Antimicrobial Activity of Chalcones with a Chlorine Atom and Their Glycosides

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Figure S135. 2′-Hydroxychalcone (**7**) physicochemical and ADME parameters prediction using the SwissADME modelling

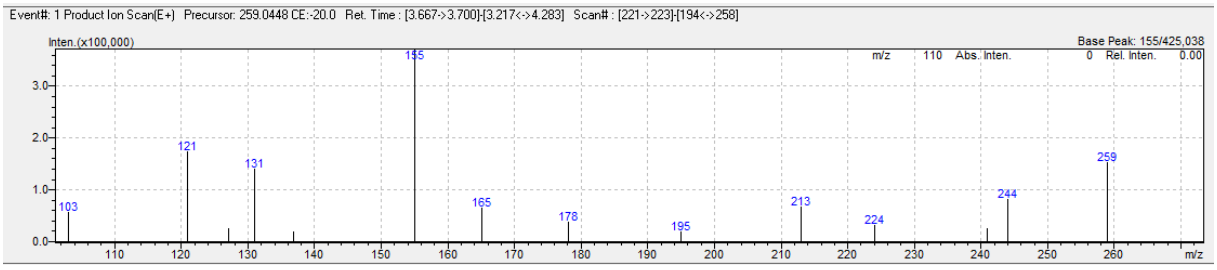


Figure S1. MS analysis of 4-chloro-2′-hydroxychalcone (**3**)

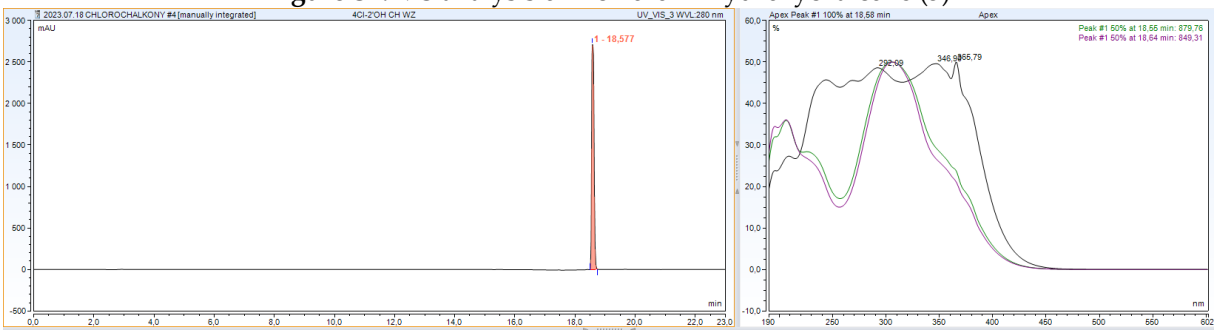


Figure S2. HPLC analysis of 4-chloro-2′-hydroxychalcone (**3**)

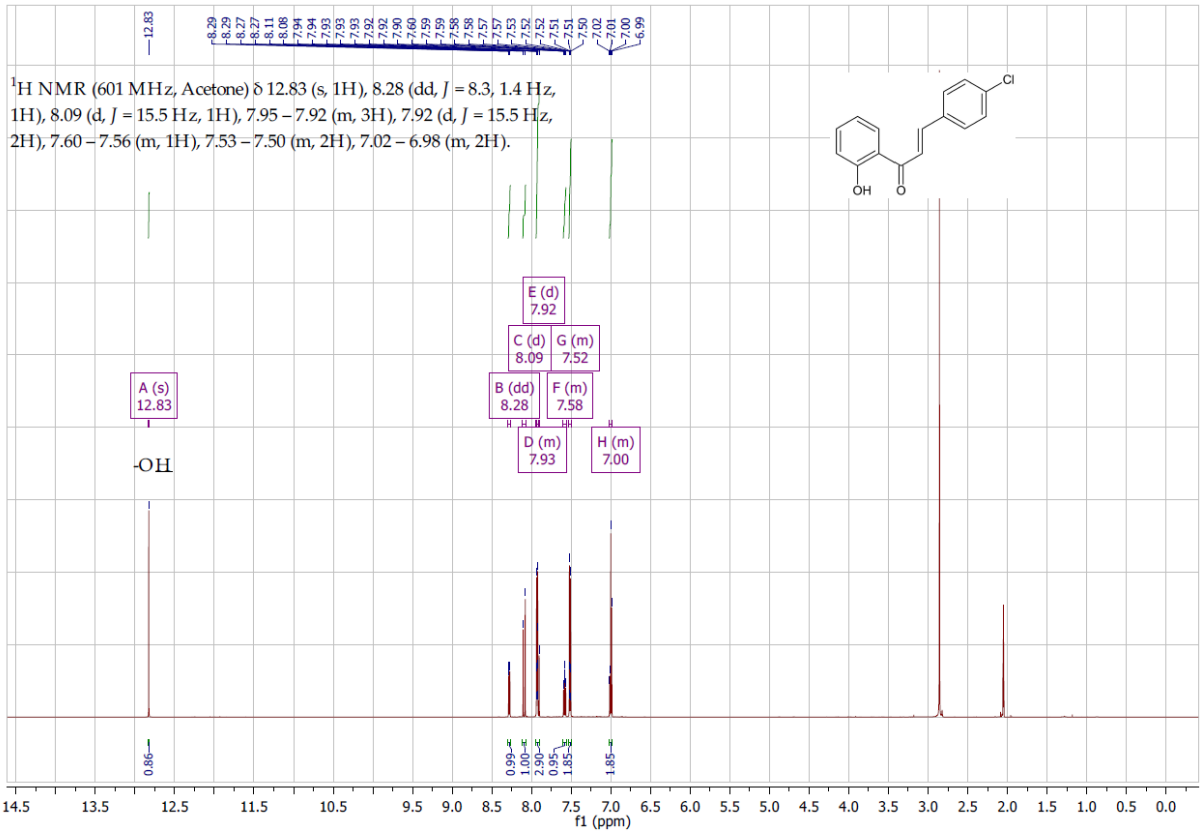


Figure S3. ^{1}H NMR spectrum (δ, acetone-d6, 600 MHz) of 4-chloro-2′-hydroxychalcone (**3**)

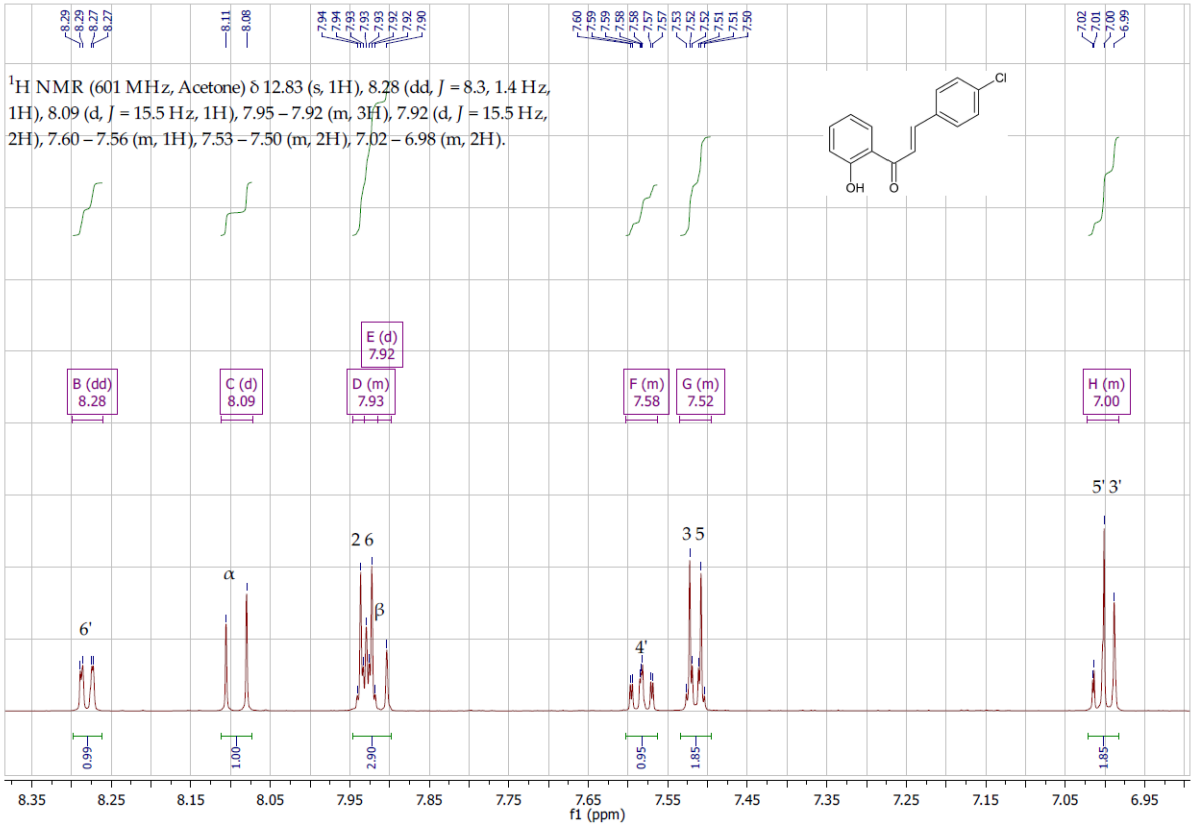


Figure S4 [1]H NMR spectrum expansion (*δ*, acetone-d6, 600 MHz) of 4-chloro-2′-hydroxychalcone (**3**)

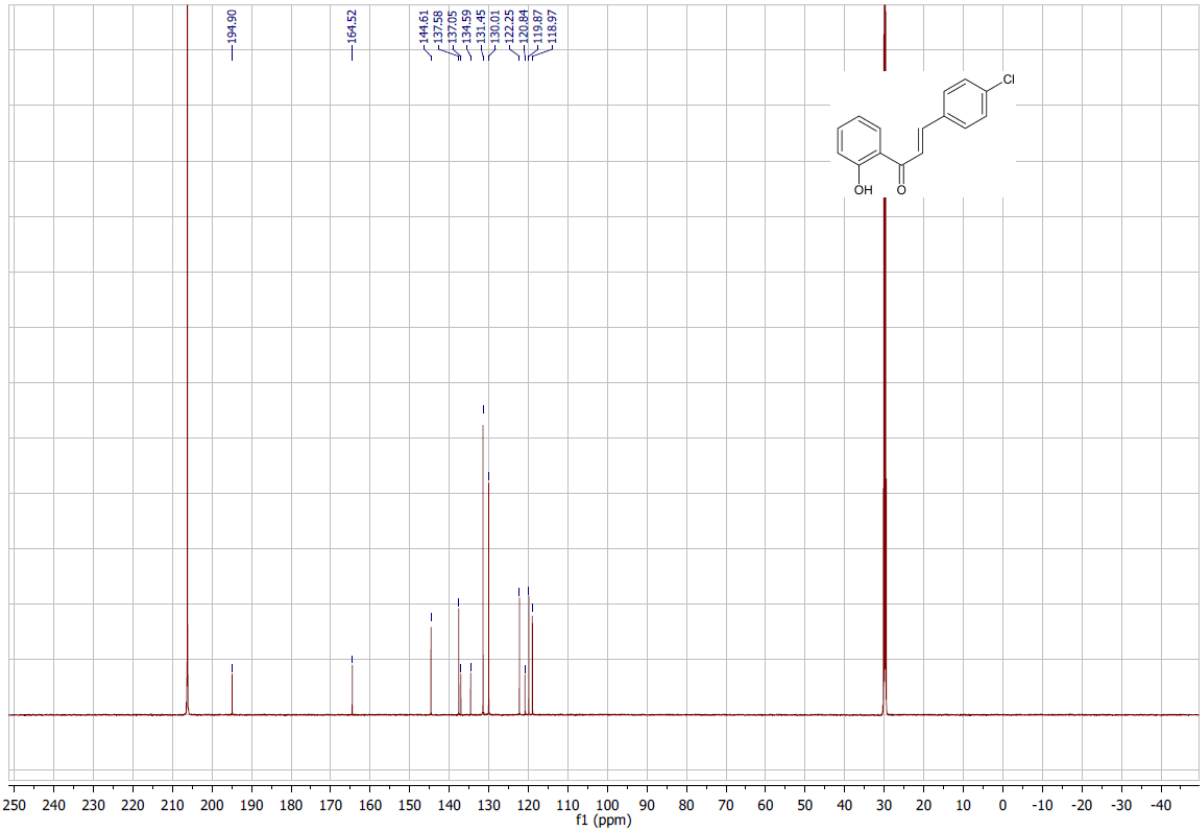


Figure S5. [13]C NMR spectrum (*δ*, acetone-d6, 151 MHz) of 4-chloro-2′-hydroxychalcone (**3**)

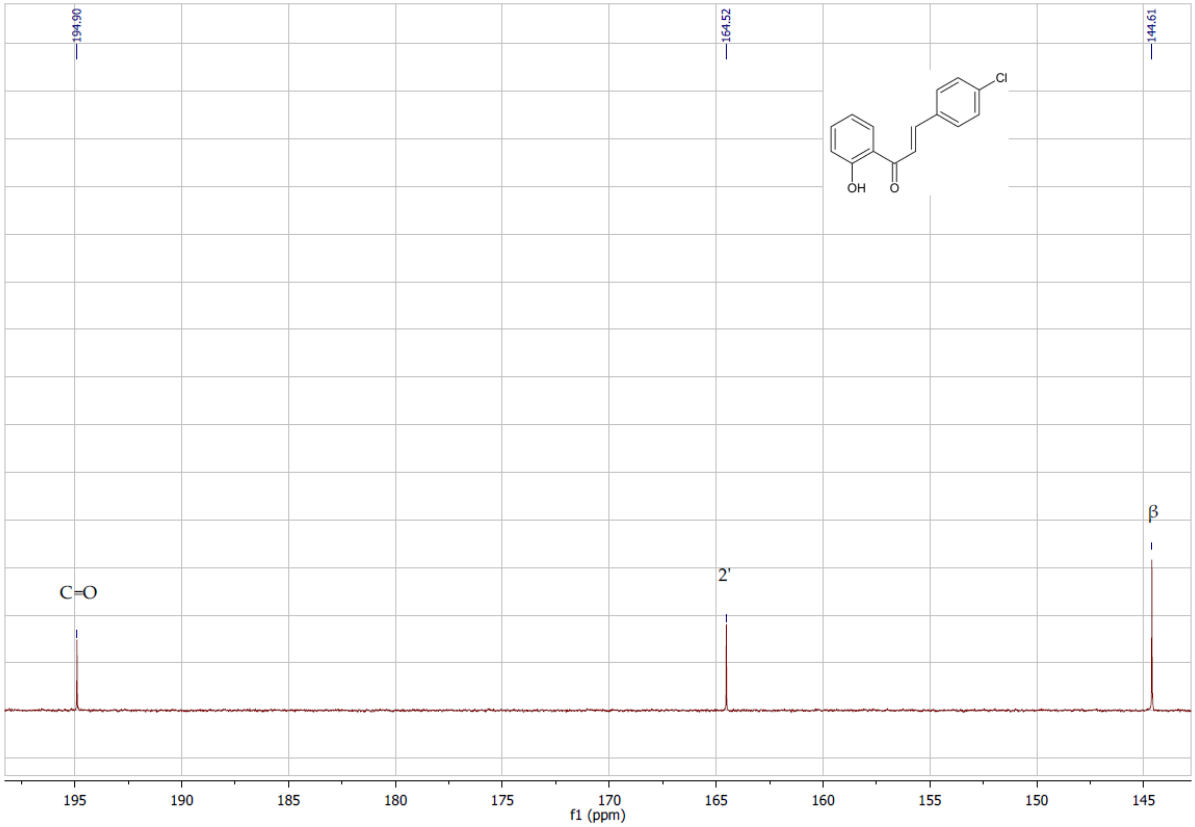


Figure S6. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 4-chloro-2′-hydroxychalcone (**3**)

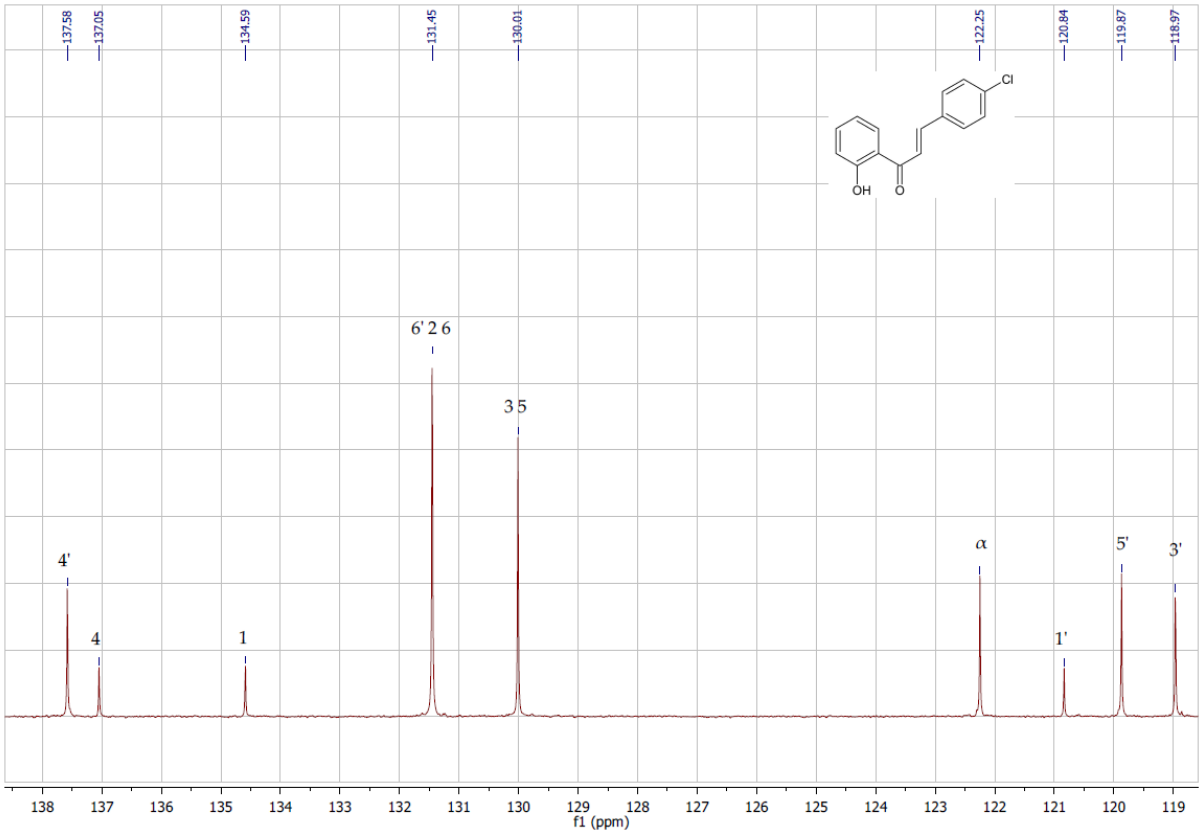


Figure S7. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 4-chloro-2′-hydroxychalcone (**3**)

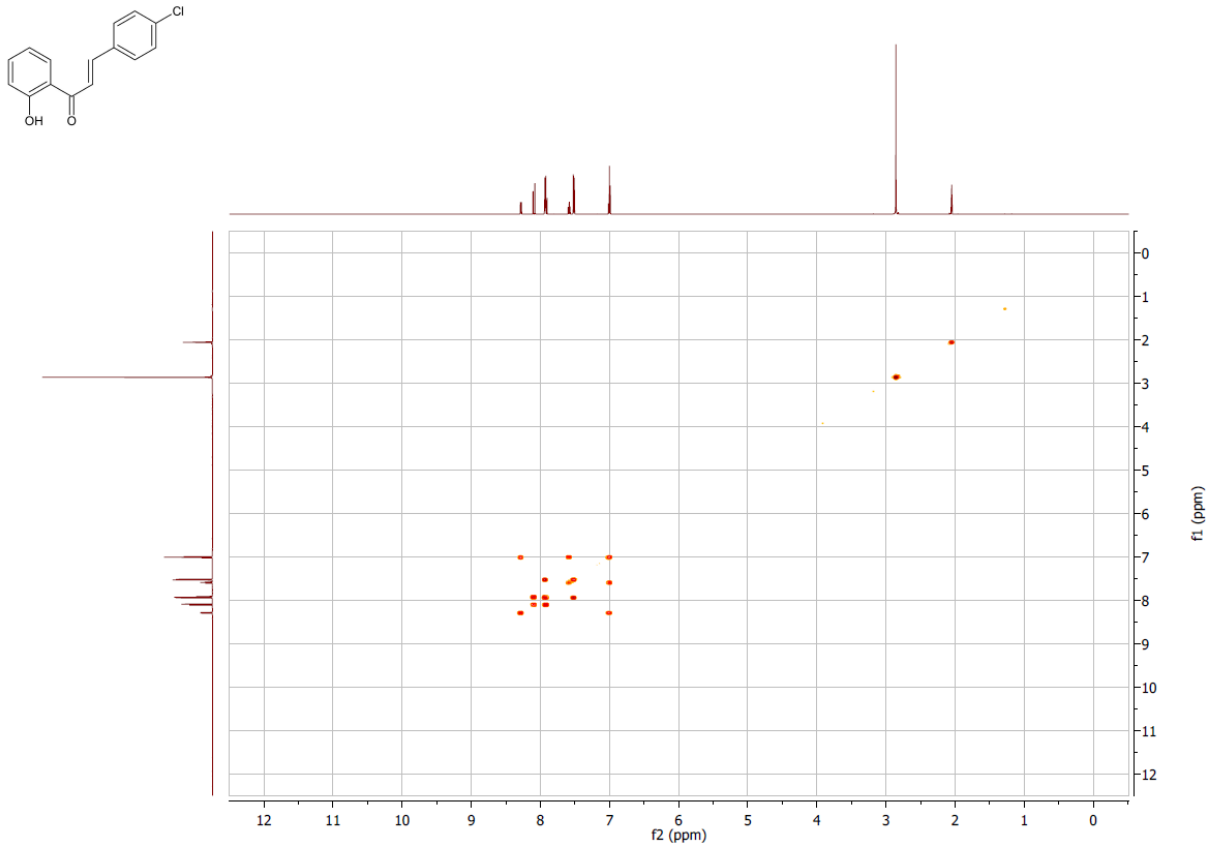


Figure S8. COSY contour map – ^{1}H x ^{1}H of 4-chloro-2′-hydroxychalcone (**3**)

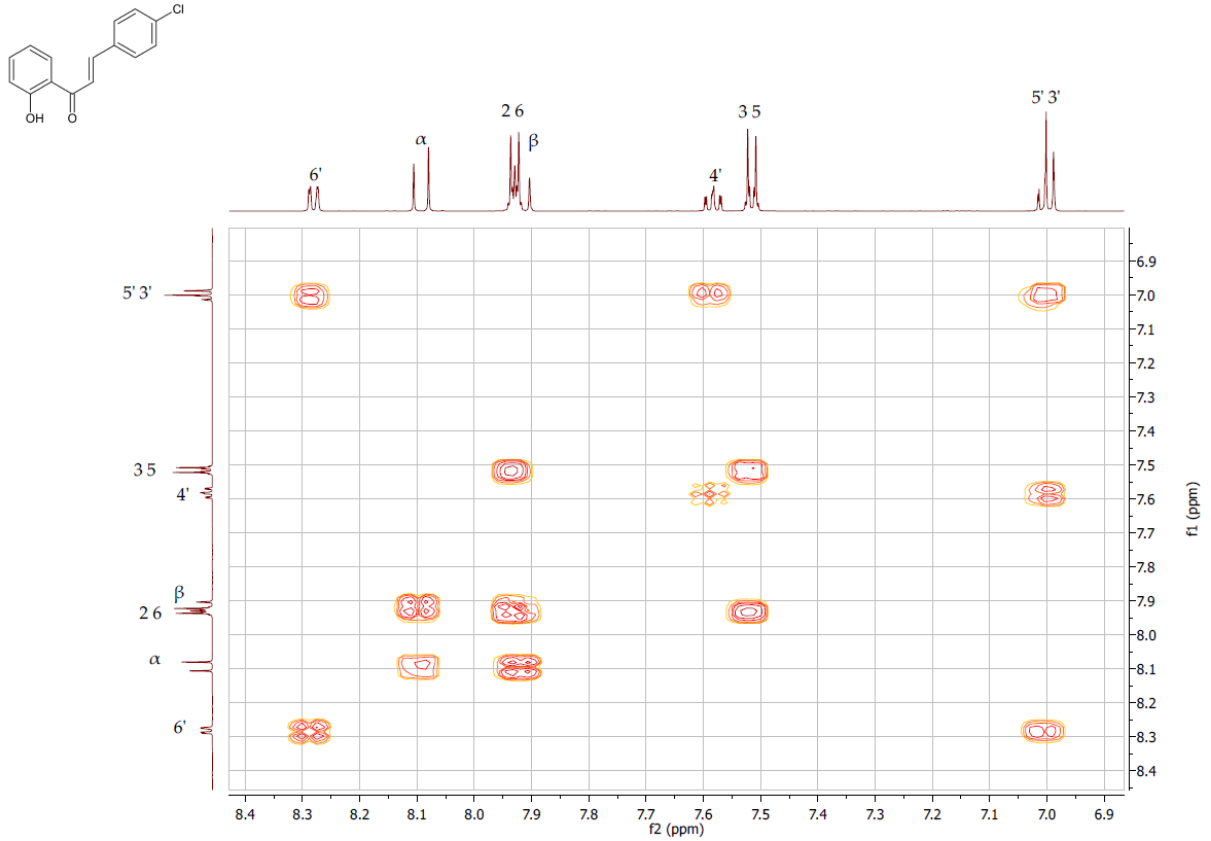


Figure S9. COSY contour map – ^{1}H x ^{1}H expansion of 4-chloro-2′-hydroxychalcone (**3**)

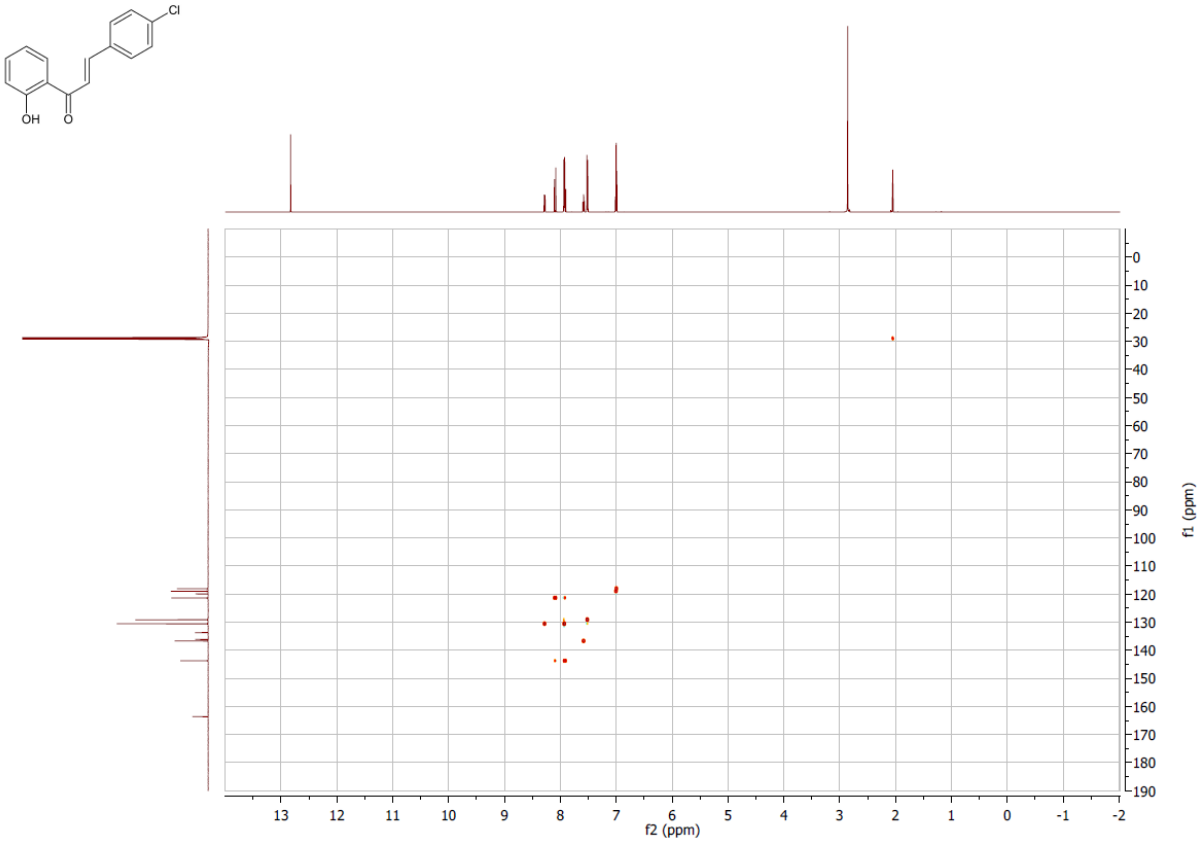


Figure S10. HMQC contour map – ^{1}H x ^{13}C of 4-chloro-2′-hydroxychalcone (**3**)

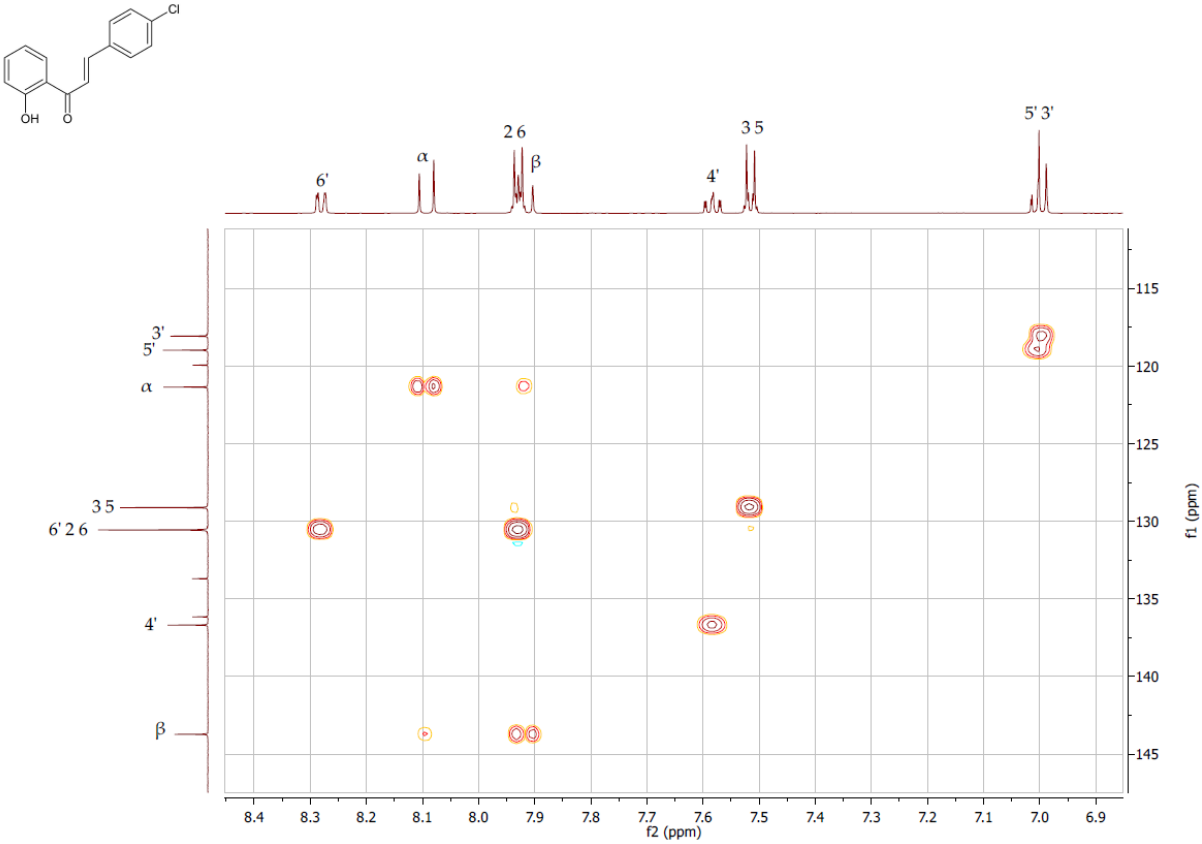


Figure S11. HMQC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxychalcone (**3**)

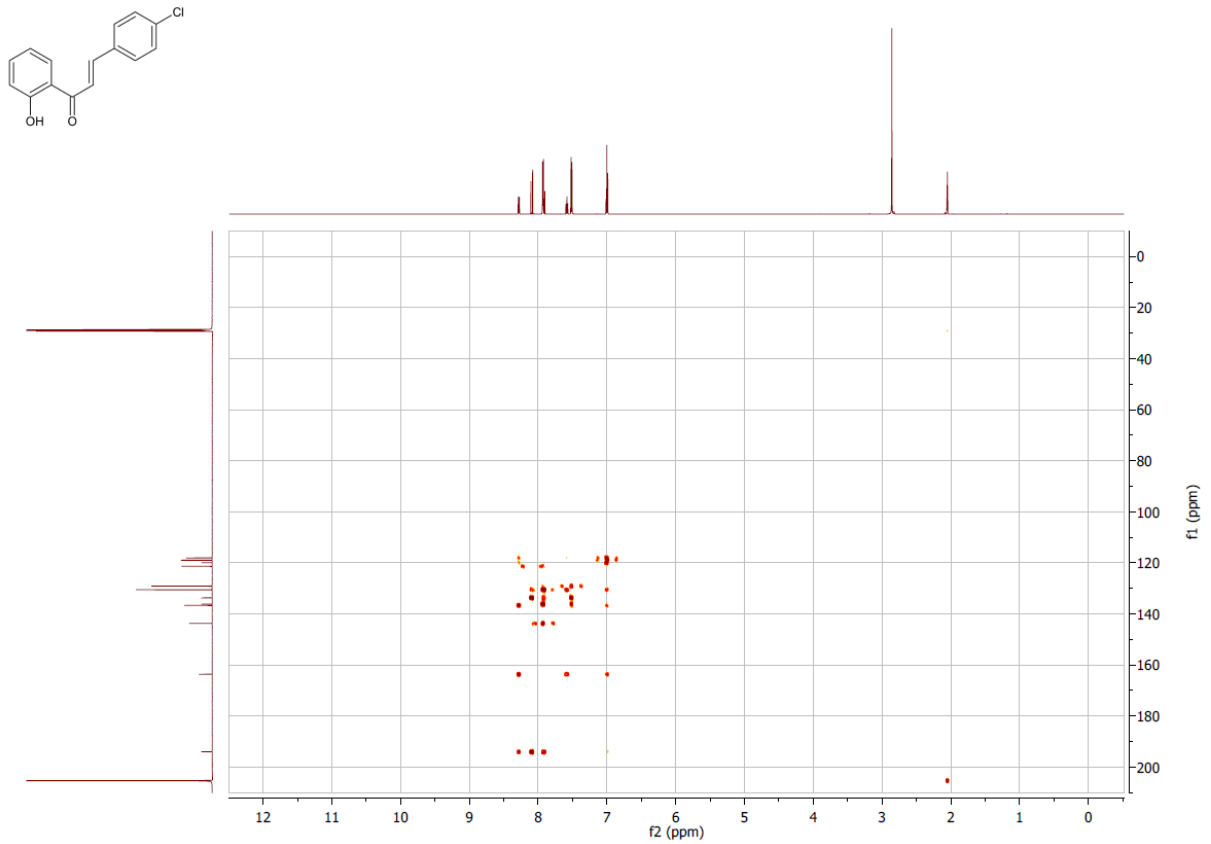


Figure S12. HMBC contour map – ^{1}H x ^{13}C of 4-chloro-2′-hydroxychalcone (**3**)

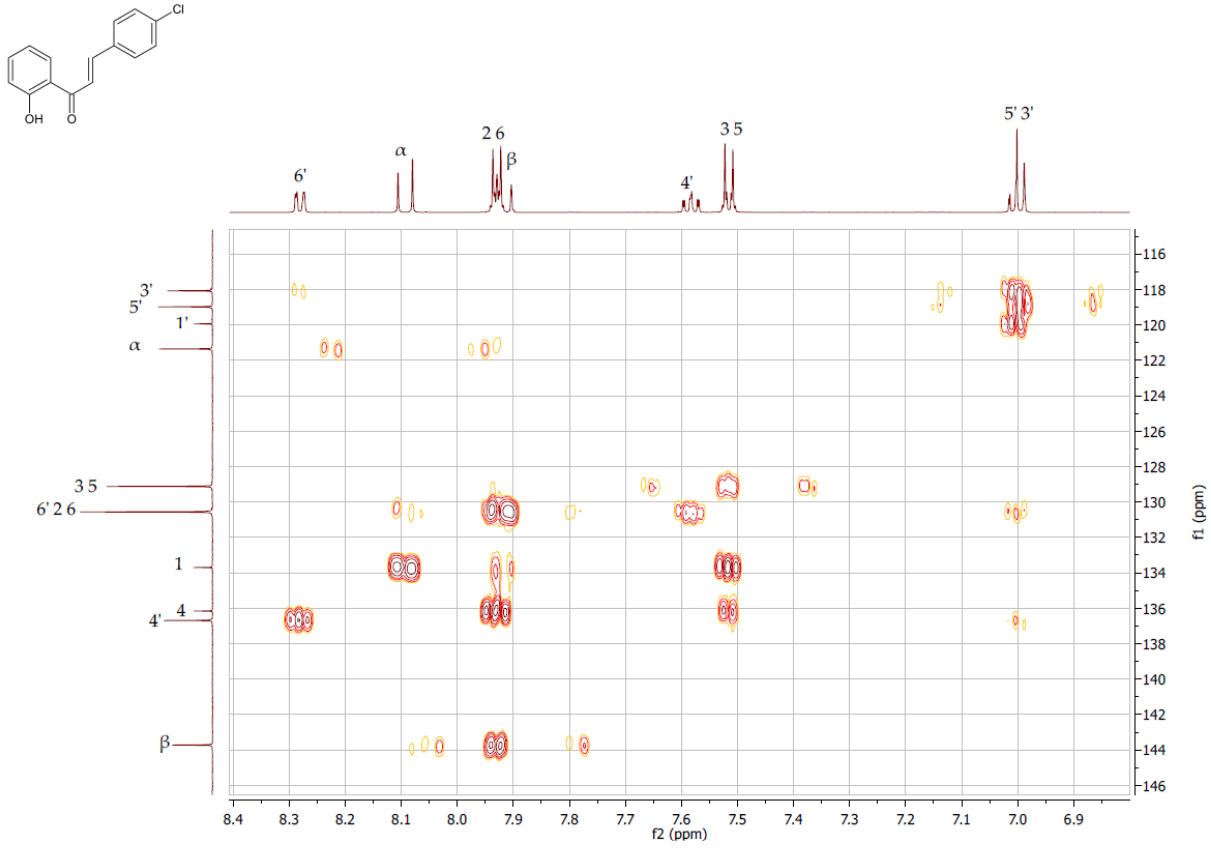


Figure S13. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxychalcone (**3**)

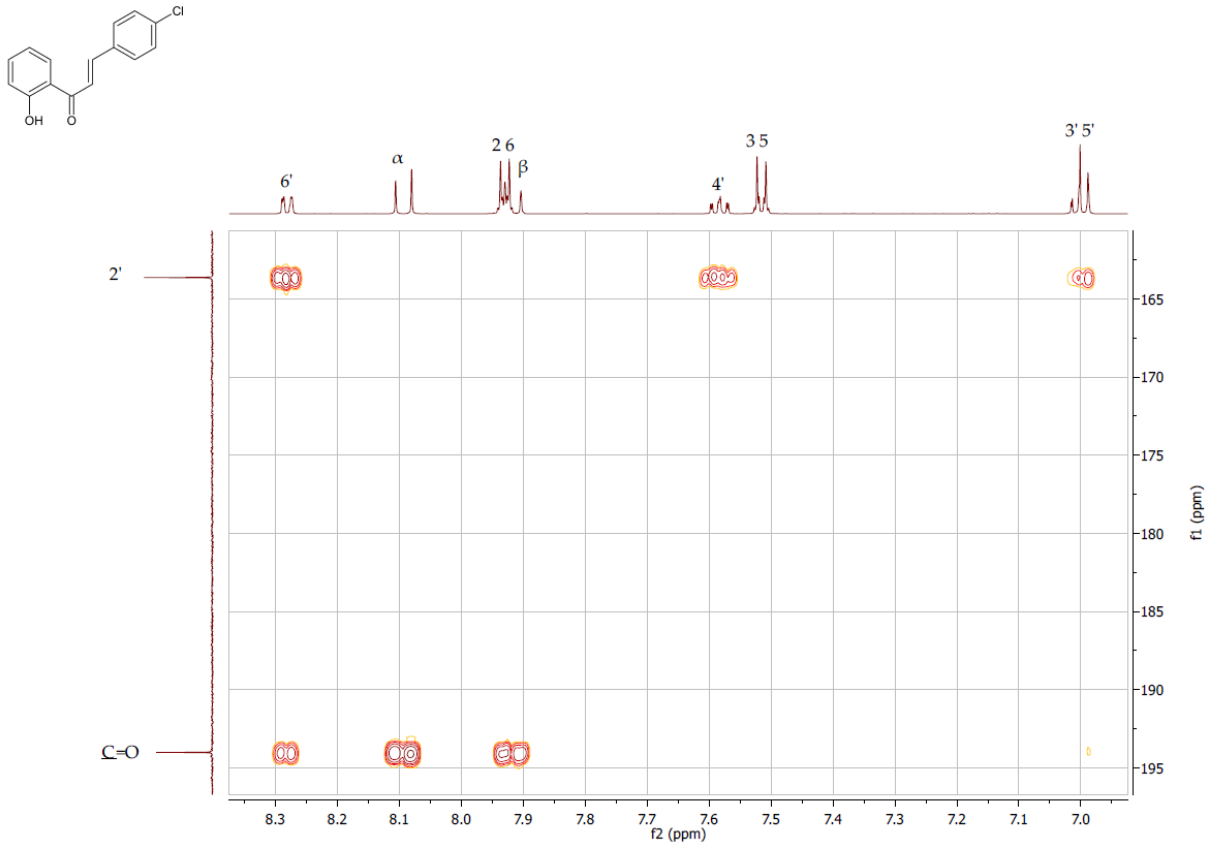
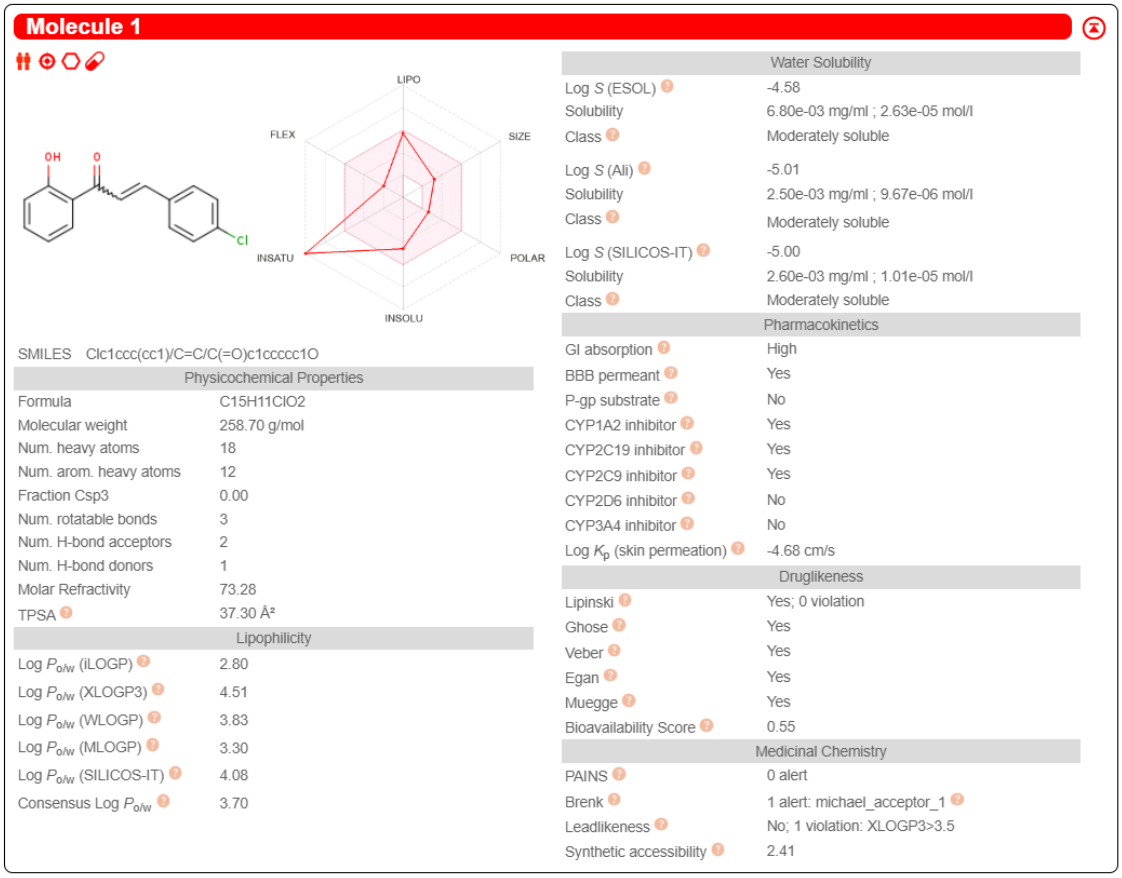


Figure S14. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxychalcone (**3**)



Molecule 1

SMILES Clc1ccc(cc1)/C=C/C(=O)c1ccccc1O

Physicochemical Properties	
Formula	C15H11ClO2
Molecular weight	258.70 g/mol
Num. heavy atoms	18
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	3
Num. H-bond acceptors	2
Num. H-bond donors	1
Molar Refractivity	73.28
TPSA	37.30 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.80
Log $P_{o/w}$ (XLOGP3)	4.51
Log $P_{o/w}$ (WLOGP)	3.83
Log $P_{o/w}$ (MLOGP)	3.30
Log $P_{o/w}$ (SILICOS-IT)	4.08
Consensus Log $P_{o/w}$	3.70

Water Solubility	
Log *S* (ESOL)	-4.58
Solubility	6.80e-03 mg/ml ; 2.63e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-5.01
Solubility	2.50e-03 mg/ml ; 9.67e-06 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-5.00
Solubility	2.60e-03 mg/ml ; 1.01e-05 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)	-4.68 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	1 alert: michael_acceptor_1
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.41

Figure S15. 4-Chloro-2′-hydroxychalcone (**3**) physicochemical and ADME parameters prediction using the SwissADME modelling

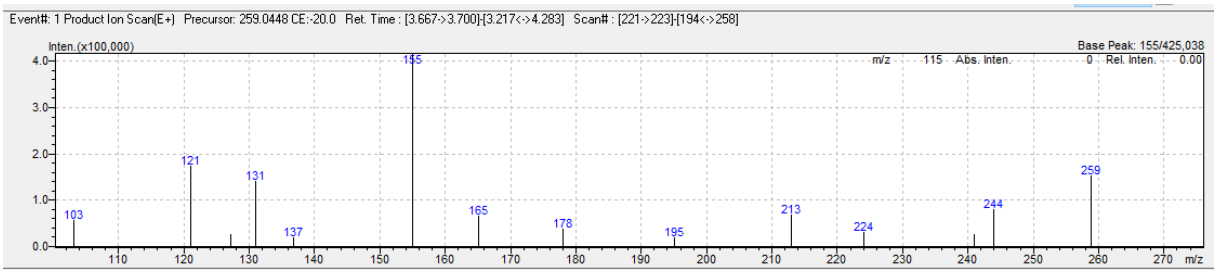


Figure S16. MS analysis of 5′-chloro-2′-hydroxychalcone (**6**)

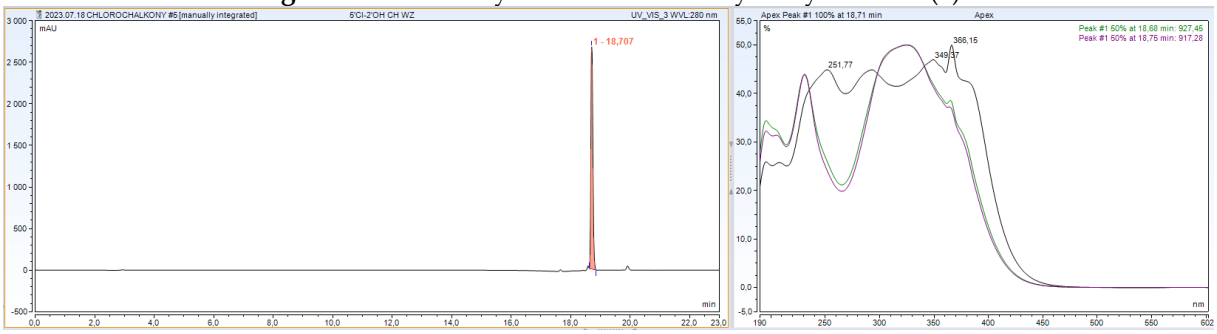


Figure S17. HPLC analysis of 5′-chloro-2′-hydroxychalcone (**6**)

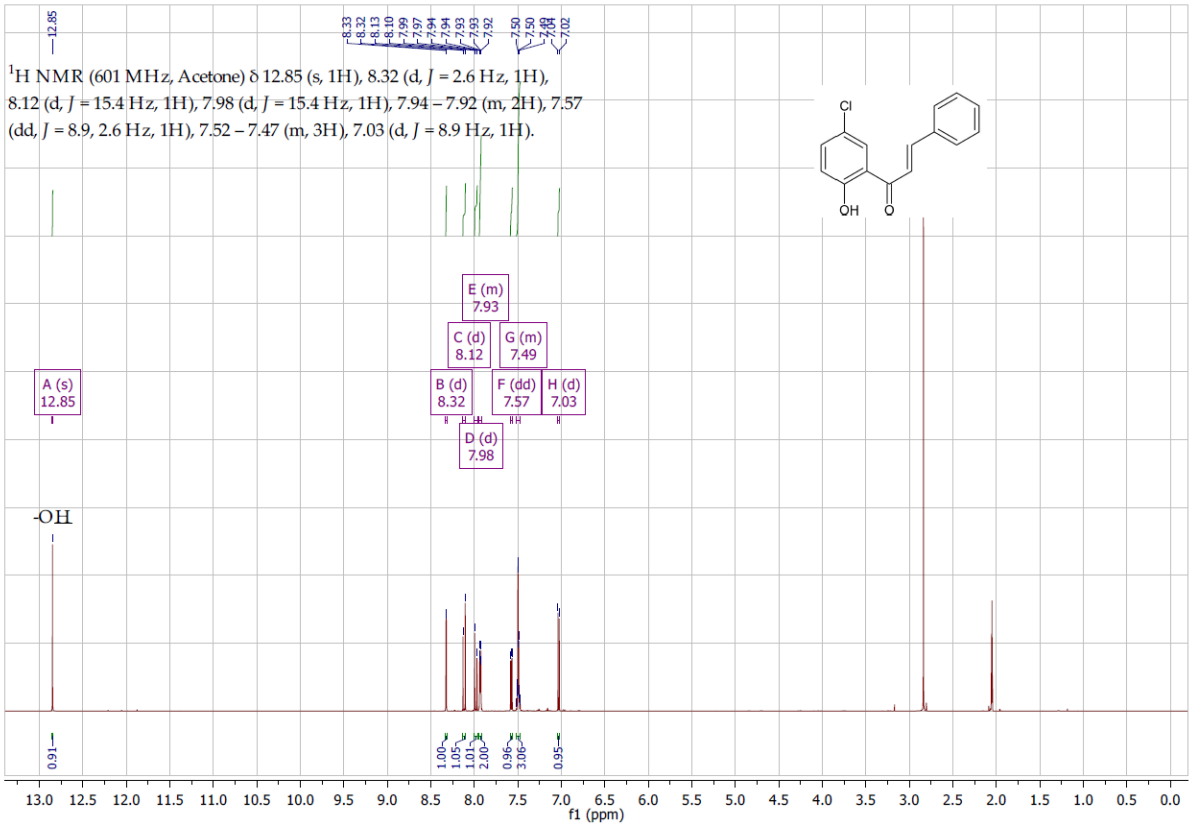


Figure S18. ¹H NMR spectrum (*δ*, acetone-d6, 600 MHz) of 5′-chloro-2′-hydroxychalcone (**6**)

