

Package ‘Chromatograms’

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Title Infrastructure for Chromatographic Mass Spectrometry Data

Version 1.0.0

Description The Chromatograms packages defines an efficient infrastructure for storing and handling of chromatographic mass spectrometry data. It provides different implementations of **backends** to store and represent the data. Such backends can be optimized for small memory footprint or fast data access/processing. A lazy evaluation queue and chunk-wise processing capabilities ensure efficient analysis of also very large data sets.

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Chromatograms	<i>The Chromatograms class to manage and access chromatographic data</i>
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Description

The Chromatograms class encapsules chromatographic data and related metadata. The chromatographic data is represented by a *backend* extending the virtual [ChromBackend](#) class which provides the raw data to the Chromatograms object. Different backends and their properties are deccribed in the [ChromBackend](#) class documentation.

Usage

```
## S4 method for signature 'ChromBackendOrMissing'
Chromatograms(object = ChromBackendMemory(), processingQueue = list(), ...)

## S4 method for signature 'Spectra'
Chromatograms(
  object,
  summarize.method = c("sum", "max"),
  chromData = data.frame(),
  factorize.by = c("msLevel", "dataOrigin"),
  spectraVariables = character(),
  ...
)

## S4 method for signature 'Chromatograms,ChromBackend'
setBackend(
```

```

    object,
    backend,
    f = processingChunkFactor(object),
    BPPARAM = SerialParam(),
    ...
)

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

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

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

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

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

## S4 method for signature 'Chromatograms'
factorize(object, factorize.by = c("msLevel", "dataOrigin"), ...)

## S4 method for signature 'Chromatograms'
chromExtract(object, peak.table, by, ...)

```

Arguments

object	A Chromatograms object.
processingQueue	list a list of processing steps (i.e. functions) to be applied to the chromatographic data. The processing steps are applied in the order they are listed in the <code>processingQueue</code> .
...	Additional arguments.
summarize.method	For <code>Chromatograms</code> created with a <code>Spectra</code> object: A character vector with the name of the function to be used to summarize the spectra data intensity. The available methods are "sum" and "max". The default is "sum".
chromData	For <code>Chromatograms()</code> build from a <code>Spectra</code> object backend, a <code>data.frame</code> with the chromatographic data. If not provided (or if empty), a default <code>data.frame</code> with the core chromatographic variables will be created.
factorize.by	A character vector with the names of the variables in the <code>Spectra</code> object and the <code>chromData</code> slot that should be used to factorize the <code>Spectra</code> object data to generate the chromatographic data.
spectraVariables	A character vector specifying which variables from the <code>Spectra</code> object should be added to the <code>chromData</code> . These will be mapped using the <code>chromSpectraIndex</code> variable.
backend	ChromBackend object providing the raw data for the <code>Chromatograms</code> object.

f	factor defining the grouping to split the Chromatograms object.
BPPARAM	Parallel setup configuration. See <code>BiocParallel::bpparam()</code> for more information.
x	A Chromatograms object.
name	A character string specifying the name of the variable to access.
value	The value to replace the variable with.
i	For <code>[]</code> : integer, logical or character to subset the object.
j	For <code>[]</code> and <code>[[]</code> : ignored.
drop	For <code>[]</code> : logical(1) default to FALSE.
peak.table	For <code>chromExtract()</code> A data frame containing the following minimum columns: - <code>rtMin</code> : Minimum retention time for each peak. Cannot be NA. - <code>rtMax</code> : Maximum retention time for each peak. Cannot be NA. - <code>mzMin</code> : Minimum m/z value for each peak. - <code>mzMax</code> : Maximum m/z value for each peak. Additionally, the <code>peak.table</code> must include columns that uniquely identify chromatograms in the object. Common choices are "msLevel" and/or "dataOrigin". These columns must also be present in the <code>chromData</code> of the object. Any extra columns in <code>peak.table</code> will be added to the <code>chromData</code> of the newly created object.
by	A character vector naming one or more columns that uniquely identify chromatograms in both <code>peak.table</code> and <code>chromData(object)</code> . The combination of these columns must be unique within <code>chromData(object)</code> . Typically includes "dataOrigin", "msLevel", or both.

Value

Refer to the individual function description for information on the return value.

Creation of objects

Chromatograms objects can be created using the `Chromatograms()` construction function. Either by providing a `ChromBackend` object or by providing a `Spectra` object. The `Spectra` object will be used to generate a `Chromatograms` object with a backend of class `ChromBackendSpectra`.

Data stored in a Chromatograms object

The `Chromatograms` object is a container for chromatographic data, which includes peaks data (*retention time* and related intensity values, also referred to as *peaks data variables* in the context of `Chromatograms`) and metadata of individual chromatogram (so called *chromatograms variables*). While a core set of chromatograms variables (the `coreChromatogramsVariables()`) and peaks data variables (the `corePeaksVariables()`) are guaranteed to be provided by a `Chromatograms`, it is possible to add arbitrary variables to a `Chromatograms` object.

The `Chromatograms` object is designed to contain chromatographic data of a (large) set of chromatograms. The data is organized *linearly* and can be thought of a list of chromatograms, i.e. each element in the `Chromatograms` is one chromatogram.

The *chromatograms variables* information in the `Chromatograms` object can be accessed using the `chromData()` function. Specific chromatograms variables can be accessed by either precisising the "columns" parameter in `chromData()` or using `$`. `chromData` can be accessed, replaced but also filtered/subsetted. Refer to the [chromData](#) documentation for more details.

The *peaks data variables* information in the `Chromatograms` object can be accessed using the `peaksData()` function. Specific peaks variables can be accessed by either precisising the "columns"

parameter in `peaksData()` or using `$`. `peaksData` can be accessed, replaced but also filtered/subsetted. Refer to the [peaksData](#) documentation for more details.

Processing of Chromatograms objects

Functions that process the chromatograms data in some ways can be applied to the object either directly or by using the `processingQueue` mechanism. The `processingQueue` is a list of processing steps that are stored within the object and only applied when needed. This was created so that the data can be processed in a single step and is very useful for larger datasets. This is even more true as this processing queue will call function that can be applied on the data in a chunk-wise manner. This allows for parallel processing of the data and reduces the memory demand. To read more about the `processingQueue`, and how to parallelize your processes, see the [processingQueue](#) documentation.

Subsetting and accessing data

The `Chromatograms` class supports subsetting by chromatogram (i.e. rows) using the `[]` operator. The `[]` operator does not support subsetting by columns. Specific chromatograms or peaks variables can be accessed using the `[[` operator or the `$` operator. The `[[` operator can also be used to replace specific chromatograms or peaks variables.

Changing the backend

The `setBackend()` function can be used to change the backend of a `Chromatograms` object. This can be useful to switch to a backend that better suits the needs of the user, for example switching to a memory-based backend for smaller datasets or to a file-based backend for larger datasets. The `setBackend()` function supports parallelization of the backend conversion using the `BPPARAM` parameter.

Extracting chromatograms based on a peak table

The `chromExtract()` function allows users to extract specific regions of interest from a `Chromatograms` object based on a user-provided peak table. Each row in the `peak.table` defines a region to extract, using minimum and maximum retention time (and m/z in the case of `chromBackendSpectra`) boundaries, and identifiers that uniquely match chromatograms in the object.

The resulting **new** `Chromatograms` object contains only chromatograms overlapping the specified regions, with updated metadata reflecting the extracted boundaries.

This function is most commonly used to subset chromatographic data around detected peaks or pre-defined time/mass ranges, for example to reprocess, visualize, or quantify extracted chromatograms corresponding to known features.

Note

This needs to be discussed, if we want for example to be able to set a backend to `ChromBackendMzR` we need to implement `backendInitialize()` better. = Support `peaksData` and `chromData` as arguments AND have a way to write `.mzml` files (which we do not have for chromatographic data).

See Also

[chromData](#) for a general description of the chromatographic metadata available in the object, as well as how to access, replace and subset them. [peaksData](#) for a general description of the chromatographic peaks data available in the object, as well as how to access, replace and subset them. [processingQueue](#) for more information on the queuing of processings and parallelization for larger dataset.

