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COMMENTARY

New Synthesis: Parallels Between Biodiversity and Chemodiversity

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A major aim of chemical ecology is to gain deeper insight into how organismic responses to the abiotic and biotic environment are regulated by naturally produced chemicals. Chemical ecologists pursue this aim by combining chemical, molecular, and ecological expertise. While many ecological studies focus on the impact of the plethora of species on community or ecosystem functions, numerous chemoecological studies aim to elucidate the ecological relevance of a comparable bounty of natural products, their biosynthesis, transfer and metabolism as well as the organismic responses to them (Hartmann 2007). Awareness of the parallels between studies of biodiversity and chemodiversity may promote finding answers to our proximate (how) and ultimate (why) questions on the chemical mediation of organismic responses to environmental stimuli.

When comparing biodiversity studies and chemoecological studies with respect to: (i) the functions of species and of natural products; (ii) the dynamics by which a community of species is established and by which a blend of chemicals is biosynthesized; and (iii) the quantification of biodiversity and chemodiversity, some informative parallels may be drawn:

(i). Numerous ecological studies have investigated the impact of biodiversity on ecosystem functions and have elucidated how the number and type of species affect the stability, elasticity, and productivity of ecosystems. Some (keystone) species have crucial effects on their community, others may be replaced by species with similar functional roles (*e.g.*, members of a pollinator guild), and many species have multiple roles (*e.g.*, plants providing the nutritional basis for phytopathogens, symbiotic organisms, pollinators, herbivores, habitats for predators of the herbivores *etc*.). In parallel, chemical ecologists have identified an enormous range of natural products, some of which clearly act as key compounds that mediate organismic interactions (*e.g.*, pheromones), or as hub metabolites for biosynthesis of other compounds. Natural products with multiple ecological roles are, for example, plant terpenoids which function as insect feeding deterrents or even toxins, but may also alert predators and parasitoids to the presence of herbivorous arthropods. Just as ecologists investigate the multifaceted roles of a species within a system and the importance of the species composition of a community for ecosystem functioning, chemical ecologists have begun to analyse the multifunctional roles of single natural products as well as the impact of specific blends of compounds on chemical mediation of organismic interactions.

(ii). For many years, ecologists have used conceptual approaches to understand the dynamics by which a community of species is established and maintained. The realized community depends on numerous factors ranging from the local availability of species and niches to the dispersal ability of species, their reproductive fitness, competitive strength, and nutritional requirements. Similarly, the realized blend of natural products detectable in an organism or emitted by it depends on a wide range of factors. The availability of enzymes and substrates required for the biosynthesis of these compounds, the mobility (dispersal) and stability of the natural products, the "productivity" of enzymatic synthesis, the ability of enzymes to compete for substrates as well as their requirements for hub metabolites and cofactors greatly affect the "community" of compounds detected in our analyses. Scientists that use genomics, proteomics, metabolomics and fluxomics data to model biosynthetic networks consider these factors in order to elucidate biosynthetic control mechanisms and to predict metabolic processes. Future studies need to show whether a combination of these system biological approaches with theoretical approaches used in studies of biodiversity dynamics (Thuiller et al. 2013) might help to elucidate the dynamics of the biosynthesis of ecologically relevant natural products.

(iii). Chemical or molecular diversity is usually considered with respect to the diversity of chemical structures and the properties that determine their bioactivity. To quantify chemodiversity, these properties (descriptor variables) are subjected to various statistical analyses (*e.g.*, (dis)similarity indices), which help detect new leads in combinatorial chemistry and high throughput screening. The numerous metrics for quantification of biodiversity range from species number to species-abundance measures (*e.g.*, Shannon and Simpson indices), to those that include species-specific traits and phylogenetic relatedness (based on species similarity). By analogy, chemodiversity may also be defined by the number of compounds and their relative abundance. While chemical ecologists often use statistical tools (*e.g.*, principal component analysis, multidimensional scaling) to disentangle the quantitative and qualitative composition of blends of compounds, diversity indices

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based on the number of compounds and their abundances are rarely applied to such data, even though they are easily adjustable to the quantification of chemodiversity (Randlkofer et al. 2010; *e.g.*, CD = chemical diversity$_{\text{(after Shannon Index)}} = -\sum p_i \times \ln p_i$; in this formula is p_i the peak area of a compound relative to the total peak area; the sum includes all compounds detected; CD increases with increasing chemodiversity). Such chemodiversity indices might help to elucidate how the diversity of a chemical blend influences organismic behavior. While a comparison of two chemical blends *via e.g.*, a principal component analysis provides information on how the blends differ, CD values based on the number of compounds and their abundances may be correlated with behavioral parameters and inform about how many “words” (compounds), and what level of “loudness” (abundance) are necessary to elicit a specific ecological interaction. Diversity of plant or animal defensive chemicals has often been interpreted as beneficial for the releasing organisms since it might pre-empt counter-adaptation by enemies; diversity of pheromones across species is obviously important for reproductive isolation through the maintenance of species-specific communication. More studies are needed to explore the impact of chemodiversity on *e.g.*, the information content or reliability of chemical signals.

The above-mentioned parallels might motivate a more intensified interdisciplinary exchange of ideas and methodological approaches between scientists studying biodiversity and chemodiversity, and eventually, a more unified understanding of complexity.

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