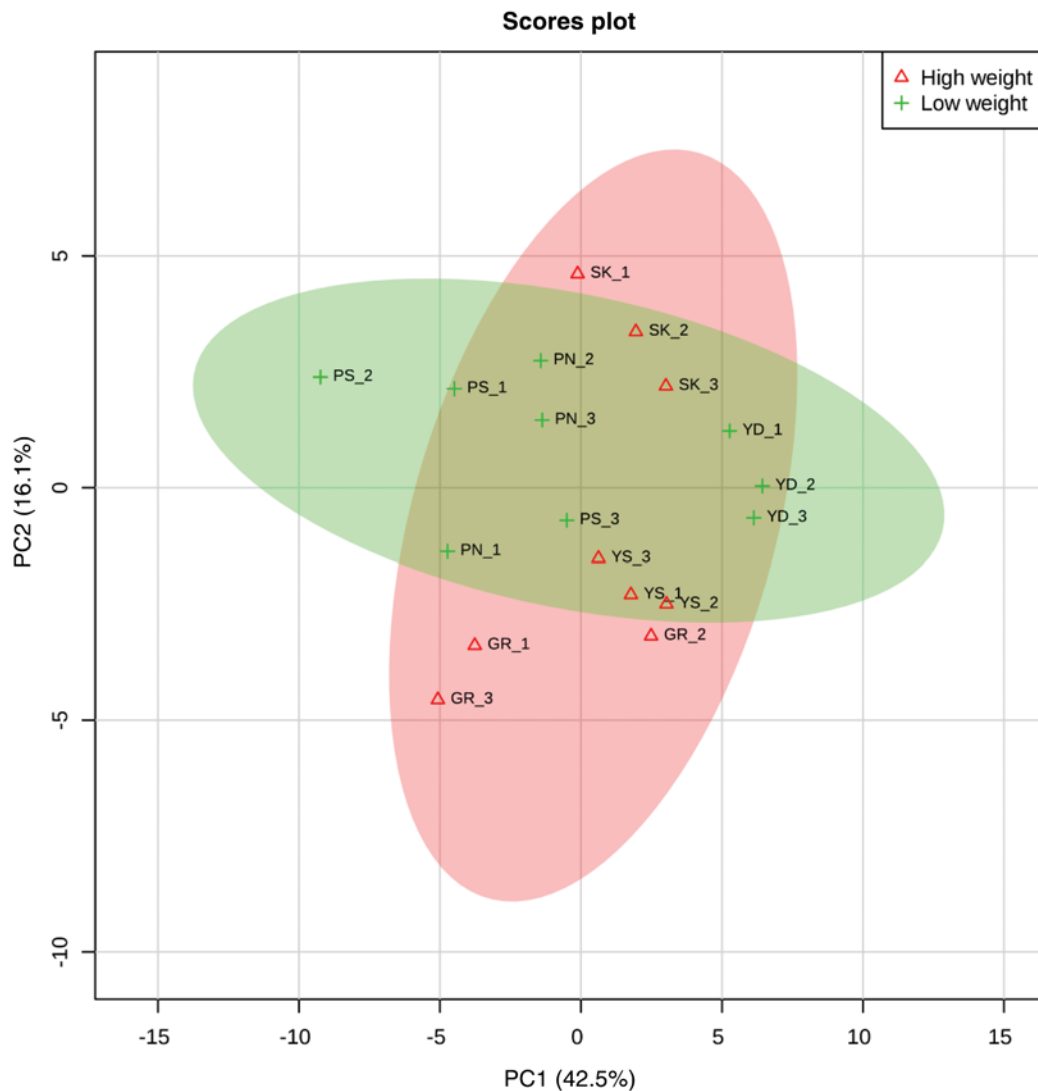


Supplemental Data for:

Maoz I, Kaplunov T, Beno-Muaem D, Lewinsohn E and Lichter A. 2018.

Variability in volatile composition of Crimson Seedless (*Vitis vinifera*) in association with maturity at harvest.

Am J Enol Vitic 69:125-132. doi: 10.5344/ajev.2017.17069.



