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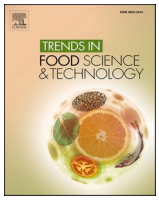

Microbial volatile organic compounds for food quality and safety: metabolic pathways, sampling and detection, and machine learning-driven insights

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ABSTRACT

Background: Microbial spoilage and contamination pose persistent threats to food safety and quality. Microbial volatile organic compounds (mVOCs), generated during microbial metabolism, are emerging as non-invasive biomarkers that allow rapid and real-time assessment of food quality, spoilage, and pathogen activity.
Scope and approach: This review outlines the metabolic origins of mVOCs from carbohydrates, proteins, and lipids pathways and evaluates their roles in food quality and safety changes. Major sampling approaches, including headspace injection, solid-phase microextraction, purge-and-trap, and needle-trap, are compared alongside analytical platforms, such as GC-MS, GC-IMS, FTIR, and e-noses. Advances in data analytics, including PCA, machine learning, and deep learning, are also discussed for interpreting complex mVOCs datasets.
Key findings and conclusions: mVOCs provide sensitive, specific, and scalable indicators of microbial dynamics in food systems, with applications in fermentation monitoring, spoilage detection, and pathogen identification. Integration with modern analytical platforms and AI-driven modeling enhances interpretability and industrial value. However, key challenges remain: lack of standardized sampling protocols and calibration methods, limited cross-laboratory reproducibility, and poor model generalizability across food types and conditions. Future work should prioritize harmonized protocols, open benchmark datasets, and explainable AI frameworks, supported by cross-disciplinary collaboration, to enable reliable, real-time, and industry-ready mVOC-based monitoring.

1. Introduction

Food safety and quality are fundamental priorities that have received growing global attention in recent years, driven by the rapid expansion of the food industry and rising consumer expectations for freshness, transparency, and safety (Shen et al., 2024). Among the many factors influencing these priorities, microbial metabolism during food production, processing, and storage plays a pivotal role in shaping both safety outcomes and sensory attributes. In this context, microbial volatile organic compounds (mVOCs), small, readily detectable molecules produced by microorganisms, have emerged as a critical focus in food science research. Due to their roles in microbial signaling, spoilage dynamics, and interactions within complex food environments, mVOCs offer valuable insight into microbial activity and contamination status (Casaburi et al., 2015). Increasingly, these compounds are being recognized as promising, non-invasive indicators for real-time assessment of food quality and safety, with potential applications in monitoring systems across the supply chain.

mVOCs are metabolic byproducts released during microbial growth and metabolism. A diverse range of chemical classes, such as alcohols, ketones, aldehydes, and esters, are formed during these processes, and their production is influenced by a variety of factors, including microbial species, nutrient composition, temperature, pH, moisture level, and oxygen availability (Wang et al., 2016). Given the well-established correlation with microbial metabolic activity, mVOCs have emerged as critical biomarkers for the dynamic monitoring of safety and spoilage processes in various food products (Ercolini et al., 2011). For instance, *Pseudomonas* species, which are closely associated with food spoilage, commonly release volatile compounds, such as dimethyl sulfide and cyclopropane, in meat-based products, whereas *Lactobacillus* species

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typically produce aromatic compounds like diacetyl and acetoin (Cera et al., 2024; Zscheppank et al., 2014). In dairy products, elevated levels of butyric acid and methyl ketones are frequently linked to spoilage-related microbial activity (Hierro et al., 2005; Zheng et al., 2021). In fish, the release of trimethylamine and alcohol serves as a typical indicator of microbial spoilage (Jørgensen et al., 2001). Changes in ester profiles in fruits and vegetables are also commonly used to detect early microbial contamination (Dong et al., 2013, 2014). Moreover, the composition and abundance of mVOCs can shift significantly throughout microbial growth phases: alcohols tend to predominate during early stages, whereas sulfur compounds and short-chain fatty acids (SCFAs) typically increase in later stages, contributing to off-odors and advanced spoilage (Yi & Xie, 2021).

mVOCs offer unique diagnostic signatures of microbial activity, driving their adoption in food safety and quality control. As a result, increasing efforts have been made to compile and systematize mVOCs profiles into comprehensive databases that support the research interest. For example, mVOC, a database originally established in 2013, has since been expanded and reached version 4.0 in 2024, now encompassing over 3500 distinct compounds (Kemmler et al., 2024). This extensive dataset serves as a foundational resource for researchers and industry professionals aiming to develop precise, high-throughput food quality and safety monitoring techniques. In addition, benefiting from recent advancements in analytical technologies and big data-driven pattern recognition, the detection and interpretation of mVOCs in food assessment have significantly improved. For example, a commercial electronic nose (e-nose) with a metal oxide semiconductor sensor array enabled accurate quantification of *Salmonella* Typhimurium in pork, with support vector machine (SVM) regression models optimized by genetic algorithms achieving an R^2 of 0.989 (Bonah et al., 2021). These applications highlight the analytical potential and the utility of mVOCs profiling combined with machine learning and multivariate methods, opening up avenues toward highly robust and scalable monitoring of foods.

This review systematically evaluates the multifaceted role of mVOCs in the monitoring of food quality and safety. It begins by outlining the key microbial metabolic pathways, including carbohydrate, protein, and lipid metabolism, that govern mVOCs production and contribute to characteristic volatile profiles. Subsequently, the review summarizes current sampling techniques and analytical detection platforms that enable accurate and sensitive mVOCs identification. Advanced data analysis approaches, including statistical modeling, machine learning, and deep learning methods, are also discussed for extracting meaningful patterns from high-dimensional mVOCs datasets. Finally, the review explores the practical applications of mVOCs monitoring in various food industry settings, from fermentation control to spoilage and contamination detection, and highlights current challenges and future directions for research and industrial implementation.

2. The metabolism pathways of microbial volatile organic compounds in food

To fully exploit mVOCs as reliable biomarkers in food safety and quality monitoring, it is essential to understand their biochemical origins. Broadly, the generation of mVOCs can be classified into three major metabolic routes: primary carbohydrate metabolism, amino acid catabolism, and lipid degradation (Fig. 1). Each pathway contributes a unique set of volatiles, which in turn reflects the underlying microbial activity and substrate utilization. Table 1 summarizes the key mVOCs, along with their primary metabolic pathways, representative microbial origins, and the food products in which they are typically found. The following sections further outline these three main metabolic pathways and their representative volatile products.

2.1. *Carbohydrate metabolism pathway*

Various mVOCs are produced in microbial carbohydrate metabolism, acting as indicators of carbohydrate breakdown, microbial fermentation and spoilage, with each compound reflecting specific metabolic stages. Carbohydrates in food are first subjected to enzymatic hydrolysis, breaking down complex polysaccharides into monosaccharides, which subsequently enter metabolic pathways like glycolysis, leading to the production of various mVOCs (Fig. 1). For example, ethanol is a well-known marker in fermented beverages and bakery products. In the fermentation of alcoholic drinks, such as beer and wine, sugars are converted into ethanol under anaerobic conditions, contributing to alcohol content (Table 1). It has also been identified as one of the key mVOCs produced by spoilage bacteria during low-temperature storage of sea bass (Table 1). Similarly, the formation of acetic acid is crucial in both desirable and undesirable microbial processes. In vinegar production, *Acetobacter* species oxidize ethanol into acetic acid, providing the characteristic sour flavor (Table 1). However, excessive acetic acid accumulation in some food products due to microbial activity can indicate product spoilage.

Through further fermentation, monosaccharides can be converted into lactic acid and acetoin as notable mVOCs (Fig. 1). Lactic acid, a key

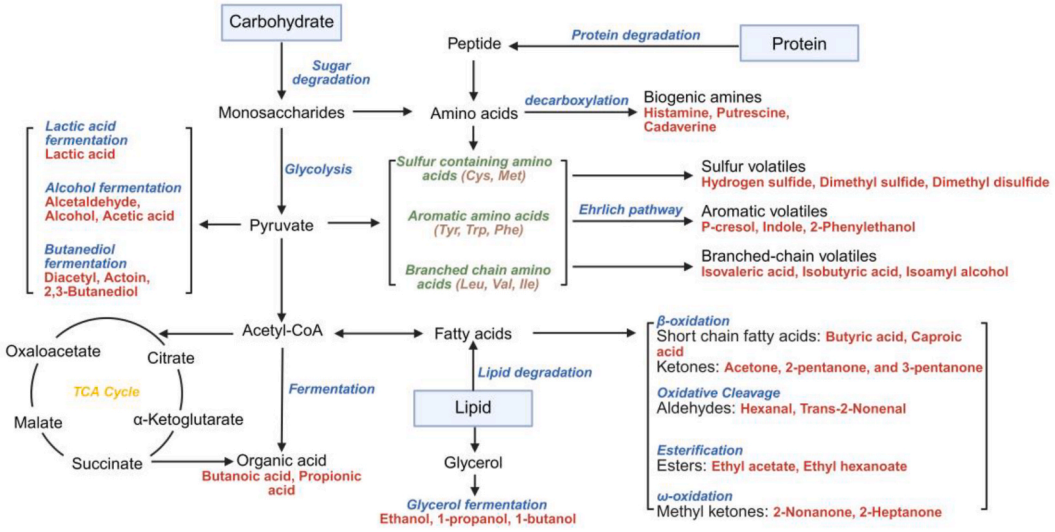

Fig. 1. Metabolic pathways of microbial volatile organic compounds (mVOCs) derived from carbohydrate, protein, and lipid metabolism.

