

*Supplementary Materials*

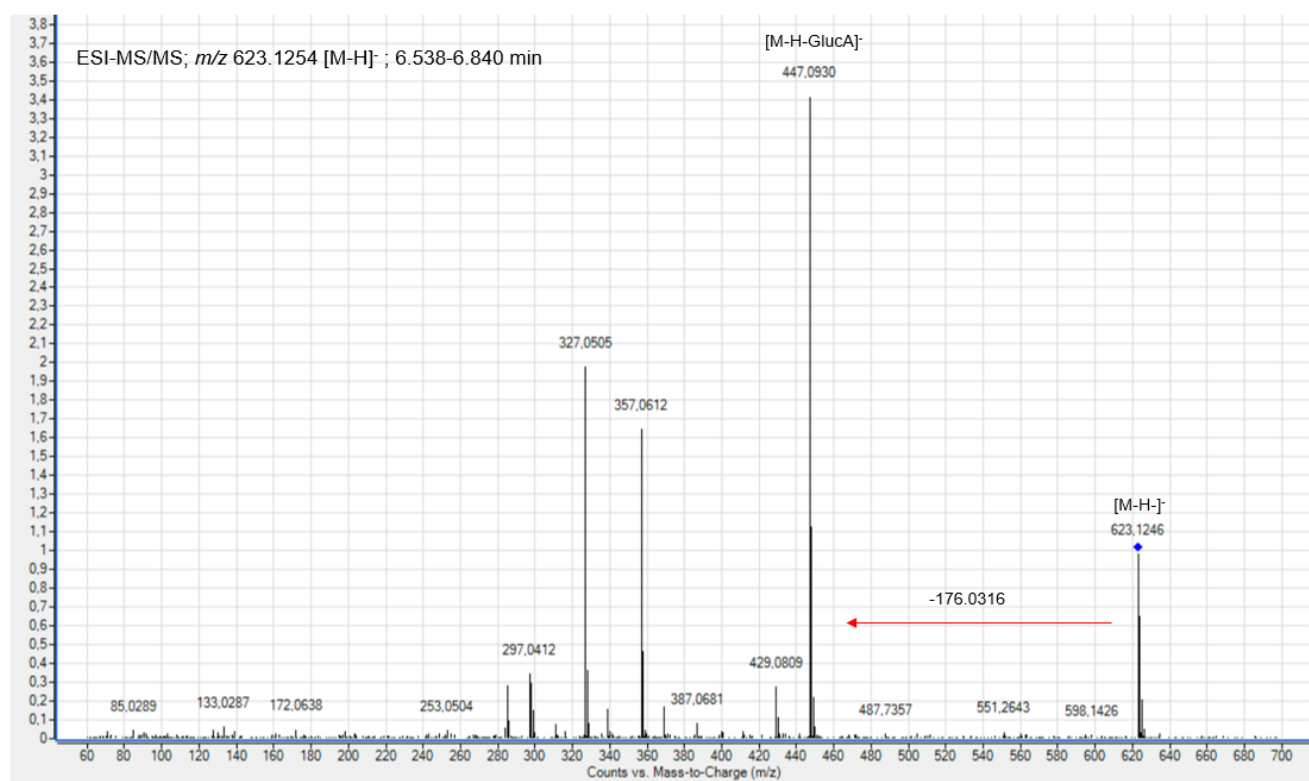
# **In Vitro Liver Metabolism of Six Flavonoid C-Glycosides**

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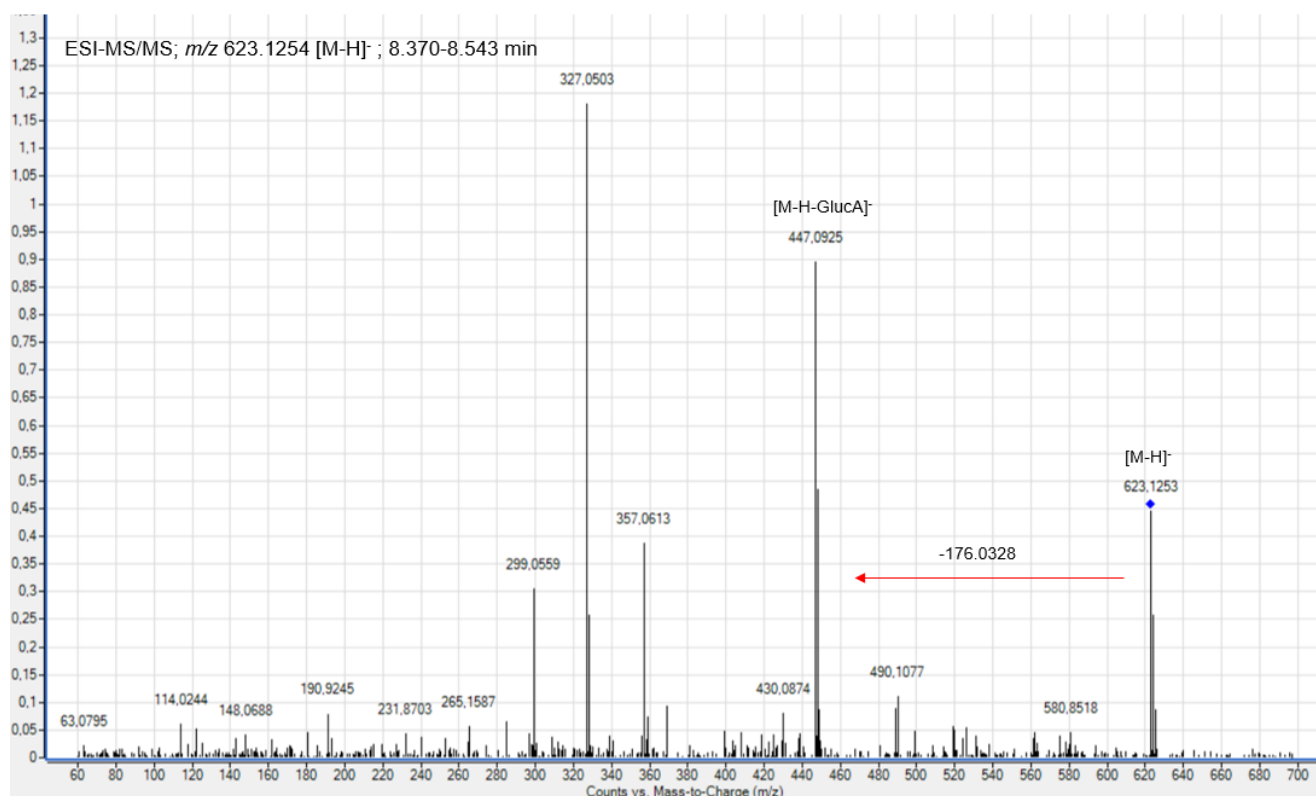
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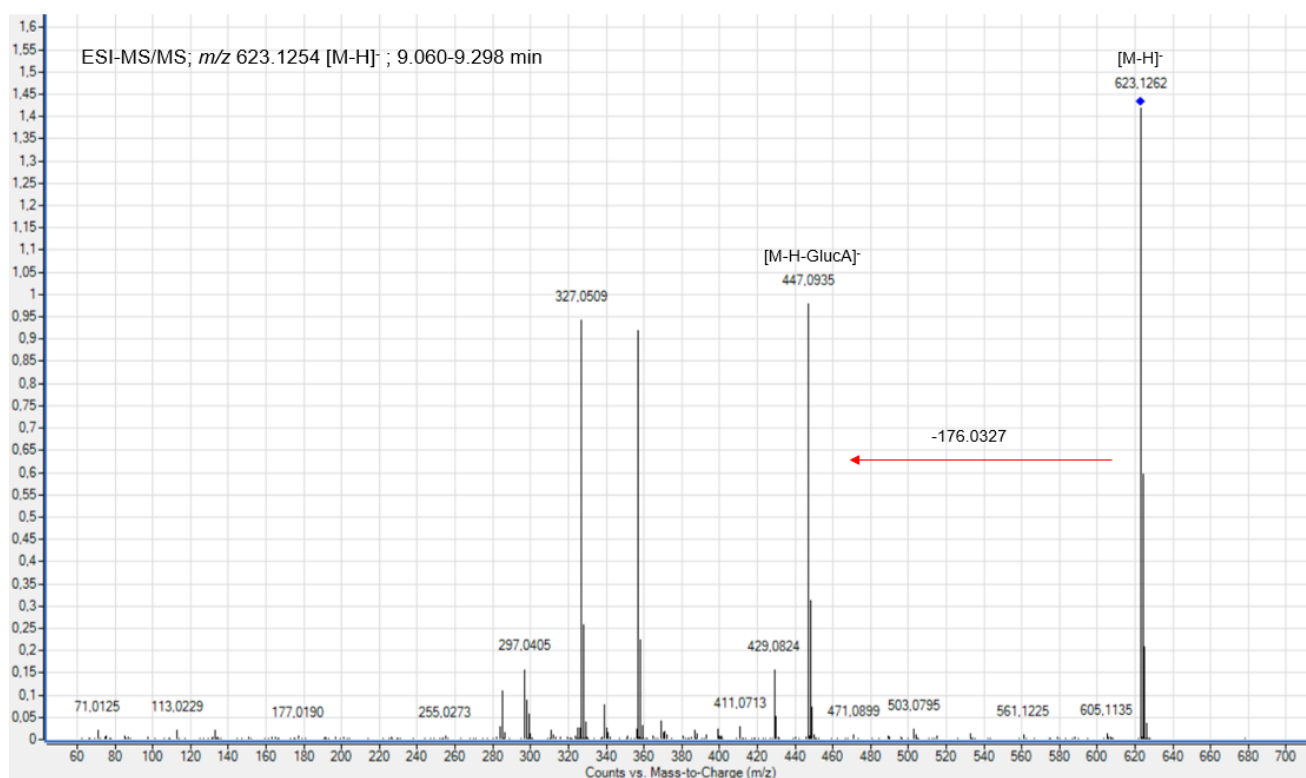
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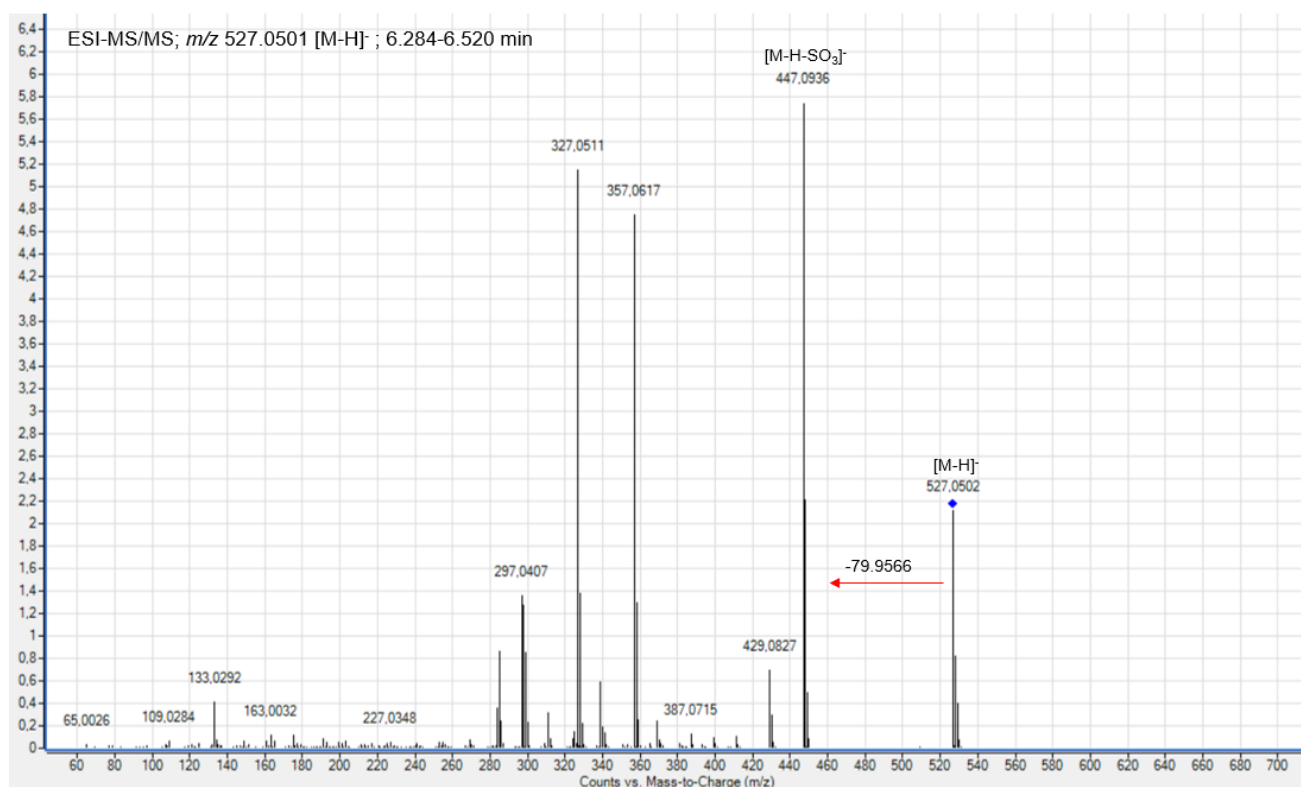
**Figure S1.** MS/MS spectrum of the extracted mass of isoorientin-G1 and its retention time with loss of dehydrated (-18 u) glucuronic acid (GlucA).



