



Metabolomics and Machine Learning for Improved Diagnostics and as a Tool to Accelerate Drug Development

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Message from the Guest Editor

Dear Colleagues,

Altered metabolism has been linked to nearly every disease, including cancer, neurodegeneration, cardiovascular disease, transplantation, aging and many more. Altered metabolites already provide powerful clinical biomarkers to diagnose diseases and guide treatments. Due to challenges in analytical measurements, most clinical assays to date only measure a limited number of metabolites, leaving the true potential largely untapped.

With advancements in technology in NMR and MS, coupled with machine learning and a deeper understanding of biology, full metabolomics studies are on the horizon. This should usher in a new era of clinical insights driving diagnostic innovation and accelerating drug development. Reproducibility concerns, sample logistics, metabolite annotations and questions around complex statistics must be addressed. In this Special Issue, we highlight technical advancements driving the field. Furthermore, we provide use cases in which metabolomics and machine learning are changing our ability to diagnose and treat disease. Finally, we provide tangible best practices and considerations for those looking to apply metabolomics and ML to their research.





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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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