

1 Multivariate statistical analysis and odour-taste network to reveal odour-taste associations

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3 Elisabeth Guichard^{1*}, Carmen Barba^{1,2}, Thierry Thomas-Danguin¹ and Anne Tromelin¹

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5 ¹Centre des Sciences du Goût et de l'Alimentation, AgroSup Dijon, CNRS, INRA, Université
6 Bourgogne Franche-Comté, F-21000 Dijon, France;

7 ²Present address: Instituto de Innovación y Sostenibilidad en la Cadena Agroalimentaria (IS-
8 FOOD), Departamento de Tecnología de Alimentos, Universidad Pública de Navarra (UPNa),
9 31006 Pamplona, Spain

10 [*elisabeth.guichard@inra.fr](mailto:elisabeth.guichard@inra.fr), 33-380693277

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12 **ABSTRACT** (100-150 mots)

13 Odour taste association has been successfully applied to enhance taste perception in foods with
14 low sugar or low salt content. Using gas chromatography/olfactometry-associated taste (GC/O-
15 AT), 68 odorant zones have been described with 41 odour descriptors and 4 taste associated
16 descriptors (sweet, salty, bitter, sour). The relationships between odour and taste descriptors
17 were analysed using multivariate analyses. A partial least square analysis allowed to visualise
18 the odours associated with a specific taste, for example fruity, sweet, strawberry, candy, floral
19 and orange with sweetness. A network representation using Cytoscape allowed visualising the
20 links between odour and taste descriptors for example the positive association of butter with
21 both saltiness and sweetness. Multidimensional scalling projection allowed allocating the
22 odorant zones to their odour and taste descriptors. Our approach provided a visualisation tool
23 of the links between odour and taste description and could be used to select odour-active
24 molecules with a potential taste enhancement effect.

25

26 **KEYWORDS** : odour-taste association, multivariate analysis, sweetness, odorant compound

27

28 **INTRODUCTION**

29 Considering the rising rate of pathologies such as diabete, obesity, which are related to
30 unbalanced diets with an excess of consumption of sugar, salt and fat, there is an urgent need
31 to decrease the content of these ingredients in food while maintaining their sensory acceptability
32 by consumers. In the present paper, we will focus on sugar reduction. Concerning sugar, a high
33 consumption of foods rich in free sugar increases the risk of tooth decay. High intake of sugar-
34 sweetened beverages is highly linked with an unhealthy diet, weight gain and increased risk of
35 noncommunicable diseases. The food industry has to integrate these nutritional criteria in the
36 formulation of food products. Different strategies have been used for sugar reduction in foods

37 as reviewed (1, 2). Simple sugars, such as fructose or sucrose, could be replaced by new
38 molecules, which confer a sweet taste to the product without the added calories, such as
39 intensive sweeteners (i.e.: acesulfame k, aspartame, neotame, cyclamate, saccharin, sucralose,
40 thaumatin, steviol, monogroside, brazzein and monatin). However, such molecules with an
41 intense sweetness are used in very small amount resulting in losses of volume and modification
42 of the final texture. Alternatively, a part of simple sugars can be replaced by soluble fibres or
43 carbohydrates, such as polyols (i.e.: sorbitol, mannitol, isomalt maltitol, lactitol, xylitol, and
44 erythritol) or fructo-oligosaccharides (i.e.: nystose, kestose and fructosylkestose), in order to
45 use as bulking agent and restore the texture. These two strategies are often combined because
46 excessive consumption of polyols and fructo-oligosaccharides may cause gastrointestinal
47 symptoms, such as gas or laxative effects, then maximum levels are regularized and also to
48 achieve a more pleasant taste. Other strategies are based on modifications of food texture and
49 structure, which impact on the dynamic of sugar release in the mouth and as a consequence on
50 taste perception (3), but the effect on sweetness perception was dependant on both the nature
51 of the texturing agent and of the taste compound (4). By varying the gel hardness using a
52 mixture of agar and gelatin, it was observed that the fracture properties of the gels affected the
53 surface area of the fragments formed during chewing and thus the rate of sugar release (5), soft
54 gels were perceived sweeter than medium gels, due to the formation of a large number of
55 fragments during chewing, which facilitated the release of sweet molecules and the stimulation
56 of the taste receptors. Moreover, in 20% sugar-reduced gelled products, a heterogeneous
57 distribution a sugar was able to enhance sweetness intensity and thus maintain consumer
58 acceptability (6). By combining these two strategies, it was observed that hard gels were
59 perceived sweeter when sugar distribution was heterogeneous due to a long-lasting in-mouth
60 sucrose concentration, the hard matrix being able to maintain the taste contrast due to different
61 sucrose concentrations, for a longer time in the mouth during chewing (7). The authors

