Package 'MALDIquantForeign'

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Title Import/Export Routines for 'MALDIquant'

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Imports base64enc, digest, readBrukerFlexData (>= 1.7), readMzXmlData (>= 2.7), XML

Suggests knitr, testthat (>= 0.8), RNetCDF (>= 1.6.1)

Description Functions for reading (tab, csv, Bruker fid, Ciphergen XML, mzXML, mzML, imzML, Analyze 7.5, CDF, mMass MSD) and writing (tab, csv, mMass MSD, mzML, imzML) different file formats of mass spectrometry data into/from 'MALDIquant' objects.

License GPL (>= 3)

URL https://strimmerlab.github.io/software/maldiquant/

https://github.com/sgibb/MALDIquantForeign/

BugReports https://github.com/sgibb/MALDIquantForeign/issues/

LazyLoad yes

VignetteBuilder knitr

RoxygenNote 7.1.2

NeedsCompilation no

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Repository CRAN

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R topics documented:

`MALDIquantForeign-package`

Import/Export routines for 'MALDIquant'

Description

This package reads and writes different file formats of mass spectrometry data into/from 'MALDIquant' objects.

Details

Package:	MALDIquantForeign
License:	GPL (>= 3)
URL:	https://strimmerlab.github.io/software/maldiquant/

Author(s)

Sebastian Gibb <mail@sebastiangibb.de>

References

https://strimmerlab.github.io/software/maldiquant/

export,AbstractMassObject-method
Export files

Description

This function provides a general interface to export AbstractMassObject-class objects (e.g. MassSpectrum-class, MassPeaks-class) into different file formats.

Usage

```
## S4 method for signature 'AbstractMassObject'
export(x, file, type="auto", force=FALSE, ...)

## S4 method for signature 'list'
export(x, path, type, force=FALSE, ...)
```

Arguments

x	a AbstractMassObject-class object or a list of AbstractMassObject-class objects.
file	character, file name.
type	character, file format. If type is set to "auto" the file extension is used.
force	logical, If TRUE the file would be overwritten or path would be created.
path	character, path to directory in which the list of AbstractMassObject-class would be exported.
...	arguments to be passed to specific export functions.

Details

Specific export functions:

tab	exportTab
csv	exportCsv
imzML	exportImzMl
msd	exportMsd
mzML	exportMzMl

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/

See Also

MassPeaks-class, MassSpectrum-class

Examples

```
## Not run:
library("MALDIquant")
library("MALDIquantForeign")

s <- list(createMassSpectrum(mass=1:5, intensity=1:5),
          createMassSpectrum(mass=1:5, intensity=1:5))

## export a single spectrum
export(s[[1]], file="spectrum.csv")
## identical to exportCsv(s[[1]], file="spectrum.csv")

## export a list of spectra
export(s, path="spectra", type="csv")
## identical to exportCsv(s, path="spectra")

## End(Not run)
```

---

exportImzMl,MassSpectrum-method

Export to imzML files

Description

This function exports MassSpectrum-class objects into imzML files.

Usage

```
## S4 method for signature 'MassSpectrum'
exportImzMl(x, file, force=FALSE, processed=TRUE,
coordinates=NULL, pixelSize=c(100, 100), ...)

## S4 method for signature 'list'
exportImzMl(x, path, force=FALSE, processed=TRUE,
coordinates=NULL, pixelSize=c(100, 100), ...)
```

Arguments

x	a AbstractMassObject-class object or a list of AbstractMassObject-class objects.
file	character, file name.
force	logical, If TRUE the file would be overwritten or path would be created.

processed	logical, If TRUE (default) the spectra will be saved in processed mode (means mass and intensity is stored for each spectra separately in contrast to continuous mode where the mass is stored only for one spectrum).
coordinates	matrix, 2 column matrix that contains the x- and y-coordinates for the spectra.
pixelSize	numeric, a vector of length 2 that contains the x and y pixel size in micrometers (default: c(100,100)).
path	character, path to directory in which the list of MassSpectrum-class would be exported. If path is a single filename all spectra will be exported to a single imzML file.
...	arguments to be passed to internal functions.