Supplemental Figure 1 Principal component analysis based on volatile compounds (ng/g FW) of the berries sampled from six vineyards divided into two groups: high weight (red) with vineyards SK, GR, and YS, or low weight (green) with vineyards YD, PN, and PS.

Supplemental Table 1 Vineyards in which Crimson Seedless table grapes were sampled.				
Region	Vineyard	Sampling date	Rootstock	Planting year
Arugot	SK	25 Aug 2014	Richter	2007
	PS	25 Aug 2014	Paulsen	2006
	PN	25 Aug 2014	Paulsen	2011
Lachish	YS	3 Sept 2014	Richter	2003
	GR	3 Sept 2014	Salt Creek	2009
	YD	3 Sept 2014	Richter	2005
Yiftach	MA	28 Aug 2014	Richter	1999

Supplemental Data for:

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Supplemental Table 2 Volatile compounds (ng/g FW) in Crimson Seedless table grapes from six vineyards in the Arugot (SK, YD, PN) and Lachish (PS, GR, YS) regions.

Compound name	ID	Main ion peak	LRI	RI	SK		YD		PN		PS		GR		YS	
					Avg	SD	Avg	SD	Avg	SD	Avg	SD	Avg	SD	Avg	SD
Alcohols																
Ethanol ^{a,b}	RI, MS, St	45	448	~477	3.57	0.96	0.59	0.25	4.01	1.12	4.60	1.90	0.89	0.45	0.92	0.51
1-Penten-3-ol	RI, MS, St	57	683	678	0.71	0.08	0.83	0.09	0.78	0.12	0.86	0.15	0.89	0.13	0.97	0.11
1-Pentanol ^a	RI, MS	42	766	763	2.06	0.31	2.36	0.31	1.81	0.08	1.69	0.72	1.79	0.27	2.26	0.21
(Z)-3-Hexenol ^a	RI, MS	67	855	854	0.48	0.10	0.38	0.05	0.57	0.12	0.65	0.10	0.33	0.05	0.65	0.11
(E)-2-Hexenol ^a	RI, MS	57	862	865	1.11	0.14	1.15	0.41	1.08	0.09	1.28	0.10	0.69	0.06	1.06	0.13
1-Hexanol	RI, MS, St	56	871	867	1.12	0.41	0.92	0.30	0.96	0.19	0.94	0.09	0.38	0.06	0.76	0.23
1-Heptanol	RI, MS, St	70	970	970	0.24	0.05	0.18	0.03	0.16	0.03	0.11	0.04	0.12	0.05	0.16	0.03
1-Octen-3-ol	RI, MS, St	57	976	979	4.47	0.53	5.47	0.51	3.72	0.58	3.20	1.21	3.21	0.81	4.51	0.44
(E)-2-Octenol ^a	RI, MS	57	1067	1068	0.16	0.02	0.19	0.02	0.10	0.03	0.09	0.02	0.11	0.08	0.14	0.03
1-Octanol	RI, MS, St	56	1068	1071	0.33	0.03	0.32	0.02	0.23	0.07	0.18	0.07	0.20	0.08	0.30	0.05
Aldehydes																
1-Butanal ^a	RI, MS	44	595	592	0.20	0.01	0.22	0.05	0.18	0.03	0.23	0.06	0.19	0.06	0.28	0.08
1-Pentanal ^a	RI, MS	44	697	696	6.85	1.57	9.17	1.90	5.89	0.58	5.17	2.81	5.12	0.95	7.92	2.03
(E)-2-Pentenal ^a	RI, MS	84	754	749	0.22	0.04	0.26	0.03	0.15	0.03	0.16	0.07	0.16	0.06	0.26	0.08
1-Hexanal	RI, MS, St	44	799	801	69.18	4.20	71.32	11.67	73.78	6.58	68.92	9.48	65.61	4.28	71.63	4.31
(Z)-2-Hexenal ^a	RI	41	841	844	0.62	0.09	0.60	0.05	0.52	0.06	0.56	0.10	0.65	0.05	0.68	0.07
(E)-2-Hexenal	RI, MS, St	41	851	853	35.02	3.65	33.19	1.93	28.02	1.37	33.55	2.34	36.94	1.87	37.79	3.75
1-Heptanal ^a	RI, MS	70	901	902	0.72	0.15	0.89	0.13	0.60	0.09	0.55	0.21	0.53	0.05	0.80	0.04
