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# Neuronal network analyses reveal novel associations between volatile organic compounds and sensory properties of tomato fruits

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## Abstract

**Introduction** The process of tomato (*Solanum lycopersicum*) breeding has affected negatively the fruit organoleptic properties and this is evident when comparing modern cultivars with heirloom varieties. Flavor of tomato fruit is determined by a complex combination of volatile and nonvolatile metabolites that is not yet understood.

**Objectives** The aim of this work was to provide an alternative approach to exploring the relationship between tomato odour/taste and volatile organic compounds (VOCs).

**Methods** VOC composition and organoleptic properties of seven Andean tomato landraces along with an edible wild species (*Solanum pimpinellifolium*) and four commercial varieties were characterized. Six hedonic traits were analyzed by a semitrained sensory panel to describe the organoleptic properties. Ninety-four VOCs were analyzed by headspace solid phase microextraction/gas chromatography–mass spectrometry (HS/SPME/GC–MS). The relationship between sensory data and VOCs was explored using an Artificial Neural Networks model (*Kohonen Self Organizing Maps*, omeSOM).

**Results and Conclusion** The results showed a strong preference by panelists for tomatoes of landraces than for commercial varieties and wild species. The predictive analysis by omeSOM showed 15 VOCs significantly associated to the typical and atypical tomato odour and taste. Moreover, omeSOM was used to predict the relationship of VOC ratios with sensory data. A total of 108 VOC ratios out of 8837 VOC ratios were predicted to be contributing to the typical and atypical tomato odour and taste. The metabolic origin of these flavor-associated VOCs and the metabolic point or target for breeding strategies were discussed.

**Keywords** VOC · Tomato flavor · Artificial neural network · GC–MS · SPME

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## 1 Introduction

Tomato (*Solanum lycopersicum*) is one of the most important food crops in the world at present. Its economic interest is based on a worldwide high yield production area and the important nutritional benefits associated with the fruit regular intake. (Bergougnoux 2014; Dorais et al. 2008).

Currently, tomato is the product of an extensive breeding program with the purpose of improving traits such as yield, synchronized harvest time, pest resistance, homogeneity in size, shape and ripening. However, it has shown detrimental effects on other important traits such as flavor and nutrient content (Klee and Tieman 2013).

The germplasm of commercial tomato showed a narrow genetic diversity compared to wild relatives, limiting crop improvement (Tanksley and McCouch 1997; Klee and Tieman 2013). Wild species and heirloom varieties such as landraces are major sources of genetic diversity (Peralta and Spooner 2007). Fruits from these kinds of genetic resources show different attributes compared with those in modern hybrids. For instance, some tomato landraces are particularly appreciated in local markets due to their important quality characteristics, such as intense flavor. Landraces can be often produced at a community or familiar scale in Andean regions of South America (Occhiuto et al. 2014).

The flavor of the tomato fruit is a complex combination of volatile and nonvolatile metabolites present in variable amounts depending on the environmental conditions and genetic background of the variety (Klee 2010). Its flavor is strongly influenced by the volatile organic compounds (VOCs) produced during the fruit development and ripening. Approximately 400 VOCs have been identified in tomatoes (Petro-Turza 1986). Within the chemodiversity of tomato VOCs, a little set of volatile compounds has been specifically associated with the characteristic tomato odour by a combination of their significant concentration in the fruit and their low odour threshold (Buttery and Ling 1993; Goff and Klee 2006; Tandon et al. 2000). This traditional approach does not include important variables such as retronasal odour threshold, tomato matrix, VOC interactions and nonvolatile metabolites that impact on the perception of taste and odour (Rambla et al. 2014). Therefore, predictive models tend to remedy these limitations (Tandon et al. 2000, 2003; Piombino et al. 2013; Tieman et al. 2012).

In recent years data mining has taken a more active role in resolving data treatment in order to discover hidden patterns among variables (Tsugawa et al. 2011; Van Meulebroek et al. 2015). Computational intelligence has been recently implemented in this task using diverse strategies such as artificial neural networks, evolutionary algorithms and fuzzy systems. Artificial Neural Networks (ANN)/Kohonen Self Organizing Maps (SOMs) have been applied in systems biology, transcriptomics and metabolomics for exploratory analysis, data integration and discovery of new relationships in large datasets (Stegmayer et al. 2009; Milone et al. 2010, 2013).

In this work, a collection of Andean tomato landraces have been analyzed along with a wild species (*Solanum pimpinellifolium*) and four commercial varieties with the aim of: (1) characterizing different tomato accessions by their volatile composition obtained by Headspace solid phase microextraction/gas chromatography–mass spectrometry (HS/SPME/GC–MS) and by their organoleptic characteristics by sensorial panels. (2) Finding relationships between sensory data and VOCs using a predictive model based on artificial neural networks. This approach allowed identifying numerous VOCs and VOC ratio with potential contribution to the typical and atypical tomato odour and taste, thus showing metabolic points or targets for breeding strategies.

## 2 Materials and methods

### 2.1 Plant material and growth conditions

Seeds of traditional tomatoes or landraces were collected in the Andean valleys of Cuyo and Northwestern Argentina (Asprelli et al. 2011) and maintained in the Horticulture Germplasm Bank of La Consulta Agricultural Experimental Station, National Institute of Agricultural Technology (INTA), Mendoza, Argentina. These landraces have been evaluated and characterized by their agronomic performance, plant morphology and fruit quality traits (Asprelli et al. 2017).

Eleven different tomato varieties of *S. lycopersicum* and the genotype LA1589 of *S. pimpinellifolium* (germplasm passport 4739) were used in this study (Supplementary Table S1). The selected tomato landraces (germplasm passport 572, 571, 569, 4750, 3806, 3836, and 3812) are highly appreciated for their intense flavor, flesh quality, colour and texture. Furthermore, the study included different commercial varieties: A cherry tomato group (CheAmPer, CheAmRed) and two modern commercial varieties, BIGUA and ELPIDA.

Tomato seeds were provided by the Horticulture Germplasm Bank and ten plants per accession were cultivated randomly in a field trial according to a random design, in comparative field parcels of the Institute of Horticulture, School of Agronomy, National University of Cuyo, Mendoza, Argentina (32°50′S, 68°52′O, 900 MASL). Mature fruits (fully red and firm slightly to finger pressure) were harvested at the beginning of March 2010. In all cases, six to ten fruits per plant of each accession for the case of VOC determination and 10–15 fruits per plant for the case of sensory analyses were harvested from three plants, randomly distributed in the experimental parcel. Each fruit was immediately chopped, frozen in liquid nitrogen and stored in ultra-freezer at − 80 °C for VOC analysis.

### 2.2 Descriptive sensory evaluation

A semi-trained sensory panel of twenty people at the National University of Cuyo was used to evaluate the

sensory profiles of tomato samples. They were women and men ranging from 20 to 50 years old including smokers and non-smokers. An average of ten panelists evaluated four to six tomato varieties in a sensory evaluation session.

For the sensory analysis, fruits were smelled and tasted to evaluate odour, taste, sweetness, sourness, juiciness and flesh amount. Each sensory variable was scored in a five-category system using a five point structured hedonic scale, ranging from 1: (non-characteristic odour and taste, low sweet, acid, juiciness and flesh amount) to 5: (very characteristic odour and taste, and very sweet, acid, juiciness and high flesh amount). The frequency of each point was used to score accessions and applied for statistical analysis (Supplementary Table S3). Moreover, to rank accessions according to odour and taste attributes, each sensory variable was simplified as a unique score [unique score $= (fs1 \times 0.1 + fs2 \times 0.25 + fs3 \times 0.5 + fs4 \times 0.75 + fs5 \times 1)$; fs: frequency of each point].

