Food Chemistry 522 (2026) 150065

Contents lists available at ScienceDirect

Food Chemistry

journal homepage: www.elsevier.com/locate/foodchem

Application of Flash GC and linear and non-linear chemometric techniques as a rapid screening tool to discriminate monovarietal *Grappa* distillates

Silvia Arduini [a,*], Chiara Cevoli [b,c], Enrico Valli [b,c], Alessandra Bendini [b,c], Fabio Chinnici [a,c]

[a] Department of Agricultural and Food Sciences, Alma Mater Studiorum-University of Bologna, Viale Fanin 40, 40127 Bologna, Italy
[b] Department of Agricultural and Food Science, Alma Mater Studiorum- University of Bologna, Piazza Goidanich 60, 47521 Cesena, Italy
[c] Interdepartmental Center for Agri-Food Industrial Research (Ciri-Agro), Via Quinto Bucci 336, 47521 Cesena, Italy

ARTICLE INFO

Keywords:
Monovarietal *Grappa*
Geographical indication
Volatile fingerprint
Grape variety discrimination
Flash gas chromatography (Flash GC)
Partial least squares-discriminant analysis (PLS-DA)
Support vector machine (SVM)

ABSTRACT

Grappa is a traditional Italian grape marc spirit protected by geographical indication. Monovarietal *Grappa,* from a single grape variety, exhibits distinctive compositional and sensory characteristics linked to the selected raw materials, including denominations such as *Grappa di Barolo*. Rapid screening methods are essential for product authentication. This study analyzed the volatile fingerprints of 45 *Grappa* samples from four grape varieties (Muscat, Prosecco, Barolo, Brunello) using Flash GC. Multivariate linear (PCA and PLS-DA) and non-linear (C-SVM) techniques were applied to different data representations including full chromatographic profiles, selected chromatographic regions and peak-area data to determine which representation offered the highest discriminant power. Comparable classification results were obtained using both PLS-DA and SVM models, reporting overall accuracy ranging from 77.8 to 84.1% in cross-validation. Tentative identification of discriminating compounds was also performed. The results suggest the potential of Flash GC and chemometrics as a rapid screening tool to discriminate monovarietal *Grappa*.

1. Introduction

The Geographical Indication (GI) *Grappa* is a traditional Italian spirit with deep cultural and historical roots, widely recognized both nationally and internationally for its unique production process, strong territorial identity, and significance in Italian gastronomy and heritage. It is obtained from the distillation of grape pomace, a by-product of vinification, derived from grapes grown and vinified in Italy, with all distillation and processing carried out within the national territory, as established by its official product specification (Ministero delle politiche agricole, alimentari e forestali, 2016; The European Parliament and the Council of the European Union, 2019).

The *Grappa* aroma profile typically reflects a complex interplay of hundreds of volatile compounds generated throughout the various stages of its production process. Beyond the key role of fermentation-derived aroma compounds, such as higher alcohols, volatile esters, acids, and aldehydes, the distinctive aroma of the distillate is also influenced by varietal compounds originally present in the grapes (Diéguez et al., 2003; Lukić et al., 2010). When all stages of production are carefully managed, these grape-derived aromatic compounds can be effectively carried over into the final distillate, contributing to the specific sensory profile associated with the grape variety used (Battistutta et al., 1995; Lukić et al., 2010). This aspect is particularly relevant in the case of monovarietal *Grappa*, where the expression of varietal aroma is essential to define the product identity. One notable example is *Grappa di Barolo*, which carries GI status and is obtained exclusively from cv Nebbiolo pomace used to produce Barolo wine. The growing interest in such products is driven by their potential to reflect the distinctive sensory characteristics of the grape variety and terroir. Consequently, verifying the authenticity of monovarietal *Grappa* has become increasingly important, not only for regulatory compliance and quality assurance, but also to safeguard market value and consumer confidence. Despite this growing interest, studies on *Grappa* authentication are very limited. Most have focused on its differentiation from other distilled spirits (Arduini et al., 2021; Giannetti et al., 2019), while the aromatic composition of monovarietal *Grappa* has received comparatively little attention. Some studies have been performed to differentiate *Grappa* samples obtained from various grape varieties. Examples include Cabernet Sauvignon, Ribolla, Picolit, Verduzzo, Sauvignon, Zibibbo di Pantelleria, Traminer, and Refosco (Di Stefano & Borsa, 2006), Müller

* Corresponding author.
E-mail addresses: silvia.arduini2@unibo.it (S. Arduini), chiara.cevoli3@unibo.it (C. Cevoli), enrico.valli4@unibo.it (E. Valli), alessandra.bendini@unibo.it (A. Bendini), fabio.chinnici@unibo.it (F. Chinnici).

https://doi.org/10.1016/j.foodchem.2026.150065
Received 22 December 2025; Received in revised form 3 April 2026; Accepted 12 June 2026
Available online 13 June 2026

Thurgau, Yellow Muscat, Gewürztraminer, and Rose Muscat (Versini et al., 1994) or Nebbiolo, Barbera, and Muscat (Borsa et al., 2008), based on their varietal aroma composition. However, these studies were mostly carried out using analytical methods such as gas chromatography–mass spectrometry (GC–MS), which, although highly accurate and widely used, present a major limitation due to their time-consuming nature, particularly when dealing with large numbers of samples or requiring rapid screening (Arduini & Chinnici, 2024). In this context, there is a growing demand for faster and high-throughput analytical techniques that can provide reliable results in shorter timeframes (Chen et al., 2025). To date, no studies have reported the use of rapid analytical techniques for the varietal discrimination of *Grappa* or, more generally, grape marc distillates.

In the food sector, a significant amount of research has been published on the application of Flash GC combined with chemometrics for the rapid authentication of various parameters, including geographical origin (Cheng et al., 2013; Melucci et al., 2016; Yu et al., 2022), botanical origin (Gan et al., 2016; Wu et al., 2022) and quality grade (Barbieri et al., 2020) in different food matrices. Regarding the spirits sector, studies applying Flash GC remain very limited, and have focused on cocoa liquors, plum distillates, and grain distillates, mainly addressing classification parameters such as geographical provenance or botanical origin (Rottiers et al., 2019; Śliwińska et al., 2016; Wiśniewska et al., 2016). To the best of our knowledge, this technique has not yet been applied to *Grappa* or, more generally, to grape marc distillates, nor has it been used to investigate differences at the grape cultivar level in these highly processed matrices. This is particularly relevant considering that the extent to which varietal signatures persist after distillation remains poorly understood.

One of the main advantages of this technique is its rapid analysis time (approximately 200 s) combined with minimal sample preparation. Furthermore, developed classification models can be easily transferred across laboratories and industries (Barbieri et al., 2020). Nevertheless, some limitations of Flash GC should be considered when comparing it with conventional GC–MS. In particular, it provides lower chromatographic resolution, which may limit the separation of co-eluting analytes, and compound identification is generally tentative (Level 3), as it only relies on retention indices and database matching, without mass spectral confirmation.

Based on the above considerations, this study aims to evaluate the effectiveness of Flash GC combined with chemometric analysis as a rapid screening tool for differentiating monovarietal *Grappa* produced in four renowned Italian geographical indications, Barolo (cv. Nebbiolo), Brunello (cv. Sangiovese), Muscat, and Prosecco (cv. Glera). A non-targeted fingerprinting approach was employed, in which the chromatographic signal was treated as a multivariate dataset for the classification of monovarietal *Grappa* samples according to their varietal origin. Principal Component Analysis (PCA) was applied for exploratory data analysis and pattern recognition, while Partial Least Squares Discriminant Analysis (PLS-DA) and Support Vector Machine (SVM) were used for linear and non-linear classification. To evaluate the impact of different data representations on discrimination performance, classification models were developed using either full chromatograms or peak-area data. Moreover, PLS-DA was applied to selected chromatographic regions identified based on variable importance in projection (VIP) scores. Tentative identification of the key discriminating volatile compounds was also carried out, based on experimental linear retention indices and comparison with relevant databases and literature.

