

Supplementary Information

Metabolic Profiling of Absciscic Acid, Ascorbate, and Phenolic Compounds across Strawberry Fruit Development

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Table S1. Complementary correlation analysis between key metabolites from strawberry

Compound	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
1	1.00	0.22	0.20	0.60	0.73	0.47	0.58	0.50	0.41	0.43	0.40	0.31	0.64	0.42	0.45	0.40	0.44	-0.02	0.18	-0.38	-0.70	-0.42	-0.37
2	0.22	1.00	0.88	0.75	0.81	0.86	0.88	0.82	0.91	0.90	0.96	0.97	-0.52	-0.67	-0.65	-0.72	-0.69	-0.88	-0.58	0.18	-0.63	-0.40	-0.51
3	0.20	0.88	1.00	0.74	0.74	0.83	0.83	0.59	0.73	0.75	0.78	0.79	-0.52	-0.67	-0.66	-0.72	-0.66	-0.79	-0.44	0.44	-0.42	-0.06	-0.17
4	0.60	0.75	0.74	1.00	0.87	0.81	0.83	0.72	0.67	0.68	0.78	0.74	-0.19	-0.40	-0.36	-0.42	-0.35	-0.53	-0.08	0.02	-0.65	-0.36	-0.25
5	0.73	0.81	0.74	0.87	1.00	0.89	0.96	0.85	0.86	0.87	0.89	0.85	0.01	-0.21	-0.18	-0.26	-0.22	-0.61	-0.30	-0.07	-0.83	-0.50	-0.55
6	0.47	0.86	0.83	0.81	0.89	1.00	0.94	0.79	0.79	0.81	0.86	0.84	-0.26	-0.40	-0.36	-0.45	-0.45	-0.66	-0.29	0.10	-0.72	-0.40	-0.46
7	0.58	0.88	0.83	0.83	0.96	0.94	1.00	0.80	0.88	0.89	0.90	0.88	-0.14	-0.32	-0.30	-0.39	-0.38	-0.68	-0.44	0.11	-0.75	-0.38	-0.51
8	0.50	0.82	0.59	0.72	0.85	0.79	0.80	1.00	0.91	0.89	0.93	0.91	-0.13	-0.28	-0.23	-0.32	-0.28	-0.68	-0.34	-0.35	-0.92	-0.81	-0.81
9	0.41	0.91	0.73	0.67	0.86	0.79	0.88	0.91	1.00	0.97	0.96	0.96	-0.25	-0.38	-0.36	-0.45	-0.42	-0.80	-0.63	-0.07	-0.81	-0.59	-0.74
10	0.43	0.90	0.75	0.68	0.87	0.81	0.89	0.89	0.97	1.00	0.95	0.94	-0.23	-0.36	-0.34	-0.43	-0.38	-0.82	-0.59	-0.02	-0.80	-0.55	-0.71
11	0.40	0.96	0.78	0.78	0.89	0.86	0.90	0.93	0.96	0.95	1.00	0.98	-0.32	-0.50	-0.46	-0.54	-0.50	-0.84	-0.49	-0.03	-0.81	-0.58	-0.65
12	0.31	0.97	0.79	0.74	0.85	0.84	0.88	0.91	0.96	0.94	0.98	1.00	-0.41	-0.55	-0.52	-0.61	-0.57	-0.84	-0.59	-0.01	-0.75	-0.57	-0.67
13	0.64	-0.52	-0.52	-0.19	0.01	-0.26	-0.14	-0.13	-0.25	-0.23	-0.32	-0.41	1.00	0.91	0.91	0.92	0.91	0.57	0.44	-0.47	-0.18	-0.13	-0.09
14	0.42	-0.67	-0.67	-0.40	-0.21	-0.40	-0.32	-0.28	-0.38	-0.36	-0.50	-0.55	0.91	1.00	0.99	0.98	0.93	0.73	0.39	-0.50	-0.03	-0.09	-0.07
15	0.45	-0.65	-0.66	-0.36	-0.18	-0.36	-0.30	-0.23	-0.36	-0.34	-0.46	-0.52	0.91	0.99	1.00	0.99	0.93	0.72	0.43	-0.55	-0.09	-0.15	-0.10
16	0.40	-0.72	-0.72	-0.42	-0.26	-0.45	-0.39	-0.32	-0.45	-0.43	-0.54	-0.61	0.92	0.98	0.99	1.00	0.96	0.75	0.50	-0.53	0.00	-0.08	-0.02
17	0.44	-0.69	-0.66	-0.35	-0.22	-0.45	-0.38	-0.28	-0.42	-0.38	-0.50	-0.57	0.91	0.93	0.93	0.96	1.00	0.65	0.54	-0.56	-0.03	-0.10	-0.01
18	-0.02	-0.88	-0.79	-0.53	-0.61	-0.66	-0.68	-0.68	-0.80	-0.82	-0.84	-0.84	0.57	0.73	0.72	0.75	0.65	1.00	0.60	-0.27	0.48	0.28	0.43
19	0.18	-0.58	-0.44	-0.08	-0.30	-0.29	-0.44	-0.34	-0.63	-0.59	-0.49	-0.59	0.44	0.39	0.43	0.50	0.54	0.60	1.00	-0.30	0.15	0.11	0.44
20	-0.38	0.18	0.44	0.02	-0.07	0.10	0.11	-0.35	-0.07	-0.02	-0.03	-0.01	-0.47	-0.50	-0.55	-0.53	-0.56	-0.27	-0.30	1.00	0.47	0.80	0.58
21	-0.70	-0.63	-0.42	-0.65	-0.83	-0.72	-0.75	-0.92	-0.81	-0.80	-0.81	-0.75	-0.18	-0.03	-0.09	0.00	-0.03	0.48	0.15	0.47	1.00	0.82	0.82
22	-0.42	-0.40	-0.06	-0.36	-0.50	-0.40	-0.38	-0.81	-0.59	-0.55	-0.58	-0.57	-0.13	-0.09	-0.15	-0.08	-0.10	0.28	0.11	0.80	0.82	1.00	0.88
23	-0.37	-0.51	-0.17	-0.25	-0.55	-0.46	-0.51	-0.81	-0.74	-0.71	-0.65	-0.67	-0.09	-0.07	-0.10	-0.02	-0.01	0.43	0.44	0.58	0.82	0.88	1.00

