

Grapevine extracts and their effect on selected gut-associated microbiota: *In vitro* study

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Electronic supplementary material

Supplementary Figure S1

Table S1. Suggested identification of compounds in *Vitis vinifera* cane extract by the HRMS/MS in ESI⁺ in MS^e mode

	t_R (min)	Ion mode	Calculated m/z	Measured m/z	Mass error (ppm)	Description	Formula
1	1.4	[M+H] ⁺	166.0868	166.0866	−1.2	L-phenylalanine	C ₉ H ₁₁ NO ₂
2	2.2	[M+H] ⁺	205.0977	205.0977	0	Tryptophan	C ₁₁ H ₁₂ N ₂ O ₂
3	2.4	[M+H] ⁺	579.1503	579.1503	0	procyanidin	C ₃₀ H ₂₆ O ₁₂
4	2.5	[M+H] ⁺	579.1503	579.1503	0	procyanidin	C ₃₀ H ₂₆ O ₁₂
5	2.8	[M+H] ⁺	291.0869	291.0870	0.3	epicatechin/catechin	C ₁₅ H ₁₄ O ₆
6	3.3	[M+H] ⁺	185.0814	185.081	−1.6	antiarol	C ₉ H ₁₂ O ₄
7	3.4	[M+H] ⁺	579.1503	579.1503	0	procyanidin	C ₃₀ H ₂₆ O ₁₂
8	3.6	[M+H] ⁺	231.1134	231.1133	−0.4	1,2-dihydroxytacrine	C ₁₃ H ₁₄ N ₂ O ₂
9	3.9	[M+H] ⁺	291.0869	291.0874	1.7	epicatechin/catechin	C ₁₅ H ₁₄ O ₆
10	4.6	[M+H] ⁺	402.1665	402.1665	0	C ₂₀ H ₂₃ N ₃ O ₆	C ₂₀ H ₂₃ N ₃ O ₆
11	4.8	[M+H] ⁺	180.1025	180.1023	−1.1	fusaric acid	C ₁₀ H ₁₃ NO ₂
12	4.9	[M+H] ⁺	402.1665	402.1665	0	C ₂₀ H ₂₃ N ₃ O ₆	C ₂₀ H ₂₃ N ₃ O ₆
13	5.6	[M+H] ⁺	455.1495	455.1489	−1.3	<i>trans</i> -δ-viniferin/ ε-viniferin	C ₂₈ H ₂₂ O ₆
14	5.7	[M+H] ⁺	241.0865	241.0858	−2.9	chrysophanic acid- 9-anthrone	C ₁₅ H ₁₂ O ₃
15	5.9	[M+H] ⁺	479.0826	479.0817	−1.8	quercetin-glucuronide	C ₂₁ H ₁₈ O ₁₃
16	6.1	[M+H] ⁺	241.0865	241.0859	−2.5	chrysarobin	C ₁₅ H ₁₂ O ₃
17	6.2	[M+H] ⁺	453.1338	453.1333	−1.1	viniferifuran	C ₂₈ H ₂₀ O ₆
18	6.4	[M+H] ⁺	249.1127	249.1123	−1.6	citreoivrenone	C ₁₄ H ₁₆ O ₄
19	7.0	[M+H] ⁺	487.2139	487.2153	2.9	C ₁₈ H ₃₄ N ₂ O ₁₃	C ₁₈ H ₃₄ N ₂ O ₁₃
20	7.2	[M+H] ⁺	455.1495	455.1495	0	<i>trans</i> -δ-viniferin/ ε-viniferin	C ₂₈ H ₂₂ O ₆
21	7.7	[M+H] ⁺	273.1127	273.1127	0	angolensin	C ₁₆ H ₁₆ O ₄
22	7.9	[M+H] ⁺	229.0865	229.0863	−0.9	resveratrol	C ₁₄ H ₁₂ O ₃
23	8.3	[M+H] ⁺	249.1127	249.1123	−1.6	citreoivrenone	C ₁₄ H ₁₆ O ₄
24	9.2	[M+Na] ⁺	287.1259	287.1255	−1.4	abscisic acid	C ₁₅ H ₂₀ O ₄ Na
25	9.5	[M+H] ⁺	907.2755	907.2751	−0.4	viniferol A/r-viniferin	C ₅₆ H ₄₂ O ₁₂
26	9.7	[M+H] ⁺	907.2755	907.2751	−0.4	viniferol A/r-viniferin	C ₅₆ H ₄₂ O ₁₂
27	10.0	[M+H] ⁺	907.2755	907.2751	−0.4	viniferol A/r-viniferin	C ₅₆ H ₄₂ O ₁₂
28	10.3	[M+H] ⁺	907.2755	907.2751	−0.4	viniferol A/r-viniferin	C ₅₆ H ₄₂ O ₁₂
29	10.9	[M+H] ⁺	308.2226	308.2225	−0.3	C ₁₈ H ₂₉ NO ₃	C ₁₈ H ₂₉ NO ₃
30	11.3	[M+H] ⁺	455.1495	455.1495	0	<i>trans</i> -δ-viniferin/ ε-viniferin	C ₂₈ H ₂₂ O ₆
31	11.5	[M+Na] ⁺	429.1678	429.1700	5.1	C ₂₅ H ₂₆ O ₅	C ₂₅ H ₂₆ O ₅
32	11.8	[M+H] ⁺	681.2125	681.2125	0	copalliferol B	C ₄₂ H ₃₂ O ₉
33	12.3	[M+H] ⁺	455.1495	455.1495	0	<i>trans</i> -δ-viniferin/ ε-viniferin	C ₂₈ H ₂₂ O ₆
34	12.5	[M+Na] ⁺	351.2147	351.2143	1.1	C ₁₈ H ₃₂ O ₅	C ₁₈ H ₃₂ O ₅
35	13.1	[M+H] ⁺	681.2125	681.2134	1.3	copalliferol B	C ₄₂ H ₃₂ O ₉
36	13.6	[M+Na] ⁺	353.2304	353.2295	−2.55	C ₁₈ H ₃₄ O ₅	C ₁₈ H ₃₄ O ₅
37	14.2	[M+H] ⁺	907.2755	907.2751	−0.4	viniferol A/r-viniferin	C ₅₆ H ₄₂ O ₁₂
38	14.9	[M+H] ⁺	249.1127	249.1123	−1.6	C ₁₄ H ₁₆ O ₄	C ₁₄ H ₁₆ O ₄
39	15.2	[M+H] ⁺	249.1127	249.1123	−1.6	C ₁₄ H ₁₆ O ₄	C ₁₄ H ₁₆ O ₄