Package 'mzR'

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Type Package

Title parser for netCDF, mzXML and mzML and mzIdentML files (mass spectrometry data)

Version 2.42.0

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Description mzR provides a unified API to the common file formats and parsers available for mass spectrometry data. It comes with a subset of the proteowizard library for mzXML, mzML and mzIdentML. The netCDF reading code has previously been used in XCMS.

License Artistic-2.0

LazyLoad yes

Depends R (>= 4.0.0), Rcpp (>= 0.10.1), methods, utils

Imports Biobase, BiocGenerics (>= 0.13.6), ProtGenerics (>= 1.17.3), ncdf4

Suggests msdata (>= 0.15.1), RUnit, mzID, BiocStyle (>= 2.5.19), knitr, XML, rmarkdown

VignetteBuilder knitr

LinkingTo Rcpp, Rhdf5lib (>= 1.1.4)

RcppModules Pwiz, Ident

SystemRequirements C++11, GNU make

URL https://github.com/sneumann/mzR/

BugReports https://github.com/sneumann/mzR/issues/

biocViews ImmunoOncology, Infrastructure, DataImport, Proteomics, Metabolomics, MassSpectrometry

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Contents

copyWriteMSData	*Write MS spectrum data to a MS file copying metadata from the originating file*

Description

Copy general information from the originating MS file and write this, along with the provided spectra data, to a new file. The expected workflow is the following: data is first loaded from an MS file, e.g. using [peaks](#) and [header](#) methods, processed in R and then saved again to an MS file providing the (eventually) manipulated spectra and header data with arguments header and data.

Usage

```
copyWriteMSData(object, file, original_file, header, backend =
  "pwiz", outformat = "mzml", rtime_seconds = TRUE, software_processing)
```

Arguments

object	list containing for each spectrum one matrix with columns mz (first column) and intensity (second column). See also [peaks](#) for the method that reads such data from an MS file.
file	character(1) defining the name of the file.
original_file	character(1) with the name of the original file from which the spectrum data was first read.
header	data.frame with the header data for the spectra. Has to be in the format as the data.frame returned by the [header](#) method.
backend	character(1) defining the backend that should be used for writing. Currently only "pwiz" backend is supported.

outformat   `character(1)` the format of the output file. One of `"mzml"` or `"mzxml"`.

rtime_seconds   `logical(1)` whether the retention time is provided in seconds or minutes (defaults to `TRUE`).

software_processing

> `list` of `character` vectors (or single `character` vector). Each `character` vector providing information about the software that was used to process the data with optional additional description of processing steps. The length of each `character` vector has to be >= 3: the first element being the name of the software, the second string its version and the third element the MS CV ID of the software (or `"MS:-1"` if not known). All additional elements are optional and represent the MS CV ID of each processing step performed with the software.

Note

`copyWriteMSData` supports at present copying data from `mzXML` and `mzML` and exporting to `mzML`. Copying and exporting to `mzXML` can fail for some input files.

The intention of this function is to copy data from an existing file and save it along with eventually modified data to a new file. To write new MS data files use the [writeMSData](#) function instead.

Author(s)

Johannes Rainer

See Also

[writeMSData](#) for a function to save MS data to a new mzML or mzXML file.

Examples

```
## Open a MS file and read the spectrum and header information
library(msdata)
fl <- system.file("threonine", "threonine_i2_e35_pH_tree.mzXML",
    package = "msdata")
ms_fl <- openMSfile(fl, backend = "pwiz")

## Get the spectra
pks <- spectra(ms_fl)
## Get the header
hdr <- header(ms_fl)

## Modify the spectrum data adding 100 to each intensity.
pks <- lapply(pks, function(z) {
    z[, 2] <- z[, 2] + 100
    z
})

## Copy metadata and additional information from the originating file
## and save it, along with the modified data, to a new mzML file.
out_file <- tempfile()
copyWriteMSData(pks, file = out_file, original_file = fl,
    header = hdr)
```

`isolationWindow-methods`

Returns the ion selection isolation window

Description

The methods return matrices of lower (column `low`) and upper (column `high`) isolation window
offsets. Matrices are returned as a list of length equal to the number of input files (provided as file
names of raw mass spectrometry data objects, see below). By default (i.e when `unique. = TRUE`),
only unique offsets are returned, as they are expected to identical for all spectra per acquisition. If
this is not the case, a message is displayed.

