Optimization of roasting conditions in hydroSOStainable almonds using volatile and descriptive sensory profiles and consumer acceptance

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Abstract: HydroSOStainable almonds are harvested from trees cultivated under controlled water stress by using a regulated deficit irrigation (RDI) strategy. The aim of this study was to investigate consumers' perception to select the best roasting temperature for the hydroSOStainable almonds and its correlation with volatile compounds, descriptive sensory attributes, instrumental color, and texture. Thirty-five volatile compounds were identified and the key compounds for the roasting process were 2,5-dimethylpyrazine, furfural, and trimethyl pyrazine. Pyrazines, furans and, in general, volatiles were higher in hydroSOStainable almonds than in control. Instrumental color and trained panel showed that almonds roasted at 190 °C presented intense color and burnt notes in both irrigation treatments, while almonds roasted at 150 °C were under-roasted. Principal component analysis (PCA) grouped together the samples of the same irrigation treatment, but separated samples roasted at different temperatures. Partial least square regression (PLS) results indicated that consumers overall liking was positively linked to specific volatiles (alkanes, alcohols, aldehydes, and furans) and sensory attributes (sweetness, roasted, almond ID, nutty, hardness, and crispiness), but, negatively correlated with pyrazines, bitterness, astringency, woody, and burnt flavor notes. Penalty analysis showed that almonds roasted at 150 and 190 °C were penalized due to low roasted aroma and soft almonds, and over-roasted samples with too intense color and burn notes, respectively. While no penalization being found for almonds roasted at 170 °C. Overall, roasting at 170 °C for 10 min in a convective oven were the optimum conditions for roasting *Vairo* almonds.

Keywords: liking drivers, Prunus dulcis, pyrazines, regulated deficit irrigation, volatile compounds, water stress

Practical Application: This research describes the link between physicochemical and sensory analysis of roasted almonds giving evidence about possible sensory quality markers. Besides, it provides valuable information for the food industry to produce roasted almonds that meet consumer demands and for the agricultural sector by encouraging reduction of irrigation water consumption by almond trees.

1. INTRODUCTION

Many areas of the world are currently experiencing an unprecedented drought which has extreme consequences in all sectors including farming. Water limitations for irrigation in southeastern Spain (provinces of Alicante and Murcia) reach worrying dimensions and seriously jeopardize biodiversity (e.g. loss of traditional minor crops) (García-Tejero, Durán-Zuazo, & Muriel-Fernández, 2014). In this context, agriculture needs to implement deficit irrigation strategies, select drought tolerant, and less-water-demanding species leading to sustainable fruits and vegetables (García-Tejero et al., 2014).

Almond (*Prunus dulcis*) is the third most cultivated tree in Spain after olive trees and grape vines, and although it is a drought resistant crop, for a profitable production, irrigation water is needed (Egea et al., 2013; FAOSTAT, 2018). The regions of southeastern Spain have low or no rainfall and high evaporative demands during most of the phenological growth of the almond tree (Egea et al., 2013). Cutting off irrigation water during kernel filling (when the plant is less sensitive to water stress) is a regulated deficit irrigation (RDI) strategy aimed to reduce water consumption with minimal production losses (Girona, Mata, & Marsal, 2005). The fruits obtained under RDI conditions are called hydroSOStainable (*hydroSOS*) products and are characterized by higher contents of C-secondary metabolites in plant and of bioactive compounds in edible fruits (Lipan, Cano-Lamadrid, et al., 2019; Lipan,

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Martín-Palomo, et al., 2019; Lipan, Moriana, et al., 2019; Noguera-Artiaga et al., 2016; Sánchez-Rodríguez et al., 2019).

Nuts are widely used in the Mediterranean cuisine and can be consumed as fresh products (raw or roasted) but also can be used as ingredient for confectionery, bakery, etc., due to their desirable and characteristic flavor, and high nutritional values (Xiao et al., 2014). Almond roasting is the key unit operation in the processing of this nut; for instance, in the production of the most popular Spanish Christmas confection "*turron*" (a typical Spanish sweet made from roasted almonds and honey)(Vázquez-Araújo, Verdú, Navarro, Martínez-Sánchez, & Carbonell-Barrachina, 2009). In the food industry, roasting is not only used to enhance sensory attributes (leading to product acceptance) but also to extend product shelf-life (Youn & Chung, 2012).

Volatile compounds are key markers in evaluating the effectiveness of the roasting process and the quality of the roasted products, as they determine the characteristic flavor of the roasted almonds. No information on the aroma profile of hydroSOStainable roasted almonds is available in literature. However, volatile aldehydes, ketones, alcohols, alkanes, and terpenes have been reported in "raw" almonds, and aldehydes, such as hexanal, nonanal, and benzaldehyde, were the main aromatics (Erten & Cadwallader, 2017; Lipan et al., 2019). The authors have previously reported 26 volatile compounds in raw almonds (cultivar *Vairo*), with alcohols being the main chemical family (Lipan et al., 2019). With regard to dry "roasted" almonds, a previous study reported that aldehydes, ketones, alcohols, aromatic hydrocarbons, terpenes, and linear hydrocarbons were the main volatile compounds (Erten & Cadwallader, 2017). However, other authors reported that pyrazines, pyrroles, furans, and aldehydes were the main groups in this same matrix (Takei & Yamanishi, 1974; Takei, Shimada, Watanabe, & Yamanishi, 1974; Valdés et al., 2015; Vázquez-Araújo, Chambers, & Carbonell-Barrachina, 2012; Vázquez-Araújo, Enguix, Verdú, García-García, & Carbonell-Barrachina, 2008; Yang et al., 2013).

The moisture content is essential in establishing proper roasting conditions, with drier almonds reaching their optimal quality before than wet ones (Vázquez-Araújo et al., 2009). Almond cultivar and growing conditions (especially irrigation strategies and water stress) can influence the almond moisture and, therefore, the optimal roasting conditions (Vázquez-Araújo et al., 2009).

In this context, the aim of this study was to determine the best roasting conditions (time and temperature) for almonds grown under different irrigation strategies. To reach the decision on which roasting parameters were the best ones, data on volatile compounds, descriptive sensory profiles, and consumer's acceptance were considered.

2. MATERIALS AND METHODS

2.1 Samples

Almonds were harvested from hydroSOStainable fields during 2019 season, in a commercial orchard "La Florida," located in Dos Hermanas (Seville, Spain). The irrigation treatments were those previously described by Lipan et al. (2019). Briefly, $T1$ treatment consisted of irrigation being provided to assure crop needs, and $T2$ consists of moderate RDI, in which trees during the kernel filling period were only irrigated when the stem water potential was below −1.5 MPa. The stem water potential was measured using a pressure chamber (PMS Instrument Co., Albany, OR, USA). The monitored trees were harvested (28 weeks after blossom) with a self-propelled trunk shaker with collector. Samples were exposed horizontally to sun light until a moisture content below 5%. This operation (either by natural or artificial drying) is essential to avoid the damage produced by mold and insects (when a higher moisture content is presented by almonds), as well as to increase the oil stability and overall edible quality (Schirra & Agabbio, 1989). Later, in-shell almonds were sent to Miguel Hernández University for quality analysis and affective tests.

2.2 Roasting of almonds

$T1$ and $T2$ almonds with similar size (length = 25.0 ± 1.37 mm; width = 15.5 ± 1.00 mm; thickness = 8.98 ± 0.57 mm) and moisture content (2.34 ± 0.07%) were selected to have a uniform material for the roasting process. Roasting conditions were chosen based on published literature (Lin et al., 2016; Lukac et al., 2007; Vázquez-Araújo et al., 2008) and after preliminary experiments, the time (10 min) was considered as constant variable. The moisture content was determined from 2 g of ground almonds dried to constant mass in a stove at 60 °C. Roasting experiments were carried out using a hot-air circulation drying oven Distform My Chef (Lleida, Spain), equipped with temperatures probes to measure the air temperature inside the roasting chamber. After the heating period, roasted almonds were immediately cooled until reaching a temperature of 50 °C. Batches of 200 g were roasted in one layer for a constant time (10 min), at three temperatures: 150, 170, and 190 °C at an air velocity of 3 m/s. Once the cooling temperature was achieved, almonds were removed from the oven and kept in a stainless-steel tray at 24.4 ± 1.0 °C and 47.4 ± 0.5% relative humidity until 25 °C was achieved.

2.3 Determination of color

Color determination was carried out at 25 ± 1 °C using a Minolta Colorimeter CR-300 (Osaka, Japan). Outside color was directly measured on the skin of 10 individual almond kernels, which afterwards were half cut, and the inside color kernel was measured for each of them. The color data was presented as CIE $L^{\star}a^{\star}b^{\star}$coordinates explaining the color in a three-dimensional space. The degree of color difference (ΔE) was calculated as previously described (Cano-Lamadrid et al., 2017).

2.4 Determination of texture

The texture of 10 almonds per roasting treatment was measured at 20 ± 1 °C using a texture analyzer (Stable Micro Systems, model TA-XT2i, Godalming, UK) with a 30 kg load cell and a probe Volodkevich Bite Jaw (HDP/VB) using the following conditions: trigger was placed at 15 g, test speed was 1 mm/s over a specific distance of 3 mm. The almonds were oriented in a way that the probe perpendicularly cut the almond and all almonds were positioned with the same orientation (Figure 1). Fracturability (mm), hardness (N), work done to shear (Ns), average force (N), and number of fractures (peaks count) were the parameters analyzed.

