

Supplementary data

High-Throughput Screening and Characterization of Phenolic Compounds in Stone Fruits Waste by LC-ESI-QTOF-MS/MS and their Potential Antioxidant Activities

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Abstract: Stone fruits, including peach (*Prunus persica* L.), nectarine (*Prunus nucipersica* L.), plum (*Prunus domestica* L.) and apricot (*Prunus armeniaca* L.) are common commercial fruits in the market. However, a huge amount of stone fruits waste is produced throughout the food supply chain during picking, handling, processing, packaging, storage, transportation, retailing and final consumption. These stone fruits waste contain high phenolic content which are the main contributors to the antioxidant potential and associated health benefits. The antioxidant results showed that plum waste contained higher concentrations of total phenolic content (TPC) (0.94 ± 0.07 mg gallic acid equivalents (GAE)/g) and total flavonoid content (TFC) (0.34 ± 0.01 mg quercetin equivalents (QE)/g), while apricot waste contained a higher concentration of total tannin content (TTC) (0.19 ± 0.03 mg catechin equivalents (CE)/g) and DPPH activity (1.47 ± 0.12 mg ascorbic acid equivalents (AAE)/g). However, nectarine waste had higher antioxidant capacity in ferric reducing-antioxidant power (FRAP) (0.98 ± 0.02 mg AAE/g) and total antioxidant capacity (TAC) (0.91 ± 0.09 mg AAE/g) assays, while peach waste showed higher antioxidant capacity in 2,2'-azino-bis-(3-ethylbenzothiazoline-6-sulfonic acid (ABTS) assay (0.43 ± 0.09 mg AAE/g) as compared to other stone fruits waste. Qualitative and quantitative phenolic analysis of Australian grown stone fruits waste were conducted by liquid chromatography coupled with electrospray-ionization quadrupole time-of-flight mass spectrometry (LC-ESI-QTOF-MS/MS) and HPLC-photodiode array detection (PDA). The LC-ESI-QTOF-MS/MS result indicates that 59 phenolic compounds were tentatively characterized in peach (33 compounds), nectarine (28), plum (38) and apricot (23). The HPLC-PDA indicated that *p*-hydroxybenzoic acid (18.64 ± 1.30 mg/g) was detected to be the most dominant phenolic acid and quercetin (19.68 ± 1.38 mg/g) was the most significant flavonoid in stone fruits waste. Hence, it could be concluded that stone fruit waste contains various phenolic compounds and have antioxidant potential. The results could support the applications of these stone fruit wastes in other food, feed, nutraceutical and pharmaceutical industries.

Keywords: Fruit waste; stone fruits; phenolic compounds; LC-ESI-QTOF-MS/MS; HPLC-PDA

