Virgin Olive Oil Aroma: Relationship between Volatile Compounds and Sensory Attributes by Chemometrics

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Volatile compounds are responsible for virgin olive oil aroma, and this paper demonstrates that basic sensory perceptions (green, fruity, sweet, ripe, over-ripe, undesirable, pungent) can be totally explained by volatile compounds with R^2-adjusted >0.85. Thirty-two samples of 6 European varieties of virgin olive oil were characterized by 55 chemical compounds and 55 sensory attributes evaluated by 6 different panels of the United Kingdom, Spain, the Netherlands, Greece, and Italy. Multidimensional scaling was used to bring out inter–intra dissimilarities from datasets of sensory attributes and volatile compounds.

Keywords: *Olive oil; flavor; sensory analysis; volatiles; statistics*

INTRODUCTION

Virgin olive oil, a gourmet oil, is highly prized for its delicious taste and aroma. It is particularly important in the basic Mediterranean diet. Today there are increasing opportunities for the export of olive oil because of an awareness of its excellent flavor in countries where olive oil has been a relatively underused commodity; for example, northern European and American countries are an increasing market for olive oil, and there have been preliminary studies into what attributes are appreciated in olive oil by an untrained palate in contrast to the qualities valued by regular users (McEwan, 1994).

Thus, sensory quality plays an important role in the overall quality of olive oil and, hence, in the preference of consumers. Volatile, and some nonvolatile, chemical compounds give rise to the sensory attributes that can be detected by consumers. Many attempts have been made to assess the role of different volatile compounds in the flavor matrix of foodstuffs, but it is not always easy to assign the volatiles responsible for a given sensory attribute produced by the whole food matrix. The method most often applied to establish the role of the volatiles is the HRGC sniffing technique (Kiritsakis, 1991; Morales et al., 1994), which consists of direct olfaction of the chromatographic eluent (Guichard, 1992). This technique allows each volatile odor to be almost perfectly characterized and the flavor impact zones assigned in the chromatogram but does not take into account the synergism and antagonism processes that occur in the complex matrix of the foodstuff. In fact, the results of the sniffing can be seen as a collection of particular solutions of a complex equation with all the pros and cons that this has compared with a general solution.

Since synergism and antagonism processes occur, it is desirable to achieve a multivariate statistical procedure that allows the sensory attributes from the volatile compounds to be explained. The procedure selected was multidimensional scaling (MDS) (Schiffman et al., 1981; Schiffman and Beeker, 1986). This procedure is based on the study of the similarities among variables, gathering them according to their major or minor similarity and showing the results spatially as a map. MDS has been successfully used to investigate sensory properties (Robertson Rosett et al., 1994; Damasio et al., 1994), to study the similarity of odors of chemicals (Schiffman et al., 1977; MacRae et al., 1990), and to correlate sensory and instrumental data (Vélez et al., 1993; Tuorila et al., 1989).

Thus, the aim of this work is to clarify the relationships between the sensory attributes produced by the whole virgin olive oil matrix and its volatile compounds using MDS. The results have been compared with those of a sniffing study to establish the role of the volatile compounds in the sensory characteristics of virgin olive oil samples. Volatiles responsible for the sensory attributes most valuable for trained and untrained assessors are also pointed out.

Table 1. Characteristics of Virgin Olive Oil Samples

codes	variety	maturity[a]	system[b]
1 (17)	Koroneiki	U	C
2 (18)	Koroneiki	N	C
3 (19)	Koroneiki	O	C
4 (20)	Koroneiki	N	P
5 (21)	Tzunnati	N	C
6 (22)	Coratina	U	C
7 (23)	Coratina	N	C
8 (24)	Coratina	O	C
9 (25)	Coratina	N	E
10 (26)	Cima di Bitonto	N	C
11 (27)	Picual	U	C
12 (28)	Picual	N	C
13 (29)	Picual	O	C
14 (30)	Arbequina	U	C
15 (31)	Arbequina	N	C
16 (32)	Arbequina	O	C

[a] N, normal ripeness; O, over-ripe; U, unripe. [b] C, centrifugation system; P, percolation system; E, pressing system.