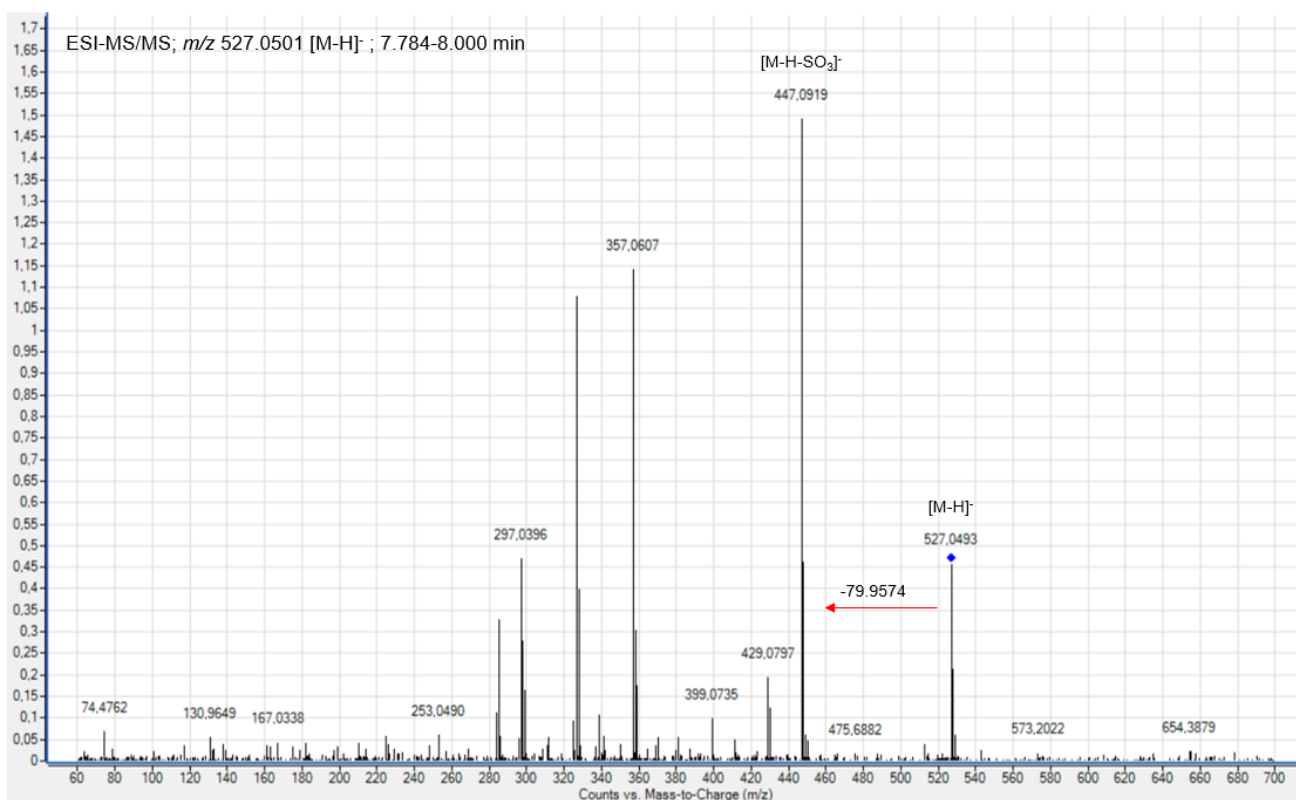
**Figure S2.** MS/MS spectrum of the extracted mass of isoorientin-G2 and its retention time with loss of dehydrated (-18 u) glucuronic acid (GlucA).



