

# Perfumery Radar 2.0: A Step toward Fragrance Design and Classification

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**ABSTRACT:** Product design and engineering is one of the novel paradigms of the 21st century, aiming for the development of novel added-value products for consumers. Its application to the fragrance business for the purpose of enhancing the design and performance of perfumed products is of prime interest because nowadays three-fourths of consumer goods contain fragrances in their composition. Furthermore, fragrance design and classification is still performed on a trial-and-error basis which consequently increases products' time to market and consumption of raw materials. The Perfumery Radar methodology was developed in the recent past as a tool for fragrance design and classification with predictive capabilities. In this study, we extend it to the Perfumery Radar 2.0, which uses typical olfactory families used by the industry but also introduces outer and inner layers for a detailed description of the odor space of fine fragrances. Furthermore, we fully validated this methodology with sensorial classifications of perfumers using several formulated fragrances with known compositions and physicochemical properties with very good predictive accuracy. Finally, and for the first time, we applied the Perfumery Radar 2.0 to 36 commercial fragrances differing in gender (feminine, masculine, and unisex) and covering the odor space. Correlations between olfactory families or odor descriptors with gender trends as well as with richer olfactory families such as chypre and fougère were also derived.

## 1. INTRODUCTION

Interpretation of the olfactory sense has been explored for a long time, but recently its horizons have been largely expanded. Smell differs from vision, hearing, or touch because it is a chemical sense (remote chemoreception) as is taste (contact chemoreception). However, differences do not end here: whatever the physiology behind olfactory detection, recognition, and classification is, the sense of smell is keener than any other. In vision, for instance, there are three broadly tuned receptors responsible for perceiving the entire visible range of wavelengths, while in olfaction we have about 391 olfactory receptors (which may be specific or generic to odorant binding)<sup>1</sup> and there are several known receptor agonists and antagonists.<sup>2</sup> This complex and highly combinatorial coding scheme to encode odor identities is the starting point for the perception of thousands of different odorant chemicals.<sup>3</sup> However, although human beings possess an extraordinary capacity for detecting odors (as low as 1 part per 50 billion), we are also very limited at identifying/recognizing them.<sup>4</sup> Conversely, when people with good visual acuity are asked to describe colors they see, they usually use only one or two words. Still, when one tries to describe the smell elicited by a rose, it often requires multiple words and some of those actually represent feelings, emotions, or past memories of the individual rather than scents. This is so because we are not taught odors as we are colors, shapes, or sounds. Furthermore, there are large interpersonal variability, different social habits, and large complexity at the olfactory system level (together with neuronal encoding) which clouds fragrance design and classification. Conversely, different people will use different descriptors or classes to classify odors (either for single odorants or for mixtures).<sup>5</sup> However, materializing perceived scents by words or qualities is better achieved by experts in the art of smell, the so-called perfumers.

Nonetheless, one issue found within the fragrance industry relies on the difficulty of knowing a priori the behavior of a multicomponent mixture of perfumery raw materials dissolved in any matrix and, ultimately, its resulting odor. Conversely, fragrance design is still based on the combination of art with acquired perfumers' experience and some scientific knowledge, though the former dominates the creation process. Indeed, it is quite common to find significant differences between olfactory classifications of commercial fragrances even when done by experts in the business, as we will see below.

In order to reduce these discrepancies and establish methodologies for both odor design and classification, we have shown in the recent past that product design can be applied through perfume engineering to speed up the preformulation of high performance fragrances. We have done so by combining knowledge from different scientific fields such as thermodynamics and transport phenomena (physicochemical) with psychophysics (sensory).<sup>6–8</sup> Furthermore, product design and engineering is already an established discipline for sustainable development of novel products.<sup>9–11</sup> Following this line of thought, the Perfumery Radar is a methodology developed for the prediction of the odor space, with application in perfume design and classification within preformulation stages of product development.

**1.1. Fragrance Classification: Approaches and Constraints.** As previously said, fragrance design and classification is still performed in the industry by perfumers who are capable of recognizing hundreds of different odorant chemicals, keeping

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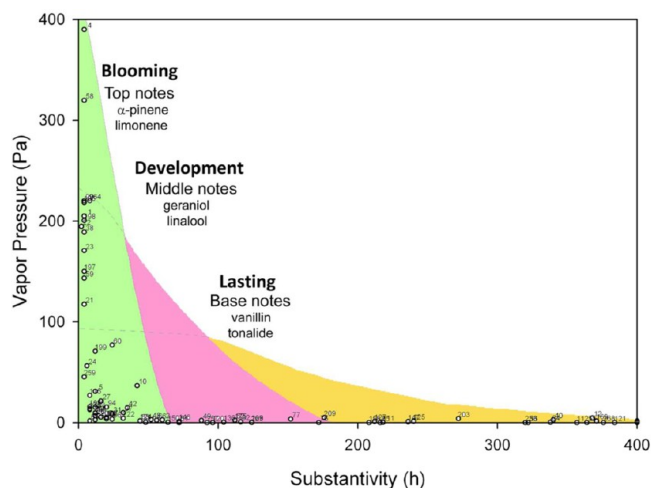


their relevant characteristics within a memory database. The process for fragrance classification generally consists of assigning odors to specific olfactory families or classes (e.g., citrus, floral, musk, *chypre*, or *fougère*) and often includes “nuances”.<sup>6</sup> A *nuance* is a subtle or secondary odor elicited apart from the main olfactory sensation of a perfumery raw material or a mixture of odorant chemicals. Those classes can be seen as semantic descriptors for each type of odor and are commonly sided by other sensorial descriptors such as spicy or sweet, fresh, or warm and (not so commonly) by quality terms such as heavy or light, sharp or round, among others.<sup>12,13</sup> Such sensations, which arise when chemical compounds activate receptor mechanisms for other senses, are within chemesthesis. This is the result from trigeminal nerve receptors located in the human nasal cavity which are responsible for sensations such as pressure, temperature, or pain (also associated with pungency and irritability). It is a common effect in different perceptual continua, occurring also for odorants: for example, minty odors often produce a trigeminal effect that is perceived as cooling and fresh sensations.

Nevertheless, this complexity in fragrance assignment and its nomenclature is interpreted with difficulty by an untrained person—the typical consumer—who is not familiar with the terminology. Even among perfumers and fragrance houses there is not complete agreement about which olfactory families should be used or how to assign odorants to each. The reason why perfumery ingredients or commercial fragrances have so detailed descriptions of odor qualities as described by perfumers may be understood by the (untrained) reader as “the expression of all the odorant faces or nuances” as stated by recognized perfumer E. Roudnitska.<sup>14</sup> Again, such terminology is complex for consumers, but any attempt to correlate it with ratings from untrained panelists is still fuzzy. Additionally, care should be taken when performing comparisons of classifications because the odor of a rose, for instance, may vary from species to species, so one may have a clear floral note or a slightly green note. Conversely, possible combinations within the odor space may be completely different and present very singular nuances.

From a simple point of view, classification of scents may be considered from two different perspectives: it can be related to fragrance release/intensity or to fragrance character/hedonics. The former has to do with the typical perfume pyramid structure as proposed by Carles<sup>15</sup> which considers that well-designed fragrances typically have a combination of top, middle, and base notes within solvent(s) and other chemicals. Top notes are the most volatile ones and are perceived in the first impact and last for some minutes. Then middle notes began to be more strongly perceived, bridging between top and base notes, which are the least volatile and can last for hours such as some musk or woody notes. Some of these base notes present extraordinary properties, especially when they have very low vapor pressures and large molecular structures, showing great affinity to bind with other notes, thus retaining them in solution and so increasing fragrance lastingness—the so-called fixatives.<sup>15</sup> However, if we look at fragrance hedonics, then olfactory families come into play. These also present some general trends with the previous perfume pyramidal structure. Typically, green, fruity, and citrus scents are usually related to top notes while florals are within heart notes and woody is often associated with base notes.<sup>16</sup> Curiously, we have found that if we represent vapor pressure versus fragrance substantivity, which is the persistence of the odor on a paper blotter measured over time, for the raw materials in our database, we observe a correlation

between these physicochemical properties and the perceived odor as defined by Carles. This relationship was obtained by gathering information from the classification of fragrance raw materials<sup>17</sup> and their corresponding substantivity values,<sup>18</sup> and it is represented in Figure 1.



**Figure 1.** Graphical representation of the typical pyramid structure of a perfume comprising top (green), middle (pink), and base (yellow) notes together with the relationship between their vapor pressure and substantivity. Open circles represent perfumery raw materials (from our proprietary database—data not shown) which clearly follow the process for release/evaporation over time from a paper blotter.

However, despite this interesting relationship established between chemical compounds' properties and the nature of olfactory perception, a similar analogy cannot be applied when evaluating fragrance mixtures once chemical interactions at the molecular level will strongly influence both release and perceived smell.

**1.2. Classification Systems for the Odor Space.** Several classification systems have been proposed, being based on semantic classifications, olfactory descriptors, odor similarities, statistical analysis, or olfactory profiles (detailed reviews on this topic can be found in recent literature).<sup>6,8,13,19,20</sup> Although it is indisputable that these many attempts to describe the odor space have contributed to increase the portfolio for mapping the odor space, agreement among them has not yet been attained. Such disagreement is even observed at lower levels, as for example in the classification of reference substances: the international standard for training the recognition of odors has defined 24 reference substances,<sup>21</sup> while Arctander used nearly 260 odor descriptors distributed throughout 88 classes of odors.<sup>22</sup> Jaubert et al.<sup>23,24</sup> described 42 different descriptors for pure raw materials, while E. Roudnitska proposed a system with 15 olfactory classes which covered the most of the odor space for training apprentices in perfumery.<sup>23</sup> It should be highlighted here that the Fragrance Wheel, which is a recognized fragrance classification system, was developed by M. Edwards to stress the similarities/dissimilarities between perfumes across 14 fragrance families.<sup>25</sup> Also, an interesting study from Zarzo and Stanton applying principal component statistical analysis in two databases, together with a comparison between the Fragrance Wheel, the odor effects diagram (from Calkin and Jellinek), and the Boelens-Haring and Thiboud databases, revealed interesting similarities between sensory maps and fragrance ingredients.<sup>13,26</sup> Unfortunately, it is also observed in this study that

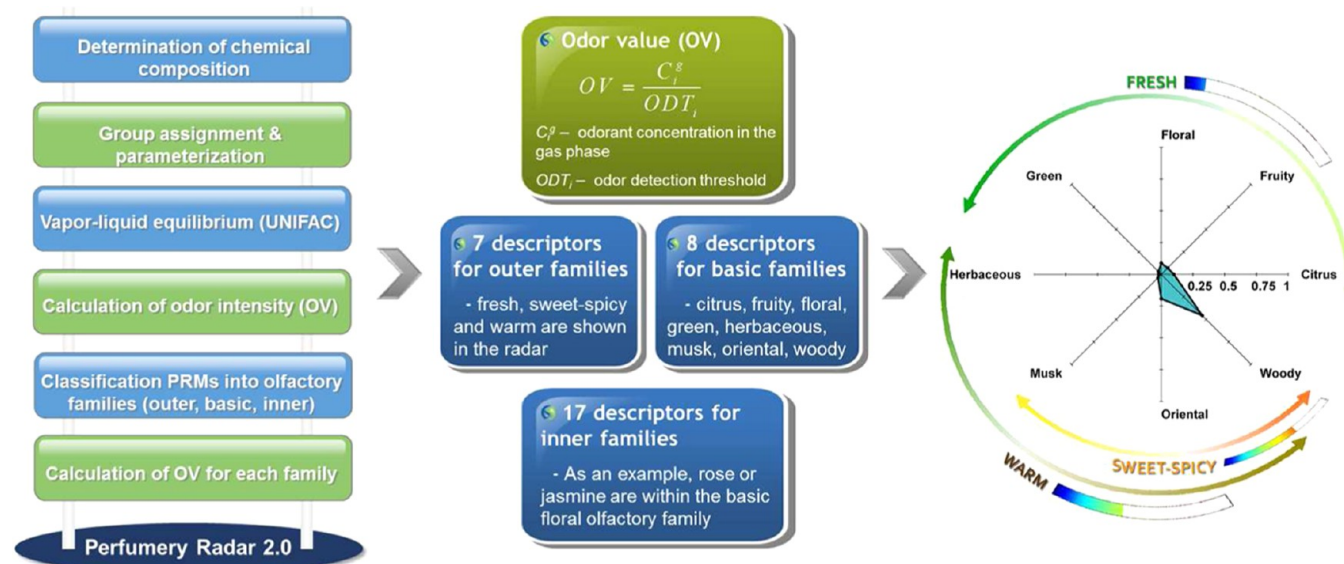


Figure 2. Schematic representation of the typical structure of the Perfumery Radar 2.0.

some of its conclusions are difficult to extrapolate. Further, the authors even report that large discrepancies are observed between previous databases and the results they obtained (possibly due to broadening the scope of analysis to extremely different databases on odor classification). Apart from these classifications, each fragrance company or specialized perfumer has also proposed their tailored, sensory-based classification system over the years (some of which we will use in this study), but it is still doubtful that a universally accepted classification for odors will ever be found. Consequently, fragrance classification remains (at least) partially based on sensory evaluation, subjected to interpersonal variability and strongly dependent on the selection of reference materials.

