UMPIRE: A Reproducible Pipeline for Scalable Metabolomics Data Analysis

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**Background:** Metabolomics includes the study of small molecules (molecular weight < 1500Da) acting as middle or end products of cellular metabolism. Large-scale epidemiological studies are increasingly collecting metabolomics data in biologically relevant tissues to understand metabolic variation in the development of health and disease. However, reproducibility is vital in science, and metabolomics data analysis still remains difficult to reproduce on different host systems. Although an increasing number of open source software packages have been developed to complete metabolomics analysis, most of these programs were designed for single desktop users and lack high-throughput scalability and reproducibility. Currently, software containers are able to package up all codes and dependencies of an application to ensure application portability, infrastructure flexibility and reproducibility. Applications running with the container will depend on the environment pre-built in the container regardless of the environment in the host machine. Nextflow is a pipeline development tool supporting containerization and high performance computing, which improves the scalability and reproducibility of bioinformatics research

**Objective**: The goal of our project is to develop an open-source tool using Nextflow to facilitate reproducible and scalable metabolomic data analysis.

**Findings**: UMPIRE can be executed on any UNIX-like systems with a specific focus on implementing UMPIRE within large-scale computing environments. We have developed UMPIRE to run in paralleled common metabolites analysis software packages including MzMine and XCMS for peak detection to enhance precision. Moreover, UMPIRE provides users multiple statistical analysis algorithms including SECIMtools, principle component analysis, volcano plots and hierarchical clustering. To facilitate dynamic and transparent data processing, we have included MultiQC reports to visualize the result of data processing and summarize metabolomics output.

**Conclusion**: UMPIRE is a container-based platform that has potential to facilitate high-throughput and scalable metabolomic data analysis with high levels of reproducibility and transparency.