Trends in Food Science & Technology 147 (2024) 104430

Contents lists available at ScienceDirect

Trends in Food Science & Technology

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

Proven traceability strategies using chemometrics for organic food authenticity

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ARTICLE INFO

Keywords:
HRMS
NMR
Elemental analysis
Food fraud detection
Inductively coupled plasma mass spectrometry
Isotope ratio mass spectrometry

ABSTRACT

Background: risk of fraudulent mislabeling of organic food, driven by higher prices and a more favorable consumer perception, underscores the necessity for accurate authentication of organic products. Different analytical approaches and statistical analysis have been developed to classify between organic and conventional food.

Scope and approach: In this review the current analytical approaches to detect organic food mislabeling are described. Potential and validated markers of organic traceability are explained, together with the techniques and statistical analysis employed. In this article, all the different foods have been reviewed and are presented by type of food.

Key findings and conclusions: Variations in the elemental and stable isotopic ratios of fertilizers lead to differences in plant food ratios. In the case of animal food products, the distinct ratio in organic results in a final product with a unique elemental and stable isotopic composition. Those could be used for authenticating organic food. In addition, the different fertilization promotes different metabolic pathways leaving a distinct metabolic signature, hence targeted and untargeted metabolomic analysis permits the traceability of organic food. Finally, the use of soft classification models such as SIMCA, PLS-DA or OPLS-DA permits the classification of organic food and enables prediction of whether a new sample is conventional or organic.

1. Introduction

The demand for organic food is increasing, as consumers perceive it to be healthier, safer, and more environmentally friendly. This tendency, together with the fact that organic products command a higher price on the market than the conventional equivalents, creates a significant risk of fraudulent practices, such as deliberate mislabeling. From 1999 to 2020, the total global land area devoted to organic agriculture experienced a substantial increase, surging from 11 million hectares to 74.9 million hectares (Willer, Trávníček, Meier, & Schlatter, 2022). Furthermore, the European Union has made a significant commitment to bolster organic production, aiming to allocate 25% of all agricultural land to organic farming by 2030 as an integral part of its farm-to-fork strategy for sustainable food systems. In parallel, sales of organic food products have more than doubled over the last decade, with Canada, China, and Germany experiencing notable market growth percentages of 26.1%, 23.0%, and 22.3%, respectively (Willer et al., 2022). This continuing expansion underscores the urgency of developing analytical tools to authenticate organic products and thwart fraudulent activities that seek to blur the lines between different agricultural and farming systems and food producers (Pettoello-Mantovani and Olivieri, 2022). To achieve this, it is imperative to include organic food traceability in existing food safety regulations and trade agreements. In Europe, in response to the swiftly evolving landscape of the organic sector, new legislation for organic products became effective on January 1, 2022, after a one-year delay in its implementation. The purpose of this regulation is to promote equitable competition for farmers, whilst preventing fraud and maintaining consumer trust.

As differences in fertilization practices between organic and conventional agriculture can significantly impact the elemental and isotopic

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https://doi.org/10.1016/j.tifs.2024.104430
Received 29 November 2023; Received in revised form 4 February 2024; Accepted 10 March 2024

composition of crops (vegetables, fruits, cereals, etc.), various atomic spectroscopy techniques have been successfully implemented to verify compliance with organic regulations. (Bateman & Kelly, 2007; Laursen, Schjoerring, Kelly, & Husted, 2014). Organic crop systems rely on compost and farmyard manure and avoid the use of pesticides, whereas conventional farming uses inorganic fertilizers and pesticides, both of which often contain heavy metals (Hassanpourfard, Mane, & Banerjee, 2023). Inorganic fertilizers have higher concentrations of rare-earth elements, such as La, Ce, Th, and Yb, and their frequent application can lead to increased levels of these elements in the soil, subsequently affecting the composition of plants and seeds (Turra et al., 2013). In addition, the differences in C/N ratios between organic and conventional fertilizers promote different biological pathways in plant organisms, resulting in contrasting metabolic signatures (González-Coria et al., 2022). Differences in the stable isotopic ratio, elemental distribution, and nutrient profile of animal feed are transferred to meat and other animal products (Pustjens, Boerrigter-Eenling, Koot, Rozijn, & van Ruth, 2017). These signatures can be determined by targeted profiling or whole fingerprint analysis, the latter providing a more accurate classification (Quintanilla-Casas et al., 2020). Additionally, due to the diverse fertilizer management practices used in both organic and conventional systems, relying on a single method for authentication is challenging. Therefore, the generation of multivariate fingerprints using multiple complementary atomic spectroscopy techniques combined with chemometric analysis of spectral data is strongly recommended.

Comprehensive and in-depth traceability analysis of organic food has scope for considerable improvement. In this article, we review English language publications on the authentication of organic vegetable and animal foods for human consumption, spanning from 2013 to the present, with the aim of providing pertinent and novel insights into food traceability. The different sections correspond to food types, which are presented in the order of the food recommendations on the Mediterranean diet pyramid (Willett et al., 1995). In addition, the vegetable and fruit sections are divided by colour, reflecting current recommendations from Harvard and other medical schools that emphasize the importance of eating foods of a broad colour palette (McManus, 2019).

2. Methodologies for organic food authentication

2.1. Analytical techniques

The analytical approaches to verify the organic status of organic food can be classed within four groups: elemental analysis, stable isotopes analysis, targeted profiling of characteristic compounds, or untargeted profiling. In elemental analysis, the concentration of each target element is measured by inductively coupled plasma mass spectrometry (ICP-MS) or ICP-optical emission spectrometry (OES). ICP apparatus is based on the use of high energy electric currents that atomize the sample, then those atoms are detected by the MS or the OES (Lee, 2018).

In isotopic analysis, the difference between the stable isotopes is determined by isotope ratio mass spectrometry (IRMS) and expressed as $\delta^{x}E$. For example, $\delta^{15}N$ is a measure of the ratio of $^{15}N/^{14}N$ in the samples to the $^{15}N/^{14}N$ in a reference material, or more precisely, it represents the per mil (‰) variation in the sample ratio compared to the standard ratio. Thus, a negative $\delta^{15}N$ value indicates that the sample ratio of $^{15}N/^{14}N$ is lower than the standard ratio (Novak, Adler, Husted, Fromberg, & Laursen, 2019). The calculation follows the equation:

$$\delta^{x}E_{sample/standard} = 1000*(Ratio_{sample}-Ratio_{standard})/\ Ratio_{standard}$$

In targeted profiling, different approaches are needed depending on the target chemicals. For example, the fatty acid profile is determined by triglyceride transesterification followed by a volatilization, and then the analysis of the resulting mixture is carried out by gas-chromatography coupled to flame ionisation detection (GC-FID) (Capuano, Gravink, Boerrigter-Eenling, & van Ruth, 2015). On the other hand, the volatile profile is analysed by a headspace solid-phase microextraction coupled to GC-mass spectrometry (HS-SPME-GC-MS) (Cuevas, Pereira-Caro, Moreno-Rojas, Muñoz-Redondo, & Ruiz-Moreno, 2017). In this analytical technique, the volatile compounds from a sample are captured by an adsorbent and then desorbed in the GC for their analysis. Other targeted profiling could be the phenolic profile, which could be achieved by different means, but mainly are determined by liquid chromatography (LC) coupled to photodiode array detector (PDA) or to MS detector (Lozano-Castellón et al., 2022). However, PDA detector could led to identification errors, as it is just based in the retention time and absorbance wavelength, which is shared by some compounds, such as quercetin-3-*O*-glucuronide and rutin, for example.

In untargeted analysis, spectral analyses are carried out in order to have a whole image of the samples. The most commonly used techniques in untargeted analysis are HRMS, nuclear magnetic resonance (NMR), and infra-red (IR) spectra. HRMS consists of an MS detector that determines the exact mass of the compounds, which can be used to determine the formula and a probable structure if fragmentation analysis is also performed (Duncan, 2012). NMR spectra are based on the magnetic activity of a molecule and provide information about the structure of the molecules, it is used to detect if a group (organic or conventional) is richer in phenolic compounds than the other group, for example (Harris, Becker, Cabral de Menezes, Goodfellow, & Granger, 2001). In addition, IR also provides information about functional groups, but it is based on the vibrational pattern of these substituents with infrared radiation (General survey of vibrational spectroscopy, 1995).

In untargeted analysis, the spectral peaks can be identified before the statistical analysis. Alternatively, all the peaks can be analysed without identification, which is restricted to any emerging marker peaks. When tracing organic food, it may be more useful to work with the whole fingerprint, doing the statistical analysis before the identification, which contains more information and therefore facilitates the separation of groups, such as organic *versus* conventional (Quintanilla-Casas et al., 2020). In this case, the compounds responsible for the differences between groups might not be identified at the end, but since the main objective is to discriminate between groups, these details might seem less important.

To choose the most suitable analytical methods, it is crucial to consider the type of sample and the available equipment. If spectral techniques are available, they are preferable as they yield high-information output, enhancing the potential to develop and validate a model for distinguishing between organic and conventional food. It is worth noting that while elemental analysis and isotopic ratio assessments may generate smaller result matrices, they still demonstrate effective group separation.

Considering the nature of the food sample, the volatile fingerprint can serve as a valuable source of information. However, it is essential to know that certain foods have minimal odor, diminishing the possibility that the volatile profile alone would offer substantial information. In such cases, alternative analyses may yield more robust results and provide a more comprehensive understanding of the sample. As food matrices are so diverse, each case should be studied to select the best analytical method for tracing the organic samples.

2.2. Statistical approaches

The obtained analytical data are evaluated by different statistical procedures to accurately classify the organic samples. Prior to the formal analysis, the data could be transformed, scaled and normalized in order to improve the classification. Scaling the data is a transformation that changes the range of the data, but the differences between samples for each variable remains. The result is data fitted between a smaller range, which is helpful as it allows to easily compare between different variables, as all of them have similar values after the scalation process. If there is no scaling step, the model would mainly focus on variables with high values, then the contribution of some variables with low values could be minimal, which can result in a loss of classification power of the model. Some examples of scaling are mean-centered, auto-scaling, and Pareto scaling, for more information see: van den Berg, Hoefsloot, Westerhuis, Smilde, and van der Werf (2006). Depending on the data, some transformations will improve more the model separation than others. On the other hand, normalizing the data is useful when parametric tests are applied, as those require data normally distributed. As the data matrices could be immense and the best preprocessing option could not be clear, some authors try all the preprocessing possibilities, and finally select the one that provides better classification between groups (de Andrade et al., 2023).

After the data pretreatment, the formal analysis is carried out. First, the differences between supervised and unsupervised models should be highlighted. An unsupervised approach is an exploratory tool that will reveal the natural distribution of the samples, allowing emerging groups to be identified. In contrast, supervised analysis forces the separation of samples into selected groups or classes, making it a useful approach for discriminating between organic and conventional foods. The most common unsupervised methods are principal component analysis (PCA) and hierarchical cluster analysis (HCA). PCA is a mathematical tool that reduces the dimensions of a data set, resulting in data that can be easily analysed for variations. The data are transformed into new dimensions (PCs) that are linear polynomials of the original variables. The result is a set of new dimensions, each explaining a percentage of the variability between the samples, which could be easily interpreted, since all the information could be graphically represented in 2 or 3 dimensions (2 or 3 PCs). In the end, the researcher has a graph in which the samples are distributed in hyperspace. Samples that have similarities tend to group together and knowing the coefficient for each variable for the PCs, one could determine why those variables are grouped together and why they are separated from the others (Jolliffe & Cadima, 2016). In the case of the HCA, it is also an unsupervised model that allows to detect the natural cluster between groups, but it works differently. In the case of the HCA, it uses a dendrogram for representing the grouping. Samples that are together in the dendrogram, are similar, and those samples that are not together are different. For building this dendrogram, different methods can be used, one is building a heatmap using the Euclidean distance. This distance is the difference between the mean and the value of the sample for a variable. And then in the heatmap, the samples are grouped according to those values (Nielsen, 2016, pp. 195–211).

In the classification of organic and conventional foods, the most used supervised techniques are partial least squares discriminant analysis (PLS-DA), soft independent modelling of class analogy (SIMCA), and support vector machines (SVM). The latter is useful when the dataset is small, SVM is based on the maximum margin hyperplane finding procedure, a type of linear model. Considering a dataset with two classes (organic and conventional samples) where the classes are linearly separable, then a hyperplane in the input space can classify the samples between the groups. The final hyperplane selected by the model is the one that minimize the errors in classifying the samples (Barbosa et al., 2016). In the case of SIMCA, it is often used as a one-class classifying model, although it could be used as discriminant model sometimes. It works as follows, first a model for each group is created, concretely a PCA (Pomerantsev & Rodionova, 2020). Then using the residuals of each group, the orthogonal and score distances, it is assessed if a sample belongs to that group or not. For checking these residuals, different methods have been developed, one of which is the data-driven SIMCA (DD-SIMCA) (Pomerantsev & Rodionova, 2020).

Finally, the PLS-DA is a discriminant method that uses the PLS-regression to search for latent variables with a maximum covariance with the Y-variables (the groups). These latent variables are linear combinations of the original variables (Ballabio & Consonni, 2013). Then, similarly to the PCA, it is possible to represent in a new hyperspace the samples according to their latent variables and visually check the group separation. In this case, this separation is forced by the model, and not natural as in the PCA.