Table 1
Summary of representative microbial volatile organic compounds (mVOCs) pathways, microbial sources, and indicative food products.

mVOCs	Primary pathways	Representative microbial sources	Representative food products	References
Ethanol	C	*Saccharomyces* spp,, *Pseudomonas* spp.	Beer, wine, bread, sea bass	(Lončarić et al., 2025; Nguyen et al., 2024; Parlapani et al., 2015)
Acetic acid	C	*Acetobacter* spp.	Vinegar, pickles	Maske et al. (2024)
Lactic acid	C	LAB, *Streptococcus* spp.	Yogurt, cheese, sausages	(El Bouchikhi et al., 2019; Santos et al., 2025)
Acetoin/diacetyl	C + P + L	LAB, yeasts, *Brochothrix*, *Serratia*	Yogurt, beer, butter, beef sausage	(Cera et al., 2024; Han et al., 2025; Tapia et al., 2025)
Butyric acid	C + L	*Clostridium* spp.	Cheese, dairy, spoiled fish	Floris et al. (2024)
Propionic acid	C	*Propionibacterium* spp.	Swiss cheese	Thierry et al. (2015)
Acetaldehyde	C + P + L	LAB, yeasts, *Pseudomonas* spp.	Yogurt, wine, cider, pork meat	(Gong et al., 2023; Papadopoulou et al., 2020)
2,3-butanediol	C	LAB, yeasts		Li et al. (2023)
Amines (e.g., histamine, putrescine, cadaverine)	P	LAB, *Pseudomonas* spp., Enterobacteriaceae	Fish, sausages, meat, cured meats	(Hernández-Jover et al., 1997; Rezaei et al., 2007; Tosukhowong et al., 2011)
Hydrogen sulfide	P	*Shewanella* spp., *Escherichia coli, Pseudomonas* spp.	Seafood	Yan et al. (2024)
Dimethyl sulfide	P	*Staphylococcus aureus, E. coli*	Mastitis milk	Hettinga et al. (2009)
Dimethyl disulfide	P	*Shewanella putrefaciens, Psychrobacter*	Vacuum-packed salmon	Claus et al. (2022)
Phenylethyl alcohol	P	*Saccharomyces* spp.	Wine, whiskey	(Guo et al., 2024; Lončarić et al., 2025)
Indole	P	*E. coli*	Shrimp, meat	Federico-Perez and Xue (2018)
p-cresol	P	*Clostridium* spp.	Baijiu	(Ji et al., 2020; Oshiro et al., 2022)
Isovaleric/isobutyric acids	P	*Penicillium* spp.	Dry-cured sausage	Hettinga et al. (2009)
Isoamyl alcohol	C + P + L	LAB, yeasts, *Staphylococcus* spp.	Dairy, sausages	Hierro et al. (2005)
Ethyl acetate	C + L	LAB, yeasts	Wine, cheese, sausages	(Abeijón Mukdsi et al., 2009; Hierro et al., 2005)
Hexanal	L	LAB, molds, *Brochothrix*, *Serratia*	Smoked fish, meat, beef sausage	(Han et al., 2025; Varlet et al., 2007)
2-Heptanone/2-nonanone	L + P	*Penicillium* spp., LAB	Blue cheese, dry-cured meat	Hierro et al. (2005)
1-Propanol/1-butanol	L + C	LAB, yeasts, *Clostridium* spp.	Baijiu, wine, sausages	(Chung et al., 2015; Zhao et al., 2025)
Methyl ketones	L + P	*Penicillium* spp., LAB	Ripened cheese, butter	(Hierro et al., 2005; Zheng et al., 2021)

Note: C, carbohydrate metabolism pathway; L, lipid metabolism pathway; P, protein metabolism pathway; LAB, *Lactic acid bacteria.*

product of lactic acid bacteria (LAB), signifies anaerobic carbohydrate metabolism and is commonly detected in fermented foods, signaling microbial activity associated with both desirable and spoilage processes. For example, in dairy fermentation, *Lactobacillus* and *Streptococcus* species metabolize sugars into lactic acid, which enhances the texture and acidity of yogurt and cheese (Table 1). However, excessive accumulation of lactic acid may lead to undesired changes in flavor, texture, or even inhibit the growth of beneficial microbes, thus compromising product quality. For instance, in yogurt production, overproduction of lactic acid results in excessive sourness and syneresis (whey separation), negatively affecting consumer acceptance (El Bouchikhi et al., 2019). On the other hand, acetoin and diacetyl, byproducts of the breakdown of glucose or other sugars during mixed acid fermentation by various bacterial strains, contributes a mild buttery aroma and indicates ongoing carbohydrate fermentation (Fernández-Varela et al., 2024; Tapia et al., 2025). It is commonly observed in dairy fermentations and some grain-based foods (Table 1). Additionally, in sourdough fermentation, *Lactobacillus sanfranciscensis* produces acetoin as an intermediate in sugar metabolism, contributing a mild buttery aroma (Cera et al., 2024).

Under anaerobic conditions, the breakdown of carbohydrates can further yield butyric acid and propionic acid (Fig. 1), both of which are associated with later stages of carbohydrate fermentation (Turgay et al., 2018). Indeed, butyric acid is strongly associated with anaerobic spoilage, particularly in dairy products, where *Clostridium butyricum* and *C. sporogenes* produce this compound, leading to rancid and unpleasant odors (Table 1). While propionic acid, produced by propionibacteria, is a key indicator in cheese (particularly in Swiss cheese) fermentation, contributing to the characteristic flavors. In this process, *Propionibacterium freudenreichii* converts lactate into propionic acid and CO_2, forming the characteristic holes and imparting a nutty flavor (Table 1). Additionally, anaerobic carbohydrate metabolism may result in the production of acetaldehyde and 2,3-butanediol (Table 1). Acetaldehyde is an intermediate product of pyruvate metabolism and is often detectable in fruit and dairy fermentations, marking active microbial carbohydrate metabolism (Gong et al., 2023). It was also identified as one of the compounds most strongly correlated with spoilage during pork storage (Table 1). Meanwhile, 2,3-butanediol, arising from acetoin reduction (Li et al., 2023), is frequently produced by LAB and certain yeasts, serving as a marker for advanced fermentation stages.

These mVOCs, including ethanol, acetic acid, lactic acid, acetoin, butyric acid, propionic acid, acetaldehyde and 2,3-butanediol, collectively represent different stages and conditions of microbial carbohydrate metabolism, offering insights into both the fermentation processes and the onset of spoilage. Their presence thus serves as a valuable indicator for monitoring microbial activity, supporting the assessment of food quality and safety, and characterizing fermentation processes in carbohydrate-rich products, such as fruits, vegetables, baked goods, and jams or syrups.

2.2. Protein metabolic pathway

In microbial protein metabolism, a range of mVOCs are produced as characteristic indicators of protein degradation and microbial activity, each associated with distinct metabolic stages (Fig. 1). During the decarboxylation of amino acids, specific biogenic amines are enzymatically generated: histamine from histidine, putrescine from ornithine, and cadaverine from lysine (Alvarez & Moreno-Arribas, 2014). These compounds are closely linked to microbial spoilage and are commonly detected in protein-rich foods. In fermented meat products, such as Nham, a traditional Thai pork sausage, putrescine and cadaverine accumulate during fermentation, especially when microbial hygiene is poor or starter cultures are not well controlled (Table 1). In ice-stored rainbow trout, putrescine and cadaverine levels increase progressively with storage time and show strong correlations with the growth of *Pseudomonas* spp. (Table 1). Histamine is typically detected only in later stages, making it less suitable as a freshness indicator in early spoilage. In ripened meat products, high levels of histamine, putrescine, and cadaverine are frequently observed, with substantial variability among commercial samples. Moreover, amine accumulation is often influenced by the hygienic quality of raw meat and the conditions of fermentation

and ripening, posing risks particularly in products with high tyramine or histamine content (Hernández-Jover et al., 1997).

Sulfur volatiles (e.g., hydrogen sulfide, dimethyl sulfide, and dimethyl disulfide), another class of mVOCs derived from protein metabolism, can be released during the degradation of sulfur-containing amino acids, such as methionine and cysteine (Fig. 1). Sulfur volatiles are typically produced under anaerobic conditions during spoilage, serving as indicators of microbial activity and degradation in certain foods. For instance, hydrogen sulfide is a typical indicator in aquatic products, primarily generated by the degradation of cysteine through both endogenous enzymes and microbial activity (Table 1). Similarly, in mastitis milk, *Staphylococcus aureus* produces dimethyl sulfide by metabolizing methionine through specific enzymatic pathways, imparting an unpleasant odor that affects sensory quality (Table 1). In vacuum-packed salmon, the accumulation of dimethyl disulfide is strongly correlated with the growth of spoilage bacteria *Shewanella putrefaciens* and *Psychrobacter* under refrigeration (Table 1).

Aromatic volatiles, such as phenylethyl alcohol, indole, and p-cresol, are produced from microbial metabolism of aromatic amino acids, specifically phenylalanine and tryptophan in food (Fig. 1). Phenylethyl alcohol, with its faintly floral aroma, is commonly produced during fermentation. For instance, *S. cerevisiae* contributes to desirable aroma in fermented products like whiskey (Table 1). Indole is a clear indicator of food spoilage and adherence to good manufacturing practices. Its accumulation, a byproduct of bacterial degradation of tryptophan, signals decomposition by microbes like *Escherichia coli*, seen in US FDA shrimp assessments (Federico-Perez & Xue, 2018). Moreover, p-cresol exhibits a complex role, indicating both specific flavor profiles in foods like grilled cheese and smoked products, and potential toxicity to humans as food spoilage (Oshiro et al., 2022). Research shows its levels increase in smoked foods show potential as an indicator to ensure safety and quality, with studies on its microbial origin in fermented foods like baijiu have identified several microbial genera, such as *Clostridium*, as potential p-cresol producers, offering insights for control (Ji et al., 2020; Oshiro et al., 2022).

In addition to amines, sulfur and aromatic volatiles, volatile fatty acids and alcohols, such as isovaleric acid, isobutyric acid, and isoamyl alcohol, can be generated from the metabolism of branched-chain amino acids, including leucine, isoleucine, and valine (Zhang et al., 2024). These compounds are common byproducts in both fermentation and spoilage environments, where their sour and pungent odors can signal microbial breakdown of protein substrates. For instance, in dry-cured sausage, *Penicillium aurantiogriseum* and *P. camemberti* produce high concentrations of isovaleric and isobutyric acids, contributing to the characteristic aged aroma (Hierro et al., 2005). However, excessive accumulation of these acids results in strong, unpleasant pungent odors, indicating spoilage. Similarly, in fresh dairy products, the growth and metabolism of *S. aureus* leads to the accumulation of isovaleric acid and isoamyl alcohol, producing a strong sweaty odor indicative of microbial spoilage (Hettinga et al., 2009).

