Package ‘MsBackendSql’

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Title SQL-based Mass Spectrometry Data Backend

Version 1.4.0

Description SQL-based mass spectrometry (MS) data backend supporting also storange and handling of very large data sets. Objects from this package are supposed to be used with the Spectra Bioconductor package. Through the MsBackendSql with its minimal memory footprint, this package thus provides an alternative MS data representation for very large or remote MS data sets.

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`MsBackendOfflineSql` *SQL-based MS backend without active database connection*

Description

The `MsBackendOfflineSql` backend extends the `MsBackendSql()` backend directly and inherits thus all of its functions as well as properties. The only difference between the two backend is that `MsBackendSql` keeps an active connection to the SQL database inside the object while the `MsBackendOfflineSql` backends reconnects to the SQL database for each query. While the performance of the latter is slightly lower (due to the need to connect/disconnect to the database for each function call) it can also be used in a parallel processing environment.

Usage

```
MsBackendOfflineSql()

## S4 method for signature 'MsBackendOfflineSql'
backendInitialize(
  object,
  drv = NULL,
  dbname = character(),
  user = character(),
  password = character(),
  host = character(),
  port = NA_integer_,
  data,
  ...
)
```

Arguments

`object`	A `MsBackendOfflineSql` object.

drv	A *DBI* database driver object (such as `SQLite()` from the `RSQLite` package or `MariaDB()` from the `RMariaDB` package). See `dbConnect()` for more information.
dbname	`character(1)` with the name of the database. Passed directly to `dbConnect()`.
user	`character(1)` with the user name for the database. Passed directly to `dbConnect()`.
password	`character(1)` with the password for the database. Note that this password is stored (unencrypted) within the object. Passed directly to `dbConnect()`.
host	`character(1)` with the host running the database. Passed directly to `dbConnect()`.
port	`integer(1)` with the port number (optional). Passed directly to `dbConnect()`.
data	For `backendInitialize()`: optional `DataFrame` with the full spectra data that should be inserted into a (new) `MsBackendSql` database. If provided, it is assumed that the provided database connection information if for a (writeable) empty database into which `data` should be inserted. `data` could be the output of `spectraData` from another backend.
...	ignored.

Creation of backend objects

An empty instance of an `MsBackendOfflineSql` class can be created using the `MsBackendOfflineSql()` function. An existing *MsBackendSql* SQL database can be loaded with the `backendInitialize()` function. This function takes parameters `drv`, `dbname`, `user`, `password`, `host` and `port`, all parameters that are passed to the `dbConnect()` function to connect to the (**existing**) SQL database.

See `MsBackendSql()` for information on how to create a *MsBackend* SQL database.

Author(s)

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MsBackendSql `Spectra` *MS backend storing data in a SQL database*

Description

The `MsBackendSql` is an implementation for the `MsBackend()` class for `Spectra()` objects which stores and retrieves MS data from a SQL database. New databases can be created from raw MS data files using `createMsBackendSqlDatabase()`.

Usage

```
MsBackendSql()

createMsBackendSqlDatabase(
  dbcon,
  x = character(),
  backend = MsBackendMzR(),
```

```
  chunksize = 10L,
  blob = TRUE,
  partitionBy = c("none", "spectrum", "chunk"),
  partitionNumber = 10L
)

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

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

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

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

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

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

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

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

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

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

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

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

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

## S4 method for signature 'MsBackendSql'
filterMsLevel(object, msLevel = uniqueMsLevels(object))
```

```
## S4 method for signature 'MsBackendSql'
filterRt(object, rt = numeric(), msLevel. = integer())

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

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

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

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

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

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

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

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

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

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

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

## S4 method for signature 'MsBackendSql'
dbconn(x)
```

Arguments

dbcon	Connection to a database.
x	For `createMsBackendSqlDatabase()`: `character` with the names of the raw data files from which the data should be imported. For other methods an `MsqlBackend` instance.
backend	For `createMsBackendSqlDatabase()`: MS backend that can be used to import MS data from the raw files specified with parameter `x`.
chunksize	For `createMsBackendSqlDatabase()`: `integer(1)` defining the number of

input that should be processed per iteration. With `chunksize = 1` each file specified with `x` will be imported and its data inserted to the database. With `chunksize = 5` data from 5 files will be imported (in parallel) and inserted to the database. Thus, higher values might result in faster database creation, but require also more memory.

`blob` For `createMsBackendSqlDatabase()`: `logical(1)` whether individual m/z and intensity values should be stored separately (`blob = FALSE`) or if the m/z and intensity values for each spectrum should be stored as a single *BLOB* SQL data type (`blob = TRUE`, the default).

