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A novel chemometric approach for classifying whole fruit juices, reconstituted juices, and nectars

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Abstract

Fruit juices are widely enjoyed beverages, valued for their organoleptic qualities, chemical composition, and nutritional benefits. They are commonly sold as whole juices (WJs), reconstituted juices, or nectars, with WJs particularly favored by consumers seeking healthier, more balanced dietary options, often commanding a higher market value. However, these desirable characteristics make them vulnerable to fraud and adulteration. To address this issue, a novel strategy has been proposed to classify juices into two categories: WJs and nectar/reconstituted juices (NERJs). This approach combines key chemical markers––such as reducing sugars (RS), sodium (Na), and potassium (K)––with advanced chemometric techniques, including unsupervised methods like principal component analysis (PCA) and supervised methods, such as machine learning algorithms (random forest [RF] and extreme gradient boosting (XGBoost)). The models developed demonstrated remarkable accuracy, achieving 100% classification accuracy for WJs and good performance for NERJs, with accuracy rates > 91.7%. This fast, accurate, and easily implementable strategy is vital for the quality control and authentication of fruit juices by regulatory bodies. It provides essential tools for detecting fraud and adulteration in the beverage industry, ultimately helping ensure the quality and consistency of products available to consumers.

Keywords: whole juice; nectar; reconstituted juice; chemical markers; machine learning; classification.

Practical Application: Key chemical characteristics were used to enhance the classification of fruit juices; good discrimination between whole juices and nectar/reconstituted juices was achieved; and a cost-effective strategy for identifying adulteration in fruit juices was developed.

1 INTRODUCTION

Recently, consumers have increasingly turned to fruit juices as a substitute for fresh fruits. This trend can be explained by the practicality and convenience of their consumption, especially in light of the fast-paced lifestyles of a large part of the world's population. The organoleptic characteristics of these beverages and their health benefits and nutritional value have also contributed to their popularity (Lan et al., 2023; Mac et al., 2023; Markowski et al., 2009). Additionally, the rise in fruit juice consumption is linked to the adoption of healthier lifestyles and the embrace of specialized diets, such as vegetarian, vegan, or those aimed at preventing food allergies or intolerances (Lan et al., 2023; Lepaus et al., 2023).

Fruit juices are highly valued and widely consumed due to their organoleptic, compositional, and nutritional characteristics, which can vary based on the type of fruit, processing methods, and the soil and climate conditions of the growing region (Kersh et al., 2023; Liu et al., 2022; Markowski et al., 2009; Rajauria & Tiwari, 2018; Rinke & Jamin, 2018). Additionally, the processing conditions (such as the addition of water, sugars, and other additives) allow juices to be offered in various forms, including whole juices (WJs), reconstituted juices, mixed juices, and nectars (Lan et al., 2023). These factors primarily influence the sugar content and mineral profile of the beverage, affecting its flavor and aroma (Kersh et al., 2023; Liu et al., 2022).

The label "whole" refers to juices that have not been concentrated or altered in any way and contain no added sugars or preservatives (Brasil, 2009; 2018). Reconstituted juices are made by rehydrating concentrated or dehydrated juice with water to match the original concentration of WJs (Brasil, 2009; 2018; Codex Alimentarius, 2005). Mixed juices are created by combining two or more different types of fruit juices (Brasil, 2009; Codex Alimentarius, 2005), with or without the addition of water, sugars, or additives. Nectars are unfermented but fermentable beverages produced by adding water and sugars to juices (Brasil, 2009; Codex Alimentarius, 2005).

To protect consumers, various regulations have established identity and quality standards for these beverages, as they are among the most commonly adulterated or fraudulently marketed food products (Brasil, 2009; 2014; Codex Alimentarius, 2005; Moore et al., 2012). Given these concerns, developing cost-effective and accurate analytical strategies for classifying

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different fruit juice forms (WJs, reconstituted juices, and nectars) is essential to ensure the integrity and quality of the consumer's beverage purchase.

The increasing demand for fruit juices, particularly WJs, enhances the commercial value of these beverages, making them more vulnerable to fraud and adulteration. Among the most commonly fraudulent foods are apple and orange juices, as well as olive oil, honey, milk, coffee, and saffron (Banti, 2020; Moore et al., 2012; Wójcik & Jakubowska, 2021). However, detecting adulteration or fraud that involves minimal changes in the composition of fruit juices is more challenging with traditional strategies, necessitating the development of new quality control methods (Mac et al., 2023; Rinke & Jamin, 2018).

