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Review

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Review

Advancements in food authentication using soft independent modelling of class analogy (SIMCA): a review

Davide De Angelis[*], Carmine Summo, Antonella Pasqualone, Michele Faccia, and Giacomo Squeo

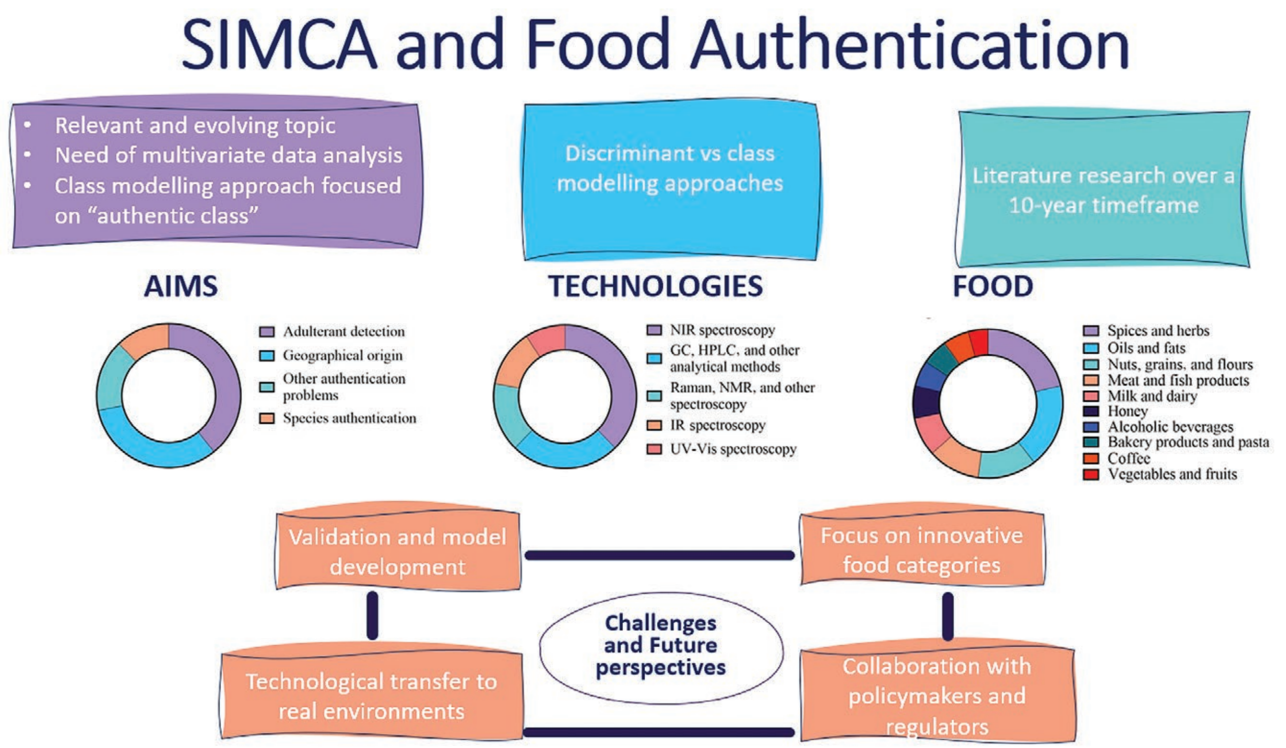
Department of Soil, Plant and Food Science (DISSPA), University of Bari 'Aldo Moro', Bari, Italy

[*]*Correspondence to:* Davide De Angelis, Department of Soil, Plant and Food Science (DISSPA), University of Bari 'Aldo Moro', Via Amendola, 165/A, 70126 Bari, Italy. E-mail: Davide.deangelis@uniba.it

Abstract

Food authentication verifies the match between product characteristics and claims and it is crucial in a globalized and complex food sector. Currently, class-modelling approaches, such as soft independent modelling of class analogy (SIMCA), are powerful tools for assessing food authenticity. The aim of this review is to discuss the application of SIMCA for food authentication and to describe the conceptual differences between discriminant and class-modelling approaches. The discussion of research articles is organized around three elements: (i) the research objectives, (ii) the analytical methodologies, and (iii) the food products investigated. Moreover, the challenges and future perspectives considering the development of innovative food products are discussed. Adulteration is the most investigated food authentication issue, followed by verification of geographical origin. Food authenticity appeared to be predominantly evaluated using non-destructive spectroscopy. Overall, the articles collectively cover a broad spectrum of food categories, representing those most prone to adulteration. However, there is a notable lack of food authentication studies on innovative food products, underscoring the urgency for further research in this field.

Graphical Abstract



Keywords: Soft independent modelling of class analogy (SIMCA); class modelling; food authentication; geographical origin; adulteration.

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Introduction

Food authentication is a vast and complex issue that refers to the process of verifying whether a food product is authentic or genuine. A comprehensive definition of 'authentic food' is given in Robson *et al.* (2021) and is described as the match between the food product characteristics and the corresponding claims. The same authors also specify that the food authenticity issue regards not only intentional acts that make the product non-authentic, but also accidental misdescription. In the first case, intentional acts are defined as "food frauds". Food fraud is triggered by globalization and complexity of food supply chains (Kendall *et al.*, 2019; Spink *et al.*, 2019; Robson *et al.*, 2021). Moreover, it was recently reported that the Corona Virus Disease 2019 (COVID-19) pandemic played a role in food fraud incidents in 2020 (Frera *et al.*, 2021), suggesting that the emergency period may be the cause of vulnerabilities in the food supply chain. Robson *et al.* (2021) reported several definitions of food fraud, pointing out that the lack of standardization and inconsistency in definition can hinder the fight against food fraud. However, most definitions agree that food fraud is an intentional act for economic gain using food (Robson *et al.*, 2021). Therefore, it is a deliberate act to deceive consumers or gain unfair economic advantage. Food fraud can have a negative impact on several aspects related to food products, including quality, safety, and ethical concerns. For example, the dilution of extra virgin olive oil with other food-grade oils like refined olive oil or seed oil has an impact on the overall quality of the product, whereas the ingestion of a fuel oil for industrial use fraudulently sold as olive oil caused deaths and hospitalizations in Spain in 1981 (Kendall *et al.*, 2019; Visciano and Schirone, 2021). Finally, ethical implications of food fraud may affect consumers following dietary guidelines established by religion and may be related to the presence of non-declared alcohol or pork meat in a product destined for Muslims and certified as Halal (Ng *et al.*, 2022).

From this context, it is clear that food authentication is a relevant issue in the food sector, and it is constantly evolving. With the increasing complexity of global supply chains and the sophistication of fraudulent practices, there is a growing recognition of the need for robust measures to ensure the authenticity and quality of food products. Various efforts and technologies are being developed and implemented to address these challenges. For instance, implementing innovative solutions such as blockchain (Creydt and Fisher, 2019) can guarantee the authenticity of foods and their traceability through verified and immutable documentation processes.

By contrast, from an analytical point of view, various technologies have been developed to detect adulterations and verify the authenticity of foods, ranging from advanced molecular approaches (Di Rienzo *et al.*, 2016) to analytical techniques such as chromatography combined with mass spectrometry (Dou *et al.*, 2023). Innovations in algorithms and data-processing techniques like artificial intelligence have also been under development (Goyal *et al.*, 2022). Moreover, technologies based on spectroscopic methods such as infrared (Liang *et al.*, 2022), Raman (Xu *et al.*, 2020) or nuclear magnetic resonance (NMR) (Consonni and Cagliani, 2019) have demonstrated high reliability when used for food authentication purposes. With this respect, the Italian scientific community is widely involved in the development of innovative solutions that can better guarantee food authenticity and protect the agri-food chain (https://agritechcenter.it/spokes/).

In general, a wide use of untargeted analytical approaches to the scope of authenticity safeguard is observed. These methods are usually much more informative than targeted approaches, although they are more complicated to treat. In fact, all the above-mentioned technologies produce multivariate data sets that must be properly treated by chemometric/multivariate tools to extract relevant information and develop suitable models to assess food genuineness. With this respect, it is important to distinguish between discriminant and class-modelling approaches because both are frequently used for food authentication purposes, and often some incorrect applications are found in the literature (Rodionova *et al.*, 2016a; Oliveri, 2017).

The purpose of this review is to discuss the application of class-modelling approaches, particularly soft independent modelling of class analogy (SIMCA), in the context of food authentication. The focus on SIMCA was chosen because this technique is recognized as the most popular for authentication purposes (Vitale *et al.*, 2023). Although there are other reviews aimed at discussing this topic (Rodionova *et al.*, 2016a, 2024; Oliveri, 2017; Medina *et al.*, 2019; Vitale *et al.*, 2023), most of them focus on the analytical techniques or the chemometric/statistical aspects of class-modelling approaches without addressing a food technology perspective. Therefore, this review aims to present to the readers the applications of SIMCA studied so far in the specific and wide context of food authentication, highlighting the contribution that this tool could make to ensuring food genuineness. Moreover, the challenges and future perspectives considering the development of innovative food products are discussed. First, a brief description of SIMCA model and of the conceptual differences between discrimination and class-modelling approaches is given in the next sections.

A brief description of the SIMCA model

In order to provide readers with a general understanding of the working principle of SIMCA and facilitate comprehension of this review article, a short and general description of the SIMCA model is provided. For a comprehensive explanation of this methodology, readers are warmly invited to refer to other articles (Rodionova *et al.*, 2016a, 2024; Oliveri, 2017; Medina *et al.*, 2019; Vitale *et al.*, 2023).

Briefly, SIMCA is based on the assumption that the similarities within objects can be explained and modelled using principal components (Oliveri, 2017; Vitale *et al.*, 2023). Thus, in SIMCA, a principal component (PC) model is computed independently for each class of interest defining a class subspace, whose complexity (i.e., number of PCs) should be optimized, and the objects are then classified on the basis of their distances from this space, with larger distances indicating a higher probability that the observation does not belong to the specific class under study (Oliveri, 2017; Vitale *et al.*, 2023). The capability of the principal component analysis (PCA) model to grasp and represent the main features of the class, and consequently the goodness of the classification, strictly depends on the representativeness of the samples used for model calibration, which is a critical aspect to consider in authentication studies. A sound model calibration ensures that the characteristics of each class are adequately captured, independently from that of other classes.

The model can be further optimized working on data pre-processing, which is aimed at the reduction of the noise and the influence of unwanted source of variability from the analytical signal (Yi *et al.*, 2016; Oliveri, 2017; Oliveri *et al.*, 2019). Pre-processing is often necessary for multivariate data sets generated with different analytical procedures, including mass spectrometry (Yi *et al.*, 2016), infrared spectroscopy (Rinnan *et al.*, 2009), Raman, X-ray fluorescence or ultraviolet–visible spectroscopy (UV–Vis) spectroscopy (Oliveri *et al.*, 2019). Selecting the best pre-processing methods depends on the type of data and allows the user to achieve the most reliable and interpretable results. For example, normalization, alignment, peak deconvolution, and baseline corrections are usually carried out for data obtained with chromatographic techniques (Yi *et al.*, 2016). Conversely, averaging and filtering methods or polynomial smoothing can be used to minimize random noise (Oliveri *et al.*, 2019) in spectroscopic studies. However, unwanted signal variations, such as baseline drifts and shifts or global intensity effects, are corrected with standard normal variate (SNV), multiplicative scatter correction (MSC) or derivative functions, among others (Oliveri *et al.*, 2019).

