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Chemical and Sensory Analysis of Commercial Tomato Juices Present on the Italian and Spanish Markets

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ABSTRACT: A quantitative descriptive analysis was developed to characterize the sensory quality of a set of 12 organic and conventional tomato juices sold in Spanish and Italian markets. The volatile compounds of tomato juices were also studied. Twelve sensory descriptors, selected by a trained panel, evaluated the sensory profile of the samples. Some tomato juices were characterized by dominant positive notes typical of tomatoes (tomato paste, vegetable notes), whereas others by negative sensory attributes (off-flavors, high intensity of acidity, and sweetness). The volatile pattern of the samples, studied by SPME/GC-MS, was correlated with the sensory results: basically, organic tomato juices were characterized by vegetable notes and higher volatile compounds than conventional samples, regardless of their geographical origin. Conventional tomato juices were grouped in a closer cluster, whereas organic tomato juices were more diversified. Moreover, "defective" samples showed higher amounts of 3-methyl-1-butanol.

KEYWORDS: *farming system, Italian and Spanish market, sensory analysis, tomato juices, volatile compounds*

INTRODUCTION

Tomato (*Solanum lycopersicum* L.) consumption is strongly associated with a reduced risk of chronic degenerative diseases.[1] To date, at least 400 volatile compounds have been identified in tomatoes. However, only some of these, such as (*E*)-2-hexenal, (*Z*)-3-hexenal, 1-hexanal, (*Z*)-3-hexen-1-ol, 1-hexanol, 2-isobutylthiazole, and 6-methyl-5-hepten-2-one,[2] are considered to have a high impact on tomato aroma due to their level and threshold of perception by humans.[3] Tomatoes described as full-flavored are characterized by a low level of titratable acidity, high contents of total sugars and soluble solids, and intermediate contents of 1-hexanal, (*Z*)-3-hexenal, 2- and 3-methyl-1-butanol, (*E*)-2-hexenal, (*Z*)-3-hexen-1-ol, geranyl acetone, β-ionone, and 1-penten-3-one.[4] Volatile compounds are formed in the intact tomato fruit during ripening or upon tissue disruption, and new volatiles are formed when cell disruption occurs. These compounds originate from many substrates, including carotenoids, terpenoids, amino acids, lipids, and lignin.[4]

There are many volatile compounds that contribute to the different flavors detectable in tomato juice, such as earthy, musty, vine, green aroma, and the fruity, tropical, floral, ripe tomato, and sweet tomato flavors.[5] The levels of sugars and acids in tomato affect gustative attributes, such as sweetness and sourness, as well as flavor as perceived by trained sensory judges.[6] The presence of 1-hexanal, (*E*)-2-hexenal, (*E*,*E*)-2,4-decadienal, (*Z*)-3-hexenol, linalool, 1-penten-3-one, 6-methyl-5-hepten-2-one, geranyl acetone, and 2-isobutylthiazole have previously been identified as the major contributors to tomato aroma.[7,8] Floral essences are attributed to the terpene alcohol linalool, which is considered to be a contributor to the fresh aroma of tomato.[3,9] Moreover, 6-methyl-5-hepten-2-one and geranyl acetone have been reported to be carotenoid-related volatile compounds that are characteristic of tomato aroma.[10] Lastly, 2-isobutylthiazole is the only alkylthiazole often found in tomatoes and has a grassy and sweet fruity odor.[11] Another study suggested that alcoholic processed or enzymatic flavors become dominant when the effect of 2-isobutylthiazole diminishes.[12]

It is extremely important to determine the volatile compounds and sensory characteristics of tomato juices to satisfy consumers' acceptance, because there is an increasing demand for processed tomato products.[13] Juice is an intermediate product in the processing of tomato paste, obtained in a juice extraction step in a process that eventually results in the production of tomato concentrate. The pulp can be separated from tomato juice by filtering, but more commonly the entire pulp is used as juice. The juice is formulated according to the characteristics demanded by the market: in Italy and Spain, the most common is juice with extra virgin olive oil, salt, and citric juice. The product is then bottled and pasteurized to extend its shelf life.[14]

The formation of volatile compounds depends on the wide range of tomato species, stage of ripeness, and growing conditions.[2,12] The nutritive composition of vegetables may be

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affected by different soil fertility managements, such as farming techniques. Conventional and organic systems differ in the amount of irrigation received, in nutrients applied as fertilizers, and in organic matter applied to the soil as crop residues, winter legume cover crops, or composted manure.[15]

Many consumers believe that organic vegetables have higher sensory qualities and vitamins than conventionally grown vegetables.[5] Therefore, the aim of this investigation was to determine if it is possible to distinguish among 12 different samples of tomato juices from the Italian and Spanish markets, according to their individual sensory characteristics and their aromatic/volatile profiles. Moreover, the volatile compounds determined by SPME/GC-MS were studied to highlight the presence of specific molecules responsible for characteristic sensory notes. To our knowledge, this is the first study investigating differences between samples of tomato juices from the Italian and Spanish markets in terms of volatile compounds and sensory characteristics.

■ MATERIALS AND METHODS

Reagents and Samples. All chemical standards were purchased from Sigma-Aldrich (St. Louis, MO, USA). Sodium chloride, citric acid, and sucrose (used to build references for sensory analysis) were of food grade. Different types of tomato juices were purchased from Italian and Spanish markets: five were tomato juices from organic tomatoes (S 8−12) and seven were tomato juices from conventional tomatoes (S 1−7). Samples were stored at 15 °C and protected from light before analysis. For all samples the expiration dates were at least 3 months later than the analysis. In Table 1, the information contained on the labels is summarized.