To prevent fraud and adulteration, various analytical strategies have been proposed for the effective and accurate classification of fruit juices, considering factors, such as their presentation forms, processing and production methods, and geographical origins (Borges et al., 2015; Cristea et al., 2020; Gutiérrez-Capitán et al., 2013; Junges et al., 2024; Liu, et al., 2022; Wen et al., 2023; Włodarska, et al., 2017; Wójcik & Jakubowska, 2021). Within this context, two groups of strategies are particularly noteworthy. The first group includes destructive methods, such as analyzing chemical characteristics and conducting isotopic, elemental, and chromatographic analyses of the fruit juice composition. The second group consists of non-destructive methods that utilize spectroscopic, electrochemical, and imaging techniques, often combined with chemometric methods for the classification or quantification of components in these beverages (Dasenaki & Thomaidis, 2019; Mac et al., 2023).

The primary advantages of non-destructive analytical strategies include speed, minimal sample requirements, and reduced waste generation. However, their drawbacks include the handling of large amounts of data that must be processed and appropriately analyzed using chemometric and machine learning tools. Additionally, these methods necessitate highly trained analysts and entail costs for equipment acquisition and maintenance, making their implementation less feasible in small- and medium-sized laboratories (Dasenaki & Thomaidis, 2019; Mac et al., 2023).

On the other hand, using chemical characteristics to verify the authenticity of fruit juices has advantages, as the methods employed are straightforward, cost-effective, and already integrated into industry quality control practices, being recognized by relevant regulations. However, several researchers have conducted classification studies on various fruit juices, utilizing a wide range of chemical characteristics to achieve greater accuracy in classifying these beverages. The extensive amount of data typically necessitates the use of unsupervised and/or supervised data analysis methods (Dasenaki & Thomaidis, 2019; Mac et al., 2023; Rizzon & Miele, 2012; Włodarska, et al., 2016; Włodarska, et al., 2017). Furthermore, this approach indicates a need for additional analytical work, leading to increased costs.

An interesting approach to address these challenges in fruit juice classification and authenticity assurance is to select the most effective chemical characteristics with strong discriminatory power and combine them with chemometric tools. By narrowing down the number of chemical characteristics, there is less noise in the modeling process, resulting in greater accuracy in classification (Mac et al., 2023). Additionally, employing supervised strategies to model data based on chemical characteristics enables the identification of hidden patterns in complex samples, such as fruit juices, particularly those with similar compositional traits, like WJs and reconstituted juices. This can significantly enhance the discrimination and classification of fruit juices across their various forms of presentation and formulation (Rajauria & Tiwari, 2018; Rinke & Jamin, 2018).

Considering all these factors, this study utilized chemical characteristics such as reducing sugars (RS) and titers of Na and K to model the classification of grape, white grape, apple, and mixed grape–apple juices into two categories: WJs and nectar/reconstituted juices (NERJs). The classification was performed using unsupervised (principal component analysis (PCA)) and supervised (random forest (RF) and extreme gradient boosting (XGBoost)) chemometric tools. The decision to group reconstituted juices and nectars from various fruits into a single category was based on the differences in processing methods used to produce reconstituted juices compared to WJs. Given the compositional similarities between these juices, unscrupulous manufacturers could market reconstituted juices as WJs. Therefore, developing a strategy to differentiate nectars and reconstituted juices from WJs of different fruits is crucial.

2 MATERIALS AND METHODS

2.1 Juice sampling

Sixty-six samples of different fruit juices with varying degrees of processing were purchased from supermarkets, wineries, and other commercial sources, including 33 samples of WJs (grape (n = 11); apple (n = 9); white grape (n = 11); and mixed grape and apple (n = 2)), 8 samples of reconstituted juices (grape (n = 2); white grape (n = 2); and apple (n = 4)), and 25 samples of nectars (grape (n = 4); white grape (n = 1); apple (n = 5); and mixed grape and apple (n = 15)). The samples were coded based on the type of fruit (grape (G), white grape (WG), and apple (A)) and the type of beverage processing (WJs and NERJs), with Arabic numerals indicating the order in which they entered the laboratory. Juice concentrations varied based on the type of fruit and the processing methods used to produce the beverages. According to Brazilian legislation, WJs have a natural concentration and are therefore considered to be 100% (Brasil, 2009; 2018). Grape nectars must contain 50% grape pulp or juice, while apple nectars and mixed juices must contain 20 or 30% fruit pulp or juice, respectively (Brasil, 2013). All samples were stored at a temperature of 6 to 8°C in their respective packaging until the chemical analyses were performed.

