Phytochemical characterization of *Philipendula vulgaris* extracts for potential uses as cosmetic ingredients

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Table S1. Phenolic compounds identified: CAS number, molecular mass (Mm), retention times (Rt), ionization mode, MS/MS transitions and coefficients of determination (R^2).

***Table S1**. Phenolic compounds identified: CAS number, molecular mass (Mm), retention times (Rt), ionization mode, MS/MS transitions and coefficients of determination (R^2).*

Phenolic compound	**CAS**	**Mm (g mol $^{-1}$)**	**Rt (min)**	**Ionization mode[a]**	**MS/MS transitions[b]**	**R^2**
Gallic acid	149-91-7	170.1	2.34	-	169.02 → 125.04 (17) 169.02 → 153.1 (15)	0.9965
Phloroglucinic acid	71989-93-0	188.1	3.28	+	168.98 → 150.99 (17) 168.98 → 83.02 (23) 168.98 → 107.02 (22)	0.9945
3,4-dihydroxybenzaldehyde	139-85-5	138.1	4.69	+	137.07 → 136.11 (21) 137.07→ 91.09 (24) 137.07 → 92.13 (25)	0.9948
Gentisic acid	490-79-9	117.1	4.85	+	152.96 → 108.00 (24) 152.96 → 81.02 (21) 152.96 → 109.01 (16)	0.9949
3- hydroxybenzoic acid	99-06-9	138.1	5.23	-	136.94 → 93.07 (14) 136.94 → 65.10 (24) 136.94 → 91.01 (32)	0.9969
4-hydroxybenzoic acid	99-96-7	138.1	5.24	-	137.00 → 93.00 (17) 137.00 → 65.00 (27)	0.9985
Catechin	18829-70-4	290.3	5.25	-	289.01 → 245.02 (17) 289.01 → 203.12 (22)	0.9868
Procyanidin B1	20315-25-7	578.5	5.30	-	577.03→ 407.06 (26) 577.03 → 288.93 (25) 577.03 → 424.98 (26)	0.9958
γ-resorcylic acid[c]	303-07-1	154.1	5.54	+	153.00 →109.05 (17) 153.00 → 65.09 (21) 153.00 → 135.02 (16)	0.9996
Procyanidin B2	29106-49-8	578.5	5.74	-	577.03 → 407.06 (26) 577.03 → 288.93 (25) 577.03 → 424.98 (26)	0.9946
4-Hydroxybenzaldehyde	123-08-0	122.1	5.75	+	122.97→ 95.05 (13) 122.97 → 51.10 (36) 122.97 → 77.05 (20)	0.9887
Caffeic acid	331-39-5	180.2	6.11	-	178.98 → 135.03 (19) 178.98 → 134.01 (28)	0.9876
Procyanidin C1	37064-30-5	866.8	6.30	-	577.03 → 288.93 (25) 577.03 → 407.07 (26) 577.03 → 424.98 (26)	0.9994
4-hydroxycinnamic acid	501-98-4	164.2	7.29	+	163.02 → 119.07 (18) 163.02 → 93.07 (37) 163.02 → 117.05 (38)	0.9951
Quercetin-3-glucuronide	22688-79-5	478.4	9.54	+	479.09 → 461.50 (14) 479.09 → 302.96 (18)	0.9955
Quercetin-3-glucoside	482-35-9	464.4	9.80	+	465.07 → 256.90 (41) 465.07 → 302.97 (14)	0.9924

***Table S1**. cont.*

Phenolic compound	**CAS**	**Mm (g mol $^{-1}$)**	**Rt (min)**	**Ionization mode[a]**	**MS/MS transitions[b]**	**R^2**
Ellagic acid	476-66-4	302.2	10.05	-	301.00 → 145.1 (39) 301.00 → 185.1 (29) 301.00 → 173.1 (36)	0.9916
Rosmarinic acid	20283-92-5	360.3	10.29	-	359.07 → 161.1 (23) 359.07 → 133.1 (42) 359.07 → 135.1 (38)	0.9954
Astragalin	480-10-4	448.4	11.15	-	447.09 → 284.1 (28) 447.09 → 255.1 (40) 447.09 → 227.1 (49)	0.9960
Quercetin	117-39-5	302.2	11.81	+	303.09 → 229.10 (28) 303.09→153.04 (33)	0.9863
Naringenin	480-41-1	272.3	12.04	+	273.00 → 119.00 (20) 273.00 → 147.00 (20)	0.9902
Luteolin	491-70-3	286.2	12.09	-	285.04 → 199.00 (20) 285.04 → 175.00 (20) 285.04 → 241.00 (20)	0.9930
Kaempferol	520-18-3	286.2	12.40	-	285.07 → 184.91 (30) 285.07 → 239.12 (35)	0.9883

[a] "-"and "+" indicate negative and positive ionization modes, respectively. [b] Underlined MS/MS transition used for quantification purpose. [c] Isomers (γ and α).