In the quest for a methodology that could unify scientifically based classification systems of odors, we have extended our Perfumery Radar tool to accurately predict sensorial perception at detailed levels. In this work, the former Perfumery Radar methodology is improved by introducing more detail in the description of the odor space with inner and outer layers of classification, the extension to all gender classes, and further validation with experimental sensory data. Indeed, the novel Perfumery Radar 2.0 tool was corroborated with five in-house designed perfume mixtures and one other whose exact composition is disclosed. In this way, compositions are known with precision instead of relying on chromatographic analysis. Then, it was applied to 36 commercial perfumes (feminine, masculine, and unisex) for the prediction of the olfactory character as it is done by the human nose. The results are compared with several empirical classifications used in the perfume industry.

## 2. METHODOLOGY

**2.1. Perfumery Radar 2.0.** The Perfumery Radar 2.0 methodology is a novel tool for the prediction of the olfactory space from the composition of the liquid mixture (concentration or mole fraction) and the molecular structure of each chemical ingredient together with their corresponding olfactory qualities. It can be structured into the following steps: (1) determination of chemical composition; (2) assignment of the UNIFAC functional groups<sup>27</sup> to each perfumery raw material and their parametrization; (3) computation of the vapor–liquid equilibrium for all species present at the gas–liquid interface

using the UNIFAC method; (4) calculation of the odor intensity for each fragrance chemical using, for example, the odor value (OV) concept (which is the ratio between the odorant concentration in the gas phase and the minimum detectable concentration by the nose—known as the odor detection threshold);<sup>28,29</sup> (5) classification of each perfumery raw material into olfactory families (for the outer, basic, and inner families); (6) determination of the OV for each olfactory family (for the basic layer there are weighing factors while for the other it is calculated based on a relative percentage) and representation in the perfumery radar. Further details on the previous version of the methodology can be found in the literature.<sup>8</sup> Conversely, the Perfumery Radar 2.0 uses the basic layer (the radar itself, taken from its predecessor) with eight olfactory families, and two additional classification layers: an outer layer with seven descriptors and an inner layer with 17 descriptors as exemplified in Figure 2.

One controversial topic within fragrance classification systems relies on the selection of descriptors and/or fragrance classes to map the whole olfactory space. There are some detailed studies in the literature addressing this particular issue, but these also show significant discrepancies across olfactory classifications from experts and fragrance houses.<sup>8,13,23,30</sup> A compilation of the most used descriptors or classes used by fragrance companies and experts is presented in Table 1. In analogy with the previous version of the Perfumery Radar, we consider that the selection of descriptors or classes in which fragrance ingredients have to be assigned should have to do with sensory evaluations from experts. This is so because perfumers are educated and trained for olfaction, and tend to use a reduced set of descriptors. Having said that, it is fundamental to use the most common descriptors found in perfume classification but also those that are most used for fragrance ingredients. Keeping this in mind, it is observed in Table 1 that olfactory classes such as floral, woody, citrus, fruity, green, and oriental are often part of the olfactory space for the majority of the classification systems (which is in agreement with previous studies<sup>8,30</sup>). Nevertheless, it is also seen that each fragrance house follows its own classification system to map the olfactory space.

Table 1. Typical Olfactory Families Used by Fragrance Houses and Experts for the Classification of Perfumes

	Givaudan <sup>31 a</sup>	Osmoz <sup>32</sup>	IFF <sup>33</sup>	Symrise <sup>34</sup>	Frutarom <sup>35</sup>	MANE <sup>36</sup>	SFP <sup>37</sup>	TFF <sup>38</sup>	Avon <sup>39</sup>	Fragrantica <sup>40</sup>	LaLoff <sup>41</sup>
floral	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
woody	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
citrus	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
fruity			✓	✓	✓	✓		✓			✓
green			✓	✓	✓	✓		✓			✓
oriental	✓	✓						✓	✓	✓	✓
chypre	✓	✓					✓		✓	✓	✓
aromatic		✓	✓	✓		✓		✓ <sup>b</sup>		✓	
fougère	✓						✓	✓ <sup>b</sup>	✓		✓
musk <sup>c</sup>			✓	✓	✓	✓					✓
spicy			✓		✓	✓					✓
ambery			✓	✓			✓				
marine <sup>d</sup>						✓		✓			✓

<sup>a</sup>Givaudan uses these families to classify perfumes but has 14 families for fragrance ingredients, including fruity, green, herbal, musky, spicy, ambery, and marine. <sup>b</sup>The Fragrance Foundation (TFF) uses the aromatic-fougère family. IFF, International Flavors & Fragrances; SFP, Société Française des Parfumeurs; TFF, The Fragrance Foundation/M. Edwards Fragrance Wheel. Other less common variations such as leather, gourmand, aldehydic, balsamic, and herbal are used two times. Descriptors salient in only one dimension are tobacco, modern chypre, floral oriental, soft oriental, mossy woods, dry woods, and mint, among others. <sup>c</sup>Musk or animalic. <sup>d</sup>Marine or watery.

Table 2. Distribution of the Number of Commercial Fragrances by Gender within Each Olfactory Family, by Olfactory Family and by Gender Alone (Women, Men, and Unisex) Listed under the 14 Categories of 2008 Edwards' Guide for a Total of 5233 Commercial Perfumes

olfactory family	no. of fragrances			% of fragrances by gender in olfactory family			% of olfactory family	% of fragrances by gender		
	women	men	unisex	women	men	unisex		women	men	unisex
fruity	75	0	14	84.3	0.0	15.7	1.7	2.4	0.0	1.7
green	31	7	23	50.8	11.5	37.7	1.2	1.0	0.6	2.7
water (marine)	34	76	31	24.1	53.9	22.0	2.7	1.1	6.1	3.7
floral	1331	9	112	91.7	0.6	7.7	27.7	42.3	0.7	13.3
soft floral	282	12	40	84.4	3.6	12.0	6.4	9.0	1.0	4.8
floral-oriental	436	2	16	96.0	0.4	3.5	8.7	13.8	0.2	1.9
soft oriental	98	8	39	67.6	5.5	26.9	2.8	3.1	0.6	4.6
oriental	97	28	58	53.0	15.3	31.7	3.5	3.1	2.3	6.9
woody-oriental	300	256	96	46.0	39.3	14.7	12.5	9.5	20.6	11.4
woods	153	284	128	27.1	50.3	22.7	10.8	4.9	22.9	15.2
mossy woods	161	52	38	64.1	20.7	15.1	4.8	5.1	4.2	4.5
dry woods	39	90	69	19.7	45.5	34.8	3.8	1.2	7.3	8.2
citrus	106	103	160	28.7	27.9	43.4	7.1	3.4	8.3	19.0
aromatic <sup>a</sup>	7	314	18	2.1	92.6	5.3	6.5	0.2	25.3	2.1
total	3150	1241	842					100.0	100.0	100.0

<sup>a</sup>Aromatic is similar to herbaceous in many cases, and it is commonly used as a powerful descriptor within the fougère olfactory family.

In what concerns the classification of perfumery raw materials, it is observed within our in-house database that descriptors such as floral, woody, herbaceous, oriental, and green when combined represent more than 75% of the odor space. Consequently, we have used the same eight olfactory classes from our previous work as follows: citrus, fruity, green, floral, herbaceous, musk, oriental, and woody (further details on their descriptions can be found elsewhere<sup>8</sup>).

**2.2. Family Attributes: Gender Association.** The distribution of the families within the Perfumery Radar 2.0 has to do with similarities/dissimilarities between them, but it should also agree with gender associations as discussed below. For that purpose, we analyzed the olfactory classification of a large sample of commercial perfumes available on the market and evaluated the number of women's, men's, and unisex fragrances together with their corresponding olfactory descriptors as presented in Table 2.

Although Table 2 uses as a database all fragrances available until 2008, we performed a recent evaluation on the 2013 Edwards guide, which includes more than the double of fragrances, but we observed no significant differences within fragrance distribution. Among the differences, the woods family suffered a reduction by 1.1% while floral-oriental and aromatic increased 1.0 and 1.1%, respectively. All other olfactory classes revealed very small changes (below 0.5%). Furthermore, distribution by gender only remained very similar between 2008 and 2013 with feminine, masculine, and unisex categories changing from 60.2, 23.7, and 16.1% to 61.3, 26.2, and 12.5%, respectively.

However, we also observed that nearly all olfactory families have commercial perfumes on the market for women, men, and unisex categories, with the exception of floral-oriental and fruity families which have very few to none for the masculine gender. Conversely, whether an olfactory family or descriptor remains dominant in one gender needs to be evaluated considering all

three categories. Thus, considering data in Table 2 for a given olfactory family, we assumed that if the percentage difference in the number of women's perfumes to that of men's was equal to or higher than 10% and equal to or higher than 10% of unisex's as well, it was regarded as feminine; if the first condition was not met but the percentage of men's perfumes was equal to or higher than 10% of unisex's and women's perfumes, then it would be typically masculine; finally, if none of the above coupled conditions was met, then it would be considered within unisex gender. Taking into account this analysis, we observed that water (marine), woods, dry woods, and aromatic are typically masculine while citrus and woody-oriental are unisex. All remaining families are within the feminine gender. Conversely, if we analyze these results in the light of the Perfumery Radar, we observe that olfactory families placed on the top of the diagram (fruity, floral, and green) are feminine; families such as citrus (herbaceous is not a specific family in Edwards' wheel though from our definition it should be close to aromatic) should be unisex, so they are positioned in the middle axis of the Perfumery Radar; and families on the bottom of the diagram such as woody and oriental (and musk, which is not a specific family within Edwards' wheel) should appeal more to the masculine gender. The only exception observed in this context is the oriental family which according to Table 2 should be more feminine, though the coupled percentage of men and unisex is nearly the same as for feminine category, which may indicate that this category might be transversal to gender (the relatively near family of woody-oriental also resulted within the unisex category). Zarzo and Stanton positioned the oriental family near the boundary between masculinity and femininity, but it is characterized by balsamic resins, ambergris odors, opulent flowers, sweet vanilla, and musks which are primarily masculine descriptors according to their work.<sup>13</sup> This discrepancy is probably due to the fact that the oriental family combines very different perfumery raw materials. Thus, depending on their relative weights and type, it may be linked with femininity (florals and orientals) or masculinity (woody-orientals). Another discrepancy found was that Zarzo and Stanton clearly correlated citrus with masculine, which does not reproduce reality, but they also reported that the number of citrus fragrances was slightly higher within the feminine gender than in the masculine, though the majority of them falls in the unisex category.

**2.3. Outer Layer Level of Classification.** The novel Perfumery Radar 2.0 uses the original assumptions from its predecessor, but it is extended here to outer and inner levels for the classification of fragrances. This is so because in fragrance evaluation it is not unusual to observe the use of odor descriptors such as warm, fresh, or sweet, which are often associated with other senses, as previously discussed. Such behavior evidences the presence of both weak synesthesia (simple cross-sensory correspondence) and strong synesthesia (the experience of one sense by stimulation of another) in odor perception, as happens in other modalities. In order to be able to predict the odor character at such levels, we have extended our database of perfumery raw materials and introduced an outer layer of classification comprising seven salient descriptors: fresh, warm, sweet-spicy, powdery, cool/mint, watery, and ethereal. From our database it is observed that fragrance ingredients having the fresh descriptor are within the citrus, green, and floral (and occasionally fruity) olfactory families, which is in agreement with Zarzo and Edwards, who included citrus, green, water, and fruity subfamilies.<sup>12,25</sup> Consequently,

we placed the fresh dimension on the top part of our radar as shown in Figure 2. We found sweet to be typically within musk, oriental, floral, and woody families, while spicy is correlated only with the oriental category. Although Zarzo and Stanton stated that sweet–feminine and dry–masculine associations can be derived from perfumery and that many florals are sweet, they also add that floral and sweet are independent dimensions of odor character. Additionally, upon analysis of Jellinek's reference material for floral (hydroxycitronellal), it was observed that its sweet score was extremely low. Moreover, Zarzo and Stanton also reported that sweet generally corresponds to base notes (which are highly correlated with musk, oriental, and woody olfactory families) as happens in our radar. Consequently, we placed sweet-spicy in the bottom of the perfumery radar as shown in Figure 2. The descriptor “warm” includes herbaceous, musk, oriental, and woody as previously stated by Zarzo and Stanton,<sup>13</sup> so it is represented in the bottom part of our radar as well, but it is broader than sweet-spicy. We found that cool/mint correlates with herbaceous and green families, while Zarzo and Stanton defined it as green-citrus undertones. Powdery, for its part, is related to soft and smooth scents of floral and sometimes musk notes, and finally, watery is associated with marine and aquatic environments (although we know that water alone is odorless). Finally, ethereal was considered in the past as an independent category by some authors.<sup>42</sup> However, these descriptors are much less commonly found in perfume classification than within fragrance raw materials (considering the data set used in this work as well) so we used them in the calculations, but they are not graphically represented in the perfumery radar.

