Review Article : Open Access

Decoding horticultural crops from genome to metabolome: DNA and chemical fingerprinting perspectives

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Article Info

Abstract

Horticultural crops constitute a vital component of global food and nutritional security, owing to their rich diversity of bioactive compounds, sensory attributes and economic value. Accurate identification, quality assurance and sustainable utilization of these crops have become increasingly important in the context of globalized trade, climate variability and rising consumer demand for high-quality and functional plant-based products. Conventional morphological and agronomic characterization methods are often limited by environmental influence, phenotypic plasticity and low discriminatory power, particularly among closely related cultivars and processed products. In this context, DNA fingerprinting and chemical fingerprinting have emerged as powerful complementary tools for precise crop characterization.This review provides a comprehensive synthesis of advances in DNA fingerprinting, chemical fingerprinting and integrative genome-metabolome approaches in horticultural crop research. It discusses the principles and applications of major molecular marker systems, including RAPD, AFLP, ISSR, SSR, SNPs, organelle markers and DNA barcoding, highlighting their roles in genetic diversity analysis, cultivar identification, germplasm conservation and marker-assisted breeding. The review further examines chemical fingerprinting and phytochemical profiling, emphasizing major metabolite classes such as phenolics, flavonoids, alkaloids, terpenoids, pigments, glucosinolates and volatiles, along with advanced analytical platforms used for their characterization.

A central focus of the review is the integration of genomic and metabolomic data through multiomics and systems biology approaches. Linking DNA markers with metabolite profiles enables deeper understanding of the genetic control of metabolite accumulation, quality traits and stress responses. Case studies from fruits, vegetables, spices and medicinal and aromatic plants demonstrate the practical value of integrative genome-metabolome fingerprinting in crop improvement, authentication, traceability and value addition. The review also addresses current challenges, including high costs, environmental effects on metabolomic signatures, data integration complexity and limited reference databases, while highlighting emerging trends such as artificial intelligence, next-generation metabolomics and portable fingerprinting tools. Overall, this review underscores the importance of integrative genome-metabolome fingerprinting as a robust and forward-looking strategy for sustainable, precise and quality-driven horticulture, with significant implications for research, breeding, industry and policy.

1. Introduction

Horticultural crops, which include fruits, vegetables, spices, plantation crops and medicinal and aromatic plants, occupy a central position in global food systems due to their indispensable contributions to human nutrition, economic development and biodiversity conservation. Unlike staple cereal crops that primarily serve as sources of calories, horticultural crops are rich repositories of essential vitamins, minerals, dietary fiber and a diverse array of bioactive phytochemicals. These components play a critical role in maintaining human health by supporting immune function, regulating metabolic processes and reducing the risk of micronutrient deficiencies and chronic non-communicable diseases. Fruits and vegetables supply vitamins such as vitamin C, vitamin A precursors, folates and vitamin K, along with minerals including potassium, calcium, magnesium and iron. Spices and medicinal plants, though consumed in smaller quantities, are concentrated sources of phenolics, flavonoids, alkaloids, terpenoids and volatile compounds that exhibit potent antioxidant, anti-inflammatory, antimicrobial and therapeutic properties. As a result, horticultural crops are increasingly recognized not only as food commodities but also as functional foods and nutraceutical resources that link agriculture with health and wellness. From an economic perspective, the horticulture sector is one of the

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most dynamic and high-value segments of agriculture. It generates substantial income per unit area, provides employment opportunities across production, processing, transportation and marketing chains and contributes significantly to national economies through domestic markets and export trade. Small holder farmers in many developing countries depend heavily on horticultural crops as cash crops that support household livelihoods and rural development. The expanding global demand for fresh produce, organic foods, specialty cultivars and value-added horticultural products has intensified the need for efficient production systems and robust quality assurance mechanisms (Nybom *et al.*, 2014). At the same time, increased international trade and longer supply chains have introduced complex challenges related to product authenticity, safety and traceability, particularly for high-value fruits, spices and plant-based products.

DNA fingerprinting has emerged as a powerful molecular approach to overcome many of the limitations associated with conventional characterization methods. By detecting variations directly at the genome level, DNA-based markers provide stable and reproducible signatures that are largely unaffected by environmental conditions or developmental stage. A wide range of molecular marker systems has been developed and applied in horticultural crops, enabling reliable identification, genetic diversity assessment and phylogenetic analysis. DNA fingerprinting facilitates unambiguous discrimination among closely related species and cultivars, supports effective management of germplasm collections and provides scientific evidence for cultivar registration and protection. These attributes make DNA-based approaches indispensable tools in modern horticultural research, breeding and regulatory frameworks. Despite their robustness, DNA markers primarily reveal genetic identity and relatedness and do not directly reflect the biochemical or functional attributes that determine crop quality, nutritional value, flavor, aroma and therapeutic potential. Many of the traits that define the commercial and nutritional value of horticultural crops are controlled by complex metabolic pathways and are expressed as specific profiles of primary and secondary metabolites. Chemical fingerprinting addresses this dimension by focusing on the comprehensive profiling of metabolites present in plant tissues. Advances in analytical technologies have enabled high-resolution characterization of complex metabolite mixtures, capturing the unique chemical signatures associated with specific species, cultivars, or geographical origins. Chemical fingerprinting plays a critical role in quality control, standardization, authentication and detection of adulteration, particularly in fruits, vegetables, spices and medicinal plant products.

Integrating DNA and chemical fingerprinting within a genome-metabolome framework offers a holistic strategy for horticultural crop characterization. The genome encodes the biosynthetic machinery and regulatory networks responsible for metabolite production, while the metabolome reflects the functional expression of these genetic instructions under specific conditions. By linking genetic markers with metabolite profiles, researchers can gain insights into how genetic variation translates into differences in nutritional quality, sensory attributes and stress responses. Such integrative approaches enable the identification of genotype-specific metabolic signatures and support more precise selection of superior cultivars with enhanced quality traits.The concept of genome-metabolome linkage represents a significant shift toward systems-level under standing in horticultural science (Collard and Mackill, 2009). Integrative analyses allow the exploration of relationships between genetic variation and metabolite accumulation, facilitating the discovery of genetic determinants of key quality and nutritional traits. This approach is particularly valuable in horticultural crops, where consumer acceptance and market value are strongly influenced by attributes such as taste, aroma, color and health-promoting properties. Genome-metabolome integration also enhances the effectiveness of crop improvement programs by enabling the selection of genotypes that combine desirable agronomic performance with superior phytochemical profiles.

Despite significant technological advances, several challenges continue to limit the widespread adoption of integrative fingerprinting approaches in horticulture. These include the high cost of advanced analytical platforms, the need for specialized technical expertise, variability in metabolite expression due to environmental factors and the lack of standardized protocols and comprehensive reference databases (Powell *et al.*, 1996). Addressing these challenges requires coordinated efforts in method standardization, data integration and capacity building, as well as interdisciplinary collaboration among molecular biologists, analytical chemists, breeders and horticulturists. Against this background, the present review aims to provide a comprehensive overview of DNA and chemical fingerprinting approaches in horticultural crop research, with a particular emphasis on their integration from genome to metabolome. The objectives of this review are to examine the principles and applications of DNA fingerprinting techniques, discuss chemical and phytochemical fingerprinting strategies relevant to crop quality and authentication and highlight the conceptual framework and practical potential of genome-metabolome integration. By synthesizing advances across molecular genetics, phytochemistry and analytical sciences, this review seeks to contribute to the development of reliable, science-based tools for sustainable horticultural production, quality assurance and biodiversity conservation.