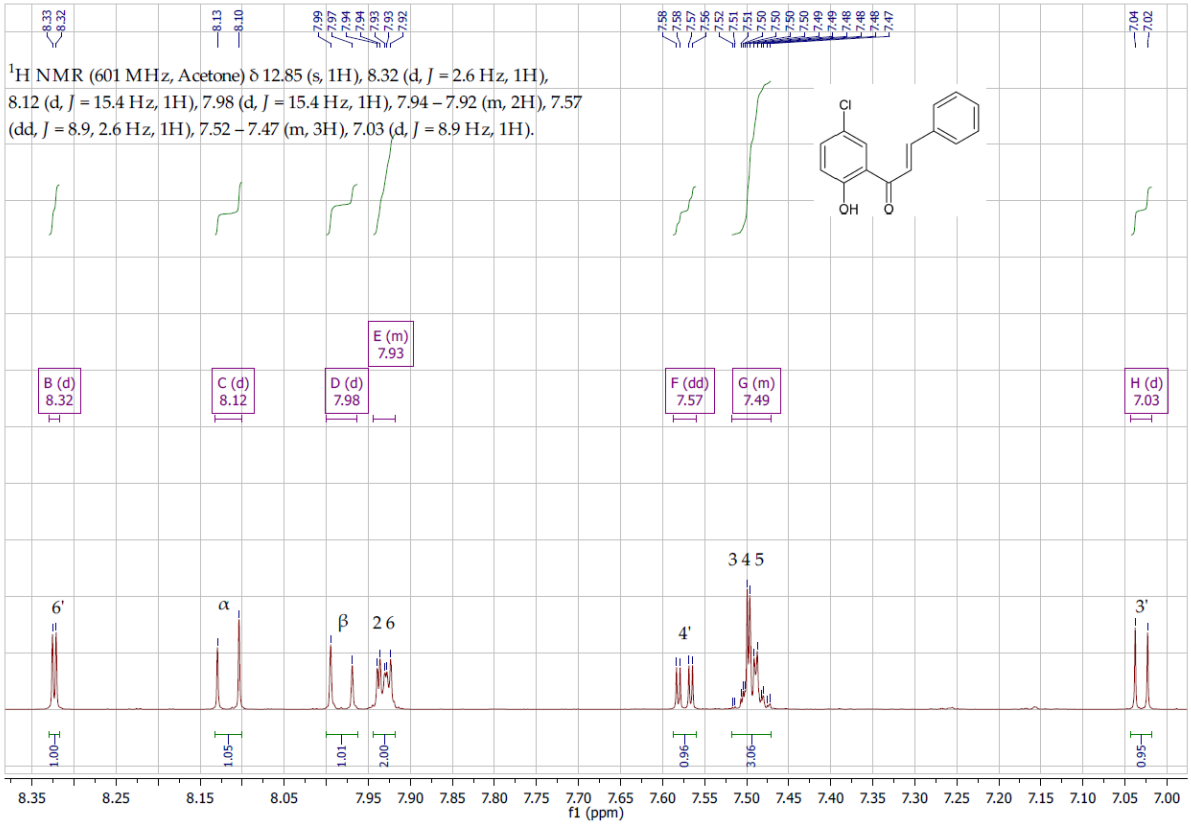


Figure S19. [1]H NMR spectrum expansion (*δ*, acetone-d6, 600 MHz) of 5′-chloro-2′-hydroxychalcone (**6**)

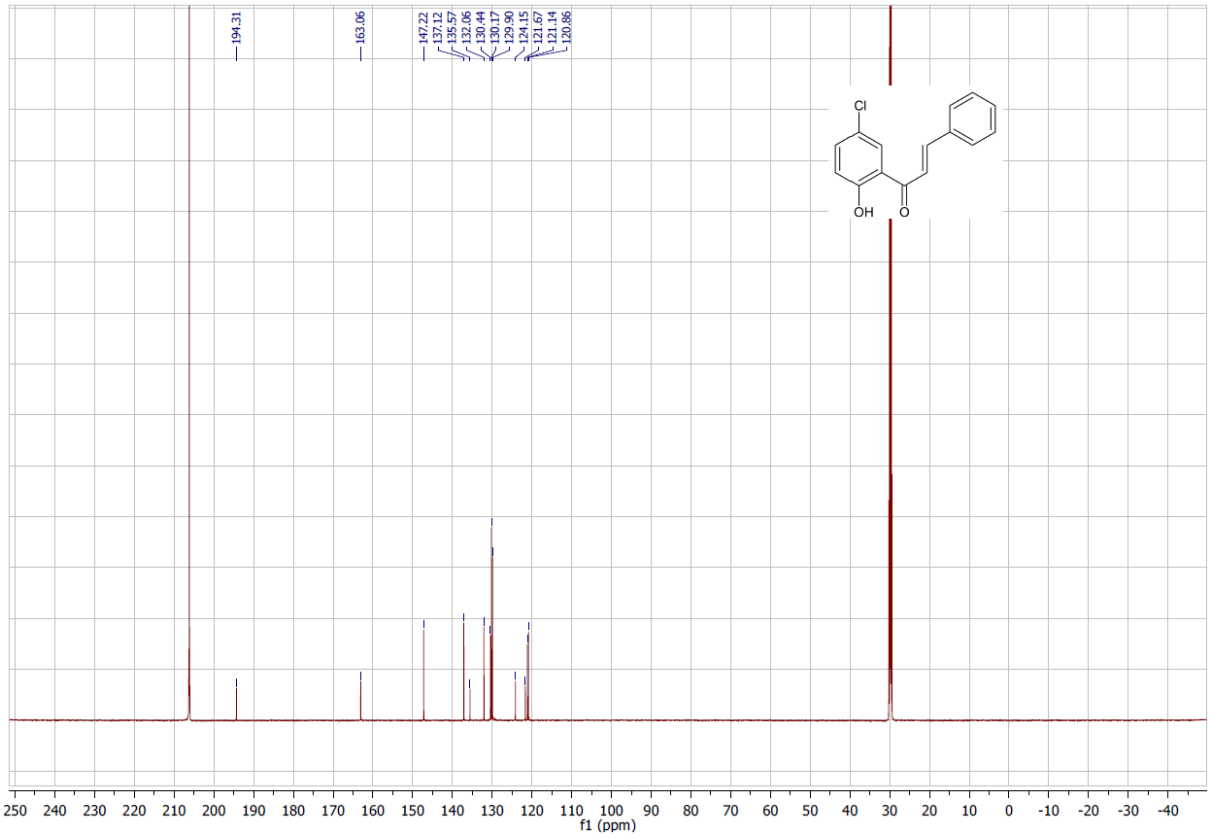


Figure S20. [13]C NMR spectrum (*δ*, acetone-d6, 151 MHz) of 5′-chloro-2′-hydroxychalcone (**6**)

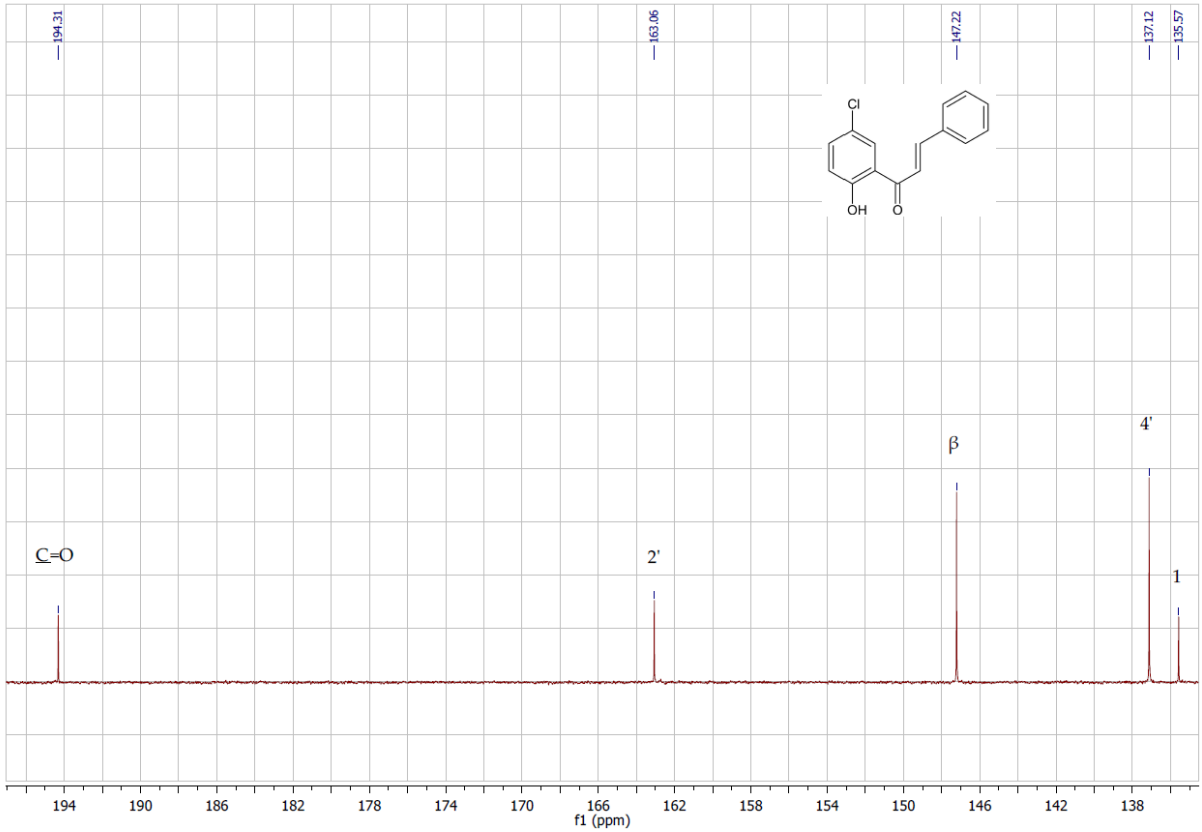


Figure S21. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 5′-chloro-2′-hydroxychalcone (**6**)

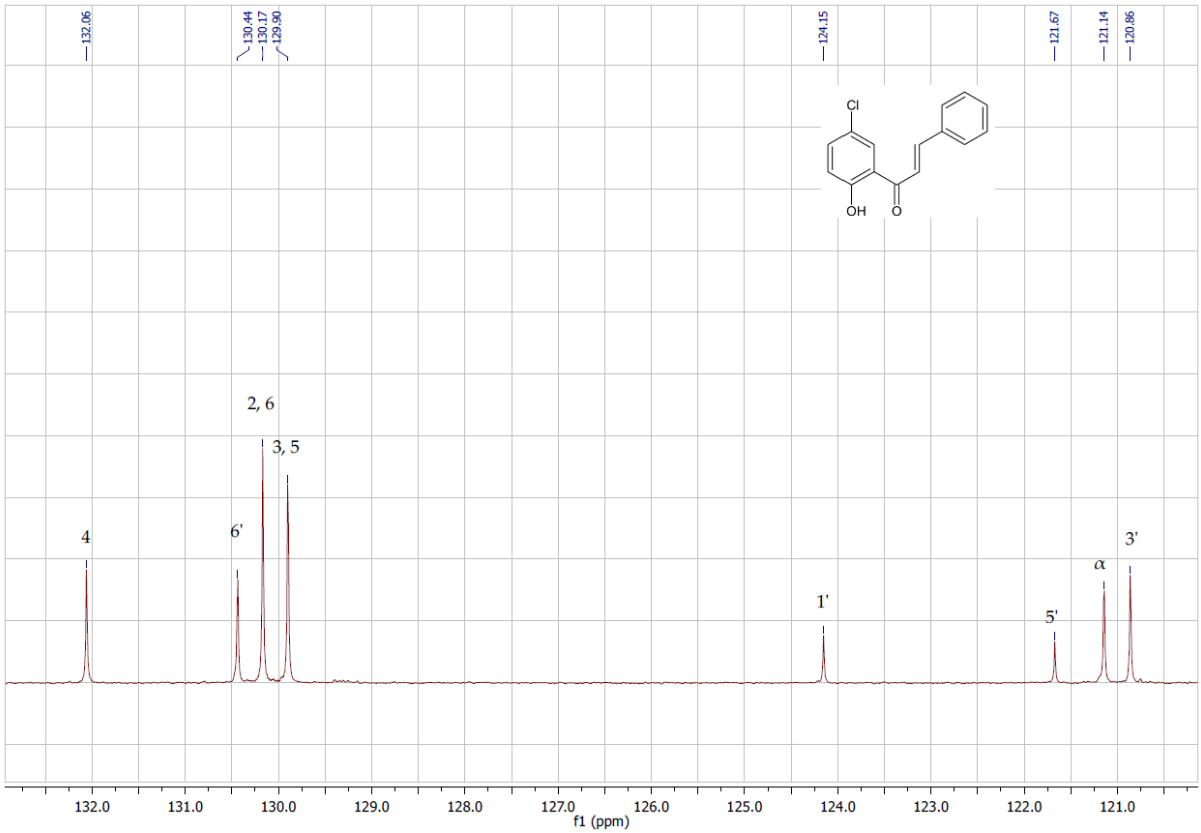


Figure S22. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 5′-chloro-2′-hydroxychalcone (**6**)

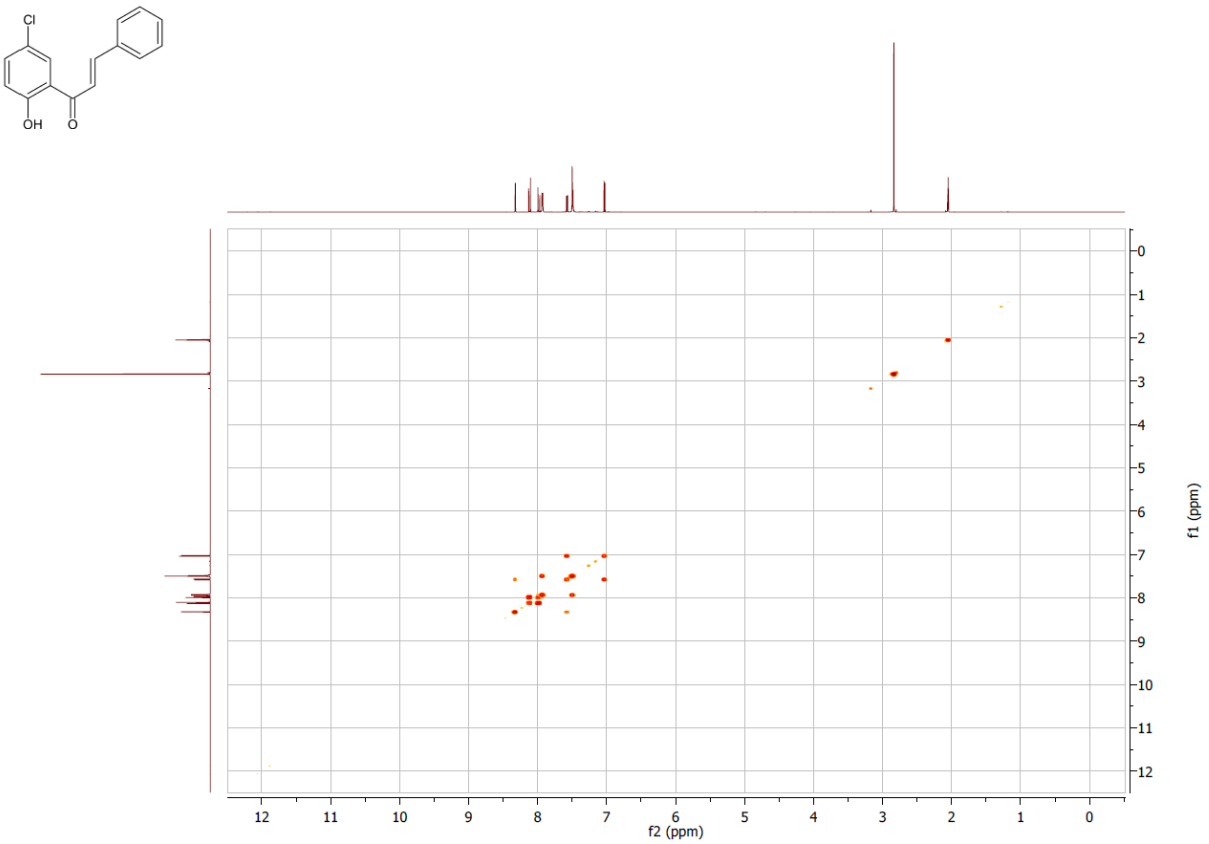


Figure S23. COSY contour map – ^{1}H x ^{1}H of 5′-chloro-2′-hydroxychalcone (**6**)

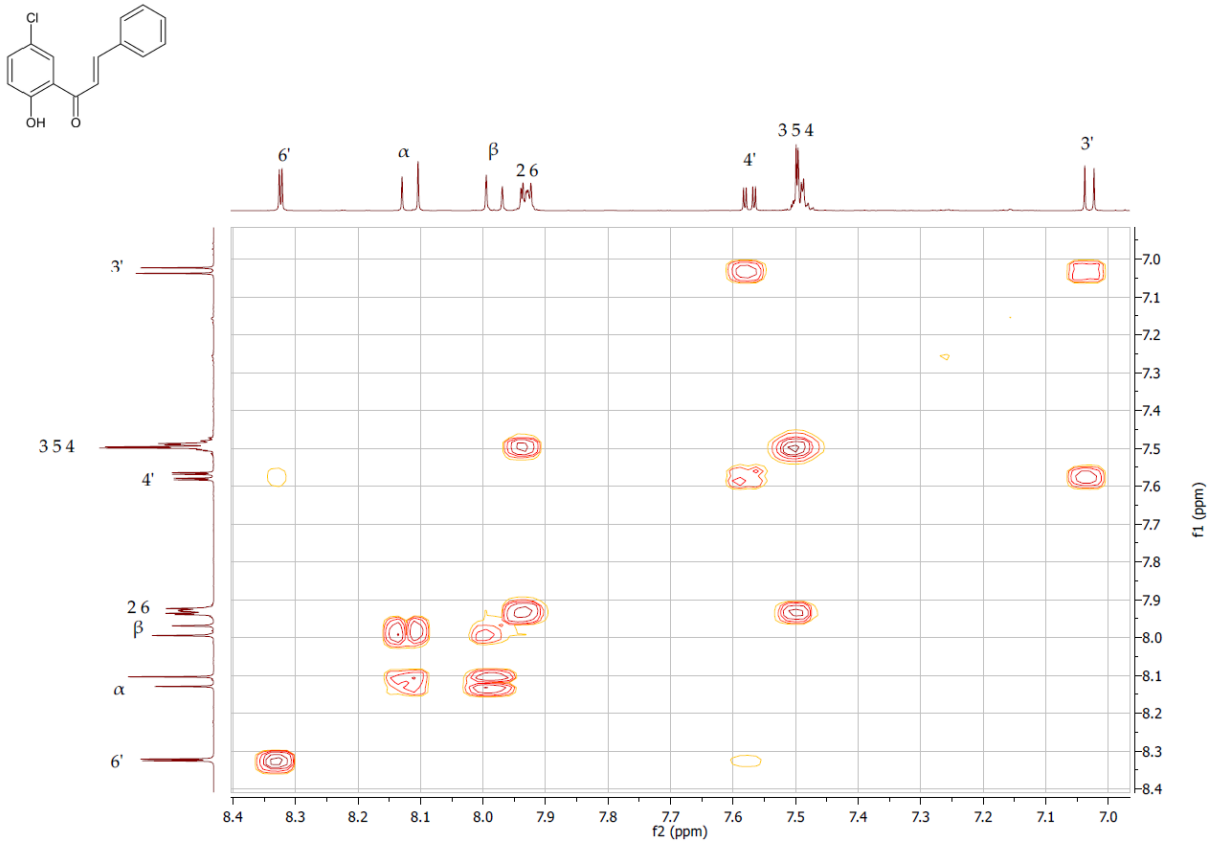


Figure S24. COSY contour map – ^{1}H x ^{1}H expansion of 5′-chloro-2′-hydroxychalcone (**6**)

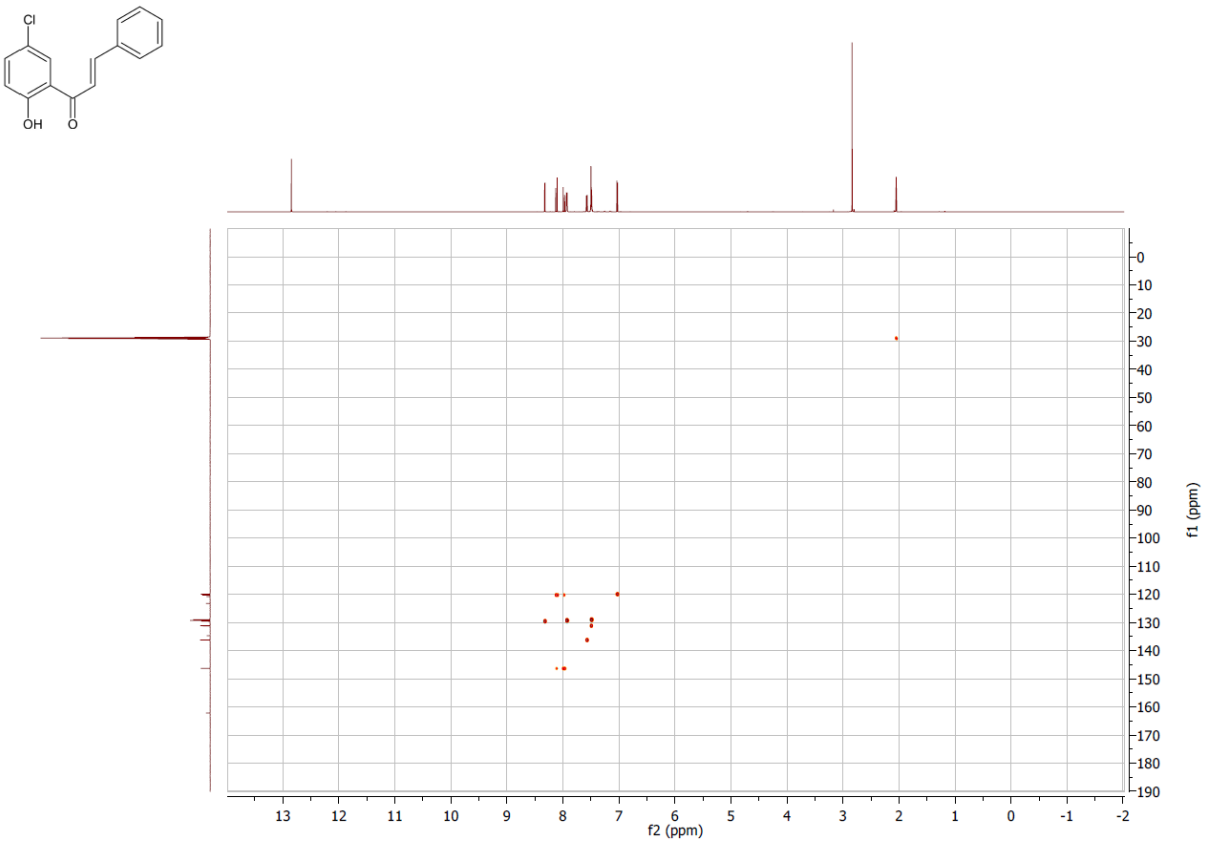


Figure S25. HMQC contour map – ^{1}H x ^{13}C of 5′-chloro-2′-hydroxychalcone (**6**)

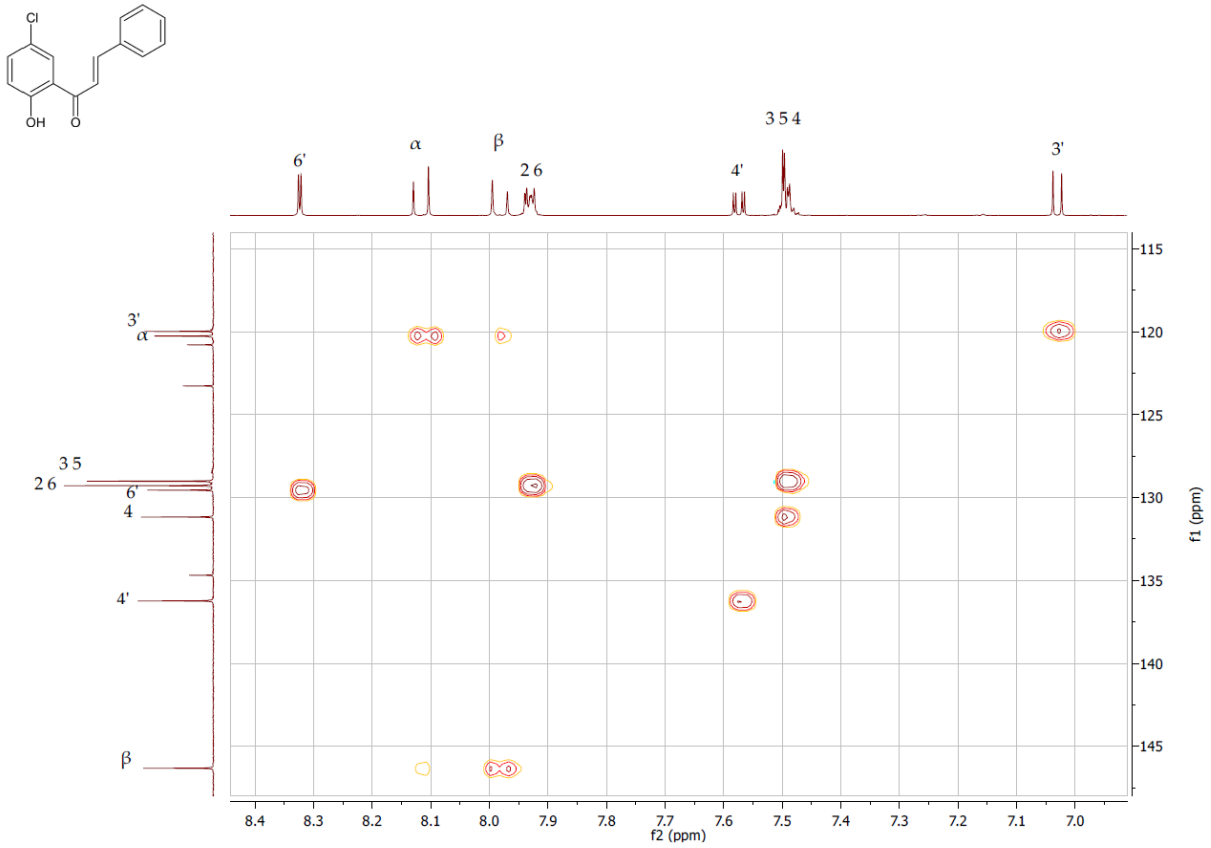


Figure S26. HMQC contour map – ^{1}H x ^{13}C expansion of 5′-chloro-2′-hydroxychalcone (**6**)

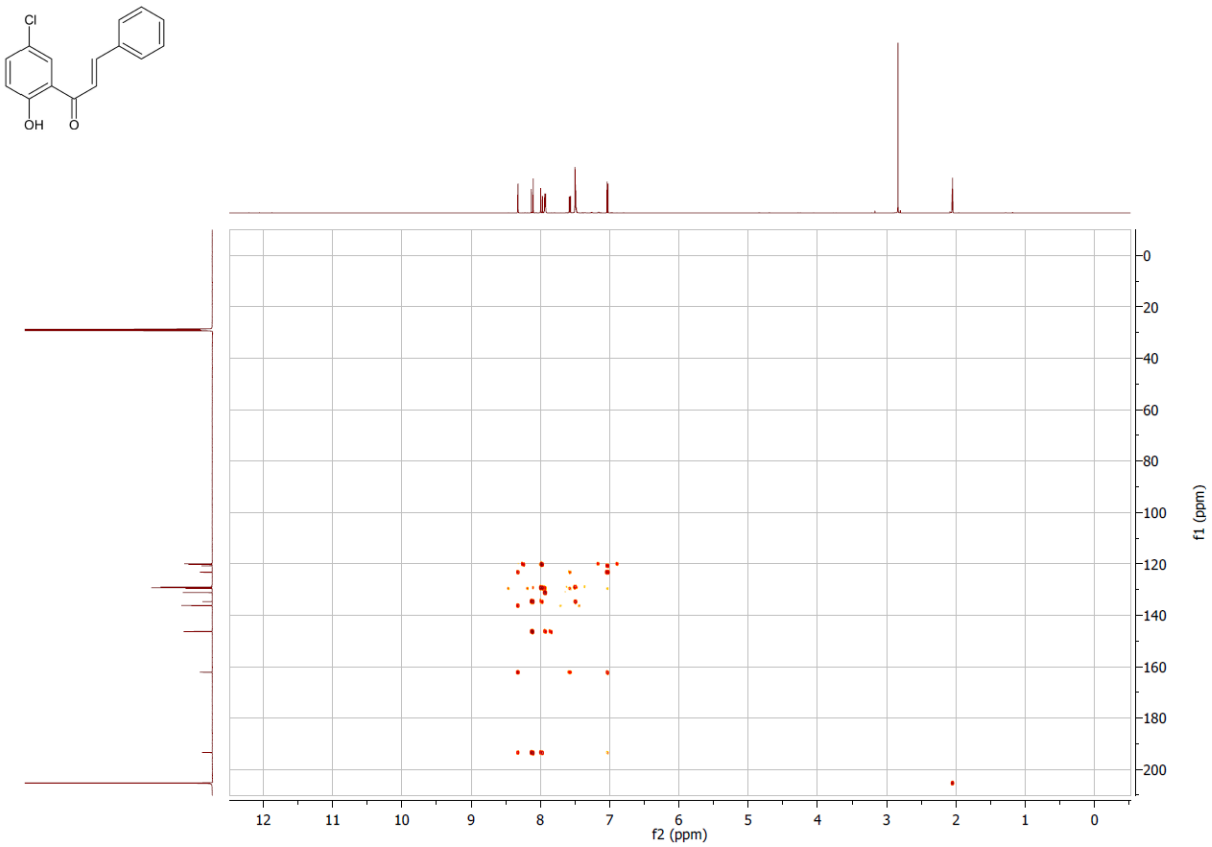


Figure S27. HMBC contour map – ^{1}H x ^{13}C of 5′-chloro-2′-hydroxychalcone (**6**)

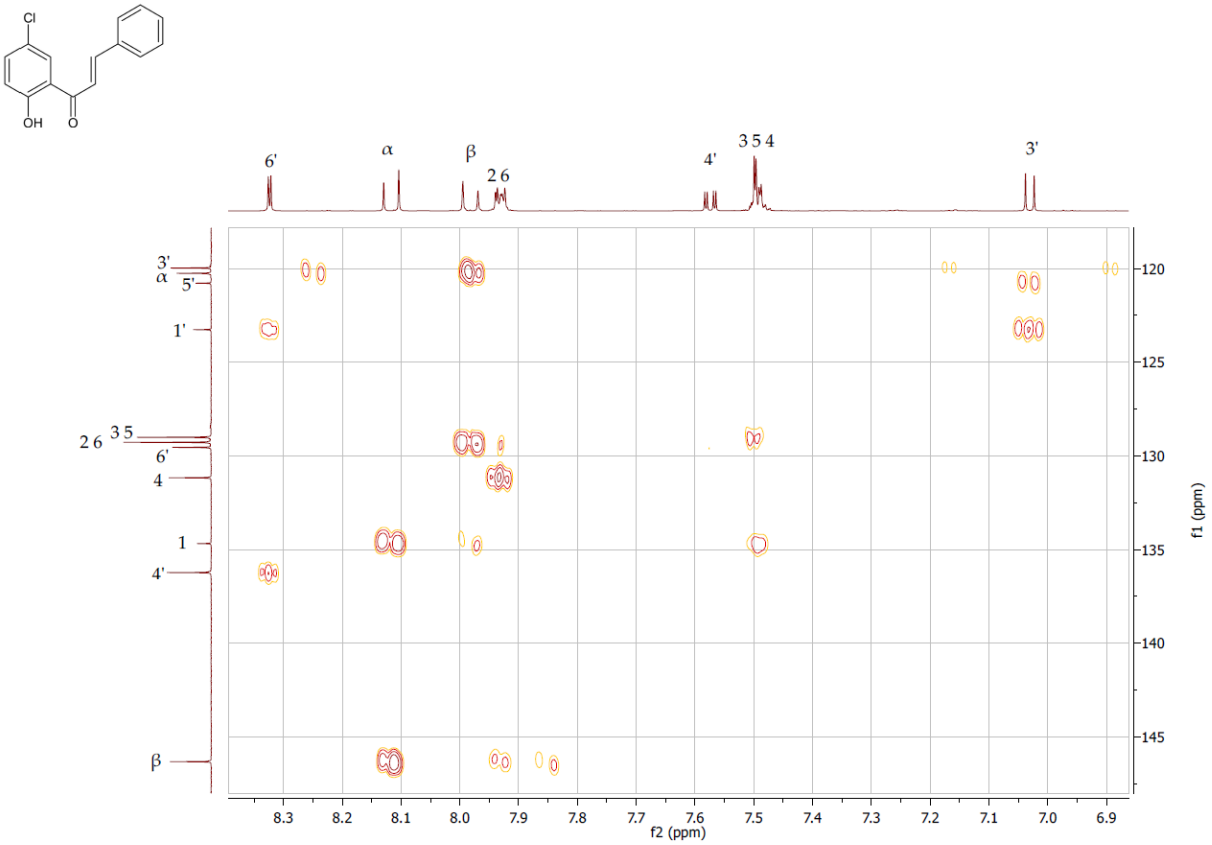


Figure S28. HMBC contour map – ^{1}H x ^{13}C expansion of 5′-chloro-2′-hydroxychalcone (**6**)

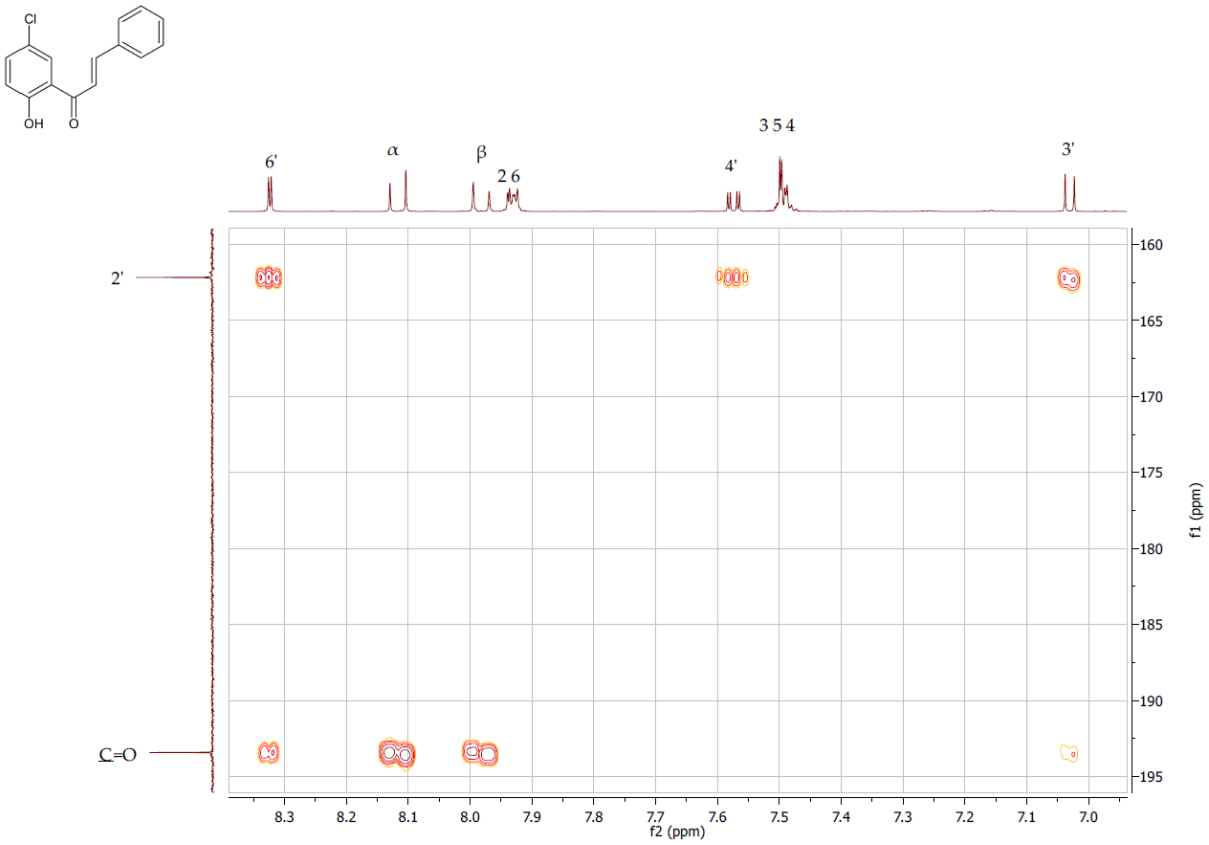


Figure S29. HMBC contour map – ^{1}H x ^{13}C expansion of 5′-chloro-2′-hydroxychalcone (**6**)

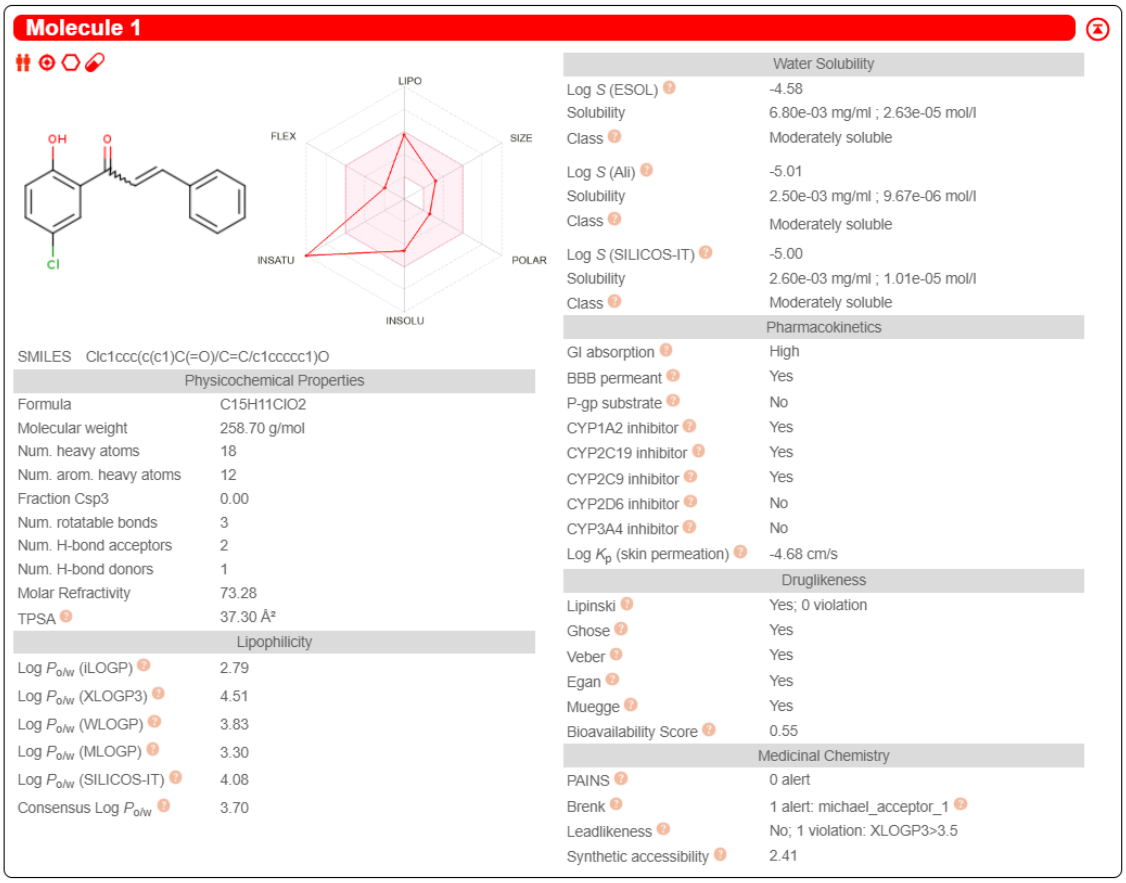


Figure S30. 5′-Chloro-2′-hydroxychalcone (**6**) physicochemical and ADME parameters prediction using the SwissADME modelling

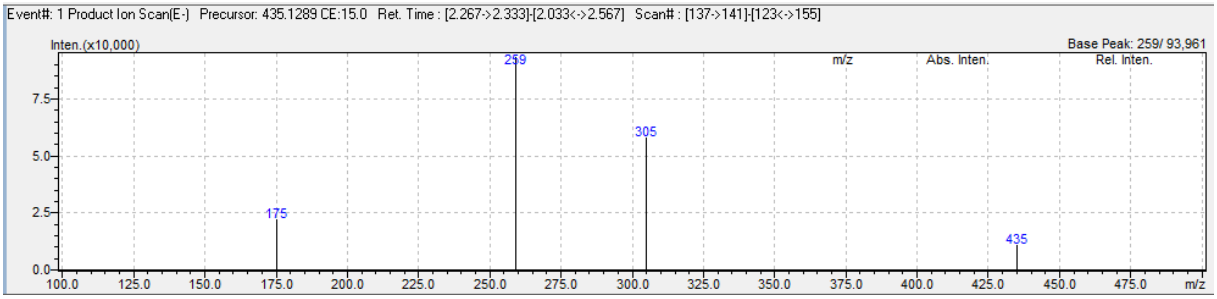
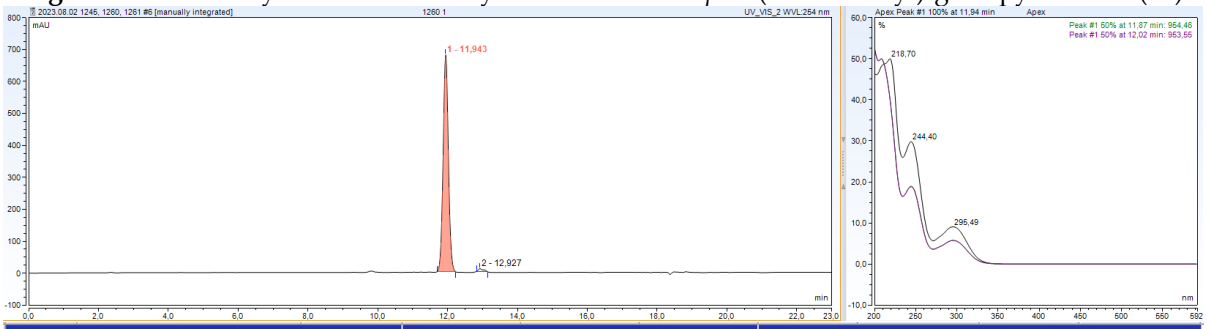


Figure S31. MS analysis of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)



Peak No.	Peak Name	Ret.Time min	Rel.Area %	Area mAU*min	Height mAU	Match	RSD Match %	PPI nm	RSD PPI %
1		*11,943*	*98,63*	*117,2608*	*679,23*	*955*	*3,88*	*216,7*	*1,58*
2		12,927	1,37	1,6334	8,95	993	0,33	212,2	0,41
Maximum			98,63	117,2608	679,23	993	3,88		1,58
Minimum			1,37	1,6334	8,95	955	0,33		0,41

Figure S32. HPLC analysis of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

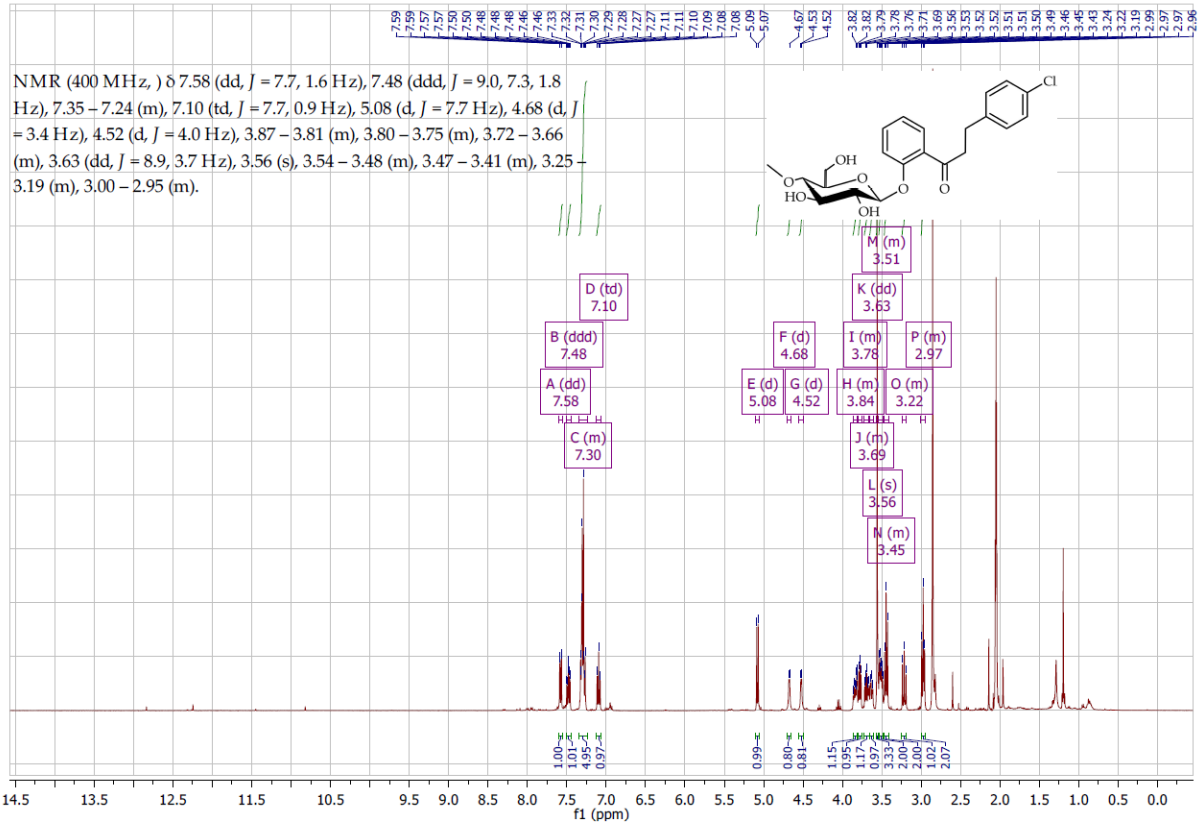


Figure S33. ^{1}H NMR spectrum (*δ*, acetone-d6, 600 MHz) of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

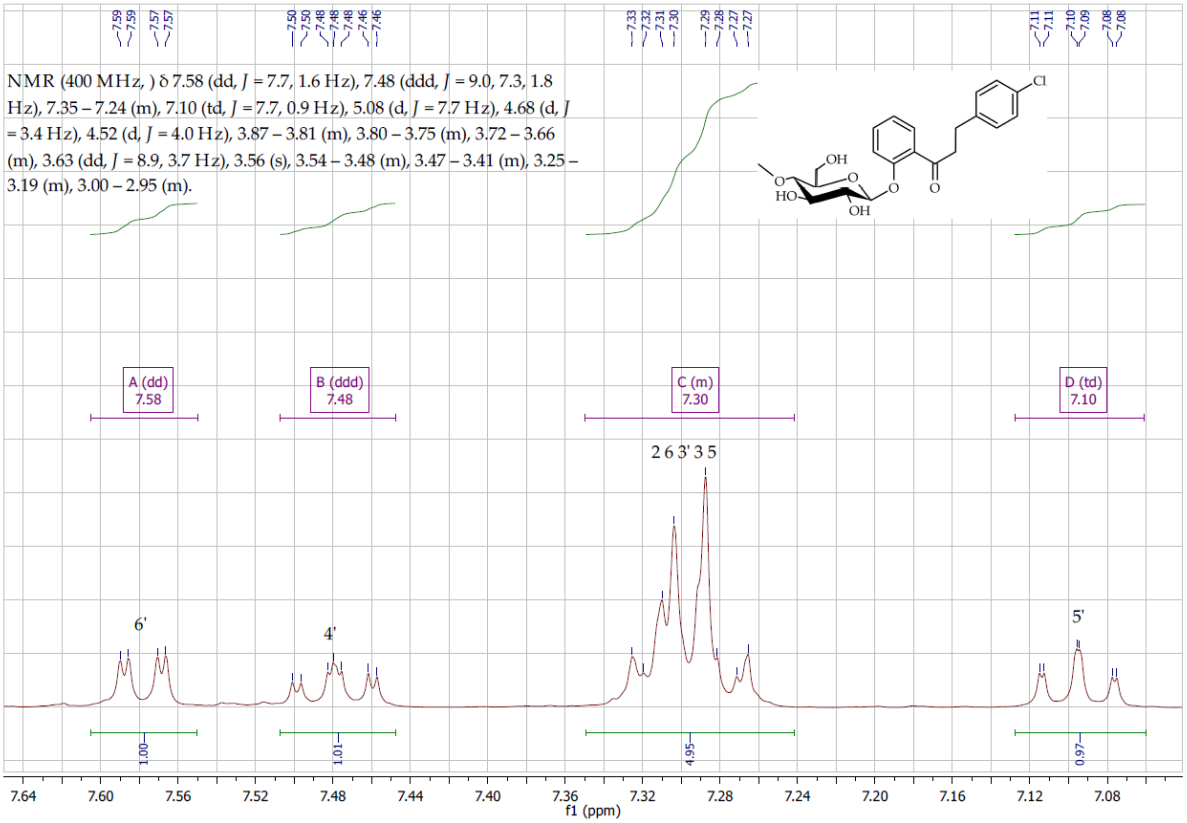


Figure S34. [1]H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

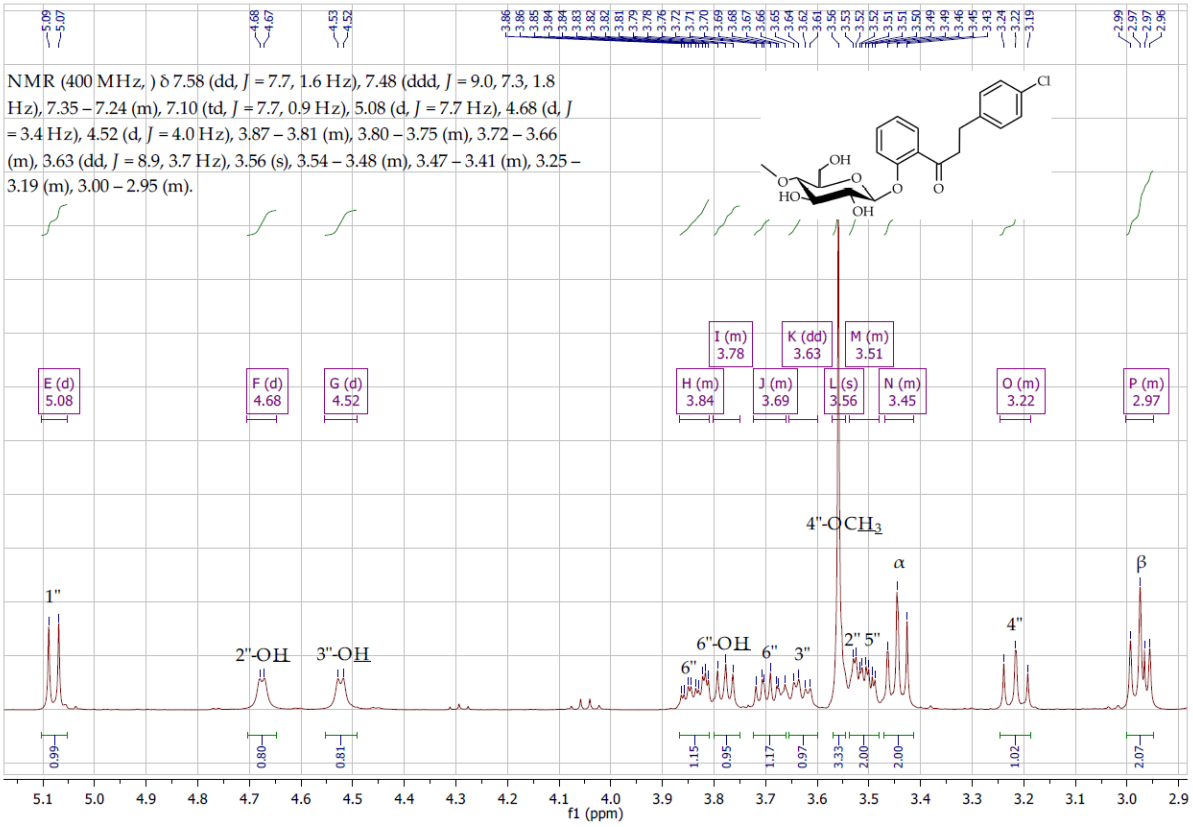


Figure S35. [1]H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

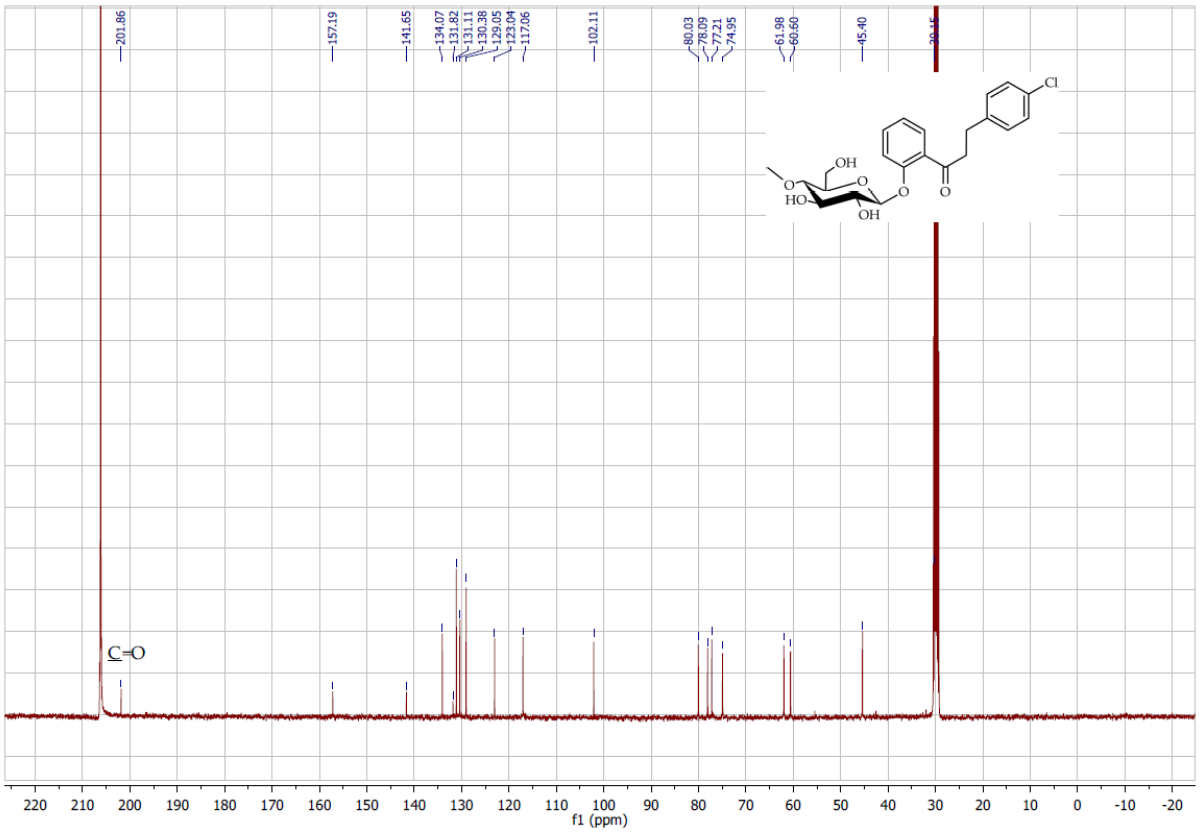


Figure S36. ^{13}C NMR spectrum (δ, acetone-d6, 151 MHz) of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

