

Article

Multivariate Analysis of Olfactory Profiles for 140 Perfumes as a Basis to Derive a Sensory Wheel for the Classification of Feminine Fragrances

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Abstract: In order to guide consumers in their purchase of a new fragrance, one approach is to visualize the spectrum of men's or women's fragrances on a two-dimensional plot. One of such sensory maps available is the Hexagon of Fragrance Families. It displays 91 women's perfumes inside a polygon, so that each side accounts for a different olfactory class. In order to discuss this chart, odor profiles were obtained for these fragrances and additional feminine ones (140 in total, launched from 1912 to 1990). An olfactory dataset was arranged by coding numerically the descriptions obtained from *Fragrantica* and *Osmoz* websites, as well as from a perfume guide. By applying principal component analysis, a sensory map was obtained that properly reflected the similarities between odor descriptors. Such representation was equivalent to the map of feminine fragrances called *Givaudan Analogies*, comprised of five major categories. Based on the results, a modified version of the Hexagon based on 14 categories was proposed. The first principal component explained preference for daytime versus nighttime wear, and regression models were fitted in order to estimate such preferences according to the odor profiles. The second component basically discriminated floral versus chypre (mossy-woody) fragrances. Results provide a fundamental basis to develop standard sensory maps of women's fragrances.

Keywords: odor analysis; fragrance; olfactory psychophysics; smell perception; odor descriptor

1. Introduction

The perceptual space of smells is highly dimensional. As a consequence, odors are difficult to measure and describe. Different reviews about aroma classification [1,2] reveal the troubles in trying to achieve certain consensus. The same difficulties are encountered when attempting to classify perfumes, which is a matter of interest because the number of commercial fragrances has increased considerably in the last decades. This issue is reflected by the size of different perfume compilations publicly available. For example, years ago the French Society of Perfumers (FSP) published a catalog comprising 807 items [3]. A directory compiled in 1991 by the company Haarmann and Reimer (H&R) displays 820 perfumes [4]. A few years later, another handbook classified about 1800 perfumes sold in the UK market [5]. A fragrance directory re-edited every year by Michael Edwards since 1984 [6] listed 2700 products in 2001, but the online version contains over 19,500 perfumes (www.fragrancesoftheworld.info). The websites of *Osmoz* [7] and *Fragrantica* [8] display olfactory descriptions for more than 8000 and 50,000 commercial perfumes, respectively.

Consumers often feel overwhelmed when entering a fragrance store due to the enormous amount of items on sale. The guidance of shop assistants is necessary in most cases, and clients have to rely on their experience. Different guides and web resources like the ones mentioned above are available, but odor description and classification is rarely displayed at the traditional perfumery stores. It seems that

the market trend in the near future will be to facilitate the olfactory information to customers. For this purpose, one option is to arrange the fragrances on sale depending on their smell, not by brand. The H&R Genealogy [9] shows a graphical taxonomy of women's perfumes structured in seven families and different subfamilies, as well as according to the year when they first appeared in the market. Similar diagrams have also been developed by other companies [10].

The classification of commercial fragrances in olfactory categories is helpful for consumers in their purchase of a new perfume. Another approach is to describe graphically the olfactory spectrum offered by a store by means of a two-dimensional (2D) sensory map, like the one called Analogies of Fragrances, developed by the Swiss company Givaudan [11] (p. 276). Perfumes close to each other in such representations are supposed to smell alike, while those located far apart would smell quite different.

One of the most popular perfume charts, and probably the most trusted in the industry, is the Fragrance Wheel developed by Edwards [12], which displays 14 categories organized around a central hub (www.fragrancesoftheworld.com). This wheel is based on two contrasting polarities: "fresh" versus "oriental", and "floral" versus "woody". A Spanish company of generic fragrances is currently using Edwards's Wheel to show consumers the olfactory classes of items on sale [13]. An experiment performed by the company Dragoco using 94 fragrances led to a sensory map structured on similar dimensions [14]. The same polarities can also be matched more or less with the two axes of another fragrance map [11] (p. 279) and 2D plots reflecting the similarities between odor descriptors commonly used in perfumeries [15,16]. Other sensory wheels have been developed in the field of perfumery like the Drom Fragrance Circle [17] and the Discodor [18]. One reported study has proposed a methodology to obtain graphic profiles of scents, which was applied to 36 commercial fragrances [19].

Most of these sensory representations are intended for fragrances in general but, excluding unisex ones, commercial perfumes are targeted either to men or women. Thus, a specific chart of women's fragrances would be more useful for a lady when purchasing a new product than a sensory chart of general scents. Regarding this issue, an experiment based on sorting tasks obtained a 2D projection of 12 commercial women's perfumes on a plot [20], and further research using the same fragrances led to similar results [21]. Another work obtained sensory maps for 15 female perfumes based on semantic methods of odor description [22]. These studies are of relevant scientific interest, but the number of samples assessed was very low and, hence, it is not representative of the huge population of perfumes in the market.

Fragrance companies have obtained sensory charts with a higher number of items. For example, Dragoco mapped 91 perfumes inside a representation called the Hexagon of Fragrance Families [23], so that each side of the hexagon accounts for a different odor class. Although this sensory wheel was developed 30 years ago, it has not been discussed yet in detail. For this purpose, odor profiles were obtained by numerically coding the olfactory descriptions of fragrances from different sources that were publicly available. Such profiles were analyzed by applying principal component analysis. The resulting 2D projection was discussed and compared with an equivalent chart developed by Givaudan. Moreover, an effort was carried out to adapt the Fragrance Wheel for the classification of women's fragrances. In a previous study [24], the same methodology was successfully applied to prove that Edwards's Wheel properly exemplifies the olfactory spectrum of fragrances. One target of the present work was to discuss how such a sensory wheel should be reorganized in order to better illustrate the perceptual space of feminine scents.

2. Materials and Methods

2.1. Sample of 140 Feminine Fragrances under Study

A set of 91 women's perfumes are displayed inside Dragoco's Hexagon, 73% of which first appeared in the market between 1981 and 1989. Two of them, Moschus Love Dream and Donna, were disregarded because they were not found in any of the perfume compilations used in the present

research: H&R guide [4], Osmoz [7], and Fragrantica [8]. The coordinates of items inside this polygon were measured from the original publication [23] using a graduated scale from -5 to 5 . Such coordinates will be referred to hereafter as X_{hexag} and Y_{hexag} . Taking into account the standard skewness coefficient (SS) and by means of a normal probability plot, it was checked that X_{hexag} follows reasonably a normal distribution (SS = 0.9) as well as Y_{hexag} , though the latter is slightly negatively skewed (SS = -0.7) due to the presence of seven values very close to the maximum.

At the time when the Hexagon was published, a sensory experiment was carried out at Dragoco with 140 commercial perfumes, which were mapped on a 2D plot [25]. The vertical axis was interpreted as “warm” versus “cool”, while the orthogonal dimension basically discriminated floral versus nonfloral scents. The coordinate of each fragrance along this vertical axis was measured by using a graduated scale ranging from -5 (warm) to $+5$ (cool). Such values will be denoted as “cool” scores (S_{cool}). Analogously, the coordinate position along the x axis was measured on a scale from -5 (nonfloral) to $+5$ (floral), and it was named as S_{floral} [24].

Further research by Jellinek [14] led to a similar sensory representation based on the same dimensions, depicting 94 perfumes. Again, their x and y coordinates were quantified on a scale from -5 to $+5$, which were called S_{floral} and S_{cool} , as in the previous case. As expected, S_{floral} scores appeared positively correlated for the 58 fragrances contained in both studies [14,25], which supports using their average to improve the accuracy; their mean S_{cool} was also computed accordingly [24].

It was checked that the statistical distribution of S_{cool} was close to normality, though slightly positively skewed (SS = 1.3). Conversely, the distribution of S_{floral} was negatively skewed (SS = -2). Given that both parameters provide relevant sensory information on a continuous scale, all women’s perfumes assessed by Jellinek [14,25] were also considered here, 67 of which are contained in the Hexagon. Altogether, 89 from the Hexagon plus 51 additional ones from Jellinek’s studies, makes a set of 140 feminine fragrances studied in the present work.

2.2. Olfactory Descriptions from Fragrantica’s Website

All these 140 fragrances except three are contained in Fragrantica [8]. This website indicates, by means of a bar chart, the percentage of users who consider a given perfume more appropriate for nighttime versus daytime wear. As the exact value of such percentages is not indicated numerically, they were obtained by measuring the length of each bar, which will be called P_{night} and P_{day} , respectively. The bar chart also displays the percentage of users who voted the fragrance more suitable for summer or winter, which were denoted as P_{summer} and P_{winter} , respectively [24]. The relationship P_{night} versus P_{winter} was studied, as well as P_{day} versus P_{summer} . The distribution of P_{day} was approximately normal (SS = 0.3), as well as for P_{winter} (SS = -0.5 , median = 31.2%). However, it was positively skewed in the case of P_{summer} (SS = 6) because the median was rather low (14.3%).

Another bar chart called “main accords” indicates the set of 5 or 6 odor descriptors supposed to be perceptible most clearly in the smell. The length of each bar in this chart was measured and expressed on a numeric scale from 0 to 5. The value 5 was consigned to the largest bar, which had the same length for all fragrances [24]. These ratings will be denoted as X , being for example X_{floral} and X_{fruity} , the ratings for “floral” and “fruity”, respectively. Fragrantica’s main accords lead to quantitative odor profiles. For example, Moods by Krizia (1989) is described as: $X_{floral} = 5$, $X_{green} = 2$, $X_{fruity} = 1.3$, $X_{powdery} = 1$, $X_{warm-spicy} = 0.9$, and $X_{woody} = 0.9$. All remaining terms not contained in the “main accords” should be rated as ≤ 0.9 (i.e., below the score of X_{woody} in this case); their exact values were unknown, and they were coded as zero. As a result of this, the pattern of these variables cannot be fitted to the most common models of statistical distribution.

