

Figure S1. Pictures of plum seed oils obtained in the different stages of plum brandy processing. **a)** plum seed oil before fermentation, **b)** plum seed oil after fermentation, **c)** plum seed oil after both fermentation and distillation.

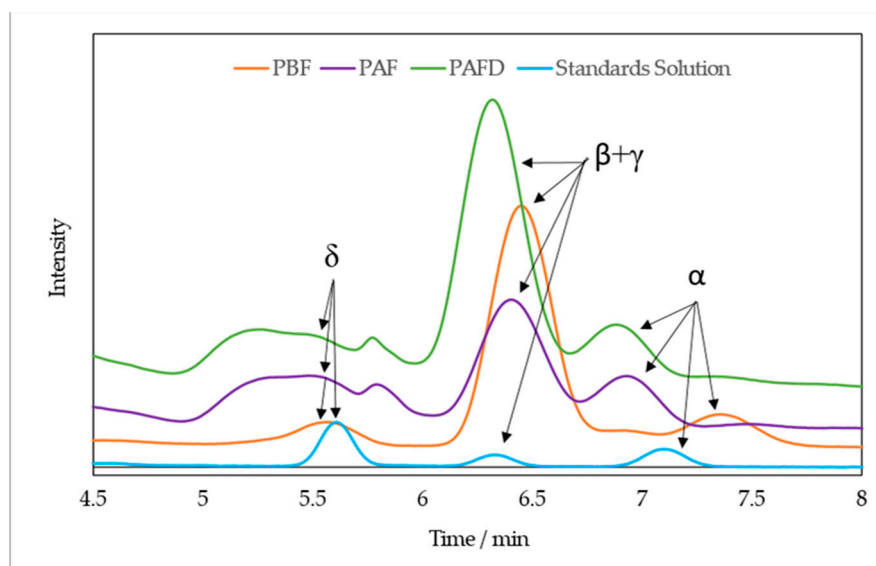


Figure S2. Comparative chromatogram at 292 nm between tocopherols in plum seed oils and standards solution by liquid chromatography coupled to ultraviolet-visible spectroscopy (HPLC-PDA). Intensity scale has been shifted for all signals. PAFD: plum seed oil after both fermentation and distillation; PAF: plum seed oil after fermentation; PBF: plum seed oil before fermentation. Standards solution at 5.0, 2.0 and 10.0 mg·L⁻¹ of α -, γ - and δ -tocopherol, respectively. Peaks were identified by spiking standards solution onto the sample.

Table S1. Identification of phenolic compounds by high-resolution liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (HPLC-ESI-QTOF-MS) in plum seed phenolic extracts.

Peak Number	Compound	RT (min)	Molecular Formula	[M-H] ⁻ (m/z)	MS/MS Fragments (m/z)
1	Gallic acid ^a	2.7	C ₇ H ₆ O ₅	169.1128	125.0306 ; 97.0302; 79.0243; 51.0305
2	2,3-Dihydroxybenzoic acid ^a	4.9	C ₇ H ₆ O ₄	153.1138	125.5103; 109.0303 ; 91.0201; 65.006
3	Neochlorogenic acid ^b	4.9	C ₁₆ H ₁₈ O ₉	353.0879	191.0433 ; 179.0335; 161.1005; 135.0433; 107.0429
4	Protocatechuate ^c	5.0	C ₇ H ₆ O ₄	153.0194	153.0159; 120.5030; 109.0351; 91.0221; 81.0410
5	Catechin ^a	7.5	C ₁₅ H ₁₄ O ₆	289.2609	289.0584; 245.0703; 203.0567; 151.0285; 109.0185; 57.0262

6	Chlorogenic acid ^a	7.8	C ₁₆ H ₁₈ O ₉	353.3015	319.6037; 257.5812, 191.0613 ; 161.0299; 85.0372
7	Vanillic acid ^a	9.2	C ₈ H ₈ O ₄	167.0351	151.0007; 108.0227 ; 91.0128; 80.5217
8	Epicatechin ^a	9.8	C ₁₅ H ₁₄ O ₆	289.2609	289.0701; 245.0839; 203.0711; 151.0428; 109.0343; 57.0379
9	Caffeic acid ^a	9.6	C ₉ H ₈ O ₄	179.1502	135.0469; 117.0299, 89.0406; 65.0374
10	Syringic acid ^a	9.7	C ₉ H ₁₀ O ₅	197.0456	181.0194; 167.0176; 151.9915; 138.0294; 123.0072 ; 95.0121
11	<i>p</i> -Coumaric acid ^a	13.8	C ₉ H ₈ O ₃	163.1508	119.0516 ; 93.0364; 65.0359
12	<i>trans</i> -Ferulic acid ^a	15.2	C ₁₀ H ₁₀ O ₄	193.1768	150.0655; 134.0400 ; 106.0488; 89.0389
13	Kaempferol 3-rutinoside ^b	17.7	C ₂₇ H ₃₀ O ₁₅	593.1513	423.0438; 367.7453; 285.0372 ; 195.1208; 61.9900
14	Isorhamnetin 3-rutinoside ^c	17.9	C ₂₈ H ₃₂ O ₁₆	623.1618	577.2840; 315.0504 ; 300.0258; 271.6939; 243.0098
15	Hesperidin ^a	18.4	C ₂₈ H ₃₄ O ₁₅	609.5534	609.1852; 527.2731; 459.0930; 301.0707; 257.0955; 136.0119
16	Quercetin ^a	27.0	C ₁₅ H ₁₀ O ₇	301.2285	273.0425; 229.0516; 179.0033; 151.0081 ; 121.0317
17	Kaempferol ^a	32.6	C ₁₅ H ₁₀ O ₆	285.2291	255.0218; 229.0400; 185.0529; 151.0335; 93.0308

Bold fragments are the ones, employed for quantitation purposes. Compared with MS data obtained from standard ^a, FooDB database ^b, and MassBank database ^c. RT means retention time.

