Package 'Spectra'

September 19, 2024

Title Spectra Infrastructure for Mass Spectrometry Data

Version 1.15.8

Description The Spectra package defines an efficient infrastructure for storing and handling mass spectrometry spectra and functionality to subset, process, visualize and compare spectra data. It provides different implementations (backends) to store mass spectrometry data. These comprise backends tuned for fast data access and processing and backends for very large data sets ensuring a small memory footprint.

Depends R (>= 4.0.0), S4Vectors, BiocParallel, ProtGenerics (>= 1.37.1)

Imports methods, IRanges, MsCoreUtils (>= 1.7.5), graphics, grDevices, stats, tools, utils, fs, BiocGenerics, MetaboCoreUtils

Suggests testthat, knitr (>= 1.1.0), msdata (>= 0.19.3), roxygen2, BiocStyle (>= 2.5.19), mzR (>= 2.19.6), rhdf5 (>= 2.32.0), rmarkdown, vdiffr (>= 1.0.0), msentropy, patrick

License Artistic-2.0

LazyData false

VignetteBuilder knitr

BugReports https://github.com/RforMassSpectrometry/Spectra/issues

URL https://github.com/RforMassSpectrometry/Spectra

biocViews Infrastructure, Proteomics, MassSpectrometry, Metabolomics

Encoding UTF-8

RoxygenNote 7.3.2

Roxygen list(markdown=TRUE)

Collate 'hidden_aliases.R' 'AllGenerics.R' 'MsBackend-functions.R'
'MsBackend.R' 'MsBackendCached.R'
'MsBackendDataFrame-functions.R' 'MsBackendDataFrame.R'
'MsBackendHdf5Peaks-functions.R' 'MsBackendHdf5Peaks.R'
'MsBackendMemory-functions.R' 'MsBackendMemory.R'
'MsBackendMzR-functions.R' 'MsBackendMzR.R'
'Spectra-estimatePrecursorMz.R' 'Spectra-functions.R'
'Spectra.R' 'Spectra-neutralLoss.R' 'countIdentifications.R'
'fft_spectrum.R' 'functions-util.R' 'mz-delta-functions.R'
'peak-list-functions.R' 'peaks-functions.R'
'plotting-functions.R' 'zzz.R'

git_url https://git.bioconductor.org/packages/Spectra

git_branch devel

git_last_commit f37fb1d

git_last_commit_date 2024-09-13

Repository Bioconductor 3.20

Date/Publication 2024-09-18

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Contents

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applyProcessing   *The Spectra class to manage and access MS data*

Description

The Spectra class encapsules spectral mass spectrometry data and related metadata.

It supports multiple data backends, e.g. in-memory ([MsBackendMemory](), [MsBackendDataFrame()]()),
on-disk as mzML ([MsBackendMzR()]()) or HDF5 ([MsBackendHdf5Peaks()]()).

Usage

```
applyProcessing(
  object,
  f = processingChunkFactor(object),
  BPPARAM = bpparam(),
  ...
)

concatenateSpectra(x, ...)

combineSpectra(
  x,
  f = x$dataStorage,
  p = x$dataStorage,
  FUN = combinePeaksData,
  ...,
  BPPARAM = bpparam()
)

joinSpectraData(x, y, by.x = "spectrumId", by.y, suffix.y = ".y")

processingLog(x)

deisotopeSpectra(
  x,
  substDefinition = isotopicSubstitutionMatrix("HMDB_NEUTRAL"),
  tolerance = 0,
  ppm = 20,
  charge = 1
)

reduceSpectra(x, tolerance = 0, ppm = 20)

filterPrecursorMaxIntensity(x, tolerance = 0, ppm = 20)

filterPrecursorIsotopes(
  x,
  tolerance = 0,
  ppm = 20,
  substDefinition = isotopicSubstitutionMatrix("HMDB_NEUTRAL")
)

scalePeaks(x, by = sum, msLevel. = uniqueMsLevels(x))

filterPrecursorPeaks(
  object,
  tolerance = 0,
  ppm = 20,
  mz = c("==", ">="),
  msLevel. = uniqueMsLevels(object)
)
```

```
## S4 method for signature 'missing'
Spectra(
  object,
  processingQueue = list(),
  metadata = list(),
  ...,
  backend = MsBackendMemory(),
  BPPARAM = bpparam()
)

## S4 method for signature 'MsBackend'
Spectra(
  object,
  processingQueue = list(),
  metadata = list(),
  ...,
  BPPARAM = bpparam()
)

## S4 method for signature 'character'
Spectra(
  object,
  processingQueue = list(),
  metadata = list(),
  source = MsBackendMzR(),
  backend = source,
  ...,
  BPPARAM = bpparam()
)

## S4 method for signature 'ANY'
Spectra(
  object,
  processingQueue = list(),
  metadata = list(),
  source = MsBackendMemory(),
  backend = source,
  ...,
  BPPARAM = bpparam()
)

## S4 method for signature 'Spectra,MsBackend'
setBackend(
  object,
  backend,
  f = processingChunkFactor(object),
  ...,
  BPPARAM = bpparam()
)

## S4 method for signature 'Spectra'
c(x, ...)
```

```
## S4 method for signature 'Spectra,ANY'
split(x, f, drop = FALSE, ...)

## S4 method for signature 'Spectra'
export(object, backend, ...)

## S4 method for signature 'Spectra'
acquisitionNum(object)

## S4 method for signature 'Spectra'
peaksData(
  object,
  columns = c("mz", "intensity"),
  f = processingChunkFactor(object),
  ...,
  BPPARAM = bpparam()
)

## S4 method for signature 'Spectra'
peaksVariables(object)

## S4 method for signature 'Spectra'
centroided(object)

## S4 replacement method for signature 'Spectra'
centroided(object) <- value

## S4 method for signature 'Spectra'
collisionEnergy(object)

## S4 replacement method for signature 'Spectra'
collisionEnergy(object) <- value

## S4 method for signature 'Spectra'
dataOrigin(object)

## S4 replacement method for signature 'Spectra'
dataOrigin(object) <- value

## S4 method for signature 'Spectra'
dataStorage(object)

## S4 method for signature 'Spectra'
dropNaSpectraVariables(object)

## S4 method for signature 'Spectra'
intensity(object, f = processingChunkFactor(object), ...)

## S4 method for signature 'Spectra'
ionCount(object)
```

```
## S4 method for signature 'Spectra'
isCentroided(object, ...)

## S4 method for signature 'Spectra'
isEmpty(x)

## S4 method for signature 'Spectra'
isolationWindowLowerMz(object)

## S4 replacement method for signature 'Spectra'
isolationWindowLowerMz(object) <- value

## S4 method for signature 'Spectra'
isolationWindowTargetMz(object)

## S4 replacement method for signature 'Spectra'
isolationWindowTargetMz(object) <- value

## S4 method for signature 'Spectra'
isolationWindowUpperMz(object)

## S4 replacement method for signature 'Spectra'
isolationWindowUpperMz(object) <- value

## S4 method for signature 'Spectra'
containsMz(
  object,
  mz = numeric(),
  tolerance = 0,
  ppm = 20,
  which = c("any", "all"),
  BPPARAM = bpparam()
)

## S4 method for signature 'Spectra'
containsNeutralLoss(
  object,
  neutralLoss = 0,
  tolerance = 0,
  ppm = 20,
  BPPARAM = bpparam()
)

## S4 method for signature 'Spectra'
spectrapply(
  object,
  FUN,
  ...,
  chunkSize = integer(),
  f = factor(),
  BPPARAM = SerialParam()
)
```

```
## S4 method for signature 'Spectra'
length(x)

## S4 method for signature 'Spectra'
msLevel(object)

## S4 method for signature 'Spectra'
mz(object, f = processingChunkFactor(object), ...)

## S4 method for signature 'Spectra'
lengths(x, use.names = FALSE)

## S4 method for signature 'Spectra'
polarity(object)

## S4 replacement method for signature 'Spectra'
polarity(object) <- value

## S4 method for signature 'Spectra'
precScanNum(object)

## S4 method for signature 'Spectra'
precursorCharge(object)

## S4 method for signature 'Spectra'
precursorIntensity(object)

## S4 method for signature 'Spectra'
precursorMz(object)

## S4 method for signature 'Spectra'
rtime(object)

## S4 replacement method for signature 'Spectra'
rtime(object) <- value

## S4 method for signature 'Spectra'
scanIndex(object)

## S4 method for signature 'Spectra'
selectSpectraVariables(
  object,
  spectraVariables = union(spectraVariables(object), peaksVariables(object))
)

## S4 method for signature 'Spectra'
smoothed(object)

## S4 replacement method for signature 'Spectra'
smoothed(object) <- value
```

```
## S4 method for signature 'Spectra'
spectraData(object, columns = spectraVariables(object))

## S4 replacement method for signature 'Spectra'
spectraData(object) <- value

## S4 method for signature 'Spectra'
spectraNames(object)

## S4 replacement method for signature 'Spectra'
spectraNames(object) <- value

## S4 method for signature 'Spectra'
spectraVariables(object)

## S4 method for signature 'Spectra'
tic(object, initial = TRUE)

## S4 method for signature 'Spectra'
x$name

## S4 replacement method for signature 'Spectra'
x$name <- value

## S4 method for signature 'Spectra'
x[[i, j, ...]]

## S4 replacement method for signature 'Spectra'
x[[i, j, ...]] <- value

## S4 method for signature 'Spectra'
x[i, j, ..., drop = FALSE]

## S4 method for signature 'Spectra'
filterAcquisitionNum(
  object,
  n = integer(),
  dataStorage = character(),
  dataOrigin = character()
)

## S4 method for signature 'Spectra'
filterEmptySpectra(object)

## S4 method for signature 'Spectra'
filterDataOrigin(object, dataOrigin = character())

## S4 method for signature 'Spectra'
filterDataStorage(object, dataStorage = character())

## S4 method for signature 'Spectra'
filterFourierTransformArtefacts(
```

```
  object,
  halfWindowSize = 0.05,
  threshold = 0.2,
  keepIsotopes = TRUE,
  maxCharge = 5,
  isotopeTolerance = 0.005
)

## S4 method for signature 'Spectra'
filterIntensity(
  object,
  intensity = c(0, Inf),
  msLevel. = uniqueMsLevels(object),
  ...
)

## S4 method for signature 'Spectra'
filterIsolationWindow(object, mz = numeric())

## S4 method for signature 'Spectra'
filterMsLevel(object, msLevel. = integer())

## S4 method for signature 'Spectra'
filterMzRange(
  object,
  mz = numeric(),
  msLevel. = uniqueMsLevels(object),
  keep = TRUE
)

## S4 method for signature 'Spectra'
filterMzValues(
  object,
  mz = numeric(),
  tolerance = 0,
  ppm = 20,
  msLevel. = uniqueMsLevels(object),
  keep = TRUE
)

## S4 method for signature 'Spectra'
filterPolarity(object, polarity = integer())

## S4 method for signature 'Spectra'
filterPrecursorMz(object, mz = numeric())

## S4 method for signature 'Spectra'
filterPrecursorMzRange(object, mz = numeric())

## S4 method for signature 'Spectra'
filterPrecursorMzValues(object, mz = numeric(), ppm = 20, tolerance = 0)
```

```
## S4 method for signature 'Spectra'
filterPrecursorCharge(object, z = integer())

## S4 method for signature 'Spectra'
filterPrecursorScan(object, acquisitionNum = integer(), f = dataOrigin(object))

## S4 method for signature 'Spectra'
filterRt(object, rt = numeric(), msLevel. = uniqueMsLevels(object))

## S4 method for signature 'Spectra'
reset(object, ...)

## S4 method for signature 'Spectra'
filterRanges(
  object,
  spectraVariables = character(),
  ranges = numeric(),
  match = c("all", "any")
)

## S4 method for signature 'Spectra'
filterValues(
  object,
  spectraVariables = character(),
  values = numeric(),
  ppm = 0,
  tolerance = 0,
  match = c("all", "any")
)

## S4 method for signature 'Spectra'
bin(
  x,
  binSize = 1L,
  breaks = NULL,
  msLevel. = uniqueMsLevels(x),
  FUN = sum,
  zero.rm = TRUE
)

## S4 method for signature 'Spectra,Spectra'
compareSpectra(
  x,
  y,
  MAPFUN = joinPeaks,
  tolerance = 0,
  ppm = 20,
  FUN = ndotproduct,
  ...,
  SIMPLIFY = TRUE
)
```

```
## S4 method for signature 'Spectra,missing'
compareSpectra(
  x,
  y = NULL,
  MAPFUN = joinPeaks,
  tolerance = 0,
  ppm = 20,
  FUN = ndotproduct,
  ...,
  SIMPLIFY = TRUE
)

## S4 method for signature 'Spectra'
pickPeaks(
  object,
  halfWindowSize = 2L,
  method = c("MAD", "SuperSmoother"),
  snr = 0,
  k = 0L,
  descending = FALSE,
  threshold = 0,
  msLevel. = uniqueMsLevels(object),
  ...
)

## S4 method for signature 'Spectra'
replaceIntensitiesBelow(
  object,
  threshold = min,
  value = 0,
  msLevel. = uniqueMsLevels(object)
)

## S4 method for signature 'Spectra'
smooth(
  x,
  halfWindowSize = 2L,
  method = c("MovingAverage", "WeightedMovingAverage", "SavitzkyGolay"),
  msLevel. = uniqueMsLevels(x),
  ...
)

## S4 method for signature 'Spectra'
addProcessing(object, FUN, ..., spectraVariables = character())

coreSpectraVariables()

## S4 method for signature 'Spectra'
uniqueMsLevels(object, ...)

## S4 method for signature 'Spectra'
backendBpparam(object, BPPARAM = bpparam())
```

```
## S4 method for signature 'Spectra'
combinePeaks(
  object,
  tolerance = 0,
  ppm = 20,
  intensityFun = base::mean,
  mzFun = base::mean,
  weighted = TRUE,
  msLevel. = uniqueMsLevels(object),
  ...
)

## S4 method for signature 'Spectra'
entropy(object, normalized = TRUE)

## S4 method for signature 'ANY'
entropy(object, ...)

## S4 method for signature 'Spectra'
dataStorageBasePath(object)

## S4 replacement method for signature 'Spectra'
dataStorageBasePath(object) <- value

asDataFrame(
  object,
  i = seq_along(object),
  spectraVars = spectraVariables(object)
)
```

Arguments

object	For Spectra(): either a DataFrame or missing. See section on creation of Spectra objects for details. For all other methods a Spectra object.
f	For split(): factor defining how to split x. See base::split() for details. For setBackend(): factor defining how to split the data for parallelized copying of the spectra data to the new backend. For some backends changing this parameter can lead to errors. For combineSpectra(): factor defining the grouping of the spectra that should be combined. For spectrapply(): factor how object should be splitted. For filterPrecursorScan(): defining which spectra belong to the same original data file (sample): Defaults to f = dataOrigin(x). For intensity(), mz() and peaksData(): factor defining how data should be chunk-wise loaded an processed. Defaults to processingChunkFactor().
BPPARAM	Parallel setup configuration. See bpparam() for more information. This is passed directly to the backendInitialize() method of the MsBackend.
...	Additional arguments.
x	A Spectra object.
p	For combineSpectra(): factor defining how to split the input Spectra for parallel processing. Defaults to x$dataStorage, i.e., depending on the used backend, per-file parallel processing will be performed.

FUN
: For addProcessing(): function to be applied to the peak matrix of each spectrum in object. For compareSpectra(): function to compare intensities of peaks between two spectra with each other. For combineSpectra(): function to combine the (peak matrices) of the spectra. See section *Data manipulations* and examples below for more details. For bin(): function to aggregate intensity values of peaks falling into the same bin. Defaults to FUN = sum thus summing up intensities. For spectrapply() and chunkapply(): function to be applied to Spectra.

y
: A Spectra object. A DataFrame for joinSpectraData().

by.x
: A character(1) specifying the spectra variable used for merging. Default is "spectrumId".

by.y
: A character(1) specifying the column used for merging. Set to by.x if missing.

suffix.y
: A character(1) specifying the suffix to be used for making the names of columns in the merged spectra variables unique. This suffix will be used to amend names(y), while spectraVariables(x) will remain unchanged.

substDefinition
: For deisotopeSpectra() and filterPrecursorIsotopes(): matrix or data.frame with definitions of isotopic substitutions. Uses by default isotopic substitutions defined from all compounds in the Human Metabolome Database (HMDB). See isotopologues() or isotopicSubstitutionMatrix() for details.

tolerance
: For compareSpectra(), containsMz(), deisotopeSpectra(), filterMzValues() and reduceSpectra(): numeric(1) allowing to define a constant maximal accepted difference between m/z values for peaks to be matched (or grouped). For containsMz() it can also be of length equal mz to specify a different tolerance for each m/z value. For filterPrecursorMaxIntensity(): numeric(1) defining the (constant) maximal accepted difference of precursor m/z values of spectra for grouping them into *precursor groups*. For filterPrecursorIsotopes(): passed directly to the isotopologues() function. For filterValues(): numeric of any length allowing to define a maximal accepted difference between user input values and the spectraVariables values. If it is not equal to the length of the value provided with parameter spectraVariables, tolerance[1] will be recycled. Default is tolerance = 0

ppm
: For compareSpectra(), containsMz(), deisotopeSpectra(), filterMzValues() and reduceSpectra(): numeric(1) defining a relative, m/z-dependent, maximal accepted difference between m/z values for peaks to be matched (or grouped). For filterPrecursorMaxIntensity(): numeric(1) defining the relative maximal accepted difference of precursor m/z values of spectra for grouping them into *precursor groups*. For filterPrecursorIsotopes(): passed directly to the isotopologues() function. For filterValues(): numeric of any length allowing to define a maximal accepted difference between user input values and the spectraVariables values. If it is not equal to the length of the value provided with parameter spectraVariables, ppm[1] will be recycled.

charge
: For deisotopeSpectra(): expected charge of the ionized compounds. See isotopologues() for details.

by
: For scalePeaks(): function to calculate a single numeric from intensity values of a spectrum by which all intensities (of that spectrum) should be divided by. The default by = sum will divide intensities of each spectrum by the sum of intensities of that spectrum.

msLevel.   integer defining the MS level(s) of the spectra to which the function should be applied (defaults to all MS levels of object. For filterMsLevel(): the MS level to which object should be subsetted.

mz   For filterIsolationWindow(): numeric(1) with the m/z value to filter the object. For filterPrecursorMz() and filterMzRange(): numeric(2) defining the lower and upper m/z boundary. For filterMzValues() and filterPrecursorMzValues(): numeric with the m/z values to match peaks or precursor m/z against.

processingQueue
                  For Spectra(): optional list of [ProcessingStep](#) objects.

metadata   For Spectra(): optional list with metadata information.

backend   For Spectra(): [MsBackend](#) to be used as backend. See section on creation of Spectra objects for details. For setBackend(): instance of [MsBackend](#) that supports setBackend() (i.e. for which supportsSetBackend() returns TRUE). Such backends have a parameter data in their backendInitialize() function that support passing the full spectra data to the initialize method. See section on creation of Spectra objects for details. For export(): [MsBackend](#) to be used to export the data.

source   For Spectra(): instance of [MsBackend](#) that can be used to import spectrum data from the provided files. See section *Creation of objects, conversion and changing the backend* for more details.

drop   For [, split(): not considered.

columns   For spectraData() accessor: optional character with column names (spectra variables) that should be included in the returned DataFrame. By default, all columns are returned. For peaksData() accessor: optional character with requested columns in the individual matrix of the returned list. Defaults to c("mz", "value") but any values returned by peaksVariables(object) with object being the Spectra object are supported.

value   replacement value for <- methods. See individual method description or expected data type.

which   for containsMz(): either "any" or "all" defining whether any (the default) or all provided mz have to be present in the spectrum.

neutralLoss   for containsNeutralLoss(): numeric(1) defining the value which should be subtracted from the spectrum's precursor m/z.

chunkSize   For spectrapply(): size of the chunks into which Spectra should be split. This parameter overrides parameters f and BPPARAM.

use.names   For lengths(): ignored.

spectraVariables
                  • For selectSpectraVariables(): character with the names of the spectra variables to which the backend should be subsetted.
                      – For addProcessing(): character with additional spectra variables that should be passed along to the function defined with FUN. See function description for details.
                      – For filterRanges() and filterValues(): character vector specifying the column(s) from spectraData(object) on which to filter the data and that correspond to the the names of the spectra variables that should be used for the filtering.

initial   For tic(): logical(1) whether the initially reported total ion current should be reported, or whether the total ion current should be (re)calculated on the actual data (initial = FALSE, same as ionCount()).

name	For $ and $<-: the name of the spectra variable to return or set.
i	For [: integer, logical or character to subset the object. For asDataFrame() an numeric indicating which scans to coerce to a DataFrame (default is seq_along(object)).
j	For [: not supported.
n	for filterAcquisitionNum(): integer with the acquisition numbers to filter for.
dataStorage	For filterDataStorage(): character to define which spectra to keep. For filterAcquisitionNum(): optionally specify if filtering should occur only for spectra of selected dataStorage.
dataOrigin	For filterDataOrigin(): character to define which spectra to keep. For filterAcquisitionNum(): optionally specify if filtering should occurr only for spectra of selected dataOrigin.
halfWindowSize	• For pickPeaks(): integer(1), used in the identification of the mass peaks: a local maximum has to be the maximum in the window from (i - halfWindowSize):(i + halfWindowSize).
	– For smooth(): integer(1), used in the smoothing algorithm, the window reaches from (i - halfWindowSize):(i + halfWindowSize).
	– For filterFourierTransformArtefacts(): numeric(1) defining the m/z window left and right of a peak where to remove fourier transform artefacts.
threshold	• For pickPeaks(): a double(1) defining the proportion of the maximal peak intensity. Just values above are used for the weighted mean calculation.
	– For replaceIntensitiesBelow(): a numeric(1) defining the threshold or a function to calculate the threshold for each spectrum on its intensity values. Defaults to threshold = min.
	– For filterFourierTransformArtefacts(): the relative intensity (to a peak) below which peaks are considered fourier artefacts. Defaults to threshold = 0.2 hence removing peaks that have an intensity below 0.2 times the intensity of the tested peak (within the selected halfWindowSize).
keepIsotopes	For filterFourierTransformArtefacts(): whether isotope peaks should not be removed as fourier artefacts.
maxCharge	For filterFourierTransformArtefacts(): the maximum charge to be considered for isotopes.
isotopeTolerance	
	For filterFourierTransformArtefacts(): the m/z tolerance to be used to define whether peaks might be isotopes of the current tested peak.
intensity	For filterIntensity(): numeric of length 1 or 2 defining either the lower or the lower and upper intensity limit for the filtering, or a function that takes the intensities as input and returns a logical (same length then peaks in the spectrum) whether the peak should be retained or not. Defaults to intensity = c(0, Inf) thus only peaks with NA intensity are removed.
keep	For filterMzValues() and filterMzRange(): logical(1) whether the matching peaks should be retained (keep = TRUE, the default) or dropped (keep = FALSE).
polarity	for filterPolarity(): integer specifying the polarity to to subset object.
z	For filterPrecursorCharge(): integer() with the precursor charges to be used as filter.

acquisitionNum	for filterPrecursorScan(): integer with the acquisition number of the spectra to which the object should be subsetted.
rt	for filterRt(): numeric(2) defining the retention time range to be used to subset/filter object.
ranges	for filterRanges(): A numeric vector of paired values (upper and lower boundary) that define the ranges to filter the object. These paired values need to be in the same order as the spectraVariables parameter (see below).
match	For filterRanges() and filterValues(): character(1) defining whether the condition has to match for all provided ranges/values (match = "all"; the default), or for any of them (match = "any") for spectra to be retained.
values	for filterValues(): A numeric vector that define the values to filter the Spectra data. These values need to be in the same order as the spectraVariables parameter.
binSize	For bin(): numeric(1) defining the size for the m/z bins. Defaults to binSize = 1.
breaks	For bin(): numeric defining the m/z breakpoints between bins.
zero.rm	logical. For bin(): indicating whether to remove bins with zero intensity. Defaults to TRUE, meaning the function will discard bins created with an intensity of 0 to enhance memory efficiency.
MAPFUN	For compareSpectra(): function to map/match peaks between the two compared spectra. See joinPeaks() for more information and possible functions.
SIMPLIFY	For compareSpectra() whether the result matrix should be *simplified* to a numeric if possible (i.e. if either x or y is of length 1).
method	• For pickPeaks(): character(1), the noise estimators that should be used, currently the the *M*edian *A*bsolute *D*eviation (method = "MAD") and Friedman's Super Smoother (method = "SuperSmoother") are supported. – For smooth(): character(1), the smoothing function that should be used, currently, the Moving-Average- (method = "MovingAverage"), Weighted-Moving-Average- (method = "WeightedMovingAverage"), Savitzky-Golay-Smoothing (method = "SavitzkyGolay") are supported.
snr	For pickPeaks(): double(1) defining the *S*ignal-to-*N*oise-*R*atio. The intensity of a local maximum has to be higher than snr * noise to be considered as peak.
k	For pickPeaks(): integer(1), number of values left and right of the peak that should be considered in the weighted mean calculation.
descending	For pickPeaks(): logical, if TRUE just values between the nearest valleys around the peak centroids are used.
intensityFun	For combinePeaks(): function to be used to aggregate intensities for all peaks in each peak group into a single intensity value.
mzFun	For combinePeaks(): function to aggregate m/z values for all peaks within each peak group into a single m/z value. This parameter is ignored if weighted = TRUE (the default).
weighted	For combinePeaks(): logical(1) whether m/z values of peaks within each peak group should be aggregated into a single m/z value using an intensity-weighted mean. Defaults to weighted = TRUE.
normalized	for entropy(): logical(1) whether the normalized entropy should be calculated (default). See also nentropy() for details.
spectraVars	character() indicating what spectra variables to add to the DataFrame. Default is spectraVariables(object), i.e. all available variables.

