

Nutrimetabolomics: Biomarker Discover, Data Quality Control, Bioinformatics Tools and Computing Hardware

Tu Hu*

Sep, 2019

*Supervised by Lars Ove Dragsted and Gözde Gürdeniz

Contents

Preface	4
Introduction	5
0.1 Biomarker Discovery	5
1 A Mini-review on Biomarkers of Whole Grain Barley and Whole Grain Wheat Intake	6
2 Discovering Barley Intake Biomarkers in Urine by UPLC-MS Based Untargeted Metabolomics	7
3 Barley Intake Biomarker: Compound Identification and Structure Elucidation	8
4 Discovering Novel Intake Biomarkers of Whole Grain Wheat Intake by LC-MS Based Untargeted Metabolomics	9
5 Data Quality Control (QC) and Quality Assurance (QA) in LC-MS Based Untargeted Metabolomics	10
5.1 Introduction	12
6 Several R Functions Facilitating LC-MS Based Metabolomics Data Analysis Workflow	13
6.1 abstract	13
6.2 "Tidy" High-throughout Analysis Data, Exemplified by RNA sequencing data	13
6.3 m2r	13
6.4 plot_excretion	13
6.5 plot_intervention	13
7 Implementing A Streamlined Metabolomics Data Analysis Workflow (EZMS) Based on R Programming Language	14
8 Using a Budgeted Device to Compute High-throughout Metabolomics Data	15
8.1 Abstract	15
8.2 Introduction	15
Closing Remarks	16

Acronyms

GC-MS Gas Chromatography-Mass Spectrometry. 4

LC-MS Liquid Chromatography-Mass Spectrometry. 4

Preface

Introduction

0.1 Biomarker Discovery

Definition of Biomarker

Biomarker Classification

Biomarker Systematic review

Credibility of BFIs: Putative biomarker, Candidate biomarker, partially validated biomarker and fully-validated biomarker

Biomarker Validation

1 A Mini-review on Biomarkers of Whole Grain Barley and Whole Grain Wheat Intake

2 Discovering Barley Intake Biomarkers in Urine by UPLC-MS Based Untargeted Metabolomics

3 Barley Intake Biomarker: Compound Identification and Structure Elucidation

4 Discovering Novel Intake Biomarkers of Whole Grain Wheat Intake by LC-MS Based Untargeted Metabolomics

5 Data Quality Control (QC) and Quality Assurance (QA) in LC-MS Based Untargeted Metabolomics

This is an abstract

Keywords:

5.1 Introduction

6 Several R Functions Facilitating LC-MS Based Metabolomics Data Analysis Workflow

6.1 abstract

I would like to test whether it's possible to input an abstract here.,

6.2 "Tidy" High-throughout Analysis Data, Exemplified by RNA sequencing data

6.3 m2r

6.4 plot_excretion

6.5 plot_intervention

7 Implementing A Streamlined Metabolomics Data Analysis Workflow (EZMS) Based on R Programming Language

8 Using a Budgeted Device to Compute High-throughout Metabolomics Data

8.1 Abstract

High-throughout metabolomics data is characterized as high computing and storage resource demanding.

How to compute the data locally (without sending it to a high-performance server) with a budgeted device could be an interesting topic to explore. Because this would provide possibilities to protect privacies in home-appliance or fulfil the real-time analysis tasks in some extreme conditions (such as in polar region or some areas with poor Internet connectivity)

why do i do this? because in the future, metabolomics analysis could become smart-home appliance, such as smart toilet or smart mirror. people can get their metabolome examined daily in their home. such a good vision raised several problems. data privacy problem and cost. because metabolome is considered as personal privacy. therefore, leak these privacy could result in bad results. however, if computed locally, whether it's possible to control the cost.

In this study, we simulated a computing task.

Not only limited to human metabolome for risk analysis. it could also be applied in the fridge for example, to detect microorganisms' characteristic metabolome.

in less developed countries, or in portable devices, transmitting the data could be very expensive (via satellite for example, in polar areas), therefore, computing such a dataset whether it's possible.

8.2 Introduction

Potential Use environment

hello

Closing Remarks