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

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Alice Roche[1], Nathalie Mejean Perrot[2] and Thierry Thomas-Danguin[1]

1. Centre des Sciences du Goût et de l'Alimentation, AgroSup Dijon, CNRS, INRA, Université Bourgogne Franche-Comté, F-21000 Dijon, France
2. UMR MIA 518, AgroParisTech, INRAE, Université Paris Saclay, F-75015 Paris, France

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

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

1. Introduction

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

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

Several databases are compiling OD of large sets of odorants: Arctander's handbook ([11]), Atlas of odor character profiles ([12]), Fenaroli's handbook ([13]), Flavor-Base (Leffingwell & Associates, http://www.leffingwell.com/flavbase.htm), Flavornet ([14]), Flavors and Fragrances of Sigma-Aldrich (http://www.sigmaaldrich.com/industries/flavors-and-fragrances.html), The good scents company ([15]). However, the vocabulary used in describing odor is extensive and ambiguous. As a matter of fact, are "citrus odor" and "odor of citrus" referring to the same odor descriptors? ([16]). Moreover, there is no agreement about the number of OD essential to cover the complete range of odor stimuli which varies from 4 to 146 ([17]). Though several teams worked on the different relationships, associations, or similarities between OD, none of them had yet gained wide acceptance ([18]; [19]; [20]).

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

To overcome these issues, this paper had for aim to use the ontology approach to make the link between OQ, the concepts manipulated by experts and OD, the odor descriptors used to qualify odorants. With the help of an expert flavorist, we developed and formalized the Ontology for Odor Perceptual Space (OOPS) to organize the vocabulary of the odor perceptual space and to describe the relationships between the OD and OQ. The aim was to fusion the information expressed by OD in order to formally characterize odors into a conceptual and generic annotation of OQ, namely not associated to a specific food product. We further used the OOPS to predict the odor profiles of two red wines, that is to say the OSA used by a trained panel to describe these wines ([25]).

2. Materials and methods

2.1. Wines

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

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

Table 2. Molecular space of the 16 red wines identified by GC-MS-O. List of the 49 odorants identified 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 guaïacol
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	Whyskeylactone

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

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

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

$$OSA = Exp1[OQ(OSA)] \cup Exp2[OQ(OSA)] \cup Exp3[OQ(OSA)] \cup Exp4[OQ(OSA)] \quad \text{Equation 1}$$

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

Table 3: Link between the 20 OQ (rows) and the 15 OSA (columns), represented as a binary 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**

2.3. Quantitative description of the odorants

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

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

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

$$OD\ database(M) = Arct[OD(M)] \cup FlavorBase[OD(M)] \cup Goodscent[OD(M)] \qquad \text{Equation 2}$$

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

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

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

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

Table 4. Link between the nine OD of Ethyl butanoate (rows) and the 20 OQ (columns), represented as 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