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/

Schramm T, Hester A, Klinkert I, Both J-P, Heeren RMA, Brunelle A, Laprevote O, Desbenoit N, Robbe M-F, Stoeckli M, Spengler B, Roempp A (2012)
imzML - A common data format for the flexible exchange and processing of mass spectrometry imaging data.
Journal of Proteomics 75 (16):5106-5110.
doi: 10.1016/j.jprot.2012.07.026

See Also

MassSpectrum-class

Examples

```
## Not run:
library("MALDIquant")
library("MALDIquantForeign")

s <- list(createMassSpectrum(mass=1:5, intensity=1:5),
          createMassSpectrum(mass=1:5, intensity=1:5))

## export a list of spectra
exportImzMl(s, path="processed.imzML", coordinates=cbind(x=1:2, y=c(1, 1)))

## End(Not run)
```

exportMsd,MassSpectrum-method
Export to MSD files

Description

This function exports AbstractMassObject-class objects (e.g. MassSpectrum-class, MassPeaks-class) into mMass MSD files.

Usage

```
## S4 method for signature 'MassSpectrum'
exportMsd(x, file, force=FALSE, peaks, ...)

## S4 method for signature 'list'
exportMsd(x, path, force=FALSE, peaks, ...)
```

Arguments

x	a MassSpectrum-class object or a list of MassSpectrum-class objects.
file	character, file name.
force	logical, If TRUE the file would be overwritten or path would be created.
peaks	a MassPeaks-class object or a list of MassPeaks-class objects.
path	character, path to directory in which the list of AbstractMassObject-class would be exported.
...	arguments to be passed to write.table.

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/,
mMass homepage: http://mmass.org/

See Also

MassPeaks-class, MassSpectrum-class

Examples

```
## Not run:
library("MALDIquant")
library("MALDIquantForeign")

s <- list(createMassSpectrum(mass=1:5, intensity=1:5),
          createMassSpectrum(mass=1:5, intensity=1:5))
p <- list(createMassPeaks(mass=4:5, intensity=4:5, snr=1:2),
          createMassPeaks(mass=4:5, intensity=4:5, snr=1:2))

## export a single spectrum
exportMsd(s[[1]], file="spectrum.msd")

## export a single spectrum with corresponding peaks
exportMsd(s[[1]], file="spectrum.msd", peaks=p[[1]])

## export a list of spectra with corresponding peaks
exportMsd(s, path="spectra", peaks=p, force=TRUE)

## End(Not run)
```

---

exportMzMl,MassSpectrum-method

Export to mzML files

Description

This function exports MassSpectrum-class objects into mzML files.

Usage

```
## S4 method for signature 'MassSpectrum'
exportMzMl(x, file, force=FALSE, ...)

## S4 method for signature 'list'
exportMzMl(x, path, force=FALSE, ...)
```

Arguments

x	a AbstractMassObject-class object or a list of AbstractMassObject-class objects.
file	character, file name.
force	logical, If TRUE the file would be overwritten or path would be created.
path	character, path to directory in which the list of MassSpectrum-class would be exported. If path is a single filename all spectra will be exported to a single mzML file.
...	arguments to be passed to internal functions.

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/,
HUPO Proteomics Standards Inititative mzML 1.1.0 Specification: https://www.psidev.info/mzML

See Also

MassSpectrum-class

Examples

```
## Not run:
library("MALDIquant")
library("MALDIquantForeign")

s <- list(createMassSpectrum(mass=1:5, intensity=1:5),
          createMassSpectrum(mass=1:5, intensity=1:5))

## export a single spectrum
exportMzMl(s[[1]], file="spectrum.mzML")

## export a list of spectra
exportMzMl(s, path="spectra.mzML")

## End(Not run)
```

---

exportTab,AbstractMassObject-method

Export to text files

Description

This function exports AbstractMassObject-class objects (e.g. MassSpectrum-class, MassPeaks-class) into different text file formats.

Usage

```
## S4 method for signature 'AbstractMassObject'
exportTab(x, file, force=FALSE, ...)

## S4 method for signature 'list'
exportTab(x, path, force=FALSE, ...)
```

```
## S4 method for signature 'AbstractMassObject'
exportCsv(x, file, force=FALSE, ...)

## S4 method for signature 'list'
exportCsv(x, path, force=FALSE, ...)
```

Arguments

x	a AbstractMassObject-class object or a list of AbstractMassObject-class objects.
file	character, file name.
force	logical, If TRUE the file would be overwritten or path would be created.
path	character, path to directory in which the list of AbstractMassObject-class would be exported.
...	arguments to be passed to write.table.