(E,E)-2,4-Hexadienal	RI, MS, St	81	911	912	0.46	0.17	0.40	0.07	0.33	0.08	0.40	0.15	0.40	0.03	0.50	0.13
(Z)-2-Heptenal ^a	RI, MS	41	951	956	1.34	0.22	1.77	0.30	0.87	0.25	0.95	0.52	0.87	0.18	1.36	0.16
(E,Z)-2,4-Heptadienal ^a	RI, MS	81	998	998	0.28	0.05	0.37	0.06	0.19	0.02	0.21	0.06	0.25	0.07	0.31	0.05
(E,E)-2,4-Heptadienal ^a	RI, MS	81	1012	1012	0.45	0.13	0.63	0.11	0.25	0.14	0.25	0.15	0.31	0.22	0.49	0.08
(E)-2-Octenal ^a	RI, MS	41	1060	1059	0.87	0.18	0.96	0.18	0.45	0.10	0.48	0.20	0.44	0.17	0.66	0.04
1-Nonanal	RI, MS, St	57	1102	1105	0.53	0.08	0.45	0.05	0.37	0.05	0.33	0.10	0.31	0.10	0.41	0.04
(E,Z)-2,6-Nonadienal	RI, MS, St	41	1146	1155	0.03	0.01	0.02	0.01	0.03	0.01	0.01	0.02	0.02	0.01	0.03	0.01
(E)-2-Nonenal ^a	RI, MS	41	1165	1161	0.07	0.03	0.08	0.01	0.04	0.02	0.03	0.03	0.04	0.02	0.05	0.01
1-Decanal ^a	RI, MS	43	1206	1207	0.14	0.06	0.12	0.01	0.07	0.01	0.09	0.03	0.07	0.02	0.10	0.01
Benzenoids																
Benzaldehyde	RI, MS, St	77	961	960	0.16	0.02	0.12	0.02	0.12	0.01	0.11	0.01	0.09	0.01	0.10	0.02
Esters																
Ethyl acetate	RI, MS, St	43	628	625	1.89	0.77	0.19	0.02	2.72	1.56	2.24	0.97	0.72	0.03	0.31	0.13
Methyl valerate	RI, MS, St	74	823	824	0.15	0.04	0.20	0.04	0.12	0.02	0.11	0.06	0.09	0.02	0.13	0.01
Methyl hexanoate	RI, MS, St	74	934	925	1.47	0.40	2.31	0.35	1.35	0.05	1.23	0.53	1.01	0.26	1.54	0.15
Methyl heptanoate ^a	RI, MS	74	1026	1026	0.11	0.01	0.14	0.01	0.14	0.02	0.12	0.06	0.13	0.04	0.15	0.03
Methyl octanoate	RI, MS, St	74	1126	1126	0.13	0.03	0.19	0.02	0.19	0.03	0.13	0.09	0.19	0.05	0.21	0.04
Methyl nonanoate	RI, MS, St	74	1225	1225	0.10	0.08	0.16	0.05	0.12	0.01	0.05	0.06	0.12	0.06	0.17	0.05
Furans																
2-Methylfuran	RI, MS, St	82	598	603	0.11	0.01	0.12	0.03	0.11	0.02	0.11	0.03	0.09	0.03	0.11	0.01
2-Ethylfuran	RI, MS, St	81	702	703	0.59	0.08	0.80	0.14	0.59	0.05	0.51	0.15	0.59	0.08	0.74	0.11
2-Butylfuran	RI, MS, St	81	885	892	0.85	0.14	1.19	0.34	0.70	0.08	0.61	0.34	0.51	0.10	0.76	0.07
2-Pentylfuran ^a	RI, MS	81	993	992	1.66	0.23	2.22	0.43	1.40	0.30	1.20	0.42	1.02	0.25	1.55	0.25
Ketones																
1-Penten-3-one ^a	RI, MS	55	684	684	2.27	0.24	2.49	0.38	1.69	0.13	1.50	0.59	1.79	0.20	2.35	0.24
(E)-3-Octen-2-one ^a	RI, MS	55	1036	1040	0.13	0.01	0.17	0.01	0.10	0.02	0.09	0.03	0.09	0.02	0.14	0.02
Oxygenated monoterpenes																
Linalool ^a	RI, St	71	1104	1101	0.14	0.03	0.13	0.02	0.12	0.02	0.12	0.01	0.12	0.02	0.12	0.03
Norisoprenoids																
6-Methyl-5-hepten-2-one	RI, MS, St	43	987	988	0.32	0.05	0.37	0.02	0.32	0.05	0.29	0.07	0.28	0.03	0.37	0.05
β -Damascenone	RI, MS, St	69	1388	1390	0.12	0.06	0.13	0.04	0.13	0.12	0.08	0.08	0.03	0.04	0.12	0.12
β -Ionone ^a	RI, MS	177	1490	1491	0.08	0.01	0.06	0.01	0.07	0.00	0.08	0.01	0.04	0.00	0.06	0.01

