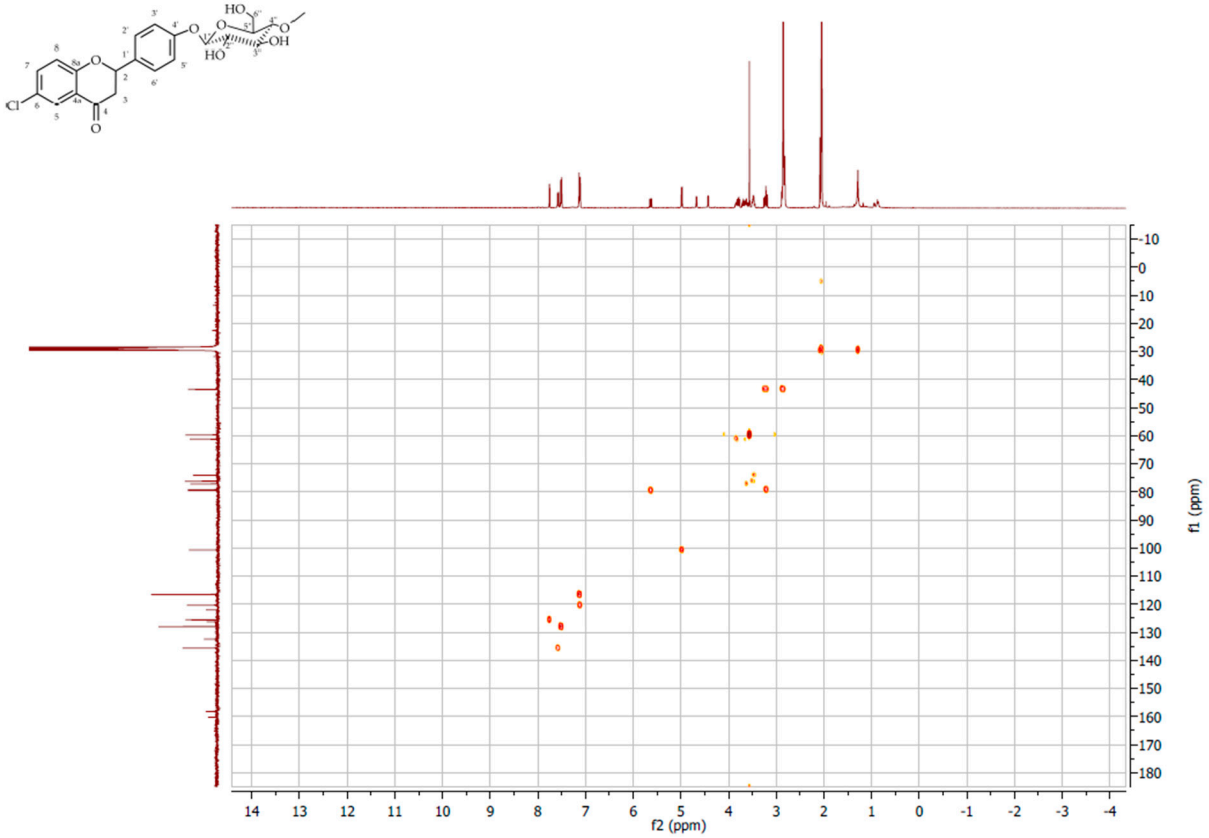


Figure S133. HMQC contour map – ^{1}H x ^{13}C of 6-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