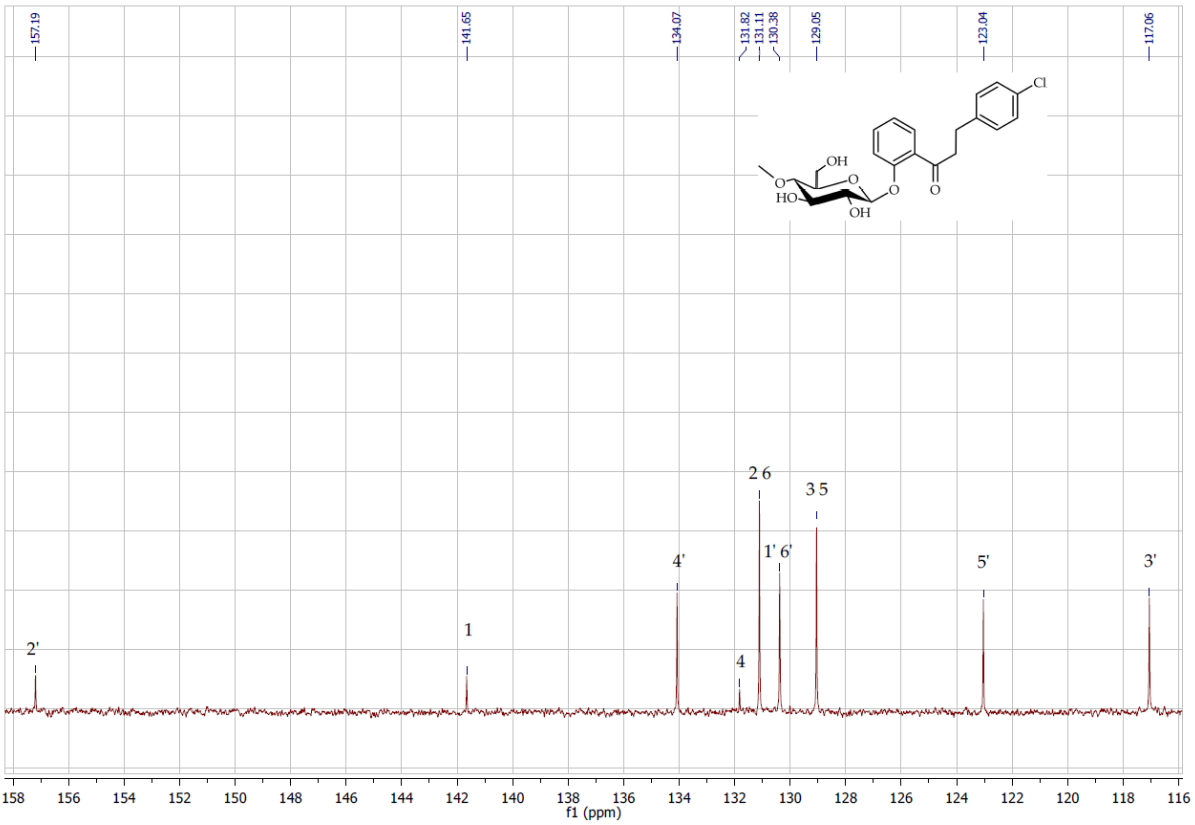


Figure S37. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

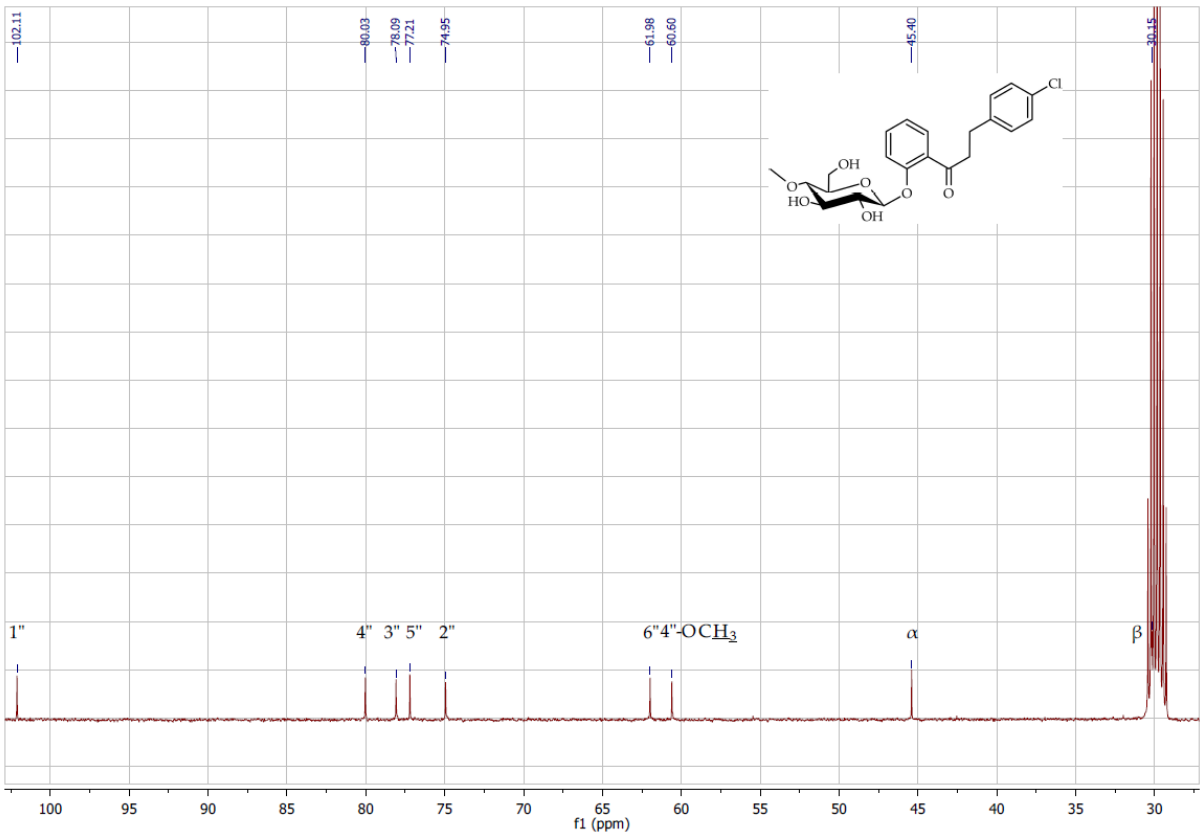


Figure S38. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

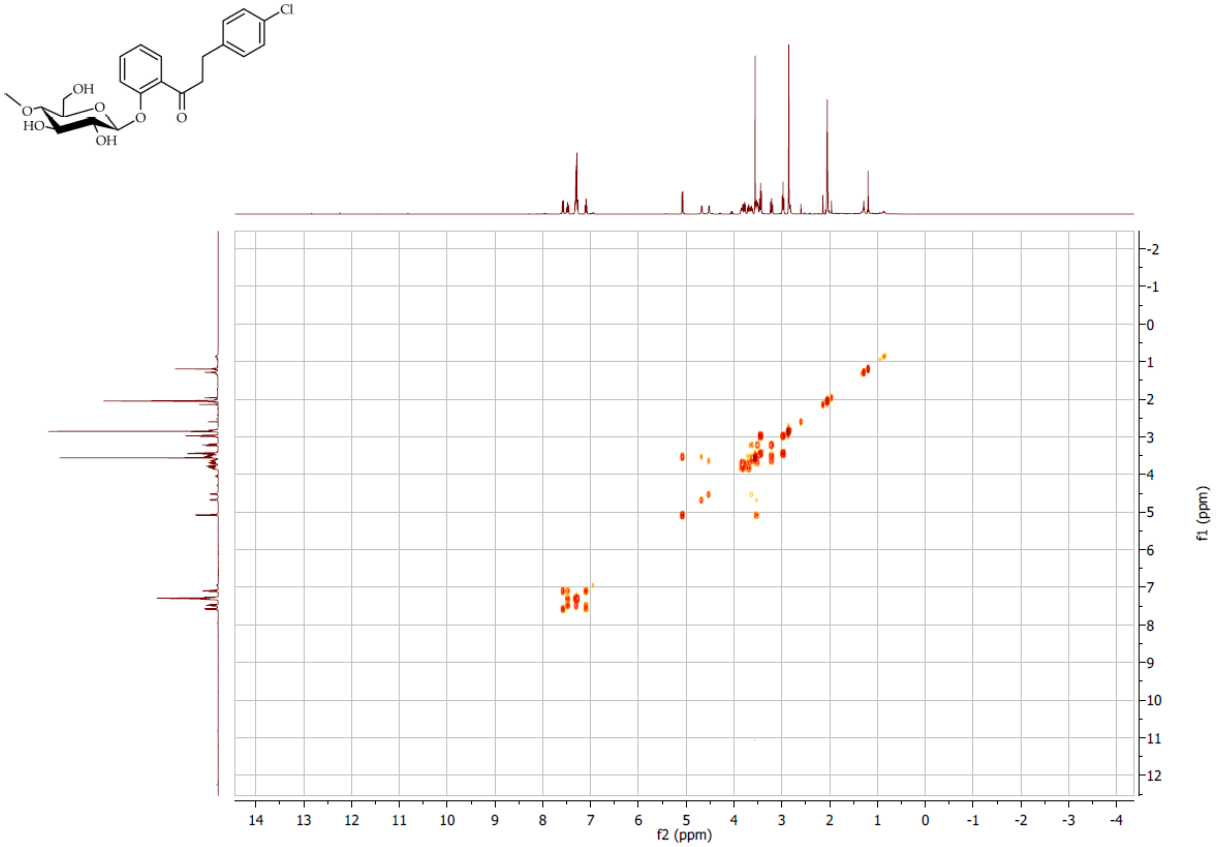


Figure S39. COSY contour map – ^{1}H x ^{1}H of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

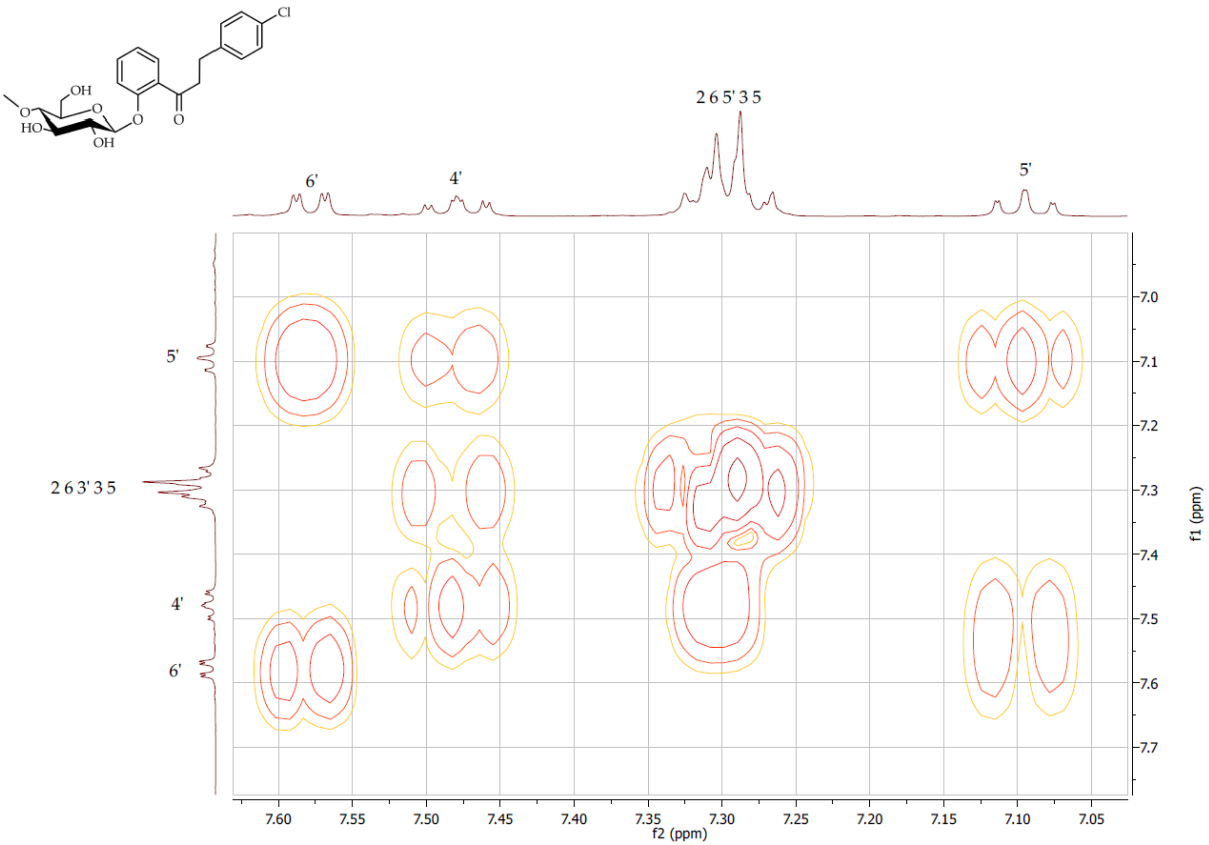


Figure S40. COSY contour map – ^{1}H x ^{1}H expansion of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

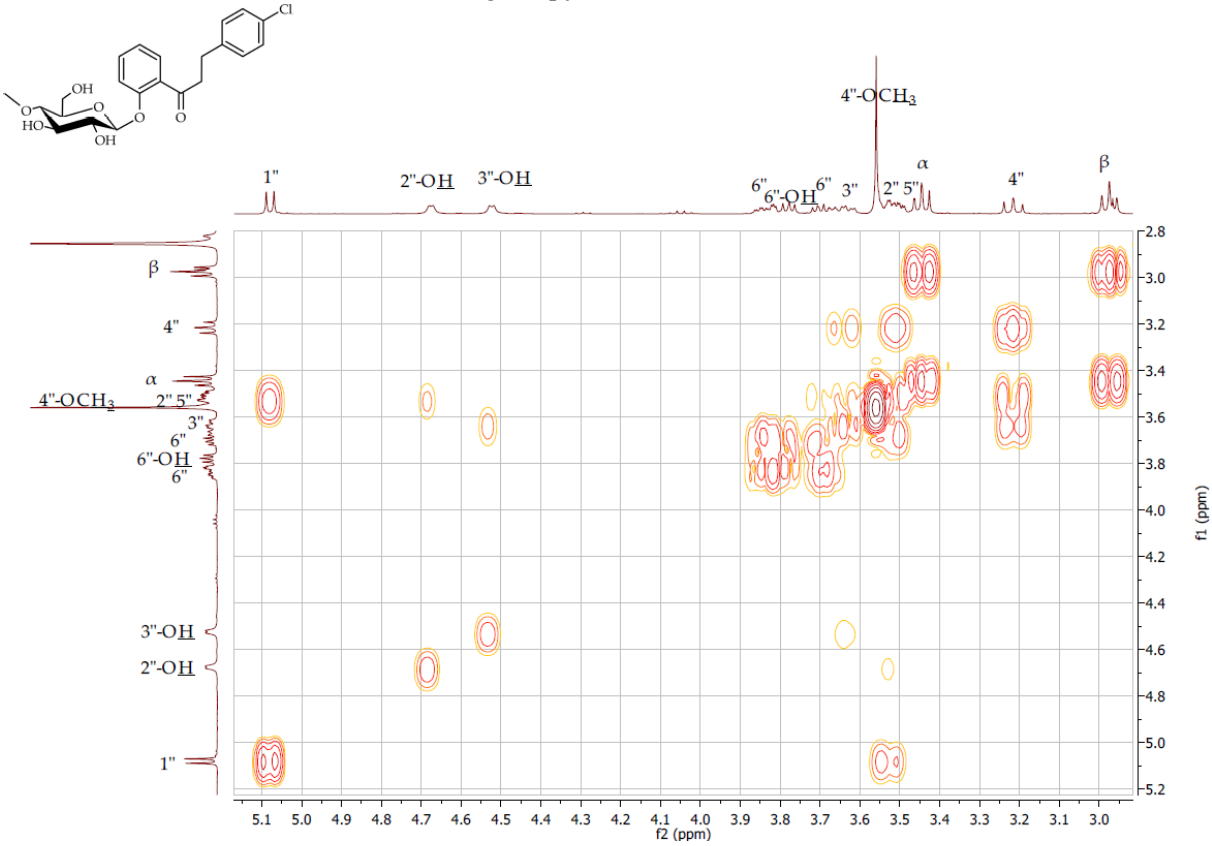


Figure S41. COSY contour map – ^{1}H x ^{1}H expansion of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

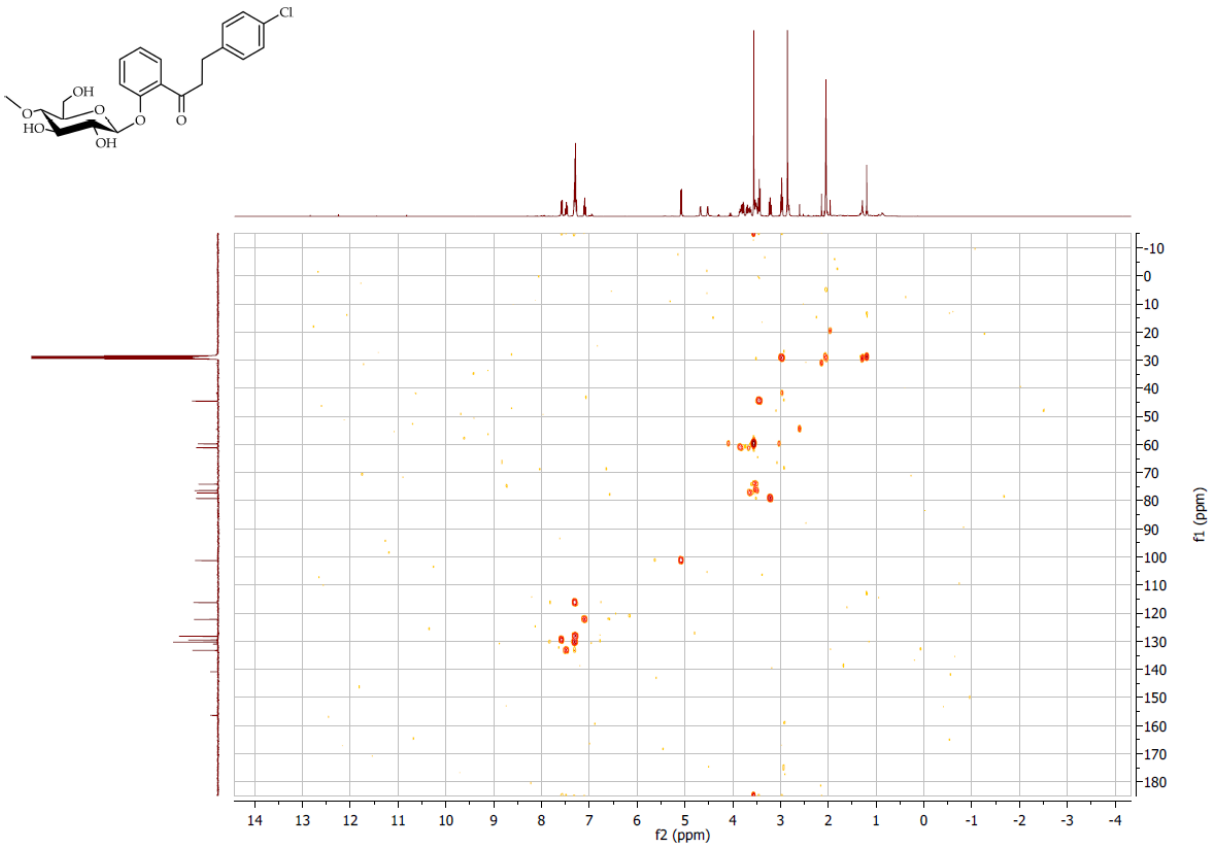


Figure S42. HMQC contour map – ^{1}H x ^{13}C of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

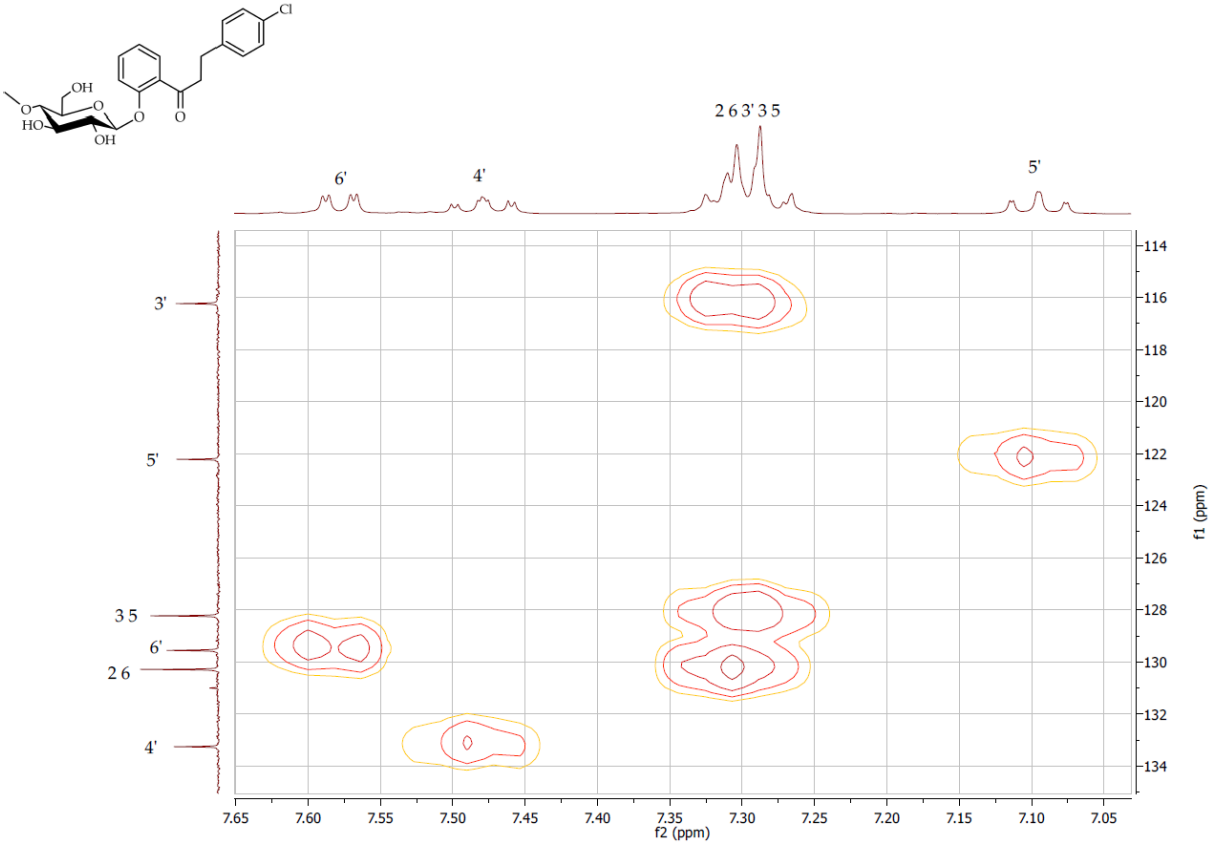


Figure S43. HMQC contour map – ^{1}H x ^{13}C expansion of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

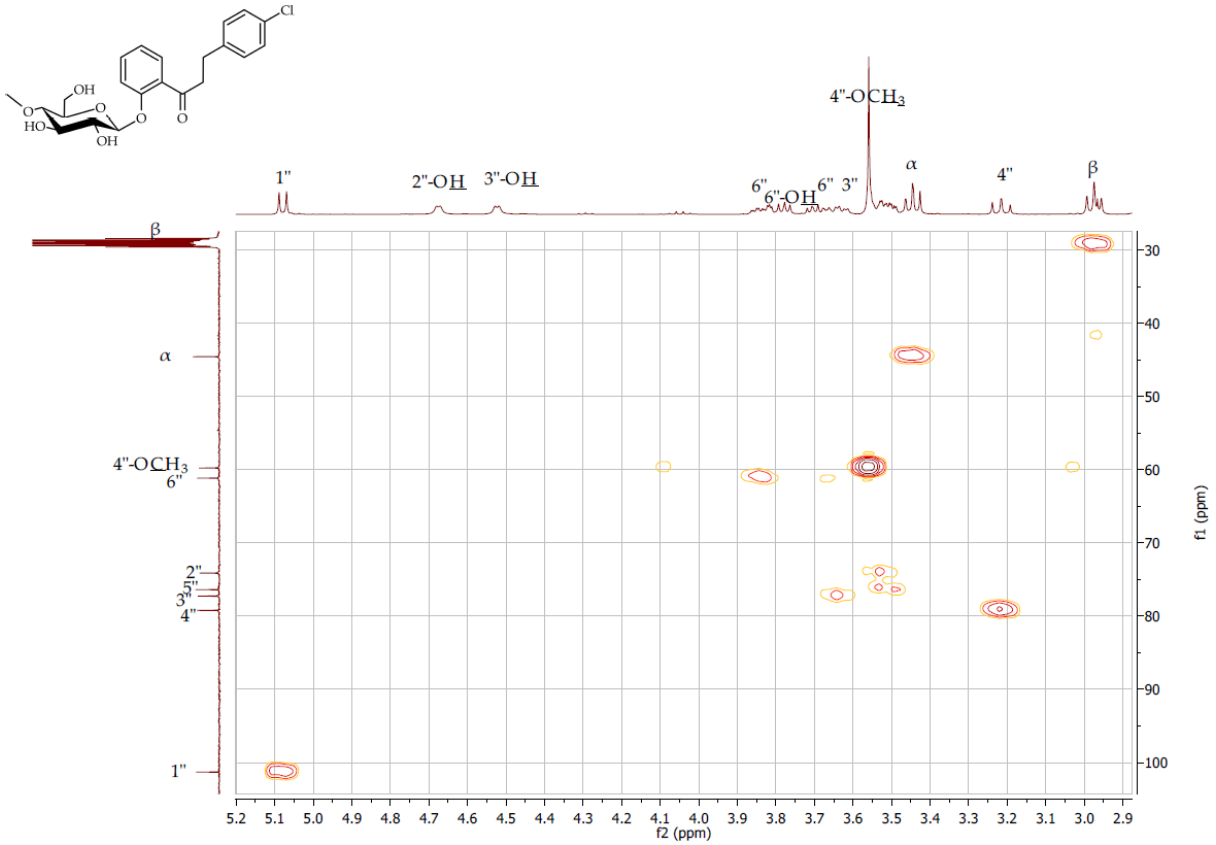


Figure S44. HMQC contour map – ^{1}H x ^{13}C expansion of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

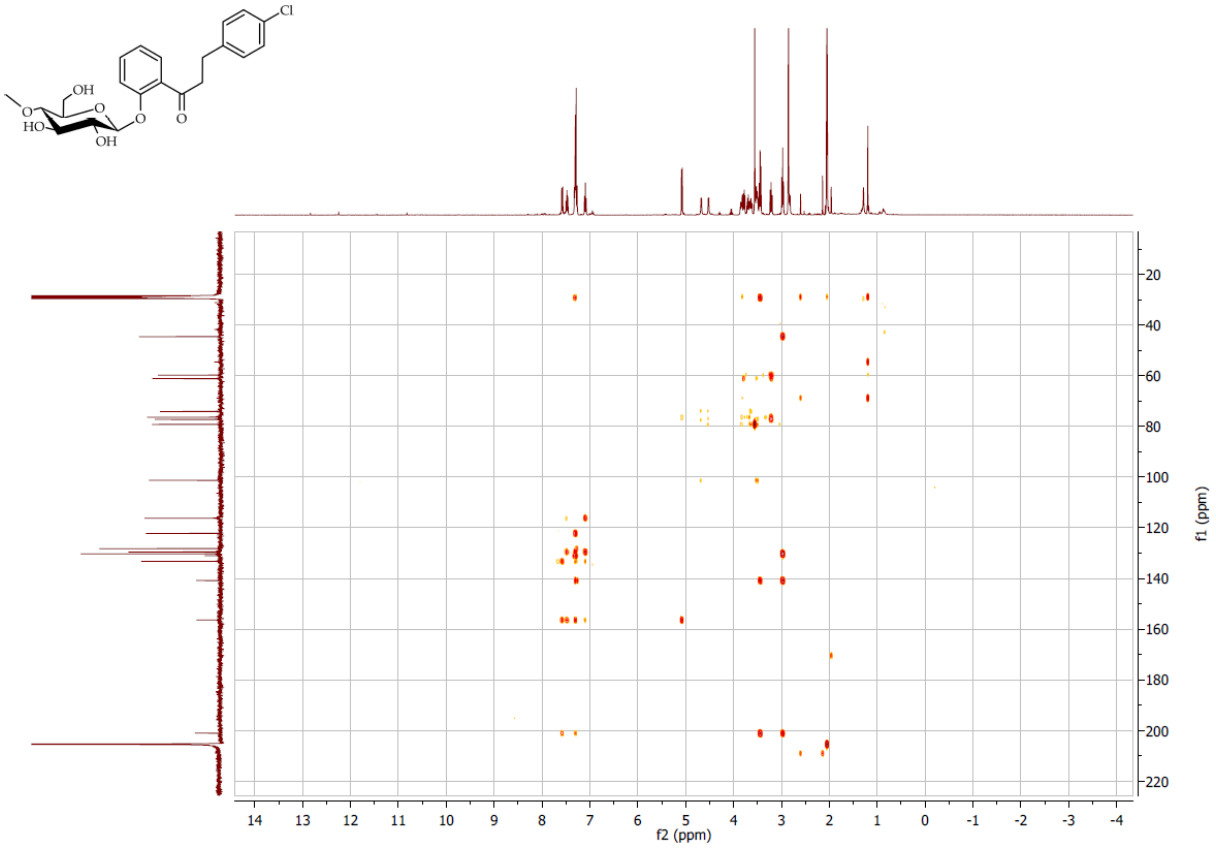


Figure S45. HMBC contour map – ^{1}H x ^{13}C of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

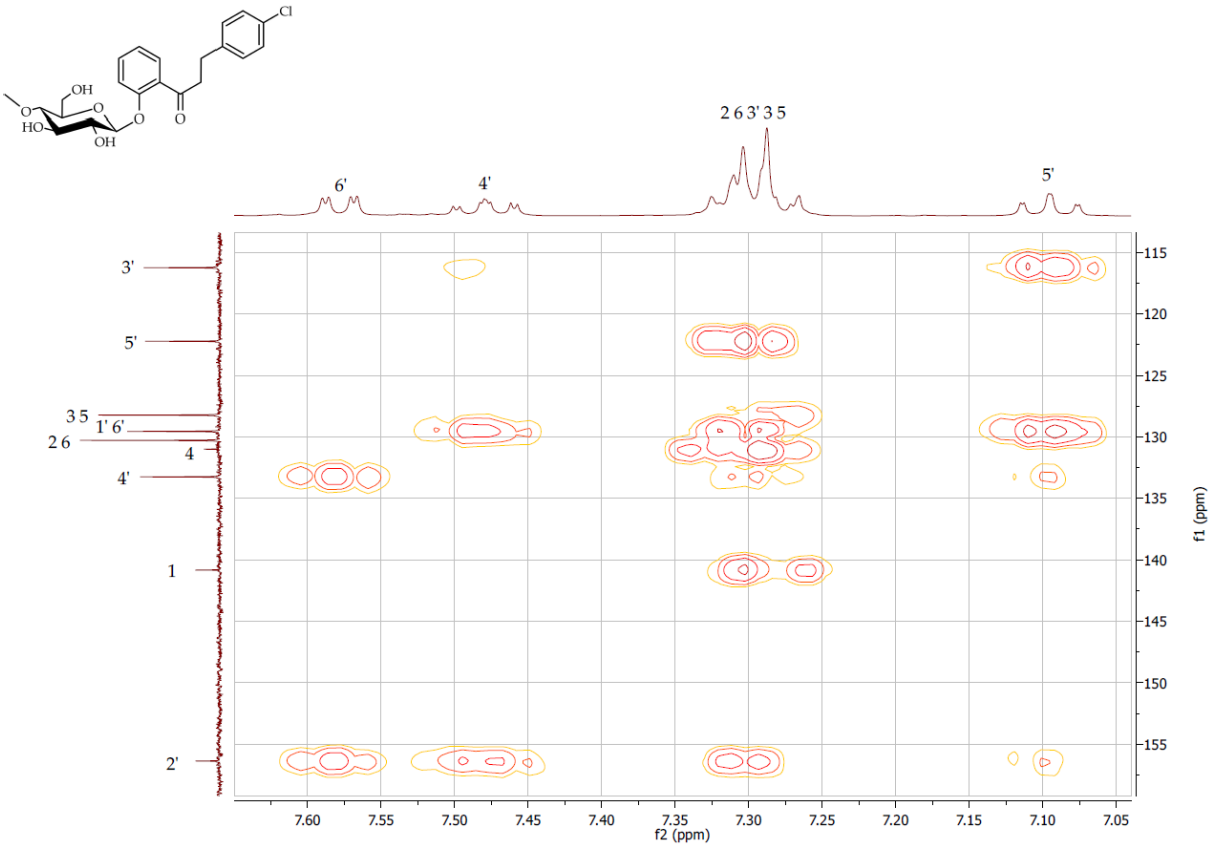


Figure S46. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

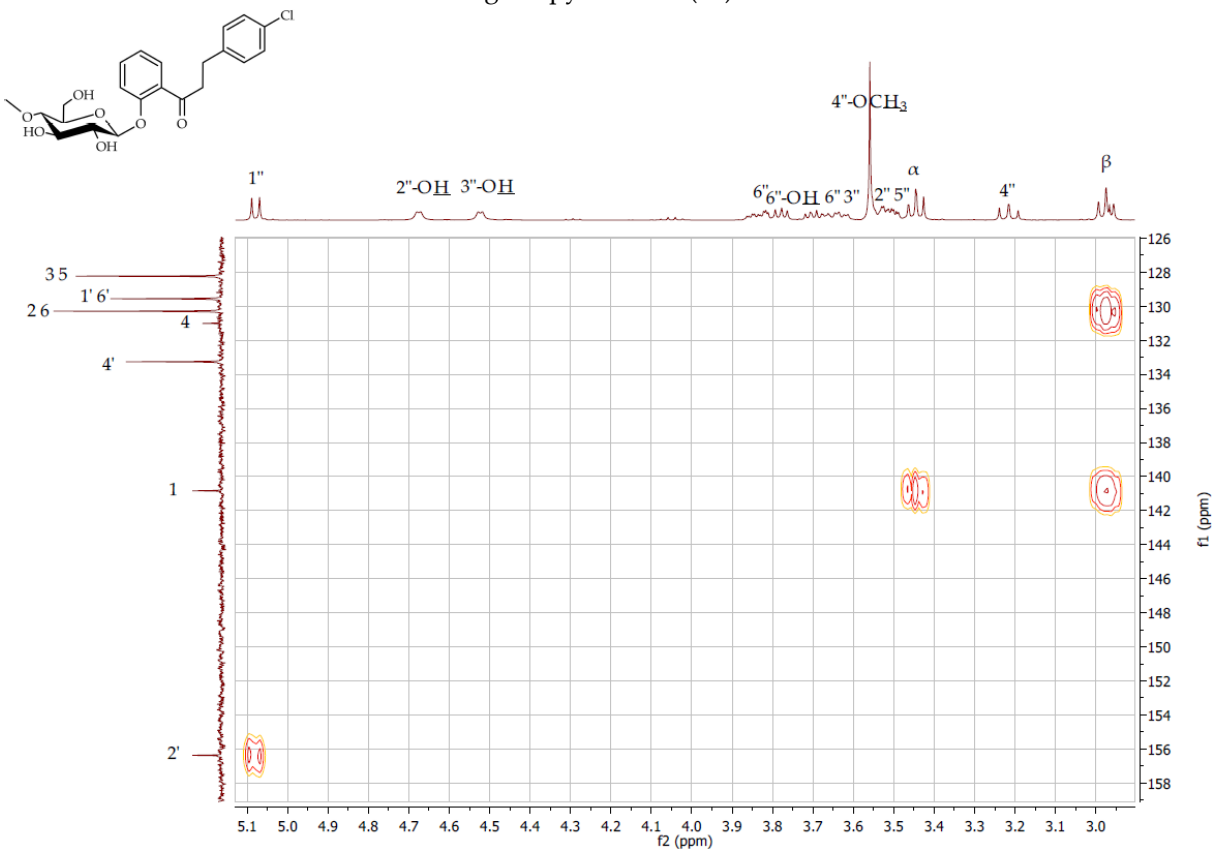


Figure S47. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

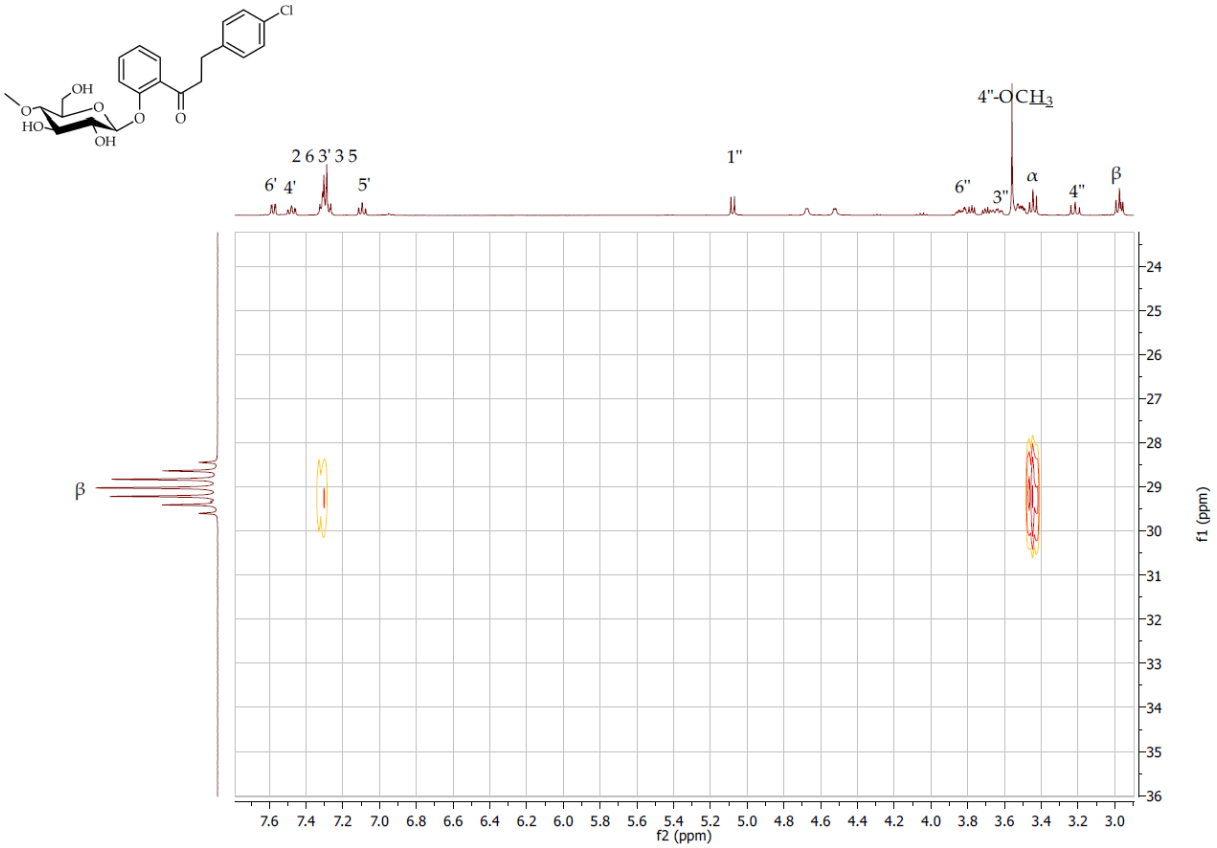


Figure S48. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

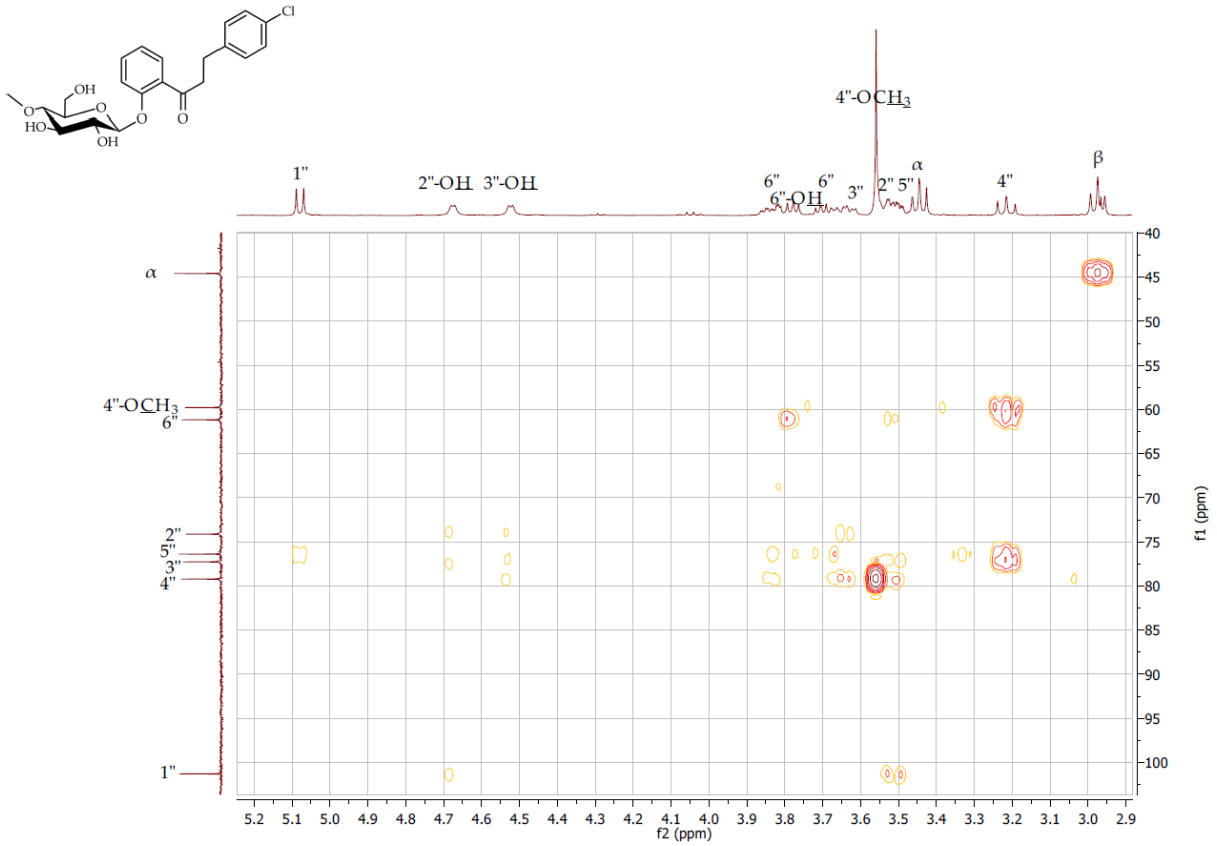


Figure S49. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

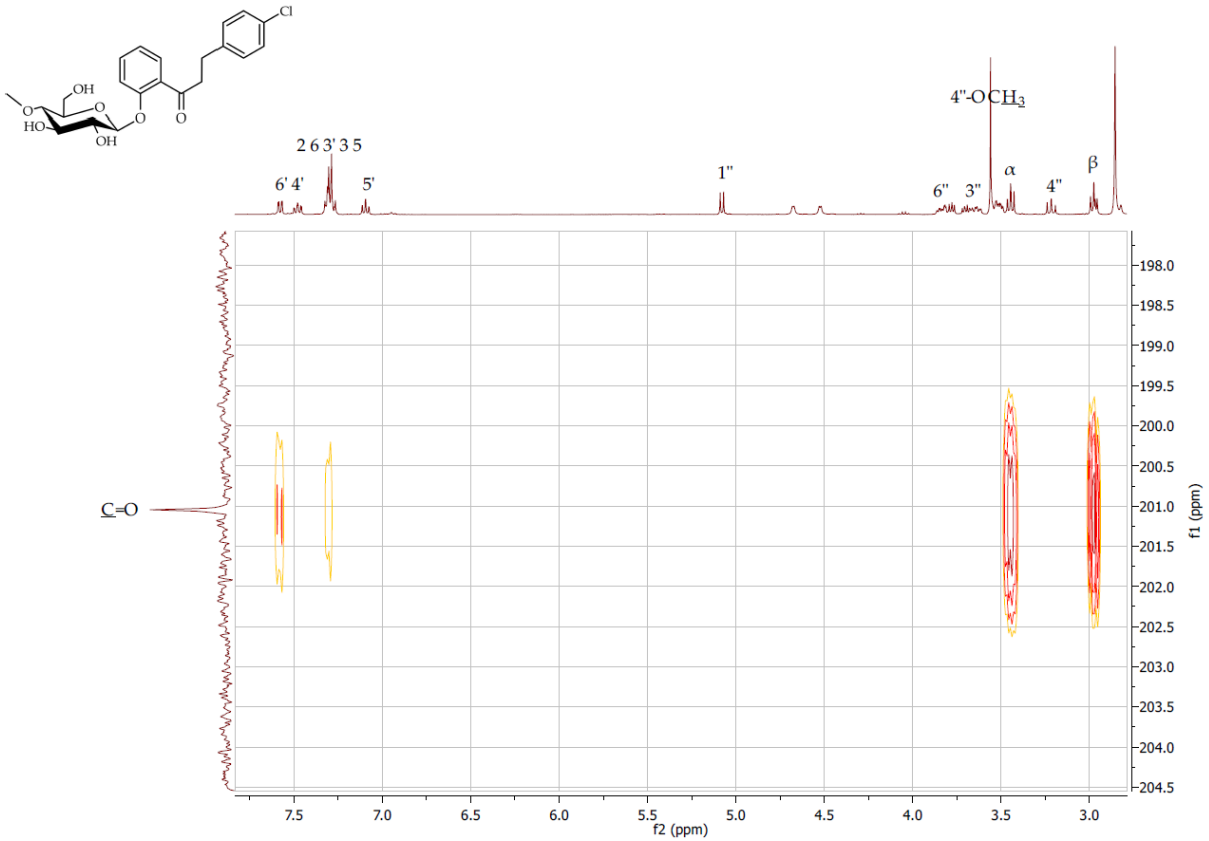


Figure S50. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**)

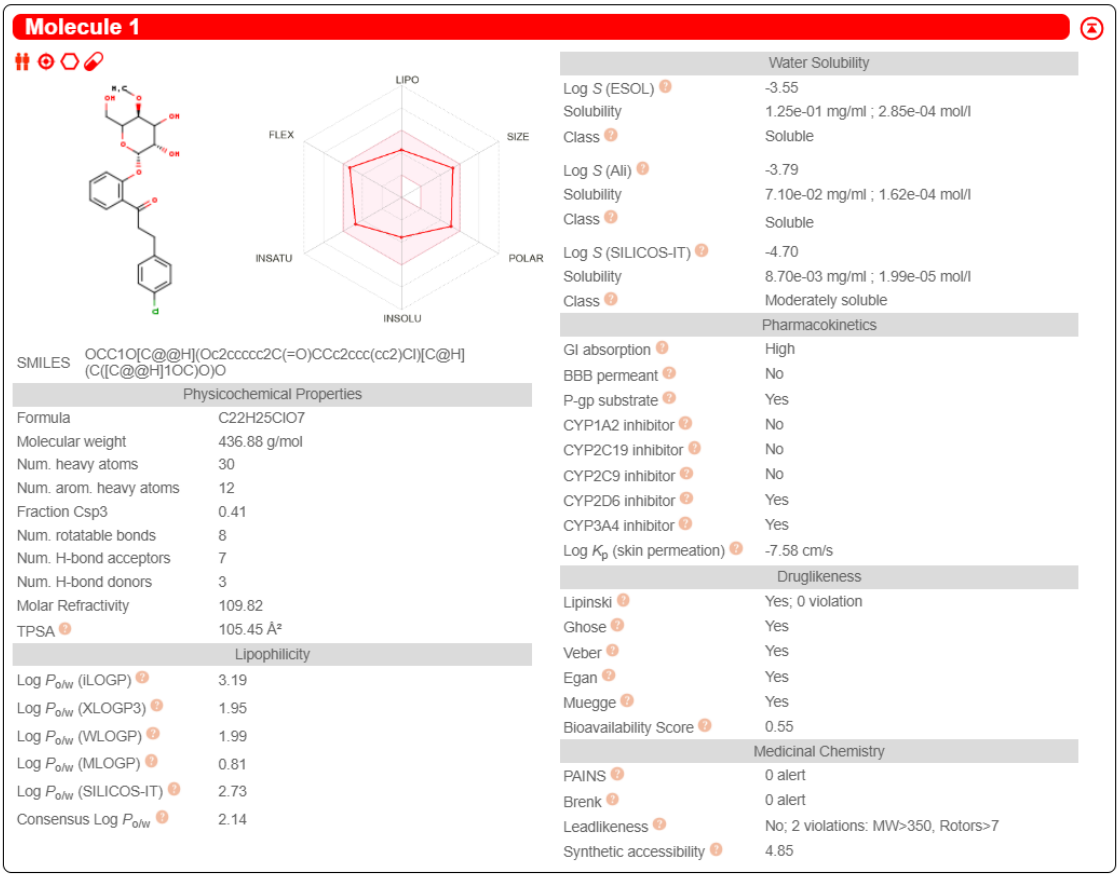


Figure S51. 4-Chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3a**) physicochemical and ADME parameters prediction using the SwissADME modelling