1: abscisic acid (ABA), 2: epicatechin epicatechin catechin, 3: ellagic acid 2-rhamnose, 4: rutin, 5: glycosylated abscisic acid (ABA-GE), 6: phaseic acid (PA), 7: dihydrophaseic acid (DPA), 8: hydroxybenzoic acid, 9: epigallocatechin catechin, 10: ellagic acid, 11: catechin, 12: epicatechin, 13: methylsyringin, 14: eriodictyol 7-*O*-glucoside, 15: apigenin, 16: pelargonidin 3-*O*-rutinoside, 17: apigenin 4-glucoside, 18: pelargonidin 3-glucoside, 19: luteolin 3-glucuronide, 20: kaempferol 3-*O*-acetylglucoside, 21: *L*-ascorbic acid (AsA), 22: cyanidin 3-(6'-malonylglucoside), 23: quercetin 4-glucuronide.

Table S2. *p*-Values from the correlation analysis between key metabolites from strawberry

Compound	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
1	NA	0.2724	0.3124	0.0010	0.0000	0.0143	0.0015	0.0074	0.0343	0.0257	0.0381	0.1131	0.0002	0.0312	0.0183	0.0383	0.0201	0.9299	0.3623	0.0534	0.0000	0.0274	0.0557
2	0.2724	NA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0050	0.0001	0.0002	0.0000	0.0000	0.0000	0.0015	0.3741	0.0003	0.0397	0.0066
3	0.3124	0.0000	NA	0.0000	0.0000	0.0000	0.0000	0.0013	0.0000	0.0000	0.0000	0.0000	0.0054	0.0001	0.0001	0.0000	0.0001	0.0000	0.0217	0.0218	0.0277	0.7630	0.3960
4	0.0010	0.0000	0.0000	NA	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.3506	0.0394	0.0659	0.0281	0.0731	0.0046	0.6915	0.9203	0.0002	0.0624	0.2003
5	0.0000	0.0000	0.0000	0.0000	NA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9569	0.2969	0.3803	0.1940	0.2761	0.0008	0.1277	0.7402	0.0000	0.0081	0.0031
6	0.0143	0.0000	0.0000	0.0000	0.0000	NA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1978	0.0364	0.0622	0.0185	0.0171	0.0002	0.1468	0.6144	0.0000	0.0397	0.0157
7	0.0015	0.0000	0.0000	0.0000	0.0000	0.0000	NA	0.0000	0.0000	0.0000	0.0000	0.0000	0.4803	0.0996	0.1284	0.0438	0.0520	0.0001	0.0224	0.5864	0.0000	0.0494	0.0067
8	0.0074	0.0000	0.0013	0.0000	0.0000	0.0000	0.0000	NA	0.0000	0.0000	0.0000	0.0000	0.5241	0.1513	0.2421	0.1029	0.1580	0.0000	0.0816	0.0729	0.0000	0.0000	0.0000
9	0.0343	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	NA	0.0000	0.0000	0.0000	0.2135	0.0504	0.0653	0.0180	0.0279	0.0000	0.0004	0.7440	0.0000	0.0011	0.0000
