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1 **OOPS, the Ontology for Odor Perceptual Space: from molecular composition to sensory**
2 **attributes of odor objects**

3
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5
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9
10 **Abstract.** When creating a flavor to elicit a specific odor object characterized by odor sensory attributes
11 (OSA), expert perfumers or flavorists use mental combinations of odor qualities (OQ) such as Fruity,
12 Green, Smoky. However, OSA and OQ are not directly related to the molecular composition in terms
13 of odorants that constitute the chemical stimuli supporting odor object perception because of the
14 complex non-linear integration of odor mixtures within the olfactory system. Indeed, single odorants are
15 described with odor descriptors (OD), which can be found in various databases. Although classifications
16 and aroma wheels studied the relationships between OD and OQ, the results are highly dependent of the
17 studied products. Nevertheless, ontologies have proved to be very useful in sharing concepts across
18 applications in a generic way but also to allow experts' knowledge integration implying non-linear
19 cognitive processes. In this paper we constructed the Ontology for Odor Perceptual Space (OOPS) to
20 merge OD into a set of OQ best characterizing the odor further translated in a set of OSA thanks to
21 expert knowledge integration. Results showed that OOPS can help to bridge molecular composition to
22 odor perception and description as demonstrated in the case of wines.

23
24 **Keywords:** Odor perceptual space, odor quality, odor descriptor, odorant, wine, expert knowledge

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29 **1. Introduction**

30 Within the physical world, colors are characterized by light wavelength, tones by sound frequency,
31 and odors by the chemical composition of the stimulus. Within the perceptual space, colors are defined
32 by specific words like red or blue, tones are referred to by dedicated notes like C or Eb, while odors are
33 usually identified by naming their sources like rose or lemon [1]. Therefore, if colors and tones can be
34 well defined experimentally, odors are difficult to describe with a consensual vocabulary but also
35 difficult to measure physically because they mostly results from the coding, by the olfactory system, of
36 complex mixtures of odorants, which are volatile organic compounds varying in chemical nature and
37 concentration [2].

38 Olfactory coding induce perceptual interactions, which can take place at several steps of the olfactory
39 information processing, and the odor perceived from mixtures of odorants is not a simple sum of the
40 odors of each odorant embedded in the mixture [2]. Synergy and masking effects have been often
41 reported ([3]; [4]; [5]; [6]), but also perceptual dominance [7], or configural and elemental perception
42 ([8]; [9]). For instance, a ternary mixture, composed of three odorants respectively described as
43 “strawberry”, “caramel” and “violet”, elicits, at a specific proportion of each compound, the perception
44 of a “pineapple” odor ([10]). The mechanisms behind these perceptual interactions are not well
45 understood yet and still poorly investigated. As a consequence, the description of the perceptual outcome
46 of a complex mixture using odor sensory attributes (OSA), is not straightforward. The global odor
47 percept is especially hardly predictable on the basis of the mixtures’ chemical composition, namely each
48 single odorant odor description, which relies on specific odor descriptors (OD).

49 Several databases are compiling OD of large sets of odorants: Arctander’s handbook ([11]), Atlas of
50 odor character profiles ([12]), Fenaroli’s handbook ([13]), Flavor-Base (Leffingwell & Associates,
51 <http://www.leffingwell.com/flavbase.htm>), Flavournet ([14]), Flavors and Fragrances of Sigma-Aldrich
52 (<http://www.sigmaaldrich.com/industries/flavors-and-fragrances.html>), The good scents company
53 ([15]). However, the vocabulary used in describing odor is extensive and ambiguous. As a matter of
54 fact, are “citrus odor” and “odor of citrus” referring to the same odor descriptors? ([16]). Moreover,
55 there is no agreement about the number of OD essential to cover the complete range of odor stimuli

56 which varies from 4 to 146 ([17]). Though several teams worked on the different relationships,
57 associations, or similarities between OD, none of them had yet gained wide acceptance ([18]; [19]; [20]).