62 concluded that the fracture properties of food can be modulated to enhance sweetness
63 perception, in association with heterogeneous distribution (5). Another innovative strategy is
64 the use of aroma-taste interactions and multimodal integration, based on the fact that an odour
65 may evoke a taste (8, 9) but are not able to activate taste receptors and the metabolisms that
66 entails. This strategy has been used with success to develop low-salt food while maintaining
67 saltiness and consumer acceptability (10), to enhance fat perception in real foods varying in
68 structure-texture properties (11) and to enhance sweet perception in sugar-reduced fruit juices
69 (12). Using such an approach needs an adequate selection of odours. As food odours can evoke
70 a specific taste through mental imagery, it has been possible to select promising odours for
71 saltiness enhancement based on the expectation taste profiles of food products being evoked by
72 their names (13). In different volatile compounds databases, such as Flavor-Base (14) or
73 Volatile Compounds in Foods (15), the word “sweet” is often used as odorant descriptor.
74 Considering this observation that some odours are described with a “smelled taste”, Stevenson
75 et al (16) calculated the correlation between odour sweetness and taste sweetness for 10 odorant
76 molecules and found that the degree to which an odour smelled sweet was a good predictor for
77 taste tasting. This association was also used to select odorants able to enhance sweetness in fruit
78 juices, using gas chromatography/olfactometry-associated taste (GC/O-AT) (12), showing that
79 odorants described with a “smelled sweet taste” were able to enhance the perceived sweetness
80 odour of a fruit juice. Moreover, other odorants not described with a “smelled sweet taste” were
81 also found to be good candidates for sweetness enhancement. In the aim to look for volatile
82 compounds able to enhance some specific taste, we tried to find links between taste descriptors
83 and odour descriptors, starting from the whole set of data previously obtained using gas
84 chromatography/olfactometry-associated taste (GC/O-AT) (12). The aim of the present work
85 was to perform different multivariate analyses to search for the links between odorant
86 descriptors and taste associated descriptors, starting from a total of 68 odorant zones (identified

87 and non-identified), which have been described first with odorant descriptors and second with
88 taste associated descriptors (sweetness, sourness, saltiness, bitterness). These links could then
89 be used for a first selection of molecules susceptible to enhance taste perception.

90

91 **MATERIALS AND METHODS**

92 **Sample preparation**

93 We used the raw data previously obtained after the extraction of volatile compounds from a
94 commercial multi-fruit juice provided by Eckes Granini (France), following the vacuum
95 distillation procedure and dichloromethane extraction described by Barba et al. (17). The extract
96 was then concentrated with a Kuderna-Danish apparatus to a final volume of approximately
97 200 μL and 1 μL (splitless mode for 0.5 min) submitted to gas-chromatography/mass-
98 spectrometry (GC/MS) for compounds identification and to GC/O-AT for odour description
99 (12) using the same column (30m x 0.32 mm i.d. fused silica capillary column coated with a
100 0.5 μm layer of polyethylene glycol, DB-Wax, Agilent, Agilent Technologies, Santa Clara,
101 CA). GC/O-AT was done with 12 panellists used to GC/O experiments. In a first run (first
102 injection of the extract), panellists were asked to indicate the detection of an odour using a
103 buzzer and to give an odorant descriptor. In a second run (second injection of the same extract),
104 panellists were asked to attribute for each odour, one of the four associated taste descriptors:
105 sweet, salty, sour or bitter. Detection times, odour descriptors and taste associated descriptors
106 were recorded using AcquiSniff software (Saint Genès Champanelle, France). The detection
107 frequency (DF) was calculated for both odour descriptors and taste associated descriptors (18).
108 Only the odorant zones with a DF higher than 30% were selected, to limit the false detection
109 risk. For each selected odorant zone, we took into account all the odour descriptors given by
110 the 12 panellists. For taste associated descriptors, we also calculated the DF for each specific
111 taste: sweetness (%), sourness (%), saltiness (%), bitterness (%).

112

113 **Data preparations**

114 From the whole set of data, we selected 68 odorant zones, with the name of the corresponding
115 identified compound if known or mention that this compound is unknown (uki). We identified
116 70 odorant descriptor, of which 7 are present only in the description of one odorant zone and
117 are not retained for the analyse. We validated a list of 63 odorant descriptors and 4 taste
118 associated descriptors. In a second step, odour descriptors only present in 1 or 2 odorant zones
119 were deleted. The multivariate analyses were done with 45 variables, the 41 remaining odorant
120 descriptors and the 4 associated taste descriptors. A co-occurrence matrix was built with, for
121 the 68 odorant zones, the number of occurrences of the 41 odorant descriptors and the DF for
122 the 4 associated tastes. Additionally, we also use a binary version of this matrix: 1 when the
123 odour descriptor or the taste associated descriptors appears in the odour description, 0
124 otherwise.

125

126 **Computational analysis and statistical methods**

127 Multivariate statistical analyses were performed using XLStat (Addinsoft). A Partial Least
128 Square (PLS) analysis was done, on the 68 odorant zones, to explain the taste association
129 descriptors (Y variables: DF for each associated taste) by the odorant descriptors (X block:
130 number of occurrence of the 63 odorant descriptors).

131

132 The multidimensional scaling (MDS) approach allows the visualisation of the similarity
133 between elements of a dataset by disposing them in an N-dimensional space. MDS is one of the
134 methods that allow dimensionality reduction and producing meaningful representations of high-
135 dimensional data into a lower-dimensional space (usually two or three dimensions space).

