

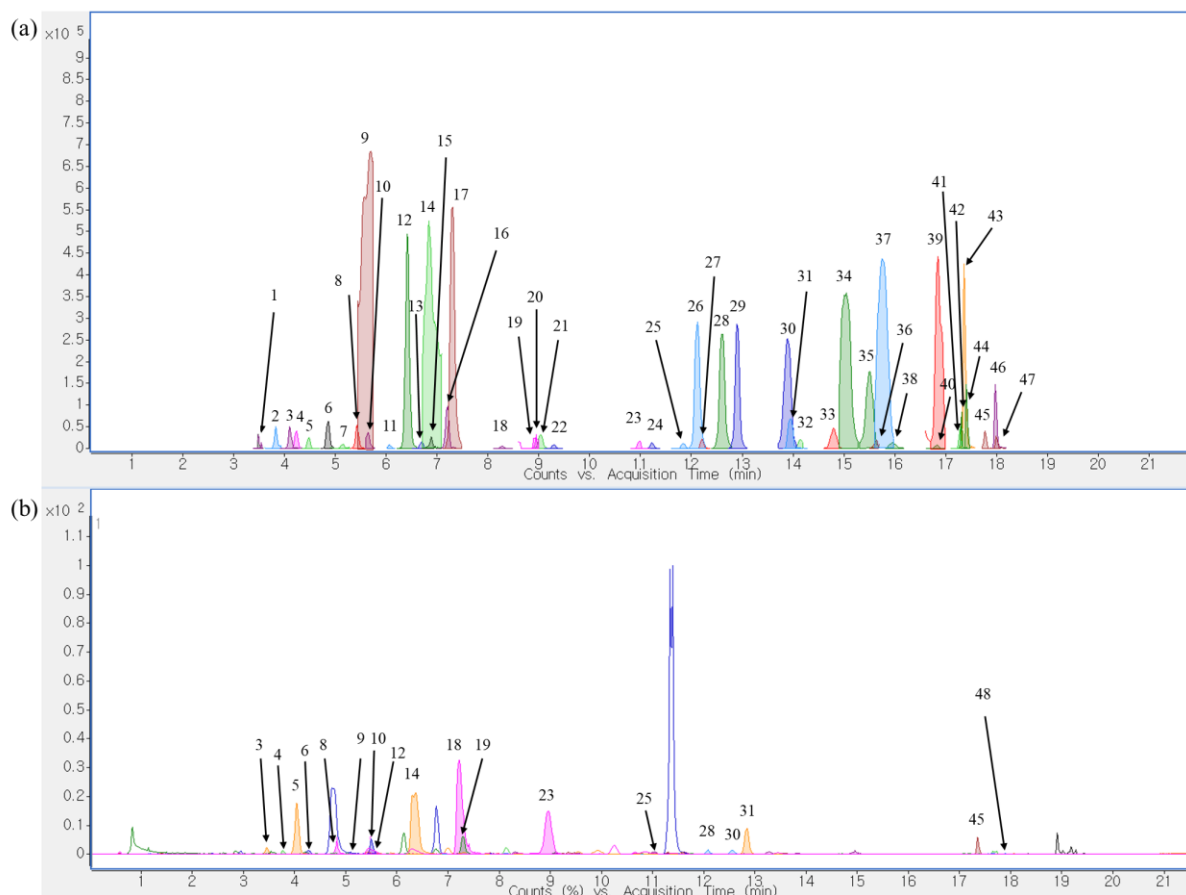


Figure S1. Extracted ion chromatogram (EIC) of the identified phenolic compounds by UHPLC-(ESI)-qTOF in the peel (a) and pulp (b) of Decobell apples. Peak numbers are annotated in Table S1.