58 In most cases, it is not possible to make a direct link between the OD of the odorants released from
59 an odor source, e.g. a food product, and its perceived odor. This is probably the reason why flavorists,
60 who are experts in creating specific odors from combinations of odor active raw materials such as
61 molecules, are not using OD but a rather different set of descriptors to organize their practical knowledge
62 acquired along with experience ([21]). Indeed, to conceptualize the perception of a specific odor trait of
63 an odor source, further called odor sensory attribute (OSA), flavorists are combining a specific set of
64 odor qualities (OQ). For example, according to an expert flavorist, the OSA “Cherry cooked” is
65 composed of the OQ “Almond”, “Cooked”, “Floral”, “Fruity”, “Green”, “Peel” and “Spicy”, which may
66 be considered as “blocks”, where each block could be composed of several molecules referring to
67 different OD (e.g. [22]). In a sense, OQ could be considered as broad categories, related more to odor
68 material than to molecules. Classifications and flavor wheels usually dedicated to a specific category of
69 food products such as wine or coffee have been established and could help to make links between OD
70 and OQ. However, these classifications are highly dependent of the studied databases and/or food
71 product and are hardly reconcilable ([12]; [19]; caramel: [23]; honey: International Honey Commission
72 (IHC) <http://www.ihc-platform.net/reports.html>; wine: [24]). For example, whereas the OD “Apple” is
73 classified in the OQ “Fruity” in the five above cited sources, the OD “Vanilla” is classified in five
74 different OQ “Spicy”, “Balsamic”, “Warm”, “Wood/Phenolic” or “Caramel/Vanilla” depending on the
75 source.

76
77 To overcome these issues, this paper had for aim to use the ontology approach to make the link
78 between OQ, the concepts manipulated by experts and OD, the odor descriptors used to qualify odorants.
79 With the help of an expert flavorist, we developed and formalized the Ontology for Odor Perceptual
80 Space (OOPS) to organize the vocabulary of the odor perceptual space and to describe the relationships
81 between the OD and OQ. The aim was to fusion the information expressed by OD in order to formally
82 characterize odors into a conceptual and generic annotation of OQ, namely not associated to a specific

83 food product. We further used the OOPS to predict the odor profiles of two red wines, that is to say the
84 OSA used by a trained panel to describe these wines ([25]).

85

86 2. Materials and methods

87

88 2.1. Wines

89 Villière et al. ([25]) studied the sensory profiles and the chemical composition in terms of odor-active
90 compounds of sixteen red wines (8 Pinot Noir and 8 Cabernet Franc), varying according to their
91 exemplarity for the grape variety ([26]). Sensory profiles resulted in the identification of 15 discriminant
92 OSA between the wines according to their grape varieties (Table 1). The results of Gas Chromatography
93 - Mass Spectrometry - Olfactometry (GC-MS-O) analyses led to identify 46 odorant zones (molecules
94 and mixtures of molecules) which corresponded to 49 identified odorants (Table 2). Raw data are
95 available on an open-source repository ([27]).

96

97 **Table 1.** List of the 15 odor sensory attributes (OSA).

Bell pepper
Blackcurrant bud
Blackcurrant fresh
Cherry cooked
Cherry fresh
Cherry stone
Cut-grass
Leather
Prune
Smoky
Strawberry fresh
Toasty
Vanilla
Violet
Woody

98

99 **Table 2.** Molecular space of the 16 red wines identified by GC-MS-O. List of the 49 odorants identified
100 by their CAS number and name.

CAS	Odorant
4312-99-6	1-Octen-3-one

431-3-8	2,3-Butanedione
600-14-6	2,3-Pentanedione
91-10-1	2,6-Dimethoxyphenol
90-05-1	2-Methoxyphenol
110-19-0	2-Methylpropyl acetate
620-17-7	3-Ethylphenol
24683-00-9	3-Isobutyl-2-methoxypyrazine
25773-40-4	3-Isopropyl-2-methoxypyrazine
51755-83-0	3-Mercapto-1-hexanol
123-51-3	3-Methyl-1-butanol
590-86-3	3-Methylbutanal
123-92-2	3-Methylbutyl acetate
2785-89-9	4-Ethyl guaiacol
123-07-9	4-Ethylphenol
626-89-1	4-Methyl-1-pentanol
75-07-0	Acetaldehyde
64-19-7	Acetic acid
100-52-7	Benzaldehyde
122-78-1	Benzene acetaldehyde
60-12-8	Benzene ethanol
100-51-6	Benzene methanol
107-92-6	Butyric acid
96-48-0	Butyrolactone
334-48-5	Decanoic acid
75-18-3	Dimethyl sulfide
64-17-5	Ethanol
141-78-6	Ethyl acetate
105-54-4	Ethyl butanoate
110-38-3	Ethyl decanoate
106-33-2	Ethyl dodecanoate
123-66-0	Ethyl hexanoate
106-32-1	Ethyl octanoate
105-37-3	Ethyl propanoate
7452-79-1	Ethyl-2-methylbutanoate
97-62-1	Ethyl-2-methylpropanoate
108-64-5	Ethyl-3-methylbutanoate
142-62-1	Hexanoic acid
503-74-2	Isovaleric acid
108-39-4	m-Cresol
74-93-1	Methanethiol
3268-49-3	Methional
505-10-2	Methionol
80-62-6	Methyl-2-methylpropenoate
106-44-5	p-Cresol
103-45-7	Phenethyl acetate
108-95-2	Phenol
7446-09-5	Sulphur dioxide
39212-23-2	Whiskeylactone