Table 1. Sample Information Reported on the Labels

sample	ingredients	packaging	price (euros L^{-1})	origin
S 1	tomato juice, salt	dark plastic bottle (1 L)	0.69	Spain
S 2	tomato juice, salt	dark plastic bottle (0.2 L)	2.00	Spain
S 3	tomato juice, salt	dark plastic bottle (1 L)	0.65	Spain
S 4	tomato juice, salt	clear glass bottle (0.125 L)	3.06	Italy
S 5	tomato juice, salt	clear glass bottle (0.125 L)	2.72	Italy
S 6	tomato juice, salt, vitamin C	dark plastic bottle (1 L)	0.74	Spain
S 7	tomato juice, lemon juice, salt	clear glass bottle (0.2 L)	6.12	Spain
S 8	tomato juice	clear glass bottle (0.2 L)	4.83	Spain
S 9	tomato juice	clear glass bottle (1 L)	2.85	Spain
S 10	tomato juice, salt	clear glass bottle (0.125 L)	2.92	Italy
S 11	tomato juice, salt, apple juice, lemon juice, herbs, celery	clear glass bottle (0.2 L)	5.00	Spain
S 12	tomato juice, carrot juice, wheat germ, salt	clear glass bottle (0.475 L)	4.00	Spain

Tomato juices had specific characteristics that permitted a good balance when sensory characteristics of products were compared: (i) 10 samples were obtained using only tomatoes, salt, lemon juice or ascorbic acid as preservative, and 2 samples contained also other ingredients such as carrot or apple juice, herbs, or wheat germ (S 11 and S 12); (ii) tomato juices were produced following similar processing steps (washing, sorting, shredding, juice extraction, dosage mixing, homogenization, sterilization, refrigeration, packaging); (iii) tomato juices were manufactured by Italian and Spanish companies and widely distributed in supermarkets; (iv) 5 samples (S 8−12) were produced according to standards for organic agriculture (brand leader in large retail for organic products); (v) 4 samples (S 2, S 5−7) were produced by primary Italian and Spanish companies and commercialized with national brands; (vi) 4 samples (S 1, S 3, S 4m and S 10) were commercialized with the private label of the distributor chains.

Sensory Evaluation. Procedures for selecting, training, and monitoring of assessors, choice of optimal descriptors and appropriate measurement scale, and evaluation of results were developed according to ISO 13299: 2010.[16] A total of 12 samples with 2 replicates were evaluated by panelists. Eight trained judges (four females and four males aged 20−50 years old) participated in the sensory analysis sessions. Panelists were recruited on the basis of their previous experience in descriptive sensory analysis (staff and Ph.D. students at the Campus of Food Science, University of Bologna, Cesena, Italy). The panel worked in a closed room, and each assessor carried out sensory analysis in a single booth. Data acquisition was carried out using Fizz software (Biosystemes, Dijon, France). Assessors were trained and samples were evaluated using a quantitative descriptive method. During the training phase, each judge received tomato juice samples and found perceivable product attributes, by identification of appearance, odor, taste, and texture attributes that can be used to describe tomato juice samples. The panel decided if descriptors were redundant and should be removed from the list or if there were additional terms that should be added. The final list of terms was written, and the panel defined each attribute. Panelists also identified possible reference standards on which the rating of the generated attributes was based. The identified references were presented to each assessor, and specific training sessions were carried out.[17] During the training sessions, reference tomato juice samples were presented to assessors. The panel leader entered the assessment data and checked if the robust coefficient of variation evaluated for each attribute was ≤20%. When the panel leader found anomalous values, the analysis was repeated. After the calibration session, all samples were presented to judges for evaluation. The panelists rated the samples indicating the intensity of each attribute on a scale from 0 (not perceivable) to 10 (perceivable at the level of saturation). Well-defined anchor points were also used for training judges. A small white plastic cup, usually used for coffee, was employed for the evaluation of appearance, odor, and taste attributes. Around 10 g of tomato juice was poured into plastic cups. Panelists were advised to spit out the tomato juice after tasting, and between one analysis and the following assessors rinsed their mouths carefully with sparkling or natural water.

Analysis of Volatile Compounds. Tomato juice (1.5 g) was weighed and placed in a 10 mL vial, fitted with a silicone septum, and spiked with 0.15 g of 4-methyl-2-pentanone (internal standard dissolved in water) at a concentration of 2.5 mg kg^{-1}. The vial was immersed in a water bath at 40 °C, and the tomato juice was maintained under magnetic stirring. After 2 min of sample conditioning with divinylbenzene/carboxen/polydimethylsiloxane (DVB/CAR/PDMS) fiber (50/30 mm, 2 cm long from Supelco Ltd., Bellefonte, PA, USA), it was exposed to the sample headspace for 30 min and immediately desorbed for 3 min at 250 °C in the injector of the GC coupled with a quadrupolar mass-selective spectrometer (Agilent 6890N Network gas chromatograph and Agilent 5973 Network detector, Agilent Technologies, Palo Alto, CA, USA). Analytes were separated on a ZB-WAX column, 30 m × 0.25 mm i.d., 1.00 mm film thickness (Phenomenex, Torrance, CA, USA). Column temperature was held at 40 °C for 10 min and increased to 200 °C at 38 °C/min. The FID temperature was set at 250 °C, and the ion source and the transfer line were at 180 and 230 °C, respectively. Electron impact mass spectra were recorded at 70 eV ionization energy in the 20−250 amu mass range, with 2 scan/s.[17] Moreover, the volatile identification of the compounds was obtained by comparison of their mass spectral data with the information from the National Institute of Standards and Technology (NIST) library (2005 version). The identification was confirmed by the identification of pure standards (α-caryophyllene, pentanal, hexanal, 1-pentanol, 3-methyl-1-butanol, 2-isobutylthyazole, (*Z*)-2-penten-1-ol, limonene, eucalyptol, geraniol,

