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Review

From molecular fingerprints to predictive flavour: a critical review of integrated, sustainable, and chemometrics-driven food and aroma profiling

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Abstract: Flavour analysis plays a crucial role in food science, enabling the identification, quantification, and characterisation of volatile and non-volatile compounds responsible for sensory perception. This review provides a critical evaluation of traditional and modern analytical techniques, including sensory evaluation, gas chromatography-mass spectrometry (GC-MS), and high-performance liquid chromatography (HPLC). It goes beyond description to provide a comparative evaluation of instrumental platforms, tackling important issues in industrial scalability, cost, and reproducibility. The emergence of machine learning and databases such as FlavorDB has further advanced the field, with this review systematically exploring the integration of chemometrics and artificial intelligence with instrumental data to enhance predictive accuracy and pattern recognition. Furthermore, sustainable analytical approaches aligned with green chemistry principles are examined, and key standardisation challenges are discussed, with actionable frameworks proposed to enhance reproducibility and cross-laboratory flavour profiling. This approach bridges the gap between academic research and real-world food innovation by connecting molecular-level findings to practical applications in food product development and quality control. The convergence of computational models with advanced chemical profiling not only deepens the understanding of complex flavour interactions but also offers transformative potential for product development, quality control, and sustainable food systems.

Keywors: Flavour analysis, Chemometrics, Machine learning, Sustainability, Standardisation, GC-MS, HPLC

1. Introduction

Food flavour is a critical driver of consumer preference, product acceptance, and market success in the global food industry. Beyond nutritional value, flavour determines whether foods are enjoyed, remembered,

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and repurchased. Flavour is a sensory perception experienced during ingestion, involving gustatory and olfactory stimuli, alongside tactile, thermal, painful, and kinaesthetic effects. These perceptions are critical in determining consumer acceptability, as they arise from the combined responses of olfaction, taste, and somatosensory inputs, along with cognitive processing in the brain [1, 2]. Flavour compounds contribute to taste attributes such as sourness, sweetness, bitterness, astringency, and spiciness [1]. Furthermore, these compounds exhibit diverse chemical structures and properties, which contribute to the distinct flavours of various foods.

Flavour compounds can generally be classified into two major categories based on their contribution to sensory perception: volatile compounds responsible for aroma and non-volatile compounds associated with taste. Volatile compounds, including esters, aldehydes, ketones, alcohols, terpenes, and sulphur-containing compounds, are typically present at low concentrations but contribute significantly to characteristic aroma notes such as fruity, floral, roasted, and meaty sensations in foods [3]. These compounds are primarily detected by the olfactory system. In contrast, non-volatile compounds such as sugars, organic acids, amino acids, and phenolic compounds contribute to basic taste perceptions, including sweetness, sourness, bitterness, umami, and astringency, which are detected by taste receptors on the tongue [4]. Together, the interaction of these volatile and non-volatile components forms the overall flavour perception of food [1, 2].

Food aromas are complex mixtures of molecules, making it challenging to analyse their composition comprehensively. Techniques for flavour analysis are used to detect and measure flavour compounds in food products, with the aim of understanding, characterising, and enhancing the sensory experience. Flavour analysis is generally carried out using two main approaches: sensory evaluation and instrumental analysis. Sensory analysis focuses on human perception of flavour and often employs descriptive methods to evaluate flavour attributes [5]. Although sensory evaluation is essential for understanding how flavours are perceived, it is limited by subjectivity and individual variability. Consequently, instrumental analytical techniques have gained importance because they allow the identification and quantification of the chemical compounds responsible for flavour with greater precision, reproducibility, and sensitivity. In recent years, various analytical techniques have emerged for analysing food flavour compounds, including chromatographic methods, solid-phase extraction, electronic noses and tongues, sensor arrays, fluorescence detection with DNA barcoding, and conformational relationship studies [6]. Techniques such as solid-phase microextraction (SPME) and stir-bar sorptive extraction (SBSE) are commonly used to isolate volatile and non-volatile compounds. Methods such as gas chromatography-olfactometry (GC-O) and solvent-assisted flavour evaporation (SAFE) are widely employed to identify key aroma-active compounds [7].

Gas chromatography (GC) and its variants, including GC–mass spectrometry (GC-MS) and GC-O, are widely used for the analysis of volatile flavour compounds due to their high separation efficiency. In contrast, liquid chromatography (LC) techniques are particularly suited for analysing non-volatile, thermally labile, or highly polar compounds such as sugars, capsaicin, and peptides [7]. Among these techniques, GC-MS remains one of the most widely applied tools for aroma analysis, enabling the identification of odour-active compounds, off-flavours, and volatile organic compounds in food and environmental samples [7].

This review critically examines the evolution of analytical methods in flavour analysis, from traditional sensory and chromatographic techniques to modern computational and database-driven approaches. While methods such as GC-MS and HPLC remain foundational, persistent challenges in reproducibility, sensitivity, and high-throughput analysis necessitate continued methodological refinement. The emergence of resources such as FlavorDB, a curated repository of over 25,000 flavour molecules integrated from authoritative sources including *Fenaroli's Handbook of Flavour Ingredients and contemporary literature*, exemplifies the shift toward data-enhanced flavour science [8].

