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Multivariate Statistical Analysis and Odor-taste Network to Reveal Odor-taste Associations

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ABSTRACT

Odor taste association has been successfully applied to enhance taste perception in foods with low sugar or low salt content. Nevertheless, selecting odor descriptors with a given associated taste remains a challenge. In the aim to look for odors able to enhance some specific taste, we tested different multivariate analyses to find links between taste descriptors and odor descriptors, starting from a set of data previously obtained using gas chromatography/olfactometry-associated taste: 68 odorant zones described with 41 odor descriptors and 4 taste associated descriptors (sweetness, saltiness, bitterness, sourness). A partial least square analysis allowed identifying odors associated with a specific taste. For instance, odors described as either fruity, sweet, strawberry, candy, floral or orange are associated to sweetness, while odors described as either toasted, potato, sulfur or mushroom are associated to saltiness. A network representation allowed visualizing the links between odor and taste descriptors. As an example a positive association was found between butter odor and both saltiness and sweetness. Our approach provided a visualization tool of the links between odor and taste description and could be used to select odor-active molecules with a potential taste enhancement effect, based on their odor descriptors.

KEYWORDS : odor-taste association, odor descriptors, multivariate analysis, sweetness, saltiness, bitterness, sourness, partial least square analysis, multidimensional scaling.

INTRODUCTION

Considering the rising rate of pathologies such as diabetes or obesity, which are related to unbalanced diets with an excess consumption of sugar, salt and fat, there is an urgent need to decrease the content of these ingredients in food while maintaining their sensory acceptability by consumers. Excessive intake of sodium has undesirable effects on health such as hypertension and may contribute to other diseases such as cancer and osteoporosis.[1] Concerning sugar, a high consumption of foods rich in free sugar increases the risk of tooth decay. High intake of sugar-sweetened beverages is highly linked with an unhealthy diet, weight gain and increased risk of health diseases. The food industry has to integrate these nutritional criteria in the formulation of food products.

Different strategies have been used for salt and sugar reduction in foods as reviewed.[2, 3] One of the most proposed reduction strategy is the substitution of sodium chloride or sugars by other molecules. In the case of salt reduction, the substitution of sodium chloride by potassium chloride often induced the perception of undesired tastes such as bitterness and metallic.[4, 5] Simple sugars, such as fructose or sucrose, could be replaced by new molecules, which confer a sweet taste to the product without the added calories, such as intensive sweeteners. However, such molecules with an intense sweetness are used in very small amount resulting in losses of bulk and modification of the final texture. Alternatively, a part of simple sugars can be replaced by soluble fibres or carbohydrates, as bulking agent, in order to restore the texture.

Other strategies are based on modifications of food texture and structure, which impact on the dynamic of salt/sugar release in the mouth and as a consequence on taste perception.[3, 6] However, in the case of sugar, the effect on sweetness perception was dependent on both the nature of the texturing agent and of the taste compound.[7]

Another strategy is to increase the heterogeneity of the food matrix, which was able to increase both salty and sweet taste without compromising consumer acceptability.[8] It was thus observed that hard gels were perceived sweeter when sugar distribution was heterogeneous due to a long-lasting in-mouth sucrose concentration, the hard matrix being able to maintain the taste contrast due to different sucrose concentrations, for a longer time in the mouth during chewing.[9] The authors concluded that the fracture properties of food can be modulated to enhance sweetness perception, in association with heterogeneous distribution.[10]

Another innovative strategy relies on the use of aroma-taste interactions and multimodal integration. This strategy is based on the observation that an odor may evoke a taste [11, 12] while it does not activate taste receptors.[13] This phenomenon results from the co-occurrence of odors and tastes during food tasting, which, through associative learning, contributes to the acquisition of taste qualities by odors.[13] It has been reported that mentally imagined odor-taste mixtures showed the same patterns of interaction that actually perceived odor-taste mixtures, thus demonstrating that taste and odor perception interact at a cognitive level during holistic flavor processing in the brain.[14] This strategy has been applied with success to develop low-salt foods while maintaining saltiness and consumer acceptability,[15] to enhance fat perception in real foods varying in structure-texture properties[16] and to enhance sweet taste perception in foods [17] especially in sugar-reduced fruit juices.[18]

Using such an approach needs an adequate selection of odors. As food odors can evoke a specific taste through mental imagery, it has been possible to select promising odors for saltiness enhancement based on the expectation taste profiles of food products being evoked by their names.[19] In different volatile compounds databases, such as Flavor-Base[20] or Volatile Compounds in Foods.[21] the word “sweet” is often used as odorant descriptor. Considering this observation that some odors are described with a “smelled taste”, Stevenson et al[22] calculated the correlation between odor sweetness and taste sweetness for 10 odorant molecules and found that the degree to which an odor smelled sweet was a good predictor for taste tasting. This association was also used to select odorants able to enhance sweetness in fruit juices, using gas chromatography/olfactometry-associated taste (GC/O-AT),[18] showing that many molecules described with a "smelled sweet taste" were able to enhance the perceived sweetness odor of a fruit juice. However some molecules, such as phenyl methanol, described with a sweet odor, were not able to enhance a perceived sweetness. Moreover, looking at the data gathered in the Flavor base,[20] most of the molecules described with a sweet taste are also described with a sweet odor, but some molecules such as bornyl formate, linalyl formate, methyl crotonate or hydroxyl methyl furfural possess a sweet taste without being described with a sweet odor. There is thus a need to look for the impact of other odor descriptors than sweet in the odor-taste associations. We thus propose to apply different complementary multivariate statistical tools to explore more deeply the links between odor descriptors and taste associated descriptors.

In the aim to look for odors able to enhance some specific taste, we tried to find links between taste descriptors and odor descriptors, starting from the whole set of data previously obtained using gas chromatography/olfactometry-associated taste (GC/O-AT).[18] The aim of the present work was to perform multivariate analyses to search for the links between odor descriptors and taste associated descriptors, starting from a total of 68 odorant zones detected by gas-chromatography/olfactometry of a fruit juice extract, which have been described first with odor descriptors and second with taste associated descriptors (sweetness, sourness, saltiness, bitterness). Using natural extracts, we expect to identify new targets and unravel unknown odor taste associations. These links could then be used for a first selection of odors susceptible to enhance taste perception. These odor descriptors could then be used to select either single molecules, mixture of molecules or aromas to be tested for their potential impact on taste perception.

MATERIALS AND METHODS

Sample preparation

We used the raw data previously obtained after the extraction of volatile compounds from a commercial multi-fruit juice provided by Eckes Granini (France), following the vacuum distillation procedure and dichloromethane extraction described by Barba et al.[23]

Chemicals

Standards for identification purposes were obtained from Sigma-Aldrich (Saint-Quentin Falavier, France): 2-pentanone, methyl-2-methyl-butanoate, ethyl butanoate, ethyl-2-methyl-butanoate, butyl acetate, hexanal, isobutyl alcohol, 3-methyl-1-butylacetate, n-butanol, β-myrcene, limonene, 2-methyl-1-butanol, γ-terpinene, 3-hydroxy-2-butanone, octanal, n-hexanol, 3-hexanol, 2-hexen-1-ol, furfural, decanal, propyl octanoate, linalool, fenchol, pentanoic acid, α-terpineol, 3-methylthioptopanol, valencene, carvone, β-damascenone, geraniol, hexanoic acid, phenyl methanol, 2-phenylethanol, β-ionone, furaneol, γ-decalactone.