MATERIALS AND METHODS

Sampling. Table 1 describes the basic characteristics of 32 samples of virgin olive oil harvested in two different years (16 × 2) and collected from Greece (Heraklion, Crete), Italy (Bitonto, Puglia), and Spain (Córdoba and Jaén, Andalusia). The varieties were selected for their high percentage of the bottled virgin olive oil trade (Hermoso et al., 1991; Aparicio and Alonso, 1994). Virgin olive oils were extracted by three different extraction systems: centrifugation, percolation, and pressing (Aparicio et al., 1994b). Oils were delivered within

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Table 2. Basic Characteristics of Panels

	Spanish	Italian	Greek	Italian	British	Dutch
no. of assessors	10	10	14	11	9	8
assessors' level[a]	F	T	T	F	T	T
consumer[b]	H	H	H	H	P	P
no. of attributes[c]	15	16	15	18	26	68
scale	S	S	S	S	U	U
scores	1–5	1–5	1–5	1–9	100 mm	130 mm

[a] F, fully trained; T, trained for this work. [b] H, habitual; P, potential. [c] S, structured; U, unstructured.

24 h of harvesting, and the samples were stored frozen until the moment of analysis.

Sensory Analysis. Samples were evaluated by six different panels constituted by assessors of five different nationalities: Spanish (A), Italian (B and D), Greek (C), British (E), and Dutch (F). All panels used quantitative descriptive analysis (Stone et al., 1974; Aparicio et al., 1994a) to evaluate sensory attributes of samples, but they can be divided into two groups on the basis of how each attribute was perceived.

Panels A–C strictly followed the EU regulation (EU, 1991), and the score for each attribute is the result of the whole gustatory–olfactory–tactile perception. Panels A and B were constituted by fully trained assessors with more than 5 years of experience in evaluating all types of olive oil (virgin, pure, lampant...) using the COI test (Aparicio et al., 1992), and they worked at research centers. Assessors of panel C were habitual consumers of this foodstuff working at an olive oil plant. Panels D–F judged the samples by applying freely a quantitative descriptive sensory profiling. Assessors of panel D were trained using mixtures of different olive oil types. The assessors were students at an Italian university. British assessors (panel E) were trained using different oils (sunflowers, nuts, sesame, olive, etc.), while the Dutch panel (F) trained its assessors by evaluating different olive oil brands.

The presentation of samples was fully randomized, and all samples were evaluated in triplicate. Table 2 summarizes the basic characteristics of these panels.

Fifty-five sensory attributes, categorized into aroma, odor, taste, aftertaste, mouthfeel, and after-mouthfeel, were considered in this study. Attributes have been numbered in Table 3, and their numbers (codes) will be used throughout this paper when they are referred to.

Instrumental Analysis. *Dynamic Headspace Gas Chromatography.* Volatile compounds of virgin olive oil samples were analyzed according to a dynamic headspace technique under determined optimized conditions as described by Morales and Aparicio (1993). Samples of 0.5 g were heated at 40 °C and swept with N_2 (200 mL/min) for 15 min. Tenax TA (Chrompack) was used as the trap. Volatiles were thermally desorbed by means of a thermal desorption cold trap injector (TCT, Chrompack) at 220 °C onto a fused silica trap cooled at −110 °C for 5 min just before injection, which was carried out by flash heating of the cold trap at 170 °C for 5 min. The volatiles were transferred onto a fused silica Supelcowax 10 capillary column (60 m, 0.32 mm i.d., 0.5 μm film thickness). The oven temperature was held at 40 °C for 4 min and programmed to rise at 4 °C/min to a final temperature of 240 °C, at which it was held for 10 min. A Hewlett-Packard 5890 Series II with a FID detector was employed. Isobutyl acetate was used as internal standard. Volatiles were isolated and analyzed in duplicate.

Dynamic Headspace Gas Chromatography–Mass Spectrometry. A MS 30/70 VG mass spectrometer (VG Analytical, Manchester, U.K.) and a VG 11/250 data system coupled to the TCT-GC were used for mass spectrometric analysis. Operating conditions were as in a previous work (Morales et al., 1994).

A set of 49 volatiles have been identified, while the rest are being identified using either the MS libraries or chemical standards. Table 4 shows the whole set of volatiles used in this study, their codes, and the approximate mean concentration in samples.