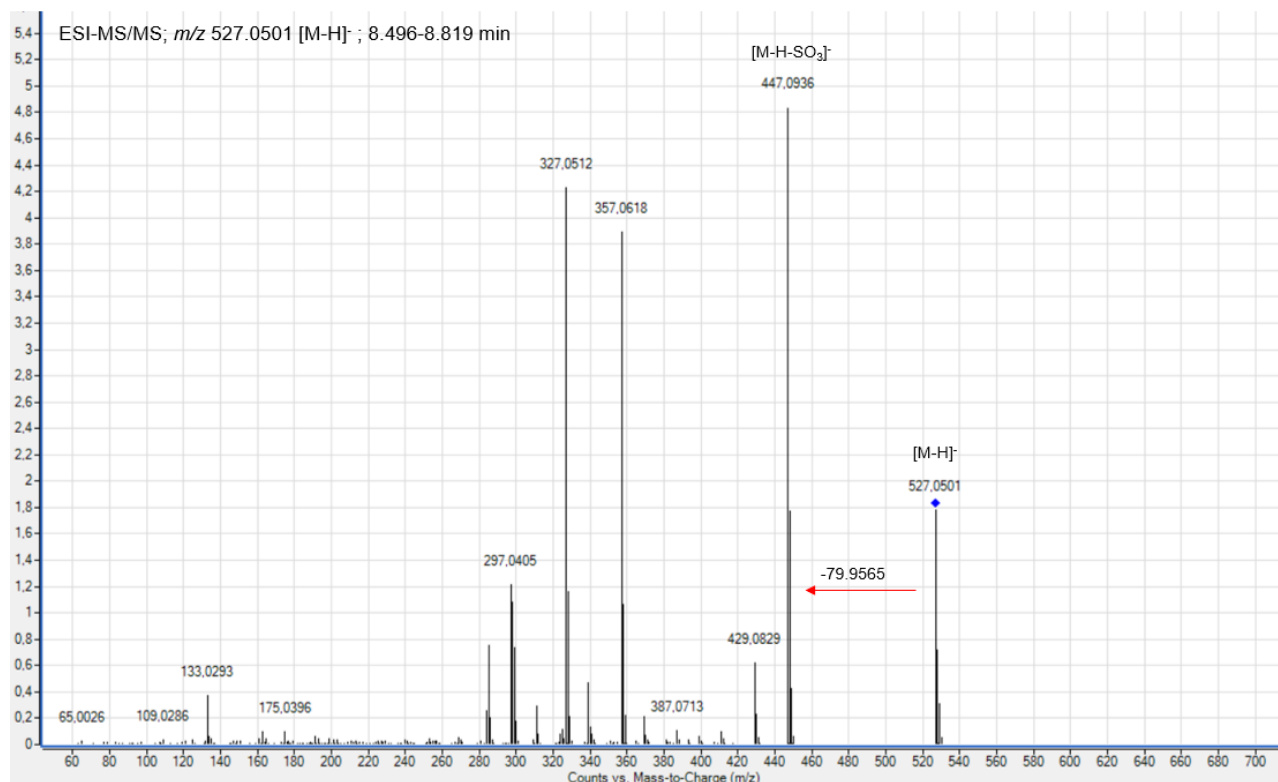
**Figure S3.** MS/MS spectrum of the extracted mass of isoorientin-G3 and its retention time with loss of dehydrated (-18 u) glucuronic acid (GlucA).



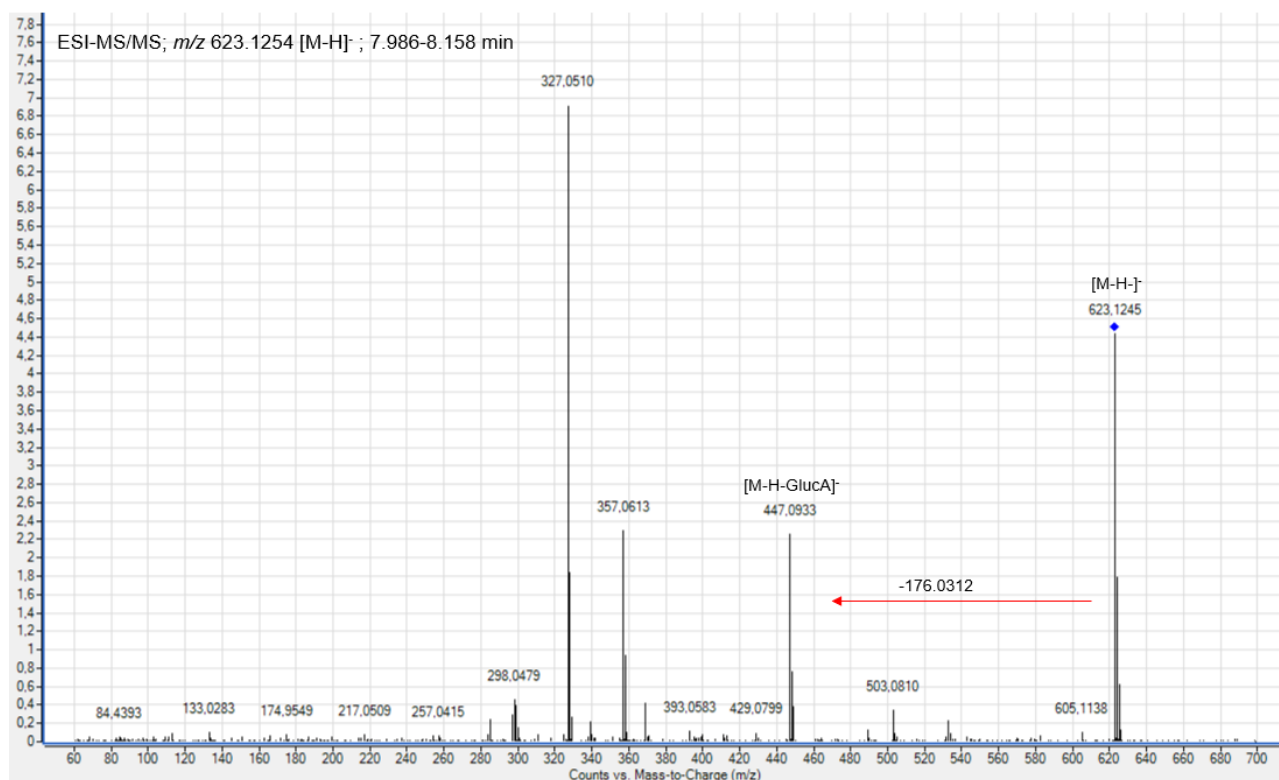
**Figure S4.** MS/MS spectrum of the extracted mass of isoorientin-S1 and its retention time with neutral loss of SO<sub>3</sub>.



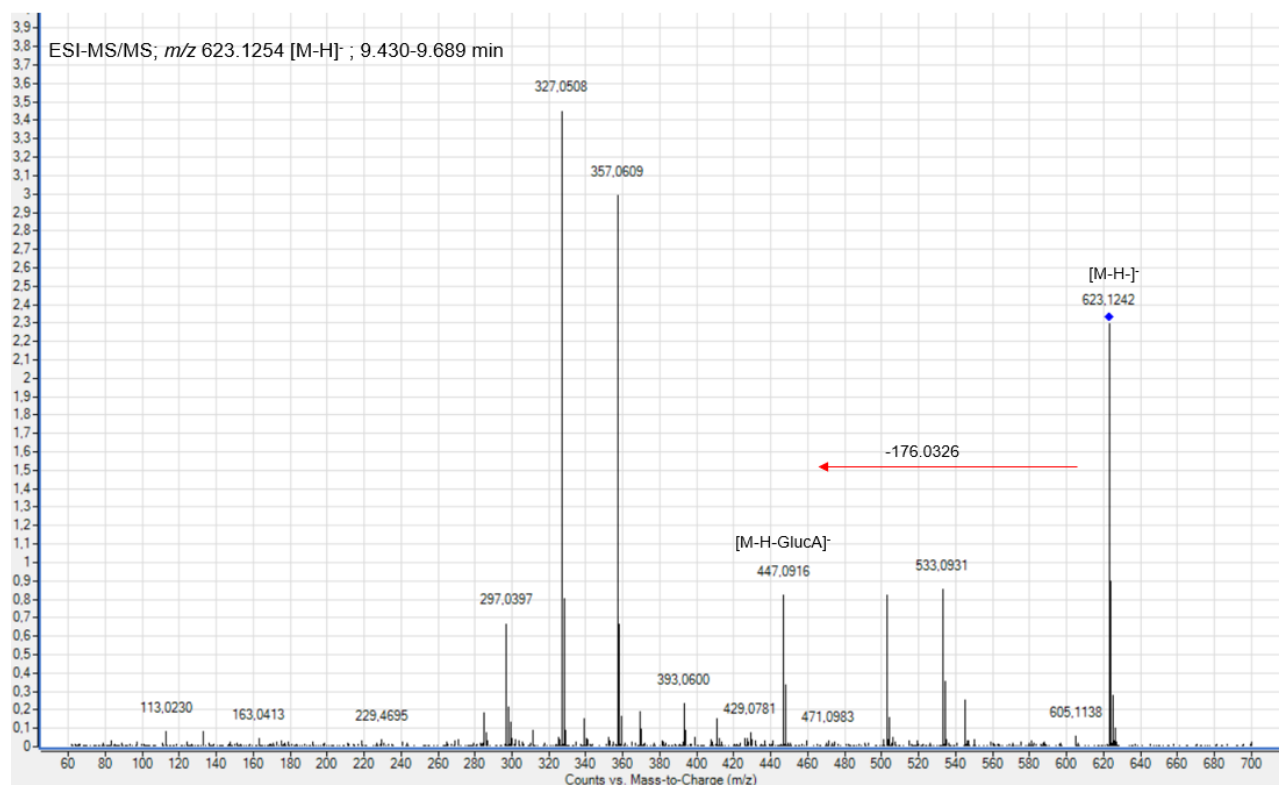
**Figure S5.** MS/MS spectrum of the extracted mass of isoorientin-S2 and its retention time with neutral loss of SO<sub>3</sub>.



