

Package ‘MsBackendMassbank’

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Title Mass Spectrometry Data Backend for MassBank record Files

Version 1.0.0

Description Mass spectrometry (MS) data backend supporting import and export of MS/MS library spectra from MassBank record files. Different backends are available that allow handling of data in plain MassBank text file format or allow also to interact directly with MassBank SQL databases. Objects from this package are supposed to be used with the Spectra Bioconductor package. This package thus adds MassBank support to the Spectra package.

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metaDataBlocks	<i>Metadata blocks to be read</i>
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Description

metaDataBlocks returns a data.frame with the MassBank metadata blocks and whether they should be imported by default from the MassBank text files.

Usage

```
metaDataBlocks()
```

Value

A data.frame with metadata blocks.

Author(s)

Michael Witting

Examples

```
metaDataBlocks()
```

MsBackendMassbank *MS data backend for mgf files*

Description

The MsBackendMassbank class supports import of MS/MS spectra data from MS/MS spectrum data from **Massbank** files. After initial import, the full MS data is kept in memory. MsBackendMassbank extends the `MsBackendDataFrame()` backend directly and supports thus the `applyProcessing()` function to make data manipulations persistent.

New objects are created with the MsBackendMassbank function. The backendInitialize method has to be subsequently called to initialize the object and import MS/MS data from (one or more) MassBank files. Optional parameter nonStop allows to specify whether the import returns with an error if one of the text files lacks required data, such as mz and intensity values (default nonStop = FALSE), or whether only affected file(s) is(are) skipped and a warning is shown (nonStop = TRUE). Note that any other error will abort import regardless of parameter nonStop.

Usage

```
## S4 method for signature 'MsBackendMassbank'
backendInitialize(
  object,
  files,
  metaBlocks = metaDataBlocks(),
  nonStop = FALSE,
  ...,
  BPPARAM = bpparam()
)

MsBackendMassbank()

spectraVariableMapping(format = c("Massbank"))

## S4 method for signature 'MsBackendMassbank'
export(object, x, file = tempfile(), mapping = spectraVariableMapping(), ...)
```

Arguments

object	Instance of MsBackendMassbank class.
files	character with the (full) file name(s) of the MassBank file(s) from which MS/MS data should be imported.
metaBlocks	data.frame indicating which metadata shall be imported. Default is <code>metaDataBlocks()</code> .
nonStop	logical(1) whether import should be stopped if an xml file does not contain all required fields. Defaults to nonStop = FALSE.
...	Currently ignored.

BPPARAM	Parameter object defining the parallel processing setup to import data in parallel. Defaults to BPPARAM = <code>bpparam()</code> . See <code>bpparam()</code> for more information.
format	for <code>spectraVariableMapping</code> : character(1) defining the format to be used. Currently only <code>format = "Massbank"</code> is supported.
x	<code>Spectra()</code> object that should be exported.
file	for export: character(1) defining the output file.
mapping	for export: named character vector allowing to specify how fields from the Massbank file should be renamed. Names are supposed to be the spectra variable name and values of the vector the field names in the Massbank file. See output of <code>spectraVariableMapping()</code> for the expected format.

Value

`backendInitialize` and `MsBackendMassbank` return an instance of `MsBackendMassbank-class`.

Author(s)

Michael Witting

Examples

```
## Create an MsBackendMassbank backend and import data from a test file.
fls <- dir(system.file("extdata", package = "MsBackendMassbank"),
           full.names = TRUE, pattern = "txt$")
be <- backendInitialize(MsBackendMassbank(), fls)
be

be$msLevel
be$intensity
be$mz

## Initializing a backend reading additional metadata columns/information
mb <- metaDataBlocks()
mb
mb[1, 2] <- TRUE

be <- backendInitialize(MsBackendMassbank(), fls, metaBlocks = mb)
spectraVariables(be)
be$instrument
```

Description

The MsBackendMassbankSql provides access to mass spectrometry data from **MassBank** by directly accessing its MySQL/MariaDb database. In addition it supports adding new spectra variables or *locally* changing spectra variables provided by MassBank (without changing the original values in the database).

Note that MsBackendMassbankSql requires a local installation of the MassBank database since direct database access is not supported for the *main* MassBank instance.

Also, some of the fields in the MassBank database are not directly compatible with Spectra, such as the *collision energy* which is not available as a numeric value. The collision energy as available in MassBank is reported as spectra variable "collision_energy_text". Also, precursor m/z values reported for some spectra can not be converted to a numeric and hence NA is reported with the spectra variable precursorMz for these spectra. The variable "precursor_mz_text" can be used to get the *original* precursor m/z reported in MassBank.

Usage

```
MsBackendMassbankSql()

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

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

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

## S4 method for signature 'MsBackendMassbankSql'
peaksData(object)

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

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

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

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

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

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

```
## S4 method for signature 'MsBackendMassbankSql'  
dataStorage(object)  
  