`partitionBy` For `createMsBackendSqlDatabase()`: `character(1)` defining if and how the peak data table should be partitioned. `"none"` (default): no partitioning, `"spectrum"`: peaks are assigned to the partition based on the spectrum ID (number), i.e. spectra are evenly (consecutively) assigned across partitions. For `partitionNumber = 3`, the first spectrum is assigned to the first partition, the second to the second, the third to the third and the fourth spectrum again to the first partition. `"chunk"`: spectra processed as part of the same *chunk* are placed into the same partition. All spectra from the next processed chunk are assigned to the next partition. Note that this is only available for MySQL/MariaDB databases, i.e., if `con` is a `MariaDBConnection`. See details for more information.

`partitionNumber`
For `createMsBackendSqlDatabase()`: `integer(1)` defining the number of partitions the database table will be partitioned into (only supported for MySQL/MariaDB databases).

`object` A `MsBackendSql` instance.

`data` For `backendInitialize()`: optional `DataFrame` with the full spectra data that should be inserted into a (new) `MsBackendSql` database. If provided, it is assumed that `dbcon` is a (writeable) connection to an empty database into which `data` should be inserted. `data` could be the output of `spectraData` from another backend.

`...` For `[`: ignored. For `backendInitialize`, if parameter `data` is used: additional parameters to be passed to the function creating the database such as `blob`.

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

`j` For `[`: ignored.

`drop` For `[`: `logical(1)`, ignored.

`columns` For `spectraData()`: `character()` optionally defining a subset of spectra variables that should be returned. Defaults to `columns = spectraVariables(object)` hence all variables are returned. For `peaksData` accessor: optional `character` with requested columns in the individual `matrix` of the returned `list`. Defaults to `columns = c("mz", "intensity")` but all columns listed by `peaksVariables` would be supported.

`value` For all setter methods: replacement value.

`name` For `<-`: `character(1)` with the name of the spectra variable to replace.

`msLevel` For `filterMsLevel()`: `integer` specifying the MS levels to filter the data.

`rt` For `filterRt()`: `numeric(2)` with the lower and upper retention time. Spectra with a retention time `>= rt[1]` and `<= rt[2]` are returned.

msLevel. For filterRt(): integerwith the MS level(s) on which the retention time filter should be a

dataOrigin For filterDataOrigin(): character with *data origin* values to which the data should be subsetted.

mz For filterPrecursorMzRange(): numeric(2) with the desired lower and upper limit of the precursor m/z range. For filterPrecursorMzValues(): numeric with the m/z value(s) to filter the object.

ppm For filterPrecursorMzValues(): numeric with the m/z-relative maximal acceptable difference for a m/z value to be considered matching. Can be of length 1 or equal to length(mz).

tolerance For filterPrecursorMzValues(): numeric with the absolute difference for m/z values to be considered matching. Can be of length 1 or equal to length(mz).

initial For tic(): logical(1) whether the original total ion count should be returned (initial = TRUE, the default) or whether it should be calculated on the spectras' intensities (initial = FALSE).

BPPARAM for backendBpparam(): BiocParallel parallel processing setup. See bpparam() for more information.

Details

The MsBackendSql class is principally a *read-only* backend but by extending the MsBackendCached() backend from the Spectra package it allows changing and adding (**temporarily**) spectra variables **without** changing the original data in the SQL database.

Value

See documentation of respective function.

Creation of backend objects

New backend objects can be created with the MsBackendSql() function. SQL databases can be created and filled with MS data from raw data files using the createMsBackendSqlDatabase() function or using backendInitialize() and providing all data with parameter data. In addition it is possible to create a database from a Spectra object changing its backend to a MsBackendSql or MsBackendOfflineSql using the setBackend() function. Existing SQL databases (created previously with createMsBackendSqlDatabase() or backendInitialize() with the data parameter) can be loaded using the *conventional* way to create/initialize MsBackend classes, i.e. using backendInitialize().

