

Package ‘tartare’

October 12, 2020

Type Package

Title Raw ground spectra recorded on Thermo Fisher Scientific mass spectrometers

Version 1.2.0

Depends R (>= 3.6), AnnotationHub (>= 2.16), ExperimentHub (>= 1.0)

Imports utils

Suggests BiocStyle, knitr, testthat, tools

Description provides raw files (size=278MBytes) recorded on different Liquid Chromatography Mass Spectrometry (LC-MS) instruments. All included MS instruments are manufactured by Thermo Fisher Scientific and belong to the Orbitrap Tribrid or Q Exactive Orbitrap family of instruments. Despite their common origin and shared hardware components (e.g. Orbitrap mass analyser), the above instruments tend to write data in different “dialects” in a shared binary file format (.raw). The intention behind tartare is to provide complex but slim real-world files that can be used to make code robust with respect to this diversity. In other words, it is intended for enhanced unit testing. The package is considered to be used with the rawDiag package (Trachsel, 2018 <doi:10.1021/acs.jproteome.8b00173>) and the Spectra MsBackends.

URL <https://github.com/cpanse/tartare>

BugReports <https://github.com/cpanse/tartare/issues>

Encoding UTF-8

NeedsCompilation no

biocViews ExperimentData, MassSpectrometryData, ExperimentHub

RoxygenNote 6.1.1

License GPL-3

VignetteBuilder knitr

Collate tartare.R zzz.R

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getFilename	<i>downloads files from aws storage and returns local filepath</i>
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Description

calls the `query` method of an `ExperimentHub` object query and returns the local filenames. Of note: for proprietary reasons, a `file.link` is set to the cached files. It seems that the New RawfileReader .Net library is only accepting files ending with raw. The overall file size is 285MB.

Usage

```
getFilename(eh, query = c("tartare"))
```

Arguments

eh	ExperimentHub object.
query	a query string, e.g., <code>c('tartar', '20190710_003_PierceHeLaProteinDigestStd.raw')</code>

Value

returns file(s) contained in the tartare package.

Author(s)

Christian Panse <cp@fgcz.ethz.ch>, 2019-10

See Also

- `browseVignettes('tartare')`
- `query`

Examples

```
library(ExperimentHub)
eh <- ExperimentHub()
query(eh, c('tartare'))

## Not run:
(files <- getFilename(eh))
library(MsBackendRawFileReader)

be <- lapply(files, function(f){
```

```
if (grepl("mzXML$", f))
  backendInitialize(MsBackendMzR(), files = f)
else
  backendInitialize(MsBackendRawFileReader(), files = f, extra=FALSE)
})

## End(Not run)

## Not run:
hfx.filename <- .query(eh, c('tartar', '20190710_003_PierceHeLaProteinDigestStd.raw'))
x <- .cnew ("Rawfile", hfx.filename)
x$GetInfoValues()

## End(Not run)
```

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