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1 How the experimental design associated with 2 objectivized sensory analysis can be used to 3 predict odor quality of gaseous mixtures?

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13 **Abstract**

14 From environmental nuisances to perfumes and aromas, the need to understand odorous
15 interactions is growing. In this context, sensory analysis is often used but faces an obstacle
16 when dealing with odor mixtures. Indeed, sensory approaches provide data on the global
17 nature and intensity of these mixtures, but these methods cannot reveal the various
18 interactions taking place when perceiving an odor. To address this issue, modeling the
19 variations in odor nature and intensity according to the composition of complex mixtures
20 offers insight into sensory interactions as well as a tool to predict odor nature and intensity.
21 While several models have been developed for odor intensity, models for odor nature are
22 scarce. In this study, an experimental mixture design is combined with sensory analysis with
23 the aim of developing new numerical models that transform chemical data into sensory data.
24 Mixtures of four odorants, dimethyl disulfide (DMDS), toluene, furfuryl mercaptan, and
25 cyclopentanone are composed of multiple values of the Odor Activity Value (OAV) for each
26 odorant. The odor nature of each mixture is described using Langage des Nez[®] (LdN), an
27 objectivized odor nature description method. The variation in odor nature with the
28 composition of the mixture is modeled using the experimental mixture design. The yielded
29 models are shown to be valid and of relatively good descriptive (adjusted R^2) between 0.610-
30 0.925) and predictive (predictive R^2 between 0.390-0.886) qualities. The models provide

31 insight into the individual contributions and binary and ternary interactions among the
32 odorants impacting the global odor nature. Moreover, the models allow the odor nature of a
33 mixture to be predicted by transforming the chemical concentration of each odorant into an
34 odor nature description. These results may be an answer to the question raised by the odor
35 mixture effect.

36 **Keywords:** odor nature, experimental mixture design, odor quality, odor modeling, Langage
37 des Nez[®]

38 **1 Introduction**

39 Odor perception is the result of cascading events beginning with the interaction of complex
40 mixtures of gaseous compounds (or odorants) with the olfactory mucosa and leading to the
41 interpretation of the induced neurological signal by the brain. The intensity and nature of the
42 perceived odors from these complex mixtures are affected by the sensory interactions between
43 the individual components of the mixture [1,2]. Understanding these interactions remains an
44 active research domain.

45 From perfumes to food flavors to annoying environmental odorants, odors affect several
46 aspects of everyday life. Odor releases are usually studied by combining instrumental
47 approaches and/or using sensory analysis which relies on a human panel to smell and analyze
48 perception [3–5]. Instrumental analysis has limitations regarding perception contribution and
49 sensitivity [6,7]. Indeed, the relevance of the sensory approach lies in the capacity of the panel
50 to detect odors at significantly low concentrations, sometimes exceeding physio-chemical
51 analysis thresholds, but also globally taking into account quantitative e.g. intensity (the
52 strength of the odor) and qualitative e.g. odor nature (what does the odor smell like)
53 synergies among odorants [8].

54 If sensory approaches are used to analyze the overall nature and intensity of mixtures, they do
55 not directly facilitate an understanding of the various interactions occurring, such as masking,
56 synergism, or total independent effects. Mixture effects may affect sensory results and make
57 the reading of the results from diverse fields of applications more complex. The same
58 question is raised in domains such as wines [9,10] or perfumes and fragrances [11], to
59 understand the contributions of odorants and the impact of their interactions on the final
60 organoleptic properties of the product. This issue is all the more crucial in the field of
61 environmental nuisances. Odor sources may be geographically adjacent; thus, their odorous

62 emissions are mixed in the atmosphere. Mixture effects such as masking and synergetic
63 effects may cover or intensify certain odor notes affecting the sensory analysis results [12]. In
64 the same way, mixture effects may affect the identification of odorants in the context of
65 indoor air studies [13]. Hence, understanding the effect of mixtures on overall quality and
66 quantity is a requirement to move forward in odor source combination interpretation and
67 environmental odor prediction or modeling.

68 For decades, psychophysicists have studied hundreds of mixtures, mostly binary mixtures
69 focusing on intensity. Ferreira revisited published papers, from 1964 to 2009, and came out
70 with a conclusion on sensory interactions in mixtures [1,2]: the highest individual intensity
71 dominates the global intensity of the mixture. If the odorants are mixed at the same individual
72 intensity (iso-intense mixtures), the intensity of the mixture will be just slightly higher (19%
73 on average) than the individual intensity of the constituents. When more compounds are
74 added to the mixture, the overall intensity remains nearly constant [2]. Moreover, studies
75 predicting the intensity of mixtures based on the chemical concentrations of the constituents
76 have advanced in the last decade; offering approaches that yield predicted values of odor
77 intensity that are coherent with odor intensity determined by sensory approaches [14]. Several
78 mathematical approaches have been developed and tested by human assessors and electronic
79 noses in different research centers like the sum of odor intensities [14,15], the vector model
80 which considers the odor intensity as vectors [16,17], and other models adapted for electronic
81 noses application [18,19].

82 However, concerning the effect of a mixture on the odor nature, the interactions are not fully
83 understood. Indeed, for binary mixtures, there is a global consensus: the odor nature of the
84 most intense constituent dominates [1]. For more complex mixtures, disagreements due to
85 proposed protocols are noted. In fact, studies have focused more on identifying odorants in a
86 mixture instead of describing the global perceived odor nature [1]. Moreover, past studies
87 have shown that, as humans, we are limited to identifying the odor of 3-4 components in a
88 complex mixture [20]. Hence, the contribution of odorants to the global odor nature of
89 complex mixtures remains unclear.

90 In addition to a lack of understanding, most studies are based on protocols using mixtures
91 presented to assessors in a solution form: odorants are generally dissolved in a liquid. Under
92 these conditions, it is obvious that the results are not representative of the equivalent mixtures
93 perceived at the gaseous state. The diffusion mechanisms and interactions of constituents may

94 be different and may influence the perceived odors [21]. In the application framework of
95 home fragrances, indoor air quality, or atmospheric odorous nuisances, studying mixtures in
96 the gaseous state is required. However, it is a challenge: sample preparation is highly
97 complicated implying the generation of individual vaporized constituents, mixing gases at
98 accurate and low quantities, and maintaining gaseous state stability in delivery systems
99 without losses. Hence, if sampling bags (such as Tedlar or Nalophan bags[®]) are generally
100 used, odorants may react with or adsorb to surfaces [22].

101 Therefore, modeling sensory interactions between odorants in the gaseous state is an essential
102 research topic. Several numerical models have been proposed to predict the odor intensities of
103 binary and complex mixtures [11,23–25]. However, few models have been developed for the
104 odor nature of mixtures. The most well-known is a model proposed by Olsson in 1998
105 [26,27]. Olsson considered the intensities of single substances as vectors, summed them
106 (vector summation model), and predicted the odor nature based on the resultant vector. The
107 model, even if it showed good accuracy, the models proposed by Olsson were limited to
108 binary mixtures and could predict the probability of perceiving one or both odorant(s), which
109 may not totally describe the odor nature of a mixture. Besides, the models are based on vector
110 model which does not take into consideration any form of “hyper additivity” interaction that
111 affects the odor intensity of odorants [16]. Hence, any form of synergism may not be
112 predicted.

113 Moreover, the experimental mixture design offers a method to study the effect of each
114 constituent and their interactions, with a limited number of experiments. The method has
115 already been applied in malt mixtures [28], ceramics [29,30], pharmaceuticals [31], extraction
116 by solvents [32], etc. However, there have been no previous attempts to combine the
117 experimental mixture design with sensory analysis and odor mixture studies.

118 Regrettably, Olsson’s model described only binary mixtures. It would be interesting to study
119 mixtures of four or more constituents [33]. In contrast, the experimental mixture design
120 permits to study more complex mixtures with a relatively lesser number of experiments.

121 Therefore, in this paper, we combined the experimental mixture design with sensory analysis
122 to study the effect of a mixture of four odorants at two different intensities. Sample
123 preparation was optimized to study mixtures of odorants in the gaseous state. The aims are (i)
124 to model the variation of the odor nature with the mixture composition, (ii) to use the obtained
125 models to understand the contribution of the odorants to the odor nature and their different

126 interactions, and (iii) to validate the capacity of these models to predict the odor nature of a
127 mixture. The purpose of this paper is also to highlight the use of the experimental mixture
128 design as a promising tool for studying odor mixtures. We have chosen to base this first study
129 on compounds whose odorous notes are frequently found in the environment of industrial
130 areas.

131 **2 Materials and Methods**

132 Experimental mixture design investigates the influence of the proportion of constituents in a
133 mixture on the manifestation of a response. Hence, it allows understanding and modeling of
134 the variation of a specific phenomenon with the variation of the mixture composition.

