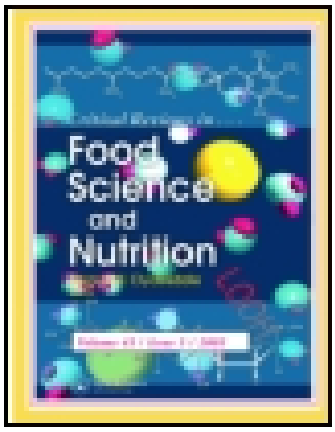




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# Challenges in Relating Concentrations of Aromas and Tastes with Flavour Features of Foods

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# Challenges in relating concentrations of aromas and tastes with flavour features of foods

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**ABSTRACT**

Flavour sensations in food are highly influenced by the aroma and taste compounds. Reviewing the extensive literature of recent years in this field has shown that the reconstitution of flavour based on aroma and taste compounds poses numerous problems. These are of different nature and include among others (a) chemical transformations among these compounds, (b) changes in the concentrations of the compounds responsible for the perceived flavour, (c) interactions among the chemical compounds that enhance or reduce a specific flavour sensation, and finally, (d) the complexity of the different food matrices and its influence in the flavour perception. Another difficulty that flavour scientists must face is how to properly model and visualize the complex relationships existing between the chemical composition of foods and the flavour

 

perception. These problems have repercussions on the reconstitution of the flavour signature of food based on the natural concentrations of its key aroma and taste compounds. Therefore, the main aim of this review is to deal with all these issues to propose potential solutions for a robust transformation in a science-based quality approach.

**Keywords**

odorants, tastants, sensory analysis, instrumental analysis, multivariate analysis

## FLAVOUR AND ITS IMPORTANCE IN FOOD

Human senses, in particular the chemical senses, protects us from eating spoiled or otherwise unfit items and encourages eating nutritious or otherwise beneficial items instead (Breslin and Spector, 2008). While flavour is considered as the result of a multisensory perception involving gustatory, olfactory and somatosensory systems, (Auvray and Spence, 2008; Small, 2012), it is generally accepted that taste and retronasal olfaction, also known as "mouth smell", play a major role in this sensory impression of food (Gotow et al., 2013). Visual cues may also alter a food flavour (**Figure 1**). For instance, food colour has been shown to affect the flavour perception (intensity and/or identification) by influencing the olfactory qualities of the food, the oral-somatosensory attributes of the food, and/or the overall flavour percept (Spence et al., 2010). However, from a practical point of view, the impressions of a food in the mouth perceived via the chemical senses can be restricted to:

a) *Retronasal odour,* the olfactory perception caused by volatile substances released from a product in the mouth via the stimulation of the posterior nares of the pharynx.
b) *Taste*, gustatory perceptions (salty, sweet, sour, bitteré ) caused by soluble substances in the mouth, and
c) *Chemical feeling factors*, which stimulate nerve ends in the soft membranes of the buccal and nasal cavities (spice heat/cooling, astringency, bite, metallic flavour, umami taste).

Recent studies have suggested that orthonasal olfaction (inhalation of food aromas through the nose in the absence of an oral stimulus) can be referred to the mouth, forming also part of the core flavour percept (Small, 2012; Stevenson et al., 2011; Tham et al., 2011).

In order to stimulate the olfactory receptors, odorants must be volatile and hydrophobic so they can permeate the air near the sensory area, penetrate surrounding layers, and interact with olfactory neurons. Furthermore, to be recognized as an odour, these compounds must be present at concentrations exceeding their odour threshold. The threshold concentrations for aroma compounds are dependent on their vapour pressure, which is affected by both temperature and medium. Thus, great differences exist between individual aroma compounds, with an odour potency range of several orders of magnitude. The values are also influenced by the assay procedure and/or performance of the sensory panel (Stevenson, 2012). The frequent discrepancies in threshold values in the literature are basically due to such differences.

The amount of volatile substances in food is extremely low, generally only 1 to 50 mg/kg. However, their number reaches several hundreds. Especially foods subjected to thermal processes, alone (e.g., coffee) or in combination with a fermentation process (e.g., bread, beer, cocoa, or tea), contain more than 800 volatile compounds (Belitz et al., 2009). The discrimination of the odorants from the other volatile compounds in food is also an important issue, as not all volatile compounds present perceivable odours. While it is possible to detect hundreds of volatile substances in a food product, only few of them may contribute substantially to the overall flavour.

Among these aroma compounds, particularly important are those bearing the unique flavour character of the food, the so-called ñcharacter-impact compoundsò (**Table 1)**(Belitz et al., 2009). Often, the character-impact of a food is the result of a synergistic blend of a group of aroma chemicals. Thus, in terms of aroma compounds, food can be classified into four groups (Molnár, 2009):

a) *Group 1*, the aroma is decisively determined by one character-impact compound. The presence of other components have little importance and serves only to round off the characteristic aroma of the food.

b) *Group 2*, the characteristic aroma is due to a mixture of a small number of compounds, one of which may play a major role.

c) *Group 3*, the aroma can only be simulated or reproduced with quite a large number of compounds. A character-impact compound is unlikely to be present.

d) *Group 4*, the food aroma cannot be satisfactorily reproduced even with a large number of aroma compounds. No character-impact compounds have been discovered.

For instance, banana aroma is definitively due to the character-impact compound isopentylacetate (Group 1), whereas butter aroma is mainly determined by 2,3-butanedione and supported by ethanol and dimethylsulfide, being a suitable example of Group 2. Thermally processed and fermented foods constitute typical examples of Groups 3 (roasted meat, coffee, bread, etc.) and Group 4 (red wine, beer, cocoa, etc.). The importance of these key odorants is such that their loss or even a small change in their composition will result in an aroma defect or off-flavour, which often occurs during food processing and/or storage.

Food flavour is the one of the major determinants of food choice and usually overrides other factors that influence food selection (Clark, 1998). If one considers the complaints received in the food industry, unsatisfactory flavour undoubtedly accounts for the largest percentage of these complaints. While we can appreciate the value of fibre, vitamins, protein quality, etc., it would be rather unusual to receive a consumer complaint in this area. The sensory aspects of a food are extremely visible to the consumer and essential for consumer satisfaction (Reineccius, 1991).

Consequently, to increase the appeal of their products, food and beverage manufacturers need to understand what flavour attributes affect flavour acceptability and then devise ways to control these critical flavour attributes **(Figure 2)**.

Since product flavour quality drives consumer acceptance and demand, modern product development and hard competition within food industry require clear understanding of sensory aspects of foods, and the ability to measure sensory attributes characteristic of high-quality products that meet consumer expectations. Thus, sensory analysis of food has become a powerful tool for (1) lowering products costs, (2) recipe optimization, (3) innovation & product development, (4) quality monitoring and comparison of products, and (5) analysis of the ñdrivers or likeabilityò.



**MEASURING THE AROMA OF FLAVOUR**

Although it is difficult to arrive at a precise estimate of the aroma contribution to flavour perception, a figure often quoted in the literature is that around 80 % of what we commonly think of as flavour comes from the information transduced by the olfactory receptors in the nose (Spence, 2013). Indeed, a food's flavour can be easily modified by changing its smell while keeping its taste similar. By considering this figure, it is easy to understand the enormous importance of aroma analysis in flavour science.

One of the crucial issues in this field is to identify and quantify all the volatile compounds responsible to a greater or lesser extent for a particular flavour. The potential number of aroma compounds one could conceivably encounter is immense, as well as their chemical diversity, which highly complicates the analytical task. Required methods must be able to distinguish trace quantities of aroma compounds from food components such as proteins, lipids and

carbohydrates, quantifying all of the former while ignoring, removing, or otherwise distinguishing the latter. These food constituents may react with flavour molecules in a variety of ways, influencing their binding and kinetic release from the food matrix. An additional difficulty arises from the low odour thresholds of many of these compounds, which makes necessary to develop methods able to measure them at very low concentrations. Keeping in mind this complex scenario, two main approaches are so far being applied for the characterization of food aroma:



***Sensory methods***

Sensory evaluation comprises a set of well-established methods providing useful information about the human perception of food flavour. Main sensory tests focus on the evaluation of overall differences among products (discrimination tests), the characterization of their sensorial attributes (descriptive tests) and the degree of consumer acceptance and satisfaction regarding product attributes (affective or hedonic tests)(Lawless and Heymann, 2010). Therefore, sensory analysis plays a key role in food industry to reduce risk and uncertainty regarding ingredient modifications, new product launches, shelf-life stability, etc.