Details

exportTab and exportCsv use write.table with different defaults (sep="\t" in exportTab and sep="," in exportCsv).

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/

See Also

MassPeaks-class, MassSpectrum-class, write.table

Examples

```
## Not run:
library("MALDIquant")
library("MALDIquantForeign")

s <- list(createMassSpectrum(mass=1:5, intensity=1:5),
          createMassSpectrum(mass=1:5, intensity=1:5))

## export a single spectrum
exportTab(s[[1]], file="spectrum.tab")

## export a list of spectra and use ; as separator
exportCsv(s, path="spectra", sep=";", force=TRUE)
```

```
## End(Not run)
```

`import` *Import files*

Description

This function provides a general interface to import different file formats into `MassSpectrum-class` or `MassPeaks-class` objects.

Usage

```
import(
  path,
  type = "auto",
  pattern,
  excludePattern = NULL,
  removeEmptySpectra = TRUE,
  centroided = FALSE,
  massRange = c(0, Inf),
  minIntensity = 0,
  mc.cores = 1L,
  verbose = interactive(),
  ...
)
```

Arguments

`path`	`character`, path to directory or file which should be read in.
`type`	`character`, file format. If `type` is set to "auto" MALDIquant tries to detect the correct file type automatically. It often depends on the file extension (if `path` is a directory the most represented file extension is used; `pattern` argument is ignored).
`pattern`	`character`, a regular expression to find files in a directory (see details).
`excludePattern`	`character`, a regular expression to exclude files in a directory (see details).
`removeEmptySpectra`	`logical`, should empty spectra excluded?
`centroided`	`logical`, if `centroided=FALSE` (default) the data are treated as not centroided and a list of `MassSpectrum-class` objects is returned. Use `centroided=TRUE` to assume centroided data and get a list of `MassPeaks-class` objects.
`massRange`	`double`, limits of mass import (left/minimal mass, right/maximal mass).
`minIntensity`	`double`, minimal intensity to import.
`mc.cores`	number of cores to use (default 1; only unix-based platforms are supported, see `MALDIquantForeign-parallel` for details).
`verbose`	`logical`, verbose output?
`...`	arguments to be passed to specific import functions.

Details

Specific import functions:

txt	importTxt
tab	importTab
csv	importCsv
fid	importBrukerFlex
ciphergen	importCiphergenXml
mzXML	importMzXml
mzML	importMzMl
imzML	importImzMl
analyze	importAnalyze
cdf	importCdf
msd	importMsd

`path`: In addition to the above mentioned file types the following (compressed) archives are supported, too: zip, tar, tar.gz, tar.bz2, tar.xz. The archives are uncompressed in a temporary directory. Afterwards the `import` function is called (with `type="auto"`).

`pattern`: Sometimes unusual file extensions are used (e.g. `"*.xml"` for mzXML files). In this case a specific `pattern` could be defined to import files with an unusual file extension (e.g. `pattern="^.*\.xml$"` to read all `*.xml` files in a directory; see `regexp` for details).

`excludePattern`: Sometimes some files should be excluded. E.g. to ignore additional aquired Bruker LIFT spectra (MALDI-TOF/TOF; which are not support, yet) you could use `excludePattern="([[:digit:]\.]+)L`

Value

a `list` of `MassSpectrum-class` or `MassPeaks-class` objects (depending on the `centroided` argument).

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/

See Also

`MassSpectrum-class`, `MassPeaks-class` `MALDIquantForeign-parallel`

Examples

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

## get example directory
```

```
exampleDirectory <- system.file("exampledata", package="MALDIquantForeign")

## import mzXML files
s <- import(exampleDirectory, type="mzXML")

## import tab delimited file with different file extension (default: *.tab)
s <- import(exampleDirectory, type="tab", pattern="^.*\\.txt")

## import single mzML file
s <- import(file.path(exampleDirectory, "tiny1.mzML1.1.mzML"))

## import gzipped csv file
s <- import(file.path(exampleDirectory, "compressed", "csv1.csv.gz"))
```

`importAnalyze` *Import Analyze 7.5 files*

Description

This function imports files in Analyze 7.5 file format into `MassSpectrum-class` or `MassPeaks-class` objects.

Usage

