

Short-term CO₂ treatment of harvested grapes (*Vitis vinifera* L., cv. Trebbiano) before partial dehydration affects berry secondary metabolism and the aromatic profile of the resulting wine

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Table S1 - Carotenoids, chlorophylls e xanthophylls in Trebbiano grape skin during postharvest storage inside the dehydration chamber

	T0	T1		T2	
		Control	Treated	Control	Treated
Beta-carotene	1.91 ± 0.16 a	1.28 ± 0.05 b	2.293 ± 0.09 a	1.02 ± 0.02 b	1.285 ± 0.098 b
Lutein	0.51 ± 0.14 a	0.67 ± 0.39 a	0.69 ± 0.05 a	0.49 ± 0.006 a	0.48 ± 0.01 a
Zeaxanthin	0.42 ± 0.024 a	0.065 ± 0.037 b	0.076 ± 0.0098 b	0.058 ± 0.0075 b	0.054 ± 0.02 b
Neoxanthin	0.14 ± 0.054 a	0.037 ± 0.009 b	0.045 ± 0.0037 b	0.03 ± 0.0028 b	0.028 ± 0.0023 b
Violaxanthin	0.15 ± 0.02 a	0.078 ± 0.013 b	0.153 ± 0.019 a	0.069 ± 0.0094 b	0.036 ± 0.0306 b
Anteraxanthin	0.24 ± 0.015 a	0.017 ± 0.0065 b	0.013 ± 0.014 b	0.022 ± 0.0078 b	0.0056 ± 0.0055 b
Chlorophyll a	8.06 ± 0.59 ab	5.747 ± 0.136 bc	9.813 ± 0.086 a	3.806 ± 0.131 c	5.678 ± 0.294 c
Chlorophyll b	1.74 ± 0.13 ab	1.23 ± 0.02 c	2.09 ± 0.14 a	0.79 ± 0.05 d	1.34 ± 0.07 c

Table S1 - Carotenoids, chlorophylls and xanthophylls content (µg/g fresh weight) in Trebbiano berry skin of control and treated berries allowed to wither inside a dehydration chamber, at harvest time (T0), at 30% weight loss (T1), and at the end of the drying period (T2) when berries lost about 50% of weight. Treated berries were incubated for 24 h with CO₂ (30%, 14° C), and then allowed to wither at this temperature, while control berries were not subjected to the treatment and allowed to wither at the same environmental parameters. Statistically significant differences were evaluated by one-way ANOVA ($p \leq 0.05$), and different letters indicate significantly different values according to Tukey–Kramer test.

Table S2 - Phenolic classes in Trebbiano grape skin (2008) during post-harvest storage inside the dehydration chamber

	T0	T1		T2	
		Control	Treated	Control	Treated
Total phenols (mg GAE/g d.w.)	9.99±0.	14.47±1.84 a	11.33±0.64 ab	9.9±2.63 b	7.99±0.516 b
Flavonoids (mg CTCE/g d.w.)	6.99±0.	11.56±0.17 a	8.64±0.47 b	5.89±0.43 c	3.71±1.076 d
Flavonols (mg QCTE/g d.w.)	0.56±0.	0.83±0.049 a	0.64±0.005 ab	0.22±0.07 c	0.41±0.069 bc
Proanthocyanidins (mg CYAE/g d.w.)	0.99±0.	1.74±0.17 a	1.51±0.11 a	1.18±0.075 ab	0.70±0.12 b
Flavan-3-ols (mg CTCE/g d.w.)	3.87±0.	5.45±0.044 a	4.19±0.37 a	2.69±0.13 ab	1.56±0.37 b
Tartaric acid esters (mg CAE/g d.w.)	0.51±0.	0.92±0.1 a	0.61±0.067 a	0.32±0.0024 a	0.40±0.082 a

Table S2 - Phenol content in Trebbiano berry skin of control and treated berries allowed to wither inside a dehydration chamber, at harvest time (T0), at 30% weight loss (T1), and at the end of the drying period (T2) when berries lost about 50% of weight. Treated berries were incubated for 24 h with CO₂ (30%, 14° C), and then allowed to wither at this temperature, while control berries were not subjected to the treatment and allowed to wither at the same environmental parameters. Statistically significant differences were evaluated by one-way ANOVA ($p \leq 0.05$) and different letters indicate significantly different values according to Tukey–Kramer test. GAE: gallic acid equivalents; CTCE: catechin equivalents; QCTE: quercetin equivalents; CYAE: cyanidin equivalents; CAE: caffeic acid equivalents; d.w.: dry weight.