Once generated, the supervised model is generally verified by cross-validation, in which the model is tested and trained using different subsets of data in multiple iterations. The aim of this statistical treatment is to evaluate the real-world performance of a predictive model with optimum accuracy, and it is the most used technique for predictive models (Allen, 1974). One type of cross-validation usually employed is the *k*-fold cross-validation. It consists in dividing equally the sample set in *k* subsets. Then each time one subset is left out for testing and the others are used for building the model. This procedure is repeated *k* times until all subsets have been used for testing. The final error is the sum of the errors of each procedure (Barbosa et al., 2016). A summary of the possible methodologies for organic traceability is shown in Fig. 1. In addition, a flowchart for the development and validation of a supervised discriminant model is presented in Fig. 2.

This review also includes studies that exclusively employed unsupervised models to find marker compounds for discrimination. Table 1 and Table 2 present all the articles covered, listing the target foods, the marker compounds (or potential marker compounds), statistical procedures, and if a validated supervised model was used to authenticate the organic product.

3. Vegetables

3.1. Red vegetables

Two studies on organic and conventional tomatoes and sweet peppers cultivated in different Brazilian regions evaluated techniques to discriminate between agronomic practices and geographic origin. de Andrade et al. (2023) reported that near-infrared (NIR) spectrometry combined with various chemometric methods, including PCA, DD-SIMCA, and PLS-DA, constitutes a useful system to verify the authenticity of organic products based on the profile of non-volatile components such as fibres, sugars, or fatty acids. Promising results were also obtained by Galvan et al. (2023) using energy-dispersive X-Ray fluorescence (EDXRF) combined with chemometric tools, an approach that does not require complex sample preparation steps and is fast and relatively inexpensive compared to chromatographic or spectrometric analytical techniques.

Zappi et al. (2022) developed a fast, cost-effective, and green procedure to verify the label information of tomato sauces by the analysis of volatile organic compounds (VOCs) and the colloidal fraction via multivariate statistical analysis. VOCs in tomato sauce were determined by GC-FID and GC-ion mobility spectrometry (GC-IMS), whereas the colloidal fraction was evaluated by asymmetric flow field-fractionation (AF4). The data obtained by both methods were useful for food-quality control: AF4 yielded comparable or better results than GC-IMS and offered complementary information to distinguish between brands of tomato sauce and certify their organic authenticity.

Ways to detect the fraudulent branding of conventional tomatoes as organic were investigated in a study with *Solanum lycopersicum* cv. *Ramyle* (Díaz-Galiano, Heinzen, Martínez-Bueno, Rajski, & Fernández-Alba, 2022). This tomato cultivar was grown using different amounts of synthetic or natural crop protection agents, combined with chemical or organic fertilisers, and the metabolic profile of the tomatoes was analysed by LC coupled to Orbitrap mass spectrometry (LC-Q-Orbitrap-MS) combined with chemometrics. A polyketide phytoalexin identified as gerberin ($[M+H]^+$ at m/z 291.1075) was found to be a potential marker to distinguish between organic and conventional cultivation, as its levels correlated negatively with the presence of synthetic chemicals. In contrast, the use of $\delta^{15}N$- IRMS alone proved to be insufficient to discern between agricultural practices.

The mineral profiling of tomatoes can identify chemical markers of the farming system. With this aim, a study carried out by Cvijanović et al. (2021) analysed eight varieties of four types of tomatoes (beef, cluster, cherry and plum), cultivated by integrated or organic farming

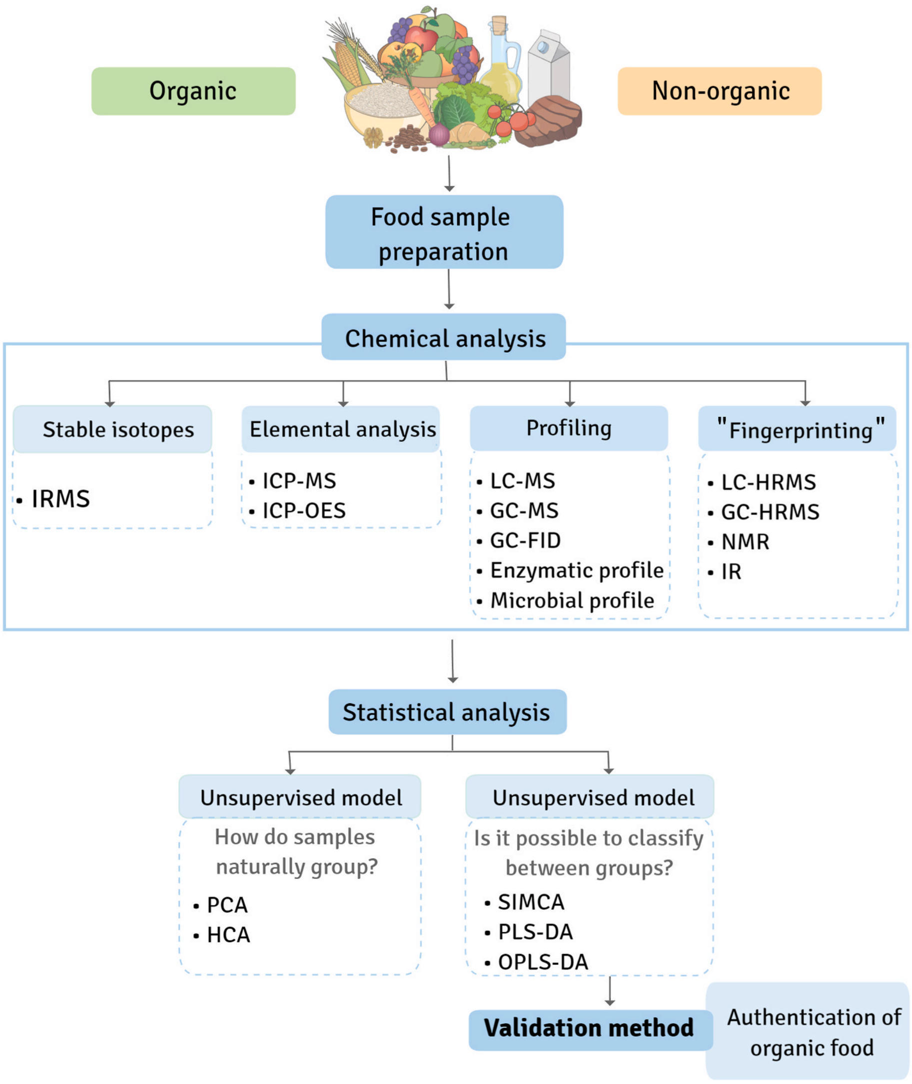

Fig. 1. Proposed methodologies for organic traceability.

regimes. Integrated farming falls between organic and conventional, as it applies minimum amounts of pesticides and synthetic fertilizers (Worth, 2012). A total of 44 elements were quantified using ICP-MS and chemometric techniques, among which the contents of Al, Mn, As, Pb, and some rare-earth elements distinguished between the two agricultural systems. In another study, the contents of 25 elements were identified as differentiators between organic and conventional practices tomato and bell pepper cultivations (*Capsicum annuum*) (Araújo, de Lima, Barbosa, & Alleoni, 2019). Discrimination models developed using data mining techniques and feature selection combined with classification algorithms resulted in accuracy rates of 100% in bell pepper and 97% in tomato. These high success rates suggest that multi-element analysis supported by the use of algorithms is a useful strategy to authenticate organic products.

Taking a different approach, the enzymatic profiles of tomatoes were examined to distinguish the impacts of organic and conventional farming (Rodrigues et al., 2021). The enzymatic activity in three tomato varieties (khaki, Italian and cherry) collected in different seasons was measured. The determined enzymes were invertases (INV), polygalacturonases (PG), peroxidases (PO), polyphenoloxidases (PPO), catalases (CAT) and phenylalanine ammonia lyase (PAL), and correlations with the farming systems were determined by PCA. The activities of PO, PPO, CAT, and PAL proved to be useful for tomato certification and traceability, particularly PO and CAT, the latter correlating better with conventional farming.

Metabolomic fingerprinting provides a comprehensive characterization of plant metabolomes, reflecting the impact of both endogenous and exogenous factors. Advanced technologies based on high performance liquid chromatography coupled with high-resolution accurate mass spectrometry (HPLC-HRAMS) were used to screen organic and conventional tomatoes grown in a greenhouse under controlled conditions (Martínez Bueno, Díaz-Galiano, Rajski, Cutillas, & Fernández-Alba, 2018). In addition, stable nitrogen isotopes ($\delta^{15}N$) and pesticide residues were analysed as possible indicators of production systems. Chemometric analysis of the HRAMS and $\delta^{15}N$ data provided a robust classification model. PCA showed sample clustering according to the farming system and significant differences in the content of six compounds (L-tyrosyl-L-isoleucyl-L-threonyl-L-threonine, trilobatin, phloridzin, tomatine, phloretin and echinenone). In a study by Bontempo et al. (2020), stable isotope ratios of hydrogen ($\delta^{2}H$), carbon ($\delta^{13}C$), nitrogen ($\delta^{15}N$), oxygen ($\delta^{18}O$) and sulfur ($\delta^{34}S$) were analysed in organic and conventional tomatoes and tomato passata. A method based on GC-combustion-IRMS (GC-C-IRMS) was developed for the analysis of C and N isotope ratios in tomato-derived amino acids. The most significant parameter to distinguish between organic and conventional products was the $\delta^{15}N$ value of amino acids. The authors proposed isotopic analysis of amino acids as a novel tool to be used in addition to existing certification and control procedures for organic tomatoes.

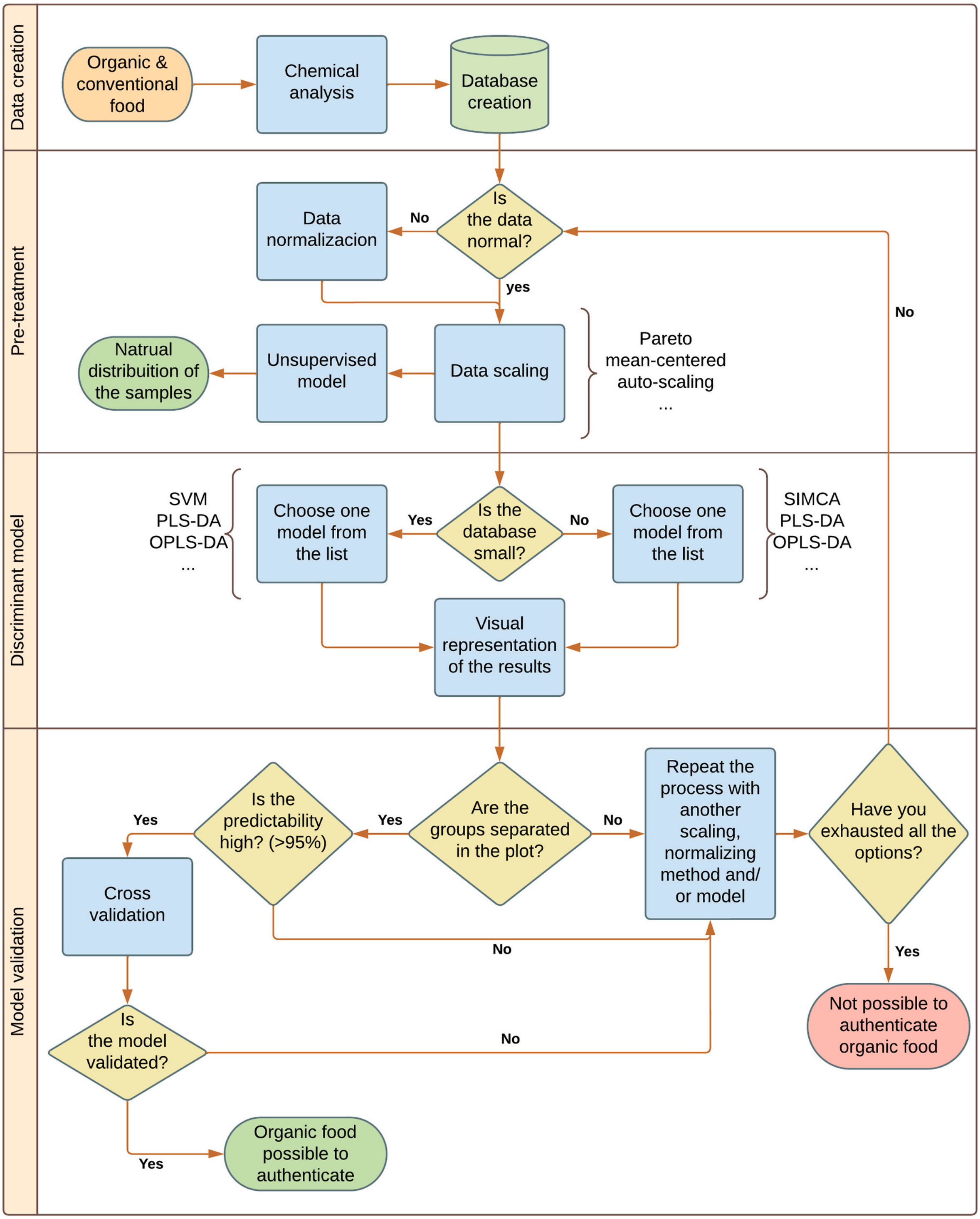

Fig. 2. Flowchart for the development and validation of a supervised discriminant model.

