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Italian and Spanish commercial tomato sauces for pasta dressing:  
study of sensory and head-space profiles by Flash Profiling and SPME-GC-MS

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Sensory and head-space profiles of Italian and Spanish tomato sauces for pasta dressing

## Abstract

**BACKGROUND** The sensory and head-space profiles of Italian and Spanish commercial tomato sauces have been studied. The Flash Profiling method was used to evaluate the sensory characteristics and samples within each set and were ranked according to selected descriptors. A hundred volatile compounds were identified by SPME-GC-MS.

**RESULTS** For Italian samples, the sensory notes of basil/aromatic herbs, acid and cooked tomato were among the most perceived by assessors, whereas in Spanish ones the sensory attributes of garlic/onion, onion/sweet pepper and, as for the Italian ones, cooked tomato were among the most frequently found. Data

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were elaborated by multivariate statistical approaches and interesting correlations were seen among different sensory attributes and related volatile compounds.

**CONCLUSIONS** Spanish samples were characterized by highest content of volatiles linked to thermal treatment of tomatoes and to raw and sautéed garlic and onion, whereas the Italian ones by terpenic compounds typical of basil and volatile molecules derived from fresh tomato. These results confirm the influence of formulation and production processes on the aromatic profile (sensory attributes and volatile compounds) of tomato products probably linked to different eating habits and culinary tradition in Italy and Spain.

**Key words:** tomato sauce, sensory profile, head-space volatiles, Flash Profiling, SPME-GC-MS

## INTRODUCTION

Europeans consume many products derived from tomatoes, for example ready-to-eat sauces used for pasta dressing or sandwiches, meat, and salad (ketchup) and the flavor of these products is an important criteria to satisfy consumer acceptance. The most widely used ingredients include: olive oil or sunflower oil, onion, garlic, basil, parsley, vegetables (celery, carrot, eggplant, zucchini), spices (pepper), salt, sugar, thickeners, and stabilizers. Tomato sauce is normally packaged in glass bottles, jars, or in bricks and then sterilized.<sup>1</sup>

Volatile compounds are formed in the intact tomato fruit upon tissue disruption or during ripening, and new volatiles are formed when cell disruption occurs. These compounds originate from many substrates, including terpenoids, carotenoids, amino acids, lipids, and lignin.<sup>2,3</sup> More than 400 volatile compounds have been identified in tomatoes, but only some are considered to have a substantial impact on tomato aroma due to their amount and threshold of perception by humans, for example (*E*)-2-hexenal, (*Z*)-3-hexenal, hexanal, (*Z*)-3-hexen-1-ol, hexanol, 2-isobutylthiazole, and 6-methyl-5-hepten-2-one.<sup>4,5</sup>

All these compounds contribute to the different flavours detectable in tomato paste such as green aroma and the fruity, tropical, floral, earthy, musty, ripe tomato, and sweet tomato flavors.<sup>6</sup> 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.<sup>7</sup> 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.<sup>8,9</sup>

Many volatile compounds derive from amino acids of tomato, in particular from valine, leucine, isoleucine, and phenylalanine. These amino acids are subjected to transaminase enzyme action with formation of the related  $\alpha$ -ketoacids, decarboxylated to aldehydes, and finally reduced to alcohols.<sup>3,10</sup> Other volatile compounds are derived from hydrolysis and enzymatic oxidation of lipids (LOX pathway) as a consequence of the tissue damage. The C6 molecules from the LOX pathway, such as 1-hexanal, (*E*)-2-hexenal, and (*Z*)-3-hexenol, contribute to the “green note” typical of fresh tomatoes.<sup>10</sup>

The volatile fraction of tomato products (juices, sauces, and concentrated tomato) also includes molecules derived from thermal treatments that are able to deactivate enzymes (blanching) or stabilize products

(sterilization). These modifications are mainly due to oxidation of carotenoids and the Maillard reaction that occurs at high temperature.<sup>11</sup>

Floral essences are attributed to the terpene alcohol linalool, which is a contributor to the fresh aroma of tomato.<sup>4</sup> Moreover, 6-methyl-5-hepten-2-one and geranyl-acetone have been reported to be carotenoid-related volatile compounds characteristic of tomato aroma.<sup>12</sup>

In ready-to-eat tomato sauces both onion or garlic are sautéed with vegetable oils at high temperature and several volatile sulfides such as propyl sulfide, methyl propyl sulfide, allyl propyl sulfide, allyl disulfide are produced. Terpenes characterize the volatile fraction of vegetables and spices.<sup>13-15</sup>