Table - S3 Free aroma compounds in Trebbiano wine (µg/L)					
Aromatic families		Control	Treated	Odor threshold (µg/L)	Reference
Acids	Propanoic acid	176.57 ± 28.5	192.65 ± 58.5	20000	[1]
	Isovaleric acid + 2-methylbutyric acid	554.72 ± 1.3	717.91 ± 127.1	700*	[1]
	Hexanoic acid (caproic acid)	1223.52 ± 61.3	1132.02 ± 41.1	1000-10000, 8800	[1,2]
	Octanoic acid (caprylic acid)	1167.00 ± 517.7	977.33 ± 153.9	15000	[1]
	Decanoic acid (capric acid)	963.99 ± 102.5 a	72.97 ± 10.2 b	8200	[1]
	Hexadecanoic acid (palmitic acid)	552.43 ± 76.4	n.d.	-	
	Isobutyric acid	401.73 ± 290.7	694.01 ± 79.5	8100	[1]
Dioxanes and dioxolanes	N-ethylacetamide	118.74 ± 8.9	198.61 ± 117.5	-	
Alcohols	1-propanol	7183.62 ± 796.3	5784.30 ± 2010.5	-	
	Isobutanol	7950.99 ± 4625.4	8893.60 ± 1349.8	75000 40000	[2,3]
	1-butanol	377.03 ± 98.8	309.00 ± 50.2	40000	[4]
	Isoamyl alcohol	75094.42 ± 53935.9	87152.11 ± 3223.0	7000	[1]
	3-methyl-1-pentanol	105.20 ± 23.0	74.50 ± 30.4	-	
	3-ethoxy-1-propanol	1320.42 ± 311.4	1998.30 ± 348.3	-	
	2,3-butanediol	3318.60 ± 514.6 b	32459.2 ± 2956.9 a	40000	[5]
	1,2-propanediol	444.28 ± 163.3 b	1207.75 ± 507.3 a	-	
	2-furanmethanol	1791.57 ± 212.1	1534.49 ± 208.9	-	
	2-phenylethanol	17433.69 ± 3063.0	20937.82 ± 426.8	7500	[1]
	Glycerol	533.43 ± 202.7	677.20 ± 180.2	-	
	Tyrosol	1505.55 ± 724.8	2406.2 ± 303.3	-	
Esters	Isoamyl acetate	316.48 ± 92.6	308.80 ± 10.2	200	[1]
	Ethyl hexanoate	437.40 ± 62.2	415.20 ± 293.6	65, 14, 5	[3,6,7]
	Ethyl lactate	256.46 ± 50.7	236.50 ± 32.8	14000	[1]
	Acetic acid+ethyl octanoate	23608.34 ± 12429.6	24100.30 ± 11186.6	250**	[1]
	Ethyl-3-hydroxy butyrate	103.00 ± 72.8	313.57 ± 163.1	-	