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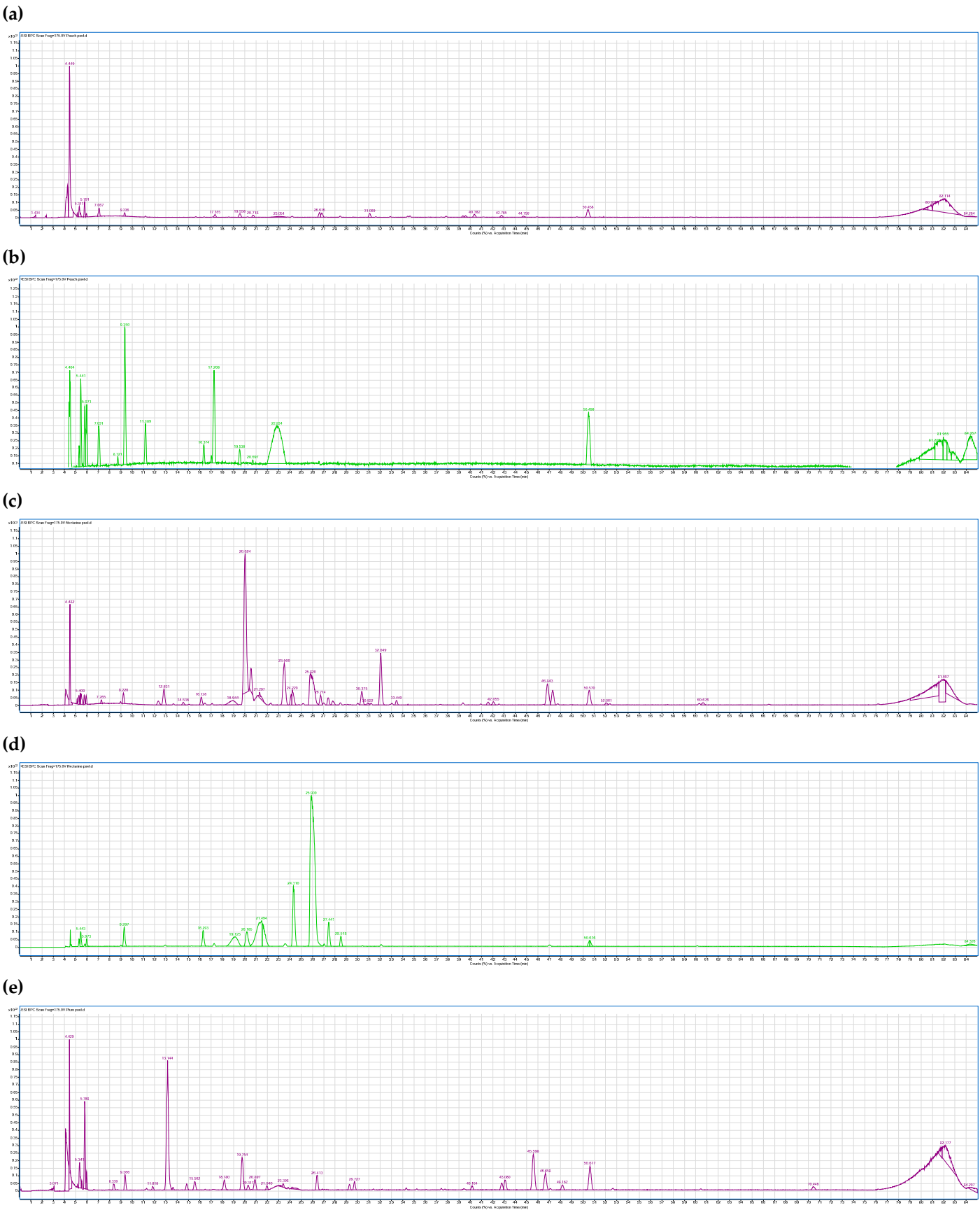
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