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ECOLOGICAL DRIVERS AND EVOLUTIONARY SIGNIFICANCE OF CHEMICAL DIVERSITY IN PLANT SECONDARY METABOLITES

Rajesh Gajanan Dagor *

Dayal Institute of Pharmaceutical Sciences, Lucknow, India.

* Corresponding Author

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ABSTRACT

Plant secondary metabolites represent one of the most diverse and functionally sophisticated groups of bioactive molecules found in nature. This chemical diversity, encompassing alkaloids, terpenoids, phenolics, and countless other specialized compounds, is not merely a taxonomic artifact but arises from complex interactions between ecological pressures, evolutionary innovation, and multi-organism interactions that shape biosynthetic pathways over time. This review provides a comprehensive synthesis of the ecological and evolutionary drivers that generate and maintain chemodiversity in plants. We critically examine how abiotic factors—including light, temperature, water availability, soil nutrients, and UV radiation—shape secondary metabolite profiles, and how biotic interactions with herbivores, pathogens, pollinators, and neighboring plants drive chemical diversification through coevolutionary arms races and mutualistic associations. Furthermore, we explore the evolutionary mechanisms underlying chemical diversity, including gene duplication, neofunctionalization, positive selection, and the role of biosynthetic gene clusters in facilitating adaptive evolution. Recent advances in metabolomics, genomics, and chemical ecology have fundamentally redefined our understanding of how these compounds are generated, regulated, and functionally deployed in nature. Despite significant progress, substantial gaps remain in understanding the interplay between phylogenetic constraints and ecological adaptation. This review identifies emerging research directions and discusses the implications of chemodiversity for ecosystem functioning, conservation, and bioprospecting.

Keywords: Chemodiversity; Plant Secondary Metabolites; Ecological Drivers; Coevolution; Biosynthetic Gene Clusters; Adaptive Evolution

1 INTRODUCTION

Plants produce an extraordinary diversity of secondary metabolites, estimated to exceed 200,000 compounds, making them the most prolific chemists on Earth (Zhan et al., 2022). These specialized metabolites—including alkaloids, terpenoids, phenolics, glucosinolates, and countless other classes—are not merely byproducts of primary metabolism but serve essential ecological functions in plant adaptation, defense, and reproduction (Zhan et al., 2022). Plant specialized metabolites (PSMs) play essential roles in the adaptation to harsh environments and function in plant defense responses, acting as key components of defense-related signaling pathways and triggering the extensive expression of defense-related genes (Zhan et al., 2022). In addition, PSMs serve as antioxidants, participating in the

scavenging of rapidly rising reactive oxygen species, and as chelators, participating in the chelation of toxins under stress conditions (Zhan et al., 2022).

Natural products represent one of the most diverse and functionally sophisticated groups of bioactive molecules found across plants, fungi, bacteria, and marine organisms (Flores et al., 2025). Recent advances in genomics, metabolomics, and chemical ecology have fundamentally redefined how these compounds are generated, regulated, and functionally deployed in nature. Increasing evidence reveals that chemical diversity arises not solely from taxonomic lineage but from ecological pressures, evolutionary innovation, and multi-organism interactions that shape biosynthetic pathways over time (Flores et al., 2025). Hybrid metabolic architectures, context-dependent activation of biosynthetic gene clusters, and cross-kingdom metabolic integration collectively portray a biosynthetic landscape far more dynamic and interconnected than previously understood (Flores et al., 2025).

Natural biodiversity is one of the primary drivers of chemical innovation in both terrestrial and marine ecosystems (Flores et al., 2025). Classic examples such as morphine, quinine, digitoxin, and artemisinin illustrate how ecological pressures, including herbivory, microbial antagonism, symbiosis, and environmental stress, shape secondary metabolism and generate compounds with potent biological activities (Flores et al., 2025). Over the past decades, natural-product research has undergone a profound transformation, with advances in extraction technologies and high-resolution analytical platforms shifting the discovery pipeline from traditional empirical screening toward data-driven strategies rooted in metabolomics, chemoinformatics, and systems biology (Flores et al., 2025).