## 2.3 Sample preparation and VOC analysis

Fruit volatile analysis was carried out according to Cortina et al. (2017). The methodology by HS–SPME–GCMS was based on Tikunov et al. (2005) with modifications on concentrations, times and temperatures. Briefly, frozen samples were ground with liquid nitrogen until obtaining a homogeneous and fine powder. A known amount of tomato powder was incubated at 35 °C for a short time, followed by the addition of an aliquot of methanolic solution of 2-methylcyclohexanone as an internal standard in a concentration of 23 mg/L. A solution of EDTA-NaOH and solid $CaCl_2$ was then added. The sample mix was sonicated for 15 min in an ultrasonic bath; later 1 mL of the processed sample was transferred to a 10 mL screw caped glass vial. Finally, the samples were introduced into a Combi Pal (Varian Inc.) autosampler for HS–SPME–GCMS analysis.

VOCs were measured using gas chromatography coupled to mass spectrometry (GC–MS) by capillary GC (Varian 3800 gas chromatograph equipped with a VF-5 ms column, 30 m × 0.25 mm i.d., 0.25 μm film thickness) and analyzed by MS using an ion trap detector (Varian Saturn 2000 MS). The MS trap temperature was set at 200 °C, the manifold was heated at 100 °C and the transfer line at 230 °C. Electron impact mass spectra were recorded at 10 V ionization energy in the 33–300 amu mass range with 1 scan/seg. Column oven temperature conditions were 35 °C for 5 min, 3 °C/min ramp until 45 °C and 1.5 °C/min ramp until 50 °C, held for 1.5 min, 3 °C/min ramp until 68 °C, held for 2 min, 3 °C/min ramp until 131 °C, held for 1 min, 10 °C/min ramp until 250 °C, and then held isothermally at 250 °C for 2.93 min using helium 5.0 ultrapure as a carrier gas at 1 mL/min. The runtime for a single chromatographic analysis was 58 min. Mass spectra were analyzed

with the Varian MS Workstation Software (Version 6.6). Despite the extensive chromatographic program used, it was necessary to implement extracted ion chromatogram (EIC) (Hübschmann 2009) to identify individual signals in coelution zones (Tikunov et al. 2005; Zanor et al. 2009). Volatile metabolites were identified by comparing their mass spectra with the NIST Mass Spectral Library (NIST 05). When available, volatile metabolite signals were compared with pure standards by retention times and mass spectra. Signals designated as UNK could not be identified (matching < 70%). All signals, VOCs and UNK, were quantified using an internal standard and expressed as relative area units considering 1 g of sample.

## 2.4 Data analysis

The integrated area of each metabolite or signal was normalized to the sample weight (1 g) and the integrated area of the internal standard Eq. (1), where *Ion area* is the selected m/z area chosen for a given metabolite or signal, *weight* is the sample amount and *Std area* is the m/z = 112 area for the internal standard.

$$Normalized\ area\ (NA) = \left[ \frac{Ion\ area/weight}{Std\ area} \right] \times 100 \qquad (1)$$

To find significant differences ($P < 0.05$) in the VOC levels among accessions, variance analysis (ANOVA) and multiple comparison method DGC were used (Di Rienzo et al. 2002). To explore VOC composition among accessions, principal component analysis (PCA) was applied. To define the accessions grouped in the biplot graphic of PCA, cluster analysis (Ward's method) was run based on PCA latent variables (Everitt et al. 2011). All the above mentioned analyses were carried out with the statistical software Infostat (2013 version) (Infostat 2013).

To identify relationships between VOCs and sensory variables, ANN/SOM analyses was used. The study of ANN/SOM was run with the programming package omeSOM* tool (version 2.27.15, available in http://sourcesinc.sourceforge.net/omesom/) implemented in the programming language of MATLAB (MATLAB 8.0 and Statistics Toolbox 8.1, The Math Works Inc., Natick, Massachusetts, United States.) (Miloneet al. 2010).

The metabolic and sensory data for ANN/SOM analysis were standardized to Z score scaling by Eq. (2):

$$Z = \frac{(Xmv = i - AVXmv = i..j)}{SXmv = i..j} \qquad (2)$$

where Z is the standardized VOC or sensory variable, *Xm* is the VOC area normalized by Eq. (1) or sensory variable score, *v* is the tomato accession; AV*X*mv$= i…j$ is the average value of *Xm* in the tomato population ($v = i…j$) and

S$X$mv$=$i…j is the standard deviation of $Xm$ in the tomato population ($v=i…j$).

omeSOM software builds self-organizing maps (SOMs) that represent a special class of neural networks that use competitive learning (which is based on the idea of units (neurons) that competing to respond to a given subset of inputs). They represent complex high-dimensional input patterns in the form of simple low-dimensional discrete maps, with neurons that can be visualized in a two-dimensional lattice structure, while preserving the proximity relationships of the original data as much as possible. A neighborhood function (Vn) is defined for each neuron and when competition among the neurons is complete, SOMs update a set of weight vectors within the neighborhood of the winning neuron. An appropriate visualization of the resulting map, painting the neurons according to the type of data grouped, is proposed for helping in the rapid identification of combined data types. When a Vn is defined, all the neurons in the neighborhood of radius Vn are considered as a group and

treated altogether accordingly (for additional information see Milone et al. 2010).

# 3 Results

## 3.1 Tomato accession characterization

### 3.1.1 Sensory analysis

Six hedonic traits (odour, taste, sweetness, sourness, juiciness and flesh amount) were evaluated by a panel of 20 semi-trained volunteers. Five score categories (1 = non-characteristic to 5 = very-characteristic) for each sensory variable were used, obtaining a total of 30 score frequencies (variables × score categories) for data analysis (Supplementary Table S3). Accessions were evaluated by PCA to identify associations between sensory scores and accession groups. Cluster analysis performed with latent variables of the first three principal components (69%
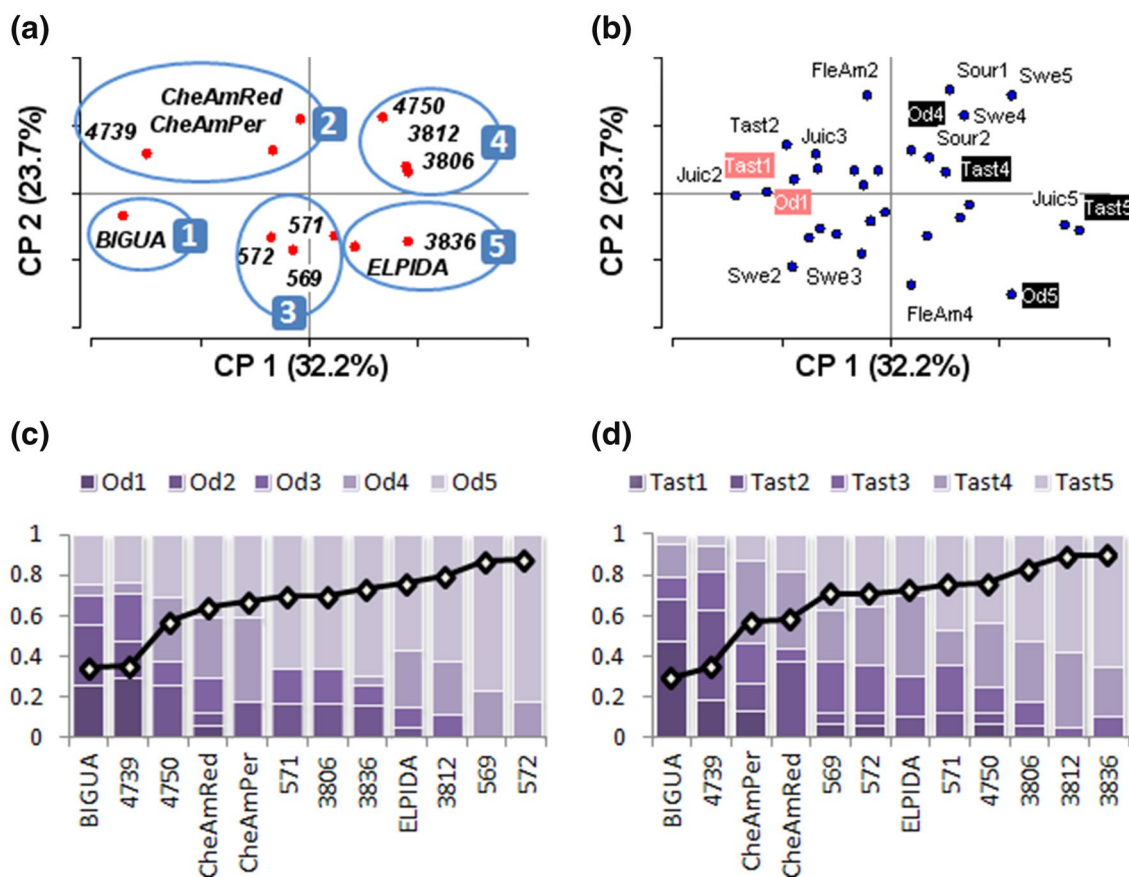


