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

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1 ABSTRACT

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

17

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

20

21

22 INTRODUCTION

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

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

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

45 Another strategy is to increase the heterogeneity of the food matrix, which was able to increase
46 both salty and sweet taste without compromising consumer acceptability.⁸ It was thus observed

47 that hard gels were perceived sweeter when sugar distribution was heterogeneous due to a long-
48 lasting in-mouth sucrose concentration, the hard matrix being able to maintain the taste contrast
49 due to different sucrose concentrations, for a longer time in the mouth during chewing.⁹ The
50 authors concluded that the fracture properties of food can be modulated to enhance sweetness
51 perception, in association with heterogeneous distribution.¹⁰

52 Another innovative strategy relies on the use of aroma-taste interactions and multimodal
53 integration. This strategy is based on the observation that an odor may evoke a taste^{11, 12} while
54 it does not activate taste receptors.¹³ This phenomenon results from the co-occurrence of odors
55 and tastes during food tasting, which, through associative learning, contributes to the
56 acquisition of taste qualities by odors.¹³ It has been reported that mentally imagined odor-taste
57 mixtures showed the same patterns of interaction that actually perceived odor-taste mixtures,
58 thus demonstrating that taste and odor perception interact at a cognitive level during holistic
59 flavor processing in the brain.¹⁴ This strategy has been applied with success to develop low-salt
60 foods while maintaining saltiness and consumer acceptability,¹⁵ to enhance fat perception in
61 real foods varying in structure-texture properties¹⁶ and to enhance sweet taste perception in
62 foods¹⁷ especially in sugar-reduced fruit juices.¹⁸

63 Using such an approach needs an adequate selection of odors. As food odors can evoke a
64 specific taste through mental imagery, it has been possible to select promising odors for
65 saltiness enhancement based on the expectation taste profiles of food products being evoked by
66 their names.¹⁹ In different volatile compounds databases, such as Flavor-Base²⁰ or Volatile
67 Compounds in Foods,²¹ the word “sweet” is often used as odorant descriptor. Considering this
68 observation that some odors are described with a “smelled taste”, Stevenson et al²² calculated
69 the correlation between odor sweetness and taste sweetness for 10 odorant molecules and found
70 that the degree to which an odor smelled sweet was a good predictor for taste tasting. This
71 association was also used to select odorants able to enhance sweetness in fruit juices, using gas

72 chromatography/olfactometry-associated taste (GC/O-AT),¹⁸ showing that many molecules
73 described with a “smelled sweet taste” were able to enhance the perceived sweetness odor of a
74 fruit juice. However some molecules, such as phenyl methanol, described with a sweet odor,
75 were not able to enhance a perceived sweetness. Moreover, looking at the data gathered in the
76 Flavor base,²⁰ most of the molecules described with a sweet taste are also described with a
77 sweet odor, but some molecules such as bornyl formate, linalyl formate, methyl crotonate or
78 hydroxyl methyl furfural possess a sweet taste without being described with a sweet odor. There
79 is thus a need to look for the impact of other odor descriptors than sweet in the odor-taste
80 associations. We thus propose to apply different complementary multivariate statistical tools to
81 explore more deeply the links between odor descriptors and taste associated descriptors.

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

94

95 **MATERIALS AND METHODS**

96 **Sample preparation**

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

100

101 **Chemicals**

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

109

110 **Gas chromatography analysis**

111 The extract was then concentrated with a Kuderna-Danish apparatus and 1 μ L (splitless mode
112 for 0.5 min) was submitted to gas-chromatography/mass-spectrometry (GC/MS) for
113 compounds identification and to GC/O-AT for odor description¹⁸ using the same column (30 m
114 x 0.32 mm i.d. fused silica capillary column coated with a 0.5 μ m layer of polyethylene glycol,
115 DB-Wax, Agilent, Agilent Technologies, Santa Clara, CA). GC/O-AT was done with 12
116 panelists used to GC/O experiments. In a first run (first injection of the extract), panelists were
117 asked to indicate the detection of an odor using a buzzer and to give an odor descriptor. In a
118 second run (second injection of the same extract), panelists were asked to attribute for each
119 odor, one of the four associated taste descriptors: sweetness, saltiness, sourness or bitterness.
120 Detection times, odor descriptors and taste associated descriptors were recorded using
121 AcquiSniff software (Saint Genès Champanelle, France). The detection frequency (DF) was

