Supplementary Materials

Table S1. Weight, width, length, and peel thickness of Haruka, Kiyomi, and Yellowball.

	Weight (g)	Width (cm)	Length (cm)	Peel thickness (cm)
Haruka	331.49 ± 29.46	10.63 ± 0.38	10.09 ± 0.42	0.90 ± 0.09
Kiyomi	250.69 ± 18.83	9.39 ± 0.39	8.92 ± 0.37	0.68 ± 0.12
Yellowball	273.74 ± 15.47	9.76 ± 0.60	9.32 ± 0.37	0.44 ± 0.03

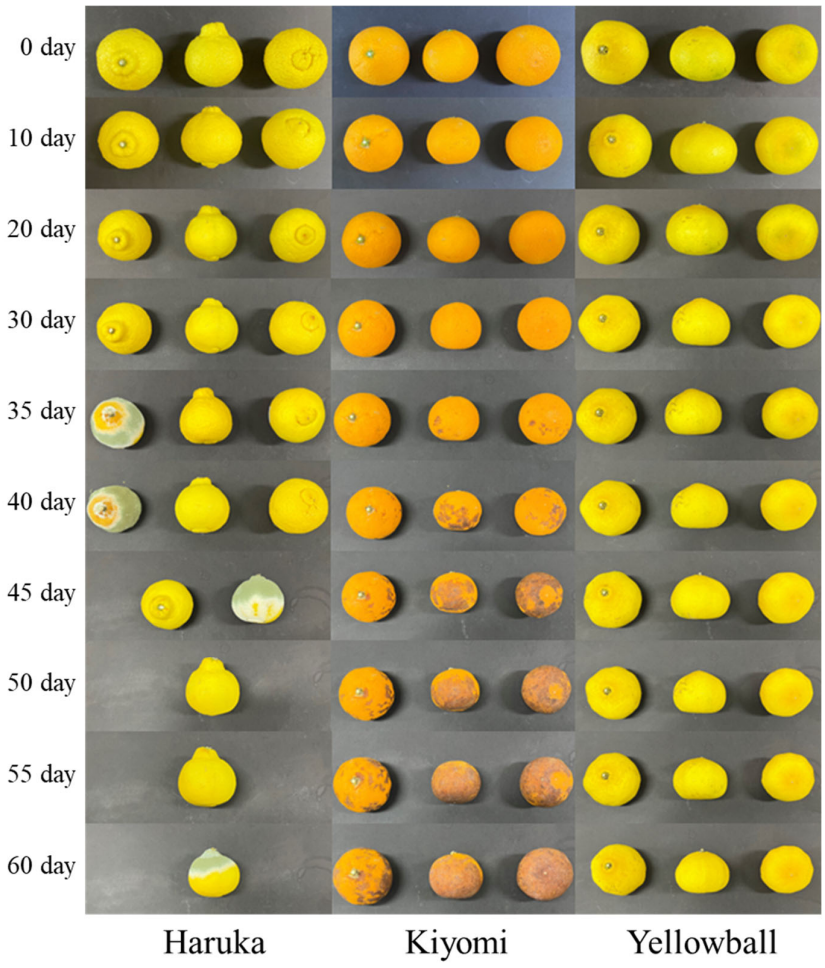

Figure S1. Appearance changes in Haruka, Kiyomi, and Yellowball during storage for 60 days at 25 °C.