135 In our case, we wanted to model the variation of the odor nature with the variation of the
136 composition of gaseous odorant mixtures. For that, the experimental design was adapted for
137 four chosen constituents: DMDS, toluene, furfuryl mercaptan, and cyclopentanone. Binary,
138 tertiary, and quaternary mixtures of these components were considered. These odorants were
139 selected according to three crucial criteria (i) their distinctive odor nature, (ii) the occurrence
140 of their odor nature in the environment [34], and (iii) the feasibility of generating accurate and
141 stable gas mixtures.

142 **2.1 Experimental mixture design**

143 **2.1.1 Mixture domain and design**

144 One of the most frequent designs is what is called a simplex-centroid design [30]. Hence, our
145 experimental domain has 3 dimensions ($q-1$ dimensions with q the number of constituents)
146 and can be represented as a regular tetrahedron, whose faces are composed of ternary plots
147 (Figure 1). The experimental design includes 15 experimental points that correspond to 15
148 mixtures with distinct compositions: four pure constituents (the vertexes; mixtures labeled 1
149 to 4), six binary mixtures (mid-edge points; mixtures from 5 to 10), four ternary mixtures
150 (face centroids; mixtures from 11 to 14) and one quaternary mixture (the center of the
151 tetrahedron, mixture 15). It also includes four test points corresponding to quaternary
152 mixtures of different compositions: their role is clarified in the following section (part 2.4).

153 **To ensure the reliability of the result, the gaseous mixture composition was established**
154 **in such a way that all compositions of the pure mixtures** (the vertexes; mixtures labeled 1
155 **to 4) are equivalent in terms of odor activity value (OAV) with no consideration for the**
156 **effective gaseous concentrations.** Thereby, the isointense complex mixture issue may be

157 studied. OAV is defined as the ratio of the chemical concentration to the odor perception
158 threshold (OPT) [35]. This approach permits us to eliminate the diverse odorization capacities
159 of each chosen odorant but implies determining the specific olfactory thresholds. The odor
160 perception threshold from the literature was shown to be inaccurate [35,36]. The differences
161 between OPTs from various references can achieve several orders of magnitude. For this
162 reason, our experiments were based on OPTs relative to the panel in charge of the sensory
163 analysis. The method, whereby the experimental olfactory thresholds were established, is
164 described in the following section (part 2.3.2). Thus, the composition of a given mixture j is
165 determined following Equation 1:

166 Equation 1: $\sum_{i=1}^n X_{ij} = \sum_{i=1}^n \frac{OAV_{ij}}{\sum_1^i OAV_{ij}} = 1$;

167 X_{ij} represents the contribution to the overall odor activity of each component i in mixture j
168 (relative OAV), and $OAV_{i,j}$ is the odor activity value of compound i in mixture j .

169 The gaseous concentrations of the mixtures were determined following Equation 2:

170 Equation 2 : $C_{i,j} = OAV_{i,j} \times OPT_{E,i}$

171 $C_{i,j}$ is the gaseous concentration of constituent i in mixture j , and $OPT_{E,i}$ is the experimentally
172 determined odor perception threshold of i . Both are expressed in terms of mass/L where the
173 mass depends on the $OPT_{E,i}$ if it is in orders of $\mu\text{g L}^{-1}$ or ng L^{-1} .

174 Two distinct experimental designs were set up: (i) the first one corresponding to a low OAV
175 (i.e., 30) related to a low-intensity scenario (LI); and (ii) the second one corresponding to a
176 high OAV (i.e., 300) related to a high-intensity scenario (HI). The OAV=30 was chosen in
177 order to be above the recognition threshold (the concentration needed to recognize an odor
178 nature [37]). The HI value was chosen to be ten folds the LI. Table 1 describes the
179 experimental matrices that frame the two scenarios: it gives the X_i and OAV_i values for each
180 experimental point and test mixture.

181 **2.1.2 Model construction**

182 To model the interactions, the results from the natural assessment of the 15 mixtures are taken
183 into consideration. Starting from the sensory evaluation of the odor nature by an expert panel
184 (see part 2.3.1), a score, “Y”, is determined for an odor nature attribute and each odorous
185 mixture. The methodology to build this score Y is detailed in the following section (part
186 2.3.3). Then, a system of reduced third-order polynomial equations is used (Equation 3):

187 Equation 3 : $Y_{a,j} = b_D X_{Dj} + b_T X_{Tj} + b_F X_{Fj} + b_C X_{Cj} + b_{DT} X_{Dj} X_{Tj} + b_{DF} X_{Dj} X_{Fj} +$
 188 $b_{DC} X_{Dj} X_{Cj} + b_{TF} X_{Tj} X_{Fj} + b_{TC} X_{Tj} X_{Cj} + b_{FC} X_{Fj} X_{Cj} + b_{DTF} X_{Dj} X_{Tj} X_{Fj} + b_{DTC} X_{Dj} X_{Tj} X_{Cj} +$
 189 $b_{DFC} X_{Dj} X_{Fj} X_{Cj} + b_{TFC} X_{Tj} X_{Fj} X_{Cj}$

190 where $Y_{a,j}$ is the score of an odor nature attribute (explained in part 2.3.3) for a mixture j , X_D
 191 is related to the OAV of DMDS, X_T to the OAV of toluene, X_F the OAV of furfuryl
 192 mercaptan, and X_C to the OAV of cyclopentanone; b_D represents the main contribution of the
 193 variable X_D , b_{DT} is the effect of the binary interaction $X_D X_T$ and b_{DTF} is the effect of the
 194 ternary interaction $X_D X_T X_F$. Obviously, the coefficients do not have the same weight, i.e., the
 195 comparison of their values should be performed only between the same level of interactions
 196 (individual, binary, and ternary). Quaternary interaction monomial term was not considered
 197 due to the minimal effect it could have on the result since it is based on a multiplication of 4
 198 OAV proportions X

199 Individual contributions b_T , b_D , b_F , and b_C and the effects of binary and tertiary interactions
 200 are determined by solving the equation system emerging from the odor nature assessment of
 201 the 15 mixtures.

202 The generation of experimental designs, the construction of models, and the statistical
 203 analysis were performed using NEMRODW[®] software [38].

204 **2.2 Preparing the mixtures**

205 **2.2.1 Odorants**

206 Gaseous mixtures of DMDS ((methylsulfanyl)methane), toluene, furfuryl mercaptan
 207 (Furan-2-ylmethanethiol), and cyclopentanone were prepared in the lab, starting from pure
 208 chemical standards, in commercially available liquid form. Table 2 gathers the characteristics
 209 of the odorants: CAS number, supplier and chemical purity, odor perception thresholds, and
 210 odor nature (evocations usually found in the bibliography). The commercial standard odorants
 211 were analyzed using gas chromatography-olfactometry (GC-O) to ensure the absence of any
 212 impurities. No impurities were either present or perceived.

213 **2.2.2 Preparation of gaseous mixtures**

214 The quantities of liquid needed to reach the targeted OAV values were calculated. These
 215 quantities (consisting of a few microliters of each toluene and cyclopentanone, and 1 μ L of a
 216 solution in methanol containing the exact mass needed for DMDS and furfuryl mercaptan),
 217 were injected separately under liquid form in a 6 L Silicocan canister (Restek[®]) under vacuum

218 (10^{-3} torr). This ensures the gentle vaporization of the compound without the need to apply
219 heat. The canister was kept under vacuum for an hour to ensure complete vaporization.
220 Afterward, the canister was filled with 12 L of pure nitrogen (alpagaz 2 Nitrogen, Air
221 Liquide, P \geq 99.9999%). The canisters were used as gas storage for the evaporated odorants
222 from which definitive volumes were later taken and diluted to produce gaseous mixtures. The
223 concentrations of DMDS, toluene, furfuryl mercaptan, and cyclopentanone were 6; 635;
224 0.091, and 476 $\mu\text{g L}^{-1}$, respectively, in the respective canisters.

225 Diluted gas mixtures were prepared in 10 L Nalophan[®] bags (Sense trading); their
226 composition fulfills the requirements given in section 2.1.1. Definitive volumes of each
227 evaporated gas from the canisters were introduced into the bags (Equation 4), which were
228 then filled with nitrogen. The volumes were adjusted in order to obtain the desired final
229 concentrations following Equation 4.

230 Equation 4 :
$$V_{\text{canister},i} = \frac{OAV_{i,j} \times OPT_{E,i} \times 10}{C_{\text{canister},i}}$$

231 where $V_{\text{canister},i}$ is the volume taken from the canister containing constituent i and introduced in
232 the bag, 10 is the volume of the bag in L, and $C_{\text{canister},i}$ is the concentration of i in the canister
233 in units of mass L^{-1} .

234 Bags were prepared one hour before the analyses to ensure the homogeneity of the mixtures.

235 At each step of mixture preparation, the stability of the odorants and the accuracy of the
236 obtained concentrations were verified using gas chromatography (DATA IN BRIEF).