2. Conceptual framework: From genome to metabolome

Understanding horticultural crop identity, quality and performance require a comprehensive conceptual framework that links genetic information with biochemical outcomes. The transition from genome to metabolome represents a systems-level perspective in which molecular variation is traced through successive biological layers to observable traits and functional metabolites. While the genome provides the fundamental blueprint for plant development and metabolism, the final phenotype and metabolite composition arise through complex regulatory processes influenced by both intrinsic genetic factors and extrinsic environmental conditions. In horticultural crops, where quality attributes such as flavor, color, aroma, nutritional value and bioactive compound content are critical determinants of market value and consumer acceptance, the genome-to-metabolome continuum offers a powerful approach to understanding crop diversity and functionality. Gene expression is a key process that translates genetic information into metabolic outcomes. Genes encoding enzymes, transporters and regulatory proteins define the metabolic capacity of a plant. Transcriptional regulation determines when and where genes are expressed, while post-transcriptional, translational and post-translational mechanisms modulate enzyme abundance, activity and stability (Kalia *et al.*, 2011). These regulatory layers collectively govern metabolic fluxes and shape the overall metabolome. In horticultural crops, pathways associated with carbohydrate metabolism, organic acid synthesis, pigment biosynthesis and secondary metabolite production are especially

important, as they directly influence fruit sweetness, acidity, color intensity, aroma and health-promoting properties. Understanding these regulatory relationships is therefore essential for elucidating the biological basis of horticultural crop quality.

The biosynthesis of primary and secondary metabolites is under strong genetic control, although these two classes differ in their roles and regulatory complexity. Primary metabolites, including sugars, amino acids, organic acids and lipids, are indispensable for basic cellular functions, growth and reproduction. Their metabolic pathways are largely conserved across plant species and are tightly regulated to ensure cellular homeostasis. In horticultural crops, primary metabolites largely determine attributes such as sweetness, acidity, texture and energy value. For instance, the balance between sugars and organic acids is a major determinant of fruit taste and consumer preference and genetic variation affecting key enzymes in these pathways can lead to substantial differences in eating quality among cultivars.Although, genetic factors establish the potential for metabolite production, environmental conditions exert a profound influence on metabolomic profiles. The metabolome is highly dynamic and responsive to external factors such as temperature, light, water availability, soil nutrient status and biotic interactions. Developmental stage and tissue type further affect metabolite accumulation, as different organs prioritize distinct metabolic functions. In horticultural crops, environmental modulation of metabolites is evident in processes such as color development during fruit ripening, accumulation of sugars and organic acids, synthesis of aroma compounds and induction of stress-related secondary metabolites. Agronomic practices, including fertilization, irrigation, pruning and post-harvest handling, also play a significant role in shaping metabolite composition. This environmental sensitivity presents both opportunities and challenges. On one hand, growers can manipulate environmental and management factors to enhance desirable quality traits, such as improving sweetness, color, or phytochemical content. On the other hand, such variability complicates the use of metabolite profiles for reliable identification and authentication, as the same genotype may exhibit different chemical fingerprints under different growing conditions. Distinguishing genetically determined variation from environmentally induced changes therefore remains a major challenge, emphasizing the need to integrate metabolomic data with stable genetic information.The rationale for integrating molecular and chemical fingerprints stems from the complementary nature of genomic and metabolomic information. Molecular fingerprints based on DNA markers provide stable, environment-independent indicators of genetic identity and relatedness, making them highly effective for cultivar discrimination, germplasm characterization and protection of plant varieties (Hebert *et al*., 2003). However, DNA markers do not directly reflect functional traits or quality attributes expressed at the metabolic level. Chemical fingerprints, in contrast, directly capture the biochemical composition that defines crop quality, nutritional value and sensory properties, but they are influenced by environmental and developmental factors. Integrating molecular and chemical fingerprints allows variable metabolite profiles to be anchored to stable genetic backgrounds, enhancing the reliability of identification, quality assessment and traceability.

3. DNA fingerprinting techniques in horticultural crops

DNA fingerprinting has emerged as one of the most powerful and reliable tools for understanding, managing and improving horticultural crops. The extraordinary diversity observed in fruits, vegetables, spices, plantation crops and medicinal and aromatic plants is the outcome of long domestication histories, natural selection, human-mediated breeding and environmental adaptation. While this diversity underpins horticulture's nutritional, economic and ecological value, it also presents significant challenges in accurate identification, characterization and utilization of genetic resources. DNA fingerprinting addresses these challenges by enabling precise, reproducible and environment-independent analysis of genetic variation, thereby forming a cornerstone of modern horticultural research and practice.Traditional methods of crop characterization based on morphological, phenological and agronomic traits have been widely used for decades. However, these approaches are constrained by phenotypic plasticity, long evaluation periods and limited resolution, particularly among closely related cultivars or clonal materials. DNA fingerprinting overcomes these limitations by directly interrogating the genome, revealing polymorphisms that reflect true genetic differences rather than environmentally induced variation. As a result, DNA-based methods are now routinely applied in horticulture for genetic diversity assessment, cultivar identification, varietal protection, germplasm conservation and breeding.

3.1 Principles of DNA fingerprinting

The fundamental principle underlying DNA fingerprinting is genetic polymorphism, defined as heritable variation in DNA sequence among individuals of a species or between species. Genetic polymorphisms arise through mutations such as base substitutions, insertions, deletions, duplications, transposable element activity and chromosomal rearrangements. Over time, these variations accumulate within populations and are shaped by evolutionary forces including natural selection, genetic drift, migration and human-mediated selection. In horticultural crops, genetic polymorphism is often extensive due to diverse origins, wide geographical distribution, frequent hybridization, vegetative propagation and intensive breeding. DNA fingerprinting exploits this variation by targeting specific polymorphic regions of the genome using molecular markers. These markers generate distinct DNA profiles that can be used to identify individuals, distinguish cultivars, assess genetic relationships and infer population structure. Marker-based identification involves the detection of polymorphic DNA fragments or sequence variants through molecular techniques such as polymerase chain reaction (PCR), restriction enzyme digestion, or high-throughput sequencing. The resulting marker patternsbands on a gel, allele sizes, or nucleotide cells constitute a genetic fingerprint unique to each genotype. Because these patterns are inherited according to Mendelian principles, they can be used to trace parentage, confirm hybridity and study inheritance of traits. A critical feature of DNA fingerprinting is its stability (Hollingsworth *et al*., 2011). DNA polymorphisms are largely unaffected by environmental conditions, developmental stage, or tissue type, making DNA-based identification highly reliable across locations and seasons. This stability is particularly important in horticulture, where crops are grown under diverse agroclimatic conditions and often evaluated for traits that are highly environment-sensitive.

DNA fingerprinting offers numerous advantages over phenotypic and biochemical markers traditionally used in horticultural research. Phenotypic traits such as plant height, leaf morphology, fruit shape andcolor are influenced by environmental conditions, crop management and developmental stage. This phenotypic plasticity

can mask underlying genetic differences, leading to misclassification or unreliable identification. In contrast, DNA markers provide direct access to genetic variation and are not influenced by external factors. Another major advantage is resolution. DNA fingerprinting can discriminate between closely related cultivars, somatic mutants and clonal selections that are morphologically indistinguishable. This is particularly relevant in horticultural crops propagated vegetatively, such as banana, grape, citrus, potato and many ornamentals, where subtle genetic differences can have major implications for quality, disease resistance and market value. DNA-based techniques also allow identification at early developmental stages, including seedlings or in vitro plantlets, thereby accelerating breeding and selection processes. Moreover, DNA fingerprinting can be applied to small amounts of tissue and to processed materials, enabling authentication of planting material, harvested produce and value-added products where morphological traits are absent (Fernie *et al.*, 2004). From a practical perspective, DNA fingerprinting generates digital and reproducible data that can be stored in databases, compared across laboratories and used for long-term documentation of genetic resources. Advances in automation and high-throughput genotyping have further enhanced the efficiency, scalability and cost-effectiveness of DNA finger printing, making it accessible for large-scale horticultural applications.