## S4 method for signature 'MsBackendMassbankSql'  
intensity(object)  
  
## S4 replacement method for signature 'MsBackendMassbankSql'  
intensity(object) <- value  
  
## S4 method for signature 'MsBackendMassbankSql'  
ionCount(object)  
  
## S4 method for signature 'MsBackendMassbankSql'  
isEmpty(x)  
  
## S4 method for signature 'MsBackendMassbankSql'  
isolationWindowLowerMz(object)  
  
## S4 replacement method for signature 'MsBackendMassbankSql'  
isolationWindowLowerMz(object) <- value  
  
## S4 method for signature 'MsBackendMassbankSql'  
isolationWindowTargetMz(object)  
  
## S4 replacement method for signature 'MsBackendMassbankSql'  
isolationWindowTargetMz(object) <- value  
  
## S4 method for signature 'MsBackendMassbankSql'  
isolationWindowUpperMz(object)  
  
## S4 replacement method for signature 'MsBackendMassbankSql'  
isolationWindowUpperMz(object) <- value  
  
## S4 method for signature 'MsBackendMassbankSql'  
length(x)  
  
## S4 method for signature 'MsBackendMassbankSql'  
msLevel(object)  
  
## S4 method for signature 'MsBackendMassbankSql'  
mz(object)  
  
## S4 replacement method for signature 'MsBackendMassbankSql'  
mz(object) <- value  
  
## S4 method for signature 'MsBackendMassbankSql'  
lengths(x, use.names = FALSE)
```

```
## S4 method for signature 'MsBackendMassbankSql'  
polarity(object)  
  
## S4 replacement method for signature 'MsBackendMassbankSql'  
polarity(object) <- value  
  
## S4 method for signature 'MsBackendMassbankSql'  
precursorCharge(object)  
  
## S4 method for signature 'MsBackendMassbankSql'  
precursorIntensity(object)  
  
## S4 method for signature 'MsBackendMassbankSql'  
precursorMz(object)  
  
## S4 method for signature 'MsBackendMassbankSql'  
reset(object)  
  
## S4 method for signature 'MsBackendMassbankSql'  
runtime(object)  
  
## S4 replacement method for signature 'MsBackendMassbankSql'  
runtime(object) <- value  
  
## S4 method for signature 'MsBackendMassbankSql'  
scanIndex(object)  
  
## S4 method for signature 'MsBackendMassbankSql'  
selectSpectraVariables(object, spectraVariables = spectraVariables(object))  
  
## S4 method for signature 'MsBackendMassbankSql'  
smoothed(object)  
  
## S4 replacement method for signature 'MsBackendMassbankSql'  
smoothed(object) <- value  
  
## S4 method for signature 'MsBackendMassbankSql'  
spectraData(object, columns = spectraVariables(object))  
  
## S4 replacement method for signature 'MsBackendMassbankSql'  
spectraData(object) <- value  
  
## S4 method for signature 'MsBackendMassbankSql'  
spectraNames(object)  
  
## S4 replacement method for signature 'MsBackendMassbankSql'  
spectraNames(object) <- value
```

```

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

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

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

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

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

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

## S4 method for signature 'MsBackendMassbankSql'
compounds(object, ...)

```

Arguments

object	Object extending MsBackendMassbankSql.
dbcon	For backendInitialize, MsBackendMassbankSql: SQL database connection to the MassBank (MariaDb) database.
...	Additional arguments.
value	replacement value for <- methods. See individual method description or expected data type.
x	Object extending MsBackendMassbankSql.
use.names	For lengths: whether spectrum names should be used.
spectraVariables	For selectSpectraVariables: character with the names of the spectra variables to which the backend should be subsetted.
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.
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.
drop	For [: not considered.
name	For \$ and \$<-: the name of the spectra variable to return or set.

Value

See documentation of respective function.

Supported Backend functions

The following functions are supported by the MsBackendMassbankSqlMassbankDb.

- `[]`: subset the backend. Only subsetting by element (*row/i*) is allowed
- `$, $<-`: 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).
- `peaksData` returns a list with the spectra's peak data. The length of the list is equal to the number of spectra in object. Each element of the list is a matrix with columns "mz" and "intensity". For an empty spectrum, a matrix with 0 rows and two columns (named `mz` and `intensity`) is returned.
- `backendInitialize`: initialises the backend by retrieving the IDs of all spectra in the database. Parameter `dbcon` with the connection to the MassBank MySQL database is required.
- `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`: returns "<MassBank>" for all spectra.
- `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. Note that the collision energy description from MassBank are provided as spectra variable "collisionEnergyText".
- `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 `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:::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.
- `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.
- `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 (integer) 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 if no precursor information is available.
- `reset`: restores the backend to its original state, i.e. deletes all locally modified data and reinitializes the backend to the full data available in the database.
- `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.
- `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 replacing the spectra data with `spectraData<-` is not supported.
- `spectraNames`: returns a character vector with the names of the spectra in object.
- `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).
- `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.

Not supported Backend functions

The following functions are not supported by the MsBackendMassbankSql since the original data can not be changed.

backendMerge, export, filterDataStorage, filterPrecursorScan, peaksData<-, filterAcquisitionNum, intensity<-, mz<-, precScanNum, spectraData<-, spectraNames<-.

Retrieving compound annotations for spectra

While compound annotations are also provided *via* the spectraVariables of the backend, it would also be possible to use the compounds function on a Spectra object (that uses a MsBackendMassbankSql backend) to retrieve compound annotations for the specific spectra.

Author(s)

Johannes Rainer

Examples

```
## Create a connection to a database with MassBank data - in the present
## example we connect to a tiny SQLite database bundled in this package
## as public access to the MassBank MySQL is not (yet) supported. See the
## vignette for more information on how to install MassBank locally and
## enable MySQL database connections
library(RSQLite)
con <- dbConnect(SQLite(), system.file("sql", "minimassbank.sqlite",
  package = "MsBackendMassbank"))

## Given that we have the connection to a MassBank databas we can
## initialize the backend:
be <- backendInitialize(MsBackendMassbankSql(), dbcon = con)
be

## Access MS level
msLevel(be)
be$msLevel

## Access m/z values
be$mz

## Access the full spectra data (including m/z and intensity values)
spectraData(be)

## Add a new spectra variable
be$new_variable <- "b"
be$new_variable

## Subset the backend
be_sub <- be[c(3, 1)]

spectraNames(be)
spectraNames(be_sub)
```

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