136 In the present study, we used the Euclidian distance to obtain a similarity matrix between 68
137 odorant zones on the basis of the frequency of 63 odorant descriptors. Then the MDS was
138 achieved on the matrix to derive Euclidian coordinates and distances. We used the coordinates
139 of the first three dimensions to display the odorant zones in a three-dimensional scatterplot. The
140 3D graphical visualisation was obtained using Miner3D (version 7).

141

142 **Network visualisation**

143 We aimed to explore the associations between odour descriptors and taste descriptors using a
144 network of odorant and taste descriptors. For that purpose, we first calculated the co-occurrence
145 matrix of the odorant and taste descriptors using the binary matrix of 68 odorant zones and 67
146 descriptors (63 odorant and 4 associated tastes). The co-occurrence matrix is a square 67x67
147 matrix in which the off-diagonal terms are the number of the odorant-taste pairs in the
148 description of an odorant zone, while the diagonal terms are the number of all occurrences of
149 each odorant and taste descriptors.

150 The calculations of MDS and co-occurrence matrix were conducted using R version 3.0.1 (19).
151 The odorant and taste descriptors were considered to be variables in the context of odorant
152 zones.

153 Cytoscape (20) was used to build a network of the links between odour descriptors and taste
154 associated descriptors. This required the square matrix to be transformed into a twoway data
155 table, which was performed via Statistica (TIBCO Software Inc. 2017).

156

157 **RESULTS AND DISCUSSION**

158 The 68 selected odorant zones with DF odour values higher than 30% are listed in Table 1 with
159 the name of the corresponding volatile compounds, if identified, or the number of the unknown
160 compound. For each odorant zone, all the odour descriptors given by the 12 panellists are listed

161 with the number of occurrence when higher than the unity. We have deleted from the list the
162 descriptor “unknown”, which was given by panellist who was not able to describe the odour.
163 This list of descriptor was used to build the Euclidian matrix. For each odorant zone, 2 values
164 are given for DF, the detection frequency for the odour (DF odour %) which is the percentage
165 of panellists having smelled the odour during the first run of GO/O and the detection frequency
166 for the associated taste descriptor (DF taste %) during the second GC/O-AT run. We then
167 calculated the DF for each of the four taste attributes, sweetness (%), sourness (%), saltiness
168 (%), bitterness (%), these values are used for the statistical analyses. The value is in bold for
169 the main associated taste. A total number of 33 odorant zones are more associated with
170 sweetness (13 with a value higher than 40%), 16 odorant zones are more associated with
171 sourness (5 with a value higher than 40%), 10 odorant zones are more associated with saltiness
172 (3 with a value higher than 40%) and 21 odorant zones are more associated with bitterness (3
173 with a value higher than 40%).

174

175 **Explanation of taste association by odour descriptors using PLS.**

176 The PLS was done on the 68 odorant zones, using the occurrences of each of the 41 odour
177 descriptors as X variables and the DF for each associated taste as Y variables. We verified that
178 the representation of the remaining 41 variables is the same as on the PLS realised with the 63
179 odour descriptors (supplementary files). Figure 1 shows the projection of the variables on the
180 two main components. The 4 associated tastes are well discriminated in the first plan, the
181 sweetness on the positive part of component 1, bitterness on the negative part of component 1,
182 sourness on the positive part of component 2 and saltiness on the negative part of component
183 2. The odour descriptors fruity, sweet, strawberry, candy, floral, orange are positively correlated
184 with component 1 and thus contribute to sweetness perception. The odour descriptors sour,
185 unpleasant, cheese, acid are positively correlated with component 2 and thus contribute to

186 sourness. The odour descriptors hot plastic, plastic, spicy are negatively correlated with
187 component 1 and thus contribute to bitterness. The odour descriptors toasted, potatoe,
188 mushroom, sulphur are negatively correlated with component 2 and thus contribute to saltiness.
189 A model has been built to predict the taste association by a linear combination of the odour
190 descriptors. Table 2 presents the coefficients affected to each odour descriptor to explain one
191 taste descriptor. The odour descriptors are ranked according to the decreasing number of their
192 total occurrences. The odours with the highest impact on sweetness are strawberry, red fruits,
193 sweet, citrus, leather, butter, orange, foot, chemical, candy, fruity, floral and those with the
194 highest negative impact are sour, sulphur, hot plastic, land, plastic, wood, metallic, toasted,
195 potatoe, smoky. The odours with the highest impact on sourness are sour, sweaty, hot plastic,
196 metallic, lemon, land, solvent and those with the highest negative impact are peanut, strawberry,
197 toasted, leather, foot, chemical, butter. The odours with the highest impact on saltiness are
198 sulphur, potatoe, toasted, smoky, land, butter, mushroom and those with the highest negative
199 impact are citrus, animal, peanut, strawberry, dust, metallic, grass, vegetal, unpleasant, plastic,
200 red fruits, foot, sweet, chemical. The odours with the highest impact on bitterness are animal,
201 metallic, peanut, plastic, wood, grass, hot plastic, vegetal, dust and those with the highest
202 negative impact are butter, strawberry, orange, cake, acid, red fruits, leather, lemon.

