

Supplementary material

Evaluation of cosmetic and dermatological properties of kombucha-fermented berry leaf extracts considered as by-products

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Table S1. Characterization of metabolites identified in *Rubus fruticosus* extract by HPLC-MS in negative ion mode

Rt (min.)	m/z-H	Error (ppm)	Fragmen ts	Formula	Compound	Identification
4.82	169.0146	2.08	125	C ₇ H ₆ O ₅	gallic acid	[1] (std)
12.02	353.0870	-2.28	179, 191	C ₁₆ H ₁₈ O ₉	neochlorogenic acid	[2] (std)
17.13	341.0861	-4.99	179	C ₁₅ H ₁₈ O ₉	caffeoyl hexoside (I)	[2]*
17.58	341.0875	-0.89	179	C ₁₅ H ₁₈ O ₉	caffeoyl hexoside (II)	[2]*
19.75	341.0869	-2.65	179	C ₁₅ H ₁₈ O ₉	caffeoyl hexoside (III)	[2]*
22.52	353.0870	-2.28	179, 191	C ₁₆ H ₁₈ O ₉	chlorogenic acid	[2] (std)
46.35	609.1460	-0.18	301	C ₂₇ H ₃₀ O ₁₆	rutoside	[2] (std)
48.12	433.0417	1.04	301	C ₁₉ H ₁₄ O ₁₂	ellagic acid pentoside	[1-3]**
48.97	300.9991	0.36		C ₁₄ H ₆ O ₈	ellagic acid	[1-3] (std)
49.96	477.0678	0.7	301	C ₂₁ H ₁₈ O ₁₃	quercetin-3-O-glucuronide	[1-3] (std)
51.11	461.0720	-1.19	285	C ₂₁ H ₁₈ O ₁₂	luteolin 3-O-glucuronide	[2]***
51.59	593.154	4.72	285	C ₂₇ H ₃₀ O ₁₅	kaempferol-3-O-rutinoside	[2]****
54.04	461.0720	-1.19	285	C ₂₁ H ₁₈ O ₁₂	kaempferol-3-O-glucuronide	[2]****
54.67	445.0770	-1.42	269	C ₂₁ H ₁₈ O ₁₁	apigenin-3-O-glucuronide	[2]*****

*Quantification was based on calibration curve for caffeic acid, ** Quantification was based on calibration curve for ellagic acid, *** Quantification was based on calibration curve for luteolin glucoside, **** Quantification was based on calibration curve for kaempferol glucoside, ***** Quantification was based on calibration curve for apigenin glucoside

Table S2. Characterization of metabolites identified in *Ribes nigrum* .extract by HPLC-MS in negative ion mode

Rt (min.)	m/z-H	Error (ppm)	Fragmen ts	Formula	Compound	Identification
5.01	169.0135	-4.39	125	C ₇ H ₆ O ₅	gallic acid	[4] (std)
8.95	153.0190	-2.16	127	C ₇ H ₆ O ₄	protocatechuic acid	standard
21.84	353.0867	-3.12	179, 191	C ₁₆ H ₁₈ O ₉	chlorogenic acid	[4] (std)
22.44	353.0863	-4.25	179, 191	C ₁₆ H ₁₈ O ₉	cryptochlorogenic acid	[5] (std)
31.85	163.0405	2.64		C ₉ H ₈ O ₃	p-coumaric acid	[5] (std)
46.34	609.1465	0.64	301	C ₂₇ H ₃₀ O ₁₆	rutoside	[4,5] (std)
50.34	463.0900	3.88	301	C ₂₁ H ₂₀ O ₁₂	quercetin 3-O-glucoside	[4] (std)
52.89	549.0889	0.56	301	C ₂₄ H ₂₂ O ₁₅	quercetin malonyl glucoside	[4,5]*
54.22	447.0936	0.7	285	C ₂₁ H ₂₀ O ₁₁	kaempferol glucoside	[4] (std)
56.37	532.0852	-1.23	301	C ₂₄ H ₂₁ O ₁₄	quercetin malonyl rhamnoside	[4]*