237 **2.3 Sensory analysis**

238 **2.3.1 Panel characteristics**

239 The panel consisted of 7 assessors between 25 and 52 years old. The assessors were 5 females
240 and 2 males. All assessors had 32 hours of initial training designed for the Langage des Nez[®]
241 method, described just below. The assessors attended a one-hour training session every month
242 minimum (the majority had upkeep once a week). Hence, assessors are considered experts, as
243 described by ISO 8586 [39]. The panel was all volunteers with their consent obtained before
244 the analysis which was reviewed by the ethical committee of Le Havre University.

245 Sensory analyses were conducted in a standardized ISO/DIS 8589 room [40]. Each session
246 lasted one hour with a 10-minute pause mid-session to limit panel fatigue.

247 **2.3.2 Odor perception threshold determination**

248 The OPT of each odorant was determined by the panel participating in the sensory analysis
249 using the triangle odor bag method as described in Ueno et al., 2009 with a forced-choice
250 (EN13725, 2003). This also permits the evaluation of the individual sensitivity of each
251 assessor toward the odorants. To determine their OPTs, a precise concentration of each
252 odorant was vaporized in Nalophan bags (as explained in part 2.2.2). The concentrations of
253 each odorant were based on odor perception thresholds reported in the literature (OPT_L).
254 Seven concentration levels were prepared so that concentrations of the samples were regularly
255 distributed in a range between 625 and 0.04 OPT_L . The concentrations are selected broadly
256 around the OPT_L due to the wide ranges of OPTs found in the literature.

257 **2.3.3 Odor nature description**

258 Descriptive analysis of the odor of each mixture was performed using the Langage des Nez[®]
259 (LdN) method. This is a methodology used to describe the odor nature using a collection of 26
260 odor referents (Figure 2). The referents are pure chemical compounds. Description of the odor
261 nature is achieved by comparing the odor of interest to the least different odor of referents
262 from the collection. Matching the odor to a referent relatively reduces the subjectivity linked
263 to odor assessment and offers a univocal lexicon repeatable by an assessor [34,43].

264 The referents are distributed in a 3D space (presented in 2-D) in 7 poles: terpenic, alkyl, ester,
265 amine, phenolic/pyrogenic, sulfurous, and aromatic. These poles are built around a nucleus,
266 consisting of 1 to 3 referent(s) (represented on the first concentric circle) and gathering 1 to 3
267 satellite referents (represented on the second and third concentric circles) as seen in Figure 2.
268 In the 3D olfactory space, the closer an odorant is to a pole, the more similar they are. For
269 example, acetic acid is attached to the alkyl pole but tends toward the ester pole. Hence, acetic
270 acid has an odor mainly similar to alkyl-like referents but also a milder ester-like facet [34].

271 The panel was asked to choose one, two, three, or four poles from eight preselected attributes:
272 phenol-like, pyrogenic-like, sulfurous-like, terpenic-like, alkyl-like, aromatic-like, ester-like,
273 and amine-like odors. The assessors gave each attribute a total score over 9. If one attribute
274 was used, the score would be 9, if two, three, or four attributes were used, the sum of the
275 given scores must be 9. The score was used as a degree of representativity.

276 The means for each attribute for a mixture were calculated after screening the assessors.
277 **These means are the experimental scores $Y_{a,1}$ - $Y_{a,15}$ which were used to establish the**
278 **models.**

279 **2.4 Model validation and quality evaluation**

280 After the model was built considering the results of mixtures 1 to 15, it was validated using
281 the experimental attribute scores $Y_{\text{test } 1} - Y_{\text{test } 4}$ related to the odor nature assessment of the so-
282 called test points. The test mixtures are quaternary mixtures with the aim of better
283 representing the inner space of the experimental domain in Figure 1. Predicted odor attribute
284 scores ($\hat{Y}_{\text{test } 1} - \hat{Y}_{\text{test } 4}$) were calculated using the established equation system (Equation 3).
285 Then, the predicted odor attribute scores were compared to the experimental attribute scores
286 $Y_{\text{test } 1} - Y_{\text{test } 4}$. A two-sample t-test score was used with a risk α of 5%. If no difference was
287 observed between the predicted and experimental results, the model was considered validated.

288 Once a model was validated, its quality was assessed. The quality was based on the
289 comparison between experimental results obtained from the sensory analysis and the
290 predicted results obtained from calculations using the model and the difference between them,
291 called residues.

292 The descriptive quality of the model was determined using R^2 (Equation 5) [30]

293 Equation 5 :
$$R^2 = \frac{\text{Sum Squared Model (SSM)}}{\text{Sum Squared Total (SST)}} = \frac{\sum_{j=1}^n (\hat{Y}_j - \bar{Y})^2}{\sum_{j=1}^n (Y_j - \bar{Y})^2}$$

294 where \hat{Y}_j is the predicted odor attribute score given by the model of a mixture j, and \bar{Y} is the
295 mean of Y_j , which are the experimental odor attribute scores.

296 The R^2 reflects the correlation between experimental results (Y) and the theoretical results
297 (\hat{Y}). Thus, the closer R^2 is to 1, the more Y and \hat{Y} are correlated and the better the descriptive
298 quality.

299 Since R^2 is sensitive to the number of experiments - in our case, 28 experiments were
300 necessary to construct the model (14 mixtures analyzed two times) and 8 experiments were
301 needed to validate it (4 test points analyzed two times); the adjusted R^2 , or R_a^2 , was used
302 (Equation 6).

303 Equation 6 :
$$R_a^2 = 1 - (1 - R^2) \frac{(n-1)}{(n-p)}$$

304 where n is the number of experiments and p is the number of coefficients, b, of the model.

305 To describe the predictive quality of the model, a predictive R^2 , R_{pred}^2 (Equation 7) was used
306 and is based on Allen's predicted residual error sum of squares (PRESS) [44].

307 Equation 7 : $R_{pred}^2 = 1 - \frac{PRESS}{SST}$

308 The R^2 factors always respect the following relation: $R_{pred}^2 \leq R_a^2 \leq R^2 \leq 1$

309 **3 Results and discussion**

310 The later parts from 3.1 to 3.4 focus on the sensory analysis results, validation, and quality of
311 the models.

312 **3.1 Panel odor perception thresholds**

313 First, the $OPT_{E,i}$ values of the panel of the four targeted odorants were determined
314 experimentally and compared with the OPTs taken from the literature (OPT_L) (Table 2). The
315 mean values of the panel are presented in Table 3; the difference between $OPT_{E,i}$, and OPT_L
316 was maximal for furfuryl mercaptan but did not exceed one order of magnitude. For DMDS
317 and toluene, OPT_L was determined using the same approach as those used in this work.
318 Differences may be explained by the differences in the sensitivities of the panel: a Japanese
319 panel was used in the study by Nagata [45] while the panel in this study was composed mostly
320 of European assessors. Differences in populations have been reported in the literature before
321 [46]. For the OPT of furfuryl mercaptan and cyclopentanone, beyond the difference in the
322 panels, gaps may be explained due to the use of different methodologies for sample
323 preparation: GC-O and dynamic olfactometry.

324 Using the obtained OPT_E and the OAV in Table 1 for each odorant, the concentration
325 introduced in the bag was calculated according to Equation 4 and Equation 2. Concentrations
326 used to construct the experimental plan are shown in Table 3 at low (LI) and high (HI)
327 intensities.

328 **3.2 Sensory Analysis results**

329 **3.2.1 Odor nature description**

330 Regarding odor nature description, for each mixture, the mean of the scores given by the
331 assessors for each attribute of the LDN was calculated, for two replicates. Only four attributes
332 among seven (Figure 1) were used by the assessors: pyrogenic, terpenic, sulfurous, and
333 esteric. To investigate the performance of the panel, a three-way analysis of variance

334 (ANOVA) was performed on the data. For each attribute, the mixture (M), assessor (A) and
335 replicate (R) were considered factors, and their interactions were also considered. The effects
336 of each factor in terms of probabilities (p-values) are presented in Table 4.

337 On the one hand, one can observe that the mixture effect was highly significant ($P < 0.0001$)
338 for each attribute in both scenarios. This result demonstrates the assessors' power to
339 discriminate the different mixtures, as this effect depends on the samples themselves, the
340 selection of relevant attributes, and the abilities of the panel. In addition, the assessor effect
341 for both scenarios was significant for each attribute. A significant assessor effect showed that
342 the global means (all mixtures and replicates taken together) were not homogeneous among
343 the assessors. This effect is generally significant and persistent even with intensive training
344 but does not offer real information on panelists' performance. This is rather the
345 mixture \times assessor interaction that well characterizes the performance of a sensory panel [47].
346 A significant interaction implies that assessors do not perceive the same differences between
347 mixtures. Table 4 shows that the p-values for the M*A interaction were significant for each
348 attribute ($\alpha=0.05$) except for the sulfurous attribute in the HI scenario. This can be explained
349 by the mixtures, especially the ternary and quaternary mixtures, being close to the odor
350 identification threshold explained in detail in part 3.5.