Details

The Spectra class uses by default a lazy data manipulation strategy, i.e. data manipulations such as performed with replaceIntensitiesBelow() are not applied immediately to the data, but applied on-the-fly to the spectrum data once it is retrieved. For some backends that allow to write data back to the data storage (such as the MsBackendMemory(), MsBackendDataFrame() and MsBackendHdf5Peaks()) it is possible to apply to queue with the applyProcessing function. See the *Data manipulation and analysis *methods* section below for more details.

For more information on parallel or chunk-wise processing (especially helpful for very large data sets) see processingChunkSize().

To apply arbitrary functions to a Spectra use the spectrapply() function (or directly chunkapply() for chunk-wise processing). See description of the spectrapply() function below for details.

For details on plotting spectra, see plotSpectra().

Clarifications regarding scan/acquisition numbers and indices:

- A spectrumId (or spectrumID) is a vendor specific field in the mzML file that contains some information about the run/spectrum, e.g.: controllerType=0 controllerNumber=1 scan=5281 file=2

- acquisitionNum is a more a less sanitize spectrum id generated from the spectrumId field by mzR (see here).

- scanIndex is the mzR generated sequence number of the spectrum in the raw file (which doesn't have to be the same as the acquisitionNum)

See also this issue.

Value

See individual method description for the return value.

Creation of objects, conversion, changing the backend and export

Spectra classes can be created with the Spectra() constructor function which supports the following formats:

- parameter object is a data.frame or DataFrame containing the spectrum data. The provided backend (by default a MsBackendMemory) will be initialized with that data.

- parameter object is a MsBackend (assumed to be already initialized).

- parameter object is missing, in which case it is supposed that the data is provided by the MsBackend class passed along with the backend argument.

- parameter object is of type character and is expected to be the file names(s) from which spectra should be imported. Parameter source allows to define a MsBackend that is able to import the data from the provided source files. The default value for source is MsBackendMzR() which allows to import spectra data from mzML, mzXML or CDF files.

With ... additional arguments can be passed to the backend's backendInitialize() method. Parameter backend allows to specify which MsBackend should be used for data storage.

The backend of a Spectra object can be changed with the setBackend() method that takes an instance of the new backend as second parameter backend. A call to setBackend(sps, backend = MsBackendDataFrame()) would for example change the backend of sps to the *in-memory* MsBackendDataFrame. Changing to a backend is only supported if that backend has a data parameter in its backendInitialize() method and if supportsSetBackend() returns TRUE for that backend. setBackend() will transfer

the full spectra data from the originating backend as a DataFrame to the new backend. Most *read-only* backends do not support setBackend(). It is for example not possible to change the backend to a *read-only* backend (such as the MsBackendMzR() backend).

The definition of the function is: setBackend(object, backend, ..., f = dataStorage(object), BPPARAM = bpparam()) and its parameters are:

- parameter object: the Spectra object.

- parameter backend: an instance of the new backend, e.g. [MsBackendMemory()].

- parameter f: factor allowing to parallelize the change of the backends. By default the process of copying the spectra data from the original to the new backend is performed separately (and in parallel) for each file. Users are advised to use the default setting.

- parameter ...: optional additional arguments passed to the backendInitialize() method of the new backend.

- parameter BPPARAM: setup for the parallel processing. See bpparam() for details.

Data from a Spectra object can be **exported** to a file with the export() function. The actual export of the data has to be performed by the export method of the MsBackend class defined with the mandatory parameter backend. Note however that not all backend classes support export of data. From the MsBackend classes in the Spectra package currently only the MsBackendMzR backend supports data export (to mzML/mzXML file(s)); see the help page of the MsBackend for information on its arguments or the examples below or the vignette for examples.

The definition of the function is export(object, backend, ...) and its parameters are:

- object: the Spectra object to be exported.

- backend: instance of a class extending MsBackend which supports export of the data (i.e. which has a defined export method).

- ...: additional parameters specific for the MsBackend passed with parameter backend.

The dataStorageBasePath() and dataStorageBasePath<- functions allow, for backend classes that support this operation, to get or change the *base* path to the directory where the backend stores the data. In-memory backends such as MsBackendMemory or MsBackendDataFrame keeping all MS data in memory don't support, and need, this function, but for MsBackendMzR this function can be used to update/adapt the path to the directory containing the original data files. Thus, for Spectra objects (using this backend) that were moved to another file system or computer, these functions allow to adjust/adapt the base file path.

Accessing spectra data

- $, $<-: gets (or sets) a spectra variable for all spectra in object. See examples for details. Note that replacing values of a peaks variable is not supported with a non-empty processing queue, i.e. if any filtering or data manipulations on the peaks data was performed. In these cases applyProcessing() needs to be called first to apply all cached data operations.

- [[, [[<-: access or set/add a single spectrum variable (column) in the backend.

- acquisitionNum(): returns the acquisition number of each spectrum. Returns an integer of length equal to the number of spectra (with NA_integer_ if not available).

- centroided(), centroided<-: gets or sets the centroiding information of the spectra. centroided() returns a logical vector of length equal to the number of spectra with TRUE if a spectrum is centroided, FALSE if it is in profile mode and NA if it is undefined. See also isCentroided() for estimating from the spectrum data whether the spectrum is centroided. value for centroided<- is either a single logical or a logical of length equal to the number of spectra in object.

- collisionEnergy(), collisionEnergy<-: gets or sets the collision energy for all spectra in object. collisionEnergy() returns a numeric with length equal to the number of spectra (NA_real_ if not present/defined), collisionEnergy<- takes a numeric of length equal to the number of spectra in object.

- coreSpectraVariables(): returns the *core* spectra variables along with their expected data type.

- dataOrigin(), dataOrigin<-: gets or sets the *data origin* for each spectrum. dataOrigin() returns a character vector (same length than object) with the origin of the spectra. dataOrigin<- expects a character vector (same length than object) with the replacement values for the data origin of each spectrum.

- dataStorage(): returns a character vector (same length than object) with the data storage location of each spectrum.

- intensity(): gets the intensity values from the spectra. Returns a NumericList() of numeric vectors (intensity values for each spectrum). The length of the list is equal to the number of spectra in object.

- ionCount(): returns a numeric with the sum of intensities for each spectrum. If the spectrum is empty (see isEmpty()), NA_real_ is returned.

- isCentroided(): a heuristic approach assessing if the spectra in object are in profile or centroided mode. The function takes the qtlth quantile top peaks, then calculates the difference between adjacent m/z value and returns TRUE if the first quartile is greater than k. (See Spectra:::.isCentroided() for the code.)

- isEmpty(): checks whether a spectrum in object is empty (i.e. does not contain any peaks). Returns a logical vector of length equal number of spectra.

- isolationWindowLowerMz(), isolationWindowLowerMz<-: gets or sets the lower m/z boundary of the isolation window.

- isolationWindowTargetMz(), isolationWindowTargetMz<-: gets or sets the target m/z of the isolation window.

- isolationWindowUpperMz(), isolationWindowUpperMz<-: gets or sets the upper m/z boundary of the isolation window.

- containsMz(): checks for each of the spectra whether they contain mass peaks with an m/z equal to mz (given acceptable difference as defined by parameters tolerance and ppm - see common() for details). Parameter which allows to define whether any (which = "any", the default) or all (which = "all") of the mz have to match. The function returns NA if mz is of length 0 or is NA.

- containsNeutralLoss(): checks for each spectrum in object if it has a peak with an m/z value equal to its precursor m/z - neutralLoss (given acceptable difference as defined by parameters tolerance and ppm). Returns NA for MS1 spectra (or spectra without a precursor m/z).

- length(): gets the number of spectra in the object.

- lengths(): gets the number of peaks (m/z-intensity values) per spectrum. Returns an integer vector (length equal to the number of spectra). For empty spectra, 0 is returned.

- msLevel(): gets the spectra's MS level. Returns an integer vector (names being spectrum names, length equal to the number of spectra) with the MS level for each spectrum.

- mz(): gets the mass-to-charge ratios (m/z) from the spectra. Returns a NumericList() or length equal to the number of spectra, each element a numeric vector with the m/z values of one spectrum.

- peaksData(): gets the *peaks* data for all spectra in object. Peaks data consist of the m/z and intensity values as well as possible additional annotations (variables) of all peaks of each spectrum. The function returns a [SimpleList()](#) of two dimensional arrays (either matrix or data.frame), with each array providing the values for the requested *peak variables* (by default "mz" and "intensity"). Optional parameter columns is passed to the backend's peaksData() function to allow the selection of specific (or additional) peaks variables (columns) that should be extracted (if available). Importantly, it is **not** guaranteed that each backend supports this parameter (while each backend must support extraction of "mz" and "intensity" columns). Parameter columns defaults to c("mz", "intensity") but any value returned by peaksVariables(object) is supported. Note also that it is possible to extract the peak data with as(x, "list") and as(x, "SimpleList") as a list and SimpleList, respectively. Note however that, in contrast to peaksData(), as() does not support the parameter columns.

- peaksVariables(): lists the available variables for mass peaks provided by the backend. Default peak variables are "mz" and "intensity" (which all backends need to support and provide), but some backends might provide additional variables. These variables correspond to the column names of the peak data array returned by peaksData().

- polarity(), polarity<-: gets or sets the polarity for each spectrum. polarity() returns an integer vector (length equal to the number of spectra), with 0 and 1 representing negative and positive polarities, respectively. polarity<- expects an integer vector of length 1 or equal to the number of spectra.

- precursorCharge(), precursorIntensity(), precursorMz(), precScanNum(), precAcquisitionNum(): gets the charge (integer), intensity (numeric), m/z (numeric), scan index (integer) and acquisition number (interger) of the precursor for MS level > 2 spectra from the object. Returns a vector of length equal to the number of spectra in object. NA are reported for MS1 spectra of if no precursor information is available.

- rtime(), rtime<-: gets or sets the retention times (in seconds) for each spectrum. rtime() returns a numeric vector (length equal to the number of spectra) with the retention time for each spectrum. rtime<- expects a numeric vector with length equal to the number of spectra.

- scanIndex(): returns an integer vector with the *scan index* for each spectrum. This represents the relative index of the spectrum within each file. Note that this can be different to the acquisitionNum of the spectrum which represents the index of the spectrum during acquisition/measurement (as reported in the mzML file).

- smoothed(),smoothed<-: gets or sets whether a spectrum is *smoothed*. smoothed() returns a logical vector of length equal to the number of spectra. smoothed<- takes a logical vector of length 1 or equal to the number of spectra in object.

- spectraData(): gets general spectrum metadata (annotation, also called header). spectraData() returns a DataFrame. Note that this method does by default **not** return m/z or intensity values.

- spectraData<-: **replaces** the full spectra data of the Spectra object with the one provided with value. The spectraData<- function expects a DataFrame to be passed as value with the same number of rows as there a spectra in object. Note that replacing values of peaks variables is not supported with a non-empty processing queue, i.e. if any filtering or data manipulations on the peaks data was performed. In these cases [applyProcessing()](#) needs to be called first to apply all cached data operations and empty the processing queue.

- spectraNames(), spectraNames<-: gets or sets the spectra names.

- spectraVariables(): returns a character vector with the available spectra variables (columns, fields or attributes of each spectrum) available in object. Note that spectraVariables() does not list the *peak variables* ("mz", "intensity" and eventual additional annotations for each MS peak). Peak variables are returned by peaksVariables().

- `tic()`: gets the total ion current/count (sum of signal of a spectrum) for all spectra in `object`. By default, the value reported in the original raw data file is returned. For an empty spectrum, `0` is returned.
- `uniqueMsLevels()`: get the unique MS levels available in `object`. This function is supposed to be more efficient than `unique(msLevel(object))`.

Filter spectra data

Filter a `Spectra` object based on the spectra data. This includes subset operations that immediately reduce the number of spectra in the object as well as filters that reduce the *content* of the `Spectra` object. See section *Filter peaks data* below for functions that filter the peaks data of a `Spectra`.

- `[`: subsets the spectra keeping only selected elements (i). The method **always** returns a `Spectra` object.
- `dropNaSpectraVariables()`: removes spectra variables (i.e. columns in the object's `spectraData` that contain only missing values (NA). Note that while columns with only NAs are removed, a `spectraData()` call after `dropNaSpectraVariables()` might still show columns containing NA values for *core* spectra variables. The total number of spectra is not changed by this function.
- `filterAcquisitionNum()`: filters the object keeping only spectra matching the provided acquisition numbers (argument n). If `dataOrigin` or `dataStorage` is also provided, `object` is subsetted to the spectra with an acquisition number equal to n **in spectra with matching dataOrigin or dataStorage values** retaining all other spectra. Returns the filtered `Spectra`.
- `filterDataOrigin()`: filters the object retaining spectra matching the provided `dataOrigin`. Parameter `dataOrigin` has to be of type `character` and needs to match exactly the data origin value of the spectra to subset. Returns the filtered `Spectra` object (with spectra ordered according to the provided `dataOrigin` parameter).
- `filterDataStorage()`: filters the object retaining spectra stored in the specified `dataStorage`. Parameter `dataStorage` has to be of type `character` and needs to match exactly the data storage value of the spectra to subset. Returns the filtered `Spectra` object (with spectra ordered according to the provided `dataStorage` parameter).
- `filterEmptySpectra()`: removes empty spectra (i.e. spectra without peaks). Returns the filtered `Spectra` object (with spectra in their original order).
- `filterIsolationWindow()`: retains spectra that contain mz in their isolation window m/z range (i.e. with an `isolationWindowLowerMz <= mz` and `isolationWindowUpperMz >= mz`. Returns the filtered `Spectra` object (with spectra in their original order).
- `filterMsLevel()`: filters object by MS level keeping only spectra matching the MS level specified with argument `msLevel`. Returns the filtered `Spectra` (with spectra in their original order).
- `filterPolarity()`: filters the object keeping only spectra matching the provided polarity. Returns the filtered `Spectra` (with spectra in their original order).
- `filterPrecursorCharge()`: retains spectra with the defined precursor charge(s).
- `filterPrecursorIsotopes()`: groups MS2 spectra based on their precursor m/z and precursor intensity into predicted isotope groups and keep for each only the spectrum representing the monoisotopic precursor. MS1 spectra are returned as is. See documentation for `deisotopeSpectra()` below for details on isotope prediction and parameter description.
- `filterPrecursorMaxIntensity()`: filters the `Spectra` keeping for groups of (MS2) spectra with similar precursor m/z values (given parameters ppm and `tolerance`) the one with the highest precursor intensity. The function filters only MS2 spectra and returns all MS1 spectra.

If precursor intensities are NA for all spectra within a spectra group, the first spectrum of that groups is returned. Note: some manufacturers don't provide precursor intensities. These can however also be estimated with estimatePrecursorIntensity().

- filterPrecursorMzRange() (previously filterPrecursorMz() which is now deprecated): retains spectra with a precursor m/z within the provided m/z range. See examples for details on selecting spectra with a precursor m/z for a target m/z accepting a small difference in *ppm*.

- filterPrecursorMzValues(): retains spectra with precursor m/z matching any of the provided m/z values (given ppm and tolerance). Spectra with missing precursor m/z value (e.g. MS1 spectra) are dropped.

- filterPrecursorScan(): retains parent (e.g. MS1) and children scans (e.g. MS2) of acquisition number acquisitionNum. Returns the filtered Spectra (with spectra in their original order). Parameter f allows to define which spectra belong to the same sample or original data file (defaults to f = dataOrigin(object)).

- filterRanges(): allows filtering of the Spectra object based on user defined *numeric* ranges (parameter ranges) for one or more available spectra variables in object (spectra variable names can be specified with parameter spectraVariables). Spectra for which the value of a spectra variable is within it's defined range are retained. If multiple ranges/spectra variables are defined, the match parameter can be used to specify whether all conditions (match = "all"; the default) or if any of the conditions must match (match = "any"; all spectra for which values are within any of the provided ranges are retained).

- filterRt(): retains spectra of MS level msLevel with retention times (in seconds) within (>=) rt[1] and (<=) rt[2]. Returns the filtered Spectra (with spectra in their original order).

- filterValues(): allows filtering of the Spectra object based on similarities of *numeric* values of one or more spectraVariables(object) (parameter spectraVariables) to provided values (parameter values) given acceptable differences (parameters tolerance and ppm). If multiple values/spectra variables are defined, the match parameter can be used to specify whether all conditions (match = "all"; the default) or if any of the conditions must match (match = "any"; all spectra for which values are within any of the provided ranges are retained).

- selectSpectraVariables(): reduces the information within the object to the selected spectra variables: all data for variables not specified will be dropped. For mandatory columns (i.e., those listed by coreSpectraVariables(), such as *msLevel*, *rtime* ...) only the values will be dropped but not the variable itself. Additional (or user defined) spectra variables will be completely removed. Returns the filtered Spectra.

Filter or aggregate mass peak data

Operations that filter or aggregate the mass peak data from each spectrum without changing the number of spectra in a Spectra object. Also, the actual subsetting/aggregation operation is only executed once peaks data is accessed (through peaksData(), mz() or intensity()) or applyProcessing() is called.

- combinePeaks(): combines mass peaks **within each spectrum** with a difference in their m/z values that is smaller than the maximal acceptable difference defined by ppm and tolerance. Parameters intensityFun and mzFun allow to define functions to aggregate the intensity and m/z values for each such group of peaks. With weighted = TRUE (the default), the m/z value of the combined peak is calculated using an intensity-weighted mean and parameter mzFun is ignored. The MsCoreUtils::group() function is used for the grouping of mass peaks. Parameter msLevel. allows to define selected MS levels for which peaks should be combined. This function returns a Spectra with the same number of spectra than the input object, but with possibly combined peaks within each spectrum. dropped (i.e. their values are replaced

with NA) for combined peaks unless they are constant across the combined peaks. See also `reduceSpectra()` for a function to select a single *representative* mass peak for each peak group.

- `deisotopeSpectra()`: *deisotopes* each spectrum keeping only the monoisotopic peak for groups of isotopologues. Isotopologues are estimated using the `isotopologues()` function from the *MetaboCoreUtils* package. Note that the default parameters for isotope prediction/detection have been determined using data from the Human Metabolome Database (HMDB) and isotopes for elements other than CHNOPS might not be detected. See parameter `substDefinition` in the documentation of `isotopologues()` for more information. The approach and code to define the parameters for isotope prediction is described here.

- `filterFourierTransformArtefacts()`: removes (Orbitrap) fast fourier artefact peaks from spectra (see examples below). The function iterates through all intensity ordered peaks in a spectrum and removes all peaks with an m/z within +/- `halfWindowSize` of the current peak if their intensity is lower than `threshold` times the current peak's intensity. Additional parameters `keepIsotopes`, `maxCharge` and `isotopeTolerance` allow to avoid removing of potential ^{13}C isotope peaks (`maxCharge` being the maximum charge that should be considered and `isotopeTolerance` the absolute acceptable tolerance for matching their m/z). See `filterFourierTransformArtefacts()` for details and background and `deisitopeSpectra()` for an alternative.

- `filterIntensity()`: filters mass peaks in each spectrum keeping only those with intensities that are within the provided range or match the criteria of the provided function. For the former, parameter `intensity` has to be a `numeric` defining the intensity range, for the latter a `function` that takes the intensity values of the spectrum and returns a `logical` whether the peak should be retained or not (see examples below for details) - additional parameters to the function can be passed with `...`. To remove only peaks with intensities below a certain threshold, say 100, use `intensity = c(100, Inf)`. Note: also a single value can be passed with the `intensity` parameter in which case an upper limit of `Inf` is used. Note that this function removes also peaks with missing intensities (i.e. an intensity of `NA`). Parameter `msLevel.` allows to restrict the filtering to spectra of the specified MS level(s).

- `filterMzRange()`: filters mass peaks in the object keeping or removing those in each spectrum that are within the provided m/z range. Whether peaks are retained or removed can be configured with parameter `keep` (default `keep = TRUE`).

- `filterMzValues()`: filters mass peaks in the object keeping all peaks in each spectrum that match the provided m/z value(s) (for `keep = TRUE`, the default) or removing all of them (for `keep = FALSE`). The m/z matching considers also the absolute `tolerance` and m/z-relative `ppm` values. `tolerance` and `ppm` have to be of length 1.

- `filterPeaksRanges()`: filters mass peaks of a `Spectra` object using any set of range-based filters on numeric spectra or peaks variables. See `filterPeaksRanges()` for more information.

- `filterPrecursorPeaks()`: removes peaks from each spectrum in `object` with an m/z equal or larger than the m/z of the precursor, depending on the value of parameter `mz`: for `mz = =="` (the default) peaks eranceandppm, respectively) are removed. For `mz = ">="`all peaks with an m/z larger or equal to th (e.g. typically for MS1 spectra).

- `reduceSpectra()`: keeps for groups of peaks with similar m/z values in (given `ppm` and `tolerance`) in each spectrum only the peak with the highest intensity removing all other peaks hence *reducing* each spectrum to the highest intensity peaks per *peak group*. Peak groups are defined using the `group()` function from the *MsCoreUtils* package. See also the `combinePeaks()` function for an alternative function to combine peaks within each spectrum.

Merging, aggregating and splitting

Several Spectra objects can be concatenated into a single object with the c() or the concatenateSpectra() function. Concatenation will fail if the processing queue of any of the Spectra objects is not empty or if different backends are used in the Spectra objects. Thus, in these cases, prior to merging Spectra object it is suggested to change the backend to a MsBackendMemory using the setBackend() function, and to *apply* all data processing steps using applyProcessing(). The spectra variables of the resulting Spectra object is the union of the spectra variables of the individual Spectra objects.