2.5 Descriptive sensory analysis

Sensory evaluation with a trained panel was used to describe and quantify the roasted almonds appearance, basic tastes, and flavor intensities of both irrigation treatments. Ten highly trained panelists (five females and five males) from the Food Quality and Safety Group (Miguel Hernández University of Elche, Orihuela, Alicante, Spain) with ages between 25 and 62 years (median age 32) conducted the descriptive analysis. The reference products and lexicon used were based on those previously reported by other authors working with almonds and *turrón* (Lipan, Cano-Lamadrid et al., 2019; Vázquez-Araújo et al., 2012). Once finished the orientation

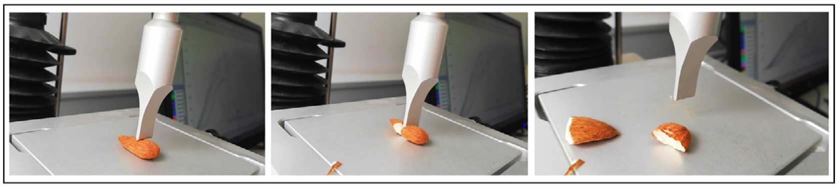

Figure 1–Texture analysis of the roasted almonds.

sessions (4), the panel was asked to evaluate the six samples corresponding to the different irrigation and roasting treatments (2 × 3); the analysis was run in triplicate. The samples were presented in 30 mL covered plastic cups using a randomized block design to avoid biases. To cleanse the palate between samples, water and unsalted crackers were available. A tasting room with individual booths (controlled temperature of 21 ± 2 °C and combined natural/artificial light) was used for the descriptive tests. A structured scale from 0 to 10 and 0.5 increments was used to quantify the intensity of the almond attributes, where 0 represents *no intensity* and 10 *extremely strong*.

2.6 Affective sensory analysis

Affective sensory analysis was carried out with 100 recruited consumers from the SensoFood Solutions consumer database (UMH). Demographic questions concerning gender, age, nuts consumption frequency, allergies, intolerances, and diet restrictions were also included in the questionnaire. The consumers profile was: 41% male and 59% female, 25% belonging to the 18 to 25 years old, 35% to 26 to 35 years old, 22% to 36 to 45 years old, and 18% to >45 years old group. Also, nuts frequency consumption was asked, and the answer was as following: 74% daily, 6% several times a week, 10% weekly, 6% several times a month, 4% once per month or less.

The samples were distributed, labeled with 3-digit codes, and served in the same recipients as described in the descriptive section. A 9-point hedonic scale was used to rate consumer liking (1 meaning "dislike extremely" and 9 meaning "like extremely"). Also, Just About Right (JAR) scales, where 1 corresponded to "not enough at all," 5 to "Just About Right," and 9 to "too much," were used to assess the attributes intensity appropriateness. Consumers were also asked to rank samples according to their preference and to check all reasons for them to choose that sample as the best (due to the color, flavor sweetness, crispiness, etc.) by using a Check All That Apply (CATA) question. The tests were also carried out in special tasting rooms with individual portable booths and using a randomized block design.

2.7 Volatile compounds

Headspace solid phase microextraction (HS-SPME) was used to determine the volatile composition of the roasted almonds. Approximately, 1 g of ground sample in a Moulinex grinder, model AR110830 (Alençon, France) for 20 seconds was placed in a hermetic vial with polypropylene cap and PTFE (polytetrafluoroethylene)/silicone septa, together with 500 μL of 12.5% aqueous NaCl and 2.5 μL of 2-acethylthiazole (1,000 mg/L) used as internal standard. This internal standard was used for the semiquantification of the volatile compounds, because no calibration curve was done for each one of the single compounds reported in this study. The vial was heated to 40 °C simulating the mouth temperature when chewing almonds as previously described by Lipan, Moriana, et al. (2019). After a stabilization period of 40 min, a 50 of 30 μm Divinylbenzene/Carboxen/Polydimethylsiloxane (DVB/CAR/PDMS) fiber was introduced in the headspace of the vial for 35 min. The fiber was specially chosen for its high capacity of trapping volatile compounds from fruits and nuts (Xiao et al., 2014). The isolation, identification, and semiquantification of the volatile compounds were performed in a gas chromatograph Shimadzu GC-17A (Shimadzu Corporation, Kyoto, Japan) coupled with a mass spectrometer (MS) detector Shimadzu GC-MS QP-5050A (identification) and a flame ionization detector, FID (semiquantification). The fiber was desorbed for 3 min in the injector port of the GC-MS. The GC was equipped with a SLB-5 ms Fused Silica Capillary Column of 30 m × 0.25 mm × 0.25 μm film thickness, 5% diphenyl, and 95% dimethyl siloxane (Supelco Analytical). Helium was used as gas carrier at a flow rate of 0.9 mL/min in a split ratio of 1:5. The oven program was: (a) initial temperature 50 °C, (b) rate of 4.0 °C/min to 130 °C, (c) rate of 10 °C/min from 130 to 180 °C, (d) rate of 20 °C from 180 °C to 280 °C. The injector and the detector were kept at 250 °C. The identification of the volatile compounds was performed using three methods: (a) retention indices, (b) retention times of standards, and (c) mass spectra (authentic chemicals and NIST69 spectral library collection) (NIST, 2020).

2.8 Statistical analysis

Data were analyzed using two-way analysis of variance (ANOVA), using "irrigation treatment" and "roasting temperature" as factors, followed by Tukey's multiple range test. Statistically significant differences were considered when $P < 0.05$. Partial least square regression (PLS) analysis was done to study the relationship of the descriptive sensory parameters and volatile compounds (x: independent variables) with the consumers overall liking data (y: dependent variable). Principal component analysis (PCA regression map) was conducted to project the samples depending on the instrumental parameters, sensory descriptors, and chemical families of the volatile compounds. Penalty analysis was also conducted, using the JAR data, to provide information about the attributes which penalized the liking of the samples under analyses and can be improved by optimizing the roasting conditions (Lawless & Heymann, 2010). Statistical analysis was performed using XLSTAT Premium 2016 and Statgraphics Plus (Version 3.1).

3. RESULTS AND DISCUSSION

3.1 Instrumental color

Almonds outside and inside instrumental color was evaluated (Table 1). Values of almonds lightness (L^*) of the outside and inside color significantly decreased ($P < 0.01$) by increasing the roasting temperature, indicating that samples became darker due to browning reactions. The characteristic golden brown color occurs due to the Maillard reaction, caramelization of sugars and dextrins to furfural and hydroxymethyl furfural and carbonization of sugars fats and protein (Skovgaard, 2004). Simultaneously, a^*, b^*, and C^*

Table 1–Instrumental color and texture of roasted almonds as affected by roasting temperature and irrigation treatments.

	Outside color						Inside color						Texture				
	L^*	a^*	b^*	C^*	h	ΔE	L^*	a^*	b^*	C^*	h	ΔE	F (mm)	H (N)	WS (Ns)	AF (N)	NF
							ANOVA[a]										
Irrigation	**	***	***	***	***	NS	NS	***	***	***	*	***	NS	***	**	NS	NS
Roasting	**	***	***	***	***	***	*	***	***	***	*	***	*	***	**	***	NS
Irrigation × Roasting	**	***	***	***	***	***	*	***	***	***	**	***	*	***	**	***	NS
							Tukey Multiple Range Test[b]										
Irrigation × Roasting																	
*T*1-150 °C	43.3a	18.1a	28.3ab	33.6a	57.4ab	4.94b	79.5a	1.53b	13.3c	13.4c	83.3a	6.59c	1.40a	59.6ab	42.1ab	29.8ab	16.8
*T*2-150 °C	46.0a	18.0a	31.7a	36.5a	60.4a	6.01b	76.9a	1.76b	11.7c	11.9c	80.9ab	9.21bc	1.41a	67.8a	47.1a	32.8a	18.5
*T*1-170 °C	41.9ab	18.1a	26.9ab	32.4a	56.0b	5.56b	79.0a	3.03b	21.5b	21.7b	82.5a	11.20b	1.38b	53.2abc	34.4ab	24.3abc	12.9
*T*2-170 °C	41.1ab	16.6a	25.1b	30.6a	54.9b	6.67b	80.1a	3.53b	22.9b	23.2b	81.5ab	11.81b	1.50a	46.1bc	29.2ab	19.1c	15.2
*T*1-190 °C	36.1b	13.3b	15.8c	20.6b	50.0c	15.0a	71.3b	6.75a	31.9a	32.6a	78.0ab	24.60a	1.18b	41.0c	24.1b	19.9c	14.6
*T*2-190 °C	41.0ab	12.6b	15.3c	19.8b	50.3c	12.9a	71.6b	6.95a	29.2a	30.0a	76.8b	22.44a	1.20b	43.4bc	25.6ab	20.8bc	15.9

[a] NS, not significant at $P < 0.05$; *, **, and *** significant at $P < 0.05$,0.01, and 0.001, respectively.
[b] Values (mean of 10 repetitions per roasting treatment) followed by the same letter, within the same column and factor, were not significantly different ($P < 0.05$), according to Tukey's least significant difference test.
L^*, 0-black and L^*, 100-white, a^*, reddish and -a^*, greenish, b^*, yellowish and -b/*, blueish, C, Chroma, h, Hue, ΔE, the degree of color difference; F , fracturability, H, hardness, WS, work to shear, AF, average force, NF, number of fractures.

increased inside the kernel, implying a more intense and brownish (mix of red and yellow color coordinates) color as result of increasing roasting temperature. The decrease in L^* values and increase in a^* values were previously also reported in roasted peanuts and the phenomenon was related to the higher melanoidin production from Maillard reactions and with a lower finished moisture content (Lykomitros, Fogliano, & Capuano, 2018). However, the outside color was characterized by lower values of a^*, b^*, and C^* which meant that red and yellow notes decreased in the almond skin exposed to the highest temperature, 190 °C. Other authors have reported different results, maybe because they have measured color in ground almonds (Vázquez-Araújo et al., 2009), while in the present study it was measured directly on the almonds skin. The skin polyphenols might have had also an impact, because each almond cultivar has a unique polyphenol profile that can affect the almond color (Bolling, 2017); they also contribute to the degree of browning developed during roasting, as polyphenols may appear to affect Maillard browning (Bolling, 2017). For instance, a negative correlation has been previously reported between polyphenols and the browning reaction precursors (sugars and amino acids) (Noor-Soffalina, Jinap, Nazamid, & Nazimah, 2009). Because the polyphenols have a high tendency to form complexes with protein, polysaccharide and alkaloid; and consequently, to influence color and to reduce the flavor due to binding of polyphenol on aroma precursors (free amino acids and sugars) and aroma compounds formed during roasting (Misnawi, Jinap, Jamilah, & Nazamid, 2004).