Although sensory evaluation is normally carried out by trained panellists, there are some limitations such as low repeatability and reproducibility of the obtained results because of many subjective (e.g., sensory susceptibility of the person, health, fatigue) and objective (conditions under which the analysis is performed) parameters (Stone et al., 2012), as well as the time needed for its implementation (Ares, 2015). Another important drawback is the limited capacity of humans to distinguish components of mixtures. Indeed, it is unlikely that humans can identify any more than three or four components in odour or taste mixtures (Laing, 1991).

***Instrumental methods***

While sensory evaluation has been regularly used by food industry for several decades, great strides in flavour science have been made in recent years due to the development of different instrumental techniques. Most of these approaches aim at characterizing, qualitative and quantitatively, the chemical composition of flavour by either obtaining the full volatile profile of a food (fingerprint) or by targeted analysis of those aroma compounds known to be responsible for a specific flavour or off-flavour.

The isolation of aroma compounds from food is typically based on their volatility and/or solubility. Nevertheless, no single method yields a whole accurate picture of the aroma constituents in a food. Every method produces a picture of the aroma profile, where the profile is strongly determined by the methodology itself (Reineccius, 2010). For instance, all the methods based on volatility will be strongly biased towards those aroma compounds that are most volatile in the food system, whereas for solvent extraction methods the aroma profile will be inevitably biased by the relative solubility of the aroma compounds in the selected solvent. Care must be taken not to alter the aroma composition during the sample preparation, especially when analysing foods containing active enzymes (fruits, vegetables, etc.) or prone to undergo significant modifications during thermal treatments (Maillard reactions, peroxides breakdown, etc.)(Etiévant, 1996). An example could be the formation of 5-hydroxymethylfurfural, 2-methyl-furane and furfural in honeys due to the hydrolysis and thermal decomposition of native components (Rivellino et al., 2013).

Several extraction methods for isolating aroma compounds from food have been described in the literature; among them simultaneous extraction/distillation (SDE) (Collin et al., 2008; Lee and

Ahn, 2009) or headspace methods such as static and dynamic headspace (Mehinagic et al., 2004; Reboredo-Rodríguez et al., 2012, 2013) have been widely used. To avoid artefacts formation, solvent-assisted flavour evaporation (SAFE), which is based on high-vacuum distillation at reduced temperatures, is one of the techniques of choice (Majcher and JeleŒ, 2009; Mayuoni-kirshinbaum et al., 2012). Solid-phase microextraction (SPME) has become one the most popular extraction techniques for volatile compounds with a fast growing number of applications in flavour analysis. Particularly, headspace SPME (HS-SPME) allows avoiding possible contamination by non-volatile food components (Fratini et al., 2012; Noguerol-Pato et al., 2009; Panseri et al., 2011). SPME is an equilibrium technique and, therefore, the volatiles profile one obtains is strongly dependent on sample composition, sampling parameters and the absorption/adsorption properties (selectivity and capacity) of the fibre coating (Reineccius, 2010). Other techniques such as solid-phase extraction (SPE), stir bar sorptive extraction (SBSE) and liquid-phase microextraction (LPME) have also been applied for the preconcentration of aroma compounds, especially in liquid foodstuffs (Alves et al., 2005; González-Álvarez et al., 2011; González-Álvarez et al., 2012; Tsuji and Mizuno, 2010). Recently, Jelen *et al.* (2012) comprehensively reviewed the use of microextraction techniques in the analysis of food flavour compounds.

Once extracted, the volatile compounds must be identified and quantified so the flavour profile of the analysed food can be conveniently assessed. To this end, different detection techniques can be used, which can be broadly classified into the following categories:

*Chromatographic techniques*

Major advances in the analysis of flavour compounds during the past decades have been possible due to the developments in gas chromatography (GC), particularly in its hyphenation with mass spectrometry (GC/MS), but also with other information-rich detectors such as nuclear magnetic resonance (NMR) spectroscopy and Fourier-Transform infrared (FTIR) spectroscopy (Biniecka and Caroli, 2011). Capillary GC is a powerful technique for separating complex mixtures of compounds as those constituting most of food flavours. Once separated, aroma compounds are determined in a suitable detector, which ideally must be able to provide qualitative and quantitative information on those individual components.

The coupling of GC with olfactometry (GC/O) enables the discrimination of relevant odour-active components in complex mixtures of volatile compounds. The eluted substances are measured simultaneously by two detectors, one of them being the human olfactory system, so the perceived attributes can be correlated with the chromatographic peaks of interest (Zellner et al., 2008). The applicability of this technique is highly improved in combination with dilution analysis methods such as aroma extract dilution analysis (AEDA)(Culleré et al., 2010; Grosch, 1993).

The great development of comprehensive two-dimensional gas chromatography (GC×GC) in recent years has opened new horizons in flavour analysis by providing higher separation power and sensitivity that can be fundamental for (1) accurate aroma fingerprints of complex samples (e.g., processed food) and (2) a better aroma blueprints of food, i.e., the distribution of key aroma compounds, in particular when present in trace amounts (Cordero et al., 2015). In a GC×GC system, two columns, with different selectivities, are connected in series through a special

interface, known as modulator. The modulator collects the effluent from the primary column and then periodically injects the collected fractions into the secondary column for further separation (Ryan and Marriott, 2003). The detector records a continuous signal, which is further transformed into a two-dimensional contour plot, where the primary and secondary retention times are plotted along the X- and Y-axes (**Figure 3**). This technique is finding the greatest application in flavour analysis when interfaced with time-of-flight mass spectrometry (TOF-MS) (Duan et al., 2015; Weldegergis et al., 2011; Welke et al., 2012). The combination of GC/O with GC×GC/MS analysis allows improving significantly the identification of odour-active compounds in complex flavour mixtures (Chin et al., 2011; Kiefl et al., 2013; Majcher et al., 2013).

*Direct mass spectrometric techniques*

In recent years, the development of rapid, non-invasive, direct mass spectrometric techniques has obtained an increasing interest in flavour analysis due their potential for studying flavour release processes (Biasioli et al., 2011; Déléris et al., 2013). It is known that flavour release and perception is changing over the time due to different physicochemical, biochemical and physiological phenomena occurring in-mouth (salivation, changes of temperature, mastication, tongue movements, breathing, swallowing, etc.)(Buettner and Beauchamp, 2010; Piggott, 2000). Therefore, real-time flavour analysis may also notably contribute to better understand the release of aroma compounds during food consumption and thus their perception in relation with food characteristics.

While chromatographic methods allow the detailed composition of many flavours to be elucidated in terms of compound identification and quantification, they are not suitable to

examine temporal changes in fast release processes as they necessarily encompass a time-based separation. There are several requirements for an instrument to perform real-time analysis of flavour release, which primarily are a high sensitivity for detection of aroma compounds and a fast analytical response time without the need for sample pre-treatment. Among the various options available to address these needs, direct MS techniques have become the most promising ones (Biasioli et al., 2011). Several approaches have been used for this purpose, including proton transfer reaction mass spectrometry (PTR-MS), atmospheric pressure chemical ionisation mass spectrometry (APCI-MS) and selected ion flow tube mass spectrometry (SIFT-MS). PTR-MS uses a soft chemical ionisation based on proton transfer from a protonated reagent, most commonly $H_3O^+$ provided by a hollow-cathode ion source, so the odour compounds with higher proton affinity than $H_2O$ will be ionised (Biasioli et al., 2011). In APCI-MS, the volatile sample is introduced via a Venturi interface or equivalent in a specially modified APCI source and molecules are ionized in the gas phase by a corona discharge plasma (Taylor et al., 2000). SIFT-MS uses a microwave-discharge plasma to generate a mixture of reagent ions, mainly $H_3O^+$, $NO^+$ and $O_2^+$, one of which is further selected by a quadrupole mass filter and injected into an inert carrier gas for reaction with the gaseous sample (Biasioli et al., 2011). Another direct MS technique with a great potential in real-time flavour analysis is direct analysis in real time mass spectrometry (DART-MS), where molecules from the sample (solid, liquid or gas) are ionised by a beam of neutral metastable species generated by a glow discharge plasma (Cody et al., 2005). When interfaced to a TOF analyser, direct MS techniques further offer increased capabilities regarding speed and structural information. A number of applications in flavour analysis have been recently published, some of which are listed in **Table 1**. For instance, Feron *et al.* (2014)

measured *in vivo* aroma release (nose-space analysis) during cheese consumption by APCI-MS aiming to correlate aroma release with different characteristics of the oral processing events that can be involved (**Figure 4**). In another recent study, Charles *et al.* (2015) used PTR-MS to investigate the release kinetics of aroma compounds during consumption of coffee and its correlation with the sensory responses by a trained panel. The results underlined the presence of multisensory taste-smell interactions during coffee drinking. Direct MS approaches have become useful tools for on-line monitoring of aroma release during food storage and/or processing; for example, Gloess *et al.* (2014) used PTR-MS to study the influence of time-temperature roasting profiles of coffee beans on the aroma formation (**Figure 5**).