To systematically address existing research gaps, this review pursues five core objectives: (1) comparing instrumental techniques including GC-MS, HPLC, ambient MS, and electronic sensors in terms of reproducibility, cost, and suitability for complex food samples; (2) exploring the integration of chemometrics and artificial intelligence with instrumental data to improve flavour prediction and analysis; (3) examining standardisation challenges and proposing practical solutions such as benchmark datasets and open-access flavour databases; (4) evaluating sustainable analytical approaches including solvent-free extraction methods and bio-based solvents; and (5) linking molecular insights to industrial applications through relevant case studies. These objectives reflect the ongoing transformation of flavour science towards a more data-driven and interconnected analytical framework, consistent with the principles of Industry 4.0, where artificial intelligence, big data analytics, and automation support more efficient interpretation of complex analytical datasets [8]. Through this perspective, this review aims to provide a future-focused resource that connects molecular fingerprints with predictive, sustainable, and chemometrics-driven flavour analysis.

2. Historical overview of analytical techniques in flavour analysis

The evolution of flavour analysis techniques has seen significant advancements over the decades, progressing from sensory evaluations to the application of machine learning. This progression closely parallels the advancements brought about by the Industry 4.0 revolution; an era characterised by technological integration driving industrial transformation. Industry 4.0 enables enhanced accessibility, connectivity, and efficiency along the value chain, thereby improving supply chains. In flavour analysis, this has led to advancements such as GC-MS with automated sample preparation, artificial intelligence (AI)-driven data processing for complex flavour profiling, and the integration of electronic sensing technologies like the electronic nose (E-nose) and electronic tongue (E-tongue) for real-time quality monitoring [9]. The industrial revolutions have unfolded in four stages: the first driven by steam power, the second by electricity, the third by preliminary automation and machinery, and the fourth shaped by cyber-physical systems and intelligent systems. Similarly, the development of flavour analysis techniques can be divided into four stages: sensory analysis, instrumental analysis, a combination of sensory and instrumental analyses, and automatic analysis integrated with machine learning [10]. Each industrial revolution has contributed to the availability of advanced instruments, which in turn have enabled significant progress in analytical methods, as illustrated in Figure 1.

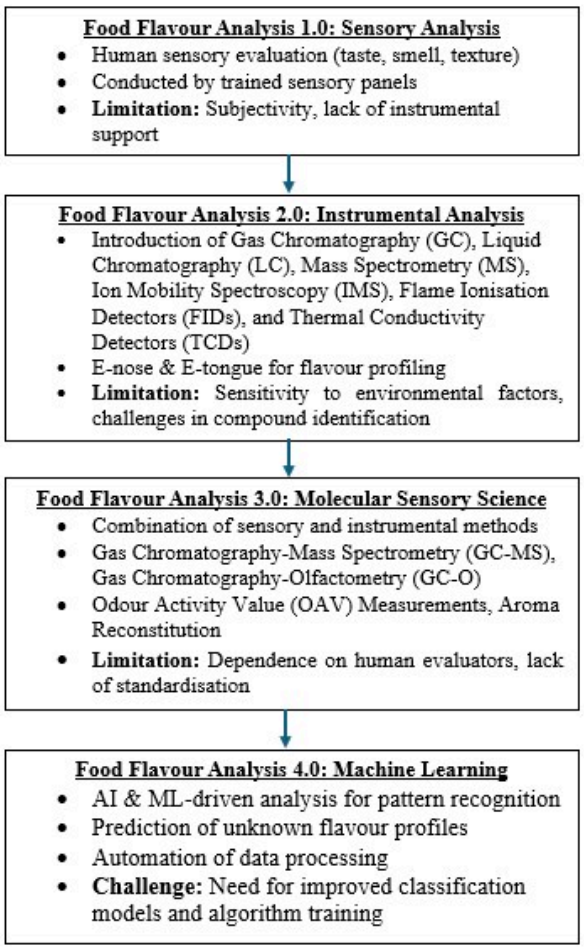

Figure 1. Evolution of food flavour analysis techniques

2.1 Food flavour analysis 1.0: sensory analysis

The first stage, referred to as Food Flavour Analysis 1.0, relied solely on sensory analysis performed by trained experts using human sensory organs to evaluate food characteristics. While sensory analysis provided valuable insights, it was limited by its inability to detect harmful gases in food or to elucidate the mechanisms underlying flavour formation. The lack of instruments during this stage restricted the effectiveness and scope of

sensory evaluations [10].

2.2 Food flavour analysis 2.0: instrumental analysis

The introduction of instrumental analysis in the second stage, Food Flavour Analysis 2.0, was facilitated by technological advancements during the second industrial revolution. Techniques such as chromatography and sensor technologies allowed researchers to study volatile and soluble components of food and beverages in greater depth. Instruments such as GC and LC, combined with detectors like mass spectrometry (MS), ion mobility spectroscopy (IMS), flame ionisation detectors (FIDs), and thermal conductivity detectors (TCDs), enabled precise flavour profiling. Additionally, E-nose and E-tongue provided specific flavour fingerprints with high reliability, complementing or even replacing GC in some cases. However, these technologies were sensitive to environmental changes, and their responses to compounds with specific functional groups were sometimes weakened, limiting their effectiveness during manual identification [10].

2.3 Food flavour analysis 3.0: molecular sensory science

The third stage, Food Flavour Analysis 3.0, marked the integration of sensory and instrumental analyses, leading to the development of molecular sensory science. Techniques such as GC-MS and GC-O were combined with odour activity value (OAV) measurements, omission tests, and aroma reconstitution experiments to quantify, describe, and elucidate the molecular basis of key flavours at a deeper level. Despite these advancements, the results of olfactometry analyses were often dependent on sensory evaluators, making it difficult to establish uniform standards [10].