3.2 Marker systems used in horticulture

A wide array of DNA marker systems has been developed and applied in horticultural crops, each with distinct molecular bases, advantages and limitations. Selection of an appropriate marker system depends on the objectives of the study, the biology of the crop, available resources and the level of resolution required. Random amplified polymorphic DNA (RAPD) markers were among the earliest PCR-based marker systems adopted in horticultural research. RAPD uses short, arbitrary primers to amplify random segments of genomic DNA, generating banding patterns that reveal polymorphisms as presence or absence of bands. RAPD markers are attractive due to their simplicity, low cost and lack of requirement for prior sequence information.In horticulture, RAPD markers have been widely used for preliminary assessment of genetic diversity, cultivar differentiation and evaluation of clonal variation in tissue culture-derived plants. They have also been applied to study genetic stability in clonal propagation systems and to characterize wild relatives and landraces. However, RAPD markers have significant limitations, most notably poor reproducibility due to sensitivity to PCR conditions and reaction components. Their dominant inheritance also prevents discrimination between homozygous and heterozygous genotypes. As a result, RAPD markers are now largely used for exploratory studies or in combination with more robust marker systems (Haall *et al.*, 2008).

Amplified fragment length polymorphism (AFLP) markers combine restriction enzyme digestion of genomic DNA with selective PCR amplification, producing highly polymorphic and reproducible fingerprints. AFLP markers generate a large number of loci distributed across the genome, making them particularly useful for high-resolution genetic analysis. In horticultural crops, AFLP markers have been extensively used for genetic diversity analysis, phylogenetic studies, population structure analysis and assessment of genetic relationships among cultivars and species. They are especially valuable for crops with limited genomic resources, as they do not require prior sequence information. Despite their high resolution, AFLP markers are technically demanding, relatively expensive and dominant in nature.

Interpretation of AFLP data can be complex and the method is less amenable to automation compared with newer marker systems. Nevertheless, AFLP remains a powerful tool for detailed genetic analysis in horticulture. Inter simple sequence repeat (ISSR) markers amplify regions between microsatellite sequences using primers anchored in simple sequence repeats. ISSR markers offer several advantages over RAPD, including higher reproducibility and greater polymorphism. They do not require prior genomic information and generate multilocus profiles suitable for genetic diversity analysis. ISSR markers have been widely applied in horticultural crops to assess genetic diversity, evaluate clonal fidelity, characterize germplasm collections and study population structure. Their relatively simple protocol and moderate cost make them suitable for laboratories with limited resources (de Vos *et al.*, 2007). Like RAPD and AFLP, ISSR markers are generally dominant, limiting their usefulness for detailed genetic analysis such as parentage studies. Nonetheless, ISSR markers remain popular for diversity assessment and preliminary characterization in horticulture.

Simple sequence repeat (SSR) markers, also known as microsatellites, are based on variation in the number of tandem repeats of short DNA motifs. SSR markers are highly polymorphic, co-dominant, locus-specific and reproducible, making them among the most informative marker systems in horticulture. SSR markers allow discrimination between homozygous and heterozygous alleles, enabling detailed genetic analysis including parentage determination, population genetics and linkage mapping. They have been extensively developed and applied in major horticultural crops such as apple, grape, citrus, tomato, pepper, onion and banana. The main limitation of SSR markers is the requirement for prior sequence information and the cost associated with marker development. However, once developed, SSR markers are highly transferable and provide long-term value for germplasm characterization, cultivar identification and breeding.Single nucleotide polymorphisms (SNPs) represent variation at a single nucleotide position and are the most abundant form of genetic variation in plant genomes. Advances in next-generation sequencing have enabled rapid discovery and genotyping of SNPs at genome-wide scale, transforming horticultural genetics. SNP markers are highly stable, amenable to automation and suitable for high-throughput platforms such as SNP arrays, genotyping-by-sequencing and targeted genotyping assays. In horticulture, SNPs are increasingly used for cultivar fingerprinting, genome-wide association studies, genetic diversity analysis and marker-assisted breeding (Verpoorte *et al.*, 2005). Although, individual SNPs are typically bi-allelic and less informative than SSRs, their high density and scalability provide unparalleled resolution for genomic analysis. SNP-based finger printing is now considered the gold standard for many horticultural applications, particularly in crops with available genome sequences.

3.3 Applications of DNA fingerprinting

Genetic diversity underpinscrop resilience, adaptability and long-term sustainability. DNA markers enable quantification of genetic variation within and among populations, identification of genetically distinct groups and analysis of population structure. Population genetic analysis provides insights into domestication, gene flow, selection and evolutionary relationships. Such information is essential for designing effective breeding strategies, conserving genetic resources and avoiding genetic erosion. DNA fingerprinting has been widely used to characterize diversity in landraces, wild relatives and cultivated varieties of horticultural crops. DNA fingerprinting plays

a central role in cultivar identification and varietal protection. Accurate identification ensures varietal purity, prevents mislabelling and supports quality assurance in horticultural value chains. DNA fingerprints serve as genetic passports that uniquely identify cultivars, even when morphological differences are minimal. In legal and regulatory contexts, DNA fingerprinting provides objective evidence for plant variety protection, breeders' rights and intellectual property claims. DNA-based identification is increasingly required for cultivar registration and certification, particularly for high-value horticultural crops. Effective conservation of horticultural germplasm requires accurate characterization and documentation of genetic resources. DNA fingerprinting enables identification of duplicates, assessment of genetic redundancy and development of core collections representing maximum diversity. DNA markers also facilitate characterization of wild relatives and underutilized species, supporting their conservation and utilization in breeding. By revealing genetic relationships and diversity patterns, DNA fingerprinting informs conservation priorities and sustainable use strategies. DNA fingerprinting is indispensable for parentage analysis and breeding. Co-dominant markers such as SSRs and SNPs allow precise determination of parent-offspring relationships, verification of hybrids and detection of unintended crosses (Dixon and Strack, 2003). Marker-assisted breeding uses DNA markers linked to desirable traits to accelerate selection and reduce breeding cycles. DNA fingerprinting supports early selection, integration of genomic information with phenotypic and metabolomic data and development of superior horticultural cultivars.

4. Chemical fingerprinting and phytochemical profiling

Chemical fingerprinting and phytochemical profiling have become central components of modern horticultural research, complementing molecular approaches by providing direct insights into the biochemical composition that underlies crop quality, nutritional value, sensory attributes and functional properties. While DNA fingerprinting establishes genetic identity, chemical fingerprinting captures the dynamic metabolic expression of that genetic potential as influenced by developmental stage, environment and management practices. In horticultural cropswhere consumer acceptance and market value are strongly determined by flavor, color, aroma and health-promoting compounds chemical fingerprinting provides indispensable information for authentication, quality control, value addition and crop improvement. This section elaborates the conceptual basis of chemical fingerprinting, major phytochemical classes in horticultural crops, analytical techniques employed and key applications in horticulture.

