Food Research International 54 (2013) 1579–1588

Contents lists available at ScienceDirect

Food Research International

journal homepage: www.elsevier.com/locate/foodres

Aroma volatile release kinetics of tomato genotypes measured by PTR-MS following artificial chewing

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ARTICLE INFO

Article history:
Received 25 June 2013
Accepted 15 September 2013

Keywords:
Tomato aroma volatiles
Quantitative descriptive analysis
SPME–GC–MS
PTR-MS
Chewing device
Retronasal perception

ABSTRACT

The aim of this study was to develop an analytical system to study the tomato aroma profile. An artificial chewing device coupled to a PTR-MS was developed to mimic, as close as possible, the release of volatiles during chewing in the human mouth and the retronasal olfaction perception.
VOC profiles of 9 tomato lines, selected based on flavor characteristics by a sensory panel, were acquired by both a PTR-MS system following artificial chewing and by SPME–GC–MS and compared to the quantitative descriptive analysis (QDA) measured by the trained sensory panel.
Based on multivariate statistical analysis, data obtained by the PTR-MS system showed a better correlation to the outcome of the QDA than SPME–GC–MS, especially for the descriptive parameters "tomato fragrance" and "tomato flavor".
The great advantage of such an analytical system was the possibility to study the release kinetics of volatiles during eating and the possibility to consider volatile concentration similar to in vivo condition resulting to an improved characterization of the aroma profile.

1. Introduction

The characteristic tomato fruit flavor is determined by a complex mixture of sugars, acids, minerals and volatile compounds (Baldwin, Goodner, & Plotto, 2008, 1991; Baldwin, Nisperos-Carriedo, & Moshonas, 1991; Baldwin, Nisperos-Carriedo, Baker, & Scott, 1991). From over 400 volatile compounds identified in tomato fruits, less than 20 compounds are considered important for flavor based on their odor thresholds (Abegaz, Tandon, Scott, Baldwin, & Shewfelt, 2004). These volatiles are derived from a diverse set of precursors that includes branched-chain and aromatic amino acids, fatty acids, and carotenoids (Klee & Tieman, 2013). Tomato volatiles can be mainly classified into two classes: one class comprises of compounds formed in the fruit during ripening (e.g. isobutylthiazole, 3-methylnitrobutane, geranylacetone, β-ionone (Buttery & Ling, 1993)) and another class comprises of compounds formed when the fruit is macerated either by cutting or by eating (Brauss, Linforth, & Taylor, 1998; Gaillard, Matthew, Wright, & Fishwick, 1977). Among them, six carbon (C6) compounds, produced by the lipid oxidation pathway, play a major role giving tomato its fresh 'top-note' (Boukobza, Dunphy, & Taylor, 2001).

It is expected that, following chewing, volatiles will be released at different rates determined by the number of enzymatic steps required and by the activity of specific enzymes (Brauss et al., 1998). The release behavior will also be affected by the volatile compounds' rate of partitioning between air and liquid according to Henry's law (Xu & Barringer, 2010). Boukobza et al. (2001) differentiated two clear types of release behavior: some compounds (such as isobutylthiazole, 6-methyl-5-hepten-2-one, methylbutanal, methylbutanol and acetaldehyde) showed rapid release immediately after maceration, reaching maximum concentration within the first 30 s whereas the concentration of other compounds (the C6 compounds such as hexenal, hexanal and hexenol) increased at a steady rate, reaching a maximum concentration after 2 min. These different release behaviors of VOCs may influence the human aroma perception during food consumption. Aroma perception depends not only on food chemical composition but also on food structure and on the oral physiology parameters (Foster et al., 2011; Poinot, Arvisenet, Grua-Priol, Fillonneau, & Prost, 2009; Taylor, 2002) since flavor compounds are released from the matrix and then transported to the receptors in the mouth and nose (Buettner et al., 2008).

The perception of food flavor and odor is a complicated physiological and psychological process resulting from the concurrent chemical stimulation of orthonasal and retronasal receptors (Shepherd, 2006). Orthonasal olfaction is the perception of odors that occurs during sniffing as opposed to retronasal olfaction, commonly associated with

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http://dx.doi.org/10.1016/j.foodres.2013.09.015

the sense of taste, which is the perception of odors emanating from the oral cavity during eating and drinking (Shepherd, 2006). Volatiles delivered by these two pathways are not perceived by the brain in the same way. It is retronasal olfaction, and not orthonasal olfaction, that is essential to flavor (Klee & Tieman, 2013). The perception of the odor and flavor cannot be exhaustively explained by simple linear models since human olfactory receptors are simultaneously influenced by hundreds of compounds interacting with each other.

Right now, flavor research has mainly prioritized aroma volatiles present at levels exceeding the orthonasally measured odor threshold ignoring the variation in the rate at which odor intensities increase above threshold (Tieman et al., 2012). During eating, a solid food product is crushed and mixed with saliva; its structure is modified and the diffusion of its volatiles from the resulting bolus to the headspace is affected. With mastication, the food surface area exposed to the air increases, and the food matrix is separated from the water it contained initially (Arvisenet et al., 2008; De Roos, 2003). The chewing process, which is directly related to the textural and physicochemical properties of the food matrix, has been reported as a substantial parameter affecting the in vivo flavor release (Foster et al., 2011; Mestres, Kieffer, & Buettner, 2006; Taylor, 2002).

