Challenges in Environmental Metabolomics

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Environmental metabolomics is a recent experimental method that is used to analyze the metabolites of living organisms (such as plants, aquatics, and other invertebrates) when exposed to external stress factors like pollution and climate change.

Nuclear magnetic resonance (NMR) and mass spectroscopy (MS) are vital tools used to measure metabolite levels. These tools are applied in the field of aquatic and terrestrial toxicology, aquaculture, and environmental supervising, and its risk evaluation.

City Pollution. Image Credit: grynold/Shutterstock.com

Challenging aspects of environmental metabolomics

Various challenges and obstacles in environmental metabolomics prevent its wide-ranging access to ecological sciences.

Interaction among analysts

Since the ecological system is multi-subject oriented, it requires analysts with distinct qualifications such as in chemistry, biology, mathematics, and computer science. So, the communication between such scientists can contribute to the development of the better experimental design. Sadly, this aspect is very challenging as the present scenario involves many barriers in bringing together the concerned people from their respective disciplines.

Additional improvement of tools to assess metabolites

There is continuing development of devices such as NMR and MS as they both do not provide a single analytical platform to perform a complete quantification and identification of all metabolites within a single sample.

> Although the working of these tools is an essential procedure, it initiates substantial confusion for new analysts in the field. So, considerable practice is required in the professional handling of NMR and mass spectroscopy. There is a demand to launch centers of superiority in this field to expedite the greater widespread utilization of this approach.

i. **Limitations of NMR spectroscopy:** Due to the narrow range of chemical shifts, NMR spectra persist in overlapped signals that result in changeableness in the spectral assignments.
ii. **Limitation of mass spectroscopy:** It finds challenges in detecting atmospheric gases such as CO_2, N_2, O_2, etc., and in evaluating extracts obtained from plastics.

The development of tools and software databases that permit full-scan analysis along with NMR and MS in the same analytical trial is another way forward.

Analytical challenges in environmental metabolomics

The amalgamation of metabolites might also be a reason for the comprehensive characterization of an organism. In examining the metabolite characterization, the challenges faced by the analytical part are mentioned below:

i. **Chemical diversity:** The chemical difference in a typical metabolome (number of metabolites in an organism) is huge and requires numerous general approaches for compound identification, quantification, and localization. Currently, metabolomics is constrained by these analytical obstacles and can be largely brought about by the tremendous extent of chemical diversity across metabolite populations.
ii. **Effective separation procedure:** The vital range of metabolite concentration is huge in some organisms, especially in plants. We need efficient separation strategies so that the minor metabolites are also isolated completely along with the vital ones.

Validation and standardization of environmental metabolomics

i. **Validation:** Presently, distinct research squads are using different experimental designs, contrasting data analysis, and analytical tools in order to conduct their investigation on environmental metabolomics. Thus, this method of validation makes it hard to study the consequences between various analyses. Even if environmental research scientists use the same device, there has been no validation to prove that the same outcome will be obtained. Aspects of these issues are currently being addressed.
ii. **Standardization:** Generally, in several experiments, standardization of protocols is a beneficial method for reducing data variation. This being said, there is no unified scheme emerging from the scientific community regarding MS-based metabolomics and today a large variety of analytical strategies still exists. So, there is an immediate requirement for standardization of procedures which allows the comparison of results in order to enhance the potential of metabolomics.

Obstacles faced during identification of metabolites

NMR and MS can identify a large number of metabolites but most detected metabolites have an unknown chemical nature. This part is a real challenge and constitutes another limitation of the widespread approach. In fact, studies have revealed that in the best cases, only 30% of the total MS signals detected in an experiment are identified. The remaining 70% represents data on changes in metabolic profiles which remain unknown.

The obvious recognition of metabolites is a critical constituent of several metabolomic studies. This facilitates the requirement to provide a vast available supply of biological data and exclusive intelligence on environmental metabolomics. Nevertheless, few commonly accessible libraries exist which comprises the data needed to attain this, especially for “exotic” metabolites that may appear in invertebrate organisms.

Regarding metabolite identification, the use of databases has become well-structured and more straightforward as these initiatives are currently working on detailing the standardization methods through merging several databases available on the Internet. Also, there is a need to create further databases that contain a range of pure metabolites to enable a clear recognition of

environmental metabolites.

Furthermore, the effects of environmental factors such as temperature, PH of water as well as soil, pesticide usage, etc., need to be explored in order to advance the understanding of the ecological metabolome and thereby improve the data interpretation.

Sources:

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