



Master Thesis

Tu Hu

Investigation of Whole Grain Wheat Intake Biomarkers

Supervisor: Gözde Gürdenz

Jun, 2019

Contents

1	Preface	4
2	Introduction	4
3	Materials and methods	4
3.1	Software	4
3.2	Data-preprocessing	4
3.3	Data conversion from MATLAB to R	4

Acronyms

GC-MS Gas Chromatography-Mass Spectrometry. 4

LC-MS Liquid Chromatography-Mass Spectrometry. 4

1 Preface

2 Introduction

3 Materials and methods

3.1 Software

Several software packages were used for different purposes.

MATLAB R2018a (9.4.0.813654) coupled with PLS toolbox was used for data processing, modeling.

MZmine 2.31, an open source data processing software for LC-MS and GC-MS.

MassLynx was used to check mass spectra.

DataBridge, an LC-MS data file conversion program built-in MassLynx developed by Waters.

3.2 Data-preprocessing

Data-preprocessing consists x steps.

First, data format was converted by DataBridge from '.raw' to '.cdf'. '.raw' was the format directly generated by Waters analytical platform. In order to be readable by MZmine, data was converted¹.

Then, the data was preprocessed by MZmine (2.31) following the steps: peak detection, deisotoping, alignment and gap filling.

Positive mode and negative were separately processed because of different noise level and in-source reaction. Blank samples were also excluded in pre-processing.

In the end, the detected features, including information of mass to charge ratio (m/z), retention time (rt) and intensities were output as '.csv' files for further investigation.

3.3 Data conversion from MATLAB to R

'm2r.R'² can convert a matlab dataset into R tidy form.

¹N.B. Although in MZmine manual, '.raw' file is described as a compatible format, in practice some weird errors were generated when '.raw' format was input into MZmine.

²codes were repositied on GitHub: <https://github.com/tuhulab/bfi-wholegrain/blob/master/r/m2r.R>