2.2 Chemical analysis

RS were determined using the Lane–Eynon volumetric method, following the procedure outlined in Method 239/IV of the Physicochemical Methods for Food Analysis (IAL, 2008), which is equivalent to OIV-MA-AS311-01A (International Organization of Vine and Wine [OIV], 2022) with some

modifications. RS were assessed from the diluted solutions of the beverages. A concentration of 5.0% (v/v) was used for the grape, white grape, and mixed grape–apple juice samples, while a concentration of 10% (v/v) was used for the apple juice samples. The analyses were conducted in triplicate ($n = 3$). The Na and K contents were determined according to the official methods for juices (OIV-MA-AS322-02B/OIV-MA-AS322-03B) (OIV, 2022) and Association of Official Analytical Chemists (AOAC) 963.13 (AOAC, 1964). An Analyser® Model 910MS flame photometer, previously calibrated with a mixed standard of 100 ppm Na and K, was employed to measure the absorbance of these elements. Samples were analyzed at their original concentration and diluted 1:10 and 1:100 (v/v) when necessary. The analyses were performed in duplicate ($n = 2$).

2.3 Principal component analysis

PCA was conducted on the averages of contents to evaluate the correlation between the chemical characteristics (RS, Na, and K) and the respective samples of WJs (W), reconstituted juices (R), and nectars (N). The open-source software R was utilized for the statistical analysis of the data (Team R Core, 2022).

2.4 Modeling the classification using machine learning algorithms

To classify the fruit juices as WJs or NERJs, the concentrations of RS, Na, and K found in the samples were utilized (Figure 1). The dataset ($n = 132$) was then divided into two subsets to reduce the risk of overfitting the classification models generated. Specifically, 70% of the data ($n = 92$) was used to construct the training model, while the remaining 30% ($n = 40$) comprised the testing model (Figure 1).

The RF and XGBoost machine learning algorithms were employed to build and validate the classification models, which were executed using the Python v. 3.8 software (Google Colaboratory, 2023).

The performance of the generated classification models was assessed using data derived from the confusion matrix, and various figures of merit, including accuracy, precision, recall, and F1-score, were calculated. These figures of merit were obtained using the number of errors and successes predicted by the classification model (Castro et al., 2019; Sokolova & Lapalme, 2009).

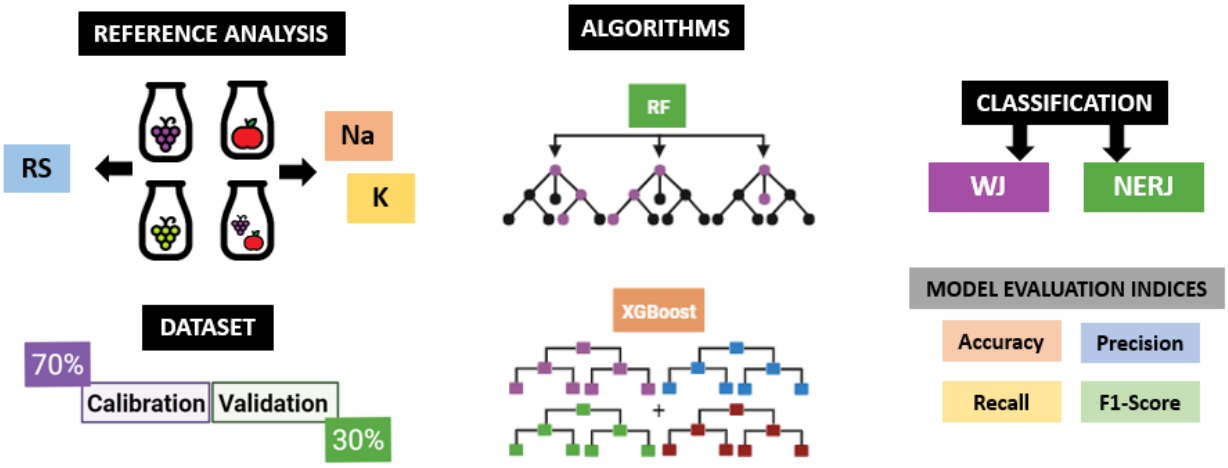
3 RESULTS AND DISCUSSION

3.1 Classification of fruit juices using PCA

PCA was conducted on the average contents of Na, K, and RS to evaluate the potential for grouping different fruit juice samples (apple, grape, white grape, and mixed grape–apple) based on their presentation forms: WJs (W), nectars (N), and reconstituted juices (R) (Figure 2). The first two principal components (PC1 and PC2) together accounted for 82.0% of the variability observed in the chemical composition of these beverages.

