chemosensors

Review

From Volatile Profiling to Sensory Prediction: Recent Advances in Wine Aroma Modeling Using Chemometrics and Sensor Technologies

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Abstract

Wine quality is closely linked to sensory attributes such as aroma, taste, and mouthfeel, all of which are influenced by grape variety, "terroir", and vinification practices. Among these, aroma is particularly important for consumer preference, and it results from a complex interplay of numerous volatile compounds. Conventional sensory methods, such as descriptive analysis (DA) performed by trained panels, offer valuable insights but are often time-consuming, resource-intensive, and subject to individual variability. Recent advances in sensor technologies—including electronic nose (E-nose) and electronic tongue (E-tongue)—combined with chemometric techniques and machine learning algorithms, offer more efficient, objective, and predictive approaches to wine aroma profiling. These tools integrate analytical and sensory data to predict aromatic characteristics and quality traits across diverse wine styles. Complementary techniques, including gas chromatography (GC), near-infrared (NIR) spectroscopy, and quantitative structure–odor relationship (QSOR) modeling, when integrated with multivariate statistical methods such as partial least squares regression (PLSR) and neural networks, have shown high predictive accuracy in assessing wine aroma and quality. Such approaches facilitate real-time monitoring, strengthen quality control, and support informed decision-making in enology. However, aligning instrumental outputs with human sensory perception remains a challenge, highlighting the need for further refinement of hybrid models. This review highlights the emerging role of predictive modeling and sensor-based technologies in advancing wine aroma evaluation and quality management.

Keywords: wine aroma; sensory analysis; volatile compounds; chemometrics; predictive modeling; machine learning; quality control; chemosensors; off-flavors

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1. Introduction

Wine is a complex alcoholic beverage containing hundreds of compounds at varying concentrations. Its quality is a multidimensional concept shaped by the dynamic interplay of sensory attributes, with aroma playing a central role in consumer perception and preference. The aromatic profile results from a diverse range of volatile compounds—including esters, alcohols, acids, aldehydes, and terpenes—whose presence and concentration are influenced by grape variety, "terroir", fermentation, and aging processes [1].

Quality assessment is traditionally carried out through sensory evaluation by trained experts, who assess flavor, taste, and color throughout the production process. While such evaluations provide valuable insights, they are costly, time-consuming, and not always readily available. As a complement, chemical methods such as gas chromatography, liquid chromatography, and spectrophotometry are used to identify and quantify specific components. Nonetheless, the inherent complexity of wine poses challenges for chemical analysis, as even minor variations in compound concentrations—or interactions among them—can significantly affect sensory characteristics [2].

Recent technological advancements have enabled more objective and efficient evaluation of wine aroma. Instrumental tools such as E-nose and E-tongue, inspired by human sensory systems, have shown strong potential in detecting complex chemical signatures. However, these devices are not yet fully accurate analytical instruments and remain limited in their ability to replicate the subtleties of human perception. While they cannot yet replace sensory panels, E-tongue and E-nose offer valuable supplementary data for profiling aroma and flavor in food and beverages. When combined with chemometric techniques and machine learning algorithms, these sensor-based systems facilitate the integration of chemical and sensory data, enabling predictive modeling of aroma attributes and overall wine quality.

To address the gap between instrumental outputs and human perception, hybrid modeling strategies can be applied through multisensor fusion [3–5]. At the feature level, raw or preprocessed outputs from multiple modalities (e.g., E-nose combined with E-tongue) can be merged into a single dataset prior to model training, enabling algorithms such as PLSR or Support Vector Machines (SVM) to capture cross-modal patterns linked to sensory descriptors [3,4,6,7]. At the decision level, independent models can be developed for each sensor type, with their predictions combined through weighted voting or Bayesian inference to enhance classification and quantification accuracy [8]. Calibration transfer can also be achieved by using sensory panel scores as reference labels while applying methods like multiblock PLS or canonical correlation analysis (CCA) to align sensor signals with human perception despite threshold variability [9,10]. For dynamic aroma or flavor release, time-series alignment between sensor response curves and temporal sensory data can further refine predictive performance under real consumption conditions [10,11].

In this context, predictive modeling offers a powerful approach to link chemical profiles with sensory outcomes, enabling more objective, reproducible, and efficient assessments. Advances in chemometrics and sensor technologies such as E-nose, E-tongue, and spectroscopy, coupled with machine learning, provide promising tools to decode volatile complexity and move towards accurate volatile-to-sensory prediction [12].

A major challenge in applying machine learning effectively is the availability of sufficient, high-quality data for model training. This issue is particularly difficult in wine aroma research, given the scarcity and heterogeneity existing databases [13–16]. While wine quality is ultimately judged by human perception, typically evaluated by trained expert panels who assign scores across multiple attributes, the outputs of E-nose and E-tongue, being inspired by human senses, could theoretically correspond to these scores. However, establishing such correlations is difficult because electronic senses detect all chemical compounds, not just those perceived by humans, and sensory perception does not always scale proportionally with compound concentration. Moreover, synergistic interactions among compounds and textural factors such as astringency or viscosity further complicate these relationships. Despite these challenges, with carefully designed sensor arrays and appropriate chemometric tools such as PLS regression, strong correlations with sensory scores or specific aromas attributes have been demonstrated [14]. Table 1 summarizes the technological evolution of E-nose and E-tongue systems.

Table 1. Advances in E-nose and E-tongue technologies.

Year/Period	Technology	Contribution/Development	Notes	References
Early 1900s	E-nose (concept)	Demonstrated detection of small amounts of aromatic compounds by non-biological means	Early concept of artificial olfaction	[17]
1954	E-nose	First odor measurement tool: microelectrode (platinum wire) and millivoltmeter	First instrumental approach	[18]
Late 1950s	E-nose	Mechanical olfactory system discriminating between simple and complex aromas	Early mechanical sensing	[19,20]
1979	E-nose	Introduction of acoustic wave chemical vapor sensors	Bulk Acoustic Wave and Surface Acoustic Wave sensors, operating at 1–500 MHz	[21]
1982	E-nose	First intelligent artificial nose with three metal oxide sensors, identifying up to 20 odorants	Milestone in E-nose development. Defined E-nose as sensor array and pattern recognition	[22]
Mid-1980s	E-nose	Integrated sensor with 6 metal oxide semiconductors	Quantified and identified scents s	[23]
1985	E-tongue	First liquid analysis system using a sensor array	Foundation of E-tongue technology	[24]
1988	E-nose	Coined the term “electronic nose”	Standard terminology established	[25]
1990	E-tongue	First system with partially selective sensors for qualitative liquid analysis	Enabled classification of liquids	[26]
1990	E-tongue	Pioneering concept of taste sensors	Marked the start of modern E-tongue development	[27]
Early 1990s	E-tongue	“E-tongue” using potentiometric electrodes with non-specific and cross-sensitive sensors	Key E-tongue breakthrough	[28]
1990s	E-tongue	Active global research on liquid sensor arrays	Enabled commercialization around 2000	[29]
Early 1990s	E-nose	First commercial electronic noses	Market introduction	[30,31]
1997	E-tongue	Voltammetric E-tongue with multiple metal electrodes reference, and auxiliary electrodes	Expanded sensing materials. Added reference and auxiliary electrodes	[32,33]
1990s–Present	E-tongue	Development of multiple operational modes: electrochemical, enzymatic, optical, and mass-based	Tailored sensor arrays for target samples	[34]
1990s–Present	E-tongue	Widespread use of potentiometric E-tongues (ion-selective electrodes)	Cost-effective, flexible, high selectivity; limited by temperature and adsorption effects	[35]
1990s–Present	E-tongue	Development of voltammetric sensors for redox-active constituents	High selectivity, low detection limits; limited by temperature fluctuations and surface degradation	[36]
2000s	E-nose	Portable E-nose developed	Enabled on-site analysis	[37]
Early 2000s	E-tongue	Introduction of impedimetric E-tongues	No reference electrode required; chemosensitive electrodes	[38]

Table 1. *Cont.*

Year/Period	Technology	Contribution/Development	Notes	References
2010–2020	E-nose	Nanoparticle-based sensors with higher sensitivity/selectivity	Significant performance improvements	[21]
2010s	E-nose and E-tongue	Fusion of E-nose and E-tongue	Better classification accuracy	[39,40]
2000s–present	E-nose	Bioelectronic noses and tongues integrating biosensors into sensor arrays	Use same chemometric tools as conventional systems	[41–43]
Recent years	E-nose	Integration with gas chromatography (including ultrafast and miniaturized headspace GC)	Improved identification capabilities	[44–48]

This review examines the current state of predictive approaches in wine aroma analysis, with particular focus on sensor technologies and multivariate data analysis. The discussion highlights the potential of these tools to complement traditional sensory methods, improve quality control, and support decision-making in enology.

2. Profiling of Volatile Compounds in Wine

The profiling of volatile compounds is a fundamental component of wine aroma research, as these molecules play a decisive role in defining the sensory identity and overall character of a wine. They are key contributors to both aroma and flavor, and their presence, concentration, and complex interactions strongly influence consumer perception, preference, and the perceived quality of the final product [49,50].

The complexity of wine's volatile fraction arises from multiple sources, including grape variety, viticultural practices, microbial activity during fermentation, and aging processes [51–57]. Each of these factors contributes to the chemical diversity and sensory richness that define a wine's unique profile.