3.2. *Green vegetables*

Araújo et al. (2019) also determined the differences in elemental composition between organic and conventional lettuces. As in tomatoes, bell peppers, and onions, the contents of 25 elements were determined by ICP-OES using the conventional sample introduction system. For lettuce, the predictive accuracy obtained with the discriminatory model was 92%, with a 90% hit rate for organic samples. Similarly, the previously described method of Novak et al. (2019) for organic authentication (see previous section 3.2. Brown/orange vegetables), based on stable isotope ratio analysis, was also able to discriminate between organic and conventional cabbage.

A comparative study evaluated the functional and bioactive compounds of *Asparagus officinalis* L. cultivated with conventional or organic systems, comparing greenhouse and conventional open–field farming (Ku et al., 2018). Antioxidant capacity, total polyphenols and chlorophylls *a* and *b*, and total carotenoids (xanthophylls + carotenes) were determined spectrophotometrically. Higher phenolic content in cladodes was associated with conventional regime. In contrast, organic spears had higher levels of total phenolics and flavonoids and showed

Table 1
Analytical and statistical approaches for organic traceability in vegetables, fruits and cereals.

Food	Key Variables	Statistical analysis	Validated method	References
VEGETABLES				
tomato, sweet pepper	NIR spectra	PCA, PLS-DA, SIMCA	Yes	de Andrade et al. (2023)
tomato, sweet pepper	EDXRF spectra	ComDim, PLS-DA	Yes	Galvan et al. (2023)
tomato	VOCs (GC-FID and GC-IMS) and colloidal fraction (AF4)	PCA	No	Zappi et al. (2022)
tomato	Metabolome profile (LC-Q-Orbitrap-MS)	Direct comparison	No	Díaz-Galiano et al. (2022)
tomato	Elemental composition (ICP-MS)	PCA	No	Cvijanović et al. (2021)
tomato, bell pepper	Elemental composition (ICP-OES)	PCA, LDA, SVM, ANN, RF	Yes	Araújo et al. (2019)
tomato	Enzimatic activity (INV, PG, PO, PPO, CAT, PAL)	PCA	No	Rodrigues et al. (2021)
tomato	Metabolomic fingerprint (HPLC-HRAMS) and $\delta^{15}N$	PCA	No	Martínez Bueno et al. (2018)
tomato	$\delta^{15}N$ + GC-C-IRMS	PCA, ANOVA	No	Bontempo et al. (2020)
carrot	Metabolomic profile (UHPLC-HRMS)	PLS-DA, OPLS-DA, ANOVA	Yes	Dinis et al. (2023)
carrot, potato	$\delta^{18}O$ (IRMS)	ANOVA, QDA	Yes	Novak et al. (2019)
carrot	Metabolomic profile (UHPLC-MS)	OPLS-DA	Yes	Cubero-Leon et al. (2018)
potato	$\delta^{15}N$	ANOVA	No	Gatzert et al. (2021)
potato	Transcriptomic profile	HCA, ORA	No	Pacifico et al. (2017)
onion	Elemental composition (ICP-OES)	PCA, LDA, SVM, ANN, RF	Yes	Araújo et al. (2019)
lettuce	Elemental composition (ICP-OES)	PCA, LDA, SVM, ANN, RF	Yes	Araújo et al. (2019)
cabbage	$\delta^{18}O$	ANOVA, QDA	Yes	Novak et al. (2019)
asparagus	Phenolic compounds	ANOVA	No	Ku et al. (2018)
FRUITS				
banana	$\delta^{15}N$	ANOVA, PCA	No	Wang et al. (2021)
banana	Microbial genetic fingerprint (PCR-DGGE)	PLS-DA	Yes	Bigot et al. (2020)
orange juice	Metabolomic profile (HPLC-HRMS), VOCs (HS-SPME-GC-MS)	PCA, PLS-DA, HCA	Yes	Cuevas, Pereira-Caro, et al. (2017)
orange leaves	Elemental composition (ICP-MS)	SVM, ANN	Yes	Maione et al. (2017)
orange fruit	VOCs (HS-SPME-GC-MS)	PLS-DA	Yes	Cuevas, Moreno-Rojas, and Ruiz-Moreno (2017)
nectarine, peach	Microbial genetic fingerprint (PCR-DGGE)	PLS-DA	Yes	Bigot et al. (2015)
apple juice	Metabolomic profile (UHPLC-HRMS)	PCA, PLS-DA, OPLS-DA, ANOVA	Yes	Dinis et al. (2022)
strawberry	Nitrate isotopic composition $(\delta^{15}N, \delta^{18}O)$	SIMCA	Yes	Wassenaar et al. (2022)
red grape	Vibrational spectroscopy (ATR-FTIR, Raman spectroscopy)	PCA, AHC, DA,PC-DA	Yes	Radulescu et al. (2021)
apple	VOCs (HS-SPME/GC-MS)	PLS-DA	Yes	Giannetti et al. (2017)
strawberry	FT-NIR spectra	PCA, PLSR, PLS-DA,	Yes	Amodio et al. (2017)
grape juice	Elemental composition (ICP-MS)	SVM, Decision trees, ANN	Yes	Maione et al. (2016)
grape juice	Elemental composition (ICP-MS)	PCA, SIMCA	Yes	Borges et al. (2016)
goldenberry	Metabolomic fingerprint (UPLC-QToF-MS)	PCA	No	Llano et al. (2018)
CEREALS				
Rice	Elemental composition (ICP-MS)	PSA, SIMCA, HCA, *KNN*	Yes	Borges, Gelinski, de Oliveira Souza, Barbosa, and Batista (2015)
Rice	Elemental composition (ICP-MS)	*t*-test, SVM	Yes	Barbosa et al. (2016)
Rice	$\delta^{13}C$ and $\delta^{15}N$	LSD (ANOVA)	No	Chung, Park, et al. (2017)
Rice	$\delta^{13}C$ and $\delta^{15}N$ (Compound-specific)	HCA, PSA, OPLS-DA	No	Chung, Kim, An, et al. (2019)
Rice	$\delta^{13}C$ and $\delta^{15}N$	SVM	Yes	Chung et al. (2021)
Rice	$\delta^{13}C$ and $\delta^{15}N$ + elemental composition (ICP-MS/MS)	ANOVA, PCA, PLS-DA	Yes	Liu et al. (2020)
Rice	$\delta^{13}C$ and $\delta^{15}N$ + elemental composition (ICP-MS)	ANOVA, PCA, PLS-DA	Yes	Yuan et al. (2018)
Rice	Metabolomic fingerprint (UHPLC-QToF MS)	PCA, PLS-DA, HCA, OPLS-DA	Yes	Xiao et al. (2018)
Rice	NIR spectra	PCA, PLS regression	Yes	Xiao et al. (2019)
Rice	Phenolic compounds	ANOVA, LSD	No	Prabakaran et al. (2018)
Wheat and barley	Elemental composition (ICP-OES)	PCA	No	Laursen et al. (2011)
Wheat and barley	$\delta^{2}H$ and $\delta^{15}N$	mean ± error	No	Laursen et al. (2013)
Wheat	$\delta^{13}C$ and $\delta^{15}N$ (Compound-specific)	SD, HSD turkey	No	Paolini et al. (2015)
Wheat	$\delta^{13}C$	mean ± SD	No	Gatzert et al. (2021)
Wheat	Metabolomic profile (GC-MS)	*t*-test PCA	No	Bonte et al. (2014)
wheat	Metabolomic profile (GC-MS)	machine learning	Yes	Kessler et al. (2015)

(*continued on next page*)

Table 1 (*continued*)

Food	Key Variables	Statistical analysis	Validated method	References
		(MeltGB 2.0)		
wheat	Crystallization patterns	PCA, k-nearest-neighbour method	Yes	Kahl et al. (2015)
wheat	Phenolic acids	PCA, ANOVA	No	Weesepoel et al. (2016)
corn	NIR and MIR spectra	PLSR, SIMCA	Yes	Ayvaz et al. (2015)

Abbreviations: EDXRF = Energy-Dispersive X-Ray Fluorescence, ICP = Inductively coupled plasma, PCA = Principal Component Analysis, SIMCA = Soft Independent Modeling of Class Analogy, HCA = Hierarchical Cluster Analysis, KNN=K-nearest neighbours, SVM = support vector machine, OPLS-DA = Orthogonal Projections to Latent Structures Discriminant Analysis, LSD = least significant difference, PLSR = partial least squares regression, ComDim = Common Dimension Analysis, VOCs = Volatile organic compounds, AF4 = asymmetric flow field-fractionation, ICP-OES = inductively coupled plasma/ optical emission spectroscopy, LDA = linear discriminant analysis, ANN = artificial neural networks, RF = random forest, INV = invertases, PG = polygalacturonases, PO = peroxidases, PPO = polyphenoloxidases, CAT = catalases, PAL = phenylalanine ammonia lyase, HPLC-HRAMS =High-performance liquid chromatography/high-resolution accurate mass spectrometry, GC-C-IRMS = gas chromatography-combustion-isotope ratio mass spectrometry, QDA = quadratic discriminant analysis, REIMS = rapid evaporative ionisation mass spectrometry, QToF = quantitative time of flight, PCA= Principal component analysis, FAMEs = fatty acids methyl esters, DGGE = PCR-Denaturing Gradient Gel Electrophoresis, ATR-FTIR = attenuated total reflectance-Fourier transform infrared spectroscopy, AHC=Agglomerative Hierarchical Clustering, DA = discriminant analysis, PC-DA = combination of principal component and discriminant analysis, MANOVA = multivariate analysis of variance, HS-SPME/GC-MS=Head Space-Solid Phase Micro Extraction/Gas Chromatography Mass Spectrometry, ORA= Over-Representation Analysis.

higher antioxidant activities in three radical scavenging assays compared to the conventional counterparts. Multivariate analysis partially differentiated between the organic and conventional samples.

3.3. *Brown/orange vegetables*

Several efforts have also been made to authenticate organic carrots (*Daucus carrota*) and potatoes (*Solanum tuberosum*). In a study by Dinis, Tsamba, Jamin, and Camel (2023), an orthogonal projections to latent structures-discriminant analysis (OLPS-DA) model generated from untargeted ultra-high performance liquid chromatography-HRMS (UHPLC-HRMS) data was able to differentiate between carrots produced in different regions, but not according to the farming regime. A novel method for organic authentication was developed by Novak et al. (2019). based on the analysis of oxygen stable isotope ratios in plant-derived sulphate compounds. Its application, together with isotopic analysis of bulk plant tissue and plant-derived nitrate, allowed discrimination between organic and conventional potatoes and carrots. Oxygen isotope ratios of sulphate in organic vegetables were found to be significantly lower compared to those of conventional products, and the values were directly correlated with the type of fertilisation. Moreover, sulphate isotope analysis had superior classification power compared to known bulk tissue isotope markers and nitrate isotope values (Cubero-Leon, De Rudder, & Maquet, 2018). In a study based on large-scale comparative metabolomics, OPLS-DA models accurately predicted whether carrots were conventionally or organically produced based on LC–MS data. When the training set used to build the OPLS-DA models contained samples representative of each harvest year, 100% correct classification of carrots was achieved, indicating that the farming system modulates the carrot metabolome.

Gatzert et al. (2021) was able to separate potatoes from different regions in Germany according to their provenance after analysing their stable isotope compositions of oxygen, hydrogen, carbon, nitrogen, and sulfur using single-variate authentication methods. Effective isotope tracers of origin were $\delta\,^{18}$O, $\delta\,^{2}$H, $\delta\,^{15}$N, $\delta\,^{13}$C and $\delta\,^{34}$S. However, only protein $\delta\,^{15}$N could differentiate between organic and conventional potato samples. The study verified that food authenticity tracking requires the analysis of a broad range of isotopes. Pacifico, Onofri, Parisi, Ostano, and Mandolino (2017) analysed the transcriptomic profile of a potato cultivar grown for two years using organic or conventional farming practices. The transcriptomic raw data were obtained through Potato Oligo Chip Initiative (POCI) microarrays and processed using unsupervised coupling multivariate statistical analysis and bioinformatics (MapMan software). Transcriptome changes detected in the potato tubers in response to organic management were associated with nutrition (e.g., the content of phenylpropanoids, flavonoids, glycoalkaloids, asparagine, and ascorbic acid). Several candidate genes were identified as potential markers of organically grown potatoes.

Araújo et al. (2019) demonstrated the efficiency of machine learning techniques in the classification of vegetables produced under organic or conventional systems in the state of Pernambuco, Brazil. The contents of 25 elements were determined in onions by ICP-OES using the conventional sample introduction system. Data mining techniques were applied to develop discrimination models based on organic vegetable samples, which were analysed by feature selection combined with classification algorithms. For onions (*Allium cepa Hysam*), 100% accuracy was obtained, indicating that elemental quantification can be used to authenticate organic and conventional onions.

4. Fruits

The lack of reliable analytical techniques to differentiate between organic and conventional foods has resulted in the exploration of innovative methodologies. For example, differences in chemical composition between organic and conventional fruits have been identified using omics approaches, whereas microbial fingerprinting has led to the proposed use of microorganisms as organic biomarkers.