Table S1. Phenolic compounds identified by UHPLC-(ESI)-qTOF in the apple peel and pulp

Code (peak no.)	Rt (min)	Compound assigned	Molecular formula	Predicted MS1 m/z	Fragment m/z	Error (ppm)	Subclass	Found in peel or pulp
<i>Phenolic acid</i>								
PA1 (1)	3.5	hydroxy benzoic acid	C ₇ H ₆ O ₃	137.0244	119 [M – H ₂ O – H] ⁻ 108 [M – CO (-28) – H] ⁻	-5.1	hydroxybenzoic acid	peel, pulp
PA2 (15)	6.9	dihydroxy benzoic acid	C ₇ H ₆ O ₄	153.0193	137 [M – CO (-28) – H] ⁻ 109 [M – CO ₂ (-44) – H] ⁻	-0.8	hydroxybenzoic acid	peel
PA3 (4)	4.2	chlorogenic acid*	C ₁₆ H ₁₈ O ₉	353.0878	191 [M – caf (-162) – H] ⁻ 179 [M – qa (-174) – H] ⁻	-2.0	hydroxycinnamic acid	peel, pulp
PA4 (8)	5.4	caffeoylquinic acid	C ₁₆ H ₁₈ O ₉	353.0878	191 [M – caf (-162) – H] ⁻ 179 [M – qa (-174) – H] ⁻	0.3	hydroxycinnamic acid	peel, pulp
PA5 (13)	6.7	coumaroylquinic acid	C ₁₆ H ₁₈ O ₈	337.0929	191 [M – cu (-146) – H] ⁻ 173 [M – cu (-146) – H ₂ O – H] ⁻	0.1	hydroxycinnamic acid	peel
PA6 (16)	7.2	coumaroylquinic acid	C ₁₆ H ₁₈ O ₈	337.0929	191 [M – cu (-146) – H] ⁻	0.5	hydroxycinnamic acid	peel, pulp
PA7 (20)	8.9	coumaroylquinic acid	C ₁₆ H ₁₈ O ₈	337.0929	191 [M – cu (-146) – H] ⁻	-2.9	hydroxycinnamic acid	peel
<i>Flavan-3-ols</i>								
P1 (2)	3.8	catechin-O-hexoside	C ₂₁ H ₂₄ O ₁₁	451.1246	289 [M – h (-162) – H] ⁻	-3.3	flavan-3-ol	peel, pulp
P2 (3)	4.1	procyanidin dimer B type	C ₃₀ H ₂₆ O ₁₂	577.1351	289 [M – cat (-288) – H] ⁻	-2.3	proanthocyanidins	peel, pulp
P3 (5)	4.5	catechin-O-hexoside	C ₂₁ H ₂₄ O ₁₁	451.1246	289 [M – h (-162) – H] ⁻ 245 [M – h (-162) – C ₂ H ₄ O – H] ⁻	3.6	flavan-3-ol	peel
P4 (6)	4.9	catechin*	C ₁₅ H ₁₄ O ₆	289.0718	203 [M – C ₄ H ₆ O ₂ – H] ⁻ 151 [M – C ₇ H ₆ O ₃ – H] ⁻ 109 [M – C ₉ H ₈ O ₄ – H] ⁻	-1.2	flavan-3-ol	peel, pulp
P5 (7)	5.1	(epi)gallocatechin	C ₁₅ H ₁₄ O ₇	305.0667		1.8	flavan-3-ol	peel, pulp
P6 (10)	5.7	procyanidin trimer B type	C ₄₅ H ₃₈ O ₁₈	865.1985		1.9	proanthocyanidins	peel, pulp
P7 (11)	6.1	(epi)gallocatechin	C ₁₅ H ₁₄ O ₇	305.0667	125 [M – C ₉ H ₈ O ₄ – H] ⁻	0.1	flavan-3-ol	peel
P8 (12)	6.4	procyanidin dimer B type	C ₃₀ H ₂₆ O ₁₂	577.1351	289 [M – cat (-288) – H] ⁻	0.0	proanthocyanidins	peel, pulp
P9 (17)	7.3	epicatechin*	C ₁₅ H ₁₄ O ₆	289.0718	245 [M – CO ₂ (-44) – H] ⁻	1.5	flavan-3-ol	peel, pulp
P10 (21)	9.0	procyanidin trimer B type	C ₄₅ H ₃₈ O ₁₈	865.1985	577 [M – cat (-288) – H] ⁻ 289 [M – cat (-288) – cat (-288) – H] ⁻	-3.7	proanthocyanidins	peel, pulp

