

Supplementary data for article:

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Supporting Information

Highly efficient enzymatic acetylation of flavonoids: Development of solvent-free process and kinetic evaluation

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1. Kinetic model

Set of ordinary differential equations (Eqs. S1-S3) that describes the rate of formation of each species

$$\frac{d([F])}{dt} = - \left(\frac{Vf_1 \cdot [F] - Vr_1 \cdot [FA]}{1 + \frac{[F]}{Kms_1} + \frac{[FA]}{Kmp_1}} \right) \quad (S1)$$

$$\frac{d([FA])}{dt} = \left(\frac{Vf_1 \cdot [F] - Vr_1 \cdot [FA]}{1 + \frac{[F]}{Kms_1} + \frac{[FA]}{Kmp_1}} \right) - \left(\frac{Vf_2 \cdot [FA] - Vr_2 \cdot [FDA]}{1 + \frac{[FA]}{Kms_2} + \frac{[FDA]}{Kmp_2}} \right) \quad (S2)$$

$$\frac{d([FDA])}{dt} = \left(\frac{Vf_2 \cdot [FA] - Vr_2 \cdot [FDA]}{1 + \frac{[FA]}{Kms_2} + \frac{[FDA]}{Kmp_2}} \right) \quad (S3)$$

where the letters inside the square brackets represent the concentrations of the respective species, while subscripts 1 and 2 of parameter names indicate the first (Eq. 2) and second (Eq. 3) reaction of kinetic model.

2. NMR analyses

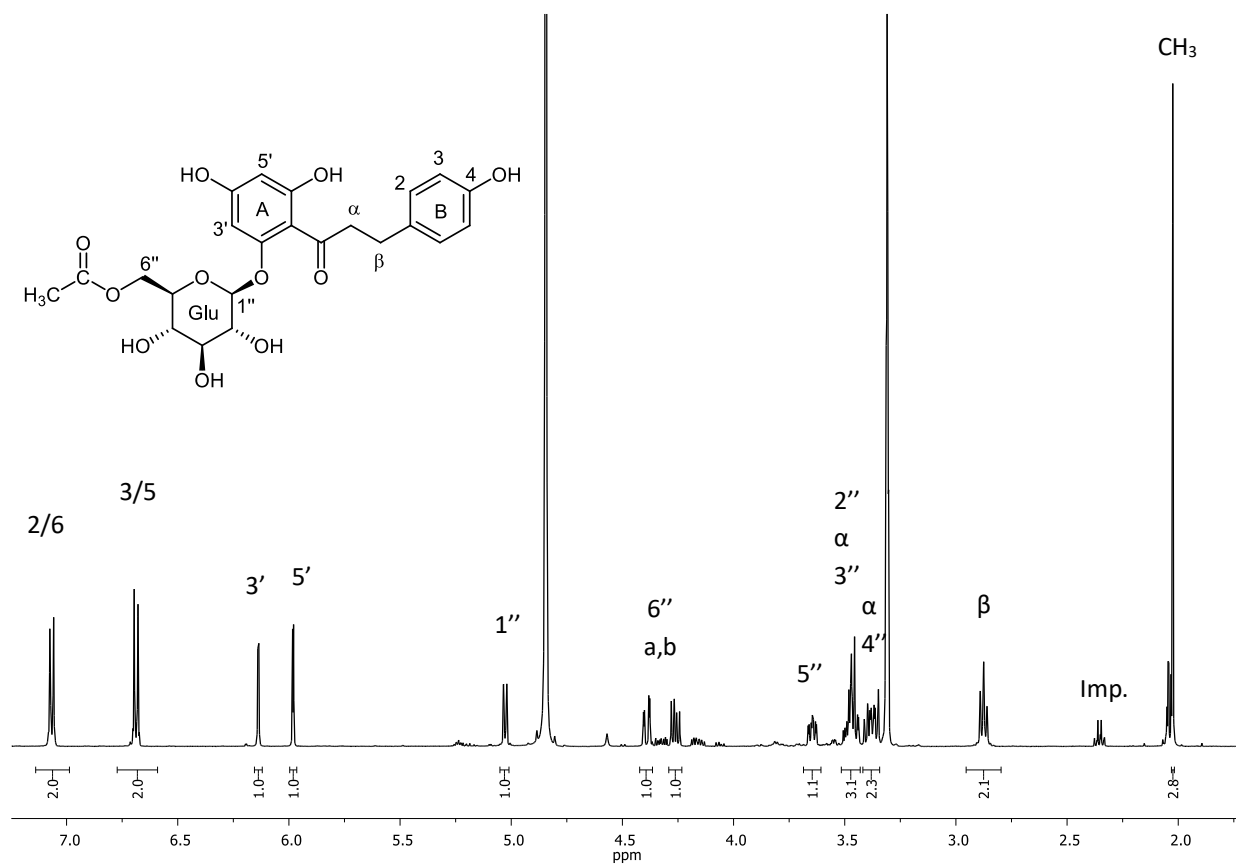


Figure S1. ¹H NMR (500 MHz, CD₃OD) spectrum of phloridzin-6''-O-acetate with complete assignments.