Table 3. Sensory Attributes Evaluated in Virgin Olive Oil Samples

panel	attribute	perception	code
A	olive fruity (green)	olfactory–gustatory	1
A	apple	olfactory–gustatory	2
A	other ripe fruits	olfactory–gustatory	3
A	green	olfactory–gustatory	4
A	bitter	olfactory–gustatory	5
A	pungent	olfactory–gustatory	6
A	winey	olfactory–gustatory	7
A	olive fruity (ripe)	olfactory–gustatory	8
B	olive fruity (green)	olfactory–gustatory	9
B	green	olfactory–gustatory	10
B	bitter	olfactory–gustatory	11
B	pungent	olfactory–gustatory	12
B	sweet	olfactory–gustatory	13
B	rough	olfactory–gustatory	14
C	olive fruity (green)	olfactory–gustatory	15
C	apple	olfactory–gustatory	16
C	other ripe fruits	olfactory–gustatory	17
C	green	olfactory–gustatory	18
C	bitter	olfactory–gustatory	19
C	pungent	olfactory–gustatory	20
C	sweet	olfactory–gustatory	21
C	rancid	olfactory–gustatory	22
D	tomato	aroma	23
D	ripe black olives	aroma	24
D	green olives	aroma	25
D	cut green grassy	aroma	26
D	artichoke	aroma	27
D	apple	aroma	28
D	yeast	aroma	29
D	bitter	taste	30
D	pungent	mouthfeel	31
D	astringent	mouthfeel	32
E	strength of olive	odor	33
E	banana skins	odor	34
E	tomato	odor	35
E	hay/composty	odor	36
E	perfumey	odor	37
E	grassy	odor	38
E	almond	odor	39
E	throatcatching	mouthfeel	40
F	twig	smell	41
F	grass	taste	42
F	green leaf	taste	43
F	green	aftertaste	44
F	sea breeze on the beach	smell	45
F	butter/cream	taste	46
F	green banana	taste	47
F	coconut	taste	48
F	dried green herbs	taste	49
F	grotty	taste	50
F	nuts	smell	51
F	olives	taste	52
F	rancid	smell	53
F	dry wood	smell	54
F	soft fruits	smell	55

GC Sniffing. DHS and GC were performed as described above, the odor-active regions of the eluate were evaluated, and the aroma notes of these regions were assigned by five assessors, two of whom had more than 10 years of experience and the other three who, while not being experienced, were habitual consumers of virgin olive oil. The assessors used a free profile to describe the odor of volatiles.

Organoleptic Testings. Ethyl acetate, hexan-1-ol (Merck, Darmstadt, Germany), and 6-methyl-5-hepten-2-one (Sigma, St. Louis, MO) were diluted with water or paraffin oil to the same concentration as found in virgin olive oil samples and tested at room temperature by the assessors to establish their tastes.

Data Manipulation. Gas chromatographic data were acquired by a personal computer, and ASCII files were manipulated by a Fortran V program for elimination of unwanted information in the chromatographic reports. An automated peak recognition subroutine performed a peak matching and recognition based on retention time ranges after

