

Package ‘readBrukerFlexData’

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Title Reads Mass Spectrometry Data in Bruker *flex Format

Depends R (>= 3.3.0)

Suggests testthat

Description Reads data files acquired by Bruker Daltonics' matrix-assisted laser desorption/ionization-time-of-flight mass spectrometer of the *flex series.

License GPL (>= 3)

URL <https://strimmerlab.github.io/software/maldiquant/>
<https://github.com/sgibb/readBrukerFlexData/>

BugReports <https://github.com/sgibb/readBrukerFlexData/issues/>

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readBrukerFlexData-package

The readBrukerFlexData Package

Description

The readBrukerFlexData package reads data files acquired by MALDI-TOF MS on Bruker Daltonics machines of the *flex series. (autoflex, microflex, ultraflex).

The package was developed *without* any knowledge nor even support by Bruker Daltonics.

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References

<https://github.com/sgibb/readBrukerFlexData>

cpSpecHpcMzXml

Mass spectrum generated by Bruker Daltonics CompassXport

Description

This dataset was generated by Bruker Daltonics CompassXport and imported by [readMzXmlFile](#) to R. It is only needed for comparison between Bruker Daltonics' HPC and [.hpc](#).

Format

A list containing a mass and an intensity vector.

Source

Examples/hpc/mzXML/hpc.mzXML

See Also

[.hpc](#), [readMzXmlFile](#)

readBrukerFlexDir	<i>Reads recursively mass spectrometry data in Bruker Daltonics XMASS format.</i>
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Description

This function leads recursively all mass spectrometry data in Bruker Daltonics XMASS format in a specified directory.

Usage

```
readBrukerFlexDir(  
  BrukerFlexDir,  
  removeCalibrationScans = TRUE,  
  removeMetaData = FALSE,  
  useHpc = TRUE,  
  useSpectraNames = TRUE,  
  filterZeroIntensities = FALSE,  
  verbose = FALSE  
)
```

Arguments

BrukerFlexDir	character, path to <i>directory</i> which should be read recursively.
removeCalibrationScans	logical, if TRUE all scans in directories called [Cc]alibration will be ignored.
removeMetaData	logical, to calculate mass data a lot of meta data are needed. To save memory they could be deleted after calculation.
useHpc	logical, should Bruker Daltonics' High Precision Calibration be used if available? (see also: .hpc)
useSpectraNames	logical, if TRUE all list elements get an unique name from metaData otherwise file path is used. (If 'removeMetaData' is TRUE 'useSpectraNames' has no effect.)
filterZeroIntensities	logical, don't change it. If TRUE all intensities equal 0.0 are removed. (see also: readBrukerFlexFile)
verbose	logical, print verbose messages?

Details

See [readBrukerFlexFile](#).

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.

See Also

[importBrukerFlex](#), [readBrukerFlexFile](#), [.hpc](#)

Examples

```
## load library
library("readBrukerFlexData")

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

## read example spectra
spec <- readBrukerFlexDir(file.path(exampleDirectory,
  "2010_05_19_Gibb_C8_A1"))

## 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] <- spec[[i]]$metaData$fullName
}

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

`readBrukerFlexFile` *Reads mass spectrometry data in Bruker Daltonics XMASS format.*

Description

This function reads mass spectrometry data in Bruker Daltonics XMASS format used by Bruker Daltonics mass spectrometer of *flex series (autoflex, microflex, ultraflex).

Usage