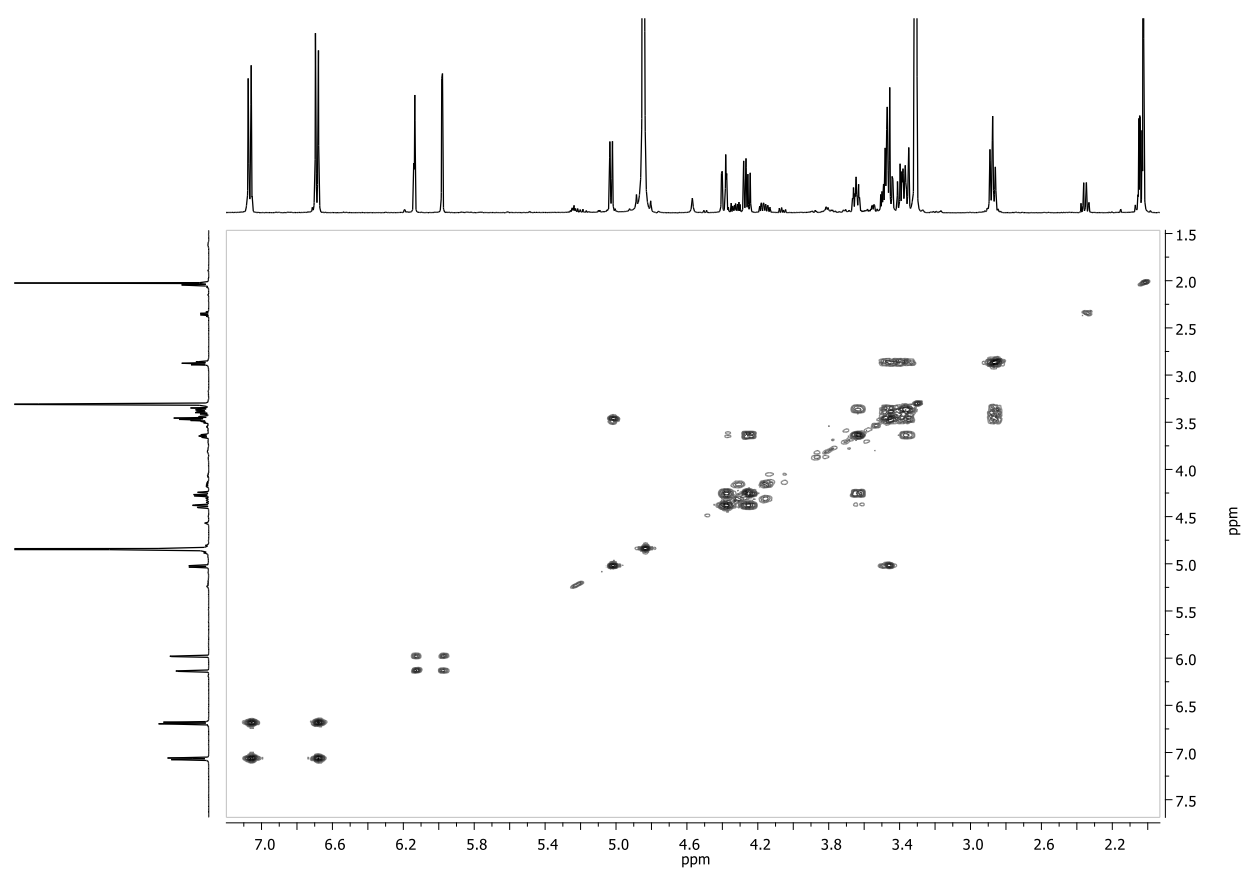


Figure S2. ^1H - ^1H COSY (500 MHz, CD_3OD) NMR spectrum of phloridzin-6''-O-acetate.