Considering such conditions, it seems not reasonable to compare human sensory perception with volatile compounds quantified with the traditional methodologies such as SPME–GC–MS using frozen tissue samples, long incubation times at high temperature and often the addition of salts. These methodologies, apart from measuring only the maximum amount of volatiles emitted under artificial conditions, do not consider the different release kinetics of individual volatiles from a food matrix. In vivo measurements, such as sampling out of the human mouth or nose during eating, are desirable since they more closely reflect the volatile profile interacting with the olfactory receptors and therefore such measurements may relate better to sensory perception (Boukobza et al., 2001). The high variability generally observed in consumer characteristics does not allow sensory measurement in vivo to be accepted as a standard and repeatable method unless made by an expensive trained panelist. Consequently, there is interest in the development of methods for rapid, repeatable and sensitive monitoring of volatile compounds emitted from food samples in a way that mimics the release in the human mouth during eating (Benjamin et al., 2012; Poinot et al., 2009; Arvisenet et al., 2008; Salles et al., 2007; Rabe, Krings, & Berger, 2004; van Ruth & Buhr, 2004; van Ruth & Roozen, 2000; Roberts & Acree, 1995; van Ruth, Roozen, & Cozijnsen, 1995).

From a technical point of view, gas chromatography is the reference method for the analysis of food volatiles but it is still a time-consuming procedure and it generally does not allow kinetic measurements. Among the various possibilities proposed and investigated for rapid quantification and identification of VOCs, proton transfer reaction mass spectrometry (PTR-MS) is one of the most used since it allows to measure on-line, with high sensitivity, a mixture of volatile compounds in a straightforward and fast way (Biasioli, Gasperi, Yeretzian, & Märk, 2011). Precise identification of peaks is, however, not possible with PTR-MS. Without attempting to assign chemical names to the mass peaks, PTR-MS is considered as the equivalent of an array of sensors giving a finger print of the total volatile mixture (Biasioli et al., 2011; Granitto et al., 2007).

The aim of this work was to develop a fast and reliable system to study the volatile aroma profile of tomato fruits that mimics, as close as possible, the release of volatiles during chewing in the human mouth. The system may be used for initial screening of genotypes in breeding programs or to quantify the effects of e.g. cultivation or postharvest conditions on volatile emission. We combined PTR-MS with a "chewing device". This allowed us to quantify the VOC production occurring during the chewing of tomato and to study the kinetics of the release of the most significant tomato VOCs to better define their organoleptic importance. In addition, the VOC profiles obtained with the PTR-MS system and SPME–GC–MS were compared to the quantitative descriptive analysis (QDA) of sensory attributes of the eating quality of tomatoes measured by a trained panel.

2. Material and methods

2.1. Plant material

Tomatoes (*Solanum lycopersicum*) were obtained in the summer of 2010 from an experimental-greenhouse in Wageningen (The Netherlands). All cherry tomato selections were grown under identical conditions and were part of an F6 population derived from a breeding program focused on the improvement of tomato flavor. We screened nine of these genotypes that we coded lines 1 to 9. Homogenous batches of tomatoes from each genotype were selected on the basis of fruit size, color and firmness, measured non-destructively.

2.2. Tomato quality characteristics

Total soluble solids (TSS) were measured using a digital refractometer (Atago).

Tomato firmness was measured at two orthogonal selected spots using a Zwick Z2.5/TS1S material testing machine (Ulm, Germany) with a cylindrical probe (Ø 15 mm). Tomatoes were placed on a plastic ring to keep the tomatoes upright during measurement. Firmness was determined as the maximum force needed to compress the tomato to 1 mm at 40 mm/min, after lowering the probe until the tomato skin was touched (Schouten, Huijben, Tijskens, & van Kooten, 2007).

L*, a*, b* system chromaticity values were measured using a tristimulus chromameter (CR-400, Minolta, Japan) in two orthogonal spots of the fruit. Tomato color was expressed as either a* or a*/b*.

2.3. Sensory analysis

A panel of nine selected panelists carried out the profiling of the different tomato lines. Selection of panelists was firstly based on performance in the recognition of basic taste and odor components and on their verbal creativity. The panelists received a sensory training program based on the recognition and quantification of the most important taste and flavor attributes of tomato fruit.

The panel, in the same session, rated the intensity of 28 sensory attributes on a 10 cm unstructured scale, anchored at each end.

A balanced-block serving order across products and panelists was used, and the products (three fruits) were presented at room temperature in transparent plastic-covered cups coded with a three digit random number.

In this paper we consider only the attributes, scored by the panelists, related to odor and flavor such as odor strength, tomato fragrance, spicy fragrance, sweet odor, sharp odor, flavor intensity, tomato flavor, earthy flavor, green/unripe flavor and spicy flavor.

2.4. SPME–GC–MS analysis

Samples of fresh tomatoes (five fruits of each tomato line) were quickly cut into quarters and immediately frozen with liquid nitrogen. The samples were stored at −80 °C and ground into powder in a metal electric grinder prior to analysis.

The profiling of volatiles was performed in four replicates using a modification of the headspace solid-phase microextraction gas chromatography (SPME–GC–MS) method of Tikunov et al. (2005) described by Farneti, Cristescu, Costa, Harren, and Woltering (2012). Frozen fruit powder (1 g fresh weight) was weighed into a 20 mL crimp cap vial, and the vial was closed and incubated at 30 °C for 10 min. The closed vials were then sonificated for 5 min. Thereafter, the samples were incubated at 60 °C with agitation for 30 min and the headspace volatiles were extracted from the vial headspace and injected into the GC–MS apparatus (Trace GC Ultra, Thermo Scientific, IL, USA) equipped with a