

Table S1. Concentrations ($\mu\text{g}\cdot\text{g}^{-1}$ FW) of the major polar metabolites detected in leaves of C2-5-12 Pummelo (*Citrus maxima*), *C. latipes*, and three corresponding sexual hybrids after derivatization with TMS and using gas chromatography-mass spectrometry ($n=4$)^z.

Peak No.	TMS Metabolite ^y	<i>Citrus maxima</i>	<i>Citrus latipes</i>	Hybrid 1	Hybrid II	Hybrid III	<i>p</i> -value ^x
1	Pyruvic acid	2.19±1.65	1.91±1.52	2.43±1.65	2.23±1.73	2.13±1.67	0.1304
2	Lactic acid ^w	4.10±1.99 ^{ab}	4.87±2.89 ^a	2.45±1.86 ^b	2.43±1.85 ^b	2.84±1.84 ^b	0.0043
3	L-Alanine ^w	6.65±2.26	8.56±3.29	7.55±3.44	10.82±3.97	8.88±2.36	0.2384
4	N-methyl proline	4.71±1.55	8.22±3.79	4.97±1.37	8.01±3.05	5.47±1.66	0.0614
5	L-Valine ^w	2.70±1.39	3.68±1.37	3.47±1.64	3.58±1.52	3.17±1.93	0.3536
6	Benzoic acid ^w	7.96±2.45	6.78±2.06	7.32±3.53	8.85±3.16	7.72±2.40	0.7105
7	Phosphoric acid ^w	42.30±14.83 ^{ab}	58.12±17.97 ^a	24.46±10.89 ^b	25.96±12.03 ^b	34.28±8.74 ^{ab}	0.0205
8	Glycerol ^w	18.30±3.94	19.42±2.28	19.25±4.97	23.76±3.98	20.47±3.95	0.3037
9	L-Proline ^w	100.03±30.94 ^{ab}	159.74±44.55 ^a	71.98±12.82 ^b	102.99±14.59 ^{ab}	85.72±23.29 ^b	0.0127
10	Propanoic acid, 1-oxo	7.94±4.73	7.43±3.07	5.91±2.53	7.45±3.40	6.42±3.02	0.7391
11	L-Serine ^w	50.87±23.77	55.78±15.54	41.23±5.40	51.74±9.40	42.97±10.90	0.6157
12	L-Threonine ^w	120.42±40.88 ^a	36.01±13.94 ^b	67.18±19.97 ^{ab}	69.47±23.70 ^{ab}	89.90±14.80 ^{ab}	0.0067
13	Malic acid ^w	161.81±54.91 ^a	48.36±18.71 ^b	90.26±26.82 ^{ab}	93.33±31.83 ^{ab}	120.79±19.87 ^{ab}	0.0067
14	L-Aspartic acid ^w	7.96±3.12 ^b	32.45±12.69 ^a	4.60±2.81 ^b	7.05±4.44 ^b	8.29±4.11 ^b	<0.0001
15	γ -Aminobutyric acid ^w	67.82±12.58	83.91±20.93	76.95±17.40	82.67±11.12	83.26±23.40	0.7724
16	Arabinofuranose	5.93±2.02	6.53±2.29	4.31±2.17	6.34±2.04	4.47±1.54	0.0665
17	Threonic acid ^w	157.79±37.37 ^a	25.39±13.11 ^c	76.56±34.92 ^b	48.00±25.68 ^{bc}	70.00±33.50 ^{bc}	<0.0001
18, 19	Xylose ^w	31.09±13.08	32.27±14.51	19.92±9.47	27.40±11.08	23.89±10.45	0.6356