The number of descriptors compiled was 31. Five of them were discarded given their low occurrence ($n < 3$). Other minority attributes like $X_{tobacco}$ ($n = 1$) and X_{smoky} ($n = 5$) were also disregarded after transferring their nonzero values to $X_{leather}$ ($n = 7$) because they are related notes [12]. The three perfumes labeled as “cinnamon” were also rated as “warm-spicy” but not as “sweet”, which is not consistent with the sweet-spicy odor of cinnamon. Hence, taking into account that $X_{cinnamon}$

($n = 3$), $X_{vanilla}$ ($n = 7$), and X_{honey} ($n = 2$) refer to natural materials with a sweet smell, such ratings were consigned to X_{sweet} ($n = 40$). The following flowery descriptors were combined into a single variable called $X_{floral-total}$ as following: $X_{floral-total} = \max\{X_{yellow-floral}, X_{white-floral}, X_{floral}, X_{rose}, X_{tuberose}\}$. Moreover, the ratings of X_{rose} ($n = 13$) and X_{floral} ($n = 84$) were merged as a new descriptor, which was named as $X_{light-floral}$ for the reason explained in Section 3.7. Further details about this approach applied to the minority descriptors can be found in a previous work [24]. The final list contained 19 terms.

2.3. Olfactory Descriptions from the H&R Guide

All fragrances under study except four are contained in the H&R catalog [4]. By checking their odor description it turns out that about half of them are labeled as “woody”, either in the top, middle, or base note. In order to account for this information, an indicator variable called I_{woody} was created by coding such fragrances as one, and zero if “woody” was absent in the description. The same procedure was applied to the rest of odor character attributes, resulting a set of 27 dichotomous (dummy) variables that were called I_{green} , I_{floral} , etc. The name “dichotomous” means that the variable only contains two possible values: one or zero; the former is applied when a given perfume is labeled with the descriptor.

Terms with 10 or less occurrences were removed because a preliminary analysis suggested that the similarities and dissimilarities with other descriptors were not consistent with the experience of perfumers. This step is necessary because, otherwise, descriptors with very few occurrences might take an excessive influence in the multivariate statistical analysis. “Elegant” and “exotic” were also disregarded given their subjectivity, as well as “floral”, because it was applied to all fragrances except one, which is not surprising because floral scents are the most typically feminine. After discarding these descriptors, the final set contained 13 indicator variables computed from the H&R catalog. For the four fragrances not contained in this guide, the values (0 or 1) of these 13 variables were estimated by means of regression methods using *Fragrantica*’s profiles as predictors.

2.4. Olfactory Descriptions from Osmoz

The Osmoz website [7] contains semantic descriptions about the olfactory pyramid (i.e., top, heart, and base notes) of commercial fragrances. Regarding the sample under study, in most cases (91%) the total number of terms applied to a given perfume ranged from 10 to 12. A few descriptors (e.g., “aldehyde”, “green notes”, “citrus oils”, “amber”, or “leather”) have a direct correspondence with variables of *Fragrantica*’s profiles, but most terms refer to perfumery materials. For example, instead of “floral”, the Osmoz pyramid indicates which floral materials best apply to the perceived smell (e.g., rose, jasmine, tuberose, lily-of-the-valley, etc.). These descriptions were also coded by means of dichotomous variables, which were named starting with “O” (Osmoz) for clarity purposes (e.g., O_{rose} , $O_{jasmine}$, and so on). Thus, O_{rose} takes the value one for those fragrances described as “rose” either in the top, heart or base note, and zero otherwise. The resulting list comprised 96 terms, but those with less than 10 occurrences were discarded for the reason stated in the previous section, as well as $O_{narcissus}$ ($n = 12$) due to the reduced number of occurrences.

The semantic descriptions from Osmoz were retrieved for 93 out of the 140 perfumes considered here. Regarding the rest not contained in this directory, their missing values were inferred for most variables based on related descriptors with available information. For example, missing values of O_{green} were coded as one for perfumes described as “green” in the H&R guide, and zero otherwise. The same criterion was applied to $O_{aldehyde}$, O_{peach} , and $O_{oakmoss}$, for items labeled as “aldehydic”, “fruity”, and “mossy”, respectively. Fragrances rated as $X_{sweet} > 2$ in *Fragrantica*’s profiles were assumed to smell like benzoin and tonka beans (i.e., $O_{benzoin} = O_{tonka} = 1$), given the sweet odor of both materials [26].

2.5. Additional Variables Computed and Final Matrix of Olfactory Descriptors

The compilation of Edwards [12], apart from classifying fragrances into 14 families, also indicates if a given perfume is perceived as fresh, crisp, classical, or rich. These categories provide qualitative information, but “fresh” and “rich” are opposite concepts in perfumery [15]. “Crisp” and “fresh” are

used in the sense of invigorating, while “classical” refers to the balanced notes, i.e., not too fresh nor too rich. Therefore, a new quantitative variable called Ed_{fresh} was created by coding: rich = 0, classical = 1, crisp = 2, and fresh = 3.

Taking into account that 125 out of the 140 fragrances studied are contained in Edwards’s guide, some supplementary indicator variables were generated as following:

- Ed_{chypre} was created by coding as one the set of 29 fragrances regarded as “mossy woods” (chypre) by Edwards [12], and zero otherwise.
- $Ed_{leather}$ was coded as one for fragrances regarded as “dry woods”, which feature leathery notes [12].
- Ed_{floral} was created by coding as one those perfumes ($n = 72$) classified as floral, floral–oriental, or soft floral. The purpose was to highlight perfumes with a patent floral character.
- $Ed_{oriental}$ takes the value one for the set of 49 perfumes regarded as oriental, soft–oriental, woody–oriental, or floral–oriental.

For fragrances not contained in Edwards’s catalog, the values of these variables were estimated based on the information provided by the remaining descriptors. Some additional indicator variables were created taking into account the olfactory descriptions from different sources:

- Z_{chypre} was computed to account for those perfumes ($n = 55$) described as chypre (as a category or subcategory) in at least one of these compilations: FSP [3], H&R [4], Groom [5], and Fragrantica [8].
- $Z_{aldehyde}$ was coded as one for fragrances ($n = 42$) described as soft floral by Edwards [12] or “aldehydic” in at least one of these directories.
- $Z_{leather}$ and Z_{fruity} were created accordingly.

The final data matrix contained 140 observations (perfumes) in rows by 80 variables (in columns), but seven of them were discarded as explained below (Section 3.2). The final list of 73 variables is indicated in Table 1. Once this matrix was arranged, stepwise multiple regression was applied in order to estimate P_{night} as a function of odor descriptors. Additional models were fitted for P_{winter} , Ed_{fresh} , P_{day} , P_{summer} , S_{cool} , and S_{floral} . The software used was Statgraphics 5.1.

2.6. Multivariate Statistical Analysis

The dataset was studied by means of principal component analysis (PCA) using the software SIMCA-P 10.0 (www.umetrics.com). Prior to this analysis, all data columns were mean-centered and scaled to unit variance, which is the most common data pretreatment. The first principal component (PC1) can be interpreted as a direction in the multivariate space that best explains the overall data variability. The projection of observations (fragrances) onto PC1 and PC2 are called $t(1)$ and $t(2)$ scores, respectively. The correlation between these scores versus X_{hexag} and Y_{hexag} was studied in order to discuss if the position of fragrances inside the Hexagon had a direct correspondence with the multivariate projection.

PC1 is the linear combination of variables explaining the maximum amount of data variability. Coefficients of this linear combination are called $p(1)$ loadings. Similarly, $p(2)$ are the contributions of odor descriptors in the formation of PC2, and so on. The scatterplot depicting $p(2)$ versus $p(1)$, which will be denoted as PC1/PC2 loading plot, can be regarded as a 2D sensory map that reflects the main relationships between odor attributes. The correspondence of this plot with the relative position of fragrance families in the Hexagon was studied by checking the correlation of $t(1)$ versus X_{hexag} , and $t(2)$ versus Y_{hexag} . The same approach was used for comparing the five categories in the perfume map of feminine fragrances called Analogies of Givaudan [11] (p. 276).

Taking into account that results are highly determined by the sample set, it was checked how this set is classified according to the Fragrance Wheel, and if the resulting percentages of items within each category are similar to those of the global fragrance market in 2008.

Table 1. Variables compiled from *Fragrantica* [8] (FrD) and different catalogs for a set of 140 fragrances: number of observations retrieved from the source (N_{obs}), number of variables excluded (N_{excl}), and list of variables included in the multivariate analysis (73 in total).

Source	Variables					Code ¹
	N_{obs}	Values	N_{excl}	$N_{included}$		
Hexagon of Fragrances [23]	89	−5 to 5	0	2	X_{hexag}, Y_{hexag}	□
Jellinek [14,25]	118 ²	−5 to 5	0	2	S_{cool}, S_{floral}	□
FrD: from preferences	137	in %	0	4	$P_{day}, P_{night}, P_{summer}, P_{winter}$	▲
FrD: from main accords	137	0 to 5	12	19	$X_{aldehydic}, X_{amber}, X_{animalic}, X_{aromatic}, X_{balsamic}, X_{citrus}, X_{earthy}, X_{floral-total}, X_{fresh-spicy}, X_{fruity}, X_{green}, X_{leather}, X_{musky}, X_{light-floral}, X_{powdery}, X_{sweet}, X_{warm-spicy}, X_{white-floral}, X_{woody}$	▲
H&R guide [5]	136	0 or 1	16	11	$I_{aldehydic}, I_{ambery}, I_{balsamic}, I_{fresh}, I_{fruity}, I_{green}, I_{mossy}, I_{powdery}, I_{spicy}, I_{sweet}, I_{woody}$	◆
Osmoz website [7]	93	0 or 1	70	26	$O_{aldehyde}, O_{benzoin}, O_{bergamot}, O_{carnation}, O_{civet}, O_{galbanum}, O_{green}, O_{heliotrope}, O_{hyacinth}, O_{iris}, O_{jasmine}, O_{leather}, O_{lemon}, O_{lily-valley}, O_{mandarin}, O_{oakmoss}, O_{orange-blossom}, O_{patchouli}, O_{peach}, O_{rose}, O_{tonka-bean}, O_{tuberose}, O_{vanilla}, O_{vetiver}, O_{violet-blossom}, O_{ylang-ylang}$	●
Edwards's guide (EdG) [12]	125	0 or 1 ³	-	5	$Ed_{chypre}, Ed_{leather}, Ed_{floral}, Ed_{oriental}, Ed_{fresh}$	○
Several sources ⁴	140	0 or 1	-	4	$Z_{chypre}, Z_{leather}, Z_{aldehyde}, Z_{fruity}$	■

¹ Code of points for the multivariate analysis (Figure 2). ² 67 contained in the Hexagon plus 51 additional ones. ³ Except for Ed_{fresh} . ⁴ From different fragrance directories: FSP [3], H&R [4], Groom [5], Frd [8], and EdG [12].