4.1. *Red fruits*

NIR spectroscopy offers great potential not only for selecting high-quality fruit products but also for improving the traceability and authentication of organic produce. In a study by Amodio, Ceglie, Chaudhry, Piazzolla, and Colelli (2017), NIR spectroscopy was applied to differentiate between various categories of strawberries grown under three distinct fertility management systems: conventional, organic with input substitution, and organic using manure and cover crop amendment. Reflectance spectra were collected using Fourier transform (FT)-NIR. PLS analysis was performed to build predictive models of chemical quality, including factors such as total soluble solids, ascorbic acid and phenolic compound content, pH and titratable acidity. Additionally, PLS-DA was used for classification models. The study successfully discriminated between the three production systems with over 95% sensitivity and more than 94% specificity, highlighting the potential of NIR methodologies for classifying organic food products. In addition, Wassenaar et al. (2022) used an innovative Ti(III) reduction method for rapid and cost-effective isotopic analysis of nitrate in organic and conventional strawberries. The distinctive isotopic signatures of synthetic nitrate fertilizers, marked by elevated $\delta\,^{18}$O values and reduced $\delta\,^{15}$N values, proved indicative of conventional agriculture. Using chemometric analysis (DD-SIMCA), nitrate δ^{18}O values were found to be a robust primary discriminator between organic and conventional strawberry production. It was concluded that this method is useful for evaluating nitrate fertilization practices in organic and conventional production and can support existing authenticity verification techniques.

FTIR and Raman spectroscopic screening methods with multivariate

Table 2
Analytical and statistical approaches for organic traceability in animal products, oils, stimulant foods and miscellanea.

Food	Key Variables	Statistical analysis	Validated method	References
ANIMAL PRODUCTS				
Beef meat	Lipidomic profile (REIMS-QToF)	PCA-LDA	Yes	Robson et al. (2022)
Pork meat	FA profile	SIMCA	Yes	Oliveira et al. (2015)
Pork meat	δ^{13}C, δ^{15}N, δ^{2}H and δ^{18}O and elemental composition (ICP-MS)	OPLS-DA	Yes	Zhao et al. (2020)
Fish (salmon and trout)	δ^{13}C and δ^{15}N, FA profile, carotenoids	*t*-test or mann-whitney test	No	Molkentin et al. (2015)
Eggs	Elemental composition (ICP-MS)	SIMCA	Yes	Borges, Volmer, et al. (2015)
Eggs	δ^{13}C and δ^{15}N	MANOVA, LSD	No	Rogers et al. (2015)
Eggs	Physical parameters, fat content, FA profile	PCA	No	Marelli et al. (2021)
Milk	δ^{13}C and δ^{15}N	LSD	No	Chung et al. (2014)
Milk	^{13}C NMR spectra of the manure	Direct comparison	No	He et al. (2015)
Milk	FA profile and TAG profile	Kruskal–Wallis and pairwise Mann–Whitney *U* test	No	Capuano et al. (2015)
Butter	Fat content, Free fatty acid, FA profile and TAG profile	Kruskal–Wallis and pairwise Mann–Whitney *U* test	No	Pustjens et al. (2017)
Milk	δ^{13}C and δ^{15}N, FA profile and vitamin E	PCA OPLS-DA	Yes	Chung et al. (2018)
Milk	δ^{13}C and δ^{15}N from fatty acids and aminoacids	PLS-DA	Yes	Chung, Kim, Yarnes, et al. (2019)
Milk	Metobolomic profile (^{1}H NMR)	PLS-DA	Yes	Phuenpong et al. (2021)
Milk powder	δ^{13}C, δ^{15}N and δ^{18}O, Elemental composition (ICP-OES and ICP-MS) and FA profile	OPLS-DA	Yes	Xu et al. (2021)
Milk	FA profile	OPLS-DA	Yes	Hou et al. (2023)
OILS				
walnut oils	Volatile compounds (GC-MS)	AHC, PCA, sPLS-DA	Yes	Kalogiouri et al. (2021)
EVOO	Calorimetric analysis	PCA	No	Mallamace et al. (2017)
STIMULANT FOOD				
Coffee	Aroma, flavor, aftertaste, body, and acidity	Hierarchical clustering	No	David et al. (2023)
Coffee	Elemental composition (ICP-MS)	Mann–Whitney test	No	Barbosa et al. (2014)
Ginseng	δ^{13}C, δ^{15}N and δ^{34}S	GLM	No	Chung, Lee, et al. (2017)
MISCELLANEA				
Hen feed	FA profile	PLS-DA	Yes	Alewijn et al. (2016)
Hemp	δ^{15}N	Kruskal-Wallis	No	Calvi et al. (2022)
Saffron	NMR	PLS-DA	Yes	Musio et al. (2022)

Abbreviations: EDXRF = Energy-Dispersive X-Ray Fluorescence, ICP = Inductively coupled plasma, PCA = Principal Component Analysis, SIMCA = Soft Independent Modeling of Class Analogy, HCA = Hierarchical Cluster Analysis, KNN=K-nearest neighbours, SVM = support vector machine, OPLS-DA = Orthogonal Projections to Latent Structures Discriminant Analysis, LSD = least significant difference, PLSR = partial least squares regression, ComDim = Common Dimension Analysis, VOCs = Volatile organic compounds, AF4 = asymmetric flow field-fractionation, ICP-OES = inductively coupled plasma/optical emission spectroscopy, LDA = linear discriminant analysis, ANN = artificial neural networks, RF = random forest, INV = invertases, PG = polygalacturonases, PO = peroxidases, PPO = polyphenoloxidases, CAT = catalases, PAL = phenylalanine ammonia lyase, HPLC-HRAMS =High-performance liquid chromatography/high-resolution accurate mass spectrometry, GC-C-IRMS = gas chromatography-combustion-isotope ratio mass spectrometry, QDA = quadratic discriminant analysis, REIMS = rapid evaporative ionisation mass spectrometry, QToF = quantitative time of flight, PCA= Principal component analysis, FAMEs = fatty acids methyl esters, DGGE = PCR-Denaturing Gradient Gel Electrophoresis, ATR-FTIR = attenuated total reflectance-Fourier transform infrared spectroscopy, AHC=Agglomerative Hierarchical Clustering, DA = discriminant analysis, PC-DA = combination of principal component and discriminant analysis, MANOVA = multivariate analysis of variance, HS-SPME/GC-MS=Head Space-Solid Phase Micro Extraction/Gas Chromatography Mass Spectrometry, ORA= Over-Representation Analysis.

statistical techniques (PCA and HCA) were applied to hydroalcoholic extracts from different grape components (skin, seeds, and pulp), in a range of grape varieties. Distinct chemical patterns were identified, which distinguished between organic and conventional vineyard practices (Radulescu et al., 2021).

In two separate studies, data mining techniques were employed to differentiate between organic and conventional grape juices based on their mineral composition. Using ICP-MS, 44 elements were identified in 37 grape juice samples, both organic and conventional, from various locations in Brazil (Maione et al., 2016). Predictive models developed with SVM, ANN, and decision trees effectively distinguished between the two types of grape juice. In the differentiation, Na, Sn, P, K, Sm, and Nd emerged as key variables, whereas Ag, Zn, Cr, Be, and Pd were the least important.

Also using ICP-MS, the other study determined the concentration of 24 elements in 19 organic and 17 conventional grape juices produced in Brazil. Concentrations of Ba, Ce, La, Mg, P, Pb, Rb, Sn, and Ti were found to be higher in organic samples, while those of Na and V were higher in conventional samples (Borges et al., 2016). Analysis of these data by PCA and SIMCA statistical techniques accurately discriminated between the two sample types. This research indicates that multi-element profiling methods are suitable alternatives for assessing potential adulteration in grape juice.

4.2. Orange/yellow/white fruits

The molecular analysis of microbial ecology has become a pivotal technique to determine the origin of certain foods. This approach is based on identifying microorganisms on the external surface of food and establishing their links with specific geographical regions. Two insightful studies have used this strategy to differentiate between conventional and organic fruits, examining the rDNA fingerprint of microorganisms. In the work of Bigot, Meile, Kapitan, and Montet (2015), a robust methodology was developed that combines the analysis of yeast and bacteria species using PCR-denaturing gradient gel electrophoresis (DGGE) with chemometric methods (PLS-DA). This tool proved highly effective in predicting organic practices for nectarines and peaches. The same techniques successfully differentiated between organic and conventional banana samples, regardless of differences in other factors such as farming methods, fruit varieties, and geographical origin, demonstrating the validity of this innovative method (Bigot et al., 2020).

Conventional and organic bananas were also differentiated by determining their stable isotopic ratios and elemental composition, followed by statistical analysis (PCA and correlation), using samples collected from six countries (Colombia, Costa Rica, Dominica Republic, Ecuador, Panama, and Peru). Significant isotopic differences indicated that $\delta^{15}N$ is a potential marker of organically produced bananas, constituting a traceability tool for commercial fruits (Wang, Erasmus, & van Ruth, 2021). In another study this determination was also proposed for organic banana traceability, concretely $\delta^{15}N$ was higher for organic banana than for conventional ones (Tixier, Loeillet, Coulis, Lescot, & de Lapeyre de Bellaire, 2022).

Differences in the phytochemical composition of conventional and organic goldenberries (*Physalis peruviana*), particularly in withanolide glycosides, were observed by Llano et al. Using a fingerprinting approach, they identified higher levels of withanolides in organic than in conventional fruit. This difference may be associated with a chemical defence mechanism, as withanolides act as immunosuppressants and insect repellents. Thus, withanolides were proposed as a useful authenticity marker for organic (pesticide-free) goldenberries (Llano, Muñoz-Jiménez, Jiménez-Cartagena, Londoño-Londoño, & Medina, 2018).

Data mining with ICP-MS was employed by Maione et al. (2017) to investigate the elemental composition of organic citrus leaves in Brazil, the world's top orange producer, where organic citriculture is currently expanding. Classification models based on SVM and artificial neural networks (ANN) were generated to predict the authenticity of organic leaves based on the concentrations of fourteen chemical elements. The best model achieved 88% accuracy, with Mn, Mg, and Rb being the most relevant elements. The methodology could therefore be useful to authenticate organic citrus leaves and potentially has wider application in certifying other organic food products.

Fruit juice authentication traditionally relies on targeted analytical methods, focusing on specific components, such as sugars, organic acids, and volatile compounds. However, these techniques may overlook more complex forms of fraud, including false organic claims. Untargeted methods for juice authentication can provide a more comprehensive analysis, detecting numerous compounds. For instance, untargeted UHPLC-HRMS analysis combined with various chemometric tools, including PCA, PLS-DA, OPLS-DA, and analysis of variance (ANOVA), successfully discriminated between apple juice samples produced by organic and conventional farming systems. The reproducibility of the method and the effectiveness of batch correction procedures were established (Dinis, Tsamba, Thomas, Jamin, & Camel, 2022).

Cuevas, Pereira-Caro, Moreno-Rojas, Muñoz-Redondo, and Ruiz-Moreno (2017). developed a chemometric approach to authenticate organic orange juices commercially available in Europe. Metabolomic fingerprints and volatile profiles were obtained using HPLC-HRMS and HS-SPME-GC-MS, and the data were analysed by PCA, HCA, and PLS-DA. Key compounds, including flavonoids, fatty acids, aldehydes, and esters, were identified as potential markers for distinguishing organic juices. Finally, data fusion strategies yielded an optimal model for classifying organic and conventional orange juices, achieving an impressive 100% sensitivity and specificity.

In a related study by the same group, HS-SPME-GC-MS was employed to compare the aromatic profiles of oranges from two cultivars grown under organic or conventional farming systems (Cuevas, Moreno-Rojas, & Ruiz-Moreno, 2017). The analysis revealed that both varieties of conventional oranges had higher concentrations of ester compounds, whereas the organic samples showed elevated levels of neryl and geranyl acetates, associated with the geranyl-diphosphate pathway, along with some terpenoids. Moreover, the application of PLS-DA proved highly effective in classifying oranges according to the farming system based on their volatile profiles, achieving an accuracy rate of 90% and 100%.

In a study aimed at discriminating between organic and conventional apples grown in north-eastern Italy, volatile profiles were evaluated using HS-SPME-GC-MS and chemometric methods (Giannetti, Boccacci Mariani, Mannino, & Marini, 2017). The study included 42 apple cultivars, ranging from ancient to new hybrid varieties, grown in different regions with different cultivation methods. After the identification of 118 volatile compounds, PLS-DA models were used to classify the apples based on origin and type of cultivation, achieving an accuracy of over 90%. Ethyl acetate and 1-methoxy-2-methyl butane were key compounds in the differentiation of apple growing systems.

5. Cereals

Differences in fertilization practices between organic and conventional agriculture can alter the chemical composition of cereals. Although atomic spectroscopy techniques have proved useful in monitoring organic compliance, the diversity in fertilizer management systems means that effective analysis depends on combining various techniques with chemometrics to create multivariate fingerprints.

5.1. Rice

Organic rice from Brazil was accurately classified by elemental profiling using quadrupole-ICP-MS followed by data analysis by PCA, SIMCA, HCA, and K-nearest neighbours statistical techniques (Borges, Gelinski, de Oliveira Souza, Barbosa, & Batista, 2015). The concentrations of 20 chemical elements (macro and micro) were measured in 50 rice samples (18 organic and 32 conventional). Conventional rice samples had a significantly higher content of As, B, Ba, Co, Cr, Cu, Mn, P and Zn and lower levels of K, Ca, Mo, Rb and Se compared to the organic samples. Therefore, in this simple and robust methodology, only 14 elements (As, B, Ba, Cd, Co, Cr, Cu, Fe, K, Mg, Mn, P, Rb, and Zn) need to be measured. The same group went on to optimize the methodology by applying SVM, analysing 19 elements (As, B, Ba, Ca, Cd, Ce, Cr, Co, Cu, Fe, La, Mg, Mn, Mo, P, Pb, Rb, Se and Zn) in organic ($n = 17$) and conventional ($n = 33$) rice samples. The authenticity of organic rice samples was predicted with an accuracy of 98% when using the 19 elements, remaining as high as 96% when including only Ca and Cd (Barbosa et al., 2016).