2.4 Food flavour analysis 4.0: machine learning

The fourth stage, Food Flavour Analysis 4.0, is characterised by the application of machine learning in the food industry. Machine learning algorithms can identify patterns, recognise similarities, and differentiate variations in sample characteristics. Supervised learning algorithms, when combined with traditional flavour analysis techniques, enable the prediction of flavours in unknown food samples with greater speed and objectivity than manual methods. Furthermore, machine learning facilitates the processing of large datasets, reducing analysis time and improving efficiency. It can identify complex patterns in high-dimensional variable spaces and automatically optimise algorithms to predict outcomes based on new data [11]. However, there remains a need for further research to summarise the advances in using different machine learning algorithms as classification criteria for food flavour analysis [10].

In addition to machine learning, Industry 4.0 technologies such as real-time data transmission and cloud-based platforms further enhance flavour analysis capabilities. These systems enable continuous monitoring and seamless sharing of analytical data across laboratories, facilitating instrument synchronisation and large-scale data integration. Such connectivity allows analytical outputs from techniques like GC-MS and electronic noses to be integrated into centralised databases for rapid interpretation and model training. Consequently, the combination of advanced analytics and interconnected systems supports the development of more efficient, reproducible, and predictive flavour analysis workflows [10, 11].

3. Analytical techniques for flavour analysis

Flavour analysis presents several key challenges, including accurate measurement of volatile and non-volatile compounds, effective data interpretation, and practical implementation in industrial settings.

3.1 Sensory analytical techniques

The primary sensory analytical technique is descriptive sensory analysis, which is performed by trained sensory panels. Descriptive analysis applies a flavour lexicon, a set of words used to describe the flavour of a product based on the sensory physiological perception of the panels. The qualitative descriptions include the appearance, odour, taste, and texture of the product [5]. Two other sensory analytical techniques include discrimination tests, which assess whether products are similar or different in terms of general or specific characteristics, and consumer tests, which focus on the hedonic and emotional responses of consumers towards products to understand consumer acceptability [12].

Taste perception can differ between individuals, including trained sensory panel members. Both flavour and texture perception influence how taste is experienced. Flavour is affected by a combination of taste, aroma, and chemesthetic sensations, which can also be influenced by cognitive descriptions and attention [5]. While taste primarily encompasses sweet, sour, bitter, salty, and umami, aroma adds layers of complexity, distinguishing between floral, fruity, earthy, spicy, and countless other descriptors. Texture plays a crucial role in defining sensations such as creaminess, crunchiness, or chewiness, adding to the mouthfeel of a product. Moreover, individual preferences, genetic variations in taste perception, and cultural upbringing further shape how flavours are perceived and interpreted, often

introducing a degree of cognitive bias.

Flavour descriptions frequently rely on metaphors, serving as conceptual guides for both spoken and written accounts. Within the domain of flavour analysis, various metaphorical frameworks are employed, including discourse metaphors that perceive flavour as an event, a dimensional entity, a balance, a living entity, or an art form [13]. For example, wine connoisseurs may use terms such as "oaky", "buttery", or "fruity" to articulate the characteristics of a particular vintage. Similarly, chefs might describe a dish as "savoury", "spicy", or "succulent", capturing its flavour profile and mouthfeel. In addition to standard descriptors, metaphors, analogies, and cultural references are frequently used to evoke specific sensations and emotions associated with flavours. Categorising flavours is a complex task that involves classification based on various criteria, such as taste, aroma, origin, and culinary use. The flavour wheel, a visual representation of flavour categories, is a common tool used by professionals in the food and beverage industry to organise and comprehend the vast spectrum of flavours [14]. Furthermore, describing complex flavours often requires a rich and diverse vocabulary encompassing a wide range of taste, aroma, and texture descriptors. The effectiveness of teaching methods may vary in influencing one's ability to analyse and describe complex flavours.

Sensory techniques can be coupled with instrumental flavour analysis methods, such as GCO. This combination can elucidate the relative impacts of many volatile compounds on flavour characteristics [15]. The E-nose and E-tongue are instrumental analytical techniques designed to mimic human sensory perception, specifically olfaction and taste. The E-nose is used to analyse volatile food flavour compounds and reveal aroma differences in food while eliminating operator fatigue, as the instrument can obtain repeatable measurements. The E-nose comprises a group of chemical sensors associated with a pattern-recognition system that detects and processes odours [7, 15, 16]. The sensors exhibit varying sensitivity to different odours due to chemical interactions between compounds and sensors. Changes in physical or chemical properties result in electrical signals recorded by a computer system. These signals are then analysed using chemometric tools, and when the sensor compares patterns from a series of samples, the acquired differences can be correlated with perceived aromas [15].

The E-tongue is based on the tongue's ability to differentiate between distinct taste qualities, such as sourness, saltiness, sweetness, bitterness, and umami. E-tongue is a non-specific sensor composed of sensing elements, including enzymes, lipids, and metallic particles, which have low selectivity but can analyse and differentiate between liquid samples based on their unique characteristics [16, 17]. The principle behind the E-tongue involves combining signals from specific, non-specific, and overlapping sensors with pattern recognition when detecting polyphenols and predicting sensory attributes. Similar to human taste receptor cells, amperometry sensors composed of metals, conducting polymers, phthalocyanine films, and biosensors analyse the sensory properties of food instead of sensory receptors. The sensors then release data on food properties, which is ultimately interpreted as perceived taste [18].