Peak No.	TMS Metabolite ^y	<i>Citrus maxima</i>	<i>Citrus latipes</i>	Hybrid 1	Hybrid II	Hybrid III	<i>p</i> -value ^x
20	L-Asparagine ^w	12.38±3.73	11.80±6.84	7.50±4.71	8.76±3.46	8.65±5.03	0.2495
21	Xylitol ^w	5.63±2.59	11.30±2.79	10.28±4.07	9.81±4.01	9.15±2.72	0.1425
22	Ribonic acid	88.45±20.40 ^a	37.26±12.22 ^b	53.58±18.13 ^{ab}	71.62±20.66 ^{ab}	46.34±10.23 ^b	0.0051
23	Shikimic acid	100.37±6.95 ^a	33.23±12.15 ^c	43.02±17.49 ^{bc}	69.94±21.32 ^{ab}	56.22±20.05 ^{bc}	0.0004
24	Citric acid ^w	332.30±94.74 ^b	592.90±154.40 ^a	318.40±55.03 ^b	386.93±58.18 ^{ab}	382.70±110.12 ^{ab}	0.0271
25	Unknown sugar 1	54.46±15.96	54.03±10.42	55.02±17.37	59.04±4.56	57.00±13.06	0.9849
26	Quinic acid ^w	593.01±185.00 ^a	115.36±43.02 ^b	416.96±173.37 ^{ab}	224.81±125.74 ^b	212.45±69.26 ^b	0.0030
27, 28	Fructose ^w	52.66±19.71	66.51±15.82	56.93±14.18	50.58±12.77	77.97±3.59	0.1248
29, 31	Glucose ^w	92.88±32.10	90.03±15.93	125.67±53.53	93.53±11.40	143.29±66.20	0.4185
30, 32	Mannose ^w	33.15±6.54	31.33±7.65	32.84±3.82	41.22±7.46	32.12±11.17	0.4154
33	Galactose ^w	23.52±12.47	19.82±5.90	29.90±6.07	13.47±5.29	40.71±23.51	0.1095
34	<i>chiro</i> -Inositol ^w	2.64±1.83 ^c	20.22±4.65 ^a	18.19±6.49 ^{ab}	21.83±3.43 ^a	12.55±3.83 ^b	<0.0001
35	Gluconic acid ^w	10.21±1.71 ^a	6.59±1.82 ^b	5.86±2.15 ^b	5.09±2.40 ^b	6.55±1.29 ^b	0.0008
36	Saccharic acid ^w	6.05±2.89 ^b	22.29±5.46 ^a	6.82±1.22 ^b	8.82±2.72 ^b	10.19±2.43 ^b	<0.0001
37	<i>scyllo</i> -Inositol ^w	37.47±6.76 ^a	17.50±4.69 ^c	24.67±6.53 ^{bc}	33.59±5.07 ^{ab}	28.27±6.55 ^{abc}	0.0006
38	Galactaric acid ^w	1.21±0.88 ^b	2.70±0.25 ^a	1.13±0.81 ^b	1.18±0.85 ^b	1.27±0.84 ^b	0.0490
39	Palmitic acid ^w	1.73±0.85	1.40±0.98	1.67±1.05	1.99±1.07	1.61±1.19	0.1865
40	<i>myo</i> -Inositol ^w	17.63±5.54	9.85±3.20	16.04±6.10	12.89±4.82	15.99±4.97	0.1053
41	Arabino-hexaric acid	60.60±8.03	46.35±4.52	52.86±10.16	50.42±11.33	59.38±13.10	0.1883
43	Stearic acid ^w	1.92±1.36	2.07±1.10	2.15±0.91	2.15±1.29	2.13±1.57	0.9793
44	Glyceryl-glycoside	6.46±1.64	5.78±1.75	6.34±2.16	6.97±1.63	7.63±2.16	0.3639

Peak No.	TMS Metabolite ^y	<i>Citrus maxima</i>	<i>Citrus latipes</i>	Hybrid 1	Hybrid II	Hybrid III	<i>p</i> -value ^x
45	Sucrose ^w	172.55±35.04 ^b	461.72±106.29 ^a	420.13±57.16 ^a	416.76±58.51 ^a	470.09±76.92 ^a	0.0004

^z Values represent means±SD (*n*=4). ^y Quantification of leaf metabolites was based on calibration curves obtained from standards of known concentration injected into the GC-MS (Perkin Elmer Elite-5ms, 30 m × 0.25 mm × 0.25 µm) under the same chromatographic conditions as the samples. ^x *p*-values are bolded if less than 0.05. Different letters indicate statistically significant differences among the studied varieties (*p* < 0.05), while cells without letters or with the same letter signify no significant differences among them using Tukey-Kramer honestly significant different test (Tukey HSD). ^w Metabolites have been confirmed using authentic reference standard.