2. Materials and methods

2.1. Grappa samples

A total of 45 monovarietal *Grappa* samples were analyzed, comprising four types from the main production regions: 13 Muscat samples (Piemonte, Veneto, Toscana and Trentino-Alto Adige); 11 Prosecco samples (Veneto, Trentino-Alto Adige and Friuli Venezia Giulia); 11 Barolo samples (Piemonte and Lombardia); and 10 Brunello samples (Toscana). All samples were unaged, produced in 2024, and sourced from multiple distilleries to reflect variability encountered in real-world production. Thirty-three samples were provided directly by the producers through the National Association of Industrial Distillers of Alcohol and Spirits (AssoDistil, Rome, Italy). Distillates were stored in stainless steel tanks and sampled at the production site prior to delivery. Eight additional samples were supplied by the producing distilleries upon request, and four were purchased from store shelves based on commercial availability. All bottles were original, unopened, and labelled as certified monovarietal *Grappa* at the time of acquisition.

Upon receipt, bottles were stored under controlled laboratory conditions (dark environment, 18–20 °C) until analysis.

2.2. Sample preparation and analysis

Sample preparation was performed immediately after bottle opening. One millilitre of each *Grappa* sample was transferred directly into a vial and diluted to a final volume of 3 mL with ultrapure water, without any chemical pre-treatment. Two vials per sample were prepared to allow duplicate analysis. Each vial was sealed with a magnetic airtight cap and placed in the instrument's sample holder for analysis.

Chromatographic analysis was carried out using a Heracles II Flash Gas Chromatograph (Alpha MOS, Toulouse, France), an integrated system combining an automatic headspace sampler, a dual-column gas chromatographic module, and a thermal desorption unit. The instrument is equipped with two columns connected in parallel: a non-polar MXT-5 column and a slightly polar MXT-1701 column (both 10 m × 0.18 mm ID). Each column is coupled to an independent flame ionization detector (FID), enabling simultaneous detection of eluted compounds. Prior to injection, sample vials were incubated at 40 °C for 20 min under agitation (500 rpm) to promote the accumulation of volatile compounds in the headspace. A 5 mL headspace aliquot was then adsorbed onto an internal Carbowax trap at 40 °C for 60 s. The trap was subsequently heated to 240 °C for 93 s to thermally desorb the volatiles and inject them into the chromatographic columns. Hydrogen was used as the carrier gas throughout the analysis.

The oven temperature program was as follows: an initial temperature of 40 °C held for 2 s, ramped to 80 °C at 1 °C/s, then increased to 250 °C at 3 °C/s and held for 101 s, resulting in a total runtime of 200 s.

2.3. Volatile compounds tentative identification

A standard mixture of *n*-alkanes (C6–C16) was injected under the same chromatographic conditions as the samples to calculate the experimental Linear Retention Indices (LRI) for each detected peak. Tentative identification of volatile compounds was then based on AroChemBase (Heracles software, Alpha M.O·S, Toulouse, France), NIST, and Flavornet (Arn & Acree, 1998) LRI databases as well as published literature.

2.4. Data analysis

Preliminary tests showed that chromatograms obtained from the MXT-5 column exhibited a higher discriminant power than those obtained from the MXT-1701 column. Therefore, all subsequent classification models were developed using data from the MXT-5 column only.

A non-targeted chemometric approach was adopted, in which classification models were developed using either the full chromatograms, selected chromatographic sections, or peak area data. The use of full chromatograms offers several advantages, as it minimizes errors associated with peak integration and avoids the risk of discarding potentially relevant information when pre-selection is applied (Melucci et al., 2016). However, models were also built using integrated peak areas to assess whether this approach could improve the discrimination

performance.

Before chemometric analysis, the chromatograms were aligned using the Correlation Optimized Warping (COW) algorithm (Tomasi et al., 2004) and pre-processed using Pareto-scaling. Pareto-scaling was preferred over standard auto-scaling because it provides a balance between emphasizing all variables and preventing excessive amplification of minor noisy signals, which could otherwise obscure relevant information (Aliakbarzadeh et al., 2016). In addition, this pre-processing method preserves the overall chromatographic profile (van den Berg et al., 2006). In Pareto-scaling, the square root of the standard deviation is used as a scaling factor, according to the following equation:

$$\widetilde{x}_{ij} = \frac{x_{ij} - \overline{x_i}}{\sqrt{SD_i}} \quad (1)$$

where x_{ij} and $\widetilde{x}_{ij}$ represent the raw and scaled data, respectively. The mean ($\overline{x_i}$) and standard deviation (SD_i) are calculated as:

$$\overline{x_i} = \frac{1}{J}\sum_{j=1}^{J} x_{ij} \quad (2)$$

$$SD_i = \sqrt{\frac{\sum_{j=1}^{J}\left(x_{ij} - \overline{x_i}\right)^2}{J-1}} \quad (3)$$

Principal Component Analysis (PCA) was first performed on all replicates to identify potential outliers and to visualize the natural clustering of samples. Subsequently, two different classification strategies were applied to discriminate samples according to monovarietal *Grappa* distillates (Muscat, Prosecco, Barolo, and Brunello): Partial Least Squares Discriminant Analysis (PLS-DA), a linear method, and Support Vector Machine (SVM), a non-linear approach. In both cases, the analysis was carried out using data averaged across the two replicates.

2.4.1. PLS-DA

PLS-DA was then applied on averaged data to differentiate monovarietal *Grappa* distillates (Muscat, Prosecco, Barolo, and Brunello). Given the limited number of samples (45), PLS-DA model validation was carried out using the Venetian blinds cross-validation method (5 segments). To prevent model overfitting, the optimal number of latent variables (LVs) was determined by identifying the global minimum of the Root Mean Square Error in Cross-Validation (RMSECV). Model robustness and statistical significance were further assessed through permutation testing, which evaluates whether the obtained model performs significantly better than models built under identical conditions using randomly permuted class labels.

To refine the PLS-DA models developed from the full chromatograms, a variable selection procedure was applied using the Variable Importance in Projection (VIP) criterion. In multivariate modeling, a large proportion of the variables may carry little relevant information for class discrimination, often representing background noise or redundant chromatographic regions. Eliminating such variables can simplify the model structure without compromising, and in some cases even enhancing, its predictive performance.

Selecting the most influential variables helps improve both model accuracy and interpretability, by focusing on the subset of predictors that contribute most significantly to the model response (Farrés et al., 2015). Among the various strategies for variable reduction, the VIP-based approach is particularly suitable for PLS-DA, as it quantifies the overall contribution of each predictor to the model. VIP scores are computed as a weighted sum of squares of the PLS weights, adjusted for the amount of Y-variance explained by each latent variable.

The VIP score for variable j is given by:

$$\mathrm{VIP_j} = \sqrt{\frac{\sum_{f=1}^{F} w_{jf}^2 \bullet \mathrm{SSY_f} \bullet J}{\mathrm{SSY_{tot}} \bullet F}} \quad (4)$$

where w_{jf} is the weight of the j-th variable in the f-th component, SSY_f is the portion of Y-variance explained by component f, J is the number of X-variables, SSY_{tot} is the total Y-variance explained, and F is the number of latent components. Variables with VIP values greater than 1 were considered relevant for class discrimination. Based on this criterion, refined PLS-DA models were reconstructed using only the selected variables.

The data analyses were conducted using PLS Toolbox for Matlab2023a®.

2.4.2. SVM

Support Vector Machine (SVM) was applied as a non-linear classification approach to discriminate among monovarietal *Grappa* distillates (Muscat, Prosecco, Barolo, and Brunello). To ensure consistency with the PLS-DA modeling strategy, SVM models were developed using data averaged across replicates and validated using a 5-fold cross-validation procedure.

A C-Support Vector Classification (C-SVC) framework was adopted, with the box constraint parameter (C) set to 1. Preliminary tests were carried out using different values of the box constraint parameter. Although a slightly higher classification accuracy was obtained with C = 10, the improvement corresponded to only one additional correctly classified sample compared to C = 1. Therefore, C = 1 was retained as a more conservative choice to reduce model complexity and limit the risk of overfitting. Classification was performed using a one-vs-one scheme, in which binary classifiers were constructed for all pairwise class combinations. Two polynomial kernel functions were evaluated, quadratic and cubic kernels, to account for potential non-linear relationships in the data.