3.2 Gas chromatography and mass spectrometry

GC is a separation technique used to analyse volatile and semi-volatile compounds. In GC, analytes are vaporised and transported by an inert carrier gas through a capillary column containing a stationary phase, where compounds are separated based on their volatility and interactions with the column phase. The components of a sample are separated by dissolving and vaporising them within the GC system, using two phases: the stationary and mobile phases [19]. The advantages and disadvantages of GC are summarised in Table 1.

Table 1. Advantages and disadvantages of gas chromatography

Advantages of gas chromatography	Disadvantages of gas chromatography
High efficiency, allowing rapid analysis due to fast separation [20].	Requires analytes to be sufficiently volatile or derivatised prior to analysis [21].
Adaptable for various applications, such as environmental monitoring and safety through different detectors and stationary phases [19].	Unsuitable for analysing samples degraded at elevated temperatures, as the analyte may decompose [22].
High quantitative accuracy [23].	Requires thermal stability to prevent temperature fluctuations during analysis [21].
Requires small sample sizes, usually less than 1 mL, and can detect extremely low concentrations [24].	Time-consuming and requires specialised expertise due to intricate data interpretation [23].
High sensitivity in detecting components in complex mixtures [23].	Limited to low-to-medium molecular weight compounds [22].

MS is a powerful technique used for identifying novel molecules, quantifying known compounds, and elucidating the structural and chemical properties of various substances [25]. Mass spectrometry (MS) is an analytical technique that identifies compounds by measuring the mass-to-charge ratio of ionised molecules. In MS analysis, compounds are ionised, fragmented, and separated in a mass analyser, generating characteristic mass spectra that enable compound identification. The advantages and disadvantages of MS are summarised in Table 2.

Table 2. Advantages and disadvantages of mass spectrometry

Advantages of mass spectrometry	Disadvantages of mass spectrometry
Rapid analysis with ultrafast liquid chromatography and high-throughput techniques, enabling quick evaluation of multiple compounds [26].	Data interpretation can be affected by matrix effects or co-eluting substances [27].
Enables both quantitative and qualitative analysis, ensuring accurate concentration measurements and molecular identification [26].	High initial instrument costs [28].
Enables tentative compound identification via spectral library matching; confirmation may require reference standards or additional methods [29].	Requires highly skilled personnel due to its technical complexity [28].
Versatile, with applications in forensic science, toxicology, and metabolomics [27, 30].	Complexity of MS-based methods and lengthy execution times make them impractical for routine clinical use [28].
High sensitivity and selectivity, allowing detection of compounds at low concentrations, making it ideal for complex sample analysis [26].	Limited sample throughput, requiring additional processes or alternative analytical methods for high-volume testing [28].

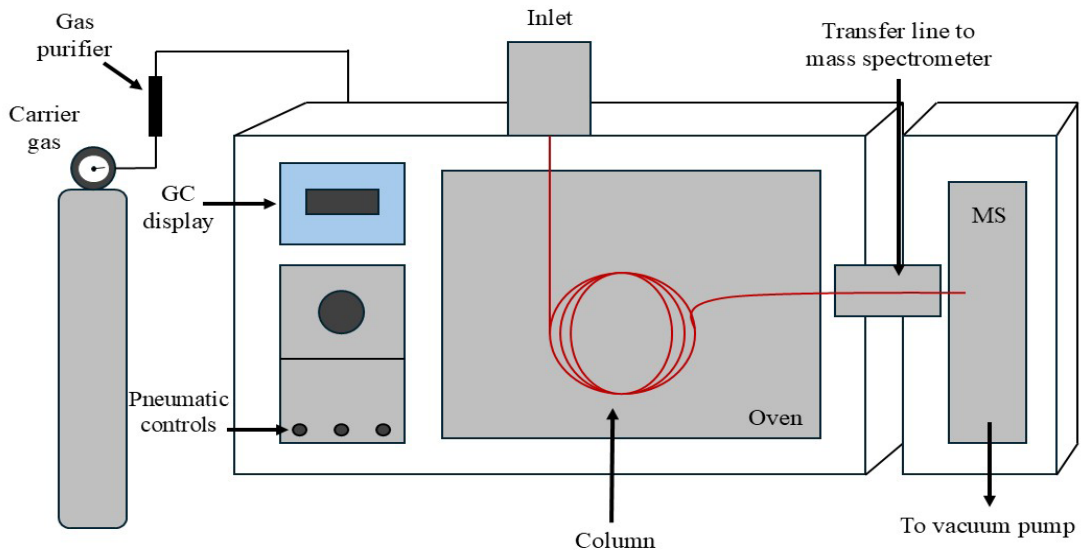

Figure 2. The GC-MS instruments

GC-MS plays a crucial role in flavour analysis, offering unmatched capabilities for identifying and characterising volatile and semi-volatile flavour compounds. GC separates complex mixtures by exploiting differences in boiling points, allowing individual flavours to be analysed sequentially [31]. Once separated, the compounds enter the MS system, where they are ionised and fragmented to generate unique mass-to-charge ratio fingerprints for identification [32], as shown in Figure 2. This synergy enables precise identification of specific flavour compounds and their relative abundance.

In flavour analysis, volatile compounds are often

extracted prior to GC-MS analysis using techniques such as SPME or SBSE. These extraction approaches allow the analysis of both known aroma compounds and broader volatile profiles present in food samples. However, the complexity of food matrices can present analytical challenges, including matrix effects, co-elution of compounds, and uncertainties in compound identification. As a result, confirmation of compound identities often requires comparison with reference standards or retention indices [7].