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Table 2. Main Volatile Compounds (Mean Values) of Analyzed (A) Organic and (B) Conventional Samples[a]

(A) Organic Samples							
volatile compound	S 8	S 9	S 10	S 11	S 12	KI	threshold value in water (mg/kg)
dimethyl sulfide	1.18d ± 0.07	1.80b ± 0.06	1.46c ± 0.08	1.01e ± 0.05	2.50a ± 0.21	787	
acetone	0.23d ± 0.05	0.44c ± 0.04	1.61a ± 0.11	0.25d ± 0.01	1.14b ± 0.08	833	
acetic acid	0.61a ± 0.01	0.59a ± 0.02	0.48b ± 0.02	0.45b ± 0.02	0.35c ± 0.03	941	
pentanal	2.61a ± 0.19	2.50b ± 0.17	nd	nd	nd	1005	
hexanal	0.43c ± 0.05	nd	0.39c ± 0.02	0.81a ± 0.01	0.64b ± 0.06	1111	4.5×10^{-3}, 5.8×10^{-3}
3-carene	nd	nd	nd	nd	6.10a ± 0.52	1153	
β-myrcene	nd	0.79b ± 0.08	nd	0.88a ± 0.09	nd	1186	13×10^{-3}, 36×10^{-3}
limonene	2.33d ± 0.16	2.80c ± 0.09	nd	5.94b ± 0.50	15.30a ± 1.11	1215	10×10^{-3}, 60×10^{-3}
eucalyptol	nd	nd	nd	0.27a ± 0.02	nd	1234	
3-methyl-1-butanol	0.50a ± 0.03	0.30b ± 0.02	nd	nd	nd	1238	0.17×10^{-3}
2-pentene	nd	nd	0.33b ± 0.02	nd	2.09a ± 0.15	1243	
(E)-2-hexenal	0.20c ± 0.02	nd	0.32b ± 0.02	2.42a ± 0.20	nd	1248	17×10^{-3}
furan-2-pentyl	nd	0.25a ± 0.03	nd	0.21b ± 0.02	nd	1260	
1-pentanol	nd	1.50c ± 0.08	1.86b ± 0.10	0.11d ± 0.01	2.24a ± 0.21	1282	
octanal	1.80a ± 0.10	nd	nd	nd	nd	1318	0.7×10^{-3}, 1.41×10^{-3}
2-penten-1-ol	nd	nd	nd	nd	0.56a ± 0.03	1354	0.4×10^{-3}
6-methyl-5-hepten-2-one	8.29d ± 0.78	0.25e ± 0.02	13.33b ± 1.10	11.34c ± 0.90	18.69a ± 1.18	1368	0.05×10^{-3}
1-hexanol	0.69e ± 0.08	1.01d ± 0.21	3.55b ± 0.31	1.56c ± 0.30	12.83a ± 1.20	1381	0.5×10^{-3}
3-penten-1-ol-3-methyl	nd	nd	0.77a ± 0.05	nd	0.48b ± 0.04	1393	
(Z)-3-hexen-1-ol	nd	5.40b ± 0.29	9.48a ± 0.55	0.89d ± 0.02	0.98c ± 0.09	1414	
nonanal	3.88b ± 0.23	2.50c ± 0.21	5.38a ± 0.24	nd	nd	1421	1×10^{-3}, 2.53×10^{-3}
2-isobutylthiazole	2.67d ± 0.12	3.20c ± 0.21	3.95b ± 0.22	3.36c ± 0.01	4.27a ± 0.35	1437	0.0035×10^{-3}
6-methyl-5-hepten-1-ol	nd	1.40a ± 0.11	1.43a ± 0.12	nd	0.37b ± 0.05	1493	
furfural	2.03b ± 0.09	1.89c ± 0.16	1.20d ± 0.13	0.27e ± 0.02	4.20a ± 0.18	1506	
2-ethyl-1-hexanol	2.09a ± 0.10	0.97b ± 0.05	0.56e ± 0.03	0.81c ± 0.01	0.67d ± 0.06	1518	
1,6-octadien-3-ol-3,7-dimethyl	1.28c ± 0.05	1.90b ± 0.10	2.65a ± 0.21	0.73e ± 0.04	1.07d ± 0.06	1575	
1-nonanol	0.73a ± 0.09	nd	nd	nd	0.31b ± 0.04	1585	
6-methyl-3,5-heptadien-2-one	0.59b ± 0.06	nd	3.16a ± 0.31	nd	0.36c ± 0.02	1629	
α-caryophyllene	nd	0.15b ± 0.09	nd	nd	0.37a ± 0.04	1700	
(E)-geranyl acetone	1.55b ± 0.02	1.09d ± 0.06	1.48b ± 0.03	1.35c ± 0.12	2.25a ± 0.05	1889	0.06×10^{-3}

