



The quality of EVOOs through the determination of VOCs coupled with SIMCA analysis

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ABSTRACT

Determining the quality of the oil is essential to discriminate EVOOs from oils labeled as such but not having the chemical and physical characteristics to be EVOOs. The purpose of this study was to determine a metric based on multivariate Soft Independent Modeling of Class Analogy (SIMCA), to identify "Premium quality" versus "Standard quality", 792 EVOO samples throughout VOCs and sensory analysis data. The result of SIMCA showed a correct classification of the "Premium quality" samples and only few samples were excluded from the SIMCA model (95.4 % sensitivity). The combination of VOCs collected by PTR-ToF-MS and SIMCA analysis allowed us to perfectly distinguish EVOO oils from non-EVOO oils. The proposed method could allow a secure, quick and reliable control of the EVOO quality within the global market.

1. Introduction

Extra virgin olive oil (EVOO) is a food that, thanks to its high nutritional value, organoleptic and antioxidant properties is widely used by consumers and represents one of the most valuable ingredients of the Mediterranean diet [1]. Since the EVOOs value is very high, international rules have been adopted for the consumer safe, which guarantee the genuineness and purity of the product. Nowadays olive oils characterized by different quality level (EVOO, VOO, Lampante) are available on the global market which are classified by the rules proposed by the International Olive Council (IOC) and EU, based on chemically parameters and on sensory evaluation (SE). Although sensory evaluation is essential and mandatory, this method is time-consuming, involves a limited number of specialized panelists and have many other inconveniences particularly when the panelists judgment come from by different locality [2]. Moreover, since the EVOO organoleptic and sensory characteristics are affected by many factors such as: cultivar, ripening stage, geographical origin, processing systems [3–7], within the EVOO category we find products characterized by flavour, bitter and spicy notes with different level intensity. Therefore, it seems obvious that the rules provided by these supranational institutions, are not enough to avoid fraud and adulterations which are common and represent a serious problem for the EVOO industry [2,8,9]. Thus, since

flavor and off-flavors are linked to volatile organic compounds (VOCs), research has long sought more rapid objective methods [2,10,11] able to help the panelist and to support their judgment, through innovative analytical technologies based on the analysis of volatile compounds.

However, both the sensory evaluation and the analytical methods mentioned above made it possible to split the oil samples into different categories without discriminating the different quality levels within the EVOO category. Indeed, some acceptability studies [12,13] have shown how a little amount of EVOO are identified as "premium quality" by the consumers that are willing to pay a "premium price" compared to the standard quality ones. The IOC has attempted to overcome this limitation by proposing a form for the organoleptic evaluation of quality oils that is not binding for marketing purposes and can be used for granting designation of origin (DO) [14]. In this case the profile sheet only considers descriptors linked to flavors. The (DO) authority shall the maximum and minimum limits of the median for each descriptor included in the profile sheet and it shall establish the limits for the robust coefficient of variation of each descriptor. However, this method also is slow, expensive, time consuming and still too subjective because requires numerous groups of adequately trained panelists [14].

To discriminate in real time oils of higher quality (EVOOs) from those of lower value in order to streamline the sensory procedure and improve its reliability there is a technique that could be a valuable