PC1, which explained 54.9% of the total variability, effectively separated nectar (N) samples from WJ (W) samples, primarily based on differences in the Na content, as shown by the two groupings in the opposite quadrants of the PCA plot (Figure 2). This distinction can be attributed to the presence of additional components, such as sugars and additives, commonly included during the dilution process of this beverage, in nectar samples. Manufacturers often incorporate sodium (Na)-based compounds, such as sodium benzoate, sodium cyclamate, and sodium citrate, as declared on the labels of most fruit nectars (Cristea et al., 2020; Maione et al., 2016; Rizzon & Miele, 2012). This practice accounts for the higher Na content observed in the nectar samples, as highlighted in the PCA (Figure 2).

The second principal component (PC2) accounted for 27.1% of the variability of the dataset. The PCA (Figure 2) revealed two overlapping groupings characterized by high levels of RS and potassium (K). One grouping comprised WJ samples, while the other included reconstituted juice samples. These groupings were positioned in the quadrant opposite to



RS: reducing sugars; RF: random forest; XGBoost: extreme gradient boosting; WJ: whole juice; NERJ: nectar/reconstituted juice; Na: sodium; K: potassium.

Figure 1. Illustration of the approach used to classify grape, white grape, apple, and mixed grape–apple juices into WJs and NERJs using machine learning algorithms.

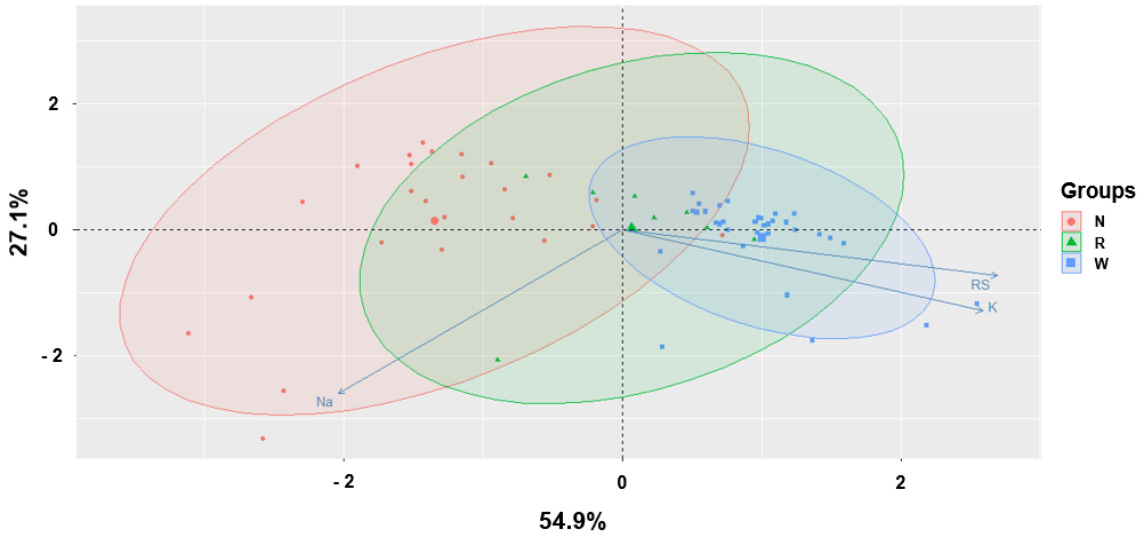


Figure 2. Projection of loadings and scores on the first two principal components, PC1 and PC2, for grouping of nectars (N), reconstituted juices (R), and WJs (W) of apple, grape, white grape, and mixed apple–grape juice samples.

the nectar samples in the PCA plot. According to legislation (Brasil, 2018; Codex Alimentarius, 2005), the incorporation of any exogenous components during the production of WJs is explicitly prohibited. As a result, it can be anticipated that WJs will contain higher levels of RS and K, along with organic acids and phenolic compounds.

