

Supplementary material

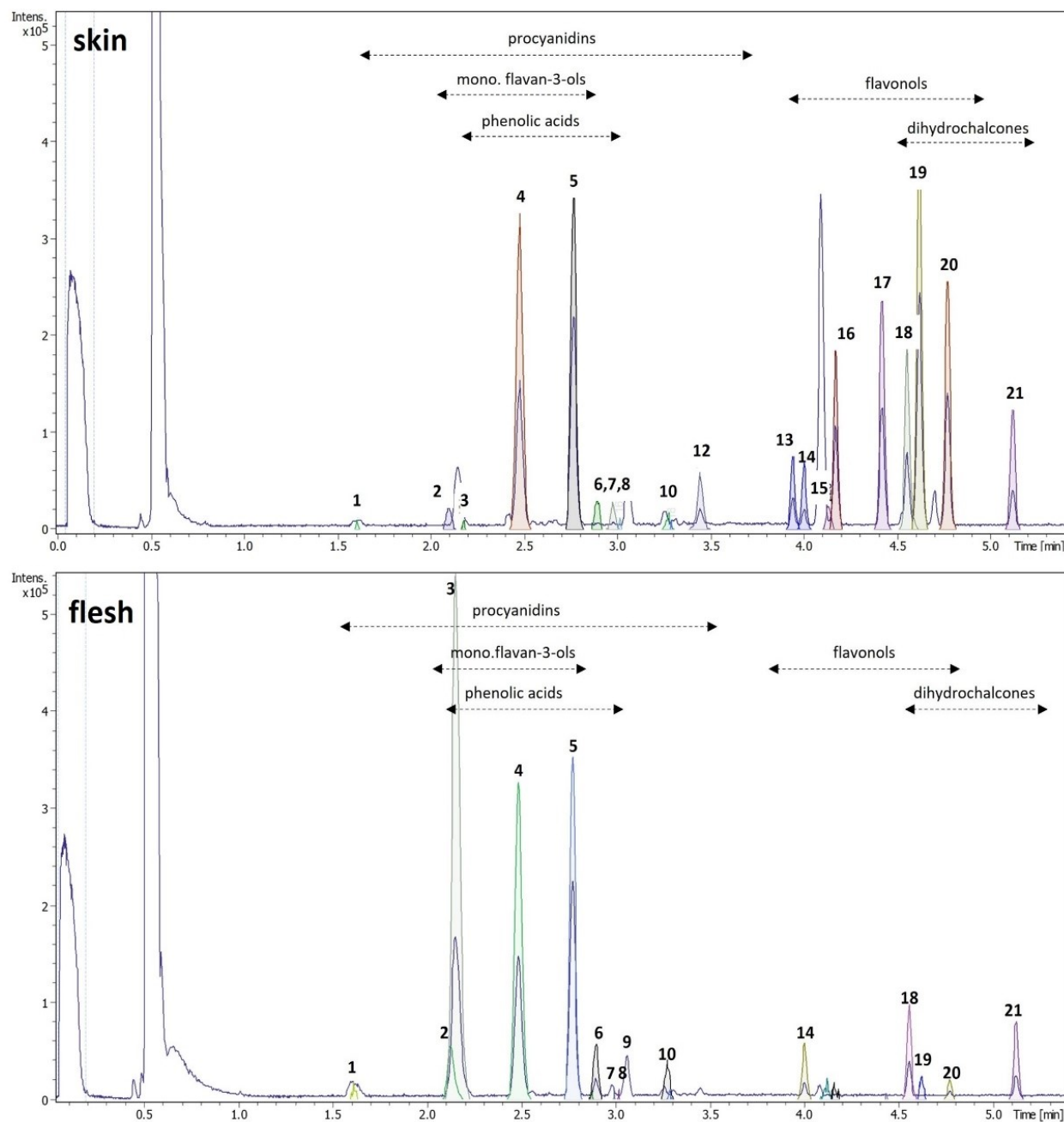


Fig. S1. Extracted ion chromatograms of Monty's Surprise skin and flesh samples analysed by LC-HRAM-MS. The chromatogram shows phytochemical compounds in Monty's Surprise apple skin and flesh. The numbers correspond to the different compounds summarised in Table S1, compound classes are shown in the chromatogram. The blue line represents the base peak chromatogram.