102 **2.2. Elicitation of odor qualities (OQ) by expert flavorists**

103 Four senior flavorists participated in the expert knowledge collection. The elicitation process was
 104 based on a 1-hour private guided interview. Flavorists were not aware of the studied food matrix in order
 105 to collect unbiased data regarding the food product.

106 The experts received monadically the 15 OSA used in the wines' sensory profiles (Table 1) and were
 107 asked i) if the OSA was composed of a single OQ or of more than one OQ and ii) in case the considered
 108 OSA was composed of several OQ, to enumerate the OQ that were needed to construct the OSA. Then
 109 we aggregated the information of the four flavorists following Equation 1, *OSA* being a given odor
 110 sensory attribute, $Exp1[OQ(OSA)]$, $Exp2[OQ(OSA)]$, $Exp3[OQ(OSA)]$ and $Exp4[OQ(OSA)]$ being the
 111 sets of OQ used to describe an OSA by the four experts.

112

113 $OSA = Exp1[OQ(OSA)] \cup Exp2[OQ(OSA)] \cup Exp3[OQ(OSA)] \cup Exp4[OQ(OSA)]$ Equation 1

114

115 As a result, we obtained a binary matrix made of in rows the 20 OQ elicited (Almond, Cooked, Cut-
 116 Grass, Floral, Fresh, Fruity, Green, Honey, Lactony, Leather, Peel, Smoky, Spicy, Sulfurous, Toasty,
 117 Vanilla, Vegetable, Violet, Wine-like and Woody) and in columns the target OSA (Table 3).

118

119 **Table 3: Link between the 20 OQ (rows) and the 15 OSA (columns), represented as a binary**
 120 **matrix.** The value 1 indicates that the OQ was part of the composition of the OSA.

OQ	Bell pepper	Blackcurrant	Blackcurrant	Cherry	Cherry fresh	Cherry stone	Cut-grass	Leather	Prune	Smoky	Strawberry	Toasty	Vanilla	Violet	Woody
Almond				1	1	1			1						
Cooked				1	1	1			1		1				
Cut-grass							1								
Floral	1	1	1	1	1	1					1				
Fresh	1	1	1												
Fruity		1	1						1		1				
Green	1	1	1	1	1	1					1				
Honey									1						

Lactoniy									1						
Leather								1							
Peel				1	1	1									
Smoky										1					
Spicy				1	1	1									
Sulfurous	1	1	1												
Toasty	1											1			
Vanilla		1											1		
Vegetable	1														
Violet															
Wine-like		1	1												
Woody															1

121

122 2.3. Quantitative description of the odorants

123 We compiled the data of three databases to collect the odor descriptors (OD) of the 49 odorants
124 identified in the wines: Arctander’s handbook (3102 chemicals described by Steffen Arctander himself),
125 Flavor-Base (commercially available Leffingwell & Associates database, marketed as Flavor-Base Pro
126 © 2010, flavor descriptions collected from many sources over the course of more than 40 years) and
127 The good scents company (publicly available database, the odor descriptions from one to several sources
128 are listed in the "Organoleptic Properties" section).

129 We extracted manually the OD from these databases. The words describing the odorants were
130 tokenized. Suffixes (e.g. “like”, “note”), auxiliary verbs (e.g. “has”) and some other words that did not
131 rely on olfactory information (e.g. “powerful”) were discarded. Unlike the analysis of the Arctander
132 database proposed by [17], we kept all the OD into account and we did not combine very similar
133 descriptors (like Leather/Leathery or Wine/Winey) For instance, the odor of Ethyl butanoate (CAS 105-
134 54-4) was specified in Arctander as “Powerful, ethereal-fruity odor suggestive of Banana and Pineapple,
135 and very diffusive” these annotations resulted in the set of OD: “ethereal-fruity”, “banana” and
136 “pineapple”.

