

Table S1. Tentative identification of major phenolic compound of mango criollo peel and pulp by HPLC-DAD-ESI-QTOF-MS/MS

Compound n°	Compound name	Formula	Family	RT (min)	MI	[M-H] ⁻	Major fragment ions m/z	Peel	Pulp
1	Quinic acid	C ₇ H ₁₂ O ₆	Org Acid	3.73	192.0634	191.0572	127.93	√	√
2	Galloyl glucoside isomer I	C ₁₃ H ₁₆ O ₁₀	Gall	3.82	332.0743	331.0687	331.0636, 169.0112, 151.0038, 123.0075	√	√
3	Citric acid	C ₆ H ₈ O ₇	Org Acid	5.03	192.0270	191.0202		√	√
4	Vanillic acid glucoside	C ₁₄ H ₁₈ O ₉	Phen Acid	5.72	330.0950	329.0880	167.0357, 152.0124, 108.0208	√	√
5	Galloyl glucoside isomer II	C ₁₃ H ₁₆ O ₁₀	Gall	6.38	332.0744	331.0687	211.0224, 169.0112, 123.0086, 59.0141	√	√
6	p-Hydroxy benzoic acid glucoside	C ₁₃ H ₁₆ O ₈	Phen Acid	14.11	300.0845	299.078	137.0235, 93.0347	√	√
7	Di-galloyl-glucoside	C ₂₀ H ₂₀ O ₁₄	Gall	14.52	484.0853	483.0770	169.0138, 125.0208, 331.0615	√	√
8	Maclurin-3-C-β-D-glucoside	C ₁₉ H ₂₀ O ₁₁	Benz	14.63	424.1006	423.0935	303.0492, 233.0315, 209.0447, 333.0645, 193.0053	√	√
9	Maclurin-3-C-β-D-glucoside	C ₁₉ H ₂₀ O ₁₁	Benz	15.84	424.1006	401.1094	401.1089, 383.0984, 225.0768, 207.0663	√	√

10	Maclurin-3-C-(2-O-galloyl)-β-D-glucoside	C ₂₆ H ₂₄ O ₁₅	Benz	16.45	576.1115	575.1049	575.1049, 423.0922, 303.0492, 285.0409, 169.0144	√	tr
11	Jasminoside R	C ₂₂ H ₃₄ O ₁₂	Terpenoid	16.89	490.2050	489.1885	443.1897, 375.0408, 323.1465, 281.1385	√	√
12	Trigalloyl glucosa	C ₂₇ H ₂₄ O ₁₈	Gall	18.62	636.0963	635.089	483, 465,423,313, 295, 169	√	√
13	(-)-Catechin	C ₁₅ H ₁₄ O ₆	Flav	17.43	290.0790	289.0729	123.0435, 109.0248, 175.0779, 205.0547	√	√
14	Mangiferin	C ₁₉ H ₁₈ O ₁₁	Xant	18.09	422.0849	421.0777	331.0455, 301.0355, 259.0209, 421.0734	√	√
15	Iriflophenone-3-C-(2-O-galloyl)-β-D-glucoside	C ₂₆ H ₂₄ O ₁₄	Xant	18.92	560.1166	559.1094	287.0585, 269.0424, 470.0979, 169.0136	√	√
16	Dihydrophaseic acid glucoside	C ₂₁ H ₃₂ O ₁₀	Terpenoid	18.97	444.1995	443.1930	281.1, 237.0	√	√
17	Maclurin-3-C-(2,3-di-O-galloyl)-β-D-glucoside	C ₃₃ H ₂₈ O ₁₉	Benz	19.04	728.1225	727.1157	727.1157, 575.1038, 405.0760, 303.0475	√	√
18	Cumaroyl gGalloyl gGlucoside	C ₂₂ H ₂₂ O ₁₂	Gall	19.29	478.1111	477.1051	727.01157, 575.1038, 405.0760,	√	√