2.1. Origins and Chemical Diversity of Volatile Compounds

Volatile compounds in wine originate from grape metabolism, fermentation, and post-fermentation processes [53,58,59]. Each contributes distinct aromatic signatures that together define the wine's bouquet and overall sensory complexity [57] (Figure 1).

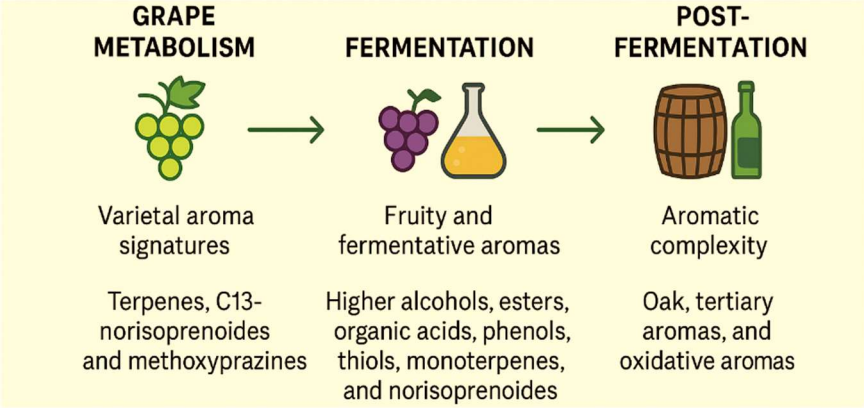


Figure 1. Evolution of volatile compounds during winemaking.

Grapes are the primary source of varietal aroma compounds [55,60], which are determined by the grapevine's genetic makeup and associated biochemical pathways [61]. During ripening, compounds such as terpenes, C13-norisoprenoids, and methoxypyrazines

accumulate in the grape berries, contributing to the varietal typicity of the resulting wine [62,63] (Figure 2). For instance, 'Muscat' and 'Gewürztraminer' grape varieties are particularly rich in monoterpenes such as linalool and geraniol, which impart their characteristic floral, citrus, and spicy aromas [62,64].

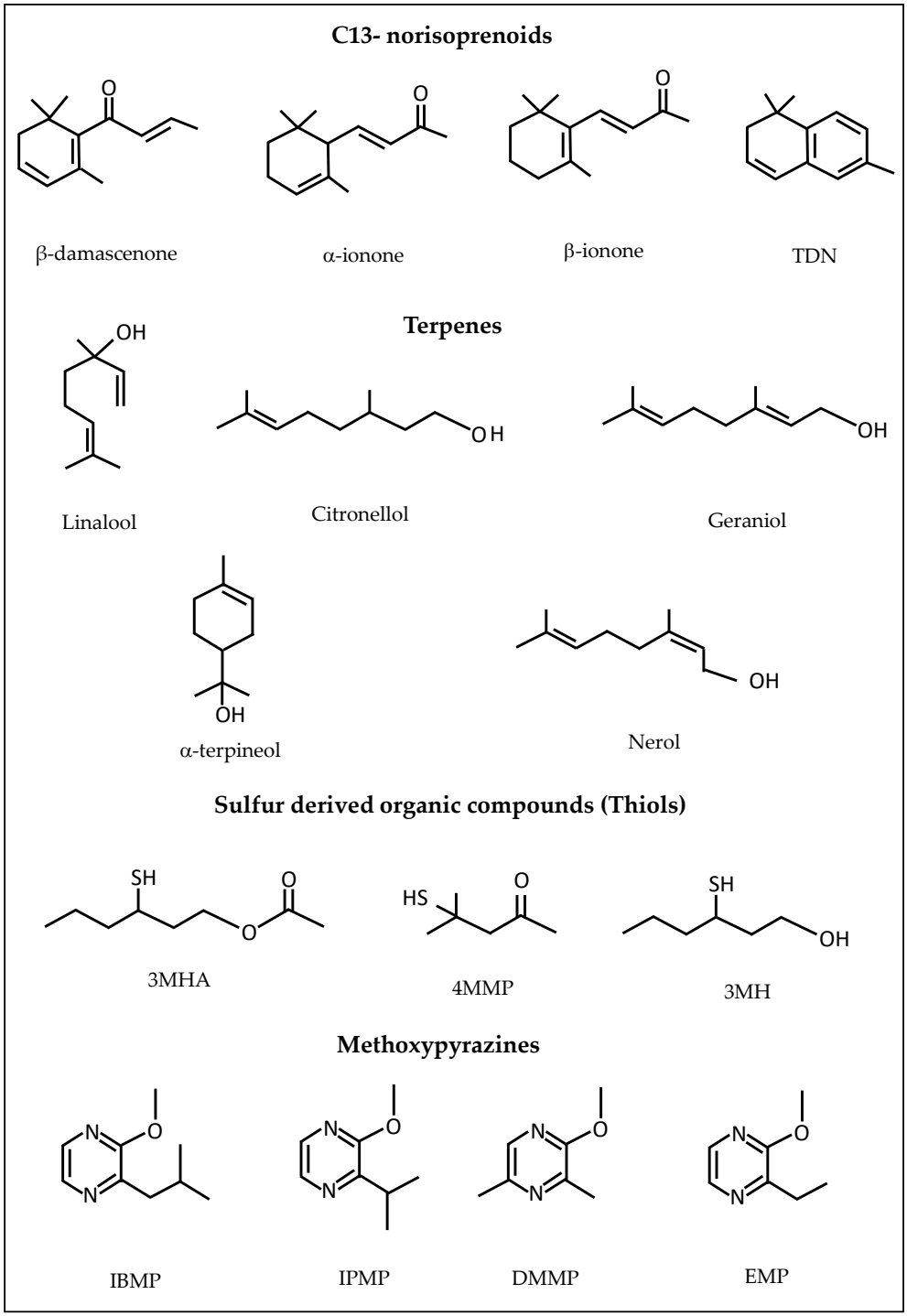


Figure 2. Chemical structures of key aromatic compounds present in grapes.

In addition to genetics, environmental factors, such as climate, soil ("terroir"), and viticultural practices, play a significant role in modulating the synthesis and expression of these compounds [65,66].

During alcoholic fermentation, *Saccharomyces cerevisiae* and other yeast species metabolize grape sugars, producing ethanol along with a diverse range of volatile compounds [67]. These include higher alcohols, esters, organic acids, phenols, thiols, monoterpenes, and norisoprenoids, all of which contribute significantly to the fruity and fermentative aromas of wine [59,68]. The specific yeast strain, fermentation temperature, nutrient availability, and oxygen exposure strongly influence both the type and concentration of volatiles produced [69]. For example, isoamyl acetate imparts banana-like aromas, whereas ethyl hexanoate contributes apple-like aromas [70]. Thus, yeast selection serves as a critical tool for modulating wine aromatic profile.

Following primary fermentation, additional processes further shape the aromatic complexity of wine. Malolactic fermentation, conducted by lactic acid bacteria, converts malic acid into lactic acid and produces buttery aromas (e.g., diacetyl) [71]. Oak aging introduces compounds such as vanillin, eugenol, and lactones, which contribute vanilla, spice, and woody notes [72,73]. Moreover, extended bottle aging promotes the development of tertiary aromas through gradual oxidation, esterification, and polymerization reactions, enhancing depth, complexity, and elegance in the final wine [74,75].

2.2. Classification of Volatile Compounds

Wine aroma results from a complex interplay of volatile compounds, which can be grouped into several chemical classes, each making a distinctive sensory contribution [50,76].

Among the most influential are terpenes, particularly monoterpenes such as linalool and geraniol, which are responsible for the floral and citrus nuances typical of aromatic varieties like 'Muscat' and 'Gewürztraminer' [77,78]. Their abundance is shaped by grape genotype, vineyard management, and winemaking techniques [53,79].

Esters, predominantly formed through yeast metabolism during fermentation, contribute to fruity and floral notes. Ethyl acetate and isoamyl acetate are prime examples, evoking ripe peaches, strawberries, and fragrant blossoms [80]. The balance of these compounds is critical, as moderate levels enhance the bouquet, whereas excess may lead to undesirable off-flavors [81,82].

Adding further complexity, volatile phenols such as eugenol and guaiacol impart spicy, smoky, or clove-like aromas. These compounds may originate from grape precursors or form during fermentation and maturation via microbial activity [83–85]. A related group, the volatile sulfur compounds, includes hydrogen sulfide and various mercaptans. In 'Sauvignon Blanc', specific thiols contribute tropical fruit and zesty citrus notes [86]; however, in excess, they can cause sensory defects reminiscent of rotten eggs or burnt rubber [87,88].

During fermentation, yeast also generates higher alcohols like propanol and isobutanol. At moderate levels, these enhance aromatic complexity, but at high concentrations, they can impart solvent-like aromas [89,90]. Other aroma-defining molecules include C_{13}-norisoprenoids, such as β-damascenone—formed from carotenoid degradation. These compounds are especially prominent in aged Riesling, where they add notable depth and richness [91]. Finally, methoxypyrazines, characteristic of 'Sauvignon Blanc', 'Cabernet Sauvignon', and 'Pinot Noir', lend herbaceous, green notes reminiscent of bell pepper and fresh-cut herbs [92,93].