137 Then we created the OD database by aggregating the information of the three databases following
138 Equation 2, M being a given odorant, $Arct[OD(M)]$, $FlavorBase[OD(M)]$ and $Goodscent[OD(M)]$ being
139 the sets of OD of the odorant M by the Arctander, Flavor-Base and Goodscent databases. We ended up
140 with 175 different OD for the 49 odorants.

141

142 $OD\ database(M) = Arct[OD(M)] \cup FlavorBase[OD(M)] \cup Goodscent[OD(M)]$ Equation 2

143

144 For a given odorant, a description was thus provided by the OD database as a set of terms in which each
145 term may be associated to an “intensity”. We defined this intensity as the number of citation of the same
146 OD for a given odorant across the databases: the higher the number of citation, the more “intense” the
147 smell related to this OD was expected for the odorant. As an example, the odorant description of Ethyl
148 butanoate was {ethereal-fruity; banana; pineapple} by Arctander, {ethereal; fruity; buttery; pineapple;
149 banana; ripe fruit; juicy} by Flavor-base and {fruity; juicy; pineapple; cognac} by GoodScents. The
150 resulting quantitative description of Ethyl butanoate in the OD database was the following: OD(Ethyl
151 butanoate) = [(banana, 2); (buttery, 1); (cognac, 1); (ethereal, 1); (ethereal-fruity, 1); (fruity, 2); (juicy,
152 2); (pineapple, 3); (ripe fruit, 1)].

153

154 **2.4. Relationships between odor descriptors (OD) and odor qualities (OQ)**

155 The correspondence between an OD and one or several OQ was obtained thanks to the expertise of
156 a junior flavorist. This expert was not one of the four flavorists previously interviewed for OQ elicitation.
157 The methodology used to obtain the relationships was based on a check-all-that-apply (CATA)
158 questionnaire (Dooley et al., 2010). The CATA list consisted of the 20 OQ defined by the experts during
159 the elicitation step (see 2.2 above). For each OD of the OD database, the flavorist was asked if the OD
160 supported none, one, or several OQ. For instance for the OD “Apple”, the flavorist was asked to tick all
161 the OQ that correspond e.g. “Fruity”.

162 We obtained a binary matrix with the OQ in columns and OD in rows. These results allowed us to
163 translate each OD sets into OQ sets. For example with Ethyl butanoate, described as OD(Ethyl
164 butanoate) = [(banana, 2); (buttery, 1); (cognac, 1); (ethereal, 1); (ethereal-fruity, 1); (fruity, 2); (juicy,
165 2); (pineapple, 3); (ripe fruit, 1)], we could now assume that the OQ set of Ethyl butanoate is the
166 following (Table 4): OQ(Ethyl butanoate) = [(Almond, 0); (Cooked, 0); (Cut-grass, 0); (Floral, 0);
167 (Fresh, 0); (Fruity, 9); (Green, 0); (Honey, 0); (Lactony, 0); (Leather, 0); (Peel, 0); (Smoky, 0); (Spicy,
168 0); (Sulfurous, 0); (Toasty, 0); (Vanilla, 0); (Vegetable, 0); (Violet, 0); (Wine-like, 0); (Woody, 0)]

169

170 **Table 4.** Link between the nine OD of Ethyl butanoate (rows) and the 20 OQ (columns), represented as
171 a binary matrix. The intensity of each OD is specified in the second column.

OD	Intensity	Almond	Cooked	Cut-grass	Floral	Fresh	Fruity	Green	Honey	Lactonic	Leather	Peel	Smoky	Spicy	Sulfurous	Toasty	Vanilla	Vegetable	Violet	Wine-like	Woody
banana	2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
buttery	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
cognac	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ethereal	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ethereal-fruity	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fruity	2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
juicy	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
pineapple	3	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ripe fruit	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0

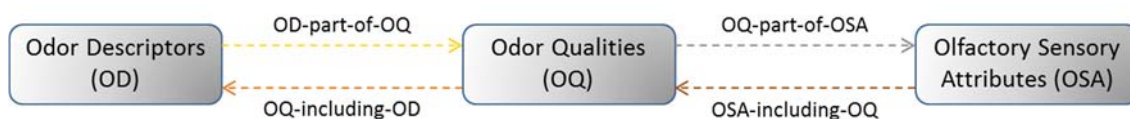
172

173 3. The Ontology for Odor Perceptual Space (OOPS)

174

175 We formalized the Ontology for Odor Perceptual Space (OOPS) as a tuple {C, R, P}, where C
176 corresponded to the three classes OD, OQ and OSA with respectively 175 sub-classes from the databases
177 aggregation, 20 sub-classes from the expertise collection and 15 sub-classes from the sensory evaluation
178 of the wines; R represented the hierarchical relations among the classes by “is-a” relations; and P, as
179 properties, represented the non-hierarchical associative relations between classes as shown in Figure 1.