This review provides a comprehensive synthesis of the ecological and evolutionary drivers that generate and maintain chemodiversity in plants. We critically examine how abiotic and biotic factors shape secondary metabolite profiles, explore the evolutionary mechanisms underlying chemical diversity, and identify emerging research directions for understanding the interplay between phylogenetic constraints and ecological adaptation.

2 ABIOTIC DRIVERS OF CHEMICAL DIVERSITY

2.1 Light and UV Radiation

Light is one of the most critical environmental factors influencing plant secondary metabolism. Plants exposed to high light intensities and UV radiation typically exhibit enhanced production of phenolic compounds, particularly flavonoids and anthocyanins, which function as UV screens and antioxidants. The production of these UV-absorbing compounds represents an adaptive response to protect photosynthetic tissues from damage caused by excessive radiation.

Studies have demonstrated that UV-B radiation specifically induces the accumulation of flavonoids and other phenolic compounds through the activation of phenylpropanoid pathway enzymes. The regulatory mechanisms involve photoreceptors and downstream signaling cascades that coordinate the expression of biosynthetic genes. The intensity and spectral composition of light also influence the production of terpenoids and alkaloids, with blue and red light wavelengths having differential effects on specific metabolic pathways.

2.2 Temperature Extremes

Temperature is a major abiotic stressor that profoundly affects plant secondary metabolism. Both heat and cold stress trigger the accumulation of specialized metabolites that function in stress tolerance. Heat stress typically induces the production of heat-shock proteins and compatible solutes, while also modulating the accumulation of phenolic compounds and terpenoids that protect cellular membranes from oxidative damage.

Cold stress, on the other hand, often leads to the accumulation of anthocyanins and other phenolic compounds that provide photoprotection during periods of low temperature when photosynthetic efficiency is reduced. The biosynthesis of these compounds is regulated by complex signaling networks involving hormones such as abscisic acid and jasmonic acid, which integrate temperature signals with metabolic responses.

2.3 Water Availability and Drought

Drought stress is one of the most significant environmental constraints on plant growth and productivity, and it profoundly influences secondary metabolite profiles. Plants experiencing water deficit typically accumulate osmolytes, including proline and glycine betaine, along with phenolic compounds and terpenoids that function in osmotic adjustment and oxidative stress protection. The production of these compounds is regulated by abscisic acid signaling and involves the activation of specific transcription factors that coordinate stress responses.

The relationship between drought and secondary metabolism is complex, with the magnitude and direction of metabolic changes depending on the severity and duration of stress, as well as the species and developmental stage. Moderate drought stress often enhances the accumulation of bioactive compounds in medicinal plants, while severe drought may inhibit biosynthesis due to photosynthetic limitations.

2.4 Soil Nutrients

Nutrient availability, particularly nitrogen and phosphorus, significantly influences plant secondary metabolism. Nitrogen availability affects the production of nitrogen-containing secondary metabolites, including alkaloids and glucosinolates, with higher nitrogen levels typically promoting their accumulation. Conversely, phosphorus deficiency often enhances the production of phenolic compounds and terpenoids, reflecting the carbon-based nature of these metabolites under nutrient limitation.

The plant's response to changes in nutrient supply relies heavily on ecological constraints that limit plant productivity. The allocation of resources between primary and secondary metabolism is governed by trade-offs that reflect the plant's evolutionary history and ecological context. Understanding these nutrient-mediated responses is essential for predicting how environmental changes will affect plant chemodiversity.

2.5 Multiple Stress Interactions

In nature, plants rarely experience single stress factors in isolation. The combined effects of multiple abiotic stresses—such as drought combined with high temperature or UV radiation—can have synergistic or antagonistic effects on secondary metabolism. The integration of multiple stress signals through shared signaling pathways and transcription factors results in metabolic responses that are often distinct from those induced by individual stresses.

