

Special Issue

Mechanism-Aware Machine Learning in Metabolomics and Clinical Translation: Signatures, Pathways, and Patient Impact

Message from the Guest Editor

This Special Issue invites contributions at the intersection of clinical metabolomics and machine learning (ML), highlighting how data-driven methods are advancing the discovery, validation, and translation of metabolic biomarkers into tools for diagnosis, prognosis, and therapeutic decision-making. We seek studies that cover the entire pipeline, from raw data to clinically actionable models, emphasizing methodological rigor, biological interpretability, and reproducibility in clinical settings. We particularly welcome studies that leverage LC/GC-MS, MS/MS, NMR, and imaging mass spectrometry to generate high-quality, harmonized datasets across sites and instruments.

Guest Editor

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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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