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Ecometabolomics: a new instrument for ecological research

Metabolomic techniques aim to determine the maximum number of metabolites present in an organism at a given time. These techniques have been used for a long time in the context of biomedicine and now are starting to be used in the field of ecology. Researchers at the Global Ecology Unit CREAF-CSIC-UAB have studied the existing literature in this field as well as technical advances leading to elucidate further the contributions that metabolomics has already made to ecology and particularly to determine future research lines in this area where the application of metabolomics studies could lead to important advances.

Metabolomics analytical techniques aim to analyse the complete metabolome (all the metabolites that one organism produces) at one particular moment and both at qualitative and at quantitative level. They thus show the phenotypical response to environment at metabolic level in a particular environmental circumstance. Metabolomics has been mainly developed coupled to biomedical studies but now the possibility of using progressively improved metabolomic techniques in ecophysiological and ecological studies is gaining importance. The use of modern hydrogen nuclear magnetic resonance (HNMR) spectrometers and gas or liquid chromatography on-line with mass spectrograph (GC-MS) coupled to bioinformatic advances has opened up a new way to advance in the knowledge of organism's and ecosystem's responses to environmental shifts. These rapid improvements in analytical methods and in the ability of computer hardware and software to interpret and visualize large datasets have multiplied the possibilities of rapidly identifying and quantifying simultaneously an increasing number of compounds (e.g. carbohydrates, amino acids and peptides, lipids, phenolics, and terpenoids). These advances will enable us not only to take 'static pictures' or snapshots of the metabolome, but also to capture and to 'film' its dynamic nature.

The challenge metabolomics opens in ecology is great, it may help to better understand the causes and evolution of ecosystem structure and function in response to environmental (climate, soil type) gradients and temporal changes and the underlying feed-backs mechanisms. The studies that have beginning to explore this field are still scarce and in most cases they are limited to the direct effects of a single abiotic factor or of biotic interactions between two trophic levels under controlled conditions. But these studies should be analyzed jointly to establish the current and potential global contributions of metabolomic studies in ecology and to explore the future possibilities of coupling metabolomic studies with complex field ecological studies (ecometabolomics).

To reach these objectives, researchers of the Global Ecology Unit CSIC-CREAF-UAB have conducted a review analysis of current bibliography of the studies that have used metabolomic techniques to study organisms' responses to environmental changes and have discussed the possibility to apply metabolomics to other diverse key fields of ecological research.

The studies available demonstrate ecometabolomic techniques have great sensitivity in detecting the phenotypic mechanisms and key molecules underlying organism responses to abiotic environmental changes and to biotic interactions. The study highlights that the treatment of the large temporal and individual variability found in metabolomes helps to unmask the sources of variation that are of interest for ecologists. This objective can be successfully approached by trying to 'film' temporal changes in metabolite levels using the continuous development of new advances in in vivo NMR spectroscopy and imaging, proton-transfer-reaction mass spectrometry, or isotope labelling. The treatment of large data sets in bioinformatics will be of great assistance in this line of work.

Several exciting challenges remain to be achieved through the use of ecometabolomics in field conditions, involving more than two trophic levels, or combining the effects of abiotic gradients with intra and inter-specific relationships. The coupling of ecometabolomic studies with genomics, transcriptomics, ecosystem stoichiometry, community biology and biogeochemistry may provide a further step forward in many areas of ecological sciences, including stress responses, species life style, life history variation, ecological stoichiometry, population structure, trophic interaction, nutrient cycling, ecological niche and global change.

But these possibilities still present some caveats. The different metabolomic analytical techniques have different capacity to determine different analytical groups (polar-non polar, volatiles-non volatiles) and different sensitivity and elucidation power. On the other hand, there is a lack of extensive data bases to help in the molecular structure determination. This specially applies to the study of plant metabolome due to the large number of secondary metabolites. But these caveats are increasingly being solved. The lack of data bases is increasingly been improved by the continuous enhancement of available commercial offer of informatics programs and databases. The use of several analytical methods to analyze the same organism extracts has been successfully used in some recent studies using 1HNMR and GC-MS and 1HNMR and HPLC-MS by thus coupling the greater sensitivity of chromatographic methods with the greater elucidation power of HNMR. At this regard the recent HPLC-DAD-MS-SPE-NMR provide high sensitivity and elucidation power at once.

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. For example, the temporal and spatial characterization 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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