203 It can be noticed that most of the odours positively associated with sweetness are negatively
204 associated with saltiness, except butter, spicy and leather which are positively associated to
205 both sweetness and saltiness.

206 Looking at the odorant zones (Figure 2), the compounds with a high positive correlation with
207 component 1 are the most associated with sweetness, ethyl2-methylbutanoate (E2MB) is
208 described with fruity, apple, strawberry, candy and sweet odour descriptors (Table 1), methyl-
209 2-methylbutanoate (M2MB) is described with fruity and sweet notes, linalool is described with
210 floral, fruity, sweet and candy notes, (E)- β -ocimene (β -Oci) is described with fruity, floral,

211 strawberry notes, phenylmethanol (PhM) is described with floral, fruity, sweet, candy notes, β -
212 damascenone (β -Dam) is described with fruity, floral and sweet notes, γ -decalactone (γ -Dec) is
213 described with floral, fruity and sweet notes, ethyl butanoate (EB) is described with fruity, floral
214 and sweet notes. The compounds the most associated with sourness (positive correlation with
215 component 2) are pentanoic acid (PA), described as acid, sharp, cheese, unpleasant, allo-
216 ocimene (allo-O), described as green, metallic, sour, hexanal (HEXA) described as green, herb,
217 floral. The compounds the most associated with bitterness (negative correlation with
218 component 1) are tricosane, described as plastic, petrol, isobutylalcohol (IBA), described as
219 plastic, hot plastic, spicy, wood. The compounds the most associated with saltiness (negative
220 correlation with component 2) are furfural, described as potatoe, toasted, sulphur, 2-hexen-1-ol
221 (2Hexe), described as mushroom, toasted, sulphur, 1-octen-3-one (1o3o), described as
222 mushroom and n-butanol (Buta), described as toasted, peanut.

223

224 **Visualisation of the links between odour descriptors and associated tastes**

225 In order to better understand the associations between odour descriptors and tastes, we build a
226 network characterized in terms of nodes and edges or links, following the approach used for
227 odour notes (21). In our case, the nodes are odour and taste descriptors and the edges are the
228 odorant zones. We used a total of 45 descriptors (41 odorant descriptors and 4 taste descriptors).
229 We obtained a list of 2025 pairs of descriptors by stacking the 45x45 co-occurrence matrix.
230 After excluding the diagonal elements and the pairs zero values link, it remained 1098 pairs.
231 We considered only the pairs between odour and taste descriptors, and after removing the
232 entries below the main diagonal (for any X and Y odor notes, the pairs XY and YX are
233 equivalent), the network displayed 143 odour-taste pairs.
234 Figure 3 represents the links between the odour and the tastes descriptors. This representation
235 allows a rapid visualisation of the odour taste associations.

236 Many odour descriptors are linked to all tastes, but some are only linked to one, two or three
237 tastes, as can be seen in Figure 3 by the lines between odour descriptors and tastes. Plain lines
238 are used for more than 4 occurrences, different types of discrete lines are used for 1, 2, 3 or 4
239 occurrences as indicated in the legend. The size of each odour descriptor depends on the number
240 of odorant zones in which they are present. The fill colour of each odour descriptor is that of
241 the main associated taste and the border colour is that of the second associated taste. In case the
242 odour is equally associated with every taste, the colour is grey.

243 One odour descriptor is only linked to one taste, strawberry, which is only linked to sweetness.
244 This explains its high positive value in the regression to sweetness perception.

245 Three odour descriptors are only linked to two tastes, they are orange, candy and red fruits
246 linked mainly to sweetness and then to sourness.

247 The descriptors linked to three tastes can be discriminated by the taste to which they are not
248 linked to. Caramel is not linked to bitterness. Butter, mushroom and peanut are not linked to
249 sourness. Hot plastic, potatoe and sour are not linked to sweetness. Grass, citrus, lemon, metallic
250 and dust are not linked to saltiness.

251 The other odour descriptors are linked to all the tastes. Fruity and floral are the most cited
252 descriptors with respectively 79 and 70 total number of occurrence and present in respectively
253 35 and 37 odorant zones. They are mainly linked to sweetness, then to the three other tastes
254 without any distinction. Cake and rose are mainly associated to sweetness but with only few
255 occurrences. Among the other odour descriptors mainly associated to sweetness, the second
256 associated taste is sourness for sweet and solvent, bitterness for vegetal, chemical and foot and
257 saltiness for leather. Only sweaty is first associated to sourness. Green, plastic, herb, wood and
258 animal are first associated to bitterness, the second associated taste is saltiness for wood,
259 sourness for animal and both sourness and sweetness for green and herb. Toasted, cheese,
260 sulphur, smoky and land are first associated to saltiness and toasted, sulphur and land are also

261 associated to bitterness. Unpleasant, sharp, spicy and acid do not present any specificity towards
262 a specific taste.