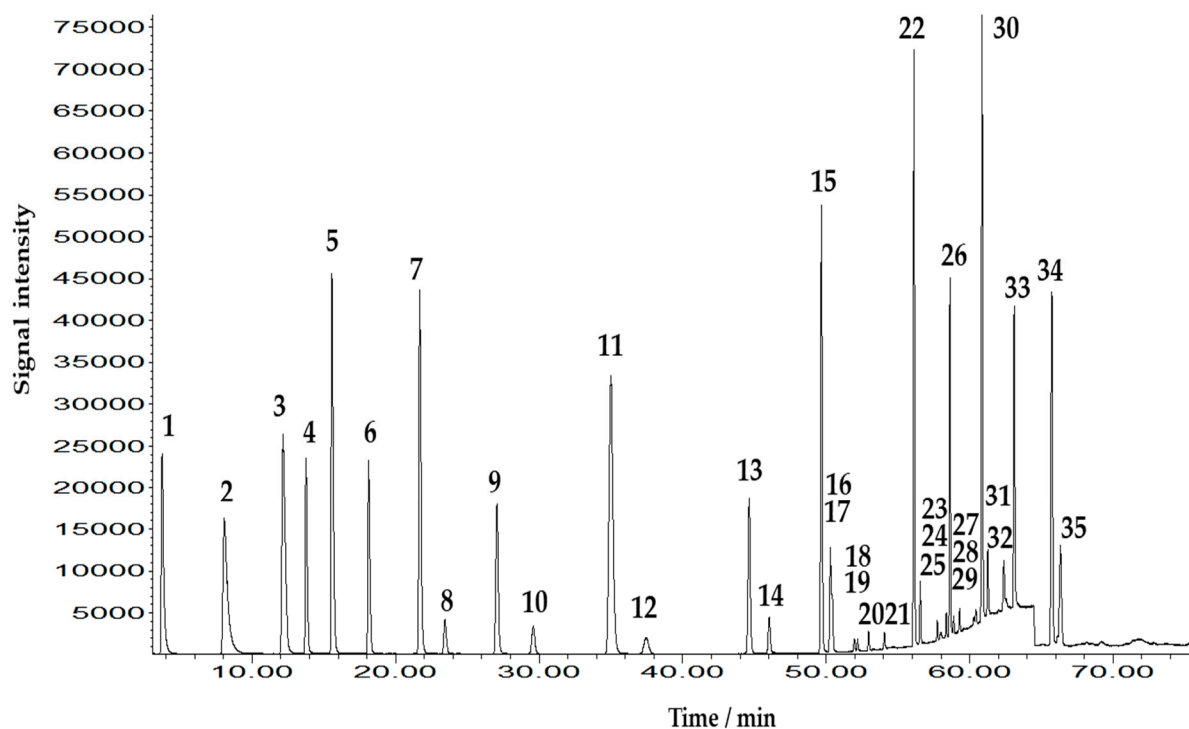


Figure S3. Chromatogram of the standard mixture of FAME 37 component SUPELCO Ref CRM47885 by gas chromatography coupled to mass spectrometry (GC- MS). Peak identification: (1) methyl hexanoate (C6:0; 400 µg·mL⁻¹); (2) methyl octanoate (C8:0; 400 µg·mL⁻¹); (3) methyl decanoate (C10:0; 400 µg·mL⁻¹); (4) methyl undecanoate (C11:0; 200 µg·mL⁻¹); (5) methyl laurate (C12:0; 400 µg·mL⁻¹); (6) methyl tridecanoate (C13:0; 200 µg·mL⁻¹); (7) methyl myristate (C14:0; 400 µg·mL⁻¹); (8) methyl myristoleate (C14:1n5; 200 µg·mL⁻¹); (9) methyl pentadecanoate (C15:0; 200 µg·mL⁻¹); (10) methyl cis-10-pentadecenoate (C15:1n5; 200 µg·mL⁻¹); (11) methyl palmitate (C16:0; 600 µg·mL⁻¹); (12) methyl palmitoleate (C16:1n7; 200 µg·mL⁻¹); (13) methyl heptadecanoate (margarate, C17:0; 200 µg·mL⁻¹); (14) cis-10-heptadecanoic acid methyl ester (C17:1n7c; 200 µg·mL⁻¹); (15) methyl stearate (C18:0; 400 µg·mL⁻¹); (16) cis-9-oleic acid methyl ester (C18:1n9c; 400 µg·mL⁻¹); (17) trans-9-elaidic

acid methyl ester (C18:1n9t; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (18) methyl linolelaidate (C18:2n6t; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (19) methyl linoleate (C18:2n6c; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (20) methyl γ -linolenate (C18:3n6; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (21) methyl linolenate (C18:3n3; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (22) methyl arachidate (C20:0; 400 $\mu\text{g}\cdot\text{mL}^{-1}$); (23) methyl cis-11-eicosenoate (C20:1n9; $\leq 200 \mu\text{g}\cdot\text{mL}^{-1}$); (24) cis 11,14-Eicosadienoic acid methyl ester (C20:2n6; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (25) cis-8,11,14-eicosatrienoic acid methyl ester (C20:3n6; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (26) methyl heneicosanoate (C21:0; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (27) cis-5,8,11,14-eicosatetraenoic acid methyl ester (C20:4n6; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (28) cis-11,14,17-eicosatrienoic acid methyl ester (C20:3n3; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (29) cis-5,8,11,14,17-Eicosapentaenoic acid methyl ester (C20:5n3; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (30) methyl behenate (C22:0; 400 $\mu\text{g}\cdot\text{mL}^{-1}$); (31) methyl erucate (C22:1n9; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (32) cis-13,16-docosadienoic acid methyl ester (C22:2n6; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (33) methyl tricosanoate (C23:0; 200 $\mu\text{g}\cdot\text{mL}^{-1}$); (34) methyl lignocerate (C24:0; 400 $\mu\text{g}\cdot\text{mL}^{-1}$); (35) methyl nervonate (C24:1n9; 200 $\mu\text{g}\cdot\text{mL}^{-1}$).

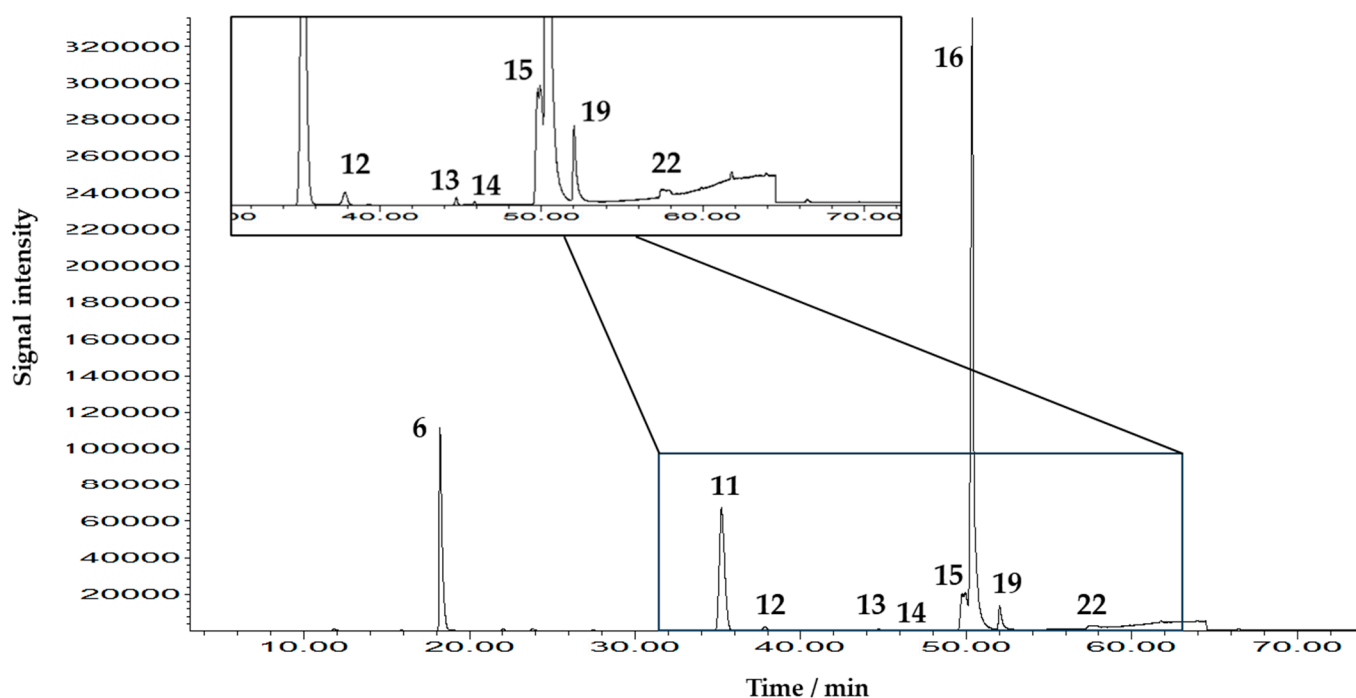


Figure S4. Chromatogram of plum seed oil before fermentation (PBF), which includes an ampliation aiming for easier appreciation of the peaks. Peak identification: (6) methyl methyl tridecanoate (C13:0) internal standard; (11) methyl palmitate (C16:0); (12) methyl palmitoleate (C16:1n7); (13) methyl heptadecanoate (margarate, C17:0); (14) cis-10-heptadecanoic acid methyl ester (C17:1n7c); (15) methyl stearate (C18:0); (16) cis-9-oleic acid methyl ester (C18:1n9c); (19) methyl linoleate (C18:2n6c); (22) methyl arachidate (C20:0).