The PCA also showed that some nectar samples were included in the WJ group. This can be attributed to grape nectar samples containing 50% or more added juices, resulting in RS and K levels similar to those of WJ samples (Figure 2). Conversely, some grape and white grape reconstituted juice samples were grouped with nectar samples. This behavior is related to the manufacturing process, where producers determine the degree of the reconstitution of concentrated or dehydrated fruit juice with water in the formulation of reconstituted juices. This process can reduce RS and K levels, aligning the composition of these samples more closely with that of nectars.

The observed variations in RS, Na, and K levels among the different presentations of fruit juices (whole, reconstituted, mixed, and nectar) for grape, white grape, apple, and mixed grape–apple (Figure 2) suggest that these chemical characteristics can effectively distinguish WJ samples (W) from nectar (N) and reconstituted juice (R) samples across various fruits.

Based on the processing differences used to formulate these beverages, this study established two distinct classes of fruit juices: WJs and NERJs. Reconstituted juices were grouped with nectars for two reasons. First, their production process involves diluting concentrated or dehydrated juices with water, which is similar to the process used for nectar production (Rajauria & Tiwari, 2018; Rinke & Jamin, 2018). Second, this classification aimed to evaluate whether reconstituted juices could be differentiated from WJs, particularly given their compositional similarities in RS and K levels.

Other authors have also achieved highly accurate classifications using these chemical characteristics (RS, Na, and K) as key variables for differentiating various types of fruit juices based on geographical origin, fruit species, production or processing methods, or fruit type (Borges et al., 2015; Cristea et al., 2020; Gutiérrez-Capitán et al., 2013; Liu et al., 2022; Maione et al., 2016; Włodarska et al., 2017). However, a review of the literature revealed no studies specifically focused on classifying WJs and NERJs. Therefore, these findings underscore the potential of these features (RS, Na, and K) for classifying fruit juices in these forms of presentation through modeling with machine learning algorithms.

3.2 Modeling using machine learning algorithms

In light of these considerations, this work generated classification models for fruit juices (grape, white grape, apple, and mixed grape–apple) into two categories: WJs and NERJs based on their RS, Na, and K content, using two machine learning algorithms (RF and XGBoost). The classification results for each algorithm are presented in the form of a confusion matrix (Table 1), which displays the number of correct and incorrect predictions of the classification model for each class investigated (Ballabio et al., 2018).

As shown in the confusion matrix (Table 1), the data indicate that the RF algorithm exhibited superior performance in classifying WJs, achieving 100% accuracy with all instances correctly classified. In contrast, the classification of NERJs was less accurate, with a few instances mistakenly classified as WJs. This outcome may stem from the closer compositional similarities that some reconstituted juices and nectars share with WJs, as outlined in the PCA plot (Figure 2). On the other hand, the XGBoost model demonstrated enhanced performance in classifying NERJ samples across both modeling stages (Table 1), indicating its efficacy in differentiating between these classes.

The performance of the models generated by the RF and XGBoost algorithms was further assessed by calculating various merit figures, including accuracy, precision, recall, and F1-score estimates (Table 2). These metrics provide a comprehensive evaluation of the models' effectiveness in classifying fruit juices into their respective categories.

The figures of merit illustrate that both the RF and XGBoost algorithms produced highly effective classification models for grape, white grape, apple, and mixed grape–apple juices, categorizing them into "WJs" and "NERJs." Specifically, the RF model demonstrated remarkable performance, achieving accuracy and precision estimates exceeding 90.5%, an F1-score above 95.0%, and an overall accuracy of 95.5% (Table 2).

The model's very strong performance, particularly for the WJ class, can be attributed to the inherent characteristics of the RF algorithm. This machine learning technique is favored in the food industry due to its straightforward training process and its ability to adjust complex non-linear models effectively. Additionally, RF handles unbalanced datasets well, leading to excellent classification outcomes. The model operates through a collection of decision trees, where each tree votes for a specific class. The tree leaves represent the classes to which the samples are assigned, while the nodes on the tree branches delineate the rules guiding each sample's classification. Approximately two-thirds of the samples are employed for growing the trees (training), while the remaining one-third is reserved for model validation and performance estimation (Breiman, 2001).

