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EDITORIAL

Ecology and evolution of plant chemodiversity

Plants produce an extraordinary variety of specialized (secondary) metabolites, a phenomenon known as phytochemical diversity, or in short, chemodiversity. This diversity is now recognized as a key component of plant ecology and evolution (Wetzel & Whitehead 2020; Petrén *et al.* 2024; Thon *et al.* 2024). Chemical traits and their diversity are functionally as important as morphological or physiological traits and should be considered integral components of a plant's ecological niche (Müller & Junker 2022; Walker *et al.* 2022). The composition of plant metabolites can vary widely across different species, between various tissues and organs, during different development stages, among individual plants, and between different populations. Moreover, the quality and quantity of plant metabolites are highly influenced by the environment, where various abiotic and biotic factors modulate the plant metabolism and chemodiversity in a fine-tuned way. In turn, these metabolites influence interactions with mutualists such as pollinators, antagonists such as herbivores, microorganisms functioning as mutualists or antagonists, and other plant species. This special issue compiles research that systematically explores these dimensions of chemodiversity.

Variation within individuals arises between organs or tissues and across development stages. For example, within herbaceous species, such as *Tanacetum vulgare* (Asteraceae) and *Solanum dulcamara* (Solanaceae), substantial differences have been found in both volatile and non-volatile compounds across plant parts, with roots generally differing in plant metabolite composition and exhibiting lower chemodiversity than leaves and flowers (Anaia *et al.* 2024; Rahimova *et al.* 2024; Ziaja & Müller 2025). Chemical patterns also change over ontogeny, as shown for volatile terpenes from the same organs sampled repeatedly, which become more chemodiverse over time (Ziaja & Müller 2025). Similar trends were reported for *Erysimum cheiranthoides* (Brassicaceae), where non-volatile cardenolides became more abundant between leaves of different ages over time (Wang & Züst 2025). Organ-specific metabolites were also found in fruits, leaves and roots of the neotropical shrubs *Psychotria* and *Palicourea* (Rubiaceae), changing across ontogeny (Schneider & Beckman 2025). In contrast, the composition of metabolites in the secretory ducts, newly described for the shrub *Baccharis platypoda* (Asteraceae), were found to be similar between female and male inflorescences (Cassola *et al.* 2024). As in herbs, in trees, such as *Populus nigra* (Salicaceae), significant chemical differences of both primary and specialized metabolites exist between organs, including shoot tips, wood, bark, leaves and roots (Bose *et al.* 2024; Yepes Vivas *et al.* 2025).

The expanding toolbox of metabolomics, including targeted and non-targeted approaches using different GC- and LC–MS techniques, has tremendously enhanced our ability to analyze plant chemistry. Non-invasive sampling of volatile organic compounds enables us to capture chemical pattern at high temporal resolution (Ziaja & Müller 2025). Statistical tools, such as the R package *chemodiv*, facilitate the quantification of chemodiversity (Petrén *et al.* 2023). Integrating metabolomics with genomics and transcriptomics advances decoding of the biosynthetic pathways underlying chemical traits (Wyatt *et al.* 2024; Aboshi *et al.* 2025; Zenchyzen *et al.* 2025). Electron microscopy and histochemical staining offer fine-scale anatomical mapping of the morphological structures in which these metabolites are stored (Cassola *et al.* 2024; Zenchyzen *et al.* 2025). Characterizing the organ- and tissue-level metabolite profiles across different plant genotypes paves the way for development of metabolic atlases (e.g., for terpenoids) for plant species (Rahimova *et al.* 2024).