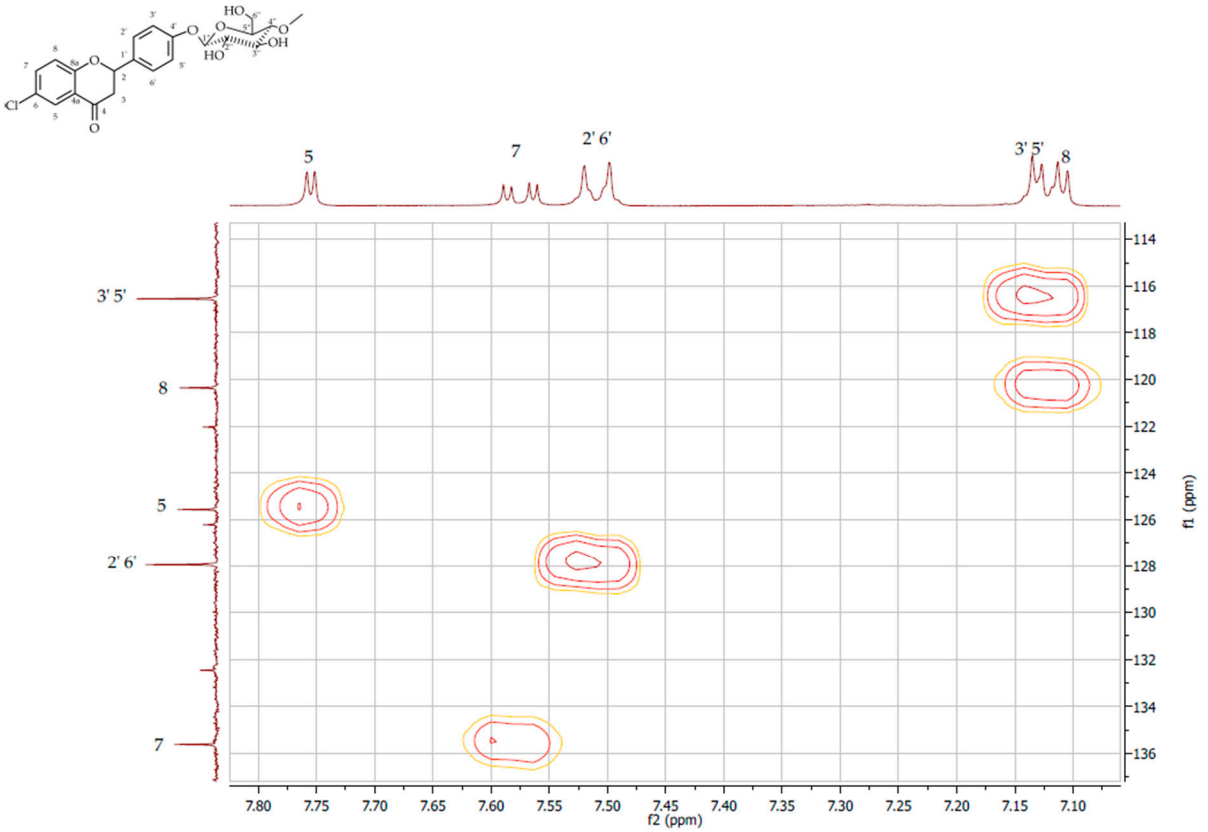


Figure S134. HMQC contour map – ^{1}H x ^{13}C expansion of 6-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