- combineSpectra(): combines MS data (i.e. mass peaks) from sets of spectra into a single spectrum per set (in contrast to combinePeaks() or reduceSpectra() that combine mass peaks **within each spectrum**). For each spectrum group (set), spectra variables from the first spectrum are used and the peak matrices are combined using the function specified with FUN, which defaults to combinePeaksData(). Please refer to the combinePeaksData() help page for details and options of the actual combination of peaks across the sets of spectra and to the package vignette for examples and alternative ways to aggregate spectra. The sets of spectra can be specified with parameter f. In addition it is possible to define, with parameter p if and how to split the input data for parallel processing. This defaults to p = x$dataStorage and hence a per-file parallel processing is applied for Spectra with file-based backends (such as the MsBackendMzR()). Prior combination of the spectra all processings queued in the lazy evaluation queue are applied. Be aware that calling combineSpectra() on a Spectra object with certain backends that allow modifications might **overwrite** the original data. This does not happen with a MsBackendMemory or MsBackendDataFrame backend, but with a MsBackendHdf5Peaks backend the m/z and intensity values in the original hdf5 file(s) will be overwritten. The function returns a Spectra of length equal to the unique levels of f.

- joinSpectraData(): Individual spectra variables can be directly added with the $<- or [[<- syntax. The joinSpectraData() function allows to merge a DataFrame to the existing spectra data. This function diverges from the merge() method in two main ways:

  - The by.x and by.y column names must be of length 1.
  - If variable names are shared in x and y, the spectra variables of x are not modified. It's only the y variables that are appended the suffix defined in suffix.y. This is to avoid modifying any core spectra variables that would lead to an invalid object.
  - Duplicated Spectra keys (i.e. x[[by.x]]) are not allowed. Duplicated keys in the DataFrame (i.e y[[by.y]]) throw a warning and only the last occurrence is kept. These should be explored and ideally be removed using for QFeatures::reduceDataFrame(), PMS::reducePSMs() or similar functions.

- split(): splits the Spectra object based on parameter f into a list of Spectra objects.

Data manipulation and analysis methods

Many data manipulation operations, such as those listed in this section, are not applied immediately to the spectra, but added to a *lazy processing/manipulation queue*. Operations stored in this queue are applied on-the-fly to spectra data each time it is accessed. This lazy execution guarantees the same functionality for Spectra objects with any backend, i.e. backends supporting to save changes to spectrum data (MsBackendMemory(), MsBackendDataFrame() or MsBackendHdf5Peaks()) as well as read-only backends (such as the MsBackendMzR()). Note that for the former it is possible to apply the processing queue and write the modified peak data back to the data storage with the applyProcessing() function.

- addProcessing(): adds an arbitrary function that should be applied to the peaks matrix of every spectrum in object. The function (can be passed with parameter FUN) is expected to take a peaks matrix as input and to return a peaks matrix. A peaks matrix is a numeric matrix with

two columns, the first containing the m/z values of the peaks and the second the corresponding intensities. The function has to have ... in its definition. Additional arguments can be passed with .... With parameter spectraVariables it is possible to define additional spectra variables from object that should be passed to the function FUN. These will be passed by their name (e.g. specifying spectraVariables = "precursorMz" will pass the spectra's precursor m/z as a parameter named precursorMz to the function. The only exception is the spectra's MS level, these will be passed to the function as a parameter called spectrumMsLevel (i.e. with spectraVariables = "msLevel" the MS levels of each spectrum will be submitted to the function as a parameter called spectrumMsLevel). Examples are provided in the package vignette.

- applyProcessing(): for Spectra objects that use a **writeable** backend only: apply all steps from the lazy processing queue to the peak data and write it back to the data storage. Parameter f allows to specify how object should be split for parallel processing. This should either be equal to the dataStorage, or f = rep(1, length(object)) to disable parallel processing alltogether. Other partitionings might result in errors (especially if a MsBackendHdf5Peaks backend is used).

- bin(): aggregates individual spectra into discrete (m/z) bins. Binning is performed only on spectra of the specified MS level(s) (parameter msLevel, by default all MS levels of x). The bins can be defined with parameter breaks which by default are equally sized bins, with size being defined by parameter binSize, from the minimal to the maximal m/z of all spectra (of MS level msLevel) within x. The same bins are used for all spectra in x. All intensity values for peaks falling into the same bin are aggregated using the function provided with parameter FUN (defaults to FUN = sum, i.e. all intensities are summed up). Note that the binning operation is applied to the peak data on-the-fly upon data access and it is possible to *revert* the operation with the reset() function (see description of reset() above).

- compareSpectra(): compares each spectrum in x with each spectrum in y using the function provided with FUN (defaults to [ndotproduct()](#)). If y is missing, each spectrum in x is compared with each other spectrum in x. The matching/mapping of peaks between the compared spectra is done with the MAPFUN function. The default [joinPeaks()](#) matches peaks of both spectra and allows to keep all peaks from the first spectrum (type = "left"), from the second (type = "right"), from both (type = "outer") and to keep only matching peaks (type = "inner"); see [joinPeaks()](#) for more information and examples). The MAPFUN function should have parameters x, y, xPrecursorMz and yPrecursorMz as these values are passed to the function. In addition to joinPeaks() also [joinPeaksGnps()](#) is supported for GNPS-like similarity score calculations. Note that joinPeaksGnps() should only be used in combination with FUN = MsCoreUtils::gnps (see [joinPeaksGnps()](#) for more information and details). Use MAPFUN = joinPeaksNone to disable internal peak matching/mapping if a similarity scoring function is used that performs the matching internally. FUN is supposed to be a function to compare intensities of (matched) peaks of the two spectra that are compared. The function needs to take two matrices with columns "mz" and "intensity" as input and is supposed to return a single numeric as result. In addition to the two peak matrices the spectra's precursor m/z values are passed to the function as parameters xPrecursorMz (precursor m/z of the x peak matrix) and yPrecursorMz (precursor m/z of the y peak matrix). Additional parameters to functions FUN and MAPFUN can be passed with .... Parameters ppm and tolerance are passed to both MAPFUN and FUN. The function returns a matrix with the results of FUN for each comparison, number of rows equal to length(x) and number of columns equal length(y) (i.e. element in row 2 and column 3 is the result from the comparison of x[2] with y[3]). If SIMPLIFY = TRUE the matrix is *simplified* to a numeric if length of x or y is one. See also the vignette for additional examples, such as using spectral entropy similarity in the scoring.

- entropy(): calculates the entropy of each spectra based on the metrics suggested by Li et al. (https://doi.org/10.1038/s41592-021-01331-z). See also [nentropy()](#) in the *MsCoreUtils* package for details.

- estimatePrecursorIntensity(): defines the precursor intensities for MS2 spectra using the intensity of the matching MS1 peak from the closest MS1 spectrum (i.e. the last MS1 spectrum measured before the respective MS2 spectrum). With method = "interpolation" it is also possible to calculate the precursor intensity based on an interpolation of intensity values (and retention times) of the matching MS1 peaks from the previous and next MS1 spectrum. See estimatePrecursorIntensity() for examples and more details.

- estimatePrecursorMz(): **for DDA data**: allows to estimate a fragment spectra's precursor m/z based on the reported precursor m/z and the data from the previous MS1 spectrum. See estimatePrecursorMz() for details.

- neutralLoss(): calculates neutral loss spectra for fragment spectra. See neutralLoss() for detailed documentation.

- processingLog(): returns a character vector with the processing log messages.

- reset(): restores the data to its original state (as much as possible): removes any processing steps from the lazy processing queue and calls reset() on the backend which, depending on the backend, can also undo e.g. data filtering operations. Note that a reset*(call after applyProcessing() will not have any effect. See examples below for more information.

- scalePeaks(): scales intensities of peaks within each spectrum depending on parameter by. With by = sum (the default) peak intensities are divided by the sum of peak intensities within each spectrum. The sum of intensities is thus 1 for each spectrum after scaling. Parameter msLevel. allows to apply the scaling of spectra of a certain MS level. By default (msLevel. = uniqueMsLevels(x)) intensities for all spectra will be scaled.

- spectrapply(): applies a given function to each individual spectrum or sets of a Spectra object. By default, the Spectra is split into individual spectra (i.e. Spectra of length 1) and the function FUN is applied to each of them. An alternative splitting can be defined with parameter f. Parameters for FUN can be passed using .... The returned result and its order depend on the function FUN and how object is split (hence on f, if provided). Parallel processing is supported and can be configured with parameter BPPARAM, is however only suggested for computational intense FUN. As an alternative to the (eventual parallel) processing of the full Spectra, spectrapply() supports also a chunk-wise processing. For this, parameter chunkSize needs to be specified. object is then split into chunks of size chunkSize which are then (stepwise) processed by FUN. This guarantees a lower memory demand (especially for on-disk backends) since only the data for one chunk needs to be loaded into memory in each iteration. Note that by specifying chunkSize, parameters f and BPPARAM will be ignored. See also chunkapply() or examples below for details on chunk-wise processing.

- smooth(): smooths individual spectra using a moving window-based approach (window size = 2 * halfWindowSize). Currently, the Moving-Average- (method = "MovingAverage"), Weighted-Moving-Average- (method = "WeightedMovingAverage"), weights depending on the distance of the center and calculated 1/2^(-halfWindowSize:halfWindowSize)) and Savitzky-Golay-Smoothing (method = "SavitzkyGolay") are supported. For details how to choose the correct halfWindowSize please see MsCoreUtils::smooth().

- pickPeaks(): picks peaks on individual spectra using a moving window-based approach (window size = 2 * halfWindowSize). For noisy spectra there are currently two different noise estimators available, the *M*edian *A*bsolute *D*eviation (method = "MAD") and Friedman's Super Smoother (method = "SuperSmoother"), as implemented in the MsCoreUtils::noise(). The method supports also to optionally *refine* the m/z value of the identified centroids by considering data points that belong (most likely) to the same mass peak. Therefore the m/z value is calculated as an intensity weighted average of the m/z values within the peak region. The peak region is defined as the m/z values (and their respective intensities) of the 2 * k closest signals to the centroid or the closest valleys (descending = TRUE) in the 2 * k region. For the latter the k has to be chosen general larger. See MsCoreUtils::refineCentroids() for

details. If the ratio of the signal to the highest intensity of the peak is below threshold it will be ignored for the weighted average.

- replaceIntensitiesBelow(): replaces intensities below a specified threshold with the provided value. Parameter threshold can be either a single numeric value or a function which is applied to all non-NA intensities of each spectrum to determine a threshold value for each spectrum. The default is threshold = min which replaces all values which are <= the minimum intensity in a spectrum with value (the default for value is 0). Note that the function specified with threshold is expected to have a parameter na.rm since na.rm = TRUE will be passed to the function. If the spectrum is in profile mode, ranges of successive non-0 peaks <= threshold are set to 0. Parameter msLevel. allows to apply this to only spectra of certain MS level(s).

Author(s)

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Examples

```
## Create a Spectra providing a `DataFrame` containing the spectrum data.

spd <- DataFrame(msLevel = c(1L, 2L), rtime = c(1.1, 1.2))
spd$mz <- list(c(100, 103.2, 104.3, 106.5), c(45.6, 120.4, 190.2))
spd$intensity <- list(c(200, 400, 34.2, 17), c(12.3, 15.2, 6.8))

data <- Spectra(spd)
data

## Get the number of spectra
length(data)

## Get the number of peaks per spectrum
lengths(data)

## Create a Spectra from mzML files and use the `MsBackendMzR` on-disk
## backend.
sciex_file <- dir(system.file("sciex", package = "msdata"),
    full.names = TRUE)
sciex <- Spectra(sciex_file, backend = MsBackendMzR())
sciex

## The MS data is on disk and will be read into memory on-demand. We can
## however change the backend to a MsBackendMemory backend which will
## keep all of the data in memory.
sciex_im <- setBackend(sciex, MsBackendMemory())
sciex_im

## The `MsBackendMemory()` supports the `setBackend()` method:
supportsSetBackend(MsBackendMemory())

## Thus, it is possible to change to that backend with `setBackend()`. Most
## read-only backends however don't support that, such as the
```

```
## `MsBackendMzR` and `setBackend()` would fail to change to that backend.
supportsSetBackend(MsBackendMzR())

## The on-disk object `sciex` is light-weight, because it does not keep the
## MS peak data in memory. The `sciex_im` object in contrast keeps all the
## data in memory and its size is thus much larger.
object.size(sciex)
object.size(sciex_im)

## The spectra variable `dataStorage` returns for each spectrum the location
## where the data is stored. For in-memory objects:
head(dataStorage(sciex_im))

## While objects that use an on-disk backend will list the files where the
## data is stored.
head(dataStorage(sciex))

## The spectra variable `dataOrigin` returns for each spectrum the *origin*
## of the data. If the data is read from e.g. mzML files, this will be the
## original mzML file name:
head(dataOrigin(sciex))
head(dataOrigin(sciex_im))


## ---- ACCESSING AND ADDING DATA ----

## Get the MS level for each spectrum.
msLevel(data)

## Alternatively, we could also use $ to access a specific spectra variable.
## This could also be used to add additional spectra variables to the
## object (see further below).
data$msLevel

## Get the intensity and m/z values.
intensity(data)
mz(data)

## Determine whether one of the spectra has a specific m/z value
containsMz(data, mz = 120.4)

## Accessing spectra variables works for all backends:
intensity(sciex)
intensity(sciex_im)

## Get the m/z for the first spectrum.
mz(data)[[1]]

## Get the peak data (m/z and intensity values).
pks <- peaksData(data)
pks
pks[[1]]
pks[[2]]

## Note that we could get the same resulb by coercing the `Spectra` to
## a `list` or `SimpleList`:
as(data, "list")
```

```
as(data, "SimpleList")

## List all available spectra variables (i.e. spectrum data and metadata).
spectraVariables(data)

## For all *core* spectrum variables accessor functions are available. These
## return NA if the variable was not set.
centroided(data)
dataStorage(data)
rtime(data)
precursorMz(data)

## The core spectra variables are:
coreSpectraVariables()

## Add an additional metadata column.
data$spectrum_id <- c("sp_1", "sp_2")

## List spectra variables, "spectrum_id" is now also listed
spectraVariables(data)

## Get the values for the new spectra variable
data$spectrum_id

## Extract specific spectra variables.
spectraData(data, columns = c("spectrum_id", "msLevel"))

## Drop spectra variable data and/or columns.
res <- selectSpectraVariables(data, c("mz", "intensity"))

## This removed the additional columns "spectrum_id" and deleted all values
## for all spectra variables, except "mz" and "intensity".
spectraData(res)

## Compared to the data before selectSpectraVariables.
spectraData(data)


## ---- SUBSETTING, FILTERING AND COMBINING

## Subset to all MS2 spectra.
data[msLevel(data) == 2]

## Same with the filterMsLevel function
filterMsLevel(data, 2)

## Below we combine the `data` and `sciex_im` objects into a single one.
data_comb <- c(data, sciex_im)

## The combined Spectra contains a union of all spectra variables:
head(data_comb$spectrum_id)
head(data_comb$rtime)
head(data_comb$dataStorage)
head(data_comb$dataOrigin)

## Filter a Spectra for a target precursor m/z with a tolerance of 10ppm
spd$precursorMz <- c(323.4, 543.2302)
```

```
data_filt <- Spectra(spd)
filterPrecursorMzRange(data_filt, mz = 543.23 + ppm(c(-543.23, 543.23), 10))

## Filter a Spectra keeping only peaks matching certain m/z values
sps_sub <- filterMzValues(data, mz = c(103, 104), tolerance = 0.3)
mz(sps_sub)

## This function can also be used to remove specific peaks from a spectrum
## by setting `keep = FALSE`.
sps_sub <- filterMzValues(data, mz = c(103, 104),
    tolerance = 0.3, keep = FALSE)
mz(sps_sub)

## Note that `filterMzValues()` keeps or removes all peaks with a matching
## m/z given the provided `ppm` and `tolerance` parameters.

## Filter a Spectra keeping only peaks within a m/z range
sps_sub <- filterMzRange(data, mz = c(100, 300))
mz(sps_sub)

## Remove empty spectra variables
sciex_noNA <- dropNaSpectraVariables(sciex)

## Available spectra variables before and after `dropNaSpectraVariables()`
spectraVariables(sciex)
spectraVariables(sciex_noNA)


## Adding new spectra variables
sciex1 <- filterDataOrigin(sciex, dataOrigin(sciex)[1])
spv <- DataFrame(spectrumId = sciex1$spectrumId[3:12], ## used for merging
                 var1 = rnorm(10),
                 var2 = sample(letters, 10))
spv

sciex2 <- joinSpectraData(sciex1, spv, by.y = "spectrumId")

spectraVariables(sciex2)
spectraData(sciex2)[1:13, c("spectrumId", "var1", "var2")]

## Removing fourier transform artefacts seen in Orbitra data.

## Loading an Orbitrap spectrum with artefacts.
data(fft_spectrum)
plotSpectra(fft_spectrum, xlim = c(264.5, 265.5))
plotSpectra(fft_spectrum, xlim = c(264.5, 265.5), ylim = c(0, 5e6))

fft_spectrum <- filterFourierTransformArtefacts(fft_spectrum)
fft_spectrum
plotSpectra(fft_spectrum, xlim = c(264.5, 265.5), ylim = c(0, 5e6))

## Using a few examples peaks in your data you can optimize the parameters
fft_spectrum_filtered <- filterFourierTransformArtefacts(fft_spectrum,
                                             halfWindowSize = 0.2,
                                             threshold = 0.005,
                                             keepIsotopes = TRUE,
                                             maxCharge = 5,
```

```
                                              isotopeTolerance = 0.005
                                              )

fft_spectrum_filtered
length(mz(fft_spectrum_filtered)[[1]])
plotSpectra(fft_spectrum_filtered, xlim = c(264.5, 265.5), ylim = c(0, 5e6))

## Using filterRanges to filter spectra object based on variables available
## in `spectraData`.
## First, determine the variable(s) on which to base the filtering:
sv <- c("rtime", "precursorMz", "peaksCount")
## Note that ANY variables can be chosen here, and as many as wanted.

## Define the ranges (pairs of values with lower and upper boundary) to be
## used for the individual spectra variables. The first two values will be
## used for the first spectra variable (e.g., rtime here), the next two for
## the second (e.g. precursorMz here) and so on:
ranges <- c(30, 350, 200,500, 350, 600)

## Input the parameters within the filterRanges function:
filt_spectra <- filterRanges(sciex, spectraVariables = sv,
                ranges = ranges)

## Using `filterRanges()` to filter spectra object with multiple ranges for
## the same `spectraVariable` (e.g, here rtime)
sv <- c("rtime", "rtime")
ranges <- c(30, 100, 200, 300)
filt_spectra <- filterRanges(sciex, spectraVariables = sv,
                ranges = ranges, match = "any")

## Using filterValues in a similar way to a filter spectra object based on
## variables available in `spectraData`. However, this time not based on
## ranges but similarities to user input single values with given
## tolerance/ppm
## First determine the variable(s) on which to base the filtering:
sv <- c("rtime", "precursorMz")
## Note that ANY variables can be chosen here, and as many as wanted.

## Define the values that will be used to filter the spectra based on their
## similarities to their respective spectraVariables.
## The first values in the parameters values, tolerance and ppm will be
## used for the first spectra variable (e.g. rtime here), the next for the
## second (e.g. precursorMz here) and so on:
values <- c(350, 400)
tolerance <- c(100, 0)
ppm <- c(0,50)

## Input the parameters within the `filterValues()` function:
filt_spectra <- filterValues(sciex, spectraVariables = sv,
                values = values, tolerance = tolerance, ppm = ppm)

## ---- DATA MANIPULATIONS AND OTHER OPERATIONS ----

## Set the data to be centroided
centroided(data) <- TRUE

## Replace peak intensities below 40 with 3.
```

```
res <- replaceIntensitiesBelow(data, threshold = 40, value = 3)
res

## Get the intensities of the first and second spectrum.
intensity(res)[[1]]
intensity(res)[[2]]

## Remove all peaks with an intensity below 40.
res <- filterIntensity(res, intensity = c(40, Inf))

## Get the intensities of the first and second spectrum.
intensity(res)[[1]]
intensity(res)[[2]]

## Lengths of spectra is now different
lengths(mz(res))
lengths(mz(data))

## In addition it is possible to pass a function to `filterIntensity()`: in
## the example below we want to keep only peaks that have an intensity which
## is larger than one third of the maximal peak intensity in that spectrum.
keep_peaks <- function(x, prop = 3) {
    x > max(x, na.rm = TRUE) / prop
}
res2 <- filterIntensity(data, intensity = keep_peaks)
intensity(res2)[[1L]]
intensity(data)[[1L]]

## We can also change the proportion by simply passing the `prop` parameter
## to the function. To keep only peaks that have an intensity which is
## larger than half of the maximum intensity:
res2 <- filterIntensity(data, intensity = keep_peaks, prop = 2)
intensity(res2)[[1L]]
intensity(data)[[1L]]

## Since data manipulation operations are by default not directly applied to
## the data but only added to the internal lazy evaluation queue, it is also
## possible to remove these data manipulations with the `reset()` function:
res_rest <- reset(res)
res_rest
lengths(mz(res_rest))
lengths(mz(res))
lengths(mz(data))

## `reset()` after a `applyProcessing()` can not restore the data, because
## the data in the backend was changed. Similarly, `reset()` after any
## filter operations can not restore data for a `Spectra` with a
## `MsBackendMemory` or `MsBackendDataFrame`.
res_2 <- applyProcessing(res)
res_rest <- reset(res_2)
lengths(mz(res))
lengths(mz(res_rest))


## Compare spectra: comparing spectra 2 and 3 against spectra 10:20 using
## the normalized dotproduct method.
res <- compareSpectra(sciex_im[2:3], sciex_im[10:20])
```

```
## first row contains comparisons of spectrum 2 with spectra 10 to 20 and
## the second row comparisons of spectrum 3 with spectra 10 to 20
res

## To use a simple Pearson correlation instead we can define a function
## that takes the two peak matrices and calculates the correlation for
## their second columns (containing the intensity values).
correlateSpectra <- function(x, y, use = "pairwise.complete.obs", ...) {
    cor(x[, 2], y[, 2], use = use)
}
res <- compareSpectra(sciex_im[2:3], sciex_im[10:20],
    FUN = correlateSpectra)
res

## Use compareSpectra to determine the number of common (matching) peaks
## with a ppm of 10:
## type = "inner" uses a *inner join* to match peaks, i.e. keeps only
## peaks that can be mapped betwen both spectra. The provided FUN returns
## simply the number of matching peaks.
compareSpectra(sciex_im[2:3], sciex_im[10:20], ppm = 10, type = "inner",
    FUN = function(x, y, ...) nrow(x))

## Apply an arbitrary function to each spectrum in a Spectra.
## In the example below we calculate the mean intensity for each spectrum
## in a subset of the sciex_im data. Note that we can access all variables
## of each individual spectrum either with the `$` operator or the
## corresponding method.
res <- spectrapply(sciex_im[1:20], FUN = function(x) mean(x$intensity[[1]]))
head(res)

## It is however important to note that dedicated methods to access the
## data (such as `intensity`) are much more efficient than using `lapply()`:
res <- lapply(intensity(sciex_im[1:20]), mean)
head(res)

## As an alternative, applying a function `FUN` to a `Spectra` can be
## performed *chunk-wise*. The advantage of this is, that only the data for
## one chunk at a time needs to be loaded into memory reducing the memory
## demand. This type of processing can be performed by specifying the size
## of the chunks (i.e. number of spectra per chunk) with the `chunkSize`
## parameter
spectrapply(sciex_im[1:20], lengths, chunkSize = 5L)

## ---- DATA EXPORT ----

## Some `MsBackend` classes provide an `export()` method to export the data
## to the file format supported by the backend.
## The `MsBackendMzR` for example allows to export MS data to mzML or
## mzXML file(s), the `MsBackendMgf` (defined in the MsBackendMgf R package)
## would allow to export the data in mgf file format.
## Below we export the MS data in `data`. We call the `export()` method on
## this object, specify the backend that should be used to export the data
## (and which also defines the output format) and provide a file name.
fl <- tempfile()
export(data, MsBackendMzR(), file = fl)

## This exported our data in mzML format. Below we read the first 6 lines
```

```
## from that file.
readLines(fl, n = 6)

## If only a single file name is provided, all spectra are exported to that
## file. To export data with the `MsBackendMzR` backend to different files, a
## file name for each individual spectrum has to be provided.
## Below we export each spectrum to its own file.
fls <- c(tempfile(), tempfile())
export(data, MsBackendMzR(), file = fls)

## Reading the data from the first file
res <- Spectra(backendInitialize(MsBackendMzR(), fls[1]))

mz(res)
mz(data)

## ---- PEAKS VARIABLES AND DATA ----

## Some `MsBackend` classes provide support for arbitrary peaks variables
## (in addition to the mandatory `"mz"` and `"intensity"` values. Below
## we create a simple data frame with an additional peak variable `"pk_ann"`
## and create a `Spectra` with a `MsBackendMemory` for that data.
## Importantly the number of values (per spectrum) need to be the same
## for all peak variables.

tmp <- data.frame(msLevel = c(2L, 2L), rtime = c(123.2, 123.5))
tmp$mz <- list(c(103.1, 110.4, 303.1), c(343.2, 453.1))
tmp$intensity <- list(c(130.1, 543.1, 40), c(0.9, 0.45))
tmp$pk_ann <- list(c(NA_character_, "A", "P"), c("B", "P"))

## Create the Spectra. With parameter `peaksVariables` we can define
## the columns in `tmp` that contain peaks variables.
sps <- Spectra(tmp, source = MsBackendMemory(),
    peaksVariables = c("mz", "intensity", "pk_ann"))
peaksVariables(sps)

## Extract just the m/z and intensity values
peaksData(sps)[[1L]]

## Extract the full peaks data
peaksData(sps, columns = peaksVariables(sps))[[1L]]

## Access just the pk_ann variable
sps$pk_ann

## Convert a subset of the Spectra object to a long DataFrame.
asDataFrame(sciex, i = 1:3, spectraVars = c("rtime", "msLevel"))
```

---

chunkapply   *Apply a function stepwise to chunks of data*

Description

chunkapply() splits x into chunks and applies the function FUN stepwise to each of these chunks.
Depending on the object it is called, this function might reduce memory demand considerably, if

for example only the full data for a single chunk needs to be loaded into memory at a time (e.g., for Spectra objects with on-disk or similar backends).