351 On the other hand, the replicate effect was not significant for all attributes in both scenarios.
352 Thus, the use of an olfactory space based on referents to describe the odor nature yields a
353 reproducible approach among sessions. Finally, no significant interactions were notable for
354 M*R (except for the esteric attribute at HI and the pyrogenic attribute at LI) and A*R.

355 **3.3 Model validation**

356 Using the sensory results obtained for the first 15 mixtures presented in Table 3, models were
357 constructed and needed to be validated. For the model validation, four test points for each
358 scenario were used (Table 3). The odor nature, described as a score for the four attributes (the
359 other poles were not used by the panel), was determined both experimentally ($Y_{\text{Test 1 - Test 4}}$),
360 following the same sensory protocol as for construction points, and theoretically ($\hat{Y}_{\text{Test 1 - Test 4}}$),
361 by calculating the scores for each attribute using the constructed models and the
362 proportions of the odorants in each test mixture (Table 5). For each scenario and each
363 attribute, two series of 4 scores were obtained. All p-values largely exceeded 5%; hence, there
364 was no significant difference between the experimental and theoretical results. Therefore, the
365 models were validated.

366 Once the models are validated, the results of the test points may be added to the construction
367 of the models to refine them and obtain final model equations, including 15 construction, and
368 4 test points. The addition of such results is not obligatory but, as will be shown in this
369 example, it may affect the descriptive and predictive quality of the models. Depending on the
370 decrease in the quality, the choice of whether to add the test point results will be discussed.

371 **3.4 Descriptive and predictive quality of the models**

372 For each of the 8 models, R^2 , R_a^2 , and R_{Pred}^2 were calculated before (A) and after (B) adding
373 the results of test points to construct the models (Table 5).

374 In Table 5, the descriptive quality is high for all attribute models at LI and HI. Indeed, R^2 and
375 R_a^2 are relatively close to 1 with values ranging from 0.610 to 0.973. However, an overall
376 decrease is notably observed for the LI scenario. Notably, the precision of the odor nature
377 sensory analysis is affected for low-intensity samples. Moreover, it must be noted that R_a^2
378 values as high as those reported with physicochemical analysis cannot be expected in this
379 work due to the variable sensitivity related to the human panel. For example, in the study on
380 ceramics by Ngun et al., R_a^2 values were at a minimum of 0.955 [30], while for this work the
381 minimum value was obtained for the terpenic attribute model in the LI scenario: R_a^2 was 0.610
382 after adding the test points results.

383 Furthermore, regardless of the intensity or attribute, R^2 and R_a^2 decreased with the addition of
384 the test points results (Table 5). In our particular case, this might be due to the nature of the
385 test points. Actually, test points were the more complex mixtures evaluated by the assessors
386 with four odorants. However, it is well known that the description of a complex odor is a
387 difficult task for assessors, increasing with the number of constituents. As described before,
388 humans are capable of identifying a maximum of three to four odorants in a mixture [20].
389 This threshold is independent of the training level of the assessors [48], the method used [49],
390 the type of odor blend [50], or whether it is a mixture of pure odorants or complex “object
391 odors” such as chocolate odor or sewage odor [51]. Therefore, when asking the assessors to
392 describe the odor nature of the test point mixtures, the results may also vary from one assessor
393 to another due to sensitivity variations.

394 R_{Pred}^2 Table 5 values obtained under both scenarios show a relatively good predictive quality.

395 Once again, the difference in the quality of the models between HI and LI is clear (Table 5).
396 This decrease in quality when intensity also decreased may be explained by the potential

397 proximity of the LI scenario mixture to the recognition threshold. Thus, if some odorants are
398 present at a concentration that may be close to or slightly above the recognition threshold,
399 assessors may smell them but are not able to recognize them.

400 The addition of the test points results makes the models more robust to future variations by
401 adding more data to their construction, especially, in our case, data issued from studying
402 quaternary mixtures. Therefore, test-points results were added to the models regardless of
403 the decrease in the descriptive and predictive qualities.

404 *What can be concluded?*

405 The panel was capable of distinguishing the mixtures and evaluating their odor natures in
406 reproducible analyses from one session to another. Nevertheless, variations among
407 assessors were observed. In contrast, in previous work evaluating the odor nature of single
408 molecules, repeatability among assessors was observed [34]. This leads to the conclusion
409 that the panel is proficient when using the LdN but is still subject to differences in
410 perception from one person to another, especially when dealing with mixtures. Thus, one
411 can consider that the models are constructed based on average perceptions.

412 Concerning the quality of the constructed models, the descriptive and predictive quality of
413 the models was satisfactory for sensory analyses even if it tended to be lower in
414 comparison with other studies involving physico-chemical analyses as explained earlier.
415 On the other hand, the quality tended to decrease with the intensity which can be explained
416 by the proximity to the recognition threshold of the odorants, interfering with the analysis.

417 The parts from 3.5 to 3.6 are dedicated to the obtained models, their coefficients, and the way
418 of use

419 **3.5 Model coefficients and 2-D representations**

420 After validating the quality of the models, this section discusses the olfactory qualitative
421 interactions between the four targeted constituents based on the experimental design
422 coefficients.

423 The coefficients of the 8 models (Equation 3) were calculated and are presented in Table 6. It
424 is important to note that the 8 models are presented after the addition of test points results in
425 the construction of the models.

426 The model obtained for the pyrogenic attribute for the LI scenario is chosen to illustrate how
427 to interpret the model coefficients (Equation 8) and how to read the 2D- representations given
428 in Figure 3 and Figure 4.

429 Equation 8 : $Y_{\text{pyrogenic attribute}} = -0.32 X_D + 0.08 X_T + 3.99 X_F + 0.23 X_C + 9.06 X_D X_T + 1.15$
430 $X_D X_F + 8.23 X_T X_F + 0.25 X_D X_C + 1.33 X_T X_C - 1.53 X_F X_C + 6.08 X_D X_T X_F - 21.03 X_D X_T X_C +$
431 $27.31 X_D X_F X_C + 1.61 X_T X_F X_C$

432 *What do the contribution coefficients tell us?* The higher the coefficients, the more important
433 the contribution is. For example, the b_D value is -0.32 while it is approximately 4 for the b_F
434 value. This indicates that DMDS has a low contribution to the pyrogenic-like odor nature (or
435 pyrogenic attribute) of the mixture, while furfuryl mercaptan is the main contributor to this
436 attribute.

437 *What about the interaction coefficients?* The first point to consider for the interaction
438 coefficient is its sign which indicates the type of contribution. A positive coefficient indicates
439 a synergetic effect while a negative coefficient indicates a masking effect. For example, b_{TC} is
440 positive while b_{FC} is negative. This means that the interaction between furfuryl mercaptan and
441 cyclopentanone masks the pyrogenic attribute while the interaction between toluene and
442 cyclopentanone intensifies it. Analogous to the contribution coefficient, the higher the
443 coefficient is, the more impactful the interaction.

444 Additionally, for ternary interactions, only coefficients with a magnitude of tens and higher
445 were considered significant because the value of the interaction is the result of a
446 multiplication of three proportions $0 \leq X \leq 1$ (Equation 3) with the coefficient. If the threshold
447 was not reached, the coefficient was considered negligible; hence, the interactions are not
448 significant. Here the D-T-F and D-T-C interactions were considered (equation 8).

449 To help the visualization of the results, the 8 models are represented by selected 2D plots
450 presented in Figure 3 for the LI scenario and Figure 4 for the HI scenario. To facilitate
451 reading, each model is represented by a series of 2D-ternary plots, (facets of the tetrahedron
452 from Figure 1). The isochrone plots show the variation of the odor nature, for an attribute,
453 with the composition of the mixture. Only the 2D plots showing the higher contributor to the
454 attribute are selected.

455 *How to read the 2D plots?* Each isovalue curve marks the score magnitude of an attribute. In
456 our example, the isochrone plot (Figure 3.a) concerns the pyrogenic attribute of a mixture of

457 DMDS, furfuryl mercaptan, and toluene; the proportion of cyclopentanone is fixed to zero.
458 We can read that: (i) when the mixture contains only furfuryl mercaptan, the pyrogenic
459 attribute is around 4/9; (ii) the pyrogenic attribute achieves a maximal score of 4.5/9 for a
460 mixture containing around 80% furfuryl mercaptan and 20% toluene; (iii) the pyrogenic
461 attribute decreases to a score of 3/9 for binary mixtures either containing approximately 70%
462 toluene and 30% furfuryl mercaptan, or 28% DMDS and 72% furfuryl mercaptan, or for a
463 ternary mixture of 33% furfuryl mercaptan and 20% toluene and 47% DMDS; (iv) if the score
464 is below 1/9 at 100% DMDS or toluene, the DMDS and toluene vertexes are beyond the
465 isovalue curve of 1.

466 For the rest of this section, and for each attribute, the contributions and interactions of
467 odorants are interpreted in the same way as explained just before based on the coefficient
468 values and isochrone plots.