(B) Conventional Samples							
volatile compound	S 1	S 2	S 3	S 4	S 5	S 6	S 7
dimethyl sulfide	0.81d ± 0.03	3.50a ± 0.16	nd	0.47e ± 0.02	1.65c ± 0.10	2.43b ± 0.10	0.27f ± 0.02
acetone	0.21d ± 0.02	0.18d ± 0.01	1.17a ± 0.04	0.13d ± 0.01	0.37c ± 0.02	0.62b ± 0.05	0.18d ± 0.01
acetic acid	0.50d ± 0.05	0.54d ± 0.02	nd	0.77c ± 0.04	1.77b ± 0.05	2.73a ± 0.12	nd
pentanal	nd	nd	nd	nd	nd	nd	0.45a ± 0.04
hexanal	0.20b ± 0.02	0.23a ± 0.01	0.25a ± 0.01	0.20b ± 0.01	nd	0.18b ± 0.01	nd
3-carene	nd	nd	nd	nd	nd	nd	nd
β-myrcene	nd	nd	nd	nd	nd	nd	nd
limonene	0.80b ± 0.05	1.41a ± 0.09	0.43c ± 0.02	0.40c ± 0.03	nd	0.33d ± 0.05	0.45c ± 0.03
eucalyptol	0.40b ± 0.02	0.47a ± 0.03	nd	nd	0.38b ± 0.02	nd	nd
3-methyl-1-butanol	nd	nd	nd	nd	nd	nd	nd
2-pentene	0.25b ± 0.01	0.34a ± 0.03	0.35a ± 0.02	0.30a ± 0.03	0.15c ± 0.01	0.33a ± 0.01	nd
(E)-2-hexenal	nd	0.30a ± 0.01	nd	nd	0.24b ± 0.02	0.28a ± 0.02	0.19c ± 0.01
furan-2-pentile	nd	nd	nd	nd	nd	0.27a ± 0.01	nd
1-pentanol	0.20b ± 0.01	0.17c ± 0.02	nd	0.22b ± 0.02	0.30a ± 0.03	nd	nd
octanal	0.29b ± 0.02	nd	0.17d ± 0.01	0.14d ± 0.01	nd	0.25c ± 0.02	1.30a ± 0.09
2-penten-1-ol	nd	nd	nd	nd	nd	nd	nd
6-methyl-5-hepten-2-one	2.05b ± 0.14	1.97b ± 0.05	1.76c ± 0.05	1.20d ± 0.10	1.15d ± 0.09	2.32a ± 0.12	1.77c ± 0.06
1-hexanol	nd	nd	nd	nd	0.28a ± 0.01	0.14c ± 0.01	0.25b ± 0.02
3-penten-1-ol-3-methyl	nd	nd	nd	nd	nd	nd	nd
(Z)-3-hexen-1-ol	nd	nd	nd	0.25a ± 0.01	0.21b ± 0.01	0.11c ± 0.01	nd
nonanal	0.26e ± 0.02	0.18f ± 0.01	0.70b ± 0.03	0.43d ± 0.01	0.18f ± 0.01	0.49c ± 0.03	0.85a ± 0.05
2-isobutylthiazole	0.61d ± 0.02	0.11f ± 0.01	0.10f ± 0.01	0.51e ± 0.02	0.89a ± 0.03	0.70c ± 0.04	0.80b ± 0.06
6-methyl-5-hepten-1-ol	0.51c ± 0.01	0.75a ± 0.02	nd	0.29e ± 0.02	0.44d ± 0.02	0.75a ± 0.03	0.60b ± 0.04
furfural	2.01a ± 0.09	1.29b ± 0.14	0.30e ± 0.02	0.40d ± 0.02	1.12c ± 0.10	nd	nd
2-ethyl-1-hexanol	0.15c ± 0.01	nd	nd	0.22b ± 0.03	0.54a ± 0.03	nd	0.21b ± 0.01
1,6-octadien-3-ol-3,7-dimethyl	0.25c ± 0.02	0.30b ± 0.02	0.36a ± 0.03	0.15e ± 0.01	0.17e ± 0.01	0.21d ± 0.02	0.20d ± 0.01

Table 2. continued

	(B) Conventional Samples						
volatile compound	S 1	S 2	S 3	S 4	S 5	S 6	S 7
1-nonanol	nd	nd	nd	nd	nd	nd	nd
6-methyl-3,5-heptadien-2-one	0.15c ± 0.01	nd	0.20b ± 0.01	0.25a ± 0.02	nd	0.24a ± 0.01	0.15c ± 0.01
α-caryophyllene	nd	nd	nd	nd	0.26a ± 0.01	0.25a ± 0.02	nd
(*E*)-geranyl acetone	nd	nd	nd	0.12b ± 0.01	nd	nd	0.15a ± 0.01

[a]Results are expressed as mg of 4-methyl-2-pentanone per kg of tomato juice. Different letters in the same column represent statistically significant differences.

and β-myrcene). Relative amounts of volatile compounds were expressed with respect to the internal standard as milligrams per kilogram of tomato juice. The Kovats indices were calculated using an appropriate mixture of *n*-alkanes. We have performed three replicates for each sample.

Statistical Treatment of Data. The software XLSTAT 7.5.2 version (Addinsoft, Belmont, MA, USA) was used to elaborate both the sensory and chemical results by analysis of variance (ANOVA) (LSD Fisher, $p < 0.05$) and principal component analysis (PCA).

RESULTS AND DISCUSSION

Characterization and Quality of Samples. In Table 1, the main information presented on the tomato juice labels is reported. The 12 tomato juices differed for farming systems, ingredients, and packaging. In particular, seven samples were obtained from conventional tomatoes (S 1−7), whereas five samples were produced from organic tomatoes (S 8−12). Clear information on the technological processes carried out was not reported. Tomato juices were bought at the supermarket and then stored at room temperature until their analysis.

Volatile Profiles. The concentrations of individual volatile compounds in headspace samples of tomato juices are given in Table 2. The threshold value is shown in Table 2A. All of the compounds reported have a contribution to tomato aroma as the threshold value is lower than the content reported for tomato juices. In total, 31 volatile compounds were tentatively identified from headspace samples of organic and conventional tomato juices. 1-Hexanal, (*E*)-2-hexenal, (*Z*)-3-hexen-1-ol, and geranyl acetone are considered to be important for tomato flavor.[4] The amount of each volatile compound was quantified by adding an internal standard to samples. Conventional tomato juices were very low in the total amount of volatiles compared to organic tomato juices. For instance, 3-carene, 3-methyl-1-butanol, β-myrcene, 1-nonanol, and 2-penten-1-ol were present at detectable levels only in organic tomato juices, and some other compounds, such as 6-methyl-5-hepten-2-one, 2-isobutylthiazole, limonene, and (*E*)-geranyl acetone, were significantly higher in organic tomato juices than in conventional alternatives (Table 2).