3.3 High-performance liquid chromatography

High-performance liquid chromatography (HPLC) is a technique used to separate, identify, and quantify components within a mixture using the principles of column chromatography. It is an advanced form of liquid chromatography in which solvents are forced through a column under high pressure, up to 400 atmospheres. In HPLC, separation occurs in a separation column, where the stationary phase consists of granular materials with minute porous particles, and the mobile phase comprises solvents moving under high pressure. The sample is injected into the mobile phase and transported through the separation column, where different components interact with the stationary phase at varying degrees. A detector then records the separated components, and the resulting chromatogram allows for identification and quantification [33]. In flavour research, HPLC-based systems such as HPLC-UV or LC-MS are commonly used to analyse non-volatile taste compounds, including organic acids, polyphenols, peptides, and other polar metabolites present in complex food matrices. The advantages and limitations of HPLC are presented in Table 3.

Table 3. Advantages and disadvantages of high-performance liquid chromatography

Advantages of HPLC	Disadvantages of HPLC
Provides rapid results, improving efficiency in laboratories [34].	High equipment and operational costs, limiting access to HPLC in some laboratories [35].
Versatile and precise in identifying and quantifying chemical components [33].	Requires skilled personnel for operation and maintenance due to its complexity [35].
High resolution and reproducibility, allowing efficient compound separation [36].	Low sensitivity for certain compounds, meaning some substances may not be detected [33].

3.4 Comparison of GC-MS and HPLC

GC-MS and liquid chromatography-based techniques differ in their analytical principles and typical applications. Both techniques rely on pressure-driven flow for separation; however, GC uses an inert carrier gas to transport vaporised compounds through the column, whereas HPLC employs high-pressure liquid solvents to achieve separation. GC-MS integrates chromatographic separation with mass spectrometric detection for volatile compounds. Similarly, liquid chromatography can also be coupled with mass spectrometry (LC–MS) for compound identification, particularly for non-volatile and thermally labile compounds. In contrast, HPLC is primarily a separation technique and is commonly coupled with detectors such as ultraviolet (HPLC–UV) or mass spectrometry (LC–MS) for compound identification and quantification. These LC-based systems are particularly suitable for analysing non-volatile, thermally labile, or highly polar compounds in complex food matrices [31].

Since chromatography itself performs compound separation, reliable compound identification typically requires coupling with appropriate detection systems such as UV detectors or mass spectrometry. Due to these differences, GC-MS is widely used for analysing volatile aroma compounds like aldehydes, esters, and terpenes found in essential oils, fruits, and spices. Meanwhile, HPLC-based systems are better suited for analysing non-volatile or thermally labile taste compounds dissolved in liquid solvents prior to analysis, including organic acids, polyphenols, and amino acids, which contribute to sensory attributes such as bitterness, astringency, sweetness, and umami [37].

In flavour analysis, GC-MS is ideal for detecting volatile compounds in fresh and processed foods, while HPLC is preferred for non-volatile taste components. For complex food matrices, both techniques are often combined to achieve a complete flavour profile [38]. Given the diversity of available platforms, a comparative evaluation of their performance metrics is essential for informed method selection.

In practical flavour studies, volatile compounds are

commonly extracted prior to GC-MS analysis using techniques such as SPME or SBSE. These approaches allow efficient concentration of volatile molecules from complex food matrices before chromatographic analysis. For example, in coffee aroma research, SPME coupled with GC-MS has been widely applied to characterise volatile compounds responsible for coffee aroma. Studies have identified furans and pyrazines as the predominant classes of volatile compounds contributing to the characteristic roasted, caramel, and nutty aroma notes of coffee [39].

3.5 Critical comparative assessment of instrumental platforms

For both research and industrial flavour analysis, a careful comparison of instrumental platforms is necessary to assist well-informed method selection. Their usefulness is significantly impacted by differences in sensitivity, reproducibility, cost, analytical throughput, and suitability for volatile and non-volatile substances. A comparison of critical performance metrics for the main analytical platforms used in flavour profiling is shown in Table 4.

Table 4. Comparative evaluation of instrumental platforms for flavour analysis

Technique	Sensitivity	Reproducibility	Cost	Throughput	Ideal for	Key limitations	References
GC-MS	High	Moderate to High	High	Low to Moderate	Volatile aroma compounds	Requires volatile samples; thermal degradation risk; skilled operator needed	[22]
HPLC–UV/ LC–MS	Moderate	High	High	Low to Moderate	Non-volatile, polar, thermally labile compounds	Less suited for volatile aromas; often requires derivatisation	[40]
E-nose/ E-tongue	Low to Moderate	Low to Moderate	Low to Moderate	High	Rapid screening, real-time monitoring	Sensor drift; affected by environment; qualitative more than quantitative	[15]
Ambient MS (e.g., DART)	Moderate	Moderate	Moderate	High	Rapid, minimal prep screening	Limited quantitative reproducibility; database dependency	[41]
SPME-GC-MS	Very High	Moderate	Moderate	Moderate	Trace-level volatiles	Fibre variability; sample carryover; optimisation required	[42]

GC-MS remains the benchmark technique for volatile aroma analysis due to its high sensitivity, comprehensive spectral libraries, and strong separation capability for complex mixtures [22]. However, column ageing, detector drift, and variations in sample preparation techniques, especially during solid phase microextraction fibre conditioning, may have an impact on reproducibility. Although the identification of trace-level aroma-active chemicals frequently necessitates derivatisation, which increases analytical complexity and processing time [43], HPLC remains widely used for the analysis of non-volatile taste-related compounds, including polyphenols, amino acids, and organic acids [37]. Ambient ionisation mass spectrometry techniques such as Direct Analysis in Real Time (DART) and Desorption Electrospray Ionization (DESI) enable rapid chemical profiling with minimal sample preparation. These techniques ionise compounds directly from sample surfaces under atmospheric conditions, allowing fast screening of food samples. However, their applications in flavour analysis are often limited by lower quantitative reproducibility and dependence on spectral databases for compound

identification [44].