469 *Pyrogenic attribute models*

470 The main contributor to the pyrogenic attribute is furfuryl mercaptan for both intensity
471 scenarios (Table 6). Hence, if $X_F = 1$, the pyrogenic attribute (Y_{AP}) will be approximately 4/9.
472 Notably, a score of 9/9 cannot be achieved with the considered component. The models
473 confirm that two attributes are needed (double facet) to characterize the odorous nature of
474 furfuryl mercaptan (the second attribute is the sulfurous one since b_F is 4.03 at HI and 4.54 at
475 LI), even if its smell is isolated.

476 For the LI scenario, the binary interactions between almost all of the odorants contribute
477 positively to the pyrogenic attribute. Only the F-C interaction has a masking effect on the
478 pyrogenic attribute. This is expected since the odorous natures of these isolated odorants are
479 different in the olfactory space (Figure 2). What is remarkable is the synergetic contribution
480 of the binary interaction F-T at LI, which has the highest contribution among binary
481 interactions. This can be visualized in Figure 3.a. A maximum score of $>4.5/9$ was obtained
482 (the small curve near the right corner of the triangle), not for $X_F=1$ as expected, but for a
483 mixture of furfuryl mercaptan ($0.66 < X_F < 0.78$) with DMDS ($0 < X_D < 0.03$) and toluene (0.19
484 $< X_T < 0.32$).

485 However, for HI, some interactions seem to change. For example, the D-F-C interaction
486 changes from synergetic to masking (b_{DFC} being equal to +27.31 at LI and -14.82 at HI). This
487 effect change can also be observed with DTC (from masking to insignificant), while some

488 coefficients including furfuryl mercaptan b_F , the major contributor of the pyrogenic attribute,
489 in binary mixture (b_{DF} for example) increase at high intensity. One hypothesis could be that
490 the cyclopentanone at HI becomes more easily recognizable and thus, has a more intense
491 masking effect when mixed with furfuryl mercaptan.

492 *Terpenic attribute models*

493 The main contributor to the terpenic attribute is toluene (Table 6). With $b_T < 9$, the results
494 suggest that toluene has a terpenic odor but also another esteric facet.

495 Binary interaction coefficients show that D-T interaction has a synergetic effect for both
496 intensities. The synergetic interaction between toluene and DMDS can be compared to the
497 synergetic interaction between styrene (which odor nature and chemical structure are close to
498 those of toluene) and H_2S found in the study of Wu et al. [52]. It is not surprising to observe
499 b_{DF} at HI close to 0 and negative at LI since DMDS and furfuryl mercaptan are positioned far
500 from the terpenic pole (Figure 2). Thus, D-F interaction is not expected to be positive. The T-
501 C interaction at HI is negative. This may be explained by the cyclopentanone intensifying the
502 esteric facet of the toluene at the expense of the terpenic facet. This explanation is supported
503 by the fact that b_{T-C} is positive for the esteric attribute model at HI.

504 The ternary interactions coefficients show that the interactions of DMDS with toluene are
505 often synergetic even with a third odorant since b_{DTC} is positive at LI and HI and b_{DTF} is
506 positive at LI. This can be observed in figure 4.e with the curves shifting towards DMDS, i.e.
507 for the same X_T , if X_D increases, the terpenic attribute increases.

508 *Sulfurous attribute models*

509 As expected, the main contributor to the sulfurous attribute was DMDS (Table 6), which is
510 representative of the sulfurous pole (Figure 2). Moreover, as mentioned before, the second
511 facet of furfuryl mercaptan appeared with a b_F of approximately 4.

512 At HI, only synergetic interactions were unexpectedly found with T-C interaction, while all of
513 the DMDS interactions with other odorants were masking interactions. The latter observation
514 was also observed at LI, except for the D-F and T-C interactions.

515 The ternary interactions all shifted from positive to negative and vice versa from LI to HI.
516 This shows the complexity of odor mixture studies due to the unpredictability of the nature of
517 interactions among odorants.

519 The main contributor to the esteric attribute was cyclopentanone (Table 6). A coefficient b_C of
520 7 at LI is not surprising since cyclopentanone is attached to the esteric pole but tends to go
521 further from the nuclei of the pole (Figure 2). Moreover, the esteric facet of toluene appears in
522 these models. Nevertheless, the esteric facet of the toluene decreased with increasing intensity
523 while its terpenic facet became more perceptible.

524 At LI, binary and ternary interactions were majorly negative or close to 0 suggesting that
525 cyclopentanone was nearly masked by all the other studied odorants except for the DMDS
526 ($b_{DC} = 7.22$). However, at HI, cyclopentanone was less masked. This can be visualized by
527 comparing Figure 3.1 and Figure 4.1. At LI, the esteric attribute achieved a score of 4/9 with
528 $X_C \geq 0.61$ when mixed with toluene and furfuryl mercaptan, whereas, at HI, a score of 4/9
529 was achieved for $X_C \geq 0.43$. The masking effect that changed at different intensity levels for
530 the same odorant in the same mixture was not surprising. It has been reported before by Kim
531 in 2010 when a mixture of acetaldehyde and H_2S showed a dominance of acetaldehyde at low
532 intensities but a dominance of H_2S at high intensities [15].

533 **3.6 Methodology for the use of the mixture model**

534 The constructed models aim to predict the odor nature of a mixture of odorants. This can be
535 done by marking the three parts of this approach: the input data, the model equation necessary
536 for calculation, and the output data. The input data of the model are the relative OAV of each
537 odorant (X_i). This can be obtained by dividing the chemical concentration by the OPT_E
538 (Equation 2) and later the X_i is calculated using (Equation 1). Once the sum of OAV is
539 calculated, the intensity scenario is determined: around 30, it is considered LI, and around
540 300, it can be considered HI. Once the X_i are calculated, and the intensity scenario is defined,
541 the models can be chosen. The output data, \hat{Y} , can be calculated following Equation 3 using
542 the calculated X_i and the corresponding b coefficients from Table 6. \hat{Y} are calculated for the
543 four attributes. After calculating the \hat{Y} , the obtained results are interpreted as odor nature as
544 the $\hat{Y}/9$ of each attribute.

545 An example of a mixture composed of 190 ng L^{-1} DMDS, $22 \text{ } \mu\text{g L}^{-1}$ toluene, 0.35 ng L^{-1}
546 furfuryl mercaptan, and $10 \text{ } \mu\text{g L}^{-1}$ cyclopentanone is shown. By dividing the concentration of
547 each odorant by its respective OPT_E (Equation 2), the OAV of each odorant is obtained. In
548 this case, they are, respectively, around 15, 5, 5, and 5. The sum of OAVs of 30 means that a

549 LI scenario is considered. An SOAV of 30 yields the following proportions: $X_D = 0.5$ and X_T
550 $= X_F = X_C = 0.17$. By substituting each proportion in the constructed models presented above,
551 e.g., Equation 8 becomes:

$$\begin{aligned} 552 \hat{Y}_{\text{pyrogenic attribute}} &= -0.32 (0.50) + 0.08 (0.17) + 3.99 (0.17) + 0.23 (0.17) + 9.06 (0.50) (0.17) + \\ 553 &1.15 (0.50) (0.17) + 8.23 (0.17) (0.17) + 0.25 (0.50) (0.17) + 1.33 (0.17) (0.17) - 1.53 (0.17) \\ 554 &(0.17) + 6.08 (0.50) (0.17) (0.17) - 21.03 (0.50) (0.17) (0.17) + 27.31 (0.50) (0.17) (0.17) + \\ 555 &1.61 (0.17) (0.17) (0.17) \end{aligned}$$

556 Thus, the results will be $\hat{Y}_{\text{pyrogenic attribute}} = 3.4$; $\hat{Y}_{\text{terpenic attribute}} = 1.7$; $\hat{Y}_{\text{sulfurous attribute}} = 2.9$; and
557 $\hat{Y}_{\text{esteric attribute}} = 1$. The odor of this mixture will be described with scores of 3.4/9 pyrogenic,
558 1.7/9 terpenic, 2.9/9 sulfurous and pyrogenic, and 1/9 esteric.

559 *What can be concluded?*

560 The interactions were shown to be dependent not only on the odorants and their individual
561 intensity ratios, as explained in the work of Ferreira [1], but also, on the intensity level as
562 observed by the changes in the interaction coefficients when intensity changed and sometimes
563 with sign conversions. The most notable change was for cyclopentanone, which was almost
564 masked by other odorants at LI but became more perceptible and more prominent at HI.

565 The coefficients offered by the models helped to highlight various aspects of the odor of the
566 mixtures. The contribution coefficients of the constructed models helped shed light on the
567 double facets of furfuryl mercaptan and toluene. Furthermore, the ternary interactions did not
568 impact all odorants; however, some interactions were unexpected, highlighting the difficulty
569 of predicting these interactions by relying only on chemical analyses and the importance of
570 understanding the mixture effects on odors. Nevertheless, it is important to mention that the
571 usage of these models is still limited to these four odorants and intensity levels. It is difficult
572 to predict the efficiency of their application to other mixtures containing similar odorants or at
573 different intensity levels. Therefore, more work is needed including studying other similar
574 odorants and intensity levels.