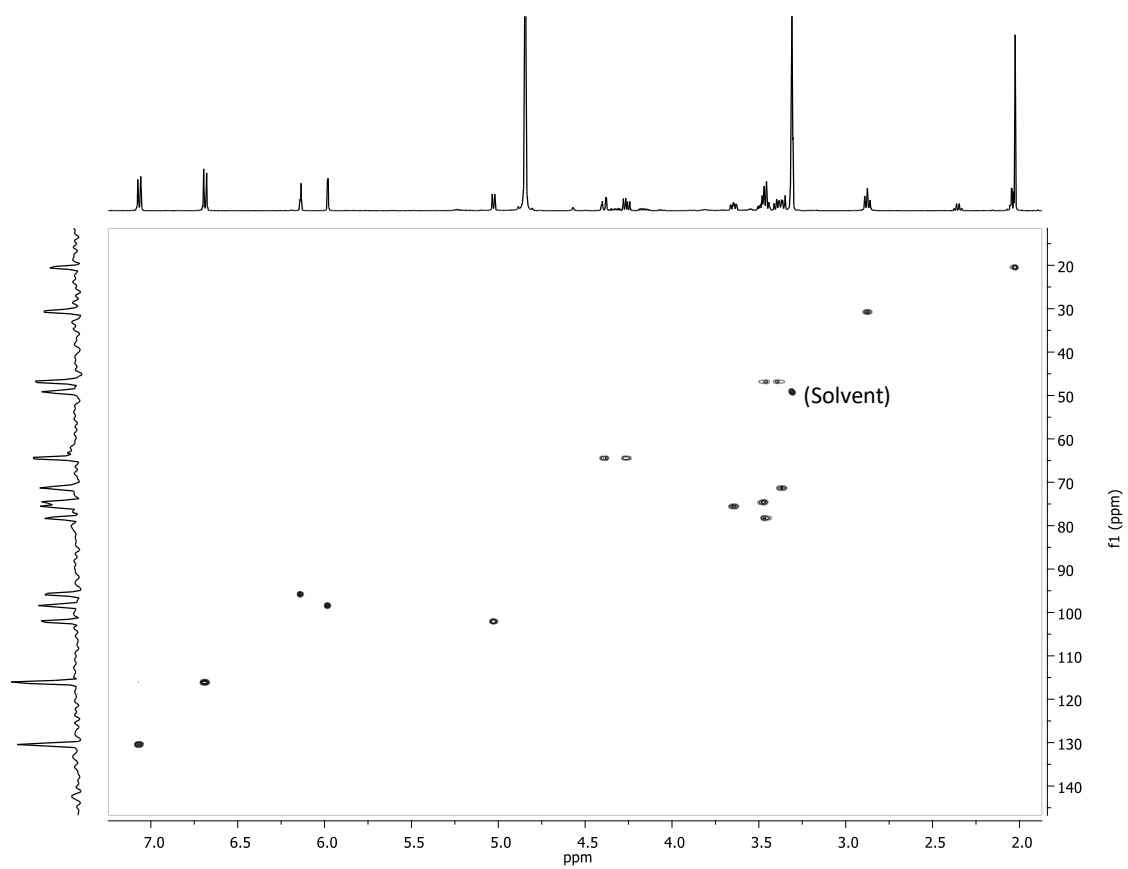


Figure S3. HSQC (500 MHz, CD₃OD) NMR spectrum of phloridzin-6''-O-acetate was used for assignments of 13 protonated carbons (nine CH, three CH₂ and one CH₃)

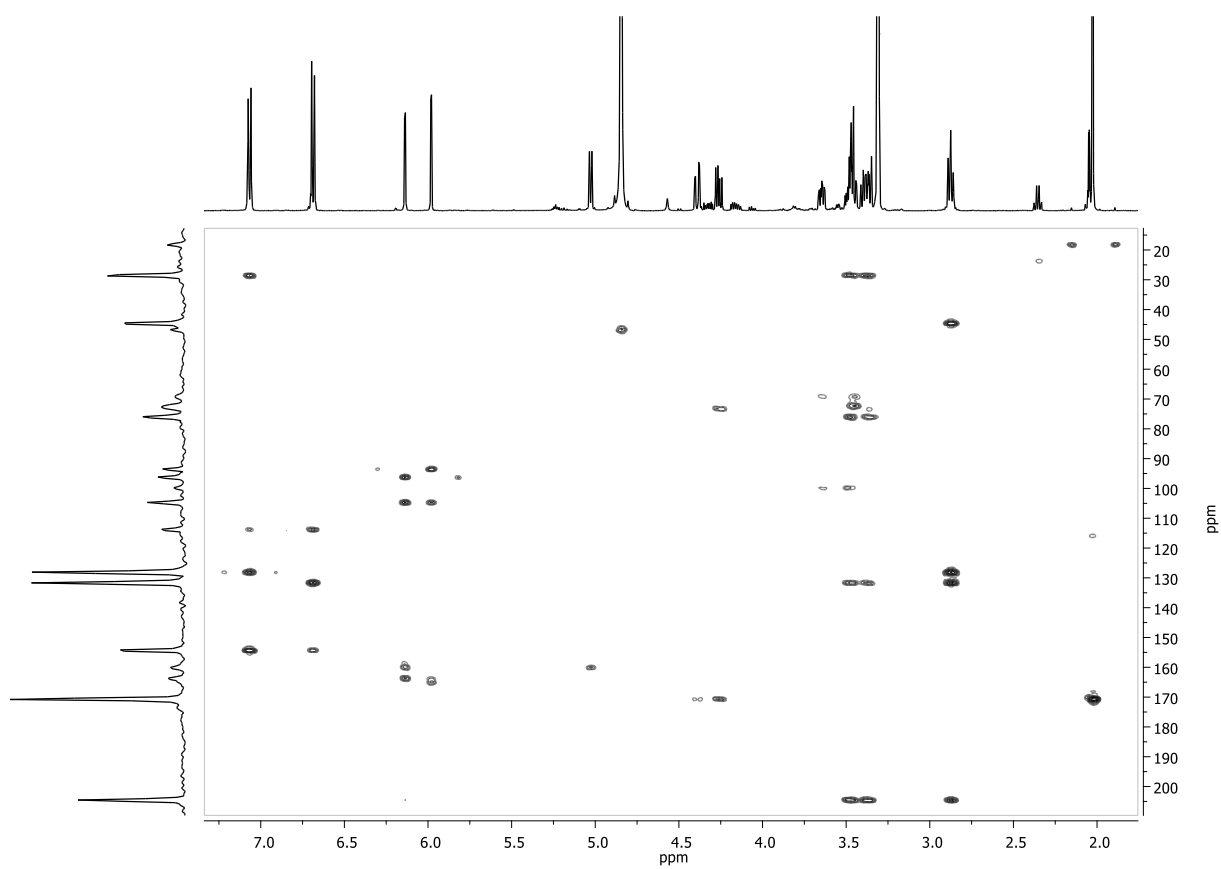


Figure S4. HMBC (500 MHz, CD₃OD) NMR spectrum of phloridzin-6''-O-acetate.