Gas chromatography analysis

The extract was then concentrated with a Kuderna-Danish apparatus and 1 μL (splitless mode for 0.5 min) was submitted to gas-chromatography/mass-spectrometry (GC/MS) for compounds identification and to GC/O-AT for odor description[18] using the same column (30 m x 0.32 mm i.d. fused silica capillary column coated with a 0.5 μm layer of polyethylene glycol, DB-Wax, Agilent, Agilent Technologies, Santa Clara, CA). GC/O-AT was done with 12 panelists used to GC/O experiments. In a first run (first injection of the extract), panelists were asked to indicate the detection of an odor using a buzzer and to give an odor descriptor. In a second run (second injection of the same extract), panelists were asked to attribute for each odor, one of the four associated taste descriptors: sweetness, saltiness, sourness or bitterness. Detection times, odor descriptors and taste associated descriptors were recorded using AcquiSniff software (Saint Genès Champanelle, France). The detection frequency (DF) was calculated for each odorant zone, for both odor descriptors and taste associated descriptors, as the percentage of panelists having detected an odor. Only the odorant zones with a DF higher than 30% were selected, to limit the false detection risk.[24] For each selected odorant zone, we took into account all the odor descriptors given by the 12 panelists. For taste associated descriptors, we also calculated the DF for each specific taste: sweetness (%), sourness (%), saltiness (%), bitterness (%), these values are used in the multivariate analyses.

Data preparations

From the whole set of data previously published, we selected 68 odorant zones (Table 1). A total of 48 compounds have been identified by their mass spectra and injection of standard compounds[18] and the 20 remaining zones correspond to unknown compounds or compounds present in trace amount. Even if the molecules present in some of the odorant zones have not all been identified, in the present paper, we used the odor descriptors given by the panelist for each odorant zone, to find links between these odor descriptors and the taste associated descriptors. From the odor descriptors given by the 12 panelists in the 68 odorant zones, a list of 70 odor descriptors was extracted, of which 7 were present only in the description of one odorant zone and 12 in only 2 odorant zones. Odor descriptors only present in one or two odorant zones were not considered for further analyses. The multivariate analyses were done with 45 variables, the number of occurrences of each of the 41 remaining odorant descriptors and the DF of each of the 4 associated taste descriptors (sweetness, saltiness, bitterness, sourness).

This first matrix (Supplementary Table S1) was transformed into a binary matrix (1 when the odor descriptor or the taste associated descriptors appeared in the odor description and a 0 otherwise). This binary matrix was used to build a co-occurrence matrix (Supplementary Table S2).

Computational analysis and statistical methods

A Partial Least Square (PLS) analysis was performed on the 68 odorant zones, to explain the taste association descriptors (Y variables: DF for each associated taste) by the odor descriptors (X variables: number of occurrence of the 41 odor descriptors) (Supplementary Table S1).

A multidimensional scaling (MDS) was performed to determine the level of similarity of the odorant zones based on their odor descriptors. The calculation involves a dissimilarity matrix obtained using the Euclidian distances between the odorant zones and based on the frequency of odor descriptors. We used the coordinates of the first three dimensions of the MDS to display the odorant zones in a three-dimensional scatterplot. The 3D graphical visualization was obtained using Miner3D Enterprise (version 7.3.3). In addition, the DF for each of the four taste descriptors were used for graph depictions.

PLS was performed with XLStat (Addinsoft, Paris, France) and MDS with R version 3.0.1.[25]

Network visualization

The associations between odor descriptors and taste descriptors were visualized using a network of odorant and taste descriptors. For that purpose, we first calculated the co-occurrence matrix (R 3.0.1 [25]) of the odorant and taste descriptors using the binary matrix made of the 68 odorant zones and the 45 descriptors (41 odor descriptors and 4 taste descriptors). The co-occurrence matrix is a square 45x45 matrix in which the off-diagonal terms are the number of odor-taste pairs in the description of an odorant zone, while the diagonal terms are the number of all occurrences of each odor and taste descriptors (Supplementary Table S2). Cytoscape[26] was used to build a network of the links between odor descriptors and taste-associated descriptors. To do so, the square matrix was transformed into a two-way table using Statistica (TIBCO Software Inc. 2017).

RESULTS

The 68 selected odorant zones with DF odor values higher than 30% are listed in Table 1 with their retention indices, the name of the corresponding volatile compounds, if identified, or the number of the unknown compound. For each odorant zone, all the odor descriptors given by the 12 panelists are listed with the number of occurrence when higher than the unity. We have removed from the list the descriptor "unknown", which was given by panelists who were not able to describe the perceived odor. This list of descriptor was used to build the Euclidian matrix. For each odorant zone, two values are given for DF. First, the detection frequency for the odor (DF odor %), which is the percentage of panelists having smelled the odor during the first run of GO/O and the detection frequency for the associated taste descriptor (DF taste %) during the second GC/O-AT run. Second, we calculated the DF for each of the four taste attributes, sweetness (%), sourness (%), saltiness (%), bitterness (%) and used these values for the statistical analyses. The values in bold refer to the main associated taste. A total number of 33 odorant zones were mostly associated with sweetness (13 with a value higher than 40%), 16 with sourness (5 with a value higher than 40%), 10 with saltiness (3 with a value higher than 40%) and 21 with bitterness (3 with a value higher than 40%).

Evaluation of taste association by odor descriptors using PLS

The PLS analysis was done on the 68 odorant zones, using the occurrences of each of the 41 odor descriptors as X variables and the DF for each associated taste as Y variables. We verified that the representation of the remaining 41 odor descriptors was the same as on the PLS performed with the 63 odor descriptors present in at least 2 odorant zones (supplementary Figure S1). Figure 1A shows the projection of the variables on the two first components. Even if the model does not account for a high level of variation, the 4 associated tastes are well discriminated in the first plane of the PLS map represented by the two first components, sweetness on the positive part of component 1, bitterness on the negative part of component 1, sourness and saltiness on the positive part of component 2 and also on the negative part of component 1. Sweetness is better represented on this first plane than the other tastes. This can be explained by the fact that the odorant zones are separated from a fruit juice extract and that most of them are described as fruity. The odor descriptors fruity, sweet, strawberry, candy, floral, orange are positively correlated with component 1 and thus associated to sweet taste perception. The odor descriptors toasted, potato, mushroom and sulfur are negatively correlated with component 2 and thus associated to saltiness. The odor descriptors sour, unpleasant, cheese and acid are positively correlated with component 2 and thus associated to sourness. The odor descriptors hot plastic, plastic and spicy are negatively correlated with component 1 and thus associated to bitterness. A PLS model was built to predict the taste association by a linear combination of the odor descriptors. Table 2 presents the coefficients affected to each odor descriptor to explain one taste descriptor. The odor descriptors are ranked according to the decreasing number of their total occurrences. The odors with the highest association with sweetness are strawberry, red fruits, sweet, citrus, leather, butter, orange, foot, chemical, candy, fruity and floral; the odors with the highest negative association with sweetness are sour, sulfur, hot plastic, land, plastic, wood, metallic, toasted, potato and smoky. The odors with the highest association with saltiness are sulfur, potato, toasted, smoky, land, butter and mushroom: the odors with the highest negative association with saltiness are citrus, animal, peanut, strawberry, dust, metallic, grass, vegetal, unpleasant, plastic, red fruits, foot, sweet and chemical. The odors with the highest association with sourness are sour, sweaty, hot plastic, metallic, lemon, land and solvent; the odors with the highest negative association with sourness are peanut, strawberry, toasted, leather, foot, chemical and butter. The odors with the highest association with bitterness are animal, metallic, peanut, plastic, wood, grass, hot plastic, vegetal and dust;

the odors with the highest association with bitterness are butter, strawberry, orange, cake, acid, red fruits, leather and lemon. These associations are only indicative but can be used to predict a potential effect on taste modulation. Most of the odors positively associated with sweetness are negatively associated with saltiness, except butter, spicy and leather which are positively associated to both sweetness and saltiness. These associations were verified on the plane represented by component 1 and 3 (Supplementary Figure S2).