Usage

```
chunkapply(x, FUN, ..., chunkSize = 1000L, chunks = factor())
```

Arguments

x	object to which FUN should be applied. Can be any object that supports split.
FUN	the function to apply to x.
...	additional parameters to FUN.
chunkSize	integer(1) defining the size of each chunk into which x should be splitted.
chunks	optional factor or length equal to length(x) defining the chunks into which x should be splitted.

Value

Depending on FUN, but in most cases a vector/result object of length equal to length(x).

Author(s)

Johannes Rainer

Examples

```
## Apply a function (`sqrt`) to each element in `x`, processed in chunks of
## size 200.
x <- rnorm(n = 1000, mean = 500)
res <- chunkapply(x, sqrt, chunkSize = 200)
length(res)
head(res)

## For such a calculation the vectorized `sqrt` would however be recommended
system.time(sqrt(x))
system.time(chunkapply(x, sqrt, chunkSize = 200))

## Simple example splitting a numeric vector into chunks of 200 and
## aggregating the values within the chunk using the `mean`. Due to the
## `unsplit` the result has the same length than the input with the mean
## value repeated.
x <- 1:1000
res <- chunkapply(x, mean, chunkSize = 200)
length(res)
head(res)
```

combinePeaksData	*Combine peaks with similar m/z across spectra*

Description

combinePeaksData() aggregates provided peak matrices into a single peak matrix. Peaks are grouped by their m/z values with the group() function from the MsCoreUtils package. In brief, all peaks in all provided spectra are first ordered by their m/z and consecutively grouped into one group if the (pairwise) difference between them is smaller than specified with parameter tolerance and ppm (see [group()](#) for grouping details and examples).

The m/z and intensity values for the resulting peak matrix are calculated using the mzFun and intensityFun on the grouped m/z and intensity values.

Note that only the grouped m/z and intensity values are used in the aggregation functions (mzFun and intensityFun) but not the number of spectra.

The function supports also different strategies for peak combinations which can be specified with the peaks parameter:

- peaks = "union" (default): report all peaks from all input spectra.
- peaks = "intersect": keep only peaks in the resulting peak matrix that are present in >= minProp proportion of input spectra. This would generate a *consensus* or *representative* spectra from a set of e.g. fragment spectra measured from the same precursor ion.

As a special case it is possible to report only peaks in the resulting matrix from peak groups that contain a peak from one of the input spectra, which can be specified with parameter main. Thus, if e.g. main = 2 is specified, only (grouped) peaks that have a peak in the second input matrix are returned.

Setting timeDomain to TRUE causes grouping to be performed on the square root of the m/z values (assuming a TOF instrument was used to create the data).

Usage

```
combinePeaksData(
  x,
  intensityFun = base::mean,
  mzFun = base::mean,
  weighted = FALSE,
  tolerance = 0,
  ppm = 0,
  timeDomain = FALSE,
  peaks = c("union", "intersect"),
  main = integer(),
  minProp = 0.5,
  ...
)
```

Arguments

x	list of peak matrices.
intensityFun	function to be used to combine intensity values for matching peaks. By default the mean intensity value is returned.

mzFun	`function` to be used to combine m/z values for matching peaks. By default the mean m/z value is returned.
weighted	`logical(1)` defining whether m/z values for matching peaks should be calculated by an intensity-weighted average of the individuak m/z values. This overrides parameter `mzFun`.
tolerance	`numeric(1)` defining the (absolute) maximal accepted difference between mass peaks to group them into the same final peak.
ppm	`numeric(1)` defining the m/z-relative maximal accepted difference between mass peaks (expressed in parts-per-million) to group them into the same final peak.
timeDomain	`logical(1)` whether grouping of mass peaks is performed on the m/z values (`timeDomain = FALSE`) or on `sqrt(mz)` (`timeDomain = TRUE`).
peaks	`character(1)` specifying how peaks should be combined. Can be either `"peaks = "union"` (default) or `peaks = "intersect"`. See function description for details.
main	optional `integer(1)` to force the resulting peak list to contain only peaks that are present in the specified input spectrum. See description for details.
minProp	`numeric(1)` for 'peaks = "intersect"`: the minimal required proportion of input spectra (peak matrices) a mass peak has to be present to be included in the consensus peak matrix.
...	additional parameters to the `mzFun` and `intensityFun` functions.

Details

For general merging of spectra, the `tolerance` and/or `ppm` should be manually specified based on the precision of the MS instrument. Peaks from spectra with a difference in their m/z being smaller than `tolerance` or smaller than `ppm` of their m/z are grouped into the same final peak.

Some details for the combination of consecutive spectra of an LC-MS run:

The m/z values of the same ion in consecutive scans (spectra) of a LC-MS run will not be identical. Assuming that this random variation is much smaller than the resolution of the MS instrument (i.e. the difference between m/z values within each single spectrum), m/z value groups are defined across the spectra and those containing m/z values of the `main` spectrum are retained. Intensities and m/z values falling within each of these m/z groups are aggregated using the `intensityFun` and `mzFun`, respectively. It is highly likely that all QTOF profile data is collected with a timing circuit that collects data points with regular intervals of time that are then later converted into m/z values based on the relationship `t = k * sqrt(m/z)`. The m/z scale is thus non-linear and the m/z scattering (which is in fact caused by small variations in the time circuit) will thus be different in the lower and upper m/z scale. m/z-intensity pairs from consecutive scans to be combined are therefore defined by default on the square root of the m/z values. With `timeDomain = FALSE`, the actual m/z values will be used.

Value

Peaks `matrix` with m/z and intensity values representing the aggregated values across the provided peak matrices.

Author(s)

Johannes Rainer

Examples

```
set.seed(123)
mzs <- seq(1, 20, 0.1)
ints1 <- abs(rnorm(length(mzs), 10))
ints1[11:20] <- c(15, 30, 90, 200, 500, 300, 100, 70, 40, 20) # add peak
ints2 <- abs(rnorm(length(mzs), 10))
ints2[11:20] <- c(15, 30, 60, 120, 300, 200, 90, 60, 30, 23)
ints3 <- abs(rnorm(length(mzs), 10))
ints3[11:20] <- c(13, 20, 50, 100, 200, 100, 80, 40, 30, 20)

## Create the peaks matrices
p1 <- cbind(mz = mzs + rnorm(length(mzs), sd = 0.01),
    intensity = ints1)
p2 <- cbind(mz = mzs + rnorm(length(mzs), sd = 0.01),
    intensity = ints2)
p3 <- cbind(mz = mzs + rnorm(length(mzs), sd = 0.009),
    intensity = ints3)

## Combine the spectra. With `tolerance = 0` and `ppm = 0` only peaks with
## **identical** m/z are combined. The result will be a single spectrum
## containing the *union* of mass peaks from the individual input spectra.
p <- combinePeaksData(list(p1, p2, p3))

## Plot the spectra before and after combining
par(mfrow = c(2, 1), mar = c(4.3, 4, 1, 1))
plot(p1[, 1], p1[, 2], xlim = range(mzs[5:25]), type = "h", col = "red")
points(p2[, 1], p2[, 2], type = "h", col = "green")
points(p3[, 1], p3[, 2], type = "h", col = "blue")

plot(p[, 1], p[, 2], xlim = range(mzs[5:25]), type = "h",
    col = "black")
## The peaks were not merged, because their m/z differs too much.

## Combine spectra with `tolerance = 0.05`. This will merge all triplets.
p <- combinePeaksData(list(p1, p2, p3), tolerance = 0.05)

## Plot the spectra before and after combining
par(mfrow = c(2, 1), mar = c(4.3, 4, 1, 1))
plot(p1[, 1], p1[, 2], xlim = range(mzs[5:25]), type = "h", col = "red")
points(p2[, 1], p2[, 2], type = "h", col = "green")
points(p3[, 1], p3[, 2], type = "h", col = "blue")

plot(p[, 1], p[, 2], xlim = range(mzs[5:25]), type = "h",
    col = "black")

## With `intensityFun = max` the maximal intensity per peak is reported.
p <- combinePeaksData(list(p1, p2, p3), tolerance = 0.05,
    intensityFun = max)

## Create *consensus*/representative spectrum from a set of spectra

p1 <- cbind(mz = c(12, 45, 64, 70), intensity = c(10, 20, 30, 40))
p2 <- cbind(mz = c(17, 45.1, 63.9, 70.2), intensity = c(11, 21, 31, 41))
p3 <- cbind(mz = c(12.1, 44.9, 63), intensity = c(12, 22, 32))

## No mass peaks identical thus consensus peaks are empty
```

```
combinePeaksData(list(p1, p2, p3), peaks = "intersect")

## Reducing the minProp to 0.2. The consensus spectrum will contain all
## peaks
combinePeaksData(list(p1, p2, p3), peaks = "intersect", minProp = 0.2)

## With a tolerance of 0.1 mass peaks can be matched across spectra
combinePeaksData(list(p1, p2, p3), peaks = "intersect", tolerance = 0.1)

## Report the minimal m/z and intensity
combinePeaksData(list(p1, p2, p3), peaks = "intersect", tolerance = 0.1,
    intensityFun = min, mzFun = min)
```

---

countIdentifications   *Count the number of identifications per scan*

Description

The function takes a Spectra object containing identification results as input. It then counts the number of identifications each scan (or their descendants) has lead to - this is either 0 or 1 for MS2 scans, or, for MS1 scans, the number of MS2 scans originating from any MS1 peak that lead to an identification.

This function can be used to generate id-annotated total ion chromatograms, as can illustrated here.

Usage

```
countIdentifications(
  object,
  identification = "sequence",
  f = dataStorage(object),
  BPPARAM = bpparam()
)
```

Arguments

object	An instance of class Spectra that contains identification data, as defined by the sequence argument.
identification	character(1) with the name of the spectra variable that defines whether a scan lead to an identification (typically containing the idenfified peptides sequence in proteomics). The absence of identification is encode by an NA. Default is "sequence".
f	A factor defining how to split object for parallelized processing. Default is dataOrigin(x), i.e. each raw data files is processed in parallel.
BPPARAM	Parallel setup configuration. See BiocParallel::bpparam() for details.

Details

The computed number of identifications is stored in a new spectra variables named "countIdentifications". If it already exists, the function throws a message and returns the object unchanged. To force the recomputation of the "countIdentifications" variable, users should either delete or rename it.

Value

An updated Spectra() object that now contains an integer spectra variable `countIdentifications`
with the number of identification for each scan.

Author(s)

Laurent Gatto

Examples

```
spdf <- new("DFrame", rownames = NULL, nrows = 86L,
   listData = list(
       msLevel = c(1L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L,
                   2L, 2L, 2L, 2L, 2L, 2L, 2L, 1L, 2L, 2L, 2L, 2L,
                   2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L,
                   2L, 1L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L,
                   2L, 2L, 2L, 1L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L,
                   2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 1L, 2L,
                   2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L,
                   2L, 2L),
       acquisitionNum = 8975:9060,
       precScanNum = c(NA, 8956L, 8956L, 8956L, 8956L, 8956L, 8956L,
                       8956L, 8956L, 8956L, 8956L, 8956L, 8956L,
                       8956L, 8956L, 8956L, 8956L, 8956L, 8956L, NA,
                       8975L, 8975L, 8975L, 8975L, 8975L, 8975L,
                       8975L, 8975L, 8975L, 8975L, 8975L, 8975L,
                       8975L, 8975L, 8975L, 8975L, 8975L, NA, 8994L,
                       8994L, 8994L, 8994L, 8994L, 8994L, 8994L,
                       8994L, 8994L, 8994L, 8994L, 8994L, 8994L, NA,
                       9012L, 9012L, 9012L, 9012L, 9012L, 9012L,
                       9012L, 9012L, 9012L, 9012L, 9012L, 9012L,
                       9012L, 9012L, 9012L, 9012L, 9012L, 9012L, NA,
                       9026L, 9026L, 9026L, 9026L, 9026L, 9026L,
                       9026L, 9026L, 9026L, 9026L, 9026L, 9026L,
                       9026L, 9026L, 9026L),
       sequence = c(NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA,
                    NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA,
                    "LSEHATAPTR", NA, NA, NA, NA, NA, NA, NA,
                    "EGSDATGDGTK", NA, NA, "NEDEDSPNK", NA, NA, NA,
                    NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA,
                    NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA,
                    NA, NA, NA, NA, NA, NA, NA, NA, NA, "GLTLAQGGVK",
                    NA, NA, NA, NA, "STLPDADRER", NA, NA, NA, NA, NA,
                    NA, NA, NA)),
   elementType = "ANY", elementMetadata = NULL, metadata = list())

sp <- Spectra(spdf)

## We have in this data 5 MS1 and 81 MS2 scans
table(msLevel(sp))

## The acquisition number of the MS1 scans
acquisitionNum(filterMsLevel(sp, 1))

## And the number of MS2 scans with precursor ions selected
## from MS1 scans (those in the data and others)
```

```
table(precScanNum(sp))

## Count number of sequences/identifications per scan
sp <- countIdentifications(sp)

## MS2 scans either lead to an identification (5 instances) or none
## (76). Among the five MS1 scans in the experiment, 3 lead to MS2
## scans being matched to no peptides and two MS1 scans produced two
## and three PSMs respectively.
table(sp$countIdentifications, sp$msLevel)
```

---

estimatePrecursorIntensity,Spectra-method
Estimate Precursor Intensities

Description

Some MS instrument manufacturers don't provide precursor intensities for fragment spectra. These can however be estimated, given that also MS1 spectra are available. The `estimatePrecursorIntensity()` funtion defines the precursor intensities for MS2 spectra using the intensity of the matching MS1 peak from the closest MS1 spectrum (i.e. the last MS1 spectrum measured before the respective MS2 spectrum). With `method = "interpolation"` it is also possible to calculate the precursor intensity based on an interpolation of intensity values (and retention times) of the matching MS1 peaks from the previous and next MS1 spectrum. See below for an example.

Usage

```
## S4 method for signature 'Spectra'
estimatePrecursorIntensity(
  object,
  ppm = 20,
  tolerance = 0,
  method = c("previous", "interpolation"),
  msLevel. = 2L,
  f = dataOrigin(object),
  BPPARAM = bpparam()
)
```

Arguments

object	Spectra with MS1 and MS2 spectra.
ppm	numeric(1) with the maximal allowed relative difference of m/z values between the precursor m/z of a spectrum and the m/z of the respective ion on the MS1 scan.
tolerance	numeric(1) with the maximal allowed difference of m/z values between the precursor m/z of a spectrum and the m/z of the respective ion on the MS1 scan.
method	character(1) defining whether the precursor intensity should be estimated on the previous MS1 spectrum (method = "previous", the default) or based on an interpolation on the previous and next MS1 spectrum (method = "interpolation").
msLevel.	integer(1) the MS level for which precursor intensities should be estimated. Defaults to 2L.

f   factor (or vector to be coerced to factor) defining which spectra belong to the
                           same original data file (sample). Defaults to f = dataOrigin(x).

BPPARAM   Parallel setup configuration. See bpparam() for more information. This is
                           passed directly to the backendInitialize() method of the MsBackend.

Author(s)

Johannes Rainer with feedback and suggestions from Corey Broeckling

Examples

```
#' ## Calculating the precursor intensity for MS2 spectra:
##
## Some MS instrument manufacturer don't report the precursor intensities
## for MS2 spectra. The `estimatePrecursorIntensity` function can be used
## in these cases to calculate the precursor intensity on MS1 data. Below
## we load an mzML file from a vendor providing precursor intensities and
## compare the estimated and reported precursor intensities.
tmt <- Spectra(msdata::proteomics(full.names = TRUE)[5],
    backend = MsBackendMzR())
pmi <- estimatePrecursorIntensity(tmt)
plot(pmi, precursorIntensity(tmt))

## We can also replace the original precursor intensity values with the
## newly calculated ones
tmt$precursorIntensity <- pmi
```

---

estimatePrecursorMz   *Estimating precursor m/z valus for DDA data*

Description

MS data from Waters instruments are calibrated through the *Lock Mass*, but, while all m/z values
of mass peaks in each spectrum will be calibrated by this method, the reported precursor m/z might
not. The precursor m/z in the converted mzML file will have m/z values from quadrupole isolation
windows instead of accurate m/z values. See also the GNPS documentation for more information.

The estimatePrecursorMz() function estimates/adjusts the reported precursor m/z of a fragment
spectrum using the following approach: in data dependent acquisition (DDA) mode, the MS instru-
ment will select ions with the highest intensities in one MS scan for fragmentation. Thus, for each
fragment spectrum, this method identifies in the previous MS1 spectrum the peak with the highest
intensity and an m/z value similar to the fragment spectrum's reported precursor m/z (given param-
eters tolerance and ppm). This m/z value is then reported. Since the fragment spectrum's potential
MS1 mass peak is selected based on its intensity, this method should **only be used for DDA data**.

Usage

```
estimatePrecursorMz(object, tolerance = 0.3, ppm = 10, BPPARAM = SerialParam())
```

Arguments

object	Spectra() object with **DDA** data.
tolerance	numeric(1) defining an absolute acceptable difference in m/z between the fragment spectra's reported precursor m/z and the MS1 peaks considered as the precursor peak. All MS1 peaks from the previous MS1 scan with an m/z between the fragment spectrum's precursorMz +/- (tolerance + ppm(precursorMz, ppm)) are considered.
ppm	numeric(1) defining the m/z dependent acceptable difference in m/z. See documentation of parameter tolerance for more information.
BPPARAM	parallel processing setup. Defaults to BPPARAM = SerialParam(). See SerialParam() for more information.

Value

numeric of length equal to the number of spectra in object with the fragment spectra's estimated precursor m/z values. For MS1 spectra NA_real_ values are returned. The original precursor m/z is reported for MS2 spectra for which no matching MS1 peak was found.

Note

This approach is applicable only when fragment spectra are obtained through data-dependent acquisition (DDA), as it assumes that the peak with the highest intensity within the given isolation m/z window (from the previous MS1 spectrum) corresponds to the precursor ion.

The spectra in object have to be ordered by their retention time.

Users of this function should evaluate and compare the estimated precursor m/z values with the originally reported one and only consider adjusted values they feel comfortable with.

Author(s)

Mar Garcia-Aloy, Johannes Rainer

Examples

```
## Load a DDA test data set. For the present data set no large differences
## between the reported and the *actual* precursor m/z are expected.
fl <- system.file("TripleTOF-SWATH", "PestMix1_DDA.mzML", package = "msdata")
s <- Spectra(fl)

pmz <- estimatePrecursorMz(s)

## plot the reported and estimated precursor m/z values against each other
plot(precursorMz(s), pmz)
abline(0, 1)

## They seem highly similar, but are they identical?
identical(precursorMz(s), pmz)
all.equal(precursorMz(s), pmz)

## Plot also the difference of m/z values against the m/z value
plot(precursorMz(s), precursorMz(s) - pmz, xlab = "precursor m/z",
    ylab = "difference reported - estimated precursor m/z")

## we could then replace the reported precursor m/z values
s$precursorMz <- pmz
```

filterFourierTransformArtefacts

Fast fourier transform artefact filter

Description

The `filterFourierTransformArtefacts()` function removes (Orbitrap) fast fourier artefact peaks from spectra. Such artefacts (also referred to as *ripples*) seem to be related to the *ringing* phenomenon and are frequently seen in Orbitrap data as small random mass peaks ~ 0.01 Da from a main peak with a very large intensity. See also here for more details and information. The data set `fft_spectrum` represents a `Spectra()` object with a single Orbitrap spectrum with such artefacts (see examples below).

See also `Spectra()` (section *Data subsetting, filtering and merging) for the definition of the function.

Details

The current implementation iterates through all intensity ordered peaks in a spectrum and removes all peaks with an m/z within +/- `halfWindowSize` of the current peak if their intensity is lower than `threshold` times the current peak's intensity. Additional parameters `keepIsotopes`, `maxCharge` and `isotopeTolerance` allow to avoid removing of potential `[13]C` isotope peaks (`maxCharge` being the maximum charge that should be considered and `isotopeTolerance` the absolute acceptable tolerance for matching their m/z).