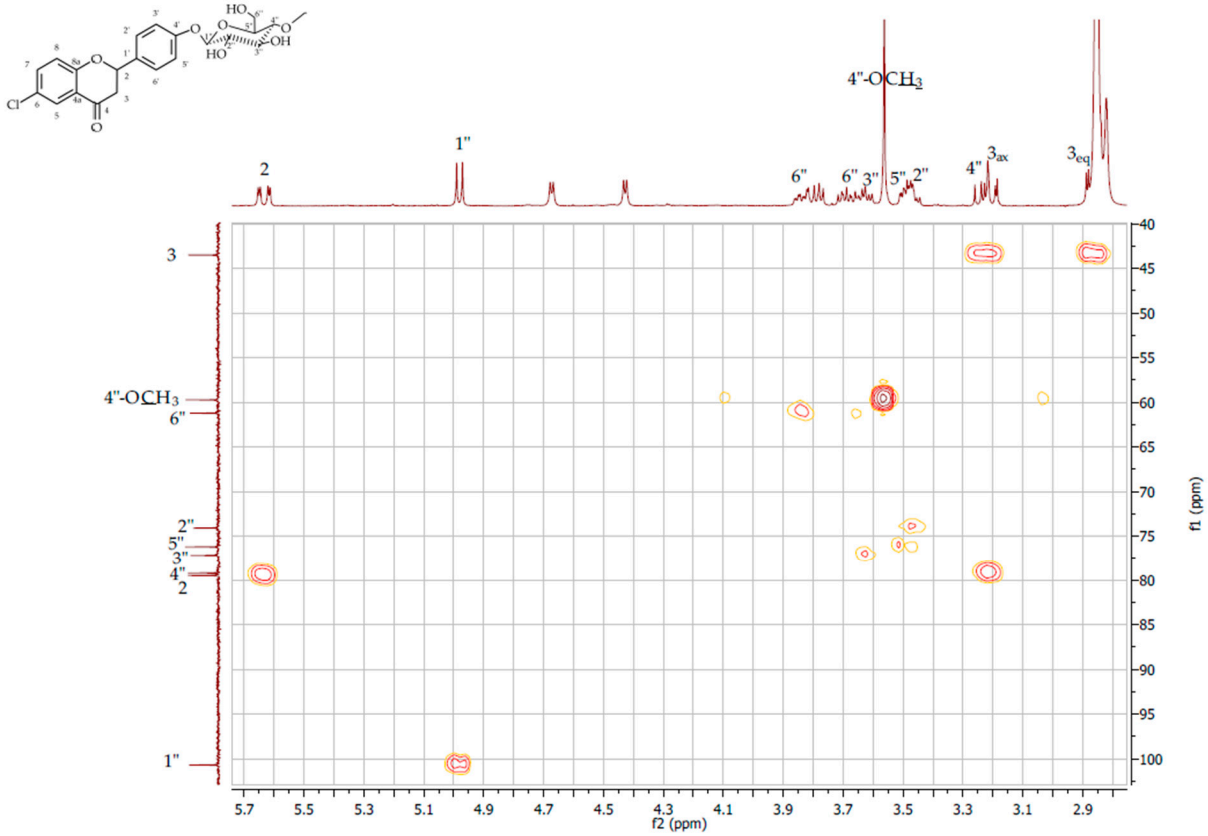


Figure S135. HMQC contour map – ^{1}H x ^{13}C expansion of 6-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