Stable carbon ($\delta^{13}C$) and nitrogen ($\delta^{15}N$) isotope analysis has proven to be a valuable method for authenticating organic agricultural products, including rice. $\delta^{13}C$ values indicate the type of photosynthetic pathway, being higher in C4 plants (Badeck, Tcherkez, Nogués, Piel, & Ghashghaie, 2005). Various factors such as water, nutrients, and organic farming affect $\delta^{13}C$ values due to their impact on soil microbe activity. On the other hand, $\delta^{15}N$ values in agriculture reflect the usage of nitrogen fertilizers, being −6 to 6‰ in conventional fertilizers and 1–37‰ in organic fertilizers (often >5‰) (Mukome, Doane, Silva, Parikh, & Horwath, 2013). These differences enable organic produce to be distinguished from conventionally grown items.

The analysis of $\delta^{13}C$ and $\delta^{15}N$ using IRMS in various rice grains successfully distinguished environment-friendly (organic and pesticide-free) from conventional rice (Chung, Park, et al., 2017). However, it was found that other elemental isotope ratios would be needed for a clearer discrimination between pesticide-free and organic rice samples. In subsequent research, an alternative method was developed using compound-specific $\delta^{13}C$ and $\delta^{15}N$ analysis of fatty acids and amino acids, along with OPLS-DA (Chung, Kim, An, et al., 2019). This new approach successfully differentiated organic, pesticide-free, and conventional rice samples, although the number of tested rice samples was limited. The OPLS-DA models highlighted the significance of $\delta^{13}C$ values of tyrosine, isoleucine, and alanine (variable importance in projection values > 1) for distinguishing organic from pesticide-free rice, with $\delta^{13}C$-lysine playing a major role. In a recent five-year study of variations in $\delta^{13}C$ and $\delta^{15}N$ values in environment-friendly and conventional rice sold in retail markets in Korea, the feasibility of discriminant models for organic rice authentication was assessed (Chung, Kim, Moon, Chi, & Kim, 2021). SVM analysis provided 4.4–14.6% better overall predictability of rice types than discriminant analysis and was effective in distinguishing organic (95.9%) and conventional (93.6%) from pesticide-free rice, potentially enabling high-throughput screening for reliable certification of organic rice.

A promising scientific tool to authenticate rice farming methods has been developed in China. A combination of stable isotope analysis and elemental profiling using chemometric methods, PCA, and linear discriminant analysis (LDA) correctly distinguished organically grown rice cultivars fertilized with animal manures from conventional rice grown with green compost or synthetic fertilizers (Yuan et al., 2018). Later, this isotopic and multi-element strategy was employed in a four-year experimental field trial with the three farming systems (Liu et al., 2020). The study involved the analysis of δ^{13}C and δ^{15}N values, along with the contents of 27 elements (including Na, K, Ca, Fe, and Zn) in both rice and soil samples. The data were evaluated by one-way ANOVA, multivariable correlation analysis, and partial LDA modelling. The influence of various factors such as cultivar, soil fertilization over multiple years, and agroclimatic variations impact on the δ^{13}C and δ^{15}N values. Hence, it was not feasible to accurately differentiate organic rice from green and conventional rice based solely on δ^{13}C and δ^{15}N values. However, significant differences were observed, particularly higher levels of K and Ca in green and conventional rice due to the use of synthetic fertilizers (e.g., KNO_3, KH_2PO_4, and $CaHPO_4$). Therefore, the combination of isotopic and elemental signatures with partial LDA modelling was able to classify organic rice with an impressive accuracy of up to 100%.

A different approach developed by Xiao, Ma, Zhang, and Qian (2018), based on the metabolite fingerprinting of rice samples from different cultivation practices, involved the use of UHPLC coupled to quadrupole time-of-flight MS (UHPLC-QTOF) in combination with statistical analyses (PCA, PLS-DA, HCA). In addition, an OPLS-DA model identified 30 key constituents that efficiently distinguished between organic and conventional cultivation. Among them, 8 metabolites (malvin, pinoresinol, lagochiline, 4-methylumbelliferyl glucuronide, coumarin 106, benzoyl-L-arginine, and hydrocinchonine) were proposed as potential biomarkers for authentication purposes.

In an alternative strategy, NIR spectroscopy with an absorption mode range of 12000–4000 cm^{-1} together with multivariate PCA and PLS regression (PLSR) discriminated between organic and conventional rice samples with a prediction accuracy of 87.5% (Xiao, Liu, Zhang, Ma, & Ngadi, 2019). Although the results indicated the models performed well, further research with a larger sample size is warranted to improve the predictions. In addition, the authors conclude the application of this methodology on an industrial scale would require the use of more tailored training sets and more in-depth knowledge of spectrum-associated chemical and structural characteristics.

A preliminary study was conducted to investigate variations in phenolic compounds in rice cultivated with different systems, as their contents are known to be influenced by the use of organic or synthetic pesticides and chemical fertilizers (Prabakaran et al., 2018). Ferulic acid was found to be the most abundant compound in three types of studied rice: (in decreasing order) pesticide-free > conventional > organic rice ($p < 0.0001$). Although the contents of individual phenolic compounds in polished rice samples were particularly low, they acquired statistical significance when analysed collectively. Despite the promising results, the researchers recognised that further studies were needed to guarantee the robustness of the experiments.

5.2. Wheat

Among cereal crops, wheat (*Triticum aestivum* L.) is considered the most important, constituting a basic dietary staple across the globe. The authentication of wheat has been the focus of considerable research in the last decades, addressing the need to verify its precise geographical origin, variety, and organic attributes, and to distinguish wheat flour from that of other cereals. In this context, multi-elemental profiling, combining ICP-MS and chemometrics, was able to confirm the organic status of wheat and barley (Laursen et al., 2011). No variations in essential plant nutrients were observed, but 14 elements allowed discrimination, particularly Cd from inorganic fertilizers. Discriminative power was enhanced by the use of semi-quantitative ICP-MS, which identified up to 25 elements, showing promise as a cost-efficient method for organic and conventional crop differentiation.

The same research group conducted carefully controlled long-term field trials, including the production of wheat and barley, with the aim of authenticating organic *versus* conventional plants. Stable isotopes of H, C, N, O, Mg, and S together with compound-specific N and O isotopes were analysed (Laursen et al., 2013). δ^{15}N values provided insights into the use of animal manure but failed to differentiate between plants produced with synthetic nitrogen fertilizers or green manures (mixtures of grasses and N_2-fixing legumes). However, this limitation was overcome by measuring δ^{2}H, which effectively distinguished between organic and conventional wheat and barley grains. Using a similar method, a recent study analysed 132 wheat samples from various regions in Germany to track their authenticity regarding production method and origin (Gatzert et al., 2021). Among the isotopes studied (of O, H, C, N, and S), δ^{13}C was the only tracer that exhibited statistically significant differences between the organic and conventional wheat samples.

Alternatively, looking for new and more sensitive markers to verify the crop fertilization regime, Paolini, Ziller, Laursen, Husted, and Camin (2015) analysed wheat-derived amino acids after protein hydrolysis and derivatization using advanced GC-C-IRMS techniques. Common and durum wheat samples grown with synthetic nitrogen fertilizers, animal manures, or green manures based on nitrogen-fixing legumes were studied. Measurements of δ^{13}C values of glutamic acid and glutamine, along with δ^{15}N and δ^{13}C values of ten amino acids (Ala, Val, Ile, Leu, Gly, Pro, Thr, Asx, Glx, and Phe), effectively differentiated organic and conventional wheat. This differentiation persisted even in cases of organic wheat production involving nitrogen-fixing plant fertilization and crop rotation.

Another approach involves the profiling of metabolites or specific nutrients. Metabolite profiling was employed to identify biomarkers in organic and conventional wheat grain from 11 diverse cultivars (Bonte et al., 2014). GC-MS analysis of methanol extracts revealed that the cultivar had a stronger impact on metabolite concentration than the farming system, although a *t*-test showed significant differences in five metabolites and 11 TAGs between organic and conventional wheat for all cultivars. The effectiveness of this approach was only demonstrated when analysing an individual cultivar, due to the significant genetic impact on the metabolite profile. The methodology was subsequently improved by the use of machine-learning algorithms to analyse the GC-MS data, proving able to differentiate between organic and conventional cultivation for a specific year and wheat cultivar (Kessler et al., 2015). The dataset was derived from more than 300 GC-MS measurements of the same 11 wheat cultivars grown over 3 years and was processed using the MeltDB 2.0 metabolomics analysis platform. The unsupervised techniques of t-distributed stochastic neighbour embedding (t-SNE) and PCA, and supervised SVM were used to visualize and classify the samples.

Similarly, phenolic acids were analysed by LC in search of biomarkers of organic wheat grown in Denmark (Weesepoel et al., 2016). By combining baseline and retention-time correction pre-treatments and PCA, organic and conventional samples were differentiated by the first principal component (93%). Wheat grown in three different locations and harvested over two years was accurately categorized into organic and conventional groups according to the levels of protocatechuic acid measured by LC analysis at 280 nm (ANOVA, $P < 0.05$).

In a different fingerprinting approach, crystallization with additives showed promise as an authentication tool for organic wheat, identifying unique structural variables (Kahl et al., 2015). The k-nearest-neighbour classification method distinguished between organic and non-organic wheat with 84% accuracy for *Runal* cv. and 95% for *Titlis* cv.

5.3. Corn

Cornmeal is a primary ingredient in the production of diverse extruded snack products, and its intrinsic properties, in combination with the processing parameters, exert a substantial influence on the ultimate quality of the extruded product. In this context, Ayvaz, Plans, Towers, Auer, and Rodriguez-Saona (2015) evaluated techniques that can rapidly authenticate organic cornmeal by distinguishing it from conventional equivalents. The accurate classification of 11 organic and 27 conventional cornmeal samples was achieved through the utilization of IR spectra in combination with several chemometric models, including SIMCA and PLSR. In concrete, benchtop and handheld NIR spectrometers, as well as portable mid-infrared (MIR) spectrometers were used. The IR data analysis revealed that differences in acidic amino acids (glutamic and aspartic acid) and amide regions attributed to proteins had a substantial impact on the classification process.

6. Animal products

In contrast with organic agriculture, the production of organic animal products must comply with other regulations besides restrictions on the use of synthetic substances. Livestock should be raised in environments that closely resemble their natural living conditions, with space for moving and grazing, and access to natural air and light (UE, FDA). Also, the use of antibiotics is restricted, while the use of hormones is prohibited, and all animal feed must be organic (European Parliament & European Council, 2018; United States Department of Agriculture, 2022).

Among the different approaches to the authentication of organic animal products, the most explored are based on the fingerprint left by organic feed, including a distinct stable isotopic ratio, elemental distribution, and fatty acid profile. In this section, the different strategies for distinguishing organic and non-organic animal products are discussed, focusing on some of the challenges faced by researchers.

In authentication research, the most studied organic animal product is milk and its derivatives. Stable isotopes have been proposed as promising markers. The combination of δ^{13}C and δ^{15}N values was found to be more effective than either value alone in distinguishing organic from conventional milk (Chung, Park, Yoon, Yang, & Kim, 2014). This research was extended by the analysis of fatty acid profiles and vitamin E as well as stable isotopes (Chung et al., 2018), all of which showed stronger seasonal variation in organic than conventional milk. The combined measurement of δ^{13}C and δ^{15}N values, fatty acid contents, and vitamin E was proposed as an accurate system for establishing organic authenticity. This approach was improved in a subsequent study in which the stable isotopic ratio of fatty acids and amino acids permitted organic milk differentiation (Chung et al., 2019). A multivariate OPLS-DA model based on stable isotope ratios, elements, and fatty acids was also satisfactorily employed to discern between organic and conventional milk (Xu et al., 2021).

Another approach to authenticate organic milk is based on NMR spectra of the organic matter of the dairy manure. He et al. (2015) studied the ^{13}C NMR spectra of the dairy manure from organic and conventional farming systems, and found that the region at 30 ppm, corresponding to cutan and cutin from the outer cuticle of herbaceous plants, had a higher peak in the former. This difference was attributed to the higher consumption of forage by organically farmed cows. In another study, the whole ^{1}H NMR metabolite profile was used to build a PLS-DA model, which correctly classified organic and conventional milk (Phuenpong et al., 2021).

The results have been less clear when using fatty acid and triglyceride profiles for the discrimination of dairy products, as proposed by Capuano et al. (2015). As the fatty acid content depends on the nutrition of the cow, the model developed by Pustjens et al. (2017), using this approach failed to discern between butters originating from organically raised and grass-fed cows, although those groups were differentiated from conventional butter. In a recent study, organic and conventional milk (both raw and retail) were correctly classified using the fatty acid profile determined by GC-MS/FID and an OPLS-DA model (Hou et al., 2023). However, it would be interesting to test the capacity of this model to differentiate between organic milk and milk produced from grass-fed cows in non-organic systems, which was not analysed.