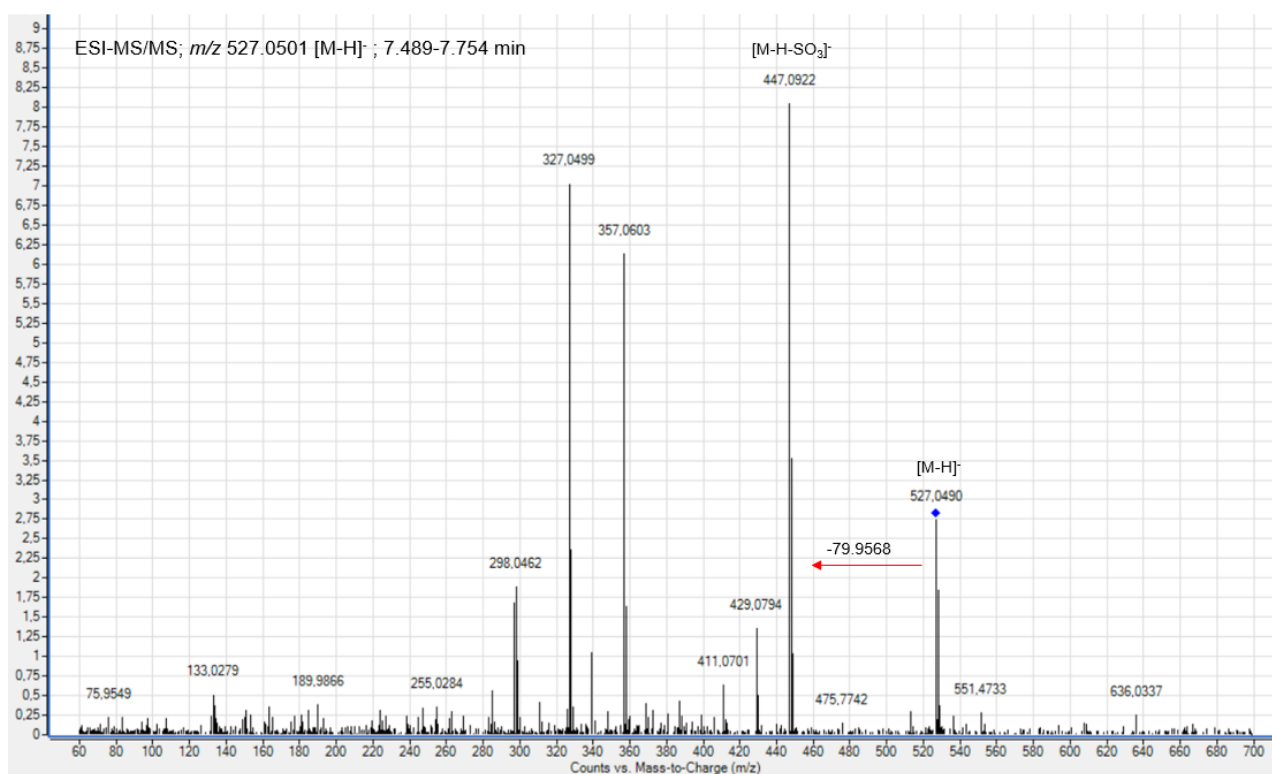
**Figure S6.** MS/MS spectrum of the extracted mass of isoorientin-S3 and its retention time with neutral loss of SO<sub>3</sub>.



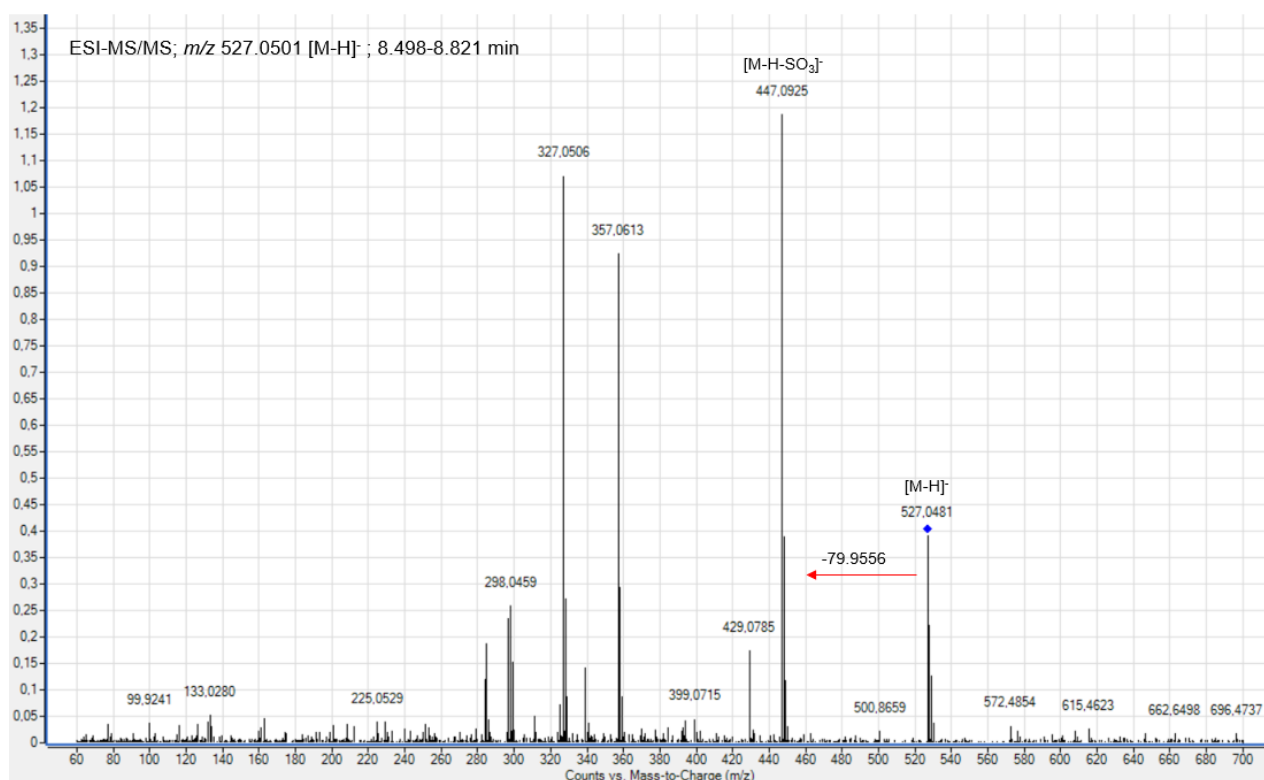
**Figure S7.** MS/MS spectrum of the extracted mass of orientin-G1 and its retention time with loss of dehydrated (-18 u) glucuronic acid (GlucA).