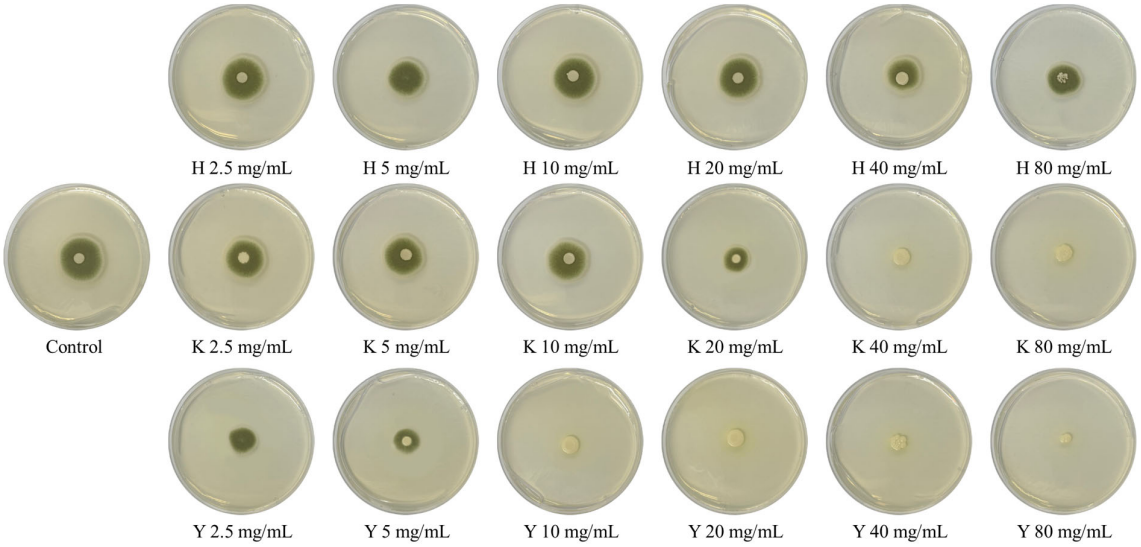

Figure S2. Growth inhibition test of peel extracts on citrus green mold (*Penicillium digitatum*) at different concentration (2.5–80 mg/mL). H, haruka; K, Kiyomi; Y, Yellowball.

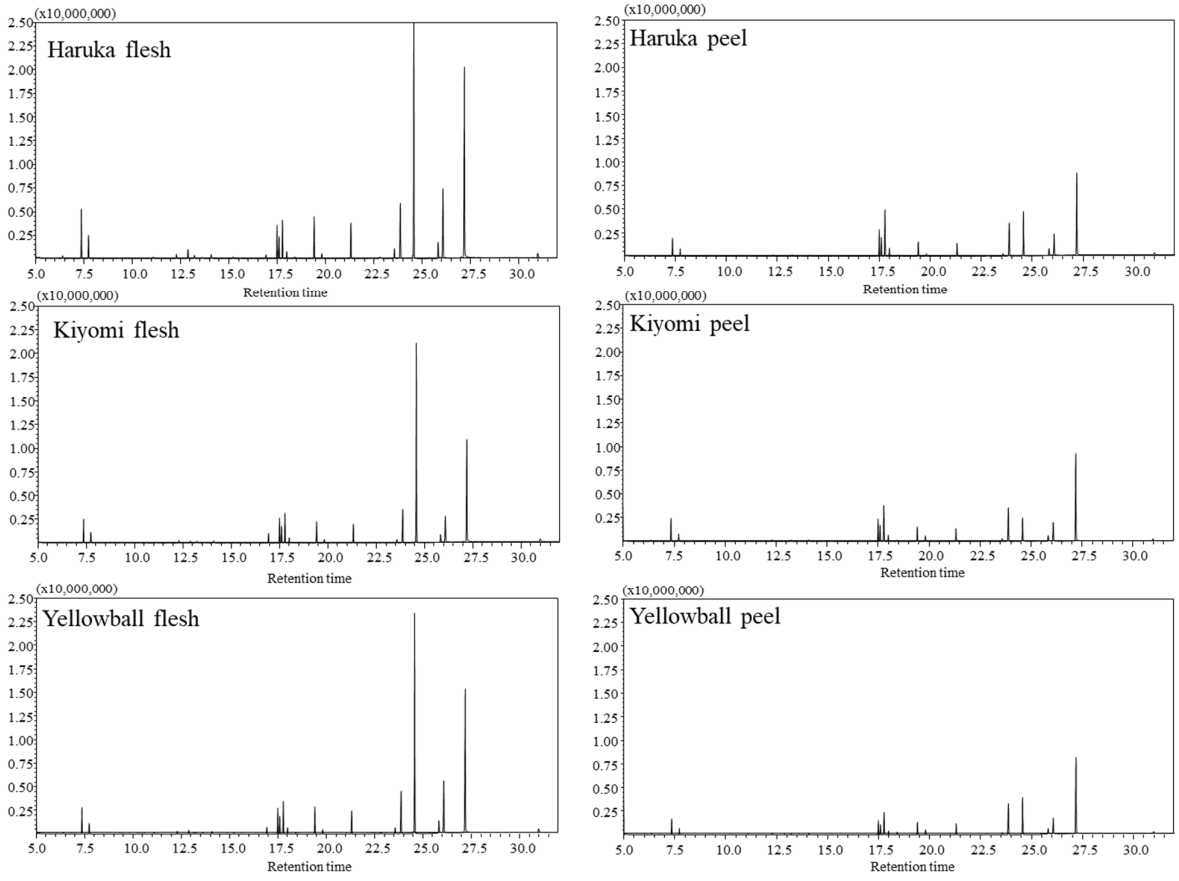

Figure S3. Representative chromatograms of citrus metabolites analyzed by GC-MS.