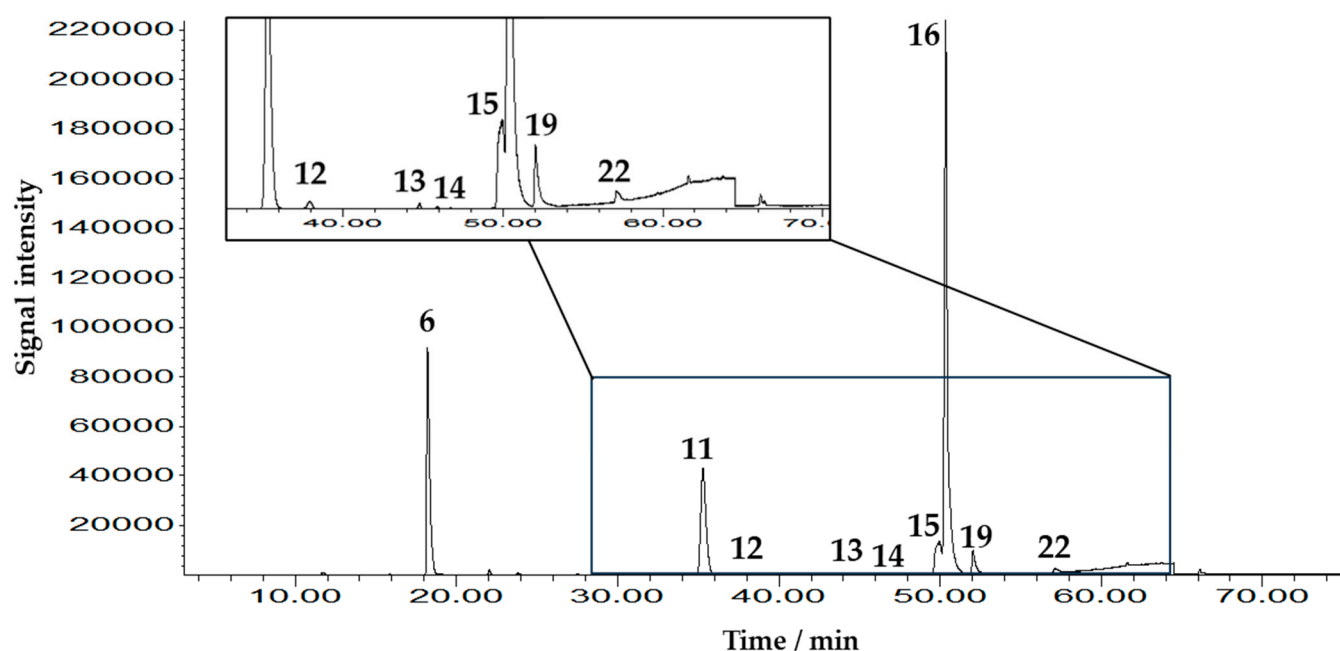


Figure S5. Chromatogram of plum seed oil after fermentation (PAF), which includes an ampliation aiming for easier appreciation of the peaks. Peak identification: (6) methyl methyl tridecanoate (C13:0) internal standard; (11) methyl palmitate (C16:0); (12) methyl palmitoleate (C16:1n7); (13) methyl heptadecanoate (margarate, C17:0); (14) cis-10-heptadecanoic acid methyl ester (C17:1n7c); (15) methyl stearate (C18:0); (16) cis-9-oleic acid methyl ester (C18:1n9c); (19) methyl linoleate (C18:2n6c); (22) methyl arachidate (C20:0).

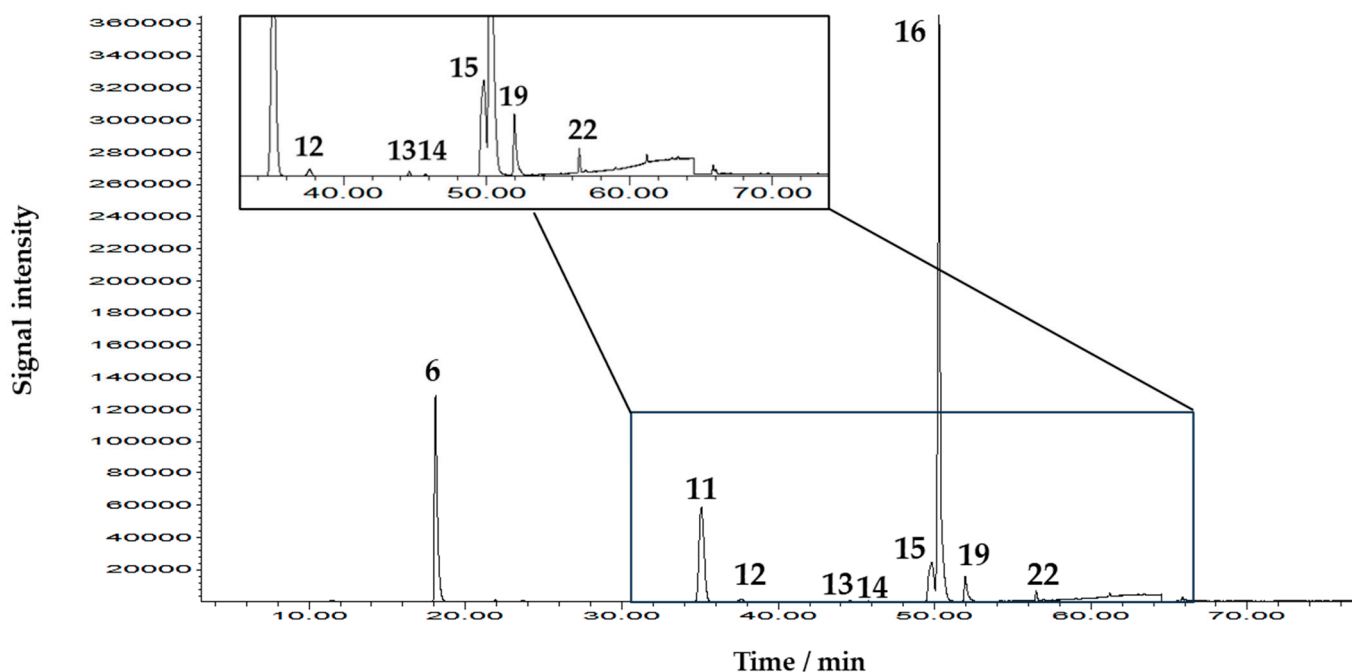


Figure S6. Chromatogram of plum seed oil after both fermentation and distillation (PAFD), which includes an ampliation aiming for easier appreciation of the peaks. Peak identification: (6) methyl methyl tridecanoate (C13:0) internal standard; (11) methyl palmitate (C16:0); (12) methyl palmitoleate (C16:1n7); (13) methyl heptadecanoate (margarate, C17:0); (14) cis-10-heptadecanoic acid methyl ester (C17:1n7c); (15) methyl stearate (C18:0); (16) cis-9-oleic acid methyl ester (C18:1n9c); (19) methyl linoleate (C18:2n6c); (22) methyl arachidate (C20:0).

Table S2. Response factors and limits of detection and quantification of FAME 37 standard mixture SUPELCO Ref CRM47885 by gas chromatography coupled to mass spectrometry (GC- MS).

