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REVIEW

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Understanding the chemodiversity of plants: Quantification, variation and ecological function

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Abstract

Plants produce a great number of phytochemicals serving a variety of different functions. Recently, the chemodiversity of these compounds (i.e., the diversity of compounds produced by a plant) has been suggested to be an important aspect of the plant phenotype that may shape interactions between plants, their environment, and other organisms. However, we lack an agreement on how to quantify chemodiversity, which complicates conclusions about the functional importance of it. Here, we discuss how chemodiversity (deconstructed into components of richness, evenness and disparity) may relate to different ecologically relevant aspects of the phenotype. Then, we systematically review the literature on chemodiversity to examine methodological practices, explore patterns

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of variability in diversity across different levels of biological organization, and investigate the functional role of this diversity in interactions between plants and other organisms. Overall, the reviewed literature suggests that high chemodiversity is often beneficial for plants, although a heterogeneity of methodological approaches partly limits what general conclusions can be drawn. Importantly, to support future research on this topic, we provide a framework with a decision tree facilitating choices on which measures of chemodiversity are best used in different contexts and outline key questions and avenues for future research. A more thorough understanding of chemodiversity will provide insights into its evolution and functional role in ecological interactions between plants and their environment.

KEYWORDS
chemical ecology, chemodiversity, metabolite biosynthesis, metabolome, phytochemical phenotype, phytochemicals, plant defense, plant–insect interactions, secondary metabolites

INTRODUCTION

Phytochemicals, also referred to as secondary or specialized metabolites, are crucial for shaping interactions between plants and their environment (Fraenkel, 1959; Hartmann, 2007). Individual compounds can be considered functional traits that impact the physiology, interactions, and fitness of plants (Müller & Junker, 2022; Walker et al., 2022). Together, a mixture of phytochemicals in a plant forms a complex phenotype that may vary along multiple dimensions (Marion et al., 2015). These dimensions include the total number of phytochemicals, quantitative variation in the abundance of those compounds, and qualitative variation given by their biosynthetic origins and molecular structures. Traditionally, most studies on the function of phytochemicals have, however, focused on the effect of individual compounds in interactions between a plant and specific organisms (Richards et al., 2010). Only more recently have studies aiming to comprehensively measure the phytochemical phenotype found that other aspects of it, such as the number and relative abundances of compounds, are important for different functions, and ultimately plant fitness (e.g., Dyer et al., 2018; Junker et al., 2018). However, due to its complex nature, we lack a more complete understanding of which of these aspects are important for different functions in various ecological interactions.

An increasingly common way of characterizing the phytochemical phenotype is to quantify its diversity (Wetzel & Whitehead, 2020). By using diversity indices, a complex multivariate phenotype can be condensed into a simpler univariate measure of diversity, reflecting a particular aspect of it (Marion et al., 2015; Petrén et al., 2023). Such a measure of chemodiversity, also called phytochemical diversity (see Box 1 for a glossary), may be useful if it encompasses a biologically relevant variation that is associated with fitness-related functions of a plant. In this article, we review chemodiversity, examine how it has been measured in published studies, and provide recommendations for how to analyze it. Although primary metabolites are certainly also relevant in ecological interactions (e.g., Forister et al., 2020), here, we focus on specialized metabolites only, as these have been the focus of chemodiversity studies.

THE PHYTOCHEMICAL PHENOTYPE

At least 200,000 phytochemicals have been described, and many more are presumed to exist (Kessler & Kalske, 2018; Wang et al., 2019). Depending on the plant species, which part of the plant is examined, and the method by which compounds are extracted and identified, anything from just a few to several thousand compounds may be found in a single sample (Li & Gaquerel, 2021; Uthe et al., 2021). Regardless of the context, phytochemicals typically occur in mixtures of multiple compounds, where each compound is present at a certain abundance, originates from a specific biosynthetic pathway, and has a particular molecular structure. Useful measures of quantifying and summarizing this multivariate phenotype are needed (Petrén et al., 2023). Any such measure of the phenotype should, ideally, be linked to its function, so that it may be associated with plant performance or fitness. Unraveling which dimensions of the phenotype are most important for function will increase our understanding of how phytochemicals

BOX 1 Glossary of central terms

Chemodiversity (phytochemical diversity)—the diversity of a set of phytochemicals, which (if the set is from an individual plant) represents an aspect of the phytochemical phenotype. Diversity itself is a multifaceted concept, and in this study, we regard diversity as some combination of richness, evenness, and disparity.

Diversity index—a quantitative measure of diversity. There are many different diversity indices, which in different ways quantify diversity as a function of richness, evenness, and/or disparity.

Functional diversity—although a term with varying meanings, we use the following definition: for species diversity, functional diversity describes the diversity of functional traits of species in a community. For chemodiversity, it describes the diversity of (functional) properties of compounds in a sample. In practice, here we regard a diversity index to quantify functional diversity if it includes a disparity component in the measure, where disparity is based on the structural or biosynthetic properties of compounds. Assuming a link between dissimilarity in structure/biosynthesis and dissimilarity in function, such a measure then quantifies the diversity of functions of the compounds in a sample.

Hill diversity—also called Hill numbers or effective number of species. A type of diversity indices, expressed in units of effective numbers (the number of equally abundant species/compounds that are needed to give the same value of diversity). Hill diversity represents a more generalized version of traditionally constructed indices such as Shannon's entropy or the Simpson index (also often referred to as diversities), and has multiple advantages over them, including the use of a parameter, q, which controls its sensitivity to the relative abundances of compounds. With the use of (functional) Hill diversity, each of the three components of diversity can be quantified separately, as well as combined.

Phytochemical phenotype—the combined set of phytochemicals found in, or emitted by (part of) a plant, with each compound representing a "trait" making up the complete multivariate phenotype.

Phytochemical richness—a measure of the number of compounds in a sample.

Phytochemical evenness—a measure of the equitability of the relative abundances of compounds in a sample. Evenness is high when all compounds have equal abundances, and low when one compound has a high abundance and others have a low abundance.

Phytochemical disparity—a measure of how dissimilar the compounds in a sample are. We also refer to this as compound dissimilarity, and this can be quantified based on, among others, the biosynthetic classification or structural properties of the compounds. A pair of compounds has a pairwise dissimilarity, and all the pairwise dissimilarities for a set of compounds can be used to construct a compound dissimilarity matrix.

Phytochemicals—also referred to as plant secondary or specialized metabolites. These are compounds produced by plants, which function predominantly in interactions between plants and their (a)biotic environment, rather than being part of primary metabolic functions.

shape interactions between plants and their biotic and abiotic environment.

Many studies have shown that various aspects of the phytochemical phenotype are important for plant function. Often, such studies focus on a univariate dimension of the phenotype. Most commonly, this is the presence or abundance of specific compounds. For example, single compounds have been shown to limit bacterial growth, reduce herbivory, or increase pollination success (Burdon et al., 2018; Lankau, 2007; Zhou et al., 2017). In other cases, function is linked to the total abundance of compounds, or derives from combinations of compounds (Calf et al., 2018; Duffey & Stout, 1996; Gershenzon et al., 2012). For example, a combination of several compounds may be necessary for optimal herbivore defense or pollinator attraction (Berenbaum et al., 1991; Byers et al., 2014). Other studies have linked function to principal components of mixtures of phytochemicals (Poelman et al., 2009) or observed that, for example, toxicity or information content of volatiles may depend on compounds occurring in specific ratios (Berenbaum & Neal, 1985; Ghirardo et al., 2012; Junker et al., 2018; Orlando et al., 2022). In the past decade, interest in summarizing the phytochemical phenotype by using measures of chemodiversity has increased (Dyer et al., 2014; Hilker, 2014; Kessler & Kalske, 2018; Marion et al., 2015; Moore et al., 2014; Müller et al., 2020; Petrén et al., 2023; Wetzel & Whitehead, 2020). In this way, chemodiversity, measured for phytochemicals found in plants (most often leaves), has been linked to ecological function in a number of studies. For example, a higher diversity of phytoalexins was associated with a lower risk of fungal infection in *Phaseolus* seedlings (Lindig-Cisneros et al., 2002). Together, these examples illustrate that there is substantial variation with regard to which aspects of the phytochemical phenotype are associated with function, and how these influence ecological interactions. Overall, an increasing number of studies suggest that chemodiversity is often a key part of the phytochemical phenotype (Appendix S1: Table S1). However, most studies have not considered that this diversity can be measured in different ways, which impedes efforts linking phytochemical variation to biological function. Therefore, a closer evaluation of what different measures of diversity actually quantify, and their usefulness in different contexts is needed. In the following sections, we compare and contextualize methods of quantifying the diversity of the phytochemical phenotype; systematically review the literature on chemodiversity, elucidating general patterns on its importance for different ecological interactions; provide a framework with recommendations for how to optimally measure chemodiversity in different ecological contexts; and propose avenues for future research on the subject.