3. Results

3.1. Olfactory Profiles from *Fragrantica* and the H&R Guide

The frequency of terms used by *Fragrantica* for the main accords of perfumes studied here is shown in Table 2, as well as the occurrence of attributes for the description of all 453 feminine fragrances contained in the H&R guide. Interestingly, the set of recurrent descriptors was basically the same, as well as those applied with a lower frequency. As an exception, the occurrence of “fruity” was much higher in the H&R guide (33.1%) than in *Fragrantica* (7.1%), while the opposite applied to “citrus”, which might be explained by the semantic and sensory similarity of both descriptors. Actually, as citrus is a type of fruit, they were presumably used interchangeably to a certain extent.

It turns out that $X_{balsamic}$ and X_{amber} are correlated ($r_{137} = 0.22, p = 0.009$; the subscript of Pearson's correlation coefficient indicates the number of observations). Curiously, “balsamic” was applied more often by *Fragrantica* (36.4%) than by the H&R guide (13.9%), while the opposite applied to “amber” (Table 2). The reason seems to be that both descriptors refer to oriental scents and, hence, they were applied indifferently to some extent, like in the case of “fruity” and “citrus”. Consistent with this interpretation, an online fragrance guide [27] contains a major class called “ambery–oriental”. Moreover, $Ed_{oriental}$ yielded the highest correlation with I_{sweet} ($r_{140} = 0.53$), $O_{vanilla}$ ($r_{140} = 0.53$), and $X_{balsamic}$ (r_{137}

= 0.44, $p < 0.0001$). Oriental perfumes often contain heavy blends of balsamic resins, opulent flowers, sweet vanilla, and musks [12].

Table 2. Number of occurrence (N) and relative frequency in percentage (P) of odor descriptors compiled from two perfume directories: from *Fragrantica* [8] (terms encountered in the description of 140 perfumes) and from the *H&R* guide [4] (terms applied to 453 women’s fragrances).

From <i>Fragrantica</i> ¹ (n = 140)	N_{Frag}	P_{Frag}	From <i>H&R</i> ² (n = 453)	$N_{H\&R}$	$P_{H\&R}$
Woody	117	83.6	Woody	178	39.3
Floral (84) or related descriptors ³	113	80.7	Floral (447) or rosy (17)	448	98.9
Aromatic (46) or fresh spicy (24)	59	42.1	Fresh (239) or cool (23)	250	55.2
Powdery	56	40.0	Powdery	241	53.2
Green	55	39.3	Green	155	34.2
Balsamic	51	36.4	Balsamic	63	13.9
Sweet (36) or vanilla (7)	40	28.6	Sweet	124	27.4
Warm spicy (38) or cinnamon (3)	38	27.1	Spicy	86	19.0
Musky (17) or animalic (26)	34	24.3	Musky (3) or sensual (70)	73	16.1
Earthy	30	21.4	Mossy	72	15.9
Citrus	22	15.7	Citrus (16) or related ⁴	22	4.9
Aldehydic	19	13.6	Aldehydic	133	29.4
Fruity	10	7.1	Fruity	150	33.1
Amber	9	6.4	Ambery	62	13.7
Leather	7	5.0	Leathery	12	2.6
Smoky	5	3.6	Smoky	0	0.0
Honey	2	1.4	Honey	1	0.2
Herbal	1	0.7	Herbaceous	10	2.2
Marine	1	0.7	Marine	1	0.2
Tobacco	1	0.7	Tobacco	0	0.0
Tropical	1	0.7	Tropical	0	0.0
Dry	0	0.0	Dry	20	4.4

¹ Sorted in decreasing order of occurrence. Similar descriptors were grouped together to ease the comparison (e.g., “sweet (36) or vanilla (7)”; the number of occurrences is indicated within parentheses). ² Descriptors applied either to the top, middle, or base note. ³ White floral (67), yellow floral (7), rose (13), or tuberose (8). ⁴ Orange (1) or agrumy (5).

The use of Pearson’s correlation coefficient here is arguable because it measures the strength of linear relationship between two variables with a normal distribution. When using dichotomous variables, it seems more convenient a priori to apply similarity coefficients [28]. Different coefficients of this type have been proposed in the literature, and several statistical tests like ANOSIM are available. A detailed discussion about which method best applies here is out of the scope of the present work. Furthermore, the issue becomes more complex here because some variables are continuous and others are dichotomous. Thus, in order to find those descriptors that yield the strongest similarity with a given variable, it was decided to compute Pearson’s correlation coefficient for simplicity, assuming the limitations of this method.

The relative frequency of “floral” in the *H&R* guide was 98.9%, which agrees with the marked feminine character of floral scents. However, “woody” was labeled more often (83.6%) than flowery descriptors (80.7%) in *Fragrantica* (Table 2), which was unexpected because woody notes are more typically found in men’s fragrances. Nevertheless, woody ratings computed from this website seem to be reliable because X_{woody} yields the highest correlation with Z_{chypre} ($r_{137} = 0.42$) and X_{earthy} ($r_{137} = 0.38$, $p < 0.0001$), which is consistent with the correlation of “woody” versus “earthy” ($r_{309} = 0.39$, $p < 0.0001$) in the olfactory profiles compiled by Boelens and Haring [29]. A multivariate analysis of this directory, which will be referred to hereafter as the BH database, allowed the classification of 309 compounds into 27 groups [30], and a further study attempted to establish structure–activity relationships [31].

3.2. Olfactory Profiles from Osmoz and the H&R Guide

The H&R catalog indicates which attributes best apply to describe the odor character of a fragrance (Table 2). Moreover, it also provides the main ingredients that are supposed to be responsible for the scent. The list of such ingredients (Table 3) is basically coincident with the 96 terms encountered in Osmoz descriptions. Frequencies are highly skewed to particular materials labeled very frequently. It is noteworthy that “amber” and “aldehyde” were more recurrent in the H&R guide (Table 3), which is consistent with Table 2.

A few unexpected similarities were identified, which are not consistent with the experience of perfumers (n is the number of occurrences of the descriptor):

- O_{amber} ($n = 40$) was neither significantly correlated with $X_{balsamic}$ ($p = 0.9$) nor $E_{oriental}$ ($p = 0.6$), which is nonsense because amber and balsamic scents are related and characteristic of oriental perfumes.
- O_{musk} ($n = 45$) was not correlated with $X_{animalic}$ ($p = 0.8$) but it yielded certain association with P_{summer} ($r_{137} = 0.19$, $p = 0.02$), which was unexpected because “musk” and “animalic” refer to similar scents that are preferred for wintertime, as discussed in Section 3.3.
- $I_{sensual}$ ($n = 19$) was supposed to be correlated with X_{musky} or $X_{animalic}$ given the sensual character of such scents, but this was not the case ($p > 0.4$).
- $O_{coriander}$ ($n = 27$) was neither correlated with $X_{fresh-spicy}$ ($p = 0.3$), S_{cool} ($p = 0.09$), nor X_{citrus} ($p = 0.9$), being associated with X_{musky} ($r_{137} = 0.32$, $p = 0.0002$). These relationships are not consistent with the fresh–spicy smell of coriander essential oil, resembling lavender and linalool (citrus).
- $O_{sandalwood}$ ($n = 81$) yielded a slight correlation with $X_{floral-total}$ ($r_{137} = 0.22$, $p = 0.01$) but not with X_{woody} ($p = 0.6$), which is not consistent with the woody smell of sandalwood oil.
- O_{cedar} ($n = 52$), likewise, was associated with S_{floral} ($r_{118} = 0.37$, $p < 0.0001$) but not with X_{woody} ($p = 0.5$), which does not agree with the smell of cedarwood oil.
- I_{warm} ($n = 32$) was correlated with $O_{patchouli}$ ($r_{140} = 0.54$) and Z_{chypre} ($r_{140} = 0.47$, $p < 0.0001$) but, unexpectedly, neither with $X_{warm-spicy}$ ($p = 0.2$) nor with P_{night} ($p = 0.1$).

These seven dichotomous variables mentioned (O_{amber} , O_{musk} , $I_{sensual}$, $O_{coriander}$, $O_{sandalwood}$, O_{cedar} , and I_{warm}) were removed due to the unclear interpretation of their similarities. A much higher sample size should be necessary for an accurate study of these relationships, but it is out of the scope of the present work. We should keep in mind that dichotomous variables are less suitable for characterizing the similarities between variables, compared with descriptors rated on a continuous scale [15].

3.3. Preference for Nighttime versus Wintertime Wear

A positive correlation was found between P_{night} and P_{winter} ($r_{137} = 0.83$, $p < 0.0001$) (Figure 1a), which is intuitively appealing because oriental perfumes smell warm and are ideal for cool weather and formal nighttime wear [14,26,32]. Accordingly, P_{night} yielded an inverse correlation with P_{summer} ($r_{137} = -0.63$, $p < 0.0001$). These relationships were affected by the presence of outliers; many of them correspond to perfumes rated by a number of votes (N_{votes}) too low (Figure 1a) because they were not available commercially in 2007 when Fragrantica’s website was created. As discussed in a previous study [24], it seems that at least 70 votes are required to assume that consumer preference from Fragrantica is reliable enough. By discarding 20 outlying fragrances rated by < 70 people, the correlation coefficient in Figure 1a became $r_{117} = 0.92$ ($R^2 = 0.86$).