Methods

`signature(object = "character", unique. = "logical", simplify = "logical")` Returns the
isolation window for the file `object`. By default, only unique isolation windows are returned
per file (`unique = TRUE`); if set to `FALSE`, a `matrix` with as many rows as there are MS2 spec-
tra. If only one file passed an input and `simplify` is set to `TRUE` (default), the resulting `list`
of length 1 is simplified to a `matrix`.

`signature(object = "mzRpwiz", unique. = "logical", simplify = "logical")` As above for
`mzRpwiz` objects.

Author(s)

Laurent Gatto <lg390@cam.ac.uk> based on the functionality from the `msPurity:::get_isolation_offsets`
function.

Examples

```
library("msdata")
f <- msdata::proteomics(full.names = TRUE,
                        pattern = "TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01.mzML.gz")
isolationWindow(f)

rw <- openMSfile(f)
isolationWindow(rw)
str(isolationWindow(rw, unique = FALSE))
```

`metadata`   *Access the metadata from an* `mzR` *object.*

Description

Accessors to the analytical setup metadata of a run. runInfo will show a summary of the experiment as a named list, including scanCount, lowMZ, highMZ, dStartTime, dEndTime and startTimeStamp. Note that startTimeStamp can only be extracted from *mzML* files using the *pwiz* backend or from *CDF* files. A NA is reported if its value is not available. The instrumentInfo method returns a named list including instrument manufacturer, model, ionisation technique, analyzer and detector. mzRpwiz will give more additional information including information on sample, software using and original source file. These individual pieces of information can also be directly accessed by the specific methods. mzidInfo is used for the mzR object created from a mzid file. It returns basic information on this mzid file including file provider, creation date, software, database, enzymes and spectra data format. The mzidInfo will return the scoring results in identification. It will return different results for different searching software used.

Usage

```
runInfo(object)
chromatogramsInfo(object)
analyzer(object)
detector(object)
instrumentInfo(object)
ionisation(object)
softwareInfo(object)
sampleInfo(object)
sourceInfo(object)
model(object)
mzidInfo(object)
modifications(object, ...)
psms(object, ...)
substitutions(object)
database(object, ...)
enzymes(object)
tolerance(object, ...)
score(x, ...)
para(object)
specParams(object)
```

Arguments

object	An instantiated mzR object.
x	An instantiated mzR object.
...	Additional arguments, currently ignored.

Author(s)

Steffen Neumann, Laurent Gatto and Qiang Kou

See Also

See for example [peaks](#) to access the data for the spectra in a "[mzR](#)" class.

Examples

```
library(msdata)

file <- system.file("microtofq/MM8.mzML", package = "msdata")
mz <- openMSfile(file)
fileName(mz)
instrumentInfo(mz)
runInfo(mz)
close(mz)

file <- system.file("cdf/ko15.CDF", package = "msdata")
mz <- openMSfile(file, backend = "netCDF")
fileName(mz)
instrumentInfo(mz)
runInfo(mz)
close(mz)

file <- system.file("mzid", "Tandem.mzid.gz", package="msdata")
mzid <- openIDfile(file)
softwareInfo(mzid)
enzymes(mzid)
```

---

mzR-class   *Class* mzR *and sub-classes*

Description

The class mzR is the main class for the common mass spectrometry formats. It is a virtual class and thus not supposed to be instanciated directly.

The sub-classes implement specific APIs to access the underlying data and metadata in the files. Currently mzRpwiz is available. mzRpwiz uses Proteowizard to access the relevant information in mzXML and mzML files. mzRident is used as an interface to mzIdentML files.

IMPORTANT: New developers that need to access and manipulate raw mass spectrometry data are advised against using this infrastucture directly. They are invited to use the corresponding MSnExp (with *on disk* mode) from the MSnbase package instead. The latter supports reading multiple files at once and offers access to the spectra data (m/z and intensity) as well as all the spectra metadata using a coherent interface. The MSnbase infrastructure itself used the low level classes in mzR, thus offering fast and efficient access.

Objects from the Class

mzR is a virtual class, so instances cannot be created.

Objects can be created by calls of the form new("mzRpwiz", ...), but more often they will be created with openMSfile.

After creating an mzR object, one can write it into a new file. mzXML, mzML, mgf formats are supported.

