

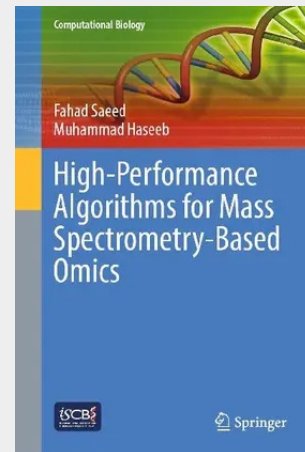
High-Performance Algorithms for Mass Spectrometry-Based Omics

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Mass spectrometry is a diverse and versatile technology for high-throughput functional characterization of proteins, small molecules and metabolites in complex biological mixtures. In the recent years the technology has rapidly evolved and is now capable of generating increasingly large (multiple tera-bytes per experiment) and complex (multiple species/microbiome/high-dimensional) data sets. This rapid advance in MS instrumentation must be matched by equally fast and rapid evolution of scalable methods developed for analysis of these complex data sets. Ideally, the new methods should leverage the rich heterogeneous computational resources available in a ubiquitous fashion in the form of multicore, manycore, CPU-GPU, CPU-FPGA, and IntelPhi architectures.

The absence of these high-performance computing algorithms now hinders scientific advancements for mass spectrometry research. In this book we illustrate the need for high-performance computing algorithms for MS based proteomics, and proteogenomics and showcase our progress in developing these high-performance algorithms.

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