Compound	m/z relation	RF	RSD (%)	LOD ($\mu\text{g}\cdot\text{g}^{-1}$)	LOQ ($\mu\text{g}\cdot\text{g}^{-1}$)
Methyl hexanoate (C6:0)	74	1.2	11.6	13.3	40.3
Methyl octanoate (C8:0)	74	1.4	11.0	24.5	74.3
Methyl decanoate (C10:0)	74	1.7	11.2	5.5	16.5
Methyl undecanoate (C11:0)	74	1.7	9.4	2.8	8.4
Methyl laurate (C12:0)	74	1.8	6.6	4.7	14.2
Methyl tridecanoate (C13:0)	74	1.8	5.3	2.9	8.8
Methyl myristate (C14:0)	74	1.75	2.26	4.0	12.1
Methyl myristoleate (C14:1n5)	74	0.38	4.57	27.3	82.8
Methyl pentadecanoate (C15:0)	74	1.65	3.01	3.4	10.4
Methyl cis-10-pentadecenoate (C15:1n5)	74	0.37	4.67	18.4	55.6
Methyl palmitate (C16:0)	74	1.7	3.8	7.3	22.1
Methyl palmitoleate (C16:1n7)	74	0.35	6.45	21.6	65.6
Methyl heptadecanoate (margarate, C17:0)	74	1.6	5.5	3.8	11.4
Cis-10-heptadecanoic acid methyl ester (C17:1n7c)	74	0.34	4.69	14.2	43.0
Methyl stearate (C18:0)	74	1.7	5.8	4.9	14.9
Cis-9-oleic acid methyl ester (C18:1n9c)	74	0.36	1.46	20.7	62.7
Trans-9-elaidic acid methyl ester (C18:1n9t)	74	0.34	7.44	16.1	48.7
Methyl linolelaidate (C18:2n6t)	74	0.071	5.186	31.4	95.2
Methyl linoleate (C18:2n6c)	74	0.07	7.41	29.6	89.7
Methyl γ -linolenate (C18:3n6)	74	0.067	5.220	61.3	185.6
Methyl linolenate (C18:3n3)	74	0.069	6.742	54.8	165.9
Methyl arachidate (C20:0)	74	1.7	7.6	10.4	31.6
Methyl cis-11-eicosenoate (C20:1n9)	74	0.34	6.75	41.5	125.8
Cis 11,14-Eicosadienoic acid methyl ester (C20:2n6)	74	0.10	7.70	71.5	216.8
Cis-8,11,14-eicosatrienoic acid methyl ester (C20:3n6)	74	0.064	3.813	54.5	165.2
Methyl heneicosanoate (C21:0)	74	1.7	8.3	7.8	23.6
Cis-5,8,11,14-eicosatetraenoic acid methyl ester (C20:4n6)	74	0.09	9.53	85.3	258.6
Cis-11,14,17-eicosatrienoic acid methyl ester (C20:3n3)	74	0.09	6.86	66.9	202.7
Cis-5,8,11,14,17-Eicosapentaenoic acid methyl ester (C20:5n3)	74	0.08	7.17	95.9	290.7
Methyl behenate (C22:0)	74	1.8	8.1	12.1	36.7
Methyl erucate (C22:1n9)	74	0.36	7.32	33.0	100.0
Cis-13,16-docosadienoic acid methyl ester (C22:2n6)	74	0.16	19.93	79.8	241.9
Methyl tricosanoate (C23:0)	74	1.8	7.8	9.5	28.7
Methyl lignocerate (C24:0)	382	0.6	8.6	13.9	42.4
Methyl nervonate (C24:1n9)	348	0.44	8.40	38.7	117.2

*Response factors (RF), expressed as mean value, were calculated for the methylated esters subsequently found in the plum seed oil samples. RSD means relative standard deviation; LOD means limit of detection; LOQ means limit of quantitation. The values of the response factor (RF) and relative standard deviation (RSD) were calculated as the average of 3 replicates. The limits of detection and quantification for each analyte corresponded to the concentration of the compounds that give a chromatographic signal (calculated as peak height), 3.3 and 10 times, respectively, higher than background noises. Bold letters are used for the corresponding data of those fatty acids present in the plum seed oil samples.

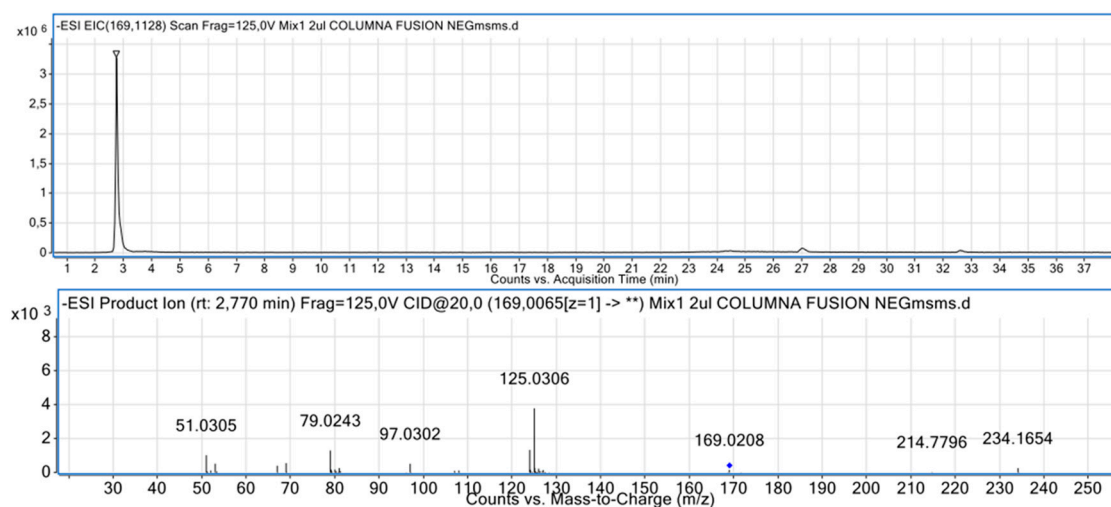


Figure S7. Gallic acid (standard solution 33 mg·L⁻¹) chromatogram and mass spectrum obtained by high-resolution liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (HPLC-ESI-QTOF-MS) in SIM scan mode (Frag=125.0V). RT= 2.770 min.

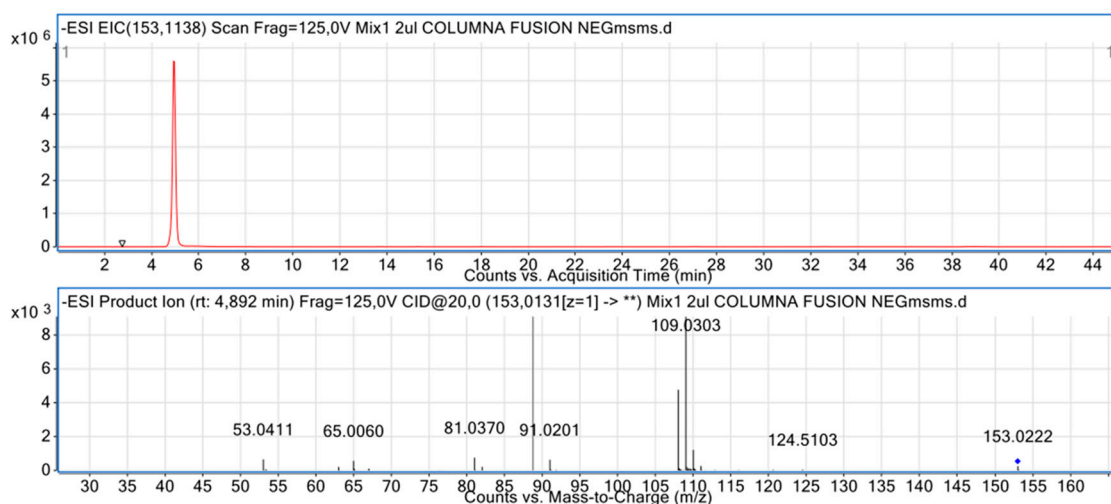


Figure S8. 2,3-Dihydroxybenzoic acid (standard solution 33 mg·L⁻¹) chromatogram and mass spectrum obtained by high-resolution liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (HPLC-ESI-QTOF-MS) in SIM scan mode (Frag=125.0V). RT= 4.892 min.

