

Package ‘MsBackendMsp’

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Title Mass Spectrometry Data Backend for NIST msp Files

Version 1.7.3

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)

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URL <https://github.com/RforMassSpectrometry/MsBackendMsp>

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Contents

| | |
|--------------------------|---|
| hidden_aliases | 2 |
| MsBackendMsp | 2 |
| readMsp | 5 |

| | |
|--------------|----------|
| Index | 7 |
|--------------|----------|

| | |
|----------------|---|
| hidden_aliases | <i>Internal page for hidden aliases</i> |
|----------------|---|

Description

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

| | |
|--------------|--------------------------------------|
| MsBackendMsp | <i>MS data backend for msp files</i> |
|--------------|--------------------------------------|

Description

The MsBackendMsp class supports import of MS/MS spectra data from files in NIST MSP file format. MsBackendMsp extends the `MsBackendDataFrame()` backend directly and supports thus the `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()` 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

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

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| ... | Currently ignored. |
| BPPARAM | Parameter object defining the parallel processing setup to import data in parallel. Defaults to BPPARAM = SerialParam(). See <code>bpparam()</code> 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 <code>spectraVariableMapping()</code> : character(1) specifying for which MSP <i>flavour</i> 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 <code>export()</code> : a <code>Spectra()</code> 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 [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()). This allows to correctly import also custom fields or data from files with different MSP <i>flavors</i> . |
| BPPARAM | parallel processing setup. See 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)
```

Index

* **internal**

- hidden_aliases, [2](#)
- [, MsBackendDataFrame-method
 - (hidden_aliases), [2](#)
- applyProcessing(), [2](#)
- backendInitialize, MsBackendMsp-method
 - (MsBackendMsp), [2](#)
- bpparam(), [4](#), [6](#)
- DataFrame(), [5](#)
- export, MsBackendMsp-method
 - (MsBackendMsp), [2](#)
- hidden_aliases, [2](#)
- MsBackendDataFrame(), [2](#)
- MsBackendMsp, [2](#)
- MsBackendMsp-class (MsBackendMsp), [2](#)
- readMsp, [5](#)
- Spectra(), [3](#), [4](#)
- spectraVariableMapping(), [3](#), [6](#)
- spectraVariableMapping, MsBackendMsp-method
 - (MsBackendMsp), [2](#)