In S 8−12 (Table 2A), the quantities of 6-methyl-5-hepten-2-one, 2-isobutylthiazole, limonene, and (*E*)-geranyl acetone ranged from 0.36 to 18.69 mg kg^{-1} of tomato juice (calculated using the internal standard 4-methyl-2-pentanone), whereas for the other tomato juices (S 1−7) the concentrations of 6-methyl-5-hepten-2-one, 2-isobutylthiazole, limonene, and (*E*)-geranyl acetone were lower than 2.32 mg kg^{-1} (Table 2B).

Another compound found in tomato juices was 2-isobutylthiazole, which is the only alkylthiazole found in tomatoes and has been associated with grassy and sweet fruity odors.[11] In organic tomato juices, 2-isobutylthiazole ranged from 2.67 to 4.27 mg kg^{-1} (Table 2A), whereas in conventional tomato juices it ranged from 0.10 to 0.89 mg kg^{-1} (Table 2B). Volatile compounds contributing to tomato aroma change according to stage of maturity, cultivar, and climatic conditions. The compounds responsible for the aroma and flavor of tomatoes are present in low amounts. Organic and conventional cultivation may also affect fruit quality.[18] Abiotic and biotic factors change plant physiology and also induce secondary metabolite synthesis, leading to important changes in the physicochemical characteristics and in the composition of the volatile compounds.[19]

Moreover, (*E*)-2-hexenal and hexanal are aroma components of many fruits and vegetables through the LOX pathway contributing to green notes.[20] In this study, (*E*)-2-hexenal was found at <0.32 mg kg^{-1} (calculated using the internal standard 4-methyl-2-pentanone) in all tomato juices except for S 11, which contained 2.42 mg kg^{-1} (Table 2Z). This fact could be due to the addition of herbs to this sample of tomato juice.

Two volatile compounds, 6-methyl-5-hepten-2-one and (*E*)-geranyl acetone, have been reported to be carotenoid-related volatile compounds that are characteristic of tomato aroma. Most of the alcohols may have resulted from reductase conversions of the corresponding aldehydes formed from the metabolism of fatty acids and amino acids.[21] These two compounds have been found in higher quantities in organic tomato juices than in conventional ones. Moreover, S 12 contained greater amounts of 6-methyl-5-hepten-2-one and (*E*)-geranyl acetone compared with S 8−11. This fact can be attributed to the addition of carrot juice to S 12.

Other compounds such as dimethyl sulfide, acetone, acetic acid, furfural, and furan-2-pentile do not help to discriminate between organic and conventional tomato juices. Wong and Carson[22] have reported that dimethyl sulfide found in heated tomato is formed by thermal decomposition of the natural fresh tomato component (3-amino-3-carboxypropyl)-dimethylsulfonium ion, $(CH_3)_2S(+)CH_2CH_2CH(NH_2)$-COOH.[8] Furfural and furan-2-pentile have been identified in a wide range of processed products.[23]

Plants release volatile compounds that can vary depending on the environmental conditions. For example, some species respond to reduced light (due to either lower light intensity or shorter daylength) with a decline in the release of herbivore-induced volatiles.[24] Moreover, water stress affects also volatile release. When a plant has less water available, elevated levels of volatiles are released from infested individuals relative to non-water-stressed controls.[25] Correlating this with organic and conventional agriculture, the addition of high levels of mineral and/or organic nitrogen fertilizers in conventional plants significantly decreased the constitutive volatiles extracted from celery.[26]

Sensory Evaluation. At present, there are no scientific studies that have analyzed both volatile compounds and sensory data by a quantitative descriptive analysis (QDA) to characterize commercial tomato juices from Italian and Spanish markets. Moreover, only very few studies in the literature have assessed

Table 3. Sensory Descriptors of Conventional and Organic Tomato Juices, Descriptions, Anchor Points, and Specific References Used during the Training of Panelists

descriptor	definition	references	anchor point	concentration of references
appearance				
red intensity	intensity of red color from light to dark	measured using a color scaling ruler		
homogeneity	absence or presence of particles	measured with a glass rotation		
odor				
intensity of tomato paste	odor reminiscent of tomato sauce	tomato sauce in a glass	strong (10)	
vegetable notes	intensity of odor reminiscent of vegetal notes	carrot, celery, potato, basil, oregano, thyme		
acidulous	acidulous sensation generated by heat treatments; reminiscent of concentrated tomato	concentrated tomato paste in a glass	strong (10)	
taste				
intensity of tomato paste	olfactory sensation reminiscent of tomato sauce and tomato concentrated paste	concentrated tomato paste in a glass	strong (10)	
saltness	basic taste from NaCl, glutamate, and others	NaCl in handmade tomato juice	weak (2); strong (8)	weak, 0.5 g/L; strong, 1 g/L
sweetness	basic taste from sucrose, fructose, glucose, and others	sucrose in handmade tomato juice	weak (2); strong (8)	weak, 0.4 g/L; strong, 0.8 g/L
acid	basic taste from citric, malic, and other acids	citric acid in handmade tomato juice	weak (2); strong (8)	weak, 0.08 g/L; strong, 0.16 g/L
vegetable notes	intensity of taste reminiscent of vegetal notes	carrot, celery, potato, basil, oregano, thyme		
texture				
density	product viscosity	liquid and creamy tomato juice		
off-flavors				
off-flavors	anomalous, unlikely scents	cheese, metal, smoked, and others		

tomato-based products that differ for farming systems.[14,15] As a consequence of the training session, the intensity of the red color and homogeneity were selected as appearance attributes. With regard to odor and taste, the panel distinguished eight different attributes perceived by orthonasal routes during the smelling phase and some other attributes perceived by retronasal routes during the tasting phase. Assessors considered as typical odor descriptors intensity of tomato paste, intensity of vegetable notes, and acidulous odor. For taste, the attributes were intensity of tomato paste, sweetness, saltiness, acidity, and vegetable notes.