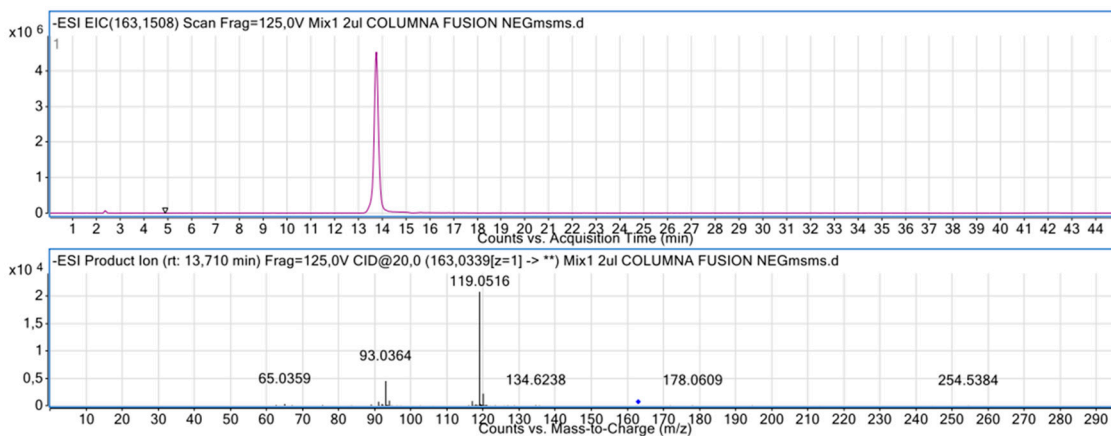


Figure S9. *p*-coumaric acid (standard solution 33 mg·L⁻¹) chromatogram and mass spectrum obtained by high-resolution liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (HPLC-ESI-QTOF-MS) in SIM scan mode (Frag=125.0V). RT= 13.710 min.

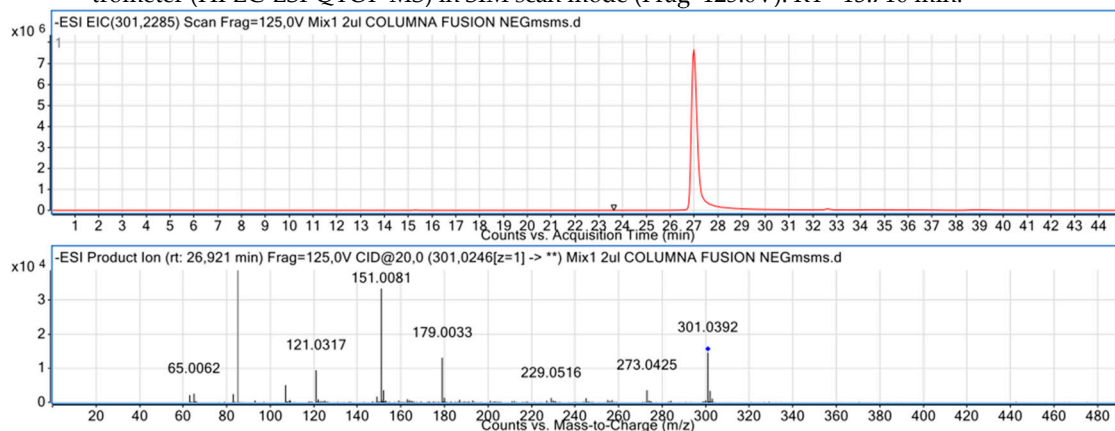


Figure S10. Quercetin (standard solution 33 mg·L⁻¹) chromatogram and mass spectrum obtained by high-resolution liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (HPLC-ESI-QTOF-MS) in SIM scan mode (Frag=125.0V). RT= 26.921 min.

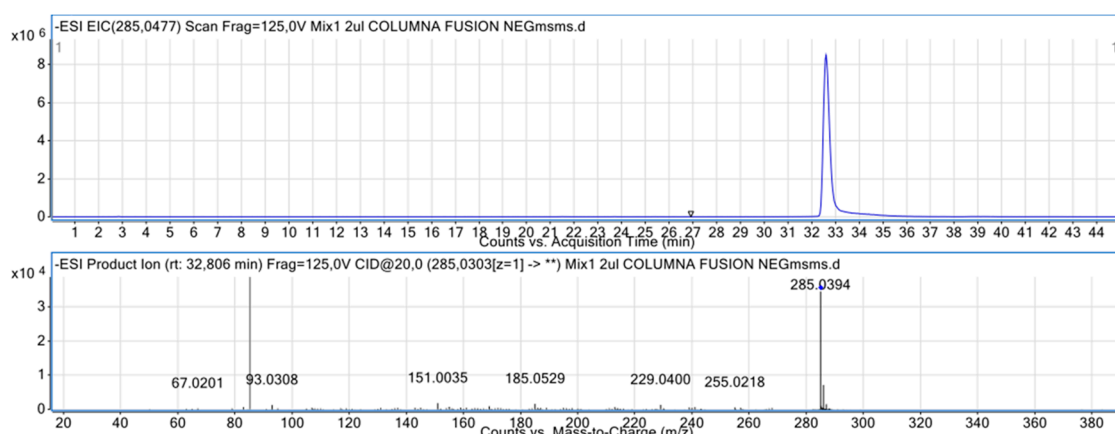


Figure S11. Kaempferol (standard solution 33 mg·L⁻¹) chromatogram and mass spectrum obtained by high-resolution liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (HPLC-ESI-QTOF-MS) in SIM scan mode (Frag=125.0V). RT= 32.806 min.

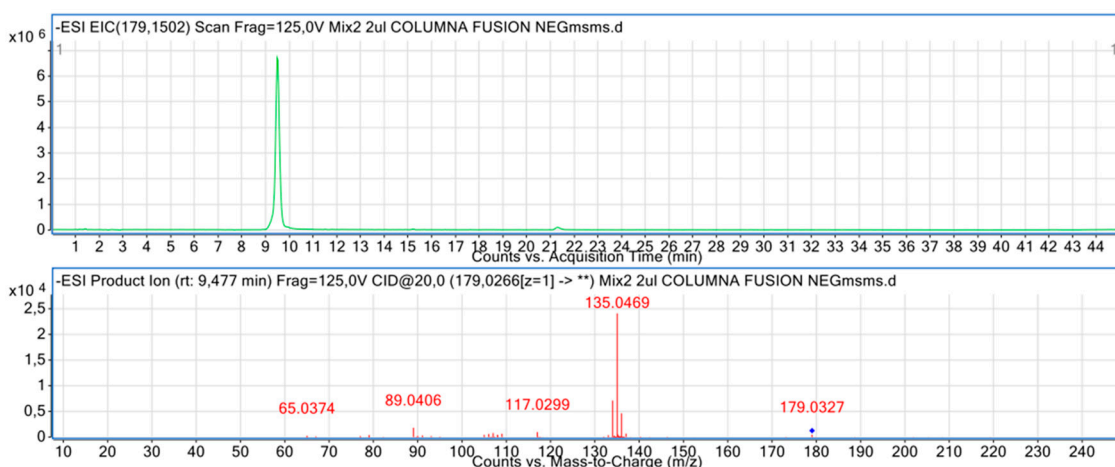


Figure S12. Caffeic acid (standard solution 33 mg·L⁻¹) chromatogram and mass spectrum obtained by high-resolution liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (HPLC-ESI-QTOF-MS) in SIM scan mode (Frag=125.0V). RT= 9.477 min.