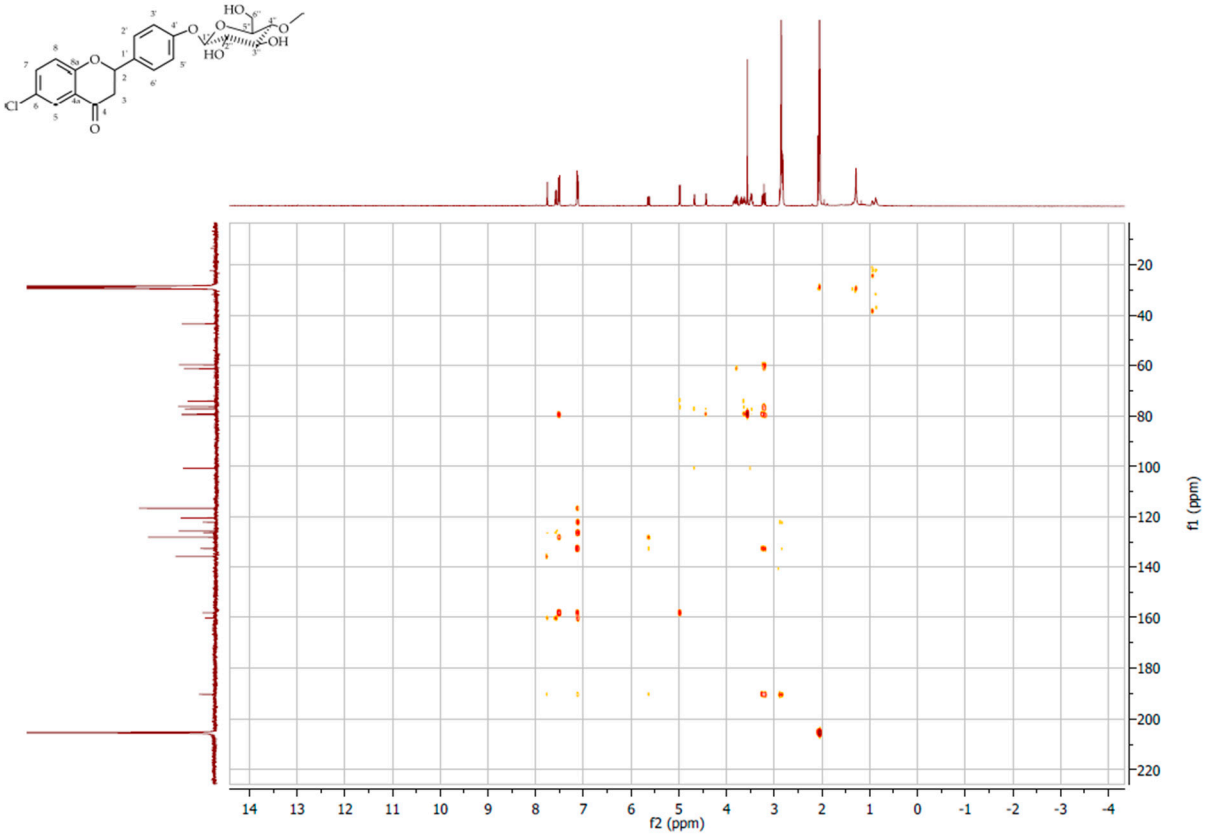


Figure S136. HMBC contour map – ^{1}H x ^{13}C of 6-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

