

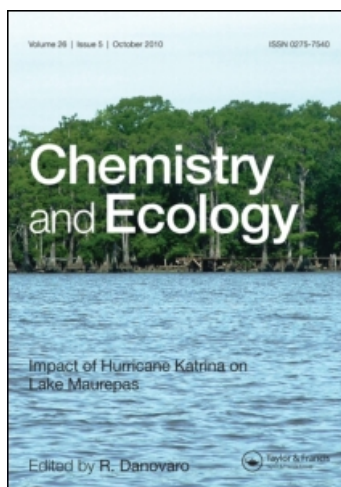
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IDEAS

Ecological metabolomics

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1. Introduction

Ecology is developing genomics-based approaches to ecological questions by using the ever-accumulating knowledge of an organism's genome, i.e. their whole hereditary information encoded in their DNA [1]. At the same time, ecology is trying to put to use the transcriptome (all the expressed genes of an organism, in the form of mRNA) and the proteome (all the translated peptides). And now, when still immersed in these developments, ecology is increasingly discovering the metabolome, the entirety of molecules present in an organism and the ultimate expression of the genotype as a response to environmental conditions [2]. Recent rapid improvements in analytical methods and in the ability of computer hardware and software to interpret large datasets have multiplied the possibilities of rapidly identifying and quantifying simultaneously an increasing number of compounds (e.g. carbohydrates, aminoacids and peptides, lipids, phenolics, and terpenoids). These advances will allow us to not only take 'static pictures' or snapshots of the metabolome, but also to capture and to 'film' its dynamic nature. All in all, we may now be able to achieve a dynamic, holistic view of the metabolism and health of an organism, a population, or an ecosystem, and in this fashion open the door to exciting new insights in ecology.

2. Metabolomics

Metabolomics allows the assessment of an organism's energetic, oxidative, reproductive, defensive and health statuses and their dynamics (for example, through measurements of concentrations of ATP, glycogen, glutathione, ascorbate, steroids, alkaloids and poliphenols). The metabolome is often the first to respond to natural daily events such as light intensity in plants or feeding in animals, or to anthropogenic stressors including pollutant exposure, even though in some cases no changes in the transcriptome and proteome actually occur. On the other hand, the transcriptome

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and proteome may change while the metabolome remains unaltered, leading to mistaken assignments of functional changes at organism level. Another interesting advantage of metabolomics is the flexibility with which it can be applied to any organism, irrespective of the knowledge of the genome of that species, which in many cases is still poor or non-existent. In all cases, metabolomic databases can be combined with datasets from other ‘omic’ technologies [3] to enhance data value and permit a system-wide analysis from genome to phenome (just as the *genome* and *proteome* signify all of an organism’s genes and proteins, the *phenome* represents the sum total of its phenotypic traits). This combination thus provides greater biological insight than any single ‘omic’ technique studying the ‘complete’ genome, proteome or metabolome alone can offer. Metabolome analysis is an additional measure of phenotype and it has advantages for ecological studies, given the universal nature of metabolites [4]. Metabolomic studies give information that can improve the assessment of biological function because frequently there is no quantitative relationship between mRNA levels and biological function [5].

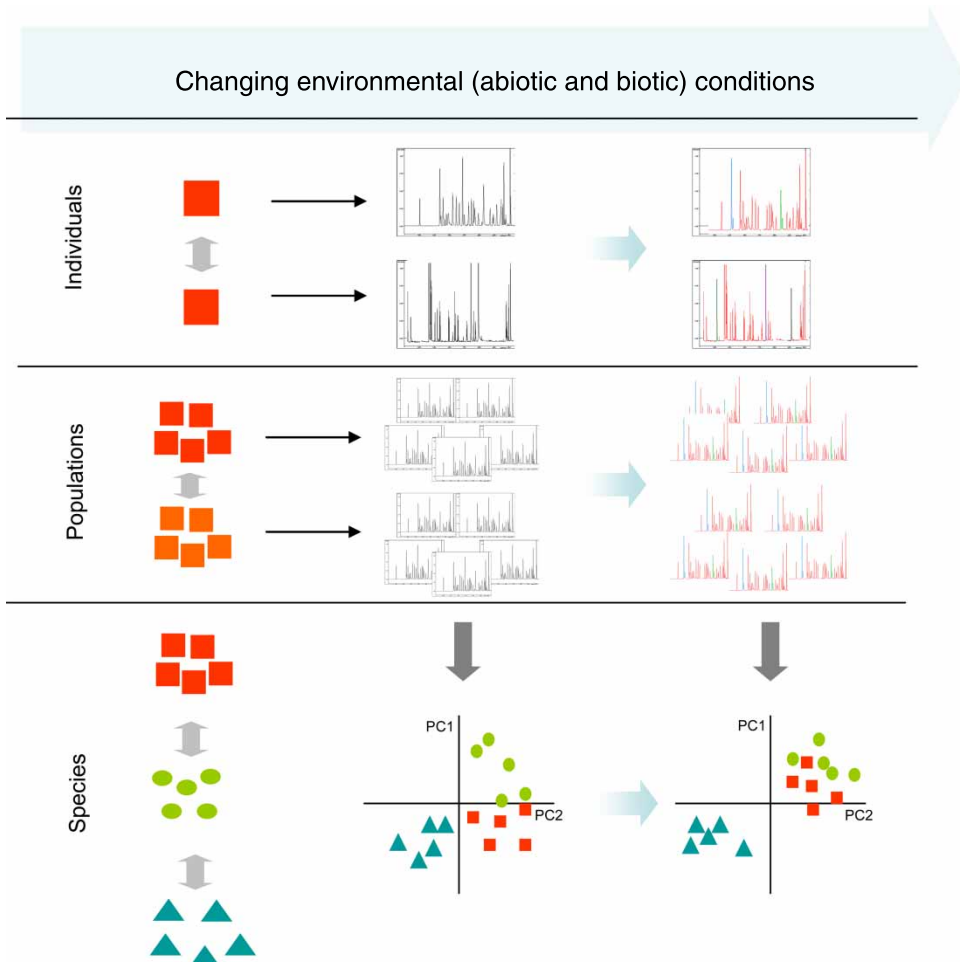


Figure 1. Metabolome analyses can be used to identify phenotypic differences between individuals, between populations and between species, and to follow such differences through time in response to environmental changes. Multivariate analyses of large datasets are needed to deal with metabolomic studies. The lower panels of the figure depict schematically the results of principal component analyses of metabolites (depicted in upper panels) from different individuals of different species in an ecosystem at different times and under different environmental conditions.