Some studies have been carried out in tomatoes and tomato juices with the aim to evaluate the sensory quality of different tomato products (e.g. conventional vs. organic, treated vs. untreated) and to identify possible correlations between volatile compounds and sensory characteristics. Vallverdu-Queralt et al. developed a quantitative descriptive analysis to characterize the sensory quality of 12 organic and conventional tomato juices sold in the Spanish and Italian markets.<sup>16</sup> Some tomato juices were characterized by dominant positive notes typical of tomatoes (tomato paste, vegetable notes), while others by negative sensory attributes (off-flavors, high intensity of acidity, and sweetness). In another study by the same researchers, quantitative descriptive analysis was developed to characterize the sensory quality of tomato juices processed with pulse electric fields.<sup>17</sup> Tomatoes subjected to moderate intensity pulsed electric fields treatments led to tomato juices with a higher content of volatile compounds and more favorable sensory properties than those prepared with untreated tomatoes. However, no studies have been focused on the sensory analysis and head space volatile profile of commercial tomato sauces for pasta dressing. These products are based on tomato paste and are formulated according to the characteristics demanded by the market: in Italy and Spain, the most common is tomato with extra virgin olive oil, salt, onions, and garlic.<sup>18</sup>

Therefore, the aim of this investigation was to study the sensory characteristics and head-space profile of ready-to-eat tomato sauces for pasta dressing, purchased from the Italian and Spanish markets. Moreover, possible relationships between the volatile compounds identified by SPME-GC-MS and sensory notes by the Flash Profiling, a rapid method based on the Free-choice profiling, were studied. To our knowledge, this is the

first study characterizing Italian and Spanish tomato sauces for pasta dressing in terms of volatile compounds and sensory characteristics and investigating the relationship between sensory attributes and instrumental data related to aromatic fractions.

## EXPERIMENTAL

### Samples

The study focused on a set consisting of 18 ready-to-eat tomato sauces samples purchased from Italian and Spanish supermarkets considering the most widely known brands. Italian samples were coded from S1 to S9 and Spanish samples from S10 to S18. All samples were stored at room temperature and protected from light before analyses. The samples differed in terms of packaging (brick, glass, and tinplate), weight (from 120 g to 570 g), tomato content (%), and ingredients added to tomatoes in the formulation. Table 1 shows the frequency of ingredients with a potential contribution to flavor for all samples.

### Analysis of head-space volatile compounds by SPME-GC-MS

An aliquot of 3 g of each sample, previously homogenized for 3 min with a mixer, was weighed into a 20 mL vial. The vial was closed with a silicone septum and conditioned at 40°C for 2 min without magnetic stirring. After 2 min of sample conditioning, a divinylbenzene/carboxen/polydimethylsiloxane (DVB/CAR/PDMS) fiber (50/30  $\mu$ m, 2 cm long from Supelco Ltd., Bellefonte, PA) was exposed to the sample headspace for 30 min and immediately desorbed for 5 min at 240°C in the injector with a split ratio of 1:10. Analytes were separated on a ZB-WAX column 30 m  $\times$  0.25 mm ID, 1.00  $\mu$ m film thickness (Phenomenex, Torrance, CA, USA). Column temperature was held at 40°C for 10 min and increased to 200°C at 3°C min<sup>-1</sup>. After 3 min, the temperature increased to 240°C at 10°C min<sup>-1</sup> and remained stable for 5 min. Helium was used as a carrier gas with a flow of 1 mL min<sup>-1</sup>. Volatile compounds were analyzed by quadrupolar mass-selective spectrometry (in the 30–250 amu mass range) coupled with GC, using a GCMS-QP2010 gas chromatograph (Shimadzu Co., Kyoto, Japan) coupled with an Autosampler AOC-5000 Plus (Shimadzu Co., Kyoto, Japan). Peaks identification was based on comparison of mass spectrum data with spectra present in the National Institute of

Standards and Technology (NIST) library (2008 version) and only identification matching more than 90% were taking into account. Being not possible the use of an internal standard (due to the difficulty to solubilized a standard molecule in a thick semi-liquid sample) a quantitative evaluation was applied and expressed as percentage composition of each peak with respect to the entire volatile fraction. Three replicates for each sample were performed.

### Sensory analysis by Flash Profiling method

The Flash Profiling (FP) method has been proposed by Dairou and Sieffermann as a rapid approach based on the Free-choice profiling.<sup>19,20</sup> FP is a descriptive technique used to describe a food product according to its sensory characteristics (appearance, flavor, aroma, texture). The training of judges is not necessary and each assessor applies an own list of sensory attributes based on their own perception.<sup>21</sup> In this way, each judge can use his list of sensory attributes to order (rank) the products for each descriptor and, at the same time, the assessor can evaluate the entire set of samples to perceive and focus only on those attributes that better discriminate the products.

FP was carried out in two different sessions by 10 assessors: in the first session the Italian samples (S1 – S9) were evaluated and the Spanish products (S10 – S11) in the second. All judges (age 21 – 47 years) were recruited among employees of the Campus of Food Science of University of Bologna who had experience in sensory description of different food products.