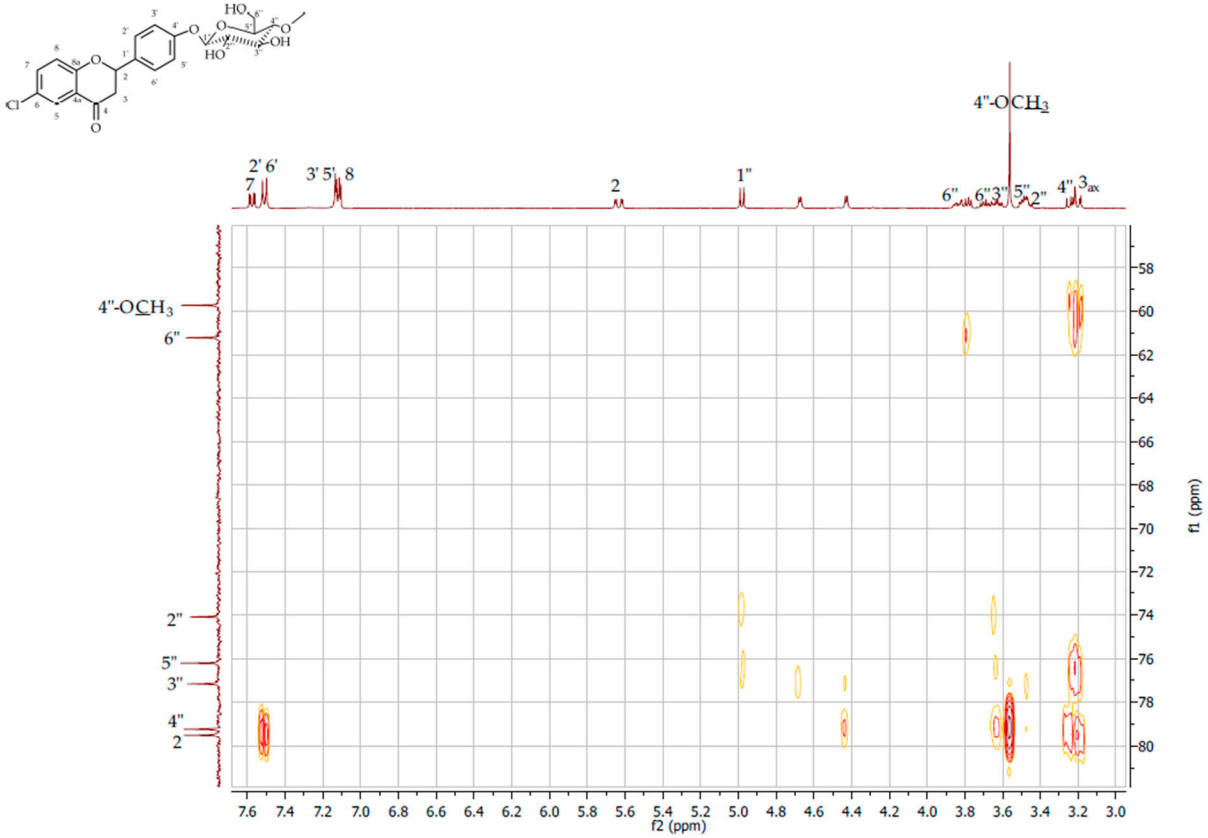


Figure S137. HMBC contour map – ^{1}H x ^{13}C expansion of 6-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