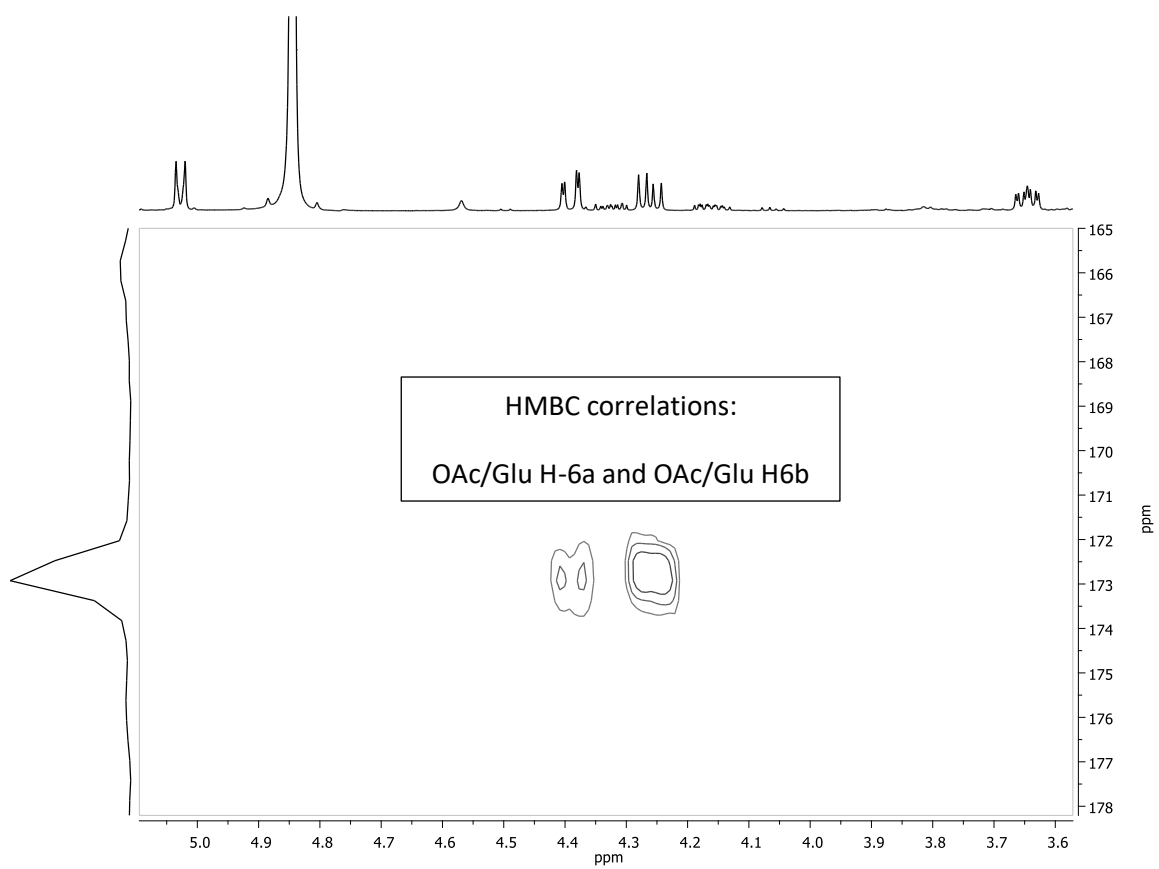


Figure S5. Partial HMBC (CD₃OD) NMR spectrum of phloridzin-6''-O-acetate showing the most important correlations between ester carbon and both Glu H-6 protons.