```
importAnalyze(path, ...)
```

Arguments

`path`	`character`, path to directory or file which should be read in.
`...`	arguments to be passed to `import`.

Value

a `list` of `MassSpectrum-class` or `MassPeaks-class` objects (depending on the `centroided` argument).

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/
http://www.grahamwideman.com/gw/brain/analyze/formatdoc.htm, http://eeg.sourceforge.net/ANALYZE75.pdf

See Also

`MassSpectrum-class`, `MassPeaks-class`

importBrukerFlex *Import Bruker Daltonics *flex files*

Description

This function imports files in Bruker Daltonics *flex-series file format into MassSpectrum-class or MassPeaks-class objects.

Usage

```
importBrukerFlex(path, ...)
```

Arguments

path	character, path to directory or file which should be read in.
...	arguments to be passed to readBrukerFlexFile.

Value

a list of MassSpectrum-class or MassPeaks-class objects (depending on the centroided argument).

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/

See Also

MassSpectrum-class, MassPeaks-class, readBrukerFlexFile

Examples

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

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

s <- importBrukerFlex(exampleDirectory)
```

importCdf *Import CDF files*

Description

This function imports files in NetCDF file format into MassSpectrum-class or MassPeaks-class objects.
Please note that the *RNetCDF* is needed.

Usage

```
importCdf(path, ...)
```

Arguments

path	character, path to directory or file which should be read in.
...	arguments to be passed to import.

Value

a list of MassSpectrum-class or MassPeaks-class objects (depending on the centroided argument).

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/

See Also

MassSpectrum-class, MassPeaks-class

Examples

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

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

## import
if (requireNamespace("RNetCDF", quietly=TRUE)) {
  s <- importCdf(exampleDirectory)
} else {
  message("You have to install the RNetCDF package to use importCdf.")
```

```
}
```

`importCiphergenXml` *Import Ciphergen XML files*

Description

This function imports files in Ciphergen XML file format into `MassSpectrum-class` or `MassPeaks-class` objects.

Usage

```
importCiphergenXml(path, ...)
```

Arguments

`path`	`character`, path to directory or file which should be read in.
`...`	arguments to be passed to `import`.

Value

a `list` of `MassSpectrum-class` or `MassPeaks-class` objects (depending on the `centroided` argument).

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/

See Also

`MassSpectrum-class`, `MassPeaks-class`

Examples

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

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

## import
s <- importCiphergenXml(exampleDirectory)
```

importImzMl *Import imzML files*

Description

This function imports files in imzML file format into MassSpectrum-class or MassPeaks-class objects.

Usage

```
importImzMl(path, coordinates = NULL, ...)
```

Arguments

path	character, path to directory or file which should be read in.
coordinates	matrix, 2 column matrix that contains the x- and y-coordinates for spectra that should be imported. Other spectra would be ignored.
...	arguments to be passed to import.

Value

a list of MassSpectrum-class or MassPeaks-class objects (depending on the centroided argument).

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/,
Definition of imzML format: https://ms-imaging.org/imzml/

See Also

MassSpectrum-class, MassPeaks-class

Examples

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

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

## import
s <- importImzMl(file.path(exampleDirectory, "tiny_continuous.imzML"))
```

```
## import only spectra for pixel 1,1 and 2,1
s <- importImzMl(file.path(exampleDirectory, "tiny_continuous.imzML"),
                 coordinates = cbind(1:2, c(1, 1)))
```

`importMsd` *Import MSD files*

Description

This function imports files in mMass MSD file format into `MassSpectrum-class` or `MassPeaks-class` objects.

Usage

```
importMsd(path, ...)
```

Arguments

`path`	`character`, path to directory or file which should be read in.
`...`	arguments to be passed to `import`.

Value

a `list` of `MassSpectrum-class` or `MassPeaks-class` objects (depending on the `centroided` argument).

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/,
mMass homepage: http://mmass.org/

See Also

`MassSpectrum-class`, `MassPeaks-class`

Examples

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

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

## import
s <- importMsd(exampleDirectory)
```

`importMzMl` *Import mzML files*

Description

This function imports files in mzML file format into `MassSpectrum-class` or `MassPeaks-class` objects.

Usage

```
importMzMl(path, ...)
```

Arguments

`path`	`character`, path to directory or file which should be read in.
`...`	arguments to be passed to `import`.