122 calculated for each odorant zone, for both odor descriptors and taste associated descriptors, as
123 the percentage of panelists having detected an odor. Only the odorant zones with a DF higher
124 than 30% were selected, to limit the false detection risk.²⁴ For each selected odorant zone, we
125 took into account all the odor descriptors given by the 12 panelists. For taste associated
126 descriptors, we also calculated the DF for each specific taste: sweetness (%), sourness (%),
127 saltiness (%), bitterness (%), these values are used in the multivariate analyses.

128

129 **Data preparations**

130 From the whole set of data previously published, we selected 68 odorant zones (Table 1). A
131 total of 48 compounds have been identified by their mass spectra and injection of standard
132 compounds¹⁸ and the 20 remaining zones correspond to unknown compounds or compounds
133 present in trace amount. Even if the molecules present in some of the odorant zones have not
134 all been identified, in the present paper, we used the odor descriptors given by the panelist for
135 each odorant zone, to find links between these odor descriptors and the taste associated
136 descriptors. From the odor descriptors given by the 12 panelists in the 68 odorant zones, a list
137 of 70 odor descriptors was extracted, of which 7 were present only in the description of one
138 odorant zone and 12 in only 2 odorant zones. Odor descriptors only present in one or two
139 odorant zones were not considered for further analyses. The multivariate analyses were done
140 with 45 variables, the number of occurrences of each of the 41 remaining odorant descriptors
141 and the DF of each of the 4 associated taste descriptors (sweetness, saltiness, bitterness,
142 sourness).

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

147

148 Computational analysis and statistical methods

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

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

159 PLS was performed with XLStat (Addinsoft, Paris, France) and MDS with R version 3.0.1.²⁵

160

161 Network visualization

162 The associations between odor descriptors and taste descriptors were visualized using a network
163 of odorant and taste descriptors. For that purpose, we first calculated the co-occurrence matrix
164 (R 3.0.1 ²⁵) of the odorant and taste descriptors using the binary matrix made of the 68 odorant
165 zones and the 45 descriptors (41 odor descriptors and 4 taste descriptors). The co-occurrence
166 matrix is a square 45x45 matrix in which the off-diagonal terms are the number of odor-taste
167 pairs in the description of an odorant zone, while the diagonal terms are the number of all
168 occurrences of each odor and taste descriptors (Supplementary Table S2). Cytoscape²⁶ was used
169 to build a network of the links between odor descriptors and taste-associated descriptors. To do
170 so, the square matrix was transformed into a two-way table using Statistica (TIBCO Software
171 Inc. 2017).

172

173 RESULTS

174 The 68 selected odorant zones with DF odor values higher than 30% are listed in Table 1 with
175 their retention indices, the name of the corresponding volatile compounds, if identified, or the
176 number of the unknown compound. For each odorant zone, all the odor descriptors given by
177 the 12 panelists are listed with the number of occurrence when higher than the unity. We have
178 removed from the list the descriptor “unknown”, which was given by panelists who were not
179 able to describe the perceived odor. This list of descriptor was used to build the Euclidian
180 matrix. For each odorant zone, two values are given for DF. First, the detection frequency for
181 the odor (DF odor %), which is the percentage of panelists having smelled the odor during the
182 first run of GO/O and the detection frequency for the associated taste descriptor (DF taste %)
183 during the second GC/O-AT run. Second, we calculated the DF for each of the four taste
184 attributes, sweetness (%), sourness (%), saltiness (%), bitterness (%) and used these values for
185 the statistical analyses. The values in bold refer to the main associated taste. A total number of
186 33 odorant zones were mostly associated with sweetness (13 with a value higher than 40%), 16
187 with sourness (5 with a value higher than 40%), 10 with saltiness (3 with a value higher than
188 40%) and 21 with bitterness (3 with a value higher than 40%).