Regarding the irrigation treatment, lower L^* value was observed in almonds irrigated at the optimum plant needs (*T*1). Almonds of *T*1 became darker before those of *T*2 at 190 °C roasting temperature, while the other two roasting temperatures showed similar results between the irrigation treatments. This might be related to the differences in chemical composition of hydroSOStainable almonds (*T*2), which had been reported to have a higher sugar content, etc. (Lipan, Moriana, et al., 2019; Lipan et al., 2020).

High ΔE (which represents the total color difference) values indicated a higher color change with respect to the raw almonds (Table 1). In general, the outside color did not significantly change when the roasting temperature was increased from 150 to 170 °C, but significantly increased at 190 °C. While the inside color increased with each roasting temperature. Conventional and hydroSOStainable almonds exhibit statistically similar behavior in inside color parameter in each roasting temperature. However, the hydroSOStainable almonds recorded a higher inside color change for the lowest roasting temperature, and no changes between conventional and hydroSOStainable almonds were observed at 170 and 190 °C.

3.2 Instrumental texture

Fruit texture is important as it is a primary determinant of consumer acceptance and the rejection of roasted almonds is mainly due to inappropriate textural attributes (e.g. not crunchy products) (Cheely et al., 2018). Hardness, work done to shear, and average force were significantly reduced with increasing roasting temperatures, while no significant differences were observed for fracturability and number of fractures (Table 1). Authors working with raw *Vairo* almonds reported higher values of facturability (1.87 mm), hardness (73.2 N), and lower numbers of fractures (9) (Lipan et al., 2019) than those found in roasted almonds from the same cultivar ($F = 1.35$ mm, $H = 52$ N, and NF = 16, respectively); as roasted almonds are less hard but more fracturable and crispy than the raw ones (Lipan, Martín-Palomo, et al., 2019). Crunchiness is a textural characteristic important for consumer acceptability (Cheely et al., 2018), and an increment in crunchiness mainly occurs due to dehydration, browning, lipid oxidation, and other structural changes (Varela, Chen, Fiszman, & Povey, 2006). The degradation of the structure during roasting cause changes in textural attributes such as crispiness, grittiness, porosity, and fracturability (Varela et al., 2006).

Significant differences ($P < 0.001$) were detected between the irrigation treatments (*T*1 and *T*2) and also among the roasting temperatures for the hardness attribute. HydroSOStainable almonds (*T*2) had the hardest texture, which decreased when the roasting temperature increased. Some authors have reported that water deficit can impact the texture of the nut due to the water stress effect on cell size, cell turgor, solute transport, and the accumulation of osmotically active solutes at the cell level (Ripoll et al., 2014). Thus, a reduction in turgor and moisture content which is directly affected by the roasting process, because this involved dehydration, with effect on color, flavor, and texture (Huang, 2014; Perren & Escher, 2013). Moreover, water deficit has also been shown to cause alteration in the chemical composition and the physical properties of the cell wall (Lipan, Martín-Palomo, et al., 2019; Lipan, Moriana, et al., 2019; Peleman et al., 1989). It has also been reported that the accumulation on antioxidants might prevent oxidative damage with a positive effect on the tomatoes texture (Dumville & Fry,

Table 2–Volatile compounds profile in roasted almonds of Vairo cultivar, retention index, and main odor and aroma descriptors (The Good Scent Company, 2018; National Center for Biotechnology Information, 2018).

Compound	Chemical family	Code	RT (min)	Retention Index[b]		Odor descriptor
				Experimental	Literature[c]	
Pentanal	Aldehyde	V1	2.194	723	715	Bready, fruity, nutty berry, cocoa chocolate notes, coffee
Hexanal	Aldehyde	V2	3.901	804	804	Fresh green fatty aldehydic grassy leafy fruity sweaty
2-Methyl pyrazine	Pyrazine	V3	4.608	832	833	Nutty, brown, nut skin, roasted
Furfural	Furan	V4	4.679	842	845	Almond, caramel, sweet, woody, baked bread
2-Heptanone	Ketone	V5	5.800	895	892	Cheese, banana like, fruity odor
Nonane	Alkane	V6	5.907	900	900	Gasoline
Heptanal	Aldehyde	V7	6.083	906	906	Fresh, fatty green herbal, citrus
2,5-Dimethylpyrazine	Pyrazine	V8	6.595	923	922	Cocoa, roasted nuts, woody
2-Heptenal	Aldehyde	V9	7.716	961	959	Green, fatty
Benzaldehyde	Aldehyde	V10	7.965	970	967	Almond, fruity, powdery, nutty, cherry, sweet, bitter
Heptanol	Alcohol	V11	8.197	978	970	Musty, leafy green, fruity, apple, banana and nutty and fatty notes
2,2,4,6,6-Pentamethylheptane[a]	Alkane	V12	8.557	990	997	
Decane	Alkane	V13	8.860	1,000	1,000	
2-Ethyl-3-Methylpyrazine	Pyrazine	V14	9.094	1,007	1,001	Roasted, nutty, potato, corn, peanut, raw
Trimethylpyrazine	Pyrazine	V15	9.244	1,011	1,018	Cocoa, earthy, musty, nutty, roasted peanut hazelnut
2-Ethylhexanol	Alcohol	V16	10.032	1,034	1,030	Citrus, fresh, floral oily sweet
Benzeneacetaldehyde	Aldehyde	V17	10.649	1,052	1,048	Green, sweet, floral, hyacinth, rose, chocolate
1-Octanol	Alcohol	V18	11.597	1,079	1,074	Waxy, green, orange, rose, mushroom, sweet fatty, coconut
2,5-Dimethyl-3-Ethylpyrazine	Pyrazine	V19	11.770	1,085	1,079	Potato, cocoa, roasted, nutty
2,3-Dimethyl-5-Ethylpyrazine	Pyrazine	V20	12.018	1,091	1,090	Burnt, popcorn, roasted, cocoa
2,6-Dimethyl-3-Ethylpyrazine	Pyrazine	V21	12.115	1,094	1,094	Burnt, almond, roasted nuts, coffee, caramel, peanut
Undecane	Alkane	V22	12.336	1,100	1,100	Waxy, fruity, creamy, fatty, floral, pineapple
2,3-Diethyl-5-methylpyrazine	Pyrazine	V23	12.530	1,104	1,094	Musty, nutty, meaty, vegetable, roasted hazelnut, nut skin
Nonanal	Aldehyde	V24	12.653	1,109	1,107	Waxy, aldehydic, citrus, green lemon peel, orange peel
Furaneol	Furan	V25	14.311	1,155	1,159	Sweet cotton candy, burnt brown caramel, strawberry, sugar
2,6-Diethyl-3-Methylpyrazine	Pyrazine	V26	11.551	1,161	1,163	Green, nutty, meaty, vegetable
3-Methylundecane	Alkane	V27	14.885	1,170	1,169	Mild aliphatic hydrocarbon odor
1-Nonanol	Alcohol	V28	15.409	1,184	1,174	Fresh, clean, fatty, floral, rose, orange, dusty, wet, oily
Dodecane	Alkane	V29	15.969	1,200	1,200	
2-Decenal	Aldehyde	V30	18.417	1,269	1,266	Fatty, orange, rose, floral, green
Tridecane	Alkane	V31	19.552	1,300	1,300	
2,4-Decadienal	Aldehyde	V32	20.444	1,331	1,323	Fatty, oily, citrus, green, chicken skin-like
Tetradecane	Alkane	V33	22.493	1,400	1,400	Mild waxy
Hexadecane	Alkane	V34	26.187	1,600	1,600	
1-Tetradecanol	Alcohol	V35	26.867	1,664	1,671	Fruity, waxy, coconut

[a] Tentatively identified (identification only based on spectral database).
[b] RT, retention time.
[c] NIST (National Institute of Standards and Technology) (NIST, 2020).

2003). In this way, the nuts texture was reported to be correlated to the fat content in walnuts, showing that when the fat content is reduced, the hardness is also reduced due to the cell wall collapse (Crowe & White, 2003).

3.3 Volatile composition

Many volatile compounds are generated through Maillard reaction and lipid oxidation during the roasting process (Vázquez-Araújo et al., 2008; Vázquez-Araújo et al., 2009). A total of 35 volatile compounds were identified in roasted almonds: aldehydes ($n = 9$), pyrazines (9), alkanes (9), alcohols (5), furans (2), and ketone (1). Table 2 shows the retention time, the retention indexes used for the identification of the aroma compounds and their odor descriptors. Similar results were previously reported by others with pyrazines and aldehydes being the chemical families in roasted almonds (Takei & Yamanishi, 1974; Takei et al., 1974; Valdés et al., 2015; Vázquez-Araújo et al., 2008; Vázquez-Araújo et al., 2012; Yang et al., 2013), and also linear hydrocarbons (Erten & Cadwallader, 2017). In this way, the previously identified chemical families in nuts aroma include (Alasalvar, Shahidi, & Cadwallader, 2003): (i) alcohols (heptanol, 1-octanol), (ii) ketones (2-heptanone), (iii) aldehydes (heptanal), (iv) aromatic hydrocarbons (benzaldehyde), (v) furans (furfural), (vi) pyrazines (2-methyl pyrazine), and (vii) linear hydrocarbons (nonane, dodecane, etc.).

Table 3–Volatile compounds (mg/kg) found in roasted almonds as affected by water stress and roasting process.