Examples

```

library(MsBackendMetaboLights)
library(Spectra)

## Create a Chromatograms object from a Spectra object.
be <- backendInitialize(MsBackendMetaboLights(),
  mtblsId = "MTBLS39",
  filePattern = c("63B.cdf")
)
s <- Spectra(be)
s <- setBackend(s, MsBackendMemory())
be <- backendInitialize(new("ChromBackendSpectra"), s)
chr <- Chromatograms(be)

## Subset
chr[1:2]

## access a specific variables
chr[["msLevel"]]
chr$msLevel

## Replace data of a specific variable
chr$msLevel <- c(2L, 2L, 2L)

## Can re factorize the data
chr <- factorize(chr)

## Can also change the backend into memory
chr <- setBackend(chr, ChromBackendMemory())

chr

```

ChromBackendMemory *Improved in-memory Chromatographic data backend*

Description

ChromBackendMemory: This backend stores chromatographic data directly in memory, making it ideal for small datasets or testing. It can be initialized with a `data.frame` of chromatographic data via the `chromData` parameter and a list of `data.frame` entries for peaks data using the `peaksData` parameter. These data can be accessed with the `chromData()` and `peaksData()` functions.

Usage

```

ChromBackendMemory()

## S4 method for signature 'ChromBackendMemory'
backendInitialize(
  object,
  chromData = fillCoreChromVariables(data.frame()),
  peaksData = list(.EMPTY_PEAKS_DATA),
  ...
)

```

Arguments

object	A ChromBackendMemory object.
chromData	For backendInitialize() of a ChromBackendMemory backend, a data.frame with the chromatographic data. If not provided (or if empty), a default data.frame with the core chromatographic variables will be created.
peaksData	For backendInitialize() of a ChromBackendMemory backend, a list of data.frame with the peaks data. If not provided (or if empty), a default list of empty data.frame with the core peaks variables will be created. The length of the list should match the number of chromatograms in the chromData parameter.
...	Additional parameters to be passed.

Value

Refer to the individual function description for information on the return value.

Author(s)

Philippine Louail

Examples

```
## Create a ChromBackendMemory object
cbm <- ChromBackendMemory()

## Initialize the ChromBackendMemory object with a data.frame of
## chromatographic data and a list of data.frame of peaks data
cdata <- data.frame(
  msLevel = c(1L, 1L, 1L),
  mz = c(112.2, 123.3, 134.4),
  dataOrigin = c("mem1", "mem2", "mem3")
)

pdata <- list(
  data.frame(
    rtime = c(12.4, 12.8, 13.2, 14.6),
    intensity = c(123.3, 153.6, 2354.3, 243.4)
  ),
  data.frame(
    rtime = c(45.1, 46.2),
    intensity = c(100, 80.1)
  ),
  data.frame(
    rtime = c(12.4, 12.8, 13.2, 14.6),
    intensity = c(123.3, 153.6, 2354.3, 243.4)
  )
)

cbm <- backendInitialize(cbm, chromData = cdata, peaksData = pdata)
cbm
```

Description

The ChromBackendMzR inherits all slots and methods from the base ChromBackendMemory backend, providing additional functionality for reading chromatographic data from mzML files.

Unlike the ChromBackendMemory backend, the ChromBackendMzR backend should have the *dataOrigin* chromatographic variables populated with the file path of the mzML file from which the chromatographic data was read.

Note that the ChromBackendMzR backend is read-only and does not support direct modification of chromatographic data. However, it does support peaksData slot replacement, which will modify the peaksData slot but not the local mzML files. This is indicated by the "inMemory" slot being set to TRUE.

Implementing functionalities with the ChromBackendMzR backend should be simplified as much as possible and reuse the methods already implemented for ChromBackendMemory when possible.

Usage

```
ChromBackendMzR()
```

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

Arguments

object	A ChromBackendMzR object.
files	A character vector of file paths to mzML files.
BPPARAM	Parallel setup configuration. See BiocParallel::bpparam() for more information.
...	Additional parameters to be passed.

Value

Refer to the individual function description for information on the return value.

Author(s)

Philippine Louail

Examples

```
library(mzR)  
library(msdata)  
  
## Load an mzML file  
MRM_file <- system.file("proteomics", "MRM-standmix-5.mzML.gz",  
  package = "msdata"  
)
```

```
## Initialize the ChromBackendMzR object
be_empty <- ChromBackendMzR()
be <- backendInitialize(be_empty, files = MRM_file, BPPARAM = SerialParam())
```

ChromBackendSpectra *Chromatographic Data Backend for Spectra Objects*

Description

The `ChromBackendSpectra` class extends `ChromBackendMemory`, inheriting all its slots and methods while providing additional functionality for summarizing chromatographic data from `Spectra::Spectra()` objects.

It can be initialized with a `Spectra` object, which is stored in the `spectra` slot of the backend. Users can also provide a `data.frame` containing chromatographic metadata, stored in `chromData`. This metadata filters the `Spectra` object and generates `peaksData`. If `chromData` is not provided, a default `data.frame` is created from the `Spectra` data. An "rtMin", "rtMax", "mzMin", and "mzMax" column will be created by condensing the `Spectra` data corresponding to each unique combination of the `factorize.by` variables.

The `dataOrigin` core chromatogram variable should reflect the `dataOrigin` of the `Spectra` object. The `factorize.by` parameter defines the variables for grouping `Spectra` data into chromatographic data. The default is `c("msLevel", "dataOrigin")`, which will define separate chromatograms for each combination of `msLevel` and `dataOrigin`. These variables must be in both `Spectra` and `chromData` (if provided).

The `summarize.method` parameter defines how spectral data intensity is summarized:

- **"sum"**: Sums intensity to create a Total Ion Chromatogram (TIC).
- **"max"**: Takes max intensity for a Base Peak Chromatogram (BPC).

If `chromData` or its factorization columns are modified, the `factorize()` method must be called to update `chromSpectraIndex`.

Usage

```
ChromBackendSpectra()

## S4 method for signature 'ChromBackendSpectra'
backendInitialize(
  object,
  spectra = Spectra(),
  factorize.by = c("msLevel", "dataOrigin"),
  summarize.method = c("sum", "max"),
  chromData = fillCoreChromVariables(),
  spectraVariables = character(),
  ...
)

chromSpectraIndex(object)
```

Arguments

<code>object</code>	A ChromBackendSpectra object.
<code>spectra</code>	A Spectra object.
<code>factorize.by</code>	A character vector of variables for grouping Spectra data into chromatographic data. Default: <code>c("msLevel", "dataOrigin")</code> . If <code>chromData</code> is provided, it must contain these columns.
<code>summarize.method</code>	A character string specifying intensity summary: <code>"sum"</code> (default) or <code>"max"</code> .
<code>chromData</code>	A data.frame with chromatographic data for use in <code>backendInitialize()</code> . If missing, a default is generated. Columns like <code>rtMin</code> , <code>rtMax</code> , <code>mzMin</code> , and <code>mzMax</code> must be provided and not contain NA values. Use <code>-Inf/Inf</code> for unspecified values. The <code>"dataOrigin"</code> column must match the Spectra object's <code>"dataOrigin"</code> .
<code>spectraVariables</code>	A character vector specifying which variables from the Spectra object should be added to the <code>chromData</code> . These will be mapped using the <code>chromSpectraIndex</code> variable.
<code>...</code>	Additional parameters.

Details

No `peaksData` is stored until the user calls a function that generates it (e.g., `rtime()`, `peaksData()`, `intensity()`). The `peaksData` slot replacement is unsupported — modifications are temporary to optimize memory. The `inMemory` slot indicates this with `TRUE`.

ChromBackendSpectra should reuse ChromBackendMemory methods whenever possible to keep implementations simple.

Value

Refer to the individual function description for information on the return value.

Note

ensure that it returns a factor

Author(s)

Philippine Louail, Johannes Rainer.