ID, identification; LRI, literature retention index; RI, retention index; MS, mass spectrometry; St, authentic standard.

Compounds are presented relative to the internal standard (S)-(+)-2-octanol.

^aTentative identification.

^bEthanol retention index was extrapolated.

Supplemental Data for:

Maoz I, Kaplunov T, Beno-Muaem D, Lewinsohn E and Lichter A. 2018.

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Am J Enol Vitic 69:125-132. doi: 10.5344/ajev.2017.17069.

Supplemental Table 3 Analysis of volatile compounds that differed significantly among six vineyards of Crimson Seedless table grapes from the Arugot and Lachish regions. *P*-values are given for one-way analysis of variance/non-parametric Kruskal-Wallis tests.

Compound name	<i>p</i> -value	$-\log_{10}$ (<i>p</i> -value)
Ethyl acetate	0.011	1.967
(<i>E</i>)-3-Octen-2-one	0.012	1.910
(<i>E</i>)-2-Octenal	0.018	1.742
Ethanol	0.022	1.652
β -ionone	0.024	1.627
(<i>Z</i>)-3-Hexenol	0.027	1.570
1-Penten-3-one	0.030	1.530
1-Octanol	0.040	1.402
(<i>E,Z</i>)-2,4-Heptadienal	0.040	1.394
Benzaldehyde	0.044	1.360
2-Pentylfuran	0.048	1.315
Methyl hexanoate	0.049	1.306
<i>p</i>-value cut off	0.050	1.301
1-Decanal	0.053	1.277
1-Octen-3-ol	0.056	1.252
2-Butylfuran	0.056	1.252
1-Heptanol	0.057	1.246
1-Heptanal	0.062	1.206
(<i>Z</i>)-2-Heptenal	0.063	1.201
(<i>E</i>)-2-Hexenal	0.063	1.198
Methyl valerate	0.064	1.192
(<i>E</i>)-2-Pentenal	0.071	1.151
(<i>E</i>)-2-Nonenal	0.073	1.135
1-Nonanal	0.076	1.122
1-Pentanal	0.080	1.098
2-Ethylfuran	0.081	1.090
(<i>E</i>)-2-Hexenol	0.082	1.086
(<i>E</i>)-2-Octenol	0.096	1.019
(<i>E,E</i>)-2,4-Heptadienal	0.102	0.992
1-Hexanol	0.127	0.896
(<i>Z</i>)-2-Hexenal	0.153	0.815
6-Methyl-5-hepten-2-one	0.194	0.713
Methyl octanoate	0.208	0.682
1-Penten-3-ol	0.234	0.631
Methyl nonanoate	0.234	0.631
1-Pentanol	0.279	0.554
Methyl heptanoate	0.367	0.436
1-Butanal	0.377	0.423
β -Damascenone	0.422	0.375
(<i>E,E</i>)-2,4-Hexadienal	0.535	0.271
(<i>E,Z</i>)-2,6-Nonadienal	0.569	0.245
2-Methylfuran	0.616	0.210
1-Hexanal	0.713	0.147
Linalool	0.805	0.094

