

Supplementary Material

Coumaroyl Flavonol Glycosides and more in marketed green teas: an intrinsic value beyond much-lauded catechins

Lorenzo Candela, Marialuisa Formato, Giuseppina Crescente, Simona Piccolella, and Severina Pacifico*

Figure S1. Total Ion Chromatograms (TICs) of alcoholic extracts ● TeaTWF; ● TeaGNP; ● TeaSNC; ● TeaBNC; ● TeaMTC; ● TeaCEC

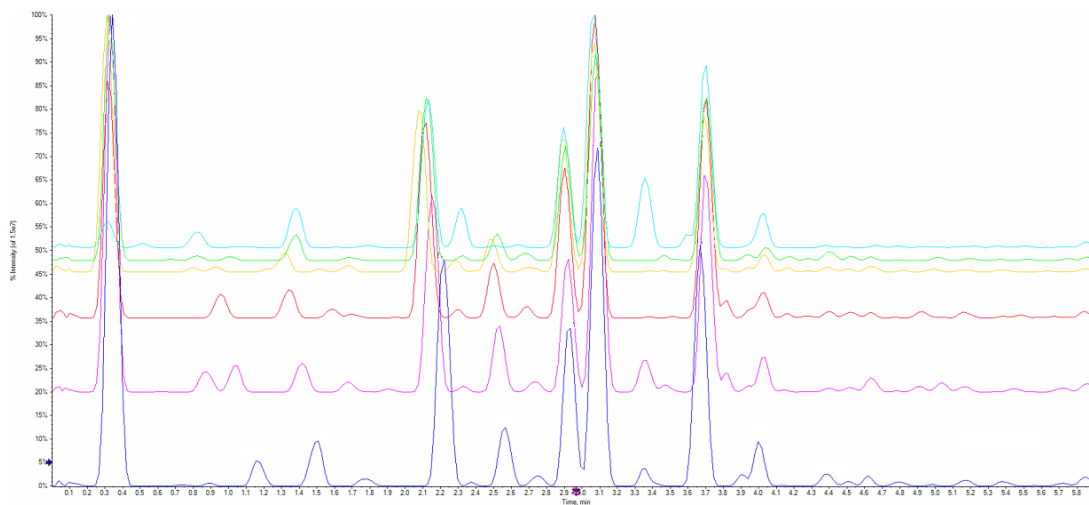


Figure S2. TOF-MS/MS spectra of deprotonated compound **1** (**A**), and $[M+Cl]^-$ adducts of compounds **4** (**B**) and **5** (**C**). In D panel, the formation of the ion at m/z 221 is proposed based on raffinose trihexose; m/z values, below each structure, are the calculated ones