E-nose and E-tongue are frequently used for real-time monitoring in industrial settings because they provide quick, high-throughput screening [15]. Although they have potential for process control due to their ease of deployment and comparatively low cost, sensor responses are sensitive to environmental conditions such as temperature and humidity. Furthermore, the need for regular recalibration limits cross-laboratory standardisation and lowers long-term stability [45].

Overall, this comparative evaluation demonstrates that no single analytical platform is universally optimal for flavour profiling. More accurate and thorough flavour characterisation is frequently produced by integrated analytical techniques, such as combining targeted GC-MS confirmation with electronic sensor screening. In industrial applications, practical considerations such as operational cost, staff training requirements, and analysis time frequently outweigh maximal analytical resolution. These factors emphasise the significance of structured method-selection frameworks that strike a compromise between analytical rigour and practical feasibility when dealing with complex food matrices.

While each analytical technique offers distinct advantages, its suitability is highly dependent on the intended application. For rapid screening and real-time monitoring, E-nose systems provide fast and cost-effective analysis, although they lack compound-specific identification. In contrast, GC-MS remains the preferred approach for regulatory and confirmatory analysis due to its high sensitivity and ability to identify individual volatile compounds. HPLC-based techniques are more suitable for non-volatile and thermally labile compounds. Therefore, the optimal analytical strategy is not universal but application-driven, requiring a balance between speed, sensitivity, cost, and analytical specificity [22].

3.6 Integration of chemometrics and machine learning with instrumental data

Building on these instrumental foundations, the integration of chemometrics and machine learning represents a shift from descriptive to predictive flavour analysis [46]. Principal Component Analysis and Partial Least Squares Regression are two chemometric techniques that make it possible to uncover significant patterns from complex datasets generated by chromatography-based methodologies and electronic sensing platforms [47]. These methods improve classification, prediction, and feature selection when paired with machine learning algorithms such as Random Forest, Support Vector Machines, and neural networks.

Key aroma active chemical identification, sensory score prediction, and geographical origin authentication are examples of practical applications. For example, by identifying volatile indicators, machine learning models applied to GC-MS data have successfully categorised olive oil sources with above 95% accuracy [48]. Unsupervised methods help to visualise sample groupings and spot anomalies, whereas supervised approaches correlate chemical profiles with sensory qualities. Predictive flavour analysis typically follows a structured workflow involving the acquisition of analytical data, such as GC-MS spectra or sensor responses, followed by data pre-processing and feature extraction prior to model development. Machine learning algorithms are then trained and validated using independent datasets before being applied to predict the flavour profiles of new samples. However, accurate prediction remains challenging due to the inherently multimodal nature of flavour, where chemical composition, sensory perception, and human subjectivity are closely interconnected. Unlike other omics fields, flavour perception is influenced by complex interactions among compounds, making prediction less straightforward and requiring the integration of both chemical and sensory datasets to improve reliability [46].

Despite these advancements, difficulties remain. Machine learning models frequently demand big, curated datasets, which are limited in flavour science. Industrial adoption is hampered by problems with cross-platform reproducibility, overfitting with limited samples, and model interpretability (commonly referred to as "black box" effects) [49]. Although machine learning has been increasingly applied in flavour analysis, the issue of model interpretability remains a significant challenge. To address the "black box" nature of complex models, interpretability approaches such as SHAP (Shapley Additive Explanations) and LIME (Local Interpretable Model-Agnostic Explanations) have been introduced, allowing the contribution of individual variables to model predictions to be examined more clearly [50]. Moreover, the selection of machine learning algorithms should be aligned with the type of flavour data being analysed. Deep learning approaches are generally more suitable for handling high-dimensional datasets such as GC-MS spectra, whereas conventional models, including support vector machines and random forests, are often more effective for structured datasets such as electronic nose sensor responses [50]. Therefore, appropriate model selection should consider data complexity, interpretability requirements, and the specific objectives of the analysis. Improved data sharing, explainable AI frameworks, and hybrid modelling techniques that incorporate sensory, chemical, and processing elements are essential for future advancements. Overall, these analytical and computational approaches collectively demonstrate the transition towards a more integrated and data-driven framework in flavour analysis.

4. FlavorDB and the role in flavour analysis

FlavorDB provides insights into the chemical composition of flavour molecules found in various food sources, offering detailed information essential for flavour analysis and exploration. As a curated database containing over 25,000 flavour molecules, FlavorDB integrates data from authoritative sources such as *Fenaroli's Handbook of Flavour Ingredients* and contemporary scientific literature, serving as a bridge between traditional flavour knowledge and modern computational research [8]. FlavorDB facilitates a comprehensive understanding of aromatic compounds, encompassing their chemical structure, sensory profiles, and potential health implications. Additionally, it serves as a valuable resource for taste compounds, stimulating research, fostering scientific breakthroughs, and driving innovation in ingredient combinations. Furthermore, its systematic organisational structure enhances data management and retrieval, enabling users to explore the intricacies of the flavour landscape with precision and efficiency [8, 51].