**Fig. 1** Sensory analysis of tomato accessions by tasting panelist. **a** Biplot graph of principal components analysis of sensory data from tomato accessions. Ellipses represent the accessions grouped by cluster analysis using the PCA latent variants (PC1, PC2 and PC3). **b** Biplot graph with loading of sensory score. **c** Stacked bar graph representing the score frequency of five odour categories in each accession. **d** Stacked bar graph representing the score frequency of five taste categories in each accession. Diamonds and Line represent the standardized unique score of odour and taste of the different tomato accessions

of total variance) produced five accession groups represented in the biplot of Fig. 1a. The PCA loadings (sensory scores) are shown in Fig. 1b. The first component (PC1) (contributing with 32.2% of total variance) allowed separation of group 1 (Bigua) and 2 (4739, CheAmPer and CheAmRed) from group 4 (4750, 3812 and 3806) and 5 (3836 and ELPIDA) (Fig. 1a). Group 1 was mainly associated with the lowest scores and group 2 to the highest score of all sensory variables (Fig. 1b). The sensory variables that contributed most to this PC1 distribution were taste and juiciness. In the second component (PC2) (contributing with 23.7% of total variance), groups 2 and 4 differed from groups 3 and 5. The sensory variables that contributed most to PC2 distribution were odour, flesh amount and sweetness. Accessions of group 3 (572, 571 and 569) and group 5 were mainly associated with the high score of odour and intermediate score of sweetness. Accessions of group 4 were clustered by the lowest sourness, the highest sweetness and medium–high odour and taste score. Accessions of group 2 (cherry group) were associated with high score of sweetness, low score of flesh amount and sourness and intermediated-low juice, odour and taste.

Because odor and taste are directly influenced by VOCs and are the sensory variables more representatives of tomato flavor (Klee 2010; Rambla et al. 2014), a zooming in their frequency distribution for each accession is shown in Fig. 1c, d, respectively. Here the accessions were ordered by the standardized unique score and they showed a distribution to similar that in PCA. Characteristic (score 4) and very characteristic (score 5) tomato odour and taste and non-characteristic (score 1) tomato odour and taste were able to discriminate accession groups. Andean landraces were more frequently scored by panelists with a typical odour and taste (scores 4 and 5) while the commercial variety CheAmPer, CheAmRed

with intermediate odour and taste and the wild accession 4739 and commercial variety Bigua as having an atypical tomato odour and taste.

### 3.1.2 Analysis of VOCs

The volatile profile obtained from HS/SPME/GC–MS produced 94 VOC signals listed in Supplementary Table S2 with their corresponding elution time and selected (m/z) ion for extracted ion chromatogram. The areas of each VOC are informed in Supplementary Table S4.

VOC data were analyzed by PCA. Four accession groups were defined by cluster analysis of latent variant of three first PCs (representing 59% of total variance). Figure 2 shows a biplot graph of PC1 vs. PC2 with the four groups. VOC distribution in each quarter of biplot is represented by pie chart according to biosynthetic origin. PC1 mainly differed between groups II and III and groups I and IV. PC2 differed between groups I and II and groups III and IV.

The VOCs that contributed most to these differentiations are listed in Table 1. They were chosen according to an eigenvalue > 50% of the greatest eigenvalue and according to levels with significant difference ($P < 0.05$) between groups (Supplementary Tables S5). Group I (accession 4739 of *S. pimpinellifolium*) and group IV (accessions 3836, 569, 571, 3806 and 4750) showed higher levels of 14 VOCs made up 28.5% fatty acid-derived VOCs, 21.4% aminoacid-derived VOCs, 21.4% terpene-derived VOCs, 7.2% carotene-derived VOCs and 21.4% unknown VOCs. Moreover, group I differed from group IV by higher levels of 15 metabolites with a high abundance (60%) of fatty acid-derived VOCs (13.3% aminoacid derived VOCs, 6.7% carotene-derived VOCs, 6.7% terpene-derived VOC and 13.3% unknown VOCs).

Group II (accession 3812) and group III [ELPIDA, BIGUA and the three cherry type varieties (572, CheAmPer and CheAmRed)] were characterized by 15 VOCs with high

**Fig. 2** Biplot graph of principal components analysis of VOC composition from tomato accessions. Ellipses represent the accessions grouped by cluster analysis using the PCA latent variants (PC1, PC2 and PC3). Pie chart represents the VOC composition (according to their metabolic origin, *AA* aminoacids, *FA* fatty acids, *TER* terpenes, *CAR* carotenes and *UNK* unknown) distributed in each quarter of biplot
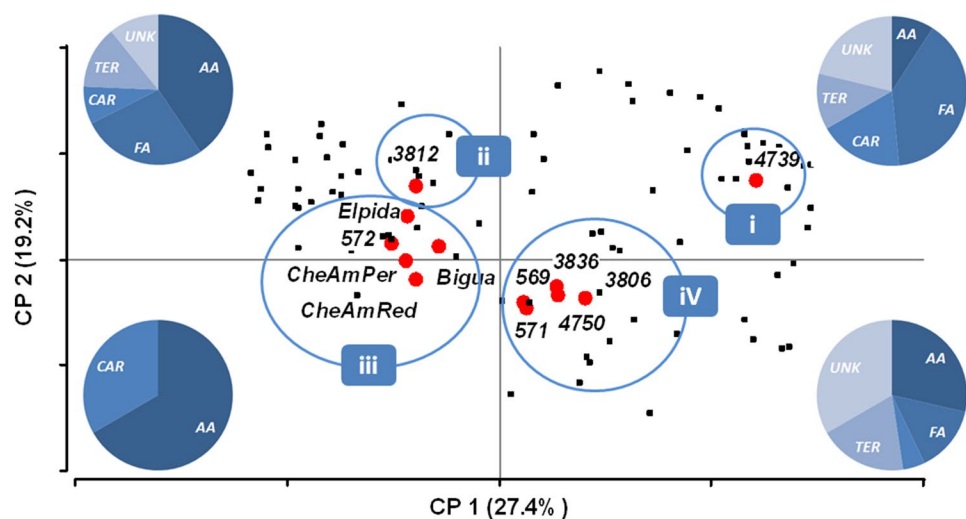
**Table 1** VOCs contributing to accessions group differentiation

| Group | VOC | Group | VOC |
|---|---|---|---|
| I/IV | *cis*-3-hexenal | I | Hexanal |
| | *cis*-2-hexenal | | *trans*-2-hexenal |
| | 2-Octenal | | 2-Ethylfuran |
| | 2-Ethyl-1-hexanol | | 1-Penten-3-one |
| | Duraldehyde | | *cis*, *cis*-1,4-pentadiene |
| | 2-Phenylethyl acetate | | *trans*-2-heptenal |
| | Benzyl acetate | | 2-Decenal |
| | Verdyl acetate | | *trans*-4-pentenal |
| | *cis*-Linalyl oxide | | 2-Nonen-1-ol |
| | *trans*-Linalyl oxide | | Benzylnitrile |
| | 6-Methyl-5-hepten-2-ol | | 2-Phenylethanol |
| | UNK m/z 57-2 | | Limonene |
| | UNK m/z 57-3 | | 6-Methyl-5-hepten-2-one |
| | UNK m/z 115 | | UNK m/z 58 |
| | | | UNK m/z 57-1 |
| II/III | Methyl butanoate | II | 2-Methyl-2-octen-4-one |
| | 2-Methyl-2-octen-4-one | | 2-Undecanone |
| | 2-Undecanone | | 3-Methylheptyl acetate |
| | 2-Dodecanone | | 2-Methylacetophenone |
| | Benzophenone | | 2-Methyl-3-phenyl-1-Propene |
| | 2-Methylacetophenone | | Terpinolene |
| | a-Hexylcinnamaldehyde | | Eugenol |
| | Benzaldehyde | | *a*-Terpineol |
| | 3-Methyl-1-butanol | | Lilial |
| | 2-Isobutylthiazole | | Linalool |
| | p-Methoxytoluene | | *b*-Damascenone |
| | *a*-Isophorone | | UNK m/z 131 |
| | UNK m/z 147 | | UNK m/z 147 |
| | UNK m/z 131 | | UNK m/z 68 |
| | UNK m/z 68 | | |