	ANOVA[a]			Irrigation x Roasting					
Code	**Irrigation**	**Roasting**	**Irrigation x Roasting**	***T*1 150 °C**	***T*2 150 °C**	***T*1 170 °C**	***T*2 170 °C**	***T*1 190 °C**	***T*2 190 °C**
				mg/kg					
V1	***	***	***	0.04de	0.02e	0.15b	0.06cd	0.08c	0.25a
V2	NS	***	***	0.22b	0.10c	0.27b	0.15c	0.30a	0.35a
V3	***	***	***	Nd	Nd	0.02b	nd[c]	0.40a	0.19b
V4	***	***	***	Nd	0.02e	0.34d	0.62c	0.97b	1.47a
V5	***	***	***	0.01c	0.04a	0.02c	0.01c	0.03b	0.02b
V6	***	***	***	0.03b	0.04a	0.02c	0.01d	0.01d	0.04a
V7	***	***	***	0.01d	0.02bc	0.02bc	0.02cd	0.03b	0.06a
V8	***	***	***	0.04c	0.02c	0.87b	0.84b	2.65a	2.93a
V9	***	***	***	0.01c	0.01c	0.03b	0.03b	0.03b	0.07a
V10	***	***	***	0.13c	0.12c	0.16c	0.18c	0.24b	0.41a
V11	***	***	***	0.02c	0.02b	0.02b	0.02b	0.03b	0.03a
V12[b]	*	*	*	2.70b	3.54a	3.00ab	3.22ab	2.74b	2.87ab
V13	NS	NS	NS	0.12	0.11	0.13	0.11	0.12	0.11
V14	***	***	***	0.01d	Nd	0.05d	0.11c	0.28a	0.16b
V15	***	***	***	0.02d	0.02d	0.19cd	0.33c	1.03b	1.23a
V16	***	***	**	0.16ab	0.16ab	0.16ab	0.13bc	0.12c	0.19a
V17	***	***	***	0.04d	0.03d	0.24c	0.30ab	0.26bc	0.34a
V18	NS	***	***	0.02cd	0.01d	0.03bc	0.03b	0.03b	0.04a
V19	***	***	***	0.07d	0.05d	0.21c	0.25c	0.54b	0.64a
V20	***	***	***	Nd	Nd	0.01c	0.01c	0.04a	0.03b
V21	***	***	***	Nd	Nd	0.04c	0.04c	0.07b	0.09a
V22	**	**	**	0.13c	0.16bc	0.21a	0.16abc	0.17ab	0.16bc
V23	***	***	***	0.01d	0.01d	0.04c	0.06c	0.08b	0.11a
V24	***	***	***	0.11d	0.07d	0.20c	0.22c	0.29b	0.44a
V25	***	***	***	0.01c	0.01c	0.01c	0.02a	0.01bc	0.02ab
V26	***	***	***	0.03c	0.02c	0.01d	0.01d	0.05b	0.08a
V27	NS	***	***	0.03cd	0.02d	0.03bcd	0.04a	0.03abc	0.04ab
V28	***	***	***	0.05bc	0.04c	0.05bc	0.07a	0.06ab	0.08a
V29	***	***	**	0.13c	0.16bc	0.19ab	0.22a	0.16bc	0.16bc
V30	NS	***	***	Nd	0.01c	0.01c	0.02b	0.03a	0.02b
V31	***	***	***	0.09c	0.14b	0.12bc	0.17a	0.10c	0.11c
V32	***	***	***	0.01d	0.02c	0.01cd	0.02b	0.02b	0.05a
V33	***	***	***	0.03c	0.03c	0.03c	0.06a	0.04bc	0.05b
V34	NS	NS	***	0.01bc	0.01b	0.01c	0.02a	0.01b	0.01b
V35	NS	NS	***	0.01cd	0.03a	0.01d	0.02c	0.03b	0.01cd
Σ	***	***	***	4.31d	5.06cd	6.90b	7.55b	11.1a	12.8a

[a] NS, not significant at $P < 0.05$; *, **, ***, significant at $P < 0.05$, 0.01, and 0.001, respectively.

[b] Tentatively identified.

[c] Values (mean of three replications) followed by the same letter, within the same row and factor, were not significantly different ($P < 0.05$), according to Tukey's least significant difference test.

The quantification of these volatile compounds is based on the use of 2-acethylthiazole as internal standard.

The total content of volatile compounds was significantly different among samples (Table 3). Almonds roasted at 150 °C showed the lowest total content of volatile compounds (4.77 mg/kg), followed by those roasted at 170 °C (7.32 mg/kg) and at 190 °C (11.9 mg/kg). Almonds roasted at 150 °C showed similar volatile content to those reported in raw almond for *Vairo* (4.39 mg/kg) (Lipan et al., 2019), and *Bute* and *Padre*cultivars (4.36 mg/kg), which meant that almonds roasted at 150 °C temperature showed very similar volatile profile to the raw almonds and were under-roasted. Generally, the aroma of raw almonds is weak and a low total content of volatile compounds is expected (Lipan, Martín-Palomo, et al., 2019); however, as observed, the roasting process increases the generation of volatile organic compounds in almonds if a threshold temperature is reached; 150 °C is below this threshold. This might happen because Maillard reaction, which is responsible for the increasing in volatile compounds, generally begins at temperatures above 140 °C (Ghaderi & Monajjemzadeh, 2020). The total volatile content in almonds roasted at 170 and 190 °C were similar to those reported by other authors, who showed similar results (in the range between 6.17 and 16.0 mg/kg) in *Marcona* and *Comuna* cultivars roasted at 200 °C for 12, 15, 17, 20, 23 min (Vázquez-Araújo et al., 2009) and *Bute/Padre* cultivars roasted at 138 °C for 28, 33, and 38 min (Xiao et al., 2014), using convection ovens in both studies.

In general, the contents of aldehydes, pyrazines, furans, ketones, alkanes, alcohols, and consequently the total volatile content of hydroSOStainable almonds (*T*2) were significantly higher than in *T*1 samples. *T*2 samples were characterized by a higher content of volatiles having sensory descriptors such as almond, nutty, bready, and chocolate notes (Table 2). An increase in volatile compounds in hydroSOStainable almonds may occur due to the alteration in the chemical composition under water stress conditions (Ju et al., 2018).

Aldehydes were one of the main chemical family found, with hexanal (V2), benzaldehyde (V10), benzeneacetaldehyde (V17), and nonanal (V24) being the predominant aldehydes; all three compounds increased with the roasting temperature. Aldehydes, as well as ketones may be formed by degradation and auto-oxidation of fatty acids during roasting process and storage, because 48 to 67% of kernel is oil, composed by 63 to 78% oleic acid, and 12 to 27% linoleic acid among others with roasting temperature and storage (Erten & Cadwallader, 2017; Lipan, Martín-Palomo, et al., 2019; Xiao et al., 2014). The unsaturated fatty acids are precursors of nonanal and hexanal aldehydes, which in high concentrations (more than 2.1 and 6.0 μg/kg hexanal) are responsible for the fat oxidation and consequently for the off-flavors and inedible almonds (Perren & Escher, 2013; Yang et al., 2013). Thus, the present values of hexanal, even those obtained in almonds roasted at the highest roasting temperature 190 °C (0.33 mg/kg) were way below than those previous reported in roasted almonds at the end of shelf life (Yang et al., 2013), demonstrating the freshness of the samples.

Benzaldehyde (V10), is a breakdown product of amygdalin (cyanogenic glycoside naturally generated in almond) and so the predominant volatile compound mainly in raw bitter almond (Kwak et al., 2015). Although it was reported that roasting process might reduce the benzaldehyde level for about 90% in sweet and bitter almonds (Hojjati, Lipan, & Carbonell-Barrachina, 2016; Xiao et al., 2014), the opposite was observed in the present study, in which benzaldehyde increased with the heating treatment being higher in *T*2 samples. Other authors also reported an increase in V10 with the roasting conditions (time and temperature) in roasted sunflower seeds. This phenomenon might occur as a consequence of lipid oxidation in which a carbonyl-amine reaction (Strecker degradation) is required to produce compounds that would be later degraded by the free radicals produced in the decomposition of lipid hydroperoxides to benzaldehyde and other compounds (Hidalgo & Zamora, 2019). In addition, "Vario" cultivar is characterized by very low levels of benzaldehyde in raw almonds (Lipan et al., 2019).

Pyrazines were also one of the main volatiles found in these roasted nuts. Pyrazines, such as 2,5-dimethylpyrazine (V8), 2-ethyl-3-methylpyrazine (V14), trimethylpyrazine (V15), 2,5-dimethyl-3-ethylpyrazine (V19), 2,3-diethyl-5-methylpyrazine (V23), and 2,6-diethyl-3-methylpyrazine (V26), were already present in samples roasted at 150 °C; however, different pyrazines appeared in the aroma profile of roasted almonds only after reaching temperatures of 170 and 190 °C; these were 2-methyl pyrazine (V3), 2,3-dimethyl-5-ethylpyrazine (V20), and 2,6-dimethyl-3-ethylpyrazine (V21). The most abundant pyrazine found in this study was V8 (1.22 mg/kg mean value for all samples), followed by V15 (0.47 mg/kg) and V19 (0.29 mg/kg) and their contents increased with increasing roasting temperatures. Similar results were also reported by other authors working with roasted almonds from *Marcona* and *Comuna* cultivars roasted at 200 °C for 12, 15, 17, 20, and 23 min (Vázquez-Araújo et al., 2009). These compounds are formed during heating *via* Maillard sugar-amine reactions and Strecker degradation and contribute to the nutty and roasted notes of the roasted-almond aroma (Alasalvar et al., 2003). Pyrazines might be considered key compounds in the roasted almonds aroma with a positive correlation between pyrazines and roasted-almond odor (Vázquez-Araújo et al., 2009), when the sample does not present burn notes (Vázquez-Araújo et al., 2009). However, as shown in Table 3, 2,6-dimethyl-3-ethylpyrazine (V21), which is a pyrazine with "burn," almond and coffee notes (The Good Scent Company, 2018), was not found at 150 °C, appeared at 170 °C, and doubled its concentration at 190 °C. This could be expected to be described as burn notes by the trained and consumer panels that will evaluate the samples later on. Regarding irrigation treatments, in general pyrazine tend to increase in hydroSOStainable almonds and similar results were also observed in pistachios when a moderate RDI was applied (Carbonell-Barrachina et al., 2015). However, the pyrazines were reduced in pistachios when the stressed was increased. This increase in pyrazine of fruits growth under moderate water stress, might be related to the sugars and amino pyrazine precursors acids which were reported to increase in deficit irrigation conditions (Ju et al., 2018; Lipan et al., 2020). Moreover, authors found a close relationship between the accumulation of the volatile compounds and amino acids concentration in grapes (Ju et al., 2018).