263

264 **Allocation of odorant zones according to their odour descriptors and associated taste**

265 A MDS realised on the dissimilarity matrix obtained using the Euclidian distance allowed to
266 determine the level of similarity of odorant zones based on their odour descriptors. The
267 distances and coordinates calculation was performed using the frequency of odour descriptors;
268 nevertheless, the data used for graph depictions involves also ~~the taste descriptors and~~ the DF
269 for each of the four taste descriptors.

270 Figure 4 and 5 present the projection of the MDS 3D space of odorant zones. We decided to
271 focus only on the links between the different taste attributes and two odorant descriptors, fruity
272 and floral which have the greater total number of occurrences. The shape of the plots depends
273 on the associated taste, sphere for sweetness (4A, 4B), cone for sourness (4C, 4D), diamond for
274 saltiness (5A, 5B) and star for bitterness (5C, 5D), their size depends on the percentage of taste
275 DF. The fruity odours are represented by a colour gradient depending on their occurrence in the
276 odorant zone (4A, 4C, 5A, 5D). They are more perceived in the odorant zones present on the
277 negative part of axis 1. The floral odours are represented by a colour gradient depending on
278 their occurrence in the odorant zone (4B, 4D, 5B, 5D), they are more perceived in the odorant
279 zones present on the positive part of axis 3 and negative part of axis 2. The odorant zones with
280 a high DF for sweetness (4A, 4B) are mainly located on negative part of V1, due to a greater
281 number of occurrence for fruity and some on the positive part of axis 2, due to the presence of
282 floral odours, but some are in the middle of the space due to links between sweetness and other
283 odour descriptors as was highlighted by Cytoscape Network. The odorant zones with a high DF
284 for sourness (4C, 4D) are located on the negative part of axis 3 and positive part of axis 1. They
285 have low occurrences for both fruity and floral. However, some odorant zones perceived as

286 fruity or floral are also associated to sourness. On Figure 5, it can be noticed that the odorant
287 zones with a high DF for saltiness and bitterness have low occurrence of fruity and floral odours.
288

289 **DISCUSSION AND CONCLUSION**

290 The different tools involved in this study allowed finding links between odour descriptors and
291 taste descriptors. As the data used in this study are from an extraction of volatile compounds
292 from a fruit juice, the odour descriptors cover a specific domain. However, we were able to find
293 links with not only sweetness and sourness, which are the main taste descriptors in fruit juices,
294 but also with saltiness and bitterness.

295 A lot of the literature on odour-taste interactions relies on sweetness perception. A review by
296 Valentin et al (22) presents the different studies reporting an effect of odour on sweet
297 perception. The most studied aroma is strawberry which has been reported to enhance sweetness
298 perception for example in model systems (23, 24), in whip cream (25) and in fruit juice (12).
299 Our results show that the strawberry descriptor is only associated with sweetness and has a high
300 positive value in the regression to sweetness perception. This can be explained by associative
301 learning (16), due to simultaneous exposition of strawberry odour and sweet taste in a great
302 variety of food products such as jams, jellies, marmalades, yogurts, ice creams or candies. Other
303 odour descriptors are mainly associated with sweetness, such as caramel, which was already
304 found to increase sweetness perception in model solutions (16) or ciders (26). Fruit odours,
305 such as orange, redfruits and lemon are potential candidates for sweetness enhancement. They
306 have a high positive value in the regression to sweetness perception and a negative value for
307 saltiness and bitterness. A sweetness enhancement has been observed for orange and raspberry
308 (27). The odour descriptor sweet is, as expected, associated with sweetness but also with
309 sourness, which can be explained by the fact that fruit products are often perceived sweet and
310 sour.

311 Concerning lemon odour, Schifferstein and Verlegh (24) observed that the sweetness enhancing
312 effect was lower than with strawberry odour. Our results show that lemon odour was mainly
313 associated with sweetness but also with sourness. In water solution, a significant enhancement
314 of both sweetness and sourness was observed by addition of lemon flavour (28), whereas in
315 acidic solutions, other authors did not find any effect of the addition of lemon odour on
316 sourness perception (29). These different results are in agreement with other observations, that
317 the effect of odour on sweetness/saltiness enhancement is higher at low to medium intensities
318 of the tastes (26, 30, 31). It can be noticed that even if lemon and citrus are both associated with
319 sweetness, with a positive contribution in the regression, lemon is secondly associated with
320 sourness with a higher contribution to sourness and a negative contribution to bitterness in the
321 regression, whereas citrus is secondly associated with bitterness, with a positive contribution to
322 bitterness in the regression. These results can be explained by the fact that lemon extract are
323 perceived as sour and sweet (32) and that some citrus fruit drinks such as grapefruit are
324 perceived sweet and bitter (33).

325 Only few odours have been mainly associated with sourness. As expected, the odour descriptor
326 sour is mainly associated with sourness, but not with sweetness. Metallic is also associated with
327 bitterness and sweaty also associated with sweetness. There is no information in the literature
328 on the effect of addition of such odours on sourness perception.

