Package: MsBackendSql (via r-universe)

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Title SQL-based Mass Spectrometry Data Backend

Version 1.14.0

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 `DBI::dbConnect()` for more information.
`dbname`	`character(1)` with the name of the database. Passed directly to `DBI::dbConnect()`.
`user`	`character(1)` with the user name for the database. Passed directly to `DBI::dbConnect()`.
`password`	`character(1)` with the password for the database. Note that this password is stored (unencrypted) within the object. Passed directly to `DBI::dbConnect()`.
`host`	`character(1)` with the host running the database. Passed directly to `DBI::dbConnect()`.

port	integer(1) with the port number (optional). Passed directly to DBI::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)

Johannes Rainer

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

Description

The MsBackendSql is an implementation for the Spectra::MsBackend() class for Spectra::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,
  peaksStorageMode = c("blob2", "long", "blob"),
  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,ANY'
extractByIndex(object, i)

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

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

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

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

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

## 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)

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

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(), setBackend(): logical(1) whether individual m/z and intensity values should be stored separately (blob = FALSE) or if the peaks data should be stored as data type *BLOB* into the database (blob = TRUE, the default). See also parameter peaksStorageMode for different data storage options.

peaksStorageMode

character(1) defining how peaks variables are stored in the database. The default peaksStorageMode = "blob2" stores the full peaks matrix of each spectrum as data type *BLOB* as one entry into a single database table column. peaksStorageMode = "blob" stores in contrast the m/z and intensity vectors as separate BLOB types into two database tables. peaksStorageMode = "long" allows to store the data in *long mode*, i.e. each intensity and m/z value is stored individually in the database.

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 or peaksStorageMode. For setBackend(): any parameters supported by backendInitialize() or createMsBackendSqlDatabase().

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 ap
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 BiocParallel::bpparam() for more information.

Details

The MsBackendSql class is principally a *read-only* backend but by extending the Spectra::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 `Spectra::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. For `blob = TRUE`, the peaks data can be stored in two different ways which can be selected with the additional parameter `peaksStorageMode`. The default `peaksStorageMode = "blob2"` stores the full peaks matrix of a spectrum as a single entry to the database (into a single database table column) while `peaksStorageMode = "blob"` (which was the default until version 1.7.2) stores the m/z and intensity vectors as BLOB data type into two separate database table columns. Performance for `peaksData()` is thus about twice as fast for `peaksStorageMode = "blob2"`. 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()`). To initialize a `MsBackendOfflineSql()` all information required for a `DBI::dbConnect()` call to connect to a database need to be provided.

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 and peaks 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. The MsBackendSql and MsBackendOfflineSql objects support the Spectra::setBackend() method from Spectra to change from (any) backend to a MsBackendSql. Any parameters to the backendInitialize() function can be passed to setBackend(). 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 BiocParallel::bpparam() for details) as input and always returns a BiocParallel::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 [or extractByIndex() functions. 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 Spectra::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 `Spectra::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.
- `longForm()`: extract the MS data in *long form* as a `data.frame`. Parameter `columns` allows to specify the columns (spectra and/or peaks variables) that should be included in the result. If MS peaks data are stored in long form in the database (i.e., `peaksStorageMode = "long"` is used), the data is extracted using a dedicated SQL query. Otherwise the default implementation of the `longForm()` method from the *Spectra* package that is based on the `spectraData()` function is used instead. Note that the performance of the SQL-based `longForm()` function is not necessarily higher than the default implementation, mostly because data extraction from the database layouts that store the MS peaks data as *BLOB* datatype (i.e., `peaksStorageMode = "blob"` or `peaksStorageMode = "blob2"`) is faster.
- `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 `Spectra::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 `BiocParallel::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 <- MsDataHub::X20171016_POOL_POS_3_105.134.mzML()

## 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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