Aimed at further understanding the correlation between P_{night} and P_{winter} , stepwise regression was applied for fitting P_{night} as a function of P_{winter} and further variables. The resulting model (Equation (1), $R^2 = 0.88$) revealed that musky scents increase the preference for nighttime wear, while the opposite applies to perfumes rated as $X_{green} > 1$, which were coded by means of the indicator variable $I_{green>1}$. In this model, the p -value of regression coefficients (p_{rc}) was very low ($p_{rc} < 0.006$).

$$P_{night} = 11.54 + 1.25 P_{winter} + 2.29 X_{musky} - 4.0 I_{green>1} \quad (1)$$

Table 3. Relative frequency of occurrence (P_{OSM} : in percentage) of terms used by Osmoz to describe the top, heart, and base note (olfactory pyramid) of 93 women's perfumes. The percentage of these terms used to describe all 453 feminine fragrances contained in the H&R guide is also shown ($P_{H\&R}$).

Base Note Descriptor ¹	P_{OSM}		Heart Note Descriptor ¹	$P_{H\&R}$		Top Note Descriptor ¹	P_{OSM}		Top Note (Minority Terms)		
	P_{OSM}	$P_{H\&R}$		P_{OSM}	$P_{H\&R}$		P_{OSM}	$P_{H\&R}$	Descriptor ¹	P_{OSM}	$P_{H\&R}$
Sandalwood	62.4	70.4	Rose	66.7	87.9	Bergamot	58.1	81.7	Melon	3.2	2.9
Vanilla	36.6	41.9	Jasmine	59.1	95.1	Aldehyde	26.9	52.8	Grapefruit	3.2	0.7
Patchouli	34.4	34.2	Tuberose	37.6	34.4	Peach	26.9	32.9	Raspberry	2.2	8.6
Oakmoss	32.3	57.0 ²	Iris (orris) ⁵	34.4	70.6	Lemon	24.7	32.7	Pimento ⁶	2.2	4.0
Vetiver	32.3	43.7	Lily-of-the-valley	33.3	57.8	Hyacinth	22.6	24.7	Reseda	2.2	1.3
Cedar	30.1	51.7 ³	Ylang ylang	23.7	62.3	Orange blossom	22.6	19.4	Pepper	2.2	0.9
Musks	25.8	83.4	Carnation	21.5	52.5	Mandarin	20.4	15.0	Coconut	2.2	0.9
Amber	24.7	71.3	Narcissus	12.9	13.2	Galbanum	18.3	16.3	Angelica	2.2	0.7
Benzoin	20.4	38.9	Violet	10.8	10.2	Coriander	16.1	18.3	Cassie	1.1	8.8
Civet	17.2	39.3	Geranium	9.7	7.5	Green notes	15.1	44.6	Chalice flower	1.1	2.9
Tonka bean	11.8	20.3	Cloves	9.7	5.3	Rosewood	9.7	20.1	Mace	1.1	2.4
Heliotrope	11.8	14.3	Cinnamon	8.6	9.9	Neroli	9.7	10.4	Artemisia	1.1	2.4
Leather	6.5	13.9	Gardenia	7.5	11.9	Blackcurrant	8.6	0.2	Cumin	1.1	1.8
Labdanum ciste	6.5	10.8 ⁴	Cyclamen	7.5	11.9	Plum	7.5	6.8	Lavender	1.1	1.5
Styrax	5.4	9.7	Honeysuckle	6.5	2.6	Citrus oil	6.5	6.0	Petitgrain	1.1	1.1
Castoreum	4.3	7.1	Honey	4.3	11.7	Pineapple	6.5	5.5	Laurel leaves	1.1	1.1
Olibanum	2.2	5.5	Lily	4.3	5.3	Orange	5.4	6.6	Pine needle	1.1	0.4
Oppoponax	2.2	4.6	Mimosa	3.2	1.3	Basil	5.4	6.6	Marigold	1.1	0.2
Peru balsam	2.2	1.8	Orchid	1.1	17.0	Anise	5.4	2.2	Chamomile	1.1	0.2
Myrrh	1.1	4.0	Lilac	1.1	7.5	Clary sage	4.3	4.0	Rosemary	1.1	0.2
Marine note	1.1	0.4	Thyme	1.1	1.8	Cardamom seed	4.3	3.1	Tagetes	0.0	7.1
Tolu	0.0	4.0	Linden	1.1	0.9	Tarragon	3.2	4.2	Strawberry	0.0	1.1
			Magnolia	1.1	0.9	Spearmint	3.2	3.5	Marjoram	0.0	0.4
			Ginger	1.1	0.4	Apricot	3.2	2.9			

¹ Sorted by decreasing order of P_{OSM} . Each descriptor is listed under the olfactory phase (i.e., base, heart, or top note) where it appears more often, but frequencies were calculated taking into account the occurrence either in the top, heart, or base notes. ² Sum of "oakmoss" (23.0%) and "moss" (34.0%). ³ Sum of "cedar" (32.7%) and "cedarwood" (19%), which are supposed to be equivalent. ⁴ Sum of "labdanum" (2.6%) and "cistus" (8.2%) as both refer to "cistus ladanifer". ⁵ Orris oil is derived from the rhizomes of iris plants and, hence, both "orris" and "iris" are equivalent descriptors. The former was the term used by the H&R guide and the latter by Osmoz. ⁶ Jamaica pepper, also called allspice.

Equation (2) was fitted to estimate P_{winter} ($R^2 = 0.59$, $p_{rc} < 0.002$), not considering the effect of P_{night} . Nine outlying fragrances were removed, eight of them rated by <59 consumers. Variables summed together corresponded to related odors with similar regression coefficients.

$$P_{winter} = 32.7 - 1.84 (X_{green} + X_{citrus}) - 4.8 (I_{green} + O_{bergamot}) + 3.02 X_{balsamic} + 1.11 (X_{warm-spicy} + X_{animalic} + X_{musky}) \quad (2)$$

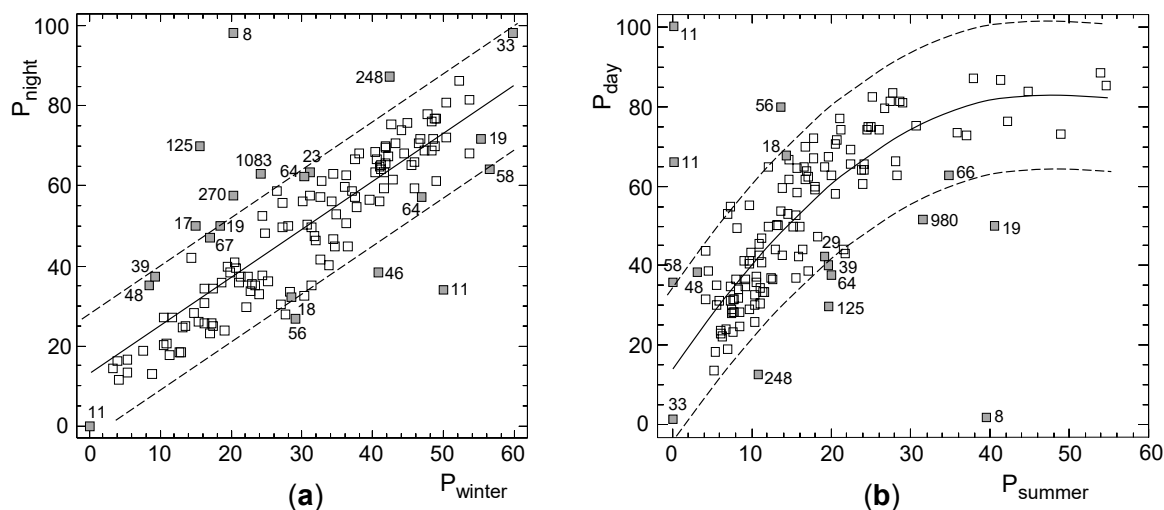


Figure 1. Consumer preferences about 140 perfumes (data from [8]). (a) Percentage of subjects who considered the fragrance more suitable for nighttime wear (P_{night}) versus for the winter season (P_{winter}); (b) preference for daytime wear (P_{day}) versus preference for summertime (P_{summer}). Values next to each observation indicate the number of subjects who voted to provide this information. Dashed lines: prediction limits (confidence level: 95%) calculated after discarding 8 outlying observations.

Similarly, Equation (3) predicted P_{night} ($R^2 = 0.53$, $p_{rc} < 0.0009$), not including P_{winter} . Eight outliers were removed, seven of them assessed by <49 people. Descriptors in Equations (2) and (3) are basically equivalent given the tight association shown in Figure 1a, which supports the notion that warm balsamic and animalic scents increase the preference for wintertime, while “green” and “citrus” odors are ideal for daytime wear. These effects are well known by perfumers, but few studies have quantified such relationships statistically [24].

“Green” is applied to describe the smell of recently cut leaves or grass. Such scents are usually regarded as fresh, invigorating, nature inspired, and reminiscent of the outdoors [11], which is consistent with Equations (3) and (4). Curiously, different studies have reported that fresh scents are associated with the leafy green color [33,34]. Another piece of research carried out with 21 fragrances found that extroverted subjects preferred fresh perfumes that evoked green and yellow colors [35].

$$P_{night} = 46.7 - 3.48 X_{green} - 2.74 X_{citrus} + 2.65 X_{balsamic} + 11.0 E_{oriental} + 2.21 (X_{animalic} + X_{musky}) \quad (3)$$

“Warm” and “fresh” refer to dissimilar odor categories [19], with the former being associated with balsamic/oriental fragrances. This polarity is consistent with the negative regression coefficients of X_{green} and X_{citrus} (fresh scents) in Equations (2) and (3), while positive coefficients refer to warm odors. The Fragrance Wheel is based on 14 categories structured in four main groups; two of them, “fresh” and “oriental”, appear as opposite classes of the same underlying polarity. Furthermore, the categories “green”, “citrus”, “fruity”, and “watery” are grouped within the “fresh” group [12], which is a common criterion in perfumery. Equation (3) suggests that P_{night} could be considered as an indirect assessment of the warm character of a given fragrance. Conversely, since $P_{day} = 100 - P_{night}$, it could be inferred that preference for daytime wear is associated with the “fresh” odor character, which is well established in perfumery [14], though this term is somewhat subjective for naive subjects.

