ASHBi SEMINAR

Computational mass spectrometry to deepen the understanding of metabolisms

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Date Monday, 14 February 2022

Time 14:00 – 15:00

Venue Zoom Online Meeting*

*Register via the right QR code

Abstract

The metabolome is the complete set of small molecules present within a living organism, formed as a result of metabolism reflecting biological phenotypes. Untargeted metabolomics studies using mass spectrometry (MS) show that metabolites are deeply involved in the body's physiology and homeostasis. Yet, only 100-200 metabolites out of thousands of ions detected by MS are identified by modern computational techniques. Currently, most metabolomics data are "dark matter" and biological mechanisms are discussed based on information from only 2-3% of the metabolome (#1). Small biomolecules are thought to comprise over one million chemical species. Illuminating the 'dark matter of metabolomes' will expand our understanding of metabolic diseases and lead to the discovery of innovative drugs. Here I have established a new field of research called computational MS (CompMS) (#2-6). Employing CompMS, I was able to (A) develop a data processing pipeline for complex MS data and (B) identify unknown metabolites. Advancing CompMS can improve our knowledge of fundamental biology and open the door to the development of new biomarkers, drugs, and clinical applications.

References

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