Together, these mVOCs, such as biogenic amines, sulfur-containing compounds, aromatic volatiles, fatty acids, and alcohols, reflect the complex and multifaceted pathways of microbial protein metabolism. Their production is closely associated with microbial enzymatic activity during the breakdown and transformation of amino acids and proteins under different environmental conditions. As such, these volatiles not only provide valuable insights into the underlying metabolic processes but also serve as meaningful indicators for monitoring microbial dynamics, assessing product quality, and ensuring safety in protein-rich food systems.

2.3. Microbial volatile organic compounds in fat metabolic pathway

In the microbial metabolism of fats, mVOCs are produced at distinct stages of lipid degradation, serving as critical indicators of both food safety and quality attributes. The initial phase of lipid catabolism, lipolysis, involves the enzymatic hydrolysis of triglycerides into glycerol and free fatty acids (Fig. 1). This process is also associated with the release of esters, such as ethyl acetate and ethyl hexanoate, which contribute fruity and buttery aromas in fermented food products (Table 1). However, these compounds can also serve as indicators of early lipid oxidation in rancid foods. For example, in cheese ripening, the production of short-chain esters is linked to beneficial microbial activity, particularly from LAB and yeasts, which contribute to desirable flavor complexity (Abeijón Mukdsi et al., 2009). On the other hand, excessive ester formation in lipid-rich fermented sausage can also indicate microbial contamination or uncontrolled fermentation, leading to off-flavors (Hierro et al., 2005).

The metabolic pathway of glycerol, an important byproduct of lipolysis, varies depending on microbial species and environmental conditions. Under anaerobic conditions, microbial fermentation of glycerol can yield ethanol, 1-propanol, and 1-butanol, which are frequently detected in fermented beverages, such as wine and baijiu (Table 1). These alcohols also serve as important flavor contributors in fermented dairy and meat products, where specific bacterial strains regulate their formation to enhance flavor complexity rather than produce off-flavors. For instance, propanol has been identified as a key component in aged cheeses, contributing mild alcoholic notes (You et al., 2024). In contrast, under aerobic conditions, glycerol is more likely to be completely oxidized through central metabolic pathways, such as glycolysis and the tricarboxylic acid cycle (TCA) cycle, leading to the production of non-volatile end-products like carbon dioxide and water, and resulting in significantly lower levels of volatile alcohols.

The β-oxidation of free fatty acids, a primary pathway in fat metabolism, leads to the formation of volatile ketone compounds, such as acetone, 2-pentanone, and 3-pentanone, often via subsequent metabolic steps or microbial activity, which contribute to the characteristic fruity, buttery, or solvent-like aromas found in various foods (Fig. 1). However, in the context of food spoilage, intensified β-oxidation leads to an excessive buildup of ketones, resulting in undesirable solvent-like odors. Additionally, lipid metabolism also produces a distinct class of compounds known as SCFAs, typically defined as volatile fatty acids containing fewer than six carbon atoms. The accumulation of SCFAs, such as butyric acid, a metabolic byproduct of butyrate-producing Clostridia, contributes to strong rancid and putrid odors in dairy spoilage but is also responsible for the characteristic sharp flavor in certain fermented cheeses, such as Limburger and Swiss varieties (Zheng et al., 2021). Caproic acid (hexanoic acid), another SCFA, produces pungent, goaty aromas commonly observed in both spoiled and aged dairy products. Additional oxidation processes, such as oxidative cleavage, generate volatile aldehydes. For instance, hexanal, contributes to grassy or fatty notes, while trans-2-nonenal, is often responsible for undesirable fishy or stale aromas, particularly significant in lipid-rich smoked fish products (Varlet et al., 2007). Moreover, ω-oxidation pathways yield methyl ketones, such as 2-nonanone and 2-heptanone, further contributing to the volatile profile of lipid-containing foods (Hierro et al., 2005).

The production of mVOCs derived from microbial lipid metabolism highlights the dynamic transformation of fats under microbial influence. Their formation reflects both the metabolic potential of specific microorganisms and the surrounding environmental conditions. The production of these volatiles is a double-edged sword: controlled microbial activity can enhance desirable flavors in fermented foods, while unregulated processes may lead to quality deterioration. As such, they serve as useful indicators for monitoring microbial activity and maintaining the quality and safety of fat-containing food systems.

2.4. Multi-pathway interactions and cross talk

Multi-pathway interactions are increasingly recognized as a defining feature of mVOCs production. Intermediates generated in one pathway frequently enter another, collectively shaping the volatile profile of types of food. For example, carbohydrate catabolism supplies pyruvate

for ethanol and acetaldehyde formation but also generates acetyl-CoA, which connects to lipid metabolism and contributes to fatty acid-derived volatiles. Protein metabolism is similarly integrated with central carbon fluxes, as exemplified by the Ehrlich pathway, where amino acids are converted into higher alcohols, such as isoamyl alcohol and 1-propanol (Gong et al., 2023; Li et al., 2023; Zhang et al., 2024; Zhao et al., 2025). Table 1 also summarizes some representative mVOCs that arise through multi-pathway interactions, in different foods. For instance, acetoin and diacetyl are classic multi-pathway compounds, deriving from carbohydrate precursors, amino acid transamination, and lipid-derived acetyl-CoA, and are important flavor notes in yogurt, beer, and butter (Table 1). Isoamyl alcohol is produced via both carbohydrate metabolism and the Ehrlich pathway from leucine, with additional input from lipid metabolism, explaining its occurrence across dairy and fermented sausages (Hierro et al., 2005). Ethyl acetate forms when ethanol from carbohydrate fermentation reacts with free fatty acids from lipid hydrolysis, linking carbohydrate and lipid metabolism in wine, cheese, and sausages (Abeijón Mukdsi et al., 2009; Hierro et al., 2005). Likewise, butyric acid can originate from carbohydrate fermentation by *Clostridium* spp. as well as lipid β-oxidation, and methyl ketones (e.g., 2-heptanone) arise from lipid breakdown but depend on amino acid-derived intermediates (Floris et al., 2024; Hierro et al., 2005; Zheng et al., 2021). In complex fermentations, such as baijiu, cheese ripening, or sausage fermentation, these multi-pathway interactions enable microbes to redirect metabolic fluxes depending on substrate availability and community composition. Recognizing such interactions is therefore critical for understanding the diversity and abundance of mVOCs in food fermentations and spoilage processes.

3. Sampling and detection method

Sampling is a critical step in mVOCs analysis, as it directly influences detection sensitivity, selectivity, and the integrity of the sample. A range of techniques has been developed to accommodate different food matrices and analytical objectives. Common methods include headspace injection (HS), which captures volatiles from the gas phase above the sample; solid-phase microextraction (SPME), which employs a coated fiber to absorb analytes without solvents; purge and trap (P&T), which uses inert gas to extract volatiles and retain them on sorbents; and needle trap (NT), which directly collects volatiles using adsorbent-packed needles. Each method presents distinct advantages in food-related mVOCs monitoring. These sampling techniques are typically coupled with detection platforms to assess spoilage, monitor fermentation, and evaluate product quality (Fig. 2). Common detection methods include gas chromatography-mass spectrometry (GC-MS), gas chromatography-ion mobility spectrometry (GC-IMS), fourier transform infrared spectroscopy (FTIR), and e-nose systems, each with unique strengths depending on analytical needs. Table 2 summarizes the analysis of mVOCs from various food samples using different combinations of sampling and detection methods.

3.1. Sampling method

3.1.1. Headspace injection method

HS is a widely used technique for analyzing mVOCs in food products. This method is based on the principle of equilibrium partitioning, where volatile compounds distribute between the sample matrix and the gas phase above it (Fig. 2). This partitioning is governed by factors, such as temperature, the volatility of the compounds, and the nature of the sample matrix. HS GC-MS analysis has been used for the identification of mVOCs in food samples, with matrix-matched calibration curves being necessary for accurate results. In cheese, HS mVOCs analysis has been employed to detect a range of volatile compounds, including aldehydes, acids, and esters, during the ripening process, enabling the monitoring of flavor profile changes and the detection of undesirable propionic acid fermentation (Table 2). Similarly, the combination of headspace sampling with gas chromatography-flame ionization detection has enabled the detection of volatile ketones in fermented oat milk, facilitating the optimization of starter cultures for improved fermentation performance (Table 2). Advances in scientific techniques have allowed for the detection of odors as primary source evidence in various fields. The use of HS has been highlighted as a simple, solvent-free, and low in cost technique, making it widely adopted for food mVOCs analysis in the past decades. However, HS generally shows low sensitivity for poorly volatile compounds, and its performance is strongly affected by temperature and matrix effects, which can reduce reproducibility in complex food systems (Gu et al., 2025).

