Package 'MsBackendMsp'

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Title Mass Spectrometry Data Backend for NIST msp Files

Version 1.12.0

Description Mass spectrometry (MS) data backend supporting import and handling of MS/MS spectra from NIST MSP Format (msp) files. Import of data from files with different MSP *flavours* is supported. Objects from this package add support for MSP files to Bioconductor's Spectra package. This package is thus not supposed to be used without the Spectra package that provides a complete infrastructure for MS data handling.

Depends R (>= 4.1.0), Spectra (>= 1.5.14)

Imports ProtGenerics (>= 1.35.3), BiocParallel, S4Vectors, IRanges, MsCoreUtils, methods, stats

Suggests testthat, knitr (>= 1.1.0), roxygen2, BiocStyle (>= 2.5.19), rmarkdown

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`hidden_aliases` *Internal page for hidden aliases*

Description

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

`MsBackendMsp` *MS data backend for msp files*

Description

The `MsBackendMsp` class supports import of MS/MS spectra data from files in NIST MSP file format. `MsBackendMsp` extends the `Spectra::MsBackendDataFrame()` backend directly and supports thus the `Spectra::applyProcessing()` function to make data manipulations persistent.

New objects are created with the `MsBackendMsp()` function. The `backendInitialize()` method has to be subsequently called to initialize the object and import MS/MS data from (one or more) msp files.

The `MsBackendMsp` backend provides an `export()` method that allows to export the data from the `Spectra` object (parameter `x`) to a file in MSP format.

Parameters to this function are:

- `x`: the `Spectra` object that should be exported.
- `file`: `character(1)` with the desired file name.
- `mapping`: named `character` providing the mapping between spectra variables and MSP data fields. Defaults to `mapping = spectraVariableMapping(MsBackendMsp())`.
- `allVariables`: `logical(1)` whether all spectra variables in `x` should be exported or only those defined with `mapping`.

- exportName: logical(1) whether a NAME field should always be exported even if not provided in x.

See the package vignette for details and examples.

The spectraVariableMapping() function allows to provide the mapping between spectra variable names (i.e. the names that will be used for the spectra variables in the Spectra::Spectra() object) and the data field names of the MSP file. Parameter format allows to select pre-defined mappings. Currently supported mapping flavors are:

- format = "msp": default MSP field names. Should work with standard NIST MSP files or MSP files exported from MS-DIAL.
- format = "mona": MSP file format from MoNA including LipidBlast.

Usage

```
## S4 method for signature 'MsBackendMsp'
backendInitialize(
  object,
  file,
  mapping = spectraVariableMapping(object),
  ...,
  BPPARAM = SerialParam()
)

MsBackendMsp()

## S4 method for signature 'MsBackendMsp'
spectraVariableMapping(object, format = c("msp", "mona"))

## S4 method for signature 'MsBackendMsp'
export(
  object,
  x,
  file = tempfile(),
  mapping = spectraVariableMapping(MsBackendMsp()),
  allVariables = TRUE,
  exportName = TRUE,
  ...
)
```

Arguments

object	Instance of MsBackendMsp class.
file	character with the (full) file name(s) of the msp file(s) from which MS/MS data should be imported or exported.
mapping	named character vector to rename MSP fields to spectra variables. This allows to correctly import also custom fields or data from files with different MSP *flavors*.

...	Currently ignored.
BPPARAM	Parameter object defining the parallel processing setup to import data in parallel. Defaults to BPPARAM = SerialParam(). See BiocParallel::bpparam() for more information. Parallel processing would make most sense for import from a large set of individual MSP files, but could also improve performance for import from a (very large) single MSP file.
format	For spectraVariableMapping(): character(1) specifying for which MSP *flavour* the mapping should be returned. Currently supported are: format = "msp" (generic MSP format, for example for MS-DIAL MSP files) and format = "mona" (MSP files in MoNA flavour).
x	For export(): a Spectra::Spectra() object that should be exported to the specified MSP file.
allVariables	logical(1) whether all spectra variables in x should be exported or only those defined with mapping.
exportName	logical(1) whether a NAME field should always be exported even if not provided in x.

Value

MsBackendMsp() and backendInitialize() return an instance of a MsBackendMsp class. spectraVariableMapping() a named character vector with the mapping between spectra variables and MSP data fields.

Note

Format requirements/assumptions of MSP files:

- Comment lines are expected to start with a #.
- Multiple spectra within the same MSP file are separated by an empty line.
- The first n lines of a spectrum entry represent metadata.
- Metadata is provided as "name: value" pairs (i.e. name and value separated by a ":").
- One line per mass peak, with values separated by a whitespace or tabulator.
- Each line is expected to contain at least the m/z and intensity values (in that order) of a peak. Additional values are currently ignored.

Author(s)

Steffen Neumann, Michael Witting, Laurent Gatto and Johannes Rainer

Examples

```
## Import spectra from a MSP file from LipidBlast
f <- system.file("extdata", "small-export-LipidBlast.msp",
    package = "MsBackendMsp")
be <- backendInitialize(MsBackendMsp(), f)
be

be$msLevel
```

```
be$intensity
be$mz

## precursor m/z are however all missing
be$precursorMz

## Default spectra variable mapping
spectraVariableMapping(MsBackendMsp())

## In fact, to read MSP files in "LipidBlast flavour" (same as MoNA) we
## should use a different spectra variable mapping
spectraVariableMapping(MsBackendMsp(), "mona")

## Importing the data with this will correctly retrieve data
be <- backendInitialize(MsBackendMsp(), f,
    mapping = spectraVariableMapping(MsBackendMsp(), "mona"))
be$precursorMz

## Other fields are also correctly mapped, but might need to be converted
## to e.g. numeric, such as "exactmass"
be$exactmass

be$exactmass <- as.numeric(be$exactmass)

be$adduct
be$formula

## Exporting Spectra objects in MSP format.

sps <- Spectra(be)
export(MsBackendMsp(), sps, file = stdout())
```

`readMsp` *Reading MSP files*

Description

The `readMsp()` function imports the data from a file in MGF format reading all specified fields and returning the data as a `S4Vectors::DataFrame()`.

Format constraints for MSP files:

- Comment lines are expected to start with a #.
- Multiple spectra within the same MSP file are separated by an empty line.
- The first n lines of a spectrum entry represent metadata.
- Metadata is provided as "name: value" pairs (i.e. name and value separated by a ":").
- One line per mass peak, with values separated by a whitespace or tabulator.
- Each line is expected to contain at least the m/z and intensity values (in that order) of a peak. Additional values are currently ignored.

Usage

```
readMsp(
  f,
  msLevel = 2L,
  mapping = spectraVariableMapping(MsBackendMsp()),
  BPPARAM = SerialParam(),
  ...
)
```

Arguments

f	`character(1)` with the path to an MSP file.
msLevel	`numeric(1)` with the MS level. Default is 2. This value will be reported as the spectra's MS level **unless** the source MSP file defines the MS level.
mapping	named `character` vector to rename MSP fields to spectra variables (see `spectraVariableMapping()` help). This allows to correctly import also custom fields or data from files with different MSP *flavors*.
BPPARAM	parallel processing setup. See `BiocParallel::bpparam()` for more details.
...	Additional parameters, currently ignored.

Value

A `DataFrame` with each row containing the data from one spectrum in the MSP file. m/z and intensity values are available in columns `"mz"` and `"intensity"` in a list representation.

Author(s)

Laurent Gatto, Steffen Neumann, Johannes Rainer

Examples

```
f <- system.file("extdata", "minimona.msp", package = "MsBackendMsp")

readMsp(f)
```

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