**[Name]: A Container-based Reproducible Untargeted Metabolomics Data Processing Pipeline**

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Keywords: febrile neutropenia; machine learning; mortality; cancer; HCUP

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Abstract word count: 238

Abstract word limit: 250

Target Journal: GigaScience

Reference limit: not mention in the guideline

Reference count:

Total word limit: not mention in the guideline

Current word count:

**ABSTRACT**

***Background:***Untargeted metabolomics data processing remains a challenge due to the large size of metabolomics data files as well as the extensive steps and computational power required to process the data. The goal of our study is to build a containerized workflow that can enhance computational reproducibility of untargeted metabolomics data processing.

***Findings****:* Nextflow, a pipeline development tool supporting containerization, parallelization and high performance computing, was used to build the pipeline. Several tools and codes were connected and incorporated into the pipeline. [Name] can be executed on any UNIX-like system and job schedulers for high-performance computing are supported.

***Conclusions****:* A highly-reproducible containerized untargeted metabolomics data processing tool was developed to facilitate collaborative research.

**1.1 Background**

**1.2 Findings**

1.2.1 The [Name] workflow

(A figure describing the workflow)

1.2.2 Implementation

1.2.3 [Name] Input/Output

(A screenshot of log file)

(A screenshot of execution profile)

1.2.4 Results

1.2.4.1 Simulation study

Reproducibility test among different operating systems

1.2.4.2 Real-world case study

1.2.5 Discussion

**1.3 Methods**

1.3.1 Data availability

1.3.1.1 Simulation study

1.3.1.2 Real-world case study

1.3.2 Data analysis

1.3.2.1 Simulation study

1.3.2.2 Real-world study

**1.7 Availability of source code**

**1.8 Availability of supporting data**

**1.9 Abbreviations**

**1.10 Competing interests**

The authors have no financial or personal relationships with other people or organizations that could inappropriately influence (bias) their work.

**1.11 Funding**

This work was supported by the National Institute of Diabetes and Digestive and Kidney Diseases [K01DK115632] and the University of Florida Clinical and Translational Science Institute [UL1TR001427]. The content is solely the responsibility of the authors and does not necessarily represent the official views the University of Florida’s Clinical and Translational Science Institute, or the National Institutes of Health.

**1.7 Author contributions**

**1.8 Acknowledgements**

**1.8 References**

**FIGURES**

Screenshot of log file

Relationship between input size and memory cost

Relationship between input number of samples and memory cost

**TABLES**

**SUPPLEMENTARY MATERIAL**