
SUPPLEMENTARY MATERIALS

Physico-Chemical, Nutritional, and Sensory Evaluation of Two New Commercial Tomato Hybrids and Their Parental Lines

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Table S1. Mean relative concentrations (expressed as % of total peak areas) and standard deviations (SD) of volatile compounds from tomato varieties analysed by headspace ITEX/GC-MS technique

No.	Compound name	Genotype / Mean \pm SD							
		Precos F1	AS 300 F1	AS 30 ♀ (F7)	AS 31 ♂ (F7)	Addalyn F1	AS 400 F1	AS 09 ♀ (F7)	AS 10 ♂ (F7)
1	1-Penten-3-ol							4.10 \pm 0.38	10.01 \pm 0.53
2	3-Pentanone					6.51 \pm 0.44	8.20 \pm 0.80	4.37 \pm 0.42	7.32 \pm 0.23
3	Pentanal	3.78 \pm 0.16	5.11 \pm 0.72	6.64 \pm 0.36	4.81 \pm 0.52				
4	n-Propyl acetate				1.19 \pm 0.65				
5	1-Butanol, 3-methyl-	2.13 \pm 0.01	2.48 \pm 0.35	0.95 \pm 0.14	8.67 \pm 0.69			20.96 \pm 0.56	
6	1-Butanol, 2-methyl-	1.43 \pm 0.14	1.23 \pm 0.38	1.61 \pm 0.10	2.07 \pm 0.05			4.93 \pm 0.45	
7	Pentanal, 2-methyl-	0.18 \pm 0.33			0.45 \pm 0.08				
8	Propanoic acid, 2-methyl-, ethyl ester	0.74 \pm 0.16		0.35 \pm 0.14	0.45 \pm 0.14				
9	1-Pentanol	0.68 \pm 0.16		1.35 \pm 0.37	1.77 \pm 0.15	1.70 \pm 0.30		1.41 \pm 0.63	
10	Acetic acid, 2-methylpropyl ester				1.27 \pm 0.10			0.45 \pm 0.15	
11	Butanoic acid, 3-methyl-, methyl ester								
12	Hexanal	29.85 \pm 1.28	24.11 \pm 0.86	12.97 \pm 0.41	30.02 \pm 0.41	8.58 \pm 0.87	4.11 \pm 0.47	0.83 \pm 0.33	1.41 \pm 0.36
13	Furfural								1.66 \pm 0.34
14	Butanoic acid, 3-methyl-, ethyl ester		0.90 \pm 0.17	0.19 \pm 0.18					
15	1-Hexanol	0.25 \pm 0.20		1.08 \pm 0.14	1.61 \pm 0.12	2.54 \pm 0.78	1.30 \pm 0.58	1.62 \pm 0.36	2.14 \pm 0.60
16	1-Butanol, 3-methyl-, acetate				4.51 \pm 0.58			17.68 \pm 1.42	
17	1-Butanol, 2-methyl-, acetate				0.65 \pm 0.33			1.17 \pm 0.67	
18	Heptanal	2.08 \pm 0.07	0.75 \pm 0.26	1.06 \pm 0.62	1.76 \pm 0.21				
19	1-Butanol, 2-ethyl-						1.54 \pm 0.42	5.11 \pm 0.73	2.90 \pm 0.35
20	Acetic acid, pentyl ester				0.19 \pm 0.40			1.06 \pm 0.36	
21	Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)- *	0.34 \pm 0.22			0.23 \pm 0.45				
22	Hexanoic acid, methyl ester	0.12 \pm 0.14		0.22 \pm 0.23	0.07 \pm 0.19				
23	.alpha.-Pinene	0.85 \pm 0.19		0.15 \pm 0.14	0.26 \pm 0.36				
24	Benzene, 1-methoxy-4-methyl- *			0.75 \pm 0.34	0.12 \pm 0.30	0.92 \pm 0.55			
25	2-Heptanone, 6-methyl-	0.33 \pm 0.40		0.28 \pm 0.33		0.20 \pm 0.04	0.28 \pm 0.58		
26	2-Heptenal, (Z)-	0.80 \pm 0.14	1.13 \pm 0.45	0.71 \pm 0.17	0.84 \pm 0.20	0.36 \pm 0.02			
27	Benzaldehyde	1.34 \pm 0.30	2.76 \pm 0.15	2.70 \pm 0.14	0.77 \pm 0.48	2.45 \pm 0.33	2.84 \pm 0.43	1.11 \pm 0.31	2.99 \pm 0.38