Examples

```
library(Spectra)
library(MsBackendMetaboLights)

## Get Spectra data from MetaboLights
be <- backendInitialize(MsBackendMetaboLights(),
  mtblsId = "MTBLS39",
  filePattern = c("63B.cdf")
)
s <- Spectra(be)

s <- setBackend(s, MsBackendMemory())
```

```

## Initialize ChromBackendSpectra
be_empty <- new("ChromBackendSpectra")
be <- backendInitialize(be_empty, s)

## replace the msLevel data
msLevel(be) <- c(1L, 2L, 3L)

## re-factorize the data
be <- factorize(be)

## Create BPC : we summarize the intensity present in the Spectra object
## by the maximum value, thus creating a Base Peak Chromatogram.
be <- backendInitialize(be_empty, s, summarize.method = "max")

## Can now see the details of this bpc by looking at the chromData of our
## object
chromData(be)

## Another possibilities is to create eics from the Spectra object.
## Here we create an EIC with a specific m/z and retention time window.
df <- data.frame(mzMin = 100.01, mzMax = 100.02 , rtMin = 50, rtMax = 100)
be <- backendInitialize(be_empty, s, summarize.method = "sum")
chromData(be) <- cbind(chromData(be), df)

## now when we call the peaksData function, we will get the intensity
## of the spectra object that are in the m/z and retention time window
## defined in the chromData.
peaksData(be)

```

chromData

Chromatographic Peaks Metadata.

Description

As explained in the [Chromatograms](#) class documentation, the Chromatograms object is a container for chromatogram data that includes chromatographic peaks data (*retention time* and related intensity values, also referred to as *peaks data variables* in the context of Chromatograms) and metadata of individual chromatograms (so called *chromatograms variables*).

The *chromatograms variables* information can be accessed using the `chromData()` function. it is also possible to access specific chromatograms variables using `$`.

`chromData` can be accessed, replaced but also filtered/subsetted. Refer to the sections below for more details.

Usage

```

## S4 method for signature 'Chromatograms'
chromData(object, columns = chromVariables(object), drop = FALSE)

## S4 replacement method for signature 'Chromatograms'
chromData(object) <- value

```

```
## S4 method for signature 'Chromatograms'  
chromVariables(object)  
  
## S4 method for signature 'Chromatograms'  
chromIndex(object)  
  
## S4 replacement method for signature 'Chromatograms'  
chromIndex(object) <- value  
  
## S4 method for signature 'Chromatograms'  
collisionEnergy(object)  
  
## S4 replacement method for signature 'Chromatograms'  
collisionEnergy(object) <- value  
  
## S4 method for signature 'Chromatograms'  
dataOrigin(object)  
  
## S4 replacement method for signature 'Chromatograms'  
dataOrigin(object) <- value  
  
## S4 method for signature 'Chromatograms'  
msLevel(object)  
  
## S4 replacement method for signature 'Chromatograms'  
msLevel(object) <- value  
  
## S4 method for signature 'Chromatograms'  
mz(object)  
  
## S4 replacement method for signature 'Chromatograms'  
mz(object) <- value  
  
## S4 method for signature 'Chromatograms'  
mzMax(object)  
  
## S4 replacement method for signature 'Chromatograms'  
mzMax(object) <- value  
  
## S4 method for signature 'Chromatograms'  
mzMin(object)  
  
## S4 replacement method for signature 'Chromatograms'  
mzMin(object) <- value  
  
## S4 method for signature 'Chromatograms'  
length(x)  
  
## S4 method for signature 'Chromatograms'  
precursorMz(object)  
  
## S4 replacement method for signature 'Chromatograms'
```

```

precursorMz(object) <- value

## S4 method for signature 'Chromatograms'
precursorMzMin(object)

## S4 replacement method for signature 'Chromatograms'
precursorMzMin(object) <- value

## S4 method for signature 'Chromatograms'
precursorMzMax(object)

## S4 replacement method for signature 'Chromatograms'
precursorMzMax(object) <- value

## S4 method for signature 'Chromatograms'
productMz(object)

## S4 replacement method for signature 'Chromatograms'
productMz(object) <- value

## S4 method for signature 'Chromatograms'
productMzMin(object)

## S4 replacement method for signature 'Chromatograms'
productMzMin(object) <- value

## S4 method for signature 'Chromatograms'
productMzMax(object)

## S4 replacement method for signature 'Chromatograms'
productMzMax(object) <- value

## S4 method for signature 'Chromatograms'
filterChromData(
  object,
  variables = character(),
  ranges = numeric(),
  match = c("any", "all"),
  keep = TRUE
)

```

Arguments

object	A Chromatograms object.
columns	A character vector of chromatograms variables to extract.
drop	A logical indicating whether to drop dimensions when extracting a single variable.
value	replacement value for <- methods. See individual method description or expected data type.
x	A Chromatograms object.
variables	For filterChromData(): character vector with the names of the chromatogram

	variables to filter for. The list of available chromatogram variables can be obtained with <code>chromVariables()</code> .
ranges	For <code>filterChromData()</code> : 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 <code>variables</code> parameter (see below).
match	For <code>filterChromData()</code> : character(1) defining whether the condition has to match for all provided ranges (<code>match = "all"</code> ; the default), or for any of them (<code>match = "any"</code>) for chromatogram data to be retained.
keep	For <code>filterChromData()</code> : logical(1) defining whether to keep (<code>keep = TRUE</code>) or remove (<code>keep = FALSE</code>) the chromatogram data that match the condition.

Value

Refer to the individual function description for information on the return value.

Chromatograms variables and accessor functions

The following chromatograms variables are guaranteed to be provided by a Chromatograms object and to be accessible with either the `chromData()` or a specific function named after the variables names:

- `chromIndex`: an integer with the index of the chromatogram in the original source file (e.g. *mzML* file).
- `collisionEnergy`: for SRM data, numeric with the collision energy of the precursor.
- `dataOrigin`: optional character with the origin of the data.
- `msLevel`: integer defining the MS level of the data.
- `mz`: optional numeric with the (target) m/z value for the chromatographic data.
- `mzMin`: optional numeric with the lower m/z value of the m/z range in case the data (e.g. an extracted ion chromatogram EIC) was extracted from a Spectra object.
- `mzMax`: optional numeric with the upper m/z value of the m/z range.
- `precursorMz`: for SRM data, numeric with the target m/z of the precursor (parent).
- `precursorMzMin`: for SRM data, optional numeric with the lower m/z of the precursor's isolation window.
- `precursorMzMax`: for SRM data, optional numeric with the upper m/z of the precursor's isolation window.
- `productMz` for SRM data, numeric with the target m/z of the product ion.
- `productMzMin`: for SRM data, optional numeric with the lower m/z of the product's isolation window.
- `productMzMax`: for SRM data, optional numeric with the upper m/z of the product's isolation window.

Filter Chromatograms variables

Functions that filter Chromatograms based on chromatograms variables (i.e. `chromData`) will remove chromatographic data that do not meet the specified conditions. This means that if a chromatogram is filtered out, its corresponding `chromData` and `peaksData` will be removed from the object immediately.

The available functions to filter chromatogram data are:

- `filterChromData()`: Filters numerical chromatographic data variables based on the provided numerical ranges. The method returns a `Chromatograms` object containing only the chromatograms that match the specified conditions. This function results in an object with fewer chromatograms than the original.

Author(s)

Philippine Louail

See Also

[Chromatograms](#) for a general description of the `Chromatograms` object. [peaksData](#) for a general description of the chromatographic peaks data available in the object, as well as how to access, replace and subset them. [processingQueue](#) for more information on the queuing of processings and parallelization for larger dataset processing.

Examples

```
# Create a Chromatograms object
cdata <- data.frame(
  msLevel = c(1L, 1L, 1L),
  mz = c(112.2, 123.3, 134.4),
  chromIndex = c(1L, 2L, 3L)
)

be <- backendInitialize(new("ChromBackendMemory"), chromData = cdata)

chr <- Chromatograms(be)

# Access chromatograms variables
chromData(chr)

# Access specific chromatograms variables
chromData(chr, columns = "msLevel")

msLevel(chr)

# Replace chromatograms variables
msLevel(chr) <- c(1L, 2L, 2L)

# Filter chromatograms variables
filterChromData(chr,
  variables = "msLevel", ranges = c(1L, 1L),
  keep = FALSE
)
```

Description

ChromBackend is a virtual class that defines what different backends need to provide to be used by the Chromatograms package and classes.

The backend should provide access to the chromatographic data which mainly consists of (paired) intensity and retention time values. Additional chromatographic metadata such as MS level and precursor and product m/z should also be provided.