4.1 Concept of chemical fingerprinting

Chemical fingerprinting is a holistic analytical strategy that aims to capture the overall chemical composition of a plant material in the form of a reproducible and characteristic profile. Rather than focusing on individual compounds in isolation, chemical fingerprinting emphasizes the collective behaviour of metabolites, recognizing that biological function, quality and identity emerge from complex interactions among multiple chemical constituents. In horticultural crops, where biochemical composition directly influences nutritional quality, sensory attributes, shelf-life and therapeutic value, chemical fingerprinting provides an integrative perspective that aligns closely with real-world quality assessment and crop utilization. At its core, chemical fingerprinting is grounded in metabolomics principles,

although, it is often applied with more targeted objectives such as authentication, standardization, or quality control. A chemical fingerprint may consist of chromatographic peak patterns, spectral signatures, or mass spectral features that together represent the biochemical "identity card" of a crop or product. These patterns are generated using standardized analytical conditions and can be compared across samples using chemometric or multivariate statistical approaches to detect similarities, differences and deviations. In horticulture, such comparisons are essential for distinguishing cultivars, identifying geographical origin and detecting adulteration or quality deterioration.

The importance of chemical fingerprinting in crop authentication has increased dramatically with the globalization of horticultural trade and the expansion of value-added plant products. Many horticultural commodities are marketed in processed formssuch as dried fruits, powders, extracts, juices, oils and nutraceutical formulations where morphological traits are absent and visual inspection is insufficient. Chemical fingerprinting enables authentication at the biochemical level by verifying the presence of characteristic metabolite patterns associated with authentic raw materials. Even when individual marker compounds are present, their relative proportions and co-occurrence patterns within the fingerprint provide stronger evidence of authenticity than single-compound analysis alone. Chemical fingerprinting is particularly relevant for distinguishing closely related species and cultivars that share similar genetic backgrounds but differ in quality attributes. In fruits and vegetables, minor variations in sugar composition, organic acid ratios, phenolic profiles, or volatile compounds can significantly alter taste, aroma and consumer preference (Fernie and yan, 2019). Chemical fingerprints capture these subtle yet functionally important differences, allowing discrimination that may not be achievable through genetic or morphological markers alone. This capability is especially valuable in horticultural breeding programs focused on quality improvement rather than yield enhancement.

From a regulatory and commercial perspective, chemical fingerprinting supports evidence-based quality assurance and certification. Regulatory agencies and industry stakeholders increasingly require comprehensive quality profiles rather than reliance on single marker compounds. Chemical fingerprinting meets this requirement by capturing the overall biochemical integrity of products, reducing the risk of false authentication based on isolated markers. This is especially important for medicinal and aromatic crops, where efficacy and safety depend on complex mixtures of bioactive compounds rather than single constituents.

4.2 Major phytochemical classes in horticultural crops

Horticultural crops are distinguished from staple food crops by their extraordinary diversity of phytochemicals, which collectively define their nutritional quality, sensory characteristics, therapeutic potential and market value. Phytochemicals are naturally occurring, biologically active compounds produced by plants as part of their primary and secondary metabolism. In horticultural crops, these compounds are not only central to plant growth, defense and adaptation but also play a decisive role in human health, food quality and functional applications (Alseekh *et al*., 2021). Chemical fingerprinting relies heavily on these phytochemical classes because their presence, relative abundance and structural diversity generate distinctive biochemical signatures that enable crop differentiation, authentication and quality evaluation.

4.2.1 Phenolic compounds

Phenolic compounds represent one of the largest and most ubiquitous classes of phytochemicals in horticultural crops. Structurally characterized by one or more hydroxyl groups attached to aromatic rings, phenolics are synthesized primarily through the phenylpropanoid pathway. They are widely distributed across fruits, vegetables, spices and medicinal plants, occurring in free or conjugated forms.Phenolics include simple phenolic acids (such as hydroxybenzoic and hydroxycinnamic acids), complex polyphenols and polymeric compounds such as tannins and lignins. In horticultural crops, phenolic acids contribute to antioxidant activity, color stability and resistance to biotic and abiotic stresses. For example, chlorogenic acid is abundant in crops such as coffee, potato and eggplant and plays a role in antioxidant defense and browning reactions. Caffeic and ferulic acids are common in fruits and vegetables and influence flavor, shelf life and nutritional value. From a chemical fingerprinting perspective, phenolic profiles are highly informative because they vary significantly among species, cultivars, tissues and developmental stages (Razzag *et al.*, 2019). Fruits such as apples, grapes, berries and pomegranates exhibit rich and diverse phenolic compositions that contribute to astringency, bitterness and antioxidant capacity. Vegetables such as onions, leafy greens and brassicas also contain distinctive phenolic patterns that can be exploited for cultivar discrimination and quality assessment. The complexity and variability of phenolic compounds make them central markers in chemical fingerprinting studies.

4.2.2 Flavonoids

Flavonoids are a major subclass of phenolic compounds and are among the most intensively studied phytochemicals in horticultural crops. Structurally, flavonoids are characterized by a common C6-C3-C6 skeleton and are further classified into flavonols, flavones, flavanols (catechins), flavanones, isoflavones and anthocyanins. Their biosynthesis is tightly regulated and highly responsive to genetic and environmental factors. In horticultural crops, flavonoids play multiple roles, including pigmentation, UV protection, defense against pathogens and modulation of flavor. Flavonols such as quercetin and kaempferol are abundant in onions, apples, kale and berries and contribute to antioxidant and anti-inflammatory properties. Flavanols, including catechins and epicatechins, are prominent in tea, grapes and certain fruits and influence bitterness and astringency. Flavones and flavanones are characteristic of citrus fruits, where they contribute to flavor and health-promoting effects. Anthocyanins, a highly visible group of flavonoids, are responsible for red, purple and blue pigmentation in fruits and vegetables such as grapes, berries, red cabbage, purple sweet potato andcolored carrots. Beyond their aesthetic value, anthocyanins are associated with strong antioxidant activity and have been linked to various health benefits (Tohge and fernie, 2015). The composition and relative abundance of anthocyanin derivatives are often cultivar-specific, making them powerful chemical markers for fingerprinting-colored horticultural crops.

4.2.3 Alkaloids

Alkaloids are nitrogen-containing secondary metabolites with diverse chemical structures and pronounced biological activity. Although, less ubiquitous than phenolics, alkaloids are particularly important in certain horticultural crops and medicinal plants. They often exhibit strong physiological effects, contributing to bitterness, pungency, toxicity, or therapeutic activity. In horticultural crops, alkaloids are especially prominent in the Solanaceae family. For instance, solanine and chaconine in potato, capsaicinoids in chili peppers and nicotine-related compounds in certain species play defensive roles and influence sensory properties. Capsaicinoids, responsible for pungency in chili peppers, are classic examples of alkaloids that define crop identity and market classification. Variation in capsaicinoid composition and concentration is used to differentiate pepper cultivars and assess quality (Oikawa *et al.*, 2006). Alkaloids are also key constituents of many medicinal and aromatic plants cultivated within horticulture. Their profiles are often species- or even cultivar-specific, making them valuable markers for authentication and standardization. However, because alkaloids can have toxic effects at high concentrations, chemical fingerprinting of alkaloids is also critical for safety evaluation and regulatory compliance.

4.2.4 Terpenoids

Terpenoids constitute one of the most structurally diverse and functionally significant classes of phytochemicals in horticultural crops. Derived from isoprene units, terpenoids include monoterpenes, sesquiterpenes, diterpenes, triterpenes, tetraterpenes (carotenoids) and polyterpenes. They play essential roles in aroma, flavor, pigmentation anddefense. In fruits and aromatic crops, volatile monoterpenes and sesquiterpenes are major contributors to characteristic aromas. For example, limonene, linalool and pinene are key aroma compounds in citrus fruits, grapes and herbs. These volatile terpenoids form complex aroma profiles that are highly sensitive to genetic background, environmental conditions and post-harvest handling. As a result, terpene fingerprints are widely used to authenticate aromatic horticultural products and assess sensory quality. Non-volatile terpenoids, such as triterpenes and sterols, also contribute to nutritional and pharmacological properties (Wishart *et al.*, 2018). Triterpenes found in fruits like apple and olive are associated with anti-inflammatory and cardioprotective effects. The diversity of terpenoid structures and their functional relevance make them central to chemical fingerprinting, particularly in spices, aromatic plants and fruits.