The primary figures of merit derived from the SIMCA model are sensitivity and specificity (Ballabio *et al.*, 2018). Sensitivity is the true positive rate of the model, calculated as the percentage of samples of the target class correctly classified in that class. Consequently, sensitivity decreases if authentic samples are erroneously rejected from the authentic class. In contrast, specificity is the percentage ratio of true negative samples to the total number of actual negative samples. It measures the ability of the model to correctly reject objects that do not belong to the class they represent. Consequently, specificity decreases if samples extraneous to the target class are recognized as belonging to it.

After the original development of SIMCA (Wolde, 1976), new variants have been proposed that basically change the way distances are calculated. The excellent work of Vitale *et al.* (2023) provides a comprehensive overview of all the currently available SIMCA variants.

Conceptual differences between class-modelling and discrimination approaches in the context of food authentication

Discriminant and class-modelling approaches are often misused terms that might create a sort of confusion because, generally speaking, they both assign objects to defined classes (Rodionova *et al.*, 2016a); therefore, they are both grouped in the classification methods in chemometrics. However, they answer different questions. A summary of the differences between the two approaches is depicted in Figure 1. Briefly, the object of discriminant techniques is to find a mathematical function (i.e., a delimiter) able to divide the multivariate space into as many regions as the number of classes (or categories) of the data set (Oliveri, 2017; Vitale *et al.*, 2023; Rodionova *et al.*, 2024). In other words, each object of the data set is always assigned to one of the categories under consideration. The consequences are remarkable. In fact, such a discriminant model, once properly calibrated and validated, is suitable for discriminating samples that must belong to one of the classes in which the model has been trained. Hence, discriminant analysis can be thought of as a proper solution only when the data set comprises well-defined and representative classes, and the end-users are sure that, in the future, the samples to be tested will always be consistent with those classes. A useful feature of types of discriminant analysis, like partial least squares-discriminant analysis (PLS-DA), is that they allow understanding of the contribution of the variables in the discrimination of samples belonging to predefined and well-defined classes (Rodionova *et al.*, 2024). Therefore, it might help in identifying which variables cause the classification. However, apart from those scenarios in which the classes are well defined and limited in number, it is practically impossible to collect or reproduce representative samples from all the possible non-authentic classes that might be encountered as adulterants in an authentication problem. Therefore, it may happen that a new sample whose category was not initially included in the calibration set will be classified in one of classes modelled with a discriminant approach. Consequently, the results of discriminant methods could be biased when applied

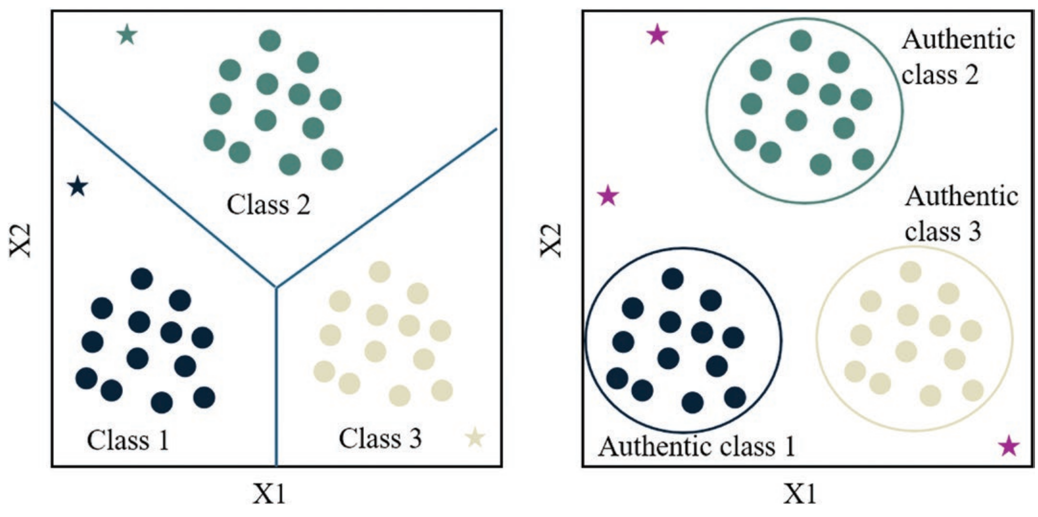

Figure 1. Differences between discriminant (left) and class-modelling (right) approaches built considering three classes. The stars represent hypothetical new samples that do not belong to the modelled classes. In discriminant analysis, these samples could be erroneously classified as belonging to one of the classes, whereas in class modelling, they could be rejected by the model and remain unclassified (Oliveri, 2017; Vitale *et al.*, 2023; Rodionova *et al.*, 2024).

to verify food authenticity (Oliveri, 2017; Vitale *et al.*, 2023; Rodionova *et al.*, 2024), because they cannot correctly classify new samples not belonging to predefined (i.e., calibrated) classes.

Considering the task of establishing the authenticity of a food product, it appears evident that there is just one class of interest, that is, the class 'authentic'. For this reason, one-class classification methods, also known as class-modelling approaches, are recognized as the most suitable in the context of food authentication (Rodionova *et al.*, 2016b, 2024; Oliveri, 2017; de Araújo Gomes *et al.*, 2023; Vitale *et al.*, 2023). These methods basically define a region of the target class (i.e., a class subspace) where samples belonging to it are more likely to be found (Vitale *et al.*, 2023). In other words, the focus is only on one class, the one to be authenticated, and if an object does not match that class' characteristics, it is rejected without necessarily postulating any category for it (i.e., it is not classified but just rejected by the model). For these reasons, one-class classification methods are also defined as 'soft' models with respect to 'hard' discrimination models (Cruz-Tirado *et al.*, 2023).

Examples of discriminant analysis used for food authentication purposes are PLS-DA, linear discriminant analysis (LDA), and support-vector machine (SVM) (Table 1). PLS-DA is one of the most often used, with several articles reporting a comparison between it and class-modelling approaches (Biancolillo *et al.*, 2018; Firmani *et al.*, 2020; Rodionova and Pomerantsev, 2020; Shawky *et al.*, 2020; Le Nguyen Doan *et al.*, 2021; Kharbach *et al.*, 2022; Małyjurek *et al.*, 2022). For a comprehensive discussion of the differences between the algorithms and the purposes of each approach, the readers are warmly invited to explore what has been previously reported in other works (Rodionova *et al.*, 2016a, 2024; Oliveri, 2017; de Araújo Gomes *et al.*, 2023; Vitale *et al.*, 2023).

Sampling is one of the most crucial aspects to consider in food authentication studies. In fact, it is suggested that when using discriminant analysis, each class must be constituted by a significant and representative set of samples, whereas if the target class is only the authentic one, sampling procedures can be focused on just one class (Oliveri, 2017). From a practical point of view, this is a tangible advantage of SIMCA compared to discrimination approaches, because it can be particularly difficult for researchers to plan and collect representative samples of non-authentic food such as all the possible variations of adulteration (Vitale *et al.*, 2023) or food representative of several geographical areas or other non-authentic categories (Oliveri, 2017).

The suitability of SIMCA for food authentication is not only based on the theory behind this algorithm but also supported by several references that identified SIMCA as the best model due to its higher performance compared to others. For example, Biancolillo *et al.* (2018) worked on protected designation of origin (PDO) hazelnut authentication and reported that SIMCA has proven to be especially effective in rejecting samples that do not belong to the target class, suggesting that it is slightly more preferable than the discriminant approach (PLS-DA).

The performance of a model may vary across different samples. For instance, in their work on the determination of adulterated insect flours, Foschi *et al.* (2022) compared SIMCA to sequential preprocessing through orthogonalization discriminant analysis (SPORT-DA). They found that SPORT-DA yielded the best results for cricket flour, correctly classifying all examined samples. However, the classification of buffalo flour was more complex, likely due to its closer composition to whole wheat flour than that of cricket flour. In this case, the SIMCA model was more accurate than the SPORT-DA model, achieving a correct classification rate of 90% for the test samples (Foschi *et al.*, 2022).

Another scenario may occur when the performance of different models varies depending on the data set used as an input. In fact, Dou *et al.* (2024) worked on geographical origin identification of camellia oil based on fatty acid and mineral element profiles and reported comparable results for SIMCA and one-class partial least squares (OC-PLS) when only fatty acid composition was used as the data set, whereas they found even superior performances for OC-PLS when the data were constituted by both fatty acid and mineral element compositions. Another important example is given by Małyjurek *et al.* (2022). The authors worked on three different species of tea and evaluated the models created by PLS-DA and SIMCA. At first glance, the authors reported high performance for both SIMCA and PLS-DA. However, when one of the classes was excluded from the process of model optimization, SIMCA outperformed PLS-DA. This emphasizes the key difference between discriminant and class-modelling analysis.

These examples point out important considerations related to the choice of the models. In fact, it is evident that certain features or variables within the data significantly influence the performance of the model, suggesting that model adaptability to different samples is a critical concern. Then, the importance of proper sampling of the target class emerges, together with the absolute importance of the validation procedures using a well-designed external data set. Moreover, excessive tailoring of the model on the available data set may cause overfitting, which implies exceptional performances on specific data sets but struggling with new or unseen data. In this respect, Brendel *et al.* (2021) reported that SIMCA had comparable performance compared to LDA when a test set was used. However, the advantages of SIMCA emerged when an external test set was introduced into the model, due to its ability to identify outliers. This, again, corroborates the importance of the validation and it underscores the importance of working on the modelling of a single class, following one-class classification approaches.

Cruz-Tirado *et al.* (2023) conducted research on authenticating Sacha inchi oil and compared the performance of two class-modelling approaches, SIMCA and OC-PLS. The study reported that SIMCA exhibited more robust and reliable outcomes compared to the OC-PLS model. The authors suggested that the capability of SIMCA to identify extreme or unusual samples in the test set may have contributed to its superior performance. Similar results were observed by de Souza *et al.* (2021) in their study on adulterant detection in honey.