```
readBrukerFlexFile(
  fidFile,
  removeMetaData = FALSE,
  useHpc = TRUE,
  filterZeroIntensities = FALSE,
  keepNegativeIntensities = FALSE,
  verbose = FALSE
)
```

Arguments

`fidFile` character, path to *fid* file which should be read.

`removeMetaData`, logical, to calculate mass data a lot of meta data are needed. To save memory they could be deleted after calculation.

`useHpc` logical, should Bruker Daltonics' High Precision Calibration be used if available? (see also: [.hpc](#))

`filterZeroIntensities` logical, don't change it. If TRUE all intensities equal 0.0 are removed. (see also: 'Details' section)

`keepNegativeIntensities` logical, don't change it. If FALSE all intensities less than zero are replaced by zero. (see also: 'Details' section)

`verbose` logical, print verbose messages?

Details

`readBrukerFlexFile` has to import the following data to calculating mass from *acqu* file:

acqu-value	becomes metaData	description
\$BYTORDA	metaData\$byteOrder	endianness of fid file
\$TD	metaData\$number	total number of measured time periods
\$DELAY	metaData\$timeDelay	first measured intensity after <i>metaData\$timeDelay</i> ns
\$DW	metaData\$timeDelta	ns between measured time periods
\$ML1	metaData\$calibrationConstants[1]	mass calibration constant
\$ML2	metaData\$calibrationConstants[2]	mass calibration constant
\$ML3	metaData\$calibrationConstants[3]	mass calibration constant

If High Precision Calibration (HPC) is used, `readBrukerFlexFile` needs:

acqu-value	becomes metaData	description
\$HPCIBHi	metaData\$hpc\$limits["maxMass"]	upper mass threshold
\$HPCIBLo	metaData\$hpc\$limits["minMass"]	lower mass threshold
\$HPCIOrd	metaData\$hpc\$order	polynomial order

\$HPCUse	metaData\$hpc\$use	maybe using of HPC? (seems to be always “yes” in our test data)
\$HPCStr	metaData\$hpc\$coefficients	polynomial coefficients in a string

readBrukerFlexFile tries also to import [optional]:

value	becomes metaData	description
acqu-value	metaData\$data	e.g. CONTINUOUS MASS
DATATYPE	metaData\$dataType	e.g. Bruker Flex Series
SPECTROMETER/DATASYSTEM	metaData\$dataSystem	e.g. TOF
.SPECTROMETER TYPE	metaData\$spectrometerType	DIRECT
.INLET	metaData\$inlet	e.g. LD+
.IONIZATION MODE	metaData\$ionizationMode	same as \$AQ_DATE but of
\$DATE	metaData\$date	path to method file
\$ACQMETH	metaData\$acquisitionMethod	acquisition date
\$AQ_DATE	metaData\$acquisitionDate	acquisition mode
\$AQ_mod	metaData\$acquisitionMode	LINEAR / REFLECTOR
\$AQOP_m	metaData\$acquisitionOperatorMode, metaData\$tofMode	laser beam attenuation
\$ATTEN	metaData\$laserAttenuation	comments
\$CMT[1:4]	metaData\$comments	deflection ON/OFF
\$DEFLON	metaData\$deflection	type of digitizer
\$DIGTYP	metaData\$digitizerType	deflection pulser cal 1
\$DPCAL1	metaData\$deflectionPulserCal1	deflection pulser mass
\$DPMASS	metaData\$deflectionPulserMass	Version of Bruker Daltonic
\$FCVer	metaData\$flexControlVersion	spectrum id
\$ID_raw	metaData\$id	e.g. AUTOFLEX
\$INSTRUM	metaData\$instrument	ID of mass spectrometer
\$InstrID	metaData\$instrumentId	instrument type
\$InstTyp	metaData\$instrumentType	LIFT constant?
\$Lift1	metaData\$lift[1]	LIFT constant?
\$Lift2	metaData\$lift[2]	initial mass error in ppm
\$Masserr	metaData\$massError	number of applied laser shots
\$NoSHOTS	metaData\$laserShots	sample position on target
\$PATCHNO	metaData\$patch	original file path (on Bruker)
\$PATH	metaData\$path	laser repetition rate in Hz
\$REPHZ	metaData\$laserRepetition	same as \$PATCHNO (in old)
\$SPOTNO	metaData\$spot	e.g. TOF
\$SPTyp	metaData\$spectrumType	target ids
\$TgIDS	metaData\$target\$id	number of measurements v
\$TgCount	metaData\$target\$count	target serial number
\$TgSer	metaData\$target\$serialNumber	target type number
\$TgTyp	metaData\$target\$typeNumber	LIFT constant?
\$TLift	metaData\$tlift	

import from file path:

value	becomes metaData	description
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full current path to fid file	metaData\$file	path on local machine
sample name	metaData\$sampleName	-

`filterZeroIntensities`: Change default value is **not recommended!** If TRUE all intensities equal zero are removed. This parameter exists only to be compatible to Bruker Daltonics CompassXport's `mzXML` export function. For details see: 'Release Notes for CompassXport 3.0.3', cap. 6 'Filtering of Zero Intensities': "Bruker Daltonics' Acquisition Software will compress Analysis raw data. To save on operation time and to keep export file sizes small, CompassXport 3.0.3 will filter out zero (0.0) intensities when exporting to `mzXML` or `mzData` ..."

`keepNegativeIntensities`: Change default value is **not recommended!** If TRUE negative intensity values are not replaced by zero. This parameter exists only to be compatible to Bruker Daltonics CompassXport.

Value

A list of spectra and metadata.

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

See Also

<https://github.com/sgibb/readBrukerFlexData/wiki>, `importBrukerFlex`, `readBrukerFlexDir`, `.hpc`

Examples

```
## load library
library("readBrukerFlexData")

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

## read example spectrum
spec <- readBrukerFlexFile(file.path(exampleDirectory,
  "2010_05_19_Gibb_C8_A1/0_A1/1/1SLin/fid"))

## print metaData
print(spec$metaData)

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

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