LC-MS based Metabolomics:
Biomarker Discover,
Data Quality Control,
Bioinformatics Tools
Computing Performance and Hardware,
Tutorial

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

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

Chapter 3

Barley Intake Biomarker: Compound Identification and Structure Elucidation

3.1 Abstract

3.2 Introduction

Phytosterol and Fragmentation Behaviour

Phytosterols ubiquitously occur in plant-based food[1]. They were claimed to have health beneficial effects, such as lowering cholesterol. They occur in food as free sterols (FS), steryl esters (SE), and glycosylated conjugates comprised of steryl glucosides (SG) and acylated steryl glucosides (ASG).

Specific sterol profiles characteristic to certain plant families have been identified showing that a broad range ofminor sterols occurs as free sterols or glycosylated conjugates

This ion could be stanol (a sub-type of phytosterol with a saturated B-ring) derivative inferred from its C-ring fragmentation behaviour:

- higher intensities of m/z 149 than both 147 and 145
- higher intensities of m/z 161 than both 159 and 163

3.3 Materials and methods

Chemicals

Sitostanol standard (CAS Number 83-45-4, Avanti Polar Lipids Inc., USA) was transported and stored in -20 °C. Ethanol

Apparatus

UPLC-MS system (column C18, QTOF (VION, Waters, Milford, USA)

UPLC-MS/MS analysis of Sitostanol

3.4 Retention Time (RT) and m/z in Different Matrix

Matrix	RT	m/z (ESI+)	Annotation
Whole Grain Barley	6.88	291.2683	Unknown
Urine	6.71	291.2683	Unknown
Standard	8.60	399.3989	[Sitostanol-H2O+H]-

Chapter 4

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

Chapter 5

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

Abstract

This is an abstract

Keywords:

5.1 Introduction

Chapter 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, Examplified by RNA sequencing data

6.3 m2r

6.4 plot_excretion

6.5 plot_intervention

Chapter 7

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

Chapter 8

Using a Budgeted Device to Compute High-throughout Metabolomics Data

"MetaboPi"

8.1 Abstract

Handling high-throughout metabolomics data demands high computing and storage resource.

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 satalliate for example, in polar areas), therefore, computing such a dataset whether it's possible.

8.2 Introduction

Potential Use environment

hello

8.3 Solution

8.4 Business Model