Specialized metabolites can also vary spatially in composition within species across regions, as nicely shown for alkaloids in *Senecio pterophorus* (Asteraceae) (Castells & Sanchez-Martinez 2024) and for floral scents of the leafy vegetable *Gynandropsis gynandra* (Cleomaceae) (Zenchyzen *et al.* 2025), both sampled across continents. In the latter species, variation in floral scents across accessions could be correlated to variations in flower morphology and supported by transcriptomic data (Zenchyzen *et al.* 2025). Furthermore, the distinct flowers are pollinated by different insect species, suggesting that subspecies of *G. gynandra* may be distinguished on the basis of these large differences (Zenchyzen *et al.* 2025). Even in gymnosperms, volatile profiles vary geographically, as shown in the fruit-scented cones of *Cycas revoluta* (Cycadaceae). Here, the chemodiversity of the volatiles matches the genetic boundaries of this species (Chang *et al.* 2025). Variation in chemical and genetic diversity within wild populations may also provide valuable insights into the utilization and conservation of species important for brewing and traditional medicine, as demonstrated, for example, in wild hop (*Humulus lupulus*, Cannabaceae), which is rich in several essential oils (Salihu *et al.* 2024). Chemical dissimilarity has been found to correlate with phylogenetic distance, although these relationships appear to be tissue-specific, as revealed in ripe pericarps and leaves of *Psychotria* and *Palicourea* (Schneider & Beckman 2025). Furthermore, chemodiversity may be modified by hybridization, offering a tool for hybrid identification when combined with genetic and morphological data. In hybrids of *Cenostigma* trees, compounds were detected that were absent in the parent species (Aecyo *et al.* 2024), while overall chemodiversity did not increase. Phylogenetic correlations with chemical distance (Schneider & Beckman 2025), together with links between genetic and chemical diversity (Salihu *et al.* 2024), provide multi-layered perspectives on chemodiversity at different levels and help in deciphering evolutionary trajectories.

From an ecological perspective, plant chemodiversity is also of crucial importance. Changes in the composition of alkaloids and their chemodiversity were found in *S. pterophorus* along an aridity gradient, indicating adaptive differentiation, as demonstrated in plants growing under both natural and common garden conditions (Castells & Sanchez-Martinez 2024). Evolutionary neutral processes as drivers of this pattern could be excluded in this study (Castells & Sanchez-Martinez 2024). Similarly, high concentrations of certain phenolics in *Baccharia platypoda* suggest adaptation to extreme UV exposure at high altitudes (Cassola *et al.* 2024). Distinct metabolite profiles were also found in both natural and experimental populations of the perennial grass *Festuca rubra* (Poaceae) along an altitudinal gradient, with plants at mid-elevations showing highest chemodiversity (Nomoto *et al.* 2025). Rapid shifts in the environmental conditions related to climate change may affect intraspecific chemodiversity and accelerate shifts in metabolomes.

The specific chemical composition and overall chemodiversity are probably key drivers in shaping plant interactions with other organisms. Terpenoid chemodiversity in individuals and groups of *T. vulgare* revealed impacts on growth and reproductive traits, being thus involved in plant–plant interactions (Ojeda-Prieto *et al.* 2024). Root exudates of several cereals showed different potential to suppress growth of an arable weed, black-grass (*Alopecurus myosuroides*, Poaceae), but these differences could not be explained by variation in individual benzoxazinoids and may therefore be related to (mixtures of) other metabolites with allelopathic potential (Hickman *et al.* 2025).

Insect herbivory can lead to distinct, often highly organ-specific, changes in plant chemistry, as revealed in several studies in this special issue, including trees (*Populus nigra*, *Buxus sempervirens*) (Hay *et al.* 2024; Yepes Vivas *et al.* 2025) and herbaceous species (within Cucurbitaceae) (Thompson *et al.* 2024). Changes were more pronounced in above- compared to belowground organs in all those species. In addition, responses to herbivory were more pronounced in primary metabolites as compared to specialized metabolites, as found in *Populus nigra* infested with the generalist herbivore *Lymantria dispar* (Yepes Vivas *et al.* 2025), as well as in *Buxus sempervirens* infested with the invasive box tree moth, *Cydalima perspectalis*, with increases in most amino acids and decreases in carbohydrates (Hay *et al.* 2024). Herbivory also led to enhanced biosynthesis and diversification of triterpenoids and alkaloids in *B. sempervirens*, underscoring fine-tuned metabolic orchestration in both leaves and roots (Hay *et al.* 2024). Herbivore-induced volatile emissions in leaves and roots were compared across six Cucurbitaceae species, differing in domestication status. Notably, domesticated species exhibited greater volatile diversity in leaves than their wild counterparts, highlighting the role of domestication in modulating plant defences and shaping chemodiversity (Thompson *et al.* 2024).