Other compounds, such as furans (e.g. furfural and furaneol), resulting from sugars degradation (glucose and fructose) (Vázquez-Araújo et al., 2008; Xiao et al., 2014), were also found as the roasting process was more intense (higher temperatures). Furfural was not detected at 150 °C for the *T*1 almonds but appeared at 170 °C (0.48 mg/kg) and increased at 190 °C (1.22 mg/kg). This phenomenon was expected because furfural is a compound of Maillard reaction and is a marker of the severity of heat treatments (Agila & Barringer, 2012). This compound was not reported in raw *Vairo* (Lipan, Moriana, et al., 2019) cultivar, neither in *Nonpareil* (Kwak et al., 2015), *Bute*, or *Padre* cultivars in previous studies, and is a byproduct of Maillard reactions initiated with the roasting process (Xiao et al., 2014). In raw fruits, furfural was reported in wild almonds (Hojjati et al., 2016) and sunflower seeds (Guo, Jom, & Ge, 2019). It was also reported that increased with the roasting time, temperature, and microwave power due to the acid hydrolysis or heating of fruits polysaccharides containing hexoses or pentoses (Petisca, Pérez-Palacios, Farah, Pinho, & Ferreira, 2013; Skovgaard, 2004). Regarding the irrigation treatment, in *T*2 treatment appeared even from the lowest heating temperature (150 °C) being always higher than in *T*1 samples (4.1-, 1.8-, and 1.5-fold at 150, 170, and 190 °C, respectively). This might be related to the sugars content which was reported to be raised in fruits grown under water stress conditions due to the osmotic adjustments (Lipan, Moriana, et al., 2019).

3.4 Descriptive sensory analysis

Descriptive sensory analysis was performed to establish the sensory profile of the roasted almonds. Fourteen flavor and texture attributes were evaluated in roasted almonds and their intensities are summarized in Table 4. As shown, all the assessed attributes, except benzaldehyde and cohesiveness, were significantly affected by the roasting temperatures and irrigation treatment. The higher the oven temperature, the higher the intensity of the following attributes: bitterness, astringency, roasted, burnt, woody, and aftertaste. The opposite was shown for sweetness, which significantly decreased with increasing temperature; the same trend was also observed for the overall nut and almond-ID flavor attributes. Hardness, crispiness, and adhesiveness were the texture attributes evaluated; hardness and crispiness had similar intensities in samples roasted at 150 and 170 °C and lower in those roasted at 190 °C. Finally, adhesiveness was slightly reduced from 4.1 to 3.0 when the roasting temperature increased.

Sweetness, overall nuts, almond-ID, hardness, and crispiness intensities were higher in hydroSOStainable samples (*T*2) than in full irrigated almonds (*T*1). This sensory finding agreed with previously discussed findings showing that volatile compounds with nutty (pentanal and 2,6-dimethyl-3-ethylpyrazine) and almond (benzaldehyde, furfural, etc.) descriptors having also higher contents in hydroSOStainable almonds. Roasted notes, however, were higher in fully irrigated samples, as found by the trained panel and the analytical analysis (2-ethyl-3-methylpyrazine).

Table 4–Descriptive sensory analysis of roasted almonds as affected by roasting temperature and deficit irrigation.

	Sweetness	Bitterness	Astringency	Overall nut	Almond-ID	Roasted	Brunt	Benzaldehyde	Woody	Hardness	Cohesiveness	Crispiness	Adhesiveness	Aftertaste
						ANOVA Test[a]								
Irrigation	***	***	***	***	***	***	***	NS	*	**	NS	*	*	***
Roasting	***	***	***	***	***	***	***	NS	*	**	NS	*	*	***
Irrigation × Roasting	***	***	***	***	***	***	***	NS	*	**	NS	*	*	***
						Tukey Multiple Range Test[b]								
Irrigation x Roasting														
*T*1-150 °C	4.90a	0.10c	0.40bc	7.00a	7.30a	3.20c	nd^c	0.10	2.95ab	5.20ab	1.75	6.80b	4.05a	7.00abc
*T*2-150 °C	4.75a	0.15c	0.30c	6.25ab	6.55ab	2.45c	nd^c	0.10	2.20b	5.40a	2.15	7.30a	4.05a	6.15c
*T*1-170 °C	3.50b	2.10b	1.10bc	5.70b	4.90c	5.90b	nd^c	0.15	2.45ab	5.35ab	1.85	7.80a	3.55ab	6.90bc
*T*2-170 °C	4.95a	2.00b	0.90bc	6.40ab	5.95b	6.75ab	nd^c	0.20	2.90ab	5.45a	2.25	7.70a	3.80ab	6.75bc
*T*1-190 °C	2.75b	3.40a	2.45a	4.40c	3.50d	7.85a	2.80^a	0.50	3.35a	4.35b	1.95	6.50b	2.75b	8.05a
*T*2-190 °C	3.45b	2.85a	1.50ab	4.90c	3.60d	7.40a	2.10^b	0.25	2.70ab	4.15b	2.10	6.40b	3.15ab	7.40ab

[a] NS, not significant at $P < 0.05$; *, **, and *** significant at $P < 0.05$, 0.01, and 0.001, respectively.
[b] Values (mean of 10 trained panelists) followed by the same letter, within the same column and factor, were not significantly different ($P < 0.05$), according to Tukey's least significant difference test.
The used scale ranged from 0 = no intensity to 10 = extremely strong intensity.

3.5 Principal component analysis

For an easy visualization of the relationships among all variables of the roasted almonds at different temperatures, a PCA was run for all six samples, including only significantly different variables: color coordinates, volatile compounds, and descriptive sensory attributes. Figure 2 shows the two principal components which explained 84.96% of the samples variation. As observed, samples roasted at different temperatures were grouped separately, but the irrigation treatments roasted at the same temperature were grouped together. Samples roasted at 150 °C were mainly described by ketones, alcohols, alkanes, adhesiveness, sweetness and almond ID; these chemical families were those very close to raw almonds (fresh, fruity, herbal, sweet, and green notes) (Lipan, Moriana, et al., 2019). Sensory attributes also demonstrated the proximity between 150 °C almonds with the raw ones, being high intensities of adherence to teeth, sweetness, and fresh almond-ID. Almonds roasted at 170 °C were described as hard, with nutty flavor and aldehydes aromatics, and with light inside color. Aldehydes was the chemical family closer to the 170 °C almonds, with descriptors such as nutty, chocolate, bready, and almond notes (The Good Scent Company, 2018; Lu Xiao et al., 2014). Finally, 190 °C roasted almonds were characterized by burnt, woody, benzaldehyde, and roasted notes, long aftertaste, due to their astringency and bitterness and volatiles such as pyrazines and furans. As shown, these samples presented burnt notes which were clearly identified by the sensory panel, and also detected using analytical techniques such as GC-MS. Some pyrazines (2,5-dimethyl-3-ethylpyrazine, 2,3-dimethyl-5-ethylpyrazine) and volatile compounds derived from furans (e.g. furaneol) have been reported to contribute to flavor notes such as burnt, roasted, coffee, and burnt brown (The Good Scent Company, 2018). Burnt notes in roasted almonds are not desirable and roasting conditions must be adjusted to avoid their generation (Hojjati et al., 2016). In this context, "the higher the volatile compounds, the better the odor and aroma of roasted almonds" statement (Hojjati et al., 2016) is not valid due to the burnt notes generated by the excessive heat treatment at 190 °C for 10 min.

3.6 Consumers acceptability and driving sensory attributes

A consumer study was carried out to determine the drivers of liking for roasted almonds, and to offer industries processing almonds relevant information regarding the temperature guidelines. For the samples preference, most consumers chose *T*1 (27 %) and *T*2 (24 %) samples roasted at 170 °C as the best almonds due to their roasted almond flavor (62%), aftertaste (43%), texture (38%), and sweetness (29%). Regarding the purchase intention:

i.) 61% (*T*1) and 59% (*T*2) of consumers were willing to buy almonds roasted at 150 °C;
ii.) 78% (*T*1) and 82% (*T*2) of consumers were willing to buy almonds roasted at 170 °C; and,
iii.) Only 25% (*T*1) and 42% (*T*2) of consumers were willing to buy almonds roasted at 190 °C.

