Chromatoplots Manual

Tengfei Yin

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1 Introduction

Metabolomics experiments often rely on Gas Chromatography - Mass Spectrometry (GC-MS) instruments for measuring the levels of metabolites. We have developed numerical methods and graphical diagnostics for converting raw GC-MS data into a dataset specifying the amount of each metabolite in each sample. In this manual, we present basic workflow and diagnosic windows.

This manual doesn't include the GUI yet, will be added later. And this manual doesn't focus on the algrithm, algrithm will be elucidated in another document later.

Now it's just for developer's communication, will be fullfilled while developing this package.

2 Installation

Please use the latest version of the following package, you can check out "commandr" and "chromatoplots" from their svn, and "xcms" ,"irange", from Bioconductor[1] dev 2.6 pool.

chromatoplots svn://had.co.nz/statgraphics/chromatoplots/trunk/chromatoplots

commandr svn://had.co.nz/statgraphics/commandr/trunk/commandr

xcms http://www.bioconductor.org/packages/2.6/bioc/html/xcms.html

IRanges http://www.bioconductor.org/packages/2.6/bioc/html/IRanges.html

Check the system and package dependencies before you install chromatoplots, install xcms first, then commandr, install chromatoplots last.

3 Workflow

3.1 Arrange Your File

First of all, you need to arrange all your raw data based on your experimental design.

In this study, my experimental design looks like this.

So I arranged my file in the following way.

[1] http://www.bioconductor.org

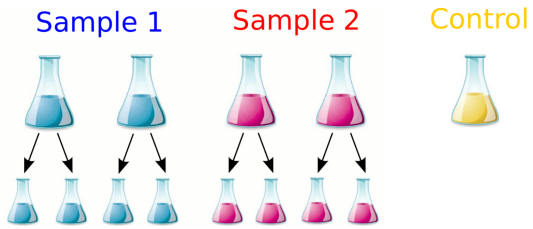

Figure 1: My calibrated data has two treatment, each treatment has four replicates.

```
./raw/s1:
M0101A.CDF  M0101B.CDF  M0102A.CDF  M0102B.CDF

./raw/s2:
M0201A.CDF  M0201B.CDF  M0202A.CDF  M0202B.CDF
```

3.2 Raw Data Input

Command Line

Specify a CDF data which contains GC-MS processed raw data by using the following command, and generate *profile matrix*[1].

[1]Profile matrix has a row for each mass and a column for each scan, in order of time.