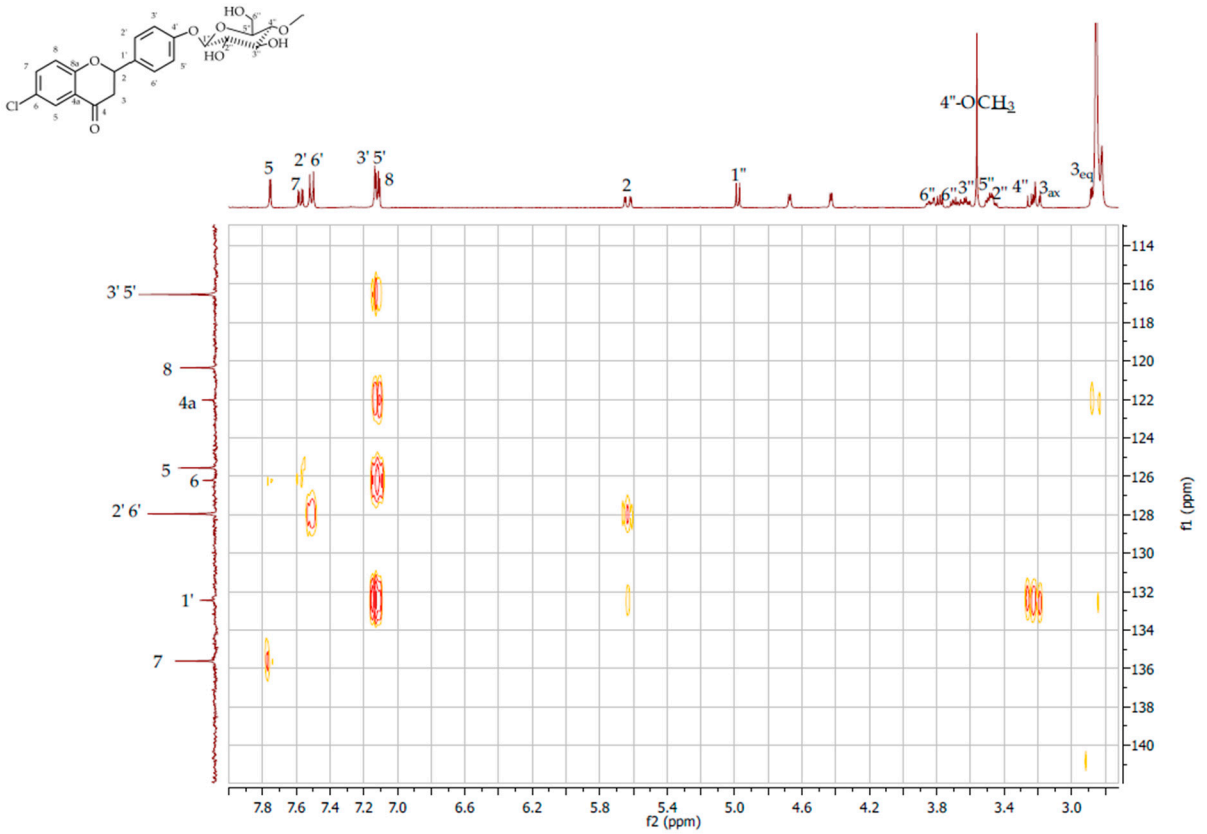


Figure S138. HMBC contour map – ^{1}H x ^{13}C expansion of 6-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

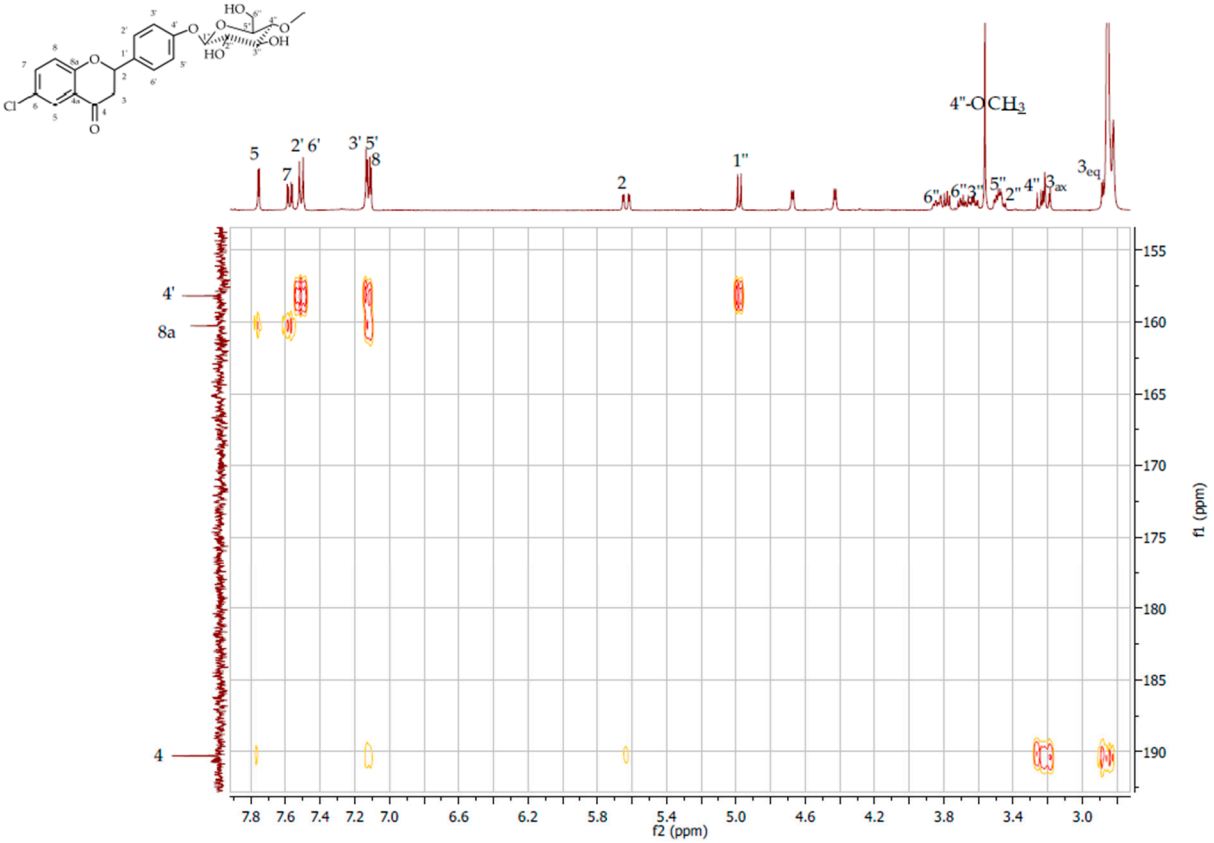


Figure S139. HMBC contour map – ^{1}H x ^{13}C expansion of 6-chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**4a**).