*Electronic noses*

Electronic noses (e-noses) are different from most other instruments used in flavour analyses since they are mainly designed to recognize gas mixtures as a whole without identifying individual chemical species within the mixture (Wilson, 2013). They attempts to mimic the human olfactory system by using an array of chemical sensors with partial specificity to a wide range of odorants and an appropriate pattern recognition system (Brattoli et al., 2011). Therefore, any odour stimulus results in a distinctive electronic pattern or fingerprint, which is further classified by comparisons with reference electronic patterns in a database. In spite of some drawbacks (e.g. sensor poisoning, sensitivity to moisture, poor linearity, etc.) the applicability of e-noses in food industry is rather high, allowing to perform objective quality assessments in a variety of applications such as evaluation of food-preservation state, off-flavour detection and prevention of food frauds (Baietto and Wilson, 2015; Song et al., 2013; Wilson et al., 2013; Xiao et al., 2015). In the last few years, mass spectrometry-based e-noses (MS-e-noses) are becoming

an increasingly used alternative (or complement) to gas sensor-based e-noses in food flavour applications (Cynkar et al., 2007; Vera et al., 2011; Vinaixa et al., 2005). In these systems, the volatile compounds are introduced into the ionization chamber of a MS instrument without prior chromatographic separation to produce a MS fingerprint, which is used in a pattern recognition system (Biasioli et al., 2011).

Despite the recent developments in the analysis of food odorants, more powerful analysis capabilities are still needed, to both further improve the data acquisition (ease of automation, accuracy, sensitivity, etc.) and to find the connection between instrumental and sensory information. Aroma analysis presents enormous difficulties (complex matrices, low concentrations and odour thresholds, the instability and reactivity of flavour compounds), which makes it a challenge for analytical chemists.

Further investigations to relate flavour release and perception are still needed (Salles et al., 2010). Thus, the study of flavour release during *in vivo* processes (eating and drinking) by means of direct MS techniques is of primary importance to better understand the flavour perception. Furthermore, flavour perception should be investigated from a higher level in order to identify the key factors driving flavour perception, which requires of multidisciplinary research teams. It is perhaps not surprising that a ñmultimodalò research team is needed to study the multimodal phenomenon that is flavour perception (Taylor and Linforth, 2010).

***UNDERSTANDING THE MECHANISMS FOR TASTES***

Taste assessment in food industry is generally implemented by human panellists. The human tongue can generate unique signal patterns of a variety of substances to the human brain. Then

the brain interprets these signals and makes a judgment or classification to identify the substances concerned, based on the experiences or neural network pattern recognition (Ha et al., 2015). However, sensory evaluation using a human panel is highly influenced by physical and psychological conditions as well as individual preference of the panellist, which may result in low objectivity and reproducibility. Therefore, the great challenge is to develop artificial systems mimicking the chemical senses of humans, aiming to obtain a sensing system for the quality control of taste (Ghasemi-Varnamkhasti et al., 2010; Singh et al., 2009). There are systems that can be used for a variety of applications in which accurate stimulus control is desired (Ashkenazi et al., 2004; Bagla et al., 1997; Hebhardt et al., 1999; Tunsuriyawong et al., 2000), e.g., in studies of the spatial and temporal properties of gustatory functions of various tongue regions. In this regard, some of the most popular biomimetic systems are the electronic tongues (e-tongues), which involve the use of a non-specific sensors array coupled with an appropriate chemometric tool for data processing (**Figure 6**). They have been widely used in a variety of applications in food science including process monitoring, freshness evaluation and authenticity assessment (Bagnasco et al., 2014; Escuder-Gilabert and Peris, 2010; Sousa et al., 2014; Teye et al., 2014). Among the various applications of the e-tongues recently reported, worth mentioning the suitable discrimination between processed orange juices from fruit harvested from healthy trees and those harvested from Huanglongbing diseased trees, symptomatic and asymptomatic (**Figure 7**) (Baldwin et al., 2011). Recently, the concept of bioelectronic tongue is emerging and has been used for taste evaluation. This one is characterized by including one or several biosensors (e.g. enzymes, antigens, antibodies, receptor proteins, cells or tissues) into the sensor array (Ha et al., 2015; Hui et al., 2014).

In order to understand the influence of taste in flavour perception, it is of key importance to know the mechanisms underlying the different tastes. The taste buds contain taste-receptor cells (TRC) that transduce chemical signals in food into electrical signals that travel to the brain through the nervous system, allowing the sensation of taste (Chandrashekar et al., 2006). Thus, distinct cell types expressing unique receptors are tuned to detect each of the different tastes (Laaksonen, 2011):

***Sweetness***

From a genetics perspective, sweetness is closely related to liking and is therefore a complex taste quality (Reed and Knaapila, 2010). The sweet taste receptor is a combination of subunits from the receptors TAS1R2 and TAS1R3. The tight relationship between sensory quality, positive hedonic value and behavioural acceptance illustrates how sweet taste detection evolved to help with the recognition of the most basic sources of metabolic energy. Omission of various sweet compounds, such as sugars (aldoses and ketoses) and sugar alcohols (alditols), may have significant effects on several sensory attributes of foods. For instance, in a model of red wine (Hufnagel and Hofmann, 2008), the omission of sweet compounds resulted in significant losses of sweetness and mouthfulness and slight increases in both drying and puckering astringent properties, as well as bitterness and sourness. Instead, the omission of key astringent phenolic compounds resulted in an increase in sweetness. However, the omission of sweet compounds in black tea (Scharbert and Hofmann, 2005) or in roasted cocoa (Stark et al., 2006) did not significantly affect the sensory properties of these food models. This can be explained because sweetness was not among the key sensory characteristics of these foods.

***Umami***

The umami taste, whose Japanese characters can be translated as ñpleasant savoury tasteò, can be described as a brothy or meaty taste with a long lasting, mouthwatering and coating sensation over the tongue. This taste is also considered to be intended for the detection of energy as various proteins, amino acids and ribonucleotides elicit an umami taste. Umami is perceived through a heterodimeric receptor composed of TAS1R1 and TAS1R3 (Reed and Knaapila, 2010). ɔ-Aminobutyric acid has been identified as a mouthdrying compound in mushroom fractions with a relatively low detection threshold (0.02 mmol/L). Chicken broth also induces a very strong umami taste (Dunkel and Hofmann, 2009). Some ɓ-alanyl peptides in the broth elicited a slightly sour taste and somewhat astringent properties when tasted individually. In beef broth, similar ɓ-alanyl peptides along with some amino acid derivatives generated in the Maillard reaction contributed to mouth-drying properties (Sonntag et al., 2010).

***Bitterness***

In contrast to sweet and umami taste, which evolved to recognize a limited subset of nutrients, the task of bitter taste can be considered the detection of a large number of structurally distinct toxic compounds in food. Bitter compounds are detected by various TAS2R receptors which are coded by TAS2R genes (Kim et al., 2004; Kim et al., 2003; Meyerhof et al., 2010). At least 25 different TAS2R receptors are so far known. For instance, TAS2R38, is related to the detection of compounds containing the thiocyanate (N=C=S) moiety, such as glucosinolates (Bufe et al., 2005; Sandell and Breslin, 2006; Sandell and Breslin, 2010). They can be found in various vegetables, such as genus Brassica (e.g. broccoli and rutabaga). Certain bitter phenolic compounds in hops (*Humulus lupulus*) activate the receptors TAS2R1, -14 and -40 (Intelmann et

al., 2009). Tea catechins were recently reported to activate a different bitterness receptor, TAS2R39 (Narukawa et al., 2011). Although bitter receptors for various isolated compounds have been identified, fewer receptors have been reported for actual bitter components in foods (Hofmann, 2009).