All tomato sauces were presented in a white plastic cup identified by an alphanumerical code. Samples were heated up to around 40°C for 10 min and then evaluated for gustative and olfactory characteristics. In the first phase, each assessor created their own list of sensory attributes perceived in all samples of the same set (Italian or Spanish) and then, after a brief discussion regarding the sensory characteristics perceived by all judges and the lexicon used to describe them, each assessor ordered samples according to increasing of intensities of their selected sensory attributes.<sup>22</sup>

### Statistical analysis

The software XLSTAT 7.5.2 version (Addinsoft, U.S.A) was used to elaborate the sensory and chemical results by analysis of variance (ANOVA) and multivariate approaches as Generalized Procrustes Analysis (GPA) and Multifactorial Analysis (MFA). Pearson's correlations ( $p < 0.05$ ) were also evaluated to investigate the relationships between volatile compounds and sensory notes.

## RESULTS AND DISCUSSION

### Analysis of the head-space volatile compounds by SPME-GC-MS

As shown in Table 1, ingredients such as tomato pulp and concentrate, basil, celery, and carrots were among those prevalent in Italian ready-to-eat tomato sauces for pasta dressing, while Spanish samples were characterized by other ingredients, including pepper, zucchini, eggplant, spices, and almonds. The variability in their formulation, shown in Table 1, was responsible for some differences in terms of headspace volatile profiles and sensory perceptions.

The odor that is perceived when a bottle of ready-to-eat tomato sauce for pasta dressing is opened is generally intense and pleasant and is determined by several volatile molecules from mixed and cooked ingredients. One hundred compounds of the headspace profiles of all samples were tentatively identified by SPME-GC-MS. These molecules belonged to different chemical classes: acids, alcohols, aldehydes, benzene derivatives, ketones, esters, furans, hydrocarbons, lactones, sulfides, sulfide derivatives, and terpenes.

In Tables 2 and 3, the percentages of molecules related to the most frequent ingredients (named category), for the Italian and Spanish samples, are shown. For each category, the volatile compounds responsible for that olfactory attribute according to the existing literature were considered. For example, in case of "sautéed garlic/onion", "thermal treated tomatoes" and "Maillard compounds", the molecules that originate from each of these thermal processes were selected based on literature data.<sup>9,12,23</sup> However, in some cases, it was not possible to find a correspondence between the presence of a specific ingredient and the related volatile compounds because the amounts of these molecules were very close to the limit of quantitation (eg. all samples declare to contain onion but in three of them there are not volatile compounds typical of this



ingredient). In fact, it is important to take into the mind that, depending on the conditions (time-temperature, ratio between sample quantity and the head-space volume) of the applied method, only a part of the molecules responsible of some specific aroma can volatilize and an equilibrium between the concentration of the molecules in the sample and in the head-space of the sample is established. However, the use of the SPME-GC-MS determination, performed by heating the samples at the same temperature applied during the sensory sessions, permits to obtain a profile in volatile compounds that are reasonably directly involved also in the tasters' smell perception (olfactory phase). On the other hand, a solvent extraction phase (e.g. with heptane) before the GC-MS analysis could surely help to better quantify the molecules linked to the ingredients of the samples but it would not help to understand what it is perceived by assessors during the sensory test. It is possible to highlight that a larger number of Spanish samples (S10-S18) were characterized by high content of compounds due to thermal treatments used for their preparation, whereas only two Italian samples (S1-S9) reported a quantifiable amount of these compounds and other molecules linked to the presence of garlic and onion among ingredients (garlic, garlic/onion, sautéed garlic/onion categories). In the headspace profiles of Italian samples, molecules due to the presence of basil (eucalyptol,  $\beta$ -linalol,  $\alpha$ -bergamotene, *p*-menth-1-en-4-ol, *p*-menth-1-en-8-ol, estragol) were found in widely variable percentages (from 2% to 80%): in particular, the highest percentage of this category was seen in S8, the only tomato sauce that also indicated the presence of natural aroma of basil among ingredients. On the other hand, in only 5 of 9 Spanish samples, the volatile compounds linked with basil were quantified and the amount was around 24% only in S16, whereas in other samples it did not reach 2%. S2, S3, and S11 showed elevated quantities of compounds linked to thermal treated tomatoes, whereas in S2, S5, S7, and S17 higher than 20% of molecules linked to the fresh tomato category were found. High quantities of molecules related to the presence of parsley were seen in S4 and S14, as expected considering the ingredients specified in the respective labels. A considerable percentage of molecules due to pepper (3-carene, 1-R- $\alpha$ -pinene,  $\beta$ -pinene, D-limonene, caryophyllene) was a peculiarity of S7. Terpenic compounds related to the presence of celery and carrot were identified in 6 Italian samples and only in one Spanish product (samples S16). S15 showed the highest

percentage (38.1%) of compounds associated with the garlic/onion attribute and S18 showed the highest percentages of volatiles responsible for the sautéed garlic/onion category.