Author(s)

Jan Stanstrup, Johannes Rainer

Examples

```
library(Spectra)
data(fft_spectrum)

plotSpectra(fft_spectrum)

## Focus on an artefact
plotSpectra(fft_spectrum, xlim = c(264.5, 265.5))
plotSpectra(fft_spectrum, xlim = c(264.5, 265.5), ylim = c(0, 5e6))

fft_spectrum <- filterFourierTransformArtefacts(fft_spectrum)
fft_spectrum
plotSpectra(fft_spectrum, xlim = c(264.5, 265.5), ylim = c(0, 5e6))

## R code to download/extract the data.

## Not run:
library(Spectra)
# get orbitrap data
download.file("https://ftp.ebi.ac.uk/pub/databases/metabolights/studies/public/MTBLS469/AV_01_v2_male_arm1_
data <- Spectra("AV_01_v2_male_arm1_juice.mzXML")
extracted_spectrum <- data[195]

## End(Not run)
```

---

filterPeaksRanges   *Filter peaks based on spectra and peaks variable ranges*

Description

The filterPeaksRanges() function allows to filter the peaks matrices of a [Spectra](#) object using any set of range-based filters on numeric spectra variables or peaks variables. These ranges can be passed to the function using the ... as <variable name> = <range> pairs. <variable name> has to be an available spectra or peaks variable. <range> can be a numeric of length 2 defining the lower and upper boundary, or a numeric two-column matrix (multi-row matrices are also supported, see further below). filterPeaksRanges(s, mz = c(200, 300)) would for example reduce the peaks matrices of the Spectra object s to mass peaks with an m/z value between 200 and 300. filterPeaksRanges() returns the original Spectra object with the filter operation added to the processing queue. Thus, the filter gets **only** applied when the peaks data gets extracted with mz(), intensity() or peaksData(). If ranges for both spectra **and** peaks variables are defined, the function evaluates first whether the spectra variable value for a spectrum is within the provided range and, if so, applies also the peaks variable-based filter (otherwise an empty peaks matrix is returned).

If more than one spectra variable and/or peaks variable are defined, their filter results are combined with a logical AND: a peak matrix is only returned for a spectrum if all values of spectra variables are within the provided (respective) ranges for spectra variables, and this matrix is further filtered to contain only those peaks which values are within the provided peaks variable ranges.

Filtering with multiple ranges per spectra and peaks variables is also supported: ranges can also be provided as multi-row numeric (two-column) matrices. In this case, the above described procedure is applied for each row separately and their results are combined with a logical OR, i.e. peaks matrices are returned that match any of the conditions/filters of a row. The number of rows of the provided ranges (being it for spectra or peaks variables) have to match.

Missing value handling: any comparison which involves a missing value (being it a spectra variable value, a peaks variable value or a value in one of the provided ranges) is treated as a logical FALSE. For example, if the retention time of a spectrum is NA and the data is filtered using a retention time range, an empty peaks matrix is returned (for keep = TRUE, for keep = FALSE the full peaks matrix is returned).

Usage

```
filterPeaksRanges(object, ..., keep = TRUE)
```

Arguments

object   A [Spectra](#) object.

...   the ranges for the spectra and/or peaks variables. Has to be provided as <name> = <range> pairs with <name> being the name of a spectra or peaks variable (of numeric data type) and <range> being either a numeric of length 2 or a numeric two column matrix (see function desription above for details),

keep   logical(1) whether to keep (default) or remove peaks that match the provided range(s).

Note

In contrast to some other *filter* functions, this function does not provide a `msLevel` parameter that allows to define the MS level of spectra on which the filter should be applied. The filter(s) will always be applied to **all** spectra (irrespectively of their MS level). Through combination of multiple filter ranges it is however possible to apply MS level-dependent filters (see examples below for details).

The filter will not be applied immediately to the data but only executed when the mass peak data is accessed (through `peaksData()`, `mz()` or `intensity()`) or by calling `applyProcessing()`.

Author(s)

Johannes Rainer

Examples

```
## Define a test Spectra
d <- data.frame(rtime = c(123.2, 134.2), msLevel = c(1L, 2L))
d$mz <- list(c(100.1, 100.2, 100.3, 200.1, 200.2, 300.3),
    c(100.3, 100.4, 200.2, 400.3, 400.4))
## Use the index of the mass peak within the spectrum as index for
## better illustration of filtering results
d$intensity <- list(c(1:6), 1:5)
s <- Spectra(d)
s

## Filter peaks removing all mass peaks with an m/z between 200 and 300
res <- filterPeaksRanges(s, mz = c(200, 300), keep = FALSE)
res

## The Spectra object has still the same length and spectra variables
length(res)
res$rtime

## The filter gets applied when mass peak data gets extracted, using either
## `mz()`, `intensity()` or `peaksData()`. The filtered peaks data does
## not contain any mass peaks with m/z values between 200 and 300:
peaksData(res)[[1L]]
peaksData(res)[[2L]]

## We next combine spectra and filter variables. We want to keep only mass
## peaks of MS2 spectra that have an m/z between 100 and 110.
res <- filterPeaksRanges(s, mz = c(100, 110), msLevel = c(2, 2))
res
length(res)

## Only data for peaks are returned for which the spectra's MS level is
## between 2 and 2 and with an m/z between 100 and 110. The peaks data for
## the first spectrum, that has MS level 1, is thus empty:
peaksData(res)[[1L]]

## While the peaks matrix for the second spectrum (with MS level 2) contains
## the mass peaks with m/z between 100 and 110.
peaksData(res)[[2L]]

## To keep also the peaks data for the first spectrum, we need to define
```

```
## an additional set of ranges, which we define using a second row in each
## ranges matrix. We use the same filter as above, i.e. keeping only mass
## peaks with an m/z between 100 and 110 for spectra with MS level 2, but
## add an additional row for MS level 1 spectra keeping mass peaks with an
## m/z between 0 and 2000. Filter results of different rows are combined
## using a logical OR, i.e. peaks matrices with mass peaks are returned
## matching either the first, or the second row.
res <- filterPeaksRanges(s, mz = rbind(c(100, 110), c(0, 1000)),
    msLevel = rbind(c(2, 2), c(1, 1)))

## The results for the MS level 2 spectrum are the same as before, but with
## the additional row we keep the full peaks matrix of the MS1 spectrum:
peaksData(res)[[1L]]
peaksData(res)[[2L]]

## As a last example we define a filter that keeps all mass peaks with an
## m/z either between 100 and 200, or between 300 and 400.
res <- filterPeaksRanges(s, mz = rbind(c(100, 200), c(300, 400)))
peaksData(res)[[1L]]
peaksData(res)[[2L]]

## Such filters could thus be defined to restrict/filter the MS data to
## specific e.g. retention time and m/z ranges.
```

---

hidden_aliases   *Internal page for hidden aliases*

Description

For S4 methods that require a documentation entry but only clutter the index.

Usage

```
## S4 method for signature 'numeric'
bin(
  x,
  y,
  size = 1,
  breaks = seq(floor(min(y)), ceiling(max(y)), by = size),
  FUN = max,
  returnMids = TRUE,
  .check = TRUE
)

containsMz(object, ...)

containsNeutralLoss(object, ...)

dropNaSpectraVariables(object, ...)

entropy(object, ...)

export(object, ...)
```

```
pickPeaks(object, ...)

replaceIntensitiesBelow(object, threshold = min, ...)

reset(object, ...)

selectSpectraVariables(object, ...)

## S4 method for signature 'MsBackendDataFrame'
show(object)

## S4 method for signature 'MsBackendDataFrame'
backendMerge(object, ...)

## S4 method for signature 'MsBackendDataFrame'
acquisitionNum(object)

## S4 method for signature 'MsBackendDataFrame'
peaksData(object, columns = c("mz", "intensity"))

## S4 method for signature 'MsBackendDataFrame'
centroided(object)

## S4 replacement method for signature 'MsBackendDataFrame'
centroided(object) <- value

## S4 method for signature 'MsBackendDataFrame'
collisionEnergy(object)

## S4 replacement method for signature 'MsBackendDataFrame'
collisionEnergy(object) <- value

## S4 method for signature 'MsBackendDataFrame'
dataOrigin(object)

## S4 replacement method for signature 'MsBackendDataFrame'
dataOrigin(object) <- value

## S4 method for signature 'MsBackendDataFrame'
dataStorage(object)

## S4 replacement method for signature 'MsBackendDataFrame'
dataStorage(object) <- value

## S4 method for signature 'MsBackendDataFrame'
intensity(object)

## S4 replacement method for signature 'MsBackendDataFrame'
intensity(object) <- value

## S4 method for signature 'MsBackendDataFrame'
```

```
isEmpty(x)

## S4 method for signature 'MsBackendDataFrame'
isolationWindowLowerMz(object)

## S4 replacement method for signature 'MsBackendDataFrame'
isolationWindowLowerMz(object) <- value

## S4 method for signature 'MsBackendDataFrame'
isolationWindowTargetMz(object)

## S4 replacement method for signature 'MsBackendDataFrame'
isolationWindowTargetMz(object) <- value

## S4 method for signature 'MsBackendDataFrame'
isolationWindowUpperMz(object)

## S4 replacement method for signature 'MsBackendDataFrame'
isolationWindowUpperMz(object) <- value

## S4 method for signature 'MsBackendDataFrame'
length(x)

## S4 method for signature 'MsBackendDataFrame'
lengths(x, use.names = FALSE)

## S4 method for signature 'MsBackendDataFrame'
msLevel(object, ...)

## S4 replacement method for signature 'MsBackendDataFrame'
msLevel(object) <- value

## S4 method for signature 'MsBackendDataFrame'
mz(object)

## S4 replacement method for signature 'MsBackendDataFrame'
mz(object) <- value

## S4 method for signature 'MsBackendDataFrame'
polarity(object)

## S4 replacement method for signature 'MsBackendDataFrame'
polarity(object) <- value

## S4 method for signature 'MsBackendDataFrame'
precScanNum(object)

## S4 method for signature 'MsBackendDataFrame'
precursorCharge(object)

## S4 method for signature 'MsBackendDataFrame'
precursorIntensity(object)
```

```
## S4 method for signature 'MsBackendDataFrame'
precursorMz(object)

## S4 replacement method for signature 'MsBackendDataFrame'
peaksData(object) <- value

## S4 method for signature 'MsBackendDataFrame'
peaksVariables(object)

## S4 method for signature 'MsBackendDataFrame'
rtime(object)

## S4 replacement method for signature 'MsBackendDataFrame'
rtime(object) <- value

## S4 method for signature 'MsBackendDataFrame'
scanIndex(object)

## S4 method for signature 'MsBackendDataFrame'
selectSpectraVariables(object, spectraVariables = spectraVariables(object))

## S4 method for signature 'MsBackendDataFrame'
smoothed(object)

## S4 replacement method for signature 'MsBackendDataFrame'
smoothed(object) <- value

## S4 method for signature 'MsBackendDataFrame'
spectraData(object, columns = spectraVariables(object))

## S4 replacement method for signature 'MsBackendDataFrame'
spectraData(object) <- value

## S4 method for signature 'MsBackendDataFrame'
spectraNames(object)

## S4 replacement method for signature 'MsBackendDataFrame'
spectraNames(object) <- value

## S4 method for signature 'MsBackendDataFrame'
spectraVariables(object)

## S4 method for signature 'MsBackendDataFrame'
tic(object, initial = TRUE)

## S4 method for signature 'MsBackendDataFrame'
x$name

## S4 replacement method for signature 'MsBackendDataFrame'
x$name <- value
```

```
## S4 method for signature 'MsBackendDataFrame'
x[i, j, ..., drop = FALSE]

## S4 method for signature 'MsBackendDataFrame,ANY'
split(x, f, drop = FALSE, ...)

## S4 method for signature 'MsBackendDataFrame'
filterAcquisitionNum(
  object,
  n = integer(),
  dataStorage = character(),
  dataOrigin = character()
)

## S4 method for signature 'MsBackendHdf5Peaks'
backendInitialize(
  object,
  files = character(),
  data = DataFrame(),
  hdf5path = character(),
  ...,
  BPPARAM = bpparam()
)

## S4 method for signature 'MsBackendHdf5Peaks'
show(object)

## S4 method for signature 'MsBackendHdf5Peaks'
peaksData(object, columns = peaksVariables(object))

## S4 method for signature 'MsBackendHdf5Peaks'
intensity(object)

## S4 replacement method for signature 'MsBackendHdf5Peaks'
intensity(object) <- value

## S4 method for signature 'MsBackendHdf5Peaks'
ionCount(object)

## S4 method for signature 'MsBackendHdf5Peaks'
isCentroided(object, ...)

## S4 method for signature 'MsBackendHdf5Peaks'
isEmpty(x)

## S4 method for signature 'MsBackendHdf5Peaks'
lengths(x, use.names = FALSE)

## S4 method for signature 'MsBackendHdf5Peaks'
mz(object)

## S4 replacement method for signature 'MsBackendHdf5Peaks'
```

```
mz(object) <- value

## S4 replacement method for signature 'MsBackendHdf5Peaks'
peaksData(object) <- value

## S4 method for signature 'MsBackendHdf5Peaks'
spectraData(object, columns = spectraVariables(object))

## S4 replacement method for signature 'MsBackendHdf5Peaks'
spectraData(object) <- value

## S4 replacement method for signature 'MsBackendHdf5Peaks'
x$name <- value

## S4 method for signature 'MsBackendHdf5Peaks'
x[i, j, ..., drop = FALSE]

## S4 method for signature 'MsBackendHdf5Peaks'
backendMerge(object, ...)

## S4 method for signature 'MsBackendMemory'
show(object)

## S4 method for signature 'MsBackendMemory'
backendMerge(object, ...)

## S4 method for signature 'MsBackendMemory'
acquisitionNum(object)

## S4 method for signature 'MsBackendMemory'
centroided(object)

## S4 replacement method for signature 'MsBackendMemory'
centroided(object) <- value

## S4 method for signature 'MsBackendMemory'
collisionEnergy(object)

## S4 replacement method for signature 'MsBackendMemory'
collisionEnergy(object) <- value

## S4 method for signature 'MsBackendMemory'
dataOrigin(object)

## S4 replacement method for signature 'MsBackendMemory'
dataOrigin(object) <- value

## S4 method for signature 'MsBackendMemory'
dataStorage(object)

## S4 replacement method for signature 'MsBackendMemory'
dataStorage(object) <- value
```

```
## S4 method for signature 'MsBackendMemory'
intensity(object)

## S4 replacement method for signature 'MsBackendMemory'
intensity(object) <- value

## S4 method for signature 'MsBackendMemory'
ionCount(object)

## S4 method for signature 'MsBackendMemory'
isEmpty(x)

## S4 method for signature 'MsBackendMemory'
isolationWindowLowerMz(object)

## S4 replacement method for signature 'MsBackendMemory'
isolationWindowLowerMz(object) <- value

## S4 method for signature 'MsBackendMemory'
isolationWindowTargetMz(object)

## S4 replacement method for signature 'MsBackendMemory'
isolationWindowTargetMz(object) <- value

## S4 method for signature 'MsBackendMemory'
isolationWindowUpperMz(object)

## S4 replacement method for signature 'MsBackendMemory'
isolationWindowUpperMz(object) <- value

## S4 method for signature 'MsBackendMemory'
length(x)

## S4 method for signature 'MsBackendMemory'
lengths(x, use.names = FALSE)

## S4 method for signature 'MsBackendMemory'
msLevel(object, ...)

## S4 replacement method for signature 'MsBackendMemory'
msLevel(object) <- value

## S4 method for signature 'MsBackendMemory'
mz(object)

## S4 replacement method for signature 'MsBackendMemory'
mz(object) <- value

## S4 method for signature 'MsBackendMemory'
peaksData(object, columns = c("mz", "intensity"))
```

```
## S4 replacement method for signature 'MsBackendMemory'
peaksData(object) <- value

## S4 method for signature 'MsBackendMemory'
polarity(object)

## S4 replacement method for signature 'MsBackendMemory'
polarity(object) <- value

## S4 method for signature 'MsBackendMemory'
precScanNum(object)

## S4 method for signature 'MsBackendMemory'
precursorCharge(object)

## S4 method for signature 'MsBackendMemory'
precursorIntensity(object)

## S4 method for signature 'MsBackendMemory'
precursorMz(object)

## S4 method for signature 'MsBackendMemory'
rtime(object)

## S4 replacement method for signature 'MsBackendMemory'
rtime(object) <- value

## S4 method for signature 'MsBackendMemory'
scanIndex(object)

## S4 method for signature 'MsBackendMemory'
selectSpectraVariables(object, spectraVariables = spectraVariables(object))

## S4 method for signature 'MsBackendMemory'
smoothed(object)

## S4 replacement method for signature 'MsBackendMemory'
smoothed(object) <- value

## S4 method for signature 'MsBackendMemory'
spectraData(object, columns = spectraVariables(object))

## S4 replacement method for signature 'MsBackendMemory'
spectraData(object) <- value

## S4 method for signature 'MsBackendMemory'
spectraNames(object)

## S4 replacement method for signature 'MsBackendMemory'
spectraNames(object) <- value

## S4 method for signature 'MsBackendMemory'
```

```
spectraVariables(object)

## S4 method for signature 'MsBackendMemory'
peaksVariables(object)

## S4 method for signature 'MsBackendMemory'
tic(object, initial = TRUE)

## S4 method for signature 'MsBackendMemory'
x$name

## S4 replacement method for signature 'MsBackendMemory'
x$name <- value

## S4 method for signature 'MsBackendMemory'
x[i, j, ..., drop = FALSE]

## S4 method for signature 'MsBackendMemory,ANY'
split(x, f, drop = FALSE, ...)

## S4 method for signature 'MsBackendMemory'
filterAcquisitionNum(
  object,
  n = integer(),
  dataStorage = character(),
  dataOrigin = character()
)

## S4 method for signature 'MsBackendMzR'
backendInitialize(object, files, ..., BPPARAM = bpparam())

## S4 method for signature 'MsBackendMzR'
show(object)

## S4 method for signature 'MsBackendMzR'
peaksData(object, columns = peaksVariables(object))

## S4 method for signature 'MsBackendMzR'
intensity(object)

## S4 replacement method for signature 'MsBackendMzR'
intensity(object) <- value

## S4 method for signature 'MsBackendMzR'
ionCount(object)

## S4 method for signature 'MsBackendMzR'
isCentroided(object, ...)

## S4 method for signature 'MsBackendMzR'
isEmpty(x)
```

```
## S4 method for signature 'MsBackendMzR'
lengths(x, use.names = FALSE)

## S4 method for signature 'MsBackendMzR'
mz(object)

## S4 replacement method for signature 'MsBackendMzR'
mz(object) <- value

## S4 method for signature 'MsBackendMzR'
spectraData(object, columns = spectraVariables(object))

## S4 replacement method for signature 'MsBackendMzR'
spectraData(object) <- value

## S4 method for signature 'MsBackendMzR'
spectraNames(object)

## S4 replacement method for signature 'MsBackendMzR'
spectraNames(object) <- value

## S4 method for signature 'MsBackendMzR'
spectraVariables(object)

## S4 replacement method for signature 'MsBackendMzR'
x$name <- value

## S4 method for signature 'MsBackendMzR'
export(
  object,
  x,
  file = tempfile(),
  format = c("mzML", "mzXML"),
  copy = FALSE,
  BPPARAM = bpparam()
)

## S4 method for signature 'Spectra'
show(object)

## S4 method for signature 'list'
combinePeaks(object, ...)
```

Value

Not applicable

Note

: this replaces **all** the data in the backend.

joinPeaks   *Join (map) peaks of two spectra*

Description

These functions map peaks from two spectra with each other if the difference between their m/z
values is smaller than defined with parameters tolerance and ppm. All functions take two matrices

- joinPeaks(): maps peaks from two spectra allowing to specify the type of *join* that should be
  performed: type = "outer" each peak in x will be matched with each peak in y, for peaks that
  do not match any peak in the other spectra an NA intensity is returned. With type = "left"
  all peaks from the left spectrum (x) will be matched with peaks in y. Peaks in y that do not
  match any peak in x are omitted. type = "right" is the same as type = "left" only for y.
  Only peaks that can be matched between x and y are returned by type = "inner", i.e. only
  peaks present in both spectra are reported.

- joinPeaksGnps(): matches/maps peaks between spectra with the same approach used in
  GNPS: peaks are considered matching if a) the difference in their m/z values is smaller than
  defined by tolerance and ppm (this is the same as joinPeaks) **and** b) the difference of
  their m/z *adjusted* for the difference of the spectras' precursor is smaller than defined by
  tolerance and ppm. Based on this definition, peaks in x can match up to two peaks in y
  hence peaks in the returned matrices might be reported multiple times. Note that if one of
  xPrecursorMz or yPrecursorMz are NA or if both are the same, the results are the same as
  with [joinPeaks()](). To calculate GNPS similarity scores, [gnps()]() should be called on the
  aligned peak matrices (i.e. compareSpectra should be called with MAPFUN = joinPeaksGnps
  and FUN = MsCoreUtils::gnps).

- joinPeaksNone(): does not perform any peak matching but simply returns the peak matrices
  in a list. This function should be used with the MAPFUN parameter of [compareSpectra()]() if
  the spectra similarity function used (parameter FUN of compareSpectra()) performs its own
  peak matching and does hence not expect matched peak matrices as an input.

Usage

```
joinPeaks(x, y, type = "outer", tolerance = 0, ppm = 10, ...)

joinPeaksGnps(
  x,
  y,
  xPrecursorMz = NA_real_,
  yPrecursorMz = NA_real_,
  tolerance = 0,
  ppm = 0,
  type = "outer",
  ...
)

joinPeaksNone(x, y, ...)
```

Arguments

x   matrix with two columns "mz" and "intensity" containing the m/z and inten-
                     sity values of the mass peaks of a spectrum.

y	matrix with two columns "mz" and "intensity" containing the m/z and intensity values of the mass peaks of a spectrum.
type	For joinPeaks() and joinPeaksGnps(): character(1) specifying the type of join that should be performed. See function description for details.
tolerance	numeric(1) defining a constant maximal accepted difference between m/z values of peaks from the two spectra to be matched/mapped.
ppm	numeric(1) defining a relative, m/z-dependent, maximal accepted difference between m/z values of peaks from the two spectra to be matched/mapped.
...	optional parameters passed to the MsCoreUtils::join() function.
xPrecursorMz	for joinPeaksGnps(): numeric(1) with the precursor m/z of the spectrum x.
yPrecursorMz	for joinPeaksGnps(): numeric(1) with the precursor m/z of the spectrum y.

Value

All functions return a list of elements "x" and "y" each being a two column matrix with m/z (first column) and intensity values (second column). The two matrices contain the matched peaks between input matrices x and y and hence have the same number of rows. Peaks present in x but not in the y input matrix have m/z and intensity values of NA in the result matrix for y (and *vice versa*).

Implementation notes

A mapping function must take two numeric matrices x and y as input and must return list with two elements named "x" and "y" that represent the aligned input matrices. The function should also have ... in its definition. Parameters ppm and tolerance are suggested but not required.

Author(s)

Johannes Rainer, Michael Witting

See Also

gnps()

Examples

```
x <- cbind(c(31.34, 50.14, 60.3, 120.9, 230, 514.13, 874.1),
    1:7)
y <- cbind(c(12, 31.35, 70.3, 120.9 + ppm(120.9, 5),
    230 + ppm(230, 10), 315, 514.14, 901, 1202),
    1:9)

## No peaks with identical m/z
joinPeaks(x, y, ppm = 0, type = "inner")

## With ppm 10 two peaks are overlapping
joinPeaks(x, y, ppm = 10, type = "inner")

## Outer join: contain all peaks from x and y
joinPeaks(x, y, ppm = 10, type = "outer")

## Left join: keep all peaks from x and those from y that match
joinPeaks(x, y, ppm = 10, type = "left")
```

```
## Right join: keep all peaks from y and those from x that match. Using
## a constant tolerance of 0.01
joinPeaks(x, y, tolerance = 0.01, type = "right")

## GNPS-like peak matching

## Define spectra
x <- cbind(mz = c(10, 36, 63, 91, 93), intensity = c(14, 15, 999, 650, 1))
y <- cbind(mz = c(10, 12, 50, 63, 105), intensity = c(35, 5, 16, 999, 450))
## The precursor m/z
pmz_x <- 91
pmz_y <- 105

## Plain joinPeaks identifies only 2 matching peaks: 1 and 5
joinPeaks(x, y)

## joinPeaksGnps finds 4 matches
joinPeaksGnps(x, y, pmz_x, pmz_y)

## with one of the two precursor m/z being NA, the result are the same as
## with joinPeaks (with type = "left").
joinPeaksGnps(x, y, pmz_x, yPrecursorMz = NA)
```

MsBackend   *Mass spectrometry data backends*

Description

Note that the classes described here are not meant to be used directly by the end-users and the material in this man page is aimed at package developers.