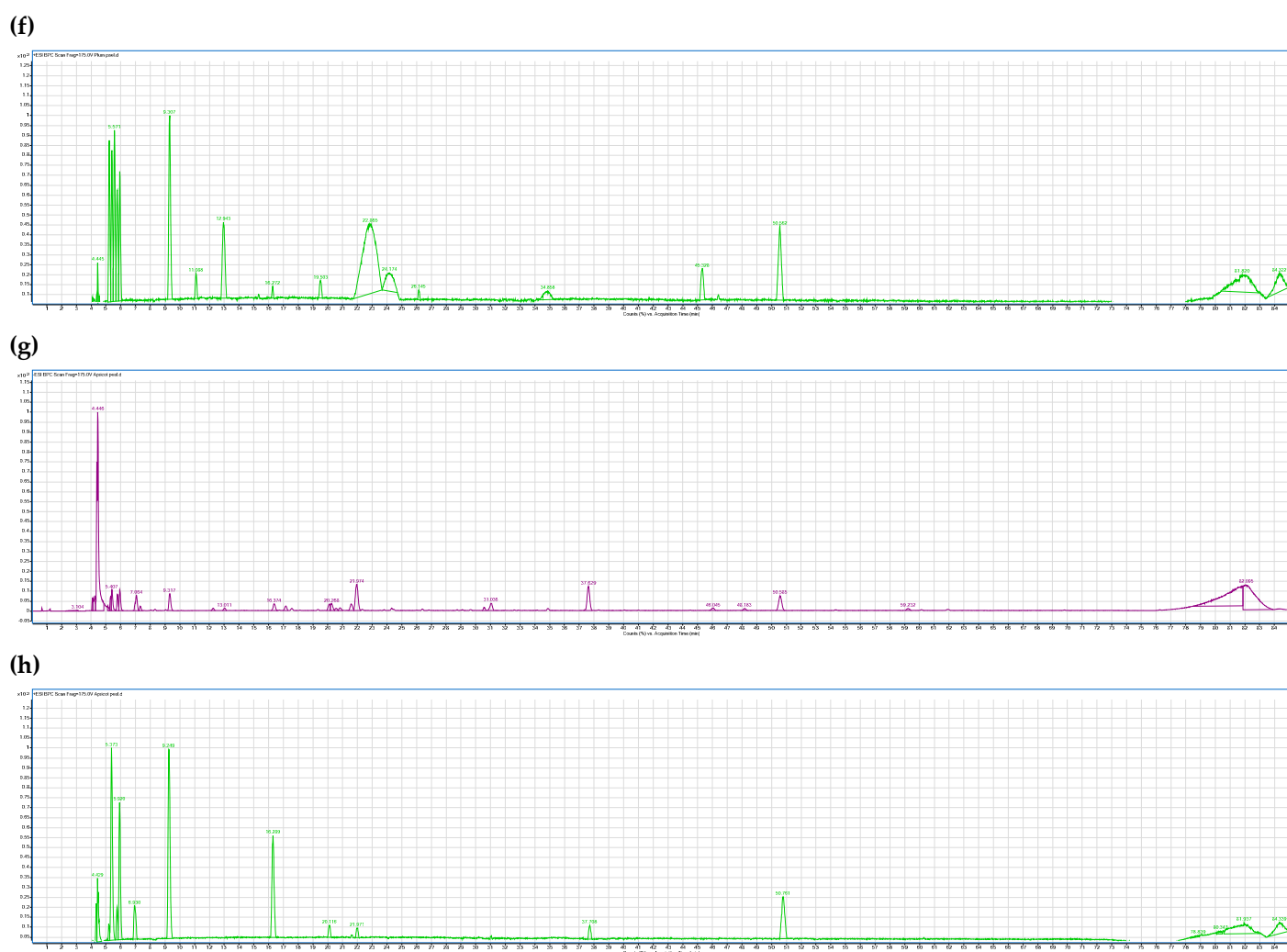
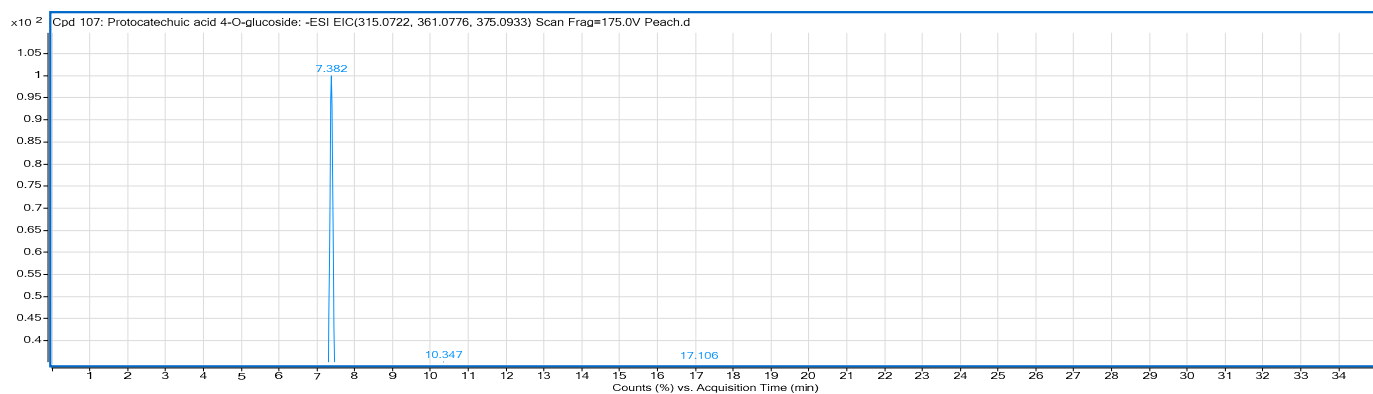
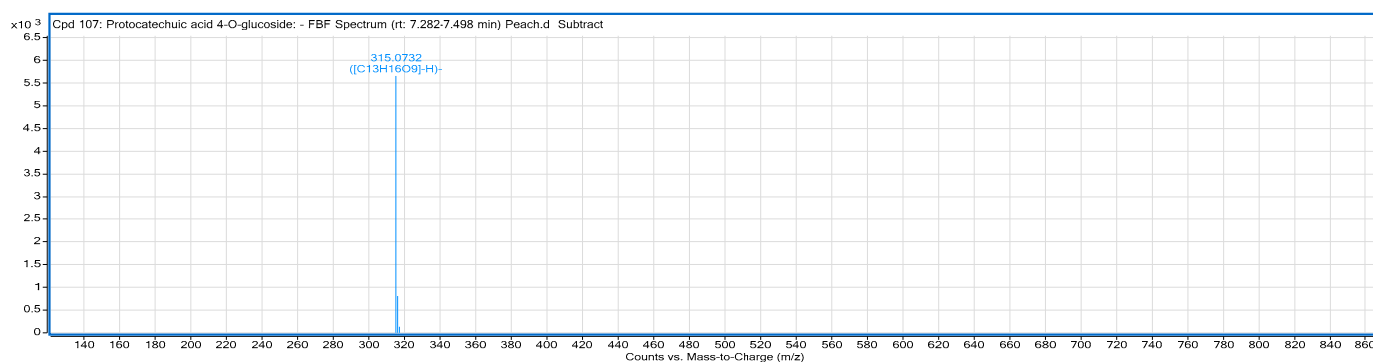