Profiling volatile compounds is not only essential for understanding wine aroma but also plays a critical role in assessing and ensuring wine quality [94,95]. By correlating chemical profiles with sensory data, winemakers can identify the compounds responsible for both desirable and undesirable aromas, optimize production processes, and maintain consistent quality across vintages [96,97].

In summary, volatile compound profiling is a multifaceted process that integrates advanced analytical techniques with deep understanding of wine chemistry. It is fundamental to unraveling the complexity of wine aroma, supporting quality control, and driving innovation in modern winemaking.

2.3. Evolution of Volatile Compounds During Winemaking

A substantial proportion of volatile compounds are generated during alcoholic fermentation, primarily through the metabolic activity of the yeast *Saccharomyces cerevisiae*. These include esters, higher alcohols, volatile acids, and, to a lesser extent, certain terpenes and thiols [98–100].

For fermentation to proceed efficiently, yeasts require a nutritionally balanced environment. Deficiencies in essential nutrients—such as nitrogen and key vitamins like thiamine and pantothenic acid—are well-documented risk factor. Such imbalances can promote the growth of undesirable microorganisms and lead to sluggish or even stuck fermentations [101], often resulting in the formation of unwanted compounds that negatively affect the wine's sensory profile [102,103].

To mitigate nutritional deficiencies in grape must, optimize fermentation performance, and prevent technical issues that may compromise wine quality, winemakers often use yeast nutritional activators, also known as oenological nutrients [99,104–106]. These supplements typically contain a mixture of macro- and micronutrients, including assimilable nitrogen, vitamins, sugars, phosphorus, potassium, magnesium, calcium, copper, iron, manganese, and zinc [107]. Some formulations also incorporate yeast cell wall derivatives, which assist in toxin adsorption and help protect against fermentation stress [108].

The evolution of volatile compounds during winemaking and aging is a critical determinant of wine quality and sensory attributes. Compounds such as esters, terpenes, higher alcohols, and phenolics, make significant contributions to aroma and flavor [109], directly influencing consumer preferences and marketability. The interconnected origins of these aromatic compounds highlight the importance of each stage of wine production—from vineyard management to fermentation and aging—in crafting the final aromatic profile of the wine.

2.4. Chemical and Sensory Modifications of Wine During Aging

2.4.1. The Influence of Barrels, Wood Fragments, and Alternative Wood Species on Wine Quality

Wine aging is a practice used not only to extend shelf life but also to improve sensory characteristics. This stage is highly valued both for the qualitative improvements it imparts and for its commercial significance in the wine industry. Whether in barrels or bottles, aging profoundly modifies the volatile compound profile, contributing to the development of complex aromas [110,111].

The evolution of volatile compounds during aging is influenced by several factors, including temperature, oxygen exposure, light, microbial activity, storage time, and the wine's chemical composition [110]. As highlighted by Jordão and Cosme [111], the interaction between wine and barrel wood plays a key role in this process. The gradual transfer of phenolic and aromatic compounds from the wood, combined with the controlled ingress of oxygen through the pores, promotes chemical reactions that progressively enhance wine quality.

In recent years, some wineries have returned to the use of wooden vats for both fermentation and storage, recognizing the positive impact of wood on the final product. Studies have shown that conducting both alcoholic and malolactic fermentation in wooden barrels can enhance varietal expression and contribute to greater aromatic and gustatory complexity in red wines [112].

Aging wine in wooden barrels remains one of the most established oenological practice, contributing significantly to color stabilization and the enhancement of sensory properties. This process improves color intensity and stability while also enhancing mouthfeel—particularly volume and texture—resulting in a higher-quality final product. Moreover, barrels aging increases aromatic complexity, primarily due to the gradual extraction of compounds from the wood matrix.

Key components released during barrel aging include cellulose, hemicellulose, lignin, organic acids, sugars, terpenes, volatile phenols, and lactones (Figure 3). These compounds, which vary widely in molecular weight, interact with wine constituents and promote chemical reactions that profoundly influence the wine's sensory profile [110].

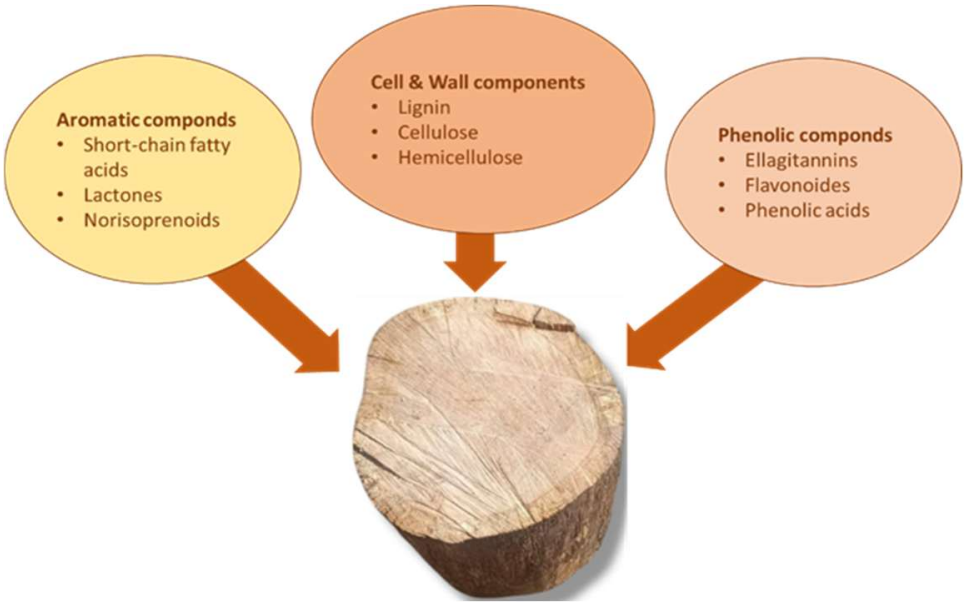


Figure 3. Main compounds present in the wood matrix.

The woods traditionally used in cooperage are mainly French or American oak, specifically from the species *Quercus petraea*, *Q. alba*, or *Q. robur*, as well as chestnut [111]. There are only species allowed for oenological use under Resolution OENO 4/2005 of the International Organization of Vine and Wine [113].

Nonetheless, other wood species are currently being investigated for their potential applications in winemaking, including brown robinia, ash, other oak species, and cherry wood [114–116].

Table 2 summarizes the main wood species used in cooperage and their associated effects on wine properties.

In recent decades, several scientific studies have investigated the impact of oak wood on the chemical composition, and sensory properties of wine, with particular focus on red wines, but also including rosé wines, white wines, and wine spirits [133]. This research covers both traditional practices, such as the use of barrels, staves, and wood powders, and alternative aging methods, including the incorporation of wood fragments in various shapes and sizes. The latter approach has become increasingly common in Europe, particularly after its authorization and regulation by the European Commission [134] and the OIV.

Table 2. Characteristics of the main wood species used in cooperage and their impact on wine properties.

Species	Chemical Composition	Resulting Wine Properties	References
Traditional Woods Used in Cooperage			
American oak (*Q. alba*) East USA	Contribution to whiskey-lactones	Slight risk of green taste, low tannin content, sugary character, fast wood intake	[117]
French oak (*Q. petraea or Q. robur*) North France	Higher content in phenols and flavonoids	Green taste with too short drying, high tannin content, limited aromatic contribution, slow wood intake	[117]
Non-traditional Woods in Cooperage from Oak Species			
Q. pyrenaica Western Atlantic–Mediterranean regions	Ellagitannins, low-weight compounds, and aromatic compounds	Higher aromatic intensity and complexity. Woody, balsamic and cocoa notes. High levels of eugenol, guaiacol, *cis*-β-methyl-γ-octalactone, and other volatile phenols	[118–121]
Q. faginea Iberian Peninsula and North Africa	Castalagin and vescalagin are the main ellagitannins	Wines related to trans-resveratrol, *p*-hydroxybenzaldehyde, syringic acid, ellagic acid, and 5–HMF	[122,123]
Q. frainetto Balkan Peninsula, South Italy, and Northwest Turkey	High content in ellagitannins	High bitterness and particular and indefinable aromas. The natural drying and toasting of the wood can cushion both attributes.	[124]
Q. humboldtii Colombia	Phenolic acids, aldehydes, and ellagitannins	Balanced syringaldehyde/vanillin relationship. Higher concentrations of 5-methylfurfural, guaiacol, isoeugenol, *trans*-isoeugenol, and syringol. Lower furfural, 5–HMF, trans-β-methyl-γ-octalactone, and cis-β-methyl-γ-octalactone content	[115,125]
Q. oocarpa South America	Monomers of ellagitannins	Regarding the gustatory aspect, it is similar to *Q. petraea*	[124]
Untraditional Woods in Cooperage: Different from Oak Species			
Castanea sativa Southern Europe and Asia	Low content of oxidizable polyphenols (less suitable for prolonged aging)	Higher content of total phenolic compounds and low molecular weight compounds. Higher antioxidant activities. Vanilla notes	[126,127]
Robinia pseudoacacia USA, Europe	Rich in mono and di-methoxyphenols, acetosyringone and ethyl vanillate. High content of simple volatile phenolic compounds	Red wines with higher smoky, spicy, and fruity notes	[128,129]
Fraxinus spp. Europe, Asia Minor, and North Africa	High content of 3-ethyl and 3,5-dimethylcyclotene, *o*-cresol, α-methylcrotonalactone, and vanillin. Low content of furanic derivatives	Less vanilla notes than oak	[128]

Table 2. *Cont.*

Species	Chemical Composition	Resulting Wine Properties	References
Morus spp. Asia, Africa, Europe, and North, Central, and South America	Decrease in fruity-note ethyl esters and ethyl-guaiacol and the high concentration of ethyl-phenol (a horsey-odor defect)	Hardly suitable for wine aging	[126,130]
P. avium and *P. cerasus* Europe and western Asia	Aromadendrin, naringenin, taxifolin, isosakuranetin, eriodictyol, and prunin	Greater oxygen penetration through their staves	[126,131,132]

These studies also explore the impact of different wood types—including oak, false acacia, and cherry—on the final chemical composition and sensory profile of various wine categories [135,136].