Looking at the odorant zones (Figure 1B), the molecules, when identified, with a high positive correlation with component 1 are the most associated with sweetness, ethyl 2-methylbutanoate (E2MB) is described with fruity, apple, strawberry, candy and sweet odor descriptors (Table 1); methyl 2-methylbutanoate (M2MB) is described with fruity and sweet notes; linalool is described with floral, fruity, sweet and candy notes; (E)-β-ocimene (β-Oci) is described with fruity, floral and strawberry notes; phenylmethanol (PhM) is described with floral, fruity, sweet and candy notes; β-damascenone (β-Dam) is described with fruity, floral and sweet notes; γ-decalactone (γ-Dec) is described with floral, fruity and sweet notes; ethyl butanoate (EB) is described with fruity, floral and sweet notes. The compounds the most associated with sourness (positive correlation with component 2) are pentanoic acid (PA), described as acid, sharp, cheese and unpleasant; allo-ocimene (allo-O), described as green, metallic and sour; hexanal (HEXA) described as green, herb and floral. The compounds the most associated with bitterness (negative correlation with component 1) are tricosane, described as plastic and petrol; isobutyl alcohol (IBA), described as plastic, hot plastic, spicy and wood. The compounds the most associated with saltiness (negative correlation with component 2) are furfural, described as potato, toasted and sulfur; 2-hexen-1-ol (2Hexe), described as mushroom, toasted and sulfur; 1-octen-3-one (1o3o), described as mushroom and n-butanol (Buta), described as toasted and peanut.

Visualization of the relationships between odor descriptors and associated tastes

In order to better understand the associations between odor descriptors and tastes, we build a network characterized in terms of nodes and edges or links, following a previous approach on odor notes.[27] In our case, the nodes are odor and taste descriptors and the edges are the odorant zones. We used a total of 45 descriptors (41 odorant descriptors and 4 taste descriptors) to produce a list of 2025 pairs of descriptors by stacking the 45x45 co-occurrence matrix. After excluding the diagonal elements and the pairs zero without links, 1098 pairs remained. We considered only the pairs between odor and taste descriptors, and after removing the duplicate pairs below the main diagonal (for any X and Y odor descriptors, the pairs XY and YX are equivalent), the network displayed 143 odor-taste pairs. The network is illustrated in Figure 2, which represents the relationships between the odor and the taste descriptors. This representation allows a rapid visualization of the odor taste associations.

Many odor descriptors are linked to all tastes, some are linked to several but not all tastes, but some are linked to only one taste dimension. In Figure 2 the size of each odor descriptor depends on the number of odorant zones in which it was present. The color used to fill the circle of each odor descriptor reflects the main associated taste and the color used for the border reflects the second most associated taste. In those cases in which the odor is equally associated with every taste, the color is grey. Different types of lines are used to illustrate the number of occurrences of the odor-taste associations.

Only the strawberry odor descriptor is linked to one single taste (sweetness), which explains its high positive value in the regression to sweetness perception. Three odor descriptors are only linked to two tastes: orange, candy and red fruits, which are linked mainly to sweetness and to a lesser extent to sourness. The descriptors linked to three tastes can be discriminated by the taste to which they are not linked to. Caramel is not linked to bitterness. Butter, mushroom and peanut are not linked to sourness. Hot plastic, potato and sour are not linked to sweetness. Grass, citrus, lemon, metallic and dust are not linked to saltiness.

The other odor descriptors are linked to all the tastes. Fruity and floral are the most cited descriptors with respectively 79 and 70 total number of occurrence and present in respectively 35 and 37 odorant zones. They are mainly linked to sweetness, then to the three other tastes without any distinction. Cake and rose are mainly associated to sweetness but with only few occurrences. Among the other odor descriptors mainly associated to sweetness, the second associated taste is sourness for sweet and solvent, bitterness for vegetal, chemical and foot and saltiness for leather. Only sweaty is associated to sourness in the first place. The odors green, plastic, herb, wood and animal are associated to bitterness, while they are also associated to saltiness for wood, sourness for animal and both sourness and sweetness for green and herb. Toasted, cheese, sulphur, smoky and land odors are mainly associated to saltiness and toasted, sulphur and land are also associated to bitterness. Unpleasant, sharp, spicy and acid do not present any specificity towards a given taste.

Allocation of odorant zones according to their odor descriptors and associated taste

The multidimensional scaling (MDS) approach allows the visualization of the similarity between elements of a dataset dispatched in an N-dimensional space. MDS is one of the methods that allows dimensionality reduction and producing meaningful representations of high-dimensional data into a lower-dimensional space (usually two or three dimensions). MDS carried out on the dissimilarity matrix obtained using the Euclidian distance between the odorant zones, allowed to determine the level of similarity of the odorant zones based on their odor descriptors. The distances and coordinates calculations were performed using the frequency of odor descriptors; in addition, the DF for each of the four taste descriptors were used for graph depictions.

Figure 3A and 3B present the projection of the MDS 3D space of odorant zones. We decided to focus only on the links between sweetness and two odorant descriptors, fruity and floral which have the greater total number of occurrences. The size of the plots depends on the percentage of sweetness DF. The fruity odors are represented on Figure 3A by a color gradient depending on their occurrence in the odorant zone. They are more perceived in the odorant zones present on the negative part of axis 1. The floral odors (3B) are represented by a color gradient depending on their occurrence in the odorant zone, they are more perceived in the odorant zones present on the positive part of axis 3 and negative part of axis 2. The odorant zones with a high DF for sweetness are mainly located on negative part of V1, due to a greater number of occurrence for fruity and some on the positive part of axis 2, due to the presence of floral odors, but some are in the middle of the space due to links between sweetness and other odor descriptors as was highlighted by Cytoscape Network.

DISCUSSION

The different data analysis approaches followed in this study allowed finding consistent relationships between odor descriptors and taste descriptors. As the data used come from an extraction of volatile compounds from a fruit juice, the odor descriptors cover a specific domain. Most of the odors are associated with sweetness, which explains that sweetness is more explained in the PLS regression than the other taste descriptors. However, we were also able to find links with sourness, saltiness and bitterness, but starting from another type of extract than fruit juice described with another set of descriptors, we could find other associations, which could lead to other links between odor descriptors and tastes.

A lot of the literature on odor-taste interactions relies on sweetness perception. A review by Valentin et al[28] presents the different studies reporting an effect of odor on sweet perception. The most studied aroma is strawberry which has been reported to enhance sweetness perception for example in model systems,[29, 30] in whip cream[31] and in fruit juice.[18] Our results show that the strawberry descriptor is only associated with sweetness and has a high positive value in the regression to sweetness perception. Such a strong association between strawberry odor and sweet taste can be explained by associative learning,[22] due to simultaneous exposition of strawberry odor and sweet taste in a great variety of food products such as jams, jellies, marmalades, yogurts, ice creams or candies. Other odor descriptors are mainly associated with sweetness, such as caramel, which was already found to increase sweetness perception in model solutions[22] or ciders,[32] but the link between caramel and sourness is not surprising as caramel odor was previously found to increase both sweetness and sourness perception.[22] Fruity odors, such as orange, red.fruits and lemon are potential candidates for sweetness enhancement. They have a high positive value in the regression to sweetness perception and a negative value for saltiness and bitterness. Indeed, a sweetness enhancement has been observed for orange and raspberry.[28] The odor descriptor sweet is, as expected, associated with sweetness but also with sourness, which can be explained by the fact that fruit products are often perceived both sweet and sour.