575 **Conclusion**

576 This work shows the relevance of the methodology to apprehend the problem of the
577 perception of mixtures of odorous compounds. The proposed methodology is based on three
578 main pillars: (i) the generation of mixtures in the gaseous state in order to limit any

579 experimental biases, (ii) the objective olfactory analyses to limit the psychological biases, and
580 finally (iii) the experimental mixture design. This study focused on mixtures of four different
581 odorants in various proportions chosen to be representative of environmental nuisances. The
582 mixtures were at two different odor intensity levels, in a gaseous state. Each mixture had its
583 odor described using the Langage des Nez[®] olfactory space. The variation in odor nature with
584 the composition of the mixtures was modeled. This was achieved using the experimental
585 mixture design approach.

586 The combination of the experimental mixture design with Langage des Nez[®] allowed the
587 transformation of chemical data into sensory data. The yielded models enabled the prediction
588 of a certain odorant mixture just by knowing the chemical concentration. After a
589 transformation of chemical concentrations in OAV, the models provide scores for each
590 attribute. In addition to prediction ability, the models permitted understanding the different
591 sensory interactions taking place in the mixture. Thus, the present study permits a better
592 understanding of the complex mixture effects i.e., unraveling the masking and synergetic
593 interactions.

594 This approach may be helpful in various domains: it might be used in perfumery to directly
595 predict the final odor of a product even before mixing; but also, for environmental studies
596 where odor emission sources are mixed and interacted. Modeling such mixtures helps to
597 identify which odorants are dominating, which are masked, and which have a synergetic
598 effect, intensifying other odors.

599 This novel work combines the experimental mixture design with sensory analysis, more
600 specifically odor nature description, for the first time. Indeed, the proposed methodology is
601 limited to four odorants. However, it might be interesting to study whether other odorants,
602 with odors similar to those of the studied odorants, behave in the same way if mixed.
603 Moreover, as the methodology offers promising results, nothing prevents the study of other
604 odorant combinations.

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608 participation.

609 **Table 1:** Experimental matrices for simplex-centroid designs with four constituents with the
 610 proportions (X_i), and odor activity values (OAVs) at high and low intensities

| Mixture number | DMDS | Toluene | Furfuryl mercaptan | Cyclopentanone |
|----------------|-------------------------------------|-------------------------------------|-------------------------------|-------------------------------|
| | $X_D/OAV_{D, LI}$ $/OAV_{D, HI}$ | $X_T/OAV_{T, LI}$ $/OAV_{T, HI}$ | $X_F/OAV_{F, LI}/OAV_{F, HI}$ | $X_C/OAV_{C, LI}/OAV_{C, HI}$ |
| 1 | 1/30/300 | 0/0/0 | 0/0/0 | 0/0/0 |
| 2 | 0/0/0 | 1/30/300 | 0/0/0 | 0/0/0 |
| 3 | 0/0/0 | 0/0/0 | 1/30/300 | 0/0/0 |
| 4 | 0/0/0 | 0/0/0 | 0/0/0 | 1/30/300 |
| 5 | 0.5/15/150 | 0.5/15/150 | 0/0/0 | 0/0/0 |
| 6 | 0.5/15/150 | 0/0/0 | 0.5/15/150 | 0/0/0 |
| 7 | 0.5/15/150 | 0/0/0 | 0/0/0 | 0.5/15/150 |
| 8 | 0/0/0 | 0.5/15/150 | 0.5/15/150 | 0/0/0 |
| 9 | 0/0/0 | 0.5/15/150 | 0/0/0 | 0.5/15/150 |
| 10 | 0/0/0 | 0/0/0 | 0.5/15/150 | 0.5/15/150 |
| 11 | 0.33/10/100 | 0.33/10/100 | 0.33/10/100 | 0/0/0 |
| 12 | 0.33/10/100 | 0.33/10/100 | 0/0/0 | 0.33/10/100 |
| 13 | 0.33/10/100 | 0/0/0 | 0.33/10/100 | 0.33/10/100 |
| 14 | 0/0/0 | 0.33/10/100 | 0.33/10/100 | 0.33/10/100 |
| 15 | 0.25/7.5/75 | 0.25/7.5/75 | 0.25/7.5/75 | 0.25/7.5/75 |
| Test 1 | 0.625/18.75/187.5 | 0.125/3.75/37.5 | 0.125/3.75/37.5 | 0.125/3.75/37.5 |
| Test 2 | 0.125/3.75/37.5 | 0.625/18.75/187.5 | 0.125/3.75/37.5 | 0.125/3.75/37.5 |
| Test 3 | 0.125/3.75/37.5 | 0.125/3.75/37.5 | 0.625/18.75/187.5 | 0.125/3.75/37.5 |
| Test 4 | 0.125/3.75/37.5 | 0.125/3.75/37.5 | 0.125/3.75/37.5 | 0.625/18.75/187.5 |

611

612 **Table 2:** The chemical compounds used with their odor perception threshold in air (OPT_L – taken
 613 from the literature), and their respective odor nature descriptions using evocations.

| Odorant | Cas number | Supplier and chemical purity | OPT_L | Odor nature – examples of evocations |
|--------------------|------------|------------------------------|------------------------------|--------------------------------------|
| DMDS | 624-92-0 | ACROS organics, 99% | 8.48 ng L ⁻¹ (1) | Garlicky, sulfurous |
| Toluene | 108-88-3 | Fisher, 99.99% | 1.24 µg L ⁻¹ (1) | Sweet, plastic |
| Furfuryl mercaptan | 98-02-2 | ACROS organics, 97% | 0.023 ng L ⁻¹ (2) | Roasted coffee |
| Cyclopentanone | 120-92-3 | ACROS organics, +99% | 0.93 µg L ⁻¹ (3) | Solventy |

614 1- [45]/ 2- [53]/ 3-[35]

615

616

617 **Table 3:** concentration in bags ($C_{i, \text{bag}}$) used in the experimental plan for the low (LI) and high-
 618 intensity (HI) scenarios based on the odor perception threshold determined experimentally by the
 619 panel

| | DMDS | Toluene | | Furfuryl mercaptan | | Cyclopentanone | | |
|---|--------------------------|-------------------------|-------------------------|--------------------------|-----|-------------------------|------------------------|-----------------------|
| OPT _L | 8.48 ng L ⁻¹ | 1.24 μg L ⁻¹ | | 0.023 ng L ⁻¹ | | 0.93 μg L ⁻¹ | | |
| OPT _{E,i} | 12.25 ng L ⁻¹ | 4.45 μg L ⁻¹ | | 0.073 ng L ⁻¹ | | 1.90 μg L ⁻¹ | | |
| Concentration in bags (ng L ⁻¹) | | | | | | | | |
| Mixture number | LI | HI | LI | HI | LI | HI | LI | HI |
| 1 | 368 | 3675 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2 | 0 | 0 | 133.6 x 10 ³ | 1336 x 10 ³ | 0 | 0 | 0 | 0 |
| 3 | 0 | 0 | 0 | 0 | 2.2 | 22 | 0 | 0 |
| 4 | 0 | 0 | 0 | 0 | 0 | 0 | 57 x 10 ³ | 570 x 10 ³ |
| 5 | 184 | 1838 | 66.8 x 10 ³ | 668 x 10 ³ | 0 | 0 | 0 | 0 |
| 6 | 184 | 1838 | 0 | 0 | 1.1 | 11 | 0 | 0 |
| 7 | 184 | 1838 | 0 | 0 | 0 | 0 | 28.5 x 10 ³ | 285 x 10 ³ |
| 8 | 0 | 0 | 66.8 x 10 ³ | 668 x 10 ³ | 1.1 | 11 | 0 | 0 |
| 9 | 0 | 0 | 66.8 x 10 ³ | 668 x 10 ³ | 0 | 0 | 28.5 x 10 ³ | 285 x 10 ³ |
| 10 | 0 | 0 | 0 | 0 | 1.1 | 11 | 28.5 x 10 ³ | 285 x 10 ³ |
| 11 | 123 | 1225 | 44.5 x 10 ³ | 445 x 10 ³ | 0.7 | 7 | 0 | 0 |
| 12 | 123 | 1225 | 44.5 x 10 ³ | 445 x 10 ³ | 0 | 0 | 19 x 10 ³ | 190 x 10 ³ |
| 13 | 123 | 1225 | 0 | 0 | 0.7 | 7 | 19 x 10 ³ | 190 x 10 ³ |
| 14 | 0 | 0 | 44.5 x 10 ³ | 445 x 10 ³ | 0.7 | 7 | 19 x 10 ³ | 190 x 10 ³ |
| 15 | 92 | 919 | 33.4 x 10 ³ | 334 x 10 ³ | 0.6 | 5.5 | 14.3 x 10 ³ | 143 x 10 ³ |
| Test 1 | 230 | 2297 | 16.7 x 10 ³ | 167 x 10 ³ | 0.3 | 3 | 7.1 x 10 ³ | 71 x 10 ³ |
| Test 2 | 46 | 459 | 83.5 x 10 ³ | 835 x 10 ³ | 0.3 | 3 | 7.1 x 10 ³ | 71 x 10 ³ |
| Test 3 | 46 | 459 | 16.7 x 10 ³ | 167 x 10 ³ | 1.4 | 14 | 7.1 x 10 ³ | 71 x 10 ³ |
| Test 4 | 46 | 460 | 16.7 x 10 ³ | 167 x 10 ³ | 0.3 | 3 | 35.5 x 10 ³ | 355 x 10 ³ |

