Package 'mzR'

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Type Package

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

Version 2.46.0

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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

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SystemRequirements C++11, GNU make

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

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

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`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
fl <- MsDataHub::PestMix1_DDA.mzML()
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 spectra. 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

```
f <- MsDataHub::PestMix1_DDA.mzML()
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

```
file <- MsDataHub::PestMix1_DDA.mzML()
mz <- openMSfile(file)
```

```
fileName(mz)
instrumentInfo(mz)
runInfo(mz)
close(mz)

file <- MsDataHub::ko15.CDF()
mz <- openMSfile(file, backend = "netCDF")
fileName(mz)
instrumentInfo(mz)
runInfo(mz)
close(mz)
```

---

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.

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

```
file <- MsDataHub::PestMix1_DDA.mzML()
mzml <- openMSfile(file)
close(mzml)
```

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

```
file <- MsDataHub::PestMix1_DDA.mzML()
mz <- openMSfile(file)
fileName(mz)
runInfo(mz)
close(mz)

## Not run:
```

```
    ## to use another backend
    mz <- openMSfile(file, backend = "pwiz")
    mz

## End(Not run)
```

---

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

```
file <- MsDataHub::PestMix1_DDA.mzML()
mz <- openMSfile(file)
runInfo(mz)
colnames(header(mz))
close(mz)

## A shotgun LCMSMS experiment
f <- MsDataHub::TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01.20141210.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 <- MsDataHub::MRM.standmix.5.mzML()
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
fl <- MsDataHub::PestMix1_DDA.mzML()
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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