2.4.2. Influence of Extractable Wood Compounds on the Chemical and Sensory Profile of Wine

Wines may be aged in oak barrel or in contact with oak chips, and subsequently stored in bottles for varying periods depending on the desired style [137]. During aging, volatile compounds are extracted from the wood, significantly influencing the final sensory profile (Table 2). Among the most influential are phenolic aldehydes and phenylketones, particularly vanilla, which is strongly associated with vanilla aromas [138,139]. Vanillin is especially notable for its low sensory threshold and its significant contribution to the characteristic aroma of green wood [140].

Furanic compounds, such as furfural, 5-methylfurfural, hydroxymethylfurfural, and furfuryl alcohol, impart toasted and almond-like aromas [138]. Other important contributors include guaiacol, eugenol, methyl-4-guaiacol, ethyl-4-guaiacol, and phenol, which generate a wide range of sensory impressions including toast, smoke, spice, clove, burnt wood, and ink.

Maltol and related oxygenated heterocycles contribute caramelized and toasted aromas typical of aged wines [141]. Additionally, β-methyl-γ-octalactones, particularly the *cis* isomer, are responsible for coconut-like notes, with each isomer exhibiting distinct sensory thresholds [142]. Lactones form a significant class of aromatic compounds found not only in aged wines but also in other wood-aged alcoholic beverages such as cognac and whiskey [143].

Beyond their aromatic contribution, several extractable wood compounds also serve important technological roles. Notably, ellagitannins enhance the oxidative stability of wine due to their strong antioxidant properties [144,145].

2.4.3. Influence of Contact Time, Wood Type, and Barrel Condition on Wine Aging

The wood used in wine aging contributes not only volatile compounds but also non-volatile components, such as phenolic acids, coumarins, and ellagitannins. These compounds play a significant role in shaping wine structure and tactile sensations—namely, body and astringency—while also contributing to its preservation and long-term quality [110].

As reported by de Simón et al. [128], the botanical origin of the wood significantly affects both the intensity and nature of sensory attributes imparted to wine, since different species release compounds with distinct aromatic and structural properties. For example, oak-aged red wines are typically characterized by classic notes of vanilla, caramel, almond, and toast. False acacia, by contrast, enhances smoky, fruity, and spicy aromas; ash contributes balsamic notes; mulberry wood reduces fruity ethyl esters but increases

4-ethylphenol, associated with off-flavors such as leather and horse, while cherry wood promotes polyphenol oxidation, limiting its suitability for long-term aging [126,146–149].

The duration of wine contact with wood is another critical factor, directly affecting the extraction of compounds and thus the chemical and sensory profile of the wine. Compounds located closer to the barrel inner surface are extracted more rapidly, notable examples include linear γ- and δ-lactones, β-damascenone, and ionones, which are found across multiple wood species [150].

Aging duration also depends on the origin, type, and quality of the wine. Barrel age further modulates this process. During shorter aging periods (6 to 9 months), substantial differences are observed between wines aged in new versus previously used barrels, particularly in the concentration of extracted compounds. Over extended aging (12 to 15 months), these differences diminish due to the progressive depletion of extractable components. The compounds most affected by barrel reuse include furanic aldehydes, alcohols, phenolic aldehydes, and characteristic oak lactones [151].

The presence of 4-ethylphenol, 4-ethylguaiacol, and 4-ethylcatechol in wine is associated with contamination by the yeast *Brettanomyces* sp., regarded as a spoilage organism in oenology. This yeast metabolizes phenolic compounds, producing undesirable aromas. These molecules serve as biomarkers of both *Brettanomyces* contamination and barrel degradation. Their occurrence can be mitigated through sulfite addition, currently the most widespread approach due to its efficiency and low cost—or by filtration, both of which inhibit microbial activity [148,152,153].

Analyses of hydroalcoholic extracts from different wood species show that oak, chestnut, and mulberry exhibit the highest levels of total polyphenols. With respect to oxidative potential, chestnut ranks highest, followed by acacia, oak, mulberry, and cherry. Across all extracts, dominant volatile compounds include benzene derivatives with guaiacol residues and medium- to long-chain fatty acids (C6–C18), both of which contribute notably to wine aroma [151].

In summary, the evolution of volatile compounds during wine aging is a dynamic and multifactorial process, crucial to the sensory quality of the final product. A detailed understanding of these mechanisms enables winemakers to optimize vinification and aging strategies, ensuring the consistent development of desirable aromatic profiles.

2.5. Varietal and Regional Aromatic Fingerprinting in Wine: The Role of Volatile Compounds in Defining Aroma, Authenticity, and "Terroir"

The aromatic profile of wine is a critical determinant of its sensory characteristics, serving not only to define identity but also to signal authenticity and economic value. By integrating volatile compound profiling with multivariate statistical analysis researchers can identify characteristic aromatic patterns that distinguish grapevine cultivars and delineate their geographic origins [154,155]. Recent advancements in analytical chemistry and data science [156–159] have further enabled the establishment of varietal and regional aromatic "fingerprints," providing robust tools for authentication and quality control.

Studies consistently show that wines produced from different grapevine cultivars exhibit distinct aromatic profiles that shape their unique sensory attributes. These varietal differences are primarily driven from genetic variation, which influences the biosynthesis and accumulation of volatile precursors. For example, 'Muscat' varieties exhibit high expression of terpene synthase genes, resulting in elevated levels of linalool, geraniol, and nerol [85]. In contrast, 'Sauvignon Blanc' accumulates glutathione-conjugated thiol precursors [160], while 'Syrah'/'Shiraz' is particularly rich in rotundone, the sesquiterpene responsible for its characteristic peppery aroma [161]. Such varietal fingerprints persist across different winemaking styles and vintages, allowing classification even in blended or aged wines.

The genetic background of each grapevine cultivar not only determines the composition but also the concentration of volatile compounds. Each grape variety possesses a distinct biosynthetic capacity to produce, store, and release aroma precursors, thereby establishing cultivar-specific aromatic signatures.

Regional fingerprinting builds on this varietal framework by incorporating environmental influences, including climate, soil composition, topography, altitude, and viticultural practices, all of which affect grape development. This integrated framework, collectively referred to as "terroir" reflects the combined effects of these variables on grapevine physiology, microbial ecology, and the metabolic pathways involved in aroma precursor biosynthesis. These interactions ultimately give rise to distinct, region-specific chemical and sensory profiles.

For instance, cool-climate regions such as the Loire Valley and Marlborough favor the preservation of volatile thiols and acidity, producing fresh and zesty aromatic profiles [162]. Conversely, warmer regions enhance the formation of norisoprenoids and esters, which are associated with ripe or baked fruit aromas [163]. In Portugal's Douro Valley, the combination of hot, dry summers and cold winters, combined with intense solar radiation and pronounced diurnal temperature shifts, promotes sugar and phenolic accumulation, intensifying aromatic expression. Grapes from warmer subregions such as Douro Superior often exhibit aromas of ripe dark fruits, figs, plums, dried fruit, and spices [164].

3. Integration of Analytical Data with Sensory Analysis and Sensomics

The integrating of analytical data with sensory analysis and sensomics represents a cutting-edge approach in food science, aiming to directly link chemical composition with human sensory perception. This integration enables a deeper understanding into how specific molecular compounds influence flavor, aroma, and consumer preferences, thereby supporting product optimization and quality control. When combined with advanced statistical and machine learning techniques, these approaches allow for more accurate prediction, classification, and optimization of sensory attributes and overall product quality.

Sensomics is an innovative methodology that integrates advanced analytical techniques, such as Comprehensive Two-Dimensional Gas Chromatography (GC × GC), Ultra-High Performance Liquid Chromatography coupled with High-Resolution Mass Spectrometry (UHPLC-HRMS), Liquid Chromatography-Mass Spectrometry (LC-MS), and Nuclear Magnetic Resonance (NMR), with sensory evaluation. It is specifically designed to identify, quantify, and validate the key sensory-active compounds that determine taste and aroma profiles across a wide range of foods. This approach encompasses both volatile and non-volatile compounds, providing a comprehensive view of how chemical constituents contribute to flavor perception. To confirm the sensory relevance of individual compounds, sensomics often employs reconstitution and omission tests, which reveal the intricate connections between molecular composition and sensory experience [165–169].