Several studies have reported on the influence of thermal treatment on the composition of the aroma of the product because heating can modify many molecules to produce new compounds (e.g. Maillard reactions).<sup>9,12</sup> In Tables 2 and 3, it can be seen that Maillard compounds were present in all samples, even if the highest amounts were found in S3, S4, S11, S13, and S18; in particular, S3 and S13 were characterized by an important amount of dimethyl sulfide and others, such as 2-pentilfuran, furfural, 3-furaldehyde, acetylfuran, 5-methylfurfural, and 3-furanmethanol.<sup>9,12</sup>

### Sensory analysis by Flash Profiling method

As described above, in the first phase of each sensory session, each assessor created an own list of sensory attributes perceived in all samples of the same set (Italian or Spanish). In particular, for Italian samples a total of 9 attributes (fresh tomato, basil/aromatic herbs, garlic/onion, cooked tomato, sweet, acid, pungency, salty, rancid) were selected. The Spanish products were described by a total of 11 attributes (fresh tomato, basil/aromatic herbs, garlic/onion, cooked tomato, sweet, acid, pungency, salty, spices, onion/sweet pepper, onion or garlic sautéed). After the second phase of FP method, data obtained by the ranking of samples for all selected attributes were statistically elaborated by GPA. In particular, GPA provides results as residuals related to objects (samples) and configurations (assessors). High configuration residual values indicate assessors that classified samples differently than the general consensus. On the other hand, the objects with the lowest residuals have the highest agreements among assessors about the ranking position of those samples.<sup>21,24</sup> S1 and S8 as well as S10, S15, and S16 were, respectively, Italian and Spanish samples with major consensus (data not shown). The residual values for Spanish samples showed a lower range (69-103) than the Italian ones (86-129), indicating less difficulty for assessors in ranking the first set of samples. GPA was helpful in verifying that all samples were generally classified for their sensory characteristics with a satisfactory agreement among assessors.

### Sensory and instrumental data: an integrated approach

After GPA, a MFA using sensory results and volatile composition of samples was carried out for the Italian and Spanish samples. In particular, to perform this statistical elaboration, only the most frequent sensory attributes (at least perceived and ranked by 5 of 10 assessors, data not shown) and categories of volatiles (at least detected in 5 of 9 samples for each set, see Tables 2 and 3) were selected. To obtain results that are less influenced by the data on the extremes, median values of the sensory ranking - instead of mean - were calculated and used as input data for the MFA. Spanish samples were mainly characterized by sensory attributes of cooked and fresh tomato, sweet, garlic/onion, and sautéed onion/sweet pepper, while Italian samples by basil/aromatic herbs, cooked tomato, sweet, and acid. It is interesting to highlight that compounds linked to the olfactory notes typical of raw and sautéed garlic/onion and fresh/thermal treated tomatoes were detected in most of the Spanish samples, whereas the aromatic profiles of all the Italian samples were highly characterized by volatile compounds linked to basil and fresh tomatoes; moreover, volatile compounds related to the Maillard reaction were detected in all samples. Some significant positive correlations between the presence of categories of the volatile molecules considered as being responsible for sensory attributes and the sensory results (ranking) of the related perceived olfactory notes were found (data not shown). For example, considering the Italian samples, a correlation was found between the volatile compounds linked to the Maillard reaction with sensory attributes of cooked tomato ( $r=0.699$ ,  $p<0.05$ ). Similarly, this latter correlation was also detected in the Spanish group ( $r=0.701$ ,  $p<0.05$ ) in which another positive correlation was found between sweet (gustatory attribute) and volatile compounds responsible for sautéed onion/garlic ( $r=0.612$ ,  $p<0.05$ ): in reality, onions and other vegetables are widely used in their preparation (Table 1). Moreover, in the Italian samples, the volatile compounds related to basil were positively correlated with the related sensory attribute of basil ( $r = 0.515$ ,  $p<0.05$ ), whereas for the Spanish samples a positive correlation was found between the garlic/onion sensory attribute and volatile category ( $r=0.688$ ,  $p<0.05$ ). Considering the projection of variables in the factorial plan for each of the two groups (see Figures 1 and 2), the vectors related to the sensory attributes “sweet” and “cooked tomato” are located near to one other as were the volatile compounds related to Maillard reaction. In fact, this latter reaction pathway is one of the main processes that contribute to the

development of the aromatic fraction of thermally treated foodstuffs.<sup>12</sup> Moreover, thermal treatment could contribute to the degradation of polysaccharides naturally present in these products, increasing the perceived overall sweetness.

In Figure 1 is also interesting to note the presence of the acid taste. This attribute was generally perceived by assessors in Italian samples, whereas in Spanish ones (Figure 2) this taste, commonly found in fresh tomatoes and tomato based products, was not so characterizing.

