

# Package ‘MALDIquantForeign’

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**Title** Import/Export routines for MALDIquant

**Depends** R (>= 3.0.0), methods, MALDIquant (>= 1.8)

**Imports**

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

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

**Description** This package reads (tab, csv, Bruker fid, CIPHERgen XML,mzXML, mzML, imzML, Analyze 7.5, CDF) and writes (tab, csv,msd, mzML) different file formats of mass spectrometry data into/from MALDIquant objects.

**License** GPL (>= 3)

**URL** <http://strimmerlab.org/software/maldiquant/>  
<https://github.com/sgibb/MALDIquantForeign/>

**BugReports** <https://github.com/sgibb/MALDIquantForeign/issues/>

**LazyLoad** yes

**VignetteBuilder** knitr

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**NeedsCompilation** no

**Repository** CRAN

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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: <http://strimmerlab.org/software/malDIquant/>

## Author(s)

Sebastian Gibb <[mail@sebastiangibb.de](mailto:mail@sebastiangibb.de)>

## References

<http://strimmerlab.org/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 <a href="#">AbstractMassObject-class</a> object or a list of <a href="#">AbstractMassObject-class</a> objects.
file	character, file name.
path	character, path to directory in which the list of <a href="#">AbstractMassObject-class</a> would be exported.
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.
...	arguments to be passed to specific export functions.

## Details

Specific export functions:

tab	<a href="#">exportTab</a>
csv	<a href="#">exportCsv</a>
msd	<a href="#">exportMsd</a>
mzML	<a href="#">exportMzML</a>

## Author(s)

Sebastian Gibb

## References

<http://strimmerlab.org/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)
```

---

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

**Author(s)**

Sebastian Gibb

**References**

<http://strimmerlab.org/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 [AbstractMassObject-class](#) objects (e.g. [MassSpectrum-class](#), [MassPeaks-class](#)) 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 <a href="#">MassSpectrum-class</a> object or a list of <a href="#">MassSpectrum-class</a> objects.
file	character, file name.
path	character, path to directory in which the list of <a href="#">AbstractMassObject-class</a> would be exported.
force	logical, If TRUE the file would be overwritten or path would be created.
...	arguments to be passed to <a href="#">write.table</a> .

**Author(s)**

Sebastian Gibb

**References**

<http://strimmerlab.org/software/maldiquant/>,  
HUPO Proteomics Standards Initiative mzML 1.1.0 Specification: [http://www.psdev.info/mzml\\_1\\_0\\_0](http://www.psdev.info/mzml_1_0_0)

**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
exportMzML(s[[1]], file="spectrum.mzML")

## export a list of spectra with corresponding peaks
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 <a href="#">AbstractMassObject-class</a> object or a list of <a href="#">AbstractMassObject-class</a> objects.
file	character, file name.
path	character, path to directory in which the list of <a href="#">AbstractMassObject-class</a> would be exported.
force	logical, If TRUE the file would be overwritten or path would be created.
...	arguments to be passed to <a href="#">write.table</a> .

## Details

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

## Author(s)

Sebastian Gibb

## References

<http://strimmerlab.org/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, verbose = TRUE, ...)
```

## 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 <a href="#">MassSpectrum-class</a> objects is returned. Use centroided=TRUE to assume centroided data and get a list of <a href="#">MassPeaks-class</a> objects.
massRange	double, limits of mass import (left/minimal mass, right/maximal mass).
minIntensity	double, minimal intensity to import.
verbose	logical, verbose output?
...	arguments to be passed to specific import functions.



