

Package ‘MsBackendRawFileReader’

March 22, 2022

Type Package

Title Mass Spectrometry Backend for Reading Thermo Fisher Scientific raw Files

Version 1.0.0

Depends R (>= 4.1), methods, Spectra (>= 1.2)

Imports MsCoreUtils, S4Vectors, IRanges, rawrr (>= 1.1.14), utils, BiocParallel

Suggests BiocStyle (>= 2.5), ExperimentHub, knitr, lattice, mzR, protViz (>= 0.7), rmarkdown, tartare (>= 1.5), testthat

Description implements a MsBackend for the Spectra package using Thermo Fisher Scientific's NewRawFileReader .Net libraries. The package is generalizing the functionality introduced by the rawrr package (Kockmann T. et al. (2020) <doi:10.1101/2020.10.30.362533>) Methods defined in this package are supposed to extend the Spectra Bioconductor package.

URL <https://github.com/fgcz/MsBackendRawFileReader>

BugReports <https://github.com/fgcz/MsBackendRawFileReader/issues>

Encoding UTF-8

NeedsCompilation yes

biocViews MassSpectrometry, Proteomics, Metabolomics

RoxygenNote 7.1.2

License GPL-3

SystemRequirements mono-runtime 4.x or higher (including System.Data library) on Linux/macOS, .Net Framework (>= 4.5.1) on Microsoft Windows.

VignetteBuilder knitr

Collate 'hidden_aliases.R' 'AllGenerics.R'
'MsBackendRawFileReader-functions.R' 'MsBackendRawFileReader.R'
'benchmark.R' 'zzz.R'

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ioBenchmark	<i>RawFileReader_read_peaks benchmark</i>
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Description

derives numbers to evaluate time performance for reading a single spectrum in dependency from the chunk size (how many spectra are read in one function call) for reading different numbers of overall spectra.

Usage

```
ioBenchmark(  
  nv = c(1000, 5000, 10000),  
  sizev = c(8, 16, 32, 64, 128, 256, 8, 16, 32, 64, 128, 256, 8, 16, 32, 64, 128, 256,  
    8, 16, 32, 64, 128, 256, 8, 16, 32, 64, 128, 256, 8, 16, 32, 64, 128, 256),  
  rawfile  
)
```

Arguments

- nv number of spectra to be read.
- sizev number of spectra write and parsed in one single junk.
- rawfile the Thermo Fisher Scientific raw file.

Value

data.frame

Examples

```
eh <- ExperimentHub::ExperimentHub()
EH4547 <- normalizePath(eh[["EH4547"]])
(rawfileEH4547 <- paste0(EH4547 , ".raw"))
if (!file.exists(rawfileEH4547 )){
  file.link(EH4547 , rawfileEH4547)
}
S <- ioBenchmark(1000, c(128, 256, 128, 256), rawfile=rawfileEH4547)
```

MsBackendRawFileReader

MsBackendRawFileReader

Description

MsBackendRawFileReader

Usage

```
MsBackendRawFileReader()

## S4 method for signature 'MsBackendRawFileReader'
filterScan(object, filter = character(), ...)

## S4 method for signature 'MsBackendRawFileReader'
scanType(object, ...)
```

Arguments

object	MsBackendRawFileReader object
filter	filter string
...	Arguments to be passed to methods.

Value

a MsBackendRawFileReader object.
a character vector of scan types.

Examples

```
beRaw <- Spectra::backendInitialize(MsBackendRawFileReader::MsBackendRawFileReader(),
  files = rawrr::sampleFilePath())
beRaw |> MsBackendRawFileReader::filterScan('Ms')
beRaw <- Spectra::backendInitialize(MsBackendRawFileReader::MsBackendRawFileReader(),
  files = rawrr::sampleFilePath())
scanType(beRaw) |> head()
```

`MsBackendRawFileReader-class`*RawFileReader-based backend*

Description

The ‘`MsBackendRawFileReader`’ inherits all slots and methods from the base ‘`MsBackendDataFrame`’ (in-memory) backend. It overrides the base ‘`mz`’ and ‘`intensity`’ methods as well as ‘`peaksData`’ to read the respective data from the original raw data files.

The validator function has to ensure that the files exist and that required column names are present.

The ‘`backendInitialize`’ method reads the header data from the raw files and hence fills the ‘`spectraData`’ slot.

Author(s)

Christian Panse (2019-2021)

Examples

```
beRaw <- Spectra::backendInitialize(MsBackendRawFileReader::MsBackendRawFileReader(),
  files = rawrr::sampleFilePath())
beRaw
Spectra::msLevel(beRaw)
```

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