4.2.5 Glucosinolates

In horticultural crops, glucosinolate composition varies widely among species, cultivars and growing conditions. Specific glucosinolates are associated with characteristic flavors and consumer acceptance, as well as with potential health benefits related to detoxification and cancer prevention. Chemical fingerprinting of glucosinolates is therefore valuable for cultivar differentiation, quality assessment and breeding for improved nutritional attributes (Misra *et al.*, 2019). Because glucosinolate profiles are strongly genotype-dependent but also modulated by environment and agronomic practices, they provide rich information for chemical fingerprinting while highlighting the need for integrated genotype-environment analysis.

4.2.6 Volatile compounds

Volatile compounds represent a critical component of phytochemical diversity and are central to aroma and flavor perception in horticultural crops. These compounds include esters, aldehydes, alcohols, ketones, terpenes andsulfur-containing compounds. Even at low concentrations, volatiles can have a profound impact on consumer acceptance.Volatile profiles are among the most complex and dynamic chemical fingerprints, reflecting interactions between

genetic factors, environmental conditions and post-harvest processes (Sakurai *et al.*, 2022). Fruits such as apple, banana, strawberry and mango exhibit complex volatile bouquets that differentiate cultivars and define market classes. In spices and aromatic plants, volatile fingerprints are used extensively for authentication and quality grading.

4.3 Analytical techniques for chemical fingerprinting

Chemical fingerprinting of horticultural crops relies on advanced analytical techniques capable of separating, detecting, identifying and quantifying a wide spectrum of metabolites present in complex plant matrices. Because horticultural crops contain hundreds to thousands of chemically diverse compounds varying in polarity, volatility, molecular weight and stability, no single analytical technique is sufficient to comprehensively capture the entire metabolome. Instead, a combination of chromatographic, spectroscopic and mass spectrometry-based platforms is employed, each contributing complementary information. Instrument selection depends on the nature of target metabolites, the purpose of analysis (authentication, quality control, metabolomics), sensitivity requirements and available infrastructure. This section provides an in-depth, instrument-wise discussion of the major analytical techniques used in chemical fingerprinting of horticultural crops.

4.3.1 Chromatographic techniques

Chromatography forms the backbone of chemical fingerprinting by enabling the separation of complex mixtures into individual components prior to detection and identification. Separation reduces matrix interference, enhances analytical resolution and allows reproducible profiling of metabolites.

4.3.1.1 High-performance liquid chromatography (HPLC)

High-performance liquid chromatography is one of the most widely used techniques for chemical fingerprinting in horticultural research. HPLC separates compounds based on their interaction with a stationary phase and a liquid mobile phase under high pressure. It is particularly suitable for non-volatile, thermally labile and moderately polar compounds commonly found in horticultural crops. HPLC is extensively used for profiling phenolic acids, flavonoids, alkaloids, organic acids, sugars and pigments such as carotenoids and anthocyanins. Reversed-phase HPLC, using C18 columns, is the most common configuration due to its versatility and compatibility with a wide range of phytochemicals. Gradient elution enables effective separation of complex metabolite mixtures, generating characteristic chromatographic patterns that serve as chemical fingerprints. In quality control and authentication, HPLC fingerprints are often generated by overlaying chromatograms of reference and test samples to assess similarity or detect deviations. Peak retention times, relative peak areas and overall chromatographic profiles are used as fingerprint parameters. Although, HPLC provides high reproducibility and robustness, its resolution and sensitivity are limited compared to newer ultra-high-pressure systems (Zhang *et al.*, 2023).

4.3.1.2 Ultra-high-performance liquid chromatography (UHPLC)

Ultra-high-performance liquid chromatography represents an advancement over conventional HPLC, operating at higher pressures with smaller particle-size columns. UHPLC offers significantly improved separation efficiency, faster analysis times and enhanced sensitivity, making it particularly suitable for high-throughput chemical fingerprinting and metabolomics. In horticultural crop analysis, UHPLC is widely used for detailed profiling of polyphenols, flavonoids, alkaloids, glucosinolates and pigments. The sharper peaks and higher resolution achieved with UHPLC enable better discrimination among closely related compounds, which is critical for cultivar differentiation and detection of subtle compositional differences (Zhang *et al.*, 2023). UHPLC fingerprints are especially valuable in comparative studies involving multiple cultivars, growing locations, or post-harvest treatments.

4.3.1.3 Gas chromatography (GC)

Gas chromatography is the method of choice for analyzing volatile and semi-volatile compounds. Separation is based on differences in volatility and interaction with the stationary phase of the GC column. GC is indispensable for chemical fingerprinting of aroma and flavor compounds in fruits, vegetables, spices and aromatic plants. GC is widely used to profile esters, aldehydes, alcohols, ketones, terpenes andsulfur-containing compounds that define sensory attributes. In horticultural crops, GC-based fingerprints are central to aroma characterization, cultivar discrimination and assessment of ripening and storage effects. Because many primary metabolites are non-volatile, GC analysis often requires derivatization to convert polar compounds into volatile derivatives, particularly for sugar and organic acid profiling.The major strengths of GC include high separation efficiency, excellent reproducibility and compatibility with sensitive detectors. However, its application is limited to volatile or derivatizable compounds, restricting its coverage of the full metabolome (Zhang *et al.*, 2023).

4.3.1.4 Thin-layer chromatography (TLC)

Thin-layer chromatography is a simple, cost-effective technique that remains relevant for preliminary screening, quality control and standardization of horticultural and medicinal plant materials. TLC separates compounds on a thin layer of adsorbent material using a solvent system, producing visual banding patterns (Zhang *et al.*, 2023). Although, TLC lacks the resolution and quantitative precision of HPLC or GC, it is widely used for rapid fingerprinting of herbal materials, detection of adulterants and routine quality checks. High-performance thin-layer chromatography (HPTLC), an advanced form of TLC, offers improved resolution, reproducibility and digital documentation, making it suitable for standardized fingerprinting in regulatory and industrial settings.

4.3.2 Spectroscopic techniques

Spectroscopic methods provide rapid, non-destructive and often minimal-sample-preparation approaches to chemical fingerprinting. Rather than separating individual compounds, spectroscopy captures collective molecular information based on interaction with electromagnetic radiation.

4.3.2.1 Fourier-transform infrared spectroscopy (FTIR)

FTIR spectroscopy measures molecular vibrations arising from functional groups, generating spectra that represent the overall chemical composition of a sample. In horticultural fingerprinting, FTIR is widely used for rapid screening, quality control and adulteration detection. FTIR fingerprints reflect the presence of carbohydrates, lipids, proteins, phenolics and other major compound classes. Because spectra are highly reproducible, multivariate analysis

of FTIR data enables classification of samples based on cultivar, origin, or processing method. FTIR is particularly attractive for routine analysis due to its speed, low cost and minimal sample preparation (Kumar *et al.*, 2024). However, it provides limited compound-specific information and is best suited for pattern recognition rather than detailed metabolite identification.

4.3.2.2 Ultraviolet-visible (UV-Vis) spectroscopy

UV-Vis spectroscopy is commonly used for the detection and quantification of chromophoric compounds that absorb light in the ultraviolet or visible range. In horticultural research, UV-Vis spectroscopy is widely applied to estimate total phenolics, flavonoids, anthocyanins, carotenoids and chlorophylls.While UV-Vis spectroscopy lacks selectivity for individual compounds, it is valuable for generating bulk chemical fingerprints and for comparative quality evaluation. When combined with chemometric analysis, UV-Vis spectral patterns can be used to classify samples and assess overall phytochemical content (Kumar *et al.*, 2024).