For each sample of the two groups, it is possible to sum the volatile compounds linked to thermal treatment of tomatoes and the Maillard reaction ones reported in Tables 2 and 3 and to compare these sums with the results related to the cooked tomato sensory attribute. As shown in Figure 3, both the Italian and Spanish samples with the highest content in Maillard and thermal treated tomatoes volatile compounds (respectively S2, S3, S4, S6, S7 among the Italian and S10, S11, S13, S14, S15 and S18 among the Spanish) were also the ones with the highest intensities of the sensory attribute of cooked tomato.

## CONCLUSIONS

The aroma analyzed by both sensory and chemical approaches was different for Italian and Spanish ready-to-eat tomato sauces for pasta dressing: Spanish samples were characterized by the highest content of volatiles linked to thermal treatment of tomatoes and to raw and sautéed garlic and onion, whereas the Italian ones by terpenic compounds typical of basil and volatile molecules derived from fresh tomatoes. At the same time, assessors more frequently perceived the sensory attributes of garlic, onion, and sweet pepper in Spanish samples, whereas more basil/aromatic herbs and acid in the Italian ones.

These results confirm the influence of formulation and production processes on the aromatic profile (sensory attributes and volatile compounds) of tomato products and highlighted an interesting agreement between sensory and instrumental data.

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## REFERENCES

1. Cosmai L, Summo C, Caponio F, Paradiso VM and Gomes T, Investigation on volatile profile, lipid fraction degradation and antioxidant content of tomato-based pâtés as a function of ingredient formulation. *Int. Food Res. J.* 20: 3141-3148 (2013).
2. Tandon KS, Baldwin EA, Scott JW and Shewfelt RL, Linking sensory descriptors to volatile and non-volatile components of fresh tomato flavour. *J. Food Sci.* 68: 2366-2371 (2003).
3. Wang L, Baldwin EA and Bai J, Recent Advance in Aromatic Volatile Research in Tomato Fruit: The Metabolisms and Regulations. *Food Bioprocess Technol.* 9: 203-216 (2016).
4. Aguilo-Aguayo I, Soliva-Fortuny R and 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.* 90: 1597-1604 (2010).
5. Wang L, Baldwin EA, Zhao W, Plotto A, Sun X, Wang Z, Brecht JK, Bai J and Yu Z, Suppression of volatile production in tomato fruit exposed to chilling temperature and alleviation of chilling injury by a pre-chilling heat treatment. *LWT-Food Sci. Technol.*, 62: 115-121 (2015).
6. Thybo AK, Edlenbos M, Christensen LP, Sørensen JN and Thorup-Kristensen K, Effect of organic growing systems on sensory quality and chemical composition of tomatoes. *LWT-Food Sci. Technol.* 39: 835-843 (2006).
7. Malundo TMM, Shewfelt RL and Scott JW, Flavor quality of fresh tomato (*Lycopersicon esculentum* Mill.) as affected by sugar and acid levels. *Postharvest Biol. Technol.* 6: 103-110 (1995).
8. Buttery RG and Ling L.C. Volatile components of tomato fruit and plant. In *Bioactive volatile compounds from plants*, (Eds: R. Teranishi, G.R Buttery, H. Sugisawa); ACS Symposium Series: Washington, DC, pp. 23-34 (1993).
9. Buttery RG, Teranishi R, Ling LC and Turnbaugh JG, Quantitative and sensory studies on tomato paste volatiles. *J. Agric. Food Chem.* 38: 336-340 (1990).
10. Salles C, *Tomatoes and Tomato Products*, (Eds: V. R. Preedy, R. R. Watson), Science Publishers, Enfield, New Hampshire, USA, pp. 85-110 (2008).
11. Servilli M, Selvaggini R, Taticchi A, Begliomini AL and Montedoro G, Relationships between the volatile compounds evaluated by solid phase microextraction and the thermal treatment of tomato juice: optimization of the blanching parameters *Food Chem.* 71: 407-415 (2000).
12. Buttery GR and Ling LC, *Bioactive volatile compounds from plants*, (Eds: R. Teranishi, G. R. Buttery, H. Sugisawa), ACS Symposium Series, Washington, DC, pp. 23-34 (1993).
13. Kjeldsen F, Christensen LP and Edelenbos M, Changes in volatile compounds of carrots (*Daucus carota* L.) during refrigerated and frozen storage. *J. Agric. Food Chem.* 51: 5400-5407 (2003).