The co-occurrence of stresses can lead to the activation of overlapping sets of biosynthetic genes, resulting in the accumulation of compounds that provide protection against multiple stressors simultaneously. Understanding these complex interactions is essential for predicting how climate change and other environmental perturbations will affect plant chemodiversity.

Table 1: Abiotic Stress Factors and Their Effects on Plant Secondary Metabolism

Stress Factor	Primary Response	Secondary Metabolites Affected	Regulatory Mechanisms	Adaptive Significance
High Light / UV	Photoprotection & ROS dissipation	Flavonoids, anthocyanins, phenolic acids	Phenylpropanoid pathway upregulation, UVR8 photoreceptor signaling	UV screening/absorption, ROS scavenging, cellular photoprotection
Heat Stress	Thermotolerance & protein stabilization	Heat shock proteins (HSPs), phenolics, terpenoids	Heat shock factors (HSFs), ABA-mediated signaling pathways	Cell membrane stabilization, protection against oxidative denaturation
Drought	Osmotic adjustment & stomatal regulation	Proline, glycine betaine, phenolics, terpenoids	ABA signaling cascade, stress-responsive TFs (<i>MYB</i> , <i>WRKY</i> , <i>bZIP</i>)	Osmoprotection, ROS scavenging, maintenance of cell turgor
Cold Stress	Cryoprotection & membrane fluidity maintenance	Anthocyanins, phenolics, compatible solutes (<i>sugars</i>)	CBF/DREB regulon activation, ABA & calcium signaling	Photoinhibition defense, cell membrane stabilization, freezing tolerance
Nutrient Limitation	Resource allocation shift (<i>C/N balance</i>)	Phenolics, terpenoids (<i>N limit</i>); Alkaloids, glucosinolates (<i>P limit</i>)	Nutrient sensing pathways (<i>TOR/SnRK1</i>), hormonal crosstalk	Resource optimization, defense molecule trade-off, metabolic reprogramming

3 BIOTIC DRIVERS OF CHEMICAL DIVERSITY

3.1 Plant-Herbivore Coevolution

The coevolutionary arms race between plants and herbivorous insects is perhaps the most powerful driver of chemical diversity in plants. Ehrlich and Raven's metaphors of coevolution encompass both the mechanism and outcomes of evolution, functioning at different hierarchical scales (Plant-herbivore interactions, 2018). The "arms race" represents the explanatory process of patterns that emerge at ecological or phylogenetic scales, while the "escape and radiation" represents the outcome, i.e., the phylogenetic patterns (Plant-herbivore interactions, 2018).

Over the course of evolution, plants have evolved mechanisms to defend themselves against herbivory, whereas herbivorous insects have evolved counter-mechanisms to overcome these defenses in co-evolutionary arms races (Genetic variation in plant chemistry, 2024). Plant chemical defenses play a central role in this coevolutionary arms race with herbivorous insects (Independent evolution of ancestral and novel defenses, 2024). In response to diverse environmental challenges, plants have evolved a plethora of structurally diverse organic compounds with repellent, antinutritive, and toxic properties (Independent evolution of ancestral and novel defenses, 2024).

Plants produce a diverse array of secondary metabolites, including terpenes, phenolics, nitrogen-containing compounds, and sulfur-containing compounds, to deter herbivorous insects (Figure 2, 2025). The expression of secondary metabolites is governed both by evolution (i.e., one-way adaptation in response to generalized herbivory) and coevolution (i.e., specific reciprocal adaptation between the interacting host and a herbivore species) (Combining Evolutionary Inference, 2019).