It is curious to observe that our (sensorial) outer layer descriptors appear in the study of Zarzo and Stanton, where a clear statistical dimension with contrasting polarities between rich/fresh, warm/cool, and powdery/watery was reported. The rich/fresh dichotomy is evident in our perfumery radar between the bottom (rich) and upper (fresh) halves, while the latter two opposite couples were also found to be relevant descriptors for the characterization of the odor space. While warm and cool/mint are semantically opposite concepts, the proximity between sweet and spicy found in our sensorial database can be partially supported by Zarzo and Stanton's study, where they reported both sweet and spicy to be most similar to aromatic. As a final remark, it should be pointed out that, in analogy with the variability found within olfactory family assignment, the same may be observed in this outer layer of classification. For instance, freshness emanating from a green note of green leaves or from cut grass is quite different from the one released from a citrus-fruity note from apricot, melon, or any other exotic fruit. The latter resembles more a spicy freshness, whereas the former is perceived as sharper green notes.

**2.4. Inner Layer Level of Classification.** An inner layer level of classification with 17 salient descriptors was also introduced to describe more specific and detailed nuances of each fragrance. In order to fine-tune the classification of the odor space, the following subfamily descriptors were included in our database: camphor, rose, pine, lemon, earthy, apple, jasmine, sandalwood, orange, vanilla, mushroom, lilac, cinnamon, pepper, banana, honey, cherry, leather, orris, chocolate, tobacco, lavender, smoky, grass, lime, myrrh, and anise. The selection of these descriptors was based on sensory descriptors from Brechbill<sup>17</sup> and Scent Direct<sup>18</sup> for each perfumery raw material, as happened for the outer layer category. Nevertheless, within classification systems for commercial fragrances, it is not

**Table 3. Physicochemical and Sensory Properties for the Fragrance Chemicals Used in This Work: Molecular Weight (MW), Vapor Pressure at 296 K ( $P^{\text{sat}}$ ), and Odor Detection Threshold (ODT) in Air; Chemical Compositions for the Five Fragrance Mixtures (Mole Fraction)**

chem component	MW (g/mol)	$P^{\text{sat}}$ <sup>45</sup> (Pa)	ODT <sup>46,47</sup> (mg/m <sup>3</sup> )	fragrance 1	fragrance 2	fragrance 3	fragrance 4	fragrance 5
(+)-(R)-limonene	136.2	205	2.45	$1.41 \times 10^{-2}$	$1.72 \times 10^{-2}$	$1.70 \times 10^{-3}$	$1.66 \times 10^{-3}$	$5.20 \times 10^{-4}$
benzyl acetate	150.2	189	$3.32 \times 10^{-1}$	$3.56 \times 10^{-4}$	$4.09 \times 10^{-3}$	$8.21 \times 10^{-5}$	$1.00 \times 10^{-2}$	$4.89 \times 10^{-4}$
eugenol	164.2	3.01	$2.56 \times 10^{-3}$	$2.68 \times 10^{-3}$	$5.80 \times 10^{-3}$	$1.02 \times 10^{-3}$	$1.39 \times 10^{-3}$	$9.23 \times 10^{-3}$
coumarin	146.1	0.13	$3.09 \times 10^{-4}$	$2.27 \times 10^{-3}$	$1.10 \times 10^{-3}$	$1.92 \times 10^{-2}$	$2.29 \times 10^{-3}$	$1.85 \times 10^{-3}$
citral	152.2	9.49	$3.69 \times 10^{-2}$	$7.38 \times 10^{-3}$	$1.02 \times 10^{-2}$	$1.57 \times 10^{-3}$	$8.02 \times 10^{-4}$	$4.29 \times 10^{-4}$
geranyl acetate	196.3	3.47	$1.47 \times 10^1$	$6.11 \times 10^{-3}$	$6.68 \times 10^{-3}$	$2.98 \times 10^{-3}$	$6.56 \times 10^{-3}$	$8.49 \times 10^{-3}$
styrallyl acetate	164.2	27.1	$5.01 \times 10^{-2}$	$7.49 \times 10^{-3}$	$3.74 \times 10^{-4}$	$9.46 \times 10^{-4}$	$4.68 \times 10^{-4}$	$5.76 \times 10^{-4}$
musk ketone	294.3	0.0016	$3.46 \times 10^{-4}$	$2.59 \times 10^{-3}$	$1.02 \times 10^{-3}$	$2.16 \times 10^{-3}$	$1.96 \times 10^{-3}$	$9.55 \times 10^{-4}$
$\beta$ -ionone	192.3	2.27	$2.09 \times 10^{-2}$	$6.22 \times 10^{-3}$	$5.43 \times 10^{-3}$	$2.17 \times 10^{-3}$	$4.61 \times 10^{-3}$	$4.17 \times 10^{-3}$
water	18.0	3170	odorless	$2.80 \times 10^{-1}$	$3.19 \times 10^{-1}$	$3.04 \times 10^{-1}$	$3.97 \times 10^{-1}$	$3.99 \times 10^{-1}$
ethanol	46.0	7270	$5.53 \times 10^1$	$6.71 \times 10^{-1}$	$6.29 \times 10^{-1}$	$6.64 \times 10^{-1}$	$5.73 \times 10^{-1}$	$5.74 \times 10^{-1}$

common to find such a detailed description. Instead, main olfactory families are used (as happens for the eight we use in the center of the perfumery radar), but when specific accords or notes are strongly perceived, perfumers also report them in their classifications.

Conversely, as in the former version of the Perfumery Radar, the only sensorial inputs for the calculations are the odor descriptors used for fragrance ingredients.<sup>8</sup> We have based this assumption on the fact that assignment of quality/character descriptors for pure reference materials shows greater agreement among perfumers (further discussion on this topic was presented elsewhere<sup>8</sup>). It should be pointed out that all odors are based on inputs at the olfactory receptor level, but as made clear by Wilson and Stevenson, whether the initial activation pattern is due to interaction with a single pure chemical or a complex mixture, the neural process is still one of pattern recognition.<sup>43</sup> Conversely, mixtures can excite neural pathways which are not activated by individual components which can, in turn, enhance or diminish fragrance recognition.<sup>44</sup> For example, the association of jasmine accord to jasmine oil will be much easier than if we use hedione, a pure chemical that represents a great part of the jasmine complex. Having said that, it results that standardized classifications of odors or mixtures of them will have to rely on homogeneous data sets which are originated from a single source. Furthermore, such a standardized classification system will have to prove on its own to have the capability of agreement with a significant number of classifications derived from experts.<sup>23</sup>

### 3. MATERIALS AND METHODS

Commercial fragrances studied in this work are from recognized brands and were in a perfect state of preservation. For the in-house formulated fragrances, the following perfumery raw materials were used: (+)-R-limonene (CAS Registry Number 5989-27-5, >97%, >98% ee), benzyl acetate (CAS Registry Number 140-11-4, >99%),  $\beta$ -ionone (CAS Registry Number 79-77-6, 96%), citral (CAS Registry Number 5392-40-5, 85%, cis/trans), coumarin (CAS Registry Number 91-64-5, 99%, HPLC), musk ketone (CAS Registry Number 81-14-1, >98%), and styrallyl acetate (CAS Registry Number 93-92-5, >98%, FG) were supplied by Sigma-Aldrich. Eugenol (CAS Registry Number 97-53-0, 99%) was purchased from ACROS, and geranyl acetate (CAS Registry Number 105-87-3, >97%, ee) was supplied by Fluka. Ethanol (absolute GR for analysis, >99.9%) was supplied by Merck, and deionized water ( $\sigma < 2 \mu\text{S/cm}$ ) was produced in the LSRE laboratory using a

two-column packed bed with ion exchange resins. All reagents were used as received without further purification. Some relevant physicochemical properties of these components are presented in Table 3.

Chemical analysis for determination of liquid and/or head-space compositions of samples was performed by gas chromatography coupled with mass spectroscopy (GC–MS) to quantify and identify compounds, respectively. The simultaneous analyses were carried out in a Varian CP-3800 instrument equipped with two parallel split/splitless injectors and two CP-Wax 52 CB bonded fused silica polar columns of 50 m length, 0.25 mm i.d., and 0.2  $\mu\text{m}$  film thickness. The detection system was composed by a Varian flame ionization detector (FID) and a Varian Saturn 2000 MS ion-trap mass spectrometer, both controlled by the Saturn 2000 workstation acquiring software. The oven was initially set at 50 °C for 5 min, then raised to 200 °C at a rate of 2 °C/min, and finally held isothermally for 40 min. The temperature of both injectors was 240 °C, with a split ratio of 1:50 for FID and 1:200 for MS. The FID detector was set at 250 °C, and helium N60 was used as carrier gas with a flow rate of 1 mL/min. The sample volume injected in the GC equipment was 0.1  $\mu\text{L}$ .

For the FID data, a lower-limit value for peak area (<2000 counts) was considered in the integration process to quantify a large number of fragrance ingredients but to avoid very low peak areas where the noise-to-signal ratio is high, thus introducing errors in the chemical analysis (peak identification by MS is also more difficult whenever the noise versus chromatographic peaks is significant). However, care should be taken with this rejection criterion, once powerful odorants may be present in trace amounts. Nevertheless, a lower limit is necessary to avoid misidentification of peaks in the analysis of the samples. The analysis of the MS data for pure component identification was performed using the mass spectral database of Flavors and Fragrances of Natural and Synthetic Compounds 2 (FFNSC 2) from Wiley, the NIST98 spectral library (upgraded), our in-house library (with pure reference species), and literature data. Moreover, linear retention indexes (LRI) were calculated relative to  $\text{C}_6$ – $\text{C}_{40}$  *n*-alkanes (purchased from Aldrich) using the same GC conditions and compared with available literature data.<sup>48–54</sup> Pure standards of several components were used. All calculations done throughout this work for the UNIFAC method and the radar plots within the Perfumery Radar 2.0 tool were run using the MATLAB software.<sup>8</sup>

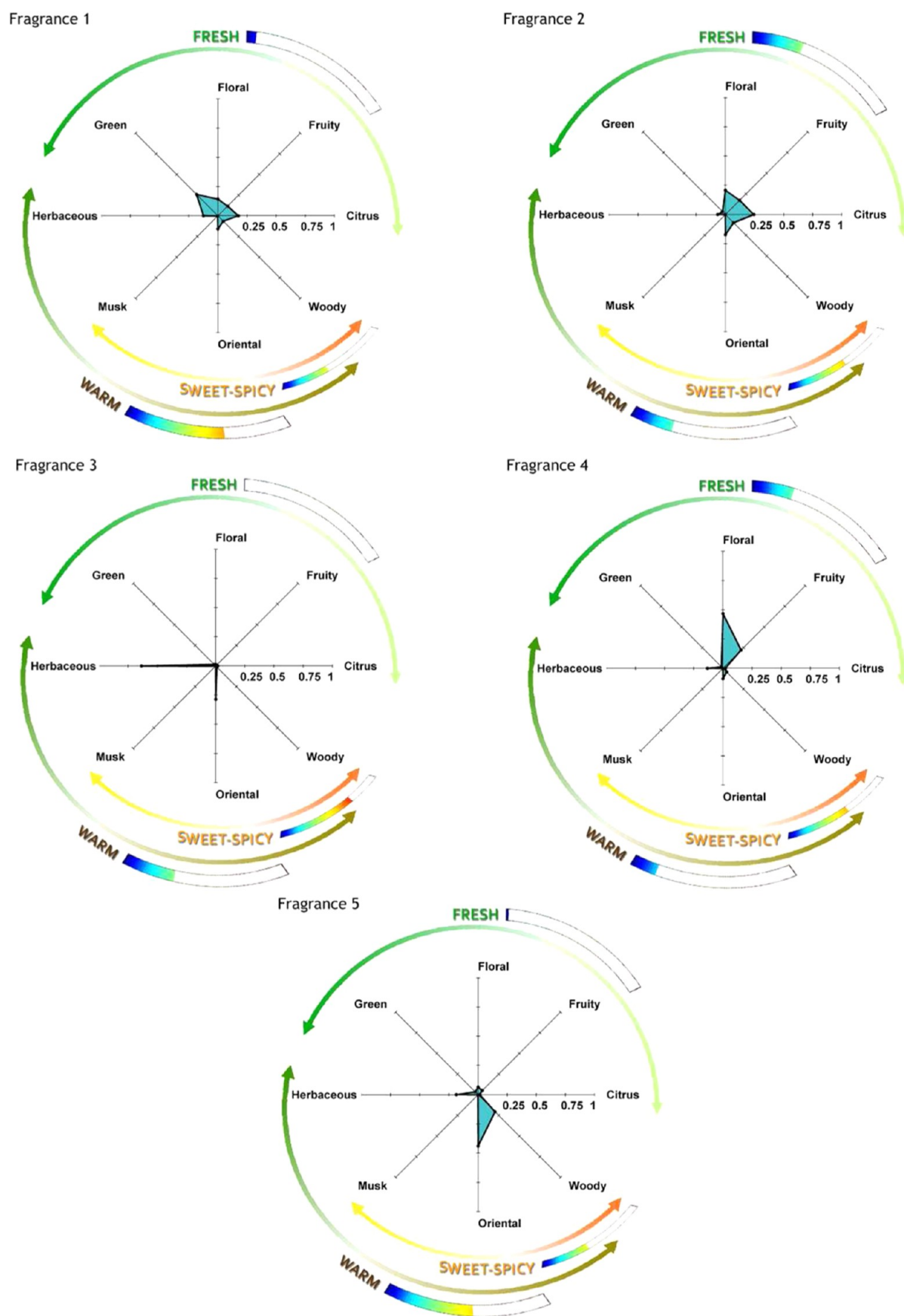


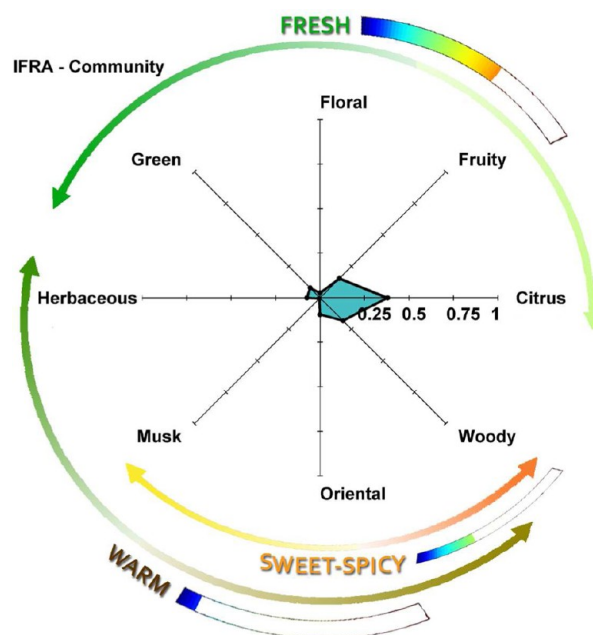
Figure 3. Perfumery radars for in-house developed fragrances 1–5.