The XGBoost algorithm demonstrated superior performance in classifying and discriminating between WJ and NERJ classes. All figures of merit assessed during the training stage yielded metrics of 100%. In the testing stage, the accuracy exceeded 95.8%, and the F1-score surpassed 97.9%. The overall accuracy reached by XGBoost models (99.0%) (Table 2) is significantly higher than the 95.5% observed for the RF models. Furthermore, XGBoost exhibited greater accuracy in classifying NERJ samples compared to the RF algorithm.

Like RF, XGBoost is a complex algorithm based on decision trees, recognized for its integrated approach, high training efficiency, and predictive performance. XGBoost effectively optimizes both the dataset and the model while maintaining high computational efficiency and avoiding overfitting.

While both algorithms use trees for classification, XGBoost enhances the decision tree model, resulting in weaker individual predictors that collectively minimize classification errors through corrective measures applied in subsequent trees. This iterative correction process leads to classification models with exceptional accuracy and precision, along with minimal residuals when classifying unknown samples (Wen et al., 2023; You et al., 2024). The robust performance of XGBoost in this study underlines its potential as a valuable tool for accurately distinguishing between different forms of fruit juices, particularly in contexts where compositional similarities may otherwise complicate classification efforts.

In comparison to the existing literature, the classification models generated by XGBoost in this work demonstrated significantly higher accuracy estimates than those previously reported for the classification of Chinese dates, which ranged from 92.7 to 97.6% (Wen et al., 2023). Additionally, the accuracy estimates surpassed those noted by Armstrong et al. (2023) in their classification of grapeseed ripeness, which ranged from 82.5 to 91.6%. This improvement underscores the effectiveness of the XGBoost algorithm in achieving robust classification outcomes in complex datasets, particularly in the context of differentiating between various forms of fruit juices based on their chemical characteristics.

Table 1. Confusion matrices for the calibration and external validation models generated by RF and XGBoost algorithms for the WJ and NERJ target classes.

Algorithms	Models	Classes' predicted values	Classes' reference values	
			WJ	NERJ
RF	Training	WJ	50	0
		NERJ	4	38
	Testing	WJ	16	0
		NERJ	2	22
XGBoost	Training	WJ	50	0
		NERJ	0	42
	Testing	WJ	16	0
		NERJ	1	23

WJ: whole juice; NERJ: nectar/reconstituted juice; RF: random forest; XGBoost: extreme gradient boosting.

5 CONCLUSIONS

Classification strategies, such as the one developed in this study, are both innovative and essential for effectively categorizing fruit juices. These strategies play a key role in ensuring the quality and consistency of beverages offered to consumers while addressing unscrupulous practices by producers, thus minimizing

Table 2. Performance expressed in percentage (%) of the classification models for fruit juice generated by the RF and XGBoost algorithms.

Model	Algorithms	Class	Precision	Recall	F1-score	Accuracy
Training	RF	WJ	100	100	100	100
		NERJ	90.5	100	95.0	90.5
	XGBoost	WJ	100	100	100	100
		NERJ	100	100	100	100
Global accuracy: 95.5						
Testing	RF	WJ	100	100	100	100
		NERJ	91.7	100	95.7	91.7
	XGBoost	WJ	100	100	100	100
		NERJ	95.8	100	97.9	95.8
Global accuracy: 99.0						

WJ: whole juice; NERJ: nectar/reconstituted juice; RF: random forest; XGBoost: extreme gradient boosting.

the risks of fraud and adulteration. By utilizing chemical characteristics such as RS and the titers of Na and K, which are already well established in the beverage industry, this approach provides a practical solution that small- and medium-sized laboratories can easily integrate into their routine analyses. These characteristics are recognized by regulatory bodies and can be determined relatively simply and quickly, making them ideal for incorporation into classification models for new samples.

The classification models combining these chemical characteristics with machine learning algorithms, such as RF and XGBoost, demonstrated excellent performance, enabling accurate classification of fruit juices into two categories: WJs and NERJs, with overall accuracy exceeding 95.5%. It is important to note that the compositional similarity between reconstituted juices and WJs presents challenges for accurate categorization, highlighting the need to employ machine learning strategies to identify complex patterns in fruit juice samples. The integration of chemical characteristics with machine learning offers significant advantages over traditional classification methods that rely solely on unsupervised techniques, including increased speed, simplicity, and cost-effectiveness, as it utilizes low-cost instrumentation and accessible software tools.

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