3.1.2. Solid phase microextraction

SPME has been widely used for extracting volatile and semi-volatile organic compounds from environmental, biological, and food matrices. By employing a coated fiber to absorb mVOCs, SPME significantly enhances the effectiveness of headspace analysis (Fig. 2). When coupled with GC-MS, it has proven effective for profiling mVOCs in complex

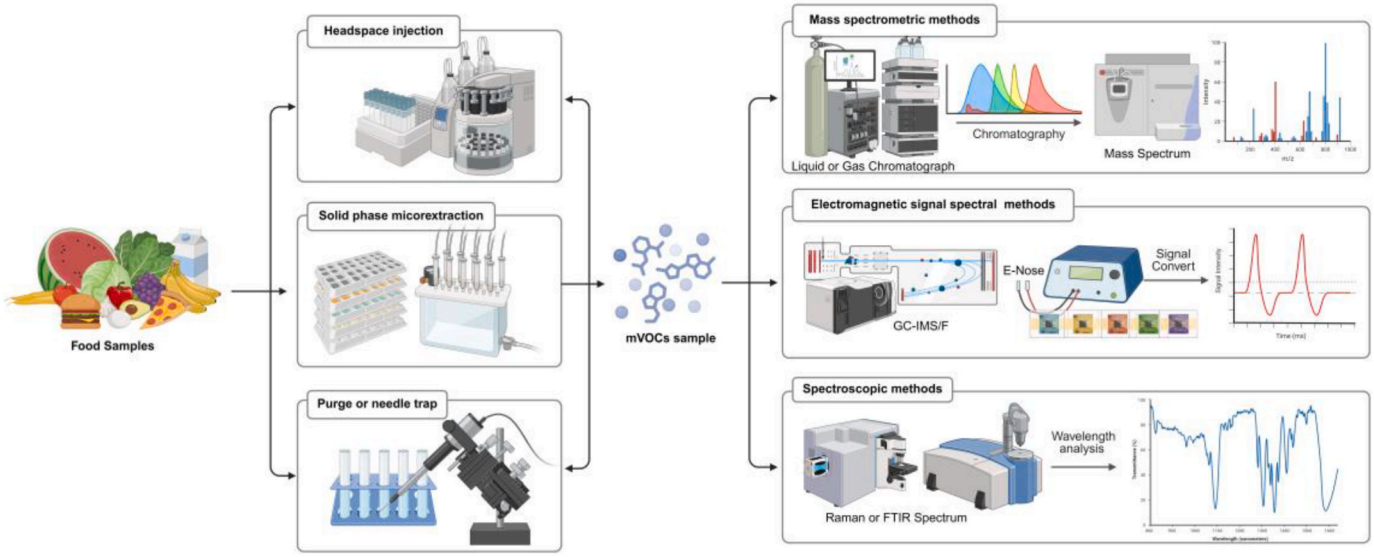

Fig. 2. Overview of sampling and detection methods for microbial volatile organic compounds (mVOCs) extracted from food samples.

Table 2
Analysis of microbial volatile organic compounds (mVOCs) from various food samples using different combinations of sampling and detection methods.

Food type	mVOCs chemical class	Sampling method	Detection method	References
Cheese	Esters	–	GC-FID	Abeijón Mukdsi et al. (2009)
Cheese	Acids	HS	GC-FID	Turgay et al. (2018)
Fermented oat milk	Ketones	HS	GC-FID	Tapia et al. (2025)
Cheeses	Aldehydes, acids, esters, etc.	HS	E-nose, GC-MS, GC-IMS	You et al. (2024)
Sausage	Alcohols, aldehydes, esters, etc.	HS	GC-IMS	Ma, Gao, et al. (2023)
Whiskey	Esters, ketones, etc.	SPME	GC-MS	Guo et al. (2024)
Pork meat	Aldehydes, ketones	SPME	GC-MS	Papadopoulou et al. (2020)
Beef and pork meat	Alcohols, aldehydes, ketones	SPME	GC-MS	Pavlidis et al. (2019)
Legumes	Ketones	SPME	GC-MS	Fernández-Varela et al. (2024)
Whiskey	Esters, alcohols, phenols, etc.	SPME	GC-MS	Lončarić et al. (2025)
Milk	Esters, acids, etc.	SPME	GC-MS	Hettinga et al. (2009)
Beef	Alcohols, aldehydes, ketones, acids	SPME	E-nose, GC-MS	Ferrocino et al. (2013)
Beef, salmon	Esters, sulfur compounds	P&T	GC-MS	Claus et al. (2022)
Salmon	Alcohols, ketones, etc.	P&T	GC-MS	Jørgensen et al. (2001)
Golden pomfret	Acids	–	GC-MS	Wang et al. (2022)
Smoked meat	Phenols	–	GC-MS	Oshiro et al. (2022)
Chicken	Acids, ketones, etc.	–	FTIR, GC-MS	Muthusamy et al. (2024)
Vinegar	Esters, alcohols, etc.	–	FTIR	Jiao et al. (2019)
Strawberry	Alcohols, esters, etc.	–	FTIR	Dong et al. (2013)
Grape	Alcohols, esters, etc.	–	FTIR	Dong et al. (2014)
Fish	Alcohols, esters, etc.	–	FTIR	Govari et al. (2021)

Noted: GC-FID, gas chromatography with flame ionization detection; HS, headspace injection; E-nose, electronic nose; GC-MS, gas chromatography-mass spectrometry; GC-IMS, gas chromatography-ion mobility spectrometry; SPME, solid phase microextraction; P&T, purge and trap; FTIR, fourier transform infrared spectroscopy.

samples. For instance, SPME GC-MS has successfully identified key mVOCs associated with spoilage during sterile pork storage, and to discriminate between minced beef and pork based on distinct volatile profiles (Table 2), highlighting its potential application in monitoring food quality and safety. Additionally, this method has been employed to detect and analyze mVOCs, such as esters, ketones, and acids, in various fermented products including whiskey, legumes, milk, sausage, alcohols, and phenols, providing valuable insight into their fermentation characteristics (Table 2). Furthermore, recent studies have utilized SPME GC-MS to rapidly detect microbial enzyme activity by measuring mVOCs generated via enzymatic hydrolysis. Thompson et al. (2020) reported a rapid and universal microbial detection approach based on nitroreductase activity, where pathogenic microorganisms converted nitrobenzene substrates into detectable aniline compounds within 6–8 h, underscoring the method's sensitivity and practicality for microbial screening in food safety, healthcare, and environmental monitoring. Given its efficiency in isolating and enriching analytes from intricate matrices, SPME remains a preferred analytical method in mVOCs research (Lytou et al., 2019). Nevertheless, SPME suffers from fiber coating degradation after repeated use, potential adsorption bias toward certain analytes, and relatively high consumable costs, which limit its robustness for long-term monitoring (Spietelun et al., 2010).

3.1.3. *Purge and trap sampling method*

P&T sampling operates on the principle of volatilization and adsorption. During the purging phase, an inert gas flows through the sample, stripping volatile compounds from the matrix into the gas phase (Fig. 2). This makes P&T particularly suitable for profiling mVOCs in applications where precision and reproducibility are essential. In a comparative study assessing spoilage in beef and salmon under various storage conditions, P&T combined with GC-MS effectively identified key spoilage markers, such as dimethyl disulfide, methyl thioacetate, and acetoin, demonstrating its strong discriminatory power and consistency with e-nose data (Table 2). In another application, P&T GC-MS was used to monitor changes in 38 volatile compounds during chilled storage of vacuum-packed cold-smoked salmon. The study identified key spoilage markers, such as 1-propanol, 2-butanone, and 2-furancarboxaldehyde, that correlated with sensory degradation, and highlighted compounds like trimethylamine and 3-methylbutanal as major contributors to off-flavors (Table 2). P&T offers high recovery efficiency with minimum loss and reproducibility, enabling detection of trace-level volatiles with strong discriminatory power. Despite these strengths, P&T systems are limited by moisture interference, which can cause analyte loss, and by strong dependence on purge parameters, such as flow rate, purge time, and temperature, making the method vulnerable to bias without careful optimization. These limitations also mean that P&T is not always well suited for complex or high-moisture food matrices, where reproducibility and practicality become challenging (Fernandez-Villarrenaga et al., 2006).

3.1.4. *Needle trap sampling method*

NT technique is a solvent-free extraction method that uses a constant-current pump to actively draw headspace air through the adsorption bed, enabling dynamic headspace extraction. It employs a hollow needle packed with adsorbent material, such as activated carbon, porous polymers, or molecular sieves. During sampling, the needle is exposed to the sample headspace or directly inserted into the sample matrix (Fig. 2). Volatile compounds are absorbed onto the packing material due to interactions based on polarity, volatility, and molecular size. This approach ensures efficient collection and concentration of volatiles while maintaining the integrity of the sample. In a recent study, NT was used to extract mVOCs from ham samples and outperformed other techniques, such as SPME and solvent-assisted flavor evaporation (SAFE), detecting a total of 205 volatile compounds, significantly more than the other methods. This superior performance is attributed to both the dynamic flow and longer enrichment time, making NT a powerful tool for comprehensive mVOCs profiling (Liu et al., 2022). In another study, a growth-dependent headspace analysis method based on NT was developed for monitoring different mVOCs. Using this method, specific metabolites from *Pseudomonas aeruginosa* and *E. coli* were successfully detected and quantified. By comparing the headspace profiles of inoculated and uninoculated media, microbial products could be clearly distinguished from background compounds, further demonstrating the applicability of NT for mVOCs analysis in food settings (Zscheppank et al., 2014). Despite their high sensitivity and suitability for rapid on-site analysis, NT technologies suffer from limited field validation, lack of standardized protocols, and inconsistent reproducibility across studies. Challenges related to sorbent stability, environmental variability, matrix interferences, and cost further restrict their reliability for routine large-scale monitoring (Baimatova & Gionfriddo, 2025).

3.2. Detection method

3.2.1. Gas chromatography-mass spectrometry

GC-MS is considered the gold standard for the analysis of mVOCs. It provides exceptional capability for the separation and identification of volatile and semi-volatile organic compounds in complex mixtures. It also demonstrates high sensitivity, enabling the detection of mVOCs at trace concentrations with remarkable specificity (Xu et al., 2021). Due to its precision, it is extensively employed in food science, environmental monitoring, and industrial applications for the detection and quantification of mVOCs. For instance, in a study on fermented golden pomfret, GC-MS was used to identify 95 volatile compounds generated during fermentation (Table 2). The analysis revealed a strong link between lipid oxidation, particularly the degradation of fatty acids like oleic, linoleic, and palmitic acids, and the formation of these volatiles. This study demonstrated how GC-MS can effectively profile dynamic chemical transformations in complex food systems and identify the lipid-derived precursors that contribute to the sensory characteristics of fermented foods. GC-MS offers excellent sensitivity, specificity, and compound identification, but it is limited by cost, speed, portability, and matrix interferences, which restrict its suitability for rapid or routine field-based monitoring of mVOCs in food.