4.3.2.3 Nuclear magnetic resonance (NMR) spectroscopy

NMR spectroscopy provides detailed structural and quantitative information on metabolites based on magnetic properties of atomic nuclei. NMR is a powerful tool for both targeted and untargeted metabolite profiling and offers exceptional reproducibility. In chemical fingerprinting, NMR generates holistic metabolic profiles that capture a broad range of compounds simultaneously without extensive sample preparation. NMR fingerprints are particularly useful for authenticity studies, geographical origin discrimination and metabolomic comparisons. Unlike mass spectrometry, NMR provides absolute quantification and structural elucidation without the need for reference standards (Kumar *et al.*, 2024). However, its lower sensitivity and higher operational costs limit its routine use in some horticultural laboratories.

4.3.3 Mass spectrometry-based platforms

Mass spectrometry-based techniques represent the most powerful and versatile tools for chemical fingerprinting and metabolomics due to their high sensitivity, selectivity and capacity for compound identification.

4.3.3.1 Gas chromatography-mass spectrometry (GC-MS)

GC-MS combines the separation capability of GC with the molecular identification power of mass spectrometry. It is the gold standard for profiling volatile and semi-volatile compounds in horticultural crops. GC-MS generates detailed fingerprints based on retention times and mass spectral fragmentation patterns, enabling identification of aroma compounds and essential oil constituents. It is widely used for cultivar discrimination, flavor profiling, detection of adulteration and assessment of post-harvest changes (Gupta *et al.*, 2024). The availability of extensive mass spectral libraries enhances compound identification and comparability across studies.

4.3.3.2 Liquid chromatography-mass spectrometry (LC-MS)

LC-MS extends mass spectrometric analysis to non-volatile and thermally unstable compounds. It is one of the most widely used platforms for phytochemical profiling in horticulture. LC-MS enables sensitive detection of phenolics, flavonoids, alkaloids, glucosinolates, pigments and other secondary metabolites. Chemical fingerprints generated by LC-MS include retention time, mass-to-charge ratio and ion intensity information, allowing comprehensive metabolite profiling (Gupta *et al.*, 2024). LC-MS is highly versatile and supports both targeted analysis of known compounds and untargeted metabolomics for discovery-based studies.

4.3.3.3 Tandem mass spectrometry (LC-MS/MS)

LC-MS/MS enhances analytical specificity by incorporating multiple stages of mass analysis. Fragmentation patterns provide structural information that improves compound identification and quantification.In chemical fingerprinting, LC-MS/MS is particularly valuable for confirming marker compounds, resolving isomeric metabolites and quantifying trace-level phytochemicals. It is widely used in standardization of medicinal and aromatic crops and in regulatory quality control (Gupta *et al.*, 2024).

4.3.3.4 High-resolution mass spectrometry (HRMS)

High-resolution mass spectrometry offers accurate mass measurements that enable elemental composition determination and improved identification of unknown metabolites. HRMS platforms are increasingly used in untargeted metabolomics and advanced fingerprinting studies in horticulture. HRMS-based fingerprints provide unparalleled chemical coverage and resolution, making them ideal for comprehensive profiling and biomarker discovery. However, data complexity and analytical costs necessitate advanced expertise and computational resources (Gupta *et al.*, 2024).

4.3.4 Integration of techniques in chemical fingerprinting

No single analytical technique can comprehensively characterize the complex phytochemical landscape of horticultural crops. Effective chemical fingerprinting therefore relies on integrating multiple analytical platforms. Chromatographic techniques provide separation, spectroscopic methods enable rapid screening and mass spectrometry offers sensitive detection and identification. Instrument integration, combined with standardized protocols and chemometric analysis, enables robust fingerprint generation that captures both qualitative and quantitative aspects of crop chemistry (Mukherjee *et al.*, 2024). Such integrated analytical strategies form the foundation of reliable chemical fingerprinting for quality assessment, authentication and crop improvement.

4.4 Applications of chemical fingerprinting in horticultural crops

Chemical fingerprinting has wide-ranging applications across horticultural research, crop production, post-harvest management, processing industries and regulatory frameworks. By capturing comprehensive metabolite profiles rather than relying on single marker compounds, chemical fingerprinting provides a robust and functionally meaningful basis for evaluating quality, authenticity, nutritional value and safety of horticultural commodities. Its applications span fresh and processed products, conventional and organic systems, food and nutraceutical industries and local as well as global supply chains. This section presents an expanded, crop-wise and industry-wise discussion of the major applications of chemical fingerprinting in horticulture.

4.4.1 Quality evaluation and nutritional profiling

One of the most important applications of chemical fingerprinting in horticulture is the objective evaluation of crop quality. Quality in horticultural crops is a multidimensional attribute encompassing

nutritional composition, sensory characteristics, functional properties and shelf-life stability. Many of these attributes are directly governed by metabolite composition, making chemical fingerprinting an ideal tool for comprehensive quality assessment. In fruits, chemical fingerprinting is extensively used to evaluate sugar profiles, organic acid composition, phenolic content, pigment concentration and volatile aroma compounds. The balance between sugars and acids determines sweetness and acidity, while phenolics and flavonoids contribute to antioxidant capacity and mouthfeel. Pigments such as carotenoids and anthocyanins define visual appeal and nutritional value, whereas volatile compounds shape aroma and flavor complexity. Chemical fingerprints integrate all these components, enabling differentiation of cultivars, assessment of maturity stages and monitoring of quality changes during ripening and storage. In vegetables, chemical fingerprinting supports quality evaluation by profiling nutrients such as vitamins, minerals (indirectly *via* chelated organic compounds), amino acids and bioactive phytochemicals. Leafy vegetables are often evaluated for chlorophyll content, phenolics and flavonoids, which are linked to freshness, nutritional value and antioxidant potential. Root and tuber crops are fingerprinted for carbohydrate composition, organic acids and secondary metabolites that influence taste, texture and health benefits. Such comprehensive profiling helps identify nutritionally superior cultivars and supports breeding programs aimed at enhancing dietary quality (Rai *et al*., 2025). Chemical fingerprinting is also widely applied to assess post-harvest quality and shelf-life. During storage and processing, biochemical changes such as sugar degradation, acid metabolism, pigment breakdown and volatile loss can significantly affect quality. Fingerprint-based monitoring enables detection of subtle biochemical shifts that precede visible deterioration, supporting improved post-harvest handling strategies and reducing losses.

4.4.2 Crop authentication and cultivar discrimination

Crop authentication is a critical application of chemical fingerprinting, particularly for high-value horticultural commodities. Authentication involves verifying that a product corresponds to its declared species, cultivar, or variety and has not been substituted or mixed with inferior materials. Chemical fingerprints provide biochemical evidence of authenticity by capturing characteristic metabolite patterns associated with specific crops and cultivars. In fruit crops, cultivar-specific chemical fingerprints are used to differentiate premium varieties from standard ones. Subtle differences in phenolic composition, aroma profiles, or pigment patterns can be sufficient to distinguish cultivars with similar morphology. This is especially important in fruits marketed under varietal names associated with superior quality or higher price. Chemical fingerprinting thus supports transparent labeling and consumer confidence (Mishra *et al*., 2025). In vegetables, chemical fingerprints are applied to discriminate cultivars with specific functional or sensory attributes, such as pungency in peppers, bitterness in leafy greens, or sweetness in carrots and sweet corn. These biochemical traits often define market classes and consumer preferences, making fingerprint-based discrimination valuable for quality assurance and breeding. In clonal crops and vegetatively propagated species, chemical fingerprinting complements genetic methods by capturing somatic variation and physiological differences that may not be reflected at the DNA level. This is particularly relevant for crops where clonal selection has produced lines with distinct quality attributes.