Concerning lemon odor, Schifferstein and Verlegh[30] observed that the sweetness enhancing effect was lower than with strawberry odor. Our results show that lemon odor was mainly associated with sweetness but also with sourness. In water solution, a significant enhancement of both sweetness and sourness was observed by addition of lemon flavor ,[33] whereas in acidic solutions, other authors did not found any effect of the addition of lemon odor on sourness perception.[34] These different results are in agreement with other observations, that the effect of odor on sweetness/saltiness enhancement is higher at low to medium intensities of the tastes.[16, 32, 35] It can be noticed that even if lemon and citrus are both associated with sweetness, as illustrated by the positive contribution in the regression, lemon is secondly associated with sourness with a positive contribution to sourness and a negative contribution to bitterness in the regression, whereas citrus is secondly associated with bitterness, with a positive contribution to bitterness in the regression. These results can be explained by the fact that lemon extract are perceived as sour and sweet[36] and that some citrus fruit drinks such as grapefruit are perceived sweet and bitter.[37]

Only few odors were found to be mainly associated with sourness. As expected, the odor descriptor sour is mainly associated with sourness, but not with sweetness. Metallic and sweaty odor descriptor are associated with sour taste, metallic is also associated with bitterness and sweaty also associated with sweetness. To the best of our knowledge, there is no information in the literature on the effect of addition of such odors on sourness perception. The links observed in the present study could then be used to test the effect of molecules described with strong metallic odor on sourness enhancement.

Even if the odorant zones, which served as a basis for this study, were isolated from a fruit extract, some odorant zones were described with odor descriptors mainly associated with saltiness, such as toasted, smoky, sulfur, cheese, potato, butter, leather and mushroom. This association was already mentioned for similar odors such as bacon, cheese or peanuts and was used to enhance saltiness intensity in water solution by orthonasal and retronasal perception [19]. Another study on odor induced saltiness enhancement showed that at least 15% salt reduction can be compensated by addition of either beef or chicken bouillon aroma and that the odor descriptors mainly contributing to this enhancement were broth, meaty and roasted [38]. Soy sauce odor was also able to induce salty taste in water solution with a very low amount of sodium chloride, below the detection threshold.[39] It can be noticed that some odor descriptors such as smoky, sulfur, potato could also be associated to umami. This taste has not been described by our panel due to a lack of familiarity for this specific taste. The associations evidenced in the present paper could be used to select molecules or mixtures of molecules with smoky, potato or sulfur odors and test their potential enhancement effect on both saltiness and umami perception.

The positive association of the butter odor with both sweetness and saltiness can be explained by the consumption of both fat-sweet and fat-salty foods. Actually, addition of a butter aroma was found to enhance fat perception in model cheeses with an additional small effect on saltiness enhancement.[16] In a similar way, spicy descriptor is linked to sweetness and saltiness likely because of the consumption of both spicy-sweet and spicy-salty foods.

The links we observed between some odors (green, grass, vegetal) and bitterness have already been reported through the increase in bitterness perception in a model olive oil after addition of cis-3-hexenol, a compound with a grass odor.[40] Considering our results, other odor descriptors could be good candidates for bitterness enhancement, such as plastic, wood, herb and animal. The impact of odors on bitterness has not been the subject of many studies.[41]s In the case of bitterness reduction in food products, such odors have to be discarded from the product. In the aim to reduce bitterness in foods, our network representation can allow to select odors which have no link or only few links with bitterness and then test the effect of the corresponding odor-active compounds.

A focus was done in the present paper on two odor descriptors with the greatest number of occurrence in our odorant zones, fruity and floral, due to the nature of the extract, from a multifruit juice. Sweetness perception can be linked either with fruity or with floral, depending on the odorant zone.

Our results also point out other negative associations. Orange, candy and red fruits are not linked with saltiness and bitterness, which explains their negative value in the regression for saltiness and bitterness. Some descriptors are not linked with one specific taste. Caramel is not linked with bitterness, which explains its negative impact on bitterness. Butter, mushroom and peanut are not linked to sourness and have all a negative impact on sourness. Hot plastic, potato and sour are not linked to sweetness and have all a high significant negative impact on sweetness. Grass, citrus, lemon, metallic and dust are not linked to saltiness and have all a high significant negative impact on saltiness, except lemon, which has a moderate negative impact on saltiness. These odors could be then tested for an eventual masking effect of undesirable tastes such as an excess of bitterness or sourness.

In the present paper the odor descriptors analyzed for their taste association have been generated from a multifruit juice extract. The use of different multivariate analyses allowed us to highlight some general trends on odor-taste associations, some of which have already been used in experiments to enhance taste perception. The PLS model was used to find the odor descriptors which explain one specific taste descriptor, in a multidimensional space. The network representation using Cytoscape allowed visualizing all the links between odor descriptors and taste associated descriptors, with their occurrences and thus facilitated the interpretation of the PLS representation. The MDS representation, focused on the distances between the odorant zones, allowed a better visualization of the impact of specific odor descriptors on sweetness perception. A generalization of this approach to other extracts obtained from different products (fruits, vegetables) could increase the number of odor descriptors and their links with taste descriptors. The proposed approach is simple to handle and could be a good way for the selection of odor-active molecules with an impact, either positive or negative, on taste perception. The relationships thus formalized between odor and taste descriptors could then be used to predict a potential odor-induced taste enhancement or odor-induced taste masking in model system or real foods. These predictions could then be validated in model systems using pure molecules, mixture of molecules or natural extracts.

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SUPPORTING INFORMATION

Supplementary Figure S1: Partial least square (PLS) regression with 67 variables and 68 individuals. **1A:** projection of the 4 taste descriptors (Y variables) and the 63 odor descriptors (X variables) on components 1-2. **1B:** projection of the 68 odorant zones (individuals) on components 1-2.

Supplementary Figure S2: Partial least square (PLS) regression with 45 variables and 68 individuals. **A:** projection of the 4 taste descriptors (Y variables) and the 41 odor descriptors (X variables) on components 1-2. **B:** projection of the 68 odorant zones (individuals) on components 1-2.

Supplementary Table S1: matrix used for partial least square (PLS) analysis and multidimensional scaling (MDS), 68 odorant zones as lines and 41 odor descriptors and 4 associated taste descriptors as columns.

Supplementary Table S2: co-occurrence matrix build from Table SI and used for Cytoscape network.

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Figure caption

Figure 1: Partial least square (PLS) regression with 45 variables and 68 individuals. **1A**: projection of the 4 taste descriptors (Y variables) and the 41 odor descriptors (X variables) on components 1 and 2. **1B**: projection of the 68 odorant zones (individuals) on components 1-2.

Figure 2: Network representation of the links between odor descriptors (circle) and taste associated descriptors (octagon). The nature of the line varies as a function of the number of occurrences. The size of each odor descriptor depends on the number of odorant zones in which it is present. The file color of the odor descriptors varies as a function of the number of occurrences with each taste: blue if the odor is mainly associated with sweetness, green for saltiness, violet for sourness, light brown for bitterness. The border color is that of the second associated taste, it is grey if the odor is equally associated to the three other tastes and dark blue if the second associated taste is equally sourness and sweetness.