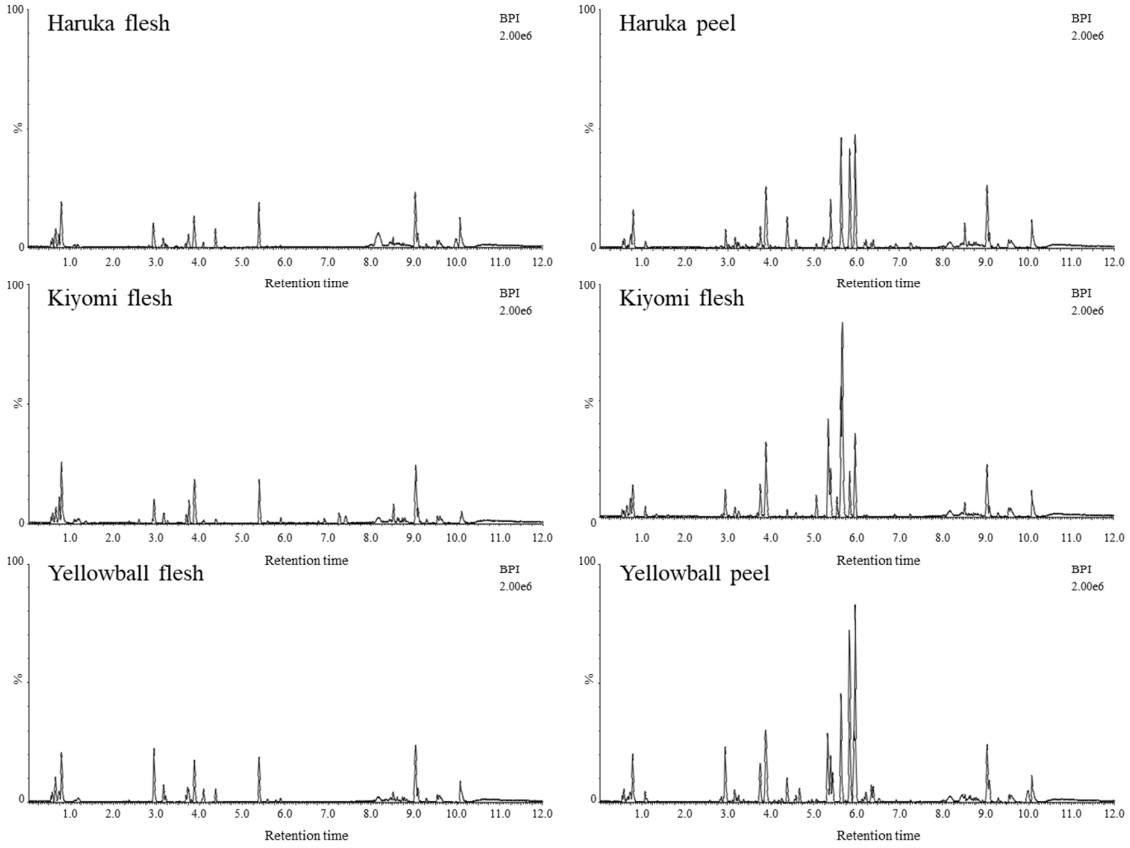

Figure S4. Representative chromatograms of citrus metabolites analyzed by UPLC-Q-TOF MS.