189

190 Evaluation of taste association by odor descriptors using PLS

191 The PLS analysis was done on the 68 odorant zones, using the occurrences of each of the 41
192 odor descriptors as X variables and the DF for each associated taste as Y variables. We verified
193 that the representation of the remaining 41 odor descriptors was the same as on the PLS
194 performed with the 63 odor descriptors present in at least 2 odorant zones (supplementary
195 Figure S1). Figure 1A shows the projection of the variables on the two first components. Even
196 if the model does not account for a high level of variation, the 4 associated tastes are well

197 discriminated in the first plane of the PLS map represented by the two first components,
198 sweetness on the positive part of component 1, bitterness on the negative part of component 1,
199 sourness and saltiness on the positive part of component 2 and also on the negative part of
200 component 1. Sweetness is better represented on this first plane than the other tastes. This can
201 be explained by the fact that the odorant zones are separated from a fruit juice extract and that
202 most of them are described as fruity. The odor descriptors fruity, sweet, strawberry, candy,
203 floral, orange are positively correlated with component 1 and thus associated to sweet taste
204 perception. The odor descriptors toasted, potato, mushroom and sulfur are negatively correlated
205 with component 2 and thus associated to saltiness. The odor descriptors sour, unpleasant, cheese
206 and acid are positively correlated with component 2 and thus associated to sourness. The odor
207 descriptors hot plastic, plastic and spicy are negatively correlated with component 1 and thus
208 associated to bitterness. A PLS model was built to predict the taste association by a linear
209 combination of the odor descriptors. Table 2 presents the coefficients affected to each odor
210 descriptor to explain one taste descriptor. The odor descriptors are ranked according to the
211 decreasing number of their total occurrences. The odors with the highest association with
212 sweetness are strawberry, red fruits, sweet, citrus, leather, butter, orange, foot, chemical, candy,
213 fruity and floral; the odors with the highest negative association with sweetness are sour, sulfur,
214 hot plastic, land, plastic, wood, metallic, toasted, potato and smoky. The odors with the highest
215 association with saltiness are sulfur, potato, toasted, smoky, land, butter and mushroom: the
216 odors with the highest negative association with saltiness are citrus, animal, peanut, strawberry,
217 dust, metallic, grass, vegetal, unpleasant, plastic, red fruits, foot, sweet and chemical. The odors
218 with the highest association with sourness are sour, sweaty, hot plastic, metallic, lemon, land
219 and solvent; the odors with the highest negative association with sourness are peanut,
220 strawberry, toasted, leather, foot, chemical and butter. The odors with the highest association
221 with bitterness are animal, metallic, peanut, plastic, wood, grass, hot plastic, vegetal and dust;

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

228 Looking at the odorant zones (Figure 1B), the molecules, when identified, with a high positive
229 correlation with component 1 are the most associated with sweetness, ethyl 2-methylbutanoate
230 (E2MB) is described with fruity, apple, strawberry, candy and sweet odor descriptors (Table
231 1); methyl 2-methylbutanoate (M2MB) is described with fruity and sweet notes; linalool is
232 described with floral, fruity, sweet and candy notes; (E)- β -ocimene (β -Oci) is described with
233 fruity, floral and strawberry notes; phenylmethanol (PhM) is described with floral, fruity, sweet
234 and candy notes; β -damascenone (β -Dam) is described with fruity, floral and sweet notes; γ -
235 decalactone (γ -Dec) is described with floral, fruity and sweet notes; ethyl butanoate (EB) is
236 described with fruity, floral and sweet notes. The compounds the most associated with sourness
237 (positive correlation with component 2) are pentanoic acid (PA), described as acid, sharp,
238 cheese and unpleasant; allo-ocimene (allo-O), described as green, metallic and sour; hexanal
239 (HEXA) described as green, herb and floral. The compounds the most associated with bitterness
240 (negative correlation with component 1) are tricosane, described as plastic and petrol; isobutyl
241 alcohol (IBA), described as plastic, hot plastic, spicy and wood. The compounds the most
242 associated with saltiness (negative correlation with component 2) are furfural, described as
243 potato, toasted and sulfur; 2-hexen-1-ol (2Hexe), described as mushroom, toasted and sulfur;
244 1-octen-3-one (1o3o), described as mushroom and n-butanol (Buta), described as toasted and
245 peanut.

