

Supplementary material:

Table S1. Metabolites derived from GC-MS and LC-MS/MS.

Nob	RT (min)	Metabolites	$m/z[M + H]^+$	Main Fragments	References
Amino Acids and Amines					
1	4.22	Alanine ^a	--	147, 73, 116, 79	STD and NIST
2	6.43	Acetamide ^a	--	220, 73, 79, 58, 147	NIST
3	6.57	Valine ^a	--	144, 73, 147, 79	STD and NIST
4	1.86	Leucine ^b	132	86, 55	Ref 57
5	8.73	proline ^a	--	73, 142, 79, 158, 52	STD and NIST
6	9.05	Glycine ^a	--	248, 174, 73, 79, 147,	STD and NIST
7	10.89	Serine ^a	--	100, 147, 204, 218	STD and NIST
8	11.81	Threonine ^a	--	73, 79, 117, 147	STD and NIST
9	12.97	Lysine ^a	--	290, 73, 174, 147, 79	NIST
10	16.46	Aspartic Acid ^a	--	232, 73, 147, 100, 156	STD and NIST
11	16.55	GABA ^a	--	304, 174, 73, 147, 86	STD and NIST
12	9.98	Glutamic Acid ^a	--	246, 73, 147, 128, 192	STD and NIST
13	23.81	1,4 -Butanediamine ^a	--	174, 73, 59	NIST
14	25.32	Glutamine ^a	--	147, 84, 102, 130	STD and NIST
15	1.39	Isoleucine ^b	132	86, 55	Ref 57
16	1.11	Arginine ^b	175	116, 60	Ref 57
17	6.13	Tryptamine ^b	161	144, 117, 91, 65	Ref 57
18	1.35	Tyramine ^b	138	121, 103	Ref 57
19	1.82	Tyrosine ^b	182	91, 136, 119	Ref 57
20	1.87	Methionine ^b	150	61, 104, 75, 81, 54	Ref 567
21	2.96	Phenylalanine ^b	166	120, 103, 93, 72	Ref 57
22	5.67	Tryptophan ^b	205	146, 118, 188	Ref 57
Sugars and Sugar Alcohols					
23	29.28	Fructose ^a	--	217, 103, 147, 133	STD and NIST
24	30.13	Glucose ^a	--	217, 147, 191, 204	STD and NIST
25	52.89	Sucrose ^a	--	361, 73, 103, 147, 217	STD and NIST
26	30.72	Sorbose ^a	--	319, 73, 147, 205, 103,	STD and NIST
27	23.17	Ribitol ^a	--	217, 73, 103, 147	NIST
28	28.03	Sorbitol ^a	--	259, 73, 147, 190, 129,	NIST
29	29.90	Mannose ^a	--	319, 73, 147, 103, 160,	NIST
30	35.99	Glycoside ^a	--	319, 73, 204, 147, 103,	NIST
31	52.43	Fucose ^a	--	333, 73, 117, 147, 219	NIST
32	52.19	Mannobiose ^a	--	361, 73, 204, 147, 129,	NIST
33	33.70	Glucopyranose ^a	--	217, 73, 191, 147, 129	NIST
34	27.24	Fructopyranose ^a	--	217, 73, 204, 147	NIST
35	29.85	Talopyranose ^a	--	73, 204, 191, 147, 217	NIST
36	26.99	Tagatofuranose ^a	--	257, 73, 217, 147	NIST
37	21.86	Xylose ^a	--	147, 91, 204, 217	NIST
38	38.44	Myo-Inositol ^a	--	147, 217, 305, 308	NIST
Organic Acids and Fatty Acids					
39	15.37	Malic Acid ^a	--	189, 113, 175, 219	STD and NIST
40	14.69	Citramalic Acid ^a	--	247, 73, 75, 115, 147	STD and NIST
41	9.17	Succinic Acid ^a	--	249, 147, 73, 75, 79, 58	STD and NIST
42	10.23	Fumaric Acid ^a	--	127, 71, 69, 99, 56	STD and NIST
43	27.20	Citrus Acid ^a	--	347, 73, 147, 273	STD and NIST
44	28.75	Quinic Acid ^a	--	345, 73, 147, 75, 55	STD and NIST
45	19.64	Tartaric Acid ^a	--	292, 73, 147, 117	STD and NIST
46	27.89	2-ketoglutaric Acid ^a	--	245, 73, 147, 173, 55	NIST
47	34.76	Hexadecanoic Acid ^a	--	313, 73, 117, 132, 55	NIST