Prior to modeling, peak area data were standardized to ensure that all variables contributed equally to the model, preventing variables with larger magnitudes from dominating the classification process.

SVM models were implemented using the Classification Learner app in MATLAB (R2023a®), with kernel scale set to automatic. In this setting, the kernel scale is determined using a heuristic procedure based on subsampling; therefore, a fixed random number seed was set to ensure reproducibility of the results.

3. Results and discussion

All chromatograms, grouped according to the monovarietal *Grappa* distillates (Barol = BA, Brunello = BR, Muscat = MU, and Prosecco = PR), are presented in Fig. S1 (Supplementary material). The main peaks are located in the initial section of the chromatogram, with retention times between 18 and 130 s. As expected, the volatile profiles of the four *Grappa* types differ markedly in both overall shape and number of peaks. Clear variations are also evident in peak intensities, confirming the discriminating capability of the volatile profile with respect to the monovarietal origin. Based on the chromatographic data, the areas corresponding to peaks shared among all *Grappa* samples were extracted and used for subsequent chemometric evaluation.

3.1. PCA exploratory analysis

PCA was first performed on the full chromatographic data (retention time between 18 and 130 s) to identify possible outliers and to visualize the natural clustering among samples (Pareto scaling pretreatment). The analysis was carried out using 11,200 X-variables corresponding to the data points of the chromatograms. Fig. 1 shows the score plots for PC1 vs. PC2 and PC1 vs. PC3, which together account for more than 64% of the total variance, indicating a satisfactory level of data representation considering the high dimensionality of the dataset. Two samples, along with their respective replicates (43–44 and 85–86), are positioned outside the 95% confidence limit in the score plots and can therefore be considered as outliers. Along the PC1 axis, a clear separation can be

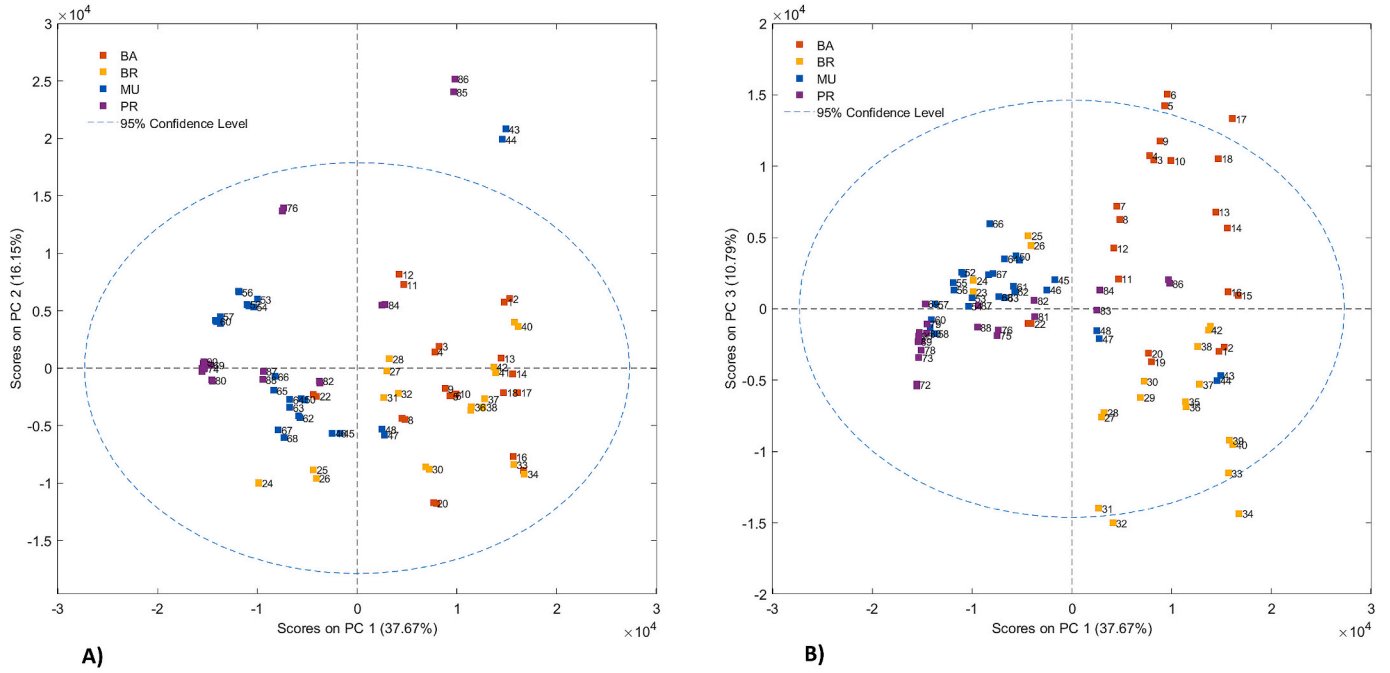

Fig. 1. Score plots for PC1 vs. PC2 (A) and PC1 vs. PC3 (B) obtained from PCA performed on the full chromatographic dataset. BA = Barolo; BR = Brunello; MU = Muscat; PR = Prosecco.

observed between BA and BR samples (positive PC1 scores) and MU and PR samples (negative PC1 scores). Examination of PC3 further highlights a distinction between BA (positive PC3 scores) and BR (negative PC3 scores), while the other samples are grouped near the y-axis, showing scores close to zero. The analysis of the x-loading plots (Fig. 2) indicates that the samples located in the first and fourth quadrants (BA and BR, showing positive PC1 values) are associated with higher intensities of chromatographic peaks around 35, 50, 97, and 110 s compared to MU and PR. The differentiation between BR and BA is mainly described by PC3: BR samples show higher values for the peak at 50 s, whereas BA samples are associated with higher intensities for peaks around 35 and 70 s.

A similar approach was employed using the data derived from the integration of the selected peak areas (22 peaks as a total), with the aim of assessing whether this dataset would yield results consistent with those obtained from the full chromatograms. PCA was performed after applying Pareto scaling and mean-centering as pre-processing methods. The resulting score plots for PC1 vs. PC2 and PC1 vs. PC3 are shown in Fig. 3, explaining a total variance of 73.8%. The clustering pattern observed is comparable to that obtained from the PCA based on the full chromatograms, but no distinct outliers are evident in this case. This difference likely arises from the complexity of the full chromatogram data: the high-dimensional signal may capture subtle variations that locate some samples outside the confidence ellipse, identifying them as statistical outliers, probably as a consequence of discrete specificities in their volatile profile. When, selected peak areas are used to carry out the same pre-processing and PCA statistical evaluation, the reduced dimensionality and variability may mask these differences, so such samples are less likely to be flagged as outliers. Examination of the x-loading plots (Fig. 4) was then carried out to identify which peak areas

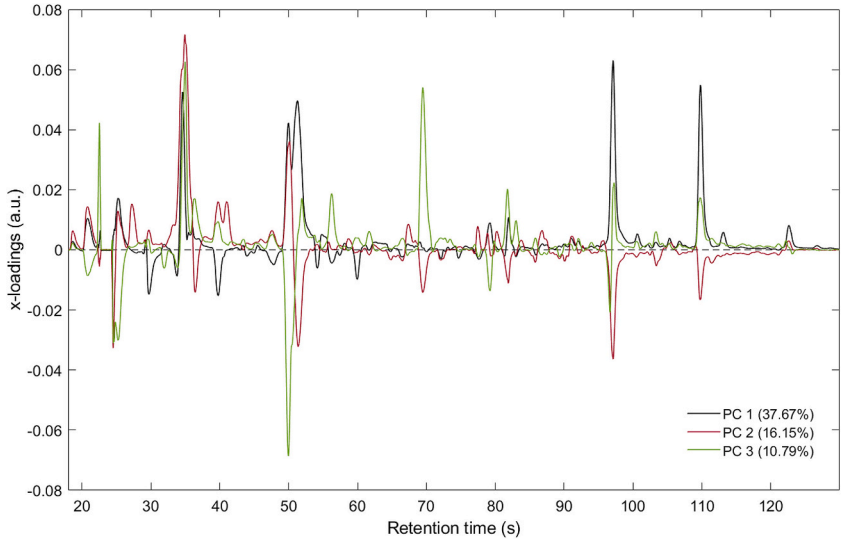

Fig. 2. X-loading plots obtained from PCA performed on the full chromatographic dataset.