3. The Ontology for Odor Perceptual Space (OOPS)

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

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

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

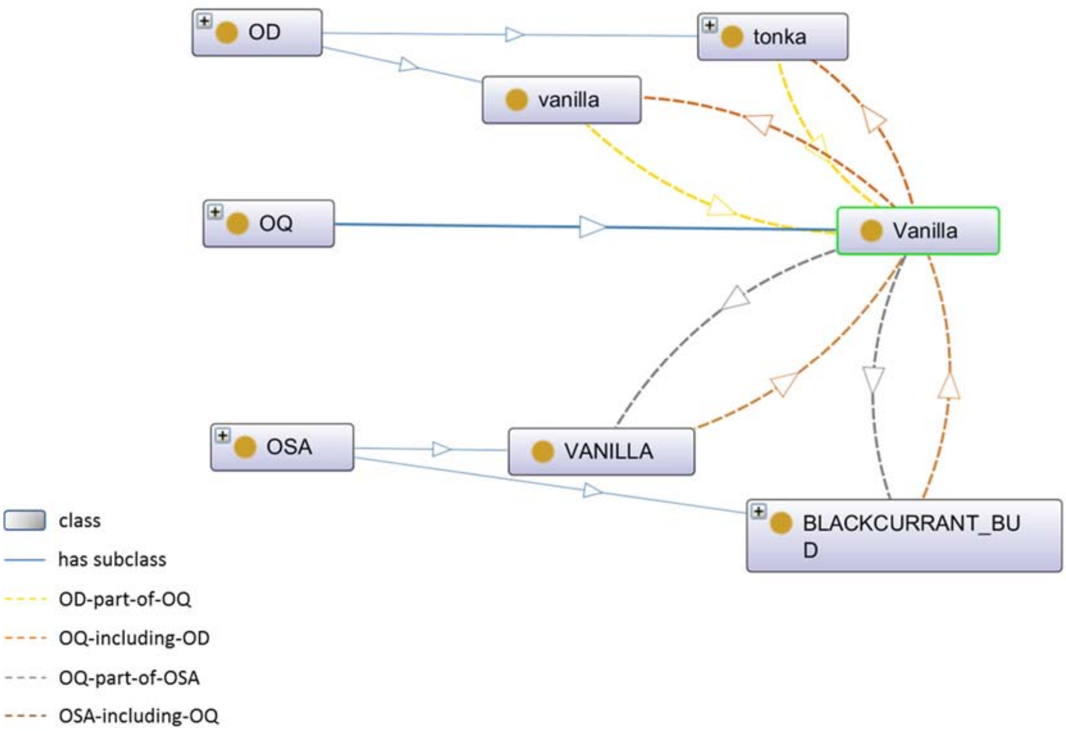

Figure 2. Properties and relationships among the classes OD, OQ and OSA considering the OQ Vanilla.

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

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

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

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

<OD-part-of-OQ some Almond>:“almond”