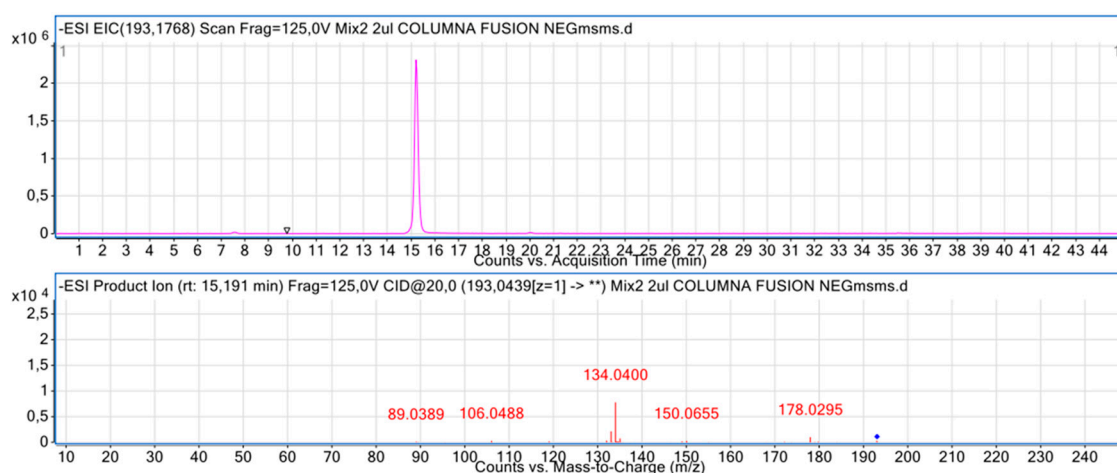


Figure S13. *trans*-ferulic acid (standard solution 33 mg·L⁻¹) chromatogram and mass spectrum obtained by high-resolution liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (HPLC-ESI-QTOF-MS) in SIM scan mode (Frag=125.0V). RT= 15.191 min.

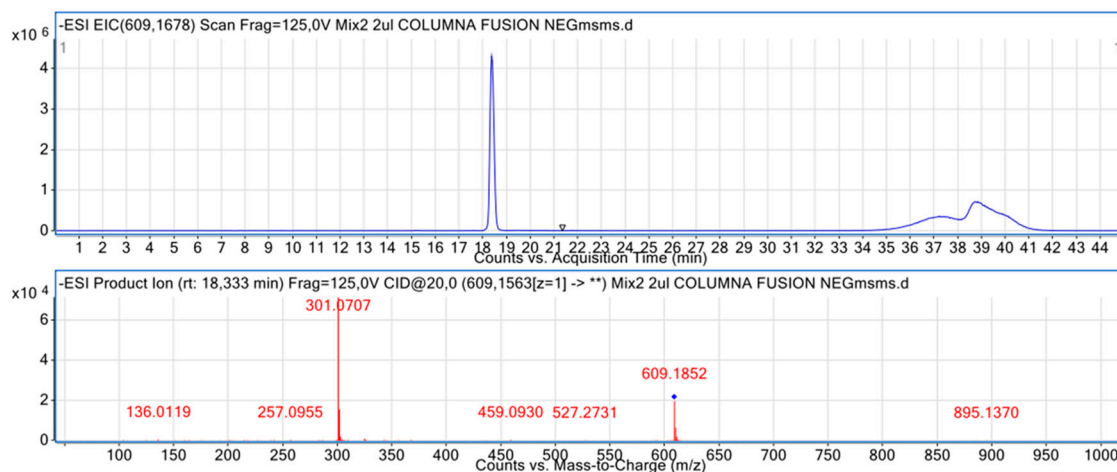


Figure S14. Hesperidin (standard solution 33 mg·L⁻¹) chromatogram and mass spectrum obtained by high-resolution liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (HPLC-ESI-QTOF-MS) in SIM scan mode (Frag=125.0V). RT= 18.333 min.

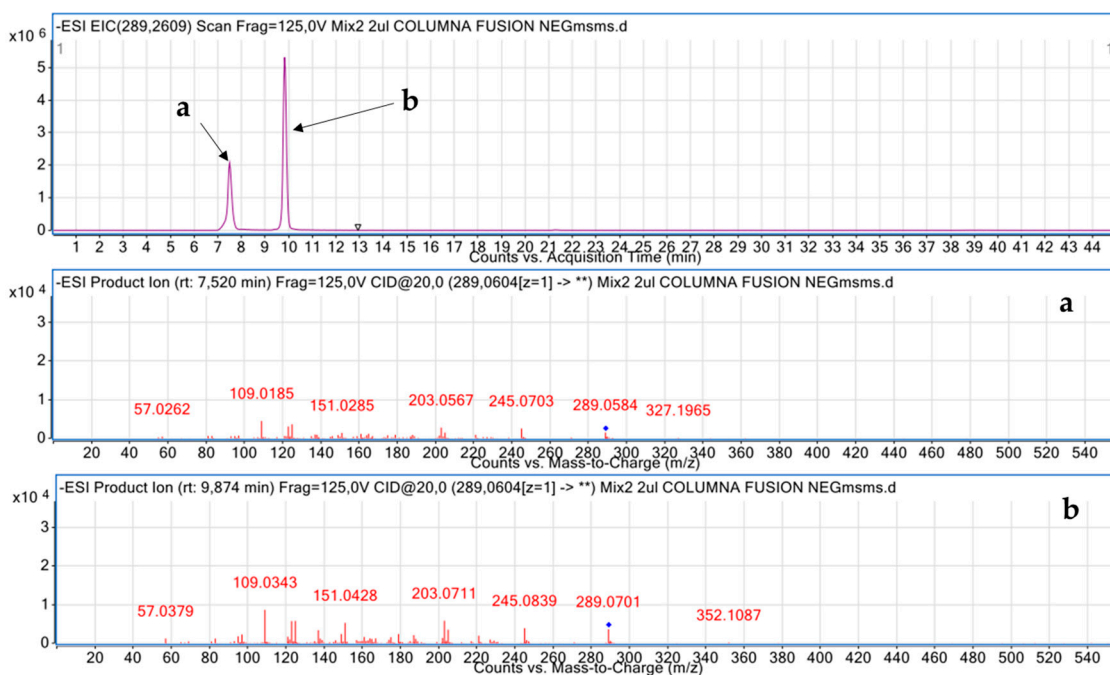


Figure S15. Catechin and epicatechin (standard solution 33 mg·L⁻¹) chromatogram and mass spectra obtained by high-resolution liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (HPLC-ESI-QTOF-MS) in SIM scan mode (Frag= 125.0V). **a)** Catechin (RT= 7.502 min; m/z= 289.0584) and **b)** Epicatechin (RT= 9.874 min; m/z= 289.0701).

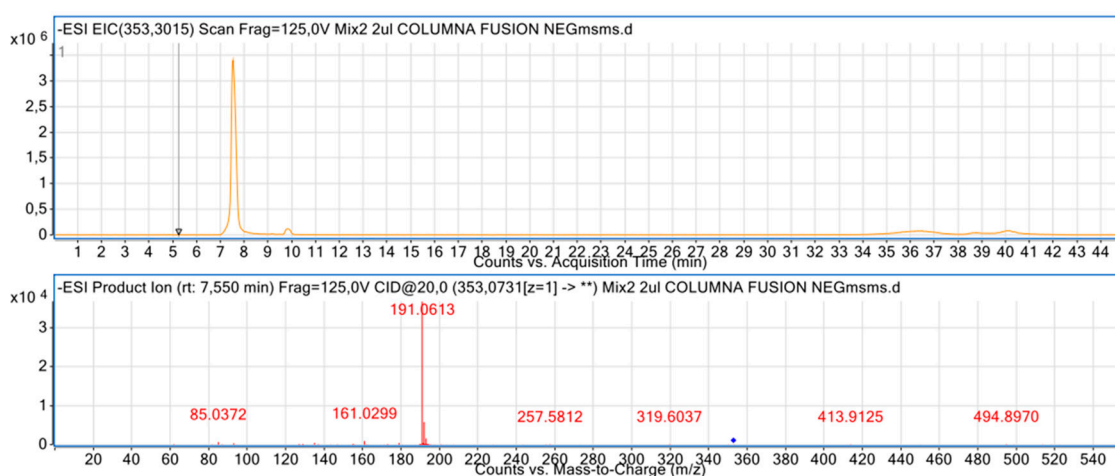


Figure S16. Chlorogenic acid (standard solution 33 mg·L⁻¹) chromatogram and mass spectrum obtained by high-resolution liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (HPLC-ESI-QTOF-MS) in SIM scan mode (Frag= 125.0V). RT= 7.550 min.