246

247 **Visualization of the relationships between odor descriptors and associated tastes**

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

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

266 Only the strawberry odor descriptor is linked to one single taste (sweetness), which explains its
267 high positive value in the regression to sweetness perception. Three odor descriptors are only
268 linked to two tastes: orange, candy and red fruits, which are linked mainly to sweetness and to
269 a lesser extent to sourness. The descriptors linked to three tastes can be discriminated by the
270 taste to which they are not linked to. Caramel is not linked to bitterness. Butter, mushroom and

271 peanut are not linked to sourness. Hot plastic, potato and sour are not linked to sweetness. Grass,
272 citrus, lemon, metallic and dust are not linked to saltiness.
273 The other odor descriptors are linked to all the tastes. Fruity and floral are the most cited
274 descriptors with respectively 79 and 70 total number of occurrence and present in respectively
275 35 and 37 odorant zones. They are mainly linked to sweetness, then to the three other tastes
276 without any distinction. Cake and rose are mainly associated to sweetness but with only few
277 occurrences. Among the other odor descriptors mainly associated to sweetness, the second
278 associated taste is sourness for sweet and solvent, bitterness for vegetal, chemical and foot and
279 saltiness for leather. Only sweaty is associated to sourness in the first place. The odors green,
280 plastic, herb, wood and animal are associated to bitterness, while they are also associated to
281 saltiness for wood, sourness for animal and both sourness and sweetness for green and herb.
282 Toasted, cheese, sulphur, smoky and land odors are mainly associated to saltiness and toasted,
283 sulphur and land are also associated to bitterness. Unpleasant, sharp, spicy and acid do not
284 present any specificity towards a given taste.

285

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

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

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

308

309 **DISCUSSION**

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

318 A lot of the literature on odor-taste interactions relies on sweetness perception. A review by
319 Valentin et al²⁸ presents the different studies reporting an effect of odor on sweet perception.
320 The most studied aroma is strawberry which has been reported to enhance sweetness perception

321 for example in model systems,^{29, 30} in whip cream³¹ and in fruit juice.¹⁸ Our results show that
322 the strawberry descriptor is only associated with sweetness and has a high positive value in the
323 regression to sweetness perception. Such a strong association between strawberry odor and
324 sweet taste can be explained by associative learning,²² due to simultaneous exposition of
325 strawberry odor and sweet taste in a great variety of food products such as jams, jellies,
326 marmalades, yogurts, ice creams or candies. Other odor descriptors are mainly associated with
327 sweetness, such as caramel, which was already found to increase sweetness perception in model
328 solutions²² or ciders,³² but the link between caramel and sourness is not surprising as caramel
329 odor was previously found to increase both sweetness and sourness perception.²² Fruity odors,
330 such as orange, red.fruits and lemon are potential candidates for sweetness enhancement. They
331 have a high positive value in the regression to sweetness perception and a negative value for
332 saltiness and bitterness. Indeed, a sweetness enhancement has been observed for orange and
333 raspberry.²⁸ The odor descriptor sweet is, as expected, associated with sweetness but also with
334 sourness, which can be explained by the fact that fruit products are often perceived both sweet
335 and sour.

336 Concerning lemon odor, Schifferstein and Verlegh³⁰ observed that the sweetness enhancing
337 effect was lower than with strawberry odor. Our results show that lemon odor was mainly
338 associated with sweetness but also with sourness. In water solution, a significant enhancement
339 of both sweetness and sourness was observed by addition of lemon flavor,³³ whereas in acidic
340 solutions, other authors did not find any effect of the addition of lemon odor on sourness
341 perception.³⁴ These different results are in agreement with other observations, that the effect of
342 odor on sweetness/saltiness enhancement is higher at low to medium intensities of the tastes.^{16,}
343 ^{32, 35} It can be noticed that even if lemon and citrus are both associated with sweetness, as
344 illustrated by the positive contribution in the regression, lemon is secondly associated with
345 sourness with a positive contribution to sourness and a negative contribution to bitterness in the