180

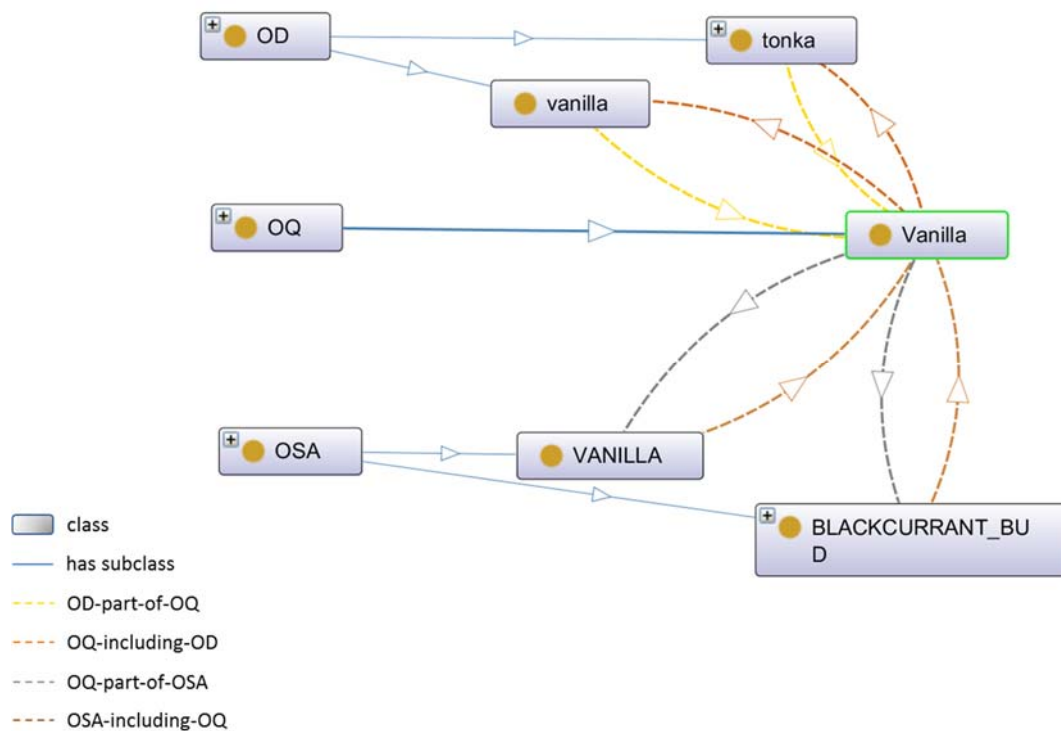


181

182 **Figure 1.** Object properties between the classes OD, OQ and OSA of the OOPS ontology.

183

184 Results from the data collection in table forms, were implemented in OWL using the software Protégé
 185 (open-source ontology editor, version 5.2.0; [28]). This allowed the visualization of the properties
 186 among the classes OD, OQ and OSA; an example is shown in Figure 2 for the OQ “Vanilla”. Such
 187 representation highlighted that the OD “vanilla” and “tonka” are part of the OQ “Vanilla”. Moreover,
 188 the OQ “Vanilla” is part of the OSA “VANILLA” and “BLACKCURRANT BUD”. From a practical
 189 point of view, these relationships illustrated that an odorant described as “vanilla” or “tonka” were part
 190 of the OQ category “Vanilla” and should contribute to the perceptual construction of the odor of Vanilla
 191 and Blackcurrant bud, which are OSA.
 192



193
 194 **Figure 2.** Properties and relationships among the classes OD, OQ and OSA considering the OQ Vanilla.

195

196 The implementation of the OOPS in OWL conferred the ability to mine the data through queries such
 197 as:

198 - In which OQ, the OD “almond” is included?

199 <OQ-including-OD some almond>:"Almond"

200 - Which OD are parts of the OQ “Almond”?

201 <OD-part-of-OQ some Almond>:“almond”

202 - In which OSA, the OQ “Almond” is included?

203 <OSA-including-OQ some Almond>: “CHERRY_COOKED”, “CHERRY_FRESH”,
204 “CHERRY_STONE”, “PRUNE”

205 - Which OQ are parts of the OSA “Prune”?