In contrast, Shawky *et al.* (2020) applied SIMCA class modelling for the authentication of saffron and found that 10% of samples were incorrectly classified as 'unadulterated'. Therefore, the authors proposed PLS-DA as an alternative and more efficient classification modelling technique compared to SIMCA. An interesting methodology approach to utilize both the algorithms can be found in Chen *et al.* (2023). In fact, the authors used SIMCA to classify the edibility categories of wild mushrooms, whereas three other types of discriminant models, that is PLS-DA, random forest (RF), and SVM, were

Table 1. List of the selected articles using the SIMCA model for food authentication

Topic	Food class	Food	Techniques	Type of samples	Algorithms	Main analytes for class modelling	Reference
Adulteration	Alcoholic beverages	Distillate of *Rosa damascena*	Colorimetric sensor arrays and liquid–liquid microextraction–GC-MS	Mixtures	SIMCA, PLS-DA	Colorimetric data and volatile compounds	Mahboubifar *et al.* (2021)
Adulteration	Coffee	Roasted and ground coffee	^{1}H-NMR	Mixtures	SIMCA	Untargeted	Milani *et al.* (2020)
Adulteration	Honey	Honey	LED-based fluorescence spectroscopy (portable)	Mixtures	SIMCA	Untargeted	Suhandy *et al.* (2023)
Adulteration	Honey	Honey	UV–Vis spectroscopy	Mixtures	SIMCA, OC-PLS	Untargeted	de Souza *et al.* (2021)
Adulteration	Milk and dairy	Nigerian fat-filled milk powders	NIR	Mixtures	SIMCA	Untargeted	Ejeahalaka *et al.* (2021)
Adulteration	Milk and dairy	Milk powder	NIR	Mixtures	SIMCA, MCR-ALS	Untargeted	Mazivila *et al.* (2020)
Adulteration	Milk and dairy	Milk powder	NIR	Mixtures	SIMCA	Untargeted	Karunathilaka *et al.* (2018)
Adulteration	Milk and dairy	Milk	NIR (portable) and energy-dispersive X-ray fluorescence (portable)	Mixtures	SIMCA, PLS-DA, C-SVC	Untargeted	Galvan *et al.* (2022)
Adulteration	Milk and dairy	Goat milk	Visible image-based fingerprint	Mixtures	SIMCA, OC-PLS	Untargeted	dos Santos Pereira *et al.* (2022)
Adulteration	Nuts, grains, and flours	Insect flours	ATR-FTIR	Mixtures	SIMCA, SPORT-DA	Untargeted	Foschi *et al.* (2022)
Adulteration	Nuts, grains, and flours	Pistachio	ATR-FTIR (portable) and NIR (portable)	Mixtures	SIMCA	Untargeted	Aykas and Menevseoglu (2021)
Adulteration	Nuts, grains, and flours	Rice	NIR	Mixtures	SIMCA, PLS-DA	Untargeted	Le Nguyen Doan *et al.* (2021)
Adulteration	Nuts, grains, and flours	Almond flour	NIR (portable)	Mixtures	SIMCA, OC-PLS	Untargeted	Netto *et al.* (2023)
Adulteration	Spices and herbs	Cumin powder	NIR hyperspectral imaging	Mixtures	SIMCA	Untargeted	Florián-Huamán *et al.* (2022)
Adulteration	Nuts, grains, and flours	Cassava starch	Raman	Mixtures	SIMCA, OC-SVM	Untargeted	Cardoso and Poppi (2021)
Adulteration	Oils and fats	Avocado oil	ATR-FTIR	Mixtures	SIMCA	Untargeted	Jiménez-Sotelo *et al.* (2016)
Adulteration	Oils and fats	Extra virgin olive oil	NIR	Mixtures	SIMCA	Untargeted	Karunathilaka *et al.* (2016)
Adulteration	Oils and fats	Sacha inchi oil	NIR (portable)	Mixtures	SIMCA, OC-PLS	Untargeted	Cruz-Tirado *et al.* (2023)
Adulteration	Oils and fats	Extra virgin argan oil	Selected-ion flow-tube mass spectrometry (SIFT-MS)	Mixtures	SIMCA, PLS-DA, SVM	Volatile compounds	Kharbach *et al.* (2022)
Adulteration	Spices and herbs	Cinnamon	ATR-FTIR	Mixtures	SIMCA, PLS-DA	Untargeted	Lixourgioti *et al.* (2022)
Adulteration	Spices and herbs	Turmeric powder	ATR-FTIR	Mixtures	SIMCA, PLS-DA	Untargeted	Khodabakhshian *et al.* (2021)
Adulteration	Spices and herbs	Saffron	Elemental analyser; isotopic ratio mass spectrometry (IRMS) and GC–combustion–IRMS	Mixtures	SIMCA, LDA, QDA, PLS-DA	Elemental composition	Ghiasi and Parastar (2021)

Table 1. Continued

Topic	Food class	Food	Techniques	Type of samples	Algorithms	Main analytes for class modelling	Reference
Adulteration	Spices and herbs	Chinese oolong teas	Atmospheric solids analysis probe mass spectrometry	Mixtures	SIMCA, LDA, SVM, kNN	Mass spectral profiles	Tan *et al.* (2022)
Adulteration	Spices and herbs	Oregano	NIR	Authentic, suspicious and mixtures	SIMCA, PLS-DA	Untargeted	Rodionova and Pomerantsev (2020)
Adulteration	Spices and herbs	Saffron	NIR	Mixtures	SIMCA, PLS-DA	Untargeted	Shawky *et al.* (2020)
Adulteration	Spices and herbs	Paprika powder	^{1}H-NMR 400 MHz	Mixtures	SIMCA, OPLS, ROBPCA	Untargeted	Horn *et al.* (2021)
Adulteration	Spices and herbs	Saffron	^{1}H-NMR 60 MHz	Mixtures	SIMCA, OCC-NN, IF	Untargeted	Gunning *et al.* (2023)
Adulteration	Vegetables and fruits	Orange juice	NIR (portable)	Mixtures	SIMCA, PLS-DA	Untargeted	Ehsani *et al.* (2023)
Adulteration and Geographical origin	Meat and fish products	Edible bird's nests	ATR-FTIR	Mixtures	SIMCA	Untargeted	Adenan *et al.* (2020)
Authentication (other)	Alcoholic beverages	Trappist beer	^{1}H-NMR 600 MHz	Authentic	SIMCA, PLS-DA	NMR compound profile	Mannina *et al.* (2016)
Authentication (other)	Bakery products and pasta	Bread from refined flour and whole wheat	UHPLC-HRMS	Authentic	SIMCA	Analytes from mass spectral profiles	Geng *et al.* (2016)
Authentication (other)	Coffee	Instant coffee (expired and decaffeinated)	NIR (portable) and UV–Vis spectroscopy	Authentic	SIMCA	Untargeted	de Araújo *et al.* (2024)
Authentication (other)	Coffee	Gourmet ground roasted coffees	NIR and digital images	Authentic	SIMCA, OC-PLS	Untargeted	de Araújo *et al.* (2021)
Authentication (other)	Meat and fish products	Extensive vs intensive reared pork meat	NIR	Authentic	SIMCA	Untargeted	Totaro *et al.* (2023)
Authentication (other)	Meat and fish products	Pre-sliced MAP Iberian dry-cured loin (commercial categories and storage time)	NIR	Authentic	SIMCA, PLS-DA, LDA	Untargeted	Tejerina *et al.* (2021)
Authentication (other)	Meat and fish products	Tissue origin of bovine gelatin	Raman	Mixtures	SIMCA, PLS-DA	Untargeted	Forooghi *et al.* (2023)
Authentication (other)	Oils and fats	Fish oil supplements	GC×GC-MS	Authentic	SIMCA, OPLS-DA	Fatty acids	Lima *et al.* (2023)
Authentication (other)	Oils and fats	Different categories of olive oils	UHPLC-UV-Vis	Authentic and blends	SIMCA, PLS-DA, SVM	Untargeted	Pérez-Beltrán *et al.* (2022)
Authentication (other)	Spices and herbs	Pure and mixed organic and conventional red pepper powders	Colorimeter (CIE Lab)	Mixtures	SIMCA	Color coordinates	Keskin *et al.* (2022)
Authentication (other)	Vegetables and fruits	Organic tomato and organic sweet pepper	NIR (portable)	Authentic	SIMCA, PLS-DA	Untargeted	de Andrade *et al.* (2023)
Authentication (other)	Vegetables and fruits	Wild bolete mushrooms (edibility and species)	NIR combined with RGB imaging	Authentic	SIMCA, PLS-DA, RF	Untargeted	Chen *et al.* (2023)

Table 1. Continued

Topic	Food class	Food	Techniques	Type of samples	Algorithms	Main analytes for class modelling	Reference
Authentication (species)	Bakery products and pasta	Raw doughs and baked 3D-printed snacks with different insect flours	ATR-FTIR (portable)	Mixtures	SIMCA	Untargeted	García-Gutiérrez *et al.* (2021)
Authentication (species)	Honey	Honey (botanical origin)	MIR spectroscopy vs MALDI-TOF MS	Authentic	SIMCA, PCA-LDA, kNN	Untargeted	Brendel *et al.* (2021)
Authentication (species)	Meat and fish products	Ground meat (beef, pork, and lamb)	NIR	Authentic	SIMCA, OC-PLS	Untargeted	Pieszczek *et al.* (2018)
Authentication (species)	Meat and fish products	Fish fillets and patties (Atlantic cod and haddock)	NIR (portable)	Authentic	SIMCA, LDA	Untargeted	Grassi *et al.* (2018)
Authentication (species)	Milk and dairy	Plastic-packaged cheese slices (cow, sheep, and/or goat)	Raman	Authentic	SIMCA	Untargeted	Arroyo-Cerezo *et al.* (2023)
Authentication (species)	Spices and herbs	Eight types of spice and herbs	HPLC-UV	Authentic	SIMCA, PLS-DA	Phenolic profile	Pages-Rebull *et al.* (2023)
Authentication (species)	Spices and herbs	Three *Cyclopia* species	NIR hyperspectral imaging	Authentic	SIMCA, PLS-DA	Untargeted	Małyjurek *et al.* (2022)
Geographical origin and species authentication	Nuts, grains, and flours	Edible insect powders	ATR-FTIR	Authentic	SIMCA	Untargeted	Mellado-Carretero *et al.* (2020)
Geographical origin	Alcoholic beverages	Pinot noir wine	MP-AES, ICP-MS	Authentic	SIMCA	Elemental composition	Tanabe *et al.* (2020)
Geographical origin	Alcoholic beverages	Sugarcane spirit	NIR	Authentic	SIMCA, OC-PLS	Untargeted	Oliveira *et al.* (2023)
Geographical origin	Bakery products and pasta	PGI pasta	GC-MS	Authentic	SIMCA, UNEQ	Volatile compounds	Giannetti *et al.* (2016)
Geographical origin	Bakery products and pasta	PGI pasta	NIR	Authentic	SIMCA, PLS-DA	Untargeted	Firmani *et al.* (2020)
Geographical origin	Coffee	PDO Brazilian green coffee beans	UV–Vis spectroscopy	Authentic	SIMCA, OC-PLS	Untargeted	dos Santos *et al.* (2023)
Geographical origin	Honey	Argentinean honey	ATR-FTIR, NIR, Raman	Authentic	SIMCA, PLS-DA	Untargeted	Damiani *et al.* (2020)
Geographical origin	Meat and fish products	Baltic sea salmon	GC-MS	Authentic	SIMCA	Dioxin and PCB profiles	Wilde *et al.* (2023)
Geographical origin	Meat and fish products	Amazon stingray	UV–Vis spectral reflectance	Authentic	SIMCA, PLS-DA	Untargeted	de Andrade *et al.* (2024)
Geographical origin	Nuts, grains, and flours	PDO chestnut	NIR	Authentic	SIMCA, PLS-DA	Untargeted	Nardecchia *et al.* (2020)
Geographical origin	Nuts, grains, and flours	Almond avola	NIR	Authentic	SIMCA, PLS-DA	Untargeted	Firmani *et al.* (2019)
Geographical origin	Nuts, grains, and flours	PDO hazelnut	NIR	Authentic	SIMCA, PLS-DA	Untargeted	Biancolillo *et al.* (2018)