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support for sensory evaluation, providing a comprehensive overview of the quality level of EVOOs available on the national and international market [2]. This technique is proton transfer reaction time-of-flight mass spectrometry (PTR-ToF-MS provides information in seconds) and is based on soft chemical ionization by proton transfer from hydronium ions [15]. In addition, PTR-ToF-MS does not involve sample preparation or alteration and is a more state-of-the-art technology than other tools for analyzing huge quantities of extra virgin olive oils produced and marketed worldwide. The PTR-ToF-MS technique has been used in conjunction with a statistical modeling framework namely Soft Independent Class Analogy (SIMCA), to classify EVOO and to assess their quality [16]. Moreover, SIMCA analysis has been used (1) to distinguish olive oil from other vegetable oils and to assess its quality category [17, 18]; (2) in conjunction with the HS-SPME-GC-MS method to verify the volatile profile of virgin olive oils [19]. PTR-MS spectrometry is important when there is a need to use rapid instruments for authentication and quality control of oils. This analysis allows the analysis of a complex oil matrix, namely VOCs composed of triacylglycerols (TAGs) and other components such as fatty acids (FA), hydrocarbons, sterols, phenolic compounds or fatty alcohols [20]. As reported by Cecchi et al. [21], SIMCA analysis was successfully used to determine the geographical origin of 65 Arbequina cv samples from three Spanish regions. Ortega-Gavilán et al. [22] used the two-class classification method SIMCA based on the detection of changes in the spectrochromatographic fingerprints of oils to identify adulterations of EVOO. SIMCA successfully identified blends made from virgin olive oils with a greenish hue (high chlorophyll/phytin content). The SIMCA analysis was used by Forina et al. [23] to trace the geographical origin of EVOO from different regions of the Mediterranean (in particular the Liguria region). SIMCA coupled with spectroscopy showed excellent discrimination in the geographical characterization of samples. In particular, samples from Western Liguria showed 100 % sensitivity and specificity.

Therefore, the work aim is to verify the possibility of discriminating, within the commercial class of EVOO, the different levels of organoleptic quality (standard quality and premium quality) of 792 samples of EVOO (obtained during five harvesting campaigns from 2014/15 to 2018/2019), by applying a robust statistical analysis model (SIMCA) to the data obtained from the VOCs analysis collected by PTR-ToF-MS.

2. Materials and methods

2.1. EVOO samples

A total of 792 samples both monocultivar and blend labeled as EVOO and belonging to five consecutive harvest years (from 2014/15 to 2018/2019) were analyzed. Samples were either purchased from large commercial stores or obtained directly from the farm or mill or aged 3/5 years from different cultivars and/or origins. Among the monocultivars, the most representative are Coratina, Koroneiki, Frantoio, Arbequina, Leccino, Carolea and Picual. For each sample, two bottles of 250 or 500 ml were collected and stored rapidly in a climate-controlled room maintained at 17 °C in the dark until the time of analysis. Each sample was analyzed before the expiration date indicated on the label (except for aged oils). For each analysis session, eight different samples of EVOO were taken from the climate chamber and left at room temperature for 60 min and then subjected to sensory evaluation. In parallel, the same samples were subjected to VOC analysis performed by PTR-ToF-MS. This procedure was replicated twice during each VOC analysis session.

2.2. EVOO sensory evaluation (SE)

The SE was performed according to the methods proposed by the IOC on sensory analysis of olive oil [24–27]. The analysis protocol is reported in detail by Taiti et al. [2] with some modifications. In brief, all panel sessions were held at the Department of Agri-food and

Environmental Sciences (DAGRI) of the University of Florence, Italy. In this way, about 160 samples were evaluated for a total of 20 tasting sessions per year. 40 different tasters were recruited from Italy and other countries. Firstly, the samples were classified as “non-defective” and “defective” and subsequently the true (non-defective) EVOO have been divided into two classes: Standard and Premium, respectively.

2.3. PTR-ToF-MS measurements and data analysis

Headspace analysis was performed following the method and instrumental setting previously proposed by Taiti et al. [28]. Each sample (15 g of oil) was placed in a sealed glass jar (3/4 L Bormioli) and analyzed rapidly and without any sample modifications. The higher resolution of PTR-ToF-MS provides a summed formula and tentative identification of each detected mass peak. Data were acquired, recorded and analyzed using TofDaq software (Tofwerk AG, Thun, Switzerland) and were expressed as ppbv. Finally, all VOC data were filtered using a threshold of 0.50 ppbv and removing all signals attributable to water chemistry and/or interfering ions, which were considered difficult to quantify accurately. The filtered data were subjected to statistical analysis.

