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

Tu Hu[*]

Sep, 2019

[*]Supervised by Lars Ove Dragsted and Gözde Gürdeniz

Contents

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

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

8 Computing Metabolomics Data on a 219 kr Device

Closing Remarks