- createMsBackendSqlDatabase(): create a database and fill it with MS data. Parameter dbcon is expected to be a database connection, parameter x a character vector with the file names from which to import the data. Parameter backend is used for the actual data import and defaults to backend = MsBackendMzR() hence allowing to import data from mzML, mzXML or netCDF files. Parameter chunksize allows to define the number of files (x) from which the data should be imported in one iteration. With the default chunksize = 10L data is imported from 10 files in x at the same time (if backend supports it even in parallel) and this data is then inserted into the database. Larger chunk sizes will require more memory and also larger disk space (as data import is performed through temporary files) but might eventually be faster. Parameter blob allows to define whether m/z and intensity values from a spectrum should be

stored as a *BLOB* SQL data type in the database (`blob = TRUE`, the default) or if individual m/z and intensity values for each peak should be stored separately (`blob = FALSE`). The latter case results in a much larger database and slower performance of the `peaksData` function, but would allow to define custom (manual) SQL queries on individual peak values. While data can be stored in any SQL database, at present it is suggested to use MySQL/MariaDB databases. For `dbcon` being a connection to a MySQL/MariaDB database, the tables will use the *ARIA* engine providing faster data access and will use *table partitioning*: tables are splitted into multiple partitions which can improve data insertion and index generation. Partitioning can be defined with the parameters `partitionBy` and `partitionNumber`. By default `partitionBy = "none"` no partitioning is performed. For `blob = TRUE` partitioning is usually not required. Only for `blob = FALSE` and very large datasets it is suggested to enable table partitioning by selecting either `partitionBy = "spectrum"` or `partitionBy = "chunk"`. The first option assignes consecutive spectra to different partitions while the latter puts spectra from files part of the same *chunk* into the same partition. Both options have about the same performance but `partitionBy = "spectrum"` requires less disk space. Note that, while inserting the data takes a considerable amount of time, also the subsequent creation of database indices can take very long (even longer than data insertion for `blob = FALSE`).

- `backendInitialize()`: get access and initialize a `MsBackendSql` object. Parameter `object` is supposed to be a `MsBackendSql` instance, created e.g. with `MsBackendSql()`. Parameter `dbcon` is expected to be a connection to an existing *MsBackendSql* SQL database (created e.g. with `createMsBackendSqlDatabase()`). `backendInitialize()` can alternatively also be used to create a **new** `MsBackendSql` database using the optional `data` parameter. In this case, `dbcon` is expected to be a writeable connection to an empty database and `data` a `DataFrame` with the **full** spectra data to be inserted into this database. The format of `data` should match the format of the `DataFrame` returned by the `spectraData()` function and requires columns `"mz"` and `"intensity"` with the m/z and intensity values of each spectrum. The `backendInitialize()` call will then create all necessary tables in the database, will fill these tables with the provided data and will return an `MsBackendSql` for this database. Thus, the `MsBackendSql` supports the `setBackend` method from `Spectra` to change from (any) backend to a `MsBackendSql`. Note however that chunk-wise (or parallel) processing needs to be disabled in this case by passing eventually `f = factor()` to the `setBackend()` call.
- `supportsSetBackend()`: whether `MsBackendSql` supports the `setBackend()` method to change the `MsBackend` of a `Spectra` object to a `MsBackendSql`. Returns `TRUE`, thus, changing the backend to a `MsBackendSql` is supported **if** a writeable database connection is provided in addition with parameter `dbcon` (i.e. `setBackend(sps, MsBackendSql(), dbcon = con)` with `con` being a connection to an **empty** database would store the full spectra data from the `Spectra` object `sps` into the specified database and would return a `Spectra` object that uses a `MsBackendSql`).
- `backendBpparam()`: whether a `MsBackendSql` supports parallel processing. Takes a `MsBackendSql` and a parallel processing setup (see `bpparam()` for details) as input and always returns a `SerialParam()` since `MsBackendSql` does **not** support parallel processing.
- `dbconn()`: returns the connection to the database.

Subsetting, merging and filtering data

`MsBackendSql` objects can be subsetted using the `[` function. Internally, this will simply subset the `integer` vector of the primary keys and eventually cached data. The original data in the database **is not** affected by any subsetting operation. Any subsetting operation can be *undone* by resetting

the object with the `reset()` function. Subsetting in arbitrary order as well as index replication is supported.

Multiple `MsBackendSql` objects can also be merged (combined) with the `backendMerge()` function. Note that this requires that all `MsBackendSql` objects are connected to the **same** database. This function is thus mostly used for combining `MsBackendSql` objects that were previously splitted using e.g. `split()`.

In addition, `MsBackendSql` supports all other filtering methods available through `MsBackendCached()`. Implementation of filter functions optimized for `MsBackendSql` objects are:

- `filterDataOrigin()`: filter the object retaining spectra with `dataOrigin` spectra variable values matching the provided ones with parameter `dataOrigin`. The function returns the results in the order of the values provided with parameter `dataOrigin`.
- `filterMsLevel()`: filter the object based on the MS levels specified with parameter `msLevel`. The function does the filtering using SQL queries. If `"msLevel"` is a *local* variable stored within the object (and hence in memory) the default implementation in `MsBackendCached` is used instead.
- `filterPrecursorMzRange()`: filters the data keeping only spectra with a `precursorMz` within the m/z value range provided with parameter `mz` (i.e. all spectra with a precursor m/z >= `mz[1L]` and <= `mz[2L]`).
- filterPrecursorMzValues(): `filters the data keeping only spectra with precursor m/z values matching the` to use different values for ppm and tolerance for each provided m/z value.
- `filterRt()`: filter the object keeping only spectra with retention times within the specified retention time range (parameter `rt`). Optional parameter `msLevel.` allows to restrict the retention time filter only on the provided MS level(s) returning all spectra from other MS levels.