Supplemental Table 4 Volatile compounds (ng/g FW) in Crimson Seedless table grapes from vineyard MA, divided into groups with low total soluble solids (TSS) (<16.0 Brix) and high TSS (>17.5 Brix). *P*-values are given for analysis of variance/non-parametric Mann-Whitney tests.

TSS group	Low TSS		High TSS		<i>p</i> -value
	Avg	SD	Avg	SD	
Alcohols					
Ethanol ^{a,b}	2.49	0.49	8.57	2.13	0.0463
1-Penten-3-ol	0.79	0.06	0.95	0.09	0.0463
1-Pentanol ^a	2.03	0.16	2.96	0.12	0.0495
(<i>Z</i>)-3-Hexenol ^a	0.52	0.08	0.43	0.07	0.1266
(<i>E</i>)-2-Hexenol ^a	1.06	0.10	0.69	0.12	0.0495
1-Hexanol	0.44	0.02	0.81	0.05	0.0495
1-Heptanol	0.28	0.01	0.37	0.00	0.0495
1-Octen-3-ol	5.58	0.45	8.73	0.44	0.0495
(<i>E</i>)-2-Octenol ^a	0.21	0.05	0.36	0.05	0.0495
1-Octanol	0.36	0.03	0.55	0.07	0.0495
Aldehydes					
1-Butanal ^a	0.26	0.01	0.29	0.07	0.5127
1-Pentanal ^a	12.72	0.78	13.92	1.20	0.1266
(<i>E</i>)-2-Pentenal ^a	0.63	0.04	0.58	0.09	0.5127
1-Hexanal	80.91	2.85	99.83	5.11	0.0495
(<i>Z</i>)-2-Hexenal ^a	1.15	0.11	0.75	0.07	0.0495
(<i>E</i>)-2-Hexenal	66.05	4.99	43.92	7.76	0.0495
1-Heptanal ^a	1.31	0.14	1.63	0.11	0.0463
(<i>E,E</i>)-2,4-Hexadienal	0.93	0.08	0.66	0.08	0.0495
(<i>Z</i>)-2-Heptenal ^a	2.97	0.07	3.28	0.15	0.0495
(<i>E,Z</i>)-2,4-Heptadienal ^a	0.35	0.02	0.64	0.11	0.0495
(<i>E,E</i>)-2,4-Heptadienal ^a	1.45	0.03	1.75	0.18	0.0495
(<i>E</i>)-2-Octenal ^a	2.34	0.11	2.52	0.28	0.2752
1-Nonanal	0.63	0.09	0.84	0.19	0.1266
(<i>E,Z</i>)-2,6-Nonadienal	0.04	0.01	0.05	0.01	0.6579
(<i>E</i>)-2-Nonenal ^a	0.09	0.03	0.13	0.04	0.1266
1-Decanal ^a	0.11	0.02	0.20	0.07	0.1266
Benzenoids					
Benzaldehyde	0.27	0.03	0.33	0.09	0.5127
Esters					
Ethyl acetate	0.20	0.04	1.07	0.50	0.0495
Methyl valerate	0.34	0.01	0.30	0.01	0.0495
Methyl hexanoate	2.23	0.08	2.65	0.08	0.0495
Methyl heptanoate ^a	0.08	0.02	0.11	0.01	0.1266
Methyl octanoate	0.12	0.03	0.14	0.02	0.2752
Methyl nonanoate	0.13	0.05	0.13	0.04	0.8273
Furans					
2-Methylfuran	0.09	0.01	0.16	0.02	0.0495
2-Ethylfuran	0.86	0.05	0.80	0.12	0.6579
2-Butylfuran	1.31	0.08	1.41	0.05	0.1266
2-Pentylfuran ^a	3.12	0.25	3.07	0.30	0.8273
Ketones					
1-Penten-3-one ^a	2.84	0.60	4.86	0.20	0.0495
(<i>E</i>)-3-Octen-2-one ^a	0.19	0.03	0.27	0.01	0.0495
Oxygenated monoterpenes					
Linalool ^a	0.14	0.01	0.17	0.02	0.0495
Norisoprenoids					
6-Methyl-5-hepten-2-one	0.64	0.02	0.62	0.03	0.3758
β -Damascenone	0.49	0.20	0.29	0.16	0.2752
β -Ionone ^a	0.10	0.01	0.10	0.01	0.5127