Regarding Ed_{fresh} , it yielded the strongest correlation with P_{day} ($r_{125} = 0.24$, $p = 0.007$), which agrees with the resulting model (Equation (4), $R^2 = 0.45$, $p_{rc} < 0.004$). Ed_{fresh} ranges from 0 to 3, and the constant 0.6 is nearly coincident with the midpoint of this interval. This equation confirms the fresh character of “green” and “fruity” scents [15]. The presence of $O_{galbanum}$ in Equation (4) is intuitively appealing because this material smells leafy green.

$$Ed_{fresh} = 0.6 + 0.15 X_{green} + 0.6 (I_{green} + O_{galbanum}) + 0.6 I_{fresh} + 0.7 Z_{fruity} \quad (4)$$

3.4. Preference for Daytime versus Summertime Wear

The relationship shown in Figure 1a is purely linear but, curiously, it becomes quadratic by comparing P_{day} versus P_{summer} (Figure 1b). After discarding eight outlying perfumes ($N_{votes} < 59$), X_{green} was the only additional variable entering in Equation (5) ($R^2 = 0.75$, $p_{rc} < 0.0003$).

$$P_{day} = 14.5 + 2.45 P_{summer} - 0.022 (P_{summer})^2 + 2.56 X_{green} \quad (5)$$

The predictive model for P_{summer} (Equation (6), $R^2 = 0.48$, $p_{rc} < 0.003$) is quite similar to Equation (2) and it was obtained after discarding basically the same nine outliers. $X_{animalic}$ and $X_{leather}$ were summed given their similar regression coefficient and because the latter presents certain animalic notes. Likewise, X_{woody} was merged with $X_{warm-spicy}$ because both refer to odors sharing a warm character; actually, “woody” is correlated with “balsamic” ($r_{309} = 0.37$) and with “spicy” ($r_{309} = 0.32$, $p < 0.0001$) in the BH database. Results evidence that warm balsamic and animalic scents decrease P_{summer} and, hence, increase the preference for wintertime.

$$P_{summer} = 24.8 + 2.57 X_{citrus} - 1.22 X_{balsamic} - 5.2 (Ed_{oriental} + I_{ambery}) - 0.98 (X_{warm-spicy} + X_{woody}) - 1.78 \cdot (X_{animalic} + X_{leather}) \quad (6)$$

The variable X_{green} was included in Equations (2)–(5), but its effect was not statistically significant in Equation (6), nor in the case of I_{green} ($p > 0.2$). This result suggests that green notes are more powerful to evoke daytime conditions than citrus notes, according to Equation (5). Actually, by excluding perfumes rated by less than 70 people, it turns out that P_{day} was more strongly correlated with X_{green} ($r_{110} = 0.48$, $p < 0.0001$) than X_{citrus} ($r_{110} = 0.16$, $p = 0.09$). Conversely, citrus scents present a higher refreshing character (i.e., more suitable for summertime) according to Equation (6).

3.5. Multivariate Analysis of the Olfactory Matrix

The final matrix of olfactory descriptors was heterogeneous regarding the statistical distribution of variables, because some were continuous and others were categorical. Hence, it is uncertain if multivariate tools adapted to nonlinear data (e.g., multiple correspondence analysis or nonlinear PCA) might be more appropriate rather than standard PCA. It was decided to use the latter because PCA is one of the most common multivariate approaches for the analysis of olfactory profiles [2], and it does not require a particular model of distribution for the variables.

The final dataset was comprised by 80 descriptors, seven of which were removed as explained in Section 3.2. It was found that $Ed_{oriental}$ and P_{winter} exerted an excessive influence in PC1, and the same occurred with Ed_{floral} and Z_{chypre} in the case of PC2. They appeared in the loading plot as extreme points, which might be confusing and is not convenient for the purpose of obtaining a meaningful sensory map. Thus, a coefficient of 0.9 was applied in order to reduce the variance of these descriptors so that they appear closer to the rest of variables. Next, a new PCA was fitted. PC1, PC2, PC3, and PC4 explained 11.3%, 9.5%, 5.4%, and 4.4%, respectively, of the overall data variability. Higher values were obtained in the analysis of the BH database (PC1: 17.5%; PC2: 14.2%; PC3: 8.4%; PC4: 6.6%) because odor descriptors were measured on a continuous 0–9 scale [15], which allowed a better characterization of the relationships between variables.

The PC1/PC2 loading plot (Figure 2) reflects the similarities and dissimilarities between variables. Descriptors appearing close to each other are expected to be positively correlated, which implies

that they are often applied together in the description of scents. It is intuitively appealing that those variables from different sources referring to the same smell (e.g., $X_{aldehydic}$, $I_{aldehydic}$, $O_{aldehydic}$, and $Z_{aldehyde}$) are located near to each other in Figure 2. Thus, such descriptors were joined together by means of a polygon, and the legend “aldehydic” was indicated only once inside the plot.

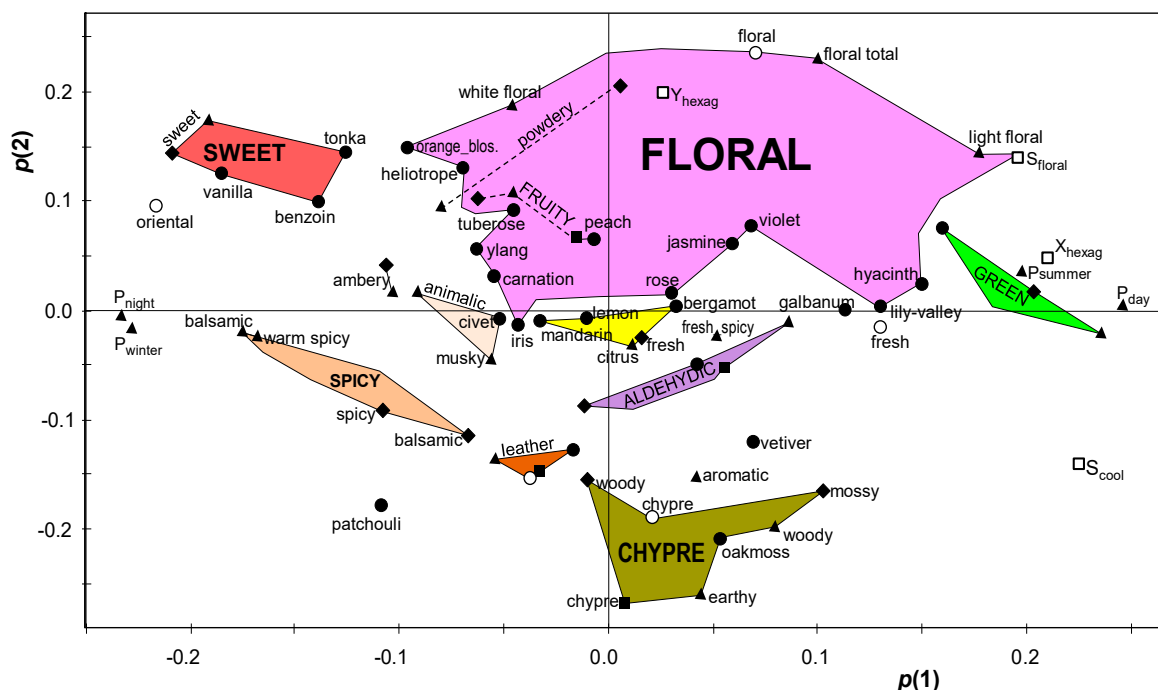


Figure 2. Loading plot ($p(2)$ versus $p(1)$) of the PCA applied to the olfactory profiles (73 variables) obtained for the set of 140 perfumes. Odor descriptors obtained from *Fragrantica* and additional catalogs (see Table 1 for list of variables included and point codes). Equivalent or related odor descriptors are joined with lines. Polygons are colored to highlight the main olfactory classes.

PC1 basically describes the preference for daytime versus nighttime wear, while PC2 discriminates floral versus chypre perfumes. The latter are characterized by the presence of oakmoss, which smells mossy–woody and explains the correlation between Z_{chypre} and $O_{oakmoss}$ ($r_{140} = 0.55$, $p < 0.0001$). The woody–earthy odor of vetiver [26] agrees with the position of $O_{vetiver}$ close to chypre descriptors (Figure 2). The location of $O_{patchouli}$, intermediate of chypre and sweet descriptors, is intuitively appealing because the scent of patchouli oil is woody–earthy and sweet–balsamic [26]. Galbanum oil smells leafy green, which justifies the similarity of $O_{galbanum}$ versus X_{green} ($r_{137} = 0.38$, $p < 0.0001$) and its position in the plot close to the “green” cluster; but it presents spicy–woody and balsamic undertones [26], which might explain the lower correlation with P_{day} ($r_{137} = 0.24$, $p = 0.005$). The position of O_{tonka} agrees with the warm, sweet caramelic odor of tonka beans. It appears next to $O_{benzoin}$ in Figure 2, which is consistent with the balsamic, sweet chocolate odor of benzoin resinoid [26]. Although perfumers usually choose sweet-smelling materials as a standard for “balsamic” [36], some other references for this descriptor, like olibanum, do not smell sweet, which would explain why $I_{balsamic}$ was not correlated with X_{sweet} ($p = 0.6$) and, hence, it is located far away from $Ed_{oriental}$.

Next, $t(1)$ and $t(2)$ scores were obtained with the software for all 140 perfumes. It turned out that $t(1)$ was correlated with X_{hexag} ($r_{89} = 0.62$, $p < 0.0001$) but not with Y_{hexag} ($p = 0.3$). Conversely, $t(2)$ had a reasonable correspondence with Y_{hexag} ($r_{89} = 0.54$, $p < 0.0001$). Thus, the projection of perfumes onto PC1 and PC2 had a rather good agreement with their position in Dragoco’s Hexagon. Nevertheless, the correlation was not very strong, which implies that the Hexagon could be improved. The location of “chypre” next to “oriental” in the original Hexagon (Figure 3a) is not consistent with Figure 2, and a better match would result by swapping “chypre” and “floral–spicy”. A new class called “light floral”

was incorporated in the modified version proposed of the Hexagon (Figure 3a), becoming a sensory wheel with seven families. As the floral–green category accounts for the most “refreshing” (daytime) fragrances, a different position, slightly rotated, was proposed in the modified Hexagon to make it coincident with the horizontal axis. Hence, this axis can be interpreted as a factor discriminating fragrances preferred for daytime versus nighttime wear. The “floral–fruity” category was renamed as “white-floral–fruity”, which refers to sweet–floral odors as discussed below.