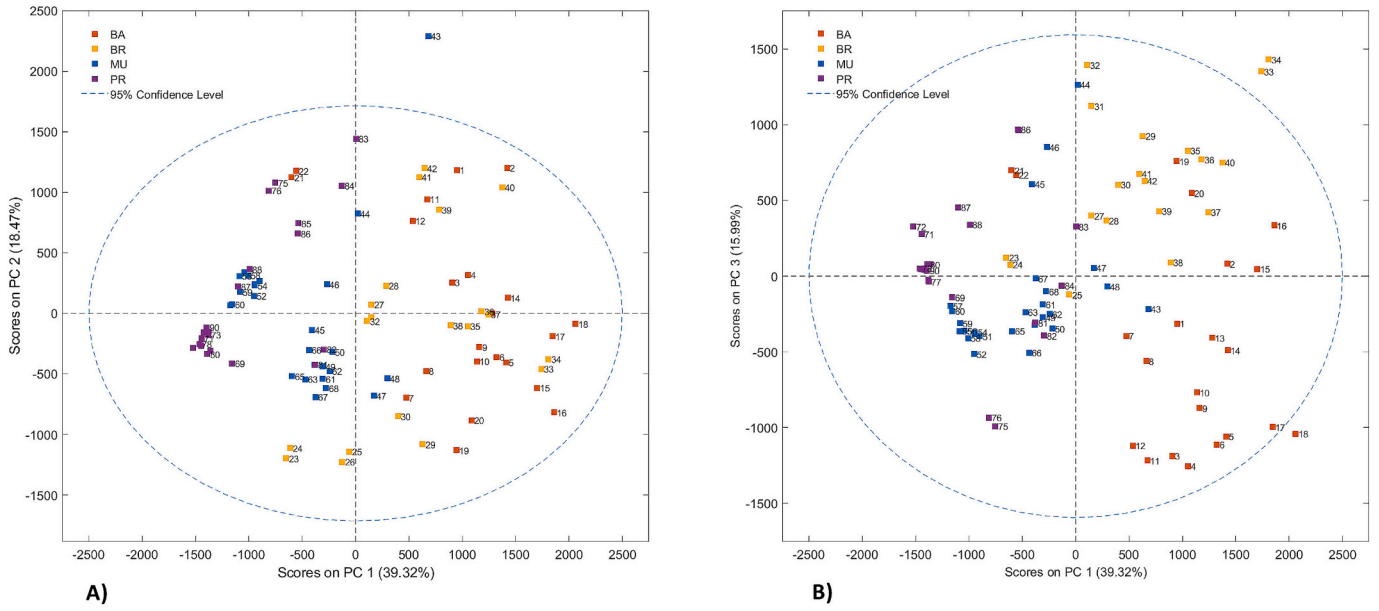

Fig. 3. Score plots for PC1 vs. PC2 (A) and PC1 vs. PC3 (B) obtained from PCA applied to the dataset derived from the integration of 22 selected peak areas. BA = Barolo; BR = Brunello; MU = Muscat; PR = Prosecco.

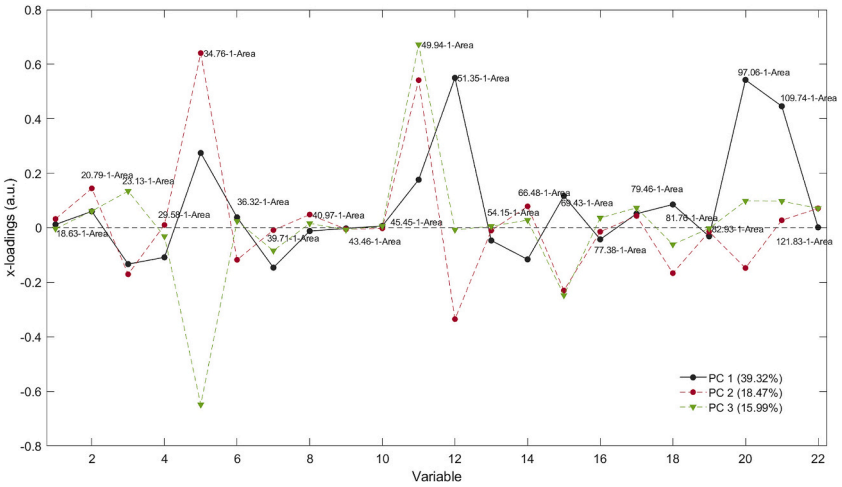

Fig. 4. X-loading plots obtained from PCA performed on the dataset derived from the integration of 22 selected peak areas.

contributed most to the observed discrimination among the samples. The plot indicates that the areas most influential in the discrimination between BA and BR versus MU and PR along PC1 are associated with retention times around 35, 51, 97, and 110 s. The separation between BA and BR along PC3 is mainly driven by the areas at approximately 35, 50, and 70 s. Overall, these results are in very good agreement with those obtained from the PCA of the full chromatograms.

3.2. PLS-DA models

PLS-DA model with four classes were developed using the chromatographic data (*Pareto scaling*) obtained from the first GC column, and their performance was evaluated through cross-validation.

The optimal number of latent variables (LVs) (8) was determined by identifying the global minimum of the RMSECV, as reported in Fig. S2 (Supplementary material). Sample classification was performed by applying the *most probable* decision rule in which each observation is assigned to the class corresponding to the highest probability value (*Bayes rule*) among the four one-vs-rest models. This criterion ensures a consistent evaluation of class membership, regardless of the absolute magnitude of the predicted responses, and allows the overall classification performance to be derived from the four individual models. The confusion matrix from cross-validation is shown in Fig. 5A. To provide a comprehensive assessment of model performance, the statistical metrics derived from the confusion matrix are summarized in Table 1. These include true positive rate (TPR), false positive rate (FPR), true negative rate (TNR), false negative rate (FNR), precision (P), and F1-score (Brown et al., 2020). TPR values ranged from 0.73 to 1.00 with PR and BA showing the lowest values. The classification results demonstrated overall good performance (overall accuracy = 80%), as confirmed by the predominance of correct predictions along the diagonal of the confusion matrix and the generally high values of recall and F1-score across most classes. In particular, the model achieved near-perfect performance for one class, indicating well-separated feature representations. However, performance was not uniform across all categories. The class PR exhibited the weakest performance, as reflected by its lower precision (0.62) and F1-score (0.67), as well as a relatively higher false positive rate. Moreover, the misclassification pattern was not uniformly