## 4. RESULTS AND DISCUSSION

**4.1. Methodology Validation.** The proof of concept was achieved by application of the Perfumery Radar 2.0 methodology to five fragrance formulations with exact known compositions and compared with olfactory evaluations performed by experts. These samples were subjected to blank sensory analysis performed by perfumers and also validated with five reference materials for a total of 10 samples. In this way, we do not rely on gas chromatography coupled with mass spectroscopy techniques to estimate real compositions of fragrance mixtures which we know are subjected to slight deviations (e.g., sensor detection may be more sensitive to some chemicals than others). Conversely, we have formulated five multicomponent fragrance mixtures with 11 chemicals, comprising top, middle, and base notes, with specific compositions presented in Table 3. The predicted perfumery radars for fragrances 1–5 are represented in Figure 3. It should be highlighted that these formulated fragrances cover most of the odor space, thus belonging to different (main) olfactory families (and consequently avoiding possible bias in our study). These five fragrances were classified by perfumers as citrus, citrus, herbaceous (slightly warm), floral, and oriental-spicy from fragrance 1 to fragrance 5, respectively. Comparison between predicted perfumery radars (shown in Figure 3) and sensory evaluations have shown a very good agreement in the dominant olfactory family, except for fragrance 1, where a green-citrus character with some other nuances was predicted but perfumers' character ratings caught the citrus odor as the most clearly dominant scent. In these particular mixtures, perfumers were not able to identify significant nuances in most of the cases, although the Perfumery Radar 2.0 methodology has predicted some secondary families.

We also applied our Perfumery Radar 2.0 to a fragrance developed by Firmenich whose formula was revealed by the International Fragrance Association (IFRA) in an act of promotion for defense of trade secrets.<sup>55</sup> As it was stated, "the formula was distributed with the fragrance and has been widely publicized to show the unique complexity and artistry that intellectual property protections are meant to preserve". The authors of this work would like to note that it is not our intention to disclose any formula of a commercial fragrance here, but to show the applicability and potentialities of the Perfumery Radar 2.0 tool. Once the formula was made out publicly, we had the opportunity to know its exact composition and use it to fully validate our methodology.

This fragrance, called Community, was designed to celebrate the European Union and it is described as rich citrus-based with a fresh scent, having notes of bergamot and mandarin developing into a fresh and elegant middle note.<sup>55</sup> In the application of the Perfumery Radar 2.0 methodology to this specific fragrance, some of the essential oils (called pours) within its composition were approximated to one or more fragrance ingredients that are extremely relevant for its scent. For example, natural bergamot oil appears in its composition and it is a combination of more than 100 chemicals, of which 15–20 are responsible for its overall odor. The predicted radar for fragrance Community is shown in Figure 4. A distinct citrus character with a strong fresh scent and a fruity nuance (typical of bergamot) was obtained, which completely agrees with the sensory description disclosed in the literature. Furthermore, it is also predicted that orange and cinnamon descriptors were the



**Figure 4.** Perfumery Radar for the fragrance Community designed by perfumer Christophe Laudamiel. The formula was revealed by IFRA in 2011.

strongest within the inner layer category, with the former dominating nearly 80% of it.

**4.2. Feminine Perfumes.** As previously discussed, fine fragrance business may be divided between typical masculine and feminine products with unisex fragrances as a transversal class in between. How people define olfactory profile trends based on gender or how they differentiate those classes may be achieved through smelling, but it is, simultaneously, much more complex to unravel at scientific levels. Here, we applied the Perfumery Radar 2.0 methodology to predict the dominant character, considering outer and inner layer categories, for 13 typical feminine commercial perfumes. Table 4 presents the commercial names and brands for these fragrances together with the most relevant sensory classifications from fragrance houses and experts in the art of perfumery (extended sensory classifications are presented in Appendix A). From simple inspection of Figures 5 and 6, it is possible to observe that, once more, selected fragrances cover a broad spectra of the olfactory space since obtained radars are widely spread in terms of families. Furthermore, the predicted perfumery radars are in very good to excellent agreement with experts' sensory classifications as we will discuss below. First and foremost, it can be seen from Figure 5 that fragrances F1–F7 show a larger consent within classifications from fragrance houses where they are either typically floral (F1–F4) or oriental (F5–F7). Our Perfumery Radar 2.0 methodology predicted a clear floral character for the former group of fragrances (F1–F4) and a dominant oriental odor for the latter three (F5–F7). Additionally, a predicted clear floral scent with sweet-spicy in the outer category was observed for F1, which matches classifications from Osmoz, LT & TS, and the Fragrantica Web site (see Table 4 and Appendix A). However, if we extend our analysis to the inner layer of classification, we observe that for F3 the perfumery radar predicts a strong (91%) leather scent with a slight (6%) rose character. Such a result reveals that a richer scent within spicy-orientals (typical of leather) is perceived at inner levels. The scent of F2 is clearly floral which, peculiarly,

Table 4. Commercial Name, Brand, Year of Launch on the Market, Family Classification and Typical Gender Association for the Selected Commercial Perfumes in This Study<sup>a,b</sup>

ref	perfume name	brand	year	Osmoz	Scent Direct	H & R <sup>56</sup>	Octagon	iPerfumer	SFP	TFF/Fragrance Wheel	LT & TS	PR2.0
Feminine												
F1	L'air du Temps	Nina Ricci	1948	floral-spicy	floral	floral	floral bouquet	floral-spicy-woody	floral bouquet	floral	floral-spicy-green-fresh	floral
F2	Paris	YSL	1983	floral-rose violet	floral		floral simple-rose	floral	floral bouquet	floral	fruity-powdery-woody	floral
F3	Chanel 19	Chanel	1970	floral-green	floral-green	floral-green	floral simple-green	floral-green-woody	floral-green	soft floral	green-floral	floral-woody
F4	Eau de Givenchy	Givenchy	1980	citrus- aromatic	floral-fruity	floral-fruity	floral transparent	floral-green-citrus	floral-green	floral	green-floral	floral-green
F5	Addict	Dior	2002	oriental-vanilla	oriental floral-fresh			oriental-green-spicy		oriental	floral-oriental	oriental
F6	Addict Eau de Fraîche	Dior	2004	oriental-floral				floral-green-oriental		floral		oriental-fruity
F7	Gloria	Cacharel	2002	oriental-woody	oriental-fresh			oriental-woody-floral	amber-woody-floral		amber-rose	oriental-woody
F8	Eau de Rochas	Rochas	1970	citrus-aromatic	chypre-fresh	chypre- fresh		citrus-chypre-woody	floral-chypre-citrus		citrus-mossy-chypre	chypre-herbaceous
F9	Ô de Lancôme	Lancôme	1969	citrus-aromatic	chypre-fresh	chypre-fresh		citrus-chypre-green	floral-chypre-citrus		fresh citrus	floral-chypre
F10	Miss Dior	Dior	1947	chypre-floral	chypre-floral-animalic	chypre-animalic	chypre-green	chypre-green	green-chypre	mossy woods	aldehydic-chypre	chypre-green
F11	Ma Griffe	Carven	1945	chypre-floral	chypre- floral	chypre-animalic	chypre-green	chypre-green-floral	floral-aldehydic-chypre	mossy woods	green-chypre	floral-green
F12	Jungle Le Tigre	Kenzo	1997	oriental-spicy		chypre-fruity	floral-fruity	oriental-fruity-spicy				oriental-woody
F13	Le Feu d'Issey Light	I. Miyake	2000	floral-woody musk		oriental-spicy		floral-woody-musk		soft floral		floral-woody
Unisex <sup>c</sup>												
U1	Aqua Allegoria Herba Fresca	Guerlain	1999					citrus-green-aromatic <sup>F</sup>	aromatic-citrus	green	weird mint	fougère
U2	Aqua Allegoria Pamplelune	Guerlain	1999	Citrus-aromatic				citrus-green-fruity <sup>F</sup>			citrus-woody-grapefruit	citrus-floral-fruity
U3	Bulgari Extrême	Bulgari	1999	woody-aromatic <sup>M</sup>		fougère-woody <sup>M</sup>		woody-aromatic-citrus <sup>M</sup>	floral-woody-citrus		woody-spicy	floral-woody-oriental
U4	CK Be	Calvin Klein	1997	floral-woody musk		fougère-woody <sup>M</sup>		floral-musky-aromatic	floral-musk	aromatic-fougère	fougère	floral-fruity-woody
U5	Cologne	T. Mugler	2001	citrus-aromatic		chypre-citrus <sup>M</sup>		citrus-musky-floral	musk-citrus		citrus-woody-floral	floral-citrus-fruity
U6	Gaultier 2	J.P. Gaultier	2005	oriental-vanilla				oriental-floral-powdery	floriental	woody-oriental	powdery-musk-floral	fougère-oriental
U7	Eau de Cartier	Cartier	2001	citrus-aromatic	floral-fresh <sup>F</sup>	chypre-fresh <sup>F</sup>		floral-woody-citrus <sup>F</sup>	floral-woody-citrus		violet leaf-woods-citrus	floral-woody
U8	Voyage d'Hermès	Hermès	2010	woody-floral musk				citrus-woody-spicy		woods		woody-citrus
U9	Eau de Gentiane Blanche	Hermès	2009	woody-floral musk <sup>M</sup>				woody-musky-green		woods		woody-oriental-musk
U10	Eau de Campagne	Sisley	1976	floral-green				citrus-chypre-green <sup>F</sup>				floral-chypre
U11	CK One	Calvin Klein	1995	citrus-aromatic	chypre-fresh	chypre-fresh	floral transparent	citrus-floral-aromatic	floral-woody-citrus			floral-woody-citrus

Table 4. continued

ref	perfume name	brand	year	Osmoz	Scent Direct	H & R <sup>56</sup>	Octagon	iPerfumer	SFP	TFF/Fragrance Wheel	LT & TS	PR2.0
<b>Masculine</b>												
M1	Acqua di gio man	G. Armani	1996	aromatic-aquatic	chypre-fresh	chypre-fresh	fresh natural	citrus-marine-woody	floral-marine	water		floral-chypre
M2	Agua Brava	Puig	1968		fougère-lavender	fougère-fresh		fougère-aromatic-woody	woody-spicy	woods		fougère-woody
M3	Armani Mania	G. Armani	2002	woody-spicy				woody-musk-ambry		woods		woody-floral-oriental
M4	Azzaro	Azzaro	1978	aromatic-fougère	fougère-fresh	fougère-woody	fougère-aromatic	fougère-aromatic	aromatic-fougère	aromatic-fougère	fougère-aromatic	floral-fruity
M5	Euphoria Intense	Calvin Klein	2008	oriental-woody				woody-oriental-aromatic		woody-oriental		fougère-woody-oriental
M6	Furyo	Bogart	1988	oriental-woody	fougère-woody ambry	fougère-ambry			floral-chypre			fougère-oriental
M7	Boss Bottled	Hugo Boss	1998	woody spicy		fougère-ambry	oriental	oriental-woody-fruity		woody-oriental		woody-oriental
M8	Monsieur Léonard	Léonard	1992	oriental-fougère	fougère-woody ambry	fougère-ambry						woody-oriental
M9	No. 1 le bateleur	D&G	2009	aromatic-aquatic				woody-citrus-spicy		citrus		herbaceous-fougère
M10	New West	Aramis	1988	aromatic-rustic	chypre-leathery	chypre-leathery	aromatic-woody	fougère-citrus-marine	aromatic-chypre	water		woody-chypre
M11	Paco Rabanne	Paco Rabanne	1973	aromatic-fougère	fougère-woody ambry	fougère-woody	fougère-aromatic	fougère-woody-chypre		aromatic-fougère	citrus-woody	fougère-woody
M12	Quorum	Puig	1982			chypre-leathery	aromatic-woody	chypre-animalic-aromatic	aromatic-chypre	dry woods		chypre-herbaceous

<sup>a</sup>F, feminine; U, unisex; M, masculine. <sup>b</sup>These classifications were compiled from the literature and correspond to Osmoz (by Firmenich), Scent Direct, Haarman & Reimer (H&R), Octagon (by former Dragoco), iPerfumer (by Givaudan), Société Française des Parfumeurs (SFP), developed with ISIPCA Institute), The Fragrance Foundation (TFF), and Luca Turin & Tania Sanchez (LT & TS) experts. Further sensory classifications can be found in Appendix A. <sup>c</sup>Whenever a company or expert classification does not agree with gender distribution within the table, it is indicated as superscript "F", feminine, or "M", masculine.