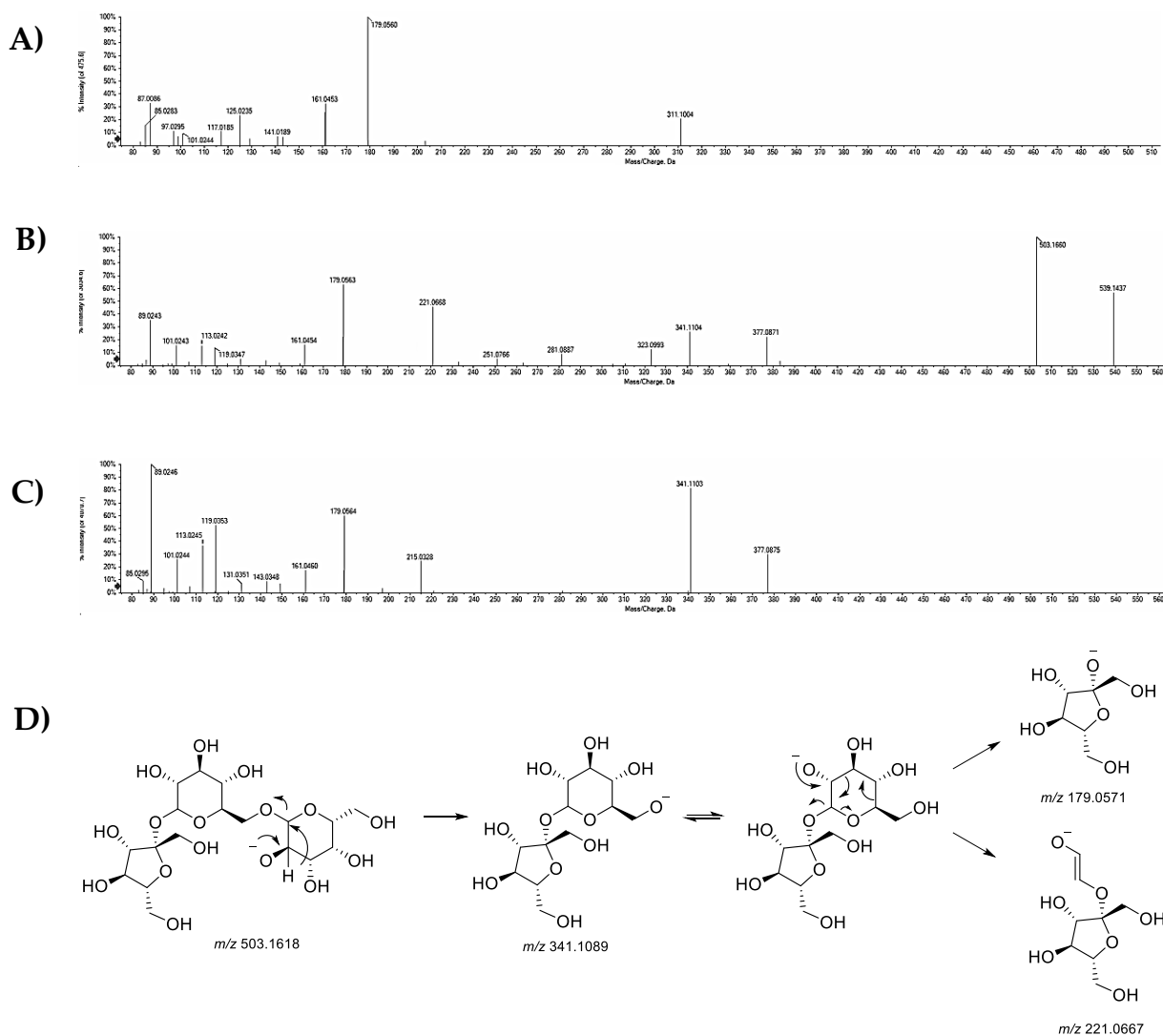


Figure S3. TOF-MS/MS spectra of $[M-H]^-$ ion of compound **A) 8**, and **C) 10**. In panel B the fragmentation pattern that leads to the HRF-mediated formation of the fragment ion at m/z 125.0244 (calcd) is exemplified (in blue), whereas RDA reaction gives the fragment ions at m/z 137.0244 e 167.0350 (calcd). This latter fragment ion is diagnostic for gallo catechins and all the derivatives showing pyrogallol B-ring.