Table 1. Chemical composition of the essential oil of <i>Thymus serpyllifolius</i> L. (Lamiaceae) by GC-MS analysis									
Peak number	Chemical name	Retention time (min)	Area (%)	Area (%)	Area (%)	Area (%)	Area (%)	Area (%)	Area (%)
28	Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)-*	1.20 ± 0.16		0.20 ± 0.14	0.19 ± 0.32				
29	Heptanol							0.49 ± 0.10	
30	.beta.-Pinene	3.34 ± 0.55		0.92 ± 0.29	0.64 ± 0.34	0.27 ± 0.12			
31	1-Octen-3-one	0.25 ± 0.28			0.26 ± 0.36				
32	Phenol	1.19 ± 0.03	2.09 ± 0.04	2.58 ± 0.13	0.71 ± 0.16	2.47 ± 0.21	1.72 ± 0.49	1.12 ± 0.38	2.25 ± 0.34
33	5-Hepten-2-one, 6-methyl-	4.82 ± 0.42	5.62 ± 0.25	11.88 ± 0.40	6.13 ± 0.70	10.81 ± 1.11	19.52 ± 0.73	6.80 ± 0.28	19.72 ± 0.74
34	.beta.-Myrcene	10.59 ± 0.50							
35	Furan, 2-pentyl-		15.03 ± 1.07	13.99 ± 0.62	8.83 ± 0.42	19.59 ± 1.59	10.07 ± 0.69	7.28 ± 0.43	16.06 ± 0.43
36	5-Hepten-2-ol, 6-methyl-			0.28 ± 0.33	0.08 ± 0.40	0.15 ± 0.08			
37	trans-2-(2-Pentenyl)furan *	0.28 ± 0.42		1.65 ± 0.21	0.16 ± 0.20	0.25 ± 0.36	0.52 ± 0.24	0.23 ± 0.46	0.35 ± 0.07
38	Hexanoic acid, ethyl ester	0.24 ± 0.22	0.28 ± 0.19		0.53 ± 0.14				
39	Octanal	2.79 ± 0.24	0.75 ± 0.14		1.15 ± 0.16	1.25 ± 0.29		0.37 ± 0.26	0.86 ± 0.21
40	3-Carene	0.41 ± 0.18					1.32 ± 0.16		
41	Acetic acid, hexyl ester				0.12 ± 0.13			0.83 ± 0.24	0.44 ± 0.06
42	.alpha.-Terpinene	0.29 ± 0.09							
43	p-Cymene	10.1 ± 0.45	1.74 ± 0.26	6.22 ± 0.63	4.64 ± 0.14	7.39 ± 0.67	0.99 ± 0.32	2.50 ± 0.44	0.23 ± 0.08
44	1,3,7-Octatriene, 3,7-dimethyl- *	0.13 ± 0.01							
45	.gamma.-Terpinene	5.12 ± 0.55		3.55 ± 0.14		4.16 ± 0.50		1.19 ± 0.67	
46	2-Octenal, (E)-		4.31 ± 0.57		2.13 ± 0.48		1.26 ± 0.43		0.69 ± 0.24
47	Acetophenone	1.22 ± 0.15	2.40 ± 0.21	2.27 ± 0.19	0.70 ± 0.14	2.38 ± 0.19	2.97 ± 0.33	0.58 ± 0.14	2.33 ± 0.15
48	2-Octen-1-ol					0.99 ± 0.46			
49	1-Octanol	0.29 ± 0.11		1.72 ± 0.28	0.70 ± 0.14	0.77 ± 0.14	1.05 ± 0.07	2.06 ± 0.35	2.18 ± 0.16
50	.alpha.- Terpinolene	0.32 ± 0.12							
51	Furan, 3-(4-methyl-3-pentenyl)-			1.28 ± 0.35		1.06 ± 0.19	3.70 ± 0.31	1.02 ± 0.40	3.06 ± 0.36
52	Nonanal	1.13 ± 0.24	0.64 ± 0.14	1.11 ± 0.31	0.89 ± 0.15	1.07 ± 0.42	1.69 ± 0.45	0.35 ± 0.06	0.94 ± 0.14
53	Octanoic acid, methyl ester	0.38 ± 0.12	0.41 ± 0.16	0.28 ± 0.29	0.18 ± 0.33	0.35 ± 0.62			
54	2-Nonenal, (E)-			5.24 ± 0.45	0.85 ± 0.25				
55	Benzoic Acid		16.08 ± 0.73	3.05 ± 0.35	2.09 ± 0.08	6.60 ± 0.8	23.25 ± 0.84	6.13 ± 0.10	4.12 ± 0.45
56	Octanoic Acid			0.48 ± 0.45	1.00 ± 0.46				
57	1-Nonanol								
58	2-Dodecanone*	0.15 ± 0.12		0.18 ± 0.38	0.08 ± 0.09		0.13 ± 0.29		
59	Methyl Salicylate					3.32 ± 0.39			3.01 ± 0.38
60	Octanoic acid, ethyl ester	0.57 ± 0.13	0.63 ± 0.09		2.00 ± 0.31				
61	Decanal	0.61 ± 0.12	0.62 ± 0.25	0.81 ± 0.29	0.24 ± 0.22	0.78 ± 0.15	0.88 ± 0.16	0.35 ± 0.07	0.24 ± 0.22
62	Acetic acid, octyl ester							0.78 ± 0.16	
63	5-Hydrxoymethylfurfural	0.58 ± 0.18	2.97 ± 0.19						2.98 ± 0.48