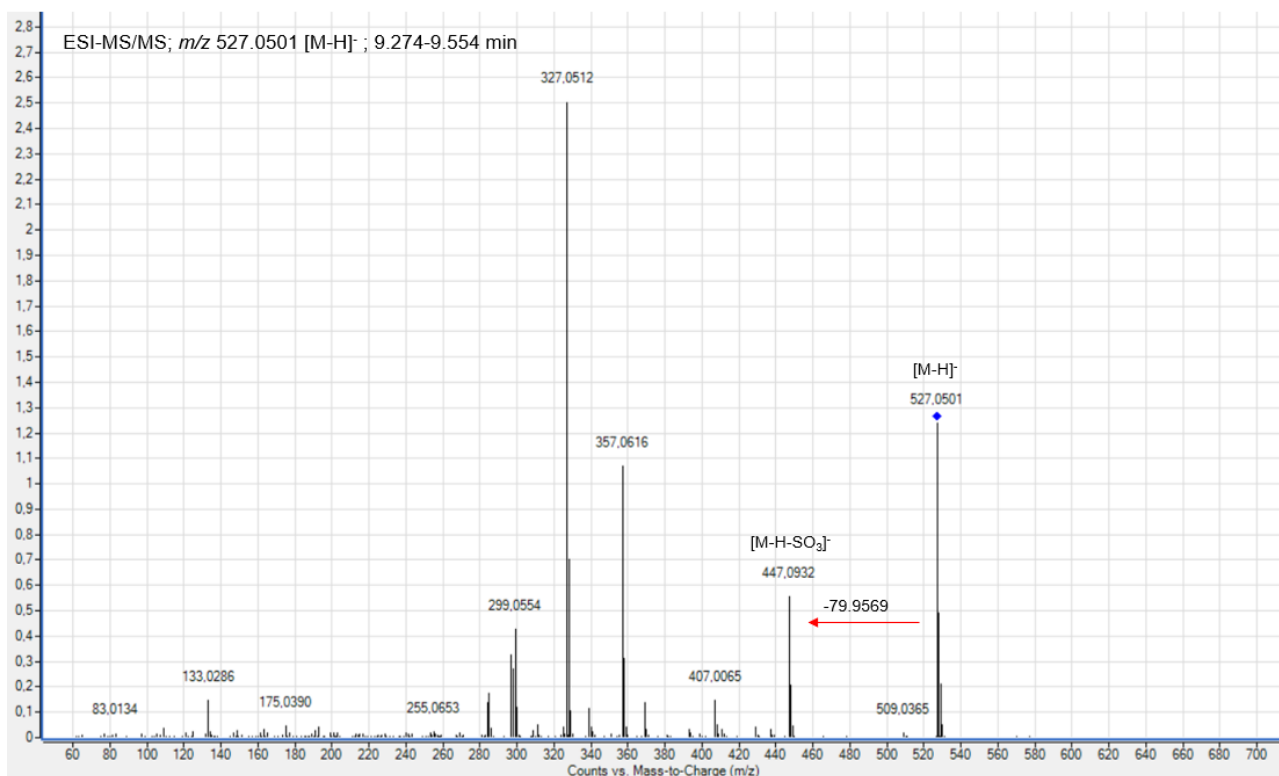
**Figure S8.** MS/MS spectrum of the extracted mass of orientin-G2 and its retention time with loss of dehydrated (-18 u) glucuronic acid (GlucA).



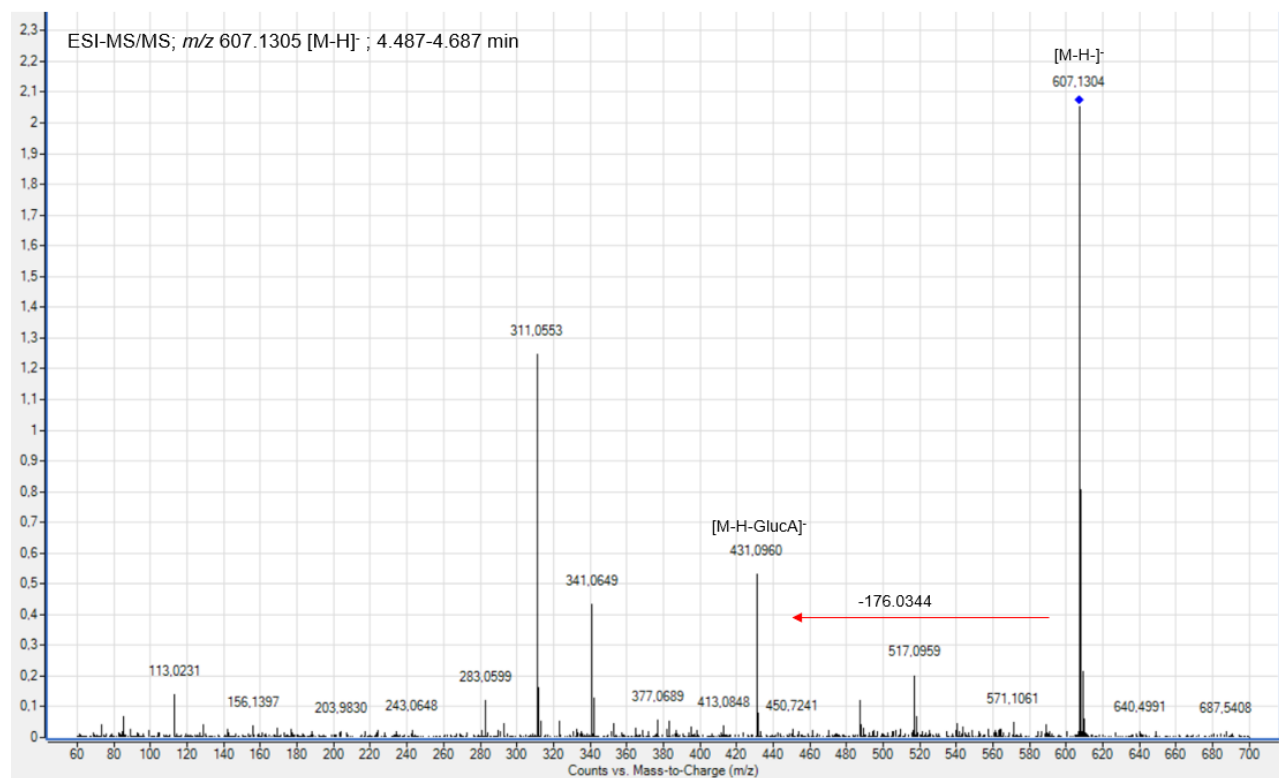
**Figure S9.** MS/MS spectrum of the extracted mass of orientin-S1 and its retention time with neutral loss of SO<sub>3</sub>.



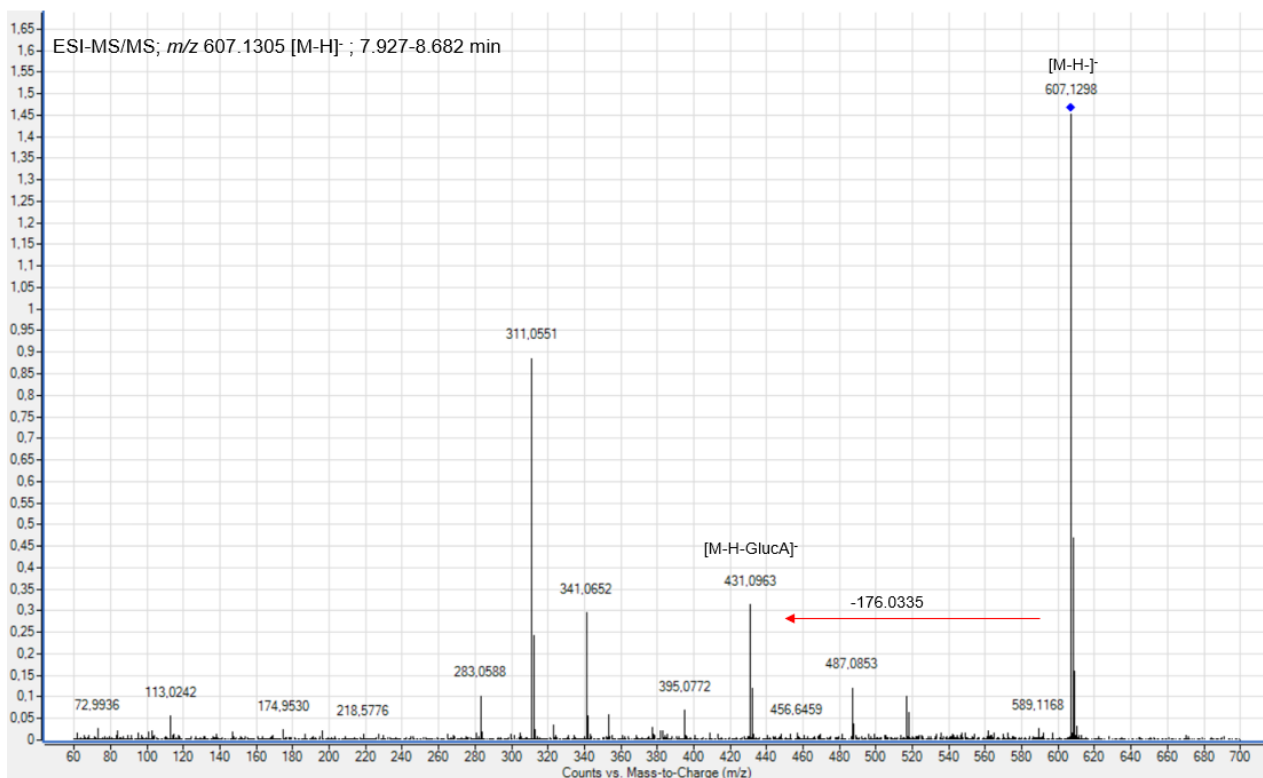
**Figure S10.** MS/MS spectrum of the extracted mass of orientin-S2 and its retention time with neutral loss of SO<sub>3</sub>.