In the context of wine, sensomics is particularly valuable for identifying the key odorants that define their aromatic character (Figure 4). This is achieved by combining targeted chemical analysis with rigorous sensory evaluation. Recent advances in expert systems have further enhanced this process, enabling the prediction of key aroma compounds and their sensory impact directly from analytical data. These tools reduce reliance on extensive human sensory panels, allowing for faster and more efficient assessments [168,170].

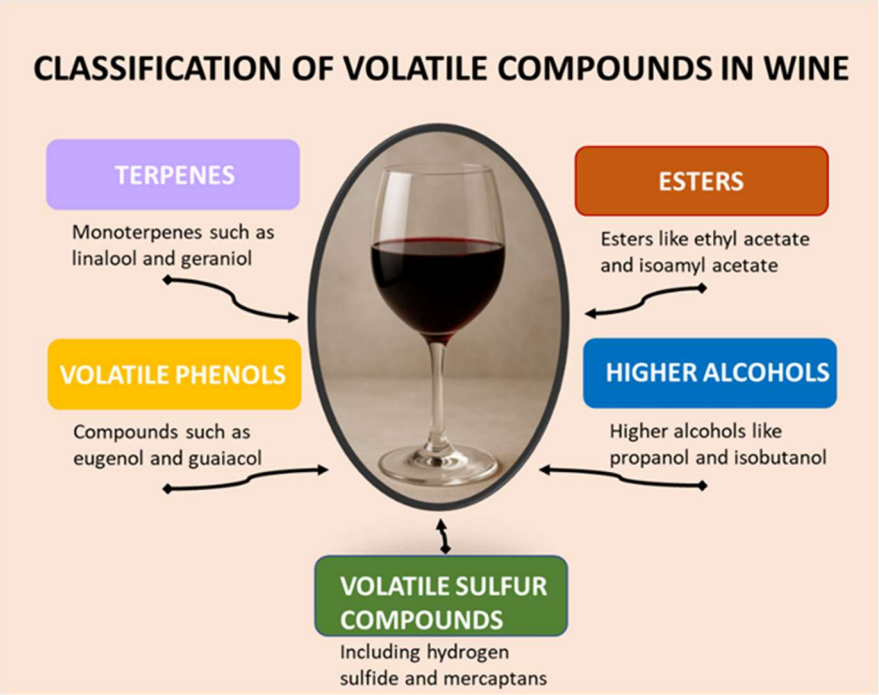


Figure 4. Classification of volatile compounds in wine.

The integration of analytical data, including compound identity, concentration, and physicochemical properties, with sensory data such as odor quality, taste descriptors and perception thresholds is facilitated by chemometrics and multivariate analysis techniques. This combined approach enables precise sensory profiling and supports robust predictions of product characteristics across the food and beverage sectors [163,167,169,171].

Furthermore, the development of expert systems and machine learning models has transformed the prediction and classification of key odorants and overall product profiles. By leveraging both analytical and sensory datasets, these models provide more reliable predictions, reducing reliance on traditional sensory panels and significantly accelerating the evaluation process [168,169,172]. This technology not only improves the precision of product development but also ensures a more consistent and high-quality sensory experience for consumers.

3.1. Applications and Benefits

The integration of analytical data with sensory analysis and sensomics offers numerous practical applications and advantages, as outlined in Table 3. These methodologies enable researchers to identify the chemical compounds with the greatest impact on consumer preferences, thereby directly guiding formulation and processing decisions to enhance product appeal and overall consumer satisfaction [167,169,172].

In terms of product origin and quality control, the combination of sensomics and chemometric analysis facilitates accurate differentiation between product types, such as distinct cocoa varieties, and allows for reliable prediction of sensory profiles. This capability supports efforts to ensure authenticity and maintain consistent quality standards across food products [169].

Furthermore, the integration of sensory analysis with biometric data—including physiological responses such as heart rate, facial expressions [173,174], and electroencephalogram (EEG) readings—offers a more holistic perspective on consumer reactions. This multi-dimensional approach not only strengthens product testing methodologies but also

provides deeper insights for market research, ultimately supporting more informed and strategic product development [172].

Table 3. Practical examples of integrating analytical data with sensory analysis and sensomics in diverse food matrices.

Application Area	Analytical Tools Used	Sensory Integration Method	Key Benefit	References
Dairy and Bakery	GC × GC, LC-MS, NMR	Sensory reconstitution, omission	Flavor optimization, blueprinting	[165,167]
Cocoa/Chocolate	UHPLC-HRMS, Chemometrics	Sensory prediction, origin mapping	Quality control, origin screening	[169]
Beer	Video, IRTI, EEG, ANN	Biometric + sensory data	Consumer acceptability modeling, sensory pleasantness	[172]
General Food Products	GC-O-MS, Chemometrics	Machine perception, artificial intelligence (AI)	Rapid aroma profiling, automation	[166,168]
Wine	GC-MS, GC × GC-MS, HPLC-MS	Trained panels, MRATA, and volatile profile analysis	Marker identification, quality prediction	[170,175,176]
Wine	Spectrofluorometry, SHS-GC-IMS	Rate-all-that-apply, sensory prediction	Sensory trait prediction, classification	[6,177–179]
Wine	Video, FaceReader, ANN	Biometric + sensory data	Consumer acceptability, sensory pleasantness	[173,174]

3.2. Chemometrics Methods for Flavor Prediction

Chemometrics encompasses a wide range of statistical and machine learning techniques that are increasingly applied to the prediction and evaluation of flavors in food and beverages. By processing complex datasets generated by instruments such as GC-MS, E-nose, E-tongue, and various spectroscopic methods, chemometrics, objective, rapid, and accurate flavor profiling and prediction are enabled. The most commonly used chemometric approaches for flavor prediction are described in the next point.

3.2.1. Multivariate Regression and Machine Learning

Partial Least Squares Regression (PLSR) is widely applied to correlate instrumental data (e.g., volatile compounds profiles, NIR spectra) with sensory attributes such as acidity, bitterness, flavor, and overall quality in products like coffee. PLSR models achieve predictive performance comparable to that of expert sensory panels [180,181].

Support Vector Machine Regression (SVR) often outperforms PLSR in predicting specific flavor components (e.g., esters, acids, sugars), achieving high correlation coefficients (Rp values up to 0.96) [182–184].

Deep neural approaches, including deep neural networks and momentum deep belief networks, have shown superior accuracy in predicting volatile compound concentrations and classifying product brands, with R^2 values exceeding 0.96 and low root mean squared error (RMSE) [185]. Similarly, artificial neural networks (ANN) have proven highly effective in differentiating processing stages and predicting odor quality, often surpassing traditional pattern recognition techniques [184].

In the wine industry, machine learning models, particularly ANN and quantitative structure–odor relationship (QSOR) approaches, are increasingly employed to predict sensory quality scores and aroma profiles directly from analytical data. These tools provide valuable support for winemaking decisions and quality control [177,178]. However, the

broader application of such models remains constrained by the limited availability of large, standardized datasets that comprehensively link sensory and chemical information [179].

3.2.2. Pattern Recognition and Classification

Principal Component Analysis (PCA) and Categorical PCA (CATPCA) are widely applied for dimensionality reduction and visualization, enabling the clustering of samples based on their flavor profiles [182,184].

Linear Discriminant Analysis (LDA) has demonstrated excellent performance in classifying products according to flavor, with reported accuracies exceeding 97% [183].

Cluster Analysis is frequently used to group samples based on similarities in flavor profile, supporting product differentiation. This approach has been successfully applied to a variety of food products [184] as well as wines [186].

Structural Equation Modeling (SEM) also finds application in sensory science. For example, Vilela et al. [187] employed second-order factor analysis models to evaluate sensory attributes in wines produced from various grape varieties in the Vinho Verde region of Portugal, providing new insights into their sensory profiles.

3.2.3. Data Fusion and Sensor Integration

Combining Multiple Sensors and integrating data from E-nose, E-tongue, GC-MS, and colorimetric sensors with chemometric models significantly enhances prediction accuracy and provides a more comprehensive characterization of flavor profile [15,182–185]. The fusion of datasets from different analytical platforms enhances both qualitative and quantitative evaluations of flavor [182,184,185].

For instance, E-nose can detect low-concentration compounds, like 2,4,6-trichloroanisole (TCA), responsible for cork taint in wine, that are often masked to humans due to higher sensory thresholds and different detection mechanisms.

E-nose use arrays of chemical sensors (e.g., metal-oxide, polymer, or acoustic wave sensors) that respond to volatile compounds by generating electrical signals. These signals are then processed using pattern recognition algorithms or machine learning models to identify and quantify specific compounds, even at trace levels. E-nose are capable of detecting TCA at concentrations as low as 1.4 ng/L, well below typical human detection thresholds [188]. Unlike human olfaction, E-nose are not subject to biological adaptation or sensory fatigue and can be engineered for high sensitivity to target molecules [188,189].

By contrast, human olfactory detection relies on odorant molecules binding to specific olfactory receptors in the nose. Perception occurs only when compound concentrations exceed individual detection threshold, which varies among people and are influenced by adaptation, mixture suppression, and cognitive factors. As a result, compounds such as TCA may remain undetectable by smell when present below threshold levels [18,190,191].