USE OF DIVERSITY INDICES IN CHEMICAL ECOLOGY

Diversity indices have a long tradition in community ecology where they are used to quantify species diversity, which is subsequently associated with community and ecosystem functions (Magurran, 2004; Box 2). Recently, these measures have become more widely applied in biology to quantify the diversity of, for example, elements, molecules, genes, transcriptomes, phenotypes, and soundscapes (Fernández-Martínez, 2022; Kellerman et al., 2014; Luypaert et al., 2022; Marion et al., 2015; Martínez & Reyes-Valdés, 2008; Sherwin et al., 2017). In chemical ecology, measuring chemodiversity is becoming increasingly popular, but with a few exceptions (Bakhtiari et al., 2021; Petrén et al., 2023; Ramos et al., 2023; Wetzel & Whitehead, 2020), little attention has been paid to how it is actually quantified, and how this is relevant to its function in various ecological contexts.

What diversity is and how it can best be measured is a much-discussed topic (Chao et al., 2014; Jost, 2006; Morris et al., 2014; Tuomisto, 2010). In this review, we focus on measures of α-diversity, which, in the case of chemodiversity, is the diversity of a single sampling unit, most often an individual plant. This contrasts with γ-diversity, which is the total diversity at the scale of a group of sampling units, and β-diversity, which is derived from the other two measures and represents the variation, turnover, or dissimilarity between sampling units (Anderson et al., 2011; Ellison, 2010). On a fundamental level, this α-diversity can be deconstructed into three components: richness, evenness, and disparity (Daly et al., 2018; Purvis & Hector, 2000) (Figure 1a). In a (phyto)chemical context, richness simply represents the number of compounds found in a sample. The second component, evenness, is a function of relative abundances of the compounds present in a sample. For a set of compounds, evenness is maximized when all compounds are equally abundant, and decreases as some compounds become more abundant than others. The third component, disparity, describes how different objects in a sample are to each other for some defined property. For chemical compounds, disparity, which we will also refer to as compound dissimilarity, can be based on a property of the compounds that is considered relevant, such as their molecular structure or the biosynthetic pathways by which they are produced (Junker, 2018; Junker et al., 2018; Petrén et al., 2023; Sedio, 2017; Whitehead et al., 2021). In practice, direct measures of disparity have only rarely been used in chemodiversity studies.

Chemodiversity can be quantified in a number of different ways (Figure 1b). Each of the three components can be quantified individually, with richness being the most straightforward measure. The most common approach, however, is to use an index that combines richness and evenness, such as Shannon's diversity or the inverse Simpson diversity. Functional diversity indices, which include the disparity component (in the form of a compound dissimilarity matrix), have only rarely been used. Such indices include mean pairwise dissimilarity (MPD; the mean of values in the dissimilarity matrix), which constitutes only the disparity component and indices such as Rao's Q (Rao, 1982), which is dependent on all three components of diversity. A more detailed mathematical description of these indices in the context of chemodiversity is available in Petrén et al. (2023).

An underestimated problem in many studies is that different diversity indices measure different things (Wetzel & Whitehead, 2020). An index necessarily emphasizes some components of diversity while de-emphasizing others, which may affect results (Steel et al., 2013; Tuomisto, 2010). For example, Bakhtiari et al. (2021) found that only some measures of chemodiversity of glucosinolates in *Cardamine* species were associated with herbivore performance, and this also depended on the type of herbivore studied. This, the authors argue, indicates that only some aspects of the diversity might be predictive of ecological effects in specific cases. Most studies however calculate only a single index, often without justifying the choice. This is not ideal, since a certain index

BOX 2 Similarities of, and links between, species diversity and chemodiversity

In this paper, we review the application of the concept of diversity, most often used to measure the diversity of species, to instead measure the diversity of phytochemicals. There are several conceptual similarities between these applications.

The diversity of species is of interest both as a measure in itself, and because of the effect of biodiversity on ecosystem functioning. A large body of literature has demonstrated positive effects of biodiversity, mostly in plants, on a wide range of ecosystem functions in a wide range of systems (Cardinale et al., 2012; Loreau et al., 2001; van der Plas, 2019). These studies indicate that different components of species diversity, including the richness, evenness, and disparity, can be important for ecosystem function in different contexts (Tilman et al., 2014). Generally, functional diversity is often found to be more important for ecosystem functioning than species diversity (Tilman et al., 1997; van der Plas, 2019). Mechanistically, diversity might have positive effects on ecosystem functions in different ways, including "complementarity effects" where the functioning of individual species is higher when grown in communities rather than monocultures, and "selection effects," where communities with high species richness are more likely to include (high abundances of) species that provide high function levels (Loreau & Hector, 2001). Additionally, the functional composition of species, that is the presence of certain functional groups, is also often a major factor affecting ecosystem function (van der Plas, 2019).

The diversity of phytochemicals, and its effects on plant function, works in analogous ways. We have demonstrated (see Section "*Systematic literature review*") how different components of diversity can influence plant functioning, and argued that measures of functional diversity, which include a disparity component, might be more predictive of function than measures based on only richness and/or evenness. Mechanistically, there are connections as well. The "synergy hypothesis" (synergistic effects between compounds, see Section "*Phytochemical richness*") is comparable to the "complementarity effects." The "screening hypothesis" (only few compounds are functional) is related to the "selection effects." The "interaction diversity hypothesis" (different compounds are effective against different interacting organisms), is related to the concept of ecosystem multifunctionality, where different species affect different ecosystem processes (Hector & Bagchi, 2007). Similarly, in addition to the diversity, also the composition of compounds is likely often important for function as well. The similarities between effects of species diversity and chemodiversity demonstrate an interesting generality of diversity-function relationships.

While we have considered species diversity and chemodiversity separately so far, the concepts can also be linked to each other. Phytochemicals can, similar to morphological traits, be regarded as (functional) traits (Müller & Junker, 2022; Walker et al., 2022). For measures of chemodiversity, these traits collectively make up the phenotype, which can be quantified as a measure of its diversity. In contrast, for calculations of the functional diversity of species in a community, these traits are, instead, included in calculations of the functional (chemo)diversity of species. Studies utilizing phytochemicals as functional traits to study the functional diversity of species, or studies simply quantifying chemodiversity on a community rather than individual plant level, have found effects of this diversity on plant functions such as herbivore resistance, which itself can be regarded as an ecosystem function (Fernandez-Conradi et al., 2022; Ristok et al., 2023; Salazar et al., 2016; Schuldt et al., 2018). In this way, the diversity of the phytochemicals that plants produce constitutes a part of the mechanistic link between plant diversity and ecosystem function.

might emphasize an aspect of the phenotype that happens to be less ecologically relevant (Wetzel & Whitehead, 2020). Instead, we argue, it is more meaningful to quantify diversity using measures where it is clear which component(s) of diversity is(are) actually measured.