14. Van Wassenhove F, Dirinck P, Vulsteke G and Schamp N, Aromatic volatile composition of celery and celeriac cultivars *Hort Science*, 25: 556-559 (1990).
15. Jelen HH and Gracka A, Analysis of black pepper volatiles by solid phase microextraction – gas chromatography. A comparison of terpenes profiles with hydrodistillation. *J. Chromatogr. A*. 1418: 200-209 (2015).
16. Vallverdú-Queralt A, Bendini A, Tesini F, Valli E, Lamuela-Raventós RM and Gallina Toschi T, Chemical and Sensory Analysis of Commercial Tomato Juices Present on the Italian and Spanish Markets. *J. Agr. Food Chem.* 61: 1044-1050 (2013).
17. Vallverdú-Queralt A, Bendini A, Barbieri S, Di Lecce G, Martin-Belloso O and Gallina Toschi T, Volatile Profile and Sensory Evaluation of Tomato Juices Treated with Pulsed Electric Fields. *J. Agr. Food Chem.* 61: 1977-1984 (2013).
18. Vallverdú-Queralt A, Rinaldi de Alvarenga JF, Estruch R and Lamuela-Raventós RM, Bioactive compounds present in the Mediterranean sofrito. *Food Chem.* 141: 3365-3372 (2013).
19. Dairou V and Siefferman JM, A comparison of 14 jams characterized by conventional profile and a quick original method, the Flash Profile. *J. Food Sci.* 37: 826-837 (2002).
20. Williams AA and Langron SE, The use of free-choice profiling for the evaluation of commercial ports. *J. Sci. Food Agric.* 35: 558-568 (1984).
21. Tàrraga A and Tarancón P, *Novel techniques in sensory characterization and consumer profiling*, (Eds: P. Varela, G. Ares) CRC Press, Taylor & Francis Group, Boca Raton, Florida, USA, pp.157-174 (2012).
22. Delarue J, *Novel techniques in sensory characterization and consumer profiling*; (Eds: P. Varela, G. Ares) CRC Press, Taylor & Francis Group, Boca Raton, Florida, USA, pp.176-205 (2012).
23. Yu T, Chung-May W and Chi-Tang H, Volatile compounds of deep-oil fried, microwave-heated and oven-baked garlic slices. *J. Agric. Food Chem.* 41: 800-805 (1993).
24. Nokels L, Fhamy T and Chrocmore S, *Handbook of Partial Least Squares - Concepts, methods and applications*, (Eds: E. V. Vinzi, W. W. Chin, J. Henseler, H. Wang), Springer-Verlag Berlin Heidelberg, Berlin, Germany, pp. 775-789 (2010).
25. Lanzotti V, The analysis of onion and garlic. *J. Chromatogr. A*, 1112: 3-22 (2006).
26. Reineccius G, *Flavor chemistry and technology*, (Eds: G. Reineccius), CRC Press, Taylor & Francis Group, Boca Raton, Florida, USA, pp. 73-101 (2005).
27. Lee S, Umamo K, Shibamoto T and Lee K, Identification of volatile components in basil (*Ocimum basilicum* L.) and thyme leaves (*Thymus vulgaris* L.) and their antioxidant properties. *Food Chem.* 91: 131-137 (2005).

## Tables

**Table 1** List of ingredients with potential contribution to the flavor of samples (for simplification, other ingredients, such as corn starch and acid lactate, have been excluded) and their frequency in all samples (18): the value in each row, for each set of samples, indicates the number of Italian (S1 - S9) and Spanish (S10 - S11) tomato sauces that contain each ingredient.

INGREDIENTS	S1 – S9 (Italian samples)	S10 – S18 (Spanish samples)
Tomatoes	3	8
Tomato pulp	5	1
Tomato concentrate	6	2
Garlic	3	4
Onion	9	9
Olive oil	6	6
Sunflower oil	-	2
Basil	4	-
Parsley	2	1
Carrot	2	-
Celery	4	-
Hot pepper	1	-
Chive	1	-
Natural aroma of basil	2	-
Pepper	1	4
Zucchini	-	2
Eggplant	-	1
Almond	-	1
Spices	-	1
Sugar	8	7
Salt	9	9



Table 2. Percentages of volatile molecules related to the most frequent ingredient (named category) in Italian samples. The categories were defined on the basis of the volatile compounds related to the ingredients reported in Table 1 and typically detected as markers of thermal processes (Maillard compounds, thermal treated tomatoes).