Table 4. Volatile Compounds Quantified in the Virgin Olive Oil Samples

code	compound	mean concn (mg L^{-1})	sniffing	MDS
1	methyl acetate	0.012		green (nuts)
2	octene	0.011	solvent-like	green (grass)
3	ethyl acetate	0.091	sweet, aromatic	slightly bitter/pungent
4	2-butanone	0.004	fragrant, pleasant	tomato, apple
5	3-methylbutanal	0.052	sweet, fruity	apple
6	1,3-hexadien-5-yne	0.017		green (green olives)
7	an alcohol	0.048	sweet, apple	other ripe fruit
8	ethylfuran	0.056	sweet	sweet
9	ethyl propanoate	0.047	sweet, strawberry, apple	sweet
10	an alcohol + hydrocarbon	0.222	pungent, acid	fruit[a]
11	3-pentanone	<0.001	sweet	sweet[a]
12	4-methylpentan-2-one	<0.001	sweet	green
13	pent-1-en-3-one	0.204	sweet, strawberry	sweet
14	2-methylbut-2-enal	0.064	solvent-like	ripe fruit (olives, dry wood)
15	2-methylbut-3-enol	0.006		slightly bitter
16	a hydrocarbon	0.229	sweet, apple	sweet
17	methylbenzene	<0.001	glue, solvent-like	other ripe fruit
18	butyl acetate	0.098	green, pungent, sweet	sweet
19	hexanal	0.178	green, apple	sweet
20	a hydrocarbon	0.140	sweet, aromatic	sweet
21	2-methylbutyl propanoate	0.006	aromatic, ketone	strength of olives, apple
22	2-methyl-1-propanol	0.043	ethyl acetate-like	green
23	(*E*)-2-pentenal	0.016	green, apple	ripe fruit (soft fruit)
24	an alcohol	0.013	greasy	undesirable (rancid)
25	(*Z*)-2-pentenal	0.022	green, pleasant, caramel	over-ripe fruit
26	ethylbenzene	0.078	strong	bitter taste (dried green herbs)
27	(*E*)-3-hexenal	0.058	artichoke, green, flowers	artichoke
28	(*Z*)-3-hexenal	0.377	green, green leaves, grassy	green
29	1-penten-3-ol	0.599	wet earth	undesirable
30	3-methylbutyl acetate	0.055	banana	slightly fruity
31	heptan-2-one	0.011	fruity	ripe fruit
32	(*E*)-2-hexenal	11.479	bitter almonds, green-fruity	almond odor, bitter taste
33	(*Z*)-2-hexenal	0.038	fruity, almonds	almond odor, bitter taste
34	2-methylbutan-1-ol	0.023	fish oil	ripe olives (over-ripe)
35	3-methyl-2-butenyl acetate	0.026	putty-like unpleasant	ripe fruit
36	dodecene	0.099		slightly bitter/taste
37	pentan-1-ol	0.004	pungent	ripe fruit
38	ethenylbenzene	0.017		fruity
39	3-methyl-butanol	0.005		undesirable (yeast)
40	hexyl acetate	0.196	sweet, fruity	green (grassy)
41	a C_8 ketone	0.003	fruity, mushroom-like	green[a]
42	octan-2-one	0.008	moldy	undesirable
43	3-(4-methyl-3-pentenyl)furan	0.055	paint-like strong	over-ripe
44	3-hexenyl acetate	0.091	green banana, green leaves	green
45	(*Z*)-2-penten-1-ol	0.518	banana	green (grass)
46	6-methyl-5-hepten-2-one	0.028	fruity	bitter taste (dried green herbs)
47	nonan-2-one	0.025	fruity	apple
48	hexan-1-ol	0.723	fruity, aromatic, soft	rough mouthfeel and rancid odor
49	(*E*)-3-hexen-1-ol	0.019		green leaf, nuts
50	2,4-hexadienal	0.001		ripe fruit
51	(*E*)-2-hexen-1-ol	0.893	green, grassy	green (cut green grassy)
52	acetic acid	0.029		undesirable
53	methyl decanoate	0.028	fresh	green leaf, nuts
54	tridecene	0.166		bitter (almond)
55	(*Z*)-3-hexen-1-ol	0.604	banana	green banana

[a] Poor information.

visual recognition of a standard chromatogram. The automated peak recognition subroutine corrected peak areas when there was more than one peak matching a certain retention time range. Retention time and areas of selected peaks, including the internal standard, were stored in a database (dBase IV). Ratios of each of the selected peak areas to the area of the internal standard were used for statistical analysis. Datasets were imported to the STATISTICA (1992) software package by which multivariate statistical studies were carried out. The information of each sample consisting of both gas chromatographic and sensory data was checked for skewness, and the study of outliers was made by Mahalanobis distance, evaluated as χ^2.

Statistical Analysis. The STATISTICA (1992) procedures used were canonical correlation, cluster analysis, and multidimensional scaling. In each multivariate analysis, each of the 55 log transformations of standardized peak areas from a chromatogram was considered a variable for a given virgin olive oil sample corresponding to the dataset of sensory attributes. First, all variables were standardized by *Z*-score since there is a great difference between figures of volatiles and sensory attributes. Once the data were standardized, cluster analysis was used to build a square matrix of distances for multidimensional scaling through two steps of cluster analysis. In the first step a matrix of distances is calculated by a tree clustering classification algorithm under a complete linkage amalgamation rule and city-block (Manhattan) distance (Schiffman et al., 1981). The second step allows the square matrix of dissimilarities to be built.

MDS can be considered an alternative to factor analysis, whose main goal is to detect meaningful underlying dimensions that allow the researcher to explain observed similarities and dissimilarities between variables. The measurement that has been used to evaluate how well the final configuration reproduces the observed distance matrix is the stress measurement. The raw stress value of a configuration is defined

