Special Issue

Machine Learning in Metabolomics: Unlocking the Future of Data Analysis

Message from the Guest Editors

Machine learning (ML) is transforming the landscape of metabolomics, building on its revolutionary impact in precision medicine and other omics fields.

A key breakthrough lies in the application of ML to compound annotation, where it has dramatically improved the identification of unknown small molecules. Another pivotal area is biomarker discovery. ML algorithms excel at processing large datasets, identifying specific metabolic signatures that indicate diseases. Moreover, ML is a cornerstone in multiomics integration—combining data from genomics, transcriptomics, proteomics, and metabolomics. This holistic approach provides a comprehensive view of biological systems, with ML enhancing both data interpretation and analytical precision.

As the field evolves, such innovations are critical for addressing data complexity, advancing our understanding of biological systems, and driving innovative personalized medicine solutions.

Guest Editors

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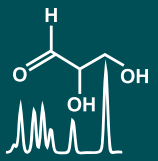

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About the Journal

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.

Editor-in-Chief

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