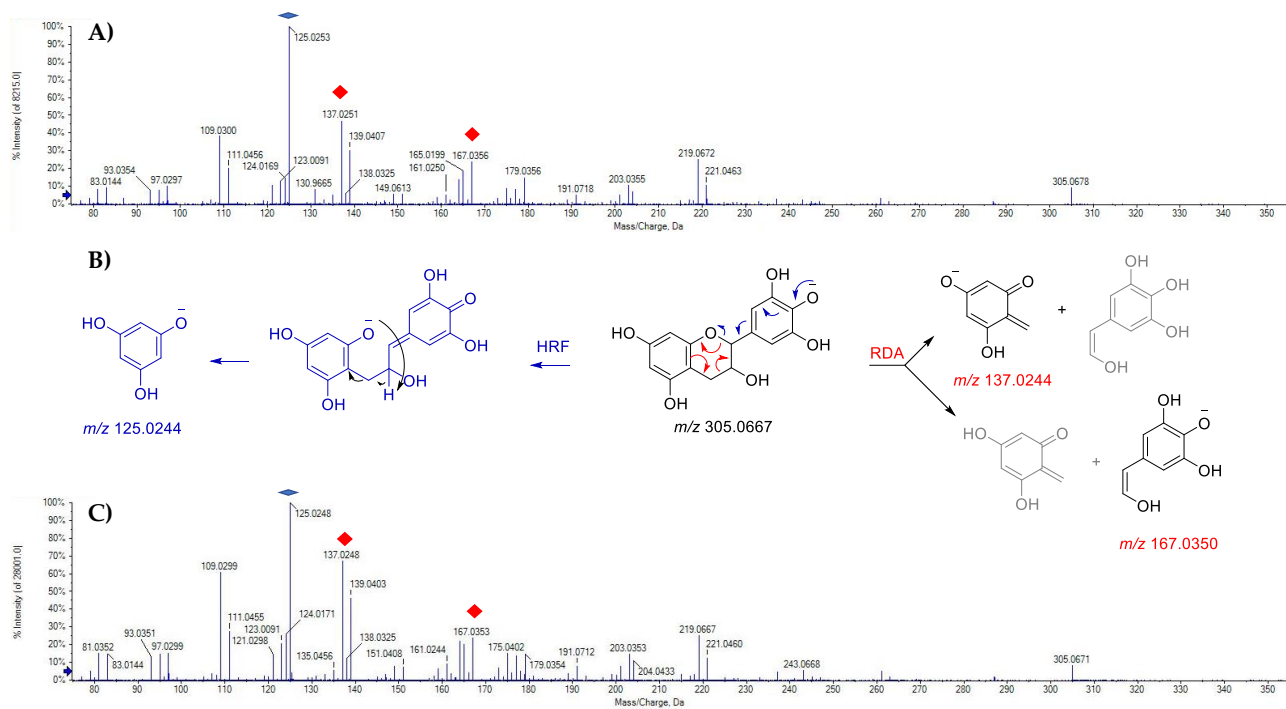


Figure S4. TOF-MS/MS spectra of [M-H]⁻ ion of compound **A) 15**, and **B) 26**. The structure of the main fragment ions is highlighted; *m/z* values, below each structure, are the calculated ones.

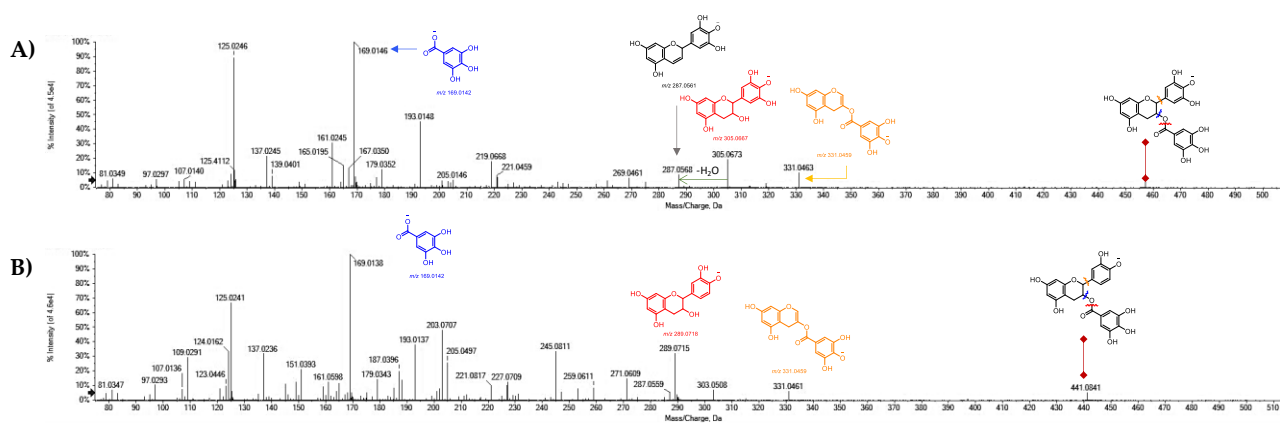


Figure S5. TOF-MS/MS spectrum of [M-H]⁻ ion of compound **35**. The neutral loss of dehydrated gallic acid residue is highlighted; *m/z* values, below each structure, are the calculated ones.

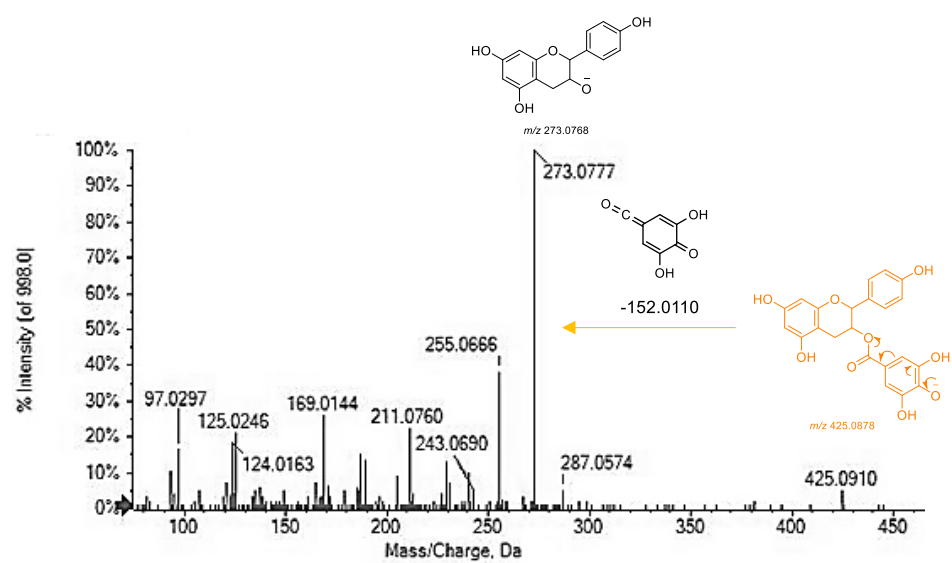


Figure S6. TOF-MS/MS spectra of [M-H]⁻ ion of compound **A) 16**, and **B) 19**. The structures assigned to the compounds are reported in the grey panel.