3.2.2. Gas chromatography-ion mobility spectrometry

GC-IMS is an emerging analytical method for the detection of mVOCs in food systems. It integrates GC for the initial separation of compounds with IMS, which distinguishes ionized molecules based on their drift times in a weak electric field under ambient pressure (Ma, Gao, et al., 2023; You et al., 2024). This dual approach enables both qualitative and quantitative assessment of complex volatile profiles with high resolution. One of the major advantages of GC-IMS is its minimal sample preparation requirement and rapid analysis time, making it highly suitable for real-time, on-site, and high-throughput food quality monitoring. It offers excellent sensitivity and repeatability, even for trace-level volatiles, which is particularly valuable in spoilage detection and aroma profiling. GC-IMS has been successfully applied to detect spoilage markers in seafood, distinguish aroma profiles in fermented dairy products, and mildew gradation based on volatile compound patterns (Gu et al., 2021). These applications underscore its growing utility in modern food safety and quality control systems. While GC-MS remains the benchmark for accurate and comprehensive mVOCs profiling, GC-IMS offers a complementary approach that is faster, more portable, and better suited to real-time food quality monitoring, albeit with reduced structural resolution and less robust compound identification (Schanzmann et al., 2025).

3.2.3. Electronic nose

The e-nose, modeled after the human olfactory system, has been widely adopted in food safety and quality monitoring due to its high sensitivity, cost-effectiveness, portability, and ease of operation in detecting mVOCs (Mohareb et al., 2016; Papadopoulou et al., 2013). Bonah et al. (2021) demonstrated the effectiveness of a commercial e-nose equipped with a ten-sensor metal oxide semiconductor array in detecting and quantifying *S.* Typhimurium contamination in pork. The device accurately differentiated samples with varying contamination levels and showed strong agreement with conventional microbial tests. Similarly, Ferrocino et al. (2013) employed an SPME GC-MS integrated with an e-nose to monitor beef during vacuum storage, showcasing its ability to discriminate storage time points and assess the impact of antimicrobial packaging on microbial growth and volatile metabolite production (Table 2). These advancements underscore the growing utility of e-nose systems as rapid, objective, and reliable tools for food quality assessment, positioning them as key components in future smart food monitoring solutions. However, their limitations include sensor drift requiring frequent recalibration, cross-sensitivity that reduces compound specificity, and poor reproducibility across different devices or environmental conditions. In addition, the interpretation of e-nose data often relies on chemometric or machine learning models, which may lack robustness if training datasets are limited (Wilson & Baietto, 2009).

3.2.4. Infrared spectroscopy

FTIR is an advanced vibrational spectroscopic method increasingly utilized for detecting different mVOCs in food matrices (Table 2). Unlike conventional infrared spectroscopy, which measures absorption at individual wavelengths sequentially, FTIR simultaneously acquires a comprehensive infrared spectrum using an interferometer and generates high-resolution molecular fingerprints via Fourier transformation. These spectra provide characteristic vibrational patterns corresponding to specific chemical structures, facilitating identification of microbially derived volatiles, such as alcohols, aldehydes, ketones, and related organic compounds (Jiao et al., 2019). Although initially developed for applications in environmental and clinical microbiology, FTIR has proven valuable in food analysis due to its ability to detect gaseous metabolic byproducts. This capability makes it a useful tool for assessing microbial spoilage and fermentation in a variety of food products, including chicken, vinegar, strawberries, grapes, and fish (Table 2). Nevertheless, its relatively low sensitivity makes it less suitable for trace-level mVOCs detection. In complex food matrices, overlapping vibrational bands can hinder accurate interpretation, and FTIR alone cannot provide unambiguous compound identification. Reliable application often requires chemometric modeling and complementary analytical techniques, which may limit its practicality for routine use. For example, FTIR spectroscopy can been applied to estimate microbial spoilage in sea bass fillets when combined with partial least squares regression (PLS-R) by detecting volatile metabolites associated with total viable counts under different packaging and temperature conditions (Govari et al., 2021).

3.3. Comparative evaluation of sampling and detection methods

While each sampling and detection technique has unique advantages, their practical suitability for food-related mVOCs analysis differs in terms of sensitivity, reproducibility, cost, and field applicability. For sampling methods, HS offers the simplest and most economical approach, making it widely adopted for routine screening; however, its relatively low sensitivity for poorly volatile compounds and dependence on temperature and matrix conditions reduce reproducibility in complex foods (Gu et al., 2025). SPME substantially improves sensitivity and selectivity while remaining solvent-free, yet fiber degradation, adsorption bias, and relatively high consumable costs restrict its robustness for long-term monitoring (Spietelun et al., 2010). P&T provides high recovery efficiency and reproducibility, enabling trace-level detection of spoilage markers, but the complexity of the system, strong dependence on purge parameters, and susceptibility to moisture interference make it less suited for rapid or field applications, particularly in high-moisture food matrices (Fernandez-Villarrenaga et al., 2006). NT combines solvent-free dynamic sampling with strong enrichment capacity and has outperformed SPME and other techniques in some cases, highlighting its potential for on-site profiling; nevertheless, limited field validation, lack of standardized protocols, sorbent stability concerns, and cost issues continue to challenge its reproducibility and routine adoption (Baimatova & Gionfriddo, 2025). Collectively, HS and SPME remain more practical for cost-effective routine monitoring, while P&T and NT offer superior sensitivity and comprehensiveness but at the expense of complexity, cost, and field applicability.

For detection methods, they also present distinct strengths and limitations in food-related mVOCs analysis. GC-MS remains the gold standard, offering unmatched specificity, sensitivity, and compound identification, but its high cost, slow throughput, and lack of portability limit its suitability for routine or field-based applications (Xu et al., 2021). GC-IMS provides faster, more portable analysis with minimal

sample preparation, making it well suited for real-time quality monitoring, though it delivers lower structural resolution and less reliable compound identification compared with GC-MS (Schanzmann et al., 2025). E-noses are attractive for their low cost, portability, and rapid screening capabilities, especially in spoilage detection, but they suffer from sensor drift, cross-sensitivity, and dependence on chemometric or machine learning models, which may reduce reproducibility across settings (Wilson & Baietto, 2009). FTIR spectroscopy enables rapid, non-destructive fingerprinting of volatile profiles and can be powerful when combined with chemometrics, yet its relatively low sensitivity, overlapping vibrational bands, and inability to unambiguously identify compounds limit its role as a stand-alone method. Taken together, GC-MS and GC-IMS remain preferred for high-precision applications, whereas e-noses and FTIR provide complementary options for cost-effective, real-time, or non-destructive food quality assessment.

Overall, these comparisons highlight that no single method is universally optimal; the choice largely depends on the analytical objective, the characteristics of the food matrix, and the available resources. In practice, combining different sampling and detection techniques often yields more robust and reliable insights into mVOCs in food systems.

4. Data analysis and machine learning modeling for mVOCs

With the growing availability of high throughput mVOCs data and their rapid detectability as reliable biomarkers, these compounds offer significant potential for monitoring of food quality and microbial dynamics, such as fermentation, contamination, and spoilage. However, fully leveraging this potential requires advanced data analysis and modeling strategies capable of handling complex, high-dimensional, and often non-linear datasets. In this context, machine learning has emerged as a powerful tool for extracting meaningful patterns from mVOCs data, enabling classification and predictive modeling beyond the capabilities of traditional statistical approaches. Table 3 outlines key applications of various machine learning techniques in food quality and safety assessment using diverse data inputs, including mVOCs.

4.1. Data preprocessing

The analysis of mVOCs data presents significant challenges due to its high dimensionality, stemming from complex mass spectrometry (MS) outputs and sensor-derived signals. These datasets are typically characterized by overlapping signals, background noise, and many variables, making accurate interpretation difficult. To address this, robust preprocessing and feature extraction techniques are essential. Feature extraction can simplify these datasets by reducing dimensionality while retaining critical information. Among the commonly used methods, Principal Component Analysis (PCA) and independent component analysis (ICA) are effective in highlighting the underlying structure of the data by emphasizing key sources of variability (Fig. 3). These techniques make the dataset more manageable and suitable for downstream analysis by enhancing the signal-to-noise ratio and reducing complexity.

PCA transforms the original data into a set of orthogonal components ranked by the variance they explain, thereby reducing redundancy and emphasizing dominant patterns within the dataset. PCA-based unsupervised feature extraction has demonstrated effectiveness across various bioinformatics applications, including DNA methylation analysis and biomarker identification (Taguchi, 2016). In the context of mVOCs gas recognition, PCA can be used as a feature extraction method alongside other techniques to improve classification accuracy when applying machine learning algorithms. Moreover, PCA can serve as a feature learning approach in multiple learning models, enhancing the extraction of relevant features from raw data (Pavlidis et al., 2019). For example, in spoiled beef and salmon, PCA effectively reduces dimensionality, generating simplified principal components. These enhance input for various downstream classification models, enabling high-accuracy discrimination of distinct sample categories (Claus et al., 2022).

On the other hand, ICA is used to decompose multivariate signals into statistically independent, non-Gaussian components. It has demonstrated strong potential as an effective feature extraction technique for analyzing mVOCs using e-nose systems. Compared to PCA, ICA

Table 3
Applications of microbial volatile organic compounds (mVOCs) and machine learning in the food industry.