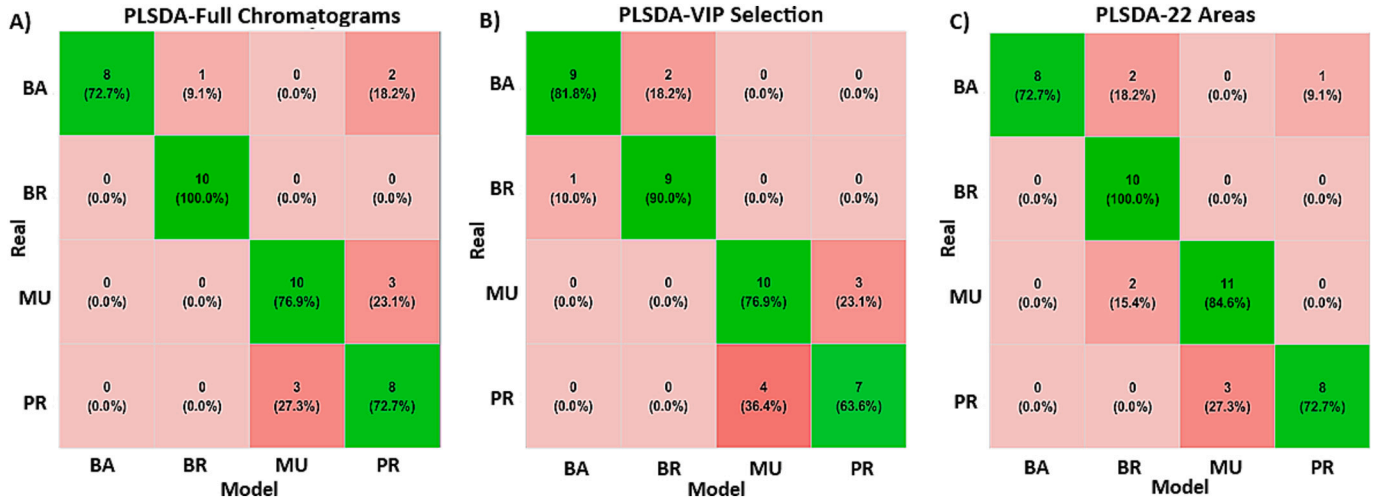

Fig. 5. PLS-DA confusion matrices for models based on (A) full chromatograms, (B) VIP-selected variables, and (C) 22 peak areas.

Table 1
PLS-DA models performance in cross-validation (CV).

		TPR	*FPR*	*TNR*	*FNR*	*Precision*	*F1*
Chromatograms							
(8 LVs)	BA	0.73	0.00	1.00	0.27	1.00	0.84
	BR	1.00	0.03	0.97	0.00	0.91	0.95
	MU	0.77	0.09	0.91	0.23	0.77	0.77
	PR	0.73	0.15	0.85	0.27	0.62	0.67
	Overall accuracy	*80.0%*					
VIP selection							
(8 LVs)	BA	0.82	0.03	0.97	0.18	0.90	0.86
	BR	0.90	0.06	0.94	0.10	0.82	0.86
	MU	0.77	0.13	0.88	0.23	0.71	0.74
	PR	0.64	0.09	0.91	0.36	0.70	0.67
	Overall accuracy	*77.8%*					
22 Areas							
(6 LVs)	BA	0.73	0.00	1.00	0.27	1.00	0.84
	BR	1.00	0.11	0.89	0.00	0.71	0.83
	MU	0.85	0.09	0.91	0.15	0.79	0.81
	PR	0.73	0.03	0.97	0.27	0.89	0.80
	Overall accuracy	*82.2%*					

BA = Barolo; BR = Brunello; MU = Muscat; PR = Prosecco. TPR = true positive rate; FPR = false positive rate; TNR = true negative rate; FNR = false negative rate;. LVs = Latent Variables.

distributed, but was predominantly concentrated between specific classes. In particular, a pronounced confusion was observed between MU and PR, as evidenced by their reciprocal misclassification in the confusion matrix. This behaviour is consistent with the preliminary PCA analysis, which indicated a partial overlap between these two classes in the feature space, thus confirming their reduced separability.

Variable selection was then performed using the VIP criterion, and new PLS-DA models were subsequently developed based on the reduced set of variables. Applying the threshold VIP ≥ 1 (Fig. S3, Supplementary material), resulted in the selection of 2951 data points out of the initial 13,000 chromatographic points thus retaining only the most informative regions of the chromatogram for class discrimination. When examining the VIP profiles calculated separately for each class PLS-DA (BA, BR, MU and PR), the overall shape of the curves appears remarkably similar across classes. However, the absolute VIP values differ noticeably, indicating that each class is primarily characterized by different chromatographic peaks. This confirms that, although the informative regions occur in comparable retention-time intervals, the variables contributing most to class discrimination are not the same for all classes. The performance of the PLS-DA models (8 LVs, Fig. S2 of the Supplementary material) built on the VIP-selected variables was evaluated following the same multi-class decision strategy used for the full chromatogram analysis, and the results are summarized in Fig. 5B (confusion matrix) and Table 1.

The VIP-based model, while slightly reducing the overall accuracy (77.8%), led to class-specific variations. In particular, the BA class benefited from variable selection, with an increase in correct classification (TPR increased from 0.73 to 0.82 and F1 from 0.84 to 0.86), and a complete removal of misclassification toward PR, suggesting that variable selection could enhance the discriminative power for this category. However, this improvement comes at the expense of other classes. The most critical behaviour was observed for the PR class, where the recall (TPR) decreased (from 0.73 to 0.64) and the false negative rate increased, confirming that this class remains the most challenging to model. Despite a slight improvement in precision, the overall F1-score remained unchanged, indicating that VIP selection does not effectively improve its classification.

These results suggest that, while VIP-based variable selection can simplify the model and improve class-specific performance (e.g., BA), the full chromatographic dataset retains a higher and more stable discriminative capability, particularly for classes characterized by subtle differences. This behaviour is consistent with the previously observed overlap between MU and PR, where reducing the feature space may further limit class separability.

Finally, the PLS-DA models (6 LVs, Fig. S2 of the Supplementary material) were developed using the 22 selected peak areas, and their performance was assessed following the same procedure adopted for the chromatogram-based models. The confusion matrix is shown in Fig. 5C, while the statistical metrics are reported in Table 1.

The PLS-DA model developed using peak areas (22 variables) showed overall comparable performance to the model based on the full chromatographic profiles, with a similar accuracy (82.2%). The classification remained well balanced across classes, with improved performance for the PR class (F1 = 0.80), indicating a better discrimination compared to the chromatogram-based model. In contrast to the full model, where a reciprocal confusion between MU and PR was observed, the peak-based model reduced this overlap, with PR samples misclassified only as MU. Conversely, MU misclassifications were mainly directed toward BR, indicating a shift in class boundaries.

The BR class remained perfectly classified (100%), confirming that the reduced representation preserves the key discriminative information for this category.

The use of peak area selection may reduce the contribution of highly specific chromatographic features associated with certain classes, potentially affecting class-specific discrimination. At the same time, it may reduce non-discriminative or redundant variability present in the full chromatographic profiles, which could contribute to improved class separation for some categories.

To further verify the reliability of the PLS-DA models and ensure that the observed class separations were not the result of random chance, permutation tests were carried out for all models developed in this study (full chromatograms, VIP-selected variables, and peak areas). These tests evaluate whether the predictive performance of the original model is significantly better than that obtained after randomly shuffling the class labels (y-block). Three complementary statistical procedures were applied: the pairwise Wilcoxon signed-rank test, the pairwise sign test, and the randomization *t*-test. All PLS-DA models produced *p*-values below 0.05 for the three tests (cross-validation), confirming their statistical significance at the 95% confidence level. These results demonstrate that the discriminant structures identified by the models are not artifactually generated by random data arrangement but reflect genuine and reproducible differences among the monovarietal *Grappa* samples.

3.3. SVM models

SVM models based on a C-Support Vector Classification (C-SVC) approach with a cubic kernel were evaluated, as they provided the best performance among the tested configurations. The corresponding performance metrics are reported in Table 2, while the confusion matrices are shown in Fig. 6. The model based on full chromatographic profiles achieved an overall accuracy of 84.1%, with well-balanced performance across all classes. In particular, the BR class was perfectly classified (F1 = 1.00), while BA also showed high classification performance (TPR = 0.90, F1 = 0.90). The MU class exhibited good performance (F1 = 0.80), although some misclassification toward PR was observed. The PR class remained the most challenging, with lower precision (0.67) and F1-score (0.69), mainly due to confusion with MU. When the model was built using peak areas (22 variables), a slight reduction in overall accuracy was observed (80.0%), while maintaining comparable performance across classes. BA and PR showed similar F1-scores (0.84 and 0.80, respectively), whereas BR exhibited a decrease in precision and F1-score (0.78). The MU class maintained stable performance (F1 = 0.79).

Regarding the misclassification patterns, the chromatogram-based model showed errors mainly involving MU and PR samples, while in the peak-based model MU samples were more frequently misclassified as BR, and PR samples as MU.