In community ecology, many agree that diversity is optimally quantified using Hill diversity (Ellison, 2010). Hill diversity, also called Hill numbers or effective numbers, is closely related to traditional diversity indices such as Shannon's diversity, but offers several advantages (Chao et al., 2014; Hill, 1973; Jost, 2006). This includes intuitive units, easy partitioning into α-, β-, and γ-diversity, and options to quantify functional diversity (Chao et al., 2014; Chiu & Chao, 2014). Additionally, Hill diversity includes a parameter, *q*, called the diversity

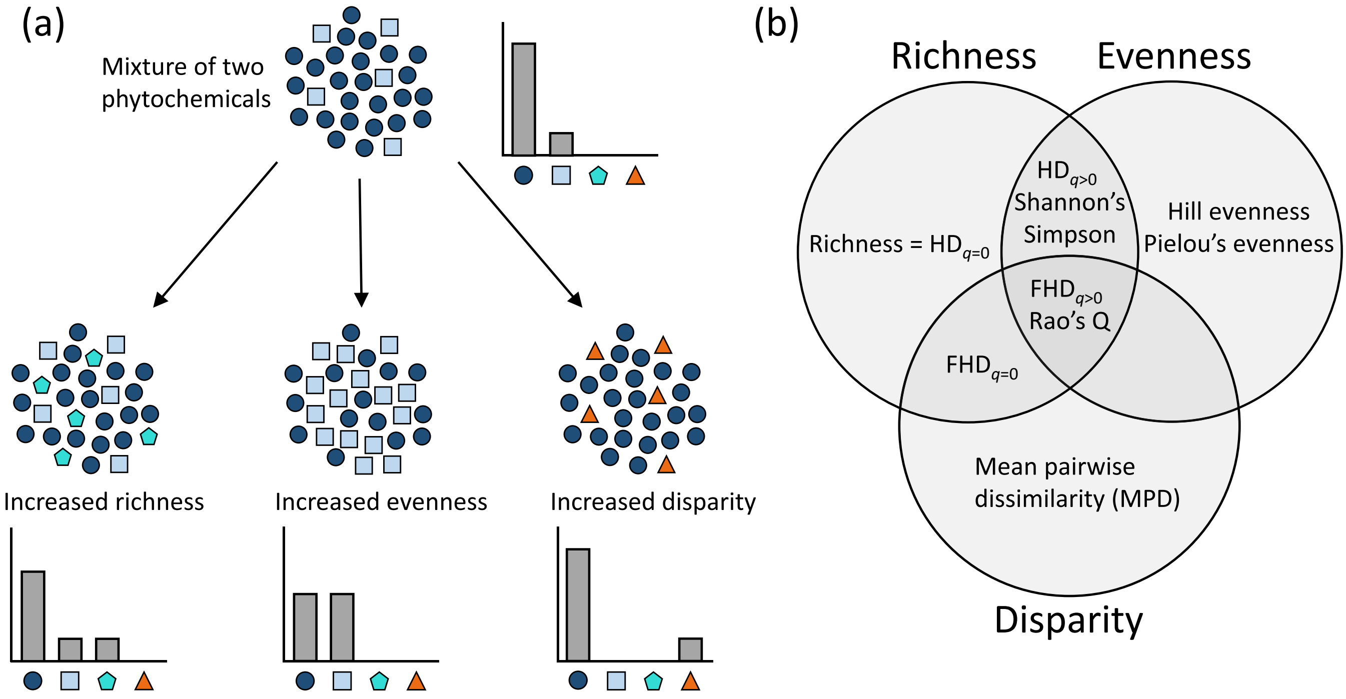

FIGURE 1 An illustration of (a) different components of diversity, and (b) indices used to measure diversity that are mentioned in the main text. (a) Diversity can be deconstructed into components of richness, evenness, and disparity. Here, individual phytochemical molecules are illustrated as shapes of different color. Those of the same color and shape are the same type of compound. Bar plots next to groups of shapes indicate the relative abundances of each type. The top group contains two different compounds with uneven abundances. Richness increases if the number of different phytochemicals increases. Evenness increases if the relative abundances of the phytochemicals become more equal. Disparity increases if the phytochemicals present in a mixture are more dissimilar, for example in regard to molecular structure or biosynthesis, here represented as replacing the light blue squares with the more dissimilar orange triangles. (b) Diversity can be measured by quantifying its components, or combinations thereof. Each circle represents one component of diversity. Indices in overlapping areas measure combinations of these components. There exists a multitude of diversity indices, and we have only included those that are considered in the main text. HD$_{q=0}$. Hill diversity at $q = 0$, which is equal to the richness; HD$_{q>0}$, Hill diversity at $q > 0$, which is a function of richness and evenness; FHD$_{q=0}$, Functional Hill diversity at $q = 0$, which is a function of richness and disparity; FHD$_{q>0}$, Functional Hill diversity at $q > 0$, which is a function of all three components of diversity.

order, which controls its sensitivity to the relative abundances of compounds. By selecting the type of Hill diversity and its q value(s), one can calculate measures of diversity that focus on any combination of its three components. This enables easier and more extensive analyses of diversity compared with using a single traditional index.

While chemodiversity has primarily been measured using traditional indices, Hill diversity has been increasingly used in recent years. Marion et al. (2015) introduced the concept to characterize phenotypic complexity, and other studies followed in measuring chemodiversity in this way (Cosmo et al., 2021; Glassmire et al., 2016; Harrison et al., 2016, 2018; Philbin et al., 2021, 2022). Functional Hill diversity, which includes compound dissimilarities in diversity calculations, has only very recently been used to quantify chemodiversity (Forrister et al., 2022). Petrén et al. (2023) developed the R-package *chemodiv*, which provides functions to aid chemical ecologists to more comprehensively quantify chemodiversity for a wide range of datasets. This includes functional Hill diversity, where compound dissimilarities calculated based on molecular and/or biosynthetic properties of the compounds, are included in diversity calculations. Since chemodiversity is increasingly often quantified (Figure 2a), there is a need to more closely examine what components of this diversity are most ecologically relevant, and consider the mechanisms by which they are important for function (Bakhtiari et al., 2021; Wetzel & Whitehead, 2020).

SYSTEMATIC LITERATURE REVIEW

To compile information on the use of diversity indices in quantifying chemodiversity, we conducted a systematic search of literature on the subject. In February 2023, we searched Web of Science for studies on chemodiversity