Moreover, E-nose apply advanced algorithms (e.g., neural networks, PCA) to distinguish subtle changes in sensor responses, enabling detection and quantification of com-pounds even in complex mixtures [188,189].

These chemometric approaches enable fast, reproducible, and objective assessments of flavor, reducing reliance on traditional human sensory panels [182,185,192]. Table 4 summarizes key applications of data fusion and sensor integration.

Combining chemical data (e.g., GC-MS, HPLC-MS) and sensory data through multivariate statistical methods (such as multiple factor analysis (MFA), Partial Least Squares Discriminant Analysis (PLS-DA), and CCA) provides deeper insights into how specific compounds influence sensory perception. This integration facilitates the identification of varietal markers, enabling optimized product development and marketing strategies tailored to consumer preferences [6,10,175,177].

Table 4. Comparison of chemometric approaches and sensory panels in wine assessment.

Feature	Chemometric Approaches	Human Sensory Panels	References
Speed	Rapid, high-throughput	Slow, labor-intensive	[193,194]
Reproducibility	High, protocol-driven	Variable, subjective	[193–195]
Objectivity	Data-driven, unbiased	Prone to human bias	[193,194]
Scalability	Easily automated	Limited by panel size	[193,194]

These methods are widely applied across various food matrices beyond wine [180–185,192]. Additionally, they play a critical role in routine quality assessment and in the design of targeted flavor profiles [153,180,181].

3.3. Can Combining Chemometrics and Sensomics Improve Flavor Prediction Accuracy?

The integration of chemometrics with sensomics significantly improves the accuracy of flavor prediction. This integration enables the precise identification and quantification of key flavor compounds, as well as their impact on sensory perception (Table 5). A notable example is the study by Lee et al. [196], who developed "SERS superprofiles" by combining receptor–flavor Surface-Enhanced Raman Spectroscopy (SERS) data with chemometrics models. Their approach uncovered molecular interactions relevant to flavor identification and enabled the differentiation of alcohol functionalities. Remarkably, the SERS-based system achieved perfect accuracy in quantifying multiple flavor compounds in an artificial wine matrix [196].

Table 5. Applications and Case Studies of the Integration of Chemometrics and Sensomics for Enhanced Flavor Prediction Accuracy.

Food Matrix	Approach Used	Prediction/Classification Accuracy	References
Wine	SERS (Surface-Enhanced Raman Scattering) + chemometrics + machine learning	Perfect accuracy in flavor quantification	[196]
Soybean Paste	E-nose/E-tongue + chemometrics + data fusion	Rp up to 0.96 for overall flavor prediction	[182,183]
Lamb Shashliks	GC-MS, E-nose, E-tongue + deep learning	R^2 above 0.96 for VOCs and brand ID	[185]
Cocoa	UHPLC-HRMS + sensomics + chemometrics	Strong correlation with sensory descriptors	[169]
Dairy Products	Sensomics + chemometrics	Identification of key flavor compounds for reconstitution	[165]

By integrating multiple sensor technologies (e.g., E-nose, E-tongue, GC-MS) with advanced chemometric tools such as support vector regression (SVR), deep neural networks (DNN), and PCA, researchers can achieve exceptionally high prediction accuracy for both qualitative and quantitative sensory attributes. For example, models have achieved correlation coefficients exceeding 0.96 and exceptional classification performance [153,181–183,185]. Sensomics further strengthens this integration by identifying and quantifying key odor- and taste-active compounds, thereby improving the inputs for the chemometric model. This synergy allows the construction of reliable "flavor blueprints" for complex products such as wine [165,166,169].

Thus, sensory prediction can be significantly improved through the integration of chemometrics and sensomics. This combined approach enables accurate mapping of chemical markers to sensory attributes, thereby supporting both product development and quality control processes [165,166,169,196]

The methodology is applicable across a wide range of food matrices [165,169,181–183,185,196] and offers the advantage of reducing reliance on human sensory panels while accelerating flavor profiling through automated, data-driven methodologies [182,185,192,196]. However, effective data management remains critical, as inadequate handling of datasets can markedly reduce the reliability and predictive power of integrated sensory-chemical models [10,197].

3.4. Comparative Analysis: Chemometrics vs. Sensory Panels in Flavor Evaluation

As previously mentioned, chemometrics relies on data from analytical instruments (e.g., E-nose, E-tongue, spectroscopy) combined with advanced statistical modeling to objectively assess and predict flavor attributes. These methods offer rapid, high-throughput analysis—sometimes evaluating samples in under a minute—and are capable of efficiently handling large and complex datasets [182,185,198–201].

In contrast, sensory panels depend on trained human assessors to evaluate aroma, taste, and other sensory characteristics. While providing direct insight into human perception, sensory evaluation is time-consuming, requires extensive training, and can be subject to assessor fatigue as well as inter-individual variability [198,201–203].

Recent advances in machine learning, such as support vector regression, deep neural networks, and PLSR, have shown strong predictive power for sensory attributes, in some cases surpassing the accuracy of sensory panels in discrimination and classification tasks. For example, chemometric models achieved identification rates of up to 98.3% compared to sensory panels' 89.2% in beer flavor discrimination [199]. Similar levels of predictive success have been reported in coffee and olive oil flavor profiling [198,201,203,204].

Despite these technological advances, sensory panels remain the gold standard for capturing the full complexity of human flavor perception—particularly for novel, subtle, or multidimensional sensory experiences. However, their results are often more subjective and less reproducible than instrument-based evaluations [201–203].

The most robust flavor evaluations often emerge from a hybrid approach that integrates chemometric tools with sensory panel insights. Chemometrics can rapidly screen, classify, and predict sensory attributes, while sensory panels provide human-centered validation and nuanced interpretation. Data fusion strategies further enhance accuracy and facilitate more comprehensive product characterization [182,185,198,201–205].

In the wine industry, for instance, combining trained sensory panels assessments with detailed chemical profiling has enabled the refinement of predictive models that relate sensory descriptors—such as astringency, fruitiness, or earthy notes—to specific molecular markers. This integrated approach enhances understanding of wine typicity and supports alignment between production practices and consumer preferences [175,177,178].

4. Advances in Wine Aroma Profiling: Integrating Sensor Technologies, Chemometrics, and Machine Learning for Quality Prediction

A variety of sensory attributes, including aroma, taste, and mouthfeel, contribute to wine quality. These characteristics vary widely across wine styles and are described using a broad and nuanced sensory vocabulary [206]. Wine quality is influenced by multiple factors, with geographical origin playing a particularly significant role [207]. To reflect this, the European Union and other wine-producing regions have established appellation system, which classify wines based on their geographical origin and traditional production practices. This system considers variables such as soil type, climate, grape variety, and vinification techniques. Under this framework, wines are categorized into three groups: those without a designation of origin, wines with a protected geographical indication (PGI), and those with a protected designation of origin (PDO) [159].

Among wine quality parameters, aroma is especially critical to consumer preference [208]. The aromatic profile of a wine is primarily determined by grape variety, as many volatile compounds persist throughout the vinification process [1]. Wine aroma is composed of more than 1,300 volatile compounds—including alcohols, esters, acids, aldehydes, isoprenoids, lactones, and ketones—found across a wide concentration range [209]. Differences in compound type, ratios, and concentrations largely account for aroma variability [210].

Descriptive Analysis (DA) by trained sensory panels remains the most widely adopted method for wine aroma characterization [211]. Although DA provides detailed and reproducible results, maintaining expert panels is both time-consuming and financially burdensome [212]. Moreover, trained assessors may perceive aromas differently from average consumers [213].

To address these limitations, sensor technologies such as E-nose and E-tongue have been developed [16,214]. Modeled after human sensory mechanisms, these instruments offer rapid and cost-effective alternatives for wine analysis. However, directly correlation between sensor outputs and human perception remains a challenging. These devices can detect compounds at concentrations below human sensory thresholds, sometimes producing intensity readings that do not correspond to perceived strength. Additionally, synergistic and masking effects between volatile compounds complicate predictions of aroma perceptions that are not predictable from individual concentrations. Furthermore, key mouthfeel attributes such as astringency, viscosity, and heat perception are not yet detectable by current sensor technologies [14]. Despite these limitations, E-nose and E-tongue systems have been successfully applied to distinguish aging techniques [215–217], differentiate wines by geographic origin or grape variety [218], and predict sensory descriptors [4].

Notably, wine aroma cannot be fully explained by individual compound concentrations due to complex molecular interactions. Statistical modeling addresses this challenge by identifying which analytical variables most strongly influence sensory attributes. Typically, models are trained on samples with known sensory classifications and then applied to predict the sensory properties of new samples [206].

Predictive approaches integrate chemical data with multivariate statistical methods to model the relationships between compounds and sensory perception. Key methodologies include chemometric regression (e.g., PLSR), machine learning (e.g., neural networks, random forests, support-vector machines), and sensor-based spectroscopy (e.g., E-nose, near/mid-IR, fluorescence) combined with advanced data analytics [219,220].