620

621 **Table 4:** p-values as a result of an ANOVA for high and low-intensity scenarios. Significant
 622 p-values are highlighted in bold letters with their level of significance shown as asterisks

| | Attribute | Mixture (M) | Assessor (A) | Replicate (R) | M*A | M*R | A*R |
|-----------|-----------|---------------------|---------------------|---------------|------------------|----------------|-------|
| HI | Pyrogenic | < 0.0001 *** | < 0.0001 *** | 0.442 | 0.009 ** | 0.441 | 0.707 |
| | Terpenic | < 0.0001 *** | < 0.042 * | 0.486 | 0.015 * | 0.357 | 0.753 |
| | Sulfurous | < 0.0001 *** | < 0.0001 *** | 0.286 | 0.441 | 0.091 | 0.402 |
| | Esteric | < 0.0001 *** | < 0.0001 *** | 0.189 | 0.000 *** | 0.042 * | 0.849 |
| LI | Pyrogenic | < 0.0001 *** | < 0.0001 *** | 0.311 | 0.006 ** | 0.019 * | 0.103 |
| | Terpenic | < 0.0001 *** | < 0.0001 *** | 0.408 | 0.002 ** | 0.095 | 0.830 |
| | Sulfurous | < 0.0001 *** | < 0.0001 *** | 0.888 | 0.000 *** | 0.061 | 0.847 |
| | Esteric | < 0.0001 *** | < 0.0001 *** | 0.864 | 0.007 ** | 0.995 | 0.669 |

623 * Significant ($\alpha=5\%$). ** very significant ($\alpha=1\%$). *** highly significant ($\alpha=0.1\%$)

624 **Table 5:** The experimental (Y) and theoretical (\hat{Y}) attributes scores for each test point used to
 625 validate the models along with R^2 , R_a^2 , and R_{Pred}^2 of the models for the four odor attributes at
 626 low and high intensities. (A) is the quality before and (B) is after adding the experimental
 627 results of the test point to the construction of the models

| | Low intensity | | | | | | | | High intensity | | | | | | | | | | |
|----------|---------------------|-----------|--------------------|-----------|---------------------|-----------|-------------------|-----------|---------------------|--------------|--------------------|-----------|---------------------|-----------|-------------------|-----------|-------|-------|-------|
| | Pyrogenic Attribute | | Terpenic Attribute | | Sulfurous Attribute | | Esteric Attribute | | Pyrogenic Attribute | | Terpenic Attribute | | Sulfurous Attribute | | Esteric Attribute | | | | |
| | Y | \hat{Y} | Y | \hat{Y} | Y | \hat{Y} | Y | \hat{Y} | Y | \hat{Y} | Y | \hat{Y} | Y | \hat{Y} | Y | \hat{Y} | | | |
| Test 1 | 0.0 | 1.8 | 1.9 | 1.6 | 4.8 | 4.1 | 2.4 | 1.5 | 1.3 | 1.4 | 2.4 | 2.5 | 4.1 | 3.8 | 1.2 | 1.2 | | | |
| Test 2 | 0.9 | 2.2 | 5.6 | 3.5 | 1.3 | 1.1 | 1.1 | 2.2 | 1.4 | 0.9 | 5.7 | 6.1 | 0.9 | 0.7 | 1.0 | 1.2 | | | |
| Test 3 | 4.4 | 3.6 | 1.4 | 1.2 | 2.8 | 3.3 | 0.4 | 0.9 | 1.9 | 2.7 | 1.7 | 2.2 | 2.8 | 2.4 | 2.7 | 1.7 | | | |
| Test 4 | 0.6 | 1.2 | 1.6 | 1.8 | 2.1 | 1.1 | 4.6 | 4.9 | 0.1 | 0.3 | 1.8 | 2.4 | 0.8 | 0.8 | 6.3 | 5.5 | | | |
| A | R^2 | 0.830 | 0.845 | 0.924 | 0.973 | 0.909 | 0.952 | 0.893 | 0.971 | R^2_a | 0.691 | 0.719 | 0.862 | 0.951 | 0.835 | 0.913 | 0.807 | 0.947 | |
| | R^2_{pred} | 0.360 | 0.446 | 0.739 | 0.913 | 0.661 | 0.823 | 0.609 | 0.900 | B | R^2 | 0.758 | 0.747 | 0.891 | 0.951 | 0.859 | 0.938 | 0.881 | 0.947 |
| | R^2_a | 0.626 | 0.610 | 0.832 | 0.925 | 0.783 | 0.904 | 0.816 | 0.918 | R^2_{pred} | 0.390 | 0.451 | 0.726 | 0.829 | 0.647 | 0.828 | 0.650 | 0.886 | |

628

629 **Table 6:** model coefficients for each attribute for the LI and HI scenarios with the significant ternary
 630 interactions highlighted.

| Coefficients | Pyrogenic attribute model | | Terpenic attribute model | | Sulfurous attribute model | | Esteric attribute model | |
|--------------|---------------------------|---------------|--------------------------|---------------|---------------------------|--------------|-------------------------|---------------|
| | LI | HI | LI | HI | LI | HI | LI | HI |
| b_D | -0.32 | 0.33 | 1.26 | 0.00 | 7.84 | 8.25 | 0.22 | 0.43 |
| b_T | 0.08 | 0.24 | 4.79 | 7.39 | 0.50 | 0.08 | 3.63 | 1.28 |
| b_F | 3.99 | 4.09 | 0.55 | 0.67 | 4.54 | 4.03 | -0.08 | 0.21 |
| b_C | 0.23 | 0.10 | 0.95 | 1.18 | 0.35 | -0.08 | 7.46 | 7.81 |
| b_{DT} | 9.06 | -0.04 | 2.21 | 9.33 | -9.43 | -10.11 | -1.84 | 0.82 |
| b_{DF} | 1.15 | 7.85 | -2.06 | -0.52 | 0.56 | -7.75 | 0.35 | 0.42 |
| b_{TF} | 8.23 | 1.58 | -3.17 | 1.64 | -0.85 | -2.68 | -4.21 | -0.55 |
| b_{DC} | 0.25 | 1.15 | -3.90 | 3.19 | -3.57 | -10.00 | 7.22 | 5.67 |
| b_{TC} | 1.33 | 1.54 | 3.04 | -7.03 | 2.40 | 3.45 | -6.77 | 2.03 |
| b_{FC} | -1.53 | -4.95 | 5.05 | 1.21 | -3.79 | -5.13 | 0.28 | 8.87 |
| b_{DTF} | 6.08 | -0.39 | 18.84 | -4.34 | -17.63 | 6.74 | -7.28 | -2.00 |
| b_{DTC} | -21.03 | -2.97 | 29.36 | 45.70 | -3.10 | 29.33 | -5.23 | -72.06 |
| b_{DFC} | 27.31 | -14.82 | -5.31 | -27.11 | -17.24 | 34.51 | -4.75 | 7.44 |
| b_{TFC} | 1.61 | -3.34 | -7.10 | 41.79 | 22.37 | -8.92 | -16.86 | -29.53 |