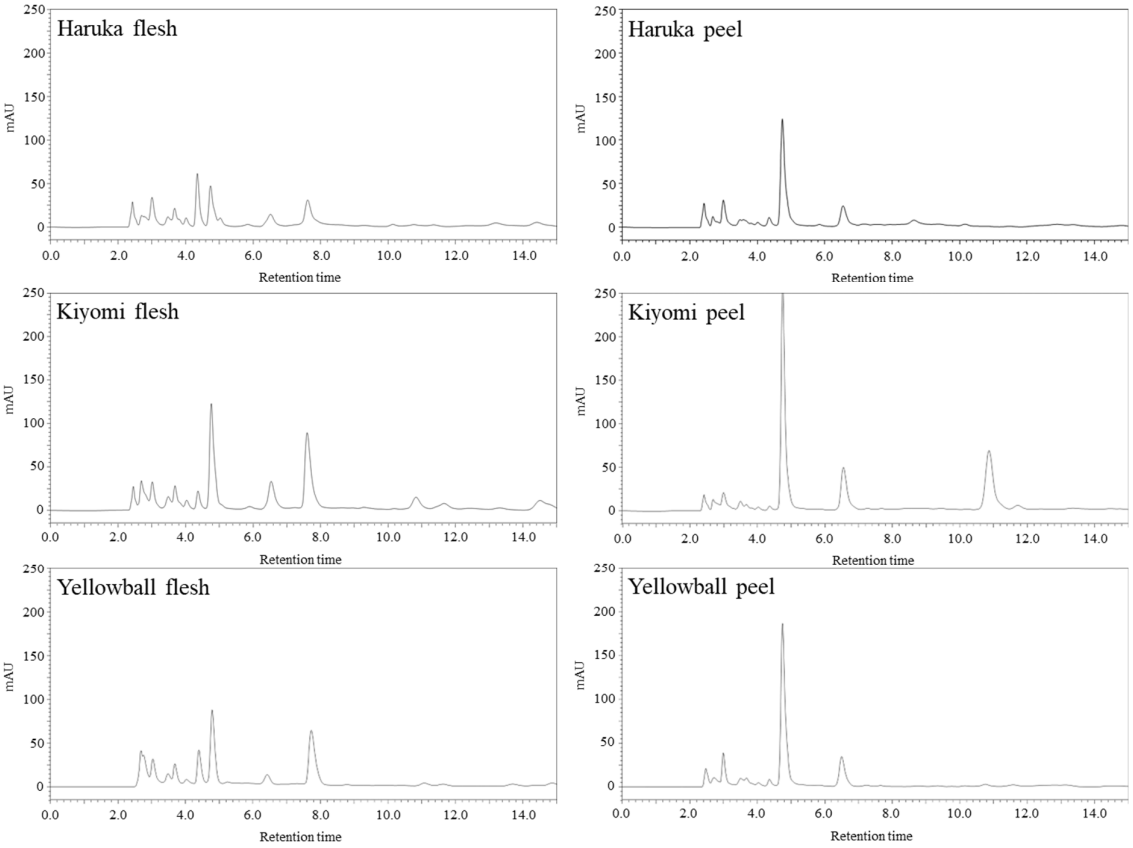

Figure S5. Representative chromatograms of organic acids analyzed by HPLC at 220 nm.