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

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

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

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

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

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

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

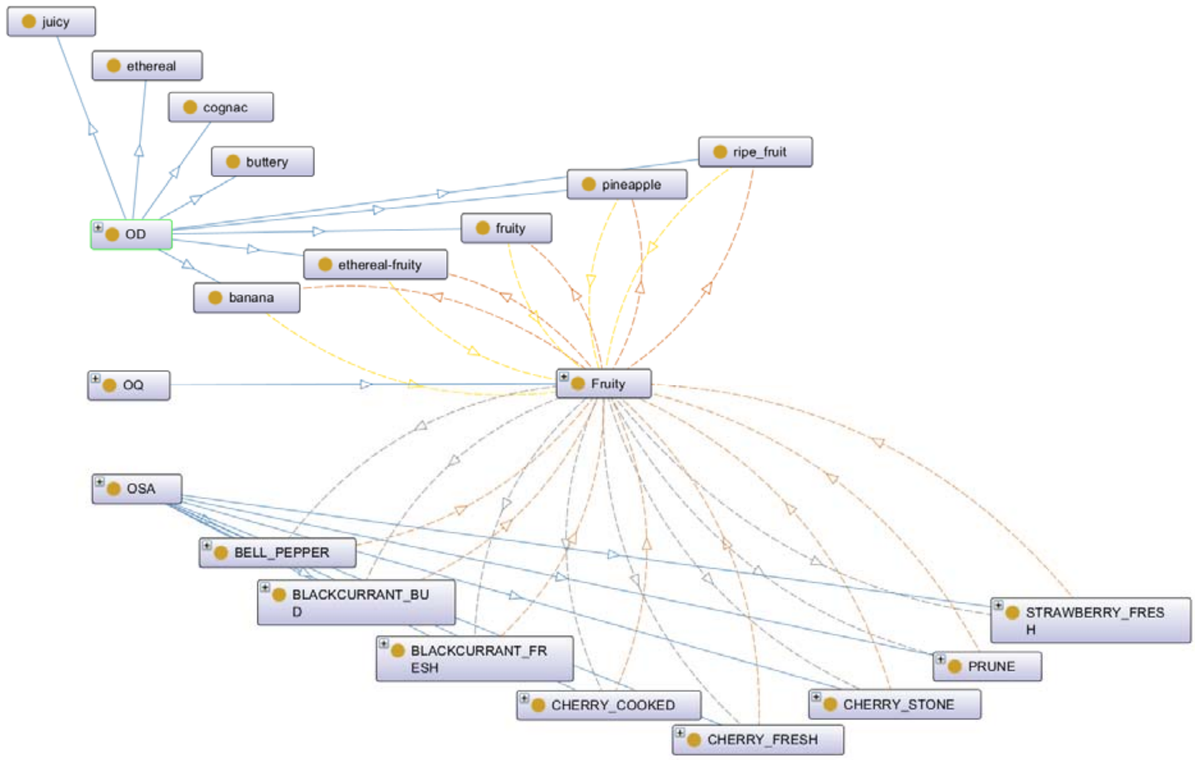

Figure 3. Properties and relationships among the classes OD, OQ and OSA considering the OD of the odorant Ethyl butanoate.

4. Application of the OOPS to wines

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

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

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

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

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

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

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

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

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

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

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

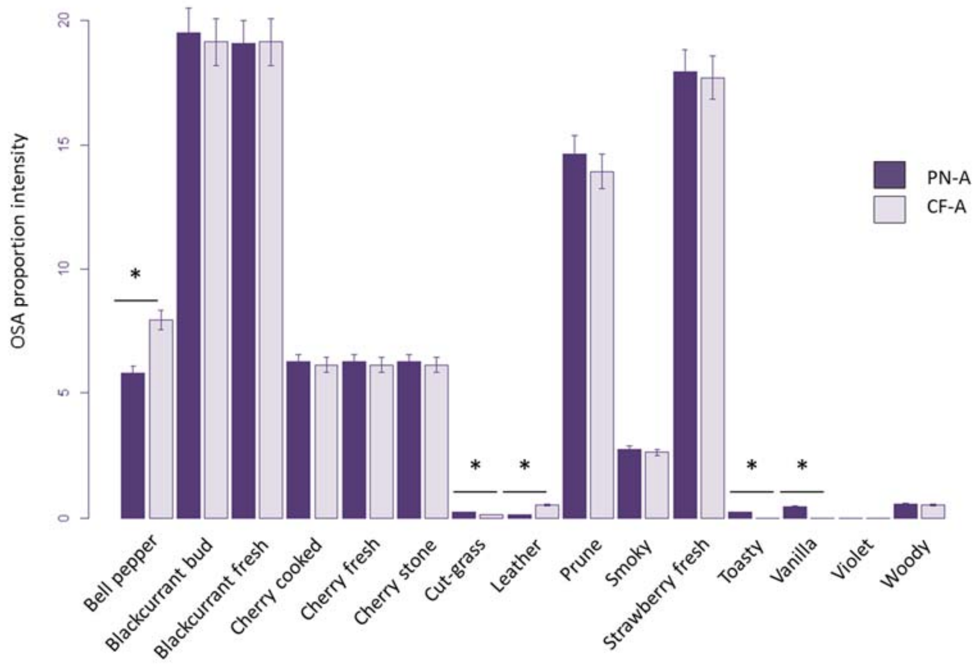

Figure 4. OSA proportions in the PN-A and CF-A wines. Bars display proportion of OSAs, and wines are indicated by the dark (PN-A) or light (CF-A) shading. The horizontal line on the top of the bars indicates significantly different proportion of OSA between the two wines (* = 5%).

5. Conclusions and future work

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

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

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

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

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

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References

[14] Acree T. & Arn H. (2004). Flavornet. Retrieved from http://www.flavornet.org/ flavornet.html

[11] Arctander S. (1969). *Perfume and flavor chemicals*. Volumes 1 and 2. Montclair, NJ: S. Arctander publisher.