329 Even if the odorant zones were isolated from a fruit extract, which cannot be associated with
330 saltiness itself, some odorant zones were described with odour descriptors mainly associated
331 with saltiness, such as toasted, smoky, sulphur, cheese, potatoe, butter, leather and mushroom.
332 This association was already mentioned for similar odours such as bacon, cheese or peanuts
333 and were able to enhance saltiness intensity in water solution by orthonasal and retronasal
334 perception (13). Another study on odour induced saltiness enhancement showed that at least
335 15% salt reduction can be compensated by addition of either beef or chicken bouillon aroma

336 and that the odour descriptors mainly contributing to this enhancement were brothy, meaty and
337 roasted (34). Soysauce odour was also able to induce salty taste in water solution with a very
338 amount of sodium chloride, below the detection threshold (35). These observation confirm that
339 the odour descriptors found in this study associated with saltiness could have an impact on
340 saltiness enhancement.

341 The positive association for butter with both sweetness and saltiness can be explained by the
342 consumption of both fat-sweet and fat-salty foods and for spicy by the consumption of both
343 spicy-sweet and spicy-salty foods. In fact, the addition of butter aroma was found to enhance
344 fat perception in model cheeses with an additional small effect on saltiness enhancement (31).

345 The links we observed between some odours (green, grass, vegetal) and bitterness have already
346 been used to increase bitterness perception in a model olive oil by addition of cis-3-hexenol, a
347 cut grass odorant compound (36). Considering our results, other odour descriptors could be
348 good candidates for bitterness enhancement, such as plastic, wood, herb and animal. In the case
349 of bitterness reduction in food products, such odours have to be discarded from the product.
350 However the impact of odours on bitterness has not been the subject of many studies. In the
351 aim to reduce bitterness in foods, our network representation can allow to select odours which
352 have no link or only few links with bitterness and then test the effect of the corresponding
353 odorant compounds.

354 A focus was done on the present paper on two odour descriptors with the greatest number of
355 occurrence in our odorant zones, due to the nature of the extract, from a multifruit juice. These
356 two odours are mainly associated with sweetness on the network representation and then to the
357 three other tastes. However the MDS projection allowed to differentiate the links between these
358 two odours and the taste descriptors. Sweetness perception can be linked either with fruity or
359 with floral. Both odours are negatively correlated with saltiness and bitterness, which means

360 that an addition of molecules perceived fruity and/or floral could decrease saltiness and/or
361 bitterness.

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

372

373 In the present manuscript the descriptors have been generated from a multifruit juice extract, a
374 generalisation of the approach to other extracts could increase the number of odour descriptors
375 and their links with taste descriptors. The proposed approach is simple to handle and could be
376 a good way for the selection of odorant molecules with an impact on taste perception. The links
377 formalised between odour and taste descriptors could then be used to predict a potential odour-
378 induced taste enhancement in model system or real foods or even an eventual masking effect.

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383 **REFERENCES.**

384 1. Di Monaco, R.; Miele, N. A.; Cabisidan, E. K.; Cavella, S., Strategies to reduce sugars in food.
385 *Current Opinion in Food Science* **2018**, *19*, 92-97.