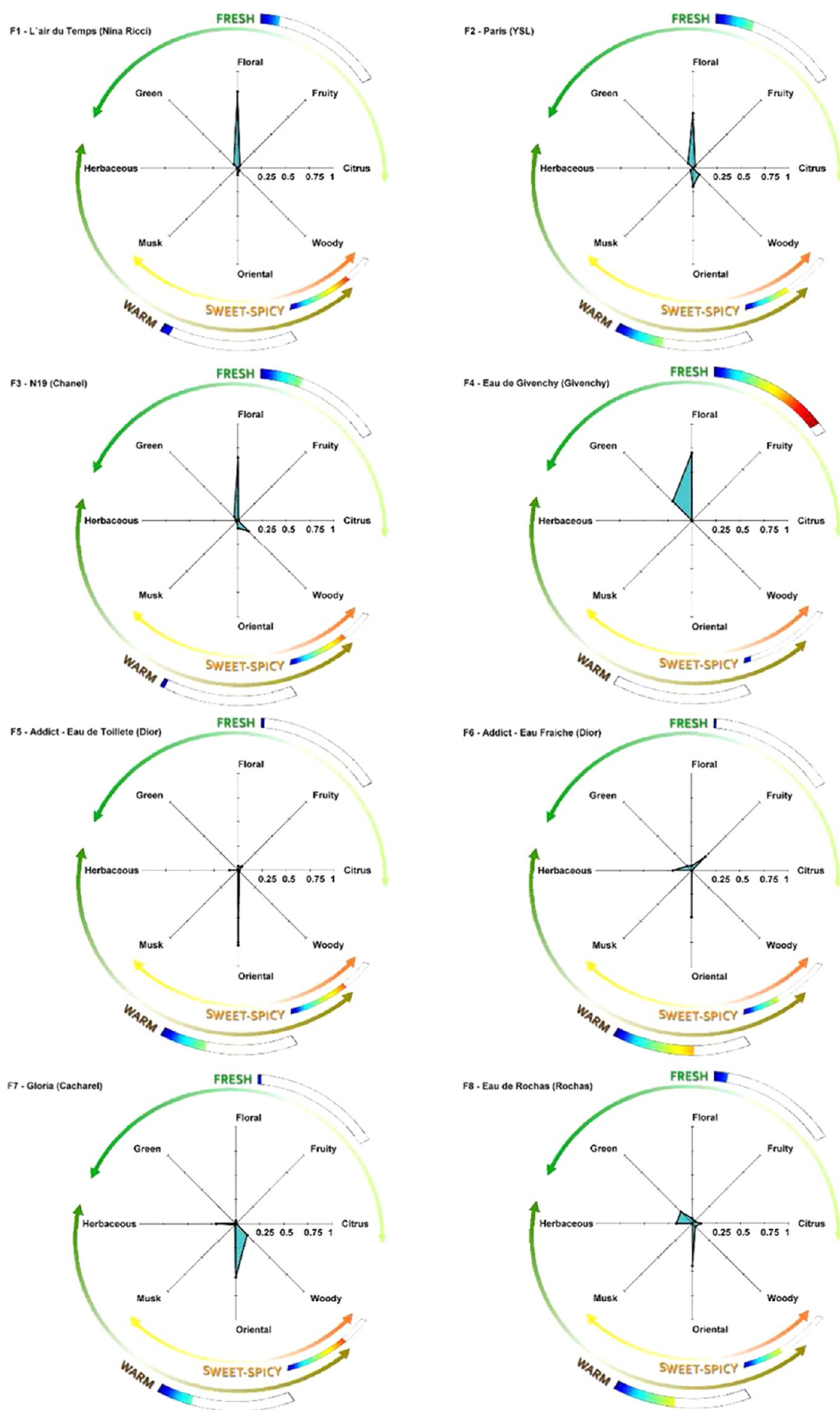


Figure 5. Perfumery radars for feminine commercial fragrances F1–F8.

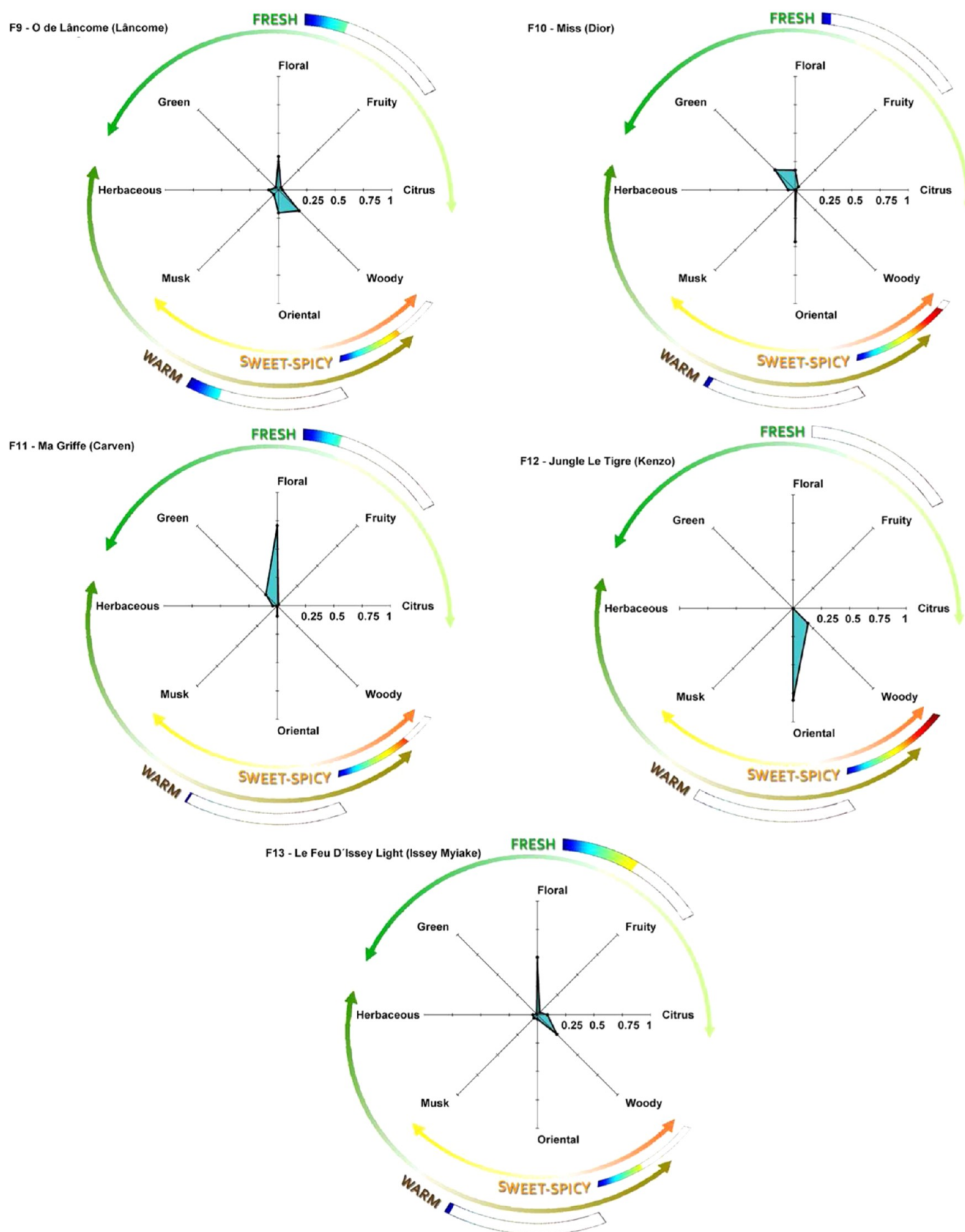


Figure 6. Perfumery radars for feminine commercial fragrances F9–F13.

agrees with the detailed classification from Osmoz, highlighting scents of rose (within middle notes) and leather (within base notes). For instance, fragrance F4 is described as, “the heart note is round, sweet and voluptuous with honeysuckle, jasmine, rose, ylang-ylang and tuberose”, which agrees with our predictions that revealed an inner layer composed of jasmine (46%), cinnamon (31%), and rose (23%) descriptors. However, we would like to note an important caveat: these relative percentages are merely indicative, being the result of the predicted Perfumery Radar 2.0 methodology and should not be taken as exact measures of the olfactory space.

On the other hand, classifications attributed to fragrances F8–F13 present large discrepancies among fragrance companies and experts. Within these commercial fragrances the chypre olfactory family appears several times. Chypre owns its name to its homonymous famous perfume dating from 1917. It consists of a combination of oak moss, *cistus labdanum*, patchouli, and bergamot as the main accord which can be somehow translated into woody, oriental, citrus, and fresh olfactory families.<sup>12</sup> Note, however, that several chypres can also have an aldehydic spike, as some green florals (which again reveals the complexity within fragrance classification). It is also analogous to the mossy woods category in Edwards’ fragrance wheel. Having said that, it is expected that fragrances within the chypre family may differ in their nuances (in terms of both character and magnitude) because it results from a combination of scents belonging to different families. Consequently or not, we observed larger divergences within experts’ classifications for this olfactory family (see Table 4 and Appendix A) than, for instance, for the single floral fragrances. It should be highlighted that it is known that fragrance classification is a very complex, subjective, and highly sensorial phenomenon, requiring much expertise and training. Despite that fact, it is also extremely difficult to quantify the magnitude of scents within a mixture, so a fragrance may be described as chypre-green or green-chypre (as happens for F10, for example).

We have developed a decision criterion for the assignment of a fragrance within the chypre family based on the definition of typical descriptors for that specific family and quantitative intensities for each descriptor or family within it. This was achieved through optimization of each criterion which resulted in the procedure presented in Appendix B. However, it should be highlighted that this decision criterion serves just as a guideline for fragrance classification that was obtained with a limited number of fragrances, as used in this study (so it should not be considered as a restrictive quantitative determination for chypre family classification). Accordingly, it was possible to see that the Perfumery Radar 2.0 accurately predicted the chypre dominant character for F8 and F10 with an average-to-good match on the nuances. For F9 we predicted a less dominant chypre in the odor space, having a floral-chypre classification while the majority of the experts’ evaluations compiled in Table 4 reported citrus-chypre (although SFP classified it as floral-chypre in accordance with what we achieved). Once more, it was possible to observe a good predictability for the inner layers of the odor space where, for example, F12 revealed a strong oriental-spicy character in line with most of the sensory descriptions (see Table 4). Finally, it is observed that, for the set of commercial perfumes studied here, feminine fragrances are typically dominant in floral and chypre families with oriental appearing as a salient dimension as well. This is in agreement with the analysis carried out in section 2 when evaluating results from Table 2.

**4.3. Masculine Perfumes.** For the typical masculine fragrances we have used the same methodology to predict the odor space of 12 commercial perfumes. Figures 7 and 8 represent the obtained predicted radars for the selected fragrances which can be compared with sensory classifications in Table 4. Within these fragrances (M1–M12) it is possible to observe that the fougère family appears several times in sensory classifications. Fougère has held its name since the iconic perfume Fougère Royale (Houbigant, 1882), eliciting “sexy cool-warm notes of citrus and lavender, sweet spices and oriental woods” as described by M. Edwards. The typical accord for a fougère fragrance contains lavender, coumarin, and oakmoss.<sup>25,32</sup> Since this traditional family is the result of a combination of others together with different nuances or accords, we have also developed a decision criterion for the assignment of a fragrance within the fougère family in analogy with that for chypre (see Appendix B). In fact, these two olfactory families are very important within fragrance design and classification, with the former being typically feminine while the latter is masculine (with few exceptions, as shown in Table 2).