346 regression, whereas citrus is secondly associated with bitterness, with a positive contribution to
347 bitterness in the regression. These results can be explained by the fact that lemon extract are
348 perceived as sour and sweet³⁶ and that some citrus fruit drinks such as grapefruit are perceived
349 sweet and bitter.³⁷

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

357 Even if the odorant zones, which served as a basis for this study, were isolated from a fruit
358 extract, some odorant zones were described with odor descriptors mainly associated with
359 saltiness, such as toasted, smoky, sulfur, cheese, potato, butter, leather and mushroom. This
360 association was already mentioned for similar odors such as bacon, cheese or peanuts and was
361 used to enhance saltiness intensity in water solution by orthonasal and retronasal perception¹⁹.
362 Another study on odor induced saltiness enhancement showed that at least 15% salt reduction
363 can be compensated by addition of either beef or chicken bouillon aroma and that the odor
364 descriptors mainly contributing to this enhancement were broth, meaty and roasted³⁸. Soy sauce
365 odor was also able to induce salty taste in water solution with a very low amount of sodium
366 chloride, below the detection threshold.³⁹ It can be noticed that some odor descriptors such as
367 smoky, sulfur, potato could also be associated to umami. This taste has not been described by
368 our panel due to a lack of familiarity for this specific taste. The associations evidenced in the
369 present paper could be used to select molecules or mixtures of molecules with smoky, potato

370 or sulfur odors and test their potential enhancement effect on both saltiness and umami
371 perception.

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

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

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

390 Our results also point out other negative associations. Orange, candy and red fruits are not
391 linked with saltiness and bitterness, which explains their negative value in the regression for
392 saltiness and bitterness. Some descriptors are not linked with one specific taste. Caramel is not
393 linked with bitterness, which explains its negative impact on bitterness. Butter, mushroom and
394 peanut are not linked to sourness and have all a negative impact on sourness. Hot plastic, potato

395 and sour are not linked to sweetness and have all a high significant negative impact on
396 sweetness. Grass, citrus, lemon, metallic and dust are not linked to saltiness and have all a high
397 significant negative impact on saltiness, except lemon, which has a moderate negative impact
398 on saltiness. These odors could be then tested for an eventual masking effect of undesirable
399 tastes such as an excess of bitterness or sourness.

400

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

418

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423

424 SUPPORTING INFORMATION

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

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

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

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

438

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539

540

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 fill 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 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	α Terp	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.