Partial least square regression (PLS) analysis was conducted to determine the drivers of liking of the samples and was explained by 93% of the variation in Y variables (volatiles and sensory descriptive results) and 87% of the variation in X variables (consumers) (Calín-Sánchez et al., 2011; Cano-Lamadrid, Vázquez-Araújo, Sánchez-Rodríguez, Wodyło, & Carbonell-Barrachina, 2018; Vázquez-Araújo, Chambers, Adhikari, & Carbonell-Barrachina, 2010; Vázquez-Araújo, Koppel, Iv, E., & Carbonell-Barrachina,

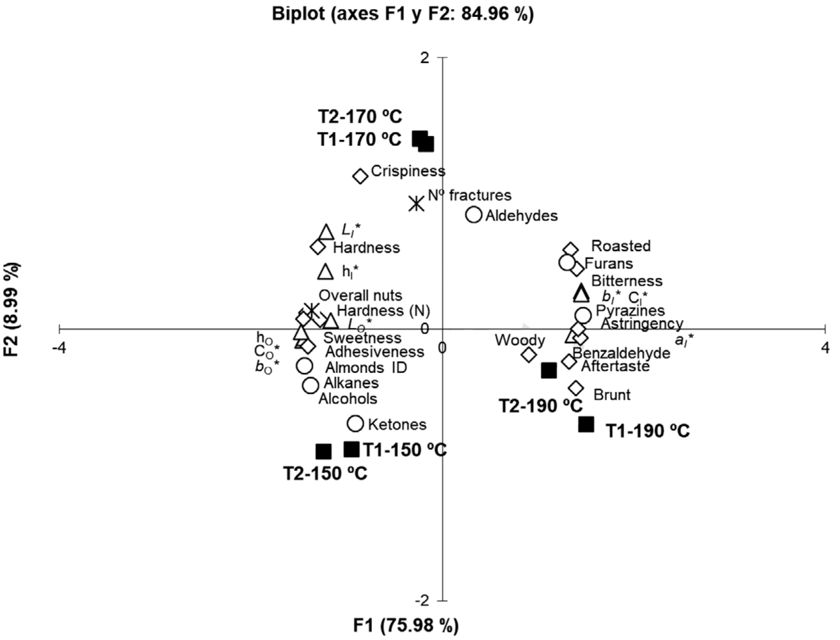

Figure 2–Principal Components Analysis (PCA) scores biplot showing the relationship among instrumental color, texture, volatile chemical family, and descriptive sensory attributes. Legend: ■ roasting treatments; △ color coordinates outside (*L**o, *a**o, *b**o) and inside (*L**i, *a**i, *b**i) kernel; ○ volatile compounds; ◇ sensory attributes.

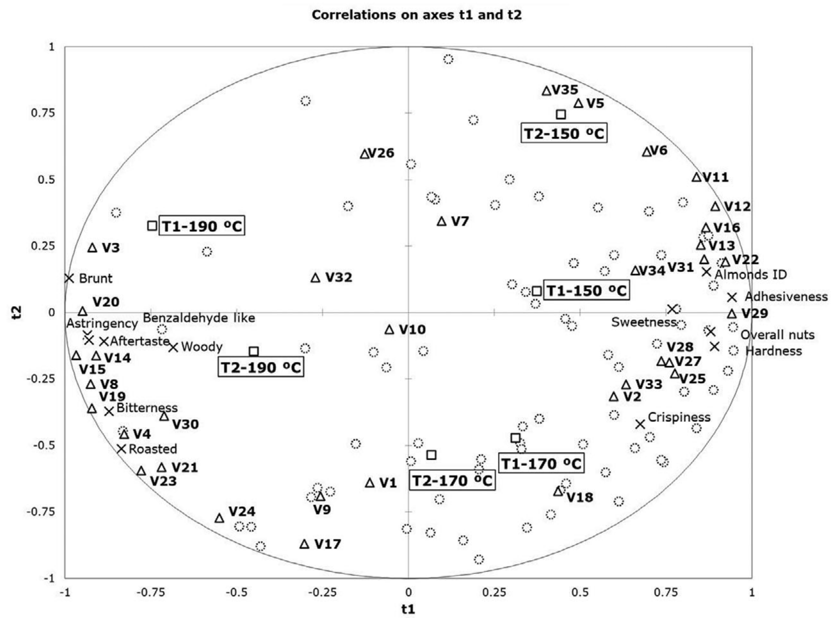

Figure 3–Partial Least Squares (PLS) regression of volatile compounds and descriptive sensory attributes (Y) and consumers overall liking (X) of roasted almonds. Legend: □ roasting treatments; △ volatile compounds, × sensory attributes, ○ consumers' overall liking.

2011). Data are represented using a map to provide information of consumers overall liking with the 35 detected volatile compounds and descriptive sensory parameters (Figure 3); only statistically significant parameters ($P < 0.05$) were included in this analysis. Figure 3 shows how almost all consumers were close to volatiles corresponding to alkane (V6, V12, V13, V22, V27, V29, V31, V33, and V34), alcohol (V11, V16, V18, V28, and V35), aldehyde (V1, V2, and V7), and ketone (V25) families. These compounds are characterized by fruity, creamy, fresh, fatty, bready, nutty, caramel-like and cocoa chocolate notes; aromas mainly related to a mild roasting. On the other side, there were those compounds belonging to the pyrazines family. Pyrazines together with furans and pyrroles are considered key compounds of roasted almonds formed during heating via Mallard sugar-amine reactions (Hojjati et al., 2016); they contribute to desirable nutty and toasty odors in roasted hazelnuts and almonds, if they are in a proper concentration (Alasalvar et al., 2003; Vázquez-Araújo et al., 2009). However, a high content of pyrazines is not associated to high quality roasted almonds, if they smell and taste burnt (Vázquez-Araújo et al., 2009). Regarding the consumer overall liking and the relationship with different descriptive sensory attributes, the main group of consumers was located close to the attributes: sweetness, almond-ID, overall nut, hardness, and crispiness showing that these descriptors are good drivers of consumer liking. While, roasted, burnt, Sensory & Consumer Sciences

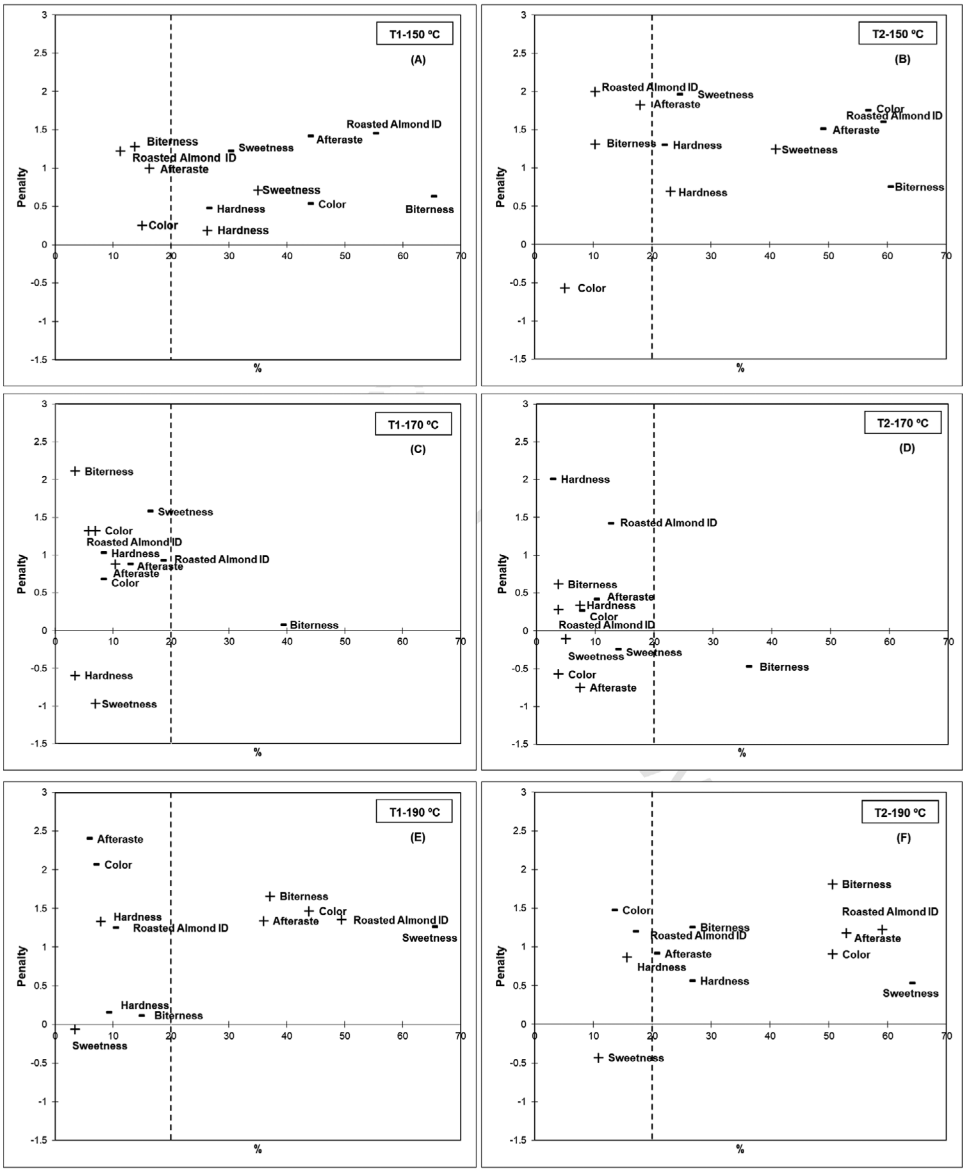

Figure 4–Penalty analysis of roasted almonds attributes intensities assessed by consumers (sample code indicated on the top right of each figure; "too low intensity" is indicated by the symbol "-" and "too high intensity" is indicated by the symbol "+").

woody, astringency, and bitterness were shown to be the less liked attributes.

In general, consumers overall liking was positively linked to specific volatiles (alkanes, alcohols, aldehydes, and furans) and sensory attributes (sweetness, roasted, almond ID, overall nut flavors together with a hard and crispy texture). On the contrary, a negative correlation was observed between consumers overall liking and pyrazines, bitterness, astringency, and woody and burnt flavor notes. Similar results were also reported for roasted peanuts revealing that the consumers drivers of liking were even similar across different countries (Spain, Netherlands, and Turkey), with color, sweetness, roasted peanut parameters increasing the liking and the contrary for bitterness (Lykomitros et al., 2018).