Finally, the panel added two attributes, density, as a texture attribute, and off-flavors. Positive attributes, high intensity of tomato paste and vegetable notes, were also considered, and negative ones were off-flavors and high intensity of acidity and sweetness.

Special references (Table 3) of known flavors were selected to have standards for the training and calibration of the panel and to make unambiguous assignment of sensations and attributes possible. Therefore, two different concentrations of saccharose, sodium chloride, and citric acid were added to a neutral tomato juice. Each concentration corresponded to an anchor point with a value of 2 or 8 situated in the graduated scale (10 point scale).

Sensory results and the content of volatile compounds were analyzed by PCA to perform a characterization of the samples according to these variables and to check eventual correlations among them. The first two components were responsible for 68.60% of variance (40.81% for PC1 and 27.80% for PC2). As shown in Figure 1, it is possible to highlight that PC1 was associated, in the positive direction, with 1-nonanol, 2-ethyl-1-hexanol, furfural, 1,6-octadien-3,7-dimethyl-3-ol, 3-methyl-1-butanol, 2-isobutylthiazole, and (*E*)-geranyl acetone; in the negative direction, PC1 was related to red intensity, saltiness, and intensity of tomato paste (odor). PC2 was correlated positively with hexanal, (*Z*)-3-hexenol, and vegetable notes.

With regard to the location of products, S 10−12 were characterized by a higher content of 2-isobutylthiazole, (*E*)-geranyl acetone, 6-methyl-5-hepten-2-one, hexanal, (*Z*)-3-hexenol, and vegetable notes, whereas S 1−7 contained a low concentration of these compounds and were also characterized by a higher red intensity. S 8 and S 9 were correlated with sweetness, off-flavors, 3-methyl-1-butanol, and 1-nonanol. The off-flavors resembled cheese, both smoked and rancid. Some factors that could contribute to the formation of off-flavors are environmental pollutants, the growth of microorganisms, oxidation of lipids, or endogenous enzymatic decomposition.[27] S 10−12 were characterized by lower amounts of these negative attributes, whereas they contained higher amounts of hexanal, (*Z*)-3-hexenol, and vegetable notes in comparison with S 8 and S 9.

In general, higher concentrations of volatile compounds were detected in the organic tomato juices. This could be due to a higher level of plant stress in organic tomatoes. Organic farming systems receive lower amounts of nutrients such as fertilizers, and this could be considered as the reason why organic tomatoes produced a higher amount of secondary metabolites.[15] These differences may be linked to a different ripening period or release of the supplied nutrients.[14] Existing studies show that organic fertilization practices produce crops with higher levels of ascorbic acid and lower levels of nitrate compared with conventionally grown crops.[28]

In extra virgin olive oil, higher concentrations of volatiles in organic products have also been detected compared to