Accessing and *modifying* data

The functions listed here are specifically implemented for `MsBackendSql`. In addition, `MsBackendSql` inherits and supports all data accessor, filtering functions and data manipulation functions from `MsBackendCached()`.

- `$`, `$<-`: access or set (add) spectra variables in `object`. Spectra variables added or modified using the `$<-` are *cached* locally within the object (data in the database is never changed). To restore an object (i.e. drop all cached values) the `reset` function can be used.
- `dataStorage()`: returns a `character` vector same length as there are spectra in `object` with the name of the database containing the data.
- `intensity<-`: not supported.
- `mz<-`: not supported.
- `peaksData()`: returns a `list` with the spectras' 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 according to parameter `columns`. For an empty spectrum, a `matrix` with 0 rows is returned. Use `peaksVariables(object)` to list supported values for parameter `columns`.
- `peaksVariables()`: returns a `character` with the available peak variables, i.e. columns that could be queried with `peaksData()`.
- `reset()`: *restores* an `MsBackendSql` by re-initializing it with the data from the database. Any subsetting or cached spectra variables will be lost.

- `spectraData()`: gets general spectrum metadata. `spectraData()` returns a `DataFrame` with the same number of rows as there are spectra in `object`. Parameter `columns` allows to select specific spectra variables.
- `spectraNames()`, `spectraNames<-`: returns a `character` of length equal to the number of spectra in `object` with the primary keys of the spectra from the database (converted to `character`). Replacing spectra names with `spectraNames<-` is not supported.
- `uniqueMsLevels()`: returns the unique MS levels of all spectra in `object`.
- `tic()`: returns the originally reported total ion count (for `initial = TRUE`) or calculates the total ion count from the intensities of each spectrum (for `initial = FALSE`).

Implementation notes

Internally, the `MsBackendSql` class contains only the primary keys for all spectra stored in the SQL database. Keeping only these `integer` in memory guarantees a minimal memory footpring of the object. Still, depending of the number of spectra in the database, this `integer` vector might become very large. Any data access will involve SQL calls to retrieve the data from the database. By extending the `MsBackendCached()` object from the `Spectra` package, the `MsBackendSql` supports to (temporarily, i.e. for the duration of the R session) add or modify spectra variables. These are however stored in a `data.frame` within the object thus increasing the memory demand of the object.

Note

The `MsBackendSql` backend keeps an (open) connection to the SQL database with the data and hence does not support saving/loading of a backend to disk (e.g. using `save` or `saveRDS`). Also, for the same reason, the `MsBackendSql` does not support parallel processing. The `backendBpparam()` method for `MsBackendSql` will thus always return a `SerialParam()` object.

The `MsBackendOfflineSql()` could be used as an alternative as it supports saving/loading the data to/from disk and supports also parallel processing.

Author(s)

Johannes Rainer

Examples

```
####
## Create a new MsBackendSql database

## Define a file from which to import the data
data_file <- system.file("microtofq", "MM8.mzML", package = "msdata")

## Create a database/connection to a database
library(RSQLite)
db_file <- tempfile()
dbc <- dbConnect(SQLite(), db_file)

## Import the data from the file into the database
createMsBackendSqlDatabase(dbc, data_file)
dbDisconnect(dbc)
```

```
## Initialize a MsBackendSql
dbc <- dbConnect(SQLite(), db_file)
be <- backendInitialize(MsBackendSql(), dbc)

be

## Original data source
head(be$dataOrigin)

## Data storage
head(dataStorage(be))

## Access all spectra data
spd <- spectraData(be)
spd

## Available variables
spectraVariables(be)

## Access mz values
mz(be)

## Subset the object to spectra in arbitrary order
be_sub <- be[c(5, 1, 1, 2, 4, 100)]
be_sub

## The internal spectrum IDs (primary keys from the database)
be_sub$spectrum_id_

## Add additional spectra variables
be_sub$new_variable <- "B"

## This variable is *cached* locally within the object (not inserted into
## the database)
be_sub$new_variable
```

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