Colors represents the metabolic origin of VOC, Light color to dark color means fatty acid, aminoacid, terpene and carotene, respectively

abundance (46.7%) of aminoacid-derived VOCs (26.7% of fatty acid-derived VOCs, 20% of unknown VOCs and 6.6% of carotene-derived VOCs). Moreover, group II differed from group III by 14 VOCs made up 35.7% terpene-derived VOCs, 21.5% the fatty acid-derived VOCs, 21.4% unknown VOCs, 14.3% the aminoacid-derived VOCs, and 7.1% the carotene-derived VOCs.

## 3.2  Association of VOCs and sensory descriptors

An analysis based on computational intelligence, ANN/SOMs, provides a different way to analyze and visualize the relationship between sensory scores and VOCs. At a glance, omeSOM provide a simple visualization interfaces (two-dimensional lattice structure or neuron map) for the identification of co-varying metabolites and sensory score. Neurons grouping both types of data are easily highlighted. Figure 3a shows the activation map resulting from the integrated analysis of 94 metabolites and 25 sensory score data within a map of $7 \times 7$ neurons topology. Direct patterns and a neighborhood function Vn = 0 were defined as parameter to activate the map and only the neurons in the neighborhood of Vn = 0 are considered as a group and treated accordingly. The neurons containing the ratings for the score of typical and atypical tomato odour and taste were selected. The highest score (5) of taste and odour variables was in N 12 and N 19, respectively, and in N 21 for taste 4 and odour 4. The lowest score (1) of odour and taste was found in N 38 and N47, respectively (Fig. 3a). Inside the neurons mentioned (Vicinity 0), other variables, metabolic or sensory, are located, showing a highly similar behavior pattern through the accessions (Fig. 3b). In addition to the neurons highlighted, immediate neighbourhood (+ 1) must be considered since it also presents similar pattern profiles, such as N19 and N12 (Fig. 3a, b), showing associations between the highest score of taste and odour.

**Fig. 3** Output layer of ANN/ SOM analysis of tomato accessions resulting from the integrated analysis of 94 metabolites and 25 sensory score from 12 tomato accessions. **a** Map of 7×7 neurons with Vn=0. **b** Details of normalized cluster patterns values clustered together in neurons containing typical and atypical score of tomato odour and taste. *Od* odour, *Tast* taste, *Sour* sourness, *Swe* sweetness, *M49* camphor, *M91 b*-methylionone, *M46* 2-methylacetophenone, *M92* benzophenone
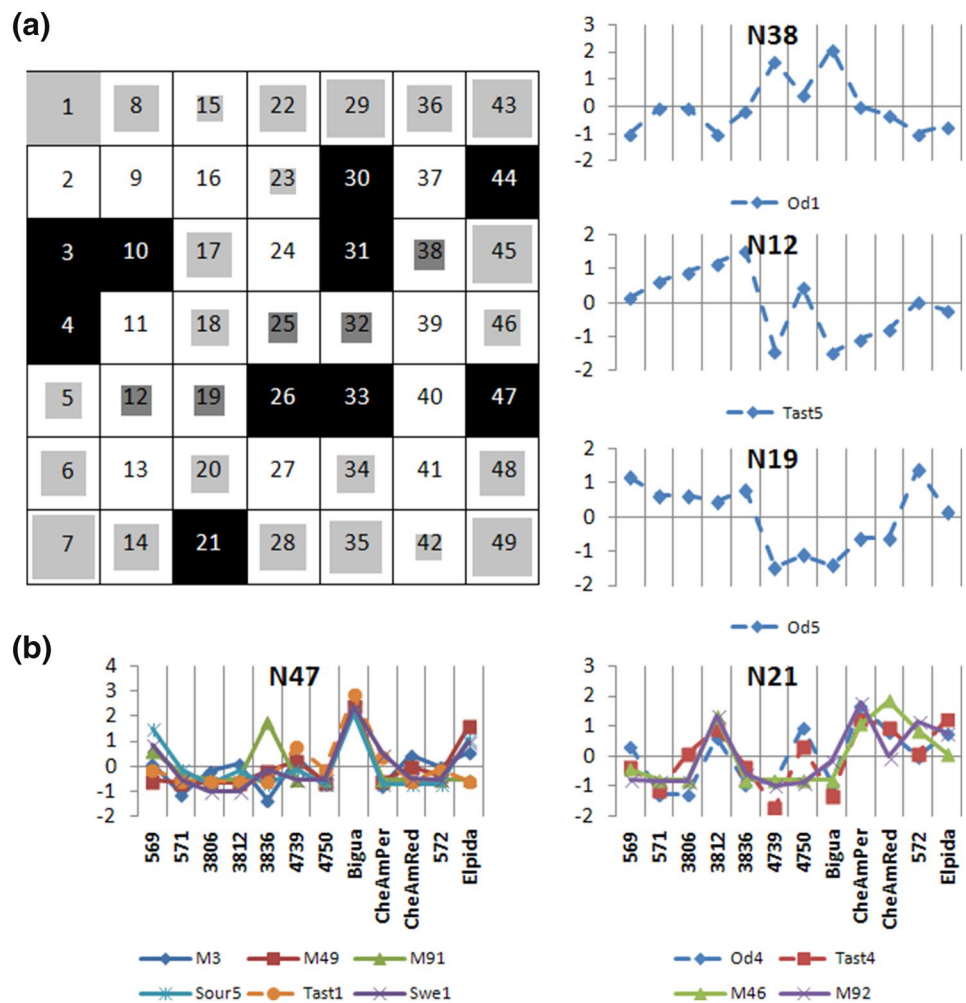


Pearson correlation was performed to identify significant correlation ($P<0.05$) between the variables associated. A total of 6 VOCs were correlated to typical tomato odour and taste (scores 4 and 5) and 9 VOCs were correlated to the atypical tomato odour and taste (score 1) (Table 2).

Similarly, associations of VOC ratios and typical and atypical odour and taste were performed. Figure 3b shows a new 30×30 Neurons map considering 8837 VOC ratios and 25 sensory score data. Neurons 412 and N 266 contain the variables of typical tomato odour (scores 5 and 4, respectively) and N 161 and N 236 contain the variables of typical tomato taste (scores 5 and 4 respectively). Neurons 578 and N 580 contain the variables of atypical tomato odour and taste (score 1), respectively. Figure 4 shows the profile of these variables and associated VOC ratio in each neuron. Table 3 lists only the significant correlations ($P<0.05$) between sensory variables and those VOC ratios in the same neuron and neighboring neurons. A total of 55 VOC ratios were significantly correlated to typical tomato odour and/or taste (Fig. 5a). On the other hand, 42 VOC

ratios were correlated to atypical tomato odour and taste and 8 VOC ratios were correlated to atypical tomato odour (Fig. 5a). In addition, 94 VOC ratios with unknown VOCs were also correlated to typical and atypical tomato odour and taste (Supplementary Table S6).

## 4 Discussion and conclusion

The process of tomato domestication and breeding resulted in a dramatic reduction of the variability available in the genus and, indeed, provides an example of severe genetic bottleneck (Bai and Lindhou 2007). Particularly, the deterioration of organoleptic properties of modern cultivars is evident when compared with heirloom varieties (Tieman et al. 2017).