3. Ecometabolomics

Ecologists are starting to apply metabolomics to the study of plant and animal metabolic responses to changing abiotic and biotic environmental conditions [6–9]. In an example of these ‘ecometabolomic’ applications, Alvarez et al. (2008) have screened and quantified the changes in sap constituents under extended drought conditions [10]. They have detected changes in the concentration of 31 compounds, including hormones such as abscisic acid and cytokinin, involved in the regulation of stomatal aperture, several phenylpropanoid compounds such as coumaric, caffeic and ferulic acids and several enzymes such as cationic peroxidases involved in lignin biosynthesis in the xylem vessels and therefore in lignification and cell wall stiffening. They have thus provided not only insights into the range of compounds in sap, but also into how alterations in composition may lead to changes in signaling and development during adaptations to drought: a pressing issue in these times of climate change. Moreover, metabolomic studies can provide information of biotic relationships between species, e.g. how infection can lead to individual responses [11–13], or how grazing injury leads to defensive responses [14].

Nonetheless, ecometabolomic applications are not only limited to the ecophysiology of organisms. A few studies exist that upscale the use of metabolomics from individual to population and ecosystem levels (Figure 1). For example, Davey et al. (2008) [15] have shown that metabolite fingerprinting and profiling is sufficiently sensitive to be able to identify the metabolic differences between populations of *Arabidopsis petraea*. They found fold differences in many free amino acid concentrations among different populations. Many free carbohydrate concentrations were also different, while polyhydric alcohol concentrations were not. A principal component analysis of metabolite fingerprints revealed different metabolic phenotypes for each population. At the landscape level, Gidman et al. (2006) [16] have shown that different metabolic fingerprints measured with rapid Fourier transform-infrared spectroscopy in tissue samples of *Galium saxatile* are correlated with a gradient of N deposition across the entire UK landscape. Metabolomics thus allows the investigation of complex ecological systems and provides a rapid and sensitive indicator of ecosystem health. Viant (2007) [17] has gone a step further, and has proposed that by using the same argument as in the origin of metabolomics, that is, that the measurement of multiple metabolites (versus one) can provide a more robust assessment of the metabolic health of an organism, characterising the health of multiple species will provide a more complete assessment of the ecosystem responses to environmental stressors, and even of the nature of the stressor.

4. Challenges

A serious challenge for ecometabolomics is the large number of metabolites and the lack of a fully described and annotated metabolome for any plant or animal species. It is estimated that the plant kingdom produces 100,000–200,000 different metabolites [18], although the actual number present in any individual plant species is still unknown. The exact number of metabolites remains a mystery, even in the case of micro-organisms with simple and well-understood metabolisms; typical non-plant eukaryotic organisms are estimated to contain from 4,000–20,000 metabolites [19]. Furthermore, the metabolome changes continuously, an additional challenge that is accentuated when measuring the metabolomes of several individuals from a free-living population, which will necessarily include considerable metabolic variation. There will be high levels of variations in metabolite concentrations between individuals, owing to differences in individual genetics, gender, age, organ, health status and spatial and temporal environmental changes: simple issues such as the time since the animal last ate or the plant last received sunlight may also be determinant.

The treatment of the large temporal and individual variability found in metabolomes, which may tend to mask the sources of variation that are of interest for ecologists, can be successfully

approached by trying to ‘film’ temporal changes in metabolite levels and their turnover rates [20] instead of merely taking ‘snapshots’ of metabolite levels, and by multiplying the number of individuals sampled. The continuous development of new advances in *in vivo* NMR spectroscopy and imaging, proton-transfer-reaction mass spectrometry, or isotope labelling and in the treatment of large data sets in bioinformatics will help in this line of work.

Another challenge to face up to is the risk that, despite its value, the overwhelming ‘-omics-type’ information reaches a field which it is conceptually not properly prepared for, thereby leading to the loss of an opportunity to advance ecological knowledge. Certain explanatory principles accounting for the complexity of living organisms and their populations and ecosystems, as well as of their responses to the environment, are still lacking. Ecometabolomics will need thus to focus on conceptual advancement and functional trait discovery and not just on technological development if it is to shed light on the fundamental system-biological mechanisms at work at scales ranging from the individual to the ecosystem.

5. Perspectives

If ecological metabolomics succeeds in overcoming these challenges and uses them as opportunities for advancing knowledge, we can expect to see stimulating new developments and applications in the near future in many areas of ecological sciences, including issues of stress responses, life-history variation, population structure, trophic interaction, nutrient cycling, and the ecological niche. For example, the temporal and spatial characterisation of the responses of individuals, populations and ecosystems to perturbations such as global change and the disentangling of evolutionary aspects of plant and animal communities both offer ecological metabolomics an immediate opportunity as a new and exciting application. In turn, ecology can provide a unique insight and a significant contribution to the study of functional metabolomics by helping to understand the ecological basis for interactions among metabolites.

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