Slots

fileName: Object of class character storing the original filename used when the instance was created.

backend: One of the implemented backens or NULL.

.__classVersion__: Object of class "Versioned", from Biobase.

Extends

Class "Versioned", directly.

Methods

For methods to access raw data (spectra and chromatograms), see peaks.

Methods currently implemented for mzR

fileName signature(object = "mzR"): ...

Methods currently implemented for mzRpwiz

analyzer signature(object = "mzRpwiz"): ...

detector signature(object = "mzRpwiz"): ...

instrumentInfo signature(object = "mzRpwiz"): ...

ionisation signature(object = "mzRpwiz"): ...

length signature(x = "mzRpwiz"): ...

manufacturer signature(object = "mzRpwiz"): ...

model signature(object = "mzRpwiz"): ...

runInfo signature(object = "mzRpwiz"): ...

chromatogramsInfo signature(object = "mzRpwiz"): ...

Methods currently implemented for mzRident

mzidInfo signature(object = "mzRident"): ...

psms signature(object = "mzRident"): ...

modifications signature(object = "mzRident"): ...

substitutions signature(object = "mzRident"): ...

database signature(x = "mzRident"): ...

enzymes signature(object = "mzRident"): ...

sourceInfo signature(object = "mzRident"): ...

tolerance signature(object = "mzRident"): ...

score signature(object = "mzRident"): ...

para signature(object = "mzRident"): ...

specParams signature(object = "mzRident"): ...

Author(s)

Steffen Neumann, Laurent Gatto, Qiang Kou

References

Proteowizard: http://proteowizard.sourceforge.net/

Examples

```
library(msdata)
filepath <- system.file("microtofq", package = "msdata")
file <- list.files(filepath, pattern="MM14.mzML",
                    full.names=TRUE, recursive = TRUE)
mzml <- openMSfile(file)
close(mzml)

## using the pwiz backend
mzml <- openMSfile(file, backend = "pwiz")
```

---

openMSfile   *Create and check mzR objects from netCDF, mzXML or mzML files.*

Description

The openMSfile constructor will create a new format-specifc mzR object by loading the 'filename' file. All header information is loaded as a Rcpp module and made accessible through the pwiz slot of the resulting object.

The openIDfile constructor will create a new format-specifc mzR object by loading the 'filename' file. All information is loaded as a Rcpp module. The mzid format is supported throught pwiz backend. Only mzIdentML 1.1 is supported.

Usage

```
openMSfile(filename, backend = NULL, verbose = FALSE)

isInitialized(object)

fileName(object, ...)

openIDfile(filename, verbose = FALSE)
```

Arguments

filename   Path name of the netCDF, mzXML or mzML file to read/write.

backend	A character(1) specifiying which backend API to use. Currently 'netCDF' and 'pwiz' are supported. If backend = NULL (the default), the function tries to determine the backend to be used based on either the file extension of the file content.
object	An instantiated mzR object.
verbose	Enable verbose output.
...	Additional arguments, currently ignored.

Author(s)

Steffen Neumann, Laurent Gatto, Qiang Kou

Examples

```
library(msdata)
filepath <- system.file("microtofq", package = "msdata")
file <- list.files(filepath, pattern="MM14.mzML",
                   full.names=TRUE, recursive = TRUE)
mz <- openMSfile(file)
fileName(mz)
runInfo(mz)
close(mz)

## Not run:
   ## to use another backend
   mz <- openMSfile(file, backend = "pwiz")
   mz

## End(Not run)

file <- system.file("mzid", "Tandem.mzid.gz", package="msdata")
mzid <- openIDfile(file)
softwareInfo(mzid)
enzymes(mzid)
```

---

peaks   *Access the raw data from an* mzR *object.*

Description

Access the MS raw data. The peaks, spectra (can be used interchangeably) and peaksCount functions return the (m/z, intensity) pairs and the number peaks in the spectrum/spectra. peaks and spectra return a single matrix if scans is a numeric of length 1 and a list of matrices if several scans are asked for or no scans argument is provided (i.e all spectra in the oject are retured). peaksCount will return a numeric of length n.