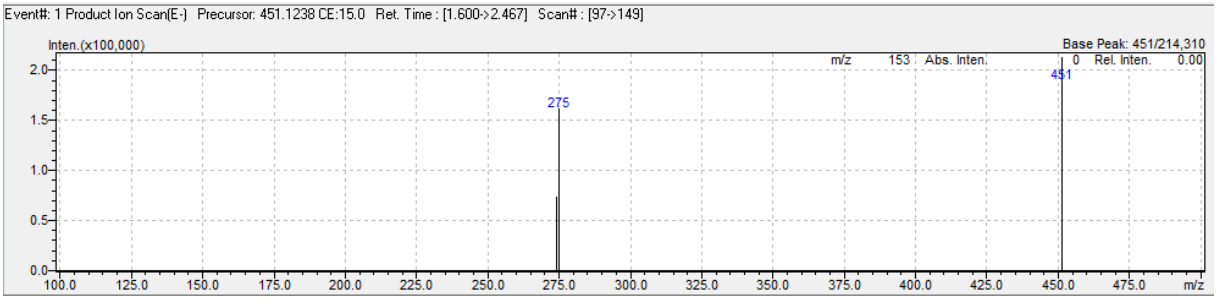
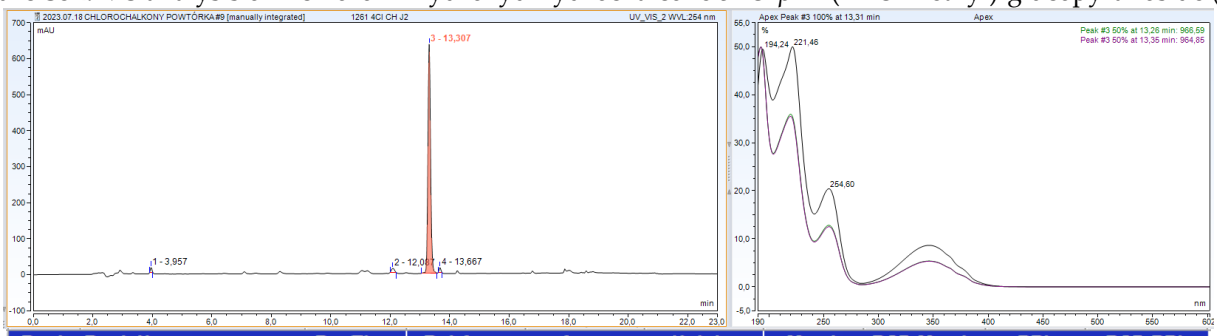


Figure S52. MS analysis of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)



Peak No.	Peak Name	Ret.Time min	Rel.Area %	Area mAU*min	Height mAU	Match	RSD Match %	PPI nm	RSD PPI %
1		3,957	1,40	0,9341	15,17	999	0,07	229,5	0,50
2		12,087	2,01	1,3428	11,57	1000	0,02	200,1	0,12
3		*13,307*	*95,21*	*63,5668*	*636,27*	*955*	*4,31*	*211,8*	*2,00*
4		13,667	1,38	0,9216	13,75	1000	0,01	266,8	0,23
Maximum			95,21	63,5668	636,27	1000	4,31		2,00
Minimum			1,38	0,9216	11,57	955	0,01		0,12

Figure S53. HPLC analysis of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

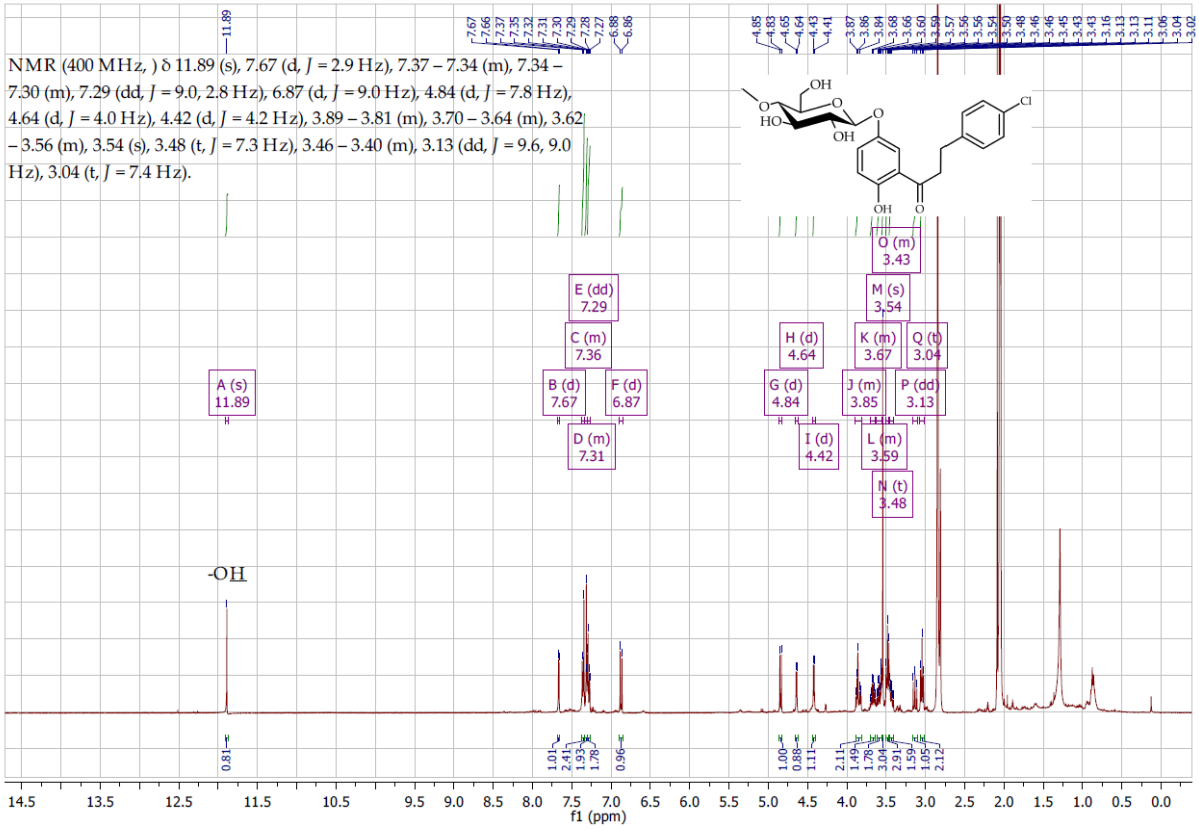


Figure S54. ^{1}H NMR spectrum (*δ*, acetone-d6, 600 MHz) of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

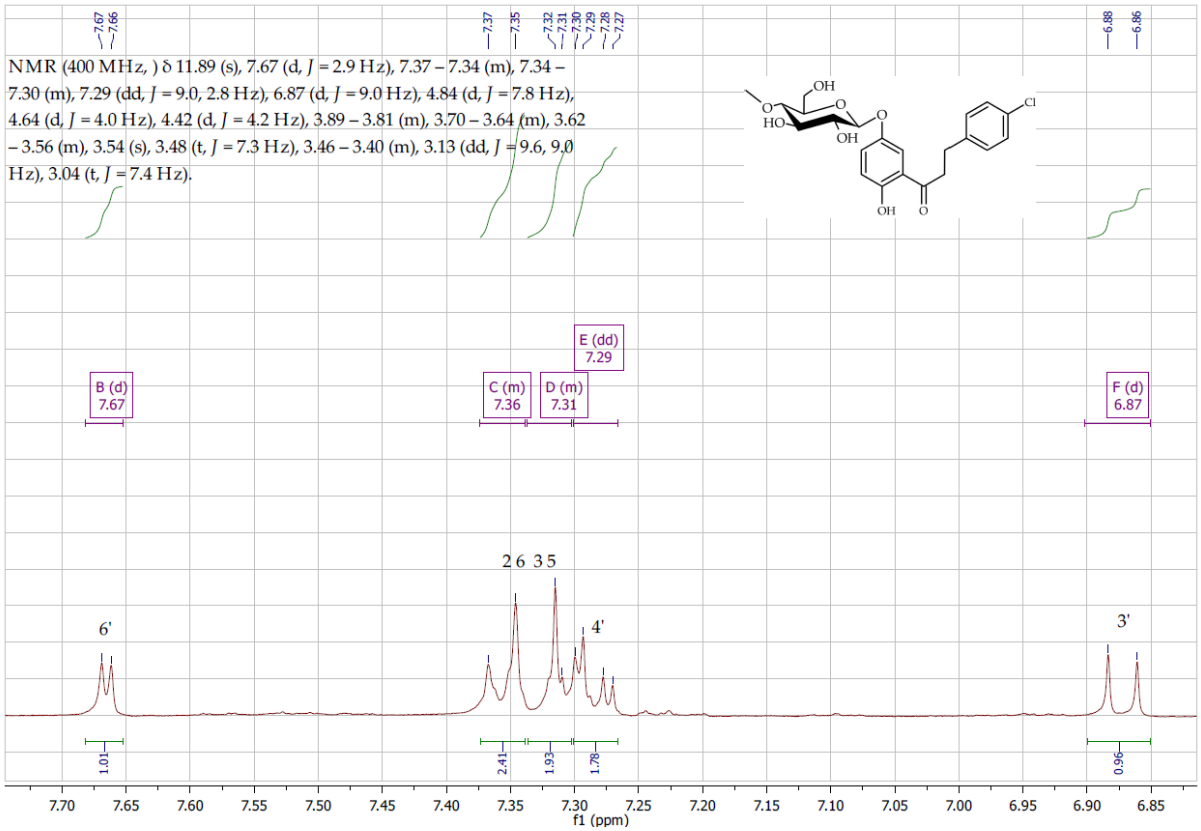


Figure S55. [1]H NMR spectrum expansion (*δ*, acetone-d6, 600 MHz) of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

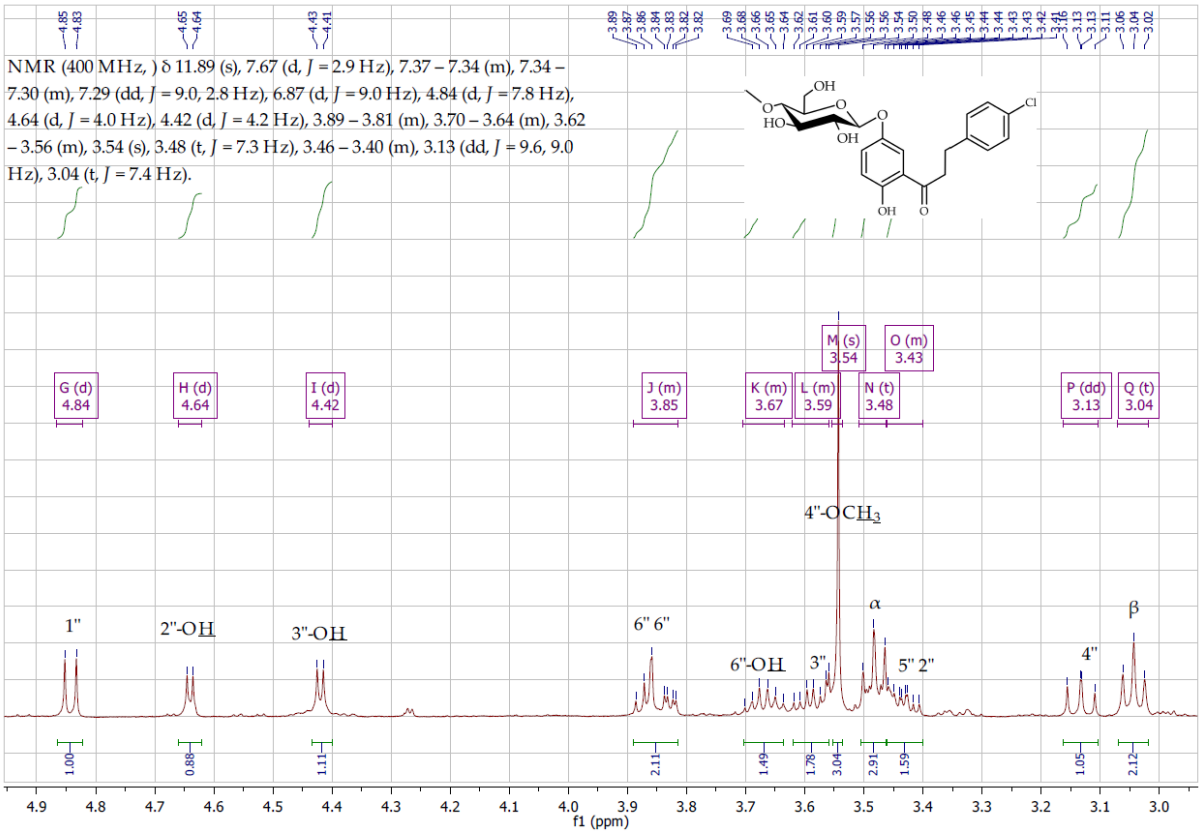


Figure S56. [1]H NMR spectrum expansion (*δ*, acetone-d6, 600 MHz) of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

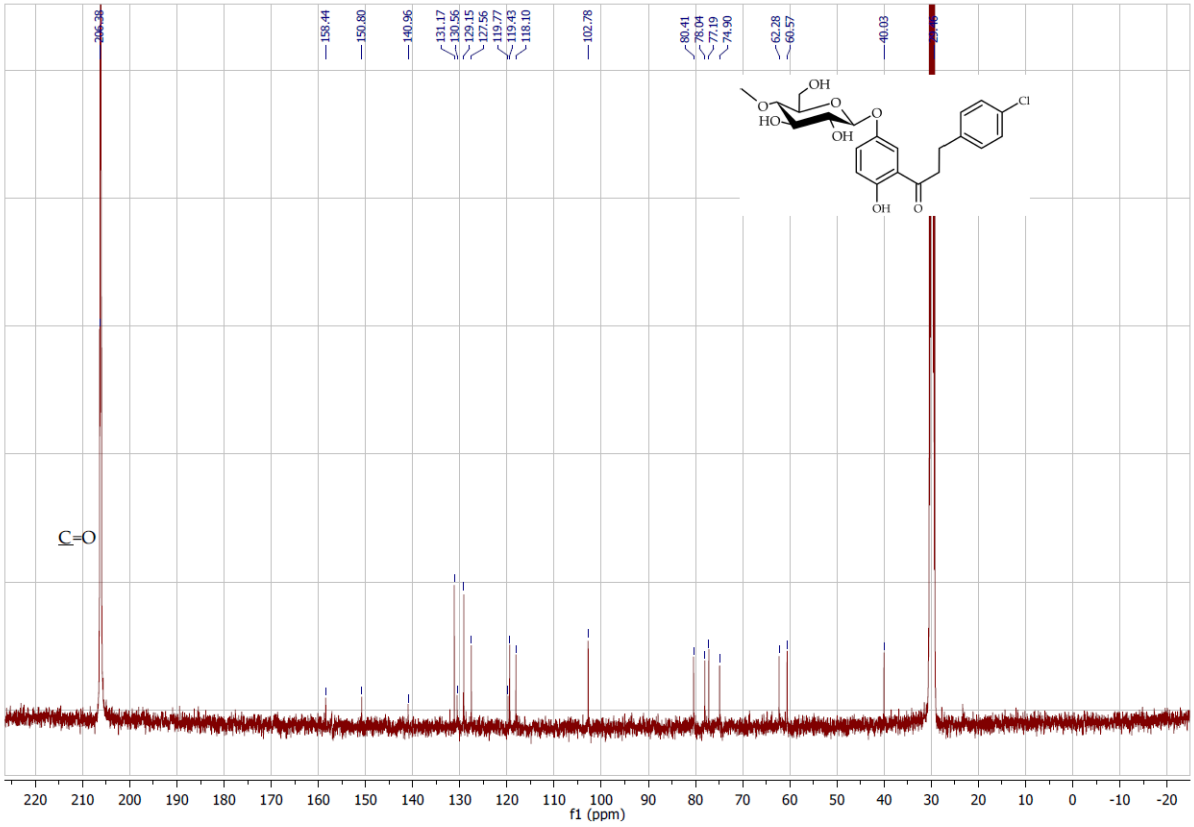


Figure S57. ^{13}C NMR spectrum (δ, acetone-d6, 151 MHz) of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

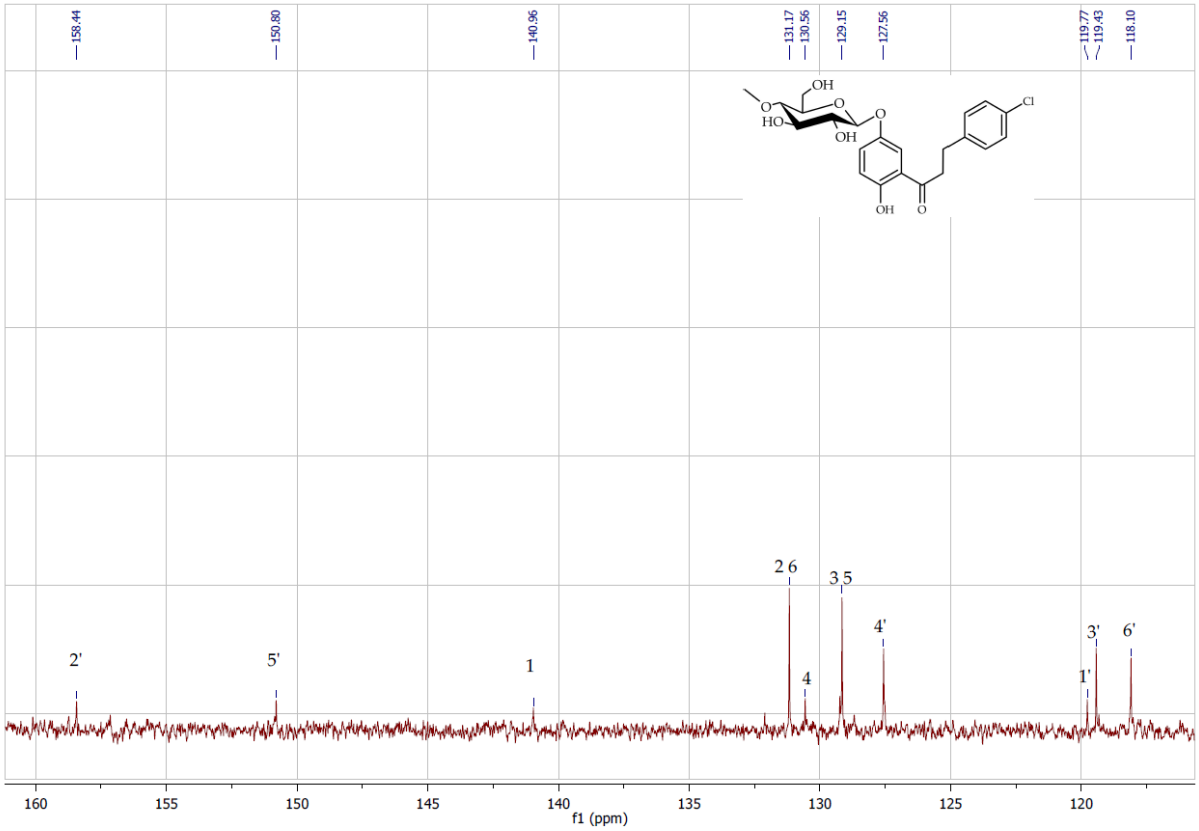


Figure S58. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

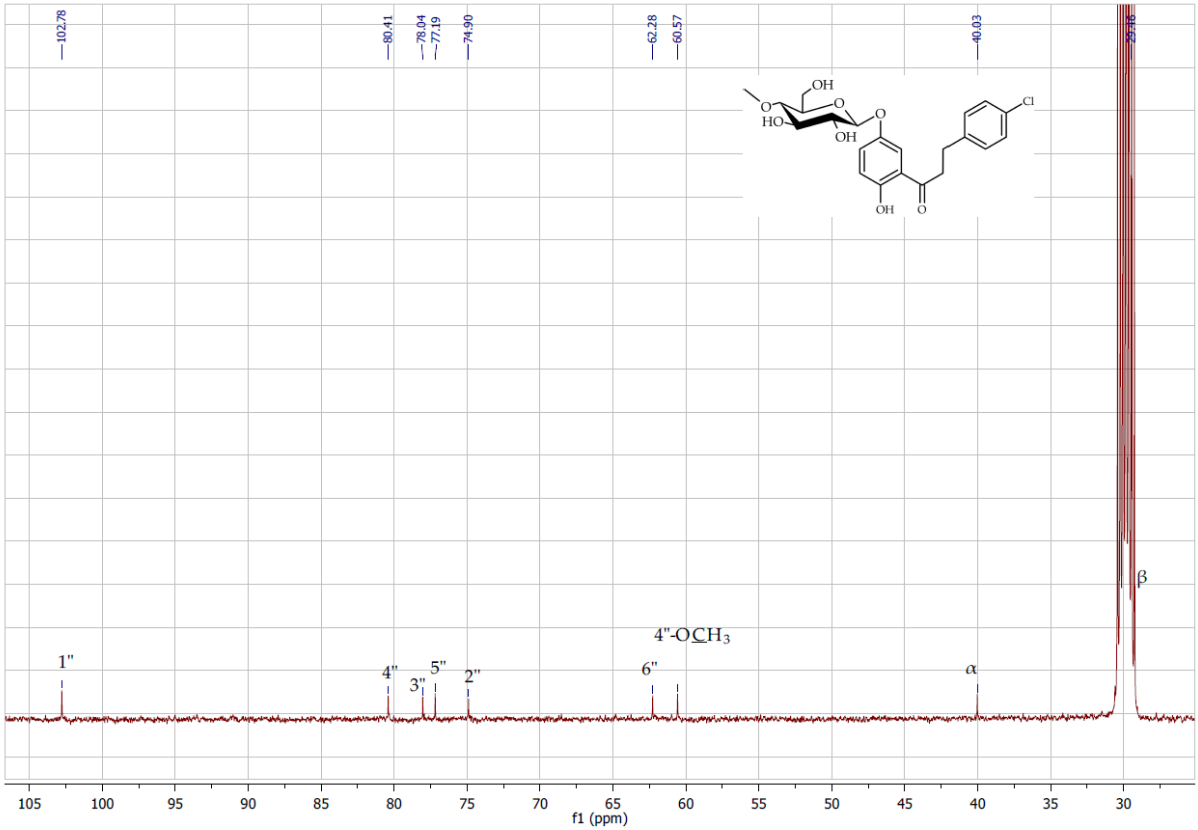


Figure S59. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

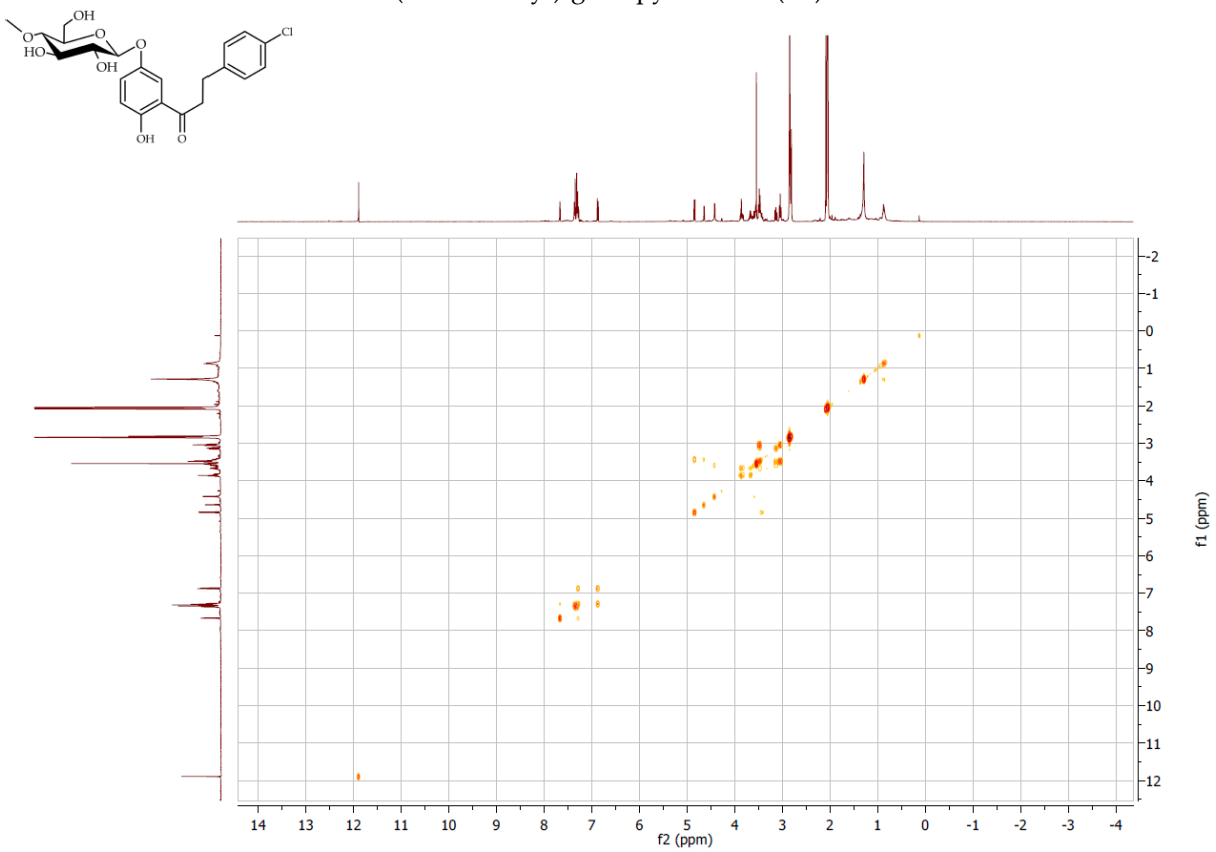


Figure S60. COSY contour map – ^{1}H x ^{1}H of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

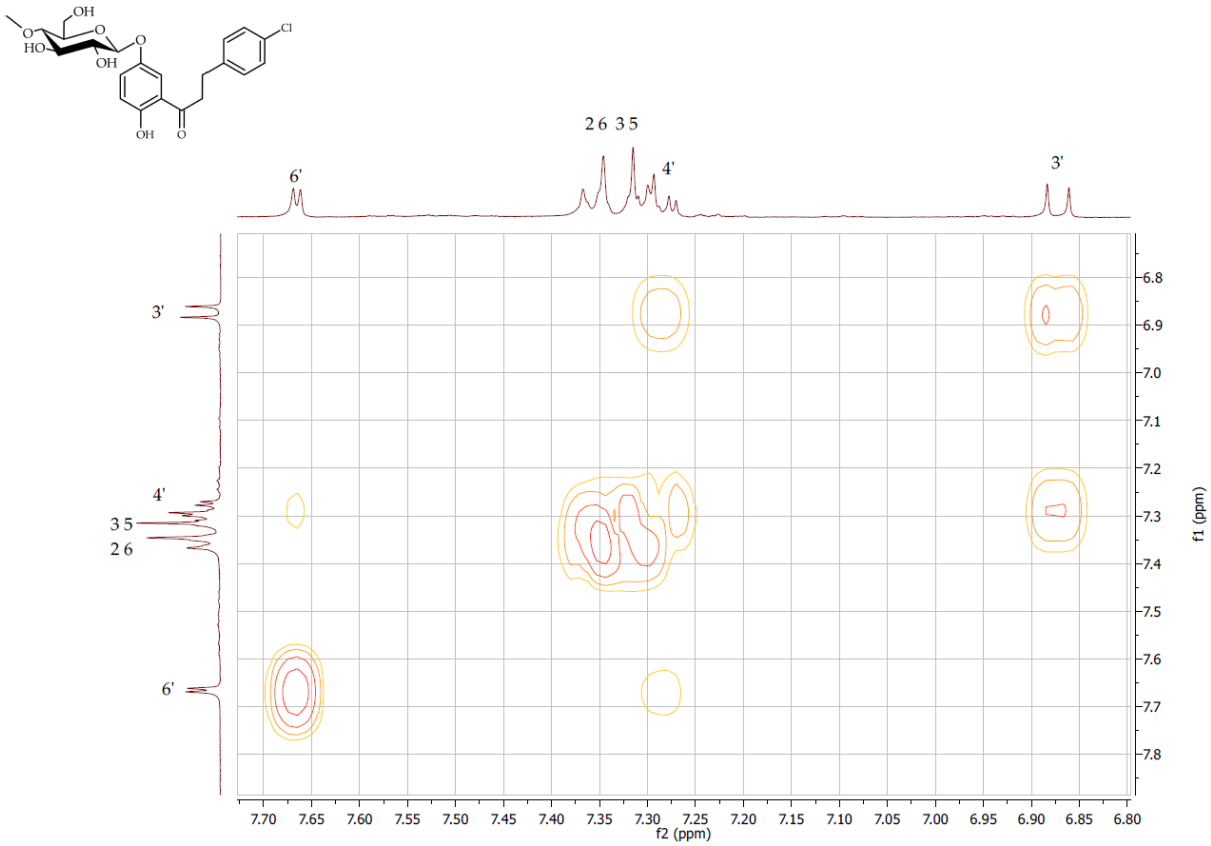


Figure S61. COSY contour map – ^{1}H x ^{1}H expansion of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

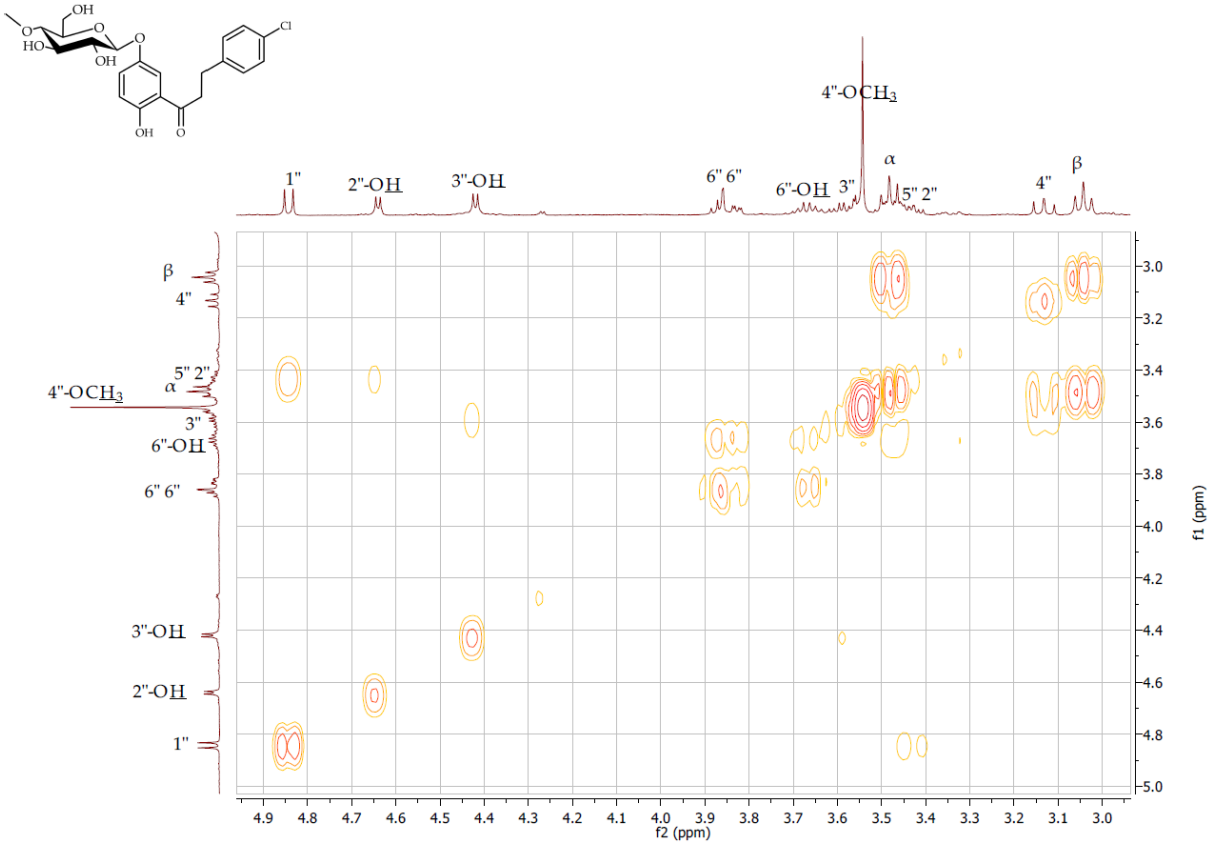


Figure S62. COSY contour map – ^{1}H x ^{1}H expansion of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

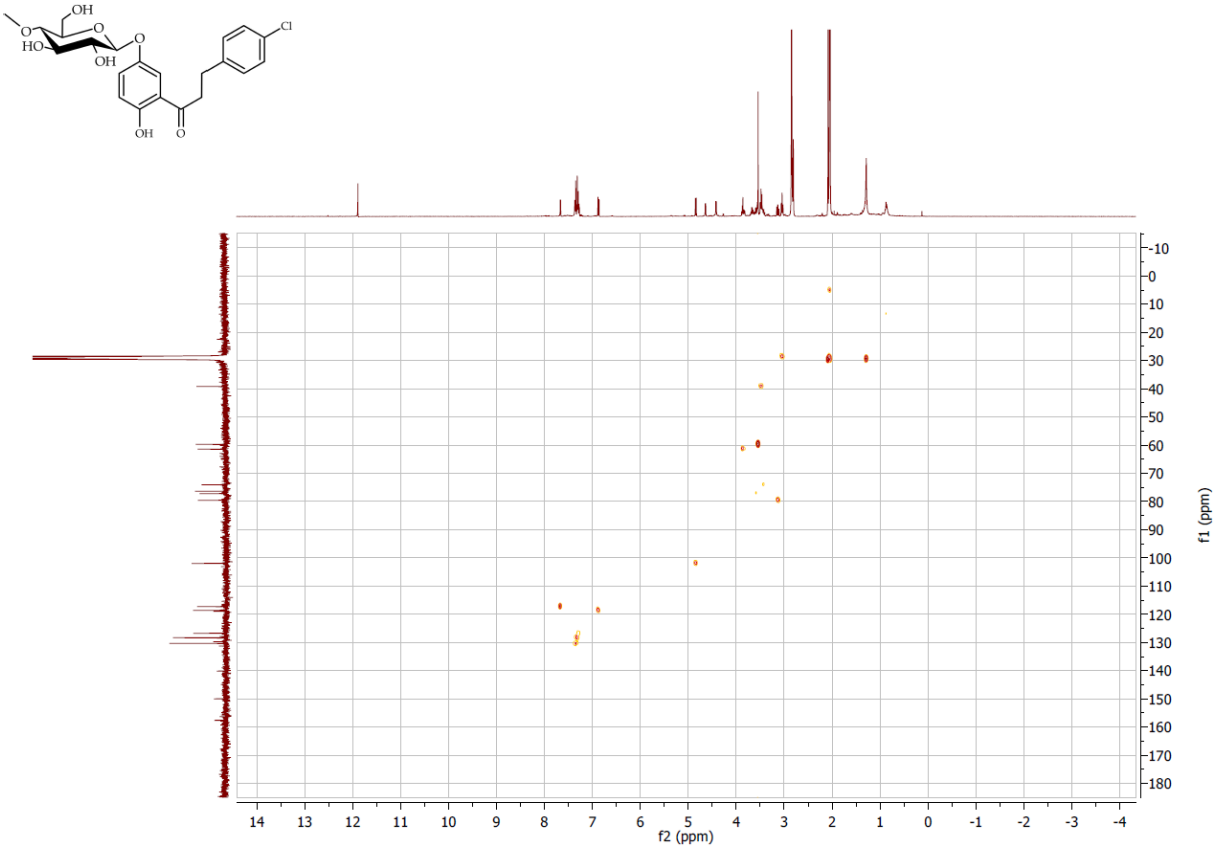


Figure S63. HMQC contour map – ^{1}H x ^{13}C of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

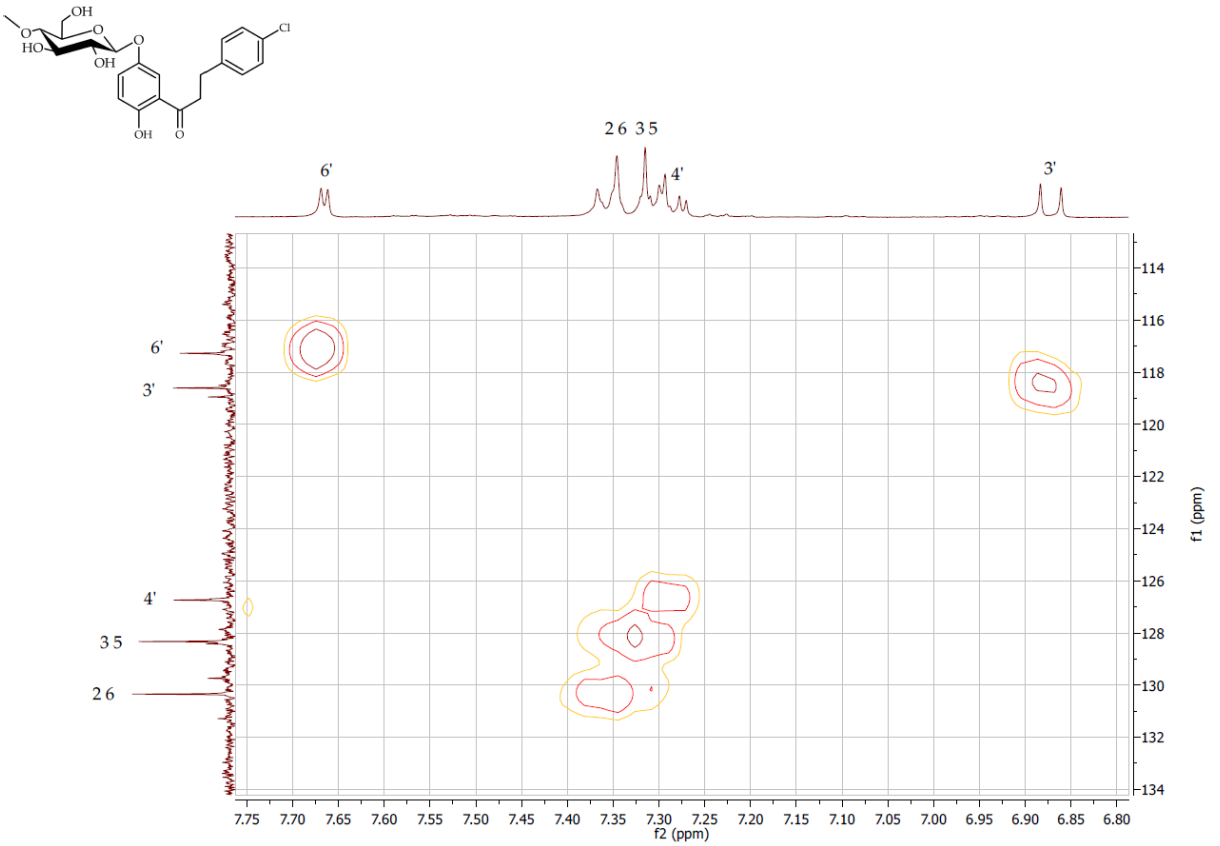


Figure S64. HMQC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

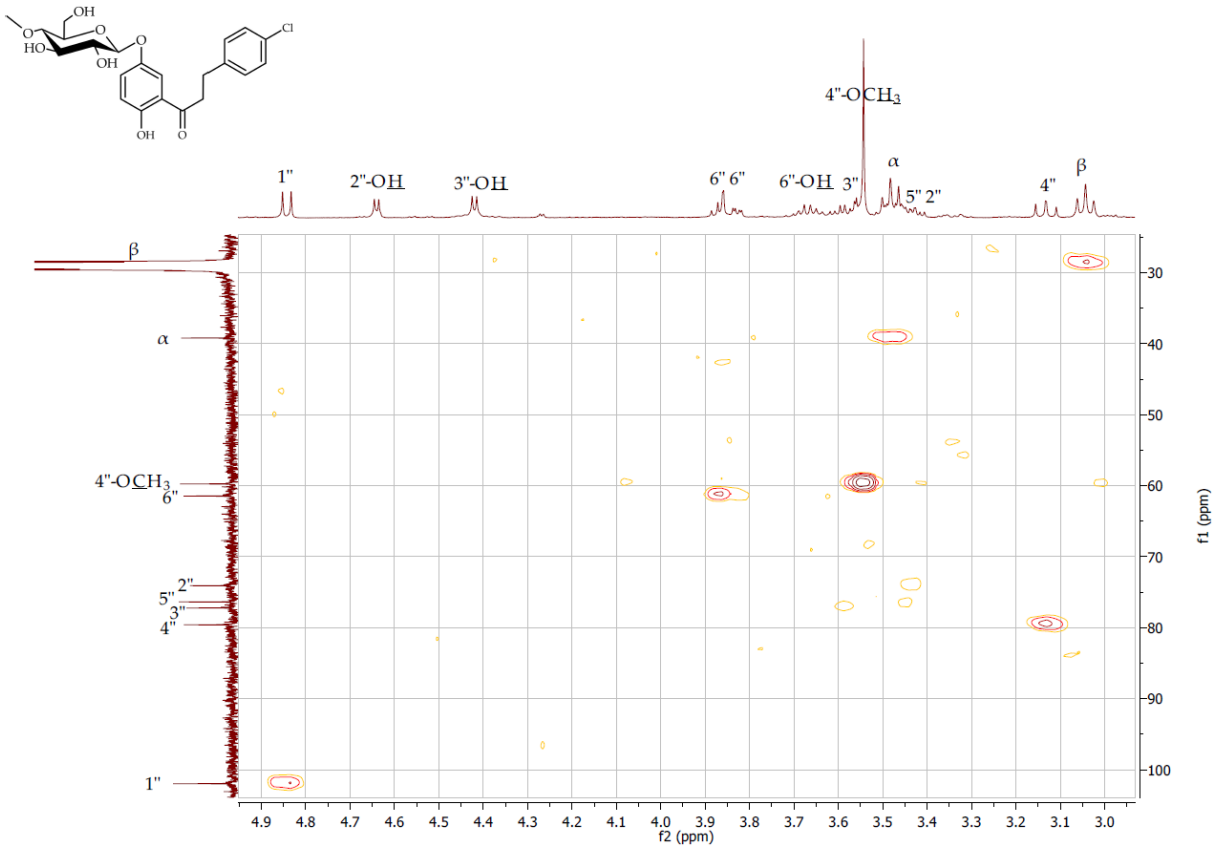


Figure S65. HMQC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

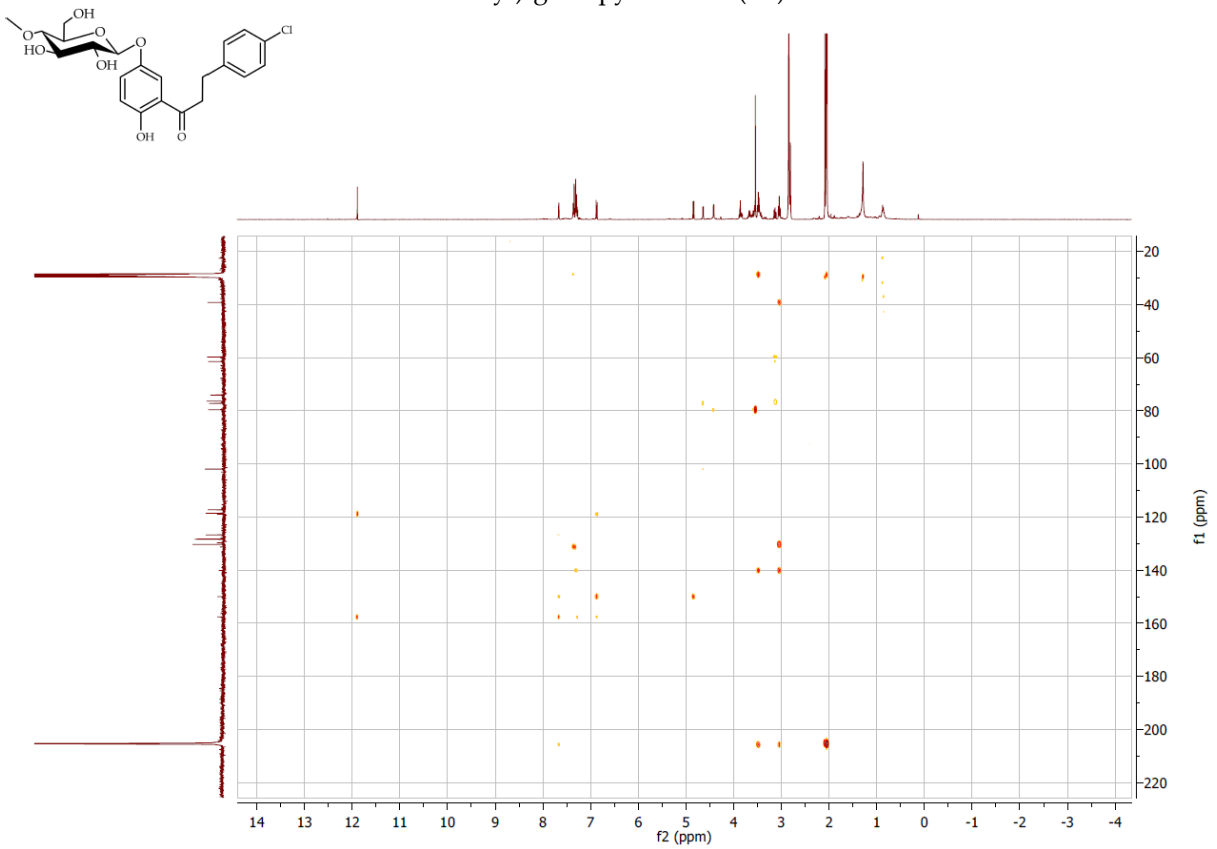


Figure S66. HMBC contour map – ^{1}H x ^{13}C of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