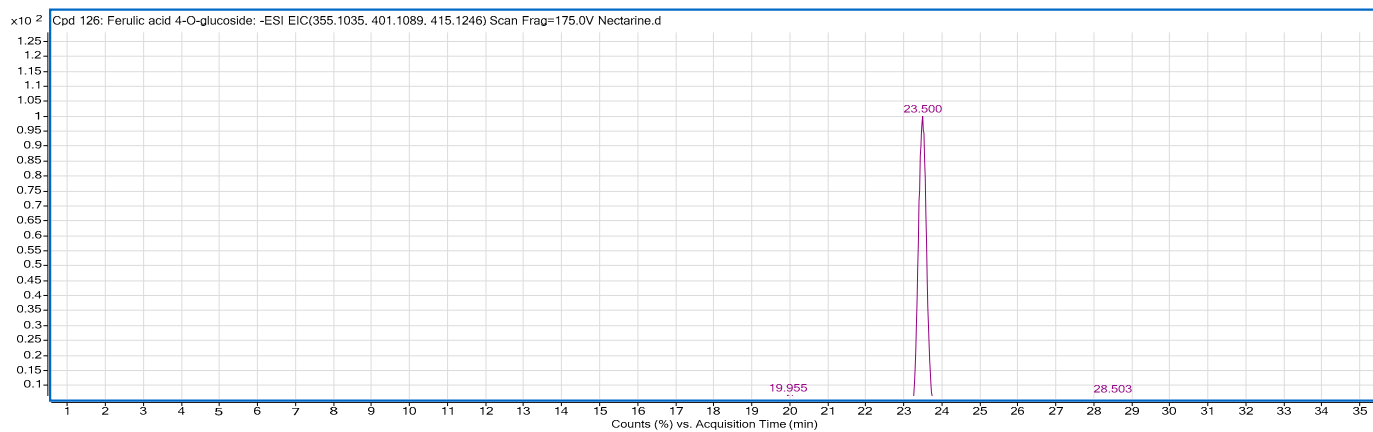
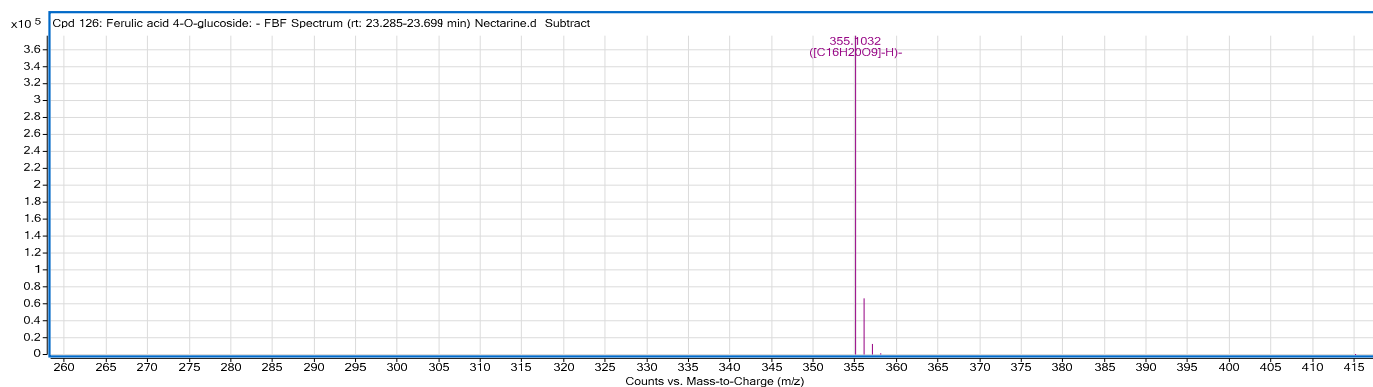
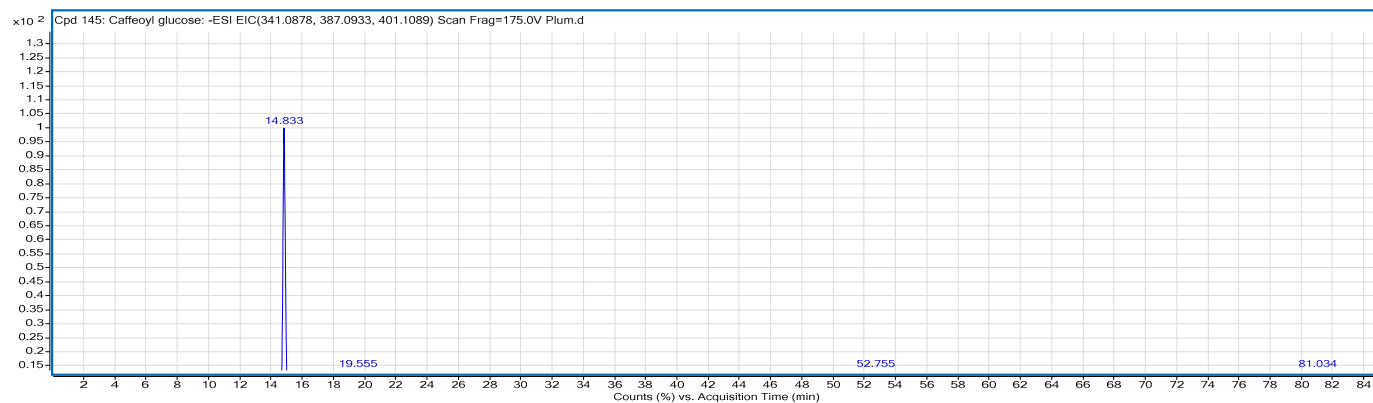