Furthermore, predicted radars for masculine fragrances resulted in very good agreement in the vast majority of perfumes for the dominant olfactory family and in many cases for nuances. The major exception is observed for M4, which fragrance companies, in this particular case, classify as aromatic-fougère although we predicted a significant floral character in the headspace due to a strong jasmine note observed at inner layers. In fact, this is reported by Osmoz, which states that this fragrance has some “zesty notes like hedione” (typical jasmine scent) in its odor space, though these should be less intense while revealing its powerful oriental-woody character (as well as a leather note which we predicted in the inner layer with a relative dominance of 20%). Furthermore, it is possible to observe that masculine fragrances having fresh as a sensory descriptor such as M1 and M2 were accurately predicted in terms of both main olfactory families (floral-chypre and fougère-woody, respectively) but also at outer and inner layers of the odor space. The corresponding radars predicted a clearly dominant fresh category at the outer layer (Figure 6) which agrees with fragrance classifications, but we also predicted an inner layer rich in orange for M1 and camphor-pine for M2 in concordance with experts’ reviews.<sup>40</sup> Similarly, fragrances having a spicy descriptor from sensory evaluations as happens with M3, M7, M8, and M9 resulted in predicted radars with the sweet-spicy dimension being dominant at the outer layer. Concerning fragrance M10, sensory classifications diverge from aromatic-woody to chypre-leather and the predicted radar resulted as woody-chypre with leather dominance at the inner layer dimension. Analogously, fragrance M12 also shows large discrepancies among sensory classifications ranging from chypre-leather to aromatic-woody and our predictions resulted in chypre-herbaceous, which is in general agreement with SFP or the Perfume Intelligence Web site (see Appendix A). Finally, fragrance M11 is typically described as aromatic-fougère or fougère-woody, with the latter being in perfect agreement with our predictions. Again, it is important to note that the set of masculine fragrances studied here presented some typical olfactory families such as fougère, aromatic, and woody, which is in agreement with previous discussion in section 2, related to Table 2.

**4.4. Unisex Perfumes.** So far, we have separately analyzed the Perfumery Radar 2.0 in the light of gender with feminine and masculine fragrances. Light and floral scents are typically

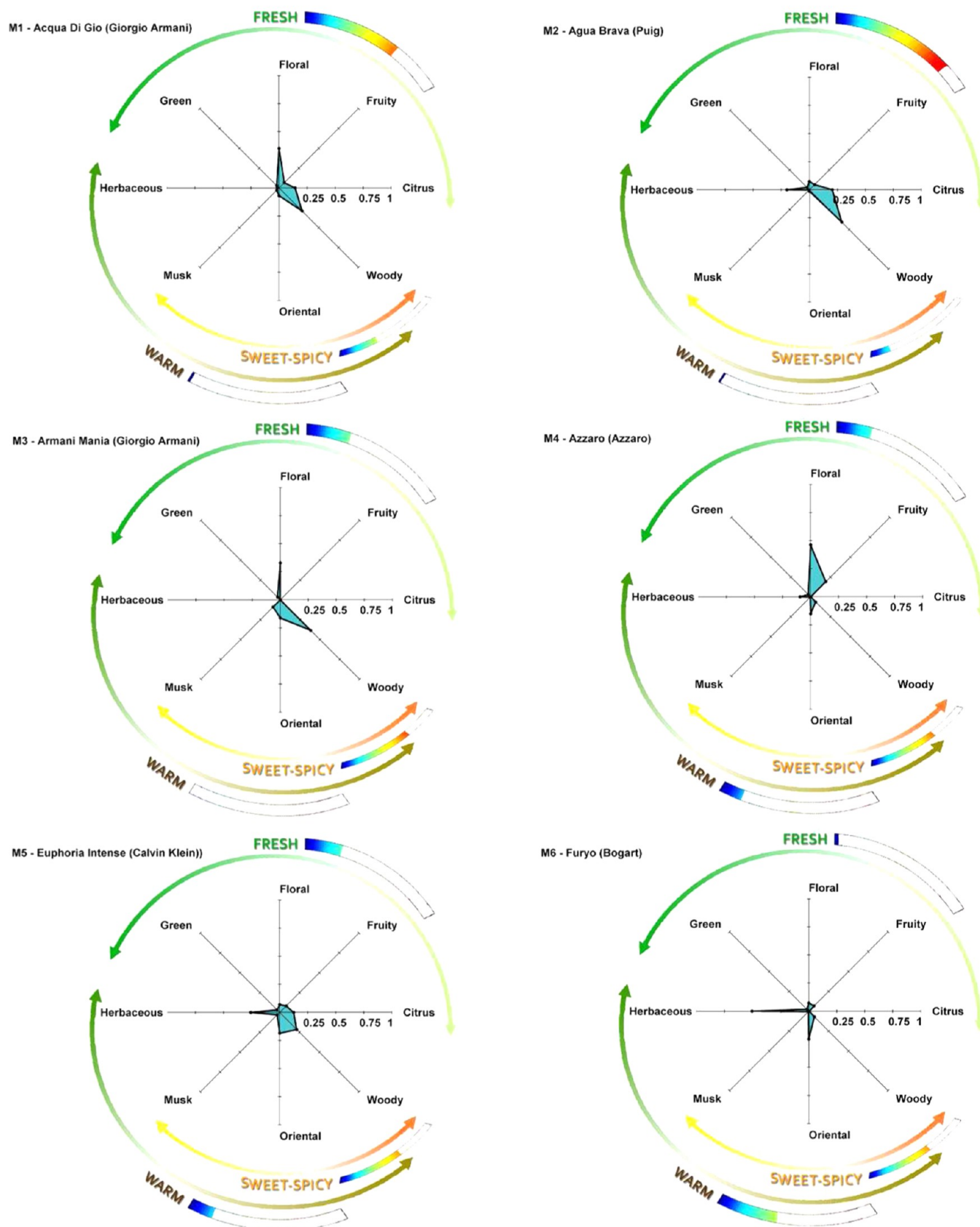


Figure 7. Perfumery radars for masculine commercial fragrances M1–M6.

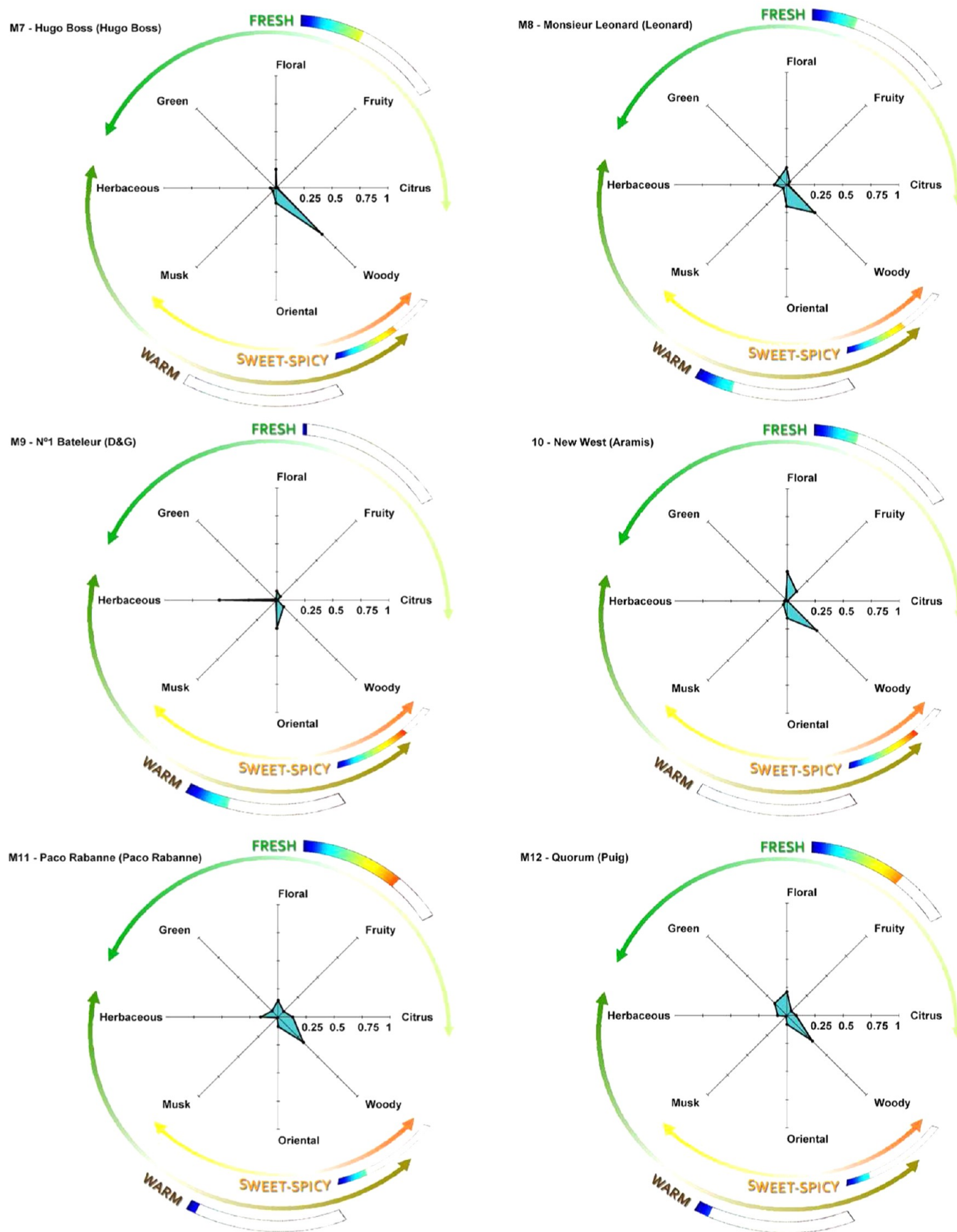


Figure 8. Perfumery radars for masculine commercial fragrances M7–M12.

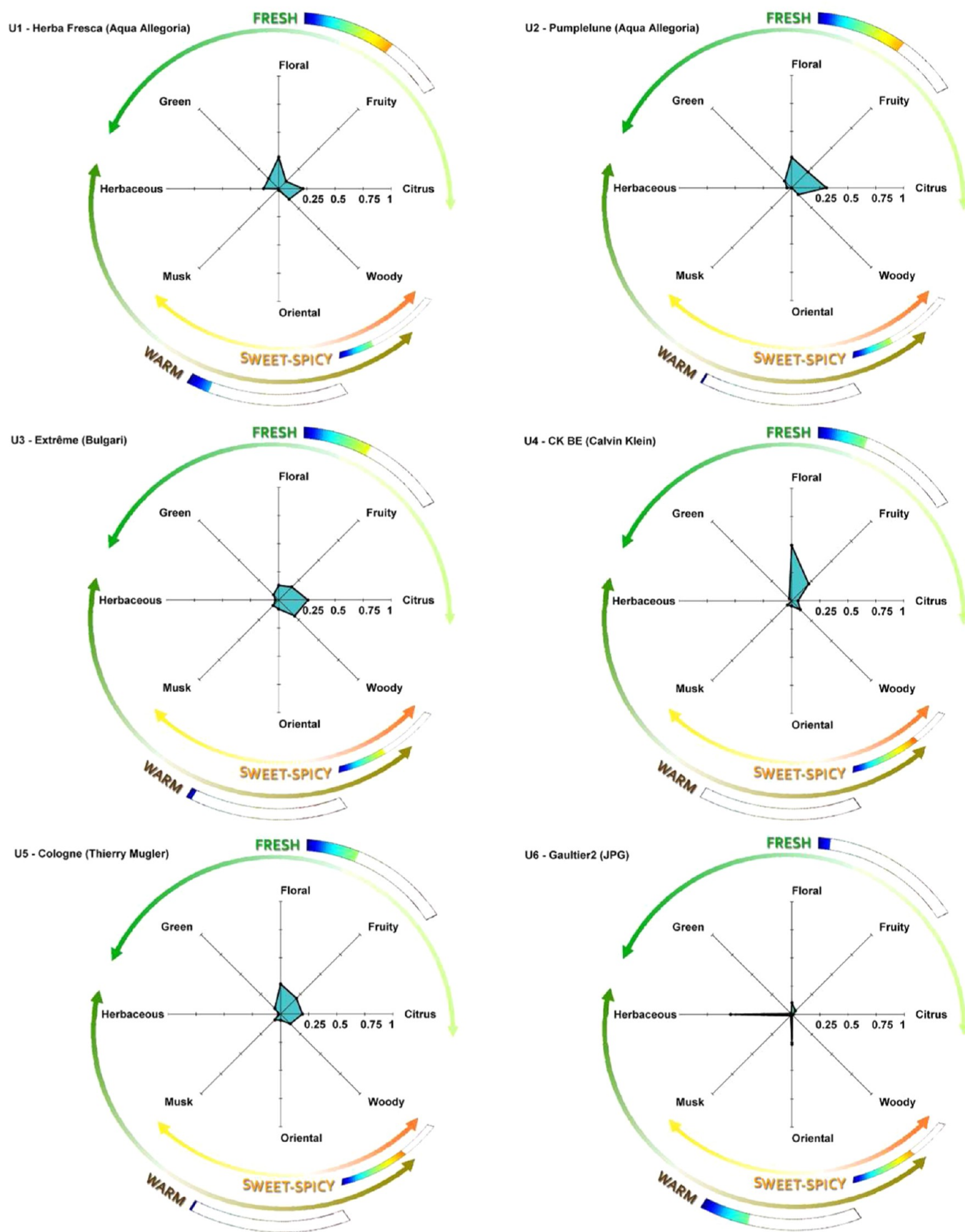


Figure 9. Perfumery radars for unisex commercial fragrances U1–U6.