With the aim of detecting associations between hedonic traits and VOC composition in tomato fruit, in the present work we report data from a characterization of the fruit organoleptic properties of seven Andean landrace (heirloom

**Table 2** Metabolites associated to high and low odor and taste in tomato accession by omeSOM analysis

| Metabolites associated to characteristic tomato taste and odour | OmeSOM analysis | | | | Odor type[a] |
|---|---|---|---|---|---|
| | Neuron | Vicinity | Associated variable | R ($p < 0.05$) | |
| 2-Methylacetophenone | 21 | 0 | Tast4/Od4 | 0.71/0.67 | Floral |
| Benzophenone | 21 | 0 | Tast4 | 0.67 | Balsamic |
| α-Hexylcinnamaldehyde | 20 | 1 | Tast4 | 0.6 | Fruity |
| α-Isophorone | 28 | 1 | Tast4/Od4 | 0.66/0.58 | Woody |
| 2-Undecanone | 28 | 1 | Tast4 | 0.63 | Fruity |
| 2-Methyl-2-octen-4-one | 28 | 1 | Tast4 | 0.63 | |
| Taste 5 | 12 | 1 | Od5 | 0.69 | |
| Odour 5 | 19 | 1 | Tast5 | 0.69 | |
| Odour 4 | 28 | 0 | Tast4 | 0.8 | |
| Taste 4 | 28 | 0 | Od4 | 0.8 | |

| Metabolites associated to non-characteristic tomato taste and odour | OmeSOM analysis | | | | Odor type[a] |
|---|---|---|---|---|---|
| | Neuron | Vicinity | Associated variable | R ($p < 0.05$) | |
| 2-Phenylethanol | 44 | 1 | Od1 | 0.72 | Floral |
| 3-Methylbutanal | 48 | 1 | Tast1/Od1 | 0.73/0.65 | Fermented |
| Phenylacetaldehyde | 44 | 1 | Od1 | 0.58 | Green |
| β-Ionone | 44 | 1 | Od1 | 0.74 | Floral |
| *cis*-2-hexenal | 30 | 1 | Od1 | 0.79 | Green |
| Camphor | 47 | 0 | Tast1/Od1 | 0.67/0.58 | Camphoreous |
| UNK m/z 55 | 31 | 1 | Tast1 | 0.83 | |
| UNK m/z 105 | 31 | 1 | Tast1 | 0.67 | |
| UNK m/z 95 | 48 | 1 | Tast1 | 0.76 | |
| Sweetness 1 | 47 | 0 | Tast1 | 0.72 | |
| Sourness 5 | 47 | 0 | Tast1 | 0.59 | |
| Odour 1 | 38 | 2 | Tast1 | 0.78 | |
| Odour 2 | 31 | 1 | Tast1 | 0.6 | |
| Taste 2 | 44 | 1 | Od1 | 0.75 | |
| Taste 1 | 47 | 2 | Od1 | 0.78 | |

[a]Odour type reported in http://www.thegoodscentscompany.com

varieties) along with four commercial varieties and one wild species. Among the sensory variables analyzed, taste, odour and juiciness were those that contributed more to discriminating accessions. In comparison with the wild species *S. pimpinellifolium* and the commercial cultivars, especially Bigua, the Andean landraces showed the highest score in terms of characteristic tomato taste and odour. These results agree with the fact that these accessions were selected and maintained by Andean communities based on their organoleptic properties (Peralta et al. 2008), while the commercial varieties were selected by modern breeding practice based on agronomic traits such as productivity, pest resistance, long shelf life and fruit shape (Bai and Lindhou 2007). Notwithstanding, the commercial cultivar Elpida showed a high score in terms of taste and odour, similar to that recorded for the Andean landrace. Contrary to other wild tomato species, *S. pimpinellifolium* produced edible fruits that were perceived as not unpleasant by panelists, but rather different to the characteristic tomato flavor.

In the present study, a Neural Network analysis (omeSOM; Milone et al. 2010) was applied to explore associations between VOCs and tomato taste and odour. Results revealed 15 VOCs significantly associated with a typical or atypical tomato taste and odour (Table 2). The odour type of pure VOCs evidences the contribution of the associated VOCs to tomato flavor. VOCs associated with typical tomato odour were described as floral and fruity while VOCs associated with atypical odour/taste showed a diverse odour type such as green, fermented, fatty, chemical-like, etc. (data obtained in http://www.thegoodscentscompany.com, Table 2). In addition to VOCs, sugars and organic acids also contribute to tomato flavor. Fruit sweetness and sourness are the most influenced sensory traits by these metabolites (Baldwin et al. 2008). In general, results showed that the accessions mostly preferred were scored with intermediate
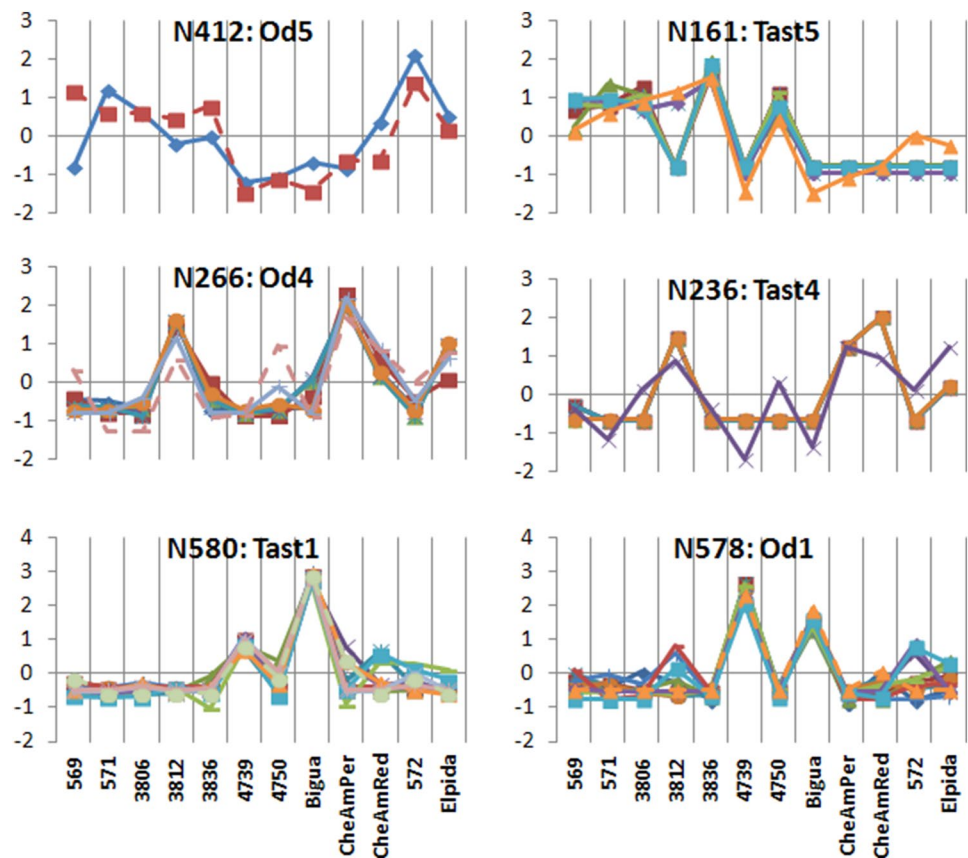
sourness (score 3) and higher sweetness (scores 4 and 5). However, omeSOM analyses found no significant associations between sweetness/sourness scores and the typical taste and odour of tomato. Lack of association between these sensory variables was also reported in previous studies in tomato (Baldwin et al. 1998; Piombino et al. 2013). By contrast, significant association between low sweetness (score 1)/high sourness (score 5) and atypical taste was found, evidencing the complexity of sweetness/sourness balance in the sensory perception.