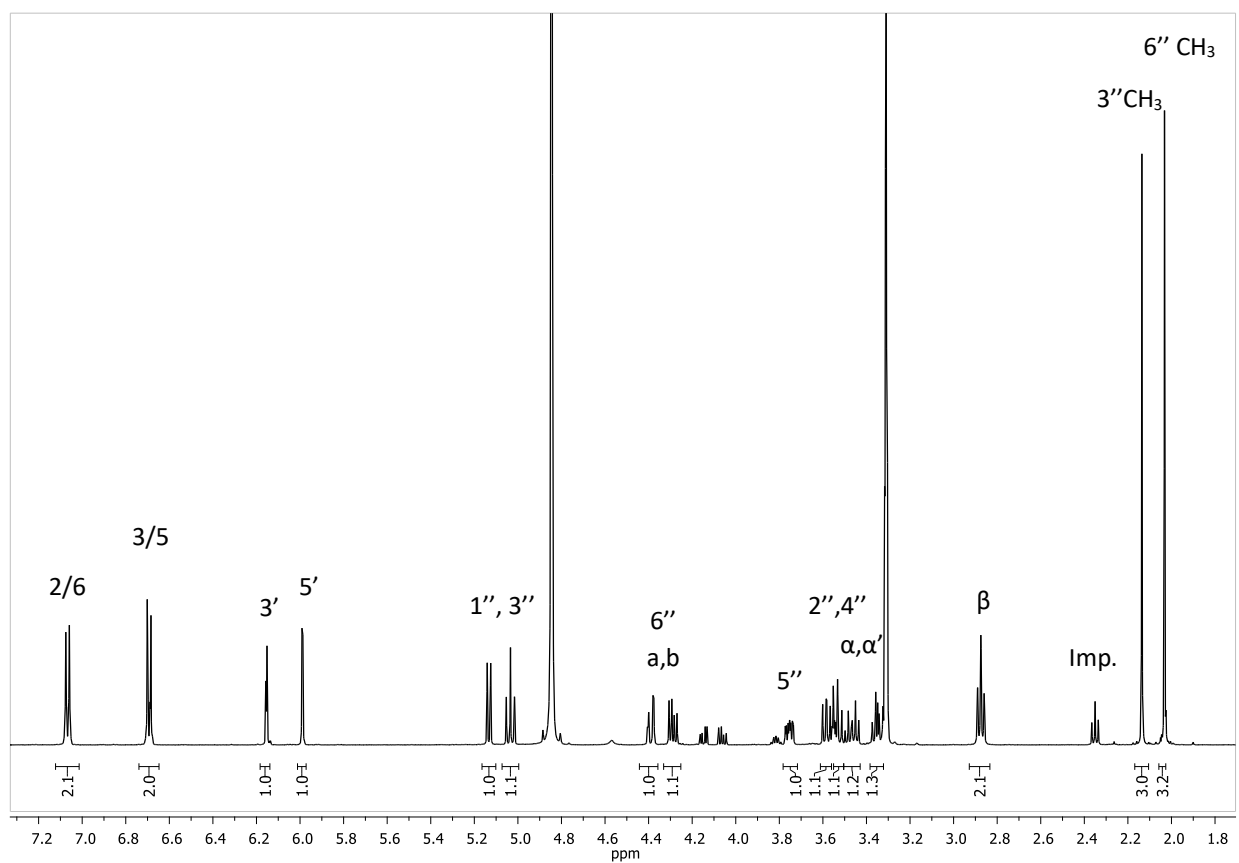
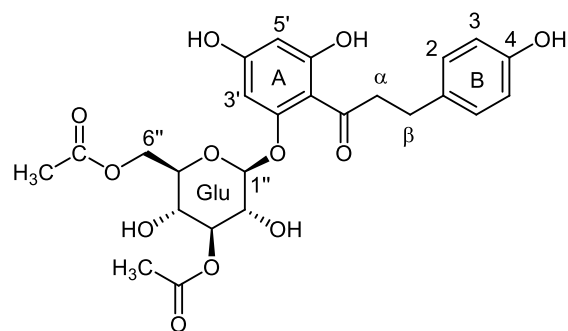


Figure S6. ^1H NMR (500 MHz, CD_3OD) spectrum of phloridzin-3'',6''-O-diacetate with complete assignments.