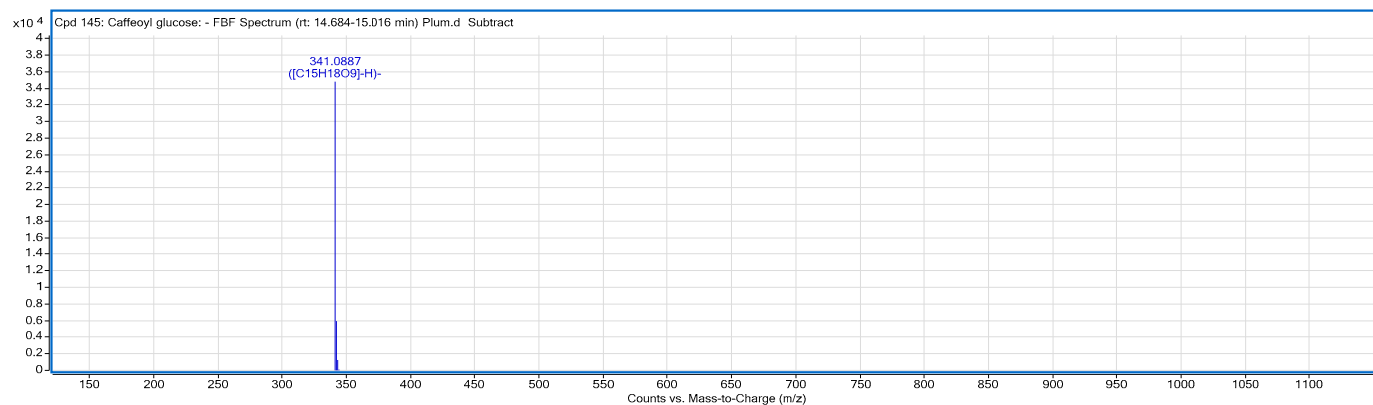
Figure 1S1. LC-ESI-QTOF-MS/MS basic peak chromatograph (BPC) for characterization of phenolic compounds of stone fruit waste samples; (a) Peach in negative ionization mode; (b) Peach in positive ionization mode; (c) Nectarine in negative ionization mode; (d) Nectarine in positive ionization mode; (e) Plum in negative ionization mode; (f) Plum in positive ionization mode; (g) Apricot in negative ionization mode; (h) Apricot in positive ionization mode.