Food type	Input data type	Algorithm	Model performance	Reference
Pork	E-nose	SVM-R	The optimal model achieved: $R^2 = 0.989$, root mean square error of prediction = 0.137, residual predictive deviation = 14.93	Bonah et al. (2021)
Beef fillet	E-nose	SVM	Correlations above 0.96 and 0.86 were obtained between observed and predicted microbial counts for the training and test data sets, respectively.	Papadopoulou et al. (2013)
Wheat	Whole-cell biosensor	ANN, SVM	Achieved 97.24 % accuracy of mold detection for early-warning	Li et al. (2025)
Pork patties	Color, e-nose data, texture, pH	PLS-DA, SVM, ANN	PLS-DA: $R^2 = 89.4$ %, Permutation test (200 iterations); SVM: $R^2 = 90.84$ %, 5-fold cross-validation; BP-ANN: $R^2 = 93.50$ %, optimal prediction model saved, *t*-test for validation	Lu et al. (2025)
Coffea canephora	GC-MS	RF	Normalized relative frequency >50 %, odor activity value > 1	Messias et al. (2025)
Peanuts & maize	GC-MS	RF	100 % accuracy in discriminating healthy from moldy foods. 95 % and 98 % accuracy in discriminating pre-mold stages for infected foods	Ma, Guan, et al. (2023)
Seafood	Chromogenic array	NN	90–99 % accuracy in differentiating pathogenic microorganisms from spoilage microflora on seafood	Yang et al. (2022)
Cheddar cheese	Color pattern shift	ANN	Pathogen detection from a high background microflora with accuracies ranging from 72 ± 11 % to 92 ± 3 %	Jia et al. (2024)
Fresh pork	GC-IMS	ANN	ANN-based method outperformed other employed models, when total plate count exceeded 6 log CFU/g	Chen et al. (2024)
Apple	E-nose	K-means clustering, KNNs	Achieved up to 100 % accuracy in predicting apple ripening stages, with consistent classification performance validated across new independent experiments	Trebar et al. (2024)
Shrimp & fish	Color pattern shift	CNN	Achieved 99 % accuracy for determining freshness levels	Jiang et al. (2024)
Wine	E-nose	LSTM	Achieved 87.8 %–99.41 % accuracy for predicting wine quality	Nguyen et al. (2024)
Salted goose	GC-MS, GC-IMS, e-nose, e-tongue, sensory evaluation	GAN	Achieved 95 % accuracy and strong generalization capability for discriminating salted goose breeds	(Shen et al., 2024)

Noted: E-nose, electronic nose; SVM-R, support vector machine regression; ANN, artificial neural network; SVM, support vector machine; PLS-DA, partial least squares discriminant analysis; BP-ANN, back propagating-artificial neural network; GC-MS, gas chromatography-mass spectrometry; RF, random forest; GC-IMS, gas chromatography-ion mobility spectrometry; NN, neural network; KNN, k-nearest neighbors; CNN, convolutional neural network; LSTM, long short-term memory; GAN, generative adversarial network.

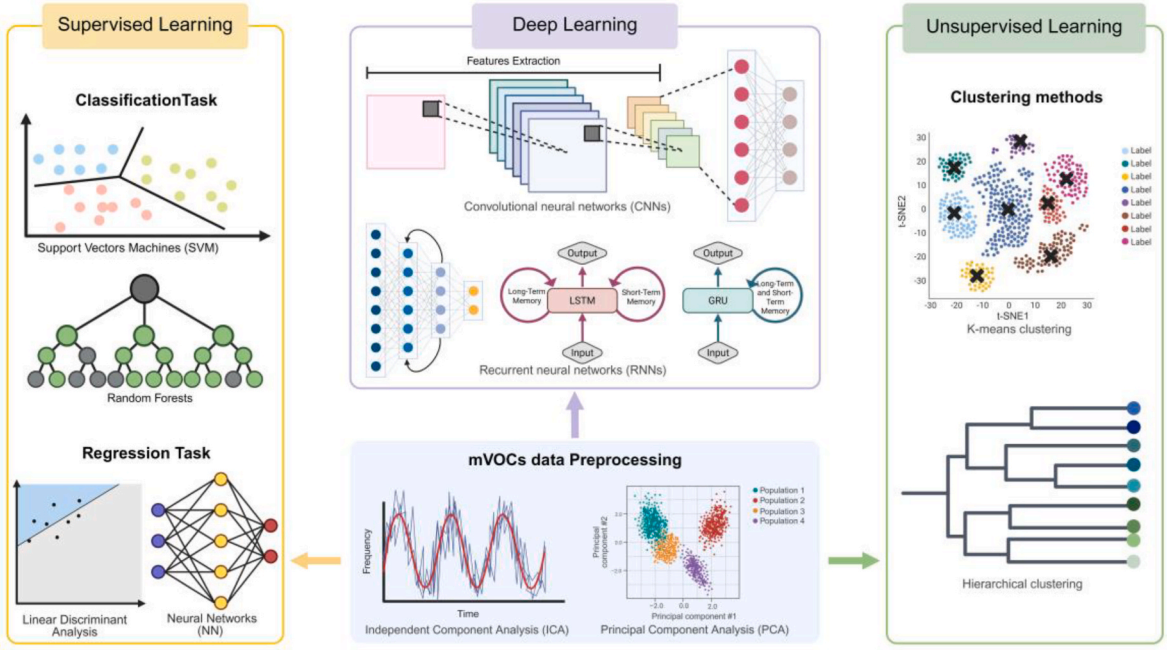

Fig. 3. Machine learning-based data processing approaches for microbial volatile organic compounds (mVOCs).

often achieves higher classification and regression accuracy for mVOCs datasets, offering superior predictive performance. As a feature learning approach, ICA can be implemented into deep learning models to automatically extract relevant features from raw sensor data, reducing reliance on manual feature engineering (Ibrahim & Al-jumaily, 2016). When combined with supervised machine learning algorithm, ICA has been successfully applied to eliminate noise and interference from mixed gas signals from e-nose sensors, thereby improving the accuracy and reliability of gas composition analysis (Meng, 2010).

4.2. Supervised learning models in mVOCs analysis

Supervised learning models are widely used in the analysis of mVOCs data in various food science applications due to their ability to learn from labeled datasets and generalize effectively to unseen data. These models are typically categorized into classification and regression tasks based on the type of output (or target variable) they are designed to predict. They provide a robust and effective framework for addressing diverse challenges, ranging from food quality monitoring to predictive modeling in mVOCs-related research.

4.2.1. Classification tasks

SVMs are a type of supervised learning algorithm widely used for classification tasks (Fig. 3). Known for their efficiency and versatility, SVMs have gained increasing prominence in food science research (Lytou et al., 2023). In particular, SVMs can identify characteristic mVOCs patterns associated with specific pathogens, enabling the development of rapid and non-invasive diagnostic tools. For example, SVMs have demonstrated excellent predictive performance in detecting *Salmonella* contamination in pork, achieving an R^2 of 0.989, a Root Mean Square Error (RMSE) of prediction of 0.137, and a residual predictive deviation of 14.93, indicating strong model fit and accuracy. Similarly, SVM-based methods have been applied for mold detection in wheat (Table 3). Beyond food safety, SVMs have also shown great potential in assessing freshness (Mohareb et al., 2016; Papadopoulou et al., 2013). In a recent study on pork patties stored at 4 °C, an e-nose combined with SVMs was used to predict freshness based on volatile profiles. The model achieved over 91 % prediction accuracy for total volatile basic nitrogen, with predicted values closely aligning with experimental results (Table 3). These applications highlight the effectiveness of SVMs in monitoring both microbial safety and quality deterioration, underscoring their value as non-destructive, efficient alternatives to conventional, labor-intensive methods. Their ability to model nonlinear relationships through kernel functions and adapt to various data types further reinforces their utility in analyzing complex biological food systems.

Random forest (RF) is another popular supervised learning model used for classification tasks (Fig. 3). It is an ensemble learning method that constructs a multitude of decision trees during training and outputs the mode of the classes of the individual trees. RF is known for its robustness, ability to handle large datasets with high dimensionality, and resistance to overfitting, especially when dealing with complex datasets. The strength of RF lies in its ability to aggregate multiple weak learners (decision trees) to improve the model's overall accuracy and generalization ability. It has been employed to identify disease-related mVOCs patterns in paratuberculosis detection, showcasing its potential in medical diagnostics (Kasbohm et al., 2017). Additionally, RF methodology has been successfully applied in various food science fields. For instance, it was applied to analyze the volatile profiles of *Coffea canephora* beverages fermented with *S. cerevisiae*, enabling the differentiation of sensory attributes associated with various fermentation treatments (Table 3). Among the 94 mVOCs identified, about 10 % were found to significantly influence the sensory characteristics. RF analysis effectively pinpointed key compounds responsible for flavor enhancement in samples treated with glucose and fructose, demonstrating its utility in optimizing fermentation processes and assessing product quality. In food safety, RF has also shown impressive performance in detecting microbial contamination. It achieved 100 % accuracy in distinguishing health from mold-infected samples and 95 %–98 % accuracy in identifying pre-mold stages, allowing for early spoilage detection and timely intervention (Table 3). These applications highlight RF's versatility and reliability in analyzing complex food systems across both sensory and safety domains.

4.2.2. Regression tasks

Linear regression models, a type of supervised learning algorithm, are widely used in predictive microbiology to simulate microbial growth under various environmental conditions. As part of regression tasks,

these models predict continuous outcomes based on input variables (Fig. 3). In food microbiology, linear regression can be applied to analyze percentage data, such as growth probability and inactivation rates. For example, linear regression analysis has revealed how organic acids, which are key microbial metabolites, significantly influence the microbial community structure in fermented grains. This influence subsequently affects the overall volatile component concentrations and product quality (He et al., 2024). Recent advancements in microbial analysis have focused on mVOCs as indicators, enabling early identification of microbial contamination.

For more complex regression tasks, such as predicting mVOCs concentration levels affected by multiple interacting factors, neural networks (NNs) provide an effective alternative (Fig. 3). NNs have been utilized in various food science applications, including modeling microbial growth and forecasting food safety outcomes. In one study, artificial neural networks (ANNs) outperformed other models in predicting total microbial counts in fresh pork (Table 3). More recently, a paper-based chromogenic array coupled with an NN achieved high accuracy (90–99 %) in distinguishing pathogenic microorganisms from spoilage microflora in seafood by detecting mVOCs (Table 3). Additionally, pathogen detection in shredded Cheddar cheese, despite a complex background microflora, yielded accuracies ranging from 72 ± 11 % to 92 ± 3 % using an ANN integrated with a paper chromogenic array (Table 3). This non-destructive approach, combined with NN analysis, effectively predicted pathogens in cod and salmon samples even in the presence of spoilage bacteria and background microflora, demonstrating the strength of supervised learning models in addressing complex regression challenges in food safety.

Although these traditional machine learning methods have been proved to be feasible, they can encounter scalability issues when applied to large datasets, which may limit their effectiveness in real-world scenarios that involve complex biological interactions (Khan et al., 2022). These challenges become particularly evident as the volume and complexity of the data increase, making it difficult for these methods to maintain high performance and accuracy. Nevertheless, the integration of supervised learning models into food science and mVOCs analysis remains a key driver of advancements in predictive modeling. Ongoing research is focused on improving the scalability, interpretability, and computational efficiency of these models, striving to overcome these limitations and unlock their full potential in addressing complex food safety and microbiological concerns.