Regarding the authentication of organic eggs, they were effectively distinguished by multi-element analysis and a SIMCA model (Borges, Volmer, et al., 2015). In a comparison of stable isotope ratios, δ^{15}N was proposed as a possible marker of traceability, as values differed between organic and conventional eggs (Rogers, van Ruth, Alewijn, Philips, & Rogers, 2015). Another study used physical parameters (total weight, plus the weights of the albumen, yolk, and shell) together with the fatty acid profile and content to build a PCA model that accurately separated the two egg types (Marelli, Madeddu, Mangiagalli, Cerolini, & Zaniboni, 2021).

Attempts to authenticate organic beef and pork have had positive outcomes. Oliveira, Alewijn, Boerrigter-Eenling, and van Ruth (2015) developed a SIMCA model based on fatty acid and volatile/non-volatile organic compound fingerprints to distinguish between organic, free-range, and conventional pork meat. The fatty acid profile gave the best results, achieving 100% correct prediction. Accurate organic pork authentication was also achieved by combining multi-element and isotopic data obtained from defatted meat and developing PCA and OPLS-DA models (Zhao et al., 2020). Organic and conventional beef were differentiated by HRMS lipidomic analysis and the use of PCA-LDA models, with 84% accuracy (Robson, Birse, Chevallier, & Elliott, 2022). It was concluded that this system was more accurate than isotopic analysis, as well as being cheaper and quicker.

Farmed fish can also be labelled as organic. As in animal farming, organic aquaculture is characterized by the provision of organic feed, natural light, and adequate space. With the purpose of tracing this kind of fish, Molkentin, Lehmann, Ostermeyer, and Rehbein (2015) studied the fatty acid profile and stable isotope ratios in wild, organic, and conventional salmon and trout. Among the fatty acids, the linoleic acid content (highest in conventional salmon) distinguished between the three types of fish. The combined δ^{13}C and δ^{15}N values in defatted matter differentiated organic from conventional but not wild fish, which was eventually achieved by measuring δ^{13}C in the fish lipids.

7. Oils

7.1. Extra virgin olive oils

Due to the widespread incorporation of extra virgin olive oils (EVOOs) into healthy diets in recent years, there has been a growing need to authenticate their geographical origin and assess their quality (Lozano-Castellón et al., 2022). Several advanced analytical techniques have been employed to investigate the physical and chemical properties of EVOOs, including NMR spectroscopy, X-ray diffraction (XRD), ultraviolet (UV) spectroscopy, HPLC, and GC (Lozano-Castellón et al., 2022). Notably, differential scanning calorimetry (DSC) has recently found application in the analysis of various foodstuffs, including EVOO, to establish a distinct thermal fingerprint capable of characterizing individual samples (Mallamace et al., 2017).

In 2015, an Italian research team used DSC in an extensive investigation into the thermal properties of 39 organic EVOOs sourced from diverse regions worldwide. This analytical technique generates distinctive thermal profiles, known as thermograms, by subjecting the sample to a series of heating and cooling cycles. Variations stemming from different cultivars, geographical origin, or chemical composition manifest as noticeable alterations within the corresponding thermograms, based on the melting profiles of triacylglycerol constituents (Mallamace et al., 2017).

7.2. Walnut oil

The volatile metabolome of walnut oils from both conventional and organic farming practices was comprehensively studied with HS-SPME-GC-MS (Kalogiouri et al., 2021). The solid-phase microextraction protocol was optimized, taking into account the impact of extraction time and temperature and sample mass, and the optimal conditions for extracting 0.5 g of walnut oil were established as 40 °C for a duration of 60 min. The analysis of twenty Greek walnut oil samples (ten conventional and ten organic) led to the identification of 41 volatile compounds, which constituted a diverse range of chemical classes such as aldehydes, ketones, alcohols, monocarboxylic acids, as well as heterocyclic compounds, including pyrazines, pyrazine derivatives and furan derivatives. Based on these data, a robust classification model was developed using sparse-PLS-DA, which provided 100% accuracy in classification of the two types of walnut oils. The compounds responsible for the variability were three alcohols, 2-hexenal, hexanol, pentanol; and two aldehydes, pentanal and 2,4-heptadienal (Kalogiouri et al., 2021).

8. Coffee and stimulant beverages

Coffee stands as one of the world's most widely traded commodities. Projections indicate that the global organic coffee market is on a trajectory to reach $20.78 billion by 2030, with a predicted annual growth rate of 10.6% from 2020 to 2030 (David, Intania, Purnama, & Iswaldi, 2023), which is largely attributed to the rising demand for health-promoting products. Notably, organically cultivated coffee beans exhibit significantly higher concentrations of total phenols and phenolic compounds in comparison with their conventionally grown counterparts (Król, Gantner, Tatarak, & Hallmann, 2020).

Melgaço Barbosa et al. combined advanced data mining techniques with the assessment of trace element concentrations to evaluate the authenticity of organic coffee, identifying 38 elements in a total of 54 samples of Brazilian coffee (20 organic and 34 nonorganic). Opposing the concept that organic food is inherently richer in essential elements, higher levels were found in conventional coffee samples, with the exception of Cs, Tl and W (Barbosa et al., 2014). Furthermore, the levels of essential elements found in the coffee samples closely align with data of previous studies of coffee grown in Brazil and other global regions (Amorim Filho, Polito, & Gomes Neto, 2007; Zaidi, Fatima, Arif, & Qureshi, 2005). With these data, the three classification algorithms were used, multilayer perceptron (MLP), SVM, and naïve Bayes (NB), MLP and SVM achieved a predictive accuracy of 96.3%. In the case of NB, the predictive accuracy increased to 98.2% when only eight of the elements (Zn, Se, Ba, U, Dy, Tl, Th, and Mo) were included in the chemometric analysis (Barbosa et al., 2014). The levels of trace elements in coffee are influenced by various factors, including the cultivar, soil type, and fertilization practices, and can constitute a unique fingerprint. The high level of accuracy achieved in the study underscores the potential of employing trace element concentrations in conjunction with data mining techniques as a robust and versatile tool for authenticity assessment of organic coffee.

Isotopic analysis has also been proposed as a way of detecting fraud in organic ginseng. The $\delta^{15}N$ value was found to be consistently lower in conventional than in organic ginseng, regardless of the type of organic fertilization (Chung, Lee, et al., 2017).

9. Miscellaneous

Some other foods and products that do not fit into the previous sections have been the subject of authentication studies, although with scarce data produced to date. For example, the authentication of organic animal feed has been studied, as its use is one of the main requisites in the production of organic animal products. Thus, organic laying hen feed was discriminated from conventional feed by a PLS-DA model using the fatty acid profile (Alewijn, van der Voet, & van Ruth, 2016). Organic and conventional saffron were also discriminated by a PLS-DA model using the whole NMR fingerprint (Musio et al., 2022). Finally, stable isotope ratios were proposed as possible markers to classify organic and conventional hemp for food use, as the isotopic pattern differs according to the growing system (Calvi et al., 2022).

10. Conclusion

In this review, we have looked at the studies exploring cutting-edge techniques to differentiate between organic and conventional foods. The application of molecular microbial analysis, advanced chemometrics, and a range of spectroscopic methods has provided invaluable insights into the origins and authenticity of food products. After this comprehensive survey, several key conclusions can be drawn.

Elemental analysis and stable isotopes analysis together with chemometrics have proven the ability to classify between organic and conventional samples. In addition, molecular analysis, particularly rDNA fingerprinting of microorganisms, is emerging as a key tool for the authentication of a wide variety of fruits, accurately predicting cultivation practices and thereby enhancing product credibility. False organic claims can also be uncovered using untargeted metabolomic fingerprinting and the comprehensive analysis of volatile profiles. Finally, the combination of techniques such as UHPLC-HRMS and HS-SPME-GC-HRMS with advanced statistical treatment of data is proving to be highly effective in differentiating between organic and conventional food, with guaranteed reliability of results.

11. Future perspectives

The challenge with these methods lies in the fact that the chemical composition of the food is not solely determined by fertilization. Therefore, a wide range of samples should be incorporated into the model development to ensure the predictability of the model.

Organic food analysis holds great promise with the development of more accurate and accessible tools to verify product authenticity and quality. The efficiency and accuracy of existing techniques will be further improved through automation and integration of AI and machine learning. Research should also be expanded to include a wider range of products and regions. The commercial application of more efficient methods to control quality, detect fraud, and verify product labeling will ensure consumer confidence and industry standards.

Author contributions

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Funding

This research was funded by PID2020-114022RB-I00 and CIBEROBN from the Instituto de Salud Carlos III, ISCIII from the Ministerio de Ciencia, Innovación y Universidades, (AEI/FEDER, UE), Generalitat de Catalunya (GC) [2021-SGR-00334]. INSA-UB is María de Maeztu Unit of Excellence (grant CEX2021-001234-M funded by MICIN/AEI/FEDER,

UE).

Declaration of competing interest

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

Data availability

No data was used for the research described in the article.

Acknowledgments

Julián Lozano-Castellón thanks the CIBER for the post-doctoral contract (2528/2958). Emily P. Laveriano-Santo. thanks FI-SDUR (EMC/503/2021) fellowship program from the Generalitat de Catalunya. Mohamed M. Abuhabib is grateful for the predoctoral scholarship FI-SDUR (REU/551/2022) from the Agency of Management of University and Research Grants (AGAUR, Generalitat de Catalunya).

References

Alewijn, M., van der Voet, H., & van Ruth, S. (2016). Validation of multivariate classification methods using analytical fingerprints – concept and case study on organic feed for laying hens. *Journal of Food Composition and Analysis, 51*, 15–23. https://doi.org/10.1016/j.jfca.2016.06.003

Allen, D. M. (1974). The relationship between variable selection and data agumentation and a method for prediction. *Technometrics, 16*(1), 125–127. https://doi.org/10.1080/00401706.1974.10489157

Amodio, M. L., Ceglie, F., Chaudhry, M. M. A., Piazzolla, F., & Colelli, G. (2017). Potential of NIR spectroscopy for predicting internal quality and discriminating among strawberry fruits from different production systems. *Postharvest Biology and Technology, 125*, 112–121. https://doi.org/10.1016/j.postharvbio.2016.11.013

Amorim Filho, V. R., Polito, W. L., & Gomes Neto, J. A. (2007). Comparative studies of the sample decomposition of green and roasted coffee for determination of nutrients and data exploratory analysis. *Journal of the Brazilian Chemical Society, 18*(1), 47–53. https://doi.org/10.1590/S0103-50532007000100005

Araújo, E. M., de Lima, M. D., Barbosa, R., & Alleoni, L. R. F. (2019). Using machine learning and multi-element analysis to evaluate the authenticity of organic and conventional vegetables. *Food Analytical Methods, 12*(11), 2542–2554. https://doi.org/10.1007/s12161-019-01597-2

Ayvaz, H., Plans, M., Towers, B. N., Auer, A., & Rodriguez-Saona, L. E. (2015). The use of infrared spectrometers to predict quality parameters of cornmeal (corn grits) and differentiate between organic and conventional practices. *Journal of Cereal Science, 62*, 22–30. https://doi.org/10.1016/j.jcs.2014.12.004

Badeck, F., Tcherkez, G., Nogués, S., Piel, C., & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. *Rapid Communications in Mass Spectrometry, 19*(11), 1381–1391. https://doi.org/10.1002/rcm.1912

Ballabio, D., & Consonni, V. (2013). Classification tools in chemistry. Part 1: Linear models. PLS-DA. *Analytical Methods, 5*(16), 3790. https://doi.org/10.1039/c3ay40582f

Barbosa, R. M., Batista, B. L., Varrique, R. M., Coelho, V. A., Campiglia, A. D., & Barbosa, F. (2014). The use of advanced chemometric techniques and trace element levels for controlling the authenticity of organic coffee. *Food Research International, 61*, 246–251. https://doi.org/10.1016/j.foodres.2013.07.060

Barbosa, R. M., de Paula, E. S., Paulelli, A. C., Moore, A. F., Souza, J. M. O., Batista, B. L., et al. (2016). Recognition of organic rice samples based on trace elements and support vector machines. *Journal of Food Composition and Analysis, 45*, 95–100. https://doi.org/10.1016/j.jfca.2015.09.010

Bateman, A. S., & Kelly, S. D. (2007). Fertilizer nitrogen isotope signatures. *Isotopes in Environmental and Health Studies, 43*(3), 237–247. https://doi.org/10.1080/10256010701550732

Bigot, C., Bugaud, C., Camilo, J., Kapitan, A., Montet, D., & Meile, J.-C. (2020). Impact of farming type, variety and geographical origin on bananas bacterial community. *Food Control, 109*, Article 106925. https://doi.org/10.1016/j.foodcont.2019.106925

Bigot, C., Meile, J.-C., Kapitan, A., & Montet, D. (2015). Discriminating organic and conventional foods by analysis of their microbial ecology: An application on fruits. *Food Control, 48*, 123–129. https://doi.org/10.1016/j.foodcont.2014.03.035

Bonte, A., Neuweger, H., Goesmann, A., Thonar, C., Mäder, P., Langenkämper, G., et al. (2014). Metabolite profiling on wheat grain to enable a distinction of samples from organic and conventional farming systems. *Journal of the Science of Food and Agriculture, 94*(13), 2605–2612. https://doi.org/10.1002/jsfa.6566

Bontempo, L., van Leeuwen, K. A., Paolini, M., Holst Laursen, K., Micheloni, C., Prenzler, P. D., et al. (2020). Bulk and compound-specific stable isotope ratio analysis for authenticity testing of organically grown tomatoes. *Food Chemistry, 318*, Article 126426. https://doi.org/10.1016/j.foodchem.2020.126426