Table 1. Continued

Topic	Food class	Food	Techniques	Type of samples	Algorithms	Main analytes for class modelling	Reference
Geographical origin	Oils and fats	Italian extra virgin olive oil	GC×GC-ToF MS	Authentic	SIMCA	Targeted and untargeted volatile compounds	Stilo *et al.* (2021)
Geographical origin	Oils and fats	Changshan camellia oil	GC-MS, ICP-MS	Authentic	SIMCA, OC-PLS, PLS-LDA	Mineral elements and fatty acid profiles	Dou *et al.* (2024)
Geographical origin	Oils and fats	Arbequina extra virgin olive oil	HPLC and GC	Authentic	SIMCA, PLS-DA	Chromatographic fingerprint	Vera *et al.* (2019)
Geographical origin	Oils and fats	Margarines and fat spreads	HPLC-DAD	Authentic	SIMCA, PLS-DA	Fatty acids finger-print	Bikrani *et al.* (2019)
Geographical origin	Oils and fats	Tunisians virgin olive oils	NIR and GC-FID	Authentic	SIMCA	NIR spectra and fatty acids	Laroussi-Mezghani *et al.* (2015)
Geographical origin	Oils and fats	Les Garrigues extra virgin olive oil	Raman	Authentic	SIMCA	Untargeted	Ruisánchez *et al.* (2021)
Geographical origin	Oils and fats	Packaged margarines and spreads	Raman	Authentic	SIMCA, PLS-DA, SVM	Untargeted	Jimenez-Carvelo *et al.* (2022)
Geographical origin	Spices and herbs	PDO saffron	ICP-MS	Authentic	SIMCA, UNEQ, LDA	Elemental composition	D'Archivio *et al.* (2019)
Geographical origin	Spices and herbs	Italian bell pepper	ICP-OES	Authentic	SIMCA	Elemental composition	Di Donato *et al.* (2023)
Geographical origin	Spices and herbs	Spanish PDO paprika types	Differential mobility spectrometry coupled to MS	Authentic	SIMCA, PLS-DA	Untargeted	Campmajó *et al.* (2022)
Geographical origin and species authentication	Honey	Honeys of different botanical, entomological and geographical Origins	UV spectroscopy	Authentic	SIMCA	Untargeted	Suhandy and Yulia (2021)

ATR-FTIR: attenuated total reflectance-Fourier transform infrared spectroscopy; CIE: International Commission on Illumination; C-SVC: C-support vector classification; ICP-MS: Inductively coupled plasma mass spectrometry; ICP-OES: inductively coupled plasma optical emission spectrometry; IF: isolation forests; GC: gas chromatography; GC-FID: gas chromatography-flame ionization detector; GC×GC-ToF MS: comprehensive two-dimensional gas chromatography with time of flight mass spectrometry; GC-MS: gas chromatography-mass spectrometry; 1H-NMR: proton nuclear magnetic resonance; HPLC-DAD: high-performance liquid chromatography with diode-array detection; HPLC-UV: high-performance liquid chromatography-ultraviolet; kNN: k-nearest neighbors; MCR-ALS: multivariate curve resolution–alternating least squares; MP-AES: microwave plasma atomic emission spectrometry; OCC-NN: one-class classification using nearest neighbors; OPLS: orthogonal partial least square; OPLS-DA: orthogonalized partial least square discriminant analysis; QDA: quadratic discriminant analysis; RF: random forests; RGB: red, green, blue; ROBPCA: robust principal component analysis; UHPLC-HRMS: ultra-high performance liquid chromatography coupled with high-resolution mass spectrometry; UNEQ: unequal dispersed classes.

used for the discrimination of multiple species. In the end, although comparisons of the different chemometric approaches at disposal for addressing classification issues are undoubtedly useful, we should recall that these comparisons could be misleading. Indeed, as reported by Rodionova *et al.* (2024), SIMCA and PLS-DA, the most commonly used algorithms, belong to different areas and are not comparable. As already mentioned, SIMCA, and more generally, class-modelling approaches, are the most appropriate in the authentication context, and in accordance with this conclusion, this review is focused on the use of SIMCA in the food context.

Literature search and data elaboration

This review is based on a literature search carried out using the Scopus scientific database, considering all the works published in a ten-year range from 2015 to present (1 January 2024). Specifically, the terms 'SIMCA' and 'Food' and 'Authentication' were searched within the title, abstract, and keywords of the articles. The outcome of this search yielded a total of 76 articles, comprising 71 research papers, 3 reviews, and 1 conference paper. One article was excluded because it did not use the SIMCA model for food authentication. To ensure a focused discussion, the review primarily concentrates on 71 research papers, excluding reviews and conference paper from the detailed analysis.

Food authentication research using SIMCA: aims, methodologies, and food products

The discussion of the research articles selected for this review is structured around three significant aspects, (i) the aims of the research, (ii) the technologies used for food authentication, and (iii) the food products under investigation. By structuring the review around these key elements, we aim to offer readers a comprehensive and insightful exploration of the research landscape related to SIMCA and food authentication over the specified ten-year period.

Aims and scope of the research articles

The research conducted within the context of food authentication addresses several scopes, as shown in the pie charts depicted in Figure 2. Overall, the application of SIMCA can be considered as a versatile tool in the field of food authentication and can be applied in a wide range of cases to address the multifaceted aspects of the authenticity of food products throughout several supply chains. At least three distinct aspects emerge as key topics for food authentication efforts, whereas there are other authentication problems that regard various foods and aims.

Adulterant detection has emerged as the most extensively investigated issue in the reviewed research articles, constituting a total of 29 of 71 articles. Adulteration is the fraudulent practice of intentionally adding a component to food which is not the result of food production (Robson *et al.*, 2021). The term 'adulteration' commonly refers to the addition of a foreign or inferior substance to the product, and may be also associated with the term 'tempering' (Robson *et al.*, 2021). However, they have slightly different meanings. In fact, the European Committee for Standardization (CEN) defines 'tempering' as subjecting a product to an undeclared process involving the removal of a component that should have been present in a product (Robson *et al.*, 2021). In order to detect adulteration in food, the common strategy is to add the adulterant substance into the authentic product using predefined or increasing concentrations. This approach also aims to increase the number of samples available for the analysis, which is fundamental to ensure robustness of the model. For example, Lixourgioti *et al.* (2022) evaluated the adulteration of cinnamon designing two different scenarios, namely two species of cinnamon adulterated with the by-product of cinnamon essential oil extraction at concentrations of 1%–99% (volume fraction), reaching 110 mixtures. The strategy of using increasing concentration of adulterants was similar to that used by other authors for detecting the adulteration of heterogeneous mixtures like spices and herbs (Shawky *et al.*, 2020; Khodabakhshian *et al.*, 2021; Florián-Huamán *et al.*, 2022; Tan *et al.*, 2022), rice grains (Le Nguyen Doan *et al.*, 2021), and almond flours (Netto *et al.*, 2023). This approach can also be used for homogeneous mixtures containing adulterant substance, such as vegetable oils (Jiménez-Sotelo *et al.*, 2016; Karunathilaka *et al.*, 2016; Kharbach *et al.*, 2022), honey (de Souza *et al.*, 2021; Suhandy *et al.*, 2023), or milk (Galvan *et al.*, 2022). This emphasis underscores the significance of fighting adulteration practices within the food industry. In fact, the number of articles focusing on adulterant detection may be explained by the relevance of adulteration practices in the food industry. For instance, a recent report evaluated food authenticity issues in the beef supply chain, finding that adulteration, together with counterfeiting, was the most diffuse food fraud in that sector (Robson *et al.*, 2020). Counterfeiting is the fraudulent and complete replication of a food product, including packaging (Robson *et al.*, 2020); therefore, it may happen in a broader number of occasions compared to adulteration.

The verification of geographical origin was the objects of 24 articles. The verification of the product categories or of the raw materials used for food production can be considered to be related to counterfeiting and mislabelling.

In the case of geographical authentication, the analytical approach for sampling appeared to be different from that for the adulterant detection. In fact, in the reviewed articles, the usual sampling methods consist of the collection of authentic products from the geographical area of interest, without producing blends or mixtures of products. This implies that the collection must be carried out with trusted companies and suppliers to build a robust and truthful model. Following this kind of sampling, the application of SIMCA algorithms to the data allowed correct authentication of the geographical origin of a wide range of food categories such as vegetable oils (Laroussi-Mezghani *et al.*, 2015; Vera *et al.*, 2019; Stilo *et al.*, 2021; Dou *et al.*, 2024), honey (Damiani *et al.*, 2020; Suhandy and Yulia, 2021), fish and fish products (Wilde *et al.*, 2023; de Andrade *et al.*, 2024), and several other food categories, as discussed in the next section. Moreover, the geographical origin of products has a relevant importance, especially from an economic point of view. For instance, some food products are protected by geographical indications quality marks that are regulated by the European Union. These marks enable consumers to trust and distinguish quality products while also helping producers market their products more easily and with greater remunerability. This principle can also be extended to all products made with peculiar raw materials or using distinctive processing that enhances their value. For example, studies have demonstrated that applying the SIMCA algorithm to volatile compounds (Giannetti *et al.*, 2016) or

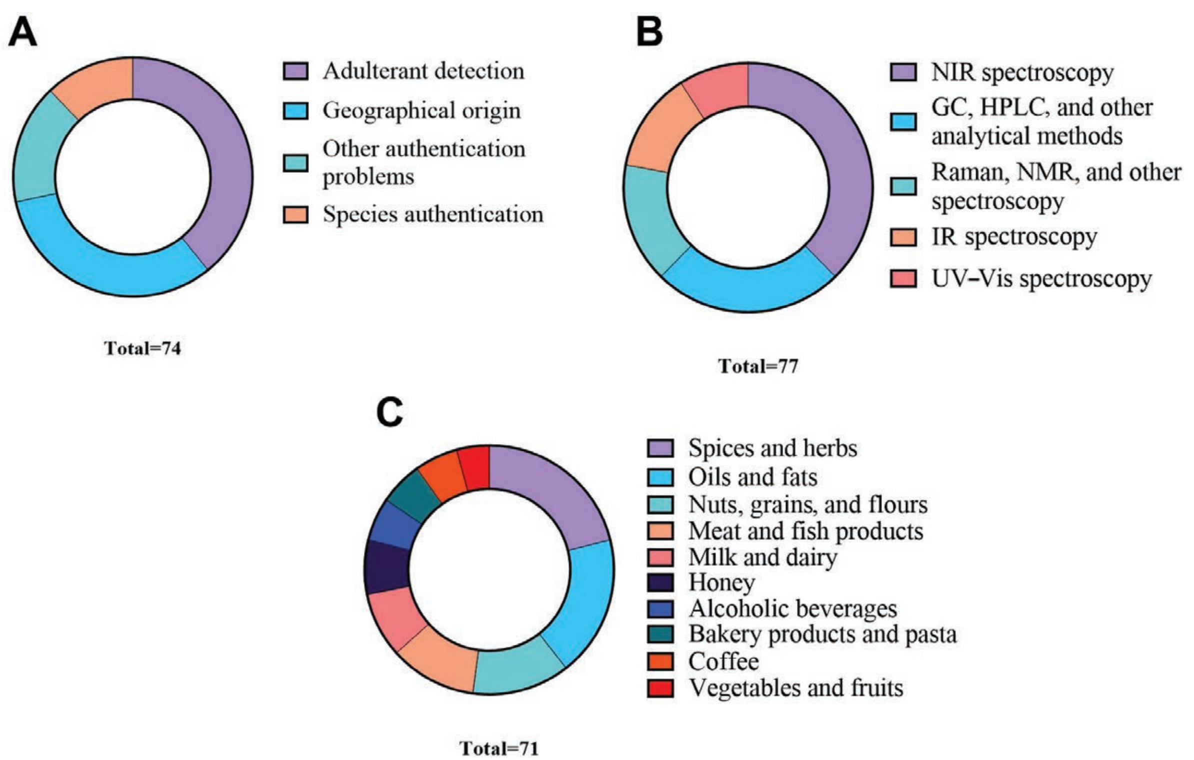

Figure 2. Pie charts depicting the results of the literature search, dividing the articles by authentication topics (A), utilized techniques (B), and food classes (C). The legend items are listed in decreasing order. GC: gas chromatography; HPLC: high-performance liquid chromatography.

near-infrared (NIR) spectra (Firmani *et al.*, 2020) enables the accurate classification of protected geographical indication (PGI) pasta di Gragnano from common pasta. Additional examples that include product with geographical indication marks are the PDO products such as paprika (Campmajó *et al.*, 2022) or hazelnut (Biancolillo *et al.*, 2018).