4.3. Unsupervised learning models in mVOCs analysis

Unlike supervised learning models, which rely on labeled data to train algorithms, unsupervised learning models are used when labeled data are unavailable, allowing for the exploration of hidden patterns and structures within datasets. In the context of mVOCs analysis in food science, unsupervised learning can uncover natural groupings of food samples based on their intrinsic characteristics. One common approach within unsupervised learning is clustering, which segments data into groups, or clusters, based on similarity metrics, offering insights into the underlying distribution and relationships of the data. Anomalous samples can be uncovered with hidden relationships and generate hypotheses for further investigation. Popular clustering methods include K-means, which partitions the dataset into a predefined number of clusters, and hierarchical clustering, which builds a tree-like structure to represent data relationships at different levels of similarity (Fig. 3). These approaches are especially beneficial in exploratory data analysis, where the primary objective is to identify underlying patterns that may inform subsequent supervised modeling or provide domain-specific insights.

K-means clustering has been applied in food science for various types of analyses. In an olive oil study, it was used to group extra virgin olive oils based on sensory profiles and volatile compounds, helping to differentiate monovarietal samples. Notably, K-means combined with K-nearest neighbors (KNN) has demonstrated strong performance in predicting the ripening stages of apple fruits. By clustering sensor data and principal components from volatile compound analysis, followed by classification using KNN, this approach achieved up to 100 % accuracy across multiple independent experiments, effectively distinguishing between less-ripe, ripe, and overripe apples (Table 3). Additionally, mVOCs have gained attention as key indicators of food contamination, and K-means clustering has been employed to analyze mVOCs profiles in various food safety assessments. In human gut microbiome studies, K-means clustering of 16S rRNA sequences has also contributed to understanding intestinal microbiota composition and identifying potential disease indicators (Taie et al., 2018).

Hierarchical clustering is another method used to analyze mVOCs emitted by various microorganisms, revealing consistency between mVOCs-based and pathogenicity-based classifications. This technique can also distinguish between different microalgal strains based on their mVOCs profiles (Deng et al., 2023). Unlike K-means, hierarchical clustering does not require a pre-specified number of clusters, making it particularly well-suited for exploratory studies where the optimal number of groups is unknown. In mVOCs profiling, studies have shown that species-level discrimination of bacterial isolates can be achieved based on emission patterns of volatile compounds. Although not always explicitly analyzed using hierarchical clustering, such mVOCs datasets present structured variability well-suited for this method. In food research, hierarchical clustering has been used to distinguish grapes and corresponding wine samples processed under different postharvest cooling treatments, based on distinct mVOCs profiles that correlate with sensory properties (Modesti et al., 2021).

4.4. Deep learning models in mVOCs analysis and time-series data processing

Deep learning models, as a form of representation-learning, are particularly effective in analyzing complex and high-dimensional datasets, such as those involved in mVOCs analysis. These models automatically learn features from raw data, refining multilevel representations to capture intricate patterns. Deep learning can be applied in both supervised learning tasks, such as classification and regression, and unsupervised tasks, such as clustering or anomaly detection, offering flexibility depending on whether labeled data is available (Shen et al., 2025). In mVOCs analysis, deep learning models help to uncover hidden relationships between volatile compounds, improving the accuracy of predictions related to microbial contamination, spoilage, and food safety.

Convolutional neural networks (CNNs) have shown promising applications in food science and related fields. For example, they have been employed in monitoring the freshness of seafood. In a recent study, colorimetric sensor arrays composed of 16 chemo-responsive dyes were used to detect mVOCs released during spoilage. The resulting color changes were digitized and analyzed using a CNN model, which successfully classified the seafood into four freshness levels, fresh, less fresh, slightly spoiled, and spoiled, with an accuracy of 99 %. (Table 3). On the other hand, recurrent neural networks (RNNs), designed to model sequential data, are particularly effective at capturing temporal dependencies in mVOCs time-series datasets. Unlike feedforward networks, RNNs incorporate loops that allow information to persist across time steps, enabling them to analyze data where the order of observations is critical. Advanced techniques, such as long short-term memory (LSTM) networks, have shown promise in predicting food allergies from longitudinal gut microbiome profiles, outperforming traditional machine learning models (Metwally et al., 2019). Additionally, in food quality evaluation, LSTM networks analyzing e-nose mVOCs signals with have achieved high accuracy (87.8–99.41 %) in wine quality recognition (Table 3). Another prominent variant of deep learning is generative adversarial networks (GANs), which are particularly powerful for data augmentation and capturing complex multimodal

food data (Shen, Wang, Nawazish, et al., 2024). For instance, Shen, Wang, Jin, et al. (2024) developed a GAN-based integrated framework that combined GC-MS, GC-IMS, e-nose, e-tongue, and sensory evaluation to discriminate salted goose breeds (Table 3). By generating synthetic data to overcome limited sample sizes and fusing heterogeneous datasets, the GAN-enhanced model achieved 95 % accuracy and strong generalization capability. This example underscores GANs' potential not only to solve the challenge of small datasets but also to integrate multi-sensor and chemometric data streams for robust food authentication and mVOCs analysis.

4.5. Critical perspectives in machine learning-based mVOCs analysis

Despite notable advances, significant challenges remain in applying machine learning to mVOCs-based food analysis. A persistent concern is the risk of overfitting, as many studies are based on relatively small but high-dimensional datasets. Such models may report deceptively high accuracies in training or cross-validation but lack robustness during external validation or real-world deployment (Khan et al., 2022; Taguchi, 2016). Closely related is the issue of generalizability, since models optimized for specific foods: models trained on specific foods, microbial communities, or sensor platforms often fail when transferred to other contexts (Ibrahim & Al-jumaily, 2016; Ma, Guan, et al., 2023). Addressing these limitations requires access to larger and more diverse datasets, rigorous external validation, and advanced strategies, such as transfer learning, domain adaptation, and federated learning, which can help models adapt to heterogeneous data without compromising privacy. As a positive example, the MeatReg study employed Monte-Carlo cross-validation and reported RMSE/accuracy across packaging types and temperatures, illustrating robust model comparison practices that help curb overfitting in small, high-dimensional settings (Estelles-Lopez et al., 2017).

Practical implementation barriers also constrain progress. Deploying machine learning for real-time monitoring in industrial environments requires computationally efficient models that are resilient to sensor drift, environmental noise, and matrix variability. Yet most existing systems remain research prototypes rather than industry-ready solutions (Bonah et al., 2021). The problem is compounded by data heterogeneity, with inconsistencies across laboratories, sensor platforms, and preprocessing protocols leading to poor reproducibility and difficult cross-study comparisons. Standardized protocols and harmonized evaluation metrics are urgently needed to ensure comparability and robustness across applications. Another critical barrier is interpretability. Many advanced models, particularly deep NNs, function as "black boxes," limiting transparency and trust in regulatory and industrial settings. Since food safety monitoring requires traceable reasoning, models that lack interpretability risk rejection. The application of explainable AI (XAI) tools, such as SHapley Additive exPlanations (SHAP) values, attention maps, or surrogate models can provide greater transparency. Furthermore, hybrid models that combine mechanistic insights with machine learning predictions could help improve both accuracy and biological interpretability (Okyere et al., 2023).

Beyond these methodological and operational challenges, several data-related limitations must be addressed. Data imbalance remains common: certain spoilage organisms, food types, or mVOCs classes are overrepresented, biasing model predictions. Similarly, the temporal dynamics of mVOCs, critical for tracking spoilage and fermentation stages, are often underexplored, with most models focusing on static snapshots rather than longitudinal signals. Integrating multimodal data (e.g., mVOCs with omics, imaging, and environmental metadata) has shown promise (Estelles-Lopez et al., 2017; Govari et al., 2021; Lytou et al., 2023). Moreover, recent perspectives in food AI highlight broader systemic barriers that are equally relevant to mVOCs research. As Zhang et al. (2025) emphasize, progress will depend on tighter integration of domain knowledge into model frameworks, ensuring that predictions are guided by an understanding of microbial metabolism, food chemistry, and processing dynamics rather than solely data-driven correlations. Moreover, the field lacks transparent and reusable workflows: many published models do not release code, datasets, or pipelines, hindering reproducibility and slowing collective progress. The absence of benchmark datasets and evaluation initiatives, comparable to Critical Assessment of Protein Structure Prediction (CASP) in protein structure prediction, makes it difficult to fairly assess whether new models represent real advances. Finally, the lack of robust data standards and infrastructure, alongside geographic biases in existing datasets, undermines global applicability and risks reinforcing inequities across food systems.

In summary, while machine learning offers transformative opportunities for mVOC-based food analysis, its advancement requires moving beyond proof-of-concept demonstrations toward scalable, interpretable, and industry-ready solutions. This will require larger collaborative datasets, standardized protocols, explainable modeling approaches, multimodal integration, and cross-disciplinary partnerships between food scientists, data scientists, and industry stakeholders. By addressing these methodological, practical, and systemic challenges, machine learning-based mVOCs analysis can evolve into a reliable tool for food quality monitoring, microbial safety, and sustainable production systems.

5. Applications of mVOCs analysis in food industry

Fig. 4a illustrates the end-to-end workflow of mVOCs analysis, starting from microbial generation and volatile release, followed by sampling and detection (e.g., GC-MS, GC-IMS, e-nose), and extending to machine learning modeling and final decision-making for food quality and safety management. This framework demonstrates how mVOCs can be systematically captured and analyzed to enable real-time interventions in fermentation, spoilage detection, foodborne pathogen monitoring, and control of undesirable microbial growth (Fig. 4b). These mVOCs play a crucial role in regulating microbial interactions during food fermentation, influencing community succession and the accumulation of metabolic products. For example, during baijiu fermentation, *Pichia* yeast releases 2-phenylethanol, which inhibits the growth of *Monascus*, thereby altering the microbial community structure and affecting flavor formation (Zhang et al., 2021). In natural vinegar fermentation, the metabolic activity of *Saccharomyces*, *Leuconostoc*, and *Acetobacter* determines the accumulation of ethanol, esters, and acetic acid, with mVOCs potentially influencing microbial regulation (Maske et al., 2024). During Qu starter preparation, *Rhizopus microsporus* produces benzyl alcohol, which promotes the growth of *Lactobacillus fermentum* and enhances microbial stability through amino acid metabolism (Hao et al., 2022). These findings suggest that mVOCs significantly shape the microbial ecology of food fermentation while influencing the synthesis of flavor precursors and fermentation dynamics. By controlling the release of mVOCs, it is possible to optimize microbial interactions, improve fermentation efficiency, and enhance the flavor and quality of the final product.