Several studies described interactions between volatile and non-volatile compounds affecting sensory perception (Tandon et al. 2003; Baldwin et al. 2008); however, the effects of VOC interaction on sensory perception are barely known. In this sense, a neuronal network analysis between VOC ratio and tomato taste and odour was assessed. VOC ratio profile fitted better to sensory variable profile than that of individual VOCs (Figs. 4, 5). VOC ratio associated with odour and taste contained most of the individually associated VOCs and exposed other VOCs not associated before. In general, typical or atypical tomato odour and taste seem to be driven for a balance between defined VOC groups contributing positively or negatively to odour and taste (Table 3). To gain greater understanding of these relations, the VOCs were grouped by metabolic origin. The distribution of VOC ratios

associated to typical odour and taste showed a predominance of aminoacid-derived VOC over fatty acid- or carotene- or aminoacid-derived VOC and fatty acid-derived VOC over fatty acid-derived VOC (Fig. 5b). On the other hand, the distribution of VOC ratios associated to atypical odour and taste showed predominance of fatty acid-derived VOC over aminoacid- or fatty acid- or terpene-derived VOC and carotene-derived VOC over aminoacid-derived VOC (Fig. 5c). The contributions of VOCs more frequently found in the ratios are highlighting:

(A) VOCs derived from phenylalanine through the phenyl ammonia lyase pathway such as methyl salicylate, α-hexylcinnamaldehyde, benzyl acetate, 2-methyl acetophenone, eugenol and benzophenone (Tieman et al. 2010; Koeduka et al. 2006) were the VOCs mainly associated with the typical tomato odour and taste.

Similarly, VOCs derived from phenylalanine through the phenylacetaldehyde synthase route (PAAS) (Tieman et al. 2006), such as phenylacetaldehyde and 2-phenylethyl acetate, were also correlated with typical tomato odour and taste. However, 2-phenylethanol, a product of phenylacetaldehyde reductase (PAR) (Tieman et al. 2007), correlated with the atypical tomato odour and taste, agreeing with the malodorous properties of fruit with high levels of this VOC (Tadmor et al. 2002). In addition, the association

**Table 3** Metabolites ratios associated by omeSOM analysis to characteristic and non characteristic tomato odor and taste score

Neurons associated to characteristic tomato odour (Od4:N266)

| Neuron location | Vicinity | Metabolite ratio a/b | | Pearson correlation | Metabolic origin | |
|---|---|---|---|---|---|---|
| | | a | b | R ($p < 0.05$) | a | b |
| 235 | 1 | Taste 4 | | 0.8 | | |
| 296 | 1 | Eugenol | Toluene | 0.59 | AA | AA |
| 267 | 1 | Methyl salicylate | Hexanal | 0.66 | AA | FA |
| 297 | 1 | *p*-Menth-1-en-9-al | Geranyl acetone | 0.58 | TER | CAR |

Neurons associated to characteristic tomato taste (Tast4:N236)

| Neuron location | Vicinity | Metabolite ratio a/b | | Pearson correlation | Metabolic origin | |
|---|---|---|---|---|---|---|
| | | a | b | R ($p < 0.05$) | a | b |
| 266 | 1 | Odour4 | | 0.8 | | |
| 205 | 1 | α-Hexylcinnamaldehyde | Duraldehyde | 0.58 | AA | AA |
| 205 | 1 | α-Hexylcinnamaldehyde | Isoamyl salicylate | 0.61 | AA | AA |
| 205 | 1 | 3-Methylbutanal | β-Ionone epoxide | 0.81 | AA | CAR |
| 205 | 1 | 3-Methyl-1-butanol | β-Ionone epoxide | 0.75 | AA | CAR |
| 205 | 1 | 3-Methyl-1-butanol | β-Methylionone | 0.74 | AA | CAR |
| 295 | 2 | Dimethylbenzaldehyde | β-Ionone epoxide | 0.63 | AA | CAR |
| 205 | 1 | α-Hexylcinnamaldehyde | β-Methylionone | 0.8 | AA | CAR |
| 265 | 1 | β-Damascenone | β-Ionone epoxide | 0.7 | CAR | CAR |
| 206 | 1 | 2-Dodecanone | β-Ionone epoxide | 0.69 | FA | CAR |

Neurons associated to characteristic tomato taste and odour

| Neuron location | Vicinity | Metabolite ratio a/b | | Pearson correlation | Metabolic origin | |
|---|---|---|---|---|---|---|
| | | a | b | R:tast/R:od ($p < 0.05$) | a | b |
| 205 | 1 | α-Hexylcinnamaldehyde | 2-Phenylethyl acetate | 0.71/0.58 | AA | AA |
| 237 | 1 | 2-Methylacetophenone | Benzaldehyde | 0.65/0.72 | AA | AA |
| 237 | 1 | 2-Methylacetophenone | Toluene | 0.63/0.69 | AA | AA |
| 207 | | 2,5-Ditertbutylbenzoquinone | β-Methylionone | 0.6/0.58 | AA | CAR |
| 236 | 0 | 2-Methylacetophenone | β-Ionone epoxide | 0.71/0.66 | AA | CAR |
| 266 | 0 | Benzophenone | β-Ionone epoxide | 0.77/0.7 | AA | CAR |
| 295 | 1 | Methyl salicylate | β-Ionone epoxide | 0.73/0.61 | AA | CAR |
| 206 | 1 | Methyl butanoate | β-Ionone epoxide | 0.78/0.75 | AA | CAR |
| 205 | 1 | α-Hexylcinnamaldehyde | Heptanal | 0.71/0.58 | AA | FA |
| 267 | 1 | Methyl salicylate | *trans*-2-heptenal | 0.63/0.67 | AA | FA |
| 237 | 1 | Eugenol | *cis*-3-hexenal | 0.77/0.73 | AA | FA |
| 266 | 0 | Eugenol | Hexanal | 0.67/0.67 | AA | FA |
| 205 | 1 | α-Hexylcinnamaldehyde | Verdyl acetate | 0.71/0.58 | AA | TER |
| 206 | 1 | 2-Dodecanone | β-Methylionone | 0.67/0.59 | FA | CAR |
| 206 | 1 | 2-Dodecanone | *cis*-2-hexenal | 0.7/0.58 | FA | FA |
| 267 | 1 | β-Damascenone | Hexanal | 0.63/0.66 | CAR | FA |

Neurons associated to very characteristic tomato odour (Od5, N:412)

| Neuron location | Vicinity | Metabolite ratio a/b | | Pearson correlation | Metabolic origin | |
|---|---|---|---|---|---|---|
| | | a | b | R ($p < 0.05$) | a | b |
| 412 | 0 | α-Hexylcinnamaldehyde | Methyl salicylate | 0.66 | AA | AA |
| 442 | 1 | Phenylacetaldehyde | *trans,trans*-2,4-decadienal | 0.6 | AA | FA |
| 442 | 1 | α-Hexylcinnamaldehyde | *trans,trans*-2,4-decadienal | 0.6 | AA | FA |

**Table 3** (continued)

Neurons associated to very characteristic tomato taste (Tast5, N:161)

| Neuron location | Vicinity | Metabolite ratio a/b | | Pearson correlation | Metabolic origin | |
|---|---|---|---|---|---|---|
| | | a | b | R ($p < 0.05$) | a | b |
| 161 | 0 | 2-Phenylethyl acetate | 2-Ethylfuran | 0.69 | AA | FA |
| 131 | 1 | 2-Phenylethyl acetate | 1-Penten-3-one | 0.64 | AA | FA |
| 131 | 1 | 2-Phenylethyl acetate | 2-Ethylfuran | 0.68 | AA | FA |
| 131 | 1 | Benzyl acetate | 2-Ethylfuran | 0.64 | AA | FA |
| 161 | 0 | 2-Phenylethyl acetate | β-Citral | 0.69 | AA | TER |
| 130 | 1 | Benzyl acetate | β-Citral | 0.62 | AA | TER |
| 193 | 1 | 6-Methyl-5-hepten-2-ol | 2-Ethylfuran | 0.66 | CAR | FA |
| 192 | 1 | 6-Methyl-5-hepten-2-ol | β-Ionone epoxide | 0.64 | CAR | CAR |
| 163 | 1 | 6-Methyl-5-hepten-2-ol | Pseudoionone | 0.62 | CAR | CAR |
| 130 | 1 | β-Damascenone | 2-Undecanone | 0.61 | CAR | FA |
| 162 | 1 | 6-Methyl-5-hepten-2-ol | β-Citral | 0.7 | CAR | TER |
| 161 | 0 | Heptanal | | 0.69 | FA | |
| 161 | 0 | Heptanal | 2-Ethylfuran | 0.71 | FA | FA |
| 161 | 0 | Heptanal | 1-Penten-3-one | 0.7 | FA | FA |
| 160 | 1 | Heptanal | cis-3-hexenal | 0.62 | FA | FA |
| 130 | 1 | Heptanal | Hexanal | 0.6 | FA | FA |
| 130 | 1 | Heptanal | trans-2-hexenal | 0.68 | FA | FA |
| 160 | 1 | Heptanal | 2-Undecanone | 0.66 | FA | FA |
| 160 | 1 | Heptanal | Camphor | 0.64 | FA | TER |
| 191 | 1 | Hexanal | β-Citral | 0.74 | FA | TER |
| 161 | 0 | Heptanal | β-Citral | 0.69 | FA | TER |
| 161 | 0 | Heptanal | p-Methoxytoluene | 0.69 | FA | AA |
| 160 | 1 | Heptanal | Benzophenone | 0.59 | FA | AA |
| 160 | 1 | Heptanal | β-Damascenone | 0.61 | FA | CAR |