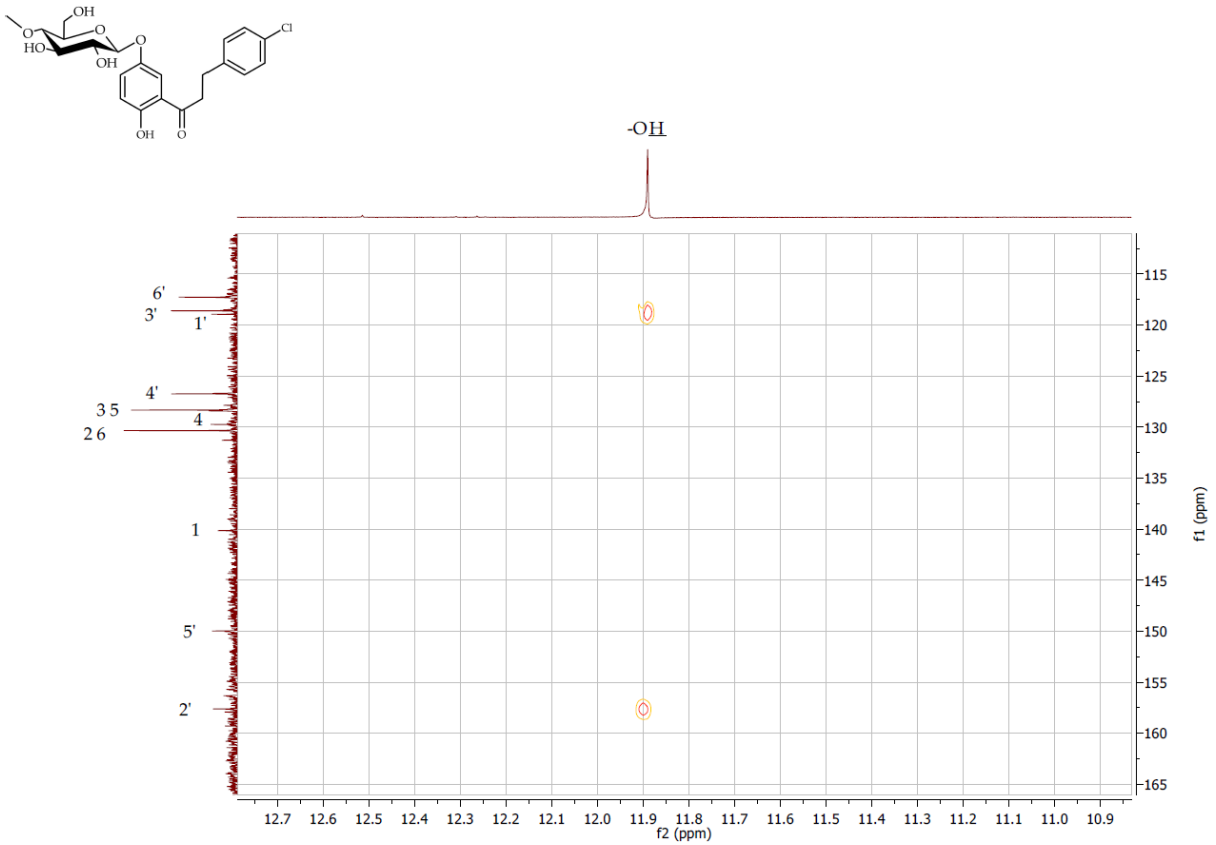


Figure S67. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

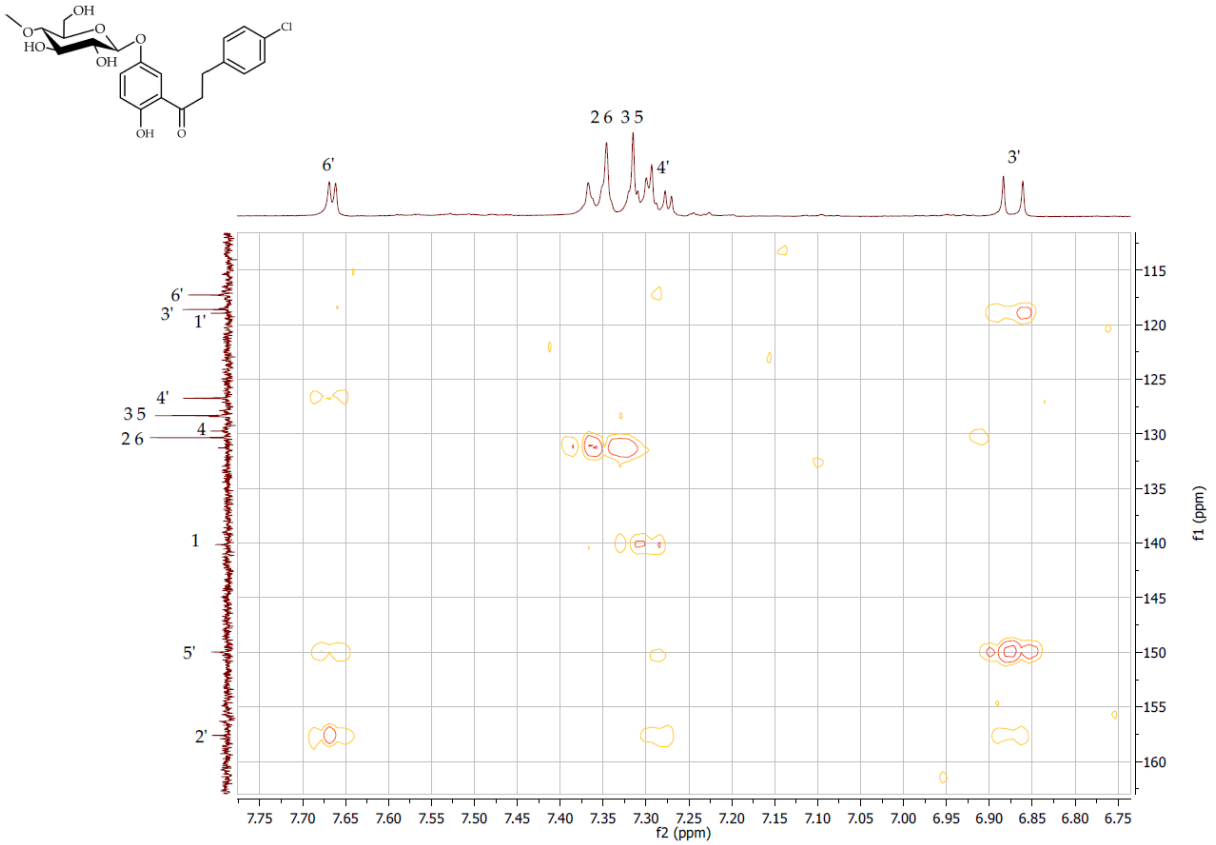


Figure S68. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

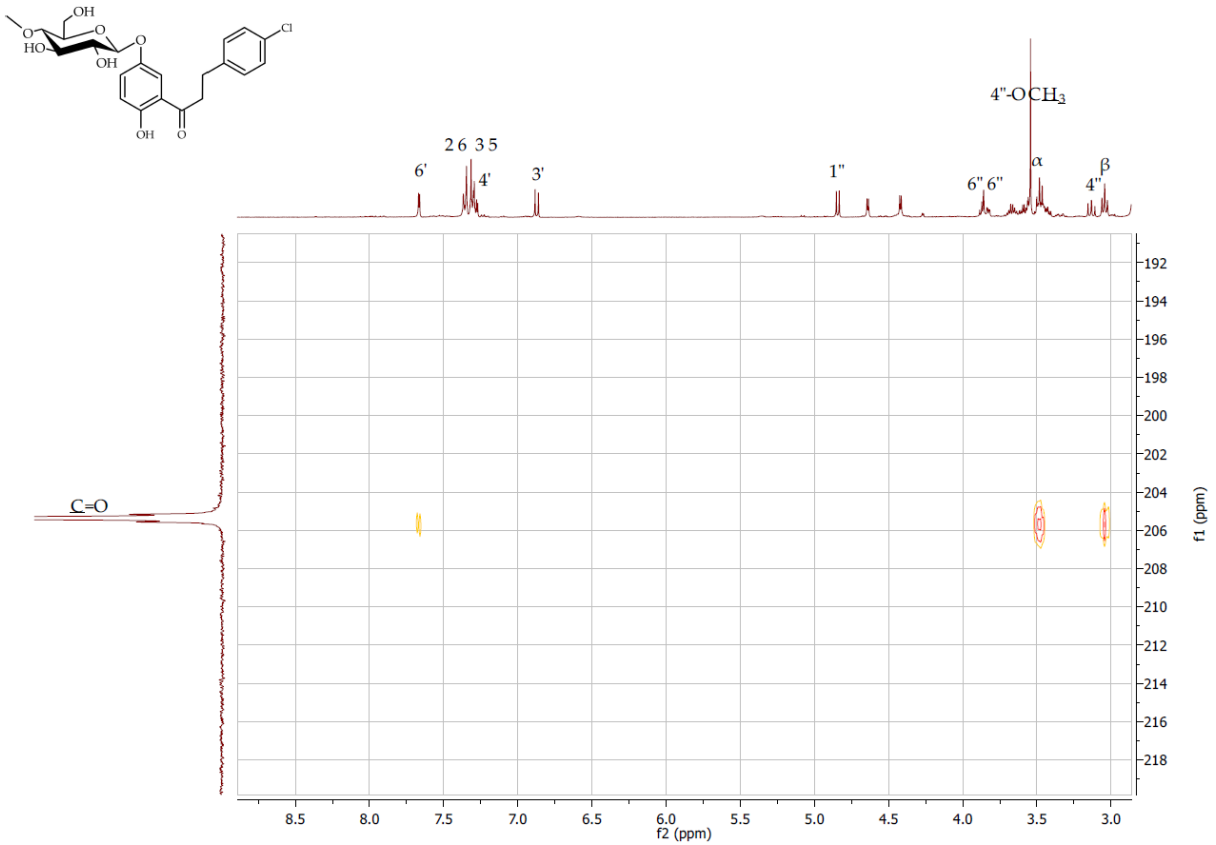


Figure S69. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

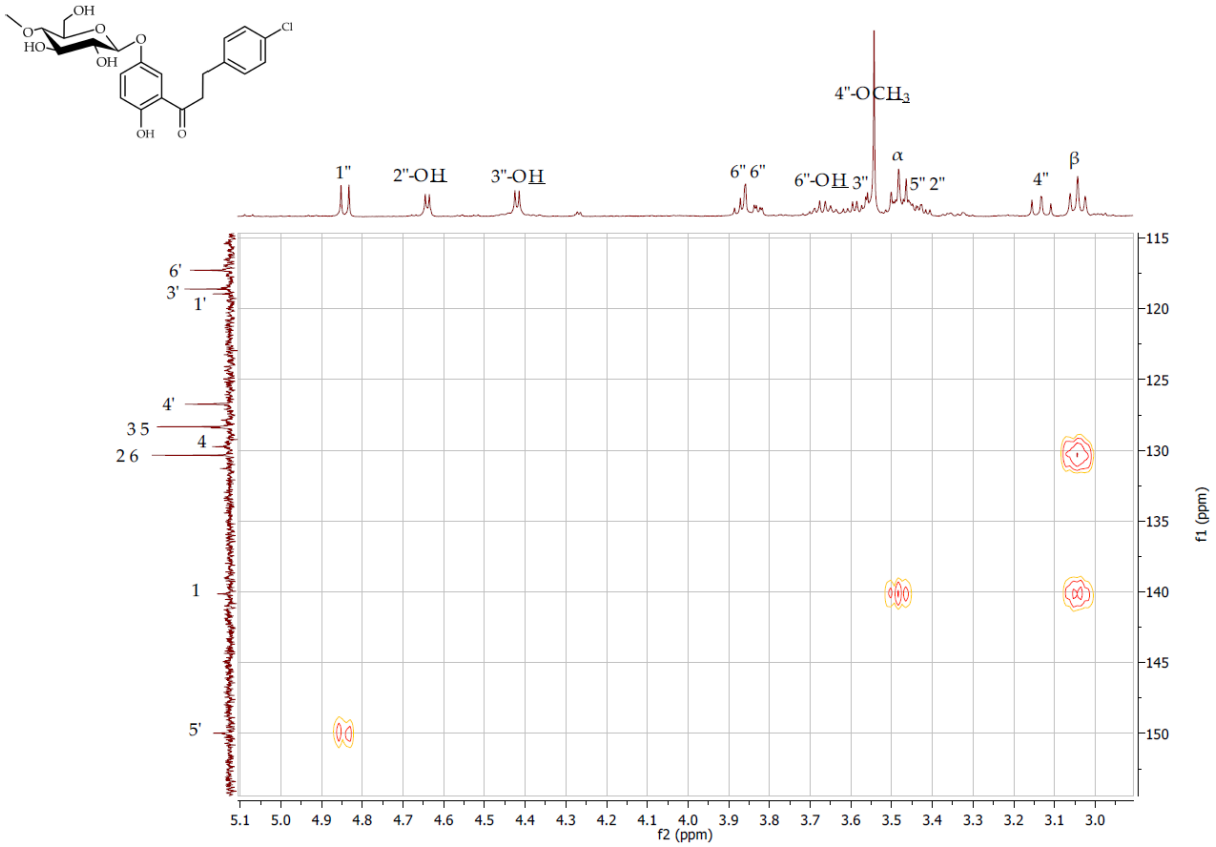


Figure S70. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

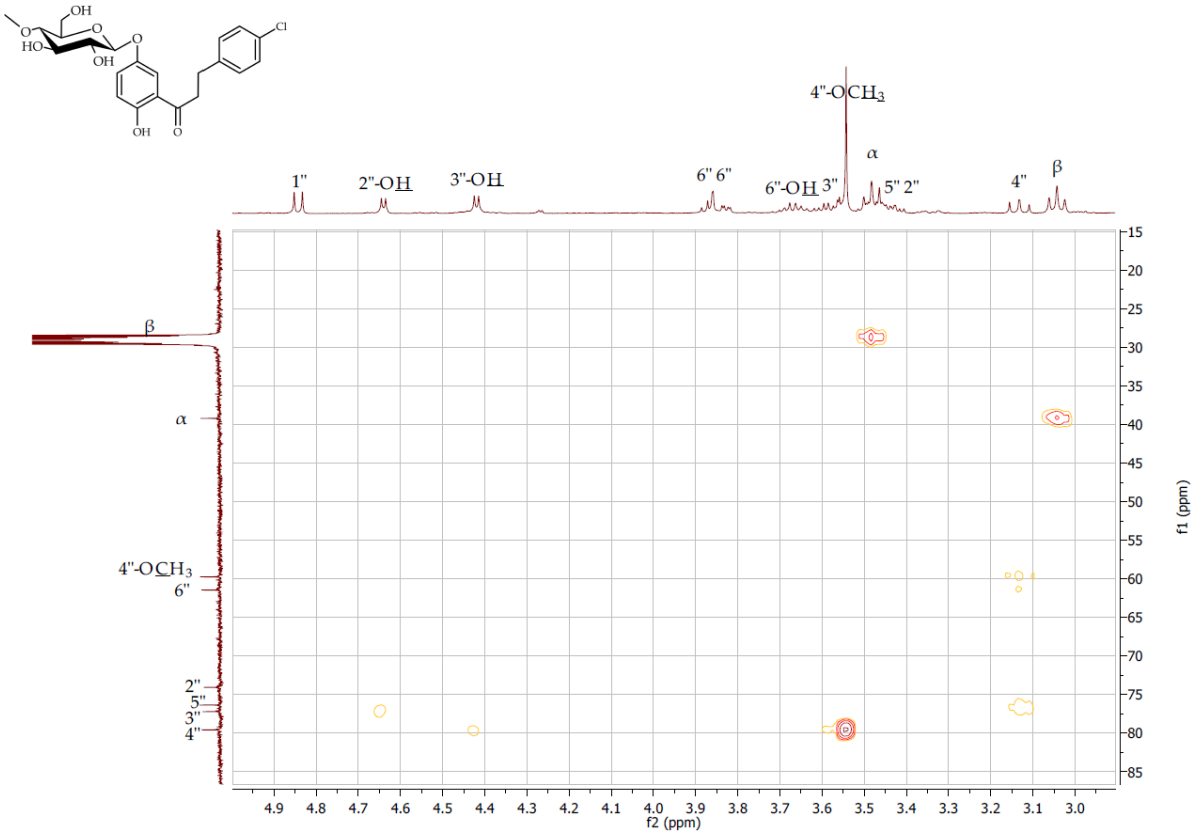


Figure S71. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**)

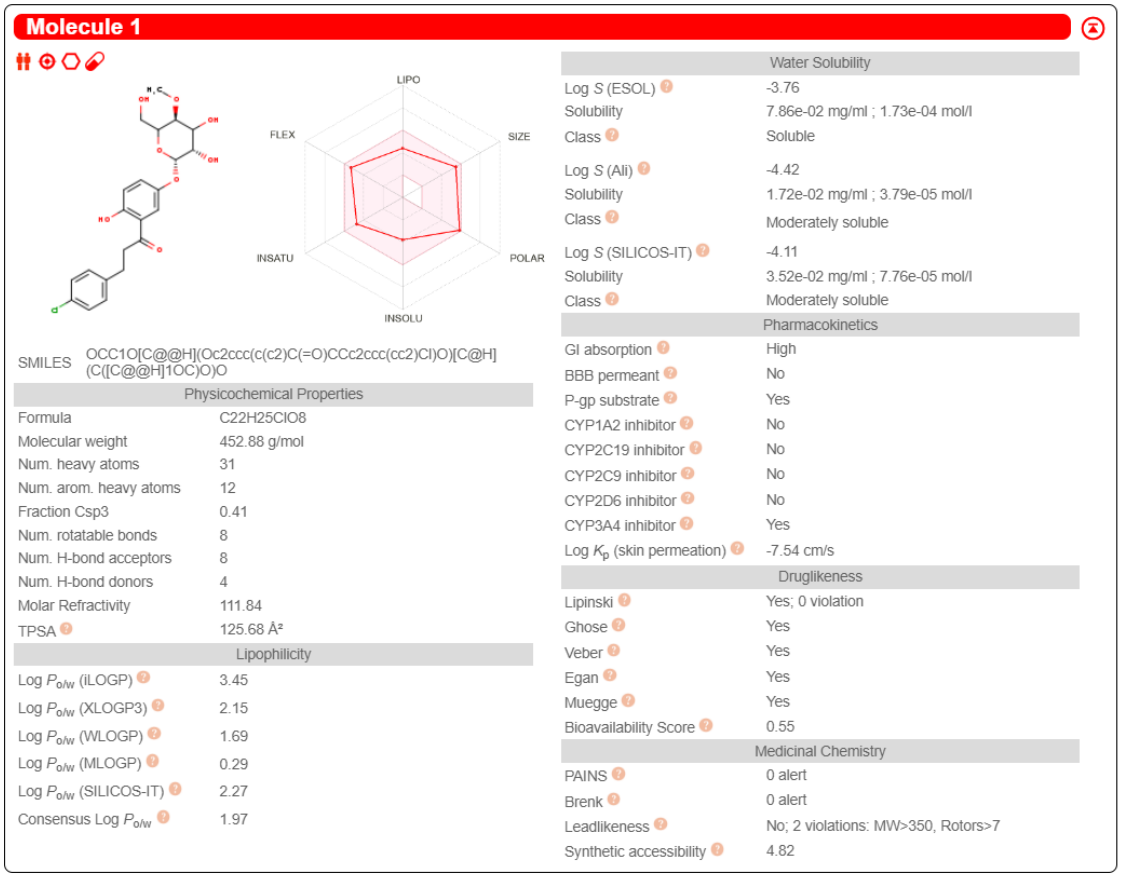


Figure S72. 4-Chloro-2′-hydroxydihydrochalcone 5′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3b**) physicochemical and ADME parameters prediction using the SwissADME modelling

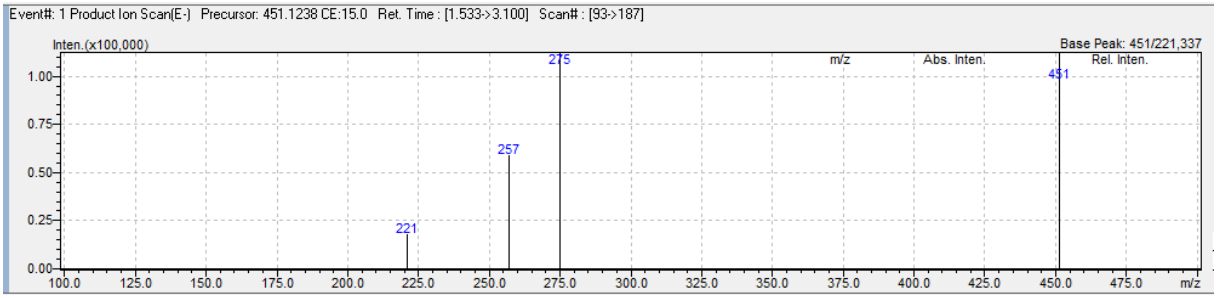
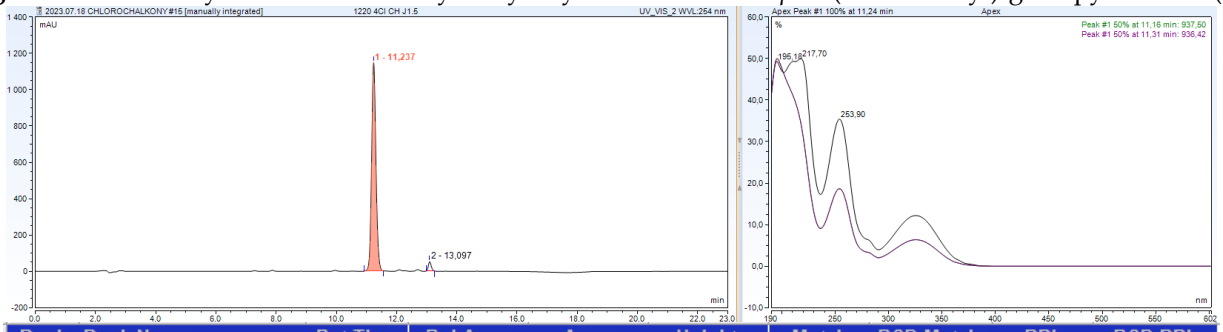


Figure S73. MS analysis of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)



Peak No.	Peak Name	Ret.Time min	Rel.Area %	Area mAU*min	Height mAU	Match	RSD Match %	PPI nm	RSD PPI %
1		11,237	97,03	188,7442	1148,41	924	7,34	212,9	3,07
2		13,097	2,97	5,7721	52,39	999	0,09	204,4	0,24
Maximum			97,03	188,7442	1148,41	999	7,34		3,07
Minimum			2,97	5,7721	52,39	924	0,09		0,24

Figure S74. HPLC analysis of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

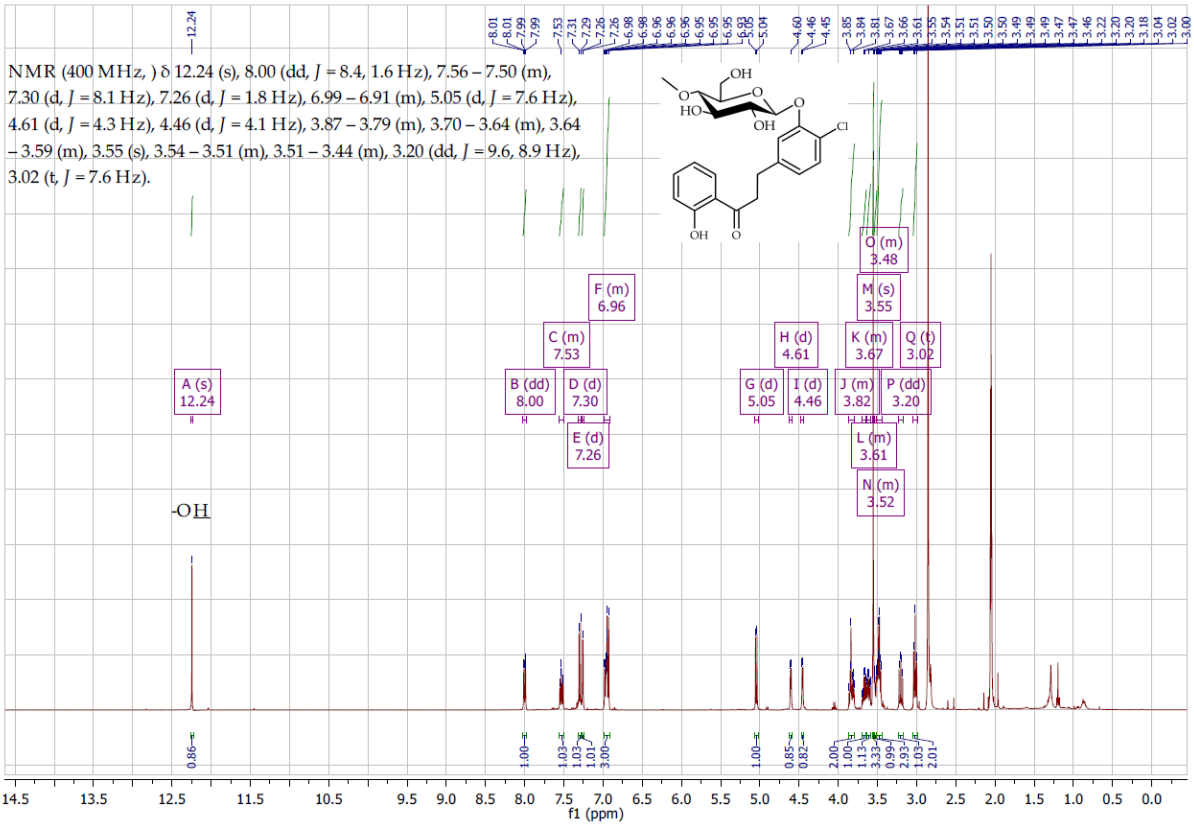


Figure S75. ^{1}H NMR spectrum (*δ*, acetone-d6, 600 MHz) of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

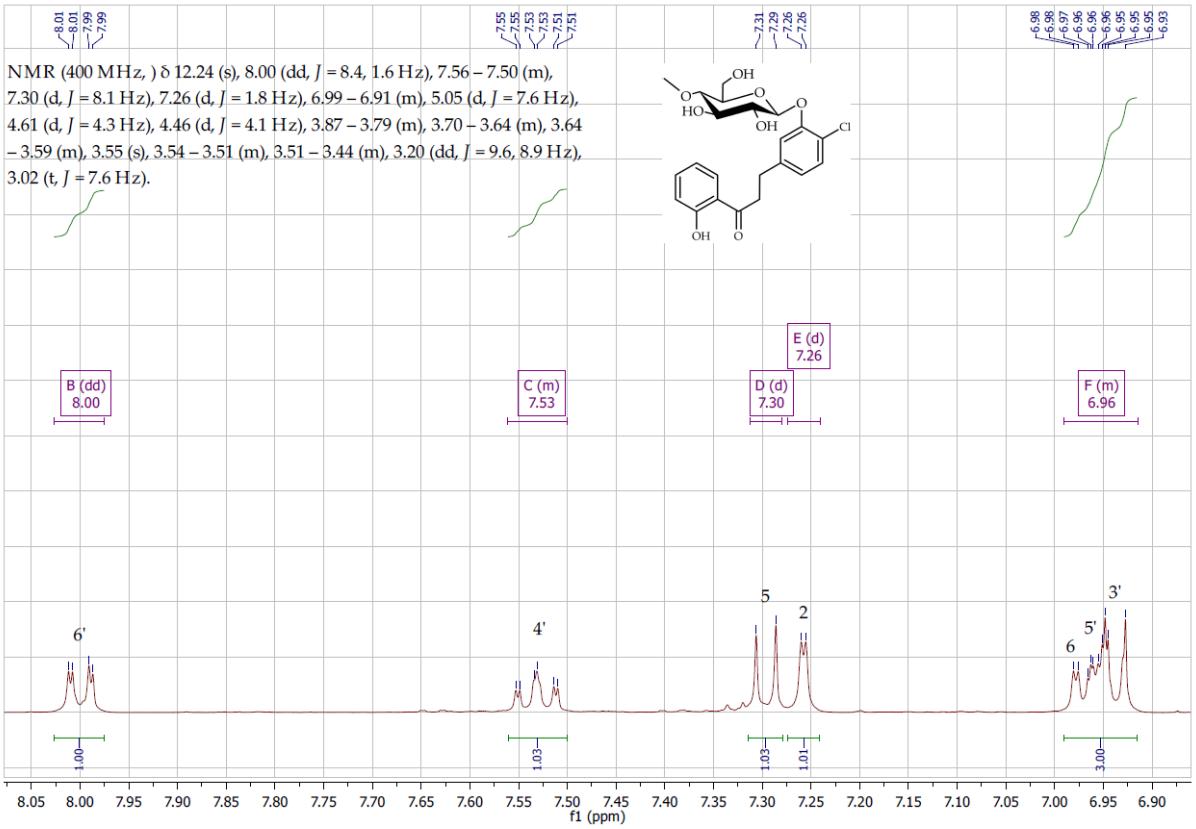


Figure S76. [1]H NMR spectrum expansion (*δ*, acetone-d6, 600 MHz) of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

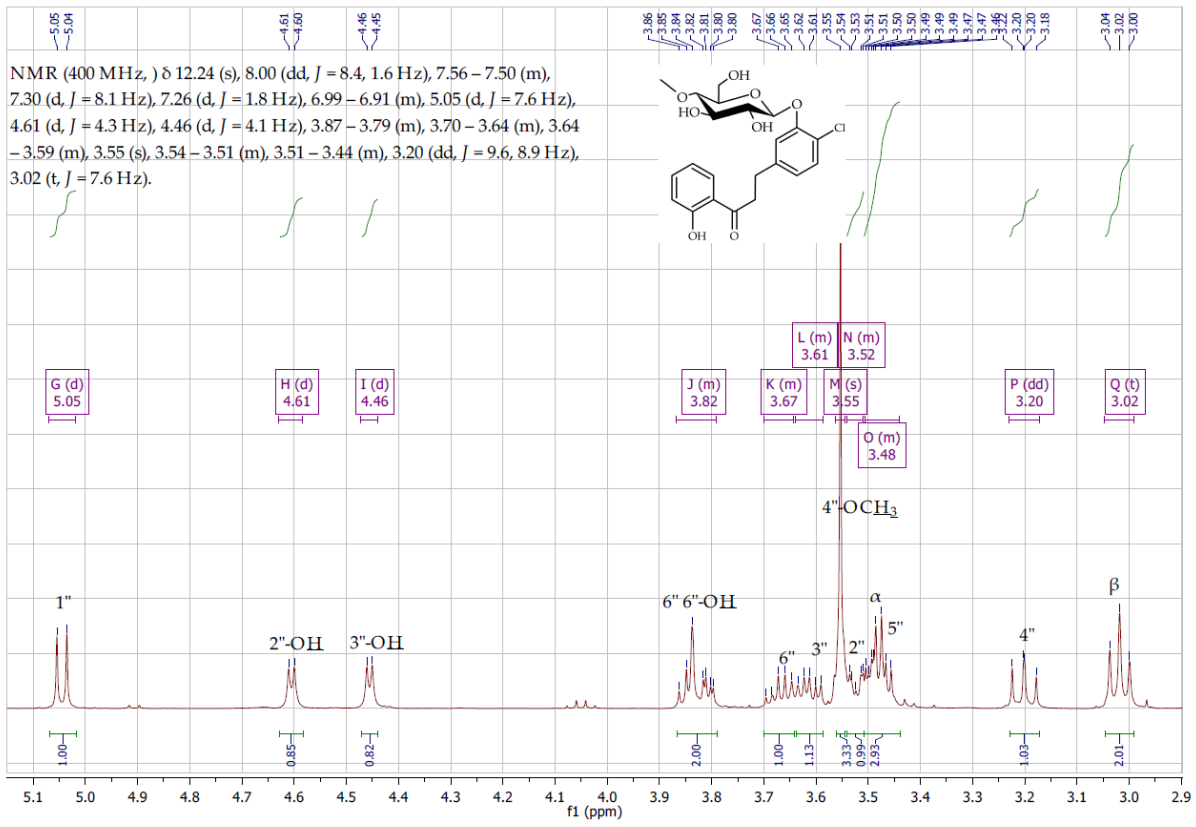


Figure S77. [1]H NMR spectrum expansion (*δ*, acetone-d6, 600 MHz) of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

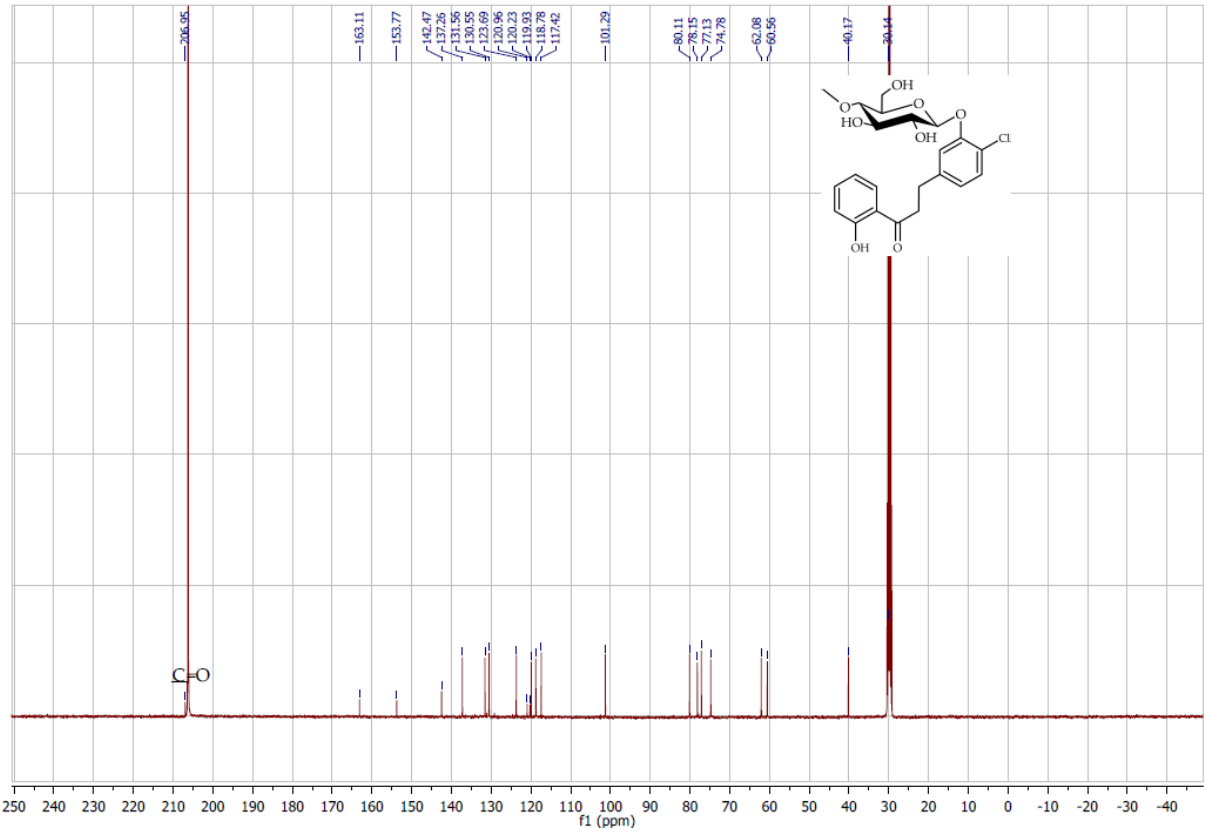


Figure S78. ^{13}C NMR spectrum (δ, acetone-d6, 151 MHz) of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

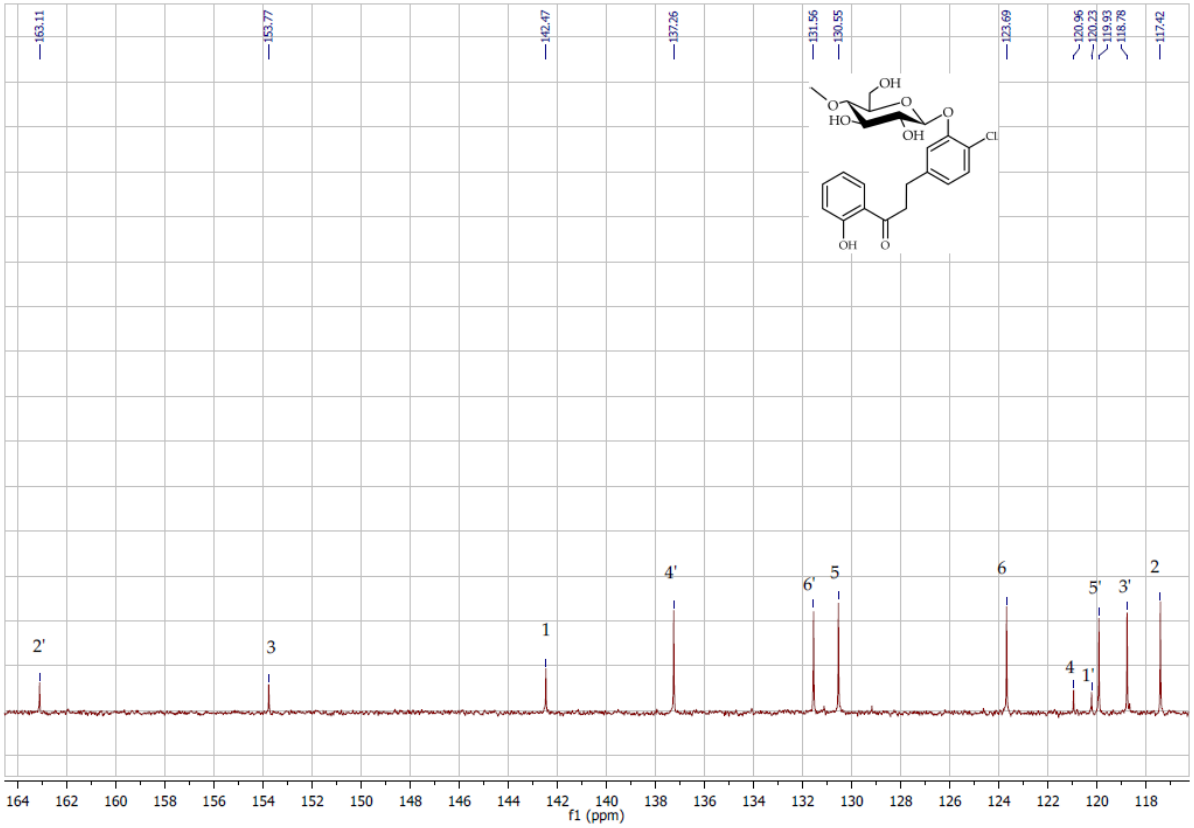


Figure S79. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

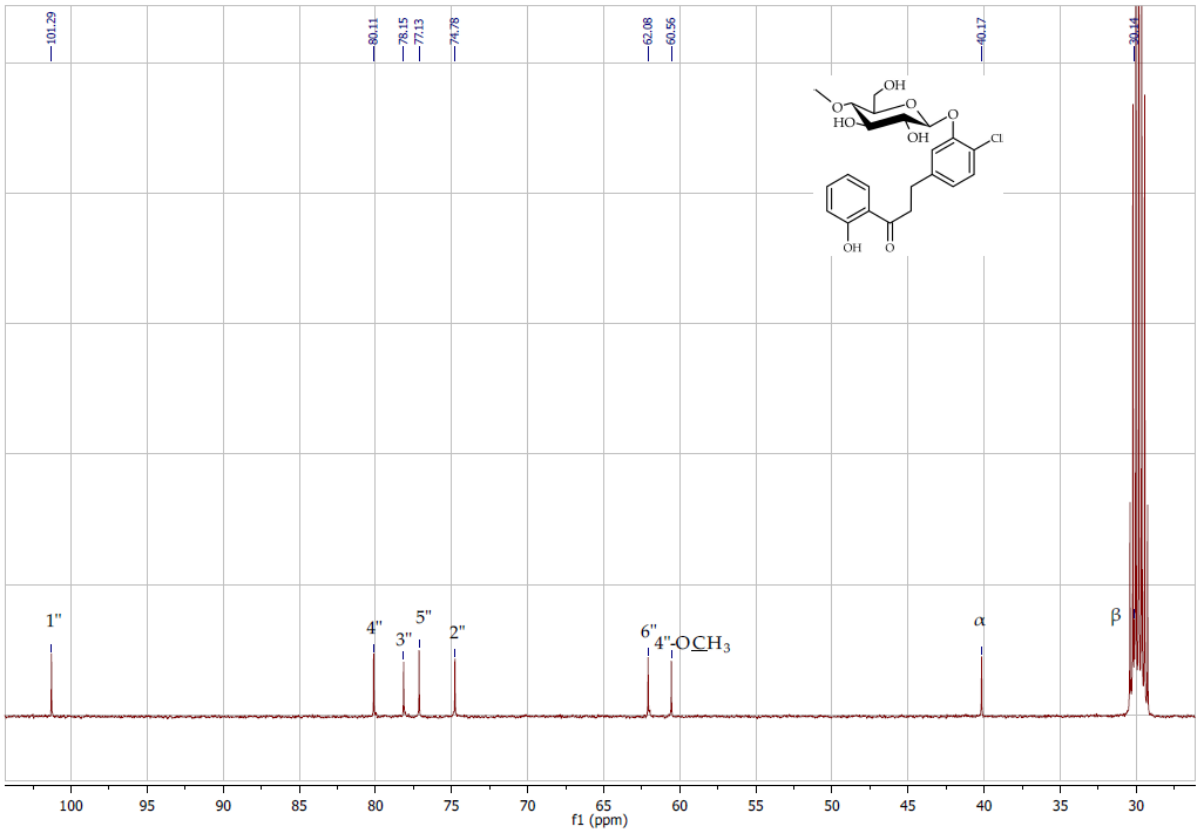


Figure S80. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

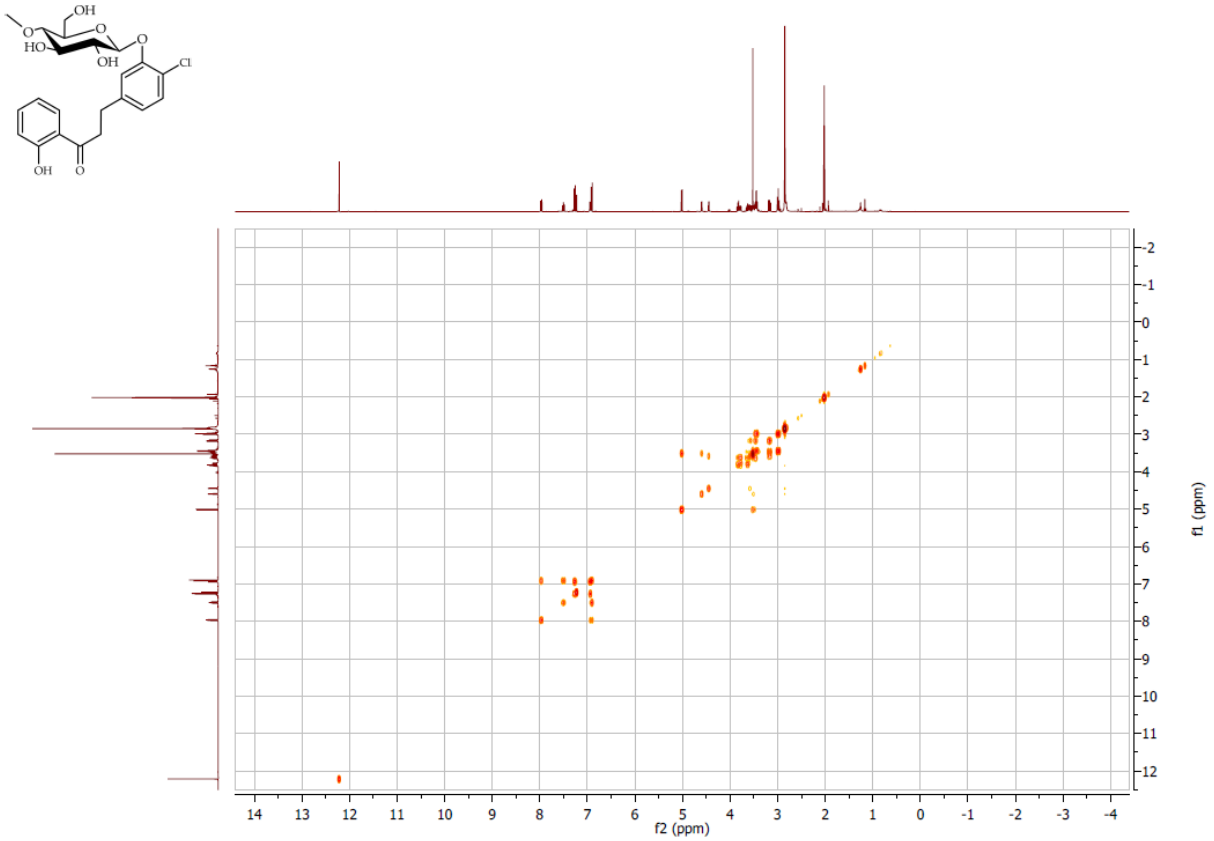


Figure S81. COSY contour map – ^{1}H x ^{1}H of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

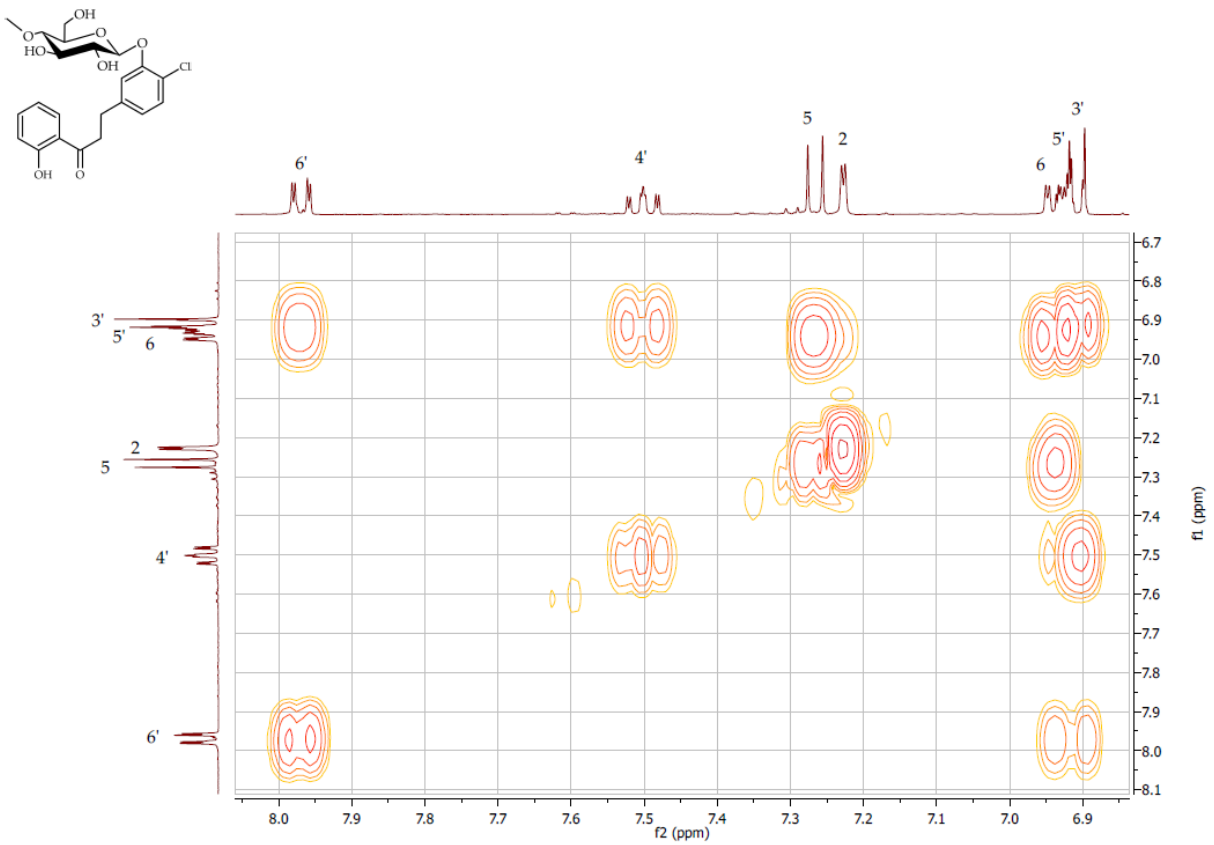


Figure S82. COSY contour map – ^{1}H x ^{1}H expansion of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

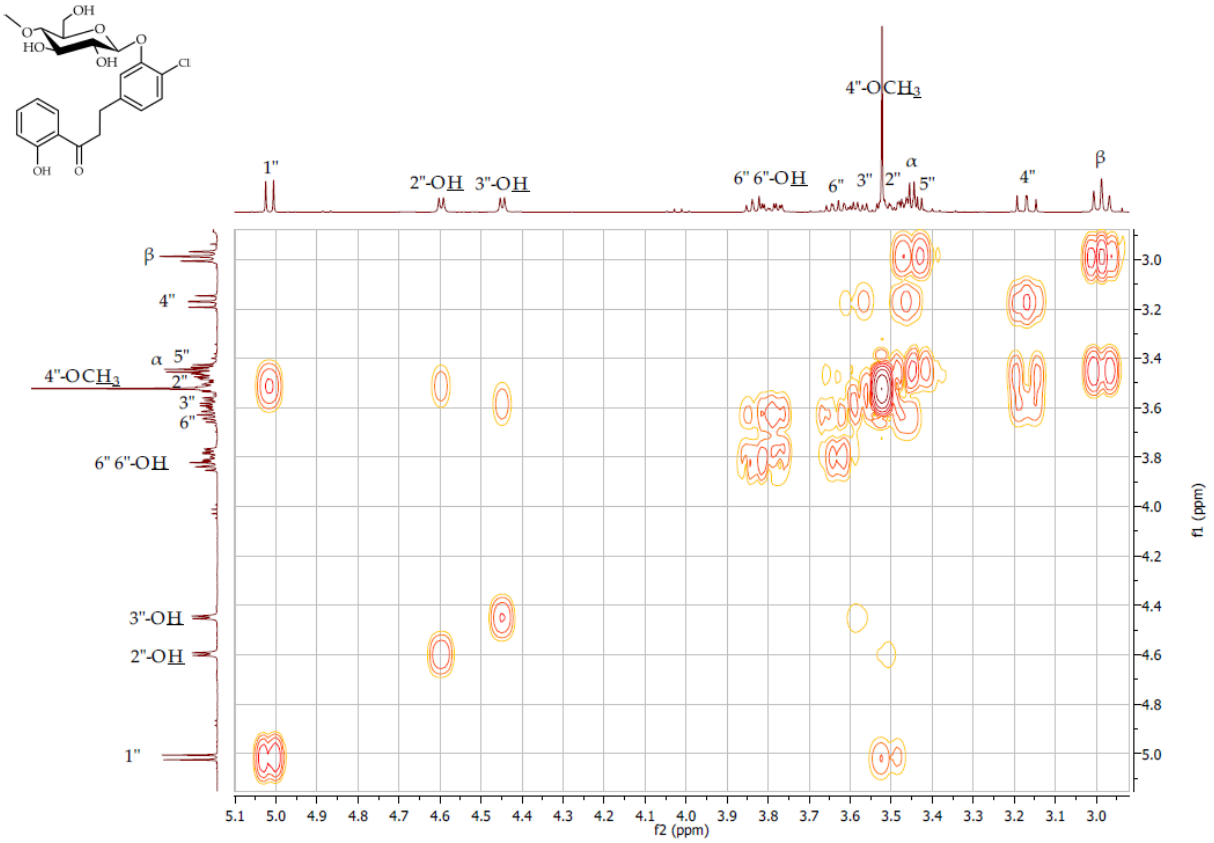


Figure S83. COSY contour map – ^{1}H x ^{1}H expansion of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

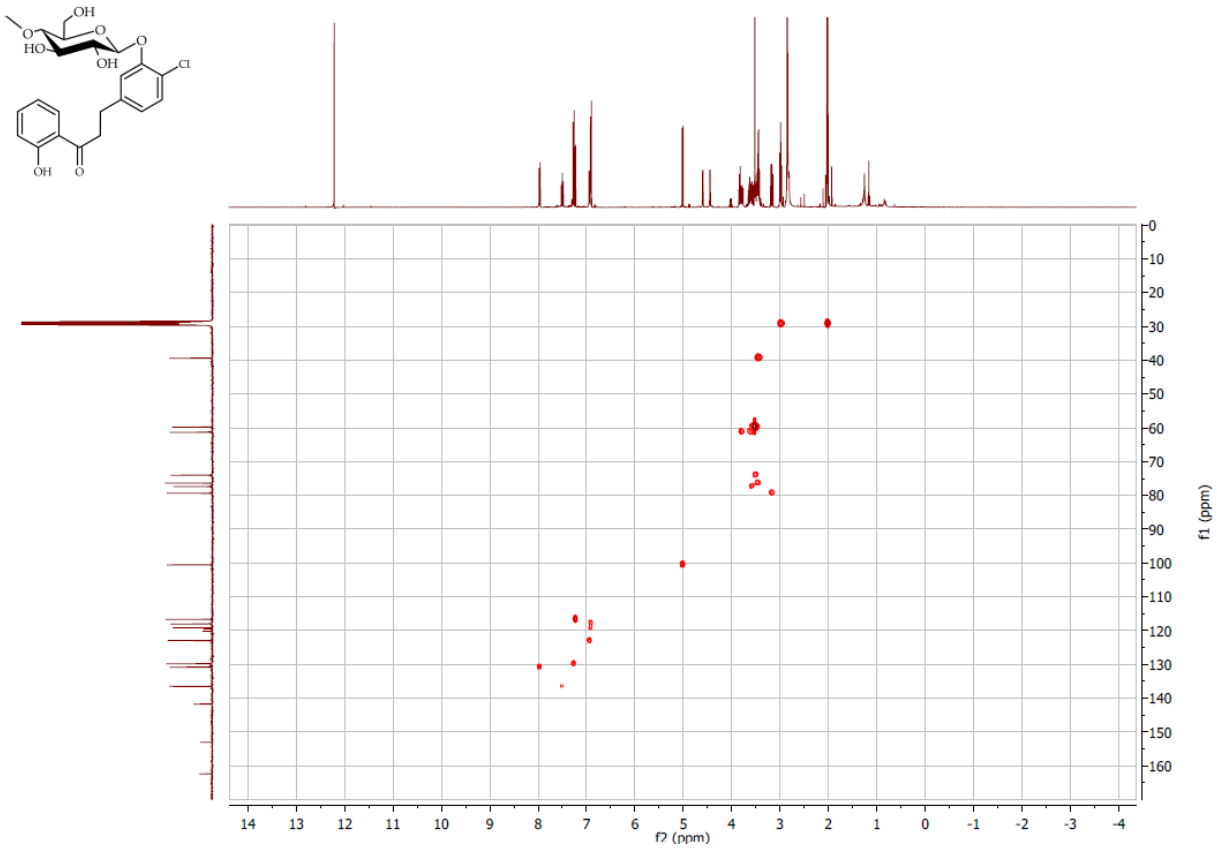


Figure S84. HMQC contour map – ^{1}H x ^{13}C of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