2.4. Metric scale definition

Soft Independent Modeling of Class Analogy (SIMCA), [16] was used with a single-class modeling approach [29] to determine the quality of 792 EVOO samples on a metric scale. Considering the 792 samples, only 108 (classified as Premium quality by SE) were used to train the SIMCA single class model. SIMCA was computed with V-Parvus 2010 software and represents a set of PCA models (NIPALS algorithm), one for each class in the dataset (one model in this case), after a separate category autoscale. SIMCA performs a cross-validation of the PCA model of each class (training set) by dividing the data (evaluation set) into 3 contiguous groups (cross-validation groups). The efficiency was evaluated through the classification (training set) and prediction (evaluation set) matrices, which report the percentage of correct classification for each class considered. SIMCA also expressed statistical parameters indicating modeling efficiency (e.g., sensitivity, modeling power for each variable). SIMCA squared distances were linearized by converting mean and maximum values to a logarithmic scale and then translating them by adding some value to have all positive values.

The 108 samples classified as “Premium quality” by SE were divided into a 95 % (training set; 103 samples) and a 5 % evaluation set (5 samples). The subdivision of the artificial data sets was chosen optimally with Euclidean distances, based on Kennard and Stone’s algorithm [30] that selects items without a priori knowledge of a regression model (i.e., the assumption is that a flat distribution of data is preferable for a regression model). The remaining 684 samples, classified by SE as “Standard quality” ($N = 263$) and “defective sample” ($N = 421$) were considered as external tests.

The final output of SIMCA is the linearized SIMCA distance squared, considered as a metric scale. Samples with linearized SIMCA distance squared less than the critical distance obtained from the single-class model can be considered “Premium quality”, conversely, with values above the critical distance can be considered as standard quality and defective sample, and the higher the value the worse the quality. The modelling power of each variable, which represents the influence of that variable in the definition of the model [31], was expressed.

3. Results and discussions

Considering the SE, the panel test showed 108 Premium quality, 263 standard quality and 421 defective sample ($N = 792$). In particular, the SE result reported in this paper come from previous work performed on the same samples [2]. A total of 792 oil samples were analyzed over the course of 5 years through SE. Defective oils were considered as

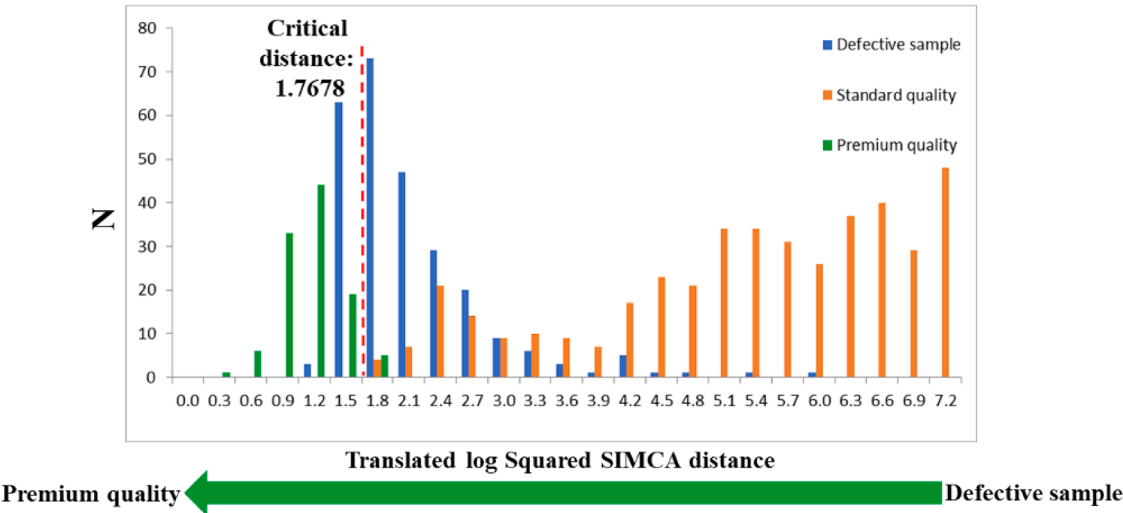


Fig. 1. Soft Independent Modeling of Class Analogy histogram by frequency class of the SIMCA translational log square performed on the spectral dataset and tested on the mean values for each EVOO sample, considering three classes (“Premium quality”, “Standard quality” and “defective sample”). The dashed line represents the critical value (i.e., the model boundary).

Table 1
Results of the Sensory Evaluation for the classification into EVOO quality classes (Premium quality, Standard quality and defective sample); Number of samples accepted by the SIMCA model as Premium quality; percentage of samples included within the SIMCA Premium quality model.