4.4.3 Geographical origin and terroir authentication

Geographical origin plays a crucial role in defining the quality, reputation and market value of many horticultural crops. Environmental factors such as climate, soil composition, altitude and agronomic practices collectively shape metabolite composition, giving rise to location-specific chemical signatures often referred to as "terroir." Chemical fingerprinting is widely used to authenticate geographical origin by identifying metabolite patterns characteristic of specific regions. In fruit crops, variations in phenolic composition, sugar-acid balance and volatile profiles can reflect growing location and climatic conditions. Such fingerprints are valuable for verifying origin claims, supporting geographical indication status and preventing fraudulent labelling (Wang *et al*., 2025). In spices, aromatic crops and plantation horticulture, geographical origin strongly influences essential oil composition and bioactive content. Chemical fingerprinting enables differentiation of products from different regions, even when they belong to the same species or cultivar. This application has significant commercial importance in protecting premium regional products and maintaining market integrity.

4.4.4 Standardization of medicinal and aromatic horticultural crops

Standardization is a critical requirement for medicinal and aromatic crops cultivated within horticulture, as consistency in phytochemical composition directly affects efficacy, safety and regulatory acceptance. Traditional quality control methods based on single marker compounds are often insufficient to capture the complexity of plant-derived products. Chemical fingerprinting provides a comprehensive approach to standardization by representing the overall chemical profile rather than focusing on isolated constituents. This holistic strategy ensures batch-to-batch consistency and accounts for synergistic interactions among multiple compounds. In medicinal horticulture, fingerprint-based standardization supports quality assurance, dosage consistency and compliance with pharmacopeial standards. In aromatic crops used for essential oils, perfumes andflavoring agents, chemical fingerprinting is essential for quality grading and market classification (Wolters *et al*., 2024). Variations in volatile composition can significantly affect aroma quality and commercial value. Fingerprint-based approaches enable objective assessment and classification of aromatic products.

5. Integrative genome-metabolome fingerprinting approaches

Integrative genome-metabolome fingerprinting represents an advanced and holistic framework for understanding horticultural crop identity, quality and functionality by linking genetic variation with biochemical expression. While DNA fingerprinting provides stable and environment-independent information on genetic identity, metabolite profiling captures the dynamic biochemical outcomes that determine sensory attributes, nutritional value and functional properties. Integrating these two layers enables a more comprehensive characterization of horticultural crops, bridging the gap between genotype and phenotype (Oh *et al*., 2023). This approach supports deeper insights into the genetic control of metabolite accumulation, enhances the precision of crop authentication and quality assessment and provides powerful tools for modern breeding, conservation and value addition in horticulture.

5.1 Linking DNA markers with metabolite profiles

The integration of genomic and metabolomic information represents a transformative approach in horticultural research, enabling a direct connection between genetic variation and biochemical phenotype. While DNA fingerprinting establishes genetic identity and relatedness, metabolite profiling reveals the functional expression of that genetic information in the form of primary and secondary metabolites. Linking these two layers provides a mechanistic understanding of how genetic variation governs metabolite accumulation, quality traits and adaptive responses in horticultural crops. This integrative genome-metabolome fingerprinting framework is particularly valuable in horticulture, where crop value is closely linked to biochemical attributes such as flavor, color, nutritional quality and bioactivity. At the biological level, metabolite accumulation is under strong genetic control, mediated by genes encoding enzymes, transporters, transcription factors and regulatory proteins. These genes collectively define the biosynthetic capacity of a plant and determine which metabolic pathways are active, when they are expressed and to what extent metabolites accumulate. Variations in gene sequence, copy number, regulatory regions, or epigenetic status can alter enzyme activity or pathway flux, leading to quantitative and qualitative differences in metabolite profiles. In horticultural crops, such genetic variation explains why cultivars within the same species often display markedly different phytochemical compositions despite similar morphology. Quantitative trait locus (QTL) mapping has played a central role in linking DNA markers with metabolite profiles. In QTL mapping, segregating populations derived from controlled crosses are genotyped using molecular markers and phenotype for metabolite concentrations. Statistical analysis identifies genomic regions associated with variation in specific metabolites or metabolite classes. In horticultural crops, QTLs have been identified for sugars, organic acids, pigments, phenolics, volatile compounds and other quality-related metabolites. These metabolite QTLs often co-localize with genes encoding key enzymes or regulators of metabolic pathways, providing biological insight into the genetic basis of metabolite variation (Singh *et al.*, 2023). The identification of metabolite-associated markers enables the development of genetic fingerprints that reflect not only identity but also functional biochemical potential. Such markers can be used to predict metabolite composition early in plant development, long before metabolites are fully expressed. This is especially valuable in perennial horticultural crops, where breeding cycles are long and early selection for quality traits can significantly accelerate improvement programs. By selecting individuals carrying favorable alleles linked to desirable metabolite profiles, breeders can enhance nutritional quality, flavor and functional attributes more efficiently.

Another important dimension of genome-metabolome linkage is the role of gene-environment interactions. While genetic markers define the potential for metabolite production, environmental conditions modulate gene expression and pathway activity. Integrative approaches that combine genetic data with metabolite profiling across environments allow identification of stable marker-metabolite associations as well as environment-specific effects. This information is crucial for developing cultivars with consistent quality across diverse growing conditions. From a fingerprinting perspective, linking DNA markers with metabolite profiles enhances the robustness and interpretability of both datasets. Genetic fingerprints provide stable identifiers, while metabolite fingerprints capture functional expression. When combined, they generate multilayered signatures that are more reliable for authentication, quality assessment and traceability than either approach alone. This integrated strategy reduces ambiguity arising from environmental variability in metabolite profiles and increases confidence in crop identification and classification.

5.2 Multiomics and systems biology approaches

Multiomics and systems biology approaches represent a paradigm shift in horticultural research, enabling comprehensive understanding of biological complexity by integrating information across multiple molecular layers. Unlike single-level analyses that examine genes or metabolites in isolation, multiomics approaches simultaneously consider genomics, transcriptomics, proteomics and metabolomics to elucidate how genetic information is transduced into biochemical and phenotypic outcomes. In the context of integrative genome-metabolome fingerprinting, these approaches provide the conceptual and analytical framework necessary to link DNA variation with metabolite accumulation, quality traits and functional attributes in horticultural crops. Proteomics adds another layer of complexity by capturing the abundance, modification and interaction of proteins that execute cellular functions. While transcript levels provide an indication of gene activity, protein abundance and activity are influenced by translational efficiency, post-translational modifications and protein turnover. In metabolic pathways, enzymes and transporters represented in the proteome directly control metabolic flux and metabolite accumulation. Integrating proteomic data therefore enhances the accuracy of genome-metabolome linkages by accounting for regulatory processes that occur beyond transcription (Kumar *et al.*, 2024). Systems biology provides the conceptual framework for integrating these omics layers into coherent models of biological function. Rather than viewing biological components as independent entities, systems biology emphasizes interactions, feedback loops and network behavior. In genome-metabolome fingerprinting, this perspective enables identification of regulatory networks that connect genes, transcripts, proteins and metabolites. For example, co-expression network analysis can reveal clusters of genes whose expression patterns are tightly correlated with specific metabolite profiles, suggesting shared regulatory control. Such networks often highlight key transcription factors or regulatory nodes that orchestrate entire metabolic pathways.