Machine learning techniques are proving increasingly effective for wine sensory evaluation, enabling rapid, objective, and accurate prediction of sensory attributes and overall quality. A wide range of algorithms has been applied to wine sensory evaluation, including: (i) Extreme Gradient Boosting (XGBoost), used to predict multiple sensory attributes (aroma, color, taste, flavor, mouthfeel) from spectral data, achieving R^2 values above 0.7 for several attributes and above 0.5 for most, demonstrating strong predictive performance for complex sensory profiles [177,221]; (ii) Random Forests and SVM, frequently outperform other models in predicting wine quality from physicochemical and sensory data. Random Forests, in particular, often achieve the highest accuracy, with reported values of up to 94.7% for white wine and 88.6% for red wine [222–226]; (iii) Ensemble and Stacking Methods: improved stacking ensemble learning further enhances prediction accuracy and robustness, reaching up to 91.7% accuracy [227]; (iv)Active Learning Approaches, reducing the need for extensive labeled data by strategically selecting the most informative samples for expert labeling, thereby increasing efficiency and accuracy in sensory classification tasks [228]; PLSR and Chemometrics, used for linking chemical composition to sensory traits, especially for complex attributes like astringency [177,229] (Table 6).

Table 6. Comparison of machine learning techniques for wine sensory evaluation.

Technique	Application Area	Notable Outcomes	References
XGBoost	Sensory attribute prediction	High R^2 for multiple attributes	[177,221,224,225]
Random Forest	Quality classification	Highest accuracy in many studies	[222–226]
SVM	Quality and astringency modeling	Strong regression/classification	[223,224,226,229,230]
Ensemble/Stacking	Quality prediction	Enhanced accuracy/robustness	[223,225,227]
Active Learning	Sensory evaluation	Reduced labeling effort, high accuracy	[228]

Despite significant advances, several research trends and limitations remain in applying machine learning to wine sensory evaluation. For instance, combining spectral and chemical data has been shown to improve model performance [177,221] while identifying key chemical variables (e.g., procyanidins, ethanol) enhances both interpretability and accuracy [225,229–231]. However, the lack of large, standardized sensory-chemical datasets and the inherent subjectivity of sensory data remain major challenges [228,232].

Most AI and machine learning methods, particularly deep learning, require large datasets to capture complex patterns and avoid fitting to noise. In wine sensory science, datasets are often relatively small, sometimes containing fewer than 100 wines, tasters, or sensory attributes. This limitation increases the risk of overfitting, where a model memorizes the training data rather than learning generalizable patterns. For instance, with fewer than 100 samples, an ANN may have far more parameters than available data points. As a result, it might achieve nearly perfect accuracy on training data but perform poorly when applied to new wines.

Sensory datasets often include numerous aroma, taste, and chemical features. When the number of wines is less than 100, the number of features may exceed the number of samples, creating what is known as the "p >> n" problem. This situation increases the likelihood of overfitting. A model trained on such a small dataset may produce drastically different results if even a few wines are added or removed. Additionally, in small datasets, the ANN might learn spurious relationships, such as linking "alcohol content" to "quality" based on only a handful of wines, which will not generalize to real-world tastings.

Wine researchers typically address this challenge by using simpler models such as linear regression, PCA, and decision trees are often more reliable than ANNs in contexts with fewer than 100 samples. Additional strategies include using cross-validation and bootstrapping to estimate model's stability, applying regularization techniques to limit overfitting, and leveraging larger external datasets for model pre-training [228,232].

So, for a better decision, the following decision tree can be used (Figure 5):

Quantitative structure–activity relationship (QSAR) models establish correlations between molecular features and odor potency. Trained on both analytical and sensory data, these models can predict aroma attributes, detect potential defects, and support winemaking decisions [233]. Several studies have demonstrated the predictive potential of these approaches. For example, Fuentes et al. [234] combined NIR spectra with weather and vineyard management data to train ANN, successfully predicted the sensory profiles of 'Pinot Noir'. Similarly, Gehlken et al. [219] showed that online NIR spectroscopy of fermenting grapes could predict key aroma attributes (fruity, floral, "green", etc.) with $R^2 > 0.97$. These findings highlight how spectroscopic fingerprints (derived from grapes or finished wine) can be integrated with machine-learning to forecast aroma-related traits accurately and rapidly, even before bottling.

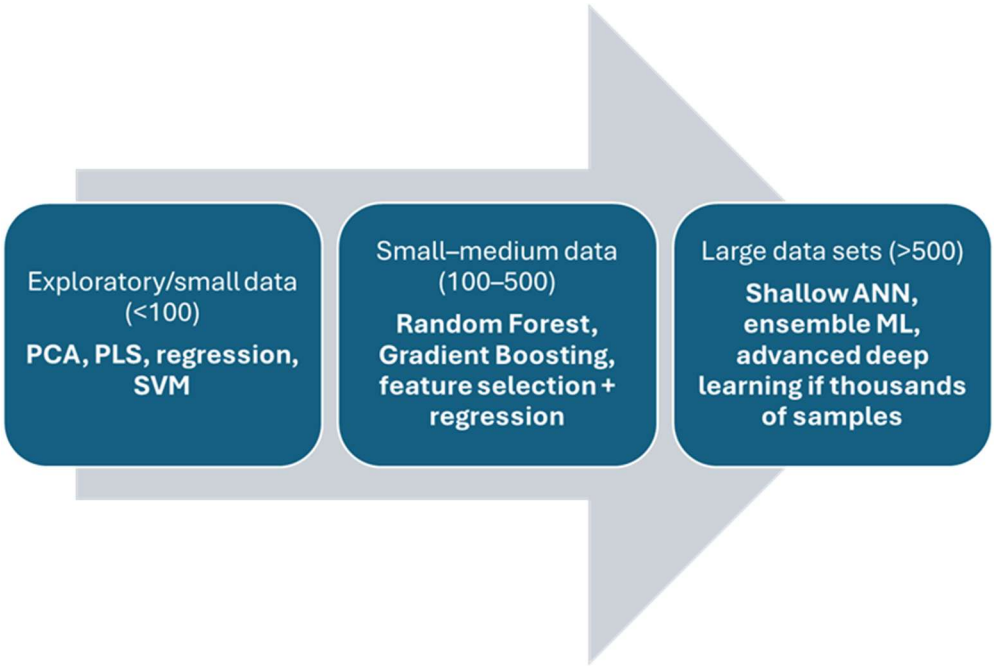


Figure 5. Summary of model choice based on the number of data points.

The reliability of any QSAR model depends on multiple factors, including the quality of the input dataset, the selection of relevant descriptors, method of dataset partitioning, the statistical tools applied, and most importantly, the validation approach. Validation is the most critical step in QSAR development, as it ensures the trustworthiness of the models and the robustness of the entire modeling process [235]. It also provides insights into data quality, diversity, and predictive ability. Validation generally falls into two categories: internal validation, which assesses how well the model predicts the data it was trained on, and external validation, which evaluates predictive performance on new, unseen compounds. When sufficient new data are not available, subsets of the original dataset may be reserved for validation purposes [236].

Several statistical parameters are commonly used to assess model performance, including the determination coefficient (R^2), variance ratio (F), standard error of estimate (s), adjusted R^2 (Ra^2) or classical metrics such as the leave-one-out cross-validated correlation coefficient (q^2), $Rpred^2$, Q^2_{F2} and the concordance correlation coefficient (CCC), can be used to judge the quality and predictive ability of the models [237,238]. Care must be taken, however, as results can sometimes be misleading depending on the validation method chosen [239]. Both internal and external validation strategies can employ various models, but the choice must account for dataset size and composition as well as the strengths and weaknesses of each method [235].

Molecular descriptors are numerical values encoding information about a molecule's structure. These descriptors can represent experimental physicochemical properties or theoretical indices derived from mathematical equations or computational methods. Therefore, molecular descriptors are intrinsically linked to the concept of molecular structure, and, therefore to QSAR. Developing models for QSAR/QSPR involves several challenges, one of the most important being the selection of the most relevant molecular descriptors for the target property or activity. Chemical structures can be represented using various types of descriptors, including functional groups, topological, constitutional, thermodynamic, and quantum mechanical descriptors. However, some descriptors may provide overlapping information or may be unrelated to the biological activity of interest, potentially masking the relationship between structure and activity. Therefore, selecting the most rele-

vant descriptors is considered one of the most critical and complex steps in QSAR/QSPR modeling [240,241].

There are various approaches to address the descriptor selection challenge, but most can be grouped into two main categories: classical methods—such as multiple linear regression or VSMP, and AI based techniques, including those inspired by genetic algorithms, ANN, and fuzzy logic [242], with the latter being more able to record nonlinear relationships between descriptors and a specific activity or property, while overcoming some of the limitations to classical selection techniques [243]. Descriptors are numerical representations of the chemical characteristics of a molecule, widely used in QSAR/QSPR studies, providing a mathematical description of molecular properties. The information they convey typically depends on the type of molecular representation used and the specific algorithm applied for their calculation. Common types of descriptors include topological indices, as well as geometrical, constitutional, and physicochemical descriptors [244,245]. Among these, constitutional descriptors are the simplest and most commonly used. They capture basic information about a compound's composition—such as the number of atoms, types of atoms, bond count, ring count, and molecular weight—without providing details about molecular topology. Because constitutional descriptors are unaffected by changes in molecular conformation, they cannot differentiate between isomers. Each selection methods have its own advantages and disadvantages, that should be carefully weighed when starting these procedures [245].