Compounds are presented relative to the internal standard (*S*)-(+)-2-octanol.

^aTentative identification.

^bEthanol retention index was extrapolated.

Supplemental Data for:

Maoz I, Kaplunov T, Beno-Muaem D, Lewinsohn E and Lichter A. 2018.

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Am J Enol Vitic 69:125-132. doi: 10.5344/ajev.2017.17069.

Supplemental Table 5 Volatile compounds (ng/g FW) in Crimson Seedless table grapes from six vineyards from Arugot and Lachish, divided into two groups: low total soluble solids (TSS), <17.5 Brix, and high TSS, >17.5 Brix. *P*-values are given for one-way analysis of variance/non-parametric Mann-Whitney test.

	Low TSS		High TSS		<i>p</i> -value
	Avg	SD	Avg	SD	
Alcohols					
Ethanol ^{a,b}	2.13	0.76	2.60	0.52	0.2752
1-Penten-3-ol	0.91	0.06	0.77	0.08	0.1266
1-Pentanol ^a	1.91	0.16	2.14	0.25	0.2752
(<i>Z</i>)-3-Hexenol ^a	0.54	0.02	0.48	0.01	0.0495
(<i>E</i>)-2-Hexenol ^a	1.01	0.09	1.17	0.24	0.2752
1-Hexanol	0.69	0.08	1.08	0.30	0.0495
1-Heptanol	0.13	0.02	0.20	0.01	0.0495
1-Octen-3-ol	3.64	0.24	4.77	0.20	0.0495
(<i>E</i>)-2-Octenol ^a	0.11	0.03	0.16	0.02	0.1266
1-Octanol	0.23	0.03	0.31	0.01	0.0495
Aldehydes					
1-Butanal ^a	0.23	0.02	0.21	0.04	0.5127
1-Pentanal ^a	6.07	0.58	7.71	1.05	0.0495
(<i>E</i>)-2-Pentenal ^a	0.19	0.03	0.22	0.03	0.2752
1-Hexanal	68.79	4.15	71.01	4.74	0.2752
(<i>Z</i>)-2-Hexenal ^a	0.63	0.05	0.59	0.01	0.5127
(<i>E</i>)-2-Hexenal	36.13	0.79	32.82	0.29	0.0495
1-Heptanal ^a	0.62	0.07	0.77	0.07	0.0495
(<i>E,E</i>)-2,4-Hexadienal	0.43	0.10	0.41	0.06	0.8273
(<i>Z</i>)-2-Heptenal ^a	1.06	0.18	1.45	0.22	0.0495
(<i>E,Z</i>)-2,4-Heptadienal ^a	0.26	0.02	0.30	0.03	0.0495
(<i>E,E</i>)-2,4-Heptadienal ^a	0.35	0.04	0.49	0.13	0.2752
(<i>E</i>)-2-Octenal ^a	0.53	0.03	0.83	0.08	0.0495
1-Nonanal	0.35	0.01	0.47	0.01	0.0495
(<i>E,Z</i>)-2,6-Nonadienal	0.02	0.01	0.03	0.00	0.5127
(<i>E</i>)-2-Nonenal ^a	0.04	0.01	0.07	0.01	0.0495
1-Decanal ^a	0.08	0.01	0.12	0.02	0.0495
Benzenoids					
Benzaldehyde	0.10	0.01	0.14	0.02	0.0495
Esters					
Ethyl acetate	1.09	0.31	1.55	0.56	0.1266
Methyl valerate	0.11	0.01	0.16	0.02	0.0495
Methyl hexanoate	1.26	0.09	1.77	0.13	0.0495
Methyl heptanoate ^a	0.14	0.01	0.13	0.00	0.2752
Methyl octanoate	0.18	0.01	0.16	0.01	0.2752
Methyl nonanoate	0.11	0.02	0.13	0.03	0.8273
Furans					
2-Methylfuran	0.10	0.02	0.12	0.01	0.3758
2-Ethylfuran	0.61	0.05	0.67	0.06	0.2752
2-Butylfuran	0.63	0.08	0.98	0.18	0.0495
2-Pentylfuran ^a	1.26	0.14	1.88	0.24	0.0495
Ketones					
1-Penten-3-one ^a	1.88	0.16	2.25	0.25	0.0495
(<i>E</i>)-3-Octen-2-one ^a	0.10	0.00	0.14	0.00	0.0495
Oxygenated monoterpenes					
Linalool ^a	0.12	0.00	0.13	0.02	0.0495
Norisoprenoids					
6-Methyl-5-hepten-2-one	0.31	0.01	0.34	0.01	0.0495
β-Damascenone	0.08	0.07	0.14	0.04	0.2752
β-Ionone ^a	0.06	0.01	0.07	0.01	0.2752