Conversely, plant chemistry also has pronounced impacts on insect herbivores. The within-plant distribution of defensive metabolites, such as cardenolides and glucosinolates, along with variation in macronutrient content and physical defenses, such as trichomes, all play crucial roles in influencing feeding preferences. This is exemplified by the interaction between *Erysimum cheiranthoides* (Brassicaceae) and the specialist diamondback moth, *Plutella xylostella* (Wang & Züst 2025). Interestingly, different cardenolide levels, manipulated either by addition or genetic knockout, did not significantly affect the feeding behaviour of *Plutella xylostella*. In contrast, in genetically different cultivars of rice, *Oryza sativa* (Poaceae), different levels of isopentylamine influenced feeding patterns of the planthopper *Nilaparvata lugens*. The underlying biosynthetic gene was identified and studied using knock-out plants (Aboshi *et al.* 2025). Blending volatiles from different plant species can also influence herbivore behaviour. For example, volatile mixtures of cabbage (*Brassica oleracea* var. *capitata*) and faba bean (*Vicia faba*) had repellent effects on cabbage pests, such as the flea beetle *Phyllotreta* spp., while results for *Plutella xylostella* remain inconclusive (Mäkinen *et al.* 2024). These findings suggest that enhancing or manipulating chemodiversity through the use of different crop varieties or intercropping strategies holds promise for pest control. However, this potential remains largely underexplored in agricultural practice.

For pollinators, at least some implications of chemodiversity are presented in this special issue. Distinct flower morphs of *Gynandropsis gynandra*, which also differ in odour profiles, are visited by different insect pollinators (Zenchyzen *et al.* 2025). The fruit-scented cones of the cycad *C. revoluta* may act as fruit mimicry to attract frugivorous pollinators (Chang *et al.* 2025). Previous studies and reviews present various consequences of flower chemodiversity on pollinators as well as flower-feeders (Kessler & Kalske 2018; Sasidharan *et al.* 2023, 2024).

Chemodiversity also plays a role in interactions of plants belowground and with microbial communities. For example, inducing systemic resistance in *Tanacetum vulgare* using pipecolic acid led to enhanced terpenoid concentrations and compositional changes in both root parts and aboveground tissues, but not in rhizomes (Rahimova *et al.* 2024). These tissue-specific changes may reflect different roles in interactions with above- and belowground antagonists or mutualists. In *Populus nigra*, variation in metabolite profiles across organs influenced bacterial biodiversity (Bose *et al.* 2024), suggesting that individual plant organs can represent distinct microbial niches. In contrast, in *T. vulgare* pronounced intraspecific variation in foliar terpenoids did not correlate with differences in leaf-associated bacterial communities (Malacrinò *et al.* 2025). However, other metabolites beyond terpenoids may be important drivers of the bacterial community in this species, as clear differences were found in bacterial composition among plants of different maternal origin, which are also known to differ in various other metabolites apart from terpenoids (Malacrinò *et al.* 2025). Overall, not only different individuals within a plant species but also different organs within a plant may offer distinct niches for microbiomes. Depending on the metabolite profiles of the plant organ, bacteria with different life history strategies (r- of K-selected) may dominate, as observed in *P. nigra* (Bose *et al.* 2024). Microbiota may also reciprocally influence the plant chemical composition, emphasizing the bidirectional nature of these interactions.

The cuticular wax layer on aboveground plant parts represents a key interface for such interactions. In *Eucalyptus* cultivars, variation in wax composition affected susceptibility to the fungal leaf pathogen *Teratosphaeria destructans* (Solís *et al.* 2024). By combining state-of-the art metabolomics approaches with controlled manipulations of the environment or laboratory bioassays, the ecological and physiological consequences of plant chemodiversity can now be studied in large detail. Together with modelling approaches, such investigations can significantly advance our understanding of this important dimension of biodiversity.

Overall, a better understanding of the HOW and WHY of chemodiversity is urgently needed, highlighting potential similarities but also divergences from impacts of biodiversity. Studies of different life history strategies, movement capabilities, and types of species interactions may elucidate mechanisms that influence chemodiversity (Schneider & Beckman 2025). Environmental drivers of chemical evolution may allow predictions of how plants will respond to climate change and cascading effects in trophic networks (Castells & Sanchez-Martinez 2024). Chemodiversity could help plants to cope with global change, possibly through a bet-hedging strategy. Chemodiversity may also play a role in invasion processes or enhance the resilience of crop plants, thereby improving sustainable plant production. The research presented in this special issue will stimulate further research in these areas.

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CM wrote a draft of the editorial, all other authors edited the draft.

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REFERENCES

Aboshi T., Teraishi M., Galis I., Yoshikawa T., Shinya T. (2025) Natural variation-based genetic screen in rice identified the isopentylamine biosynthetic gene that modulates brown planthopper behavior. *Plant Biology*, **27**(5), 873–882.

Aecyo P., Costa L., Jacobina U.P., Harand W., Leal I.R., Souza G., Pedrosa-Harand A. (2024) Integrative evidence on the hybridization between *Cenostigma microphyllum* and *C. pyramidale* (Leguminosae) in the Caatinga dry forest. *Plant Biology*, **27**(5), 749–760.