Figure 3: Allocation of odorant zones according to their odor descriptors and associated sweetness: Multidimensional scanning (MDS) representation in a 3 dimensional space. The color represents the occurrence of fruity (3A) floral (3B), the size of the plots depends on the percentage of sweetness detection frequency in the odorant zone.

Table 1: Odorant zones detected by gas chromatography/olfactometry (GC/O) and gas chromatography/olfactometry-associated taste (GC/O-AT), with the list of odour descriptors, the detection frequency (DF) (percentage of panellists having given an odorant descriptor) during the GC/O run, the detection frequency (percentage of panellists having given a taste associated descriptor) during the GC/O-AT run and the detection frequency for each associated taste. Values in bold refer to the main associated taste.

RI[a]	Abbrev.	Compound[b]	Odor descriptors[c]	DF odor (%)	DF taste (%)	sweetness (%)	sourness (%)	saltiness (%)
989	uk1	unknown	fruity (3), apple, grenadine, peach, caramel, sweet, strawberry (2), butter, floral	83	67	**67**	0	0
993	2PE	2-pentanone (St)	fruity, cheese (3), caramel, green (3), butter (2)	92	67	25	8	**33**
1001	uk4	unknown	plastic (3), solvent, unpleasant, almond, toasted	75	67	0	8	8
1015	M2MB	methyl-2-methyl butanoate (St)	fruity (8), banana, sweet, candy, acid, floral (2)	92	75	**58**	17	0
1043	EB	Ethyl butanoate (St)	fruity (4), orange, floral (2) sweet, cheese, red fruits, ripe fruit, sweaty, foot	100	75	**50**	17	0
1058	E2MB	ethyl-2-methyl butanoate (St)	fruity (6), apple (3), strawberry, candy (2), sweet (2), lemon, fusil	100	75	**58**	8	0
1081	BA	butyl acetate (St)	lemon, solvent (4), alcohol, sour, sweet, caramel	75	67	8	**42**	8
1087	HEXA	hexanal (ST)	green (7), herb (5), floral (2), fresh, herbal, solvent , cut grass,	100	75	8	**25**	17
1103	IBA	Isobutyl alcohol (St)	spicy, vegetal, wood (2), plastic, glue, hot plastic, burnt, glue	100	83	0	17	17
1112	uk6	n.d.	unpleasant, toasted, sulfur, plastic, herb, green, leek, hot plastic, asparagus,	75	67	0	25	8
1130	M3BA	3-methyl-1-butyl acetate (St)	fruity (4), banana (3), solvent (2), sweet, candy (3)	75	67	25	**33**	0
1147	uk7	n.d.	green (3), vegetal, herb, grass, leather	42	42	**25**	0	8
1157	Buta	n-butanol (St)	toasted, peanut, solvent, chocolate, foot	33	42	**17**	0	8
1171	β-Myr	β-myrcene (St)	herb (2), green, sour, floral, sweet	50	67	0	**42**	0
1206	Limone	limonene (St)	spicy, green, lemon (2), citrus, metallic, aromatic herbs, sulfur	67	58	**17**	**17**	8

1218	M2B	2-methyl-1-butanol (St)	acid, cheese, wool, chocolate, paint, rose, nutty, solvent (2), chemical, toasted, sport room, foot, fruity	92	50	**17**	0	**17**
1242	β-Oci	(E)-β-ocimene (MS)	fruity (6), strawberry, floral (2), lemon, ripe fruit, solvent	67	75	**75**	0	0
1248	γ-Ter	γ-terpinene (St)	green, green tea, potatoe, animal, bread, plastic	50	33	0	8	8
1291	3H2B	3-hydroxy-2-butanone (St)	fruity, cream (2), cheese, toasted, baked, green, floral, butter, wood	67	50	**25**	8	17
1295	Octa	octanal (St)	sharp, green, floral (3), lemon, fruity, citrus,	58	42	**25**	8	8
1307	1o3o	1-octen-3-one (MS)	floral, mushroom (10), plastic	100	83	0	8	**50**
1332	uk8	unknown	toasted, peanut, mushroom (2), land, sweet, floral, unpleasant	75	58	**25**	0	17
1361	Cyclop	2-cyclopenten-1-one (MS)	fruity, floral, rose	33	33	**17**	8	0
1367	Hexa	n-hexanol (St)	floral (6), green (3), grass, herb (2), solvent, white flower, violet, fruity	92	67	**33**	17	0
1381	allo-O	allo-ocimene (MS)	green (3), metallic (2), aldehyde, floral, animal, plastic, herbal, bitter, sour, vegetal	100	83	0	25	8
1388	3Hexe	3-hexenol (St)	green (4), grass, land, herb, unpleasant, gas, rotten, drain, sweet, fruity	83	33	0	8	0
1401	uk9	n.d.	floral (3), cork, herb, plastic	50	42	**25**	8	0
1406	uk10	n.d.	fruity (2), floral, medicine, aspirin, leather, citrus, solvent	75	42	**17**	8	0
1412	2Hexe	2-hexen-1-ol (St)	toasted, mushroom (6), floral, sulfur	75	50	0	8	**25**
1438	uk3	unknown	fruity, mushroom, potatoe (3), mold, sulfur	67	58	0	0	**42**
1442	Lin-Ox	linalool-oxide (MS)	green (2), grass, wood, earth, dust, potatoe, floral, opium poppy, butter, earth	75	33	0	8	8
1461	furfural	furfural (St)	toasted, fruity, potatoe (5), mash potatoes, exotic fruit, sulfur	83	67	0	0	**58**
1492	Deca	decanal (St)	fruity (3), floral, solvent, chemical, burnt meat	50	50	**17**	8	8
1515	PO	Propyl octanoate (St)	green (2), land, paper, warm plastic	58	75	8	**42**	25

1544	M3MTP	methyl-3-methylthio propionate (MS)	green, wood, paper (2), dust, animal, unpleasant	75	50	0	8	0
1557	linalool	linalool (St)	floral (6), pleasant, fruity (2), sweet, pineapple, apricot, cake, candy, butter	92	75	**67**	8	0
1573	E3MTP	ethyl-3-methylthio propionate (MS)	acid, floral (2), medicine, aspirin, candy, fruity (3), orange	58	42	**25**	17	0
1594	Fenchol	fenchol (St)	floral, green (2), melon, green vegetable, grass	58	67	8	**25**	8
1603	4M2-5DF	4-methoxy-2,5-dimethyl furanone (MS)	sharp, green, vegetal, sweet, fruity (3), caramel (2), cereal, muesli, cake, hot bread	75	83	**25**	**25**	17
1637	4Ter	4-terpineol (MS)	mushroom, wood, humid, meat, toasted	42	33	0	8	**25**
1648	uk5	unknown	unpleasant (2), acid, floral, rose, cheese (4), urine, sour, lemon, dust, dry flowers, sweaty	92	58	0	**50**	8
1654	uk11	n.d.	toasted, cheese, fruity	42	42	0	8	**17**
1688	PA	pentanoic acid (St)	acid (4), sharp, cheese (9), animal, unpleasant (3), vomit, sour, spicy, plastic warm	100	75	0	**42**	25
1703	αTerp	α -terpineol (St)	floral (2), green, hot plastic, peanut, hot bread	50	42	0	8	0
1710	3MTP	3-methylthio propanol (St)	wood, aromatic herbs, hot plastic	33	33	8	0	**17**
1726	Valencene	valencene (St)	green, anise (3), floral (2), fruity	50	58	17	**25**	17
1730	uk12	n.d.	green (3), vegetal, fruity (2), cat urine (2), herb, sweaty, unpleasant, mustard, urine, leaves cassis, floral, passion fruit	92	58	17	**33**	0
1740	Carvone	carvone (St)	green, insect, plastic, red fruit, fruity	33	33	8	8	8
1780	uk13	n.d.	floral (4), rose (2), green (2), vegetal (2), lemon	58	75	**25**	**25**	8
1821	uk14	n.d.	floral (2), vegetal, wood, toasted, fruity, acid	67	58	17	0	17
1829	β-Dam	β-damascenone (St)	fruity (6), sweet, peach, floral, old fruit, cherry, red fruit	75	50	**50**	0	0