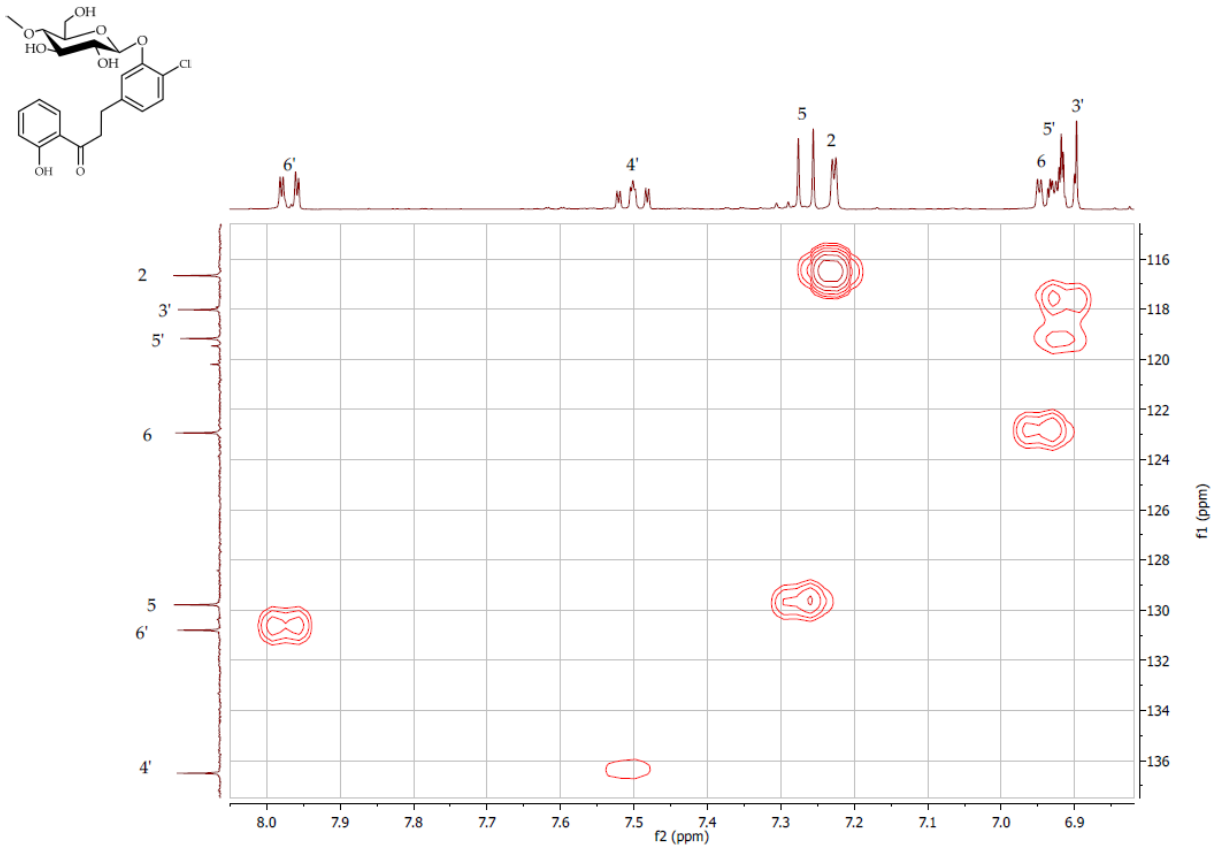


Figure S85. HMQC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

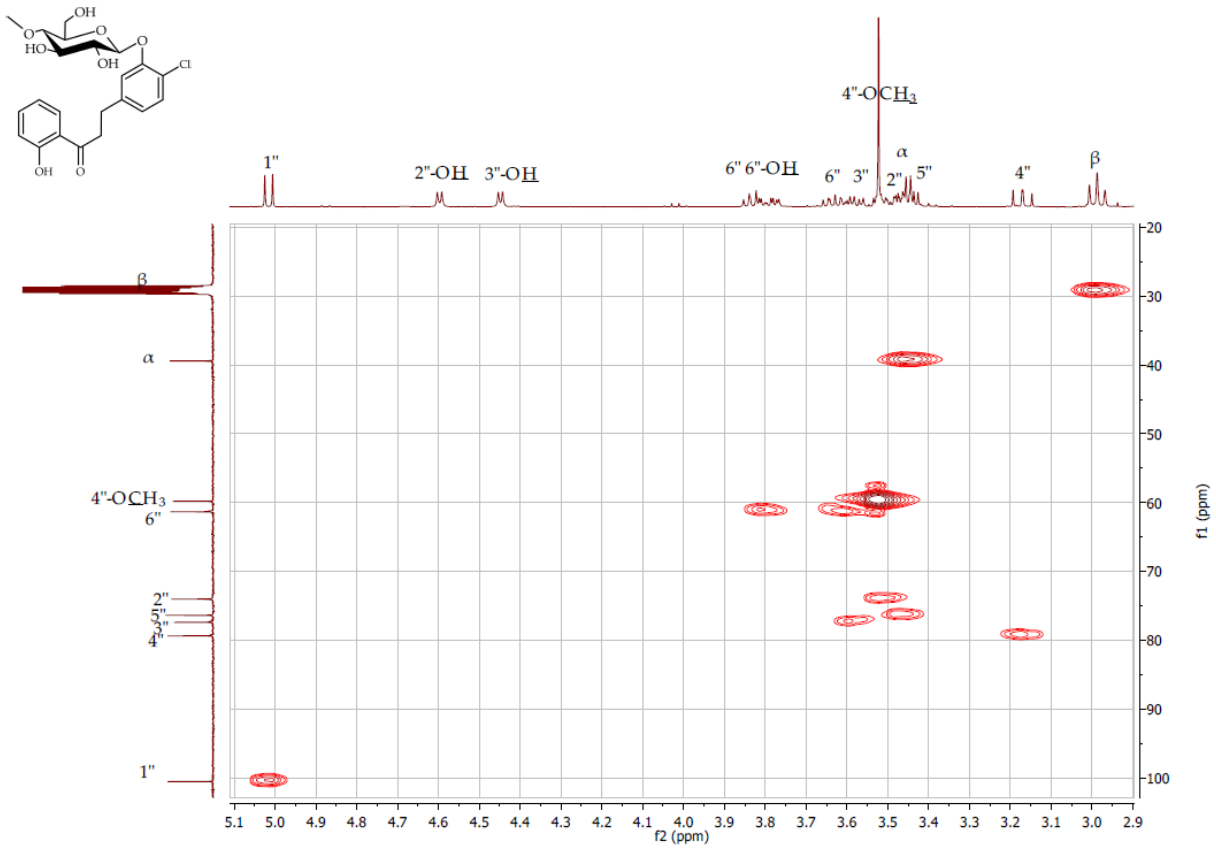


Figure S86. HMQC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

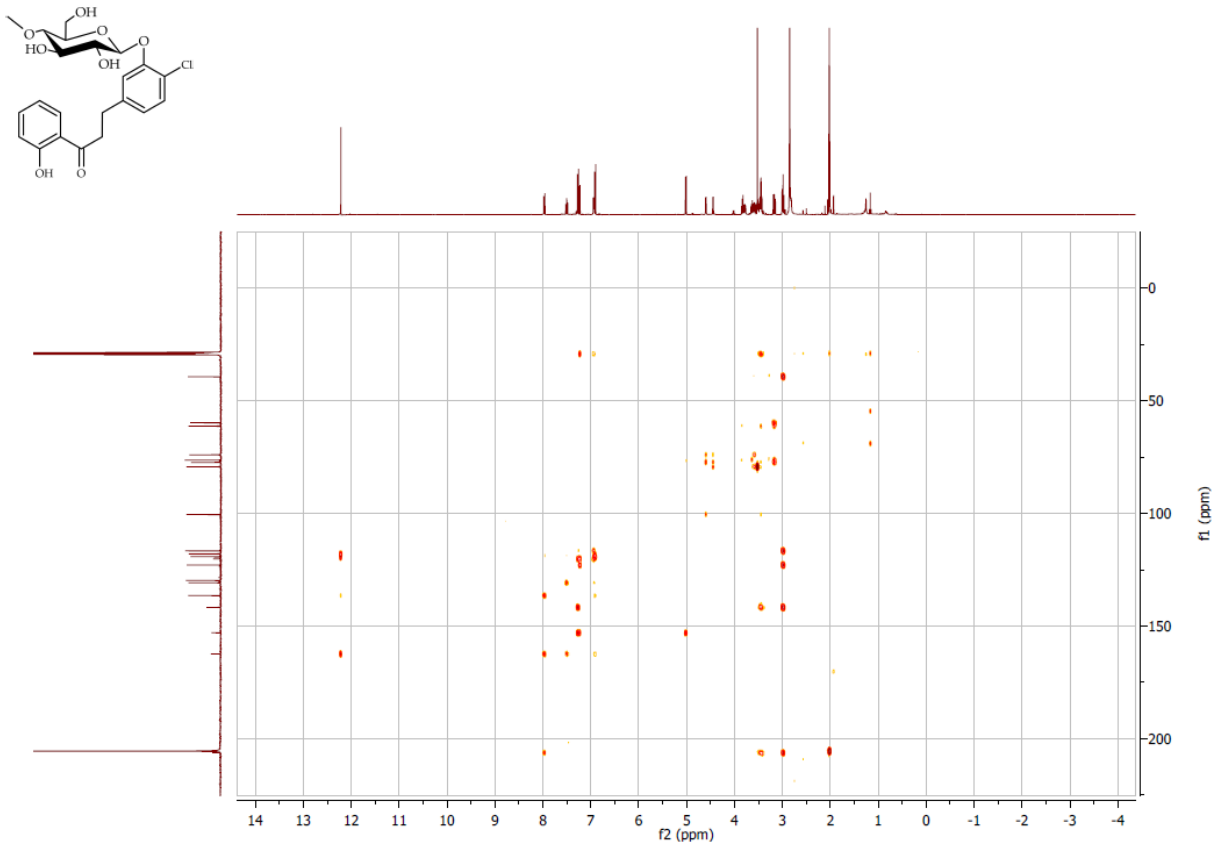


Figure S87. HMBC contour map – ^{1}H x ^{13}C of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

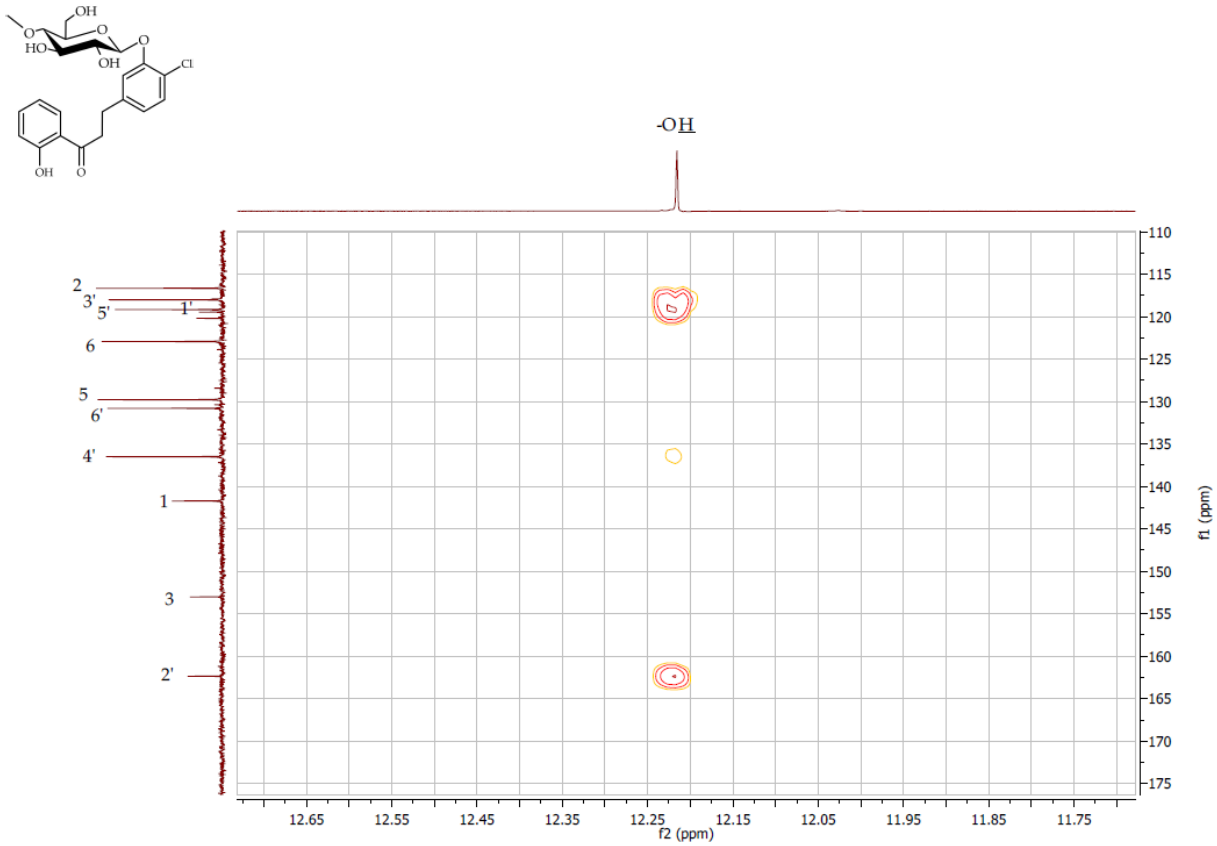


Figure S88. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

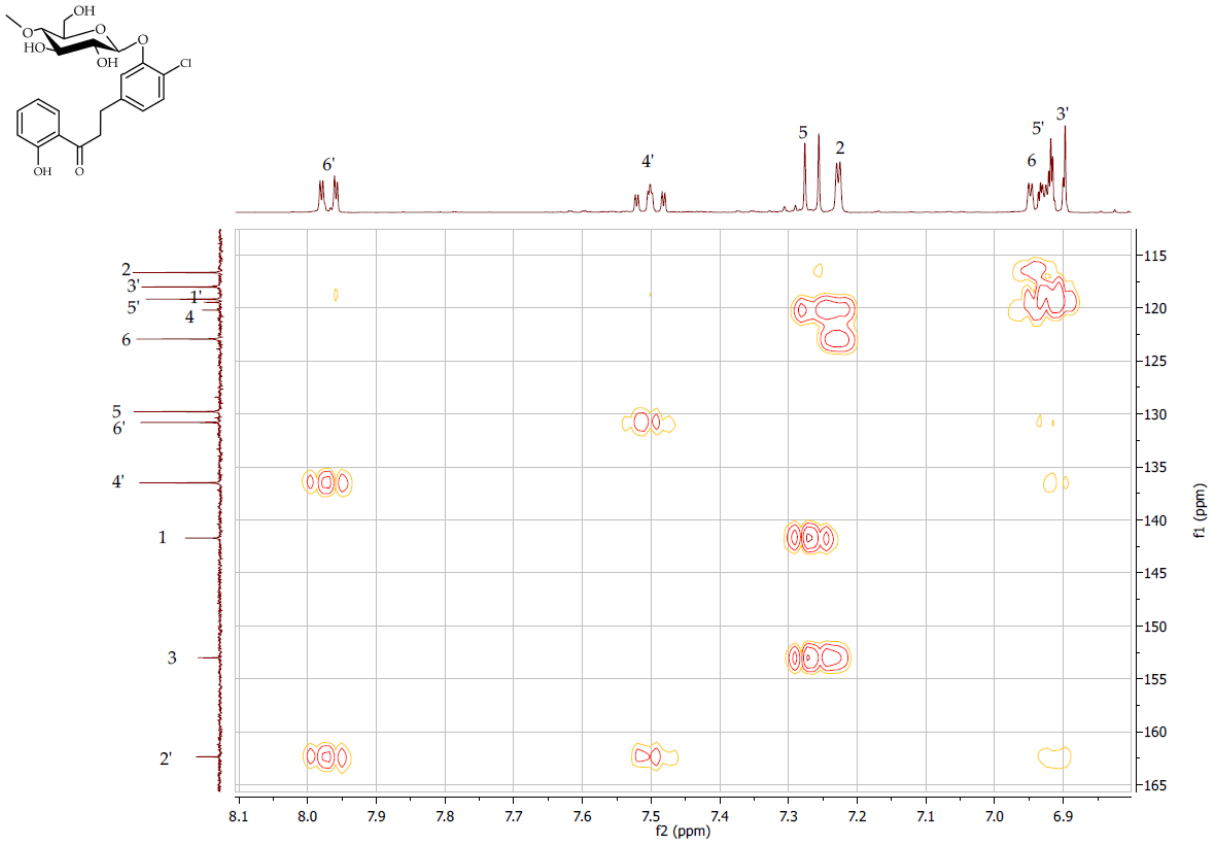


Figure S89. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

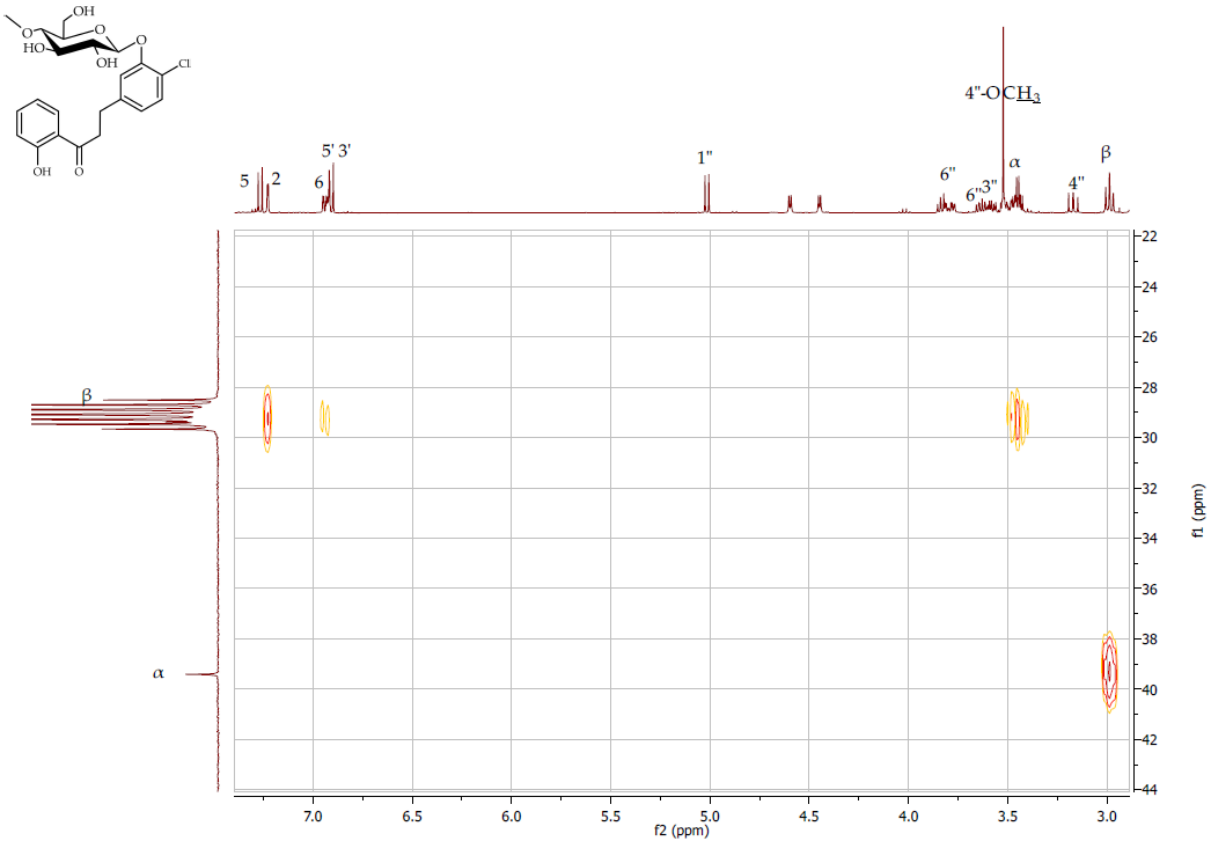


Figure S90. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

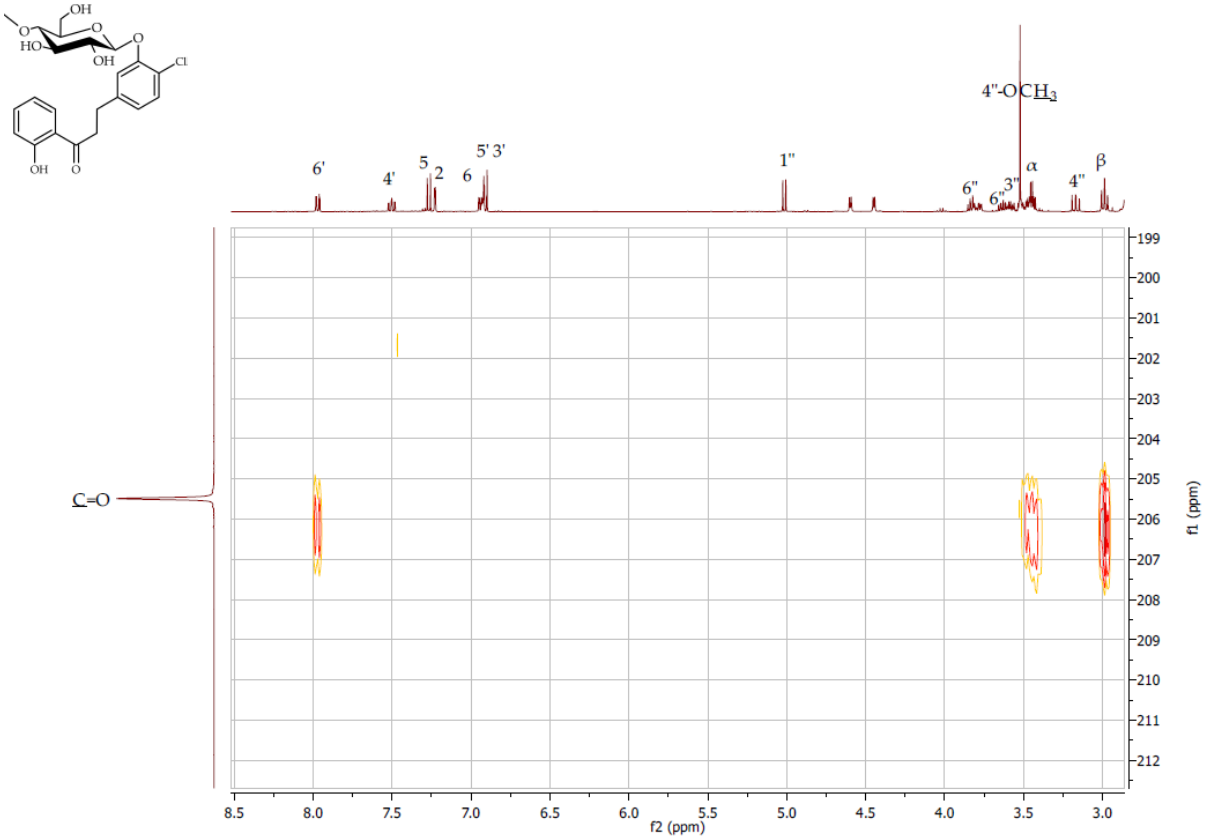


Figure S91. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

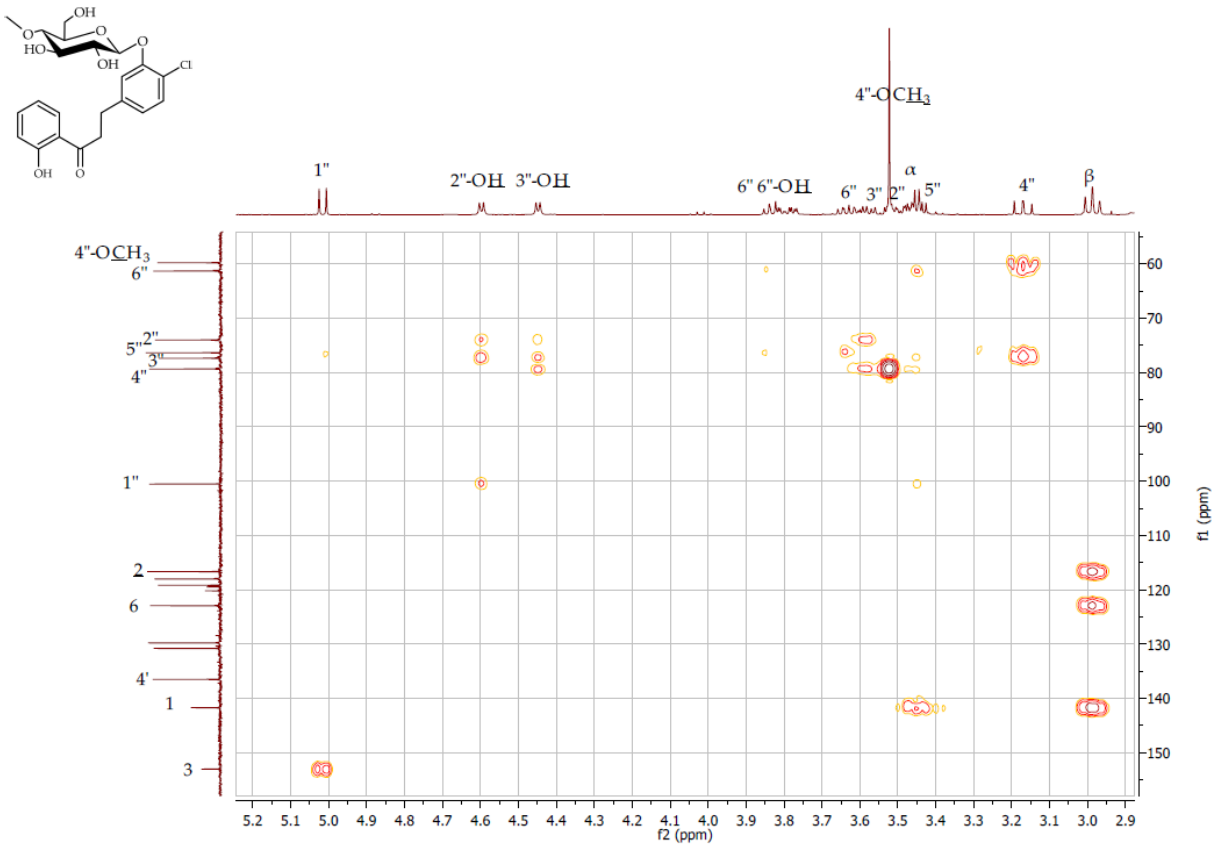


Figure S92. HMBC contour map – ^{1}H x ^{13}C expansion of 4-chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**)

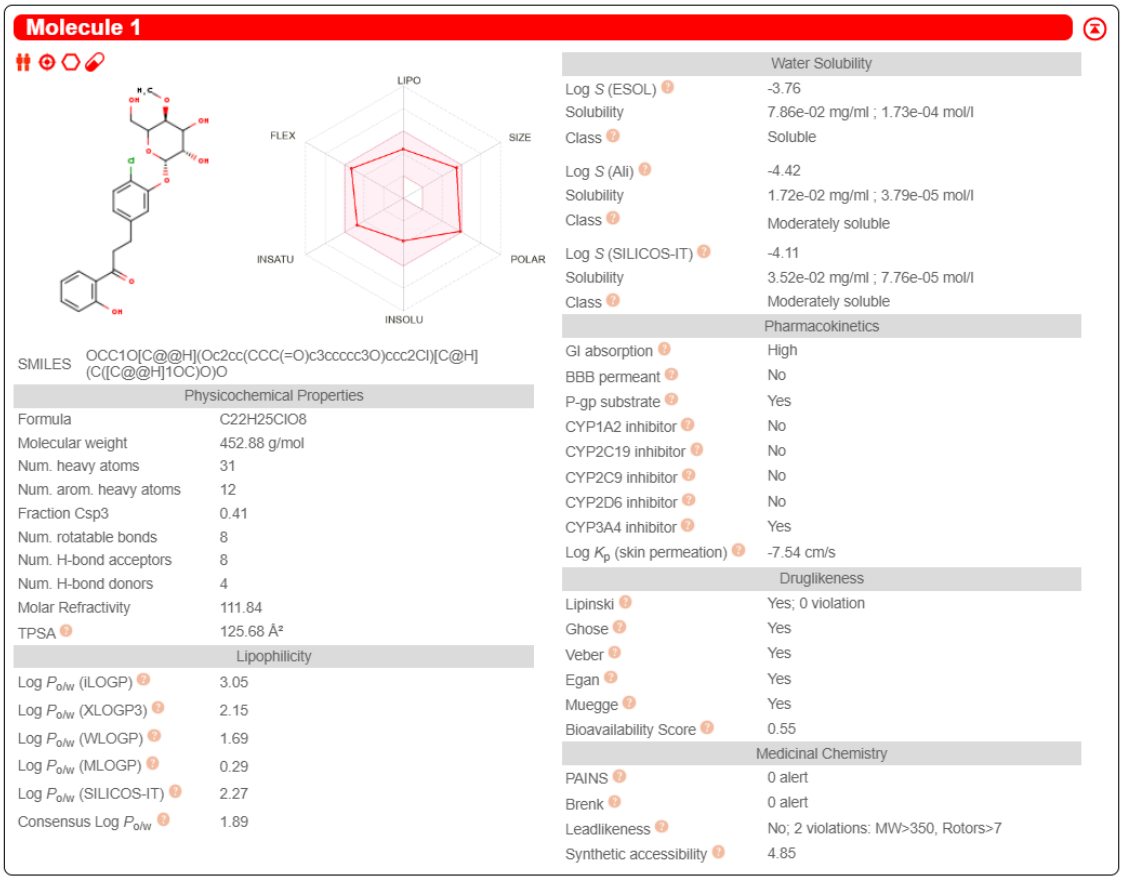


Figure S93. 4-Chloro-2′-hydroxydihydrochalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**3c**) physicochemical and ADME parameters prediction using the SwissADME modelling

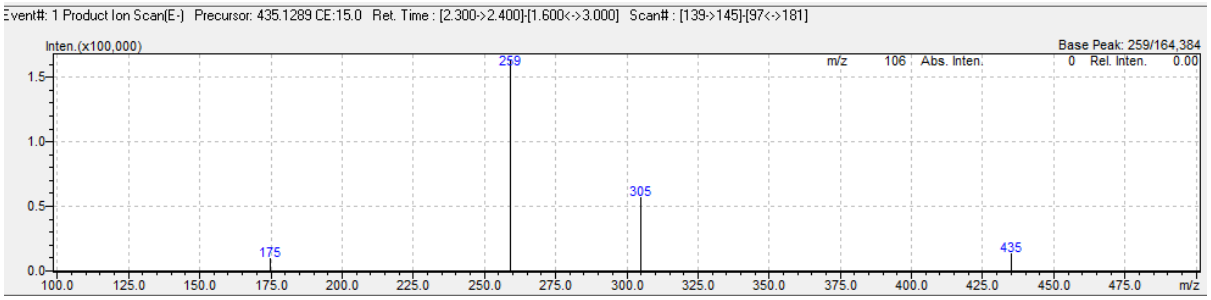
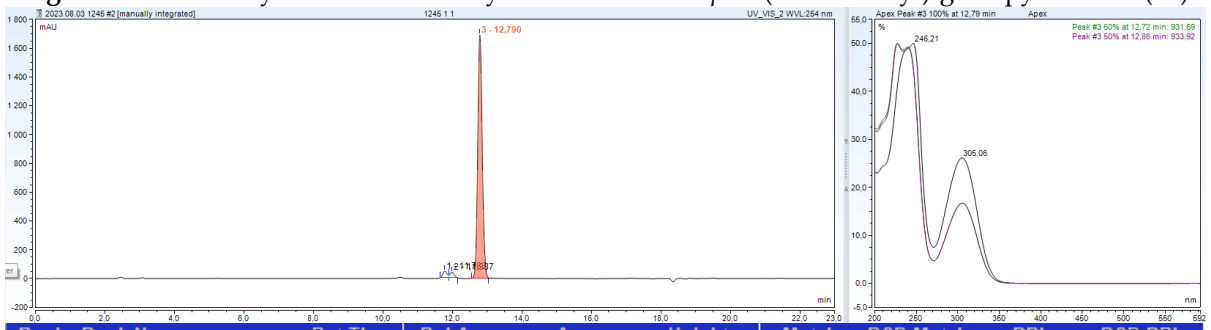


Figure S94. MS analysis of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)



Peak No.	Peak Name	Ret.Time min	Rel.Area %	Area mAU*min	Height mAU	Match	RSD Match %	PPI nm	RSD PPI %
1		11,783	2,49	6,5172	45,34	1000	0,01	214,4	0,05
2		11,987	2,19	5,7189	38,21	997	0,49	215,1	0,62
3		*12,790*	*95,32*	*249,3451*	*1687,39*	*858*	*19,18*	*234,5*	*4,78*
Maximum			95,32	249,3451	1687,39	1000	19,18		4,78
Minimum			2,19	5,7189	38,21	858	0,01		0,05

Figure S95. HPLC analysis of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

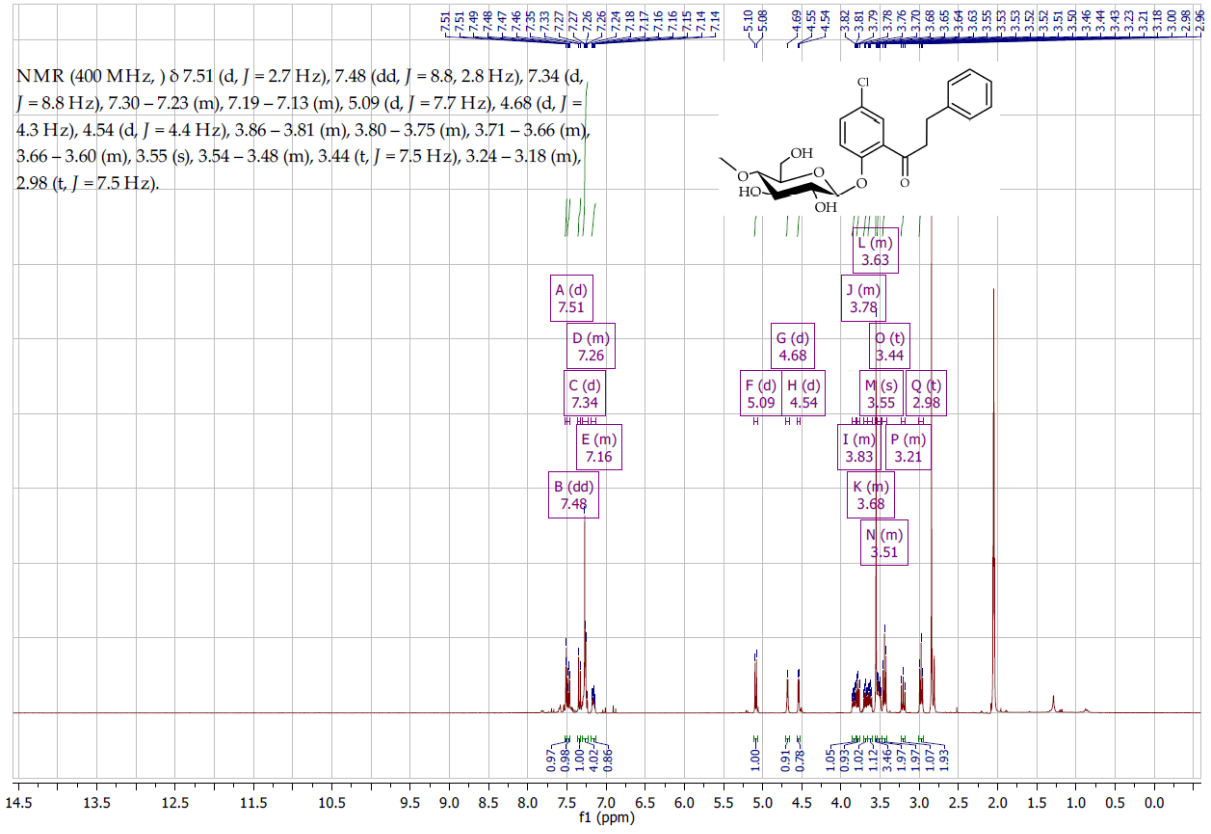


Figure S96. ^{1}H NMR spectrum (*δ*, acetone-d6, 600 MHz) of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

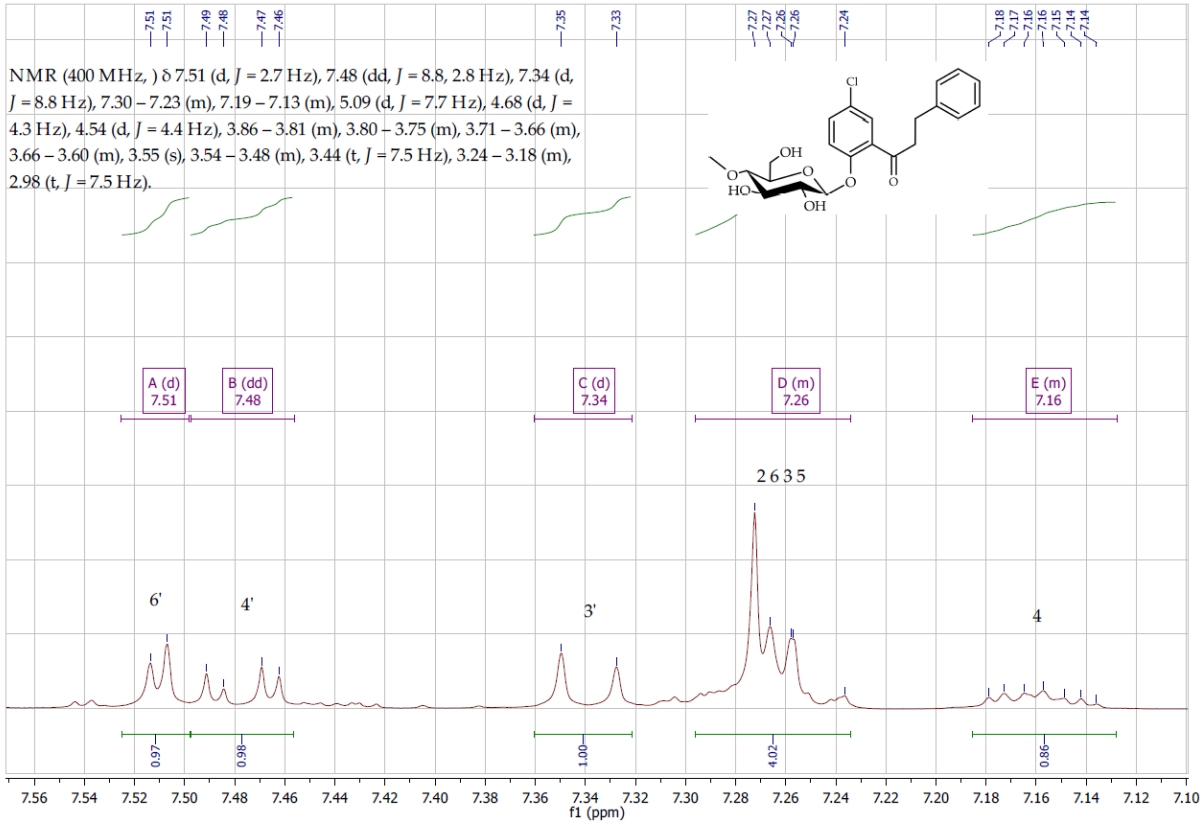


Figure S97. [1]H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

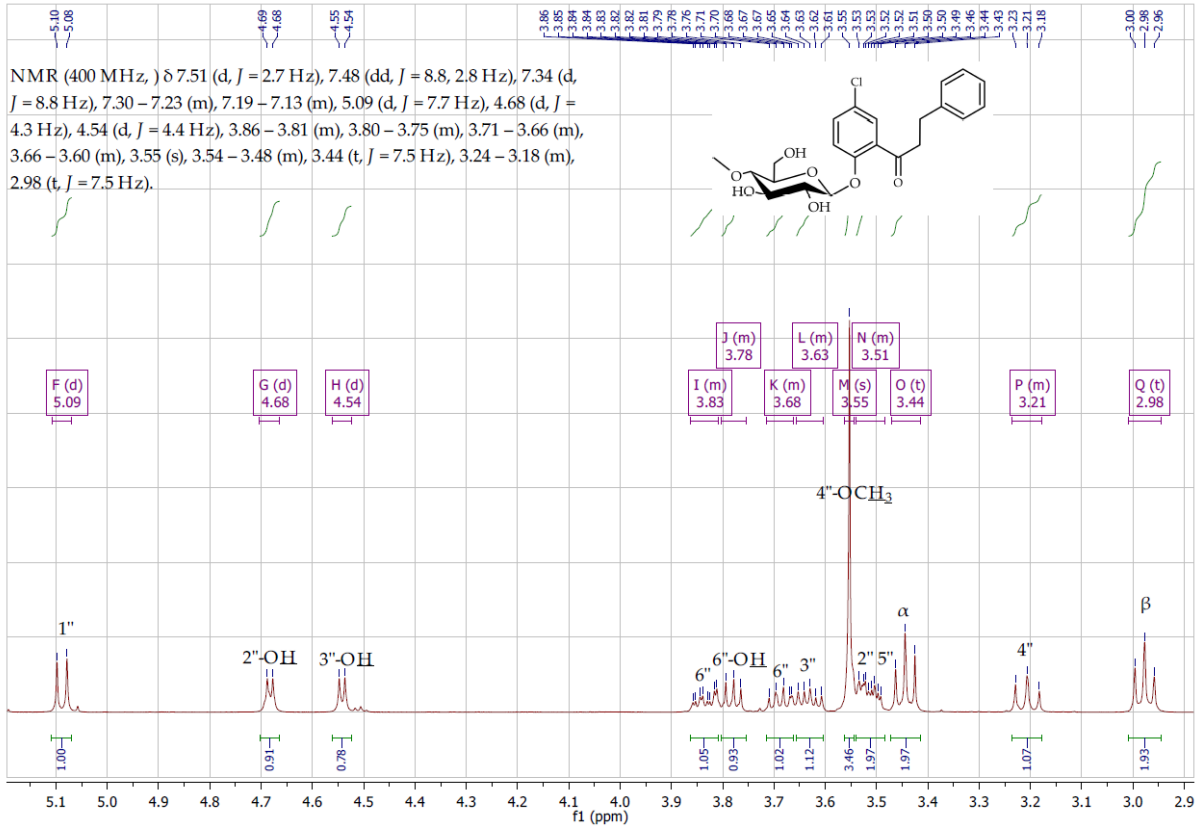


Figure S98. [1]H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

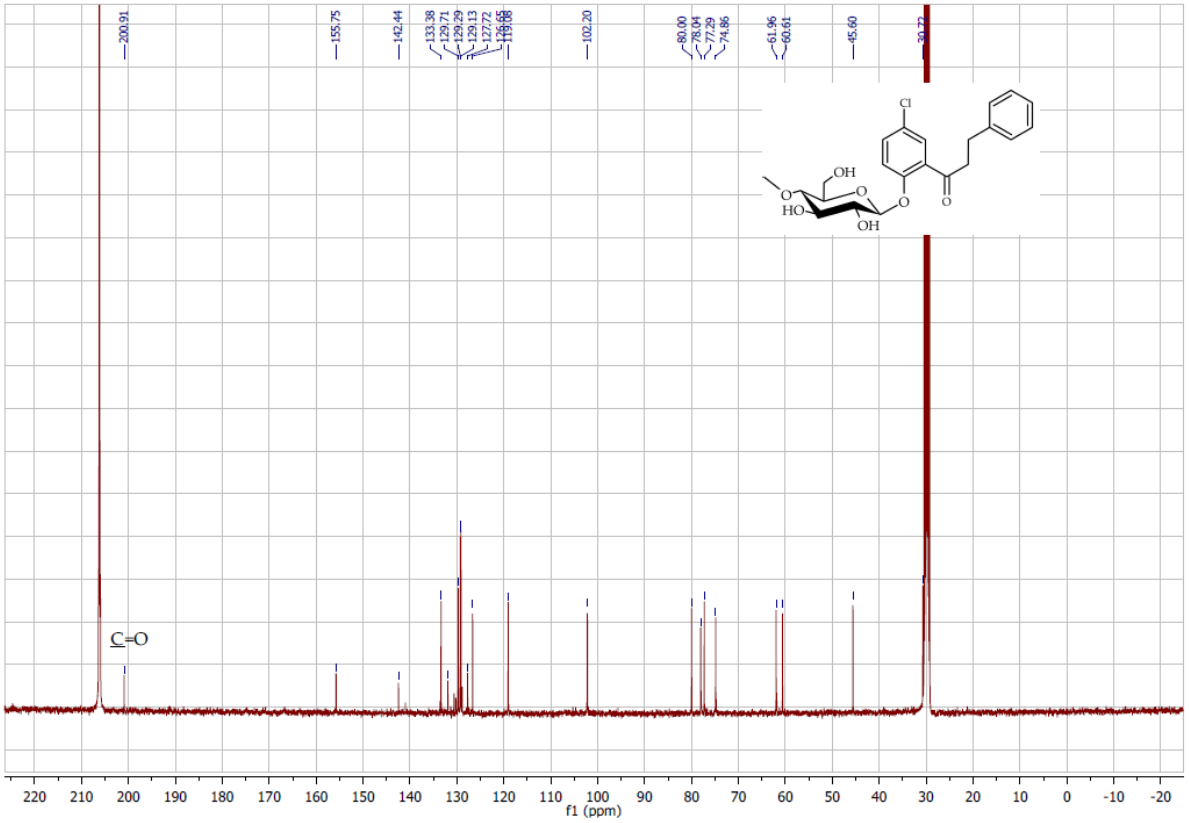


Figure S99. ^{13}C NMR spectrum (δ, acetone-d6, 151 MHz) of 5′-chlorodihydrochalcone 2′-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

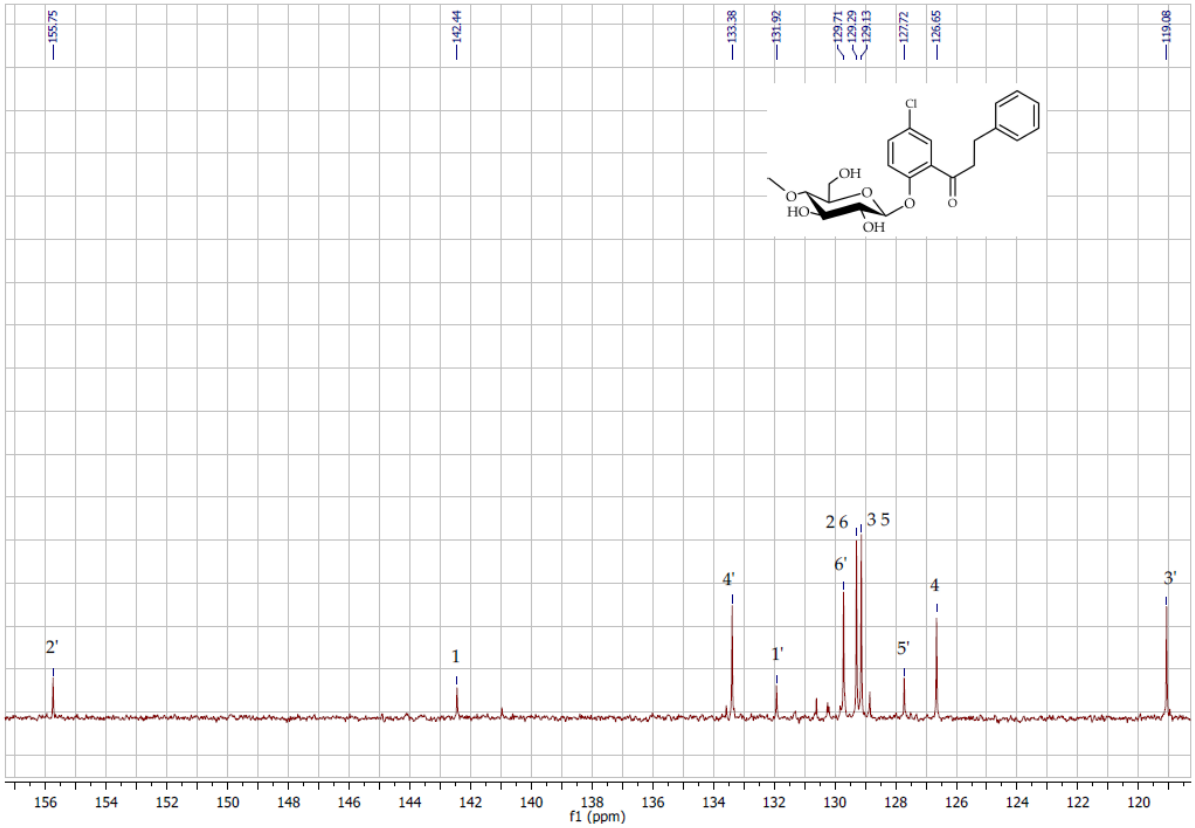


Figure S100. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 5′-chlorodihydrochalcone 2′-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

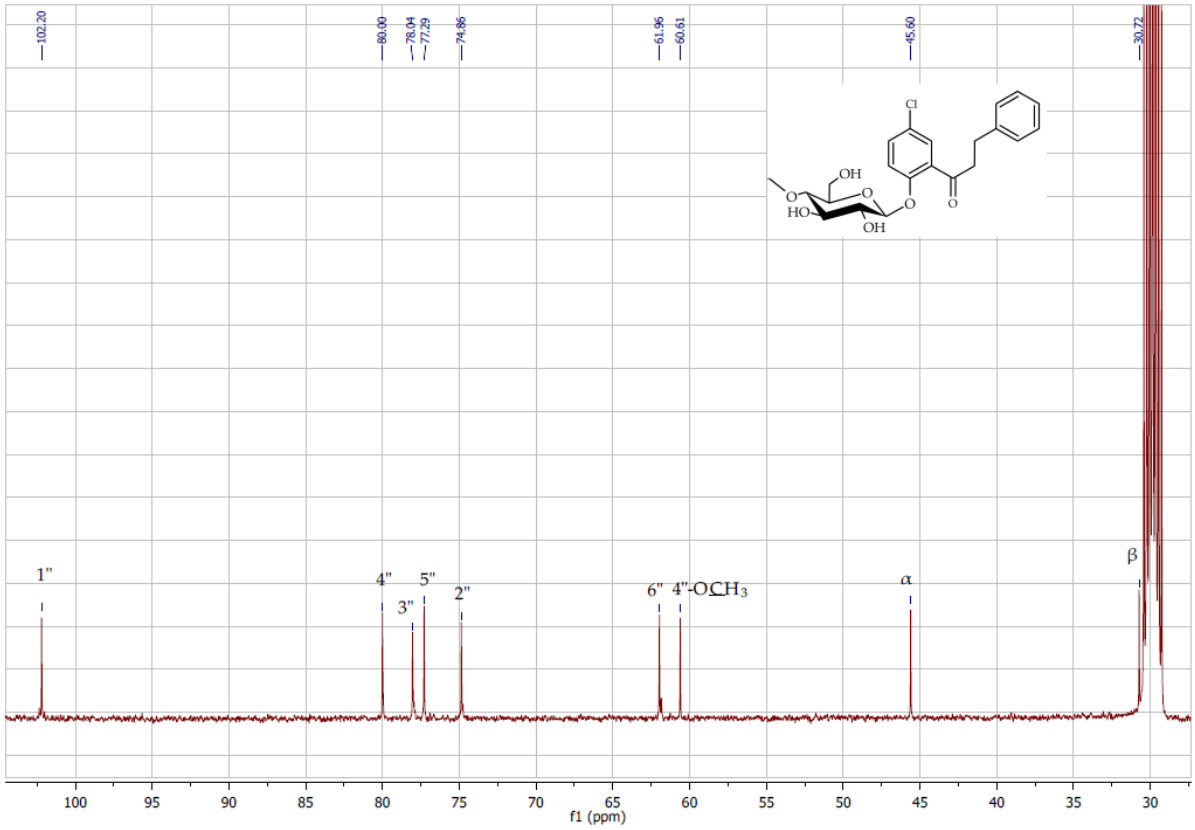


Figure S101. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

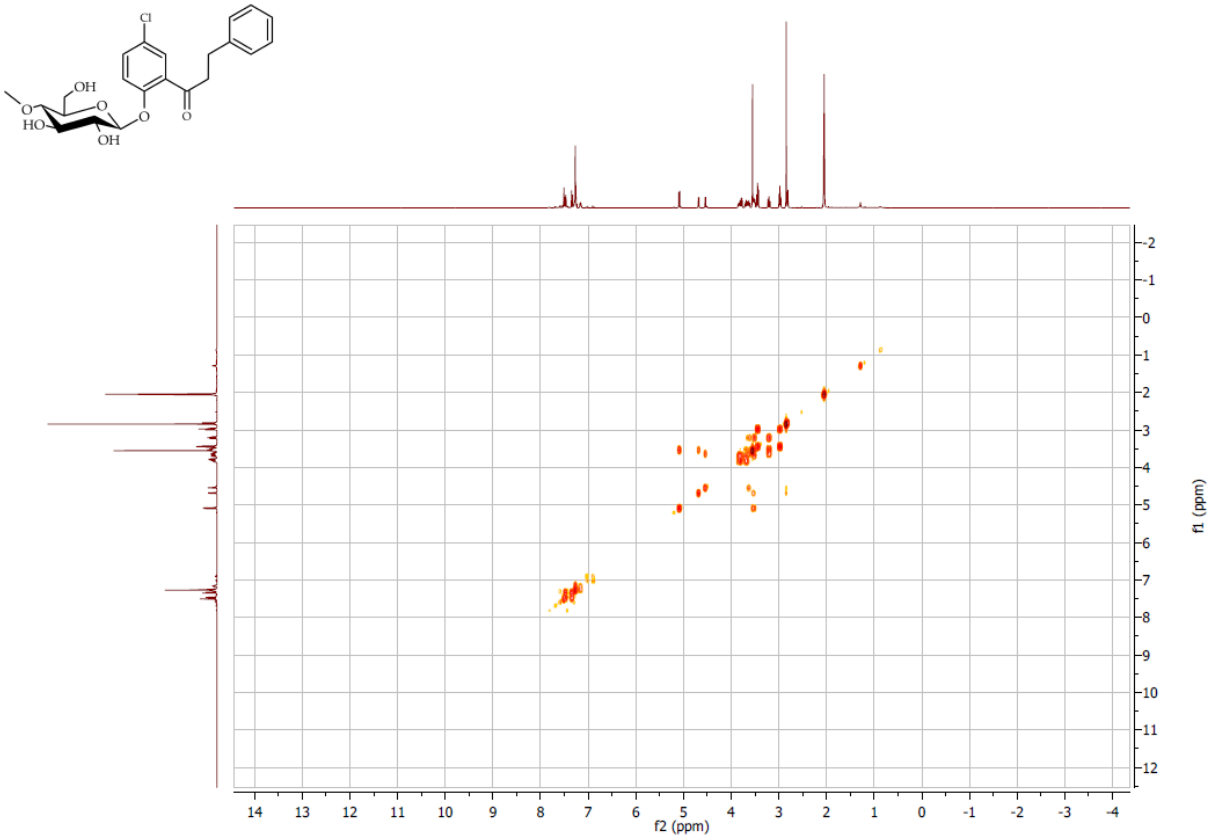


Figure S102. COSY contour map – ^{1}H x ^{1}H of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