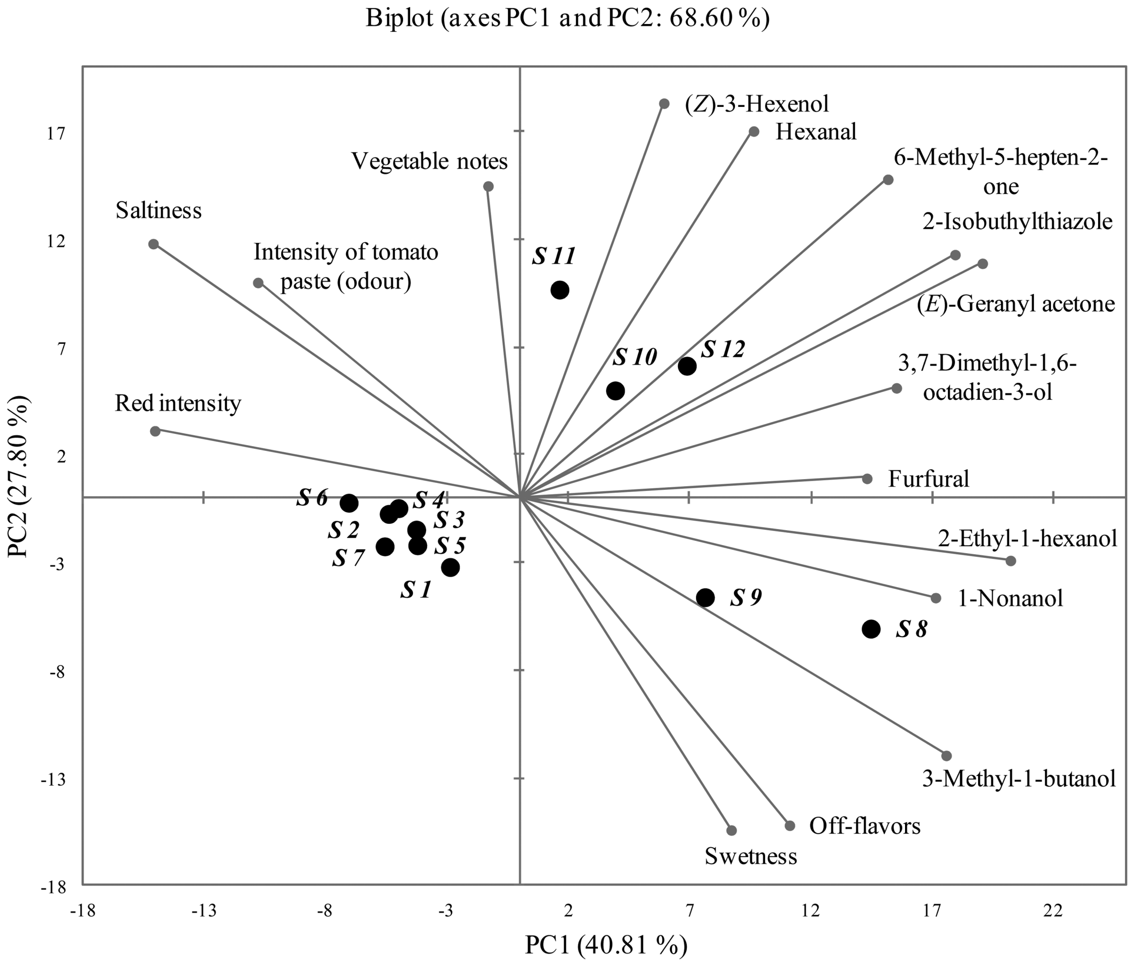

Figure 1. PCA of tomato juices (S 1−12, see Table 1 for sample information).

conventional ones. In an earlier report, Gutierrez et al.[29] compared the quality of conventional and organic extra virgin olive oils extracted from olives harvested at increasing stages of ripeness. These authors found that the organic oils were of superior quality compared to the conventional oils in all of the quality parameters analyzed. However, Ninfali et al.[30] reported that the volatile compounds, which are correlated with positive or negative sensory attributes, differed occasionally but not consistently between organic and conventional oils, suggesting that aroma depends on a wide number of variables, making it difficult to find a relationship between volatile compounds and agricultural practices. Moreover, some studies have reported that consumers do not detect sensory differences between organic and conventional vegetables.[30−32] Similarly, the differences between organic and conventional tomato juices for individual sensory characteristics show no clear patterns. Haglund et al.[33] found that conventionally grown carrots had a higher carrot taste, whereas organic carrots were more bitter. Similarly, Caussiol and Joyce[34] reported no flavor differences between organic and conventional bananas, and Zhao et al. showed that consumers did not perceive differences among leafy greens grown in organic versus conventional alternatives.[32]

In conclusion, in this study the group of conventional tomato juices was characterized by lower amounts of volatile compound than organic ones regardless of Italian or Spanish origin. Conventional tomato juices appeared as a more homogeneous cluster, whereas organic tomato juices were more diversified due to both desirable (olfactory and gustative vegetable notes) and undesirable compounds (off-flavors). Juices produced by conventional tomatoes showed a wide range of prices (from 0.69 to 6.12 euros L^{-1} of product), and these differences can be mainly justified by different brands and packaging materials (plastic or glass bottles) because similar results were found for sensory and volatile profiles. On the other hand, organic juices were characterized by a higher mean price (from 2.85 to 5.00 euros L^{-1} of product): this can be supported by both the major cost and the added value of the raw material as well by peculiar sensory attributes that can meet consumer expectations.

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Notes

The authors declare no competing financial interest.

REFERENCES

(1) Weisburger, J. H. Lycopene and tomato products in health promotion. *Exp. Biol. Med.* **2002**, *227*, 924−927.

(2) Ruiz, J. J.; Alonso, A.; Garcia-Martinez, S.; Valero, M.; Blasco, P.; Ruiz-Bevia, F. Quantitative analysis of flavour volatiles detects differences among closely related traditional cultivars of tomato. *J. Sci. Food Agric.* **2005**, *85*, 54−60.

(3) Aguilo-Aguayo, I.; Soliva-Fortuny, R.; Martin-Belloso, O. Volatile compounds and changes in flavour-related enzymes during cold storage of high-intensity pulsed electric field- and heat-processed tomato juices. *J. Sci. Food Agric.* **2010**, *90*, 1597−1604.

(4) Tandon, K. S.; Baldwin, E. A.; Scott, J. W.; Shewfelt, R. L. Linking sensory descriptors to volatile and nonvolatile components of fresh tomato flavor. *J. Food Sci.* **2003**, *68*, 2366−2371.

(5) Thybo, A. K.; Edlenbos, M.; Christensen, L. P.; Sørensen, J. N.; Thorup-Kristensen, K. Effect of organic growing systems on sensory quality and chemical composition of tomatoes. *LWT−Food Sci. Technol.* **2006**, *39*, 835−843.

(6) Malundo, T. M. M.; Shewfelt, R. L.; Scott, J. W. Flavor quality of fresh tomato (*Lycopersicon esculentum* Mill.) as affected by sugar and acid levels. *Postharvest Biol. Technol.* **1995**, *6*, 103−110.

(7) Buttery, R. G.; Teranishi, R.; Ling, L. C. Fresh tomato aroma volatiles: a quantitative study. *J. Agric. Food Chem.* **1987**, *35*, 540−544.

(8) Buttery, R. G.; Teranishi, R.; Ling, L. C.; Turnbaugh, J. G. Quantitative and sensory studies on tomato paste volatiles. *J. Agric. Food Chem.* **1990**, *38*, 336−340.

(9) Galliard, T.; Matthew, J. A.; Wright, A. J.; Fishwick, M. J. The enzymic breakdown of lipids to volatile and non-volatile carbonyl fragments in disrupted tomato fruits. *J. Sci. Food Agric.* **1977**, *28*, 863−868.

(10) Buttery, R. G.; Ling, L. Enzymatic production of volatiles in tomatoes. In *Progress in Flavor Precursor Studies*, Schreier, P., Winterhalter, P., Eds.; Allured Publishing: Carol Stream, IL, 1993; pp 137−146.