Through their implementation different backends can be either optimized for minimal memory requirements or performance. Each backend needs to implement data access methods listed in section *Backend functions*: below.

And example implementation and more details and descriptions are provided in the *Creating new ChromBackend classes for Chromatograms* vignette.

Currently available backends are:

- ChromBackendMemory: This backend stores chromatographic data directly in memory, making it ideal for small datasets or testing. It can be initialized with a `data.frame` of chromatographic data via the `chromData` parameter and a list of `data.frame` entries for peaks data using the `peaksData` parameter. These data can be accessed with the `chromData()` and `peaksData()` functions.
- ChromBackendMzR: The ChromBackendMzR inherits all slots and methods from the base ChromBackendMemory backend, providing additional functionality for reading chromatographic data from mzML files.
- ChromBackendSpectra: The ChromBackendSpectra inherits all slots and methods from the base ChromBackendMemory backend, providing additional functionality for reading chromatographic data from Spectra objects.

Filter the peak data based on the provided ranges for the given variables.

Usage

```

coreChromVariables()

corePeaksVariables()

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

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

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

## S4 method for signature 'ChromBackend'
chromData(object, columns = chromVariables(object), drop = FALSE)

## S4 replacement method for signature 'ChromBackend'
chromData(object) <- value

## S4 method for signature 'ChromBackend'
chromExtract(object, peak.table, by)

```

```
## S4 method for signature 'ChromBackend'  
factorize(object, ...)  
  
## S4 method for signature 'ChromBackend'  
peaksData(object, columns = c("rttime", "intensity"), drop = FALSE, ...)  
  
## S4 replacement method for signature 'ChromBackend'  
peaksData(object) <- value  
  
## S4 method for signature 'ChromBackend'  
x[i, j, ..., drop = FALSE]  
  
## S4 method for signature 'ChromBackend'  
x[[i, j, ...]]  
  
## S4 replacement method for signature 'ChromBackend'  
x[[i, j, ...]] <- value  
  
## S4 method for signature 'ChromBackend'  
backendBpparam(object, BPPARAM = bpparam())  
  
## S4 method for signature 'ChromBackend'  
backendInitialize(object, ...)  
  
## S4 method for signature 'ChromBackend'  
backendParallelFactor(object, ...)  
  
## S4 method for signature 'list'  
backendMerge(object, ...)  
  
## S4 method for signature 'ChromBackend'  
chromIndex(object)  
  
## S4 replacement method for signature 'ChromBackend'  
chromIndex(object) <- value  
  
## S4 method for signature 'ChromBackend'  
chromVariables(object)  
  
## S4 method for signature 'ChromBackend'  
collisionEnergy(object)  
  
## S4 replacement method for signature 'ChromBackend'  
collisionEnergy(object) <- value  
  
## S4 method for signature 'ChromBackend'  
dataOrigin(object)  
  
## S4 replacement method for signature 'ChromBackend'  
dataOrigin(object) <- value  
  
## S4 method for signature 'ChromBackend,ANY'
```

```
extractByIndex(object, i)

## S4 method for signature 'ChromBackend,missing'
extractByIndex(object, i)

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

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

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

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

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

## S4 method for signature 'ChromBackend'
lengths(x)

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

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

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

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

## S4 method for signature 'ChromBackend'
mzMax(object)

## S4 replacement method for signature 'ChromBackend'
mzMax(object) <- value

## S4 method for signature 'ChromBackend'
mzMin(object)

## S4 replacement method for signature 'ChromBackend'
mzMin(object) <- value

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

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

```
## S4 replacement method for signature 'ChromBackend'  
precursorMz(object) <- value  
  
## S4 method for signature 'ChromBackend'  
precursorMzMax(object)  
  
## S4 replacement method for signature 'ChromBackend'  
precursorMzMax(object) <- value  
  
## S4 method for signature 'ChromBackend'  
precursorMzMin(object)  
  
## S4 replacement method for signature 'ChromBackend'  
precursorMzMin(object) <- value  
  
## S4 method for signature 'ChromBackend'  
productMz(object)  
  
## S4 replacement method for signature 'ChromBackend'  
productMz(object) <- value  
  
## S4 method for signature 'ChromBackend'  
productMzMax(object)  
  
## S4 replacement method for signature 'ChromBackend'  
productMzMax(object) <- value  
  
## S4 method for signature 'ChromBackend'  
productMzMin(object)  
  
## S4 replacement method for signature 'ChromBackend'  
productMzMin(object) <- value  
  
## S4 method for signature 'ChromBackend'  
reset(object)  
  
## S4 method for signature 'ChromBackend'  
rtime(object)  
  
## S4 replacement method for signature 'ChromBackend'  
rtime(object) <- value  
  
## S4 method for signature 'ChromBackend,ANY'  
split(x, f, drop = FALSE, ...)  
  
## S4 method for signature 'ChromBackend'  
filterChromData(  
  object,  
  variables = character(),  
  ranges = numeric(),  
  match = c("any", "all"),
```

```

    keep = TRUE
  )

## S4 method for signature 'ChromBackend'
filterPeaksData(
  object,
  variables = character(),
  ranges = numeric(),
  match = c("any", "all"),
  keep = TRUE
)