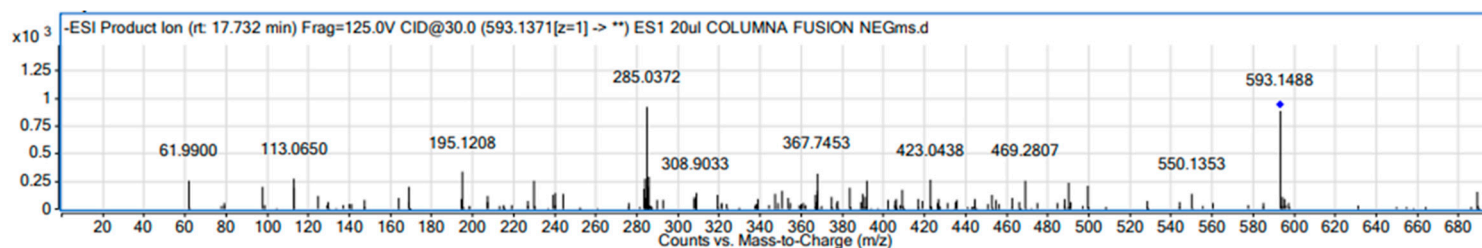


Figure S17. Kaempferol 3-rutinoside mass spectrum provided by FooDB database. RT= 17.232 min.

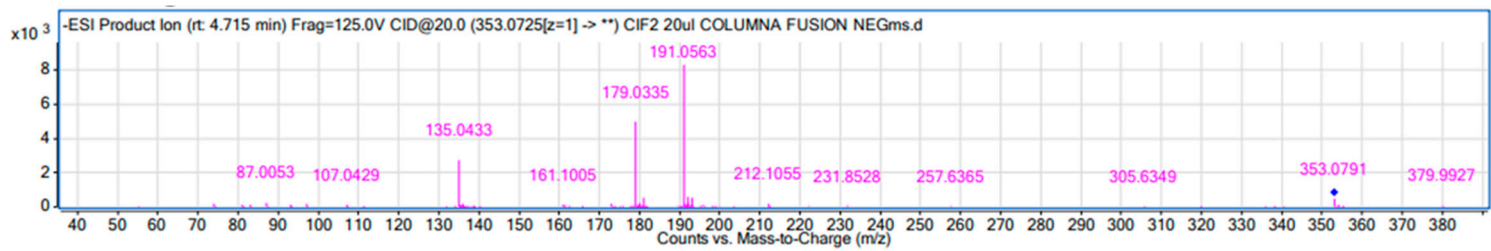


Figure S18. Neochlorogenic acid mass spectrum provided by FooDB database. RT= 4.715 min.

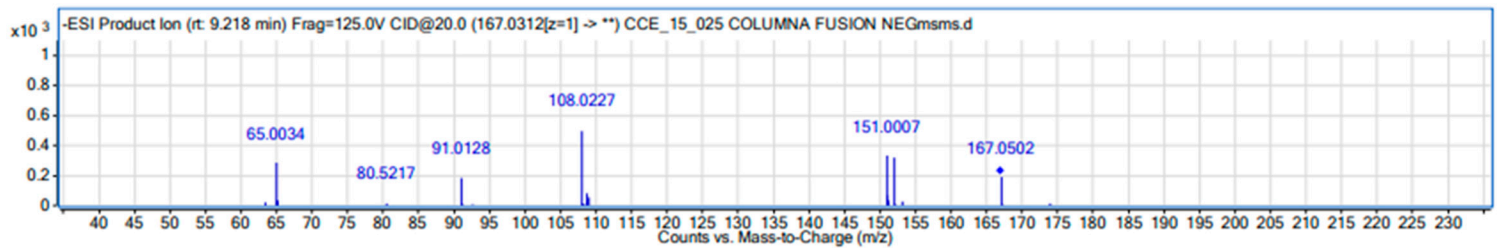


Figure S19. Vanillic acid mass spectrum standard solution. RT= 9.218 min.

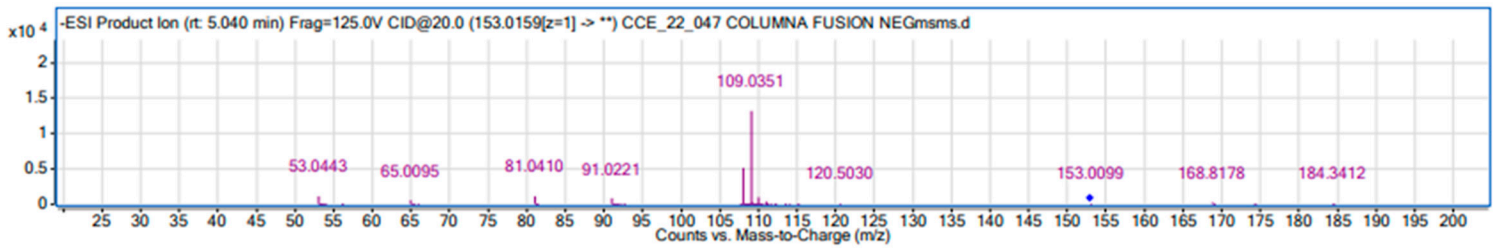


Figure S20. Protocatechuic acid mass spectrum provided by MassBank database. RT= 5.040 min.

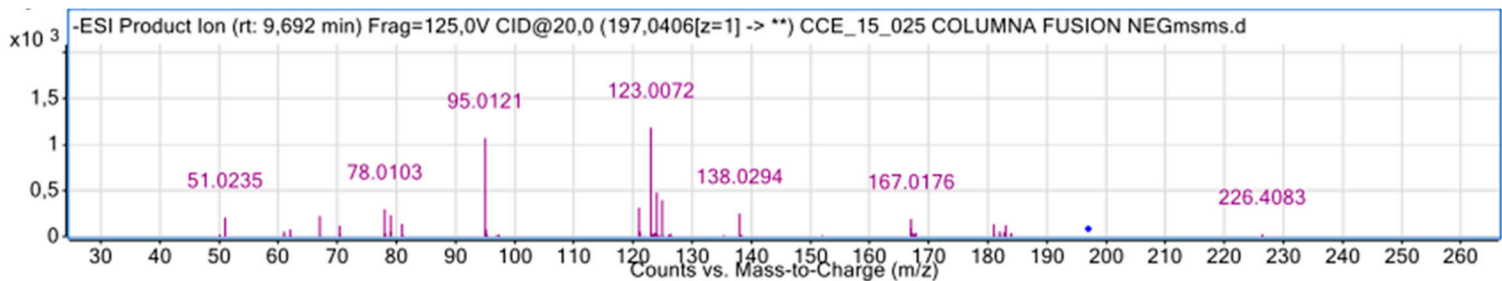


Figure S21. Syringic acid mass spectrum standard solution. RT= 9.692 min.