The defensive function of plant secondary compounds has been extensively documented. Besides pathogens and nematodes, chemical defenses of plants are usually induced by herbivorous insect attack (Plant-herbivore interactions, 2018). Plants of the genus *Bursera* produce a set of monoterpenes distributed in a network of channels in the stems and leaves, with leaf damage resulting in a rapid release of fluids toxic to herbivores at the site of damage (Plant-herbivore interactions, 2018). Other substances released after the attack of herbivores, such as some resins in latex, besides being toxic, may reduce digestibility (Plant-herbivore interactions, 2018).

3.2 Pathogen Interactions

Plant-pathogen interactions represent another significant driver of chemical diversity. Pathogens, including fungi, bacteria, and viruses, exert strong selective pressure on plants to develop chemical defenses. Plants produce phytoalexins—antimicrobial compounds synthesized *de novo* in response to pathogen attack—along with constitutive antimicrobial compounds such as saponins and phenolic compounds.

The recognition of pathogen-associated molecular patterns triggers immune responses that include the production of antimicrobial secondary metabolites. The diversity of plant-pathogen interactions has driven the evolution of an extensive array of antimicrobial compounds with diverse modes of action. The coevolutionary dynamics between plants and pathogens continue to shape the chemical diversity of both partners.

3.3 Pollinator and Mutualist Interactions

While much attention has focused on defensive secondary metabolites, many plant compounds have evolved to attract pollinators and mutualists. Floral volatile compounds, including terpenoids and benzenoids, serve as attractants for insect pollinators, while nectar compounds may deter non-pollinating visitors. The chemical diversity of floral volatiles reflects the diverse sensory preferences of different pollinator taxa.

Similarly, compounds involved in plant-microbe mutualisms, including flavonoids that signal to nitrogen-fixing rhizobia and strigolactones that attract mycorrhizal fungi, contribute to the overall chemical diversity of plants. These mutualistic interactions have driven the evolution of specific chemical signals that mediate beneficial associations, adding another dimension to plant chemodiversity.

3.4 Plant-Plant Interactions and Allelopathy

Plants also interact chemically with neighboring plants through allelopathy—the release of compounds that inhibit the growth of competing species. Allelopathic compounds, including phenolics, terpenoids, and alkaloids, contribute to the chemical diversity of plant communities and influence species composition and ecosystem dynamics.

The production of allelopathic compounds can vary with environmental conditions and may be influenced by the presence of competing species. This chemical interference represents an additional selective pressure that has contributed to the evolution of diverse secondary metabolites. The role of plant-plant signaling through volatile

compounds, where damaged plants release signals that alert neighboring plants to impending threats, further illustrates the complexity of chemical interactions in plant communities.

3.5 Multi-Organism Interactions and Meta-Organismal Chemistry

Increasing evidence reveals that chemical diversity arises not solely from taxonomic lineage but from ecological pressures, evolutionary innovation, and multi-organism interactions that shape biosynthetic pathways over time (Flores et al., 2025). Hybrid metabolic architectures, context-dependent activation of biosynthetic gene clusters, and cross-kingdom metabolic integration collectively portray a biosynthetic landscape far more dynamic and interconnected than previously understood (Flores et al., 2025).

The concept of meta-organismal chemistry recognizes that the chemical repertoire of a plant includes compounds produced by associated microorganisms, including endophytes and rhizosphere microbes. These microbial partners can contribute to the production of bioactive compounds, modify plant-produced metabolites, or induce changes in plant metabolism. This multi-organismal dimension of chemodiversity adds significant complexity to our understanding of chemical diversity in nature.