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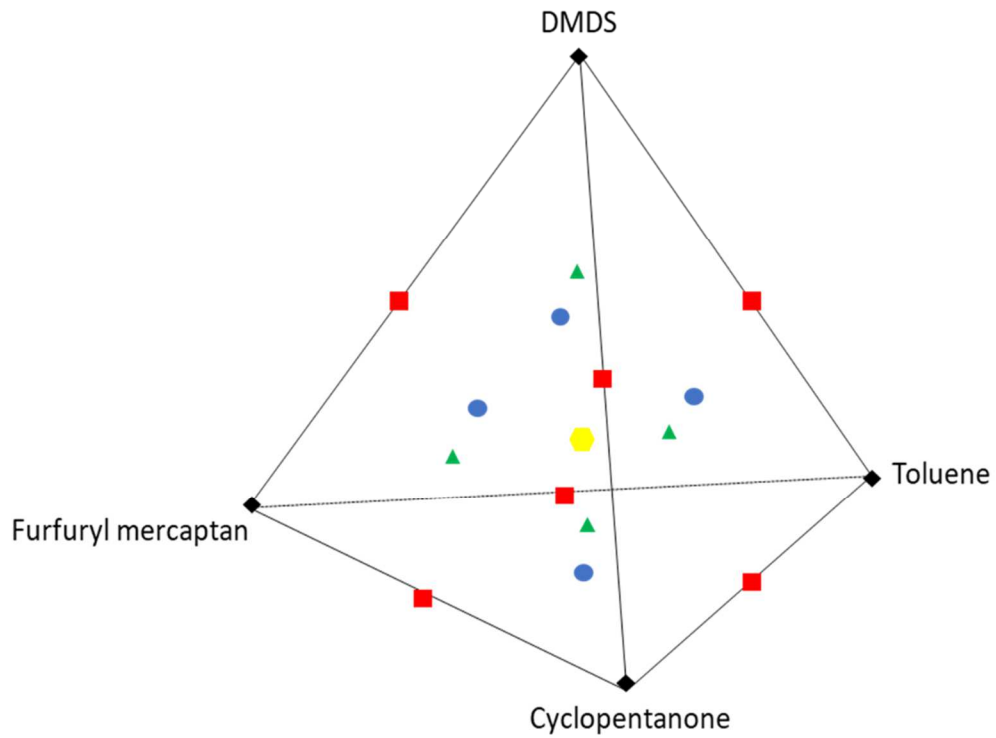


Figure 1: Experimental mixture design comprised of four constituents in their pure form (black diamonds), six binary mixtures (red squares), four equiproportional mixtures (in terms of OAV) of the three constituents (blue dots), and one equiproportional mixture of the four constituents (yellow hexagon). Green triangles are test points located in the center of the tetrahedrons formed by one vertex and three adjacent mid-edge points.

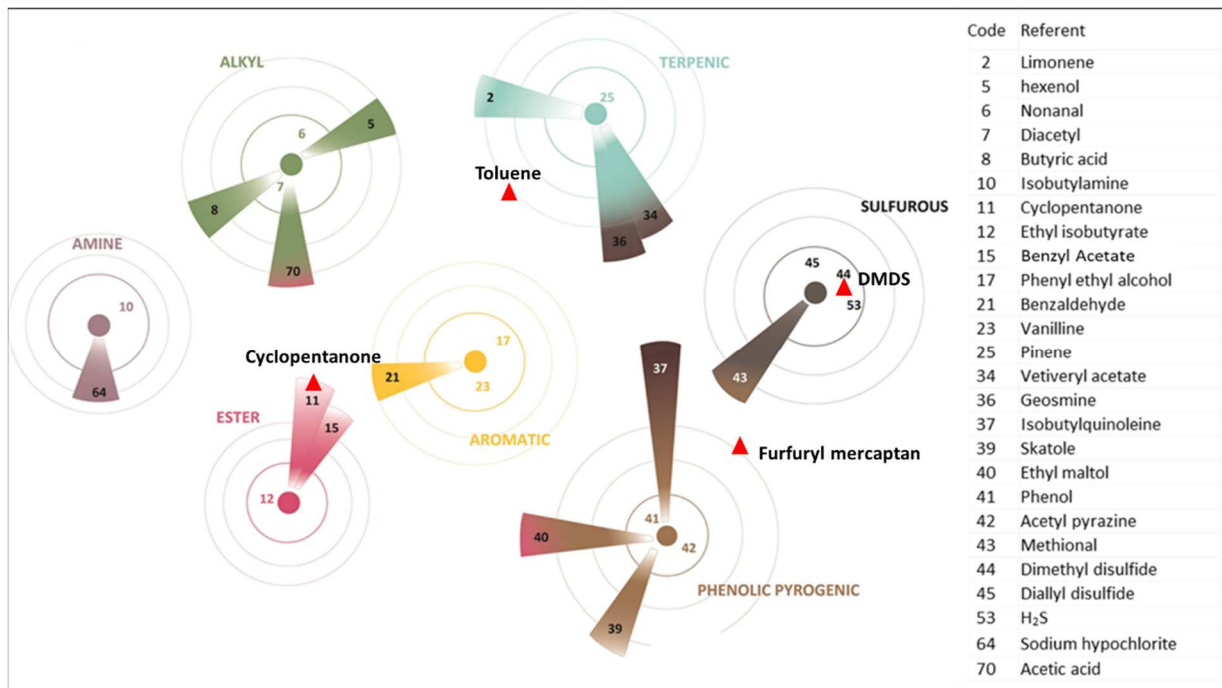


Figure 2: The 2-D representation of the 3D olfactory space with the referent collection of LdN. Red triangles represent the positioning of the studied compounds: toluene, cyclopentanone, DMDS, and furfuryl mercaptan

Figure 3: Isochrone 2-D presentation of the four models for LI scenario. In each figure, the proportion of one compound was fixed at 0 for easier visualization. Only the compounds with maximum effects on the model were not set to 0%.

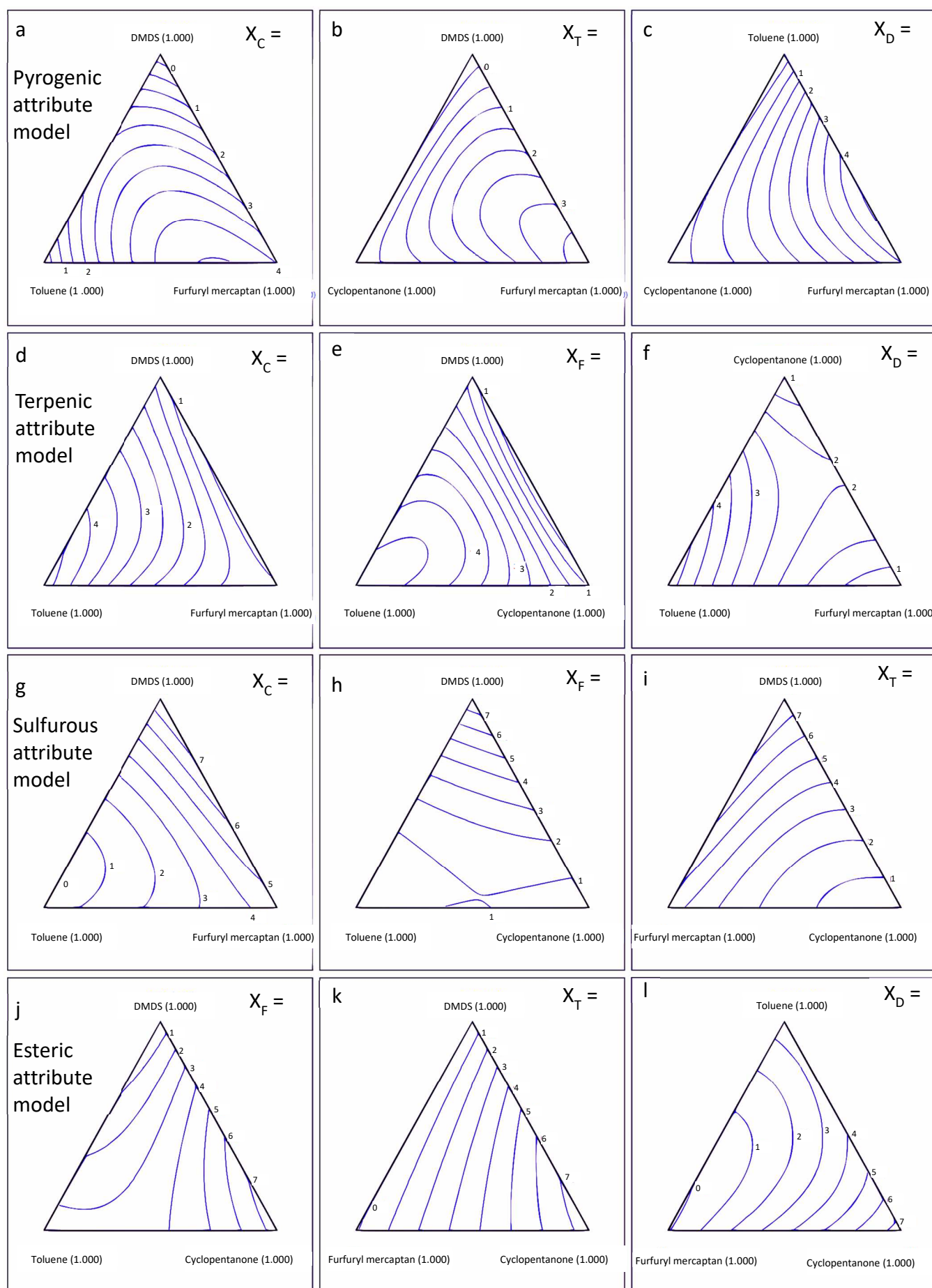


Figure 4: Isochrone 2-D presentation of the four models at HI. In each figure, the proportion of one compound was fixed at 0 for easier visualization. Only the compounds with maximum effects on the model were not fixed at 0%.