(11) Riley, J. C. M.; Thompson, J. E. Subcellular generation and distribution of lipid-derived volatiles in the ripe tomato. *J. Plant Physiol.* **1997**, *150*, 546−551.

(12) Yilmaz, E. Oxylipin pathway in the biosynthesis of fresh tomato volatiles. *Turk. J. Biol.* **2000**, *25*, 351−360.

(13) Vallverdu-Queralt, A.; Jauregui, O.; Di Lecce, G.; Andres-Lacueva, C.; Lamuela-Raventos, R. M. Screening of the polyphenol content of tomato-based products through accurate-mass spectrometry (HPLC-ESI-QTOF). *Food Chem.* **2011**, *129*, 877−883.

(14) Vallverdú-Queralt, A.; Medina-Remón, A.; Casals-Ribes, I.; Lamuela-Raventos, R. M. Is there any difference between the phenolic content of organic and conventional tomato juices? *Food Chem.* **2012**, *130*, 222−227.

(15) Vallverdu-Queralt, A.; Medina-Remon, A.; Casals-Ribes, I.; Amat, M.; Lamuela-Raventos, R. M. A metabolomic approach differentiates between conventional and organic ketchups. *J. Agric. Food Chem.* **2011**, *59*, 11703−11710.

(16) Sensory analysis – Methodology – General guidance for establishing a sensory profile (ISO 13299: 2003) approved by CEN as a EN ISO 13299:2010.

(17) Bendini, A.; Barbieri, S.; Valli, E.; Buchecker, K.; Canavari, M.; Toschi, T. G. Quality evaluation of cold pressed sunflower oils by sensory and chemical analysis. *Eur. J. Lipid Sci. Technol.* **2011**, *113*, 1375−1384.

(18) Willer, H.; Yussefi-Menzler, M.; Sorensen, N. *The World of Organic Agriculture - Statistics and Emerging Trends 2008*; IFOAM: Bonn, Germany, 2008.

(19) Serrão Macoris, M.; Soares Janzantti, N.; dos Santos Garruti, V.; Monteiro, M. Volatile compounds from organic and conventional passion fruit (*Passiflora edulis* F. flavicarpa) pulp. *Cienc. Tecnol. Aliment. Campinas* **2010**, *31*, 430−435.

(20) Neri, F.; Mari, M.; Brigati, S. Control of *Penicillium expansum* by plant volatile compounds. *Plant Pathol.* **2006**, *55*, 100−105.

(21) Sucan, M. K.; Russell, G. F. Effects of processing on tomato bioactive volatile compounds. In *Bioactive Compounds in Foods*; ACS Symposium Series 816; American Chemical Society: Washington, DC, 2002; pp 155−172.

(22) Wong, F. F.; Carson, J. F. Isolation of S-methyl methionine sulfonium salt from fresh tomatoes. *J. Agr Food Chem* **1966**, *14*, 247−249.

(23) Fagerson, I. S. Thermal degradation of carbohydrates; a review. *J. Agric. Food Chem.* **1969**, *17*, 747−750.

(24) Paré, P. W.; Tumlinson, J. H. Plant volatiles as a defense against insect herbivores. *Plant Physiol.* **1999**, *121*, 325−332.

(25) Takabayashi, J.; Dicke, M.; Posthumus, M. A. Volatile herbivore-induced terpenoids in plant-mite interactions: variation caused by biotic and abiotic factors. *J. Chem. Ecol.* **1994**, *20*, 1329−1354.

(26) Van Wassenhove, F. A.; Dirinck, P. J.; Schamp, N. M.; Vulsteke, G. A. Effect of nitrogen fertilizers on celery volatiles. *J. Agric. Food Chem.* **1990**, *38*, 220−226.

(27) Wilkes, J. G.; Conte, E. D.; Kim, Y.; Holcomb, M.; Sutherland, J. B.; Miller, D. W. Sample preparation for the analysis of flavors and off-flavors in foods. *J. Chromatogr., A* **2000**, *880*, 3−33.

(28) Worthington, V. Effect of agricultural methods on nutritional quality: a comparison of organic with conventional crops. *Altern. Ther. Health Med.* **1998**, *4*, 58−69.

(29) Gutierrez, F.; Arnaud, T.; Albi, M. Influence of ecological cultivation on virgin olive oil quality. *J. Am. Oil Chem. Soc.* **1999**, *76*, 617−621.

(30) Ninfali, P.; Bacchiocca, M.; Biagiotti, E.; Esposto, S.; Servili, M.; Rosati, A.; Montedoro, G. A 3-year study on quality, nutritional and organoleptic evaluation of organic and conventional extra-virgin olive oils. *J. Am. Oil Chem. Soc.* **2008**, *85*, 151−158.

(31) Schutz, H. G.; Lorenz, O. A. Consumer preferences for vegetables grown under 'commercial' and 'organic' condition. *J. Food Sci.* **1976**, *41*, 70−73.

(32) Zhao, X.; Chambers, E.; Matta, Z.; Loughin, T. M.; Carey, E. E. Consumer sensory analysis of organically and conventionally grown vegetables. *J. Food Sci.* **2007**, *72*, S87−S91.

(33) Haglund, A.; Johansson, L.; Berglund, L.; Dahlstedt, L. Sensory evaluation of carrots from ecological and conventional growing systems. *Food Qual. Pref.* **1999**, *10*, 23−29.

(34) Caussiol, L. P.; Joyce, D. C. Characteristics of banana fruit from nearby organic versus conventional plantations: a case study. *J. Hortic. Sci. Biotechnol.* **2004**, *79*, 678−682.