[16] Barkat-Defradas, M., Motte-Florac, E., (2016). *Words for Odours: Language Skills and Cultural Insights*. Newcastle: Cambridge Scholars Publishing.

[13] Burdock G.A., 2010. *Fenaroli's handbook of flavor ingredients*. 5th ed. Boca Raton, FL: CRC Press.

[3] Cain, W.S., Drexler, M., (1974). Scope and evaluation of odor counteraction and masking. Annals of the New York academy of sciences, 237: 427-439. Doi: 10.1111/j. 1749-6632.1974.tb49876.x.

[18] Chastrette, M., Elmouaffek, A., Sauvegrain, P. (1988). A multidimensional statistical study of similarities between 74 notes used in perfumery. *Chemical Senses*, 13(2), 295–305. doi: 10.1093/chemse/13.2.295

[17] Chastrette M., 2002. Classification of odors and structure-odor relationships, 100-116, in Rouby C., *Olfaction, Taste, and Cognition*, New-York: Cambridge University Press.

[12] Dravnieks A., (1985). *Atlas of Odor Character Profiles*. Philadelphia, PA: American Society for Testing and Materials.

Dubois, D. (2006). Des catégories d'odorants à la sémantique des odeurs: Une approche cognitive de l'olfaction. *Terrain*, 47, 89–106. doi: 10.4000/terrain.4263

[5] Ferreira, V. (2012a). Revisiting psychophysical work on the quantitative and qualitative odour properties of simple odour mixtures: A flavour chemistry view. Part 1: Intensity and detectability. A review. Flavour and fragrance journal, 27:124-140. doi:10.1002/ffj.2090

[7] Ferreira, V. (2012b). Revisiting psychophysical work on the quantitative and qualitative odour properties of simple odour mixtures: A flavour chemistry view. Part 2: Qualitative aspects. A review. Flavour and fragrance journal, 27:201-215. doi:10.1002/ffj.2091

[4] Ishii, A., Roudnitzky, N., Beno, N., Bensafi, M., Hummel, T., Rouby, C., Thomas-Danguin, T. (2008). Synergy and masking in odor mixtures: An electrophysiological study of orthonasal V.S retronasal perception. Chemical senses, 33(6): 553-561. Doi: 10.1093/chemse/bjn022

[22] Jaubert, J. N., Gordon, G., Dore, J.-C. (1987). Une organisation du champ des odeurs. Première partie : recherche de critères objectifs. *Parfums, Cosmétiques, Arômes*, 77, 53–56.

[8] Jinks, A & Laing, DG. 2001. The analysis of odor mixtures by humans: Evidence for a configurational process. Physiology and behavior, 72(1-2):51-63. doi:10.1016/S0031-9384(00)00407-8

[30] Keller, A. & Vosshall, L.B. Human (2004) Olfactory Psychophysics. *Current Biology* , 14, R875–R878. doi: 10.1016/j.cub.2004.09.066

[20] Kumar, R., Kaur, R., Auffarth, B., Bhondekar, A. P. (2015). Understanding the odour spaces: A step towards solving olfactory stimulus-percept problem. *PLoS ONE*, 10(10), 1–19. doi: 10.1371/journal.pone.0141263

[21] Langlois, J., Dacremont, C., Peyron, D., Valentin, D., Dubois, D. (2011). Lexicon and types of discourse in wine expertise: The case of vin de garde. Food Quality and Preferences. 22, 491-498.