MsBackend is a virtual class that defines what each different backend needs to provide. MsBackend objects provide access to mass spectrometry data. Such backends can be classified into *in-memory* or *on-disk* backends, depending on where the data, i.e spectra (m/z and intensities) and spectra annotation (MS level, charge, polarity, ...) are stored.

Typically, in-memory backends keep all data in memory ensuring fast data access, while on-disk backends store (parts of) their data on disk and retrieve it on demand.

The *Backend functions and implementation notes for new backend classes* section documents the API that a backend must implement.

Currently available backends are:

- MsBackendMemory and MsBackendDataFrame: store all data in memory. The MsBackendMemory is optimized for accessing and processing the peak data (i.e. the numerical matrices with the m/z and intensity values) while the MsBackendDataFrame keeps all data in a DataFrame.

- MsBackendMzR: stores the m/z and intensities on-disk in raw data files (typically mzML or mzXML) and the spectra annotation information (header) in memory in a DataFrame. This backend requires the mzR package.

- MsBackendHdf5Peaks: stores the m/z and intensities on-disk in custom hdf5 data files and the remaining spectra variables in memory (in a DataFrame). This backend requires the rhdf5 package.

See below for more details about individual backends.

Usage

```
## S4 method for signature 'MsBackend'
backendBpparam(object, BPPARAM = bpparam())

## S4 method for signature 'MsBackend'
backendInitialize(object, ...)

## S4 method for signature 'list'
backendMerge(object, ...)

## S4 method for signature 'MsBackend'
backendMerge(object, ...)

## S4 method for signature 'MsBackend'
backendParallelFactor(object, ...)

## S4 method for signature 'MsBackend'
export(object, ...)

## S4 method for signature 'MsBackend'
acquisitionNum(object)

## S4 method for signature 'MsBackend'
peaksData(object, columns = c("mz", "intensity"))

## S4 method for signature 'MsBackend'
peaksVariables(object)

## S4 method for signature 'MsBackend'
centroided(object)

## S4 replacement method for signature 'MsBackend'
centroided(object) <- value

## S4 method for signature 'MsBackend'
collisionEnergy(object)

## S4 replacement method for signature 'MsBackend'
collisionEnergy(object) <- value

## S4 method for signature 'MsBackend'
dataOrigin(object)

## S4 replacement method for signature 'MsBackend'
dataOrigin(object) <- value

## S4 method for signature 'MsBackend'
dataStorage(object)

## S4 replacement method for signature 'MsBackend'
dataStorage(object) <- value
```

```
## S4 method for signature 'MsBackend'
dropNaSpectraVariables(object)

## S4 method for signature 'MsBackend'
filterAcquisitionNum(object, n, file, ...)

## S4 method for signature 'MsBackend'
filterDataOrigin(object, dataOrigin = character())

## S4 method for signature 'MsBackend'
filterDataStorage(object, dataStorage = character())

## S4 method for signature 'MsBackend'
filterEmptySpectra(object, ...)

## S4 method for signature 'MsBackend'
filterIsolationWindow(object, mz = numeric(), ...)

## S4 method for signature 'MsBackend'
filterMsLevel(object, msLevel = integer())

## S4 method for signature 'MsBackend'
filterPolarity(object, polarity = integer())

## S4 method for signature 'MsBackend'
filterPrecursorMzRange(object, mz = numeric())

## S4 method for signature 'MsBackend'
filterPrecursorMz(object, mz = numeric())

## S4 method for signature 'MsBackend'
filterPrecursorMzValues(object, mz = numeric(), ppm = 20, tolerance = 0)

## S4 method for signature 'MsBackend'
filterPrecursorCharge(object, z = integer())

## S4 method for signature 'MsBackend'
filterPrecursorScan(object, acquisitionNum = integer(), f = dataOrigin(object))

## S4 method for signature 'MsBackend'
filterRanges(
  object,
  spectraVariables = character(),
  ranges = numeric(),
  match = c("all", "any")
)

## S4 method for signature 'MsBackend'
filterRt(object, rt = numeric(), msLevel. = uniqueMsLevels(object))

## S4 method for signature 'MsBackend'
filterValues(
```

```
  object,
  spectraVariables = character(),
  values = numeric(),
  ppm = 0,
  tolerance = 0,
  match = c("all", "any")
)

## S4 method for signature 'MsBackend'
intensity(object)

## S4 replacement method for signature 'MsBackend'
intensity(object) <- value

## S4 method for signature 'MsBackend'
ionCount(object)

## S4 method for signature 'MsBackend'
isCentroided(object, ...)

## S4 method for signature 'MsBackend'
isEmpty(x)

## S4 method for signature 'MsBackend'
isolationWindowLowerMz(object)

## S4 replacement method for signature 'MsBackend'
isolationWindowLowerMz(object) <- value

## S4 method for signature 'MsBackend'
isolationWindowTargetMz(object)

## S4 replacement method for signature 'MsBackend'
isolationWindowTargetMz(object) <- value

## S4 method for signature 'MsBackend'
isolationWindowUpperMz(object)

## S4 replacement method for signature 'MsBackend'
isolationWindowUpperMz(object) <- value

## S4 method for signature 'MsBackend'
isReadOnly(object)

## S4 method for signature 'MsBackend'
length(x)

## S4 method for signature 'MsBackend'
msLevel(object)

## S4 method for signature 'MsBackend'
mz(object)
```

```
## S4 replacement method for signature 'MsBackend'
mz(object) <- value

## S4 method for signature 'MsBackend'
lengths(x, use.names = FALSE)

## S4 method for signature 'MsBackend'
polarity(object)

## S4 replacement method for signature 'MsBackend'
polarity(object) <- value

## S4 method for signature 'MsBackend'
precScanNum(object)

## S4 method for signature 'MsBackend'
precursorCharge(object)

## S4 method for signature 'MsBackend'
precursorIntensity(object)

## S4 method for signature 'MsBackend'
precursorMz(object)

## S4 replacement method for signature 'MsBackend'
peaksData(object) <- value

## S4 method for signature 'MsBackend'
reset(object)

## S4 method for signature 'MsBackend'
rtime(object)

## S4 replacement method for signature 'MsBackend'
rtime(object) <- value

## S4 method for signature 'MsBackend'
scanIndex(object)

## S4 method for signature 'MsBackend'
selectSpectraVariables(object, spectraVariables = spectraVariables(object))

## S4 method for signature 'MsBackend'
smoothed(object)

## S4 replacement method for signature 'MsBackend'
smoothed(object) <- value

## S4 method for signature 'MsBackend'
spectraData(object, columns = spectraVariables(object))
```

```
## S4 replacement method for signature 'MsBackend'
spectraData(object) <- value

## S4 method for signature 'MsBackend'
spectraNames(object)

## S4 replacement method for signature 'MsBackend'
spectraNames(object) <- value

## S4 method for signature 'MsBackend'
spectraVariables(object)

## S4 method for signature 'MsBackend,ANY'
split(x, f, drop = FALSE, ...)

## S4 method for signature 'MsBackend'
supportsSetBackend(object, ...)

## S4 method for signature 'MsBackend'
tic(object, initial = TRUE)

## S4 method for signature 'MsBackend'
x[i, j, ..., drop = FALSE]

## S4 method for signature 'MsBackend'
x$name

## S4 replacement method for signature 'MsBackend'
x$name <- value

## S4 method for signature 'MsBackend'
x[[i, j, ...]]

## S4 replacement method for signature 'MsBackend'
x[[i, j, ...]] <- value

## S4 method for signature 'MsBackend'
uniqueMsLevels(object, ...)

## S4 method for signature 'MsBackend'
dataStorageBasePath(object)

## S4 replacement method for signature 'MsBackend'
dataStorageBasePath(object) <- value

MsBackendDataFrame()

## S4 method for signature 'MsBackendDataFrame'
backendInitialize(object, data, peaksVariables = c("mz", "intensity"), ...)

MsBackendHdf5Peaks()
```

```
MsBackendMemory()

## S4 method for signature 'MsBackendMemory'
backendInitialize(object, data, peaksVariables = c("mz", "intensity"), ...)

MsBackendMzR()
```

Arguments

`object`	Object extending MsBackend.
`BPPARAM`	for backendBpparam(): parameter object from the BiocParallel package defining the parallel processing setup. Defaults to BPPARAM = bpparam(). See bpparam() for more information.
`...`	Additional arguments.
`columns`	For spectraData() accessor: optional character with column names (spectra variables) that should be included in the returned DataFrame. By default, all columns are returned. For peaksData() accessor: optional character with requested columns in the individual matrix of the returned list. Defaults to peaksVariables(object) and depends on what *peaks variables* the backend provides.
`value`	replacement value for <- methods. See individual method description or expected data type.
`n`	for filterAcquisitionNum(): integer with the acquisition numbers to filter for.
`file`	For filterFile(): index or name of the file(s) to which the data should be subsetted. For export(): character of length 1 or equal to the number of spectra.
`dataOrigin`	For filterDataOrigin(): character to define which spectra to keep. For filterAcquisitionNum(): optionally specify if filtering should occur only for spectra of selected dataOrigin.
`dataStorage`	For filterDataStorage(): character to define which spectra to keep. For filterAcquisitionNum(): optionally specify if filtering should occur only for spectra of selected dataStorage.
`mz`	For filterIsolationWindow(): numeric(1) with the m/z value to filter the object. For filterPrecursorMzRange(): numeric(2) with the lower and upper m/z boundary. For filterPrecursorMzValues(): numeric with the m/z value(s) to filter the object.
`msLevel`	integer defining the MS level of the spectra to which the function should be applied. For filterMsLevel(): the MS level to which object should be subsetted.
`polarity`	For filterPolarity(): integer specifying the polarity to to subset object.
`ppm`	For filterPrecursorMzValues(): numeric(1) with the m/z-relative maximal acceptable difference for a m/z to be considered matching. See closest() for details. For filterValues(): numeric of any length allowing to define a maximal accepted difference between user input values and the spectraVariables values. If it is not equal to the length of the value provided with parameter spectraVariables, ppm[1] will be recycled.

tolerance   For filterPrecursorMzValues(): numeric(1) with the maximal absolute ac-
                 ceptable difference for a m/z value to be considered matching. See [closest()](#)
                 for details. For filterValues(): numeric accepted tolerance between the
                 values and the spectra variables. Defaults to tolerance = 0. If it is not equal to
                 the length of the value provided with parameter spectraVariables, tolerance[1]
                 will be recycled.

z   For filterPrecursorCharge(): integer() with the precursor charges to be
                 used as filter.

acquisitionNum   for filterPrecursorScan(): integer with the acquisition number of the spec-
                 tra to which the object should be subsetted.

f   factor defining the grouping to split x. See [split()](#). For filterPrecursorScan():
                 factor defining from which original data files the spectra derive to avoid select-
                 ing spectra from different samples/files. Defaults to f = dataOrigin(object).

spectraVariables
                 For selectSpectraVariables(): character with the names of the spectra
                 variables to which the backend should be subsetted. For filterRanges() and
                 filterValues(): character vector specifying the column(s) from spectraData(object)
                 on which to filter the data and that correspond to the the names of the spectra
                 variables that should be used for the filtering.

ranges   for filterRanges(): A numeric vector of paired values (upper and lower
                 boundary) that define the ranges to filter the object. These paired values need
                 to be in the same order as the spectraVariables parameter (see below).

match   For filterRanges() and filterValues(): character(1) defining whether
                 the condition has to match for all provided ranges/values (match = "all"; the
                 default), or for any of them (match = "any") for spectra to be retained.

rt   for filterRt(): numeric(2) defining the retention time range to be used to
                 subset/filter object.

msLevel.   same as msLevel above.

values   for filterValues(): A numeric vector that define the values to filter the
                 object. values needs to be of same length than parameter spectraVariables
                 and in the same order.

x   Object extending MsBackend.

use.names   For lengths(): whether spectrum names should be used.

drop   For [: not considered.

initial   For tic(): logical(1) whether the initially reported total ion current should be
                 reported, or whether the total ion current should be (re)calculated on the actual
                 data (initial = FALSE).

i   For [: integer, logical or character to subset the object.

j   For [: not supported.

name   For $ and $<-: the name of the spectra variable to return or set.

data   For backendInitialize(): DataFrame with spectrum metadata/data. This pa-
                 rameter can be empty for MsBackendMzR backends but needs to be provided for
                 MsBackendDataFrame backends.

peaksVariables   For backendInitialize() for MsBackendMemory: character specifying which
                 of the columns of the provided data contain *peaks variables* (i.e. information
                 for individual mass peaks). Defaults to peaksVariables = c("mz", "intensity").
                 "mz" and "intensity" should **always** be specified.

Value

See documentation of respective function.

Implementation notes

Backends extending MsBackend **must** implement all of its methods (listed above). Developers of new MsBackends should follow the MsBackendMemory implementation. To ensure a new implementation being conform with the MsBackend definition, developers should included test suites provided by this package in their unit test setup. For that a variable be should be created in the package's "testthat.R" file that represents a (initialized) instance of the developed backend. Then the path to the test suites should be defined with test_suite <- system.file("test_backends", "test_MsBackend", package = "Spectra") followed by test_dir(test_suite) to run all test files in that directory. Individual unit test files could be run with test_file(file.path(test_suite, "test_spectra_variables.R"), stop_on_failure = TRUE) (note that without stop_on_failure = TRUE tests would fail silently) . Adding this code to the packages "testthat.R" file ensures that all tests checking the validity of an MsBackend instance defined in the Spectra package are also run on the newly develped backend class.

The MsBackend defines the following slots:

- @readonly: logical(1) whether the backend supports writing/replacing of m/z or intensity values.

Backends extending MsBackend **must** implement all of its methods (listed above). Developers of new MsBackends should follow the MsBackendDataFrame implementation.

The [MsBackendCached()](#) backend provides a caching mechanism to allow *read only* backends to add or change spectra variables. This backend shouldn't be used on its own, but is meant to be extended. See [MsBackendCached()](#) for details.

The MsBackend defines the following slots:

- @readonly: logical(1) whether the backend supports writing/replacing of m/z or intensity values.

Backend functions

New backend classes **must** extend the base MsBackend class will have to implement some of the following methods (see the MsBackend vignette for detailed description and examples):

- [: subset the backend. Only subsetting by element (*row*/i) is allowed. Parameter i should support integer indices and logical and should throw an error if i is out of bounds. The MsCoreUtils::i2index could be used to check the input i. For i = integer() an empty backend should be returned.

- $, $<-: access or set/add a single spectrum variable (column) in the backend. Using a value of NULL should allow deleting the specified spectra variable. An error should be thrown if the spectra variable is not available.

- [[, [[<-: access or set/add a single spectrum variable (column) in the backend. The default implementation uses $, thus these methods don't have to be implemented for new classes extending MsBackend.

- acquisitionNum(): returns the acquisition number of each spectrum. Returns an integer of length equal to the number of spectra (with NA_integer_ if not available).

- backendBpparam(): return the parallel processing setup supported by the backend class. This function can be used by any higher level function to evaluate whether the provided parallel processing setup (or the default one returned by bpparam()) is supported by the backend.

Backends not supporting parallel processing (e.g. because they contain a connection to a database that can not be shared across processes) should extend this method to return only `SerialParam()` and hence disable parallel processing for (most) methods and functions. See also `backendParallelFactor()` for a function to provide a preferred splitting of the backend for parallel processing.

- `backendInitialize()`: initialises the backend. This method is supposed to be called rights after creating an instance of the backend class and should prepare the backend (e.g. set the data for the memory backend or read the spectra header data for the MsBackendMzR backend). Parameters can be defined freely for each backend, depending on what is needed to initialize the backend. It is however suggested to also support a parameter `data` that can be used to submit the full spectra data as a `DataFrame` to the backend. This would allow the backend to be also usable for the [setBackend()](#) function from Spectra. Note that eventually (for *read-only* backends) also the supportsSetBackend method would need to be implemented to return `TRUE`. The backendInitialize() method has also to ensure to correctly set spectra variable `dataStorage`.

- `backendMerge()`: merges (combines) MsBackend objects into a single instance. All objects to be merged have to be of the same type (e.g. [MsBackendDataFrame()](#)).

- `backendParallelFactor()`: returns a `factor` defining an optimal (preferred) way how the backend can be split for parallel processing used for all peak data accessor or data manipulation functions. The default implementation returns a factor of length 0 (`factor()`) providing thus no default splitting. `backendParallelFactor()` for MsBackendMzR on the other hand returns `factor(dataStorage(object))` hence suggesting to split the object by data file.

- `dataOrigin()`: gets a `character` of length equal to the number of spectra in `object` with the *data origin* of each spectrum. This could e.g. be the mzML file from which the data was read.

- `dataStorage()`: gets a `character` of length equal to the number of spectra in `object` with the data storage of each spectrum. Note that missing values (`NA_character_`) are not supported for `dataStorage`.

- `dataStorageBasePath()`, `dataStorageBasePath<-`: gets or sets the common *base* path of the directo acterof length 1. Most backends (such as for example theMsBackendMemorywill not support this fur BackendMzR, this function allows to get or change the path to the directory containing the orig: BackendMzR` instance gets copied to another computer or file system.

- `dropNaSpectraVariables()`: removes spectra variables (i.e. columns in the object's `spectraData` that contain only missing values (NA). Note that while columns with only NAs are removed, a `spectraData()` call after dropNaSpectraVariables() might still show columns containing NA values for *core* spectra variables.

- `centroided()`, `centroided<-`: gets or sets the centroiding information of the spectra. `centroided()` returns a `logical` vector of length equal to the number of spectra with `TRUE` if a spectrum is centroided, `FALSE` if it is in profile mode and `NA` if it is undefined. See also `isCentroided()` for estimating from the spectrum data whether the spectrum is centroided. `value` for `centroided<-` is either a single `logical` or a `logical` of length equal to the number of spectra in `object`.

- `collisionEnergy()`, `collisionEnergy<-`: gets or sets the collision energy for all spectra in `object`. `collisionEnergy()` returns a `numeric` with length equal to the number of spectra (`NA_real_` if not present/defined), `collisionEnergy<-` takes a `numeric` of length equal to the number of spectra in `object`.

- `export()`: exports data from a Spectra class to a file. This method is called by the `export,Spectra` method that passes itself as a second argument to the function. The `export,MsBackend` implementation is thus expected to take a Spectra class as second argument from which all data is exported. Taking data from a Spectra class ensures that also all eventual data manipulations (cached in the Spectra's lazy evaluation queue) are applied prior to export - this would not be possible with only a [MsBackend](#) class. An example implementation is the export()

method for the MsBackendMzR backend that supports export of the data in *mzML* or *mzXML* format. See the documentation for the MsBackendMzR class below for more information.

- filterAcquisitionNum(): filters the object keeping only spectra matching the provided acquisition numbers (argument n). If dataOrigin or dataStorage is also provided, object is subsetted to the spectra with an acquisition number equal to n **in spectra with matching dataOrigin or dataStorage values** retaining all other spectra.

- filterDataOrigin(): filters the object retaining spectra matching the provided dataOrigin. Parameter dataOrigin has to be of type character and needs to match exactly the data origin value of the spectra to subset. filterDataOrigin() should return the data ordered by the provided dataOrigin parameter, i.e. if dataOrigin = c("2", "1") was provided, the spectra in the resulting object should be ordered accordingly (first spectra from data origin "2" and then from "1"). Implementation of this method is optional since a default implementation for MsBackend is available.

- filterDataStorage(): filters the object retaining spectra matching the provided dataStorage. Parameter dataStorage has to be of type character and needs to match exactly the data storage value of the spectra to subset. filterDataStorage() should return the data ordered by the provided dataStorage parameter, i.e. if dataStorage = c("2", "1") was provided, the spectra in the resulting object should be ordered accordingly (first spectra from data storage "2" and then from "1"). Implementation of this method is optional since a default implementation for MsBackend is available.

- filterEmptySpectra(): removes empty spectra (i.e. spectra without peaks). Implementation of this method is optional since a default implementation for MsBackend is available.

- filterFile(): retains data of files matching the file index or file name provided with parameter file.

- filterIsolationWindow(): retains spectra that contain mz in their isolation window m/z range (i.e. with an isolationWindowLowerMz <= mz and isolationWindowUpperMz >= mz. Implementation of this method is optional since a default implementation for MsBackend is available.

- filterMsLevel(): retains spectra of MS level msLevel. Implementation of this method is optional since a default implementation for MsBackend is available.

- filterPolarity(): retains spectra of polarity polarity. Implementation of this method is optional since a default implementation for MsBackend is available.

- filterPrecursorMzRange() (previously filterPrecursorMz): retains spectra with a precursor m/z within the provided m/z range. Implementation of this method is optional since a default implementation for MsBackend is available.

- filterPrecursorMzValues(): retains spectra with a precursor m/z matching any of the provided m/z values (given ppm and tolerance). Implementation of this method is optional since a default implementation for MsBackend is available.

- filterPrecursorCharge(): retains spectra with the defined precursor charge(s). Implementation of this method is optional since a default implementation for MsBackend is available.

- filterPrecursorScan(): retains parent (e.g. MS1) and children scans (e.g. MS2) of acquisition number acquisitionNum. Parameter f is supposed to define the origin of the spectra (i.e. the original data file) to ensure related spectra from the same file/sample are selected and retained. Implementation of this method is optional since a default implementation for MsBackend is available.

- filterRanges(): allows filtering of the Spectra object based on user defined *numeric* ranges (parameter ranges) for one or more available spectra variables in object (spectra variable names can be specified with parameter spectraVariables). Spectra for which the value of

a spectra variable is within it's defined range are retained. If multiple ranges/spectra variables are defined, the match parameter can be used to specify whether all conditions (match = "all"; the default) or if any of the conditions must match (match = "any"; all spectra for which values are within any of the provided ranges are retained). Implementation of this method is optional since a default implementation for MsBackend is available.

- filterRt(): retains spectra of MS level msLevel with retention times within (>=) rt[1] and (<=) rt[2]. Implementation of this method is optional since a default implementation for MsBackend is available.

- filterValues(): allows filtering of the Spectra object based on similarities of *numeric* values of one or more spectraVariables(object) (parameter spectraVariables) to provided values (parameter values) given acceptable differences (parameters tolerance and ppm). If multiple values/spectra variables are defined, the match parameter can be used to specify whether all conditions (match = "all"; the default) or if any of the conditions must match (match = "any"; all spectra for which values are within any of the provided ranges are retained). Implementation of this method is optional since a default implementation for MsBackend is available.

- intensity(): gets the intensity values from the spectra. Returns a [NumericList()](#) of numeric vectors (intensity values for each spectrum). The length of the list is equal to the number of spectra in object.

- intensity<-: replaces the intensity values. value has to be a list (or [NumericList()](#)) of length equal to the number of spectra and the number of values within each list element identical to the number of peaks in each spectrum (i.e. the lengths(x)). Note that just writeable backends support this method.

- ionCount(): returns a numeric with the sum of intensities for each spectrum. If the spectrum is empty (see isEmpty()), NA_real_ is returned.