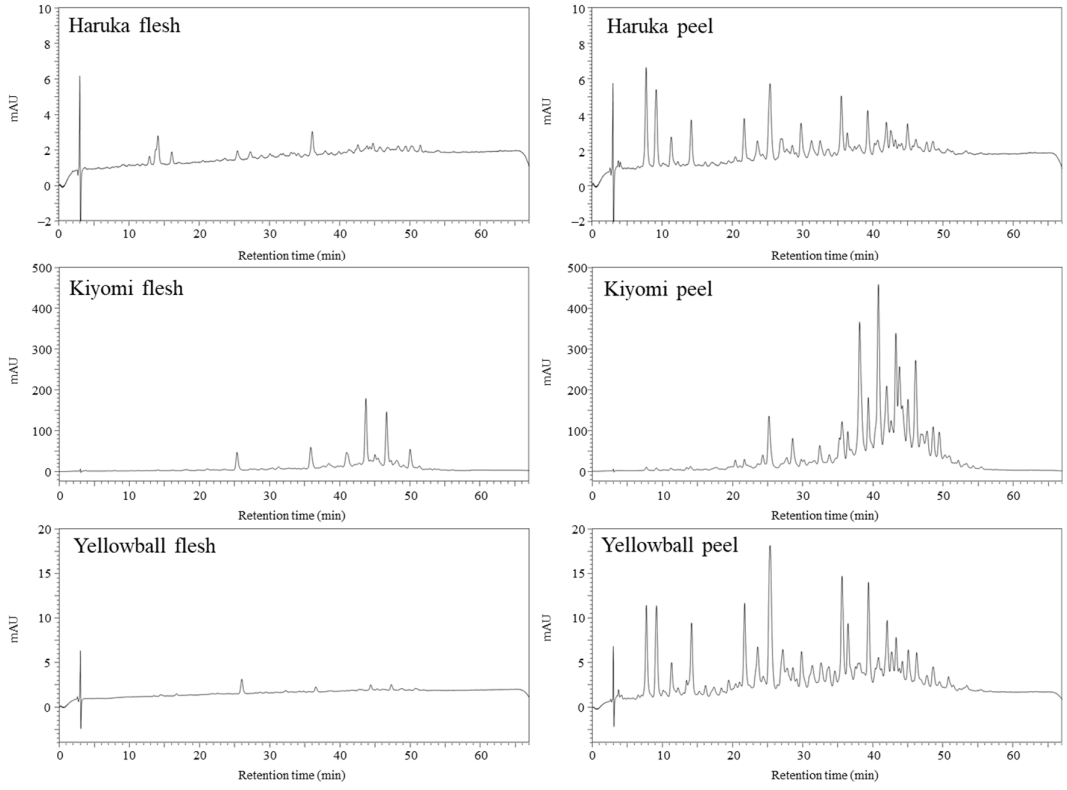

Figure S6. Representative chromatograms of carotenoids analyzed by HPLC at 450 nm.

Table S2. Identification of major metabolites by GC-MS.

RT	Compounds	RI	VIP	*p*-value
6.34	glycine	1051	1.21	2.45×10^{-2}
10.22	proline	1293	0.94	1.54×10^{-6}
13.48	4-aminobutanoic acid	1525	1.32	1.10×10^{-10}
15.21	aspartic acid	1663	1.04	1.29×10^{-8}
17.34	quinic acid	1846	1.24	7.17×10^{-20}
17.49	fructose	1860	1.16	3.90×10^{-5}
17.77	glucose	1885	1.35	7.10×10^{-7}
18.14	methyl galactoside	1920	1.06	2.17×10^{-19}
19.41	palmitic acid	2022	0.81	2.32×10^{-10}
19.80	*myo*-inositol	2042	1.25	8.03×10^{-13}
21.30	stearic acid	2240	0.84	6.09×10^{-12}
24.51	oleic acid	2615	1.31	1.09×10^{-14}
24.57	sucrose	2622	1.21	8.29×10^{-30}

RT, retention time; RI, retention indices; VIP, variable importance in the projection.
p-Values were analyzed by Duncan's test.

Table S3. Identification of major metabolites by UPLC-Q-TOF MS.