Table 2: Biotic Interactions and Their Influence on Plant Secondary Metabolism

Interaction Type	Primary Selective Pressure	Secondary Metabolites Involved	Evolutionary Dynamics	Ecological Consequences
Plant-Herbivore	Herbivory avoidance & tissue damage reduction	Alkaloids, terpenoids, phenolics, glucosinolates	Coevolutionary arms race (<i>Ehrlich-Raven model</i>)	Rapid diversification and specialized expression of defense compounds
Plant-Pathogen	Infection resistance & pathogen containment	Phytoalexins, saponins, phenolic acids	Dynamic coevolutionary interactions (<i>Gene-for-gene model</i>)	Broad-spectrum antimicrobial compound diversity and structural variation
Plant-Pollinator	Pollinator attraction & vector fidelity	Floral volatiles, monoterpenes, sesquiterpenes, benzenoids	Mutualistic coevolution & trait matching	Chemical communication diversity and floral specialization
Plant-Microbe	Mutualism establishment (<i>e.g., mycorrhizae, rhizobia</i>)	Flavonoids, strigolactones, cyclic lipopeptides	Mutualistic co-adaptation & metabolic integration	High signal molecule diversity for host-symbiont recognition
Plant-Plant	Competition for space, light, & soil nutrients	Allelopathic compounds (<i>e.g., juglone, sorgoleone</i>), volatile signals	Competitive coevolution & chemical warfare	Shifts in plant community structure, succession, and spatial patterning

4 EVOLUTIONARY MECHANISMS UNDERLYING CHEMICAL DIVERSITY

4.1 Gene Duplication and Neofunctionalization

Gene duplication provides the raw material for the evolution of new metabolic functions. Duplicated genes can acquire new functions through neofunctionalization, where one copy retains the original function while the other evolves a novel activity. This process has been instrumental in the evolution of plant secondary metabolism, where gene families involved in the biosynthesis of alkaloids, terpenoids, and phenolics have undergone extensive expansion and diversification.

Positive selection driving diversification in plant secondary metabolism has been demonstrated, with results showing that gene duplication, neofunctionalization, and positive selection provide the mechanism for biochemical adaptation in plant defense (Positive selection driving diversification, 2006). These processes occur repeatedly in the history of gene families, indicating their fundamental importance for the evolution of plant metabolic diversity both within and among species (Positive selection driving diversification, 2006).

4.2 Enzyme Promiscuity and Pathway Evolution

The evolutionary implications of enzyme promiscuity-generated pathway branchpoints are not well understood. It has been postulated that the permissiveness of an enzyme may encourage the retention of gene duplicates, which could favour subsequent functional specialization or neo-functionalization (Open data phylometabolomics, 2026). A minor metabolite may exhibit desirable activities in response to fluctuating abiotic and biotic ecological changes (Open data phylometabolomics, 2026).

Enzyme promiscuity—the ability of an enzyme to catalyze multiple reactions—provides a mechanism for the evolution of new metabolic pathways. Promiscuous enzymes can generate novel compounds that may acquire adaptive functions, providing the starting material for the evolution of new biosynthetic pathways. This process contributes to the ongoing diversification of plant secondary metabolism.

4.3 Biosynthetic Gene Clusters

Biosynthetic genes of selected secondary metabolites cluster within localized chromosomal regions (Cawood et al., 2025). The arrangement of these biosynthetic gene clusters (BGCs) challenges the long-held model of random gene order in eukaryotes, raising questions about their regulation, ecological significance, and evolution (Cawood et al., 2025). BGCs contribute to ecologically relevant plant-biotic interactions, while molecular-(epi)genetic mechanisms control their coordinated stress- and tissue-specific expression (Cawood et al., 2025).

Based on evidence that BGCs have distinct chromatin signatures and are enriched with transposable elements, emerging hypotheses into an updated evolutionary model emphasize how stress-induced epigenetic processes have shaped BGC formation (Cawood et al., 2025). The clustering of biosynthetic genes facilitates the coordinated regulation of complex metabolic pathways and may enable the horizontal transfer of entire pathways between organisms.