Databases such as FlavorDB play a critical role in this data-driven landscape, providing curated chemical and sensory data essential for machine learning-enabled flavour prediction. Distinctive flavour profiles encompass a variety of sensory characteristics, such as flavour and aroma, elevating the gastronomic experience to new levels of complexity and enhancing the appeal of food and beverages, ultimately increasing consumer satisfaction [4]. In the realm of flavour science and within the era of Food Flavour Analysis 4.0, understanding the distinct physicochemical properties of individual flavour molecules is paramount. Databases serve as meticulous repositories, documenting these variations alongside the natural origins and sensory responses elicited by these molecules [8].

FlavorDB interprets data by integrating different dimensions of flavour from the 'entity space' and 'flavour space'. The entity space incorporates facets of ingredients, representing entities from natural sources commonly used in food, whereas the flavour space consists of molecules responsible for flavour sensation and their descriptions. Through this, the database provides a comprehensive dataset via a user-friendly interface, creative visualisations, and interlinked search engines that facilitate the exploration of food characteristics contributing to flavour sensation. Thus, it paves the way for compounds with biological system applications and allied uses [8].

5. Role of food flavour analysis

Flavour analysis extends beyond simple component identification, employing comprehensive approaches to unravel the subtle interactions of chemical constituents that contribute to flavour perception [52]. Driven by the demand for high-sensitivity and user-friendly techniques, contemporary food analysis prioritises the development of simple yet powerful sensing tools for the comprehensive identification of both volatile aroma and non-volatile flavour components within a food sample. These analyses frequently rely on established methods such as GC-MS and HPLC [53]. Sensory evaluation, wherein human taste and smell play a critical role, further validates these analytical results. Flavour analysis provides valuable insights for quality control by ensuring consistent flavour profiles across production batches. Additionally, it empowers researchers and manufacturers to unravel the complexities of specific flavours, facilitating targeted manipulation and innovation in product development.

5.1 Standardisation challenges

To summarise, flavour analysis plays a critical role in ensuring the quality, safety, and sensory attributes of food products. By employing a variety of analytical techniques, such as gas chromatography-mass spectrometry, scientists can identify and quantify volatile compounds responsible for flavour and aroma, ultimately enhancing flavour profiles and increasing consumer satisfaction. However, the reproducibility of these analyses across multiple laboratories and experimental setups is still a considerable difficulty [54]. Comparative research and industrial quality control are hindered by inconsistent results that are frequently caused by variations in sample preparation, equipment calibration, data processing, and operator experience.

Differences in SPME fibre conditioning, GC column ageing, detector sensitivity drift, and the absence of widely recognised reference materials for complex food matrices are major causes of irreproducibility. Even well-known techniques like GC-MS and HPLC produce data that is challenging to compare or validate among research groups in the absence of standardised methodologies [55]. This is especially difficult when creating large-scale flavour databases for machine learning applications and in regulatory contexts. The development of standardised benchmark datasets is hindered by several technical challenges, including matrix effects, variability in sample preparation, and the instability of reference standards. Differences in instrumentation and analytical conditions across laboratories further contribute to reproducibility issues, limiting the comparability of results [56].

To solve these challenges, numerous practical solutions are proposed. First, cross-laboratory calibration and technique validation would be made possible by globally recognised benchmark datasets that include well-characterised food extracts with validated concentrations of important flavour constituents [57]. Second, academic, business, and regulatory parties should work together

to create standard operating procedures (SOPs) for data reporting, instrument settings, and sample preparation. Third, open-access, quality-controlled flavour databases supplemented with metadata on analytical circumstances would increase transparency and data reuse.

Furthermore, the integration of artificial intelligence technologies for automated quality control, such as signal alignment, predictive calibration, and outlier identification, may reduce human-related variability and enhance flavour profiling's overall dependability [58]. Therefore, emphasising standardisation and reproducibility will aid in the creation of frameworks for flavour analysis that are more reliable, compatible, and applicable to industry.

5.2 Sustainable approaches in flavour profiling

In order to lessen ecological impact, flavour analysis is increasingly using green analytical chemistry principles as part of the growing emphasis on environmental responsibility. Sustainable techniques aim to preserve analytical performance while reducing the usage of solvents, energy, and waste.

Solvent-free microextraction techniques, such as SPME and SBSE, are important green technologies that eliminate or significantly minimise the need for organic solvents [59]. Compared to traditional petroleum-based solvents, bio-based solvents made from renewable resources are more environmentally friendly. Furthermore, ambient mass spectrometry methods save energy and solvent use by enabling quick analysis with minimal sample preparation [41].

By identifying the flavour characteristics in waste streams and byproducts, flavour analysis also helps to value upcycled food ingredients and promotes circular food economies. To ensure that flavour profiling develops in an environmentally friendly way, future advancements should keep including sustainability indicators into technique validation [60].

Although green analytical techniques such as solid-phase microextraction (SPME) reduce solvent use and environmental impact, they may present limitations in sensitivity and reproducibility compared to conventional solvent-based extraction methods [61]. Additionally, the adoption of sustainable analytical approaches in industry is often constrained by equipment cost, scalability, and compatibility with existing workflows. Therefore, the implementation of green techniques requires careful consideration of the trade-offs between environmental benefits and analytical performance [62].