Category	S1	S2	S3	S4	S5	S6	S7	S8	S9
Garlic	n.d.	n.d.	n.d.	6.5 <i>a</i>	n.d.	n.d.	n.d.	n.d.	n.d.
Garlic/onion *	n.d.	n.d.	2.5 <i>c</i>	4.8 <i>b</i>	1.1 <i>d</i>	n.d.	9.8 <i>a</i>	0.5 <i>e</i>	1.2 <i>d</i>
Sautéed garlic/onion	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Basil *	78.6 <i>a</i>	2.0 <i>d</i>	19.0 <i>c</i>	4.4 <i>d</i>	2.1 <i>d</i>	34.5 <i>b</i>	2.6 <i>d</i>	80.3 <i>a</i>	36.9 <i>b</i>
Black pepper *	1.5 <i>d, e</i>	2.4 <i>d</i>	n.d.	7.1 <i>c</i>	n.d.	n.d.	14.3 <i>a</i>	0.7 <i>e</i>	11.6 <i>b</i>
Fresh tomato *	8.1 <i>d, e</i>	21.7 <i>b</i>	6.1 <i>e</i>	10.3 <i>d</i>	42.6 <i>a</i>	13.2 <i>c</i>	23.7 <i>b</i>	6.6 <i>e</i>	13.8 <i>c</i>
Parsley	n.d.	n.d.	n.d.	10.4 <i>a</i>	n.d.	n.d.	n.d.	n.d.	n.d.
Celery/carrot *	3.2 <i>c</i>	2.4 <i>c</i>	n.d.	11.5 <i>b</i>	n.d.	n.d.	14.3 <i>a</i>	0.7 <i>d</i>	12.8 <i>b</i>
Maillard compounds *	2.8 <i>d</i>	9.1 <i>c</i>	29.3 <i>a</i>	16.4 <i>b</i>	3.0 <i>d</i>	10.7 <i>c</i>	10.2 <i>c</i>	2.0 <i>d</i>	2.7 <i>d</i>
Thermal treated tomatoes	n.d.	13.3 <i>b</i>	23.1 <i>a</i>	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

n.d. = not detectable (<LOD); \* = detected in 5 or more Italian samples and used as input data for the MFA.

Garlic: 3-vinyl-1,2-dithiacyclohex-4-ene, 3-vinyl-1,2-dithiacyclohex-5-ene.<sup>23</sup> Garlic/onion: 2-methylbutanal, allyl-methyl-sulfide, allyl sulfide, 2-methyl-2-pentenal, 2,4-dimethylthiophene, methyl 2-propenyl disulfide, dimethyl trisulfide, dimethyl disulfide, diallyl disulfide, allyl methyl sulfide, allyl trisulfide (all these compounds are common to both garlic and onion volatile profiles).<sup>25,26</sup> Sautéed garlic/onion: methyl propyl sulfide, dipropyl disulfide, dipropyl trisulfide, 1-propyl-2-(4-thiopent-2-en-5-yl)-disulfide.<sup>23</sup> Basil: eucaliptol,  $\beta$ -linalol,  $\alpha$ -bergamotene, *p*-menth-1-en-4-ol, *p*-menth-1-en-8-ol, estragol.<sup>27</sup> Pepper: 3-carene, 1-R- $\alpha$ -pinene,  $\beta$ -pinene, D-limonene, cariophyllene.<sup>15</sup> Fresh tomato: 3-methylbutanal, hexanal, 3-methyl-1-butanol, 6-methyl-5-hepten-2-one, (*E*)-3-hexen-1-ol, (*Z*)-3-hexen-1-ol.<sup>8,10</sup> Parsley:  $\alpha$ -phellandrene,  $\beta$ -phellandrene, 1,3,8-*p*-menthatriene. Celery/carrot: 1-R- $\alpha$ -pinene,  $\beta$ -pinene,  $\beta$ -myrcene,  $\alpha$ -terpinene, D-limonene,  $\gamma$ -terpinene, cariophyllene.<sup>13,14</sup> Maillard compounds: 2-pentylfuran, furfural, 3-furadehyde, 2-acetylfuran, 5-methylfurfural, 3-furanmethanol.<sup>9,12</sup> Thermal treated tomatoes: dimethyl sulfide.<sup>9</sup>

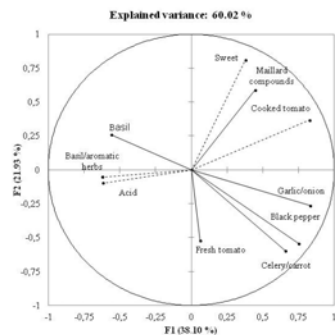
Table 3. Percentages of volatile molecules related to the most frequent ingredient (named category) in Spanish samples. The categories were defined on the basis of the volatile compounds related to the ingredients reported in Table 1 and typically detected as markers of thermal processes (Maillard compounds, thermal treated tomatoes).