64	Nonanoic acid	0.26 ± 0.05				0.29 ± 0.12			
65	2,6-Octadienal, 3,7-dimethyl-, (E)- *	0.24 ± 0.03	0.24 ± 0.17	0.57 ± 0.40	0.18 ± 0.19	0.26 ± 0.10	0.66 ± 0.07		0.35 ± 0.06
66	Benzoic acid, 2-hydroxy-, ethyl ester		0.77 ± 0.26						
67	Ethanone, 1-[4-(1-methylethyl)phenyl]-								
68	Undecanal	0.16 ± 0.11							
69	2-Undecenal	0.19 ± 0.06			0.38 ± 0.19				
70	Dodecanal	0.17 ± 0.57							
71	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	1.85 ± 0.19	3.22 ± 0.47	3.45 ± 0.48	1.49 ± 0.33	3.61 ± 0.45	4.10 ± 0.46	2.12 ± 0.16	4.51 ± 0.26
72	1-Dodecanol	1.90 ± 0.31	0.65 ± 0.35						
73	Dodecanoic acid	4.32 ± 0.75	3.10 ± 0.56	7.29 ± 0.60	1.92 ± 0.50	8.94 ± 1.2	7.90 ± 0.38	2.14 ± 0.45	7.25 ± 0.43

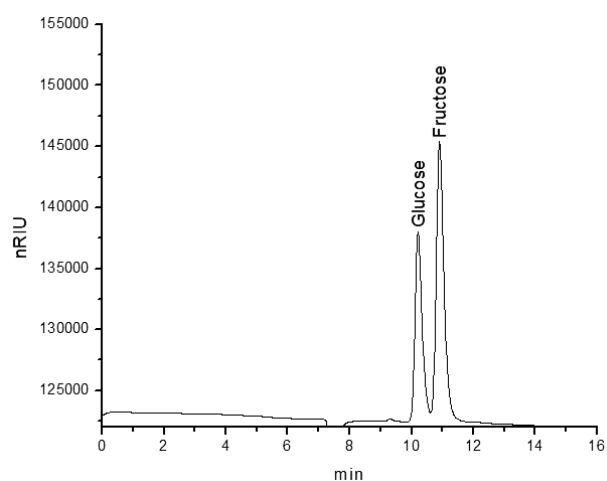
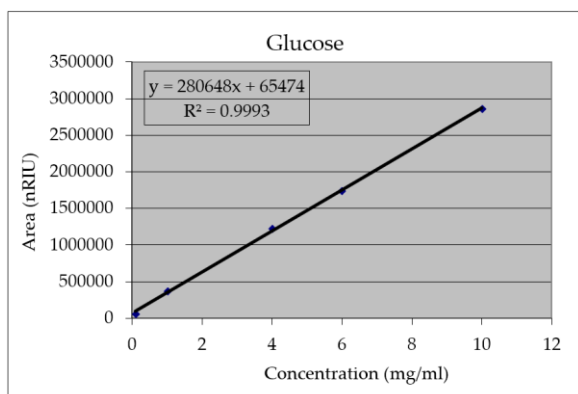
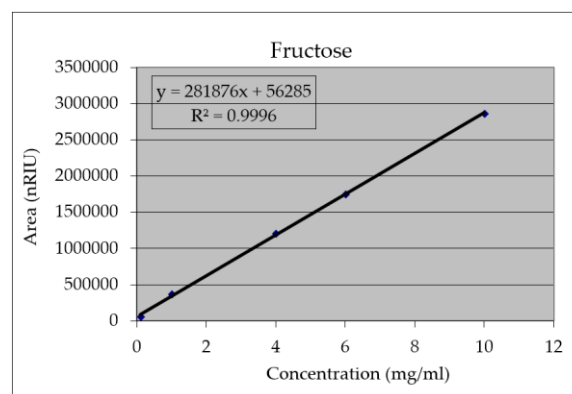


Figure S1. Chromatogram of carbohydrate standards and retention time: glucose $R_t = 10.22$ min; fructose $R_t = 10.87$ min



(a)



(b)

Figure S2. Calibration curves with glucose and fructose standards of 99% purity, with mg/ml concentration: (a) fructose $R^2 = 0.9996$; (b) glucose $R^2 = 0.9993$; $P < 0.05$)

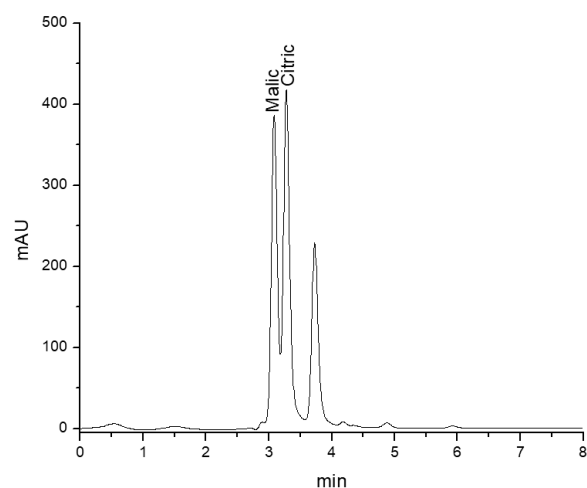


Figure S3. Chromatogram of organic acid standards and retention time: malic acid $R_t = 3.08$ min, citric acid $R_t = 3.32$ min