The [header](#) function returns a data.frame containing seqNum, acquisitionNum, msLevel, peaksCount, totIonCurrent, retentionTime (in seconds), basePeakMZ, basePeakIntensity, collisionEnergy, ionisationEnergy, lowM, highMZ, precursorScanNum, precursorMZ, precursorCharge, precursorIntensity,

mergedScan, mergedResultScanNum, mergedResultStartScanNum, mergedResultEndScanNum, filterString, spectrumId, centroided (logical whether the data of the spectrum is in centroid mode or profile mode; only for pwiz backend), injectionTime (ion injection time, in milliseconds), ionMobilityDriftTime (in milliseconds), isolationWindowTargetMZ, isolationWindowLowerOffset, isolationWindowUpperOffset, scanWindowLowerLimit and scanWindowUpperLimit. If multiple scans are queried, a data.frame is returned with the scans reported along the rows. For missing or not defined spectrum variables NA is reported.

The get3Dmap function performs a simple resampling between lowMz and highMz with reMz resolution. A matrix of dimensions length(scans) times seq(lowMz,highMz,resMz) is returned.

The chromatogram (chromatograms) accessors return chromatograms for the MS file handle. If a single index is provided, as data.frame containing the retention time ("rtime", first column) and intensities ("intensity", second column) is returned.

If more than 1 or no chromatogram indices are provided, then a list of chromatograms is returned; either those passed as argument or all of them. By default, the first (and possibly only) chromatogram is the total ion count, which can also be accessed with the tic method.

The nChrom function returns the number of chromatograms, including the total ion chromatogram.

The chromatogramHeader returns (similar to the header function for spectra) a data.frame with metadata information for the individual chromatograms. The data.frame has the columns: "chromatogramId" (the ID of the chromatogram as specified in the file), "chromatogramIndex" (the index of the chromatogram within the file), "polarity" (the polarity for the chromatogram, 0 for negative, +1 for positive and -1 for not set), "precursorIsolationWindowTargetMZ" (the isolation window m/z of the precursor), "precursorIsolationWindowLowerOffset", "precursorIsolationWindowUpperOffset" (lower and upper offset for the isolation window m/z), "precursorCollisionEnergy" (collision energy), "productIsolationWindowTargetMZ", "productIsolationWindowLowerOffset" and "productIsolationWindowUpperOffset" (definition of the m/z isolation window for the product).

Note that access to chromatograms is only supported in the pwiz backend.

Usage

```
 header(object, scans, ...)

 peaksCount(object, scans, ...)

 ## S4 method for signature 'mzRpwiz'
peaks(object, scans)
 ## S4 method for signature 'mzRnetCDF'
peaks(object, scans)

 ## S4 method for signature 'mzRpwiz'
spectra(object, scans)    ## same as peaks
 ## S4 method for signature 'mzRnetCDF'
spectra(object, scans)

 get3Dmap(object, scans, lowMz, highMz, resMz, ...)

 ## S4 method for signature 'mzRpwiz'
```

```
chromatogram(object, chrom, drop = TRUE)

 ## S4 method for signature 'mzRpwiz'
chromatograms(object, chrom, drop = TRUE)  ## same as chromatogram

 ## S4 method for signature 'mzRpwiz'
chromatogramHeader(object, chrom)

 tic(object, ...)

 nChrom(object)
```

Arguments

`object`	An instantiated `mzR` object.
`scans`	A `numeric` specifying which scans to return. Optional for the `header`, `peaks`, `spectra` and `peaksCount` methods. If ommited, the requested data for all peaks is returned.
`lowMz, highMz`	`Numerics` defining the m/z range to be returned.
`resMz`	a `numeric` defining the m/z resolution.
`chrom`	For `chromatogram`, `chromatograms` and `chromatogramHeader`: numeric specifying the index of the chromatograms to be extracted from the file. If omitted, data for all chromatograms is returned.
`drop`	For `chromatogram()`, `chromatograms()`: `logical(1)` whether the result should always be a `list` of `data.frame` (drop = FALSE), even if data from a single chromatogram is requested, or if, in such cases, a `data.frame` should be returned (drop = TRUE, the default).
`...`	Other arguments. A scan parameter can be passed to `peaks`.

Details

The column `acquisitionNum` in the `data.frame` returned by the `header` method contains the index during the scan in which the signal from the spectrum was measured. The `pwiz` backend extracts this number from the spectrum's ID provided in the mzML file. In contrast, column `seqNum` contains the index of each spectrum within the file and is thus consecutively numbered. Spectra from files with multiple MS levels are linked to each other *via* their `acquisitionNum`: column `precursorScanNum` of an e.g. MS level 2 spectrum contains the `acquisitionNum` of the related MS level 1 spectrum.