Value

a `list` of `MassSpectrum-class` or `MassPeaks-class` objects (depending on the `centroided` argument).

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/,
Definition of `mzML` format: https://www.psidev.info/mzML

See Also

`MassSpectrum-class`, `MassPeaks-class`

Examples

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

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

## import
s <- importMzMl(exampleDirectory)
```

`importMzXml` *Import mzXML files*

Description

This function imports files in mzXML file format into `MassSpectrum-class` or `MassPeaks-class` objects.

Usage

```
importMzXml(path, ...)
```

Arguments

`path`	`character`, path to directory or file which should be read in.
`...`	arguments to be passed to `readMzXmlFile`.

Value

a `list` of `MassSpectrum-class` or `MassPeaks-class` objects (depending on the `centroided` argument).

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/,
Definition of `mzXML` format: http://tools.proteomecenter.org/wiki/index.php?title=Formats:mzXML

See Also

`MassSpectrum-class`, `MassPeaks-class`, `readMzXmlFile`

Examples

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

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

## import
s <- importMzXml(exampleDirectory)
```

`importTxt` *Import text files*

Description

This function imports different text file formats into `MassSpectrum-class` or `MassPeaks-class` objects.

Usage

```
importTxt(path, ...)

importTab(path, ...)

importCsv(path, ...)
```

Arguments

`path`	`character`, path to directory or file which should be read in.
`...`	arguments to be passed to `read.table`.

Details

`importTab`, `importTxt` and `importCsv` use `read.table` with different defaults.

Value

a `list` of `MassSpectrum-class` or `MassPeaks-class` objects (depending on the `centroided` argument).

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/

See Also

MassSpectrum-class, MassPeaks-class, read.table

Examples

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

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

## import txt files
s <- importTxt(exampleDirectory)

## import csv files
s <- importCsv(exampleDirectory)
```

MALDIquantForeign-parallel

Parallel Support in Package **MALDIquantForeign**

Description

MALDIquantForeign-package offers multi-core support using mclapply and mcmapply. This approach is limited to unix-based platforms.

Details

Please note that not all import functions benfit from parallelisation. The current implementation is limited to run the parallelisation over different files. That's why only imports of multiple files could be run on multiple cores. E.g. a single mzML file containing 4 spectra would always be read on a single core. In contrast 4 mzML files each containing just one spectra could be read in using 4 cores.

The improvement in the runtime depends on the amount of data to read, the proportion of parsing/decoding of the data, the amount of memory and the speed of the hard disk.

Please note: It is possible that using parallelisation results in a worse runtime!

Author(s)

Sebastian Gibb <mail@sebastiangibb.de>

References

https://strimmerlab.github.io/software/maldiquant/

See Also

MALDIquant-parallel, mclapply, mcmapply

Examples

```
## load packages
library("MALDIquant")
library("MALDIquantForeign")

exampleDirectory <- system.file("exampledata", package="MALDIquantForeign")

## run single-core import
print(system.time(
  s1 <- importMzMl(exampleDirectory, centroided=TRUE, verbose=FALSE)
))

if(.Platform$OS.type == "unix") {
  ## run multi-core import
  ## (because the example spectra are very small (just 5 data points) the
  ## multi-core solution is slower on most systems)
  print(system.time(
    s2 <- importMzMl(exampleDirectory, centroided=TRUE, mc.cores=2,
                     verbose=FALSE)
  ))
  stopifnot(all.equal(s1, s2))
}
```

---

supportedFileFormats *Supported file formats*

Description

This function prints all file formats supported by MALDIquantForeign-package.

Usage

```
supportedFileFormats()
```

Details

Import:

txt	importTxt
tab	importTab
csv	importCsv
fid	importBrukerFlex
ciphergen	importCiphergenXml
mzXML	importMzXml
mzML	importMzMl

imzML	importImzMl
analyze	importAnalyze
cdf	importCdf
msd	importMsd

Export:

tab	exportTab
csv	exportCsv
imzML	exportImzMl
msd	exportMsd
mzML	exportMzMl

Value

a `list` with two named elements (`import` and `export`) containing a `character` vector of supported file types.

Author(s)

Sebastian Gibb

References

https://strimmerlab.github.io/software/maldiquant/

See Also

export, import

Examples

```
library("MALDIquantForeign")

supportedFileFormats()
```

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