## Details

Specific import functions:

txt	<a href="#">importTxt</a>
tab	<a href="#">importTab</a>
csv	<a href="#">importCsv</a>
fid	<a href="#">importBrukerFlex</a>
ciphergen	<a href="#">importCiphergenXml</a>
mzXML	<a href="#">importMzXml</a>
mzML	<a href="#">importMzMl</a>
imzML	<a href="#">importImzMl</a>
analyze	<a href="#">importAnalyze</a>
cdf	<a href="#">importCdf</a>

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 acquired Bruker LIFT spectra (MALDI-TOF/TOF; which are not supported, yet) you could use excludePattern="([[:digit:]]\\.[ ]+)

## Value

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

## Author(s)

Sebastian Gibb

## References

<http://strimmerlab.org/software/maldiquant/>

## See Also

[MassSpectrum-class](#), [MassPeaks-class](#)

## 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 <a href="#">import</a> .

## Value

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

## Author(s)

Sebastian Gibb

## References

<http://strimmerlab.org/software/maldiquant/>  
<http://www.grahamwideman.com/gw/brain/analyze/formatdoc.htm>, <http://eeg.sourceforge.net/ANALYZE75.pdf>

## See Also

[MassSpectrum-class](#), [MassPeaks-class](#)

---

importBrukerFlex	<i>Import Bruker Daltonics *flex files</i>
------------------	--

---

### 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 <a href="#">readBrukerFlexFile</a> .

### Value

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

### Author(s)

Sebastian Gibb

### References

<http://strimmerlab.org/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	<i>Import CDF files</i>
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---

### 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 <code>import</code> .

### Value

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

### Author(s)

Sebastian Gibb

### References

<http://strimmerlab.org/software/maldiquant/>

### See Also

`MassSpectrum-class`, `MassPeaks-class`

### Examples

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

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

## import
if (require("RNetCDF")) {
  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

<http://strimmerlab.org/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	<i>Import imzML files</i>
-------------	---------------------------

---

### Description

This function imports files in imzML file format into [MassSpectrum-class](#) or [MassPeaks-class](#) objects.

### Usage

```
importImzML(path, ...)
```

### Arguments

path	character, path to directory or file which should be read in.
...	arguments to be passed to <a href="#">import</a> .

### Value

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

### Author(s)

Sebastian Gibb

### References

<http://strimmerlab.org/software/malDIquant/>,  
Definition of imzML format: <http://www.imzml.org/>

### See Also

[MassSpectrum-class](#), [MassPeaks-class](#)

### Examples

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

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

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

---

importMzML	<i>Import mzML files</i>
------------	--------------------------

---

### 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 <a href="#">import</a> .

### Value

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

### Author(s)

Sebastian Gibb

### References

<http://strimmerlab.org/software/malDIquant/>,  
Definition of mzML format: [http://www.psidev.info/mzml\\_1\\_0\\_0%20](http://www.psidev.info/mzml_1_0_0%20)

### 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**

<code>path</code>	character, path to directory or file which should be read in.
<code>...</code>	arguments to be passed to <code>readMzXmlFile</code> .

**Value**

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

**Author(s)**

Sebastian Gibb

**References**

<http://strimmerlab.org/software/malDIquant/>,  
Definition of mzXML format: <http://tools.proteomecenter.org/mzXMLschema.php>

**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	<i>Import text files</i>
-----------	--------------------------

---

## 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 <a href="#">read.table</a> .

## 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

<http://strimmerlab.org/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)
```

---

supportedFileFormats *Supported file formats*

---

## Description

This function prints all file formats supported by [MALDIquantForeign-package](#).

## Usage

```
supportedFileFormats()
```

## Details

### Import:

txt	<a href="#">importTxt</a>
tab	<a href="#">importTab</a>
csv	<a href="#">importCsv</a>
fid	<a href="#">importBrukerFlex</a>
ciphergen	<a href="#">importCiphergenXml</a>
mzXML	<a href="#">importMzXml</a>
mzML	<a href="#">importMzML</a>
imzML	<a href="#">importImzML</a>
analyze	<a href="#">importAnalyze</a>
cdf	<a href="#">importCdf</a>

### Export:

tab	<a href="#">exportTab</a>
csv	<a href="#">exportCsv</a>
msd	<a href="#">exportMsd</a>
mzML	<a href="#">exportMzML</a>

**Value**

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

**Author(s)**

Sebastian Gibb

**References**

<http://strimmerlab.org/software/maldiquant/>

**See Also**

[export](#), [import](#)

**Examples**

```
library("MALDIquantForeign")  
  
supportedFileFormats()
```

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