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

## S4 method for signature 'ChromBackend'
imputePeaksData(
  object,
  method = c("linear", "spline", "gaussian", "loess"),
  span = 0.3,
  sd = 1,
  window = 2,
  ...
)

```

Arguments

x	Object extending ChromBackend.
name	For \$ and \$<-: the name of the chromatogram variable to return or set.
value	Replacement value for <- methods. See individual method description or expected data type.
object	Object extending ChromBackend.
...	Additional arguments.
columns	For chromData() accessor: optional character with column names (chromatogram variables) that should be included in the returned data.frame. By default, all columns are returned.
drop	For chromData() and peaksData(): logical(1) default to FALSE. If TRUE, and one column is requested by the user, the method should return a vector (or list of vector for peaksData()) of the single column requested.
peak.table	For chromExtract() A data frame containing the following minimum columns: - rtMin: Minimum retention time for each peak. Cannot be NA. - rtMax: Maximum retention time for each peak. Cannot be NA. - mzMin: Minimum m/z value for each peak. - mzMax: Maximum m/z value for each peak. Additionally, the peak.table must include columns that uniquely identify chromatograms in the object. Common choices are "msLevel" and/or "dataOrigin". These columns must also be present in the chromData of the object. Any extra columns in peak.table will be added to the chromData of the newly created object.
by	for chromExtract() A character vector specifying one or more column names that are present in both peak.table and chromData(object). These columns

	uniquely identify chromatograms. The combination of these columns must be unique in <code>chromData(object)</code> . Can be of length 1 or greater.
<code>i</code>	For <code>[]</code> : integer, logical or character to subset the object.
<code>j</code>	For <code>[]</code> and <code>[[</code> : ignored.
<code>BPPARAM</code>	Parallel setup configuration. See <code>BiocParallel::bpparam()</code> for more information.
<code>f</code>	factor defining the grouping to split <code>x</code> . See <code>split()</code> .
<code>variables</code>	For <code>filterChromData()</code> : character vector with the names of the chromatogram variables to filter for. The list of available chromatogram variables can be obtained with <code>chromVariables()</code> .
<code>ranges</code>	For <code>filterChromData()</code> : 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 <code>variables</code> parameter (see below).
<code>match</code>	For <code>filterChromData()</code> : <code>character(1)</code> defining whether the condition has to match for all provided ranges (<code>match = "all"</code> ; the default), or for any of them (<code>match = "any"</code>) for chromatogram data to be retained.
<code>keep</code>	For <code>filterChromData()</code> : <code>logical(1)</code> defining whether to keep (<code>keep = TRUE</code>) or remove (<code>keep = FALSE</code>) the chromatogram data that match the condition.
<code>method</code>	For <code>imputePeaksData()</code> : <code>character(1)</code> : Imputation method ("linear", "spline", "gaussian", "loess")
<code>span</code>	For <code>imputePeaksData</code> : <code>numeric(1)</code> , for the loess method: Smoothing parameter (only used if <code>method == "loess"</code>)
<code>sd</code>	For <code>imputePeaksData</code> : <code>numeric(1)</code> , for the gaussian method: Standard deviation for Gaussian kernel (only used if <code>method == "gaussian"</code>)
<code>window</code>	For <code>imputePeaksData</code> : integer, for the gaussian method: Half-width of Gaussian kernel window (e.g., 2 gives window size 5)

Value

Refer to the individual function description for information on the return value.

Core chromatogram variables

The *core* chromatogram variables are variables (metadata) that can/should be provided by a backend. For each of these variables a value needs to be returned, if none is defined, a missing value (of the correct data type) should be returned. The names of the chromatogram variables in your current chromatogram object are returned with the `chromVariables()` function.

For each core chromatogram variable a dedicated access method exists. In contrast to the peaks data described below, a single value should be returned for each chromatogram.

The `coreChromVariables()` function returns the core chromatogram variables along with their expected (defined) data type.

The core chromatogram variables (in alphabetical order) are:

- `chromIndex`: an integer with the index of the chromatogram in the original source file (e.g. *mzML* file). In backedn with no original source file, this variable should be set to `NA_integer_`.
- `collisionEnergy`: for SRM data, numeric with the collision energy of the precursor.
- `dataOrigin`: optional character with the origin of a chromatogram.

- `msLevel`: integer defining the MS level of the data.
- `mz`: optional numeric with the (target) m/z value for the chromatographic data.
- `mzMin`: optional numeric with the lower m/z value of the m/z range in case the data (e.g. an extracted ion chromatogram EIC) was extracted from a `Spectra` object.
- `mzMax`: optional numeric with the upper m/z value of the m/z range.
- `precursorMz`: for SRM data, numeric with the target m/z of the precursor (parent).
- `precursorMzMin`: for SRM data, optional numeric with the lower m/z of the precursor's isolation window.
- `precursorMzMax`: for SRM data, optional numeric with the upper m/z of the precursor's isolation window.
- `productMz` for SRM data, numeric with the target m/z of the product ion.
- `productMzMin`: for SRM data, optional numeric with the lower m/z of the product's isolation window.
- `productMzMax`: for SRM data, optional numeric with the upper m/z of the product's isolation window.

Core Peaks variables

Similar to the *core* chromatogram variables, *core* peaks variables represent metadata that should be provided by a backend. Each of these variables should return a value, and if undefined, a missing value (with the appropriate data type) is returned. The number of values for a peaks variable in a single chromatogram can vary, from none to multiple, and may differ between chromatograms.

The names of peaks variables in the current chromatogram object can be obtained with the `peaksVariables()` function.

Each core peaks variable has a dedicated accessor method.

The `corePeaksVariables()` function returns the core peaks variables along with their expected (defined) data type.

The core peaks variables, listed in the required order for `peaksData`, are:

- `rttime`: A numeric vector containing retention time values.
- `intensity`: A numeric vector containing intensity values.

They should be provided for each chromatogram in the backend, **in this order**. No NAs are allowed for the `rttime` values. These characteristics will be checked with the `validPeaksData()` function.

Mandatory methods

New backend classes **must** extend the base `ChromBackend` class and implement the following mandatory methods:

- `backendInitialize()`: initialises the backend. This method is supposed to be called right after creating an instance of the backend class and should prepare the backend. Parameters can be defined freely for each backend, depending on what is needed to initialize the backend. This method has to ensure to set the chromatogram variable `dataOrigin` correctly.
- `backendBpparam()`: returns 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.

- 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 ChromBackendMzR on the other hand returns factor(dataOrigin(object)) hence suggesting to split the object by data file.
- chromData(), chromData<-: gets or sets general chromatogram metadata (annotation). chromData() returns a data.frame, chromData<- expects a data.frame with the same number of rows as there are chromatograms in object. Read-only backends might not need to implement the replacement method chromData<- (unless some internal caching mechanism could be used). chromData() should be implemented with the parameter drop set to FALSE as default. With drop = FALSE the method should return a data.frame even if one column is requested. If drop = TRUE is specified, the output will be a vector of the single column requested. New backends should be implemented such as if empty, the method returns a data.frame with 0 rows and the columns defined by chromVariables(). By default, the function *should* return at minimum the coreChromVariables, even if NAs.
- chromExtract(): return A new Chrombackend object containing separated chromatographic area as individual chromatograms. The chromatographic areas are defined by the peak.table parameter. The new object will contain chromatograms that match the conditions defined in peak.table. If no chromatograms match the conditions, an empty ChromBackend object should be returned.
- extractByIndex(): function to subset a backend to selected elements defined by the provided index. Similar to [], this method should allow extracting (or to subset) the data in any order. In contrast to [], however, i is expected to be an integer (while [] should also support logical and eventually character). While being apparently redundant to [], this methods avoids package namespace errors/problems that can result in implementations of [] being not found by R (which can happen sometimes in parallel processing using the BiocParallel::SnowParam()). This method is used internally to extract/subset its backend. Implementation of this method is mandatory.
- peaksData(): returns a list of data.frame with the data (e.g. retention time - intensity pairs) from each chromatogram. The length of the list is equal to the number of chromatograms in object. For an empty chromatogram a data.frame with 0 rows and two columns (named "rtime" and "intensity") has to be returned. The optional parameter columns, if supported by the backend allows to define which peak variables should be returned in each array. As default (minimum) columns "rtime" and "intensity" have to be provided. peaksData() should be implemented with the parameter drop set to FALSE as default. With drop = FALSE the method should return a data.frame even if only one column is requested. If drop = TRUE is specified, the output will be a vector of the single column requested.
- peaksData<- replaces the peak data (retention time and intensity values) of the backend. This method expects a list of two-dimensional arrays (data.frame) with columns representing the peak variables. All existing peaks data are expected to be replaced with these new values. The length of the list has to match the number of chromatogram of object. Note that only writeable backends need to support this method.
- []: subset the backend. Only subsetting by element (row/i) is allowed. This method should be implemented as to support empty integer.
- \$, \$<-: access or set/add a single chromatogram variable (column) in the backend.
- backendMerge(): merges (combines) ChromBackend objects into a single instance. All objects to be merged have to be of the same type.

Optional methods with default implementations

Additional methods that might be implemented, but for which default implementations are already present are:

- `[]`
- `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.
- `chromIndex()`: returns an integer vector with the index of the chromatograms in the original source file.
- `chromVariables()`: returns a character vector with the available chromatogram variables (columns, fields or attributes) available in object. Variables listed by this function are expected to be returned (if requested) by the `chromData()` function.
- `collisionEnergy()`, `collisionEnergy<-`: gets or sets the collision energy for the precursor (for SRM data). `collisionEnergy()` returns a numeric of length equal to the number of chromatograms in object.
- `dataOrigin()`, `dataOrigin<-`: gets or sets the *data origin* variable. `dataOrigin()` returns a character of length equal to the number of chromatograms, `dataOrigin<-` expects a character of length equal `length(object)`.
- `filterChromData()`: filters any numerical chromatographic data variables based on the provided numerical ranges. The method should return a `ChromBackend` object with the chromatograms that match the condition. This function will result in an object with less chromatogram than the original.
- `intensity()`: gets the intensity values from the chromatograms. Returns a list of numeric vectors (intensity values for each chromatogram). The length of the list is equal to the number of chromatograms in object.
- `intensity<-`: replaces the intensity values. `value` has to be a list of length equal to the number of chromatograms and the number of values within each list element identical to the number of data pairs in each chromatogram. Note that just writeable backends need to support this method.
- `imputePeaksData()`: Imputes missing intensity values in the chromatographic peaks data using various methods such as linear interpolation, spline interpolation, Gaussian kernel smoothing, or LOESS smoothing. This method modifies the peaks data in place and returns the same `ChromBackend` object with imputed values.
- `isReadOnly()`: returns a `logical(1)` whether the backend is *read only* or does allow also to write/update data. Defaults to `FALSE`.
- `isEmpty()`: returns a `logical` of length equal to the number of chromatograms with `TRUE` for chromatograms without any data pairs.
- `length()`: returns the number of chromatograms in the object.
- `lengths()`: returns the number of data pairs (retention time and intensity values) per chromatogram.
- `msLevel()`: gets the chromatogram's MS level. Returns an integer vector (of length equal to the number of chromatograms) with the MS level for each chromatogram (or `NA_integer_` if not available).
- `mz()`, `mz<-`: gets or sets the m/z value of the chromatograms. `mz()` returns a numeric of length equal to the number of chromatograms in object, `mz<-` expects a numeric of length `length(object)`.

- `mzMax()`, `mzMax<-`: gets or sets the upper m/z of the mass-to-charge range from which a chromatogram contains signal (e.g. if the chromatogram was extracted from MS data in spectra format and a m/z range was provided). `mzMax()` returns a numeric of length equal to the number of chromatograms in object, `mzMax<-` expects a numeric of length equal to the number of chromatograms in object.
- `mzMin()`, `mzMin<-`: gets or sets the lower m/z of the mass-to-charge range from which a chromatogram contains signal (e.g. if the chromatogram was extracted from MS data in spectra format and a m/z range was provided). `mzMin()` returns a numeric of length equal to the number of chromatograms in object, `mzMin<-` expects a numeric of length equal to the number of chromatograms in object.
- `peaksVariables()`: lists the available data variables for the chromatograms. Default peak variables are "rttime" and "intensity" (which all backends need to support and provide), but some backends might provide additional variables. Variables listed by this function are expected to be returned (if requested) by the `peaksData()` function.
- `precursorMz()`, `precursorMz<-`: gets or sets the (target) m/z of the precursor (for SRM data). `precursorMz()` returns a numeric of length equal to the number of chromatograms in object. `precursorMz<-` expects a numeric of length equal to the number of chromatograms.
- `precursorMzMin()`, `precursorMzMax()`, `productMzMin()`, `productMzMax()`: gets the lower and upper margin for the precursor or product isolation windows. These functions might return the value of `productMz()` if the respective minimal or maximal m/z values are not defined in object.
- `productMz()`, `productMz<-`: gets or sets the (target) m/z of the product (for SRM data). `productMz()` returns a numeric of length equal to the number of chromatograms in object. `productMz<-` expects a numeric of length equal to the number of chromatograms.
- `rttime()`: gets the retention times from the chromatograms. returns a list of numeric vectors (retention times for each chromatogram). The length of the returned list is equal to the number of chromatograms in object.
- `rttime<-`: replaces the retention times. value has to be a list of length equal to the number of chromatograms and the number of values within each list element identical to the number of data pairs in each chromatogram. Note that just writeable backends support this method.
- `split()`: splits the backend into a list of backends (depending on parameter f). The default method for `ChromBackend` uses `split.default()`, thus backends extending `ChromBackend` don't necessarily need to implement this method.
- `supportsSetBackend()`: whether a `ChromBackend` supports the `Chromatograms setBackend()` function. The default function will take the `peaksData()` and `chromData()` of the user's backend and pass it to the new backend. If the backend does not support this function, it should return `FALSE`. Therefore both backend in question should have a adequate `peaksData()` and `chromData()` method as well as their respective replacement method.

Implementation notes

Backends extending `ChromBackend` **must** implement all of its methods (listed above). A guide to create new backend classes is provided as a dedicated vignette. Additional information and an example for a backend implementation is provided in the respective vignette.

Author(s)

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Examples