***Sourness***

Sour taste can be considered as a mechanism of detection for spoiled (fermented) foods and also for optimally ripe foods, as sourness usually decreases during the ripening of fruits and berries along with increasing sweetness (Kim et al., 2004). Sour taste has some correlation with pH, specifically with pH of inorganic acids (Kim et al., 2004). Non-phenolic organic (e.g. lactic, citric, tartaric, malic, quinic and acetic acids) and some inorganic acids (e.g. hydrochloric and phosphoric acids) can elicit astringent sensations in addition to a sour taste (Bajec and Pickering, 2008). Lawless *et al.* (1996) concluded that the astringency elicited by acids is not due to hydrogen bonding between the acid and oral proteins, but due to the sourness itself. Sourness may be perceived through specific ion channels (PKD2L1) in taste cells (Huang et al., 2006).

***Metallic saltiness***

The mechanisms highly depend on the specific salts. Aluminium sulphates elicit strong astringent sensations (Bajec and Pickering, 2008). De Wijk and Prinz (2005) showed that alum does not decrease the viscosity of saliva. Copper and zinc sulphates have bitter and astringent characteristics, while ferrous sulphate does not have these properties and is perceived as metallic (Lawless et al., 2004b). Zinc sulphate and chloride also have some umami properties similar to monosodiumglutamate (Keast, 2003; Yang and Lawless, 2005). Calcium chloride is perceived mainly as bitter, but it may have also metallic, astringent and irritating properties (Lawless et al.,

2003). Calcium chloride has a slightly attenuating effect on the astringency of citric acid (Lawless et al., 2004a).

***Kokumi***

Kokumi is a Japanese term used to describe some sensory properties such as richness, mouthfulness, thickness and complexity (Dunkel et al., 2007). Kokumi compounds have only a minimal flavour in water, but if added to some foods, they can substantially enhance the thickness, continuity, and mouthfulness of the food to which they have been added (Miyaki et al., 2015). Recently, it was reported that kokumi substances such as GSH are perceived through the calcium-sensing receptor (CaSR) in humans (Ohsu et al., 2010). Several peptides in edible beans (Dunkel et al., 2007) and in Gouda cheese (Toelstede et al., 2009; Toelstede and Hofmann, 2008), as well as oxylipins in avocado (Degenhardt and Hofmann, 2010), have been reported to contribute to kokumi perception. The taste active compounds in avocado were bitterer and more kokumi enhancing than astringent, but the thermal treatment of the food had a significantly increasing effect on astringency (Degenhardt and Hofmann, 2010). The glutamyl dipeptides contributed to kokumi properties in beans (*Phaseolus vulgaris*). Dairy foods with fatty or creamy texture may lubricate the oral cavity and thus mask the astringent properties (De Wijk et al., 2003; De Wijk and Prinz, 2005, 2006; Prinz et al., 2007). The masking of astringency (and corresponding bitterness) may be one reason for adding milk to tea or coffee.

It is then clear that the relevance of determining intensities of tastants dissolved in water for the ñreal lifeò perception of taste in complex food is then rather limited (Mojet et al., 2003).

## MULTISENSORY FLAVOUR PERCEPTION AS DISTINCT OF EATING HEDONICS

The taste and smell systems are distinct in both their anatomy and their neural processing of inputs. The advantage of the human sensory system over artificial systems is that the brain can receive signals from both olfactory and gustatory receptors and integrate both sets of data to form classifications and/or judgments (Baldwin et al., 2011). There have been attempts to integrate electronic noses and tongues to obtain improved classifications of foods (Di Natale et al., 2000; Winquist et al., 1999). A combination of the nose and tongue was also found to markedly improve classification properties (Deisingh et al., 2004). Recently, Banerjee *et al.* (2012) showed that the integration of e-nose and e-tongue systems improved the classification accuracy in tea quality assessment.

As flavour is the result of a multisensory perception, understanding the different ways that the integration between the various sensory stimuli is performed in humans can help to draw different possibilities for the integration in artificial systems. Although explaining multisensory integration is not a simple task, the literature contains many suggestions of the sorts of rules and properties that may be involved in multisensory integration. Prominent amongst these are the following (Smith, 2013):

### *Spatio-temporal Unity*

The hypothesis is that the unity of flavour comes from the fact that sensory information of various kinds, or from various origins, is put together when presented as close in time and space. However, the interaction between the multimodal components goes beyond mere co-occurrence in consciousness.

***Superadditivity***

Combining vanilla aroma with a sucrose solution, where the aroma is sensed orthonasally by inhaling, will make that solution taste sweeter. This is the sweetness enhancement effect (Cliff and Noble, 1990; Dalton et al., 2000; Frank et al., 1991). This cross-modal effect results in a conscious experience but is not the result of conscious combining. Other factors affect the perception of sweetness, such as a creamy texture, which can enhance the perceived sweetness, and there are interactions between odours and textures (Bult et al., 2007).

Moreover, if space and time were the only factors of unity for a flavour, then all information that is processed or perceived as close enough in time and space, or attributed to a single cause in space and time, would be components of such a flavour. So are the sounds heard during crunching an apple or a carrot part of its flavour? They can certainly affect the overall experience of the food (Zampini and Spence, 2004), but they should not be treated as components of flavour (Spence et al., 2010). Surely, we should say that these factors can causally affect our perception of flavours, but they are not constitutive flavour perceptions. We need to distinguish causally affecting versus constitutive features of our experience of tasting. This is true for hedonics too, because we could ask on the spatio-temporal unity hypothesis whether the hedonic or affective component of eating and drinking is a constitutive part of flavour or flavour perception (Smith, 2013). Some have said yes (Verhagen, 2007) and others no (Smith, 2007, 2012), while for others it is indeterminate, though they go together and are tested together (Yeomans et al., 2008).

If force-fed the same food repetitively, even a food we like such as chocolate, we may suddenly find the hedonics switching around from like to dislike. This is stimulus specific satiety. The identity of the stimuli stays the same even when the hedonics vary, because if you were suddenly

offered a different type of chocolate you would notice (Kringelbach and Stein, 2010; O'doherty et al., 2000). In the other side, mixture suppression is the perception that tastes or aromas in combination are less intense than when perceived individually, whereas release from suppression is a temporal sensory phenomenon that occurs while we eat. In other words the sequence in which we eat foods impacts our perceived intensity of flavour in those foods (Delwiche, 2010).

***Sensory Dominance***

In the sensory and food literature, expectations can have a big impact on perceived flavours. Expectations generated by the colour of a food or beverage, experienced before it is tasted (and stimulation occurs) can lead to enhanced (or diminished) perceptions of sweetness or sourness (Spence et al., 2010), because linked to the recognition of a certain kind of food giving rise to expectations of corresponding kinds of flavours. For instance, the more intense the colour, the more intense the flavour is. Expectations generated by different linguistic description of the same food (Yeomans et al., 2008) with smoked salmon ice cream tasting saltier and more savoury when labelled as a novel flavour of ice cream rather than as a ñfrozen savoury mousseò (Smith, 2013).

***Semantic Congruence***

Congruency could explain the role of expectation in flavour experiences. Colour-smell expectations depend on the congruency of the two pieces of information. Sweetness enhancement effects are specific to certain congruent odour-tasting pairs (Prescott, 2004). Lim and Maxwell (2012) gave preliminary results in which, when a congruent taste was added to an odour, referral to the oral cavity and tongue were significantly enhanced. So congruency could help to explain localisation too.