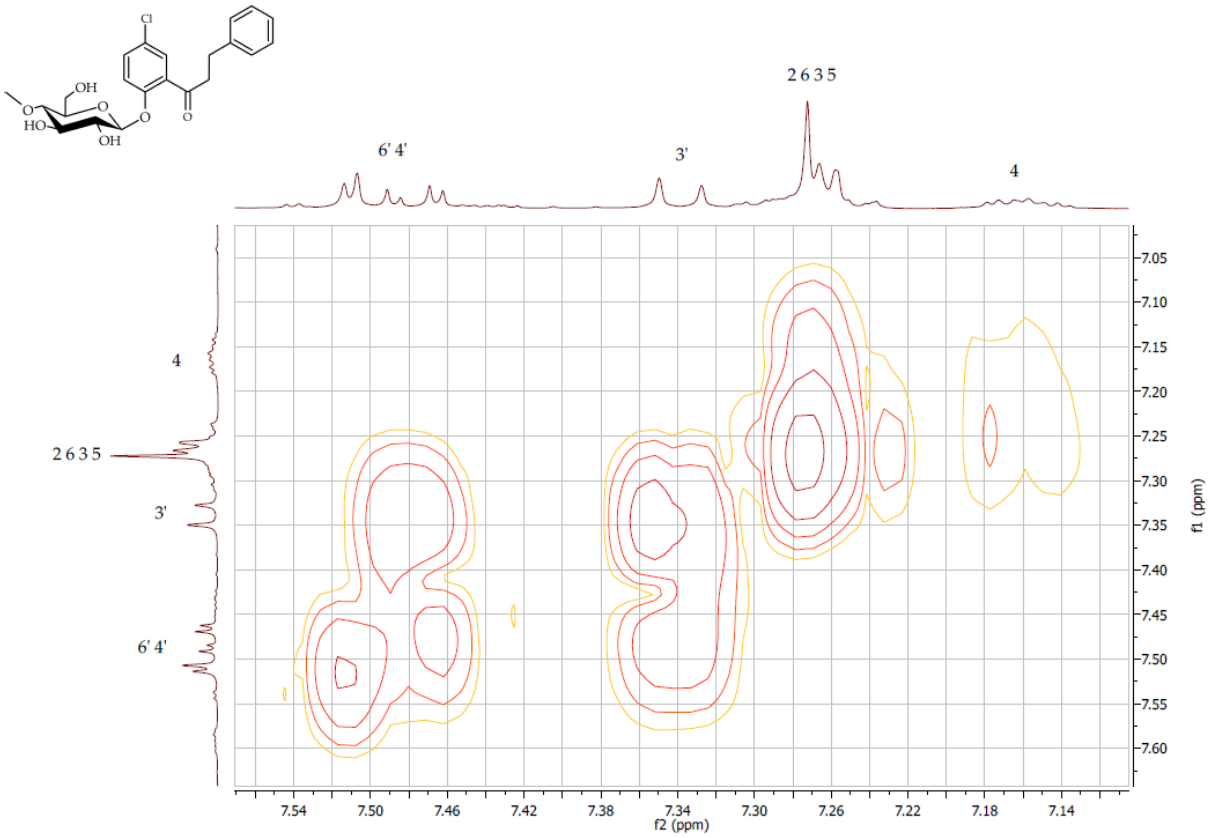


Figure S103. COSY contour map – ^{1}H x ^{1}H expansion of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

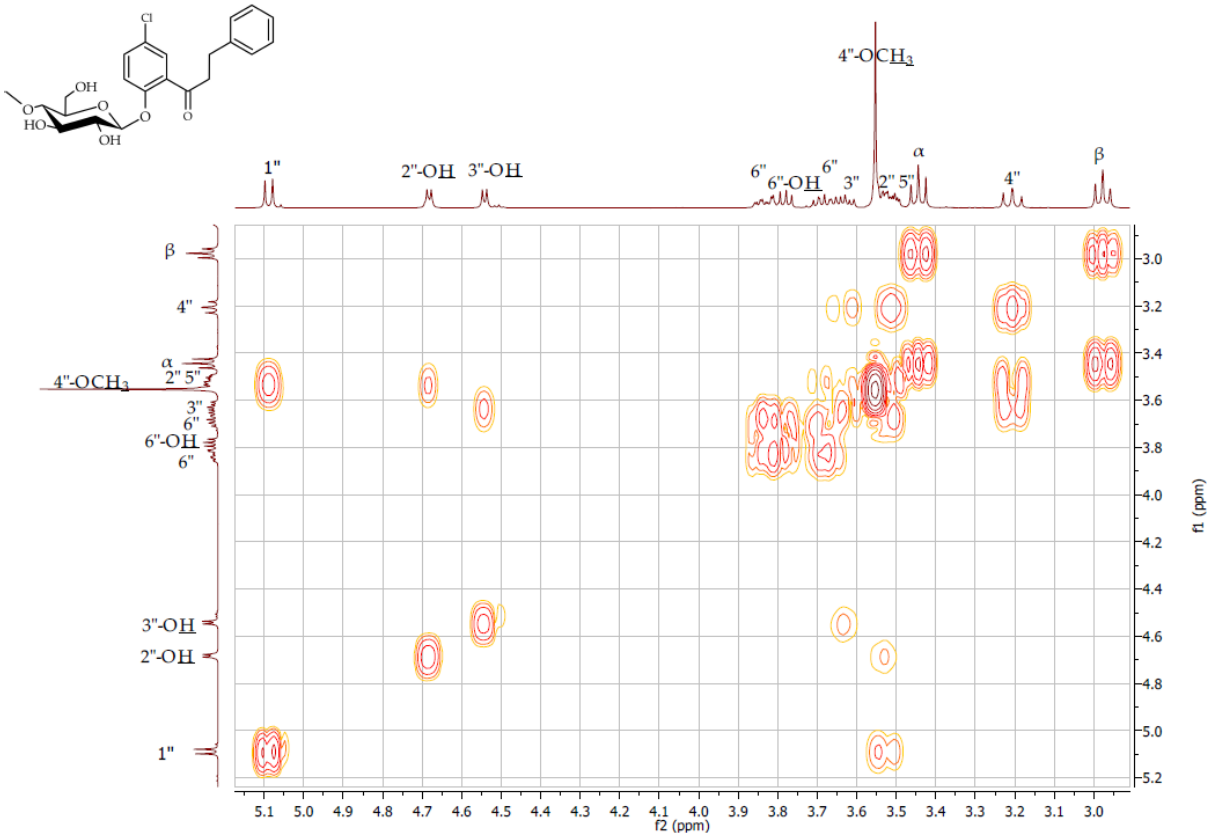


Figure S104. COSY contour map – ^{1}H x ^{1}H expansion of 4-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

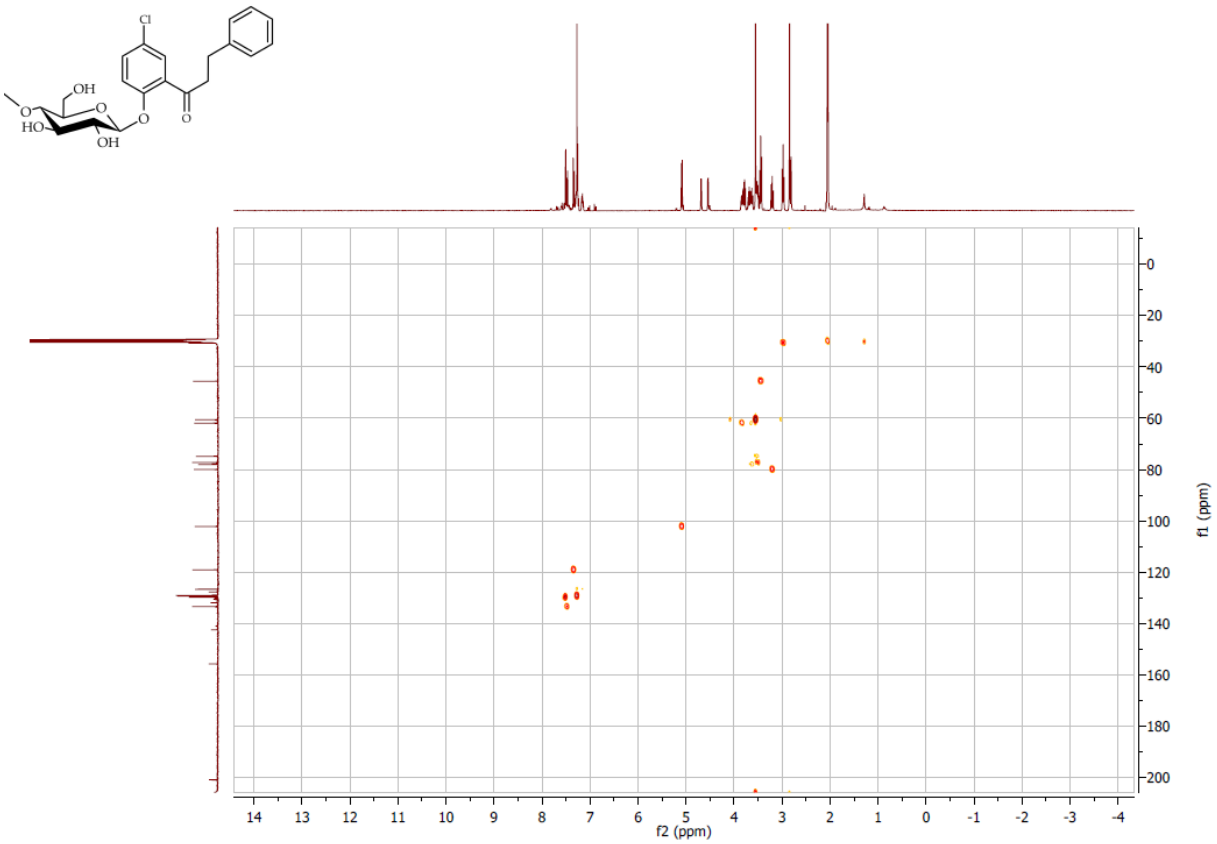


Figure S105. HMQC contour map – ^{1}H x ^{13}C of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

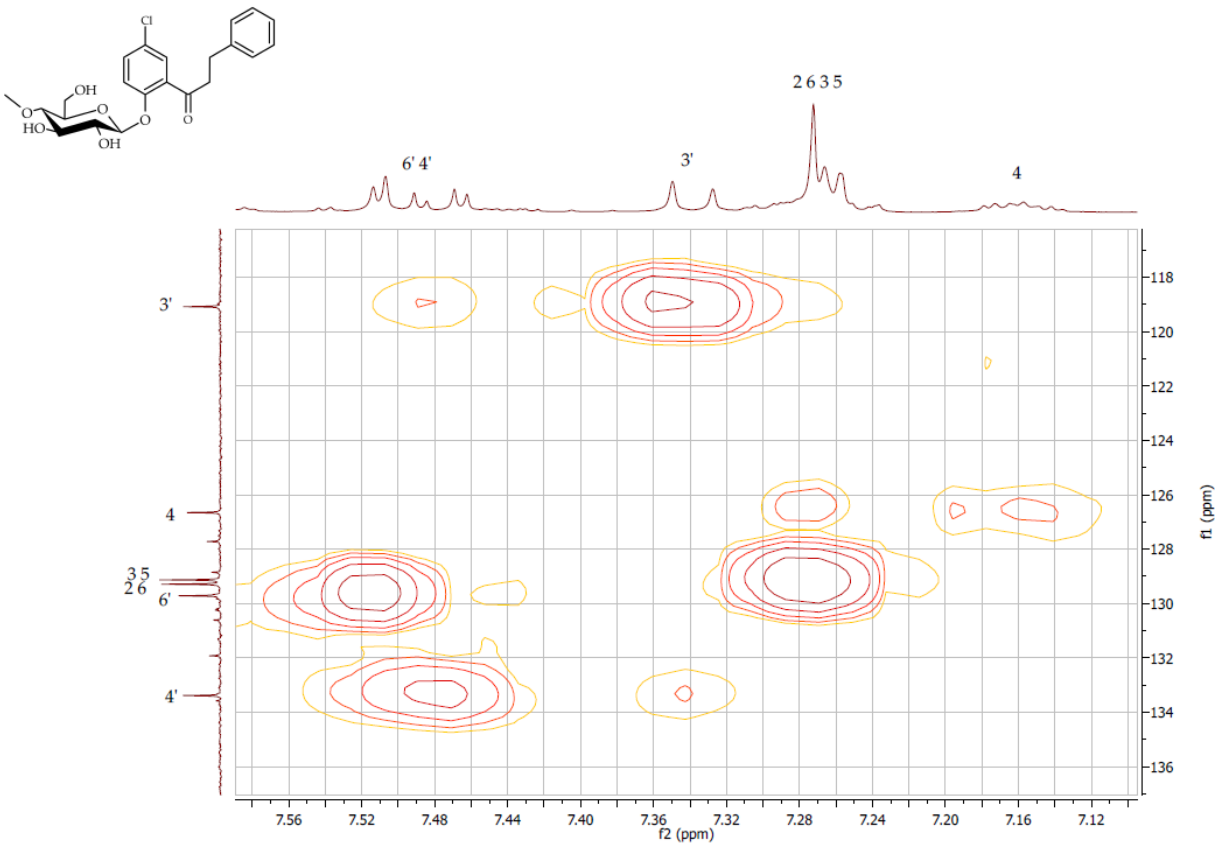


Figure S106. HMQC contour map – ^{1}H x ^{13}C expansion of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

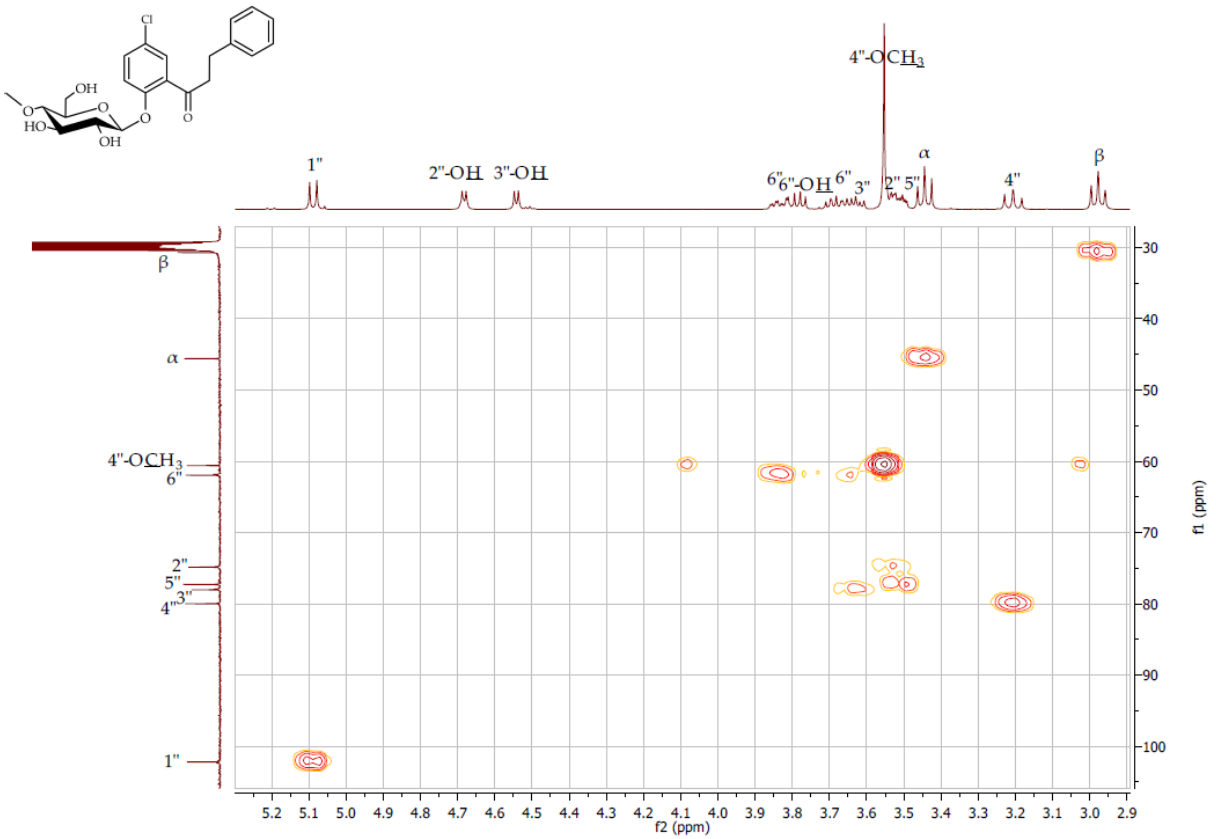


Figure S107. HMQC contour map – ^{1}H x ^{13}C expansion of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

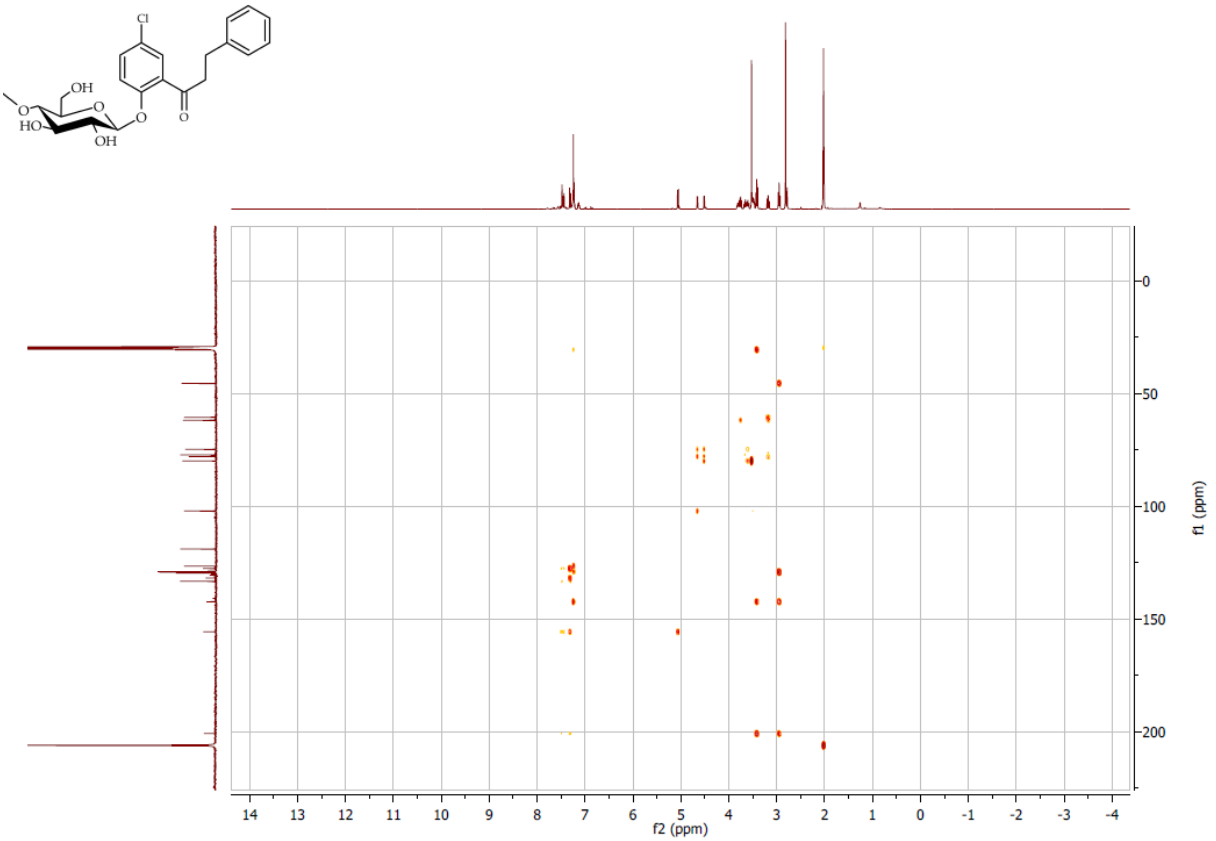


Figure S108. HMBC contour map – ^{1}H x ^{13}C of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

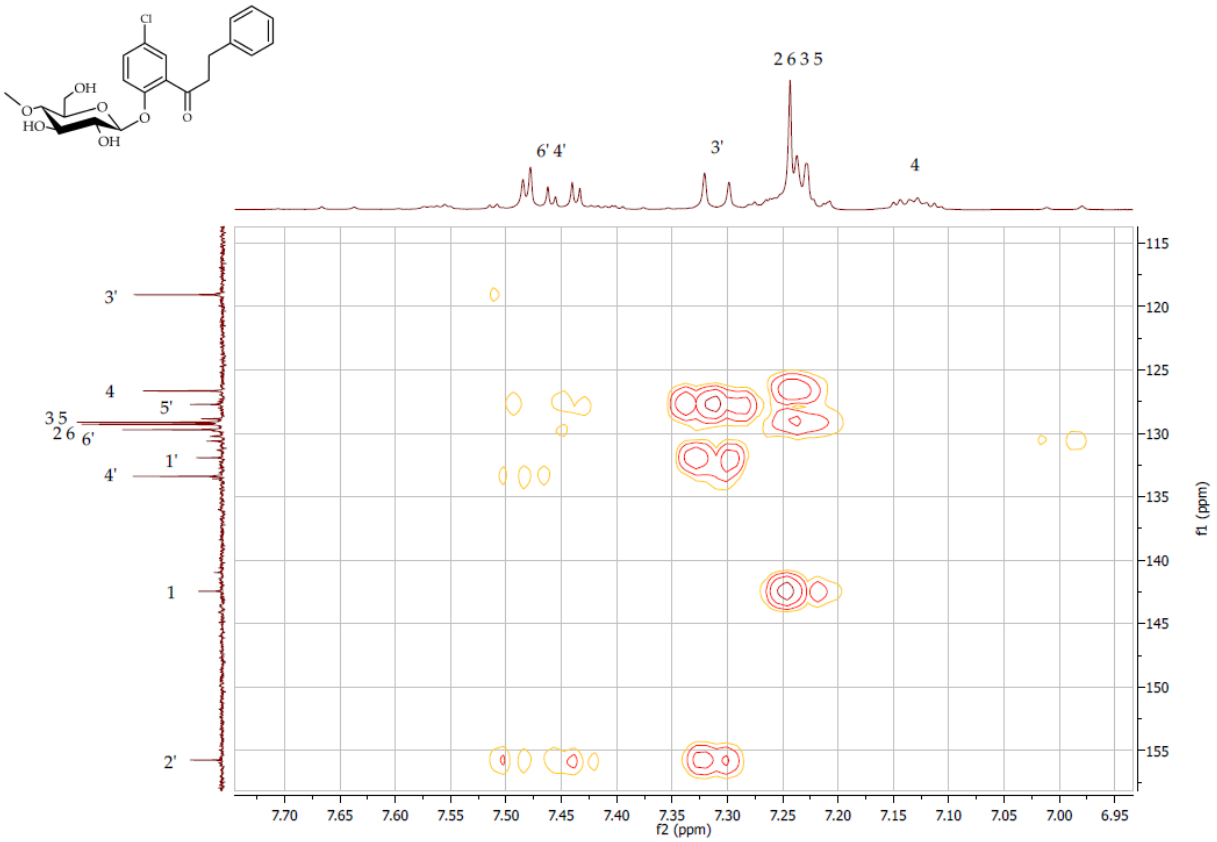


Figure S109. HMBC contour map – ^{1}H x ^{13}C expansion of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

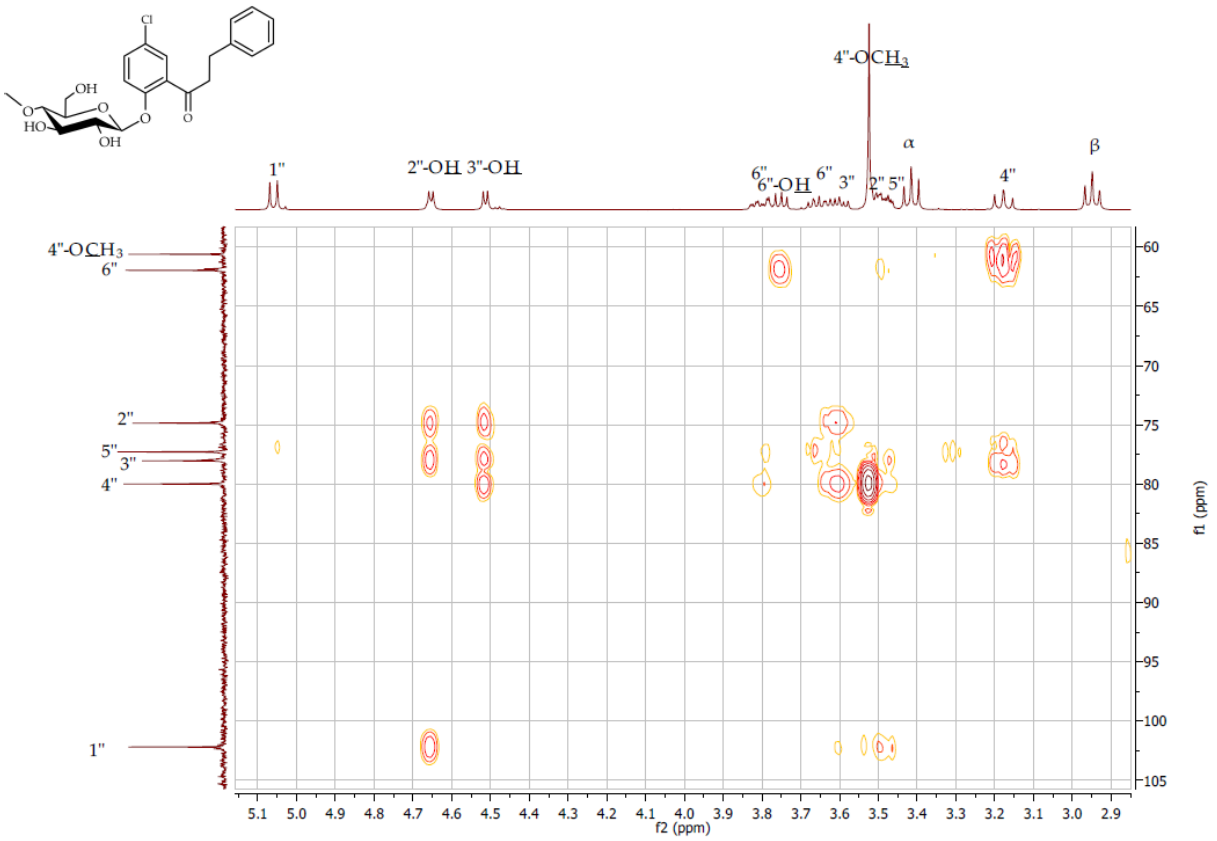


Figure S110. HMBC contour map – ^{1}H x ^{13}C expansion of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

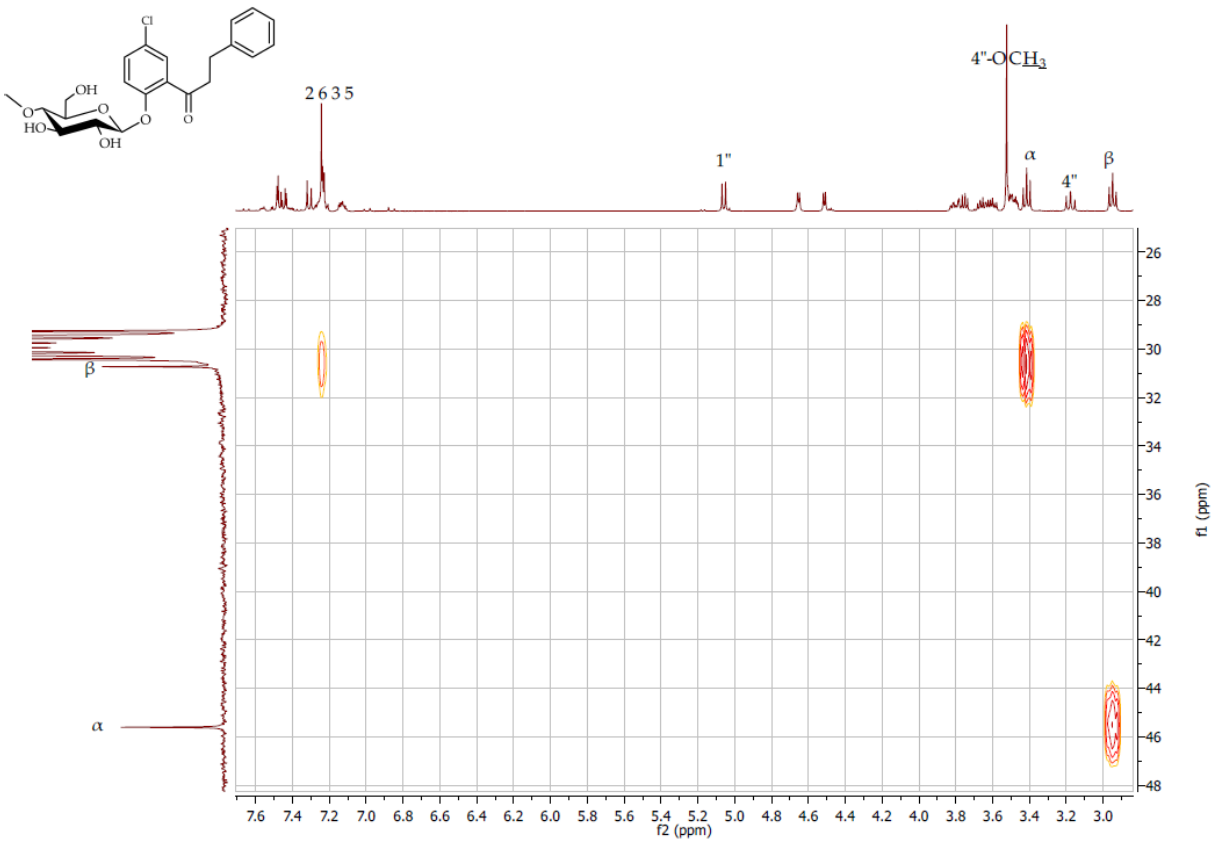


Figure S111. HMBC contour map – ^{1}H x ^{13}C expansion of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

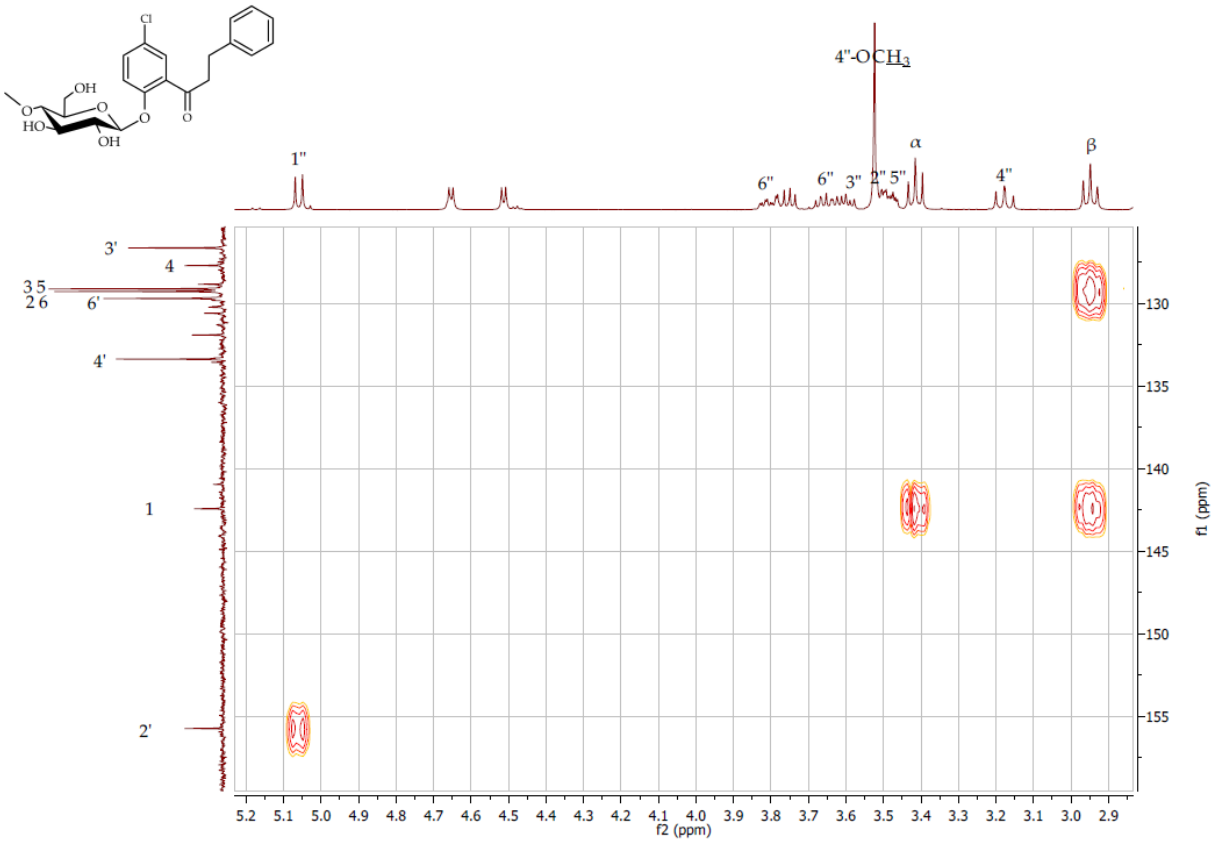


Figure S112. HMBC contour map – ^{1}H x ^{13}C expansion of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

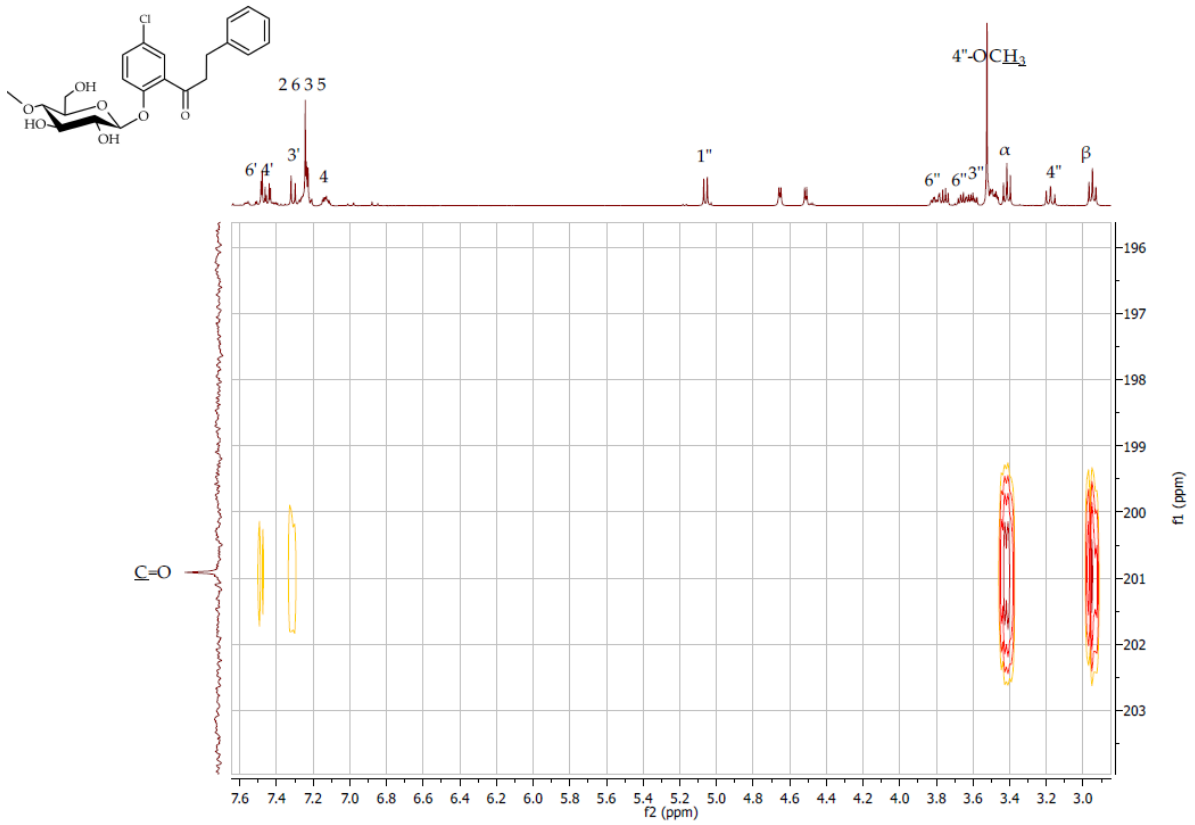


Figure S113. HMBC contour map – ^{1}H x ^{13}C expansion of 5′-chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**)

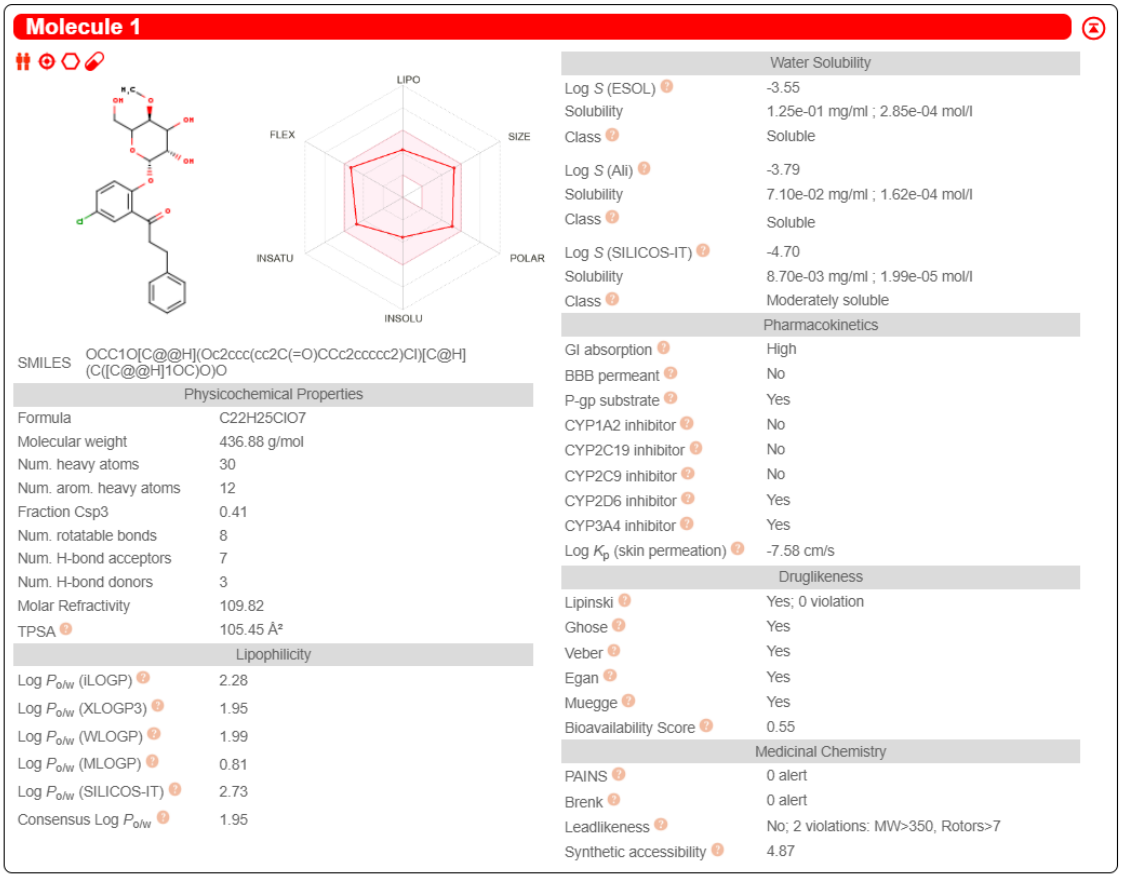


Figure S114. 5′-Chlorodihydrochalcone 2′-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6a**) physicochemical and ADME parameters prediction using the SwissADME modelling

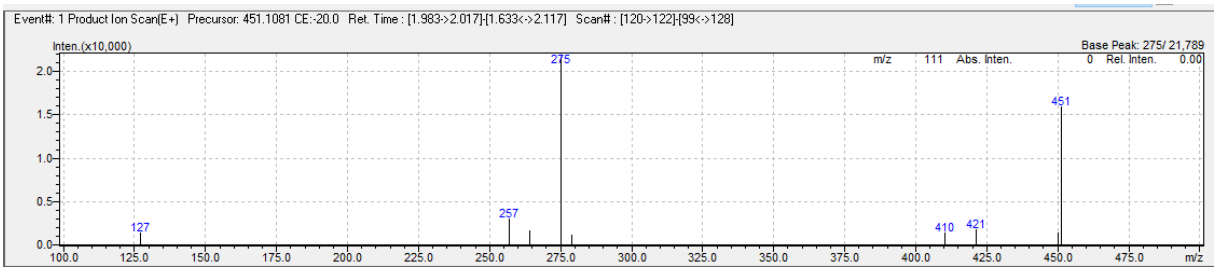
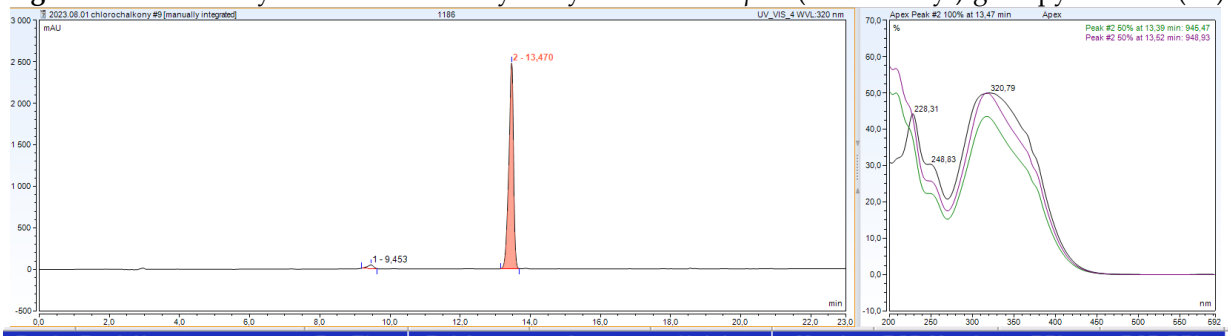


Figure S115. MS analysis of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)



Peak No.	Peak Name	Ret.Time min	Rel.Area %	Area mAU*min	Height mAU	Match	RSD Match %	PPI nm	RSD PPI %
1		9,453	2,36	9,1893	44,06	1000	0,03	218,3	0,04
2		*13,470*	*97,64*	*379,5331*	*2477,05*	*941*	*5,11*	*286,3*	*3,83*
Maximum			97,64	379,5331	2477,05	1000	5,11		3,83
Minimum			2,36	9,1893	44,06	941	0,03		0,04

Figure S116. HPLC analysis of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

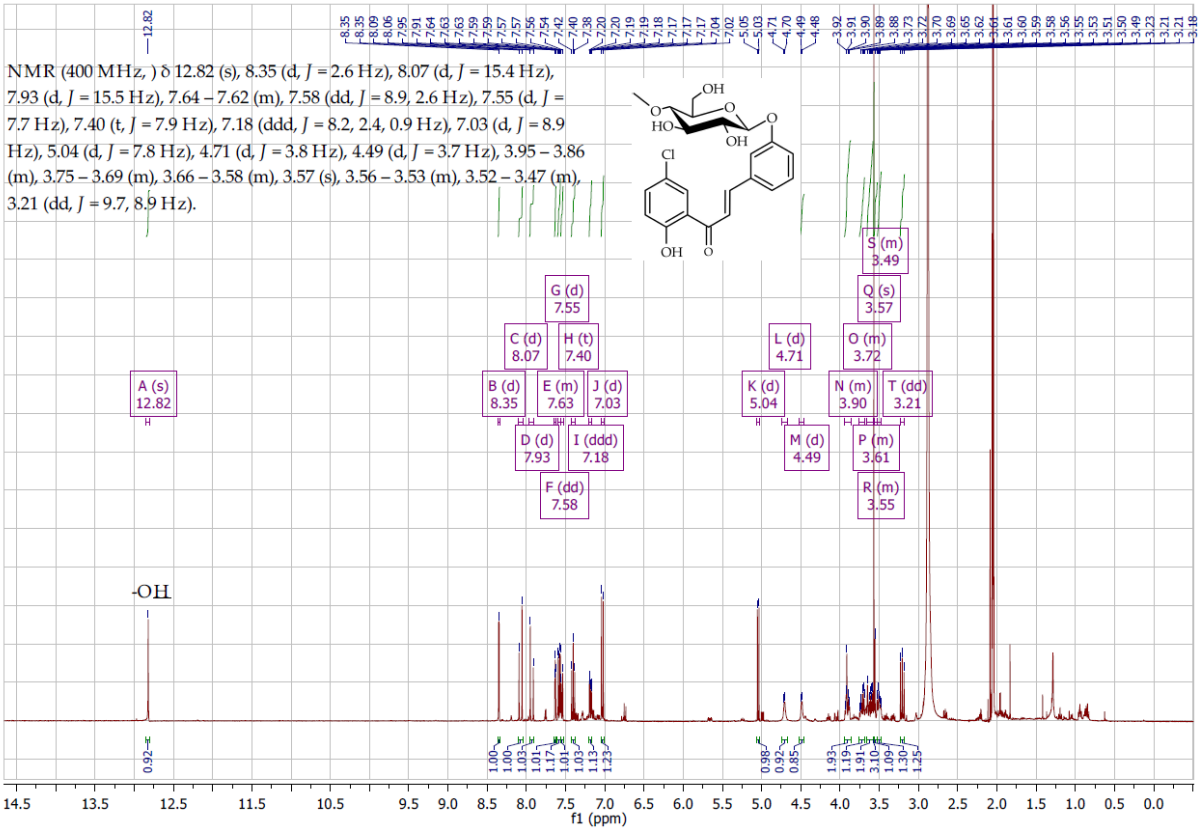


Figure S117. ^{1}H NMR spectrum (*δ*, acetone-d6, 600 MHz) of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

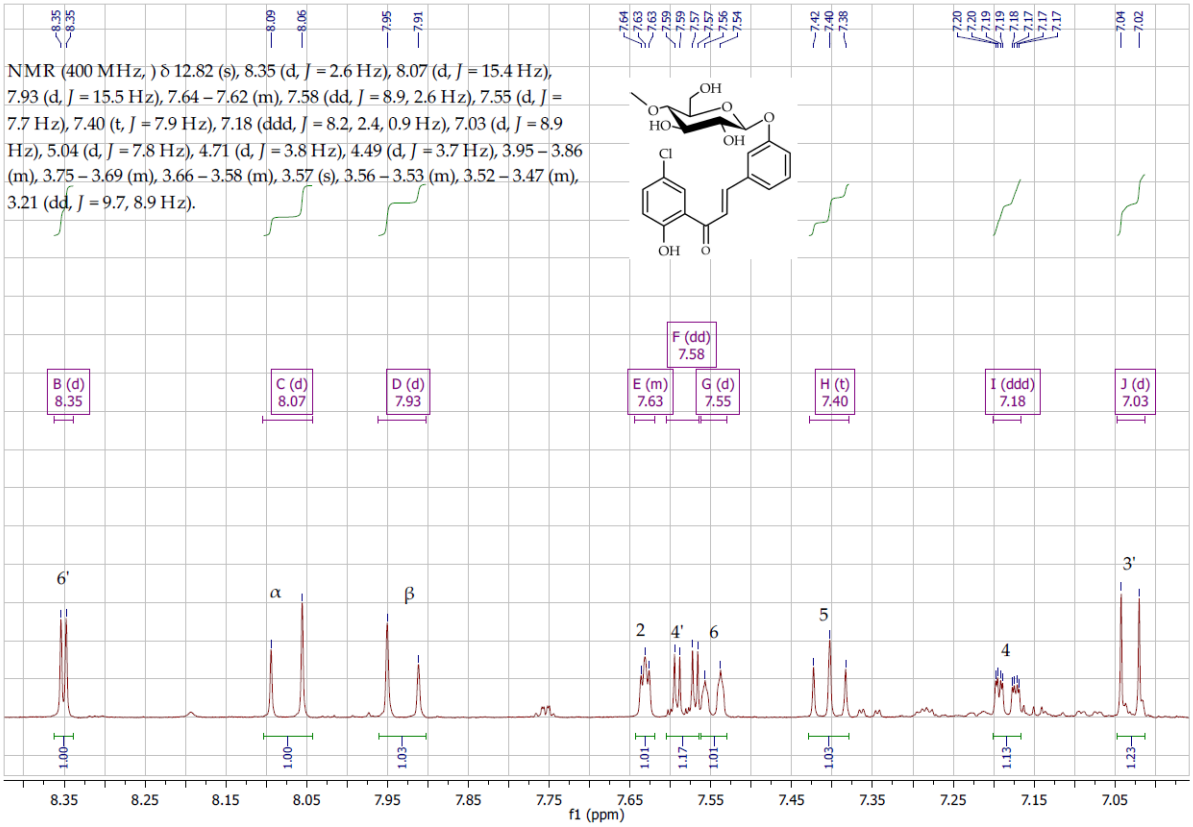


Figure S118. [1]H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

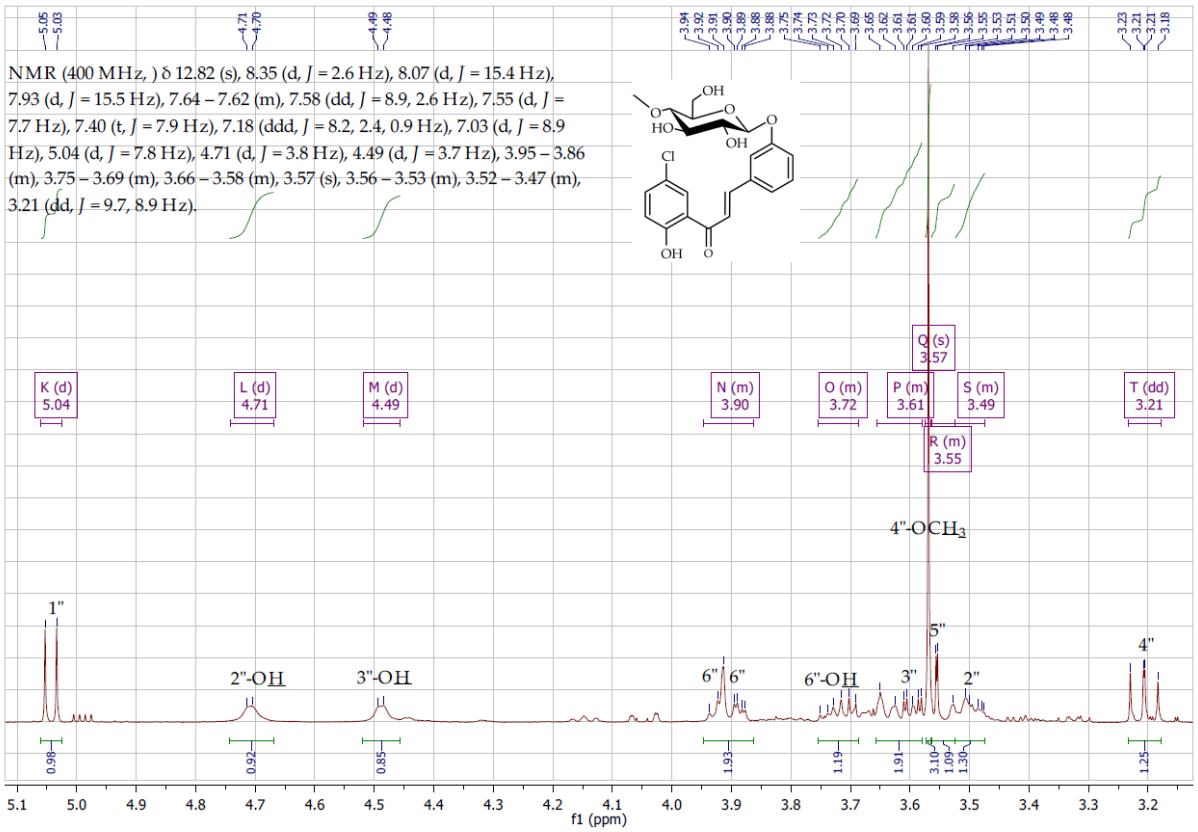


Figure S119. [1]H NMR spectrum expansion (δ, acetone-d6, 600 MHz) of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