Borges, E. M., Gelinski, J. M. L. N., de Oliveira Souza, V. C., Barbosa, F., Jr., & Batista, B. L. (2015). Monitoring the authenticity of organic rice via chemometric analysis of elemental data. *Food Research International, 77*, 299–309. https://doi.org/10.1016/j.foodres.2015.06.008

Borges, E. M., Volmer, D. A., Brandelero, E., Gelinski, J. M. L. N., Gallimberti, M., & Barbosa, F. (2016). Monitoring the authenticity of organic grape juice via chemometric analysis of elemental data. *Food Analytical Methods, 9*(2), 362–369. https://doi.org/10.1007/s12161-015-0191-x

Borges, E. M., Volmer, D. A., Gallimberti, M., Ferreira de Souza, D., Luiz de Souza, E., & Barbosa, F. (2015). Evaluation of macro- and microelement levels for verifying the authenticity of organic eggs by using chemometric techniques. *Analytical Methods, 7*(6), 2577–2584. https://doi.org/10.1039/C4AY02986K

Calvi, M., Bontempo, L., Pizzini, S., Cucinotta, L., Camin, F., & Stenni, B. (2022). Isotopic characterization of Italian industrial hemp (Cannabis sativa L.) intended for food use: A first exploratory study. *Separations, 9*(6), 136. https://doi.org/10.3390/separations9060136

Capuano, E., Gravink, R., Boerrigter-Eenling, R., & van Ruth, S. M. (2015). Fatty acid and triglycerides profiling of retail organic, conventional and pasture milk: Implications for health and authenticity. *International Dairy Journal, 42*, 58–63. https://doi.org/10.1016/j.idairyj.2014.11.002

Chung, I.-M., Kim, J.-K., An, Y.-J., Kwon, C., Kim, S.-Y., Yang, Y.-J., et al. (2019). Compound-specific δ13C and δ15N analyses of fatty acids and amino acids for discrimination of organic, pesticide-free, and conventional rice (Oryza sativa L). *Food Chemistry, 283*, 305–314. https://doi.org/10.1016/j.foodchem.2018.12.129

Chung, I.-M., Kim, J.-K., Lee, K.-J., Son, N.-Y., An, M.-J., Lee, J.-H., et al. (2018). Discrimination of organic milk by stable isotope ratio, vitamin E, and fatty acid profiling combined with multivariate analysis: A case study of monthly and seasonal variation in Korea for 2016–2017. *Food Chemistry, 261*, 112–123. https://doi.org/10.1016/j.foodchem.2018.04.017

Chung, I.-M., Kim, Y.-J., Moon, H.-S., Chi, H.-Y., & Kim, S.-H. (2021). Long-term isotopic model study for ecofriendly rice (Oryza sativa L.) authentication: Updating a case study in South Korea. *Food Chemistry, 362*, Article 130215. https://doi.org/10.1016/j.foodchem.2021.130215

Chung, I.-M., Kim, J.-K., Yarnes, C. T., An, Y.-J., Kwon, C., Kim, S.-Y., et al. (2019). Fatty acid- and amino acid-specific isotope analysis for accurate authentication and traceability in organic milk. *Journal of Agricultural and Food Chemistry, 67*(2), 711–722. https://doi.org/10.1021/acs.jafc.8b05063

Chung, I.-M., Lee, T.-J., Oh, Y.-T., Ghimire, B. K., Jang, I.-B., & Kim, S.-H. (2017). Ginseng authenticity testing by measuring carbon, nitrogen, and sulfur stable isotope compositions that differ based on cultivation land and organic fertilizer type. *Journal of Ginseng Research, 41*(2), 195–200. https://doi.org/10.1016/j.jgr.2016.03.004

Chung, I.-M., Park, S.-K., Lee, K.-J., An, M.-J., Lee, J.-H., Oh, Y.-T., et al. (2017). Authenticity testing of environment-friendly Korean rice (Oryza sativa L.) using carbon and nitrogen stable isotope ratio analysis. *Food Chemistry, 234*, 425–430. https://doi.org/10.1016/j.foodchem.2017.05.014

Chung, I.-M., Park, I., Yoon, J.-Y., Yang, Y.-S., & Kim, S.-H. (2014). Determination of organic milk authenticity using carbon and nitrogen natural isotopes. *Food Chemistry, 160*, 214–218. https://doi.org/10.1016/j.foodchem.2014.01.061

Cubero-Leon, E., De Rudder, O., & Maquet, A. (2018). Metabolomics for organic food authentication: Results from a long-term field study in carrots. *Food Chemistry, 239*, 760–770. https://doi.org/10.1016/j.foodchem.2017.06.161

Cuevas, F. J., Moreno-Rojas, J. M., & Ruiz-Moreno, M. J. (2017). Assessing a traceability technique in fresh oranges (Citrus sinensis L. Osbeck) with an HS-SPME-GC-MS method. Towards a volatile characterisation of organic oranges. *Food Chemistry, 221*, 1930–1938. https://doi.org/10.1016/j.foodchem.2016.11.156

Cuevas, F. J., Pereira-Caro, G., Moreno-Rojas, J. M., Muñoz-Redondo, J. M., & Ruiz-Moreno, M. J. (2017). Assessment of premium organic orange juices authenticity using HPLC-HR-MS and HS-SPME-GC-MS combining data fusion and chemometrics. *Food Control, 82*, 203–211. https://doi.org/10.1016/j.foodcont.2017.06.031

Cvijanović, V., Sarić, B., Dramićanin, A., Kodranov, I., Manojlović, D., Momirović, N., et al. (2021). Content and distribution of macroelements, microelements, and rare-earth elements in different tomato varieties as a promising tool for monitoring the distinction between the integral and organic systems of production in zeleni hit—official enza and vitalis trial and breeding station. *Agriculture, 11*(10), 1009. https://doi.org/10.3390/agriculture11101009

David, W., Intania, M., Purnama, P., & Iswaldi, I. (2023). Characteristics of commercial single-origin organic coffee in Indonesia. *Food Science and Technology, 43*. https://doi.org/10.1590/fst.118522

de Andrade, J. C., Galvan, D., Effting, L., Lelis, C., Melquiades, F. L., Bona, E., 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. https://doi.org/10.1007/s12161-022-02439-4

Díaz-Galiano, F. J., Heinzen, H., Martínez-Bueno, M. J., Rajski, Ł., & Fernández-Alba, A. R. (2022). Use of high-resolution mass spectrometry for the first-time identification of gerberin as a tentative marker of the fraudulent organic production of tomatoes. *Journal of Food Composition and Analysis, 112*, Article 104662. https://doi.org/10.1016/j.jfca.2022.104662

Dinis, K., Tsamba, L., Jamin, E., & Camel, V. (2023). Untargeted metabolomics-based approach using UHPLC-HRMS to authenticate carrots (Daucus carota L.) based on geographical origin and production mode. *Food Chemistry, 423*, Article 136273. https://doi.org/10.1016/j.foodchem.2023.136273

Dinis, K., Tsamba, L., Thomas, F., Jamin, E., & Camel, V. (2022). Preliminary authentication of apple juices using untargeted UHPLC-HRMS analysis combined to chemometrics. *Food Control, 139*, Article 109098. https://doi.org/10.1016/j.foodcont.2022.109098

Duncan, M. W. (2012). Good mass spectrometry and its place in good science. *Journal of Mass Spectrometry, 47*(6), 795–809. https://doi.org/10.1002/jms.3038

European Parliament, & European Council. (2018). Regulation (EU) 2018/848. In *Official journal of the European union* (pp. 1–92). European Comission.

Galvan, D., de Andrade, J. C., Effting, L., Lelis, C. A., Melquiades, F. L., Bona, E., et al. (2023). Energy-dispersive X-ray fluorescence combined with chemometric tools applied to tomato and sweet pepper classification. *Food Control, 143*, Article 109326. https://doi.org/10.1016/j.foodcont.2022.109326

Gatzert, X., Chun, K. P., Boner, M., Hermanowski, R., Mäder, R., Breuer, L., et al. (2021). Assessment of multiple stable isotopes for tracking regional and organic authenticity of plant products in Hesse, Germany. *Isotopes in Environmental and Health Studies, 57*(3), 281–300. https://doi.org/10.1080/10256016.2021.1905635

General survey of vibrational spectroscopy. (1995). In *Infrared and Raman spectroscopy* (pp. 7–61). Wiley. https://doi.org/10.1002/9783527615438.ch02.

Giannetti, V., Boccacci Mariani, M., Mannino, P., & Marini, F. (2017). Volatile fraction analysis by HS-SPME/GC-MS and chemometric modeling for traceability of apples cultivated in the Northeast Italy. *Food Control, 78*, 215–221. https://doi.org/10.1016/j.foodcont.2017.02.036

González-Coria, J., Lozano-Castellón, J., Jaime-Rodríguez, C., Olmo-Cunillera, A., Laveriano-Santos, E. P., Pérez, M., et al. (2022). The effects of differentiated organic fertilization on tomato production and phenolic content in traditional and high-yielding varieties. *Antioxidants, 11*(11). https://doi.org/10.3390/antiox11112127

Harris, R. K., Becker, E. D., Cabral de Menezes, S. M., Goodfellow, R., & Granger, P. (2001). NMR nomenclature. Nuclear spin properties and conventions for chemical shifts(IUPAC Recommendations 2001). *Pure and Applied Chemistry, 73*(11), 1795–1818. https://doi.org/10.1351/pac200173111795

Hassanpourfard, P., Mane, A. V., & Banerjee, K. (2023). Studies on the contamination of heavy metals and their chemical speciation in sediment from selected locations of Pune district. *Nature Environment and Pollution Technology, 22*(4), 1941–1950. https://doi.org/10.46488/NEPT.2023.v22i04.020

He, Z., Zhang, M., Cao, X., Li, Y., Mao, J., & Waldrip, H. M. (2015). Potential traceable markers of organic matter in organic and conventional dairy manure using ultraviolet–visible and solid-state 13C nuclear magnetic resonance spectroscopy. *Organic Agriculture, 5*(2), 113–122. https://doi.org/10.1007/s13165-014-0092-0

Hou, H., Tang, Y., Zhao, J., Debrah, A. A., Shen, Z., Li, C., et al. (2023). Authentication of organically produced cow milk by fatty acid profile combined with chemometrics: A case study in China. *Journal of Food Composition and Analysis, 120*, Article 105297. https://doi.org/10.1016/j.jfca.2023.105297

Jolliffe, I. T., & Cadima, J. (2016). Principal component analysis: A review and recent developments. *Philosophical Transactions of the Royal Society A: Mathematical, Physical & Engineering Sciences, 374*(2065), Article 20150202. https://doi.org/10.1098/rsta.2015.0202

Kahl, J., Busscher, N., Mergardt, G., Mäder, P., Torp, T., & Ploeger, A. (2015). Differentiation of organic and non-organic winter wheat cultivars from a controlled field trial by crystallization patterns. *Journal of the Science of Food and Agriculture, 95*(1), 53–58. https://doi.org/10.1002/jsfa.6818

Kalogiouri, N. P., Manousi, N., Rosenberg, E., Zachariadis, G. A., Paraskevopoulou, A., & Samanidou, V. (2021). Exploring the volatile metabolome of conventional and organic walnut oils by solid-phase microextraction and analysis by GC-MS combined with chemometrics. *Food Chemistry, 363*, Article 130331. https://doi.org/10.1016/j.foodchem.2021.130331

Kessler, N., Bonte, A., Albaum, S. P., Mã¤der, P., Messmer, M., Goesmann, A., et al. (2015). Learning to classify organic and conventional wheat – A machine learning driven approach using the MeltDB 2.0 metabolomics analysis platform. *Frontiers in Bioengineering and Biotechnology, 3*. https://doi.org/10.3389/fbioe.2015.00035

Król, K., Gantner, M., Tatarak, A., & Hallmann, E. (2020). The content of polyphenols in coffee beans as roasting, origin and storage effect. *European Food Research and Technology, 246*(1), 33–39. https://doi.org/10.1007/s00217-019-03388-9

Ku, Y. G., Kang, D. H., Lee, C. K., Lee, S. Y., Ryu, C. S., Kim, D. E., et al. (2018). Influence of different cultivation systems on bioactivity of asparagus. *Food Chemistry, 244*, 349–358. https://doi.org/10.1016/j.foodchem.2017.10.044

Laursen, K. H., Mihailova, A., Kelly, S. D., Epov, V. N., Bérail, S., Schjoerring, J. K., et al. (2013). Is it really organic? – Multi-isotopic analysis as a tool to discriminate between organic and conventional plants. *Food Chemistry, 141*(3), 2812–2820. https://doi.org/10.1016/j.foodchem.2013.05.068

Laursen, K. H., Schjoerring, J. K., Kelly, S. D., & Husted, S. (2014). Authentication of organically grown plants – advantages and limitations of atomic spectroscopy for multi-element and stable isotope analysis. *TrAC, Trends in Analytical Chemistry, 59*, 73–82. https://doi.org/10.1016/j.trac.2014.04.008

Laursen, K. H., Schjoerring, J. K., Olesen, J. E., Askegaard, M., Halekoh, U., & Husted, S. (2011). Multielemental fingerprinting as a tool for authentication of organic wheat, barley, faba bean, and potato. *Journal of Agricultural and Food Chemistry, 59*(9), 4385–4396. https://doi.org/10.1021/jf104928r