Tasting is the activity by which we assess what we ingest or imbibe hedonically, but this is done of the basis of perceptual experiences and these are perceptions of flavours. Each act of tasting is a snapshot of a flavour profile that we may explore by repeated tasting or experiments with flavours. The term flavour does not describe a construct of the brain, but it is a technical term used to describe the sapid and odorous properties of a solid or liquid, including properties of its temperature and texture, as well as the power to irritate the trigeminal nerve. Configurations of these properties are flavours and we use multiple senses to track them. Multisensory integration unites information from different sensory inputs into perceptual experiences of flavour, where the exact nature of these experiences depends on the precise arrangements of textures, odours, and tastings/irritants that generate the sensory inputs. The more unified the configurations that make up flavours, the more unified but complex are the flavour experience whose parts we are unable to distinguish. Finally, we must distinguish the hedonics of eating from the perceptual experience of tasting. Eating experience overflows flavour perception. The sound of the crispness of an apple is not part of flavour, but it is part of the pleasurable experience of eating it. Many aspects that contribute to the hedonic responses that we suppose to be bound up with, and revealing of, the flavour or taste of something may overflow flavour and professional tasters often have to set them aside (Smith, 2013).



***RELATING INSTRUMENTAL MEASURES WITH SENSORY ATTRIBUTES***

We have assisted in recent years to great developments in the field of flavour analysis, allowing us to obtain large data sets containing valuable information on the chemical composition, both qualitative and quantitative, of foods. Nevertheless, one of the major challenges is how to match this chemical knowledge with the multimodal perception which is the flavour. Thus, the study of

the relationship between instrumental and sensory data is of paramount importance in flavour science. For instance, one can desire (1) to replace sensory measurements, regarded as not very reliable because of their high variability, by instrumental measurements or (2) to enhance the interpretation of the sensory data by showing how the physical and chemical properties are reflected by specific sensations (Pagés and Husson, 2005).

The use of GC/O, especially in combination with GC/MS or GC×GC/MS may help in the identification of the most potent odorants contributing to the aroma, describing the sensory attribute related to the compounds identified (Chin et al., 2011; Zellner et al., 2008). However, odour characteristics of some compounds tend to vary as a function of concentration, which complicates to establish a proper correlation. A remarkable example is skatole, which has a flowery smell at a low concentration, but it is perceived as faecal at high concentrations. This phenomenon is explained by the combinatorial coding scheme, because the same odorant could be represented as different combinations of olfactory receptors depending on its concentration, given that the threshold for the activation of receptors are variable (Niimura, 2012). On the other hand, GC/O-based approaches do not account for the interactions between the different flavour components. Thus, most of times an odour is the result of the combination of different odorants which can present synergetic or masking effects on the overall perception. For instance, Thomas-Danguin *et al.* (2007) showed that a mixture of specific proportions of ethyl isobutyrate (strawberry-like odour), ethylmaltol (caramel-like odour), and allyl-Ŭ-ionone (violet-like odour) was judged more typical of a pineapple odour than were the individual components.

Therefore, although GC/O has been proven as a very useful tool in flavour analysis, we should be cautious so the quality attribute of a single volatile compound is hardly related to the flavour attribute identified in a complex system.

Due to these reasons, multivariate approaches are normally more suited to explore the relationship between volatile compounds and the sensory attributes. Although a good correlation between instrumental measures and sensory flavour characteristics may not indicate a cause and effect relationship because there may be other reasons for the correlation, it is an indication that both variables change in same manner. For instance, the presence of a high level of an identified odorant may also be an indication of a high intensity of a flavour attribute with which it is correlated (Owusu et al., 2013).

Multivariate analysis (MVA) has been frequently used to find patterns and correlations within samples and variables, and between instrumental and sensory data in a variety of food/beverages including wine (González-Álvarez et al., 2011; Quijada-Morín et al., 2012; Rudnitskaya et al., 2010), chocolate (Owusu et al., 2013), cheese (Biasioli et al., 2006) and bread (Heenan et al., 2009). The most common MVA techniques used for this purpose are principal component analysis (PCA), partial least squares (PLS) and general procrustes analysis (GPA) (Chambers and Koppel, 2013). Briefly, PCA is an unsupervised method in the sense that no additional knowledge (e.g. sample class) besides raw data is required to describe the data set. PCA gives an overview of the data which is useful to detect outliers, common groupings between samples and to evaluate the relationships between samples and variables (i.e. compounds measured), and between variables themselves (Charve et al., 2011). PLS is frequently used to understand relationships between the two data sets by predicting one data set from the other set. Thus, PLS

can be applied to investigate the relationship between instrumental and sensory data (Chung et al., 2003). Both PCA and PLS can perform this kind of analysis when used as dimension reduction before discriminant analysis (DA), forming the methods PCA-DA and PLS-DA respectively. These hyphenated methods are both highly effective supervised classification methods for application to multivariate data. However, as with all supervised techniques particular emphasis should always be given to model validation, as an important step of the model building (Kalogeropoulou, 2011).

General procrustes analysis (GPA) extracts a common structure from multiple data sets composed of non-identical variables among the data sets (Dijksterhuis, 1994). It involves a series of transformations (translation, rotation/reflection and rescaling) of the individual data matrices to increase their comparability. GPA is especially useful for free choice profiling (FCP), since it can accommodate different numbers and kinds of attributes among panellists. Moreover, GPA can be used to visually describe different effects, such as product differences, assessor agreement, and repeatability (Xiong et al., 2008). However, this method is also suited for understanding the relationship between sensory responses and instrumental measurements and it has been widely used in this way (Berna et al., 2005; Chung et al., 2003; King et al., 2014).

Relating the chemical composition with the flavour attributes of a food is a difficult task. With more complete and accurate information, our understanding of the relationship between aroma and taste compounds and the perceived flavour should be improved. If meaningful relationships are to be obtained, the first prerequisite is that chemical and sensory information are as precise and as meaningful as possible. On the sensory side, this would involve reducing response variation or examining data on an individual basis, as well as clearly defining the sensory aspect

being described by the attribute used in the description (Chambers and Koppel, 2013; Williams, 1994). A flavour wheel could be a good tool to systematically categorise and define sensory characteristics of any food. Analytically, the information should either be comprehensive or provided in a form that reflects the composition of the stimulus as it reaches the receptor (Williams, 1994). Recent instrumental techniques allow obtaining large sets of data that need to be properly analysed. As a first approach, it should be extracted the information that be gained from simple correlations, but always bearing in mind that relationships between chemical composition and flavour perception may not be linear. Therefore, the use of multivariate approaches, able to reflect more complex relationships, is crucial in succeeding in this challenge.



## *FUTURE PROSPECTS TO BE ADDRESSED TO RELATE AROMAS AND TASTES WITH FLAVOURS*

Understanding flavour perception is a complex task, which requires to distinguish flavours from flavour experiences. Such experiences are mostly unified and yet hard to extricate the overall experience of eating or drinking, which includes a hedonic response. Therefore, we face a challenge to say how the integrations of sensory information in brain gives rise to unified precepts in conscious experience, and what the ultimate nature of those conscious mental items is (Smith, 2013).

Flavour is one of the most important quality attributes influencing consumer food choices, perceptions and purchase behaviour. In consequence, it is essential to provide tools to assist food technologists in sensory quality of foods, based not only on sensory analysis but also on instrumental analysis of the product to guarantee the consumer´s requirements. During the last decades flavour research has evolved, passing through the stages of identifying volatiles in

foods, searching for key odorants via olfactory approaches, investigating food-flavour interactions and more recently exploring *in vivo* flavour release processes. However, advances in extraction and analytical techniques with the use of increasingly sensitive detection equipment technologies to determinate all key compounds with robustness are still necessary. Also, specific scientific investigations are required for understanding the connection between instrumental and sensory analysis in food commodities. In this context, it is noteworthy to mention the emerging field of flavoromics, a new discipline aimed at linking the chemical composition of foods with flavour through the application of omics techniques (Reineccius, 2008). As an ñomicsò approach, it ideally considers all low molecular weight compounds in food systems (volatiles and non-volatiles) as candidate chemical stimuli in flavour perception, which potentially allows identifying new flavour contributors, as well as a better prediction of flavour since it includes inputs from more chemical compounds (Charve et al., 2011). As well, a push in metabolomics to understand the interplay effects of aroma and taste compounds would be of paramount importance. This ñtaste nutrigenomicsò approach might stimulate the future development of innovative food products (Hofmann, 2009), with flavour signatures targeted to specific genotypes or ethnic populations.