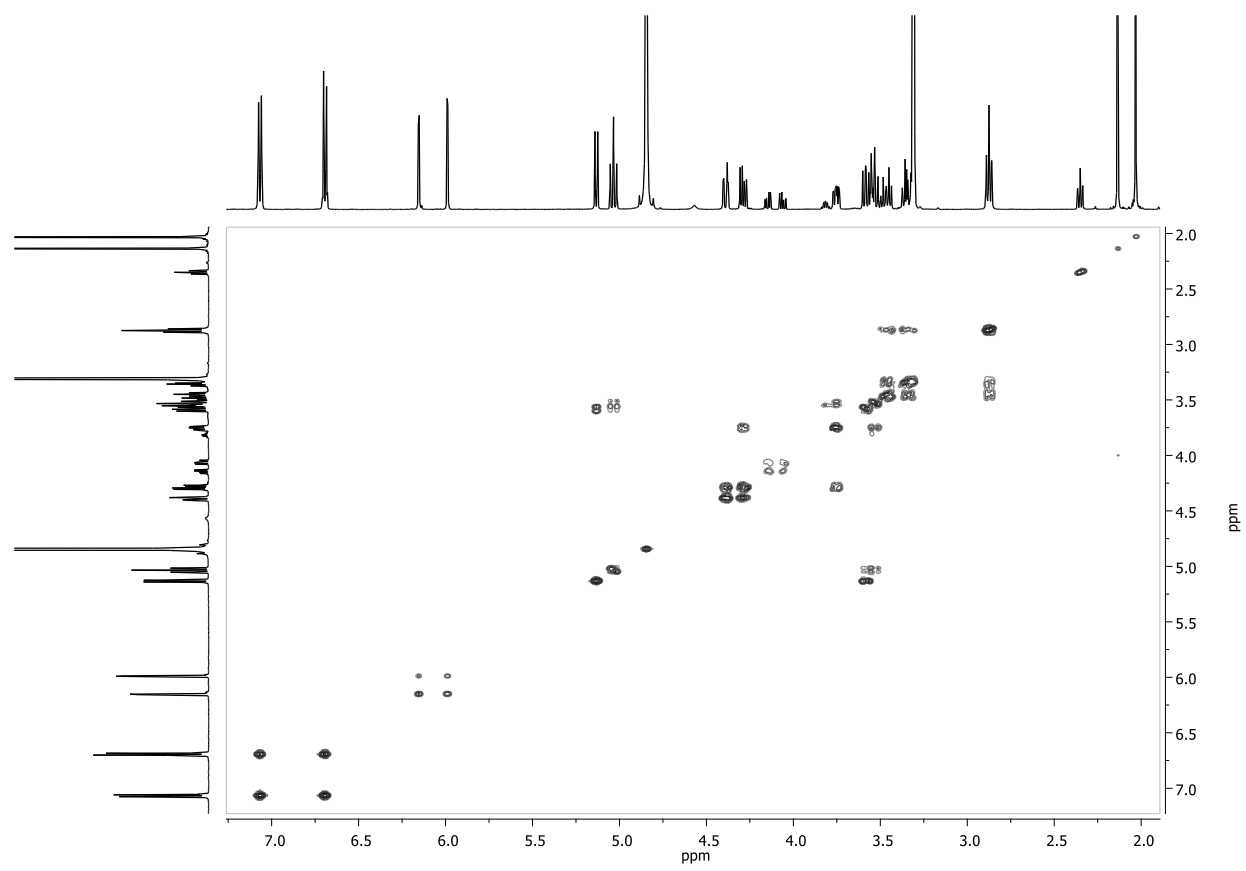


Figure S7. ^1H - ^1H COSY (500 MHz, CD_3OD) NMR spectrum of phloridzin-3'',6''-O-diacetate.

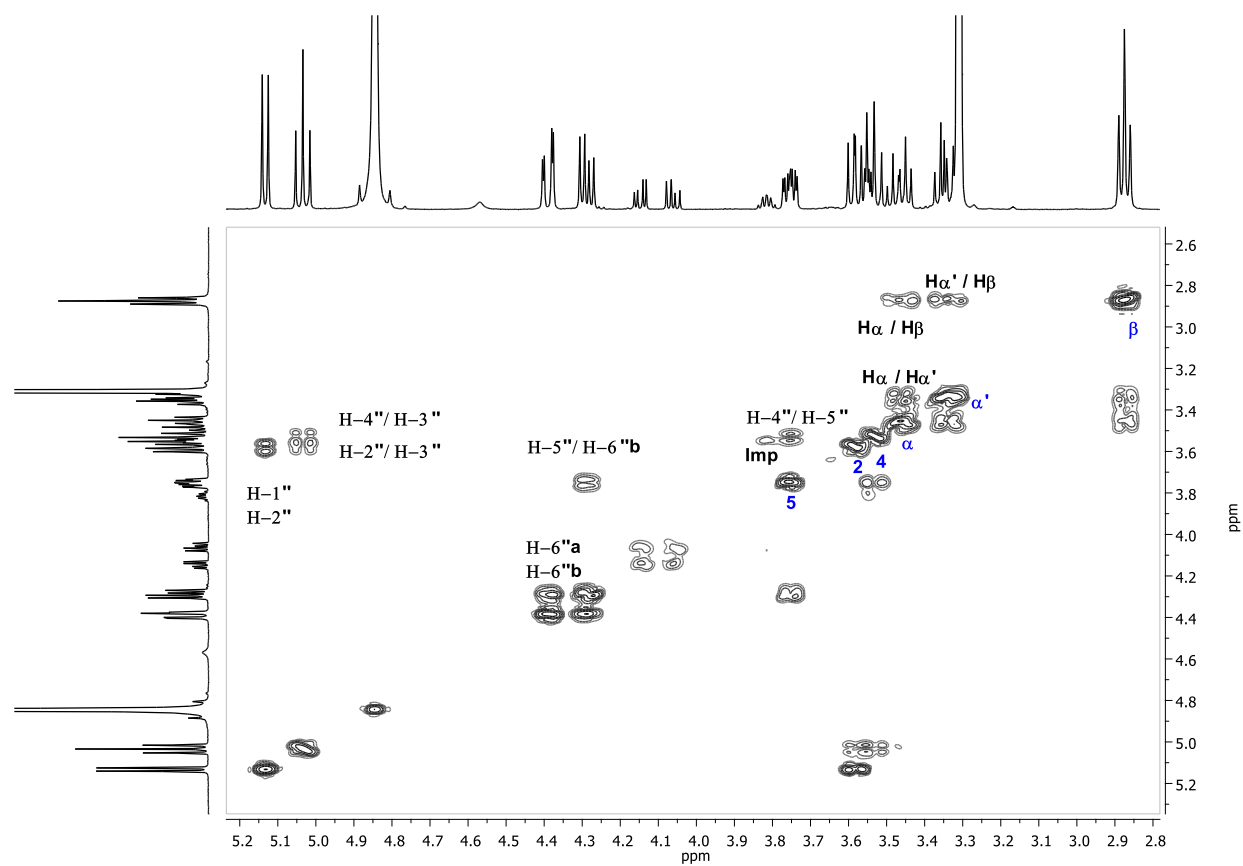


Figure S8. Partial ^1H - ^1H COSY (500 MHz, CD_3OD) NMR spectrum of phloridzin-3'',6''-O-diacetate showing the most important correlations.