Category	S10	S11	S12	S13	S14	S15	S16	S17	S18
Garlic	n.d.	n.d.	n.d.	n.d.	2.3 <i>b</i>	20.2 <i>a</i>	n.d.	n.d.	n.d.
Garlic/onion *	33.5 <i>b</i>	4.4 <i>e</i>	1.7 <i>f</i>	8.7 <i>d</i>	26.3 <i>c</i>	38.1 <i>a</i>	2.9 <i>e, f</i>	1.4 <i>f</i>	7.4 <i>d</i>
Sautéed garlic/onion *	n.d.	n.d.	19.8 <i>b</i>	1.5 <i>c, d</i>	2.6 <i>c</i>	0.6 <i>d</i>	n.d.	n.d.	38.4 <i>a</i>
Basil *	0.5 <i>b, c</i>	n.d.	0.8 <i>b, c</i>	0.7 <i>b, c</i>	n.d.	n.d.	24.2 <i>a</i>	1.7 <i>b</i>	n.d.
Black pepper	n.d.	n.d.	n.d.	n.d.	8.7 <i>a</i>	n.d.	n.d.	n.d.	n.d.
Fresh tomato *	9.4 <i>c</i>	6.8 <i>d</i>	4.3 <i>e, f</i>	16.8 <i>b</i>	2.0 <i>f</i>	5.4 <i>d, e</i>	4.0 <i>e, f</i>	29.0 <i>a</i>	2.3 <i>f</i>
Parsley	n.d.	n.d.	n.d.	n.d.	25.6 <i>a</i>	n.d.	4.0 <i>b</i>	n.d.	n.d.
Celery/carrot	n.d.	n.d.	n.d.	n.d.	8.7 <i>b</i>	n.d.	22.6 <i>a</i>	n.d.	n.d.
Maillard compounds *	6.6 <i>e</i>	19.4 <i>b</i>	3.0 <i>f</i>	30.3 <i>a</i>	3.9 <i>e, f</i>	13.8 <i>c, d</i>	14.4 <i>c</i>	11.0 <i>d</i>	27.8 <i>a</i>
Thermal treated tomatoes *	7.0 <i>b</i>	16.6 <i>a</i>	4.5 <i>c</i>	7.4 <i>b</i>	1.0 <i>d</i>	3.6 <i>c</i>	n.d.	n.d.	n.d.

n.d. = not detectable (<LOD); \* = detected in 5 or more Italian samples and used as input data for the MFA.

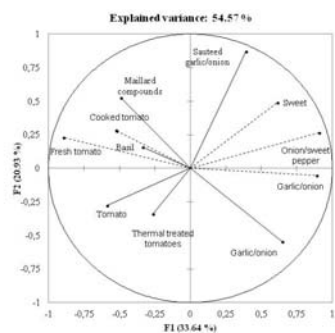
Garlic: 3-vinyl-1,2-dithiacyclohex-4-ene, 3-vinyl-1,2-dithiacyclohex-5-ene.<sup>23</sup> Garlic/onion: 2-methylbutanal, allyl-methyl-sulfide, allyl sulfide, 2-methyl-2-pentenal, 2,4-dimethylthiophene, methyl 2-propenyl disulfide, dimethyl trisulfide, dimethyl disulfide, diallyl disulfide, allyl methyl sulfide, allyl trisulfide (all these compounds are common to both garlic and onion volatile profiles).<sup>25,26</sup> Sautéed garlic/onion: methyl propyl sulfide, dipropyl disulfide, dipropyl trisulfide, 1-propyl-2-(4-thiopet-2-en-5-il)-disulfide.<sup>23</sup> Basil: eucaliptol,  $\beta$ -linalol,  $\alpha$ -bergamotene, *p*-menth-1-en-4-ol, *p*-menth-1-en-8-ol, estragol.<sup>27</sup> Pepper: 3-carene, 1-R- $\alpha$ -pinene,  $\beta$ -pinene, D-limonene, cariophyllene.<sup>15</sup> Fresh tomato: 3-methylbutanal, hexanal, 3-methyl-1-butanol, 6-methyl-5-epten-2-one, (*E*)-3-hexen-1-ol, (*Z*)-3-hexen-1-ol.<sup>8,10</sup> Parsley:  $\alpha$ -phellandrene,  $\beta$ -phellandrene, 1,3,8-*p*- menthatriene. Celery/carrot: 1-R- $\alpha$ -pinene,  $\beta$ -pinene,  $\beta$ -myrcene,  $\alpha$ -terpinene, D-limonene,  $\gamma$ -terpinene, cariophyllene.<sup>13,14</sup> Maillard compounds: 2-pentylfuran, furfural, 3-furadehyde, 2-acetylfuran, 5-methylfurfural, 3-furanmethanol.<sup>9,12</sup> Thermal treated tomatoes: dimethyl sulfide.<sup>9</sup>

Figure 1 – top of the figure



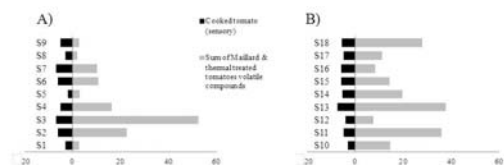
Projection of variables (sensory attributes as dot-lines and categories of volatile compounds as full lines) in the factorial plan (MFA) for Italian samples.

Figure 2 – top of the figure



Projection of variables (sensory attributes as dot-lines and categories of volatile compounds as full lines) in the factorial plan (MFA) for Spanish samples

Figure 3 – top of the figure



Sum of volatile compounds linked to the Maillard reaction and thermal treated tomatoes (see Tables 2 and 3) and rank in the Italian (A) and Spanish (B) groups.