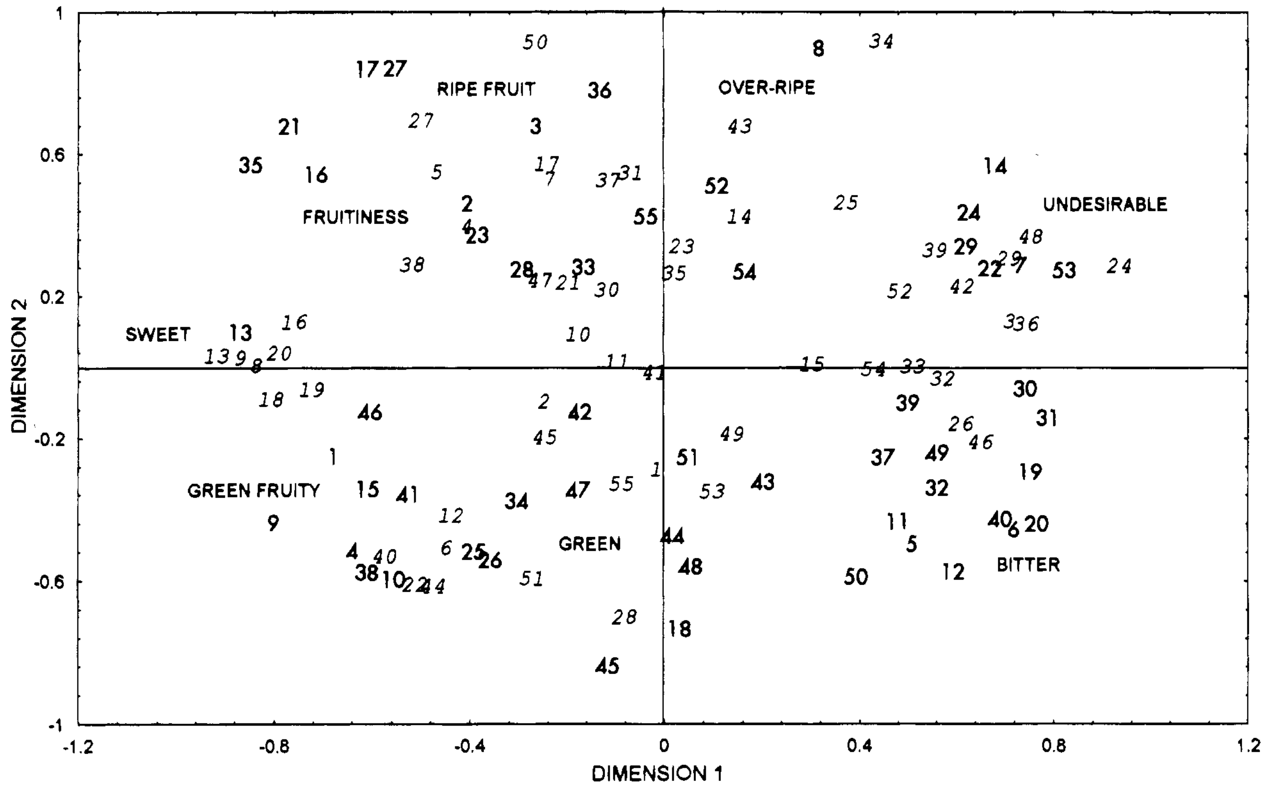

Figure 1. First two dimensions of multidimensional scaling of datasets of volatiles (italic) and sensory attributes (bold).

by

$$\Phi = \sum(d_{ij} - \Delta_{ij})^2$$

where d_{ij} stands for the observed distances and Δ_{ij} for the reproduced distances. Thus, the smaller the stress value, the better is the fit of the reproduced distance matrix to the observed distance matrix.

The number of initial dimensions (eight) provided an adequate starting configuration for the iterative fitting procedure, whilst the criterion for deciding how many final dimensions should be used to arrive at a conclusion was the clarity of the final configuration. Successive iterations are carried out to minimize the stress loss function.

To assess the fit of the sensory attributes for volatile components, a canonical correlation procedure was applied to the different clusters of those variables obtained by MDS. The goal of canonical correlation is to analyze the relationship between two sets of variables to see how the two sets relate to each other. Selection of pairs of canonical variates is made by Bartlett's test, while the interpretation of canonical variates involves assessment of overlapping variance.

The software was run on a 486 personal computer.

RESULTS AND DISCUSSION

Volatiles isolation was used as part of an integrated system for an objective measurement of virgin olive oil aroma. The analytical scheme consisted of the integration of the tools needed to permit the association of sensory responses to chemical data by multivariate statistics. Since the quality of virgin olive oil is determined by its sensory attributes or acceptability to consumers, methods relating sensory attributes and volatiles would enable the step from a more or less subjective and expensive methodology to another method that is quite objective, cheap, and easy to apply.

MDS allows objects that are judged to be experimentally similar to one another to be represented as points close to each other in the results spatial map; objects judged to be dissimilar are represented as points distant from one another. The result of applying MDS to the datasets of volatile compounds and sensory attributes is displayed in Figure 1, and this pictorial representation will allow study of the inter- and intrarelationships of sensory attributes and volatiles.