206 <OQ-part-of-OSA some Prune>: “Almond”, “Cooked”, “Fruity”, “Honey”, “Lactonic”

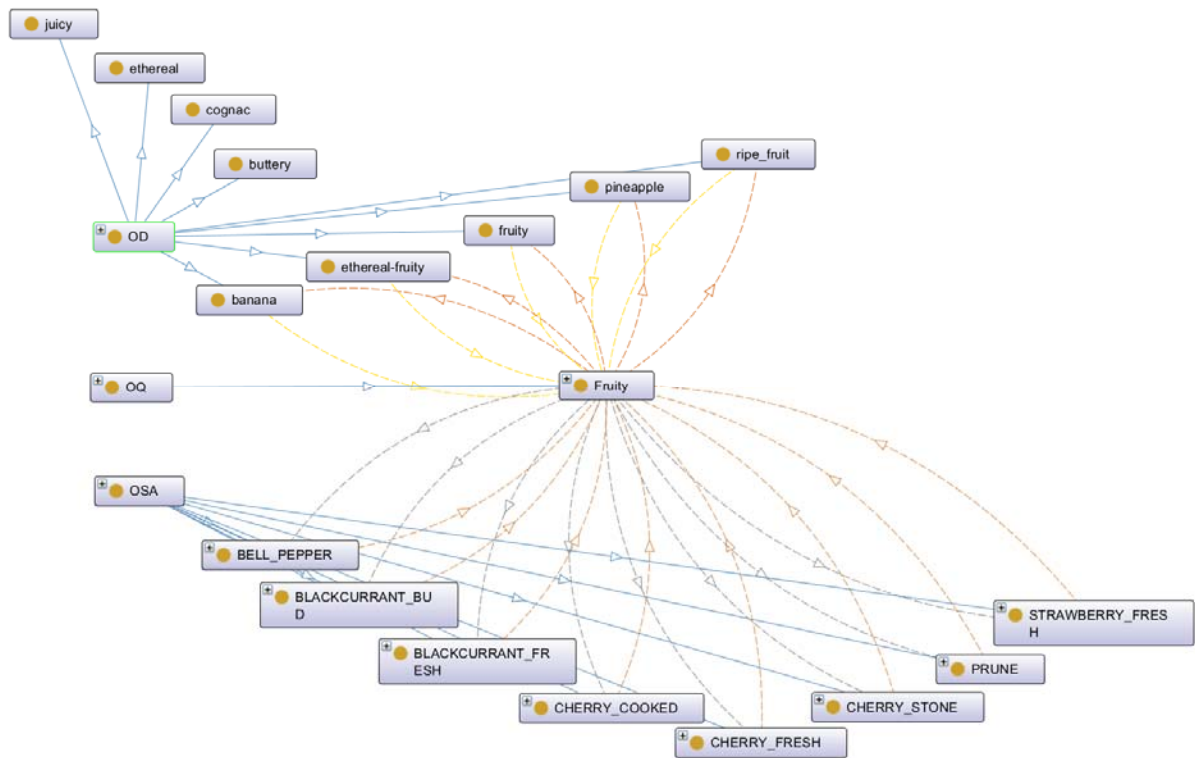
207

208 All together the OOPS led to the fast visualization of relationships among the three classes OD, OQ
209 and OSA in order to estimate the OQ or OSA profiles of odorants (Figure 3). As for example with the
210 odorant Ethyl butanoate, described by the OD(Ethyl butanoate) = [(banana, 2); (buttery, 1); (cognac, 1);
211 (ethereal, 1); (ethereal-fruity, 1); (fruity, 2); (juicy, 2); (pineapple, 3); (ripe fruit, 1)], we were able to
212 estimate its contribution to the OQ “Fruity” and then to the OSA “Bell pepper”, “Blackcurrant bud”,
213 “Blackcurrant fresh”, “Cherry cooked”, “Cherry fresh”, “Cherry stone”, “Prune” and “Strawberry
214 fresh”.

215 Intensities of the OD were spread along the relationships between OD and OQ as well as between
216 OQ and OSA. The OQ set of Ethyl butanoate was equal to OQ(Ethyl butanoate) = [(Almond, 0);
217 (Cooked, 0); (Cut-grass, 0); (Floral, 0); (Fresh, 0); (Fruity, 9); (Green, 0); (Honey, 0); (Lactony, 0);
218 (Leather, 0); (Peel, 0); (Smoky, 0); (Spicy, 0); (Sulfurous, 0); (Toasty, 0); (Vanilla, 0); (Vegetable, 0);
219 (Violet, 0); (Wine-like, 0); (Woody, 0)], as previously mentioned. Regarding the OSA set, we obtained:

220 OSA(Ethyl butanoate)= [(Bell pepper, 9); (Blackcurrant bud, 9); (Blackcurrant fresh, 9); (Cherry
221 cooked, 9); (Cherry fresh, 9); (Cherry stone, 9); (Cut-grass, 0); (Leather, 0); (Prune, 9); (Smoky, 0);
222 (Strawberry fresh, 9); (Toasty, 0); (Vanilla, 0); (Violet, 0); (Woody, 0)].