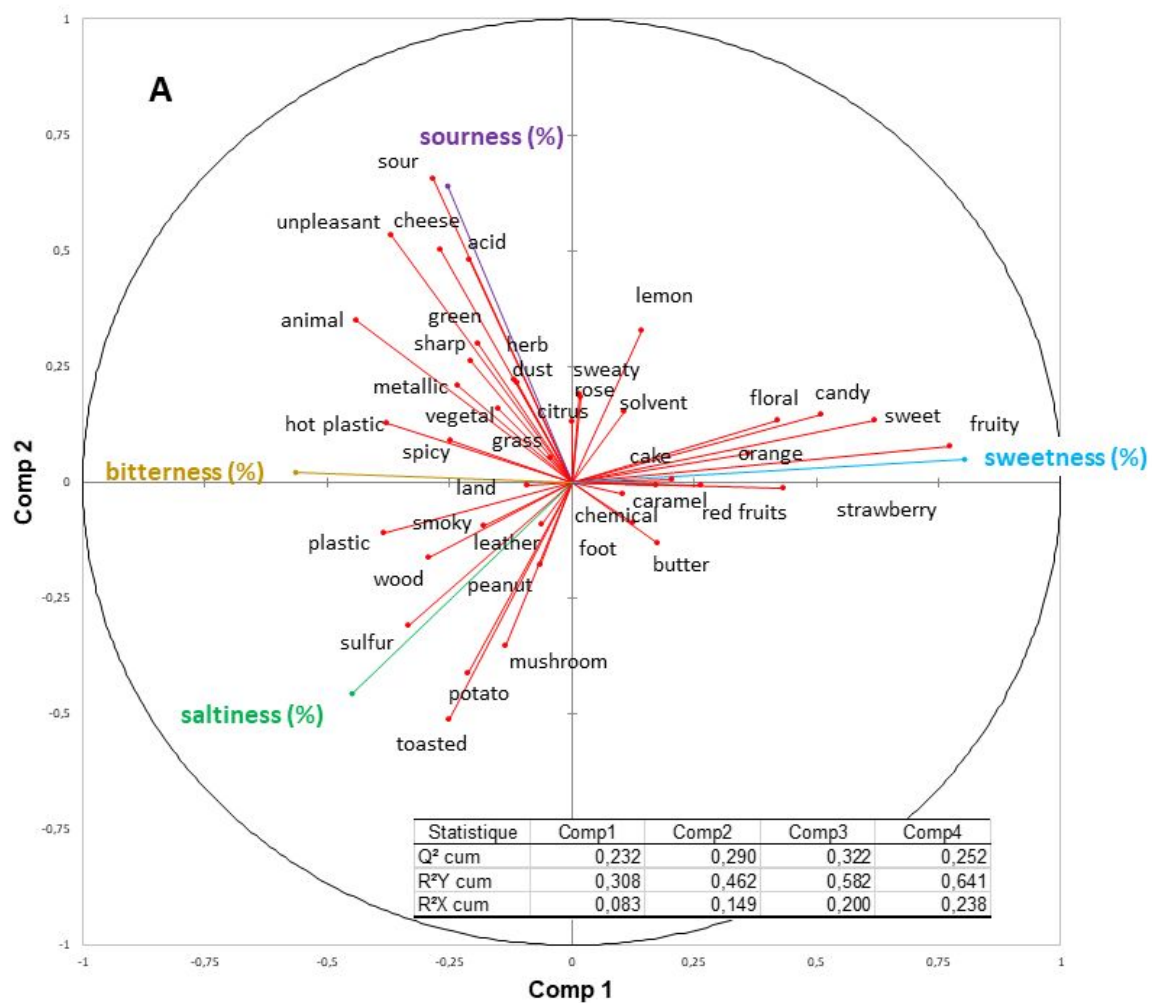
^b: mode of identification, MS: tentatively identified by retention index (RI) compared to data from VCF 16.1 and mass spectrum (MS) verified by comparison with mass spectra database (NIST; INRAMass: CSGA/J. Maratray), St: RI and MS verified with literature data and by injection of pure standard in the 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