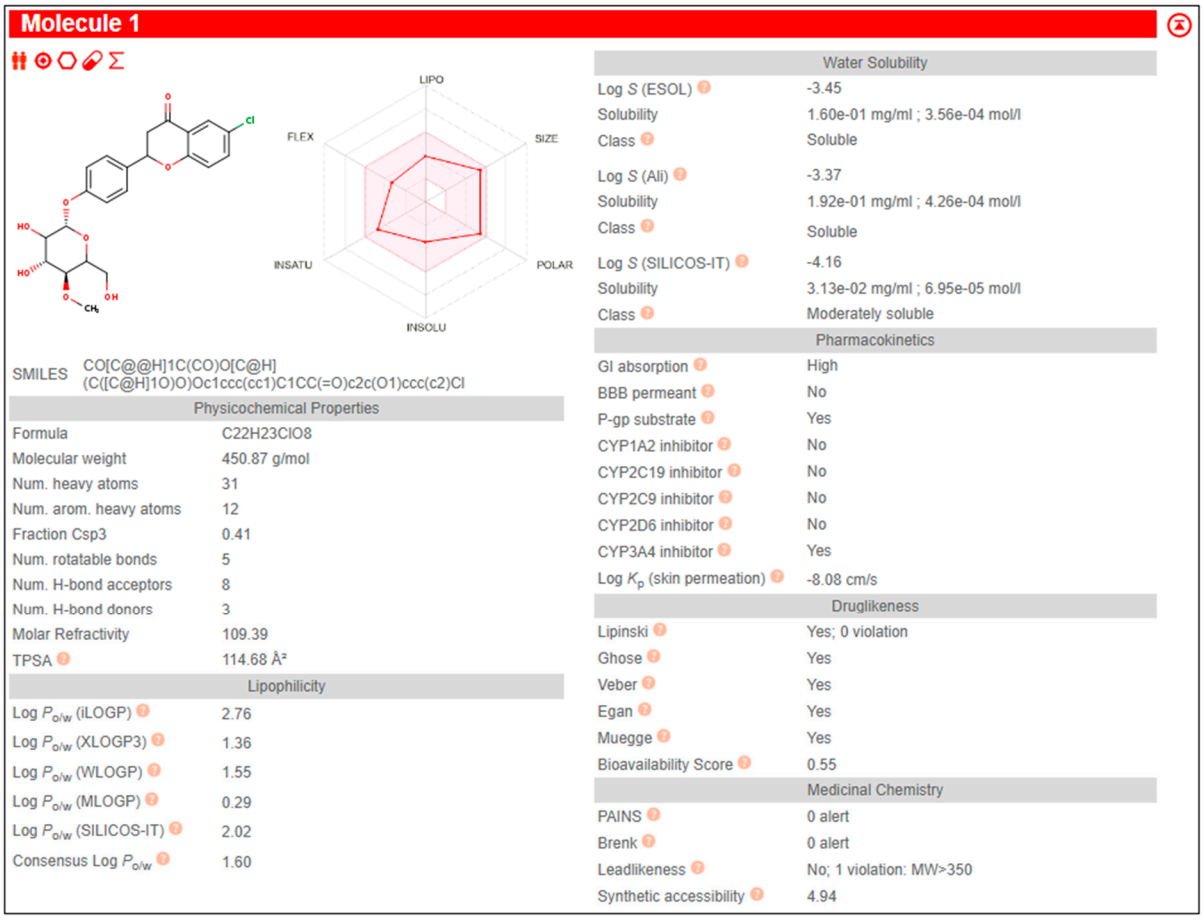


Figure S140. 6-Chloroflavanone 4′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**4a**) physicochemical and ADME parameters prediction using the SwissADME modelling.