(a)**(b)****(c)****(d)**

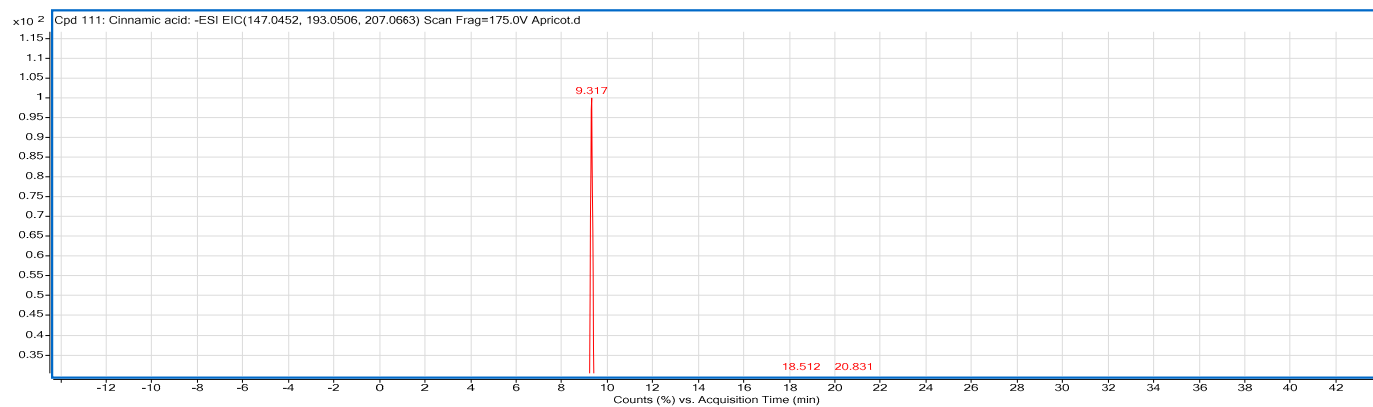
(e)