VOCs associated to non-characteristic tomato odour (Od1:N578)

| Neuron location | Vicinity | Metabolite ratio a/b | | Pearson correlation | Metabolic origin | |
|---|---|---|---|---|---|---|
| | | a | b | R ($p < 0.05$) | a | b |
| 580 | 2 | Taste1 | | 0.78 | | |
| 607 | 1 | 1-Penten-3-one | 2-Methyl-3-phenyl-1-propene | 0.69 | FA | AA |
| 579 | 1 | 2-Dodecanone | Benzophenone | 0.95 | FA | AA |
| 607 | 1 | 2-Ethylfuran | 2-Methyl-3-phenyl-1-propene | 0.81 | FA | AA |
| 547 | 1 | 2-Ethylfuran | 3-Methylheptyl acetate | 0.86 | FA | FA |
| 577 | 1 | cis-2-hexenal | 2-Pentylfuran | 0.91 | FA | FA |
| 577 | 1 | cis-2-hexenal | Heptanal | 0.91 | FA | FA |
| 547 | 1 | trans-2-hexenal | 2-Ethyl-1-hexanol | 0.83 | FA | FA |
| 577 | 1 | cis-2-hexenal | Terpinolene | 0.91 | FA | TER |

Neurons associated to non-characteristic tomato taste and odour (Tast1, N580; Od1:N578)

| Neuron | Vicinity | Metabolite ratio a/b | | Pearson correlation | Metabolic origin | |
|---|---|---|---|---|---|---|
| | | a | b | R:tast/R:od ($p < 0.05$) | a | b |
| 578 | 0 | 2-Phenylethanol | Linalool | 0.68/0.95 | AA | TER |
| 578 | 0 | 3-Methylbutanal | α-Terpineol | 0.69/0.97 | AA | TER |
| 550 | 1 | 3-Methyl-1-butanol | α-Terpineol | 0.86/0.78 | AA | TER |
| 580 | 0 | 3-Methyl-1-butanol | β-Damascenone | 0.84/0.79 | AA | CAR |
| 577 | 1 | 3-Methylbutanal | β-Damascenone | 0.61/0.94 | AA | CAR |

**Table 3** (continued)

Neurons associated to non-characteristic tomato taste and odour (Tast1, N580; Od1:N578)

| Neuron | Vicinity | Metabolite ratio a/b | | Pearson correlation | Metabolic origin | |
|---|---|---|---|---|---|---|
| | | a | b | R:tast/R:od ($p < 0.05$) | a | b |
| 578 | 0 | 2-Phenylethanol | 3-Methylheptyl acetate | 0.62/0.9 | AA | FA |
| 578 | 0 | β-Methylionone | α-Hexylcinnamaldehyde | 0.84/0.95 | CAR | AA |
| 578 | 0 | Geranyl acetone | Dimethylbenzaldehyde | 0.68/0.86 | CAR | AA |
| 578 | 0 | β-Ionone | Isoamyl salicylate | 0.68/0.83 | CAR | AA |
| 579 | 1 | β-Ionone | Dimethylbenzaldehyde | 0.82/0.94 | CAR | AA |
| 611 | 1 | β-Ionone epoxide | 2-Methyl-3-phenyl-1-propene | 0.94/0.72 | CAR | AA |
| 581 | 1 | β-Ionone epoxide | Dimethylbenzaldehyde | 0.92/0.67 | CAR | AA |
| 610 | 1 | β-Ionone | 3-Methylheptyl acetate | 0.87/0.86 | CAR | FA |
| 609 | 1 | Geranyl acetone | 3-Methylheptyl acetate | 0.75/0.83 | CAR | FA |
| 579 | 1 | β-Ionone epoxide | 2-Undecanone | 0.85/0.96 | CAR | FA |
| 608 | 1 | 6-Methyl-5-hepten-2-one | Linalool | 0.66/0.91 | CAR | TER |
| 578 | 0 | β-Ionone epoxide | α-Terpineol | 0.72/0.92 | CAR | TER |
| 580 | 0 | β-Ionone epoxide | Terpinolene | 0.95/0.86 | CAR | TER |
| 578 | 0 | *trans*-4-pentenal | Dimethylbenzaldehyde | 0.61/0.88 | FA | AA |
| 577 | 1 | *cis*-2-hexenal | 2-Methyl-3-phenyl-1-propene | 0.63/0.83 | FA | AA |
| 548 | 1 | *cis*-2-hexenal | Dimethylbenzaldehyde | 0.68/0.9 | FA | AA |
| 577 | 1 | *cis*-2-hexenal | Isoamyl salicylate | 0.67/0.92 | FA | AA |
| 577 | 1 | *cis*-2-hexenal | Propyl salicylate | 0.64/0.91 | FA | AA |
| 577 | 1 | *cis*-3-hexenal | Isoamyl salicylate | 0.63/0.89 | FA | AA |
| 577 | 1 | *trans*-4-pentenal | 2-Methyl-3-phenyl-1-propene | 0.6/0.9 | FA | AA |
| 548 | 1 | *trans*-4-pentenal | 3-Methylheptyl acetate | 0.7/0.86 | FA | FA |
| 580 | 0 | 2-Dodecanone | β-Damascenone | 0.87/0.83 | FA | CAR |
| 609 | 1 | 8-Pentadecanone | β-Damascenone | 0.71/0.81 | FA | CAR |
| 578 | 0 | 2-Ethylfuran | 2-Ethyl-1-hexanol | 0.68/0.96 | FA | FA |
| 579 | 1 | 2-Ethylfuran | Hexanal | 0.68/0.76 | FA | FA |
| 549 | 1 | *trans*-4-pentenal | 2-Ethyl-1-hexanol | 0.77/0.82 | FA | FA |
| 580 | 0 | 2-Dodecanone | α-Terpineol | 0.89/0.82 | FA | TER |
| 609 | 1 | 8-Pentadecanone | α-Terpineol | 0.86/0.91 | FA | TER |
| 609 | 1 | 2-Decenal | *cis*-linalyl oxide | 0.62/0.87 | FA | TER |
| 609 | 1 | 2-Decenal | *trans*-linalyl oxide | 0.64/0.88 | FA | TER |
| 549 | 1 | *cis*-2-hexenal | *p*-Menth-1-en-9-al | 0.8/0.85 | FA | TER |
| 579 | 1 | *trans*-4-pentenal | *p*-Menth-1-en-9-al | 0.82/0.9 | FA | TER |
| 611 | 1 | *trans*-4-pentenal | *trans*-linalyl oxide | 0.81/0.61 | FA | TER |
| 608 | 1 | 2-Decenal | DMHEX | 0.47/0.83 | FA | |
| 578 | 0 | Camphor | α-Terpineol | 0.74/0.98 | TER | TER |
| 608 | 1 | Lilial | Terpinolene | 0.71/0.89 | TER | TER |
| 578 | 0 | Camphor | β-Damascenone | 0.66/0.95 | TER | CAR |

Neuron location means the position of metabolite ratio in the neuron map (Fig. S1). Vicinity means the proximity of neuron with metabolite ratio to neuron with the analyzed sensory score