1852	Geraniol	geraniol (St)	green (2), sharp, fruity, rhubarb, animal, bitter, citrus, smoked, vegetal, smoke, plastic, bitter, rhubarb, sulfur, unpleasant	92	83	17	**33**	8
1861	HA	hexanoic acid (St)	metallic, citrus, unpleasant	33	50	**25**	17	0
1870	uk15	n.d.	toasted, smoky, burnt, sweet, cotton candy, smoky, floral,	67	42	0	0	**33**
1896	PhM	Phenyl methanol (St)	sweet, candy, floral (4), fruity (3), fresh, green, orange	75	42	**42**	0	0
1921	PhE	2-phenyl ethanol (St)	fruity, floral (2), rose, mushroom (3)	67	67	**58**	0	8
1951	β-Ion	(E)-β-ionone (St)	spicy, cinnamon, food, roasted meat, solvent, floral, smoky, plastic, leather, fruity	58	92	**42**	17	33
2014	uk16	n.d.	wood, potatoe, humid, metallic (2), bread	67	67	0	**33**	0
2037	uk2	unknown	unpleasant, dust, fruity (2), candy	50	50	**42**	0	0
2046	furaneol	furaneol (St)	caramel (6), cotton candy, sweet, sugar, jam	75	42	**42**	0	0
2143	uk17	n.d.	sweet, floral, plastic, toasted, candle, fruity	50	33	**17**	**17**	0
2160	γ-Dec	γ-decalactone (St)	floral (3), menthol, fruity (3), unpleasant, sweet (2), citrus	75	58	**42**	8	0
2174	Eugenol	eugenol (MS)	petrol, spicy (2), pepper, clove (2), medicine, chemical, vegetal	50	50	**33**	8	8
2209	uk18	n.d.	mushroom, butter, cake, cinnamon, herb, vegetal	42	50	**17**	8	8
2234	Elemicin	elemicin (MS)	floral (3), green, solvent, honey, fruity	58	33	**17**	8	0
2248	uk19	unknown	mushroom, floral, fruity, chemical, citrus, wet earth, herb, vegetal	58	42	8	8	0
2284	uk20	unknown	plastic, smoky, wood, pepper, sharp, spicy, sweaty, floral, vegetable soup, leather, felt pen	67	58	8	0	17
2303	Tricosane	tricosane (MS)	petrol, animal, plastic, herb	33	50	0	8	8

[a]: RI calculated retention index of the compound using a series of n-alkanes injected on a DB-Wax column under identical chromatographic conditions.

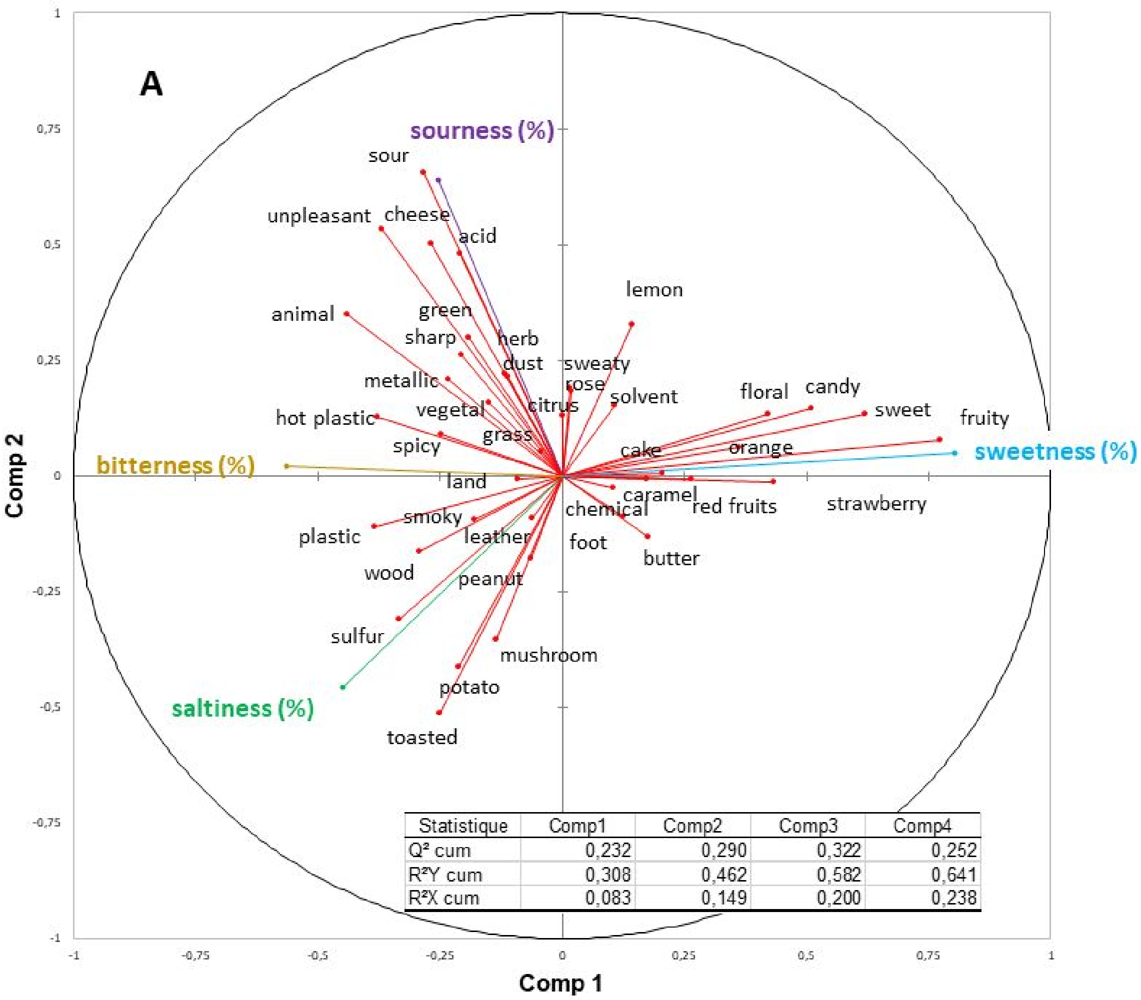
[b]: mode of identification, MS: tentatively identified by retention index (RI) compared to data from VCF 16.1 and mass spectrum (MS) verified by comparison with mass spectra database (NIST; INRAMass: CSGA/J. Maratray), St: RI and MS verified with literature data and by injection of pure standard in the same condition, (data already published in Barba et al., (16, 21), n.d. means not detected.