							303.0475		
19	Mangiferin-6'-O-gallate	C ₂₆ H ₂₂ O ₁₅	Xant	20.37	574.0959	573.0878	421.0778, 403.0760, 573.0855, 169.1056	√	√
20	Quercetin-3-O-diglycoside	C ₂₆ H ₂₈ O ₁₆	Flav	21.63	596.1377	595.1304	595.1301, 300.0251, 301.0331	√	no
21	Tetra-O-galloyl-glucoside I	C ₃₄ H ₂₈ O ₂₂	Gall	21.83	788.1072	787.1005	787.1005, 635.0782, 617.0765, 169.0189	√	√
22	Ethyl gallate	C ₉ H ₁₀ O ₅	Gall	22.98	198.0528	197.0468	169.0101, 124.0179, 103.9804	√	√
23	Octil gallate	C ₉ H ₂₂ O ₅	Gall	23.37	282.1467	281.1389	237, 189, 171, 168, 121	√	√
24	Ellagic acid	C ₁₄ H ₆ O ₆	Phen Acid	23.51	302.0062	301.0021	300.92, 257.01, 229.08	√	√
25	Quercetin-3-O-galactoside	C ₂₁ H ₂₀ O ₁₂	Flav	23.57	464.0955	463.0890	300.0260, 301.0342, 463.0890, 151.0029	√	√
26	Quercetin-3-O-glucoside (isoquercitrin)	C ₂₁ H ₂₀ O ₁₂	Flav	23.90	464.0955	463.0890	463.0890, 300.0277, 301.0333, 151.0004	√	√
27	Penta-O-galloyl-glucoside	C ₄₁ H ₃₂ O ₂₆	Gall	24.32	940.1182	939.1107	769.0687, 470.0508, 787.0760, 617.0672	√	√

28	Valonic acid dilactone	C ₂₁ H ₁₀ O ₁₃	Phen Acid	24.32	470.0121	469.0505	423, 401, 169	√	√
29	Quercetin pentoside I	C ₂₀ H ₁₈ O ₁₁	Flav	24.91	434.0849	433.0783	433.073, 301.0314, 30.0296	√	√
30	Quercetin-3-O-rhamnoside	C ₂₁ H ₂₀ O ₁₁	Flav	25.30	448.1006	447.0941	447.0941, 284.0301, 285.0387	tr	no
31	Quercetin pentoside II	C ₂₀ H ₁₈ O ₁₁	Flav	25.39	434.0849	433.0783	433.073, 301.0314, 30.0296	√	√
32	Hexagalloyl glucose isomer I	C ₄₈ H ₃₆ O ₃₀	Gall	25.79	1092.1290	1091.1200	879.9843, 770.0973, 498.4653, 169.0091, 279.0338	√	√
33	Hexagalloyl glucose isomer II	C ₄₈ H ₃₆ O ₃₀	Gall	26.06	1092.129	1091.1200	787.1257, 433.0671, 839.2524, 16.9678	√	√
34	Hexagalloyl glucose isomer III	C ₄₈ H ₃₆ O ₃₀	Gall	26.30	1092.1290	1091.1200	879.9843, 770.0973, 498.4653, 169.0091, 279.0338	√	√
35	Hexagalloyl hexose isomer IV	C ₄₈ H ₃₆ O ₃₀	Gall	26.57	1092.129	1091.1200	433.0671, 787.1257, 839.2524, 16.9678	√	√
36	Heptagalloyl glucoside isomer I	C ₅₅ H ₄₀ O ₃₄	Gall	27.59	1244.8857	1243.1330	939, 621, 545	√	tr
37	Heptagalloyl glucoside isomer I	C ₅₅ H ₄₀ O ₃₄	Gall	27.98	1244.8857	1243.1330	939, 621, 545	√	tr

38	Heptagalloyl glucoside isomer I	C ₅₅ H ₄₀ O ₃₄	Gall	28.30	1244.8857	1243.1330	939, 621, 545	√	tr
39-41	Unknown		Gall	29 - 31	>1300			√	tr
42	Abcistic acid	C ₁₅ H ₂₀ O ₄	Terpenoid	33.86	264.1362	263.1289	219.2, 153.2, 151.2	no	√

Org Acid, organic acid; Phen Acid, phenolic acid derivatives; Gall, gallates and gallotannins; Bez, benzophenones; Flav, flavonoids; Xant, xanthonenes; tr, traces.