*R* correlation coefficient of Pearson analysis of associated variables (metabolites ratio vs. sensory score frequency). Metabolic origin means the biosynthetic pathway of metabolite, *AA* amino acids, *FA* fatty acids, *CAR* carotenes, *TER* terpenes

of methyl salicylate/2 phenylethyl acetate ratio with typical odour and taste evidences that either a higher activity of PAL pathway than PAAS/PAR/alcohol acyltransferase (AAT) (Goulet et al. 2015) or a regulation of methylation/acetylation by glycosyl transferase/esterase (SlCXE, Goulet et al. 2012) would be improving taste and odour. Recent

**Fig. 5** VOC ratio associated to typical and atypical tomato odour and taste by omeSOM analysis. **a** Common and unique VOC ratio associated to typical and atypical tomato odour and/or taste. **b** Distribution of VOC ratio grouped by metabolic origin in data set associated to typical sensory variables. **c** Distribution of VOC ratio grouped by metabolic origin in data set associated to atypical sensory variables. *TER* terpenes, *AA* aminoacids, *FA* fatty acids, *CAR* carotenes
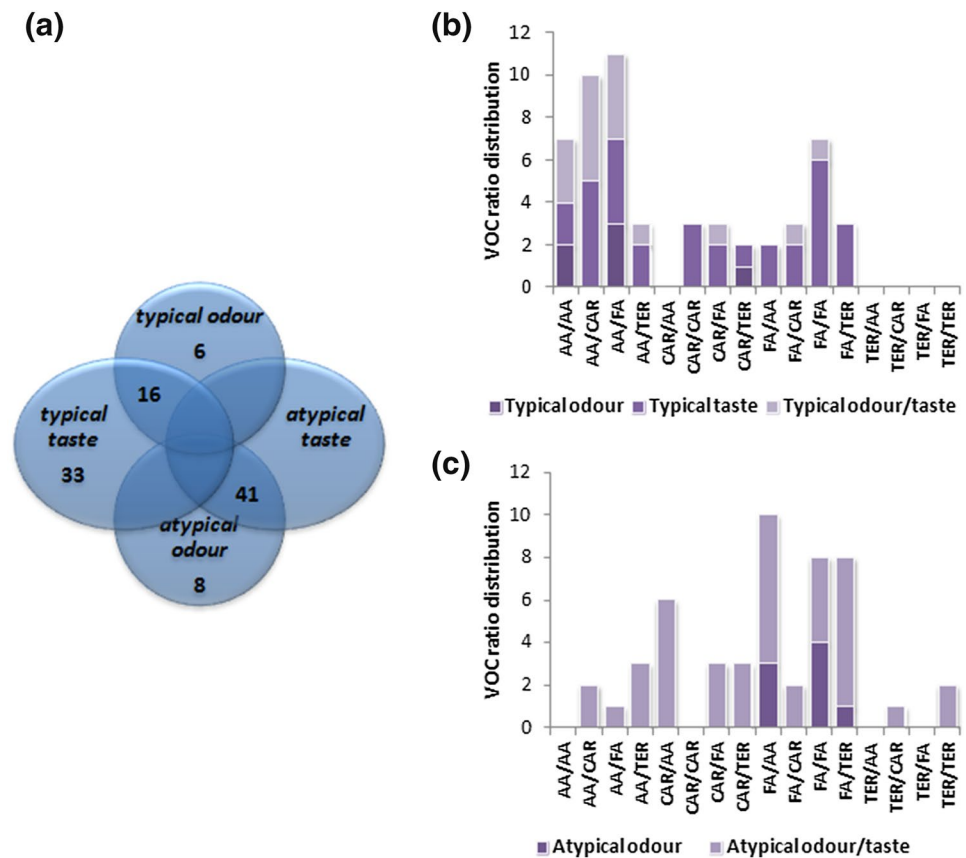


studies reported genetic *loci* for VOCs derived from this pathway, that were related to ethylene biosynthesis (Tieman et al. 2017) and probably indirectly to PAL (Singh et al. 2010), and related to a glycosil transferase (Bauchet et al. 2017).

The VOCs derived from the branched chain aminoacid: 3-methylbutanal and 3-methyl-1-butanol, correlated in the individual analysis with atypical tomato taste and odour. However, the ratio of these VOCs with ionone derivatives showed a positive correlation with typical tomato taste, while ratios with β-damascenone or α-citral or α-terpineol correlated with atypical tomato taste and odour (Table 3).

The results of VOCs derived from aromatic and branched chain aminoacids seem to be determining in the typical tomato taste and odour, agreeing with previous predictive studies (Piombino et al. 2013; Tieman et al. 2010; Vogel et al. 2010; Tandon et al. 2003).

(B) Carotenoid-derived VOCs: the relation of carotene-derived VOCs with tomato flavor was established with tomato mutant of carotenoid biosynthesis (Vogel et al. 2010). However, the contribution of individual VOCs was rather contradictory between studies. For instance, β-damascenone was defined by Buttery and Ling (1993) as one of the main contributors to tomato flavor. However, Tieman et al. (2012) showed no evidence of this VOC in

the tomato flavor contribution. β-ionone was positively correlated with tomato sourness (Tandon et al. 2003; Baldwin et al. 1998) while other studies reported a contribution to tomato sweetness (Tieman et al. 2012; Vogel et al. 2010). Here, we found β-damascenone (β-carotene derivative) correlating individually with typical tomato odour and taste and in VOC ratio with typical tomato taste, while β-ionone, β-ionone epoxide and β-methylionone (all β-carotene derivatives) together with geranylacetone (ζ-carotene derivative) showed correlation with atypical tomato taste and odour. 6-Methyl-5-hepten-2-ol (lycopene derivative) was individually correlated with atypical taste and odour while their ratio with ionone derivatives correlated with typical tomato taste. The negative contribution of these VOCs to tomato flavor was also reported (Piombino et al. 2013).

(C) Fatty acid-derived VOC: some, such as hexanal or 3-hexenal/ 2-hexenal, are abundant VOCs in tomato fruits and considered one of the major contributors to flavor (Buttery and Ling 1993). Transgenic plant with reduced lipoxygenase (LOX) activity, and therefore in VOCs derived from this pathway, was differed by flavor but not by consumer preference (Tieman et al. 2012). However, results presented here provide evidence of the differentiated contribution of LOX products to tomato flavor. Saturated aldehydes, such as heptanal and

hexanal, showed correlation with typical tomato taste, while unsaturated aldehydes, such as 2-hexenal, *trans*-4-pentenal, 2-decenal, showed correlations with atypical tomato taste and odour (all VOCs derived from LOX pathway).

(D) Terpene-derived VOCs: few terpenes are found in ripe tomato fruits and at low concentration (Rambla et al. 2014). It is well accepted that terpene production in tomato is limited and primarily formed by carotenoid degradation rather than by de novo synthesis from prenyl diphosphate (Lewinsohn et al. 2005). This has tended to underestimate the contribution of terpene to tomato flavor. However, we found that *p*-menth-1-en-9-al correlated well with typical tomato odour and taste while camphor and lilial correlated with atypical tomato taste and odour.

Overall, our results showed that the Andean landraces were highly accepted by the panelists, showing the supreme scores of odour and taste for their fruits, while the commercial varieties and the *S. pimpinellifolium* accession showed the lower preference and an atypical odour and taste. Predictive analysis by omeSOM revealed 15 VOCs contributing to the typical and atypical tomato odour and taste. Moreover, 108 VOC ratios out of the 8837 assessed were predicted to contribute to the typical and atypical tomato odour and taste by neuronal network analysis. The analysis of these VOCs by their metabolic origin highlighted the importance of these pathways and provided information for the understanding of the metabolic and genetic bases of these important traits.

## Compliance with ethical standards

**Conflict of interest**  All authors declare that they have no conflict of interest.

**Ethical approval**  The sensory study was approved by the committee of the food science department of the National University of Cuyo. This committee established ethical criteria and protocols for sensorial panels to evaluate fresh and processing products based on the legislation provided by the National Administration of Medicine, Food and Medical Technology of Argentina (ANMAT) and National Food Code.

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