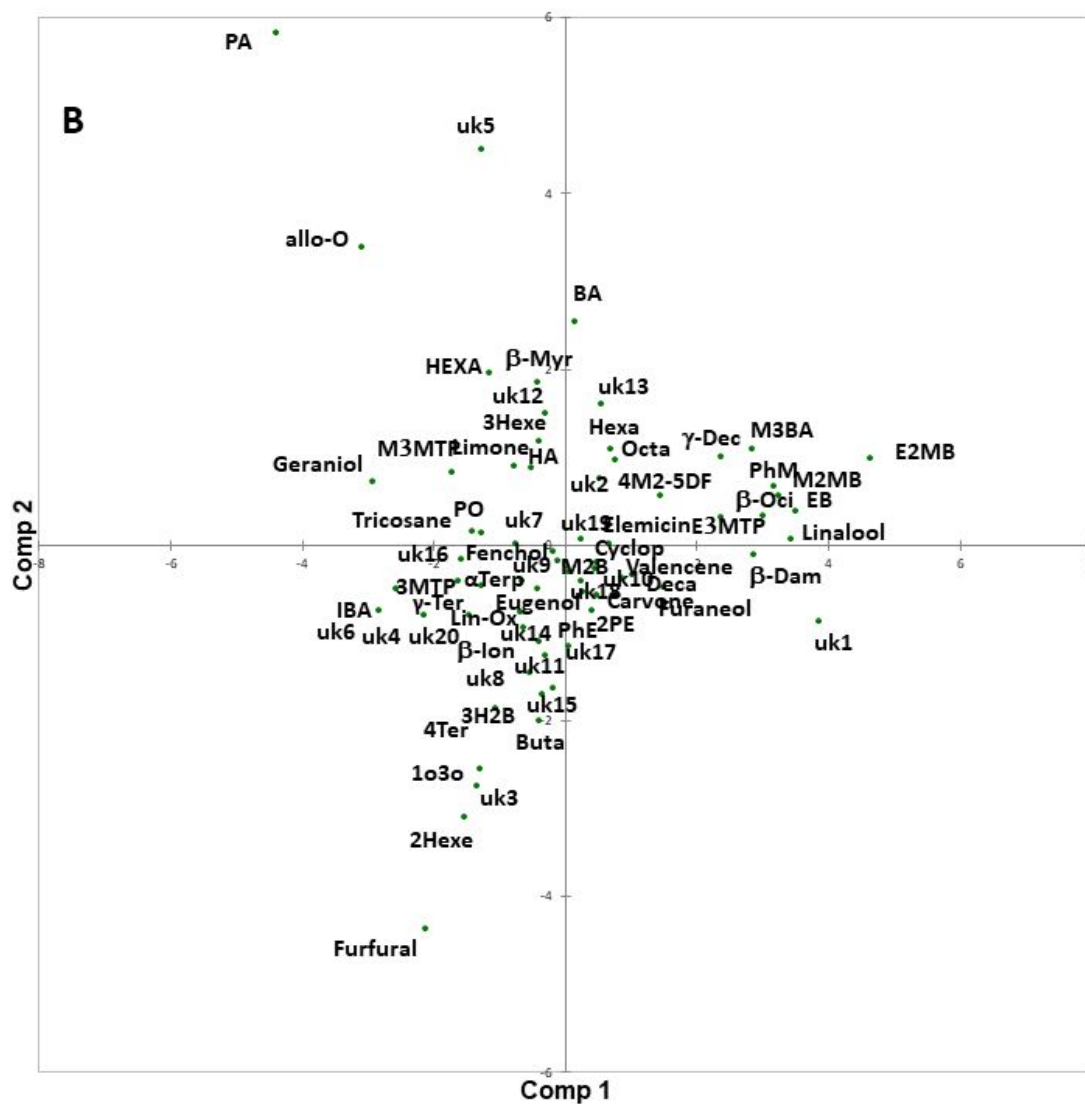


Figure 2

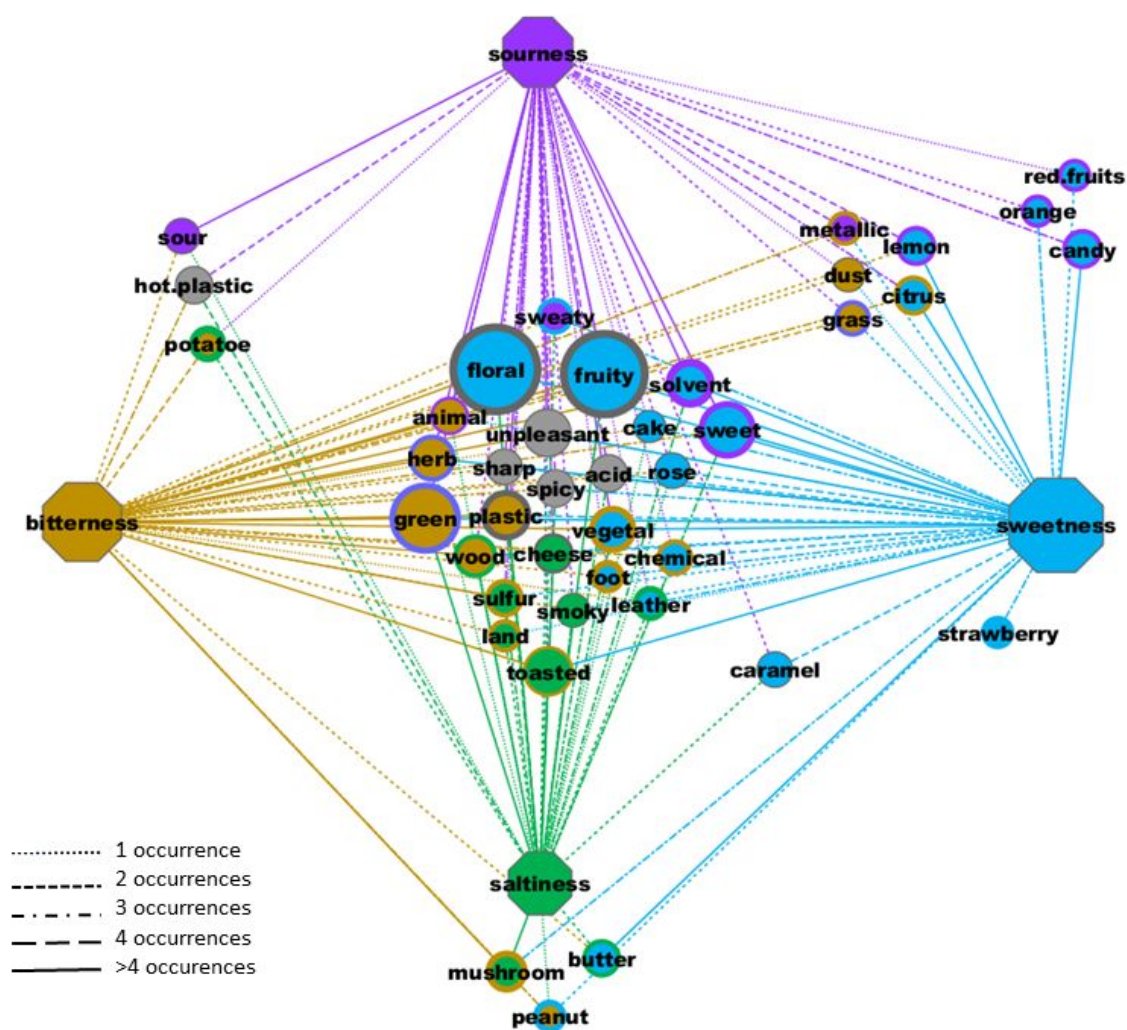