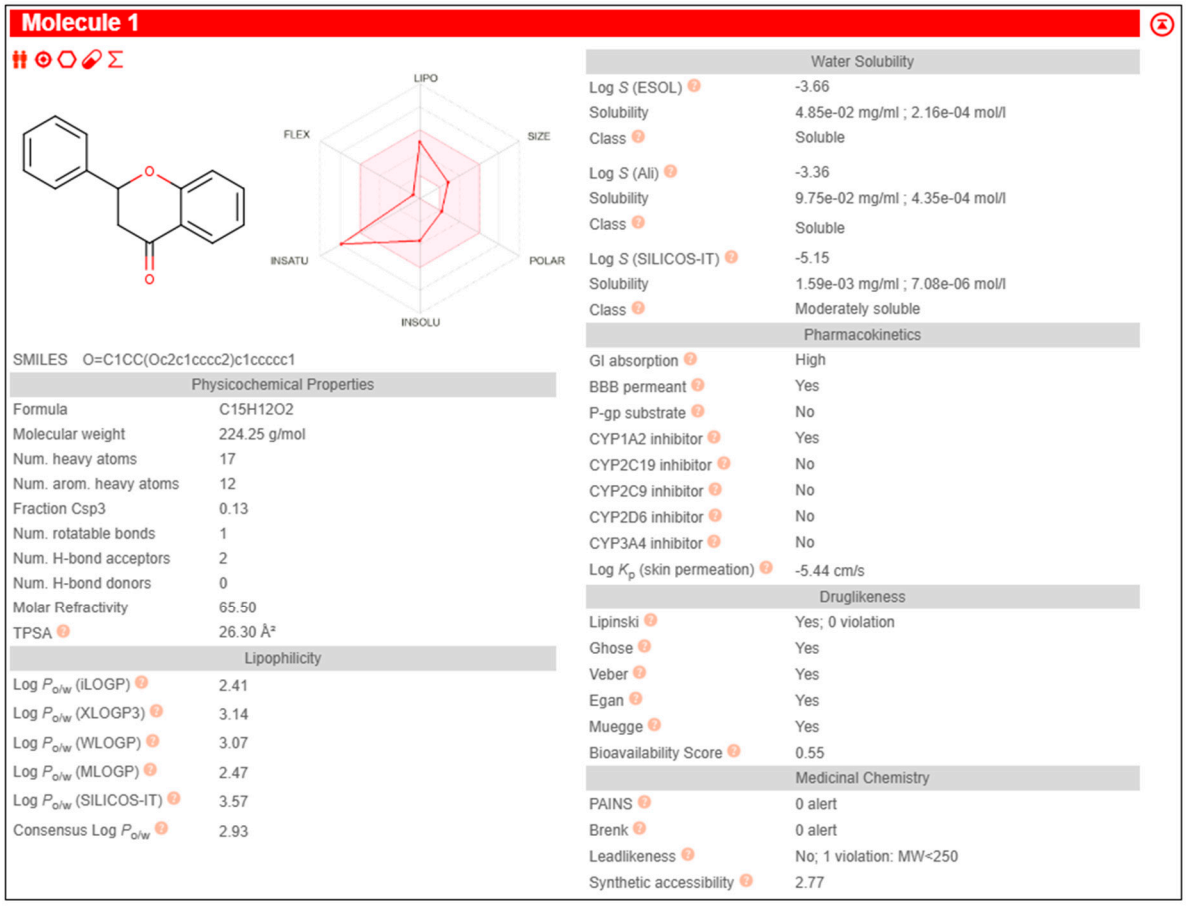


Figure S141. Flavanone (**5**) physicochemical and ADME parameters prediction using the SwissADME modelling.