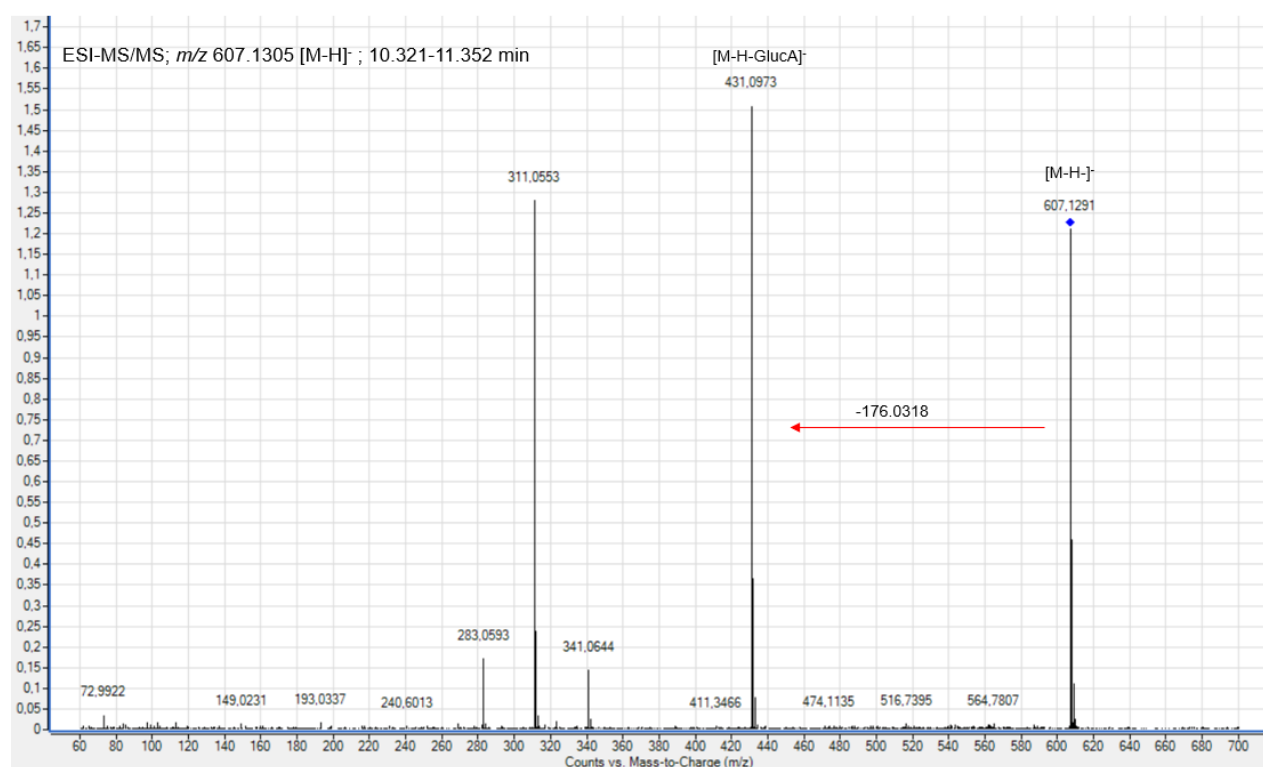
**Figure S11.** MS/MS spectrum of the extracted mass of orientin-S3 and its retention time with neutral loss of SO<sub>3</sub>.



**Figure S12.** MS/MS spectrum of the extracted mass of vitexin-G1 and its retention time with loss of dehydrated (-18 u) glucuronic acid (GlucA).

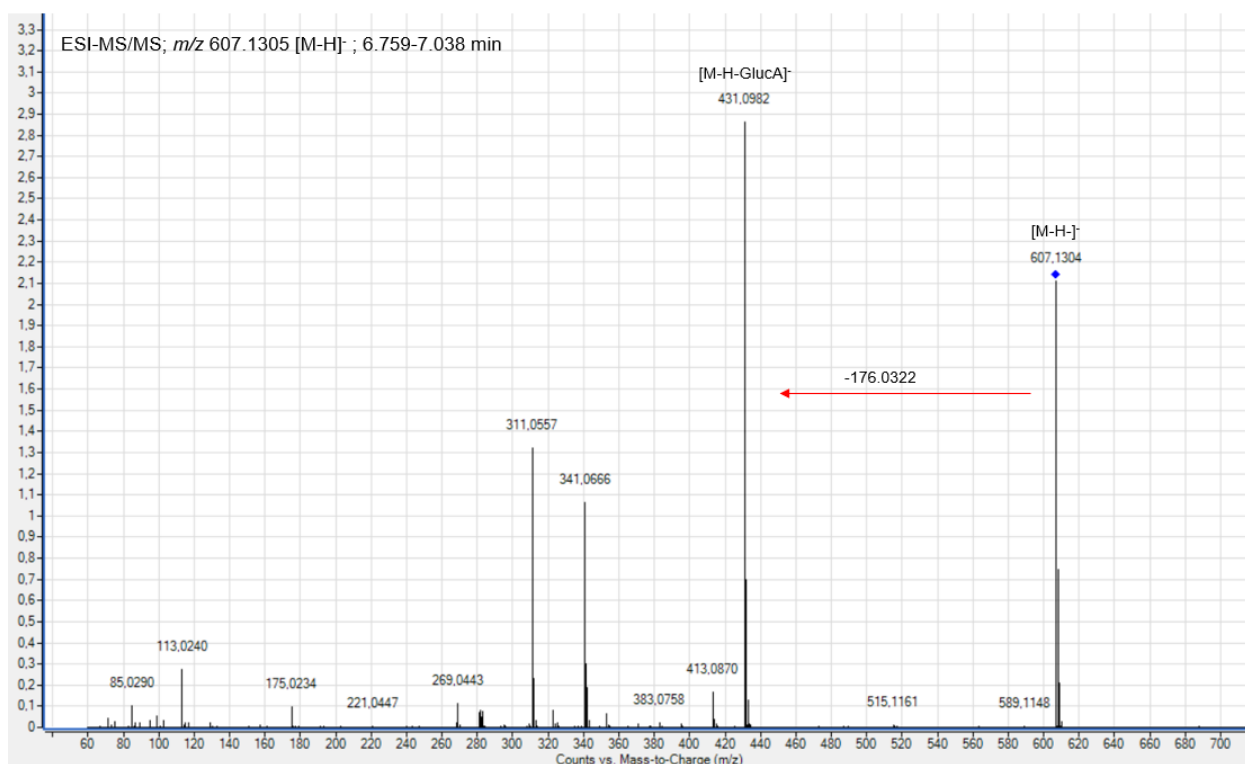


**Figure S13.** MS/MS spectrum of the extracted mass of vitexin-G2 and its retention time with loss of dehydrated (-18 u) glucuronic acid (GlucA).

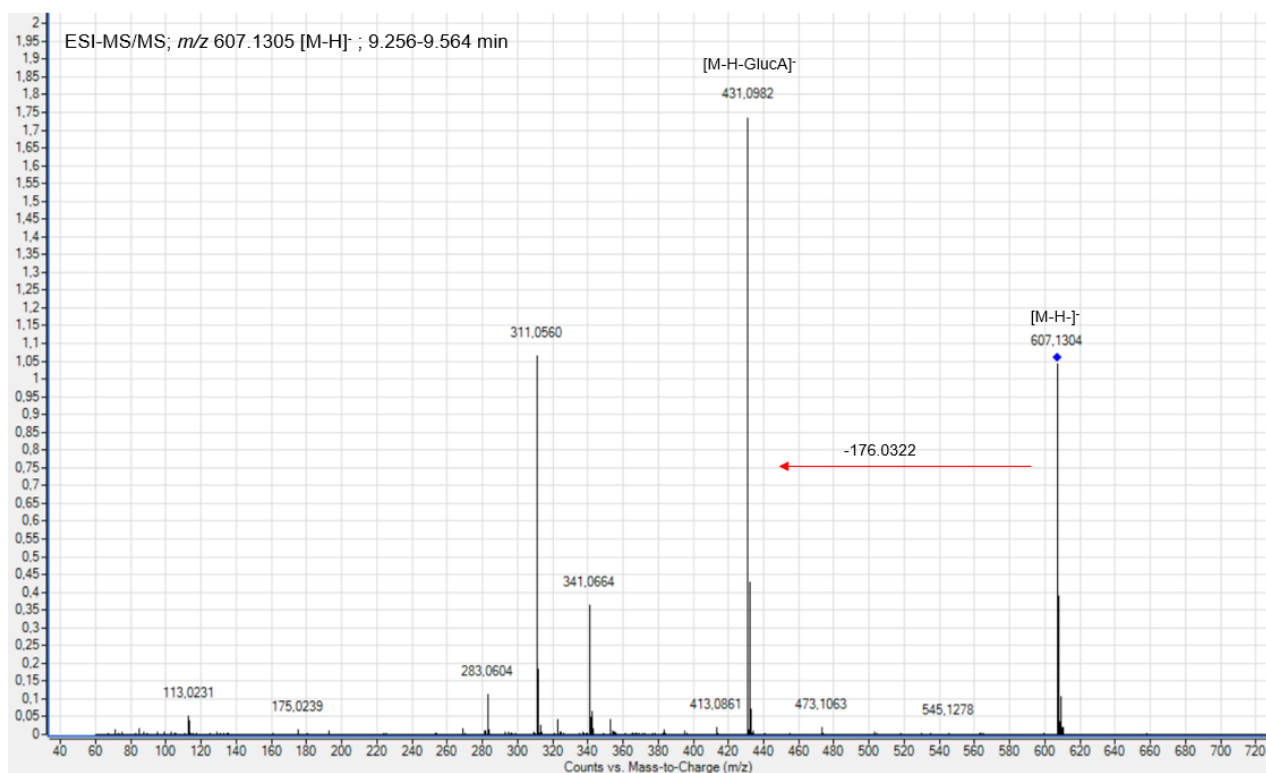


**Figure S14.** MS/MS spectrum of the extracted mass of vitexin-G3 and its retention time with loss of dehydrated (-18 u) glucuronic acid (GlucA).