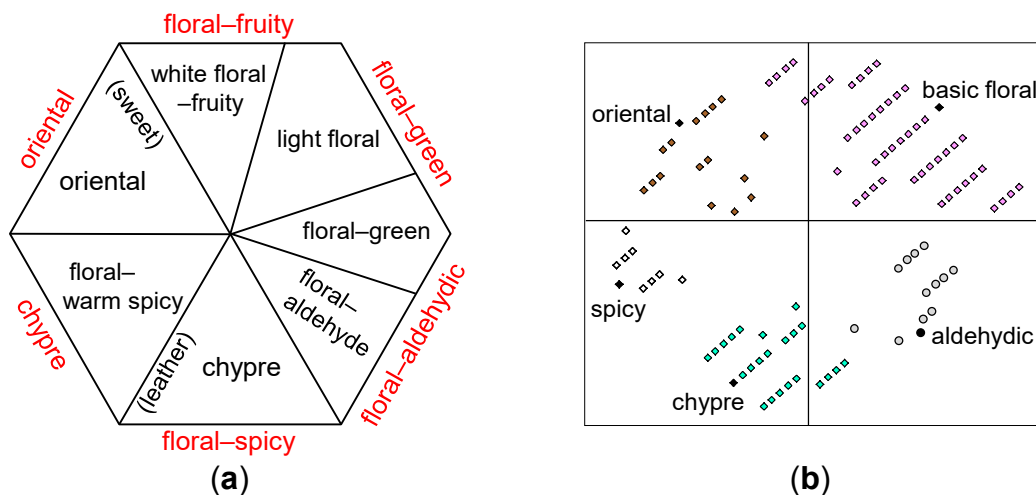


Figure 3. (a) Modified Hexagon of Fragrance Families. Categories in the original representation (indicated in red outside the polygon) were reorganized according to Figure 2; (b) Givaudan Analogies of feminine fragrances [11] (p. 276), which was properly rotated to achieve the best match with Figure 2. The fragrance most representative of each class is indicated as a black point.

The chart called Analogies of Feminine Fragrances was developed by the Swiss company Givaudan around 1985 [11] (p. 276). It displays 113 perfumes, 65 of which are included in the sample set studied here. Their coordinate position was obtained on a continuous arbitrary scale. If this odor map is rotated -45 degrees approximately (Figure 3b), it turns out that the projection of perfumes over the x axis yields the maximum correlation ($r_{65} = 0.6$, $p < 0.0001$) with $t(1)$ scores. Strikingly, the position of five major classes in Givaudan’s map (Figure 3b) is coincident with equivalent descriptors in Figure 2 and with the modified Hexagon (Figure 3a).

3.6. Study of Further Components

By visually inspecting the PC3/PC4 loading plot (Figure 4), it was found that PC3 basically reflects the contrast between “aldehydic” and “fruity” descriptors. According to Müller [26], aldehydes are used especially in perfumes that feature elegant feminine notes. This feminine character is reflected by the fact that “aldehydic” is encountered more often in women’s perfumes (in the H&R guide: 52.8% of women’s versus 25.3% of men’s). Given the preference of ladies for aldehydic and floral scents, these descriptors are usually located close to each other in perfumery odor maps [16,37], but both appear as distinctive (far apart) polygons in Figure 2. The reason seems to be the marked nonsweet (dry) odor character of aldehydes [11] (p. 278), which explains the negative correlation between $Z_{aldehyde}$ and X_{sweet} ($r_{137} = -0.26$, $p = 0.003$). Such dissimilarity of “aldehyde” versus “sweet” is also apparent in the BH database ($r_{312} = -0.36$, $p < 0.0001$) and in Figure 4.

Conversely, X_{sweet} yielded the highest similarity with X_{fruity} ($r_{137} = 0.44$, $p < 0.0001$), which explains the opposite character between fruity and aldehydic descriptors revealed by PC3. Fruity, sweet, and spicy descriptors appear with low $p(3)$ loadings, and they are typically encountered in foodstuffs. On the opposite side, aldehydes and animalic notes are characterized by a certain unpleasant character. Hence, PC3 might be interpreted in some way as an underlying dimension related with “edible” scents.

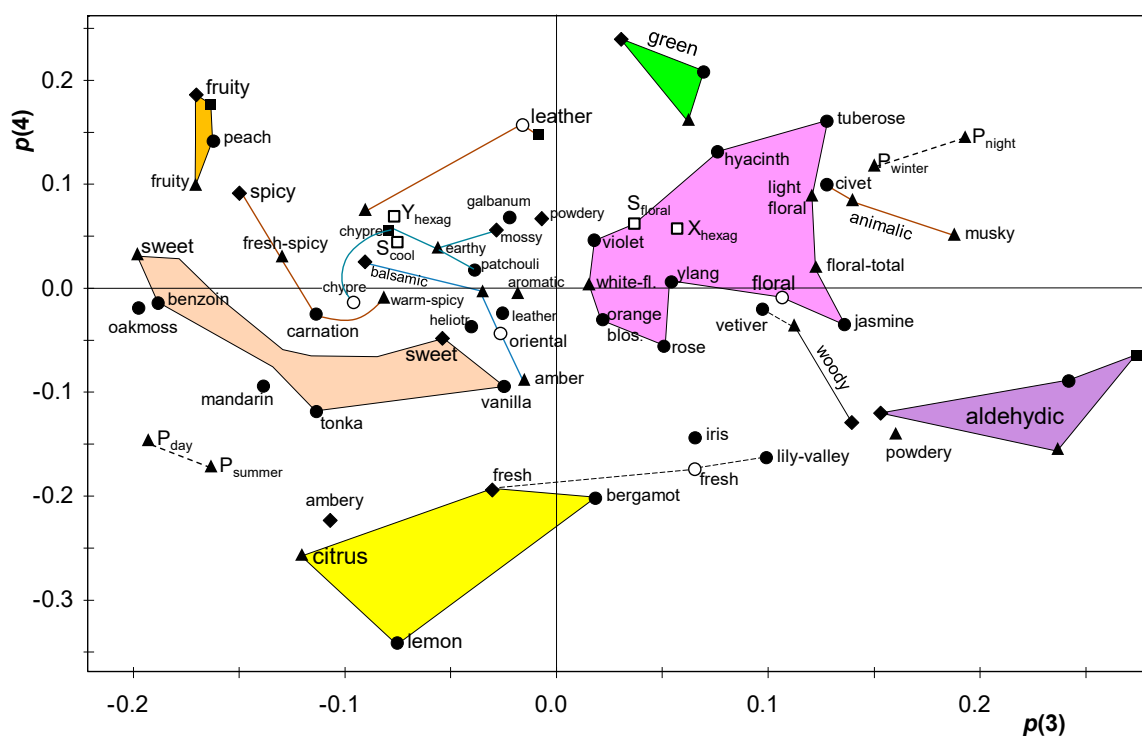


Figure 4. Loading plot ($p(4)$ versus $p(3)$) of the PCA applied to the olfactory profiles for the set of 140 perfumes. See Table 1 for list of variables included and point codes. Equivalent or related odor descriptors are joined with lines. Polygons are colored to highlight some odor classes.

PC4 basically reflects a dissimilar character between citrusy descriptors (i.e., X_{citrus} , O_{lemon} , and $O_{bergamot}$) with respect to “green” variables (I_{green} , O_{green} , and X_{green}). Both categories are usually regarded as fresh and enhance the preference for daytime wear (Equation (3)). In the BH database, “fresh” is similar to “green” ($r_{312} = 0.43$) and “citrusy” ($r_{312} = 0.43$, $p < 0.0001$), but the correlation between both variables is very weak ($r_{312} = 0.12$, $p = 0.03$), which reveals a distinct odor character. Accordingly, X_{citrus} and X_{green} are slightly dissimilar ($r_{137} = -0.18$, $p = 0.04$) in Fragrantica’s profiles, which justifies their divergent position in Figure 2; Figure 4. “Citrus” is located close to the center of Figure 2 because it is not correlated with P_{day} ($p = 0.3$). It is appealing that $O_{mandarin}$ appears in Figure 4 closer to X_{sweet} because mandarins smell much sweeter than lemons.

PC5 did not provide additional relevant information because it basically discriminated floral versus balsamic descriptors, which are distinct odors as already reflected by Figures 2 and 4. Further components are not of interest.

3.7. Study of Floral Descriptors

“Rose” was the most frequent floral term encountered in Osmoz descriptions (Table 3). Actually, rose oil is commonly considered as the preferred reference material for “floral” by perfumers [36], which implies that certain correlation should be expected between O_{rose} and $X_{floral-total}$. However, this was not the case ($p = 0.2$, $n = 93$), which is consistent with the position of O_{rose} very close to the origin of coordinates in Figure 2. Thus, it seems that the information of O_{rose} is not relevant here, probably because it was labeled too often.

“Floral” and “white floral” are different descriptors in Fragrantica. It turns out that X_{floral} is dissimilar to X_{sweet} ($r_{137} = -0.20$, $p = 0.02$) and it is associated with: X_{green} ($r_{137} = 0.33$, $p = 0.0001$), P_{day} ($r_{137} = 0.27$, $p = 0.001$), O_{violet} ($r_{137} = 0.26$, $p = 0.002$), and $O_{hyacinth}$ ($r_{137} = 0.26$). Considering that “green”, “fresh”, and “light” are related concepts in perfumery, applied to odors evoking daytime conditions, “floral” was renamed as “light floral” for clarity purposes, as explained in Section 2.2. The observed correlations indicate that violet and hyacinth are the lightest floral scents in the database.

Both materials smell leafy green [26], which justifies the similarity between $O_{hyacinth}$ and I_{green} ($r_{140} = 0.48$, $p < 0.0001$). The correlation of $O_{lily-valley}$ versus P_{day} ($r_{137} = 0.25$, $p = 0.003$) is explained by the light floral, fresh green scent of lily-of-the-valley [11] and is consistent with the proximity of Ed_{fresh} in Figure 4.