3.7 Penalty analysis

Additionally, to overall liking, JAR questions were also asked during the consumer study to see which of the attributes penalized liking. To understand the relationship between JAR scores and consumer liking, penalty analysis was conducted (Cano-Lamadrid et al., 2018; Lipan et al., 2019; Narayanan, Chinnasamy, Jin, & Clark, 2014). Figure 4 shows the proportion of consumers opinion plots against the mean drops (penalty). The aspects susceptible of improvement were those that had the greatest negative impact on the sample liking for at least 20% of consumers and caused a drop of at least 1 unit for liking. There was an apparent need to improve *T*1 samples roasted at 150 °C (Figure 4A), which were characterized by low roasted almond flavor, aftertaste, and sweetness. In the same way, samples *T*2 (Figure 4B) roasted at the same temperature needed to increase the intensity of color, roasted, and almond flavor, sweetness, and hardness. The 170 °C roasting temperature was associated with high consumer acceptance of roasted almonds from both irrigation treatments (*T*1 and *T*2), and results of penalty analysis (Figure 4C and D) suggested that this was the optimum temperature. Finally, samples roasted at 190 °C were penalized due to their too high bitterness, aftertaste, color, and roasted notes of almonds from *T*1 and *T*2 irrigation treatments (Figure 4E and F).

4. CONCLUSIONS

This is the first study reporting volatile composition, sensory profile, and consumer acceptance of roasted almonds grown under deficit irrigation conditions. Results indicated that the heat treatment of 170 °C was the optimum roasting temperature from an aromatic, descriptive, and affective point of view for the *Vairo* almonds. These samples were characterized by (i) a proper total content of volatile compounds (7.22 mg/kg), with 2.5-dimethyl pyrazine and furfural being the main predominant compounds and contributing to the almond, baked bread, roasted nuts notes; and, (ii) also by having hard and crispy texture, and intense almond and nutty flavor. Penalty analysis showed that almonds roasted at 150 °C were penalized because of their low roasted aroma and soft hardness, and almonds roasted at 190 °C were perceived as over-roasted, with too intense color and burn notes. Almonds roasted at 170 °C were not penalized and, therefore, did not need to be optimized. Regarding the irrigation treatments, hydroSOStainable almonds (*T*2) were characterized by a higher total content of volatile compounds and for being harder, sweeter, and by having a higher intensity of almond and roasted notes at the optimum roasting temperature (170 °C).

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AUTHOR CONTRIBUTIONS

Lipan run the physicochemical, sensory data, conducted part of the statistical analysis and writing the manuscript; Cano-Lamadrid helped with statistical analysis; Vázquez-Araújo helped with the design of the work, interpretation of data, and the manuscript revision; Łyczko helped with the physicochemical analysis; Moriana and Hernández prepared the samples and were the experts in irrigation strategies; García-García revised and approved the final manuscript; Carbonell-Barrachina coordinated and assisted with acquiring founding for the study.

REFERENCES

Agila, A., & Barringer, S. (2012). Effect of roasting conditions on color and volatile profile including hmf level in sweet al monds (*Prunus dulcis*). *Journal of Food Science*, 77(4), C461–C468. https://doi.org/10.1111/j.1750-3841.2012.02629.x

Alasalvar, C., Shahidi, F., & Cadwallader, K. R. (2003). Comparison of natural and roasted Turkish Tombul hazelnut (*Corylus avellana L.*) volatiles and flavor by DHA/GC/MS and descriptive sensory analysis. *Journal of Agricultural and Food Chemistry*, *51*(17), 5067–5072. https://doi.org/10.1021/jf0300846

Bolling, B. W. (2017). Almond polyphenols: Methods of analysis, contribution to food quality, and health promotion. *Comprehensive Reviews in Food Science and Food Safety*, *16*(3), 346–368. https://doi.org/10.1111/1541-4337.12260

Calín-Sánchez, Á, Martínez, J. J., Vázquez-Araújo, L., Burló, F., Melgarejo, P., & Carbonell-Barrachina, Á. A. (2011). Volatile composition and sensory quality of Spanish pomegranates (*Punica granatum L*). *Journal of the Science of Food and Agriculture*, *91*(3), 586–592. https://doi.org/10.1002/jsfa.4230

Cano-Lamadrid, M., Lech, K., Michalska, A., Wasilewska, M., Figiel, A., Wojdyło, A., & Carbonell-Barrachina, Á. A. (2017). Influence of osmotic dehydration pre-treatment and combined drying method on physico-chemical and sensory properties of pomegranate arils, cultivar Mollar de Elche. *Food Chemistry*, *232*, 306–315. https://doi.org/10.1016/j.foodchem.2017.04.033

Cano-Lamadrid, M., Vázquez-Araújo, L., Sánchez-Rodríguez, L., Wodyło, A., & Carbonell-Barrachina, Á. A. (2018). Consumers' opinion on dried pomegranate arils to determine the best processing conditions. *Joural of Food Science*, *83*(12), 3085–3091. https://doi.org/10.1111/1750-3841.14390

Carbonell-Barrachina, A. A., Memmi, H., Noguera-Artiaga, L., Gijon-Lopez, M. D., Ciapa, R., & Perez-Lopez, D. (2015). Quality attributes of pistachio nuts as affected by rootstock and deficit irrigation. *Journal of the Science of Food and Agriculture*, *95*(14), 2866–2873. https://doi.org/10.1002/jsfa.7027

Cheely, A. N., Pegg, R. B., Kerr, W. L., Swanson, R. B., Huang, G., Parrish, D. R., & Kerrihard, A. L. (2018). Modeling sensory and instrumental texture changes of dry-roasted almonds under different storage conditions. *LWT-Food Science and Technology*, *91*, 498–504. https://doi.org/10.1016/j.lwt.2018.01.069

Crowe, T. D., & White, P. J. (2003). Oxidation, flavor, and texture of walnuts reduced in fat content by supercritical carbon dioxide. JAOCS, *Journal of the American Oil Chemists' Society*, *80*(6), 569–574. https://doi.org/10.1007/s11746-003-0739-4

Dumville, J. C., & Fry, S. C. (2003). Solubilisation of tomato fruit pectins by ascorbate: A possible non-enzymic mechanism of fruit softening. *Planta*, *217*(6), 951–961. https://doi.org/10.1007/s00425-003-1061-0

Egea, G., Nortes, P. A., Domingo, R., Baille, A., Perez-Pastor, A., & Gonzalez-Real, M. M. (2013). Almond agronomic response to long-term deficit irrigation applied since orchard establishment. *Irrigation Science*, *31*(3), 445–454. https://doi.org/10.1007/s00271-012-0322-8

Erten, E. S., & Cadwallader, K. R. (2017). Identification of predominant aroma components of raw, dry roasted and oil roasted almonds. *Food Chemistry*, *217*, 244–253. https://doi.org/10.1016/j.foodchem.2016.08.091

FAOSTAT. (2018). Almond crop surface and production. Food and Agriculture Organization of the United Nations. Retrieved from http://www.fao.org

García-Tejero, I. F., Durán-Zuazo, V. H., & Muriel-Fernández, J. L. (2014). Towards sustainable irrigated Mediterranean agriculture: Implications for water conservation in semi-arid environments. *Water International*, *39*(5), 635–648. https://doi.org/10.1080/02508060.2014.931753

Ghaderi, F., & Monajjemzadeh, F. (2020). Review of the physicochemical methods applied in the investigation of the maillard reaction in pharmaceutical preparations. *Journal of Drug Delivery Science and Technology*, *55*, 101362. https://doi.org/10.1016/j.jddst.2019.101362

Girona, J., Mata, M., & Marsal, J. (2005). Regulated deficit irrigation during the kernel-filling period and optimal irrigation rates in almond. *Agricultural Water Management*, *75*, 152–167. https://doi.org/10.1016/j.agwat.2004.12.008

Guo, S., Jom, Na, & Ge, Y. (2019). Influence of roasting condition on flavor profile of sunflower seeds: A flavoromics approach. *Scientific Reports*, *9*(1). https://doi.org/10.1038/s41598-019-47811-3

Hidalgo, F. J., & Zamora, R. (2019). Formation of phenylacetic acid and benzaldehyde by degradation of phenylalanine in the presence of lipid hydroperoxides: New routes in the amino acid degradation pathways initiated by lipid oxidation products. *Food Chemistry: X*, *2*, 100037. https://doi.org/10.1016/j.fochx.2019.100037

Hojjati, M., Lipan, L., & Carbonell-Barrachina, Á. A. (2016). Effect of roasting on physicochemical properties of wild almonds (*Amygdalus scoparia*). *JAOCS, Journal of the American Oil Chemists' Society*, *93*(9), 1211–1220. https://doi.org/10.1007/s11746-016-2868-8

Huang, G. (2014). Almond shelf life factors. Technical Summary, Almond Board of California, 1–4. Retrieved from https://www.almonds.com/sites/default/files/content/attachments/2014aq0007_shelf_life_factors.pdf

Ju, Y. L., Xu, G. Q., Yue, X. F., Zhao, X. F., Tu, T. Y., Zhang, J. X., & Fang, Y. L. (2018). Effects of regulated deficit irrigation on amino acid profiles and their derived volatile compounds in cabernet sauvignon (*Vitis vinifera L.*) grapes and wines. *Molecules*, *23*(8), 1983. https://doi.org/10.3390/molecules23081983

Kwak, J., Faranda, A., Henkin, M., J., Gallagher, M., Preti, McGovern, P. G. (2015). Volatile organic compounds released by enzymatic reactions in raw nonpareil almond kernel. *European Food Research and Technollogy*, *241*(3), 441–377. https://doi.org/10.1007/s00217-015-2463-5

Lawless, H. T., & Heymann, H. (2010). *Sensory evaluation of food: principles and practices* (2nd ed.). New York, NY: Springer. https://doi.org/10.1007/978-1-4419-6488-5

Lin, J. T., Liu, S. C., Hu, C. C., Shyu, Y. S., Hsu, C. Y., & Yang, D. J. (2016). Effects of roasting temperature and duration on fatty acid composition, phenolic composition, Maillard reaction degree and antioxidant attribute of almond (*Prunus dulcis*) kernel. *Food Chemistry*, *190*, 520–528. https://doi.org/10.1016/j.foodchem.2015.06.004