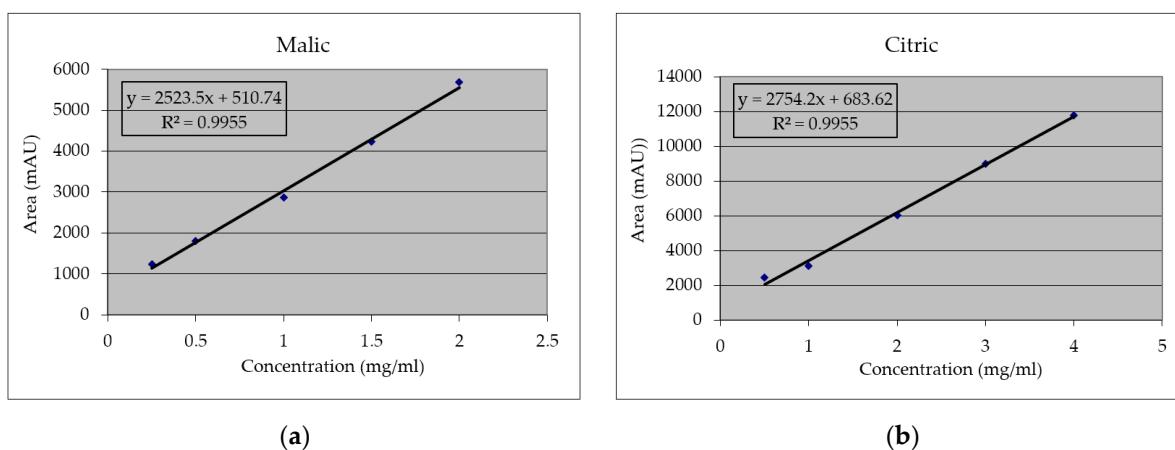


Figure S4. Calibration curves for organic acids by injecting five different concentrations of standard substance of 99% purity: (a) Malic acid $R^2 = 0.9955$; (b) Citric acid $R^2 = 0.9955$

Table S2. Identification of phenolic compounds performed after retention times, UV-Vis and mass spectra for each peak.

Peak	Rt (min)	λ_{max} (nm)	$[M+H]^+$ (m/z)	Phenolic compounds	Phenolic subclasses
1	10.87	302, 245	343	Caffeic acid-glucoside I	Hidroxicinamic acid
2	11.85	312, 248	343	Caffeic acid-glucoside I	Hidroxicinamic acid
3	12.29	326, 248	355	3-Caffeoylquinic acid	Hidroxicinamic acid
4	12.48	326, 248	355	5-Caffeoylquinic acid	Hidroxicinamic acid
5	13.64	324, 248	181	Caffeic acid	Hidroxicinamic acid