5.3 Industrial applications and molecular insights

Flavour analysis is essential for industrial product development, quality control, and innovation, especially in response to growing consumer demand for novel and sustainable foods.

In plant-based meat development, flavour optimisation focuses on key volatile compounds such as aldehydes (e.g., hexanal), ketones, and pyrazines, which contribute to desirable meaty and roasted notes. GC-MS has been widely used to identify undesirable compounds associated with lipid oxidation and plant-derived off-flavours, such as beany or grassy notes. These analytical findings enable targeted reformulation strategies, including ingredient modification and processing optimisation, to suppress off-flavours and enhance desirable aroma profiles. Such improvements have been reported to enhance sensory acceptance and consumer preference of plant-based products [63]. Similarly, in functional food systems, plant-derived bioactive compounds such as phenolics and essential oils are utilised not only for their antioxidant activity but also for their contribution to flavour enhancement and product stability. Their incorporation has supported the development of clean-label products with improved shelf life and consumer appeal [64]. These examples demonstrate how analytical techniques directly guide formulation decisions and contribute to improved product quality and market acceptance.

In industrial practice, flavour profiling guides the development of products such as plant-based meats, functional beverages, and clean-label foods [44]. HPLC helps maximise bitterness in functional teas [65], and GC-MS is utilised to discover important aroma compounds that mimic meaty notes in plant-based substitutes [66]. Real-time quality monitoring in manufacturing is made possible by electronic noses and tongues, which guarantee consistency and early detection of off flavours [67], alongside emerging nanomaterial-based immunosensors for contaminant detection [68].

At both the molecular and processing levels, flavour analysis reveals the chemical and physical foundations of sensory attributes. Studies on coffee roasting track Maillard reaction products like pyrazines and furans, which contribute to roasted flavours [38]. In fermented dairy, dynamic changes in esters and acids are monitored to control flavour development. Understanding these pathways allows for precise manipulation during processing, improving both flavour and nutritional quality [69]. Similarly, processing techniques such as enzyme pretreatment and drying can influence flavour retention and release in cereal-based products, affecting overall sensory perception [70].

The integration of databases such as FlavorDB and machine learning models supports these applications by providing predictive tools for flavour pairing and compound discovery [8]. Together, these approaches bridge molecular insight with industrial application, enabling the creation of innovative, sensorially appealing, and sustainable food products. Collectively, these developments emphasise the integration of analytical

techniques, molecular insights, and computational tools in shaping a more comprehensive and data-driven flavour analysis framework.

From an industrial standpoint, the implementation of advanced analytical techniques requires careful cost–benefit evaluation. Although GC-MS offers high analytical precision, its substantial cost and operational complexity may restrict its use, particularly among small and medium enterprises (SMEs). In comparison, electronic nose systems provide a faster and more cost-effective alternative, albeit with reduced specificity. Therefore, selecting an appropriate analytical approach involves balancing analytical accuracy, cost considerations, and application needs.

6. Conclusion

This review has traced the journey from molecular fingerprinting to predictive flavour science, highlighting the convergence of instrumental analysis, AI, and sustainability as the foundation of next-generation food systems. The analysis of food flavour compounds has evolved into an integrated discipline where instrumental techniques, chemometrics, and artificial intelligence converge to enable predictive and sustainable flavour profiling. This review has critically evaluated the progression from traditional to data-driven flavour science, emphasising the integration of chemometrics, machine learning, and sustainable practices within Food Flavour Analysis 4.0. This review highlights that while GC-MS and HPLC remain central for characterising volatiles and non-volatiles, challenges in reproducibility, cost, and standardisation persist, necessitating harmonised protocols and open access databases.

The synergy of machine learning with flavour data accelerates the shift from descriptive analysis to predictive design, enhancing applications in authenticity, product development, and quality control. Concurrently, green analytical approaches, including solvent-free microextraction and bio-based solvents, align flavour science with sustainability goals. Furthermore, addressing standardisation through benchmark datasets and AI-validated frameworks is essential for reproducible, industrially applicable analysis. Moving forward, the integration of molecular insights, computational tools, and industrial practice will drive innovation in creating sensorially appealing, safe, and environmentally conscious foods, positioning flavour analysis as a cornerstone of future food systems.

Future research in Flavour Analysis 4.0 should focus on several key priorities. First, the development of explainable artificial intelligence models is essential to improve the interpretability and reliability of predictive flavour analysis. Second, the establishment of standardised and interoperable flavour databases is needed to enhance data consistency and cross-platform integration. Third, the integration of multimodal datasets, including chemical, sensory, and omics data, will enable more comprehensive and accurate flavour prediction. Additionally, advancements in real-time monitoring technologies and automation should be explored to support scalable and efficient industrial applications. Addressing these areas will be critical to advancing the robustness, applicability, and adoption of flavour analysis technologies in the food industry.

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CRediT authorship contribution statement

Shyang Pei Hong: Formal analysis, Conceptualization, Methodology, Validation, Resources, Data curation, Writing –review & editing, Supervision, Project administration, Funding acquisition. Nur Wardina Abu Bakar: Writing –review & editing. Phuah Eng Tong: Writing –review & editing, Ummul Hasanah Hassan: Writing –review & editing, Yie Hua Tan: Conceptualization, Kae Jye Si: Validation.

Conflicts of interest

The authors declare no conflicts of interest.

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