Other issues that need to be addressed in future research are a better meta-analyses by mathematical models aimed at clarifying relationships between data matrices for an improved understanding of the relationships of flavour/aroma phenomena and chemical composition (González-Álvarez et al., 2011; González-Álvarez et al., 2013; Quijada-Morín et al., 2012; Rey-Salgueiro et al., 2013). New statistical methods that rely less on linear assumptions and move into non-linear or so-called artificial neural networks, a computational models capable of

learning complex patterns, are essential for better understanding of these complex relationships. Possibilities include analyses such as logistic regression, which is normally used to predict the presence or absence or some item, behaviour, or action (Osborne, 2012) and could be used to ñpredictò the likelihood that some sensory attributes would be present given the presence of one or more compounds. However, this method does not provide a predictive equation of intensity to concentration (Chambers and Koppel, 2013).

A next challenge in flavour research which requires of an extensive knowledge of the relationships between chemical composition and sensory characteristics, is the reconstruction of food flavour. This possibility opens new horizons in food industry, for instance, the production of customized food products flavour-tailored by using emerging technologies such as three-dimensional (3D) food printing (Sun et al., 2015). To date, no comprehensive studies have yet been targeted toward the total reconstruction of the flavour of a food product based on quantitative data of the entire set of volatile key aroma and non-volatile key taste compounds (Frank et al., 2011). Anyway, non-volatile components in foods that might be considered to have no taste per se may still exert an influence of the flavour of a food. In this case, the analyses employed are less well defined and are unique to the components one wishes to analyse (Hofmann et al., 2001; Pickenhagen, 1996).



ABBREVIATIONS

**AEDA** = aroma extract dilution analysis

**APCI** = atmospheric pressure chemical ionisation

**CaSR** = calcium-sensing receptor

**DA** = discriminant analysis

**DART** = direct analysis in real time

**e-nose** = electronic nose

**e-tongue** = electronic tongue

**FCP** = free choice profiling

**FTIR** = Fourier-Transform infrared spectroscopy

**GC** = gas chromatography

**GC/O** = gas chromatography coupled to olfactometry

**GC×GC** = comprehensive two-dimensional gas chromatography

**GPA** = general procrustes analysis

**HS** = headspace

**IT** = ion trap

**LPME** = liquid-phase microextraction

**MS** = mass spectrometry

**MVA** = multivariate analysis

**NMR** = nuclear magnetic resonance

**PCA** = principal component analysis

**PLS** = partial least squares

**PTR** = proton transfer reaction

**Q** = quadrupole

**QLIT** = quadrupole/linear ion trap

**SAFE** = solvent-assisted flavour evaporation

**SBSE** = stir bar sorptive extraction



 

**SDE** = simultaneous extraction/distillation

**SIFT** = selected ion flow tube

**SPE** = solid-phase extraction

**SPME** = solid-phase microextraction

**TOF** = time-of-flight

**TRC** = taste-receptor cells

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**Table 1**: Literature review on the most characteristic aroma chemicals of different types of foods (synthesised from (Belitz et al., 2009)).

| Food type | Aromas | Chemicals | Formation | Notes |
|---|---|---|---|---|
| Meat | Heated meat-like | Heterocyclic aroma substances | Non-enzymatic | Thiols, amines and aldehydes, get concentrated to such an extent that they condense to form heterocyclic aroma substances |
| Fish | Amine-like | Amines, such as: 2-Methylpropyl 2-Methylbutyl 3-Methylbutyl 2-Phenylethyl 3-(Methylthio)propyl | Enzymatic decarboxylation of amino acids produces the same amines as the Strecker reaction | The odour thresholds of these amines are pH dependent. |
| Dairy | Butter-like | Decalactone | Enzymatic oxidation of unsaturated fatty acids | Its sweetish odour enhances the aroma of butter |
| Eggs | Pungent-like | Allyl isothiocyanate and allyl thiocyanate | Enzymatic deamination, decarboxylation, | Fat-soluble aroma |

| | | | | |
|---|---|---|---|---|
| | | | reduction and acylation | |
| Oils | Green-like | Hydroperoxides and aldehydes | Enzymatic oxidation of unsaturated fatty acids | Volatile and non-volatile hydroperoxides fragment even at temperatures around 40 ºC |
| Cereals | Popcorn-like | Acyl thiazoles and thiazolines | Metal catalyzed oxidation | The length of the alkanoyl group influences the aroma activity |
| Vegetables | Fresh-like | Oxo acids, aldehydes and allyl alcohols | Oxidative degradation of fatty acids by lipoxygenase alone or in combination with a hydroperoxide lyase | Aldehydes formed by the Strecker degradation can also be obtained as metabolic by-products of the enzymatic transamination or oxidative deamination of amino acids |
| Fruits | Fruit-like | Essential oils | Metal-catalyzed oxidation or photooxidation | The essential oils will change with the specific fruits |

| | | | | |
|---|---|---|---|---|
| Nuts | Nut-like | Carbonyl compounds (phenols in roasted nuts) | Volatile carbonyl compounds are formed by lipid peroxidation, caramelization, and amino acid decomposition by the Strecker degradation mechanism | The impact compounds will change with the specific nuts. Carbonyl compounds show large differences between the ortho- and retronasal thresholds |

**Table 2.** Overview of some recent direct mass spectrometry applications in food flavour characterization

| Food type | Chemicals | Application | Direct MS technique | Reference |
|---|---|---|---|---|
| Coffee beans | Volatile compounds | HS measurements; influence of roasting conditions | PTR-TOF-MS | (Gloess et al., 2014) |
| Processed meat | Volatile compounds | HS measurements; monitoring of quality changes during storage | PTR-Q-MS | (Holm et al., 2013) |
| Tomatoes | Volatile compounds | HS measurements; MS fingerprinting (tomato types, ripening, storage) | PTR-Q-MS | (Farneti et al., 2012) |
| Cereal bars | 17 flavour active volatile compounds | HS measurements and *in vivo* aroma release; influence of sugar composition | PTR-TOF-MS | (Heenan et al., 2012) |
| Coffee | Volatile compounds | *In vivo* aroma release; influence of roasting degree and sugar | PTR-TOF-MS | (Charles et al., 2015) |

| | | | | |
|---|---|---|---|---|
| | | addition in espresso coffee | | |
| Honeys | Volatile compounds | HS measurements; MS fingerprinting (monofloral honeys) | SIFT-MS | (Langford et al., 2012) |
| Dry fermented sausages | 31 volatile aroma compounds | HS measurements; monitoring during sausages processing | SIFT-MS | (Olivares et al., 2010) |
| Strawberries | Lipoxygenase derived aroma compounds | HS measurements and *in vivo* aroma release; influence of storage, ripening, varieties and food oral processing | SIFT-MS | (Ozcan and Barringer, 2011) |
| Cocoa liquors | Alkylpyrazines and Strecker aldehydes | HS measurements; effect of alkalization of cocoa beans | SIFT-MS | (Huang and Barringer, 2010) |
| Cooked macaroni | 2,6-dimethylpyrazine, 2-propoxyethanol, 3-carene, 4-vinylpyridine, (E)-2-hexenal, (E)-3-hexen-1-ol, furan, heptanal, and ethyl acetate | HS measurements; influence of addition of sodium-reduced sauce | SIFT-MS | (West et al., 2013) |

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|---|---|---|---|---|
| Curry sauce products | Linalool, cuminaldehyde, Ŭ-phellandrene | *In vivo* aroma release; reformulation of spice levels in low-oil sauces | APCI-Q-MS | (Hatakeyama et al., 2014) |
| Cheese products | Ethyl propanoate, nonan-2-one | *In vivo* aroma release; influence of oral physiology and food oral processing | APCI-IT-MS | (Feron et al., 2014) |
| Flavoured emulsions | Nonan-2-one, pyrazine, 3-methylbutanol, limonene, cymene, heptan-2-one, ethyl nonanoate | *In vivo* aroma release; modelling the effect of fat in flavour release | APCI-Q-MS | (Linforth et al., 2010) |
| Candies | Pyrazine, 3-Methyl butanol, Ethyl butyrate, 2-Nonanone, p-Cymene, Ethyl nonanoate | HS measurements and *in vivo* aroma release; reformulation of flavours in candies | APCI-Q-MS | (Yang et al., 2011) |
| Beer | 14 selected alcohols and esters | HS measurements; monitoring during fermentation | APCI-Q-MS | (Ashraf et al., 2010) |
| Tea | Indole and geranic acid | Monitoring of tea fermentation and manufacture processes | DART-IT-MS | (Fraser et al., 2013) |
| Beer | Volatiles and phenolic | HS measurements; MS | DART- | (Cajka et al., |

| | | | | |
|---|---|---|---|---|
| | compounds | fingerprinting (different beer brands) | TOF-MS | 2010) |
| Chewing gums | Cyclohexanecarboxamide, N-ethyl-5-methyl-2-(1-methylethyl) | Kinetics of release of a flavour active compound into saliva | DART-QLIT-MS | (Jeckelmann and Haefliger, 2010) |