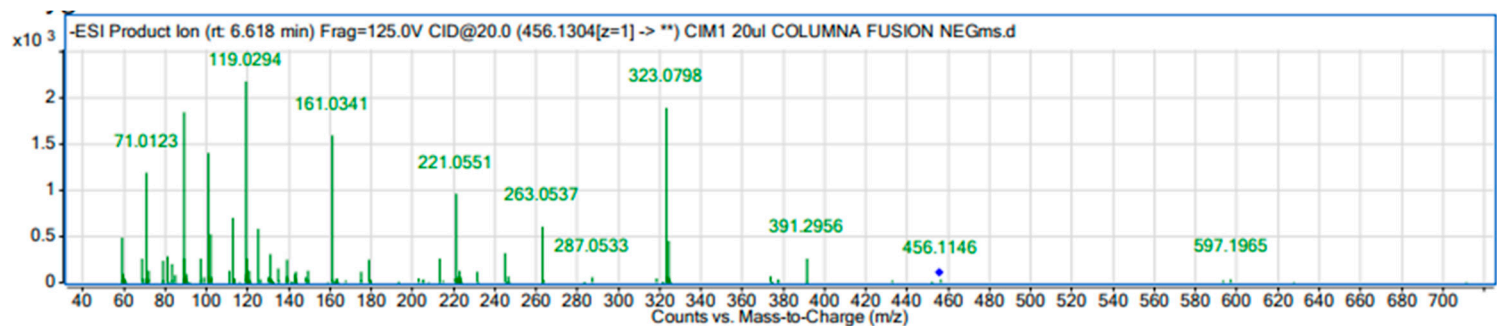


Figure S22. Amygdalin mass spectrum provided by FooDB database. RT= 6.618 min.

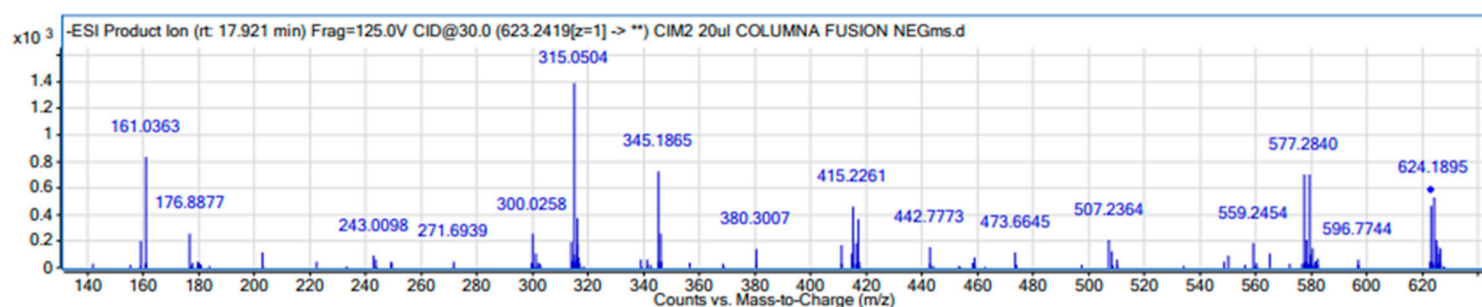


Figure S23. Isorhamnetin 3-rutinoside mass spectrum provided by MassBank database. RT= 17.921 min.

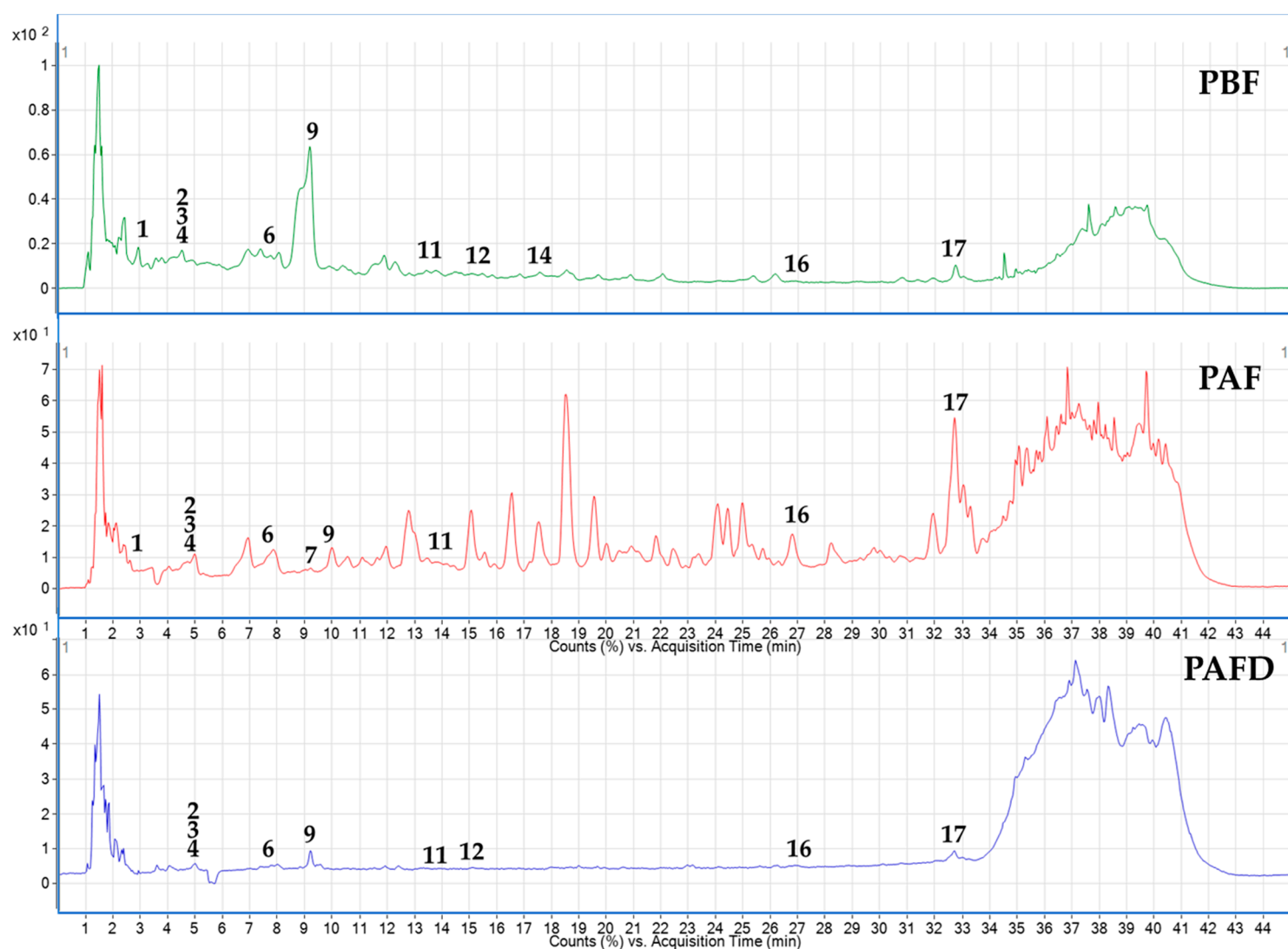


Figure S24. Chromatograms of polyphenols in defatted plum seed extracts by high-resolution liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (HPLC-ESI-QTOF-MS) in TIC negative scan mode (Frag= 125.0V). Peak identification: (1) gallic acid; (2) 2,3-dihydroxybenzoic acid; (3) neo-chlorogenic acid; (4) protocatechuate; (6) chlorogenic acid; (7) vanillic acid; (9) caffeic acid; (11) *p*-coumaric acid; (12) trans-ferulic acid; (14) isorhamnetin 3-rutinoside; (16) quercetin; (17) kaempferol.