3.4. PLS-DA vs SVM

A comparison between PLS-DA and SVM models highlighted a high degree of consistency in both classification performance and misclassification patterns, regardless of the data representation used. In both approaches, comparable results were obtained when using either full chromatographic profiles or peak area data. When full chromatographic data were used, both models showed a misclassification pattern mainly involving PR and MU samples, indicating a stable overlap between these classes. Conversely, when peak area representation was adopted, the misclassification pattern changed similarly in both models, with MU samples more frequently misclassified as BR and PR samples as MU.

Notably, several misclassified samples were shared between the two models, confirming that classification errors are not model-dependent but rather related to intrinsic similarities among samples. This is further supported by the PCA results, where these samples are located in overlapping regions of the score plots, indicating limited separability in the feature space. For example, the BA sample misclassified as PR by all models (replicates 21 and 22) was clearly separated from the main BA cluster and positioned closer to the PR region, explaining the observed classification behaviours. These findings demonstrate that the classification behaviours are mainly driven by the data representation and underlying class overlap, rather than by the choice of the classification algorithm.

3.5. Tentative compound identification

To obtain a preliminary evaluation of the compounds present in the samples, the main chromatographic peaks were subjected to tentative identification. Putative compound assignments are reported in Table 3 and were obtained by comparing LRI with multiple reference sources, including AroChemBase, NIST, Flavornet, and relevant literature data. According to the Metabolomics Standards Initiative (Sumner et al., 2007), these assignments are classified as Level 3 (putatively characterized compounds), as they are based exclusively on retention behaviour and database matching, without mass-spectral confirmation.

It is worth noting that a similar level-3 identification strategy has already been applied in previous studies using Flash GC, including the tentative identification of predominant volatile compounds in cocoa-

Table 2
SVM models performance in cross-validation (CV).

		TPR	*FPR*	*TNR*	*FNR*	*Precision*	*F1*
Chromatograms	BA	0.90	0.03	0.97	0.10	0.91	0.90
	BR	1.00	0.00	1.00	0.00	1.00	1.00
	MU	0.77	0.06	0.94	0.23	0.83	0.80
	PR	0.73	0.12	0.88	0.27	0.67	0.69
	Overall accuracy	*84.1%*					
22 Areas	BA	0.73	0.00	1.00	0.27	1.00	0.84
	BR	0.90	0.11	0.89	0.10	0.69	0.78
	MU	0.85	0.13	0.87	0.15	0.73	0.79
	PR	0.73	0.03	0.97	0.27	0.89	0.80
	Overall accuracy	*80.0%*					

BA = Barolo; BR = Brunello; MU = Muscat; PR = Prosecco. TPR = true positive rate; FPR = false positive rate; TNR = true negative rate; FNR = false negative rate.

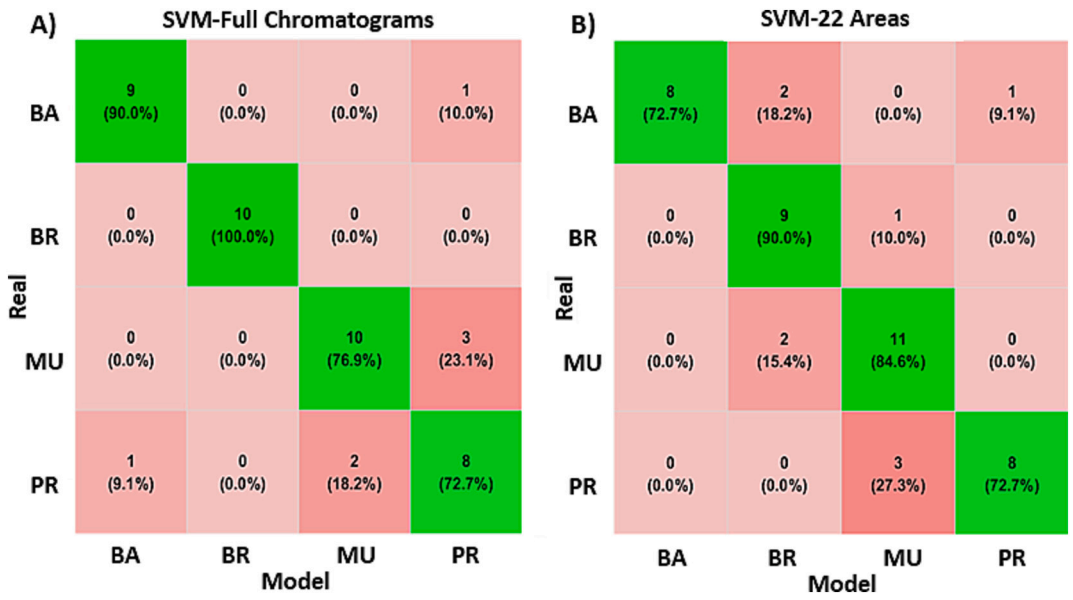

Fig. 6. SVM confusion matrices for models based on (A) full chromatograms and (B) 22 peak areas.

based liqueurs (Rottiers et al., 2019) and the characterization of discriminating molecules constituting the volatile profile of Italian Prosecco wines, associated with geographical origin, viticultural techniques, and vinification techniques (Forleo et al., 2020). However, as these identifications remain putative (Level 3), confirmation using complementary techniques, such as GC–MS, in further studies would be necessary to achieve unambiguous compound assignments and strengthen the robustness of the results.

Analysis of the PCA x-loading plots (Fig. 4) indicated that BA and BR (from red grapes) are characterized by higher intensities of peaks at approximately 35, 51, 97, and 110 s compared to MU and PR (from white grapes). Those peaks were tentatively identified as n-butanol, hexanal, γ-nonalactone, and 4-undecanolide (Table 3). In addition, when compared to BA, BR exhibited elevated peaks intensities at around 35, 50, and 70 s, corresponding to n-butanol, hexanal, and benzaldehyde. The abundance of these compounds in grape marc distillates may indeed be associated to grape variety and the corresponding production technology. For example, higher fermentation temperatures typical of red pomace can enhance yeast activity and the formation of higher alcohols (Lukić et al., 2011; Molina et al., 2008) and prolonged skin and seed contact during maceration of red grapes can increase the availability of unsaturated fatty acid precursors of C6 aldehydes (Buican et al., 2025; Kalua & Boss, 2009; Piombino et al., 2022). In addition, the frequent occurrence of malolactic fermentation in red-wine vinification can enhance lactone formation (Pozo-Bayón et al., 2005; Ugliano & Moio, 2005).

While plausible mechanisms can be inferred from previous studies on grape pomace and fermentation, these interpretations remain hypothetical, as, to the best of our knowledge, no direct comparative studies are available either on the differentiation between BA and BR versus PR and MU, or specifically between BA and BR distillates.

4. Conclusions

This preliminary study investigated the potential of Flash GC analysis of volatile compounds, combined with chemometric techniques, as a rapid analytical approach for differentiating monovarietal *Grappa* distillates. The findings derive from a representative set of monovarietal *Grappa* samples, collected from multiple distilleries across the main producing regions, trying to reflect the current market scenario, represented by a limited number of distilleries producing certified GI *Grappa*. Linear and non-linear chemometric methods and different data representations, including full chromatographic profiles, selected chromatographic regions, and selected peak areas, were used to build the chemometric models in order to determine which approach provided the best performance.

Due to the relatively limited number of available samples, model validation was performed using cross-validation to preserve the robustness of the calibration.

Comparable classification results were obtained using both PLS-DA and SVM models, indicating that the choice of the classification algorithm had a limited impact on performance. In contrast, the different type of dataset played a more relevant role: full chromatographic profiles provided a more stable discrimination, while reduced representations (VIP selection and peak areas) led to slight variations in class separation and misclassification patterns. In particular, a consistent overlap between specific classes (e.g., MU and PR) was observed in the full chromatographic data, whereas peak-based representations modified the distribution of classification errors, suggesting changes in class boundaries.