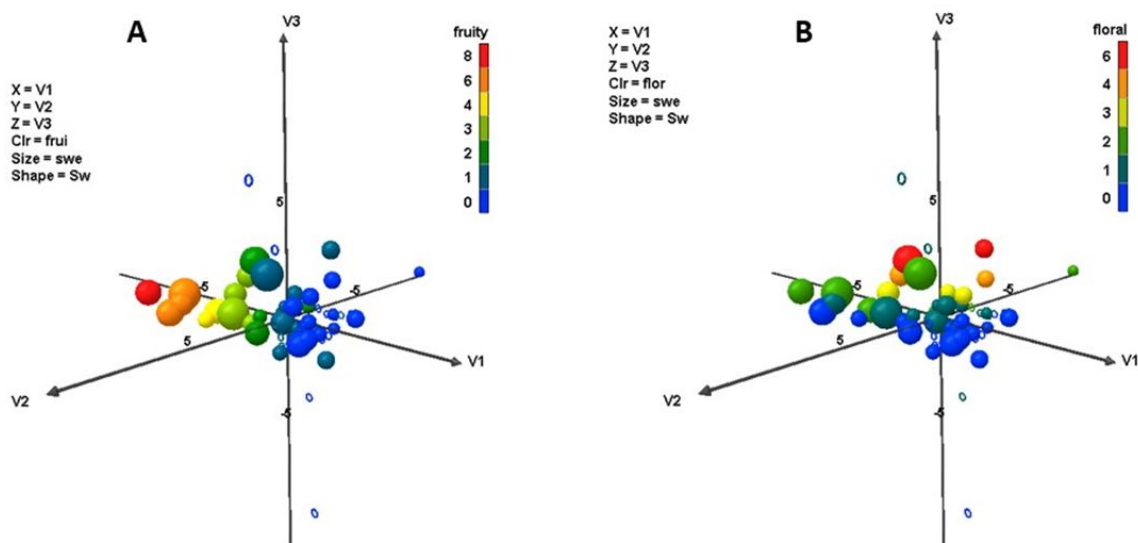


Figure 3



TOC graphic