RT	Compounds	Exact mass (M+H)	MS fragment	VIP	*p*-value
0.64	arginine	175.1181	70, 158, 116	1.27	6.60×10^{-28}
0.78	stachydrine	144.1010	116, 184, 70, 102, 58	1.15	6.02×10^{-15}
2.59	phenylalanine	166.0847	120, 103	1.39	2.22×10^{-14}
2.90	tryptophan	205.0959	188, 188, 144, 170	1.19	3.98×10^{-22}
2.93	feruloyl putrescine	265.1533	177, 145	1.81	2.19×10^{-23}
3.03	luteolin-3'-7'-diglucoside	611.1608	163, 593, 575, 325	0.90	1.41×10^{-8}
3.16	saponarin	595.1664	577, 475	1.33	1.91×10^{-4}
3.21	apigenin-7-rutinoside-4'-glucoside	741.2250	595, 433, 271, 377, 653	0.96	3.15×10^{-4}
3.48	apioside	565.1550	433, 415, 313, 521	1.31	2.36×10^{-2}
3.68	zapoterin	471.2016	425, 95	1.19	1.55×10^{-6}
3.72	apigenin-7-rutinoside	579.1719	271, 433, 519	1.77	7.64×10^{-15}
3.75	narirutin	581.1875	273, 419, 119	0.96	1.19×10^{-15}
3.88	hesperidin	611.1973	303, 449, 177	0.93	4.86×10^{-18}
4.09	xylogranatin K	515.2287	496, 409	1.50	5.87×10^{-10}
4.37	didymin	595.2021	287, 433, 559	1.19	3.53×10^{-12}
4.58	cyclonatsudamine A	728.3989	615, 587, 502, 474	0.95	2.81×10^{-7}
4.67	natsudaidain derivatives (natsudaidain 3-(4-O-3-hydroxy-3-methylglutaroylglucoside))	725.2313	419	1.05	2.97×10^{-13}
4.73	monohydroxy tetramethoxyflavone	359.1125	184	0.88	5.36×10^{-8}
5.06	isosinensetin	373.1276	343, 358	1.08	4.13×10^{-28}
5.33	sinensetin	373.1269	343, 358	1.09	4.13×10^{-25}
5.63	nobiletin	403.1379	373, 355	0.94	1.04×10^{-25}
5.66	tetramethoxyflavone	343.1163	313, 282, 299, 281	1.08	9.13×10^{-23}
5.83	heptamethoxyflavone	433.1489	403, 385, 418	0.97	4.90×10^{-34}
5.88	monohydroxy tetramethoxyflavone	359.1123	184, 326	1.03	6.07×10^{-16}
5.89	phytosphingosine	318.3003	184, 282	1.12	5.03×10^{-16}
5.93	natsudaidain	419.1335	184, 389, 371	1.17	5.29×10^{-38}
5.96	tangeretin	373.1275	343, 358	0.92	1.17×10^{-29}
6.17	monohydroxy pentamethoxyflavone-1	389.1235	359	1.00	7.52×10^{-9}
6.21	heptamethoxyflavone	403.1398	184, 373, 355	1.13	1.96×10^{-22}
6.34	monohydroxy pentamethoxyflavone-2	389.1237	359, 374, 356, 341	1.09	3.43×10^{-29}
6.38	5-hydroxy-3,6,7,8,3',4'-hexamethoxyflavone	419.1335	184, 389, 371	1.08	6.06×10^{-26}
6.90	LPE(C18:2)	478.2943	155, 337, 98, 460	1.46	2.14×10^{-10}
6.92	LPC(C18:2)	520.3410	337, 478, 104	1.16	1.39×10^{-4}
7.24	LPE(C16:0)	454.2945	184, 104, 125	1.58	1.12×10^{-18}
7.27	LPC(C16:0)	496.3406	184, 104, 125	1.49	2.20×10^{-12}
7.39	LPE(C18:1)	480.3086	155, 337, 98, 460	1.40	4.30×10^{-12}
7.41	LPC(C18:1)	522.3572	339, 341, 313, 104, 504	1.28	2.99×10^{-9}
8.63	pheophorbide A	593.2772	184	0.89	2.61×10^{-7}
9.98	cholesteryl acetate	429.3728	165, 205, 164, 219	1.23	6.61×10^{-5}

RT, retention time; VIP, variable importance in the projection; LPE, lysophosphatidylethanolamine; LPC, lysophosphatidylcholine.

p-Values were analyzed by Duncan's test.

Table S4. Identification of major metabolites by HPLC.

	RT	Compounds	λ_{max} (nm)	VIP	*p*-value
Organic acid	3.1	oxalic acid		1.39	7.11×10^{-7}
	3.5	tartaric acid		1.12	1.68×10^{-21}
	4.4	malic acid		1.59	1.73×10^{-37}
	4.8	ascorbic acid		1.04	2.64×10^{-29}
	5.4	lactic acid		1.01	6.13×10^{-5}
	5.7	acetic acid		1.45	1.68×10^{-13}
	7.7	maleic acid		1.01	3.94×10^{-25}
	7.8	citric acid		1.30	5.90×10^{-39}
	8.8	succinic acid		1.35	1.22×10^{-19}
Carotenoids	9.1	violaxanthin	421, 448	0.77	2.05×10^{-7}
	11.2	neoxanthin	436, 464	0.70	2.35×10^{-7}
	13.4	lutein	400, 422	0.92	8.33×10^{-8}
	14.1	zeaxanthin	422	0.84	7.98×10^{-5}
	25.3	β-cryptoxanthin	451, 477	1.09	4.83×10^{-8}
	35.6	*α*-carotene	446, 474	0.87	4.38×10^{-5}
	38.1	β-carotene	436, 464	1.00	3.98×10^{-14}
	39.3	9-*cis*-β-carotene	439, 469	0.84	1.79×10^{-4}

RT, retention time; VIP, variable importance in the projection.
p-Values were analyzed by Duncan's test.