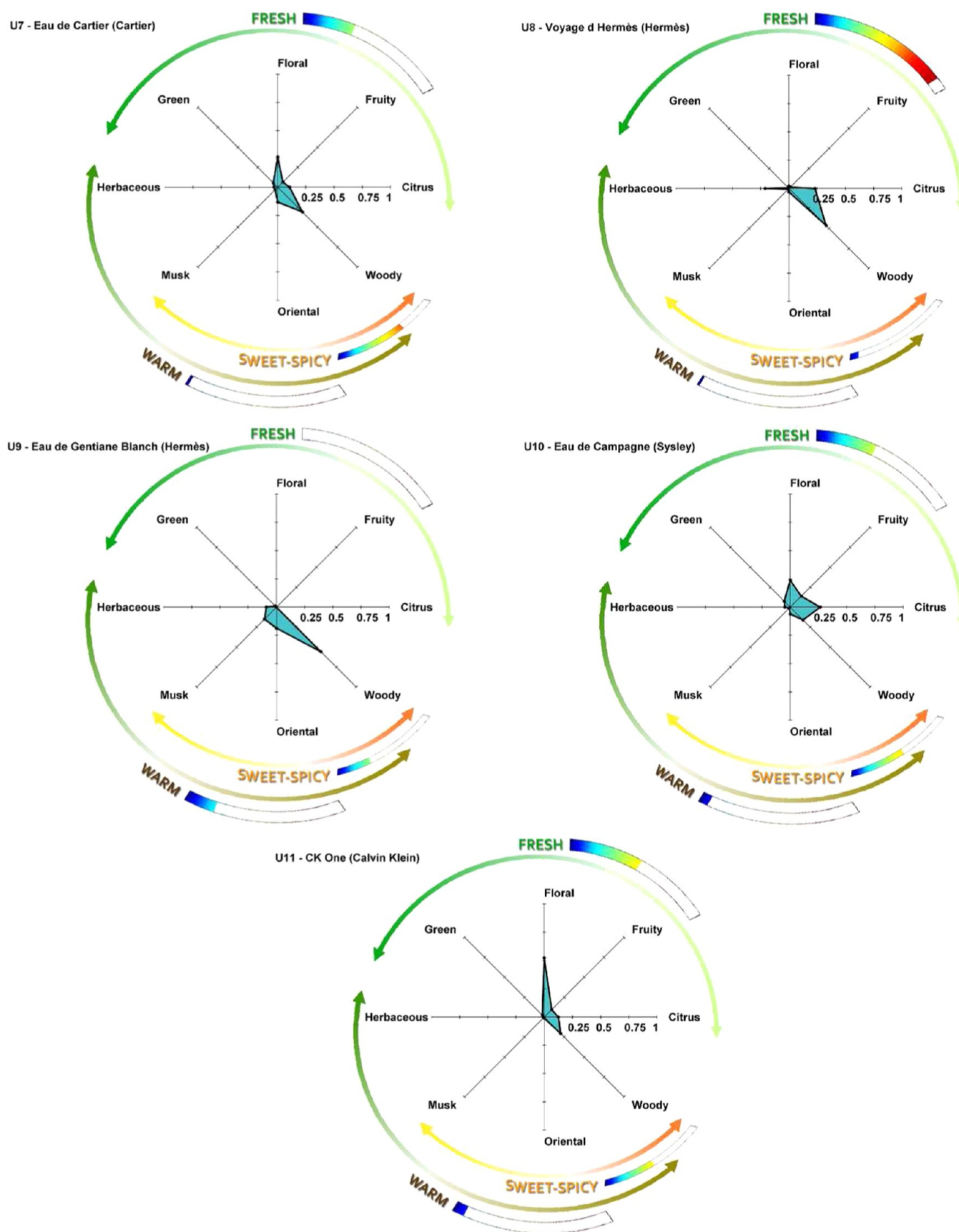
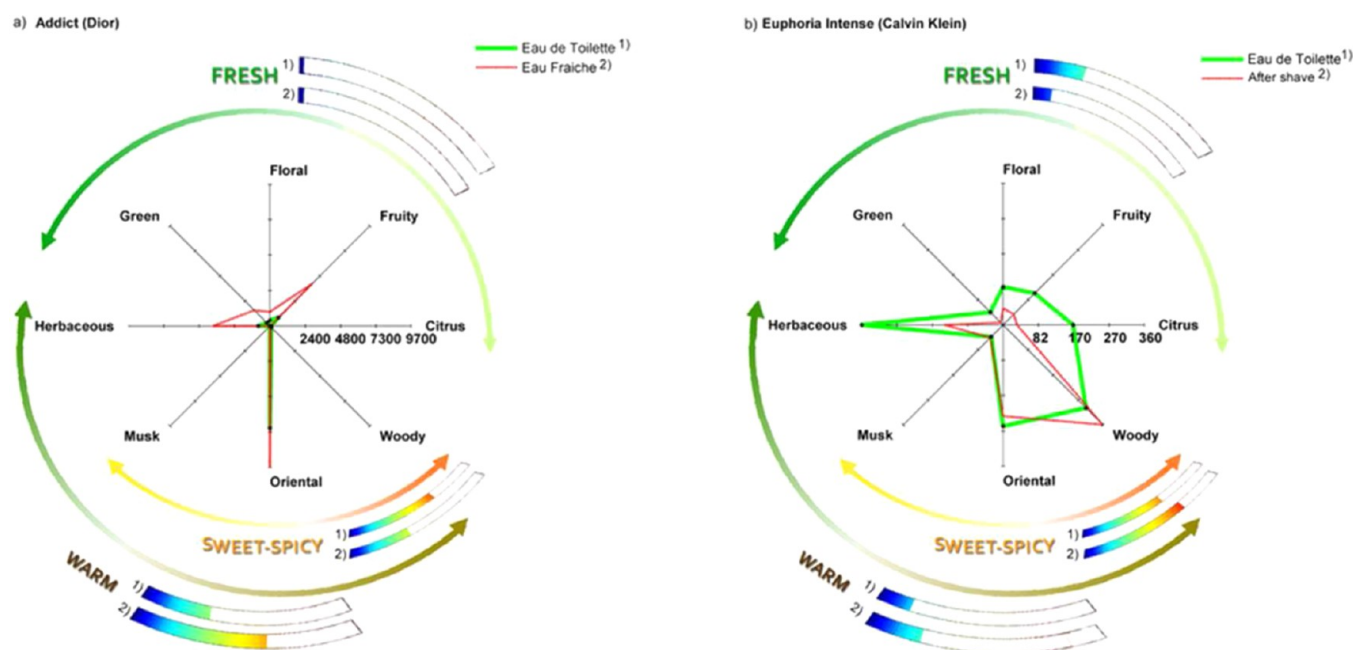


Figure 10. Perfumery radars for unisex commercial fragrances U7–U11.



**Figure 11.** Comparison between the odor intensities of the olfactory families of two different fragrances: (a) eau de toilette versus eau fraîche versions of the commercial perfume Addict (Dior) and (b) eau de toilette and aftershave versions of Euphoria Intense (Calvin Klein).

feminine, while rich aromatic-woody families are much more appellative to the masculine side. Nowadays, apart from these two genders, unisex fragrances are growing in trends and markets, aiming at simultaneously pleasing both women and men. Unisex fragrances represented in 2012 around 6.3% of the total volume in global sales, while feminine and masculine fragrances were reported to be 62.4 and 31.3%, respectively.<sup>57</sup> Consequently, as happens with colors (pink, yellow, and purple are considered more feminine, while blue, brown, and gray are appellative to masculine<sup>58</sup>), fragrances may be also gender specific. These differences within gender association are linked with fragrance composition, and that may become evident in the main olfactory families in which they fall under. For this purpose, the Perfumery Radar 2.0 methodology was applied to 11 unisex commercial fragrances from several brands (see Table 4). The predicted radars obtained for these fragrances are shown in Figures 9 and 10. As observed before with feminine and masculine perfumes, there are several discrepancies among classifications found in the literature for the same fragrance. It is also seen that some olfactory families are more prevalent in the unisex perfumes used in this study such as citrus, musk, and fresh but, for instance, spicy is rare. This is in agreement with our previous discussion on gender–character association for building up the Perfumery Radar 2.0 (see Table 2 and discussion therein). Moreover, it should be noted that for some of these commercial perfumes there is not unanimity on the classifications as to their unisex (U) character. This is shown in Table 4, and whenever different gender assignments were found, either its corresponding feminine (F) or masculine (M) category is highlighted with a superscript letter. With the exception of Gaultier 2 (by J.P. Gaultier), Voyage d'Hermès (by Hermès), and CK One (by Calvin Klein), all other perfumes present at least one divergent gender association. Conversely, within the unisex category, not only character classification but also gender assignment evidences its own difficulties in establishing family or gender frontiers, respectively.

From the comparison of the perfumery radars predicted in this work for the unisex fragrances and the classifications shown in Table 4, it is possible to observe a very good agreement. For the great majority of these selected commercial perfumes, the Perfumery Radar 2.0 methodology is able to accurately predict the odor space within the primary olfactory family, with few exceptions: Bulgari Extreme (U3, though it agrees with the SPF classification), Cologne (U5), and CK One (U11, though it agrees with the Dragoco classification), for which only secondary families were well predicted.

Nevertheless, for perfumes such as U4, U7, U8, or U9 obtained predictions perfectly match all the classifications from the experts. Curiously, the predicted outer layer for fragrance U9 shows cool/mint and powdery dimensions as dominant (not shown in Figure 9), which is in contrast to the majority of the fragrances studied here but agrees with detailed sensory descriptions from *Fragrantica*.<sup>40</sup>

However, there is still a long way to go on the classification of odors, and the prediction of their tendency toward women or men is still difficult to know a priori. Fragrance perception is highly dimensional and complex, differing from one to another. Age is also an important factor to take into account in this matter: the Fragrance Foundation reported that women under 18 have higher propensity for citrus fragrances, while in the 18–25 range they prefer fruity-floral notes, and above 35 years of age women mostly choose musky notes.<sup>59</sup>

**4.5. Evaluation of Odor Intensities of Similar Perfumes.** Fine fragrances can also be classified in terms of their chemical composition (which is a function of the desired type of application—eau de parfum, eau de toilette, aftershave, among others). Here, we will use the Perfumery Radar 2.0 to compare both the perceived odor intensity and the character of similar fragrances (same brand and model) but which differ in composition (especially in terms of alcohol and water content but sometimes in terms of ingredients as well) and type of application (which is the result of extending a product's portfolio within brands). For that purpose, we randomly selected

Table 5. Complete List of Commercial Fragrances Used in This Study with All Olfactory Family/Character Classifications Found in the Literature