Anaia R.A., Chiocchio I., Sontowski R., Swinkels B., Vergara F., van Dam N.M. (2024) Ontogeny and organ-specific steroidal glycoside diversity is associated with differential expression of steroidal glycoside pathway genes in two *Solanum dulcamara* leaf chemotypes. *Plant Biology*, **27**(5), 651–668.

Bose T., Mahomed T.G., Mbatha K.C., Joubert J.C., Hammerbacher A. (2024) Tissue ontogeny and chemical composition influence bacterial biodiversity in the wood and shoot tip of *Populus nigra*. *Plant Biology*, **27**(5), 913–923.

Cassola F., Pinheiro G.P., Alves M.F., Alves D.M., Sawaya A., Silva A.A.R., Koch I., Antunes E.R.M., Sartoratto A., Porcari A.M., Mayer J.L.S. (2024) Secretory structures in *Baccharis platypoda* DC. inflorescences (Asteraceae) and characterization of the chemical composition of its secretion. *Plant Biology*, **27**(5), 669–680.

Castells E., Sanchez-Martinez P. (2024) The influence of aridity on plant intraspecific chemical diversity supports adaptive differentiation and convergent evolution. *Plant Biology*, **27**(5), 761–772.

Chang J.-T., Lee T.-C., Valchanova A.K., Okamoto T., Liao P.-C., Kokubugata G., Okuyama Y. (2025) Match of fruit-scented cone volatile compositions with genetic boundary in *Cycas revoluta* and implications for fruit mimicry pollination. *Plant Biology*, **27**(5), 725–739.

Hay A.E., Deborde C., Dussarrat T., Moing A., Millery A., Hoang T.P.T., Touboul D., Rey M., Ledru L., Ibanez S., Pétriacq P., Vanhaverbeke C., Gallet C. (2024) Comparative metabolomics reveals how the severity of predation by the invasive insect *Cydalima perspectalis* modulates the metabolism re-orchestration of native *Buxus sempervirens*. *Plant Biology*, **27**(5), 818–833.

Hickman D.T., Withall D.M., Caulfield J.C., Comont D., Ritz K., Neve P., Rasmussen A., Birkett M.A. (2025) Variation in suppression of black-grass by modern and ancestral cereal root exudates. *Plant Biology*, **27**(5), 808–817.

Kessler A., Kalske A. (2018) Plant secondary metabolite diversity and species interactions. *Annual Review of Ecology, Evolution, and Systematics*, **49**, 115–138.

Mäkinen J.K., Saussure S., Ruhanen H., Räty E., Blande J.D. (2024) Effects of diversified volatile profiles on olfactory orientation of flea beetles *Phyllotreta* spp. and the diamondback moth *Plutella xylostella*. *Plant Biology*, **27**(5), 883–890.

Malacrinò A., Jakobs R., Xu S., Müller C. (2025) Influences of plant maternal effects, chemotype, and environment on the leaf bacterial community. *Plant Biology*, **27**(5), 903–912.

Müller C., Junker R.R. (2022) Chemical phenotype as important and dynamic niche dimension of plants. *New Phytologist*, **234**, 1168–1174. https://doi.org/10.1111/nph.18075

Nomoto H., Fernández-Conradi P., Kjelsberg N., Defossez E., Münzbergová Z., Glauser G., Rasmann S. (2025) Elevation drives intraspecific metabolomic differentiation in natural and experimental populations. *Plant Biology*, **10**, 11779–11786.

Ojeda-Prieto L., van Medina- Berkum P., Unsicker S.B., Heinen R., Weisser W.W. (2024) Intraspecific chemical variation of *Tanacetum vulgare* at plant and plot level affects plant growth and reproductive traits in field plant communities. *Plant Biology*, **27**(5), 785–801.

Petrén H., Anaia R.A., Aragam K.S., Bräutigam A., Eckert S., Heinen R., Jakobs R., Ojeda-Prieto L., Popp M., Sasidharan R., Schnitzler J.-P., Steppuhn A., Thon F.M., Tschikin S., Unsicker S.B., van Dam N.M., Weisser W.W., Wittmann M.J., Yepes S., Ziaja D., Müller C., Junker R.R. (2024) Understanding the phytochemical diversity of plants: Quantification, variation and ecological function. *Ecological Monographs*, **94**, e1635.