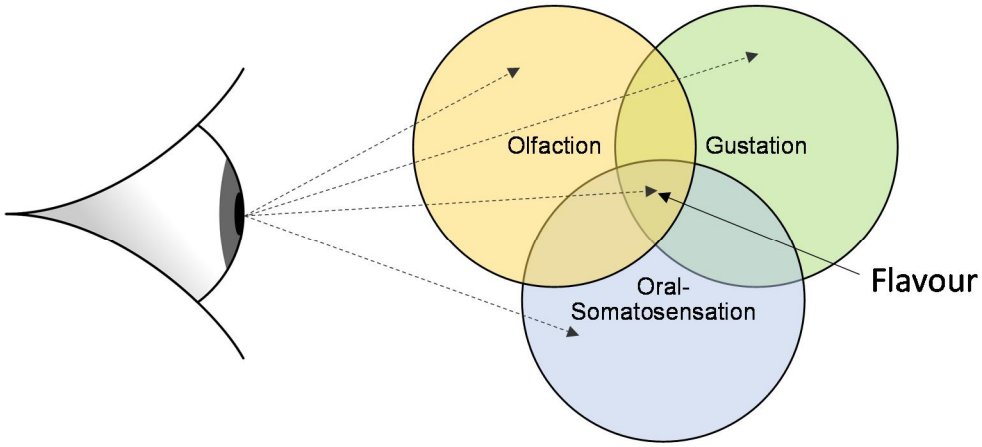



**Figure 1.** Integration of main senses in flavour perception

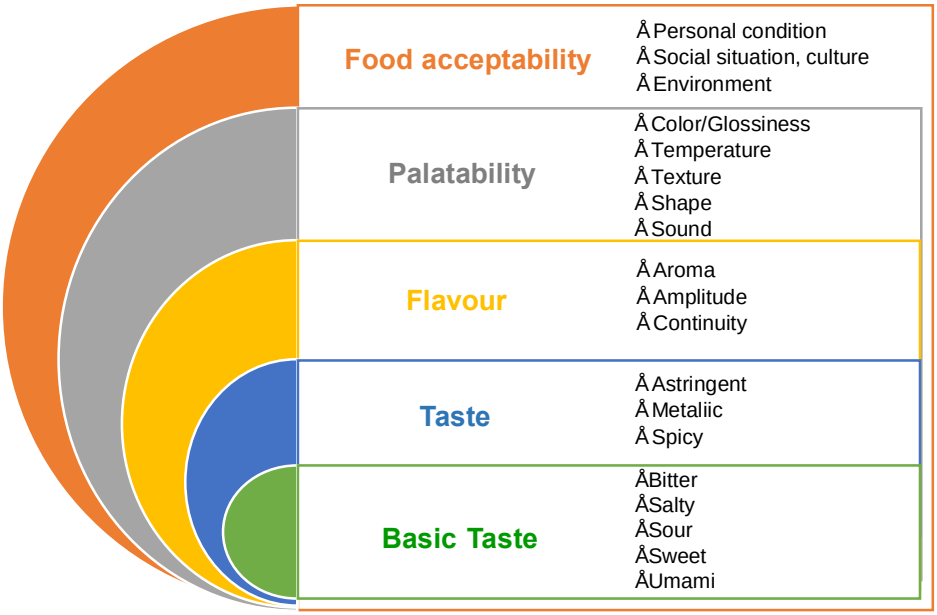



**Figure 2.** Some factors determining food acceptability

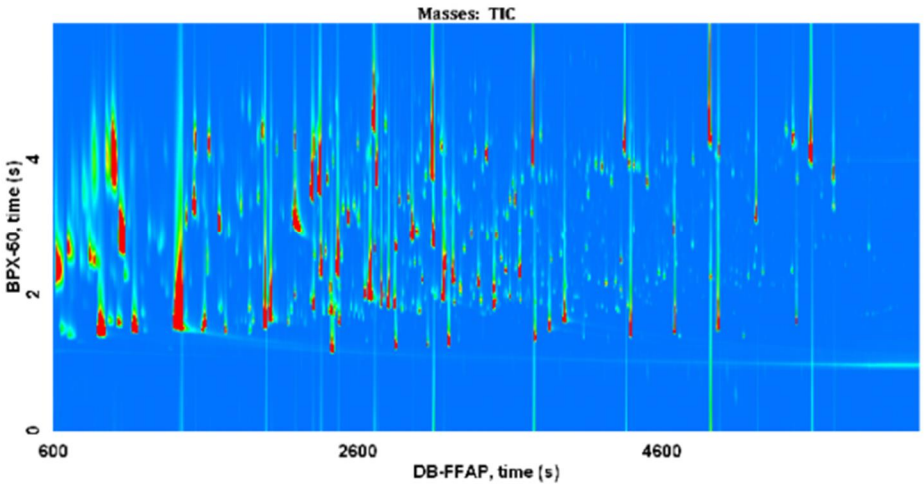



**Figure 3.** GC×GC-TOF-MS total ion current chromatogram obtained for a spirit distilled from fermented *Sorbus domestica* fruit. Reproduced from (Vyviurska et al., 2015), licensed under CC BY-NC-ND 3.0.

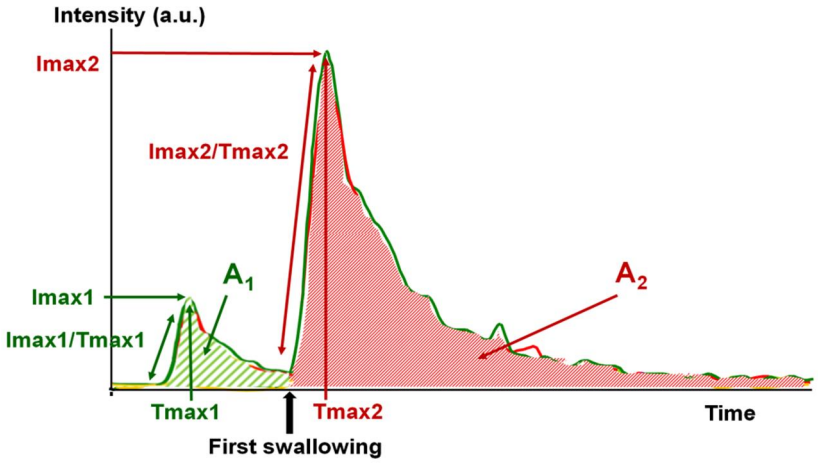



**Figure 4.** Typical aroma release curve profile obtained *in vivo* by APCI-MS during cheese consumption. The release profile was separated in two release phases: before (phase 1) and after (phase 2) first swallowing. The quantity of aroma released (A1 & A2), the maximum intensity (Imax1 & Imax2), the time to reach maximum intensity (Tmax1 & Tmax2) and the release rate (Imax1/Tmax1 & Imax2/Tmax2) were extracted from the curve for each release phase. Reproduced from (Feron et al., 2014) , licensed under CC BY 4.0.