According to Fragrantica, “white flower” refers to the heady, sweet–floral scent common in jasmine and orange blossom. Jasmine absolute was the reference for “floral” in the BH database, which yielded the highest correlation with “sweet” ($r_{312} = 0.28$, $p < 0.0001$). The variable $X_{white-floral}$ correlated with $O_{tuberose}$ ($r_{96} = 0.54$, $p < 0.0001$), $O_{orange-blossom}$ ($r_{137} = 0.42$, $p < 0.0001$), and X_{sweet} ($r_{137} = 0.34$, $p < 0.0001$), but not with $O_{jasmine}$ ($p = 0.2$), perhaps because “jasmine” was encountered too often (59.1%) in Osmoz descriptions. Jasmine, tuberose, and orange blossom are flowers of white color that display a floral–sweet, honey-like scent [26].

The flowery descriptors mentioned next (i.e., O_{iris} , $O_{carnation}$, O_{ylang} , and $O_{heliotrope}$) are neither correlated with S_{floral} nor $X_{floral-total}$ ($p > 0.1$), which indicates a lower floral character and is consistent with their position in Figures 2 and 4:

- O_{iris} correlated with $X_{powdery}$ ($r_{137} = 0.31$, $p = 0.0003$) and O_{violet} ($r_{140} = 0.15$, $p = 0.08$). These similarities are intuitively appealing because the powdery facet of orris is well known [12,38]. Moreover, orris (iris) oil displays a woody, violet-like odor [26].
- $O_{carnation}$ yielded the highest similarity with I_{spicy} ($r_{140} = 0.18$, $p = 0.03$), which agrees with the spicy, clove-like character of carnation flowers [38].
- O_{ylang} correlated with $O_{vanilla}$ ($r_{93} = 0.21$, $p = 0.04$), consistent with the floral–narcotic and sweet–spicy smell of ylang-ylang flowers.
- $O_{heliotrope}$ yields the strongest correlation with X_{sweet} ($r_{137} = 0.26$, $p = 0.002$), which can be explained by the sweet scent of heliotrope flowers, being reminiscent of marzipan, vanilla, and cherry pie.

The continuous variable S_{floral} obtained from sensory experiments [14,25] yielded the strongest correlation with $X_{floral-total}$ ($r_{116} = 0.62$) and $X_{light-floral}$ ($r_{116} = 0.52$, $p < 0.0001$), which evidences that Fragrantica’s profiles are consistent with experimental ratings. Equation (7) was obtained by applying stepwise regression ($R^2 = 0.82$, $p_{rc} < 0.006$) after removing five moderate outliers. The correlation between S_{floral} and P_{day} ($r_{116} = 0.44$, $p < 0.0001$) agrees with the position of “floral” in a reported fragrance map [11] (p. 280). By contrast, oriental and sweet scents are preferred for nighttime wear, which justifies their negative coefficients in Equation (7).

$$S_{floral} = 1.0 Ed_{floral} + 0.76 X_{floral-total} - 1.3 Ed_{oriental} - 0.9 I_{sweet} - 0.25 X_{powdery} - 0.9 I_{aldehydic} \quad (7)$$

This model reflects that aldehydic notes attenuate (i.e., “soften”) the floral character, which justifies the name “soft floral” given by Edwards [12] for aldehydic fragrances. The reason could be that the natural scent of short-chain aliphatic aldehydes is not pleasant; however, in floral fragrances, such notes combine appropriately with the powdery accents of vanilla and iris to create soft floral fragrances [12]. In perfumery, the powdery impression is associated with particular warm–sweet scents, which explains that $X_{powdery}$ yields the highest correlation with O_{iris} ($r_{137} = 0.31$, $p = 0.0003$) and $O_{vanilla}$ ($r_{137} = 0.21$, $p = 0.01$). A mixture of musk ketone and coumarin was the reference for “powdery” in the BH database [29].

3.8. Prediction of the Cool Odor Character

“Fresh” and “warm” are usually regarded as contrasting polarities in the perception of fragrances [15]. However, “cool” and “warm” are also opposite terms semantically [25]. In order to clarify these relationships, Figure 5 reveals that fragrances with higher values of S_{cool} (i.e., the most “cool” fragrances) tend to be preferred for daytime wear ($P_{day} > 50\%$) while, conversely, most sweet–oriental perfumes (black points in Figure 5) smell warm and are best suited for the night, but not always. Both variables are linearly related, but the correlation is not very strong ($r_{116} = 0.47$, $p < 0.0001$).

Considering that “fresh” basically accounts for informal daytime fragrances, as discussed above, the lack of a tight correlation reveals that “fresh” and “cool” refer to different concepts in perfumery.

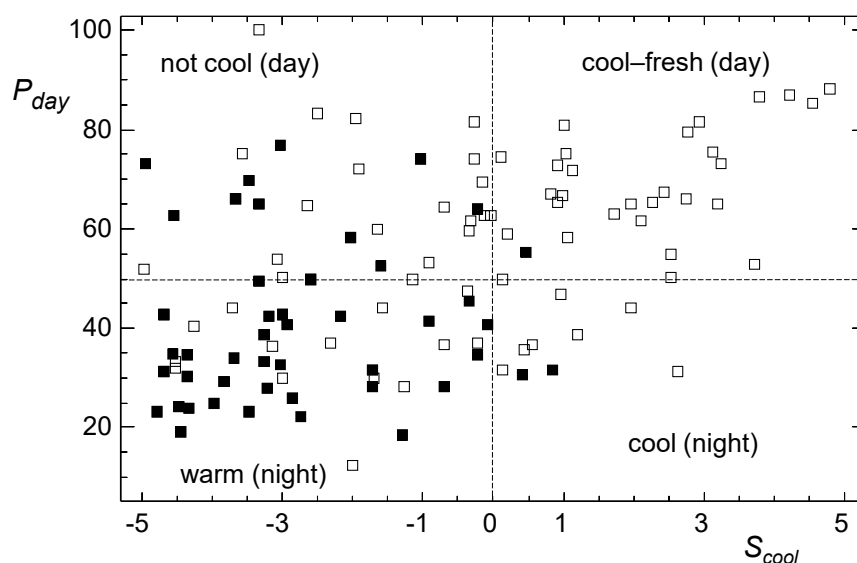


Figure 5. Scatterplot of preference for daytime wear according to *Fragrantica* (P_{day}) versus cool scores (S_{cool} : sensory ratings on a scale from -5 (warm) to 5 (cool) obtained by Jellinek [14,25] from a panel for 116 fragrances. Filled points: fragrances described as “sweet” in the H&R guide or classified as “oriental”, “woody-oriental”, “soft-oriental”, or “floral-oriental” by Edwards [12] (fragrances that do not fulfil this criterion appear as unfilled points). Dashed lines were drawn for clarity purposes to divide the scatterplot in four meaningful sections.

The variable S_{cool} obtained experimentally yielded the highest correlation with P_{day} ($r_{116} = 0.47$) and I_{mossy} ($r_{118} = 0.40$, $p < 0.0001$), which explains its position in Figure 2. The negative correlation with $Ed_{oriental}$ ($r_{118} = -0.52$) and I_{sweet} ($r_{118} = -0.48$, $p < 0.0001$) evidences the warm smell of oriental fragrances [32]. These similarities are reflected by Equation (8), which was fitted after discarding six moderate outliers rated by <68 people. The positive coefficient of P_{day} and Z_{chypre} in Equation (8) suggests that “cool” fragrances are intermediates of fresh and chypre perfumes but dissimilar to oriental scents, given the negative coefficient of $Ed_{oriental}$ and I_{ambery} . Accordingly, the aromatic/fougère category in Edwards’s wheel is located between “chypre” and fresh families but opposed to “oriental”, which agrees with the association between “cool” and “fougère” in perfumery.

$$S_{cool} = -3.9 + 0.054 P_{day} + 1.6 Z_{chypre} - 1.2 Ed_{oriental} - 1.5 I_{ambery} \quad (8)$$

The goodness-of-fit for the prediction of S_{cool} ($R^2 = 0.54$, $p_{rc} < 0.008$) was lower than the value obtained for S_{floral} ($R^2 = 0.82$), which might indicate that the cool character of a fragrance is a particular odor quality not properly captured by those descriptors considered here. The proposed hypothesis is that “cool” basically refers to the perception of camphoraceous notes, as discussed next.

“Aromatic/fougère” is the category in Edwards’s guide with highest amount of men’s fragrances in the market [15] (p. 243). Although the term “aromatic” is rather subjective, it is applied in modern perfumery as a synonym of “fougère”, a family developed after the well-known Fougère Royale launched in 1882. The fougère accord is based upon the interplay between lavender, oakmoss, and coumarin [4], which justifies that $X_{aromatic}$ yielded the strongest similarity with $O_{oakmoss}$ ($r_{137} = 0.36$, $p < 0.0001$). Lavender seems to be the key material responsible for the cool odor character of fougère accords because it presents a marked camphoraceous smell [38]. The cooling effect of camphor and mentholic odors is apparent [39]. Lavender and some fresh-spicy herbs (e.g., peppermint, rosemary, and sage) share camphoraceous notes that produce a trigeminal cooling effect, which explains the

similarity between $X_{fresh-spicy}$ and $X_{aromatic}$ ($r_{137} = 0.23$, $p = 0.007$). However, lavender and herbaceous notes are typically masculine and, hence, these scents are never dominating in women's perfumes (Table 2; Table 3).

3.9. Towards a Standard Sensory Wheel of Women's Fragrances

Taking into account the seven olfactory classes shown inside Figure 3a, it seems more convenient to think about a heptagon of feminine perfumes. If each side of this heptagon is split in two parts, it obviously becomes an odor wheel with 14 categories. Interestingly, the Fragrance Wheel of Edwards [12] is based on the same number of families, but such representation is intended to display the whole spectrum of commercial fragrances. Edwards's wheel is probably the most popular one nowadays in perfumery; it is employed, among others, by two Spanish franchise bulk perfume companies [13,40] aimed at showing their customers the palette of items on sale. Nonetheless, if we focus on the subset of women's perfume, it might be convenient to reorganize some categories of this Fragrance Wheel to better describe the perceptual space from a sensory standpoint. Accordingly, some alterations should be required to adapt such a wheel to the subset of men's fragrances; this issue will be tackled in a further work.