[c]: in brackets, the number of citations of the odor descriptors by the panelists if >1

Table 2: Partial least square (PLS) regression to explain the taste descriptors by odor descriptors: for each odor descriptor the number of total occurrences and the number of odorants zones in which it has been described are given with the regression coefficients for each associated taste.

nb occurrences	nb odorant zones	odor descriptor	taste descriptor			
			sweetness	sourness	saltiness	bitterness
		Constant	17,523	11,099	13,413	13,431
79	35	fruity	2,328	-0,353	-0,899	-1,086
70	37	floral	2,082	-0,351	-1,306	-0,579
49	25	green	-1,684	1,593	0,083	0,711
25	8	mushroom	-1,420	-0,205	2,291	-0,487
20	7	cheese	-0,121	0,881	1,386	-1,364
19	17	sweet	4,005	0,899	-2,255	-1,878
17	11	herb	-2,097	1,925	-1,110	1,845
17	12	solvent	-1,685	2,701	0,299	0,138
15	13	plastic	-3,555	-0,975	-2,484	5,228
15	12	unpleasant	0,822	1,093	-2,474	0,649
13	13	toasted	-3,708	-3,590	5,726	0,106
12	11	vegetal	-1,745	1,378	-2,630	2,911
11	5	caramel	2,015	-0,735	-0,268	-1,182
11	5	potato	-3,437	-0,417	6,095	-1,646
10	7	candy	2,387	2,068	-1,905	-1,263
10	9	wood	-3,494	-2,012	-1,117	4,541
9	6	acid	0,898	0,991	1,306	-2,257
8	7	lemon	1,543	3,176	-0,644	-2,054
7	6	butter	3,363	-2,329	3,197	-4,319
7	7	citrus	3,873	-1,017	-5,668	1,485
7	6	spicy	1,711	-1,998	0,836	-1,396
6	6	animal	-2,074	-0,335	-5,721	6,066
6	6	hot plastic	-5,895	2,952	0,767	3,044
6	4	metallic	-3,591	2,874	-5,004	5,676
6	5	rose	1,750	1,016	-0,634	-1,411
6	4	smoky	-2,498	0,068	4,055	-1,084
6	6	sulfur	-6,885	-0,295	7,439	0,087
5	5	chemical	2,402	-2,354	-2,022	0,499
5	5	grass	0,210	-0,819	-3,974	3,195
5	5	sharp	-0,005	1,059	1,268	-1,544
5	5	sour	-8,975	13,036	0,921	1,486
5	5	sweaty	-0,908	3,186	-0,914	0,175
4	4	dust	2,091	-0,487	-5,041	2,215
4	4	leather	3,507	-5,016	1,363	-2,036
4	3	strawberry	11,448	-5,259	-5,237	-3,395
3	3	cake	2,645	1,188	-0,009	-2,593
3	3	foot	3,385	-3,862	-2,208	0,444
3	3	land	-4,686	3,251	3,781	-0,274
3	3	orange	5,095	1,502	-2,592	-2,716
3	3	peanut	2,097	-6,944	-5,584	5,267
3	3	red fruits	5,416	-0,960	-2,534	-2,092

Figure 1



Statistique	Comp1	Comp2	Comp3	Comp4
Q² cum	0,232	0,290	0,322	0,252
R²Y cum	0,308	0,462	0,582	0,641
R²X cum	0,083	0,149	0,200	0,238

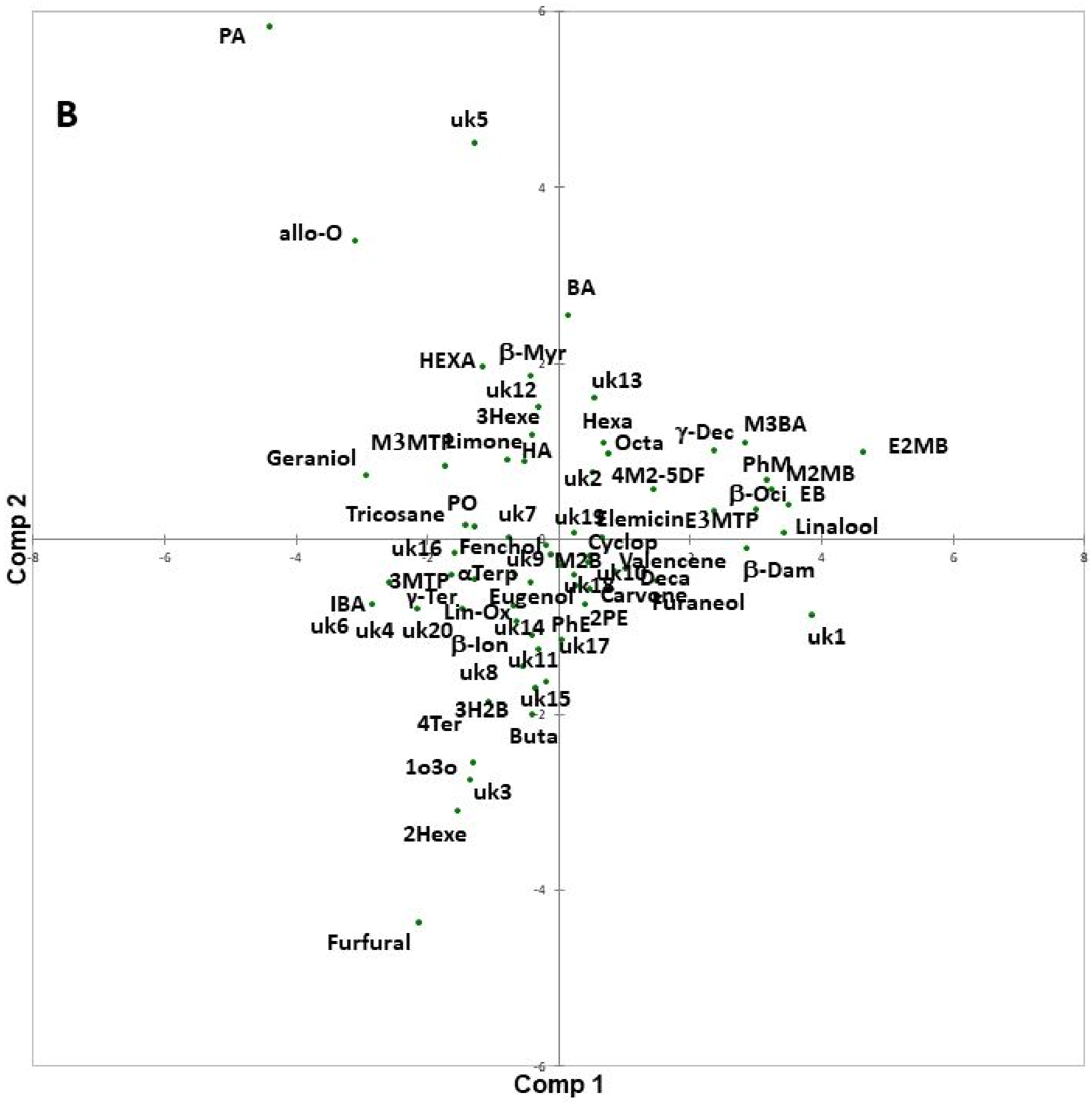

B
PA
uk5
allo-O
BA
HEXA
β-Myr
uk12
uk13
3Hexe
Hexa
γ-Dec
M3BA
Geraniol
M3MTP
Limone
HA
Octa
E2MB
uk2
4M2-5DF
PhM
M2MB
β-Oci
EB
Tricosane
PO
uk7
uk19
Elemicin
E3MTP
Linalool
uk16
Fenchol
Cyclop
uk9
M2B
Valencene
β-Dam
3MTP
αTerp
uk10
Deca
IBA
γ-Ter
Eugenol
uk18
Carvone
Furaneol
Lin-Ox
uk6
uk4
uk20
uk14
PhE
2PE
uk1
β-Ion
uk17
uk11
uk8
uk15
3H2B
4Ter
Buta
1o3o
uk3
2Hexe
Furfural
Comp 1
Comp 2