10	0.0257	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	NA	0.0000	0.0000	0.2490	0.0647	0.0830	0.0263	0.0492	0.0000	0.0011	0.9185	0.0000	0.0028	0.0000
11	0.0381	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	NA	0.0000	0.1040	0.0081	0.0145	0.0036	0.0086	0.0000	0.0100	0.8727	0.0000	0.0016	0.0002
12	0.1131	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	NA	0.0352	0.0030	0.0050	0.0007	0.0018	0.0000	0.0011	0.9483	0.0000	0.0019	0.0001
13	0.0002	0.0050	0.0054	0.3506	0.9569	0.1978	0.4803	0.5241	0.2135	0.2490	0.1040	0.0352	NA	0.0000	0.0000	0.0000	0.0000	0.0018	0.0202	0.0127	0.3613	0.5339	0.6432
14	0.0312	0.0001	0.0001	0.0394	0.2969	0.0364	0.0996	0.1513	0.0504	0.0647	0.0081	0.0030	0.0000	NA	0.0000	0.0000	0.0000	0.0000	0.0420	0.0077	0.8740	0.6473	0.7344
15	0.0183	0.0002	0.0001	0.0659	0.3803	0.0622	0.1284	0.2421	0.0653	0.0830	0.0145	0.0050	0.0000	0.0000	NA	0.0000	0.0000	0.0000	0.0235	0.0030	0.6576	0.4564	0.6130
16	0.0383	0.0000	0.0000	0.0281	0.1940	0.0185	0.0438	0.1029	0.0180	0.0263	0.0036	0.0007	0.0000	0.0000	0.0000	NA	0.0000	0.0000	0.0078	0.0048	0.9838	0.7001	0.9179
17	0.0201	0.0000	0.0001	0.0731	0.2761	0.0171	0.0520	0.1580	0.0279	0.0492	0.0086	0.0018	0.0000	0.0000	0.0000	0.0000	NA	0.0002	0.0036	0.0025	0.8858	0.6040	0.9778
18	0.9299	0.0000	0.0000	0.0046	0.0008	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0018	0.0000	0.0000	0.0000	0.0002	NA	0.0009	0.1715	0.0113	0.1595	0.0255
19	0.3623	0.0015	0.0217	0.6915	0.1277	0.1468	0.0224	0.0816	0.0004	0.0011	0.0100	0.0011	0.0202	0.0420	0.0235	0.0078	0.0036	0.0009	NA	0.1278	0.4444	0.5846	0.0216
20	0.0534	0.3741	0.0218	0.9203	0.7402	0.6144	0.5864	0.0729	0.7440	0.9185	0.8727	0.9483	0.0127	0.0077	0.0030	0.0048	0.0025	0.1715	0.1278	NA	0.0127	0.0000	0.0014
21	0.0000	0.0003	0.0277	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3613	0.8740	0.6576	0.9838	0.8858	0.0113	0.4444	0.0127	NA	0.0000	0.0000
22	0.0274	0.0397	0.7630	0.0624	0.0081	0.0397	0.0494	0.0000	0.0011	0.0028	0.0016	0.0019	0.5339	0.6473	0.4564	0.7001	0.6040	0.1595	0.5846	0.0000	0.0000	NA	0.0000
23	0.0557	0.0066	0.3960	0.2003	0.0031	0.0157	0.0067	0.0000	0.0000	0.0000	0.0002	0.0001	0.6432	0.7344	0.6130	0.9179	0.9778	0.0255	0.0216	0.0014	0.0000	0.0000	NA