Bioinformatics plays a central role in enabling multiomics integration and interpretation. Multiomics datasets are typically large, high-dimensional and heterogeneous, requiring advanced computational tools for data processing, normalization and analysis. Bioinformatic pipelines integrate genomic marker data with transcript abundance, protein profiles and metabolite intensities, allowing statistical association and network inference. Multivariate statistical methods, machine learning algorithms and pathway analysis tools are commonly employed to extract meaningful biological insights from complex datasets. Data-driven interpretation is particularly important in horticultural applications, where quality traits are often controlled by multiple genes and influenced by environmental interactions (Hall *et al.*, 2023). Integrative analysis can identify key genetic determinants of metabolite accumulation, reveal pathway-level regulation and uncover genotype-environment interactions that shape crop quality. These insights support the development of predictive models that link genetic profiles with expected metabolite composition and quality outcomes, enabling informed selection and management decisions.

Multiomics integration also enhances the robustness of fingerprinting approaches. Genetic data provide stable identifiers, while transcriptomic and metabolomic data capture functional expression. When combined, these layers generate multilayered fingerprints that are more informative and reliable for crop authentication, quality evaluation and traceability than single-omics approaches. Such integrated fingerprints are particularly valuable for distinguishing closely related cultivars, verifying geographical origin and assessing consistency in high-value horticultural products. From a practical perspective, multiomics and systems biology approaches support precision horticulture and targeted crop improvement. By identifying key regulatory genes and metabolic pathways associated with desirable quality traits, breeders can design more efficient selection strategies. Integrative datasets also facilitate the discovery of biomarkers that can be used for early-stage selection, reducing breeding cycles and resource investment. In perennial horticultural crops, where long generation times pose significant challenges, these approaches offer substantial advantages. Despite their potential, multi-omics approaches in horticulture face several challenges, including high costs, data integration complexity and the need for interdisciplinary expertise. Standardization of experimental design, data acquisition and analysis remains a critical requirement for reproducibility and comparability across studies. Continued advances in analytical technologies, bioinformatics tools and data-sharing platforms are expected to further enhance the accessibility and impact of multiomics approaches in horticultural research.

6. Applications in modern horticulture

The integration of genomic and metabolomic fingerprinting approaches has significantly expanded the scope and effectiveness of modern horticulture. Beyond their value in fundamental research, these approaches have found practical applications across crop improvement, quality assurance, intellectual property protection, value addition and biodiversity conservation. As horticulture increasingly shifts toward quality-driven, market-oriented and sustainability-focused production systems, integrative fingerprinting provides science-based tools to address contemporary challenges and opportunities. This section highlights key applications of genome-metabolome fingerprinting in modern horticulture. Crop improvement in horticulture has traditionally emphasized yield, appearance and adaptability. However, growing consumer awareness of nutrition, health and environmental sustainability has shifted breeding priorities toward quality attributes, nutritional enhancement and stress tolerance. Integrative genome-metabolome fingerprinting supports precision breeding by enabling the selection of genotypes that combine desirable genetic traits with superior biochemical profiles. By linking DNA markers with metabolite traits, breeders can identify nutritionally superior genotypes enriched in vitamins, antioxidants, phenolics, carotenoids and other health-promoting compounds. Such metabolite-informed selection allows early identification of elite lines, reducing reliance on time-consuming phenotypic evaluation (Alseekh *et al.*, 2024). Integrative approaches are particularly valuable in perennial horticultural crops, where long generation times make early selection critical for breeding efficiency.

Authentication and traceability have become essential components of modern horticultural value chains, particularly for high-value crops and products traded in global markets. Integrative genome-metabolome fingerprinting provides a robust framework for verifying crop identity and origin by combining stable genetic signatures with characteristic biochemical profiles. DNA fingerprinting enables unambiguous identification of species and cultivars, supporting protection of elite varieties and breeders' rights. Chemical finger printing complements this by capturing functional attributes linked to quality and geographical origin. Together, these approaches strengthen traceability systems and reduce the risk of mislabeling, substitution and fraud.

7. Emerging trends and future perspectives

Rapid technological innovation is reshaping the landscape of genome-metabolome fingerprinting and offers promising solutions to many existing limitations. One of the most influential trends is the continued advancement of high-throughput sequencing technologies and next-generation metabolomics. Declining sequencing costs and improved analytical sensitivity are enabling large-scale genomic and metabolomic profiling across diverse horticultural crops. These developments are expected to expand coverage beyond major crops to include underutilized species, landraces and wild relatives, enriching reference datasets and supporting broader application of integrative fingerprinting. Next-generation metabolomics platforms, including high-resolution and ultra-fast mass spectrometry systems, are enhancing metabolite coverage, detection sensitivity and analytical throughput. Coupled with improved sample preparation and automation, these technologies will facilitate routine metabolomic fingerprinting in breeding programs, quality control laboratories and supply chains. The integration of targeted and untargeted metabolomics approaches is expected to improve both compound identification and functional interpretation.

Artificial intelligence (AI) and machine learning are emerging as powerful tools for fingerprint analysis and interpretation. These data-driven approaches can handle high-dimensional multi-omics datasets, identify complex patterns and uncover non-linear relationships between genetic variation, metabolite profiles and phenotypic traits. In horticulture, AI-based models have the potential to improve cultivar classification, predict quality attributes, detect adulteration and forecast crop performance under different environmental scenarios. As computational tools become more accessible and user-friendly, AI-driven fingerprinting is likely to become an integral component of precision horticulture. Another important trend is the development of portable and rapid fingerprinting tools. Miniaturized spectroscopic devices, handheld sensors and field-deployable analytical platforms are increasingly capable of generating rapid chemical or spectral fingerprints without extensive sample preparation. While these tools may not match the resolution of laboratory-based instruments, they offer significant advantages for on-site quality assessment, traceability and decision-making in real time. Integration of portable tools with cloud-based databases and AI analytics could enable decentralized and scalable fingerprinting applications across horticultural value chains. Integrative genome-metabolome fingerprinting is also expected to play a crucial role in climate-resilient horticulture. As climate change intensifies environmental stresses and variability, understanding how genetic diversity translates into metabolic resilience will be essential for developing robust cultivars. Integrated approaches can identify genetic and metabolic traits associated with stress tolerance, nutritional stability and adaptive capacity, supporting the breeding and deployment of climate-resilient horticultural crops. In this context, integrative fingerprinting moves beyond characterization toward predictive and adaptive crop management.

8. Conclusion

Over the past decades, significant advances in DNA fingerprinting and chemical fingerprinting have transformed horticultural research and practice. DNA-based markers have provided robust tools for genetic identification, diversity analysis, cultivar protection and breeding, while chemical fingerprinting has enabled comprehensive assessment of quality, nutrition, authenticity and functional properties. Together, these approaches have addressed many limitations of conventional morphological and biochemical characterization methods. The integration of genomic and metabolomic information represents a major conceptual and practical advancement. Integrative genome-metabolome fingerprinting bridges the gap between genetic potential and biochemical expression, offering a systems-level understanding of horticultural crop identity and quality. By linking DNA markers with metabolite profiles through multiomics and bioinformatics frameworks, this approach enhances the precision, reliability and functional relevance of crop characterization. Looking ahead, continued technological innovation, improved data integration and wider accessibility will further expand the impact of genome-metabolome fingerprinting. Emerging tools such as AI-driven analytics, next-generation metabolomics and portable fingerprinting devices are expected to accelerate translation from research to practice. Ultimately, integrative fingerprinting approaches hold strong promise for shaping a future of horticulture that is more precise, resilient and capable of meeting global demands for high-quality, nutritious and authentic plant-based products.

Acknowledgements

Conflict of interest

The authors declare no conflicts of interest relevant to this article.

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