Lee, H.-C. (2018). Review of inductively coupled plasmas: Nano-applications and bistable hysteresis physics. *Applied Physics Reviews, 5*(1). https://doi.org/10.1063/1.5012001

Liu, Z., Yuan, Y., Xie, T., Zhang, Y., Shao, S., Nie, J., et al. (2020). Long-term agricultural effects on the authentication accuracy of organic, green, and conventional rice using isotopic and elemental chemometric analyses. *Journal of Agricultural and Food Chemistry, 68*(5), 1213–1225. https://doi.org/10.1021/acs.jafc.9b06847

Llano, S. M., Muñoz-Jiménez, A. M., Jiménez-Cartagena, C., Londoño-Londoño, J., & Medina, S. (2018). Untargeted metabolomics reveals specific withanolides and fatty acyl glycoside as tentative metabolites to differentiate organic and conventional Physalis peruviana fruits. *Food Chemistry, 244*, 120–127. https://doi.org/10.1016/j.foodchem.2017.10.026

Lozano-Castellón, J., López-Yerena, A., Domínguez-López, I., Siscart-Serra, A., Fraga, N., Sámano, S., et al. (2022). Extra virgin olive oil: A comprehensive review of efforts to ensure its authenticity, traceability, and safety. *Comprehensive Reviews in Food Science and Food Safety, 21*(3). https://doi.org/10.1111/1541-4337.12949

Maione, C., de Paula, E. S., Gallimberti, M., Batista, B. L., Campiglia, A. D., Jr, F. B., et al. (2016). Comparative study of data mining techniques for the authentication of organic grape juice based on ICP-MS analysis. *Expert Systems with Applications, 49*, 60–73. https://doi.org/10.1016/j.eswa.2015.11.024

Maione, C., Turra, C., Fernandes, E. A. D. N., Bacchi, M. A., Barbosa, F., & Barbosa, R. M. (2017). Finding the most significant elements for the classification of organic orange leaves: A data mining approach. *Analytical Letters, 50*(14), 2292–2307. https://doi.org/10.1080/00032719.2017.1286667

Mallamace, D., Vasi, S., Corsaro, C., Naccari, C., Clodoveo, M. L., Dugo, G., et al. (2017). Calorimetric analysis points out the physical-chemistry of organic olive oils and reveals the geographical origin. *Physica A: Statistical Mechanics and its Applications, 486*, 925–932. https://doi.org/10.1016/j.physa.2017.06.015

Marelli, S. P., Madeddu, M., Mangiagalli, M. G., Cerolini, S., & Zaniboni, L. (2021). Egg production systems, open space allowance and their effects on physical parameters and fatty acid profile in commercial eggs. *Animals, 11*(2), 265. https://doi.org/10.3390/ani11020265

Martínez Bueno, M. J., Díaz-Galiano, F. J., Rajski, Ł., Cutillas, V., & Fernández-Alba, A. R. (2018). A non-targeted metabolomic approach to identify food markers to support discrimination between organic and conventional tomato crops. *Journal of Chromatography A, 1546*, 66–76. https://doi.org/10.1016/j.chroma.2018.03.002

McManus, K. D. (2019). *Phytonutrients: Paint your plate with the colors of the rainbow*. Harvard Health Publishing- Harvard Medical School.

Molkentin, J., Lehmann, I., Ostermeyer, U., & Rehbein, H. (2015). Traceability of organic fish – authenticating the production origin of salmonids by chemical and isotopic analyses. *Food Control, 53*, 55–66. https://doi.org/10.1016/j.foodcont.2015.01.003

Mukome, F. N. D., Doane, T. A., Silva, L. C. R., Parikh, S. J., & Horwath, W. R. (2013). Testing protocol ensures the authenticity of organic fertilizers. *California Agriculture, 67*(4), 210–216. https://doi.org/10.3733/ca.v067n04p210

Musio, B., Todisco, S., Antonicelli, M., Garino, C., Arlorio, M., Mastrorilli, P., et al. (2022). Non-targeted NMR method to assess the authenticity of saffron and trace the agronomic practices applied for its production. *Applied Sciences, 12*(5), 2583. https://doi.org/10.3390/app12052583

Nielsen, F. (2016). *Hierarchical clustering*. https://doi.org/10.1007/978-3-319-21903-5_8

Novak, V., Adler, J., Husted, S., Fromberg, A., & Laursen, K. H. (2019). Authenticity testing of organically grown vegetables by stable isotope ratio analysis of oxygen in plant-derived sulphate. *Food Chemistry, 291*, 59–67. https://doi.org/10.1016/j.foodchem.2019.03.125

Oliveira, G., Alewijn, M., Boerrigter-Eenling, R., & van Ruth, S. (2015). Compositional signatures of conventional, free range, and organic pork meat using fingerprint techniques. *Foods, 4*(4), 359–375. https://doi.org/10.3390/foods4030359

Pacifico, D., Onofri, C., Parisi, B., Ostano, P., & Mandolino, G. (2017). Influence of organic farming on the potato transcriptome. *Sustainability, 9*(5), 779. https://doi.org/10.3390/su9050779

Paolini, M., Ziller, L., Laursen, K. H., Husted, S., & Camin, F. (2015). Compound-specific δ^{15}N and δ^{13}C analyses of amino acids for potential discrimination between organically and conventionally grown wheat. *Journal of Agricultural and Food Chemistry, 63*(25), 5841–5850. https://doi.org/10.1021/acs.jafc.5b00662

Pettoello-Mantovani, C., & Olivieri, B. (2022). Food safety and public health within the frame of the EU legislation. *Global Pediatrics, 2*, Article 100020. https://doi.org/10.1016/j.gpeds.2022.100020

Phuenpong, T., Kongboonkird, M., Duangmal, K., Lerdvorasap, W., Suksawwawimon, M., Mekboonsonglarp, W., et al. (2021). Molecular discrimination between organic and conventional liquid milk products in Thailand using 1H-NMR metabolomics approach. *Tropical Animal Science Journal, 44*(4), 478–488. https://doi.org/10.5398/tasj.2021.44.4.478

Pomerantsev, A. L., & Rodionova, O. Y. (2020). Popular decision rules in SIMCA: Critical review. *Journal of Chemometrics, 34*(8). https://doi.org/10.1002/cem.3250

Prabakaran, M., Chung, I.-M., Son, N.-Y., Chi, H.-Y., Kim, S.-Y., Yang, Y.-J., et al. (2018). Analysis of selected phenolic compounds in organic, pesticide-free, conventional rice (oryza sativa L.) using LC-ESI-MS/MS. *Molecules, 24*(1), 67. https://doi.org/10.3390/molecules24010067

Pustjens, A., Boerrigter-Eenling, R., Koot, A., Rozijn, M., & van Ruth, S. (2017). Characterization of retail conventional, organic, and grass full-fat butters by their fat contents, free fatty acid contents, and triglyceride and fatty acid profiling. *Foods, 6*(4), 26. https://doi.org/10.3390/foods6040026

Quintanilla-Casas, B., Bertin, S., Leik, K., Bustamante, J., Guardiola, F., Valli, E., et al. (2020). Profiling versus fingerprinting analysis of sesquiterpene hydrocarbons for the geographical authentication of extra virgin olive oils. *Food Chemistry, 307*, Article 125556. https://doi.org/10.1016/j.foodchem.2019.125556

Radulescu, C., Olteanu, R. L., Nicolescu, C. M., Bumbac, M., Buruleanu, L. C., & Holban, G. C. (2021). Vibrational spectroscopy combined with chemometrics as tool for discriminating organic vs. Conventional culture systems for red grape extracts. *Foods, 10*(8), 1856. https://doi.org/10.3390/foods10081856

Robson, K., Birse, N., Chevallier, O., & Elliott, C. (2022). Metabolomic profiling to detect different forms of beef fraud using rapid evaporative ionisation mass spectrometry (REIMS). *Npj Science of Food, 6*(1), 9. https://doi.org/10.1038/s41538-022-00125-7

Rodrigues, M. H. P., Collazzo, C. C., Marques, C. G., Senna, C. de A., Souza, T. D. de, & Badiale-Furlong, E. (2021). Traceability of tomatoes (Solanun lycopersicum) based on their enzymatic profile. *Food Bioscience, 43*, Article 101269. https://doi.org/10.1016/j.fbio.2021.101269

Rogers, K. M., van Ruth, S., Alewijn, M., Philips, A., & Rogers, P. (2015). Verification of egg farming systems from The Netherlands and New Zealand using stable isotopes.

Journal of Agricultural and Food Chemistry, 63(38), 8372–8380. https://doi.org/10.1021/acs.jafc.5b01975

Tixier, P., Loeillet, D., Coulis, M., Lescot, T., & de Lapeyre de Bellaire, L. (2022). Isotopes Don't Lie, differentiating organic from conventional banana (Musa AAA, Cavendish subgroup) fruits using C and N stable isotopes. *Food Chemistry, 394*, Article 133491. https://doi.org/10.1016/j.foodchem.2022.133491

Turra, C., De Nadai Fernandes, E. A., Bacchi, M. A., Sarriés, G. A., Júnior, F. B., & Reyes, A. E. L. (2013). Rare earth elements in citrus production systems. *Journal of Plant Nutrition, 36*(5), 762–771. https://doi.org/10.1080/01904167.2012.754040

United States Department of Agriculture. (2022). National organic program. *Agricultural Marketing Service, 3*(7), 396–449. USDA.

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

Wang, Z., Erasmus, S. W., & van Ruth, S. M. (2021). Preliminary study on tracing the origin and exploring the relations between growing conditions and isotopic and elemental fingerprints of organic and conventional cavendish bananas (musa spp). *Foods, 10*(5), 1021. https://doi.org/10.3390/foods10051021

Wassenaar, L. I., Kelly, S. D., Douence, C., Islam, M., Monteiro, L., Abrahim, A., et al. (2022). Assessment of rapid low-cost isotope (δ ^{15}N, δ ^{18}O) analyses of nitrate in fruit extracts by Ti(III) reduction to differentiate organic from conventional production. *Rapid Communications in Mass Spectrometry, 36*(7). https://doi.org/10.1002/rcm.9259

Weesepoel, Y., Heenan, S., Boerrigter-Eenling, R., Venderink, T., Blokland, M., & Van Ruth, S. (2016). Protocatechuic acid levels discriminate between organic and conventional wheat from Denmark. *CHIMIA, 70*(5), 360. https://doi.org/10.2533/chimia.2016.360

Willer, H., Trávníček, J., Meier, C., & Schlatter, B. (2022). The World of organic agriculture-STATISTICS & EMERGING TRENDS 2022. *IFOAM and FiBL*. https://knowledge4policy.ec.europa.eu/publication/world-organic-agriculture-statistics-emerging-trends-2022_en.

Willett, W., Sacks, F., Trichopoulou, A., Drescher, G., Ferro-Luzzi, A., Helsing, E., et al. (1995). Mediterranean diet pyramid: A cultural model for healthy eating. *The American Journal of Clinical Nutrition, 61*(6), 1402S–1406S. https://doi.org/10.1093/ajcn/61.6.1402S

Worth, T. (2012). *European integrated farming framework*.

Xiao, R., Liu, L., Zhang, D., Ma, Y., & Ngadi, M. O. (2019). Discrimination of organic and conventional rice by chemometric analysis of NIR spectra: A pilot study. *Journal of Food Measurement and Characterization, 13*(1), 238–249. https://doi.org/10.1007/s11694-018-9937-7

Xiao, R., Ma, Y., Zhang, D., & Qian, L. (2018). Discrimination of conventional and organic rice using untargeted LC-MS-based metabolomics. *Journal of Cereal Science, 82*, 73–81. https://doi.org/10.1016/j.jcs.2018.05.012

Xu, S., Zhao, C., Deng, X., Zhang, R., Qu, L., Wang, M., et al. (2021). Multivariate analysis for organic milk authentication. *Journal of Chromatography B, 1186*, Article 123029. https://doi.org/10.1016/j.jchromb.2021.123029

Yuan, Y., Zhang, W., Zhang, Y., Liu, Z., Shao, S., Zhou, L., et al. (2018). Differentiating organically farmed rice from conventional and green rice harvested from an experimental field trial using stable isotopes and multi-element chemometrics. *Journal of Agricultural and Food Chemistry, 66*(11), 2607–2615. https://doi.org/10.1021/acs.jafc.7b05422

Zaidi, J. H., Fatima, I., Arif, M., & Qureshi, I. H. (2005). Determination of trace elements in coffee beans and instant coffee of various origins by INAA. *Journal of Radioanalytical and Nuclear Chemistry, 267*(1), 109–112. https://doi.org/10.1007/s10967-006-0015-y

Zappi, A., Marassi, V., Kassouf, N., Giordani, S., Pasqualucci, G., Garbini, D., et al. (2022). A green analytical method combined with chemometrics for traceability of tomato sauce based on colloidal and volatile fingerprinting. *Molecules, 27*(17), 5507. https://doi.org/10.3390/molecules27175507

Zhao, Y., Tu, T., Tang, X., Zhao, S., Qie, M., Chen, A., et al. (2020). Authentication of organic pork and identification of geographical origins of pork in four regions of China by combined analysis of stable isotopes and multi-elements. *Meat Science, 165*, Article 108129. https://doi.org/10.1016/j.meatsci.2020.108129