1: abscisic acid (ABA), 2: epicatechin epicatechin catechin, 3: ellagic acid 2-rhamnose, 4: rutin, 5: glycosylated abscisic acid (ABA-GE), 6: phaseic acid (PA), 7: dihydrophaseic acid (DPA), 8: hydroxybenzoic acid, 9: epigallocatechin catechin, 10: ellagic acid, 11: catechin, 12: epicatechin, 13: methylsyringin, 14: eriodictyol 7-*O*-glucoside, 15: apigenin, 16: pelargonidin 3-*O*-rutinoside, 17: apigenin 4-glucoside, 18: pelargonidin 3-glucoside, 19: luteolin 3-glucuronide, 20: kaempferol 3-*O*-acetylglucoside, 21: *L*-ascorbic acid (AsA), 22: cyanidin 3-(6'-malonylglucoside), 23: quercetin 4-glucuronide; NA: not applicable.

Table S3. Detailed information on the identified compounds

Compound	Ionization mode	Molecular formula	t _R / min	Theoretical mass	Experimental mass	Error / ppm	mSigma	MS/MS fragments	CE / eV
4-Hydroxybenzoic acid/salicylic acid	[M – H] [–]	C ₇ H ₆ O ₃	8.77	137.02	137.02	1.60	6.20	93.03	16.90
(–)-Epicatechin	[M – H] [–]	C ₁₅ H ₁₄ O ₆	6.44	289.07	289.07	–0.30	39.30	109.03	24.50
Catechin	[M – H] [–]	C ₁₅ H ₁₄ O ₆	4.60	289.07	289.07	–1.70	8.90	109.0290; 125.0230; 123.0438; 203.0717; 151.0396	24.50
Cyanidin-3-(6''-malonylglucoside)	[M] ⁺	C ₂₄ H ₂₃ O ₁₄ ⁺	8.03	535.11	535.11	–0.90	47.10	287.06	36.10
Ellagic acid	[M – H] [–]	C ₁₄ H ₆ O ₈	7.50	301.00	301.00	0.50	38.10	301.00	25.00
Epicatechin-(4β→6)-epicatechin-(4β→8)-catechin	[M – H] [–]	C ₄₅ H ₃₈ O ₁₈	6.60	865.20	865.20	0.60	99.00	125.0238; 289.0720; 287.0565	46.00
Eriodictyol 7-glucoside/Taxifolin 3-rhamnoside	[M – H] [–]	C ₂₁ H ₂₂ O ₁₁	6.76	449.11	449.11	0.30	31.40	not matched	n.f.
Kaempferol 3-(<i>p</i> -coumaroyl-glucoside)	[M – H] [–]	C ₃₀ H ₂₆ O ₁₃	8.77	593.13	593.13	0.90	9.30	285.04	37.80
Kaempferol 3- <i>O</i> -acetyl-glucoside/queracetin 3- <i>O</i> -acetyl-rhamnoside	[M – H] [–]	C ₂₃ H ₂₂ O ₁₂	8.05	489.10	489.10	1.10	28.90	285.04	34.50
Luteolin	[M – H] [–]	C ₁₅ H ₁₀ O ₆	9.83	285.04	285.04	1.80	5.70	not matched	n.f.
Luteolin 3'-glucuronide/kaempferol 3-glucuronide	[M – H] [–]	C ₂₁ H ₁₈ O ₁₂	7.85	461.07	461.07	0.50	28.70	258.04	33.10
Octadecadienoic acid	[M – H] [–]	C ₁₈ H ₃₂ O ₂	19.61	279.23	279.23	1.70	21.20	not matched	n.f.
<i>p</i> -Coumaric acid	[M – H] [–]	C ₉ H ₈ O ₃	7.13	163.04	163.04	0.50	6.20	not matched	n.f.
Pelargonidin 3-glucoside	[M] ⁺	C ₂₁ H ₂₁ O ₁₀	6.29	433.11	433.11	–1.10	1.80	271.06	31.70
Pelargonidin-3- <i>O</i> -rutinoside	[M] ⁺	C ₂₇ H ₃₁ O ₁₄	6.54	579.17	579.17	–1.10	12.00	271.06	37.40
Phloridzin	[M – H] [–]	C ₂₁ H ₂₄ O ₁₀	7.72	435.13	435.13	–0.10	43.90	315.09	27.10
Quercetin 4'-glucuronide	[M – H] [–]	C ₂₁ H ₁₈ O ₁₃	7.47	477.07	477.07	–1.00	47.60	301.03	29.00

n.f.: no fragments observed in MS/MS experiment; CE: collision energy.