Figure 1 shows there are basically seven groups of sensory perceptions (undesirable, bitter-pungent, green, sweet, fruitiness, ripe fruit, and over-ripe) which agree with the conclusions of the virgin olive oil sensory wheel (Aparicio and Morales, 1995), a robust statistical procedure that has allowed clustering of up to 139 sensory attributes evaluated by habitual and potential consumers (Aparicio et al., 1994a). This figure displays the volatile components quantified in the samples, while characterization by their place in the figure and by sniffing (Morales et al., 1994) is summarized in Table 4.

Figure 1 also shows that the sensory attributes surround the volatiles, thereby showing that the former are the consequence of the latter; therefore, volatiles should explain the sensory attributes characterizing these groups that they have been clustered with. Thus, mathematical and sensory studies have been used to give broad answers to the relationships between volatiles and sensory attributes.

The place of the basic perceptions in the figure is quite logical since the cycle "bitter–green–sweet–fruit-ripe–over-ripe–undesirable" can be associated with the sensory perceptions expected from the maturity of olives. In relation to the place of these groups, the first quadrant clusters sensory attributes and volatile components related to undesirable or unallowable (over-ripe) perceptions. Bitter–pungent–astringent attributes and volatile components appear alone in the second quadrant; they go from an undesirable taste perception [bitter almonds, (*E*)-2-hexenal (**32**)] (Bauer et al., 1990) to a perception of green odor with a bitter taste [green leaf, (*E*)-3-hexen-1-ol (**49**)] (Aldrich Catalog, 1995), since

Table 5. Results of Canonical Correlations of Some Basic Sensory Perceptions and the Attributes Classified within These Groups

perception	sensory attributes	volatile compounds	R^2-adjusted
green	1, 4, 9, 10, 15, 18, 25, 26, 34, 39, 42, 46	**1, 6, 12, 22, 28, 40, 44, 45, 51, 55**	0.97
sweet	13	**8, 9, 13, 16, 18, 19, 20**	0.91
bitter-pungent	5, 6, 11, 12, 19, 20, 30, 31, 32, 40, 41	**26, 32, 33, 46, 54**	0.95
undesirable	7, 14, 22, 29, 54	**24, 29, 39, 42, 48, 52**	0.95
fruitiness	2, 16, 21, 23, 28, 35	**4, 5, 21, 38, 47**	0.87

attribute 18 has been characterized as "green slightly bitter" (Aparicio et al., 1994a). This quadrant can also be thought of as the taste/mouthfeel quadrant, since perceptions bitter, pungent, and astringent are not odor evaluation.

The third quadrant, full of the green sensory attributes and volatiles associated with this perception, goes from a strong green perception [(*Z*)-3-hexenal (**28**) (Kuentzel and Bahri, 1991), (*Z*)-3-hexen-1-ol (**55**)] (Hatanaka et al., 1992) to olive fruity. In the boundaries of this and the fourth quadrant there is a sweet perception characterized as green-sweety by Aparicio et al. (1994a). It is interesting to point out that several volatile compounds (**8, 9, 13, 16, 20**) appear close to this attribute and all of them gave a sweet description by sniffing. In fact, volatile components butyl acetate (**18**) and hexanal (**19**) are the only ones of this group that were also characterized as green by sniffing (Table 4).

Sensory attributes and volatile components related to normal and slightly ripe olives appear in the fourth quadrant. The groups of this quadrant can be characterized as fruity since there are no clear limits between groups and they are totally opposite to bitter taste, between the green and over-ripe—undesirable sectors.

From a statistical viewpoint, the first dimension (*X*-axis) divides the figure into two parts: desirable (left side) and undesirable (right side) sensory attributes and volatiles. The second dimension (*Y*-axis) shows at the bottom (from right to left) the unripe (bitter) and ripe (fruity) characteristics of olives and, at the top (from left to right), the ripe (other ripe fruit) to off-flavors (undesirable) characteristics.

Finally, Figure 1 shows that sensory attributes with the same semantic term are differently evaluated by panels despite the facts that they followed the same procedure and that assessors were well-trained (Aparicio et al., 1994a). This means that there is nothing in the experimental paradigm to convince the authors that different assessors are using the response scale in exactly the same fashion since the meaning of the numbers is conditional upon how the assessor is responding. Thus, although "apple", "tomato", and "other ripe fruit" show some discrepancies when they are evaluated by different panels, sweet is the perception most differently evaluated by panels. Thus, panel B evaluated sweet (13) as green-sweety, while panel C evaluated sweet (21) as sweet-fruity. Another important discrepancy is how panel C evaluated green (18), since it means a green slightly bitter.