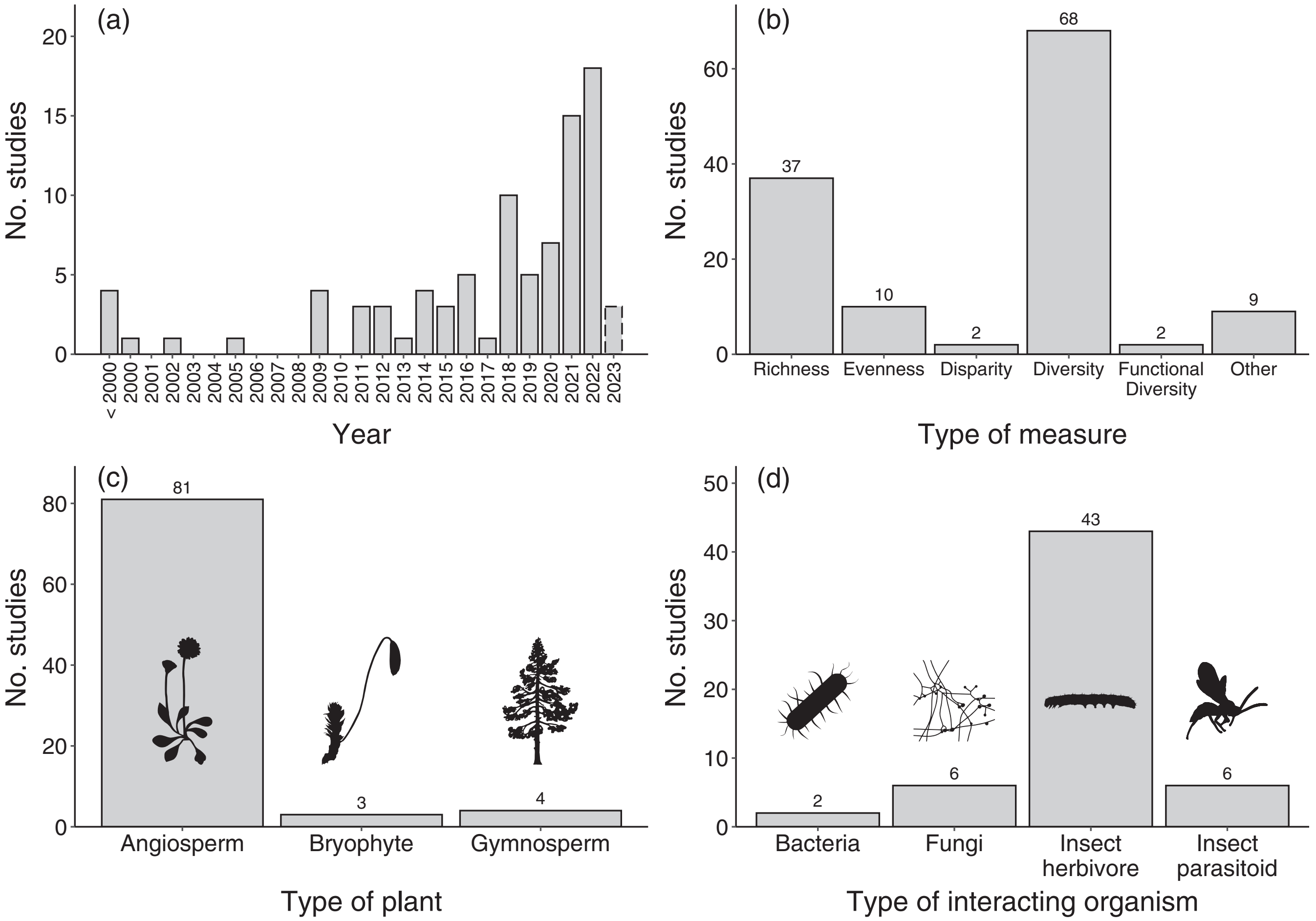

FIGURE 2 Some general patterns of studies on chemodiversity in plants. (a) A total of 89 studies were found in the systematic literature search, with an increased number of studies published in recent years. Studies conducted before the year 2000 are merged in the "<2000" bar. For 2023 the line around the bar is dashed, as only studies published up until February were included because that is when the literature search was done. (b) Number of studies using different measures of chemodiversity. "Richness," "Evenness" and "Disparity" are the components of diversity as described in the main text; "Diversity" includes Shannon's, Simpson and Hill diversity; "Functional Diversity" includes Rao's Q and functional Hill diversity; "Other" includes other measures of diversity, and diversity measured on the level of populations or communities rather than individuals. (c) Number of studies done on different types of plants. (d) Number of studies that tested effects of chemodiversity on different types of interacting organisms. Numbers above bars in (b), (c), and (d) indicate the number of studies. Individual studies, all of which are included in Appendix S1: Table S1, may occur in multiple or no categories in these plots. Images of organisms were obtained from PhyloPic (https://www.phylopic.org/) under the CC0 1.0 Universal Public Domain Dedication license.

with four separate searches of "*chemical diversity*" *AND plant**, *chemodiversity AND plant**, "*secondary compound*" *OR* "*secondary metabolite*" *AND diversity AND plant**, and "*voc diversity*" *OR* "*scent diversity*" *OR* "*volatile diversity*" *AND plant**. This returned a total of 2106 scientific articles. These were screened by title and abstract, and potentially relevant papers were examined in detail for the use of diversity indices quantifying mixtures of phytochemicals. In addition, we also screened all papers cited by, and all papers that cited a number of key papers in the field (Bakhtiari et al., 2021; Cosmo et al., 2021; Hilker, 2014; Kessler & Kalske, 2018; Marion et al., 2015; Moore et al., 2014; Philbin et al., 2022; Wetzel & Whitehead, 2020; Whitehead et al., 2021), and included a small number of additional papers and preprints known to the authors but not found in our systematic search. We included studies quantifying α-diversity or some component (richness, evenness, disparity) of it. Most often, this represents the chemodiversity of individual plants, and is, therefore, a measure of their phenotype. In a few cases, this included lower (within-plant) or higher (population or community) level variation, and such studies were included if this level was considered as the sampling unit by the authors. Studies quantifying only β-diversity or dissimilarity were not included, as that was beyond the scope of this study. Although we believe our search to be exhaustive with regard to finding studies that use diversity indices, it should be noted that many studies reporting only phytochemical richness were likely not included. Richness is often not framed in the context of diversity, but is frequently reported in result sections simply noting how many compounds were found in total in a set of samples. We only included studies quantifying richness if they did so in the context of diversity. Our collection of studies includes both those examining variation in chemodiversity (using it as a response variable in comparing, e.g., populations, species or treatments) and studies examining function through the effect of chemodiversity on interacting organisms (using it as a predictor variable to test effects on, e.g., herbivore performance or fungal growth). In total, we found 89 studies in our systematic search that fit the criteria, many of which were published in recent years (Figure 2a). Appendix S1: Table S1 lists these studies, including the study system, type of phytochemicals measured, analytical method, type of measures calculated, type of plant, type of interacting organism, and whether variation in or an effect of the diversity was found. Below, we review these studies, and consider theoretical aspects of each diversity component separately and combined.

Phytochemical richness

Richness, the number of compounds, is the most straightforward component of chemodiversity. It is a frequently reported measure, and was used in 42% of the compiled studies (Figure 2b). Variation in richness has been documented on all levels of biological organization, including among tissues/organs (Elser et al., 2023; Whitehead et al., 2013), individuals (Ziaja & Müller, 2023), populations (Eisen et al., 2022; Zeng et al., 2022), species (Macel et al., 2014; Schweiger et al., 2021; Züst et al., 2020), orders (Courtois et al., 2009), and communities (Peguero et al., 2021), as well as across herbivory treatments (Agrawal, 2000), phylogenies (Becerra et al., 2009; Cacho et al., 2015) and landscapes (Defossez et al., 2021). Here, richness varies from a handful of compounds of a specific biosynthetic class, to several thousand metabolic features that are assumed to represent unidentified individual compounds. Whereas some studies solely document variation in phytochemical richness, others go a step further and investigate the functional importance of this variation. For example, a higher phytochemical richness has been shown to reduce preference and/or performance of specific herbivores in a number of study systems (Adams & Bernays, 1978; Agrawal, 2000; Castellanos & Espinosa-García, 1997). In natural environments, phytochemical richness, both on the level of individual plants and whole communities, has been found to shape ecological interactions, with effects such as reducing species richness of herbivores (Salazar et al., 2018), decreasing arthropod abundances (Defossez et al., 2021) and reducing levels of herbivore damage (Whitehead et al., 2013). Hence, phytochemical richness may be important for plants in both single interactions and contexts in which plants experience pressures from whole herbivore communities.

From an ecological perspective, producing a high number of phytochemicals may benefit a plant through various mechanisms. These mechanisms are linked to hypotheses explaining how chemodiversity is maintained by natural selection (Thon et al., 2024; Wetzel & Whitehead, 2020; Whitehead et al., 2021), and we present three major hypotheses here. According to the "interaction diversity hypothesis", for a plant experiencing a multitude of interactions, for example, being attacked by multiple herbivores, producing more compounds is useful if different compounds are effective against different herbivores. This would then result in selection toward increased phytochemical richness (Berenbaum & Zangerl, 1996; Iason et al., 2011; Junker, 2016). If, as suggested by the "screening hypothesis," most compounds are instead nonfunctional, a high richness may increase the probability that at least some compounds in a mixture are functional (Jones & Firn, 1991, Firn & Jones, 2003, but see Pichersky et al., 2006). For this, and especially the interaction diversity hypothesis, a higher richness may benefit plants experiencing multiple interactions. Importantly, function still originates from effects of individual compounds. In contrast, according to the "synergy hypothesis," phytochemical richness, per se, may be mechanistically important in single interactions. Synergistic effects, where the effect of a mixture of compounds is greater than the combined effects of individual compounds, have been documented in a number of systems, and may emerge via several different mechanisms (Richards et al., 2016). The probability of synergistic effects occurring may increase with the number of compounds present in a mixture, thereby creating selection for increased phytochemical richness. Similarly, these hypotheses can also explain selection for increased evenness or disparity (see below), thereby explaining why chemodiversity may be functionally important.

The main advantage of quantifying chemodiversity as compound richness is that it is easy to measure. However, there are some disadvantages. First, levels of measured richness may vary widely depending on which methods are used for extraction and detection (e.g., targeted or untargeted analyses) of compounds, and be further affected by post-analytical choices such as signal-to-noise cut-offs (Li & Gaquerel, 2021; Uthe et al., 2021). Additionally, levels of detected richness may increase with the total amount of plant material used and the total abundance of phytochemicals in a plant for both technical and biological reasons (Wetzel & Whitehead, 2020). This can restrict comparisons of phytochemical richness to situations where similar analytical methods and data-processing routines have been used. Second, measures of richness disregard the relative abundances of compounds. This means that compounds occurring at low abundances, which may be functionally less important in some contexts, contribute as much to the measure of richness as highly abundant compounds.

Phytochemical evenness

Evenness is dependent on the relative abundances of compounds. Compared with richness, measures of evenness are rarer in the literature. Among the studies that have quantified it (11% of the compiled studies; Figure 2b), there is evidence of variation in evenness between bryophyte species (Peters et al., 2019, 2021), wild type and mutant *Erysimum cheiranthoides* (Mirzaei et al., 2020), and types of maize (Bernal et al., 2023). Pais et al. (2018) found that an increased evenness of leaf metabolites in *Cornus florida* was associated with a higher probability of plants being diseased. In contrast, Feng et al. (2021) noted a positive association between evenness and antibacterial activity for *Juniperus rigida* essential oils, and Whitehead et al. (2021) found that increasing the evenness of phenolics in the diet of different insect and fungi consumers increased how many of them were negatively affected by the phenolics. Measuring covariation in the diversity of plants, fungi, and arthropods, as well as chemical and genetic diversity associated with *Plantago lanceolata* individuals, Morris et al. (2014) found that evenness showed different patterns compared with richness and, for example, Shannon's diversity, suggesting that it represents different information not captured by other diversity indices.