Based on the results reported here, an effort was carried out to conveniently arrange the 14 Edwards's families inside this novel Heptagon (Figure 6). The order of categories appearing in the original Fragrance Wheel is indicated numerically close to the central hub. Following this sequence, it becomes apparent that the main difference with respect to Edwards's wheel is the position of "fruity" and "soft floral". The former was placed next to "green" by Edwards [12], but fruity descriptors appear in Figures 2 and 4 closer to "sweet" rather than to "green", which evidences the sweet character of fruity scents as discussed in Section 3.6. Based on this result, the fruity category was placed closer to the sweet polarity in Figure 6. Regarding "soft floral" that accounts for aldehydic perfumes, it appears in Edwards's wheel next to "floral oriental", but Figure 2 suggests a better position in between chypre/aromatic and citrus/green due to the nonsweet character of such perfumes, as already discussed.

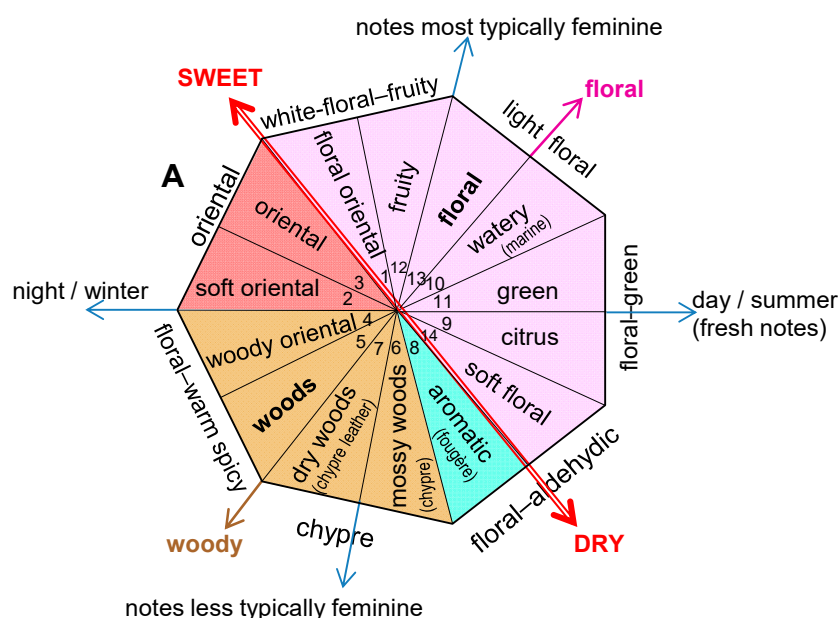


Figure 6. The Heptagon Wheel of Women's Fragrances. Names of the 14 categories inside the heptagon correspond to the olfactory families of Edwards's Fragrance Wheel [12]. Names outside the polygon basically correspond to Figure 3a. Four underlying polarities are indicated.

Apart from this remarkable reorganization of categories with respect to the Fragrance Wheel, some contrasting polarities were also indicated in an effort to achieve a sensory wheel based on meaningful underlying dimensions. The horizontal axis explains preference for daytime versus nighttime wear, which is directly related with preference for summertime versus wintertime wear. Another polarity is “sweet” versus “nonsweet” (dry). Interestingly, this axis divides the chart in two parts; all floral categories are located on the upper right side, and they basically account for those scents most typically feminine. On the other hand, “woody” appears as opposite to “floral”, which agrees with Edwards’s wheel. Regarding the contrasting polarity of notes most typically feminine versus those less feminine, it does not seem to be exactly equivalent to the divergence of “floral” versus “woody”.

3.10. Representativeness of the Sample of 140 Perfumes

The sample under study corresponds to quite old perfumes, which obviously constrains the results because the market of women’s fragrances has evolved since the 1990s. Taking into account that 125 out of the 140 fragrances are contained in Edwards’s guide, Table 4 displays the number of items listed under each class of this guide (24th edition of 2008), as well as the classification corresponding to the set of perfumes under study. By comparing the relative frequencies P_{ED} and P_{125} , it turned out that the percentage of perfumes classified as “floral” in the sample was about half of the percentage in Edwards’s directory. Conversely, the ratio for “mossy woods” (chypre) was much higher in the sample. Interestingly, both categories are properly discriminated by PC2 and appear as opposed odor classes in Figures 2 and 6. As the polygon of floral descriptors is broad enough, it is unclear if a larger proportion of floral perfumes in the sample might lead to a better characterization of such perceptual spectrum.

Table 4. Number of feminine fragrances (N_{ED}) listed under each class of the directory published by Edwards in 2008 (3463 in total). Classification of those 125 perfumes studied here that are contained in this directory (number of occurrences: N_{125}). Frequencies in percentage are also indicated.

Class	Occurrences		Percentages		Class	Occurrence		Percentage	
	N_{ED}	N_{125}	P_{ED}	P_{125}		N_{ED}	N_{125}	P_{ED}	P_{125}
Floral	1446	27	41.8	21.6	Citrus	146	2	4.2	1.6
Floral oriental	533	19	15.4	15.2	Dry woods	47	7	1.4	5.6
Soft floral	354	14	10.2	11.2	Woods	71	0	2.1	0
Woody oriental	352	12	10.2	9.6	Green	33	5	1.0	4.0
Mossy woods	175	24	5.1	19.2	Watery	35	1	1.0	0.8
Oriental	145	5	4.2	4.0	Fruity	21	0	0.6	0
Soft oriental	97	9	2.8	7.2	Fougère	8	0	0.2	0

After discarding the categories “floral” and “mossy woods”, a chi-squared test was carried out with the values N_{ED} and N_{125} in Table 4. As this test requires an occurrence >4 , some classes appearing next to each other in the Fragrance Wheel (e.g., “woods” and “woody oriental”) were summed together prior to the test in order to achieve this condition. It turned out that the null hypothesis of independence could be accepted ($\chi^2(6) = 9.6, p = 0.14$). Hence, this test suggests that except for “floral” and “chypre”, none of the remaining categories in the Fragrance Wheel were underrepresented in the sample. It can be assumed that Figure 6 properly exemplifies the perceptual spectrum of women’s fragrances currently in the market. Nevertheless, a further study would be necessary to confirm this hypothesis, and to take into consideration some new trends like “gourmand” scents that have become popular in recent years.

4. Discussion

The idea that perfumers have in mind when creating a new formulation can be different to the actual olfactory “image” that naive consumers perceive when trying the scent. Thus, understanding consumer perception and preference based on the smell is important for the creation of successful

fragrances. Equations obtained here are consistent with the experience of perfumers and provide quantitative models that might be useful for an appropriate design of marketing strategies.

Given the enormous amount of perfumes available in the market, the shopping decision for a new fragrance is a complex task for consumers. Classification systems of these products by means of 2D sensory charts are valuable tools to visualize the olfactory spectrum, which may facilitate the communication between consumers and retailers. Generally speaking, there is a reasonable agreement between different studies that have projected perfumery scents on a 2D plot. This coincidence implies an opportunity for a universal system for fragrance classification [41]. The Odor Effects Diagram [42] displays odor descriptors commonly encountered in perfumery; the two axes of this diagram can be approximately matched with the PC1/PC2 loading plot derived from the BH database [15], as well as with similar 2D plots [11,16,43].

One axis of these sensory representations discriminates descriptors most typically feminine (i.e., “floral”, “sweet”, and “fruity”) versus those mostly encountered in men’s fragrances (i.e., “aromatic”, “earthy”, and “woody”). This dimension reflects the major commercial classification of perfumes as targeted either to men or women. One study [44] has attempted to further understand the olfactory differences associated to this classification, but only 12 fragrances were used. As the 140 fragrances studied here are targeted to women, it was unexpected to find that PC2 in Figure 2 is basically determined by the chypre (earthy–woody) versus floral polarity, which further supports that this dissimilarity is strongly marked in our perceptual space of scents. Strikingly, the position of “leathery”, “spicy”, and “animalic” descriptors is also consistent with other sensory maps of perfumery scents [15]. Floral–powdery fragrances are the ones most dissimilar to chypre perfumes, which agrees with the negative correlation of $I_{powdery}$ versus Z_{chypre} ($r_{140} = -0.34$, $p < 0.0001$).

The orthogonal dimension of reported 2D perfumery maps usually discriminates “fresh” versus “warm” scents, as it is also the case here for PC1 (Figure 2). Such polarity was also found in a multivariate analysis of odor profiles obtained for 37 aroma chemicals [45]. In perfumery, “fresh” is usually applied to invigorating odors reminiscent of the outdoors like the clean scent of early morning air, the green note of recently cut leaves, or citrus scents [11]. The terms “refreshing” and “invigorating”, which are synonymous in English, were associated by Richardson [43] with green and citrus scents.

In a previous study that applied the same methodology used here [24], it was shown that Edwards’s Fragrance Wheel properly exemplifies the spectrum of perfumes on sale. One dimension of the multivariate analysis discriminated masculine versus feminine fragrances, which is intuitively appealing. However, results reported here suggest that some reorganization of categories in the Fragrance Wheel, particularly regarding “fruity” and “soft floral”, should be necessary in order to obtain a more accurate sensory wheel for women’s perfumes. In the sensory wheel developed by Edwards [12], the author indicated that it is based on two contrasting polarities: “fresh” versus “oriental”, and “floral” versus “woody”. The same underlying dimensions are reflected by Figure 6, but two additional poles are indicated: “sweet” versus “dry”, and notes most typically feminine versus those that are less feminine. The four polarities shown in Figure 6 are intended to better understand the relationships between odor categories.

Despite the difficulties in obtaining reliable descriptions of scents, it is striking that the projection of olfactory profiles onto PC1 and PC2 (Figure 2) has a reasonable agreement with Dragoco’s Hexagon and Givaudan’s map (Figure 3). The resulting Heptagon (Figure 6) might be a valuable tool to better understand the contrasting polarities in the perceptual space of feminine fragrances. Results presented here might be somewhat limited by the amount of items studied and, hence, further research should be carried out with a larger sample. Nevertheless, the reported evidence suggests that it is possible to reach certain consensus about how to develop a standard sensory wheel for women’s perfumes. Such representations would be of practical interest for marketing purposes.

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