```

## Create a simple backend implementation
ChromBackendDummy <- setClass("ChromBackendDummy",
  contains = "ChromBackend"
)

## We will show examples on a `ChromBackendMemory` backend.
be <- ChromBackendMemory()

## 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.
cdata <- data.frame(
  msLevel = c(1L, 1L, 1L),
  mz = c(112.2, 123.3, 134.4),
  dataOrigin = c("mem1", "mem2", "mem3")
)

pdata <- list(
  data.frame(
    rtime = c(12.4, 12.8, 13.2, 14.6),
    intensity = c(123.3, 153.6, 2354.3, 243.4)
  ),
  data.frame(
    rtime = c(45.1, 46.2),
    intensity = c(100, 80.1)
  ),
  data.frame(
    rtime = c(12.4, 12.8, 13.2, 14.6),
    intensity = c(123.3, 153.6, 2354.3, 243.4)
  )
)
be <- backendInitialize(be, chromData = cdata, peaksData = pdata)

be

## Data can be accessed with the accessor methods
msLevel(be)

rtime(be)

## Even if no data was provided for all chromatogram variables, its accessor
## methods are supposed to return a value.
precursorMz(be)

## The `peaksData()` method is supposed to return data/frames of rtime and
## intensity pairs as a `list`.
peaksData(be)

## Use columns to extract specific peaks variables. Below we extract rtime
## and intensity values, but in reversed order to the default.
peaksData(be, columns = c("intensity", "rtime"))

## List available chromatographic variables
chromVariables(be)

```

```

## List available peak variables
peaksVariables(be)

## Extract multiple chromatographic variables
chromData(be, c("dataOrigin", "mz", "msLevel"))

## Single variables can also be accessed and replaced
mz(be)
mz(be) <- c(123.4, 134.5, 145.6)

be$msLevel
be$msLevel <- c(2L, 2L, 2L)

be[["rttime"]]
be[["rttime"]] <- list(
  c(12.4, 12.8, 13.2, 14.6),
  c(45.1, 46.2),
  c(12.4, 12.8, 13.2, 14.6)
)

```

peaksData

*Chromatographic peaks data***Description**

As explained in the [Chromatograms](#) class documentation, the `Chromatograms` object is a container for chromatographic data that includes chromatographic peaks data (*retention time* and related intensity values, also referred to as *peaks data variables* in the context of `Chromatograms`) and meta-data of individual chromatograms (so called *chromatograms variables*).

The *peaks data variables* information can be accessed using the `peaksData()` function. It is also possible to access specific peaks variables using `$`.

The peaks data can be accessed, replaced but also filtered/subsetted. Refer to the sections below for more details.

Usage

```

## S4 method for signature 'Chromatograms'
imputePeaksData(
  object,
  method = c("linear", "spline", "gaussian", "loess"),
  span = 0.3,
  sd = 1,
  window = 2,
  ...
)

## S4 method for signature 'Chromatograms'
filterPeaksData(
  object,
  variables = character(),
  ranges = numeric(),
  match = c("any", "all"),

```

```

    keep = TRUE
  )

## S4 method for signature 'Chromatograms'
intensity(object, ...)

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

## S4 method for signature 'Chromatograms'
peaksData(
  object,
  columns = peaksVariables(object),
  f = processingChunkFactor(object),
  BPPARAM = bpparam(),
  drop = FALSE,
  ...
)