Mechanistically, evenness might be important for function in different ways. If function is dependent on synergies between compounds occurring in similar abundances, a set of compounds with high evenness might enable more or stronger synergies than a set of compounds with low evenness. On the other hand, if function comes from only a few specific compounds, a high evenness may be disadvantageous if it reflects a lower abundance of those compounds (Pais et al., 2018; Wetzel & Whitehead, 2020).

Although a potentially interesting measure, evenness has a number of disadvantages. First, accurately quantifying the relative abundances of structurally different molecules in a chromatogram can be difficult (Walker et al., 2022), making comparisons across different sets of compounds and different studies challenging. Second, if the bioactivity of compounds varies widely, such that also compounds present in low abundance are important for function, measuring evenness is less relevant (Clavijo McCormick et al., 2014). Third, although it seems like a straightforward measure, there is no consensus on how to best quantify evenness (Chao & Ricotta, 2019; Jost, 2010; Smith & Wilson, 1996; Tuomisto, 2012). The most popular measure is likely Pielou's evenness (Pielou, 1966), but evenness can also be calculated in the Hill diversity framework (Hill, 1973). The behavior of these two indices can differ, with the former measure not being truly independent of richness (Alatalo, 1981; DeBenedictis, 1973), and there is no agreement on which method is most suitable (Jost, 2010; Tuomisto, 2012). Overall, the limited evidence so far suggests that the effects of phytochemical evenness differ between study systems. Since basically any change in the phytochemical phenotype will affect evenness, more research is needed to investigate its ecological relevance and potential mechanisms. Notably, four different evenness indices were used in the studies cited above. Consequently, measured effects of evenness could differ depending on the index used. This illustrates the challenges of measuring this aspect of the phytochemical phenotype.

Phytochemical disparity

Disparity (compound dissimilarity) is rarely quantified in studies of chemodiversity, but may often be an important component of it. We are aware of two studies (2% of the compiled studies; Figure 2b) that have specifically quantified the disparity of sets of phytochemicals as a measure of their structural diversity. Similar to results on evenness, Whitehead et al. (2021) found that an increased structural diversity of phenolics, quantified as the MPD of all compounds in a mixture, increased the proportion of consumers that were negatively affected by the compounds. Studying different *Salix* species along elevational gradients, Volf et al. (2022) found an increase in the MPD of salicinoids with altitude, but a decrease in the MPD of flavonoids, which may result from variation in abiotic factors. Although evidence is limited, these studies suggest that the level of disparity can be an important aspect of the phytochemical phenotype that affects function and varies with environmental conditions.

To quantify disparity, dissimilarities between identified chemical compounds may be calculated in different ways based on, for example, their molecular substructures (Cao et al., 2008), physicochemical properties (Dowell & Mason, 2020), molecular fingerprints (Cereto-Massagué et al., 2015) or what biosynthetic pathways or enzymes produce them (Junker, 2018;

Petrén et al., 2023). Additionally, recently developed methods in the web-based GNPS mass spectrometry platform (Wang et al., 2016) enable calculations of compound dissimilarities for unidentified compounds for which mass spectral data are available. Here, cosine dissimilarities are calculated based on comparisons of mass spectra (Aksenov et al., 2021; Wang et al., 2016). Such dissimilarity measures have been used in chemical ecology (Sedio, 2017), also in combination with other methods that incorporate molecular substructures (Ernst et al., 2019). Notably, the question of whether a compound is identified or not may often be a matter of probability rather than a binary decision (Hoffmann et al., 2023; Uthe et al., 2021), and researchers will have to make judgments on which methods are most suitable in different cases.

In an ecological context, a crucial assumption for why compound dissimilarities are relevant is that there is an association between the structure/biosynthetic origin of a compound and its function. Generally, molecules with a similar chemical structure can be expected to, on average, have a more similar biological activity/function compared with molecules with a more different structure (Berenbaum & Zangerl, 1996; Martin et al., 2002). Dissimilarity in chemical structures may, however, not always be associated with dissimilarity in biological function, as exceptions to this assumption exist (e.g., He et al., 2019). Instead, associations between structure and function may be more prevalent at the level of mixtures containing multiple compounds. More dissimilar compounds may also be more likely to function synergistically than less dissimilar compounds (Liu & Zhao, 2016). Therefore, a structurally diverse set of phytochemicals may be more functionally diverse (in line with the interaction diversity hypothesis) and/or potent (in line with the synergy hypothesis) (Philbin et al., 2022). Biosynthetically based compound dissimilarities may also be useful (although structural and biosynthetic similarity are often correlated) because different classes of compounds may, on a general level, have partly different functions in plant–insect interactions (Glassmire et al., 2019; Junker & Blüthgen, 2010; Kantsa et al., 2019; Schiestl, 2010). Therefore, a set of biosynthetically dissimilar compounds could be more multifunctional than a set of compounds produced in the same biosynthetic pathway. Biosynthetically based dissimilarities may also be relevant in evolutionary studies. In this case, if a plant species produces a set of compounds with a high average compound dissimilarity, this indicates that these are produced in multiple biosynthetic pathways, indicating that the species has an extensive metabolic machinery for producing phytochemicals. Comparing such compound dissimilarities across phylogenies may generate insights into the evolution of phytochemicals, as has previously been done in similar ways (Becerra et al., 2009).

We believe that including compound dissimilarities in measures of chemodiversity can be meaningful. However, there are also a number of challenges associated with it. First, as mentioned, the ecological usefulness of including compound dissimilarities rests on the assumption of a link between structure and function, such that two compounds that are structurally dissimilar are also functionally dissimilar. Although this may not be the case for all pairs of phytochemicals in a set of compounds, an association between the structural diversity (level of disparity) for the whole set of compounds and its diversity in function may be more likely. Second, compound dissimilarity can be quantified in many different ways. We have made a distinction between methods based on biosynthesis and molecular structure, but there are also different ways of quantifying compound dissimilarities based on their structures (Cao et al., 2008; Cereto-Massagué et al., 2015). Overall, more research is needed to examine links between (different measures of) the structure and function of phytochemicals, and to determine the most appropriate measure of disparity for a given research question.

In addition to using compound dissimilarities to examine structural diversity, it should be noted that other studies have quantified dissimilarities or properties of phytochemicals in other ways. Sternberg et al. (2012) and Rasmann (2014) examined the effects of the polarity of phytochemicals on herbivore resistance, finding that nonpolar cardenolides may be more toxic to herbivores than polar cardenolides. Cosine dissimilarities between MS/MS spectra of compounds have been included in measures that integrate structural and compositional dissimilarities of sets of phytochemicals, in order to quantify such differences within and between species at different scales (Endara et al., 2022; Ernst et al., 2019; Forrister et al., 2022; Sedio et al., 2017, 2018, 2020, 2021). Although these examples regard dissimilarity between, rather than diversity within, sets of phytochemicals, they similarly point to the importance of structural variation of phytochemicals at different levels.

Phytochemical diversity—Measures of combined components

While each of the three components of diversity may be measured separately, many diversity indices combine two or more components (Figure 1b). Shannon's, Simpson and Hill diversity combine richness and evenness into a single measure. Richness and disparity may be combined as the sum of all the pairwise dissimilarities in a dissimilarity matrix (Walker et al., 1999). Richness, evenness and disparity can be combined with the use of functional diversity indices such as functional Hill diversity.