	Diethyl succinate	374.60 ± 2.3 b	463.42 ± 36.2 a	100000	[5]
	Ethyl-9-decanoate	27.70 ± 19.6	n. d.	200	[6]
	1,3 propanediol monoacetate	459.82 ± 43.2 b	894.12 ± 315.4 a	-	
	Ethyl 4-hydroxybutanoate	13458.93 ± 1015.5	17427.80 ± 4017.1	-	
	Ethyl decanoate	341.71 ± 81.0 a	171.58 ± 58.3 b	200	[6]
	Diethyl malate	58.40 ± 41.3	n. d.	760000	[5]
	4-hydroxy-isopentyl butanoate	185.59 ± 26.5	260.68 ± 65.4	-	
	Ethyl c16	988.82 ± 601.7 a	134.40 ± 95.0 b	-	
	Ethyl-γ-hexadecanoate	178.39 ± 89.3 a	42.20 ± 29.8 b	-	
	Mono ethyl succinate	5010.88 ± 1302.1	4150.00 ± 1792.5	1000000	[5]
	Ethyl c18	334.58 ± 37.4	n. d.	-	
	Ethyl oleate	303.17 ± 24.4	n. d.	-	
	Ethyl linoleate	218.77 ± 178.7	n. d.	-	
Volatile phenols	4-vinyl guaiacol	126.03 ± 8.2	217.14 ± 127.9	10, 40	[7,8]
	Vanillin	16.88 ± 3.9	n. d.	200	[3]
	Methyl vanillate	4.36 ± 2.2	n. d.	-	
	Ethyl vanillate	53.75 ± 6.0	n. d.	-	
	Acetovanillone	150.35 ± 43.0	n. d.	-	
	Zingerone (vanillylacetone)	13.79 ± 9.5	n. d.	-	
	Guaiacyl propanol	351.64 ± 164.7	n. d.	-	
	Guaiacyl ethanol	295.35 ± 213.2	n. d.	-	
Other molecules	Acetoin	1694.85 ± 618.2	2029.29 ± 1036.1	150000	[7]
	1-hexanal	529.87 ± 90.9	486.72 ± 3.2	5	[9]
	Furfural	2331.91 ± 490.6	1308.34 ± 543.8	770	[5]
	γ-butyrolactone + acid c4	1663.11 ± 148.6 a	1201.35 ± 217.0 b	1000***	[5]
	Methionol	75.73 ± 9.3 a	25.48 ± 36.0 b	1000	[7]
	2-hydroxy-4-piranone	249.50 ± 57.7	1021.1 ± 932.9	-	
	Pentalactone	24.43 ± 4.5	n. d.	-	
	4-carbethoxy-γ-butyrolactone precursor	62.34 ± 21.6 a	24.81 ± 5.1 b	-	
	4-carbethoxy-γ-butyrolactone	18.17 ± 11.7	6.95 ± 2.8	-	
	26.30 ± 7.2 3-oxo-α-ionol	26.30 ± 7.2	n. d.	-	

