

Imaging Mass Spectrometry using MALDIquant

Sebastian Gibb*

May 20, 2014

Abstract

This vignette describes how to load Imaging Mass Spectrometry Data and plot them using using MALDIquant

Contents

1	Foreword	2
2	Dataset	2
3	Plotting	2
3.1	Setup	2
3.2	Import Raw Data	3
3.3	Plot Image	3
3.4	IMS Shiny Example	4
4	Session Information	4

*mail@sebastiangibb.de

1 Foreword

MALDIquant is free and open source software for the R (R Core Team, 2014) environment and under active development. If you use it, please support the project by citing it in publications:

Gibb, S. and Strimmer, K. (2012). MALDIquant: a versatile R package for the analysis of mass spectrometry data. *Bioinformatics*, 28(17):2270–2271

If you have any questions, bugs, or suggestions do not hesitate to contact me (mail@sebastiangibb.de). Please visit <http://strimmerlab.org/software/malDIquant/>.

2 Dataset

In this vignette we use the *imzML* example dataset of an urinary bladder from http://www.maldi-msi.org/index.php?option=com_content&view=article&id=186&Itemid=68.

3 Plotting

3.1 Setup

First we need to install the necessary packages (you can skip this part if you have already done this). You can install MALDIquant (Gibb and Strimmer, 2012), MALDIquantForeign (Gibb, 2014) directly from CRAN. To install this example package from <http://github.com/sgibb/MALDIquantExamples> you need the devtools (Wickham and Chang, 2014) package.

```
install.packages(c("MALDIquant", "MALDIquantForeign", "devtools"))
library("devtools")
install_github("sgibb/MALDIquantExamples")
```

Next we load the packages.

```
library("MALDIquant")
library("MALDIquantForeign")

library("MALDIquantExamples")
```

3.2 Import Raw Data

We use the `importImzMl` function provided by `MALDIquantForeign` to import the *imzML* file from http://www.maldi-msi.org/download/imzml/s043_processed.zip.

```
spectra <- import("http://www.maldi-msi.org/download/imzml/s043_processed.zip",
                  verbose=FALSE)
```

3.3 Plot Image

We use the same mass range as in *Example 2* on http://www.maldi-msi.org/index.php?option=com_content&view=article&id=186&Itemid=68

```
plotImzSlice(spectra, range=c(156.95, 157.45), main="urinary bladder")
```

urinary bladder (m/z: 156.95–157.45)



3.4 IMS Shiny Example

Please have a look at <https://github.com/sgibb/ims-shiny/>.

4 Session Information

- R version 3.1.0 (2014-04-10), x86_64-pc-linux-gnu
- Base packages: base, datasets, grDevices, graphics, methods, stats, utils
- Other packages: MALDIquant~1.10.1, MALDIquantExamples~0.1, MALDIquantForeign~0.7, corpcor~1.6.6, crossval~1.0.1, entropy~1.2.0, fdrtool~1.2.12, knitr~1.5, sda~1.3.3, xtable~1.7-3
- Loaded via a namespace (and not attached): XML~3.98-1.1, base64enc~0.1-1, digest~0.6.4, downloader~0.3, evaluate~0.5.5, formatR~0.10, highr~0.3, readBrukerFlexData~1.7, readMzXmlData~2.7, stringr~0.6.2, tools~3.1.0

References

- Gibb, S. (2014). *MALDIquantForeign: Import/Export routines for MALDIquant*. R package version 0.6.2.
- Gibb, S. and Strimmer, K. (2012). MALDIquant: a versatile R package for the analysis of mass spectrometry data. *Bioinformatics*, 28(17):2270–2271.
- R Core Team (2014). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria.
- Wickham, H. and Chang, W. (2014). *devtools: Tools to make developing R code easier*. R package version 1.5.