Package 'readMzXmlData'

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Title Reads Mass Spectrometry Data in mzXML Format

Depends R (>= 4.2.0)

Imports base64enc, digest, XML

Description Functions for reading mass spectrometry data in mzXML format.

License GPL (>= 3)

URL https://strimmerlab.github.io/software/maldiquant/
https://github.com/sgibb/readMzXmlData/

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

LazyLoad yes

RoxygenNote 7.2.3

NeedsCompilation no

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Contents

readMzXmlData-package *The readMzXmlData Package*

Description

The package reads mass spectrometry data in mzXML format.

Details

Main functions:

`readMzXmlFile`: Reads mass spectrometry data in mzXML format.

`readMzXmlDir`: Reads recursively mass spectrometry data in mzXML format in a specific directory.

`mqReadMzXml`: Reads mass spectrometry data into MALDIquant.

Author(s)

Sebastian Gibb <mail@sebastiangibb.de>

References

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

See Also

`readMzXmlDir`, `readMzXmlFile`

readMzXmlDir *Reads recursively mass spectrometry data in mzXML format.*

Description

Reads recursively all mass spectrometry data in mzXML format in a specified directory.

Usage

```
readMzXmlDir(
  mzXmlDir,
  removeCalibrationScans = TRUE,
  removeMetaData = FALSE,
  rewriteNames = TRUE,
  fileExtension = "mzXML",
  verbose = FALSE
)
```

Arguments

mzXmlDir	character, path to *directory* which should be read recursively.
removeCalibrationScans	logical, if TRUE all scans in directories called "[Cc]alibration" will be ignored.
removeMetaData	logical, to save memory metadata could be deleted.
rewriteNames	logical, if TRUE all list elements get an unique name from metadata otherwise file path is used.
fileExtension	character, file extension of mzXML formatted files. The directory is only searched for *fileExtension* files. In most cases it would be ""mzXML"" but sometimes you have to use "xml".
verbose	logical, verbose output?

Details

See readMzXmlFile.

Value

A list of spectra.

- [[1]]spectrum$mass: A vector of calculated mass.
- [[1]]spectrum$intensity: A vector of intensity values.
- [[1]]metaData: A list of metaData depending on read spectrum.

Author(s)

Sebastian Gibb <mail@sebastiangibb.de>

See Also

readMzXmlFile, importMzXml

Examples

```
## load library
library("readMzXmlData")

## get examples directory
exampleDirectory <- system.file("Examples", package="readMzXmlData")

## read example spectra
spec <- readMzXmlDir(exampleDirectory)

## plot spectra
plot(spec[[1]]$spectrum$mass, spec[[1]]$spectrum$intensity, type="n")

l <- length(spec)
legendStr <- character(l)
for (i in seq(along=spec)) {
```

```
  lines(spec[[i]]$spectrum$mass, spec[[i]]$spectrum$intensity, type="l",
        col=rainbow(l)[i])
  legendStr[i] <- basename(spec[[i]]$metaData$file)
}

## draw legend
legend(x="topright", legend=legendStr, col=rainbow(l), lwd=1)
```

`readMzXmlFile` *Reads mass spectrometry data in mzXML format.*

Description

Reads mass spectrometry data in mzXML format defined in http://tools.proteomecenter.org/wiki/index.php?title=Formats:mzXML

Usage

```
readMzXmlFile(mzXmlFile, removeMetaData = FALSE, verbose = FALSE)
```

Arguments

`mzXmlFile`	`character`, path to *mzXML* file which should be read.
`removeMetaData`	`logical`, to save memory metadata could be deleted.
`verbose`	`logical`, verbose output?

Value

A list of spectra and metadata.

- `spectrum$mass`: A vector of calculated mass.
- `spectrum$intensity`: A vector of intensity values.
- `metaData`: A list of metaData depending on read spectrum.

Author(s)

Sebastian Gibb <mail@sebastiangibb.de>

References

Definition of `mzXML` format: http://tools.proteomecenter.org/wiki/index.php?title=Formats:mzXML

See Also

`readMzXmlDir`, `importMzXml`

Examples

```
## load library
library("readMzXmlData")

## get examples directory
exampleDirectory <- system.file("Examples", package="readMzXmlData")

## read example spectrum
spec <- readMzXmlFile(file.path(exampleDirectory, "A1-0_A1.mzXML"))

## print metaData
print(spec$metaData)

## plot spectrum
plot(spec$spectrum$mass, spec$spectrum$intensity, type="l")
```

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