223



224
 225 **Figure 3.** Properties and relationships among the classes OD, OQ and OSA considering the OD of the
 226 odorant Ethyl butanoate.

227
 228 **4. Application of the OOPS to wines**

229
 230 We applied the OOPS to establish the OQ and OSA profiles of two wines from their molecular
 231 composition. Two wines were selected among the sixteen used to build the ontology: one good example
 232 of the grape variety Pinot Noir (PN-A) and one good example of the grape variety Cabernet Franc (CF-
 233 A).

234 We estimated the OQ and OSA sets of each odorant present in the two wines. For a given wine, we
 235 summed the OQ and OSA sets of the odorants included in the wine weighted by their intensities.

236 Firstly, we obtained the OQ profiles of the wines PN-A and CF-A, respectively OQ(PN-A) and
 237 OQ(CF-A):

238

239 OQ(PN-A) = [(Almond, 1); (Cooked, 3); (Cut-grass, 2); (**Floral, 25**); (Fresh, 1); (**Fruity, 118**); (**Green,**
240 **12**); (Honey, 6); (Lactony, 1); (Leather, 1); (Peel, 4); (**Smoky, 24**); (Spicy, 10); (Sulfurous, 3); (Toasty,
241 2); (Vanilla, 4); (Vegetable, 8); (Violet, 0); (Wine-like, 9); (Woody, 5)]

242

243 OQ(CF-A) = [(Almond, 3); (Cooked, 4); (Cut-grass, 1); (**Floral, 20**); (Fresh, 1); (**Fruity, 97**); (**Green,**
244 **15**); (Honey, 3); (Lactony, 0); (Leather, 4); (Peel, 4); (**Smoky, 20**); (Spicy, 1); (Sulfurous, 4); (Toasty,
245 0); (Vanilla, 0); (**Vegetable, 21**); (Violet, 0); (Wine-like, 10); (Woody, 4)]

246

247 Values in bold corresponded to OQ with an intensity higher than 5% of the total intensity of the OQ in
248 the corresponding wine. At this step, the two wines were described as Fruity wines with Floral, Green
249 and Smoky notes, and CF-A differed from PN-A with its Vegetable note.

250 Then, we obtained the OSA profiles of the wines PN-A and CF-A, respectively OSA(PN-A) and
251 OSA(CF-A):

252

253 OSA(PN-A) = [(**Bell pepper, 51**); (**Blackcurrant bud, 172**); (**Blackcurrant fresh, 168**); (**Cherry**
254 **cooked, 55**); (**Cherry fresh, 55**); (**Cherry stone, 55**); (Cut-grass, 2); (Leather, 1); (**Prune, 129**);
255 (Smoky, 24); (**Strawberry fresh, 158**); (Toasty, 2); (Vanilla, 4); (Violet, 0); (Woody, 5)]