- 386 2. Stieger, M.; van de Velde, F., Microstructure, texture and oral processing: New ways to reduce
387 sugar and salt in foods. *Current Opinion in Colloid & Interface Science* **2013**, *18*, 334-348.
- 388 3. Pangborn, R. M.; Trabue, I. M.; Szczesniak, A. S., Effect of hydrocolloids on oral viscosity and
389 basic taste intensities. *Journal of Texture Studies* **1973**, *4*, 224-241.
- 390 4. Tournier, C.; Sulmont-Rossé, C.; Guichard, E., Flavour perception: aroma, taste and texture
391 interactions. In *Food, Books*, G. S., Ed. Global Science Books Ltd.: England (Great Britain), 2007; Vol. 1,
392 pp 246-257.
- 393 5. Mosca, A. C.; de Velde, F. V.; Bult, J. H. F.; van Boekel, M.; Stieger, M., Taste enhancement in
394 food gels: Effect of fracture properties on oral breakdown, bolus formation and sweetness intensity.
395 *Food Hydrocolloids* **2015**, *43*, 794-802.
- 396 6. Mosca, A. C.; Bult, J. H. F.; Stieger, M., Effect of spatial distribution of tastants on taste intensity,
397 fluctuation of taste intensity and consumer preference of (semi-)solid food products. *Food. Qual.*
398 *Prefer.* **2013**, *28*, 182-187.
- 399 7. Mosca, A. C.; van de Velde, F.; Bult, J. H. F.; van Boekel, M.; Stieger, M., Effect of gel texture
400 and sucrose spatial distribution on sweetness perception. *Lwt-Food Science and Technology* **2012**, *46*,
401 183-188.
- 402 8. Small, D. M.; Prescott, J., Odor/taste integration and the perception of flavor. *Exp. Brain Res.*
403 **2005**, *166*, 345-357.
- 404 9. Thomas-Danguin, T.; Sinding, C.; Tournier, C.; Saint-Eve, A., Multimodal interactions. In *Flavor:*
405 *From Food to Behaviors, Wellbeing and Health (460 p.)*, Etiévant, P.; Guichard, E.; Salles, C.; Voilley, A.,
406 Eds. Elsevier Ltd.: Cambridge (England), 2016; Vol. WPF 299, pp 121-141.
- 407 10. Thomas-Danguin, T.; Lawrence, G.; Emorine, M.; Nasri, N.; Boisard, L.; Guichard, E.; Salles, C.,
408 Strategies to enhance saltiness in food involving cross modal interactions. In *The Chemical Sensory*
409 *Informatics of Food: Measurement, Analysis, Integration*, Guthrie, B.; Beauchamp, J.; Buettner, A.;
410 Lavine, B. K., Eds. ACS Division of Agricultural Food and Chemistry, Inc.: Washington, DC (United
411 States), 2015; pp 27-40.
- 412 11. Syarifuddin, A.; Septier, C.; Salles, C.; Thomas-Danguin, T., Reducing salt and fat while
413 maintaining taste: An approach on a model food system. *Food Quality and Preference* **2016**, *48*, 59-69.
- 414 12. Barba, C.; Béno, N.; Guichard, E.; Thomas-Danguin, T., Selecting odorant compounds to
415 enhance sweet flavor perception by gas chromatography/olfactometry-associated taste (GC/O-AT).
416 *Food Chemistry* **2018**, *257*, 172-181.
- 417 13. Lawrence, G.; Salles, C.; Septier, C.; Busch, J.; Thomas-Danguin, T., Odour-taste interactions: A
418 way to enhance saltiness in low-salt content solutions. *Food Quality and Preference* **2009**, *20*, 241-248.
- 419 14. Flavor-Base, Flavor-Base. In 9th edition ed.; Associate, L., Ed. 2013.
- 420 15. Nijssen, L. M.; Ingen-Visscher, C. A.; van Donders, J. J. H., Volatile compounds in food: database
421 - Version 16.2. In Triskelion, T., Ed. Zeist (The Netherlands), 2016.
- 422 16. Stevenson, R. J.; Prescott, J.; Boakes, R. A., Confusing tastes and smells : how odours can
423 influence the perception of sweet and sour tastes. *Chemical Senses* **1999**, *24*, 627-635.
- 424 17. Barba, C.; Thomas-Danguin, T.; Guichard, E., Comparison of stir bar sorptive extraction in the
425 liquid and vapour phases, solvent-assisted flavor evaporation and headspace solid-phase
426 microextraction for the (non)-targeted analysis of volatiles in fruit juice. *Lwt-Food Science and*
427 *Technology* **2017**, *85*, 334-344.
- 428 18. Pollien, P.; Ott, A.; Montigon, F.; Baumgartner, M.; Muñoz-Box, R.; Chaintreau, A., Hyphenated
429 headspace-gas chromatography-sniffing technique: screening of impact odorants and quantitative
430 aromagram comparisons. *J. Agric. Food Chem.* **1997**, *45*, 2630-2637.
- 431 19. Team, R. C., R 3.0.1: R: A language and environment for statistical computing In R Foundation
432 for Statistical Computing: Vienna, Austria, 2013.
- 433 20. Shannon, P.; Markiel, A.; Ozier, O.; Baliga, N. S.; Wang, J. T.; Ramage, D.; Amin, N.; Schwikowski,
434 B.; Ideker, T., Cytoscape: A software environment for integrated models of biomolecular interaction
435 networks. *Genome Research* **2003**, *13*, 2498-2504.