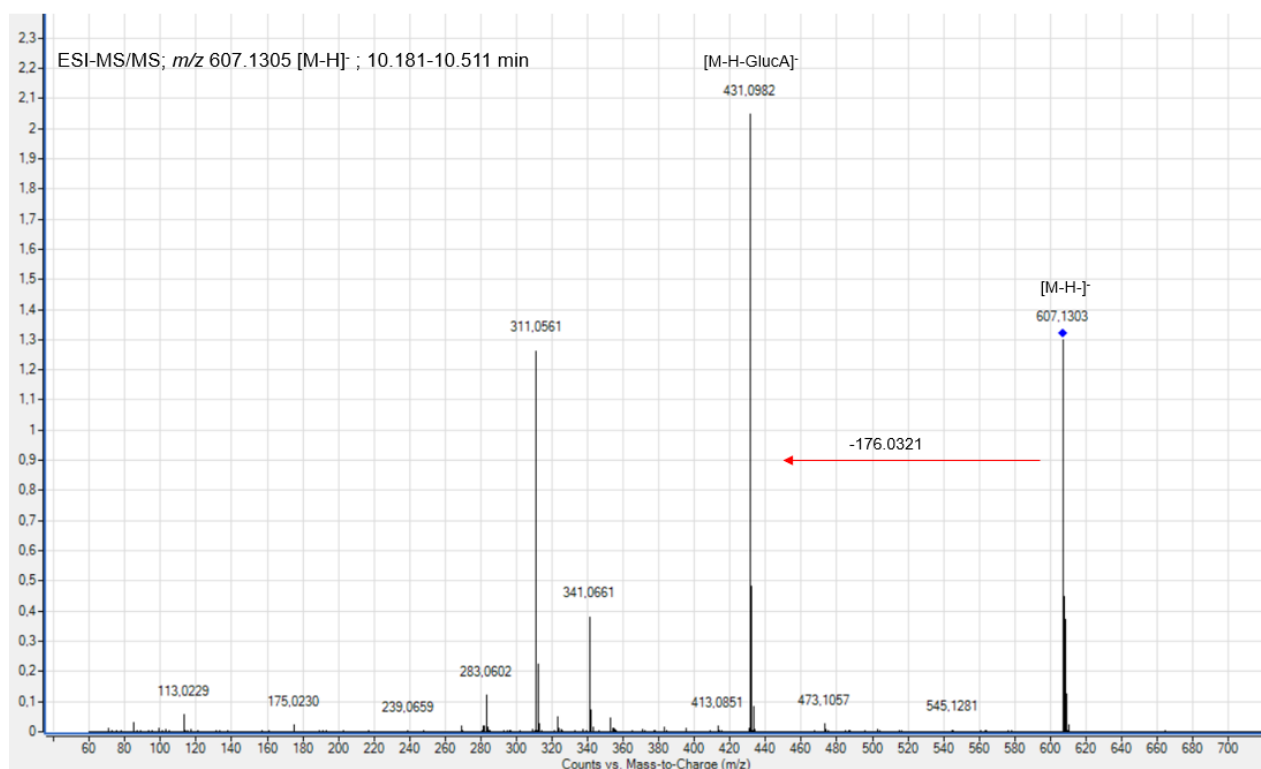




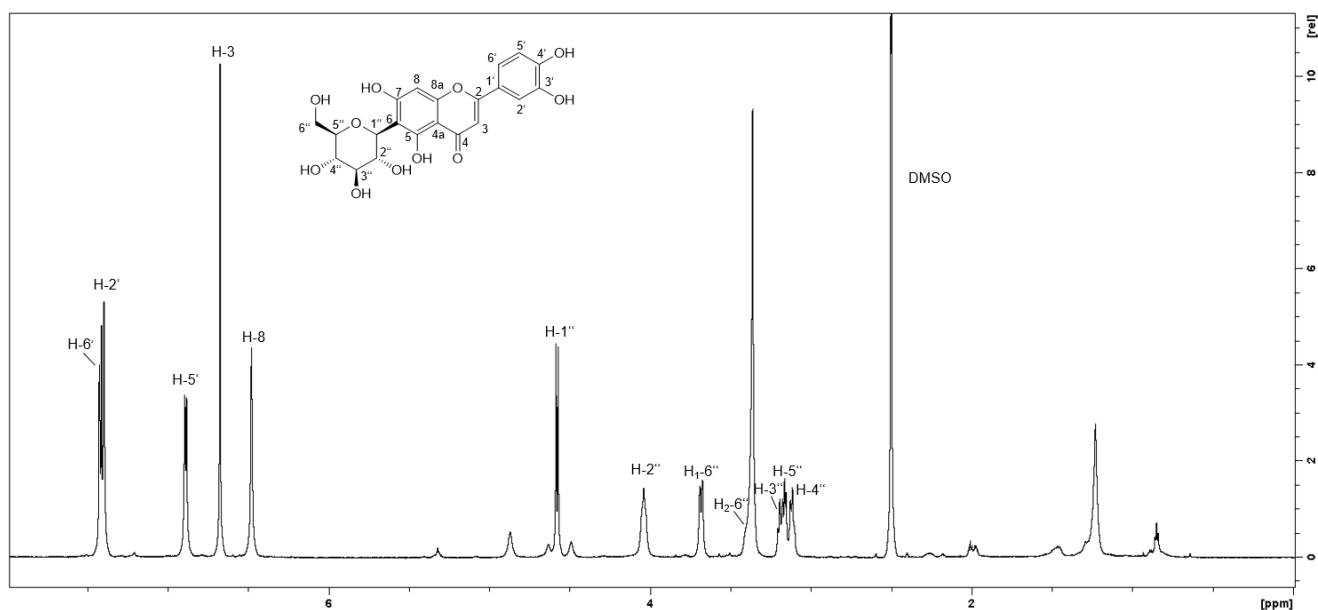
**Figure S15.** MS/MS spectrum of the extracted mass of isovitexin-G1 and its retention time with loss of dehydrated (-18 u) glucuronic acid (GlucA).



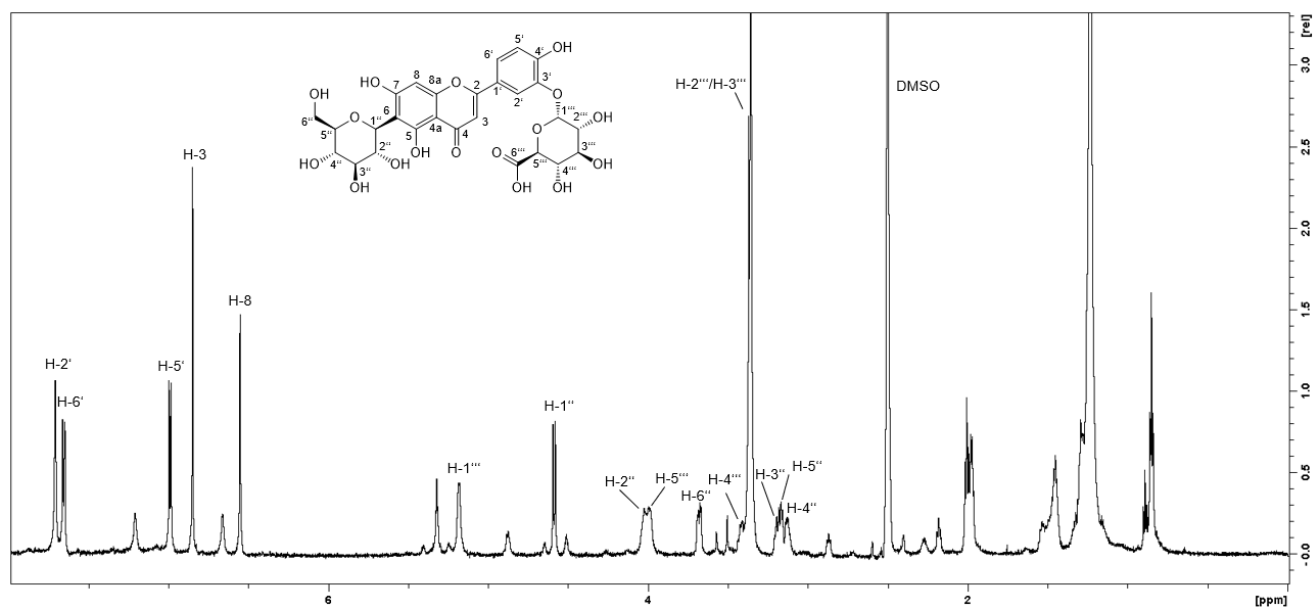
**Figure S16.** MS/MS spectrum of the extracted mass of isovitexin-G2 and its retention time with loss of dehydrated (-18 u) glucuronic acid (GlucA).