* The threshold value is referred only to isovaleric acid.

**The threshold value is referred only to ethyl octanoate.

***The threshold value is referred only to γ-butyrolactone.

Table S3 - Free aroma compound content in Trebbiano wine (µg/L) obtained from totally air-stored berries (control) and CO₂-treated berries (treated), together with the odor threshold values (µg/L) found in the literature. Control and treated berries were allowed to wither inside a dehydration chamber. Treated berries were incubated for 24 h with CO₂ (30%, 14° C), and then allowed to wither at this temperature, while control berries were not subjected to the treatment and allowed to wither at the same environmental parameters. Different letters indicate statistically significant differences according to t-test ($p \leq 0.05$). Means not followed by any letters are not statistically different (t-test, $p \leq 0.05$).

Table S4 - Glycosylated bound aroma compounds in Trebbiano wine (µg/L)					
Aromatic families		Control	Treated	Odor threshold (µg/L)	Reference
Alcohols	Hexanol	5.40 ± 3.0 b	13.19 ± 2.3 a	2500	[5]
	Octanol	11.76 ± 1.9	11.41 ± 1.5	-	
	Myrtenol	2.11 ± 0.3	2.31 ± 0.2	-	
	2-(2-butoxyethoxy)-ethanol	6.88 ± 0.7	7.94 ± 1.1	-	
	Benzyl alcohol	8.82 ± 0.1	8.67 ± 0.2	-	
	2-phenyl ethanol	10.84 ± 0.8	10.72 ± 0.6	-	
Volatile phenols	Eugenol	1.71 ± 0.1	2.04 ± 0.3	6, 5	[3,7]
	Methyl vanillate	7.48 ± 1.1	6.60 ± 1.2	-	
	Acetovanillone	7.77 ± 0.7	8.40 ± 1.3	-	
	Zingerone (vanillylacetone)	12.88 ± 1.5	15.43 ± 2.6	-	
Terpenes	linalool oxide furanoid (LOF) CIS	n. d.	0.47 ± 0.1	6000	[5]
	LOF TRANS	n. d.	0.63 ± 0.2	6000	[5]
	Linalool	3.02 ± 1.4 b	6.40 ± 0.4 a	50	[5]
	α -terpineol	7.04 ± 0.8 b	12.50 ± 1.3 a	250	[7]
	LOP (linalool oxide pyranic) TRANS	0.69 ± 0.3	0.73 ± 1.0	-	
	LOP CIS+ methyl salicylate	1.09 ± 0.4	1.40 ± 0.6	-	
	3,7-diol	1.03 ± 0.2	1.00 ± 0.0	-	
	<i>p</i> -cymen- α -ol	3.06 ± 0.2	3.57 ± 0.9	-	
	<i>p</i> -1-menthen-7,8-diol	10.02 ± 0.6	9.82 ± 0.1	-	
	Citronellol	5.69 ± 0.9	8.10 ± 0.6	100	[3]
	Nerol	28.90 ± 0.8	27.20 ± 1.5	60	[10]
	Geraniol	148.10 ± 15.6	171.95 ± 35.0	30	[3]
	Exo-2-hydroxycineole	10.84 ± 1.0	10.81 ± 1.5	-	
	Linalool hydrate	0.92 ± 0.1	1.03 ± 0.3	-	
	Citronellol hydrate	17.37 ± 0.5 b	24.40 ± 2.7 a	-	
	3,8-diol + nerol hydrate	n. d.	7.60 ± 0.9	-	
	(Z)-8-hydroxylinalool + geraniol hydrate	14.93 ± 0.0 b	21.02 ± 1.3 a	-	
Esters	Ethyl caprate	0.94 ± 0.1	1.20 ± 0.3	-	
	Isopropyl myristate	9.91 ± 1.1	9.80 ± 1.9	-	
C13	3,4-dihydro-3-oxo-actinidol I (ACTI I)	4.37 ± 0.3	5.65 ± 1.0	-	
	ACTI II	5.52 ± 0.5	5.60 ± 1.0	-	
	ACTI III	6.92 ± 0.3	7.68 ± 1.0	-	
	ACTI IIII + 3 hydroxy- β -damascone	53.71 ± 0.5	56.48 ± 10.2	-	
	3-hydroxy-7,8-dihydro- β -ionone	9.90 ± 0.5	11.31 ± 1.9	-	
	3-oxo- α -ionol + 4-oxo- β -ionol	118.64 ± 7.8	133.29 ± 24.9	-	
	3-hydroxy-7,8-dihydro- β -ionol	55.30 ± 6.1 b	100.20 ± 11.7 a	-	
	4-oxo-7,8-dihydro- β -ionol + hydroxy- β -ionone	20.76 ± 2.6	19.51 ± 3.0	-	
	3-oxo-7,8-dihydro- α -ionol	6.72 ± 0.3 b	9.35 ± 1.6 a	-	
	3-oxo-retro- α -ionol	6.10 ± 0.5	6.66 ± 0.3	-	
	7,8-dihydrovomifoliol	23.69 ± 3.4	18.73 ± 5.8	-	
	Vomifoliol	4.90 ± 1.2	4.15 ± 2.1	-	

Table S4 - Glycosylated-bound aroma compound content in Trebbiano wine (µg/L) obtained from totally air-stored berries (control) and CO₂-treated berries (treated), together with the odor threshold values (µg/L) found in the literature. Control and treated berries were allowed to wither inside a dehydration chamber. Treated berries were incubated for 24 h with CO₂ (30%, 14° C), and then allowed to wither at this temperature, while control berries were not subjected to the treatment and allowed to wither at the same environmental parameters. Different letters indicate statistically significant differences according to t-test ($p \leq 0.05$). Means not followed by any letters are not statistically different (t-test, $p \leq 0.05$).