Tentative identification of key discriminating compounds further highlighted potential links between production technology parameters, grape variety, and differences in aroma profiles, particularly between distillates from white and red varieties. Confirmation of these compounds by complementary techniques, such as GC–MS, is however recommended to ensure their definitive identification.

Overall, this study shows Flash GC as a promising rapid analytical screening tool that may contribute to improve authenticity control procedures of spirit drinks with composition claims, potentially relevant for both industry stakeholders and control authorities.

To confirm its practical applicability, future studies should focus on the collection of additional samples to enable external validation of the proposed models assessing their predictive performance on truly independent datasets and better capturing natural and seasonal sample variability. Additionally, exploring relationships with sensory techniques could provide further technological insights.

CRediT authorship contribution statement

Silvia Arduini: Writing – original draft, Investigation, Data curation, Conceptualization. **Chiara Cevoli:** Writing – review & editing, Writing – original draft, Visualization, Formal analysis, Data curation. **Enrico**

Table 3
Tentative identification of predominant volatile compounds.

RT[a] column MXT-5	LRI[b] column MXT-5	Compound name	Identification by database[c]	Identification by literature
20.79	444	Acetaldehyde	A	(Forleo et al., 2020; Rottiers et al., 2019)
22.69	479	Ethanol	A, N	(Forleo et al., 2020; Rottiers et al., 2019)
23.15	483	2-Propanol	A, N	
29.20	588	Butane-2,3-dione	A, N	
32.86	623	Ethyl acetate	A, N, F	(Forleo et al., 2020; Rottiers et al., 2019)
34.10	639	Isopropyl acetate	A, N	(Rottiers et al., 2019)
34.98	653	n-Butanol	A, N	
39.05	684	Pentan-2-one	A, N	
42.77	714	Ethyl propanoate	A, N	
46.65	744	Pyrrole	A, N	
51.35	773	Hexanal	A, N	
54.12	794	Ethyl butyrate	A, N, F	
56.14	810	Propyl propanoate	A, N, F	
59.83	842	Furfural	A, N, F	
61.58	858	3-Methylbutanoic acid	A, N	(Forleo et al., 2020)
66.43	900	3-Heptanone	A, N	
68.22	919	2,3-Dimethylpyrazine	A, N	
70.48	944	Benzaldehyde	A, N, F	
74.36	987	Myrcene	A, N, F	
77.24	1022	Acetylpyrazine	A, N, F	
79.09	1047	ʟ-Limonene	A, N	
81.66	1082	Pentyl butanoate	A, N, F	
85.72	1144	(*E*, *Z*)-2,6-nonadienal	A, N	
89.85	1211	Ethyl Octanoate	A, N, F	(Forleo et al., 2020)
90.87	1229	Nerol	A, N, F	
93.76	1281	4-Ethylguaiacol	A, N, F	
94.71	1298	Ethyl nonanoate	A, N,	
96.97	1341	γ-Nonalactone	A, N	
100.50	1409	Methyl eugenol	A, N, F	
103.32	1465	Cinnamic acid	A, F	
105.15	1501	δ-Decalactone	A, N	
109.65	1588	4-Undecanolide	A, N	
112.98	1653	γ-Dodecanolactone	A, N	
121.00	1808	Ethyl tetradecanoate	A, N	

[a] RT = Retention times.
[b] LRI = Linear Retention Index values calculated by comparison of the retention times of the analytes with a homologous series of normal alkanes (C6–C16) analyzed with the same GC method.
[c] Identification by database: A = AroChemBase (Heracles software, Alpha M. O·S, Toulouse, France); N = NIST database; F = Flavornet database.

Valli: Writing – review & editing, Validation. **Alessandra Bendini:** Writing – review & editing, Validation, Supervision, Resources, Conceptualization. **Fabio Chinnici:** Writing – review & editing, Supervision, Resources, Conceptualization.

Funding sources

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

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.

Acknowledgements

The authors gratefully acknowledge the National Association of Industrial Distillers of Alcohol and Spirits (AssoDistil) for providing the majority of the samples used in this study.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.foodchem.2026.150065.

Data availability

The data supporting the findings of this study are available in the Institutional Research Repository (AMS-Acta) of the Alma Mater Studiorum - University of Bologna with the identifier: https://doi.org/10.6092/unibo/amsacta/8833.

References

Aliakbarzadeh, G., Parastar, H., & Sereshti, H. (2016). Classification of gas chromatographic fingerprints of saffron using partial least squares discriminant analysis together with different variable selection methods. *Chemometrics and Intelligent Laboratory Systems, 158*, 165–173. https://doi.org/10.1016/j.chemolab.2016.09.002

Arduini, S., & Chinnici, F. (2024). Advancements in analytical strategies for authentication and quality control of grappa and wine brandy with geographical indications. *Applied Sciences, 14*(17). https://doi.org/10.3390/app14178092

Arduini, S., Zappi, A., Locatelli, M., Sgrò, S., & Melucci, D. (2021). An authentication study on grappa Spirit: The use of Chemometrics to detect a food fraud. *Analytica, 2*(3), 84–92. https://doi.org/10.3390/analytica2030010

Arn, H., & Acree, T. E. (1998). Flavornet: A database of aroma compounds based on odor potency in natural products. *Developments in Food Science, 40*, 27. https://doi.org/10.1016/S0167-4501(98)80029-0

Barbieri, S., Cevoli, C., Bendini, A., Quintanilla-Casas, B., García-González, D. L., & Gallina Toschi, T. (2020). Flash gas chromatography in tandem with Chemometrics: A rapid screening tool for quality grades of virgin olive oils. *Foods, 9*(7). https://doi.org/10.3390/foods9070862

Battistutta, F., Da Porto, C., & Sensidoni, A. (1995). Composition and flavour of Muscat of canelli grape distillates obtained using different oenological techniques and unconventional distillation processes. *Italian Journal of Food Science, 7*(1), 47–56.

van den Berg, R. A., Hoefsloot, H. C. J., Westerhuis, J. A., Smilde, A. K., & van der Werf, M. J. (2006). Centering, scaling, and transformations: Improving the biological information content of metabolomics data. *BMC Genomics, 7*(1), 142. https://doi.org/10.1186/1471-2164-7-142

Borsa, D., Monticelli, L., Bonello, F., Pazo Alvarez, M. C., Dell'Oro, V., & Cravero, M. C. (2008). Caractérisation chimique et sensorielle des distillats de marc Italiens "Grappa" produits en Piémont. In A. Bertrand (Ed.), *Les eaux-de-vie traditionnelles d'origine viticole* (pp. 209–216). Lavoisier Tec & Doc.

Brown, S., Tauler, R., & Walczak, B. (2020). *Comprehensive chemometrics: Chemical and biochemical data analysis*. Elsevier.

Buican, B.-C., Luchian, C. E., Colibaba, L. C., Niculaua, M., Bordean, M.-E., Kallithraka, S., & Cotea, V. V. (2025). Aroma compounds from grape pomace: Investigation of key winemaking factors for future extraction applications—A review. *Horticulturae, 11*(3), 302. https://doi.org/10.3390/horticulturae11030302

Chen, X., Sun, B., Deng, Q., Dong, W., & Sun, X. (2025). Current trends and perspectives on the roles of multi-analytical methodologies in spirit authentication: Perspectives, challenges, and opportunities. *Food Chemistry, 493*. https://doi.org/10.1016/j.foodchem.2025.145898

Cheng, H., Qin, Z. H., Guo, X. F., Hu, X. S., & Wu, J. H. (2013). Geographical origin identification of propolis using GC-MS and electronic nose combined with principal component analysis. *Food Research International, 51*(2), 813–822. https://doi.org/10.1016/j.foodres.2013.01.053

Di Stefano, R., & Borsa, D. (2006). Composti aromatici varietali di grappe e distillati d'uva da monovitigno. *Rivista Di Viticoltura e Di Enologia, 59*(1), 37–56.