(f)



(g)



(h)

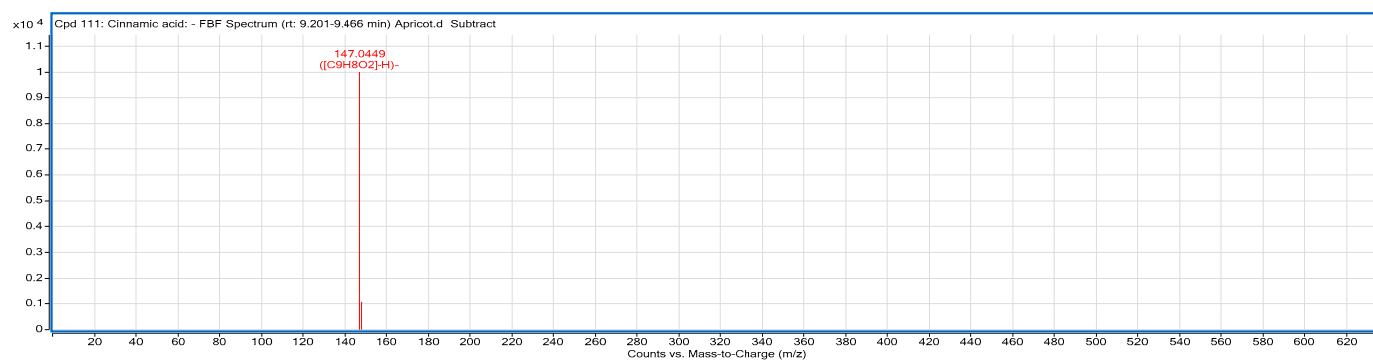


Figure S2. Extracted ion chromatogram of stone fruits waste samples and their mass spectrum. (a) A chromatograph of protocatechuic acid 4-*O*-glucoside (Compound 19, Table 3), retention time (RT = 7.382 min) in the negative mode of ionization (ESI/[M-H]⁻) identified and characterized in peach waste; **(b)** Mass spectra of protocatechuic acid 4-*O*-glucoside showing an observed *m/z* 315.0732; **(c)** A chromatograph of ferulic acid 4-*O*-glucoside (Compound 10, Table 3), retention time (RT = 23.500 min) in the negative mode of ionization (ESI/[M-H]⁻) identified and characterized in nectarine waste; **(d)** Mass spectra of ferulic acid 4-*O*-glucoside showing an observed *m/z* 355.1032; **(e)** A chromatograph of caffeoyl glucose (Compound 4, Table 3), retention time (RT = 14.833 min) in the negative mode of ionization (ESI/[M-H]⁻) identified and characterized in plum waste; **(f)** Mass spectra of caffeoyl glucose showing an observed *m/z* 341.0887; **(g)** A chromatograph of cinnamic acid (Compound 3, Table 3), retention time (RT = 9.317 min) in the negative mode of ionization (ESI/[M-H]⁻) identified and characterized in apricot waste; **(h)** Mass spectra of cinnamic acid showing an observed *m/z* 147.0449.