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**A Reproducible Pipeline for Scalable Untargeted Metabolomics Data Analysis**

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##### ABSTRACT

**Background:** Untargeted metabolomics data is increasingly collected by epidemiological studies to investigate population-level variation in the development of health and disease. Reproducibility of untargeted metabolomics data analysis remains a challenge. Containerization of analysis workflows is the process of packaging all codes and dependencies of an application to ensure portability, infrastructure flexibility and reproducibility. 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 a container-based open-source tool to facilitate reproducible and scalable untargeted metabolomic data analysis.

**Findings**: The pipeline can be executed on any UNIX-like systems with a specific focus on implementation within large-scale computing environments. We have embedded common metabolomics analysis software (i.e Mzmine) within a Nextflow workflow for the purpose of enhancing reproducibility. Moreover, we used Python for statistical tests, as well as providing users multiple visualization methods including principle component analysis, and hierarchical clustering. To facilitate dynamic and transparent data processing, we have included MultiQC interactive reports to visualize the result of data processing and summarize metabolomics output. To test our pipeline, we used two different operating systems in which the MZmine versions were also different to do peak detection for four sample metabolomics data. This simulates the situation that one researcher wants to reproduce the other researcher’s published work with a different machine. We got very different peak numbers from MZmine of the two machines, but the exact same peak numbers when using our Nextflow pipeline.

**Conclusion**: We have developed a container-based platform that has potential to facilitate high-throughput and scalable untargeted metabolomics data analysis with high levels of reproducibility and transparency.