Diéguez, S. C., de la Peña, M., & L. G., & Gómez, E. F.. (2003). Approaches to Spirit aroma: Contribution of some aromatic compounds to the primary aroma in samples of Orujo spirits. *Journal of Agricultural and Food Chemistry, 51*(25), 7385–7390. https://doi.org/10.1021/jf0302916

Farrés, M., Platikanov, S., Tsakovski, S. L., & Tauler, R. (2015). Comparison of the variable importance in projection (VIP) and of the selectivity ratio (SR) methods for variable selection and interpretation. *Journal of Chemometrics, 29*(10), 528–536. https://doi.org/10.1002/cem.2736

Forleo, T., Zappi, A., Gottardi, F., & Melucci, D. (2020). Rapid discrimination of Italian prosecco wines by head-space gas-chromatography basing on the volatile profile as a chemometric fingerprint. *European Food Research and Technology, 246*(9), 1805–1816. https://doi.org/10.1007/s00217-020-03534-8

Gan, Z., Yang, Y., Li, J., Wen, X., Zhu, M., Jiang, Y., & Ni, Y. (2016). Using sensor and spectral analysis to classify botanical origin and determine adulteration of raw

honey. *Journal of Food Engineering, 178*, 151–158. https://doi.org/10.1016/j.jfoodeng.2016.01.016

Giannetti, V., Mariani, M. B., Marini, F., Torrelli, P., & Biancolillo, A. (2019). Flavour fingerprint for the differentiation of grappa from other Italian distillates by GC-MS and chemometrics. *Food Control, 105*, 123–130. https://doi.org/10.1016/j.foodcont.2019.05.028

Kalua, C. M., & Boss, P. K. (2009). Evolution of volatile compounds during the development of cabernet sauvignon grapes (Vitis vinifera L.). *Journal of Agricultural and Food Chemistry, 57*(9), 3818–3830. https://doi.org/10.1021/jf803471n

Lukić, I., Miličević, B., Banović, M., Tomas, S., Radeka, S., & Peršurić, Đ. (2010). Characterization and differentiation of Monovarietal grape Marc distillates on the basis of varietal aroma compound composition. *Journal of Agricultural and Food Chemistry, 58*(12), 7351–7360. https://doi.org/10.1021/jf100214k

Lukić, I., Milicevic, B., Banović, M., Tomas, S., Radeka, S., & Peršurić, Đ. (2011). Secondary aroma compounds in fresh grape Marc distillates as a result of variety and corresponding production technology. *Food Technology and Biotechnology, 49*, 214–227.

Melucci, D., Bendini, A., Tesini, F., Barbieri, S., Zappi, A., Vichi, S., Conte, L., & Gallina Toschi, T. (2016). Rapid direct analysis to discriminate geographic origin of extra virgin olive oils by flash gas chromatography electronic nose and chemometrics. *Food Chemistry, 204*, 263–273. https://doi.org/10.1016/j.foodchem.2016.02.131

Ministero delle politiche agricole, alimentari e forestali. (2016). *Modifica del decreto 1° agosto 2011, n. 5389, recante disposizioni in materia di «Attuazione dell'articolo 17 del regolamento (CE) n. 110/2008 del Parlamento europeo e del Consiglio, del 15 gennaio 2008, concernente la definizione, la designazione, la presentazione, l'etichettatura e la protezione delle indicazioni geografiche delle bevande spiritose - Scheda tecnica della "Grappa"»*. Gazzetta Ufficiale Della Repubblica Italiana Serie Generale, 31 (08/02/2016). https://www.gazzettaufficiale.it/atto/serie_generale/caricaDettaglioAtto/originario?atto.codiceRedazionale=16A00865&atto.dataPubblicazioneGazzetta=2016-02-08.

Molina, A., Swiegers, J., Varela, C., Pretorius, I., & Agosin, E. (2008). Influence of wine fermentation temperature on the synthesis of yeast-derived volatile aroma compounds. *Applied Microbiology and Biotechnology, 77*, 675–687. https://doi.org/10.1007/s00253-007-1194-3

Piombino, P., Genovese, A., Rustioni, L., Moio, L., Failla, O., Bellincontro, A., & Mencarelli, F. (2022). Free and glycosylated green leaf volatiles, lipoxygenase and alcohol dehydrogenase in defoliated Nebbiolo grapes during postharvest dehydration. *Australian Journal of Grape and Wine Research, 28*(1), 107–118. https://doi.org/10.1111/ajgw.12521

Pozo-Bayón, M. A., G-Alegría, E., Polo, M. C., Tenorio, C., Martín-Álvarez, P. J., Calvo de la Banda, M. T., Ruiz-Larrea, F., & Moreno-Arribas, M. V. (2005). Wine volatile and amino acid composition after malolactic fermentation: Effect of Oenococcus oeni and Lactobacillus plantarum starter cultures. *Journal of Agricultural and Food Chemistry, 53*(22), 8729–8735. https://doi.org/10.1021/jf050739y

Rottiers, H., Tzompa Sosa, D. A., Van de Vyver, L., Hinneh, M., Everaert, H., De Wever, J., … Dewettinck, K. (2019). Discrimination of cocoa liquors based on their odor fingerprint: A fast GC electronic nose suitability study. *Food Analytical Methods, 12*(2), 475–488. https://doi.org/10.1007/s12161-018-1379-7

Śliwińska, M., Wiśniewska, P., Dymerski, T., Wardencki, W., & Namieśnik, J. (2016). Evaluation of the suitability of electronic nose based on fast GC for distinguishing between the plum spirits of different geographical origins. *European Food Research and Technology, 242*(11), 1813–1819. https://doi.org/10.1007/s00217-016-2680-6

Sumner, L. W., Amberg, A., Barrett, D., Beale, M. H., Beger, R., Daykin, C. A., … Viant, M. R. (2007). Proposed minimum reporting standards for chemical analysis. *Metabolomics, 3*(3), 211–221. https://doi.org/10.1007/s11306-007-0082-2

The European Parliament and the Council of the European Union. (2019). Regulation (EU) 2019/787 of the European Parliament and of the council of 17 April 2019 on the definition, description, presentation and labelling of spirit drinks, the use of the names of spirit drinks in the presentation and labelling of other foodstuffs, the protection of geographical indications for spirit drinks, the use of ethyl alcohol and distillates of agricultural origin in alcoholic beverages, and repealing regulation (EC) no 110/2008. *Official Journal of the European Union, L130*(III), 17–27. https://eur-lex.europa.eu/eli/reg/2019/787/oj/eng.

Tomasi, G., Van Den Berg, F., & Andersson, C. (2004). Correlation optimized warping and dynamic time warping as preprocessing methods for chromatographic data. *Journal of Chemometrics, 18*(5), 231–241. https://doi.org/10.1002/cem.859

Ugliano, M., & Moio, L. (2005). Changes in the concentration of yeast-derived volatile compounds of red wine during malolactic fermentation with four commercial starter cultures of Oenococcus oeni. *Journal of Agricultural and Food Chemistry, 53*(26), 10134–10139. https://doi.org/10.1021/jf0514672

Versini, G., Rapp, A., Dalla Serra, A., Pichler, U., & Ramponi, M. (1994). Methyl trans geranate and farnesoate as markers for Gewurztraminer grape skins and related distillates. *Vitis, 33*, 139–142. https://doi.org/10.5073/vitis.1994.33.139-142

Wiśniewska, P., Śliwińska, M., Dymerski, T., Wardencki, W., & Namieśnik, J. (2016). Differentiation between spirits according to their botanical origin. *Food Analytical Methods, 9*(4), 1029–1035. https://doi.org/10.1007/s12161-015-0280-x

Wu, X., Fauconnier, M.-L., & Bi, J. (2022). Characterization and discrimination of apples by flash GC E-nose: Geographical regions and botanical origins studies in China. *Foods, 11*(11). https://doi.org/10.3390/foods11111631

Yu, D. X., Zhang, X., Guo, S., Yan, H., Wang, J. M., Zhou, J. Q., Yang, J., & Duan, J. A. (2022). Headspace GC/MS and fast GC e-nose combined with chemometric analysis to identify the varieties and geographical origins of ginger (Zingiber officinale Roscoe). *Food Chemistry, 396*, Article 133672. https://doi.org/10.1016/j.foodchem.2022.133672