EVOO Samples	SE	N. samples accepted by the SIMCA Premium quality model	% samples included within the SIMCA Premium quality model
Premium quality	108	103	95.4
Standard quality	263	66	25.1
Defective sample	421	0	0

“non-EVOO”, while the others were called true “EVOO”. Thus, although many oils were labelled and sold as EVOO, by applying an independent SE they were not found to be such. In fact, ~53 % of all samples analyzed (421 samples) were found not to be true EVOO, as they had perceivable off-flavours and were identified as defective [2]. On the contrary, among the EVOO samples, 9 were acquired from retail outlets and 361 provided

by mills or farms; of these, 169 (46.4 %) were blended while 201 (50.6 %) were monocultivar samples. Among the EVOO sample, 109 were identified based on their intensity flavor as “Premium” samples. Thus, we found that a large proportion of EVOOs sold worldwide (including top-selling brands) and purchased at different retail outlets do not meet the IOC sensory standards for extra virgin olive oil [2].

The results obtained by the SE [2] have been used in this study to train a SIMCA model to assess the Premium quality class while the other two classes have been used as external test. Fig. 1 shows the SIMCA model applied to the VOCs dataset of the 108 EVOO Premium quality samples and tested on the remaining 263 standard quality and 421 defective EVOO samples.

The SIMCA logarithmic translated critical distance obtained by the model Premium quality was 1.7678. This identifies the boundary between samples belonging to the “Premium quality” class (i.e., values below the critical distance; green histograms) and those belonging to the other classes (blue and orange histograms in Fig. 1). Values below the critical distance are included within the Premium quality model, while those above the critical distance (i.e., rejected by the model) have a lower quality (i.e., the more the distance increases the worse the quality).

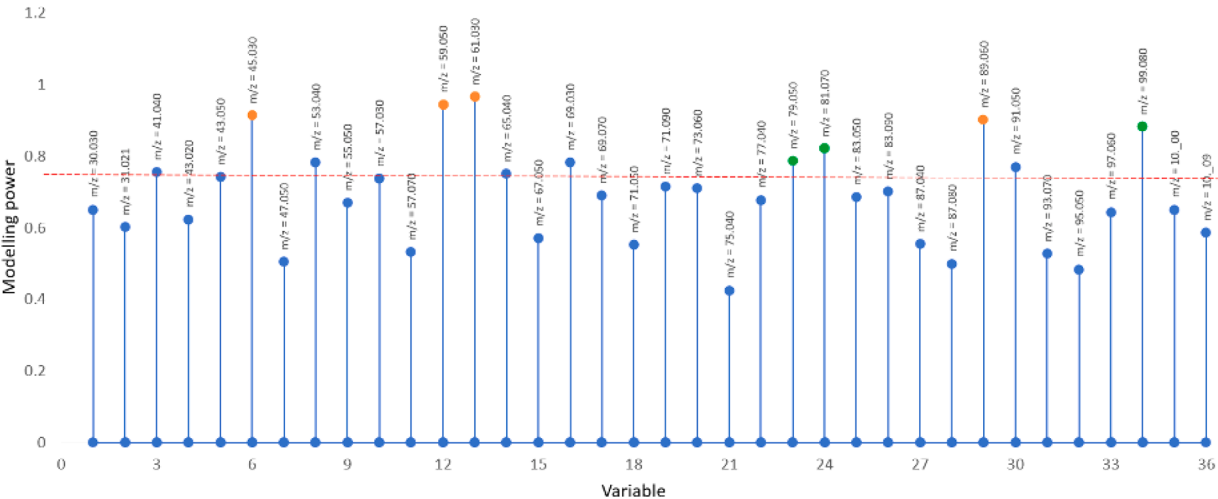


Fig. 2. Modelling power obtained by the SIMCA model used to assess EVOO Premium quality. Red dashed line highlights values > 1.75; the orange points highlight the best defect markers while the green points indicate quality markers as evidenced by Taiti et al. [2].

