

MALDIquantForeign: Import/Export routines for MALDIquant

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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" "mzxml"
[7] "mzml"     "imzml"    "analyze"  "cdf"      "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           : 8.859 KiB
Name                   : brukerflex.
File                   : /tmp/Rtmp1oHRqa/Rinst9507e138643/MALDIquantForeign/exam

```

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           : 8.859 KiB
Name                   : brukerflex.
File                   : /tmp/Rtmp1oHRqa/Rinst9507e138643/MALDIquantForeign/exam

```

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            : 1.492 KiB
File                    : /tmp/RtmpvYI4Uq/MALDIquantForeign_uncompress/csv_a06604

> 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            : 1.492 KiB
File                    : /tmp/RtmpvYI4Uq/MALDIquantForeign_uncompress/csv_a0627k

```

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            : 1.695 KiB
File                    : /tmp/Rtmp1oHRqa/Rinst9507e138643/MALDIquantForeign/exam

```

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           : 1.492 KiB  
File                   : /tmp/Rtmp1oHRqa/Rbuild9504c8bb7ba/MALDIquantForeign/vig
```

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 4.4.1 (2024-06-14), x86_64-pc-linux-gnu
- Running under: Ubuntu 24.04.1 LTS
- Matrix products: default
- BLAS:
/usr/lib/x86_64-linux-gnu/openblas-pthread/libblas.so.3
- LAPACK:
/usr/lib/x86_64-linux-gnu/openblas-pthread/libopenblas-p0.3.26.so
; LAPACK version3.12.0
- Base packages: base, datasets, grDevices, graphics, methods, stats, utils
- Other packages: MALDIquant 1.22.3, MALDIquantForeign 0.14.1, knitr 1.48
- Loaded via a namespace (and not attached): XML 3.99-0.17, base64enc 0.1-3, buildtools 1.0.0, compiler 4.4.1, digest 0.6.37, evaluate 1.0.0, highr 0.11, maketools 1.3.0, parallel 4.4.1, readBrukerFlexData 1.9.2, readMzXmlData 2.8.3, sys 3.4.2, tools 4.4.1, xfun 0.47

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.