6	14.03	328, 248	357	Ferulic acid-glucoside	Hidroxicinamic
7	14.68	355, 255	743	Quercetin-triglucoside	Flavonol
8	15.69	354, 256	611	Quercetin-rutinoside	Flavonol
9	16.03	330, 280	580	Naringin	Flavanone
10	17.32	326, 248	195	Ferulic acid	Hidroxicinamic

*Spectral values were recorded in the range 200-600 nm for all peaks, and chromatograms were recorded at the wavelength $\lambda = 340$ nm. For the retention time (Rt) values were recorded between 10.87-17.32 min, and the mass spectrum $[M + H]^+$ had values between 181-743 m/z.

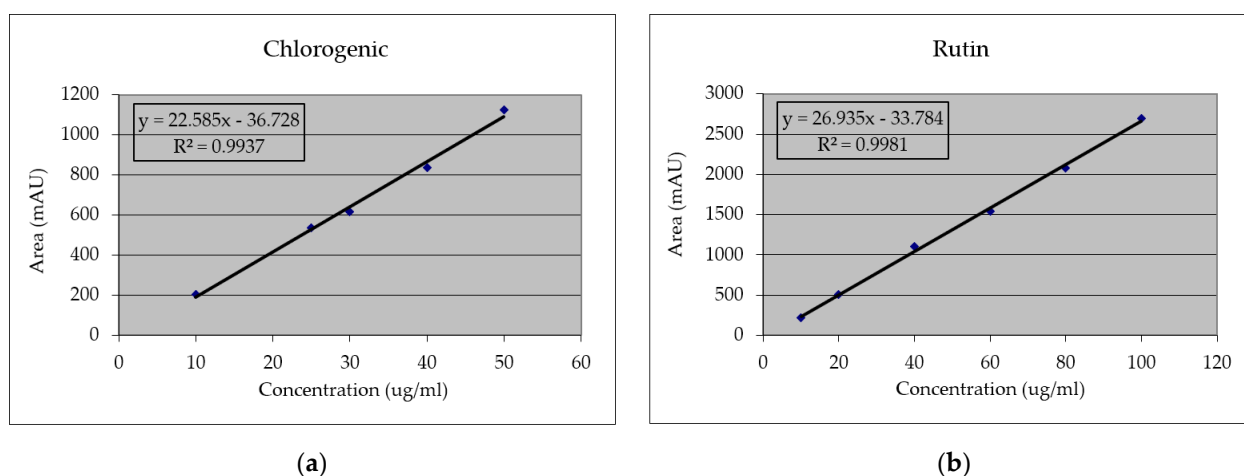


Figure S5. Calibration curves for total phenolic content with chlorogenic and rutin standard of 99% purity, with ug/ml concentration: (a) Chlorogenic $R^2=0.9937$; (b) Rutin $R^2=0.9981$, $P<0,05$)