For the authentication of the geographical origin, other authentication problems are not usually addressed by preparing artificial mixtures of non-authentic product to increase the data set for class modelling. Hence, in this scenario, meaningful and representative sampling remains crucial for the development of the model. Again, as previously discussed, the working principle of SIMCA may facilitate sampling, being solely focused on the target class. Furthermore, SIMCA has shown the ability to authenticate a wide range of food categories, such as the classification of Trappist beer with respect to conventional beer (Mannina *et al.*, 2016), fat of pork meat derived from extensive rearing systems with respect to intensive ones (Totaro *et al.*, 2023), and non-expired or decaffeinated coffee samples against expired and non-decaffeinated ones (de Araújo *et al.*, 2024).

The verification of the species used in a food product is another aspect of food authentication that can be explored using analytical technologies combined with the SIMCA algorithm. This scope becomes particularly relevant when a specific species confers added value to the product. This may be the case for honeys (Brendel *et al.*, 2021; Suhandy and Yulia, 2021), peculiar spices and herbs (Małyjurek *et al.*, 2022; Pages-Rebull *et al.*, 2023), and meat (Pieszczek *et al.*, 2018) and fish (Grassi *et al.*, 2018) products.

Technologies used for food authentication

Various technologies play a crucial role in ensuring the authenticity of food products, employing a diverse range of analytical methods for the determination of chemical properties or the acquisition of untargeted chemical profiles. Figure 2 illustrates the technologies utilized in the selected articles, whereas Table 1 provides a detailed overview of the technologies employed in each article considered for this review. There is a noteworthy prevalence of non-destructive spectroscopic technologies, with NIR spectroscopy being particularly dominant. In fact, 29 research articles studied food authentication by means of NIR spectroscopy. Additionally, other rapid and non-destructive techniques include UV–Vis spectroscopy, Fourier transform infrared (FTIR), Raman, and nuclear magnetic resonance (NMR).

Traditional analytical methods also commonly used to obtain specific chemical information for food authentication. Chromatographic methods, among others, are frequently employed for authentication purposes. In particular, the combination of chromatographic separation with mass spectrometers has emerged as a widely utilized approach for food authentication. Dou *et al.* (2023) comprehensively reviewed the use of mass spectrometry for food authentication. In fact, mass spectrometry allows quantification and identification of analytes with high sensitivity and resolution, which makes it suitable for metabolomic fingerprinting (Dou *et al.*, 2023).

However, spectroscopic techniques in the context of food authentication offer distinct advantages, explaining the large focus on these technologies in the majority of the reviewed articles. In particular, they are rapid, non-destructive, and low-cost, and do not require any solvent or sample preparation, with consequent benefits for the environment and for the applicability in the agri-food supply chain. One of the main strengths of these spectroscopic techniques is that the common approach used for this kind of analysis is untargeted, meaning that only spectral elaboration is needed to construct a model that can guarantee the authentication of food. Examples of untargeted approaches can be found in Karunathilaka *et al.* (2016, 2018), Grassi *et al.* (2018), Rodionova and Pomerantsev (2020), and Suhandy *et al.* (2023). However, as reported in Table 1, untargeted approaches were also utilized with data obtained via chromatography or other analytical techniques.

Interestingly, Brendel *et al.* (2021) compared the class models for honey authentication, using infrared (IR) spectra and the data acquired with matrix-assisted laser desorption ionization–time of flight mass spectrometry (MALDI-ToF MS) and found better performance in validating the IR data compared to the MALDI-ToF MS data. The authors also pointed out that the higher reproducibility of spectroscopic analysis can better guarantee the authenticity control in the supply chain. By contrast, Laroussi-Mezghani *et al.* (2015) evaluated the performance of SIMCA for the classification of olive oils based on NIR spectra and fatty acid composition, finding more accurate classifications using conventional analysis than using NIR. Most likely, fatty acid composition is a very specific and targeted analysis for oils and fat, and this can guarantee better performance compared to untargeted analysis.

Another interesting point of spectroscopic technologies is related to the possibility of acquiring spectra using handheld portable instruments. In fact, numerous studies have demonstrated that successful SIMCA models can be built using the data obtained with portable devices. In particular, according to the analysis of the articles selected for this review, the majority of the studies focusing on portable instruments have prominently utilized NIR technology (Grassi *et al.*, 2018; Karunathilaka *et al.*, 2018; Le Nguyen Doan *et al.*, 2021; Cruz-Tirado *et al.*, 2023; de Andrade *et al.*, 2023; Ehsani *et al.*, 2023; Netto *et al.*, 2023; de Araújo *et al.*, 2024). Furthermore, examples of applications of other portable equipments include (i) portable Raman spectrometers used for the authentication of margarines (Jimenez-Carvelo *et al.*, 2022) or sliced cheeses (Arroyo-Cerezo *et al.*, 2023); (ii) portable energy-dispersive X-ray fluorescence spectrometer utilized for milk authentication (Galvan *et al.*, 2022); and (iii) a portable Fourier-transform mid-infrared (FT-MIR) instrument to detect adulteration in pistachio (Aykas and Menevseoglu, 2021). It is noteworthy that most of the articles discussing the use of portable instruments are very recent, demonstrating that technology improvements have been made in recent years. These advancements support the utilization of portable spectroscopic devices at different points of the supply chain, starting from the fields of process monitoring and quality control during manufacturing and distribution. Moreover, the cost-effectiveness of portable devices should be emphasized, because they are more accessible than conventional bench spectrometers (Galvan *et al.*, 2022; de Andrade *et al.*, 2023).

Other innovative applications that exploit IR or NIR radiation involve the utilization of imaging techniques such as hyperspectral imaging. The advantage of this technology consists in the acquisition of both spatial and spectral information, providing insights into the distribution of the components in a food matrix (Squeo *et al.*, 2022), which is valuable for food authentication purposes. For instance, Florián-Huamán *et al.* (2022) used hyperspectral imaging combined with NIR for the quantitative detection of peanut shell, pecan shell and walnut shell in cumin powder, because they are common adulterants in this spice. Małyjurek *et al.* (2022) worked on the authentication of three *Cyclopia* species, *C. intermedia*, *C. genistoides*, and *C. subternata*, which are used for the production of honeybush tea. In both cases, high sensitivity and specificity were reached by the authors.

In addition to the application of the class modelling for food authentication, the advantages of using spectroscopic technologies include the possibility of predicting the amount of adulterant in food through multivariate regression modelling, such as PLS (Jiménez-Sotelo *et al.*, 2016; Shawky *et al.*, 2020; Florián-Huamán *et al.*, 2022; Kharbach *et al.*, 2022; Netto *et al.*, 2023) or principal component regression (PCR) (Suhandy *et al.*, 2023).

Food product object of authentication using SIMCA

The food products addressed in the selected articles are illustrated in Figure 2, and most of the case studies have been discussed in the previous sections, providing insights into the context of SIMCA and of the analytical methods used for the authentication purposes.

Spices and herbs emerge as the most extensively investigated food categories, with 15 articles, followed by oils and fats (13 articles), and nuts, grains, and flour (9 articles). In fact, spices and herbs, together with oils and fats, are particularly susceptible to adulteration and food fraud (Van Ruth *et al.*, 2018). The motivations behind the need to authenticate such products are often related to their economic value. For instance, among spices and herbs, saffron (*Crocus sativus* L.) has attracted particular interest, because it is one of the most expensive spices and it is very easy to adulterate with foreign plant materials. In fact, SIMCA has been applied to detect adulteration of saffron by Shawky *et al.* (2020), Ghiasi and Parastar (2021), and Gunning *et al.* (2023), whereas only D'Archivio *et al.* (2019) authenticated the geographical origin of the products, focusing on the denominated 'Zafferano dell'Aquila', which is one of the five saffron spices produced in Europe that has the PDO quality mark.

Among oils and fat, the authentication of extra virgin olive oil is predominant, especially to detect adulteration with other oils with lower quality and from other species (Karunathilaka *et al.*, 2016) or verify the geographical origin (Laroussi-Mezghani *et al.*, 2015; Vera *et al.*, 2019; Stilo *et al.*, 2021), which is a quality marker for this kind of product.

Most of the research carried out on nuts, grains, and flours has been aimed at adulterant detection (Aykas and Menevseoglu, 2021; Le Nguyen Doan *et al.*, 2021; Foschi *et al.*, 2022; Netto *et al.*, 2023), but there are examples of the successful application of SIMCA to authenticate products with geographical quality marks, such as a PDO hazelnut (Biancolillo *et al.*, 2018), PDO chestnut (Nardecchia *et al.*, 2020), and prodotto agroalimentare tradizionale (PAT, traditional Italian agri-food product) almond (Firmani *et al.*, 2019).

Six articles focused on milk and dairy products, five of which were aimed at identifying adulterants in the products (Karunathilaka *et al.*, 2018; Mazivila *et al.*, 2020; Ejeahalaka *et al.*, 2021; dos Santos Pereira *et al.*, 2022; Galvan *et al.*, 2022). Therefore, the relevance of adulterant practices is again highlighted.

Honey is the object of five articles. It has been reported that honey is susceptible to at least five distinct food frauds, including adulteration with sugar-based syrups, mislabelling concerning geographical origin or botanical species, and non-declared practices in bee feeding and illegal practices in product processing (de Souza *et al.*, 2021). However, among these, adulteration is the most prevalent food fraud (de Souza *et al.*, 2021).

Interestingly, Chen *et al.* (2023) used NIR spectroscopy in combination with SIMCA to authenticate wild mushrooms, having edibility/non-edibility as a target class.

Overall, the articles collectively cover a broad spectrum of food categories, representing those most prone to adulteration globally (Van Ruth *et al.*, 2018; Aslam *et al.*, 2023). For more in-depth insights into prevalent food fraud, interested readers are invited to refer to detailed reports elsewhere (Tähkäpää *et al.*, 2015; Zhang and Xue, 2016; Van Ruth *et al.*, 2018; Visciano and Schirone, 2021; Aslam *et al.*, 2023).