4.4 Phylogenetic Constraints and Functional Convergence

Although phylogenetic relatedness influences plant chemodiversity, functional convergence of tissue-specific metabolites may be a major evolutionary driver (Sources of variation, 2025). Studies using model systems have examined the extent to which phytochemical diversity is shaped by tissue-specific function and the degree to which phylogenetic relatedness explains variation in chemodiversity (Sources of variation, 2025). Fruit and leaf metabolomes were more similar to the same organ in other species than to the other organs within the same species, indicating that functional convergence of tissue-specific metabolites may be a major evolutionary driver (Sources of variation, 2025).

Macroevolution of plant chemistry integrates both diversification and constraint (Open data phylometabolomics, 2026). While lineages replace most of their metabolites through extreme turnover, they do so within the boundaries of clade-specific constraints, but diversification remains channeled by inherited constraints that keep each lineage within characteristic physicochemical and biosynthetic neighborhoods (Open data phylometabolomics, 2026).

4.5 Beyond Ecological Drivers: Intrinsic Functions

Traditionally, the evolution of specialized metabolites has been studied primarily through the lens of plants' ecological interactions with herbivores, pathogens, and pollinators, as many of them exhibit defense and/or attraction functions (Xu and Gaquerel, 2025). However, increasing evidence suggests that many specialized metabolites, along with their precursors, also act as cellular signals that regulate cell growth and differentiation (Xu and Gaquerel, 2025). These intrinsic functions are at least equally important factors in shaping the evolution of plant chemical defenses (Xu and Gaquerel, 2025).

The recognition that specialized metabolites have intrinsic cellular functions beyond their ecological roles has expanded our understanding of the forces shaping chemodiversity. These intracellular functions may represent the ancestral functions of many specialized metabolites, with ecological roles evolving later as plants adapted to diverse environments and interactions.