The release of mVOCs during food spoilage acts as a reliable indicator of deterioration, providing a solid foundation for food quality monitoring. In seafood, the accumulation of methanethiol and dimethyl disulfide results from the enzymatic degradation of methionine and cysteine, while the increase in ethyl acetate and ethyl propionate is associated with fatty acid metabolism. These mVOCs have been identified as key markers of seafood spoilage (Chang & Urban, 2018). In poultry, ethanol, 3-methyl-1-butanol, and acetic acid concentrations rise significantly with microbial growth. Ethanol is primarily produced by *Pseudomonas* spp., whereas 3-methyl-1-butanol and acetic acid are linked to the metabolic activity of LAB and *Brochothrix thermosphacta*. The presence of these mVOCs correlates with spoilage progression, making them effective indicators for poultry quality assessment (Mikš-Krajnik et al., 2016). In red meat products such as beef sausages, GC-MS analysis revealed hexanal, acetoin, and 1-octen-3-ol as the main

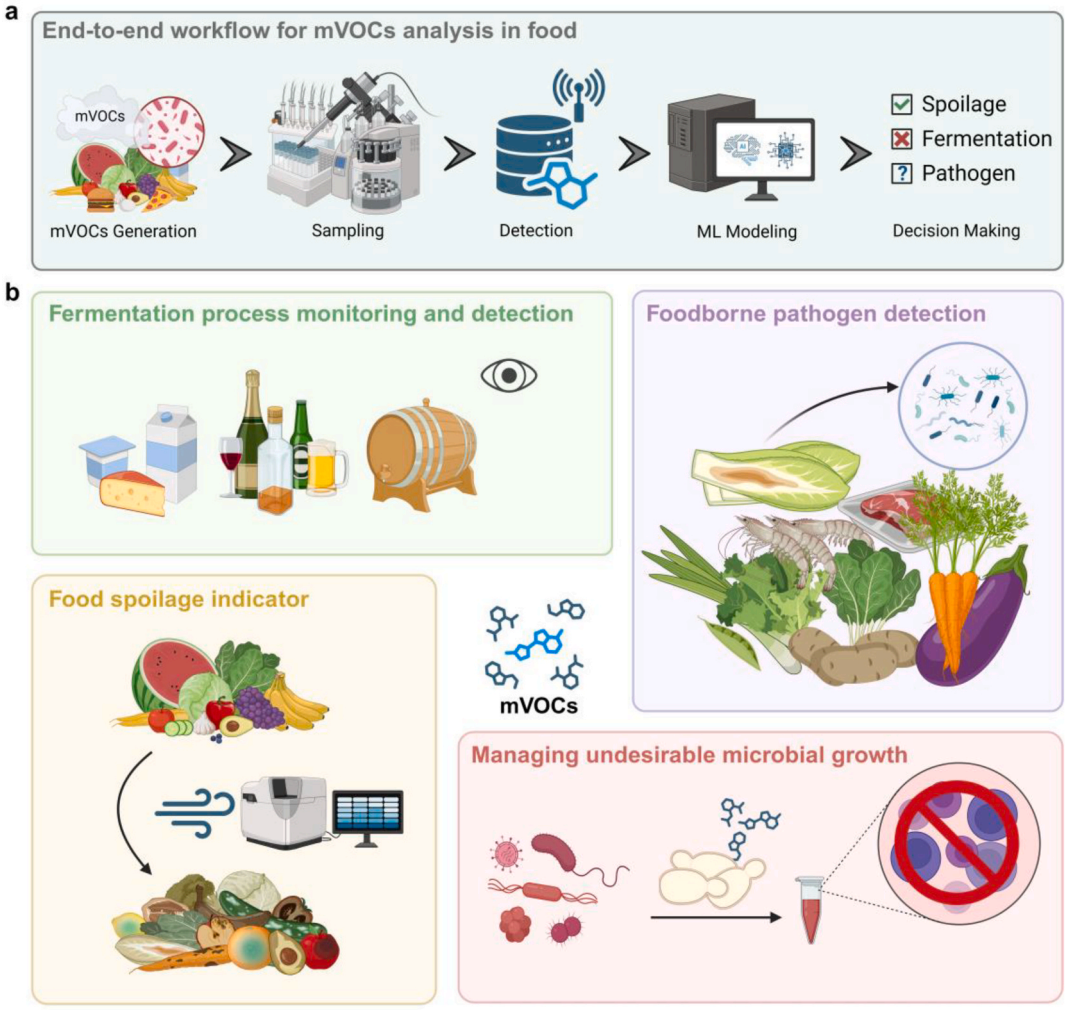

Fig. 4. End-to-end workflow (a) for microbial volatile organic compounds (mVOCs) analysis and its applications (b) in the food industry.

mVOCs during refrigerated storage, with their concentrations positively correlated to the dominant spoilage bacteria *Brochothrix* and *Serratia* (Table 1), underscoring their value as spoilage indicators (Han et al., 2025). These studies demonstrate the potential of mVOCs to signal the onset of spoilage and differentiate stages of deterioration, supporting their use in food quality evaluation and spoilage monitoring.

mVOCs contribute to food safety by inhibiting pathogenic microorganisms and minimizing contamination risks. For example, *Bacillus*-derived mVOCs have expanded their application in food safety control. Studies show that mVOCs from *B. subtilis, B. amyloliquefaciens,* and *B. cereus* inhibit pathogens, such as *Moniliophthora perniciosa* and *Fusarium oxysporum*, with key inhibitory compounds, including propanone, 1-butanol, 3-methyl-1-butanol, acetic acid, and ethyl acetate (Chaves-López et al., 2015). Furthermore, pathogen-emitted mVOCs are emerging as reliable biomarkers for pathogen detection and identification in complex food matrices. Recent studies have demonstrated distinct mVOCs fingerprints specific to pathogens, such as *E. coli, S.* Typhimurium*, S. aureus, Vibrio parahaemolyticus* and *Shigella sonnei* (Fang et al., 2021; Wang et al., 2018; Yang et al., 2021). For example, mVOCs released by pathogens were used to differentiate rapidly and simultaneously between living *E. coli* O157:H7 and *Listeria monocytogenes* in fresh-cut romaine lettuce without the need for culturing or enrichment, maintaining the promise of mVOCs as valuable biomarkers for monitoring food safety (Yang et al., 2021). Similarly, diagnostic volatile metabolite profiles of pathogens *S. sonnei* and *S. aureus* were efficiently sensed in contaminated foods, further validating the practicability of pathogen-specific mVOCs in premature detection of contamination (Fang et al., 2021; Wang et al., 2018). Collectively, the multifunctionality of mVOCs, as both antimicrobial agents and precise biomarkers for pathogen identification, represents a promising avenue for sustainable and innovative food safety and quality management strategies.

6. Conclusion

mVOCs have emerged as powerful non-invasive indicators for assessing food quality and safety, enabling early detection of spoilage, contamination, and fermentation dynamics. This review summarizes their metabolic origins across carbohydrate, protein, and lipid pathways, which generate characteristic volatile signatures linked to microbial activities in diverse food matrices. The effectiveness of mVOCs analysis depends heavily on optimized sampling methods, such as HS, SPME, P&T, and NT, each offering unique advantages in cost, sensitivity, selectivity, and applicability to various food systems. For detection, GC-MS remains the gold standard for sensitivity and specificity, while GC-IMS enables rapid and portable profiling, FTIR offers non-destructive molecular fingerprints, and e-nose systems provide fast, sensor-based classification. Equally critical is the role of data analysis and machine learning. Raw mVOCs datasets are typically high-dimensional, noisy, and matrix-dependent, requiring careful preprocessing and feature extraction to ensure meaningful interpretation. Supervised learning models like SVMs, RFs, and NNs have been widely applied to classify

pathogens and predict spoilage stages, while unsupervised approaches (e.g., clustering and PCA/ICA) uncover hidden patterns in unlabeled data. More advanced deep learning architectures, such as CNNs and RNNs, are particularly useful for handling complex and time-series mVOCs signals, enabling dynamic monitoring of microbial activity. To fully realize their potential, future studies must prioritize data harmonization, standardized workflows, and the creation of benchmark datasets to reduce overfitting risks and enhance reproducibility across laboratories and food systems.

Despite substantial progress, several critical challenges remain. Standardization of experimental protocols is urgently needed, including calibration procedures for GC-MS and GC-IMS, harmonized quality control measures, and cross-laboratory reproducibility studies to ensure comparability of results. Moreover, model interpretability, robustness to sensor drift, and integration of multimodal data streams (e.g., metabolomics, imaging, and sensor data) remain open challenges that must be addressed before industrial adoption. Looking ahead, future perspectives should emphasize: (i) protocol standardization and reference material development to support regulatory adoption and cross-industry comparability; (ii) scalable and cost-effective sensing solutions that enable both laboratory and industrial deployment; (iii) robust data infrastructures and open repositories to promote transparency, benchmarking, and cross-study comparability; and (iv) interdisciplinary collaboration between microbiologists, analytical chemists, data scientists, and industry partners to accelerate translation into practice. By addressing these methodological, computational, and translational challenges, the field can move toward reliable, scalable, and real-time applications of mVOCs in ensuring food quality, safety, and sustainability.

Author contribution form

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#Use author initials to declare the contributions to the manuscript.

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Competing interests

All authors declare that they have no competing interests.

Data availability

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

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