48	31.87	Glucuronic Acid ^a	--	333, 73, 147, 160, 189	NIST
49	46.49	Octadecanoic Acid ^a	--	341, 73, 117, 129, 55	NIST
50	47.96	9,12,15-Octadecatrienoic Acid ^a	--	319, 73, 147, 93, 207	NIST
51	10.82	2-Piperidinecarboxylic Acid ^a	--	156, 73, 79, 147	NIST
52	4.49	Oxalic Acid ^a	--	147, 73, 133	STD and NIST
53	18.23	Threonic Acid ^a	--	292, 73, 147, 220, 117	NIST
Betalains and Betalain Precursors					
54	4.53	Betain ^b	551	389	Ref. 1
55	5.94	Isobetain ^b	551	188, 389	Ref. 1
56	6.52	Phyllocatin ^b	637	593, 551, 389	Ref. 58
57	13.06	Betalamic Acid ^b	212,	168, 194, 105	Ref. 1
58	8.89	Hylocerin ^b	695	651, 551, 389	Ref. 58
59	8.97	Quercetin 3-O-rutinoside ^b	611	303, 465	Ref. 57
60	17.43	Cyclo-5-O-glucoside ^b	358	340, 106, 88, 70, 57	Ref. 1
Other Metabolites					
61	7.91	H ₃ PO ₄ ^a	--	186, 174, 73, 147, 100,	NIST
62	18.95	Butane ^a	--	306, 73, 117, 147, 205	NIST
63	10.06	Vebronol ^b	453	322, 209, 114	Ref. 59
64	18.14	Sespendole ^b	520	184	Ref. 59
65	18.04	Vapiprost ^b	478	337	Ref. 59

Note: Metabolites ^(a), Metabolites derived from GC-MS. Metabolites ^(b), Metabolites derived from LC-MS/MS. STD, standard compound. Ref, reference. --, Data unlisted.

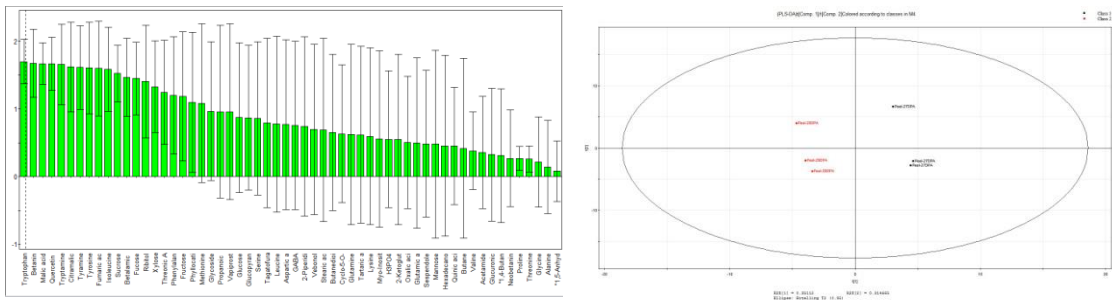


Figure S1. Peel-29DPA vs. Peel-27DPA.

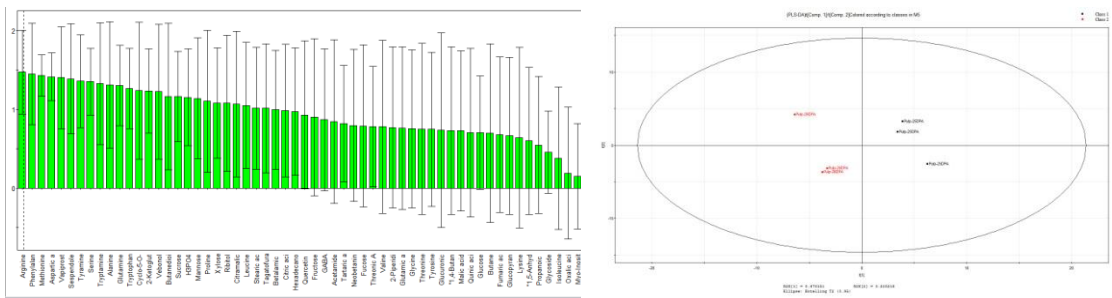


Figure S2. Pulp-26DPA vs. Pulp-25DPA.

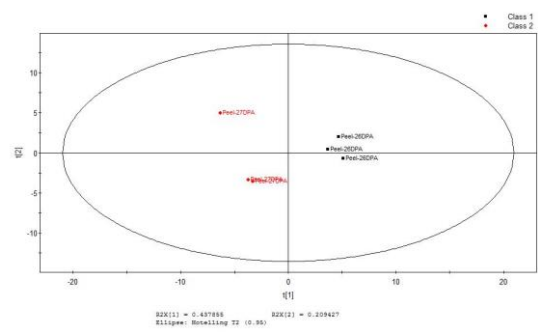
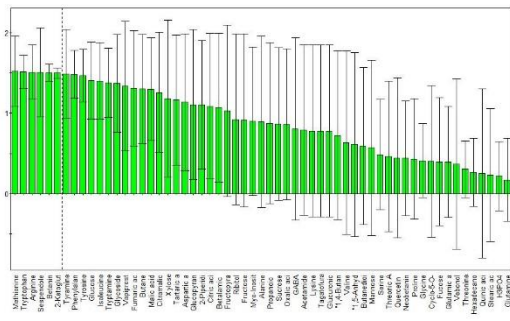


Figure S3. Pulp-26DPA vs. Pulp-27DPA.