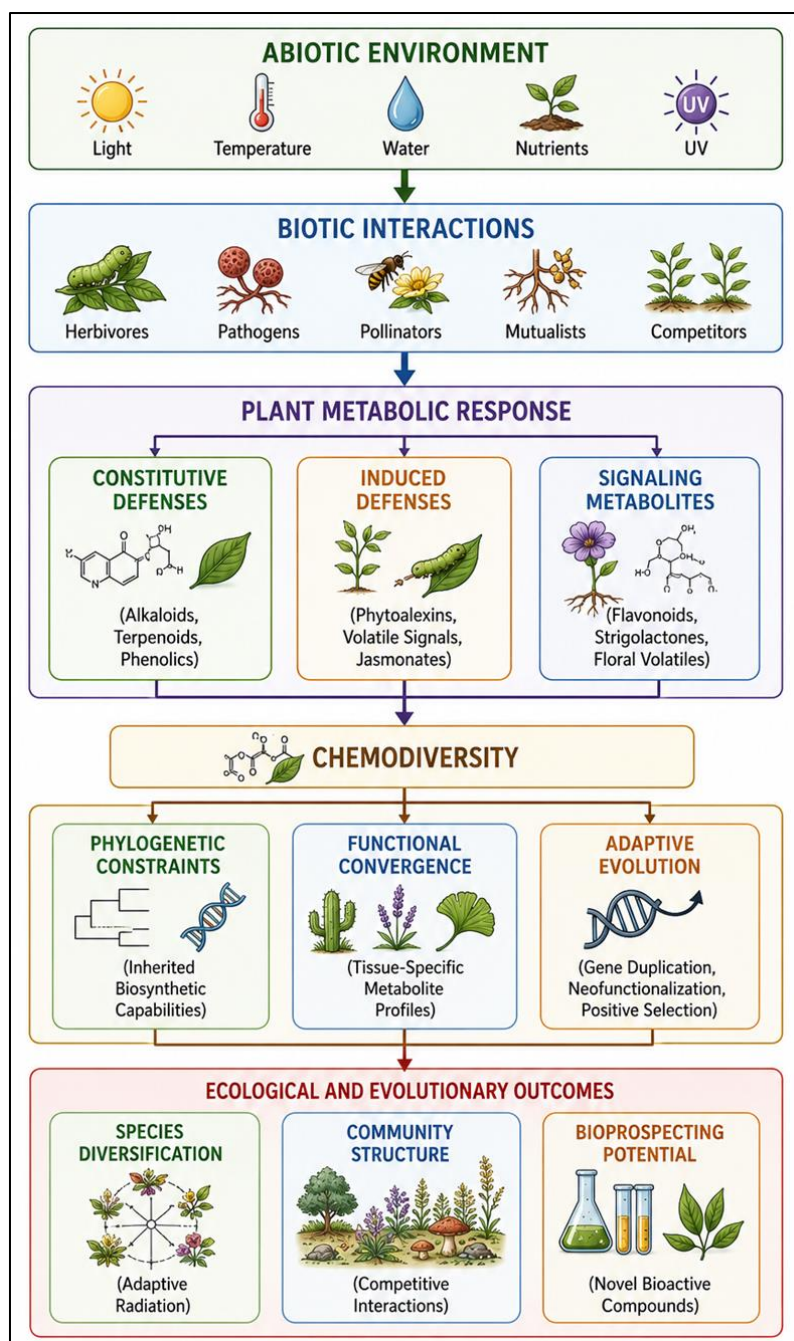


Figure 1: Conceptual Framework for Ecological and Evolutionary Drivers of Plant Chemodiversity

5 CONSEQUENCES OF CHEMODIVERSITY FOR ECOSYSTEM FUNCTIONING

5.1 Community Structure and Dynamics

The chemical diversity of plant communities influences species composition, competitive interactions, and ecosystem dynamics. Chemically diverse plant communities may be more resistant to herbivore outbreaks and pathogen spread, as the diversity of defense compounds creates a heterogeneous chemical landscape that limits the ability of specialized herbivores to exploit host plants.

Phytochemical diversity is an important aspect of the functional diversity of plants and the biodiversity of ecosystems (Beyond phylogeny, 2025). Studies have detected thousands of unique phytochemical features across regenerating woody species, revealing chemically heterogeneous plant communities dominated by alkaloids and terpenoids (Phytochemical diversity, 2026). The diversity of chemical defenses at the community level contributes to ecosystem stability and resilience.

5.2 Ecosystem Services

Plant chemodiversity underpins numerous ecosystem services, including pollination, pest regulation, and nutrient cycling. The chemical diversity of floral volatiles supports diverse pollinator communities, while the diversity of antimicrobial compounds contributes to disease suppression in plant communities. The production of allelopathic compounds influences plant community composition and succession.

The medicinal and nutritional value of plant communities is also directly related to their chemical diversity. Chemically diverse plant communities provide a wider range of bioactive compounds with potential applications in medicine, agriculture, and industry.

5.3 Implications for Conservation and Bioprospecting

Understanding the ecological and evolutionary drivers of chemodiversity has important implications for conservation and bioprospecting. The loss of biodiversity threatens not only species but also the chemical diversity they harbor. Conserving chemically diverse plant communities is essential for maintaining the full spectrum of bioactive compounds that may have future pharmaceutical or agricultural applications.

Bioprospecting efforts that are informed by ecological and evolutionary knowledge may be more successful in identifying novel bioactive compounds. Species that have evolved under strong selective pressures, such as those in biodiversity hotspots or extreme environments, may be particularly rich sources of novel chemistry. However, bioprospecting must be conducted sustainably, with respect for biodiversity conservation and indigenous knowledge rights.

6 CHALLENGES AND RESEARCH GAPS

6.1 Integrating Multiple Drivers

A major challenge in understanding plant chemodiversity is integrating the multiple ecological and evolutionary drivers that operate simultaneously. The interplay between a vast array of factors driving plant chemodiversity remains unclear, mainly because most studies have focused on a single organ—mostly leaves—or, when comparing different organs, have been limited to single taxa (Sources of variation, 2025). Thus, the relationship between functional and phylogenetic factors remains unresolved (Sources of variation, 2025).