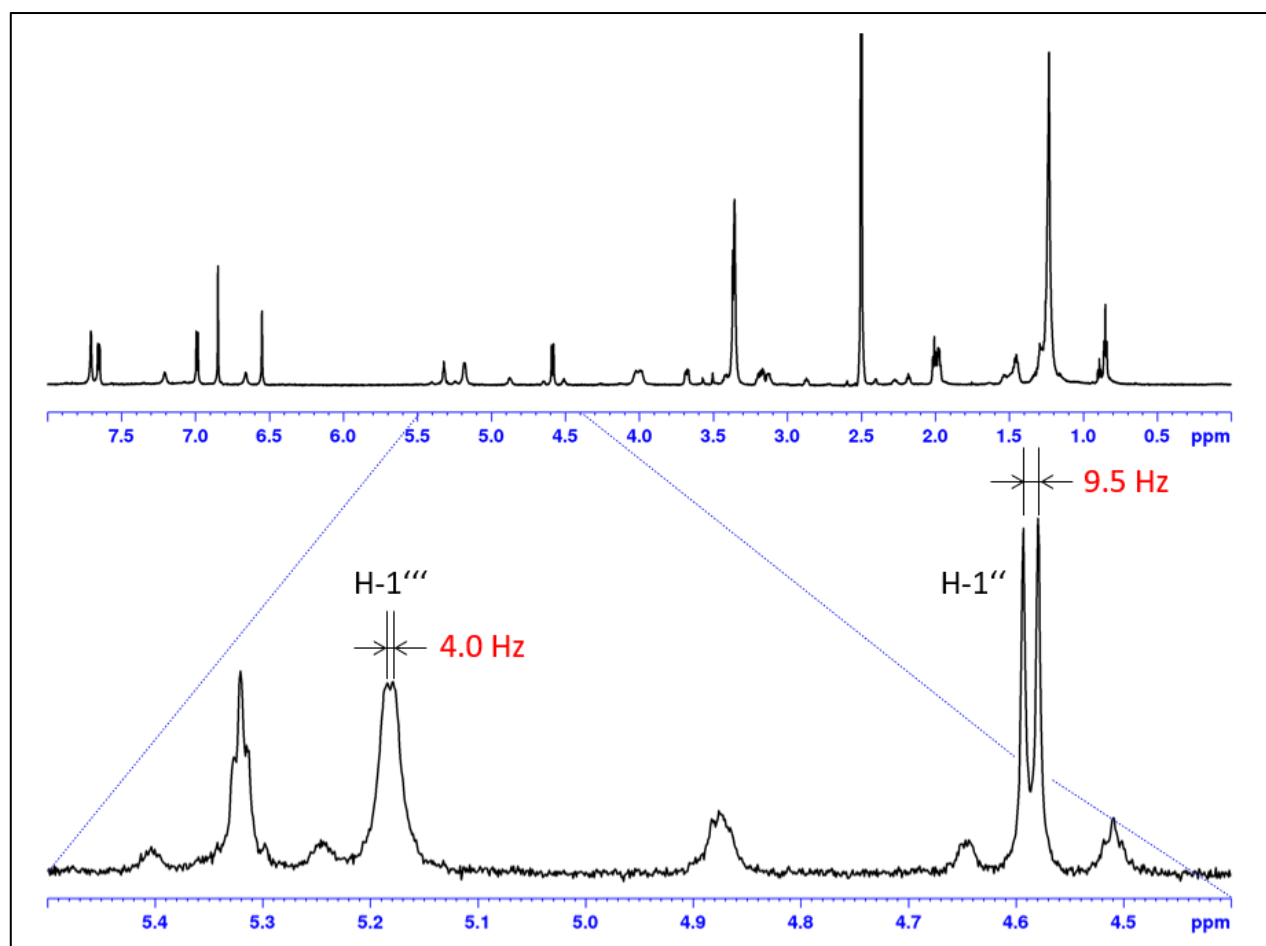
**Figure S17.** MS/MS spectrum of the extracted mass of isovitexin-G3 and its retention time with loss of dehydrated (-18 u) glucuronic acid (GlucA).



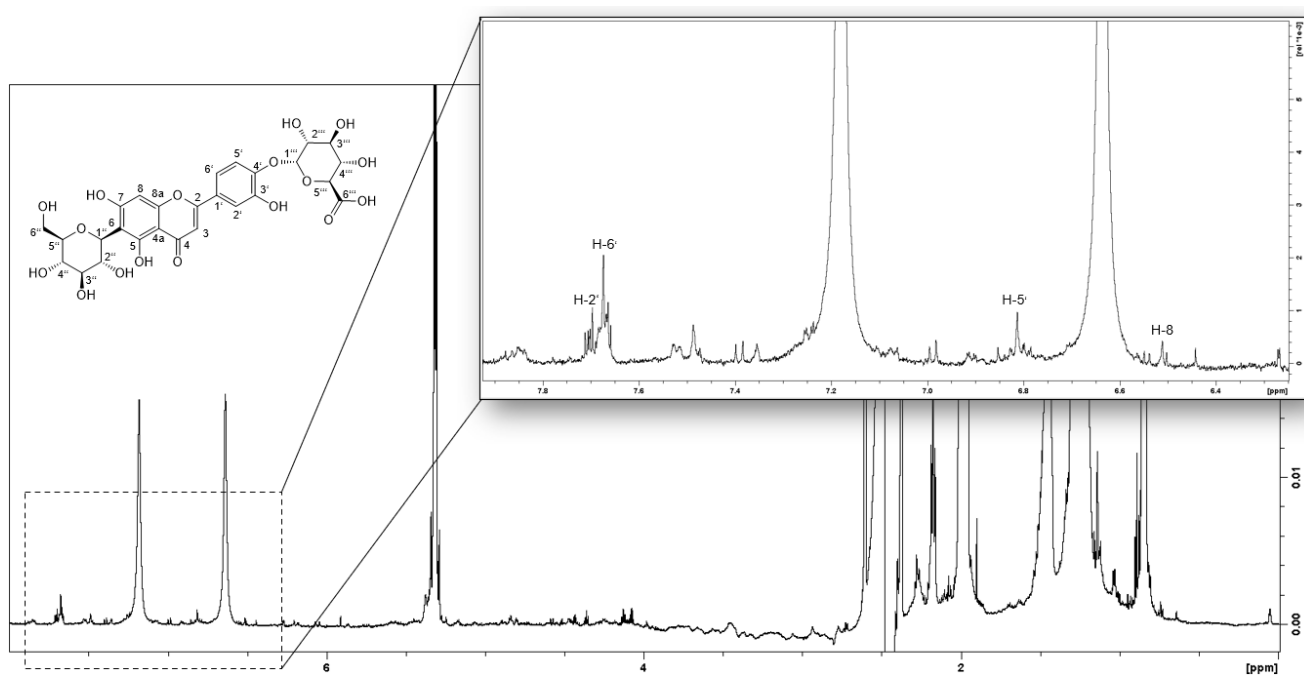
**Figure S18.**  $^1H$ -NMR spectrum of isoorientin in  $DMSO-d_6$  at 298 K, 700 MHz.



**Figure S19.**  $^1\text{H}$ -NMR spectrum of isoorientin-3'-O- $\alpha$ -glucuronide in  $\text{DMSO}-d_6$  at 298 K, 700 MHz.



**Figure S20.** Expanded  $^1\text{H}$  NMR spectrum of isoorientin-3'-O- $\alpha$ -glucuronide with coupling constants of H-1''' and H-1''.



**Figure S21.** <sup>1</sup>H-NMR spectrum of isoorientin-4'-O-α-glucuronide in DMSO-*d*<sub>6</sub> at 298 K, 700 MHz.