Using diversity indices that are a function of richness and evenness is the most common way to quantify chemodiversity (76% of the compiled studies; Figure 2b, Appendix S1: Table S1). Similar to richness, variation in diversity has been documented at different levels of biological organization, including different plant tissues (Eilers, 2021; Elser et al., 2023), populations (Bravo-Monzón et al., 2014, 2018) and species (Ortiz et al., 2019; Peguero et al., 2021). There is also variation along altitudinal gradients (Glassmire et al., 2016; Philbin et al., 2021; Volf et al., 2020) and for different levels/types of herbivory (Li et al., 2020; Philbin et al., 2022). Among studies that have examined functional effects, results indicate that an increased chemodiversity can decrease levels of herbivory (Glassmire et al., 2019; Richards et al., 2015), decrease herbivore performance (Tewes et al., 2018; Whitehead & Poveda, 2019) and increase resistance to fungi and bacteria (De-la-Cruz-Chacón et al., 2019; Feng et al., 2021; Lindig-Cisneros et al., 1997, 2002). It can also affect the diversity or structure of the community of herbivores feeding on host plants (Cosmo et al., 2021; Harrison et al., 2018; Richards et al., 2015; Volf et al., 2018), affect tri-trophic interactions (Slinn et al., 2018; Wan et al., 2017), and shape the diversity of the surrounding plant and microbe communities (Iason et al., 2005; Zhang et al., 2024). Other studies have instead found that intermediate or high levels of chemodiversity might be disadvantageous (Pais et al., 2018; Sternberg et al., 2012) or found no/limited effects on herbivory (Espinosa-García et al., 2021; Schuldt et al., 2012; Torres-Gurrola et al., 2011). Taken together, results from these studies suggest that an increased chemodiversity is often, but not always, beneficial for plants (Appendix S1: Table S1). Given the limited number of studies, the very diverse set of contexts and measured ecological effects, and the potential for publication bias, it is difficult to make more general conclusions about exactly what factors may affect whether chemodiversity is beneficial or not.

Only two studies (2% of the compiled studies; Figure 2b, Appendix S1: Table S1) have measured chemodiversity with indices that directly include also the disparity component. Bakhtiari et al. (2021) measured chemodiversity of glucosinolates in *Cardamine* plants with the Rao's Q index, where compound dissimilarities were quantified based on chemical classes and molecular weights. They found variation in this measure of diversity among groups of *Cardamine* species, but no association between chemodiversity and the level of resistance to different herbivores. Investigating leaf metabolites from around 100 *Inga* species, Forrister et al. (2022) measured functional Hill diversity and compared it to a null model, concluding that plants invested in producing structurally diverse sets of compounds. It should also be noted that some studies (e.g., Cosmo et al., 2021; Philbin et al., 2022; Richards et al., 2015) have measured chemodiversity in a way that indirectly takes compound structure into account by calculating diversity from ^{1}H-NMR spectra, instead of the more commonly used mass spectrometry data. This has the advantage that the measures partly depend on both the intra- and intermolecular complexity of compounds in a sample, compared with mass spectrometry-based measures of disparity, which only consider differences between molecules. A disadvantage of NMR-based measures is that the different components of diversity cannot be as easily separated. Combining both methods in the same study could be fruitful in quantifying chemodiversity more fully (Philbin et al., 2022).

By combining multiple components of diversity, indices are advantageous because they summarize different aspects of the phytochemical phenotype in a single measure, which can be associated with function. This can be especially useful if the function of a mixture of phytochemicals depend on a combination of richness, evenness, and/or disparity. For example, a higher number of compounds could increase herbivore resistance, but only if the compounds occur at similar abundances, and/or are structurally dissimilar. In such a scenario, richness alone may not, or only weakly, correlate with herbivore resistance, while an index that also includes evenness and/or disparity will. There are also potential disadvantages of using indices. By combining multiple components of diversity, they may conceal independent variation in single components. Additionally, the relative weights of different components in different indices can vary. For example, Simpson diversity puts less weight on low-abundance compounds than Shannon's diversity, and a choice has to be made about which index is most appropriate. This is made easier by using Hill diversity, where the selection of the diversity order (q) controls the index's sensitivity to the relative abundances of compounds. More than anything, understanding the properties of the calculated indices is crucial.

FRAMEWORK FOR MEASURING CHEMODIVERSITY IN DIFFERENT CONTEXTS

There is often a lack of justification as to why diversity is measured in a certain way in a particular study. This limits our understanding of what aspects of the phytochemical phenotype are most important for function. Although the issue of how to best measure chemodiversity is complex, some general practices should be considered. Therefore, we provide a guide and recommendations on how to appropriately measure chemodiversity for different types of datasets.

An overview of our recommendations for measuring chemodiversity is presented in Figure 3. We believe that, although diversity may be measured with an appropriate index, it should also be deconstructed into separate measures of each component. Which components this includes depends on the dataset, and the data collected will depend on the research question considered. Data may consist of presence/absence data or quantitative data with compound abundances. Setting aside disparity for now, in the former case the only applicable measure of chemodiversity is the richness component. In the latter case, the evenness of the compounds can also be considered if their relative abundances have been adequately quantified. In this case, the chemodiversity may be quantified as Hill diversity, and the diversity order parameter (q) can be adjusted to control the measure's sensitivity to the relative abundance of compounds. Although any value of $q > 0$ can be used to include evenness as a component, we recommend using $q = 1$ by default, as compounds are then weighted in proportion to their abundances. In addition, diversity profile plots, where diversity is plotted as a function of different q values (e.g., in the range of $q = 0$ to $q = 3$ or higher), can be constructed to illustrate how diversity varies depending