*Quantification was based on calibration curve for rutoside

Table S3. Characterization of metabolites identified in *Fragaria vesca*.extract by HPLC-MS in negative ion mode

Rt (min.)	m/z-H	Error (ppm)	Fragmen ts	Formula	Compound	Identification
4.97	169.0139	-2.04	125	C ₇ H ₆ O ₅	gallic acid	[6] (std)
22.01	353.0872	-1.71	179, 191	C ₁₆ H ₁₈ O ₉	chlorogenic acid	[6,7] (std)
45.66	623.1270	2.61	285	C ₂₇ H ₂₈ O ₁₇	kaempferol hexoside glucuronide	[6,7]*
46.67	609.1460	-0.18	301	C ₂₇ H ₃₀ O ₁₆	rutoside	[6,7] (std)
48.05	433.0413	0.12	301	C ₁₉ H ₁₄ O ₁₂	ellagic acid pentoside	[6,7]**
49.41	300.9982	-2.62		C ₁₄ H ₆ O ₈	ellagic acid	[6,7] (std)
49.48	477.0676	0.28	301	C ₂₁ H ₁₈ O ₁₃	quercetin glucuronide	[6,7] (std)
50.33	607.1311	1.06	301	C ₂₇ H ₂₈ O ₁₆	quercetin hydroxymethylglutaroyl hexoside	[6,7]***
51.50	593.1296	-0.78	285	C ₃₀ H ₂₆ O ₁₃	kaempferol coumaroyl hexoside	[6,7]*
54.32	461.0746	4.44	285	C ₂₁ H ₁₈ O ₁₂	kaempferolglucuronide	[6,7]*
55.01	461.0720	-1.19	315	C ₂₁ H ₁₈ O ₁₂	dimethyl ellagic acid pentoside	[6,7]**

*Quantification was based on calibration curve for kaempferol glucoside, ** Quantification was based on calibration curve for ellagic acid,

***Quantification was based on calibration curve for quercetin glucoside,

Table S4. Characterization of metabolites identified in *Vaccinium myrtillus* .extract by HPLC-MS in negative ion mode

Rt (min.)	m/z-H	Error (ppm)	Frag- ments	Formula	Compound	Identification
4.68	169.0144	0.9	125	C ₇ H ₆ O ₅	gallic acid	standard
8.93	153.0197	2.39	127	C ₇ H ₆ O ₄	protocatechuic acid	[8] (std)
21.88	353.0891	3.66	179, 191	C ₁₆ H ₁₈ O ₉	chlorogenic acid	[3] (std)
22.42	353.0888	2.81	179, 191	C ₁₆ H ₁₈ O ₉	cryptochlorogenic acid	[3] (std)
35,40	337.0934	1.51	191	C ₁₆ H ₁₈ O ₈	p-coumaroylquinic acid II	[3]*
47.72	535.1461	0.72	311,371	C ₂₅ H ₂₈ O ₁₃	p-Coumaroyl monotropein	[8]*
49.22	463.0889	1.51	301	C ₂₁ H ₂₀ O ₁₂	quercetin-3-O-galactoside	[3] (std)
49.63	477.0669	-1.18	301	C ₂₁ H ₁₈ O ₁₃	quercetin glucuronide	[3] (std)
51.93	409.1149	2.14	163	C ₁₉ H ₂₂ O ₁₀	p-Coumaroyl diacetylhexoside	[8]*
53.92	461.0719	-1.41	285	C ₂₁ H ₁₈ O ₁₂	kaempferol glucuronide	[3]**
55.43	411.1680	4.72	163	C ₂₀ H ₂₈ O ₉	p-Coumaroyl malonylhexoside I	[8]*
56.63	411.1677	3.99	163	C ₂₀ H ₂₈ O ₉	p-Coumaroyl malonylhexoside II	[8]*

*Quantification was based on calibration curve for p-coumaric acid, ** Quantification was based on calibration curve for kaempferol glucoside

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