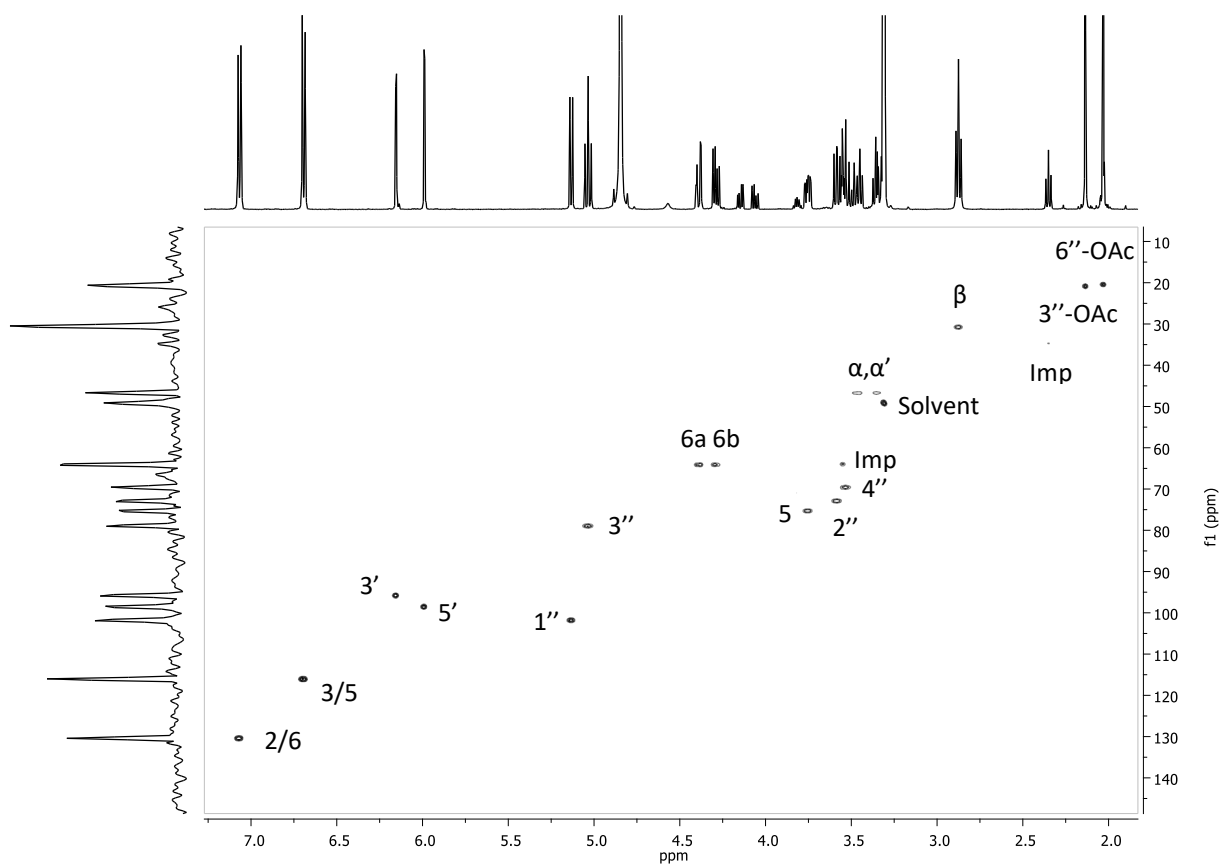


Figure S9. HSQC (500 MHz, CD₃OD) NMR spectrum of phloridzin-3'',6''-O-diacetate showing all assignments of protonated carbons.