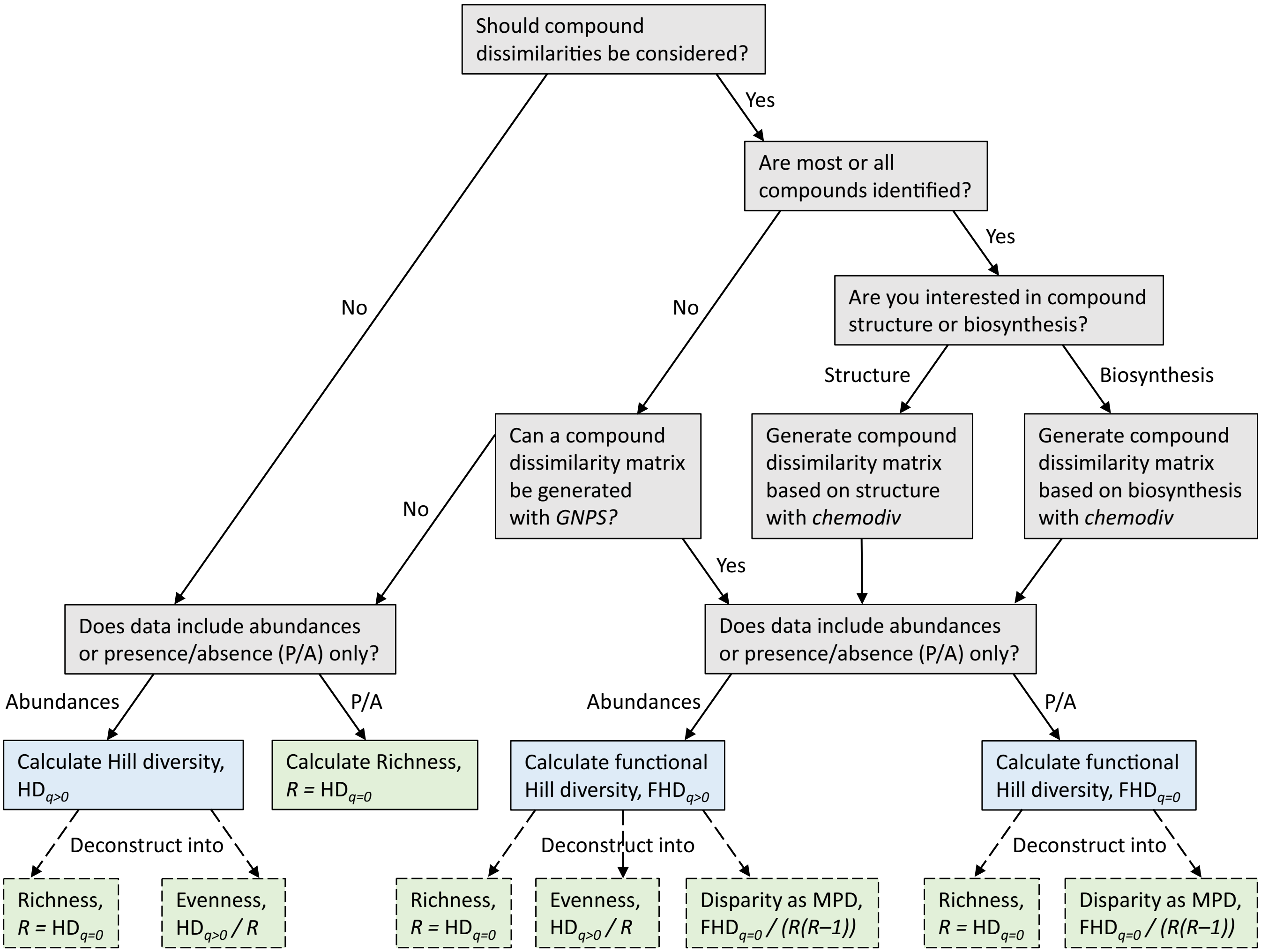

FIGURE 3 Decision tree for quantifying chemodiversity. The choice of measure depends on whether compound dissimilarity for the measured phytochemicals should be considered, and if abundance data, or only presence/absence data, is available. Gray boxes mark steps in the decision tree. Blue boxes represent measures of diversity in the Hill diversity framework. Dashed green boxes mark components into which measures of (functional) Hill diversity can be deconstructed. R, compound richness; $\text{HD}_{q=0}$, Hill diversity at $q = 0$; $\text{HD}_{q>0}$, Hill diversity at $q > 0$; $\text{FHD}_{q=0}$, functional Hill diversity at $q = 0$; $\text{FHD}_{q>0}$, functional Hill diversity at $q > 0$; MPD, mean pairwise dissimilarity. For measuring HD or FHD at $q > 0$, we recommend using $q = 1$ by default. All steps in the decision tree, except generating a compound dissimilarity matrix with GNPS, can be done with the chemodiv R package (Petrén et al., 2023).

on the sensitivity of the index to the relative abundances of compounds. Such profiles then allow for further insights into relative levels of chemodiversity of different groups and how that might depend on the extent to which compound abundance is taken into account (Chao & Jost, 2015; Wetzel & Whitehead, 2020). Since indices may conceal independent variation in their components, we recommend also quantifying richness and evenness separately to examine variation in or effects of each component.

In line with the increasing evidence for the importance of compound structure for function, we recommend that the disparity (compound dissimilarity) should be considered if possible. This can be done in multiple ways. For datasets where most or all compounds are unidentified, compound dissimilarities can be calculated, for example, as cosine scores based directly on mass spectra, by use of the GNPS platform (Aksenov et al., 2021; Wang et al., 2016), although the suitability of such methods for quantifying biologically relevant variation needs further investigation. For datasets where most or all compounds have been identified, we have previously developed the *chemodiv* R package (Petrén et al., 2023), which can be used to calculate compound dissimilarities based on either their structure or biosynthetic classification. Once a dissimilarity matrix of the compounds has been constructed, we recommend calculating functional Hill diversity (with $q = 1$ by default) to generate an overall measure of chemodiversity. Thereafter, this may be deconstructed into the three components. Richness and evenness are calculated as before, while disparity may be quantified as the MPD. Additionally, diversity profiles may be constructed. The *chemodiv* package provides functions for these calculations.

ASPECTS OF THE FUNCTIONAL ROLE OF CHEMODIVERSITY

The recommendations above represent a general way to quantify chemodiversity. However, the importance and relevance of this diversity may vary depending on the type of compounds analyzed and the ecological context. Below, we discuss some important but underappreciated aspects of the potential importance of chemodiversity in ecological, evolutionary, and phenotypic plasticity contexts.

Perspectives on chemodiversity and ecological interactions

First, it is important to note that when phytochemicals are analyzed, and calculations of chemodiversity are made, this usually includes only a subset of the metabolites of a plant (Li & Gaquerel, 2021). Often, there are biological reasons to suspect that a class of compounds, for example, terpenoids or glucosinolates, are ecologically important in a given case. It may then be suitable to base calculations of chemodiversity on such subsets of compounds. On the other hand, other groups of phytochemicals or primary metabolites (Walker et al., 2023) that were not quantified may also be important, potentially complicating the effects of the measured chemodiversity. Choosing an appropriately delimited set of compounds is an important first step before quantifying chemodiversity.

In general, specialist herbivores are often less affected by chemical defenses than generalist herbivores (Hopkins et al., 2009; Mithöfer & Boland, 2012). This may be true also for chemodiversity (Dyer, 2018). Several studies have found that chemodiversity can have a stronger negative effect on generalists than on specialists (Agrawal, 2000; Bakhtiari et al., 2021; Kozel et al., 2022; Li et al., 2020; Volf et al., 2018). Chemodiversity might also be more predictive of function in comparisons within rather than between plant species (Schuldt et al., 2012). Within species, there may be limited variation in what compounds are found in different individuals, and function might thereby be more dependent on diversity. Across species, larger variation in which compounds are present may be of greater importance for function than the diversity itself. Phytochemical variation on the level of whole plant communities may also be ecologically important, including community-level similarity, diversity, and uniqueness affecting herbivore diversity, levels of herbivory, plant survival, and ecosystem functioning (Lavandero et al., 2009; Massad et al., 2017; Salazar & Marquis, 2022; Schuldt et al., 2018) (Box 2). From the plant's perspective, chemodiversity might be more predictive of function under natural conditions, where plants experience a multitude of interactions, compared with single interactions. The value of chemodiversity for single interactions rests on the assumption that diversity, per se, is important for function, with synergistic effects of combinations of compounds. While such effects might be common (Richards et al., 2016), there are also examples where synergies are lacking (Liu et al., 2017; Whitehead et al., 2021), or where instead antagonistic effects are found (Heiling et al., 2022; Whitehead & Bowers, 2014). In contrast, for multiple interactions, chemodiversity can be predictive of function without direct synergistic effects, if different compounds are effective against different interacting organisms (Berenbaum & Zangerl, 1996; Iason et al., 2011).

In interactions between plants and insects, a potentially useful distinction between types of phytochemicals is between volatile and non-volatile compounds (Salazar et al., 2016). Such a division is a simplification, but on a general level, the role of chemodiversity might differ between non-volatile compounds that, when consumed, have direct negative physiological effects on consumers (Wari et al., 2021), and volatile compounds acting as information cues or signals to herbivores and pollinators from a distance (Wilson et al., 2015). For example, phytochemical richness might be more relevant than evenness in the latter case, as volatiles present in low abundance can still be highly attractive or repellent to insects (Clavijo McCormick et al., 2014). A few chemodiversity studies have been performed in the context of volatile information (Appendix S1: Table S1), examining how the diversity of volatiles can act to repel herbivores or attract herbivore parasitoids (e.g., Doyle, 2009; Wan et al., 2017; Zu et al., 2020, 2022). For phytochemicals functioning as floral scent to attract pollinators, some studies have examined variation in richness between, for example, different populations (Eisen et al., 2022; Zeng et al., 2022) or between plants pollinated by different groups of pollinators (Farré-Armengol et al., 2020). Sasidharan et al. (2023) found a positive correlation between pollinator visitation and plot-level chemodiversity in *Tanacetum vulgare*, but no clear effect of chemotype. To our knowledge, no study has directly tested for a correlation between the level of chemodiversity and pollinator attraction in individual plants.

Evolutionary patterns

From an ecological perspective, phytochemicals affect the organisms interacting with plants. From an evolutionary perspective, the interacting organisms are agents of selection, affecting what phytochemicals plants produce. By examining macroevolutionary patterns and microevolutionary processes, we can learn how natural selection and other evolutionary forces generate chemodiversity on different levels (Thon et al., 2024).

Assuming a coevolutionary escape-and-radiate process between plants and herbivores (Ehrlich & Raven, 1964), the diversity of phytochemicals may increase over time as new plant species evolve. A few studies have found evidence of this. Becerra et al. (2009) found that the chemodiversity in *Bursera* species escalated over macroevolutionary timescales. Similarly, Volf et al. (2018) found an increase in alkaloid diversity over time among *Ficus* species, and Defossez et al. (2021) discovered an increase in the richness of molecular families over time in a large set of vascular plants. In contrast, Cacho et al. (2015) found an evolutionary decline in glucosinolate diversity in *Streptanthus* plants, suggesting potential trade-offs with other kinds of defense (Agrawal & Fishbein, 2008). These studies suggest that chemodiversity may often, but not always, increase over evolutionary time. This may include new compounds in existing biosynthetic pathways, or, potentially more effective but less common, compounds in new biosynthetic pathways (Becerra et al., 2009). Overall, phylogenetic patterns are often complex and might differ for different aspects of the phytochemical phenotype or different classes of compounds (Courtois et al., 2016; Forrister et al., 2022; Zhang et al., 2021; Züst et al., 2020). Therefore, the disparity component of chemodiversity, based on biosynthetic classifications, should be considered in macroevolutionary studies.