Challenges and future perspectives of food authentication

From the analysis of the literature, the challenges and some points of interest for future research can be highlighted, as summarized in Figure 3. One of the main challenges with authentication models (but in general with predictive models) is assessing their performances when applied to new samples, confirming their reliability in real-case scenarios. In other words, the models should be properly validated. The importance of validation has already been emphasized in other review articles (Oliveri, 2017; Pomerantsev and Rodionova, 2021; Lopez *et al.*, 2023; Vitale *et al.*, 2023). The recommended strategy for validating a model is to use an external test set of samples. The test set can be randomly selected from the entire data set or, preferably, selected using specific algorithms such as Kennard-Stone (Oliveri, 2017; Lopez *et al.*, 2023). Typically, 10%–50% of the samples are used for the test set (Oliveri, 2017), and these samples should represent the largest variability within the data set (Vitale *et al.*, 2023). To mitigate the risk of overfitting, Oliveri (2017) suggested using three data subsets: a training set, an optimization set (for model tuning), and a test set for validation. Cross-validation or other resampling methods (e.g. jackknife and bootstrap) can be employed, and are even suggested, when the number of samples is limited (Pomerantsev and Rodionova, 2021; Lopez *et al.*, 2023). However, it should be considered that the predictive ability of the model might be overestimated. In the particular case of the optimization and validation of one-class models, a methodological and theoretical debate has arisen leading to the identification of two distinct approaches: rigorous and compliant (Rodionova *et al.*, 2016b). The former requires that the model should be trained and optimized only based on the target class under study, in accordance with the specific aim of one-class classification study. On the other hand, the compliant approach makes use of samples from the alien class(es), both to optimize the model and to evaluate its performance, particularly its specificity. The rigorous approach has been identified as the most appropriate in the context of food authentication, although, depending on the cases, the compliant could provide more reliable results (Rodionova *et al.*, 2016b), but the challenge moves to how the alien class should be chosen. Some hints about this aspect have been reported in the literature (Rodionova *et al.*, 2019, 2024).

Regarding the food product object of authentication studies, it is worth noting that most of the articles focus on well-established food products, with limited attention given to innovative foods incorporating novel ingredients or technologies. For example, only three articles specifically address the authentication of insect flours (Mellado-Carretero *et al.*, 2020; Foschi *et al.*, 2022) or bakery products made with insect flour (García-Gutiérrez *et al.*, 2021).

Surprisingly, there is a notable lack of articles investigating potential adulteration or authentication issues in foods made with alternative protein sources like meat analogues and dairy alternatives, despite the rapid growth and development of such products. In fact, to the best of the authors' knowledge, only

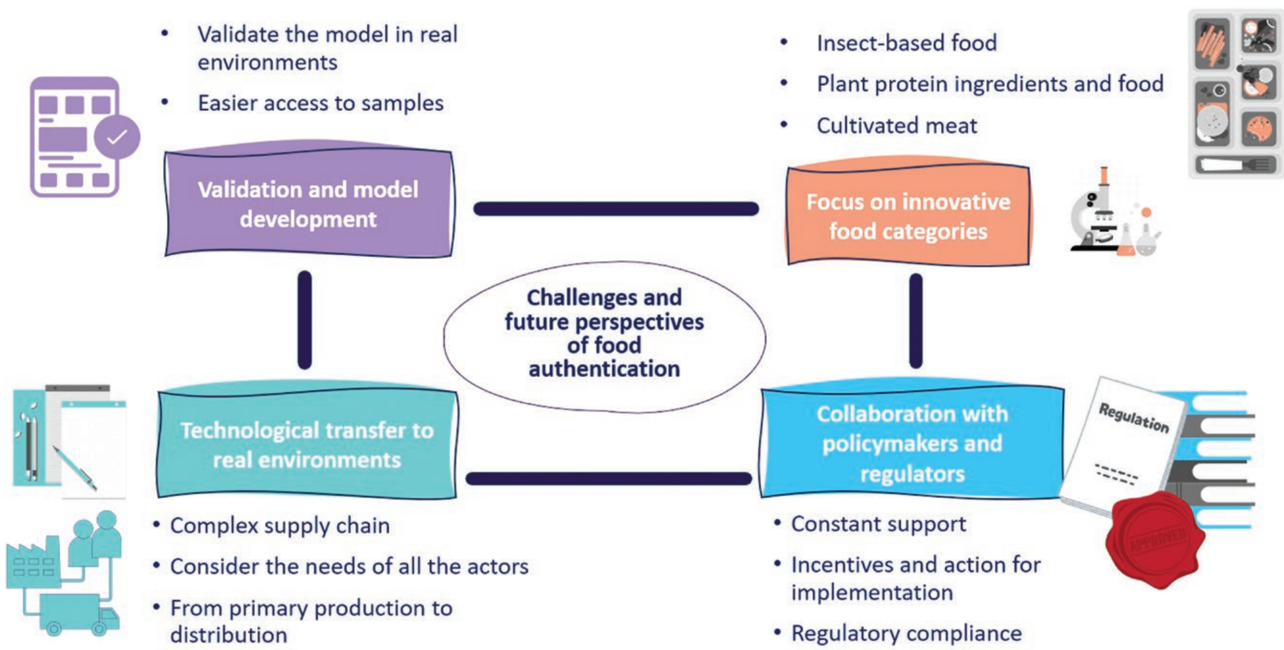

Figure 3. Summary of the challenges and future perspectives for food authentication studies.

Neves *et al.* (2022) worked on the detection of adulterants in plant-based proteins using FT-NIR. However, the authors did not use SIMCA, but reported the results for OC-PLS and PLS-DA. Some authors have highlighted the lack of regulations in this sector (Wickramasinghe *et al.*, 2021), underscoring the urgency for further research in this field. Authentication issues in innovative food products may manifest in various ways, such as the presence of undeclared protein sources that could potentially trigger allergies or intolerances. Common examples include soy protein and wheat gluten, which are prevalent ingredients in the preparation of alternative foods. Furthermore, the evaluation of food derived from cellular agriculture remains largely unexplored within the context of food authentication. For example, future requirements may involve verifying the presence of cultivated meat in traditional meat products and vice versa. This aspect is particularly relevant considering both the skepticism and the concerns related to this kind of product as well as the motivated interest in developing sustainable food alternatives (Rasmussen *et al.*, 2024).

The dynamic nature of these markets and the evolving regulatory landscape highlight the critical need for ongoing research to ensure the authenticity and safety of emerging food products.

Other aspects that could be further explored include strategies for validating models for food authenticity in the relevant environments of supply chains. For instance, as recently noted by McVey *et al.* (2021), technological advancements in food authentication may lack significance if they cannot be integrated into digitalization networks that facilitate comprehensive traceability, transparency, and fraud prevention across the entirety of the food supply chain, even with real-time output generation capabilities. Implementing such systems would pose particular challenges, given the diverse needs and infrastructures across different segments of the food supply chain. For instance, primary producers may have vastly different requirements compared to the food industry and retailers and distributors. Access to information technologies and the Internet in agricultural fields may be given as a simple example in this context and highlights logistical challenges across the supply chain.

Moreover, the implementation of such technologies in a real environment must be accompanied by constant discussion with policymakers and regulators. Their decisions and actions can have a significant impact on the development and implementation of innovative solutions for food authentication. Such actors should promote initiatives, incentives, and programs that enable the technological transfer across the supply chain, as well as support innovations in food authenticity to achieve regulatory compliance.

Conclusions

The application of SIMCA in the context of food authentication demonstrated successful applications. SIMCA, as other class-modelling approaches, emphasizes the characterization of each class, focusing on the similarities among samples and capturing the characteristics of each class of interest. This advantage of SIMCA over other discriminant methods is a key feature that allows to have robust but simple classification models, even when data set is modified after model building. This aspect has been discussed in this review and it has been proven by the given references.

The predominant use of non-destructive technologies in food authentication research underscores the industry's emphasis on rapid, efficient, and environmentally friendly analytical methods. In particular, recent advancements in portable devices for spectroscopic analysis have shown high potential for guaranteeing food authenticity. However, the current literature research revealed limited studies and applications, suggesting the need for a further focus on this topic.

Adulteration studies often involve the creation of artificial adulterated mixtures, but it is crucial to recognize the significance of authentic sample collection for addressing various purposes in the context of food authentication.

One of the main challenges of the models is validation in real-case applications. Moreover, as future perspectives, a clear need to shift attention towards emerging food products, including insects, meat analogues, alternative proteins, and food derived from cellular agriculture has emerged. In fact, the dynamic nature of the food supply chain requires continuous adaptation, and future research should be aimed at addressing the authentication needs of these innovative products. Additional efforts should be taken to promote the transfer of the analytical methodologies and SIMCA models in the real and relevant environments of the supply chain, considering the challenges given by the complexity of the systems and the needs of constant collaboration with policymakers and regulators.

Author Contributions

Davide De Angelis: Conceptualization, investigation, visualization, writing original draft, and review and editing; Antonella Pasqualone: Review and editing; Michele Faccia: Project administration and review and editing; Carmine Summo: Project administration and review and editing; Giacomo Squeo: Conceptualization, investigation, writing original draft, and review and editing

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Conflicts of Interest

The authors declare no conflict of interest.

References

Adenan, M. N. H., Moosa, S., Muhammad, S. A., *et al.* (2020). Screening Malaysian edible bird's nests for structural adulterants and geographical origin using Mid-Infrared–Attenuated Total Reflectance (MIR-ATR) spectroscopy combined with chemometric analysis by Data-Driven–Soft Independent Modelling of Class Analogy (DD-SIMCA). *Forensic Chemistry*, 17: 100197.

Arroyo-Cerezo, A., Jiménez-Carvelo, A. M., González-Casado, A., *et al.* (2023). The potential of the spatially offset Raman spectroscopy (SORS) for implementing rapid and non-invasive in-situ authentication methods of plastic-packaged commodity foods—application to sliced cheeses. *Food Control*, 146: 109522.

Aslam, R., Sharma, S. R., Kaur, J., *et al*. (2023). A systematic account of food adulteration and recent trends in the non-destructive analysis of food fraud detection. *Journal of Food Measurement and Characterization*, 17(3): 3094–3114.

Aykas, D. P., Menevseoglu, A. (2021). A rapid method to detect green pea and peanut adulteration in pistachio by using portable FT-MIR and FT-NIR spectroscopy combined with chemometrics. *Food Control*, 121: 107670.

Ballabio, D., Grisoni, F., Todeschini, R. (2018). Multivariate comparison of classification performance measures. *Chemometrics and Intelligent Laboratory Systems*, 174: 33–44.

Biancolillo, A., De Luca, S., Bassi, S., *et al*. (2018). Authentication of an Italian PDO hazelnut ('Nocciola Romana') by NIR spectroscopy. *Environmental Science and Pollution Research*, 25: 28780–28786.

Bikrani, S., Jiménez-Carvelo, A. M., Nechar, M., *et al*. (2019). Authentication of the geographical origin of margarines and fat-spread products from liquid chromatographic UV-absorption fingerprints and chemometrics. *Foods*, 8(11): 588.

Brendel, R., Schwolow, S., Gerhardt, N., *et al*. (2021). MIR spectroscopy versus MALDI-ToF-MS for authenticity control of honeys from different botanical origins based on soft independent modelling by class analogy (SIMCA)—a clash of techniques? *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 263: 120225.

Campmajó, G., Saurina, J., Núñez, O., *et al*. (2022). Differential mobility spectrometry coupled to mass spectrometry (DMS–MS) for the classification of Spanish PDO paprika. *Food Chemistry*, 390: 133141.

Cardoso, V. G. K., Poppi, R. J. (2021). Cleaner and faster method to detect adulteration in cassava starch using Raman spectroscopy and one-class support vector machine. *Food Control*, 125: 107917.

Chen, J., Liu, H., Li, T., *et al*. (2023). Edibility and species discrimination of wild bolete mushrooms using FT-NIR spectroscopy combined with DD-SIMCA and RF models. *LWT-Food Science and Technology*, 180: 114701.

Consonni, R., Cagliani, L. R. (2019). The potentiality of NMR-based metabolomics in food science and food authentication assessment. *Magnetic Resonance in Chemistry*, 57(9): 558–578.

Creydt, M., Fischer, M. (2019). Blockchain and more—algorithm driven food traceability. *Food Control*, 105: 45–51.