Petrén H., Köllner T., Junker R.R. (2023) Quantifying chemodiversity considering biochemical and structural properties of compounds with the R package chemodiv. *New Phytologist*, **237**, 2478–2492.

Rahimova H., Heinen R., Weber B., Weisser W.W., Schnitzler J.P. (2024) Exogenous stimulation of *Tanacetum vulgare* roots with pipecolic acid leads to tissue-specific responses in terpenoid composition. *Plant Biology*, **27**(5), 891–902.

Salihu B., Samarakoon T., Pulaj B., Quave C.L., Mustafa B., Hajdari A. (2024) Analysis of chemical and genetic variability in wild hop (*Humulus lupulus* L.) populations of Kosovo. *Plant Biology*, **27**(5), 740–748.

Sasidharan R., Brokate L., Eilers E.J., Müller C. (2023) Chemodiversity in flowers of *Tanacetum vulgare* has consequences on a florivorous beetle. *Plant Biology*, **25**, 1071–1082.

Sasidharan R., Grond S.G., Champion S., Eilers E.J., Müller C. (2024) Intraspecific plant chemodiversity at the individual and plot levels influences flower visitor groups with consequences for germination success. *Functional Ecology*, **38**, 2665–2678.

Schneider G., Beckman N. (2025) Different tools for different trades: Contrasts in specialized metabolite chemodiversity and phylogenetic dispersion in fruit, leaves, and roots of the neotropical shrubs *Psychotria* and *Palicourea* (Rubiaceae). *Plant Biology*, **27**(5), 681–697.

Solís M., Naidoo S., Wingfield M.J., Joubert J.C., Hammerbacher A. (2024) First line of defence: *Eucalyptus* leaf waxes influence infection by an aggressive fungal leaf pathogen. *Plant Biology*, **27**(5), 924–932.

Thompson M.N., Cohen Z.P., Merrell D., Helms A.M. (2024) Eco-evolutionary factors contribute to chemodiversity in aboveground and belowground cucurbit herbivore-induced plant volatiles. *Plant Biology*, **27**(5), 847–860.

Thon F.M., Müller C., Wittmann M.J. (2024) Evolution of chemodiversity – From verbal to quantitative models. *Ecology Letters*, **27**, e14365. https://doi.org/10.1111/ele.14365

Walker T.W.N., Alexander J.M., Allard P.-M., Baines O., Baldy V., Bardgett R.D., Capdevila P., Coley P.D., David B., Defossez E., Endara M.-J., Ernst M., Fernandez C., Forrister D., Gargallo-Garriga A., Jassey V.E.J., Marr S., Neumann S., Pellissier L., Peñuelas J., Peters K., Rasmann S., Roessner U., Sardans J., Schrodt F., Schuman M.C., Soule A., Uthe H., Weckwerth W., Wolfender J.-L., van Dam N.M., Salguero-Gómez R. (2022) Functional traits 2.0: The power of the metabolome for ecology. *Journal of Ecology*, **110**, 4–20.

Wang K., Züst T. (2025) Within-plant variation in chemical defence of *Erysimum cheiranthoides* does not explain Plutella xylostella feeding preference. *Plant Biology*, **27**(5), 861–872.

Wetzel W.C., Whitehead S.R. (2020) The many dimensions of phytochemical diversity: Linking theory to praxis. *Ecology Letters*, **23**, 16–32.

Wyatt G., Zerbe P., Tiedge K. (2024) Characterization of switchgrass (*Panicum virgatum* L.) PvKSL1 as a levopimaradiene/abietadiene-type diterpene synthase. *Plant Biology*, **27**(5), 698–709.

Yepes Vivas S.A., Popp M., Reichelt M., Gershenzon J., Schnitzler J., Unsicker S. (2025) Deciphering organ-specific chemical changes following insect herbivory in *Populus nigra* using comparative metabolomics. *Plant Biology*, **27**(5), 834–846.

Zenchyzen B., Schmidt S.A., Carey S., Merkosky K., de la Mata A.P., Harynuk J.J., Hall J.C. (2025) Chemical, morphological, and genetic characterization of the floral scent and scent-releasing structures of *Gynandropsis gynandra* (Cleomaceae, Brassicales). *Plant Biology*, **27**(5), 710–724.

Ziaja D., Müller C. (2025) Intraspecific and intra-individual chemodiversity and phenotypic integration of terpenes across plant parts and developmental stages in an aromatic plant species. *Plant Biology*, **27**(5), 637–650.