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Editorial: Perspectives in omics 2022

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Editorial on the Research Topic Perspectives in omics 2022

Introduction

Omics-based studies, encompassing various disciplines such as genomics, transcriptomics, proteomics, lipidomics, and metabolomics, along with related fields, have burgeoned over the past 2 decades. These studies aim to offer a comprehensive and holistic understanding of biological systems by simultaneously exploring multiple layers of molecular information. Researchers employ these approaches to unravel fundamental biological mechanisms, identify disease biomarkers in clinical studies, investigate genetic and environmental factors, and explore potential therapeutic targets.

Mass spectrometry (MS) stands as an analytical tool across various omics sciences. Its unmatched sensitivity, precision, speed, and selectivity, combined with a wide dynamic range, make it exceptionally powerful. When integrated with separation methods, tandem experiments, and informative approaches, MS becomes a highly effective tool, enabling comprehensive research.

In this Research Topic, we, along with our contributing authors, endeavor to provide an overview of the omics field, focusing on small molecules such as Lipidomics and Metabolomics. Additionally, we delve into the combined omics approaches for clinical and environmental applications. Furthermore, we detail recent MS-based developments, ensuring accurate data acquisition in Lipidomics.

The aquatic environment stands out as one of the most intricate biosystems, where organisms at all trophic levels face exposure to a myriad of pollutants. Ecotoxicology, with its primary objective being the examination of the impact of toxic substances on ecosystems, typically focuses on studying sentinel organisms like freshwater organisms also called sentinel species, reflecting the river health (*Daphnia magna*, *Gammarus fossarum* ...). In recent decades, MS-based omics techniques have been applied to these sentinel species under both laboratory and field exposure conditions. Single-omics approaches facilitate the identification of biomarkers reflecting an organism's health status. However, these methods, while illuminating a portion of the molecular cascade, offer only a partial comprehension of the intricate ecotoxicological effects. In contrast, a more comprehensive understanding of ecotoxicity pathways can be achieved through multi-omics approaches. These methodologies delve deeper into the intricate web of interactions, providing a holistic view of the complex effects of pollutants on aquatic ecosystems. In their contributed

perspective, [Calabrese et al.](#) deliver a critical assessment of future advancements in MS-based single and multi-omics studies in aquatic ecotoxicology. As an illustrative case, the authors conducted a thorough examination of the literature relating to omics and multi-omics method developments on Gammarids, freshwater amphipods serving as non-model sentinel organisms highly responsive to pollutants and environmental changes.

Untargeted omics applied to small molecules such as lipidomics aims to provide an exhaustive catalogue of lipids. To achieve this objective, untargeted lipidomics workflow typically implicates the coupling of separation methods to high-resolution mass spectrometry (HRMS). Getting an exhaustive coverage of the lipidome with a high confidence in structure identification is still highly challenging due to the wide concentration range of lipids in complex matrices and the presence of numerous isobaric and isomeric species. The development of innovative separation methods and HRMS(/MS) acquisition workflows helped improving the situation, but issues still remain regarding confident structure characterization. To overcome these issues, thoroughly optimized MS/MS acquisition methods are needed. For this purpose, different methodologies have been developed to enable MS and MS/MS acquisition in parallel. Those methodologies, derived from the proteomics, are referred to Data Dependent Acquisition (DDA) and Data Independent Acquisition (DIA). In this context, [Valmori et al.](#) provided in their perspective paper the latest developments of DDA- and DIA-based lipidomic workflows and listed available bioinformatic tools for the analysis of resulting spectral data.

In the same field of application, [Schwudke](#), in his minireview discussed about the considerations for interpreting membrane and storage lipid profile changes that are often the central focus of untargeted Lipidomics studies. Insights into how the most conserved molecular patterns are formed in eukaryotic systems and the consequences for the perturbation of lipid homeostasis were also addressed. The implications of lipid identification specificity and experimental variability on modeling membrane structure and systemic responses were discussed.

Metabolomics aims to comprehensively analyze and identify small molecules to gain insights into the metabolic processes occurring within biological systems. Since metabolomics involves the characterization of multivariate metabolic phenotypes, such a field requires specific data analysis tools to fully exploit the relevant information considering the different factors, as well as their respective impact on metabolite levels. [Boccard and Rudaz](#), in their perspective discussed about the challenges opened by the investigation of such a high-dimensional multifactorial data and pointed out the requirement of the development of innovative experimental strategies involving structured designs of experiments to assess cause-effect associations to reach deeper insight into relevant biological information.

In a clinical point of view, [Le Gouellec et al.](#), in their mini review discussed about how metabolomics can be useful and

implemented in clinical studies for the discovery of biomarkers, but also to propose the assays of biomarkers called “signatures,” which can be composite biomarkers or fingerprints, which will ultimately guide the clinician. They exemplified their arguments by the illustration of trimethylamine N-oxide found as a biomarker for cardiovascular diseases.

Ultimately, [Lazari et al.](#), in their mini-review surveyed literature that have combined mass spectrometry-based omics techniques (proteomics, lipidomics, and metabolomics) and artificial intelligence to understand COVID-19 pathogenesis. They made an exhaustive bibliography studies pointed out the pros and the cons of used MS-based strategies as well as data analysis.

We would like to acknowledge all the authors who have made invaluable contributions to shaping this Research Topic. We would also like to express our gratitude to the diligent reviewers who have played a pivotal role in upholding the quality of the manuscripts. We have striven to incorporate a diverse spectrum of opinions, representing various geographic regions and career stages. Ultimately, we hope that this Research Topic will serve as a valuable reservoir of knowledge, catering to both novices and experts, offering insights into the current advancements and future trajectories in the “Omics” field.

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