- isCentroided(): a heuristic approach assessing if the spectra in object are in profile or centroided mode. The function takes the qtl th quantile top peaks, then calculates the difference between adjacent m/z value and returns TRUE if the first quartile is greater than k. (See Spectra:::.peaks_is_centroided for the code.)

- isEmpty(): checks whether a spectrum in object is empty (i.e. does not contain any peaks). Returns a logical vector of length equal number of spectra.

- isolationWindowLowerMz(), isolationWindowLowerMz<-: gets or sets the lower m/z boundary of the isolation window.

- isolationWindowTargetMz(), isolationWindowTargetMz<-: gets or sets the target m/z of the isolation window.

- isolationWindowUpperMz(), isolationWindowUpperMz<-: gets or sets the upper m/z boundary of the isolation window.

- isReadOnly(): returns a logical(1) whether the backend is *read only* or does allow also to write/update data.

- length(): returns the number of spectra in the object.

- lengths(): gets the number of peaks (m/z-intensity values) per spectrum. Returns an integer vector (length equal to the number of spectra). For empty spectra, 0 is returned.

- msLevel(): gets the spectra's MS level. Returns an integer vector (of length equal to the number of spectra) with the MS level for each spectrum (or NA_integer_ if not available).

- mz(): gets the mass-to-charge ratios (m/z) from the spectra. Returns a [NumericList()](#) or length equal to the number of spectra, each element a numeric vector with the m/z values of one spectrum.

- `mz<-`: replaces the m/z values. `value` has to be a `list` of length equal to the number of spectra and the number of values within each list element identical to the number of peaks in each spectrum (i.e. the `lengths(x)`). Note that just writeable backends support this method.

- `polarity()`, `polarity<-`: gets or sets the polarity for each spectrum. `polarity()` returns an `integer` vector (length equal to the number of spectra), with `0` and `1` representing negative and positive polarities, respectively. `polarity<-` expects an integer vector of length 1 or equal to the number of spectra.

- `precursorCharge()`, `precursorIntensity()`, `precursorMz()`, `precScanNum()`, `precAcquisitionNum()`: get the charge (`integer`), intensity (`numeric`), m/z (`numeric`), scan index (`integer`) and acquisition number (`interger`) of the precursor for MS level 2 and above spectra from the object. Returns a vector of length equal to the number of spectra in `object`. `NA` are reported for MS1 spectra of if no precursor information is available.

- `peaksData()` returns a `list` with the spectras' peak data, i.e. m/z and intensity values or other *peak variables*. The length of the list is equal to the number of spectra in `object`. Each element of the list has to be a two-dimensional array (`matrix` or `data.frame`) with columns depending on the provided `columns` parameter (by default `"mz"` and `"intensity"`, but depends on the backend's available `peaksVariables`). For an empty spectrum, a `matrix` (`data.frame`) with 0 rows and columns according to `columns` is returned. The optional parameter `columns`, if supported by the backend, allows to define which peak variables should be returned in the `numeric` peak `matrix`. As a default `c("mz", "intensity")` should be used.

- `peaksData<-` replaces the peak data (m/z and intensity values) of the backend. This method expects a `list` of two dimensional arrays (`matrix` or `data.frame`) with columns representing the peak variables. All existing peaks data is expected to be replaced with these new values. The length of the `list` has to match the number of spectra of `object`. Note that only writeable backends need to support this method.

- `peaksVariables()`: lists the available variables for mass peaks. Default peak variables are `"mz"` and `"intensity"` (which all backends need to support and provide), but some backends might provide additional variables. All these variables are expected to be returned (if requested) by the `peaksData()` function.

- `reset()` a backend (if supported). This method will be called on the backend by the `reset,Spectra` method that is supposed to restore the data to its original state (see `reset,Spectra` for more details). The function returns the *reset* backend. The default implementation for `MsBackend` returns the backend as-is.

- `rtime()`, `rtime<-`: gets or sets the retention times for each spectrum (in seconds). `rtime()` returns a `numeric` vector (length equal to the number of spectra) with the retention time for each spectrum. `rtime<-` expects a numeric vector with length equal to the number of spectra.

- `scanIndex()`: returns an `integer` vector with the *scan index* for each spectrum. This represents the relative index of the spectrum within each file. Note that this can be different to the `acquisitionNum()` of the spectrum which is the index of the spectrum as reported in the mzML file.

- `selectSpectraVariables()`: reduces the information within the backend to the selected spectra variables. It is suggested to **not** remove values for the `"dataStorage"` variable, since this might be required for some backends to work properly (such as the `MsBackendMzR`).

- `smoothed()`,`smoothed<-`: gets or sets whether a spectrum is *smoothed*. `smoothed()` returns a `logical` vector of length equal to the number of spectra. `smoothed<-` takes a `logical` vector of length 1 or equal to the number of spectra in `object`.

- `spectraData()`, `spectraData<-`: gets or sets general spectrum metadata (annotation, also called header). `spectraData()` returns a `DataFrame`, `spectraData<-` expects a `DataFrame`

with the same number of rows as there are spectra in object. Note that spectraData() has to return the full data, i.e. also the m/z and intensity values (as a list or SimpleList in columns "mz" and "intensity".

- spectraNames(): returns a character vector with the names of the spectra in object or NULL if not set. spectraNames<- allows to set spectra names (if the object is not read-only).

- spectraVariables(): returns a character vector with the available spectra variables (columns, fields or attributes) available in object. This should return **all** spectra variables which are present in object, also "mz" and "intensity" (which are by default not returned by the spectraVariables,Spectra method).

- split(): splits the backend into a list of backends (depending on parameter f). The default method for MsBackend uses [split.default()](), thus backends extending MsBackend don't necessarily need to implement this method.

- supportsSetBackend(): whether a MsBackend supports the Spectra setBackend() function. For a MsBackend to support setBackend() it needs to have a parameter called data in its backendInitialize() method that support receiving all spectra data as a DataFrame from another backend and to initialize the backend with this data. In general *read-only* backends do not support setBackend() hence, the default implementation of supportsSetBackend() returns !isReadOnly(object). If a read-only backend would support the setBackend() and being initialized with a DataFrame an implementation of this method for that backend could be defined that returns TRUE (see also the MsBackend vignette for details and examples).

- tic(): gets the total ion current/count (sum of signal of a spectrum) for all spectra in object. By default, the value reported in the original raw data file is returned. For an empty spectrum, NA_real_ is returned.

- uniqueMsLevels(): gets the unique MS levels of all spectra in object. The default implementation calls unique(msLevel(object)) but more efficient implementations could be defined for specific backends.

Subsetting and merging backend classes

Backend classes must support (implement) the [method to subset the object. This method should only support subsetting by spectra (rows, i) and has to return a MsBackend class.

Backends extending MsBackend should also implement the backendMerge() method to support combining backend instances (only backend classes of the same type should be merged). Merging should follow the following rules:

- The whole spectrum data of the various objects should be merged. The resulting merged object should contain the union of the individual objects' spectra variables (columns/fields), with eventually missing variables in one object being filled with NA.

In-memory data backends

MsBackendMemory and MsBackendDataFrame:

The MsBackendMemory and MsBackendDataFrame objects keep all MS data in memory are thus ideal for fast data processing. Due to their large memory footprint they are however not suited for large scale experiments. The two backends store the data different. The MsBackendDataFrame stores all data in a DataFrame and thus supports also S4-classes as spectra variables. Also, sepratate access to m/z or intensity values (i.e. using the mz() and intensity() methods) is faster for the MsBackendDataFrame. The MsBackendMemory on the other hand, due to the way the data is organized internally, provides much faster access to the full peak data (i.e. the numerical matrices of m/z and intensity values). Also subsetting and access to any spectra variable (except "mz" and "intensity") is fastest for the MsBackendMemory.

Thus, for most use cases, the MsBackendMemory provides a higher performance and flexibility than the MsBackendDataFrame and should thus be preferred. See also issue 246 for a performance comparison.

New objects can be created with the MsBackendMemory() and MsBackendDataFrame() function, respectively. Both backends can be subsequently initialized with the backendInitialize() method, taking a DataFrame (or data.frame) with the (full) MS data as first parameter data. The second parameter peaksVariables allows to define which columns in data contain *peak variables* such as the m/z and intensity values of individual peaks per spectrum. The default for this parameter is peaksVariables = c("mz", "intensity"). Note that it is not supported to provide either "mz" or "intensity", if provided, both need to be present in the data frame. Alternatively, the function also supports a data frame without m/z and intensity values, in which case a Spectra without mass peaks is created.

Suggested columns of this DataFrame are:

- "msLevel": integer with MS levels of the spectra.
- "rt": numeric with retention times of the spectra.
- "acquisitionNum": integer with the acquisition number of the spectrum.
- "scanIndex": integer with the index of the scan/spectrum within the *mzML/mzXML/CDF* file.
- "dataOrigin": character defining the *data origin*.
- "dataStorage": character indicating grouping of spectra in different e.g. input files. Note that missing values are not supported.
- "centroided": logical whether the spectrum is centroided.
- "smoothed": logical whether the spectrum was smoothed.
- "polarity": integer with the polarity information of the spectra.
- "precScanNum": integer specifying the index of the (MS1) spectrum containing the precursor of a (MS2) spectrum.
- "precursorMz": numeric with the m/z value of the precursor.
- "precursorIntensity": numeric with the intensity value of the precursor.
- "precursorCharge": integer with the charge of the precursor.
- "collisionEnergy": numeric with the collision energy.
- "mz": NumericList() of numeric vectors representing the m/z values for each spectrum.
- "intensity": NumericList() of numeric vectors representing the intensity values for each spectrum.

Additional columns are allowed too.

The peaksData() function for MsBackendMemory and MsBackendDataFrame returns a list of numeric matrix by default (with parameter columns = c("mz", "intensity")). If other peak variables are requested, a list of data.frame is returned (ensuring m/z and intensity values are always numeric).

MsBackendMzR, on-disk MS data backend

The MsBackendMzR keeps only a limited amount of data in memory, while the spectra data (m/z and intensity values) are fetched from the raw files on-demand. This backend uses the mzR package for data import and retrieval and hence requires that package to be installed. Also, it can only be used to import and represent data stored in *mzML*, *mzXML* and *CDF* files.

The `MsBackendMzR` backend extends the `MsBackendDataFrame` backend using its `DataFrame` to keep spectra variables (except m/z and intensity) in memory.

New objects can be created with the `MsBackendMzR()` function which can be subsequently filled with data by calling `backendInitialize()` passing the file names of the input data files with argument `files`.

This backend provides an `export()` method to export data from a `Spectra` in *mzML* or *mzXML* format. The definition of the function is:

`export(object, x, file = tempfile(), format = c("mzML", "mzXML"), copy = FALSE)`

The parameters are:

- `object`: an instance of the `MsBackendMzR` class.

- `x`: the [Spectra](#) object to be exported.

- `file`: `character` with the (full) output file name(s). Should be of length 1 or equal `length(x)`. If a single file is specified, all spectra are exported to that file. Alternatively it is possible to specify for each spectrum in `x` the name of the file to which it should be exported (and hence `file` has to be of length equal `length(x)`).

- `format`: `character(1)`, either `"mzML"` or `"mzXML"` defining the output file format.

- `copy`: `logical(1)` whether general file information should be copied from the original MS data files. This only works if `x` uses a `MsBackendMzR` backend and if `dataOrigin(x)` contains the original MS data file names.

- `BPPARAM`: parallel processing settings.

See examples in [Spectra](#) or the vignette for more details and examples.

The `MsBackendMzR` ignores parameter `columns` of the `peaksData()` function and returns **always** m/z and intensity values.

`MsBackendHdf5Peaks`, on-disk MS data backend

The `MsBackendHdf5Peaks` keeps, similar to the `MsBackendMzR`, peak data (i.e. m/z and intensity values) in custom data files (in HDF5 format) on disk while the remaining spectra variables are kept in memory. This backend supports updating and writing of manipulated peak data to the data files.

New objects can be created with the `MsBackendHdf5Peaks()` function which can be subsequently filled with data by calling the object's `backendInitialize()` method passing the desired file names of the HDF5 data files along with the spectra variables in form of a `DataFrame` (see `MsBackendDataFrame` for the expected format). An optional parameter `hdf5path` allows to specify the folder where the HDF5 data files should be stored to. If provided, this is added as the path to the submitted file names (parameter `files`).

By default `backendInitialize()` will store all peak data into a single HDF5 file which name has to be provided with the parameter `files`. To store peak data across several HDF5 files `data` has to contain a column `"dataStorage"` that defines the grouping of spectra/peaks into files: peaks for spectra with the same value in `"dataStorage"` are saved into the same HDF5 file. If parameter `files` is omitted, the value in `dataStorage` is used as file name (replacing any file ending with `".h5"`. To specify the file names, `files`' length has to match the number of unique elements in `"dataStorage"`.

For details see examples on the [Spectra()](#) help page.

The `MsBackendHdf5Peaks` ignores parameter `columns` of the `peaksData()` function and returns **always** m/z and intensity values.

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Examples

```
## The MsBackend class is a virtual class and can not be instantiated
## directly. Below we define a new backend class extending this virtual
## class
MsBackendDummy <- setClass("MsBackendDummy", contains = "MsBackend")
MsBackendDummy()

## This class inherits now all methods from `MsBackend`, all of which
## however throw an error. These methods would have to be implemented
## for the new backend class.
try(mz(MsBackendDummy()))

## See `MsBackendDataFrame` as a reference implementation for a backend
## class (in the *R/MsBackendDataFrame.R* file).

## MsBackendDataFrame
##
## The `MsBackendDataFrame` uses a `S4Vectors::DataFrame` to store all MS
## data. Below we create such a backend by passing a `DataFrame` with all
## data to it.
data <- DataFrame(msLevel = c(1L, 2L, 1L), scanIndex = 1:3)
data$mz <- list(c(1.1, 1.2, 1.3), c(1.4, 54.2, 56.4, 122.1), c(15.3, 23.2))
data$intensity <- list(c(3, 2, 3), c(45, 100, 12.2, 1), c(123, 12324.2))

## Backends are supposed to be created with their specific constructor
## function
be <- MsBackendDataFrame()

be

## The `backendInitialize()` method initializes the backend filling it with
## data. This method can take any parameters needed for the backend to
## get loaded with the data (e.g. a file name from which to load the data,
## a database connection or, in this case, a data frame containing the data).
be <- backendInitialize(be, data)

be

## Data can be accessed with the accessor methods
msLevel(be)

mz(be)

## Even if no data was provided for all spectra variables, its accessor
## methods are supposed to return a value.
precursorMz(be)

## The `peaksData()` method is supposed to return the peaks of the spectra as
## a `list`.
peaksData(be)

## List available peaks variables
```

```
peaksVariables(be)

## Use columns to extract specific peaks variables. Below we extract m/z and
## intensity values, but in reversed order to the default.
peaksData(be, columns = c("intensity", "mz"))

## List available spectra variables (i.e. spectrum metadata)
spectraVariables(be)

## Extract precursor m/z, rtime, MS level spectra variables
spectraData(be, c("precursorMz", "rtime", "msLevel"))

## MsBackendMemory
##
## The `MsBackendMemory` uses a more efficient internal data organization
## and allows also adding arbitrary additional peaks variables (annotations)
## Below we thus add a column "peak_ann" with arbitrary names/ids for each
## peak and add the name of this column to the `peaksVariables` parameter
## of the `backendInitialize()` method (in addition to `"mz"` and
## `"intensity"` that should **always** be specified.
data$peak_ann <- list(c("a", "", "d"), c("", "d", "e", "f"), c("h", "i"))
be <- backendInitialize(MsBackendMemory(), data,
    peaksVariables = c("mz", "intensity", "peak_ann"))
be

spectraVariables(be)

## peak_ann is also listed as a peaks variable
peaksVariables(be)

## The additional peaks variable can be accessed using the `peaksData()`
## function
peaksData(be, "peak_ann")

## The $<- method can be used to replace values of an existing peaks
## variable. It is important that the number of elements matches the
## number of peaks per spectrum.
be$peak_ann <- list(1:3, 1:4, 1:2)

## A peaks variable can again be removed by setting it to NULL
be$peak_ann <- NULL

peaksVariables(be)
```

MsBackendCached   *Base MsBackend class providing data caching mechanism*

Description

The MsBackendCached class is a rudimentary implementation of the [MsBackend](#) providing a simple mechanism to cache spectra data locally. This class is thought to be used as a base class for other MsBackend implementations to reuse its caching mechanism and avoid having to re-implement commonly used methods. This class is thus not thought to be used directly by a user.

The MsBackendCached caching mechanism allows MsBackend instances to add or replace spectra variables even if the backend used by them does not allow to alter values (e.g. if a SQL database is used as a backend). Any replacement operation with $<- will add the specified values to a local data.frame within the MsBackendCached class that allows to *cache* these values (increasing obviously the memory demand of the object).

Any data accessor functions of the extending MsBackend class (such as $ or msLevel() or spectraData()) should first use callNextMethod() to call the respective accessor of MsBackendCached that will evaluate if the requested spectra variable(s) are in the local cache and return these. If the requested spectra variables are neither in the local cache, nor listed in the @spectraVariables slot (which defines all spectra variables that can be requested from the extending MsBackend class) but are *core spectra variables* then missing values of the correct data type are returned.

Usage

```
MsBackendCached()

## S4 method for signature 'MsBackendCached'
backendInitialize(
  object,
  data = data.frame(),
  nspectra = 0L,
  spectraVariables = character(),
  ...
)

## S4 method for signature 'MsBackendCached'
dataStorage(object)

## S4 method for signature 'MsBackendCached'
length(x)

## S4 method for signature 'MsBackendCached'
spectraVariables(object)

## S4 method for signature 'MsBackendCached'
spectraData(object, columns = spectraVariables(object))

## S4 replacement method for signature 'MsBackendCached'
spectraData(object) <- value

## S4 method for signature 'MsBackendCached'
x[i, j, ..., drop = FALSE]

## S4 method for signature 'MsBackendCached'
x$name

## S4 replacement method for signature 'MsBackendCached'
x$name <- value

## S4 method for signature 'MsBackendCached'
selectSpectraVariables(object, spectraVariables = spectraVariables(object))
```

```
## S4 method for signature 'MsBackendCached'
show(object)

## S4 method for signature 'MsBackendCached'
acquisitionNum(object)

## S4 method for signature 'MsBackendCached'
centroided(object)

## S4 replacement method for signature 'MsBackendCached'
centroided(object) <- value

## S4 method for signature 'MsBackendCached'
collisionEnergy(object)

## S4 replacement method for signature 'MsBackendCached'
collisionEnergy(object) <- value

## S4 method for signature 'MsBackendCached'
dataOrigin(object)

## S4 replacement method for signature 'MsBackendCached'
dataOrigin(object) <- value

## S4 method for signature 'MsBackendCached'
msLevel(object)

## S4 method for signature 'MsBackendCached'
intensity(object)

## S4 method for signature 'MsBackendCached'
ionCount(object)

## S4 method for signature 'MsBackendCached'
isEmpty(x)

## S4 method for signature 'MsBackendCached'
isolationWindowLowerMz(object)

## S4 replacement method for signature 'MsBackendCached'
isolationWindowLowerMz(object) <- value

## S4 method for signature 'MsBackendCached'
isolationWindowTargetMz(object)

## S4 replacement method for signature 'MsBackendCached'
isolationWindowTargetMz(object) <- value

## S4 method for signature 'MsBackendCached'
isolationWindowUpperMz(object)

## S4 replacement method for signature 'MsBackendCached'
```

```
isolationWindowUpperMz(object) <- value

## S4 method for signature 'MsBackendCached'
lengths(x, use.names = FALSE)

## S4 method for signature 'MsBackendCached'
mz(object)

## S4 method for signature 'MsBackendCached'
polarity(object)

## S4 replacement method for signature 'MsBackendCached'
polarity(object) <- value

## S4 method for signature 'MsBackendCached'
precursorCharge(object)

## S4 method for signature 'MsBackendCached'
precursorIntensity(object)

## S4 method for signature 'MsBackendCached'
precursorMz(object)

## S4 method for signature 'MsBackendCached'
rtime(object)

## S4 replacement method for signature 'MsBackendCached'
rtime(object) <- value

## S4 method for signature 'MsBackendCached'
scanIndex(object)

## S4 method for signature 'MsBackendCached'
smoothed(object)

## S4 replacement method for signature 'MsBackendCached'
smoothed(object) <- value
```

Arguments

object	A MsBackendCached object.
data	For backendInitialize(): (optional) data.frame with cached values. The number of rows (and their order) has to match the number of spectra.
nspectra	For backendInitialize(): integer with the number of spectra.
spectraVariables	
	For backendInitialize(): character with the names of the spectra variables that are provided by the extending backend. For selectSpectraVariables(): character specifying the spectra variables to keep.
...	ignored
x	A MsBackendCached object.
columns	For spectraData(): character with the names of the spectra variables to retrieve.

value	replacement value for <- methods. See individual method description or expected data type.
i	For [: integer with the indices to subset the object.
j	For [: ignored.
drop	For [: not considered.
name	For $<-: the name of the spectra variable to set.
use.names	For lengths(): whether spectrum names should be used.

Value

See documentation of respective function.

Implementation notes

Classes extending the MsBackendCached need to

- call the backendInitialize() method of this class in their own backendInitialize() method and set at least the number of spectra with the nspectra parameter and the spectraVariables that are available to the (extending) backend class.

- implement the spectraData() method that also calls the spectraData() method from MsBackendCached to also retrieve cached values (e.g. using res <- callNextMethod() at the beginning of the spectraData function). The spectraData,MsBackendCached method will return NULL if the selected spectra variables were not cached and are not *core spectra variables* not being provided by the extending backend. Thus, the extending backend can then proceed to retrieve the respective values from its own backend/data storage.

- implement eventually the [method that calls in addition the [from the MsBackendCached.

All other methods accessing or setting spectra variables don't need to be implemented by the extending backend class (the default implementations of the MsBackendCached will then be used instead; these ensure that cached values are returned first). Spectra variables can be modified or added using the $<- method of the MsBackendCached. Replacing or adding multiple variables using the spectraData<- is not supported by MsBackendCached. The extending backend might however implement such a method that internally uses $<- to add/replace single variables.

The MsBackendCached has the following slots:

- nspectra: integer(1) defining the number of spectra of the backend. This variable needs to be set and must match the number of rows of localData and the actual number of spectra in the (extending) backend.

- localData: data.frame with the cached local data. Any replacement operation with $<- will set/add a column with the respective values.

- spectraVariables: character defining the spectra variables that are provided by the extending MsBackend class (e.g. all spectra variables that can be retrieved from the data base or original data files).

Available methods

- acquisitionNum(): returns the acquisition number of each spectrum. Returns an integer of length equal to the number of spectra (with NA_integer_ if not available).

- backendInitialize(): *initializes* the backend. The method takes parameters data (data.frame with cached data), nspectra (integer defining the number of spectra) and spectraVariables (character with the spectra variables that are provided by the extending backend.

- `centroided()`, `centroided<-`: gets or sets the centroiding information of the spectra. `centroided` returns a `logical` vector of length equal to the number of spectra with `TRUE` if a spectrum is centroided, `FALSE` if it is in profile mode and `NA` if it is undefined. See also `isCentroided` for estimating from the spectrum data whether the spectrum is centroided. `value` for `centroided<-` is either a single `logical` or a `logical` of length equal to the number of spectra in `object`.

- `collisionEnergy()`, `collisionEnergy<-`: gets or sets the collision energy for all spectra in `object`. `collisionEnergy()` returns a `numeric` with length equal to the number of spectra (`NA_real_` if not present/defined), `collisionEnergy<-` takes a `numeric` of length equal to the number of spectra in `object`.

- `dataOrigin()`: gets a `character` of length equal to the number of spectra in `object` with the *data origin* of each spectrum. This could e.g. be the mzML file from which the data was read.