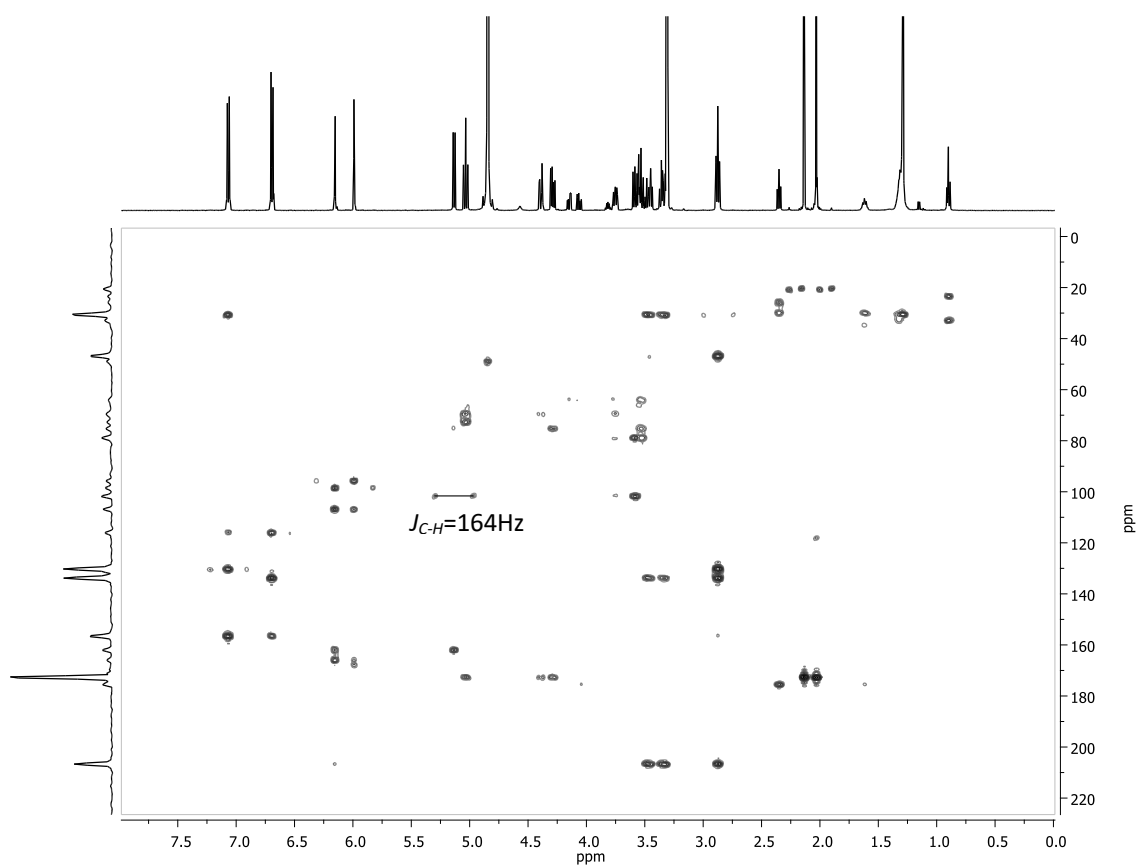


Figure S10. HMBC (500 MHz, CD₃OD) NMR spectrum of phloridzin-3'',6''-O-diacetate. Label is showing HSQC artefact of anomeric signal with coupling constant of 164 Hz between proton and carbon, characteristic for β -anomers.

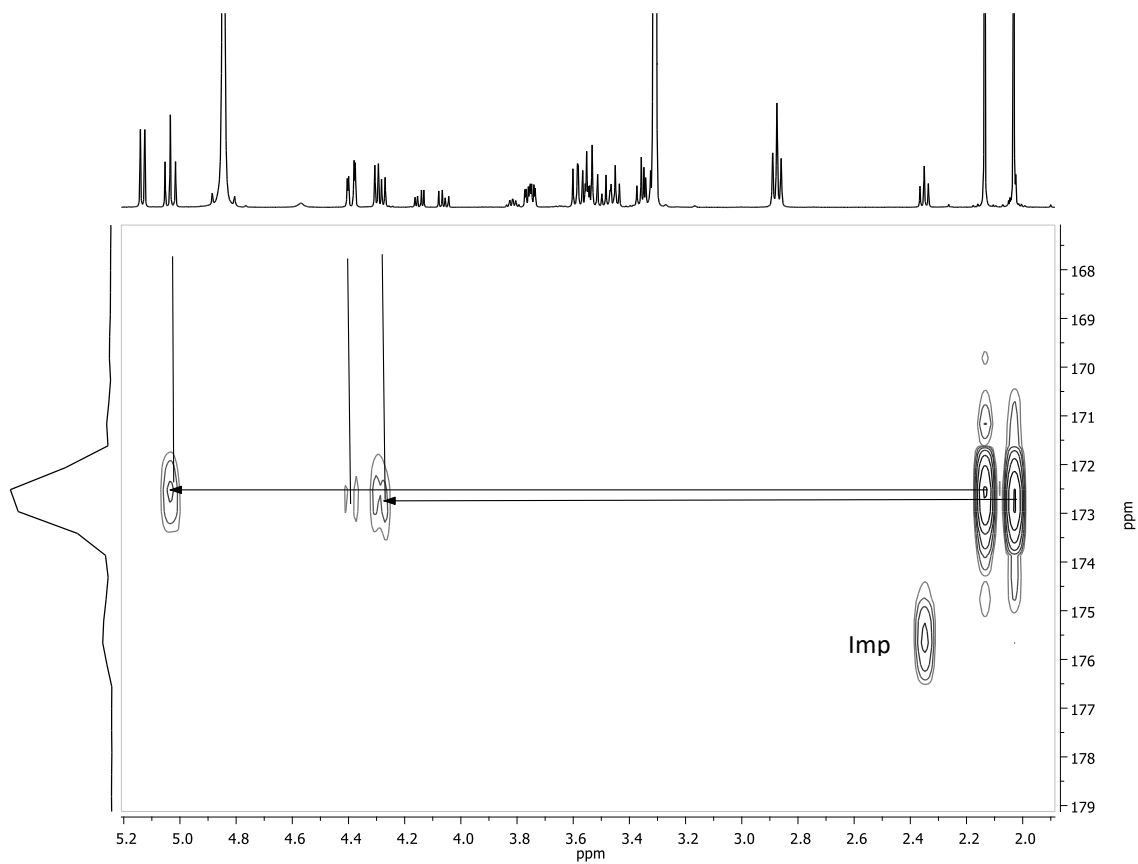


Figure S11. Partial HMBC (CD_3OD) NMR spectrum of phloridzin-3'',6''-O-diacetate showing the most important correlations between ester carbons and Glu H-3 and H-6 protons.

Table S1 Calculated values of coefficient of determination (R^2) for all variables in all experiment with model flavonoid used for kinetic modeling purposes.

	Initial concentration of phloridzin, mM			
	30	50	75	100
R^2 (Ph)	0.995	0.997	0.997	0.998
R^2 (PhAc)	0.978	0.983	0.987	0.994
R^2 (PhDAc)	0.997	0.998	0.998	0.998

*Ph, PhAc, PhDAc refer to phloridzin, phloridzin acetate and phloridzin diacetate, respectively.