Figure 2

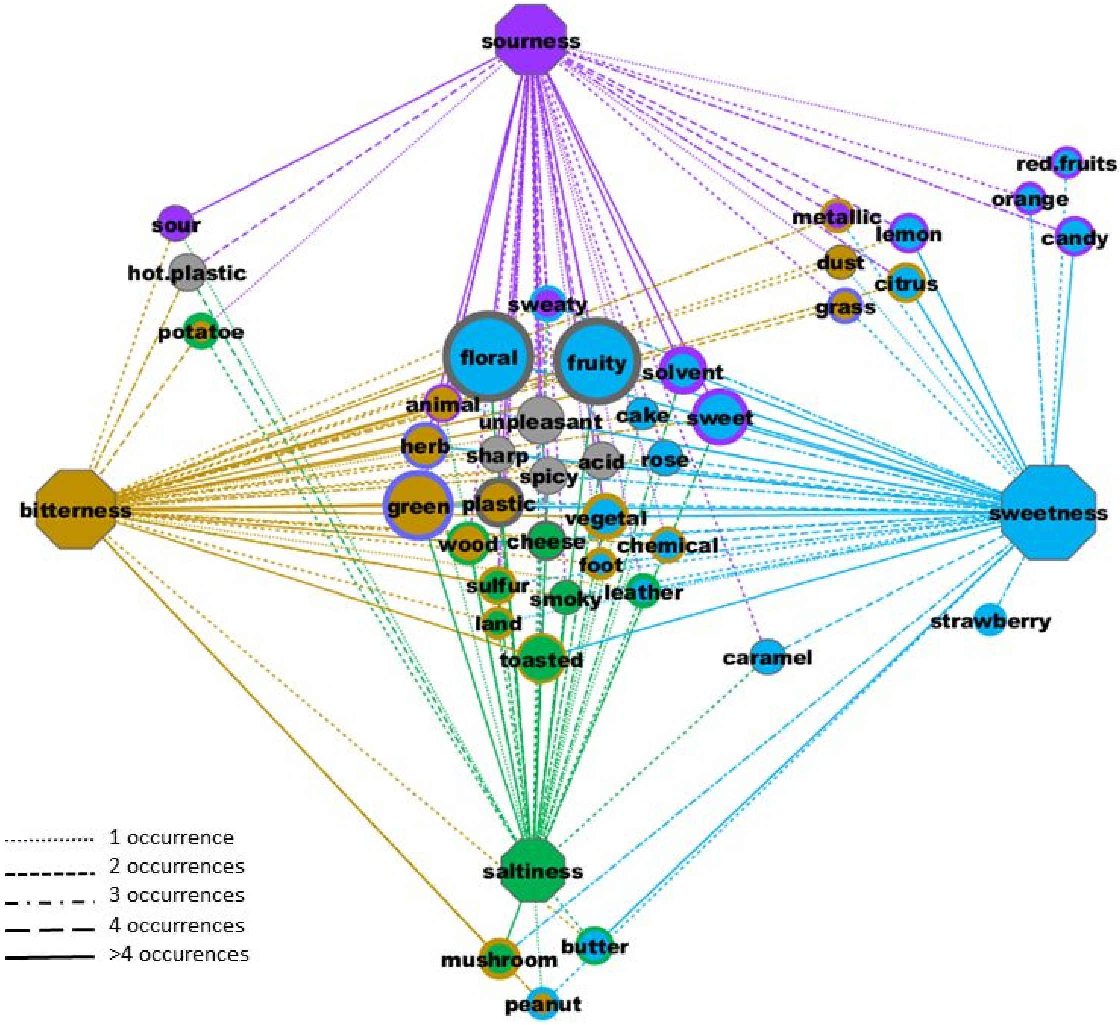
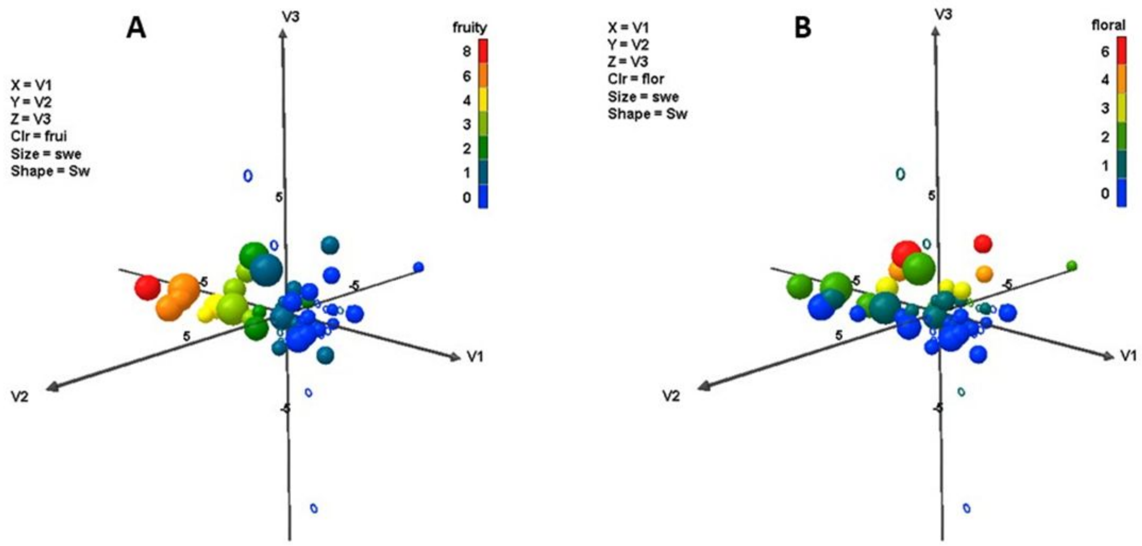
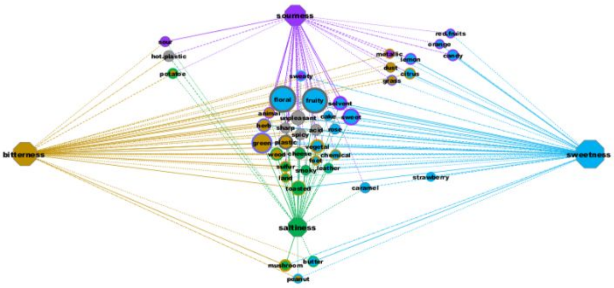

sourness
red.fruits
orange
candy
metallic
lemon
dust
citrus
grass
sour
hot.plastic
potatoe
sweaty
floral
fruity
solvent
animal
unpleasant
cake
sweet
herb
sharp
acid
rose
spicy
bitterness
green
plastic
vegetal
sweetness
wood
cheese
chemical
foot
sulfur
smoky
leather
land
toasted
strawberry
caramel
1 occurrence
2 occurrences
3 occurrences
4 occurrences
>4 occurences
saltiness
mushroom
butter
peanut

Figure 3


A
X = V1
Y = V2
Z = V3
Clr = frui
Size = swe
Shape = Sw
fruity
V1
V2
V3
B
X = V1
Y = V2
Z = V3
Clr = flor
Size = swe
Shape = Sw
floral

TOC graphic


sourness
bitterness
sweetness
saltiness
sour
hot.plastic
potatoe
red.fruits
orange
candy
metallic
lemon
dust
citrus
grass
sweaty
floral
fruity
solvent
sweet
animal
unpleasant
cake
herb
sharp
acid
rose
spicy
green
plastic
vegetal
wood
cheese
chemical
foot
sulfur
smoky
leather
land
toasted
strawberry
caramel
mushroom
butter
peanut