- `intensity()`: gets the intensity values from the spectra. Returns a NumericList() of numeric vectors (intensity values for each spectrum). The length of the `list` is equal to the number of `spectra` in `object`.

- `ionCount()`: returns a `numeric` with the sum of intensities for each spectrum. If the spectrum is empty (see `isEmpty()`), `NA_real_` is returned.

- `isEmpty()`: checks whether a spectrum in `object` is empty (i.e. does not contain any peaks). Returns a `logical` vector of length equal number of spectra.

- `isolationWindowLowerMz()`, `isolationWindowLowerMz<-`: gets or sets the lower m/z boundary of the isolation window.

- `isolationWindowTargetMz()`, `isolationWindowTargetMz<-`: gets or sets the target m/z of the isolation window.

- `isolationWindowUpperMz()`, `isolationWindowUpperMz<-`: gets or sets the upper m/z boundary of the isolation window.

- `length()`: returns the number of spectra (i.e. the @nspectra).

- `lengths()`: gets the number of peaks (m/z-intensity values) per spectrum. Returns an `integer` vector (length equal to the number of spectra). For empty spectra, `0` is returned.

- `msLevel()`: gets the spectra's MS level. Returns an `integer` vector (of length equal to the number of spectra) with the MS level for each spectrum (or `NA_integer_` if not available).

- `mz()`: gets the mass-to-charge ratios (m/z) from the spectra. Returns a NumericList() or length equal to the number of spectra, each element a `numeric` vector with the m/z values of one spectrum.

- `polarity()`, `polarity<-`: gets or sets the polarity for each spectrum. `polarity` returns an `integer` vector (length equal to the number of spectra), with `0` and `1` representing negative and positive polarities, respectively. `polarity<-` expects an integer vector of length 1 or equal to the number of spectra.

- `precursorCharge()`, `precursorIntensity()`, `precursorMz()`, `precScanNum()`, `precAcquisitionNum()`: get the charge (`integer`), intensity (`numeric`), m/z (`numeric`), scan index (`integer`) and acquisition number (`interger`) of the precursor for MS level 2 and above spectra from the object. Returns a vector of length equal to the number of spectra in `object`. NA are reported for MS1 spectra of if no precursor information is available.

- `rtime()`, `rtime<-`: gets or sets the retention times for each spectrum (in seconds). `rtime()` returns a `numeric` vector (length equal to the number of spectra) with the retention time for each spectrum. `rtime<-` expects a numeric vector with length equal to the number of spectra.

- `scanIndex()`: returns an `integer` vector with the *scan index* for each spectrum. This represents the relative index of the spectrum within each file. Note that this can be different to the `acquisitionNum()` of the spectrum which is the index of the spectrum as reported in the mzML file.

- selectSpectraVariables(): subset the object to specified spectra variables. This will eventually remove spectra variables listed in @spectraVariables and will also drop columns from the local cache if not among spectraVariables.

- smoothed(),smoothed<-: gets or sets whether a spectrum is *smoothed*. smoothed() returns a logical vector of length equal to the number of spectra. smoothed<- takes a logical vector of length 1 or equal to the number of spectra in object.

- spectraVariables(): returns the available spectra variables, i.e. the unique set of *core spectra variables*, cached spectra variables and spectra variables defined in the @spectraVariables slot (i.e. spectra variables thought to be provided by the extending MsBackend instance).

- spectraData(): returns a DataFrame with cached spectra variablers or initialized *core spectra variables*. Parameter spectraVariables allows to specify the variables to retrieve. The function returns NULL if the requested variables are not cached and are not provided by the extending backend. Note that this method **only** returns cached spectra variables or core spectra variables **not** provided by the extending backend. It is the responsibility of the extending backend to add/provide these.

- [: subsets the cached data. Parameter i needs to be an integer vector.

- $, $<-: access or set/add a single spectrum variable (column) in the backend.

Author(s)

Johannes Rainer

See Also

MsBackend for the documentation of MS backends.

---

neutralLoss	*Calculate Neutral Loss Spectra*

Description

This help page lists functions that convert MS/MS spectra to neutral loss spectra. The main function for this is neutralLoss and the specific algorithm to be used is defined (and configured) with dedicated *parameter* objects (paramer param of the neutralLoss() function).

The parameter objects for the different algorithms are:

- PrecursorMzParam(): calculates neutral loss spectra as in Aisporna *et al.* 2022 by subtracting the (fragment's) peak m/z value from the precursor m/z value of each spectrum (precursor m/z - fragment m/z). Parameter msLevel allows to restrict calculation of neutral loss spectra to specified MS level(s). Spectra from other MS level(s) are returned as-is. Parameter filterPeaks allows to remove certain peaks from the neutral loss spectra. By default (filterPeaks = "none") no filtering takes place. With filterPeaks = "removePrecursor" all fragment peaks with an m/z value matching the precursor m/z (considering also ppm and tolerance are removed. With filterPeaks = "abovePrecursor", all fragment peaks with an m/z larger than the precursor m/z (m/z > precursor m/z - tolerance - ppm of the precursor m/z) are removed (thus removing also in most cases the fragment peaks representing the precursor). Finally, with filterPeaks = "belowPrecursor" all fragment peaks with an m/z smaller than the precursor m/z (m/z < precursor m/z + tolerance + ppm of the precursor m/z) are removed. Also in this case the precursor fragment peak is (depending on the values of ppm and tolerance) removed.

Usage

```
neutralLoss(object, param, ...)

PrecursorMzParam(
 filterPeaks = c("none", "abovePrecursor", "belowPrecursor", "removePrecursor"),
  msLevel = c(2L, NA_integer_),
  ppm = 10,
  tolerance = 0
)

## S4 method for signature 'Spectra,PrecursorMzParam'
neutralLoss(object, param, ...)
```

Arguments

object	[Spectra()](#) object with the fragment spectra for which neutral loss spectra should be calculated.
param	One of the *parameter* objects discussed below.
...	Currently ignored.
filterPeaks	For PrecursorMzParam(): character(1) or function defining if and how fragment peaks should be filtered before calculation. Pre-defined options are: "none" (keep all peaks), "abovePrecursor" (removes all fragment peaks with an m/z >= precursor m/z), "belowPrecursor" (removes all fragment peaks with an m/z <= precursor m/z). In addition, it is possible to pass a custom function with this parameter with arguments x (two column peak matrix) and precursorMz (the precursor m/z) that returns the sub-setted two column peak matrix.
msLevel	integer defining for which MS level(s) the neutral loss spectra should be calculated. Defaults to msLevel = c(2L, NA) thus, neutral loss spectra will be calculated for all spectra with MS level equal to 2 or with missing/undefined MS level. All spectra with a MS level different than msLevel will be returned unchanged.
ppm	numeric(1) with m/z-relative acceptable difference in m/z values to filter peaks. Defaults to ppm = 10. See function description for details.
tolerance	numeric(1) with absolute acceptable difference in m/z values to filter peaks. Defaults to tolerance = 0. See function description for details.

Value

A [Spectra()](#) object with calculated neutral loss spectra.

Note

By definition, mass peaks in a Spectra object need to be ordered by their m/z value (in increasing order). Thus, the order of the peaks in the calculated neutral loss spectra might not be the same than in the original Spectra object.

Note also that for spectra with a missing precursor m/z empty spectra are returned (i.e. spectra without peaks) since it is not possible to calcualte the neutral loss spectra.

Author(s)

Johannes Rainer

References

Aisporna A, Benton PH, Chen A, Derks RJE, Galano JM, Giera M and Siuzdak G (2022). Neu-
tral Loss Mass Spectral Data Enhances Molecular Similarity Analysis in METLIN. Journal of the
American Society for Mass Spectrometry. doi:10.1021/jasms.1c00343

Examples

```
## Create a simple example Spectra object with some MS1, MS2 and MS3 spectra.
DF <- DataFrame(msLevel = c(1L, 2L, 3L, 1L, 2L, 3L),
                precursorMz = c(NA, 40, 20, NA, 300, 200))
DF$mz <- IRanges::NumericList(
                    c(3, 12, 14, 15, 16, 200),
                    c(13, 23, 39, 86),
                    c(5, 7, 20, 34, 50),
                    c(5, 7, 9, 20, 100),
                    c(15, 53, 299, 300),
                    c(34, 56, 100, 200, 204, 309)
                  , compress = FALSE)
DF$intensity <- IRanges::NumericList(1:6, 1:4, 1:5, 1:5, 1:4, 1:6,
                                     compress = FALSE)
sps <- Spectra(DF, backend = MsBackendDataFrame())

## Calculate neutral loss spectra for all MS2 spectra, keeping MS1 and MS3
## spectra unchanged.
sps_nl <- neutralLoss(sps, PrecursorMzParam(msLevel = 2L))
mz(sps)
mz(sps_nl)

## Calculate neutral loss spectra for MS2 and MS3 spectra, removing peaks
## with an m/z >= precursorMz
sps_nl <- neutralLoss(sps, PrecursorMzParam(
    filterPeaks = "abovePrecursor", msLevel = 2:3))
mz(sps_nl)
## This removed also the peak with m/z 39 from the second spectrum

## Removing all fragment peaks matching the precursor m/z with a tolerance
## of 1 and ppm 10
sps_nl <- neutralLoss(sps, PrecursorMzParam(
    filterPeaks = "removePrecursor", tolerance = 1, ppm = 10, msLevel = 2:3))
mz(sps_nl)

## Empty spectra are returned for MS 2 spectra with undefined precursor m/z.
sps$precursorMz <- NA_real_
sps_nl <- neutralLoss(sps, PrecursorMzParam())
mz(sps_nl)
```

---

plotMzDelta   *MZ delta Quality Control*

Description

The M/Z delta plot illustrates the suitability of MS2 spectra for identification by plotting the M/Z
differences of the most intense peaks. The resulting histogram should optimally show modes at
amino acid residu masses. The plots have been described in Foster et al. 2011.

Only a certain percentage of most intense MS2 peaks are taken into account to use the most significant signal. Default value is 20% (see `percentage` argument). The difference between peaks is then computed for all individual spectra and their distribution is plotted as a histogram. Delta M/Z between 40 and 200 are plotted by default, to encompass the residue masses of all amino acids and several common contaminants, although this can be changes with the `mzRange` argument.

In addition to the processing described above, isobaric reporter tag peaks and the precursor peak can also be removed from the MS2 spectrum, to avoid interence with the fragment peaks.

Note that figures in Foster et al. 2011 have been produced and optimised for centroided data. While running the function on profile mode is likely fine, it is recommended to use centroided data.

A `ggplot2` based function called `ggMzDeltaPlot()` to visualise the M/Z delta distributions is available at <https://gist.github.com/lgatto/c72b1ff5a4116118dbb34d9d2bc3470a>.

Usage

```
computeMzDeltas(
  object,
  percentage = 0.2,
  mzRange = c(40, 200),
  BPPARAM = BiocParallel::bpparam()
)

plotMzDelta(x, aaLabels = TRUE)
```

Arguments

`object`	An instance of class `Spectra()`.
`percentage`	`numeric(1)` between 0 and 1 indicating the percentage of the most intense peaks in each MS2 spectrum to include in the calculation. Default is 0.2.
`mzRange`	`numeric(2)` with the upper and lower M/Z to be used to the MZ deltas. Default is `c(40, 200)`.
`BPPARAM`	An optional `BiocParallelParam` instance determining the parallel back-end to be used during evaluation. Default is to use `BiocParallel::bpparam()`. See `?BiocParallel::bpparam` for details.
`x`	A list of M/Z delta values, as returned by `computeMzDeltas()`.
`aaLabels`	`logical(1)` defining whether the amino acids should be labelled on the histogram. Default is `TRUE`.

Value

`computeMzDeltas()` returns a `list` of numeric vectors. `plotMzDelta()` is used to visualise of M/Z delta distributions.

Author(s)

Laurent Gatto with contributions (to MSnbase) of Guangchuang Yu.

References

Foster JM, Degroeve S, Gatto L, Visser M, Wang R, Griss J, et al. A posteriori quality control for the curation and reuse of public proteomics data. Proteomics. 2011;11: 2182-2194. http://dx.doi.org/10.1002/pmic.201000602

Examples

```
library(msdata)
f <- proteomics(pattern = "TMT.+20141210.mzML.gz", full.names = TRUE)
sp <- Spectra(f)

d <- computeMzDeltas(sp[1:1000])
plotMzDelta(d)
```

---

processingChunkSize   *Parallel and chunk-wise processing of* Spectra

---

Description

Many operations on Spectra objects, specifically those working with the actual MS data (peaks data), allow a chunk-wise processing in which the Spectra is splitted into smaller parts (chunks) that are iteratively processed. This enables parallel processing of the data (by data chunk) and also reduces the memory demand since only the MS data of the currently processed subset is loaded into memory and processed. This chunk-wise processing, which is by default disabled, can be enabled by setting the processing chunk size of a Spectra with the processingChunkSize() function to a value which is smaller than the length of the Spectra object. Setting processingChunkSize(sps) <- 1000 will cause any data manipulation operation on the sps, such as filterIntensity() or bin(), to be performed eventually in parallel for sets of 1000 spectra in each iteration.

Such chunk-wise processing is specifically useful for Spectra objects using an *on-disk* backend or for very large experiments. For small data sets or Spectra using an in-memory backend, a direct processing might however be more efficient. Setting the chunk size to Inf will disable the chunk-wise processing.

For some backends a certain type of splitting and chunk-wise processing might be preferable. The MsBackendMzR backend for example needs to load the MS data from the original (mzML) files, hence chunk-wise processing on a per-file basis would be ideal. The [backendParallelFactor()](#) function for MsBackend allows backends to suggest a preferred splitting of the data by returning a factor defining the respective data chunks. The MsBackendMzR returns for example a factor based on the *dataStorage* spectra variable. A factor of length 0 is returned if no particular preferred splitting should be performed. The suggested chunk definition will be used if no finite processingChunkSize() is defined. Setting the processingChunkSize overrides backendParallelFactor.

See the *Large-scale data handling and processing with Spectra* for more information and examples.

Functions to configure parallel or chunk-wise processing:

- processingChunkSize(): allows to get or set the size of the chunks for parallel processing or chunk-wise processing of a Spectra in general. With a value of Inf (the default) no chunk-wise processing will be performed.

- processingChunkFactor(): returns a factor defining the chunks into which a Spectra will be split for chunk-wise (parallel) processing. A factor of length 0 indicates that no chunk-wise processing will be performed.

Usage

```
processingChunkSize(x)

processingChunkSize(x) <- value

processingChunkFactor(x)
```

Arguments

x	Spectra.
value	integer(1) defining the chunk size.

Value

processingChunkSize() returns the currently defined processing chunk size (or Inf if it is not defined). processingChunkFactor() returns a factor defining the chunks into which x will be split for (parallel) chunk-wise processing or a factor of length 0 if no splitting is defined.

Note

Some backends might not support parallel processing at all. For these, the backendBpparam() function will always return a SerialParam() independently on how parallel processing was defined.

Author(s)

Johannes Rainer

---

spectra-plotting   *Plotting Spectra*

Description

[Spectra()](#) can be plotted with one of the following functions

- plotSpectra(): plots each spectrum in its separate plot by splitting the plot area into as many panels as there are spectra.
- plotSpectraOverlay(): plots all spectra in x **into the same** plot (as an overlay).
- plotSpectraMirror(): plots a pair of spectra as a *mirror plot*. Parameters x and y both have to be a Spectra of length 1. Matching peaks (considering ppm and tolerance) are highlighted. See [common()](#) for details on peak matching. Parameters matchCol, matchLty, matchLwd and matchPch allow to customize how matching peaks are indicated.

Usage

```
plotSpectra(
  x,
  xlab = "m/z",
  ylab = "intensity",
  type = "h",
  xlim = numeric(),
  ylim = numeric(),
  main = character(),
  col = "#00000080",
  labels = character(),
  labelCex = 1,
  labelSrt = 0,
  labelAdj = NULL,
```

```
    labelPos = NULL,
    labelOffset = 0.5,
    labelCol = "#00000080",
    asp = 1,
    ...
)

plotSpectraOverlay(
    x,
    xlab = "m/z",
    ylab = "intensity",
    type = "h",
    xlim = numeric(),
    ylim = numeric(),
    main = paste(length(x), "spectra"),
    col = "#00000080",
    labels = character(),
    labelCex = 1,
    labelSrt = 0,
    labelAdj = NULL,
    labelPos = NULL,
    labelOffset = 0.5,
    labelCol = "#00000080",
    axes = TRUE,
    frame.plot = axes,
    ...
)

## S4 method for signature 'Spectra'
plotSpectraMirror(
    x,
    y,
    xlab = "m/z",
    ylab = "intensity",
    type = "h",
    xlim = numeric(),
    ylim = numeric(),
    main = character(),
    col = "#00000080",
    labels = character(),
    labelCex = 1,
    labelSrt = 0,
    labelAdj = NULL,
    labelPos = NULL,
    labelOffset = 0.5,
    labelCol = "#00000080",
    axes = TRUE,
    frame.plot = axes,
    ppm = 20,
    tolerance = 0,
    matchCol = "#80B1D3",
    matchLwd = 1,
```

```
    matchLty = 1,
    matchPch = 16,
    ...
)
```

Arguments

x	a [Spectra()](#) object. For plotSpectraMirror() it has to be an object of length 2.
xlab	character(1) with the label for the x-axis (by default xlab = "m/z").
ylab	character(1) with the label for the y-axis (by default ylab = "intensity").
type	character(1) specifying the type of plot. See [plot.default()](#) for details. Defaults to type = "h" which draws each peak as a line.
xlim	numeric(2) defining the x-axis limits. The range of m/z values are used by default.
ylim	numeric(2) defining the y-axis limits. The range of intensity values are used by default.
main	character(1) with the title for the plot. By default the spectrum's MS level and retention time (in seconds) is used.
col	color to be used to draw the peaks. Should be either of length 1, or equal to the number of spectra (to plot each spectrum in a different color) or be a list with colors for each individual peak in each spectrum.
labels	allows to specify a label for each peak. Can be a character with length equal to the number of peaks, or, ideally, a function that uses one of the Spectra's variables (see examples below). plotSpectraMirror() supports only labels of type *function*.
labelCex	numeric(1) giving the amount by which the text should be magnified relative to the default. See parameter cex in [par()](#).
labelSrt	numeric(1) defining the rotation of the label. See parameter srt in [text()](#).
labelAdj	see parameter adj in [text()](#).
labelPos	see parameter pos in [text()](#).
labelOffset	see parameter offset in [text()](#).
labelCol	color for the label(s).
asp	for plotSpectra(): the target ratio (columns / rows) when plotting mutliple spectra (e.g. for 20 spectra use asp = 4/5 for 4 columns and 5 rows or asp = 5/4 for 5 columns and 4 rows; see [grDevices::n2mfrow()](#) for details).
...	additional parameters to be passed to the [plot.default()](#) function.
axes	logical(1) whether (x and y) axes should be drawn.
frame.plot	logical(1) whether a box should be drawn around the plotting area.
y	for plotSpectraMirror(): Spectra object of length 1 against which x should be plotted against.
ppm	for plotSpectraMirror(): m/z relative acceptable difference (in ppm) for peaks to be considered matching (see [common()](#) for more details).
tolerance	for plotSpectraMirror(): absolute acceptable difference of m/z values for peaks to be considered matching (see [common()](#) for more details).
matchCol	for plotSpectraMirror(): color for matching peaks.

matchLwd   for plotSpectraMirror(): line width (lwd) to draw matching peaks. See
                par() for more details.

matchLty   for plotSpectraMirror(): line type (lty) to draw matching peaks. See par()
                for more details.

matchPch   for plotSpectraMirror(): point character (pch) to label matching peaks. De-
                faults to matchPch = 16, set to matchPch = NA to disable. See par() for more
                details.

Value

These functions create a plot.

Author(s)

Johannes Rainer, Sebastian Gibb, Laurent Gatto

Examples

```
ints <- list(c(4.3412, 12, 8, 34, 23.4),
    c(8, 25, 16, 32))
mzs <- list(c(13.453421, 43.433122, 46.6653553, 129.111212, 322.24432),
    c(13.452, 43.5122, 129.112, 322.245))

df <- DataFrame(msLevel = c(1L, 1L), rtime = c(123.12, 124))
df$mz <- mzs
df$intensity <- ints
sp <- Spectra(df)

#### ----------------------------------------- ####
##                     plotSpectra                    ##

## Plot one spectrum.
plotSpectra(sp[1])

## Plot both spectra.
plotSpectra(sp)

## Define a color for each peak in each spectrum.
plotSpectra(sp, col = list(c(1, 2, 3, 4, 5), 1:4))

## Color peaks from each spectrum in different colors.
plotSpectra(sp, col = c("green", "blue"))

## Label each peak with its m/z.
plotSpectra(sp, labels = function(z) format(unlist(mz(z)), digits = 4))

## Rotate the labels.
plotSpectra(sp, labels = function(z) format(unlist(mz(z)), digits = 4),
    labelPos = 2, labelOffset = 0.1, labelSrt = -30)

## Add a custom annotation for each peak.
sp$label <- list(c("", "A", "B", "C", "D"),
    c("Frodo", "Bilbo", "Peregrin", "Samwise"))
## Plot each peak in a different color
plotSpectra(sp, labels = function(z) unlist(z$label),
    col = list(1:5, 1:4))
```

```
## Plot a single spectrum specifying the label.
plotSpectra(sp[2], labels = c("A", "B", "C", "D"))


#### ------------------------------------------ ####
##                plotSpectraOverlay            ##

## Plot both spectra overlaying.
plotSpectraOverlay(sp)

## Use a different color for each spectrum.
plotSpectraOverlay(sp, col = c("#ff000080", "#0000ff80"))

## Label also the peaks with their m/z if their intensity is above 15.
plotSpectraOverlay(sp, col = c("#ff000080", "#0000ff80"),
    labels = function(z) {
        lbls <- format(mz(z)[[1L]], digits = 4)
        lbls[intensity(z)[[1L]] <= 15] <- ""
        lbls
    })
abline(h = 15, lty = 2)

## Use different asp values
plotSpectra(sp, asp = 1/2)
plotSpectra(sp, asp = 2/1)

#### ------------------------------------------ ####
##                plotSpectraMirror             ##

## Plot two spectra against each other.
plotSpectraMirror(sp[1], sp[2])

## Label the peaks with their m/z
plotSpectraMirror(sp[1], sp[2],
    labels = function(z) format(mz(z)[[1L]], digits = 3),
    labelSrt = -30, labelPos = 2, labelOffset = 0.2)
grid()

## The same plot with a tolerance of 0.1 and using a different color to
## highlight matching peaks
plotSpectraMirror(sp[1], sp[2],
    labels = function(z) format(mz(z)[[1L]], digits = 3),
    labelSrt = -30, labelPos = 2, labelOffset = 0.2, tolerance = 0.1,
    matchCol = "#ff000080", matchLwd = 2)
grid()
```

---

spectraVariableMapping

Mapping between spectra variables and data file fields

Description

The spectraVariableMapping function provides the mapping between *spectra variables* of a [Spectra()](Spectra) object with data fields from a data file. Such name mapping is expected to enable

an easier import of data files with specific *dialects*, e.g. files in MGF format that use a different naming convention for core spectra variables.

MsBackend() implementations are expected to implement this function (if needed) to enable import of data from file formats with non-standardized data fields.

Usage

```
spectraVariableMapping(object, ...)
```

Arguments

object	An instance of an object extending MsBackend().
...	Optional parameters.

Value

A named character with names being spectra variable names (use spectraVariables() for a list of supported names) and values being the data field names.

Author(s)

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