Cruz-Tirado, J. P., Muñoz-Pastor, D., de Moraes, I. A., *et al*. (2023). Comparing data-driven soft independent class analogy (DD-SIMCA) and one-class partial least square (OC-PLS) to authenticate sacha inchi (*Plukenetia volubilis* L.) oil using portable NIR spectrometer. *Chemometrics and Intelligent Laboratory Systems*, 242: 105004.

D'Archivio, A. A., Di Vacri, M. L., Ferrante, M., *et al*. (2019). Geographical discrimination of saffron (*Crocus sativus* L.) using ICP-MS elemental data and class modeling of PDO Zafferano dell'Aquila produced in Abruzzo (Italy). *Food Analytical Methods*, 12(11): 2572–2581.

Damiani, T., Alonso-Salces, R. M., Aubone, I., *et al*. (2020). Vibrational spectroscopy coupled to a multivariate analysis tiered approach for Argentinean honey provenance confirmation. *Foods*, 9(10): 1450.

de Andrade, J. C., Galvan, D., Effting, L., *et al*. (2023). An easy-to-use and cheap analytical approach based on NIR and chemometrics for tomato and sweet pepper authentication by non-volatile profile. *Food Analytical Methods*, 16(3): 567–580.

de Andrade, J. C., de Oliveira, A. T., Amazonas, M. G. F. M., *et al*. (2024). Fingerprinting based on spectral reflectance and chemometrics—an analytical approach aimed at combating the illegal trade of stingray meat in the Amazon. *Food Chemistry*, 436: 137637.

de Araújo, T. K. L., Nóbrega, R. O., de Sousa Fernandes, D. D., *et al*. (2021). Non-destructive authentication of Gourmet ground roasted coffees using NIR spectroscopy and digital images. *Food Chemistry*, 364: 130452.

de Araújo, T. K. L., da Silva Lyra, W., da Silva, J. D. S., *et al*. (2024). Authentication of the shelf-life and decaffeination process of instant coffee samples using UV–Vis and NIR spectral fingerprints. *Food Control*, 155: 110098.

de Araújo Gomes, A., Azcarate, S. M., Špánik, I., *et al*. (2023). Pattern recognition techniques in food quality and authenticity: a guide on how to process multivariate data in food analysis. *TrAC Trends in Analytical Chemistry*, 164: 117105.

de Souza, R. R., de Sousa Fernandes, D. D., Diniz, P. H. G. D. (2021). Honey authentication in terms of its adulteration with sugar syrups using UV–Vis spectroscopy and one-class classifiers. *Food Chemistry*, 365: 130467.

Di Donato, F., Biancolillo, A., Foschi, M., *et al*. (2023). Authentication of typical Italian bell pepper spices by ICP-OES multi-elemental analysis combined with SIMCA class modelling. *Journal of Food Composition and Analysis*, 115: 104948.

Di Rienzo, V., Miazzi, M. M., Fanelli, V., *et al*. (2016). An enhanced analytical procedure to discover table grape DNA adulteration in industrial musts. *Food Control*, 60: 124–130.

dos Santos, L. B., Tarabal, J., Sena, M. M., *et al*. (2023). UV–Vis spectroscopy and one-class modeling for the authentication of the geographical origin of green coffee beans from Cerrado Mineiro, Brazil. *Journal of Food Composition and Analysis*, 123: 105555.

dos Santos Pereira, E. V., de Sousa Fernandes, D. D., de Almeida, L. F., *et al*. (2022). Goat milk authentication by one-class classification of digital image-based fingerprint signatures: detection of adulteration with cow milk. *Microchemical Journal*, 180: 107640.

Dou, X., Zhang, L., Yang, R., *et al*. (2023). Mass spectrometry in food authentication and origin traceability. *Mass Spectrometry Reviews*, 42(5): 1772–1807.

Dou, X., Wang, X., Ma, F., *et al*. (2024). Geographical origin identification of camellia oil based on fatty acid profiles combined with one-class classification. *Food Chemistry*, 433: 137306.

Ehsani, S., Yazdanpanah, H., Parastar, H. (2023). An innovative screening approach for orange juice authentication using dual portable/handheld NIR spectrometers and chemometrics. *Microchemical Journal*, 194: 109304.

Ejeahalaka, K. K., Mclaughlin, P., On, S. L. (2021). Monitoring the composition, authenticity and quality dynamics of commercially available Nigerian fat-filled milk powders under inclement conditions using NIRS, chemometrics, packaging and microbiological parameters. *Food Chemistry*, 339: 127844.

Firmani, P., Bucci, R., Marini, F., *et al*. (2019). Authentication of 'Avola almonds' by near infrared (NIR) spectroscopy and chemometrics. *Journal of Food Composition and Analysis*, 82: 103235.

Firmani, P., La Piscopia, G., Bucci, R., *et al*. (2020). Authentication of PGI Gragnano pasta by near infrared (NIR) spectroscopy and chemometrics. *Microchemical Journal*, 152: 104339.

Florián-Huamán, J., Cruz-Tirado, J. P., Barbin, D. F., *et al*. (2022). Detection of nutshells in cumin powder using NIR hyperspectral imaging and chemometrics tools. *Journal of Food Composition and Analysis*, 108: 104407.

Forooghi, E., Zade, S. V., Sahebi, H., *et al*. (2023). Authentication and discrimination of tissue origin of bovine gelatin using combined supervised pattern recognition strategies. *Microchemical Journal*, 187: 108417.

Foschi, M., D'Addario, A., D'Archivio, A. A., *et al*. (2022). Future foods protection: supervised chemometric approaches for the determination of adulterated insects' flours for human consumption by means of ATR-FTIR spectroscopy. *Microchemical Journal*, 183: 108021.

Frera, M., Elahi, M. S., Woolfe, S., *et al*. (2021). Has COVID-19 caused a significant increase in observed food fraud incidents? *Food Science and Technology*, 6: 1–10.

Galvan, D., Lelis, C. A., Effting, L., *et al*. (2022). Low-cost spectroscopic devices with multivariate analysis applied to milk authenticity. *Microchemical Journal*, 181: 107746.

García-Gutiérrez, N., Mellado-Carretero, J., Bengoa, C., *et al*. (2021). ATR-FTIR spectroscopy combined with multivariate analysis successfully discriminates raw doughs and baked 3D-printed snacks enriched with edible insect powder. *Foods*, 10(8): 1806.

Geng, P., Harnly, J. M., Chen, P. (2016). Differentiation of bread made with whole grain and refined wheat (*T. aestivum*) flour using LC/MS-based chromatographic fingerprinting and chemometric approaches. *Journal of Food Composition and Analysis*, 47: 92–100.

Ghiasi, S., Parastar, H. (2021). Chemometrics-assisted isotope ratio fingerprinting based on gas chromatography/combustion/isotope ratio mass spectrometry for saffron authentication. *Journal of Chromatography A*, 1657: 462587.

Giannetti, V., Boccacci Mariani, M., Mannino, P. (2016). Characterization of the authenticity of Pasta di Gragnano protected geographical indication through flavor component analysis by gas chromatography–mass spectrometry and chemometric tools. *Journal of AOAC International*, 99(5): 1279–1286.

Goyal, K., Kumar, P., Verma, K. (2022). Food adulteration detection using artificial intelligence: a systematic review. *Archives of Computational Methods in Engineering*, 29(1): 397–426.

Grassi, S., Casiraghi, E., Alamprese, C. (2018). Handheld NIR device: a non-targeted approach to assess authenticity of fish fillets and patties. *Food Chemistry*, 243: 382–388.

Gunning, Y., Davies, K. S., Kemsley, E. K. (2023). Authentication of saffron using 60 MHz ^{1}H NMR spectroscopy. *Food Chemistry*, 404(Part B): 134649.

Horn, B., Esslinger, S., Fauhl-Hassek, C., *et al.* (2021). ^{1}H NMR spectroscopy, one-class classification and outlier diagnosis: a powerful combination for adulteration detection in paprika powder. *Food Control*, 128: 108205.

Jimenez-Carvelo, A. M., Arroyo-Cerezo, A., Bikrani, S., *et al.* (2022). Rapid and non-destructive spatially offset Raman spectroscopic analysis of packaged margarines and fat-spread products. *Microchemical Journal*, 178: 107378.

Jiménez-Sotelo, P., Hernández-Martínez, M., Osorio-Revilla, G., *et al.* (2016). Use of ATR-FTIR spectroscopy coupled with chemometrics for the authentication of avocado oil in ternary mixtures with sunflower and soybean oils. *Food Additives & Contaminants Part A: Chemistry, Analysis, Control, Exposure & Risk Assessment*, 33(7): 1105–1115.

Karunathilaka, S. R., Kia, A. R. F., Srigley, C., *et al.* (2016). Nontargeted, rapid screening of extra virgin olive oil products for authenticity using near-infrared spectroscopy in combination with conformity index and multivariate statistical analyses. *Journal of Food Science*, 81(10): C2390–C2397.

Karunathilaka, S. R., Yakes, B. J., He, K., *et al.* (2018). Non-targeted NIR spectroscopy and SIMCA classification for commercial milk powder authentication: a study using eleven potential adulterants. *Heliyon*, 4(9): e00806.

Kendall, H., Clark, B., Rhymer, C., *et al.* (2019). A systematic review of consumer perceptions of food fraud and authenticity: a European perspective. *Trends in Food Science & Technology*, 94: 79–90.

Keskin, M., Arslan, A., Soysal, Y., *et al.* (2022). Feasibility of a chromameter and chemometric techniques to discriminate pure and mixed organic and conventional red pepper powders: a pilot study. *Journal of Food Processing and Preservation*, 46(6): e15846.

Kharbach, M., Yu, H., Kamal, R., *et al.* (2022). Authentication of extra virgin argan oil by selected-ion flow-tube mass-spectrometry fingerprinting and chemometrics. *Food Chemistry*, 383: 132565.

Khodabakhshian, R., Bayati, M. R., Emadi, B. (2021). An evaluation of IR spectroscopy for authentication of adulterated turmeric powder using pattern recognition. *Food Chemistry*, 364: 130406.

Laroussi-Mezghani, S., Vanloot, P., Molinet, J., *et al.* (2015). Authentication of Tunisian virgin olive oils by chemometric analysis of fatty acid compositions and NIR spectra. Comparison with Maghrebian and French virgin olive oils. *Food Chemistry*, 173: 122–132.

Le Nguyen Doan, D., Nguyen, Q. C., Marini, F., *et al.* (2021). Authentication of rice (*Oryza sativa* L.) using near infrared spectroscopy combined with different chemometric classification strategies. *Applied Sciences*, 11(1): 362.

Liang, N., Sun, S., Zhang, C., *et al.* (2022). Advances in infrared spectroscopy combined with artificial neural network for the authentication and traceability of food. *Critical Reviews in Food Science and Nutrition*, 62(11): 2963–2984.

Lima, R. A. M., Ferraz, S. M. M., Cardoso, V. G. K., *et al.* (2023). Authentication of fish oil (omega-3) supplements using class-oriented chemometrics and comprehensive two-dimensional gas chromatography coupled to mass spectrometry. *Analytical and Bioanalytical Chemistry*, 415(13): 2601–2611.

Lixourgioti, P., Goggin, K. A., Zhao, X., *et al.* (2022). Authentication of cinnamon spice samples using FT-IR spectroscopy and chemometric classification. *LWT-Food Science and Technology*, 154: 112760.