Relationship between Characterization of Volatile Components by Sniffing and MDS. As most of the attempts to relate sensory attributes and volatile components have been carried out by sniffing, Table 4 compares the results of the characterization of volatile components by sniffing and by the sensory attributes nearest to them in Figure 1. Despite the differences of these procedures (sniffing characterizes each volatile individually, and MDS does not; MDS characterizes the volatiles using standardized sensory attributes, while sniffing uses a free sensory profile), there is sufficient agreement between them since the discrepancies amount to only four volatiles: ethyl acetate (**3**), (*Z*)-2-pentenal (**25**), 6-methyl-5-hepten-2-one (**46**) and hexan-1-ol (**48**).

The sensory characterization of hexan-1-ol by sniffing, described as "fruity, aromatic, soft", disagrees with the group (undesirable) in which it is placed by MDS. However, hexan-1-ol is also described as "oxidized green bean" (Kochhar, 1993), which agrees with the rancid perception of its nearest sensory attribute, with which it has a correlation of R^2-adjusted = 0.87.

A similar explanation can be given for (*Z*)-2-pentenal, since Kochhar (1993) characterizes it as "oxidized and fishy", more or less in agreement with its position in Figure 1, between the groups undesirable and over-ripe.

No explanation has been found regarding ethyl acetate and 6-methyl-5-hepten-2-one, except that they could be classified by their taste rather than smell, as sniffing characterized them, since they appear in the bitter-pungent group whose perceptions are of mouthfeel and taste. In fact, the tasting of these compounds by the assessors gave a rough, bitter aftertaste description for ethyl acetate, a rough mouthfeel description for hexan-1-ol, and a bitter, astringent description for 6-methyl-5-hepten-2-one, which could explain their positions in the MDS plot.

On the other hand, the groups constituted by volatiles and sensory attributes can be understood, since the synergy of these chemical compounds generates the basic perception characterizing the group. From a mathematical viewpoint, the canonical correlation is the statistical procedure appropriate to analyze that process and explain if volatile components could be used instead of the basic perceptions detected by MDS.

Green, sweet, bitter, undesirable, and fruity are the most remarkable perceptions in virgin olive oil (Aparicio and Morales, 1995), and these have been the perceptions analyzed by canonical analysis. Table 5 shows that the results of applying this statistical procedure are quite satisfactory; fruity perception is the only one whose value is lower than 0.90, though this perception is understood as an aggregation of other perceptions (sweet, apple, tomato, etc.) compared with other perceptions such as ripe, over-ripe, and bitter. The correlation coefficients of table 5 mean that the basic perceptions characterizing a virgin olive oil, as found by either habitual or potential consumers, could be obtained from an easy, cheap, and objective evaluation of a certain group of volatiles instead of a complex, expensive, and perhaps subjective procedure carried out by panelists evaluating virgin olive oil.

Quality Sensory Evaluation of Virgin Olive Oil by Its Volatile Components. Figure 2 displays the sensory quality evaluation of several virgin olive oil samples. The overall gradings of habitual and potential consumers are shown.

As can be seen, habitual consumers gave higher scores than did potential consumers, probably because the latter knew the product less well. However, the tendencies in the evaluation are quite similar in both types of

Table 6. Some Normalized Values of Volatile Components Characterizing the Varieties of Virgin Olive Oil

variety	2-butanone (**4**)	butyl acetate (**18**)	hexanal (**19**)	(*E*)-3-hexenal (**27**)	(*E*)-2-hexenal (**32**)
Koroneiki	0.13	5.45	10.43	1.39	252.27
Coratina	0.02	0.87	1.38	1.50	777.39
Arbequina	0.09	3.32	6.03	4.25	235.10
Picual	0.17	2.61	4.32	0.77	92.47

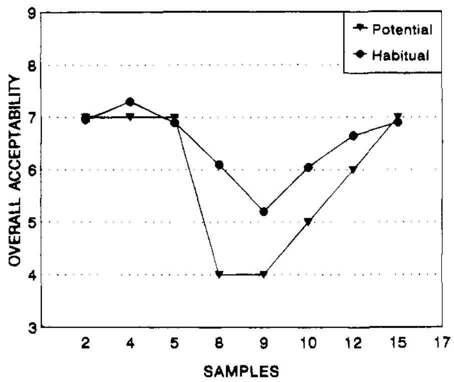

Figure 2. Sensory quality evaluation of virgin olive oil samples by habitual and potential consumers.