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

## S4 method for signature 'Chromatograms'
peaksVariables(object, ...)

## S4 method for signature 'Chromatograms'
rtime(object, ...)

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

## S4 method for signature 'Chromatograms'
lengths(x)

```

Arguments

object	A Chromatograms object.
method	For <code>imputePeaksData()</code> : character(1): Imputation method ("linear", "spline", "gaussian", "loess")
span	For <code>imputePeaksData</code> : numeric(1), for the loess method: Smoothing parameter (only used if method == "loess")
sd	For <code>imputePeaksData</code> : numeric(1), for the gaussian method: Standard deviation for Gaussian kernel (only used if method == "gaussian")
window	For <code>imputePeaksData</code> : integer, for the gaussian method: Half-width of Gaussian kernel window (e.g., 2 gives window size 5)
...	Additional arguments passed to the method.
variables	For <code>filterPeaksData()</code> : character vector with the names of the peaks data variables to filter for. The list of available peaks data variables can be obtained with <code>peaksVariables()</code> .
ranges	For <code>filterPeaksData()</code> : 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 variables parameter (see below).
match	For <code>filterPeaksData()</code> : <code>character(1)</code> defining whether the condition has to match for all provided ranges (<code>match = "all"</code> ; the default), or for any of them (<code>match = "any"</code>).
keep	For <code>filterPeaksData()</code> : <code>logical(1)</code> defining whether to keep (<code>keep = TRUE</code>) or remove (<code>keep = FALSE</code>) the chromatographic peaks data that match the condition.
value	For <code>rtime()</code> and <code>intensity()</code> : numeric vector with the values to replace the current values. The length of the vector must match the number of peaks data pairs in the <code>Chromatograms</code> object.
columns	For <code>peaksData()</code> : optional character with column names (peaks variables) that should be included in the returned <code>list</code> of <code>data.frame</code> . By default, all columns are returned. Available variables can be found by calling <code>peaksVariables()</code> on the object.
f	factor defining the grouping to split the <code>Chromatograms</code> object.
BPPARAM	Parallel setup configuration. See <code>BiocParallel::bpparam()</code> for more information.
drop	<code>logical(1)</code> For <code>peaksData()</code> , default to <code>FALSE</code> . If <code>TRUE</code> , and one column is called by the user, the method returns a list of vector of the single column requested.
x	For <code>lengths()</code> : A <code>Chromatograms</code> object.

Value

Refer to the individual function description for information on the return value.

Filter Peaks Variables

Functions that filter a `Chromatograms`'s peaks data (i.e., `peaksData`). These functions remove peaks data that do not meet the specified conditions. If a chromatogram in a `Chromatograms` object is filtered, only the corresponding peaks variable pairs (i.e., rows) in the `peaksData` are removed, while the chromatogram itself remains in the object.

The available functions to filter chromatographic peaks data include:

- `filterPeaksData()`: Filters numerical peaks data variables based on the specified numerical ranges parameter. This method returns the same input `Chromatograms` object, but the filtering step is added to the processing queue. The filtered data will be reflected when the user accesses `peaksData`. This function does *not* reduce the number of chromatograms in the object, but it removes the specified peaks data (e.g., "rtime" and "intensity" pairs) from the `peaksData`.

In the case of a read-only backend, (such as the [ChromBackendMzR](#)), the replacement of the peaks data is not possible. The peaks data can be filtered, but the filtered data will not be saved in the backend. This means the original `mzml` files will not be affected by computations performed on the [Chromatograms](#).

Impute Peaks Variables

`imputePeaksData` will impute missing values in a `Chromatograms`'s peaks data (i.e., `peaksData`). This functions replace missing peaks data values with specified imputation methods using various methods such as linear interpolation, spline interpolation, Gaussian kernel smoothing, or LOESS smoothing. This method modifies the peaks data in place and returns the same `Chromatograms` object with imputed values.

Author(s)

Philippine Louail

See Also

[Chromatograms](#) for a general description of the Chromatograms object, and [chromData](#) for accessing, substituting and filtering chromatographic variables. For more information on the queuing of processings and parallelization for larger dataset processing see [processingQueue](#).

Examples

```
# Create a Chromatograms object
cdata <- data.frame(
  msLevel = c(1L, 1L, 1L),
  mz = c(112.2, 123.3, 134.4),
  dataOrigin = c("mem1", "mem2", "mem3")
)

pdata <- list(
  data.frame(
    rtime = c(12.4, 12.8, 13.2, 14.6),
    intensity = c(123.3, 153.6, 2354.3, 243.4)
  ),
  data.frame(
    rtime = c(45.1, 46.2),
    intensity = c(100, 80.1)
  ),
  data.frame(
    rtime = c(12.4, 12.8, 13.2, 14.6),
    intensity = c(123.3, 153.6, 2354.3, 243.4)
  )
)

be <- backendInitialize(new("ChromBackendMemory"),
  chromData = cdata,
  peaksData = pdata
)

chr <- Chromatograms(be)

# Access peaks data
peaksData(chr)

# Access specific peaks data variables
peaksData(chr, columns = "rtime")
rtime(chr)

# Replace peaks data
rtime(chr)[[1]] <- c(1, 2, 3, 4)

# Filter peaks data
filterPeaksData(chr, variables = "rtime", ranges = c(12.5, 13.5))
```

plotChromatograms *Plot chromatograms*

Description

[Chromatograms\(\)](#) can be plotted with the following functions:

The `plotChromatograms()`: plots each chromatogram in its separate plot by splitting the plot area into as many panels as there are spectra.

Usage

```
plotChromatograms(  
  x,  
  xlab = "rtime (s)",  
  ylab = "intensity",  
  type = "o",  
  pch = 20,  
  cex = 0.6,  
  lwd = 1.5,  
  xlim = numeric(),  
  ylim = numeric(),  
  main = character(),  
  col = "#00000080",  
  asp = 1,  
  ...  
)  
  
plotChromatogramsOverlay(  
  x,  
  xlab = "rtime (s)",  
  ylab = "intensity",  
  type = "o",  
  pch = 20,  
  cex = 0.6,  
  lwd = 1.5,  
  xlim = numeric(),  
  ylim = numeric(),  
  main = paste(length(x), "chromatograms"),  
  col = "#00000080",  
  axes = TRUE,  
  frame.plot = axes,  
  ...  
)
```

Arguments

x	A Chromatograms object.
xlab	character(1) with the label for the x-axis (by default <code>xlab = "rtime (s)"</code>).
ylab	character(1) with the label for the y-axis (by default <code>ylab = "intensity"</code>).

type	character(1) specifying the type of plot. See <code>plot.default()</code> for details. Defaults to type = "l" which draws each peak as a line.
pch	integer(1) or character(1) specifying the plotting symbol (see <code>plot.default()</code>).
cex	numeric(1) specifying the size of the plotting symbol (see <code>plot.default()</code>).
lwd	numeric(1) specifying the line width (see <code>plot.default()</code>).
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 chromatograms (to plot each chromatograms in a different color) or be a list with colors for each individual peak in each spectrum.
asp	numeric(1) the aspect ratio of the plot, i.e. the ratio of the y-axis to the x-axis. Defaults to 1.
...	Additional arguments to be passed to <code>plot.default()</code> .
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.

Value

These functions create a plot.

Refer to the individual function description for information on the return value.

Author(s)

Philippine Louail, Johannes Rainer.

Examples

```
## Create a Chromatograms object
cdata <- data.frame(
  msLevel = c(1L, 1L, 1L),
  mz = c(112.2, 123.3, 134.4),
  chromIndex = c(1L, 2L, 3L)
)
pdata <- list(
  data.frame(
    rtime = c(12.4, 12.8, 13.2, 14.6),
    intensity = c(123.3, 153.6, 2354.3, 243.4)
  ),
  data.frame(
    rtime = c(45.1, 46.2),
    intensity = c(100, 80.1)
  ),
  data.frame(
    rtime = c(12.4, 12.8, 13.2, 14.6),
    intensity = c(123.3, 153.6, 2354.3, 243.4)
  )
)
```

```

chr <- backendInitialize(ChromBackendMemory(),
  chromData = cdata,
  peaksData = pdata
) |> Chromatograms()

## Plot one chromatogram
plotChromatograms(chr[1])

## Plot the full Chromatograms object
plotChromatograms(chr)

## Define a color for each peak in each chromatogram
plotChromatograms(chr[1:2], col = c("green", "blue"))

## Overlay all chromatograms
plotChromatogramsOverlay(chr[1:2], col = c("green", "blue"))

```

processingQueue

Efficiently processing Chromatograms objects.

Description

The processingQueue of a Chromatograms object is a list of processing steps (i.e., functions) that are stored within the object and applied only when needed. This design allows data to be processed in a single step, which is particularly useful for larger datasets. The processing queue enables functions to be applied in a chunk-wise manner, facilitating parallel processing and reducing memory demand.

Since the peaks data can be quite large, a processing queue is used to ensure efficiency. Generally, the processing queue is applied either temporarily when calling peaksData() or permanently when calling applyProcessing(). As explained below the processing efficiency can be further improved by enabling chunk-wise processing.

Usage

```

## S4 method for signature 'Chromatograms'
applyProcessing(
  object,
  f = processingChunkFactor(object),
  BPPARAM = bpparam(),
  ...
)