[29] Lawrence, G., Symoneaux, R., Maitre, I., Brossaud, F., Maestrojuan, M., Mehinagic, E. (2013). Using the free comments method for sensory characterisation of Cabernet Franc wines : Comparison with classical profiling in a professional context. *Food Quality and Preference*, 30(2), 145–155. doi: 10.1016/j.foodqual.2013.04.005

[10] Le Berre, E., Béno, N., Ishii, A., Chabanet, C., Etievant, P., Thomas-Danguin, T. (2008). Just noticeable differences in component concentrations modify the odor quality of a blending mixture. *Chemical Senses*, 33, 389–395. doi: 10. 1093/chemse/bjn006

[26] Loison, A., Symoneaux, R., Deneulin, P., Thomas-Danguin, T., Fant, C., Guérin, L., Le Fur, Y. (2015). Exemplarity measurement and estimation of the level of interjudge agreement for two categories of French red wines. *Food Quality and Preference*, 40, 240–251. doi: 10.1016/j.foodqual.2014.10.001

[15] Luebke, W. (1980). The good scents company. Retrieved from http://www.thegoodscentscompany.com/index.html

[28] Musen, M.A. (2015). The Protégé project: A look back and a look forward. *AI Matters*, 1(4). doi: 10.1145/2557001.25757003

[24] Noble, A.C., Arnold, R.A., Buechsenstein, J., Leach, E.J., Schmidt, J.O., & Stern, P.M. (1987). Modification of a Standardized System of Wine Aroma Terminology. *American Journal of Enology and Viticulture*, 38(2), 143–146. doi: 10.1073/pnas.0703993104

[23]Paravisini, L., Septier, C., Moretton, C., Nigay, H., Arvisenet, G., Guichard, E., Dacremont, C. (2014). Caramel odor: Contribution of volatile compounds according to their odor qualities to caramel typicality. *Food Research International*, 57, 79–88. doi: 10.1016/j.foodres.2014.01.009

[9] Romagny, S, Coureaud, G & Thomas-Danguin, T. 2018. Key odorants or key associations? Insights into elemental and configural odour processing. Flavour and fragrance journal, 33:97-105. doi:10.1002/ffj.3429.

[1] Rouby, C., Schaal, B., Dubois, D., Gervais, R., & Holley, A. (Eds.). (2002). *Olfaction, taste, and cognition*. Cambridge University Press.

[2] Thomas-Danguin, T., Sinding, C., Romagny, S., El Mountassir, F., Atanasova, B., Le Berre, E., Le Bon, A.-M., Coureaud, G. (2014). The perception of odor objects in everyday life: a review on the processing of odor mixtures. *Frontiers in Psychology*, 5, 504. doi: 10.3389/fpsyg.2014.00504

[6]Tempere, S, Hamtat, M-L, de Revel, G & Sicard, G. 2016. Comparison of the ability of wine experts and novices to identify odorant signals: A new insight in wine expertise. Australian journal of grape and wine research, 22(2):190-196. doi:10.1111/ajgw.12192.

[27] Villière, A., Symoneaux, R., Roche, A., Eslami, A., Perrot, N., Le Fur, Y., Prost, C., Courcoux, P., Vigneau, E.,Thomas-Danguin, T., Guérin, L. (2018a). Dataset on the characterization of the flavor of two red wine varieties using sensory descriptive analysis, volatile organic compounds quantitative analysis by GC-MS and odorant composition by GC-MS-O [Data set]. Zenodo. http://doi.org/10.5281/zenodo.1213610

[25] Villière, A., Symoneaux, R., Roche, A., Eslami, A., Perrot, N., Le Fur, Y., Prost, C., Courcoux, P., Vigneau, E.,Thomas-Danguin, T., Guérin, L. (2018b). Characterization of the flavor of two red wine varieties using sensory descriptive analysis, volatile organic compounds quantitative analysis by GC-MS and odorant composition by GC-MS-O. Data in Brief, 24 (103725) June 2019.

[19] Zarzo, M., & Stanton, D. T. (2006). Identification of latent variables in a semantic odor profile database using principal component analysis. *Chemical Senses*, 31(8), 713–724. doi: 10.1093/chemse/bjl013