Only 5 samples out of the 108 EVOO (4.6 %) identified as “Premium quality” by SE, were excluded by the SIMCA model (sensitivity 95.4 %) (Table 1), but with score proximal to the critical distance. However, the error provided by the model here applied could be linked to the non-excellent evaluation obtained by these 5 samples throughout the sensory analysis. Among the Premium oil samples result in the best three oil samples collected from Italian mills. The first sample is an Italian monocultivar oil (Coratina) belonging to the 2017 harvest year and it comes from the Puglia region in Italy. The second sample is an Italian blend oil (Leccino, Frantoio and Moraiolo) belonging to the 2018 season and it comes from Tuscany region in Italy. The third oil sample is a monocultivar oil (San Felice) from the 2017 harvest season and it comes from Umbria, in central Italy. All three EVOO samples have won national and international awards. Regarding Standard samples, 66 out of 263 samples were included by the model (25.1 %). None of the 421 Defective samples were included by the model. Among these last, those with the highest score (i.e., those with the worst quality) were six samples, all purchased from the GDO and all blended. Four samples were from EU countries another 2 were from Italy. Except for 2 samples belonging to the 2017 harvest year, the others belonged to the 2016 harvest year.

The SIMCA logarithmic squared dimensional distance represents a true metric scale in which each sample is placed. It defines the possible quality of the sample and places it in a specific level or range of quality.

Fig. 2 showed the modelling power of the SIMCA model applied to VOCs indicating which masses returned the higher contribute to the Premium quality identification. As shown in Fig. 2, it is evident that the values with higher modelling power are the same as those obtained by Taiti et al. [2] Specifically, those in orange are those defined by Taiti et al. [2] as best defects markers while those in green are indicated as quality markers. Specifically, as reported by Taiti et al. [2] the orange samples i.e., the defective ones showed high values of some compounds (detected at $m/z = 45.033$ (acetaldehyde), $m/z = 59.049$ (acetates), $m/z = 61.028$ (acetic acid) and $m/z = 89.059$ (butanoic acid)) that are linked to rancid, fusty or/and vinegary notes. Indeed, as reported elsewhere [32,33,34] acetaldehyde, acetic acid and butanoic acid are compounds that can be linked to fermentation or oxidation process. On the contrary, the VOCs that have contributed significantly to the classification as “Premium quality” were $m/z = 81.069$ and $m/z = 99.080$, both C6 compounds derived from fatty acid degradation by the LOX pathway [35] which are linked to the EVOO green notes. This result returned an optimal correspondence between the modeling power obtained by the SIMCA model and the PLS-DA VIP scores obtained by Taiti et al. [2] on the same samples, but with the advantage that the SIMCA model is based on a single class (class-modelling approach); [36,37,16] being immediately applicable and easy to be understood to assess premium quality EVOO.

4. Conclusions

Premium extra virgin olive oils (PEVOO) are oils of exceptional quality that are sold at high prices compared to the other EVOO. SIMCA classification model proposed in this study and based on the VOCs fingerprint acquired by the PTR-ToF-MS allows to clearly distinguishing olive oil samples of different organoleptic quality in a very simple and intuitive modality. Although a more extended and representative sampling (i.e., more varieties, more production area etc.) is needed to better evaluate the effectiveness of our model, this classification model could be applied as fast and reliable method to evaluate different quality inside the EVOO production. Our results are in line with the olive oil sector demands that requires analytical tools to support or integrate the Panel Test. In this we analyzed EVOO samples by SIMCA technique. Generally, SIMCA analysis with respect to machine learning techniques is a statistical classification approach that allows the handling of data consisting of categories of different sizes. In fact, with SIMCA, each category can be treated separately and independently. Furthermore, unlike

discriminant techniques, SIMCA gives information on the similarities between the samples belonging to the single category instead of the differences distinguishing the categories from one another.

CRedit authorship contribution statement

Simona Violino: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Methodology, Formal analysis, Data curation, Conceptualization. **Cosimo Taiti:** Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Data curation. **Elettra Marone:** Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Data curation. **Corrado Costa:** Writing – review & editing, Writing – original draft, Visualization, Supervision, Resources, Project administration, Formal analysis, Data curation, Conceptualization. **Stefano Mancuso:** Visualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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