



Machine Learning Applications in Metabolomics Analysis

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Message from the Guest Editors

Metabolomics research is gaining much popularity since it enables the study of biological problems at a biochemical level, and can help us to understand the induction, development and mechanisms of many diseases, complementing information from other 'omics technologies. Similar to other high-throughput biological technologies, metabolomics can produce large volumes of data, and therefore, machine learning strategies can facilitate its application, with the discovery of new biomolecular signatures, which consequently facilitate the diagnosis/prognostic monitoring of diseases, including rare metabolic disorders, etc.

This Special Issue aims to attract publications focused on the application of machine learning techniques to the analysis of multidimensional metabolomics data, including the development of methods, data augmentation procedures, preprocessing techniques, the comparisons of different methods, interpretability of results, the identification of new signatures, etc.





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Message from the Editor-in-Chief

The metabolome is the result of the combined effects of genetic and environmental influences on metabolic processes. Metabolomic studies can provide a global view of metabolism and thereby improve our understanding of the underlying biology. Advances in metabolomic technologies have shown utility for elucidating mechanisms which underlie fundamental biological processes including disease pathology. *Metabolites* is proud to be part of the development of metabolomics and we look forward to working with many of you to publish high quality metabolomic studies.

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