Future research must adopt more holistic approaches that consider the combined effects of abiotic and biotic factors, phylogenetic constraints, and developmental regulation on chemical diversity. Multi-omics approaches that integrate metabolomics, genomics, transcriptomics, and ecological data offer promising avenues for addressing this complexity.

6.2 Scaling from Molecules to Ecosystems

Bridging the gap between molecular mechanisms and ecosystem-level patterns remains a significant challenge. While we have detailed knowledge of individual biosynthetic pathways and their regulation, understanding how these pathways scale to produce the chemical diversity observed at the community and ecosystem levels requires new analytical and conceptual approaches.

The development of community metabolomics and chemical ecology approaches that can characterize the chemical diversity of entire plant communities offers opportunities for addressing this scaling challenge. These approaches can reveal patterns of chemical diversity that are not apparent from studies of individual species or pathways.

6.3 Evolutionary Dynamics in Changing Environments

Understanding how plant chemodiversity will respond to ongoing environmental changes, including climate change, habitat loss, and species invasions, is an urgent research priority. Environmental changes can alter the selective pressures that drive chemical diversity, potentially leading to the loss of chemically diverse phenotypes or the evolution of novel chemical profiles.

Long-term studies and experimental evolution approaches are needed to understand the evolutionary dynamics of plant secondary metabolism in changing environments. These studies can reveal the capacity of plant populations to adapt chemically to new environmental conditions and the consequences of chemical adaptation for ecosystem functioning.

7 FUTURE PERSPECTIVES

The future of research on ecological and evolutionary drivers of plant chemodiversity lies in the integration of multi-omics approaches and systems biology. The application of metabolomics, genomics, transcriptomics, and chemical ecology will enable comprehensive characterization of the factors that generate and maintain chemical diversity in plants. The integration of phylogenomics and metabolomics will reveal the evolutionary history of biosynthetic pathways and the constraints that shape chemical diversification.

The development of predictive models for plant chemodiversity will facilitate understanding of how environmental changes will affect chemical diversity and its ecological functions. The application of artificial intelligence and machine learning approaches to metabolomic and genomic data promises to accelerate the discovery of novel compounds and the identification of their ecological functions.

The exploration of understudied ecosystems and plant lineages may reveal novel chemical diversity and new insights into the drivers of chemodiversity. The integration of chemical ecology with conservation biology will inform strategies for preserving chemical diversity in the face of environmental change. Continued interdisciplinary collaboration between chemists, ecologists, evolutionary biologists, and conservation scientists is essential for advancing understanding of plant chemodiversity and its implications for ecosystem functioning and human well-being.

8 CONCLUSION

Plant secondary metabolites represent one of the most diverse and functionally sophisticated groups of bioactive molecules in nature. This chemical diversity arises from the complex interplay of ecological pressures and evolutionary innovations that shape biosynthetic pathways over time. Abiotic factors including light, temperature, water availability, soil nutrients, and UV radiation profoundly influence secondary metabolite profiles, while biotic interactions with herbivores, pathogens, pollinators, and neighboring plants drive chemical diversification through coevolutionary arms races and mutualistic associations.

The evolutionary mechanisms underlying chemical diversity include gene duplication and neofunctionalization, enzyme promiscuity, biosynthetic gene clusters, and the interplay between phylogenetic constraints and functional convergence. The recognition that specialized metabolites have intrinsic cellular functions beyond their ecological roles has expanded our understanding of the forces shaping chemodiversity.

Understanding the ecological and evolutionary drivers of plant chemodiversity has important implications for ecosystem functioning, conservation, and bioprospecting. Continued research, employing integrated multi-omics approaches and interdisciplinary collaboration, will advance our understanding of chemodiversity and its role in plant adaptation, ecosystem dynamics, and the discovery of novel bioactive compounds.

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