Lipan, L., Cano-Lamadrid, M., Corell, M., Sendra, E., Hernández, F., Stan, L., …Carbonell-Barrachina, Á. A. (2019). Sensory profile and acceptability of hydroSOStainable almonds. *Foods*, *8*(2), 64. https://doi.org/10.3390/foods8020064

Lipan, L., Garcia-Tejero, I. F., Gutierrez-Gordillo, S., Demirbas, N., Sendra, E., Hernandez, F., …Carbonell-Barrachina, A. A. (2020). Enhancing nut quality parameters and sensory profiles in three almond cultivars by different irrigation regimes. *Journal of Agricultural and Food Chemistry*, *68*, 2316–2328. https://doi.org/10.1021/acs.jafc.9b06854

Lipan, L., Martín-Palomo, M. J., Sánchez-Rodríguez, L., Cano-Lamadrid, M., Sendra, E., Hernández, F., …Carbonell-Barrachina, Á. A. (2019). Almond fruit quality can be improved by means of deficit irrigation strategies. *Agricultural Water Management*, *217*, 236–242. https://doi.org/10.1016/j.agwat.2019.02.041

Lipan, L., Moriana, A., Lluch López, D. B., Cano-Lamadrid, M., Sendra, E., Hernández, F., …Carbonell-Barrachina, Á. A. (2019). Nutrition quality parameters of almonds as affected by deficit irrigation strategies. *Molecules*, *24*(14), 2646. https://doi.org/10.3390/molecules24142646

Lukac, H., Amrein, T. M., Perren, R., Conde-Petit, B., Amadò, R., & Escher, F. (2007). Influence of roasting conditions on the acrylamide content and the color of roasted almonds. *Journal of Food Science*, *72*(1), C33–C38. https://doi.org/10.1111/j.1750-3841.2006.00206.x

Lykomitros, D., Fogliano, V., & Capuano, E. (2018). Drivers of preference and perception of freshness in roasted peanuts (*arachis spp.*) For european consumers. *Journal of Food Science*, *83*(4), 1103–1115. https://doi.org/10.1111/1750-3841.14095

Misnawi, A., Jinap, S., Jamilah, B., & Nazamid, S. (2004). Sensory properties of cocoa liquor as affected by polyphenol concentration and duration of roasting. *Food Quality and Preference*, *15*(5), 403–409. https://doi.org/10.1016/S0950-3293(03)00097-1

Narayanan, P., Chinnasamy, B., Jin, L., & Clark, S. (2014). Use of just-about-right scales and penalty analysis to determine appropriate concentrations of stevia sweeteners for vanilla yogurt. *Journal of Dairy Science*, *97*(6), 3262–3272. https://doi.org/10.3168/jds.2013-7365

National Center for Biotechnology Information. (2018). PubChem Open Chemistry Database. Retrieved from https://pubchem.ncbi.nlm.nih.gov

NIST. (2020). National Institute of Standards and Technology (Libro delWeb de Química del NIST. SRD69). U.S. Secretary of Commerce on behalf of the United States of America. Retreived from https://webbook.nist.gov/chemistry/

Noguera-Artiaga, L., Lipan, L., Vázquez-Araújo, L., Barber, X., Pérez-López, D., & Carbonell-Barrachina, Á (2016). Opinion of spanish consumers on hydrosustainable pistachios. *Journal of Food Science*, *81*(10), S2559–S2565. https://doi.org/10.1111/1750-3841.13501

Noor-Soffalina, S. S., Jinap, S., Nazamid, S., & Nazimah, S. A. H. (2009). Effect of polyphenol and pH on cocoa Maillard-related flavour precursors in a lipidic model system. *International Journal of Food Science and Technology*, *44*(1), 168–180. https://doi.org/10.1111/j.1365-2621.2008.01711.x

Peleman, J., Boerjan, W., Engler, G., Seurinck, J., Botterman, J., Alliotte, T., …Inzé, D. (1989). Strong cellular preference in the expression of a housekeeping gene of *Arabidopsis thaliana* encoding *S*-adenosylmethionine synthetase. *Plant Cell*, *1*(1), 81–93. https://doi.org/10.1105/tpc.1.1.81

Perren, R., & Escher, F. E. (2013). Impact of roasting on nut quality. In L. J. Harris (Ed.), *Improving the safety and quality of nuts* (pp. 173–197). Sawston, UK: Woodhead Publishing.

Petisca, C., Pérez-Palacios, T., Farah, A., Pinho, O., & Ferreira, I. M. P. L. V. O. (2013). Furans and other volatile compounds in ground roasted and espresso coffee using headspace solid-phase microextraction: Effect of roasting speed. *Food and Bioproducts Processing*, *91*(3), 233–241. https://doi.org/10.1016/j.fbp.2012.10.003

Ripoll, J., Urban, L., Staudt, M., Lopez-Lauri, F., Bidel, L. P. R., & Bertin, N. (2014). Water shortage and quality of fleshy fruits-making the most of the unavoidable. *Journal of Experimental Botany*, *65*(15), 4097–4117. https://doi.org/10.1093/jxb/eru197

Sánchez-Rodríguez, L., Lipan, L., Andreu, L., Martín-Palomo, M. J., Carbonell-Barrachina, Á. A., Hernández, F., & Sendra, E. (2019). Effect of regulated deficit irrigation on the quality of raw and table olives. *Agricultural Water Management*, *221*, 415–421. https://doi.org/10.1016/j.agwat.2019.05.014

Schirra, M., & Agabbio, M. (1989). Influence of irrigation on keeping quality of almond kernels. *Journal of Food Science*, *54*(6), 1642–1645. https://doi.org/10.1111/j.1365-2621.1989.tb05178.x

Skovgaard, N. (2004). *Food Processing Technology. Principles and Practice*. CRC Press, *International Journal of Food Microbiology*, *93*(1), 124. https://doi.org/10.1016/j.ijfoodmicro.2003.11.002

Takei, Y., Shimada, K., Watanabe, S., & Yamanishi, T. (1974). Volatile components of roasted almonds: Basic fraction. *Agricultural and Biological Chemistry*, *38*(3), 645–648. https://doi.org/10.1080/00021369.1974.10861198

Takei, Y., & Yamanishi, T. (1974). Flavor components of roasted almond. *Agricultural and Biological Chemistry*, *38*(12), 2329–2336. https://doi.org/10.1271/bbb1961.38.2329

The Good Scents Company Information System. (2018). Providing information for the Flavor, Fragrance, Food and Cosmetic industries. Retrieved from http://www.thegoodscentscompany.com/

Valdés, A., Beltrán, A., Karabagias, I., Badeka, A., Kontominas, M. G., & Garrigós, M. C. (2015). Monitoring the oxidative stability and volatiles in blanched, roasted and fried almonds under normal and accelerated storage conditions by DSC, thermogravimetric analysis and ATR-FTIR. *European Journal of Lipid Science and Technology*, *117*(8), 1199–1213. https://doi.org/10.1002/ejlt.201400384

Varela, P., Chen, J., Fiszman, S., & Povey, M. J. W. (2006). Crispness assessment of roasted almonds by an integrated approach to texture description: Texture, acoustics, sensory and structure. *Journal of Chemometrics*, *20*(6-7), 311–320. https://doi.org/10.1002/cem.1029

Vázquez-Araújo, L., Chambers, D., & Carbonell-Barrachina, Á. A. (2012). Development of a sensory lexicon and application by an industry trade panel for turrón, a European protected product. *Journal of Sensory Studies*, *27*(1), 26–36. https://doi.org/10.1111/j.1745-459X.2011.00364.x

Vázquez-Araújo, L., Chambers, E., Adhikari, K., & Carbonell-Barrachina, Á. A. (2010). Sensory and physicochemical characterization of juices made with pomegranate and blueberries, blackberries, or raspberries. *Journal of Food Science*, *75*(7), S398–S404. https://doi.org/10.1111/j.1750-3841.2010.01779.x

Vázquez-Araújo, L., Enguix, L., Verdú, A., García-García, E., & Carbonell-Barrachina, A. A. (2008). Investigation of aromatic compounds in toasted almonds used for the manufacture of turrón. *European Food Research and Technology*, *227*(1), 243–254. https://doi.org/10.1007/s00217-007-0717-6

Vázquez-Araújo, L., Koppel, K., Iv, Chambers, E., Adhikari, & K., & Carbonell-Barrachina, A. A. (2011). Instrumental and sensory aroma profile of pomegranate juices from the USA: Differences between fresh and commercial juice. *Flavour and Fragrance Journal*, *26*(2), 129–138. https://doi.org/10.1002/ffj.2035

Vázquez-Araújo, L., Verdú, A., Navarro, P., Martínez-Sánchez, F., & Carbonell-Barrachina, Á. A. (2009). Changes in volatile compounds and sensory quality during toasting of Spanish almonds. *International Journal of Food Science & Technology*, *44*(11), 2225–2233. https://doi.org/10.1111/j.1365-2621.2009.02063.x

Xiao, L., Lee, J., Zhang, G., Ebeler, S. E., Wickramasinghe, N., Seiber, J., & Mitchell, A. E. (2014). HS-SPME GC/MS characterization of volatiles in raw and dry-roasted almonds (*Prunus dulcis*). *Food Chemistry*, *151*, 31–39. https://doi.org/10.1016/j.foodchem.2013.11.052

Yang, J., Pan, Z., Takeoka, G., MacKey, B., Bingol, G., Brandl, M. T., …Wang, H. (2013). Shelf-life of infrared dry-roasted almonds. *Food Chemistry*, *138*(1), 671–678. https://doi.org/10.1016/j.foodchem.2012.09.142

Youn, K. S., & Chung, H. S. (2012). Optimization of the roasting temperature and time for preparation of coffee-like maize beverage using the response surface methodology. *LWT-Food Science and Technology*, *46*(1), 305–310. https://doi.org/10.1016/j.lwt.2011.09.014