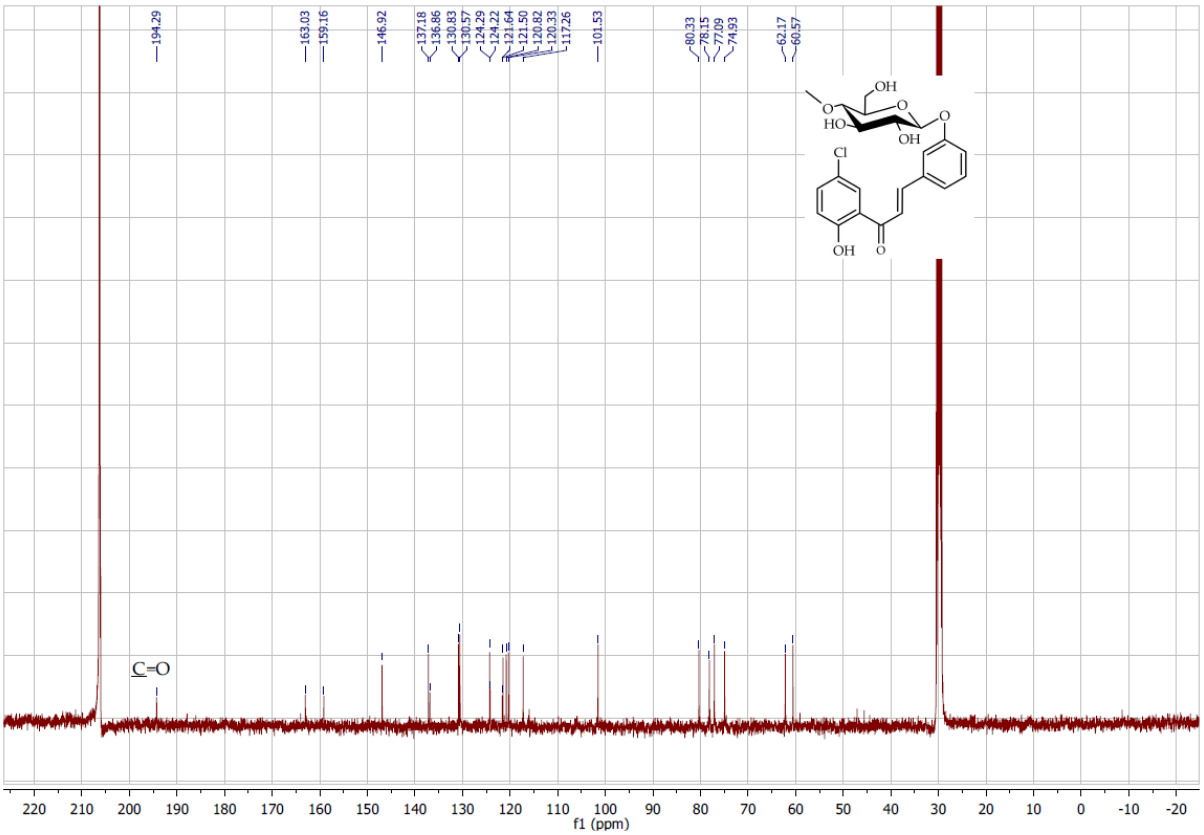


Figure S120. ^{13}C NMR spectrum (δ, acetone-d6, 151 MHz) of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

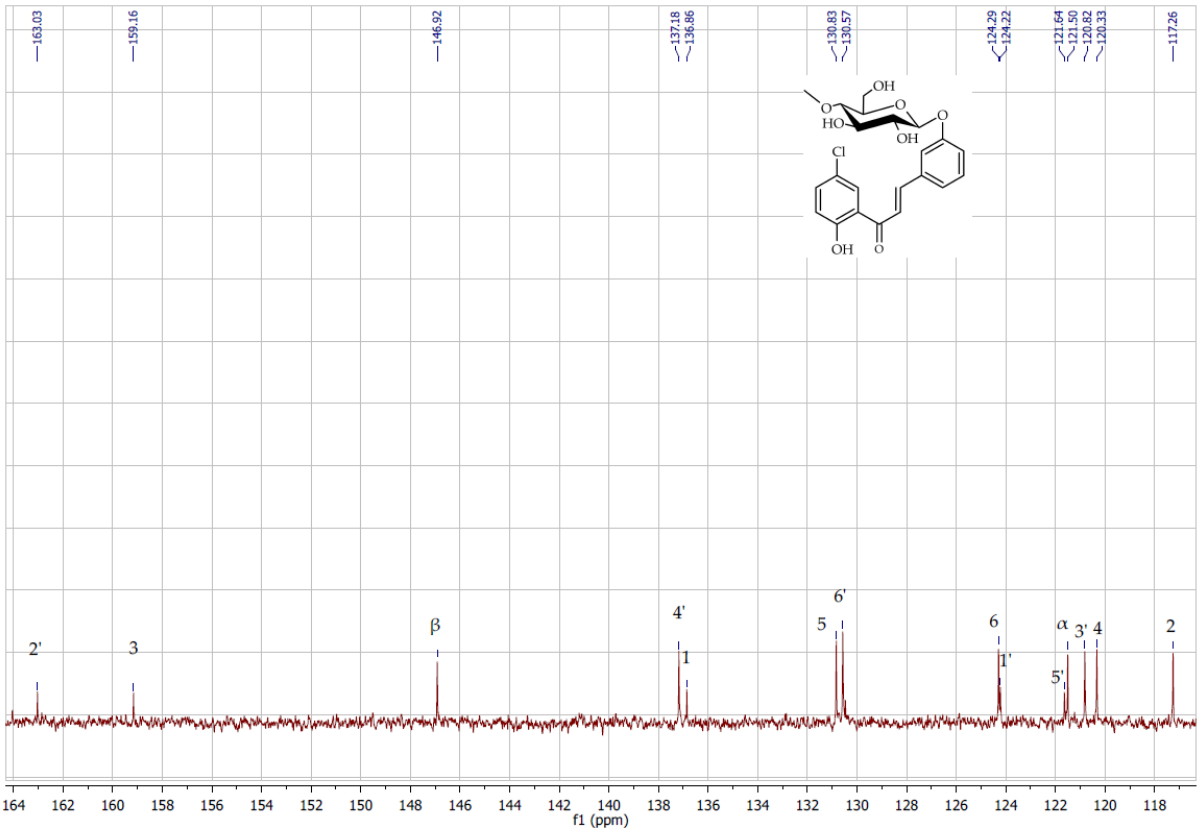


Figure S121. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

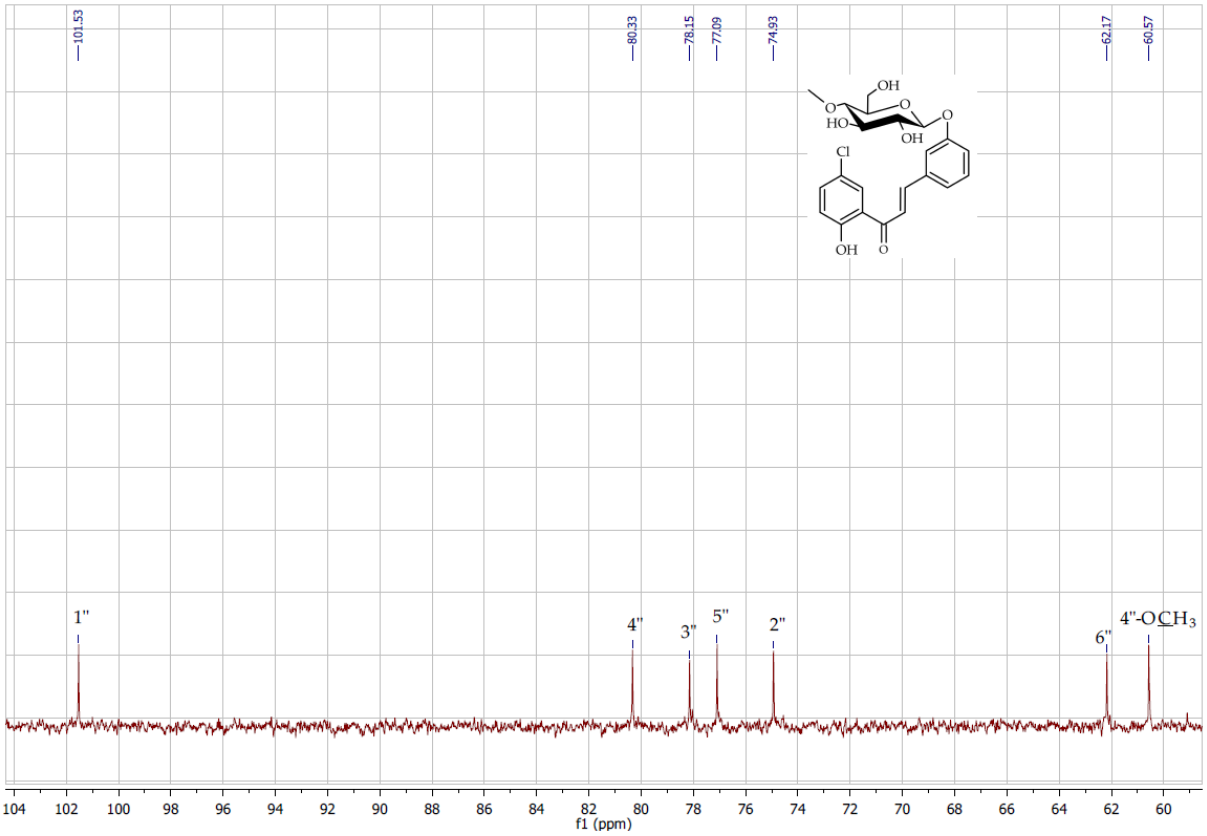


Figure S122. ^{13}C NMR spectrum expansion (δ, acetone-d6, 151 MHz) of 5′-chloro-2′-hydroxychalcone 3-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

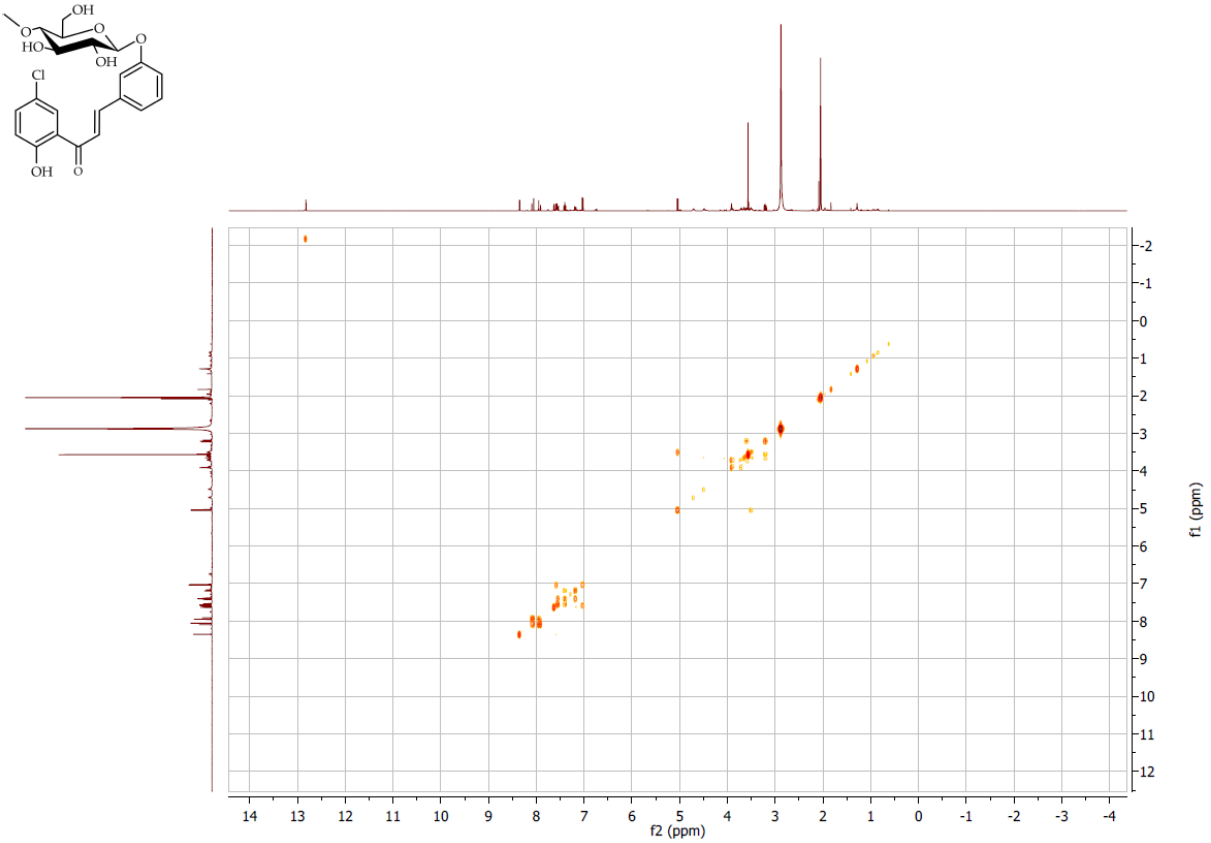


Figure S123. COSY contour map – ^{1}H x ^{1}H of 4-chloro-2′-hydroxydihydrochalcone 5′-chloro-2′-hydroxychalcone 3-*O*-β-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

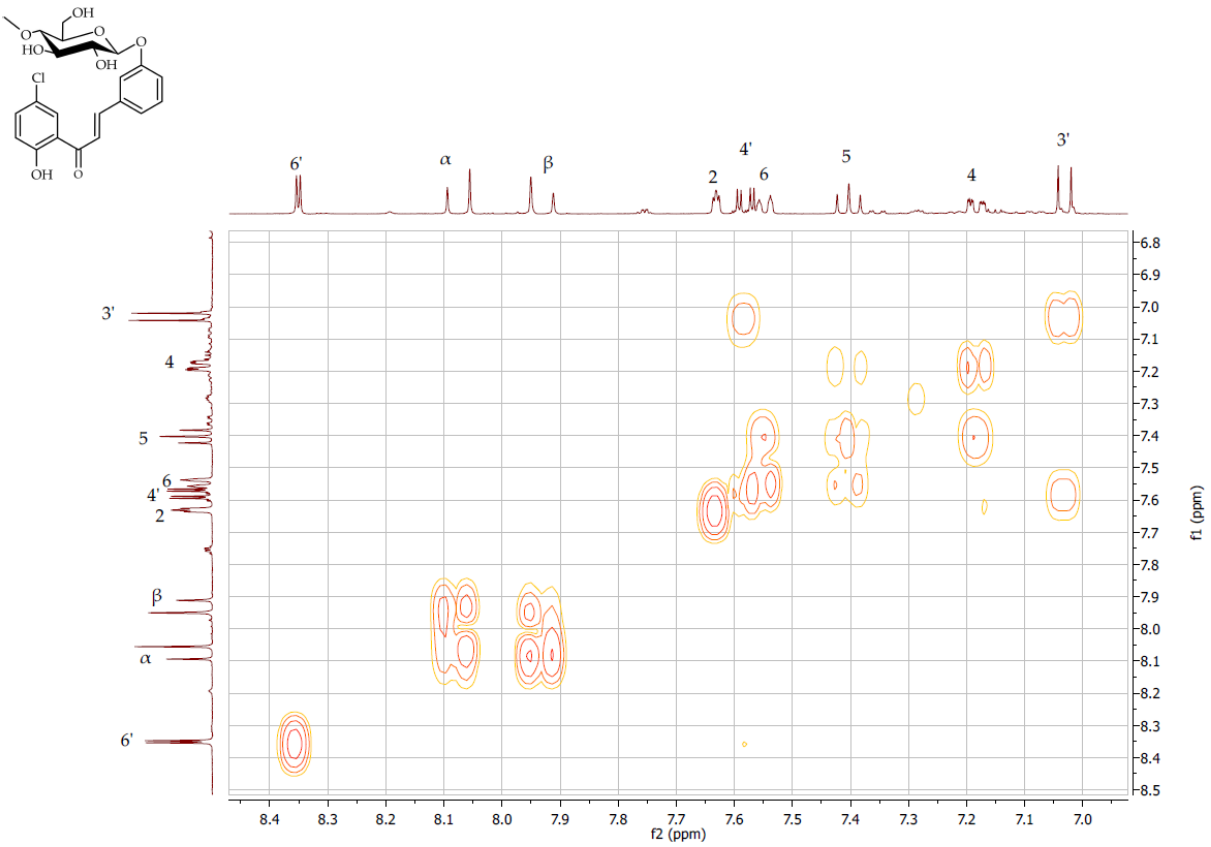


Figure S124. COSY contour map – ^{1}H x ^{1}H expansion of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

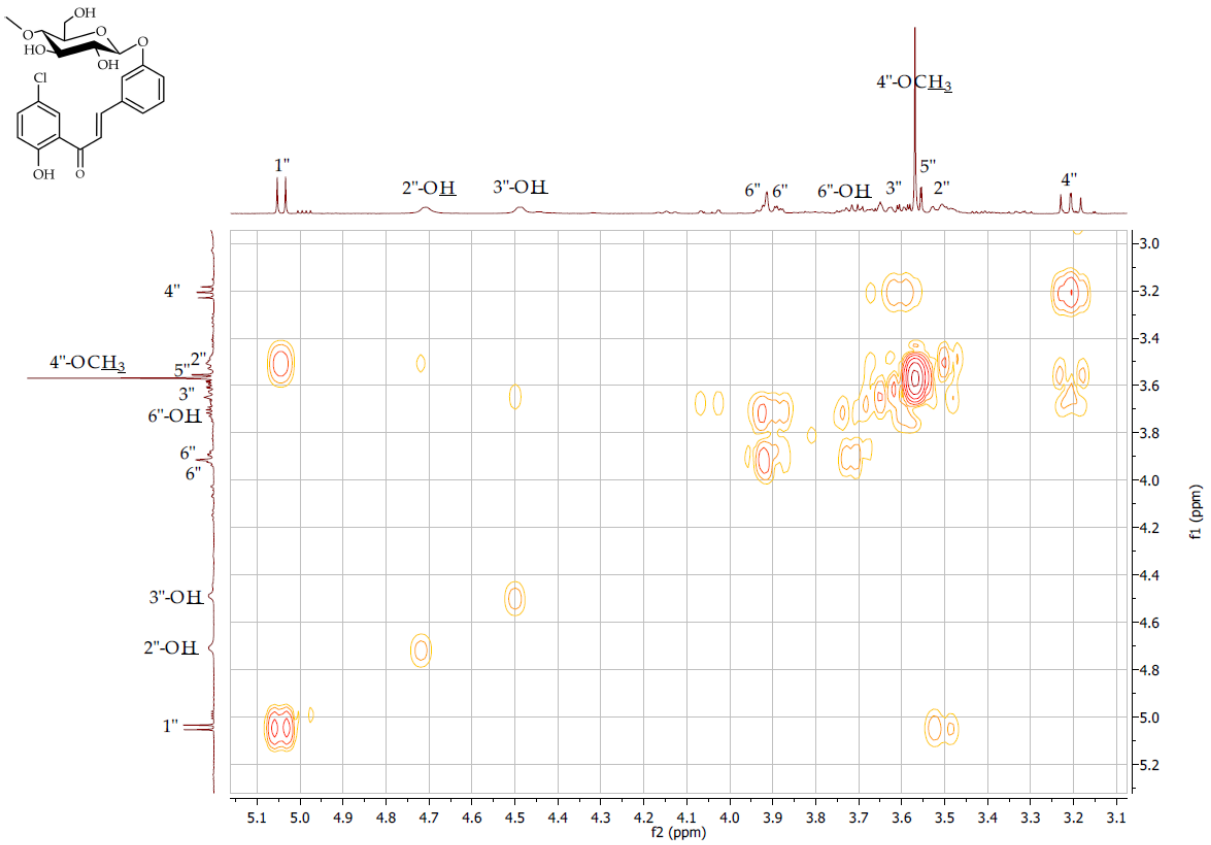


Figure S125. COSY contour map – ^{1}H x ^{1}H expansion of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

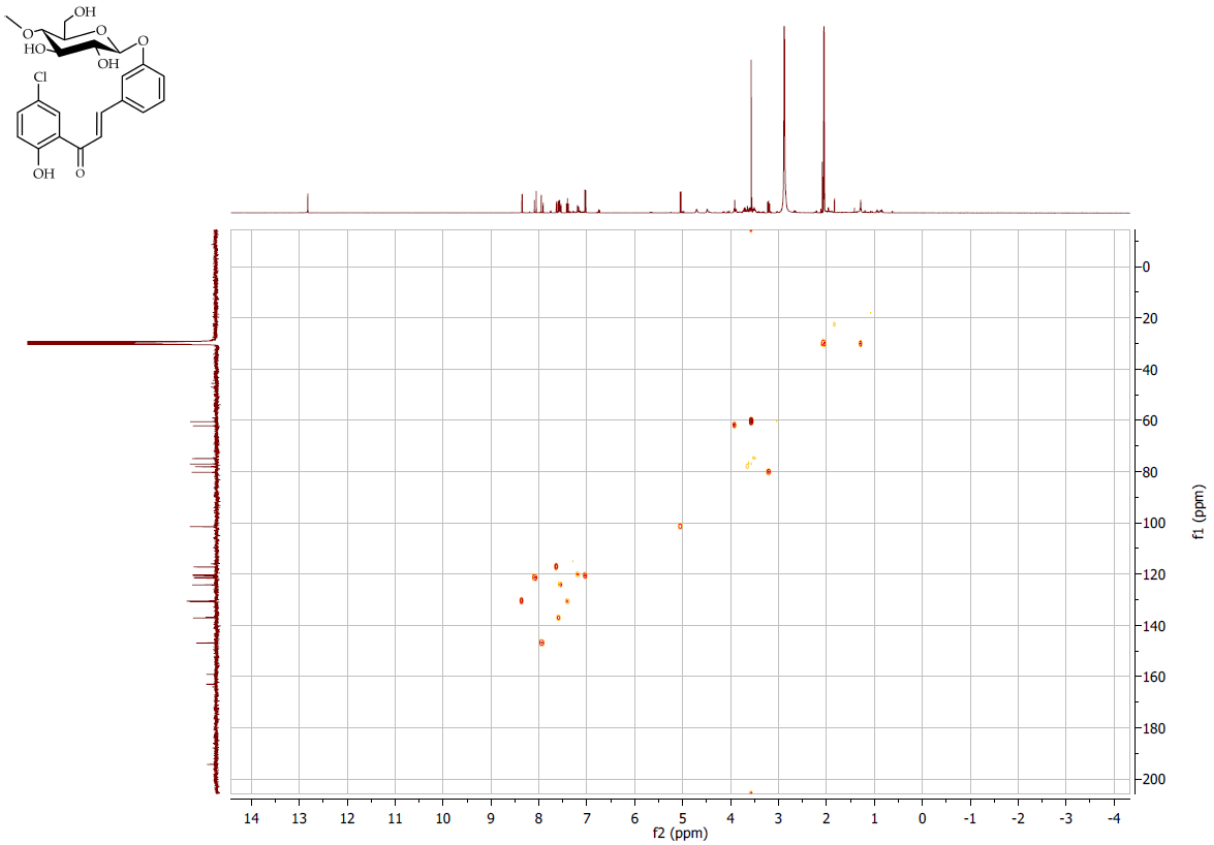


Figure S126. HMQC contour map – ^{1}H x ^{13}C of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

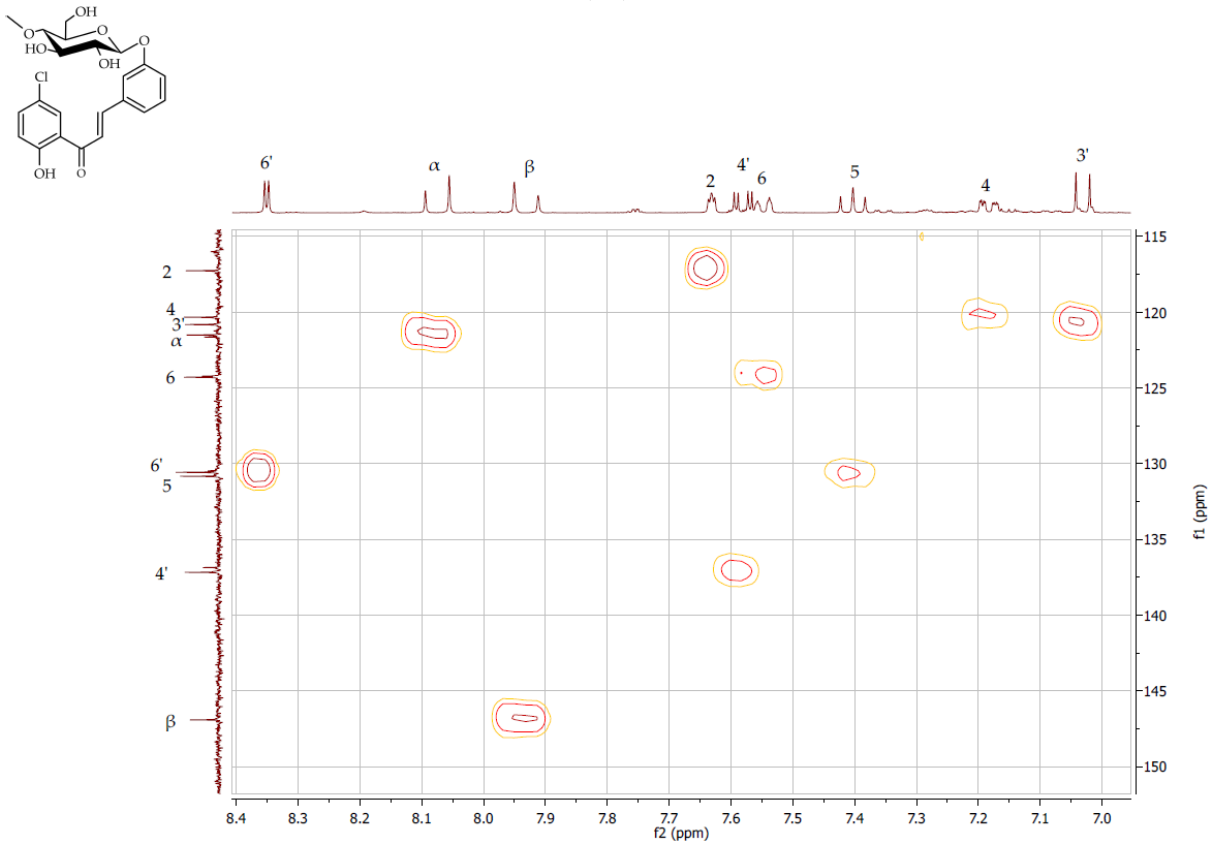


Figure S127. HMQC contour map – ^{1}H x ^{13}C expansion of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

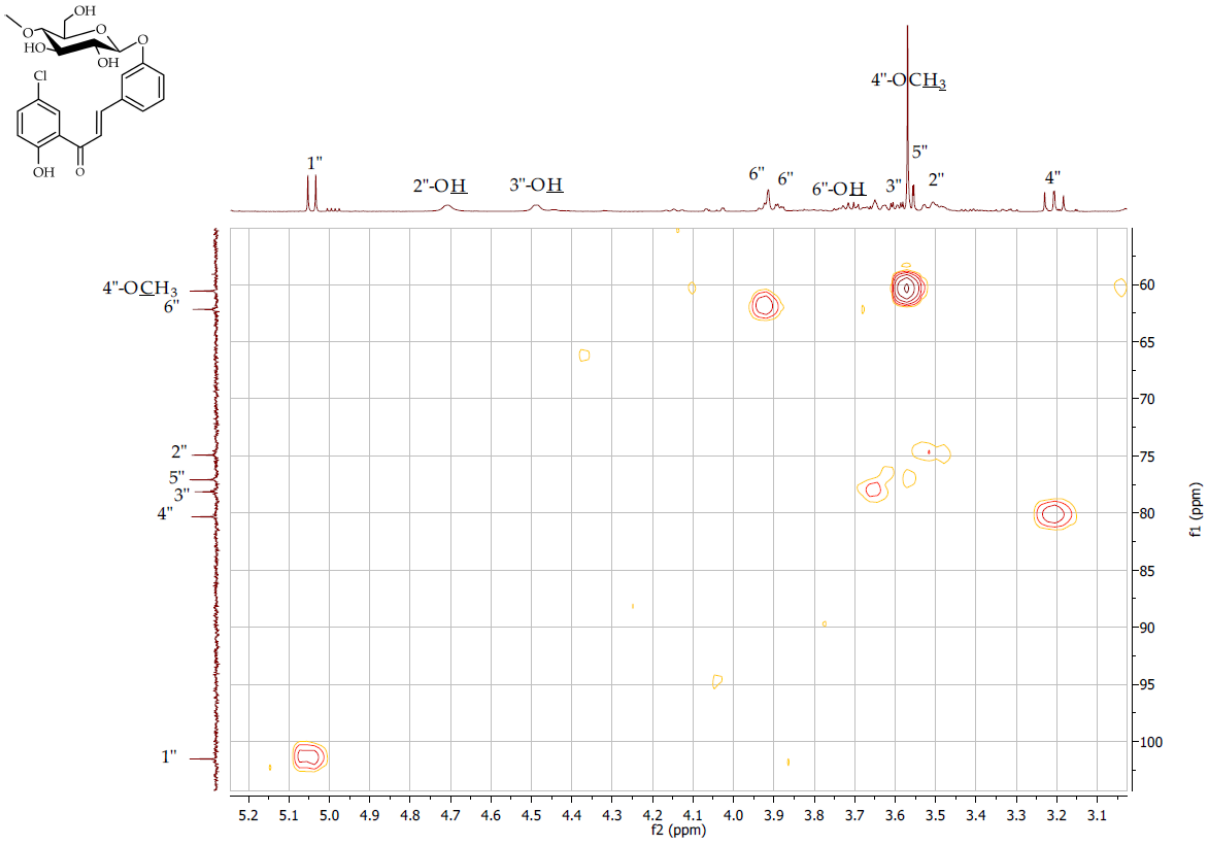


Figure S128. HMQC contour map – ^{1}H x ^{13}C expansion of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

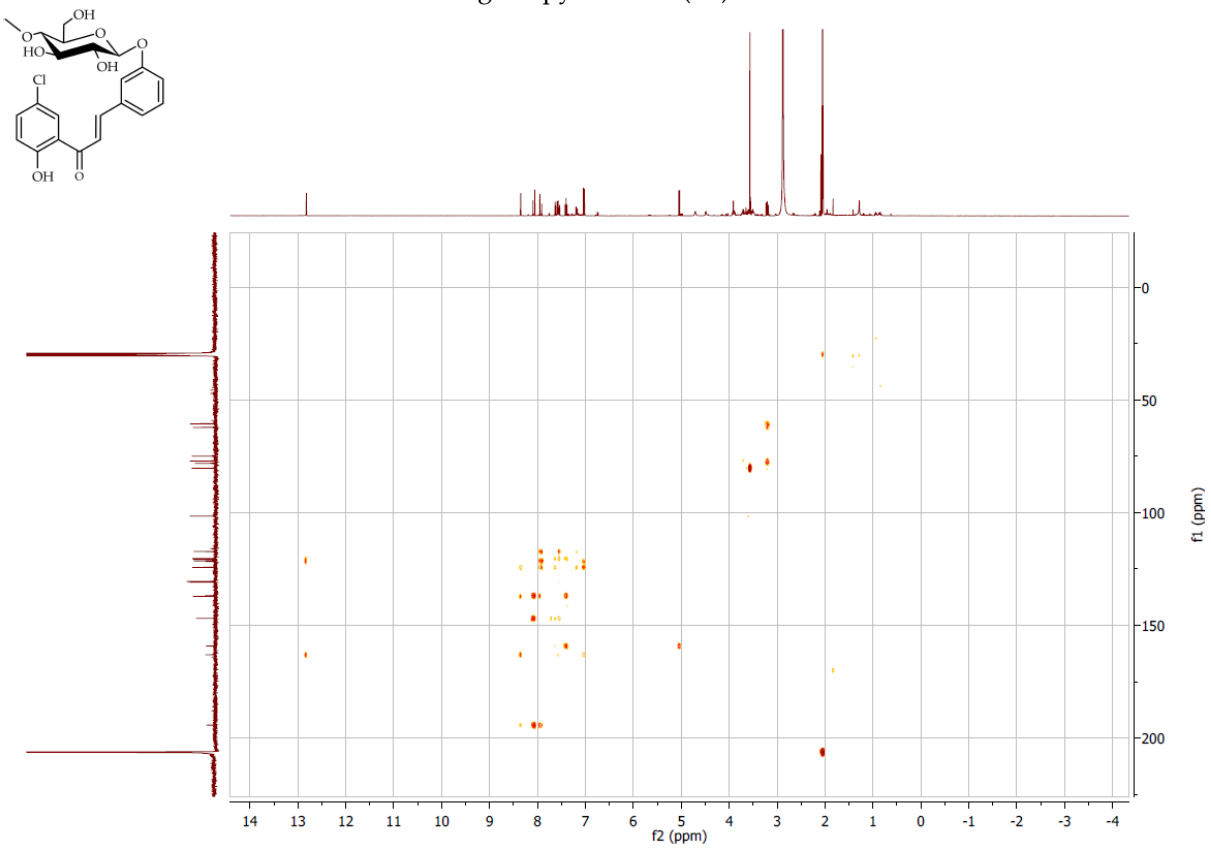


Figure S129. HMBC contour map – ^{1}H x ^{13}C of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

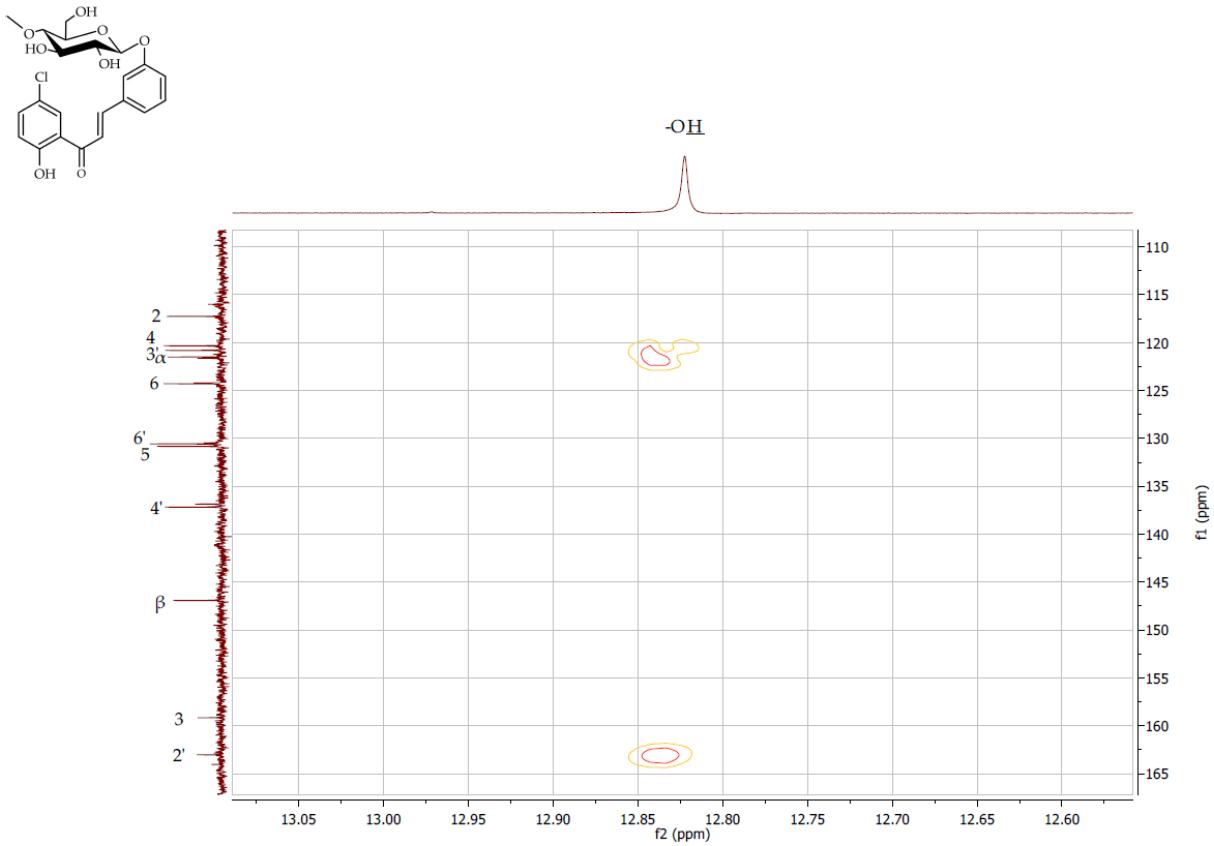


Figure S130. HMBC contour map – ^{1}H x ^{13}C expansion of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

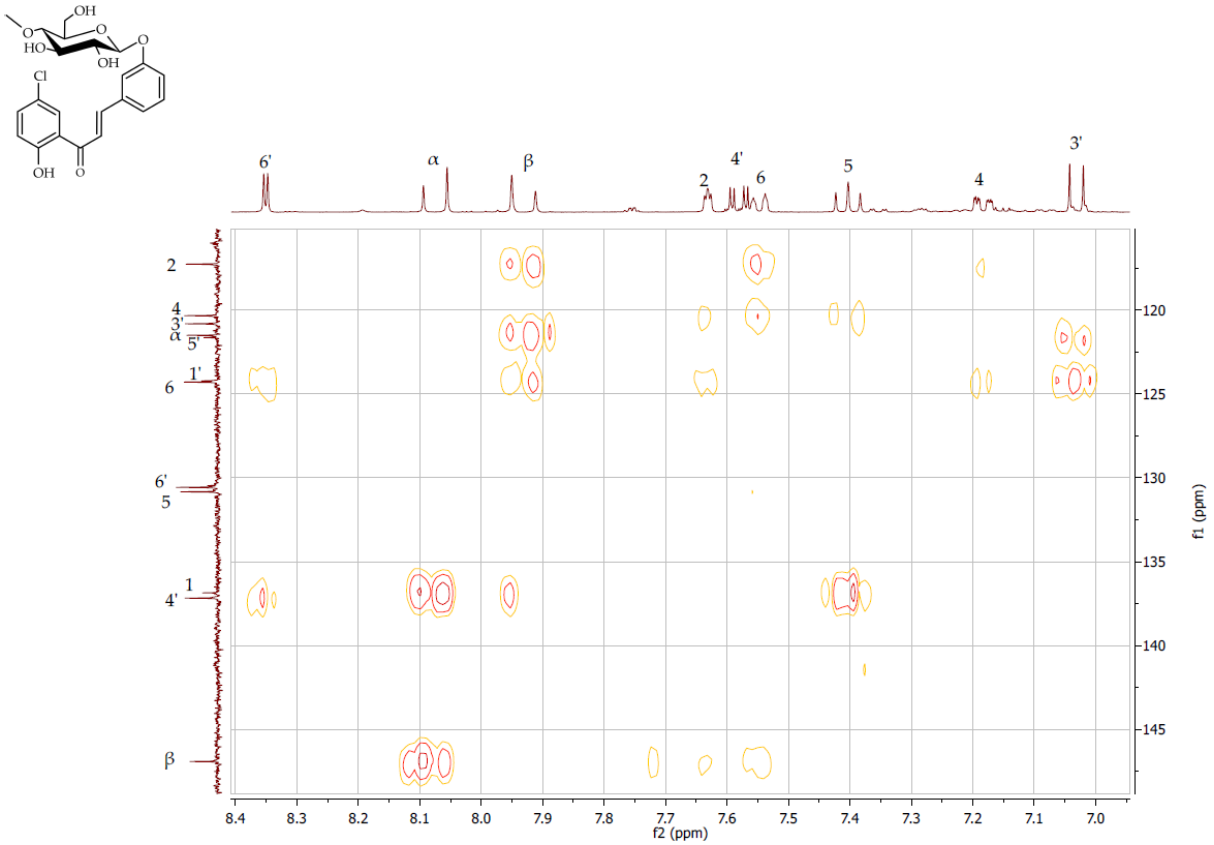


Figure S131. HMBC contour map – ^{1}H x ^{13}C expansion of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

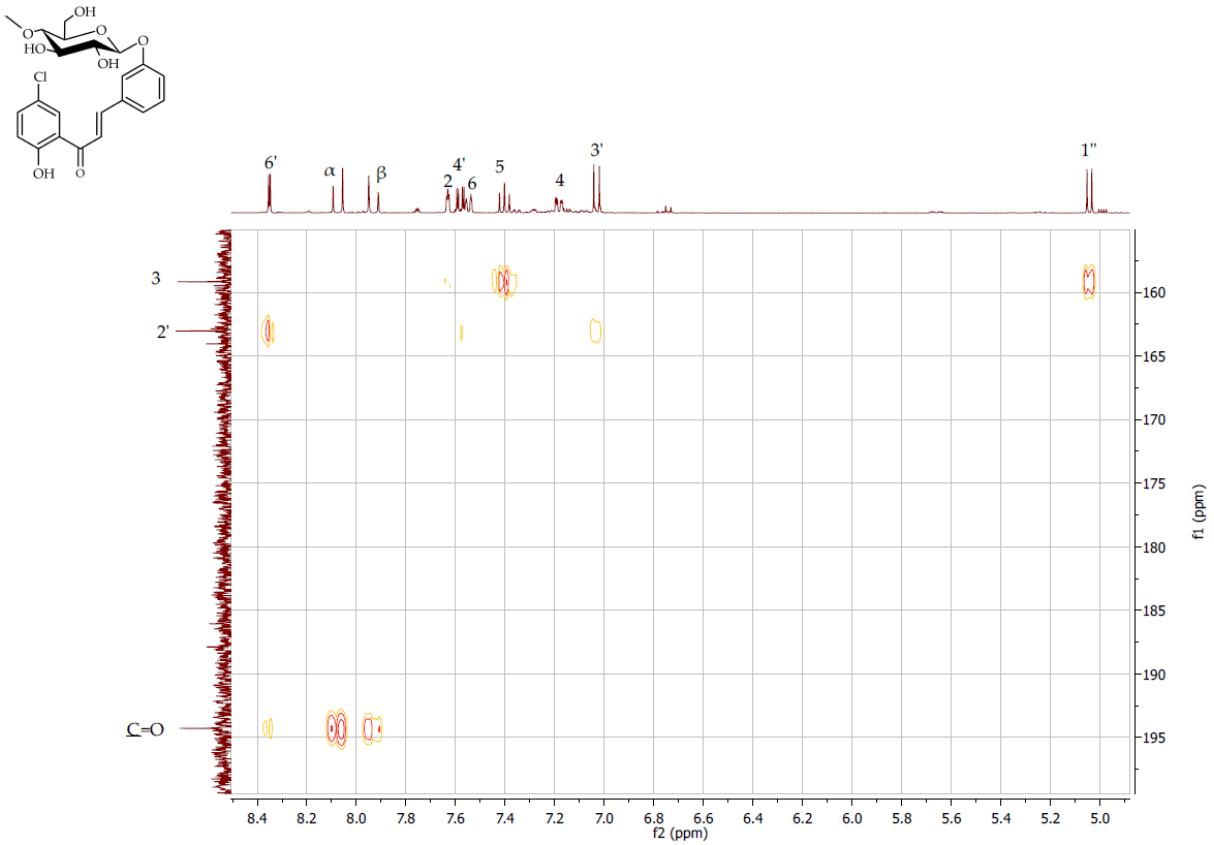


Figure S132. HMBC contour map – ^{1}H x ^{13}C expansion of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

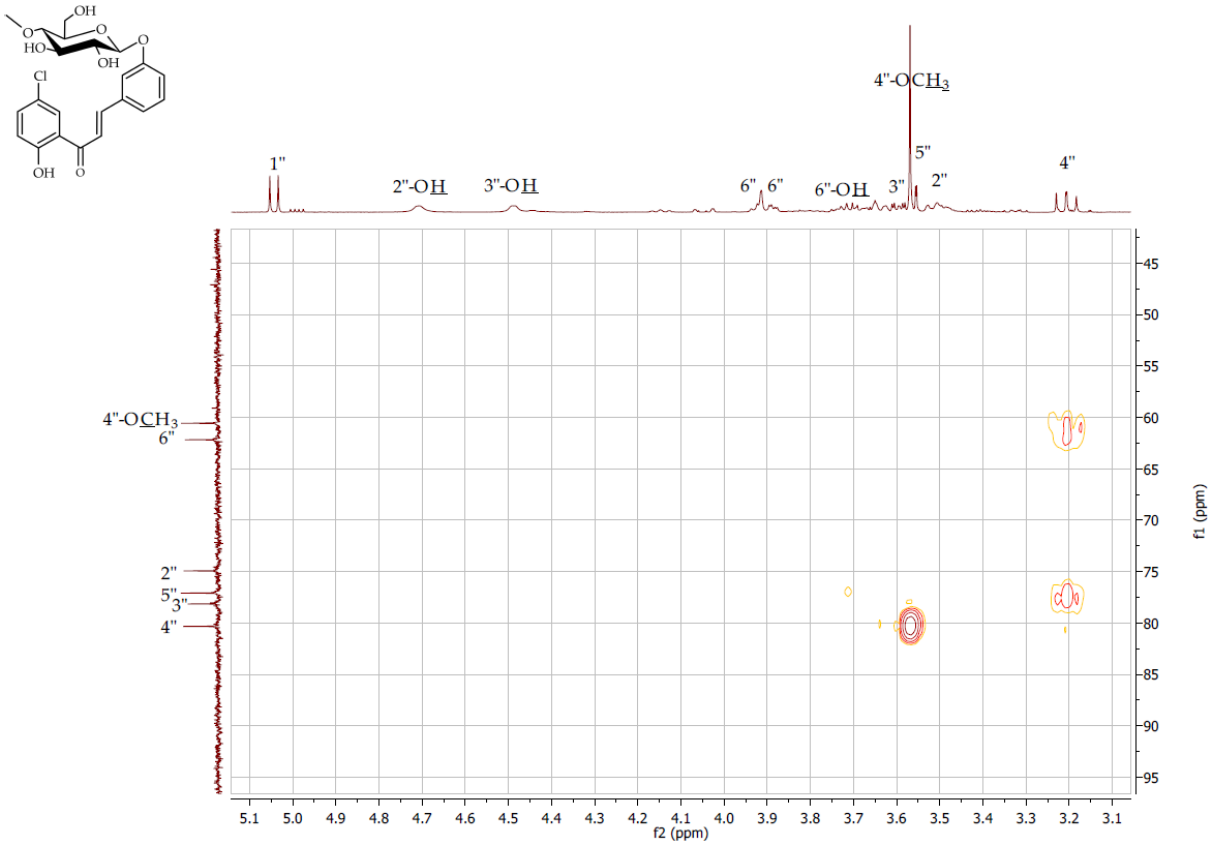


Figure S133. HMBC contour map – ^{1}H x ^{13}C expansion of 5′-chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**)

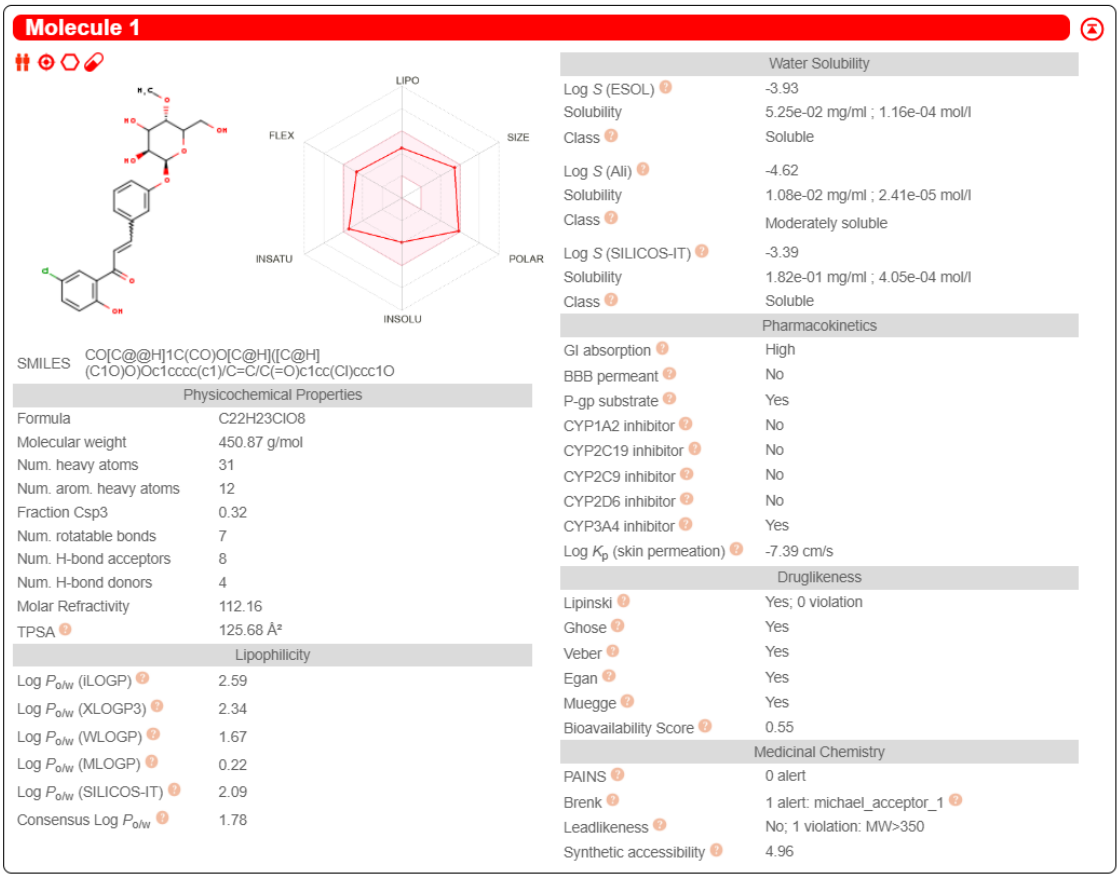


Figure S134. 5′-Chloro-2′-hydroxychalcone 3-*O*-*β*-D-(4′′-*O*-methyl)-glucopyranoside (**6b**) physicochemical and ADME parameters prediction using the SwissADME modelling

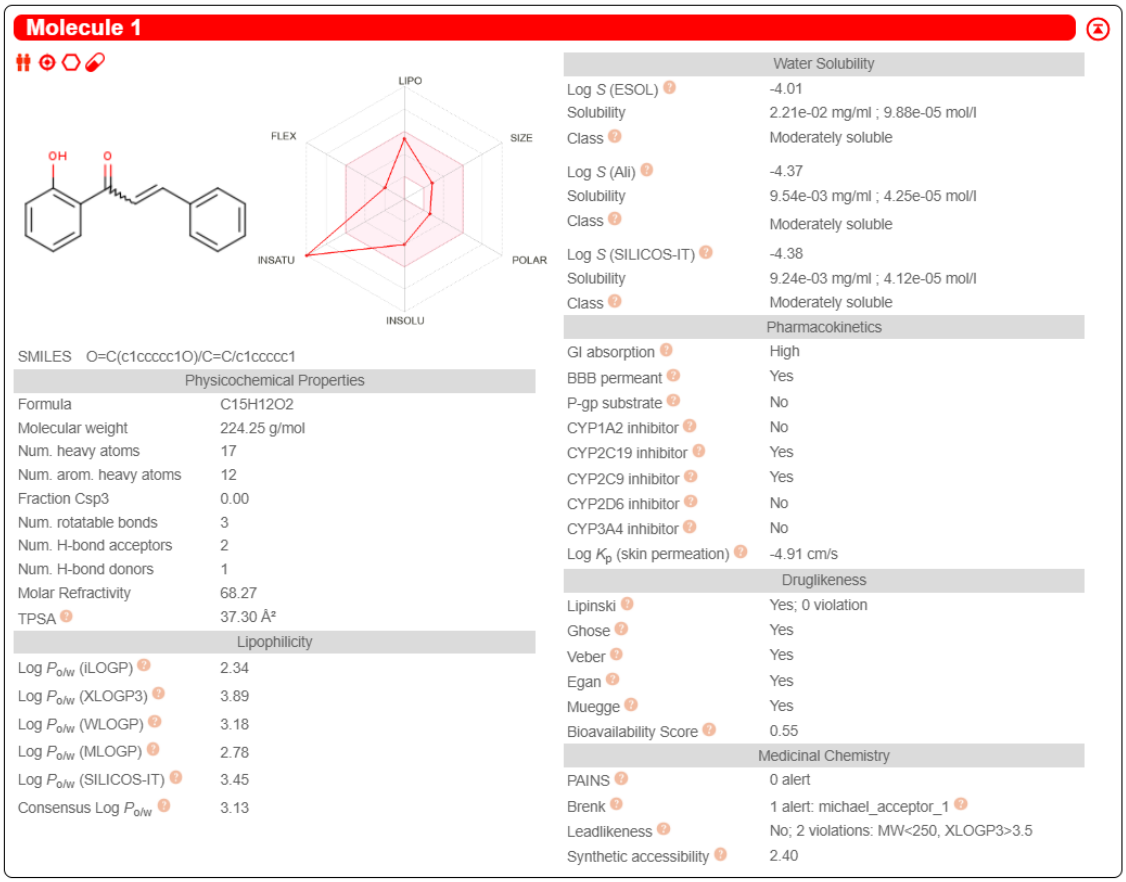


Figure S135. 2′-Hydroxychalcone (**7**) physicochemical and ADME parameters prediction using the SwissADME modelling