

MALDIquantForeign: Import/Export routines for MALDIquant

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September 6, 2017

Abstract

`MALDIquantForeign` provides routines for importing/exporting different file formats into/from `MALDIquant`.

This vignette describes the usage of the `MALDIquantForeign` package.

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Foreword

MALDIquantForeign 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/>.

1 Introduction

MALDIquant should be device and platform independent. That's why it has not any import/export functions. MALDIquantForeign fills this gap and provides import/export routines for various file formats:

```
> supportedFileFormats()
```

```

$import
[1] "txt"      "tab"      "csv"      "fid"      "ciphergen"
[6] "mzxml"    "mzml"     "imzml"    "analyze"  "cdf"
[11] "msd"

$export
[1] "tab"  "csv"  "msd"  "mzml"  "imzml"

```

2 Setup

After starting R we could install MALDIquant and MALDIquantForeign directly from CRAN using `install.packages`:

```
> install.packages(c("MALDIquant", "MALDIquantForeign"))
```

Before we can use MALDIquant and MALDIquantForeign we have to load the packages.

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

3 Import

MALDIquantForeign provides an `import` function that tries to auto-detect the correct file type. Because this would never be perfect MALDIquantForeign offers also many `import*` functions like `importBrukerFlex`, `importMzML`, etc. Please see the manual page of `import` for a complete list (`?import`).

First we try to import some example data in Bruker Daltonics *flex-series file format using the `import` function.

```

> ## get the example directory
> exampleDirectory <- system.file("exampledata",
+                                package="MALDIquantForeign")

```

```

>
> spectra <- import(file.path(exampleDirectory,
+                             "brukerflex"),
+                             verbose=FALSE)
> spectra[[1]]

S4 class type          : MassSpectrum
Number of m/z values   : 5
Range of m/z values    : 226.762 - 230.51
Range of intensity values: 1e+00 - 5e+00
Memory usage           : 7.789 KiB
Name                   : brukerflex.
File                   : /tmp/RtmprAXU3a/Rinst524977b93cfd/MALDIquantForeign/exa

```

Next we use the `importBrukerFlex` function (the result is the same as above).

```

> spectra <- importBrukerFlex(file.path(exampleDirectory,
+                                       "brukerflex"),
+                                       verbose=FALSE)
> spectra[[1]]

S4 class type          : MassSpectrum
Number of m/z values   : 5
Range of m/z values    : 226.762 - 230.51
Range of intensity values: 1e+00 - 5e+00
Memory usage           : 7.789 KiB
Name                   : brukerflex.
File                   : /tmp/RtmprAXU3a/Rinst524977b93cfd/MALDIquantForeign/exa

```

MALDIquantForeign supports compressed files, too (*zip*, *tar*.{*bz2*, *gz*,*xz*}).

```

> spectra <- importCsv(file.path(exampleDirectory, "compressed",
+                                "csv.tar.gz"), verbose=FALSE)
> spectra[[1]]

S4 class type          : MassSpectrum

```

```

Number of m/z values      : 5
Range of m/z values      : 1 - 5
Range of intensity values: 6 - 10
Memory usage             : 1.406 KiB
File                     : /tmp/RtmpnxGRHh/MALDIquantForeign_uncompress/csv_525c52

> spectra <- importCsv(file.path(exampleDirectory, "compressed",
+                          "csv.zip"), verbose=FALSE)
> spectra[[1]]

S4 class type             : MassSpectrum
Number of m/z values      : 5
Range of m/z values      : 1 - 5
Range of intensity values: 6 - 10
Memory usage             : 1.406 KiB
File                     : /tmp/RtmpnxGRHh/MALDIquantForeign_uncompress/csv_525c57

```

Remote files are supported as well. Data are taken from Tan et al. (2006).

```

> spectra <- import(paste0("http://www.meb.ki.se/",
+                          "~yudpaw/papers/spikein_xml.zip"),
+                  centroided=FALSE, verbose=TRUE)

```

If you want to read peak lists (centroided data) instead of spectra data you have to set `centroided=TRUE`.

```

> peaks <- import(file.path(exampleDirectory, "ascii.txt"),
+                  centroided=TRUE, verbose=FALSE)
> peaks

[[1]]
S4 class type             : MassPeaks
Number of m/z values      : 5
Range of m/z values      : 1 - 5
Range of intensity values: 6 - 10
Range of snr values       : NA - NA
Memory usage             : 1.602 KiB
File                     : /tmp/RtmpprAXU3a/Rinst524977b93cfd/MALDIquantForeign/exa

```

4 Export

The export routines in `MALDIquantForeign` are very similar to the import routines. Please see manual page of `export` for a complete list of supported export routines (`?export`).

First we create a simple list of `MassSpectrum` objects using `createMassSpectrum`.

```
> spectra <- list(  
+   createMassSpectrum(mass=1:5, intensity=1:5),  
+   createMassSpectrum(mass=1:5, intensity=6:10))
```

Now we want to export the first spectrum into a CSV file.

```
> export(spectra[[1]], file="spectrum1.csv")  
> import("spectrum1.csv")  
  
[[1]]  
S4 class type           : MassSpectrum  
Number of m/z values    : 5  
Range of m/z values     : 1 - 5  
Range of intensity values: 1 - 5  
Memory usage           : 1.406 KiB  
File                   : /tmp/RtmprAXU3a/Rbuild524977c1885c/MALDIquantForeign/vi
```

Exporting every file by hand is cumbersome. We want to export the whole list of spectra. Instead of `file` we use `path` now to specify a directory. Please note that we have to add the file type/format information now (we can use the `type` argument or the corresponding `export*` function). If the path doesn't exist we will get an error. To force `export` to create/overwrite the given path, we set the argument `force=TRUE`.

```
> export(spectra, type="csv", path="spectra", force=TRUE)  
> list.files("spectra")  
  
[1] "1.csv" "2.csv"
```

5 Analyse Mass Spectrometry Data

Please have a look at the corresponding vignette shipped with MALDIquant and the MALDIquant website: <http://strimmerlab.org/software/malDIquant/>.

```
> vignette(topic="MALDIquant", package="MALDIquant")
```

6 Session Information

- R version 3.3.3 (2017-03-06), x86_64-pc-linux-gnu
- Base packages: base, datasets, grDevices, graphics, methods, stats, utils
- Other packages: MALDIquant 1.16.4, MALDIquantForeign 0.11, knitr 1.17
- Loaded via a namespace (and not attached): XML 3.98-1.9, base64enc 0.1-3, digest 0.6.12, evaluate 0.10.1, highr 0.6, magrittr 1.5, parallel 3.3.3, readBrukerFlexData 1.8.5, readMzXmlData 2.8.1, stringi 1.1.5, stringr 1.2.0, tools 3.3.3

References

- 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.
- Tan, C. S., Ploner, A., Quandt, A., Lehtiö, J., and Pawitan, Y. (2006). Finding regions of significance in SELDI measurements for identifying protein biomarkers. *Bioinformatics*, 22(12):1515–1523.