A1 (9)	5.6	cyanidin-3- <i>O</i> -galactoside*	C ₂₁ H ₂₀ O ₁₁	449.1078+	287 [M-h (-162) + H] ⁺	-3.4	anthocyanin	peel, pulp
A2 (14)	6.9	cyanidin-3- <i>O</i> -arabinoside*	C ₂₀ H ₁₈ O ₁₀	419.0973+	287 [M-h (-132) + H] ⁺	-0.6	anthocyanin	peel
A3 (19)	8.8	cyanidin- <i>O</i> -pentoside	C ₂₀ H ₁₈ O ₁₀	419.0973+	287 [M - p (-132) + H] ⁺	1.1	anthocyanin	peel
A4 (31)	14.0	cyanidin- <i>O</i> -hexoside	C ₂₁ H ₂₀ O ₁₁	449.1078+	287 [M - h (-162) + H] ⁺	0.3	anthocyanin	peel
A5 (41)	17.3	cyanidin- <i>O</i> -pentoside	C ₂₀ H ₁₈ O ₁₀	419.0973+	287 [M - h (-132) + H] ⁺	-1.7	anthocyanin	peel
A6 (44)	17.4	cyanidin- <i>O</i> -rhamnoside*	C ₂₁ H ₂₀ O ₁₀	433.1129+	287 [M - dh (-146) + H] ⁺	-2.0	anthocyanin	peel

Dihydrochalcone

PH1 (39)	16.8	phloretin- <i>O</i> -pentose hexoside	C ₂₆ H ₃₂ O ₁₄	567.1719	273 [M - h (-162) -p (-132) - H] ⁻	0.9	dihydrochalcone	peel
PH2 (43)	17.4	phloridzin*	C ₂₁ H ₂₄ O ₁₀	435.1297	273 [M - h (-162) - H] ⁻	-0.5	dihydrochalcone	peel, pulp

* identified with authentic standards.

+ indicates that the values were measured in ESI-positive mode and other m/z values were measured in ESI-negative mode.

qa-quinic, caf-caffeoyl, cu-coumaroyl, cat-catechin, h-hexose, dh-deoxyhexose, p-pentose.

Table S2. F-values and *p*-values in the analysis of variance for metabolites among the peel and pulp of apple cultivars

	Frc	Glc	Suc	Sor	Total free sugar	Mal	Cit	Shi	Total orga nic acid	Suga r/aci d	DPP H	ABT S	QTof EIC area	Cat	Epi	Phl	CA	C3gal	C3 ara	Rut	Q3gal	Q3gl c	Q3 rha	Total phen olic
<i>F value</i>																								
Peel	-	-	-	-	-	-	-	-	-	-	1834	240	148	321	61	199	5641	294	331	576	168	267	241	91
Pulp	1233	42	1283	447	231	4585	10954 1	39	5434	1517	121	423	324	1332	1166	2523	6164	14048	n.d.	103	1306	5404	n.d.	3175
<i>p-value</i>																								
Peel	-	-	-	-	-	-	-	-	-	-	**	**	**	**	**	**	**	**	**	**	**	**	**	**
Pulp	**	**	**	**	**	**	**	**	**	**	**	**	**	**	**	**	**	**	n.d.	**	**	**	n.d.	**

Frc, Glc, Suc, Sor, Mal, Cit, Shi, Cat, Epi, Phl, CA, C3gal, C3ara, Rut, Q3gal, Q3glc, and Q3rha indicate fructose, glucose, sucrose, sorbitol, malic acid, citric acid, shikimic acid, catechin, epicatechin, phloridzin, chlorogenic acid, cyanidin-3-*O*-galactoside, cyanidin-3-*O*-arabinoside, rutin, quercetin-3-*O*-galactoside, quercetin-3-*O*-glucoside, and quercetin-3-*O*-rhamnoside, respectively. –, n.d., and ** indicate not determined, not detected, and significant differences at $p < 0.01$, respectively.