Table S1. Compounds detected in Monty's Surprise apple skin and flesh ethanolic extracts by LC-HRAM-MS.

peak number	phenolic group	compound name	standard used	formula	RT (min)*	m/z (M + H)*
1	oligomeric flavan-3-ols	procyanidin B1	procyanidin B2	C ₃₀ H ₂₆ O ₁₂	1.62	578.1424
2	monomeric flavan-3-ols	catechin	catechin	C ₁₅ H ₁₄ O ₆	2.13	290.079
3	phenolic acids	chlorogenic acid	chlorogenic acid	C ₁₆ H ₁₈ O ₉	2.16	354.0951
4	oligomeric flavan-3-ols	procyanidin B2	procyanidin B2	C ₃₀ H ₂₆ O ₁₂	2.50	578.1424
5	monomeric flavan-3-ols	epicatechin	catechin	C ₁₅ H ₁₄ O ₆	2.78	290.079
6	oligomeric flavan-3-ols	procyanidin hexamer	procyanidin B2	C ₉₀ H ₇₄ O ₃₆	2.88	1730.396
7	phenolic acids	trans-4-p-coumaroyl quinic acid	trans-4-p-coumaroyl quinic acid	C ₁₆ H ₁₈ O ₈	2.90	338.1002
		trans-5-p-coumaroyl quinic acid	trans-4-p-coumaroyl quinic acid	C ₁₆ H ₁₈ O ₈	2.99	338.1002
8	phenolic acids	procyanidin C1	procyanidin B2	C ₃₀ H ₄₆ O ₆	3.00	866.2058
9	oligomeric flavan-3-ols	procyanidin B5	procyanidin B2	C ₃₀ H ₂₆ O ₁₂	3.27	578.1425
10	oligomeric flavan-3-ols	procyanidin tetramer	procyanidin B2	C ₆₀ H ₅₀ O ₂₄	3.26	1154.2692
11	oligomeric flavan-3-ols	procyanidin pentamer	procyanidin B2	C ₇₅ H ₆₂ O ₃₀	3.45	1442.3326
12	flavonols	quercetin 3-rutinoside	quercetin 3-rutinoside	C ₂₇ H ₃₀ O ₁₆	3.94	610.1534
13	oligomeric flavan-3-ols	procyanidin B7	procyanidin B2	C ₃₀ H ₂₆ O ₁₂	4.00	578.1425
14	flavonols	quercetin 3-galactoside	quercetin 3-rutinoside	C ₂₁ H ₂₀ O ₁₂	4.09	464.0955
15	flavonols	quercetin 3-glucoside	quercetin 3-rutinoside	C ₂₁ H ₂₀ O ₁₂	4.17	464.0955
16	flavonols	quercetin 3-xylopyranoside	quercetin 3-rutinoside	C ₂₀ H ₁₈ O ₁₁	4.42	434.0849
17	flavonols	phloretin-2'-O-xyloglucoside	phloridzin	C ₂₆ H ₃₂ O ₁₄	4.57	568.1792
18	dihydrochalcones	quercetin 3-arabinopyranoside	quercetin 3-rutinoside	C ₂₀ H ₁₈ O ₁₁	4.62	434.0849
19	flavonols	quercetin 3-rhamnoside	quercetin 3-rutinoside	C ₂₁ H ₂₀ O ₁₂	4.77	448.1006
20	flavonols	phloridzin	phloridzin	C ₂₁ H ₂₄ O ₁₀	5.14	436.137
21	dihydrochalcones					

* RT – retention time, m/z – mass to charge ratio of the molecule