Lopez, E., Etxebarria-Elezgarai, J., Amigo, J. M., *et al.* (2023). The importance of choosing a proper validation strategy in predictive models. A tutorial with real examples. *Analytica Chimica Acta*, 1275: 341532.

Mahboubifar, M., Hemmateenejad, B., Jassbi, A. R. (2021). Evaluation of adulteration in distillate samples of *Rosa damascena* Mill using colorimetric sensor arrays, chemometric tools and dispersive liquid–liquid microextraction–GC-MS. *Phytochemical Analysis*, 32(6): 1027–1038.

Małyjurek, Z., de Beer, D., Joubert, E., *et al.* (2022). Combining class-modelling and discriminant methods for improvement of products authentication. *Chemometrics and Intelligent Laboratory Systems*, 228: 104620.

Mannina, L., Marini, F., Antiochia, R., *et al.* (2016). Tracing the origin of beer samples by NMR and chemometrics: Trappist beers as a case study. *Electrophoresis*, 37(20): 2710–2719.

Mazivila, S. J., Páscoa, R. N., Castro, R. C., *et al.* (2020). Detection of melamine and sucrose as adulterants in milk powder using near-infrared spectroscopy with DD-SIMCA as one-class classifier and MCR-ALS as a means to provide pure profiles of milk and of both adulterants with forensic evidence: a short communication. *Talanta*, 216: 120937.

McVey, C., Elliott, C. T., Cannavan, A., *et al.* (2021). Portable spectroscopy for high throughput food authenticity screening: advancements in technology and integration into digital traceability systems. *Trends in Food Science & Technology*, 118: 777–790.

Medina, S., Perestrelo, R., Silva, P., *et al.* (2019). Current trends and recent advances on food authenticity technologies and chemometric approaches. *Trends in Food Science & Technology*, 85: 163–176.

Mellado-Carretero, J., García-Gutiérrez, N., Ferrando, M., *et al.* (2020). Rapid discrimination and classification of edible insect powders using ATR-FTIR spectroscopy combined with multivariate analysis. *Journal of Insects as Food and Feed*, 6(2): 141–148.

Milani, M. I., Rossini, E. L., Catelani, T. A., *et al.* (2020). Authentication of roasted and ground coffee samples containing multiple adulterants using NMR and a chemometric approach. *Food Control*, 112: 107104.

Nardecchia, A., Presutto, R., Bucci, R., *et al.* (2020). Authentication of the geographical origin of 'Vallerano' chestnut by near infrared spectroscopy coupled with chemometrics. *Food Analytical Methods*, 13(9): 1782–1790.

Netto, J. M., Honorato, F. A., Celso, P. G., *et al.* (2023). Authenticity of almond flour using handheld near infrared instruments and one class classifiers. *Journal of Food Composition and Analysis*, 115: 104981.

Neves, M. D. G., Poppi, R. J., Breitkreitz, M. C. (2022). Authentication of plant-based protein powders and classification of adulterants as whey, soy protein, and wheat using FT-NIR in tandem with OC-PLS and PLS-DA models. *Food Control*, 132: 108489.

Ng, P. C., Ahmad Ruslan, N. A. S., Chin, L. X., *et al.* (2022). Recent advances in halal food authentication: challenges and strategies. *Journal of Food Science*, 87(1): 8–35.

Oliveira, S., Duarte, E., Gomes, M., *et al.* (2023). A green method for the authentication of sugarcane spirit and prediction of density and alcohol content based on near infrared spectroscopy and chemometric tools. *Food Research International*, 170: 112830.

Oliveri, P. (2017). Class-modelling in food analytical chemistry: development, sampling, optimisation and validation issues—a tutorial. *Analytica Chimica Acta*, 982: 9–19.

Oliveri, P., Malegori, C., Simonetti, R., *et al.* (2019). The impact of signal pre-processing on the final interpretation of analytical outcomes—a tutorial. *Analytica Chimica Acta*, 1058: 9–17.
Pages-Rebull, J., Pérez-Ràfols, C., Serrano, N., *et al.* (2023). Classification and authentication of spices and aromatic herbs by means of HPLC-UV and chemometrics. *Food Bioscience*, 52: 102401.
Pérez-Beltrán, C. H., Jiménez-Carvelo, A. M., Martín-Torres, S., *et al.* (2022). Instrument-agnostic multivariate models from normal phase liquid chromatographic fingerprinting. A case study: authentication of olive oil. *Food Control*, 137: 108957.
Pieszczek, L., Czarnik-Matusewicz, H., Daszykowski, M. (2018). Identification of ground meat species using near-infrared spectroscopy and class modeling techniques—aspects of optimization and validation using a one-class classification model. *Meat Science*, 139: 15–24.
Pomerantsev, A. L., Rodionova, O. Y. (2021). New trends in qualitative analysis: performance, optimization, and validation of multi-class and soft models. *Trends in Analytical Chemistry*, 143: 116372.
Rasmussen, M. K., Gold, J., Kaiser, M. W., *et al.* (2024). Critical review of cultivated meat from a Nordic perspective. *Trends in Food Science & Technology*, 144: 104336.
Rinnan, A., Van Den Berg, F., Engelsen, S. B. (2009). Review of the most common pre-processing techniques for near-infrared spectra. *Trends in Analytical Chemistry*, 28(10): 1201–1222.
Robson, K., Dean, M., Brooks, S., *et al.* (2020). A 20-year analysis of reported food fraud in the global beef supply chain. *Food Control*, 116: 107310.
Robson, K., Dean, M., Haughey, S., *et al.* (2021). A comprehensive review of food fraud terminologies and food fraud mitigation guides. *Food Control*, 120: 107516.
Rodionova, O. Y., Pomerantsev, A. L. (2020). Chemometric tools for food fraud detection: the role of target class in non-targeted analysis. *Food Chemistry*, 317: 126448.
Rodionova, O. Y., Titova, A. V., Pomerantsev, A. L. (2016a). Discriminant analysis is an inappropriate method of authentication. *TrAC Trends in Analytical Chemistry*, 78: 17–22.
Rodionova, O. Y., Oliveri, P., Pomerantsev, A. L. (2016b). Rigorous and compliant approaches to one-class classification. *Chemometrics and Intelligent Laboratory Systems*, 159: 89–96.
Rodionova, O. Y., Titova, A. V., Balyklova, K. S., *et al.* (2019). Detection of counterfeit and substandard tablets using non-invasive NIR and chemometrics—a conceptual framework for a big screening system. *Talanta*, 205: 120150.
Rodionova, O. Y., Oliveri, P., Malegori, C., *et al.* (2024). Chemometrics as an efficient tool for food authentication: golden pillars for building reliable models. *Trends in Food Science & Technology*, 147: 104429.
Ruisánchez, I., Jiménez-Carvelo, A. M., Callao, M. P. (2021). ROC curves for the optimization of one-class model parameters. A case study: authenticating extra virgin olive oil from a Catalan protected designation of origin. *Talanta*, 222: 121564.
Shawky, E., El-Khair, R. M. A., Selim, D. A. (2020). NIR spectroscopy–multivariate analysis for rapid authentication, detection and quantification of common plant adulterants in saffron (*Crocus sativus* L.) stigmas. *LWT-Food Science and Technology*, 122: 109032.
Spink, J., Bedard, B., Keogh, J., *et al.* (2019). International survey of food fraud and related terminology: preliminary results and discussion. *Journal of Food Science*, 84(10): 2705–2718.
Squeo, G., De Angelis, D., Summo, C., *et al.* (2022). Assessment of macronutrients and alpha-galactosides of texturized vegetable proteins by near infrared hyperspectral imaging. *Journal of Food Composition and Analysis*, 108: 104459.
Stilo, F., Jiménez-Carvelo, A. M., Liberto, E., *et al.* (2021). Chromatographic fingerprinting enables effective discrimination and identitation of high-quality Italian extra-virgin olive oils. *Journal of Agricultural and Food Chemistry*, 69(31): 8874–8889.
Suhandy, D., Yulia, M. (2021). The use of UV spectroscopy and SIMCA for the authentication of Indonesian honeys according to botanical, entomological and geographical origins. *Molecules*, 26(4): 915.
Suhandy, D., Al Riza, D. F., Yulia, M., *et al.* (2023). Non-targeted detection and quantification of food adulteration of high-quality stingless bee honey (SBH) via a portable LED-based fluorescence spectroscopy. *Foods*, 12(16): 3067.
Tähkäpää, S., Maijala, R., Korkeala, H., *et al.* (2015). Patterns of food frauds and adulterations reported in the EU rapid alert system for food and feed and in Finland. *Food Control*, 47: 175–184.
Tan, H. R., Chan, L. Y., Lee, H. H., *et al.* (2022). Rapid authentication of Chinese oolong teas using atmospheric solids analysis probe–mass spectrometry (ASAP-MS) combined with supervised pattern recognition models. *Food Control*, 134: 108736.
Tanabe, C. K., Nelson, J., Boulton, R. B., *et al.* (2020). The use of macro, micro, and trace elemental profiles to differentiate commercial single vineyard Pinot Noir wines at a sub-regional level. *Molecules*, 25(11): 2552.
Tejerina, D., Contador, R., Ortiz, A. (2021). Near infrared spectroscopy (NIRS) as tool for classification into official commercial categories and shelf-life storage times of pre-sliced modified atmosphere packaged Iberian dry-cured loin. *Food Chemistry*, 356: 129733.
Totaro, M. P., Squeo, G., De Angelis, D., *et al.* (2023). Application of NIR spectroscopy coupled with DD-SIMCA class modelling for the authentication of pork meat. *Journal of Food Composition and Analysis*, 118: 105211.
Van Ruth, S. M., Luning, P. A., Silvis, I. C., *et al.* (2018). Differences in fraud vulnerability in various food supply chains and their tiers. *Food Control*, 84: 375–381.
Vera, D. N., Jiménez-Carvelo, A. M., Cuadros-Rodríguez, L., *et al.* (2019). Authentication of the geographical origin of extra-virgin olive oil of the Arbequina cultivar by chromatographic fingerprinting and chemometrics. *Talanta*, 203: 194–202.
Visciano, P., Schirone, M. (2021). Food frauds: global incidents and misleading situations. *Trends in Food Science & Technology*, 114: 424–442.
Vitale, R., Cocchi, M., Biancolillo, A., *et al.* (2023). Class modelling by soft independent modelling of class analogy: why, when, how? A tutorial. *Analytica Chimica Acta*, 1270: 341304.
Wickramasinghe, K., Breda, J., Berdzuli, N., *et al.* (2021). The shift to plant-based diets: are we missing the point? *Global Food Security*, 29: 100530.
Wilde, A. S., Sørensen, S., Kucheryavskiy, S., *et al.* (2023). Patterns in official food control data—modelling dioxin and PCB profiling data for authentication of Baltic Sea salmon. *Journal of Food Composition and Analysis*, 124: 105607.
Wold, S. (1976). Pattern recognition by means of disjoint principal components models. *Pattern Recognition*, 8(3): 127–139.
Xu, Y., Zhong, P., Jiang, A., *et al.* (2020). Raman spectroscopy coupled with chemometrics for food authentication: a review. *TRAC Trends in Analytical Chemistry*, 131: 116017.
Yi, L., Dong, N., Yun, Y., *et al.* (2016). Chemometric methods in data processing of mass spectrometry-based metabolomics: a review. *Analytica Chimica Acta*, 914: 17–34.
Zhang, W., Xue, J. (2016). Economically motivated food fraud and adulteration in China: an analysis based on 1553 media reports. *Food Control*, 67: 192–198.