ref.	perfume name	brand	year	Osmoz	Scent Direct	H & R	Octagon	iPerfumer	SFP	TFF	LT & TS	AuParfum <sup>60</sup>	Prime-Beauté <sup>61</sup>	Fragrantica	Perfume Intelligence <sup>62</sup>	PR2.0
<b>Feminine</b>																
F1	L'air du Temps	Nina Ricci	1948	floral-spicy	floral	floral	floral bouquet	floral-spicy-woody	floral bouquet	floral	floral-spicy-green-fresh	floral-spicy-woody	floral-spicy	floral-spicy	floral	floral
F2	Paris	YSL	1983	floral-rose violet	floral		floral simple-rose	floral	floral bouquet	floral	fruity-powdery-woody	floral-rose violet	floral-rose violet	floral	floral	floral
F3	Chanel 19	Chanel	1970	floral-green	floral-green	floral-green	floral simple-green	floral-green-woody	floral-green	soft floral	green-floral	floral	floral-green	floral-woody-green	soft fresh green-floral	floral-woody
F4	Eau de Givenchy	Givenchy	1980	citrus-aromatic	floral-fruity	floral-fruity	floral transparent	floral-green-citrus	floral-green	floral	green-floral	floral	floral	floral-fruity	green-floral-fruity	floral-green
F5	Addict	Dior	2002	oriental-vanilla	oriental-floral-fresh			oriental-green-spicy	oriental	oriental	floral-oriental	oriental	oriental	oriental-floral	floral-oriental	oriental
F6	Addict Eau de Fraîche	Dior	2004	oriental-floral				floral-green-oriental		floral				oriental-floral	fruity-floral	oriental-fruity
F7	Gloria	Cacharel	2002	oriental-woody	oriental-fresh			oriental-woody-floral	amber-woody-floral		amber-rose		oriental-woody-warm	oriental-woody	oriental-woody	oriental-woody
F8	Eau de Rochas	Rochas	1970	citrus-aromatic	chypre-fresh	chypre-fresh		citrus-chypre-woody	floral-chypre-citrus		citrus-mossy-chypre	citrus	citrus-aromatic	citrus-chypre	chypre-herbaceous	chypre-herbaceous
F9	Ô de Lancôme	Lancôme	1969	citrus-aromatic	chypre-fresh	chypre-fresh		citrus-chypre-green	floral-chypre-citrus	citrus	fresh citrus		citrus-aromatic	citrus	fresh-citrus	floral-chypre
F10	Miss Dior	Dior	1947	chypre-floral	chypre-floral-animalic	chypre-animalic	chypre-green	chypre-green	green-chypre	mossy woods	aldehydic-chypre	chypre	oriental-chypre	chypre-floral	fresh green-mossy-woods-chypre	chypre-green
F11	Ma Griffe	Carven	1945	chypre-floral	chypre-floral	chypre-animalic	chypre-green	chypre-green-floral	floral-aldehydic-chypre	mossy woods	green-chypre		chypre	chypre-floral	crisp green-mossy-woods-chypre	floral-green
F12	Jungle Le Tigre	Kenzo	1977	oriental-spicy		chypre-fruity	floral-fruity	oriental-fruity-spicy						oriental-spicy	fresh-fruity-floral-oriental	oriental-woody
F13	Le Feu d'Issey Light	Issey Miyake	2000	floral-woody musk		oriental-spicy		floral-woody-musk		soft floral				floral	woody-oriental	floral-woody
<b>Unisex</b>																
U1	Aqua Allegoria Herba Fresca	Guerlain	1999					citrus-green-aromatic <sup>F</sup>	aromatic-citrus	green	weird mint		aromatic-citrus <sup>F</sup>	aromatic-green	fougère	
U2	Aqua Allegoria Pamplelune	Guerlain	1999	citrus-aromatic				citrus-green-fruity <sup>F</sup>	citrus	citrus	citrus-woody-grapefruit		fruity-citrus <sup>F</sup>	citrus	citrus-floral-fruity	
U3	Bulgari Extrême	Bulgari	1999	woody-aromatic <sup>M</sup>		fougère woody <sup>M</sup>		woody-aromatic-citrus <sup>M</sup>	floral-woody-citrus	citrus	woody-spicy		woody-aromatic <sup>M</sup>	woody-aromatic <sup>M</sup>	floral-woody-oriental	
U4	CK Be	Calvin Klein	1997	floral-woody musk		fougère-woody <sup>M</sup>		floral-musky-aromatic	floral-musk	aromatic-fougère	fougère	woody	fougère-fresh	floral-woody-musk	fresh woody-oriental	
U5	Cologne	Thierry Mugler	2001	citrus-aromatic		chypre-citrus <sup>M</sup>		citrus-musky-floral	musk-citrus	citrus	citrus-woody-floral		citrus-aromatic	citrus	floral-citrus-fruity	
U6	Gaultier 2	J.P. Gaultier	2005	oriental-vanilla				oriental-floral-powdery	floral	woody-oriental	powdery-musk-floral	oriental	oriental-vanilla	oriental-vanilla	fougère-oriental	
U7	Eau de Cartier	Cartier	2001	citrus-aromatic	floral-fresh <sup>F</sup>	chypre-fresh <sup>F</sup>		floral-woody-citrus <sup>F</sup>	floral-woody-citrus	citrus	violet leaf-woods		citrus-aromatic <sup>F</sup>	citrus-aromatic	aromatic-citrus	floral-woody
U8	Voyage d'Hermès	Hermès	2010	woody-floral musk				citrus-woody-spicy		woods				woody-floral-musk	fresh musk-woody	woody-citrus
U9	Eau Gentiane Blanche	Hermès	2009	woody-floral musk <sup>M</sup>				woody-musky-green		woods				aromatic	woody-oriental-musk	
U10	Eau de Campagne	Sisley	1976	floral-green				citrus-chypre-green <sup>F</sup>		woods				chypre-floral	floral-chypre	

Table S. continued

ref.	perfume name	brand	year	Osmoz	Scent Direct	H & R	Octagon	iPerfumer	SFP	TFF	LT & TS	AuParfum <sup>60</sup>	Prime-Beauté <sup>61</sup>	Fragrantica	Perfume Intelligence <sup>62</sup>	PR2.0
U11	CK One	Calvin Klein	1995	citrus-aromatic	chypre-fresh	chypre-fresh	floral transparent	citrus-floral-aromatic	floral-woody-citrus	citrus	citrus	citrus	citrus-aromatic	citrus-aromatic	fresh citrus	floral-woody-citrus
<b>Unisex</b>																
M1	Acqua di gio man	Giorgio Armani	1996	aromatic-aquatic	chypre-fresh	chypre-fresh	fresh natural	citrus-marine-woody	floral-marine	water		aromatic	aromatic-aquatic	aromatic-aquatic	crisp marine	floral-chypre
M2	Agua Brava	Puig	1968		fougère-lavender	fougère-fresh		fougère-aromatic-woody		woods				woody-chypre	mossy woods	fougère-woody
M3	Armani Mania	Giorgio Armani	2002	woody-spicy				woody-musk-ambery	woody-spicy	woods			woody-spicy	woody-spicy	aromatic-fougère	woody-floral-oriental
M4	Azzaro	Azzaro	1978	aromatic-fougère	fougère-fresh	fougère-woody	fougère-aromatic	fougère-aromatic	aromatic-fougère	aromatic-fougère		fougère	aromatic-fougère	aromatic-fougère	fresh aromatic-fougère	floral-fruity
M5	Euphoria Intense	Calvin Klein	2008	oriental-woody				woody-oriental-aromatic		woody-oriental			woody	oriental-woody	woody-oriental	fougère-woody-oriental
M6	Furyo	Bogart	1988	oriental-woody	fougère-woody-ambery	fougère-ambery		—	floral-chypre					oriental-woody	floral-chypre	fougère-oriental
M7	Boss Bottled	Hugo Boss	1998	woody-spicy		fougère ambery	oriental	oriental-woody-fruity		woody-oriental		woody	woody-spicy	woody-spicy		woody-oriental
M8	Monsieur Léonard	Léonard	1992	oriental-fougère	fougère-woody-ambery	fougère-ambery		—							aromatic-fougère	woody-oriental
M9	No. 1 le bateleur	D&G	2009	aromatic-aquatic				woody-citrus-spicy		citrus			aromatic-aquatic	aromatic-aquatic	herbaceous-fougère	
M10	New West	Aramis	1988	aromatic-rustic	chypre-leathery	chypre-leathery	aromatic-woody	fougère-citrus-marine	aromatic-chypre	water				aromatic	marine-chypre	woody-chypre
M11	Paco Rabanne	Paco Rabanne	1973	aromatic-fougère	fougère-woody-ambery	fougère-woody	fougère-aromatic	fougère-woody-chypre		aromatic-fougère		fougère	aromatic-fougère	aromatic-fougère	fougère	fougère-woody
M12	Quorum	Puig	1982			chypre-leathery	aromatic-woody	chypre-animalic-aromatic	aromatic-chypre	dry woods				woody-aromatic	aromatic-chypre	chypre-herbaceous

two fragrances from our study: one feminine—Addict (Dior)—with the versions eau de toilette and eau fraîche, and one masculine—Euphoria Intense (Calvin Klein)—in the eau de toilette and aftershave versions. A comparison between the obtained radars is shown in Figure 11.

First of all, a comparison between the compositions of these fragrances has shown that, although they have very similar fragrance ingredients, some of those are present in significantly different concentrations (meaning concentrations in the concentrated perfume or absolute, besides the obvious dilutions used in ethanol and water, as previously referred). For example, limonene and linalyl acetate are 3 and 5 times more concentrated in Addict eau de toilette than in the eau fraîche, respectively. In the same way, these chemicals have shown 8 and 4 times more concentration in the Euphoria Intense eau de toilette version than in the aftershave, respectively. Furthermore, some fragrance ingredients were found in the composition of one of the versions but not in the other. From the analysis of Figure 11, it is clear that there are differences in both intensity and character between the two versions of Addict tested here (Figure 11a) while for Euphoria Intense (Figure 11b) the odor space is similar though with small differences in the intensities of the olfactory families. Moreover, in terms of odor intensity, it is seen that the odor values for the dominant notes of each perfume are much higher in the oriental family for Addict ( $\max OV_i = 9700$ ) than in the woody family for Euphoria Intense ( $\max OV_i = 360$ ). No sensory classifications were found in the literature for the aftershave version of Euphoria Intense, though the predicted radar is very similar to the eau de toilette version as could be expected.

## 5. CONCLUSIONS

The Perfumery Radar 2.0 methodology uses scientific models combined with sensory properties from perfumery for the design and classification of perfumed products. It uses thermodynamic models for prediction of vapor–liquid equilibria and psychophysical models for olfactory perception. Altogether, it introduces scientific knowledge for a standardized way of classification of perfumes and the odor space, instead of relying only on experimental evaluations which are subjected to large interpersonal variability. In this way, the arbitrariness of the classification of fragrances is confined to experimental descriptors for pure fragrance chemicals. Furthermore, since this is a modular built methodology, it presents high flexibility: it is possible to easily change or add perfume families to the radar plots, include or exclude fragrant components, add new data, or even change the models used to account for the evaporation, odor intensity, or family character. The Perfumery Radar 2.0 methodology was fully validated in this work, and it has been

shown that it is able to accurately predict the primary olfactory family and nuances in several commercial fragrances belonging to different genders. Furthermore, the extension of the previous perfumery radar methodology allows characterizing the odor space at higher levels (outer and inner layers together with the basic olfactory families) with accuracy. It should be mentioned, though, that the Perfumery Radar 2.0 methodology, as a purely predictive tool, still has some limitations in order to explain the whole spectra of the odor space when compared to the level of screening of the human nose (this is discussed in detail elsewhere<sup>8</sup>). Nevertheless, we consider it to be a valuable tool for the preformulation stages of fragrance design and classification, thus helping perfumers in developing their work.

## ■ APPENDIX A

Table 5 contains the complete list of commercial fragrances used in this study and all olfactory family and character classifications found in the literature.

## ■ APPENDIX B

The decision criteria developed for both chypre and fougère olfactory families considers the typical classifications given in the literature for the main families or nuances which fall within these two families. Note, however, that once more, there is not a perfect agreement for the “definition” of chypre and fougère within the literature. Here, we have followed the detailed description from M. Edwards<sup>25</sup> and optimized the calculation of different criteria in order to obtain the maximum agreement with experts’ classifications of perfumes. Finally, these guidelines are the result of numerical computation using the Perfumery Radar 2.0 methodology, predicting boundaries for these two classic perfume families, though there will be exceptions.

The result of applying these criteria is that a radar plot for a particular perfume can be considered as belonging to the chypre and fougère families, rather than a combination of several families in the radar axes. Considering the relevance of the chypre and fougère families in perfumery, it is critical that the Perfumery Radar 2.0 identifies them as salient dimensions of the odor space and clearly as all other perfume classifications.

The decision criteria for the assignment of a fragrance within the chypre family are presented as depicted in Condition 1 of Chart B1.

If Condition 1 is met, the fragrance does not belong to the chypre family (see Condition 2 in Chart B1).

If Condition 2 is met, the fragrance belongs to the chypre family (and has dominant chypre character). If it is not met, the fragrance has chypre nuance but another family is dominant.

**Chart B1. Decision Criteria for the Assignment of a Fragrance within the Chypre Family**

Condition 1:

$$\text{if } \left\{ \sum \{\text{citrus, oriental, woody}\} < 45\% \vee \left\{ \begin{array}{l} \text{citrus} < 0.1\% \\ \text{oriental} < 0.1\% \\ \text{woody} < 0.1\% \end{array} \right\} \vee \left\{ \begin{array}{l} \text{citrus} > 45\% \\ \text{oriental} > 45\% \\ \text{woody} > 45\% \end{array} \right\} \vee \text{herbaceous} > 15\% \right\}$$

Condition 2:

$$\text{if } \left\{ \sum \{\text{citrus, oriental, woody}\} > 45\% \wedge \left\{ \begin{array}{l} \text{fruity} < 25\% \\ \text{floral} < 25\% \\ \text{green} < 25\% \\ \text{musk} < 25\% \end{array} \right\} \right\}$$

Chart B2. Decision Criteria for the Assignment of a Fragrance within the Fougère Family

Condition 1:

$$\text{if } \left\{ \sum \{\text{citrus, herbaceous, oriental, woody}\} < 45\% \vee \left\{ \begin{array}{l} \text{citrus} < 0.1\% \\ \text{oriental} < 0.1\% \\ \text{woody} < 0.1\% \end{array} \right\} \vee \left\{ \begin{array}{l} \text{citrus} > 45\% \\ \text{oriental} > 45\% \\ \text{woody} > 45\% \end{array} \right\} \vee \text{herbaceous} < 15\% \vee \sum \{\text{sweet, fresh}\} < 50\% \right\}$$

Condition 2:

$$\text{if } \left\{ \sum \{\text{citrus, herbaceous, oriental, woody}\} > 45\% \wedge \left\{ \begin{array}{l} \text{fruity} < 25\% \\ \text{floral} < 25\% \\ \text{green} < 25\% \\ \text{musk} < 25\% \end{array} \right\} \right\}$$

The decision criteria for the assignment of a fragrance within the fougère family are presented as depicted in Condition 1 of Chart B2.

If Condition 1 is met, the fragrance does not belong to the fougère family (see Condition 2 in Chart B2).

If Condition 2 is met, the fragrance belongs to the fougère family (and has dominant fougère character). If it is not met, the fragrance has fougère nuance but another family is dominant.

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### Notes

The authors declare no competing financial interest.

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