## S4 method for signature 'Chromatograms'
addProcessing(object, FUN, ...)

## S4 method for signature 'Chromatograms'
processingChunkSize(object, ...)

## S4 replacement method for signature 'Chromatograms'
processingChunkSize(object) <- value

```

```
## S4 method for signature 'Chromatograms'
processingChunkFactor(object, chunkSize = processingChunkSize(object), ...)
```

Arguments

object	A Chromatograms object.
f	factor defining the grouping to split the Chromatograms object.
BPPARAM	Parallel setup configuration. See <code>BiocParallel::bpparam()</code> for more information.
...	Additional arguments passed to the methods.
FUN	For <code>addProcessing()</code> , a function to be added to the Chromatograms object's processing queue.
value	<code>integer(1)</code> defining the chunk size.
chunkSize	<code>integer(1)</code> for <code>processingChunkFactor</code> defining the chunk size. The default is the value stored in the Chromatograms object's <code>processingChunkSize</code> slot.

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 object will be split for (parallel) chunk-wise processing or a factor of length 0 if no splitting is defined.

Refer to the individual function description for information on the return value.

Apply Processing

The `applyProcessing()` function applies the processing queue to the backend and returns the updated Chromatograms object. The processing queue is a list of processing steps applied to the chromatograms data. Each element in the list is a function that processes the chromatograms data. To apply processing to the peaks data, the backend must be set to a non-read-only backend using the `setBackend()` function.

Parallel and Chunk-wise Processing of Chromatograms

Many operations on Chromatograms objects, especially those involving the actual peaks data (see [peaksData](#)), support chunk-wise processing. This involves splitting the Chromatograms into smaller parts (chunks) that are processed iteratively. This enables parallel processing by data chunk and reduces memory demand since only the peak data of the currently processed subset is loaded into memory. Chunk-wise processing, which is disabled by default, can be enabled by setting the processing chunk size of a Chromatograms object using the `processingChunkSize()` function to a value smaller than the length of the Chromatograms object. For example, setting `processingChunkSize(chr) <- 1000` will cause any data manipulation operation on `chr`, such as `filterPeaksData()`, to be performed in parallel for sets of 1000 chromatograms in each iteration.

Chunk-wise processing is particularly useful for Chromatograms objects using an *on-disk* backend or for very large experiments. For small datasets or Chromatograms using an in-memory backend, direct processing might be more efficient. Setting the chunk size to `Inf` will disable chunk-wise processing.

Some backends may prefer a specific type of splitting and chunk-wise processing. For example, the `ChromBackendMzR` backend needs to load MS data from the original (mzML) files, so chunk-wise processing on a per-file basis is ideal. The `backendParallelFactor()` function for `ChromBackend` allows backends to suggest a preferred data chunking by returning a factor defining the respective data chunks. The `ChromBackendMzR` returns a factor based on the *dataOrigin* chromatograms

variable. A factor of length 0 is returned if no particular preferred splitting is needed. The suggested chunk definition will be used if no finite processingChunkSize() is defined. Setting the processingChunkSize overrides backendParallelFactor.

Functions to configure parallel or chunk-wise processing:

- processingChunkSize(): Gets or sets the size of the chunks for parallel or chunk-wise processing of a Chromatograms object. With a value of Inf (the default), no chunk-wise processing will be performed.
- processingChunkFactor(): Returns a factor defining the chunks into which a Chromatograms object will be split for chunk-wise (parallel) processing. A factor of length 0 indicates that no chunk-wise processing will be performed.

Note

Some backends might not support parallel processing. For these, the backendBpparam() function will always return a SerialParam() regardless of how parallel processing was defined.

Author(s)

Johannes Rainer, Philippine Louail

Examples

```
# Create a Chromatograms object
cdata <- data.frame(
  msLevel = c(1L, 1L, 1L),
  mz = c(112.2, 123.3, 134.4),
  chromIndex = c(1L, 2L, 3L)
)

pdata <- list(
  data.frame(
    rtime = c(12.4, 12.8, 13.2, 14.6),
    intensity = c(123.3, 153.6, 2354.3, 243.4)
  ),
  data.frame(
    rtime = c(45.1, 46.2),
    intensity = c(100, 80.1)
  ),
  data.frame(
    rtime = c(12.4, 12.8, 13.2, 14.6),
    intensity = c(123.3, 153.6, 2354.3, 243.4)
  )
)

be <- backendInitialize(new("ChromBackendMemory"),
  chromData = cdata,
  peaksData = pdata
)

chr <- Chromatograms(be)

divide_intensities <- function(x, y, ...) {
  intensity(x) <- lapply(intensity(x), `/%`, y)
  x
}
```

```
## Add the function to the processing queue
chr <- addProcessing(chr, divide_intensities, y = 2)
chr

# Apply the processing queue
chr <- applyProcessing(chr)
```

reset

Fill data.frame with columns for missing core chromatogram variables.

Description

`fillCoreChromVariables()` fills a provided `data.frame` with columns for eventually missing *core* chromatogram variables. The missing core variables are added as new columns with missing values (NA) of the correct data type. Use `coreChromVariables()` to list the set of core variables and their data types.

`validChromData()` checks that columns, representing *core* chromatogram variables are of the correct data type.

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

This method returns the chromatographic data stored in the backend. If not specified otherwise it will return all defined columns in the `chromData` slot as well as adding the `coreChromVariables` missing with NA values.

Usage

```
reset(object, ...)
```

```
fillCoreChromVariables(x = data.frame())
```

```
validChromData(x = data.frame(), error = TRUE)
```

```
validPeaksData(x = list(), error = TRUE)
```

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

```
## S4 method for signature 'ChromBackendMemory'
chromData(object, columns = chromVariables(object), drop = FALSE)
```

```
## S4 replacement method for signature 'ChromBackendMemory'
chromData(object) <- value
```

```
## S4 method for signature 'ChromBackendMemory'
chromVariables(object)
```

```
## S4 method for signature 'ChromBackendMemory'
peaksData(object, columns = peaksVariables(object), drop = FALSE, ...)
```

```
## S4 replacement method for signature 'ChromBackendMemory'  
peaksData(object) <- value  
  
## S4 method for signature 'ChromBackendMemory'  
peaksVariables(object)  
  
## S4 method for signature 'ChromBackendMemory'  
isReadOnly(object)  
  
## S4 method for signature 'ChromBackendMemory'  
show(object)  
  
## S4 method for signature 'ChromBackendMemory'  
supportsSetBackend(object, ...)  
  
## S4 method for signature 'ChromBackendMemory'  
x[i, j, ..., drop = FALSE]  
  
## S4 method for signature 'ChromBackendMemory'  
x$name  
  
## S4 replacement method for signature 'ChromBackendMemory'  
x$name <- value  
  
## S4 method for signature 'ChromBackendMemory'  
chromExtract(object, peak.table, by)  
  
## S4 method for signature 'ChromBackendMzR'  
show(object)  
  
## S4 method for signature 'ChromBackendMzR'  
backendParallelFactor(object, ...)  
  
## S4 method for signature 'ChromBackendMzR'  
isReadOnly(object)  
  
## S4 method for signature 'ChromBackendMzR'  
peaksData(  
  object,  
  columns = peaksVariables(object),  
  drop = FALSE,  
  BPPARAM = SerialParam(),  
  ...  
)  
  
## S4 replacement method for signature 'ChromBackendMzR'  
peaksData(object) <- value  
  
## S4 replacement method for signature 'ChromBackendMzR'  
chromData(object) <- value  
  
## S4 method for signature 'ChromBackendMzR'
```

```

supportsSetBackend(object, ...)

## S4 method for signature 'ChromBackendMzR'
x[i, j, ..., drop = TRUE]

## S4 method for signature 'ChromBackendMzR'
chromExtract(object, peak.table, by, ...)

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

## S4 method for signature 'ChromBackendSpectra'
factorize(object, factorize.by = c("msLevel", "dataOrigin"), ...)

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

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

## S4 method for signature 'ChromBackendSpectra'
peaksData(object, columns = peaksVariables(object), drop = FALSE, ...)

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

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

## S4 method for signature 'ChromBackendSpectra'
x[i, j, ..., drop = TRUE]

## S4 method for signature 'ChromBackendSpectra'
chromExtract(object, peak.table, by, ...)

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

```

Arguments

object	A Chromatograms object.
x	list representing the peaks data of a Chromatograms
error	logical(1) whether an error should be thrown (the default) if one or more columns don't have the correct data type.

Value

input data frame x with missing core variables added (with the correct data type).

If the core variables have all the correct data type: an empty character. If one or more core variables (columns) have the wrong data type the function either throws an error (with error = TRUE) or returns a character specifying which variables/columns don't have the correct type (for error = FALSE).

Not applicable

Examples

```
## Define a data frame
a <- data.frame(msLevel = c(1L, 1L, 2L), other_column = "b")

## Add missing core chromatogram variables to this data frame
fillCoreChromVariables(a)

## The data.frame thus contains columns for all core chromatogram
## variables in the respective expected data type (but filled with
## missing values).
```

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