Compounds are presented relative to the internal standard (*S*)-(+)-2-octanol.

^aTentative identification.

^bEthanol retention index was extrapolated.

Supplemental Table 6 Correlation coefficient analysis of volatile compounds from seven vineyards of Crimson Seedless table grapes based on total soluble solids (TSS) levels (Pearson *r* distance measurement). FDR, false discovery rate.

Compound name	Correlation	FDR
(<i>E</i>)-2-Hexenal ^a	-0.815	0.019
1-Octanol ^a	0.775	0.026
Methyl hexanoate ^a	0.813	0.019
1-Octen-3-ol ^a	0.820	0.019
(<i>Z</i>)-2-Hexenal	-0.798	0.020
β-Ionone	-0.203	0.707
1-Penten-3-ol	-0.184	0.707
β-Damascenone	-0.174	0.707
(<i>E</i>)-2-Hexenol	-0.172	0.707
6-Methyl-5-hepten-2-one	-0.110	0.829
Methyl octanoate	-0.095	0.849
(<i>E</i>)-2-Pentenal	-0.077	0.872
Methyl heptanoate	-0.021	0.971
Methyl nonanoate	-0.008	0.980
Methyl valerate ^a	0.065	0.883
(<i>E</i>)-2-Octenal	0.142	0.767
(<i>E,E</i>)-2,4-Heptadienal	0.178	0.707
(<i>Z</i>)-2-Heptenal ^a	0.220	0.682
(<i>E,Z</i>)-2,6-Nonadienal	0.222	0.682
Benzaldehyde	0.249	0.670
2-Pentylfuran	0.262	0.658
1-Pentanal	0.303	0.583
1-Hexanal	0.343	0.492
1-Heptanal ^a	0.383	0.414
Ethyl acetate	0.397	0.413
Linalool ^a	0.402	0.413
1-Hexanol ^a	0.482	0.254
(<i>E</i>)-2-Nonenal	0.487	0.254
2-Methylfuran	0.522	0.207
1-Nonanal	0.547	0.176
2-Butylfuran	0.566	0.158
1-Pentanol	0.605	0.123
(<i>E</i>)-2-Octenol	0.618	0.115
(<i>E,Z</i>)-2,4-Heptadienal ^a	0.630	0.110
1-Decanal	0.643	0.104
Ethanol	0.643	0.104
1-Heptanol ^a	0.674	0.087
1-Penten-3-one ^a	0.676	0.087
(<i>E</i>)-3-Octen-2-one ^a	0.676	0.087

^aCompounds with *p* value < 0.05 in both Supplemental Tables 4 and 5.