Note

Spectrum identifiers are only specified in *mzML* files, thus, for all other file types the column `"spectrumId"` of the result `data.frame` returned by `header` contains `"scan="` followed by the acquisition number of the spectrum. Also, only the `pwiz` backend supports extraction of the spectras' IDs from *mzML* files. Thus, only *mzML* files read with `backend = "pwiz"` provide the spectrum IDs defined in the file. The content of the spectrum identifier depends on the vendor and the instrument acquisition settings and is reported here as a character, in its raw form, without further parsing.

Author(s)

Steffen Neumann and Laurent Gatto

See Also

instrumentInfo for metadata access and the "mzR" class.

writeMSData and copyWriteMSData for functions to write MS data in *mzML* or mzXML format.

Examples

```
library(msdata)
filepath <- system.file("microtofq", package = "msdata")
file <- list.files(filepath, pattern="MM14.mzML",
                   full.names=TRUE, recursive = TRUE)
mz <- openMSfile(file)
runInfo(mz)
colnames(header(mz))
close(mz)

## A shotgun LCMSMS experiment
f <- proteomics(full.names = TRUE,
            pattern = "TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01.mzML.gz")
x <- openMSfile(f, backend = "pwiz")
x
nChrom(x)
head(tic(x))
head(chromatogram(x, 1L)) ## same as tic(x)
str(chromatogram(x)) ## as a list

p <- peaks(x) ## extract all peak information
head(peaks(x, scan=4)) ## extract just peaks from the 4th scan

## An MRM experiment
f <- proteomics(full.names = TRUE, pattern = "MRM")
x <- openMSfile(f, backend = "pwiz")
x
nChrom(x)
head(tic(x))
head(chromatogram(x, 1L)) ## same as tic(x)
str(chromatogram(x, 10:12))

## get the header information for the chromatograms
ch <- chromatogramHeader(x)
head(ch)
```

pwiz.version	*Get the version number of pwiz backend.*

Description

Get the version number of pwiz backend.

Usage

```
pwiz.version()
```

---

writeMSData   *Write MS spectrum data to an MS file*

Description

writeMSData exports the MS spectrum data provided with parameters header and data to an MS file in mzML or mzXML format.

Usage

```
## S4 method for signature 'list,character'
writeMSData(object, file, header,
    backend = "pwiz", outformat = "mzml", rtime_seconds = TRUE,
    software_processing)
```

Arguments

object	list containing for each spectrum one matrix with columns mz (first column) and intensity (second column). See also [peaks](#) for the method that reads such data from an MS file.
file	character(1) defining the name of the file.
header	data.frame with the header data for the spectra. Has to be in the format as the data.frame returned by the [header](#) method.
backend	character(1) defining the backend that should be used for writing. Currently only "pwiz" backend is supported.
outformat	character(1) the format of the output file. One of "mzml" or "mzxml".
rtime_seconds	logical(1) whether the retention time is provided in seconds or minutes (defaults to TRUE).
software_processing	
	list of character vectors (or single character vector). Each character vector providing information about the software that was used to process the data with optional additional description of processing steps. The length of each character vector has to be >= 3: the first element being the name of the software, the second string its version and the third element the MS CV ID of the software (or "MS:-1" if not known). All additional elements are optional and represent the MS CV ID of each processing step performed with the software.

Author(s)

Johannes Rainer

See Also

copyWriteMSData for a function to copy general information from a MS data file and writing eventually modified MS data from that originating file.

Examples

```
## Open a MS file and read the spectrum and header information
library(msdata)
fl <- system.file("threonine", "threonine_i2_e35_pH_tree.mzXML",
    package = "msdata")
ms_fl <- openMSfile(fl, backend = "pwiz")

## Get the spectra
pks <- spectra(ms_fl)
## Get the header
hdr <- header(ms_fl)

## Modify the spectrum data adding 100 to each intensity.
pks <- lapply(pks, function(z) {
    z[, 2] <- z[, 2] + 100
    z
})

## Write the data to a mzML file.
out_file <- tempfile()
writeMSData(object = pks, file = out_file, header = hdr)
```

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