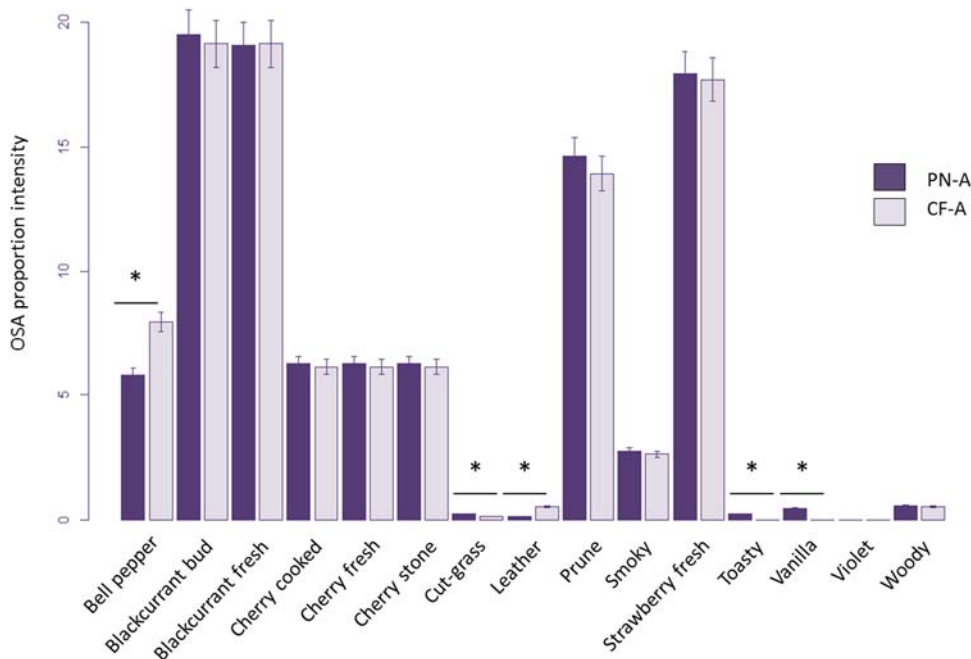
256

257 OSA(CF-A) = [(**Bell pepper, 61**); (**Blackcurrant bud, 147**); (**Blackcurrant fresh, 147**); (**Cherry**
258 **cooked, 47**); (**Cherry fresh, 47**); (**Cherry stone, 47**); (Cut-grass, 1); (Leather, 4); (**Prune, 107**);
259 (Smoky, 20); (**Strawberry fresh, 136**); (Toasty, 0); (Vanilla, 0); (Violet, 0); (Woody, 4)]

260

261 Values in bold corresponded to OSA with an intensity higher than 5% of the total intensity of the OSA
262 in the corresponding wine. From these OSA sets we were able to point out differences among the two
263 wines (Figure 4). The PN-A wine was identified with higher proportion intensity of the OSA Cut-grass,
264 Toasty and Vanilla and lower proportion intensity of the OSA Bell pepper and Leather than the CF-A
265 wine. These results were consistent with the literature because PN and CF wines are described as Fruity
266 wines. Moreover, CF wines are usually described as having a Bell pepper ([29]).

267 According to the sensory profiles of the wines ([25]), PN-A was perceived as more Toasty and
 268 Vanilla than CF-A which is also find with the OOPS approach. However some differences between the
 269 wines did not follow their sensory profiles. Indeed, from sensory evaluation the CF-A wine was
 270 perceived with a higher intensity of the OSA Cut-grass and a lower intensity of the OSA Leather than
 271 PN-A, from the OOPS approach we obtained the opposite.
 272



273
 274 **Figure 4.** OSA proportions in the PN-A and CF-A wines. Bars display proportion of OSAs, and wines
 275 are indicated by the dark (PN-A) or light (CF-A) shading. The horizontal line on the top of the bars
 276 indicates significantly different proportion of OSA between the two wines (* = 5%).

277
 278 **5. Conclusions and future work**

279
 280 In this paper we presented the building of the OOPS, the Ontology for Odor Perceptual Space,
 281 designed for fixing the vocabulary of the odor perceptual space and the relationships between the
 282 different terms involved: OD, OQ and OSA. The genericity of the OOPS was achieved by integrating
 283 flavorist's expertise.

284 An example of application of the OOPS on a food product was presented with the odorant
285 composition of two red wines to estimate their OQ and OSA profiles. We were able to obtain a good
286 prediction of the OQ and OSA profiles.

287 This work, following a semantic approach, will provide a standard tool for communication among
288 experts to increase knowledge sharing and can be helpful in training sensory panels for odor profiling.
289 Therefore this ontology might be used to establish sensory profiles of food product from their chemical
290 composition. Because of the genericity of the tool, the OOPS will be available for studying various food
291 products.

292 However we would like to precise that this approach has several ways of improvement. We should
293 keep in mind that the perception of odorants mixture is not a simple sum of each odorants' odor. Non-
294 linear combinations among the OD, OQ and OSA could then be developed from the knowledge we
295 collected and formalized. In addition, the intensity or concentration of odorants might be integrated in
296 the OOPS approach to intensity balance the OD sets and further impact OQ and OSA profiles prediction.

297 Finally, one advantage of the ontology formalization is that data could be further modified to adapt
298 to domain changes or to new usages. Indeed OD or OQ may become outdated and may be
299 incomprehensible to subjects from different cultural backgrounds or non-native English speakers [30].
300 One following work will be to increase the data and knowledge embedded in the OOPS to allow more
301 complete and accurate predictions.

302

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308

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