More recently, Muñoz-Castells et al. [220] combined an E-nose sensor array with GC–MS reference data. Using PLS-discriminant analysis and principal component regression, they achieved the prediction of "odorant series" (fruity, floral, etc.) from E-nose signals. Models demonstrated strong predictive capabilities for particular odorant series but also showed reduced performance for others, indicating the need for further refinement [220]. Other examples include QSPR models. For instance, Ojha and Roy [246] developed PLS-based QSPR models to predict the odor-threshold properties of wine aroma molecules from molecular descriptors. Their work identified structural features that lower odor thresholds and even predicted a composite odor-threshold index for different wines, thus linking molecular composition to perceived aroma.

Gas chromatography (GC–FID/MS) and GC-Olfactometry remain standard methodology for quantifying volatiles, and multivariate models often use these values to predict sensory outcomes. For example, Li et al. [247] used sensomics (SPME, LLE-GC-MS) to identify key "sweet berry" aroma compounds in red wine, then built PLS regression models to accurately predict the intensity of sweet and berry aroma notes from volatile concentrations. Other studies have used GC data to relate specific odorants to descriptors such as wood, floral, or vegetal via PLSR [7].

Current trends emphasize non-destructive, real-time approaches. Calibrated NIR or MIR spectroscopy is increasingly used to infer volatile content and sensory scores without chromatography, especially when combined with machine learning [219]. These predictive models are particularly valuable for ensuring quality control and maintaining consistency in wine style. For instance, Harris et al. [248] developed NIR-ML models to predict aroma compound levels and sensory intensity in unopened bottles. Fuentes et al. [234] demonstrated that seasonal weather conditions can accurately predict 'Pinot Noir' aroma profiles, providing growers with advanced guidance.

5. Detection of Off-Flavors in Wine Using Integrated Sensor Technologies

The presence of compounds that produce unpleasant odors in wine can result in significant economic losses for the wine industry. Wine quality is particularly susceptible to

undesirable volatile compounds that form during fermentation or storage. Early detection of these off-odors is essential for implementing corrective measures to prevent sensory defects. Electronic nose technologies have shown promising potential in identifying several key spoilage compounds (Table 7). For example, E-nose combined with machine learning have successfully detected acetic acid [249], ethyl acetate, and related compounds [250].

Additionally, the E-tongue is emerging as a valuable tool for detecting faults in red wine. It employs an array of seven cross-selective chemical sensors to monitor changes in soluble organic and inorganic compounds [251,252]. An E-tongue system based on all-solid-state potentiometric sensors has also proven effective in tracking acetic acid levels in white wines [253]. As such, the E-tongue can complement traditional sensory analysis methods in wine evaluation [252,254].

Cork taint is another common defect in wine, primarily caused by chlorinated compounds such as TCA. These compounds are tough to detect due to their extremely low odor threshold [255]. Sánchez et al. [256] introduced an innovative, non-destructive, and cost-effective E-nose method for detecting TCA in sparkling wines. Using PCA and Artificial Neural Network Discriminant Analysis (ANNDA), their system accurately classified wines based on a threshold of 2 ng/L of TCA, achieving 88% classification accuracy.

Brettanomyces bruxellensis (commonly known as Brett) is one of the most significant spoilage yeasts in red wine production, primarily due to its ability to produce volatile phenols [257]. The formation of 4-ethylphenol occurs through the decarboxylation of hydroxycinnamic acids by *Brettanomyces/Dekkera bruxellensis*, yeasts naturally present in the grape microflora [152]. These acids are first converted to hydroxystyrenes via the enzyme hydroxycinnamate decarboxylase, and then reduced to ethyl derivatives by vinylphenol reductase.

The concentration of 4-ethylphenol often increases during the aging of wine. It can continue to rise after bottling, leading to undesirable off-flavors typically described as horse sweat, stable, or varnish-like aromas [258]. This spoilage affects the wine's sensory profile by converting vinylphenols—such as 4-vinylphenol, 4-vinylcatechol, and 4-vinylguaiacol—into ethylphenols, contributing to the so-called "Brett character" marked by unpleasant phenolic and animal-like odors.

In addition to ethylphenols, Brett can also produce other spoilage metabolites, including 2-ethyltetrahydropyridine, 2-acetyltetrahydropyridine, and isovaleric acid, all of which can cause mousy off-flavors and sensory defects even at very low concentrations [258].

Given these challenges, there is growing interest in developing sensitive, rapid, and cost-effective methods for yeast detection in wine. Electrochemical biosensors offer significant promise for microbiological analysis due to their high sensitivity, specificity, portability, and low cost. These sensors often rely on affinity-based interactions to enhance selectivity and can be further optimized using disposable screen-printed electrodes and nanomaterials for improved signal amplification. Electrochemical biosensors specifically targeting *Brettanomyces* and total yeast content have been developed by Borisova et al. [259]. More recently, Villalonga et al. [260] introduced an amperometric biosensor capable of rapidly detecting and quantifying *Brettanomyces bruxellensis* and total yeast levels in wine. Additionally, Portugal-Gomez et al. [261] demonstrated the potential of modified screen-printed carbon electrodes (SPCEs) for the sensitive and selective detection of 4-ethylphenol. Among the sensors tested, the activated C60/SPCE exhibited the best performance, with detection limits ranging from 400 to 700 µg/L depending on deposition time, along with good reproducibility.

Electronic nose technologies have also been effectively employed to detect spoilage-related defects, particularly those associated with elevated levels of 4-ethylphenol and 4-ethylguaiacol [262,263]. Furthermore, González-Calabuig and del Valle [264] demonstrated the use of a voltammetric E-tongue to quantify key *Brettanomyces* metabolites—namely

4-ethylphenol, 4-ethylguaiacol, and 4-ethylcatechol—in spiked wine samples. Their system combined cyclic voltammetry using six modified graphite-epoxy electrodes, signal compression via discrete wavelet transform, and chemometric modeling with ANN to achieve accurate quantification.

Gonzalez Viejo and Fuentes [265] used NIR spectroscopy and a low-cost E-nose with machine learning to detect wine faults, achieving high accuracy for red (94–96% NIR; 92–97% E-nose) and white wines (96–97% NIR; 90–97% E-nose). Such technologies could transform winemaking by enabling predictive decisions and preserving wine quality in a changing climate.

Table 7. Electronic nose for Detection of Off-Flavors in Wine.

Application	Sensor Array	Chemometrics	Reference
Detection of Wine Spoilage Thresholds Using an Electronic Nose System: Focus on Acetic Acid	Metal Oxide Semiconductors	Principal Component Analysis, Support Vector Machines	[252]
Electronic Nose for Early Detection of Wine Spoilage	Metal Oxide Semiconductors		[266]
Enhancing Electronic Nose Performance for Wine Defect Evaluation	Metal Oxide Semiconductors	Deep Learning, Support Vector Machines	[267]
Rapid Detection of TCA (2,4,6-Trichloroanisole)	Metal Oxide Semiconductors	Principal Component Analysis	[268]
Portable Electronic Nose for TCA Detection in Wines	Metal Oxide Semiconductors	Principal Component Analysis	[269]
Artificial Diagnosis of *Brettanomyces* spp.	Quartz Crystal Microbalance	Principal Component Analysis	[270]
Detection of Phenolic Derivatives (e.g., 4-Ethylphenol, 4-Ethylguaiacol)			[260]

6. Conclusions

Integrating analytical data with sensory analysis and sensomics provides a powerful, multidimensional perspective on food flavor and consumer perception. This integrative approach enables precise flavor optimization, robust quality control, and deeper consumer insights, ultimately driving innovation in food science and the food industry.

Chemometric methods and machine learning—primarily when combined with advanced sensing technologies—provide accurate, efficient, and scalable tools for flavor prediction and characterization. These approaches are transforming the way researchers and producers address flavor research, product development, and quality assurance.

In wine analysis, the integration of analytical data, sensory evaluation, and sensomics establishes a holistic framework for understanding and predicting sensory attributes and overall wine quality. This synergy supports both scientific insight and practical decision-making in winemaking and quality management.

Electrochemical biosensors and sensor arrays—such as E-nose and E-tongue—further strengthen this integrative strategy by offering rapid, cost-effective, and often portable solutions for detecting off-flavors, contaminants, and spoilage. These technologies complement traditional human sensory panels by enabling early intervention and ensuring consistency across vintages.

Despite these advances, challenges remain. Instrumental measurements require further refinement to more closely align with human sensory perception, especially considering the complex interactions and threshold sensitivities of volatile compounds. Fu-

ture progress should emphasize the development of multi-sensor platforms, of sensory–chemical databases, and hybrid modeling strategies that integrate human expertise with machine learning.

Machine learning methods such as XGBoost, Random Forests, and ensemble techniques are already revolutionizing wine sensory evaluation by delivering rapid, objective, and accurate predictions of sensory attributes and quality. These approaches reduce reliance on human panels while offering valuable tools for both research and industry. Further refinement in wine modeling should focus on nonlinear algorithms (e.g., Random Forest, Gradient Boosting) and PLS-based models, combined with targeted feature selection to improve predictive accuracy and practical applicability.

Ultimately, the convergence of analytical data, sensor technologies, and predictive modeling provides a powerful platform for innovation in oenology. This integrative paradigm strengthens real-time quality control, preserves wine typicity, and supports sustainability in modern wine production.

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