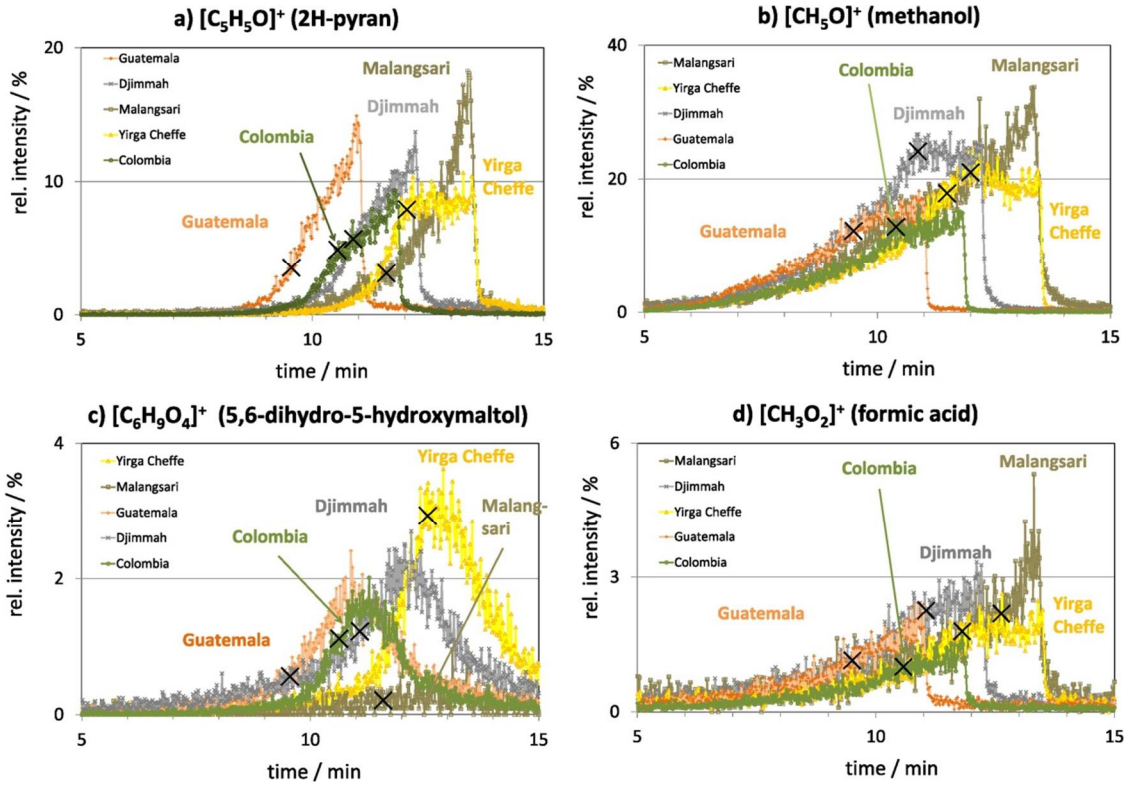



**Figure 5.** Time-intensity profiles obtained by PTR-TOF-MS during the coffee roasting process for the volatiles (a) 2H-pyran, (b) methanol, (c) 5,6-dihydro-5-hydroxymaltol, and (d) formic acid. The cross marks the respective time of the first crack (at a roasting temperature of 184 °C). Reproduced from (Gloess et al., 2014), licensed under CC BY-NC-ND 3.0.

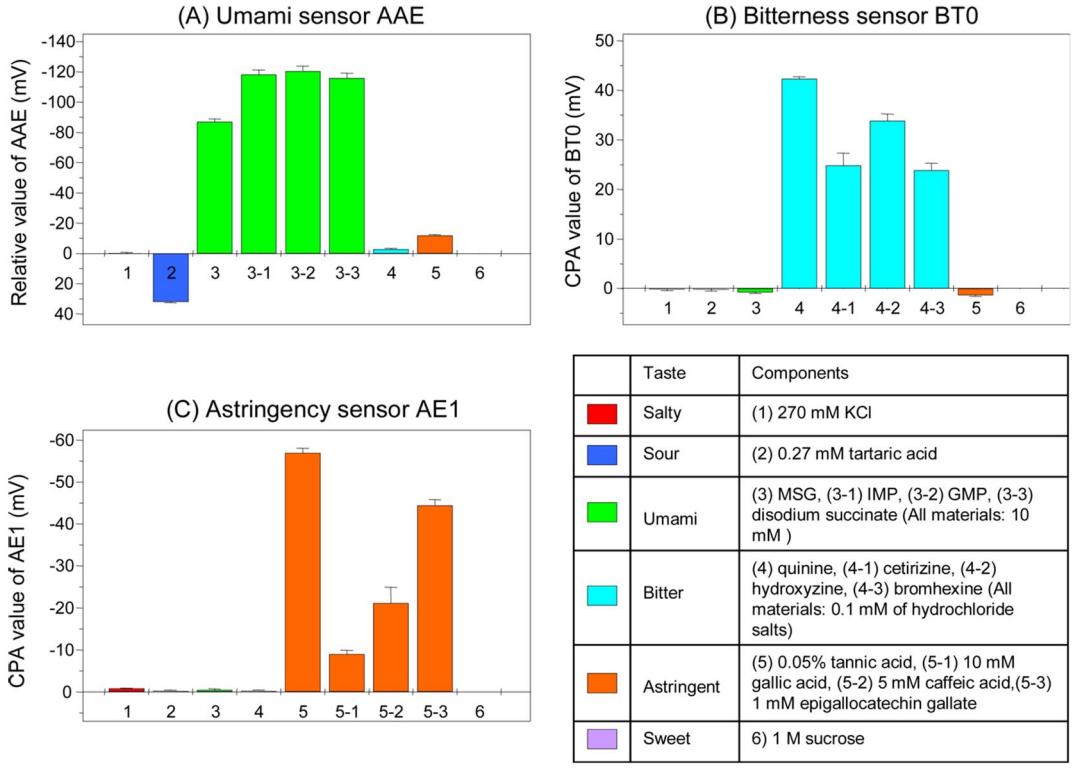
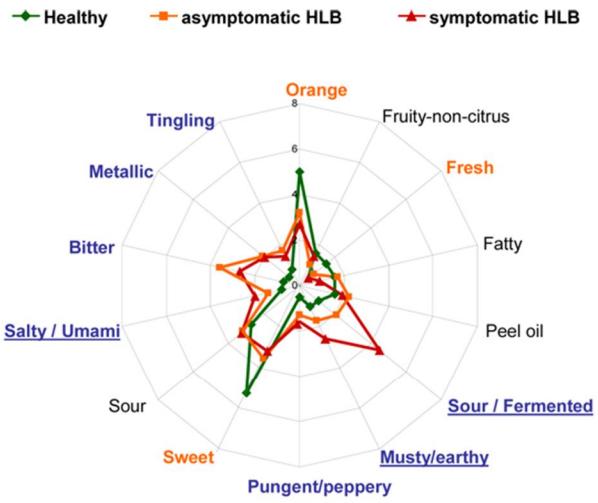
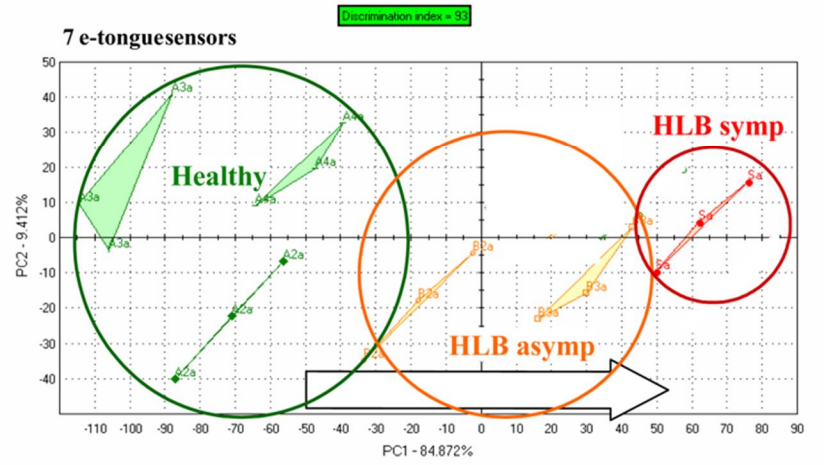



**Figure 6.** Responses of taste sensors to six tastes: (a) relative value of the umami sensor AAE, (b) the change of membrane potential caused by adsorption (CPA) value of the bitterness sensor BT0, and (c) the CPA value of the astringency sensor AE1. MSG, monosodium glutamate; IMP, disodium 5′-inosine monophosphate; GMP, disodium 5′-guanosine monophosphate. Reproduced from (Kobayashi et al., 2010), licensed under CC BY 3.0.




(A)




(B)

**Figure 7.** (a) Trained sensory panel rating of processed juice from Hamlin oranges harvested from healthy or Huanglongbing (HLB) diseased trees including juice from asymptomatic and symptomatic fruits. Healthy juice was significantly higher in orange flavour, fresh and sweet tastes, and HLB juice was higher in sour/fermented, musty/earthy and salty/umami tastes. (b) e-tongue (AlphaMOS ASTREE) PCA plot of the same juice. Reproduced from (Baldwin et al., 2011), licensed under CC BY 3.0.