Package 'MsBackendRawFileReader'

April 10, 2023

Type Package

Title Mass Spectrometry Backend for Reading Thermo Fisher Scientific raw Files

Version 1.4.0

Depends R (>= 4.1), methods, Spectra (>= 1.5.8)

Imports MsCoreUtils, S4Vectors, IRanges, rawrr (>= 1.3.6), utils, BiocParallel

Suggests BiocStyle (>= 2.5), ExperimentHub, MsBackendMgf, 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'

git_url https://git.bioconductor.org/packages/MsBackendRawFileReader

git_branch RELEASE_3_16

git_last_commit 3cffb45

git_last_commit_date 2022-11-01

Date/Publication 2023-04-10

Author Christian Panse [aut, cre] (<https://orcid.org/0000-0003-1975-3064>),
Tobias Kockmann [aut] (<https://orcid.org/0000-0002-1847-885X>)

Maintainer Christian Panse <cp@fgcz.ethz.ch>

R topics documented:

`ioBenchmark` *RawFileReader_read_peaks benchmark*

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)
```

Index