- 436 21. Tromelin, A.; Chabanet, C.; Audouze, K.; Koensgen, F.; Guichard, E., Multivariate statistical
437 analysis of a large odorants database aimed at revealing similarities and links between odorants and
438 odors. *Flavour and Fragrance Journal* **2018**, *33*, 106-126.
- 439 22. Valentin, D.; Chrea, C.; Nguyen, D. H., Taste-odour interactions in sweet taste perception. In
440 *Optimising sweet taste in foods*, Spillane, W., Ed. Woodhead Publishing Limited: Cambridge, 2006; pp
441 66-84.
- 442 23. Frank, R. A.; Vanderklaauw, N. J.; Schifferstein, H. N. J., Both perceptual and conceptual factors
443 influence taste-odor and taste-taste interactions. *Perception & Psychophysics* **1993**, *54*, 343-354.
- 444 24. Schifferstein, H. N. J.; Verlegh, P. W. J., The role of congruency and pleasantness in odor-
445 induced taste enhancement. *Acta Psychologica* **1996**, *94*, 87-105.
- 446 25. Frank, R. A.; Byram, J., Taste-smell interactions are tastant and odorant dependent. *Chemical*
447 *Senses* **1988**, *13*, 445-455.
- 448 26. Symoneaux, R.; Guichard, H.; Le Quere, J. M.; Baron, A.; Chollet, S., Could cider aroma modify
449 cider mouthfeel properties? *Food Quality and Preference* **2015**, *45*, 11-17.
- 450 27. Valentin, D.; Chrea, C.; Hoang Nguyen, D., Taste-odour interaction in sweet taste perception.
451 In *Optimising sweet taste in foods*, Spillane, W. J., Ed. Woodhead Publishing Limited: Cambridge
452 (England), 2006; pp 66-84.
- 453 28. Le Calvé, B.; Goichon, H.; Cayeux, I., CO₂ perception and its influence on flavour. In *EXpression*
454 *of multidisciplinary flavour science*, Blank, I.; Wüst, M.; Yeretian, C., Eds. Institut für chemie und
455 biologische chemie: Wissenschaften, Switzerland, 2010; pp 55-58.
- 456 29. Cayeux, I.; Mercier, C., *Sensory evaluation of interaction between smell and taste - Application*
457 *to sourness*. 2003; p 287-292.
- 458 30. Lethuaut, L.; Brossard, C.; Meynier, A.; Rousseau, F.; Llamas, G.; Bousseau, B.; Genot, C.,
459 Sweetness and aroma perceptions in dairy desserts varying in sucrose and aroma levels and in textural
460 agent. *International Dairy Journal* **2005**, *15*, 485-493.
- 461 31. Syarifuddin, A.; Septier, C.; Salles, C.; Thomas-Danguin, T., Reducing salt and fat while
462 maintaining taste: An approach on a model food system. *Food Quality and Preference* **2016**, *48*, 59-69.
- 463 32. Veldhuizen, M. G.; Siddique, A.; Rosenthal, S.; Marks, L. E., Interactions of Lemon, Sucrose and
464 Citric Acid in Enhancing Citrus, Sweet and Sour Flavors. *Chemical Senses* **2018**, *43*, 17-26.
- 465 33. Obenland, D.; Campisi-Pinto, S.; Arpaia, M. L., Determinants of sensory acceptability in
466 grapefruit. *Scientia Horticulturae* **2018**, *231*, 151-157.
- 467 34. Batenburg, M.; van der Velden, R., Saltiness Enhancement by Savory Aroma Compounds.
468 *Journal of Food Science* **2011**, *76*, S280-S288.
- 469 35. Chokumnoyporn, N.; Sriwattana, S.; Phimolsiripol, Y.; Torrico, D. D.; Prinyawiwatkul, W., Soy
470 sauce odour induces and enhances saltiness perception. *International Journal of Food Science and*
471 *Technology* **2015**, *50*, 2215-2221.
- 472 36. Caporale, G.; Policastro, S.; Monteleone, E., Bitterness enhancement induced by cut grass
473 odorant (cis-3-hexen-1-ol) in a model olive oil. *Food Quality and Preference* **2004**, *15*, 219-227.

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477 **Table 1:** Odorant zones detected by GC/O and GC/O-AT, with the list of odour descriptors,
478 the detection frequency for odorants and for each associated taste. ^a: mode of identification,
479 MS: comparison with mass spectra database and retention index, St: mass spectra and
480 retention index verified with standard injected in the same condition, refer to Barba et al., (12,
481 17), n.d. means not detected.

482

483 **Table 2:** PLS regression to explain the taste descriptors by odour descriptors: for each odour
484 descriptor the number of total occurrences and the number of odorants zones in which it has
485 been described are given with the regression coefficients for each associated taste.

486

487 **Figure 1:** PLS regression with 45 variables and 68 individuals, projection of the 4 taste
488 descriptors (Y variables) and the 41 odour descriptors (X variables) on components 1 and 2.

489 **Figure 2:** PLS regression with 45 variables and 68 individuals, projection of the 68 odorant
490 zones (individuals) on components 1-2.

491 **Figure 3:** Network representation of the links between odour descriptors (circle) and taste
492 associated descriptors (octagon). The nature of the line varies as a function of the number of
493 occurrences. The size of each odour descriptor depends on the number of odorant zones in
494 which it is present. The file colour of the odour descriptors varies as a function of the number
495 of occurrences with each taste: blue if the odour is mainly associated with sweetness, green
496 for saltiness, violet for sourness, light brown for bitterness. The border colour is that of the
497 second associated taste, it is grey if the odour is equally associated to the three other tastes
498 and dark blue if the second associated taste is equally sourness and sweetness.

499 **Figure 4:** Allocation of odorant zones according to their odour descriptors and associated
500 taste: MDS representation in a 3D space. The colour represents the occurrence of fruity (A, C)
501 floral (B, D), the shape of the plots represents the associated taste (sphere for sweetness, cone
502 for sourness and the size depends on the percentage of taste detection frequency in the odorant
503 zone.

504 **Figure 5:** Allocation of odorant zones according to their odour descriptors and associated
505 taste: MDS representation in a 3D space. The colour represents the occurrence of fruity (A, C)
506 floral (B, D), the shape of the plots represents the associated taste (diamond for saltiness, star
507 for bitterness and the size depends on the percentage of taste detection frequency in the
508 odorant zone.

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510 **Supplementary Figure 1:** PLS regression with 67 variables and 68 individuals, projection of
511 the 4 taste descriptors (Y variables) and the 63 odour descriptors (X variables) on components
512 1 and 2.

513 **Supplementary Figure 2:** PLS regression with 67 variables and 68 individuals, projection of
514 the 68 odorant zones (individuals) on components 1-2.

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