Few studies have investigated chemodiversity on a microevolutionary level. The two cases that have investigated associations between genetic diversity and chemodiversity have found different results, with Bravo-Monzón et al. (2018) finding no association between the two, but Pais et al. (2018) finding a potential positive association. Multiple studies have examined selection on individual compounds, principal components or total abundances of, for example, floral scent or herbivore defense compounds (Chapurlat et al., 2019; Joffard et al., 2020; Johnson et al., 2009). There are also multiple examples of associations between chemodiversity and various measures of plant performance, such as levels of herbivory. However, these do not take into account the potential costs for plants to produce a diverse set of compounds. Such costs, which are an important topic for future research, could diminish or outweigh benefits (Cipollini et al., 2017). Therefore, direct estimates of phenotypic selection on chemodiversity are required to investigate its potential to act on a composite trait such as chemodiversity (*c.f.* Opedal et al., 2022). We are aware of only one study that has done so (Wagner & Mitchell-Olds, 2018), where authors found that the direction of selection on glucosinolate diversity in *Boechera stricta* varied geographically among different sites. With additional studies, we may better understand how different aspects of the phytochemical phenotype experience selection and evolve over time.

Phenotypic plasticity

Chemodiversity may additionally be affected by the plant's surrounding environment. The phenotypic plasticity of phytochemicals has been examined in a broad set of contexts (Majetic et al., 2009; Metlen et al., 2009). Any phenotypic change is likely to have an effect on chemodiversity, but direct studies on this aspect are rare.

Agrawal (2000) found an increase in glucosinolate richness in *Lepidium virginicum* following herbivory, which was associated with a decreased performance in a generalist but not a specialist herbivore. In contrast, Li et al. (2020) and Bai et al. (2022) found that herbivory in *Nicotiana attenuata* had no or a negative effect on the diversity of leaf metabolomes. Instead, induced changes may act to increase metabolomic specialization if there is an increased production of certain groups of compounds that increase plant resistance. Changes to the abiotic environment could also affect levels of chemodiversity (Ramos et al., 2021), although Tewes and Müller (2018) found no effect of fertilization on glucosinolate diversity in *Bunias orientalis*. Overall, we still know comparatively little about which aspects of the phytochemical phenotype are most plastic. If plasticity involves changes in the relative abundances of compounds, this will affect evenness. But if it involves the production of novel sets of compounds, richness or disparity components may change. More studies are needed to examine the (adaptive value of) plasticity of the phenotype in the context of chemodiversity and better distinguish between genetic and environmental sources of variation.

UNANSWERED QUESTIONS AND FUTURE RESEARCH DIRECTIONS

Several aspects of chemodiversity and related topics raise questions that should be more closely investigated. First, chemodiversity is only one aspect of a multivariate phytochemical phenotype, and other aspects of this phenotype are clearly key to function in many cases. To what extent the chemodiversity, in contrast with individual compounds, specific ratios/compositions of compounds, stereochemistry of isomeric compounds, classes/modules of compounds, or the total abundance of compounds, is mechanistically important for or predictive of function will be a fundamental question to answer (Junker, 2016; Marion et al., 2015; Oduor, 2022; Torres-Gurrola et al., 2011; Yarnes et al., 2006). Studies that combine the common approach of focusing on individual compounds with diversity measures are ideally suited to answer such questions. Additionally, it will be crucial to better understand the links between molecular structure and ecological function, further examine the role of synergistic effects (Corning, 2012), and test if structurally diverse sets of compounds also have a broader function or more potent effects (Berenbaum & Zangerl, 1996; Liu & Zhao, 2016; Philbin et al., 2022). Understanding this, in turn, requires knowledge on how phytochemicals function mechanistically on molecular and physiological levels (Mithöfer & Boland, 2012; Wari et al., 2021). Furthermore, the relative importance of, and potential synergies between, chemical and morphological traits should also be studied in more detail (Edwards et al., 2022).

A second important aspect is the calculation of diversity itself. As diversity is a composite measure, we have argued for first quantifying it and then deconstructing it into its components of richness, evenness, and disparity. Many alternative ways of quantifying diversity exist, which may also provide relevant measures of the phytochemical phenotype (Chao et al., 2019; Magneville et al., 2021; Mouchet et al., 2010), although more complex measures may be more difficult to interpret. Additionally, different types and components of diversity may be mathematically correlated, and care should be taken not to confuse such mathematical associations for biological ones, as discussed by Loiseau and Gaertner (2015). Other related quantities, such as specialization and dominance, may also be important (Berger & Parker, 1970; Martínez & Reyes-Valdés, 2008), as may measures of intramolecular complexity, which are not quantified by measures of compound dissimilarity (Méndez-Lucio & Medina-Franco, 2017; Philbin et al., 2022; Richards et al., 2015). In addition to chemodiversity at the level of individual plants, also β-diversity or diversity at the within-plant, population, or community level is ecologically relevant (Glassmire et al., 2020; Robinson et al., 2022; Wetzel & Whitehead, 2020). Studies that simultaneously quantify multiple types/components of diversity are needed to examine which of these quantities are most relevant in different contexts.

Third, research on chemodiversity remains somewhat limited in scope with regard to the types of plants studied and experimental methods used. The vast majority of studies have been conducted on flowering plants, with few examples including gymnosperms or bryophytes (Figure 2c) (Feng et al., 2021; Iason et al., 2005; Peters et al., 2018, 2019, 2021; Schweiger et al., 2021; Zhang et al., 2024). Most studies are observational, comparing chemodiversity across different groups and associating this with ecological function. Experimental studies manipulating levels of diversity are rare (Fernandez-Conradi et al., 2022; Ojeda-Prieto et al., 2024; Salazar & Marquis, 2022; Sasidharan et al., 2023; Whitehead et al., 2021; Ziaja & Müller, 2023), but useful for disentangling which components of diversity are most relevant for function. Additionally, most research on the effects of chemodiversity examines effects of chemodiversity in leaves on the performance of insect herbivores or levels of herbivory (Figure 2d). Studies including other plant tissues such as roots, flowers, fruits, and seeds, and other types of interactions such as those involving fungi, bacteria, and parasitoids, have only recently become more common (De-la-Cruz-Chacón et al., 2019; Doyle, 2009; Feng et al., 2021; Lindig-Cisneros et al., 1997, 2002; Sasidharan et al., 2023; Wan et al., 2017; Whitehead et al., 2021; Zhang et al., 2024). Additionally, recent technical advances in plant metabolomics enable the use of new analytical methods (Uthe et al., 2021). These will increase the number of plant metabolites detected and identified and enable novel insights. However, it is important to acknowledge that methodological steps upstream those of diversity calculations, such as sample collection and chemical analyses, and post-analytical steps like compound identification, data processing and compound quantification, can influence results, and further work is needed to standardize these steps across studies (Walker et al., 2022). Finally, most research so far has aimed to answer fundamental ecological questions. Only a few studies have been carried out in more applied contexts, examining chemodiversity of crop species, and its potential importance for protection against pest insects (Bernal et al., 2023; Espinosa-García et al., 2021; Robinson et al., 2022; Whitehead & Poveda, 2019). Further research on this topic will increase our understanding of how chemodiversity may be utilized in agroecosystems (Espinosa-García, 2022; Silva et al., 2018).

Sixty-five years have passed since Fraenkel's (1959) seminal paper on the raison d'être of phytochemicals. Today, studying the mechanisms by which these phytochemicals function, in order to explain patterns or effects observed in nature, is central to chemical ecology (Raguso et al., 2015). However, we still have a limited knowledge of how these compounds function, alone and in mixtures, in different interactions between plants and their environment. Our literature review demonstrates that considering mixtures of phytochemicals as a complex phenotype, where aspects of its multivariate nature can be summarized into measures of diversity, may be a fruitful way to a better understanding of phytochemical function. Our framework and recommendations of how to measure chemodiversity in different contexts will allow researchers to more easily study the relevant aspects of phytochemical variation, and contribute to an increased understanding of the functional importance of the diversity of phytochemicals produced by plants.

AUTHOR CONTRIBUTIONS

Robert R. Junker and Hampus Petrén conceived of the study. All authors contributed ideas and perspectives on the topics of the paper. Hampus Petrén performed the systematic literature review and wrote the first draft with contributions from Robert R. Junker. All authors reviewed the manuscript and approved the submitted version of it.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest.

DATA AVAILABILITY STATEMENT

Data and code (Petrén et al., 2024) are available in Figshare at https://doi.org/10.6084/m9.figshare.23709072.v1.

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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