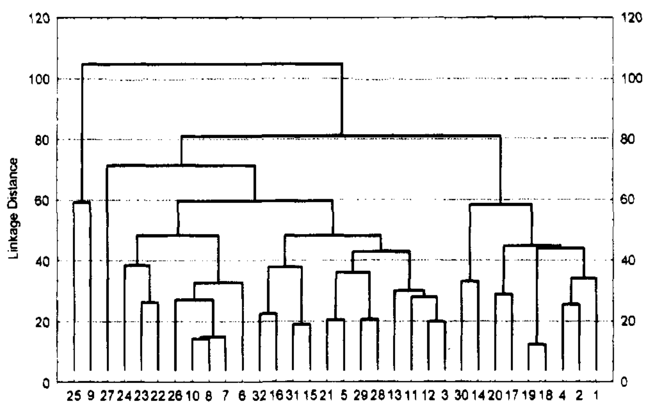

Figure 3. Dendrogram showing the clustering of the virgin olive oil samples (*X*-axis) using the volatile dataset.

consumer. Samples 8 and 9 of the Coratina variety are the lowest valued. The Coratina variety is characterized by too high an "almond odor" and a low "sweet aroma". The best scores are obtained by the Greek varieties: Koroneiki is characterized by the highest "green smell". The Arbequina sample can be characterized as "sweet artichoke aroma" and is also scored as one of the best oils; the Picual variety is considered to be at a medium level, characterized by the lowest "almond odor".

Table 6 shows some of the volatiles responsible for the differences between varieties. As can be seen, the (*E*)-2-hexenal content in Coratina samples is by far the highest, in concordance with the results of sniffing and MDS. On the other hand, butyl acetate and hexanal have very low concentrations in the samples. Picual is characterized by a low volatile content. Arbequina shows a higher content of (*E*)-3-hexenal and Koroneiki a higher content of hexanal and butyl acetate with a concentration of (*E*)-2-hexenal close to that found in Arbequina.

A cluster analysis was performed to determine whether virgin olive oil samples could be characterized by their volatile components only. A hierarchical clustering technique was used, and the similarity matrix was computed on the basis of the Manhattan (city-block) distance; the samples were clustered by the complete linkage method.

The dendrogram of Figure 3 shows that (except sample 27) the crop has no relevant influence on the production of volatiles since samples of the same variety, maturity, and extraction system, but of a different crop, have a great similarity. Regarding the other parameters, the samples from pressing (variety Coratina) are quite apart from the other samples, obtained by centrifugation and percolation. Pressing is an inappropriate technique for attaining olive oils of good quality (Aparicio et al., 1994b) as they are in intimate contact with vegetable water for a certain time. In fact, these samples can be distinguished from the others by two volatile compounds (2-methylbutan-1-ol and 1-penten-3-ol), whose contents are by far the highest in pressing samples. These volatiles were characterized by both sniffing and MDS as undesirable attributes and indicate that the time virgin olive oil is in contact with the vegetable water leaves undesirable attributes in the oil's aroma.

The dendrogram shows that the Koroneiki and unripe Arbequina samples are quite apart from the other varieties. The other great group is constituted by two subgroups—one clusters Italian samples and the other basically Spanish varieties that appear separated in the next two groups.

However, since volatile components are responsible for sensory attributes, there will be a relationship between consumers' attitudes and the volatiles quantified in the samples. The attitudes of consumers concerning overall acceptability of the evaluated samples agree with the groups of the dendrogram, as the scale of these parameters (from left to right) goes from low values (Coratina variety, pressing system) to high values (Koroneiki variety).

In an attempt to explain the acceptability of virgin olive oil samples by potential consumers from the volatile compounds, a regression study between potential consumers' overall values and volatile compounds was carried out, *F*-to-enter and *F*-to-remove at $p = 0.05$. This showed an R^2-adjusted = 0.995 (SD = 0.087) with volatiles butyl acetate, 2-butanone, 2-methylbut-2-enal, and hexyl acetate. As can be seen, one volatile compound corresponding to each of the basic virgin olive oil perceptions (sweet, green, fruitiness, and ripe fruit) was selected, so showing the usefulness of volatile components to explain the acceptability of virgin olive oils by potential consumers.

Conclusions. The statistical study of sensory attributes and volatiles of virgin olive oil has allowed the following general conclusions to be reached:

(1) MDS has allowed the basic sensory perceptions described by the sensory wheel procedure (Aparicio and Morales, 1995) to be verified.

(2) MDS is an optimal statistical procedure analyzing the inter–intrarelationships between volatiles and sensory attributes, allowing that simple analytical measures can give tentative information about virgin olive oil quality.

(3) Finally, the characterization of different varieties of virgin olive oil agrees with the acceptability of these oils by consumers of this foodstuff.

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